Full wwPDB EM Validation Report

Mar 29, 2026 – 02:51 AM UTC

PDB ID	:	7WG5 / pdb_00007wg5
EMDB ID	:	EMD-32477
Title	:	Cyclic electron transport supercomplex NDH-PSI from Arabidopsis
Authors	:	Pan, X.W.; Li, M.
Deposited on	:	2021-12-28
Resolution	:	3.89 Å(reported)

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

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

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

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

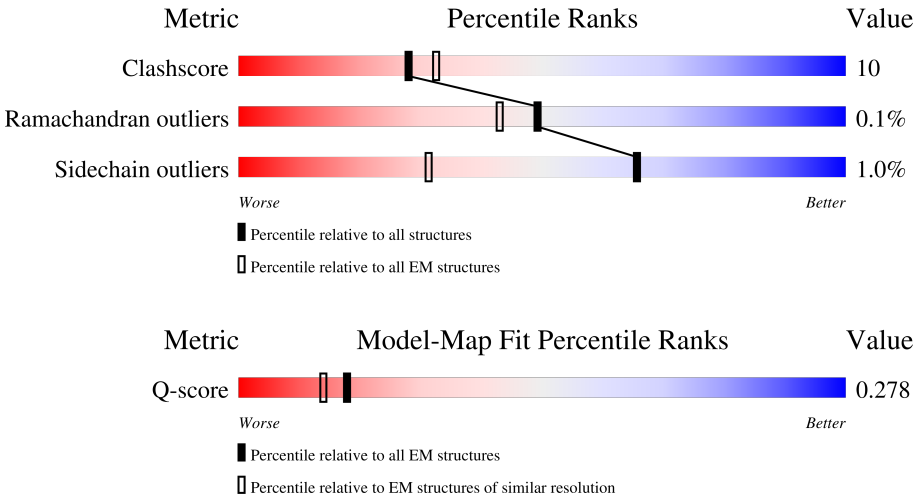
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.89 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	8712 (3.39 - 4.39)

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	AA	750	87% 11%
1	BA	750	7% 85% 13%
2	AB	734	85% 15%
2	BB	734	5% 85% 15%

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Mol	Chain	Length	Quality of chain
3	AC	81	79% 20%
3	BC	81	70% 28%
4	AD	204	58% 11% 31%
4	BD	204	8% 54% 14% 30%
5	AE	143	41% 6% 53%
5	BE	143	8% 41% 8% 52%
6	AF	221	62% 7% 31%
6	BF	221	5% 61% 9% 30%
7	AG	160	49% 12% 38%
7	BG	160	16% 45% 12% 41%
8	AH	145	5% 54% 11% 34%
8	BH	145	13% 51% 14% 34%
9	AI	37	78% 11% 11%
9	BI	37	24% 59% 30% 11%
10	AJ	44	73% 23% 5%
10	BJ	44	7% 75% 23%
11	AK	130	6% 47% 50%
11	BK	130	11% 38% 10% 51%
12	AL	219	63% 9% 28%
12	BL	219	15% 58% 14% 27%
13	A1	241	71% 11% 19%
13	B1	241	6% 56% 15% 29%
14	A3	273	74% 7% 20%
14	B3	273	13% 69% 12% 19%
15	A4	251	70% 9% 22%

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Mol	Chain	Length	Quality of chain
16	A6	270	69% 9% 21%
17	B2	257	11% 65% 16% 19%
18	B5	256	66% 14% 20%
19	A	360	15% 63% 21% 15%
20	B	512	73% 21% 5%
21	C	120	18% 55% 23% 22%
22	D	506	71% 27%
23	E	101	5% 56% 32% 12%
24	F	746	6% 68% 22% 9%
25	G	176	6% 65% 30% 5%
26	a	461	57% 17% 26%
27	b	348	5% 65% 24% 12%
28	c	204	5% 47% 15% 37%
29	d	161	38% 20% 42%
30	e	212	59% 12% 29%
31	f	238	47% 16% 36%
32	g	190	54% 7% 39%
33	h	220	53% 13% 34%
34	i	217	55% 12% 33%
35	j	255	54% 14% 32%
36	H	393	87% 67% 23% 9%
37	I	172	66% 68% 24% 7%
38	J	158	87% 73% 25%
39	K	225	59% 56% 17% 26%
40	L	191	13% 38% 60%

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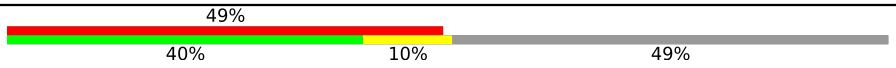
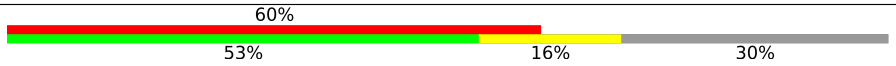
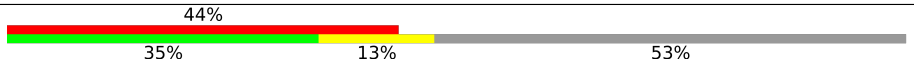
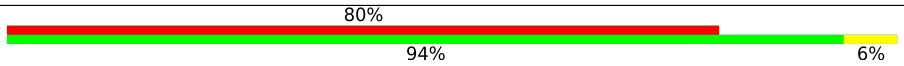
Mol	Chain	Length	Quality of chain
41	M	217	
42	N	209	
43	O	158	
44	T	122	

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
45	CLA	A1	304	X	-	-	-
45	CLA	A1	305	X	-	-	-
45	CLA	A1	306	X	-	-	-
45	CLA	A1	307	X	-	-	-
45	CLA	A1	309	X	-	-	-
45	CLA	A1	310	X	-	-	-
45	CLA	A1	311	X	-	-	-
45	CLA	A1	312	X	-	-	-
45	CLA	A1	313	X	-	-	-
45	CLA	A1	314	X	-	-	-
45	CLA	A1	315	X	-	-	-
45	CLA	A1	316	X	-	-	-
45	CLA	A3	302	X	-	-	-
45	CLA	A3	303	X	-	-	-
45	CLA	A3	304	X	-	-	-
45	CLA	A3	305	X	-	-	-
45	CLA	A3	306	X	-	-	-
45	CLA	A3	308	X	-	-	-
45	CLA	A3	309	X	-	-	-
45	CLA	A3	310	X	-	-	-
45	CLA	A3	311	X	-	-	-
45	CLA	A3	312	X	-	-	-
45	CLA	A3	314	X	-	-	-
45	CLA	A3	315	X	-	-	-
45	CLA	A4	301	X	-	-	-
45	CLA	A4	302	X	-	-	-
45	CLA	A4	303	X	-	-	-
45	CLA	A4	307	X	-	-	-
45	CLA	A4	308	X	-	-	-
45	CLA	A4	309	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	A4	310	X	-	-	-
45	CLA	A4	311	X	-	-	-
45	CLA	A4	312	X	-	-	-
45	CLA	A4	313	X	-	-	-
45	CLA	A6	601	X	-	-	-
45	CLA	A6	603	X	-	-	-
45	CLA	A6	604	X	-	-	-
45	CLA	A6	605	X	-	-	-
45	CLA	A6	609	X	-	-	-
45	CLA	A6	610	X	-	-	-
45	CLA	A6	611	X	-	-	-
45	CLA	A6	612	X	-	-	-
45	CLA	A6	613	X	-	-	-
45	CLA	A6	614	X	-	-	-
45	CLA	AA	801	X	-	-	-
45	CLA	AA	802	X	-	-	-
45	CLA	AA	803	X	-	-	-
45	CLA	AA	805	X	-	-	-
45	CLA	AA	806	X	-	-	-
45	CLA	AA	807	X	-	-	-
45	CLA	AA	808	X	-	-	-
45	CLA	AA	809	X	-	-	-
45	CLA	AA	810	X	-	-	-
45	CLA	AA	811	X	-	-	-
45	CLA	AA	812	X	-	-	-
45	CLA	AA	813	X	-	-	-
45	CLA	AA	814	X	-	-	-
45	CLA	AA	816	X	-	-	-
45	CLA	AA	817	X	-	-	-
45	CLA	AA	819	X	-	-	-
45	CLA	AA	820	X	-	-	-
45	CLA	AA	821	X	-	-	-
45	CLA	AA	822	X	-	-	-
45	CLA	AA	823	X	-	-	-
45	CLA	AA	824	X	-	-	-
45	CLA	AA	825	X	-	-	-
45	CLA	AA	826	X	-	-	-
45	CLA	AA	827	X	-	-	-
45	CLA	AA	828	X	-	-	-
45	CLA	AA	829	X	-	-	-
45	CLA	AA	830	X	-	-	-
45	CLA	AA	831	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	AA	832	X	-	-	-
45	CLA	AA	833	X	-	-	-
45	CLA	AA	835	X	-	-	-
45	CLA	AA	837	X	-	-	-
45	CLA	AA	840	X	-	-	-
45	CLA	AA	842	X	-	-	-
45	CLA	AB	801	X	-	-	-
45	CLA	AB	802	X	-	-	-
45	CLA	AB	803	X	-	-	-
45	CLA	AB	804	X	-	-	-
45	CLA	AB	805	X	-	-	-
45	CLA	AB	806	X	-	-	-
45	CLA	AB	807	X	-	-	-
45	CLA	AB	809	X	-	-	-
45	CLA	AB	810	X	-	-	-
45	CLA	AB	811	X	-	-	-
45	CLA	AB	812	X	-	-	-
45	CLA	AB	813	X	-	-	-
45	CLA	AB	814	X	-	-	-
45	CLA	AB	815	X	-	-	-
45	CLA	AB	816	X	-	-	-
45	CLA	AB	817	X	-	-	-
45	CLA	AB	818	X	-	-	-
45	CLA	AB	819	X	-	-	-
45	CLA	AB	820	X	-	-	-
45	CLA	AB	821	X	-	-	-
45	CLA	AB	822	X	-	-	-
45	CLA	AB	824	X	-	-	-
45	CLA	AB	825	X	-	-	-
45	CLA	AB	826	X	-	-	-
45	CLA	AB	827	X	-	-	-
45	CLA	AB	828	X	-	-	-
45	CLA	AB	829	X	-	-	-
45	CLA	AB	830	X	-	-	-
45	CLA	AB	831	X	-	-	-
45	CLA	AB	833	X	-	-	-
45	CLA	AB	834	X	-	-	-
45	CLA	AB	837	X	-	-	-
45	CLA	AB	839	X	-	-	-
45	CLA	AB	840	X	-	-	-
45	CLA	AB	841	X	-	-	-
45	CLA	AB	842	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	AF	802	X	-	-	-
45	CLA	AF	803	X	-	-	-
45	CLA	AF	804	X	-	-	-
45	CLA	AG	201	X	-	-	-
45	CLA	AG	203	X	-	-	-
45	CLA	AG	204	X	-	-	-
45	CLA	AH	201	X	-	-	-
45	CLA	AJ	102	X	-	-	-
45	CLA	AK	201	X	-	-	-
45	CLA	AK	202	X	-	-	-
45	CLA	AK	203	X	-	-	-
45	CLA	AL	303	X	-	-	-
45	CLA	AL	305	X	-	-	-
45	CLA	B1	304	X	-	-	-
45	CLA	B1	305	X	-	-	-
45	CLA	B1	306	X	-	-	-
45	CLA	B1	307	X	-	-	-
45	CLA	B1	310	X	-	-	-
45	CLA	B1	311	X	-	-	-
45	CLA	B1	312	X	-	-	-
45	CLA	B1	313	X	-	-	-
45	CLA	B1	314	X	-	-	-
45	CLA	B1	315	X	-	-	-
45	CLA	B2	602	X	-	-	-
45	CLA	B2	603	X	-	-	-
45	CLA	B2	604	X	-	-	-
45	CLA	B2	608	X	-	-	-
45	CLA	B2	609	X	-	-	-
45	CLA	B2	610	X	-	-	-
45	CLA	B2	611	X	-	-	-
45	CLA	B2	612	X	-	-	-
45	CLA	B2	613	X	-	-	-
45	CLA	B3	301	X	-	-	-
45	CLA	B3	302	X	-	-	-
45	CLA	B3	303	X	-	-	-
45	CLA	B3	304	X	-	-	-
45	CLA	B3	305	X	-	-	-
45	CLA	B3	307	X	-	-	-
45	CLA	B3	308	X	-	-	-
45	CLA	B3	309	X	-	-	-
45	CLA	B3	310	X	-	-	-
45	CLA	B3	311	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	B3	312	X	-	-	-
45	CLA	B3	313	X	-	-	-
45	CLA	B3	314	X	-	-	-
45	CLA	B5	601	X	-	-	-
45	CLA	B5	603	X	-	-	-
45	CLA	B5	604	X	-	-	-
45	CLA	B5	608	X	-	-	-
45	CLA	B5	609	X	-	-	-
45	CLA	B5	611	X	-	-	-
45	CLA	B5	612	X	-	-	-
45	CLA	B5	613	X	-	-	-
45	CLA	BA	801	X	-	-	-
45	CLA	BA	802	X	-	-	-
45	CLA	BA	803	X	-	-	-
45	CLA	BA	805	X	-	-	-
45	CLA	BA	806	X	-	-	-
45	CLA	BA	807	X	-	-	-
45	CLA	BA	808	X	-	-	-
45	CLA	BA	810	X	-	-	-
45	CLA	BA	811	X	-	-	-
45	CLA	BA	812	X	-	-	-
45	CLA	BA	813	X	-	-	-
45	CLA	BA	814	X	-	-	-
45	CLA	BA	816	X	-	-	-
45	CLA	BA	819	X	-	-	-
45	CLA	BA	820	X	-	-	-
45	CLA	BA	822	X	-	-	-
45	CLA	BA	823	X	-	-	-
45	CLA	BA	824	X	-	-	-
45	CLA	BA	825	X	-	-	-
45	CLA	BA	827	X	-	-	-
45	CLA	BA	828	X	-	-	-
45	CLA	BA	829	X	-	-	-
45	CLA	BA	830	X	-	-	-
45	CLA	BA	831	X	-	-	-
45	CLA	BA	833	X	-	-	-
45	CLA	BA	835	X	-	-	-
45	CLA	BA	837	X	-	-	-
45	CLA	BA	838	X	-	-	-
45	CLA	BA	840	X	-	-	-
45	CLA	BA	841	X	-	-	-
45	CLA	BA	842	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	BA	844	X	-	-	-
45	CLA	BB	801	X	-	-	-
45	CLA	BB	802	X	-	-	-
45	CLA	BB	804	X	-	-	-
45	CLA	BB	805	X	-	-	-
45	CLA	BB	806	X	-	-	-
45	CLA	BB	807	X	-	-	-
45	CLA	BB	808	X	-	-	-
45	CLA	BB	810	X	-	-	-
45	CLA	BB	811	X	-	-	-
45	CLA	BB	812	X	-	-	-
45	CLA	BB	813	X	-	-	-
45	CLA	BB	814	X	-	-	-
45	CLA	BB	815	X	-	-	-
45	CLA	BB	816	X	-	-	-
45	CLA	BB	817	X	-	-	-
45	CLA	BB	818	X	-	-	-
45	CLA	BB	819	X	-	-	-
45	CLA	BB	820	X	-	-	-
45	CLA	BB	821	X	-	-	-
45	CLA	BB	822	X	-	-	-
45	CLA	BB	823	X	-	-	-
45	CLA	BB	825	X	-	-	-
45	CLA	BB	826	X	-	-	-
45	CLA	BB	828	X	-	-	-
45	CLA	BB	829	X	-	-	-
45	CLA	BB	830	X	-	-	-
45	CLA	BB	831	X	-	-	-
45	CLA	BB	832	X	-	-	-
45	CLA	BB	835	X	-	-	-
45	CLA	BB	837	X	-	-	-
45	CLA	BB	838	X	-	-	-
45	CLA	BB	841	X	-	-	-
45	CLA	BB	842	X	-	-	-
45	CLA	BB	843	X	-	-	-
45	CLA	BF	301	X	-	-	-
45	CLA	BF	302	X	-	-	-
45	CLA	BF	303	X	-	-	-
45	CLA	BG	201	X	-	-	-
45	CLA	BG	202	X	-	X	-
45	CLA	BH	201	X	-	-	-
45	CLA	BJ	102	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
45	CLA	BK	201	X	-	-	-
45	CLA	BK	202	X	-	-	-
45	CLA	BK	203	X	-	-	-
45	CLA	BL	304	X	-	-	-
49	SF4	AC	102	-	-	X	-
49	SF4	BC	102	-	-	X	-
49	SF4	I	202	-	-	X	-
54	CHL	A1	303	X	-	-	-
54	CHL	A1	308	X	-	-	-
54	CHL	A3	307	X	-	-	-
54	CHL	A4	304	X	-	-	-
54	CHL	A4	305	X	-	-	-
54	CHL	A4	306	X	-	-	-
54	CHL	A4	314	X	-	-	-
54	CHL	A6	602	X	-	-	-
54	CHL	A6	606	X	-	-	-
54	CHL	A6	607	X	-	-	-
54	CHL	A6	608	X	-	-	-
54	CHL	B1	303	X	-	-	-
54	CHL	B1	308	X	-	-	-
54	CHL	B2	601	X	-	-	-
54	CHL	B2	605	X	-	-	-
54	CHL	B2	606	X	-	-	-
54	CHL	B2	607	X	-	-	-
54	CHL	B2	614	X	-	-	-
54	CHL	B3	306	X	-	-	-
54	CHL	B5	605	X	-	-	-
54	CHL	B5	606	X	-	-	-
54	CHL	B5	607	X	-	-	-
57	FES	c	301	-	-	X	-

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 112687 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	AA	742	Total	C	N	O	S	0	0
			5839	3826	992	1003	18		
1	BA	742	Total	C	N	O	S	0	0
			5841	3828	992	1003	18		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	AB	734	Total	C	N	O	S	0	0
			5862	3847	999	1001	15		
2	BB	733	Total	C	N	O	S	0	0
			5854	3842	998	1000	14		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	AC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		
3	BC	80	Total	C	N	O	S	0	0
			615	381	107	116	11		

- Molecule 4 is a protein called Photosystem I reaction center subunit II-2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	AD	141	Total	C	N	O	S	0	0
			1112	712	193	203	4		
4	BD	143	Total	C	N	O	S	0	0
			1127	723	195	205	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	AE	67	Total	C	N	O	0	0
			530	341	94	95		
5	BE	69	Total	C	N	O	0	0
			546	352	97	97		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AF	153	Total	C	N	O	S	0	0
			1213	792	208	210	3		
6	BF	154	Total	C	N	O	S	0	0
			1220	797	209	211	3		

- Molecule 7 is a protein called Photosystem I reaction center subunit V, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	AG	99	Total	C	N	O	0	0
			771	501	126	144		
7	BG	94	Total	C	N	O	0	0
			733	474	121	138		

- Molecule 8 is a protein called Photosystem I reaction center subunit VI-2, chloroplastic.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	AH	95	Total	C	N	O	0	0
			730	476	119	135		
8	BH	95	Total	C	N	O	0	0
			730	476	119	135		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	AI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		
9	BI	33	Total	C	N	O	S	0	0
			257	175	41	40	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	AJ	42	Total	C	N	O	S	0	0
			338	230	51	56	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	BJ	43	Total	C	N	O	S	0	0
			344	233	52	58	1		

- Molecule 11 is a protein called Photosystem I reaction center subunit psaK, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	AK	65	Total	C	N	O	S	0	0
			451	290	74	84	3		
11	BK	64	Total	C	N	O	S	0	0
			445	285	73	84	3		

- Molecule 12 is a protein called Photosystem I reaction center subunit XI, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AL	157	Total	C	N	O	S	0	0
			1173	775	187	209	2		
12	BL	159	Total	C	N	O	S	0	0
			1184	781	190	211	2		

- Molecule 13 is a protein called Chlorophyll a-b binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	A1	196	Total	C	N	O	S	0	0
			1511	984	251	271	5		
13	B1	172	Total	C	N	O	S	0	0
			1339	873	221	240	5		

- Molecule 14 is a protein called Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	A3	219	Total	C	N	O	S	0	0
			1675	1096	272	302	5		
14	B3	221	Total	C	N	O	S	0	0
			1696	1111	276	304	5		

- Molecule 15 is a protein called Chlorophyll a-b binding protein 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	A4	197	Total	C	N	O	S	0	0
			1562	1022	254	283	3		

- Molecule 16 is a protein called Photosystem I chlorophyll a/b-binding protein 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	A6	212	Total	C	N	O	S	0	0
			1671	1088	272	299	12		

- Molecule 17 is a protein called Photosystem I chlorophyll a/b-binding protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	B2	208	Total	C	N	O	S	0	0
			1607	1051	261	291	4		

- Molecule 18 is a protein called Photosystem I chlorophyll a/b-binding protein 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	B5	206	Total	C	N	O	S	0	0
			1599	1045	263	285	6		

- Molecule 19 is a protein called NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A	305	Total	C	N	O	S	0	0
			2372	1593	366	409	4		

- Molecule 20 is a protein called NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B	486	Total	C	N	O	S	0	0
			3780	2495	577	679	29		

- Molecule 21 is a protein called NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	C	94	Total	C	N	O	S	0	0
			776	544	109	121	2		

- Molecule 22 is a protein called NAD(P)H-quinone oxidoreductase chain 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	D	497	Total	C	N	O	S	0	0
			3946	2656	599	666	25		

- Molecule 23 is a protein called NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	E	89	Total	C	N	O	S	0	0
			695	458	112	119	6		

- Molecule 24 is a protein called NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	F	677	Total	C	N	O	S	0	0
			5330	3558	829	915	28		

- Molecule 25 is a protein called NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	G	167	Total	C	N	O	S	0	0
			1281	858	194	224	5		

- Molecule 26 is a protein called Photosynthetic NDH subunit of subcomplex B 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	341	Total	C	N	O	S	0	0
			2655	1692	450	500	13		

- Molecule 27 is a protein called Photosynthetic NDH subunit of subcomplex B 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	b	307	Total	C	N	O	S	0	0
			2367	1508	392	452	15		

- Molecule 28 is a protein called Photosynthetic NDH subunit of subcomplex B 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	128	Total	C	N	O	S	0	0
			1005	636	180	183	6		

- Molecule 29 is a protein called NDH dependent flow 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	93	Total	C	N	O	S	0	0
			762	497	119	138	8		

- Molecule 30 is a protein called Photosynthetic NDH subunit of subcomplex B 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	150	Total	C	N	O	S	0	0
			1206	780	183	236	7		

- Molecule 31 is a protein called Photosynthetic NDH subunit of lumenal location 1, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	f	153	Total	C	N	O	S	0	0
			1277	823	219	233	2		

- Molecule 32 is a protein called Photosynthetic NDH subunit of lumenal location 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	g	115	Total	C	N	O	S	0	0
			965	620	159	180	6		

- Molecule 33 is a protein called Photosynthetic NDH subunit of lumenal location 3, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	145	Total	C	N	O	S	0	0
			1170	753	191	221	5		

- Molecule 34 is a protein called Photosynthetic NDH subunit of lumenal location 4, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	145	Total	C	N	O	S	0	0
			1098	698	190	204	6		

- Molecule 35 is a protein called Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	173	Total	C	N	O	S	0	0
			1331	840	236	248	7		

- Molecule 36 is a protein called NAD(P)H-quinone oxidoreductase subunit H, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	H	356	Total	C	N	O	S	0	0
			2812	1830	465	499	18		

- Molecule 37 is a protein called NAD(P)H-quinone oxidoreductase subunit I, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	I	160	Total	C	N	O	S	0	0
			1236	776	214	233	13		

- Molecule 38 is a protein called NAD(P)H-quinone oxidoreductase subunit J, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	J	155	Total	C	N	O	S	0	0
			1116	722	189	202	3		

- Molecule 39 is a protein called NAD(P)H-quinone oxidoreductase subunit K, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	K	167	Total	C	N	O	S	0	0
			1199	765	203	221	10		

- Molecule 40 is a protein called NAD(P)H-quinone oxidoreductase subunit L, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	L	77	Total	C	N	O	S	0	0
			646	437	106	99	4		

- Molecule 41 is a protein called NAD(P)H-quinone oxidoreductase subunit M, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	M	110	Total	C	N	O	S	0	0
			771	494	132	143	2		

- Molecule 42 is a protein called NAD(P)H-quinone oxidoreductase subunit N, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	N	146	Total	C	N	O	S	0	0
			908	584	156	166	2		

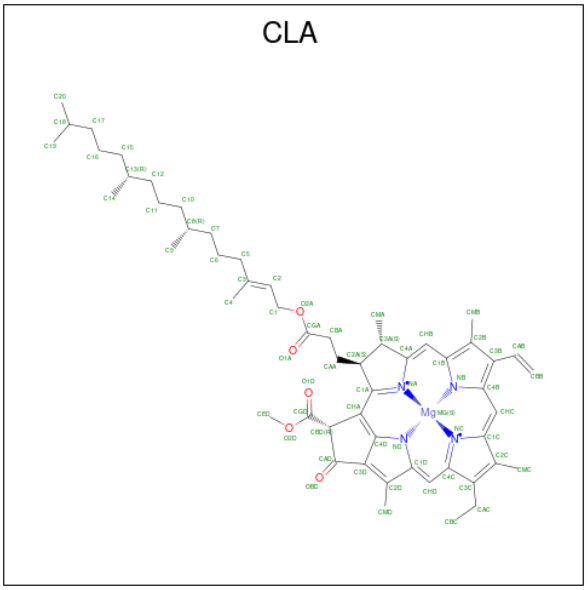
- Molecule 43 is a protein called NdhO.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	O	75	Total	C	N	O	0	0
			520	334	90	96		

- Molecule 44 is a protein called NdhT.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	T	122	Total	C	N	O	0	0
			610	366	122	122		

- Molecule 45 is CHLOROPHYLL A (CCD ID: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			51	42	1	4	4	

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Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	AB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	AF	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	AF	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AF	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AG	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	AG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	AG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
45	AK	1	Total	C	Mg	N	O	0
			35	29	1	4	1	
45	AK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	AK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	AL	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	AL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	AL	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	A1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A1	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			37	31	1	4	1	
45	A3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	A3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	A4	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A4	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	A6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	A6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	A6	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	A6	1	Total	C	Mg	N	O	0
			64	55	1	4	4	
45	A6	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			54	44	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BA	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
45	BA	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BA	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			56	46	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BB	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BB	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	BF	1	Total	C	Mg	N	O	0
			55	46	1	4	4	
45	BF	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BF	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	BG	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BG	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BH	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BJ	1	Total	C	Mg	N	O	0
			42	34	1	4	3	
45	BK	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	BK	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	BK	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	BL	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	BL	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	BL	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			54	45	1	4	4	
45	B1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			39	31	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			59	49	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B1	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
45	B2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			38	30	1	4	3	
45	B2	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
45	B2	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			42	32	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B3	1	Total	C	Mg	N	O	0
			36	30	1	4	1	
45	B3	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			43	33	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			44	34	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			42	34	1	4	3	

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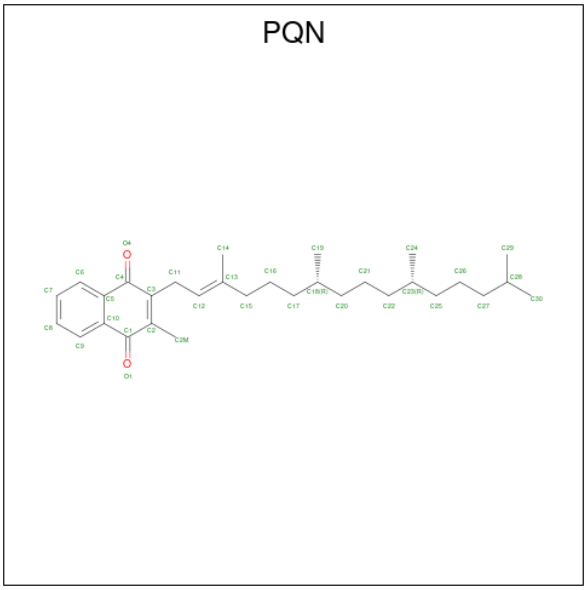
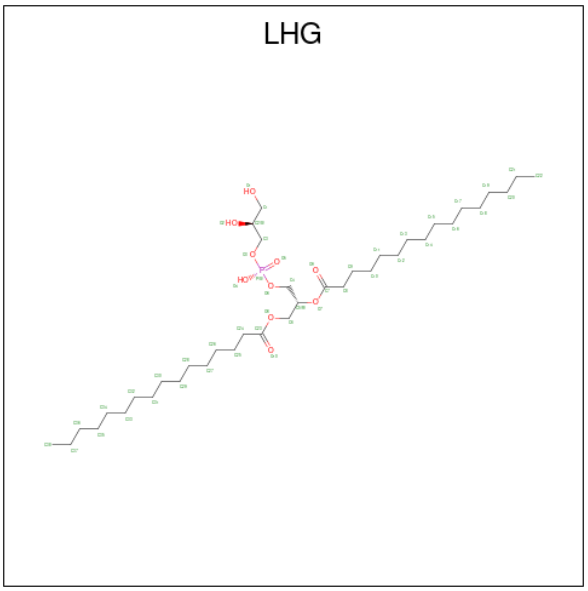
Mol	Chain	Residues	Atoms					AltConf
45	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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



Mol	Chain	Residues	Atoms			AltConf
46	AA	1	Total	C	O	0
			33	31	2	
46	AB	1	Total	C	O	0
			33	31	2	
46	BA	1	Total	C	O	0
			33	31	2	
46	BB	1	Total	C	O	0
			33	31	2	

- Molecule 47 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms				AltConf
47	AA	1	Total	C	O	P	0
			49	38	10	1	
47	AJ	1	Total	C	O	P	0
			40	29	10	1	
47	A1	1	Total	C	O	P	0
			38	27	10	1	
47	A1	1	Total	C	O	P	0
			36	25	10	1	
47	A1	1	Total	C	O	P	0
			49	38	10	1	
47	A3	1	Total	C	O	P	0
			36	25	10	1	
47	A3	1	Total	C	O	P	0
			23	12	10	1	
47	A6	1	Total	C	O	P	0
			36	25	10	1	
47	BA	1	Total	C	O	P	0
			49	38	10	1	
47	BA	1	Total	C	O	P	0
			27	16	10	1	
47	BF	1	Total	C	O	P	0
			45	34	10	1	
47	B1	1	Total	C	O	P	0
			38	27	10	1	
47	B1	1	Total	C	O	P	0
			36	25	10	1	
47	B1	1	Total	C	O	P	0
			42	31	10	1	

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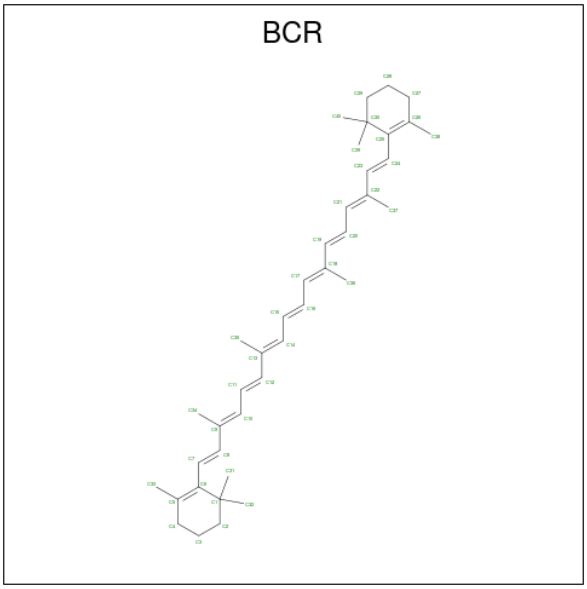
Mol	Chain	Residues	Atoms				AltConf
47	B2	1	Total	C	O	P	0
			35	24	10	1	
47	B3	1	Total	C	O	P	0
			23	12	10	1	
47	B5	1	Total	C	O	P	0
			30	19	10	1	
47	F	1	Total	C	O	P	0
			37	26	10	1	
47	a	1	Total	C	O	P	0
			29	18	10	1	

- Molecule 48 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	
48	AA	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AB	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AF	1	Total C 40 40	0
48	AG	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AI	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AJ	1	Total C 40 40	0
48	AK	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	AL	1	Total C 40 40	0
48	A1	1	Total C 40 40	0
48	A3	1	Total C 40 40	0
48	A4	1	Total C 40 40	0
48	A6	1	Total C 40 40	0
48	BA	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BF	1	Total C 40 40	0
48	BG	1	Total C 40 40	0
48	BI	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BJ	1	Total C 40 40	0
48	BK	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0
48	BL	1	Total C 40 40	0

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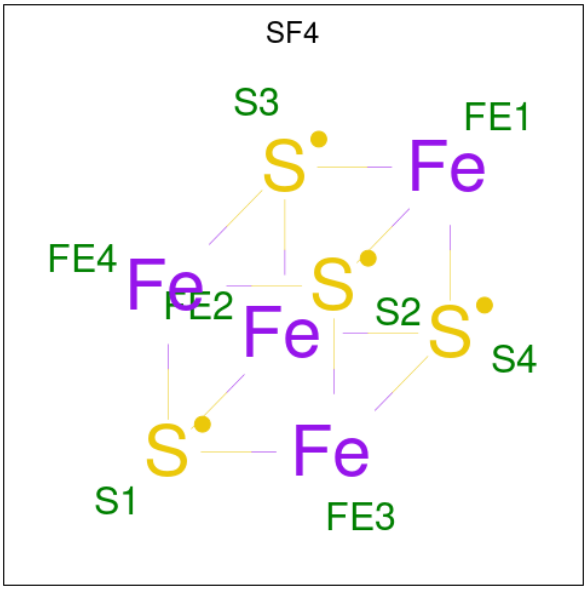
Mol	Chain	Residues	Atoms	AltConf
48	B2	1	Total C 40 40	0
48	B3	1	Total C 40 40	0
48	B5	1	Total C 40 40	0

- Molecule 49 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
49	AA	1	Total Fe S 8 4 4	0
49	AC	1	Total Fe S 8 4 4	0
49	AC	1	Total Fe S 8 4 4	0
49	BA	1	Total Fe S 8 4 4	0
49	BC	1	Total Fe S 8 4 4	0
49	BC	1	Total Fe S 8 4 4	0
49	I	1	Total Fe S 8 4 4	0
49	I	1	Total Fe S 8 4 4	0

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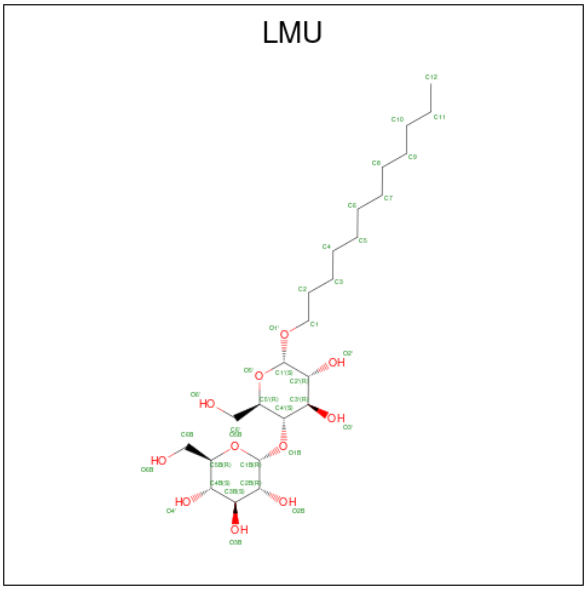
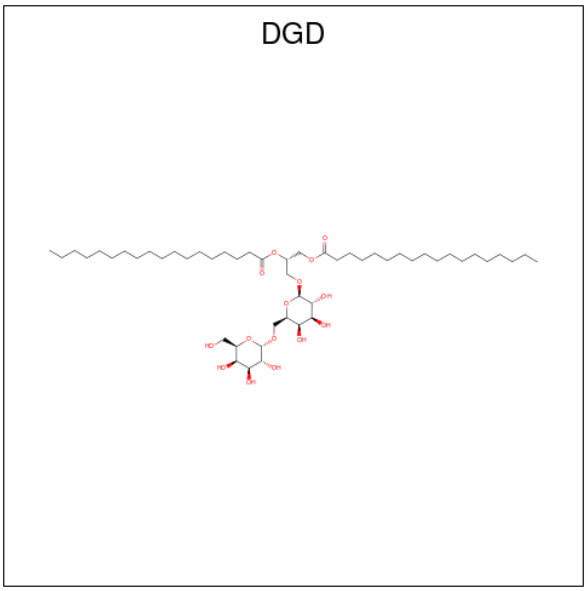
Mol	Chain	Residues	Atoms	AltConf
49	K	1	Total Fe S 8 4 4	0

- Molecule 50 is DODECYL-ALPHA-D-MALTOSIDE (CCD ID: LMU) (formula: $C_{24}H_{46}O_{11}$).



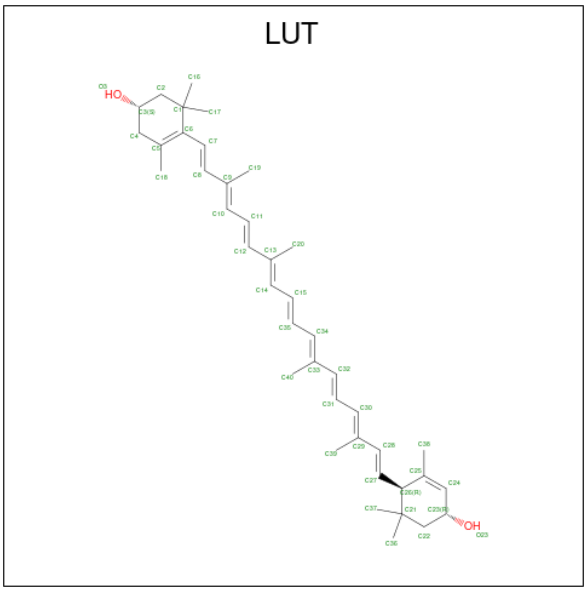
Mol	Chain	Residues	Atoms	AltConf
50	AA	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AB	1	Total C O 35 24 11	0
50	AL	1	Total C O 34 23 11	0
50	BA	1	Total C O 34 23 11	0
50	BA	1	Total C O 33 22 11	0
50	BB	1	Total C O 35 24 11	0

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



Mol	Chain	Residues	Atoms			AltConf
51	AB	1	Total	C	O	0
			66	51	15	
51	BB	1	Total	C	O	0
			66	51	15	

- Molecule 52 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3 ,3'-DIOL (CCD ID: LUT) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
52	AF	1	Total	C	O	0
			42	40	2	

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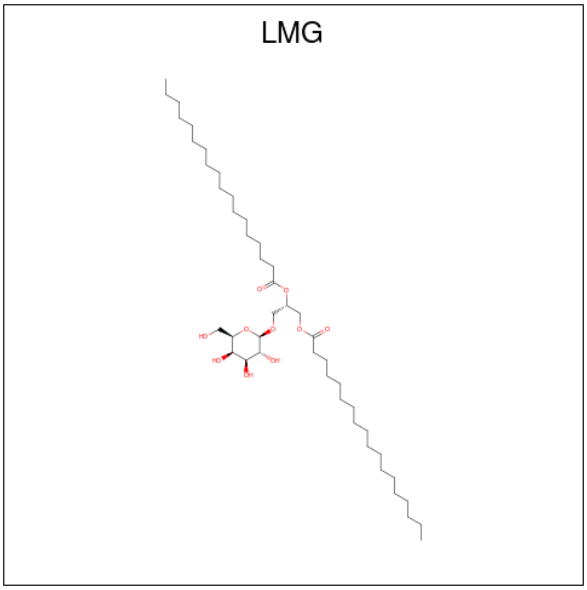
Mol	Chain	Residues	Atoms	AltConf
52	A1	1	Total C O 42 40 2	0
52	A3	1	Total C O 42 40 2	0
52	A4	1	Total C O 42 40 2	0
52	A6	1	Total C O 42 40 2	0
52	B1	1	Total C O 42 40 2	0
52	B2	1	Total C O 42 40 2	0
52	B3	1	Total C O 42 40 2	0
52	B5	1	Total C O 42 40 2	0

- Molecule 53 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



Mol	Chain	Residues	Atoms	AltConf
53	AG	1	Total C O 38 28 10	0
53	A1	1	Total C O 44 34 10	0
53	A4	1	Total C O 39 29 10	0

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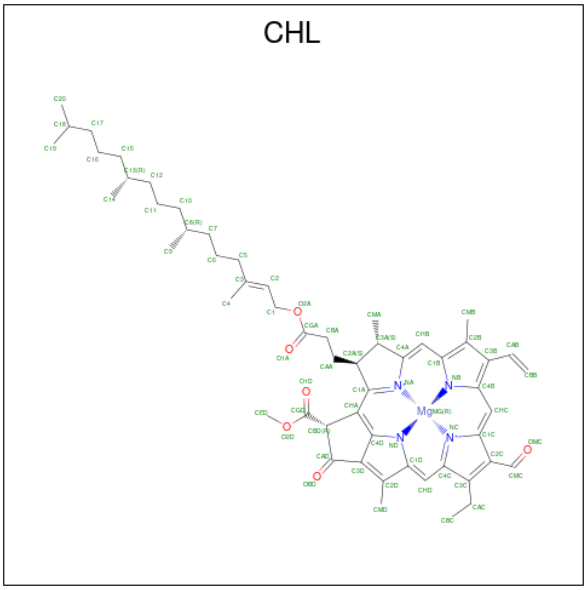
Mol	Chain	Residues	Atoms			AltConf
53	B5	1	Total	C	O	0
			33	23	10	

- Molecule 54 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
54	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
54	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
54	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A6	1	Total	C	Mg	N	O	0
			52	41	1	4	6	
54	A6	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	A6	1	Total	C	Mg	N	O	0
			43	34	1	4	4	

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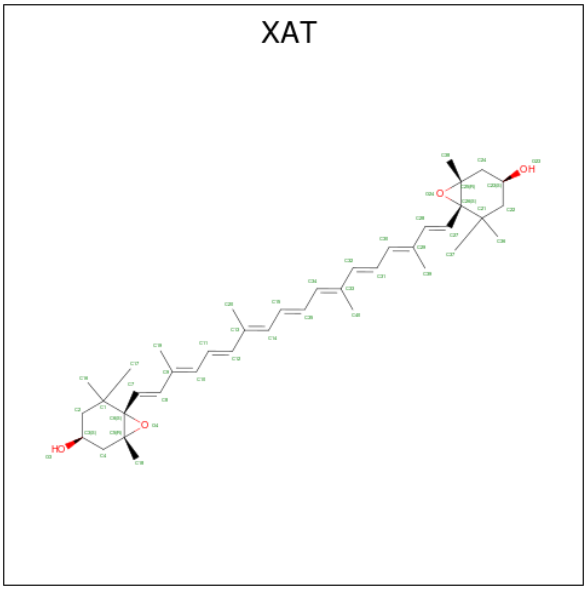
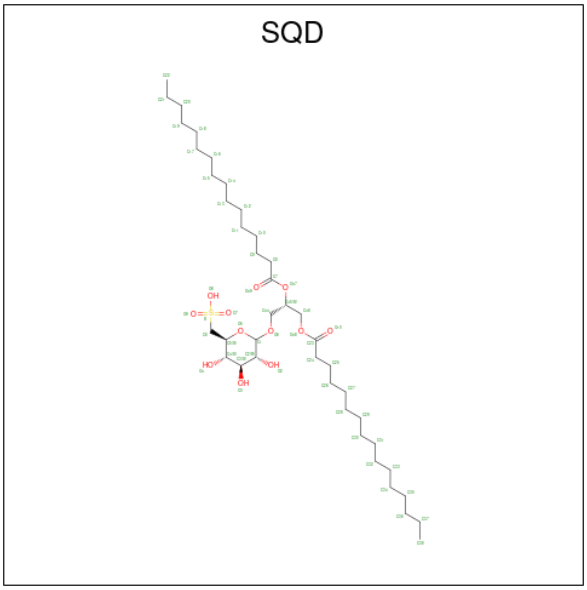
Mol	Chain	Residues	Atoms					AltConf
54	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
54	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	B5	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B5	1	Total	C	Mg	N	O	0
			40	32	1	4	3	
54	B5	1	Total	C	Mg	N	O	0
			45	34	1	4	6	

- Molecule 55 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (CCD ID: XAT) (formula: $C_{40}H_{56}O_4$).



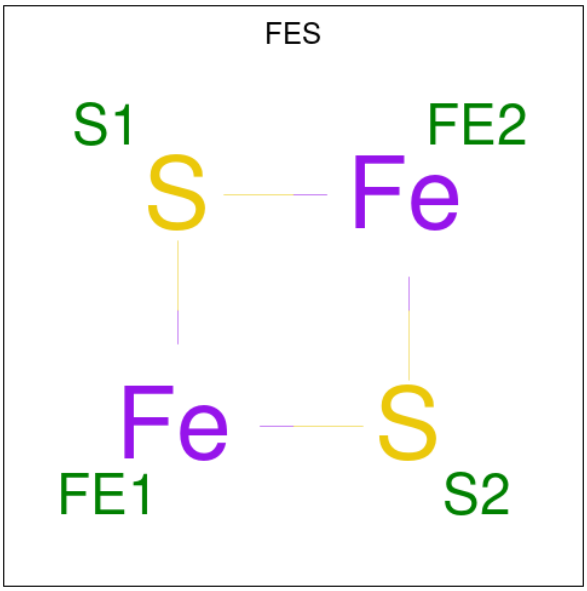
Mol	Chain	Residues	Atoms				AltConf
55	A1	1	Total	C	O		0
			44	40	4		
55	A3	1	Total	C	O		0
			44	40	4		
55	A4	1	Total	C	O		0
			44	40	4		
55	A6	1	Total	C	O		0
			44	40	4		
55	B1	1	Total	C	O		0
			44	40	4		
55	B2	1	Total	C	O		0
			44	40	4		
55	B3	1	Total	C	O		0
			44	40	4		
55	B5	1	Total	C	O		0
			44	40	4		

- Molecule 56 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms				AltConf
56	BJ	1	Total	C	O	S	0
			47	34	12	1	
56	e	1	Total	C	O	S	0
			34	21	12	1	

- Molecule 57 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



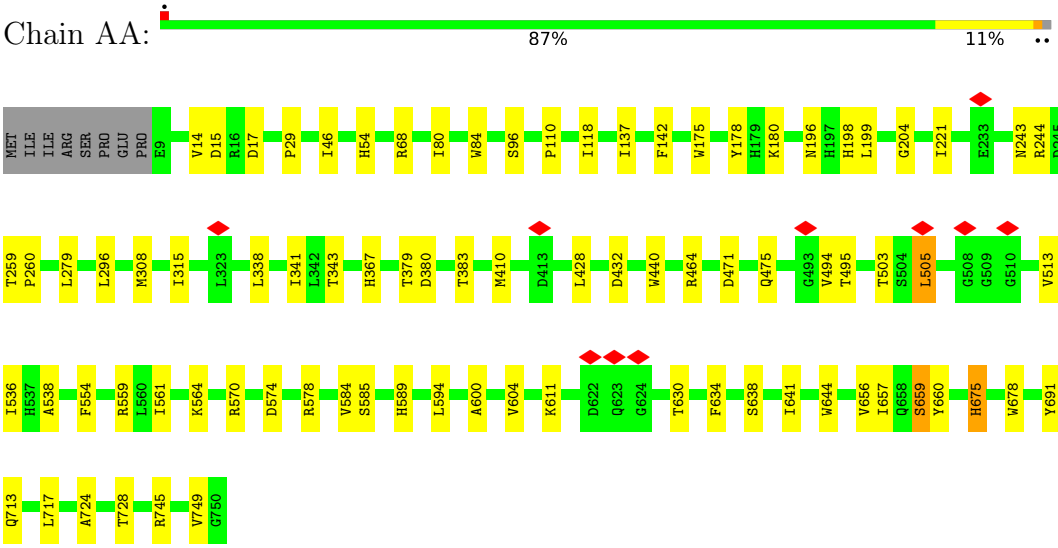
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
57	c	1	4	2	2	0

3 Residue-property plots (i)

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

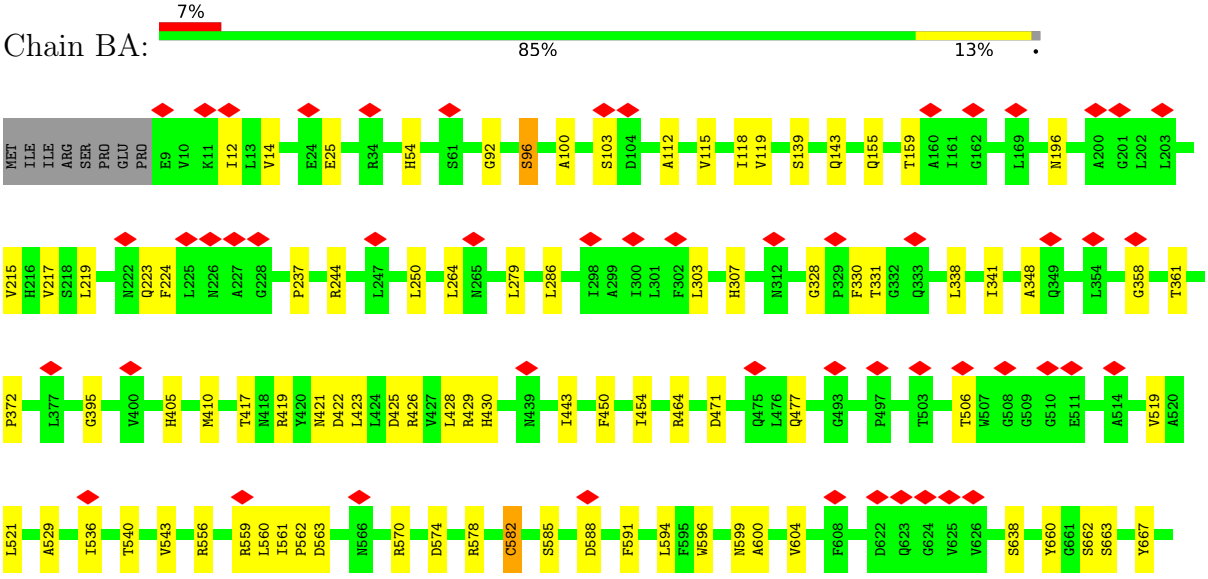
• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA:

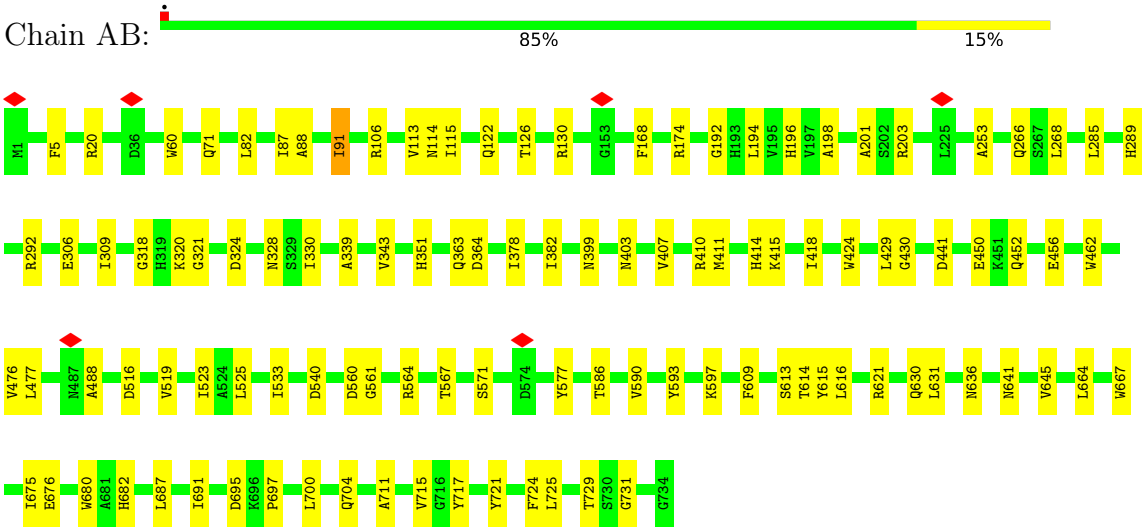


• Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

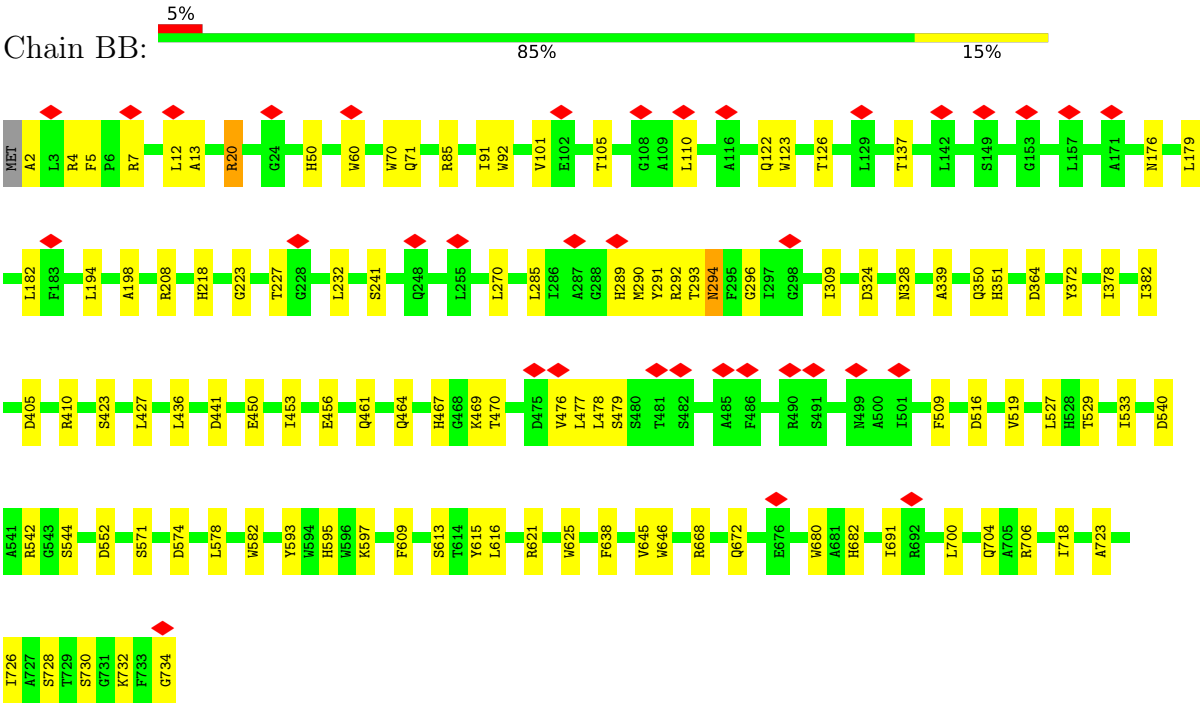
Chain BA:



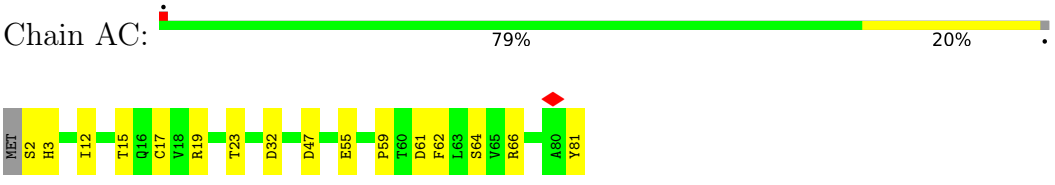
• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

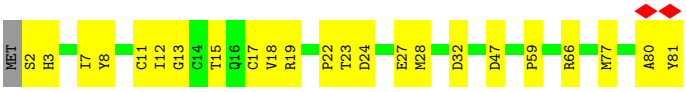


• Molecule 3: Photosystem I iron-sulfur center



• Molecule 3: Photosystem I iron-sulfur center

Chain BC:

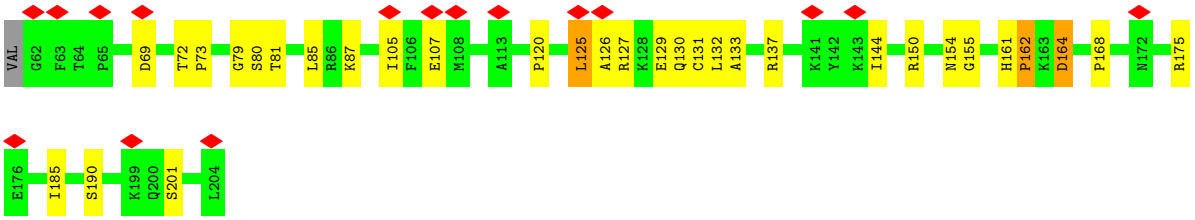


• Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain AD:

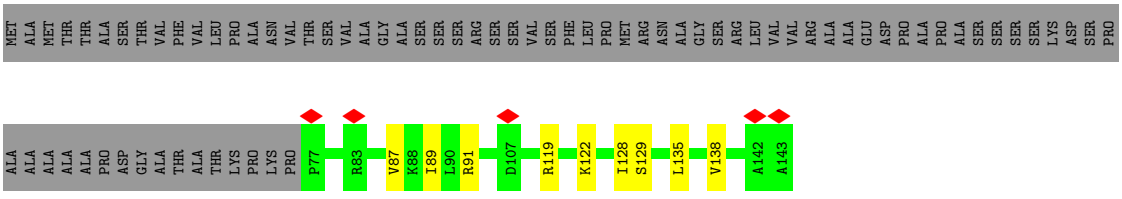
• Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD:



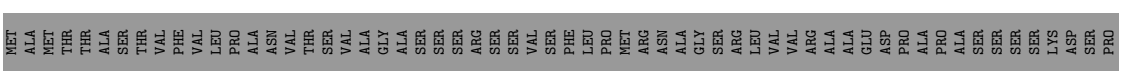
• Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

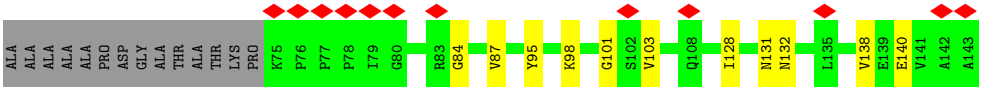
Chain AE:



• Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

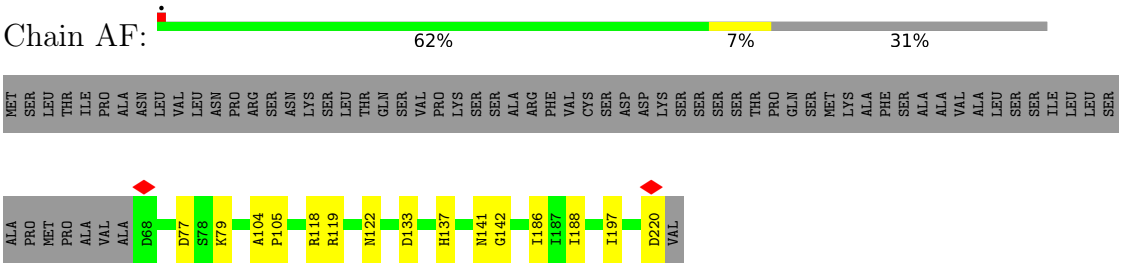
Chain BE:





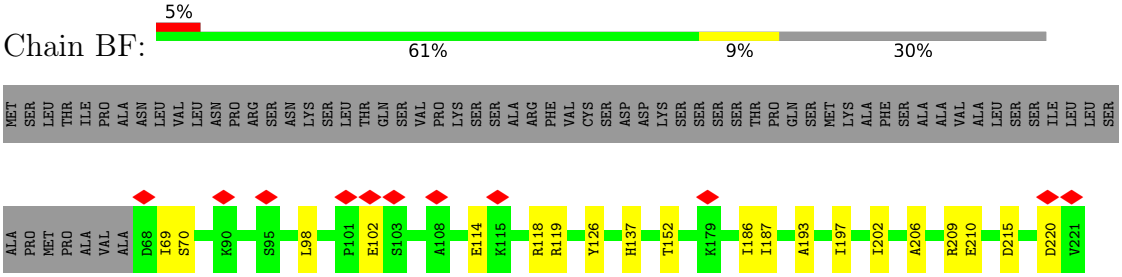
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain AF:



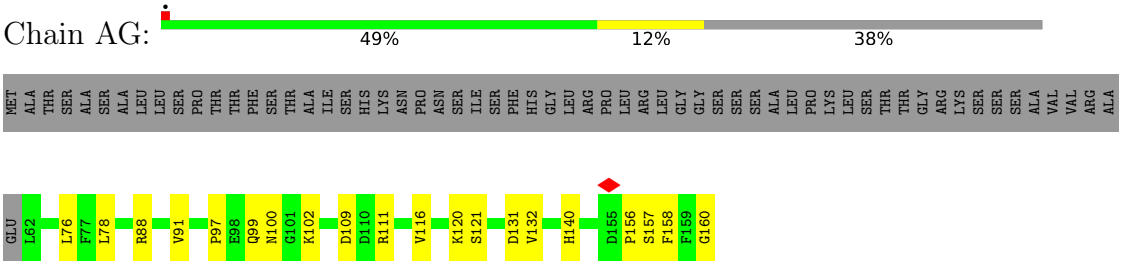
• Molecule 6: Photosystem I reaction center subunit III, chloroplastic

Chain BF:



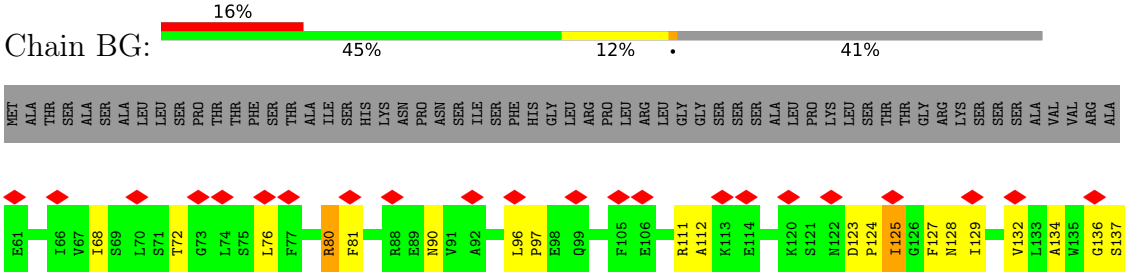
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

Chain AG:



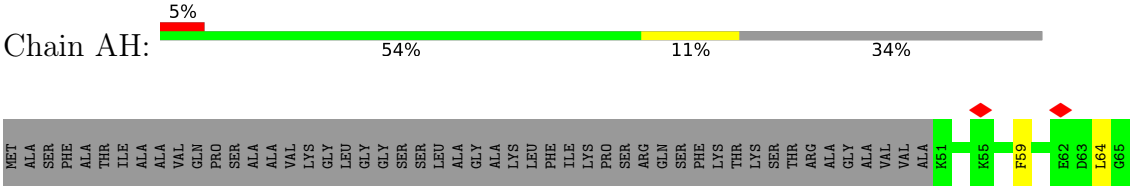
• Molecule 7: Photosystem I reaction center subunit V, chloroplastic

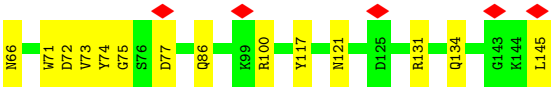
Chain BG:



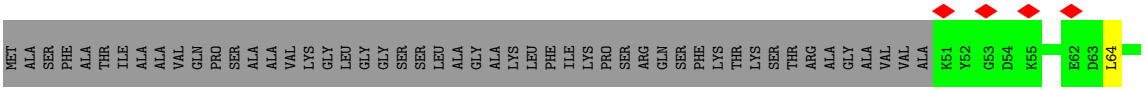
• Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

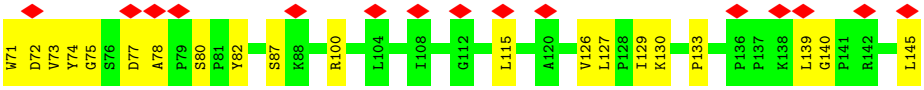
Chain AH:



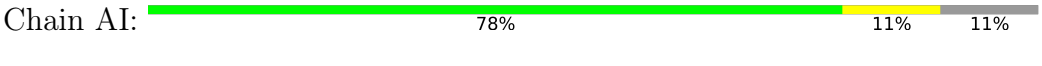


• Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

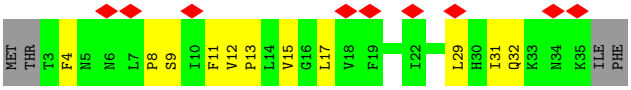




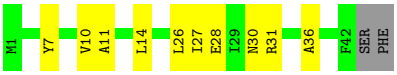
• Molecule 9: Photosystem I reaction center subunit VIII



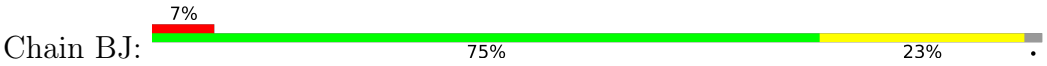
• Molecule 9: Photosystem I reaction center subunit VIII

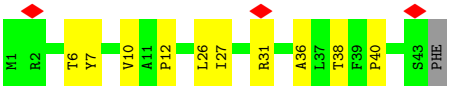


• Molecule 10: Photosystem I reaction center subunit IX

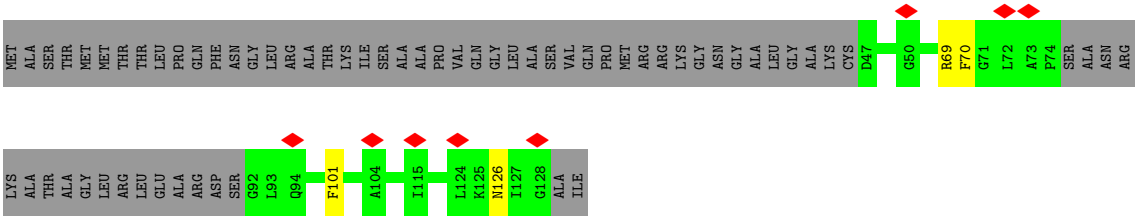


• Molecule 10: Photosystem I reaction center subunit IX



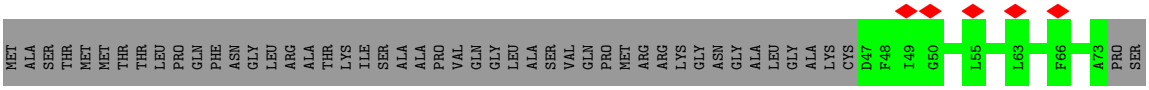


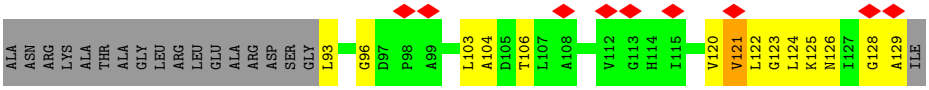
• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



• Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic

Chain BK:



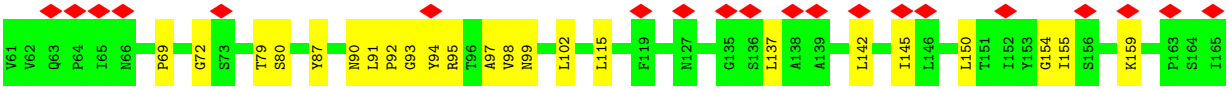


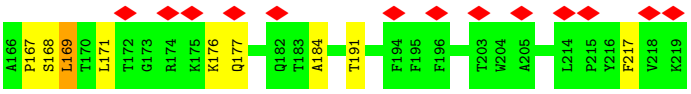
• Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

Chain AL:

• Molecule 12: Photosystem I reaction center subunit XI, chloroplastic

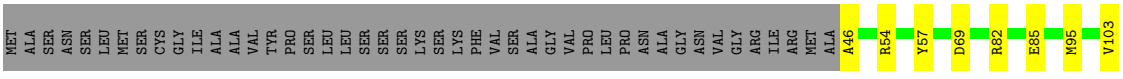
Chain BL:





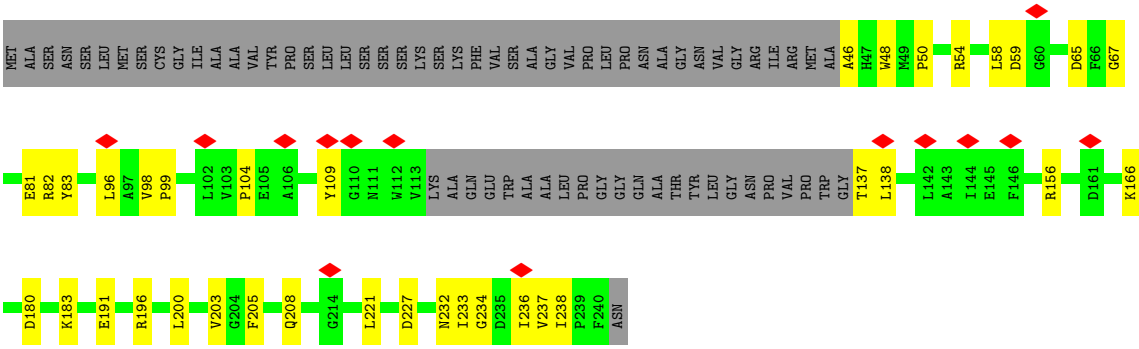
• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain A1:



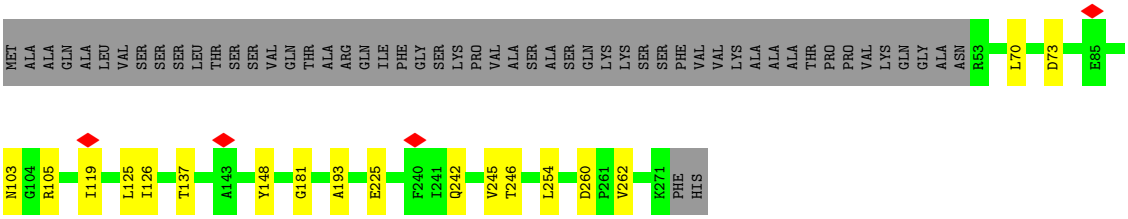
• Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

Chain B1:



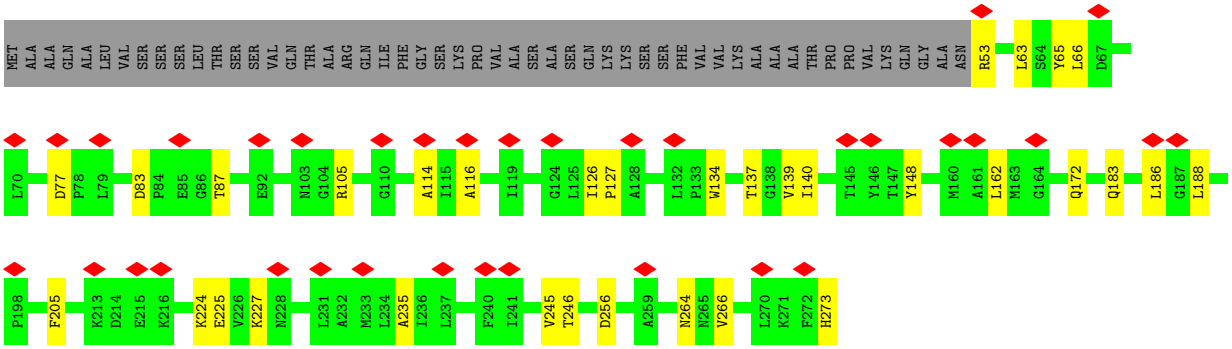
• Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain A3:



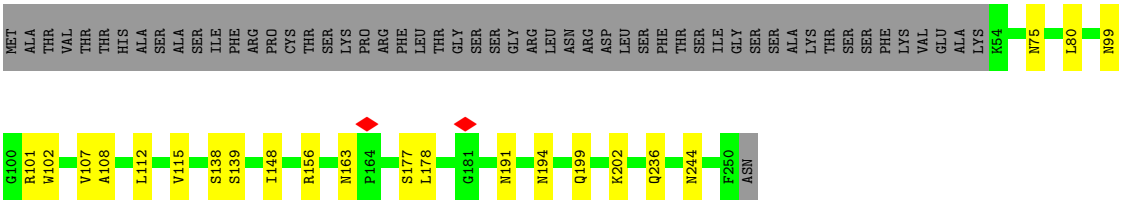
• Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic

Chain B3:



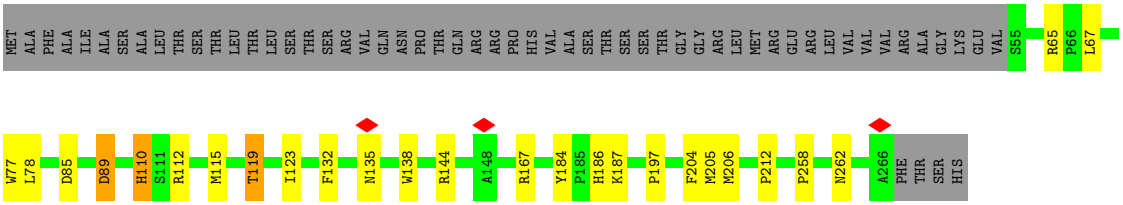
• Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic

Chain A4:



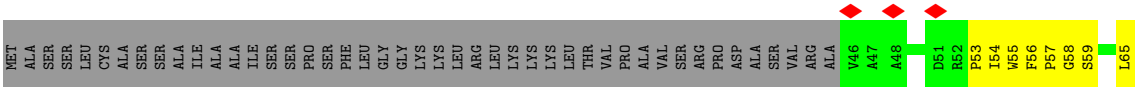
• Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

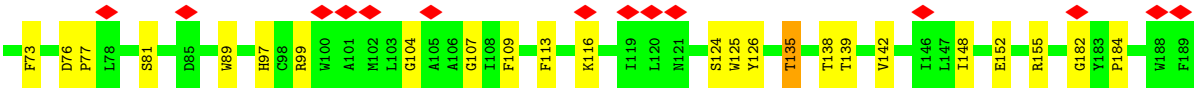
Chain A6:

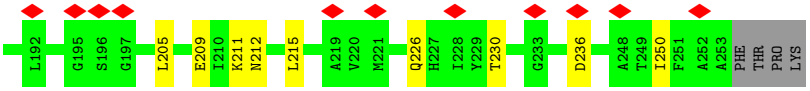


• Molecule 17: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain B2:

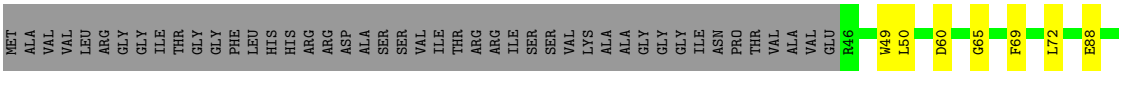


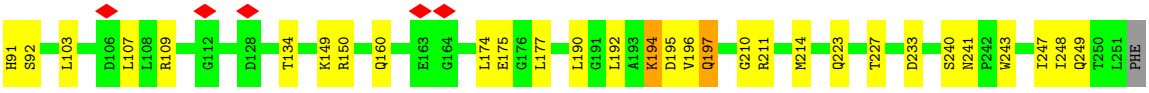




• Molecule 18: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic

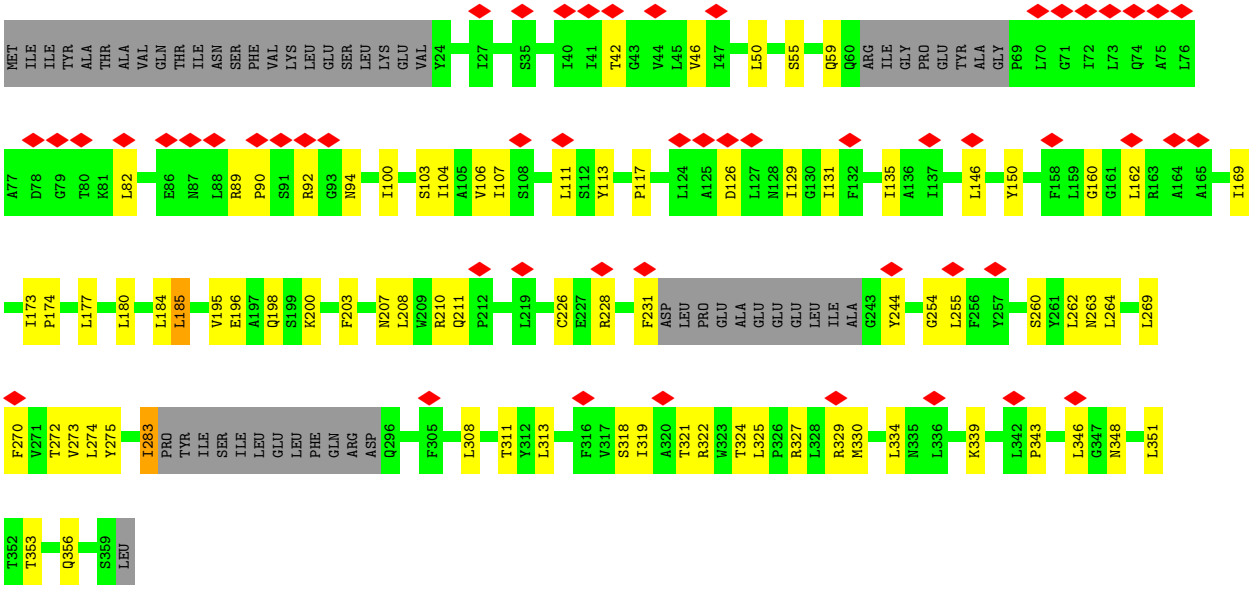
Chain B5:





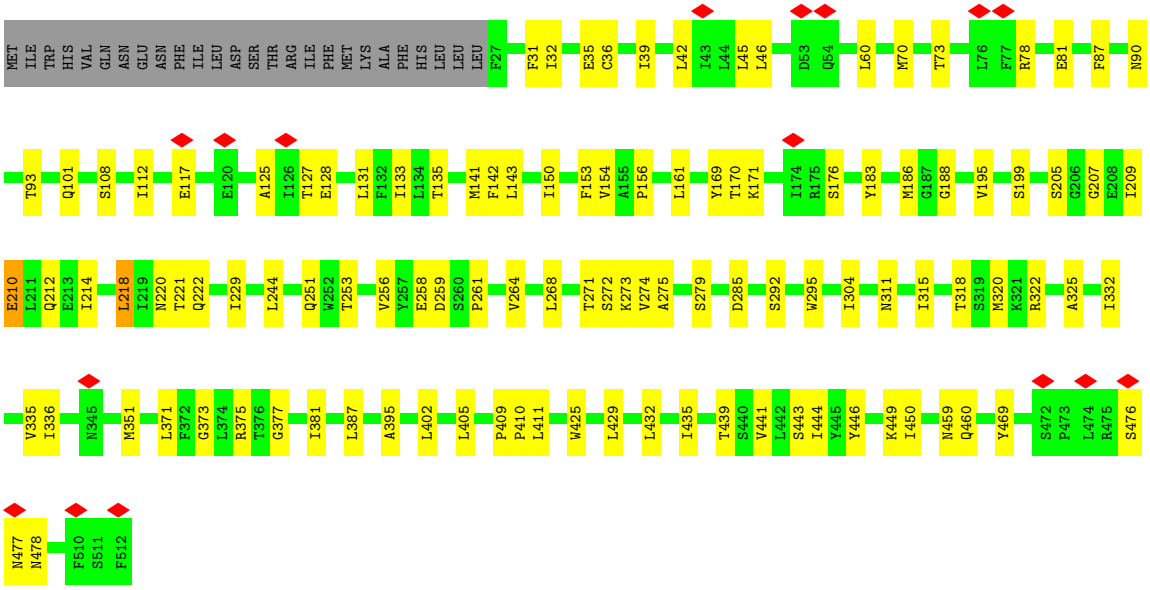
• Molecule 19: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain A:



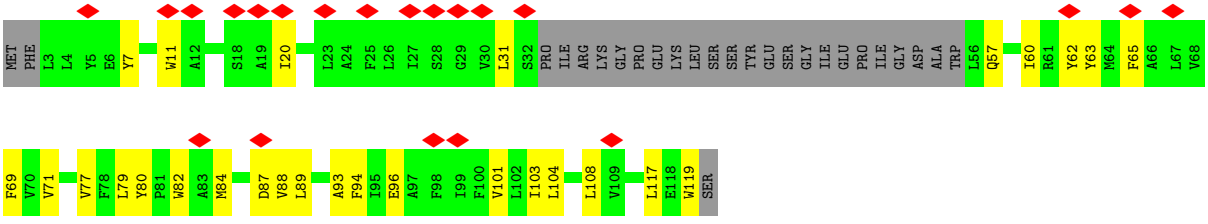
• Molecule 20: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

Chain B:



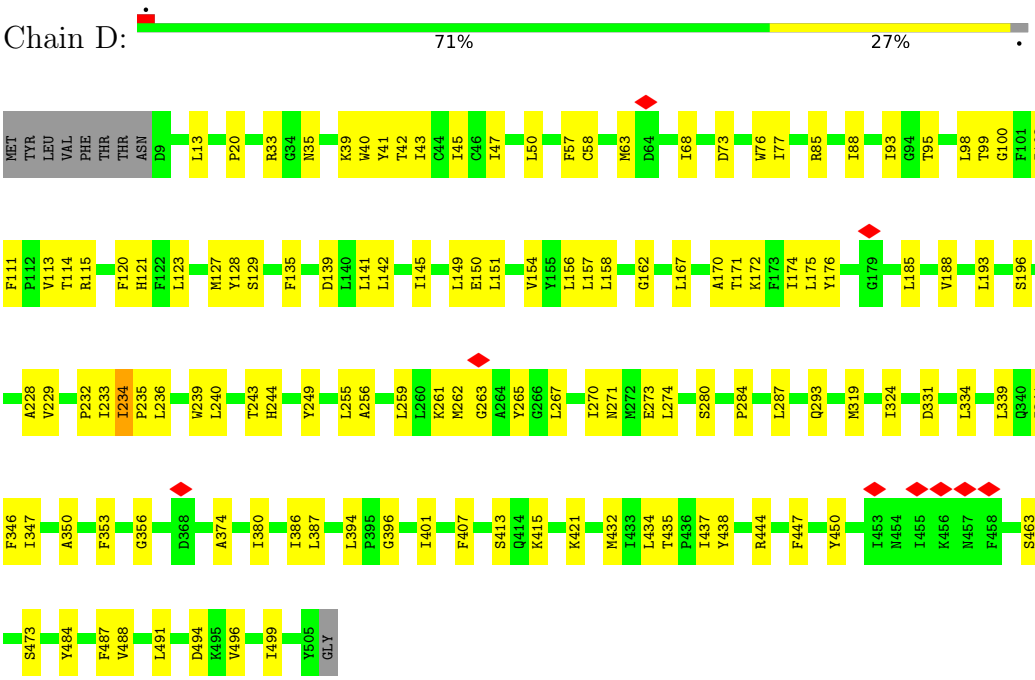
• Molecule 21: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic

Chain C:



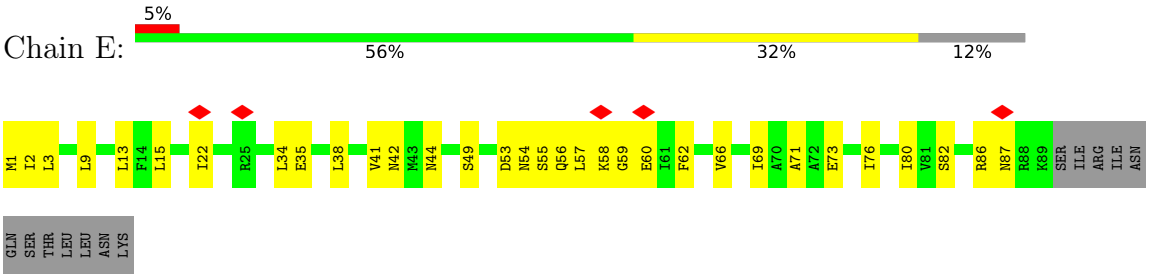
• Molecule 22: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic

Chain D:



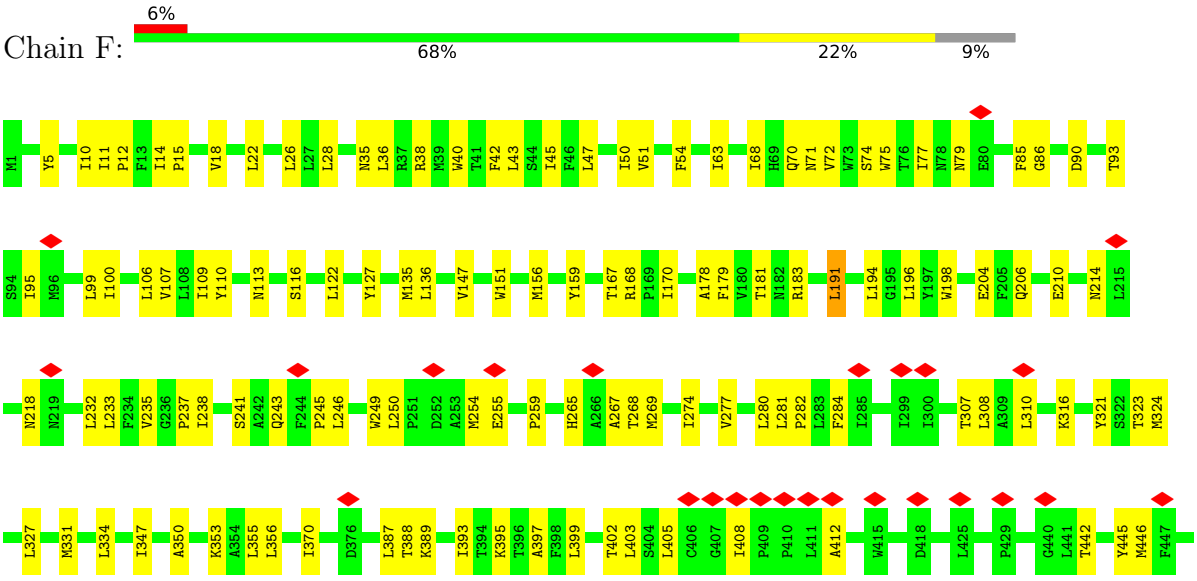
• Molecule 23: NAD(P)H-quinone oxidoreductase subunit 4L, chloroplastic

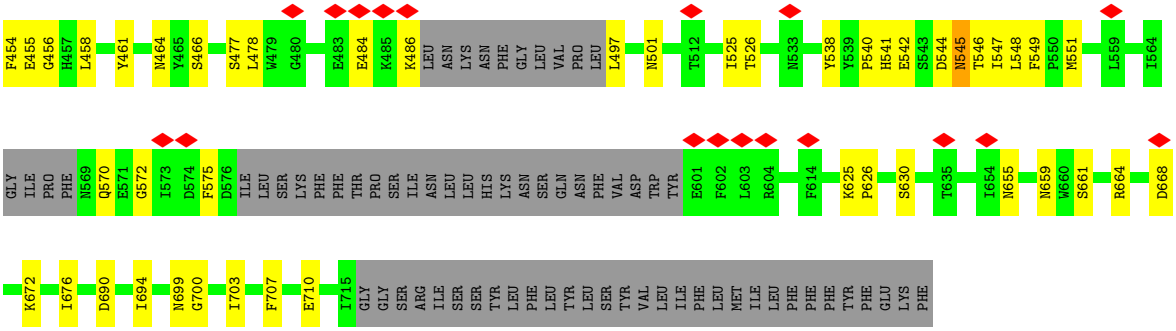
Chain E:



• Molecule 24: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

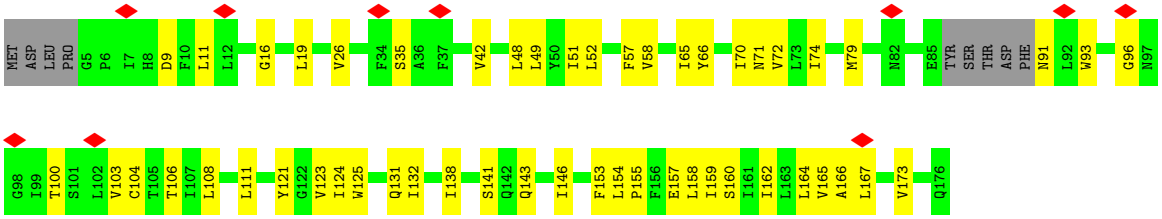
Chain F:





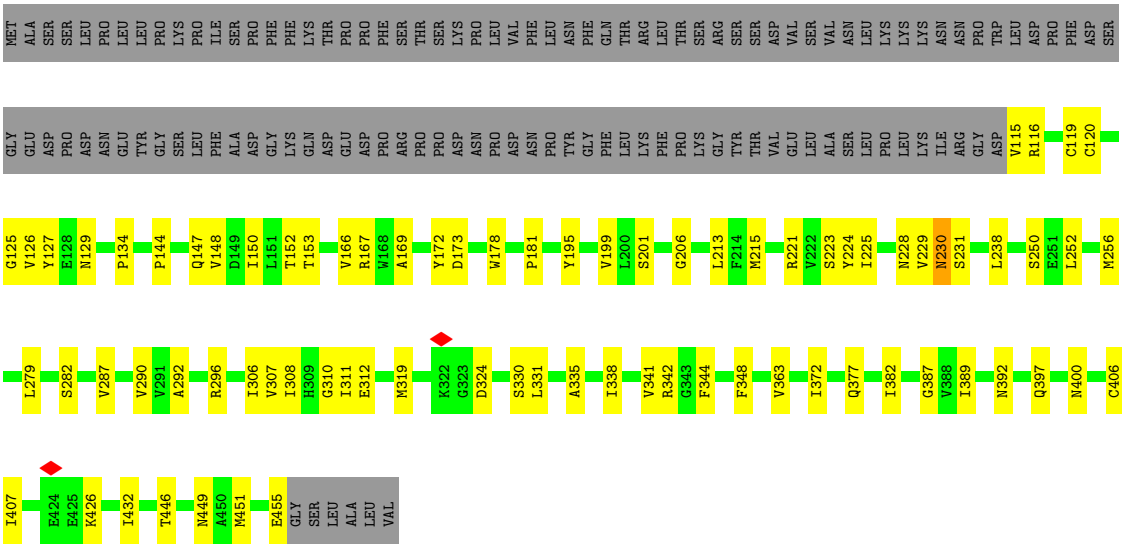
• Molecule 25: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

Chain G:



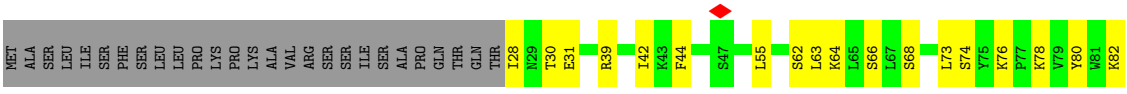
• Molecule 26: Photosynthetic NDH subunit of subcomplex B 1, chloroplastic

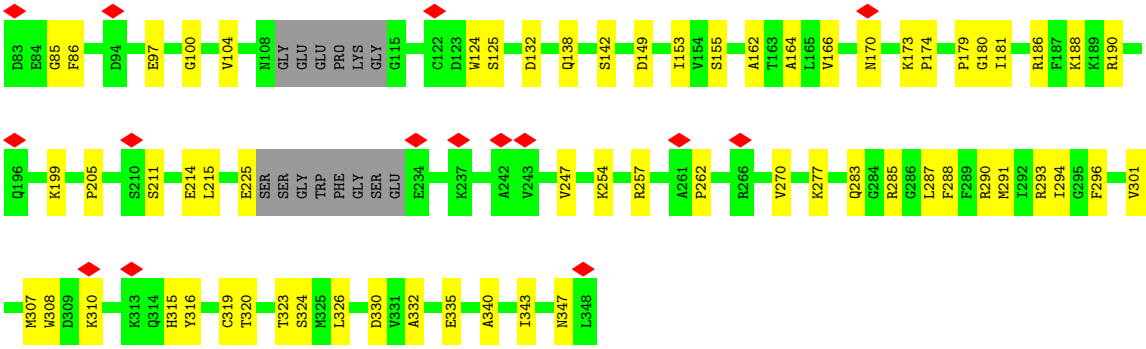
Chain a:



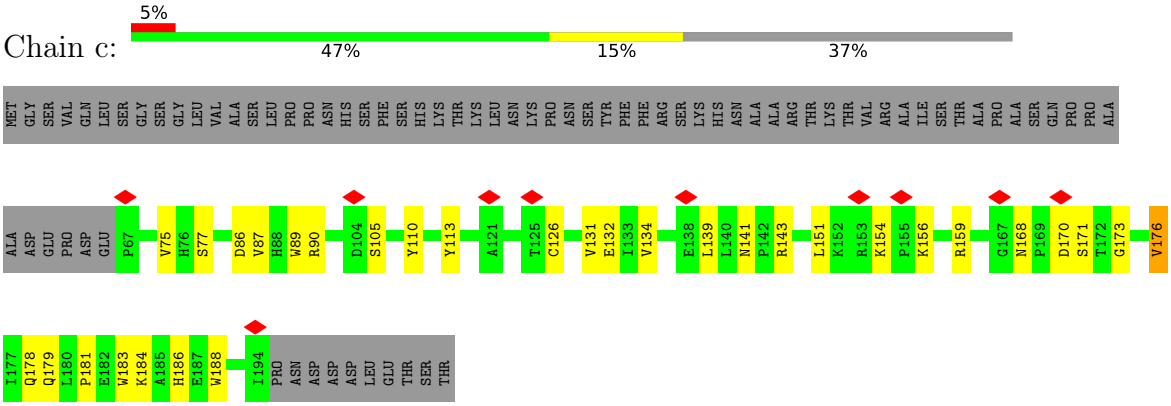
• Molecule 27: Photosynthetic NDH subunit of subcomplex B 2, chloroplastic

Chain b:

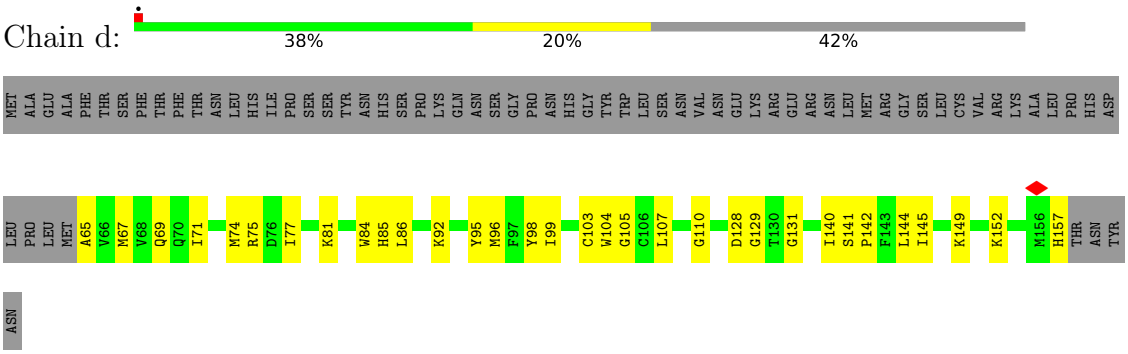




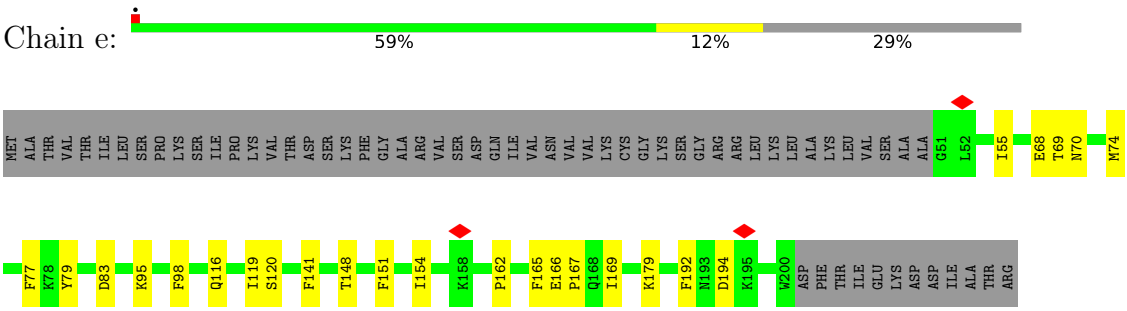
• Molecule 28: Photosynthetic NDH subunit of subcomplex B 3, chloroplastic



• Molecule 29: NDH dependent flow 6

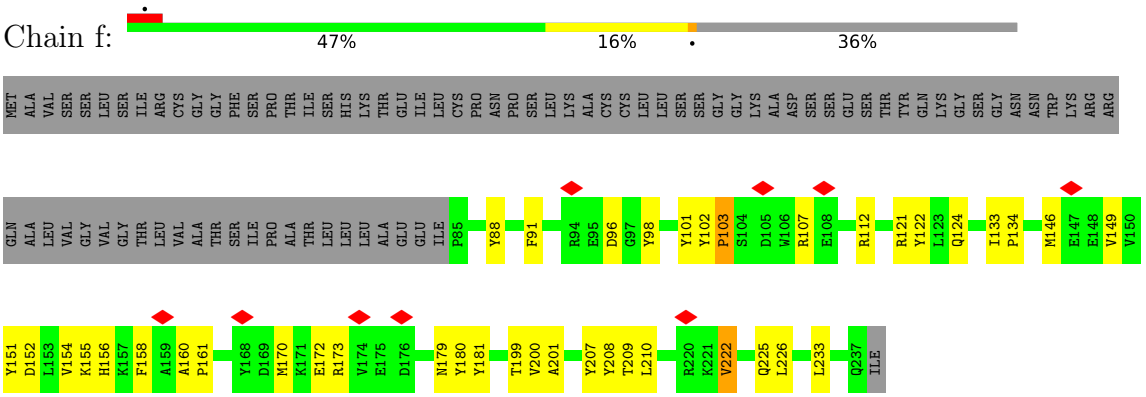


• Molecule 30: Photosynthetic NDH subunit of subcomplex B 5, chloroplastic



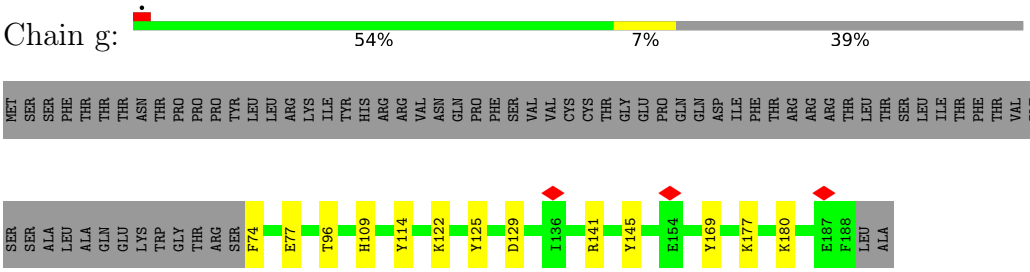
• Molecule 31: Photosynthetic NDH subunit of lumenal location 1, chloroplastic

Chain f:



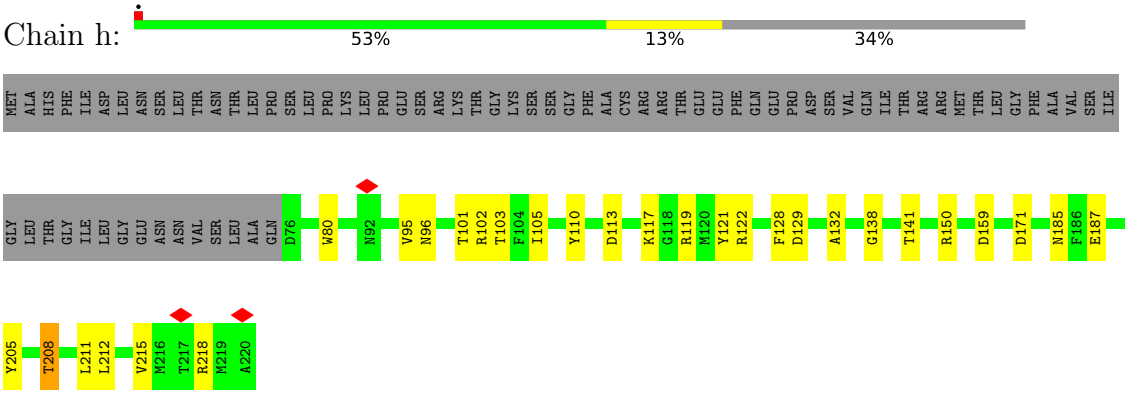
• Molecule 32: Photosynthetic NDH subunit of lumenal location 2, chloroplastic

Chain g:



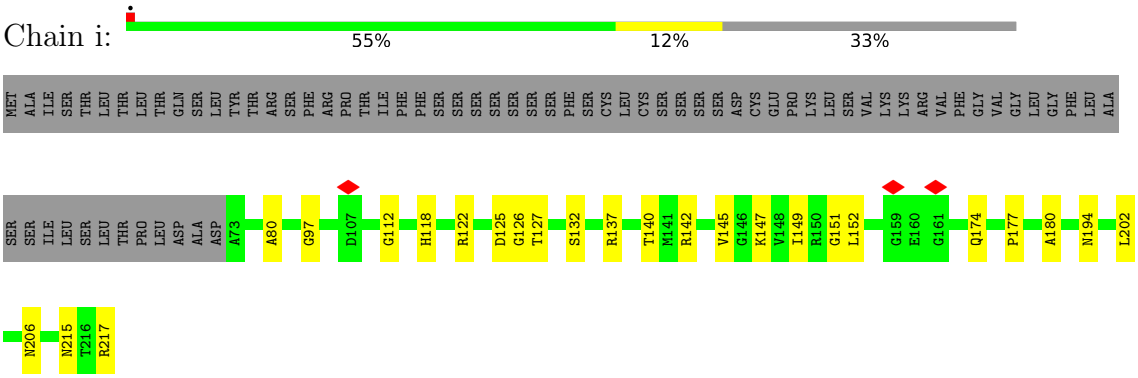
• Molecule 33: Photosynthetic NDH subunit of lumenal location 3, chloroplastic

Chain h:



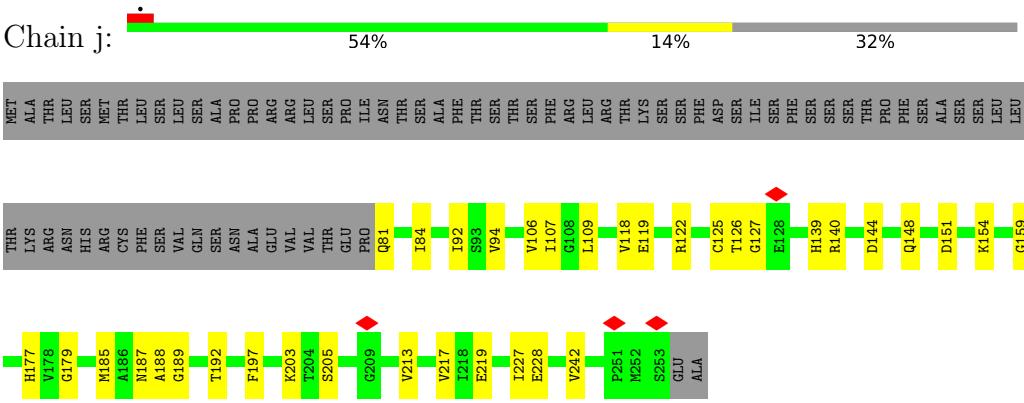
• Molecule 34: Photosynthetic NDH subunit of lumenal location 4, chloroplastic

Chain i:



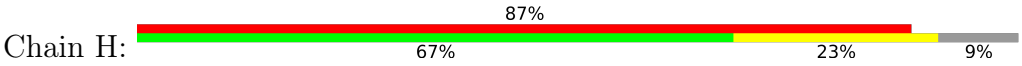
• Molecule 35: Isoform 2 of Photosynthetic NDH subunit of lumenal location 5, chloroplastic

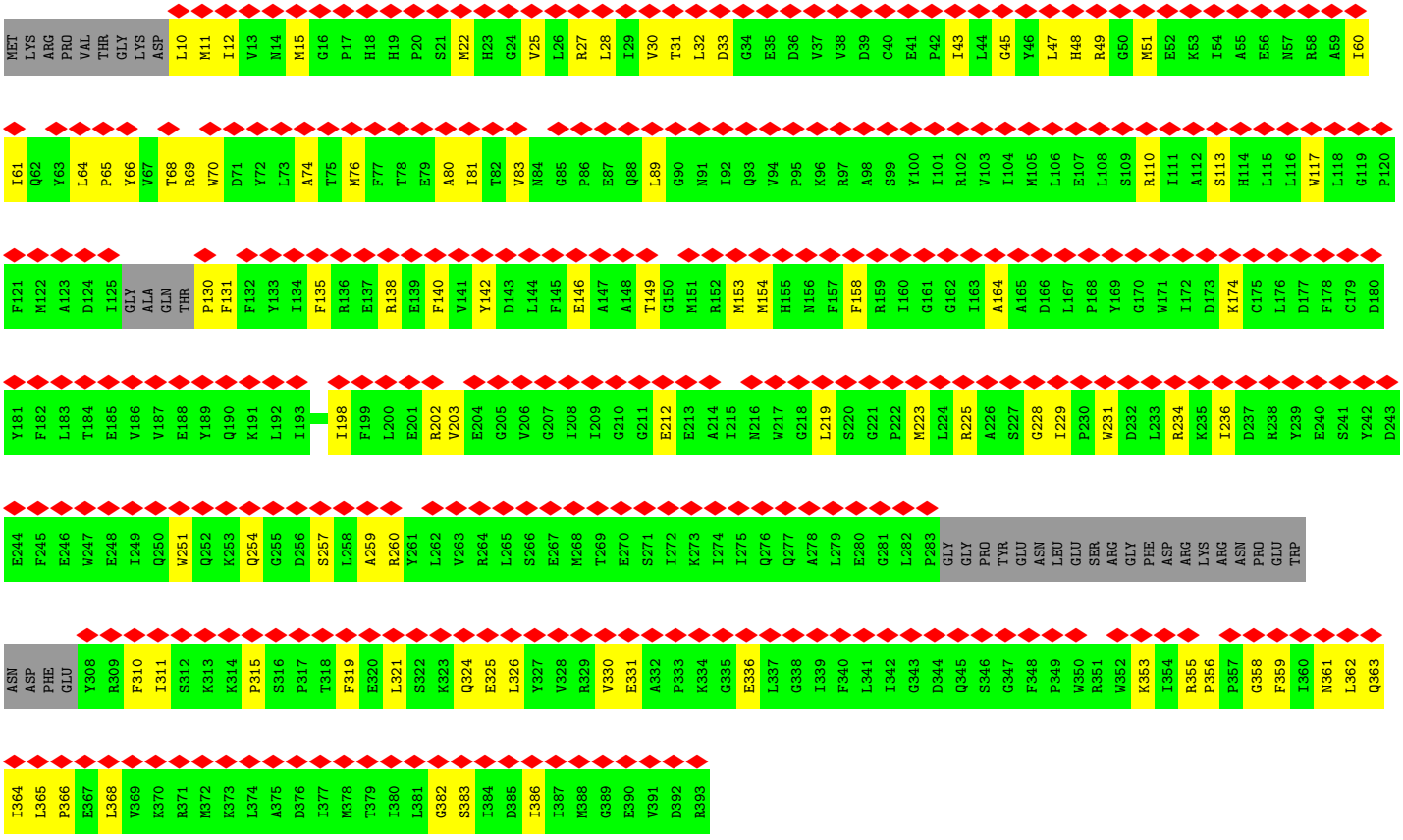
Chain j:



• Molecule 36: NAD(P)H-quinone oxidoreductase subunit H, chloroplastic

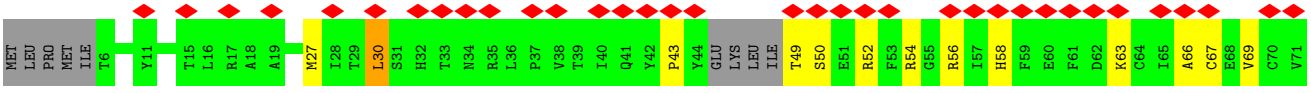
Chain H:

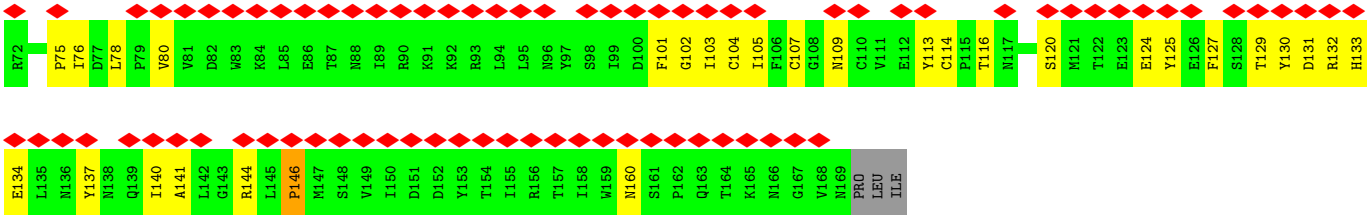




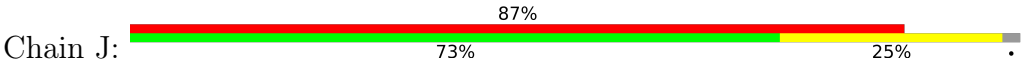
• Molecule 37: NAD(P)H-quinone oxidoreductase subunit I, chloroplastic

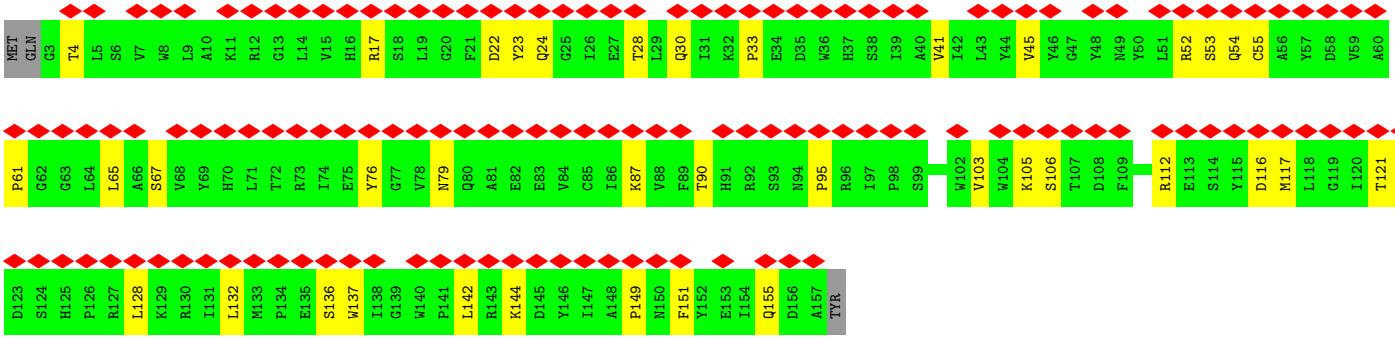
Chain I:



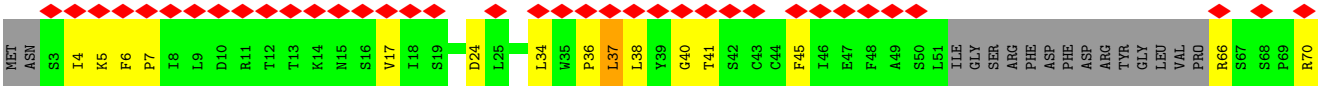


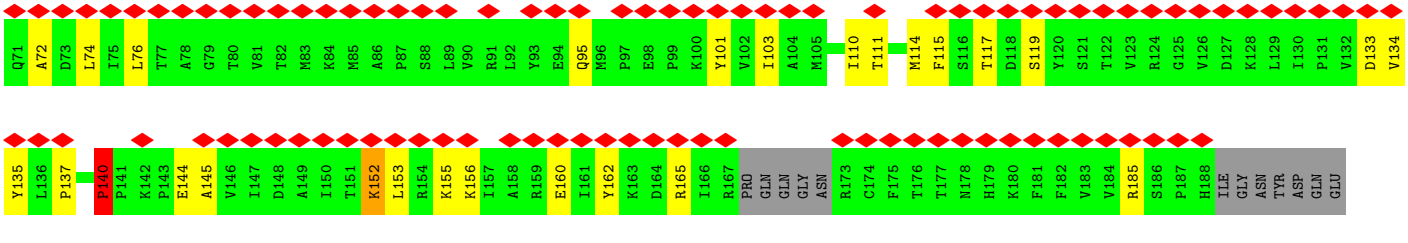
• Molecule 38: NAD(P)H-quinone oxidoreductase subunit J, chloroplastic



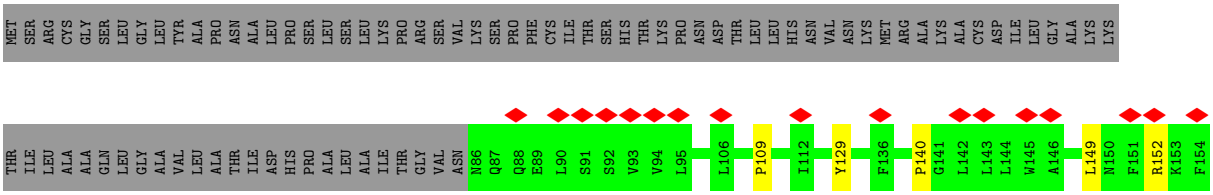


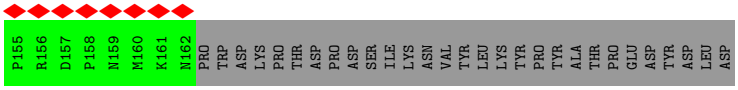
• Molecule 39: NAD(P)H-quinone oxidoreductase subunit K, chloroplastic



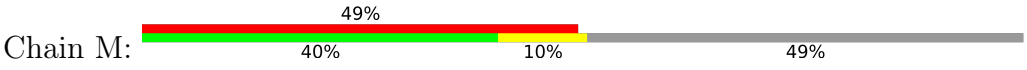


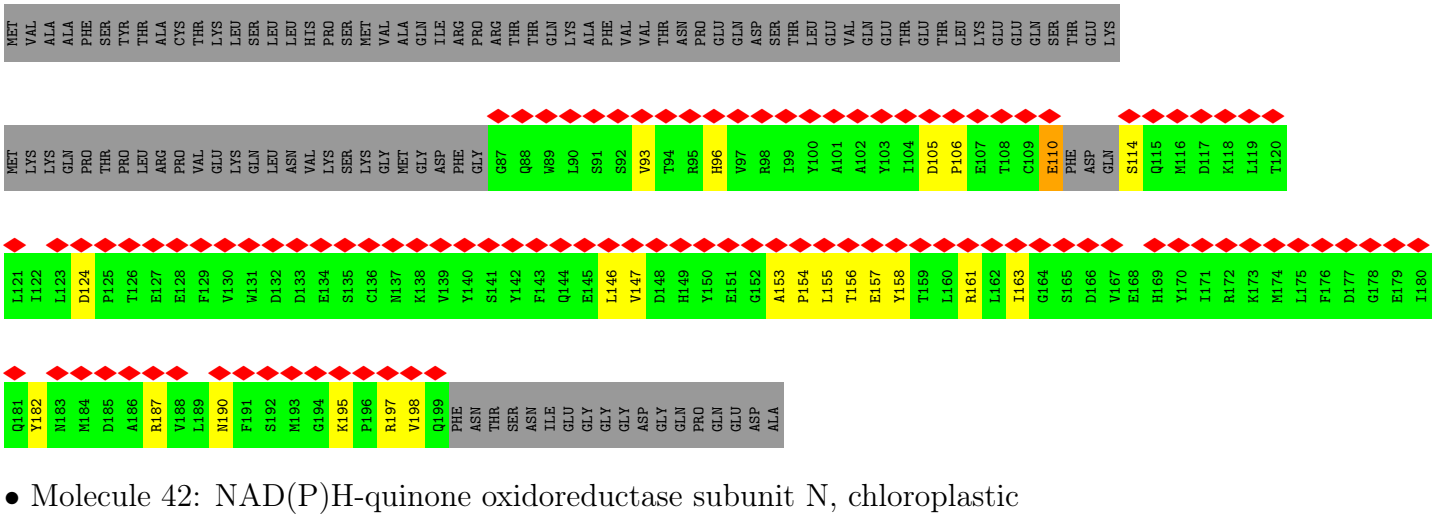
• Molecule 40: NAD(P)H-quinone oxidoreductase subunit L, chloroplastic



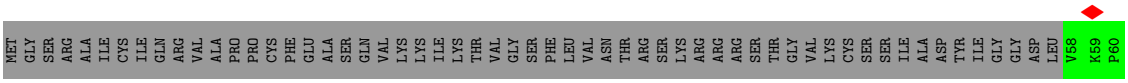


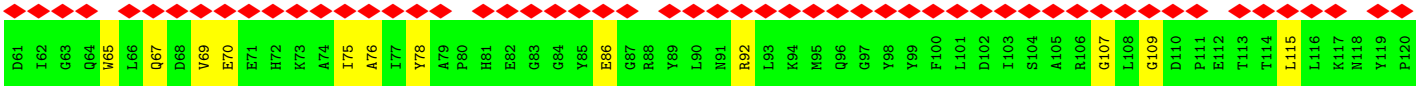
• Molecule 41: NAD(P)H-quinone oxidoreductase subunit M, chloroplastic



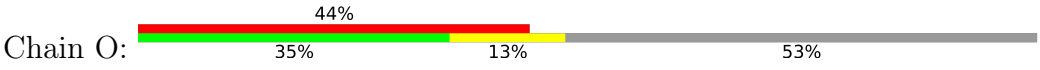


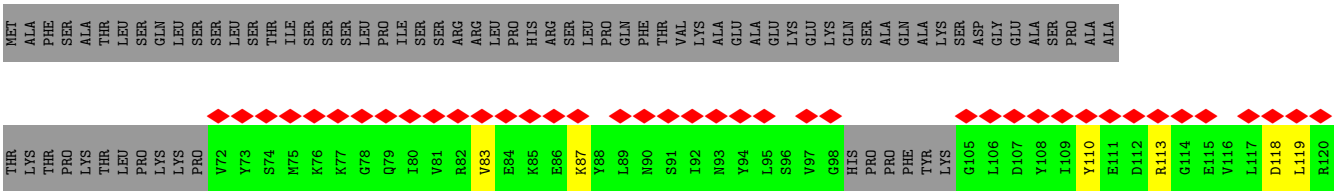
• Molecule 42: NAD(P)H-quinone oxidoreductase subunit N, chloroplastic

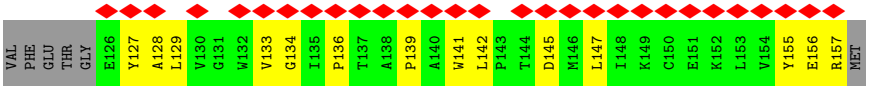




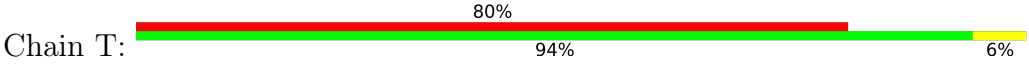
• Molecule 43: NdhO

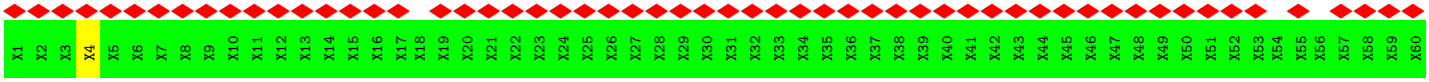


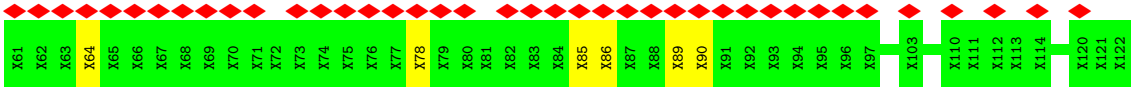




• Molecule 44: NdhT







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	136022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60.0	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.261	Depositor
Minimum map value	-0.089	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	416.0, 416.0, 416.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: XAT, LUT, LHG, SF4, SQD, PQN, FES, LMU, CLA, BCR, LMG, CHL, DGD

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	AA	0.32	1/6037 (0.0%)	0.47	0/8236
1	BA	0.31	0/6039	0.48	1/8239 (0.0%)
2	AB	0.30	0/6073	0.44	0/8291
2	BB	0.31	0/6065	0.48	1/8281 (0.0%)
3	AC	0.37	0/628	0.57	0/852
3	BC	0.39	0/628	0.63	0/852
4	AD	0.22	0/1140	0.45	0/1542
4	BD	0.32	0/1156	0.55	0/1563
5	AE	0.20	0/542	0.36	0/736
5	BE	0.20	0/559	0.37	0/760
6	AF	0.23	0/1243	0.44	0/1677
6	BF	0.25	0/1250	0.46	0/1687
7	AG	0.41	1/791 (0.1%)	0.49	0/1072
7	BG	0.31	0/750	0.54	0/1016
8	AH	0.19	0/751	0.41	0/1018
8	BH	0.25	0/751	0.48	0/1018
9	AI	0.22	0/264	0.39	0/359
9	BI	0.39	0/264	0.84	2/359 (0.6%)
10	AJ	0.31	0/348	0.54	0/474
10	BJ	0.29	0/354	0.52	0/482
11	AK	0.28	0/456	0.45	0/617
11	BK	0.40	0/449	0.68	1/607 (0.2%)
12	AL	0.26	0/1208	0.47	1/1650 (0.1%)
12	BL	0.28	0/1218	0.50	0/1663
13	A1	0.32	1/1562 (0.1%)	0.47	0/2131
13	B1	0.22	0/1381	0.43	0/1879
14	A3	0.22	0/1726	0.41	0/2347
14	B3	0.21	0/1749	0.39	0/2378
15	A4	0.27	0/1611	0.45	0/2194
16	A6	0.28	0/1732	0.49	0/2363
17	B2	0.23	0/1663	0.47	0/2277
18	B5	0.25	0/1646	0.48	1/2239 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	A	0.26	0/2430	0.60	0/3312
20	B	0.31	0/3872	0.64	2/5263 (0.0%)
21	C	0.35	1/802 (0.1%)	0.59	0/1094
22	D	0.37	0/4058	0.63	1/5509 (0.0%)
23	E	0.28	0/705	0.56	0/952
24	F	0.30	0/5478	0.63	6/7446 (0.1%)
25	G	0.27	0/1307	0.63	2/1785 (0.1%)
26	a	0.33	0/2708	0.70	0/3668
27	b	0.22	0/2417	0.60	0/3265
28	c	0.33	0/1030	0.70	0/1401
29	d	0.38	0/784	0.68	0/1057
30	e	0.26	0/1241	0.62	0/1685
31	f	0.24	0/1312	0.60	0/1777
32	g	0.22	0/986	0.51	0/1329
33	h	0.25	0/1193	0.64	0/1610
34	i	0.24	0/1124	0.53	0/1523
35	j	0.26	0/1357	0.60	0/1823
36	H	0.25	0/2877	0.53	0/3894
37	I	0.37	0/1256	0.66	1/1701 (0.1%)
38	J	0.22	0/1142	0.48	0/1545
39	K	0.34	0/1222	0.69	2/1656 (0.1%)
40	L	0.28	0/669	0.61	1/911 (0.1%)
41	M	0.31	0/783	0.54	0/1062
42	N	0.43	0/921	0.60	0/1252
43	O	0.29	0/525	0.40	0/705
All	All	0.30	4/94233 (0.0%)	0.54	22/128084 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A1	103	VAL	CA-CB	8.58	1.58	1.54
7	AG	156	PRO	C-O	-6.81	1.15	1.24
21	C	20	ILE	C-N	5.55	1.40	1.34
1	AA	17	ASP	C-O	-5.00	1.21	1.23

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	140	PRO	N-CA-C	8.24	120.75	110.70
9	BI	9	SER	CA-C-N	-7.60	114.79	122.77
9	BI	9	SER	C-N-CA	-7.60	114.79	122.77
12	AL	215	PRO	N-CA-C	-6.45	106.29	114.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
39	K	37	LEU	N-CA-C	-6.34	105.91	113.21
11	BK	124	LEU	N-CA-C	-5.98	104.57	112.34
1	BA	96	SER	N-CA-C	5.67	117.81	109.24
20	B	127	THR	CA-C-N	5.61	132.26	121.54
20	B	127	THR	C-N-CA	5.61	132.26	121.54
18	B5	194	LYS	N-CA-C	-5.40	105.09	110.97
24	F	267	ALA	CA-C-N	5.38	129.74	121.19
24	F	267	ALA	C-N-CA	5.38	129.74	121.19
25	G	96	GLY	CA-C-N	5.33	131.73	121.54
25	G	96	GLY	C-N-CA	5.33	131.73	121.54
37	I	66	ALA	CA-C-O	-5.31	115.75	121.38
40	L	109	PRO	N-CA-C	5.25	117.10	110.70
24	F	15	PRO	CA-C-N	5.14	127.37	120.58
24	F	15	PRO	C-N-CA	5.14	127.37	120.58
22	D	234	ILE	N-CA-C	5.13	119.96	108.88
2	BB	20	ARG	CB-CG-CD	-5.04	99.71	111.30
24	F	538	TYR	CA-C-N	5.01	128.26	120.60
24	F	538	TYR	C-N-CA	5.01	128.26	120.60

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	AA	5839	0	5683	76	0
1	BA	5841	0	5690	110	0
2	AB	5862	0	5649	97	0
2	BB	5854	0	5637	114	0
3	AC	615	0	593	16	0
3	BC	615	0	595	38	0
4	AD	1112	0	1122	14	0
4	BD	1127	0	1134	52	0
5	AE	530	0	536	14	0
5	BE	546	0	555	13	0
6	AF	1213	0	1243	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	BF	1220	0	1252	14	0
7	AG	771	0	749	16	0
7	BG	733	0	718	82	0
8	AH	730	0	720	25	0
8	BH	730	0	720	71	0
9	AI	257	0	274	7	0
9	BI	257	0	274	34	0
10	AJ	338	0	351	14	0
10	BJ	344	0	356	13	0
11	AK	451	0	462	11	0
11	BK	445	0	453	36	0
12	AL	1173	0	1162	27	0
12	BL	1184	0	1179	73	0
13	A1	1511	0	1464	16	0
13	B1	1339	0	1316	39	0
14	A3	1675	0	1647	11	0
14	B3	1696	0	1663	39	0
15	A4	1562	0	1516	22	0
16	A6	1671	0	1599	56	0
17	B2	1607	0	1555	56	0
18	B5	1599	0	1581	37	0
19	A	2372	0	2454	64	0
20	B	3780	0	3840	87	0
21	C	776	0	777	30	0
22	D	3946	0	4068	107	0
23	E	695	0	732	34	0
24	F	5330	0	5289	175	0
25	G	1281	0	1340	59	0
26	a	2655	0	2673	67	0
27	b	2367	0	2371	60	0
28	c	1005	0	1006	22	0
29	d	762	0	730	49	0
30	e	1206	0	1110	27	0
31	f	1277	0	1235	31	0
32	g	965	0	945	12	0
33	h	1170	0	1176	26	0
34	i	1098	0	1082	21	0
35	j	1331	0	1320	22	0
36	H	2812	0	2795	93	0
37	I	1236	0	1180	70	0
38	J	1116	0	938	65	0
39	K	1199	0	1106	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
40	L	646	0	630	12	0
41	M	771	0	652	43	0
42	N	908	0	717	59	0
43	O	520	0	438	20	0
44	T	610	0	133	12	0
45	A1	575	0	447	8	0
45	A3	575	0	420	2	0
45	A4	480	0	376	5	0
45	A6	485	0	399	14	0
45	AA	2411	0	2371	32	0
45	AB	2452	0	2461	37	0
45	AF	140	0	113	1	0
45	AG	131	0	94	5	0
45	AH	60	0	59	1	0
45	AJ	42	0	31	1	0
45	AK	126	0	88	12	0
45	AL	143	0	119	1	0
45	B1	519	0	402	8	0
45	B2	442	0	366	15	0
45	B3	578	0	422	6	0
45	B5	476	0	368	4	0
45	BA	2446	0	2387	39	0
45	BB	2422	0	2404	50	0
45	BF	138	0	110	1	0
45	BG	87	0	64	48	0
45	BH	60	0	59	0	0
45	BJ	42	0	31	0	0
45	BK	127	0	88	7	0
45	BL	148	0	125	11	0
46	AA	33	0	46	3	0
46	AB	33	0	46	2	0
46	BA	33	0	46	3	0
46	BB	33	0	46	2	0
47	A1	123	0	162	0	0
47	A3	59	0	58	1	0
47	A6	36	0	42	0	0
47	AA	49	0	74	1	0
47	AJ	40	0	53	0	0
47	B1	116	0	145	1	0
47	B2	35	0	40	2	0
47	B3	23	0	16	1	0
47	B5	30	0	30	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	BA	76	0	98	3	0
47	BF	45	0	63	1	0
47	F	37	0	44	3	0
47	a	29	0	28	2	0
48	A1	40	0	56	3	0
48	A3	40	0	56	2	0
48	A4	40	0	56	0	0
48	A6	40	0	56	3	0
48	AA	240	0	336	6	0
48	AB	240	0	336	9	0
48	AF	80	0	112	6	0
48	AG	40	0	56	1	0
48	AI	80	0	112	3	0
48	AJ	80	0	112	5	0
48	AK	40	0	56	2	0
48	AL	80	0	112	1	0
48	B2	40	0	56	2	0
48	B3	40	0	56	4	0
48	B5	40	0	56	0	0
48	BA	280	0	392	13	0
48	BB	240	0	336	13	0
48	BF	40	0	56	1	0
48	BG	40	0	56	13	0
48	BI	40	0	56	1	0
48	BJ	80	0	112	9	0
48	BK	40	0	56	0	0
48	BL	120	0	167	6	0
49	AA	8	0	0	0	0
49	AC	16	0	0	4	0
49	BA	8	0	0	1	0
49	BC	16	0	0	7	0
49	I	16	0	0	4	0
49	K	8	0	0	1	0
50	AA	35	0	46	0	0
50	AB	105	0	138	0	0
50	AL	34	0	41	1	0
50	BA	67	0	80	0	0
50	BB	35	0	46	0	0
51	AB	66	0	96	0	0
51	BB	66	0	96	1	0
52	A1	42	0	56	1	0
52	A3	42	0	56	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	A4	42	0	56	4	0
52	A6	42	0	56	4	0
52	AF	42	0	56	2	0
52	B1	42	0	56	3	0
52	B2	42	0	56	0	0
52	B3	42	0	56	3	0
52	B5	42	0	56	0	0
53	A1	44	0	58	1	0
53	A4	39	0	48	4	0
53	AG	38	0	46	0	0
53	B5	33	0	36	0	0
54	A1	92	0	60	3	0
54	A3	45	0	30	0	0
54	A4	169	0	100	2	0
54	A6	187	0	127	2	0
54	B1	91	0	58	2	0
54	B2	227	0	154	16	0
54	B3	45	0	30	1	0
54	B5	126	0	67	0	0
55	A1	44	0	56	1	0
55	A3	44	0	56	2	0
55	A4	44	0	56	2	0
55	A6	44	0	56	4	0
55	B1	44	0	56	0	0
55	B2	44	0	56	6	0
55	B3	44	0	56	1	0
55	B5	44	0	56	1	0
56	BJ	47	0	61	6	0
56	e	34	0	32	1	0
57	c	4	0	0	2	0
All	All	112687	0	110283	2142	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 10.

All (2142) 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)
40:L:149:LEU:HD21	40:L:152:ARG:CD	1.39	1.52
18:B5:175:GLU:CB	26:a:229:VAL:HG12	1.46	1.45
8:BH:100:ARG:NH1	12:BL:155:ILE:HA	1.35	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:87:ILE:HG23	2:AB:113:VAL:CG1	1.58	1.33
8:AH:71:TRP:CD1	12:AL:169:LEU:HD11	1.65	1.30
7:BG:132:VAL:HG21	45:BG:202:CLA:CMA	1.64	1.28
8:BH:82:TYR:CD2	12:BL:102:LEU:HD12	1.68	1.27
8:AH:71:TRP:HD1	12:AL:169:LEU:CD1	1.47	1.26
8:BH:82:TYR:CD2	12:BL:102:LEU:CD1	2.21	1.24
11:BK:93:LEU:CD1	11:BK:103:LEU:HB3	1.67	1.23
8:BH:75:GLY:O	12:BL:176:LYS:HE3	1.36	1.22
16:A6:205:MET:HE3	24:F:109:ILE:CD1	1.68	1.20
7:BG:124:PRO:HG3	45:BG:202:CLA:CBC	1.72	1.18
40:L:149:LEU:CD2	40:L:152:ARG:HD2	1.74	1.17
1:BA:358:GLY:O	1:BA:361:THR:HG22	1.44	1.15
42:N:128:LYS:NZ	43:O:139:PRO:HD3	1.61	1.15
8:BH:100:ARG:HD3	12:BL:155:ILE:HG12	1.27	1.15
14:B3:53:ARG:HH11	14:B3:63:LEU:CD1	1.59	1.14
2:AB:87:ILE:CG2	2:AB:113:VAL:HG11	1.78	1.14
7:BG:127:PHE:CE2	45:BG:202:CLA:HMB1	1.82	1.13
8:BH:115:LEU:HD21	9:BI:17:LEU:CD1	1.79	1.12
8:BH:126:VAL:O	8:BH:127:LEU:HD12	1.49	1.12
1:BA:506:THR:CG2	1:BA:521:LEU:HD11	1.80	1.11
7:BG:132:VAL:HG21	45:BG:202:CLA:HMA1	1.26	1.11
8:BH:115:LEU:CD2	9:BI:17:LEU:HD12	1.79	1.11
11:BK:93:LEU:HD12	11:BK:103:LEU:HB3	1.12	1.11
14:B3:53:ARG:NH1	14:B3:63:LEU:HD13	1.64	1.11
40:L:149:LEU:CD2	40:L:152:ARG:CD	2.28	1.10
39:K:37:LEU:HG	39:K:72:ALA:HB3	1.17	1.10
7:BG:123:ASP:OD1	7:BG:124:PRO:HD2	1.50	1.09
1:BA:264:LEU:HB3	11:BK:122:LEU:HD11	1.32	1.09
18:B5:175:GLU:CB	26:a:229:VAL:CG1	2.29	1.08
2:AB:106:ARG:CZ	2:AB:115:ILE:HG12	1.83	1.08
7:AG:76:LEU:HD13	45:AG:204:CLA:HMB3	1.32	1.07
7:AG:116:VAL:O	7:AG:120:LYS:HG3	1.53	1.07
13:B1:58:LEU:HD11	13:B1:67:GLY:HA2	1.16	1.07
7:BG:124:PRO:HG3	45:BG:202:CLA:HBC3	1.32	1.07
8:AH:71:TRP:HD1	12:AL:169:LEU:HD11	0.90	1.07
2:AB:87:ILE:HG23	2:AB:113:VAL:HG11	1.16	1.06
7:AG:76:LEU:HD13	45:AG:204:CLA:CMB	1.86	1.05
2:BB:405:ASP:OD1	2:BB:410:ARG:HD3	1.55	1.05
27:b:190:ARG:HD3	27:b:308:TRP:CZ2	1.93	1.03
45:A6:610:CLA:H72	24:F:42:PHE:HZ	1.21	1.03
11:BK:93:LEU:CD2	11:BK:104:ALA:HB2	1.89	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:M:195:LYS:HB3	42:N:137:PRO:HG3	1.41	1.03
8:BH:77:ASP:HB2	12:BL:177:GLN:NE2	1.73	1.03
11:BK:93:LEU:CD1	11:BK:103:LEU:HD23	1.87	1.02
37:I:76:ILE:HD11	39:K:117:THR:H	1.23	1.02
1:BA:224:PHE:CE1	1:BA:250:LEU:HD11	1.94	1.02
2:BB:467:HIS:HA	2:BB:478:LEU:HD12	1.02	1.02
37:I:43:PRO:HD3	39:K:144:GLU:HG2	1.42	1.01
2:AB:476:VAL:HG12	2:AB:477:LEU:H	1.20	1.00
16:A6:205:MET:HA	24:F:546:THR:CG2	1.90	1.00
2:BB:5:PHE:HB2	9:BI:31:ILE:HA	1.41	1.00
2:BB:467:HIS:HA	2:BB:478:LEU:CD1	1.92	1.00
1:AA:175:TRP:CH2	1:AA:180:LYS:HG3	1.96	0.99
36:H:10:LEU:HD23	36:H:31:THR:OG1	1.62	0.99
37:I:127:PHE:HB2	39:K:137:PRO:HG3	1.43	0.99
16:A6:206:MET:SD	24:F:544:ASP:HB3	2.01	0.99
12:BL:87:TYR:O	12:BL:91:LEU:HD13	1.61	0.99
13:B1:58:LEU:CD1	13:B1:67:GLY:HA2	1.91	0.99
1:AA:118:ILE:CD1	10:AJ:27:ILE:HG23	1.92	0.99
36:H:32:LEU:O	36:H:32:LEU:HD12	1.63	0.99
42:N:176:PRO:O	42:N:180:PRO:HD2	1.63	0.98
2:BB:467:HIS:CA	2:BB:478:LEU:HD12	1.92	0.98
16:A6:205:MET:HA	24:F:546:THR:HG22	1.41	0.98
16:A6:205:MET:HE2	24:F:45:ILE:HD13	1.45	0.98
1:BA:506:THR:HG23	1:BA:521:LEU:HD11	1.44	0.98
16:A6:205:MET:CE	24:F:109:ILE:CD1	2.42	0.98
2:BB:70:TRP:HZ2	9:BI:4:PHE:O	1.45	0.98
8:BH:100:ARG:NH1	12:BL:155:ILE:CA	2.26	0.97
7:BG:132:VAL:HG21	45:BG:202:CLA:HMA2	1.46	0.97
5:BE:87:VAL:HG21	5:BE:138:VAL:CG1	1.94	0.97
14:B3:53:ARG:HH11	14:B3:63:LEU:HD13	1.23	0.96
8:BH:82:TYR:CD2	12:BL:102:LEU:HD13	2.00	0.96
2:BB:292:ARG:HE	7:BG:96:LEU:HA	1.30	0.96
38:J:137:TRP:CE3	41:M:161:ARG:NH2	2.34	0.96
11:BK:93:LEU:HD23	11:BK:104:ALA:HB2	1.47	0.96
11:BK:93:LEU:HD12	11:BK:103:LEU:CB	1.96	0.95
40:L:149:LEU:HD21	40:L:152:ARG:HD2	0.97	0.95
8:AH:72:ASP:OD2	8:AH:75:GLY:HA3	1.65	0.95
8:BH:100:ARG:HH11	12:BL:155:ILE:CA	1.78	0.95
11:AK:126:ASN:HD22	45:AK:202:CLA:HMA3	1.32	0.94
8:BH:82:TYR:CG	12:BL:102:LEU:HD13	2.02	0.94
39:K:37:LEU:CG	39:K:72:ALA:HB3	1.95	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:M:195:LYS:HB3	42:N:137:PRO:CG	1.97	0.94
28:c:126:CYS:O	57:c:301:FES:S1	2.26	0.94
24:F:113:ASN:HB2	24:F:546:THR:OG1	1.67	0.94
8:BH:115:LEU:HD21	9:BI:17:LEU:HD12	0.95	0.93
2:BB:294:ASN:ND2	7:BG:112:ALA:HA	1.83	0.93
24:F:254:MET:SD	24:F:316:LYS:HB3	2.08	0.93
7:BG:127:PHE:HD2	45:BG:202:CLA:HHB	1.34	0.93
1:AA:175:TRP:CH2	1:AA:180:LYS:CG	2.52	0.92
39:K:5:LYS:O	42:N:148:PRO:HG3	1.68	0.92
11:BK:93:LEU:CD1	11:BK:103:LEU:CB	2.47	0.92
22:D:484:TYR:CE2	29:d:86:LEU:HD12	2.05	0.92
8:BH:82:TYR:HD2	12:BL:102:LEU:HD12	1.28	0.92
27:b:28:ILE:CG2	27:b:31:GLU:HB2	1.99	0.91
37:I:130:TYR:CD1	39:K:134:VAL:HG22	2.05	0.91
2:AB:687:LEU:HD21	12:AL:91:LEU:HD11	1.50	0.91
2:AB:87:ILE:CG2	2:AB:113:VAL:CG1	2.42	0.91
1:AA:175:TRP:CZ2	1:AA:180:LYS:HD3	2.06	0.90
8:BH:100:ARG:HH21	12:BL:184:ALA:HB1	1.33	0.90
8:BH:115:LEU:CD2	9:BI:17:LEU:CD1	2.45	0.90
45:A6:610:CLA:H41	24:F:42:PHE:CE2	2.06	0.90
7:BG:124:PRO:HG3	45:BG:202:CLA:HBC2	1.50	0.90
15:A4:199:GLN:HE22	15:A4:202:LYS:HZ1	1.17	0.89
27:b:28:ILE:HG21	27:b:31:GLU:HB2	1.53	0.89
16:A6:204:PHE:O	24:F:546:THR:CG2	2.20	0.88
45:A6:610:CLA:H61	24:F:42:PHE:CE2	2.08	0.88
9:BI:29:LEU:HD21	12:BL:155:ILE:HG21	1.53	0.88
15:A4:199:GLN:HE22	15:A4:202:LYS:NZ	1.71	0.88
2:BB:292:ARG:NE	7:BG:96:LEU:HA	1.89	0.88
11:BK:93:LEU:HD11	11:BK:103:LEU:CG	2.04	0.88
16:A6:204:PHE:CD1	24:F:549:PHE:CD2	2.61	0.88
1:AA:175:TRP:CZ3	1:AA:180:LYS:HG3	2.08	0.88
7:BG:127:PHE:CD2	45:BG:202:CLA:HMB1	2.08	0.88
8:BH:82:TYR:CE2	12:BL:102:LEU:HB2	2.09	0.88
7:BG:127:PHE:HD2	45:BG:202:CLA:CHB	1.86	0.88
40:L:149:LEU:HD21	40:L:152:ARG:HD3	1.52	0.87
41:M:105:ASP:CG	41:M:106:PRO:CD	2.47	0.87
7:BG:132:VAL:CG2	45:BG:202:CLA:CMA	2.52	0.87
27:b:190:ARG:CD	27:b:308:TRP:CZ2	2.56	0.87
36:H:22:MET:HE2	39:K:45:PHE:CE1	2.09	0.87
8:AH:71:TRP:CD1	12:AL:169:LEU:CD1	2.39	0.86
7:BG:132:VAL:CG1	48:BG:203:BCR:H19C	2.04	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BH:100:ARG:HD3	12:BL:155:ILE:CG1	2.04	0.86
18:B5:190:LEU:HD23	26:a:178:TRP:HH2	1.40	0.86
16:A6:205:MET:HE3	24:F:109:ILE:HD11	1.57	0.86
19:A:55:SER:O	19:A:59:GLN:HB2	1.76	0.86
16:A6:205:MET:HE3	24:F:109:ILE:HD12	1.58	0.86
7:BG:132:VAL:CG2	45:BG:202:CLA:HMA1	2.06	0.86
37:I:105:ILE:HG13	39:K:114:MET:HB3	1.57	0.85
11:BK:121:VAL:HG12	11:BK:122:LEU:HD12	1.57	0.85
19:A:226:CYS:SG	19:A:263:ASN:CG	2.60	0.85
20:B:176:SER:HA	20:B:259:ASP:CB	2.07	0.85
8:BH:77:ASP:HB2	12:BL:177:GLN:HE22	1.35	0.85
17:B2:56:PHE:CD1	54:B2:601:CHL:HMA3	2.12	0.85
42:N:128:LYS:HZ1	43:O:139:PRO:HD3	1.36	0.85
37:I:103:ILE:HD13	39:K:111:THR:HB	1.58	0.84
39:K:37:LEU:HG	39:K:72:ALA:CB	2.04	0.84
14:B3:53:ARG:HH11	14:B3:63:LEU:HD12	1.40	0.84
3:BC:18:VAL:HG21	4:BD:168:PRO:HB2	1.58	0.84
12:BL:91:LEU:HD12	45:BL:302:CLA:HMC2	1.60	0.84
4:AD:153:PRO:O	8:AH:64:LEU:HD23	1.78	0.84
45:BB:812:CLA:H191	9:BI:17:LEU:HB3	1.60	0.84
38:J:45:VAL:CB	44:T:64:UNK:O	2.25	0.84
38:J:137:TRP:CZ3	41:M:161:ARG:CZ	2.61	0.84
16:A6:204:PHE:O	24:F:546:THR:HG22	1.78	0.83
19:A:228:ARG:HD3	19:A:322:ARG:CZ	2.09	0.83
24:F:18:VAL:HG21	24:F:43:LEU:HG	1.58	0.83
45:AA:801:CLA:HED2	45:AA:801:CLA:HAA2	1.60	0.83
1:BA:506:THR:HG22	1:BA:521:LEU:HD11	1.59	0.83
18:B5:177:LEU:HD13	26:a:228:ASN:CG	2.03	0.83
45:BB:812:CLA:C19	9:BI:17:LEU:HB3	2.10	0.82
37:I:116:THR:HG23	49:I:202:SF4:S2	2.18	0.82
7:BG:80:ARG:HG2	45:BG:202:CLA:HAB	1.61	0.82
21:C:60:ILE:HD11	23:E:86:ARG:HH21	1.44	0.82
45:A6:610:CLA:H72	24:F:42:PHE:CZ	2.10	0.82
12:BL:91:LEU:HD21	45:BL:302:CLA:HAB	1.62	0.82
7:BG:127:PHE:O	45:BG:202:CLA:HAA1	1.79	0.82
11:BK:93:LEU:HG	11:BK:104:ALA:H	1.44	0.82
41:M:195:LYS:HB2	42:N:137:PRO:HD2	1.61	0.81
1:BA:361:THR:HG21	1:BA:395:GLY:CA	2.11	0.81
25:G:132:ILE:HD11	31:f:161:PRO:HD3	1.62	0.81
3:BC:27:GLU:CD	4:BD:175:ARG:HD2	2.05	0.81
7:BG:127:PHE:CD2	45:BG:202:CLA:CHB	2.63	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:28:ILE:HG22	27:b:31:GLU:H	1.46	0.81
42:N:129:GLN:CG	42:N:130:PRO:HD2	2.10	0.81
3:BC:23:THR:HG21	3:BC:47:ASP:O	1.81	0.81
41:M:105:ASP:CG	41:M:106:PRO:HD2	2.03	0.81
7:BG:129:ILE:N	45:BG:202:CLA:HBA2	1.95	0.80
11:BK:93:LEU:HD21	11:BK:104:ALA:HB2	1.63	0.80
2:AB:476:VAL:HG12	2:AB:477:LEU:N	1.95	0.80
2:AB:476:VAL:CG1	2:AB:477:LEU:H	1.94	0.80
26:a:206:GLY:HA3	26:a:231:SER:HA	1.63	0.80
38:J:137:TRP:CZ3	41:M:161:ARG:NH2	2.50	0.80
37:I:130:TYR:HD1	39:K:134:VAL:HG22	1.43	0.79
7:BG:80:ARG:HH12	7:BG:124:PRO:HG2	1.48	0.79
11:BK:93:LEU:CD1	11:BK:103:LEU:CD2	2.60	0.79
16:A6:205:MET:CE	24:F:45:ILE:HD13	2.13	0.79
36:H:236:ILE:HG12	38:J:79:ASN:CG	2.07	0.79
41:M:158:TYR:HD1	41:M:161:ARG:HH21	1.29	0.79
45:A6:610:CLA:C7	24:F:42:PHE:HZ	1.96	0.79
41:M:153:ALA:HB1	41:M:154:PRO:HD2	1.65	0.79
39:K:155:LYS:HE3	42:N:86:GLU:CD	2.06	0.79
42:N:76:ALA:O	42:N:198:PRO:HD2	1.83	0.79
1:BA:358:GLY:O	1:BA:361:THR:CG2	2.29	0.78
9:BI:15:VAL:HG11	48:BI:101:BCR:HC42	1.63	0.78
3:BC:22:PRO:C	4:BD:132:LEU:HD23	2.08	0.78
14:B3:53:ARG:NH1	14:B3:63:LEU:CD1	2.30	0.78
37:I:140:ILE:HG23	42:N:109:GLY:HA3	1.64	0.78
5:BE:87:VAL:CG2	5:BE:138:VAL:CG1	2.61	0.78
17:B2:104:GLY:HA2	55:B2:616:XAT:H181	1.66	0.78
40:L:149:LEU:HD21	40:L:152:ARG:NE	1.98	0.78
7:BG:127:PHE:CD2	45:BG:202:CLA:HHB	2.17	0.77
7:BG:76:LEU:HD11	48:BG:203:BCR:C36	2.15	0.77
8:BH:100:ARG:HH11	12:BL:155:ILE:HA	0.84	0.77
36:H:25:VAL:HG23	39:K:41:THR:HB	1.66	0.77
6:BF:114:GLU:HB3	6:BF:118:ARG:HH21	1.49	0.77
37:I:105:ILE:HG21	39:K:114:MET:HE2	1.66	0.77
3:BC:17:CYS:SG	49:BC:102:SF4:S4	2.84	0.76
18:B5:190:LEU:HD23	26:a:178:TRP:CH2	2.20	0.76
1:AA:118:ILE:HD12	10:AJ:27:ILE:HG23	1.64	0.76
36:H:149:THR:O	37:I:52:ARG:HD2	1.85	0.76
38:J:151:PHE:CE2	41:M:161:ARG:NE	2.54	0.76
5:AE:87:VAL:CG2	5:AE:138:VAL:HG22	2.15	0.76
27:b:28:ILE:HG22	27:b:31:GLU:CB	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:92:TRP:CE2	8:BH:129:ILE:CG2	2.69	0.75
37:I:131:ASP:HA	39:K:135:TYR:HE2	1.50	0.75
2:BB:92:TRP:NE1	8:BH:129:ILE:HG23	2.00	0.75
13:B1:58:LEU:HD13	13:B1:65:ASP:OD1	1.86	0.75
36:H:60:ILE:O	36:H:64:LEU:HB2	1.87	0.75
9:BI:29:LEU:HD21	12:BL:155:ILE:CG2	2.17	0.75
8:BH:100:ARG:NH2	12:BL:184:ALA:HB1	2.02	0.75
31:f:134:PRO:HB3	32:g:169:TYR:CE1	2.21	0.75
16:A6:205:MET:CE	24:F:109:ILE:HD13	2.15	0.75
41:M:195:LYS:CB	42:N:137:PRO:CD	2.64	0.75
13:B1:58:LEU:HD12	13:B1:58:LEU:O	1.85	0.75
11:BK:106:THR:HG21	45:BK:201:CLA:CAB	2.17	0.75
16:A6:204:PHE:HE1	24:F:109:ILE:HD12	1.52	0.75
37:I:76:ILE:HD11	39:K:117:THR:N	1.99	0.75
7:BG:127:PHE:CE2	45:BG:202:CLA:CMB	2.66	0.74
1:BA:264:LEU:CB	11:BK:122:LEU:HD11	2.14	0.74
24:F:210:GLU:HB2	29:d:71:ILE:HG12	1.68	0.74
5:AE:87:VAL:HG21	5:AE:138:VAL:CG2	2.17	0.74
1:BA:361:THR:CG2	1:BA:395:GLY:CA	2.64	0.74
52:A6:615:LUT:H372	24:F:42:PHE:CE1	2.23	0.74
39:K:4:ILE:HD11	42:N:148:PRO:HD3	1.69	0.74
8:BH:100:ARG:CD	12:BL:155:ILE:HG12	2.14	0.74
3:BC:27:GLU:OE2	4:BD:175:ARG:HD2	1.88	0.74
8:BH:82:TYR:CE2	12:BL:98:VAL:HG21	2.23	0.74
40:L:149:LEU:CG	40:L:152:ARG:HD2	2.17	0.74
7:BG:123:ASP:OD1	45:BG:202:CLA:NC	2.21	0.74
36:H:212:GLU:HG2	44:T:85:UNK:O	1.88	0.74
7:AG:116:VAL:HG23	7:AG:120:LYS:HE3	1.70	0.73
20:B:90:ASN:HD21	25:G:155:PRO:HD3	1.52	0.73
29:d:104:TRP:NE1	30:e:120:SER:OG	2.21	0.73
4:BD:72:THR:CG2	4:BD:73:PRO:HD2	2.17	0.73
24:F:147:VAL:O	24:F:151:TRP:HB2	1.89	0.73
4:AD:107:GLU:O	4:AD:137:ARG:NH1	2.21	0.73
11:AK:126:ASN:HD22	45:AK:202:CLA:CMA	2.01	0.73
3:BC:18:VAL:HG21	4:BD:168:PRO:O	1.89	0.73
37:I:131:ASP:HA	39:K:135:TYR:CE2	2.24	0.73
16:A6:132:PHE:CZ	24:F:54:PHE:HE1	2.07	0.73
7:BG:123:ASP:OD1	45:BG:202:CLA:C4C	2.37	0.72
8:BH:100:ARG:HH21	12:BL:184:ALA:CB	2.01	0.72
15:A4:199:GLN:NE2	15:A4:202:LYS:NZ	2.36	0.72
7:BG:136:GLY:O	7:BG:140:HIS:CD2	2.43	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:BH:126:VAL:C	8:BH:127:LEU:HD12	2.14	0.72
12:BL:91:LEU:CD1	45:BL:302:CLA:HMC2	2.19	0.72
13:B1:180:ASP:OD1	13:B1:183:LYS:HB2	1.90	0.72
3:BC:18:VAL:HG11	4:BD:168:PRO:O	1.89	0.72
45:A6:610:CLA:H61	24:F:42:PHE:HE2	1.50	0.72
45:A6:610:CLA:C4	24:F:42:PHE:CE2	2.72	0.72
3:BC:23:THR:O	3:BC:23:THR:HG22	1.88	0.72
17:B2:65:LEU:HD22	45:B2:602:CLA:O1D	1.90	0.72
1:AA:570:ARG:NH1	47:AA:844:LHG:O10	2.23	0.71
24:F:168:ARG:NH2	30:e:83:ASP:OD2	2.21	0.71
8:BH:115:LEU:HG	9:BI:13:PRO:HB3	1.70	0.71
7:AG:88:ARG:NH2	7:AG:131:ASP:OD2	2.24	0.71
11:BK:93:LEU:HD23	11:BK:104:ALA:CB	2.21	0.71
41:M:195:LYS:CB	42:N:137:PRO:CG	2.66	0.71
1:BA:594:LEU:HD21	45:BA:830:CLA:HBC1	1.70	0.71
26:a:308:ILE:HG22	26:a:310:GLY:H	1.55	0.71
11:BK:120:VAL:HG23	45:BK:202:CLA:HAB	1.70	0.71
16:A6:206:MET:SD	24:F:544:ASP:CB	2.78	0.70
11:BK:93:LEU:CD1	11:BK:103:LEU:CG	2.68	0.70
54:B1:303:CHL:OBD	18:B5:149:LYS:NZ	2.23	0.70
28:c:151:LEU:HB2	28:c:154:LYS:HG3	1.73	0.70
11:BK:93:LEU:HD11	11:BK:103:LEU:HD23	1.70	0.70
38:J:137:TRP:CE3	41:M:161:ARG:CZ	2.74	0.70
19:A:327:ARG:HG2	19:A:329:ARG:H	1.56	0.70
39:K:6:PHE:HA	42:N:148:PRO:CG	2.22	0.70
11:BK:93:LEU:HD11	11:BK:103:LEU:HG	1.73	0.70
36:H:229:ILE:HG12	38:J:76:TYR:CG	2.26	0.70
41:M:195:LYS:HB2	42:N:137:PRO:CD	2.20	0.70
2:BB:292:ARG:HE	7:BG:97:PRO:HD3	1.56	0.70
17:B2:73:PHE:N	45:B2:602:CLA:OBD	2.25	0.70
21:C:103:ILE:HG23	25:G:164:LEU:HD22	1.74	0.70
1:AA:175:TRP:CH2	1:AA:180:LYS:CD	2.75	0.69
7:BG:124:PRO:CG	45:BG:202:CLA:HBC2	2.22	0.69
11:BK:93:LEU:HD11	11:BK:103:LEU:CD2	2.20	0.69
18:B5:194:LYS:HG3	26:a:230:ASN:ND2	2.06	0.69
16:A6:204:PHE:CG	24:F:549:PHE:CD2	2.80	0.69
20:B:176:SER:CA	20:B:259:ASP:CB	2.69	0.69
24:F:210:GLU:OE1	29:d:69:GLN:NE2	2.26	0.69
2:BB:92:TRP:CE2	8:BH:129:ILE:HG21	2.28	0.69
41:M:105:ASP:CG	41:M:106:PRO:HD3	2.16	0.69
3:BC:28:MET:HE1	49:BC:102:SF4:S1	2.33	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:195:VAL:HG12	23:E:41:VAL:HG11	1.74	0.69
21:C:57:GLN:NE2	36:H:11:MET:HG2	2.08	0.69
16:A6:204:PHE:CD1	24:F:549:PHE:CE2	2.80	0.69
20:B:188:GLY:HA3	23:E:34:LEU:HD11	1.74	0.69
27:b:28:ILE:CG2	27:b:31:GLU:CB	2.71	0.69
11:AK:69:ARG:HE	45:AK:201:CLA:CHD	2.06	0.69
20:B:87:PHE:HE2	25:G:154:LEU:HD13	1.58	0.69
19:A:228:ARG:HD3	19:A:322:ARG:NH2	2.08	0.68
1:BA:361:THR:HG21	1:BA:395:GLY:HA2	1.75	0.68
38:J:155:GLN:CG	43:O:136:PRO:HD2	2.23	0.68
4:BD:72:THR:CG2	4:BD:73:PRO:CD	2.71	0.68
13:B1:180:ASP:CG	13:B1:183:LYS:HB2	2.18	0.68
45:BB:809:CLA:H42	9:BI:11:PHE:CD1	2.28	0.68
8:BH:77:ASP:HB2	12:BL:177:GLN:CD	2.19	0.68
36:H:251:TRP:O	44:T:90:UNK:HA	1.92	0.68
36:H:30:VAL:HG12	36:H:32:LEU:H	1.59	0.68
22:D:162:GLY:HA2	29:d:131:GLY:H	1.59	0.68
1:AA:118:ILE:HD11	10:AJ:27:ILE:HG23	1.76	0.68
2:AB:106:ARG:CZ	2:AB:115:ILE:CG1	2.68	0.68
4:BD:72:THR:HG23	4:BD:73:PRO:HD2	1.76	0.68
16:A6:205:MET:CA	24:F:546:THR:CG2	2.72	0.68
20:B:161:LEU:HD12	23:E:76:ILE:HD12	1.76	0.68
42:N:129:GLN:CG	43:O:134:GLY:HA2	2.24	0.68
17:B2:152:GLU:OE1	17:B2:155:ARG:NH2	2.27	0.68
18:B5:177:LEU:HD13	26:a:228:ASN:ND2	2.09	0.68
1:BA:330:PHE:O	1:BA:426:ARG:NH2	2.26	0.67
37:I:129:THR:O	39:K:135:TYR:N	2.26	0.67
40:L:149:LEU:CD2	40:L:152:ARG:HD3	2.14	0.67
16:A6:204:PHE:O	24:F:546:THR:HG23	1.94	0.67
5:BE:87:VAL:HG21	5:BE:138:VAL:HG12	1.73	0.67
36:H:61:ILE:HD11	37:I:113:TYR:OH	1.94	0.67
5:AE:87:VAL:CG2	5:AE:138:VAL:CG2	2.72	0.67
2:BB:92:TRP:CE2	8:BH:129:ILE:HG23	2.28	0.67
5:AE:87:VAL:HG21	5:AE:138:VAL:HG22	1.75	0.67
14:A3:137:THR:HG21	55:A3:317:XAT:O3	1.95	0.67
36:H:22:MET:CE	39:K:45:PHE:CE1	2.77	0.67
14:B3:245:VAL:HG23	14:B3:246:THR:HG23	1.77	0.67
18:B5:194:LYS:HA	26:a:230:ASN:ND2	2.08	0.67
8:BH:100:ARG:NH1	12:BL:154:GLY:O	2.26	0.67
8:BH:100:ARG:NH2	12:BL:184:ALA:CB	2.58	0.67
11:BK:126:ASN:HB2	45:BK:202:CLA:CMA	2.24	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:A6:132:PHE:HZ	24:F:54:PHE:HE1	1.40	0.67
13:B1:96:LEU:CD2	45:B1:306:CLA:HBB2	2.25	0.67
17:B2:54:ILE:H	14:B3:183:GLN:HE22	1.43	0.67
37:I:140:ILE:HG23	42:N:109:GLY:CA	2.24	0.67
8:AH:77:ASP:HA	12:AL:97:ALA:HB2	1.76	0.66
7:BG:76:LEU:HD11	48:BG:203:BCR:H362	1.76	0.66
13:B1:232:ASN:ND2	18:B5:134:THR:OG1	2.27	0.66
38:J:151:PHE:CE1	41:M:161:ARG:HB3	2.30	0.66
38:J:155:GLN:HG2	43:O:136:PRO:HD2	1.75	0.66
7:BG:80:ARG:HD2	7:BG:125:ILE:HG21	1.77	0.66
17:B2:97:HIS:NE2	45:B2:603:CLA:NC	2.43	0.66
22:D:232:PRO:HD2	22:D:319:MET:HG3	1.77	0.66
2:BB:70:TRP:CZ2	9:BI:4:PHE:O	2.38	0.66
2:BB:294:ASN:HD21	7:BG:112:ALA:HA	1.59	0.66
2:BB:450:GLU:OE2	6:BF:119:ARG:NE	2.28	0.66
7:AG:116:VAL:CG2	7:AG:120:LYS:HE3	2.25	0.66
1:AA:96:SER:OG	1:AA:142:PHE:HZ	1.79	0.66
15:A4:101:ARG:NH2	54:A4:306:CHL:OBD	2.29	0.66
53:A4:318:LMG:H292	48:A6:617:BCR:H332	1.77	0.66
1:BA:713:GLN:NE2	5:BE:95:TYR:OH	2.28	0.66
37:I:103:ILE:CD1	39:K:111:THR:HB	2.26	0.66
2:BB:436:LEU:HD22	2:BB:453:ILE:HG21	1.76	0.66
37:I:130:TYR:CE1	39:K:134:VAL:HG22	2.30	0.66
41:M:195:LYS:CB	42:N:137:PRO:HD2	2.24	0.66
7:AG:76:LEU:HD13	45:AG:204:CLA:HMB2	1.73	0.66
16:A6:184:TYR:HE1	24:F:393:ILE:HG12	1.60	0.66
6:BF:193:ALA:O	6:BF:197:ILE:N	2.28	0.66
3:AC:64:SER:OG	49:AC:102:SF4:S3	2.53	0.66
2:BB:350:GLN:NE2	2:BB:372:TYR:OH	2.28	0.66
22:D:444:ARG:HH22	30:e:68:GLU:HA	1.60	0.66
27:b:30:THR:HB	27:b:44:PHE:HB3	1.75	0.66
3:AC:55:GLU:OE2	3:AC:66:ARG:NH2	2.30	0.65
34:i:97:GLY:HA3	34:i:174:GLN:HB3	1.77	0.65
1:AA:338:LEU:HD23	1:AA:341:ILE:HD11	1.79	0.65
8:BH:72:ASP:N	12:BL:167:PRO:HB2	2.10	0.65
24:F:135:MET:HG2	24:F:268:THR:HB	1.79	0.65
34:i:80:ALA:O	35:j:148:GLN:NE2	2.26	0.65
38:J:137:TRP:HZ3	41:M:161:ARG:CZ	2.09	0.65
8:AH:86:GLN:HE21	45:AH:201:CLA:C4D	2.08	0.65
37:I:105:ILE:HD11	39:K:114:MET:N	2.11	0.65
2:BB:464:GLN:NE2	45:BB:838:CLA:OBD	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:38:ARG:HH22	24:F:116:SER:CB	2.09	0.65
2:BB:71:GLN:NE2	45:BB:809:CLA:O1D	2.30	0.65
7:BG:68:ILE:HG21	45:BG:201:CLA:CAD	2.26	0.65
19:A:226:CYS:SG	19:A:263:ASN:OD1	2.54	0.65
36:H:65:PRO:HG3	37:I:109:ASN:HD21	1.62	0.65
2:AB:87:ILE:HG23	2:AB:113:VAL:HG13	1.73	0.65
14:B3:186:LEU:HD22	48:B3:317:BCR:H342	1.76	0.65
37:I:103:ILE:HD13	39:K:111:THR:CB	2.25	0.65
3:AC:59:PRO:HD2	49:AC:102:SF4:S2	2.37	0.65
26:a:225:ILE:HG23	26:a:231:SER:HB2	1.77	0.65
2:AB:113:VAL:HG12	2:AB:114:ASN:N	2.10	0.65
45:BB:841:CLA:H202	9:BI:17:LEU:CD2	2.27	0.65
5:BE:87:VAL:CG2	5:BE:138:VAL:HG13	2.27	0.65
1:BA:341:ILE:HG22	1:BA:419:ARG:HB3	1.79	0.64
38:J:22:ASP:OD1	38:J:28:THR:HG23	1.97	0.64
2:AB:523:ILE:HG12	2:AB:590:VAL:HG12	1.78	0.64
1:BA:331:THR:HG22	1:BA:331:THR:O	1.95	0.64
2:BB:638:PHE:O	2:BB:638:PHE:CD1	2.50	0.64
8:BH:82:TYR:CE2	12:BL:102:LEU:CB	2.80	0.64
8:BH:82:TYR:CE2	12:BL:102:LEU:HD12	2.31	0.64
31:f:107:ARG:HB3	31:f:121:ARG:HE	1.61	0.64
13:A1:209:GLN:NE2	13:A1:213:PRO:O	2.30	0.64
13:A1:233:ILE:N	45:A1:314:CLA:O1A	2.28	0.64
36:H:355:ARG:HE	38:J:52:ARG:HB2	1.62	0.64
37:I:129:THR:O	39:K:134:VAL:HA	1.98	0.64
2:BB:4:ARG:HD2	2:BB:20:ARG:CZ	2.28	0.64
38:J:136:SER:OG	41:M:156:THR:HB	1.98	0.64
2:AB:456:GLU:OE1	6:AF:137:HIS:ND1	2.31	0.64
12:BL:115:LEU:HD22	12:BL:142:LEU:HD23	1.78	0.64
24:F:388:THR:HG23	24:F:395:LYS:HE2	1.78	0.64
35:j:106:VAL:HB	35:j:219:GLU:HB2	1.79	0.64
37:I:63:LYS:NZ	37:I:116:THR:O	2.31	0.64
1:AA:175:TRP:CH2	1:AA:180:LYS:HD3	2.33	0.64
23:E:2:ILE:HG22	25:G:9:ASP:HB2	1.79	0.64
39:K:6:PHE:CG	42:N:148:PRO:HB2	2.32	0.64
1:BA:348:ALA:HB1	48:BA:849:BCR:H393	1.78	0.64
17:B2:53:PRO:HB2	54:B2:601:CHL:HBC1	1.79	0.64
17:B2:55:TRP:HA	54:B2:601:CHL:C1C	2.28	0.64
19:A:200:LYS:HD3	31:f:122:TYR:CE2	2.33	0.64
22:D:100:GLY:HA2	22:D:128:TYR:HE1	1.62	0.64
2:BB:351:HIS:ND1	45:BB:819:CLA:OBD	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:h:185:ASN:HD22	33:h:211:LEU:HD12	1.62	0.64
41:M:158:TYR:HD1	41:M:161:ARG:NH2	1.96	0.64
7:BG:132:VAL:HG13	48:BG:203:BCR:C19	2.28	0.63
8:AH:72:ASP:CG	8:AH:75:GLY:HA3	2.22	0.63
2:BB:364:ASP:CG	8:BH:145:LEU:HD11	2.23	0.63
36:H:326:LEU:HD12	38:J:24:GLN:CG	2.27	0.63
13:B1:96:LEU:HD23	45:B1:306:CLA:HBB2	1.80	0.63
22:D:249:TYR:HB3	22:D:356:GLY:HA3	1.79	0.63
29:d:67:MET:HB2	33:h:128:PHE:CE1	2.33	0.63
16:A6:212:PRO:HB3	24:F:38:ARG:HB2	1.80	0.63
11:BK:93:LEU:HG	11:BK:104:ALA:N	2.13	0.63
26:a:400:ASN:O	26:a:426:LYS:NZ	2.31	0.63
10:AJ:28:GLU:HG3	45:AJ:102:CLA:NB	2.14	0.63
8:BH:100:ARG:HH12	12:BL:155:ILE:HA	1.54	0.63
19:A:330:MET:SD	21:C:62:TYR:OH	2.56	0.63
29:d:81:LYS:HE3	33:h:129:ASP:OD1	1.98	0.63
1:AA:503:THR:HG23	45:AA:818:CLA:CGA	2.29	0.63
15:A4:199:GLN:NE2	15:A4:202:LYS:HZ1	1.94	0.63
1:BA:12:ILE:HD11	45:BA:812:CLA:O1A	1.99	0.63
7:BG:124:PRO:CG	45:BG:202:CLA:CBC	2.64	0.63
9:BI:29:LEU:CD2	12:BL:155:ILE:CG2	2.77	0.63
19:A:196:GLU:HG3	31:f:107:ARG:HE	1.63	0.63
27:b:153:ILE:HB	27:b:164:ALA:HB3	1.81	0.63
34:i:149:ILE:HG22	34:i:151:GLY:H	1.63	0.63
35:j:125:CYS:C	35:j:127:GLY:H	2.05	0.63
17:B2:54:ILE:N	14:B3:183:GLN:HE22	1.96	0.63
45:A4:311:CLA:HMB1	52:A4:315:LUT:H7	1.80	0.63
2:BB:292:ARG:NE	7:BG:97:PRO:HD3	2.14	0.63
45:BA:840:CLA:HMD1	48:BB:803:BCR:H383	1.79	0.62
7:BG:68:ILE:HD13	45:BG:201:CLA:C3D	2.29	0.62
27:b:288:PHE:H	27:b:347:ASN:HD21	1.47	0.62
15:A4:191:ASN:ND2	15:A4:194:ASN:HA	2.14	0.62
14:B3:63:LEU:HD12	14:B3:66:LEU:O	1.99	0.62
34:i:118:HIS:HB2	34:i:206:ASN:HB3	1.80	0.62
24:F:707:PHE:HB2	26:a:215:MET:HE2	1.79	0.62
1:BA:358:GLY:C	1:BA:361:THR:HG22	2.23	0.62
3:BC:13:GLY:HA2	49:BC:102:SF4:S1	2.38	0.62
2:AB:87:ILE:HG21	2:AB:113:VAL:HG11	1.77	0.62
24:F:308:LEU:HD11	24:F:664:ARG:HA	1.79	0.62
5:BE:131:ASN:ND2	5:BE:132:ASN:O	2.33	0.62
12:BL:90:ASN:O	12:BL:95:ARG:NH1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:77:VAL:HG21	25:G:65:ILE:HD13	1.81	0.62
37:I:131:ASP:C	39:K:135:TYR:CD2	2.77	0.62
4:BD:125:LEU:HD11	4:BD:131:CYS:HB3	1.82	0.62
36:H:325:GLU:HB2	38:J:22:ASP:HA	1.81	0.62
16:A6:205:MET:HE2	24:F:45:ILE:CD1	2.25	0.62
14:B3:127:PRO:HG2	45:B3:313:CLA:C3D	2.29	0.62
22:D:42:THR:HG21	22:D:121:HIS:HB3	1.82	0.62
27:b:291:MET:HG2	27:b:343:ILE:HG12	1.81	0.62
1:AA:96:SER:OG	1:AA:142:PHE:CZ	2.53	0.62
2:AB:106:ARG:NH2	2:AB:115:ILE:HG12	2.15	0.62
19:A:169:ILE:HD11	25:G:72:VAL:HG21	1.81	0.62
41:M:197:ARG:HG2	41:M:198:VAL:H	1.64	0.62
45:BA:803:CLA:HMD1	6:BF:186:ILE:HG23	1.82	0.62
16:A6:205:MET:HE2	24:F:109:ILE:HD13	1.81	0.61
17:B2:77:PRO:HD2	55:B2:616:XAT:H222	1.82	0.61
26:a:147:GLN:OE1	26:a:167:ARG:NH1	2.33	0.61
1:AA:175:TRP:CZ2	1:AA:180:LYS:CD	2.83	0.61
1:BA:676:PHE:CG	48:BA:851:BCR:H363	2.35	0.61
3:BC:66:ARG:HD2	4:BD:185:ILE:HD11	1.83	0.61
11:BK:93:LEU:CD2	11:BK:104:ALA:CB	2.73	0.61
22:D:249:TYR:HB2	22:D:353:PHE:HA	1.82	0.61
27:b:76:LYS:HB3	27:b:86:PHE:HB2	1.83	0.61
39:K:37:LEU:HD23	39:K:66:ARG:N	2.15	0.61
4:AD:98:TRP:NE1	4:AD:116:MET:SD	2.72	0.61
28:c:134:VAL:HG23	28:c:176:VAL:HG13	1.82	0.61
42:N:180:PRO:HG2	42:N:183:ARG:CB	2.31	0.61
2:AB:87:ILE:HD12	2:AB:113:VAL:HG11	1.82	0.61
11:BK:93:LEU:CG	11:BK:103:LEU:HB3	2.31	0.61
18:B5:88:GLU:OE2	18:B5:211:ARG:NH1	2.33	0.61
19:A:318:SER:O	19:A:322:ARG:HG3	2.01	0.61
36:H:325:GLU:O	38:J:22:ASP:HB3	2.01	0.61
3:AC:12:ILE:O	3:AC:12:ILE:HG22	1.99	0.61
1:AA:494:VAL:HG13	1:AA:495:THR:HG23	1.81	0.61
29:d:69:GLN:HB3	29:d:77:ILE:HB	1.83	0.61
39:K:6:PHE:HA	42:N:148:PRO:HG2	1.83	0.61
1:BA:582:CYS:N	2:BB:668:ARG:O	2.34	0.61
27:b:155:SER:HB2	27:b:162:ALA:HB3	1.81	0.61
1:AA:536:ILE:HG23	45:AA:801:CLA:H193	1.83	0.61
2:AB:106:ARG:NH1	2:AB:115:ILE:HG12	2.15	0.61
1:BA:521:LEU:HG	1:BA:521:LEU:O	2.00	0.60
13:A1:237:VAL:O	45:A1:316:CLA:NB	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:279:LEU:HD11	1:BA:521:LEU:HD23	1.83	0.60
37:I:133:HIS:CD2	41:M:190:ASN:O	2.54	0.60
41:M:197:ARG:HG2	41:M:198:VAL:N	2.16	0.60
5:AE:119:ARG:CZ	5:AE:129:SER:OG	2.49	0.60
45:A6:610:CLA:H61	24:F:42:PHE:CZ	2.37	0.60
19:A:231:PHE:H	19:A:327:ARG:HG3	1.65	0.60
24:F:5:TYR:HB3	24:F:71:ASN:HD21	1.65	0.60
26:a:134:PRO:HG3	26:a:279:LEU:H	1.66	0.60
42:N:129:GLN:HA	43:O:133:VAL:O	2.01	0.60
1:AA:594:LEU:HD21	45:AA:830:CLA:HBC1	1.83	0.60
18:B5:92:SER:HB2	18:B5:210:GLY:HA3	1.83	0.60
45:AB:801:CLA:O1D	48:AF:801:BCR:H401	2.00	0.60
3:BC:81:TYR:HA	4:BD:87:LYS:HB2	1.82	0.60
34:i:112:GLY:O	34:i:142:ARG:NH1	2.35	0.60
39:K:24:ASP:CG	42:N:92:ARG:HH22	2.08	0.60
41:M:195:LYS:HB3	42:N:137:PRO:CD	2.29	0.60
2:AB:351:HIS:ND1	45:AB:818:CLA:OBD	2.35	0.60
16:A6:206:MET:HE1	24:F:544:ASP:OD2	2.00	0.60
19:A:343:PRO:HG3	21:C:108:LEU:HD21	1.83	0.60
20:B:150:ILE:HG12	23:E:62:PHE:HD1	1.66	0.60
2:BB:110:LEU:O	8:BH:133:PRO:HD3	2.00	0.60
24:F:214:ASN:HD22	33:h:117:LYS:HE3	1.66	0.60
36:H:32:LEU:O	36:H:32:LEU:CD1	2.46	0.60
16:A6:204:PHE:CG	24:F:549:PHE:CE2	2.89	0.60
2:BB:126:THR:HG22	2:BB:270:LEU:HD21	1.83	0.60
7:BG:132:VAL:CG1	48:BG:203:BCR:C19	2.79	0.60
22:D:33:ARG:H	30:e:179:LYS:HE3	1.67	0.60
24:F:18:VAL:HG22	24:F:43:LEU:HD23	1.83	0.60
2:BB:456:GLU:OE1	6:BF:137:HIS:ND1	2.35	0.60
36:H:117:TRP:NE1	36:H:382:GLY:O	2.34	0.60
37:I:101:PHE:HA	37:I:104:CYS:HB3	1.83	0.60
12:AL:93:GLY:N	45:AL:304:CLA:OBD	2.34	0.60
13:B1:59:ASP:OD1	13:B1:59:ASP:N	2.35	0.60
13:B1:81:GLU:OE2	13:B1:166:LYS:NZ	2.34	0.60
17:B2:139:THR:OG1	18:B5:249:GLN:NE2	2.35	0.60
22:D:233:ILE:HG22	22:D:235:PRO:HD2	1.84	0.60
26:a:342:ARG:HH22	26:a:344:PHE:HD1	1.48	0.60
8:AH:71:TRP:HA	12:AL:169:LEU:O	2.02	0.59
19:A:228:ARG:NH1	19:A:260:SER:OG	2.35	0.59
19:A:228:ARG:HG3	19:A:264:LEU:HD21	1.84	0.59
25:G:132:ILE:CD1	31:f:161:PRO:HD3	2.30	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:96:MET:HG3	30:e:141:PHE:CE1	2.36	0.59
19:A:226:CYS:SG	19:A:263:ASN:ND2	2.75	0.59
26:a:311:ILE:HG23	26:a:331:LEU:HD21	1.83	0.59
45:BB:813:CLA:HED2	7:BG:111:ARG:HH11	1.66	0.59
3:BC:22:PRO:O	4:BD:132:LEU:HD23	2.03	0.59
45:AF:803:CLA:HMB1	10:AJ:26:LEU:HD21	1.85	0.59
4:BD:72:THR:HG23	4:BD:73:PRO:CD	2.31	0.59
26:a:125:GLY:O	26:a:129:ASN:ND2	2.35	0.59
1:BA:331:THR:HG21	47:BA:846:LHG:O2	2.03	0.59
11:BK:106:THR:CG2	45:BK:201:CLA:CAB	2.79	0.59
2:AB:87:ILE:HD12	2:AB:113:VAL:CG1	2.32	0.59
27:b:225:GLU:HA	27:b:254:LYS:HB3	1.85	0.59
45:AB:822:CLA:CAD	48:AB:844:BCR:H312	2.33	0.59
13:B1:233:ILE:HD12	45:B1:314:CLA:H43	1.84	0.59
20:B:205:SER:HB3	20:B:218:LEU:HD22	1.84	0.59
24:F:18:VAL:HG22	24:F:43:LEU:CD2	2.32	0.59
16:A6:135:ASN:O	16:A6:144:ARG:NH2	2.36	0.59
25:G:125:TRP:CD1	32:g:114:TYR:HH	2.21	0.59
31:f:134:PRO:HD3	32:g:169:TYR:CD1	2.38	0.59
4:BD:72:THR:HG22	4:BD:73:PRO:HD2	1.84	0.59
7:BG:140:HIS:CE1	45:BG:201:CLA:NA	2.70	0.59
36:H:212:GLU:OE2	44:T:86:UNK:CB	2.51	0.59
5:BE:87:VAL:CG2	5:BE:138:VAL:HG12	2.32	0.58
7:BG:76:LEU:CD1	48:BG:203:BCR:H362	2.33	0.58
8:AH:117:TYR:O	8:AH:121:ASN:ND2	2.36	0.58
13:A1:119:ALA:HB1	13:A1:138:LEU:HD13	1.85	0.58
14:A3:103:ASN:ND2	45:A3:308:CLA:OBD	2.36	0.58
1:BA:223:GLN:HG2	1:BA:250:LEU:HD13	1.85	0.58
1:BA:717:LEU:N	46:BA:843:PQN:O4	2.35	0.58
45:BB:805:CLA:HBC2	45:BB:805:CLA:HHD	1.84	0.58
8:BH:115:LEU:CD2	9:BI:17:LEU:HD13	2.33	0.58
22:D:68:ILE:HG13	22:D:204:GLU:HG2	1.83	0.58
22:D:113:VAL:HA	29:d:129:GLY:HA3	1.84	0.58
1:AA:84:TRP:HZ3	48:AA:846:BCR:H322	1.68	0.58
5:AE:135:LEU:O	5:AE:138:VAL:HG12	2.03	0.58
7:BG:136:GLY:O	7:BG:140:HIS:HD2	1.85	0.58
37:I:102:GLY:O	39:K:111:THR:OG1	2.21	0.58
13:A1:237:VAL:HG23	13:A1:238:ILE:HD12	1.86	0.58
39:K:24:ASP:OD2	42:N:92:ARG:NH2	2.36	0.58
8:AH:72:ASP:OD2	12:AL:96:THR:HG21	2.04	0.58
2:BB:292:ARG:NH1	2:BB:296:GLY:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BB:841:CLA:H202	9:BI:17:LEU:HD22	1.85	0.58
33:h:122:ARG:NH2	33:h:159:ASP:OD1	2.36	0.58
22:D:484:TYR:CE2	29:d:86:LEU:CD1	2.82	0.58
1:AA:243:ASN:HB2	1:AA:246:LEU:HD12	1.84	0.58
27:b:190:ARG:HD3	27:b:308:TRP:CH2	2.36	0.58
32:g:96:THR:HG23	32:g:122:LYS:HD2	1.86	0.58
13:B1:208:GLN:HE22	52:B1:316:LUT:H42	1.68	0.58
19:A:42:THR:HG21	40:L:140:PRO:HB3	1.86	0.58
25:G:132:ILE:HD11	31:f:160:ALA:HA	1.85	0.58
26:a:221:ARG:HB3	26:a:238:LEU:HD23	1.84	0.58
2:BB:292:ARG:HH21	7:BG:96:LEU:HG	1.69	0.58
3:BC:81:TYR:CA	4:BD:87:LYS:HB2	2.34	0.58
5:BE:98:LYS:NZ	6:BF:220:ASP:OD2	2.30	0.58
20:B:220:ASN:ND2	34:i:147:LYS:O	2.37	0.58
27:b:173:LYS:NZ	27:b:174:PRO:O	2.36	0.58
38:J:54:GLN:NE2	38:J:67:SER:OG	2.37	0.58
48:BB:803:BCR:H353	45:BB:834:CLA:CGA	2.34	0.58
7:BG:76:LEU:CD1	48:BG:203:BCR:C36	2.81	0.58
8:BH:82:TYR:CB	12:BL:102:LEU:HD13	2.33	0.58
12:BL:217:PHE:HD2	45:BL:304:CLA:CGA	2.17	0.58
20:B:46:LEU:HD11	25:G:164:LEU:HD21	1.86	0.58
24:F:18:VAL:HG21	24:F:43:LEU:CG	2.32	0.58
24:F:655:ASN:OD1	24:F:659:ASN:ND2	2.37	0.58
7:BG:140:HIS:HE1	45:BG:201:CLA:NA	2.02	0.57
17:B2:89:TRP:NE1	45:B2:603:CLA:O2A	2.36	0.57
18:B5:194:LYS:HA	26:a:230:ASN:HD21	1.68	0.57
20:B:381:ILE:HD11	20:B:450:ILE:HG12	1.84	0.57
24:F:218:ASN:ND2	33:h:113:ASP:O	2.37	0.57
1:BA:426:ARG:HG2	1:BA:429:ARG:NH2	2.19	0.57
8:BH:115:LEU:HD22	9:BI:17:LEU:HD13	1.87	0.57
26:a:377:GLN:HE21	30:e:55:ILE:HD12	1.69	0.57
37:I:56:ARG:HH12	37:I:144:ARG:H	1.51	0.57
38:J:45:VAL:C	44:T:64:UNK:CB	2.77	0.57
1:AA:259:THR:HG23	1:AA:260:PRO:HD3	1.84	0.57
2:BB:339:ALA:HB2	48:BB:849:BCR:H372	1.85	0.57
20:B:135:THR:HG21	25:G:165:VAL:HG21	1.86	0.57
23:E:55:SER:O	25:G:143:GLN:NE2	2.37	0.57
36:H:236:ILE:HG12	38:J:79:ASN:CB	2.34	0.57
48:BB:803:BCR:HC31	56:BJ:104:SQD:H92	1.86	0.57
14:B3:266:VAL:N	45:B3:311:CLA:O1A	2.35	0.57
21:C:57:GLN:HE21	36:H:11:MET:HG2	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:324:ASP:OD2	26:a:392:ASN:ND2	2.36	0.57
20:B:42:LEU:HD22	20:B:131:LEU:HD12	1.86	0.57
20:B:87:PHE:CD2	25:G:154:LEU:HB2	2.39	0.57
48:AA:847:BCR:H23C	48:AA:847:BCR:H383	1.87	0.57
2:AB:122:GLN:NE2	2:AB:364:ASP:OD2	2.37	0.57
1:BA:92:GLY:HA2	1:BA:96:SER:OG	2.04	0.57
10:BJ:31:ARG:HG3	48:BJ:101:BCR:H313	1.86	0.57
22:D:339:LEU:HD21	22:D:401:ILE:HG23	1.86	0.57
24:F:238:ILE:HG22	24:F:246:LEU:HB2	1.87	0.57
38:J:105:LYS:CE	44:T:78:UNK:O	2.53	0.57
31:f:154:VAL:HA	31:f:158:PHE:HB2	1.86	0.57
7:BG:123:ASP:OD1	45:BG:202:CLA:CHD	2.53	0.57
12:BL:91:LEU:HG	45:BL:302:CLA:CHC	2.34	0.57
36:H:228:GLY:O	44:T:89:UNK:O	2.22	0.57
13:A1:46:ALA:O	13:A1:54:ARG:NH2	2.38	0.57
4:BD:155:GLY:HA2	8:BH:64:LEU:HD11	1.86	0.57
20:B:161:LEU:HD11	23:E:73:GLU:HA	1.87	0.57
27:b:55:LEU:HD12	27:b:63:LEU:HD23	1.87	0.57
36:H:325:GLU:HB2	38:J:22:ASP:CB	2.33	0.57
42:N:128:LYS:HZ3	43:O:139:PRO:HD3	1.66	0.57
5:AE:119:ARG:NH1	5:AE:129:SER:OG	2.37	0.57
1:BA:331:THR:CG2	1:BA:423:LEU:CD2	2.83	0.57
2:BB:2:ALA:O	2:BB:7:ARG:NH2	2.37	0.57
48:BL:305:BCR:H392	48:BL:305:BCR:H23C	1.87	0.56
29:d:69:GLN:NE2	33:h:121:TYR:CE1	2.72	0.56
7:BG:80:ARG:HG3	7:BG:81:PHE:N	2.19	0.56
31:f:201:ALA:HB3	31:f:208:TYR:HB2	1.85	0.56
2:AB:266:GLN:OE1	2:AB:363:GLN:NE2	2.38	0.56
11:AK:101:PHE:CD2	45:AK:201:CLA:HMC2	2.40	0.56
3:BC:15:THR:O	3:BC:19:ARG:NH2	2.38	0.56
7:BG:127:PHE:CD2	45:BG:202:CLA:CMB	2.86	0.56
17:B2:184:PRO:HB3	54:B2:607:CHL:HBC2	1.85	0.56
45:B2:603:CLA:HBC3	55:B2:616:XAT:H203	1.87	0.56
19:A:89:ARG:NH2	19:A:92:ARG:O	2.38	0.56
36:H:353:LYS:HE3	38:J:54:GLN:O	2.05	0.56
2:AB:450:GLU:OE2	6:AF:119:ARG:NE	2.38	0.56
1:BA:676:PHE:CD2	48:BA:851:BCR:H363	2.40	0.56
4:BD:155:GLY:HA2	8:BH:64:LEU:CD1	2.36	0.56
13:B1:104:PRO:O	13:B1:109:TYR:N	2.36	0.56
13:B1:191:GLU:OE1	45:B1:311:CLA:C4A	2.54	0.56
22:D:47:ILE:HD12	29:d:103:CYS:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:80:TYR:HB2	27:b:85:GLY:HA2	1.87	0.56
29:d:128:ASP:HB3	30:e:167:PRO:HG3	1.87	0.56
33:h:95:VAL:O	33:h:102:ARG:NH1	2.34	0.56
45:AA:828:CLA:H11	48:AA:849:BCR:H323	1.88	0.56
2:AB:418:ILE:HG23	45:AB:839:CLA:CBB	2.36	0.56
11:AK:101:PHE:CE2	45:AK:201:CLA:HMC2	2.40	0.56
12:AL:169:LEU:HD12	12:AL:170:THR:O	2.05	0.56
54:A1:303:CHL:OBD	15:A4:156:ARG:NH2	2.37	0.56
4:BD:107:GLU:O	4:BD:137:ARG:NH1	2.39	0.56
7:BG:132:VAL:HG13	48:BG:203:BCR:H19C	1.84	0.56
8:BH:82:TYR:HE2	12:BL:98:VAL:HG21	1.71	0.56
20:B:143:LEU:HD13	20:B:156:PRO:HG3	1.87	0.56
37:I:49:THR:N	37:I:160:ASN:OD1	2.38	0.56
1:AA:675:HIS:HD1	45:AB:802:CLA:HED2	1.69	0.56
14:A3:245:VAL:HG13	14:A3:246:THR:HG23	1.86	0.56
1:BA:361:THR:HG21	1:BA:395:GLY:N	2.18	0.56
20:B:78:ARG:HE	20:B:81:GLU:HG3	1.70	0.56
22:D:234:ILE:HG13	22:D:235:PRO:HD3	1.87	0.56
24:F:630:SER:O	27:b:283:GLN:NE2	2.31	0.56
15:A4:75:ASN:HD21	53:A4:318:LMG:HC61	1.69	0.56
1:BA:559:ARG:O	4:BD:127:ARG:NH1	2.38	0.56
2:BB:85:ARG:NH1	8:BH:140:GLY:HA3	2.21	0.56
27:b:186:ARG:HB2	27:b:315:HIS:HB3	1.87	0.56
12:AL:169:LEU:CD1	12:AL:170:THR:O	2.54	0.56
45:BB:812:CLA:H193	9:BI:17:LEU:HB3	1.86	0.56
22:D:35:ASN:O	22:D:39:LYS:CB	2.54	0.56
36:H:254:GLN:HB2	36:H:259:ALA:HB2	1.88	0.56
4:AD:203:ASP:O	4:AD:204:LEU:HG	2.04	0.56
45:AK:203:CLA:HMC3	48:AK:204:BCR:H332	1.88	0.56
17:B2:56:PHE:CD1	54:B2:601:CHL:CMA	2.88	0.56
24:F:77:ILE:HD11	29:d:85:HIS:HB2	1.87	0.56
26:a:229:VAL:C	26:a:231:SER:H	2.14	0.56
36:H:234:ARG:HE	36:H:331:GLU:HB3	1.70	0.56
12:AL:121:LYS:O	50:AL:301:LMU:O3'	2.23	0.56
4:BD:72:THR:HG22	4:BD:73:PRO:CD	2.35	0.56
9:BI:29:LEU:CD2	12:BL:155:ILE:HG21	2.29	0.56
20:B:315:ILE:O	20:B:449:LYS:NZ	2.38	0.56
24:F:389:LYS:NZ	24:F:456:GLY:O	2.38	0.56
27:b:199:LYS:HB2	27:b:247:VAL:HA	1.88	0.56
47:A3:301:LHG:O3	47:A3:301:LHG:O1	2.22	0.55
2:BB:574:ASP:OD1	2:BB:706:ARG:NH1	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:BG:201:CLA:HMC2	48:BG:203:BCR:H332	1.88	0.55
11:BK:93:LEU:HD12	11:BK:103:LEU:HD23	1.82	0.55
27:b:190:ARG:HG2	27:b:316:TYR:HB2	1.88	0.55
1:BA:536:ILE:HG23	45:BA:801:CLA:H193	1.88	0.55
13:B1:46:ALA:O	13:B1:54:ARG:NH2	2.39	0.55
17:B2:57:PRO:O	54:B2:601:CHL:HED1	2.06	0.55
24:F:387:LEU:H	24:F:454:PHE:HA	1.70	0.55
45:AB:827:CLA:H142	48:AB:847:BCR:C21	2.36	0.55
4:AD:153:PRO:C	8:AH:64:LEU:HD23	2.31	0.55
24:F:254:MET:SD	24:F:316:LYS:CB	2.91	0.55
36:H:74:ALA:HB2	36:H:113:SER:HB3	1.87	0.55
1:BA:224:PHE:CZ	1:BA:250:LEU:HD11	2.40	0.55
22:D:261:LYS:HE3	22:D:319:MET:HE1	1.88	0.55
22:D:334:LEU:HD23	22:D:496:VAL:HG13	1.88	0.55
24:F:181:THR:HG23	24:F:246:LEU:HD12	1.88	0.55
27:b:28:ILE:HG22	27:b:31:GLU:N	2.19	0.55
1:AA:96:SER:HG	1:AA:142:PHE:HZ	1.45	0.55
16:A6:184:TYR:OH	24:F:548:LEU:HD13	2.06	0.55
1:BA:562:PRO:CG	4:BD:130:GLN:HG2	2.37	0.55
13:B1:200:LEU:HA	13:B1:203:VAL:HG12	1.89	0.55
1:BA:417:THR:HA	4:BD:105:ILE:HG23	1.88	0.55
11:BK:128:GLY:O	11:BK:129:ALA:C	2.50	0.55
13:B1:137:THR:OG1	13:B1:138:LEU:N	2.39	0.55
14:B3:188:LEU:HD22	14:B3:205:PHE:CZ	2.41	0.55
34:i:177:PRO:HA	34:i:180:ALA:HB3	1.88	0.55
34:i:215:ASN:HB2	34:i:217:ARG:HE	1.71	0.55
2:AB:113:VAL:CG1	2:AB:114:ASN:N	2.70	0.55
2:AB:676:GLU:HG2	3:AC:81:TYR:HE2	1.72	0.55
3:AC:61:ASP:OD2	5:AE:91:ARG:NH1	2.40	0.55
1:BA:506:THR:HG22	1:BA:521:LEU:CD1	2.35	0.55
14:B3:227:LYS:NZ	47:B3:318:LHG:O5	2.27	0.55
2:AB:87:ILE:HG23	2:AB:113:VAL:HG12	1.76	0.55
1:BA:361:THR:CG2	1:BA:395:GLY:HA3	2.35	0.55
36:H:315:PRO:HD2	36:H:319:PHE:HZ	1.72	0.55
17:B2:55:TRP:HA	54:B2:601:CHL:NC	2.22	0.55
14:B3:137:THR:OG1	14:B3:148:TYR:OH	2.21	0.55
19:A:162:LEU:HD21	25:G:79:MET:SD	2.47	0.55
20:B:212:GLN:HB3	34:i:140:THR:HG21	1.88	0.55
24:F:547:ILE:HG22	24:F:551:MET:HE2	1.88	0.55
36:H:236:ILE:HG12	38:J:79:ASN:HB3	1.89	0.55
39:K:76:LEU:HB3	39:K:103:ILE:HB	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A1:107:LEU:HD12	13:A1:108:GLY:N	2.22	0.55
12:BL:217:PHE:CD2	45:BL:304:CLA:CGA	2.90	0.55
24:F:265:HIS:HB2	24:F:323:THR:HG21	1.88	0.55
1:AA:464:ARG:NH2	45:AA:834:CLA:O1D	2.41	0.54
15:A4:191:ASN:OD1	52:A4:315:LUT:O23	2.25	0.54
1:BA:361:THR:CG2	1:BA:395:GLY:HA2	2.33	0.54
8:BH:115:LEU:HD22	9:BI:17:LEU:CD1	2.34	0.54
22:D:203:LEU:HD22	22:D:274:LEU:HD21	1.90	0.54
36:H:47:LEU:O	36:H:49:ARG:NH1	2.40	0.54
37:I:105:ILE:CG2	39:K:114:MET:HE2	2.35	0.54
40:L:149:LEU:HD11	40:L:152:ARG:HD2	1.88	0.54
3:AC:23:THR:OG1	49:AC:101:SF4:S1	2.65	0.54
48:AK:204:BCR:H23C	48:AK:204:BCR:H383	1.88	0.54
20:B:150:ILE:HA	23:E:62:PHE:CE1	2.41	0.54
22:D:158:LEU:HD23	22:D:170:ALA:HA	1.87	0.54
24:F:5:TYR:O	24:F:71:ASN:ND2	2.41	0.54
24:F:70:GLN:NE2	24:F:204:GLU:OE2	2.39	0.54
3:AC:47:ASP:OD2	4:AD:128:LYS:NZ	2.33	0.54
18:B5:194:LYS:HG3	26:a:230:ASN:HD22	1.70	0.54
20:B:460:GLN:HE22	29:d:140:ILE:HG12	1.72	0.54
23:E:57:LEU:HD23	23:E:60:GLU:HG3	1.90	0.54
26:a:342:ARG:H	26:a:451:MET:HE1	1.72	0.54
28:c:184:LYS:NZ	28:c:186:HIS:O	2.38	0.54
39:K:110:ILE:HG12	39:K:135:TYR:HD1	1.72	0.54
2:AB:415:LYS:NZ	2:AB:540:ASP:OD1	2.32	0.54
12:BL:91:LEU:CD1	45:BL:302:CLA:CMC	2.85	0.54
18:B5:65:GLY:O	18:B5:211:ARG:NH2	2.40	0.54
27:b:301:VAL:HG12	27:b:320:THR:HG23	1.88	0.54
37:I:132:ARG:N	39:K:135:TYR:CE2	2.76	0.54
2:AB:418:ILE:HG23	45:AB:839:CLA:HBB2	1.90	0.54
2:AB:615:TYR:OH	2:AB:621:ARG:NH2	2.40	0.54
22:D:13:LEU:HD21	22:D:88:ILE:HD11	1.88	0.54
26:a:127:TYR:OH	26:a:397:GLN:NE2	2.40	0.54
1:BA:429:ARG:HD2	4:BD:79:GLY:O	2.08	0.54
22:D:432:MET:HB2	24:F:183:ARG:HH21	1.73	0.54
1:BA:92:GLY:O	1:BA:96:SER:HB2	2.08	0.54
2:BB:615:TYR:OH	2:BB:621:ARG:NH2	2.41	0.54
19:A:313:LEU:HG	40:L:129:TYR:OH	2.06	0.54
24:F:18:VAL:CG2	24:F:43:LEU:HG	2.32	0.54
29:d:67:MET:HB2	33:h:128:PHE:CD1	2.43	0.54
39:K:6:PHE:CB	42:N:148:PRO:HB2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:K:110:ILE:HG22	39:K:111:THR:HG23	1.90	0.54
1:AA:244:ARG:NH2	45:AA:815:CLA:OBD	2.41	0.54
7:AG:157:SER:O	7:AG:160:GLY:O	2.25	0.54
8:AH:71:TRP:HD1	12:AL:169:LEU:HD12	1.59	0.54
11:AK:126:ASN:ND2	45:AK:202:CLA:CMA	2.71	0.54
2:BB:110:LEU:O	8:BH:133:PRO:CD	2.56	0.54
22:D:380:ILE:HG13	22:D:463:SER:HB2	1.90	0.54
24:F:710:GLU:HG3	26:a:215:MET:HA	1.88	0.54
36:H:336:GLU:O	36:H:355:ARG:NH1	2.39	0.54
5:AE:87:VAL:HG22	5:AE:138:VAL:HG22	1.87	0.54
1:BA:338:LEU:HA	1:BA:341:ILE:HG12	1.90	0.54
2:BB:70:TRP:HE1	9:BI:4:PHE:HB3	1.73	0.54
2:BB:182:LEU:HD13	45:BB:815:CLA:HHB	1.90	0.54
2:BB:461:GLN:OE1	6:BF:70:SER:OG	2.21	0.54
4:BD:164:ASP:OD2	4:BD:175:ARG:NH1	2.41	0.54
14:B3:256:ASP:O	14:B3:264:ASN:ND2	2.41	0.54
19:A:270:PHE:HA	19:A:273:VAL:HG22	1.90	0.54
23:E:76:ILE:HD11	25:G:166:ALA:HA	1.90	0.54
24:F:274:ILE:HD13	24:F:331:MET:HE2	1.88	0.54
24:F:308:LEU:HD13	24:F:661:SER:HA	1.90	0.54
26:a:150:ILE:HB	26:a:169:ALA:HA	1.89	0.54
26:a:406:CYS:SG	26:a:407:ILE:N	2.81	0.54
31:f:146:MET:HE3	31:f:170:MET:HG2	1.91	0.54
16:A6:205:MET:HA	24:F:546:THR:HG21	1.88	0.53
8:BH:82:TYR:CZ	12:BL:102:LEU:HB2	2.42	0.53
11:BK:123:GLY:C	11:BK:125:LYS:N	2.62	0.53
35:j:140:ARG:NH1	35:j:148:GLN:OE1	2.41	0.53
38:J:151:PHE:CZ	41:M:161:ARG:NE	2.70	0.53
19:A:319:ILE:HD13	19:A:322:ARG:HD3	1.89	0.53
36:H:236:ILE:CG1	38:J:79:ASN:CG	2.80	0.53
1:AA:471:ASP:O	1:AA:475:GLN:NE2	2.42	0.53
25:G:100:THR:O	25:G:104:CYS:HB2	2.09	0.53
35:j:109:LEU:HD13	35:j:118:VAL:HG13	1.91	0.53
4:AD:100:SER:OG	4:AD:102:LYS:O	2.27	0.53
24:F:672:LYS:HA	24:F:676:ILE:HG22	1.90	0.53
28:c:143:ARG:NH1	28:c:156:LYS:O	2.42	0.53
29:d:69:GLN:NE2	33:h:121:TYR:HE1	2.06	0.53
42:N:179:ARG:HB2	42:N:180:PRO:CD	2.38	0.53
20:B:273:LYS:HD3	20:B:332:ILE:HG13	1.90	0.53
22:D:114:THR:O	30:e:166:GLU:HG3	2.08	0.53
22:D:240:LEU:HD11	22:D:244:HIS:CE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:78:LYS:NZ	27:b:82:LYS:O	2.41	0.53
3:AC:59:PRO:HA	5:AE:128:ILE:HD13	1.91	0.53
1:BA:464:ARG:NH2	45:BA:834:CLA:O1D	2.41	0.53
11:BK:93:LEU:HD11	11:BK:103:LEU:CB	2.29	0.53
12:BL:150:LEU:HB3	12:BL:191:THR:HG22	1.91	0.53
24:F:355:LEU:HD11	24:F:397:ALA:HB1	1.90	0.53
28:c:141:ASN:O	28:c:159:ARG:NH2	2.42	0.53
36:H:135:PHE:HA	36:H:138:ARG:HB2	1.91	0.53
11:AK:69:ARG:HH21	45:AK:201:CLA:C2D	2.21	0.53
45:BB:828:CLA:H142	48:BB:848:BCR:C21	2.38	0.53
7:BG:129:ILE:N	45:BG:202:CLA:CBA	2.71	0.53
19:A:169:ILE:HG13	25:G:72:VAL:HG11	1.89	0.53
22:D:374:ALA:HB2	22:D:447:PHE:HB3	1.90	0.53
2:AB:71:GLN:NE2	45:AB:808:CLA:O1D	2.40	0.53
2:AB:122:GLN:O	2:AB:126:THR:OG1	2.22	0.53
1:BA:348:ALA:HB1	48:BA:849:BCR:C39	2.38	0.53
45:BA:832:CLA:CBB	48:BL:301:BCR:H342	2.38	0.53
19:A:198:GLN:NE2	19:A:274:LEU:O	2.42	0.53
19:A:308:LEU:HA	19:A:311:THR:HG22	1.90	0.53
20:B:409:PRO:HG2	20:B:411:LEU:HG	1.90	0.53
20:B:410:PRO:HD2	22:D:149:LEU:HD13	1.91	0.53
22:D:13:LEU:HD11	22:D:88:ILE:HG13	1.90	0.53
24:F:281:LEU:HA	24:F:284:PHE:HB2	1.91	0.53
26:a:342:ARG:NH1	26:a:455:GLU:OE2	2.41	0.53
42:N:158:VAL:HA	42:N:186:ALA:HB3	1.91	0.53
11:AK:126:ASN:ND2	45:AK:202:CLA:HMA3	2.12	0.53
17:B2:73:PHE:HD2	45:B2:602:CLA:HMD2	1.74	0.53
14:B3:139:VAL:HG13	14:B3:140:ILE:HG13	1.91	0.53
29:d:96:MET:HG3	30:e:141:PHE:CZ	2.43	0.53
36:H:325:GLU:HB2	38:J:22:ASP:CA	2.38	0.53
45:BB:823:CLA:CAD	48:BB:845:BCR:H312	2.39	0.53
19:A:207:ASN:HB2	19:A:275:TYR:HA	1.90	0.53
22:D:331:ASP:HB3	24:F:79:ASN:HD22	1.73	0.53
29:d:141:SER:HA	29:d:144:LEU:HB2	1.91	0.53
30:e:116:GLN:HB2	30:e:154:ILE:HD13	1.90	0.53
38:J:155:GLN:HG3	43:O:136:PRO:HD2	1.91	0.53
42:N:128:LYS:HZ2	43:O:139:PRO:HD3	1.66	0.53
15:A4:99:ASN:ND2	45:A4:307:CLA:OBD	2.42	0.52
15:A4:138:SER:OG	15:A4:139:SER:N	2.41	0.52
10:BJ:31:ARG:HG3	48:BJ:101:BCR:C31	2.39	0.52
12:BL:87:TYR:CE1	12:BL:91:LEU:HD21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:173:ILE:HD11	21:C:69:PHE:HD1	1.75	0.52
22:D:88:ILE:HD13	22:D:93:ILE:HD13	1.89	0.52
42:N:180:PRO:HG2	42:N:183:ARG:HB3	1.92	0.52
2:AB:488:ALA:HB2	7:AG:158:PHE:CE1	2.44	0.52
3:AC:12:ILE:O	3:AC:12:ILE:CG2	2.56	0.52
11:AK:69:ARG:NH2	45:AK:201:CLA:C2D	2.73	0.52
1:BA:143:GLN:OE1	1:BA:143:GLN:N	2.42	0.52
1:BA:599:ASN:OD1	45:BA:801:CLA:H43	2.09	0.52
3:BC:17:CYS:CB	49:BC:102:SF4:S4	2.97	0.52
19:A:113:TYR:OH	19:A:262:LEU:O	2.27	0.52
22:D:484:TYR:CD2	29:d:86:LEU:HD12	2.43	0.52
24:F:68:ILE:HG13	29:d:75:ARG:HD2	1.92	0.52
27:b:28:ILE:HG22	27:b:31:GLU:HB2	1.75	0.52
38:J:22:ASP:CG	38:J:28:THR:HG23	2.34	0.52
45:AB:833:CLA:CGA	48:AF:801:BCR:H353	2.39	0.52
16:A6:65:ARG:NH2	16:A6:78:LEU:O	2.43	0.52
1:BA:585:SER:OG	1:BA:588:ASP:OD2	2.24	0.52
2:BB:122:GLN:OE1	2:BB:122:GLN:N	2.41	0.52
24:F:204:GLU:HG3	24:F:206:GLN:H	1.74	0.52
27:b:179:PRO:HD2	27:b:324:SER:HB2	1.90	0.52
2:AB:324:ASP:O	2:AB:328:ASN:ND2	2.43	0.52
3:BC:23:THR:N	4:BD:132:LEU:HD23	2.23	0.52
13:B1:180:ASP:OD2	13:B1:183:LYS:HG3	2.10	0.52
39:K:103:ILE:HG23	39:K:134:VAL:HB	1.92	0.52
2:AB:399:ASN:O	2:AB:403:ASN:ND2	2.43	0.52
2:AB:441:ASP:OD1	2:AB:616:LEU:N	2.42	0.52
1:BA:54:HIS:ND1	45:BA:806:CLA:O1A	2.39	0.52
5:BE:87:VAL:HG22	5:BE:138:VAL:HG13	1.91	0.52
13:B1:82:ARG:NH1	45:B1:305:CLA:O1D	2.43	0.52
20:B:176:SER:HB2	20:B:259:ASP:CB	2.39	0.52
22:D:255:LEU:HD23	22:D:259:LEU:HD13	1.92	0.52
33:h:205:TYR:HA	33:h:208:THR:HG22	1.92	0.52
36:H:225:ARG:NE	36:H:231:TRP:O	2.41	0.52
26:a:250:SER:HA	26:a:256:MET:HE2	1.90	0.52
36:H:225:ARG:NH1	36:H:231:TRP:O	2.42	0.52
37:I:56:ARG:NH1	37:I:141:ALA:O	2.43	0.52
38:J:112:ARG:O	38:J:116:ASP:HB2	2.10	0.52
42:N:180:PRO:HG2	42:N:183:ARG:HB2	1.91	0.52
16:A6:205:MET:HE1	24:F:45:ILE:HG21	1.92	0.52
19:A:100:ILE:HG22	19:A:104:ILE:HG12	1.92	0.52
21:C:88:VAL:HG23	21:C:89:LEU:HG	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:49:ARG:NH2	36:H:69:ARG:O	2.43	0.52
1:AA:279:LEU:HD22	1:AA:505:LEU:HD11	1.91	0.52
1:BA:223:GLN:CG	1:BA:250:LEU:HD13	2.40	0.52
2:BB:700:LEU:HD22	2:BB:704:GLN:NE2	2.25	0.52
3:BC:18:VAL:CG2	4:BD:168:PRO:HB2	2.36	0.52
22:D:229:VAL:O	22:D:239:TRP:NE1	2.42	0.52
24:F:28:LEU:O	56:e:301:SQD:O2	2.27	0.52
27:b:307:MET:SD	27:b:310:LYS:NZ	2.76	0.52
36:H:22:MET:HE2	39:K:45:PHE:HE1	1.65	0.52
16:A6:205:MET:CA	24:F:546:THR:HG22	2.29	0.52
45:A6:610:CLA:C7	24:F:42:PHE:CZ	2.83	0.52
6:BF:102:GLU:N	6:BF:102:GLU:OE2	2.42	0.52
23:E:38:LEU:O	23:E:42:ASN:HB2	2.10	0.52
24:F:254:MET:SD	24:F:316:LYS:C	2.93	0.52
28:c:168:ASN:OD1	28:c:171:SER:OG	2.27	0.52
40:L:149:LEU:CD1	40:L:152:ARG:HD2	2.38	0.52
41:M:110:GLU:HB3	41:M:114:SER:HA	1.91	0.52
26:a:389:ILE:HG23	26:a:407:ILE:HD11	1.91	0.51
29:d:107:LEU:HB3	30:e:151:PHE:CE1	2.44	0.51
31:f:133:ILE:HB	31:f:207:TYR:HB3	1.92	0.51
1:AA:503:THR:HG21	45:AA:827:CLA:HAB	1.92	0.51
1:BA:570:ARG:NH1	45:BA:830:CLA:O2D	2.43	0.51
48:BA:851:BCR:H362	45:BB:802:CLA:C4	2.40	0.51
2:BB:60:TRP:NE1	45:BB:829:CLA:OBD	2.43	0.51
48:BB:847:BCR:H23C	48:BB:847:BCR:H383	1.92	0.51
7:BG:72:THR:HG22	48:BG:203:BCR:H362	1.92	0.51
18:B5:72:LEU:HD22	55:B5:615:XAT:H372	1.92	0.51
22:D:267:LEU:HA	22:D:271:ASN:HB2	1.91	0.51
38:J:151:PHE:CE1	41:M:161:ARG:CB	2.94	0.51
20:B:441:VAL:HA	20:B:444:ILE:HD12	1.92	0.51
28:c:131:VAL:HG12	28:c:179:GLN:HA	1.93	0.51
36:H:146:GLU:OE2	37:I:50:SER:OG	2.28	0.51
36:H:356:PRO:HG2	36:H:359:PHE:HB3	1.93	0.51
39:K:7:PRO:HD3	42:N:148:PRO:HG2	1.92	0.51
3:BC:12:ILE:HG13	49:BC:102:SF4:S2	2.50	0.51
13:B1:180:ASP:OD1	13:B1:180:ASP:O	2.27	0.51
19:A:107:ILE:HG23	19:A:111:LEU:HD23	1.92	0.51
24:F:484:GLU:HG3	24:F:486:LYS:H	1.75	0.51
37:I:130:TYR:O	39:K:133:ASP:O	2.28	0.51
2:AB:641:ASN:OD1	2:AB:641:ASN:N	2.43	0.51
2:BB:92:TRP:HA	8:BH:129:ILE:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:B3:53:ARG:CZ	14:B3:63:LEU:HD13	2.37	0.51
18:B5:69:PHE:N	45:B5:602:CLA:OBD	2.38	0.51
29:d:142:PRO:HA	29:d:145:ILE:HG12	1.92	0.51
30:e:165:PHE:HB3	30:e:169:ILE:HG13	1.93	0.51
32:g:141:ARG:O	32:g:145:TYR:CB	2.59	0.51
42:N:176:PRO:O	42:N:180:PRO:CD	2.48	0.51
1:BA:338:LEU:HD23	1:BA:341:ILE:HD11	1.91	0.51
6:BF:209:ARG:NH1	47:BF:305:LHG:O4	2.43	0.51
13:B1:98:VAL:HG13	13:B1:99:PRO:HD3	1.93	0.51
13:B1:200:LEU:O	13:B1:203:VAL:HG12	2.11	0.51
20:B:222:GLN:O	34:i:194:ASN:ND2	2.44	0.51
24:F:178:ALA:HA	24:F:249:TRP:HB2	1.92	0.51
26:a:432:ILE:HD11	26:a:449:ASN:HD21	1.75	0.51
31:f:181:TYR:O	31:f:199:THR:OG1	2.25	0.51
36:H:358:GLY:HA3	36:H:386:ILE:HD13	1.93	0.51
37:I:131:ASP:CA	39:K:135:TYR:CE2	2.93	0.51
38:J:30:GLN:HA	38:J:87:LYS:HB2	1.93	0.51
1:AA:175:TRP:CZ3	1:AA:180:LYS:CG	2.85	0.51
2:AB:168:PHE:O	2:AB:174:ARG:NH1	2.41	0.51
2:AB:519:VAL:HG21	2:AB:593:TYR:HB2	1.92	0.51
22:D:63:MET:HE3	22:D:491:LEU:HB3	1.92	0.51
33:h:103:THR:HG22	33:h:187:GLU:HG2	1.92	0.51
38:J:41:VAL:HG21	44:T:4:UNK:CB	2.40	0.51
1:AA:15:ASP:OD2	1:AA:68:ARG:NH2	2.44	0.51
3:AC:15:THR:O	3:AC:19:ARG:NH2	2.43	0.51
1:BA:118:ILE:HD12	10:BJ:27:ILE:HG23	1.92	0.51
1:BA:331:THR:HG22	1:BA:423:LEU:CD2	2.40	0.51
1:BA:691:TYR:OH	2:BB:533:ILE:HA	2.11	0.51
37:I:127:PHE:C	39:K:137:PRO:HD3	2.36	0.51
21:C:82:TRP:HE1	21:C:93:ALA:HB1	1.75	0.51
24:F:210:GLU:OE1	29:d:71:ILE:HG12	2.11	0.51
24:F:241:SER:HB2	24:F:327:LEU:HD12	1.92	0.51
27:b:188:LYS:HD2	27:b:285:ARG:HH21	1.75	0.51
30:e:74:MET:SD	30:e:79:TYR:OH	2.60	0.51
45:A1:314:CLA:HMB1	52:A1:317:LUT:H7	1.92	0.51
1:BA:118:ILE:HG23	1:BA:119:VAL:HG22	1.93	0.51
9:BI:29:LEU:CD2	12:BL:155:ILE:HG22	2.41	0.51
13:B1:83:TYR:HH	47:B1:301:LHG:H02	1.56	0.51
13:B1:98:VAL:HG23	13:B1:205:PHE:CZ	2.46	0.51
22:D:232:PRO:O	22:D:293:GLN:NE2	2.43	0.51
22:D:350:ALA:HB1	22:D:387:LEU:HD13	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:110:PRO:O	1:AA:137:ILE:N	2.44	0.50
4:BD:72:THR:HG22	4:BD:73:PRO:N	2.26	0.50
20:B:373:GLY:HA2	20:B:377:GLY:H	1.75	0.50
38:J:17:ARG:HB3	38:J:30:GLN:HB3	1.93	0.50
42:N:78:TYR:HB3	42:N:192:ARG:HB2	1.93	0.50
2:AB:418:ILE:HG21	48:AB:847:BCR:H282	1.93	0.50
2:AB:452:GLN:NE2	2:AB:614:THR:OG1	2.43	0.50
11:AK:70:PHE:CZ	45:AK:201:CLA:HMD1	2.46	0.50
3:BC:17:CYS:HB3	49:BC:102:SF4:S4	2.51	0.50
5:BE:140:GLU:OE1	5:BE:140:GLU:N	2.44	0.50
52:B3:315:LUT:H381	52:B3:315:LUT:H28	1.92	0.50
19:A:92:ARG:NH2	19:A:150:TYR:OH	2.44	0.50
24:F:455:GLU:OE1	24:F:625:LYS:NZ	2.45	0.50
37:I:127:PHE:HB2	39:K:137:PRO:CG	2.28	0.50
41:M:197:ARG:CG	41:M:198:VAL:H	2.23	0.50
48:AB:845:BCR:H23C	48:AB:845:BCR:H382	1.92	0.50
7:AG:78:LEU:HD21	13:A1:147:LEU:HD13	1.93	0.50
8:AH:71:TRP:C	12:AL:167:PRO:HB3	2.37	0.50
45:A3:304:CLA:NB	48:A3:318:BCR:H392	2.27	0.50
1:BA:471:ASP:OD1	1:BA:477:GLN:NE2	2.45	0.50
1:BA:563:ASP:HB3	4:BD:133:ALA:HB1	1.92	0.50
19:A:339:LYS:HE3	21:C:117:LEU:HB2	1.93	0.50
31:f:200:VAL:HG23	31:f:209:THR:HG22	1.93	0.50
13:A1:95:MET:HE2	45:A1:311:CLA:CAB	2.41	0.50
35:j:107:ILE:HG22	35:j:217:VAL:HA	1.94	0.50
36:H:68:THR:OG1	36:H:154:MET:SD	2.69	0.50
37:I:137:TYR:CE1	42:N:107:GLY:HA3	2.46	0.50
41:M:153:ALA:HB1	41:M:154:PRO:CD	2.39	0.50
1:AA:644:TRP:HB3	45:AA:801:CLA:H101	1.94	0.50
15:A4:102:TRP:CE2	54:A4:306:CHL:HED2	2.46	0.50
7:BG:129:ILE:CA	45:BG:202:CLA:HBA2	2.40	0.50
12:BL:79:THR:OG1	12:BL:80:SER:N	2.45	0.50
17:B2:76:ASP:OD2	17:B2:81:SER:OG	2.29	0.50
22:D:344:HIS:HA	22:D:347:ILE:HB	1.94	0.50
2:AB:318:GLY:O	2:AB:407:VAL:N	2.42	0.50
1:BA:331:THR:HG22	1:BA:423:LEU:HD21	1.93	0.50
45:BA:801:CLA:H18	45:BA:802:CLA:C1B	2.42	0.50
45:BB:809:CLA:H42	9:BI:11:PHE:CE1	2.46	0.50
18:B5:223:GLN:O	18:B5:227:THR:OG1	2.29	0.50
24:F:198:TRP:O	33:h:110:TYR:OH	2.27	0.50
26:a:201:SER:HB3	26:a:223:SER:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:b:62:SER:HB2	27:b:76:LYS:HB2	1.94	0.50
36:H:228:GLY:HA2	36:H:251:TRP:C	2.37	0.50
39:K:155:LYS:HG2	42:N:86:GLU:OE1	2.10	0.50
1:AA:175:TRP:CZ2	1:AA:180:LYS:CG	2.94	0.50
2:AB:130:ARG:NH1	2:AB:201:ALA:O	2.40	0.50
15:A4:163:ASN:OD1	15:A4:163:ASN:N	2.44	0.50
2:BB:726:ILE:O	2:BB:730:SER:OG	2.22	0.50
12:BL:97:ALA:HB2	12:BL:177:GLN:HE21	1.77	0.50
17:B2:109:PHE:O	17:B2:113:PHE:N	2.45	0.50
21:C:77:VAL:CG2	25:G:65:ILE:HD13	2.41	0.50
28:c:75:VAL:HG22	28:c:87:VAL:HG22	1.93	0.50
41:M:105:ASP:CB	41:M:106:PRO:CD	2.88	0.50
2:AB:516:ASP:OD2	2:AB:597:LYS:NZ	2.42	0.50
45:BG:201:CLA:CMC	48:BG:203:BCR:H332	2.42	0.50
22:D:487:PHE:O	29:d:95:TYR:OH	2.30	0.50
24:F:110:TYR:CE1	24:F:547:ILE:HG23	2.47	0.50
27:b:262:PRO:HD2	27:b:326:LEU:HD23	1.93	0.50
31:f:134:PRO:HB3	32:g:169:TYR:HE1	1.73	0.50
16:A6:204:PHE:CE1	24:F:549:PHE:CE2	3.00	0.50
2:BB:5:PHE:HB2	9:BI:31:ILE:CA	2.29	0.50
24:F:18:VAL:CG2	24:F:43:LEU:CD2	2.89	0.50
24:F:237:PRO:O	24:F:241:SER:OG	2.30	0.50
25:G:138:ILE:HB	31:f:112:ARG:HE	1.76	0.50
45:AB:840:CLA:HAB	46:AB:843:PQN:H141	1.94	0.49
7:BG:76:LEU:HD11	48:BG:203:BCR:C18	2.42	0.49
20:B:375:ARG:NH1	20:B:469:TYR:OH	2.38	0.49
24:F:233:LEU:HD21	24:F:280:LEU:HD13	1.94	0.49
31:f:134:PRO:HD3	32:g:169:TYR:HD1	1.75	0.49
36:H:353:LYS:CD	38:J:55:CYS:HA	2.42	0.49
1:BA:674:ALA:HB1	1:BA:733:GLY:O	2.12	0.49
2:BB:718:ILE:HG21	51:BB:850:DGD:HBG3	1.93	0.49
13:B1:196:ARG:NH2	45:B1:304:CLA:O2D	2.45	0.49
36:H:324:GLN:HB3	38:J:23:TYR:CB	2.42	0.49
2:AB:410:ARG:O	2:AB:414:HIS:ND1	2.41	0.49
2:AB:676:GLU:CG	3:AC:81:TYR:HE2	2.24	0.49
45:BA:840:CLA:H2A	45:BA:840:CLA:HED3	1.94	0.49
20:B:117:GLU:OE2	20:B:478:ASN:ND2	2.45	0.49
21:C:11:TRP:CZ3	25:G:48:LEU:HD22	2.48	0.49
27:b:28:ILE:HG22	27:b:28:ILE:O	2.12	0.49
39:K:101:TYR:HE2	41:M:187:ARG:CG	2.25	0.49
1:AA:503:THR:HG21	45:AA:827:CLA:HBB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:AB:630:GLN:NE2	2:AB:731:GLY:O	2.46	0.49
7:AG:140:HIS:CD2	45:AG:203:CLA:NC	2.79	0.49
1:BA:100:ALA:O	1:BA:103:SER:OG	2.30	0.49
20:B:143:LEU:HD11	20:B:279:SER:HB2	1.94	0.49
20:B:221:THR:HB	25:G:123:VAL:HG13	1.93	0.49
21:C:62:TYR:HA	21:C:65:PHE:HD2	1.75	0.49
26:a:290:VAL:HG11	30:e:55:ILE:HD13	1.93	0.49
36:H:363:GLN:HG2	38:J:106:SER:HB2	1.94	0.49
1:AA:243:ASN:HD22	1:AA:246:LEU:CD1	2.25	0.49
7:BG:123:ASP:CG	7:BG:124:PRO:HD2	2.32	0.49
17:B2:205:LEU:HD21	45:B2:609:CLA:O1A	2.12	0.49
24:F:370:ILE:HD11	24:F:540:PRO:HD3	1.92	0.49
24:F:690:ASP:HA	24:F:694:ILE:HG22	1.95	0.49
27:b:39:ARG:H	27:b:42:ILE:HB	1.77	0.49
37:I:43:PRO:CD	39:K:144:GLU:HG2	2.28	0.49
39:K:4:ILE:CD1	42:N:146:ALA:HA	2.42	0.49
48:AB:846:BCR:H23C	48:AB:846:BCR:H383	1.94	0.49
2:BB:405:ASP:OD1	2:BB:410:ARG:CD	2.45	0.49
18:B5:103:LEU:O	18:B5:107:LEU:HD23	2.13	0.49
14:A3:181:GLY:HA3	14:A3:193:ALA:HB2	1.95	0.49
2:BB:292:ARG:HH21	7:BG:96:LEU:CG	2.26	0.49
3:BC:24:ASP:OD1	4:BD:161:HIS:O	2.30	0.49
8:BH:71:TRP:HD1	12:BL:169:LEU:HB3	1.78	0.49
18:B5:190:LEU:CD2	26:a:178:TRP:HH2	2.19	0.49
20:B:320:MET:HE1	20:B:450:ILE:HD13	1.95	0.49
24:F:238:ILE:HG23	24:F:243:GLN:HB2	1.94	0.49
27:b:104:VAL:HG12	27:b:181:ILE:HG12	1.95	0.49
36:H:326:LEU:HB2	38:J:23:TYR:CB	2.42	0.49
36:H:364:ILE:HG13	36:H:368:LEU:HD23	1.95	0.49
1:AA:54:HIS:ND1	45:AA:806:CLA:O1A	2.38	0.49
2:AB:113:VAL:CG1	2:AB:114:ASN:H	2.26	0.49
8:AH:75:GLY:HA3	12:AL:96:THR:HG21	1.95	0.49
8:AH:77:ASP:CA	12:AL:97:ALA:HB2	2.42	0.49
45:BA:842:CLA:H92	48:BL:305:BCR:H392	1.93	0.49
14:B3:105:ARG:NH2	14:B3:225:GLU:OE2	2.45	0.49
22:D:110:ALA:HB1	22:D:120:PHE:HE2	1.77	0.49
36:H:48:HIS:CD2	38:J:132:LEU:HD13	2.47	0.49
39:K:160:GLU:HG3	39:K:162:TYR:H	1.76	0.49
16:A6:119:THR:OG1	52:A6:615:LUT:H401	2.13	0.49
45:BA:803:CLA:ND	10:BJ:12:PRO:HG3	2.27	0.49
17:B2:81:SER:HB3	45:B2:602:CLA:O1A	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:402:LEU:HD23	20:B:405:LEU:HD12	1.95	0.49
22:D:98:LEU:HD22	22:D:342:ILE:HA	1.94	0.49
24:F:35:ASN:HD21	30:e:95:LYS:C	2.21	0.49
24:F:408:ILE:HB	24:F:412:ALA:HB3	1.94	0.49
26:a:432:ILE:HG21	26:a:446:THR:HB	1.94	0.49
37:I:130:TYR:OH	39:K:152:LYS:O	2.31	0.49
2:AB:339:ALA:HB2	48:AB:848:BCR:H372	1.94	0.49
2:BB:208:ARG:NH1	45:BB:816:CLA:O1D	2.46	0.49
11:BK:120:VAL:HG23	45:BK:202:CLA:CAB	2.39	0.49
19:A:160:GLY:HA3	19:A:244:TYR:HB3	1.94	0.49
22:D:50:LEU:HD21	29:d:99:ILE:HD12	1.95	0.49
24:F:310:LEU:HD23	24:F:445:TYR:HB3	1.95	0.49
27:b:68:SER:HA	27:b:124:TRP:HB2	1.94	0.49
35:j:177:HIS:HB2	35:j:205:SER:HA	1.95	0.49
39:K:34:LEU:HA	39:K:74:LEU:HD22	1.95	0.49
1:AA:644:TRP:CZ2	45:AA:801:CLA:H142	2.48	0.48
13:A1:137:THR:HG23	13:A1:138:LEU:H	1.77	0.48
16:A6:204:PHE:CD1	24:F:549:PHE:HD2	2.29	0.48
2:BB:519:VAL:HG23	45:BB:804:CLA:H141	1.94	0.48
6:BF:210:GLU:O	6:BF:215:ASP:N	2.45	0.48
22:D:73:ASP:HB3	22:D:85:ARG:HD3	1.95	0.48
42:N:128:LYS:NZ	43:O:139:PRO:CD	2.55	0.48
3:AC:2:SER:OG	3:AC:3:HIS:N	2.46	0.48
16:A6:115:MET:O	16:A6:119:THR:OG1	2.28	0.48
45:BB:823:CLA:O1D	7:BG:90:ASN:HB3	2.13	0.48
8:BH:71:TRP:C	12:BL:167:PRO:CB	2.87	0.48
20:B:264:VAL:O	20:B:268:LEU:HB2	2.12	0.48
23:E:71:ALA:HA	25:G:70:ILE:HD11	1.94	0.48
24:F:170:ILE:HG23	24:F:255:GLU:HG2	1.94	0.48
37:I:114:CYS:SG	37:I:116:THR:OG1	2.65	0.48
48:AJ:101:BCR:H403	48:AJ:101:BCR:H23C	1.96	0.48
12:AL:169:LEU:HD12	12:AL:169:LEU:C	2.38	0.48
1:BA:331:THR:O	1:BA:331:THR:CG2	2.62	0.48
48:BB:803:BCR:H382	48:BB:803:BCR:H23C	1.95	0.48
7:BG:124:PRO:CD	45:BG:202:CLA:HBC2	2.42	0.48
17:B2:57:PRO:CG	54:B2:601:CHL:C2D	2.92	0.48
20:B:31:PHE:HB3	20:B:93:THR:HG21	1.95	0.48
24:F:11:ILE:HG13	24:F:12:PRO:HD3	1.94	0.48
30:e:162:PRO:HA	30:e:165:PHE:HD2	1.77	0.48
37:I:127:PHE:CB	39:K:137:PRO:HG3	2.30	0.48
45:AB:812:CLA:HED2	7:AG:111:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:560:LEU:HD11	1:BA:578:ARG:HB3	1.95	0.48
2:BB:85:ARG:NH1	8:BH:140:GLY:CA	2.77	0.48
12:BL:145:ILE:HD12	48:BL:301:BCR:H271	1.95	0.48
17:B2:205:LEU:HG	45:B2:609:CLA:H3A	1.95	0.48
18:B5:192:LEU:HG	26:a:178:TRP:HZ2	1.79	0.48
27:b:293:ARG:NH1	27:b:296:PHE:O	2.47	0.48
34:i:149:ILE:HB	34:i:152:LEU:HD23	1.95	0.48
43:O:87:LYS:NZ	43:O:145:ASP:O	2.36	0.48
2:AB:700:LEU:HD21	46:AB:843:PQN:H152	1.94	0.48
16:A6:204:PHE:HA	24:F:545:ASN:HB2	1.95	0.48
2:BB:469:LYS:NZ	2:BB:509:PHE:O	2.41	0.48
10:BJ:40:PRO:CG	56:BJ:104:SQD:H2	2.43	0.48
48:BL:306:BCR:H371	48:BL:306:BCR:H382	1.96	0.48
17:B2:59:SER:N	14:B3:172:GLN:NE2	2.60	0.48
18:B5:177:LEU:CD1	26:a:228:ASN:ND2	2.75	0.48
20:B:125:ALA:O	20:B:169:TYR:OH	2.31	0.48
22:D:115:ARG:HB2	29:d:128:ASP:HB2	1.95	0.48
24:F:664:ARG:NH2	24:F:668:ASP:OD2	2.46	0.48
32:g:141:ARG:O	32:g:145:TYR:HB2	2.13	0.48
37:I:129:THR:O	39:K:134:VAL:HG13	2.14	0.48
1:AA:367:HIS:ND1	45:AA:818:CLA:OBD	2.47	0.48
1:BA:718:SER:OG	1:BA:721:GLN:HB2	2.13	0.48
19:A:174:PRO:HA	19:A:177:LEU:HB2	1.94	0.48
25:G:157:GLU:O	25:G:160:SER:OG	2.29	0.48
26:a:119:CYS:SG	26:a:120:CYS:N	2.87	0.48
27:b:270:VAL:HB	28:c:89:TRP:O	2.14	0.48
31:f:173:ARG:HB2	31:f:180:TYR:HD2	1.79	0.48
3:BC:11:CYS:SG	49:BC:102:SF4:S3	3.08	0.48
14:B3:162:LEU:HB3	48:B3:317:BCR:H363	1.94	0.48
18:B5:109:ARG:NH2	18:B5:233:ASP:OD2	2.46	0.48
22:D:35:ASN:O	22:D:39:LYS:HB3	2.13	0.48
22:D:111:PHE:HE2	29:d:110:GLY:HA3	1.78	0.48
25:G:11:LEU:HD23	25:G:52:LEU:HD21	1.96	0.48
27:b:39:ARG:NH1	27:b:132:ASP:O	2.43	0.48
27:b:73:LEU:HD11	27:b:97:GLU:HA	1.96	0.48
37:I:105:ILE:CG1	39:K:114:MET:HB3	2.36	0.48
38:J:137:TRP:HZ3	41:M:161:ARG:NE	2.11	0.48
43:O:156:GLU:OE2	43:O:157:ARG:NH1	2.46	0.48
2:AB:586:THR:O	2:AB:590:VAL:HG13	2.13	0.48
2:AB:609:PHE:O	2:AB:613:SER:OG	2.24	0.48
48:AL:302:BCR:H311	48:AL:302:BCR:HC8	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BA:331:THR:CG2	1:BA:423:LEU:HD21	2.44	0.48
45:BB:809:CLA:HAA1	9:BI:12:VAL:HG22	1.96	0.48
17:B2:99:ARG:NH1	54:B2:607:CHL:OBD	2.30	0.48
27:b:28:ILE:CG2	27:b:31:GLU:H	2.22	0.48
28:c:77:SER:HA	28:c:178:GLN:HE21	1.78	0.48
36:H:260:ARG:HE	36:H:383:SER:HB2	1.79	0.48
39:K:7:PRO:HD2	42:N:149:PRO:HD3	1.95	0.48
8:AH:131:ARG:NE	8:AH:134:GLN:OE1	2.46	0.48
16:A6:184:TYR:OH	24:F:393:ILE:HG13	2.14	0.48
2:BB:50:HIS:ND1	45:BB:815:CLA:OBD	2.44	0.48
2:BB:542:ARG:NH2	4:BD:190:SER:OG	2.47	0.48
13:B1:58:LEU:CD1	13:B1:67:GLY:CA	2.80	0.48
24:F:70:GLN:HE22	24:F:206:GLN:HB2	1.79	0.48
24:F:72:VAL:HA	24:F:86:GLY:HA3	1.95	0.48
24:F:72:VAL:HG12	24:F:86:GLY:HA3	1.94	0.48
24:F:405:LEU:HD12	24:F:446:MET:HE2	1.96	0.48
2:BB:378:ILE:HG22	2:BB:382:ILE:HD12	1.96	0.48
45:BB:809:CLA:HAA1	9:BI:12:VAL:CG2	2.44	0.48
7:BG:123:ASP:OD1	45:BG:202:CLA:C1D	2.62	0.48
10:BJ:26:LEU:HB2	48:BJ:103:BCR:H371	1.96	0.48
43:O:142:LEU:HD23	43:O:147:LEU:HB3	1.95	0.48
45:AB:808:CLA:OBD	9:AI:11:PHE:HB2	2.13	0.47
3:AC:61:ASP:OD1	3:AC:62:PHE:N	2.45	0.47
1:BA:578:ARG:NH1	4:BD:129:GLU:OE1	2.46	0.47
2:BB:285:LEU:O	2:BB:289:HIS:ND1	2.47	0.47
14:B3:162:LEU:HB3	48:B3:317:BCR:H16C	1.95	0.47
20:B:45:LEU:HD13	20:B:60:LEU:HD11	1.96	0.47
22:D:123:LEU:HB2	22:D:157:LEU:HD21	1.95	0.47
35:j:125:CYS:C	35:j:127:GLY:N	2.72	0.47
1:AA:196:ASN:HB3	45:AA:820:CLA:HMD1	1.95	0.47
2:AB:462:TRP:NE1	2:AB:476:VAL:HG21	2.29	0.47
9:AI:31:ILE:HD11	48:AI:102:BCR:H333	1.96	0.47
45:BB:841:CLA:C20	9:BI:17:LEU:HD22	2.44	0.47
19:A:203:PHE:HB2	19:A:283:ILE:HB	1.96	0.47
22:D:450:TYR:HB2	24:F:167:THR:HG22	1.96	0.47
26:a:116:ARG:HH12	26:a:144:PRO:HD2	1.79	0.47
45:BA:808:CLA:H92	47:BA:845:LHG:H222	1.95	0.47
48:BB:845:BCR:H23C	48:BB:845:BCR:H383	1.96	0.47
11:BK:93:LEU:HD12	11:BK:103:LEU:CD2	2.39	0.47
24:F:100:ILE:HA	24:F:268:THR:HG22	1.97	0.47
24:F:245:PRO:HB2	24:F:246:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:148:VAL:HB	26:a:166:VAL:HG12	1.96	0.47
48:AF:805:BCR:H23C	48:AF:805:BCR:H383	1.96	0.47
2:BB:218:HIS:NE2	2:BB:232:LEU:O	2.48	0.47
2:BB:578:LEU:HD22	45:BB:801:CLA:CBC	2.45	0.47
24:F:466:SER:HA	28:c:183:TRP:HB3	1.95	0.47
35:j:140:ARG:HB2	35:j:148:GLN:HB3	1.95	0.47
1:AA:243:ASN:HD22	1:AA:246:LEU:HD11	1.79	0.47
48:AF:801:BCR:H23C	48:AF:801:BCR:H383	1.96	0.47
3:BC:32:ASP:OD1	3:BC:32:ASP:N	2.47	0.47
7:BG:76:LEU:HD22	45:BG:202:CLA:CMB	2.44	0.47
21:C:84:MET:HG2	25:G:141:SER:OG	2.14	0.47
25:G:100:THR:O	25:G:104:CYS:CB	2.63	0.47
26:a:252:LEU:HD22	26:a:256:MET:HA	1.96	0.47
27:b:294:ILE:HB	27:b:340:ALA:HB3	1.96	0.47
31:f:98:TYR:HB2	31:f:233:LEU:HD11	1.96	0.47
37:I:116:THR:CG2	49:I:202:SF4:S2	2.98	0.47
1:AA:198:HIS:ND1	45:AA:825:CLA:OBD	2.47	0.47
6:AF:188:ILE:HB	10:AJ:14:LEU:HD13	1.97	0.47
16:A6:110:HIS:CE1	45:A6:604:CLA:NB	2.83	0.47
2:BB:182:LEU:HD13	45:BB:815:CLA:CHB	2.44	0.47
6:BF:187:ILE:HG21	10:BJ:6:THR:HG23	1.96	0.47
7:BG:76:LEU:HD22	45:BG:202:CLA:HMB2	1.96	0.47
19:A:126:ASP:OD1	19:A:126:ASP:N	2.47	0.47
22:D:234:ILE:HG23	22:D:293:GLN:HG3	1.96	0.47
1:AA:561:ILE:HD12	1:AA:584:VAL:HG11	1.96	0.47
2:AB:106:ARG:NH1	2:AB:115:ILE:CG1	2.77	0.47
2:AB:462:TRP:CD1	2:AB:476:VAL:HG21	2.50	0.47
4:AD:151:VAL:HG11	8:AH:59:PHE:CE1	2.50	0.47
15:A4:177:SER:OG	15:A4:178:LEU:N	2.47	0.47
45:BA:801:CLA:HBC1	2:BB:625:TRP:CD1	2.50	0.47
45:BA:801:CLA:H111	45:BA:802:CLA:CMA	2.45	0.47
45:BA:829:CLA:C2	48:BA:848:BCR:H342	2.45	0.47
2:BB:292:ARG:HH21	7:BG:96:LEU:CD2	2.27	0.47
2:BB:527:LEU:HD12	45:BB:840:CLA:HED1	1.96	0.47
2:BB:616:LEU:HD22	45:BB:802:CLA:HMA2	1.97	0.47
45:BB:815:CLA:HBC2	45:BB:815:CLA:HHD	1.97	0.47
14:B3:245:VAL:O	14:B3:273:HIS:N	2.44	0.47
19:A:269:LEU:O	19:A:272:THR:OG1	2.30	0.47
20:B:251:GLN:NE2	25:G:91:ASN:OD1	2.47	0.47
21:C:96:GLU:HG2	25:G:153:PHE:CE1	2.50	0.47
36:H:22:MET:HE2	39:K:45:PHE:CD1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:51:MET:HG3	36:H:70:TRP:HE1	1.80	0.47
37:I:137:TYR:CZ	42:N:107:GLY:HA3	2.49	0.47
43:O:113:ARG:NH1	43:O:155:TYR:O	2.46	0.47
45:AB:834:CLA:O1A	10:AJ:30:ASN:ND2	2.47	0.47
1:BA:25:GLU:OE1	1:BA:25:GLU:N	2.48	0.47
48:BA:851:BCR:H382	48:BA:851:BCR:H23C	1.97	0.47
2:BB:292:ARG:CZ	7:BG:96:LEU:HA	2.45	0.47
10:BJ:36:ALA:CB	56:BJ:104:SQD:H441	2.44	0.47
13:B1:180:ASP:OD2	13:B1:183:LYS:HB2	2.15	0.47
20:B:207:GLY:HA3	23:E:53:ASP:HB2	1.97	0.47
22:D:35:ASN:O	22:D:39:LYS:HB2	2.15	0.47
24:F:38:ARG:HH22	24:F:116:SER:HB2	1.77	0.47
24:F:90:ASP:OD1	24:F:93:THR:N	2.45	0.47
26:a:312:GLU:HB2	26:a:330:SER:HA	1.97	0.47
1:AA:14:VAL:HG11	45:AA:810:CLA:HED3	1.96	0.47
2:AB:91:ILE:HD12	45:AB:810:CLA:C2D	2.45	0.47
12:AL:188:ALA:O	12:AL:191:THR:OG1	2.26	0.47
16:A6:205:MET:CE	24:F:109:ILE:HD11	2.26	0.47
1:BA:574:ASP:OD2	1:BA:578:ARG:NH2	2.44	0.47
2:BB:4:ARG:HD2	2:BB:20:ARG:NH2	2.29	0.47
17:B2:59:SER:N	14:B3:172:GLN:HE21	2.13	0.47
20:B:176:SER:CB	20:B:259:ASP:CB	2.92	0.47
20:B:429:LEU:HB3	20:B:432:LEU:HD23	1.96	0.47
21:C:71:VAL:HG21	25:G:167:LEU:HB2	1.96	0.47
27:b:302:GLY:N	27:b:319:CYS:O	2.48	0.47
31:f:88:TYR:HB3	31:f:101:TYR:HB3	1.97	0.47
36:H:138:ARG:NH2	36:H:142:TYR:OH	2.48	0.47
42:N:188:CYS:SG	42:N:189:GLY:N	2.88	0.47
43:O:119:LEU:HA	43:O:128:ALA:HA	1.97	0.47
2:AB:700:LEU:HD22	2:AB:704:GLN:NE2	2.31	0.47
16:A6:138:TRP:HE3	55:A6:616:XAT:H173	1.81	0.47
1:BA:417:THR:HA	4:BD:105:ILE:CG2	2.44	0.47
8:BH:74:TYR:HB2	12:BL:94:TYR:CD1	2.50	0.47
17:B2:58:GLY:C	14:B3:172:GLN:NE2	2.73	0.47
17:B2:182:GLY:HA2	54:B2:607:CHL:CMD	2.45	0.47
20:B:108:SER:O	20:B:112:ILE:HB	2.14	0.47
24:F:699:ASN:HD22	26:a:181:PRO:HB2	1.80	0.47
27:b:180:GLY:HA2	27:b:323:THR:HG22	1.96	0.47
38:J:45:VAL:O	44:T:64:UNK:CB	2.63	0.47
42:N:76:ALA:N	42:N:198:PRO:O	2.45	0.47
2:AB:60:TRP:NE1	45:AB:828:CLA:OBD	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:AI:102:BCR:H392	48:AI:102:BCR:H23C	1.97	0.46
15:A4:199:GLN:OE1	15:A4:202:LYS:HE3	2.15	0.46
1:BA:286:LEU:N	1:BA:372:PRO:O	2.48	0.46
14:B3:186:LEU:HD22	48:B3:317:BCR:C34	2.45	0.46
22:D:158:LEU:HD21	22:D:243:THR:HG23	1.97	0.46
36:H:25:VAL:HG23	39:K:41:THR:CB	2.42	0.46
36:H:363:GLN:O	36:H:366:PRO:HD2	2.15	0.46
39:K:24:ASP:CG	42:N:92:ARG:NH2	2.73	0.46
41:M:96:HIS:HA	41:M:124:ASP:H	1.81	0.46
12:AL:63:GLN:O	12:AL:75:GLU:N	2.48	0.46
45:A6:610:CLA:C6	24:F:42:PHE:CZ	2.97	0.46
1:BA:328:GLY:HA3	1:BA:331:THR:HB	1.97	0.46
2:BB:571:SER:OG	2:BB:574:ASP:OD2	2.30	0.46
7:BG:132:VAL:CG2	45:BG:202:CLA:HMA2	2.32	0.46
20:B:292:SER:HA	20:B:295:TRP:HB3	1.98	0.46
45:AA:801:CLA:HMB3	45:AB:802:CLA:OBD	2.14	0.46
4:AD:138:LEU:HD22	4:AD:144:ILE:HD11	1.97	0.46
6:AF:186:ILE:O	10:AJ:11:ALA:N	2.47	0.46
1:BA:139:SER:OG	45:BA:808:CLA:OBD	2.29	0.46
1:BA:450:PHE:CZ	1:BA:454:ILE:HD11	2.50	0.46
11:BK:93:LEU:HD13	11:BK:103:LEU:HD23	1.88	0.46
12:BL:91:LEU:HD11	45:BL:302:CLA:CMC	2.46	0.46
24:F:206:GLN:HE21	29:d:69:GLN:CG	2.27	0.46
29:d:69:GLN:HE22	33:h:121:TYR:HE1	1.61	0.46
38:J:117:MET:HE3	38:J:142:LEU:HB2	1.96	0.46
39:K:24:ASP:OD1	42:N:92:ARG:NH2	2.45	0.46
2:AB:519:VAL:HG23	45:AB:803:CLA:H141	1.98	0.46
45:BB:830:CLA:H202	48:BB:846:BCR:H352	1.97	0.46
12:BL:168:SER:O	12:BL:168:SER:OG	2.33	0.46
24:F:458:LEU:HD23	24:F:461:TYR:HB2	1.97	0.46
36:H:65:PRO:CG	37:I:109:ASN:HD21	2.27	0.46
45:AA:801:CLA:HBD	45:AA:801:CLA:HED3	1.58	0.46
48:AB:844:BCR:H383	48:AB:844:BCR:H23C	1.97	0.46
16:A6:138:TRP:CE3	55:A6:616:XAT:H173	2.50	0.46
1:BA:96:SER:OG	1:BA:112:ALA:HA	2.15	0.46
1:BA:425:ASP:O	1:BA:429:ARG:HG3	2.15	0.46
3:BC:2:SER:OG	3:BC:3:HIS:N	2.48	0.46
3:BC:7:ILE:HG23	3:BC:11:CYS:SG	2.56	0.46
14:B3:134:TRP:HB2	55:B3:316:XAT:H173	1.97	0.46
20:B:112:ILE:HD13	20:B:133:ILE:HG21	1.96	0.46
22:D:224:LEU:O	22:D:228:ALA:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:280:SER:HB3	22:D:415:LYS:HZ3	1.81	0.46
39:K:4:ILE:HA	41:M:182:TYR:HB2	1.98	0.46
1:AA:440:TRP:NE1	45:AA:833:CLA:OBD	2.46	0.46
45:BA:801:CLA:HBC1	2:BB:625:TRP:HD1	1.81	0.46
2:BB:324:ASP:O	2:BB:328:ASN:ND2	2.45	0.46
13:B1:227:ASP:N	13:B1:227:ASP:OD1	2.49	0.46
20:B:311:ASN:HD22	20:B:439:THR:HB	1.81	0.46
35:j:92:ILE:HD13	35:j:227:ILE:HD11	1.98	0.46
43:O:83:VAL:HB	43:O:110:TYR:HA	1.98	0.46
1:AA:678:TRP:HZ3	45:AB:802:CLA:HMD3	1.80	0.46
48:AA:849:BCR:H362	45:AB:802:CLA:H43	1.96	0.46
7:BG:127:PHE:CD2	45:BG:202:CLA:C1B	2.99	0.46
17:B2:142:VAL:HG11	45:B5:613:CLA:HED1	1.97	0.46
14:B3:114:ALA:HB1	14:B3:134:TRP:HB3	1.98	0.46
35:j:151:ASP:OD1	35:j:151:ASP:N	2.47	0.46
1:AA:343:THR:O	45:AA:825:CLA:H192	2.16	0.46
12:AL:76:THR:O	12:AL:80:SER:OG	2.30	0.46
53:A4:318:LMG:C29	48:A6:617:BCR:H332	2.46	0.46
1:BA:430:HIS:HA	4:BD:81:THR:CG2	2.46	0.46
2:BB:540:ASP:HB3	2:BB:544:SER:OG	2.16	0.46
45:BB:828:CLA:H142	48:BB:848:BCR:C22	2.46	0.46
4:BD:154:ASN:OD1	4:BD:155:GLY:N	2.49	0.46
11:BK:123:GLY:C	11:BK:125:LYS:H	2.23	0.46
20:B:253:THR:HB	20:B:325:ALA:HB1	1.97	0.46
29:d:152:LYS:HG2	29:d:157:HIS:HA	1.98	0.46
1:AA:574:ASP:OD2	1:AA:578:ARG:NH2	2.45	0.46
48:AG:205:BCR:H383	48:AG:205:BCR:H23C	1.96	0.46
3:BC:7:ILE:CG2	3:BC:11:CYS:SG	3.04	0.46
14:B3:224:LYS:NZ	45:B3:310:CLA:O2D	2.48	0.46
20:B:32:ILE:HG22	20:B:35:GLU:HB2	1.98	0.46
22:D:466:ARG:NH1	22:D:467:GLU:OE2	2.49	0.46
26:a:307:VAL:HG21	26:a:382:ILE:HD13	1.98	0.46
29:d:65:ALA:O	33:h:128:PHE:HZ	1.99	0.46
41:M:197:ARG:CG	41:M:198:VAL:N	2.78	0.46
16:A6:77:TRP:NE1	16:A6:89:ASP:OD2	2.45	0.46
1:BA:559:ARG:NH1	4:BD:85:LEU:HD21	2.30	0.46
1:BA:578:ARG:HA	3:BC:77:MET:HA	1.98	0.46
17:B2:226:GLN:O	17:B2:230:THR:N	2.44	0.46
24:F:399:LEU:HA	24:F:402:THR:HG22	1.98	0.46
33:h:138:GLY:O	33:h:141:THR:OG1	2.29	0.46
1:AA:538:ALA:HB2	45:AA:838:CLA:HMA1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A3:137:THR:OG1	14:A3:148:TYR:OH	2.32	0.45
1:BA:303:LEU:O	1:BA:307:HIS:ND1	2.43	0.45
1:BA:662:SER:OG	1:BA:663:SER:N	2.49	0.45
1:BA:746:ILE:O	1:BA:750:GLY:HA2	2.15	0.45
2:BB:540:ASP:N	2:BB:540:ASP:OD1	2.48	0.45
3:BC:27:GLU:OE1	4:BD:175:ARG:HD2	2.15	0.45
7:BG:72:THR:HG23	7:BG:136:GLY:HA2	1.98	0.45
7:BG:127:PHE:O	45:BG:202:CLA:H3A	2.16	0.45
12:BL:91:LEU:HB3	12:BL:92:PRO:HD2	1.98	0.45
14:B3:235:ALA:HB2	52:B3:315:LUT:C10	2.46	0.45
19:A:146:LEU:HD22	25:G:79:MET:HE1	1.98	0.45
22:D:284:PRO:HB3	33:h:80:TRP:CD2	2.51	0.45
31:f:103:PRO:HB3	31:f:225:GLN:HE21	1.80	0.45
36:H:236:ILE:CD1	38:J:79:ASN:CG	2.89	0.45
43:O:128:ALA:HB3	43:O:147:LEU:HD21	1.98	0.45
1:AA:706:LEU:HD21	48:AF:805:BCR:C34	2.46	0.45
48:AA:848:BCR:H392	48:AA:848:BCR:H23C	1.97	0.45
2:AB:636:ASN:OD1	2:AB:636:ASN:N	2.47	0.45
8:AH:73:VAL:HG23	8:AH:74:TYR:CD2	2.51	0.45
10:AJ:31:ARG:HD3	48:AJ:101:BCR:H312	1.98	0.45
2:BB:519:VAL:HG21	2:BB:593:TYR:HB2	1.99	0.45
17:B2:77:PRO:HD2	55:B2:616:XAT:C22	2.45	0.45
17:B2:124:SER:OG	17:B2:125:TRP:N	2.46	0.45
19:A:106:VAL:HG21	19:A:255:LEU:HD22	1.97	0.45
19:A:180:LEU:HD21	21:C:79:LEU:HB3	1.97	0.45
20:B:142:PHE:CE2	25:G:158:LEU:HD21	2.51	0.45
22:D:256:ALA:O	22:D:261:LYS:NZ	2.42	0.45
27:b:138:GLN:HA	27:b:155:SER:HA	1.99	0.45
37:I:80:VAL:HG21	42:N:124:ALA:HA	1.97	0.45
38:J:105:LYS:HE3	44:T:78:UNK:O	2.17	0.45
43:O:118:ASP:O	43:O:129:LEU:N	2.46	0.45
1:AA:503:THR:HG21	45:AA:827:CLA:CBB	2.46	0.45
16:A6:184:TYR:HB2	16:A6:187:LYS:HB3	1.97	0.45
9:BI:32:GLN:O	12:BL:159:LYS:NZ	2.47	0.45
20:B:153:PHE:CD1	20:B:195:VAL:HG21	2.51	0.45
26:a:223:SER:OG	26:a:224:TYR:N	2.49	0.45
31:f:152:ASP:HA	31:f:156:HIS:HD2	1.81	0.45
39:K:103:ILE:HD11	39:K:153:LEU:HD13	1.97	0.45
3:AC:32:ASP:OD1	3:AC:32:ASP:N	2.44	0.45
2:BB:92:TRP:CZ2	8:BH:129:ILE:CG2	2.99	0.45
2:BB:182:LEU:HG	45:BB:815:CLA:H43	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B2:250:ILE:HA	45:B2:612:CLA:OBD	2.17	0.45
22:D:287:LEU:HD12	22:D:324:ILE:HG12	1.99	0.45
22:D:339:LEU:HA	22:D:488:VAL:HG11	1.98	0.45
24:F:282:PRO:HG3	29:d:74:MET:CE	2.46	0.45
27:b:149:ASP:OD2	27:b:170:ASN:ND2	2.39	0.45
33:h:105:ILE:O	33:h:150:ARG:NH2	2.49	0.45
35:j:119:GLU:OE1	35:j:122:ARG:NH1	2.50	0.45
1:AA:561:ILE:CD1	1:AA:584:VAL:HG11	2.47	0.45
45:AB:827:CLA:H142	48:AB:847:BCR:C22	2.46	0.45
1:BA:599:ASN:HD21	45:BA:801:CLA:H191	1.80	0.45
2:BB:364:ASP:HB2	8:BH:145:LEU:HD21	1.98	0.45
2:BB:680:TRP:NE1	12:BL:72:GLY:O	2.50	0.45
19:A:324:THR:HG23	19:A:325:LEU:HD12	1.99	0.45
42:N:179:ARG:CB	42:N:180:PRO:CD	2.94	0.45
45:AA:801:CLA:H102	45:AA:801:CLA:H62	1.69	0.45
1:BA:14:VAL:HG21	45:BA:810:CLA:HED3	1.99	0.45
20:B:171:LYS:HD2	23:E:87:ASN:HD21	1.82	0.45
20:B:443:SER:HA	20:B:446:TYR:CE2	2.52	0.45
22:D:58:CYS:O	29:d:92:LYS:HD3	2.17	0.45
22:D:494:ASP:OD1	22:D:494:ASP:N	2.49	0.45
32:g:74:PHE:HD2	32:g:77:GLU:HB3	1.82	0.45
37:I:131:ASP:HB3	37:I:134:GLU:HG3	1.99	0.45
2:AB:561:GLY:O	2:AB:567:THR:OG1	2.34	0.45
16:A6:184:TYR:OH	24:F:548:LEU:CD1	2.65	0.45
45:BA:808:CLA:H93	48:BJ:103:BCR:H343	1.98	0.45
19:A:228:ARG:HD3	19:A:322:ARG:NH1	2.29	0.45
20:B:199:SER:OG	23:E:44:ASN:HB3	2.17	0.45
22:D:40:TRP:HA	22:D:43:ILE:HG22	1.99	0.45
22:D:151:LEU:HD11	22:D:174:ILE:HA	1.98	0.45
22:D:154:VAL:O	22:D:158:LEU:HB2	2.17	0.45
24:F:77:ILE:HG13	29:d:85:HIS:HD2	1.79	0.45
25:G:132:ILE:HD12	32:g:109:HIS:ND1	2.32	0.45
25:G:155:PRO:O	25:G:159:ILE:HG12	2.17	0.45
45:AA:801:CLA:HBB1	45:AA:801:CLA:HMB1	1.98	0.45
2:AB:82:LEU:C	8:AH:145:LEU:HD23	2.42	0.45
2:AB:560:ASP:OD2	2:AB:564:ARG:NH1	2.49	0.45
15:A4:107:VAL:HG11	52:A4:315:LUT:H12	1.99	0.45
1:BA:215:VAL:HA	1:BA:219:LEU:HD12	1.99	0.45
8:BH:78:ALA:O	12:BL:97:ALA:HB3	2.16	0.45
19:A:346:LEU:HD12	21:C:108:LEU:HD22	1.97	0.45
22:D:57:PHE:HE2	29:d:95:TYR:HD2	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:G:71:ASN:HA	25:G:74:ILE:HB	1.98	0.45
5:AE:89:ILE:HG22	5:AE:91:ARG:H	1.81	0.45
13:B1:50:PRO:O	18:B5:160:GLN:NE2	2.50	0.45
17:B2:107:GLY:HA3	55:B2:616:XAT:H182	1.99	0.45
14:B3:235:ALA:CB	52:B3:315:LUT:H10	2.47	0.45
19:A:177:LEU:HD11	19:A:346:LEU:HD23	1.98	0.45
19:A:321:THR:HA	19:A:324:THR:HG22	1.99	0.45
20:B:258:GLU:OE2	20:B:322:ARG:NH1	2.50	0.45
36:H:310:PHE:HB2	36:H:311:ILE:HD12	1.99	0.45
2:AB:411:MET:HE1	45:AB:831:CLA:CHD	2.47	0.45
10:AJ:27:ILE:HG22	48:AJ:101:BCR:H343	1.98	0.45
1:BA:600:ALA:O	1:BA:604:VAL:HG23	2.17	0.45
1:BA:699:ILE:HD12	45:BA:840:CLA:HMD2	1.99	0.45
48:BJ:101:BCR:H392	48:BJ:101:BCR:H23C	1.98	0.45
19:A:89:ARG:HD2	19:A:90:PRO:HD2	1.99	0.45
22:D:20:PRO:HB2	22:D:129:SER:HB2	1.98	0.45
22:D:396:GLY:HA3	47:F:801:LHG:H352	1.98	0.45
24:F:268:THR:OG1	24:F:269:MET:N	2.50	0.45
28:c:110:TYR:HB3	28:c:113:TYR:HB2	1.99	0.45
30:e:116:GLN:HA	30:e:119:ILE:HG22	1.98	0.45
30:e:194:ASP:OD1	30:e:194:ASP:N	2.49	0.45
12:AL:91:LEU:HD12	12:AL:93:GLY:H	1.81	0.44
13:A1:121:LEU:O	13:A1:121:LEU:HD12	2.16	0.44
15:A4:75:ASN:N	45:A4:301:CLA:OBD	2.50	0.44
45:A4:309:CLA:HBC3	53:A4:318:LMG:H112	1.99	0.44
1:BA:421:ASN:OD1	1:BA:422:ASP:N	2.50	0.44
2:BB:516:ASP:OD2	2:BB:597:LYS:NZ	2.49	0.44
7:BG:127:PHE:O	45:BG:202:CLA:C3A	2.66	0.44
10:BJ:40:PRO:HG2	56:BJ:104:SQD:H2	1.99	0.44
12:BL:91:LEU:HD21	45:BL:302:CLA:CAB	2.42	0.44
20:B:101:GLN:HB3	20:B:141:MET:HE3	1.99	0.44
26:a:152:THR:OG1	26:a:153:THR:N	2.50	0.44
26:a:372:ILE:HD12	26:a:377:GLN:HB3	2.00	0.44
35:j:144:ASP:N	35:j:228:GLU:OE2	2.50	0.44
45:AB:808:CLA:H12	9:AI:15:VAL:HG21	1.99	0.44
8:AH:77:ASP:C	12:AL:97:ALA:HB2	2.42	0.44
1:BA:410:MET:O	1:BA:556:ARG:NH2	2.46	0.44
1:BA:426:ARG:HG2	1:BA:429:ARG:HH21	1.83	0.44
1:BA:674:ALA:HB2	1:BA:736:ALA:HB3	1.98	0.44
7:BG:129:ILE:H	45:BG:202:CLA:CGA	2.30	0.44
8:BH:80:SER:CB	12:BL:98:VAL:HG23	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B1:221:LEU:HD22	52:B1:316:LUT:H163	1.98	0.44
17:B2:148:ILE:HD13	48:B2:617:BCR:H361	2.00	0.44
20:B:318:THR:HG22	26:a:195:TYR:HD1	1.81	0.44
21:C:31:LEU:HD22	39:K:165:ARG:HH22	1.82	0.44
24:F:464:ASN:N	27:b:290:ARG:HH12	2.16	0.44
27:b:285:ARG:HG3	27:b:287:LEU:HD22	1.98	0.44
36:H:325:GLU:HB2	38:J:22:ASP:HB3	2.00	0.44
37:I:129:THR:O	39:K:134:VAL:CA	2.66	0.44
39:K:7:PRO:CD	42:N:148:PRO:HG2	2.46	0.44
2:AB:5:PHE:CG	9:AI:31:ILE:HD13	2.52	0.44
2:AB:645:VAL:HG21	45:AB:809:CLA:HAC1	1.98	0.44
45:AB:808:CLA:CGA	9:AI:15:VAL:HB	2.47	0.44
1:BA:529:ALA:HB1	1:BA:638:SER:OG	2.17	0.44
2:BB:646:TRP:O	2:BB:723:ALA:HB1	2.16	0.44
41:M:146:LEU:HB3	41:M:163:ILE:HD11	1.98	0.44
42:N:179:ARG:HB2	42:N:180:PRO:HD3	1.99	0.44
1:AA:656:VAL:HG13	1:AA:657:ILE:HG23	1.99	0.44
2:AB:113:VAL:HG12	2:AB:114:ASN:H	1.79	0.44
6:AF:133:ASP:OD1	6:AF:133:ASP:N	2.50	0.44
13:A1:57:TYR:OH	13:A1:69:ASP:OD2	2.25	0.44
1:BA:118:ILE:HG12	1:BA:119:VAL:HG13	1.99	0.44
1:BA:410:MET:HE1	1:BA:428:LEU:HD11	1.99	0.44
1:BA:562:PRO:HG3	4:BD:130:GLN:HG2	1.99	0.44
1:BA:717:LEU:CD2	46:BA:843:PQN:H143	2.48	0.44
45:BA:801:CLA:HMB2	45:BB:802:CLA:CAD	2.47	0.44
13:B1:48:TRP:O	54:B1:303:CHL:ND	2.50	0.44
20:B:244:LEU:HD13	20:B:336:ILE:HD11	2.00	0.44
22:D:434:LEU:HA	22:D:437:ILE:HD12	1.99	0.44
22:D:473:SER:O	29:d:98:TYR:OH	2.33	0.44
36:H:83:VAL:HG11	36:H:158:PHE:HB3	2.00	0.44
37:I:80:VAL:CG2	42:N:124:ALA:HA	2.47	0.44
8:BH:82:TYR:CZ	12:BL:102:LEU:CB	3.00	0.44
18:B5:247:ILE:N	45:B5:612:CLA:O1A	2.49	0.44
19:A:270:PHE:O	19:A:274:LEU:HB2	2.16	0.44
27:b:100:GLY:HA2	27:b:215:LEU:HD21	2.00	0.44
30:e:83:ASP:OD1	30:e:83:ASP:N	2.50	0.44
15:A4:80:LEU:HD12	55:A4:316:XAT:H372	1.98	0.44
1:BA:429:ARG:HB3	4:BD:80:SER:HA	1.99	0.44
2:BB:529:THR:HG21	2:BB:582:TRP:CE2	2.52	0.44
2:BB:578:LEU:HD22	45:BB:801:CLA:HBC1	1.99	0.44
4:BD:69:ASP:OD1	4:BD:69:ASP:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:BG:80:ARG:NH1	7:BG:124:PRO:HG2	2.25	0.44
8:BH:87:SER:HA	12:BL:102:LEU:HD21	2.00	0.44
22:D:240:LEU:HD12	22:D:240:LEU:HA	1.72	0.44
39:K:36:PRO:C	39:K:38:LEU:H	2.26	0.44
39:K:40:GLY:HA3	39:K:45:PHE:HD1	1.83	0.44
39:K:185:ARG:HA	41:M:155:LEU:HD12	1.99	0.44
1:AA:713:GLN:CD	5:AE:122:LYS:HB2	2.42	0.44
2:AB:174:ARG:HB2	45:AB:814:CLA:HBC2	1.99	0.44
2:AB:343:VAL:CG2	48:AB:848:BCR:H362	2.47	0.44
4:AD:85:LEU:O	4:AD:89:GLN:NE2	2.51	0.44
2:BB:92:TRP:HA	8:BH:129:ILE:CG1	2.48	0.44
17:B2:53:PRO:HG3	47:B2:618:LHG:O1	2.18	0.44
17:B2:56:PHE:HD1	54:B2:601:CHL:HMA3	1.75	0.44
19:A:94:ASN:ND2	19:A:150:TYR:O	2.51	0.44
20:B:36:CYS:HA	20:B:39:ILE:HG22	2.00	0.44
24:F:99:LEU:HD11	24:F:350:ALA:HB3	1.99	0.44
36:H:355:ARG:NE	38:J:52:ARG:HB2	2.32	0.44
37:I:124:GLU:HB2	37:I:146:PRO:HB3	1.99	0.44
38:J:144:LYS:HB3	43:O:141:TRP:HB2	1.98	0.44
1:AA:380:ASP:OD2	1:AA:383:THR:OG1	2.21	0.44
2:AB:721:TYR:HB2	45:AB:803:CLA:HED3	1.99	0.44
8:AH:74:TYR:HB2	12:AL:94:TYR:CD1	2.52	0.44
1:BA:196:ASN:HB3	45:BA:820:CLA:HMD2	1.98	0.44
2:BB:700:LEU:HD21	46:BB:844:PQN:H152	1.99	0.44
3:BC:59:PRO:HA	5:BE:128:ILE:CD1	2.48	0.44
8:BH:77:ASP:CB	12:BL:177:GLN:NE2	2.63	0.44
17:B2:57:PRO:HG2	54:B2:601:CHL:C2D	2.48	0.44
14:B3:126:ILE:CD1	45:B3:313:CLA:C1C	2.96	0.44
20:B:87:PHE:HD2	25:G:154:LEU:HB2	1.79	0.44
20:B:264:VAL:HB	20:B:268:LEU:HD23	2.00	0.44
22:D:47:ILE:HB	30:e:148:THR:HG21	1.99	0.44
22:D:139:ASP:HB3	22:D:142:LEU:HB3	2.00	0.44
22:D:171:THR:HA	22:D:174:ILE:HG22	1.99	0.44
23:E:15:LEU:HG	25:G:108:LEU:HB2	1.99	0.44
24:F:51:VAL:HG11	24:F:136:LEU:HD13	1.99	0.44
25:G:159:ILE:HD13	25:G:162:ILE:HD12	2.00	0.44
33:h:96:ASN:ND2	33:h:101:THR:OG1	2.51	0.44
37:I:131:ASP:C	39:K:135:TYR:CE2	2.96	0.44
2:AB:115:ILE:O	45:AB:809:CLA:HMD2	2.18	0.44
2:AB:664:LEU:O	2:AB:667:TRP:NE1	2.51	0.44
10:AJ:7:TYR:O	10:AJ:10:VAL:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
55:A6:616:XAT:H35	55:A6:616:XAT:H401	1.87	0.44
1:BA:674:ALA:CB	1:BA:736:ALA:HB3	2.48	0.44
2:BB:292:ARG:HE	7:BG:97:PRO:CD	2.26	0.44
8:BH:115:LEU:CG	9:BI:13:PRO:HB3	2.46	0.44
17:B2:53:PRO:HB2	54:B2:601:CHL:CBC	2.48	0.44
17:B2:58:GLY:HA3	14:B3:172:GLN:HB3	1.99	0.44
20:B:70:MET:HA	20:B:73:THR:HG22	2.00	0.44
20:B:335:VAL:HG13	20:B:351:MET:HG2	2.00	0.44
22:D:229:VAL:HG12	22:D:236:LEU:HB3	2.00	0.44
22:D:262:MET:HA	22:D:265:TYR:HB3	2.00	0.44
24:F:307:THR:O	24:F:661:SER:OG	2.36	0.44
24:F:486:LYS:HD3	24:F:497:LEU:HA	2.00	0.44
33:h:113:ASP:HA	33:h:119:ARG:HH21	1.82	0.44
37:I:125:TYR:CD2	39:K:145:ALA:HB2	2.53	0.44
38:J:122:TYR:HB2	38:J:128:LEU:HD22	2.00	0.44
1:AA:503:THR:HG21	45:AA:827:CLA:CAB	2.48	0.43
2:AB:268:LEU:HD13	45:AB:818:CLA:HMA2	2.00	0.43
2:AB:675:ILE:HG21	2:AB:697:PRO:O	2.18	0.43
52:AF:806:LUT:H373	53:A1:321:LMG:C28	2.48	0.43
10:AJ:27:ILE:CG2	48:AJ:101:BCR:H343	2.48	0.43
13:A1:215:THR:OG1	13:A1:216:GLY:N	2.50	0.43
14:A3:260:ASP:O	14:A3:262:VAL:N	2.47	0.43
15:A4:236:GLN:O	15:A4:244:ASN:ND2	2.50	0.43
1:BA:540:THR:HB	1:BA:600:ALA:HB2	1.99	0.43
48:BF:304:BCR:H23C	48:BF:304:BCR:H383	1.99	0.43
18:B5:240:SER:OG	18:B5:241:ASN:ND2	2.51	0.43
20:B:209:ILE:HG12	23:E:58:LYS:HD3	2.00	0.43
20:B:285:ASP:O	34:i:137:ARG:NH1	2.50	0.43
24:F:18:VAL:CG2	24:F:43:LEU:HD23	2.48	0.43
34:i:215:ASN:HD22	34:i:217:ARG:HH21	1.66	0.43
36:H:142:TYR:HE1	36:H:153:MET:HG2	1.83	0.43
36:H:219:LEU:HD11	36:H:364:ILE:HG12	2.00	0.43
39:K:115:PHE:HB3	39:K:119:SER:HB2	2.01	0.43
2:AB:20:ARG:NH2	2:AB:695:ASP:OD1	2.48	0.43
2:AB:88:ALA:N	2:AB:114:ASN:O	2.46	0.43
7:AG:99:GLN:N	7:AG:102:LYS:O	2.51	0.43
54:A1:303:CHL:HMB2	45:A4:313:CLA:O1D	2.18	0.43
45:A1:306:CLA:C1B	48:A1:319:BCR:H392	2.48	0.43
3:BC:47:ASP:OD1	4:BD:150:ARG:NH2	2.48	0.43
4:BD:72:THR:HG21	4:BD:120:PRO:HB2	1.99	0.43
8:BH:71:TRP:C	12:BL:167:PRO:HB2	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:B2:53:PRO:HA	14:B3:183:GLN:NE2	2.34	0.43
24:F:10:ILE:HD12	24:F:14:ILE:HD11	1.99	0.43
24:F:74:SER:HB3	29:d:84:TRP:H	1.81	0.43
24:F:159:TYR:HB2	24:F:179:PHE:HB2	1.99	0.43
28:c:170:ASP:OD1	28:c:170:ASP:N	2.51	0.43
36:H:81:ILE:HD12	36:H:330:VAL:HG12	1.99	0.43
37:I:125:TYR:HD2	39:K:145:ALA:HB2	1.83	0.43
1:AA:379:THR:HG21	1:AA:515:VAL:HG22	2.00	0.43
1:AA:585:SER:O	1:AA:589:HIS:ND1	2.43	0.43
2:AB:717:TYR:CE1	45:AB:803:CLA:HED1	2.54	0.43
4:AD:132:LEU:HD23	4:AD:132:LEU:O	2.18	0.43
16:A6:197:PRO:HB3	54:A6:608:CHL:HBC2	2.00	0.43
14:B3:83:ASP:O	14:B3:87:THR:HG21	2.17	0.43
24:F:36:LEU:HG	30:e:98:PHE:HB2	1.99	0.43
26:a:331:LEU:O	26:a:335:ALA:N	2.49	0.43
35:j:187:ASN:HB2	35:j:192:THR:HG23	2.00	0.43
36:H:10:LEU:HB3	36:H:31:THR:OG1	2.18	0.43
36:H:140:PHE:HE1	36:H:174:LYS:HD2	1.83	0.43
13:A1:116:GLN:OE1	54:A1:308:CHL:NA	2.52	0.43
14:A3:105:ARG:NH2	14:A3:225:GLU:OE2	2.51	0.43
45:BB:841:CLA:H202	9:BI:17:LEU:HD23	1.98	0.43
14:B3:116:ALA:HB3	45:B3:303:CLA:CHD	2.49	0.43
20:B:153:PHE:HE2	23:E:66:VAL:HA	1.83	0.43
20:B:271:THR:HA	20:B:274:VAL:HG12	2.01	0.43
22:D:435:THR:HA	22:D:438:TYR:CE2	2.54	0.43
26:a:126:VAL:HG21	26:a:319:MET:HG2	2.00	0.43
32:g:125:TYR:O	32:g:129:ASP:HB2	2.18	0.43
37:I:69:VAL:HG12	49:I:202:SF4:S3	2.58	0.43
37:I:131:ASP:CA	39:K:135:TYR:CD2	3.01	0.43
38:J:61:PRO:HG2	43:O:127:TYR:CE1	2.54	0.43
1:AA:432:ASP:OD2	1:AA:559:ARG:NH2	2.48	0.43
6:AF:118:ARG:O	6:AF:122:ASN:ND2	2.48	0.43
2:BB:293:THR:HG22	2:BB:294:ASN:H	1.83	0.43
2:BB:542:ARG:HH22	4:BD:190:SER:CB	2.32	0.43
2:BB:728:SER:O	2:BB:732:LYS:HG2	2.19	0.43
7:BG:127:PHE:HB3	45:BG:202:CLA:CHB	2.48	0.43
23:E:60:GLU:HB3	25:G:58:VAL:HG21	2.01	0.43
24:F:442:THR:HA	24:F:445:TYR:CE2	2.54	0.43
26:a:338:ILE:HA	26:a:341:VAL:HG12	2.00	0.43
27:b:28:ILE:HG22	27:b:31:GLU:HB3	1.99	0.43
34:i:127:THR:HA	35:j:189:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:H:27:ARG:HB3	36:H:43:ILE:HB	1.99	0.43
36:H:66:TYR:CE1	37:I:75:PRO:HB2	2.53	0.43
37:I:109:ASN:N	49:I:201:SF4:S1	2.67	0.43
45:AA:841:CLA:H143	46:AA:843:PQN:H291	2.00	0.43
2:AB:203:ARG:NH1	2:AB:253:ALA:O	2.47	0.43
8:AH:72:ASP:HB3	12:AL:176:LYS:HE2	1.99	0.43
2:BB:241:SER:O	2:BB:241:SER:OG	2.33	0.43
5:BE:87:VAL:O	5:BE:101:GLY:N	2.52	0.43
17:B2:97:HIS:CE1	45:B2:603:CLA:ND	2.87	0.43
14:B3:65:TYR:OH	14:B3:77:ASP:OD2	2.34	0.43
25:G:26:VAL:HA	25:G:35:SER:HB2	2.00	0.43
34:i:142:ARG:NH1	34:i:215:ASN:O	2.45	0.43
36:H:33:ASP:N	36:H:33:ASP:OD1	2.50	0.43
36:H:66:TYR:OH	37:I:75:PRO:O	2.36	0.43
38:J:22:ASP:OD2	38:J:28:THR:HG23	2.19	0.43
39:K:140:PRO:HD2	49:K:301:SF4:S4	2.59	0.43
1:AA:29:PRO:HA	45:AA:803:CLA:HBC1	2.01	0.43
45:AB:834:CLA:H41	10:AJ:26:LEU:HD23	2.00	0.43
11:AK:69:ARG:NE	45:AK:201:CLA:CHD	2.78	0.43
16:A6:184:TYR:CZ	24:F:542:GLU:HG2	2.53	0.43
52:A6:615:LUT:C37	24:F:42:PHE:CE1	2.96	0.43
48:A6:617:BCR:H321	48:A6:617:BCR:HC8	2.00	0.43
2:BB:423:SER:O	2:BB:427:LEU:HB2	2.18	0.43
7:BG:68:ILE:CG2	45:BG:201:CLA:CAD	2.94	0.43
12:BL:98:VAL:HG22	12:BL:99:ASN:N	2.34	0.43
17:B2:73:PHE:CD2	54:B2:601:CHL:CMC	3.02	0.43
17:B2:211:LYS:NZ	47:B2:618:LHG:O5	2.46	0.43
20:B:150:ILE:HA	23:E:62:PHE:HE1	1.82	0.43
22:D:263:GLY:O	22:D:267:LEU:N	2.44	0.43
31:f:96:ASP:O	31:f:208:TYR:OH	2.32	0.43
33:h:102:ARG:NH2	33:h:187:GLU:OE2	2.45	0.43
33:h:212:LEU:HA	33:h:215:VAL:HG12	2.01	0.43
35:j:81:GLN:HB3	35:j:84:ILE:HD11	2.00	0.43
36:H:110:ARG:HH22	36:H:234:ARG:HH21	1.65	0.43
37:I:27:MET:HA	37:I:30:LEU:HD23	2.01	0.43
1:AA:634:PHE:O	1:AA:638:SER:OG	2.30	0.43
5:AE:87:VAL:HG21	5:AE:138:VAL:HG21	2.00	0.43
45:BA:801:CLA:HBD	45:BA:801:CLA:HED3	1.69	0.43
4:BD:161:HIS:HB3	4:BD:162:PRO:HD3	2.00	0.43
17:B2:57:PRO:HG2	54:B2:601:CHL:C3D	2.49	0.43
14:B3:127:PRO:CG	45:B3:313:CLA:C2D	2.96	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A:334:LEU:HD13	21:C:65:PHE:CE2	2.54	0.43
20:B:183:TYR:HB2	20:B:256:VAL:HG11	2.01	0.43
27:b:125:SER:O	27:b:142:SER:N	2.52	0.43
34:i:122:ARG:HB2	34:i:202:LEU:HB2	2.01	0.43
42:N:75:ILE:HA	42:N:199:LEU:HA	2.00	0.43
1:AA:536:ILE:HD12	45:AA:801:CLA:H172	2.01	0.43
1:AA:705:LYS:NZ	6:AF:220:ASP:OD2	2.51	0.43
1:AA:745:ARG:O	1:AA:749:VAL:HG22	2.19	0.43
2:AB:292:ARG:HD3	7:AG:97:PRO:HD3	2.01	0.43
48:A1:319:BCR:H382	48:A1:319:BCR:H23C	2.01	0.43
55:A4:316:XAT:C28	55:A4:316:XAT:H381	2.49	0.43
7:BG:128:ASN:C	45:BG:202:CLA:HBA2	2.43	0.43
11:BK:96:GLY:O	45:BK:201:CLA:H3A	2.18	0.43
12:BL:95:ARG:O	12:BL:98:VAL:HG12	2.19	0.43
20:B:387:LEU:HG	20:B:395:ALA:HB2	2.00	0.43
22:D:407:PHE:HB3	24:F:194:LEU:HD11	2.01	0.43
29:d:69:GLN:CD	33:h:121:TYR:HE1	2.26	0.43
36:H:236:ILE:HG23	38:J:79:ASN:HB3	2.00	0.43
1:AA:530:ASP:OD2	1:AA:611:LYS:NZ	2.44	0.43
2:AB:429:LEU:HD11	45:AB:838:CLA:HMB2	2.01	0.43
2:AB:631:LEU:HD22	2:AB:724:PHE:HA	1.99	0.43
14:A3:125:LEU:O	14:A3:126:ILE:HG23	2.18	0.43
2:BB:101:VAL:O	2:BB:105:THR:HG23	2.19	0.43
20:B:171:LYS:HA	20:B:171:LYS:HD3	1.85	0.43
23:E:54:ASN:ND2	25:G:131:GLN:OE1	2.52	0.43
24:F:22:LEU:HD22	24:F:122:LEU:HB3	2.01	0.43
24:F:235:VAL:HA	24:F:238:ILE:HD12	2.00	0.43
27:b:39:ARG:HB2	27:b:42:ILE:HD12	2.01	0.43
27:b:211:SER:HB3	27:b:214:GLU:HG3	2.00	0.43
38:J:65:LEU:O	38:J:90:THR:N	2.45	0.43
41:M:147:VAL:HG12	41:M:163:ILE:HG12	2.01	0.43
7:AG:132:VAL:HG21	45:AG:204:CLA:CMA	2.49	0.42
2:BB:12:LEU:O	2:BB:20:ARG:HB3	2.18	0.42
17:B2:99:ARG:NH2	17:B2:209:GLU:OE2	2.49	0.42
18:B5:195:ASP:OD1	18:B5:196:VAL:N	2.52	0.42
19:A:334:LEU:HD12	21:C:119:TRP:CD1	2.54	0.42
22:D:57:PHE:CE2	29:d:95:TYR:HD2	2.37	0.42
22:D:102:ILE:HD11	22:D:346:PHE:HD1	1.84	0.42
22:D:123:LEU:HD13	22:D:156:LEU:HB2	2.01	0.42
23:E:80:ILE:HD13	25:G:173:VAL:HG11	2.01	0.42
25:G:111:LEU:HD23	25:G:111:LEU:HA	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:j:179:GLY:HA2	35:j:203:LYS:HA	2.01	0.42
37:I:133:HIS:HD2	41:M:190:ASN:O	1.98	0.42
45:BA:841:CLA:H41	46:BA:843:PQN:H191	2.00	0.42
2:BB:4:ARG:NH2	2:BB:13:ALA:O	2.52	0.42
45:BB:809:CLA:OBD	9:BI:8:PRO:HA	2.20	0.42
45:BB:841:CLA:HAB	46:BB:844:PQN:H141	2.00	0.42
3:BC:18:VAL:CG2	4:BD:168:PRO:O	2.65	0.42
4:BD:125:LEU:H	4:BD:125:LEU:HD12	1.84	0.42
18:B5:192:LEU:HG	26:a:178:TRP:CZ2	2.54	0.42
20:B:143:LEU:HD23	20:B:275:ALA:HB1	2.00	0.42
24:F:127:TYR:OH	47:F:801:LHG:O10	2.36	0.42
26:a:115:VAL:O	26:a:116:ARG:NE	2.50	0.42
26:a:153:THR:HA	26:a:173:ASP:H	1.84	0.42
26:a:306:ILE:HG12	26:a:387:GLY:HA3	2.00	0.42
27:b:330:ASP:OD1	27:b:330:ASP:N	2.52	0.42
36:H:76:MET:O	36:H:80:ALA:HB2	2.17	0.42
38:J:116:ASP:OD2	38:J:132:LEU:N	2.43	0.42
45:AA:801:CLA:H2	45:AA:802:CLA:O1D	2.20	0.42
14:A3:254:LEU:HD13	52:A3:316:LUT:H163	2.00	0.42
1:BA:155:GLN:O	1:BA:159:THR:OG1	2.34	0.42
2:BB:110:LEU:O	8:BH:133:PRO:CG	2.67	0.42
4:BD:79:GLY:HA2	12:BL:69:PRO:O	2.20	0.42
13:B1:156:ARG:HD2	45:B1:309:CLA:HMD2	2.02	0.42
13:B1:180:ASP:OD2	13:B1:183:LYS:CG	2.66	0.42
17:B2:126:TYR:CE1	54:B2:606:CHL:HMA2	2.53	0.42
19:A:129:ILE:HD13	25:G:57:PHE:HA	2.02	0.42
20:B:425:TRP:HD1	22:D:193:LEU:HD12	1.83	0.42
24:F:477:SER:OG	24:F:478:LEU:N	2.52	0.42
24:F:526:THR:HA	28:c:188:TRP:HA	2.01	0.42
28:c:139:LEU:HD21	28:c:173:GLY:HA3	2.01	0.42
31:f:222:VAL:HG12	31:f:226:LEU:HG	2.00	0.42
36:H:12:ILE:HD13	36:H:31:THR:HA	2.01	0.42
38:J:95:PRO:HB2	38:J:121:THR:H	1.84	0.42
38:J:136:SER:OG	41:M:157:GLU:N	2.49	0.42
2:AB:378:ILE:HG22	2:AB:382:ILE:HD12	2.02	0.42
45:AB:810:CLA:H202	9:AI:24:MET:HG3	2.00	0.42
13:A1:95:MET:HE2	45:A1:311:CLA:CBB	2.49	0.42
1:BA:217:VAL:HG13	1:BA:237:PRO:HB3	2.01	0.42
2:BB:441:ASP:OD1	2:BB:616:LEU:N	2.52	0.42
5:BE:84:GLY:N	5:BE:103:VAL:O	2.47	0.42
17:B2:116:LYS:NZ	17:B2:236:ASP:OD2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:D:58:CYS:HA	29:d:92:LYS:HD3	2.00	0.42
22:D:120:PHE:CD1	22:D:157:LEU:HD22	2.55	0.42
24:F:95:ILE:HD12	24:F:347:ILE:HD11	2.00	0.42
24:F:548:LEU:HD23	24:F:551:MET:HE3	2.00	0.42
25:G:103:VAL:HA	25:G:106:THR:HG22	2.00	0.42
26:a:199:VAL:HG11	26:a:213:LEU:HD22	2.00	0.42
27:b:66:SER:HB3	27:b:73:LEU:HD23	2.01	0.42
38:J:149:PRO:HG3	41:M:158:TYR:HE1	1.84	0.42
2:AB:309:ILE:HD11	2:AB:320:LYS:HB2	2.01	0.42
55:A3:317:XAT:H31	55:A3:317:XAT:H391	1.95	0.42
45:BA:806:CLA:HMD2	47:BA:845:LHG:H223	2.00	0.42
2:BB:92:TRP:NE1	8:BH:129:ILE:CG2	2.76	0.42
6:BF:126:TYR:OH	56:BJ:104:SQD:H4	2.19	0.42
22:D:73:ASP:OD1	22:D:73:ASP:N	2.52	0.42
22:D:172:LYS:O	22:D:176:TYR:HB2	2.19	0.42
24:F:63:ILE:HD13	24:F:575:PHE:HD1	1.84	0.42
24:F:548:LEU:HA	24:F:551:MET:HE3	2.00	0.42
1:AA:199:LEU:O	1:AA:204:GLY:N	2.53	0.42
1:AA:513:VAL:HG23	1:AA:513:VAL:O	2.20	0.42
2:AB:285:LEU:O	2:AB:289:HIS:ND1	2.51	0.42
2:AB:351:HIS:CE1	45:AB:827:CLA:NB	2.88	0.42
2:AB:430:GLY:HA2	2:AB:525:LEU:HD22	2.00	0.42
14:A3:70:LEU:N	14:A3:73:ASP:OD2	2.49	0.42
2:BB:609:PHE:O	2:BB:613:SER:OG	2.31	0.42
7:BG:125:ILE:HD12	7:BG:125:ILE:HA	1.94	0.42
20:B:186:MET:HE2	25:G:93:TRP:HE3	1.84	0.42
20:B:218:LEU:HD11	20:B:229:ILE:HD13	2.01	0.42
22:D:394:LEU:HD21	24:F:156:MET:HB2	2.02	0.42
24:F:18:VAL:HG13	24:F:40:TRP:CE3	2.55	0.42
26:a:287:VAL:HA	26:a:290:VAL:HG12	2.01	0.42
28:c:178:GLN:HG3	28:c:188:TRP:HE1	1.84	0.42
46:AA:843:PQN:H193	48:AF:801:BCR:H383	2.02	0.42
2:AB:725:LEU:O	2:AB:729:THR:OG1	2.29	0.42
1:BA:429:ARG:HA	4:BD:80:SER:HB2	2.01	0.42
1:BA:443:ILE:HD11	48:BA:855:BCR:H402	2.02	0.42
2:BB:123:TRP:CZ2	45:BB:815:CLA:H191	2.55	0.42
2:BB:294:ASN:N	2:BB:294:ASN:OD1	2.52	0.42
2:BB:476:VAL:HG22	2:BB:477:LEU:HG	2.00	0.42
45:BB:815:CLA:H41	45:BB:820:CLA:CBC	2.50	0.42
7:BG:80:ARG:HG2	45:BG:202:CLA:CAB	2.40	0.42
22:D:413:SER:HB3	22:D:421:LYS:HE2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:206:GLN:HE21	29:d:69:GLN:HG2	1.84	0.42
32:g:177:LYS:HA	32:g:180:LYS:HE2	2.02	0.42
42:N:65:TRP:O	42:N:69:VAL:HG23	2.20	0.42
1:AA:296:LEU:HD21	45:AA:817:CLA:HMB1	2.01	0.42
2:AB:328:ASN:ND2	7:AG:100:ASN:OD1	2.53	0.42
2:AB:519:VAL:HG11	2:AB:593:TYR:CD1	2.54	0.42
6:AF:104:ALA:HB3	6:AF:105:PRO:HD3	2.02	0.42
14:A3:242:GLN:HA	14:A3:245:VAL:HG12	2.02	0.42
1:BA:536:ILE:HD12	45:BA:801:CLA:H172	2.01	0.42
45:BA:808:CLA:H91	45:BA:811:CLA:H193	2.02	0.42
45:BB:801:CLA:O1D	48:BB:803:BCR:H401	2.19	0.42
22:D:107:THR:HA	22:D:110:ALA:HB3	2.02	0.42
22:D:175:LEU:HD13	47:a:501:LHG:H261	2.02	0.42
25:G:19:LEU:HG	25:G:42:VAL:HG13	2.00	0.42
25:G:65:ILE:HD12	25:G:65:ILE:HA	1.85	0.42
26:a:292:ALA:HB1	26:a:296:ARG:HH12	1.85	0.42
28:c:132:GLU:O	28:c:178:GLN:N	2.52	0.42
33:h:171:ASP:OD1	33:h:218:ARG:NH2	2.53	0.42
34:i:122:ARG:NH1	34:i:126:GLY:O	2.45	0.42
36:H:164:ALA:HA	36:H:311:ILE:HD11	2.00	0.42
1:BA:405:HIS:CE1	45:BA:830:CLA:NA	2.87	0.42
1:BA:543:VAL:HG11	1:BA:596:TRP:CE2	2.55	0.42
1:BA:560:LEU:HD13	2:BB:672:GLN:HG2	2.01	0.42
2:BB:194:LEU:HA	2:BB:198:ALA:HB3	2.02	0.42
19:A:208:LEU:HD22	19:A:275:TYR:HB3	2.00	0.42
20:B:150:ILE:HG12	23:E:62:PHE:CD1	2.51	0.42
22:D:33:ARG:N	30:e:179:LYS:HE3	2.33	0.42
22:D:185:LEU:HA	22:D:188:VAL:HG22	2.01	0.42
24:F:113:ASN:CB	24:F:546:THR:OG1	2.54	0.42
24:F:403:LEU:HD22	24:F:408:ILE:HG13	2.02	0.42
26:a:228:ASN:HB3	26:a:229:VAL:H	1.72	0.42
28:c:110:TYR:HE1	57:c:301:FES:S2	2.43	0.42
30:e:166:GLU:HB2	30:e:169:ILE:HG12	2.02	0.42
36:H:219:LEU:HD13	36:H:223:MET:HB3	2.02	0.42
15:A4:112:LEU:HA	15:A4:115:VAL:HG22	2.01	0.42
48:BA:855:BCR:H391	45:BB:805:CLA:O1D	2.20	0.42
3:BC:23:THR:CA	4:BD:132:LEU:HD23	2.49	0.42
7:BG:68:ILE:HD13	45:BG:201:CLA:C2D	2.50	0.42
48:BL:301:BCR:HC8	48:BL:301:BCR:H311	2.02	0.42
20:B:128:GLU:HA	20:B:131:LEU:HB3	2.02	0.42
20:B:268:LEU:HD13	20:B:268:LEU:HA	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:C:87:ASP:OD2	31:f:124:GLN:HG2	2.19	0.42
22:D:76:TRP:HD1	22:D:77:ILE:HG13	1.85	0.42
23:E:9:LEU:HD22	25:G:16:GLY:HA2	2.02	0.42
25:G:49:LEU:HD23	25:G:52:LEU:HD12	2.01	0.42
29:d:81:LYS:O	33:h:132:ALA:HB1	2.18	0.42
31:f:107:ARG:HD2	31:f:121:ARG:HG2	2.02	0.42
36:H:203:VAL:O	36:H:257:SER:OG	2.30	0.42
37:I:130:TYR:CZ	39:K:156:LYS:HB2	2.55	0.42
1:AA:724:ALA:O	1:AA:728:THR:OG1	2.34	0.41
16:A6:112:ARG:NH1	54:A6:608:CHL:OBD	2.50	0.41
48:BA:856:BCR:H23C	48:BA:856:BCR:H382	2.01	0.41
3:BC:8:TYR:O	3:BC:11:CYS:SG	2.78	0.41
8:BH:73:VAL:HG13	12:BL:171:LEU:HD21	2.01	0.41
17:B2:138:THR:HG22	18:B5:248:ILE:HG12	2.02	0.41
17:B2:250:ILE:HD12	45:B2:612:CLA:HMD3	2.02	0.41
22:D:232:PRO:HG2	22:D:240:LEU:HD22	2.01	0.41
24:F:625:LYS:HD2	24:F:626:PRO:HD2	2.02	0.41
26:a:225:ILE:HG23	26:a:231:SER:CB	2.48	0.41
28:c:86:ASP:OD1	28:c:86:ASP:N	2.49	0.41
36:H:325:GLU:CB	38:J:22:ASP:CB	2.97	0.41
36:H:325:GLU:CB	38:J:22:ASP:HB3	2.50	0.41
36:H:358:GLY:HA2	36:H:361:ASN:HB2	2.01	0.41
39:K:70:ARG:HG2	39:K:95:GLN:HB3	2.02	0.41
1:AA:178:TYR:OH	45:AA:811:CLA:O2D	2.38	0.41
1:AA:717:LEU:HD21	46:AA:843:PQN:C15	2.50	0.41
2:AB:306:GLU:OE1	2:AB:321:GLY:N	2.46	0.41
45:AB:824:CLA:HMA1	45:AB:842:CLA:O2D	2.20	0.41
16:A6:204:PHE:HB2	24:F:549:PHE:CG	2.55	0.41
1:BA:667:TYR:O	1:BA:740:ALA:HB1	2.21	0.41
3:BC:23:THR:O	3:BC:23:THR:CG2	2.59	0.41
7:BG:68:ILE:HG21	45:BG:201:CLA:OBD	2.19	0.41
8:BH:100:ARG:NH1	12:BL:154:GLY:C	2.78	0.41
10:BJ:36:ALA:HB1	56:BJ:104:SQD:H441	2.02	0.41
17:B2:139:THR:OG1	18:B5:249:GLN:CD	2.63	0.41
19:A:135:ILE:HG13	21:C:80:TYR:OH	2.20	0.41
19:A:184:LEU:HD23	19:A:356:GLN:HG3	2.02	0.41
20:B:154:VAL:HG21	25:G:155:PRO:HB3	2.02	0.41
20:B:459:ASN:ND2	30:e:192:PHE:O	2.37	0.41
23:E:22:ILE:HG21	25:G:100:THR:HB	2.02	0.41
23:E:35:GLU:OE1	25:G:66:TYR:OH	2.32	0.41
24:F:353:LYS:HE2	24:F:405:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:570:GLN:HG2	24:F:572:GLY:H	1.84	0.41
28:c:90:ARG:HD3	28:c:105:SER:HB2	2.02	0.41
35:j:154:LYS:HB2	35:j:159:GLY:H	1.85	0.41
36:H:198:ILE:O	36:H:202:ARG:HB2	2.20	0.41
39:K:6:PHE:HB2	42:N:148:PRO:HB2	2.01	0.41
1:AA:641:ILE:HG23	45:AA:801:CLA:H91	2.02	0.41
2:AB:424:TRP:NE1	45:AB:833:CLA:OBD	2.43	0.41
15:A4:199:GLN:NE2	15:A4:202:LYS:CE	2.84	0.41
6:BF:202:ILE:HD13	6:BF:206:ALA:HB2	2.02	0.41
10:BJ:27:ILE:CG2	48:BJ:101:BCR:H343	2.50	0.41
48:BJ:101:BCR:H11C	48:BJ:101:BCR:H341	1.94	0.41
13:B1:233:ILE:O	13:B1:236:ILE:HG22	2.20	0.41
19:A:82:LEU:HD23	19:A:254:GLY:HA2	2.01	0.41
19:A:185:LEU:HD11	19:A:211:GLN:HG3	2.02	0.41
19:A:207:ASN:HA	19:A:210:ARG:HB2	2.02	0.41
20:B:476:SER:OG	20:B:477:ASN:N	2.52	0.41
22:D:41:TYR:CZ	22:D:45:ILE:HD11	2.55	0.41
22:D:127:MET:HE1	22:D:150:GLU:HB2	2.02	0.41
22:D:469:PHE:CZ	29:d:105:GLY:HA3	2.54	0.41
23:E:49:SER:HB2	23:E:59:GLY:HA3	2.02	0.41
36:H:355:ARG:HB2	38:J:53:SER:HB3	2.02	0.41
1:AA:600:ALA:O	1:AA:604:VAL:HG23	2.20	0.41
1:AA:691:TYR:OH	2:AB:533:ILE:HA	2.21	0.41
4:AD:161:HIS:HB3	4:AD:162:PRO:HD3	2.02	0.41
8:AH:66:ASN:ND2	12:AL:169:LEU:HD22	2.35	0.41
48:A3:318:BCR:H23C	48:A3:318:BCR:H382	2.03	0.41
16:A6:65:ARG:NH2	16:A6:85:ASP:OD1	2.53	0.41
16:A6:110:HIS:HD1	55:A6:616:XAT:H201	1.85	0.41
45:BA:801:CLA:HED2	45:BA:801:CLA:HAA2	2.02	0.41
2:BB:645:VAL:HG21	45:BB:810:CLA:HAC1	2.02	0.41
12:BL:91:LEU:HD12	45:BL:302:CLA:CMC	2.39	0.41
12:BL:93:GLY:N	45:BL:303:CLA:OBD	2.52	0.41
12:BL:97:ALA:HB2	12:BL:177:GLN:NE2	2.35	0.41
17:B2:250:ILE:HD12	45:B2:612:CLA:CMD	2.51	0.41
18:B5:60:ASP:OD1	18:B5:60:ASP:N	2.53	0.41
19:A:46:VAL:O	19:A:50:LEU:HB2	2.19	0.41
19:A:100:ILE:HA	19:A:103:SER:HB2	2.02	0.41
20:B:332:ILE:O	20:B:336:ILE:HG12	2.20	0.41
29:d:107:LEU:HB3	30:e:151:PHE:CD1	2.54	0.41
31:f:146:MET:HA	31:f:149:VAL:HG12	2.02	0.41
36:H:212:GLU:HG2	44:T:85:UNK:C	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:I:76:ILE:HD13	39:K:114:MET:O	2.20	0.41
6:AF:141:ASN:OD1	6:AF:142:GLY:N	2.53	0.41
2:BB:176:ASN:ND2	2:BB:291:TYR:O	2.50	0.41
10:BJ:31:ARG:HB2	48:BJ:101:BCR:H313	2.01	0.41
48:BJ:103:BCR:H382	48:BJ:103:BCR:H23C	2.01	0.41
17:B2:212:ASN:O	17:B2:215:LEU:HD23	2.21	0.41
18:B5:197:GLN:H	18:B5:197:GLN:HG2	1.51	0.41
22:D:50:LEU:HG	29:d:99:ILE:HG23	2.03	0.41
22:D:167:LEU:HB2	47:a:501:LHG:HC12	2.03	0.41
23:E:1:MET:HE3	23:E:3:LEU:HB2	2.03	0.41
27:b:104:VAL:HG12	27:b:181:ILE:HG23	2.02	0.41
27:b:277:LYS:HD3	27:b:290:ARG:HH21	1.84	0.41
30:e:69:THR:OG1	30:e:70:ASN:N	2.54	0.41
34:i:122:ARG:NH1	35:j:188:ALA:O	2.52	0.41
37:I:140:ILE:CG2	42:N:109:GLY:HA3	2.44	0.41
39:K:37:LEU:CD2	39:K:66:ARG:N	2.82	0.41
4:AD:74:SER:O	4:AD:117:ARG:NE	2.49	0.41
5:AE:135:LEU:C	5:AE:138:VAL:HG12	2.45	0.41
3:BC:80:ALA:HB1	4:BD:126:ALA:HB1	2.03	0.41
24:F:250:LEU:HD23	24:F:324:MET:HB2	2.02	0.41
24:F:277:VAL:HB	24:F:334:LEU:HD13	2.03	0.41
26:a:279:LEU:HD13	26:a:397:GLN:HB3	2.03	0.41
26:a:348:PHE:HE2	26:a:363:VAL:HG21	1.86	0.41
36:H:362:LEU:HD21	36:H:386:ILE:HG21	2.03	0.41
37:I:54:ARG:NH1	37:I:107:CYS:O	2.53	0.41
2:AB:682:HIS:NE2	2:AB:691:ILE:O	2.49	0.41
2:AB:711:ALA:O	2:AB:715:VAL:HG23	2.21	0.41
4:AD:127:ARG:NH2	4:AD:129:GLU:OE1	2.50	0.41
15:A4:108:ALA:HB2	52:A4:315:LUT:H401	2.02	0.41
16:A6:258:PRO:O	16:A6:262:ASN:ND2	2.47	0.41
1:BA:426:ARG:O	1:BA:430:HIS:ND1	2.48	0.41
17:B2:135:THR:HG23	18:B5:243:TRP:O	2.21	0.41
18:B5:197:GLN:HE21	18:B5:197:GLN:HB3	1.62	0.41
19:A:348:ASN:HA	19:A:351:LEU:HB2	2.02	0.41
20:B:210:GLU:O	20:B:214:ILE:HG13	2.21	0.41
21:C:63:TYR:OH	23:E:82:SER:HB3	2.20	0.41
22:D:141:LEU:O	22:D:145:ILE:HG12	2.20	0.41
22:D:267:LEU:HD23	22:D:271:ASN:HD22	1.85	0.41
22:D:386:ILE:HG12	47:F:801:LHG:H302	2.02	0.41
23:E:13:LEU:HD11	25:G:19:LEU:HD21	2.02	0.41
24:F:107:VAL:HG13	24:F:259:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:F:196:LEU:HD11	24:F:233:LEU:HD22	2.03	0.41
27:b:332:ALA:HB3	27:b:335:GLU:H	1.86	0.41
35:j:94:VAL:HG12	35:j:242:VAL:HG22	2.02	0.41
36:H:15:MET:HG2	36:H:28:LEU:HB2	2.03	0.41
1:AA:554:PHE:O	1:AA:564:LYS:NZ	2.51	0.41
2:AB:192:GLY:O	2:AB:196:HIS:ND1	2.43	0.41
45:AB:834:CLA:O1D	10:AJ:36:ALA:N	2.53	0.41
13:A1:82:ARG:NH1	45:A1:305:CLA:O1A	2.53	0.41
16:A6:167:ARG:NE	45:A6:601:CLA:OBD	2.52	0.41
1:BA:599:ASN:OD1	45:BA:801:CLA:H201	2.20	0.41
2:BB:292:ARG:CD	7:BG:97:PRO:HD3	2.50	0.41
2:BB:595:HIS:HE1	2:BB:728:SER:OG	2.04	0.41
45:BB:827:CLA:HMA1	48:BB:849:BCR:H14C	2.02	0.41
13:B1:200:LEU:HD21	45:B1:304:CLA:HBC1	2.03	0.41
55:B2:616:XAT:C28	55:B2:616:XAT:H381	2.51	0.41
19:A:169:ILE:HG23	21:C:69:PHE:CD2	2.56	0.41
20:B:170:THR:HG23	20:B:261:PRO:HD3	2.02	0.41
24:F:106:LEU:HD23	24:F:106:LEU:HA	1.91	0.41
24:F:700:GLY:HA2	24:F:703:ILE:HB	2.03	0.41
26:a:282:SER:OG	29:d:149:LYS:HD3	2.21	0.41
27:b:205:PRO:HA	27:b:257:ARG:HA	2.03	0.41
38:J:149:PRO:HG3	41:M:158:TYR:CE1	2.55	0.41
42:N:159:LEU:HB3	42:N:187:GLU:HA	2.03	0.41
48:AA:848:BCR:H23C	48:AA:848:BCR:H403	2.02	0.41
52:AF:806:LUT:H31	52:AF:806:LUT:H391	1.93	0.41
12:AL:150:LEU:HB3	12:AL:191:THR:HG22	2.03	0.41
45:A6:613:CLA:HMB1	52:A6:615:LUT:H7	2.03	0.41
45:BA:801:CLA:H2	45:BA:802:CLA:O1D	2.21	0.41
2:BB:292:ARG:HH21	7:BG:96:LEU:HD23	1.86	0.41
2:BB:552:ASP:OD1	4:BD:201:SER:OG	2.31	0.41
3:BC:15:THR:HG22	3:BC:28:MET:HG3	2.03	0.41
48:BG:203:BCR:H20C	48:BG:203:BCR:H361	1.36	0.41
10:BJ:7:TYR:O	10:BJ:10:VAL:HG12	2.21	0.41
13:B1:98:VAL:HG11	52:B1:316:LUT:H14	2.03	0.41
13:B1:234:GLY:HA2	13:B1:237:VAL:HG22	2.02	0.41
19:A:117:PRO:HG2	19:A:195:VAL:HG21	2.02	0.41
19:A:353:THR:HG22	21:C:94:PHE:CE1	2.56	0.41
22:D:270:ILE:HA	22:D:274:LEU:HD23	2.03	0.41
24:F:47:LEU:HD23	24:F:50:ILE:HD12	2.02	0.41
26:a:152:THR:O	26:a:172:TYR:N	2.43	0.41
26:a:330:SER:OG	26:a:331:LEU:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:d:69:GLN:OE1	33:h:121:TYR:HE1	2.04	0.41
31:f:172:GLU:OE2	31:f:179:ASN:ND2	2.54	0.41
31:f:210:LEU:HD13	31:f:233:LEU:HB2	2.03	0.41
34:i:132:SER:OG	34:i:137:ARG:O	2.39	0.41
37:I:58:HIS:N	37:I:120:SER:O	2.48	0.41
38:J:105:LYS:NZ	44:T:78:UNK:O	2.54	0.41
42:N:67:GLN:HA	42:N:70:GLU:HG2	2.03	0.41
55:A1:318:XAT:H35	55:A1:318:XAT:H401	1.92	0.41
45:BA:840:CLA:H91	45:BF:302:CLA:HBC3	2.03	0.41
48:BA:847:BCR:H311	48:BA:847:BCR:C8	2.51	0.41
2:BB:290:MET:HE1	45:BB:821:CLA:CAD	2.51	0.41
13:B1:98:VAL:HG23	13:B1:205:PHE:HZ	1.84	0.41
48:B2:617:BCR:H331	48:B2:617:BCR:HC8	2.03	0.41
14:B3:105:ARG:NH1	54:B3:306:CHL:OBD	2.52	0.41
20:B:268:LEU:O	20:B:272:SER:CB	2.69	0.41
23:E:56:GLN:HB3	23:E:58:LYS:HG3	2.03	0.41
24:F:26:LEU:HD11	24:F:122:LEU:HB2	2.03	0.41
31:f:151:TYR:O	31:f:155:LYS:HB2	2.21	0.41
6:AF:77:ASP:O	6:AF:79:LYS:NZ	2.49	0.40
45:BA:803:CLA:CMD	6:BF:186:ILE:HG23	2.49	0.40
2:BB:682:HIS:NE2	2:BB:691:ILE:O	2.47	0.40
3:BC:18:VAL:CG1	4:BD:168:PRO:O	2.65	0.40
45:B2:610:CLA:HBD	45:B2:611:CLA:CAD	2.51	0.40
21:C:7:TYR:HD2	25:G:51:ILE:HG23	1.86	0.40
21:C:101:VAL:HA	21:C:104:LEU:HB3	2.03	0.40
22:D:95:THR:O	22:D:99:THR:OG1	2.30	0.40
22:D:273:GLU:HB3	22:D:499:ILE:HD12	2.03	0.40
24:F:75:TRP:HB2	24:F:85:PHE:HD1	1.86	0.40
34:i:145:VAL:HG23	34:i:147:LYS:HG2	2.03	0.40
36:H:68:THR:HG23	36:H:69:ARG:HG2	2.03	0.40
36:H:89:LEU:HD23	36:H:321:LEU:HD22	2.03	0.40
36:H:130:PRO:HB2	36:H:131:PHE:H	1.64	0.40
37:I:130:TYR:HA	39:K:134:VAL:HA	2.03	0.40
38:J:61:PRO:HB3	38:J:144:LYS:HB2	2.03	0.40
2:AB:194:LEU:HA	2:AB:198:ALA:HB3	2.03	0.40
2:AB:680:TRP:NE1	12:AL:72:GLY:O	2.51	0.40
48:AJ:103:BCR:H23C	48:AJ:103:BCR:H382	2.04	0.40
1:BA:723:ARG:NH2	49:BA:852:SF4:S1	2.95	0.40
2:BB:732:LYS:HG3	2:BB:734:GLY:H	1.87	0.40
45:BB:812:CLA:H193	8:BH:115:LEU:HD22	2.03	0.40
17:B2:65:LEU:CD2	45:B2:602:CLA:O1D	2.65	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:B5:150:ARG:NH2	45:B5:608:CLA:O1D	2.50	0.40
24:F:353:LYS:HA	24:F:356:LEU:HB2	2.03	0.40
37:I:141:ALA:HB2	42:N:109:GLY:N	2.36	0.40
1:AA:659:SER:OG	1:AA:660:TYR:N	2.53	0.40
45:AB:825:CLA:H71	45:AB:827:CLA:H42	2.03	0.40
3:AC:17:CYS:N	49:AC:102:SF4:S4	2.69	0.40
9:AI:31:ILE:HD11	48:AI:102:BCR:C33	2.51	0.40
45:BA:805:CLA:HMC1	45:BA:830:CLA:HMA1	2.03	0.40
2:BB:646:TRP:CZ2	2:BB:726:ILE:HG21	2.56	0.40
45:BB:812:CLA:C19	9:BI:17:LEU:HD13	2.51	0.40
22:D:135:PHE:O	22:D:265:TYR:OH	2.32	0.40
23:E:57:LEU:HB3	23:E:60:GLU:HB2	2.02	0.40
24:F:168:ARG:HB3	30:e:77:PHE:CE2	2.57	0.40
24:F:191:LEU:HD11	24:F:232:LEU:HD13	2.03	0.40
25:G:121:TYR:HA	25:G:124:ILE:HD12	2.04	0.40
25:G:143:GLN:HA	25:G:146:ILE:HG12	2.02	0.40
27:b:76:LYS:HD2	27:b:86:PHE:HD2	1.87	0.40
42:N:115:LEU:HB2	42:N:140:VAL:HG22	2.02	0.40
1:AA:410:MET:HE1	1:AA:428:LEU:HD11	2.03	0.40
16:A6:110:HIS:HE1	45:A6:604:CLA:NC	2.20	0.40
45:BA:801:CLA:HMB3	45:BB:804:CLA:HAA1	2.03	0.40
48:BA:851:BCR:H362	45:BB:802:CLA:H42	2.03	0.40
48:BA:851:BCR:C40	45:BB:834:CLA:HMB2	2.52	0.40
2:BB:223:GLY:O	2:BB:227:THR:OG1	2.20	0.40
7:BG:123:ASP:OD1	45:BG:202:CLA:ND	2.54	0.40
11:BK:126:ASN:HB2	45:BK:202:CLA:HMA1	2.00	0.40
18:B5:92:SER:HB3	18:B5:214:MET:HE2	2.03	0.40
19:A:131:ILE:HD12	19:A:274:LEU:HD11	2.02	0.40
20:B:304:ILE:HG23	20:B:435:ILE:HG21	2.04	0.40
20:B:371:LEU:HD23	20:B:371:LEU:HA	1.94	0.40
22:D:261:LYS:HG2	22:D:341:ILE:HG23	2.03	0.40
24:F:308:LEU:HD12	24:F:321:TYR:CZ	2.56	0.40
24:F:501:ASN:HA	24:F:525:ILE:HA	2.03	0.40
31:f:91:PHE:HB3	31:f:102:TYR:HE2	1.86	0.40
36:H:45:GLY:HA2	38:J:132:LEU:HD22	2.03	0.40
36:H:325:GLU:HB3	38:J:22:ASP:CG	2.47	0.40
45:A1:306:CLA:NB	48:A1:319:BCR:H392	2.37	0.40
16:A6:186:HIS:HD2	24:F:541:HIS:HB3	1.87	0.40
2:BB:92:TRP:CG	8:BH:129:ILE:HG12	2.57	0.40
7:BG:134:ALA:O	7:BG:137:SER:OG	2.36	0.40
21:C:11:TRP:HH2	25:G:48:LEU:HB3	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:E:69:ILE:HD11	25:G:159:ILE:HD12	2.03	0.40
24:F:18:VAL:HG13	24:F:40:TRP:HE3	1.87	0.40
27:b:64:LYS:HB3	27:b:74:SER:H	1.85	0.40
28:c:181:PRO:HA	28:c:184:LYS:HD3	2.04	0.40
34:i:125:ASP:N	34:i:125:ASP:OD1	2.54	0.40
35:j:139:HIS:CD2	35:j:140:ARG:HG3	2.56	0.40
35:j:185:MET:HA	35:j:197:PHE:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	AA	740/750 (99%)	686 (93%)	53 (7%)	1 (0%)	48 80
1	BA	740/750 (99%)	692 (94%)	48 (6%)	0	100 100
2	AB	732/734 (100%)	695 (95%)	37 (5%)	0	100 100
2	BB	731/734 (100%)	696 (95%)	35 (5%)	0	100 100
3	AC	78/81 (96%)	72 (92%)	6 (8%)	0	100 100
3	BC	78/81 (96%)	73 (94%)	5 (6%)	0	100 100
4	AD	139/204 (68%)	126 (91%)	13 (9%)	0	100 100
4	BD	141/204 (69%)	121 (86%)	18 (13%)	2 (1%)	9 38
5	AE	65/143 (46%)	58 (89%)	7 (11%)	0	100 100
5	BE	67/143 (47%)	61 (91%)	6 (9%)	0	100 100
6	AF	151/221 (68%)	144 (95%)	7 (5%)	0	100 100
6	BF	152/221 (69%)	149 (98%)	3 (2%)	0	100 100
7	AG	97/160 (61%)	90 (93%)	7 (7%)	0	100 100
7	BG	92/160 (58%)	84 (91%)	8 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	AH	93/145 (64%)	89 (96%)	4 (4%)	0	100	100
8	BH	93/145 (64%)	87 (94%)	6 (6%)	0	100	100
9	AI	31/37 (84%)	30 (97%)	1 (3%)	0	100	100
9	BI	31/37 (84%)	29 (94%)	2 (6%)	0	100	100
10	AJ	40/44 (91%)	38 (95%)	2 (5%)	0	100	100
10	BJ	41/44 (93%)	38 (93%)	3 (7%)	0	100	100
11	AK	61/130 (47%)	57 (93%)	4 (7%)	0	100	100
11	BK	60/130 (46%)	53 (88%)	7 (12%)	0	100	100
12	AL	155/219 (71%)	145 (94%)	10 (6%)	0	100	100
12	BL	157/219 (72%)	149 (95%)	8 (5%)	0	100	100
13	A1	194/241 (80%)	178 (92%)	16 (8%)	0	100	100
13	B1	168/241 (70%)	160 (95%)	8 (5%)	0	100	100
14	A3	217/273 (80%)	192 (88%)	25 (12%)	0	100	100
14	B3	219/273 (80%)	206 (94%)	13 (6%)	0	100	100
15	A4	195/251 (78%)	185 (95%)	10 (5%)	0	100	100
16	A6	210/270 (78%)	197 (94%)	13 (6%)	0	100	100
17	B2	206/257 (80%)	191 (93%)	15 (7%)	0	100	100
18	B5	204/256 (80%)	188 (92%)	15 (7%)	1 (0%)	24	59
19	A	297/360 (82%)	279 (94%)	18 (6%)	0	100	100
20	B	484/512 (94%)	443 (92%)	40 (8%)	1 (0%)	43	74
21	C	90/120 (75%)	87 (97%)	3 (3%)	0	100	100
22	D	495/506 (98%)	453 (92%)	42 (8%)	0	100	100
23	E	87/101 (86%)	79 (91%)	8 (9%)	0	100	100
24	F	669/746 (90%)	614 (92%)	55 (8%)	0	100	100
25	G	163/176 (93%)	151 (93%)	12 (7%)	0	100	100
26	a	339/461 (74%)	277 (82%)	61 (18%)	1 (0%)	36	69
27	b	301/348 (86%)	267 (89%)	34 (11%)	0	100	100
28	c	126/204 (62%)	109 (86%)	17 (14%)	0	100	100
29	d	91/161 (56%)	78 (86%)	13 (14%)	0	100	100
30	e	148/212 (70%)	122 (82%)	26 (18%)	0	100	100
31	f	151/238 (63%)	132 (87%)	18 (12%)	1 (1%)	18	53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	g	113/190 (60%)	113 (100%)	0	0	100 100
33	h	143/220 (65%)	130 (91%)	13 (9%)	0	100 100
34	i	143/217 (66%)	125 (87%)	18 (13%)	0	100 100
35	j	171/255 (67%)	150 (88%)	21 (12%)	0	100 100
36	H	350/393 (89%)	315 (90%)	35 (10%)	0	100 100
37	I	156/172 (91%)	132 (85%)	22 (14%)	2 (1%)	9 40
38	J	153/158 (97%)	134 (88%)	19 (12%)	0	100 100
39	K	161/225 (72%)	137 (85%)	23 (14%)	1 (1%)	21 55
40	L	75/191 (39%)	67 (89%)	8 (11%)	0	100 100
41	M	106/217 (49%)	94 (89%)	12 (11%)	0	100 100
42	N	144/209 (69%)	128 (89%)	15 (10%)	1 (1%)	18 53
43	O	69/158 (44%)	62 (90%)	7 (10%)	0	100 100
All	All	11603/14548 (80%)	10637 (92%)	955 (8%)	11 (0%)	49 80

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	BD	164	ASP
39	K	140	PRO
26	a	230	ASN
42	N	166	LYS
18	B5	49	TRP
37	I	67	CYS
1	AA	659	SER
4	BD	162	PRO
20	B	210	GLU
31	f	103	PRO
37	I	146	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AA	600/610 (98%)	590 (98%)	10 (2%)	53 68
1	BA	601/610 (98%)	593 (99%)	8 (1%)	61 71
2	AB	598/600 (100%)	594 (99%)	4 (1%)	76 78
2	BB	597/600 (100%)	590 (99%)	7 (1%)	63 72
3	AC	70/71 (99%)	70 (100%)	0	100 100
3	BC	70/71 (99%)	70 (100%)	0	100 100
4	AD	120/170 (71%)	118 (98%)	2 (2%)	53 68
4	BD	121/170 (71%)	119 (98%)	2 (2%)	53 68
5	AE	56/114 (49%)	56 (100%)	0	100 100
5	BE	58/114 (51%)	58 (100%)	0	100 100
6	AF	125/185 (68%)	124 (99%)	1 (1%)	73 77
6	BF	126/185 (68%)	123 (98%)	3 (2%)	43 63
7	AG	83/133 (62%)	80 (96%)	3 (4%)	31 54
7	BG	79/133 (59%)	76 (96%)	3 (4%)	29 52
8	AH	77/113 (68%)	76 (99%)	1 (1%)	61 71
8	BH	77/113 (68%)	75 (97%)	2 (3%)	40 60
9	AI	29/33 (88%)	29 (100%)	0	100 100
9	BI	29/33 (88%)	29 (100%)	0	100 100
10	AJ	37/39 (95%)	37 (100%)	0	100 100
10	BJ	38/39 (97%)	37 (97%)	1 (3%)	40 60
11	AK	47/95 (50%)	47 (100%)	0	100 100
11	BK	46/95 (48%)	45 (98%)	1 (2%)	45 64
12	AL	119/174 (68%)	119 (100%)	0	100 100
12	BL	120/174 (69%)	118 (98%)	2 (2%)	53 68
13	A1	151/190 (80%)	147 (97%)	4 (3%)	40 60
13	B1	138/190 (73%)	137 (99%)	1 (1%)	76 78
14	A3	168/211 (80%)	167 (99%)	1 (1%)	78 80
14	B3	170/211 (81%)	170 (100%)	0	100 100
15	A4	164/210 (78%)	163 (99%)	1 (1%)	78 80
16	A6	177/226 (78%)	172 (97%)	5 (3%)	38 59
17	B2	165/205 (80%)	164 (99%)	1 (1%)	78 80
18	B5	166/205 (81%)	162 (98%)	4 (2%)	43 63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	A	258/312 (83%)	256 (99%)	2 (1%)	73 77
20	B	420/446 (94%)	419 (100%)	1 (0%)	87 87
21	C	78/103 (76%)	78 (100%)	0	100 100
22	D	430/439 (98%)	428 (100%)	2 (0%)	81 82
23	E	75/87 (86%)	75 (100%)	0	100 100
24	F	561/661 (85%)	559 (100%)	2 (0%)	84 83
25	G	145/154 (94%)	145 (100%)	0	100 100
26	a	288/397 (72%)	288 (100%)	0	100 100
27	b	263/297 (89%)	262 (100%)	1 (0%)	84 83
28	c	112/177 (63%)	111 (99%)	1 (1%)	70 75
29	d	81/143 (57%)	81 (100%)	0	100 100
30	e	125/178 (70%)	125 (100%)	0	100 100
31	f	134/207 (65%)	133 (99%)	1 (1%)	76 78
32	g	104/172 (60%)	104 (100%)	0	100 100
33	h	127/192 (66%)	126 (99%)	1 (1%)	73 77
34	i	114/180 (63%)	114 (100%)	0	100 100
35	j	143/219 (65%)	141 (99%)	2 (1%)	59 71
36	H	291/342 (85%)	290 (100%)	1 (0%)	86 85
37	I	132/159 (83%)	130 (98%)	2 (2%)	57 70
38	J	87/140 (62%)	84 (97%)	3 (3%)	32 55
39	K	114/205 (56%)	112 (98%)	2 (2%)	51 67
40	L	66/171 (39%)	66 (100%)	0	100 100
41	M	58/195 (30%)	56 (97%)	2 (3%)	32 55
42	N	49/174 (28%)	48 (98%)	1 (2%)	48 65
43	O	36/138 (26%)	36 (100%)	0	100 100
All	All	9513/12210 (78%)	9422 (99%)	91 (1%)	65 75

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	46	ILE
1	AA	80	ILE
1	AA	221	ILE

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Mol	Chain	Res	Type
1	AA	247	LEU
1	AA	308	MET
1	AA	315	ILE
1	AA	505	LEU
1	AA	515	VAL
1	AA	630	THR
1	AA	675	HIS
2	AB	91	ILE
2	AB	330	ILE
2	AB	571	SER
2	AB	577	TYR
4	AD	132	LEU
4	AD	178	VAL
6	AF	197	ILE
7	AG	91	VAL
7	AG	109	ASP
7	AG	121	SER
8	AH	100	ARG
13	A1	85	GLU
13	A1	112	TRP
13	A1	142	LEU
13	A1	153	GLU
14	A3	119	ILE
15	A4	148	ILE
16	A6	67	LEU
16	A6	89	ASP
16	A6	110	HIS
16	A6	119	THR
16	A6	123	ILE
1	BA	115	VAL
1	BA	244	ARG
1	BA	519	VAL
1	BA	561	ILE
1	BA	582	CYS
1	BA	591	PHE
1	BA	660	TYR
1	BA	697	GLU
2	BB	91	ILE
2	BB	137	THR
2	BB	179	LEU
2	BB	294	ASN
2	BB	309	ILE

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Mol	Chain	Res	Type
2	BB	470	THR
2	BB	479	SER
4	BD	125	LEU
4	BD	144	ILE
6	BF	69	ILE
6	BF	98	LEU
6	BF	152	THR
7	BG	80	ARG
7	BG	125	ILE
7	BG	149	THR
8	BH	130	LYS
8	BH	139	LEU
10	BJ	38	THR
11	BK	121	VAL
12	BL	137	LEU
12	BL	169	LEU
13	B1	238	ILE
17	B2	135	THR
18	B5	50	LEU
18	B5	91	HIS
18	B5	174	LEU
18	B5	197	GLN
19	A	185	LEU
19	A	283	ILE
20	B	218	LEU
22	D	196	SER
22	D	470	LEU
24	F	191	LEU
24	F	545	ASN
27	b	166	VAL
28	c	176	VAL
31	f	222	VAL
33	h	208	THR
35	j	126	THR
35	j	213	VAL
36	H	365	LEU
37	I	30	LEU
37	I	78	LEU
38	J	4	THR
38	J	33	PRO
38	J	103	VAL
39	K	17	VAL

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Mol	Chain	Res	Type
39	K	152	LYS
41	M	93	VAL
41	M	110	GLU
42	N	176	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (106) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	243	ASN
1	AA	628	HIS
2	AB	220	GLN
2	AB	236	ASN
2	AB	363	GLN
2	AB	452	GLN
2	AB	487	ASN
2	AB	504	ASN
4	AD	71	ASN
5	AE	131	ASN
6	AF	213	ASN
7	AG	90	ASN
8	AH	83	ASN
8	AH	86	GLN
10	AJ	30	ASN
11	AK	54	ASN
11	AK	126	ASN
12	AL	66	ASN
13	A1	155	GLN
13	A1	208	GLN
13	A1	209	GLN
14	A3	103	ASN
15	A4	75	ASN
15	A4	199	GLN
15	A4	248	GLN
16	A6	186	HIS
16	A6	245	GLN
16	A6	250	ASN
1	BA	652	GLN
1	BA	713	GLN
2	BB	350	GLN
2	BB	399	ASN
2	BB	502	ASN
2	BB	704	GLN

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Mol	Chain	Res	Type
4	BD	99	ASN
4	BD	172	ASN
5	BE	127	ASN
6	BF	144	GLN
7	BG	140	HIS
11	BK	94	GLN
11	BK	114	HIS
13	B1	208	GLN
17	B2	226	GLN
14	B3	103	ASN
14	B3	152	ASN
14	B3	172	GLN
14	B3	183	GLN
14	B3	242	GLN
14	B3	253	ASN
18	B5	197	GLN
19	A	128	ASN
19	A	263	ASN
20	B	90	ASN
20	B	222	GLN
20	B	251	GLN
20	B	311	ASN
20	B	331	GLN
20	B	465	HIS
22	D	32	HIS
22	D	248	HIS
22	D	293	GLN
23	E	44	ASN
23	E	54	ASN
23	E	87	ASN
24	F	35	ASN
24	F	62	GLN
24	F	71	ASN
24	F	117	HIS
24	F	206	GLN
24	F	214	ASN
24	F	644	ASN
25	G	56	HIS
25	G	62	GLN
26	a	170	ASN
26	a	177	HIS
26	a	209	HIS

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Mol	Chain	Res	Type
26	a	230	ASN
26	a	352	HIS
26	a	400	ASN
27	b	108	ASN
27	b	347	ASN
28	c	88	HIS
29	d	93	ASN
30	e	164	ASN
30	e	185	ASN
30	e	193	ASN
31	f	124	GLN
31	f	156	HIS
31	f	179	ASN
31	f	225	GLN
32	g	135	ASN
32	g	155	ASN
33	h	93	ASN
33	h	96	ASN
33	h	126	ASN
33	h	162	ASN
34	i	116	ASN
34	i	198	ASN
34	i	206	ASN
35	j	249	GLN
36	H	84	ASN
36	H	216	ASN
37	I	109	ASN
37	I	133	HIS
38	J	54	GLN
41	M	96	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

423 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AK	203	-	50,54,73	1.34	8 (16%)	59,90,113	1.32	4 (6%)
45	CLA	BB	805	-	69,73,73	1.14	10 (14%)	82,113,113	1.45	10 (12%)
45	CLA	AA	828	-	69,73,73	1.16	7 (10%)	82,113,113	1.35	8 (9%)
45	CLA	AK	202	-	49,53,73	1.38	7 (14%)	58,89,113	1.21	4 (6%)
45	CLA	BA	811	-	69,73,73	1.15	7 (10%)	82,113,113	1.15	5 (6%)
50	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.09	4 (8%)
54	CHL	A6	608	-	43,58,74	3.68	17 (39%)	42,95,114	2.77	17 (40%)
45	CLA	AB	823	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	6 (7%)
47	LHG	B1	318	45	41,41,48	1.01	2 (4%)	44,47,54	0.97	2 (4%)
52	LUT	A3	316	-	42,43,43	0.85	0	51,60,60	1.80	15 (29%)
54	CHL	B1	303	13	44,58,74	3.97	19 (43%)	39,95,114	2.59	15 (38%)
45	CLA	A6	612	16	48,52,73	1.40	8 (16%)	57,88,113	1.21	4 (7%)
45	CLA	B3	304	-	44,49,73	1.44	6 (13%)	50,84,113	1.27	3 (6%)
48	BCR	BB	849	-	41,41,41	0.91	1 (2%)	56,56,56	1.87	15 (26%)
47	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.93	2 (4%)
45	CLA	BB	837	-	46,50,73	1.41	7 (15%)	53,85,113	1.28	3 (5%)
48	BCR	AJ	103	-	41,41,41	0.75	0	56,56,56	2.41	21 (37%)
45	CLA	A4	310	15	44,49,73	1.43	8 (18%)	50,84,113	1.28	4 (8%)
48	BCR	BK	204	-	41,41,41	0.91	1 (2%)	56,56,56	2.16	21 (37%)
48	BCR	AK	204	-	41,41,41	1.02	3 (7%)	56,56,56	2.07	15 (26%)
45	CLA	BA	844	47	45,49,73	1.41	5 (11%)	54,84,113	1.21	5 (9%)
45	CLA	AA	805	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	9 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AB	830	-	60,64,73	1.26	7 (11%)	71,102,113	1.23	4 (5%)
45	CLA	BB	823	-	49,54,73	1.33	6 (12%)	57,90,113	1.16	4 (7%)
49	SF4	BC	102	3	0,12,12	-	-	-		
45	CLA	BB	812	-	69,73,73	1.15	7 (10%)	82,113,113	1.26	7 (8%)
45	CLA	BB	843	47	69,73,73	1.18	9 (13%)	82,113,113	1.18	4 (4%)
45	CLA	B5	612	18	61,65,73	1.24	7 (11%)	72,103,113	1.12	3 (4%)
47	LHG	F	801	-	36,36,48	0.75	1 (2%)	39,42,54	1.25	3 (7%)
45	CLA	AB	813	-	47,51,73	1.35	7 (14%)	55,86,113	1.26	5 (9%)
56	SQD	BJ	104	-	45,47,54	1.23	4 (8%)	55,58,65	3.67	12 (21%)
54	CHL	A1	303	13	45,59,74	3.94	19 (42%)	39,96,114	2.73	18 (46%)
46	PQN	BB	844	-	34,34,34	3.50	11 (32%)	43,45,45	1.61	8 (18%)
45	CLA	BB	836	-	64,68,73	1.20	6 (9%)	76,107,113	1.24	5 (6%)
45	CLA	B3	301	14	64,68,73	1.20	8 (12%)	76,107,113	1.10	6 (7%)
45	CLA	BB	804	-	69,73,73	1.16	6 (8%)	82,113,113	1.17	6 (7%)
48	BCR	BA	847	-	41,41,41	1.01	2 (4%)	56,56,56	1.64	10 (17%)
45	CLA	BB	832	-	47,51,73	1.38	6 (12%)	55,86,113	1.18	4 (7%)
47	LHG	B1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.00	2 (5%)
45	CLA	B2	613	-	47,51,73	1.36	7 (14%)	55,86,113	1.21	6 (10%)
48	BCR	BA	849	-	41,41,41	0.87	0	56,56,56	2.02	19 (33%)
54	CHL	A6	606	-	36,50,74	4.08	18 (50%)	31,85,114	3.31	14 (45%)
45	CLA	A4	303	-	47,51,73	1.49	9 (19%)	58,87,113	1.36	6 (10%)
45	CLA	BA	838	-	58,62,73	1.32	8 (13%)	70,99,113	1.32	8 (11%)
45	CLA	A3	306	14	45,49,73	1.49	9 (20%)	54,84,113	1.42	6 (11%)
45	CLA	B1	310	13	42,47,73	1.54	8 (19%)	52,82,113	1.29	6 (11%)
48	BCR	BJ	101	-	41,41,41	0.90	0	56,56,56	1.73	15 (26%)
45	CLA	BA	840	-	69,73,73	1.12	6 (8%)	82,113,113	1.20	4 (4%)
45	CLA	BA	824	-	59,63,73	1.27	7 (11%)	70,101,113	1.24	4 (5%)
45	CLA	AA	824	-	57,62,73	1.29	8 (14%)	67,100,113	1.32	9 (13%)
52	LUT	B5	614	-	42,43,43	0.85	1 (2%)	51,60,60	1.91	15 (29%)
45	CLA	BA	841	-	69,73,73	1.13	8 (11%)	82,113,113	1.38	10 (12%)
55	XAT	A4	316	-	41,47,47	1.03	2 (4%)	54,74,74	2.20	16 (29%)
45	CLA	BA	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.15	4 (4%)
45	CLA	AB	819	-	64,68,73	1.20	7 (10%)	76,107,113	1.46	10 (13%)
45	CLA	A3	308	14	49,53,73	1.38	6 (12%)	58,89,113	1.23	5 (8%)
45	CLA	B5	604	-	47,51,73	1.50	9 (19%)	58,87,113	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.06	5 (10%)
57	FES	c	301	28	0,4,4	-	-	-		
45	CLA	A1	316	13	47,51,73	1.52	9 (19%)	58,87,113	1.41	6 (10%)
54	CHL	B5	607	-	39,53,74	3.98	20 (51%)	35,89,114	3.02	14 (40%)
45	CLA	BA	842	-	69,73,73	1.18	8 (11%)	82,113,113	1.19	6 (7%)
45	CLA	BA	828	-	69,73,73	1.13	6 (8%)	82,113,113	1.30	10 (12%)
45	CLA	BL	304	-	47,51,73	1.35	5 (10%)	55,86,113	1.29	5 (9%)
45	CLA	BB	818	-	59,63,73	1.24	6 (10%)	70,101,113	1.22	5 (7%)
48	BCR	BL	305	-	41,41,41	0.81	0	56,56,56	2.26	20 (35%)
45	CLA	BB	830	-	69,73,73	1.18	9 (13%)	82,113,113	1.13	6 (7%)
47	LHG	a	501	-	28,28,48	0.91	1 (3%)	31,34,54	1.28	2 (6%)
45	CLA	AB	840	-	69,73,73	1.19	8 (11%)	82,113,113	1.10	6 (7%)
49	SF4	K	301	39	0,12,12	-	-	-		
48	BCR	A6	617	-	41,41,41	1.00	2 (4%)	56,56,56	2.04	16 (28%)
45	CLA	AA	836	1	49,53,73	1.40	7 (14%)	58,89,113	1.32	6 (10%)
45	CLA	AB	816	-	47,51,73	1.37	7 (14%)	55,86,113	1.20	3 (5%)
45	CLA	BA	825	-	69,73,73	1.17	9 (13%)	82,113,113	1.19	4 (4%)
45	CLA	AL	305	-	46,50,73	1.40	7 (15%)	53,85,113	1.39	4 (7%)
49	SF4	I	201	37	0,12,12	-	-	-		
48	BCR	AF	805	-	41,41,41	0.82	0	56,56,56	1.85	14 (25%)
48	BCR	B5	616	-	41,41,41	0.82	0	56,56,56	2.33	23 (41%)
45	CLA	AA	829	-	69,73,73	1.19	7 (10%)	82,113,113	1.38	11 (13%)
45	CLA	BA	813	-	69,73,73	1.16	8 (11%)	82,113,113	1.22	5 (6%)
45	CLA	BA	821	-	69,73,73	1.14	7 (10%)	82,113,113	1.24	9 (10%)
45	CLA	BA	839	-	55,59,73	1.30	6 (10%)	64,96,113	1.30	6 (9%)
49	SF4	I	202	37	0,12,12	-	-	-		
53	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.21	4 (9%)
45	CLA	B3	310	14	47,51,73	1.38	5 (10%)	55,86,113	1.25	5 (9%)
48	BCR	AB	845	-	41,41,41	0.87	1 (2%)	56,56,56	1.90	17 (30%)
48	BCR	BB	846	-	41,41,41	0.87	1 (2%)	56,56,56	2.13	18 (32%)
47	LHG	A3	319	45	22,22,48	1.46	2 (9%)	25,28,54	1.31	2 (8%)
45	CLA	BA	835	-	49,53,73	1.38	6 (12%)	58,89,113	1.23	3 (5%)
45	CLA	BA	836	1	49,53,73	1.38	5 (10%)	58,89,113	1.37	5 (8%)
45	CLA	A6	614	-	47,51,73	1.41	6 (12%)	55,86,113	1.23	4 (7%)
45	CLA	AB	828	-	69,73,73	1.14	8 (11%)	82,113,113	1.27	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AB	826	-	66,70,73	1.17	7 (10%)	78,109,113	1.16	6 (7%)
45	CLA	AB	801	-	69,73,73	1.15	7 (10%)	82,113,113	1.46	12 (14%)
45	CLA	B1	312	47	41,46,73	1.54	7 (17%)	51,81,113	1.33	6 (11%)
48	BCR	AL	306	-	41,41,41	0.95	1 (2%)	56,56,56	2.01	21 (37%)
45	CLA	A3	305	-	44,49,73	1.44	7 (15%)	50,84,113	1.26	5 (10%)
45	CLA	BB	806	-	45,49,73	1.37	7 (15%)	54,84,113	1.33	5 (9%)
45	CLA	A3	310	47	39,45,73	1.49	7 (17%)	51,79,113	1.26	5 (9%)
48	BCR	BB	803	-	41,41,41	0.86	0	56,56,56	2.02	21 (37%)
47	LHG	B2	618	45	34,34,48	1.05	2 (5%)	37,40,54	0.97	2 (5%)
45	CLA	BB	825	-	49,53,73	1.36	7 (14%)	58,89,113	1.26	5 (8%)
45	CLA	AB	835	-	64,68,73	1.19	6 (9%)	76,107,113	1.20	6 (7%)
45	CLA	AB	808	-	55,59,73	1.29	7 (12%)	63,95,113	1.29	5 (7%)
45	CLA	BB	838	-	54,58,73	1.31	8 (14%)	64,95,113	1.34	8 (12%)
45	CLA	B3	305	-	45,49,73	1.49	8 (17%)	54,84,113	1.45	7 (12%)
45	CLA	AB	821	-	54,58,73	1.31	8 (14%)	64,95,113	1.30	6 (9%)
45	CLA	B5	602	18	64,68,73	1.24	9 (14%)	76,107,113	1.18	5 (6%)
45	CLA	A1	304	13	64,68,73	1.20	7 (10%)	75,106,113	1.17	5 (6%)
45	CLA	A1	312	47	41,46,73	1.57	8 (19%)	51,81,113	1.22	7 (13%)
45	CLA	BB	841	-	69,73,73	1.16	9 (13%)	82,113,113	1.17	7 (8%)
45	CLA	AA	838	-	59,63,73	1.22	8 (13%)	70,101,113	1.18	7 (10%)
45	CLA	BA	806	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
45	CLA	A6	604	-	45,50,73	1.44	7 (15%)	52,85,113	1.41	4 (7%)
45	CLA	A6	603	16	69,73,73	1.16	8 (11%)	82,113,113	1.17	6 (7%)
45	CLA	A1	314	-	67,72,73	1.18	7 (10%)	79,112,113	1.14	5 (6%)
45	CLA	BB	809	-	56,60,73	1.29	8 (14%)	65,97,113	1.22	4 (6%)
45	CLA	A1	311	13	63,67,73	1.22	7 (11%)	75,106,113	1.11	5 (6%)
48	BCR	AB	844	-	41,41,41	0.86	1 (2%)	56,56,56	2.32	24 (42%)
54	CHL	A4	304	-	35,49,74	4.16	18 (51%)	30,84,114	2.86	14 (46%)
45	CLA	BB	826	-	69,73,73	1.19	10 (14%)	82,113,113	1.16	5 (6%)
48	BCR	AB	848	-	41,41,41	0.90	1 (2%)	56,56,56	1.99	17 (30%)
45	CLA	AA	808	1	69,73,73	1.16	7 (10%)	82,113,113	1.19	5 (6%)
45	CLA	B3	303	-	45,50,73	1.53	7 (15%)	55,86,113	1.29	5 (9%)
45	CLA	BB	842	-	69,73,73	1.17	7 (10%)	82,113,113	1.21	5 (6%)
50	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.90	0
45	CLA	BF	303	-	45,49,73	1.40	8 (17%)	54,84,113	1.27	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
49	SF4	AC	101	3	0,12,12	-	-	-		
52	LUT	B3	315	-	42,43,43	0.98	1 (2%)	51,60,60	2.09	17 (33%)
45	CLA	A6	610	16	59,63,73	1.26	8 (13%)	70,101,113	1.19	7 (10%)
45	CLA	A1	315	-	41,46,73	1.56	8 (19%)	51,81,113	1.41	8 (15%)
45	CLA	BA	807	-	54,58,73	1.31	8 (14%)	64,95,113	1.15	5 (7%)
45	CLA	BA	833	-	69,73,73	1.19	8 (11%)	82,113,113	1.21	5 (6%)
45	CLA	AA	807	-	54,58,73	1.30	8 (14%)	64,95,113	1.23	7 (10%)
47	LHG	A3	301	-	35,35,48	1.10	2 (5%)	38,41,54	1.02	2 (5%)
45	CLA	B2	610	47	40,45,73	2.49	10 (25%)	46,76,113	1.46	6 (13%)
45	CLA	B2	612	17	69,73,73	1.18	7 (10%)	82,113,113	1.11	5 (6%)
45	CLA	AB	836	-	46,50,73	1.41	6 (13%)	53,85,113	1.32	4 (7%)
45	CLA	BA	804	-	56,60,73	1.28	8 (14%)	65,97,113	1.37	7 (10%)
50	LMU	AA	851	-	36,36,36	1.15	2 (5%)	47,47,47	1.04	2 (4%)
45	CLA	BB	824	-	69,73,73	1.13	7 (10%)	82,113,113	1.19	7 (8%)
45	CLA	A4	307	15	49,53,73	1.40	7 (14%)	58,89,113	1.20	4 (6%)
45	CLA	BB	835	-	69,73,73	1.17	7 (10%)	82,113,113	1.07	5 (6%)
47	LHG	A1	320	45	48,48,48	0.93	2 (4%)	51,54,54	0.85	2 (3%)
48	BCR	AL	302	-	41,41,41	0.80	0	56,56,56	2.23	22 (39%)
45	CLA	A6	605	-	46,51,73	1.40	7 (15%)	54,86,113	1.20	3 (5%)
45	CLA	AB	837	-	54,58,73	1.33	10 (18%)	64,95,113	1.34	6 (9%)
48	BCR	AI	102	-	41,41,41	0.88	0	56,56,56	2.60	18 (32%)
45	CLA	AA	803	-	69,73,73	1.15	7 (10%)	82,113,113	1.26	8 (9%)
56	SQD	e	301	-	32,34,54	1.21	5 (15%)	42,45,65	1.70	10 (23%)
45	CLA	BA	818	-	60,64,73	1.25	7 (11%)	71,102,113	1.20	6 (8%)
45	CLA	AL	304	-	64,68,73	1.23	7 (10%)	76,107,113	1.24	9 (11%)
48	BCR	BA	856	-	41,41,41	0.94	1 (2%)	56,56,56	2.17	18 (32%)
45	CLA	AA	815	-	43,49,73	1.35	5 (11%)	48,83,113	1.40	5 (10%)
46	PQN	BA	843	-	34,34,34	3.55	12 (35%)	43,45,45	1.58	5 (11%)
50	LMU	BA	854	-	34,34,36	1.17	2 (5%)	45,45,47	0.92	2 (4%)
45	CLA	AA	839	-	56,60,73	1.28	7 (12%)	65,97,113	1.27	6 (9%)
50	LMU	BA	853	-	35,35,36	1.14	2 (5%)	46,46,47	0.94	0
45	CLA	B3	313	-	40,44,73	1.47	7 (17%)	49,77,113	1.18	4 (8%)
45	CLA	BB	840	-	51,55,73	1.32	7 (13%)	60,91,113	1.28	5 (8%)
45	CLA	BK	203	-	50,54,73	1.32	6 (12%)	59,90,113	1.34	6 (10%)
54	CHL	B1	308	-	35,49,74	4.62	18 (51%)	28,84,114	2.57	13 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	BL	303	-	64,68,73	1.21	7 (10%)	76,107,113	1.22	8 (10%)
45	CLA	AA	810	-	68,72,73	1.23	8 (11%)	82,111,113	1.18	5 (6%)
45	CLA	BA	803	-	69,73,73	1.13	8 (11%)	82,113,113	1.24	6 (7%)
48	BCR	B3	317	-	41,41,41	0.87	0	56,56,56	3.71	29 (51%)
45	CLA	AB	817	-	59,63,73	1.25	8 (13%)	70,101,113	1.17	5 (7%)
45	CLA	A1	313	13	49,53,73	1.38	8 (16%)	58,89,113	1.37	4 (6%)
45	CLA	AG	203	-	46,50,73	1.39	7 (15%)	53,85,113	1.25	4 (7%)
45	CLA	AA	840	-	69,73,73	1.17	8 (11%)	82,113,113	1.22	6 (7%)
45	CLA	A3	303	14	59,63,73	1.29	8 (13%)	70,101,113	1.32	7 (10%)
45	CLA	BA	801	-	69,73,73	1.17	5 (7%)	82,113,113	1.12	5 (6%)
54	CHL	A6	602	16	46,60,74	3.98	19 (41%)	40,97,114	2.62	18 (45%)
45	CLA	B1	305	-	58,62,73	1.27	6 (10%)	68,99,113	1.38	6 (8%)
45	CLA	B5	613	-	49,53,73	1.37	7 (14%)	58,89,113	1.19	5 (8%)
52	LUT	A6	615	-	42,43,43	0.91	1 (2%)	51,60,60	1.69	12 (23%)
54	CHL	A4	314	15	36,49,74	4.25	16 (44%)	30,84,114	2.79	11 (36%)
49	SF4	BC	101	3	0,12,12	-	-	-		
45	CLA	A4	312	-	49,53,73	1.37	7 (14%)	58,89,113	1.22	5 (8%)
54	CHL	B5	606	-	35,48,74	3.91	16 (45%)	32,83,114	3.02	15 (46%)
45	CLA	AA	822	-	46,50,73	1.39	7 (15%)	53,85,113	1.31	4 (7%)
47	LHG	BA	845	-	48,48,48	0.88	3 (6%)	51,54,54	0.98	3 (5%)
54	CHL	A3	307	-	38,53,74	3.83	18 (47%)	36,89,114	2.90	13 (36%)
48	BCR	BL	301	-	41,41,41	0.89	1 (2%)	56,56,56	2.35	16 (28%)
45	CLA	BA	808	1	69,73,73	1.13	6 (8%)	82,113,113	1.12	5 (6%)
51	DGD	BB	850	-	67,67,67	0.82	2 (2%)	81,81,81	0.99	4 (4%)
45	CLA	BF	302	-	46,50,73	1.39	7 (15%)	53,85,113	1.36	4 (7%)
45	CLA	AA	834	-	69,73,73	1.16	7 (10%)	82,113,113	1.36	11 (13%)
45	CLA	AA	827	-	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
48	BCR	AA	847	-	41,41,41	0.99	2 (4%)	56,56,56	2.28	25 (44%)
45	CLA	A6	613	16	68,72,73	1.19	7 (10%)	80,111,113	1.10	4 (5%)
45	CLA	BB	829	-	69,73,73	1.13	7 (10%)	82,113,113	1.20	5 (6%)
45	CLA	A4	308	15	58,62,73	1.26	8 (13%)	68,99,113	1.14	5 (7%)
45	CLA	AA	801	-	69,73,73	1.16	5 (7%)	82,113,113	1.18	6 (7%)
48	BCR	AB	849	-	41,41,41	0.82	0	56,56,56	2.45	25 (44%)
45	CLA	AA	806	1	69,73,73	1.17	8 (11%)	82,113,113	1.28	5 (6%)
45	CLA	BA	816	-	49,53,73	1.38	5 (10%)	58,89,113	1.29	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	AA	852	-	41,41,41	0.94	2 (4%)	56,56,56	2.20	17 (30%)
45	CLA	AB	820	-	59,63,73	1.29	8 (13%)	70,101,113	1.14	5 (7%)
45	CLA	B1	309	-	47,52,73	1.41	7 (14%)	55,88,113	1.27	4 (7%)
48	BCR	AG	205	-	41,41,41	0.94	0	56,56,56	2.00	19 (33%)
45	CLA	BA	809	1	54,58,73	1.33	8 (14%)	64,95,113	1.32	8 (12%)
54	CHL	A4	305	-	35,49,74	3.87	16 (45%)	33,84,114	3.06	16 (48%)
45	CLA	AA	802	-	69,73,73	1.17	8 (11%)	82,113,113	1.19	5 (6%)
45	CLA	B1	306	-	45,49,73	1.39	6 (13%)	54,84,113	1.26	3 (5%)
45	CLA	AB	841	-	69,73,73	1.18	8 (11%)	82,113,113	1.14	4 (4%)
45	CLA	A4	313	-	54,58,73	1.32	7 (12%)	64,95,113	1.33	6 (9%)
52	LUT	B2	615	-	42,43,43	0.82	0	51,60,60	2.00	15 (29%)
45	CLA	BA	819	-	69,73,73	1.16	8 (11%)	82,113,113	1.20	6 (7%)
45	CLA	A6	609	16	49,53,73	1.37	8 (16%)	58,89,113	1.22	4 (6%)
54	CHL	B5	605	-	35,49,74	4.17	18 (51%)	30,84,114	2.69	13 (43%)
45	CLA	B3	314	-	43,48,73	1.42	6 (13%)	51,83,113	1.21	8 (15%)
55	XAT	A1	318	-	41,47,47	0.96	2 (4%)	54,74,74	2.25	24 (44%)
45	CLA	B3	311	-	57,62,73	1.29	7 (12%)	67,100,113	1.11	4 (5%)
45	CLA	BA	817	-	64,68,73	1.18	5 (7%)	76,107,113	1.21	8 (10%)
45	CLA	AB	829	-	69,73,73	1.18	7 (10%)	82,113,113	1.18	10 (12%)
45	CLA	BA	810	-	69,73,73	1.16	7 (10%)	82,113,113	1.12	6 (7%)
45	CLA	AA	804	-	56,60,73	1.27	8 (14%)	65,97,113	1.34	7 (10%)
49	SF4	AC	102	3	0,12,12	-	-	-		
53	LMG	AG	202	-	38,38,55	1.15	3 (7%)	46,46,63	1.07	2 (4%)
50	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.95	1 (2%)
45	CLA	BB	833	-	47,51,73	1.35	7 (14%)	55,86,113	1.40	5 (9%)
45	CLA	B5	610	47	46,50,73	1.38	7 (15%)	53,85,113	1.25	6 (11%)
52	LUT	A1	317	-	42,43,43	0.95	1 (2%)	51,60,60	1.97	14 (27%)
48	BCR	AB	847	-	41,41,41	0.89	0	56,56,56	2.03	13 (23%)
45	CLA	A1	306	-	53,57,73	1.31	8 (15%)	61,93,113	1.27	4 (6%)
45	CLA	BB	828	-	66,70,73	1.20	8 (12%)	78,109,113	1.34	9 (11%)
45	CLA	AA	811	-	69,73,73	1.16	6 (8%)	82,113,113	1.16	4 (4%)
48	BCR	BA	855	-	41,41,41	0.79	0	56,56,56	2.22	25 (44%)
45	CLA	AA	842	-	69,73,73	1.17	6 (8%)	82,113,113	1.27	9 (10%)
45	CLA	AA	823	-	45,49,73	1.46	7 (15%)	54,84,113	1.25	6 (11%)
45	CLA	B2	603	-	47,52,73	1.40	6 (12%)	55,88,113	1.33	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AF	803	-	46,50,73	1.41	8 (17%)	53,85,113	1.37	4 (7%)
45	CLA	BA	832	-	60,64,73	1.23	6 (10%)	71,102,113	1.19	6 (8%)
45	CLA	BA	822	-	46,50,73	1.37	6 (13%)	53,85,113	1.33	5 (9%)
45	CLA	AB	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.10	5 (6%)
48	BCR	BF	304	-	41,41,41	0.90	1 (2%)	56,56,56	1.93	18 (32%)
45	CLA	BK	201	11	40,44,73	1.57	8 (20%)	51,77,113	1.45	6 (11%)
45	CLA	AK	201	11	38,43,73	1.68	7 (18%)	49,75,113	1.44	7 (14%)
46	PQN	AA	843	-	34,34,34	3.51	10 (29%)	43,45,45	1.71	7 (16%)
54	CHL	A4	306	-	40,54,74	4.22	19 (47%)	34,90,114	3.06	17 (50%)
45	CLA	B2	608	17	49,53,73	1.37	7 (14%)	58,89,113	1.20	5 (8%)
45	CLA	B2	602	17	69,73,73	1.16	9 (13%)	82,113,113	1.17	7 (8%)
45	CLA	AB	802	-	68,72,73	1.29	8 (11%)	83,112,113	1.22	6 (7%)
45	CLA	AB	812	-	58,62,73	1.35	9 (15%)	71,100,113	1.34	7 (9%)
45	CLA	BB	808	2	69,73,73	1.16	8 (11%)	82,113,113	1.22	4 (4%)
45	CLA	AG	201	-	47,52,73	1.41	7 (14%)	55,88,113	1.26	3 (5%)
45	CLA	AA	833	-	69,73,73	1.19	8 (11%)	82,113,113	1.29	8 (9%)
45	CLA	BB	821	-	59,63,73	1.25	8 (13%)	70,101,113	1.07	5 (7%)
45	CLA	AB	842	47	69,73,73	1.15	8 (11%)	82,113,113	1.28	7 (8%)
45	CLA	BL	302	12	49,53,73	1.38	7 (14%)	58,89,113	1.47	8 (13%)
45	CLA	AB	809	-	69,73,73	1.15	7 (10%)	82,113,113	1.25	9 (10%)
45	CLA	BB	807	-	69,73,73	1.16	8 (11%)	82,113,113	1.20	8 (9%)
52	LUT	B1	316	-	42,43,43	1.28	8 (19%)	51,60,60	1.43	10 (19%)
45	CLA	A3	315	-	43,48,73	1.42	6 (13%)	51,83,113	1.20	5 (9%)
45	CLA	BG	201	-	46,50,73	1.37	6 (13%)	53,85,113	1.19	5 (9%)
45	CLA	AA	821	-	69,73,73	1.16	9 (13%)	82,113,113	1.22	8 (9%)
45	CLA	A3	309	14	45,49,73	1.42	8 (17%)	54,84,113	1.28	7 (12%)
48	BCR	BA	848	-	41,41,41	0.83	0	56,56,56	2.03	18 (32%)
45	CLA	BB	817	-	45,50,73	1.37	6 (13%)	52,85,113	1.25	5 (9%)
45	CLA	B5	603	-	48,52,73	1.49	9 (18%)	59,88,113	1.39	5 (8%)
48	BCR	AA	848	-	41,41,41	0.80	1 (2%)	56,56,56	1.99	17 (30%)
53	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
45	CLA	B2	604	-	46,51,73	1.40	7 (15%)	54,86,113	1.20	5 (9%)
45	CLA	AL	303	12	45,49,73	1.42	6 (13%)	54,84,113	1.25	5 (9%)
45	CLA	AA	813	-	69,73,73	1.16	8 (11%)	82,113,113	1.25	5 (6%)
54	CHL	B3	306	-	38,53,74	3.80	18 (47%)	36,89,114	2.88	13 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	A4	311	-	59,64,73	1.25	7 (11%)	69,102,113	1.16	4 (5%)
45	CLA	AF	802	-	61,65,73	1.25	8 (13%)	72,103,113	1.29	7 (9%)
45	CLA	BA	830	-	69,73,73	1.19	8 (11%)	82,113,113	1.10	4 (4%)
45	CLA	AB	814	-	69,73,73	1.18	10 (14%)	82,113,113	1.20	4 (4%)
45	CLA	BB	815	-	69,73,73	1.17	8 (11%)	82,113,113	1.41	9 (10%)
45	CLA	BB	839	-	69,73,73	1.14	8 (11%)	82,113,113	1.16	4 (4%)
55	XAT	B3	316	-	41,47,47	1.03	2 (4%)	54,74,74	2.48	20 (37%)
45	CLA	AG	204	7	49,53,73	1.41	8 (16%)	58,89,113	1.31	4 (6%)
45	CLA	B5	611	18	44,49,73	1.42	7 (15%)	50,84,113	1.27	3 (6%)
45	CLA	AF	804	-	45,49,73	1.42	7 (15%)	54,84,113	1.41	5 (9%)
55	XAT	B2	616	-	41,47,47	1.07	2 (4%)	54,74,74	2.19	20 (37%)
45	CLA	AA	817	-	64,68,73	1.20	6 (9%)	76,107,113	1.21	6 (7%)
45	CLA	B1	307	-	44,48,73	1.47	5 (11%)	51,82,113	1.36	4 (7%)
45	CLA	BA	834	-	69,73,73	1.15	7 (10%)	82,113,113	1.35	7 (8%)
48	BCR	BB	845	-	41,41,41	0.95	1 (2%)	56,56,56	2.22	20 (35%)
45	CLA	B3	307	14	49,53,73	1.37	6 (12%)	58,89,113	1.26	6 (10%)
48	BCR	A4	317	-	41,41,41	0.83	0	56,56,56	2.41	22 (39%)
55	XAT	A3	317	-	41,47,47	1.02	2 (4%)	54,74,74	2.24	18 (33%)
54	CHL	B2	607	-	40,54,74	4.24	20 (50%)	34,90,114	3.04	15 (44%)
45	CLA	BB	819	-	63,67,73	1.20	8 (12%)	74,105,113	1.27	7 (9%)
45	CLA	A1	305	-	59,63,73	1.26	6 (10%)	70,101,113	1.45	6 (8%)
45	CLA	B1	315	-	41,46,73	1.57	8 (19%)	51,81,113	1.35	7 (13%)
48	BCR	BB	847	-	41,41,41	0.89	1 (2%)	56,56,56	1.86	13 (23%)
45	CLA	AH	201	-	64,68,73	1.21	6 (9%)	76,107,113	1.25	8 (10%)
48	BCR	BA	851	-	41,41,41	0.90	1 (2%)	56,56,56	1.98	20 (35%)
45	CLA	A4	309	-	46,50,73	1.35	6 (13%)	53,85,113	1.33	4 (7%)
45	CLA	AA	814	-	49,53,73	1.38	7 (14%)	58,89,113	1.32	6 (10%)
45	CLA	BB	831	-	60,64,73	1.28	8 (13%)	71,102,113	1.20	2 (2%)
45	CLA	B3	302	14	59,63,73	1.25	7 (11%)	70,101,113	1.23	5 (7%)
47	LHG	BA	846	45	26,26,48	1.07	2 (7%)	29,32,54	1.01	1 (3%)
54	CHL	A1	308	13	35,49,74	4.40	18 (51%)	28,84,114	2.61	12 (42%)
45	CLA	B5	601	18	50,54,73	1.34	9 (18%)	59,90,113	1.23	4 (6%)
45	CLA	A1	307	-	44,48,73	1.44	8 (18%)	51,82,113	1.53	8 (15%)
45	CLA	AA	832	-	60,64,73	1.23	6 (10%)	71,102,113	1.23	6 (8%)
45	CLA	A6	601	15	50,54,73	1.34	8 (16%)	59,90,113	1.30	5 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	BA	837	-	55,59,73	1.29	9 (16%)	64,96,113	1.31	6 (9%)
45	CLA	AA	820	-	49,53,73	1.37	8 (16%)	58,89,113	1.30	3 (5%)
45	CLA	AB	807	2	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
45	CLA	AB	815	-	69,73,73	1.13	9 (13%)	82,113,113	1.24	9 (10%)
47	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.06	2 (5%)
45	CLA	AB	838	-	69,73,73	1.13	9 (13%)	82,113,113	1.19	5 (6%)
48	BCR	A1	319	-	41,41,41	0.91	1 (2%)	56,56,56	3.23	21 (37%)
45	CLA	AB	804	-	69,73,73	1.17	10 (14%)	82,113,113	1.57	13 (15%)
45	CLA	B5	609	18	58,62,73	1.26	8 (13%)	68,99,113	1.13	5 (7%)
48	BCR	BB	848	-	41,41,41	0.84	0	56,56,56	2.17	19 (33%)
45	CLA	BB	822	-	45,49,73	1.38	7 (15%)	54,84,113	1.38	5 (9%)
53	LMG	A4	318	-	39,39,55	1.01	3 (7%)	47,47,63	1.41	7 (14%)
45	CLA	AA	816	-	49,53,73	1.39	7 (14%)	58,89,113	1.36	5 (8%)
48	BCR	AF	801	-	41,41,41	0.88	1 (2%)	56,56,56	1.57	10 (17%)
48	BCR	AA	849	-	41,41,41	0.94	2 (4%)	56,56,56	2.08	21 (37%)
45	CLA	AJ	102	10	46,50,73	1.39	7 (15%)	53,85,113	1.28	3 (5%)
45	CLA	AB	811	-	69,73,73	1.16	8 (11%)	82,113,113	1.37	8 (9%)
55	XAT	A6	616	-	41,47,47	1.05	2 (4%)	54,74,74	2.37	21 (38%)
45	CLA	AA	831	-	51,55,73	1.34	8 (15%)	60,91,113	1.27	5 (8%)
45	CLA	A3	302	14	64,68,73	1.20	8 (12%)	76,107,113	1.14	6 (7%)
49	SF4	BA	852	1,2	0,12,12	-	-	-		
45	CLA	BA	827	-	69,73,73	1.15	7 (10%)	82,113,113	1.13	5 (6%)
45	CLA	B3	308	14	45,49,73	1.38	7 (15%)	54,84,113	1.25	4 (7%)
55	XAT	B1	317	-	41,47,47	1.00	2 (4%)	54,74,74	2.30	19 (35%)
49	SF4	AA	850	1,2	0,12,12	-	-	-		
54	CHL	A6	607	-	37,51,74	4.37	18 (48%)	30,86,114	3.17	15 (50%)
47	LHG	A6	618	45	35,35,48	1.06	2 (5%)	38,41,54	0.98	2 (5%)
45	CLA	AB	832	-	69,73,73	1.16	6 (8%)	82,113,113	1.18	6 (7%)
45	CLA	AA	812	-	58,62,73	1.28	8 (13%)	68,99,113	1.33	6 (8%)
46	PQN	AB	843	-	34,34,34	3.48	10 (29%)	43,45,45	1.78	6 (13%)
45	CLA	AB	803	-	69,73,73	1.16	8 (11%)	82,113,113	1.13	6 (7%)
48	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.39	20 (35%)
45	CLA	B1	314	-	64,68,73	1.23	7 (10%)	76,107,113	1.09	5 (6%)
45	CLA	AA	818	-	63,67,73	1.22	7 (11%)	74,105,113	1.23	7 (9%)
54	CHL	B2	601	17	47,61,74	3.98	20 (42%)	41,98,114	2.91	15 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
54	CHL	B2	606	-	37,51,74	4.39	18 (48%)	30,86,114	3.15	17 (56%)
45	CLA	B1	311	13	63,67,73	1.20	7 (11%)	75,106,113	1.09	5 (6%)
48	BCR	BA	850	-	41,41,41	0.79	0	56,56,56	2.11	14 (25%)
47	LHG	A1	301	45	37,37,48	1.07	2 (5%)	40,43,54	0.99	3 (7%)
45	CLA	AB	805	-	45,49,73	1.40	6 (13%)	54,84,113	1.28	6 (11%)
54	CHL	B2	605	-	36,50,74	4.09	18 (50%)	31,85,114	3.17	14 (45%)
47	LHG	B5	618	45	29,29,48	1.17	2 (6%)	32,35,54	1.22	3 (9%)
45	CLA	AA	826	-	63,67,73	1.21	9 (14%)	74,105,113	1.14	5 (6%)
45	CLA	BB	802	-	69,73,73	1.18	9 (13%)	82,113,113	1.32	8 (9%)
45	CLA	AB	833	-	69,73,73	1.15	5 (7%)	82,113,113	1.13	7 (8%)
45	CLA	AB	839	-	51,55,73	1.34	7 (13%)	60,91,113	1.39	7 (11%)
45	CLA	AB	824	-	47,51,73	1.37	8 (17%)	55,86,113	1.45	7 (12%)
45	CLA	A1	309	-	47,52,73	1.41	7 (14%)	55,88,113	1.23	5 (9%)
47	LHG	B3	318	45	22,22,48	1.51	2 (9%)	25,28,54	1.43	2 (8%)
45	CLA	AB	827	-	66,70,73	1.19	9 (13%)	78,109,113	1.36	9 (11%)
47	LHG	B1	301	45	37,37,48	1.09	2 (5%)	40,43,54	1.03	3 (7%)
45	CLA	A3	304	-	45,50,73	1.53	9 (20%)	55,86,113	1.28	5 (9%)
45	CLA	BB	834	-	69,73,73	1.16	5 (7%)	82,113,113	1.25	7 (8%)
45	CLA	BB	820	-	64,68,73	1.19	7 (10%)	76,107,113	1.45	9 (11%)
45	CLA	A3	312	-	57,62,73	1.28	7 (12%)	67,100,113	1.23	5 (7%)
47	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.90	2 (3%)
45	CLA	BA	805	-	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
45	CLA	A4	302	15	48,52,73	1.49	8 (16%)	59,88,113	1.43	7 (11%)
45	CLA	A3	314	-	40,44,73	1.49	8 (20%)	49,77,113	1.21	4 (8%)
45	CLA	BB	811	2	69,73,73	1.17	8 (11%)	82,113,113	1.21	7 (8%)
45	CLA	AA	819	-	69,73,73	1.17	8 (11%)	82,113,113	1.26	5 (6%)
45	CLA	A3	311	14	47,51,73	1.39	6 (12%)	55,86,113	1.30	5 (9%)
45	CLA	BA	815	-	46,50,73	1.38	5 (10%)	53,85,113	1.36	5 (9%)
45	CLA	BB	816	-	68,72,73	1.16	8 (11%)	81,112,113	1.20	7 (8%)
48	BCR	AJ	101	-	41,41,41	0.90	1 (2%)	56,56,56	2.00	17 (30%)
45	CLA	B2	609	17	59,63,73	1.26	8 (13%)	70,101,113	1.20	7 (10%)
45	CLA	AB	825	-	69,73,73	1.19	11 (15%)	82,113,113	1.23	7 (8%)
45	CLA	A4	301	15	64,68,73	1.18	8 (12%)	76,107,113	1.21	7 (9%)
45	CLA	B3	312	-	43,48,73	1.44	7 (16%)	51,83,113	1.19	5 (9%)
45	CLA	AA	830	-	69,73,73	1.20	7 (10%)	82,113,113	1.18	5 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
45	CLA	AA	809	1	54,58,73	1.35	8 (14%)	64,95,113	1.33	8 (12%)
45	CLA	BA	814	-	49,53,73	1.38	8 (16%)	58,89,113	1.33	4 (6%)
50	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
48	BCR	AB	846	-	41,41,41	0.88	0	56,56,56	1.99	16 (28%)
45	CLA	AB	822	-	51,55,73	1.34	7 (13%)	60,91,113	1.18	3 (5%)
54	CHL	B2	614	17	37,51,74	4.38	18 (48%)	30,86,114	3.29	12 (40%)
45	CLA	BA	820	-	49,53,73	1.36	7 (14%)	58,89,113	1.33	3 (5%)
45	CLA	BJ	102	10	46,50,73	1.39	7 (15%)	53,85,113	1.26	3 (5%)
45	CLA	AA	825	-	69,73,73	1.19	9 (13%)	82,113,113	1.18	3 (3%)
47	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.11	3 (6%)
45	CLA	AB	810	2	69,73,73	1.17	8 (11%)	82,113,113	1.22	4 (4%)
45	CLA	BB	827	-	66,70,73	1.17	7 (10%)	78,109,113	1.13	6 (7%)
45	CLA	BA	831	-	51,55,73	1.36	8 (15%)	60,91,113	1.33	8 (13%)
45	CLA	AB	806	-	69,73,73	1.17	8 (11%)	82,113,113	1.20	5 (6%)
45	CLA	B1	304	13	65,69,73	1.19	7 (10%)	77,108,113	1.25	5 (6%)
48	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	20 (35%)
45	CLA	BA	829	-	69,73,73	1.20	10 (14%)	82,113,113	1.21	7 (8%)
48	BCR	A3	318	-	41,41,41	1.00	1 (2%)	56,56,56	2.85	19 (33%)
45	CLA	B5	608	18	48,52,73	1.40	8 (16%)	57,88,113	1.26	5 (8%)
45	CLA	AA	837	-	55,59,73	1.28	8 (14%)	64,96,113	1.43	9 (14%)
55	XAT	B5	615	-	41,47,47	1.04	2 (4%)	54,74,74	2.21	18 (33%)
52	LUT	A4	315	-	42,43,43	0.96	2 (4%)	51,60,60	1.95	17 (33%)
51	DGD	AB	851	-	67,67,67	0.81	2 (2%)	81,81,81	1.00	4 (4%)
48	BCR	AA	845	-	41,41,41	1.04	2 (4%)	56,56,56	1.93	13 (23%)
45	CLA	BK	202	-	49,53,73	1.37	6 (12%)	58,89,113	1.30	5 (8%)
45	CLA	BF	301	-	58,63,73	1.25	6 (10%)	71,100,113	1.20	6 (8%)
45	CLA	BA	826	-	57,61,73	1.26	8 (14%)	67,98,113	1.24	8 (11%)
45	CLA	AB	818	-	63,67,73	1.22	8 (12%)	74,105,113	1.21	7 (9%)
45	CLA	AB	831	-	47,51,73	1.39	9 (19%)	55,86,113	1.18	5 (9%)
45	CLA	B1	313	13	49,53,73	1.38	7 (14%)	58,89,113	1.33	3 (5%)
45	CLA	BB	810	-	69,73,73	1.14	8 (11%)	82,113,113	1.22	9 (10%)
45	CLA	A3	313	-	43,48,73	1.44	7 (16%)	51,83,113	1.25	5 (9%)
48	BCR	BG	203	-	41,41,41	0.93	2 (4%)	56,56,56	6.70	27 (48%)
45	CLA	B2	611	17	48,52,73	1.41	7 (14%)	57,88,113	1.26	4 (7%)
48	BCR	BI	101	-	41,41,41	0.96	2 (4%)	56,56,56	2.17	21 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	BCR	B2	617	-	41,41,41	0.91	1 (2%)	56,56,56	2.51	23 (41%)
45	CLA	BA	823	-	45,49,73	1.40	6 (13%)	54,84,113	1.28	7 (12%)
45	CLA	BA	812	-	58,62,73	1.26	7 (12%)	68,99,113	1.26	5 (7%)
45	CLA	BB	801	-	69,73,73	1.16	8 (11%)	82,113,113	1.33	9 (10%)
45	CLA	AA	835	-	47,52,73	1.41	8 (17%)	55,88,113	1.26	4 (7%)
45	CLA	BG	202	7	49,53,73	1.40	7 (14%)	58,89,113	1.42	5 (8%)
52	LUT	AF	806	-	42,43,43	1.02	2 (4%)	51,60,60	1.75	12 (23%)
45	CLA	A6	611	47	40,45,73	2.55	9 (22%)	46,76,113	1.50	8 (17%)
45	CLA	AA	841	-	69,73,73	1.18	8 (11%)	82,113,113	1.24	5 (6%)
48	BCR	AI	101	-	41,41,41	0.95	2 (4%)	56,56,56	2.06	20 (35%)
48	BCR	BL	306	-	41,41,41	0.91	2 (4%)	56,56,56	10.70	27 (48%)
45	CLA	B3	309	47	43,48,73	1.46	6 (13%)	49,83,113	1.17	3 (6%)
45	CLA	A1	310	13	44,48,73	1.51	8 (18%)	55,83,113	1.42	7 (12%)
45	CLA	BB	814	-	47,51,73	1.37	8 (17%)	55,86,113	1.25	4 (7%)
45	CLA	BH	201	-	64,68,73	1.23	6 (9%)	76,107,113	1.19	6 (7%)
45	CLA	BB	813	-	58,62,73	1.34	8 (13%)	71,100,113	1.30	7 (9%)

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
45	CLA	AK	203	-	1/1/11/20	10/17/93/115	-
45	CLA	BB	805	-	1/1/15/20	13/39/115/115	-
45	CLA	AA	828	-	1/1/15/20	14/39/115/115	-
45	CLA	AK	202	-	1/1/11/20	8/15/91/115	-
45	CLA	BA	811	-	1/1/15/20	16/39/115/115	-
50	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
54	CHL	A6	608	-	3/3/17/26	8/19/117/137	-
45	CLA	AB	823	-	-	17/39/115/115	-
54	CHL	B1	303	13	3/3/17/26	3/19/117/137	-
47	LHG	B1	318	45	-	12/46/46/53	-
52	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
45	CLA	A6	612	16	1/1/11/20	8/13/89/115	-
45	CLA	B3	304	-	1/1/10/20	6/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
47	LHG	AJ	104	-	-	15/44/44/53	-
45	CLA	BB	837	-	1/1/10/20	5/12/88/115	-
48	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	A4	310	15	1/1/10/20	6/10/86/115	-
48	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
48	BCR	AK	204	-	-	6/29/63/63	0/2/2/2
45	CLA	BA	844	47	1/1/10/20	4/10/86/115	-
45	CLA	AA	805	-	1/1/15/20	15/39/115/115	-
45	CLA	AB	830	-	1/1/13/20	9/29/105/115	-
45	CLA	BB	823	-	1/1/11/20	4/16/92/115	-
49	SF4	BC	102	3	-	-	0/6/5/5
45	CLA	BB	812	-	1/1/15/20	11/39/115/115	-
45	CLA	BB	843	47	1/1/15/20	13/39/115/115	-
45	CLA	B5	612	18	1/1/13/20	6/30/106/115	-
47	LHG	F	801	-	-	20/41/41/53	-
45	CLA	AB	813	-	1/1/10/20	3/13/89/115	-
56	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
54	CHL	A1	303	13	3/3/17/26	3/21/119/137	-
46	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
45	CLA	B3	301	14	1/1/14/20	5/33/109/115	-
45	CLA	BB	836	-	-	11/33/109/115	-
45	CLA	BB	804	-	1/1/15/20	13/39/115/115	-
48	BCR	BA	847	-	-	4/29/63/63	0/2/2/2
45	CLA	BB	832	-	1/1/10/20	5/13/89/115	-
47	LHG	B1	302	-	-	12/40/40/53	-
45	CLA	B2	613	-	1/1/10/20	1/13/89/115	-
48	BCR	BA	849	-	-	4/29/63/63	0/2/2/2
54	CHL	A6	606	-	3/3/15/26	2/10/108/137	-
45	CLA	A4	303	-	1/1/11/20	4/11/87/115	-
45	CLA	BA	838	-	1/1/12/20	11/27/99/115	-
45	CLA	A3	306	14	1/1/10/20	0/10/86/115	-
45	CLA	B1	310	13	1/1/10/20	2/6/82/115	-
48	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
45	CLA	BA	840	-	1/1/15/20	13/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BA	824	-	1/1/13/20	9/27/103/115	-
45	CLA	AA	824	-	1/1/13/20	9/25/101/115	-
52	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
45	CLA	BA	841	-	1/1/15/20	17/39/115/115	-
55	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	802	-	1/1/15/20	5/39/115/115	-
45	CLA	AB	819	-	1/1/14/20	14/33/109/115	-
45	CLA	A3	308	14	1/1/11/20	6/15/91/115	-
45	CLA	B5	604	-	1/1/11/20	2/11/87/115	-
50	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
57	FES	c	301	28	-	-	0/1/1/1
45	CLA	A1	316	13	1/1/11/20	8/11/87/115	-
54	CHL	B5	607	-	3/3/16/26	4/13/111/137	-
45	CLA	BA	842	-	1/1/15/20	13/39/115/115	-
45	CLA	BA	828	-	1/1/15/20	14/39/115/115	-
45	CLA	BL	304	-	1/1/10/20	5/13/89/115	-
45	CLA	BB	818	-	1/1/13/20	8/27/103/115	-
48	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	830	-	1/1/15/20	11/39/115/115	-
47	LHG	a	501	-	-	16/33/33/53	-
45	CLA	AB	840	-	1/1/15/20	7/39/115/115	-
49	SF4	K	301	39	-	-	0/6/5/5
48	BCR	A6	617	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	836	1	-	7/15/91/115	-
45	CLA	AB	816	-	1/1/10/20	2/13/89/115	-
45	CLA	BA	825	-	1/1/15/20	15/39/115/115	-
45	CLA	AL	305	-	1/1/10/20	5/12/88/115	-
49	SF4	I	201	37	-	-	0/6/5/5
48	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
48	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	829	-	1/1/15/20	15/39/115/115	-
45	CLA	BA	813	-	1/1/15/20	14/39/115/115	-
45	CLA	BA	821	-	-	11/39/115/115	-
45	CLA	BA	839	-	-	7/23/99/115	-
49	SF4	I	202	37	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
45	CLA	B3	310	14	1/1/10/20	2/13/89/115	-
48	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
48	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
47	LHG	A3	319	45	-	14/26/26/53	-
45	CLA	BA	835	-	1/1/11/20	4/15/91/115	-
45	CLA	BA	836	1	-	6/15/91/115	-
45	CLA	A6	614	-	1/1/10/20	4/13/89/115	-
45	CLA	AB	828	-	1/1/15/20	12/39/115/115	-
45	CLA	AB	826	-	1/1/14/20	6/36/112/115	-
45	CLA	AB	801	-	1/1/15/20	16/39/115/115	-
45	CLA	B1	312	47	1/1/10/20	0/4/80/115	-
48	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
45	CLA	A3	305	-	1/1/10/20	5/10/86/115	-
45	CLA	BB	806	-	1/1/10/20	2/10/86/115	-
45	CLA	A3	310	47	1/1/9/20	2/2/78/115	-
48	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
47	LHG	B2	618	45	-	22/39/39/53	-
45	CLA	BB	825	-	1/1/11/20	6/15/91/115	-
45	CLA	BB	838	-	1/1/12/20	4/21/97/115	-
45	CLA	AB	808	-	-	4/22/98/115	-
45	CLA	AB	835	-	-	7/33/109/115	-
45	CLA	B3	305	-	1/1/10/20	2/10/86/115	-
45	CLA	AB	821	-	1/1/12/20	7/21/97/115	-
45	CLA	B5	602	18	-	11/33/109/115	-
45	CLA	A1	304	13	1/1/13/20	9/33/109/115	-
45	CLA	A1	312	47	1/1/10/20	0/4/80/115	-
45	CLA	BB	841	-	1/1/15/20	6/39/115/115	-
45	CLA	AA	838	-	-	8/27/103/115	-
45	CLA	BA	806	1	1/1/15/20	18/39/115/115	-
45	CLA	A6	604	-	1/1/10/20	2/11/87/115	-
45	CLA	A6	603	16	1/1/15/20	11/39/115/115	-
45	CLA	A1	314	-	1/1/15/20	12/37/113/115	-
45	CLA	BB	809	-	-	3/24/100/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A1	311	13	1/1/14/20	2/31/107/115	-
48	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
54	CHL	A4	304	-	3/3/15/26	1/8/106/137	-
45	CLA	BB	826	-	1/1/15/20	11/39/115/115	-
48	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	808	1	1/1/15/20	10/39/115/115	-
45	CLA	B3	303	-	1/1/11/20	2/9/85/115	-
45	CLA	BB	842	-	1/1/15/20	11/39/115/115	-
50	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
45	CLA	BF	303	-	1/1/10/20	2/10/86/115	-
49	SF4	AC	101	3	-	-	0/6/5/5
52	LUT	B3	315	-	-	3/29/67/67	0/2/2/2
45	CLA	A6	610	16	1/1/13/20	6/27/103/115	-
45	CLA	A1	315	-	1/1/10/20	0/4/80/115	-
45	CLA	BA	807	-	1/1/12/20	3/21/97/115	-
45	CLA	BA	833	-	1/1/15/20	15/39/115/115	-
45	CLA	AA	807	-	1/1/12/20	3/21/97/115	-
47	LHG	A3	301	-	-	10/40/40/53	-
45	CLA	B2	610	47	1/1/7/20	5/10/70/115	-
45	CLA	B2	612	17	1/1/15/20	12/39/115/115	-
45	CLA	AB	836	-	-	3/12/88/115	-
45	CLA	BA	804	-	-	4/24/100/115	-
50	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
45	CLA	BB	824	-	-	15/39/115/115	-
45	CLA	A4	307	15	1/1/11/20	2/15/91/115	-
45	CLA	BB	835	-	1/1/15/20	16/39/115/115	-
47	LHG	A1	320	45	-	15/53/53/53	-
48	BCR	AL	302	-	-	5/29/63/63	0/2/2/2
45	CLA	A6	605	-	1/1/10/20	4/12/88/115	-
45	CLA	AB	837	-	1/1/12/20	6/21/97/115	-
48	BCR	AI	102	-	-	3/29/63/63	0/2/2/2
45	CLA	AA	803	-	1/1/15/20	14/39/115/115	-
56	SQD	e	301	-	-	10/29/49/69	0/1/1/1
45	CLA	BA	818	-	-	8/29/105/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AL	304	-	-	9/33/109/115	-
48	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
45	CLA	AA	815	-	-	2/12/88/115	-
46	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
50	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
45	CLA	AA	839	-	-	3/24/100/115	-
50	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
45	CLA	B3	313	-	1/1/8/20	2/2/74/115	-
45	CLA	BB	840	-	-	4/18/94/115	-
45	CLA	BK	203	-	1/1/11/20	4/17/93/115	-
54	CHL	B1	308	-	3/3/15/26	0/8/106/137	-
45	CLA	BL	303	-	-	9/33/109/115	-
45	CLA	AA	810	-	1/1/14/20	10/39/111/115	-
45	CLA	BA	803	-	1/1/15/20	17/39/115/115	-
48	BCR	B3	317	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	817	-	1/1/13/20	7/27/103/115	-
45	CLA	A1	313	13	1/1/11/20	5/15/91/115	-
45	CLA	AG	203	-	1/1/10/20	2/12/88/115	-
45	CLA	AA	840	-	1/1/15/20	13/39/115/115	-
45	CLA	A3	303	14	1/1/13/20	10/27/103/115	-
45	CLA	BA	801	-	1/1/15/20	9/39/115/115	-
54	CHL	A6	602	16	3/3/17/26	5/22/120/137	-
45	CLA	B1	305	-	1/1/12/20	6/25/101/115	-
45	CLA	B5	613	-	1/1/11/20	7/15/91/115	-
52	LUT	A6	615	-	-	0/29/67/67	0/2/2/2
54	CHL	A4	314	15	3/3/15/26	0/10/106/137	-
49	SF4	BC	101	3	-	-	0/6/5/5
45	CLA	A4	312	-	1/1/11/20	5/15/91/115	-
54	CHL	B5	606	-	3/3/15/26	4/8/104/137	-
45	CLA	AA	822	-	1/1/10/20	6/12/88/115	-
47	LHG	BA	845	-	-	27/53/53/53	-
54	CHL	A3	307	-	3/3/16/26	4/13/111/137	-
48	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
45	CLA	BA	808	1	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
45	CLA	BF	302	-	1/1/10/20	2/12/88/115	-
45	CLA	AA	834	-	-	15/39/115/115	-
45	CLA	AA	827	-	1/1/15/20	15/39/115/115	-
48	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
45	CLA	A6	613	16	1/1/14/20	7/37/113/115	-
45	CLA	BB	829	-	1/1/15/20	17/39/115/115	-
45	CLA	A4	308	15	1/1/12/20	6/26/102/115	-
45	CLA	AA	801	-	1/1/15/20	13/39/115/115	-
48	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
45	CLA	AA	806	1	1/1/15/20	12/39/115/115	-
45	CLA	BA	816	-	1/1/11/20	4/15/91/115	-
48	BCR	AA	852	-	-	5/29/63/63	0/2/2/2
45	CLA	AB	820	-	1/1/13/20	8/27/103/115	-
45	CLA	B1	309	-	-	4/13/89/115	-
48	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
45	CLA	BA	809	1	-	9/21/97/115	-
54	CHL	A4	305	-	3/3/15/26	0/10/106/137	-
45	CLA	AA	802	-	1/1/15/20	7/39/115/115	-
45	CLA	B1	306	-	1/1/10/20	3/10/86/115	-
45	CLA	AB	841	-	1/1/15/20	10/39/115/115	-
45	CLA	A4	313	-	1/1/12/20	9/21/97/115	-
52	LUT	B2	615	-	-	0/29/67/67	0/2/2/2
45	CLA	BA	819	-	1/1/15/20	11/39/115/115	-
45	CLA	A6	609	16	1/1/11/20	3/15/91/115	-
54	CHL	B5	605	-	3/3/15/26	2/8/106/137	-
45	CLA	B3	314	-	1/1/10/20	0/8/84/115	-
55	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
45	CLA	B3	311	-	1/1/13/20	8/25/101/115	-
45	CLA	BA	817	-	-	8/33/109/115	-
45	CLA	AB	829	-	1/1/15/20	14/39/115/115	-
45	CLA	BA	810	-	1/1/15/20	10/39/115/115	-
45	CLA	AA	804	-	-	7/24/100/115	-
49	SF4	AC	102	3	-	-	0/6/5/5
53	LMG	AG	202	-	-	5/33/53/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
50	LMU	AB	852	-	-	11/21/61/61	0/2/2/2
45	CLA	BB	833	-	-	3/13/89/115	-
45	CLA	B5	610	47	-	6/12/88/115	-
52	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
48	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
45	CLA	A1	306	-	1/1/11/20	7/20/96/115	-
45	CLA	BB	828	-	1/1/14/20	9/36/112/115	-
45	CLA	AA	811	-	1/1/15/20	13/39/115/115	-
48	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
45	CLA	AA	842	-	1/1/15/20	19/39/115/115	-
45	CLA	AA	823	-	1/1/10/20	4/10/86/115	-
45	CLA	B2	603	-	1/1/11/20	4/13/89/115	-
45	CLA	AF	803	-	1/1/10/20	3/12/88/115	-
45	CLA	BA	832	-	-	6/29/105/115	-
45	CLA	BA	822	-	1/1/10/20	6/12/88/115	-
45	CLA	AB	834	-	1/1/15/20	16/39/115/115	-
48	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
45	CLA	BK	201	11	1/1/8/20	0/2/74/115	-
45	CLA	AK	201	11	1/1/8/20	0/2/74/115	-
46	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
54	CHL	A4	306	-	3/3/16/26	4/15/113/137	-
45	CLA	B2	608	17	1/1/11/20	2/15/91/115	-
45	CLA	B2	602	17	1/1/15/20	11/39/115/115	-
45	CLA	AB	802	-	1/1/15/20	14/37/113/115	-
45	CLA	AB	812	-	1/1/13/20	8/25/101/115	-
45	CLA	BB	808	2	1/1/15/20	10/39/115/115	-
45	CLA	AG	201	-	1/1/11/20	5/13/89/115	-
45	CLA	AA	833	-	1/1/15/20	19/39/115/115	-
45	CLA	BB	821	-	1/1/13/20	7/27/103/115	-
45	CLA	AB	842	47	1/1/15/20	19/39/115/115	-
45	CLA	BL	302	12	-	6/15/91/115	-
45	CLA	AB	809	-	1/1/15/20	14/39/115/115	-
45	CLA	BB	807	-	1/1/15/20	11/39/115/115	-
52	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
45	CLA	A3	315	-	1/1/10/20	0/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BG	201	-	1/1/10/20	6/12/88/115	-
45	CLA	AA	821	-	1/1/15/20	13/39/115/115	-
45	CLA	A3	309	14	1/1/10/20	4/10/86/115	-
48	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	BB	817	-	1/1/10/20	3/11/87/115	-
45	CLA	B5	603	-	1/1/11/20	4/13/89/115	-
48	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
53	LMG	A1	321	-	-	16/39/59/70	0/1/1/1
45	CLA	B2	604	-	1/1/10/20	4/12/88/115	-
45	CLA	AL	303	12	1/1/10/20	6/10/86/115	-
45	CLA	AA	813	-	1/1/15/20	16/39/115/115	-
54	CHL	B3	306	-	3/3/16/26	5/13/111/137	-
45	CLA	A4	311	-	1/1/13/20	7/28/104/115	-
45	CLA	AF	802	-	1/1/13/20	9/30/106/115	-
45	CLA	BA	830	-	1/1/15/20	12/39/115/115	-
45	CLA	AB	814	-	1/1/15/20	14/39/115/115	-
45	CLA	BB	815	-	1/1/15/20	18/39/115/115	-
45	CLA	BB	839	-	-	8/39/115/115	-
55	XAT	B3	316	-	-	0/31/93/93	0/4/4/4
45	CLA	AG	204	7	1/1/11/20	6/15/91/115	-
45	CLA	B5	611	18	1/1/10/20	3/10/86/115	-
45	CLA	AF	804	-	1/1/10/20	2/10/86/115	-
55	XAT	B2	616	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	817	-	1/1/14/20	5/33/109/115	-
45	CLA	B1	307	-	1/1/9/20	2/10/82/115	-
45	CLA	BA	834	-	-	11/39/115/115	-
48	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
45	CLA	B3	307	14	1/1/11/20	2/15/91/115	-
48	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
55	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
54	CHL	B2	607	-	3/3/16/26	4/15/113/137	-
45	CLA	BB	819	-	1/1/13/20	15/32/108/115	-
45	CLA	A1	305	-	1/1/13/20	7/27/103/115	-
45	CLA	B1	315	-	1/1/10/20	0/4/80/115	-
48	BCR	BB	847	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AH	201	-	1/1/14/20	11/33/109/115	-
48	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
45	CLA	A4	309	-	1/1/10/20	4/12/88/115	-
45	CLA	AA	814	-	1/1/11/20	4/15/91/115	-
45	CLA	BB	831	-	1/1/13/20	6/29/105/115	-
45	CLA	B3	302	14	1/1/13/20	6/27/103/115	-
47	LHG	BA	846	45	-	7/30/30/53	-
54	CHL	A1	308	13	3/3/15/26	2/8/106/137	-
45	CLA	B5	601	18	1/1/11/20	8/17/93/115	-
45	CLA	A1	307	-	1/1/9/20	4/10/82/115	-
45	CLA	AA	832	-	1/1/13/20	7/29/105/115	-
45	CLA	A6	601	15	1/1/11/20	1/17/93/115	-
45	CLA	BA	837	-	1/1/12/20	2/23/99/115	-
45	CLA	AA	820	-	1/1/11/20	6/15/91/115	-
45	CLA	AB	807	2	1/1/15/20	10/39/115/115	-
45	CLA	AB	815	-	1/1/15/20	16/39/115/115	-
47	LHG	A1	302	-	-	16/40/40/53	-
45	CLA	AB	838	-	-	7/39/115/115	-
48	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
45	CLA	AB	804	-	1/1/15/20	16/39/115/115	-
45	CLA	B5	609	18	1/1/12/20	4/26/102/115	-
48	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	822	-	1/1/10/20	3/10/86/115	-
53	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
45	CLA	AA	816	-	1/1/11/20	6/15/91/115	-
48	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
48	BCR	AA	849	-	-	7/29/63/63	0/2/2/2
45	CLA	AJ	102	10	1/1/10/20	3/12/88/115	-
45	CLA	AB	811	-	1/1/15/20	12/39/115/115	-
55	XAT	A6	616	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	831	-	1/1/11/20	10/18/94/115	-
45	CLA	A3	302	14	1/1/14/20	8/33/109/115	-
49	SF4	BA	852	1,2	-	-	0/6/5/5
45	CLA	BA	827	-	1/1/15/20	12/39/115/115	-
45	CLA	B3	308	14	1/1/10/20	4/10/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
55	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
49	SF4	AA	850	1,2	-	-	0/6/5/5
54	CHL	A6	607	-	3/3/15/26	4/12/110/137	-
47	LHG	A6	618	45	-	17/40/40/53	-
45	CLA	AB	832	-	-	9/39/115/115	-
45	CLA	AA	812	-	1/1/12/20	8/26/102/115	-
46	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
45	CLA	AB	803	-	1/1/15/20	17/39/115/115	-
54	CHL	B2	601	17	3/3/17/26	7/24/122/137	-
45	CLA	B1	314	-	1/1/14/20	8/33/109/115	-
54	CHL	B2	606	-	3/3/15/26	2/12/110/137	-
45	CLA	AA	818	-	-	8/32/108/115	-
48	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	B1	311	13	1/1/14/20	3/31/107/115	-
48	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
47	LHG	A1	301	45	-	11/42/42/53	-
45	CLA	AB	805	-	1/1/10/20	2/10/86/115	-
54	CHL	B2	605	-	3/3/15/26	4/10/108/137	-
47	LHG	B5	618	45	-	11/34/34/53	-
45	CLA	AA	826	-	1/1/13/20	11/32/108/115	-
45	CLA	BB	802	-	1/1/15/20	13/39/115/115	-
45	CLA	AB	833	-	1/1/15/20	9/39/115/115	-
45	CLA	AB	839	-	1/1/11/20	3/18/94/115	-
45	CLA	AB	824	-	1/1/10/20	3/13/89/115	-
45	CLA	A1	309	-	1/1/11/20	9/13/89/115	-
47	LHG	B3	318	45	-	11/26/26/53	-
45	CLA	AB	827	-	1/1/14/20	11/36/112/115	-
47	LHG	B1	301	45	-	7/42/42/53	-
45	CLA	A3	304	-	1/1/11/20	0/9/85/115	-
45	CLA	BB	834	-	-	11/39/115/115	-
45	CLA	BB	820	-	1/1/14/20	12/33/109/115	-
45	CLA	A3	312	-	1/1/13/20	11/25/101/115	-
47	LHG	AA	844	-	-	16/53/53/53	-
45	CLA	BA	805	-	1/1/15/20	19/39/115/115	-
45	CLA	A4	302	15	1/1/11/20	6/13/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A3	314	-	1/1/8/20	2/2/74/115	-
45	CLA	BB	811	2	1/1/15/20	14/39/115/115	-
45	CLA	AA	819	-	1/1/15/20	13/39/115/115	-
45	CLA	A3	311	14	1/1/10/20	1/13/89/115	-
45	CLA	BB	816	-	1/1/15/20	13/37/113/115	-
45	CLA	BA	815	-	-	2/12/88/115	-
48	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
45	CLA	B2	609	17	1/1/13/20	8/27/103/115	-
45	CLA	AB	825	-	1/1/15/20	13/39/115/115	-
45	CLA	A4	301	15	1/1/14/20	8/33/109/115	-
45	CLA	B3	312	-	1/1/10/20	2/8/84/115	-
45	CLA	AA	830	-	1/1/15/20	12/39/115/115	-
45	CLA	AA	809	1	1/1/12/20	6/21/97/115	-
45	CLA	BA	814	-	1/1/11/20	5/15/91/115	-
50	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
48	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	822	-	1/1/11/20	6/18/94/115	-
54	CHL	B2	614	17	3/3/15/26	0/12/110/137	-
45	CLA	BA	820	-	1/1/11/20	6/15/91/115	-
45	CLA	BJ	102	10	1/1/10/20	2/12/88/115	-
45	CLA	AA	825	-	1/1/15/20	9/39/115/115	-
47	LHG	BF	305	-	-	17/49/49/53	-
45	CLA	AB	810	2	1/1/15/20	13/39/115/115	-
45	CLA	BB	827	-	-	8/36/112/115	-
45	CLA	BA	831	-	1/1/11/20	8/18/94/115	-
45	CLA	AB	806	-	1/1/15/20	13/39/115/115	-
45	CLA	B1	304	13	1/1/14/20	8/35/111/115	-
48	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
45	CLA	BA	829	-	1/1/15/20	11/39/115/115	-
48	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
45	CLA	B5	608	18	1/1/11/20	4/13/89/115	-
45	CLA	AA	837	-	1/1/12/20	6/23/99/115	-
55	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
52	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
51	DGD	AB	851	-	-	21/55/95/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
45	CLA	BK	202	-	1/1/11/20	7/15/91/115	-
45	CLA	BF	301	-	1/1/12/20	8/26/102/115	-
45	CLA	BA	826	-	-	5/25/101/115	-
45	CLA	AB	818	-	1/1/13/20	12/32/108/115	-
45	CLA	AB	831	-	1/1/10/20	4/13/89/115	-
45	CLA	B1	313	13	1/1/11/20	4/15/91/115	-
45	CLA	BB	810	-	1/1/15/20	11/39/115/115	-
45	CLA	A3	313	-	-	3/8/84/115	-
48	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
45	CLA	B2	611	17	1/1/11/20	7/13/89/115	-
48	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
48	BCR	B2	617	-	-	0/29/63/63	0/2/2/2
45	CLA	BA	823	-	1/1/10/20	4/10/86/115	-
45	CLA	BA	812	-	1/1/12/20	6/26/102/115	-
45	CLA	BB	801	-	1/1/15/20	14/39/115/115	-
45	CLA	AA	835	-	1/1/11/20	2/13/89/115	-
45	CLA	BG	202	7	1/1/11/20	4/15/91/115	-
52	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
45	CLA	A6	611	47	1/1/7/20	4/10/70/115	-
45	CLA	AA	841	-	-	11/39/115/115	-
48	BCR	AI	101	-	-	6/29/63/63	0/2/2/2
48	BCR	BL	306	-	-	15/29/63/63	0/2/2/2
45	CLA	B3	309	47	1/1/10/20	2/8/84/115	-
45	CLA	A1	310	13	1/1/10/20	2/8/84/115	-
45	CLA	BB	814	-	1/1/10/20	0/13/89/115	-
45	CLA	BH	201	-	1/1/14/20	12/33/109/115	-
45	CLA	BB	813	-	1/1/13/20	4/25/101/115	-

All (2683) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	611	CLA	C1A-NA	12.82	1.40	1.29
45	B2	610	CLA	C1A-NA	12.33	1.40	1.29
54	B1	308	CHL	C2C-C3C	12.01	1.48	1.36
54	A4	314	CHL	C2C-C3C	11.65	1.47	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	303	CHL	C2C-C3C	11.52	1.47	1.36
54	B2	601	CHL	C2C-C3C	11.49	1.47	1.36
54	A6	602	CHL	C2C-C3C	11.47	1.47	1.36
54	B2	606	CHL	C2C-C3C	11.41	1.47	1.36
54	A1	308	CHL	C2C-C3C	11.30	1.47	1.36
54	B2	614	CHL	C2C-C3C	11.21	1.47	1.36
54	B2	607	CHL	C2C-C3C	11.02	1.47	1.36
54	A6	607	CHL	C2C-C3C	11.01	1.47	1.36
54	B1	303	CHL	C2C-C3C	10.94	1.47	1.36
54	A4	306	CHL	C2C-C3C	10.81	1.46	1.36
54	B1	308	CHL	C3B-C4B	10.31	1.51	1.41
54	B2	607	CHL	C3B-C4B	10.28	1.51	1.41
54	B5	607	CHL	C3B-C4B	10.13	1.51	1.41
46	BB	844	PQN	C12-C13	10.13	1.56	1.33
54	B5	605	CHL	C3B-C4B	10.00	1.51	1.41
54	B2	601	CHL	C3B-C4B	9.99	1.51	1.41
54	A4	306	CHL	C3B-C4B	9.97	1.51	1.41
46	AA	843	PQN	C12-C13	9.92	1.55	1.33
54	B2	614	CHL	C3B-C4B	9.91	1.51	1.41
46	BA	843	PQN	C12-C13	9.89	1.55	1.33
54	A6	607	CHL	C3B-C4B	9.85	1.51	1.41
54	B2	606	CHL	C3B-C4B	9.81	1.50	1.41
54	B1	303	CHL	C3B-C4B	9.77	1.50	1.41
54	A6	608	CHL	C3B-C4B	9.73	1.50	1.41
46	AB	843	PQN	C12-C13	9.71	1.55	1.33
54	A6	606	CHL	C3B-C4B	9.67	1.50	1.41
54	A1	303	CHL	C3B-C4B	9.60	1.50	1.41
54	B2	605	CHL	C3B-C4B	9.43	1.50	1.41
54	A6	602	CHL	C3B-C4B	9.41	1.50	1.41
54	A4	304	CHL	C1B-C2B	9.31	1.50	1.39
54	A4	305	CHL	C1B-C2B	9.23	1.50	1.39
54	A1	308	CHL	C3B-C4B	9.20	1.50	1.41
54	A3	307	CHL	C3B-C4B	9.10	1.50	1.41
54	A4	314	CHL	C1B-C2B	9.08	1.49	1.39
54	B5	606	CHL	C1B-C2B	8.97	1.49	1.39
54	B3	306	CHL	C3B-C4B	8.94	1.50	1.41
54	A6	602	CHL	C1B-C2B	8.91	1.49	1.39
54	A6	608	CHL	C1B-C2B	8.78	1.49	1.39
54	A4	304	CHL	C3B-C4B	8.78	1.49	1.41
54	A6	602	CHL	C1D-C2D	8.73	1.49	1.39
54	A6	607	CHL	C1B-C2B	8.71	1.49	1.39
54	B2	614	CHL	C1B-C2B	8.68	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B5	605	CHL	C1D-C2D	8.68	1.49	1.39
54	B1	308	CHL	C1D-C2D	8.62	1.49	1.39
54	B1	308	CHL	C1B-C2B	8.59	1.49	1.39
54	A4	314	CHL	C1D-C2D	8.58	1.49	1.39
54	B2	605	CHL	C1D-C2D	8.58	1.49	1.39
54	A4	306	CHL	C1B-C2B	8.55	1.49	1.39
54	B2	607	CHL	C1B-C2B	8.52	1.49	1.39
54	B1	303	CHL	C1B-C2B	8.50	1.49	1.39
54	A6	606	CHL	C1B-C2B	8.49	1.49	1.39
54	A6	606	CHL	C1D-C2D	8.49	1.49	1.39
54	B2	606	CHL	C1D-C2D	8.47	1.49	1.39
54	B5	607	CHL	C1B-C2B	8.47	1.49	1.39
54	B5	605	CHL	C1B-C2B	8.45	1.49	1.39
54	B2	601	CHL	C1D-C2D	8.42	1.49	1.39
54	A4	304	CHL	C1D-C2D	8.42	1.49	1.39
54	B2	601	CHL	C1B-C2B	8.37	1.49	1.39
54	B2	606	CHL	C1B-C2B	8.36	1.49	1.39
54	A4	306	CHL	C1D-C2D	8.34	1.49	1.39
54	A4	305	CHL	C1D-C2D	8.33	1.49	1.39
54	A6	607	CHL	C1D-C2D	8.32	1.49	1.39
54	A3	307	CHL	C1D-C2D	8.27	1.49	1.39
54	B2	614	CHL	C1D-C2D	8.26	1.49	1.39
54	A1	303	CHL	C1B-C2B	8.25	1.48	1.39
54	A1	308	CHL	C1B-C2B	8.21	1.48	1.39
54	A6	608	CHL	C1D-C2D	8.16	1.48	1.39
54	B5	606	CHL	C1D-C2D	8.15	1.48	1.39
54	B2	605	CHL	C1B-C2B	8.11	1.48	1.39
54	A1	308	CHL	C1D-C2D	8.10	1.48	1.39
54	B3	306	CHL	C1D-C2D	8.08	1.48	1.39
54	B2	607	CHL	C1D-C2D	8.06	1.48	1.39
54	B2	601	CHL	C1A-CHA	7.93	1.49	1.40
46	AB	843	PQN	O4-C4	7.89	1.39	1.23
46	AA	843	PQN	O4-C4	7.88	1.39	1.23
54	B5	607	CHL	C1D-C2D	7.87	1.48	1.39
54	B1	303	CHL	C1D-C2D	7.83	1.48	1.39
54	A3	307	CHL	C1B-C2B	7.82	1.48	1.39
46	BA	843	PQN	O4-C4	7.81	1.39	1.23
54	A4	305	CHL	C1A-CHA	7.76	1.48	1.40
46	BA	843	PQN	O1-C1	7.70	1.39	1.23
54	A4	305	CHL	C4B-C3B	7.69	1.48	1.39
46	BB	844	PQN	O4-C4	7.69	1.39	1.23
54	B3	306	CHL	C1B-C2B	7.69	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	BB	844	PQN	O1-C1	7.68	1.39	1.23
46	AB	843	PQN	O1-C1	7.60	1.39	1.23
46	AA	843	PQN	C9-C10	7.60	1.51	1.39
54	A1	303	CHL	C1D-C2D	7.56	1.48	1.39
54	A4	314	CHL	C4B-C3B	7.53	1.48	1.39
54	B5	606	CHL	C4B-C3B	7.52	1.48	1.39
54	A6	602	CHL	C1A-CHA	7.51	1.48	1.40
46	BA	843	PQN	C9-C10	7.51	1.51	1.39
54	B1	308	CHL	C1A-CHA	7.50	1.48	1.40
54	B2	606	CHL	C1A-CHA	7.49	1.48	1.40
54	B5	606	CHL	C1A-CHA	7.46	1.48	1.40
54	A4	314	CHL	C1A-CHA	7.44	1.48	1.40
54	A6	608	CHL	C1A-CHA	7.44	1.48	1.40
46	AA	843	PQN	O1-C1	7.44	1.38	1.23
54	A6	607	CHL	C1A-CHA	7.41	1.48	1.40
54	A4	304	CHL	C1A-CHA	7.38	1.48	1.40
54	B1	303	CHL	C1A-CHA	7.38	1.48	1.40
46	BA	843	PQN	C6-C5	7.37	1.51	1.39
54	A1	303	CHL	C1A-CHA	7.36	1.48	1.40
54	B3	306	CHL	C1A-CHA	7.29	1.48	1.40
46	AA	843	PQN	C6-C5	7.28	1.51	1.39
54	A1	308	CHL	C1A-CHA	7.20	1.48	1.40
46	AB	843	PQN	C6-C5	7.20	1.50	1.39
46	AB	843	PQN	C9-C10	7.19	1.50	1.39
54	B2	605	CHL	C1A-CHA	7.18	1.48	1.40
46	BB	844	PQN	C10-C5	-7.17	1.29	1.40
54	A3	307	CHL	C1A-CHA	7.16	1.48	1.40
54	B2	614	CHL	C1A-CHA	7.13	1.48	1.40
46	BB	844	PQN	C9-C10	7.12	1.50	1.39
54	A6	606	CHL	C1A-CHA	7.02	1.48	1.40
54	A4	306	CHL	C1A-CHA	6.94	1.47	1.40
54	B5	605	CHL	C1A-CHA	6.91	1.47	1.40
46	BA	843	PQN	C10-C5	-6.85	1.29	1.40
46	AB	843	PQN	C10-C5	-6.84	1.29	1.40
54	B2	607	CHL	C1A-CHA	6.79	1.47	1.40
46	BB	844	PQN	C6-C5	6.75	1.50	1.39
46	AA	843	PQN	C10-C5	-6.72	1.29	1.40
54	B5	607	CHL	C1A-CHA	6.49	1.47	1.40
54	A4	304	CHL	C3B-C2B	5.98	1.48	1.40
54	B2	605	CHL	C3A-C2A	-5.93	1.49	1.54
54	B5	607	CHL	C3A-C2A	-5.89	1.49	1.54
54	B2	614	CHL	C3B-C2B	5.80	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B2	607	CHL	C3A-C2A	-5.78	1.49	1.54
54	B5	607	CHL	C3B-C2B	5.72	1.48	1.40
54	A6	602	CHL	C3B-C2B	5.71	1.48	1.40
54	A6	606	CHL	C3A-C2A	-5.68	1.49	1.54
54	B3	306	CHL	CHB-C4A	-5.67	1.31	1.38
54	A6	608	CHL	C3B-C2B	5.66	1.48	1.40
54	B1	303	CHL	C3B-C2B	5.66	1.48	1.40
54	B1	308	CHL	C3B-C2B	5.65	1.48	1.40
54	A4	306	CHL	C3A-C2A	-5.61	1.49	1.54
54	B2	601	CHL	C3B-C2B	5.60	1.48	1.40
54	B5	605	CHL	C3B-C2B	5.57	1.47	1.40
54	B5	605	CHL	C3A-C2A	-5.57	1.49	1.54
54	B2	607	CHL	C3B-C2B	5.55	1.47	1.40
54	B5	606	CHL	C3D-C2D	5.52	1.49	1.39
54	B2	614	CHL	C3A-C2A	-5.52	1.49	1.54
54	B1	308	CHL	CHC-C4B	5.51	1.48	1.39
54	A4	304	CHL	C3A-C2A	-5.49	1.50	1.54
54	A6	607	CHL	C3B-C2B	5.48	1.47	1.40
54	B1	308	CHL	C3D-C2D	5.46	1.49	1.39
54	A3	307	CHL	CHB-C4A	-5.45	1.32	1.38
54	B2	605	CHL	CHB-C4A	-5.44	1.32	1.38
54	A1	303	CHL	CHB-C4A	-5.38	1.32	1.38
54	A3	307	CHL	C3A-C2A	-5.38	1.50	1.54
54	B3	306	CHL	C3A-C2A	-5.38	1.50	1.54
54	A6	606	CHL	C3B-C2B	5.36	1.47	1.40
54	B2	606	CHL	C3B-C2B	5.35	1.47	1.40
54	B2	601	CHL	C3A-C2A	-5.35	1.50	1.54
54	A4	305	CHL	C3D-C2D	5.33	1.48	1.39
54	B2	607	CHL	CHB-C4A	-5.33	1.32	1.38
54	B2	605	CHL	C3B-C2B	5.33	1.47	1.40
54	A6	607	CHL	C3A-C2A	-5.33	1.50	1.54
54	B5	607	CHL	CHB-C4A	-5.32	1.32	1.38
54	A4	306	CHL	C3B-C2B	5.31	1.47	1.40
54	A6	607	CHL	C3D-C2D	5.29	1.48	1.39
54	A4	314	CHL	C3D-C2D	5.28	1.48	1.39
54	A6	606	CHL	C3D-C2D	5.26	1.48	1.39
54	B2	601	CHL	CHB-C4A	-5.24	1.32	1.38
54	B2	606	CHL	C3D-C2D	5.23	1.48	1.39
54	A1	303	CHL	C3D-C2D	5.23	1.48	1.39
54	B5	605	CHL	C3D-C2D	5.23	1.48	1.39
54	A6	606	CHL	CHB-C4A	-5.22	1.32	1.38
54	A1	308	CHL	C2A-C3A	-5.22	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	308	CHL	C3D-C2D	5.22	1.48	1.39
54	B1	303	CHL	C3A-C2A	-5.21	1.50	1.54
54	B2	605	CHL	C3D-C2D	5.20	1.48	1.39
54	A4	306	CHL	CHB-C4A	-5.18	1.32	1.38
54	B5	606	CHL	O2D-CGD	5.17	1.45	1.33
54	B2	606	CHL	O2D-CGD	5.16	1.45	1.33
54	B2	605	CHL	O2D-CGD	5.16	1.45	1.33
54	A4	304	CHL	C3D-C2D	5.13	1.48	1.39
54	A4	305	CHL	O2D-CGD	5.13	1.45	1.33
54	A6	608	CHL	C3D-C2D	5.13	1.48	1.39
54	B5	605	CHL	CHB-C4A	-5.12	1.32	1.38
54	B2	606	CHL	CHB-C4A	-5.11	1.32	1.38
54	A6	607	CHL	O2D-CGD	5.11	1.45	1.33
54	B5	607	CHL	CHC-C4B	5.11	1.47	1.39
54	A4	305	CHL	OBD-CAD	5.10	1.29	1.22
54	B2	614	CHL	O2D-CGD	5.10	1.45	1.33
54	A1	308	CHL	CHB-C4A	-5.09	1.32	1.38
54	A3	307	CHL	C3D-C2D	5.09	1.48	1.39
54	A6	607	CHL	CHB-C4A	-5.09	1.32	1.38
54	A6	606	CHL	O2D-CGD	5.08	1.45	1.33
54	B2	614	CHL	C3D-C2D	5.08	1.48	1.39
54	B5	606	CHL	C2C-C3C	5.08	1.47	1.37
54	B2	607	CHL	CHC-C4B	5.07	1.47	1.39
54	B2	606	CHL	CHC-C4B	5.07	1.47	1.39
54	A4	304	CHL	C2C-C3C	5.07	1.47	1.37
54	B5	605	CHL	C2C-C3C	5.06	1.47	1.37
47	B3	318	LHG	O7-C7	5.05	1.46	1.35
54	A4	314	CHL	C3A-C2A	-5.05	1.50	1.54
54	B1	303	CHL	C3D-C2D	5.05	1.48	1.39
54	A1	308	CHL	OBD-CAD	5.05	1.28	1.22
54	B2	614	CHL	OBD-CAD	5.04	1.28	1.22
54	A4	304	CHL	CHC-C4B	5.04	1.47	1.39
54	B2	606	CHL	OBD-CAD	5.03	1.28	1.22
54	A6	608	CHL	O2D-CGD	5.03	1.45	1.33
54	A1	308	CHL	C3B-C2B	5.03	1.47	1.40
54	B1	303	CHL	CHB-C4A	-5.02	1.32	1.38
54	A6	602	CHL	C3D-C2D	5.02	1.48	1.39
54	B2	605	CHL	C2C-C3C	5.02	1.47	1.37
54	B1	308	CHL	OBD-CAD	5.01	1.28	1.22
54	A6	607	CHL	OBD-CAD	5.01	1.28	1.22
54	A1	303	CHL	C3B-C2B	5.01	1.47	1.40
54	A1	308	CHL	CHC-C4B	5.00	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	303	CHL	C3A-C2A	-5.00	1.50	1.54
54	A4	306	CHL	CHC-C4B	5.00	1.47	1.39
54	A3	307	CHL	C3B-C2B	4.99	1.47	1.40
54	A6	606	CHL	OBD-CAD	4.99	1.28	1.22
54	A4	306	CHL	C3D-C2D	4.99	1.48	1.39
54	A4	314	CHL	OBD-CAD	4.98	1.28	1.22
54	B5	606	CHL	C3A-C2A	-4.97	1.50	1.54
54	B2	614	CHL	CHB-C4A	-4.97	1.32	1.38
54	A4	306	CHL	O2D-CGD	4.95	1.45	1.33
54	B5	606	CHL	OBD-CAD	4.95	1.28	1.22
54	B5	607	CHL	O2D-CGD	4.94	1.45	1.33
54	B1	303	CHL	OBD-CAD	4.93	1.28	1.22
54	A4	304	CHL	OBD-CAD	4.93	1.28	1.22
54	B2	601	CHL	OBD-CAD	4.92	1.28	1.22
54	B3	306	CHL	O2D-CGD	4.92	1.45	1.33
54	A6	602	CHL	OBD-CAD	4.91	1.28	1.22
54	A6	607	CHL	CHC-C4B	4.91	1.47	1.39
54	B2	607	CHL	O2D-CGD	4.91	1.45	1.33
54	B2	614	CHL	CHC-C4B	4.91	1.47	1.39
54	B5	607	CHL	C2C-C3C	4.91	1.47	1.37
54	B3	306	CHL	C3D-C2D	4.90	1.48	1.39
54	A3	307	CHL	O2D-CGD	4.90	1.45	1.33
54	A4	304	CHL	CHB-C4A	-4.89	1.32	1.38
45	AK	201	CLA	C1B-C2B	4.89	1.49	1.41
54	B5	607	CHL	C3D-C2D	4.89	1.48	1.39
54	A6	608	CHL	OBD-CAD	4.89	1.28	1.22
54	A6	602	CHL	CHB-C1B	4.88	1.47	1.39
54	B2	601	CHL	C3D-C2D	4.88	1.48	1.39
54	A1	303	CHL	CHC-C4B	4.88	1.47	1.39
54	B1	308	CHL	CHB-C4A	-4.85	1.32	1.38
54	A4	305	CHL	C3A-C2A	-4.84	1.50	1.54
54	B2	601	CHL	CHC-C4B	4.83	1.47	1.39
47	A3	319	LHG	O7-C7	4.83	1.45	1.35
54	B1	308	CHL	C2A-C3A	-4.81	1.50	1.54
56	BJ	104	SQD	O8-S	4.81	1.65	1.47
54	B1	303	CHL	CHC-C4B	4.80	1.47	1.39
54	A6	606	CHL	C2C-C3C	4.80	1.46	1.37
54	A4	304	CHL	CHB-C1B	4.79	1.47	1.39
54	B2	605	CHL	OBD-CAD	4.79	1.28	1.22
54	A6	602	CHL	C3A-C2A	-4.78	1.50	1.54
54	B2	601	CHL	O2D-CGD	4.78	1.45	1.33
54	B1	308	CHL	O2D-CGD	4.78	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A4	314	CHL	O2D-CGD	4.76	1.45	1.30
54	B1	308	CHL	CHB-C1B	4.75	1.47	1.39
54	B2	607	CHL	C3D-C2D	4.75	1.47	1.39
54	B5	605	CHL	O2D-CGD	4.74	1.45	1.30
54	A6	602	CHL	CHB-C4A	-4.74	1.32	1.38
54	A4	304	CHL	O2D-CGD	4.74	1.45	1.30
54	A3	307	CHL	OBD-CAD	4.74	1.28	1.22
54	A1	308	CHL	O2D-CGD	4.73	1.45	1.30
54	B5	605	CHL	OBD-CAD	4.72	1.28	1.22
54	B3	306	CHL	OBD-CAD	4.72	1.28	1.22
54	B1	303	CHL	O2D-CGD	4.71	1.45	1.30
54	A4	314	CHL	CHD-C4C	4.71	1.48	1.39
54	A4	306	CHL	CHB-C1B	4.68	1.47	1.39
54	B3	306	CHL	C3B-C2B	4.68	1.46	1.40
54	B5	605	CHL	CHC-C4B	4.68	1.47	1.39
54	A6	608	CHL	CHC-C4B	4.68	1.47	1.39
54	B2	606	CHL	C3A-C2A	-4.68	1.50	1.54
54	B2	605	CHL	CHC-C4B	4.67	1.47	1.39
54	A1	303	CHL	O2D-CGD	4.67	1.45	1.30
54	B5	607	CHL	CHB-C1B	4.66	1.47	1.39
54	A3	307	CHL	CHC-C4B	4.65	1.47	1.39
54	A6	602	CHL	O2D-CGD	4.65	1.45	1.30
54	B2	606	CHL	CHD-C1D	4.63	1.47	1.39
54	B2	606	CHL	CHD-C4C	4.63	1.48	1.39
54	A6	608	CHL	CHB-C1B	4.63	1.47	1.39
54	B2	614	CHL	CHB-C1B	4.62	1.47	1.39
54	B2	607	CHL	OBD-CAD	4.62	1.28	1.22
45	AK	201	CLA	C3B-C4B	4.62	1.49	1.39
54	A6	602	CHL	CHC-C4B	4.61	1.47	1.39
54	A4	304	CHL	CHD-C4C	4.60	1.48	1.39
54	B1	308	CHL	CHD-C4C	4.59	1.48	1.39
54	A6	606	CHL	CHC-C4B	4.58	1.47	1.39
54	B2	605	CHL	CHD-C1D	4.58	1.47	1.39
54	A6	608	CHL	CHB-C4A	-4.57	1.33	1.38
54	B3	306	CHL	CHC-C4B	4.57	1.47	1.39
54	B3	306	CHL	O2A-CGA	4.57	1.45	1.30
54	B5	607	CHL	O2A-CGA	4.56	1.45	1.30
54	A1	303	CHL	OBD-CAD	4.56	1.28	1.22
54	A4	306	CHL	O2A-CGA	4.56	1.45	1.30
54	A4	314	CHL	CHB-C4A	-4.55	1.33	1.38
54	A4	305	CHL	CHB-C4A	-4.54	1.33	1.38
54	A4	305	CHL	CHB-C1B	4.54	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B5	606	CHL	CHB-C1B	4.54	1.47	1.39
54	A3	307	CHL	O2A-CGA	4.52	1.45	1.30
54	B5	605	CHL	CHB-C1B	4.52	1.46	1.39
54	A6	602	CHL	CHD-C4C	4.52	1.48	1.39
54	A4	306	CHL	OBD-CAD	4.52	1.28	1.22
54	B5	606	CHL	CHD-C1D	4.52	1.46	1.39
54	B5	605	CHL	CHD-C1D	4.51	1.46	1.39
54	B2	607	CHL	O2A-CGA	4.51	1.45	1.30
54	B5	605	CHL	CHD-C4C	4.50	1.48	1.39
54	B2	601	CHL	O2A-CGA	4.50	1.46	1.33
54	B1	308	CHL	CHD-C1D	4.50	1.46	1.39
54	B3	306	CHL	CHD-C1D	4.49	1.46	1.39
54	A4	305	CHL	CHD-C4C	4.49	1.48	1.39
54	A1	303	CHL	O2A-CGA	4.49	1.46	1.33
54	A1	308	CHL	CHD-C1D	4.49	1.46	1.39
54	A4	306	CHL	CHC-C1C	4.48	1.48	1.39
54	B2	605	CHL	CHD-C4C	4.47	1.48	1.39
54	A4	314	CHL	CHD-C1D	4.47	1.46	1.39
54	B2	601	CHL	CHD-C4C	4.47	1.47	1.39
54	A6	602	CHL	O2A-CGA	4.46	1.46	1.33
54	A1	308	CHL	CHB-C1B	4.45	1.46	1.39
54	A6	607	CHL	CHD-C4C	4.45	1.47	1.39
54	A4	314	CHL	CHB-C1B	4.45	1.46	1.39
54	B2	614	CHL	CHD-C4C	4.43	1.47	1.39
54	A1	308	CHL	CHD-C4C	4.42	1.47	1.39
54	B5	606	CHL	CHD-C4C	4.41	1.47	1.39
54	B2	606	CHL	CHB-C1B	4.41	1.46	1.39
54	B2	607	CHL	CHB-C1B	4.40	1.46	1.39
54	A6	608	CHL	CHD-C4C	4.38	1.47	1.39
54	B1	308	CHL	CHC-C1C	4.38	1.47	1.39
53	AG	202	LMG	O7-C10	4.38	1.46	1.34
54	A4	305	CHL	CHD-C1D	4.37	1.46	1.39
54	B5	607	CHL	CHD-C4C	4.37	1.47	1.39
54	A6	607	CHL	CHB-C1B	4.36	1.46	1.39
54	A4	305	CHL	CHC-C4B	4.36	1.46	1.39
54	A6	606	CHL	CHD-C4C	4.35	1.47	1.39
54	B5	606	CHL	CHC-C4B	4.35	1.46	1.39
54	A6	602	CHL	CHD-C1D	4.35	1.46	1.39
54	A3	307	CHL	CHB-C1B	4.35	1.46	1.39
54	A6	608	CHL	CHD-C1D	4.35	1.46	1.39
54	B5	606	CHL	CHB-C4A	-4.34	1.33	1.38
54	A1	303	CHL	CHD-C4C	4.34	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	B1	301	LHG	O7-C7	4.34	1.46	1.34
54	B1	303	CHL	CHB-C1B	4.34	1.46	1.39
54	B5	607	CHL	OBD-CAD	4.33	1.28	1.22
54	A6	607	CHL	CHD-C1D	4.32	1.46	1.39
54	A4	304	CHL	CHD-C1D	4.31	1.46	1.39
47	AJ	104	LHG	O8-C23	4.30	1.45	1.33
54	B2	606	CHL	CHC-C1C	4.30	1.47	1.39
53	AG	202	LMG	O8-C28	4.29	1.45	1.33
53	B5	617	LMG	O7-C10	4.29	1.46	1.34
54	A6	608	CHL	O2A-CGA	4.29	1.45	1.33
54	B2	605	CHL	CHB-C1B	4.28	1.46	1.39
54	B5	607	CHL	CHC-C1C	4.28	1.47	1.39
47	A1	302	LHG	O8-C23	4.28	1.45	1.33
47	B3	318	LHG	O8-C23	4.27	1.45	1.33
47	AA	844	LHG	O8-C23	4.27	1.45	1.33
47	A1	301	LHG	O7-C7	4.27	1.46	1.34
54	B2	601	CHL	CHD-C1D	4.27	1.46	1.39
47	AJ	104	LHG	O7-C7	4.26	1.46	1.34
53	B5	617	LMG	O8-C28	4.26	1.45	1.33
47	A3	301	LHG	O8-C23	4.26	1.45	1.33
54	B2	601	CHL	CHB-C1B	4.26	1.46	1.39
47	B1	302	LHG	O7-C7	4.26	1.46	1.34
54	A4	306	CHL	CHD-C4C	4.26	1.47	1.39
54	A3	307	CHL	CHD-C1D	4.25	1.46	1.39
47	B1	301	LHG	O8-C23	4.25	1.45	1.33
54	B2	607	CHL	CHD-C4C	4.25	1.47	1.39
47	A1	320	LHG	O8-C23	4.25	1.45	1.33
54	A6	606	CHL	CHD-C1D	4.24	1.46	1.39
47	B1	318	LHG	O7-C7	4.23	1.46	1.34
53	A1	321	LMG	O8-C28	4.23	1.45	1.33
54	A4	314	CHL	CHC-C4B	4.22	1.46	1.39
47	B5	618	LHG	O8-C23	4.22	1.45	1.33
54	A6	606	CHL	CHB-C1B	4.21	1.46	1.39
54	B1	303	CHL	O2A-CGA	4.21	1.45	1.33
47	B1	302	LHG	O8-C23	4.20	1.45	1.33
53	A1	321	LMG	O7-C10	4.20	1.46	1.34
54	B3	306	CHL	CHB-C1B	4.19	1.46	1.39
56	BJ	104	SQD	O47-C7	4.19	1.46	1.34
54	B3	306	CHL	CHD-C4C	4.18	1.47	1.39
54	A1	303	CHL	CHB-C1B	4.18	1.46	1.39
54	A6	608	CHL	C3A-C2A	-4.18	1.51	1.54
54	B2	607	CHL	CHC-C1C	4.17	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	303	CHL	CHC-C1C	4.16	1.47	1.39
51	BB	850	DGD	O1G-C1A	4.16	1.45	1.33
54	A6	606	CHL	CHC-C1C	4.16	1.47	1.39
54	B5	605	CHL	CHC-C1C	4.16	1.47	1.39
54	A4	314	CHL	CHC-C1C	4.16	1.47	1.39
47	B1	318	LHG	O8-C23	4.14	1.45	1.33
47	A1	302	LHG	O7-C7	4.13	1.46	1.34
47	BF	305	LHG	O8-C23	4.13	1.45	1.33
54	A3	307	CHL	CHD-C4C	4.13	1.47	1.39
47	A3	301	LHG	O7-C7	4.11	1.45	1.34
54	B1	303	CHL	CHD-C4C	4.11	1.47	1.39
56	BJ	104	SQD	O48-C23	4.11	1.45	1.33
47	A1	301	LHG	O8-C23	4.10	1.45	1.33
47	A3	319	LHG	O8-C23	4.10	1.45	1.33
47	BA	846	LHG	O7-C7	4.10	1.45	1.34
54	B2	601	CHL	CHC-C1C	4.08	1.47	1.39
54	A1	308	CHL	CHC-C1C	4.07	1.47	1.39
51	AB	851	DGD	O1G-C1A	4.07	1.45	1.33
54	B1	303	CHL	CHD-C1D	4.06	1.46	1.39
47	A1	320	LHG	O7-C7	4.06	1.45	1.34
47	BF	305	LHG	O7-C7	4.06	1.45	1.34
54	A6	608	CHL	CHC-C1C	4.06	1.47	1.39
54	B5	606	CHL	CHC-C1C	4.06	1.47	1.39
54	A4	305	CHL	CHC-C1C	4.05	1.47	1.39
54	B2	614	CHL	CHD-C1D	4.04	1.46	1.39
54	B2	605	CHL	CHC-C1C	4.03	1.47	1.39
54	A1	303	CHL	CHD-C1D	4.03	1.46	1.39
54	B1	303	CHL	CHC-C1C	4.03	1.47	1.39
54	B2	607	CHL	CHD-C1D	4.01	1.46	1.39
47	A6	618	LHG	O7-C7	4.01	1.45	1.34
54	B2	614	CHL	CHC-C1C	4.00	1.47	1.39
47	B2	618	LHG	O8-C23	3.99	1.45	1.33
51	BB	850	DGD	O2G-C1B	3.98	1.45	1.34
47	A6	618	LHG	O8-C23	3.96	1.44	1.33
47	B5	618	LHG	O7-C7	3.96	1.45	1.34
54	A4	304	CHL	CHC-C1C	3.95	1.47	1.39
54	B5	607	CHL	CHD-C1D	3.95	1.46	1.39
54	A6	602	CHL	CHC-C1C	3.93	1.46	1.39
53	A4	318	LMG	O8-C28	3.90	1.44	1.33
47	AA	844	LHG	O7-C7	3.90	1.45	1.34
54	A6	607	CHL	CHC-C1C	3.89	1.46	1.39
51	AB	851	DGD	O2G-C1B	3.85	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	B2	618	LHG	O7-C7	3.84	1.45	1.34
47	BA	845	LHG	O8-C23	3.82	1.44	1.33
54	A4	306	CHL	CHD-C1D	3.73	1.45	1.39
45	AA	823	CLA	C1D-ND	3.70	1.42	1.37
45	A6	614	CLA	C1D-ND	3.68	1.42	1.37
54	A3	307	CHL	CHA-CBD	-3.65	1.47	1.51
47	BA	845	LHG	O7-C7	3.64	1.44	1.34
45	BA	801	CLA	C1D-ND	3.64	1.42	1.37
50	AL	301	LMU	O5B-C1B	3.63	1.51	1.41
45	BB	837	CLA	C1D-ND	3.61	1.42	1.37
45	AA	801	CLA	C1D-ND	3.59	1.42	1.37
45	BK	201	CLA	C1D-ND	3.58	1.42	1.37
54	A6	606	CHL	CHA-CBD	-3.58	1.47	1.51
45	BL	302	CLA	C1D-ND	3.57	1.42	1.37
45	A3	311	CLA	C1D-ND	3.57	1.42	1.37
45	BA	844	CLA	C1D-ND	3.56	1.42	1.37
45	B1	307	CLA	C1D-ND	3.56	1.42	1.37
54	A3	307	CHL	CHC-C1C	3.56	1.46	1.39
53	A4	318	LMG	O7-C10	3.55	1.44	1.34
54	B3	306	CHL	CHC-C1C	3.54	1.46	1.39
45	A4	302	CLA	C1D-ND	3.54	1.42	1.37
45	B3	309	CLA	C1D-ND	3.54	1.42	1.37
45	BA	836	CLA	C1D-ND	3.53	1.42	1.37
45	AB	802	CLA	CAB-C3B	-3.53	1.43	1.50
45	A3	313	CLA	C1D-ND	3.53	1.42	1.37
45	B1	309	CLA	C1D-ND	3.52	1.42	1.37
45	AK	201	CLA	C1D-ND	3.52	1.42	1.37
45	A3	312	CLA	C1D-ND	3.51	1.42	1.37
45	A1	316	CLA	C1D-ND	3.50	1.42	1.37
45	AL	304	CLA	C1D-ND	3.50	1.42	1.37
45	A1	305	CLA	C1D-ND	3.50	1.42	1.37
45	AH	201	CLA	C1D-ND	3.50	1.42	1.37
54	B5	607	CHL	CHA-CBD	-3.49	1.47	1.51
45	AB	836	CLA	C1D-ND	3.49	1.42	1.37
45	AF	804	CLA	C1D-ND	3.49	1.42	1.37
45	BB	842	CLA	C1D-ND	3.49	1.42	1.37
45	BG	202	CLA	C1D-ND	3.49	1.42	1.37
45	B3	310	CLA	C1D-ND	3.48	1.42	1.37
45	A1	313	CLA	C1D-ND	3.48	1.42	1.37
45	AG	204	CLA	C1D-ND	3.48	1.42	1.37
45	B3	312	CLA	C1D-ND	3.48	1.42	1.37
45	BL	303	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	836	CLA	C1D-ND	3.47	1.42	1.37
45	AA	816	CLA	C1D-ND	3.47	1.42	1.37
45	BK	202	CLA	C1D-ND	3.47	1.42	1.37
45	A3	303	CLA	C1D-ND	3.47	1.42	1.37
45	AB	817	CLA	C1D-ND	3.46	1.42	1.37
45	B5	601	CLA	C1D-ND	3.46	1.42	1.37
45	BB	818	CLA	C1D-ND	3.46	1.42	1.37
45	B1	313	CLA	C1D-ND	3.45	1.42	1.37
46	BB	844	PQN	C11-C12	3.45	1.56	1.50
50	AL	301	LMU	O5'-C1'	3.45	1.50	1.41
45	AA	812	CLA	C1D-ND	3.44	1.42	1.37
45	A6	613	CLA	C1D-ND	3.44	1.42	1.37
45	BA	815	CLA	C1D-ND	3.44	1.42	1.37
45	A1	309	CLA	C1D-ND	3.44	1.42	1.37
45	A1	307	CLA	C1D-ND	3.44	1.42	1.37
45	B3	313	CLA	C1D-ND	3.44	1.42	1.37
45	B1	306	CLA	C1D-ND	3.44	1.42	1.37
45	AK	203	CLA	C1D-ND	3.43	1.42	1.37
45	BJ	102	CLA	C1D-ND	3.43	1.42	1.37
45	B2	611	CLA	C1D-ND	3.43	1.42	1.37
45	AK	202	CLA	C1D-ND	3.43	1.42	1.37
45	A3	306	CLA	C1D-ND	3.43	1.42	1.37
45	B2	609	CLA	C1D-ND	3.43	1.42	1.37
45	A1	312	CLA	CAB-C3B	-3.43	1.43	1.50
45	BA	844	CLA	C4B-NB	3.42	1.42	1.37
45	BA	832	CLA	C1D-ND	3.42	1.42	1.37
45	A1	306	CLA	C1D-ND	3.41	1.42	1.37
45	A4	310	CLA	C1D-ND	3.41	1.42	1.37
45	B3	305	CLA	C1D-ND	3.41	1.42	1.37
45	A3	305	CLA	C1D-ND	3.41	1.42	1.37
45	A6	614	CLA	C4B-NB	3.41	1.42	1.37
45	A1	315	CLA	C1D-ND	3.40	1.42	1.37
50	AB	852	LMU	O5B-C1B	3.40	1.50	1.41
54	A1	303	CHL	CHA-CBD	-3.40	1.47	1.51
45	AG	201	CLA	C1D-ND	3.40	1.42	1.37
45	A4	312	CLA	C1D-ND	3.40	1.42	1.37
45	B5	604	CLA	C1D-ND	3.40	1.42	1.37
54	B5	605	CHL	CHA-CBD	-3.40	1.47	1.51
45	B1	312	CLA	C1D-ND	3.40	1.42	1.37
45	AB	808	CLA	C1D-ND	3.39	1.42	1.37
45	B1	305	CLA	C1D-ND	3.39	1.42	1.37
45	AJ	102	CLA	C1D-ND	3.39	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	836	CLA	C1D-ND	3.39	1.42	1.37
45	AA	822	CLA	C1D-ND	3.38	1.42	1.37
45	BB	820	CLA	C1D-ND	3.38	1.42	1.37
45	B5	613	CLA	C1D-ND	3.38	1.42	1.37
45	AA	832	CLA	C1D-ND	3.38	1.42	1.37
45	A6	605	CLA	C1D-ND	3.38	1.42	1.37
50	BA	853	LMU	O5B-C1B	3.38	1.50	1.41
45	AL	305	CLA	C1D-ND	3.38	1.42	1.37
45	BF	303	CLA	C1D-ND	3.37	1.42	1.37
45	BA	812	CLA	C1D-ND	3.37	1.42	1.37
45	B5	603	CLA	C1D-ND	3.37	1.42	1.37
45	A3	314	CLA	C1D-ND	3.36	1.42	1.37
45	BB	809	CLA	C1D-ND	3.36	1.42	1.37
45	BA	816	CLA	C1D-ND	3.36	1.42	1.37
45	BA	823	CLA	C1D-ND	3.36	1.42	1.37
45	BB	828	CLA	C1D-ND	3.36	1.42	1.37
45	AA	835	CLA	C1D-ND	3.36	1.42	1.37
45	A3	310	CLA	C1D-ND	3.36	1.42	1.37
45	B5	611	CLA	C1D-ND	3.36	1.42	1.37
45	BA	838	CLA	CAD-C3D	-3.36	1.45	1.50
45	AA	819	CLA	C1D-ND	3.35	1.42	1.37
45	BB	833	CLA	C1D-ND	3.35	1.42	1.37
54	B3	306	CHL	CHA-CBD	-3.35	1.47	1.51
45	B3	303	CLA	C1D-ND	3.35	1.42	1.37
45	BA	813	CLA	C1D-ND	3.35	1.42	1.37
45	A4	308	CLA	C1D-ND	3.35	1.42	1.37
45	BA	835	CLA	C1D-ND	3.34	1.42	1.37
50	AB	853	LMU	O5'-C1'	3.34	1.50	1.41
45	B1	310	CLA	C1D-ND	3.34	1.42	1.37
45	B5	610	CLA	C1D-ND	3.34	1.42	1.37
45	BB	843	CLA	C1D-ND	3.33	1.42	1.37
45	BA	807	CLA	C1D-ND	3.33	1.42	1.37
45	B5	612	CLA	C1D-ND	3.33	1.42	1.37
45	B3	311	CLA	C4B-NB	3.33	1.42	1.37
45	BA	810	CLA	C1D-ND	3.32	1.42	1.37
45	AF	803	CLA	C4B-NB	3.32	1.42	1.37
45	AG	204	CLA	C4B-NB	3.32	1.42	1.37
45	A4	303	CLA	C1D-ND	3.32	1.42	1.37
45	AB	841	CLA	C1D-ND	3.32	1.42	1.37
45	B2	612	CLA	C1D-ND	3.31	1.42	1.37
45	BA	824	CLA	C1D-ND	3.31	1.42	1.37
54	B2	614	CHL	CHA-CBD	-3.31	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	839	CLA	CMD-C2D	-3.31	1.44	1.50
50	AA	851	LMU	O5'-C1'	3.31	1.50	1.41
45	AA	810	CLA	CAD-C3D	-3.31	1.45	1.50
45	BA	818	CLA	C1D-ND	3.31	1.42	1.37
54	B2	607	CHL	CHA-CBD	-3.30	1.47	1.51
45	A3	309	CLA	C1D-ND	3.30	1.42	1.37
45	A4	307	CLA	C1D-ND	3.30	1.42	1.37
45	AH	201	CLA	C4B-NB	3.30	1.42	1.37
45	BA	839	CLA	C1D-ND	3.30	1.42	1.37
54	B2	605	CHL	CHA-CBD	-3.30	1.47	1.51
45	BA	820	CLA	C1D-ND	3.30	1.42	1.37
45	BH	201	CLA	C1D-ND	3.30	1.42	1.37
45	AA	822	CLA	C4B-NB	3.30	1.42	1.37
45	AB	827	CLA	C1D-ND	3.30	1.42	1.37
46	BA	843	PQN	C11-C12	3.30	1.55	1.50
45	B2	611	CLA	C4B-NB	3.30	1.42	1.37
45	AA	807	CLA	C1D-ND	3.30	1.42	1.37
50	AB	853	LMU	O5B-C1B	3.30	1.50	1.41
50	BA	854	LMU	O5B-C1B	3.30	1.50	1.41
45	BA	822	CLA	C1D-ND	3.29	1.42	1.37
45	A1	311	CLA	C1D-ND	3.29	1.42	1.37
45	B3	307	CLA	C1D-ND	3.29	1.42	1.37
45	A3	304	CLA	C1D-ND	3.29	1.42	1.37
45	BA	834	CLA	C1D-ND	3.29	1.42	1.37
45	B2	604	CLA	C1D-ND	3.29	1.42	1.37
45	BF	302	CLA	C1D-ND	3.29	1.42	1.37
45	AA	809	CLA	C1D-ND	3.28	1.42	1.37
45	AA	820	CLA	C1D-ND	3.28	1.42	1.37
45	AB	812	CLA	C1D-ND	3.28	1.42	1.37
45	AB	816	CLA	C1D-ND	3.28	1.42	1.37
45	AB	819	CLA	C1D-ND	3.28	1.42	1.37
45	A4	309	CLA	C1D-ND	3.28	1.42	1.37
45	BB	813	CLA	C1D-ND	3.28	1.42	1.37
45	AB	832	CLA	C1D-ND	3.28	1.42	1.37
45	AA	806	CLA	C1D-ND	3.28	1.42	1.37
45	AL	303	CLA	C1D-ND	3.28	1.42	1.37
45	A6	610	CLA	C1D-ND	3.28	1.42	1.37
45	BG	201	CLA	C4B-NB	3.28	1.42	1.37
50	BA	854	LMU	O5'-C1'	3.27	1.50	1.41
45	BA	817	CLA	C1D-ND	3.27	1.42	1.37
45	BA	821	CLA	C1D-ND	3.27	1.42	1.37
45	B1	311	CLA	C1D-ND	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	828	CLA	C1D-ND	3.27	1.42	1.37
45	B2	613	CLA	C1D-ND	3.27	1.42	1.37
45	A6	612	CLA	C1D-ND	3.26	1.42	1.37
45	BK	203	CLA	C1D-ND	3.26	1.42	1.37
50	AB	850	LMU	O5'-C1'	3.26	1.50	1.41
45	B5	608	CLA	C1D-ND	3.26	1.42	1.37
45	B1	311	CLA	C4B-NB	3.26	1.42	1.37
45	A4	311	CLA	C1D-ND	3.26	1.42	1.37
45	B3	302	CLA	C1D-ND	3.26	1.42	1.37
45	A3	304	CLA	CAB-C3B	-3.26	1.44	1.50
45	A1	312	CLA	C1D-ND	3.26	1.42	1.37
45	AA	836	CLA	C4B-NB	3.25	1.42	1.37
45	BA	840	CLA	C1D-ND	3.25	1.42	1.37
45	A4	307	CLA	C4B-NB	3.25	1.42	1.37
54	A4	306	CHL	CHA-CBD	-3.25	1.47	1.51
45	A4	308	CLA	C4B-NB	3.25	1.42	1.37
45	AA	803	CLA	C1D-ND	3.25	1.42	1.37
45	B2	603	CLA	C1D-ND	3.25	1.42	1.37
45	B3	311	CLA	C1D-ND	3.25	1.42	1.37
45	BA	814	CLA	C1D-ND	3.25	1.42	1.37
45	AA	827	CLA	C1D-ND	3.25	1.42	1.37
45	A4	313	CLA	C1D-ND	3.25	1.42	1.37
45	BA	837	CLA	C1D-ND	3.25	1.42	1.37
45	A6	601	CLA	C1D-ND	3.25	1.42	1.37
45	AA	829	CLA	CMD-C2D	-3.24	1.44	1.50
45	AB	818	CLA	C1D-ND	3.24	1.42	1.37
45	AB	809	CLA	C4B-NB	3.24	1.42	1.37
45	B5	609	CLA	C1D-ND	3.24	1.42	1.37
45	B3	304	CLA	C1D-ND	3.24	1.42	1.37
45	BF	302	CLA	C4B-NB	3.24	1.42	1.37
45	AA	813	CLA	C1D-ND	3.24	1.42	1.37
54	A6	607	CHL	CHA-CBD	-3.24	1.47	1.51
45	A6	604	CLA	C1D-ND	3.24	1.42	1.37
45	BH	201	CLA	C4B-NB	3.24	1.42	1.37
45	AA	811	CLA	C1D-ND	3.24	1.42	1.37
45	AB	842	CLA	C1D-ND	3.24	1.42	1.37
45	AA	839	CLA	C1D-ND	3.23	1.42	1.37
45	BB	808	CLA	C1D-ND	3.23	1.42	1.37
50	BA	853	LMU	O5'-C1'	3.23	1.50	1.41
45	B1	310	CLA	CAB-C3B	-3.23	1.44	1.50
45	AA	814	CLA	C1D-ND	3.23	1.42	1.37
45	B2	604	CLA	C4B-NB	3.23	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	308	CHL	CHA-CBD	-3.23	1.47	1.51
45	B1	314	CLA	C1D-ND	3.23	1.42	1.37
45	BA	805	CLA	C1D-ND	3.22	1.42	1.37
45	AK	202	CLA	C4B-NB	3.22	1.42	1.37
45	A1	309	CLA	C4B-NB	3.22	1.42	1.37
45	B3	308	CLA	C1D-ND	3.22	1.42	1.37
45	B5	610	CLA	C4B-NB	3.22	1.42	1.37
45	A3	308	CLA	C1D-ND	3.22	1.42	1.37
45	B3	309	CLA	C4B-NB	3.22	1.42	1.37
45	A1	314	CLA	C1D-ND	3.21	1.42	1.37
45	BA	822	CLA	C4B-NB	3.21	1.42	1.37
45	BB	834	CLA	C1D-ND	3.21	1.42	1.37
45	B5	603	CLA	CAB-C3B	-3.21	1.44	1.50
50	BB	851	LMU	O5B-C1B	3.21	1.50	1.41
45	AA	831	CLA	C1D-ND	3.21	1.42	1.37
45	A4	303	CLA	CAB-C3B	-3.21	1.44	1.50
45	AF	803	CLA	C1D-ND	3.21	1.42	1.37
45	AB	806	CLA	C1D-ND	3.21	1.42	1.37
45	B2	609	CLA	C4B-NB	3.20	1.42	1.37
45	A4	302	CLA	CAB-C3B	-3.20	1.44	1.50
45	AA	823	CLA	C4B-NB	3.20	1.42	1.37
45	AB	822	CLA	C4B-NB	3.20	1.42	1.37
48	BI	101	BCR	C30-C25	-3.20	1.49	1.53
45	AB	820	CLA	C4B-NB	3.20	1.42	1.37
45	AB	837	CLA	C1D-ND	3.20	1.42	1.37
45	A6	609	CLA	C1D-ND	3.20	1.42	1.37
45	B5	604	CLA	CAB-C3B	-3.20	1.44	1.50
50	BB	851	LMU	O5'-C1'	3.20	1.50	1.41
45	AA	809	CLA	C4B-NB	3.20	1.42	1.37
45	BB	807	CLA	C1D-ND	3.19	1.42	1.37
45	BK	201	CLA	C4B-NB	3.19	1.42	1.37
45	AA	837	CLA	C1D-ND	3.19	1.42	1.37
45	AB	821	CLA	C1D-ND	3.19	1.42	1.37
45	AG	201	CLA	C4B-NB	3.19	1.42	1.37
45	B3	301	CLA	C1D-ND	3.19	1.42	1.37
45	A6	604	CLA	C4B-NB	3.19	1.42	1.37
45	BA	831	CLA	C1D-ND	3.19	1.42	1.37
45	AL	303	CLA	C4B-NB	3.19	1.42	1.37
45	AG	203	CLA	C4B-NB	3.19	1.42	1.37
45	BA	829	CLA	CMD-C2D	-3.18	1.44	1.50
45	A1	310	CLA	CAB-C3B	-3.18	1.44	1.50
45	B1	306	CLA	C4B-NB	3.18	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	608	CLA	C1D-ND	3.18	1.42	1.37
45	B3	303	CLA	CAB-C3B	-3.18	1.44	1.50
45	AA	821	CLA	C1D-ND	3.18	1.42	1.37
46	AB	843	PQN	C11-C12	3.18	1.55	1.50
45	B3	304	CLA	C4B-NB	3.18	1.42	1.37
45	B5	604	CLA	C4B-NB	3.18	1.42	1.37
45	B1	315	CLA	C1D-ND	3.18	1.42	1.37
45	B3	312	CLA	C4B-NB	3.18	1.42	1.37
45	A1	311	CLA	C4B-NB	3.17	1.42	1.37
45	A1	316	CLA	CAB-C3B	-3.17	1.44	1.50
45	AB	811	CLA	C1D-ND	3.17	1.42	1.37
45	AA	824	CLA	C4B-NB	3.17	1.42	1.37
50	AB	852	LMU	O5'-C1'	3.17	1.50	1.41
45	BB	801	CLA	CMD-C2D	-3.17	1.44	1.50
45	AB	828	CLA	C1D-ND	3.17	1.42	1.37
45	BB	817	CLA	C1D-ND	3.17	1.42	1.37
45	B2	610	CLA	C1D-ND	3.16	1.42	1.37
45	A4	311	CLA	C4B-NB	3.16	1.42	1.37
45	AB	812	CLA	CAB-C3B	-3.16	1.44	1.50
45	A3	302	CLA	C1D-ND	3.16	1.42	1.37
45	BA	827	CLA	C1D-ND	3.16	1.42	1.37
45	B1	314	CLA	C4B-NB	3.16	1.42	1.37
45	B3	310	CLA	C4B-NB	3.16	1.42	1.37
45	BB	811	CLA	C1D-ND	3.16	1.42	1.37
45	AA	818	CLA	C1D-ND	3.16	1.42	1.37
45	A3	304	CLA	C4B-NB	3.16	1.42	1.37
45	B1	310	CLA	C4B-NB	3.16	1.42	1.37
45	AB	802	CLA	C1D-ND	3.15	1.42	1.37
45	A1	305	CLA	C4B-NB	3.15	1.42	1.37
45	BA	838	CLA	C4B-NB	3.15	1.42	1.37
45	B3	303	CLA	C4B-NB	3.15	1.42	1.37
45	A1	310	CLA	C1D-ND	3.15	1.42	1.37
45	B2	603	CLA	C4B-NB	3.15	1.42	1.37
45	AA	815	CLA	C2D-C1D	3.15	1.48	1.42
45	A6	611	CLA	C4B-NB	3.15	1.42	1.37
45	BK	202	CLA	C4B-NB	3.15	1.42	1.37
45	BB	813	CLA	CAB-C3B	-3.15	1.44	1.50
50	AB	850	LMU	O5B-C1B	3.15	1.49	1.41
45	BK	201	CLA	CAB-C3B	-3.15	1.44	1.50
45	BA	836	CLA	C4B-NB	3.15	1.42	1.37
45	B5	602	CLA	C4B-NB	3.15	1.42	1.37
45	A6	610	CLA	C4B-NB	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	AA	851	LMU	O5B-C1B	3.15	1.49	1.41
54	A4	314	CHL	CHA-CBD	-3.15	1.48	1.51
45	A3	306	CLA	CAB-C3B	-3.14	1.44	1.50
45	BA	809	CLA	C1D-ND	3.14	1.42	1.37
46	AA	843	PQN	C11-C12	3.14	1.55	1.50
45	A3	314	CLA	C4B-NB	3.14	1.42	1.37
45	A4	310	CLA	C4B-NB	3.14	1.42	1.37
45	BG	201	CLA	C1D-ND	3.14	1.42	1.37
45	B1	312	CLA	CAB-C3B	-3.14	1.44	1.50
45	B3	305	CLA	CAB-C3B	-3.14	1.44	1.50
45	BB	821	CLA	C1D-ND	3.14	1.42	1.37
45	A6	611	CLA	CAB-C3B	-3.14	1.44	1.50
45	AA	805	CLA	C1D-ND	3.14	1.42	1.37
45	BA	828	CLA	C1D-ND	3.14	1.42	1.37
45	B1	315	CLA	CAB-C3B	-3.13	1.44	1.50
45	AA	810	CLA	C1D-ND	3.13	1.42	1.37
45	BA	811	CLA	C1D-ND	3.13	1.42	1.37
45	BB	819	CLA	C1D-ND	3.13	1.42	1.37
45	BB	835	CLA	C4B-NB	3.13	1.42	1.37
45	BA	804	CLA	C1D-ND	3.13	1.42	1.37
45	A3	311	CLA	C4B-NB	3.12	1.42	1.37
45	AG	203	CLA	C1D-ND	3.12	1.42	1.37
45	A3	305	CLA	C4B-NB	3.12	1.42	1.37
45	BB	827	CLA	C1D-ND	3.12	1.42	1.37
45	BB	810	CLA	C4B-NB	3.12	1.42	1.37
45	BA	808	CLA	C1D-ND	3.12	1.42	1.37
45	B2	612	CLA	C4B-NB	3.12	1.42	1.37
45	A3	310	CLA	C4B-NB	3.12	1.42	1.37
45	AB	826	CLA	C1D-ND	3.12	1.42	1.37
45	B3	314	CLA	C1D-ND	3.11	1.42	1.37
45	A6	613	CLA	C4B-NB	3.11	1.42	1.37
45	BL	304	CLA	C4B-NB	3.11	1.41	1.37
54	A6	602	CHL	CHA-CBD	-3.11	1.48	1.51
45	BL	304	CLA	C1D-ND	3.11	1.41	1.37
45	B1	307	CLA	C4B-NB	3.11	1.41	1.37
45	BA	841	CLA	C1D-ND	3.11	1.41	1.37
45	BL	302	CLA	C4B-NB	3.11	1.41	1.37
45	B5	612	CLA	C4B-NB	3.11	1.41	1.37
45	AJ	102	CLA	C4B-NB	3.11	1.41	1.37
45	B1	309	CLA	C4B-NB	3.11	1.41	1.37
45	AA	804	CLA	C1D-ND	3.11	1.41	1.37
54	A6	608	CHL	CHA-CBD	-3.11	1.48	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	e	301	SQD	O48-C23	3.11	1.42	1.33
45	B5	609	CLA	C4B-NB	3.11	1.41	1.37
45	AA	831	CLA	C4B-NB	3.10	1.41	1.37
45	BA	819	CLA	C1D-ND	3.10	1.41	1.37
45	A6	612	CLA	C4B-NB	3.10	1.41	1.37
45	A6	603	CLA	C1D-ND	3.10	1.41	1.37
45	B1	315	CLA	C4B-NB	3.10	1.41	1.37
45	BB	843	CLA	C4B-NB	3.10	1.41	1.37
45	AA	808	CLA	C4B-NB	3.10	1.41	1.37
45	AB	833	CLA	C1D-ND	3.10	1.41	1.37
45	BB	829	CLA	C1D-ND	3.10	1.41	1.37
45	A1	315	CLA	CAB-C3B	-3.10	1.44	1.50
45	AB	835	CLA	C1D-ND	3.09	1.41	1.37
45	BA	830	CLA	C1D-ND	3.09	1.41	1.37
45	BA	809	CLA	C4B-NB	3.09	1.41	1.37
45	A1	310	CLA	C4B-NB	3.09	1.41	1.37
45	BB	802	CLA	C4B-NB	3.09	1.41	1.37
45	A4	313	CLA	C4B-NB	3.09	1.41	1.37
45	BA	806	CLA	C1D-ND	3.09	1.41	1.37
45	A3	303	CLA	C4B-NB	3.09	1.41	1.37
45	AA	842	CLA	C1D-ND	3.09	1.41	1.37
45	AA	829	CLA	C1D-ND	3.08	1.41	1.37
45	BA	823	CLA	C4B-NB	3.08	1.41	1.37
45	BB	812	CLA	C1D-ND	3.08	1.41	1.37
45	BB	822	CLA	C1D-ND	3.08	1.41	1.37
45	BB	816	CLA	C1D-ND	3.08	1.41	1.37
45	AL	305	CLA	C4B-NB	3.08	1.41	1.37
54	A4	305	CHL	CHA-CBD	-3.08	1.48	1.51
45	BB	837	CLA	C4B-NB	3.08	1.41	1.37
45	BB	833	CLA	C4B-NB	3.08	1.41	1.37
45	B3	305	CLA	C4B-NB	3.08	1.41	1.37
45	AB	823	CLA	C1D-ND	3.08	1.41	1.37
45	AF	804	CLA	C4B-NB	3.08	1.41	1.37
45	B1	305	CLA	C4B-NB	3.08	1.41	1.37
45	BA	842	CLA	C1D-ND	3.07	1.41	1.37
45	BF	301	CLA	C1D-ND	3.07	1.41	1.37
45	B2	613	CLA	C4B-NB	3.07	1.41	1.37
45	BF	303	CLA	C4B-NB	3.07	1.41	1.37
45	BA	825	CLA	C1D-ND	3.07	1.41	1.37
45	AB	822	CLA	C1D-ND	3.07	1.41	1.37
45	AA	801	CLA	C4B-NB	3.07	1.41	1.37
45	A4	312	CLA	C4B-NB	3.07	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BJ	102	CLA	C4B-NB	3.07	1.41	1.37
45	BA	833	CLA	C1D-ND	3.07	1.41	1.37
45	BB	806	CLA	C1D-ND	3.06	1.41	1.37
45	BB	840	CLA	C1D-ND	3.06	1.41	1.37
45	AB	805	CLA	C1D-ND	3.06	1.41	1.37
45	AB	830	CLA	C4B-NB	3.06	1.41	1.37
45	AB	840	CLA	C4B-NB	3.06	1.41	1.37
45	A3	306	CLA	C4B-NB	3.06	1.41	1.37
45	AA	810	CLA	C4B-NB	3.06	1.41	1.37
45	B5	608	CLA	C4B-NB	3.06	1.41	1.37
54	B5	606	CHL	CHA-CBD	-3.06	1.48	1.51
45	AB	802	CLA	C4B-NB	3.06	1.41	1.37
45	AB	836	CLA	C4B-NB	3.06	1.41	1.37
45	A1	306	CLA	C4B-NB	3.06	1.41	1.37
45	A1	315	CLA	C4B-NB	3.06	1.41	1.37
45	BA	838	CLA	C1D-ND	3.05	1.41	1.37
45	BG	202	CLA	C4B-NB	3.05	1.41	1.37
45	B3	301	CLA	C4B-NB	3.05	1.41	1.37
45	B2	610	CLA	C4B-NB	3.05	1.41	1.37
45	AA	824	CLA	C1D-ND	3.05	1.41	1.37
45	BB	802	CLA	C1D-ND	3.05	1.41	1.37
48	AA	849	BCR	C30-C25	-3.05	1.49	1.53
45	AA	841	CLA	C1D-ND	3.05	1.41	1.37
45	B2	610	CLA	CAB-C3B	-3.04	1.44	1.50
45	B5	602	CLA	C1D-ND	3.04	1.41	1.37
45	BB	839	CLA	C4B-NB	3.04	1.41	1.37
45	BA	802	CLA	C1D-ND	3.04	1.41	1.37
45	B5	603	CLA	C4B-NB	3.04	1.41	1.37
48	BG	203	BCR	C1-C6	-3.04	1.49	1.53
45	BB	824	CLA	C1D-ND	3.04	1.41	1.37
45	AA	817	CLA	C1D-ND	3.04	1.41	1.37
45	AB	803	CLA	C1D-ND	3.04	1.41	1.37
45	B5	613	CLA	C4B-NB	3.04	1.41	1.37
45	AB	820	CLA	C1D-ND	3.04	1.41	1.37
54	B1	308	CHL	CHA-CBD	-3.03	1.48	1.51
45	AA	816	CLA	C4B-NB	3.03	1.41	1.37
45	BA	826	CLA	C1D-ND	3.03	1.41	1.37
54	B1	303	CHL	CHA-CBD	-3.03	1.48	1.51
45	BB	814	CLA	C1D-ND	3.02	1.41	1.37
45	A3	312	CLA	C4B-NB	3.02	1.41	1.37
45	BB	830	CLA	C1D-ND	3.02	1.41	1.37
45	A3	313	CLA	C4B-NB	3.02	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	827	CLA	C4B-NB	3.02	1.41	1.37
45	AB	813	CLA	C1D-ND	3.02	1.41	1.37
45	AB	814	CLA	C1D-ND	3.02	1.41	1.37
45	AA	838	CLA	C1D-ND	3.01	1.41	1.37
45	BB	831	CLA	C4B-NB	3.01	1.41	1.37
45	AA	811	CLA	C4B-NB	3.01	1.41	1.37
45	B3	314	CLA	C4B-NB	3.01	1.41	1.37
45	BB	804	CLA	C1D-ND	3.01	1.41	1.37
45	BA	811	CLA	C4B-NB	3.01	1.41	1.37
45	AA	833	CLA	C4B-NB	3.01	1.41	1.37
45	BA	831	CLA	C4B-NB	3.00	1.41	1.37
45	AA	808	CLA	C1D-ND	3.00	1.41	1.37
45	BB	823	CLA	C4B-NB	3.00	1.41	1.37
45	AA	834	CLA	C1D-ND	3.00	1.41	1.37
45	BA	802	CLA	C4B-NB	3.00	1.41	1.37
45	A3	315	CLA	C1D-ND	3.00	1.41	1.37
45	A4	309	CLA	C4B-NB	3.00	1.41	1.37
45	BA	801	CLA	C4B-NB	3.00	1.41	1.37
45	AA	817	CLA	C4B-NB	3.00	1.41	1.37
45	BB	836	CLA	C4B-NB	3.00	1.41	1.37
45	BK	203	CLA	C4B-NB	3.00	1.41	1.37
45	BB	813	CLA	C4B-NB	2.99	1.41	1.37
45	AA	802	CLA	C1D-ND	2.99	1.41	1.37
45	AA	827	CLA	C4B-NB	2.99	1.41	1.37
45	BA	833	CLA	C4B-NB	2.99	1.41	1.37
45	AA	830	CLA	C4B-NB	2.99	1.41	1.37
45	BA	806	CLA	C4B-NB	2.99	1.41	1.37
45	A1	312	CLA	C4B-NB	2.99	1.41	1.37
45	A6	609	CLA	C4B-NB	2.99	1.41	1.37
45	BB	838	CLA	C4B-NB	2.99	1.41	1.37
45	BA	807	CLA	C4B-NB	2.98	1.41	1.37
45	BB	824	CLA	C4B-NB	2.98	1.41	1.37
45	BA	814	CLA	C4B-NB	2.98	1.41	1.37
45	BB	822	CLA	C4B-NB	2.98	1.41	1.37
45	BB	825	CLA	C1D-ND	2.98	1.41	1.37
45	AB	830	CLA	CMD-C2D	-2.98	1.44	1.50
45	A6	605	CLA	C4B-NB	2.98	1.41	1.37
45	AA	815	CLA	C4B-NB	2.98	1.41	1.37
45	AB	829	CLA	C1D-ND	2.98	1.41	1.37
45	AB	803	CLA	C4B-NB	2.97	1.41	1.37
45	AB	837	CLA	C4B-NB	2.97	1.41	1.37
45	A3	309	CLA	C4B-NB	2.97	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	842	CLA	C4B-NB	2.97	1.41	1.37
48	A3	318	BCR	C40-C30	2.97	1.59	1.53
45	B2	602	CLA	C1D-ND	2.97	1.41	1.37
45	AA	821	CLA	C4B-NB	2.97	1.41	1.37
55	A6	616	XAT	O4-C5	-2.97	1.42	1.46
45	A1	313	CLA	C4B-NB	2.97	1.41	1.37
45	AB	810	CLA	C1D-ND	2.97	1.41	1.37
45	AB	812	CLA	C4B-NB	2.97	1.41	1.37
45	AB	821	CLA	C4B-NB	2.96	1.41	1.37
45	AK	203	CLA	C4B-NB	2.96	1.41	1.37
45	BA	830	CLA	C4B-NB	2.96	1.41	1.37
45	BA	804	CLA	C4B-NB	2.96	1.41	1.37
45	B1	313	CLA	C4B-NB	2.96	1.41	1.37
45	BA	835	CLA	C4B-NB	2.96	1.41	1.37
45	AA	828	CLA	C3B-C4B	2.96	1.51	1.42
45	AA	826	CLA	C1D-ND	2.96	1.41	1.37
45	AA	840	CLA	C1D-ND	2.96	1.41	1.37
45	AB	831	CLA	C1D-ND	2.96	1.41	1.37
45	BA	828	CLA	C4B-NB	2.96	1.41	1.37
45	A1	307	CLA	C4B-NB	2.95	1.41	1.37
45	AA	825	CLA	CMD-C2D	-2.95	1.44	1.50
45	BB	842	CLA	C1B-C2B	2.95	1.50	1.43
45	AA	825	CLA	C4B-NB	2.95	1.41	1.37
45	BF	301	CLA	C4B-NB	2.95	1.41	1.37
45	BB	838	CLA	C1D-ND	2.95	1.41	1.37
45	AB	834	CLA	C4B-NB	2.95	1.41	1.37
45	A1	316	CLA	C4B-NB	2.95	1.41	1.37
45	B1	312	CLA	C4B-NB	2.95	1.41	1.37
45	AA	833	CLA	C1D-ND	2.95	1.41	1.37
45	AA	835	CLA	C4B-NB	2.95	1.41	1.37
45	AA	820	CLA	C4B-NB	2.94	1.41	1.37
45	B5	611	CLA	C4B-NB	2.94	1.41	1.37
45	AB	841	CLA	C4B-NB	2.94	1.41	1.37
45	AA	825	CLA	C1D-ND	2.94	1.41	1.37
45	AA	814	CLA	C4B-NB	2.94	1.41	1.37
45	BA	816	CLA	C4B-NB	2.94	1.41	1.37
45	B3	302	CLA	C4B-NB	2.94	1.41	1.37
45	BB	822	CLA	C1B-C2B	2.94	1.50	1.43
45	BB	807	CLA	C4B-NB	2.94	1.41	1.37
45	B2	608	CLA	C4B-NB	2.93	1.41	1.37
45	BA	817	CLA	C4B-NB	2.93	1.41	1.37
45	BB	832	CLA	C1D-ND	2.93	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	823	CLA	C1D-ND	2.93	1.41	1.37
45	BB	815	CLA	C1D-ND	2.93	1.41	1.37
45	BB	834	CLA	C1B-C2B	2.93	1.50	1.43
45	BA	830	CLA	CMB-C2B	-2.93	1.44	1.50
45	B3	308	CLA	C4B-NB	2.93	1.41	1.37
45	A4	303	CLA	C4B-NB	2.92	1.41	1.37
45	A3	302	CLA	C4B-NB	2.92	1.41	1.37
45	BB	828	CLA	C4B-NB	2.92	1.41	1.37
45	B3	307	CLA	C4B-NB	2.92	1.41	1.37
45	AB	815	CLA	C1D-ND	2.92	1.41	1.37
45	A4	302	CLA	C4B-NB	2.92	1.41	1.37
45	AA	802	CLA	CMD-C2D	-2.92	1.44	1.50
45	AB	831	CLA	C4B-NB	2.92	1.41	1.37
45	BA	818	CLA	C4B-NB	2.92	1.41	1.37
45	AH	201	CLA	C1B-C2B	2.92	1.50	1.43
45	BA	810	CLA	C4B-NB	2.92	1.41	1.37
45	BA	824	CLA	C4B-NB	2.91	1.41	1.37
45	BB	826	CLA	C4B-NB	2.91	1.41	1.37
45	A1	316	CLA	C1B-C2B	2.91	1.50	1.43
45	AA	830	CLA	C1D-ND	2.91	1.41	1.37
45	AA	802	CLA	C4B-NB	2.90	1.41	1.37
45	B2	602	CLA	C4B-NB	2.90	1.41	1.37
45	A1	304	CLA	C1D-ND	2.90	1.41	1.37
45	BA	829	CLA	C1D-ND	2.90	1.41	1.37
45	AA	830	CLA	CMB-C2B	-2.89	1.44	1.50
45	AA	828	CLA	C4B-NB	2.89	1.41	1.37
45	B3	313	CLA	C4B-NB	2.89	1.41	1.37
45	AB	839	CLA	C1D-ND	2.89	1.41	1.37
45	AB	816	CLA	C4B-NB	2.88	1.41	1.37
45	A4	313	CLA	C1B-C2B	2.88	1.49	1.43
54	B2	601	CHL	CHA-CBD	-2.88	1.48	1.51
45	BB	812	CLA	C4B-NB	2.88	1.41	1.37
45	A3	308	CLA	C4B-NB	2.88	1.41	1.37
45	BB	831	CLA	C1D-ND	2.88	1.41	1.37
45	BB	840	CLA	C4B-NB	2.88	1.41	1.37
45	AB	823	CLA	C4B-NB	2.87	1.41	1.37
45	BB	816	CLA	C4B-NB	2.87	1.41	1.37
45	AB	838	CLA	C4B-NB	2.87	1.41	1.37
45	AB	824	CLA	C1D-ND	2.87	1.41	1.37
45	AB	840	CLA	CMD-C2D	-2.87	1.44	1.50
45	BB	827	CLA	C4B-NB	2.87	1.41	1.37
45	AB	835	CLA	C4B-NB	2.86	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	801	CLA	C1B-C2B	2.86	1.49	1.43
45	AB	834	CLA	C1D-ND	2.86	1.41	1.37
45	BB	842	CLA	C4B-NB	2.86	1.41	1.37
45	AA	841	CLA	CMC-C2C	-2.86	1.44	1.50
45	AB	840	CLA	C1D-ND	2.85	1.41	1.37
45	A4	301	CLA	C4B-NB	2.85	1.41	1.37
45	AB	813	CLA	C4B-NB	2.85	1.41	1.37
52	B1	316	LUT	C8-C9	-2.85	1.39	1.46
45	AA	804	CLA	C4B-NB	2.85	1.41	1.37
45	BA	803	CLA	CMD-C2D	-2.84	1.44	1.50
45	AB	827	CLA	C4B-NB	2.84	1.41	1.37
45	AB	820	CLA	CMB-C2B	-2.84	1.44	1.50
54	B2	601	CHL	CBD-CGD	-2.84	1.48	1.52
45	BA	825	CLA	C4B-NB	2.84	1.41	1.37
45	A1	314	CLA	C4B-NB	2.84	1.41	1.37
45	BL	303	CLA	C4B-NB	2.84	1.41	1.37
45	AB	807	CLA	C1D-ND	2.84	1.41	1.37
45	A6	603	CLA	C4B-NB	2.84	1.41	1.37
45	AA	833	CLA	CMB-C2B	-2.83	1.45	1.50
45	BB	832	CLA	C4B-NB	2.83	1.41	1.37
45	BB	835	CLA	C1D-ND	2.83	1.41	1.37
45	AA	832	CLA	C4B-NB	2.83	1.41	1.37
45	BB	841	CLA	C1D-ND	2.83	1.41	1.37
45	AF	802	CLA	CMB-C2B	-2.83	1.45	1.50
45	AB	826	CLA	C4B-NB	2.83	1.41	1.37
45	BB	819	CLA	C4B-NB	2.83	1.41	1.37
45	BA	820	CLA	C1B-C2B	2.83	1.49	1.43
45	BA	839	CLA	C4B-NB	2.83	1.41	1.37
45	BB	837	CLA	C1B-C2B	2.83	1.49	1.43
45	BB	825	CLA	C4B-NB	2.83	1.41	1.37
45	AB	801	CLA	CMD-C2D	-2.83	1.45	1.50
45	AA	839	CLA	C1B-C2B	2.82	1.49	1.43
45	AB	839	CLA	C4B-NB	2.82	1.41	1.37
45	AB	825	CLA	CMD-C2D	-2.82	1.45	1.50
45	A3	304	CLA	C4B-C3B	2.82	1.49	1.43
45	AG	203	CLA	C1B-C2B	2.82	1.49	1.43
45	B3	313	CLA	C1B-C2B	2.82	1.49	1.43
45	AB	809	CLA	C1D-ND	2.82	1.41	1.37
45	AB	817	CLA	C4B-NB	2.82	1.41	1.37
45	BB	809	CLA	C4B-NB	2.82	1.41	1.37
45	AB	838	CLA	C1D-ND	2.82	1.41	1.37
45	BB	821	CLA	C4B-NB	2.82	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	839	CLA	C4B-NB	2.82	1.41	1.37
45	B3	309	CLA	C1B-C2B	2.82	1.49	1.43
45	BB	831	CLA	CMB-C2B	-2.81	1.45	1.50
45	AA	838	CLA	C4B-NB	2.81	1.41	1.37
45	B1	304	CLA	C4B-NB	2.81	1.41	1.37
45	BB	831	CLA	C1B-C2B	2.81	1.49	1.43
45	AA	803	CLA	C4B-NB	2.81	1.41	1.37
52	B3	315	LUT	C26-C27	2.81	1.54	1.50
45	A6	611	CLA	C1D-ND	2.80	1.41	1.37
45	BB	817	CLA	C4B-NB	2.80	1.41	1.37
45	BB	814	CLA	C4B-NB	2.80	1.41	1.37
45	A1	310	CLA	C1B-C2B	2.80	1.49	1.43
45	A3	312	CLA	C1B-C2B	2.80	1.49	1.43
54	B2	606	CHL	CHA-CBD	-2.80	1.48	1.51
45	AB	829	CLA	CMB-C2B	-2.79	1.45	1.50
45	AB	807	CLA	C1B-C2B	2.79	1.49	1.43
45	BB	839	CLA	C1D-ND	2.79	1.41	1.37
45	B5	611	CLA	C1B-C2B	2.79	1.49	1.43
45	AB	825	CLA	C4B-NB	2.79	1.41	1.37
45	AB	829	CLA	CMD-C2D	-2.79	1.45	1.50
45	AB	833	CLA	C1B-C2B	2.79	1.49	1.43
45	BB	804	CLA	C4B-NB	2.79	1.41	1.37
45	BA	801	CLA	C1B-C2B	2.79	1.49	1.43
45	A3	315	CLA	C4B-NB	2.78	1.41	1.37
46	AA	843	PQN	C10-C1	2.78	1.53	1.48
45	AF	802	CLA	C1D-ND	2.78	1.41	1.37
45	AA	807	CLA	C4B-NB	2.78	1.41	1.37
45	BA	841	CLA	C4B-NB	2.78	1.41	1.37
45	BB	823	CLA	C1B-C2B	2.78	1.49	1.43
54	A4	304	CHL	CHA-CBD	-2.78	1.48	1.51
45	BA	802	CLA	CMD-C2D	-2.78	1.45	1.50
45	B1	305	CLA	C1B-C2B	2.77	1.49	1.43
45	AA	841	CLA	C4B-NB	2.77	1.41	1.37
45	A3	315	CLA	CMD-C2D	-2.77	1.45	1.50
56	e	301	SQD	O47-C7	2.77	1.42	1.34
45	BA	827	CLA	C1B-C2B	2.76	1.49	1.43
45	BB	825	CLA	C1B-C2B	2.76	1.49	1.43
45	BB	806	CLA	C4B-NB	2.76	1.41	1.37
45	BA	817	CLA	C1B-C2B	2.76	1.49	1.43
45	AL	305	CLA	C1B-C2B	2.76	1.49	1.43
45	BB	818	CLA	C4B-NB	2.76	1.41	1.37
45	AB	805	CLA	CMD-C2D	-2.76	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	830	CLA	CMB-C2B	-2.76	1.45	1.50
45	BB	834	CLA	C4B-NB	2.76	1.41	1.37
45	AA	842	CLA	C4B-NB	2.75	1.41	1.37
45	AB	806	CLA	C4B-NB	2.75	1.41	1.37
47	a	501	LHG	O7-C5	-2.75	1.40	1.46
45	AA	819	CLA	CMB-C2B	-2.75	1.45	1.50
45	BA	826	CLA	C4B-NB	2.75	1.41	1.37
45	B1	304	CLA	C1D-ND	2.75	1.41	1.37
45	AB	823	CLA	C1B-C2B	2.75	1.49	1.43
45	BA	813	CLA	C1B-C2B	2.75	1.49	1.43
45	BA	832	CLA	C4B-NB	2.75	1.41	1.37
45	AK	202	CLA	C1B-C2B	2.75	1.49	1.43
45	AA	842	CLA	C1B-C2B	2.75	1.49	1.43
45	A4	302	CLA	C1B-C2B	2.75	1.49	1.43
45	BB	841	CLA	CMD-C2D	-2.75	1.45	1.50
45	AB	832	CLA	C4B-NB	2.75	1.41	1.37
45	BA	805	CLA	C1B-C2B	2.75	1.49	1.43
45	AB	840	CLA	CMB-C2B	-2.75	1.45	1.50
45	BB	826	CLA	CMD-C2D	-2.75	1.45	1.50
45	A3	311	CLA	C1B-C2B	2.74	1.49	1.43
45	BB	831	CLA	CMD-C2D	-2.74	1.45	1.50
45	BB	840	CLA	C1B-C2B	2.74	1.49	1.43
45	BA	825	CLA	CMD-C2D	-2.74	1.45	1.50
45	AB	805	CLA	C4B-NB	2.74	1.41	1.37
45	AK	203	CLA	C1B-C2B	2.74	1.49	1.43
45	A1	306	CLA	C1B-C2B	2.74	1.49	1.43
48	AA	847	BCR	C8-C9	2.74	1.51	1.46
45	AB	815	CLA	C4B-NB	2.74	1.41	1.37
45	BA	840	CLA	C1B-C2B	2.74	1.49	1.43
45	BB	841	CLA	C4B-NB	2.73	1.41	1.37
45	A3	310	CLA	C1B-C2B	2.73	1.49	1.43
45	AB	810	CLA	CMB-C2B	-2.73	1.45	1.50
45	B2	603	CLA	C1B-C2B	2.73	1.49	1.43
45	BA	833	CLA	CMB-C2B	-2.73	1.45	1.50
45	AA	805	CLA	C1B-C2B	2.73	1.49	1.43
45	AB	803	CLA	C1B-C2B	2.73	1.49	1.43
45	BA	824	CLA	C1B-C2B	2.73	1.49	1.43
45	AJ	102	CLA	C1B-C2B	2.73	1.49	1.43
45	B3	310	CLA	C1B-C2B	2.73	1.49	1.43
45	AB	828	CLA	C4B-NB	2.72	1.41	1.37
45	AA	830	CLA	CMC-C2C	-2.72	1.45	1.50
45	B3	303	CLA	C4B-C3B	2.72	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	802	CLA	C4B-C3B	2.72	1.49	1.43
45	BA	842	CLA	CMD-C2D	-2.72	1.45	1.50
45	AB	818	CLA	C4B-NB	2.72	1.41	1.37
45	AA	826	CLA	C4B-NB	2.72	1.41	1.37
45	BA	823	CLA	C1B-C2B	2.72	1.49	1.43
48	BA	851	BCR	C1-C6	-2.72	1.50	1.53
45	B5	601	CLA	C4B-NB	2.72	1.41	1.37
45	BB	807	CLA	C1B-C2B	2.72	1.49	1.43
45	BA	813	CLA	C4B-NB	2.72	1.41	1.37
45	B2	610	CLA	C4B-C3B	2.72	1.49	1.43
45	AB	819	CLA	C4B-NB	2.71	1.41	1.37
45	A1	315	CLA	C1B-C2B	2.71	1.49	1.43
45	BB	835	CLA	CMD-C2D	-2.71	1.45	1.50
45	BB	826	CLA	C1D-ND	2.71	1.41	1.37
45	BB	817	CLA	C1B-C2B	2.71	1.49	1.43
45	BA	803	CLA	C1D-ND	2.71	1.41	1.37
45	AA	818	CLA	C4B-NB	2.70	1.41	1.37
45	A3	305	CLA	C1B-C2B	2.70	1.49	1.43
45	BB	820	CLA	C1B-C2B	2.70	1.49	1.43
45	BB	830	CLA	CMD-C2D	-2.70	1.45	1.50
45	A4	301	CLA	C1D-ND	2.70	1.41	1.37
45	AB	801	CLA	C4B-NB	2.70	1.41	1.37
45	AB	832	CLA	C1B-C2B	2.70	1.49	1.43
45	AA	814	CLA	C1B-C2B	2.70	1.49	1.43
45	B1	306	CLA	C1B-C2B	2.70	1.49	1.43
45	AA	820	CLA	C1B-C2B	2.70	1.49	1.43
45	BA	821	CLA	C4B-NB	2.70	1.41	1.37
45	BK	201	CLA	C1B-C2B	2.70	1.49	1.43
45	AB	804	CLA	CMD-C2D	-2.69	1.45	1.50
47	F	801	LHG	O7-C5	-2.69	1.40	1.46
45	AB	816	CLA	C1B-C2B	2.69	1.49	1.43
45	A1	311	CLA	C3B-C4B	2.69	1.50	1.42
45	AA	806	CLA	C4B-NB	2.69	1.41	1.37
45	A6	605	CLA	C1B-C2B	2.69	1.49	1.43
45	B3	302	CLA	C1B-C2B	2.69	1.49	1.43
45	AB	812	CLA	C4B-C3B	2.69	1.49	1.43
45	AB	830	CLA	C1B-C2B	2.69	1.49	1.43
45	A3	314	CLA	C1B-C2B	2.69	1.49	1.43
45	BB	813	CLA	C4B-C3B	2.69	1.49	1.43
45	B1	304	CLA	C1B-C2B	2.69	1.49	1.43
45	A6	611	CLA	C4B-C3B	2.68	1.49	1.43
45	B5	604	CLA	C1B-C2B	2.68	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BF	303	CLA	C1B-C2B	2.68	1.49	1.43
45	A4	309	CLA	C1B-C2B	2.68	1.49	1.43
45	B1	311	CLA	C1B-C2B	2.68	1.49	1.43
45	A6	601	CLA	CMC-C2C	-2.68	1.45	1.50
45	AB	824	CLA	C1B-C2B	2.68	1.49	1.43
45	BK	203	CLA	C1B-C2B	2.68	1.49	1.43
45	B3	311	CLA	C1B-C2B	2.68	1.49	1.43
45	AB	808	CLA	C4B-NB	2.68	1.41	1.37
45	AB	830	CLA	C1D-ND	2.68	1.41	1.37
45	AA	818	CLA	CMD-C2D	-2.68	1.45	1.50
45	BA	807	CLA	C1B-C2B	2.68	1.49	1.43
45	BJ	102	CLA	C1B-C2B	2.68	1.49	1.43
45	BA	815	CLA	C4B-NB	2.67	1.41	1.37
45	B5	612	CLA	C1B-C2B	2.67	1.49	1.43
45	B5	604	CLA	C4B-C3B	2.67	1.49	1.43
45	BB	820	CLA	C4B-NB	2.67	1.41	1.37
45	BG	202	CLA	C1B-C2B	2.67	1.49	1.43
45	BF	301	CLA	C1B-C2B	2.67	1.49	1.43
45	A1	304	CLA	C4B-NB	2.67	1.41	1.37
45	BA	819	CLA	C4B-NB	2.67	1.41	1.37
45	AB	822	CLA	C1B-C2B	2.67	1.49	1.43
45	BB	806	CLA	C1B-C2B	2.66	1.49	1.43
45	AA	822	CLA	C1B-C2B	2.66	1.49	1.43
45	B1	309	CLA	C1B-C2B	2.66	1.49	1.43
45	AA	810	CLA	C1B-C2B	2.66	1.49	1.43
45	BA	822	CLA	C1B-C2B	2.66	1.49	1.43
45	AB	833	CLA	C4B-NB	2.66	1.41	1.37
48	BF	304	BCR	C1-C6	-2.66	1.50	1.53
45	BA	839	CLA	C1B-C2B	2.66	1.49	1.43
45	AA	823	CLA	C1B-C2B	2.66	1.49	1.43
45	BA	834	CLA	C4B-NB	2.66	1.41	1.37
45	AA	827	CLA	C1B-C2B	2.66	1.49	1.43
45	BB	829	CLA	C4B-NB	2.66	1.41	1.37
45	B5	613	CLA	C1B-C2B	2.65	1.49	1.43
45	AA	830	CLA	C1B-C2B	2.65	1.49	1.43
45	B1	315	CLA	C4B-C3B	2.65	1.49	1.43
45	AA	805	CLA	C4B-NB	2.65	1.41	1.37
45	AA	811	CLA	C1B-C2B	2.65	1.49	1.43
45	BB	801	CLA	C4B-NB	2.65	1.41	1.37
45	A1	305	CLA	C1B-C2B	2.65	1.49	1.43
45	BB	830	CLA	C4B-NB	2.65	1.41	1.37
45	A6	611	CLA	C1B-C2B	2.65	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BK	201	CLA	C4B-C3B	2.65	1.49	1.43
45	B3	305	CLA	C1B-C2B	2.65	1.49	1.43
45	BA	808	CLA	C4B-NB	2.65	1.41	1.37
45	B2	610	CLA	C1B-C2B	2.65	1.49	1.43
45	BA	820	CLA	C4B-NB	2.65	1.41	1.37
45	B3	304	CLA	C1B-C2B	2.64	1.49	1.43
45	AL	304	CLA	C4B-NB	2.64	1.41	1.37
45	A1	311	CLA	C1B-C2B	2.64	1.49	1.43
45	B2	604	CLA	C1B-C2B	2.64	1.49	1.43
45	BB	811	CLA	C4B-NB	2.64	1.41	1.37
45	BB	833	CLA	C1B-C2B	2.64	1.49	1.43
45	B5	603	CLA	C1B-C2B	2.64	1.49	1.43
46	BA	843	PQN	C5-C4	2.64	1.53	1.48
45	B1	310	CLA	C1B-C2B	2.64	1.49	1.43
45	B1	313	CLA	C1B-C2B	2.64	1.49	1.43
45	AA	840	CLA	CMD-C2D	-2.64	1.45	1.50
45	B3	305	CLA	C4B-C3B	2.64	1.49	1.43
45	BA	837	CLA	C4B-NB	2.64	1.41	1.37
45	AA	834	CLA	C1B-C2B	2.64	1.49	1.43
45	BA	828	CLA	C1B-C2B	2.64	1.49	1.43
45	BG	201	CLA	C1B-C2B	2.64	1.49	1.43
45	BB	810	CLA	C1D-ND	2.63	1.41	1.37
45	BB	804	CLA	C1B-C2B	2.63	1.49	1.43
45	AA	836	CLA	CMB-C2B	-2.63	1.45	1.50
45	BB	830	CLA	CMB-C2B	-2.63	1.45	1.50
45	AB	812	CLA	C1B-C2B	2.63	1.49	1.43
45	B2	613	CLA	C1B-C2B	2.63	1.49	1.43
45	A4	303	CLA	C4B-C3B	2.63	1.49	1.43
45	BK	202	CLA	C1B-C2B	2.63	1.49	1.43
45	BA	832	CLA	C1B-C2B	2.63	1.49	1.43
45	B3	308	CLA	C1B-C2B	2.63	1.49	1.43
45	B3	303	CLA	C1B-C2B	2.63	1.49	1.43
45	A4	303	CLA	C1B-C2B	2.63	1.49	1.43
45	B1	315	CLA	C1B-C2B	2.63	1.49	1.43
45	BL	304	CLA	C1B-C2B	2.62	1.49	1.43
45	BB	828	CLA	C1B-C2B	2.62	1.49	1.43
45	BA	805	CLA	C4B-NB	2.62	1.41	1.37
45	AA	817	CLA	C1B-C2B	2.62	1.49	1.43
45	B1	312	CLA	C1B-C2B	2.62	1.49	1.43
45	AB	807	CLA	CMD-C2D	-2.62	1.45	1.50
45	A1	313	CLA	C1B-C2B	2.62	1.49	1.43
45	AB	824	CLA	C4B-NB	2.62	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AF	804	CLA	C1B-C2B	2.62	1.49	1.43
45	BA	835	CLA	C1B-C2B	2.62	1.49	1.43
45	B3	312	CLA	C1B-C2B	2.62	1.49	1.43
45	BA	844	CLA	C1B-C2B	2.62	1.49	1.43
45	A6	611	CLA	CMD-C2D	-2.62	1.45	1.50
45	A3	313	CLA	C1B-C2B	2.62	1.49	1.43
45	BB	824	CLA	C1B-C2B	2.62	1.49	1.43
46	AA	843	PQN	C5-C4	2.62	1.53	1.48
45	AB	813	CLA	C1B-C2B	2.61	1.49	1.43
45	AA	812	CLA	C1B-C2B	2.61	1.49	1.43
45	AG	201	CLA	C1B-C2B	2.61	1.49	1.43
45	B3	314	CLA	C1B-C2B	2.61	1.49	1.43
45	A1	314	CLA	C1B-C2B	2.61	1.49	1.43
45	AA	808	CLA	C1B-C2B	2.61	1.49	1.43
45	AB	801	CLA	CMB-C2B	-2.60	1.45	1.50
45	AF	802	CLA	C4B-NB	2.60	1.41	1.37
45	BA	829	CLA	MG-NB	-2.60	2.00	2.05
45	AB	841	CLA	C1B-C2B	2.60	1.49	1.43
45	BA	825	CLA	C1B-C2B	2.60	1.49	1.43
45	A4	312	CLA	C1B-C2B	2.60	1.49	1.43
45	BA	815	CLA	C1B-C2B	2.60	1.49	1.43
45	AA	824	CLA	C1B-C2B	2.60	1.49	1.43
45	A3	304	CLA	C1B-C2B	2.60	1.49	1.43
45	BA	828	CLA	C3B-C4B	2.60	1.50	1.42
45	AB	811	CLA	C4B-NB	2.60	1.41	1.37
45	AB	829	CLA	C4B-NB	2.60	1.41	1.37
45	BB	818	CLA	C1B-C2B	2.60	1.49	1.43
55	B3	316	XAT	O24-C25	-2.60	1.42	1.46
45	B2	612	CLA	CMB-C2B	-2.60	1.45	1.50
45	A3	306	CLA	C1B-C2B	2.60	1.49	1.43
45	BH	201	CLA	C1B-C2B	2.60	1.49	1.43
45	AA	829	CLA	MG-NB	-2.60	2.00	2.05
45	AA	840	CLA	C4B-NB	2.60	1.41	1.37
45	AB	834	CLA	C1B-C2B	2.59	1.49	1.43
45	BB	832	CLA	CMB-C2B	-2.59	1.45	1.50
45	AA	813	CLA	C4B-NB	2.59	1.41	1.37
45	BB	836	CLA	C1B-C2B	2.59	1.49	1.43
45	A3	306	CLA	C4B-C3B	2.59	1.49	1.43
45	AB	842	CLA	CMD-C2D	-2.59	1.45	1.50
45	A1	311	CLA	CMC-C2C	-2.59	1.45	1.50
45	BB	838	CLA	C1B-C2B	2.59	1.49	1.43
46	BB	844	PQN	C2-C1	2.59	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	821	CLA	C1B-C2B	2.59	1.49	1.43
45	AL	303	CLA	CMB-C2B	-2.58	1.45	1.50
45	AA	832	CLA	C1B-C2B	2.58	1.49	1.43
45	BB	813	CLA	C1B-C2B	2.58	1.49	1.43
45	AA	834	CLA	C4B-NB	2.58	1.41	1.37
45	BA	810	CLA	C1B-C2B	2.58	1.49	1.43
45	B1	312	CLA	C4B-C3B	2.58	1.49	1.43
45	A1	310	CLA	C4B-C3B	2.58	1.49	1.43
45	BB	808	CLA	C4B-NB	2.58	1.41	1.37
45	AA	815	CLA	C1B-C2B	2.58	1.49	1.43
46	AB	843	PQN	C5-C4	2.58	1.53	1.48
45	B1	304	CLA	CMD-C2D	-2.58	1.45	1.50
45	AB	831	CLA	CMB-C2B	-2.58	1.45	1.50
45	A1	315	CLA	C4B-C3B	2.58	1.49	1.43
45	A6	613	CLA	C1B-C2B	2.58	1.49	1.43
45	BA	819	CLA	CMB-C2B	-2.58	1.45	1.50
45	AA	812	CLA	C4B-NB	2.58	1.41	1.37
45	AB	806	CLA	C3B-C4B	2.58	1.50	1.42
45	A4	310	CLA	C1B-C2B	2.58	1.49	1.43
45	AA	803	CLA	C1B-C2B	2.58	1.49	1.43
45	AB	806	CLA	C1B-C2B	2.58	1.49	1.43
45	A6	614	CLA	C1B-C2B	2.58	1.49	1.43
45	BA	844	CLA	C3B-C4B	2.57	1.50	1.42
45	BA	803	CLA	C1B-C2B	2.57	1.49	1.43
45	AA	839	CLA	CMD-C2D	-2.57	1.45	1.50
45	BB	827	CLA	C1B-C2B	2.57	1.49	1.43
45	A4	307	CLA	CMD-C2D	-2.57	1.45	1.50
45	AA	837	CLA	C4B-NB	2.57	1.41	1.37
45	B1	310	CLA	C4B-C3B	2.57	1.49	1.43
45	BA	833	CLA	C1B-C2B	2.57	1.49	1.43
45	BA	830	CLA	C1B-C2B	2.56	1.49	1.43
45	B3	301	CLA	C1B-C2B	2.56	1.49	1.43
45	A3	308	CLA	C1B-C2B	2.56	1.49	1.43
45	BB	810	CLA	CMD-C2D	-2.56	1.45	1.50
45	AB	809	CLA	C1B-C2B	2.56	1.49	1.43
45	A3	309	CLA	CMD-C2D	-2.56	1.45	1.50
45	A1	312	CLA	C4B-C3B	2.56	1.49	1.43
45	A6	604	CLA	C1B-C2B	2.56	1.49	1.43
45	AA	809	CLA	CMD-C2D	-2.56	1.45	1.50
45	BA	831	CLA	CMB-C2B	-2.56	1.45	1.50
52	B1	316	LUT	C32-C33	-2.56	1.40	1.46
55	A4	316	XAT	O24-C25	-2.56	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	839	CLA	C1B-C2B	2.55	1.49	1.43
45	AB	842	CLA	C4B-NB	2.55	1.41	1.37
45	A1	304	CLA	C1B-C2B	2.55	1.49	1.43
45	AB	837	CLA	C1B-C2B	2.55	1.49	1.43
45	AA	829	CLA	CMB-C2B	-2.55	1.45	1.50
45	AG	204	CLA	C1B-C2B	2.55	1.49	1.43
45	BA	819	CLA	C1B-C2B	2.55	1.49	1.43
45	BA	806	CLA	C3B-C4B	2.55	1.50	1.42
45	A6	601	CLA	C4B-NB	2.55	1.41	1.37
45	BA	842	CLA	C1B-C2B	2.55	1.49	1.43
45	AB	836	CLA	CMB-C2B	-2.55	1.45	1.50
47	BA	846	LHG	O8-C23	2.55	1.45	1.33
45	AB	824	CLA	CMD-C2D	-2.55	1.45	1.50
45	AA	827	CLA	CMD-C2D	-2.54	1.45	1.50
45	BB	815	CLA	C1B-C2B	2.54	1.49	1.43
45	A1	312	CLA	C1B-C2B	2.54	1.49	1.43
45	A6	612	CLA	C1B-C2B	2.54	1.49	1.43
45	BB	839	CLA	C1B-C2B	2.54	1.49	1.43
45	AB	825	CLA	C1B-C2B	2.54	1.49	1.43
45	B1	315	CLA	CMD-C2D	-2.54	1.45	1.50
45	AB	819	CLA	C1B-C2B	2.54	1.49	1.43
45	BB	825	CLA	CMD-C2D	-2.54	1.45	1.50
45	BB	805	CLA	C1B-C2B	2.54	1.49	1.43
45	B5	601	CLA	C1B-C2B	2.54	1.49	1.43
45	B2	608	CLA	C1B-C2B	2.53	1.49	1.43
45	AB	802	CLA	C1B-C2B	2.53	1.49	1.43
45	BA	814	CLA	C1B-C2B	2.53	1.49	1.43
45	B2	609	CLA	C3B-C4B	2.53	1.50	1.42
45	BA	806	CLA	CMD-C2D	-2.53	1.45	1.50
45	BF	302	CLA	C1B-C2B	2.53	1.49	1.43
45	BA	812	CLA	C1B-C2B	2.53	1.49	1.43
45	B2	611	CLA	C3B-C4B	2.53	1.50	1.42
52	B1	316	LUT	C28-C29	-2.53	1.40	1.46
45	BA	816	CLA	C1B-C2B	2.53	1.49	1.43
45	AB	805	CLA	C1B-C2B	2.53	1.49	1.43
45	AF	802	CLA	CMD-C2D	-2.53	1.45	1.50
55	B2	616	XAT	O24-C25	-2.52	1.43	1.46
45	A1	309	CLA	C1B-C2B	2.52	1.49	1.43
45	BB	802	CLA	C1B-C2B	2.52	1.49	1.43
45	A3	315	CLA	C1B-C2B	2.52	1.49	1.43
45	AA	841	CLA	CMD-C2D	-2.52	1.45	1.50
45	BL	303	CLA	C3B-C4B	2.52	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	821	CLA	C1B-C2B	2.52	1.49	1.43
45	BB	827	CLA	CMD-C2D	-2.52	1.45	1.50
55	A1	318	XAT	O24-C25	-2.52	1.43	1.46
45	A3	309	CLA	C1B-C2B	2.51	1.49	1.43
45	B1	307	CLA	C1B-C2B	2.51	1.49	1.43
45	B5	603	CLA	C4B-C3B	2.51	1.49	1.43
48	AI	101	BCR	C30-C25	-2.51	1.50	1.53
45	BF	302	CLA	C3B-C4B	2.51	1.50	1.42
45	B1	314	CLA	C1B-C2B	2.51	1.49	1.43
45	A6	609	CLA	CMD-C2D	-2.51	1.45	1.50
45	AB	825	CLA	C1D-ND	2.51	1.41	1.37
45	A6	609	CLA	C1B-C2B	2.51	1.49	1.43
45	AB	831	CLA	CMD-C2D	-2.51	1.45	1.50
45	BA	811	CLA	C1B-C2B	2.51	1.49	1.43
45	A4	308	CLA	C1B-C2B	2.51	1.49	1.43
45	BB	810	CLA	CMC-C2C	-2.50	1.45	1.50
45	B3	307	CLA	C1B-C2B	2.50	1.49	1.43
48	AA	847	BCR	C12-C13	2.50	1.51	1.46
45	BB	834	CLA	CMC-C2C	-2.50	1.45	1.50
45	AA	819	CLA	C4B-NB	2.50	1.41	1.37
45	A4	302	CLA	C4B-C3B	2.50	1.49	1.43
45	BB	814	CLA	C1B-C2B	2.50	1.49	1.43
45	B2	612	CLA	C1B-C2B	2.50	1.49	1.43
45	BB	843	CLA	C3B-C4B	2.49	1.50	1.42
45	BA	836	CLA	C1B-C2B	2.49	1.49	1.43
45	AB	814	CLA	C4B-NB	2.49	1.41	1.37
45	AA	835	CLA	C1B-C2B	2.49	1.49	1.43
45	A6	603	CLA	C1B-C2B	2.49	1.49	1.43
45	BB	838	CLA	CMD-C2D	-2.49	1.45	1.50
45	A1	307	CLA	C1B-C2B	2.49	1.49	1.43
45	BA	803	CLA	C4B-NB	2.49	1.41	1.37
45	BB	805	CLA	CMC-C2C	-2.49	1.45	1.50
45	A6	601	CLA	C1B-C2B	2.49	1.49	1.43
45	A4	311	CLA	C1B-C2B	2.49	1.49	1.43
48	AA	849	BCR	C1-C6	-2.48	1.50	1.53
45	BB	808	CLA	C1B-C2B	2.48	1.49	1.43
45	AB	801	CLA	CMC-C2C	-2.48	1.45	1.50
45	AB	821	CLA	CMB-C2B	-2.48	1.45	1.50
45	BA	804	CLA	C1B-C2B	2.48	1.49	1.43
46	BA	843	PQN	C10-C1	2.48	1.53	1.48
45	BA	812	CLA	CMC-C2C	-2.48	1.45	1.50
48	BG	203	BCR	C30-C25	-2.48	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	840	CLA	CMB-C2B	-2.48	1.45	1.50
45	B2	611	CLA	C1B-C2B	2.48	1.48	1.43
45	AB	804	CLA	CMC-C2C	-2.48	1.45	1.50
45	BB	802	CLA	C3B-C4B	2.48	1.49	1.42
45	B1	307	CLA	CHC-C1C	2.47	1.43	1.38
45	B5	609	CLA	C3B-C4B	2.47	1.49	1.42
45	AB	819	CLA	CMB-C2B	-2.47	1.45	1.50
45	BA	812	CLA	C4B-NB	2.47	1.41	1.37
45	BA	826	CLA	C1B-C2B	2.47	1.48	1.43
45	BB	835	CLA	C1B-C2B	2.47	1.48	1.43
45	A1	316	CLA	C4B-C3B	2.47	1.48	1.43
45	BB	809	CLA	C1B-C2B	2.47	1.48	1.43
45	BB	834	CLA	CMD-C2D	-2.47	1.45	1.50
45	AB	808	CLA	C1B-C2B	2.47	1.48	1.43
45	AB	835	CLA	C1B-C2B	2.47	1.48	1.43
45	AB	814	CLA	CMB-C2B	-2.47	1.45	1.50
45	AA	808	CLA	CMD-C2D	-2.47	1.45	1.50
45	A3	308	CLA	CMD-C2D	-2.47	1.45	1.50
45	BA	829	CLA	CMB-C2B	-2.47	1.45	1.50
45	AA	841	CLA	C1B-C2B	2.47	1.48	1.43
45	AA	809	CLA	CMB-C2B	-2.47	1.45	1.50
45	BB	815	CLA	C4B-NB	2.46	1.41	1.37
45	AA	819	CLA	C1B-C2B	2.46	1.48	1.43
45	AA	816	CLA	CMB-C2B	-2.46	1.45	1.50
45	AB	826	CLA	C1B-C2B	2.46	1.48	1.43
45	BA	827	CLA	CMD-C2D	-2.46	1.45	1.50
45	BA	828	CLA	CMD-C2D	-2.46	1.45	1.50
45	AB	821	CLA	CMD-C2D	-2.46	1.45	1.50
45	AA	818	CLA	CMB-C2B	-2.46	1.45	1.50
45	AL	304	CLA	CMB-C2B	-2.46	1.45	1.50
45	BA	806	CLA	C1B-C2B	2.46	1.48	1.43
45	BA	809	CLA	CMD-C2D	-2.46	1.45	1.50
45	BB	830	CLA	MG-NB	-2.46	2.00	2.05
45	AA	821	CLA	CMB-C2B	-2.46	1.45	1.50
45	BA	818	CLA	CMD-C2D	-2.46	1.45	1.50
54	A1	308	CHL	CMC-C2C	2.46	1.49	1.44
45	AA	806	CLA	C1B-C2B	2.46	1.48	1.43
45	AB	811	CLA	C1B-C2B	2.46	1.48	1.43
45	BG	201	CLA	C3B-C4B	2.45	1.49	1.42
55	A6	616	XAT	O24-C25	-2.45	1.43	1.46
45	BB	829	CLA	C3B-C4B	2.45	1.49	1.42
45	AB	826	CLA	C3B-C4B	2.45	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B1	311	CLA	C3B-C4B	2.45	1.49	1.42
45	BB	807	CLA	C3B-C4B	2.45	1.49	1.42
45	AA	825	CLA	C1B-C2B	2.45	1.48	1.43
45	A3	302	CLA	C1B-C2B	2.45	1.48	1.43
45	AF	803	CLA	C1B-C2B	2.45	1.48	1.43
45	BB	802	CLA	CMD-C2D	-2.45	1.45	1.50
45	BB	832	CLA	CMD-C2D	-2.45	1.45	1.50
45	AB	842	CLA	C1B-C2B	2.45	1.48	1.43
45	AB	810	CLA	MG-NB	-2.45	2.00	2.05
45	AA	831	CLA	CMB-C2B	-2.45	1.45	1.50
45	A1	304	CLA	CMD-C2D	-2.45	1.45	1.50
45	AB	807	CLA	C4B-NB	2.45	1.41	1.37
45	AB	841	CLA	CMB-C2B	-2.44	1.45	1.50
45	BA	841	CLA	CMC-C2C	-2.44	1.45	1.50
45	BB	840	CLA	CMD-C2D	-2.44	1.45	1.50
45	BA	820	CLA	CMD-C2D	-2.44	1.45	1.50
55	B1	317	XAT	O24-C25	-2.44	1.43	1.46
45	AB	835	CLA	CMD-C2D	-2.44	1.45	1.50
45	A4	311	CLA	C3B-C4B	2.44	1.49	1.42
45	A6	610	CLA	C3B-C4B	2.44	1.49	1.42
45	AA	807	CLA	C1B-C2B	2.44	1.48	1.43
45	AA	831	CLA	C1B-C2B	2.44	1.48	1.43
45	AB	834	CLA	CMD-C2D	-2.44	1.45	1.50
45	A4	301	CLA	CMC-C2C	-2.44	1.45	1.50
45	BA	841	CLA	CMB-C2B	-2.44	1.45	1.50
45	BA	806	CLA	CMC-C2C	-2.43	1.45	1.50
45	AB	815	CLA	CMD-C2D	-2.43	1.45	1.50
45	B5	610	CLA	C3B-C4B	2.43	1.49	1.42
45	AB	817	CLA	C1B-C2B	2.43	1.48	1.43
45	BA	814	CLA	CMC-C2C	-2.43	1.45	1.50
45	A6	603	CLA	CMD-C2D	-2.43	1.45	1.50
45	AA	838	CLA	C1B-C2B	2.43	1.48	1.43
45	AB	838	CLA	C1B-C2B	2.43	1.48	1.43
45	BA	835	CLA	CMB-C2B	-2.43	1.45	1.50
45	BA	829	CLA	C4B-NB	2.43	1.41	1.37
45	AB	836	CLA	C1B-C2B	2.43	1.48	1.43
45	AA	821	CLA	CMD-C2D	-2.43	1.45	1.50
45	BA	809	CLA	C1B-C2B	2.43	1.48	1.43
45	B2	609	CLA	CHC-C1C	2.43	1.43	1.38
45	AA	827	CLA	C3B-C4B	2.43	1.49	1.42
45	B2	602	CLA	C1B-C2B	2.43	1.48	1.43
45	BB	827	CLA	C3B-C4B	2.43	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	805	CLA	CMD-C2D	-2.43	1.45	1.50
45	AA	811	CLA	CMD-C2D	-2.42	1.45	1.50
45	AA	826	CLA	CMD-C2D	-2.42	1.45	1.50
45	BF	301	CLA	CMB-C2B	-2.42	1.45	1.50
45	BL	302	CLA	C3B-C4B	2.42	1.49	1.42
45	AB	809	CLA	CMD-C2D	-2.42	1.45	1.50
45	BA	842	CLA	CMB-C2B	-2.42	1.45	1.50
45	AA	828	CLA	CMD-C2D	-2.42	1.45	1.50
45	BA	837	CLA	C1B-C2B	2.42	1.48	1.43
45	AA	842	CLA	CMB-C2B	-2.42	1.45	1.50
45	BB	843	CLA	CHC-C1C	2.42	1.43	1.38
55	B5	615	XAT	O24-C25	-2.42	1.43	1.46
45	AA	803	CLA	CMC-C2C	-2.42	1.45	1.50
45	AA	812	CLA	CMB-C2B	-2.42	1.45	1.50
45	BB	839	CLA	CMD-C2D	-2.42	1.45	1.50
45	AA	828	CLA	C1B-C2B	2.42	1.48	1.43
45	AB	820	CLA	CMD-C2D	-2.41	1.45	1.50
45	BB	838	CLA	C3B-C4B	2.41	1.49	1.42
46	BA	843	PQN	C2-C1	2.41	1.53	1.47
45	AB	832	CLA	CMD-C2D	-2.41	1.45	1.50
45	BB	820	CLA	CMB-C2B	-2.41	1.45	1.50
54	B1	308	CHL	CMC-C2C	2.41	1.49	1.44
45	AA	833	CLA	C1B-C2B	2.41	1.48	1.43
45	AF	802	CLA	C1B-C2B	2.41	1.48	1.43
45	AA	825	CLA	C3B-C4B	2.41	1.49	1.42
45	B3	307	CLA	CMD-C2D	-2.41	1.45	1.50
45	BA	822	CLA	C3B-C4B	2.41	1.49	1.42
45	AA	804	CLA	C1B-C2B	2.41	1.48	1.43
45	AA	806	CLA	CMD-C2D	-2.41	1.45	1.50
52	A4	315	LUT	C8-C9	2.41	1.51	1.46
45	AF	803	CLA	CMB-C2B	-2.41	1.45	1.50
45	BA	811	CLA	CMD-C2D	-2.41	1.45	1.50
45	BA	840	CLA	CMD-C2D	-2.41	1.45	1.50
45	A6	603	CLA	CMC-C2C	-2.41	1.45	1.50
45	BB	829	CLA	C1B-C2B	2.41	1.48	1.43
45	AB	804	CLA	C1B-C2B	2.41	1.48	1.43
45	BB	832	CLA	C1B-C2B	2.41	1.48	1.43
45	B1	307	CLA	C3B-C4B	2.41	1.49	1.42
45	A4	307	CLA	C1B-C2B	2.41	1.48	1.43
45	A3	303	CLA	CMB-C2B	-2.41	1.45	1.50
45	BA	802	CLA	CMC-C2C	-2.41	1.45	1.50
45	BA	827	CLA	C3B-C4B	2.40	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	604	CLA	C3B-C4B	2.40	1.49	1.42
45	BB	810	CLA	C1B-C2B	2.40	1.48	1.43
45	BB	810	CLA	C3B-C4B	2.40	1.49	1.42
48	BL	306	BCR	C1-C6	-2.40	1.50	1.53
45	AB	819	CLA	CMD-C2D	-2.40	1.45	1.50
45	BB	814	CLA	CMD-C2D	-2.40	1.45	1.50
46	AB	843	PQN	C10-C1	2.40	1.52	1.48
45	B5	610	CLA	C1B-C2B	2.40	1.48	1.43
45	B5	608	CLA	CMD-C2D	-2.40	1.45	1.50
45	AB	837	CLA	CMB-C2B	-2.40	1.45	1.50
45	BB	812	CLA	C1B-C2B	2.40	1.48	1.43
45	B3	304	CLA	CMB-C2B	-2.40	1.45	1.50
45	BB	811	CLA	C1B-C2B	2.40	1.48	1.43
45	B5	602	CLA	C3B-C4B	2.40	1.49	1.42
45	BB	812	CLA	C3B-C4B	2.40	1.49	1.42
45	BB	826	CLA	C1B-C2B	2.40	1.48	1.43
45	AL	303	CLA	C1B-C2B	2.40	1.48	1.43
45	AB	828	CLA	C1B-C2B	2.39	1.48	1.43
45	AB	802	CLA	CMD-C2D	-2.39	1.45	1.50
45	AB	826	CLA	CMD-C2D	-2.39	1.45	1.50
45	A1	304	CLA	CMB-C2B	-2.39	1.45	1.50
45	A3	303	CLA	C1B-C2B	2.39	1.48	1.43
45	AB	829	CLA	MG-NB	-2.39	2.01	2.05
45	BB	822	CLA	CMD-C2D	-2.39	1.45	1.50
45	AA	834	CLA	CMC-C2C	-2.39	1.45	1.50
45	AB	825	CLA	CMC-C2C	-2.39	1.45	1.50
45	AF	803	CLA	CMD-C2D	-2.39	1.45	1.50
45	AB	803	CLA	CMD-C2D	-2.39	1.45	1.50
45	A6	610	CLA	CMD-C2D	-2.39	1.45	1.50
45	AG	204	CLA	C3B-C4B	2.39	1.49	1.42
45	AA	812	CLA	CMD-C2D	-2.39	1.45	1.50
45	AB	835	CLA	CMB-C2B	-2.39	1.45	1.50
52	AF	806	LUT	C12-C13	2.39	1.51	1.46
45	AB	810	CLA	C4B-NB	2.39	1.41	1.37
45	A4	309	CLA	C3B-C4B	2.38	1.49	1.42
45	AA	837	CLA	C1B-C2B	2.38	1.48	1.43
45	BB	815	CLA	MG-NB	-2.38	2.01	2.05
45	BA	818	CLA	CMB-C2B	-2.38	1.45	1.50
45	BB	802	CLA	CMC-C2C	-2.38	1.45	1.50
45	BB	807	CLA	CMC-C2C	-2.38	1.45	1.50
45	A3	308	CLA	CMB-C2B	-2.38	1.45	1.50
45	AA	802	CLA	CMC-C2C	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	835	CLA	CMB-C2B	-2.38	1.45	1.50
45	AF	803	CLA	C3B-C4B	2.38	1.49	1.42
45	AA	820	CLA	CMD-C2D	-2.38	1.45	1.50
45	B3	311	CLA	C3B-C4B	2.38	1.49	1.42
45	AA	834	CLA	CMB-C2B	-2.38	1.45	1.50
45	AA	830	CLA	CMD-C2D	-2.38	1.45	1.50
45	BA	834	CLA	C1B-C2B	2.38	1.48	1.43
45	AA	803	CLA	CMD-C2D	-2.38	1.45	1.50
45	AL	304	CLA	C1B-C2B	2.38	1.48	1.43
45	B3	310	CLA	C3B-C4B	2.37	1.49	1.42
45	B3	314	CLA	CMD-C2D	-2.37	1.45	1.50
45	BB	828	CLA	C3B-C4B	2.37	1.49	1.42
45	AG	204	CLA	CMB-C2B	-2.37	1.45	1.50
45	BA	808	CLA	CMB-C2B	-2.37	1.45	1.50
45	AA	805	CLA	CMD-C2D	-2.37	1.45	1.50
45	AB	809	CLA	CMC-C2C	-2.37	1.45	1.50
45	AB	827	CLA	CMD-C2D	-2.37	1.45	1.50
45	A4	301	CLA	C1B-C2B	2.37	1.48	1.43
45	BA	818	CLA	C1B-C2B	2.37	1.48	1.43
45	BB	807	CLA	CMD-C2D	-2.37	1.45	1.50
45	AB	827	CLA	C1B-C2B	2.37	1.48	1.43
45	BF	301	CLA	CMD-C2D	-2.37	1.45	1.50
45	BA	805	CLA	CMD-C2D	-2.37	1.45	1.50
45	A4	307	CLA	C3B-C4B	2.37	1.49	1.42
45	AB	838	CLA	CMC-C2C	-2.37	1.45	1.50
45	A6	613	CLA	CMB-C2B	-2.36	1.45	1.50
45	BH	201	CLA	CMB-C2B	-2.36	1.45	1.50
45	BA	811	CLA	CMB-C2B	-2.36	1.45	1.50
45	BL	304	CLA	C3B-C4B	2.36	1.49	1.42
45	BB	801	CLA	C1D-ND	2.36	1.41	1.37
45	AB	827	CLA	C3B-C4B	2.36	1.49	1.42
45	AA	829	CLA	MG-ND	-2.36	2.01	2.05
45	AA	824	CLA	CMD-C2D	-2.36	1.45	1.50
45	AA	826	CLA	C1B-C2B	2.36	1.48	1.43
45	A6	604	CLA	CHC-C1C	2.36	1.43	1.38
45	BB	806	CLA	CMD-C2D	-2.36	1.45	1.50
45	AA	838	CLA	CMD-C2D	-2.36	1.45	1.50
45	AB	814	CLA	MG-NB	-2.36	2.01	2.05
45	AB	818	CLA	CMD-C2D	-2.36	1.45	1.50
45	BB	816	CLA	CMD-C2D	-2.36	1.45	1.50
45	BB	801	CLA	MG-ND	-2.36	2.01	2.05
45	AB	811	CLA	CMD-C2D	-2.35	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B2	605	CHL	CMC-C2C	2.35	1.49	1.44
45	AB	828	CLA	C3B-C4B	2.35	1.49	1.42
52	B1	316	LUT	C12-C13	-2.35	1.40	1.46
45	AA	807	CLA	C3B-C4B	2.35	1.49	1.42
45	BB	804	CLA	CMC-C2C	-2.35	1.45	1.50
54	A6	607	CHL	CMC-C2C	2.35	1.49	1.44
45	BA	807	CLA	C3B-C4B	2.35	1.49	1.42
45	AA	825	CLA	CMB-C2B	-2.35	1.46	1.50
45	AB	832	CLA	CMB-C2B	-2.35	1.46	1.50
45	BB	801	CLA	CMB-C2B	-2.35	1.46	1.50
45	B5	609	CLA	C1B-C2B	2.35	1.48	1.43
45	BB	833	CLA	C3B-C4B	2.35	1.49	1.42
45	BA	838	CLA	C1B-C2B	2.35	1.48	1.43
45	AA	814	CLA	CMD-C2D	-2.35	1.46	1.50
45	AA	821	CLA	C1B-C2B	2.35	1.48	1.43
55	A3	317	XAT	O24-C25	-2.35	1.43	1.46
45	B3	312	CLA	C3B-C4B	2.35	1.49	1.42
45	BL	303	CLA	CMB-C2B	-2.35	1.46	1.50
45	A1	309	CLA	C3B-C4B	2.35	1.49	1.42
45	BA	840	CLA	C4B-NB	2.34	1.40	1.37
53	AG	202	LMG	O1-C1	2.34	1.44	1.40
45	BB	811	CLA	CMC-C2C	-2.34	1.46	1.50
45	AB	810	CLA	CMD-C2D	-2.34	1.46	1.50
45	BA	804	CLA	CMD-C2D	-2.34	1.46	1.50
45	BA	817	CLA	C3B-C4B	2.34	1.49	1.42
45	B1	314	CLA	C3B-C4B	2.34	1.49	1.42
45	A4	308	CLA	C3B-C4B	2.34	1.49	1.42
45	AL	305	CLA	CMD-C2D	-2.34	1.46	1.50
45	B3	314	CLA	C3B-C4B	2.34	1.49	1.42
45	BB	805	CLA	C1D-ND	2.34	1.40	1.37
45	A3	302	CLA	C3B-C4B	2.34	1.49	1.42
45	A6	614	CLA	C3B-C4B	2.34	1.49	1.42
45	AB	837	CLA	C3B-C4B	2.34	1.49	1.42
45	AA	818	CLA	C1B-C2B	2.34	1.48	1.43
45	BA	837	CLA	CMD-C2D	-2.34	1.46	1.50
45	BA	813	CLA	C3B-C4B	2.34	1.49	1.42
45	BB	819	CLA	CMD-C2D	-2.34	1.46	1.50
45	AA	832	CLA	C3B-C4B	2.34	1.49	1.42
45	AA	813	CLA	CMB-C2B	-2.34	1.46	1.50
45	AA	813	CLA	C1B-C2B	2.34	1.48	1.43
45	BK	202	CLA	C3B-C4B	2.34	1.49	1.42
45	A6	614	CLA	CHC-C1C	2.34	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	838	CLA	C3B-C4B	2.34	1.49	1.42
45	AB	805	CLA	CMB-C2B	-2.33	1.46	1.50
45	B5	603	CLA	CMB-C2B	-2.33	1.46	1.50
45	BA	836	CLA	CMB-C2B	-2.33	1.46	1.50
45	AB	824	CLA	CMB-C2B	-2.33	1.46	1.50
45	AB	809	CLA	CMB-C2B	-2.33	1.46	1.50
45	A6	612	CLA	CMD-C2D	-2.33	1.46	1.50
45	A3	315	CLA	C3B-C4B	2.33	1.49	1.42
45	AB	818	CLA	CMB-C2B	-2.33	1.46	1.50
45	AB	837	CLA	CMC-C2C	-2.33	1.46	1.50
45	BB	824	CLA	CMD-C2D	-2.33	1.46	1.50
45	AB	817	CLA	CMD-C2D	-2.33	1.46	1.50
45	AB	801	CLA	C1D-ND	2.33	1.40	1.37
54	A4	304	CHL	CMC-C2C	2.33	1.49	1.44
45	AB	832	CLA	CMC-C2C	-2.33	1.46	1.50
45	AA	801	CLA	CMB-C2B	-2.33	1.46	1.50
45	AA	802	CLA	CMB-C2B	-2.33	1.46	1.50
45	AA	829	CLA	C1B-C2B	2.33	1.48	1.43
45	BB	840	CLA	C3B-C4B	2.33	1.49	1.42
45	AA	821	CLA	C3B-C4B	2.32	1.49	1.42
45	A4	310	CLA	CMD-C2D	-2.32	1.46	1.50
45	BA	801	CLA	CMB-C2B	-2.32	1.46	1.50
45	BA	802	CLA	CMB-C2B	-2.32	1.46	1.50
45	BA	806	CLA	CHC-C1C	2.32	1.43	1.38
45	AB	817	CLA	C3B-C4B	2.32	1.49	1.42
45	B2	608	CLA	CMD-C2D	-2.32	1.46	1.50
45	AB	841	CLA	CMD-C2D	-2.32	1.46	1.50
45	BG	201	CLA	CHC-C1C	2.32	1.43	1.38
54	B2	606	CHL	CMC-C2C	2.32	1.49	1.44
45	AB	801	CLA	MG-ND	-2.32	2.01	2.05
45	AA	807	CLA	CMC-C2C	-2.32	1.46	1.50
45	AA	823	CLA	CMD-C2D	-2.32	1.46	1.50
45	A6	604	CLA	CMB-C2B	-2.32	1.46	1.50
45	BL	302	CLA	C1B-C2B	2.32	1.48	1.43
45	AB	814	CLA	CMD-C2D	-2.32	1.46	1.50
54	B3	306	CHL	CBD-CGD	-2.32	1.49	1.52
45	B5	602	CLA	CMD-C2D	-2.32	1.46	1.50
45	A1	305	CLA	C3B-C4B	2.32	1.49	1.42
45	AA	831	CLA	CMD-C2D	-2.32	1.46	1.50
45	BB	839	CLA	CMB-C2B	-2.32	1.46	1.50
45	AA	808	CLA	C3B-C4B	2.32	1.49	1.42
45	A1	316	CLA	CMB-C2B	-2.32	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	804	CLA	CMD-C2D	-2.32	1.46	1.50
45	AF	802	CLA	MG-NB	-2.32	2.01	2.05
45	AB	813	CLA	CMD-C2D	-2.32	1.46	1.50
45	AF	803	CLA	CMC-C2C	-2.31	1.46	1.50
45	AB	809	CLA	C3B-C4B	2.31	1.49	1.42
45	AB	842	CLA	MG-NB	-2.31	2.01	2.05
45	BA	831	CLA	CMD-C2D	-2.31	1.46	1.50
45	B5	612	CLA	CMC-C2C	-2.31	1.46	1.50
48	A6	617	BCR	C8-C9	2.31	1.50	1.46
45	AL	305	CLA	CMC-C2C	-2.31	1.46	1.50
45	BA	839	CLA	CMB-C2B	-2.31	1.46	1.50
45	B5	608	CLA	C3B-C4B	2.31	1.49	1.42
45	AB	823	CLA	CMD-C2D	-2.31	1.46	1.50
45	AB	816	CLA	CMC-C2C	-2.31	1.46	1.50
45	BB	811	CLA	CMB-C2B	-2.31	1.46	1.50
45	AA	811	CLA	CMB-C2B	-2.31	1.46	1.50
45	AB	802	CLA	CMC-C2C	-2.31	1.46	1.50
45	BB	828	CLA	CMD-C2D	-2.31	1.46	1.50
45	B1	304	CLA	CMB-C2B	-2.31	1.46	1.50
45	AA	814	CLA	CMB-C2B	-2.31	1.46	1.50
45	BA	841	CLA	CMD-C2D	-2.31	1.46	1.50
45	B5	613	CLA	C3B-C4B	2.31	1.49	1.42
45	AA	842	CLA	CMD-C2D	-2.31	1.46	1.50
45	BB	801	CLA	C3B-C4B	2.30	1.49	1.42
45	A4	307	CLA	CMB-C2B	-2.30	1.46	1.50
45	AA	837	CLA	CMD-C2D	-2.30	1.46	1.50
45	B5	602	CLA	CHC-C1C	2.30	1.43	1.38
45	A4	301	CLA	CMD-C2D	-2.30	1.46	1.50
45	BA	805	CLA	CMB-C2B	-2.30	1.46	1.50
45	BA	812	CLA	CMB-C2B	-2.30	1.46	1.50
45	AA	808	CLA	CMB-C2B	-2.30	1.46	1.50
45	B2	608	CLA	CMB-C2B	-2.30	1.46	1.50
45	BB	842	CLA	CMD-C2D	-2.30	1.46	1.50
45	AA	823	CLA	CMB-C2B	-2.30	1.46	1.50
45	AB	811	CLA	C3B-C4B	2.30	1.49	1.42
48	BA	847	BCR	C8-C9	2.30	1.50	1.46
45	B1	314	CLA	CMB-C2B	-2.30	1.46	1.50
45	B5	603	CLA	CMD-C2D	-2.30	1.46	1.50
45	BB	805	CLA	C4B-NB	2.30	1.40	1.37
45	BB	842	CLA	CMB-C2B	-2.30	1.46	1.50
54	A3	307	CHL	CBD-CGD	-2.30	1.49	1.52
45	AA	833	CLA	MG-NB	-2.30	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	834	CLA	CMD-C2D	-2.30	1.46	1.50
45	BA	830	CLA	CMC-C2C	-2.30	1.46	1.50
45	AA	804	CLA	CMD-C2D	-2.30	1.46	1.50
45	AB	830	CLA	CMC-C2C	-2.29	1.46	1.50
45	B3	301	CLA	CMC-C2C	-2.29	1.46	1.50
45	BA	833	CLA	CMD-C2D	-2.29	1.46	1.50
45	AA	836	CLA	C1B-C2B	2.29	1.48	1.43
45	AB	823	CLA	CMB-C2B	-2.29	1.46	1.50
45	A3	311	CLA	C3B-C4B	2.29	1.49	1.42
45	BA	808	CLA	C1B-C2B	2.29	1.48	1.43
45	AA	805	CLA	CMB-C2B	-2.29	1.46	1.50
45	AA	819	CLA	CMD-C2D	-2.29	1.46	1.50
45	AA	834	CLA	CMD-C2D	-2.29	1.46	1.50
45	AL	304	CLA	CMD-C2D	-2.29	1.46	1.50
46	BA	843	PQN	C11-C3	2.29	1.55	1.51
45	A6	605	CLA	CMB-C2B	-2.29	1.46	1.50
45	BB	826	CLA	MG-NB	-2.29	2.01	2.05
45	AA	804	CLA	C3B-C4B	2.29	1.49	1.42
45	AB	804	CLA	C4B-NB	2.29	1.40	1.37
52	A4	315	LUT	C22-C21	-2.29	1.51	1.54
45	AB	831	CLA	C1B-C2B	2.29	1.48	1.43
45	BA	819	CLA	CMC-C2C	-2.29	1.46	1.50
45	BB	821	CLA	CMB-C2B	-2.29	1.46	1.50
55	B1	317	XAT	O4-C5	-2.29	1.43	1.46
45	AB	838	CLA	C3B-C4B	2.29	1.49	1.42
45	BB	808	CLA	CMD-C2D	-2.29	1.46	1.50
45	A1	313	CLA	C3B-C4B	2.29	1.49	1.42
45	BA	837	CLA	C3B-C4B	2.29	1.49	1.42
45	A4	312	CLA	C3B-C4B	2.29	1.49	1.42
45	AB	804	CLA	MG-ND	-2.29	2.01	2.05
45	A1	314	CLA	CMD-C2D	-2.28	1.46	1.50
45	BB	804	CLA	CMB-C2B	-2.28	1.46	1.50
45	BB	839	CLA	C3B-C4B	2.28	1.49	1.42
45	BA	830	CLA	CMD-C2D	-2.28	1.46	1.50
45	AB	813	CLA	CMB-C2B	-2.28	1.46	1.50
45	BA	834	CLA	CMB-C2B	-2.28	1.46	1.50
45	BB	823	CLA	CMD-C2D	-2.28	1.46	1.50
45	BB	835	CLA	C3B-C4B	2.28	1.49	1.42
45	A6	610	CLA	CHC-C1C	2.28	1.43	1.38
45	AB	834	CLA	CMC-C2C	-2.28	1.46	1.50
55	A4	316	XAT	O4-C5	-2.28	1.43	1.46
45	A4	313	CLA	CMD-C2D	-2.28	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	825	CLA	MG-NB	-2.28	2.01	2.05
45	B2	612	CLA	C3B-C4B	2.28	1.49	1.42
45	BA	821	CLA	C1B-C2B	2.28	1.48	1.43
45	AB	812	CLA	CMD-C2D	-2.28	1.46	1.50
45	A6	610	CLA	C1B-C2B	2.28	1.48	1.43
45	B5	609	CLA	CHC-C1C	2.28	1.43	1.38
45	AB	811	CLA	MG-NB	-2.27	2.01	2.05
45	AB	803	CLA	CMB-C2B	-2.27	1.46	1.50
45	BB	842	CLA	CMC-C2C	-2.27	1.46	1.50
45	A1	314	CLA	CMB-C2B	-2.27	1.46	1.50
45	AB	802	CLA	CHC-C1C	2.27	1.43	1.38
45	B3	311	CLA	CMD-C2D	-2.27	1.46	1.50
45	AA	822	CLA	C3B-C4B	2.27	1.49	1.42
45	BJ	102	CLA	C3B-C4B	2.27	1.49	1.42
45	BA	839	CLA	CMD-C2D	-2.27	1.46	1.50
45	BA	841	CLA	C1B-C2B	2.27	1.48	1.43
45	AB	836	CLA	CMD-C2D	-2.27	1.46	1.50
45	BA	821	CLA	CMB-C2B	-2.27	1.46	1.50
45	B3	308	CLA	CMD-C2D	-2.27	1.46	1.50
45	BA	816	CLA	CMB-C2B	-2.27	1.46	1.50
45	BA	825	CLA	CMB-C2B	-2.27	1.46	1.50
45	A3	305	CLA	CMD-C2D	-2.27	1.46	1.50
45	B5	613	CLA	CMD-C2D	-2.27	1.46	1.50
45	A1	306	CLA	C3B-C4B	2.27	1.49	1.42
45	A4	302	CLA	CMD-C2D	-2.27	1.46	1.50
45	B5	602	CLA	CMB-C2B	-2.27	1.46	1.50
45	AB	810	CLA	MG-ND	-2.27	2.01	2.05
45	AB	808	CLA	CMC-C2C	-2.27	1.46	1.50
45	A1	307	CLA	CMD-C2D	-2.27	1.46	1.50
45	BA	826	CLA	CMD-C2D	-2.27	1.46	1.50
45	BA	824	CLA	CMC-C2C	-2.27	1.46	1.50
45	BB	843	CLA	C1B-C2B	2.26	1.48	1.43
45	AA	817	CLA	CMD-C2D	-2.26	1.46	1.50
45	B2	602	CLA	CMD-C2D	-2.26	1.46	1.50
45	AB	815	CLA	C1B-C2B	2.26	1.48	1.43
45	BA	821	CLA	CMC-C2C	-2.26	1.46	1.50
45	B1	313	CLA	C3B-C4B	2.26	1.49	1.42
45	BB	836	CLA	CMB-C2B	-2.26	1.46	1.50
45	AA	809	CLA	C3B-C4B	2.26	1.49	1.42
45	B5	609	CLA	CMD-C2D	-2.26	1.46	1.50
54	B2	601	CHL	CMC-C2C	2.26	1.49	1.44
45	BG	202	CLA	CMB-C2B	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AK	202	CLA	C3B-C4B	2.26	1.49	1.42
45	AB	827	CLA	CMC-C2C	-2.26	1.46	1.50
45	AK	203	CLA	CMC-C2C	-2.26	1.46	1.50
45	BB	809	CLA	CMB-C2B	-2.26	1.46	1.50
45	B2	609	CLA	C1B-C2B	2.26	1.48	1.43
45	AB	806	CLA	CMD-C2D	-2.26	1.46	1.50
45	B3	301	CLA	C3B-C4B	2.26	1.49	1.42
45	B5	608	CLA	CMB-C2B	-2.26	1.46	1.50
45	BB	812	CLA	MG-NB	-2.26	2.01	2.05
52	B5	614	LUT	C22-C21	-2.26	1.52	1.54
45	A3	302	CLA	CHC-C1C	2.26	1.43	1.38
45	AA	813	CLA	CMC-C2C	-2.26	1.46	1.50
45	BB	817	CLA	CMD-C2D	-2.26	1.46	1.50
45	AA	816	CLA	C1B-C2B	2.26	1.48	1.43
45	A1	316	CLA	CMD-C2D	-2.26	1.46	1.50
45	BA	828	CLA	CMC-C2C	-2.26	1.46	1.50
45	AB	817	CLA	CHC-C1C	2.26	1.43	1.38
45	BF	303	CLA	C3B-C4B	2.25	1.49	1.42
45	AA	806	CLA	C3B-C4B	2.25	1.49	1.42
45	A6	601	CLA	CMB-C2B	-2.25	1.46	1.50
45	AB	816	CLA	CMD-C2D	-2.25	1.46	1.50
45	B3	307	CLA	CMB-C2B	-2.25	1.46	1.50
45	AB	808	CLA	CMD-C2D	-2.25	1.46	1.50
45	BA	812	CLA	CMD-C2D	-2.25	1.46	1.50
45	A6	612	CLA	C3B-C4B	2.25	1.49	1.42
45	BB	826	CLA	CMB-C2B	-2.25	1.46	1.50
45	A4	310	CLA	C3B-C4B	2.25	1.49	1.42
45	BB	806	CLA	C3B-C4B	2.25	1.49	1.42
45	A6	610	CLA	CMB-C2B	-2.25	1.46	1.50
45	AB	824	CLA	MG-NB	-2.25	2.01	2.05
55	B5	615	XAT	O4-C5	-2.25	1.43	1.46
45	AG	203	CLA	CMD-C2D	-2.25	1.46	1.50
45	A3	305	CLA	C3B-C4B	2.25	1.49	1.42
45	BA	809	CLA	C3B-C4B	2.25	1.49	1.42
46	BA	843	PQN	C3-C4	2.25	1.52	1.47
45	A3	313	CLA	C3B-C4B	2.25	1.49	1.42
45	AL	303	CLA	CMD-C2D	-2.25	1.46	1.50
45	A3	309	CLA	C3B-C4B	2.25	1.49	1.42
45	A4	308	CLA	CMD-C2D	-2.25	1.46	1.50
45	AA	805	CLA	CMC-C2C	-2.25	1.46	1.50
45	BB	814	CLA	CMB-C2B	-2.25	1.46	1.50
45	AB	801	CLA	C3B-C4B	2.25	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	604	CLA	CMD-C2D	-2.25	1.46	1.50
45	BB	839	CLA	CMC-C2C	-2.25	1.46	1.50
48	AK	204	BCR	C12-C13	2.25	1.50	1.46
45	AA	835	CLA	CMD-C2D	-2.24	1.46	1.50
45	BA	808	CLA	CMD-C2D	-2.24	1.46	1.50
45	A3	303	CLA	CMD-C2D	-2.24	1.46	1.50
45	AL	305	CLA	CMB-C2B	-2.24	1.46	1.50
45	AA	802	CLA	C3B-C4B	2.24	1.49	1.42
45	AA	827	CLA	CHC-C1C	2.24	1.43	1.38
45	AB	822	CLA	CMB-C2B	-2.24	1.46	1.50
45	AB	807	CLA	CMB-C2B	-2.24	1.46	1.50
45	BA	814	CLA	C3B-C4B	2.24	1.49	1.42
45	AB	812	CLA	CMB-C2B	-2.24	1.46	1.50
45	AA	838	CLA	CMB-C2B	-2.24	1.46	1.50
45	BA	814	CLA	CMD-C2D	-2.24	1.46	1.50
45	A3	314	CLA	C3B-C4B	2.24	1.49	1.42
45	A6	603	CLA	CMB-C2B	-2.24	1.46	1.50
45	AA	826	CLA	C3B-C4B	2.24	1.49	1.42
45	BA	809	CLA	CHC-C1C	2.24	1.43	1.38
45	AB	804	CLA	CMB-C2B	-2.24	1.46	1.50
45	BB	815	CLA	CMB-C2B	-2.24	1.46	1.50
45	BL	303	CLA	CMD-C2D	-2.24	1.46	1.50
45	B5	610	CLA	CMD-C2D	-2.24	1.46	1.50
54	A6	602	CHL	CMC-C2C	2.24	1.49	1.44
45	A3	315	CLA	CHC-C1C	2.24	1.43	1.38
45	A6	612	CLA	CMB-C2B	-2.24	1.46	1.50
45	AG	203	CLA	CHC-C1C	2.24	1.43	1.38
45	BA	829	CLA	MG-ND	-2.24	2.01	2.05
45	B2	602	CLA	CMB-C2B	-2.24	1.46	1.50
45	AA	819	CLA	CMC-C2C	-2.24	1.46	1.50
45	A3	306	CLA	CMD-C2D	-2.24	1.46	1.50
45	A4	307	CLA	CHC-C1C	2.24	1.43	1.38
45	AB	838	CLA	CMD-C2D	-2.23	1.46	1.50
45	AA	810	CLA	CMB-C2B	-2.23	1.46	1.50
45	AB	826	CLA	CHC-C1C	2.23	1.43	1.38
45	A1	312	CLA	CHC-C1C	2.23	1.43	1.38
45	B5	602	CLA	MG-NB	-2.23	2.01	2.05
48	A1	319	BCR	C40-C30	2.23	1.58	1.53
45	AA	813	CLA	C3B-C4B	2.23	1.49	1.42
45	AB	815	CLA	CMC-C2C	-2.23	1.46	1.50
45	AB	841	CLA	CMC-C2C	-2.23	1.46	1.50
45	BB	813	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	814	CLA	CHC-C1C	2.23	1.43	1.38
45	BA	826	CLA	C3B-C4B	2.23	1.49	1.42
45	B1	309	CLA	C3B-C4B	2.23	1.49	1.42
45	AB	811	CLA	CMC-C2C	-2.23	1.46	1.50
45	AB	842	CLA	CMB-C2B	-2.23	1.46	1.50
45	A4	313	CLA	CMB-C2B	-2.23	1.46	1.50
45	BF	302	CLA	CMD-C2D	-2.23	1.46	1.50
45	BA	838	CLA	CMD-C2D	-2.23	1.46	1.50
45	B1	306	CLA	C3B-C4B	2.23	1.49	1.42
45	B2	602	CLA	C3B-C4B	2.23	1.49	1.42
46	AB	843	PQN	C2-C1	2.23	1.52	1.47
45	BB	817	CLA	C3B-C4B	2.23	1.49	1.42
45	AB	814	CLA	CMC-C2C	-2.23	1.46	1.50
45	AG	201	CLA	CMB-C2B	-2.23	1.46	1.50
45	BA	819	CLA	CMD-C2D	-2.23	1.46	1.50
45	BA	825	CLA	MG-NB	-2.23	2.01	2.05
45	B5	612	CLA	C3B-C4B	2.23	1.49	1.42
45	AB	810	CLA	C1B-C2B	2.23	1.48	1.43
45	BB	805	CLA	CHC-C1C	2.23	1.42	1.38
45	BB	843	CLA	CMD-C2D	-2.23	1.46	1.50
54	A6	606	CHL	CMC-C2C	2.23	1.49	1.44
45	A4	311	CLA	CMD-C2D	-2.23	1.46	1.50
45	A6	601	CLA	MG-NB	-2.23	2.01	2.05
45	BB	816	CLA	C3B-C4B	2.23	1.49	1.42
45	AA	832	CLA	CMD-C2D	-2.22	1.46	1.50
45	A4	303	CLA	CMD-C2D	-2.22	1.46	1.50
55	A1	318	XAT	O4-C5	-2.22	1.43	1.46
45	BK	203	CLA	C3B-C4B	2.22	1.49	1.42
45	A1	310	CLA	CMD-C2D	-2.22	1.46	1.50
45	A1	307	CLA	C3B-C4B	2.22	1.49	1.42
45	AB	825	CLA	CHC-C1C	2.22	1.42	1.38
45	AB	807	CLA	CAC-C3C	-2.22	1.45	1.51
45	AB	804	CLA	C1D-ND	2.22	1.40	1.37
45	A6	613	CLA	CMD-C2D	-2.22	1.46	1.50
45	B2	613	CLA	C3B-C4B	2.22	1.49	1.42
45	A4	301	CLA	CMB-C2B	-2.22	1.46	1.50
45	AA	828	CLA	CMB-C2B	-2.22	1.46	1.50
45	AB	808	CLA	CMB-C2B	-2.22	1.46	1.50
45	BB	812	CLA	CMD-C2D	-2.22	1.46	1.50
45	AA	837	CLA	C3B-C4B	2.22	1.49	1.42
45	AF	804	CLA	C3B-C4B	2.22	1.49	1.42
45	BA	813	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	808	CLA	CMB-C2B	-2.22	1.46	1.50
45	BF	302	CLA	CMC-C2C	-2.22	1.46	1.50
45	AL	304	CLA	CMC-C2C	-2.22	1.46	1.50
45	A6	609	CLA	CMB-C2B	-2.22	1.46	1.50
45	B2	603	CLA	CMD-C2D	-2.22	1.46	1.50
45	B1	309	CLA	CMD-C2D	-2.22	1.46	1.50
52	B1	316	LUT	C10-C9	2.22	1.40	1.35
45	BB	819	CLA	CMB-C2B	-2.22	1.46	1.50
45	B3	301	CLA	CMB-C2B	-2.22	1.46	1.50
45	A3	309	CLA	CMB-C2B	-2.22	1.46	1.50
45	AB	820	CLA	C1B-C2B	2.22	1.48	1.43
54	B1	303	CHL	CMC-C2C	2.22	1.49	1.44
45	AA	841	CLA	CMB-C2B	-2.22	1.46	1.50
45	BA	821	CLA	CMD-C2D	-2.22	1.46	1.50
45	AA	841	CLA	C3B-C4B	2.22	1.49	1.42
45	BA	829	CLA	C1B-C2B	2.22	1.48	1.43
45	BA	810	CLA	CMB-C2B	-2.22	1.46	1.50
45	BB	819	CLA	C1B-C2B	2.22	1.48	1.43
54	B5	605	CHL	CMC-C2C	2.21	1.49	1.44
45	AJ	102	CLA	C3B-C4B	2.21	1.49	1.42
45	BB	832	CLA	MG-NB	-2.21	2.01	2.05
45	B3	309	CLA	C3B-C4B	2.21	1.49	1.42
45	A6	614	CLA	CMD-C2D	-2.21	1.46	1.50
45	BA	832	CLA	C3B-C4B	2.21	1.49	1.42
45	BH	201	CLA	CMD-C2D	-2.21	1.46	1.50
45	BA	803	CLA	CMC-C2C	-2.21	1.46	1.50
45	A6	609	CLA	C3B-C4B	2.21	1.49	1.42
55	A3	317	XAT	O4-C5	-2.21	1.43	1.46
45	BL	304	CLA	CMD-C2D	-2.21	1.46	1.50
45	A1	305	CLA	CMD-C2D	-2.21	1.46	1.50
45	AG	203	CLA	C3B-C4B	2.21	1.49	1.42
48	BB	849	BCR	C19-C18	2.21	1.50	1.46
45	AA	810	CLA	C3B-C4B	2.21	1.49	1.42
45	BB	823	CLA	C3B-C4B	2.21	1.49	1.42
45	BB	829	CLA	CMD-C2D	-2.21	1.46	1.50
45	AG	201	CLA	CMD-C2D	-2.21	1.46	1.50
45	BB	822	CLA	C3B-C4B	2.21	1.49	1.42
45	BB	821	CLA	CMD-C2D	-2.21	1.46	1.50
45	AL	303	CLA	C3B-C4B	2.21	1.49	1.42
45	AF	804	CLA	CMD-C2D	-2.21	1.46	1.50
45	BA	833	CLA	MG-NB	-2.20	2.01	2.05
45	BB	805	CLA	MG-ND	-2.20	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	807	CLA	CMC-C2C	-2.20	1.46	1.50
45	BA	813	CLA	CMD-C2D	-2.20	1.46	1.50
45	BA	824	CLA	CMB-C2B	-2.20	1.46	1.50
45	A6	601	CLA	CHC-C1C	2.20	1.42	1.38
45	BB	811	CLA	CMD-C2D	-2.20	1.46	1.50
45	A1	313	CLA	CMD-C2D	-2.20	1.46	1.50
45	AH	201	CLA	CMD-C2D	-2.20	1.46	1.50
45	AB	825	CLA	C3B-C4B	2.20	1.49	1.42
45	BA	811	CLA	CMC-C2C	-2.20	1.46	1.50
45	AF	804	CLA	CMB-C2B	-2.20	1.46	1.50
45	A1	312	CLA	CMD-C2D	-2.20	1.46	1.50
45	AA	837	CLA	MG-NB	-2.20	2.01	2.05
45	A3	310	CLA	C3B-C4B	2.20	1.49	1.42
45	BA	831	CLA	MG-NB	-2.20	2.01	2.05
45	BA	807	CLA	CMD-C2D	-2.20	1.46	1.50
45	BA	840	CLA	CMB-C2B	-2.20	1.46	1.50
45	B1	311	CLA	CHC-C1C	2.20	1.42	1.38
48	AB	848	BCR	C19-C18	2.20	1.50	1.46
45	AK	202	CLA	CMD-C2D	-2.20	1.46	1.50
45	AB	815	CLA	CHC-C1C	2.20	1.42	1.38
45	AB	811	CLA	CMB-C2B	-2.20	1.46	1.50
45	A3	305	CLA	CMB-C2B	-2.19	1.46	1.50
45	AB	834	CLA	C3B-C4B	2.19	1.49	1.42
45	BB	822	CLA	CMC-C2C	-2.19	1.46	1.50
45	A4	310	CLA	CHC-C1C	2.19	1.42	1.38
45	BA	804	CLA	C3B-C4B	2.19	1.49	1.42
45	AA	809	CLA	C1B-C2B	2.19	1.48	1.43
45	BB	815	CLA	CMD-C2D	-2.19	1.46	1.50
45	BL	302	CLA	CMD-C2D	-2.19	1.46	1.50
45	BA	841	CLA	C3B-C4B	2.19	1.49	1.42
45	AB	827	CLA	CHC-C1C	2.19	1.42	1.38
45	AG	201	CLA	C3B-C4B	2.19	1.49	1.42
45	BB	836	CLA	CMD-C2D	-2.19	1.46	1.50
45	A3	304	CLA	CHC-C1C	2.19	1.42	1.38
45	B5	602	CLA	C1B-C2B	2.19	1.48	1.43
45	AB	838	CLA	CMB-C2B	-2.19	1.46	1.50
45	B5	609	CLA	CMC-C2C	-2.19	1.46	1.50
56	e	301	SQD	O2-C2	-2.19	1.37	1.43
45	BA	838	CLA	CMB-C2B	-2.19	1.46	1.50
45	B3	311	CLA	CMB-C2B	-2.19	1.46	1.50
45	AA	839	CLA	C3B-C4B	2.19	1.49	1.42
45	BB	821	CLA	C3B-C4B	2.19	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	830	CLA	C1B-C2B	2.19	1.48	1.43
54	B5	607	CHL	CBD-CGD	-2.19	1.49	1.52
45	BB	818	CLA	CMD-C2D	-2.19	1.46	1.50
45	BA	839	CLA	C3B-C4B	2.19	1.49	1.42
45	BB	813	CLA	CMD-C2D	-2.19	1.46	1.50
45	A6	604	CLA	C3B-C4B	2.19	1.49	1.42
45	A6	613	CLA	C3B-C4B	2.19	1.49	1.42
48	AA	848	BCR	C1-C6	-2.19	1.51	1.53
45	B1	305	CLA	C3B-C4B	2.19	1.49	1.42
45	AA	810	CLA	CMD-C2D	-2.19	1.46	1.50
45	A4	312	CLA	CMB-C2B	-2.19	1.46	1.50
45	BL	303	CLA	C1B-C2B	2.19	1.48	1.43
45	BB	816	CLA	CHC-C1C	2.19	1.42	1.38
45	AB	822	CLA	CMD-C2D	-2.19	1.46	1.50
45	BA	834	CLA	CMC-C2C	-2.19	1.46	1.50
45	B1	314	CLA	CMD-C2D	-2.18	1.46	1.50
45	A6	605	CLA	CMD-C2D	-2.18	1.46	1.50
45	AA	840	CLA	C3B-C4B	2.18	1.49	1.42
45	BB	808	CLA	C3B-C4B	2.18	1.49	1.42
45	AF	802	CLA	CMC-C2C	-2.18	1.46	1.50
45	BB	841	CLA	C1B-C2B	2.18	1.48	1.43
45	AA	833	CLA	CMD-C2D	-2.18	1.46	1.50
45	A3	314	CLA	CMB-C2B	-2.18	1.46	1.50
45	AB	805	CLA	C3B-C4B	2.18	1.49	1.42
45	B5	612	CLA	CMB-C2B	-2.18	1.46	1.50
45	BB	814	CLA	C3B-C4B	2.18	1.49	1.42
48	AA	845	BCR	C8-C9	2.18	1.50	1.46
45	BA	814	CLA	CMB-C2B	-2.18	1.46	1.50
45	A3	313	CLA	CMD-C2D	-2.18	1.46	1.50
45	A6	601	CLA	CMD-C2D	-2.18	1.46	1.50
45	BB	816	CLA	CMC-C2C	-2.18	1.46	1.50
45	AB	833	CLA	CMD-C2D	-2.18	1.46	1.50
54	A1	303	CHL	CMC-C2C	2.18	1.49	1.44
45	B1	310	CLA	CMD-C2D	-2.18	1.46	1.50
48	BI	101	BCR	C1-C6	-2.18	1.51	1.53
45	A4	312	CLA	CHC-C1C	2.18	1.42	1.38
45	AA	826	CLA	CMB-C2B	-2.18	1.46	1.50
45	BA	805	CLA	CMC-C2C	-2.18	1.46	1.50
45	BA	823	CLA	CMD-C2D	-2.18	1.46	1.50
45	BB	833	CLA	CMC-C2C	-2.18	1.46	1.50
45	A3	312	CLA	C3B-C4B	2.18	1.49	1.42
46	BB	844	PQN	C11-C3	2.18	1.55	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	843	CLA	CMB-C2B	-2.18	1.46	1.50
45	BB	826	CLA	C3B-C4B	2.18	1.49	1.42
45	BA	822	CLA	CMD-C2D	-2.18	1.46	1.50
45	AB	825	CLA	MG-ND	-2.18	2.01	2.05
45	AL	305	CLA	C3B-C4B	2.18	1.49	1.42
45	A4	301	CLA	C3B-C4B	2.18	1.49	1.42
45	AB	815	CLA	CMB-C2B	-2.18	1.46	1.50
45	BA	809	CLA	CMB-C2B	-2.18	1.46	1.50
54	B2	614	CHL	CMC-C2C	2.18	1.49	1.44
45	BB	838	CLA	CMB-C2B	-2.18	1.46	1.50
45	B5	611	CLA	CMB-C2B	-2.18	1.46	1.50
45	BB	807	CLA	CHC-C1C	2.18	1.42	1.38
45	AK	201	CLA	CBD-CAD	2.18	1.56	1.51
45	AK	203	CLA	CMD-C2D	-2.18	1.46	1.50
45	A1	309	CLA	CMD-C2D	-2.18	1.46	1.50
45	BA	801	CLA	CMD-C2D	-2.18	1.46	1.50
45	BB	808	CLA	CMC-C2C	-2.18	1.46	1.50
45	AA	825	CLA	C1B-NB	-2.18	1.35	1.37
45	AB	828	CLA	CMD-C2D	-2.18	1.46	1.50
45	AA	817	CLA	C3B-C4B	2.17	1.49	1.42
45	AA	821	CLA	CMC-C2C	-2.17	1.46	1.50
45	AA	806	CLA	CMC-C2C	-2.17	1.46	1.50
45	A4	308	CLA	CHC-C1C	2.17	1.42	1.38
45	BG	202	CLA	C3B-C4B	2.17	1.49	1.42
45	AB	824	CLA	MG-ND	-2.17	2.01	2.05
45	A1	307	CLA	CMC-C2C	-2.17	1.46	1.50
45	AB	813	CLA	C3B-C4B	2.17	1.49	1.42
45	AB	820	CLA	C3B-C4B	2.17	1.49	1.42
45	BA	802	CLA	C3B-C4B	2.17	1.49	1.42
45	BB	802	CLA	CMB-C2B	-2.17	1.46	1.50
45	A3	309	CLA	CHC-C1C	2.17	1.42	1.38
45	AA	815	CLA	C3B-C4B	2.17	1.49	1.42
45	AA	838	CLA	CMC-C2C	-2.17	1.46	1.50
45	BB	809	CLA	CMD-C2D	-2.17	1.46	1.50
45	A1	315	CLA	CMB-C2B	-2.17	1.46	1.50
45	AB	820	CLA	MG-NB	-2.17	2.01	2.05
45	B3	313	CLA	CBD-CAD	2.17	1.56	1.51
45	AA	804	CLA	CMC-C2C	-2.17	1.46	1.50
45	AB	824	CLA	CMC-C2C	-2.17	1.46	1.50
45	AB	837	CLA	CMD-C2D	-2.17	1.46	1.50
45	A4	303	CLA	CMB-C2B	-2.17	1.46	1.50
45	B5	602	CLA	CMC-C2C	-2.17	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	816	CLA	CMD-C2D	-2.17	1.46	1.50
45	A3	312	CLA	CMB-C2B	-2.17	1.46	1.50
45	BA	803	CLA	C3B-C4B	2.17	1.49	1.42
45	AA	817	CLA	CMB-C2B	-2.17	1.46	1.50
45	B5	612	CLA	CMD-C2D	-2.17	1.46	1.50
45	AA	816	CLA	C3B-C4B	2.17	1.49	1.42
45	AA	806	CLA	CMB-C2B	-2.17	1.46	1.50
45	AA	823	CLA	C3B-C4B	2.16	1.49	1.42
45	B5	608	CLA	C1B-C2B	2.16	1.48	1.43
45	BK	201	CLA	CHC-C1C	2.16	1.42	1.38
45	AB	814	CLA	C3B-C4B	2.16	1.49	1.42
45	A3	303	CLA	C3B-C4B	2.16	1.49	1.42
45	BG	201	CLA	CMD-C2D	-2.16	1.46	1.50
45	B5	613	CLA	CHC-C1C	2.16	1.42	1.38
45	BA	829	CLA	CHC-C1C	2.16	1.42	1.38
45	AA	820	CLA	CMC-C2C	-2.16	1.46	1.50
45	A4	302	CLA	CMC-C2C	-2.16	1.46	1.50
45	BA	804	CLA	CMC-C2C	-2.16	1.46	1.50
45	AB	828	CLA	CMB-C2B	-2.16	1.46	1.50
45	BB	819	CLA	C3B-C4B	2.16	1.49	1.42
45	BH	201	CLA	C3B-C4B	2.16	1.49	1.42
45	A3	310	CLA	CMD-C2D	-2.16	1.46	1.50
45	B3	303	CLA	CHC-C1C	2.16	1.42	1.38
45	A3	312	CLA	CMC-C2C	-2.16	1.46	1.50
45	AB	834	CLA	CMB-C2B	-2.16	1.46	1.50
45	BA	821	CLA	C3B-C4B	2.16	1.49	1.42
45	B5	604	CLA	CHC-C1C	2.16	1.42	1.38
45	AA	828	CLA	CMC-C2C	-2.16	1.46	1.50
45	AA	824	CLA	CMB-C2B	-2.16	1.46	1.50
45	BA	825	CLA	C3B-C4B	2.16	1.49	1.42
45	BF	302	CLA	CMB-C2B	-2.16	1.46	1.50
45	AF	802	CLA	MG-ND	-2.16	2.01	2.05
45	AB	839	CLA	C3B-C4B	2.16	1.49	1.42
45	B3	302	CLA	CMD-C2D	-2.16	1.46	1.50
45	B5	604	CLA	CMB-C2B	-2.16	1.46	1.50
45	AA	840	CLA	C1B-C2B	2.16	1.48	1.43
45	AA	827	CLA	CMC-C2C	-2.16	1.46	1.50
45	AB	840	CLA	MG-NB	-2.16	2.01	2.05
45	BA	804	CLA	CMB-C2B	-2.16	1.46	1.50
45	BA	820	CLA	CMB-C2B	-2.16	1.46	1.50
45	BB	808	CLA	MG-NB	-2.16	2.01	2.05
45	AA	822	CLA	CMD-C2D	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	821	CLA	CMC-C2C	-2.15	1.46	1.50
45	BB	822	CLA	CMB-C2B	-2.15	1.46	1.50
45	BK	203	CLA	CMD-C2D	-2.15	1.46	1.50
45	AB	815	CLA	MG-NB	-2.15	2.01	2.05
45	AA	812	CLA	CMC-C2C	-2.15	1.46	1.50
45	AA	824	CLA	C3B-C4B	2.15	1.49	1.42
45	BB	841	CLA	MG-NB	-2.15	2.01	2.05
45	BA	812	CLA	C3B-C4B	2.15	1.49	1.42
45	BB	835	CLA	CMC-C2C	-2.15	1.46	1.50
45	A1	306	CLA	CMD-C2D	-2.15	1.46	1.50
45	A4	312	CLA	CMD-C2D	-2.15	1.46	1.50
45	BB	811	CLA	MG-NB	-2.15	2.01	2.05
45	A6	605	CLA	C3B-C4B	2.15	1.49	1.42
45	AB	829	CLA	C1B-C2B	2.15	1.48	1.43
45	B2	604	CLA	CMD-C2D	-2.15	1.46	1.50
45	BK	202	CLA	CHC-C1C	2.15	1.42	1.38
45	B5	608	CLA	CHC-C1C	2.15	1.42	1.38
45	BA	836	CLA	C3B-C4B	2.15	1.49	1.42
45	B3	308	CLA	CMB-C2B	-2.15	1.46	1.50
45	AG	204	CLA	CHC-C1C	2.15	1.42	1.38
45	BB	826	CLA	CHC-C1C	2.15	1.42	1.38
45	B3	302	CLA	C3B-C4B	2.15	1.49	1.42
48	BA	847	BCR	C30-C25	-2.15	1.51	1.53
45	A1	312	CLA	CMB-C2B	-2.15	1.46	1.50
45	AB	815	CLA	C3B-C4B	2.15	1.49	1.42
45	A1	313	CLA	CMC-C2C	-2.15	1.46	1.50
52	B1	316	LUT	C34-C33	2.15	1.40	1.35
45	AB	807	CLA	CMC-C2C	-2.15	1.46	1.50
45	A3	302	CLA	CMD-C2D	-2.15	1.46	1.50
45	AG	204	CLA	CMD-C2D	-2.15	1.46	1.50
45	AB	807	CLA	MG-NB	-2.15	2.01	2.05
45	BB	813	CLA	CMB-C2B	-2.15	1.46	1.50
45	BB	816	CLA	CMB-C2B	-2.15	1.46	1.50
45	B2	602	CLA	CMC-C2C	-2.15	1.46	1.50
45	AB	821	CLA	C3B-C4B	2.14	1.49	1.42
45	A1	311	CLA	CMD-C2D	-2.14	1.46	1.50
45	BB	831	CLA	CMC-C2C	-2.14	1.46	1.50
45	B2	611	CLA	CMB-C2B	-2.14	1.46	1.50
45	BB	821	CLA	CHC-C1C	2.14	1.42	1.38
45	BB	824	CLA	C3B-C4B	2.14	1.49	1.42
45	AA	820	CLA	CMB-C2B	-2.14	1.46	1.50
45	B2	609	CLA	CMD-C2D	-2.14	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	e	301	SQD	O47-C45	-2.14	1.41	1.46
45	AA	815	CLA	CMB-C2B	-2.14	1.46	1.50
45	A1	306	CLA	CMB-C2B	-2.14	1.46	1.50
45	A3	306	CLA	CMB-C2B	-2.14	1.46	1.50
45	A6	613	CLA	CMC-C2C	-2.14	1.46	1.50
45	B2	613	CLA	CMB-C2B	-2.14	1.46	1.50
45	AA	820	CLA	C3B-C4B	2.14	1.49	1.42
45	BA	811	CLA	C3B-C4B	2.14	1.49	1.42
45	B3	308	CLA	C3B-C4B	2.14	1.49	1.42
45	AA	823	CLA	CHC-C1C	2.14	1.42	1.38
45	BB	820	CLA	CMD-C2D	-2.14	1.46	1.50
45	B2	604	CLA	CHC-C1C	2.14	1.42	1.38
45	BA	815	CLA	CMD-C2D	-2.14	1.46	1.50
45	BA	819	CLA	C3B-C4B	2.14	1.49	1.42
45	BB	831	CLA	CHC-C4B	-2.14	1.34	1.39
45	AK	201	CLA	CHC-C1C	2.14	1.42	1.38
45	AA	813	CLA	CMD-C2D	-2.14	1.46	1.50
45	A1	313	CLA	CMB-C2B	-2.14	1.46	1.50
45	BB	817	CLA	CMC-C2C	-2.14	1.46	1.50
45	BA	842	CLA	MG-NB	-2.14	2.01	2.05
45	BB	816	CLA	C1B-C2B	2.14	1.48	1.43
45	BA	802	CLA	C1B-C2B	2.14	1.48	1.43
52	A6	615	LUT	C22-C21	-2.14	1.52	1.54
45	B1	305	CLA	CMB-C2B	-2.14	1.46	1.50
45	BA	834	CLA	MG-NB	-2.14	2.01	2.05
45	A4	308	CLA	CMB-C2B	-2.14	1.46	1.50
45	BF	301	CLA	C3B-C4B	2.14	1.49	1.42
45	B3	304	CLA	C3B-C4B	2.13	1.49	1.42
45	AB	814	CLA	C1B-C2B	2.13	1.48	1.43
45	AA	813	CLA	MG-NB	-2.13	2.01	2.05
45	AA	837	CLA	CMB-C2B	-2.13	1.46	1.50
45	BA	817	CLA	CMD-C2D	-2.13	1.46	1.50
45	B2	603	CLA	C3B-C4B	2.13	1.49	1.42
45	B2	603	CLA	CMB-C2B	-2.13	1.46	1.50
45	B3	314	CLA	CHC-C1C	2.13	1.42	1.38
45	AB	828	CLA	CMC-C2C	-2.13	1.46	1.50
45	AA	818	CLA	MG-NB	-2.13	2.01	2.05
45	AH	201	CLA	CMB-C2B	-2.13	1.46	1.50
48	BB	847	BCR	C8-C9	2.13	1.50	1.46
45	A3	314	CLA	CMD-C2D	-2.13	1.46	1.50
45	AB	818	CLA	CHC-C1C	2.13	1.42	1.38
45	AK	202	CLA	CHC-C1C	2.13	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	BJ	104	SQD	O6-C1	2.13	1.43	1.40
45	BA	844	CLA	CHC-C1C	2.13	1.42	1.38
45	AA	805	CLA	C3B-C4B	2.13	1.48	1.42
45	BB	805	CLA	C3B-C4B	2.13	1.48	1.42
45	B3	304	CLA	CMD-C2D	-2.13	1.46	1.50
45	AA	822	CLA	CHC-C1C	2.13	1.42	1.38
45	BB	837	CLA	C3B-C4B	2.13	1.48	1.42
45	BA	831	CLA	C3B-C4B	2.13	1.48	1.42
45	AB	837	CLA	MG-NB	-2.13	2.01	2.05
45	AB	833	CLA	CMB-C2B	-2.13	1.46	1.50
45	B2	604	CLA	CMB-C2B	-2.13	1.46	1.50
45	B2	612	CLA	CMD-C2D	-2.13	1.46	1.50
45	AA	826	CLA	CHC-C1C	2.13	1.42	1.38
45	BA	823	CLA	C3B-C4B	2.13	1.48	1.42
45	AB	831	CLA	CMC-C2C	-2.13	1.46	1.50
45	BA	809	CLA	MG-NB	-2.13	2.01	2.05
45	A1	315	CLA	CMD-C2D	-2.13	1.46	1.50
45	B5	610	CLA	CMB-C2B	-2.13	1.46	1.50
45	AB	804	CLA	CHC-C1C	2.13	1.42	1.38
45	BB	826	CLA	CMC-C2C	-2.13	1.46	1.50
45	BA	842	CLA	C3B-C4B	2.13	1.48	1.42
45	AA	839	CLA	CMB-C2B	-2.13	1.46	1.50
45	A4	310	CLA	CMB-C2B	-2.13	1.46	1.50
45	A6	605	CLA	CMC-C2C	-2.13	1.46	1.50
45	B5	611	CLA	C3B-C4B	2.12	1.48	1.42
45	A1	309	CLA	CHC-C1C	2.12	1.42	1.38
45	AB	838	CLA	CHC-C1C	2.12	1.42	1.38
45	BA	837	CLA	CMC-C2C	-2.12	1.46	1.50
45	AA	835	CLA	C3B-C4B	2.12	1.48	1.42
45	A3	313	CLA	CHC-C1C	2.12	1.42	1.38
45	AA	804	CLA	CHC-C1C	2.12	1.42	1.38
55	B3	316	XAT	O4-C5	-2.12	1.43	1.46
48	AK	204	BCR	C8-C9	2.12	1.50	1.46
45	BB	841	CLA	C3B-C4B	2.12	1.48	1.42
45	A6	603	CLA	C3B-C4B	2.12	1.48	1.42
45	AA	807	CLA	CMD-C2D	-2.12	1.46	1.50
45	A4	302	CLA	CMB-C2B	-2.12	1.46	1.50
45	B2	611	CLA	CMD-C2D	-2.12	1.46	1.50
45	B5	611	CLA	CMD-C2D	-2.12	1.46	1.50
45	AB	804	CLA	C3B-C4B	2.12	1.48	1.42
45	AA	806	CLA	CHC-C1C	2.12	1.42	1.38
45	AK	203	CLA	C3B-C4B	2.12	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	831	CLA	C3B-C4B	2.12	1.48	1.42
45	BB	836	CLA	C3B-C4B	2.12	1.48	1.42
45	AB	813	CLA	CHC-C1C	2.12	1.42	1.38
45	A3	312	CLA	CHC-C1C	2.12	1.42	1.38
45	B1	305	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	833	CLA	CMD-C2D	-2.12	1.46	1.50
45	B3	303	CLA	CMD-C2D	-2.12	1.46	1.50
45	B3	312	CLA	CHC-C1C	2.12	1.42	1.38
45	B5	609	CLA	CMB-C2B	-2.12	1.46	1.50
45	A1	311	CLA	CHC-C1C	2.12	1.42	1.38
45	BB	818	CLA	C3B-C4B	2.12	1.48	1.42
45	BA	810	CLA	CMD-C2D	-2.12	1.46	1.50
45	AB	819	CLA	CMC-C2C	-2.12	1.46	1.50
45	AL	304	CLA	C3B-C4B	2.12	1.48	1.42
45	BA	805	CLA	C3B-C4B	2.12	1.48	1.42
45	AB	839	CLA	MG-NB	-2.12	2.01	2.05
45	BA	832	CLA	CMD-C2D	-2.12	1.46	1.50
45	A1	304	CLA	MG-NB	-2.12	2.01	2.05
45	AA	803	CLA	CMB-C2B	-2.12	1.46	1.50
45	B2	608	CLA	C3B-C4B	2.12	1.48	1.42
45	AA	801	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	830	CLA	MG-ND	-2.12	2.01	2.05
45	BB	809	CLA	C3B-C4B	2.11	1.48	1.42
45	AB	818	CLA	C1B-C2B	2.11	1.48	1.43
45	AB	826	CLA	CMC-C2C	-2.11	1.46	1.50
45	B3	301	CLA	CMD-C2D	-2.11	1.46	1.50
45	AB	825	CLA	CMB-C2B	-2.11	1.46	1.50
45	AB	806	CLA	CHC-C1C	2.11	1.42	1.38
45	AA	802	CLA	C1B-C2B	2.11	1.48	1.43
45	BB	801	CLA	C1B-C2B	2.11	1.48	1.43
46	BB	844	PQN	C10-C1	2.11	1.52	1.48
45	BA	820	CLA	MG-NB	-2.11	2.01	2.05
45	A4	313	CLA	C3B-C4B	2.11	1.48	1.42
45	AB	812	CLA	CMC-C2C	-2.11	1.46	1.50
45	AB	808	CLA	C3B-C4B	2.11	1.48	1.42
45	AJ	102	CLA	CHC-C1C	2.11	1.42	1.38
45	BB	826	CLA	MG-ND	-2.11	2.01	2.05
45	BA	816	CLA	C3B-C4B	2.11	1.48	1.42
45	AA	805	CLA	CHC-C1C	2.11	1.42	1.38
45	A1	309	CLA	CMB-C2B	-2.11	1.46	1.50
45	B1	312	CLA	CMD-C2D	-2.11	1.46	1.50
45	B2	613	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	610	CLA	CMD-C2D	-2.11	1.46	1.50
45	BA	826	CLA	MG-NB	-2.11	2.01	2.05
45	BB	824	CLA	CMB-C2B	-2.11	1.46	1.50
45	AB	841	CLA	MG-NB	-2.11	2.01	2.05
45	BA	803	CLA	MG-NB	-2.11	2.01	2.05
45	AA	810	CLA	CMC-C2C	-2.11	1.46	1.50
45	A3	304	CLA	CMD-C2D	-2.11	1.46	1.50
45	AB	804	CLA	MG-NB	-2.11	2.01	2.05
45	A4	311	CLA	CHC-C1C	2.11	1.42	1.38
45	BB	806	CLA	CMC-C2C	-2.11	1.46	1.50
52	A1	317	LUT	C22-C21	-2.11	1.52	1.54
45	BB	837	CLA	CMB-C2B	-2.11	1.46	1.50
45	AB	842	CLA	C3B-C4B	2.11	1.48	1.42
45	AA	821	CLA	CHC-C1C	2.11	1.42	1.38
45	B5	601	CLA	CMD-C2D	-2.11	1.46	1.50
45	A1	314	CLA	C3B-C4B	2.11	1.48	1.42
45	A3	304	CLA	CMB-C2B	-2.11	1.46	1.50
45	BA	831	CLA	C1B-C2B	2.11	1.48	1.43
45	AG	203	CLA	CMB-C2B	-2.11	1.46	1.50
45	BB	825	CLA	CMB-C2B	-2.11	1.46	1.50
48	BL	306	BCR	C30-C25	-2.11	1.51	1.53
45	AA	825	CLA	MG-NB	-2.11	2.01	2.05
45	AA	826	CLA	CMC-C2C	-2.11	1.46	1.50
45	AB	835	CLA	C3B-C4B	2.11	1.48	1.42
45	A4	310	CLA	CMC-C2C	-2.10	1.46	1.50
45	AA	840	CLA	MG-NB	-2.10	2.01	2.05
45	BB	828	CLA	CMB-C2B	-2.10	1.46	1.50
45	BA	824	CLA	CMD-C2D	-2.10	1.46	1.50
45	BB	801	CLA	CMC-C2C	-2.10	1.46	1.50
45	B3	302	CLA	CMB-C2B	-2.10	1.46	1.50
45	AA	811	CLA	C3B-C4B	2.10	1.48	1.42
45	B3	301	CLA	CHC-C1C	2.10	1.42	1.38
53	A4	318	LMG	O7-C8	-2.10	1.41	1.46
45	BB	835	CLA	CMB-C2B	-2.10	1.46	1.50
45	B3	305	CLA	CMD-C2D	-2.10	1.46	1.50
45	B3	313	CLA	CMD-C2D	-2.10	1.46	1.50
45	AB	822	CLA	C3B-C4B	2.10	1.48	1.42
45	BB	829	CLA	CHC-C1C	2.10	1.42	1.38
45	BB	824	CLA	CMC-C2C	-2.10	1.46	1.50
45	AB	836	CLA	C3B-C4B	2.10	1.48	1.42
45	A4	309	CLA	CMB-C2B	-2.10	1.46	1.50
45	B2	609	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B1	309	CLA	CHC-C1C	2.10	1.42	1.38
45	AA	836	CLA	C3B-C4B	2.10	1.48	1.42
45	AB	830	CLA	C3B-C4B	2.10	1.48	1.42
45	AB	816	CLA	CMB-C2B	-2.10	1.46	1.50
45	BA	831	CLA	CHC-C1C	2.10	1.42	1.38
45	BA	818	CLA	C3B-C4B	2.10	1.48	1.42
48	AA	852	BCR	C12-C13	2.10	1.50	1.46
45	BB	815	CLA	CHC-C1C	2.10	1.42	1.38
45	A3	303	CLA	CMC-C2C	-2.10	1.46	1.50
45	AA	818	CLA	CMC-C2C	-2.10	1.46	1.50
45	BB	828	CLA	CMC-C2C	-2.10	1.46	1.50
45	B1	310	CLA	CMB-C2B	-2.10	1.46	1.50
45	AB	831	CLA	C3B-C4B	2.10	1.48	1.42
45	B1	315	CLA	CHC-C1C	2.10	1.42	1.38
54	A4	306	CHL	CBD-CGD	-2.10	1.49	1.52
45	BB	812	CLA	CMB-C2B	-2.09	1.46	1.50
45	AB	816	CLA	C3B-C4B	2.09	1.48	1.42
45	A3	302	CLA	CMB-C2B	-2.09	1.46	1.50
45	BB	841	CLA	CMC-C2C	-2.09	1.46	1.50
45	AK	201	CLA	CMC-C2C	-2.09	1.46	1.50
45	BB	810	CLA	CMB-C2B	-2.09	1.46	1.50
45	BA	814	CLA	CHC-C1C	2.09	1.42	1.38
45	AH	201	CLA	C3B-C4B	2.09	1.48	1.42
54	B2	607	CHL	CMC-C2C	2.09	1.49	1.44
48	BL	301	BCR	C8-C9	2.09	1.50	1.46
52	B1	316	LUT	C14-C13	2.09	1.40	1.35
45	B5	601	CLA	C3B-C4B	2.09	1.48	1.42
45	AA	824	CLA	CMC-C2C	-2.09	1.46	1.50
45	BB	841	CLA	CMB-C2B	-2.09	1.46	1.50
45	AA	807	CLA	CMB-C2B	-2.09	1.46	1.50
45	AB	829	CLA	MG-ND	-2.09	2.01	2.05
45	B3	305	CLA	CHC-C1C	2.09	1.42	1.38
45	BA	808	CLA	C3B-C4B	2.09	1.48	1.42
45	AA	831	CLA	CMC-C2C	-2.09	1.46	1.50
45	AA	826	CLA	MG-NB	-2.09	2.01	2.05
45	AB	840	CLA	C1B-C2B	2.09	1.48	1.43
45	AA	807	CLA	CHC-C1C	2.09	1.42	1.38
45	A4	313	CLA	CMC-C2C	-2.09	1.46	1.50
45	B1	313	CLA	CMB-C2B	-2.09	1.46	1.50
45	BA	827	CLA	CHC-C1C	2.09	1.42	1.38
45	BB	833	CLA	CMB-C2B	-2.09	1.46	1.50
45	AB	842	CLA	CHC-C1C	2.09	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	610	CLA	CMC-C2C	-2.09	1.46	1.50
45	B5	611	CLA	CMC-C2C	-2.09	1.46	1.50
45	AA	836	CLA	CMD-C2D	-2.09	1.46	1.50
45	B3	311	CLA	CHC-C1C	2.09	1.42	1.38
48	AB	844	BCR	C30-C25	-2.09	1.51	1.53
45	A1	306	CLA	CMC-C2C	-2.08	1.46	1.50
45	BA	807	CLA	CMB-C2B	-2.08	1.46	1.50
45	BB	806	CLA	CMB-C2B	-2.08	1.46	1.50
45	AA	803	CLA	C3B-C4B	2.08	1.48	1.42
45	BB	815	CLA	MG-ND	-2.08	2.01	2.05
45	A3	314	CLA	CBD-CAD	2.08	1.56	1.51
45	AB	803	CLA	CMC-C2C	-2.08	1.46	1.50
48	AB	845	BCR	C8-C9	2.08	1.50	1.46
45	AB	827	CLA	CMB-C2B	-2.08	1.46	1.50
45	AK	202	CLA	CMB-C2B	-2.08	1.46	1.50
45	B1	313	CLA	CMD-C2D	-2.08	1.46	1.50
45	AA	841	CLA	CHC-C1C	2.08	1.42	1.38
48	BA	856	BCR	C12-C13	2.08	1.50	1.46
45	B1	304	CLA	C3B-C4B	2.08	1.48	1.42
54	B2	607	CHL	CBD-CGD	-2.08	1.49	1.52
45	A6	612	CLA	CHC-C1C	2.08	1.42	1.38
45	A4	308	CLA	CMC-C2C	-2.08	1.46	1.50
45	AA	814	CLA	MG-NB	-2.08	2.01	2.05
45	AA	809	CLA	CHC-C1C	2.08	1.42	1.38
45	A3	313	CLA	CMB-C2B	-2.08	1.46	1.50
45	AB	828	CLA	CHC-C1C	2.08	1.42	1.38
45	A1	305	CLA	CMB-C2B	-2.08	1.46	1.50
45	BA	837	CLA	CMB-C2B	-2.08	1.46	1.50
45	B3	313	CLA	C3B-C4B	2.08	1.48	1.42
45	AG	201	CLA	CHC-C1C	2.08	1.42	1.38
45	AB	806	CLA	CMB-C2B	-2.08	1.46	1.50
45	A3	314	CLA	CHC-C1C	2.08	1.42	1.38
45	BA	833	CLA	C3B-C4B	2.08	1.48	1.42
45	AA	812	CLA	C3B-C4B	2.08	1.48	1.42
45	BB	827	CLA	CMC-C2C	-2.08	1.46	1.50
48	AF	801	BCR	C23-C22	2.08	1.50	1.46
45	A3	305	CLA	CHC-C1C	2.07	1.42	1.38
54	B5	607	CHL	CMC-C2C	2.07	1.49	1.44
45	BJ	102	CLA	CMB-C2B	-2.07	1.46	1.50
45	AA	831	CLA	CHC-C1C	2.07	1.42	1.38
45	A3	306	CLA	CHC-C1C	2.07	1.42	1.38
52	AF	806	LUT	C8-C9	2.07	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	609	CLA	CMC-C2C	-2.07	1.46	1.50
45	B1	304	CLA	MG-NB	-2.07	2.01	2.05
45	B1	311	CLA	CMD-C2D	-2.07	1.46	1.50
45	B5	604	CLA	CMD-C2D	-2.07	1.46	1.50
45	AA	830	CLA	C3B-C4B	2.07	1.48	1.42
46	AA	843	PQN	C2-C1	2.07	1.52	1.47
45	B3	313	CLA	CMB-C2B	-2.07	1.46	1.50
45	AA	840	CLA	CHC-C1C	2.07	1.42	1.38
45	BJ	102	CLA	CHC-C1C	2.07	1.42	1.38
45	BB	838	CLA	MG-ND	-2.07	2.01	2.05
45	AA	820	CLA	CHC-C1C	2.07	1.42	1.38
45	AK	201	CLA	CMD-C2D	-2.07	1.46	1.50
45	B1	315	CLA	CMB-C2B	-2.07	1.46	1.50
45	B2	602	CLA	MG-NB	-2.07	2.01	2.05
45	BK	201	CLA	CBD-CAD	2.07	1.56	1.51
45	BA	826	CLA	CMB-C2B	-2.07	1.46	1.50
45	B3	312	CLA	CMD-C2D	-2.07	1.46	1.50
45	A4	303	CLA	CHC-C1C	2.07	1.42	1.38
45	AA	809	CLA	CMC-C2C	-2.07	1.46	1.50
45	A6	603	CLA	CHC-C1C	2.07	1.42	1.38
45	BA	835	CLA	C3B-C4B	2.07	1.48	1.42
45	B1	309	CLA	CMB-C2B	-2.06	1.46	1.50
45	A1	307	CLA	CHC-C1C	2.06	1.42	1.38
45	AA	839	CLA	CMC-C2C	-2.06	1.46	1.50
45	B5	613	CLA	CMB-C2B	-2.06	1.46	1.50
45	AA	816	CLA	CMC-C2C	-2.06	1.46	1.50
45	AB	827	CLA	MG-NB	-2.06	2.01	2.05
45	BB	819	CLA	CMC-C2C	-2.06	1.46	1.50
45	AB	810	CLA	CMC-C2C	-2.06	1.46	1.50
45	BA	820	CLA	CMC-C2C	-2.06	1.46	1.50
45	AB	831	CLA	CHC-C1C	2.06	1.42	1.38
47	BA	845	LHG	O7-C5	-2.06	1.41	1.46
45	AA	804	CLA	CMB-C2B	-2.06	1.46	1.50
45	BA	832	CLA	CMC-C2C	-2.06	1.46	1.50
48	AA	845	BCR	C12-C13	2.06	1.50	1.46
45	BB	843	CLA	CMC-C2C	-2.06	1.46	1.50
45	B5	608	CLA	CMC-C2C	-2.06	1.46	1.50
45	BB	811	CLA	MG-ND	-2.06	2.01	2.05
45	AA	812	CLA	CHC-C4B	-2.06	1.34	1.39
45	AB	840	CLA	CMC-C2C	-2.06	1.46	1.50
45	BB	802	CLA	MG-ND	-2.06	2.01	2.05
45	B3	309	CLA	CHC-C1C	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	829	CLA	CMC-C2C	-2.06	1.46	1.50
45	B5	601	CLA	CMB-C2B	-2.06	1.46	1.50
45	BB	825	CLA	C3B-C4B	2.06	1.48	1.42
45	AB	823	CLA	CMC-C2C	-2.06	1.46	1.50
45	AA	808	CLA	CHC-C1C	2.06	1.42	1.38
45	AA	814	CLA	CMC-C2C	-2.06	1.46	1.50
45	AA	819	CLA	C3B-C4B	2.06	1.48	1.42
45	A3	310	CLA	CHC-C1C	2.06	1.42	1.38
45	BA	810	CLA	CMC-C2C	-2.06	1.46	1.50
45	B2	610	CLA	CMB-C2B	-2.06	1.46	1.50
45	BA	840	CLA	C3B-C4B	2.06	1.48	1.42
45	AA	842	CLA	C3B-C4B	2.06	1.48	1.42
45	BG	202	CLA	CMD-C2D	-2.05	1.46	1.50
45	B1	311	CLA	CMC-C2C	-2.05	1.46	1.50
45	A6	611	CLA	CHC-C1C	2.05	1.42	1.38
45	BB	810	CLA	CHC-C1C	2.05	1.42	1.38
45	BL	302	CLA	CHC-C1C	2.05	1.42	1.38
45	BB	823	CLA	CMC-C2C	-2.05	1.46	1.50
45	AA	825	CLA	CMC-C2C	-2.05	1.46	1.50
45	AA	837	CLA	CMC-C2C	-2.05	1.46	1.50
45	BA	838	CLA	CMC-C2C	-2.05	1.46	1.50
45	B5	601	CLA	MG-NB	-2.05	2.01	2.05
45	A4	309	CLA	CMD-C2D	-2.05	1.46	1.50
45	B1	313	CLA	CMC-C2C	-2.05	1.46	1.50
45	A1	313	CLA	CHC-C1C	2.05	1.42	1.38
45	BA	810	CLA	C3B-C4B	2.05	1.48	1.42
45	A3	309	CLA	CMC-C2C	-2.05	1.46	1.50
45	A3	310	CLA	CMB-C2B	-2.05	1.46	1.50
45	B1	310	CLA	CMC-C2C	-2.05	1.46	1.50
45	AB	803	CLA	CHC-C1C	2.05	1.42	1.38
45	BB	842	CLA	C3B-C4B	2.05	1.48	1.42
45	AA	822	CLA	CMB-C2B	-2.05	1.46	1.50
45	A3	303	CLA	MG-NB	-2.05	2.01	2.05
45	BA	815	CLA	MG-NB	-2.05	2.01	2.05
45	A3	311	CLA	CHC-C1C	2.05	1.42	1.38
45	AB	814	CLA	MG-ND	-2.05	2.01	2.05
45	BG	202	CLA	MG-NB	-2.05	2.01	2.05
45	B1	312	CLA	CMC-C2C	-2.05	1.46	1.50
45	BB	802	CLA	CHC-C1C	2.05	1.42	1.38
48	A6	617	BCR	C12-C13	2.05	1.50	1.46
45	BA	822	CLA	CHC-C1C	2.05	1.42	1.38
45	BA	813	CLA	MG-NB	-2.04	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	609	CLA	CMC-C2C	-2.04	1.46	1.50
45	B3	302	CLA	MG-NB	-2.04	2.01	2.05
45	AB	817	CLA	CMC-C2C	-2.04	1.46	1.50
45	AB	823	CLA	C3B-C4B	2.04	1.48	1.42
45	B2	611	CLA	CHC-C1C	2.04	1.42	1.38
45	BB	807	CLA	CMB-C2B	-2.04	1.46	1.50
45	BK	201	CLA	CMC-C2C	-2.04	1.46	1.50
45	BB	831	CLA	C3B-C4B	2.04	1.48	1.42
45	B2	610	CLA	CHC-C1C	2.04	1.42	1.38
45	AB	803	CLA	C3B-C4B	2.04	1.48	1.42
45	BB	819	CLA	CHC-C1C	2.04	1.42	1.38
45	AG	204	CLA	CMC-C2C	-2.04	1.46	1.50
45	BK	202	CLA	CMD-C2D	-2.04	1.46	1.50
45	B2	612	CLA	CHC-C1C	2.04	1.42	1.38
45	A6	612	CLA	CMC-C2C	-2.04	1.46	1.50
45	AA	835	CLA	CHC-C1C	2.04	1.42	1.38
45	BA	830	CLA	MG-NB	-2.04	2.01	2.05
45	AA	829	CLA	C4B-NB	2.04	1.40	1.37
45	AB	840	CLA	C3B-C4B	2.04	1.48	1.42
45	AB	837	CLA	C1B-NB	-2.04	1.35	1.37
45	B1	306	CLA	CMD-C2D	-2.04	1.46	1.50
45	B3	305	CLA	CMB-C2B	-2.04	1.46	1.50
45	B5	603	CLA	CHC-C1C	2.04	1.42	1.38
45	AA	838	CLA	C3B-C4B	2.04	1.48	1.42
45	AB	806	CLA	CMC-C2C	-2.04	1.46	1.50
45	BK	203	CLA	CHC-C1C	2.04	1.42	1.38
45	AA	824	CLA	CHC-C1C	2.04	1.42	1.38
45	A6	611	CLA	CMB-C2B	-2.04	1.46	1.50
54	A4	305	CHL	CBD-CGD	-2.04	1.49	1.52
45	BF	303	CLA	CHC-C1C	2.04	1.42	1.38
45	AA	834	CLA	C3B-C4B	2.04	1.48	1.42
45	BF	303	CLA	CMB-C2B	-2.04	1.46	1.50
45	BB	805	CLA	CMB-C2B	-2.04	1.46	1.50
45	BB	814	CLA	MG-NB	-2.04	2.01	2.05
45	BB	843	CLA	MG-NB	-2.04	2.01	2.05
45	A1	314	CLA	CHC-C1C	2.04	1.42	1.38
56	e	301	SQD	O4-C4	-2.03	1.37	1.43
45	B3	309	CLA	CMD-C2D	-2.03	1.46	1.50
45	AA	802	CLA	MG-ND	-2.03	2.01	2.05
45	AK	203	CLA	CHC-C1C	2.03	1.42	1.38
45	A1	307	CLA	CMB-C2B	-2.03	1.46	1.50
45	AJ	102	CLA	CMB-C2B	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	316	CLA	CMC-C2C	-2.03	1.46	1.50
45	BL	303	CLA	CHC-C1C	2.03	1.42	1.38
45	B2	608	CLA	CHC-C1C	2.03	1.42	1.38
45	AJ	102	CLA	CMD-C2D	-2.03	1.46	1.50
55	B2	616	XAT	O4-C5	-2.03	1.43	1.46
45	BA	827	CLA	CMC-C2C	-2.03	1.46	1.50
45	A4	303	CLA	CMC-C2C	-2.03	1.46	1.50
45	B3	310	CLA	CMD-C2D	-2.03	1.46	1.50
45	B3	308	CLA	CHC-C1C	2.03	1.42	1.38
45	BA	835	CLA	CMD-C2D	-2.03	1.46	1.50
45	A6	609	CLA	CHC-C1C	2.03	1.42	1.38
45	AB	825	CLA	CMA-C3A	-2.03	1.48	1.53
45	AB	820	CLA	CMC-C2C	-2.03	1.46	1.50
45	BB	830	CLA	CMC-C2C	-2.03	1.46	1.50
45	AF	803	CLA	CHC-C1C	2.03	1.42	1.38
45	A1	306	CLA	CHC-C1C	2.03	1.42	1.38
45	A4	301	CLA	CHC-C1C	2.03	1.42	1.38
45	BA	837	CLA	MG-NB	-2.03	2.01	2.05
45	BA	829	CLA	CMC-C2C	-2.03	1.46	1.50
45	A3	302	CLA	CMC-C2C	-2.03	1.46	1.50
45	BF	303	CLA	CMD-C2D	-2.03	1.46	1.50
45	AB	812	CLA	CHC-C1C	2.03	1.42	1.38
45	BA	841	CLA	MG-NB	-2.03	2.01	2.05
48	AJ	101	BCR	C23-C22	2.03	1.50	1.46
48	BB	845	BCR	C8-C9	2.03	1.50	1.46
48	AA	852	BCR	C23-C22	2.03	1.50	1.46
48	BB	846	BCR	C8-C9	2.03	1.50	1.46
45	AB	839	CLA	CMB-C2B	-2.03	1.46	1.50
45	AB	818	CLA	CMC-C2C	-2.03	1.46	1.50
45	BA	825	CLA	CMC-C2C	-2.03	1.46	1.50
45	AB	817	CLA	CMB-C2B	-2.03	1.46	1.50
45	AB	819	CLA	MG-NB	-2.02	2.01	2.05
45	BA	818	CLA	MG-NB	-2.02	2.01	2.05
45	AA	833	CLA	C3B-C4B	2.02	1.48	1.42
45	B2	613	CLA	CHC-C1C	2.02	1.42	1.38
48	B2	617	BCR	C8-C9	2.02	1.50	1.46
45	BA	813	CLA	CHC-C1C	2.02	1.42	1.38
45	BB	818	CLA	CHC-C1C	2.02	1.42	1.38
45	BB	837	CLA	CHC-C1C	2.02	1.42	1.38
45	BB	820	CLA	MG-NB	-2.02	2.01	2.05
45	BB	809	CLA	CMC-C2C	-2.02	1.46	1.50
45	A4	311	CLA	CMB-C2B	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	BK	204	BCR	C8-C9	2.02	1.50	1.46
45	A3	311	CLA	CMD-C2D	-2.02	1.46	1.50
45	BA	803	CLA	CMB-C2B	-2.02	1.46	1.50
45	BJ	102	CLA	CMD-C2D	-2.02	1.46	1.50
45	BB	839	CLA	CHC-C1C	2.02	1.42	1.38
45	BA	807	CLA	CHC-C1C	2.02	1.42	1.38
45	BB	837	CLA	CMD-C2D	-2.02	1.46	1.50
45	BA	826	CLA	CHC-C1C	2.02	1.42	1.38
45	AA	833	CLA	CMC-C2C	-2.02	1.46	1.50
45	BL	302	CLA	CMB-C2B	-2.02	1.46	1.50
45	AA	836	CLA	MG-NB	-2.02	2.01	2.05
48	AI	101	BCR	C1-C6	-2.02	1.51	1.53
45	AB	818	CLA	C3B-C4B	2.02	1.48	1.42
45	B1	306	CLA	CHC-C1C	2.02	1.42	1.38
45	BB	825	CLA	CHC-C1C	2.02	1.42	1.38
45	BA	833	CLA	CMC-C2C	-2.02	1.46	1.50
45	B3	312	CLA	CMB-C2B	-2.02	1.46	1.50
45	BA	804	CLA	MG-NB	-2.02	2.01	2.05
45	BB	840	CLA	CMB-C2B	-2.02	1.46	1.50
45	BB	840	CLA	MG-NB	-2.02	2.01	2.05
45	BB	814	CLA	CHC-C1C	2.02	1.42	1.38
45	B2	602	CLA	CHC-C1C	2.02	1.42	1.38
48	AL	306	BCR	C12-C13	2.02	1.50	1.46
45	AB	831	CLA	MG-NB	-2.02	2.01	2.05
45	BA	802	CLA	MG-NB	-2.02	2.01	2.05
45	BA	830	CLA	C3B-C4B	2.02	1.48	1.42
45	BB	828	CLA	CHC-C1C	2.02	1.42	1.38
45	B2	610	CLA	C1A-CHA	-2.02	1.36	1.40
45	A3	304	CLA	CMC-C2C	-2.02	1.46	1.50
45	A3	306	CLA	CMC-C2C	-2.02	1.46	1.50
45	BA	824	CLA	C3B-C4B	2.02	1.48	1.42
45	AF	804	CLA	CHC-C1C	2.02	1.42	1.38
45	BF	303	CLA	CMC-C2C	-2.02	1.46	1.50
45	B5	601	CLA	CMC-C2C	-2.02	1.46	1.50
45	BB	838	CLA	MG-NB	-2.01	2.01	2.05
45	AA	832	CLA	CHC-C1C	2.01	1.42	1.38
45	A1	310	CLA	CHC-C1C	2.01	1.42	1.38
45	AB	821	CLA	MG-NB	-2.01	2.01	2.05
45	AB	838	CLA	MG-NB	-2.01	2.01	2.05
45	BB	821	CLA	MG-NB	-2.01	2.01	2.05
45	AA	821	CLA	MG-NB	-2.01	2.01	2.05
45	BA	823	CLA	CMB-C2B	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	316	CLA	CHC-C1C	2.01	1.42	1.38
45	BA	829	CLA	C3B-C4B	2.01	1.48	1.42
45	A1	315	CLA	CHC-C1C	2.01	1.42	1.38
45	AA	819	CLA	MG-NB	-2.01	2.01	2.05
45	B5	610	CLA	CHC-C1C	2.01	1.42	1.38
45	BB	830	CLA	C3B-C4B	2.01	1.48	1.42
46	BB	844	PQN	C15-C13	2.01	1.55	1.51
45	BB	827	CLA	CHC-C1C	2.01	1.42	1.38
45	AB	837	CLA	MG-ND	-2.01	2.01	2.05
45	AB	841	CLA	C3B-C4B	2.01	1.48	1.42
45	BB	820	CLA	C3B-C4B	2.01	1.48	1.42
45	AK	203	CLA	CMB-C2B	-2.01	1.46	1.50
45	BA	825	CLA	MG-ND	-2.01	2.01	2.05
45	BB	809	CLA	MG-NB	-2.01	2.01	2.05
45	A1	304	CLA	C3B-C4B	2.01	1.48	1.42
45	A3	308	CLA	MG-NB	-2.01	2.01	2.05
45	BA	842	CLA	CMC-C2C	-2.00	1.46	1.50
45	B5	604	CLA	CMC-C2C	-2.00	1.46	1.50
45	BA	819	CLA	MG-NB	-2.00	2.01	2.05
45	B1	314	CLA	CHC-C1C	2.00	1.42	1.38
45	AB	822	CLA	CHC-C1C	2.00	1.42	1.38
48	AK	204	BCR	C19-C18	2.00	1.50	1.46
45	AA	838	CLA	MG-NB	-2.00	2.01	2.05
45	BB	805	CLA	MG-NB	-2.00	2.01	2.05
45	B5	601	CLA	CHC-C1C	2.00	1.42	1.38
45	A1	310	CLA	CMB-C2B	-2.00	1.46	1.50
45	BB	841	CLA	CHC-C1C	2.00	1.42	1.38
45	B5	603	CLA	CMC-C2C	-2.00	1.46	1.50
45	AA	835	CLA	CMC-C2C	-2.00	1.46	1.50
45	BA	806	CLA	CMB-C2B	-2.00	1.46	1.50
52	B1	316	LUT	C30-C29	2.00	1.40	1.35
45	B3	307	CLA	C3B-C4B	2.00	1.48	1.42
45	BA	837	CLA	MG-ND	-2.00	2.01	2.05

All (3336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BL	306	BCR	C37-C22-C23	-28.76	74.16	118.09
48	BL	306	BCR	C37-C22-C21	-28.03	77.40	122.82
48	BL	306	BCR	C35-C13-C14	-27.18	78.78	122.82
48	BL	306	BCR	C34-C9-C8	-26.91	76.99	118.09
48	BG	203	BCR	C35-C13-C12	-26.13	78.17	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BL	306	BCR	C35-C13-C12	-25.86	78.58	118.09
48	BL	306	BCR	C34-C9-C10	-25.80	81.01	122.82
48	BG	203	BCR	C35-C13-C14	-25.63	81.29	122.82
48	BG	203	BCR	C12-C13-C14	24.86	158.12	119.01
48	BL	306	BCR	C8-C9-C10	24.65	157.78	119.01
48	BL	306	BCR	C12-C13-C14	24.34	157.29	119.01
48	BL	306	BCR	C23-C22-C21	20.59	151.40	119.01
56	BJ	104	SQD	O9-S-C6	-15.99	82.88	106.76
48	A1	319	BCR	C40-C30-C25	-14.39	87.67	110.24
48	B3	317	BCR	C40-C30-C25	-12.88	90.04	110.24
56	BJ	104	SQD	O8-S-O9	-11.87	81.70	111.40
48	B3	317	BCR	C39-C30-C25	10.96	127.44	110.24
48	A3	318	BCR	C40-C30-C25	-10.46	93.83	110.24
48	AI	102	BCR	C7-C8-C9	-10.01	111.42	126.23
48	A1	319	BCR	C39-C30-C25	9.81	125.63	110.24
54	A6	606	CHL	O2D-CGD-CBD	9.80	121.72	110.95
48	BJ	103	BCR	C28-C27-C26	-9.80	96.58	114.06
48	BG	203	BCR	C7-C8-C9	-9.52	112.15	126.23
48	B2	617	BCR	C33-C5-C6	9.40	134.74	124.48
54	B2	614	CHL	O2D-CGD-CBD	9.37	121.24	110.95
56	BJ	104	SQD	O9-S-O7	-9.34	83.46	113.82
48	BA	850	BCR	C28-C27-C26	-9.27	97.53	114.06
48	AJ	103	BCR	C28-C27-C26	-8.86	98.26	114.06
54	B2	605	CHL	O2D-CGD-CBD	8.78	120.59	110.95
48	BG	203	BCR	C20-C21-C22	-8.70	115.08	127.28
48	AB	844	BCR	C3-C4-C5	-8.34	99.18	114.06
54	B2	601	CHL	O2D-CGD-CBD	8.30	120.07	110.95
54	A4	305	CHL	O2D-CGD-CBD	8.28	120.04	110.95
48	B3	317	BCR	C30-C25-C26	-8.21	111.41	122.64
56	BJ	104	SQD	O8-S-C6	7.96	121.34	105.97
48	BL	306	BCR	C20-C21-C22	7.93	138.41	127.28
54	B5	607	CHL	OBD-CAD-C3D	-7.87	115.62	127.89
48	B3	317	BCR	C24-C23-C22	-7.81	114.67	126.23
54	B2	607	CHL	CHA-C1A-C2A	-7.81	114.97	133.31
54	A4	306	CHL	CHA-C1A-C2A	-7.80	115.00	133.31
54	B5	605	CHL	CHA-C1A-C2A	-7.79	115.03	133.31
54	A4	304	CHL	CHA-C1A-C2A	-7.77	115.06	133.31
55	B5	615	XAT	O4-C5-C4	7.75	120.75	113.49
54	B2	614	CHL	CHA-C1A-C2A	-7.71	115.21	133.31
54	B1	303	CHL	CHA-C1A-C2A	-7.67	115.30	133.31
54	B5	606	CHL	O2D-CGD-CBD	7.66	119.37	110.95
54	A6	606	CHL	CHA-C1A-C2A	-7.66	115.33	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A4	306	CHL	OBD-CAD-C3D	-7.64	115.98	127.89
54	B5	607	CHL	CHA-C1A-C2A	-7.62	115.41	133.31
54	B5	607	CHL	O2D-CGD-CBD	7.54	119.23	110.95
54	B2	605	CHL	CHA-C1A-C2A	-7.54	115.62	133.31
54	B2	607	CHL	O2D-CGD-CBD	7.52	119.21	110.95
54	A6	602	CHL	CHA-C1A-C2A	-7.52	115.66	133.31
54	A6	607	CHL	O2D-CGD-CBD	7.51	119.19	110.95
54	A6	608	CHL	O2D-CGD-CBD	7.46	119.14	110.95
54	A4	306	CHL	O2D-CGD-CBD	7.45	119.13	110.95
54	A4	314	CHL	CHA-C1A-C2A	-7.45	115.82	133.31
48	BL	306	BCR	C19-C18-C17	7.44	130.72	119.01
54	A1	303	CHL	OBD-CAD-C3D	-7.43	116.30	127.89
54	A3	307	CHL	O2D-CGD-CBD	7.42	119.10	110.95
54	A1	303	CHL	CHA-C1A-C2A	-7.42	115.89	133.31
54	A3	307	CHL	CHA-C1A-C2A	-7.42	115.90	133.31
56	BJ	104	SQD	O7-S-C6	7.38	117.77	106.76
48	BB	845	BCR	C3-C4-C5	-7.34	100.96	114.06
54	B3	306	CHL	CHA-C1A-C2A	-7.33	116.09	133.31
54	A6	607	CHL	CHA-C1A-C2A	-7.30	116.17	133.31
54	B2	601	CHL	CHA-C1A-C2A	-7.30	116.17	133.31
48	BL	306	BCR	C20-C19-C18	-7.27	106.43	126.36
48	A3	318	BCR	C39-C30-C25	7.24	121.60	110.24
54	B2	607	CHL	OBD-CAD-C3D	-7.23	116.62	127.89
54	B3	306	CHL	O2D-CGD-CBD	7.20	118.86	110.95
55	A4	316	XAT	O4-C5-C4	7.20	120.24	113.49
54	A3	307	CHL	OBD-CAD-C3D	-7.18	116.69	127.89
48	A3	318	BCR	C40-C30-C39	-7.09	88.33	108.63
54	A4	305	CHL	CHA-C1A-C2A	-7.09	116.67	133.31
54	B5	606	CHL	CHA-C1A-C2A	-7.07	116.71	133.31
54	B1	303	CHL	OBD-CAD-C3D	-7.06	116.88	127.89
54	A6	608	CHL	OBD-CAD-C3D	-7.04	116.91	127.89
54	A6	607	CHL	OBD-CAD-C3D	-7.02	116.94	127.89
54	A6	608	CHL	CHA-C1A-C2A	-7.02	116.83	133.31
54	B1	308	CHL	OBD-CAD-C3D	-7.00	116.98	127.89
55	B3	316	XAT	O24-C25-C38	6.99	122.86	115.05
54	B2	601	CHL	OBD-CAD-C3D	-6.95	117.05	127.89
54	B2	606	CHL	OBD-CAD-C3D	-6.95	117.06	127.89
54	B3	306	CHL	OBD-CAD-C3D	-6.94	117.06	127.89
48	B3	317	BCR	C3-C4-C5	-6.94	101.69	114.06
54	A4	314	CHL	OBD-CAD-C3D	-6.93	117.08	127.89
54	B2	606	CHL	CHA-C1A-C2A	-6.91	117.08	133.31
54	A1	308	CHL	OBD-CAD-C3D	-6.90	117.12	127.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A1	319	BCR	C40-C30-C39	-6.90	88.87	108.63
54	A4	305	CHL	OBD-CAD-C3D	-6.89	117.15	127.89
54	A6	602	CHL	OBD-CAD-C3D	-6.86	117.19	127.89
54	B2	614	CHL	OBD-CAD-C3D	-6.83	117.23	127.89
54	B5	606	CHL	OBD-CAD-C3D	-6.83	117.23	127.89
55	A1	318	XAT	O4-C5-C4	6.81	119.87	113.49
55	A6	616	XAT	O4-C5-C4	6.78	119.85	113.49
45	BB	842	CLA	C4A-NA-C1A	6.76	109.77	106.68
56	BJ	104	SQD	O47-C7-C8	6.76	126.11	111.48
54	B2	605	CHL	OBD-CAD-C3D	-6.76	117.35	127.89
54	A6	606	CHL	OBD-CAD-C3D	-6.75	117.36	127.89
48	AK	204	BCR	C28-C27-C26	-6.73	102.06	114.06
52	A4	315	LUT	C8-C7-C6	-6.69	109.13	127.00
45	BB	828	CLA	C4A-NA-C1A	6.67	109.72	106.68
54	B2	606	CHL	O2D-CGD-CBD	6.59	118.19	110.95
48	AG	205	BCR	C3-C4-C5	-6.59	102.31	114.06
45	AB	811	CLA	C4A-NA-C1A	6.59	109.69	106.68
48	BL	301	BCR	C8-C7-C6	-6.56	109.48	127.00
54	A4	304	CHL	OBD-CAD-C3D	-6.55	117.67	127.89
55	B3	316	XAT	O4-C5-C18	6.55	122.36	115.05
45	A1	305	CLA	C4A-NA-C1A	6.50	109.64	106.68
48	A6	617	BCR	C40-C30-C25	-6.46	100.12	110.24
48	AA	845	BCR	C38-C26-C25	-6.44	117.46	124.48
48	AB	849	BCR	C24-C23-C22	-6.44	116.71	126.23
46	BA	843	PQN	C11-C12-C13	-6.43	115.76	126.83
54	B5	605	CHL	OBD-CAD-C3D	-6.39	117.92	127.89
45	BA	813	CLA	C4A-NA-C1A	6.39	109.59	106.68
48	AA	848	BCR	C28-C27-C26	-6.36	102.72	114.06
48	BA	849	BCR	C28-C27-C26	-6.33	102.77	114.06
48	AA	852	BCR	C3-C4-C5	-6.27	102.88	114.06
55	B2	616	XAT	O4-C5-C4	6.27	119.36	113.49
45	BB	805	CLA	C4A-NA-C1A	6.26	109.54	106.68
48	AK	204	BCR	C3-C4-C5	-6.26	102.89	114.06
52	A1	317	LUT	C17-C1-C6	-6.26	100.43	110.24
48	B5	616	BCR	C28-C27-C26	-6.24	102.93	114.06
45	AB	825	CLA	C4A-NA-C1A	6.22	109.52	106.68
45	AL	305	CLA	C4A-NA-C1A	6.22	109.52	106.68
55	A3	317	XAT	O4-C5-C4	6.21	119.31	113.49
45	B1	305	CLA	C4A-NA-C1A	6.21	109.51	106.68
45	AA	841	CLA	C4A-NA-C1A	6.21	109.51	106.68
48	A4	317	BCR	C28-C27-C26	-6.16	103.08	114.06
55	B1	317	XAT	O4-C5-C4	6.15	119.25	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	807	CLA	C4A-NA-C1A	6.14	109.48	106.68
45	BB	812	CLA	C4A-NA-C1A	6.10	109.46	106.68
45	AB	804	CLA	CAC-C3C-C4C	6.10	132.73	124.79
48	BL	306	BCR	C21-C20-C19	6.09	140.85	123.20
48	AB	849	BCR	C3-C4-C5	-6.08	103.22	114.06
45	AB	827	CLA	C4A-NA-C1A	6.06	109.45	106.68
48	AB	846	BCR	C37-C22-C21	-6.03	113.05	122.82
45	BA	840	CLA	C4A-NA-C1A	6.02	109.43	106.68
45	AA	820	CLA	C4A-NA-C1A	6.01	109.42	106.68
45	AA	813	CLA	C4A-NA-C1A	6.01	109.42	106.68
45	BA	820	CLA	C4A-NA-C1A	6.00	109.42	106.68
48	AB	849	BCR	C37-C22-C23	5.99	127.24	118.09
48	BA	856	BCR	C28-C27-C26	-5.98	103.39	114.06
52	A3	316	LUT	C17-C1-C6	-5.97	100.88	110.24
45	BG	202	CLA	C4A-NA-C1A	5.96	109.40	106.68
48	B5	616	BCR	C1-C6-C5	-5.95	114.50	122.64
48	BI	101	BCR	C38-C26-C25	-5.95	117.99	124.48
48	B2	617	BCR	C28-C27-C26	-5.94	103.46	114.06
45	B3	305	CLA	C4A-NA-C1A	5.94	109.39	106.68
45	AF	802	CLA	C4A-NA-C1A	5.93	109.38	106.68
45	BB	822	CLA	C4A-NA-C1A	5.92	109.38	106.68
45	AA	837	CLA	C4A-NA-C1A	5.91	109.38	106.68
54	B5	606	CHL	C4D-ND-C1D	5.90	109.70	105.22
48	AL	306	BCR	C38-C26-C25	-5.88	118.07	124.48
45	AB	828	CLA	C4A-NA-C1A	5.88	109.36	106.68
45	AA	806	CLA	C4A-NA-C1A	5.87	109.36	106.68
45	AF	803	CLA	C4A-NA-C1A	5.87	109.36	106.68
54	B2	606	CHL	C4D-ND-C1D	5.87	109.67	105.22
45	BK	203	CLA	C4A-NA-C1A	5.86	109.35	106.68
48	BA	855	BCR	C3-C4-C5	-5.86	103.60	114.06
55	A4	316	XAT	O24-C25-C38	5.86	121.60	115.05
54	A1	308	CHL	C4D-ND-C1D	5.86	109.66	105.22
45	A6	604	CLA	C4A-NA-C1A	5.84	109.34	106.68
45	AB	824	CLA	C4A-NA-C1A	5.82	109.33	106.68
45	BA	806	CLA	C4A-NA-C1A	5.82	109.33	106.68
48	BG	203	BCR	C33-C5-C6	-5.81	118.14	124.48
48	BA	847	BCR	C38-C26-C25	-5.80	118.15	124.48
45	BB	820	CLA	C4A-NA-C1A	5.80	109.33	106.68
45	AB	832	CLA	C4A-NA-C1A	5.79	109.32	106.68
48	B3	317	BCR	C33-C5-C6	-5.79	118.17	124.48
45	BB	815	CLA	CAC-C3C-C4C	5.79	132.32	124.79
48	BA	856	BCR	C3-C4-C5	-5.76	103.78	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	839	CLA	C4A-NA-C1A	5.75	109.30	106.68
48	BG	203	BCR	C24-C23-C22	-5.75	117.73	126.23
45	AB	810	CLA	C4A-NA-C1A	5.74	109.30	106.68
48	B3	317	BCR	C40-C30-C39	-5.73	92.22	108.63
48	BA	848	BCR	C3-C4-C5	-5.73	103.84	114.06
48	AB	847	BCR	C38-C26-C25	-5.73	118.24	124.48
45	A1	316	CLA	C4A-NA-C1A	5.71	109.28	106.68
45	BA	812	CLA	C4A-NA-C1A	5.70	109.28	106.68
45	BB	833	CLA	C4A-NA-C1A	5.70	109.28	106.68
48	AL	302	BCR	C28-C27-C26	-5.70	103.90	114.06
45	AB	842	CLA	C4A-NA-C1A	5.69	109.28	106.68
45	AB	804	CLA	C4A-NA-C1A	5.69	109.27	106.68
48	A3	318	BCR	C30-C25-C26	-5.67	114.88	122.64
54	B3	306	CHL	C4D-ND-C1D	5.67	109.52	105.22
45	BB	808	CLA	C4A-NA-C1A	5.65	109.26	106.68
45	B5	603	CLA	C4A-NA-C1A	5.65	109.25	106.68
48	AI	102	BCR	C8-C7-C6	-5.65	111.92	127.00
48	BA	855	BCR	C32-C1-C6	-5.64	101.40	110.24
48	BB	848	BCR	C28-C27-C26	-5.64	104.00	114.06
46	AB	843	PQN	C15-C13-C12	-5.63	108.53	121.17
45	AA	834	CLA	C4A-NA-C1A	5.63	109.25	106.68
45	BA	822	CLA	C4A-NA-C1A	5.62	109.24	106.68
48	BG	203	BCR	C8-C9-C10	5.61	127.83	119.01
48	BL	301	BCR	C31-C1-C6	5.61	119.04	110.24
45	AK	203	CLA	C4A-NA-C1A	5.61	109.24	106.68
45	AA	833	CLA	C4A-NA-C1A	5.60	109.23	106.68
45	AB	841	CLA	C4A-NA-C1A	5.60	109.23	106.68
48	AA	845	BCR	C23-C24-C25	-5.60	112.04	127.00
54	A4	305	CHL	C4D-ND-C1D	5.59	109.47	105.22
45	AA	808	CLA	C4A-NA-C1A	5.58	109.23	106.68
45	BF	302	CLA	C4A-NA-C1A	5.58	109.23	106.68
48	BB	847	BCR	C37-C22-C21	-5.58	113.77	122.82
45	AA	828	CLA	C4A-NA-C1A	5.58	109.22	106.68
55	A1	318	XAT	O24-C25-C24	5.58	118.72	113.49
48	A4	317	BCR	C32-C1-C6	5.58	118.99	110.24
45	AB	837	CLA	C4A-NA-C1A	5.56	109.22	106.68
45	AA	812	CLA	C4A-NA-C1A	5.56	109.21	106.68
48	AL	302	BCR	C31-C1-C6	5.55	118.94	110.24
45	BL	302	CLA	C4A-NA-C1A	5.55	109.21	106.68
45	A1	313	CLA	C4A-NA-C1A	5.54	109.21	106.68
48	AK	204	BCR	C32-C1-C6	-5.54	101.55	110.24
45	A4	313	CLA	C4A-NA-C1A	5.54	109.21	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	837	CLA	C4A-NA-C1A	5.53	109.20	106.68
48	A6	617	BCR	C28-C27-C26	-5.52	104.21	114.06
48	AB	848	BCR	C23-C24-C25	-5.51	112.27	127.00
54	B1	308	CHL	C4D-ND-C1D	5.50	109.40	105.22
45	BB	802	CLA	C4A-NA-C1A	5.50	109.19	106.68
55	A3	317	XAT	O24-C25-C38	5.50	121.19	115.05
45	BB	811	CLA	C4A-NA-C1A	5.50	109.19	106.68
45	BB	840	CLA	C4A-NA-C1A	5.50	109.19	106.68
48	AA	847	BCR	C7-C8-C9	-5.49	118.11	126.23
45	AB	830	CLA	C4A-NA-C1A	5.49	109.18	106.68
54	A6	608	CHL	C4D-ND-C1D	5.49	109.38	105.22
45	AA	842	CLA	C4A-NA-C1A	5.48	109.18	106.68
48	A3	318	BCR	C3-C4-C5	-5.48	104.29	114.06
45	AA	810	CLA	C4A-NA-C1A	5.47	109.17	106.68
48	B3	317	BCR	C1-C6-C5	-5.47	115.17	122.64
48	A4	317	BCR	C1-C6-C5	-5.46	115.18	122.64
54	A4	314	CHL	C4D-ND-C1D	5.46	109.36	105.22
48	BB	849	BCR	C23-C24-C25	-5.46	112.42	127.00
45	B2	603	CLA	C4A-NA-C1A	5.45	109.17	106.68
48	AA	847	BCR	C31-C1-C6	5.45	118.78	110.24
45	BA	814	CLA	C4A-NA-C1A	5.44	109.16	106.68
45	AK	201	CLA	C4A-NA-C1A	5.44	109.16	106.68
45	AA	814	CLA	C4A-NA-C1A	5.44	109.16	106.68
48	B3	317	BCR	C27-C26-C25	-5.44	115.36	122.70
45	A3	306	CLA	C4A-NA-C1A	5.41	109.15	106.68
45	AG	203	CLA	C4A-NA-C1A	5.38	109.13	106.68
48	BL	301	BCR	C34-C9-C10	-5.38	114.10	122.82
45	A6	601	CLA	C4A-NA-C1A	5.37	109.13	106.68
45	BA	833	CLA	C4A-NA-C1A	5.37	109.13	106.68
54	A3	307	CHL	C4D-ND-C1D	5.37	109.29	105.22
46	AA	843	PQN	C15-C13-C12	-5.35	109.15	121.17
45	AA	839	CLA	C4A-NA-C1A	5.35	109.12	106.68
52	B3	315	LUT	C17-C1-C6	-5.35	101.85	110.24
48	AI	101	BCR	C38-C26-C25	-5.35	118.65	124.48
54	B2	605	CHL	C4D-ND-C1D	5.34	109.27	105.22
45	BK	201	CLA	C4A-NA-C1A	5.33	109.11	106.68
45	AB	802	CLA	C4A-NA-C1A	5.33	109.11	106.68
45	A4	309	CLA	C4A-NA-C1A	5.32	109.11	106.68
46	AB	843	PQN	C11-C12-C13	-5.32	117.67	126.83
45	BA	805	CLA	C4A-NA-C1A	5.32	109.10	106.68
45	BA	809	CLA	C4A-NA-C1A	5.32	109.10	106.68
45	AG	201	CLA	C4A-NA-C1A	5.31	109.10	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BB	843	CLA	C4A-NA-C1A	5.31	109.10	106.68
45	AA	830	CLA	C4A-NA-C1A	5.31	109.10	106.68
48	AI	102	BCR	C27-C26-C25	-5.30	115.54	122.70
48	BB	845	BCR	C30-C25-C26	-5.30	115.39	122.64
45	AB	814	CLA	C4A-NA-C1A	5.30	109.10	106.68
45	AB	822	CLA	C4A-NA-C1A	5.30	109.10	106.68
48	BL	301	BCR	C28-C27-C26	-5.30	104.60	114.06
45	BB	826	CLA	C4A-NA-C1A	5.29	109.09	106.68
45	A1	310	CLA	C4A-NA-C1A	5.28	109.09	106.68
48	AA	847	BCR	C28-C27-C26	-5.28	104.64	114.06
45	AB	821	CLA	C4A-NA-C1A	5.27	109.08	106.68
45	AB	812	CLA	C4A-NA-C1A	5.27	109.08	106.68
45	BB	836	CLA	C4A-NA-C1A	5.27	109.08	106.68
45	BA	839	CLA	C4A-NA-C1A	5.27	109.08	106.68
54	B5	607	CHL	OBD-CAD-CBD	5.27	133.55	125.82
55	B3	316	XAT	C18-C5-C6	-5.26	113.65	122.30
48	AA	846	BCR	C36-C18-C19	5.24	126.10	118.09
45	AJ	102	CLA	C4A-NA-C1A	5.24	109.07	106.68
48	BG	203	BCR	C15-C14-C13	-5.23	119.94	127.28
54	A6	607	CHL	C4D-ND-C1D	5.23	109.19	105.22
45	BA	819	CLA	C4A-NA-C1A	5.23	109.06	106.68
45	BB	804	CLA	C4A-NA-C1A	5.23	109.06	106.68
45	AA	825	CLA	C4A-NA-C1A	5.22	109.06	106.68
45	BA	824	CLA	C4A-NA-C1A	5.22	109.06	106.68
45	BB	838	CLA	C4A-NA-C1A	5.22	109.06	106.68
45	BA	815	CLA	C4A-NA-C1A	5.22	109.06	106.68
45	BB	813	CLA	C4A-NA-C1A	5.21	109.06	106.68
45	A1	306	CLA	C4A-NA-C1A	5.21	109.05	106.68
45	BA	817	CLA	C4A-NA-C1A	5.20	109.05	106.68
45	BA	836	CLA	C4A-NA-C1A	5.20	109.05	106.68
45	AA	811	CLA	C4A-NA-C1A	5.20	109.05	106.68
48	BG	203	BCR	C15-C16-C17	-5.19	112.89	123.52
45	AA	822	CLA	C4A-NA-C1A	5.19	109.05	106.68
48	BB	846	BCR	C30-C25-C26	-5.19	115.55	122.64
45	BA	841	CLA	C4-C3-C5	5.17	124.21	115.23
46	BB	844	PQN	C15-C13-C12	-5.16	109.59	121.17
45	AB	808	CLA	C4A-NA-C1A	5.15	109.03	106.68
45	BF	301	CLA	C4A-NA-C1A	5.15	109.03	106.68
54	A4	306	CHL	OBD-CAD-CBD	5.15	133.38	125.82
45	AA	805	CLA	C4A-NA-C1A	5.13	109.02	106.68
48	AJ	103	BCR	C39-C30-C25	-5.12	102.21	110.24
45	AF	804	CLA	C4A-NA-C1A	5.12	109.02	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	841	CLA	C4A-NA-C1A	5.11	109.01	106.68
45	BA	827	CLA	C4A-NA-C1A	5.10	109.01	106.68
45	B5	612	CLA	C4A-NA-C1A	5.10	109.00	106.68
54	B1	303	CHL	C4D-ND-C1D	5.09	109.08	105.22
45	AA	804	CLA	C4A-NA-C1A	5.09	109.00	106.68
54	A1	303	CHL	C4D-ND-C1D	5.09	109.08	105.22
48	BB	803	BCR	C28-C27-C26	-5.09	104.98	114.06
48	AI	102	BCR	C33-C5-C6	5.09	130.03	124.48
45	AB	838	CLA	C4A-NA-C1A	5.08	109.00	106.68
48	BB	848	BCR	C3-C4-C5	-5.08	105.00	114.06
45	BA	834	CLA	C4A-NA-C1A	5.07	108.99	106.68
45	BB	839	CLA	C4A-NA-C1A	5.07	108.99	106.68
45	BA	842	CLA	C4A-NA-C1A	5.07	108.99	106.68
45	AA	827	CLA	C4A-NA-C1A	5.05	108.98	106.68
45	B1	304	CLA	C4A-NA-C1A	5.05	108.98	106.68
45	AA	815	CLA	C4A-NA-C1A	5.05	108.98	106.68
48	BA	851	BCR	C37-C22-C23	5.04	125.79	118.09
45	B1	313	CLA	C4A-NA-C1A	5.04	108.98	106.68
45	BB	834	CLA	C4A-NA-C1A	5.03	108.97	106.68
45	B5	611	CLA	C4A-NA-C1A	5.03	108.97	106.68
48	BB	846	BCR	C27-C26-C25	-5.03	115.91	122.70
54	A3	307	CHL	OBD-CAD-CBD	5.02	133.20	125.82
54	A6	602	CHL	C4D-ND-C1D	5.02	109.03	105.22
45	B3	304	CLA	C4A-NA-C1A	5.02	108.97	106.68
48	AA	852	BCR	C36-C18-C19	5.00	125.73	118.09
47	B3	318	LHG	O7-C7-C8	5.00	120.01	111.09
45	A3	312	CLA	C4A-NA-C1A	5.00	108.96	106.68
45	BA	804	CLA	C4A-NA-C1A	5.00	108.96	106.68
48	BF	304	BCR	C28-C27-C26	-5.00	105.14	114.06
45	BA	828	CLA	C4A-NA-C1A	4.99	108.96	106.68
54	B5	605	CHL	C4D-ND-C1D	4.98	109.00	105.22
54	B2	601	CHL	C4D-ND-C1D	4.98	109.00	105.22
48	BA	848	BCR	C36-C18-C19	4.98	125.69	118.09
48	BL	305	BCR	C28-C27-C26	-4.98	105.18	114.06
45	A4	302	CLA	C4A-NA-C1A	4.97	108.95	106.68
48	AA	852	BCR	C30-C25-C26	-4.96	115.86	122.64
45	A6	613	CLA	C4A-NA-C1A	4.96	108.94	106.68
45	BA	825	CLA	C4A-NA-C1A	4.95	108.94	106.68
48	BG	203	BCR	C20-C19-C18	-4.95	112.80	126.36
45	B1	309	CLA	C4A-NA-C1A	4.95	108.94	106.68
45	AB	819	CLA	C4A-NA-C1A	4.94	108.94	106.68
54	A4	304	CHL	C4D-ND-C1D	4.94	108.97	105.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A1	307	CLA	C4A-NA-C1A	4.94	108.93	106.68
52	B2	615	LUT	C3-C4-C5	-4.94	99.88	112.18
54	B2	607	CHL	OBD-CAD-CBD	4.93	133.06	125.82
48	AA	849	BCR	C34-C9-C10	-4.93	114.83	122.82
45	AG	204	CLA	C4A-NA-C1A	4.93	108.93	106.68
54	B5	607	CHL	C4D-ND-C1D	4.92	108.95	105.22
45	BB	837	CLA	C4A-NA-C1A	4.92	108.92	106.68
54	A6	606	CHL	C4D-ND-C1D	4.91	108.95	105.22
48	B5	616	BCR	C3-C4-C5	-4.91	105.30	114.06
45	AB	813	CLA	C4A-NA-C1A	4.91	108.92	106.68
45	A4	310	CLA	C4A-NA-C1A	4.91	108.92	106.68
45	AB	809	CLA	C4A-NA-C1A	4.91	108.92	106.68
55	B5	615	XAT	O24-C25-C24	4.90	118.09	113.49
48	A1	319	BCR	C29-C30-C25	4.90	117.55	110.44
45	AA	821	CLA	C4A-NA-C1A	4.90	108.91	106.68
54	B2	601	CHL	OBD-CAD-CBD	4.90	133.01	125.82
48	BK	204	BCR	C3-C4-C5	-4.90	105.33	114.06
45	BB	831	CLA	C4A-NA-C1A	4.89	108.91	106.68
48	BL	306	BCR	C15-C14-C13	-4.89	120.42	127.28
56	BJ	104	SQD	C45-O47-C7	-4.89	106.10	117.80
45	BJ	102	CLA	C4A-NA-C1A	4.88	108.91	106.68
45	BA	811	CLA	C4A-NA-C1A	4.87	108.90	106.68
45	BA	808	CLA	C4A-NA-C1A	4.86	108.90	106.68
54	B2	607	CHL	C4D-ND-C1D	4.86	108.91	105.22
54	A1	303	CHL	OBD-CAD-CBD	4.85	132.95	125.82
45	BF	303	CLA	C4A-NA-C1A	4.85	108.89	106.68
45	BB	823	CLA	C4A-NA-C1A	4.85	108.89	106.68
55	B3	316	XAT	O4-C5-C4	4.84	118.03	113.49
45	B3	311	CLA	C4A-NA-C1A	4.84	108.89	106.68
48	AB	847	BCR	C28-C27-C26	-4.84	105.42	114.06
45	AA	817	CLA	C4A-NA-C1A	4.84	108.89	106.68
48	BA	855	BCR	C37-C22-C23	4.84	125.48	118.09
45	BB	829	CLA	C4A-NA-C1A	4.83	108.88	106.68
45	A4	311	CLA	C4A-NA-C1A	4.83	108.88	106.68
55	B1	317	XAT	O24-C25-C24	4.82	118.00	113.49
54	B1	303	CHL	OBD-CAD-CBD	4.82	132.89	125.82
45	A3	305	CLA	C4A-NA-C1A	4.82	108.88	106.68
45	BB	806	CLA	C4A-NA-C1A	4.81	108.87	106.68
45	AA	816	CLA	C4A-NA-C1A	4.81	108.87	106.68
54	B3	306	CHL	OBD-CAD-CBD	4.80	132.87	125.82
45	A1	314	CLA	C4A-NA-C1A	4.80	108.87	106.68
45	A3	311	CLA	C4A-NA-C1A	4.80	108.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	801	CLA	C4A-NA-C1A	4.79	108.86	106.68
48	A4	317	BCR	C23-C24-C25	-4.79	114.21	127.00
48	A4	317	BCR	C40-C30-C25	-4.77	102.75	110.24
45	AB	836	CLA	C4A-NA-C1A	4.77	108.85	106.68
48	BJ	103	BCR	C36-C18-C19	4.76	125.37	118.09
54	A6	608	CHL	OBD-CAD-CBD	4.76	132.81	125.82
54	B2	614	CHL	OBD-CAD-CBD	4.75	132.80	125.82
45	AA	818	CLA	C4A-NA-C1A	4.75	108.84	106.68
52	B2	615	LUT	C39-C29-C28	4.74	125.32	118.09
45	BB	817	CLA	C4A-NA-C1A	4.73	108.83	106.68
48	BL	305	BCR	C27-C26-C25	-4.72	116.33	122.70
55	A1	318	XAT	C6-C7-C8	-4.71	116.04	125.99
48	BB	848	BCR	C38-C26-C25	-4.70	119.36	124.48
45	AB	803	CLA	C4A-NA-C1A	4.69	108.82	106.68
48	BG	203	BCR	C31-C1-C6	-4.69	102.88	110.24
48	BB	848	BCR	C37-C22-C23	4.69	125.25	118.09
45	B3	302	CLA	C4A-NA-C1A	4.68	108.82	106.68
48	BL	306	BCR	C36-C18-C17	-4.68	115.23	122.82
45	AA	803	CLA	C4A-NA-C1A	4.68	108.81	106.68
48	BB	845	BCR	C36-C18-C19	4.68	125.24	118.09
54	A4	314	CHL	OBD-CAD-CBD	4.68	132.69	125.82
45	AA	801	CLA	C4A-NA-C1A	4.68	108.81	106.68
45	AB	834	CLA	C4A-NA-C1A	4.66	108.81	106.68
45	BA	821	CLA	C4A-NA-C1A	4.65	108.80	106.68
45	BA	834	CLA	C4-C3-C5	4.65	123.29	115.23
54	A6	607	CHL	OBD-CAD-CBD	4.64	132.63	125.82
45	B3	310	CLA	C4A-NA-C1A	4.64	108.80	106.68
48	BK	204	BCR	C36-C18-C19	4.64	125.17	118.09
48	BJ	101	BCR	C8-C7-C6	-4.64	114.61	127.00
48	AJ	101	BCR	C34-C9-C8	4.63	125.16	118.09
48	AB	847	BCR	C36-C18-C19	4.63	125.16	118.09
55	A6	616	XAT	C6-C7-C8	-4.63	116.21	125.99
45	A3	303	CLA	C4A-NA-C1A	4.63	108.79	106.68
47	A3	319	LHG	O7-C7-C8	4.63	119.34	111.09
48	AB	845	BCR	C34-C9-C10	-4.63	115.32	122.82
54	B2	606	CHL	OBD-CAD-CBD	4.63	132.61	125.82
45	AA	835	CLA	C4A-NA-C1A	4.62	108.79	106.68
54	A1	308	CHL	OBD-CAD-CBD	4.62	132.61	125.82
45	AB	816	CLA	C4A-NA-C1A	4.62	108.79	106.68
54	A6	602	CHL	OBD-CAD-CBD	4.62	132.60	125.82
45	AA	831	CLA	C4A-NA-C1A	4.62	108.79	106.68
48	B5	616	BCR	C37-C22-C23	4.61	125.13	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A1	315	CLA	C4A-NA-C1A	4.61	108.78	106.68
45	AA	836	CLA	C4A-NA-C1A	4.60	108.78	106.68
45	BB	820	CLA	C4-C3-C5	4.60	123.21	115.23
45	BB	814	CLA	C4A-NA-C1A	4.60	108.78	106.68
54	A4	305	CHL	OBD-CAD-CBD	4.60	132.57	125.82
45	B5	601	CLA	C4A-NA-C1A	4.59	108.78	106.68
48	BA	856	BCR	C27-C26-C25	-4.59	116.50	122.70
48	AJ	101	BCR	C3-C4-C5	-4.59	105.88	114.06
55	A6	616	XAT	C18-C5-C6	-4.58	114.76	122.30
48	BG	203	BCR	C19-C18-C17	4.58	126.21	119.01
45	A3	304	CLA	C4A-NA-C1A	4.58	108.77	106.68
48	AA	852	BCR	C28-C27-C26	-4.58	105.89	114.06
54	B1	308	CHL	OBD-CAD-CBD	4.57	132.54	125.82
45	AA	829	CLA	C4A-NA-C1A	4.57	108.76	106.68
45	AA	809	CLA	C4A-NA-C1A	4.57	108.76	106.68
45	BA	818	CLA	C4A-NA-C1A	4.57	108.76	106.68
48	AL	306	BCR	C33-C5-C6	-4.56	119.51	124.48
48	AL	302	BCR	C8-C7-C6	-4.55	114.83	127.00
48	BL	305	BCR	C31-C1-C6	4.55	117.38	110.24
48	AI	101	BCR	C36-C18-C19	4.55	125.03	118.09
45	BA	838	CLA	C4A-NA-C1A	4.54	108.75	106.68
45	A6	603	CLA	C4A-NA-C1A	4.54	108.75	106.68
48	BL	305	BCR	C37-C22-C23	4.53	125.01	118.09
45	AH	201	CLA	C4A-NA-C1A	4.52	108.74	106.68
48	AA	846	BCR	C32-C1-C6	4.52	117.33	110.24
48	AJ	101	BCR	C32-C1-C6	-4.52	103.16	110.24
45	A3	310	CLA	C4A-NA-C1A	4.52	108.74	106.68
48	AA	847	BCR	C35-C13-C14	-4.51	115.50	122.82
48	BL	305	BCR	C40-C30-C25	-4.51	103.18	110.24
48	AB	848	BCR	C33-C5-C6	-4.50	119.57	124.48
45	A4	303	CLA	C4A-NA-C1A	4.50	108.73	106.68
48	BB	846	BCR	C37-C22-C23	4.50	124.96	118.09
48	BB	845	BCR	C27-C26-C25	-4.50	116.62	122.70
45	AA	840	CLA	C4A-NA-C1A	4.50	108.73	106.68
54	A6	606	CHL	OBD-CAD-CBD	4.49	132.41	125.82
45	AK	202	CLA	C4A-NA-C1A	4.49	108.73	106.68
45	BB	807	CLA	C4A-NA-C1A	4.49	108.73	106.68
46	AA	843	PQN	C11-C12-C13	-4.48	119.11	126.83
48	BB	849	BCR	C36-C18-C19	4.48	124.93	118.09
48	AA	845	BCR	C32-C1-C6	-4.48	103.22	110.24
48	BA	856	BCR	C36-C18-C19	4.47	124.92	118.09
45	BB	818	CLA	C4A-NA-C1A	4.47	108.72	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A6	617	BCR	C3-C4-C5	-4.47	106.08	114.06
45	B2	611	CLA	C4A-NA-C1A	4.47	108.72	106.68
45	BL	304	CLA	C4A-NA-C1A	4.46	108.72	106.68
45	A4	301	CLA	C4A-NA-C1A	4.46	108.71	106.68
45	BK	202	CLA	C4A-NA-C1A	4.46	108.71	106.68
54	B2	614	CHL	C4D-ND-C1D	4.45	108.60	105.22
45	BB	809	CLA	C4A-NA-C1A	4.45	108.71	106.68
48	BB	803	BCR	C35-C13-C12	4.44	124.88	118.09
48	AA	846	BCR	C24-C23-C22	-4.42	119.69	126.23
48	BA	850	BCR	C37-C22-C23	4.42	124.83	118.09
54	A4	304	CHL	OBD-CAD-CBD	4.41	132.30	125.82
55	B2	616	XAT	O4-C5-C18	4.41	119.98	115.05
45	BH	201	CLA	C4A-NA-C1A	4.41	108.69	106.68
54	B5	606	CHL	OBD-CAD-CBD	4.41	132.30	125.82
48	AA	852	BCR	C37-C22-C23	4.41	124.83	118.09
45	B3	301	CLA	C4A-NA-C1A	4.41	108.69	106.68
52	AF	806	LUT	C40-C33-C32	4.40	124.82	118.09
48	AJ	103	BCR	C36-C18-C19	4.40	124.81	118.09
45	BA	832	CLA	C4A-NA-C1A	4.40	108.69	106.68
55	A6	616	XAT	C39-C29-C28	4.40	124.80	118.09
48	A1	319	BCR	C1-C6-C5	-4.39	116.63	122.64
48	AB	844	BCR	C34-C9-C8	4.39	124.80	118.09
48	BL	306	BCR	C15-C16-C17	-4.38	114.55	123.52
45	AA	838	CLA	C4A-NA-C1A	4.38	108.68	106.68
45	B3	309	CLA	C4A-NA-C1A	4.38	108.68	106.68
45	AB	815	CLA	C4A-NA-C1A	4.38	108.67	106.68
54	B2	605	CHL	OBD-CAD-CBD	4.37	132.24	125.82
48	AF	805	BCR	C37-C22-C23	4.37	124.77	118.09
48	AJ	103	BCR	C32-C1-C6	-4.37	103.39	110.24
47	F	801	LHG	O4-P-O5	4.36	132.75	112.44
45	BB	801	CLA	C4A-NA-C1A	4.36	108.67	106.68
48	AA	852	BCR	C27-C26-C25	-4.36	116.81	122.70
45	A3	313	CLA	C4A-NA-C1A	4.35	108.66	106.68
48	AA	848	BCR	C37-C22-C23	4.34	124.72	118.09
48	AF	801	BCR	C37-C22-C23	4.34	124.72	118.09
45	BA	803	CLA	C4A-NA-C1A	4.34	108.66	106.68
55	A3	317	XAT	O4-C5-C18	4.34	119.90	115.05
55	B1	317	XAT	O24-C25-C38	4.34	119.90	115.05
48	B5	616	BCR	C30-C25-C26	-4.34	116.70	122.64
52	A6	615	LUT	C8-C7-C6	-4.33	115.43	127.00
48	BB	846	BCR	C34-C9-C10	-4.33	115.80	122.82
48	AL	302	BCR	C38-C26-C25	-4.33	119.76	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BB	846	BCR	C36-C18-C19	4.33	124.70	118.09
48	BL	305	BCR	C36-C18-C19	4.32	124.69	118.09
48	AA	847	BCR	C1-C6-C5	-4.32	116.73	122.64
48	AJ	103	BCR	C31-C1-C6	4.32	117.02	110.24
48	AA	846	BCR	C3-C4-C5	-4.32	106.35	114.06
45	B5	604	CLA	C4A-NA-C1A	4.32	108.65	106.68
45	A6	605	CLA	C4A-NA-C1A	4.32	108.65	106.68
45	B1	312	CLA	C4A-NA-C1A	4.32	108.65	106.68
48	AJ	101	BCR	C37-C22-C23	4.32	124.68	118.09
45	A3	308	CLA	C4A-NA-C1A	4.32	108.65	106.68
48	A6	617	BCR	C37-C22-C23	4.31	124.68	118.09
55	B1	317	XAT	C18-C5-C6	-4.31	115.20	122.30
52	B5	614	LUT	C39-C29-C28	4.31	124.67	118.09
45	B1	306	CLA	C4A-NA-C1A	4.31	108.64	106.68
45	B2	612	CLA	C4A-NA-C1A	4.31	108.64	106.68
45	AB	819	CLA	C4-C3-C5	4.30	122.70	115.23
48	AA	849	BCR	C39-C30-C25	-4.30	103.51	110.24
47	a	501	LHG	O4-P-O5	4.29	132.42	112.44
45	B3	313	CLA	C4A-NA-C1A	4.29	108.64	106.68
55	A3	317	XAT	C6-C7-C8	-4.29	116.92	125.99
55	B2	616	XAT	O24-C25-C38	4.29	119.84	115.05
52	B3	315	LUT	C21-C26-C27	-4.29	107.90	112.83
45	AB	823	CLA	C4A-NA-C1A	4.28	108.63	106.68
55	A3	317	XAT	C38-C25-C26	-4.27	115.28	122.30
46	AB	843	PQN	C14-C13-C12	-4.27	112.67	123.63
45	AA	819	CLA	C4A-NA-C1A	4.27	108.63	106.68
48	A4	317	BCR	C36-C18-C19	4.26	124.60	118.09
48	AI	102	BCR	C40-C30-C25	-4.26	103.57	110.24
48	AG	205	BCR	C28-C27-C26	-4.25	106.47	114.06
46	BA	843	PQN	C15-C13-C12	-4.25	111.63	121.17
45	BB	810	CLA	C4A-NA-C1A	4.25	108.62	106.68
55	A6	616	XAT	O24-C25-C38	4.25	119.80	115.05
52	AF	806	LUT	C39-C29-C28	4.24	124.56	118.09
45	AB	840	CLA	C4A-NA-C1A	4.23	108.61	106.68
45	B2	604	CLA	C4A-NA-C1A	4.23	108.61	106.68
54	A4	306	CHL	C4D-ND-C1D	4.23	108.43	105.22
48	A4	317	BCR	C3-C4-C5	-4.23	106.51	114.06
48	BA	849	BCR	C1-C6-C5	-4.23	116.86	122.64
55	B2	616	XAT	C6-C7-C8	-4.22	117.06	125.99
45	AB	817	CLA	C4A-NA-C1A	4.22	108.61	106.68
48	BB	803	BCR	C36-C18-C19	4.21	124.52	118.09
48	AB	847	BCR	C37-C22-C23	4.20	124.51	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A6	607	CHL	C1C-C2C-CMC	4.20	134.38	126.80
48	AF	805	BCR	C35-C13-C14	-4.20	116.01	122.82
48	BB	848	BCR	C36-C18-C19	4.20	124.51	118.09
45	AA	832	CLA	C4A-NA-C1A	4.20	108.60	106.68
48	BI	101	BCR	C36-C18-C19	4.20	124.50	118.09
45	A3	314	CLA	C4A-NA-C1A	4.20	108.59	106.68
48	AB	844	BCR	C38-C26-C25	-4.19	119.91	124.48
48	BL	305	BCR	C30-C25-C26	-4.18	116.92	122.64
45	A4	312	CLA	C4A-NA-C1A	4.18	108.59	106.68
45	BA	830	CLA	C4A-NA-C1A	4.18	108.58	106.68
48	B3	317	BCR	C40-C30-C29	-4.17	92.93	108.95
48	AL	302	BCR	C3-C4-C5	-4.17	106.62	114.06
48	BK	204	BCR	C1-C6-C5	-4.17	116.94	122.64
48	A4	317	BCR	C37-C22-C23	4.17	124.46	118.09
53	A4	318	LMG	C8-O7-C10	-4.17	107.82	117.80
48	BA	851	BCR	C1-C6-C5	-4.16	116.95	122.64
48	BI	101	BCR	C33-C5-C6	-4.16	119.95	124.48
45	AA	829	CLA	C4-C3-C5	4.16	122.44	115.23
48	BA	856	BCR	C37-C22-C23	4.15	124.43	118.09
48	AI	101	BCR	C7-C8-C9	-4.14	120.11	126.23
54	A1	308	CHL	C1C-C2C-CMC	4.14	134.27	126.80
48	AI	101	BCR	C31-C1-C6	-4.14	103.75	110.24
45	B3	308	CLA	C4A-NA-C1A	4.13	108.56	106.68
55	A4	316	XAT	C39-C29-C28	4.13	124.40	118.09
45	AA	802	CLA	C4A-NA-C1A	4.13	108.56	106.68
45	BA	816	CLA	C4A-NA-C1A	4.13	108.56	106.68
52	A1	317	LUT	C16-C1-C6	4.12	116.71	110.24
45	BA	807	CLA	C4A-NA-C1A	4.12	108.56	106.68
48	BB	845	BCR	C28-C27-C26	-4.12	106.70	114.06
48	BA	851	BCR	C33-C5-C6	-4.12	119.99	124.48
45	BB	824	CLA	C4A-NA-C1A	4.12	108.56	106.68
55	A6	616	XAT	C40-C33-C32	4.11	124.37	118.09
55	B3	316	XAT	C38-C25-C26	-4.11	115.53	122.30
54	A4	306	CHL	C1C-C2C-CMC	4.11	134.21	126.80
45	AA	824	CLA	C4-C3-C5	4.11	122.36	115.23
48	BL	301	BCR	C36-C18-C19	4.09	124.34	118.09
54	B2	606	CHL	C1A-CHA-C4D	-4.09	112.16	118.98
48	AG	205	BCR	C36-C18-C19	4.08	124.33	118.09
45	BA	810	CLA	C4A-NA-C1A	4.08	108.54	106.68
45	BB	825	CLA	C4A-NA-C1A	4.08	108.54	106.68
48	AB	849	BCR	C32-C1-C6	-4.08	103.85	110.24
48	A1	319	BCR	C30-C25-C26	-4.08	117.06	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	A3	318	BCR	C40-C30-C29	-4.07	93.31	108.95
48	AB	845	BCR	C37-C22-C23	4.07	124.31	118.09
48	AB	846	BCR	C37-C22-C23	4.07	124.31	118.09
54	B2	607	CHL	C1C-C2C-CMC	4.07	134.13	126.80
55	B3	316	XAT	C39-C29-C28	4.07	124.30	118.09
55	B1	317	XAT	C20-C13-C12	4.06	124.30	118.09
55	B3	316	XAT	C19-C9-C8	4.06	124.30	118.09
45	BA	802	CLA	C4A-NA-C1A	4.06	108.53	106.68
55	B5	615	XAT	O24-C25-C38	4.06	119.58	115.05
48	AI	102	BCR	C1-C6-C5	-4.06	117.09	122.64
48	AL	302	BCR	C37-C22-C23	4.05	124.28	118.09
48	BB	847	BCR	C34-C9-C10	-4.04	116.26	122.82
56	e	301	SQD	O9-S-O7	-4.04	100.67	113.82
45	BA	838	CLA	C4-C3-C5	4.04	122.24	115.23
45	AA	828	CLA	CMB-C2B-C1B	-4.03	119.28	125.42
45	AB	805	CLA	C4A-NA-C1A	4.03	108.52	106.68
47	BF	305	LHG	O7-C7-C8	4.03	120.20	111.48
55	B1	317	XAT	C39-C29-C28	4.02	124.24	118.09
45	BB	832	CLA	C4A-NA-C1A	4.02	108.52	106.68
48	AA	849	BCR	C37-C22-C23	4.02	124.23	118.09
48	AB	845	BCR	C36-C18-C19	4.02	124.23	118.09
45	BB	805	CLA	CHB-C4A-NA	4.02	130.20	124.40
48	AB	846	BCR	C33-C5-C6	-4.02	120.10	124.48
45	AA	826	CLA	C4A-NA-C1A	4.01	108.51	106.68
48	B2	617	BCR	C30-C25-C26	-4.01	117.15	122.64
45	AF	804	CLA	CAA-C2A-C3A	-4.01	107.03	116.23
54	B5	605	CHL	OBD-CAD-CBD	4.01	131.71	125.82
47	A3	301	LHG	O7-C7-C8	4.01	120.16	111.48
54	A6	608	CHL	C1A-CHA-C4D	-4.01	112.29	118.98
45	B1	311	CLA	C4A-NA-C1A	4.00	108.50	106.68
54	B2	614	CHL	C1A-CHA-C4D	-4.00	112.31	118.98
45	BA	823	CLA	C4A-NA-C1A	3.99	108.50	106.68
54	B2	614	CHL	C1C-C2C-CMC	3.99	134.00	126.80
48	BK	204	BCR	C30-C25-C26	-3.99	117.18	122.64
48	AB	847	BCR	C3-C4-C5	-3.99	106.94	114.06
55	B5	615	XAT	C39-C29-C28	3.99	124.18	118.09
54	B2	607	CHL	C1A-CHA-C4D	-3.99	112.33	118.98
48	AA	846	BCR	C38-C26-C25	-3.98	120.14	124.48
52	B2	615	LUT	C26-C27-C28	-3.98	118.38	124.58
48	A1	319	BCR	C37-C22-C23	3.98	124.17	118.09
54	B2	606	CHL	C1C-C2C-CMC	3.98	133.98	126.80
45	A6	612	CLA	C4A-NA-C1A	3.98	108.49	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	A1	301	LHG	O7-C7-C8	3.97	120.08	111.48
48	BL	301	BCR	C3-C4-C5	-3.97	106.97	114.06
45	BA	826	CLA	C4A-NA-C1A	3.97	108.49	106.68
48	AB	846	BCR	C34-C9-C10	-3.96	116.39	122.82
45	BA	835	CLA	C4A-NA-C1A	3.96	108.49	106.68
48	BK	204	BCR	C37-C22-C23	3.96	124.14	118.09
54	B5	607	CHL	C1A-CHA-C4D	-3.96	112.37	118.98
52	B2	615	LUT	C40-C33-C32	3.96	124.14	118.09
45	AB	833	CLA	C4A-NA-C1A	3.95	108.48	106.68
45	BA	844	CLA	C4A-NA-C1A	3.95	108.48	106.68
53	B5	617	LMG	O7-C10-C11	3.94	120.00	111.48
45	AB	835	CLA	C4A-NA-C1A	3.94	108.48	106.68
45	AA	807	CLA	C4A-NA-C1A	3.93	108.47	106.68
45	A1	309	CLA	C4A-NA-C1A	3.93	108.47	106.68
45	B1	310	CLA	C4A-NA-C1A	3.93	108.47	106.68
45	B2	613	CLA	C4A-NA-C1A	3.93	108.47	106.68
54	B1	303	CHL	C1C-C2C-CMC	3.93	133.88	126.80
54	A1	308	CHL	C1A-CHA-C4D	-3.93	112.43	118.98
48	AI	102	BCR	C28-C27-C26	-3.92	107.06	114.06
48	B2	617	BCR	C23-C24-C25	-3.92	116.51	127.00
48	AA	847	BCR	C24-C23-C22	-3.92	120.43	126.23
45	AB	811	CLA	O2D-CGD-O1D	-3.92	116.21	123.85
45	BB	841	CLA	C4A-NA-C1A	3.92	108.47	106.68
48	AJ	103	BCR	C8-C9-C10	-3.92	112.84	119.01
48	BL	301	BCR	C30-C25-C26	-3.91	117.29	122.64
54	A4	306	CHL	C1A-CHA-C4D	-3.91	112.46	118.98
54	B1	308	CHL	C1A-CHA-C4D	-3.90	112.47	118.98
45	A4	307	CLA	C4A-NA-C1A	3.90	108.46	106.68
54	A4	304	CHL	C1A-CHA-C4D	-3.90	112.47	118.98
48	BK	204	BCR	C30-C25-C24	3.90	126.22	115.65
54	A4	304	CHL	CMA-C3A-C4A	-3.89	106.22	114.61
54	A6	602	CHL	C1A-CHA-C4D	-3.89	112.49	118.98
45	BA	829	CLA	C4A-NA-C1A	3.89	108.45	106.68
48	AF	805	BCR	C7-C8-C9	-3.89	120.48	126.23
45	BA	831	CLA	C4A-NA-C1A	3.89	108.45	106.68
45	B3	307	CLA	C4A-NA-C1A	3.88	108.45	106.68
54	B2	601	CHL	C1A-CHA-C4D	-3.88	112.51	118.98
52	A4	315	LUT	C21-C26-C27	-3.88	108.37	112.83
54	A6	606	CHL	C1C-C2C-CMC	3.87	133.78	126.80
48	BG	203	BCR	C10-C11-C12	-3.87	111.97	123.20
45	A1	304	CLA	C4A-NA-C1A	3.86	108.44	106.68
47	B1	318	LHG	O7-C7-C8	3.86	119.83	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	806	CLA	C4A-NA-C1A	3.86	108.44	106.68
54	B2	605	CHL	C1C-C2C-CMC	3.86	133.76	126.80
48	A1	319	BCR	C36-C18-C19	3.86	123.98	118.09
46	AB	843	PQN	C12-C11-C3	-3.85	102.59	112.08
45	BB	815	CLA	C4A-NA-C1A	3.85	108.44	106.68
48	BG	203	BCR	C38-C26-C25	-3.85	120.28	124.48
52	B5	614	LUT	C1-C6-C5	-3.85	117.38	122.64
45	A4	308	CLA	C4A-NA-C1A	3.85	108.43	106.68
47	A1	302	LHG	O7-C7-C8	3.85	119.80	111.48
54	A1	303	CHL	C1A-CHA-C4D	-3.85	112.57	118.98
48	BJ	103	BCR	C32-C1-C6	-3.84	104.22	110.24
52	B3	315	LUT	C39-C29-C28	3.84	123.95	118.09
48	BB	849	BCR	C33-C5-C6	-3.83	120.30	124.48
54	B1	303	CHL	C1A-CHA-C4D	-3.83	112.59	118.98
48	BA	849	BCR	C36-C18-C19	3.83	123.94	118.09
48	BB	803	BCR	C30-C25-C26	-3.83	117.41	122.64
45	AL	303	CLA	C4A-NA-C1A	3.83	108.42	106.68
45	AL	304	CLA	C4A-NA-C1A	3.83	108.42	106.68
47	B5	618	LHG	O7-C7-C8	3.83	119.76	111.48
55	B2	616	XAT	C20-C13-C12	3.82	123.93	118.09
45	A6	611	CLA	O2D-CGD-O1D	-3.82	116.41	123.85
54	A1	303	CHL	O2A-CGA-CBA	3.82	123.48	111.83
54	A1	303	CHL	C1C-C2C-CMC	3.82	133.69	126.80
45	A3	302	CLA	C4A-NA-C1A	3.82	108.42	106.68
45	BB	819	CLA	C4A-NA-C1A	3.82	108.42	106.68
48	BG	203	BCR	C34-C9-C10	-3.82	116.63	122.82
48	AJ	103	BCR	C1-C6-C5	-3.82	117.42	122.64
55	B3	316	XAT	C6-C7-C8	-3.82	117.92	125.99
52	B1	316	LUT	C15-C35-C34	3.82	131.33	123.52
51	BB	850	DGD	O2G-C1B-C2B	3.82	119.73	111.48
48	BB	849	BCR	C3-C4-C5	-3.81	107.25	114.06
48	BI	101	BCR	C31-C1-C6	-3.81	104.26	110.24
48	B2	617	BCR	C40-C30-C25	-3.81	104.26	110.24
48	BA	848	BCR	C34-C9-C8	3.81	123.91	118.09
52	A4	315	LUT	C26-C27-C28	-3.81	118.66	124.58
45	B3	303	CLA	C4A-NA-C1A	3.81	108.42	106.68
48	BL	305	BCR	C30-C25-C24	3.80	125.96	115.65
45	B2	608	CLA	C4A-NA-C1A	3.80	108.41	106.68
48	BA	848	BCR	C30-C25-C26	-3.80	117.45	122.64
54	B5	605	CHL	C1A-CHA-C4D	-3.79	112.65	118.98
48	BA	850	BCR	C30-C25-C26	-3.79	117.45	122.64
54	A4	305	CHL	C1A-CHA-C4D	-3.79	112.66	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BL	305	BCR	C32-C1-C6	-3.78	104.32	110.24
55	A3	317	XAT	C39-C29-C28	3.78	123.86	118.09
48	B2	617	BCR	C32-C1-C6	-3.77	104.33	110.24
51	AB	851	DGD	O2G-C1B-C2B	3.77	119.64	111.48
48	B5	616	BCR	C33-C5-C6	-3.77	120.37	124.48
45	AA	829	CLA	C6-C5-C3	3.77	122.65	113.47
45	B2	602	CLA	C4A-NA-C1A	3.77	108.40	106.68
54	B2	601	CHL	C1C-C2C-CMC	3.77	133.59	126.80
54	A3	307	CHL	CMC-C2C-C1C	3.76	131.51	124.73
45	B3	312	CLA	C4A-NA-C1A	3.76	108.40	106.68
54	B5	606	CHL	C1A-CHA-C4D	-3.76	112.70	118.98
45	B5	610	CLA	C4A-NA-C1A	3.75	108.39	106.68
54	B5	607	CHL	C1C-C2C-CMC	3.75	133.56	126.80
48	BF	304	BCR	C35-C13-C14	-3.75	116.74	122.82
54	A6	602	CHL	C1C-C2C-CMC	3.75	133.56	126.80
54	A4	304	CHL	C1C-C2C-CMC	3.74	133.55	126.80
48	BL	301	BCR	C38-C26-C25	-3.74	120.40	124.48
48	AI	102	BCR	C37-C22-C23	3.74	123.80	118.09
51	AB	851	DGD	C2G-O2G-C1B	-3.74	108.84	117.80
52	A1	317	LUT	C26-C27-C28	-3.74	118.76	124.58
54	A6	608	CHL	CMC-C2C-C1C	3.74	131.46	124.73
48	BA	849	BCR	C38-C26-C25	-3.73	120.42	124.48
45	A6	609	CLA	C4A-NA-C1A	3.73	108.38	106.68
46	BB	844	PQN	C11-C12-C13	-3.73	120.41	126.83
48	A3	318	BCR	C39-C30-C29	3.72	123.24	108.95
54	A4	314	CHL	C1A-CHA-C4D	-3.72	112.78	118.98
54	A6	607	CHL	C1A-CHA-C4D	-3.72	112.78	118.98
54	B1	308	CHL	C1C-C2C-CMC	3.72	133.50	126.80
48	B3	317	BCR	C37-C22-C23	3.72	123.77	118.09
54	A6	606	CHL	C1A-CHA-C4D	-3.72	112.78	118.98
48	BB	845	BCR	C1-C6-C5	-3.71	117.56	122.64
45	BL	303	CLA	C4A-NA-C1A	3.71	108.37	106.68
48	B2	617	BCR	C36-C18-C19	3.71	123.76	118.09
48	AI	102	BCR	C30-C25-C26	-3.71	117.56	122.64
48	BB	803	BCR	C37-C22-C23	3.71	123.75	118.09
48	AB	844	BCR	C7-C8-C9	-3.70	120.75	126.23
52	B5	614	LUT	C36-C21-C26	3.70	115.16	109.55
45	BB	802	CLA	C4-C3-C5	3.70	121.65	115.23
45	B5	613	CLA	C4A-NA-C1A	3.70	108.37	106.68
48	BB	846	BCR	C8-C7-C6	-3.70	117.12	127.00
55	A6	616	XAT	C8-C9-C10	-3.69	113.20	119.01
54	B2	605	CHL	C1A-CHA-C4D	-3.68	112.83	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AG	205	BCR	C32-C1-C6	-3.68	104.47	110.24
48	AA	849	BCR	C27-C26-C25	-3.68	117.73	122.70
55	A6	616	XAT	O24-C25-C24	3.68	116.94	113.49
48	A3	318	BCR	C38-C26-C25	-3.67	120.48	124.48
48	AA	848	BCR	C36-C18-C19	3.67	123.70	118.09
48	BA	851	BCR	C23-C22-C21	-3.67	113.24	119.01
48	A1	319	BCR	C4-C5-C6	-3.67	117.75	122.70
46	AB	843	PQN	C11-C3-C4	-3.66	114.72	118.58
48	AL	302	BCR	C34-C9-C10	-3.66	116.88	122.82
48	A3	318	BCR	C1-C6-C5	-3.66	117.64	122.64
48	BI	101	BCR	C39-C30-C25	-3.66	104.50	110.24
48	AB	848	BCR	C36-C18-C19	3.65	123.67	118.09
48	AG	205	BCR	C36-C18-C17	-3.65	116.90	122.82
55	B1	317	XAT	O4-C5-C18	3.65	119.13	115.05
55	A3	317	XAT	C19-C9-C8	3.65	123.67	118.09
45	A6	611	CLA	O2D-CGD-CBD	3.65	117.61	111.23
45	B1	315	CLA	C4A-NA-C1A	3.65	108.34	106.68
52	B5	614	LUT	C21-C26-C27	-3.63	108.66	112.83
47	BF	305	LHG	C5-O7-C7	-3.62	109.12	117.80
54	B3	306	CHL	CMC-C2C-C1C	3.62	131.24	124.73
48	A1	319	BCR	C40-C30-C29	-3.62	95.06	108.95
48	AB	849	BCR	C23-C22-C21	-3.62	113.32	119.01
45	B5	602	CLA	C4A-NA-C1A	3.61	108.33	106.68
48	BL	306	BCR	C33-C5-C6	-3.61	120.55	124.48
48	AL	306	BCR	C28-C27-C26	-3.61	107.62	114.06
48	BG	203	BCR	C36-C18-C17	-3.61	116.97	122.82
55	B3	316	XAT	C35-C15-C14	-3.61	116.14	123.52
46	BB	844	PQN	C11-C3-C4	-3.60	114.78	118.58
54	B3	306	CHL	C1A-CHA-C4D	-3.60	112.97	118.98
48	BA	847	BCR	C30-C25-C26	-3.60	117.72	122.64
48	BA	856	BCR	C30-C25-C26	-3.60	117.72	122.64
48	BG	203	BCR	C33-C5-C4	3.60	121.27	113.60
45	AB	818	CLA	C4A-NA-C1A	3.60	108.32	106.68
45	A6	614	CLA	C4A-NA-C1A	3.59	108.32	106.68
53	A1	321	LMG	O7-C10-C11	3.59	119.25	111.48
48	BA	850	BCR	C36-C18-C19	3.59	123.57	118.09
46	BA	843	PQN	C16-C15-C13	-3.59	104.73	113.47
45	A1	311	CLA	C4A-NA-C1A	3.58	108.31	106.68
48	BJ	103	BCR	C39-C30-C25	-3.58	104.62	110.24
45	BB	821	CLA	C4A-NA-C1A	3.58	108.31	106.68
45	B3	314	CLA	C4A-NA-C1A	3.58	108.31	106.68
48	BI	101	BCR	C30-C25-C26	-3.57	117.75	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	B3	315	LUT	C40-C33-C32	3.57	123.54	118.09
45	BK	201	CLA	CAA-C2A-C3A	-3.57	108.05	116.23
45	A3	309	CLA	C4A-NA-C1A	3.56	108.31	106.68
55	B1	317	XAT	C6-C7-C8	-3.56	118.46	125.99
45	AA	803	CLA	O2D-CGD-O1D	-3.56	116.91	123.85
48	AA	848	BCR	C30-C25-C24	3.56	125.31	115.65
45	B1	304	CLA	O2D-CGD-O1D	-3.56	116.92	123.85
52	B3	315	LUT	C3-C4-C5	-3.55	103.33	112.18
45	BB	835	CLA	C4A-NA-C1A	3.55	108.30	106.68
48	BA	855	BCR	C34-C9-C8	3.55	123.51	118.09
48	BA	855	BCR	C24-C23-C22	-3.55	120.98	126.23
45	AB	801	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
48	BB	846	BCR	C3-C4-C5	-3.55	107.73	114.06
54	A6	606	CHL	O1D-CGD-CBD	-3.55	119.34	124.72
45	BB	801	CLA	O2D-CGD-O1D	-3.55	116.95	123.85
45	AA	816	CLA	O2D-CGD-O1D	-3.54	116.95	123.85
48	AL	306	BCR	C30-C25-C24	3.54	125.25	115.65
48	AB	847	BCR	C23-C24-C25	-3.54	117.55	127.00
45	BA	829	CLA	C3B-C4B-NB	-3.54	107.37	110.53
53	A4	318	LMG	O7-C10-C11	3.53	119.12	111.48
48	BB	847	BCR	C36-C18-C19	3.53	123.48	118.09
55	A1	318	XAT	C8-C9-C10	-3.53	113.46	119.01
48	AB	849	BCR	C16-C15-C14	-3.53	116.31	123.52
55	B5	615	XAT	C6-C7-C8	-3.52	118.55	125.99
55	B1	317	XAT	C40-C33-C32	3.52	123.47	118.09
45	B2	610	CLA	CHA-C1A-NA	-3.52	122.81	126.67
55	B2	616	XAT	O24-C25-C24	3.52	116.79	113.49
54	B2	601	CHL	O2A-CGA-CBA	3.52	122.56	111.83
48	AL	302	BCR	C2-C1-C6	-3.52	105.33	110.44
48	AJ	101	BCR	C8-C7-C6	-3.51	117.61	127.00
48	BA	851	BCR	C34-C9-C10	-3.51	117.13	122.82
48	BJ	101	BCR	C3-C4-C5	-3.51	107.80	114.06
52	AF	806	LUT	C15-C35-C34	-3.51	116.34	123.52
48	BF	304	BCR	C30-C25-C26	-3.51	117.84	122.64
48	AB	844	BCR	C4-C5-C6	-3.51	117.97	122.70
48	BK	204	BCR	C27-C26-C25	-3.51	117.97	122.70
55	B2	616	XAT	C39-C29-C28	3.51	123.44	118.09
45	B2	610	CLA	O2D-CGD-O1D	-3.50	117.03	123.85
48	AA	847	BCR	C36-C18-C19	3.50	123.44	118.09
48	A6	617	BCR	C23-C24-C25	-3.50	117.65	127.00
48	BA	856	BCR	C29-C30-C25	3.50	115.52	110.44
48	BA	856	BCR	C38-C26-C25	3.50	128.30	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	803	CLA	O2D-CGD-O1D	-3.49	117.05	123.85
45	B1	307	CLA	C4A-NA-C1A	3.49	108.27	106.68
48	AI	102	BCR	C30-C25-C24	3.49	125.12	115.65
48	BB	848	BCR	C39-C30-C25	-3.49	104.77	110.24
54	B2	601	CHL	CMA-C3A-C4A	-3.49	107.10	114.61
48	B2	617	BCR	C4-C5-C6	-3.49	117.99	122.70
47	B1	301	LHG	O7-C7-C8	3.48	119.02	111.48
48	BI	101	BCR	C37-C22-C23	3.48	123.40	118.09
45	BB	834	CLA	O2D-CGD-O1D	-3.47	117.08	123.85
48	BK	204	BCR	C38-C26-C27	3.47	121.00	113.60
45	BA	834	CLA	O2D-CGD-O1D	-3.47	117.09	123.85
48	BA	848	BCR	C27-C26-C25	-3.47	118.01	122.70
52	A6	615	LUT	C26-C27-C28	-3.47	119.18	124.58
52	B3	315	LUT	C19-C9-C8	3.47	123.39	118.09
55	B2	616	XAT	C40-C33-C32	3.47	123.39	118.09
54	A4	314	CHL	C1C-C2C-CMC	3.47	133.06	126.80
48	AA	849	BCR	C31-C1-C6	-3.47	104.81	110.24
48	AB	848	BCR	C15-C16-C17	-3.46	116.43	123.52
48	AA	846	BCR	C15-C16-C17	-3.46	116.43	123.52
54	A1	303	CHL	CMD-C2D-C3D	3.46	131.60	124.68
45	AB	801	CLA	CAA-C2A-C1A	-3.46	100.64	111.97
45	AA	822	CLA	O2D-CGD-O1D	-3.46	117.12	123.85
56	e	301	SQD	C4-C3-C2	3.46	116.90	110.83
48	AB	844	BCR	C37-C22-C23	3.45	123.36	118.09
52	A1	317	LUT	C3-C4-C5	-3.45	103.58	112.18
48	AI	101	BCR	C37-C22-C23	3.45	123.36	118.09
56	BJ	104	SQD	O47-C7-O49	-3.45	115.64	123.70
48	BB	845	BCR	C38-C26-C27	3.45	120.95	113.60
48	BJ	103	BCR	C8-C9-C10	-3.45	113.58	119.01
55	B5	615	XAT	C18-C5-C6	-3.45	116.63	122.30
54	A6	602	CHL	O2A-CGA-CBA	3.44	122.33	111.83
45	A3	315	CLA	C4A-NA-C1A	3.44	108.25	106.68
55	A4	316	XAT	C35-C15-C14	-3.44	116.49	123.52
45	AA	837	CLA	O2D-CGD-O1D	-3.43	117.16	123.85
48	AL	302	BCR	C35-C13-C12	3.43	123.33	118.09
45	AA	832	CLA	C4-C3-C5	3.43	121.18	115.23
52	A3	316	LUT	C39-C29-C28	3.43	123.33	118.09
45	A1	312	CLA	C4A-NA-C1A	3.43	108.24	106.68
45	BB	843	CLA	C3B-C4B-NB	-3.43	107.47	110.53
48	AA	848	BCR	C38-C26-C25	-3.42	120.75	124.48
48	AF	801	BCR	C35-C13-C12	3.42	123.32	118.09
48	AB	846	BCR	C36-C18-C19	3.42	123.31	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B2	616	XAT	C36-C21-C22	-3.42	102.96	108.97
48	BJ	101	BCR	C34-C9-C8	3.42	123.31	118.09
48	BL	306	BCR	C38-C26-C25	-3.41	120.76	124.48
54	A3	307	CHL	C1A-CHA-C4D	-3.41	113.29	118.98
56	e	301	SQD	O47-C7-C8	3.41	118.86	111.48
48	AJ	101	BCR	C4-C5-C6	-3.41	118.09	122.70
53	AG	202	LMG	O7-C10-C11	3.41	118.86	111.48
45	B2	609	CLA	C4A-NA-C1A	3.41	108.23	106.68
48	AB	845	BCR	C8-C7-C6	-3.40	117.91	127.00
55	B1	317	XAT	C38-C25-C26	-3.40	116.70	122.30
48	AB	849	BCR	C24-C25-C26	3.40	129.39	121.56
48	BB	847	BCR	C8-C9-C10	3.40	124.35	119.01
48	BG	203	BCR	C11-C10-C9	3.40	132.04	127.28
48	BA	855	BCR	C16-C15-C14	-3.39	116.58	123.52
45	BB	801	CLA	CHB-C4A-NA	3.39	129.29	124.40
52	A1	317	LUT	C8-C7-C6	-3.39	117.94	127.00
45	BB	807	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
45	A6	610	CLA	C4A-NA-C1A	3.39	108.22	106.68
45	AB	842	CLA	O2D-CGD-O1D	-3.39	117.25	123.85
55	A1	318	XAT	C18-C5-C6	-3.39	116.73	122.30
45	AB	819	CLA	O2D-CGD-O1D	-3.38	117.26	123.85
48	AF	805	BCR	C16-C15-C14	-3.38	116.60	123.52
48	AA	852	BCR	C15-C16-C17	-3.38	116.61	123.52
48	BG	203	BCR	C16-C17-C18	3.38	132.01	127.28
48	AK	204	BCR	C29-C30-C25	3.37	115.34	110.44
48	BB	803	BCR	C29-C30-C25	3.37	115.33	110.44
48	AK	204	BCR	C30-C25-C26	-3.37	118.03	122.64
45	AB	804	CLA	CHB-C4A-NA	3.37	129.26	124.40
48	AB	849	BCR	C39-C30-C25	-3.37	104.96	110.24
45	B5	608	CLA	C4A-NA-C1A	3.37	108.22	106.68
48	AG	205	BCR	C8-C7-C6	-3.36	118.01	127.00
45	BG	201	CLA	C4A-NA-C1A	3.36	108.21	106.68
48	BJ	101	BCR	C32-C1-C6	-3.36	104.98	110.24
45	AB	831	CLA	C4A-NA-C1A	3.36	108.21	106.68
48	AI	101	BCR	C24-C23-C22	-3.35	121.27	126.23
45	B5	602	CLA	C3B-C4B-NB	-3.35	107.54	110.53
45	AB	813	CLA	O2D-CGD-O1D	-3.35	117.32	123.85
45	AA	833	CLA	O2D-CGD-O1D	-3.35	117.33	123.85
52	A6	615	LUT	C21-C26-C27	-3.35	108.97	112.83
48	BB	847	BCR	C33-C5-C6	-3.35	120.83	124.48
48	AB	849	BCR	C4-C5-C6	-3.35	118.18	122.70
52	B3	315	LUT	C38-C25-C24	-3.35	115.44	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	829	CLA	C3B-C4B-NB	-3.34	107.55	110.53
48	AI	101	BCR	C39-C30-C25	-3.34	105.00	110.24
45	AB	827	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
47	B1	302	LHG	O7-C7-C8	3.34	118.70	111.48
48	BB	848	BCR	C29-C30-C25	3.33	115.28	110.44
47	BA	846	LHG	O7-C7-C8	3.33	118.69	111.48
47	A6	618	LHG	O7-C7-C8	3.33	118.68	111.48
45	BA	839	CLA	O2D-CGD-O1D	-3.32	117.38	123.85
52	AF	806	LUT	C8-C7-C6	-3.32	118.12	127.00
46	BB	844	PQN	C14-C13-C12	-3.32	115.10	123.63
55	A3	317	XAT	C26-C27-C28	-3.32	118.98	125.99
48	AA	849	BCR	C36-C18-C17	-3.32	117.44	122.82
45	AA	827	CLA	O2D-CGD-O1D	-3.32	117.39	123.85
45	BA	836	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
48	BI	101	BCR	C16-C15-C14	-3.31	116.74	123.52
55	A4	316	XAT	C38-C25-C26	-3.31	116.85	122.30
45	BB	815	CLA	CAC-C3C-C2C	-3.31	121.47	127.56
48	BA	850	BCR	C27-C26-C25	-3.31	118.23	122.70
45	AB	809	CLA	O2D-CGD-O1D	-3.31	117.40	123.85
55	B5	615	XAT	C36-C21-C22	-3.31	103.15	108.97
45	AA	809	CLA	CAA-C2A-C3A	-3.31	104.06	113.00
45	AA	819	CLA	O2D-CGD-O1D	-3.30	117.42	123.85
48	AF	801	BCR	C30-C25-C26	-3.30	118.13	122.64
45	AA	839	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
48	A1	319	BCR	C38-C26-C25	-3.30	120.88	124.48
45	AA	824	CLA	C4A-NA-C1A	3.30	108.18	106.68
53	A4	318	LMG	C7-O1-C1	-3.30	106.73	113.80
52	B5	614	LUT	C26-C27-C28	-3.30	119.45	124.58
45	AB	806	CLA	O2D-CGD-O1D	-3.29	117.44	123.85
45	B2	610	CLA	O2D-CGD-CBD	3.29	116.98	111.23
45	AA	827	CLA	CAA-CBA-CGA	-3.28	103.88	113.21
52	B1	316	LUT	C19-C9-C10	-3.28	117.50	122.82
45	AB	804	CLA	CAC-C3C-C2C	-3.28	121.53	127.56
45	AB	835	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
48	AJ	103	BCR	C15-C16-C17	-3.28	116.81	123.52
48	AB	848	BCR	C38-C26-C25	-3.28	120.91	124.48
48	BA	851	BCR	C8-C9-C10	3.28	124.16	119.01
45	AB	819	CLA	C6-C5-C3	3.27	121.44	113.47
48	BF	304	BCR	C31-C1-C6	-3.27	105.11	110.24
48	BA	848	BCR	C38-C26-C27	3.27	120.58	113.60
45	BB	840	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
48	A4	317	BCR	C33-C5-C6	-3.27	120.91	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	841	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
45	AB	839	CLA	O2D-CGD-O1D	-3.27	117.48	123.85
45	A1	307	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
45	AA	806	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
45	BA	828	CLA	O2D-CGD-O1D	-3.27	117.49	123.85
45	AA	803	CLA	O2D-CGD-CBD	3.26	116.94	111.23
48	BJ	103	BCR	C1-C6-C5	-3.26	118.18	122.64
45	AF	802	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
55	A4	316	XAT	C6-C7-C8	-3.26	119.10	125.99
45	BB	829	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
48	AL	306	BCR	C38-C26-C27	3.26	120.54	113.60
48	BB	803	BCR	C16-C15-C14	-3.25	116.86	123.52
45	AA	830	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
48	AB	848	BCR	C8-C9-C10	-3.25	113.89	119.01
55	A6	616	XAT	C15-C35-C34	-3.25	116.86	123.52
48	BA	851	BCR	C33-C5-C4	3.25	120.53	113.60
45	BA	833	CLA	O2D-CGD-O1D	-3.25	117.52	123.85
48	AB	846	BCR	C3-C4-C5	-3.25	108.26	114.06
48	AB	844	BCR	C33-C5-C6	3.25	128.03	124.48
45	BB	810	CLA	O2D-CGD-O1D	-3.25	117.53	123.85
48	BF	304	BCR	C37-C22-C23	3.25	123.05	118.09
55	A1	318	XAT	C40-C33-C32	3.24	123.05	118.09
48	BL	305	BCR	C3-C4-C5	-3.24	108.27	114.06
45	BB	812	CLA	O2D-CGD-O1D	-3.24	117.55	123.85
45	BB	816	CLA	C4A-NA-C1A	3.23	108.15	106.68
52	B1	316	LUT	C39-C29-C30	-3.23	117.58	122.82
55	A3	317	XAT	C35-C15-C14	-3.23	116.91	123.52
50	AA	851	LMU	O5B-C5B-C4B	3.23	115.51	109.70
48	BK	204	BCR	C38-C26-C25	-3.22	120.97	124.48
48	BL	301	BCR	C34-C9-C8	3.22	123.00	118.09
45	AA	836	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
56	e	301	SQD	O7-S-C6	3.22	111.56	106.76
55	A1	318	XAT	C39-C29-C28	3.21	123.00	118.09
48	B3	317	BCR	C28-C29-C30	-3.21	103.05	114.43
45	AB	801	CLA	CMD-C2D-C1D	-3.21	119.07	124.73
48	BA	847	BCR	C37-C22-C23	3.21	123.00	118.09
45	BA	804	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
45	BB	841	CLA	O2D-CGD-O1D	-3.21	117.60	123.85
45	AA	811	CLA	O2D-CGD-O1D	-3.21	117.61	123.85
48	BA	855	BCR	C4-C5-C6	-3.21	118.37	122.70
54	B2	601	CHL	CBC-CAC-C3C	-3.21	108.28	112.87
54	B2	614	CHL	O1D-CGD-CBD	-3.21	119.86	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AA	849	BCR	C28-C27-C26	-3.20	108.34	114.06
45	BG	201	CLA	O2D-CGD-O1D	-3.20	117.61	123.85
55	A4	316	XAT	C28-C29-C30	-3.20	113.97	119.01
48	AA	848	BCR	C33-C5-C6	-3.20	120.99	124.48
45	BB	819	CLA	O2D-CGD-O1D	-3.20	117.62	123.85
48	BL	301	BCR	C37-C22-C23	3.20	122.97	118.09
51	BB	850	DGD	O1G-C1A-C2A	3.20	121.58	111.83
48	AB	844	BCR	C30-C25-C26	-3.20	118.27	122.64
48	AB	846	BCR	C1-C6-C5	-3.19	118.27	122.64
45	BA	831	CLA	C3B-C4B-NB	-3.19	107.68	110.53
48	AJ	103	BCR	C7-C8-C9	-3.19	121.52	126.23
48	BF	304	BCR	C7-C8-C9	-3.19	121.52	126.23
45	A3	310	CLA	CBD-CHA-C1A	3.19	132.19	127.38
45	A4	313	CLA	O2D-CGD-O1D	-3.19	117.65	123.85
45	AA	840	CLA	C3B-C4B-NB	-3.18	107.69	110.53
45	AA	812	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
45	B1	307	CLA	C3A-C2A-C1A	-3.18	103.05	106.30
45	AB	812	CLA	O2D-CGD-O1D	-3.18	117.67	123.85
48	BA	855	BCR	C39-C30-C25	-3.18	105.26	110.24
45	BA	832	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
48	BF	304	BCR	C16-C15-C14	-3.17	117.02	123.52
48	AB	845	BCR	C3-C4-C5	-3.17	108.40	114.06
48	B5	616	BCR	C23-C24-C25	-3.17	118.52	127.00
45	AA	815	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
45	AA	824	CLA	CBA-CAA-C2A	3.17	123.23	113.79
45	A3	311	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
45	BB	830	CLA	C4A-NA-C1A	3.17	108.12	106.68
45	BB	814	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
45	BK	202	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
55	B1	317	XAT	C35-C15-C14	-3.16	117.06	123.52
48	BI	101	BCR	C38-C26-C27	3.16	120.33	113.60
45	B3	305	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
45	BB	809	CLA	O2D-CGD-O1D	-3.15	117.71	123.85
45	BA	828	CLA	O2D-CGD-CBD	3.15	116.74	111.23
46	AA	843	PQN	O1-C1-C2	-3.15	116.31	120.45
55	A4	316	XAT	O4-C5-C18	3.15	118.57	115.05
48	BG	203	BCR	C37-C22-C21	-3.15	117.72	122.82
45	AB	808	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
45	BB	825	CLA	O2D-CGD-O1D	-3.15	117.73	123.85
45	BL	304	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
45	BB	827	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
48	AB	845	BCR	C8-C9-C10	3.14	123.95	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	834	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
45	BB	828	CLA	O2D-CGD-O1D	-3.14	117.73	123.85
45	AA	823	CLA	C4A-NA-C1A	3.14	108.11	106.68
45	AB	825	CLA	O2D-CGD-O1D	-3.14	117.74	123.85
45	AB	814	CLA	C3B-C4B-NB	-3.14	107.73	110.53
48	BI	101	BCR	C1-C6-C5	-3.13	118.35	122.64
48	AL	306	BCR	C30-C25-C26	-3.13	118.36	122.64
46	AA	843	PQN	C14-C13-C12	-3.13	115.58	123.63
52	AF	806	LUT	C37-C21-C36	3.13	112.42	107.87
55	B1	317	XAT	C26-C27-C28	-3.13	119.38	125.99
56	BJ	104	SQD	C3-C4-C5	3.13	115.90	110.23
45	AB	818	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
48	B5	616	BCR	C23-C22-C21	-3.12	114.09	119.01
45	AB	817	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
45	BB	802	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
52	B2	615	LUT	C17-C1-C6	-3.12	105.35	110.24
45	A3	302	CLA	C3B-C4B-NB	-3.12	107.75	110.53
48	BB	849	BCR	C38-C26-C25	-3.12	121.08	124.48
48	AA	847	BCR	C10-C11-C12	3.12	132.24	123.20
45	AK	201	CLA	CHB-C1B-C2B	-3.12	123.91	130.51
45	A1	304	CLA	CAC-C3C-C4C	3.12	128.85	124.79
45	BB	830	CLA	C3B-C4B-NB	-3.12	107.75	110.53
48	BI	101	BCR	C28-C27-C26	-3.12	108.50	114.06
48	BA	855	BCR	C8-C9-C10	-3.11	114.11	119.01
48	BF	304	BCR	C1-C6-C5	-3.11	118.38	122.64
48	AK	204	BCR	C23-C22-C21	3.11	123.91	119.01
48	AF	805	BCR	C36-C18-C19	3.11	122.84	118.09
48	AI	102	BCR	C4-C5-C6	-3.11	118.50	122.70
48	AL	306	BCR	C36-C18-C19	3.11	122.84	118.09
45	BA	810	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
48	BB	849	BCR	C15-C16-C17	-3.11	117.16	123.52
48	AA	848	BCR	C30-C25-C26	-3.11	118.39	122.64
45	AA	832	CLA	O2D-CGD-O1D	-3.11	117.80	123.85
48	AA	849	BCR	C38-C26-C27	3.10	120.22	113.60
52	A3	316	LUT	C16-C1-C6	3.10	115.11	110.24
52	A4	315	LUT	C39-C29-C28	3.10	122.83	118.09
52	B3	315	LUT	C15-C35-C34	-3.10	117.17	123.52
45	AA	821	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
45	BB	824	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
45	BB	818	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
54	B5	606	CHL	CMC-C2C-C1C	3.10	130.31	124.73
45	AA	813	CLA	O2D-CGD-O1D	-3.10	117.82	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A3	316	LUT	C26-C27-C28	-3.10	119.76	124.58
45	A4	301	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
45	AA	828	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
45	BF	302	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
45	AB	801	CLA	CHB-C4A-NA	3.09	128.86	124.40
48	AA	849	BCR	C2-C3-C4	-3.09	104.48	111.28
45	BA	817	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
45	AB	811	CLA	CAA-C2A-C3A	-3.09	104.65	113.00
48	AJ	101	BCR	C36-C18-C19	3.09	122.81	118.09
45	BB	827	CLA	C4A-NA-C1A	3.09	108.09	106.68
55	B5	615	XAT	C40-C33-C32	3.09	122.80	118.09
45	BA	821	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
45	AA	810	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
45	BB	805	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
48	AA	849	BCR	C8-C9-C10	3.08	123.85	119.01
48	BA	850	BCR	C19-C18-C17	-3.08	114.17	119.01
48	AB	844	BCR	C32-C1-C6	-3.08	105.42	110.24
45	AB	828	CLA	CHB-C4A-NA	3.08	128.84	124.40
45	AB	806	CLA	CHB-C4A-NA	3.08	128.84	124.40
46	AA	843	PQN	C16-C15-C13	-3.08	105.98	113.47
54	A4	305	CHL	CMC-C2C-C1C	3.07	130.26	124.73
45	AA	842	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
45	BB	834	CLA	C6-C5-C3	3.07	120.95	113.47
45	BB	820	CLA	C6-C5-C3	3.07	120.95	113.47
45	BA	844	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
45	AA	821	CLA	CMB-C2B-C1B	-3.07	120.75	125.42
45	A6	605	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
47	B1	301	LHG	O8-C23-C24	3.07	121.19	111.83
48	BB	847	BCR	C37-C22-C23	3.07	122.77	118.09
54	B2	606	CHL	CBC-CAC-C3C	-3.06	108.48	112.87
45	BA	820	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
45	B1	314	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
45	AA	828	CLA	CMB-C2B-C3B	3.06	133.75	126.55
45	AB	803	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
48	A3	318	BCR	C29-C30-C25	3.06	114.88	110.44
48	BB	849	BCR	C28-C27-C26	-3.06	108.61	114.06
45	BA	806	CLA	O2D-CGD-O1D	-3.05	117.90	123.85
45	A6	611	CLA	CHA-C1A-NA	-3.05	123.32	126.67
52	A6	615	LUT	C8-C9-C10	-3.05	114.21	119.01
45	BA	842	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
45	BH	201	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
45	A4	309	CLA	O2D-CGD-O1D	-3.05	117.92	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AA	849	BCR	C30-C25-C26	-3.05	118.47	122.64
48	A4	317	BCR	C27-C26-C25	-3.05	118.59	122.70
45	BA	819	CLA	O2D-CGD-O1D	-3.05	117.92	123.85
48	A3	318	BCR	C24-C23-C22	-3.04	121.73	126.23
45	AA	817	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
45	BA	809	CLA	C3B-C4B-NB	-3.04	107.82	110.53
45	B5	609	CLA	C4A-NA-C1A	3.04	108.07	106.68
51	BB	850	DGD	C2G-O2G-C1B	-3.04	110.52	117.80
45	AA	807	CLA	O2D-CGD-O1D	-3.04	117.93	123.85
55	A4	316	XAT	C26-C27-C28	-3.04	119.57	125.99
45	AB	818	CLA	CHB-C4A-NA	3.04	128.78	124.40
48	AA	852	BCR	C37-C22-C21	-3.04	117.90	122.82
48	BB	803	BCR	C40-C30-C25	-3.04	105.48	110.24
48	B2	617	BCR	C38-C26-C25	-3.04	121.17	124.48
48	B2	617	BCR	C37-C22-C23	3.03	122.72	118.09
45	AA	841	CLA	CHB-C4A-NA	3.03	128.78	124.40
48	B2	617	BCR	C33-C5-C4	-3.03	107.14	113.60
45	BB	822	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
48	BB	803	BCR	C12-C13-C14	-3.03	114.24	119.01
45	AA	822	CLA	O2D-CGD-CBD	3.03	116.53	111.23
45	BB	813	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
45	BA	822	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
45	AA	834	CLA	C4-C3-C5	3.03	120.48	115.23
45	AL	305	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
48	BA	848	BCR	C38-C26-C25	-3.02	121.19	124.48
45	AB	815	CLA	C3B-C4B-NB	-3.02	107.84	110.53
45	BA	806	CLA	CHB-C4A-NA	3.01	128.75	124.40
45	BA	815	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
55	A6	616	XAT	C20-C13-C12	3.01	122.69	118.09
48	AB	849	BCR	C36-C18-C19	3.01	122.68	118.09
48	BK	204	BCR	C4-C5-C6	-3.01	118.64	122.70
48	BJ	103	BCR	C19-C18-C17	-3.00	114.28	119.01
48	BB	846	BCR	C38-C26-C27	3.00	120.00	113.60
45	AH	201	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
45	AB	829	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
45	A4	303	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
45	AA	820	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
45	BB	820	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
48	AA	852	BCR	C24-C23-C22	-3.00	121.80	126.23
47	F	801	LHG	O8-C23-C24	2.99	120.97	111.83
48	AA	845	BCR	C37-C22-C23	2.99	122.66	118.09
48	BA	849	BCR	C37-C22-C23	2.99	122.66	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BA	847	BCR	C38-C26-C27	2.99	119.97	113.60
45	AA	804	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
45	BB	829	CLA	CHB-C4A-NA	2.99	128.71	124.40
48	A3	318	BCR	C37-C22-C23	2.99	122.65	118.09
48	AA	846	BCR	C35-C13-C12	2.98	122.65	118.09
47	BA	845	LHG	O7-C7-C8	2.98	117.93	111.48
52	B2	615	LUT	C28-C29-C30	-2.98	114.32	119.01
45	AB	826	CLA	C4A-NA-C1A	2.98	108.04	106.68
48	A6	617	BCR	C1-C6-C5	-2.98	118.57	122.64
48	B2	617	BCR	C31-C1-C6	2.97	114.91	110.24
45	BB	836	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
45	B5	610	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
45	A1	313	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
48	BB	848	BCR	C15-C16-C17	-2.97	117.44	123.52
55	A1	318	XAT	C12-C13-C14	-2.97	114.34	119.01
45	B2	602	CLA	CAC-C3C-C4C	2.97	128.65	124.79
48	B3	317	BCR	C15-C16-C17	-2.97	117.44	123.52
48	BA	856	BCR	C15-C16-C17	-2.97	117.44	123.52
54	B2	605	CHL	O1D-CGD-CBD	-2.97	120.22	124.72
48	B5	616	BCR	C33-C5-C4	2.97	119.92	113.60
47	AA	844	LHG	O7-C7-C8	2.97	117.90	111.48
45	BA	806	CLA	C3B-C4B-NB	-2.97	107.88	110.53
54	A4	305	CHL	O1D-CGD-CBD	-2.97	120.23	124.72
56	e	301	SQD	O5-C5-C4	2.96	115.04	109.70
48	BL	305	BCR	C1-C6-C5	-2.96	118.59	122.64
48	AA	846	BCR	C31-C1-C6	-2.96	105.60	110.24
45	AA	805	CLA	CAA-C2A-C1A	-2.96	102.27	111.97
52	B5	614	LUT	C35-C15-C14	-2.96	117.46	123.52
45	B1	305	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
48	AJ	101	BCR	C16-C15-C14	-2.96	117.46	123.52
48	B5	616	BCR	C12-C13-C14	-2.96	114.36	119.01
45	B2	611	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
52	B2	615	LUT	C1-C6-C5	-2.95	118.60	122.64
45	BB	821	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
45	AA	806	CLA	CHB-C4A-NA	2.95	128.66	124.40
45	B2	602	CLA	C3B-C4B-NB	-2.95	107.89	110.53
48	B3	317	BCR	C33-C5-C4	2.95	119.89	113.60
45	AB	820	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
54	A6	608	CHL	O2A-CGA-CBA	2.95	120.83	111.83
48	BB	848	BCR	C30-C25-C26	-2.95	118.61	122.64
46	AA	843	PQN	C12-C11-C3	-2.95	104.82	112.08
48	AA	847	BCR	C32-C1-C6	-2.95	105.62	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	803	CLA	O2D-CGD-CBD	2.95	116.38	111.23
52	B3	315	LUT	C37-C21-C22	-2.94	103.92	109.41
48	BA	848	BCR	C8-C9-C10	-2.94	114.38	119.01
48	A4	317	BCR	C15-C16-C17	-2.94	117.50	123.52
45	AF	803	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
48	BA	851	BCR	C31-C1-C6	-2.94	105.63	110.24
45	A1	306	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
45	BA	825	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
48	AJ	103	BCR	C34-C9-C8	2.94	122.58	118.09
48	A6	617	BCR	C1-C6-C7	2.94	123.62	115.65
48	AB	844	BCR	C40-C30-C25	-2.94	105.64	110.24
48	BJ	103	BCR	C7-C8-C9	-2.94	121.89	126.23
45	BB	815	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
52	A4	315	LUT	C28-C29-C30	-2.93	114.40	119.01
45	AB	814	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
45	AB	824	CLA	CBA-CAA-C2A	2.93	120.10	114.05
48	BJ	103	BCR	C30-C25-C26	-2.93	118.63	122.64
45	BA	802	CLA	CMB-C2B-C1B	-2.93	120.96	125.42
48	AB	846	BCR	C8-C9-C10	2.93	123.61	119.01
45	BJ	102	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
45	BB	812	CLA	CAA-C2A-C3A	-2.93	105.09	113.00
55	B2	616	XAT	C38-C25-C26	-2.92	117.49	122.30
45	AA	831	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
52	A1	317	LUT	C1-C6-C5	-2.92	118.64	122.64
48	A4	317	BCR	C1-C6-C7	2.92	123.58	115.65
48	AB	848	BCR	C28-C27-C26	-2.92	108.84	114.06
48	AB	844	BCR	C16-C15-C14	-2.92	117.54	123.52
45	BA	811	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
52	B5	614	LUT	C8-C9-C10	-2.92	114.42	119.01
47	a	501	LHG	O8-C23-C24	2.92	120.73	111.83
45	AK	202	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
45	BA	824	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
45	AB	828	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
45	AK	203	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
45	AA	812	CLA	C4-C3-C5	2.91	120.28	115.23
45	A1	316	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
48	BJ	103	BCR	C31-C1-C6	2.91	114.81	110.24
45	AB	801	CLA	O2D-CGD-CBD	2.91	116.32	111.23
48	BA	849	BCR	C3-C4-C5	-2.91	108.86	114.06
45	A6	604	CLA	C3B-C4B-NB	-2.91	107.93	110.53
45	BB	833	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
54	A6	606	CHL	CAC-C3C-C4C	2.91	129.97	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A6	616	XAT	C10-C11-C12	-2.91	114.77	123.20
45	BB	804	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
45	BB	838	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
48	BA	856	BCR	C37-C22-C21	-2.91	118.10	122.82
45	AB	823	CLA	CHB-C4A-NA	2.91	128.60	124.40
45	AB	820	CLA	C4A-NA-C1A	2.91	108.01	106.68
45	A1	307	CLA	O2D-CGD-CBD	2.91	116.31	111.23
47	AJ	104	LHG	O8-C23-C24	2.91	120.69	111.83
48	BG	203	BCR	C38-C26-C27	2.90	119.79	113.60
52	B5	614	LUT	C40-C33-C32	2.90	122.52	118.09
45	BA	831	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
48	BK	204	BCR	C28-C27-C26	-2.90	108.88	114.06
45	B5	608	CLA	C3B-C4B-NB	-2.90	107.94	110.53
45	BA	827	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
55	B3	316	XAT	C36-C21-C22	-2.90	103.87	108.97
53	A1	321	LMG	C8-O7-C10	-2.90	110.86	117.80
45	AB	829	CLA	C3B-C4B-NB	-2.90	107.94	110.53
48	B2	617	BCR	C34-C9-C8	2.90	122.51	118.09
48	BJ	103	BCR	C16-C15-C14	-2.90	117.59	123.52
48	BA	849	BCR	C16-C15-C14	-2.90	117.59	123.52
45	BB	806	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
45	AB	801	CLA	C1-O2A-CGA	2.89	123.65	116.65
45	AB	841	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
48	BJ	103	BCR	C15-C16-C17	-2.89	117.60	123.52
45	AB	832	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
55	A1	318	XAT	O24-C25-C38	2.89	118.28	115.05
48	AB	849	BCR	C23-C24-C25	2.89	134.72	127.00
45	BA	829	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
48	AA	849	BCR	C20-C21-C22	-2.89	123.23	127.28
45	B3	308	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
45	B1	306	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
52	B3	315	LUT	C8-C9-C10	-2.89	114.47	119.01
45	B2	610	CLA	CGD-CBD-CAD	2.89	120.19	110.85
55	A6	616	XAT	C12-C13-C14	-2.89	114.47	119.01
54	A6	602	CHL	CMA-C3A-C4A	-2.89	108.39	114.61
45	BA	807	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
45	B5	602	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
48	B5	616	BCR	C36-C18-C19	2.88	122.49	118.09
52	A1	317	LUT	C21-C26-C27	-2.88	109.51	112.83
45	AA	809	CLA	CHB-C4A-NA	2.88	128.56	124.40
45	BB	809	CLA	O2D-CGD-CBD	2.88	116.26	111.23
48	A6	617	BCR	C27-C26-C25	-2.88	118.81	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BB	842	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
45	AB	802	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
45	AA	828	CLA	C14-C13-C15	2.88	121.52	111.27
48	BB	848	BCR	C23-C22-C21	-2.87	114.49	119.01
48	BB	847	BCR	C1-C6-C5	-2.87	118.71	122.64
53	AG	202	LMG	O8-C28-C29	2.87	120.60	111.83
48	BJ	101	BCR	C37-C22-C23	2.87	122.47	118.09
45	A4	302	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
45	B5	608	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
48	BF	304	BCR	C33-C5-C6	-2.87	121.36	124.48
45	A3	306	CLA	CMB-C2B-C3B	2.86	131.15	123.53
55	B1	317	XAT	C12-C13-C14	-2.86	114.50	119.01
48	AA	848	BCR	C7-C8-C9	-2.86	122.00	126.23
45	BB	801	CLA	CAA-C2A-C1A	-2.86	102.59	111.97
45	AB	842	CLA	C3B-C4B-NB	-2.86	107.97	110.53
45	B1	307	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
48	AJ	101	BCR	C8-C9-C10	-2.86	114.51	119.01
45	A3	306	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
48	BI	101	BCR	C32-C1-C6	2.86	114.72	110.24
45	B5	604	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
54	A4	305	CHL	C4C-C3C-C2C	-2.86	102.08	113.37
45	B2	609	CLA	CHB-C4A-NA	2.86	128.52	124.40
45	AA	801	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
55	A4	316	XAT	C18-C5-C6	-2.86	117.60	122.30
47	B3	318	LHG	O8-C23-C24	2.86	120.54	111.83
48	AA	848	BCR	C23-C22-C21	-2.86	114.52	119.01
45	B1	311	CLA	CHB-C4A-NA	2.86	128.52	124.40
45	B5	613	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
45	BB	826	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
48	B3	317	BCR	C23-C22-C21	-2.85	114.52	119.01
52	A6	615	LUT	C1-C6-C5	-2.85	118.74	122.64
45	BA	835	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
48	A3	318	BCR	C36-C18-C19	2.85	122.44	118.09
45	BB	837	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
56	e	301	SQD	O6-C1-C2	2.85	112.60	108.27
55	B3	316	XAT	C12-C13-C14	-2.85	114.53	119.01
48	AA	846	BCR	C40-C30-C25	-2.84	105.78	110.24
45	BB	816	CLA	C3B-C4B-NB	-2.84	107.99	110.53
45	BA	816	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
45	BA	826	CLA	C3B-C4B-NB	-2.84	107.99	110.53
55	A3	317	XAT	C8-C9-C10	-2.84	114.54	119.01
48	B3	317	BCR	C36-C18-C19	2.84	122.43	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BB	834	CLA	CHB-C4A-NA	2.84	128.50	124.40
45	AJ	102	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
48	AB	847	BCR	C15-C16-C17	-2.84	117.70	123.52
48	BK	204	BCR	C34-C9-C8	2.84	122.43	118.09
45	AB	834	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
52	A1	317	LUT	C39-C29-C28	2.84	122.43	118.09
45	AB	824	CLA	C3B-C4B-NB	-2.84	108.00	110.53
54	B2	607	CHL	CBC-CAC-C3C	-2.84	108.81	112.87
48	AA	847	BCR	C7-C6-C5	2.84	128.09	121.56
54	A1	303	CHL	O2A-CGA-O1A	-2.84	116.53	123.63
45	A6	613	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
48	BA	850	BCR	C23-C22-C21	-2.84	114.55	119.01
48	AB	849	BCR	C16-C17-C18	-2.84	123.30	127.28
45	AB	821	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
45	AG	204	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
50	AA	851	LMU	C3B-C4B-C5B	2.84	115.37	110.23
45	B1	311	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
52	A1	317	LUT	C28-C29-C30	-2.83	114.55	119.01
45	BB	812	CLA	C3B-C4B-NB	-2.83	108.00	110.53
45	BG	202	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
47	B5	618	LHG	C5-O7-C7	-2.83	111.02	117.80
48	AF	801	BCR	C16-C15-C14	-2.83	117.72	123.52
45	AA	824	CLA	C6-C5-C3	2.83	120.37	113.47
45	AB	805	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
48	B3	317	BCR	C1-C6-C7	2.83	123.33	115.65
45	AA	826	CLA	C3B-C4B-NB	-2.83	108.00	110.53
45	B1	310	CLA	CMA-C3A-C2A	-2.83	109.74	116.23
45	A6	614	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
54	A6	607	CHL	CBC-CAC-C3C	-2.83	108.82	112.87
48	AB	848	BCR	C1-C6-C5	-2.83	118.78	122.64
45	BA	838	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
48	AB	845	BCR	C38-C26-C25	2.82	127.56	124.48
45	AA	813	CLA	CHB-C4A-NA	2.82	128.47	124.40
48	AK	204	BCR	C40-C30-C25	-2.82	105.82	110.24
45	AB	807	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
48	AG	205	BCR	C37-C22-C23	2.82	122.40	118.09
54	A6	606	CHL	OMC-CMC-C2C	-2.82	120.22	125.12
45	A3	309	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
54	A6	608	CHL	C4C-C3C-C2C	-2.82	102.24	113.37
52	A3	316	LUT	C40-C33-C32	2.82	122.39	118.09
48	AA	845	BCR	C16-C15-C14	-2.82	117.76	123.52
54	A3	307	CHL	CBC-CAC-C3C	-2.82	108.84	112.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BF	303	CLA	CAA-C2A-C3A	-2.82	109.77	116.23
56	e	301	SQD	O9-S-C6	2.81	110.96	106.76
45	AB	827	CLA	CHB-C4A-NA	2.81	128.46	124.40
52	B2	615	LUT	C15-C35-C34	-2.81	117.76	123.52
45	B2	612	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
45	A4	302	CLA	CAB-C3B-C2B	2.81	131.00	123.53
45	BB	817	CLA	O2D-CGD-O1D	-2.81	117.70	124.08
45	AA	818	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
45	A1	315	CLA	CAB-C3B-C2B	2.81	131.00	123.53
45	BB	819	CLA	O2A-CGA-O1A	-2.81	116.61	123.63
45	BA	802	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
48	BJ	103	BCR	C27-C26-C25	-2.81	118.91	122.70
45	AB	820	CLA	C3B-C4B-NB	-2.81	108.03	110.53
45	B5	609	CLA	O2D-CGD-O1D	-2.81	118.39	123.85
48	B5	616	BCR	C16-C15-C14	-2.80	117.78	123.52
45	AA	802	CLA	CMB-C2B-C1B	-2.80	121.15	125.42
52	B2	615	LUT	C8-C7-C6	-2.80	119.51	127.00
48	BL	301	BCR	C2-C1-C6	-2.80	106.37	110.44
48	AB	845	BCR	C30-C25-C26	-2.80	118.81	122.64
48	AB	849	BCR	C30-C25-C26	-2.80	118.81	122.64
45	AA	804	CLA	CHB-C4A-NA	2.80	128.44	124.40
45	AB	831	CLA	C3B-C4B-NB	-2.80	108.03	110.53
52	A6	615	LUT	C28-C29-C30	-2.80	114.61	119.01
45	A3	312	CLA	O2D-CGD-O1D	-2.80	117.73	124.08
45	BB	805	CLA	C3B-C4B-NB	-2.80	108.03	110.53
45	BA	836	CLA	O2D-CGD-CBD	2.80	116.12	111.23
45	A3	302	CLA	C6-C5-C3	2.80	120.28	113.47
48	AI	101	BCR	C30-C25-C26	-2.80	118.81	122.64
48	BF	304	BCR	C34-C9-C8	2.80	122.36	118.09
45	A1	310	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
45	BB	805	CLA	CAC-C3C-C4C	2.79	128.43	124.79
52	A4	315	LUT	C40-C33-C32	2.79	122.36	118.09
45	BL	302	CLA	CHB-C4A-NA	2.79	128.43	124.40
48	B3	317	BCR	C20-C21-C22	-2.79	123.36	127.28
45	A1	304	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
45	AB	833	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
45	AB	823	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
48	A1	319	BCR	C33-C5-C4	2.79	119.54	113.60
45	A6	603	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
45	AA	838	CLA	C3B-C4B-NB	-2.79	108.04	110.53
48	BB	847	BCR	C23-C22-C21	2.79	123.39	119.01
45	BB	805	CLA	CMC-C2C-C1C	-2.78	120.68	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	801	CLA	C4A-NA-C1A	2.78	107.95	106.68
45	BB	821	CLA	C3B-C4B-NB	-2.78	108.05	110.53
48	AJ	103	BCR	C7-C6-C5	2.78	127.97	121.56
45	AA	810	CLA	CBD-CHA-C1A	2.78	132.74	127.58
45	AB	825	CLA	CHB-C4A-NA	2.78	128.41	124.40
45	BB	826	CLA	CHB-C4A-NA	2.78	128.41	124.40
45	B3	303	CLA	CMB-C2B-C3B	2.78	130.92	123.53
48	BA	855	BCR	C36-C18-C19	2.78	122.33	118.09
45	A6	610	CLA	CHB-C4A-NA	2.78	128.41	124.40
52	A4	315	LUT	C37-C21-C22	-2.78	104.23	109.41
45	AA	825	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
45	AA	809	CLA	C2A-C1A-CHA	2.78	128.69	123.87
48	AI	101	BCR	C16-C15-C14	-2.78	117.84	123.52
45	AA	806	CLA	C3B-C4B-NB	-2.78	108.05	110.53
48	BB	846	BCR	C28-C27-C26	-2.78	109.11	114.06
48	AI	101	BCR	C20-C21-C22	-2.78	123.39	127.28
48	AB	848	BCR	C8-C7-C6	-2.77	119.59	127.00
45	BB	829	CLA	C3B-C4B-NB	-2.77	108.05	110.53
45	AB	815	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
45	B3	305	CLA	CMB-C2B-C3B	2.77	130.89	123.53
45	AB	811	CLA	O1D-CGD-CBD	2.77	129.98	124.52
48	B2	617	BCR	C1-C6-C5	-2.77	118.85	122.64
45	A1	315	CLA	O2D-CGD-O1D	-2.77	117.80	124.08
52	B3	315	LUT	C32-C33-C34	-2.77	114.66	119.01
48	AA	849	BCR	C23-C22-C21	-2.77	114.66	119.01
45	AB	842	CLA	C6-C5-C3	2.77	120.21	113.47
45	BK	201	CLA	CMB-C2B-C3B	2.77	130.88	123.53
45	AB	836	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
45	B3	305	CLA	CAB-C3B-C2B	2.76	130.88	123.53
45	AB	811	CLA	C3B-C4B-NB	-2.76	108.06	110.53
45	BA	818	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
55	B3	316	XAT	C26-C27-C28	-2.76	120.15	125.99
55	B5	615	XAT	C38-C25-C26	-2.76	117.76	122.30
48	BI	101	BCR	C24-C23-C22	-2.76	122.15	126.23
48	AB	848	BCR	C37-C22-C23	2.76	122.30	118.09
48	B5	616	BCR	C8-C9-C10	-2.76	114.67	119.01
48	BL	306	BCR	C7-C8-C9	-2.76	122.16	126.23
48	AL	306	BCR	C37-C22-C23	2.76	122.30	118.09
54	B2	601	CHL	O1D-CGD-CBD	-2.76	120.54	124.72
48	AB	845	BCR	C16-C15-C14	-2.76	117.88	123.52
45	BK	201	CLA	CAB-C3B-C2B	2.76	130.86	123.53
56	e	301	SQD	O8-S-C6	2.76	111.29	105.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A4	312	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
45	AB	822	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
45	A1	316	CLA	CAB-C3B-C2B	2.75	130.85	123.53
54	A4	314	CHL	CBC-CAC-C3C	-2.75	108.93	112.87
47	AJ	104	LHG	O7-C7-C8	2.75	117.44	111.48
48	AA	847	BCR	C35-C13-C12	2.75	122.29	118.09
48	BK	204	BCR	C1-C6-C7	2.75	123.11	115.65
45	A3	302	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
45	BA	830	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
45	BA	838	CLA	C3B-C4B-NB	-2.75	108.08	110.53
45	BB	819	CLA	CHB-C4A-NA	2.75	128.36	124.40
45	AG	204	CLA	CHB-C4A-NA	2.74	128.36	124.40
48	BK	204	BCR	C36-C18-C17	-2.74	118.37	122.82
45	A4	309	CLA	CHB-C4A-NA	2.74	128.36	124.40
47	B5	618	LHG	O8-C23-C24	2.74	120.19	111.83
48	AB	844	BCR	C31-C1-C6	2.74	114.54	110.24
45	A1	307	CLA	CAC-C3C-C4C	2.74	128.35	124.79
48	BB	849	BCR	C8-C7-C6	-2.74	119.68	127.00
45	A4	307	CLA	C3B-C4B-NB	-2.74	108.09	110.53
50	AB	853	LMU	C2'-C3'-C4'	2.73	115.89	109.68
48	BA	849	BCR	C4-C5-C6	-2.73	119.01	122.70
45	AK	201	CLA	CAA-C2A-C3A	-2.73	109.96	116.23
45	AB	810	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
48	BA	847	BCR	C1-C6-C5	-2.73	118.90	122.64
45	B1	313	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
45	A4	303	CLA	CAB-C3B-C2B	2.73	130.79	123.53
45	AA	802	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
45	BA	839	CLA	O2D-CGD-CBD	2.73	116.00	111.23
52	AF	806	LUT	C26-C27-C28	-2.73	120.34	124.58
45	B5	609	CLA	CHB-C4A-NA	2.73	128.33	124.40
48	BA	850	BCR	C16-C15-C14	-2.72	117.94	123.52
48	AA	846	BCR	C36-C18-C17	-2.72	118.40	122.82
48	A3	318	BCR	C23-C22-C21	-2.72	114.73	119.01
45	A4	303	CLA	CMB-C2B-C3B	2.72	130.76	123.53
48	A4	317	BCR	C12-C13-C14	-2.72	114.73	119.01
45	A3	306	CLA	CAB-C3B-C2B	2.72	130.76	123.53
51	AB	851	DGD	O1G-C1A-C2A	2.72	120.13	111.83
52	B5	614	LUT	C28-C29-C30	-2.72	114.73	119.01
45	AA	832	CLA	C3B-C4B-NB	-2.72	108.10	110.53
52	B3	315	LUT	C7-C8-C9	-2.72	122.22	126.23
45	A3	311	CLA	CHB-C4A-NA	2.72	128.32	124.40
45	BA	801	CLA	C1D-ND-C4D	-2.72	104.41	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A6	603	CLA	CHB-C4A-NA	2.71	128.32	124.40
45	BA	813	CLA	CHB-C4A-NA	2.71	128.32	124.40
52	AF	806	LUT	C1-C6-C5	-2.71	118.93	122.64
45	B5	601	CLA	C3B-C4B-NB	-2.71	108.11	110.53
45	BB	816	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
55	B2	616	XAT	C26-C27-C28	-2.71	120.26	125.99
45	BA	805	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
45	BL	302	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
54	A3	307	CHL	C4C-C3C-C2C	-2.71	102.67	113.37
45	BB	802	CLA	O2A-CGA-O1A	-2.71	116.85	123.63
48	AF	805	BCR	C12-C13-C14	2.71	123.27	119.01
45	BL	303	CLA	O2D-CGD-CBD	2.71	115.97	111.23
48	BB	848	BCR	C40-C30-C25	-2.71	106.00	110.24
48	AL	306	BCR	C3-C4-C5	-2.71	109.23	114.06
54	A4	306	CHL	CAC-C3C-C4C	2.71	130.99	124.03
45	A6	603	CLA	CAC-C3C-C4C	2.71	128.31	124.79
45	AB	816	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
45	AF	804	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
47	A1	320	LHG	O8-C23-C24	2.71	120.08	111.83
45	BA	803	CLA	CAC-C3C-C4C	2.71	128.31	124.79
53	B5	617	LMG	O8-C28-C29	2.71	120.08	111.83
45	B2	609	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
48	BF	304	BCR	C38-C26-C25	-2.71	121.53	124.48
47	B2	618	LHG	O8-C23-C24	2.70	120.08	111.83
45	BB	822	CLA	CHB-C4A-NA	2.70	128.30	124.40
48	A1	319	BCR	C23-C22-C21	-2.70	114.75	119.01
48	BA	849	BCR	C24-C23-C22	-2.70	122.23	126.23
45	AA	805	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
55	B1	317	XAT	C36-C21-C22	-2.70	104.22	108.97
48	BG	203	BCR	C23-C22-C21	2.70	123.26	119.01
48	AA	848	BCR	C40-C30-C25	-2.70	106.00	110.24
45	AA	837	CLA	CHB-C4A-NA	2.70	128.30	124.40
45	BK	203	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
45	A1	311	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
45	B1	304	CLA	CAC-C3C-C4C	2.70	128.30	124.79
46	BB	844	PQN	O4-C4-C5	-2.70	117.26	121.57
45	AL	303	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
45	A1	305	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
45	A1	314	CLA	O2D-CGD-O1D	-2.70	117.96	124.08
45	BB	815	CLA	CBC-CAC-C3C	2.70	119.73	112.42
48	AF	801	BCR	C8-C9-C10	-2.70	114.77	119.01
54	B2	601	CHL	O2A-CGA-O1A	-2.70	116.89	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A1	307	CLA	C3A-C2A-C1A	-2.70	103.54	106.30
45	B5	603	CLA	O2D-CGD-O1D	-2.69	118.60	123.85
45	A6	609	CLA	O2D-CGD-O1D	-2.69	118.61	123.85
54	B3	306	CHL	CBC-CAC-C3C	-2.69	109.02	112.87
45	B1	315	CLA	CAB-C3B-C2B	2.69	130.69	123.53
54	B2	606	CHL	CMA-C3A-C4A	-2.69	108.81	114.61
45	AA	834	CLA	CHB-C4A-NA	2.69	128.28	124.40
45	AB	827	CLA	C3B-C4B-NB	-2.69	108.13	110.53
48	AI	102	BCR	C31-C1-C6	2.69	114.46	110.24
45	B1	315	CLA	CMB-C2B-C3B	2.69	130.68	123.53
50	AL	301	LMU	O5B-C5B-C4B	2.69	114.54	109.70
45	BA	801	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
48	BB	848	BCR	C19-C18-C17	-2.69	114.78	119.01
48	AB	847	BCR	C39-C30-C25	-2.69	106.03	110.24
48	BJ	103	BCR	C3-C4-C5	-2.69	109.26	114.06
48	A6	617	BCR	C2-C3-C4	-2.69	105.37	111.28
45	A3	315	CLA	O2D-CGD-O1D	-2.69	117.99	124.08
48	AJ	103	BCR	C3-C4-C5	-2.69	109.27	114.06
45	AB	840	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
45	A6	610	CLA	C3B-C4B-NB	-2.69	108.13	110.53
48	AB	844	BCR	C36-C18-C19	2.68	122.19	118.09
48	BB	847	BCR	C32-C1-C6	-2.68	106.03	110.24
48	AI	101	BCR	C38-C26-C27	2.68	119.31	113.60
45	BA	802	CLA	CMB-C2B-C3B	2.68	132.86	126.55
45	AA	823	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
45	AA	808	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
45	AA	814	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
45	BL	303	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
45	A4	301	CLA	C3B-C4B-NB	-2.68	108.14	110.53
45	B5	603	CLA	CAB-C3B-C2B	2.68	130.66	123.53
55	A4	316	XAT	C8-C9-C10	-2.68	114.79	119.01
45	AB	818	CLA	C3B-C4B-NB	-2.68	108.14	110.53
48	BA	848	BCR	C12-C13-C14	-2.68	114.80	119.01
45	AA	840	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
48	BA	855	BCR	C12-C13-C14	-2.68	114.80	119.01
48	BB	846	BCR	C8-C9-C10	2.68	123.22	119.01
54	A4	304	CHL	O2D-CGD-CBD	2.68	120.47	113.90
45	B3	310	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
45	AB	837	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
45	B5	611	CLA	CHB-C4A-NA	2.68	128.26	124.40
48	BA	849	BCR	C36-C18-C17	-2.68	118.48	122.82
48	AB	848	BCR	C20-C21-C22	-2.67	123.53	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	824	CLA	CHB-C4A-NA	2.67	128.26	124.40
45	AG	203	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
45	B3	310	CLA	CHB-C4A-NA	2.67	128.26	124.40
48	AA	846	BCR	C30-C25-C26	-2.67	118.98	122.64
45	BB	801	CLA	O1D-CGD-CBD	2.67	129.79	124.52
48	BA	855	BCR	C24-C25-C26	2.67	127.70	121.56
48	AB	844	BCR	C8-C9-C10	-2.67	114.81	119.01
45	AB	826	CLA	O2D-CGD-O1D	-2.67	118.65	123.85
45	A1	309	CLA	O2D-CGD-O1D	-2.67	118.03	124.08
45	BB	813	CLA	CMB-C2B-C3B	2.67	130.62	123.53
48	AF	801	BCR	C24-C25-C26	2.67	127.70	121.56
45	BB	824	CLA	CHB-C4A-NA	2.67	128.25	124.40
45	AB	808	CLA	O2D-CGD-CBD	2.67	115.89	111.23
45	BB	815	CLA	C3B-C4B-NB	-2.66	108.15	110.53
45	AB	829	CLA	C4A-NA-C1A	2.66	107.89	106.68
45	BA	823	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
45	AA	834	CLA	C6-C5-C3	2.66	119.95	113.47
48	BA	855	BCR	C29-C28-C27	-2.66	105.43	111.28
45	BA	808	CLA	O2A-CGA-O1A	-2.66	116.98	123.63
45	B1	309	CLA	O2D-CGD-O1D	-2.66	118.05	124.08
45	A3	303	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
45	AA	840	CLA	CHB-C4A-NA	2.66	128.24	124.40
47	B2	618	LHG	O7-C7-C8	2.66	117.23	111.48
53	A4	318	LMG	O7-C10-O9	-2.66	117.49	123.70
45	AA	802	CLA	CMB-C2B-C3B	2.66	132.80	126.55
47	A1	320	LHG	O7-C7-C8	2.66	117.23	111.48
45	AB	809	CLA	O2D-CGD-CBD	2.66	115.87	111.23
54	B3	306	CHL	C4C-C3C-C2C	-2.66	102.88	113.37
45	AA	803	CLA	CAC-C3C-C4C	2.66	128.25	124.79
52	B1	316	LUT	C20-C13-C14	-2.65	118.52	122.82
48	AB	848	BCR	C15-C14-C13	-2.65	123.56	127.28
48	BB	845	BCR	C16-C15-C14	-2.65	118.09	123.52
45	AB	825	CLA	C3B-C4B-NB	-2.65	108.16	110.53
45	A6	611	CLA	CGD-CBD-CAD	2.65	119.43	110.85
48	AA	849	BCR	C24-C23-C22	-2.65	122.31	126.23
45	BB	832	CLA	C3B-C4B-NB	-2.65	108.16	110.53
45	B2	604	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
46	BA	843	PQN	C21-C22-C23	-2.65	107.17	115.97
52	B2	615	LUT	C8-C9-C10	-2.65	114.85	119.01
45	AA	818	CLA	C3B-C4B-NB	-2.65	108.17	110.53
45	AA	827	CLA	C3B-C4B-NB	-2.65	108.17	110.53
54	B2	601	CHL	C1A-CHA-CBD	2.65	139.14	132.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	830	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
50	AB	850	LMU	C3B-C4B-C5B	2.65	115.03	110.23
55	A3	317	XAT	C10-C11-C12	-2.65	115.54	123.20
45	AB	824	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
45	A6	611	CLA	C1A-CHA-C4D	-2.64	122.03	125.69
52	A3	316	LUT	C3-C4-C5	-2.64	105.59	112.18
54	A4	314	CHL	O2D-CGD-CBD	2.64	120.39	113.90
45	A6	610	CLA	C6-C5-C3	2.64	119.91	113.47
54	A3	307	CHL	O1D-CGD-CBD	-2.64	120.72	124.72
45	AB	804	CLA	CBC-CAC-C3C	2.64	119.58	112.42
45	A1	313	CLA	CHB-C4A-NA	2.64	128.21	124.40
50	AL	301	LMU	O1B-C4'-C3'	2.64	113.95	107.23
48	AA	846	BCR	C20-C21-C22	-2.64	123.57	127.28
48	AB	846	BCR	C33-C5-C4	2.64	119.23	113.60
45	BB	838	CLA	CHB-C4A-NA	2.64	128.21	124.40
48	BL	306	BCR	C36-C18-C19	-2.64	114.05	118.09
48	AK	204	BCR	C27-C26-C25	-2.64	119.14	122.70
55	B3	316	XAT	C24-C23-C22	-2.64	105.85	110.79
45	BA	826	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
45	AB	835	CLA	CHB-C4A-NA	2.64	128.21	124.40
45	BB	828	CLA	CHB-C4A-NA	2.64	128.21	124.40
48	BJ	103	BCR	C12-C13-C14	-2.64	114.86	119.01
52	B2	615	LUT	C32-C33-C34	-2.64	114.86	119.01
48	B2	617	BCR	C7-C6-C5	2.64	127.63	121.56
54	B5	605	CHL	O2D-CGD-CBD	2.64	120.37	113.90
45	AF	802	CLA	CHB-C4A-NA	2.64	128.20	124.40
45	BB	811	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
45	BB	801	CLA	C1-O2A-CGA	2.63	123.03	116.65
45	BA	805	CLA	CMC-C2C-C1C	-2.63	120.92	125.03
48	BA	851	BCR	C39-C30-C25	-2.63	106.11	110.24
45	B2	608	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
45	B2	609	CLA	C3B-C4B-NB	-2.63	108.18	110.53
48	BI	101	BCR	C12-C13-C14	-2.63	114.87	119.01
47	BA	845	LHG	O8-C23-C24	2.63	119.86	111.83
45	BA	827	CLA	C3B-C4B-NB	-2.63	108.18	110.53
45	BF	303	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
52	B1	316	LUT	C40-C33-C34	-2.63	118.55	122.82
45	AB	804	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
45	B5	601	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
45	AA	819	CLA	CHB-C4A-NA	2.63	128.19	124.40
52	B3	315	LUT	C12-C13-C14	-2.63	114.87	119.01
45	AH	201	CLA	C4-C3-C5	2.63	119.79	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BB	831	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
45	A4	311	CLA	O2D-CGD-O1D	-2.63	118.12	124.08
45	AA	824	CLA	O2D-CGD-O1D	-2.63	118.12	124.08
45	A6	603	CLA	C3B-C4B-NB	-2.63	108.19	110.53
45	BB	818	CLA	C3B-C4B-NB	-2.63	108.19	110.53
48	B2	617	BCR	C29-C30-C25	2.62	114.25	110.44
48	B5	616	BCR	C1-C6-C7	2.62	122.77	115.65
45	BA	828	CLA	CAA-CBA-CGA	-2.62	105.75	113.21
45	BA	837	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
52	B2	615	LUT	C19-C9-C8	2.62	122.10	118.09
55	B5	615	XAT	C8-C9-C10	-2.62	114.89	119.01
54	A6	607	CHL	CAC-C3C-C4C	2.62	130.77	124.03
45	BL	302	CLA	C3B-C4B-NB	-2.62	108.19	110.53
45	AB	812	CLA	CAB-C3B-C2B	2.62	130.50	123.53
48	B3	317	BCR	C19-C18-C17	-2.62	114.89	119.01
45	A6	612	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
45	B1	304	CLA	O1D-CGD-CBD	2.62	129.68	124.52
48	A6	617	BCR	C23-C22-C21	-2.62	114.89	119.01
48	AL	306	BCR	C1-C6-C5	-2.62	119.06	122.64
48	BA	851	BCR	C3-C4-C5	-2.62	109.39	114.06
45	A6	604	CLA	O2D-CGD-O1D	-2.62	118.15	124.08
45	B5	611	CLA	O2D-CGD-O1D	-2.62	118.15	124.08
54	B5	606	CHL	CMD-C2D-C3D	2.62	129.91	124.68
45	B1	315	CLA	O2D-CGD-O1D	-2.61	118.15	124.08
45	BB	841	CLA	C3B-C4B-NB	-2.61	108.20	110.53
45	BA	812	CLA	O2A-CGA-O1A	-2.61	117.09	123.63
48	BJ	101	BCR	C36-C18-C19	2.61	122.08	118.09
45	B1	312	CLA	CAB-C3B-C2B	2.61	130.48	123.53
48	AJ	103	BCR	C19-C18-C17	-2.61	114.90	119.01
45	AA	838	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
45	AA	835	CLA	O2D-CGD-O1D	-2.61	118.15	124.08
54	A4	306	CHL	CBC-CAC-C3C	-2.61	109.13	112.87
48	BA	848	BCR	C15-C16-C17	-2.61	118.18	123.52
45	A4	311	CLA	C3B-C4B-NB	-2.61	108.20	110.53
48	AA	846	BCR	C8-C9-C10	-2.61	114.90	119.01
48	AF	805	BCR	C23-C22-C21	-2.61	114.90	119.01
45	AA	805	CLA	CMC-C2C-C1C	-2.61	120.96	125.03
54	A6	602	CHL	O2D-CGD-CBD	2.61	120.30	113.90
45	BB	838	CLA	C1-C2-C3	-2.61	122.54	126.76
48	B2	617	BCR	C38-C26-C27	2.61	119.16	113.60
48	AA	847	BCR	C3-C4-C5	-2.61	109.41	114.06
45	BA	813	CLA	O2D-CGD-O1D	-2.61	118.77	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	829	CLA	CHB-C4A-NA	2.61	128.16	124.40
45	BA	840	CLA	CHB-C4A-NA	2.61	128.16	124.40
45	AB	804	CLA	C3B-C4B-NB	-2.61	108.20	110.53
54	B1	303	CHL	CBC-CAC-C3C	-2.61	109.14	112.87
45	A4	302	CLA	CAC-C3C-C4C	2.61	128.18	124.79
54	A4	305	CHL	CMD-C2D-C3D	2.60	129.88	124.68
45	B1	315	CLA	CMA-C3A-C2A	-2.60	110.26	116.23
48	BL	305	BCR	C15-C16-C17	-2.60	118.20	123.52
48	BB	803	BCR	C3-C4-C5	-2.60	109.42	114.06
45	BB	823	CLA	CHB-C4A-NA	2.60	128.15	124.40
48	BA	848	BCR	C35-C13-C12	2.60	122.06	118.09
47	B1	302	LHG	O8-C23-C24	2.60	119.76	111.83
48	AA	847	BCR	C8-C9-C10	-2.60	114.92	119.01
55	B3	316	XAT	C8-C9-C10	-2.60	114.92	119.01
45	BB	825	CLA	C3B-C4B-NB	-2.60	108.21	110.53
56	e	301	SQD	O48-C23-C24	2.60	119.75	111.83
45	A1	310	CLA	CAB-C3B-C2B	2.60	130.44	123.53
45	A3	313	CLA	O2D-CGD-O1D	-2.60	118.19	124.08
45	B2	613	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
45	AA	840	CLA	O2A-CGA-O1A	-2.60	117.13	123.63
45	BF	301	CLA	CBD-CHA-C1A	2.60	132.39	127.58
45	B1	313	CLA	CHB-C4A-NA	2.60	128.15	124.40
45	BB	808	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
45	AA	833	CLA	C4-C3-C2	-2.59	116.96	123.63
48	AI	101	BCR	C15-C16-C17	-2.59	118.21	123.52
52	B1	316	LUT	C32-C33-C34	2.59	123.09	119.01
45	A4	310	CLA	CHB-C4A-NA	2.59	128.14	124.40
45	AL	304	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
45	A3	304	CLA	CMB-C2B-C3B	2.59	130.42	123.53
45	A1	305	CLA	C5-C3-C2	2.59	126.99	121.17
45	B3	314	CLA	O2D-CGD-O1D	-2.59	118.20	124.08
45	A1	314	CLA	CHB-C4A-NA	2.59	128.14	124.40
45	BA	821	CLA	C4-C3-C5	2.59	119.73	115.23
45	B3	303	CLA	CAB-C3B-C2B	2.59	130.42	123.53
48	BA	855	BCR	C30-C25-C26	-2.59	119.09	122.64
45	A1	311	CLA	CHB-C4A-NA	2.59	128.14	124.40
45	A4	308	CLA	CHB-C4A-NA	2.59	128.14	124.40
45	BA	828	CLA	C11-C10-C8	2.59	124.58	115.97
48	BJ	101	BCR	C30-C25-C26	-2.59	119.10	122.64
45	BB	816	CLA	CHB-C4A-NA	2.59	128.14	124.40
52	A1	317	LUT	C37-C21-C36	2.59	111.64	107.87
48	BJ	103	BCR	C7-C6-C5	2.59	127.52	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	842	CLA	CHB-C4A-NA	2.59	128.13	124.40
45	BA	824	CLA	CBA-CAA-C2A	2.59	121.49	113.79
45	BA	819	CLA	CHB-C4A-NA	2.59	128.13	124.40
50	AB	850	LMU	O5B-C5B-C4B	2.59	114.36	109.70
45	AL	305	CLA	CHB-C4A-NA	2.59	128.13	124.40
48	AJ	103	BCR	C38-C26-C25	-2.59	121.66	124.48
54	A4	306	CHL	OMC-CMC-C2C	-2.59	120.63	125.12
45	AB	801	CLA	CMD-C2D-C3D	2.58	133.62	127.69
45	BL	303	CLA	C3B-C4B-NB	-2.58	108.22	110.53
45	BA	809	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
45	BA	808	CLA	CHB-C4A-NA	2.58	128.13	124.40
45	BF	302	CLA	CHB-C4A-NA	2.58	128.13	124.40
45	B1	310	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
48	AF	805	BCR	C33-C5-C6	-2.58	121.67	124.48
45	A3	305	CLA	O2D-CGD-O1D	-2.58	118.22	124.08
53	A1	321	LMG	O8-C28-C29	2.58	119.71	111.83
48	AA	848	BCR	C31-C1-C6	-2.58	106.20	110.24
45	BA	814	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
55	A1	318	XAT	C26-C27-C28	-2.58	120.54	125.99
45	B3	308	CLA	CMA-C3A-C2A	-2.58	110.31	116.23
45	AA	828	CLA	CHB-C4A-NA	2.58	128.12	124.40
48	A3	318	BCR	C30-C25-C24	2.58	122.64	115.65
45	A1	315	CLA	CMB-C2B-C3B	2.58	130.38	123.53
45	BB	839	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
54	B5	605	CHL	C4C-C3C-C2C	-2.58	102.49	108.42
45	BB	810	CLA	C3B-C4B-NB	-2.58	108.23	110.53
45	B5	609	CLA	C3B-C4B-NB	-2.58	108.23	110.53
54	A6	607	CHL	O1D-CGD-CBD	-2.58	120.82	124.72
48	AA	852	BCR	C36-C18-C17	-2.57	118.65	122.82
48	AK	204	BCR	C36-C18-C19	2.57	122.02	118.09
45	AB	829	CLA	CMB-C2B-C1B	-2.57	121.50	125.42
45	BB	808	CLA	CHB-C4A-NA	2.57	128.11	124.40
45	AB	812	CLA	CMB-C2B-C3B	2.57	130.36	123.53
45	BA	808	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
45	A3	309	CLA	CHB-C4A-NA	2.57	128.11	124.40
45	AB	827	CLA	O2D-CGD-CBD	2.57	115.72	111.23
45	AA	803	CLA	C1-C2-C3	-2.57	121.99	126.20
48	AF	801	BCR	C37-C22-C21	-2.57	118.66	122.82
47	A1	302	LHG	O8-C23-C24	2.57	119.66	111.83
48	BA	849	BCR	C33-C5-C4	2.57	119.07	113.60
45	AB	802	CLA	CHB-C4A-NA	2.57	128.10	124.40
45	B5	603	CLA	CHB-C4A-NA	2.57	128.10	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	A4	315	LUT	C1-C6-C5	-2.56	119.13	122.64
45	BB	813	CLA	CAB-C3B-C2B	2.56	130.35	123.53
48	BB	848	BCR	C23-C24-C25	-2.56	120.15	127.00
48	AF	801	BCR	C12-C13-C14	-2.56	114.98	119.01
45	AA	817	CLA	C4-C3-C2	-2.56	117.05	123.63
54	B1	303	CHL	O2D-CGD-CBD	2.56	120.18	113.90
45	B5	604	CLA	CMB-C2B-C3B	2.56	130.34	123.53
55	B5	615	XAT	C26-C27-C28	-2.56	120.58	125.99
45	B5	604	CLA	CAB-C3B-C2B	2.56	130.34	123.53
45	AL	305	CLA	O2D-CGD-CBD	2.56	115.70	111.23
45	AA	827	CLA	CHB-C4A-NA	2.56	128.09	124.40
45	BB	819	CLA	C3B-C4B-NB	-2.56	108.25	110.53
48	B3	317	BCR	C29-C30-C25	2.56	114.15	110.44
48	AA	848	BCR	C15-C16-C17	-2.56	118.29	123.52
48	A1	319	BCR	C23-C24-C25	-2.56	120.17	127.00
48	AI	101	BCR	C34-C9-C8	2.56	121.99	118.09
45	AL	304	CLA	CBA-CAA-C2A	2.55	121.39	113.79
54	B5	605	CHL	CAC-C3C-C4C	2.55	129.33	124.73
48	AI	102	BCR	C39-C30-C25	2.55	114.25	110.24
48	BF	304	BCR	C12-C13-C14	2.55	123.03	119.01
47	BA	845	LHG	C5-O7-C7	-2.55	111.69	117.80
48	BB	845	BCR	C15-C16-C17	-2.55	118.30	123.52
48	AA	845	BCR	C7-C8-C9	-2.55	122.46	126.23
45	BL	302	CLA	O1A-CGA-CBA	2.55	131.19	123.09
52	B1	316	LUT	C35-C15-C14	2.55	128.74	123.52
48	BA	851	BCR	C4-C5-C6	-2.55	119.26	122.70
45	AA	839	CLA	O2D-CGD-CBD	2.55	115.69	111.23
48	B5	616	BCR	C27-C26-C25	-2.55	119.26	122.70
45	BB	820	CLA	CHB-C4A-NA	2.55	128.08	124.40
48	AB	847	BCR	C38-C26-C27	2.55	119.03	113.60
45	BA	814	CLA	C3B-C4B-NB	-2.55	108.25	110.53
55	B3	316	XAT	C4-C3-C2	-2.55	106.02	110.79
45	A4	307	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
45	B1	312	CLA	O2D-CGD-O1D	-2.55	118.30	124.08
45	B2	603	CLA	O2D-CGD-O1D	-2.55	118.30	124.08
48	AB	844	BCR	C24-C23-C22	-2.55	122.47	126.23
45	BB	842	CLA	CAC-C3C-C4C	2.55	128.10	124.79
54	B2	614	CHL	O2D-CGD-O1D	-2.55	118.89	123.85
45	BB	807	CLA	CHB-C4A-NA	2.55	128.07	124.40
48	AJ	101	BCR	C37-C22-C21	-2.54	118.69	122.82
48	AA	847	BCR	C27-C26-C25	-2.54	119.27	122.70
45	AA	841	CLA	C3B-C4B-NB	-2.54	108.26	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BJ	101	BCR	C2-C1-C6	2.54	114.13	110.44
45	B1	312	CLA	CMB-C2B-C3B	2.54	130.29	123.53
45	B2	602	CLA	C1-C2-C3	-2.54	122.03	126.20
56	BJ	104	SQD	O48-C23-C24	2.54	119.59	111.83
45	AA	812	CLA	CHB-C4A-NA	2.54	128.07	124.40
48	AB	844	BCR	C15-C16-C17	-2.54	118.32	123.52
48	BA	855	BCR	C8-C7-C6	-2.54	120.21	127.00
54	A1	303	CHL	O2D-CGD-CBD	2.54	120.13	113.90
45	AB	811	CLA	CHB-C4A-NA	2.54	128.06	124.40
45	AA	837	CLA	O2D-CGD-CBD	2.54	115.67	111.23
52	B1	316	LUT	C39-C29-C28	2.54	121.97	118.09
48	AL	302	BCR	C30-C25-C26	-2.54	119.17	122.64
48	AJ	101	BCR	C30-C25-C26	-2.54	119.17	122.64
45	A1	307	CLA	CHB-C4A-NA	2.54	128.06	124.40
45	B3	312	CLA	O2D-CGD-O1D	-2.54	118.33	124.08
45	BB	843	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
45	AB	831	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
48	AA	846	BCR	C1-C6-C5	-2.53	119.17	122.64
45	BB	808	CLA	C3B-C4B-NB	-2.53	108.27	110.53
45	AA	815	CLA	CHB-C4A-NA	2.53	128.06	124.40
45	BA	812	CLA	CHB-C4A-NA	2.53	128.06	124.40
48	A1	319	BCR	C15-C16-C17	-2.53	118.34	123.52
45	A6	601	CLA	CHB-C4A-NA	2.53	128.05	124.40
48	A6	617	BCR	C29-C30-C25	2.53	114.11	110.44
45	AB	838	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
48	BA	849	BCR	C31-C1-C6	-2.53	106.28	110.24
45	AA	814	CLA	C3B-C4B-NB	-2.53	108.27	110.53
48	AB	847	BCR	C30-C25-C26	-2.53	119.18	122.64
45	B1	307	CLA	C3B-C4B-NB	-2.53	108.27	110.53
45	A3	315	CLA	C3B-C4B-NB	-2.53	108.28	110.53
54	A1	308	CHL	O2D-CGD-CBD	2.53	120.09	113.90
45	A4	313	CLA	CHB-C4A-NA	2.53	128.04	124.40
45	A6	610	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
54	A6	606	CHL	O2D-CGD-O1D	-2.52	118.94	123.85
48	BA	855	BCR	C2-C3-C4	-2.52	105.73	111.28
45	AA	831	CLA	C3B-C4B-NB	-2.52	108.28	110.53
48	AB	845	BCR	C19-C18-C17	-2.52	115.04	119.01
48	AB	849	BCR	C29-C30-C25	2.52	114.10	110.44
45	BB	810	CLA	CBA-CAA-C2A	2.52	121.30	113.79
48	BL	301	BCR	C38-C26-C27	2.52	118.97	113.60
45	A3	312	CLA	C4-C3-C5	2.52	119.61	115.23
45	BL	304	CLA	O2D-CGD-CBD	2.52	115.64	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	834	CLA	CHB-C4A-NA	2.52	128.04	124.40
48	B2	617	BCR	C16-C15-C14	-2.52	118.36	123.52
45	BL	302	CLA	O2A-CGA-O1A	-2.52	116.85	123.33
48	B5	616	BCR	C29-C30-C25	2.52	114.10	110.44
48	AA	846	BCR	C38-C26-C27	2.52	118.97	113.60
53	A1	321	LMG	C7-O1-C1	2.52	119.20	113.80
54	B5	606	CHL	O1D-CGD-CBD	-2.52	120.90	124.72
45	A3	304	CLA	O2D-CGD-O1D	-2.52	118.37	124.08
48	AF	805	BCR	C29-C28-C27	-2.52	105.74	111.28
48	AI	102	BCR	C2-C3-C4	-2.52	105.74	111.28
48	BB	848	BCR	C2-C1-C6	2.52	114.10	110.44
45	AB	826	CLA	C3B-C4B-NB	-2.52	108.28	110.53
45	BB	817	CLA	CHB-C4A-NA	2.52	128.03	124.40
55	A1	318	XAT	C10-C11-C12	-2.52	115.91	123.20
52	A6	615	LUT	C39-C29-C28	2.52	121.93	118.09
45	B3	304	CLA	O2D-CGD-O1D	-2.52	118.37	124.08
45	A1	307	CLA	C3B-C4B-NB	-2.52	108.28	110.53
45	B2	612	CLA	CMB-C2B-C1B	-2.52	121.59	125.42
45	BA	816	CLA	CAC-C3C-C4C	2.52	128.06	124.79
45	AB	817	CLA	C3B-C4B-NB	-2.52	108.28	110.53
45	B3	311	CLA	O2D-CGD-O1D	-2.52	118.37	124.08
45	AA	815	CLA	O2D-CGD-CBD	2.52	115.63	111.23
48	AB	848	BCR	C34-C9-C8	2.52	121.93	118.09
54	B2	606	CHL	CAC-C3C-C4C	2.51	130.49	124.03
45	AA	834	CLA	CMC-C2C-C1C	-2.51	121.11	125.03
45	AB	806	CLA	CMC-C2C-C1C	-2.51	121.11	125.03
48	BK	204	BCR	C16-C15-C14	-2.51	118.38	123.52
54	A6	608	CHL	CAC-C3C-C4C	2.51	130.49	124.03
45	AH	201	CLA	CHB-C4A-NA	2.51	128.03	124.40
45	BB	813	CLA	CHB-C4A-NA	2.51	128.03	124.40
52	A3	316	LUT	C8-C7-C6	-2.51	120.29	127.00
48	AG	205	BCR	C16-C15-C14	-2.51	118.38	123.52
48	AJ	103	BCR	C10-C11-C12	-2.51	115.92	123.20
55	B3	316	XAT	C10-C11-C12	-2.51	115.93	123.20
45	B2	609	CLA	C6-C5-C3	2.51	119.58	113.47
55	A3	317	XAT	C36-C21-C22	-2.51	104.57	108.97
48	AA	852	BCR	C29-C30-C25	2.51	114.08	110.44
45	B3	309	CLA	O2D-CGD-O1D	-2.50	118.40	124.08
45	BA	837	CLA	CHB-C4A-NA	2.50	128.01	124.40
45	BK	203	CLA	CHB-C4A-NA	2.50	128.01	124.40
52	A3	316	LUT	C28-C29-C30	-2.50	115.07	119.01
48	AA	852	BCR	C40-C30-C25	-2.50	106.32	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A1	310	CLA	CHB-C4A-NA	2.50	128.01	124.40
48	BJ	103	BCR	C10-C11-C12	-2.50	115.95	123.20
45	B3	302	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
45	B2	612	CLA	CHB-C4A-NA	2.50	128.01	124.40
54	B1	308	CHL	O2D-CGD-CBD	2.50	120.03	113.90
45	A3	304	CLA	CHB-C4A-NA	2.50	128.01	124.40
45	AA	823	CLA	CAA-C2A-C3A	-2.50	110.50	116.23
45	BB	832	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
45	B2	612	CLA	O2A-CGA-O1A	-2.50	117.38	123.63
48	BA	851	BCR	C38-C26-C25	-2.50	121.76	124.48
48	B5	616	BCR	C15-C16-C17	-2.50	118.41	123.52
52	AF	806	LUT	C32-C33-C34	-2.50	115.08	119.01
45	BF	301	CLA	C6-C5-C3	2.50	119.55	113.47
45	B3	303	CLA	O2D-CGD-O1D	-2.50	118.42	124.08
48	A3	318	BCR	C33-C5-C6	-2.49	121.76	124.48
48	AB	849	BCR	C2-C1-C6	2.49	114.06	110.44
45	BG	201	CLA	C3B-C4B-NB	-2.49	108.30	110.53
46	BA	843	PQN	C14-C13-C12	-2.49	117.23	123.63
45	AK	203	CLA	CHB-C4A-NA	2.49	128.00	124.40
45	A1	305	CLA	CHB-C4A-NA	2.49	127.99	124.40
48	AB	848	BCR	C19-C18-C17	-2.49	115.09	119.01
48	A6	617	BCR	C4-C5-C6	-2.49	119.34	122.70
45	BB	811	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
48	AL	302	BCR	C19-C18-C17	-2.49	115.09	119.01
45	AF	803	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	A3	302	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	BA	841	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	BB	805	CLA	CMD-C2D-C3D	2.49	133.40	127.69
54	A6	608	CHL	C1A-CHA-CBD	2.49	138.73	132.36
45	AB	824	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	AB	838	CLA	C3B-C4B-NB	-2.49	108.31	110.53
48	BB	803	BCR	C24-C25-C26	2.49	127.28	121.56
54	B2	606	CHL	C1A-CHA-CBD	2.49	138.73	132.36
45	BB	812	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	A6	611	CLA	CAB-C3B-C2B	2.49	130.14	123.53
45	AA	813	CLA	C3B-C4B-NB	-2.49	108.31	110.53
45	A3	305	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	B5	608	CLA	CHB-C4A-NA	2.49	127.99	124.40
45	B1	305	CLA	CHB-C4A-NA	2.48	127.99	124.40
48	B5	616	BCR	C21-C20-C19	-2.48	116.00	123.20
45	BL	303	CLA	CHB-C4A-NA	2.48	127.98	124.40
48	AA	848	BCR	C38-C26-C27	2.48	118.89	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	840	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
45	A4	301	CLA	CHB-C4A-NA	2.48	127.98	124.40
45	BA	808	CLA	C3B-C4B-NB	-2.48	108.31	110.53
45	BA	832	CLA	C3B-C4B-NB	-2.48	108.32	110.53
45	B5	601	CLA	CHB-C4A-NA	2.48	127.98	124.40
45	BA	803	CLA	C1-C2-C3	-2.48	122.13	126.20
48	AG	205	BCR	C2-C1-C6	2.48	114.04	110.44
45	AB	810	CLA	CHB-C4A-NA	2.48	127.98	124.40
48	AA	846	BCR	C37-C22-C23	2.48	121.88	118.09
54	B5	607	CHL	C4C-C3C-C2C	-2.48	102.71	108.42
45	BA	839	CLA	CHB-C4A-NA	2.48	127.98	124.40
45	BB	835	CLA	C3B-C4B-NB	-2.48	108.32	110.53
45	BA	812	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
45	BA	834	CLA	O2D-CGD-CBD	2.48	115.56	111.23
45	AA	837	CLA	C3B-C4B-NB	-2.48	108.32	110.53
45	BA	821	CLA	C3B-C4B-NB	-2.48	108.32	110.53
45	AB	807	CLA	CHB-C4A-NA	2.48	127.97	124.40
54	A4	304	CHL	C1B-CHB-C4A	-2.48	119.73	121.32
54	A6	606	CHL	C4C-C3C-C2C	-2.48	102.72	108.42
45	A4	301	CLA	CAC-C3C-C4C	2.47	128.01	124.79
48	BB	846	BCR	C37-C22-C21	-2.47	118.81	122.82
48	AG	205	BCR	C20-C21-C22	-2.47	123.81	127.28
48	BB	848	BCR	C32-C1-C6	-2.47	106.36	110.24
45	BB	833	CLA	CMB-C2B-C1B	-2.47	121.65	125.42
50	AL	301	LMU	C1B-O5B-C5B	2.47	118.55	113.72
45	BA	836	CLA	CHB-C4A-NA	2.47	127.97	124.40
45	BA	831	CLA	CHB-C4A-NA	2.47	127.97	124.40
48	BG	203	BCR	C39-C30-C25	-2.47	106.37	110.24
48	AA	847	BCR	C37-C22-C23	2.47	121.86	118.09
45	BA	817	CLA	CHB-C4A-NA	2.47	127.96	124.40
48	AB	848	BCR	C24-C23-C22	-2.47	122.58	126.23
48	BA	849	BCR	C33-C5-C6	-2.47	121.79	124.48
45	A4	310	CLA	O2D-CGD-O1D	-2.47	118.48	124.08
48	AL	306	BCR	C37-C22-C21	-2.47	118.82	122.82
45	BL	304	CLA	C3B-C4B-NB	-2.47	108.33	110.53
48	A6	617	BCR	C36-C18-C19	2.47	121.86	118.09
52	A3	316	LUT	C19-C9-C8	2.47	121.86	118.09
55	A3	317	XAT	C24-C23-C22	-2.47	106.18	110.79
48	BL	301	BCR	C8-C9-C10	2.47	122.89	119.01
45	B1	310	CLA	CAB-C3B-C2B	2.47	130.09	123.53
54	B1	303	CHL	O2A-CGA-O1A	-2.47	117.46	123.63
48	BA	851	BCR	C30-C25-C26	-2.47	119.27	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	A6	616	XAT	C38-C25-C26	-2.46	118.25	122.30
45	BA	832	CLA	CHB-C4A-NA	2.46	127.96	124.40
45	BB	818	CLA	CHB-C4A-NA	2.46	127.96	124.40
45	AA	841	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
45	BB	833	CLA	CHB-C4A-NA	2.46	127.95	124.40
48	BA	847	BCR	C40-C30-C25	-2.46	106.38	110.24
48	BL	306	BCR	C16-C17-C18	2.46	130.73	127.28
45	BA	838	CLA	C4-C3-C2	-2.46	117.30	123.63
45	AA	817	CLA	CHB-C4A-NA	2.46	127.95	124.40
55	A6	616	XAT	C36-C21-C26	2.46	116.69	110.05
48	AB	849	BCR	C21-C20-C19	-2.46	116.07	123.20
45	AB	812	CLA	CHB-C4A-NA	2.46	127.95	124.40
45	B3	301	CLA	C3B-C4B-NB	-2.46	108.33	110.53
47	B1	318	LHG	O8-C23-C24	2.46	119.33	111.83
48	AA	845	BCR	C16-C17-C18	-2.46	123.83	127.28
45	BB	835	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
48	AA	847	BCR	C37-C22-C21	-2.46	118.83	122.82
54	B5	607	CHL	O1D-CGD-CBD	-2.46	121.00	124.72
45	BA	829	CLA	O2A-CGA-O1A	-2.46	117.48	123.63
45	B3	307	CLA	CHB-C4A-NA	2.46	127.94	124.40
48	AF	805	BCR	C19-C18-C17	-2.46	115.15	119.01
48	AI	101	BCR	C12-C13-C14	-2.46	115.15	119.01
48	B5	616	BCR	C38-C26-C25	-2.46	121.81	124.48
48	BL	306	BCR	C23-C24-C25	-2.45	120.44	127.00
45	A6	611	CLA	CMB-C2B-C3B	2.45	130.06	123.53
45	AB	819	CLA	O2D-CGD-CBD	2.45	115.52	111.23
45	B2	610	CLA	CMB-C2B-C3B	2.45	130.05	123.53
48	AA	847	BCR	C29-C30-C25	2.45	114.00	110.44
55	A3	317	XAT	C12-C13-C14	-2.45	115.15	119.01
45	AB	804	CLA	CMD-C2D-C1D	-2.45	120.41	124.73
45	BA	827	CLA	CHB-C4A-NA	2.45	127.94	124.40
45	AB	839	CLA	O2D-CGD-CBD	2.45	115.52	111.23
54	B5	607	CHL	OMC-CMC-C2C	-2.45	120.86	125.12
45	B5	612	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
45	AG	201	CLA	O2D-CGD-O1D	-2.45	118.52	124.08
45	A1	304	CLA	CHB-C4A-NA	2.45	127.94	124.40
45	A1	312	CLA	O2D-CGD-O1D	-2.45	118.52	124.08
54	A4	305	CHL	C1A-CHA-CBD	2.45	138.63	132.36
48	B2	617	BCR	C27-C26-C25	-2.45	119.39	122.70
54	B5	607	CHL	C3D-CAD-CBD	2.45	110.83	107.61
45	BA	813	CLA	C4-C3-C5	2.45	119.48	115.23
45	AA	818	CLA	O2A-CGA-O1A	-2.45	117.50	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	815	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
45	BA	818	CLA	O2A-CGA-O1A	-2.45	117.50	123.63
54	A1	308	CHL	CAC-C3C-C4C	2.45	130.32	124.03
45	BA	814	CLA	CHB-C4A-NA	2.45	127.93	124.40
45	AB	831	CLA	CAC-C3C-C4C	2.45	127.97	124.79
48	BB	848	BCR	C21-C20-C19	-2.44	116.12	123.20
45	A3	303	CLA	CAC-C3C-C4C	2.44	127.97	124.79
45	AB	819	CLA	CHB-C4A-NA	2.44	127.93	124.40
45	AB	801	CLA	C4-C3-C5	2.44	119.47	115.23
45	B3	311	CLA	CHB-C4A-NA	2.44	127.92	124.40
45	AH	201	CLA	CAA-C2A-C3A	2.44	119.60	113.00
45	B1	306	CLA	CAA-C2A-C3A	-2.44	110.63	116.23
45	BB	820	CLA	C5-C3-C2	-2.44	115.69	121.17
52	B5	614	LUT	C37-C21-C36	2.44	111.42	107.87
48	BA	847	BCR	C28-C27-C26	-2.44	109.70	114.06
48	BB	846	BCR	C16-C15-C14	-2.44	118.53	123.52
47	AA	844	LHG	O8-C23-C24	2.44	119.27	111.83
48	AA	845	BCR	C8-C7-C6	-2.44	120.48	127.00
48	AF	801	BCR	C36-C18-C19	2.44	121.81	118.09
52	AF	806	LUT	C8-C9-C10	-2.44	115.17	119.01
54	B2	614	CHL	CMD-C2D-C3D	2.44	129.56	124.68
45	B3	303	CLA	CHB-C4A-NA	2.44	127.92	124.40
54	A6	607	CHL	CMD-C2D-C3D	2.44	129.55	124.68
48	AB	845	BCR	C24-C25-C26	2.44	127.17	121.56
55	B5	615	XAT	C4-C3-C2	-2.44	106.23	110.79
45	AA	827	CLA	O2D-CGD-CBD	2.44	115.49	111.23
45	A3	306	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	AB	828	CLA	C3B-C4B-NB	-2.43	108.36	110.53
48	BL	305	BCR	C38-C26-C27	2.43	118.78	113.60
48	AL	302	BCR	C23-C22-C21	-2.43	115.18	119.01
48	BB	846	BCR	C12-C13-C14	-2.43	115.18	119.01
45	AA	831	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	AA	833	CLA	CMD-C2D-C3D	2.43	133.27	127.69
45	BB	829	CLA	O2A-CGA-O1A	-2.43	117.54	123.63
48	AA	852	BCR	C11-C10-C9	-2.43	123.87	127.28
45	BA	834	CLA	C3B-C4B-NB	-2.43	108.36	110.53
45	BB	806	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	A4	308	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
45	BG	201	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	AB	815	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	AF	804	CLA	CHB-C4A-NA	2.43	127.91	124.40
45	B3	308	CLA	CHB-C4A-NA	2.43	127.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	830	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
48	BA	855	BCR	C19-C18-C17	-2.43	115.19	119.01
45	AK	201	CLA	CMB-C2B-C1B	-2.43	123.52	125.94
45	BA	837	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
48	AA	849	BCR	C38-C26-C25	-2.43	121.84	124.48
48	BA	848	BCR	C36-C18-C17	-2.43	118.89	122.82
45	BB	806	CLA	CAA-C2A-C3A	-2.42	110.67	116.23
48	AI	101	BCR	C28-C27-C26	-2.42	109.73	114.06
45	AL	304	CLA	CHB-C4A-NA	2.42	127.90	124.40
45	AB	819	CLA	CMB-C2B-C1B	-2.42	121.73	125.42
45	A1	309	CLA	C3B-C4B-NB	-2.42	108.37	110.53
48	BA	855	BCR	C23-C22-C21	-2.42	115.20	119.01
48	AA	846	BCR	C15-C14-C13	-2.42	123.88	127.28
45	BK	202	CLA	C3B-C4B-NB	-2.42	108.37	110.53
48	AB	844	BCR	C12-C13-C14	-2.42	115.20	119.01
45	B2	610	CLA	CAB-C3B-C2B	2.42	129.97	123.53
48	A4	317	BCR	C21-C20-C19	-2.42	116.19	123.20
48	A4	317	BCR	C2-C1-C6	-2.42	106.92	110.44
45	BJ	102	CLA	CHB-C4A-NA	2.42	127.89	124.40
45	BA	801	CLA	C3B-C4B-NB	-2.42	108.37	110.53
45	A1	310	CLA	CAA-C2A-C3A	-2.42	110.69	116.23
45	AA	806	CLA	O2D-CGD-CBD	2.42	115.46	111.23
54	A6	602	CHL	O2A-CGA-O1A	-2.42	117.58	123.63
45	AA	809	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
54	A4	304	CHL	C4C-C3C-C2C	-2.42	102.86	108.42
48	BJ	101	BCR	C30-C25-C24	2.42	122.20	115.65
52	AF	806	LUT	C38-C25-C24	-2.42	117.64	123.36
48	BB	848	BCR	C1-C6-C5	-2.42	119.33	122.64
54	B5	606	CHL	C1B-CHB-C4A	-2.42	119.77	121.32
45	AB	842	CLA	CHB-C4A-NA	2.42	127.89	124.40
45	AB	817	CLA	CHB-C4A-NA	2.41	127.89	124.40
45	A6	604	CLA	CHB-C4A-NA	2.41	127.89	124.40
48	AB	849	BCR	C12-C13-C14	-2.41	115.21	119.01
48	AB	844	BCR	C23-C22-C21	-2.41	115.21	119.01
45	B3	307	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
45	BA	834	CLA	CHB-C4A-NA	2.41	127.88	124.40
45	A1	315	CLA	CHB-C4A-NA	2.41	127.88	124.40
48	BB	848	BCR	C38-C26-C27	2.41	118.74	113.60
45	BA	830	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
50	AB	852	LMU	C1B-O1B-C4'	-2.41	112.26	117.98
55	A3	317	XAT	C4-C3-C2	-2.41	106.28	110.79
45	BA	838	CLA	O2A-CGA-O1A	-2.41	117.59	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	B1	308	CHL	CMD-C2D-C3D	2.41	129.50	124.68
45	BB	805	CLA	C2A-C1A-CHA	2.41	128.05	123.87
52	A4	315	LUT	C35-C15-C14	-2.41	118.59	123.52
48	BL	306	BCR	C33-C5-C4	2.41	118.73	113.60
45	A1	306	CLA	O2A-CGA-O1A	-2.41	117.60	123.63
45	BA	839	CLA	C1-C2-C3	-2.41	122.25	126.20
54	A1	303	CHL	C1-O2A-CGA	2.41	122.48	116.65
45	AB	832	CLA	CHC-C4B-NB	2.41	127.66	124.05
54	B5	605	CHL	CMA-C3A-C4A	-2.41	109.42	114.61
45	B2	608	CLA	CHB-C4A-NA	2.41	127.87	124.40
48	B3	317	BCR	C24-C25-C26	2.41	127.10	121.56
45	AA	833	CLA	C3B-C4B-NB	-2.41	108.38	110.53
45	B1	305	CLA	CBC-CAC-C3C	-2.41	105.90	112.42
48	AA	847	BCR	C11-C12-C13	2.40	132.96	126.36
48	AA	849	BCR	C12-C13-C14	-2.40	115.23	119.01
45	A4	312	CLA	C3B-C4B-NB	-2.40	108.39	110.53
45	AA	805	CLA	CBA-CAA-C2A	2.40	120.94	113.79
45	BG	201	CLA	O1D-CGD-CBD	2.40	129.26	124.52
48	AB	845	BCR	C15-C16-C17	-2.40	118.60	123.52
48	B2	617	BCR	C23-C22-C21	-2.40	115.23	119.01
55	B2	616	XAT	C8-C9-C10	-2.40	115.23	119.01
45	BA	837	CLA	C3B-C4B-NB	-2.40	108.39	110.53
45	AB	809	CLA	CBA-CAA-C2A	2.40	120.94	113.79
45	AB	842	CLA	O2D-CGD-CBD	2.40	115.43	111.23
45	B1	311	CLA	C3B-C4B-NB	-2.40	108.39	110.53
45	AA	801	CLA	C1D-ND-C4D	-2.40	104.63	106.31
48	AA	845	BCR	C11-C10-C9	-2.40	123.92	127.28
54	B2	605	CHL	O2D-CGD-O1D	-2.40	119.18	123.85
45	AB	827	CLA	CMB-C2B-C1B	-2.40	121.77	125.42
45	A1	310	CLA	CMA-C3A-C2A	-2.40	110.74	116.23
48	B3	317	BCR	C39-C30-C29	2.40	118.15	108.95
54	B1	308	CHL	C1B-CHB-C4A	-2.40	119.78	121.32
45	BB	840	CLA	O2D-CGD-CBD	2.40	115.42	111.23
48	BA	856	BCR	C40-C30-C25	-2.39	106.49	110.24
54	A1	303	CHL	C3D-CAD-CBD	2.39	110.76	107.61
52	A4	315	LUT	C8-C9-C10	-2.39	115.25	119.01
48	BB	803	BCR	C29-C28-C27	-2.39	106.02	111.28
45	BA	804	CLA	CHB-C4A-NA	2.39	127.85	124.40
45	BB	834	CLA	C4-C3-C5	-2.39	111.08	115.23
48	AI	102	BCR	C38-C26-C25	2.39	127.09	124.48
45	BA	809	CLA	CHB-C4A-NA	2.39	127.85	124.40
48	B5	616	BCR	C38-C26-C27	2.39	118.69	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A1	303	CHL	C4-C3-C5	2.39	118.94	116.13
48	AA	852	BCR	C32-C1-C6	-2.39	106.49	110.24
55	B2	616	XAT	C35-C15-C14	-2.39	118.63	123.52
45	AA	819	CLA	CBA-CAA-C2A	2.39	120.90	113.79
45	AA	810	CLA	CHB-C4A-NA	2.39	127.85	124.40
48	AA	848	BCR	C19-C18-C17	-2.39	115.25	119.01
48	AJ	101	BCR	C12-C13-C14	-2.39	115.25	119.01
48	BA	847	BCR	C23-C22-C21	-2.39	115.25	119.01
48	AL	302	BCR	C8-C9-C10	2.39	122.76	119.01
45	AA	821	CLA	CMB-C2B-C3B	2.39	132.16	126.55
45	BA	813	CLA	C3B-C4B-NB	-2.38	108.40	110.53
45	AB	832	CLA	CHB-C4A-NA	2.38	127.84	124.40
45	AA	804	CLA	C3B-C4B-NB	-2.38	108.40	110.53
48	BF	304	BCR	C11-C10-C9	-2.38	123.94	127.28
55	B2	616	XAT	C19-C9-C8	2.38	121.73	118.09
45	A4	303	CLA	CHB-C4A-NA	2.38	127.84	124.40
45	B3	301	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
45	AA	835	CLA	CHB-C4A-NA	2.38	127.84	124.40
45	AB	805	CLA	CHB-C4A-NA	2.38	127.84	124.40
48	AB	847	BCR	C19-C18-C17	-2.38	115.26	119.01
45	AA	824	CLA	CHD-C1D-ND	-2.38	121.45	124.80
45	BB	826	CLA	C3B-C4B-NB	-2.38	108.41	110.53
52	B3	315	LUT	C36-C21-C26	2.38	113.15	109.55
48	BG	203	BCR	C21-C20-C19	2.38	130.09	123.20
45	BA	804	CLA	O2D-CGD-CBD	2.38	115.39	111.23
45	A3	303	CLA	C5-C3-C2	2.38	126.50	121.17
46	BB	844	PQN	C12-C11-C3	-2.38	106.22	112.08
48	BB	845	BCR	C16-C17-C18	-2.38	123.94	127.28
52	B2	615	LUT	C30-C31-C32	-2.38	116.31	123.20
45	AB	818	CLA	O2A-CGA-O1A	-2.38	117.68	123.63
45	B1	310	CLA	CMB-C2B-C3B	2.38	129.85	123.53
45	AA	829	CLA	C2D-C1D-ND	-2.38	107.77	110.13
54	B1	303	CHL	O2A-CGA-CBA	2.38	119.08	111.83
54	B3	306	CHL	O1D-CGD-CBD	-2.38	121.12	124.72
48	AA	848	BCR	C24-C25-C26	-2.38	116.08	121.56
45	BB	812	CLA	O1D-CGD-CBD	2.38	129.20	124.52
54	B2	607	CHL	CAC-C3C-C4C	2.38	130.13	124.03
55	A1	318	XAT	C20-C13-C12	2.37	121.72	118.09
52	B1	316	LUT	C12-C13-C14	2.37	122.74	119.01
48	BB	849	BCR	C15-C14-C13	-2.37	123.95	127.28
48	BA	850	BCR	C21-C20-C19	-2.37	116.32	123.20
45	AA	821	CLA	CHB-C4A-NA	2.37	127.83	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AB	845	BCR	C12-C13-C14	-2.37	115.28	119.01
45	AA	839	CLA	CHB-C4A-NA	2.37	127.82	124.40
48	AI	101	BCR	C11-C10-C9	-2.37	123.95	127.28
48	A4	317	BCR	C8-C9-C10	-2.37	115.28	119.01
45	BB	841	CLA	CHB-C4A-NA	2.37	127.82	124.40
55	B1	317	XAT	C8-C9-C10	-2.37	115.28	119.01
45	AA	820	CLA	CHB-C4A-NA	2.37	127.82	124.40
48	BB	849	BCR	C37-C22-C23	2.37	121.71	118.09
48	AB	845	BCR	C40-C30-C25	-2.37	106.53	110.24
52	B1	316	LUT	C19-C9-C8	2.37	121.71	118.09
55	A6	616	XAT	C24-C23-C22	-2.37	106.36	110.79
45	BA	816	CLA	CHB-C4A-NA	2.37	127.82	124.40
45	BF	301	CLA	CHB-C4A-NA	2.37	127.82	124.40
45	B1	312	CLA	CHB-C4A-NA	2.37	127.82	124.40
54	B1	308	CHL	C1A-CHA-CBD	2.37	138.43	132.36
48	AJ	103	BCR	C16-C15-C14	-2.37	118.67	123.52
45	B1	310	CLA	CHB-C4A-NA	2.37	127.82	124.40
48	BB	845	BCR	C19-C18-C17	-2.37	115.28	119.01
45	AA	842	CLA	C4-C3-C5	-2.37	111.12	115.23
48	BB	846	BCR	C40-C30-C25	-2.37	106.53	110.24
45	AA	826	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
45	AB	816	CLA	CHB-C4A-NA	2.37	127.81	124.40
48	BL	301	BCR	C36-C18-C17	-2.37	118.98	122.82
46	AB	843	PQN	C14-C13-C15	-2.36	111.12	115.23
45	AA	803	CLA	CHB-C4A-NA	2.36	127.81	124.40
52	A1	317	LUT	C35-C15-C14	-2.36	118.68	123.52
54	A6	602	CHL	O2D-CGD-O1D	-2.36	118.72	124.08
52	A4	315	LUT	C19-C9-C8	2.36	121.70	118.09
45	AB	829	CLA	CBA-CAA-C2A	2.36	120.82	113.79
45	AB	814	CLA	CHB-C4A-NA	2.36	127.81	124.40
48	AB	849	BCR	C7-C8-C9	-2.36	122.74	126.23
48	AB	849	BCR	C8-C9-C10	-2.36	115.30	119.01
45	B5	613	CLA	C3B-C4B-NB	-2.36	108.42	110.53
45	A4	312	CLA	CHB-C4A-NA	2.36	127.81	124.40
48	BL	305	BCR	C19-C18-C17	-2.36	115.30	119.01
45	AA	836	CLA	O2D-CGD-CBD	2.36	115.36	111.23
45	AA	836	CLA	CHB-C4A-NA	2.36	127.80	124.40
45	B3	305	CLA	CHB-C4A-NA	2.36	127.80	124.40
45	A4	311	CLA	CHB-C4A-NA	2.36	127.80	124.40
45	A1	312	CLA	CAA-C2A-C3A	-2.36	110.82	116.23
45	AB	841	CLA	O2A-CGA-O1A	-2.36	117.73	123.63
45	B5	612	CLA	CHB-C4A-NA	2.36	127.80	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	B2	602	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
48	AB	849	BCR	C29-C28-C27	-2.35	106.10	111.28
48	BJ	103	BCR	C34-C9-C8	2.35	121.68	118.09
55	A6	616	XAT	C19-C9-C8	2.35	121.68	118.09
48	AJ	101	BCR	C16-C17-C18	-2.35	123.98	127.28
45	BB	828	CLA	O2D-CGD-CBD	2.35	115.34	111.23
54	B2	606	CHL	C1B-CHB-C4A	-2.35	119.81	121.32
45	BB	801	CLA	C3B-C4B-NB	-2.35	108.43	110.53
45	BB	834	CLA	O2D-CGD-CBD	2.35	115.34	111.23
54	B2	606	CHL	CED-O2D-CGD	2.35	121.24	115.92
48	A1	319	BCR	C8-C9-C10	-2.35	115.31	119.01
45	BL	302	CLA	CBA-CAA-C2A	2.35	120.78	113.79
45	A6	605	CLA	CHB-C4A-NA	2.35	127.79	124.40
45	BA	810	CLA	CHB-C4A-NA	2.35	127.79	124.40
48	AI	101	BCR	C32-C1-C6	2.35	113.92	110.24
45	A1	305	CLA	CBC-CAC-C3C	-2.35	106.06	112.42
45	BK	202	CLA	CHB-C4A-NA	2.35	127.79	124.40
48	A6	617	BCR	C8-C9-C10	-2.35	115.32	119.01
45	BA	829	CLA	O2D-CGD-CBD	2.34	115.33	111.23
45	A1	307	CLA	C2A-C1A-CHA	2.34	126.35	122.71
45	B1	305	CLA	C5-C3-C2	2.34	126.43	121.17
47	A3	319	LHG	O8-C23-C24	2.34	118.98	111.83
48	B3	317	BCR	C38-C26-C27	2.34	118.59	113.60
45	BB	814	CLA	CHB-C4A-NA	2.34	127.78	124.40
45	BA	831	CLA	CAC-C3C-C4C	2.34	127.84	124.79
48	AB	849	BCR	C2-C3-C4	-2.34	106.13	111.28
45	BB	841	CLA	CMB-C2B-C3B	2.34	132.06	126.55
45	AB	838	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
51	AB	851	DGD	O2G-C1B-O1B	-2.34	118.23	123.70
45	BA	820	CLA	CHB-C4A-NA	2.34	127.78	124.40
45	AB	827	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
54	A6	602	CHL	C1-C2-C3	-2.34	122.36	126.20
48	AK	204	BCR	C36-C18-C17	-2.34	119.02	122.82
48	BK	204	BCR	C37-C22-C21	-2.34	119.02	122.82
54	A6	602	CHL	C1A-CHA-CBD	2.34	138.35	132.36
45	BA	833	CLA	C3B-C4B-NB	-2.34	108.44	110.53
45	BB	824	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
45	A6	613	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
48	BJ	103	BCR	C37-C22-C23	2.34	121.66	118.09
45	BA	828	CLA	CHB-C4A-NA	2.34	127.78	124.40
45	A1	310	CLA	CMB-C2B-C3B	2.34	129.75	123.53
48	BA	856	BCR	C24-C23-C22	-2.34	122.78	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	821	CLA	CHB-C4A-NA	2.34	127.77	124.40
45	AB	837	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
45	AB	827	CLA	CAA-C2A-C3A	-2.34	106.68	113.00
45	BA	815	CLA	CHB-C4A-NA	2.34	127.77	124.40
55	B1	317	XAT	C32-C33-C34	-2.34	115.33	119.01
48	AA	847	BCR	C15-C16-C17	-2.34	118.74	123.52
45	B5	603	CLA	CMB-C2B-C3B	2.34	129.74	123.53
52	A6	615	LUT	C37-C21-C22	-2.33	105.05	109.41
45	AF	803	CLA	C3B-C4B-NB	-2.33	108.45	110.53
47	BF	305	LHG	O8-C23-C24	2.33	118.95	111.83
48	AB	849	BCR	C37-C22-C21	-2.33	119.03	122.82
48	BA	847	BCR	C36-C18-C19	2.33	121.65	118.09
48	AK	204	BCR	C7-C8-C9	-2.33	122.78	126.23
45	A4	301	CLA	O2D-CGD-CBD	2.33	115.31	111.23
48	AB	845	BCR	C7-C8-C9	-2.33	122.78	126.23
52	A3	316	LUT	C15-C35-C34	-2.33	118.75	123.52
54	B5	606	CHL	CAC-C3C-C4C	2.33	128.93	124.73
45	A6	601	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
55	B2	616	XAT	C32-C33-C34	-2.33	115.34	119.01
54	A1	303	CHL	CBC-CAC-C3C	-2.33	109.54	112.87
45	B2	611	CLA	C3B-C4B-NB	-2.33	108.45	110.53
45	BA	811	CLA	CHB-C4A-NA	2.33	127.76	124.40
45	BA	818	CLA	CHB-C4A-NA	2.33	127.76	124.40
48	BB	803	BCR	C16-C17-C18	-2.33	124.01	127.28
48	BB	845	BCR	C37-C22-C23	2.33	121.64	118.09
45	A6	609	CLA	CHB-C4A-NA	2.33	127.76	124.40
45	BB	830	CLA	CBA-CAA-C2A	2.33	120.72	113.79
45	BA	829	CLA	C2D-C1D-ND	-2.33	107.82	110.13
45	BB	807	CLA	O2A-CGA-O1A	-2.33	117.81	123.63
48	BB	803	BCR	C8-C9-C10	-2.33	115.35	119.01
55	B3	316	XAT	C36-C21-C26	2.33	116.33	110.05
48	BB	803	BCR	C19-C18-C17	-2.33	115.35	119.01
47	A3	301	LHG	O8-C23-C24	2.33	118.92	111.83
45	BA	821	CLA	O2D-CGD-CBD	2.33	115.30	111.23
45	A3	312	CLA	CHB-C4A-NA	2.32	127.75	124.40
48	BA	849	BCR	C40-C30-C25	-2.32	106.60	110.24
45	BF	303	CLA	CHB-C4A-NA	2.32	127.75	124.40
54	A6	602	CHL	C4-C3-C5	2.32	119.26	115.23
45	A3	309	CLA	CMA-C3A-C2A	-2.32	110.90	116.23
48	AB	844	BCR	C35-C13-C12	2.32	121.64	118.09
52	A1	317	LUT	C8-C9-C10	-2.32	115.36	119.01
45	AB	823	CLA	CHD-C1D-ND	-2.32	121.53	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
55	B2	616	XAT	C18-C5-C6	-2.32	118.48	122.30
48	BI	101	BCR	C3-C4-C5	-2.32	109.92	114.06
54	A1	303	CHL	C1A-CHA-CBD	2.32	138.31	132.36
55	B2	616	XAT	C24-C23-C22	-2.32	106.45	110.79
48	A6	617	BCR	C15-C16-C17	-2.32	118.77	123.52
45	BB	810	CLA	O2D-CGD-CBD	2.32	115.29	111.23
48	BA	848	BCR	C16-C15-C14	-2.32	118.77	123.52
48	AB	849	BCR	C33-C5-C4	2.32	118.54	113.60
54	A4	304	CHL	O2D-CGD-O1D	-2.32	118.82	124.08
48	BA	855	BCR	C23-C24-C25	2.32	133.19	127.00
45	BB	842	CLA	CHB-C4A-NA	2.32	127.75	124.40
45	AB	821	CLA	CHB-C4A-NA	2.32	127.75	124.40
55	A6	616	XAT	C36-C21-C22	-2.32	104.89	108.97
48	A4	317	BCR	C19-C18-C17	-2.32	115.36	119.01
48	B5	616	BCR	C4-C5-C6	-2.32	119.57	122.70
45	AA	829	CLA	O2A-CGA-O1A	-2.32	117.83	123.63
45	BL	303	CLA	CHD-C1D-ND	-2.32	121.54	124.80
45	BA	821	CLA	C7-C6-C5	-2.32	107.08	113.26
52	B5	614	LUT	C16-C1-C6	2.32	113.88	110.24
45	AB	801	CLA	C3B-C4B-NB	-2.32	108.46	110.53
45	BB	809	CLA	C3B-C4B-NB	-2.32	108.46	110.53
54	B1	303	CHL	OMC-CMC-C2C	-2.32	121.10	125.12
45	A3	303	CLA	CHB-C1B-NB	2.32	127.53	124.05
45	B2	609	CLA	C4-C3-C5	2.32	119.25	115.23
45	A4	309	CLA	O2D-CGD-CBD	2.32	115.28	111.23
48	AI	101	BCR	C16-C17-C18	-2.31	124.03	127.28
48	AL	302	BCR	C7-C6-C5	-2.31	116.22	121.56
45	AF	804	CLA	C3B-C4B-NB	-2.31	108.46	110.53
45	AH	201	CLA	CBA-CAA-C2A	2.31	120.68	113.79
48	AL	302	BCR	C1-C6-C7	2.31	121.93	115.65
55	A1	318	XAT	C19-C9-C8	2.31	121.62	118.09
45	AA	808	CLA	O2D-CGD-CBD	2.31	115.28	111.23
45	A3	313	CLA	CAA-C2A-C3A	-2.31	110.92	116.23
45	AB	823	CLA	CBA-CAA-C2A	2.31	120.68	113.79
45	AA	807	CLA	CHD-C1D-ND	-2.31	121.55	124.80
48	BA	848	BCR	C28-C27-C26	-2.31	109.93	114.06
45	AB	835	CLA	C3B-C4B-NB	-2.31	108.47	110.53
45	AA	824	CLA	CHB-C4A-NA	2.31	127.74	124.40
55	A4	316	XAT	C10-C11-C12	-2.31	116.50	123.20
45	AB	815	CLA	CMB-C2B-C3B	2.31	131.99	126.55
48	AL	306	BCR	C29-C30-C25	-2.31	107.08	110.44
48	B2	617	BCR	C36-C18-C17	-2.31	119.07	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	B2	613	CLA	CHD-C1D-ND	-2.31	121.55	124.80
45	B1	309	CLA	CHB-C4A-NA	2.31	127.73	124.40
55	A1	318	XAT	C36-C21-C22	-2.31	104.91	108.97
45	AB	833	CLA	CHB-C4A-NA	2.31	127.73	124.40
48	B2	617	BCR	C8-C9-C10	-2.31	115.38	119.01
48	AL	306	BCR	C35-C13-C12	2.31	121.61	118.09
47	B1	301	LHG	O8-C23-O10	-2.31	117.86	123.63
54	A4	304	CHL	C1A-CHA-CBD	2.31	138.27	132.36
45	BA	823	CLA	CHB-C4A-NA	2.31	127.73	124.40
45	AA	809	CLA	C3B-C4B-NB	-2.31	108.47	110.53
54	B2	614	CHL	C1A-CHA-CBD	2.31	138.27	132.36
45	AA	832	CLA	CHB-C4A-NA	2.31	127.73	124.40
45	AL	303	CLA	CMA-C3A-C2A	-2.31	110.94	116.23
48	AG	205	BCR	C40-C30-C25	-2.31	106.63	110.24
45	BA	805	CLA	CHB-C4A-NA	2.31	127.73	124.40
48	BA	848	BCR	C19-C18-C17	-2.31	115.38	119.01
45	A3	315	CLA	CAA-C2A-C3A	-2.31	110.94	116.23
48	BA	847	BCR	C16-C15-C14	-2.30	118.80	123.52
45	BA	804	CLA	O2A-CGA-O1A	-2.30	117.86	123.63
45	AB	815	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
45	BA	828	CLA	C3B-C4B-NB	-2.30	108.47	110.53
45	AA	840	CLA	C1-C2-C3	-2.30	122.42	126.20
55	A1	318	XAT	C35-C15-C14	-2.30	118.81	123.52
45	A1	315	CLA	CAA-C2A-C3A	-2.30	110.95	116.23
54	A4	306	CHL	C3D-CAD-CBD	2.30	110.64	107.61
45	BA	826	CLA	C1-C2-C3	-2.30	122.42	126.20
45	BL	304	CLA	CHB-C4A-NA	2.30	127.72	124.40
55	A4	316	XAT	C35-C34-C33	-2.30	124.05	127.28
52	B3	315	LUT	C28-C29-C30	-2.30	115.39	119.01
45	A6	613	CLA	CHB-C4A-NA	2.30	127.72	124.40
45	AA	835	CLA	C3B-C4B-NB	-2.30	108.48	110.53
55	A3	317	XAT	O4-C5-C6	-2.30	57.11	58.93
45	AB	828	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
45	BB	828	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
54	A1	303	CHL	OMC-CMC-C2C	-2.30	121.13	125.12
45	AA	841	CLA	CBA-CAA-C2A	2.30	120.63	113.79
52	A3	316	LUT	C1-C6-C5	-2.30	119.50	122.64
45	AA	811	CLA	CHB-C4A-NA	2.30	127.72	124.40
54	B1	303	CHL	C1A-CHA-CBD	2.30	138.25	132.36
45	AA	819	CLA	O2D-CGD-CBD	2.30	115.25	111.23
45	BA	841	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
48	BI	101	BCR	C16-C17-C18	-2.30	124.06	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AG	201	CLA	CHB-C4A-NA	2.30	127.71	124.40
48	BB	845	BCR	C20-C21-C22	-2.30	124.06	127.28
48	AJ	101	BCR	C1-C6-C5	-2.30	119.50	122.64
45	B3	307	CLA	CMB-C2B-C1B	-2.30	121.92	125.42
45	A6	612	CLA	C3B-C4B-NB	-2.30	108.48	110.53
54	B2	607	CHL	OMC-CMC-C2C	-2.30	121.14	125.12
54	B2	607	CHL	C1A-CHA-CBD	2.29	138.24	132.36
45	B3	301	CLA	CHB-C4A-NA	2.29	127.71	124.40
45	BK	201	CLA	CHB-C4A-NA	2.29	127.71	124.40
48	AI	102	BCR	C36-C18-C19	2.29	121.59	118.09
54	B2	601	CHL	O2D-CGD-O1D	-2.29	119.39	123.85
45	A3	311	CLA	O2D-CGD-CBD	2.29	115.24	111.23
45	BB	802	CLA	O2D-CGD-CBD	2.29	115.24	111.23
48	AK	204	BCR	C2-C3-C4	-2.29	106.24	111.28
48	AJ	103	BCR	C24-C23-C22	-2.29	122.85	126.23
48	BA	851	BCR	C21-C20-C19	-2.29	116.56	123.20
45	AB	802	CLA	O2D-CGD-CBD	2.29	115.23	111.23
45	BA	841	CLA	C5-C3-C2	-2.29	116.03	121.17
48	AG	205	BCR	C29-C30-C25	2.29	113.76	110.44
45	BA	804	CLA	C3B-C4B-NB	-2.29	108.49	110.53
50	AB	850	LMU	C2'-C3'-C4'	2.29	114.87	109.68
55	B5	615	XAT	C24-C23-C22	-2.29	106.51	110.79
54	A6	608	CHL	CBC-CAC-C3C	-2.29	109.60	112.87
48	BL	306	BCR	C3-C4-C5	-2.28	109.98	114.06
45	A3	310	CLA	CHB-C4A-NA	2.28	127.70	124.40
45	AA	808	CLA	CHB-C4A-NA	2.28	127.69	124.40
45	BG	202	CLA	C3B-C4B-NB	-2.28	108.49	110.53
45	B1	305	CLA	C4-C3-C2	-2.28	117.77	123.63
52	B3	315	LUT	C30-C31-C32	-2.28	116.59	123.20
45	BB	815	CLA	C7-C6-C5	2.28	119.34	113.26
45	B3	313	CLA	CHB-C4A-NA	2.28	127.69	124.40
45	A3	308	CLA	CHB-C4A-NA	2.28	127.69	124.40
45	BL	303	CLA	CBA-CAA-C2A	2.28	120.58	113.79
45	AB	817	CLA	CHD-C1D-ND	-2.28	121.59	124.80
54	B2	605	CHL	C4C-C3C-C2C	-2.28	103.17	108.42
45	AK	201	CLA	CHB-C4A-NA	2.28	127.69	124.40
45	BB	811	CLA	CMB-C2B-C3B	2.28	131.91	126.55
54	A1	308	CHL	C1A-CHA-CBD	2.28	138.20	132.36
45	AL	304	CLA	CHD-C1D-ND	-2.28	121.60	124.80
45	BB	810	CLA	CHB-C4A-NA	2.28	127.69	124.40
55	B5	615	XAT	O4-C5-C18	2.28	117.59	115.05
45	AA	821	CLA	O2D-CGD-CBD	2.28	115.21	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	AA	843	PQN	C17-C16-C15	-2.28	107.19	113.26
53	A4	318	LMG	O8-C28-C29	2.28	118.78	111.83
45	BB	805	CLA	CMD-C2D-C1D	-2.28	120.72	124.73
55	A6	616	XAT	C40-C33-C34	-2.28	119.13	122.82
45	AB	813	CLA	C3B-C4B-NB	-2.28	108.50	110.53
45	AB	809	CLA	O2A-CGA-O1A	-2.28	117.94	123.63
48	BA	856	BCR	C36-C18-C17	-2.28	119.13	122.82
45	AA	818	CLA	CHB-C4A-NA	2.27	127.68	124.40
45	AG	203	CLA	CHB-C4A-NA	2.27	127.68	124.40
54	B3	306	CHL	C1A-CHA-CBD	2.27	138.18	132.36
45	AA	834	CLA	CBC-CAC-C3C	2.27	118.58	112.42
45	A4	310	CLA	C3B-C4B-NB	-2.27	108.50	110.53
54	B5	606	CHL	C1A-CHA-CBD	2.27	138.18	132.36
45	BB	807	CLA	CMC-C2C-C1C	-2.27	121.48	125.03
54	B2	607	CHL	O1D-CGD-CBD	-2.27	121.28	124.72
48	AI	102	BCR	C15-C16-C17	-2.27	118.87	123.52
48	AB	845	BCR	C32-C1-C6	-2.27	106.68	110.24
45	A3	314	CLA	CHB-C4A-NA	2.27	127.68	124.40
45	BA	818	CLA	C3B-C4B-NB	-2.27	108.50	110.53
48	BK	204	BCR	C20-C21-C22	-2.27	124.09	127.28
45	BB	836	CLA	C3B-C4B-NB	-2.27	108.50	110.53
52	A1	317	LUT	C37-C21-C22	-2.27	105.17	109.41
53	A1	321	LMG	O4-C4-C3	-2.27	105.03	110.38
45	AA	814	CLA	O2D-CGD-CBD	2.27	115.20	111.23
45	BB	839	CLA	C3B-C4B-NB	-2.27	108.50	110.53
48	BL	305	BCR	C23-C22-C21	-2.27	115.44	119.01
45	A3	308	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
55	B5	615	XAT	C39-C29-C30	-2.27	119.14	122.82
45	B5	610	CLA	C3B-C4B-NB	-2.27	108.51	110.53
45	AB	809	CLA	CHB-C4A-NA	2.27	127.67	124.40
45	AB	820	CLA	CHB-C1B-NB	2.27	127.45	124.05
45	AB	827	CLA	CMB-C2B-C3B	2.27	131.88	126.55
45	AB	837	CLA	O2A-CGA-O1A	-2.26	117.96	123.63
54	A4	306	CHL	C1A-CHA-CBD	2.26	138.16	132.36
50	AB	850	LMU	C1'-C2'-C3'	2.26	114.77	110.01
45	BB	821	CLA	CHB-C4A-NA	2.26	127.67	124.40
45	BB	836	CLA	CHB-C4A-NA	2.26	127.67	124.40
52	B5	614	LUT	C3-C4-C5	-2.26	106.54	112.18
45	AB	811	CLA	C2A-C1A-CHA	2.26	127.79	123.87
45	AG	203	CLA	C3B-C4B-NB	-2.26	108.51	110.53
45	B3	311	CLA	C3B-C4B-NB	-2.26	108.51	110.53
48	AL	302	BCR	C2-C3-C4	-2.26	106.30	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A6	603	CLA	O1D-CGD-CBD	2.26	128.98	124.52
48	B5	616	BCR	C19-C18-C17	-2.26	115.45	119.01
48	BB	803	BCR	C10-C11-C12	-2.26	116.65	123.20
54	B1	303	CHL	O2D-CGD-O1D	-2.26	118.95	124.08
54	A4	306	CHL	O2A-CGA-CBA	2.26	121.14	114.00
45	AB	833	CLA	C3B-C4B-NB	-2.26	108.51	110.53
45	B1	309	CLA	C3B-C4B-NB	-2.26	108.51	110.53
45	AA	833	CLA	CHB-C4A-NA	2.26	127.66	124.40
45	AA	814	CLA	O2A-CGA-O1A	-2.26	117.52	123.33
48	BJ	101	BCR	C16-C15-C14	-2.26	118.89	123.52
45	AA	805	CLA	CHB-C4A-NA	2.26	127.66	124.40
45	AB	826	CLA	CHB-C4A-NA	2.26	127.66	124.40
45	A6	614	CLA	CHB-C4A-NA	2.26	127.66	124.40
45	AB	832	CLA	O2A-CGA-O1A	-2.26	117.98	123.63
45	A4	312	CLA	CHD-C1D-ND	-2.26	121.62	124.80
53	A4	318	LMG	O1-C1-C2	2.26	111.70	108.27
53	B5	617	LMG	C6-C5-C4	-2.26	107.47	113.02
45	A1	309	CLA	CHB-C4A-NA	2.26	127.66	124.40
48	BB	849	BCR	C20-C21-C22	-2.26	124.11	127.28
45	AB	804	CLA	CMD-C2D-C3D	2.26	132.87	127.69
45	A6	609	CLA	C3B-C4B-NB	-2.26	108.52	110.53
45	B5	613	CLA	CHB-C4A-NA	2.26	127.66	124.40
45	BB	824	CLA	CBA-CAA-C2A	2.26	120.51	113.79
45	AA	834	CLA	O2D-CGD-CBD	2.26	115.17	111.23
45	AB	807	CLA	CHD-C1D-ND	-2.26	121.63	124.80
45	BA	844	CLA	C3B-C4B-NB	-2.25	108.52	110.53
45	BB	830	CLA	O2D-CGD-O1D	-2.25	119.46	123.85
55	B3	316	XAT	C16-C1-C2	-2.25	105.01	108.97
45	BB	804	CLA	CHB-C4A-NA	2.25	127.65	124.40
45	BL	302	CLA	C3A-C2A-C1A	2.25	104.72	101.34
55	A4	316	XAT	C19-C9-C8	2.25	121.53	118.09
45	A1	316	CLA	CMB-C2B-C3B	2.25	129.52	123.53
45	AA	809	CLA	CHA-C1A-NA	-2.25	121.29	126.39
54	A6	608	CHL	O1D-CGD-CBD	-2.25	121.31	124.72
45	BB	802	CLA	C7-C6-C5	-2.25	107.26	113.26
48	AA	846	BCR	C19-C18-C17	-2.25	115.47	119.01
55	B2	616	XAT	C4-C3-C2	-2.25	106.58	110.79
45	BB	814	CLA	O2D-CGD-CBD	2.25	115.17	111.23
54	B5	606	CHL	CED-O2D-CGD	2.25	121.02	115.92
45	AB	805	CLA	CMA-C3A-C2A	-2.25	111.07	116.23
45	AJ	102	CLA	CHB-C4A-NA	2.25	127.65	124.40
48	AL	306	BCR	C20-C21-C22	-2.25	124.12	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	823	CLA	CAA-C2A-C3A	-2.25	111.07	116.23
45	AA	822	CLA	CHB-C4A-NA	2.25	127.64	124.40
45	A1	305	CLA	C4-C3-C2	-2.25	117.85	123.63
45	AA	833	CLA	CMD-C2D-C1D	-2.25	120.77	124.73
52	B5	614	LUT	C12-C13-C14	-2.25	115.47	119.01
50	AL	301	LMU	O5B-C1B-C2B	2.25	114.98	110.37
55	A1	318	XAT	C36-C21-C26	2.25	116.11	110.05
52	B2	615	LUT	C12-C13-C14	-2.25	115.48	119.01
45	A4	302	CLA	CHB-C4A-NA	2.25	127.64	124.40
45	AB	841	CLA	CAC-C3C-C4C	2.24	127.71	124.79
54	A4	314	CHL	C1A-CHA-CBD	2.24	138.11	132.36
45	AA	825	CLA	CMB-C2B-C1B	-2.24	122.00	125.42
48	BF	304	BCR	C33-C5-C4	2.24	118.38	113.60
54	B2	606	CHL	CMD-C2D-C3D	2.24	129.16	124.68
48	AL	302	BCR	C38-C26-C27	2.24	118.38	113.60
45	AB	825	CLA	O2D-CGD-CBD	2.24	115.15	111.23
55	A1	318	XAT	C31-C30-C29	-2.24	124.14	127.28
48	B3	317	BCR	C12-C13-C14	-2.24	115.48	119.01
48	AJ	103	BCR	C30-C25-C26	-2.24	119.57	122.64
45	AB	809	CLA	C11-C10-C8	-2.24	108.52	115.97
48	BB	846	BCR	C33-C5-C6	-2.24	122.04	124.48
45	AB	804	CLA	CHD-C4C-C3C	2.24	128.04	124.77
45	BA	826	CLA	CHB-C4A-NA	2.24	127.63	124.40
54	A4	306	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
48	AL	306	BCR	C24-C25-C26	-2.24	116.40	121.56
54	B2	607	CHL	O2D-CGD-O1D	-2.24	119.49	123.85
48	AG	205	BCR	C34-C9-C8	2.24	121.51	118.09
45	A3	304	CLA	CAB-C3B-C2B	2.24	129.48	123.53
45	BA	805	CLA	CMC-C2C-C3C	2.24	132.20	126.15
45	AA	821	CLA	C3B-C4B-NB	-2.24	108.53	110.53
45	BB	843	CLA	CHB-C4A-NA	2.24	127.63	124.40
48	BA	856	BCR	C29-C28-C27	-2.24	106.36	111.28
45	BB	828	CLA	C2A-C1A-CHA	2.23	127.75	123.87
45	B5	604	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	AA	804	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
45	A3	308	CLA	O1D-CGD-CBD	2.23	128.92	124.52
48	BA	848	BCR	C40-C30-C25	-2.23	106.74	110.24
45	AA	816	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	A3	313	CLA	CHB-C4A-NA	2.23	127.62	124.40
52	A6	615	LUT	C15-C35-C34	-2.23	118.95	123.52
45	BB	810	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
52	AF	806	LUT	C37-C21-C22	-2.23	105.25	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A4	306	CHL	CMA-C3A-C4A	-2.23	109.81	114.61
45	A4	307	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	BH	201	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	BA	825	CLA	C3B-C4B-NB	-2.23	108.54	110.53
48	B3	317	BCR	C2-C1-C6	-2.23	107.20	110.44
45	BB	841	CLA	O2D-CGD-CBD	2.23	115.13	111.23
45	BB	811	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	BB	832	CLA	CHB-C4A-NA	2.23	127.62	124.40
45	B2	613	CLA	CHB-C4A-NA	2.23	127.62	124.40
48	B5	616	BCR	C10-C11-C12	-2.23	116.74	123.20
45	AA	807	CLA	CMB-C2B-C1B	-2.23	122.03	125.42
48	BB	849	BCR	C8-C9-C10	-2.23	115.50	119.01
45	B3	314	CLA	C3B-C4B-NB	-2.23	108.54	110.53
48	A3	318	BCR	C20-C21-C22	-2.23	124.16	127.28
52	A3	316	LUT	C38-C25-C24	-2.23	118.09	123.36
48	AJ	101	BCR	C2-C3-C4	-2.23	106.38	111.28
48	AA	852	BCR	C38-C26-C25	2.23	126.91	124.48
45	BB	836	CLA	CHD-C1D-ND	-2.23	121.67	124.80
48	AB	846	BCR	C23-C22-C21	2.23	122.51	119.01
46	BB	844	PQN	O1-C1-C10	-2.23	118.01	121.57
45	AB	830	CLA	O1D-CGD-CBD	2.22	128.91	124.52
48	AL	306	BCR	C11-C10-C9	-2.22	124.16	127.28
54	B5	605	CHL	C1C-C2C-CMC	2.22	130.81	126.80
45	AB	821	CLA	C3B-C4B-NB	-2.22	108.55	110.53
55	A1	318	XAT	C37-C21-C36	-2.22	104.14	107.37
48	AB	844	BCR	C1-C6-C5	-2.22	119.60	122.64
45	AH	201	CLA	O2A-CGA-O1A	-2.22	118.07	123.63
48	BL	305	BCR	C8-C9-C10	-2.22	115.51	119.01
48	AF	805	BCR	C11-C10-C9	-2.22	124.16	127.28
45	B3	312	CLA	C3B-C4B-NB	-2.22	108.55	110.53
45	AB	825	CLA	C1-O2A-CGA	2.22	122.03	116.65
47	A1	301	LHG	O8-C23-C24	2.22	118.61	111.83
45	BA	803	CLA	CHB-C4A-NA	2.22	127.61	124.40
45	BA	842	CLA	C3B-C4B-NB	-2.22	108.55	110.53
45	AB	829	CLA	O2D-CGD-CBD	2.22	115.11	111.23
48	BA	855	BCR	C37-C22-C21	-2.22	119.22	122.82
55	A1	318	XAT	O4-C5-C18	2.22	117.53	115.05
48	AB	844	BCR	C15-C14-C13	-2.22	124.17	127.28
45	AA	830	CLA	O1D-CGD-CBD	2.22	128.90	124.52
48	BB	847	BCR	C29-C30-C25	2.22	113.66	110.44
52	A6	615	LUT	C40-C33-C32	2.22	121.48	118.09
45	A3	302	CLA	O1D-CGD-CBD	2.22	128.89	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	BA	851	BCR	C36-C18-C17	-2.22	119.22	122.82
54	A6	602	CHL	CBC-CAC-C3C	-2.22	109.70	112.87
45	A6	612	CLA	CHB-C4A-NA	2.22	127.60	124.40
45	AA	837	CLA	CMB-C2B-C3B	2.22	131.76	126.55
45	BA	809	CLA	O1D-CGD-CBD	2.22	128.89	124.52
45	BB	807	CLA	CBA-CAA-C2A	2.22	120.39	113.79
45	AA	842	CLA	CAA-CBA-CGA	-2.22	106.92	113.21
48	AK	204	BCR	C20-C21-C22	-2.21	124.17	127.28
45	AB	829	CLA	CHB-C4A-NA	2.21	127.60	124.40
48	BB	846	BCR	C7-C8-C9	-2.21	122.96	126.23
54	A1	303	CHL	O2D-CGD-O1D	-2.21	119.06	124.08
54	A4	306	CHL	O1D-CGD-CBD	-2.21	121.36	124.72
45	BB	817	CLA	CAC-C3C-C4C	2.21	127.67	124.79
55	A1	318	XAT	C24-C23-C22	-2.21	106.65	110.79
45	AB	805	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
54	A6	608	CHL	O2D-CGD-O1D	-2.21	119.54	123.85
45	A3	309	CLA	C3B-C4B-NB	-2.21	108.56	110.53
45	BB	838	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
48	BF	304	BCR	C8-C9-C10	-2.21	115.53	119.01
45	AA	805	CLA	CHD-C1D-ND	-2.21	121.69	124.80
48	A1	319	BCR	C3-C4-C5	-2.21	110.12	114.06
45	A3	315	CLA	CHB-C4A-NA	2.21	127.59	124.40
45	BB	840	CLA	CHB-C4A-NA	2.21	127.59	124.40
45	A3	314	CLA	C3B-C4B-NB	-2.21	108.56	110.53
45	BA	810	CLA	C3B-C4B-NB	-2.21	108.56	110.53
45	BA	816	CLA	C3B-C4B-NB	-2.21	108.56	110.53
45	AA	829	CLA	CHC-C4B-NB	2.21	127.36	124.05
52	A6	615	LUT	C17-C1-C6	-2.21	106.78	110.24
53	B5	617	LMG	O6-C5-C4	2.21	113.68	109.70
48	AB	846	BCR	C24-C25-C26	2.21	126.64	121.56
45	BB	824	CLA	CHD-C1D-ND	-2.21	121.70	124.80
50	BA	854	LMU	C1-O1'-C1'	2.21	117.45	113.68
48	A4	317	BCR	C23-C22-C21	-2.20	115.54	119.01
48	BB	847	BCR	C15-C16-C17	-2.20	119.01	123.52
45	AA	809	CLA	O1D-CGD-CBD	2.20	128.87	124.52
45	BB	823	CLA	O2D-CGD-O1D	-2.20	119.08	124.08
45	BA	811	CLA	C1-C2-C3	-2.20	122.59	126.20
45	AB	823	CLA	O2A-CGA-O1A	-2.20	118.12	123.63
45	BA	818	CLA	CHC-C4B-NB	2.20	127.35	124.05
52	A6	615	LUT	C19-C9-C8	2.20	121.45	118.09
45	AB	839	CLA	CHB-C4A-NA	2.20	127.58	124.40
48	AI	102	BCR	C37-C22-C21	-2.20	119.25	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A1	312	CLA	CMB-C2B-C3B	2.20	129.38	123.53
45	BB	804	CLA	O2A-CGA-O1A	-2.20	118.13	123.63
48	BA	855	BCR	C10-C11-C12	-2.20	116.83	123.20
48	AL	302	BCR	C16-C15-C14	-2.20	119.02	123.52
55	A6	616	XAT	C39-C29-C30	-2.20	119.26	122.82
45	AB	818	CLA	O2D-CGD-CBD	2.20	115.07	111.23
48	AA	846	BCR	C28-C27-C26	-2.20	110.14	114.06
48	BJ	101	BCR	C28-C27-C26	-2.20	110.14	114.06
48	BA	849	BCR	C12-C13-C14	-2.20	115.56	119.01
45	BA	815	CLA	C3B-C4B-NB	-2.20	108.57	110.53
54	A1	308	CHL	C1B-CHB-C4A	-2.20	119.91	121.32
45	AB	837	CLA	CHA-C1A-NA	-2.19	121.42	126.39
45	BB	835	CLA	CHB-C4A-NA	2.19	127.57	124.40
45	B2	602	CLA	CHB-C4A-NA	2.19	127.57	124.40
48	BL	305	BCR	C12-C13-C14	-2.19	115.56	119.01
45	BH	201	CLA	CAC-C3C-C4C	2.19	127.64	124.79
54	A6	602	CHL	CBA-CAA-C2A	2.19	120.24	113.78
45	A1	314	CLA	CBC-CAC-C3C	2.19	118.37	112.42
45	BB	802	CLA	CHB-C4A-NA	2.19	127.56	124.40
48	BL	306	BCR	C1-C6-C5	-2.19	119.64	122.64
45	AA	842	CLA	O2D-CGD-CBD	2.19	115.06	111.23
45	BA	801	CLA	CHC-C4B-NB	2.19	127.34	124.05
45	AA	808	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
45	AA	816	CLA	O2D-CGD-CBD	2.19	115.06	111.23
45	BA	811	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
54	B1	308	CHL	C3D-CAD-CBD	2.19	110.49	107.61
45	B2	603	CLA	CBC-CAC-C3C	-2.19	106.48	112.42
55	A4	316	XAT	C12-C13-C14	-2.19	115.57	119.01
48	AI	101	BCR	C36-C18-C17	-2.19	119.27	122.82
48	A4	317	BCR	C38-C26-C27	2.19	118.26	113.60
45	B2	608	CLA	C3B-C4B-NB	-2.19	108.58	110.53
48	BK	204	BCR	C40-C30-C39	2.19	114.90	108.63
55	A4	316	XAT	C32-C33-C34	-2.19	115.57	119.01
45	AB	824	CLA	CAA-C2A-C1A	2.19	119.14	111.97
45	AA	805	CLA	O1D-CGD-CBD	2.19	128.83	124.52
45	AL	303	CLA	CHB-C4A-NA	2.19	127.56	124.40
45	A4	301	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
45	BB	811	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
45	BA	825	CLA	C6-C5-C3	2.19	118.79	113.47
45	BB	830	CLA	CHB-C4A-NA	2.19	127.56	124.40
45	BB	830	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
48	BF	304	BCR	C3-C4-C5	-2.19	110.16	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AB	846	BCR	C24-C23-C22	-2.19	123.00	126.23
48	BA	855	BCR	C29-C30-C25	2.19	113.61	110.44
45	B3	312	CLA	CHB-C4A-NA	2.18	127.55	124.40
45	B1	311	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
45	AL	303	CLA	C3B-C4B-NB	-2.18	108.58	110.53
54	A6	606	CHL	CMD-C2D-C3D	2.18	129.05	124.68
45	A1	312	CLA	CHB-C4A-NA	2.18	127.55	124.40
54	A6	607	CHL	C1A-CHA-CBD	2.18	137.95	132.36
45	BB	824	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
45	A4	302	CLA	CMB-C2B-C3B	2.18	129.33	123.53
45	BB	838	CLA	CHA-C1A-NA	-2.18	121.45	126.39
45	BA	828	CLA	C6-C7-C8	-2.18	108.71	115.97
45	B1	304	CLA	CHB-C4A-NA	2.18	127.55	124.40
54	A4	314	CHL	O2D-CGD-O1D	-2.18	119.13	124.08
45	AA	817	CLA	C3B-C4B-NB	-2.18	108.58	110.53
45	AA	829	CLA	C5-C3-C2	-2.18	116.27	121.17
45	A3	314	CLA	CAA-C2A-C3A	-2.18	111.23	116.23
45	BB	819	CLA	C6-C5-C3	2.18	118.78	113.47
45	AB	812	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
45	BF	301	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
45	AB	834	CLA	CAC-C3C-C4C	2.18	127.62	124.79
45	B5	602	CLA	CHD-C1D-ND	-2.18	121.74	124.80
52	A3	316	LUT	C35-C15-C14	-2.18	119.06	123.52
47	A6	618	LHG	O8-C23-C24	2.18	118.47	111.83
45	AB	839	CLA	C3B-C4B-NB	-2.18	108.59	110.53
55	A6	616	XAT	C26-C27-C28	-2.18	121.39	125.99
45	AA	805	CLA	CMC-C2C-C3C	2.18	132.03	126.15
45	BB	801	CLA	C2D-C1D-ND	-2.18	107.97	110.13
50	BA	854	LMU	C1B-O1B-C4'	-2.18	112.82	117.98
48	BG	203	BCR	C28-C27-C26	-2.18	110.18	114.06
48	AG	205	BCR	C1-C6-C5	-2.17	119.66	122.64
45	BK	203	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
45	BB	827	CLA	C3B-C4B-NB	-2.17	108.59	110.53
45	B2	604	CLA	C3B-C4B-NB	-2.17	108.59	110.53
52	B5	614	LUT	C8-C7-C6	-2.17	121.19	127.00
45	AA	834	CLA	CHD-C1D-ND	-2.17	121.74	124.80
45	AB	835	CLA	CHD-C1D-ND	-2.17	121.74	124.80
45	AB	834	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
54	B5	606	CHL	C3D-CAD-CBD	2.17	110.47	107.61
45	AB	802	CLA	C4-C3-C5	2.17	119.00	115.23
54	B5	607	CHL	C1A-CHA-CBD	2.17	137.92	132.36
45	AA	816	CLA	CAC-C3C-C4C	2.17	127.61	124.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A3	313	CLA	C3B-C4B-NB	-2.17	108.59	110.53
45	BA	831	CLA	O1D-CGD-CBD	2.17	128.80	124.52
48	BI	101	BCR	C33-C5-C4	2.17	118.22	113.60
45	B1	314	CLA	CAC-C3C-C4C	2.17	127.61	124.79
45	B3	314	CLA	CAA-C2A-C3A	-2.17	111.26	116.23
45	B3	313	CLA	CAA-C2A-C3A	-2.17	111.26	116.23
45	BB	828	CLA	CAA-CBA-CGA	-2.17	107.05	113.21
52	A3	316	LUT	C32-C33-C34	-2.17	115.60	119.01
45	AB	813	CLA	O2D-CGD-CBD	2.17	115.02	111.23
45	AB	831	CLA	CHB-C4A-NA	2.17	127.53	124.40
45	A6	601	CLA	CMC-C2C-C1C	-2.17	121.65	125.03
48	AA	845	BCR	C36-C18-C19	2.17	121.40	118.09
48	AA	852	BCR	C19-C18-C17	-2.17	115.60	119.01
45	AB	826	CLA	CHD-C1D-ND	-2.17	121.75	124.80
45	AB	842	CLA	C3A-C2A-C1A	2.17	104.58	101.34
48	AB	844	BCR	C20-C21-C22	-2.16	124.24	127.28
45	BA	840	CLA	O2A-CGA-O1A	-2.16	118.21	123.63
45	BA	810	CLA	CAC-C3C-C4C	2.16	127.61	124.79
45	AB	809	CLA	C3B-C4B-NB	-2.16	108.60	110.53
47	A1	301	LHG	O8-C23-O10	-2.16	118.22	123.63
45	BA	817	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
45	BB	842	CLA	O2A-CGA-O1A	-2.16	118.22	123.63
45	B2	604	CLA	CHB-C4A-NA	2.16	127.52	124.40
47	F	801	LHG	C27-C26-C25	-2.16	103.44	114.37
45	BA	838	CLA	CBD-CHA-C1A	2.16	131.59	127.58
45	AA	823	CLA	C3B-C4B-NB	-2.16	108.60	110.53
48	BK	204	BCR	C24-C25-C26	-2.16	116.58	121.56
45	BA	817	CLA	CHD-C1D-ND	-2.16	121.77	124.80
55	A1	318	XAT	C28-C29-C30	-2.16	115.61	119.01
45	AF	802	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
45	B2	609	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
45	B3	302	CLA	CAC-C3C-C4C	2.16	127.59	124.79
45	AB	813	CLA	CHB-C4A-NA	2.16	127.51	124.40
45	BB	837	CLA	CHB-C4A-NA	2.16	127.51	124.40
45	A3	309	CLA	CAA-C2A-C3A	-2.15	111.29	116.23
48	AA	847	BCR	C29-C28-C27	-2.15	106.54	111.28
48	AB	844	BCR	C16-C17-C18	-2.15	124.26	127.28
45	BB	815	CLA	O2A-CGA-O1A	-2.15	118.24	123.63
48	AL	302	BCR	C23-C24-C25	-2.15	121.24	127.00
45	AB	822	CLA	CHB-C4A-NA	2.15	127.51	124.40
54	B5	607	CHL	CMD-C2D-C3D	2.15	128.99	124.68
45	AA	804	CLA	CMB-C2B-C3B	2.15	131.62	126.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	A3	303	CLA	CHB-C1B-C2B	-2.15	121.17	127.43
45	BA	819	CLA	CBA-CAA-C2A	2.15	120.20	113.79
48	AB	847	BCR	C36-C18-C17	-2.15	119.33	122.82
48	AJ	103	BCR	C27-C26-C25	-2.15	119.80	122.70
45	BA	807	CLA	CHD-C1D-ND	-2.15	121.77	124.80
48	BB	845	BCR	C31-C1-C6	2.15	113.62	110.24
45	BA	819	CLA	O2D-CGD-CBD	2.15	114.99	111.23
45	BB	807	CLA	CHD-C1D-ND	-2.15	121.78	124.80
54	A4	305	CHL	CAC-C3C-C4C	2.15	129.56	124.03
48	AA	852	BCR	C20-C21-C22	-2.15	124.26	127.28
48	AA	849	BCR	C16-C15-C14	-2.15	119.12	123.52
45	AA	837	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
45	AA	802	CLA	C2B-C1B-NB	2.15	112.55	110.33
45	B1	315	CLA	CHB-C4A-NA	2.15	127.50	124.40
45	AA	818	CLA	CAA-C2A-C3A	2.15	118.80	113.00
45	AA	838	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
45	BB	805	CLA	O2D-CGD-CBD	2.15	114.98	111.23
54	B2	607	CHL	CMA-C3A-C4A	-2.15	109.98	114.61
45	BA	841	CLA	C1-C2-C3	-2.15	122.68	126.20
48	B3	317	BCR	C30-C25-C24	2.15	121.47	115.65
52	A4	315	LUT	C3-C4-C5	-2.15	106.83	112.18
45	AA	837	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
45	BA	842	CLA	CHB-C4A-NA	2.15	127.50	124.40
54	A3	307	CHL	CMD-C2D-C3D	2.15	128.97	124.68
45	AB	829	CLA	CMB-C2B-C3B	2.15	131.60	126.55
48	AB	845	BCR	C10-C11-C12	-2.15	116.98	123.20
45	B2	604	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
48	AB	846	BCR	C12-C13-C14	-2.15	115.64	119.01
48	BA	851	BCR	C24-C23-C22	-2.14	123.06	126.23
48	AF	805	BCR	C40-C30-C25	-2.14	106.88	110.24
45	AA	834	CLA	C7-C6-C5	-2.14	107.55	113.26
45	AB	808	CLA	C3B-C4B-NB	-2.14	108.62	110.53
45	BA	822	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
45	BB	816	CLA	CMB-C2B-C3B	2.14	131.59	126.55
45	AB	804	CLA	CMC-C2C-C1C	-2.14	121.69	125.03
54	A6	607	CHL	CMA-C3A-C4A	-2.14	110.00	114.61
48	BJ	101	BCR	C2-C3-C4	-2.14	106.57	111.28
45	BL	303	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
48	AL	306	BCR	C16-C15-C14	-2.14	119.14	123.52
55	A1	318	XAT	C17-C1-C16	-2.14	104.26	107.37
45	AA	823	CLA	CHD-C1D-ND	-2.14	121.79	124.80
45	AB	808	CLA	CHD-C1D-ND	-2.14	121.79	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	B3	309	CLA	CHB-C4A-NA	2.14	127.49	124.40
48	BA	850	BCR	C12-C13-C14	-2.14	115.64	119.01
54	A3	307	CHL	C1A-CHA-CBD	2.14	137.84	132.36
45	AA	803	CLA	CAA-CBA-CGA	-2.14	107.13	113.21
45	BB	804	CLA	CHC-C4B-NB	2.14	127.26	124.05
48	AF	805	BCR	C28-C27-C26	-2.14	110.24	114.06
45	AB	836	CLA	CHB-C4A-NA	2.14	127.49	124.40
45	BB	834	CLA	C3B-C4B-NB	-2.14	108.62	110.53
52	A4	315	LUT	C37-C21-C26	2.14	112.78	109.55
48	BA	850	BCR	C38-C26-C27	2.14	118.15	113.60
45	AA	832	CLA	O2D-CGD-CBD	2.14	114.97	111.23
54	A4	306	CHL	CMD-C2D-C3D	2.14	128.95	124.68
54	A6	607	CHL	C3D-CAD-CBD	2.14	110.42	107.61
55	A1	318	XAT	C38-C25-C26	-2.14	118.78	122.30
48	BA	851	BCR	C12-C13-C14	-2.14	115.65	119.01
45	B3	302	CLA	C5-C3-C2	2.14	125.96	121.17
45	AB	804	CLA	O2D-CGD-CBD	2.13	114.96	111.23
48	AG	205	BCR	C16-C17-C18	-2.13	124.28	127.28
48	AA	846	BCR	C2-C3-C4	-2.13	106.58	111.28
45	BB	810	CLA	CMD-C2D-C3D	2.13	132.58	127.69
48	BI	101	BCR	C20-C21-C22	-2.13	124.29	127.28
45	BB	841	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
55	A3	317	XAT	C38-C25-C24	2.13	116.64	114.24
54	A4	305	CHL	O2D-CGD-O1D	-2.13	119.70	123.85
45	BA	832	CLA	O2D-CGD-CBD	2.13	114.96	111.23
54	B1	303	CHL	CMD-C2D-C3D	2.13	128.94	124.68
45	BK	203	CLA	CMB-C2B-C3B	2.13	131.56	126.55
45	A1	313	CLA	CMB-C2B-C1B	-2.13	122.17	125.42
45	BA	844	CLA	CHB-C4A-NA	2.13	127.47	124.40
54	A6	608	CHL	CMD-C2D-C3D	2.13	128.94	124.68
45	BA	841	CLA	CAC-C3C-C4C	2.13	127.56	124.79
45	AK	201	CLA	CMA-C3A-C2A	-2.13	111.34	116.23
45	B3	314	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
45	AL	304	CLA	C3B-C4B-NB	-2.13	108.63	110.53
48	BB	849	BCR	C36-C18-C17	-2.13	119.37	122.82
45	BA	831	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
45	AA	838	CLA	O2D-CGD-CBD	2.13	114.95	111.23
48	BA	855	BCR	C20-C21-C22	-2.13	124.29	127.28
45	B2	613	CLA	C3B-C4B-NB	-2.13	108.63	110.53
54	A1	308	CHL	CMD-C2D-C3D	2.13	128.94	124.68
53	A4	318	LMG	C13-C12-C11	-2.13	105.31	113.13
45	BA	842	CLA	CAA-CBA-CGA	-2.13	107.17	113.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	805	CLA	CHD-C1D-ND	-2.13	121.81	124.80
45	AB	825	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
45	AA	826	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
45	BA	812	CLA	CMB-C2B-C1B	-2.13	122.18	125.42
45	AL	304	CLA	O2A-CGA-O1A	-2.13	118.31	123.63
45	AA	829	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
48	AA	845	BCR	C20-C21-C22	-2.13	124.30	127.28
45	A3	305	CLA	C3B-C4B-NB	-2.13	108.63	110.53
54	B2	605	CHL	C3D-CAD-CBD	2.13	110.40	107.61
55	B5	615	XAT	C36-C21-C26	2.13	115.78	110.05
48	AA	848	BCR	C1-C6-C5	-2.12	119.73	122.64
45	A1	315	CLA	CAB-C3B-C4B	-2.12	122.18	125.42
45	BF	301	CLA	CMB-C2B-C1B	-2.12	122.18	125.42
54	A1	308	CHL	O2D-CGD-O1D	-2.12	119.26	124.08
45	BA	841	CLA	O2A-CGA-O1A	-2.12	118.31	123.63
45	B1	314	CLA	C4A-NA-C1A	2.12	107.65	106.68
48	AA	845	BCR	C34-C9-C10	-2.12	119.38	122.82
45	AB	835	CLA	CAA-C2A-C3A	-2.12	107.26	113.00
48	AA	848	BCR	C21-C20-C19	-2.12	117.05	123.20
55	A1	318	XAT	C35-C34-C33	-2.12	124.30	127.28
45	B2	603	CLA	O2A-CGA-O1A	-2.12	117.88	123.33
48	BA	856	BCR	C24-C25-C26	2.12	126.44	121.56
55	A3	317	XAT	C28-C29-C30	-2.12	115.67	119.01
45	BA	833	CLA	CHB-C4A-NA	2.12	127.46	124.40
48	A6	617	BCR	C30-C25-C26	-2.12	119.74	122.64
45	B3	314	CLA	CHB-C4A-NA	2.12	127.46	124.40
45	A1	315	CLA	CMA-C3A-C2A	-2.12	111.37	116.23
48	BB	849	BCR	C19-C18-C17	-2.12	115.67	119.01
45	A1	316	CLA	CHB-C4A-NA	2.12	127.46	124.40
45	BA	829	CLA	CHB-C4A-NA	2.12	127.46	124.40
48	AA	847	BCR	C34-C9-C8	2.12	121.32	118.09
48	BL	305	BCR	C16-C15-C14	-2.12	119.19	123.52
45	A4	302	CLA	CAB-C3B-C4B	-2.12	122.19	125.42
45	BA	835	CLA	CHB-C4A-NA	2.12	127.46	124.40
45	BB	822	CLA	CMA-C3A-C2A	-2.12	111.37	116.23
48	AB	846	BCR	C16-C15-C14	-2.12	119.19	123.52
54	B5	606	CHL	O2D-CGD-O1D	-2.12	119.73	123.85
48	BA	851	BCR	C32-C1-C6	2.12	113.56	110.24
48	AA	849	BCR	C34-C9-C8	2.12	121.32	118.09
45	AB	819	CLA	CMB-C2B-C3B	2.11	131.52	126.55
48	BB	845	BCR	C12-C13-C14	-2.11	115.68	119.01
45	A3	310	CLA	CAA-C2A-C3A	-2.11	111.38	116.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
52	B3	315	LUT	C11-C10-C9	-2.11	124.31	127.28
45	B5	610	CLA	CHB-C4A-NA	2.11	127.45	124.40
45	A1	312	CLA	C3B-C4B-NB	-2.11	108.14	110.33
48	AI	101	BCR	C19-C18-C17	-2.11	115.69	119.01
45	BA	815	CLA	CHC-C4B-NB	2.11	127.22	124.05
45	AA	824	CLA	C3B-C4B-NB	-2.11	108.64	110.53
45	AB	838	CLA	CHD-C1D-ND	-2.11	121.83	124.80
54	A4	305	CHL	CBC-CAC-C3C	-2.11	109.85	112.87
48	AK	204	BCR	C8-C7-C6	-2.11	121.36	127.00
45	BK	203	CLA	C3B-C4B-NB	-2.11	108.65	110.53
45	BB	826	CLA	C1-O2A-CGA	2.11	121.76	116.65
45	AA	810	CLA	C3B-C4B-NB	-2.11	108.65	110.53
45	A3	303	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
45	AB	821	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
48	BA	848	BCR	C37-C22-C23	2.11	121.31	118.09
45	BH	201	CLA	CHC-C4B-NB	2.11	127.21	124.05
48	BB	845	BCR	C32-C1-C6	-2.11	106.94	110.24
48	BB	849	BCR	C34-C9-C8	2.11	121.31	118.09
45	BA	817	CLA	C4-C3-C2	-2.11	118.22	123.63
45	AB	819	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
45	BB	801	CLA	CMD-C2D-C1D	-2.11	121.02	124.73
45	BB	815	CLA	CHB-C4A-NA	2.11	127.44	124.40
45	A1	312	CLA	CAB-C3B-C2B	2.11	129.13	123.53
45	A4	313	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
48	BA	851	BCR	C24-C25-C26	2.11	126.41	121.56
48	B3	317	BCR	C8-C9-C10	-2.11	115.70	119.01
54	B5	605	CHL	O2D-CGD-O1D	-2.11	119.30	124.08
48	A3	318	BCR	C15-C16-C17	-2.10	119.21	123.52
45	AB	829	CLA	C2D-C1D-ND	-2.10	108.04	110.13
45	AB	833	CLA	CHC-C4B-NB	2.10	127.21	124.05
45	AA	834	CLA	CMC-C2C-C3C	2.10	131.84	126.15
45	BB	812	CLA	C2A-C1A-CHA	2.10	127.52	123.87
45	BB	818	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
45	AB	840	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
45	AB	806	CLA	CMC-C2C-C3C	2.10	131.84	126.15
45	A1	306	CLA	CHB-C4A-NA	2.10	127.44	124.40
45	AB	803	CLA	CHC-C4B-NB	2.10	127.20	124.05
45	BB	828	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
45	BA	823	CLA	CMA-C3A-C2A	-2.10	111.41	116.23
45	B2	611	CLA	CHB-C4A-NA	2.10	127.43	124.40
45	BB	816	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
45	B1	314	CLA	CHB-C4A-NA	2.10	127.43	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	B5	607	CHL	O2D-CGD-O1D	-2.10	119.76	123.85
54	B5	605	CHL	C3D-CAD-CBD	2.10	110.37	107.61
48	AA	849	BCR	C15-C16-C17	-2.10	119.22	123.52
45	AB	840	CLA	CHB-C4A-NA	2.10	127.43	124.40
48	A4	317	BCR	C35-C13-C12	2.10	121.30	118.09
45	BB	806	CLA	CAC-C3C-C4C	2.10	127.52	124.79
54	B1	308	CHL	O2D-CGD-O1D	-2.10	119.32	124.08
48	BA	849	BCR	C38-C26-C27	2.10	118.07	113.60
45	AA	842	CLA	CAC-C3C-C4C	2.10	127.52	124.79
45	BA	817	CLA	O2D-CGD-CBD	2.10	114.90	111.23
48	BL	301	BCR	C1-C6-C7	2.10	121.34	115.65
45	A3	311	CLA	CAA-C2A-C3A	-2.10	107.33	113.00
55	B2	616	XAT	C12-C13-C14	-2.10	115.71	119.01
48	BJ	101	BCR	C4-C5-C6	-2.10	119.87	122.70
45	A1	311	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
45	A1	314	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
45	AB	803	CLA	C3B-C4B-NB	-2.10	108.66	110.53
48	BL	306	BCR	C24-C25-C26	-2.10	116.73	121.56
45	AB	830	CLA	CHB-C4A-NA	2.10	127.42	124.40
48	BB	846	BCR	C36-C18-C17	-2.09	119.42	122.82
45	AB	804	CLA	C2A-C1A-CHA	2.09	127.50	123.87
45	B5	602	CLA	CHB-C1B-NB	2.09	127.19	124.05
45	BA	807	CLA	CHB-C4A-NA	2.09	127.42	124.40
48	AB	849	BCR	C8-C7-C6	-2.09	121.41	127.00
45	BB	816	CLA	CMB-C2B-C1B	-2.09	122.23	125.42
45	AB	801	CLA	C2A-C1A-CHA	2.09	127.50	123.87
48	AB	848	BCR	C3-C4-C5	-2.09	110.32	114.06
54	A4	304	CHL	CMD-C2D-C3D	2.09	128.86	124.68
45	B5	613	CLA	CHD-C1D-ND	-2.09	121.86	124.80
45	AB	837	CLA	CHB-C4A-NA	2.09	127.42	124.40
50	AL	301	LMU	C1-O1'-C1'	2.09	117.25	113.68
45	AA	801	CLA	O1D-CGD-CBD	2.09	128.64	124.52
48	BB	845	BCR	C23-C22-C21	-2.09	115.72	119.01
45	AB	840	CLA	C3B-C4B-NB	-2.09	108.66	110.53
52	A4	315	LUT	C36-C21-C26	2.09	112.71	109.55
48	AL	306	BCR	C29-C28-C27	-2.09	106.68	111.28
45	AB	807	CLA	CAA-C2A-C1A	-2.09	105.13	111.97
55	B2	616	XAT	O4-C5-C6	-2.09	57.27	58.93
48	BA	855	BCR	C35-C13-C12	2.09	121.28	118.09
48	BB	846	BCR	C15-C16-C17	-2.09	119.25	123.52
45	AA	813	CLA	CAA-C2A-C3A	-2.09	107.36	113.00
45	AA	814	CLA	CHB-C4A-NA	2.09	127.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	821	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
48	BA	849	BCR	C16-C17-C18	-2.09	124.35	127.28
45	B2	602	CLA	O1D-CGD-CBD	2.09	128.63	124.52
45	AB	811	CLA	CHA-C1A-NA	-2.09	121.67	126.39
48	AL	302	BCR	C20-C21-C22	-2.08	124.35	127.28
48	A1	319	BCR	C20-C21-C22	-2.08	124.35	127.28
54	B1	303	CHL	C1-C2-C3	-2.08	123.39	126.76
52	B2	615	LUT	C35-C15-C14	-2.08	119.25	123.52
45	BB	833	CLA	CMB-C2B-C3B	2.08	131.45	126.55
48	AA	849	BCR	C10-C11-C12	-2.08	117.16	123.20
45	BA	804	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
45	BB	827	CLA	O1D-CGD-CBD	2.08	128.63	124.52
48	BA	856	BCR	C20-C21-C22	-2.08	124.36	127.28
45	A4	313	CLA	O2D-CGD-CBD	2.08	114.87	111.23
54	A4	304	CHL	CAC-C3C-C4C	2.08	128.48	124.73
48	BB	803	BCR	C23-C22-C21	-2.08	115.73	119.01
45	BA	832	CLA	C1-C2-C3	-2.08	122.78	126.20
48	A3	318	BCR	C28-C27-C26	-2.08	110.34	114.06
45	AA	804	CLA	CHD-C1D-ND	-2.08	121.87	124.80
54	A6	607	CHL	CED-O2D-CGD	2.08	120.64	115.92
45	AB	803	CLA	O1D-CGD-CBD	2.08	128.62	124.52
52	B5	614	LUT	C7-C8-C9	-2.08	123.16	126.23
54	B2	614	CHL	CAC-C3C-C4C	2.08	129.38	124.03
48	AL	306	BCR	C34-C9-C8	2.08	121.27	118.09
45	BA	826	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
45	BA	828	CLA	CMB-C2B-C3B	2.08	131.44	126.55
45	A3	306	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
45	B1	315	CLA	CAB-C3B-C4B	-2.08	122.25	125.42
45	BA	807	CLA	C3B-C4B-NB	-2.08	108.67	110.53
45	BA	844	CLA	O2D-CGD-CBD	2.08	114.86	111.23
45	A4	308	CLA	C1D-ND-C4D	-2.08	104.85	106.31
45	AA	811	CLA	O1D-CGD-CBD	2.08	128.62	124.52
45	BA	828	CLA	C14-C13-C15	2.08	118.68	111.27
45	AA	836	CLA	C3B-C4B-NB	-2.08	108.68	110.53
45	B3	302	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
45	B1	314	CLA	CMC-C2C-C1C	-2.08	121.79	125.03
45	AB	818	CLA	CAC-C3C-C4C	2.08	127.49	124.79
48	AJ	103	BCR	C20-C21-C22	-2.08	124.37	127.28
45	BA	822	CLA	CHB-C4A-NA	2.08	127.39	124.40
54	A6	606	CHL	C1A-CHA-CBD	2.08	137.68	132.36
45	BA	809	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
48	BB	847	BCR	C21-C20-C19	-2.07	117.19	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	A4	314	CHL	CMD-C2D-C3D	2.07	128.82	124.68
48	AJ	101	BCR	C19-C18-C17	-2.07	115.75	119.01
54	B2	606	CHL	O1D-CGD-CBD	-2.07	121.58	124.72
45	AA	838	CLA	C5-C3-C2	2.07	125.82	121.17
45	AA	836	CLA	CHB-C1B-NB	2.07	127.16	124.05
45	B3	307	CLA	O1D-CGD-CBD	2.07	128.60	124.52
45	B3	310	CLA	CHA-C1A-NA	-2.07	121.70	126.39
48	BB	845	BCR	C36-C18-C17	-2.07	119.46	122.82
45	BB	827	CLA	CHB-C4A-NA	2.07	127.39	124.40
45	B3	301	CLA	O1D-CGD-CBD	2.07	128.60	124.52
45	AA	831	CLA	CHD-C1D-ND	-2.07	121.89	124.80
45	BA	838	CLA	CHB-C4A-NA	2.07	127.39	124.40
45	BB	823	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
45	AB	802	CLA	C1-O2A-CGA	2.07	121.66	116.65
48	BA	849	BCR	C20-C21-C22	-2.07	124.38	127.28
45	A4	303	CLA	CAB-C3B-C4B	-2.07	122.27	125.42
45	BA	827	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
48	AF	805	BCR	C24-C25-C26	2.07	126.32	121.56
45	BK	201	CLA	CAB-C3B-C4B	-2.07	122.27	125.42
45	AB	826	CLA	CMB-C2B-C3B	2.07	131.41	126.55
54	B2	606	CHL	C3D-CAD-CBD	2.07	110.33	107.61
45	AA	838	CLA	CHB-C4A-NA	2.07	127.38	124.40
45	BB	828	CLA	CHA-C1A-NA	-2.07	121.71	126.39
48	BF	304	BCR	C23-C22-C21	-2.07	115.76	119.01
48	A1	319	BCR	C12-C13-C14	-2.07	115.76	119.01
45	BA	821	CLA	CHD-C1D-ND	-2.07	121.89	124.80
45	A4	308	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
45	AF	802	CLA	O1D-CGD-CBD	2.07	128.59	124.52
45	B3	310	CLA	C2A-C1A-CHA	2.07	127.45	123.87
56	BJ	104	SQD	O47-C45-C44	2.06	115.75	108.34
55	B3	316	XAT	C32-C33-C34	-2.06	115.76	119.01
45	BB	804	CLA	C5-C3-C2	-2.06	116.53	121.17
45	AA	807	CLA	CMB-C2B-C3B	2.06	131.41	126.55
45	BA	830	CLA	O1D-CGD-CBD	2.06	128.59	124.52
48	B3	317	BCR	C21-C20-C19	-2.06	117.22	123.20
48	BA	849	BCR	C30-C25-C26	-2.06	119.82	122.64
45	A3	312	CLA	CHD-C1D-ND	-2.06	121.90	124.80
48	BA	856	BCR	C7-C8-C9	-2.06	123.18	126.23
45	BB	813	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
48	BL	301	BCR	C30-C25-C24	2.06	121.25	115.65
45	A6	610	CLA	CBA-CAA-C2A	2.06	119.93	113.79
55	B1	317	XAT	C10-C11-C12	-2.06	117.22	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	819	CLA	C3B-C4B-NB	-2.06	108.69	110.53
45	B2	613	CLA	O2D-CGD-CBD	2.06	114.83	111.23
45	AA	828	CLA	CAA-CBA-CGA	-2.06	107.36	113.21
48	AB	846	BCR	C32-C1-C6	-2.06	107.01	110.24
45	AH	201	CLA	C1-C2-C3	-2.06	122.82	126.20
48	AB	847	BCR	C23-C22-C21	-2.06	115.77	119.01
45	AB	801	CLA	C3A-C2A-C1A	2.06	104.42	101.34
48	A4	317	BCR	C34-C9-C8	2.06	121.23	118.09
54	B1	308	CHL	CBC-CAC-C3C	-2.06	109.92	112.87
45	AA	830	CLA	CHB-C4A-NA	2.06	127.37	124.40
45	AB	815	CLA	C1-C2-C3	-2.06	122.82	126.20
48	B2	617	BCR	C16-C17-C18	-2.06	124.39	127.28
48	BB	803	BCR	C32-C1-C2	-2.06	101.04	108.95
48	BB	803	BCR	C1-C6-C5	-2.06	119.82	122.64
45	A1	311	CLA	C3B-C4B-NB	-2.06	108.69	110.53
48	BI	101	BCR	C23-C22-C21	-2.06	115.77	119.01
54	B2	607	CHL	C3D-CAD-CBD	2.06	110.31	107.61
48	BG	203	BCR	C27-C26-C25	-2.06	119.92	122.70
45	BB	822	CLA	CAA-C2A-C3A	-2.06	111.51	116.23
54	B2	605	CHL	C1A-CHA-CBD	2.06	137.63	132.36
45	AA	818	CLA	CHC-C4B-NB	2.06	127.13	124.05
45	A6	610	CLA	O2A-CGA-O1A	-2.06	118.49	123.63
48	A1	319	BCR	C21-C20-C19	-2.06	117.25	123.20
48	BB	803	BCR	C34-C9-C8	2.05	121.23	118.09
45	AF	802	CLA	CMD-C2D-C3D	2.05	132.40	127.69
45	BA	839	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
45	AB	839	CLA	CHC-C4B-NB	2.05	127.13	124.05
45	AA	821	CLA	C7-C6-C5	-2.05	107.79	113.26
48	BA	851	BCR	C19-C18-C17	2.05	122.24	119.01
56	e	301	SQD	C1-O5-C5	2.05	117.73	113.72
45	AB	805	CLA	CAA-C2A-C3A	-2.05	111.52	116.23
48	BJ	103	BCR	C16-C17-C18	-2.05	124.40	127.28
48	BL	306	BCR	C28-C27-C26	-2.05	110.40	114.06
54	A1	303	CHL	CBA-CAA-C2A	2.05	119.81	113.78
45	AA	812	CLA	O2D-CGD-CBD	2.05	114.81	111.23
48	AA	847	BCR	C8-C7-C6	2.05	132.47	127.00
48	BK	204	BCR	C15-C16-C17	-2.05	119.33	123.52
48	BJ	101	BCR	C19-C18-C17	-2.05	115.79	119.01
45	BK	202	CLA	O2D-CGD-CBD	2.05	114.81	111.23
45	BB	835	CLA	O1D-CGD-CBD	2.05	128.56	124.52
48	AA	847	BCR	C16-C15-C14	-2.05	119.33	123.52
54	A3	307	CHL	CAC-C3C-C4C	2.05	129.29	124.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	AG	205	BCR	C29-C28-C27	-2.05	106.78	111.28
45	AA	803	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
45	AF	802	CLA	C6-C5-C3	2.05	118.45	113.47
45	AA	815	CLA	C3B-C4B-NB	-2.05	108.70	110.53
45	B3	312	CLA	CAA-C2A-C3A	-2.05	111.54	116.23
54	B5	605	CHL	C1A-CHA-CBD	2.05	137.60	132.36
48	AA	845	BCR	C4-C5-C6	2.05	125.47	122.70
45	A1	309	CLA	CAC-C3C-C4C	2.05	127.45	124.79
45	BB	821	CLA	O2A-CGA-O1A	-2.05	118.51	123.63
48	A1	319	BCR	C39-C30-C29	2.04	116.80	108.95
45	AB	832	CLA	CMC-C2C-C3C	2.04	131.68	126.15
54	B3	306	CHL	CMA-C3A-C4A	-2.04	110.21	114.61
45	AK	203	CLA	C3B-C4B-NB	-2.04	108.71	110.53
45	BB	817	CLA	C3B-C4B-NB	-2.04	108.71	110.53
45	AA	829	CLA	CMB-C2B-C3B	2.04	131.36	126.55
48	AF	801	BCR	C39-C30-C25	-2.04	107.04	110.24
50	AB	853	LMU	O5B-C5B-C4B	2.04	113.38	109.70
48	AA	849	BCR	C19-C18-C17	2.04	122.22	119.01
48	AJ	103	BCR	C12-C13-C14	-2.04	115.80	119.01
45	B3	305	CLA	C3A-C2A-C1A	2.04	104.40	101.34
48	AL	306	BCR	C12-C13-C14	-2.04	115.80	119.01
52	A4	315	LUT	C12-C13-C14	-2.04	115.80	119.01
45	B5	608	CLA	CHB-C1B-NB	2.04	127.11	124.05
54	A6	602	CHL	CAC-C3C-C4C	2.04	129.28	124.03
45	BA	836	CLA	C3B-C4B-NB	-2.04	108.71	110.53
55	B1	317	XAT	C35-C34-C33	-2.04	124.42	127.28
54	B2	605	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
45	BB	811	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
48	BI	101	BCR	C19-C18-C17	-2.04	115.80	119.01
48	BF	304	BCR	C20-C21-C22	-2.04	124.42	127.28
45	AA	839	CLA	C3B-C4B-NB	-2.04	108.71	110.53
45	AB	840	CLA	CHB-C1B-NB	2.04	127.11	124.05
55	B5	615	XAT	C15-C35-C34	-2.04	119.35	123.52
48	AL	302	BCR	C12-C13-C14	-2.04	115.80	119.01
51	BB	850	DGD	O1G-C1A-O1A	-2.04	118.53	123.63
45	AB	815	CLA	C16-C15-C13	2.04	122.74	115.97
45	BA	826	CLA	C5-C3-C2	2.04	125.74	121.17
45	AA	807	CLA	O2D-CGD-CBD	2.04	114.79	111.23
54	B1	308	CHL	OMC-CMC-C2C	-2.04	121.58	125.12
55	B1	317	XAT	C4-C3-C2	-2.04	106.98	110.79
45	AA	826	CLA	CHB-C4A-NA	2.04	127.34	124.40
48	BA	850	BCR	C34-C9-C8	2.04	121.20	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AB	824	CLA	CHC-C4B-NB	2.04	127.10	124.05
54	B2	605	CHL	CMD-C2D-C3D	2.04	128.75	124.68
55	B3	316	XAT	C28-C29-C30	-2.04	115.81	119.01
48	BB	847	BCR	C24-C25-C26	2.04	126.24	121.56
45	BB	810	CLA	CMD-C2D-C1D	-2.04	121.14	124.73
54	A4	305	CHL	CMA-C3A-C4A	-2.04	110.23	114.61
55	B5	615	XAT	C10-C11-C12	-2.03	117.30	123.20
45	BH	201	CLA	CED-O2D-CGD	2.03	120.53	115.92
45	AK	201	CLA	CMB-C2B-C3B	2.03	129.50	124.63
45	AB	809	CLA	C5-C3-C2	2.03	125.73	121.17
45	AB	820	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
45	AA	833	CLA	O2D-CGD-CBD	2.03	114.78	111.23
54	B2	601	CHL	C4-C3-C5	2.03	118.75	115.23
54	A6	608	CHL	C3D-CAD-CBD	2.03	110.28	107.61
48	BA	850	BCR	C7-C8-C9	-2.03	123.23	126.23
45	BB	827	CLA	CHD-C1D-ND	-2.03	121.94	124.80
45	A1	304	CLA	O1D-CGD-CBD	2.03	128.52	124.52
45	AA	807	CLA	C3B-C4B-NB	-2.03	108.72	110.53
45	A6	601	CLA	C3B-C4B-NB	-2.03	108.72	110.53
48	AL	306	BCR	C34-C9-C10	-2.03	119.53	122.82
45	AA	801	CLA	CHC-C4B-NB	2.03	127.09	124.05
45	BB	838	CLA	CAA-C2A-C3A	-2.03	107.51	113.00
54	B2	606	CHL	OMC-CMC-C2C	-2.03	121.60	125.12
45	BA	833	CLA	C4-C3-C2	-2.03	118.42	123.63
48	AA	847	BCR	C12-C13-C14	2.03	122.20	119.01
48	AB	846	BCR	C15-C16-C17	-2.03	119.37	123.52
45	AG	204	CLA	C3B-C4B-NB	-2.03	108.72	110.53
45	BA	831	CLA	CHB-C1B-NB	2.03	127.09	124.05
48	AG	205	BCR	C33-C5-C6	-2.03	122.27	124.48
45	BF	302	CLA	C3B-C4B-NB	-2.03	108.72	110.53
48	AG	205	BCR	C39-C30-C25	-2.03	107.06	110.24
45	BG	202	CLA	CHB-C4A-NA	2.03	127.33	124.40
45	B3	314	CLA	CMA-C3A-C2A	-2.03	111.58	116.23
45	AA	824	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
45	A3	310	CLA	C3B-C4B-NB	-2.03	108.72	110.53
45	A1	316	CLA	CAB-C3B-C4B	-2.03	122.33	125.42
48	BA	848	BCR	C24-C23-C22	-2.03	123.24	126.23
45	A4	313	CLA	CBA-CAA-C2A	2.03	119.82	113.79
48	AK	204	BCR	C4-C5-C6	-2.03	119.97	122.70
48	AG	205	BCR	C27-C26-C25	-2.02	119.97	122.70
45	BA	834	CLA	CAA-CBA-CGA	-2.02	107.46	113.21
48	AL	302	BCR	C15-C16-C17	-2.02	119.38	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	AA	837	CLA	C2A-C1A-CHA	2.02	127.38	123.87
45	AA	812	CLA	CHD-C1D-ND	-2.02	121.95	124.80
45	A3	305	CLA	CHD-C1D-ND	-2.02	121.95	124.80
48	BL	305	BCR	C37-C22-C21	-2.02	119.54	122.82
45	BA	821	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
55	A6	616	XAT	C35-C34-C33	-2.02	124.44	127.28
48	BB	848	BCR	C2-C3-C4	-2.02	106.83	111.28
54	A4	305	CHL	C3D-CAD-CBD	2.02	110.27	107.61
48	BA	855	BCR	C2-C1-C6	2.02	113.38	110.44
45	BA	826	CLA	CMB-C2B-C3B	2.02	131.31	126.55
45	B1	312	CLA	CAA-C2A-C3A	-2.02	111.59	116.23
56	BJ	104	SQD	C4-C3-C2	2.02	114.38	110.83
45	B2	608	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
48	AJ	101	BCR	C2-C1-C6	2.02	113.38	110.44
54	A1	308	CHL	C3D-CAD-CBD	2.02	110.27	107.61
45	AK	202	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
48	BJ	101	BCR	C20-C21-C22	-2.02	124.44	127.28
45	AB	829	CLA	CHC-C4B-NB	2.02	127.08	124.05
48	BB	803	BCR	C2-C3-C4	-2.02	106.83	111.28
45	AL	304	CLA	C1-O2A-CGA	2.02	121.54	116.65
52	A4	315	LUT	C15-C35-C34	-2.02	119.38	123.52
45	A3	309	CLA	O2D-CGD-CBD	2.02	114.76	111.23
45	BB	820	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
45	BA	823	CLA	C3B-C4B-NB	-2.02	108.73	110.53
45	AL	304	CLA	CHD-C1D-C2D	2.02	129.69	125.49
45	A6	611	CLA	C3B-C4B-NB	-2.02	108.23	110.33
45	AB	828	CLA	CMB-C2B-C3B	2.02	131.30	126.55
45	BB	825	CLA	CHB-C4A-NA	2.02	127.31	124.40
48	BK	204	BCR	C16-C17-C18	-2.02	124.45	127.28
45	BB	813	CLA	C5-C3-C2	2.02	125.70	121.17
45	BB	839	CLA	C1-C2-C3	-2.02	122.89	126.20
48	A4	317	BCR	C16-C15-C14	-2.02	119.39	123.52
52	AF	806	LUT	C39-C29-C30	-2.02	119.55	122.82
45	B3	313	CLA	C3B-C4B-NB	-2.02	108.73	110.53
45	AB	839	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
54	A6	608	CHL	C5-C3-C4	2.02	119.23	114.59
45	AB	833	CLA	O2A-CGA-O1A	-2.02	118.59	123.63
45	BA	823	CLA	CHD-C1D-ND	-2.02	121.97	124.80
52	A1	317	LUT	C18-C5-C6	2.02	126.68	124.48
45	AK	202	CLA	O2D-CGD-CBD	2.01	114.75	111.23
45	AB	836	CLA	CHB-C1B-NB	2.01	127.07	124.05
48	BB	845	BCR	C38-C26-C25	-2.01	122.29	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	BB	844	PQN	C6-C5-C10	2.01	121.52	119.26
45	BG	202	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
45	AA	828	CLA	C16-C15-C13	2.01	122.66	115.97
48	BI	101	BCR	C35-C13-C12	2.01	121.16	118.09
45	B3	307	CLA	CMB-C2B-C3B	2.01	131.29	126.55
48	BB	845	BCR	C33-C5-C6	2.01	126.68	124.48
45	B5	610	CLA	CHB-C1B-NB	2.01	127.07	124.05
54	B3	306	CHL	CAC-C3C-C4C	2.01	129.20	124.03
45	AA	842	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
45	AA	839	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
45	AB	812	CLA	C5-C3-C2	2.01	125.68	121.17
45	B3	305	CLA	CAB-C3B-C4B	-2.01	122.36	125.42
45	B5	609	CLA	CBA-CAA-C2A	2.01	119.78	113.79
45	BB	825	CLA	O2D-CGD-CBD	2.01	114.75	111.23
48	AB	848	BCR	C37-C22-C21	-2.01	119.56	122.82
45	AA	817	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
45	BB	840	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
45	A6	614	CLA	CHD-C1D-ND	-2.01	121.97	124.80
45	BB	820	CLA	CHD-C1D-ND	-2.01	121.97	124.80
45	AA	823	CLA	CHB-C4A-NA	2.01	127.30	124.40
45	AB	803	CLA	CHB-C4A-NA	2.01	127.30	124.40
48	AB	844	BCR	C11-C10-C9	-2.01	124.46	127.28
45	BA	810	CLA	O1D-CGD-CBD	2.01	128.48	124.52
45	AB	819	CLA	CAA-C2A-C3A	2.01	118.43	113.00
45	BA	809	CLA	CAA-C2A-C1A	2.01	118.56	111.97
45	B5	610	CLA	CMB-C2B-C1B	-2.01	122.36	125.42
45	BA	841	CLA	CMB-C2B-C3B	2.01	131.27	126.55
48	BA	856	BCR	C11-C10-C9	-2.01	124.46	127.28
45	A3	308	CLA	C3B-C4B-NB	-2.01	108.74	110.53
45	B3	304	CLA	C3B-C4B-NB	-2.01	108.74	110.53
45	B3	301	CLA	C6-C5-C3	2.01	118.36	113.47
54	A6	602	CHL	CAA-C2A-C3A	2.01	118.42	113.00
45	AB	833	CLA	C4-C3-C5	2.01	118.71	115.23
52	A4	315	LUT	C38-C25-C24	-2.01	118.61	123.36
48	BL	305	BCR	C24-C25-C26	-2.00	116.94	121.56
45	B3	314	CLA	CMB-C2B-C3B	2.00	131.26	126.55
45	BB	807	CLA	C3B-C4B-NB	-2.00	108.74	110.53
45	BA	806	CLA	O2D-CGD-CBD	2.00	114.73	111.23
45	BB	819	CLA	O2D-CGD-CBD	2.00	114.73	111.23
45	BB	802	CLA	C2A-C1A-CHA	2.00	127.34	123.87
45	BA	837	CLA	CMB-C2B-C3B	2.00	131.26	126.55
45	BA	842	CLA	C6-C5-C3	2.00	118.35	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	BA	822	CLA	CMB-C2B-C3B	2.00	131.26	126.55
45	BA	817	CLA	C5-C3-C2	2.00	125.66	121.17
48	AB	849	BCR	C15-C16-C17	-2.00	119.42	123.52
48	B3	317	BCR	C28-C27-C26	-2.00	110.48	114.06
48	BA	850	BCR	C15-C16-C17	-2.00	119.42	123.52
45	BB	838	CLA	C2A-C1A-CHA	2.00	127.34	123.87
45	BB	820	CLA	CBA-CAA-C2A	2.00	119.75	113.79
45	AA	801	CLA	O2A-CGA-O1A	-2.00	118.62	123.63
45	BA	809	CLA	CAA-CBA-CGA	-2.00	107.53	113.21
45	AA	842	CLA	C1-C2-C3	-2.00	122.92	126.20
48	AA	847	BCR	C19-C18-C17	-2.00	115.86	119.01
52	A3	316	LUT	C21-C26-C27	-2.00	110.53	112.83
45	AB	810	CLA	C2A-C1A-CHA	2.00	127.34	123.87

All (310) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
45	AA	801	CLA	ND
45	AA	802	CLA	ND
45	AA	803	CLA	ND
45	AA	805	CLA	ND
45	AA	806	CLA	ND
45	AA	807	CLA	ND
45	AA	808	CLA	ND
45	AA	809	CLA	ND
45	AA	810	CLA	ND
45	AA	811	CLA	ND
45	AA	812	CLA	ND
45	AA	813	CLA	ND
45	AA	814	CLA	ND
45	AA	816	CLA	ND
45	AA	817	CLA	ND
45	AA	819	CLA	ND
45	AA	820	CLA	ND
45	AA	821	CLA	ND
45	AA	822	CLA	ND
45	AA	823	CLA	ND
45	AA	824	CLA	ND
45	AA	825	CLA	ND
45	AA	826	CLA	ND
45	AA	827	CLA	ND
45	AA	828	CLA	ND

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Mol	Chain	Res	Type	Atom
45	AA	829	CLA	ND
45	AA	830	CLA	ND
45	AA	831	CLA	ND
45	AA	832	CLA	ND
45	AA	833	CLA	ND
45	AA	835	CLA	ND
45	AA	837	CLA	ND
45	AA	840	CLA	ND
45	AA	842	CLA	ND
45	AB	801	CLA	ND
45	AB	802	CLA	ND
45	AB	803	CLA	ND
45	AB	804	CLA	ND
45	AB	805	CLA	ND
45	AB	806	CLA	ND
45	AB	807	CLA	ND
45	AB	809	CLA	ND
45	AB	810	CLA	ND
45	AB	811	CLA	ND
45	AB	812	CLA	ND
45	AB	813	CLA	ND
45	AB	814	CLA	ND
45	AB	815	CLA	ND
45	AB	816	CLA	ND
45	AB	817	CLA	ND
45	AB	818	CLA	ND
45	AB	819	CLA	ND
45	AB	820	CLA	ND
45	AB	821	CLA	ND
45	AB	822	CLA	ND
45	AB	824	CLA	ND
45	AB	825	CLA	ND
45	AB	826	CLA	ND
45	AB	827	CLA	ND
45	AB	828	CLA	ND
45	AB	829	CLA	ND
45	AB	830	CLA	ND
45	AB	831	CLA	ND
45	AB	833	CLA	ND
45	AB	834	CLA	ND
45	AB	837	CLA	ND
45	AB	839	CLA	ND

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Mol	Chain	Res	Type	Atom
45	AB	840	CLA	ND
45	AB	841	CLA	ND
45	AB	842	CLA	ND
45	AF	802	CLA	ND
45	AF	803	CLA	ND
45	AF	804	CLA	ND
45	AG	201	CLA	ND
45	AG	203	CLA	ND
45	AG	204	CLA	ND
45	AH	201	CLA	ND
45	AJ	102	CLA	ND
45	AK	201	CLA	ND
45	AK	202	CLA	ND
45	AK	203	CLA	ND
45	AL	303	CLA	ND
45	AL	305	CLA	ND
45	A1	304	CLA	ND
45	A1	305	CLA	ND
45	A1	306	CLA	ND
45	A1	307	CLA	ND
45	A1	309	CLA	ND
45	A1	310	CLA	ND
45	A1	311	CLA	ND
45	A1	312	CLA	ND
45	A1	313	CLA	ND
45	A1	314	CLA	ND
45	A1	315	CLA	ND
45	A1	316	CLA	ND
45	A3	302	CLA	ND
45	A3	303	CLA	ND
45	A3	304	CLA	ND
45	A3	305	CLA	ND
45	A3	306	CLA	ND
45	A3	308	CLA	ND
45	A3	309	CLA	ND
45	A3	310	CLA	ND
45	A3	311	CLA	ND
45	A3	312	CLA	ND
45	A3	314	CLA	ND
45	A3	315	CLA	ND
45	A4	301	CLA	ND
45	A4	302	CLA	ND

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Mol	Chain	Res	Type	Atom
45	A4	303	CLA	ND
45	A4	307	CLA	ND
45	A4	308	CLA	ND
45	A4	309	CLA	ND
45	A4	310	CLA	ND
45	A4	311	CLA	ND
45	A4	312	CLA	ND
45	A4	313	CLA	ND
45	A6	601	CLA	ND
45	A6	603	CLA	ND
45	A6	604	CLA	ND
45	A6	605	CLA	ND
45	A6	609	CLA	ND
45	A6	610	CLA	ND
45	A6	611	CLA	ND
45	A6	612	CLA	ND
45	A6	613	CLA	ND
45	A6	614	CLA	ND
45	BA	801	CLA	ND
45	BA	802	CLA	ND
45	BA	803	CLA	ND
45	BA	805	CLA	ND
45	BA	806	CLA	ND
45	BA	807	CLA	ND
45	BA	808	CLA	ND
45	BA	810	CLA	ND
45	BA	811	CLA	ND
45	BA	812	CLA	ND
45	BA	813	CLA	ND
45	BA	814	CLA	ND
45	BA	816	CLA	ND
45	BA	819	CLA	ND
45	BA	820	CLA	ND
45	BA	822	CLA	ND
45	BA	823	CLA	ND
45	BA	824	CLA	ND
45	BA	825	CLA	ND
45	BA	827	CLA	ND
45	BA	828	CLA	ND
45	BA	829	CLA	ND
45	BA	830	CLA	ND
45	BA	831	CLA	ND

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Mol	Chain	Res	Type	Atom
45	BA	833	CLA	ND
45	BA	835	CLA	ND
45	BA	837	CLA	ND
45	BA	838	CLA	ND
45	BA	840	CLA	ND
45	BA	841	CLA	ND
45	BA	842	CLA	ND
45	BA	844	CLA	ND
45	BB	801	CLA	ND
45	BB	802	CLA	ND
45	BB	804	CLA	ND
45	BB	805	CLA	ND
45	BB	806	CLA	ND
45	BB	807	CLA	ND
45	BB	808	CLA	ND
45	BB	810	CLA	ND
45	BB	811	CLA	ND
45	BB	812	CLA	ND
45	BB	813	CLA	ND
45	BB	814	CLA	ND
45	BB	815	CLA	ND
45	BB	816	CLA	ND
45	BB	817	CLA	ND
45	BB	818	CLA	ND
45	BB	819	CLA	ND
45	BB	820	CLA	ND
45	BB	821	CLA	ND
45	BB	822	CLA	ND
45	BB	823	CLA	ND
45	BB	825	CLA	ND
45	BB	826	CLA	ND
45	BB	828	CLA	ND
45	BB	829	CLA	ND
45	BB	830	CLA	ND
45	BB	831	CLA	ND
45	BB	832	CLA	ND
45	BB	835	CLA	ND
45	BB	837	CLA	ND
45	BB	838	CLA	ND
45	BB	841	CLA	ND
45	BB	842	CLA	ND
45	BB	843	CLA	ND

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Mol	Chain	Res	Type	Atom
45	BF	301	CLA	ND
45	BF	302	CLA	ND
45	BF	303	CLA	ND
45	BG	201	CLA	ND
45	BG	202	CLA	ND
45	BH	201	CLA	ND
45	BJ	102	CLA	ND
45	BK	201	CLA	ND
45	BK	202	CLA	ND
45	BK	203	CLA	ND
45	BL	304	CLA	ND
45	B1	304	CLA	ND
45	B1	305	CLA	ND
45	B1	306	CLA	ND
45	B1	307	CLA	ND
45	B1	310	CLA	ND
45	B1	311	CLA	ND
45	B1	312	CLA	ND
45	B1	313	CLA	ND
45	B1	314	CLA	ND
45	B1	315	CLA	ND
45	B2	602	CLA	ND
45	B2	603	CLA	ND
45	B2	604	CLA	ND
45	B2	608	CLA	ND
45	B2	609	CLA	ND
45	B2	610	CLA	ND
45	B2	611	CLA	ND
45	B2	612	CLA	ND
45	B2	613	CLA	ND
45	B3	301	CLA	ND
45	B3	302	CLA	ND
45	B3	303	CLA	ND
45	B3	304	CLA	ND
45	B3	305	CLA	ND
45	B3	307	CLA	ND
45	B3	308	CLA	ND
45	B3	309	CLA	ND
45	B3	310	CLA	ND
45	B3	311	CLA	ND
45	B3	312	CLA	ND
45	B3	313	CLA	ND

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Mol	Chain	Res	Type	Atom
45	B3	314	CLA	ND
45	B5	601	CLA	ND
45	B5	603	CLA	ND
45	B5	604	CLA	ND
45	B5	608	CLA	ND
45	B5	609	CLA	ND
45	B5	611	CLA	ND
45	B5	612	CLA	ND
45	B5	613	CLA	ND
54	A1	303	CHL	ND
54	A1	303	CHL	NC
54	A1	303	CHL	NA
54	A1	308	CHL	ND
54	A1	308	CHL	NC
54	A1	308	CHL	NA
54	A3	307	CHL	ND
54	A3	307	CHL	NC
54	A3	307	CHL	NA
54	A4	304	CHL	ND
54	A4	304	CHL	NC
54	A4	304	CHL	NA
54	A4	305	CHL	ND
54	A4	305	CHL	NC
54	A4	305	CHL	NA
54	A4	306	CHL	ND
54	A4	306	CHL	NC
54	A4	306	CHL	NA
54	A4	314	CHL	ND
54	A4	314	CHL	NC
54	A4	314	CHL	NA
54	A6	602	CHL	ND
54	A6	602	CHL	NC
54	A6	602	CHL	NA
54	A6	606	CHL	ND
54	A6	606	CHL	NC
54	A6	606	CHL	NA
54	A6	607	CHL	ND
54	A6	607	CHL	NC
54	A6	607	CHL	NA
54	A6	608	CHL	ND
54	A6	608	CHL	NC
54	A6	608	CHL	NA

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Mol	Chain	Res	Type	Atom
54	B1	303	CHL	ND
54	B1	303	CHL	NC
54	B1	303	CHL	NA
54	B1	308	CHL	ND
54	B1	308	CHL	NC
54	B1	308	CHL	NA
54	B2	601	CHL	ND
54	B2	601	CHL	NC
54	B2	601	CHL	NA
54	B2	605	CHL	ND
54	B2	605	CHL	NC
54	B2	605	CHL	NA
54	B2	606	CHL	ND
54	B2	606	CHL	NC
54	B2	606	CHL	NA
54	B2	607	CHL	ND
54	B2	607	CHL	NC
54	B2	607	CHL	NA
54	B2	614	CHL	ND
54	B2	614	CHL	NC
54	B2	614	CHL	NA
54	B3	306	CHL	ND
54	B3	306	CHL	NC
54	B3	306	CHL	NA
54	B5	605	CHL	ND
54	B5	605	CHL	NC
54	B5	605	CHL	NA
54	B5	606	CHL	ND
54	B5	606	CHL	NC
54	B5	606	CHL	NA
54	B5	607	CHL	ND
54	B5	607	CHL	NC
54	B5	607	CHL	NA

All (2981) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	AA	801	CLA	CBD-CGD-O2D-CED
45	AA	802	CLA	CBD-CGD-O2D-CED
45	AA	803	CLA	CHA-CBD-CGD-O1D
45	AA	803	CLA	CHA-CBD-CGD-O2D
45	AA	804	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
45	AA	804	CLA	C3A-C2A-CAA-CBA
45	AA	805	CLA	CAD-CBD-CGD-O2D
45	AA	808	CLA	CHA-CBD-CGD-O1D
45	AA	808	CLA	CHA-CBD-CGD-O2D
45	AA	813	CLA	CAD-CBD-CGD-O1D
45	AA	813	CLA	CAD-CBD-CGD-O2D
45	AA	816	CLA	CAD-CBD-CGD-O1D
45	AA	816	CLA	CAD-CBD-CGD-O2D
45	AA	818	CLA	C3A-C2A-CAA-CBA
45	AA	818	CLA	C2B-C3B-CAB-CBB
45	AA	818	CLA	C4B-C3B-CAB-CBB
45	AA	819	CLA	C3A-C2A-CAA-CBA
45	AA	820	CLA	C2B-C3B-CAB-CBB
45	AA	820	CLA	C4B-C3B-CAB-CBB
45	AA	822	CLA	C1A-C2A-CAA-CBA
45	AA	822	CLA	C4B-C3B-CAB-CBB
45	AA	822	CLA	CHA-CBD-CGD-O2D
45	AA	823	CLA	C2B-C3B-CAB-CBB
45	AA	823	CLA	C4B-C3B-CAB-CBB
45	AA	824	CLA	C1A-C2A-CAA-CBA
45	AA	824	CLA	C3A-C2A-CAA-CBA
45	AA	825	CLA	C1A-C2A-CAA-CBA
45	AA	828	CLA	CBD-CGD-O2D-CED
45	AA	828	CLA	C14-C13-C15-C16
45	AA	831	CLA	C1A-C2A-CAA-CBA
45	AA	831	CLA	C3A-C2A-CAA-CBA
45	AA	831	CLA	CHA-CBD-CGD-O2D
45	AA	833	CLA	C2B-C3B-CAB-CBB
45	AA	833	CLA	C4B-C3B-CAB-CBB
45	AA	833	CLA	CAD-CBD-CGD-O1D
45	AA	833	CLA	CAD-CBD-CGD-O2D
45	AA	833	CLA	CBD-CGD-O2D-CED
45	AA	837	CLA	CHA-CBD-CGD-O1D
45	AA	837	CLA	CHA-CBD-CGD-O2D
45	AA	837	CLA	C4-C3-C5-C6
45	AA	840	CLA	C2B-C3B-CAB-CBB
45	AA	840	CLA	C4B-C3B-CAB-CBB
45	AA	842	CLA	C4B-C3B-CAB-CBB
45	AB	804	CLA	C1A-C2A-CAA-CBA
45	AB	804	CLA	C3A-C2A-CAA-CBA
45	AB	804	CLA	C2C-C3C-CAC-CBC
45	AB	804	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
45	AB	804	CLA	CBD-CGD-O2D-CED
45	AB	804	CLA	C11-C10-C8-C7
45	AB	806	CLA	C1A-C2A-CAA-CBA
45	AB	806	CLA	C3A-C2A-CAA-CBA
45	AB	806	CLA	CAD-CBD-CGD-O1D
45	AB	806	CLA	CAD-CBD-CGD-O2D
45	AB	807	CLA	CBD-CGD-O2D-CED
45	AB	809	CLA	C1A-C2A-CAA-CBA
45	AB	809	CLA	C3A-C2A-CAA-CBA
45	AB	809	CLA	CHA-CBD-CGD-O1D
45	AB	809	CLA	CHA-CBD-CGD-O2D
45	AB	810	CLA	CBD-CGD-O2D-CED
45	AB	811	CLA	C1A-C2A-CAA-CBA
45	AB	811	CLA	CAD-CBD-CGD-O1D
45	AB	811	CLA	CAD-CBD-CGD-O2D
45	AB	812	CLA	CBD-CGD-O2D-CED
45	AB	812	CLA	O1D-CGD-O2D-CED
45	AB	814	CLA	C1A-C2A-CAA-CBA
45	AB	814	CLA	C3A-C2A-CAA-CBA
45	AB	815	CLA	CBD-CGD-O2D-CED
45	AB	816	CLA	CBD-CGD-O2D-CED
45	AB	818	CLA	C2B-C3B-CAB-CBB
45	AB	818	CLA	C4B-C3B-CAB-CBB
45	AB	819	CLA	C3A-C2A-CAA-CBA
45	AB	820	CLA	C2B-C3B-CAB-CBB
45	AB	820	CLA	C4B-C3B-CAB-CBB
45	AB	824	CLA	C1A-C2A-CAA-CBA
45	AB	824	CLA	C3A-C2A-CAA-CBA
45	AB	825	CLA	CHA-CBD-CGD-O1D
45	AB	825	CLA	CHA-CBD-CGD-O2D
45	AB	828	CLA	C1A-C2A-CAA-CBA
45	AB	829	CLA	C1A-C2A-CAA-CBA
45	AB	834	CLA	C2B-C3B-CAB-CBB
45	AB	834	CLA	C4B-C3B-CAB-CBB
45	AB	834	CLA	CBD-CGD-O2D-CED
45	AB	834	CLA	C6-C7-C8-C9
45	AB	836	CLA	CBD-CGD-O2D-CED
45	AB	839	CLA	CHA-CBD-CGD-O1D
45	AB	839	CLA	CHA-CBD-CGD-O2D
45	AB	841	CLA	C6-C7-C8-C9
45	AF	802	CLA	C3A-C2A-CAA-CBA
45	AF	803	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	AG	203	CLA	CBD-CGD-O2D-CED
45	AG	204	CLA	CBD-CGD-O2D-CED
45	AH	201	CLA	C3A-C2A-CAA-CBA
45	AH	201	CLA	C2B-C3B-CAB-CBB
45	AH	201	CLA	C4B-C3B-CAB-CBB
45	AH	201	CLA	CBD-CGD-O2D-CED
45	AJ	102	CLA	C1A-C2A-CAA-CBA
45	AK	202	CLA	C4B-C3B-CAB-CBB
45	AK	203	CLA	C1A-C2A-CAA-CBA
45	AK	203	CLA	CBD-CGD-O2D-CED
45	AL	305	CLA	C1A-C2A-CAA-CBA
45	AL	305	CLA	CHA-CBD-CGD-O1D
45	AL	305	CLA	CHA-CBD-CGD-O2D
45	A1	306	CLA	CAD-CBD-CGD-O1D
45	A1	306	CLA	CAD-CBD-CGD-O2D
45	A1	306	CLA	CBD-CGD-O2D-CED
45	A1	307	CLA	C4B-C3B-CAB-CBB
45	A1	307	CLA	CBD-CGD-O2D-CED
45	A1	309	CLA	C1A-C2A-CAA-CBA
45	A1	310	CLA	CBD-CGD-O2D-CED
45	A1	313	CLA	CBD-CGD-O2D-CED
45	A1	314	CLA	C11-C10-C8-C9
45	A3	303	CLA	C1A-C2A-CAA-CBA
45	A3	303	CLA	C3A-C2A-CAA-CBA
45	A3	305	CLA	C1A-C2A-CAA-CBA
45	A3	305	CLA	C2B-C3B-CAB-CBB
45	A3	305	CLA	C4B-C3B-CAB-CBB
45	A3	308	CLA	C2B-C3B-CAB-CBB
45	A3	308	CLA	C4B-C3B-CAB-CBB
45	A3	309	CLA	CBD-CGD-O2D-CED
45	A3	310	CLA	C4B-C3B-CAB-CBB
45	A3	313	CLA	C2B-C3B-CAB-CBB
45	A3	313	CLA	C4B-C3B-CAB-CBB
45	A4	302	CLA	CBD-CGD-O2D-CED
45	A4	303	CLA	CBD-CGD-O2D-CED
45	A4	308	CLA	C2B-C3B-CAB-CBB
45	A4	308	CLA	C4B-C3B-CAB-CBB
45	A4	309	CLA	C1A-C2A-CAA-CBA
45	A4	309	CLA	C3A-C2A-CAA-CBA
45	A4	310	CLA	C1A-C2A-CAA-CBA
45	A4	310	CLA	C3A-C2A-CAA-CBA
45	A4	310	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
45	A4	312	CLA	C2B-C3B-CAB-CBB
45	A4	312	CLA	C4B-C3B-CAB-CBB
45	A4	312	CLA	CBD-CGD-O2D-CED
45	A4	313	CLA	C1A-C2A-CAA-CBA
45	A4	313	CLA	C4B-C3B-CAB-CBB
45	A4	313	CLA	CBD-CGD-O2D-CED
45	A6	605	CLA	CAA-CBA-CGA-O1A
45	A6	609	CLA	C1A-C2A-CAA-CBA
45	A6	609	CLA	C3A-C2A-CAA-CBA
45	A6	611	CLA	CMA-C3A-C4A-CHB
45	A6	611	CLA	CMA-C3A-C4A-NA
45	A6	611	CLA	CAD-CBD-CGD-O1D
45	A6	611	CLA	CAD-CBD-CGD-O2D
45	A6	612	CLA	C4B-C3B-CAB-CBB
45	BA	801	CLA	CBD-CGD-O2D-CED
45	BA	802	CLA	CBD-CGD-O2D-CED
45	BA	803	CLA	CHA-CBD-CGD-O1D
45	BA	803	CLA	CHA-CBD-CGD-O2D
45	BA	804	CLA	C1A-C2A-CAA-CBA
45	BA	804	CLA	C3A-C2A-CAA-CBA
45	BA	808	CLA	C2B-C3B-CAB-CBB
45	BA	808	CLA	C4B-C3B-CAB-CBB
45	BA	808	CLA	CHA-CBD-CGD-O1D
45	BA	808	CLA	CHA-CBD-CGD-O2D
45	BA	809	CLA	C1A-C2A-CAA-CBA
45	BA	809	CLA	C2B-C3B-CAB-CBB
45	BA	809	CLA	C4B-C3B-CAB-CBB
45	BA	811	CLA	C4B-C3B-CAB-CBB
45	BA	813	CLA	CAD-CBD-CGD-O2D
45	BA	816	CLA	CHA-CBD-CGD-O1D
45	BA	816	CLA	CHA-CBD-CGD-O2D
45	BA	818	CLA	C1A-C2A-CAA-CBA
45	BA	818	CLA	C3A-C2A-CAA-CBA
45	BA	818	CLA	C2B-C3B-CAB-CBB
45	BA	818	CLA	C4B-C3B-CAB-CBB
45	BA	819	CLA	C3A-C2A-CAA-CBA
45	BA	820	CLA	C2B-C3B-CAB-CBB
45	BA	820	CLA	C4B-C3B-CAB-CBB
45	BA	820	CLA	CHA-CBD-CGD-O1D
45	BA	820	CLA	CHA-CBD-CGD-O2D
45	BA	821	CLA	CBD-CGD-O2D-CED
45	BA	822	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
45	BA	822	CLA	CAD-CBD-CGD-O1D
45	BA	822	CLA	CAD-CBD-CGD-O2D
45	BA	823	CLA	C2B-C3B-CAB-CBB
45	BA	823	CLA	C4B-C3B-CAB-CBB
45	BA	824	CLA	C1A-C2A-CAA-CBA
45	BA	824	CLA	C3A-C2A-CAA-CBA
45	BA	824	CLA	C2B-C3B-CAB-CBB
45	BA	824	CLA	C4B-C3B-CAB-CBB
45	BA	827	CLA	C6-C7-C8-C9
45	BA	828	CLA	CBD-CGD-O2D-CED
45	BA	831	CLA	C2B-C3B-CAB-CBB
45	BA	831	CLA	C4B-C3B-CAB-CBB
45	BA	833	CLA	C2B-C3B-CAB-CBB
45	BA	833	CLA	C4B-C3B-CAB-CBB
45	BA	833	CLA	CAD-CBD-CGD-O1D
45	BA	833	CLA	CAD-CBD-CGD-O2D
45	BA	833	CLA	CBD-CGD-O2D-CED
45	BA	835	CLA	CBD-CGD-O2D-CED
45	BA	836	CLA	C4B-C3B-CAB-CBB
45	BA	839	CLA	CHA-CBD-CGD-O2D
45	BA	840	CLA	CBD-CGD-O2D-CED
45	BA	841	CLA	CAD-CBD-CGD-O2D
45	BA	844	CLA	CHA-CBD-CGD-O1D
45	BA	844	CLA	CHA-CBD-CGD-O2D
45	BA	844	CLA	CBD-CGD-O2D-CED
45	BB	804	CLA	CBD-CGD-O2D-CED
45	BB	805	CLA	C1A-C2A-CAA-CBA
45	BB	805	CLA	C3A-C2A-CAA-CBA
45	BB	805	CLA	CBD-CGD-O2D-CED
45	BB	807	CLA	C3A-C2A-CAA-CBA
45	BB	810	CLA	C1A-C2A-CAA-CBA
45	BB	810	CLA	CHA-CBD-CGD-O1D
45	BB	810	CLA	CHA-CBD-CGD-O2D
45	BB	811	CLA	CBD-CGD-O2D-CED
45	BB	812	CLA	C1A-C2A-CAA-CBA
45	BB	813	CLA	CBD-CGD-O2D-CED
45	BB	815	CLA	C4C-C3C-CAC-CBC
45	BB	815	CLA	CBD-CGD-O2D-CED
45	BB	816	CLA	CBD-CGD-O2D-CED
45	BB	817	CLA	CAD-CBD-CGD-O2D
45	BB	818	CLA	CBD-CGD-O2D-CED
45	BB	819	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	BB	819	CLA	C4B-C3B-CAB-CBB
45	BB	820	CLA	C3A-C2A-CAA-CBA
45	BB	821	CLA	C2B-C3B-CAB-CBB
45	BB	821	CLA	C4B-C3B-CAB-CBB
45	BB	823	CLA	C1A-C2A-CAA-CBA
45	BB	825	CLA	C1A-C2A-CAA-CBA
45	BB	825	CLA	C3A-C2A-CAA-CBA
45	BB	826	CLA	CHA-CBD-CGD-O2D
45	BB	830	CLA	C1A-C2A-CAA-CBA
45	BB	835	CLA	C2B-C3B-CAB-CBB
45	BB	835	CLA	C4B-C3B-CAB-CBB
45	BB	835	CLA	C6-C7-C8-C9
45	BB	836	CLA	CBD-CGD-O2D-CED
45	BB	837	CLA	C1A-C2A-CAA-CBA
45	BB	837	CLA	CBD-CGD-O2D-CED
45	BB	838	CLA	CBD-CGD-O2D-CED
45	BB	840	CLA	CHA-CBD-CGD-O1D
45	BB	840	CLA	CHA-CBD-CGD-O2D
45	BF	301	CLA	C1A-C2A-CAA-CBA
45	BF	301	CLA	C3A-C2A-CAA-CBA
45	BF	303	CLA	CBD-CGD-O2D-CED
45	BG	201	CLA	C1A-C2A-CAA-CBA
45	BG	201	CLA	C3A-C2A-CAA-CBA
45	BG	201	CLA	CBD-CGD-O2D-CED
45	BG	202	CLA	CBD-CGD-O2D-CED
45	BH	201	CLA	C1A-C2A-CAA-CBA
45	BH	201	CLA	CBD-CGD-O2D-CED
45	BH	201	CLA	O1D-CGD-O2D-CED
45	BL	302	CLA	C2B-C3B-CAB-CBB
45	BL	302	CLA	C4B-C3B-CAB-CBB
45	BL	303	CLA	C1A-C2A-CAA-CBA
45	BL	304	CLA	CHA-CBD-CGD-O1D
45	BL	304	CLA	CHA-CBD-CGD-O2D
45	B1	305	CLA	CHA-CBD-CGD-O1D
45	B1	305	CLA	CHA-CBD-CGD-O2D
45	B1	307	CLA	CBD-CGD-O2D-CED
45	B1	309	CLA	C2B-C3B-CAB-CBB
45	B1	309	CLA	C4B-C3B-CAB-CBB
45	B1	310	CLA	CAD-CBD-CGD-O2D
45	B1	311	CLA	CBD-CGD-O2D-CED
45	B2	602	CLA	C2B-C3B-CAB-CBB
45	B2	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	B2	603	CLA	CHA-CBD-CGD-O2D
45	B2	604	CLA	CAA-CBA-CGA-O1A
45	B2	609	CLA	C2B-C3B-CAB-CBB
45	B2	609	CLA	C4B-C3B-CAB-CBB
45	B2	610	CLA	CMA-C3A-C4A-CHB
45	B2	610	CLA	CMA-C3A-C4A-NA
45	B3	302	CLA	C1A-C2A-CAA-CBA
45	B3	302	CLA	C3A-C2A-CAA-CBA
45	B3	303	CLA	CAD-CBD-CGD-O2D
45	B3	304	CLA	C1A-C2A-CAA-CBA
45	B3	304	CLA	C3A-C2A-CAA-CBA
45	B3	304	CLA	C2B-C3B-CAB-CBB
45	B3	304	CLA	C4B-C3B-CAB-CBB
45	B3	308	CLA	C2B-C3B-CAB-CBB
45	B3	308	CLA	C4B-C3B-CAB-CBB
45	B3	309	CLA	C4B-C3B-CAB-CBB
45	B3	313	CLA	C4B-C3B-CAB-CBB
45	B5	601	CLA	C4B-C3B-CAB-CBB
45	B5	601	CLA	CAD-CBD-CGD-O1D
45	B5	601	CLA	CAD-CBD-CGD-O2D
45	B5	603	CLA	CHA-CBD-CGD-O1D
45	B5	603	CLA	CHA-CBD-CGD-O2D
45	B5	604	CLA	CBD-CGD-O2D-CED
45	B5	609	CLA	C2B-C3B-CAB-CBB
45	B5	609	CLA	C4B-C3B-CAB-CBB
45	B5	609	CLA	CBD-CGD-O2D-CED
45	B5	610	CLA	C1A-C2A-CAA-CBA
45	B5	610	CLA	C3A-C2A-CAA-CBA
45	B5	611	CLA	C1A-C2A-CAA-CBA
46	AB	843	PQN	C19-C18-C20-C21
46	BB	844	PQN	C11-C12-C13-C14
46	BB	844	PQN	C19-C18-C20-C21
47	AA	844	LHG	C4-O6-P-O4
47	AJ	104	LHG	C4-O6-P-O3
47	AJ	104	LHG	C4-O6-P-O4
47	AJ	104	LHG	C4-O6-P-O5
47	A1	302	LHG	C3-O3-P-O6
47	A1	320	LHG	C4-O6-P-O3
47	A1	320	LHG	C4-O6-P-O4
47	A1	320	LHG	C4-O6-P-O5
47	A3	301	LHG	C3-O3-P-O5
47	A3	301	LHG	C4-O6-P-O3

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Mol	Chain	Res	Type	Atoms
47	A3	301	LHG	C4-O6-P-O4
47	A3	301	LHG	C4-O6-P-O5
47	A3	319	LHG	C3-O3-P-O4
47	A3	319	LHG	C3-O3-P-O5
47	A3	319	LHG	C3-O3-P-O6
47	A6	618	LHG	C3-O3-P-O4
47	A6	618	LHG	C3-O3-P-O6
47	A6	618	LHG	C4-O6-P-O3
47	A6	618	LHG	C4-O6-P-O5
47	BA	845	LHG	C3-O3-P-O5
47	BA	846	LHG	C1-C2-C3-O3
47	BA	846	LHG	C3-O3-P-O4
47	BA	846	LHG	C3-O3-P-O5
47	BA	846	LHG	C3-O3-P-O6
47	BF	305	LHG	C3-O3-P-O5
47	BF	305	LHG	C3-O3-P-O6
47	BF	305	LHG	C4-O6-P-O5
47	BF	305	LHG	C8-C7-O7-C5
47	B1	301	LHG	O10-C23-O8-C6
47	B1	301	LHG	C24-C23-O8-C6
47	B1	302	LHG	C3-O3-P-O4
47	B1	302	LHG	C3-O3-P-O5
47	B1	302	LHG	C3-O3-P-O6
47	B1	318	LHG	C3-O3-P-O4
47	B1	318	LHG	C3-O3-P-O6
47	B1	318	LHG	C4-O6-P-O5
47	B2	618	LHG	O2-C2-C3-O3
47	B2	618	LHG	C3-O3-P-O4
47	B2	618	LHG	C3-O3-P-O5
47	B2	618	LHG	C3-O3-P-O6
47	B2	618	LHG	C4-O6-P-O3
47	B2	618	LHG	C4-O6-P-O5
47	B2	618	LHG	O7-C5-C6-O8
47	B3	318	LHG	C4-O6-P-O3
47	B3	318	LHG	C4-O6-P-O4
47	B5	618	LHG	C3-O3-P-O5
47	B5	618	LHG	C4-O6-P-O3
47	B5	618	LHG	C8-C7-O7-C5
47	F	801	LHG	C1-C2-C3-O3
47	F	801	LHG	C3-O3-P-O4
47	F	801	LHG	O6-C4-C5-O7
47	a	501	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
47	a	501	LHG	C3-O3-P-O6
48	AA	845	BCR	C7-C8-C9-C10
48	AA	846	BCR	C21-C22-C23-C24
48	AA	846	BCR	C23-C24-C25-C26
48	AA	847	BCR	C5-C6-C7-C8
48	AA	847	BCR	C7-C8-C9-C10
48	AA	847	BCR	C21-C22-C23-C24
48	AA	849	BCR	C23-C24-C25-C26
48	AA	852	BCR	C23-C24-C25-C26
48	AA	852	BCR	C23-C24-C25-C30
48	AB	844	BCR	C5-C6-C7-C8
48	AB	845	BCR	C7-C8-C9-C10
48	AB	845	BCR	C23-C24-C25-C26
48	AB	845	BCR	C23-C24-C25-C30
48	AB	848	BCR	C21-C22-C23-C24
48	AB	849	BCR	C21-C22-C23-C24
48	AB	849	BCR	C37-C22-C23-C24
48	AB	849	BCR	C23-C24-C25-C26
48	AB	849	BCR	C23-C24-C25-C30
48	AF	801	BCR	C23-C24-C25-C26
48	AF	801	BCR	C23-C24-C25-C30
48	AF	805	BCR	C7-C8-C9-C10
48	AI	101	BCR	C7-C8-C9-C10
48	AI	102	BCR	C7-C8-C9-C10
48	AI	102	BCR	C7-C8-C9-C34
48	AJ	103	BCR	C5-C6-C7-C8
48	AL	302	BCR	C1-C6-C7-C8
48	AL	302	BCR	C5-C6-C7-C8
48	A1	319	BCR	C1-C6-C7-C8
48	A1	319	BCR	C5-C6-C7-C8
48	A3	318	BCR	C21-C22-C23-C24
48	A6	617	BCR	C5-C6-C7-C8
48	BA	848	BCR	C23-C24-C25-C26
48	BA	848	BCR	C23-C24-C25-C30
48	BA	849	BCR	C1-C6-C7-C8
48	BA	849	BCR	C5-C6-C7-C8
48	BA	849	BCR	C21-C22-C23-C24
48	BA	850	BCR	C23-C24-C25-C26
48	BA	851	BCR	C5-C6-C7-C8
48	BA	851	BCR	C23-C24-C25-C26
48	BA	855	BCR	C23-C24-C25-C26
48	BA	856	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
48	BB	803	BCR	C23-C24-C25-C26
48	BB	803	BCR	C23-C24-C25-C30
48	BB	845	BCR	C1-C6-C7-C8
48	BB	845	BCR	C5-C6-C7-C8
48	BB	845	BCR	C23-C24-C25-C26
48	BB	846	BCR	C7-C8-C9-C10
48	BB	846	BCR	C23-C24-C25-C26
48	BB	846	BCR	C23-C24-C25-C30
48	BB	849	BCR	C21-C22-C23-C24
48	BF	304	BCR	C5-C6-C7-C8
48	BJ	103	BCR	C5-C6-C7-C8
48	BL	301	BCR	C1-C6-C7-C8
48	BL	305	BCR	C1-C6-C7-C8
48	BL	305	BCR	C5-C6-C7-C8
48	BL	306	BCR	C37-C22-C23-C24
48	B3	317	BCR	C37-C22-C23-C24
48	B3	317	BCR	C23-C24-C25-C26
48	B3	317	BCR	C23-C24-C25-C30
50	AA	851	LMU	O5'-C1'-O1'-C1
50	AB	852	LMU	C2'-C1'-O1'-C1
50	AB	852	LMU	O5'-C1'-O1'-C1
51	AB	851	DGD	C2B-C1B-O2G-C2G
51	AB	851	DGD	O2G-C2G-C3G-O3G
51	BB	850	DGD	C2B-C1B-O2G-C2G
51	BB	850	DGD	O1B-C1B-O2G-C2G
52	B1	316	LUT	C10-C11-C12-C13
52	B1	316	LUT	C11-C12-C13-C14
52	B1	316	LUT	C27-C28-C29-C30
52	B1	316	LUT	C27-C28-C29-C39
52	B3	315	LUT	C21-C26-C27-C28
52	B3	315	LUT	C25-C26-C27-C28
53	A1	321	LMG	O9-C10-O7-C8
53	A1	321	LMG	C11-C10-O7-C8
53	A4	318	LMG	O6-C1-O1-C7
53	A4	318	LMG	C11-C10-O7-C8
54	A1	308	CHL	CAD-CBD-CGD-O2D
54	A3	307	CHL	CBD-CGD-O2D-CED
54	A6	607	CHL	CBD-CGD-O2D-CED
54	B2	601	CHL	CAD-CBD-CGD-O1D
54	B2	601	CHL	CAD-CBD-CGD-O2D
54	B2	601	CHL	C3-C5-C6-C7
54	B3	306	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
56	BJ	104	SQD	C24-C23-O48-C46
56	BJ	104	SQD	C5-C6-S-O7
56	e	301	SQD	O5-C5-C6-S
45	BB	815	CLA	C2C-C3C-CAC-CBC
45	AA	823	CLA	O1D-CGD-O2D-CED
45	AB	803	CLA	O1D-CGD-O2D-CED
45	AH	201	CLA	O1D-CGD-O2D-CED
45	AK	203	CLA	O1D-CGD-O2D-CED
45	A1	305	CLA	O1D-CGD-O2D-CED
45	A1	307	CLA	O1D-CGD-O2D-CED
45	A1	310	CLA	O1D-CGD-O2D-CED
45	A1	311	CLA	O1D-CGD-O2D-CED
45	A3	303	CLA	O1D-CGD-O2D-CED
45	BA	801	CLA	O1D-CGD-O2D-CED
45	BB	818	CLA	O1D-CGD-O2D-CED
45	BB	833	CLA	O1D-CGD-O2D-CED
45	B1	306	CLA	O1D-CGD-O2D-CED
45	B5	602	CLA	O1D-CGD-O2D-CED
54	B2	607	CHL	O1D-CGD-O2D-CED
45	AA	834	CLA	C4C-C3C-CAC-CBC
45	AA	802	CLA	O1D-CGD-O2D-CED
45	AA	810	CLA	O1D-CGD-O2D-CED
45	AB	804	CLA	O1D-CGD-O2D-CED
45	AB	807	CLA	O1D-CGD-O2D-CED
45	AB	815	CLA	O1D-CGD-O2D-CED
45	AB	830	CLA	O1D-CGD-O2D-CED
45	AB	836	CLA	O1D-CGD-O2D-CED
45	AG	204	CLA	O1D-CGD-O2D-CED
45	A4	303	CLA	O1D-CGD-O2D-CED
45	BA	802	CLA	O1D-CGD-O2D-CED
45	BA	810	CLA	O1D-CGD-O2D-CED
45	BA	821	CLA	O1D-CGD-O2D-CED
45	BB	805	CLA	O1D-CGD-O2D-CED
45	BB	813	CLA	O1D-CGD-O2D-CED
45	BB	816	CLA	O1D-CGD-O2D-CED
45	BB	837	CLA	O1D-CGD-O2D-CED
45	BG	202	CLA	O1D-CGD-O2D-CED
45	B2	611	CLA	O1D-CGD-O2D-CED
47	A3	319	LHG	C8-C7-O7-C5
45	AA	810	CLA	CBD-CGD-O2D-CED
45	AA	811	CLA	CBD-CGD-O2D-CED
45	AA	813	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	AA	814	CLA	CBD-CGD-O2D-CED
45	AA	815	CLA	CBD-CGD-O2D-CED
45	AA	823	CLA	CBD-CGD-O2D-CED
45	AA	834	CLA	CBD-CGD-O2D-CED
45	AA	842	CLA	CBD-CGD-O2D-CED
45	AB	801	CLA	CBD-CGD-O2D-CED
45	AB	803	CLA	CBD-CGD-O2D-CED
45	AB	822	CLA	CBD-CGD-O2D-CED
45	AB	823	CLA	CBD-CGD-O2D-CED
45	AB	830	CLA	CBD-CGD-O2D-CED
45	AF	802	CLA	CBD-CGD-O2D-CED
45	A1	305	CLA	CBD-CGD-O2D-CED
45	A1	311	CLA	CBD-CGD-O2D-CED
45	A3	302	CLA	CBD-CGD-O2D-CED
45	A3	303	CLA	CBD-CGD-O2D-CED
45	A6	603	CLA	CBD-CGD-O2D-CED
45	BA	810	CLA	CBD-CGD-O2D-CED
45	BA	811	CLA	CBD-CGD-O2D-CED
45	BA	814	CLA	CBD-CGD-O2D-CED
45	BA	820	CLA	CBD-CGD-O2D-CED
45	BA	834	CLA	CBD-CGD-O2D-CED
45	BA	841	CLA	CBD-CGD-O2D-CED
45	BB	808	CLA	CBD-CGD-O2D-CED
45	BB	812	CLA	CBD-CGD-O2D-CED
45	BB	826	CLA	CBD-CGD-O2D-CED
45	BB	833	CLA	CBD-CGD-O2D-CED
45	BB	834	CLA	CBD-CGD-O2D-CED
45	BF	302	CLA	CBD-CGD-O2D-CED
45	BK	203	CLA	CBD-CGD-O2D-CED
45	B1	305	CLA	CBD-CGD-O2D-CED
45	B1	306	CLA	CBD-CGD-O2D-CED
45	B2	604	CLA	CBD-CGD-O2D-CED
45	B2	609	CLA	CBD-CGD-O2D-CED
45	B2	611	CLA	CBD-CGD-O2D-CED
45	B3	302	CLA	CBD-CGD-O2D-CED
45	B3	308	CLA	CBD-CGD-O2D-CED
45	B5	602	CLA	CBD-CGD-O2D-CED
45	B5	610	CLA	CBD-CGD-O2D-CED
54	A4	306	CHL	CBD-CGD-O2D-CED
54	A6	608	CHL	CBD-CGD-O2D-CED
54	B2	607	CHL	CBD-CGD-O2D-CED
54	B5	607	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	AB	830	CLA	O1A-CGA-O2A-C1
45	BA	832	CLA	O1A-CGA-O2A-C1
45	B3	302	CLA	O1A-CGA-O2A-C1
47	B1	302	LHG	O10-C23-O8-C6
56	BJ	104	SQD	O10-C23-O48-C46
45	BB	805	CLA	C2C-C3C-CAC-CBC
45	BB	804	CLA	O1D-CGD-O2D-CED
45	B5	604	CLA	O1D-CGD-O2D-CED
47	B3	318	LHG	C8-C7-O7-C5
45	AK	203	CLA	CBA-CGA-O2A-C1
45	BK	203	CLA	CBA-CGA-O2A-C1
45	AA	801	CLA	O1D-CGD-O2D-CED
45	AA	814	CLA	O1D-CGD-O2D-CED
45	AB	801	CLA	O1D-CGD-O2D-CED
45	BA	814	CLA	O1D-CGD-O2D-CED
45	B5	610	CLA	O1D-CGD-O2D-CED
54	A4	306	CHL	O1D-CGD-O2D-CED
54	B5	607	CHL	O1D-CGD-O2D-CED
45	BA	832	CLA	CBA-CGA-O2A-C1
47	B1	302	LHG	C24-C23-O8-C6
45	BB	843	CLA	CBD-CGD-O2D-CED
45	AA	817	CLA	O1A-CGA-O2A-C1
45	AA	821	CLA	O1A-CGA-O2A-C1
45	AL	304	CLA	O1A-CGA-O2A-C1
45	A3	303	CLA	O1A-CGA-O2A-C1
45	BA	817	CLA	O1A-CGA-O2A-C1
45	BA	821	CLA	O1A-CGA-O2A-C1
45	BA	827	CLA	O1A-CGA-O2A-C1
45	BA	833	CLA	O1A-CGA-O2A-C1
45	BA	837	CLA	O1A-CGA-O2A-C1
45	BA	838	CLA	O1A-CGA-O2A-C1
45	BB	812	CLA	O1A-CGA-O2A-C1
45	BB	843	CLA	O1A-CGA-O2A-C1
45	BL	303	CLA	O1A-CGA-O2A-C1
47	A1	301	LHG	O10-C23-O8-C6
47	A6	618	LHG	O10-C23-O8-C6
47	a	501	LHG	O10-C23-O8-C6
54	A1	303	CHL	O1A-CGA-O2A-C1
54	B1	303	CHL	O1A-CGA-O2A-C1
45	AA	834	CLA	C2C-C3C-CAC-CBC
45	AA	811	CLA	O1D-CGD-O2D-CED
45	AA	833	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	AB	816	CLA	O1D-CGD-O2D-CED
45	AF	802	CLA	O1D-CGD-O2D-CED
45	AF	803	CLA	O1D-CGD-O2D-CED
45	AG	203	CLA	O1D-CGD-O2D-CED
45	BA	833	CLA	O1D-CGD-O2D-CED
45	BA	844	CLA	O1D-CGD-O2D-CED
45	BB	826	CLA	O1D-CGD-O2D-CED
45	BF	303	CLA	O1D-CGD-O2D-CED
45	B1	307	CLA	O1D-CGD-O2D-CED
45	B1	311	CLA	O1D-CGD-O2D-CED
45	B5	609	CLA	O1D-CGD-O2D-CED
54	A3	307	CHL	O1D-CGD-O2D-CED
54	A6	608	CHL	O1D-CGD-O2D-CED
54	B3	306	CHL	O1D-CGD-O2D-CED
45	AA	828	CLA	O1D-CGD-O2D-CED
45	A1	306	CLA	O1D-CGD-O2D-CED
45	A1	313	CLA	O1D-CGD-O2D-CED
45	A4	302	CLA	O1D-CGD-O2D-CED
45	A4	312	CLA	O1D-CGD-O2D-CED
45	A4	313	CLA	O1D-CGD-O2D-CED
45	BB	836	CLA	O1D-CGD-O2D-CED
45	BB	838	CLA	O1D-CGD-O2D-CED
45	BG	201	CLA	O1D-CGD-O2D-CED
45	AB	837	CLA	CBD-CGD-O2D-CED
50	AL	301	LMU	O5B-C1B-O1B-C4'
45	AA	833	CLA	O1A-CGA-O2A-C1
47	BF	305	LHG	O9-C7-O7-C5
47	B5	618	LHG	O9-C7-O7-C5
51	AB	851	DGD	O1B-C1B-O2G-C2G
45	A3	309	CLA	O1D-CGD-O2D-CED
45	BK	203	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	C3-C5-C6-C7
45	AB	810	CLA	C3-C5-C6-C7
45	AB	812	CLA	C3-C5-C6-C7
45	AB	820	CLA	C3-C5-C6-C7
45	AB	835	CLA	C3-C5-C6-C7
45	AB	840	CLA	C3-C5-C6-C7
45	AB	841	CLA	C3-C5-C6-C7
45	AH	201	CLA	C3-C5-C6-C7
45	A1	314	CLA	C3-C5-C6-C7
45	A6	603	CLA	C3-C5-C6-C7
45	A6	613	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
45	BA	828	CLA	C3-C5-C6-C7
45	BA	832	CLA	C3-C5-C6-C7
45	BF	301	CLA	C3-C5-C6-C7
45	BH	201	CLA	C3-C5-C6-C7
45	B1	305	CLA	C3-C5-C6-C7
45	B1	314	CLA	C3-C5-C6-C7
45	B2	602	CLA	C3-C5-C6-C7
46	BA	843	PQN	C13-C15-C16-C17
45	BA	835	CLA	O1D-CGD-O2D-CED
54	A6	607	CHL	O1D-CGD-O2D-CED
45	AA	811	CLA	CBA-CGA-O2A-C1
45	AA	812	CLA	CBA-CGA-O2A-C1
45	AA	842	CLA	CBA-CGA-O2A-C1
45	AB	830	CLA	CBA-CGA-O2A-C1
45	AL	304	CLA	CBA-CGA-O2A-C1
45	A1	314	CLA	CBA-CGA-O2A-C1
45	BA	806	CLA	CBA-CGA-O2A-C1
45	BA	811	CLA	CBA-CGA-O2A-C1
45	BA	821	CLA	CBA-CGA-O2A-C1
45	BA	837	CLA	CBA-CGA-O2A-C1
45	B3	302	CLA	CBA-CGA-O2A-C1
47	A1	301	LHG	C24-C23-O8-C6
47	a	501	LHG	C24-C23-O8-C6
54	A1	303	CHL	CBA-CGA-O2A-C1
45	AA	820	CLA	CBD-CGD-O2D-CED
45	AA	821	CLA	CBD-CGD-O2D-CED
45	AA	826	CLA	CBD-CGD-O2D-CED
45	AA	829	CLA	CBD-CGD-O2D-CED
45	AA	831	CLA	CBD-CGD-O2D-CED
45	AA	836	CLA	CBD-CGD-O2D-CED
45	AB	802	CLA	CBD-CGD-O2D-CED
45	AB	811	CLA	CBD-CGD-O2D-CED
45	AB	820	CLA	CBD-CGD-O2D-CED
45	AB	832	CLA	CBD-CGD-O2D-CED
45	AB	838	CLA	CBD-CGD-O2D-CED
45	AL	305	CLA	CBD-CGD-O2D-CED
45	A4	308	CLA	CBD-CGD-O2D-CED
45	A6	613	CLA	CBD-CGD-O2D-CED
45	BA	813	CLA	CBD-CGD-O2D-CED
45	BA	817	CLA	CBD-CGD-O2D-CED
45	BA	823	CLA	CBD-CGD-O2D-CED
45	BA	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	BA	831	CLA	CBD-CGD-O2D-CED
45	BA	836	CLA	CBD-CGD-O2D-CED
45	BB	831	CLA	CBD-CGD-O2D-CED
45	BB	839	CLA	CBD-CGD-O2D-CED
45	BL	304	CLA	CBD-CGD-O2D-CED
45	B3	301	CLA	CBD-CGD-O2D-CED
45	B5	601	CLA	CBD-CGD-O2D-CED
54	B2	605	CHL	CBD-CGD-O2D-CED
45	AA	815	CLA	O1D-CGD-O2D-CED
45	AB	810	CLA	O1D-CGD-O2D-CED
45	AB	834	CLA	O1D-CGD-O2D-CED
45	BA	811	CLA	O1D-CGD-O2D-CED
45	BA	828	CLA	O1D-CGD-O2D-CED
45	BA	840	CLA	O1D-CGD-O2D-CED
45	BB	811	CLA	O1D-CGD-O2D-CED
45	BB	815	CLA	O1D-CGD-O2D-CED
45	AK	203	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	C4-C3-C5-C6
45	AA	832	CLA	C4-C3-C5-C6
45	AB	802	CLA	C4-C3-C5-C6
45	AB	819	CLA	C4-C3-C5-C6
45	BA	834	CLA	C4-C3-C5-C6
45	BA	841	CLA	C4-C3-C5-C6
45	BB	802	CLA	C4-C3-C5-C6
45	BB	820	CLA	C4-C3-C5-C6
45	AA	829	CLA	C2-C3-C5-C6
45	AA	832	CLA	C2-C3-C5-C6
45	AB	802	CLA	C2-C3-C5-C6
45	BA	841	CLA	C2-C3-C5-C6
45	BB	802	CLA	C2-C3-C5-C6
45	BB	822	CLA	CBD-CGD-O2D-CED
45	B5	612	CLA	CBD-CGD-O2D-CED
45	AB	822	CLA	O1D-CGD-O2D-CED
45	B3	302	CLA	O1D-CGD-O2D-CED
45	BA	805	CLA	C2A-CAA-CBA-CGA
45	AB	811	CLA	O1A-CGA-O2A-C1
45	AB	823	CLA	C3-C5-C6-C7
45	AB	833	CLA	C3-C5-C6-C7
45	BA	805	CLA	C3-C5-C6-C7
45	BB	824	CLA	C3-C5-C6-C7
45	BB	842	CLA	C3-C5-C6-C7
45	AA	817	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
45	AA	821	CLA	CBA-CGA-O2A-C1
45	AA	826	CLA	CBA-CGA-O2A-C1
45	AA	832	CLA	CBA-CGA-O2A-C1
45	AA	833	CLA	CBA-CGA-O2A-C1
45	AA	838	CLA	CBA-CGA-O2A-C1
45	AB	817	CLA	CBA-CGA-O2A-C1
45	A1	306	CLA	CBA-CGA-O2A-C1
45	A3	303	CLA	CBA-CGA-O2A-C1
45	BA	810	CLA	CBA-CGA-O2A-C1
45	BA	817	CLA	CBA-CGA-O2A-C1
45	BA	824	CLA	CBA-CGA-O2A-C1
45	BA	827	CLA	CBA-CGA-O2A-C1
45	BA	833	CLA	CBA-CGA-O2A-C1
45	BA	838	CLA	CBA-CGA-O2A-C1
45	BA	842	CLA	CBA-CGA-O2A-C1
45	BB	812	CLA	CBA-CGA-O2A-C1
45	BB	819	CLA	CBA-CGA-O2A-C1
45	BB	823	CLA	CBA-CGA-O2A-C1
45	BB	828	CLA	CBA-CGA-O2A-C1
45	BB	843	CLA	CBA-CGA-O2A-C1
45	BL	303	CLA	CBA-CGA-O2A-C1
47	A6	618	LHG	C24-C23-O8-C6
54	B1	303	CHL	CBA-CGA-O2A-C1
56	e	301	SQD	C24-C23-O48-C46
46	AB	843	PQN	C11-C12-C13-C14
46	BA	843	PQN	C11-C12-C13-C14
47	A3	319	LHG	O9-C7-O7-C5
47	B3	318	LHG	O9-C7-O7-C5
50	AB	852	LMU	O5'-C5'-C6'-O6'
48	BL	306	BCR	C19-C20-C21-C22
45	AA	810	CLA	O1A-CGA-O2A-C1
45	AA	811	CLA	O1A-CGA-O2A-C1
45	AA	837	CLA	O1A-CGA-O2A-C1
45	AB	803	CLA	O1A-CGA-O2A-C1
45	AB	842	CLA	O1A-CGA-O2A-C1
45	A1	314	CLA	O1A-CGA-O2A-C1
45	BA	806	CLA	O1A-CGA-O2A-C1
45	BA	810	CLA	O1A-CGA-O2A-C1
45	BA	811	CLA	O1A-CGA-O2A-C1
45	BA	842	CLA	O1A-CGA-O2A-C1
45	BB	804	CLA	O1A-CGA-O2A-C1
45	BB	819	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
45	BB	828	CLA	O1A-CGA-O2A-C1
56	e	301	SQD	O10-C23-O48-C46
53	A4	318	LMG	O9-C10-O7-C8
51	AB	851	DGD	C4E-C5E-C6E-O5E
45	BA	841	CLA	O1D-CGD-O2D-CED
45	BB	808	CLA	O1D-CGD-O2D-CED
45	B2	604	CLA	O1D-CGD-O2D-CED
45	B2	609	CLA	O1D-CGD-O2D-CED
45	AA	805	CLA	C3-C5-C6-C7
45	AA	833	CLA	C3-C5-C6-C7
45	AF	802	CLA	C3-C5-C6-C7
45	BA	829	CLA	C3-C5-C6-C7
45	BA	833	CLA	C3-C5-C6-C7
45	BB	808	CLA	C3-C5-C6-C7
45	BB	816	CLA	C3-C5-C6-C7
45	BB	836	CLA	C3-C5-C6-C7
45	BB	841	CLA	C3-C5-C6-C7
45	B2	612	CLA	C3-C5-C6-C7
45	AB	825	CLA	CBD-CGD-O2D-CED
45	A6	614	CLA	CBD-CGD-O2D-CED
45	BA	815	CLA	CBD-CGD-O2D-CED
45	B3	310	CLA	CBD-CGD-O2D-CED
54	B2	606	CHL	CBD-CGD-O2D-CED
47	AJ	104	LHG	O2-C2-C3-O3
47	BF	305	LHG	O2-C2-C3-O3
47	a	501	LHG	O2-C2-C3-O3
45	AA	813	CLA	O1D-CGD-O2D-CED
45	BB	812	CLA	O1D-CGD-O2D-CED
45	BK	203	CLA	O1D-CGD-O2D-CED
45	B3	308	CLA	O1D-CGD-O2D-CED
45	AA	810	CLA	CBA-CGA-O2A-C1
45	AA	837	CLA	CBA-CGA-O2A-C1
45	AB	827	CLA	CBA-CGA-O2A-C1
45	BA	804	CLA	CBA-CGA-O2A-C1
45	BB	804	CLA	CBA-CGA-O2A-C1
47	A3	319	LHG	C24-C23-O8-C6
45	AA	812	CLA	O1A-CGA-O2A-C1
45	AA	842	CLA	O1A-CGA-O2A-C1
45	AB	817	CLA	O1A-CGA-O2A-C1
47	B3	318	LHG	O10-C23-O8-C6
45	BF	302	CLA	O1D-CGD-O2D-CED
50	AB	850	LMU	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
50	AB	852	LMU	C4'-C5'-C6'-O6'
45	AA	832	CLA	CBD-CGD-O2D-CED
47	A3	319	LHG	O10-C23-O8-C6
50	AB	853	LMU	O5'-C5'-C6'-O6'
45	AA	842	CLA	O1D-CGD-O2D-CED
45	AB	823	CLA	O1D-CGD-O2D-CED
45	BB	834	CLA	O1D-CGD-O2D-CED
45	AA	828	CLA	C3-C5-C6-C7
45	BA	803	CLA	C3-C5-C6-C7
45	BA	827	CLA	C3-C5-C6-C7
45	AA	838	CLA	CBD-CGD-O2D-CED
45	A1	304	CLA	CBD-CGD-O2D-CED
45	A1	316	CLA	CBD-CGD-O2D-CED
45	B2	602	CLA	CBD-CGD-O2D-CED
45	B2	610	CLA	CBD-CGD-O2D-CED
45	AA	834	CLA	O1D-CGD-O2D-CED
45	A3	302	CLA	O1D-CGD-O2D-CED
45	BA	834	CLA	O1D-CGD-O2D-CED
45	B1	305	CLA	O1D-CGD-O2D-CED
45	AB	803	CLA	CBA-CGA-O2A-C1
45	AB	811	CLA	CBA-CGA-O2A-C1
45	AB	815	CLA	CBA-CGA-O2A-C1
45	AB	842	CLA	CBA-CGA-O2A-C1
47	B3	318	LHG	C24-C23-O8-C6
45	AA	812	CLA	C4-C3-C5-C6
45	AA	824	CLA	C4-C3-C5-C6
45	AA	824	CLA	C2-C3-C5-C6
45	AA	826	CLA	O1A-CGA-O2A-C1
45	AA	832	CLA	O1A-CGA-O2A-C1
45	BA	804	CLA	O1A-CGA-O2A-C1
45	BA	824	CLA	O1A-CGA-O2A-C1
50	AA	851	LMU	O5B-C5B-C6B-O6B
45	A6	603	CLA	O1D-CGD-O2D-CED
50	AB	850	LMU	C4'-C5'-C6'-O6'
45	AA	812	CLA	CBD-CGD-O2D-CED
45	AA	830	CLA	CBD-CGD-O2D-CED
45	AB	805	CLA	CBD-CGD-O2D-CED
54	B5	606	CHL	CBD-CGD-O2D-CED
45	BA	829	CLA	C2A-CAA-CBA-CGA
45	BA	820	CLA	O1D-CGD-O2D-CED
45	BB	843	CLA	O1D-CGD-O2D-CED
45	AA	838	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
45	AB	819	CLA	O1A-CGA-O2A-C1
45	AB	827	CLA	O1A-CGA-O2A-C1
45	A1	306	CLA	O1A-CGA-O2A-C1
45	BA	819	CLA	O1A-CGA-O2A-C1
45	BB	823	CLA	O1A-CGA-O2A-C1
50	BA	854	LMU	O5'-C1'-O1'-C1
51	AB	851	DGD	O6D-C1D-O3G-C3G
45	A4	308	CLA	O1D-CGD-O2D-CED
45	AA	827	CLA	CBA-CGA-O2A-C1
45	AB	819	CLA	CBA-CGA-O2A-C1
45	AB	832	CLA	CBA-CGA-O2A-C1
45	AB	838	CLA	CBA-CGA-O2A-C1
45	BA	819	CLA	CBA-CGA-O2A-C1
45	BA	826	CLA	CBA-CGA-O2A-C1
45	BB	802	CLA	CBA-CGA-O2A-C1
45	BB	807	CLA	CBA-CGA-O2A-C1
45	BB	839	CLA	CBA-CGA-O2A-C1
45	BF	301	CLA	CBA-CGA-O2A-C1
45	B5	612	CLA	CBA-CGA-O2A-C1
45	AA	819	CLA	CBD-CGD-O2D-CED
45	AA	840	CLA	CBD-CGD-O2D-CED
45	AB	814	CLA	CBD-CGD-O2D-CED
45	AB	819	CLA	CBD-CGD-O2D-CED
45	AB	840	CLA	CBD-CGD-O2D-CED
45	AB	842	CLA	CBD-CGD-O2D-CED
45	BA	803	CLA	CBD-CGD-O2D-CED
45	BA	807	CLA	CBD-CGD-O2D-CED
45	BA	838	CLA	CBD-CGD-O2D-CED
45	BB	821	CLA	CBD-CGD-O2D-CED
45	BB	824	CLA	CBD-CGD-O2D-CED
45	BB	829	CLA	CBD-CGD-O2D-CED
45	BB	835	CLA	CBD-CGD-O2D-CED
45	B1	304	CLA	CBD-CGD-O2D-CED
45	B1	313	CLA	CBD-CGD-O2D-CED
45	B2	612	CLA	CBD-CGD-O2D-CED
45	B3	305	CLA	CBD-CGD-O2D-CED
45	B5	613	CLA	CBD-CGD-O2D-CED
51	AB	851	DGD	O6E-C5E-C6E-O5E
45	BB	815	CLA	C5-C6-C7-C8
45	BA	826	CLA	O1A-CGA-O2A-C1
45	AB	815	CLA	O1A-CGA-O2A-C1
45	AB	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
45	BB	802	CLA	O1A-CGA-O2A-C1
45	BB	807	CLA	O1A-CGA-O2A-C1
45	BF	301	CLA	O1A-CGA-O2A-C1
56	e	301	SQD	O49-C7-O47-C45
47	B2	618	LHG	C1-C2-C3-O3
45	AA	806	CLA	CBA-CGA-O2A-C1
45	AA	808	CLA	CBA-CGA-O2A-C1
45	AA	819	CLA	CBA-CGA-O2A-C1
45	AA	834	CLA	CBA-CGA-O2A-C1
45	AA	839	CLA	CBA-CGA-O2A-C1
45	AB	812	CLA	CBA-CGA-O2A-C1
45	AB	818	CLA	CBA-CGA-O2A-C1
45	AB	822	CLA	CBA-CGA-O2A-C1
45	AB	829	CLA	CBA-CGA-O2A-C1
45	AB	834	CLA	CBA-CGA-O2A-C1
45	AB	841	CLA	CBA-CGA-O2A-C1
45	AF	802	CLA	CBA-CGA-O2A-C1
45	BA	808	CLA	CBA-CGA-O2A-C1
45	BA	834	CLA	CBA-CGA-O2A-C1
45	BA	840	CLA	CBA-CGA-O2A-C1
45	BB	805	CLA	CBA-CGA-O2A-C1
45	BB	813	CLA	CBA-CGA-O2A-C1
45	BB	815	CLA	CBA-CGA-O2A-C1
45	BB	816	CLA	CBA-CGA-O2A-C1
45	BB	820	CLA	CBA-CGA-O2A-C1
45	B1	314	CLA	CBA-CGA-O2A-C1
45	B2	612	CLA	CBA-CGA-O2A-C1
47	A1	302	LHG	C24-C23-O8-C6
47	BA	845	LHG	C24-C23-O8-C6
47	B2	618	LHG	C24-C23-O8-C6
54	A6	602	CHL	CBA-CGA-O2A-C1
45	AL	303	CLA	CBD-CGD-O2D-CED
45	BA	839	CLA	CBD-CGD-O2D-CED
45	BB	805	CLA	C4C-C3C-CAC-CBC
45	AA	831	CLA	O1D-CGD-O2D-CED
45	AB	832	CLA	O1D-CGD-O2D-CED
45	AB	837	CLA	O1D-CGD-O2D-CED
45	BA	836	CLA	O1D-CGD-O2D-CED
45	BB	831	CLA	O1D-CGD-O2D-CED
45	BL	304	CLA	O1D-CGD-O2D-CED
45	B5	601	CLA	O1D-CGD-O2D-CED
45	BA	838	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
45	AA	812	CLA	C2-C3-C5-C6
45	AB	819	CLA	C2-C3-C5-C6
45	BA	834	CLA	C2-C3-C5-C6
45	BA	838	CLA	C2-C3-C5-C6
45	BB	820	CLA	C2-C3-C5-C6
45	AA	813	CLA	C3-C5-C6-C7
45	AA	821	CLA	C11-C10-C8-C9
45	AA	827	CLA	C6-C7-C8-C9
45	AA	840	CLA	C11-C12-C13-C14
45	AB	801	CLA	C6-C7-C8-C9
45	AB	804	CLA	C11-C12-C13-C14
45	AB	815	CLA	C14-C13-C15-C16
45	AB	823	CLA	C6-C7-C8-C9
45	AB	829	CLA	C14-C13-C15-C16
45	AB	842	CLA	C14-C13-C15-C16
45	BA	806	CLA	C14-C13-C15-C16
45	BA	828	CLA	C14-C13-C15-C16
45	BA	840	CLA	C11-C12-C13-C14
45	BB	801	CLA	C6-C7-C8-C9
45	BB	824	CLA	C6-C7-C8-C9
45	BB	830	CLA	C14-C13-C15-C16
45	BB	842	CLA	C6-C7-C8-C9
50	AL	301	LMU	C5'-C4'-O1B-C1B
45	AA	821	CLA	O1D-CGD-O2D-CED
45	BB	839	CLA	O1D-CGD-O2D-CED
45	B3	301	CLA	O1D-CGD-O2D-CED
50	AA	851	LMU	C2'-C1'-O1'-C1
50	AL	301	LMU	C2'-C1'-O1'-C1
50	BA	854	LMU	C2'-C1'-O1'-C1
47	A3	319	LHG	O2-C2-C3-O3
47	BA	846	LHG	O2-C2-C3-O3
47	B3	318	LHG	O2-C2-C3-O3
47	F	801	LHG	O2-C2-C3-O3
45	BA	823	CLA	O1D-CGD-O2D-CED
45	BB	830	CLA	CBA-CGA-O2A-C1
45	AB	834	CLA	O1A-CGA-O2A-C1
45	BB	820	CLA	O1A-CGA-O2A-C1
47	B2	618	LHG	O10-C23-O8-C6
50	AB	853	LMU	C4'-C5'-C6'-O6'
45	AB	838	CLA	O1D-CGD-O2D-CED
45	BA	813	CLA	O1D-CGD-O2D-CED
48	AA	847	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
48	AA	847	BCR	C37-C22-C23-C24
48	AB	848	BCR	C37-C22-C23-C24
48	AF	805	BCR	C7-C8-C9-C34
48	AI	101	BCR	C7-C8-C9-C34
48	AK	204	BCR	C37-C22-C23-C24
48	BB	846	BCR	C7-C8-C9-C34
48	BL	306	BCR	C11-C12-C13-C35
52	B1	316	LUT	C11-C12-C13-C20
48	AK	204	BCR	C21-C22-C23-C24
48	B3	317	BCR	C21-C22-C23-C24
45	AA	817	CLA	C2A-CAA-CBA-CGA
45	AA	842	CLA	C2A-CAA-CBA-CGA
45	AB	810	CLA	C2A-CAA-CBA-CGA
45	BB	812	CLA	C2A-CAA-CBA-CGA
45	AA	808	CLA	O1A-CGA-O2A-C1
45	AA	819	CLA	O1A-CGA-O2A-C1
45	AB	812	CLA	O1A-CGA-O2A-C1
45	AB	818	CLA	O1A-CGA-O2A-C1
45	AF	802	CLA	O1A-CGA-O2A-C1
45	BA	834	CLA	O1A-CGA-O2A-C1
45	BA	840	CLA	O1A-CGA-O2A-C1
45	BB	816	CLA	O1A-CGA-O2A-C1
45	B2	612	CLA	O1A-CGA-O2A-C1
45	AB	807	CLA	C3-C5-C6-C7
45	AB	826	CLA	CBA-CGA-O2A-C1
45	A4	311	CLA	CBA-CGA-O2A-C1
45	BB	835	CLA	CBA-CGA-O2A-C1
45	BA	834	CLA	C5-C6-C7-C8
46	BA	843	PQN	C18-C20-C21-C22
45	AA	825	CLA	C2-C1-O2A-CGA
45	BB	805	CLA	C2-C1-O2A-CGA
45	AA	820	CLA	O1D-CGD-O2D-CED
45	AA	829	CLA	O1D-CGD-O2D-CED
45	AA	836	CLA	O1D-CGD-O2D-CED
45	AB	811	CLA	O1D-CGD-O2D-CED
45	A6	613	CLA	O1D-CGD-O2D-CED
45	BA	831	CLA	O1D-CGD-O2D-CED
54	B2	605	CHL	O1D-CGD-O2D-CED
50	BB	851	LMU	C4'-C5'-C6'-O6'
45	AA	827	CLA	C15-C16-C17-C18
45	AA	832	CLA	C5-C6-C7-C8
45	AB	838	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
50	AB	850	LMU	O5B-C1B-O1B-C4'
47	F	801	LHG	O1-C1-C2-O2
45	AA	806	CLA	C11-C12-C13-C15
45	AB	826	CLA	C11-C10-C8-C7
46	BB	844	PQN	C21-C22-C23-C25
45	AH	201	CLA	CBA-CGA-O2A-C1
45	B2	609	CLA	CBA-CGA-O2A-C1
45	AB	802	CLA	O1D-CGD-O2D-CED
45	AB	820	CLA	O1D-CGD-O2D-CED
45	AB	827	CLA	C3-C5-C6-C7
45	BB	828	CLA	C3-C5-C6-C7
45	AB	835	CLA	C8-C10-C11-C12
45	AB	838	CLA	C15-C16-C17-C18
53	A1	321	LMG	C28-C29-C30-C31
53	B5	617	LMG	C10-C11-C12-C13
45	AA	806	CLA	O1A-CGA-O2A-C1
45	AA	827	CLA	O1A-CGA-O2A-C1
45	AA	834	CLA	O1A-CGA-O2A-C1
45	AB	829	CLA	O1A-CGA-O2A-C1
45	AB	841	CLA	O1A-CGA-O2A-C1
45	BA	808	CLA	O1A-CGA-O2A-C1
45	BB	805	CLA	O1A-CGA-O2A-C1
45	BB	813	CLA	O1A-CGA-O2A-C1
47	A1	302	LHG	O10-C23-O8-C6
45	BB	842	CLA	CBD-CGD-O2D-CED
45	AA	826	CLA	O1D-CGD-O2D-CED
45	AL	305	CLA	O1D-CGD-O2D-CED
45	BA	817	CLA	O1D-CGD-O2D-CED
45	BA	825	CLA	O1D-CGD-O2D-CED
45	AA	842	CLA	C5-C6-C7-C8
45	AB	801	CLA	C13-C15-C16-C17
45	AB	823	CLA	C8-C10-C11-C12
45	AB	825	CLA	C10-C11-C12-C13
45	AB	825	CLA	C13-C15-C16-C17
45	A6	613	CLA	C13-C15-C16-C17
45	BA	811	CLA	C15-C16-C17-C18
45	BA	828	CLA	C13-C15-C16-C17
45	BA	829	CLA	C10-C11-C12-C13
45	BB	808	CLA	C10-C11-C12-C13
45	BB	826	CLA	C8-C10-C11-C12
45	BB	826	CLA	C13-C15-C16-C17
50	AL	301	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
45	AA	821	CLA	C2A-CAA-CBA-CGA
45	AA	833	CLA	C2A-CAA-CBA-CGA
45	AB	811	CLA	C2A-CAA-CBA-CGA
45	AG	201	CLA	C2A-CAA-CBA-CGA
45	A6	601	CLA	C2A-CAA-CBA-CGA
45	BA	806	CLA	C2A-CAA-CBA-CGA
45	BA	821	CLA	C2A-CAA-CBA-CGA
45	BA	827	CLA	C2A-CAA-CBA-CGA
45	BA	842	CLA	C2A-CAA-CBA-CGA
45	BB	811	CLA	C2A-CAA-CBA-CGA
45	BB	841	CLA	C2A-CAA-CBA-CGA
54	A6	602	CHL	C2A-CAA-CBA-CGA
45	BA	831	CLA	C2-C1-O2A-CGA
50	AB	852	LMU	O1'-C1-C2-C3
45	AA	803	CLA	C15-C16-C17-C18
45	AA	840	CLA	C5-C6-C7-C8
45	A6	603	CLA	C13-C15-C16-C17
45	BA	819	CLA	C13-C15-C16-C17
45	BA	827	CLA	C10-C11-C12-C13
45	BB	816	CLA	C10-C11-C12-C13
45	BB	816	CLA	C13-C15-C16-C17
45	B3	301	CLA	C10-C11-C12-C13
53	B5	617	LMG	O6-C5-C6-O5
47	F	801	LHG	C7-C8-C9-C10
56	BJ	104	SQD	C7-C8-C9-C10
45	AA	839	CLA	O1A-CGA-O2A-C1
45	AB	822	CLA	O1A-CGA-O2A-C1
45	BB	830	CLA	O1A-CGA-O2A-C1
45	BB	839	CLA	O1A-CGA-O2A-C1
54	A6	602	CHL	O1A-CGA-O2A-C1
46	AA	843	PQN	C13-C15-C16-C17
45	BA	808	CLA	CBD-CGD-O2D-CED
50	AL	301	LMU	O5'-C1'-O1'-C1
45	AA	805	CLA	C8-C10-C11-C12
45	AA	806	CLA	C5-C6-C7-C8
45	AA	833	CLA	C15-C16-C17-C18
45	AA	841	CLA	C15-C16-C17-C18
45	AB	801	CLA	C15-C16-C17-C18
45	AB	802	CLA	C15-C16-C17-C18
45	AB	803	CLA	C10-C11-C12-C13
45	AB	806	CLA	C13-C15-C16-C17
45	AB	815	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
45	A3	302	CLA	C10-C11-C12-C13
45	BA	825	CLA	C13-C15-C16-C17
45	BA	827	CLA	C15-C16-C17-C18
45	BA	833	CLA	C13-C15-C16-C17
45	BA	842	CLA	C5-C6-C7-C8
45	BB	804	CLA	C10-C11-C12-C13
45	BB	807	CLA	C10-C11-C12-C13
45	BB	826	CLA	C10-C11-C12-C13
46	AB	843	PQN	C15-C16-C17-C18
46	BB	844	PQN	C15-C16-C17-C18
46	BB	844	PQN	C25-C26-C27-C28
45	AA	830	CLA	CBA-CGA-O2A-C1
45	BB	827	CLA	CBA-CGA-O2A-C1
45	AB	833	CLA	CBD-CGD-O2D-CED
45	BB	815	CLA	O1A-CGA-O2A-C1
45	B1	314	CLA	O1A-CGA-O2A-C1
45	B5	612	CLA	O1A-CGA-O2A-C1
47	BA	845	LHG	O10-C23-O8-C6
45	B5	612	CLA	C8-C10-C11-C12
47	F	801	LHG	C23-C24-C25-C26
56	BJ	104	SQD	C23-C24-C25-C26
45	AA	810	CLA	C13-C15-C16-C17
45	AB	803	CLA	C13-C15-C16-C17
45	AB	811	CLA	C8-C10-C11-C12
45	AB	829	CLA	C8-C10-C11-C12
45	BB	839	CLA	C15-C16-C17-C18
45	BL	303	CLA	C5-C6-C7-C8
46	AB	843	PQN	C25-C26-C27-C28
45	B3	310	CLA	O1D-CGD-O2D-CED
45	BA	801	CLA	C3-C5-C6-C7
45	B5	612	CLA	O1D-CGD-O2D-CED
45	AA	805	CLA	C13-C15-C16-C17
45	BA	825	CLA	C10-C11-C12-C13
45	BB	801	CLA	C10-C11-C12-C13
46	AA	843	PQN	C25-C26-C27-C28
46	BA	843	PQN	C23-C25-C26-C27
45	BA	822	CLA	CBD-CGD-O2D-CED
45	AB	838	CLA	O1A-CGA-O2A-C1
45	AH	201	CLA	O1A-CGA-O2A-C1
45	A4	311	CLA	O1A-CGA-O2A-C1
45	BB	835	CLA	O1A-CGA-O2A-C1
47	B5	618	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
53	A1	321	LMG	C10-C11-C12-C13
45	BA	815	CLA	O1D-CGD-O2D-CED
45	BB	822	CLA	O1D-CGD-O2D-CED
54	B2	606	CHL	O1D-CGD-O2D-CED
50	AB	850	LMU	O1'-C1-C2-C3
45	AA	827	CLA	C10-C11-C12-C13
45	AB	807	CLA	C13-C15-C16-C17
45	AA	803	CLA	CBA-CGA-O2A-C1
45	A4	308	CLA	CBA-CGA-O2A-C1
54	A6	606	CHL	CBD-CGD-O2D-CED
45	BA	830	CLA	C13-C15-C16-C17
45	AB	801	CLA	C3-C5-C6-C7
45	AB	808	CLA	CAA-CBA-CGA-O2A
45	BA	829	CLA	C8-C10-C11-C12
47	AJ	104	LHG	C1-C2-C3-O3
45	AA	836	CLA	C2A-CAA-CBA-CGA
45	A4	313	CLA	C2A-CAA-CBA-CGA
45	BA	833	CLA	C2A-CAA-CBA-CGA
45	BA	840	CLA	C2A-CAA-CBA-CGA
45	BB	802	CLA	C2A-CAA-CBA-CGA
45	AB	804	CLA	CBA-CGA-O2A-C1
45	AB	823	CLA	CBA-CGA-O2A-C1
45	A4	313	CLA	CBA-CGA-O2A-C1
45	BA	830	CLA	CBA-CGA-O2A-C1
45	BB	818	CLA	CBA-CGA-O2A-C1
45	BB	824	CLA	CBA-CGA-O2A-C1
45	BB	842	CLA	CBA-CGA-O2A-C1
45	AA	828	CLA	C8-C10-C11-C12
45	AA	829	CLA	C8-C10-C11-C12
45	AA	829	CLA	C10-C11-C12-C13
45	AA	833	CLA	C5-C6-C7-C8
45	AB	829	CLA	C10-C11-C12-C13
45	AB	832	CLA	C13-C15-C16-C17
45	AB	834	CLA	C15-C16-C17-C18
45	BA	803	CLA	C13-C15-C16-C17
45	BA	810	CLA	C5-C6-C7-C8
45	BA	810	CLA	C13-C15-C16-C17
45	BA	819	CLA	C10-C11-C12-C13
45	BB	827	CLA	C8-C10-C11-C12
45	BB	831	CLA	C5-C6-C7-C8
45	BB	835	CLA	C8-C10-C11-C12
45	BB	839	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	BB	843	CLA	C8-C10-C11-C12
46	AA	843	PQN	C20-C21-C22-C23
45	A6	614	CLA	O1D-CGD-O2D-CED
45	BA	809	CLA	CBD-CGD-O2D-CED
45	BA	803	CLA	C5-C6-C7-C8
45	BA	833	CLA	C15-C16-C17-C18
45	BB	829	CLA	C10-C11-C12-C13
50	AL	301	LMU	C3'-C4'-O1B-C1B
45	AA	813	CLA	C8-C10-C11-C12
45	AA	826	CLA	C5-C6-C7-C8
45	AA	828	CLA	C10-C11-C12-C13
45	AA	841	CLA	C13-C15-C16-C17
45	AB	827	CLA	C10-C11-C12-C13
45	AB	834	CLA	C8-C10-C11-C12
45	BA	830	CLA	C10-C11-C12-C13
45	BA	840	CLA	C5-C6-C7-C8
45	BB	828	CLA	C10-C11-C12-C13
45	BB	836	CLA	C8-C10-C11-C12
45	AA	801	CLA	CBA-CGA-O2A-C1
45	BA	812	CLA	CBA-CGA-O2A-C1
45	AA	838	CLA	O1D-CGD-O2D-CED
45	AB	825	CLA	O1D-CGD-O2D-CED
45	AA	819	CLA	C13-C15-C16-C17
45	AB	842	CLA	C8-C10-C11-C12
45	BB	820	CLA	C8-C10-C11-C12
45	BB	802	CLA	CBD-CGD-O2D-CED
47	BA	845	LHG	C8-C7-O7-C5
45	AA	825	CLA	C11-C12-C13-C14
45	AA	832	CLA	O1D-CGD-O2D-CED
45	AB	826	CLA	O1A-CGA-O2A-C1
46	AA	843	PQN	C11-C12-C13-C14
47	F	801	LHG	O9-C7-O7-C5
56	BJ	104	SQD	C2-C1-O6-C44
56	e	301	SQD	C2-C1-O6-C44
45	AB	827	CLA	C5-C6-C7-C8
45	AA	809	CLA	CBA-CGA-O2A-C1
45	AB	806	CLA	CBA-CGA-O2A-C1
45	A1	305	CLA	CBA-CGA-O2A-C1
45	AA	806	CLA	C16-C17-C18-C19
52	B1	316	LUT	C11-C10-C9-C19
52	B1	316	LUT	C39-C29-C30-C31
50	BA	853	LMU	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
50	BB	851	LMU	O5'-C5'-C6'-O6'
45	AA	830	CLA	C8-C10-C11-C12
48	AA	845	BCR	C7-C8-C9-C34
48	AA	846	BCR	C37-C22-C23-C24
48	AB	845	BCR	C7-C8-C9-C34
48	BB	849	BCR	C37-C22-C23-C24
48	BL	306	BCR	C7-C8-C9-C34
48	BL	306	BCR	C21-C22-C23-C24
45	A4	313	CLA	O1A-CGA-O2A-C1
45	BB	818	CLA	O1A-CGA-O2A-C1
45	AA	802	CLA	C2A-CAA-CBA-CGA
45	AB	802	CLA	C2A-CAA-CBA-CGA
45	AB	840	CLA	C2A-CAA-CBA-CGA
45	A3	312	CLA	C2A-CAA-CBA-CGA
45	BA	802	CLA	C2A-CAA-CBA-CGA
45	BA	808	CLA	C2A-CAA-CBA-CGA
45	BA	841	CLA	C2A-CAA-CBA-CGA
45	B5	601	CLA	C2A-CAA-CBA-CGA
54	B2	601	CHL	C2A-CAA-CBA-CGA
45	AB	815	CLA	C13-C15-C16-C17
45	BA	821	CLA	C15-C16-C17-C18
47	A3	301	LHG	O1-C1-C2-C3
47	B2	618	LHG	O1-C1-C2-C3
47	F	801	LHG	O1-C1-C2-C3
45	AB	805	CLA	O1D-CGD-O2D-CED
45	AA	819	CLA	C16-C17-C18-C19
45	AA	819	CLA	C16-C17-C18-C20
45	AB	810	CLA	C16-C17-C18-C19
45	AB	817	CLA	C6-C7-C8-C10
45	BB	804	CLA	C16-C17-C18-C19
45	AA	830	CLA	O1D-CGD-O2D-CED
45	A1	304	CLA	O1D-CGD-O2D-CED
45	A1	316	CLA	O1D-CGD-O2D-CED
45	B2	609	CLA	O1A-CGA-O2A-C1
45	AA	801	CLA	C3-C5-C6-C7
45	AA	827	CLA	C3-C5-C6-C7
45	AA	828	CLA	C13-C15-C16-C17
52	B1	316	LUT	C11-C10-C9-C8
52	B1	316	LUT	C28-C29-C30-C31
47	BA	845	LHG	O9-C7-O7-C5
56	BJ	104	SQD	O5-C1-O6-C44
47	A6	618	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
45	AA	806	CLA	C13-C15-C16-C17
45	AA	825	CLA	C15-C16-C17-C18
45	BA	821	CLA	C13-C15-C16-C17
45	BA	828	CLA	C15-C16-C17-C18
45	AA	812	CLA	O1D-CGD-O2D-CED
45	B2	602	CLA	O1D-CGD-O2D-CED
54	B5	606	CHL	O1D-CGD-O2D-CED
45	BB	824	CLA	O1A-CGA-O2A-C1
45	B2	610	CLA	O1D-CGD-O2D-CED
45	AA	804	CLA	CBA-CGA-O2A-C1
45	AB	821	CLA	CBA-CGA-O2A-C1
45	BB	831	CLA	CBA-CGA-O2A-C1
45	AA	828	CLA	C15-C16-C17-C18
45	AA	833	CLA	C13-C15-C16-C17
45	AB	804	CLA	C2-C1-O2A-CGA
45	AB	810	CLA	C16-C17-C18-C20
45	AB	817	CLA	C6-C7-C8-C9
45	A3	312	CLA	C6-C7-C8-C10
45	A4	301	CLA	C11-C12-C13-C15
45	BA	806	CLA	C16-C17-C18-C19
45	BB	807	CLA	C16-C17-C18-C19
45	BA	830	CLA	O1A-CGA-O2A-C1
45	BB	827	CLA	O1A-CGA-O2A-C1
50	BA	853	LMU	O5B-C1B-O1B-C4'
47	AJ	104	LHG	C18-C19-C20-C21
53	A4	318	LMG	C12-C13-C14-C15
47	A1	320	LHG	C11-C12-C13-C14
47	BA	845	LHG	C14-C15-C16-C17
45	BA	803	CLA	O1D-CGD-O2D-CED
45	B2	612	CLA	O1D-CGD-O2D-CED
45	AB	832	CLA	C8-C10-C11-C12
45	AA	803	CLA	O1A-CGA-O2A-C1
45	AA	830	CLA	O1A-CGA-O2A-C1
45	AB	823	CLA	O1A-CGA-O2A-C1
45	A4	308	CLA	O1A-CGA-O2A-C1
45	AA	831	CLA	CBA-CGA-O2A-C1
51	AB	851	DGD	CAA-CBA-CCA-CDA
56	BJ	104	SQD	C10-C11-C12-C13
50	BA	853	LMU	C2-C1-O1'-C1'
45	AA	819	CLA	O1D-CGD-O2D-CED
45	AA	840	CLA	O1D-CGD-O2D-CED
45	BB	839	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
45	AA	809	CLA	C4B-C3B-CAB-CBB
45	AA	811	CLA	C4B-C3B-CAB-CBB
45	AA	813	CLA	C4B-C3B-CAB-CBB
45	AA	831	CLA	C4B-C3B-CAB-CBB
45	AA	834	CLA	C4B-C3B-CAB-CBB
45	AA	836	CLA	C4B-C3B-CAB-CBB
45	AB	831	CLA	C4B-C3B-CAB-CBB
45	AB	842	CLA	C4B-C3B-CAB-CBB
45	AG	201	CLA	C4B-C3B-CAB-CBB
45	AG	204	CLA	C4B-C3B-CAB-CBB
45	AK	203	CLA	C4B-C3B-CAB-CBB
45	A3	303	CLA	C4B-C3B-CAB-CBB
45	A3	309	CLA	C4B-C3B-CAB-CBB
45	A3	314	CLA	C4B-C3B-CAB-CBB
45	A4	310	CLA	C4B-C3B-CAB-CBB
45	A6	605	CLA	C4B-C3B-CAB-CBB
45	A6	610	CLA	C4B-C3B-CAB-CBB
45	BB	825	CLA	C4B-C3B-CAB-CBB
45	BB	832	CLA	C4B-C3B-CAB-CBB
45	BB	843	CLA	C4B-C3B-CAB-CBB
45	BH	201	CLA	C4B-C3B-CAB-CBB
45	BK	202	CLA	C4B-C3B-CAB-CBB
45	B5	602	CLA	C4B-C3B-CAB-CBB
45	B5	613	CLA	C4B-C3B-CAB-CBB
47	B1	318	LHG	C28-C29-C30-C31
45	AA	808	CLA	C16-C17-C18-C19
45	AB	812	CLA	C6-C7-C8-C9
45	A4	301	CLA	C11-C12-C13-C14
45	BA	825	CLA	C16-C17-C18-C19
45	BA	825	CLA	C16-C17-C18-C20
45	BB	807	CLA	C16-C17-C18-C20
45	BA	838	CLA	O1D-CGD-O2D-CED
45	BB	824	CLA	O1D-CGD-O2D-CED
45	B1	313	CLA	O1D-CGD-O2D-CED
45	AA	808	CLA	C2A-CAA-CBA-CGA
45	B2	612	CLA	C2A-CAA-CBA-CGA
54	B3	306	CHL	C2A-CAA-CBA-CGA
47	A1	301	LHG	C24-C25-C26-C27
45	AA	817	CLA	C10-C11-C12-C13
45	A6	603	CLA	C10-C11-C12-C13
45	BB	824	CLA	C8-C10-C11-C12
50	AB	850	LMU	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
47	B2	618	LHG	C8-C7-O7-C5
56	e	301	SQD	C8-C7-O47-C45
50	BB	851	LMU	C6-C7-C8-C9
45	AA	813	CLA	C6-C7-C8-C10
45	AB	834	CLA	C11-C12-C13-C15
45	BA	801	CLA	C12-C13-C15-C16
45	BA	829	CLA	C11-C10-C8-C7
45	BB	828	CLA	C11-C10-C8-C7
46	AB	843	PQN	C21-C22-C23-C25
45	AA	829	CLA	C5-C6-C7-C8
45	BB	843	CLA	C15-C16-C17-C18
51	AB	851	DGD	C3A-C4A-C5A-C6A
53	A4	318	LMG	C13-C14-C15-C16
56	BJ	104	SQD	C13-C14-C15-C16
45	A1	305	CLA	O1A-CGA-O2A-C1
45	AA	803	CLA	C3A-C2A-CAA-CBA
45	AA	825	CLA	C3A-C2A-CAA-CBA
45	AB	828	CLA	C3A-C2A-CAA-CBA
45	AB	829	CLA	C3A-C2A-CAA-CBA
45	AB	834	CLA	C3A-C2A-CAA-CBA
45	AK	203	CLA	C3A-C2A-CAA-CBA
45	A1	316	CLA	C3A-C2A-CAA-CBA
45	A6	612	CLA	C3A-C2A-CAA-CBA
45	BA	803	CLA	C3A-C2A-CAA-CBA
45	BA	805	CLA	C3A-C2A-CAA-CBA
45	BA	809	CLA	C3A-C2A-CAA-CBA
45	BB	810	CLA	C3A-C2A-CAA-CBA
45	BB	815	CLA	C3A-C2A-CAA-CBA
45	BL	303	CLA	C3A-C2A-CAA-CBA
45	B2	611	CLA	C3A-C2A-CAA-CBA
45	BB	829	CLA	O1D-CGD-O2D-CED
45	B5	613	CLA	O1D-CGD-O2D-CED
47	A1	320	LHG	C33-C34-C35-C36
47	BF	305	LHG	C11-C10-C9-C8
45	BA	802	CLA	C15-C16-C17-C18
45	B1	304	CLA	O1D-CGD-O2D-CED
47	AJ	104	LHG	C7-C8-C9-C10
45	AB	812	CLA	C6-C7-C8-C10
45	AB	835	CLA	C11-C12-C13-C14
45	AB	835	CLA	C11-C12-C13-C15
45	BA	806	CLA	C16-C17-C18-C20
45	BA	813	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
45	BB	804	CLA	C16-C17-C18-C20
45	BB	835	CLA	C16-C17-C18-C20
45	BB	836	CLA	C11-C12-C13-C14
45	BB	836	CLA	C11-C12-C13-C15
50	AB	853	LMU	O5B-C5B-C6B-O6B
45	AA	801	CLA	O1A-CGA-O2A-C1
45	AA	809	CLA	O1A-CGA-O2A-C1
45	AB	804	CLA	O1A-CGA-O2A-C1
45	AB	806	CLA	O1A-CGA-O2A-C1
45	AB	831	CLA	CBD-CGD-O2D-CED
45	BB	841	CLA	CBD-CGD-O2D-CED
45	BJ	102	CLA	CBD-CGD-O2D-CED
45	BA	805	CLA	CBA-CGA-O2A-C1
45	BB	840	CLA	CBA-CGA-O2A-C1
47	BF	305	LHG	C27-C28-C29-C30
56	BJ	104	SQD	C9-C10-C11-C12
45	BB	843	CLA	C3-C5-C6-C7
45	AB	804	CLA	C5-C6-C7-C8
45	AB	840	CLA	O1D-CGD-O2D-CED
47	AA	844	LHG	C10-C11-C12-C13
50	AA	851	LMU	C3-C4-C5-C6
53	A4	318	LMG	C29-C30-C31-C32
45	AB	821	CLA	O1A-CGA-O2A-C1
45	BA	812	CLA	O1A-CGA-O2A-C1
45	BB	842	CLA	O1A-CGA-O2A-C1
50	AA	851	LMU	C4-C5-C6-C7
45	BB	821	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	CAA-CBA-CCA-CDA
45	BA	807	CLA	O1D-CGD-O2D-CED
56	BJ	104	SQD	C11-C12-C13-C14
45	AA	805	CLA	C16-C17-C18-C19
45	AA	804	CLA	O1A-CGA-O2A-C1
45	BB	831	CLA	O1A-CGA-O2A-C1
45	AA	809	CLA	C2B-C3B-CAB-CBB
45	AA	813	CLA	C2B-C3B-CAB-CBB
45	AA	822	CLA	C2B-C3B-CAB-CBB
45	AA	834	CLA	C2B-C3B-CAB-CBB
45	AA	836	CLA	C2B-C3B-CAB-CBB
45	AA	842	CLA	C2B-C3B-CAB-CBB
45	AK	202	CLA	C2B-C3B-CAB-CBB
45	AK	203	CLA	C2B-C3B-CAB-CBB
45	A1	307	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	A3	303	CLA	C2B-C3B-CAB-CBB
45	A3	310	CLA	C2B-C3B-CAB-CBB
45	A4	313	CLA	C2B-C3B-CAB-CBB
45	A6	612	CLA	C2B-C3B-CAB-CBB
45	BA	811	CLA	C2B-C3B-CAB-CBB
45	BA	836	CLA	C2B-C3B-CAB-CBB
45	BA	842	CLA	C2B-C3B-CAB-CBB
45	BK	202	CLA	C2B-C3B-CAB-CBB
45	B3	309	CLA	C2B-C3B-CAB-CBB
45	B3	313	CLA	C2B-C3B-CAB-CBB
45	B5	601	CLA	C2B-C3B-CAB-CBB
48	AA	846	BCR	C23-C24-C25-C30
48	AA	847	BCR	C1-C6-C7-C8
48	AA	847	BCR	C23-C24-C25-C26
48	AA	848	BCR	C1-C6-C7-C8
48	AA	848	BCR	C5-C6-C7-C8
48	AA	849	BCR	C5-C6-C7-C8
48	AA	849	BCR	C23-C24-C25-C30
48	AA	852	BCR	C5-C6-C7-C8
48	AB	844	BCR	C1-C6-C7-C8
48	AB	844	BCR	C23-C24-C25-C26
48	AB	844	BCR	C23-C24-C25-C30
48	AB	846	BCR	C1-C6-C7-C8
48	AB	846	BCR	C5-C6-C7-C8
48	AF	805	BCR	C1-C6-C7-C8
48	AF	805	BCR	C5-C6-C7-C8
48	AI	101	BCR	C23-C24-C25-C26
48	AJ	103	BCR	C1-C6-C7-C8
48	AJ	103	BCR	C23-C24-C25-C26
48	AK	204	BCR	C23-C24-C25-C26
48	AK	204	BCR	C23-C24-C25-C30
48	AL	306	BCR	C1-C6-C7-C8
48	AL	306	BCR	C5-C6-C7-C8
48	A3	318	BCR	C1-C6-C7-C8
48	A3	318	BCR	C5-C6-C7-C8
48	A4	317	BCR	C1-C6-C7-C8
48	A4	317	BCR	C5-C6-C7-C8
48	A6	617	BCR	C1-C6-C7-C8
48	BA	847	BCR	C5-C6-C7-C8
48	BA	847	BCR	C23-C24-C25-C26
48	BA	850	BCR	C23-C24-C25-C30
48	BA	851	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	BA	851	BCR	C23-C24-C25-C30
48	BA	855	BCR	C23-C24-C25-C30
48	BA	856	BCR	C1-C6-C7-C8
48	BA	856	BCR	C5-C6-C7-C8
48	BA	856	BCR	C23-C24-C25-C30
48	BB	845	BCR	C23-C24-C25-C30
48	BB	847	BCR	C1-C6-C7-C8
48	BB	847	BCR	C5-C6-C7-C8
48	BF	304	BCR	C1-C6-C7-C8
48	BF	304	BCR	C23-C24-C25-C26
48	BI	101	BCR	C1-C6-C7-C8
48	BI	101	BCR	C5-C6-C7-C8
48	BI	101	BCR	C23-C24-C25-C26
48	BJ	103	BCR	C1-C6-C7-C8
48	BJ	103	BCR	C23-C24-C25-C26
48	BJ	103	BCR	C23-C24-C25-C30
48	BL	301	BCR	C5-C6-C7-C8
48	BL	301	BCR	C23-C24-C25-C26
48	BL	306	BCR	C1-C6-C7-C8
48	B3	317	BCR	C1-C6-C7-C8
48	B3	317	BCR	C5-C6-C7-C8
48	B5	616	BCR	C1-C6-C7-C8
48	B5	616	BCR	C5-C6-C7-C8
45	AB	821	CLA	CBD-CGD-O2D-CED
50	AB	850	LMU	C3'-C4'-O1B-C1B
45	AB	814	CLA	O1D-CGD-O2D-CED
45	B3	305	CLA	O1D-CGD-O2D-CED
47	F	801	LHG	C30-C31-C32-C33
45	AA	824	CLA	C2A-CAA-CBA-CGA
45	BA	817	CLA	C2A-CAA-CBA-CGA
45	AA	831	CLA	O1A-CGA-O2A-C1
50	AB	850	LMU	C5'-C4'-O1B-C1B
47	A6	618	LHG	O9-C7-O7-C5
47	BF	305	LHG	C30-C31-C32-C33
48	AA	847	BCR	C10-C11-C12-C13
45	AA	834	CLA	C2-C3-C5-C6
45	A3	312	CLA	C6-C7-C8-C9
47	AA	844	LHG	C16-C17-C18-C19
50	BA	853	LMU	C5-C6-C7-C8
45	AA	803	CLA	C3-C5-C6-C7
56	e	301	SQD	O5-C1-O6-C44
47	BA	845	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
47	B1	318	LHG	C11-C12-C13-C14
45	BA	833	CLA	C5-C6-C7-C8
50	AB	852	LMU	C11-C10-C9-C8
51	AB	851	DGD	C9B-CAB-CBB-CCB
45	AA	811	CLA	C3-C5-C6-C7
45	AB	811	CLA	C3-C5-C6-C7
45	BB	821	CLA	CBA-CGA-O2A-C1
54	B2	601	CHL	CBA-CGA-O2A-C1
45	AA	805	CLA	C16-C17-C18-C20
45	AA	806	CLA	C16-C17-C18-C20
45	AL	304	CLA	C11-C12-C13-C14
50	BB	851	LMU	O5B-C1B-O1B-C4'
47	AA	844	LHG	C8-C7-O7-C5
47	B1	318	LHG	C8-C7-O7-C5
47	a	501	LHG	C8-C7-O7-C5
53	B5	617	LMG	C11-C10-O7-C8
47	A1	301	LHG	C23-C24-C25-C26
45	AA	827	CLA	C8-C10-C11-C12
45	BA	810	CLA	C10-C11-C12-C13
47	B2	618	LHG	O9-C7-O7-C5
53	B5	617	LMG	O9-C10-O7-C8
47	BA	845	LHG	C32-C33-C34-C35
51	BB	850	DGD	CCA-CDA-CEA-CFA
48	AA	847	BCR	C11-C12-C13-C35
48	BA	849	BCR	C37-C22-C23-C24
50	AL	301	LMU	C2-C3-C4-C5
48	AI	101	BCR	C21-C22-C23-C24
48	A1	319	BCR	C21-C22-C23-C24
54	A6	608	CHL	C2A-CAA-CBA-CGA
45	AA	801	CLA	C16-C17-C18-C19
45	AB	815	CLA	C16-C17-C18-C20
45	BA	805	CLA	C16-C17-C18-C19
45	BA	805	CLA	C16-C17-C18-C20
45	BA	813	CLA	C16-C17-C18-C20
45	AA	834	CLA	C4-C3-C5-C6
47	BF	305	LHG	C11-C12-C13-C14
45	BB	835	CLA	O1D-CGD-O2D-CED
45	BA	805	CLA	O1A-CGA-O2A-C1
45	AB	809	CLA	C3-C5-C6-C7
45	AB	802	CLA	C5-C6-C7-C8
45	BB	811	CLA	C13-C15-C16-C17
45	AB	819	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
47	A1	301	LHG	C7-C8-C9-C10
56	e	301	SQD	C7-C8-C9-C10
47	AA	844	LHG	O9-C7-O7-C5
45	AB	835	CLA	CBD-CGD-O2D-CED
45	BB	820	CLA	CBD-CGD-O2D-CED
47	B1	302	LHG	C8-C7-O7-C5
45	AB	806	CLA	C8-C10-C11-C12
45	AA	810	CLA	CAD-CBD-CGD-O2D
45	BA	838	CLA	C6-C7-C8-C10
45	B3	311	CLA	C6-C7-C8-C9
51	BB	850	DGD	CDA-CEA-CFA-CGA
45	B2	602	CLA	C13-C15-C16-C17
45	B2	612	CLA	C8-C10-C11-C12
47	B1	318	LHG	C9-C10-C11-C12
45	AB	802	CLA	C3-C5-C6-C7
45	AL	304	CLA	C3-C5-C6-C7
47	a	501	LHG	O7-C5-C6-O8
45	BB	840	CLA	O1A-CGA-O2A-C1
47	BA	845	LHG	C29-C30-C31-C32
47	F	801	LHG	C32-C33-C34-C35
45	BA	830	CLA	C5-C6-C7-C8
45	BB	834	CLA	C5-C6-C7-C8
45	B1	314	CLA	C8-C10-C11-C12
45	BA	839	CLA	O1D-CGD-O2D-CED
47	AA	844	LHG	C33-C34-C35-C36
45	BA	841	CLA	C2-C1-O2A-CGA
45	AB	803	CLA	C16-C17-C18-C20
45	AB	823	CLA	C16-C17-C18-C20
45	BA	801	CLA	C16-C17-C18-C19
45	BA	811	CLA	C13-C15-C16-C17
45	BB	808	CLA	C15-C16-C17-C18
45	BB	829	CLA	C15-C16-C17-C18
47	AJ	104	LHG	C14-C15-C16-C17
45	AA	812	CLA	C2A-CAA-CBA-CGA
45	AB	814	CLA	C2A-CAA-CBA-CGA
45	BA	828	CLA	C2A-CAA-CBA-CGA
45	B1	314	CLA	C2A-CAA-CBA-CGA
45	BA	809	CLA	CBA-CGA-O2A-C1
45	A1	314	CLA	C2C-C3C-CAC-CBC
45	AB	842	CLA	O1D-CGD-O2D-CED
45	AL	303	CLA	O1D-CGD-O2D-CED
45	BB	801	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	A6	613	CLA	C2-C1-O2A-CGA
45	AB	817	CLA	C3-C5-C6-C7
45	A6	613	CLA	C2A-CAA-CBA-CGA
45	AA	803	CLA	C1A-C2A-CAA-CBA
45	AA	805	CLA	C1A-C2A-CAA-CBA
45	AA	807	CLA	C1A-C2A-CAA-CBA
45	AA	810	CLA	C1A-C2A-CAA-CBA
45	AA	818	CLA	C1A-C2A-CAA-CBA
45	AA	819	CLA	C1A-C2A-CAA-CBA
45	AA	839	CLA	C1A-C2A-CAA-CBA
45	AB	819	CLA	C1A-C2A-CAA-CBA
45	AB	821	CLA	C1A-C2A-CAA-CBA
45	AB	833	CLA	C1A-C2A-CAA-CBA
45	AB	834	CLA	C1A-C2A-CAA-CBA
45	AB	839	CLA	C1A-C2A-CAA-CBA
45	AF	802	CLA	C1A-C2A-CAA-CBA
45	AH	201	CLA	C1A-C2A-CAA-CBA
45	AL	304	CLA	C1A-C2A-CAA-CBA
45	A1	316	CLA	C1A-C2A-CAA-CBA
45	A4	312	CLA	C1A-C2A-CAA-CBA
45	A6	612	CLA	C1A-C2A-CAA-CBA
45	BA	803	CLA	C1A-C2A-CAA-CBA
45	BA	807	CLA	C1A-C2A-CAA-CBA
45	BA	810	CLA	C1A-C2A-CAA-CBA
45	BA	819	CLA	C1A-C2A-CAA-CBA
45	BA	830	CLA	C1A-C2A-CAA-CBA
45	BA	832	CLA	C1A-C2A-CAA-CBA
45	BB	807	CLA	C1A-C2A-CAA-CBA
45	BB	820	CLA	C1A-C2A-CAA-CBA
45	BB	834	CLA	C1A-C2A-CAA-CBA
45	BB	836	CLA	C1A-C2A-CAA-CBA
45	BL	304	CLA	C1A-C2A-CAA-CBA
45	B2	611	CLA	C1A-C2A-CAA-CBA
45	B2	613	CLA	C1A-C2A-CAA-CBA
45	B5	613	CLA	C1A-C2A-CAA-CBA
45	AA	803	CLA	C10-C11-C12-C13
47	A1	320	LHG	C30-C31-C32-C33
47	A6	618	LHG	C9-C10-C11-C12
47	F	801	LHG	O6-C4-C5-C6
47	F	801	LHG	C27-C28-C29-C30
53	AG	202	LMG	C10-C11-C12-C13
45	AA	801	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
45	AA	813	CLA	C11-C10-C8-C7
45	AA	819	CLA	C6-C7-C8-C10
45	AA	825	CLA	C11-C10-C8-C7
45	AA	827	CLA	C12-C13-C15-C16
45	AA	828	CLA	C6-C7-C8-C10
45	AB	802	CLA	C12-C13-C15-C16
45	AB	803	CLA	C6-C7-C8-C10
45	AB	806	CLA	C11-C10-C8-C7
45	AB	807	CLA	C11-C12-C13-C15
45	AB	819	CLA	C11-C10-C8-C7
45	AB	825	CLA	C12-C13-C15-C16
45	AB	841	CLA	C6-C7-C8-C10
45	A1	304	CLA	C11-C10-C8-C7
45	BA	813	CLA	C11-C10-C8-C7
45	BA	819	CLA	C11-C12-C13-C15
45	BB	808	CLA	C11-C10-C8-C7
45	BB	811	CLA	C6-C7-C8-C10
45	BB	811	CLA	C11-C10-C8-C7
45	BB	824	CLA	C6-C7-C8-C10
45	BB	826	CLA	C12-C13-C15-C16
45	BB	836	CLA	C11-C10-C8-C7
45	BB	843	CLA	C6-C7-C8-C10
45	BL	303	CLA	C11-C10-C8-C7
46	AB	843	PQN	C17-C18-C20-C21
45	B2	602	CLA	C16-C17-C18-C19
45	AA	822	CLA	C3A-C2A-CAA-CBA
45	A3	305	CLA	C3A-C2A-CAA-CBA
45	BA	822	CLA	C3A-C2A-CAA-CBA
45	B5	611	CLA	C3A-C2A-CAA-CBA
45	BB	811	CLA	C10-C11-C12-C13
47	BA	845	LHG	C10-C11-C12-C13
45	AA	827	CLA	C4-C3-C5-C6
45	AB	815	CLA	C4-C3-C5-C6
45	AB	815	CLA	C2-C3-C5-C6
45	BA	806	CLA	C2-C3-C5-C6
45	BA	809	CLA	O1A-CGA-O2A-C1
45	BB	821	CLA	O1A-CGA-O2A-C1
45	AA	803	CLA	C5-C6-C7-C8
45	AA	829	CLA	C15-C16-C17-C18
47	A1	320	LHG	C8-C7-O7-C5
45	A1	314	CLA	C2A-CAA-CBA-CGA
45	BB	818	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
45	BB	830	CLA	C2A-CAA-CBA-CGA
45	AA	808	CLA	C11-C12-C13-C14
45	AA	813	CLA	C11-C12-C13-C14
45	AA	825	CLA	C11-C10-C8-C9
45	AA	827	CLA	C14-C13-C15-C16
45	AA	830	CLA	C14-C13-C15-C16
45	AB	810	CLA	C11-C10-C8-C9
45	AB	826	CLA	C11-C10-C8-C9
45	BA	813	CLA	C11-C10-C8-C9
45	BA	819	CLA	C6-C7-C8-C9
45	BB	807	CLA	C11-C12-C13-C14
45	BB	811	CLA	C11-C10-C8-C9
45	BB	819	CLA	C6-C7-C8-C9
45	BB	826	CLA	C6-C7-C8-C9
45	BB	826	CLA	C14-C13-C15-C16
45	BB	843	CLA	C6-C7-C8-C9
45	BL	303	CLA	C11-C10-C8-C9
45	B1	314	CLA	C6-C7-C8-C9
47	BA	845	LHG	C34-C35-C36-C37
53	AG	202	LMG	C11-C12-C13-C14
47	B5	618	LHG	C24-C23-O8-C6
45	BB	806	CLA	C2C-C3C-CAC-CBC
50	AB	853	LMU	C2'-C1'-O1'-C1
47	A3	301	LHG	C4-C5-C6-O8
47	BA	845	LHG	C4-C5-C6-O8
47	B2	618	LHG	C4-C5-C6-O8
53	AG	202	LMG	O1-C7-C8-C9
53	A1	321	LMG	O1-C7-C8-C9
53	B5	617	LMG	O1-C7-C8-C9
47	BA	845	LHG	C15-C16-C17-C18
47	A3	301	LHG	C11-C10-C9-C8
51	AB	851	DGD	C9A-CAA-CBA-CCA
45	BB	812	CLA	C5-C6-C7-C8
50	AB	850	LMU	C5-C6-C7-C8
45	AB	801	CLA	C16-C17-C18-C20
45	AB	823	CLA	C16-C17-C18-C19
45	AL	304	CLA	C11-C12-C13-C15
45	BA	811	CLA	C16-C17-C18-C19
45	BA	838	CLA	C6-C7-C8-C9
45	B3	311	CLA	C6-C7-C8-C10
54	A4	306	CHL	CHA-CBD-CGD-O1D
54	A4	306	CHL	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
54	A6	607	CHL	CHA-CBD-CGD-O1D
54	A6	607	CHL	CHA-CBD-CGD-O2D
47	BA	845	LHG	C23-C24-C25-C26
46	AB	843	PQN	C14-C13-C15-C16
45	AA	821	CLA	C2-C3-C5-C6
45	AA	827	CLA	C2-C3-C5-C6
53	AG	202	LMG	C30-C31-C32-C33
45	BA	806	CLA	C10-C11-C12-C13
45	BA	828	CLA	C10-C11-C12-C13
47	B1	318	LHG	O9-C7-O7-C5
48	BA	855	BCR	C21-C22-C23-C24
48	BI	101	BCR	C21-C22-C23-C24
45	AL	304	CLA	C8-C10-C11-C12
45	BA	813	CLA	C15-C16-C17-C18
45	BB	830	CLA	C5-C6-C7-C8
45	BH	201	CLA	C10-C11-C12-C13
56	BJ	104	SQD	C11-C10-C9-C8
54	B2	601	CHL	O1A-CGA-O2A-C1
50	AB	852	LMU	C5-C6-C7-C8
45	AA	825	CLA	CBA-CGA-O2A-C1
45	AB	840	CLA	CBA-CGA-O2A-C1
45	A6	610	CLA	CBA-CGA-O2A-C1
45	BB	801	CLA	CBA-CGA-O2A-C1
56	BJ	104	SQD	C15-C16-C17-C18
45	A1	314	CLA	C8-C10-C11-C12
45	B2	602	CLA	C16-C17-C18-C20
45	A6	604	CLA	C2A-CAA-CBA-CGA
45	AB	801	CLA	C5-C6-C7-C8
45	AB	802	CLA	C8-C10-C11-C12
45	AB	809	CLA	CBA-CGA-O2A-C1
45	BA	818	CLA	CBA-CGA-O2A-C1
45	BA	839	CLA	CBA-CGA-O2A-C1
45	BA	841	CLA	CBA-CGA-O2A-C1
47	A1	301	LHG	C30-C31-C32-C33
45	BA	806	CLA	C4-C3-C5-C6
45	AA	826	CLA	C2-C3-C5-C6
45	BA	811	CLA	C16-C17-C18-C20
47	B2	618	LHG	C9-C10-C11-C12
50	AB	852	LMU	C4-C5-C6-C7
56	BJ	104	SQD	C19-C20-C21-C22
51	AB	851	DGD	CCA-CDA-CEA-CFA
47	A3	301	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
51	BB	850	DGD	O1G-C1G-C2G-O2G
53	A4	318	LMG	O1-C7-C8-O7
45	AA	841	CLA	CBA-CGA-O2A-C1
45	AB	828	CLA	C10-C11-C12-C13
45	BA	808	CLA	O1D-CGD-O2D-CED
53	B5	617	LMG	C31-C32-C33-C34
45	AB	829	CLA	C2A-CAA-CBA-CGA
45	AA	840	CLA	C3-C5-C6-C7
45	AB	829	CLA	C5-C6-C7-C8
45	BA	826	CLA	C5-C6-C7-C8
45	BA	806	CLA	C5-C6-C7-C8
45	AA	824	CLA	CBA-CGA-O2A-C1
45	AB	820	CLA	CBA-CGA-O2A-C1
45	BB	810	CLA	CBA-CGA-O2A-C1
51	AB	851	DGD	CDA-CEA-CFA-CGA
45	A1	314	CLA	C15-C16-C17-C18
45	BB	801	CLA	O1A-CGA-O2A-C1
45	BA	822	CLA	O1D-CGD-O2D-CED
45	AA	842	CLA	C13-C15-C16-C17
45	AB	807	CLA	C5-C6-C7-C8
45	BA	805	CLA	C8-C10-C11-C12
45	B2	612	CLA	C10-C11-C12-C13
45	BB	842	CLA	O1D-CGD-O2D-CED
45	BB	824	CLA	C16-C17-C18-C20
45	AA	804	CLA	C4-C3-C5-C6
45	AA	821	CLA	C4-C3-C5-C6
45	AB	833	CLA	C4-C3-C5-C6
45	BA	811	CLA	C4-C3-C5-C6
45	BB	836	CLA	C4-C3-C5-C6
45	AA	829	CLA	CBA-CGA-O2A-C1
45	B5	602	CLA	CBA-CGA-O2A-C1
54	A6	608	CHL	CBA-CGA-O2A-C1
47	a	501	LHG	C25-C26-C27-C28
47	B1	302	LHG	O9-C7-O7-C5
45	AB	808	CLA	C2-C1-O2A-CGA
47	A3	301	LHG	O1-C1-C2-O2
50	BB	851	LMU	C2-C1-O1'-C1'
45	AA	803	CLA	C11-C10-C8-C9
45	AA	819	CLA	C6-C7-C8-C9
45	AA	828	CLA	C6-C7-C8-C9
45	AA	842	CLA	C11-C10-C8-C9
45	AB	802	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
45	AB	803	CLA	C6-C7-C8-C9
45	AB	806	CLA	C11-C10-C8-C9
45	AB	807	CLA	C11-C12-C13-C14
45	AB	807	CLA	C14-C13-C15-C16
45	AB	819	CLA	C11-C10-C8-C9
45	AB	825	CLA	C14-C13-C15-C16
45	AB	830	CLA	C6-C7-C8-C9
45	AB	834	CLA	C11-C12-C13-C14
45	A1	304	CLA	C11-C10-C8-C9
45	BA	803	CLA	C11-C10-C8-C9
45	BA	819	CLA	C11-C12-C13-C14
45	BA	842	CLA	C11-C10-C8-C9
45	BB	807	CLA	C6-C7-C8-C9
45	BB	811	CLA	C6-C7-C8-C9
45	BB	820	CLA	C11-C10-C8-C9
45	BB	828	CLA	C11-C12-C13-C14
45	BB	829	CLA	C11-C10-C8-C9
45	BB	836	CLA	C11-C10-C8-C9
45	BA	809	CLA	O1D-CGD-O2D-CED
45	AB	826	CLA	C10-C11-C12-C13
47	a	501	LHG	C2-C3-O3-P
47	B5	618	LHG	O10-C23-O8-C6
45	AA	824	CLA	C4B-C3B-CAB-CBB
45	AA	835	CLA	C4B-C3B-CAB-CBB
45	AA	841	CLA	C4B-C3B-CAB-CBB
45	AB	803	CLA	C4B-C3B-CAB-CBB
45	AB	814	CLA	C4B-C3B-CAB-CBB
45	AB	821	CLA	C4B-C3B-CAB-CBB
45	AB	822	CLA	C4B-C3B-CAB-CBB
45	AB	832	CLA	C4B-C3B-CAB-CBB
45	AF	804	CLA	C4B-C3B-CAB-CBB
45	AL	303	CLA	C4B-C3B-CAB-CBB
45	A1	314	CLA	C4B-C3B-CAB-CBB
45	A3	302	CLA	C4B-C3B-CAB-CBB
45	A3	312	CLA	C4B-C3B-CAB-CBB
45	BA	834	CLA	C4B-C3B-CAB-CBB
45	BA	841	CLA	C4B-C3B-CAB-CBB
45	BA	842	CLA	C4B-C3B-CAB-CBB
45	BL	303	CLA	C4B-C3B-CAB-CBB
51	AB	851	DGD	CCB-CDB-CEB-CFB
45	AA	805	CLA	C10-C11-C12-C13
45	A3	303	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
45	BB	835	CLA	C16-C17-C18-C19
45	AB	809	CLA	O1A-CGA-O2A-C1
45	A4	311	CLA	C2A-CAA-CBA-CGA
45	BB	833	CLA	C2A-CAA-CBA-CGA
47	A1	320	LHG	O6-C4-C5-C6
47	BF	305	LHG	C10-C11-C12-C13
54	A6	606	CHL	O1D-CGD-O2D-CED
45	AA	803	CLA	C11-C10-C8-C7
45	AA	808	CLA	C11-C12-C13-C15
45	AA	810	CLA	C6-C7-C8-C10
45	AA	813	CLA	C11-C12-C13-C15
45	AA	827	CLA	C6-C7-C8-C10
45	AA	828	CLA	C12-C13-C15-C16
45	AA	829	CLA	C11-C12-C13-C15
45	AA	830	CLA	C12-C13-C15-C16
45	AA	842	CLA	C11-C10-C8-C7
45	AB	801	CLA	C11-C10-C8-C7
45	AB	802	CLA	C6-C7-C8-C10
45	AB	807	CLA	C12-C13-C15-C16
45	AB	810	CLA	C11-C10-C8-C7
45	AB	815	CLA	C11-C10-C8-C7
45	AB	815	CLA	C12-C13-C15-C16
45	AB	818	CLA	C6-C7-C8-C10
45	AB	823	CLA	C6-C7-C8-C10
45	AB	830	CLA	C6-C7-C8-C10
45	AB	834	CLA	C6-C7-C8-C10
45	A1	314	CLA	C11-C10-C8-C7
45	A6	603	CLA	C11-C12-C13-C15
45	BA	803	CLA	C11-C10-C8-C7
45	BA	819	CLA	C6-C7-C8-C10
45	BA	827	CLA	C6-C7-C8-C10
45	BA	828	CLA	C6-C7-C8-C10
45	BA	842	CLA	C11-C10-C8-C7
45	BB	802	CLA	C6-C7-C8-C10
45	BB	807	CLA	C11-C12-C13-C15
45	BB	819	CLA	C6-C7-C8-C10
45	BB	820	CLA	C11-C10-C8-C7
45	BB	826	CLA	C6-C7-C8-C10
45	BB	829	CLA	C11-C10-C8-C7
45	B1	314	CLA	C6-C7-C8-C10
45	B5	602	CLA	C11-C10-C8-C7
46	BB	844	PQN	C17-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
45	AB	817	CLA	C5-C6-C7-C8
45	AB	830	CLA	C5-C6-C7-C8
45	BB	825	CLA	CBD-CGD-O2D-CED
45	BA	811	CLA	C5-C6-C7-C8
45	BB	819	CLA	C11-C12-C13-C14
45	AA	805	CLA	C3A-C2A-CAA-CBA
45	AA	805	CLA	C4-C3-C5-C6
45	AA	826	CLA	C4-C3-C5-C6
45	AB	810	CLA	C3A-C2A-CAA-CBA
45	AB	842	CLA	C4-C3-C5-C6
45	AF	802	CLA	C4-C3-C5-C6
45	A1	309	CLA	C3A-C2A-CAA-CBA
45	A4	313	CLA	C3A-C2A-CAA-CBA
45	BA	825	CLA	C3A-C2A-CAA-CBA
45	BB	823	CLA	C3A-C2A-CAA-CBA
45	BB	829	CLA	C3A-C2A-CAA-CBA
45	BB	830	CLA	C3A-C2A-CAA-CBA
45	BF	301	CLA	C4-C3-C5-C6
45	BH	201	CLA	C3A-C2A-CAA-CBA
54	A6	602	CHL	C3A-C2A-CAA-CBA
45	BB	819	CLA	CAA-CBA-CGA-O2A
45	BB	836	CLA	C2-C3-C5-C6
45	AA	825	CLA	O1A-CGA-O2A-C1
45	AB	840	CLA	O1A-CGA-O2A-C1
45	BB	824	CLA	C16-C17-C18-C19
48	AA	848	BCR	C7-C8-C9-C34
48	BG	203	BCR	C11-C12-C13-C35
45	A6	610	CLA	O1A-CGA-O2A-C1
54	A6	608	CHL	O1A-CGA-O2A-C1
45	AB	833	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	O6E-C5E-C6E-O5E
48	AJ	103	BCR	C7-C8-C9-C10
51	AB	851	DGD	C4A-C5A-C6A-C7A
45	BB	834	CLA	CBA-CGA-O2A-C1
50	AA	851	LMU	C7-C8-C9-C10
45	BA	805	CLA	C15-C16-C17-C18
47	a	501	LHG	C4-C5-C6-O8
51	AB	851	DGD	C1G-C2G-C3G-O3G
56	BJ	104	SQD	O6-C44-C45-C46
45	AA	811	CLA	C13-C15-C16-C17
45	BA	842	CLA	C4-C3-C5-C6
46	BB	844	PQN	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
45	AA	804	CLA	C2-C3-C5-C6
45	AB	833	CLA	C2-C3-C5-C6
45	BB	818	CLA	C3-C5-C6-C7
45	AB	808	CLA	C2A-CAA-CBA-CGA
45	BA	801	CLA	C16-C17-C18-C20
47	A1	320	LHG	O9-C7-O7-C5
47	A1	320	LHG	O6-C4-C5-O7
45	AB	822	CLA	C2B-C3B-CAB-CBB
45	BA	841	CLA	C2B-C3B-CAB-CBB
48	AA	846	BCR	C5-C6-C7-C8
48	AA	852	BCR	C1-C6-C7-C8
48	AG	205	BCR	C23-C24-C25-C26
48	BA	848	BCR	C5-C6-C7-C8
48	BA	850	BCR	C5-C6-C7-C8
48	BB	803	BCR	C5-C6-C7-C8
48	BB	848	BCR	C5-C6-C7-C8
48	BL	306	BCR	C23-C24-C25-C30
52	A4	315	LUT	C1-C6-C7-C8
52	B1	316	LUT	C1-C6-C7-C8
50	BA	854	LMU	C1-C2-C3-C4
50	AB	850	LMU	C9-C10-C11-C12
45	AA	801	CLA	C16-C17-C18-C20
45	A3	303	CLA	C6-C7-C8-C9
47	B2	618	LHG	O8-C23-C24-C25
45	BB	819	CLA	C2A-CAA-CBA-CGA
54	B1	303	CHL	C2A-CAA-CBA-CGA
45	BA	819	CLA	C5-C6-C7-C8
47	BA	845	LHG	O7-C5-C6-O8
53	AG	202	LMG	O1-C7-C8-O7
53	A1	321	LMG	O1-C7-C8-O7
53	A1	321	LMG	O7-C8-C9-O8
53	B5	617	LMG	O7-C8-C9-O8
45	BB	820	CLA	O1D-CGD-O2D-CED
45	BB	834	CLA	C3-C5-C6-C7
45	BA	818	CLA	O1A-CGA-O2A-C1
45	BA	839	CLA	O1A-CGA-O2A-C1
47	B1	302	LHG	C10-C11-C12-C13
45	BA	805	CLA	C10-C11-C12-C13
45	AA	805	CLA	C2-C3-C5-C6
45	AB	842	CLA	C2-C3-C5-C6
45	AF	802	CLA	C2-C3-C5-C6
45	BA	811	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
45	BA	842	CLA	C2-C3-C5-C6
45	BF	301	CLA	C2-C3-C5-C6
45	AA	808	CLA	C16-C17-C18-C20
53	A4	318	LMG	C29-C28-O8-C9
45	AA	803	CLA	C11-C12-C13-C14
45	AA	840	CLA	C11-C10-C8-C9
45	AB	802	CLA	C6-C7-C8-C9
45	AB	804	CLA	C11-C10-C8-C9
45	AB	810	CLA	C11-C12-C13-C14
45	AB	814	CLA	C11-C12-C13-C14
45	AB	818	CLA	C6-C7-C8-C9
45	AB	828	CLA	C11-C10-C8-C9
45	BB	829	CLA	CAA-CBA-CGA-O2A
47	A1	320	LHG	C34-C35-C36-C37
47	F	801	LHG	C29-C30-C31-C32
51	BB	850	DGD	CAB-CBB-CCB-CDB
50	AA	851	LMU	C1-C2-C3-C4
45	BJ	102	CLA	O1D-CGD-O2D-CED
51	AB	851	DGD	C4B-C5B-C6B-C7B
45	AA	841	CLA	O1A-CGA-O2A-C1
45	AA	801	CLA	CAA-CBA-CGA-O2A
45	BB	829	CLA	C2C-C3C-CAC-CBC
45	BB	802	CLA	O1D-CGD-O2D-CED
47	AA	844	LHG	C23-C24-C25-C26
45	A1	304	CLA	CBA-CGA-O2A-C1
45	AB	819	CLA	C11-C12-C13-C15
45	AB	821	CLA	O1D-CGD-O2D-CED
45	B1	314	CLA	C2C-C3C-CAC-CBC
45	AB	818	CLA	C8-C10-C11-C12
45	AB	826	CLA	C8-C10-C11-C12
45	AB	833	CLA	C10-C11-C12-C13
45	BB	812	CLA	C15-C16-C17-C18
47	BF	305	LHG	C1-C2-C3-O3
45	BB	810	CLA	O1A-CGA-O2A-C1
45	BA	801	CLA	CAA-CBA-CGA-O2A
45	AA	840	CLA	CBA-CGA-O2A-C1
45	AA	802	CLA	C15-C16-C17-C18
51	AB	851	DGD	C7A-C8A-C9A-CAA
47	AJ	104	LHG	O6-C4-C5-C6
47	B3	318	LHG	O6-C4-C5-C6
47	a	501	LHG	O6-C4-C5-C6
45	AB	815	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
48	A3	318	BCR	C37-C22-C23-C24
53	A1	321	LMG	C11-C12-C13-C14
45	AA	803	CLA	C11-C12-C13-C15
45	AA	811	CLA	C12-C13-C15-C16
45	AA	821	CLA	C6-C7-C8-C10
45	AA	840	CLA	C11-C10-C8-C7
45	AB	801	CLA	C6-C7-C8-C10
45	AB	809	CLA	C6-C7-C8-C10
45	AB	814	CLA	C11-C12-C13-C15
45	AB	828	CLA	C11-C10-C8-C7
45	A4	301	CLA	C11-C10-C8-C7
45	BA	810	CLA	C6-C7-C8-C10
45	BA	828	CLA	C12-C13-C15-C16
45	BA	830	CLA	C12-C13-C15-C16
45	BA	840	CLA	C11-C10-C8-C7
45	BA	841	CLA	C11-C10-C8-C7
45	BB	804	CLA	C6-C7-C8-C10
45	BB	804	CLA	C12-C13-C15-C16
45	BB	815	CLA	C11-C12-C13-C15
45	BB	816	CLA	C11-C10-C8-C7
45	B1	304	CLA	C11-C12-C13-C15
50	AL	301	LMU	C1-C2-C3-C4
47	A1	320	LHG	C11-C10-C9-C8
45	AH	201	CLA	C5-C6-C7-C8
45	BB	801	CLA	C13-C15-C16-C17
48	AA	847	BCR	C11-C12-C13-C14
48	AA	848	BCR	C7-C8-C9-C10
48	AB	849	BCR	C7-C8-C9-C10
48	AJ	101	BCR	C17-C18-C19-C20
48	AK	204	BCR	C7-C8-C9-C10
48	BL	306	BCR	C7-C8-C9-C10
45	AA	829	CLA	O1A-CGA-O2A-C1
45	AB	820	CLA	O1A-CGA-O2A-C1
45	A1	304	CLA	O1A-CGA-O2A-C1
45	BA	841	CLA	O1A-CGA-O2A-C1
45	A4	301	CLA	CBD-CGD-O2D-CED
45	B1	305	CLA	C2A-CAA-CBA-CGA
50	BA	853	LMU	C3'-C4'-O1B-C1B
45	AB	831	CLA	O1D-CGD-O2D-CED
45	B3	311	CLA	C4-C3-C5-C6
45	BB	834	CLA	O1A-CGA-O2A-C1
45	B5	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
47	F	801	LHG	C33-C34-C35-C36
45	AA	816	CLA	CBD-CGD-O2D-CED
45	AB	814	CLA	C15-C16-C17-C18
45	BA	830	CLA	O2A-C1-C2-C3
47	A3	319	LHG	C6-C5-O7-C7
45	AA	824	CLA	O1A-CGA-O2A-C1
45	AB	803	CLA	C16-C17-C18-C19
50	AB	853	LMU	C3'-C4'-O1B-C1B
47	A1	320	LHG	C7-C8-C9-C10
51	AB	851	DGD	C5A-C6A-C7A-C8A
45	AA	830	CLA	C5-C6-C7-C8
45	AB	819	CLA	C5-C6-C7-C8
47	AJ	104	LHG	O6-C4-C5-O7
47	B3	318	LHG	O6-C4-C5-O7
47	a	501	LHG	O6-C4-C5-O7
45	AB	801	CLA	C16-C17-C18-C19
45	BB	838	CLA	CBA-CGA-O2A-C1
47	A1	301	LHG	C11-C12-C13-C14
45	AB	828	CLA	C4-C3-C5-C6
45	AA	830	CLA	C10-C11-C12-C13
45	AB	823	CLA	C5-C6-C7-C8
46	AA	843	PQN	C18-C20-C21-C22
45	AA	805	CLA	C2C-C3C-CAC-CBC
45	BB	802	CLA	C3-C5-C6-C7
47	A6	618	LHG	O7-C5-C6-O8
53	B5	617	LMG	O1-C7-C8-O7
45	AA	810	CLA	C6-C7-C8-C9
45	AA	811	CLA	C14-C13-C15-C16
45	AB	827	CLA	C11-C12-C13-C14
45	A4	301	CLA	C11-C10-C8-C9
45	BB	804	CLA	C6-C7-C8-C9
45	BB	815	CLA	C11-C12-C13-C14
45	B5	602	CLA	C11-C10-C8-C9
45	AB	842	CLA	C16-C17-C18-C19
50	AL	301	LMU	C5-C6-C7-C8
47	AA	844	LHG	C31-C32-C33-C34
47	A6	618	LHG	C26-C27-C28-C29
50	AL	301	LMU	C3-C4-C5-C6
45	A6	612	CLA	CBD-CGD-O2D-CED
47	AA	844	LHG	C25-C26-C27-C28
53	A1	321	LMG	C30-C31-C32-C33
45	AA	834	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
47	AA	844	LHG	C30-C31-C32-C33
47	BA	845	LHG	C12-C13-C14-C15
45	BA	803	CLA	CBA-CGA-O2A-C1
45	B3	311	CLA	CBA-CGA-O2A-C1
47	A6	618	LHG	C5-C4-O6-P
45	A6	613	CLA	CBA-CGA-O2A-C1
47	A1	302	LHG	C10-C11-C12-C13
45	B3	311	CLA	C2-C3-C5-C6
45	BB	824	CLA	C5-C6-C7-C8
47	B1	318	LHG	O2-C2-C3-O3
51	BB	850	DGD	C9B-CAB-CBB-CCB
50	AA	851	LMU	C4'-C5'-C6'-O6'
45	BB	821	CLA	C5-C6-C7-C8
45	BB	835	CLA	C10-C11-C12-C13
53	A4	318	LMG	O10-C28-O8-C9
45	BB	819	CLA	C3-C5-C6-C7
47	A1	320	LHG	C25-C26-C27-C28
47	B2	618	LHG	C29-C30-C31-C32
45	BA	803	CLA	O1A-CGA-O2A-C1
45	AA	813	CLA	CBA-CGA-O2A-C1
50	BA	853	LMU	C5'-C4'-O1B-C1B
45	AB	835	CLA	O1D-CGD-O2D-CED
50	AL	301	LMU	C2-C1-O1'-C1'
45	BB	801	CLA	C3-C5-C6-C7
45	AA	805	CLA	C5-C6-C7-C8
45	AA	830	CLA	C1A-C2A-CAA-CBA
45	AA	838	CLA	C4B-C3B-CAB-CBB
45	AB	810	CLA	C1A-C2A-CAA-CBA
45	AB	841	CLA	C1A-C2A-CAA-CBA
45	AB	841	CLA	C4B-C3B-CAB-CBB
45	A1	309	CLA	C4B-C3B-CAB-CBB
45	A3	308	CLA	C1A-C2A-CAA-CBA
45	A4	307	CLA	C4B-C3B-CAB-CBB
45	A4	309	CLA	C4B-C3B-CAB-CBB
45	BA	811	CLA	C1A-C2A-CAA-CBA
45	BB	815	CLA	C1A-C2A-CAA-CBA
45	BB	829	CLA	C1A-C2A-CAA-CBA
45	BB	842	CLA	C4B-C3B-CAB-CBB
45	B3	312	CLA	C4B-C3B-CAB-CBB
45	B5	608	CLA	C4B-C3B-CAB-CBB
45	BB	829	CLA	C4-C3-C5-C6
46	AA	843	PQN	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
47	BA	845	LHG	C35-C36-C37-C38
45	B3	311	CLA	O1A-CGA-O2A-C1
45	BB	801	CLA	C2A-CAA-CBA-CGA
45	BB	810	CLA	C2A-CAA-CBA-CGA
45	BB	841	CLA	O1D-CGD-O2D-CED
47	AJ	104	LHG	C16-C17-C18-C19
51	AB	851	DGD	C8B-C9B-CAB-CBB
45	AB	804	CLA	C15-C16-C17-C18
45	AB	829	CLA	C13-C15-C16-C17
45	BB	801	CLA	CBD-CGD-O2D-CED
45	AA	837	CLA	C2-C3-C5-C6
56	BJ	104	SQD	C5-C6-S-O9
45	AA	811	CLA	C6-C7-C8-C10
45	AA	830	CLA	C11-C10-C8-C7
45	AA	841	CLA	C11-C10-C8-C7
45	AB	815	CLA	C11-C12-C13-C15
45	AB	823	CLA	C11-C10-C8-C7
45	AB	823	CLA	C12-C13-C15-C16
45	AB	825	CLA	C6-C7-C8-C10
45	AB	829	CLA	C12-C13-C15-C16
45	BA	805	CLA	C11-C12-C13-C15
45	BA	827	CLA	C11-C10-C8-C7
45	BB	801	CLA	C6-C7-C8-C10
45	BB	808	CLA	C12-C13-C15-C16
45	BB	810	CLA	C6-C7-C8-C10
45	BB	830	CLA	C12-C13-C15-C16
53	A1	321	LMG	C33-C34-C35-C36
50	AA	851	LMU	C4B-C5B-C6B-O6B
45	AA	813	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	CAA-CBA-CGA-O2A
47	A6	618	LHG	C29-C30-C31-C32
47	F	801	LHG	C11-C10-C9-C8
45	BB	820	CLA	C5-C6-C7-C8
47	BF	305	LHG	C13-C14-C15-C16
47	F	801	LHG	C24-C25-C26-C27
45	AB	809	CLA	C4-C3-C5-C6
45	A3	308	CLA	C3A-C2A-CAA-CBA
45	BB	838	CLA	O1A-CGA-O2A-C1
45	AA	813	CLA	C11-C10-C8-C9
45	AB	801	CLA	C11-C10-C8-C9
45	AB	809	CLA	C6-C7-C8-C9
45	AB	825	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
45	A6	603	CLA	C11-C12-C13-C14
45	BA	830	CLA	C14-C13-C15-C16
45	BA	840	CLA	C11-C10-C8-C9
45	BA	841	CLA	C11-C10-C8-C9
45	BB	816	CLA	C11-C10-C8-C9
45	B1	304	CLA	C11-C12-C13-C14
45	BA	803	CLA	C8-C10-C11-C12
52	B1	316	LUT	C9-C10-C11-C12
45	AA	817	CLA	C5-C6-C7-C8
45	AB	810	CLA	C8-C10-C11-C12
45	AB	828	CLA	C15-C16-C17-C18
45	A1	306	CLA	C1-C2-C3-C4
45	A3	305	CLA	CAD-CBD-CGD-O1D
45	B3	304	CLA	CAD-CBD-CGD-O1D
45	B5	611	CLA	CAD-CBD-CGD-O1D
45	BB	812	CLA	C3-C5-C6-C7
45	BB	841	CLA	O1A-CGA-O2A-C1
56	BJ	104	SQD	O6-C44-C45-O47
47	BF	305	LHG	C14-C15-C16-C17
45	AB	829	CLA	C4-C3-C5-C6
45	BB	819	CLA	C4-C3-C5-C6
47	BA	845	LHG	C11-C12-C13-C14
47	AA	844	LHG	C35-C36-C37-C38
45	AA	814	CLA	CAD-CBD-CGD-O2D
45	AB	814	CLA	CAD-CBD-CGD-O2D
45	AB	827	CLA	CAD-CBD-CGD-O2D
45	AB	837	CLA	CAD-CBD-CGD-O2D
45	AB	842	CLA	CAD-CBD-CGD-O2D
45	AL	303	CLA	CAD-CBD-CGD-O2D
45	A1	305	CLA	CAD-CBD-CGD-O2D
45	A1	316	CLA	CAD-CBD-CGD-O2D
45	BA	805	CLA	CAD-CBD-CGD-O2D
45	BA	812	CLA	CAD-CBD-CGD-O2D
45	BA	814	CLA	CAD-CBD-CGD-O2D
45	BA	824	CLA	CAD-CBD-CGD-O2D
45	BA	831	CLA	CAD-CBD-CGD-O2D
45	BB	815	CLA	CAD-CBD-CGD-O2D
45	BG	201	CLA	CAD-CBD-CGD-O2D
45	BK	202	CLA	CAD-CBD-CGD-O2D
45	BL	302	CLA	CAD-CBD-CGD-O2D
45	AA	840	CLA	O1A-CGA-O2A-C1
45	AB	837	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
45	BB	841	CLA	CBA-CGA-O2A-C1
45	B3	311	CLA	C2A-CAA-CBA-CGA
50	AB	853	LMU	C5'-C4'-O1B-C1B
45	AB	837	CLA	O1A-CGA-O2A-C1
45	BB	825	CLA	O1D-CGD-O2D-CED
45	AA	805	CLA	CAD-CBD-CGD-O1D
45	AA	814	CLA	CAD-CBD-CGD-O1D
45	AA	820	CLA	CHA-CBD-CGD-O1D
45	AA	820	CLA	CHA-CBD-CGD-O2D
45	AA	822	CLA	CHA-CBD-CGD-O1D
45	AA	831	CLA	CHA-CBD-CGD-O1D
45	AB	814	CLA	CAD-CBD-CGD-O1D
45	AB	827	CLA	CAD-CBD-CGD-O1D
45	AB	837	CLA	CAD-CBD-CGD-O1D
45	AB	842	CLA	CAD-CBD-CGD-O1D
45	AK	202	CLA	CHA-CBD-CGD-O1D
45	AK	202	CLA	CHA-CBD-CGD-O2D
45	AK	203	CLA	CHA-CBD-CGD-O1D
45	AK	203	CLA	CHA-CBD-CGD-O2D
45	AL	303	CLA	CAD-CBD-CGD-O1D
45	A1	305	CLA	CAD-CBD-CGD-O1D
45	A1	309	CLA	CHA-CBD-CGD-O2D
45	A1	309	CLA	CAD-CBD-CGD-O2D
45	A1	313	CLA	CHA-CBD-CGD-O1D
45	A1	316	CLA	CAD-CBD-CGD-O1D
45	A4	302	CLA	CHA-CBD-CGD-O1D
45	A4	302	CLA	CHA-CBD-CGD-O2D
45	A4	310	CLA	CHA-CBD-CGD-O2D
45	BA	805	CLA	CAD-CBD-CGD-O1D
45	BA	812	CLA	CAD-CBD-CGD-O1D
45	BA	813	CLA	CAD-CBD-CGD-O1D
45	BA	814	CLA	CAD-CBD-CGD-O1D
45	BA	824	CLA	CAD-CBD-CGD-O1D
45	BA	825	CLA	CHA-CBD-CGD-O1D
45	BA	825	CLA	CHA-CBD-CGD-O2D
45	BA	831	CLA	CAD-CBD-CGD-O1D
45	BA	839	CLA	CHA-CBD-CGD-O1D
45	BA	841	CLA	CAD-CBD-CGD-O1D
45	BB	815	CLA	CAD-CBD-CGD-O1D
45	BB	819	CLA	CHA-CBD-CGD-O1D
45	BB	822	CLA	CHA-CBD-CGD-O1D
45	BB	826	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	BB	827	CLA	CAD-CBD-CGD-O1D
45	BG	201	CLA	CAD-CBD-CGD-O1D
45	BK	202	CLA	CAD-CBD-CGD-O1D
45	BL	302	CLA	CAD-CBD-CGD-O1D
45	B1	304	CLA	CHA-CBD-CGD-O1D
45	B1	304	CLA	CHA-CBD-CGD-O2D
45	B1	310	CLA	CHA-CBD-CGD-O2D
45	B3	303	CLA	CHA-CBD-CGD-O2D
45	B3	304	CLA	CAD-CBD-CGD-O2D
47	AA	844	LHG	C4-O6-P-O3
47	AJ	104	LHG	C3-O3-P-O5
47	A1	301	LHG	C3-O3-P-O4
47	A1	302	LHG	C3-O3-P-O5
47	A1	302	LHG	C4-O6-P-O3
47	A1	302	LHG	C4-O6-P-O4
47	A1	302	LHG	C4-O6-P-O5
47	A3	319	LHG	C4-O6-P-O3
47	A6	618	LHG	C4-O6-P-O4
47	BF	305	LHG	C3-O3-P-O4
47	B1	318	LHG	C4-O6-P-O3
47	B2	618	LHG	C4-O6-P-O4
47	B5	618	LHG	C4-O6-P-O5
47	a	501	LHG	C3-O3-P-O5
54	A1	308	CHL	CHA-CBD-CGD-O2D
54	A4	304	CHL	CHA-CBD-CGD-O2D
54	B5	605	CHL	CHA-CBD-CGD-O2D
54	B5	605	CHL	CAD-CBD-CGD-O2D
45	BA	840	CLA	C3-C5-C6-C7
45	A3	312	CLA	C4-C3-C5-C6
45	AA	811	CLA	C2B-C3B-CAB-CBB
45	AA	831	CLA	C2B-C3B-CAB-CBB
45	AA	838	CLA	C2B-C3B-CAB-CBB
45	AA	841	CLA	C2B-C3B-CAB-CBB
45	AB	831	CLA	C2B-C3B-CAB-CBB
45	AB	832	CLA	C2B-C3B-CAB-CBB
45	AB	842	CLA	C2B-C3B-CAB-CBB
45	AF	804	CLA	C2B-C3B-CAB-CBB
45	AG	204	CLA	C2B-C3B-CAB-CBB
45	A3	302	CLA	C2B-C3B-CAB-CBB
45	A3	309	CLA	C2B-C3B-CAB-CBB
45	A4	309	CLA	C2B-C3B-CAB-CBB
45	A4	310	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	A6	605	CLA	C2B-C3B-CAB-CBB
45	A6	610	CLA	C2B-C3B-CAB-CBB
45	BB	825	CLA	C2B-C3B-CAB-CBB
45	BB	832	CLA	C2B-C3B-CAB-CBB
45	BB	843	CLA	C2B-C3B-CAB-CBB
45	BH	201	CLA	C2B-C3B-CAB-CBB
45	BL	303	CLA	C2B-C3B-CAB-CBB
45	B3	312	CLA	C2B-C3B-CAB-CBB
45	B5	613	CLA	C2B-C3B-CAB-CBB
48	AA	847	BCR	C23-C24-C25-C30
48	AI	101	BCR	C5-C6-C7-C8
48	AJ	103	BCR	C23-C24-C25-C30
48	BF	304	BCR	C23-C24-C25-C30
47	BA	845	LHG	C31-C32-C33-C34
45	AB	809	CLA	C2-C3-C5-C6
47	A1	302	LHG	C7-C8-C9-C10
47	AJ	104	LHG	C2-C3-O3-P
47	B3	318	LHG	C5-C4-O6-P
47	F	801	LHG	C2-C3-O3-P
48	AI	101	BCR	C37-C22-C23-C24
48	AK	204	BCR	C7-C8-C9-C34
48	A1	319	BCR	C37-C22-C23-C24
48	BI	101	BCR	C37-C22-C23-C24
52	B1	316	LUT	C31-C32-C33-C40
45	AA	816	CLA	O1D-CGD-O2D-CED
45	AA	818	CLA	CAA-CBA-CGA-O2A
45	AB	828	CLA	CAA-CBA-CGA-O2A
47	AA	844	LHG	C29-C30-C31-C32
47	a	501	LHG	C7-C8-C9-C10
45	AB	818	CLA	C10-C11-C12-C13
45	BB	819	CLA	O2A-C1-C2-C3
51	AB	851	DGD	CBB-CCB-CDB-CEB
45	AB	833	CLA	CAA-CBA-CGA-O2A
45	BA	817	CLA	C5-C6-C7-C8
45	BB	819	CLA	C2-C3-C5-C6
45	AB	819	CLA	C11-C12-C13-C14
45	BA	841	CLA	C16-C17-C18-C19
45	AA	826	CLA	C8-C10-C11-C12
45	BB	808	CLA	C5-C6-C7-C8
45	BA	805	CLA	C2C-C3C-CAC-CBC
45	A3	312	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
45	AB	815	CLA	C11-C10-C8-C9
45	AB	823	CLA	C14-C13-C15-C16
45	BA	810	CLA	C6-C7-C8-C9
45	BB	802	CLA	C6-C7-C8-C9
45	BB	805	CLA	C11-C12-C13-C14
45	BB	810	CLA	C6-C7-C8-C9
46	BB	844	PQN	C21-C22-C23-C24
45	AA	842	CLA	C12-C13-C15-C16
45	BA	808	CLA	C11-C12-C13-C15
45	BB	815	CLA	C6-C7-C8-C10
47	B1	301	LHG	C28-C29-C30-C31
47	BF	305	LHG	C24-C25-C26-C27
45	A6	612	CLA	O1D-CGD-O2D-CED
45	BA	818	CLA	CAA-CBA-CGA-O2A
45	BA	821	CLA	C4-C3-C5-C6
45	AB	818	CLA	C5-C6-C7-C8
47	A1	302	LHG	O9-C7-O7-C5
50	BA	854	LMU	C6-C7-C8-C9
45	BA	829	CLA	CAA-CBA-CGA-O2A
47	AA	844	LHG	C32-C33-C34-C35
45	BB	806	CLA	C4C-C3C-CAC-CBC
45	AB	828	CLA	C2C-C3C-CAC-CBC
45	BA	830	CLA	C16-C17-C18-C20
45	AA	838	CLA	C5-C6-C7-C8
45	AB	809	CLA	C2A-CAA-CBA-CGA
45	BB	805	CLA	C5-C6-C7-C8
45	AA	828	CLA	C2-C1-O2A-CGA
45	AB	833	CLA	C2-C1-O2A-CGA
45	BA	825	CLA	C2-C1-O2A-CGA
45	AA	802	CLA	C4-C3-C5-C6
45	AA	806	CLA	C4-C3-C5-C6
45	BB	830	CLA	C4-C3-C5-C6
51	BB	850	DGD	O1G-C1G-C2G-C3G
53	A4	318	LMG	O1-C7-C8-C9
45	AB	838	CLA	C8-C10-C11-C12
45	AB	818	CLA	CAA-CBA-CGA-O2A
48	BA	855	BCR	C37-C22-C23-C24
47	BA	845	LHG	C11-C10-C9-C8
48	AA	852	BCR	C21-C22-C23-C24
48	BA	856	BCR	C21-C22-C23-C24
45	AB	806	CLA	C2C-C3C-CAC-CBC
47	AJ	104	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
45	AA	813	CLA	C2A-CAA-CBA-CGA
45	AB	817	CLA	C2A-CAA-CBA-CGA
45	BK	202	CLA	C2A-CAA-CBA-CGA
50	BA	853	LMU	C11-C10-C9-C8
50	BA	853	LMU	C3-C4-C5-C6
45	AB	830	CLA	C4-C3-C5-C6
45	BB	805	CLA	C10-C11-C12-C13
45	AB	829	CLA	C2-C3-C5-C6
50	AB	853	LMU	C3-C4-C5-C6
50	AB	853	LMU	C2-C1-O1'-C1'
50	BA	854	LMU	C2-C1-O1'-C1'
47	BA	845	LHG	C9-C10-C11-C12
45	AA	811	CLA	C6-C7-C8-C9
45	AA	830	CLA	C11-C10-C8-C9
45	A4	311	CLA	C6-C7-C8-C9
45	BB	808	CLA	C14-C13-C15-C16
45	BB	815	CLA	C6-C7-C8-C9
53	B5	617	LMG	C29-C28-O8-C9
45	A4	301	CLA	O1D-CGD-O2D-CED
45	AA	816	CLA	C4B-C3B-CAB-CBB
45	AB	808	CLA	C4B-C3B-CAB-CBB
45	A1	305	CLA	C4B-C3B-CAB-CBB
45	BB	837	CLA	C4B-C3B-CAB-CBB
47	A1	302	LHG	C23-C24-C25-C26
45	AA	826	CLA	C10-C11-C12-C13
45	A1	309	CLA	CAA-CBA-CGA-O2A
45	AA	826	CLA	C11-C12-C13-C14
45	A3	312	CLA	CBA-CGA-O2A-C1
45	BB	811	CLA	CBA-CGA-O2A-C1
50	BA	854	LMU	C3'-C4'-O1B-C1B
45	AA	806	CLA	C2-C3-C5-C6
45	AB	828	CLA	C2-C3-C5-C6
45	A3	312	CLA	C2-C3-C5-C6
45	A3	312	CLA	C3-C5-C6-C7
50	BB	851	LMU	C4B-C5B-C6B-O6B
45	BA	830	CLA	C16-C17-C18-C19
45	AB	827	CLA	C11-C10-C8-C7
45	AB	840	CLA	C11-C10-C8-C7
45	BA	805	CLA	C12-C13-C15-C16
45	BA	842	CLA	C12-C13-C15-C16
45	AA	842	CLA	C10-C11-C12-C13
45	AB	814	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	BA	840	CLA	C13-C15-C16-C17
50	BB	851	LMU	C3-C4-C5-C6
53	A1	321	LMG	C31-C32-C33-C34
45	A1	304	CLA	C2-C3-C5-C6
45	AA	809	CLA	C3A-C2A-CAA-CBA
45	AB	811	CLA	C3A-C2A-CAA-CBA
54	A6	602	CHL	C3-C5-C6-C7
50	AA	851	LMU	C2-C3-C4-C5
48	AA	847	BCR	C35-C13-C14-C15
48	AA	849	BCR	C11-C10-C9-C34
48	AA	849	BCR	C16-C17-C18-C36
48	AB	845	BCR	C11-C10-C9-C34
48	AB	846	BCR	C11-C10-C9-C34
48	AB	846	BCR	C20-C21-C22-C37
48	AF	805	BCR	C35-C13-C14-C15
48	AL	302	BCR	C11-C10-C9-C34
48	BA	851	BCR	C11-C10-C9-C34
48	BA	851	BCR	C16-C17-C18-C36
48	BB	846	BCR	C11-C10-C9-C34
48	BB	847	BCR	C11-C10-C9-C34
48	BB	847	BCR	C20-C21-C22-C37
48	BF	304	BCR	C35-C13-C14-C15
48	BG	203	BCR	C11-C10-C9-C34
48	BG	203	BCR	C35-C13-C14-C15
48	BG	203	BCR	C16-C17-C18-C36
48	BL	301	BCR	C11-C10-C9-C34
48	BL	306	BCR	C11-C10-C9-C34
48	BL	306	BCR	C35-C13-C14-C15
48	BL	306	BCR	C16-C17-C18-C36
48	BL	306	BCR	C20-C21-C22-C37
50	AB	853	LMU	O5'-C1'-O1'-C1
45	BB	843	CLA	C10-C11-C12-C13
46	BA	843	PQN	C20-C21-C22-C23
47	A3	319	LHG	C23-C24-C25-C26
45	BA	806	CLA	C15-C16-C17-C18
50	AB	853	LMU	C5-C6-C7-C8
45	AB	842	CLA	C3-C5-C6-C7
45	BA	813	CLA	C8-C10-C11-C12
54	A1	303	CHL	C4-C3-C5-C6
50	BB	851	LMU	C3'-C4'-O1B-C1B
45	A3	308	CLA	CAA-CBA-CGA-O1A
52	B3	315	LUT	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
45	BA	805	CLA	C4-C3-C5-C6
45	AA	802	CLA	C2-C3-C5-C6
45	BB	829	CLA	C2-C3-C5-C6
45	BH	201	CLA	C11-C12-C13-C14
45	BA	826	CLA	CBD-CGD-O2D-CED
45	B5	613	CLA	CAA-CBA-CGA-O1A
54	B5	607	CHL	CAA-CBA-CGA-O2A
47	A1	320	LHG	C15-C16-C17-C18
51	AB	851	DGD	CBA-CCA-CDA-CEA
45	AA	833	CLA	C8-C10-C11-C12
45	AB	841	CLA	C5-C6-C7-C8
45	AB	842	CLA	C10-C11-C12-C13
45	A1	309	CLA	CAA-CBA-CGA-O1A
54	B5	607	CHL	CAA-CBA-CGA-O1A
45	AB	803	CLA	C11-C12-C13-C14
45	BA	805	CLA	C11-C12-C13-C14
45	BA	808	CLA	C11-C12-C13-C14
45	BA	830	CLA	C11-C10-C8-C9
45	BA	842	CLA	C14-C13-C15-C16
45	BB	802	CLA	C11-C10-C8-C9
45	BB	835	CLA	C11-C12-C13-C14
45	B2	602	CLA	C11-C10-C8-C9
46	BA	843	PQN	C21-C22-C23-C24
45	BA	813	CLA	C10-C11-C12-C13
45	BB	818	CLA	C5-C6-C7-C8
47	B1	301	LHG	C11-C10-C9-C8
45	BB	834	CLA	CAA-CBA-CGA-O2A
45	BA	806	CLA	CBD-CGD-O2D-CED
45	AB	830	CLA	C2-C3-C5-C6
45	BA	821	CLA	C2-C3-C5-C6
45	BB	830	CLA	C2-C3-C5-C6
47	B2	618	LHG	O1-C1-C2-O2
45	BA	838	CLA	C2A-CAA-CBA-CGA
45	AA	841	CLA	C1A-C2A-CAA-CBA
45	AB	820	CLA	C1A-C2A-CAA-CBA
45	AK	202	CLA	C1A-C2A-CAA-CBA
45	BA	805	CLA	C1A-C2A-CAA-CBA
45	BA	825	CLA	C1A-C2A-CAA-CBA
45	BA	827	CLA	C1A-C2A-CAA-CBA
45	BB	832	CLA	C1A-C2A-CAA-CBA
48	AA	847	BCR	C12-C13-C14-C15
48	AA	849	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
48	AA	849	BCR	C16-C17-C18-C19
48	AB	845	BCR	C11-C10-C9-C8
48	AB	846	BCR	C11-C10-C9-C8
48	AB	846	BCR	C20-C21-C22-C23
48	AF	805	BCR	C12-C13-C14-C15
48	AL	302	BCR	C11-C10-C9-C8
48	BA	851	BCR	C11-C10-C9-C8
48	BA	851	BCR	C16-C17-C18-C19
48	BB	846	BCR	C11-C10-C9-C8
48	BB	847	BCR	C11-C10-C9-C8
48	BB	847	BCR	C20-C21-C22-C23
48	BF	304	BCR	C12-C13-C14-C15
48	BG	203	BCR	C11-C10-C9-C8
48	BG	203	BCR	C16-C17-C18-C19
48	BL	301	BCR	C11-C10-C9-C8
48	BL	306	BCR	C16-C17-C18-C19
45	BB	829	CLA	CBA-CGA-O2A-C1
50	AB	853	LMU	O5B-C1B-O1B-C4'
51	BB	850	DGD	C9A-CAA-CBA-CCA
56	BJ	104	SQD	C27-C28-C29-C30
45	B2	602	CLA	C8-C10-C11-C12
45	AA	835	CLA	C2B-C3B-CAB-CBB
45	AB	814	CLA	C2B-C3B-CAB-CBB
45	AB	841	CLA	C2B-C3B-CAB-CBB
45	AF	803	CLA	C2B-C3B-CAB-CBB
45	AG	201	CLA	C2B-C3B-CAB-CBB
45	AL	303	CLA	C2B-C3B-CAB-CBB
45	A1	309	CLA	C2B-C3B-CAB-CBB
45	A3	314	CLA	C2B-C3B-CAB-CBB
45	A4	301	CLA	C2B-C3B-CAB-CBB
45	A4	307	CLA	C2B-C3B-CAB-CBB
45	BB	842	CLA	C2B-C3B-CAB-CBB
45	B5	602	CLA	C2B-C3B-CAB-CBB
45	B5	610	CLA	C2B-C3B-CAB-CBB
48	AA	846	BCR	C1-C6-C7-C8
48	AI	102	BCR	C1-C6-C7-C8
48	BA	847	BCR	C1-C6-C7-C8
48	BL	306	BCR	C5-C6-C7-C8
48	BL	306	BCR	C23-C24-C25-C26
52	B1	316	LUT	C5-C6-C7-C8
47	A1	302	LHG	C8-C7-O7-C5
45	BK	202	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
50	BB	851	LMU	C2B-C1B-O1B-C4'
45	A6	610	CLA	C3-C5-C6-C7
45	A3	308	CLA	CAA-CBA-CGA-O2A
45	BA	836	CLA	CAA-CBA-CGA-O1A
45	AB	803	CLA	C4-C3-C5-C6
45	AB	827	CLA	C4-C3-C5-C6
45	BA	840	CLA	C4-C3-C5-C6
45	BK	202	CLA	CAA-CBA-CGA-O1A
45	B5	613	CLA	CAA-CBA-CGA-O2A
45	AA	833	CLA	C11-C12-C13-C15
45	AB	842	CLA	C12-C13-C15-C16
45	A4	311	CLA	C6-C7-C8-C10
45	BA	803	CLA	C11-C12-C13-C15
45	BA	806	CLA	C11-C12-C13-C15
45	BA	806	CLA	C12-C13-C15-C16
45	BA	811	CLA	C12-C13-C15-C16
45	BA	840	CLA	C12-C13-C15-C16
45	BB	816	CLA	C11-C12-C13-C15
45	BB	824	CLA	C11-C10-C8-C7
45	BB	824	CLA	C12-C13-C15-C16
45	BB	834	CLA	C11-C12-C13-C15
45	BB	842	CLA	C6-C7-C8-C10
45	B2	612	CLA	C16-C17-C18-C20
45	BB	843	CLA	C2A-CAA-CBA-CGA
53	A4	318	LMG	O7-C8-C9-O8
45	BG	202	CLA	CAA-CBA-CGA-O1A
45	BH	201	CLA	CBA-CGA-O2A-C1
45	AB	818	CLA	C3-C5-C6-C7
45	BB	810	CLA	C3-C5-C6-C7
45	BB	827	CLA	C3-C5-C6-C7
53	B5	617	LMG	O10-C28-O8-C9
47	A3	319	LHG	C1-C2-C3-O3
47	B3	318	LHG	C1-C2-C3-O3
45	AA	808	CLA	C15-C16-C17-C18
45	BB	829	CLA	O1A-CGA-O2A-C1
45	BG	202	CLA	CAA-CBA-CGA-O2A
45	BB	816	CLA	C4-C3-C5-C6
45	BB	827	CLA	C4-C3-C5-C6
54	B2	601	CHL	C4-C3-C5-C6
50	AB	852	LMU	C4B-C5B-C6B-O6B
45	B1	311	CLA	C5-C6-C7-C8
45	BA	805	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
50	BA	853	LMU	C2B-C1B-O1B-C4'
45	AB	801	CLA	C2-C1-O2A-CGA
45	BB	807	CLA	C2-C1-O2A-CGA
45	BB	832	CLA	CBD-CGD-O2D-CED
45	BF	301	CLA	C5-C6-C7-C8
54	B2	607	CHL	CAA-CBA-CGA-O2A
48	BJ	103	BCR	C7-C8-C9-C10
47	A1	302	LHG	C27-C28-C29-C30
45	AA	821	CLA	C13-C15-C16-C17
45	BB	827	CLA	C13-C15-C16-C17
45	A6	612	CLA	CAA-CBA-CGA-O1A
45	A6	612	CLA	CAA-CBA-CGA-O2A
45	BA	836	CLA	CAA-CBA-CGA-O2A
45	AB	811	CLA	C14-C13-C15-C16
45	BA	829	CLA	C14-C13-C15-C16
45	BB	824	CLA	C11-C12-C13-C14
45	BA	824	CLA	C5-C6-C7-C8
47	B2	618	LHG	O10-C23-C24-C25
45	AB	802	CLA	C10-C11-C12-C13
45	BB	804	CLA	C4-C3-C5-C6
45	BB	811	CLA	O1A-CGA-O2A-C1
45	BH	201	CLA	O1A-CGA-O2A-C1
45	BB	827	CLA	C5-C6-C7-C8
54	A3	307	CHL	CAA-CBA-CGA-O2A
45	BA	825	CLA	C8-C10-C11-C12
53	A4	318	LMG	C7-C8-C9-O8
45	BB	812	CLA	C10-C11-C12-C13
45	A1	316	CLA	CAA-CBA-CGA-O2A
45	B2	608	CLA	CAA-CBA-CGA-O2A
45	AA	810	CLA	CAD-CBD-CGD-O1D
45	AA	806	CLA	C2A-CAA-CBA-CGA
45	AB	828	CLA	C2A-CAA-CBA-CGA
45	BB	839	CLA	C2A-CAA-CBA-CGA
45	B5	612	CLA	C2A-CAA-CBA-CGA
50	BB	851	LMU	C5'-C4'-O1B-C1B
47	BA	845	LHG	O6-C4-C5-O7
47	B1	301	LHG	O6-C4-C5-O7
45	BA	813	CLA	C4-C3-C5-C6
45	B2	611	CLA	CAA-CBA-CGA-O2A
56	BJ	104	SQD	C17-C18-C19-C20
45	AB	813	CLA	C4B-C3B-CAB-CBB
45	AB	836	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	AJ	102	CLA	C4B-C3B-CAB-CBB
45	A3	311	CLA	C4B-C3B-CAB-CBB
45	A4	301	CLA	C4B-C3B-CAB-CBB
45	BA	803	CLA	C4B-C3B-CAB-CBB
45	BA	814	CLA	C4B-C3B-CAB-CBB
45	BB	809	CLA	C4B-C3B-CAB-CBB
45	BB	834	CLA	C4B-C3B-CAB-CBB
45	BB	801	CLA	C8-C10-C11-C12
45	BB	830	CLA	C13-C15-C16-C17
45	AG	204	CLA	CAA-CBA-CGA-O2A
45	AG	204	CLA	CAA-CBA-CGA-O1A
45	A4	302	CLA	CAA-CBA-CGA-O2A
45	AB	809	CLA	C16-C17-C18-C19
54	B2	605	CHL	CHA-CBD-CGD-O1D
54	B2	605	CHL	CHA-CBD-CGD-O2D
54	B5	606	CHL	CHA-CBD-CGD-O1D
54	B5	606	CHL	CHA-CBD-CGD-O2D
45	BA	841	CLA	C5-C6-C7-C8
45	BB	802	CLA	C15-C16-C17-C18
45	BA	835	CLA	CAA-CBA-CGA-O2A
45	AA	801	CLA	CAA-CBA-CGA-O1A
47	B1	301	LHG	O6-C4-C5-C6
47	B1	302	LHG	O6-C4-C5-C6
45	AA	842	CLA	C4-C3-C5-C6
45	B2	609	CLA	C4-C3-C5-C6
47	A3	319	LHG	O7-C5-C6-O8
45	BA	808	CLA	C5-C6-C7-C8
45	B1	309	CLA	CAA-CBA-CGA-O2A
45	AB	827	CLA	C2-C3-C5-C6
45	AA	828	CLA	C5-C6-C7-C8
47	a	501	LHG	C5-C4-O6-P
47	F	801	LHG	C28-C29-C30-C31
45	BA	813	CLA	C11-C12-C13-C15
45	BB	801	CLA	C12-C13-C15-C16
45	BB	824	CLA	C11-C12-C13-C15
46	BA	843	PQN	C21-C22-C23-C25
47	B2	618	LHG	C26-C27-C28-C29
45	AB	813	CLA	O1D-CGD-O2D-CED
45	AA	836	CLA	CAA-CBA-CGA-O2A
53	A1	321	LMG	C34-C35-C36-C37
45	BA	826	CLA	O1D-CGD-O2D-CED
45	B2	608	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
54	B2	607	CHL	CAA-CBA-CGA-O1A
45	BB	819	CLA	CAA-CBA-CGA-O1A
52	B5	614	LUT	C7-C8-C9-C10
45	AA	819	CLA	C11-C12-C13-C14
45	AA	821	CLA	C6-C7-C8-C9
45	AB	823	CLA	C11-C12-C13-C14
45	A1	314	CLA	C6-C7-C8-C9
45	BA	821	CLA	C11-C12-C13-C14
45	BB	808	CLA	C11-C10-C8-C9
45	BB	828	CLA	C11-C10-C8-C9
45	B2	612	CLA	C14-C13-C15-C16
53	B5	617	LMG	C4-C5-C6-O5
45	BA	806	CLA	O1D-CGD-O2D-CED
45	BA	831	CLA	C2A-CAA-CBA-CGA
45	AA	833	CLA	C2-C1-O2A-CGA
45	AB	818	CLA	C2-C1-O2A-CGA
45	AH	201	CLA	C2-C1-O2A-CGA
45	BB	818	CLA	C2-C1-O2A-CGA
54	A6	608	CHL	C2-C1-O2A-CGA
45	BH	201	CLA	C11-C12-C13-C15
45	AA	841	CLA	C3A-C2A-CAA-CBA
45	BA	827	CLA	C3A-C2A-CAA-CBA
45	B5	608	CLA	C3A-C2A-CAA-CBA
45	B5	603	CLA	CAA-CBA-CGA-O2A
54	B3	306	CHL	CAA-CBA-CGA-O2A
47	A3	301	LHG	O7-C7-C8-C9
45	AB	801	CLA	O1A-CGA-O2A-C1
45	AB	804	CLA	O2A-C1-C2-C3
47	A6	618	LHG	C4-C5-O7-C7
50	BA	854	LMU	C5'-C4'-O1B-C1B
45	BB	832	CLA	O1D-CGD-O2D-CED
45	A1	316	CLA	CAA-CBA-CGA-O1A
45	B1	313	CLA	CAA-CBA-CGA-O2A
45	B3	307	CLA	CAA-CBA-CGA-O2A
45	BA	835	CLA	CAA-CBA-CGA-O1A
45	B2	611	CLA	CAA-CBA-CGA-O1A
45	A6	603	CLA	C2A-CAA-CBA-CGA
45	BB	829	CLA	C2A-CAA-CBA-CGA
54	A3	307	CHL	CAA-CBA-CGA-O1A
45	B1	304	CLA	CBA-CGA-O2A-C1
45	AB	825	CLA	C8-C10-C11-C12
45	A4	302	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
45	B3	307	CLA	CAA-CBA-CGA-O1A
45	B5	603	CLA	CAA-CBA-CGA-O1A
54	B3	306	CHL	CAA-CBA-CGA-O1A
47	BA	846	LHG	O6-C4-C5-O7
47	B1	302	LHG	O6-C4-C5-O7
45	AA	821	CLA	C10-C11-C12-C13
45	AA	818	CLA	C10-C11-C12-C13
56	e	301	SQD	C25-C26-C27-C28
45	AK	202	CLA	CAA-CBA-CGA-O1A
47	A6	618	LHG	C4-C5-C6-O8
53	A1	321	LMG	C7-C8-C9-O8
53	B5	617	LMG	C7-C8-C9-O8
47	BA	845	LHG	C19-C20-C21-C22
45	BA	838	CLA	CAD-CBD-CGD-O2D
45	AB	842	CLA	C2A-CAA-CBA-CGA
47	B1	301	LHG	C27-C28-C29-C30
45	AA	836	CLA	CAA-CBA-CGA-O1A
46	BB	844	PQN	C12-C13-C15-C16
45	B2	612	CLA	C16-C17-C18-C19
45	BB	829	CLA	CAA-CBA-CGA-O1A
45	AB	813	CLA	CBD-CGD-O2D-CED
45	B1	313	CLA	CAA-CBA-CGA-O1A
45	A1	304	CLA	C4C-C3C-CAC-CBC
45	B1	309	CLA	CAA-CBA-CGA-O1A
45	BB	804	CLA	C5-C6-C7-C8
45	AB	801	CLA	C11-C12-C13-C14
45	AB	803	CLA	C11-C10-C8-C9
45	AL	304	CLA	C11-C10-C8-C9
45	A3	302	CLA	C6-C7-C8-C9
45	BA	825	CLA	C11-C10-C8-C9
45	BA	827	CLA	C11-C10-C8-C9
47	B2	618	LHG	C30-C31-C32-C33
45	AA	833	CLA	CAA-CBA-CGA-O2A
54	A6	608	CHL	CAA-CBA-CGA-O2A
45	B1	304	CLA	O1A-CGA-O2A-C1
47	AA	844	LHG	O6-C4-C5-C6
47	A1	301	LHG	O6-C4-C5-C6
53	B5	617	LMG	O7-C10-C11-C12
46	BA	843	PQN	C26-C27-C28-C29
45	AA	809	CLA	C2A-CAA-CBA-CGA
45	A1	304	CLA	C2A-CAA-CBA-CGA
45	AA	801	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
45	BA	821	CLA	C11-C12-C13-C15
45	BA	829	CLA	C12-C13-C15-C16
45	BB	805	CLA	C11-C10-C8-C7
45	BB	835	CLA	C11-C12-C13-C15
45	BB	842	CLA	C11-C10-C8-C7
45	B2	612	CLA	C12-C13-C15-C16
45	A3	302	CLA	C8-C10-C11-C12
45	AA	816	CLA	C2B-C3B-CAB-CBB
45	AA	824	CLA	C2B-C3B-CAB-CBB
45	AB	803	CLA	C2B-C3B-CAB-CBB
45	AB	821	CLA	C2B-C3B-CAB-CBB
45	AJ	102	CLA	C2B-C3B-CAB-CBB
45	A1	314	CLA	C2B-C3B-CAB-CBB
45	A3	312	CLA	C2B-C3B-CAB-CBB
45	A6	603	CLA	C2B-C3B-CAB-CBB
45	A6	614	CLA	C2B-C3B-CAB-CBB
45	BA	816	CLA	C2B-C3B-CAB-CBB
45	BA	834	CLA	C2B-C3B-CAB-CBB
45	BB	834	CLA	C2B-C3B-CAB-CBB
45	BB	837	CLA	C2B-C3B-CAB-CBB
45	B3	301	CLA	C2B-C3B-CAB-CBB
48	AG	205	BCR	C23-C24-C25-C30
48	AL	302	BCR	C23-C24-C25-C26
48	AL	306	BCR	C23-C24-C25-C26
48	AL	306	BCR	C23-C24-C25-C30
48	BB	803	BCR	C1-C6-C7-C8
48	BB	848	BCR	C1-C6-C7-C8
48	BI	101	BCR	C23-C24-C25-C30
48	BK	204	BCR	C5-C6-C7-C8
48	BL	301	BCR	C23-C24-C25-C30
45	BA	832	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	CEA-CFA-CGA-CHA
45	AB	812	CLA	C2-C1-O2A-CGA
45	AB	829	CLA	C2-C1-O2A-CGA
45	BA	829	CLA	C2-C1-O2A-CGA
45	BB	816	CLA	C2-C1-O2A-CGA
50	AB	853	LMU	C2-C3-C4-C5
47	BA	845	LHG	C30-C31-C32-C33
53	A4	318	LMG	O7-C10-C11-C12
45	BA	832	CLA	CBD-CGD-O2D-CED
45	AB	819	CLA	C3-C5-C6-C7
45	BB	815	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	AA	842	CLA	C2-C3-C5-C6
45	BB	811	CLA	C5-C6-C7-C8
47	F	801	LHG	C8-C7-O7-C5
45	BB	828	CLA	C5-C6-C7-C8
45	A1	313	CLA	CAA-CBA-CGA-O2A
47	BA	845	LHG	C17-C18-C19-C20
50	AB	853	LMU	C2B-C1B-O1B-C4'
56	BJ	104	SQD	C4-C5-C6-S
45	AA	834	CLA	CAA-CBA-CGA-O2A
47	B5	618	LHG	O7-C7-C8-C9
45	AG	201	CLA	CAA-CBA-CGA-O2A
45	B5	608	CLA	CAA-CBA-CGA-O2A
45	BB	829	CLA	C13-C15-C16-C17
47	AJ	104	LHG	C17-C18-C19-C20
45	AB	801	CLA	C2A-CAA-CBA-CGA
45	A4	303	CLA	CAA-CBA-CGA-O1A
45	BA	833	CLA	CAA-CBA-CGA-O2A
47	AA	844	LHG	C12-C13-C14-C15
45	BA	801	CLA	CAA-CBA-CGA-O1A
45	BA	829	CLA	C5-C6-C7-C8
45	BB	835	CLA	C15-C16-C17-C18
45	B2	603	CLA	CAA-CBA-CGA-O1A
45	AA	833	CLA	C11-C12-C13-C14
45	AA	842	CLA	C14-C13-C15-C16
45	BA	811	CLA	C14-C13-C15-C16
45	BA	828	CLA	C6-C7-C8-C9
45	BB	811	CLA	C14-C13-C15-C16
46	AB	843	PQN	C21-C22-C23-C24
45	AA	827	CLA	CAA-CBA-CGA-O2A
45	AB	834	CLA	CAA-CBA-CGA-O2A
45	BA	825	CLA	CAA-CBA-CGA-O2A
47	B1	302	LHG	O7-C7-C8-C9
53	A1	321	LMG	O8-C28-C29-C30
45	AA	834	CLA	C15-C16-C17-C18
45	AA	826	CLA	C4B-C3B-CAB-CBB
45	AA	827	CLA	C1A-C2A-CAA-CBA
45	AB	803	CLA	C1A-C2A-CAA-CBA
45	AB	824	CLA	C4B-C3B-CAB-CBB
45	A4	311	CLA	C4B-C3B-CAB-CBB
45	A6	603	CLA	C4B-C3B-CAB-CBB
45	A6	614	CLA	C4B-C3B-CAB-CBB
45	BA	816	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
45	BA	839	CLA	C4B-C3B-CAB-CBB
45	BB	817	CLA	C1A-C2A-CAA-CBA
45	B2	604	CLA	C1A-C2A-CAA-CBA
45	B3	301	CLA	C4B-C3B-CAB-CBB
45	B3	311	CLA	C4B-C3B-CAB-CBB
45	B5	610	CLA	C4B-C3B-CAB-CBB
45	BA	812	CLA	CAA-CBA-CGA-O2A
45	BA	834	CLA	CAA-CBA-CGA-O2A
47	A1	302	LHG	O8-C23-C24-C25
45	A4	303	CLA	CAA-CBA-CGA-O2A
47	B1	318	LHG	C27-C28-C29-C30
48	AB	844	BCR	C17-C18-C19-C20
48	AL	306	BCR	C7-C8-C9-C10
48	BA	847	BCR	C21-C22-C23-C24
48	BA	848	BCR	C11-C12-C13-C14
52	B1	316	LUT	C31-C32-C33-C34
45	AB	842	CLA	C16-C17-C18-C20
50	AB	852	LMU	C3'-C4'-O1B-C1B
45	BA	806	CLA	CAA-CBA-CGA-O2A
45	BA	817	CLA	CAA-CBA-CGA-O2A
45	BA	828	CLA	CAA-CBA-CGA-O2A
45	BB	801	CLA	CAA-CBA-CGA-O2A
45	BB	804	CLA	CAA-CBA-CGA-O2A
47	BA	845	LHG	O8-C23-C24-C25
45	BB	809	CLA	C2A-CAA-CBA-CGA
45	B5	602	CLA	C2A-CAA-CBA-CGA
47	BF	305	LHG	C32-C33-C34-C35
45	A3	302	CLA	C5-C6-C7-C8
50	BA	854	LMU	C4-C5-C6-C7
45	AB	842	CLA	C5-C6-C7-C8
45	AB	806	CLA	CAA-CBA-CGA-O2A
45	AB	828	CLA	C8-C10-C11-C12
45	A6	605	CLA	O1D-CGD-O2D-CED
45	AB	815	CLA	C2-C1-O2A-CGA
45	BA	828	CLA	C2-C1-O2A-CGA
45	BA	838	CLA	C2-C1-O2A-CGA
45	AA	840	CLA	C12-C13-C15-C16
45	AB	804	CLA	C11-C12-C13-C15
45	AB	823	CLA	C11-C12-C13-C15
45	AB	825	CLA	C11-C10-C8-C7
45	AB	841	CLA	C11-C12-C13-C15
45	BB	810	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
45	BB	828	CLA	C11-C12-C13-C15
45	AA	818	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	C2A-CAA-CBA-CGA
45	AK	202	CLA	CAA-CBA-CGA-O2A
47	a	501	LHG	O7-C7-C8-C9
45	A1	313	CLA	CAA-CBA-CGA-O1A
45	B2	603	CLA	CAA-CBA-CGA-O2A
45	AA	827	CLA	C3A-C2A-CAA-CBA
45	AB	823	CLA	C3A-C2A-CAA-CBA
45	AB	835	CLA	C3A-C2A-CAA-CBA
45	AL	304	CLA	C3A-C2A-CAA-CBA
45	A3	312	CLA	CHA-CBD-CGD-O1D
45	A3	313	CLA	CHA-CBD-CGD-O1D
45	BA	802	CLA	C4-C3-C5-C6
45	BB	812	CLA	C3A-C2A-CAA-CBA
45	BB	817	CLA	CHA-CBD-CGD-O1D
45	B2	603	CLA	CHA-CBD-CGD-O1D
45	BB	815	CLA	CAA-CBA-CGA-O1A
45	BB	842	CLA	C15-C16-C17-C18
45	BA	829	CLA	C16-C17-C18-C20
47	A1	301	LHG	O6-C4-C5-O7
45	BB	835	CLA	CAA-CBA-CGA-O2A
53	B5	617	LMG	O9-C10-C11-C12
45	AA	840	CLA	C2A-CAA-CBA-CGA
45	BB	815	CLA	C2A-CAA-CBA-CGA
45	AA	801	CLA	C11-C10-C8-C9
45	AA	801	CLA	C14-C13-C15-C16
45	AA	821	CLA	C11-C12-C13-C14
45	AA	841	CLA	C11-C10-C8-C9
45	AB	814	CLA	C6-C7-C8-C9
45	BA	801	CLA	C14-C13-C15-C16
45	BA	803	CLA	C11-C12-C13-C14
45	BB	816	CLA	C11-C12-C13-C14
45	AB	809	CLA	C15-C16-C17-C18
45	B5	608	CLA	CAA-CBA-CGA-O1A
45	AA	842	CLA	C8-C10-C11-C12
45	B5	602	CLA	C10-C11-C12-C13
45	A6	610	CLA	C4-C3-C5-C6
45	BA	833	CLA	CAA-CBA-CGA-O1A
45	A4	311	CLA	C2-C3-C5-C6
45	BB	831	CLA	C2-C3-C5-C6
45	B2	609	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
45	BB	811	CLA	C15-C16-C17-C18
45	A1	309	CLA	CAD-CBD-CGD-O1D
45	A6	604	CLA	CAD-CBD-CGD-O1D
56	BJ	104	SQD	O5-C5-C6-S
45	BL	302	CLA	CAA-CBA-CGA-O2A
45	AB	806	CLA	CAA-CBA-CGA-O1A
54	A6	608	CHL	CAA-CBA-CGA-O1A
56	e	301	SQD	C24-C25-C26-C27
45	AA	807	CLA	O1D-CGD-O2D-CED
47	A6	618	LHG	O8-C23-C24-C25
45	AG	201	CLA	CAA-CBA-CGA-O1A
45	BB	802	CLA	C13-C15-C16-C17
45	AA	807	CLA	CBD-CGD-O2D-CED
48	BF	304	BCR	C7-C8-C9-C10
45	AA	833	CLA	CAA-CBA-CGA-O1A
45	BA	812	CLA	CAA-CBA-CGA-O1A
47	BA	845	LHG	O10-C23-C24-C25
47	B5	618	LHG	O9-C7-C8-C9
45	A6	609	CLA	CAA-CBA-CGA-O2A
45	BA	817	CLA	CAA-CBA-CGA-O1A
45	BA	809	CLA	CAA-CBA-CGA-O2A
45	B5	601	CLA	CAA-CBA-CGA-O2A
45	AA	819	CLA	C5-C6-C7-C8
45	AA	828	CLA	C2A-CAA-CBA-CGA
45	AB	825	CLA	C2A-CAA-CBA-CGA
45	B2	611	CLA	C2A-CAA-CBA-CGA
47	A1	302	LHG	C4-C5-C6-O8
47	A3	319	LHG	C4-C5-C6-O8
45	BL	302	CLA	CAA-CBA-CGA-O1A
45	AA	834	CLA	CAA-CBA-CGA-O1A
45	BA	806	CLA	CAA-CBA-CGA-O1A
45	BA	834	CLA	CAA-CBA-CGA-O1A
47	B1	302	LHG	O9-C7-C8-C9
45	AA	802	CLA	C8-C10-C11-C12
45	AB	832	CLA	C10-C11-C12-C13
45	B5	602	CLA	C8-C10-C11-C12
45	AA	841	CLA	CAA-CBA-CGA-O2A
45	AB	803	CLA	C2-C3-C5-C6
50	AB	852	LMU	C5'-C4'-O1B-C1B
53	A4	318	LMG	O9-C10-C11-C12
45	AA	804	CLA	CAD-CBD-CGD-O2D
45	AA	806	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
45	AA	811	CLA	CAD-CBD-CGD-O2D
45	BA	818	CLA	CAD-CBD-CGD-O2D
45	BB	835	CLA	CAD-CBD-CGD-O2D
45	B1	306	CLA	CAD-CBD-CGD-O2D
45	B2	610	CLA	CAD-CBD-CGD-O2D
45	AB	810	CLA	CAA-CBA-CGA-O2A
45	BA	813	CLA	CAA-CBA-CGA-O2A
53	A1	321	LMG	C14-C15-C16-C17
45	AA	806	CLA	C3-C5-C6-C7
45	AB	834	CLA	CAA-CBA-CGA-O1A
45	BA	828	CLA	CAA-CBA-CGA-O1A
45	AK	202	CLA	O1D-CGD-O2D-CED
45	AA	834	CLA	C2-C1-O2A-CGA
45	AA	838	CLA	C2-C1-O2A-CGA
45	BA	806	CLA	C2-C1-O2A-CGA
53	A1	321	LMG	O10-C28-C29-C30
47	B1	318	LHG	C23-C24-C25-C26
45	AA	842	CLA	C16-C17-C18-C19
47	A1	301	LHG	C29-C30-C31-C32
45	BA	825	CLA	CAA-CBA-CGA-O1A
51	BB	850	DGD	C1B-C2B-C3B-C4B
45	AA	818	CLA	CBA-CGA-O2A-C1
45	AA	812	CLA	CAA-CBA-CGA-O2A
45	BB	809	CLA	CAA-CBA-CGA-O2A
45	B2	602	CLA	CAA-CBA-CGA-O2A
47	BA	846	LHG	O7-C7-C8-C9
47	B5	618	LHG	O8-C23-C24-C25
53	A4	318	LMG	O8-C28-C29-C30
47	A1	302	LHG	O10-C23-C24-C25
45	AA	805	CLA	CAA-CBA-CGA-O2A
45	AA	842	CLA	CAA-CBA-CGA-O2A
45	AB	807	CLA	CAA-CBA-CGA-O2A
45	BA	841	CLA	CAA-CBA-CGA-O2A
45	BA	842	CLA	CAA-CBA-CGA-O2A
45	BB	801	CLA	O1D-CGD-O2D-CED
45	A6	603	CLA	O1A-CGA-O2A-C1

There are no ring outliers.

224 monomers are involved in 480 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	AK	203	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	BB	805	CLA	2	0
45	AA	828	CLA	1	0
45	AK	202	CLA	4	0
45	BA	811	CLA	1	0
54	A6	608	CHL	2	0
52	A3	316	LUT	1	0
54	B1	303	CHL	2	0
48	BB	849	BCR	2	0
48	AJ	103	BCR	1	0
48	AK	204	BCR	2	0
45	BB	823	CLA	2	0
49	BC	102	SF4	7	0
45	BB	812	CLA	5	0
45	B5	612	CLA	1	0
47	F	801	LHG	3	0
56	BJ	104	SQD	6	0
54	A1	303	CHL	2	0
46	BB	844	PQN	2	0
45	BB	804	CLA	2	0
48	BA	847	BCR	1	0
48	BA	849	BCR	2	0
48	BJ	101	BCR	6	0
45	BA	840	CLA	4	0
45	BA	841	CLA	1	0
55	A4	316	XAT	2	0
45	BA	802	CLA	3	0
45	A3	308	CLA	1	0
50	AL	301	LMU	1	0
57	c	301	FES	2	0
45	A1	316	CLA	1	0
45	BA	842	CLA	1	0
45	BL	304	CLA	2	0
48	BL	305	BCR	2	0
45	BB	830	CLA	1	0
47	a	501	LHG	2	0
45	AB	840	CLA	1	0
49	K	301	SF4	1	0
48	A6	617	BCR	3	0
49	I	201	SF4	1	0
48	AF	805	BCR	2	0
49	I	202	SF4	3	0
45	B3	310	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	AB	845	BCR	1	0
48	BB	846	BCR	1	0
45	AB	828	CLA	1	0
45	AB	801	CLA	1	0
48	BB	803	BCR	5	0
47	B2	618	LHG	2	0
45	AB	808	CLA	4	0
45	BB	838	CLA	1	0
45	B5	602	CLA	1	0
45	BB	841	CLA	5	0
45	AA	838	CLA	1	0
45	BA	806	CLA	2	0
45	A6	604	CLA	2	0
45	A1	314	CLA	2	0
45	BB	809	CLA	6	0
45	A1	311	CLA	2	0
48	AB	844	BCR	2	0
48	AB	848	BCR	2	0
45	B3	303	CLA	1	0
49	AC	101	SF4	1	0
52	B3	315	LUT	3	0
45	A6	610	CLA	10	0
47	A3	301	LHG	1	0
45	B2	610	CLA	1	0
45	B2	612	CLA	3	0
45	A4	307	CLA	1	0
48	AL	302	BCR	1	0
48	AI	102	BCR	3	0
45	AA	803	CLA	1	0
56	e	301	SQD	1	0
45	AL	304	CLA	1	0
48	BA	856	BCR	1	0
45	AA	815	CLA	1	0
46	BA	843	PQN	3	0
45	B3	313	CLA	3	0
45	BB	840	CLA	1	0
45	BL	303	CLA	1	0
45	AA	810	CLA	1	0
45	BA	803	CLA	3	0
48	B3	317	BCR	4	0
45	AG	203	CLA	1	0
45	BA	801	CLA	14	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	B1	305	CLA	1	0
45	B5	613	CLA	1	0
52	A6	615	LUT	4	0
47	BA	845	LHG	2	0
48	BL	301	BCR	3	0
45	BA	808	CLA	4	0
51	BB	850	DGD	1	0
45	BF	302	CLA	1	0
45	AA	834	CLA	1	0
45	AA	827	CLA	4	0
48	AA	847	BCR	1	0
45	A6	613	CLA	1	0
45	BB	829	CLA	1	0
45	AA	801	CLA	11	0
45	AA	806	CLA	1	0
45	B1	309	CLA	1	0
48	AG	205	BCR	1	0
45	AA	802	CLA	1	0
45	B1	306	CLA	2	0
45	A4	313	CLA	1	0
55	A1	318	XAT	1	0
45	B3	311	CLA	1	0
45	BA	810	CLA	1	0
49	AC	102	SF4	3	0
52	A1	317	LUT	1	0
48	AB	847	BCR	3	0
45	A1	306	CLA	2	0
45	BB	828	CLA	2	0
45	AA	811	CLA	1	0
48	BA	855	BCR	2	0
45	B2	603	CLA	4	0
45	AF	803	CLA	1	0
45	BA	832	CLA	1	0
45	AB	834	CLA	3	0
48	BF	304	BCR	1	0
45	BK	201	CLA	3	0
45	AK	201	CLA	7	0
46	AA	843	PQN	3	0
54	A4	306	CHL	2	0
45	B2	602	CLA	5	0
45	AB	802	CLA	4	0
45	AB	812	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	AA	833	CLA	1	0
45	BB	821	CLA	1	0
45	AB	842	CLA	1	0
45	BL	302	CLA	8	0
45	AB	809	CLA	2	0
52	B1	316	LUT	3	0
45	BG	201	CLA	9	0
48	BA	848	BCR	1	0
48	AA	848	BCR	2	0
53	A1	321	LMG	1	0
54	B3	306	CHL	1	0
45	A4	311	CLA	1	0
45	BA	830	CLA	4	0
45	AB	814	CLA	1	0
45	BB	815	CLA	7	0
55	B3	316	XAT	1	0
45	AG	204	CLA	4	0
55	B2	616	XAT	6	0
45	AA	817	CLA	1	0
45	BA	834	CLA	1	0
48	BB	845	BCR	2	0
55	A3	317	XAT	2	0
54	B2	607	CHL	3	0
45	BB	819	CLA	1	0
45	A1	305	CLA	1	0
48	BB	847	BCR	1	0
45	AH	201	CLA	1	0
48	BA	851	BCR	6	0
45	A4	309	CLA	1	0
47	BA	846	LHG	1	0
54	A1	308	CHL	1	0
45	A6	601	CLA	1	0
45	AA	820	CLA	1	0
45	AB	838	CLA	1	0
48	A1	319	BCR	3	0
48	BB	848	BCR	2	0
53	A4	318	LMG	4	0
48	AF	801	BCR	4	0
48	AA	849	BCR	2	0
45	AJ	102	CLA	1	0
55	A6	616	XAT	4	0
49	BA	852	SF4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
46	AB	843	PQN	2	0
45	AB	803	CLA	3	0
48	BJ	103	BCR	3	0
45	B1	314	CLA	1	0
45	AA	818	CLA	2	0
54	B2	601	CHL	12	0
54	B2	606	CHL	1	0
45	B1	311	CLA	1	0
45	BB	802	CLA	4	0
45	AB	833	CLA	2	0
45	AB	839	CLA	2	0
45	AB	824	CLA	1	0
47	B3	318	LHG	1	0
45	AB	827	CLA	4	0
47	B1	301	LHG	1	0
45	A3	304	CLA	1	0
45	BB	834	CLA	2	0
45	BB	820	CLA	1	0
47	AA	844	LHG	1	0
45	BA	805	CLA	1	0
45	BB	816	CLA	1	0
48	AJ	101	BCR	4	0
45	B2	609	CLA	2	0
45	AB	825	CLA	1	0
45	A4	301	CLA	1	0
45	AA	830	CLA	1	0
48	AB	846	BCR	1	0
45	AB	822	CLA	1	0
45	BA	820	CLA	1	0
45	AA	825	CLA	2	0
47	BF	305	LHG	1	0
45	AB	810	CLA	2	0
45	BB	827	CLA	1	0
45	B1	304	CLA	2	0
48	AA	846	BCR	1	0
45	BA	829	CLA	1	0
48	A3	318	BCR	2	0
45	B5	608	CLA	1	0
55	B5	615	XAT	1	0
52	A4	315	LUT	4	0
45	BK	202	CLA	4	0
45	AB	818	CLA	2	0

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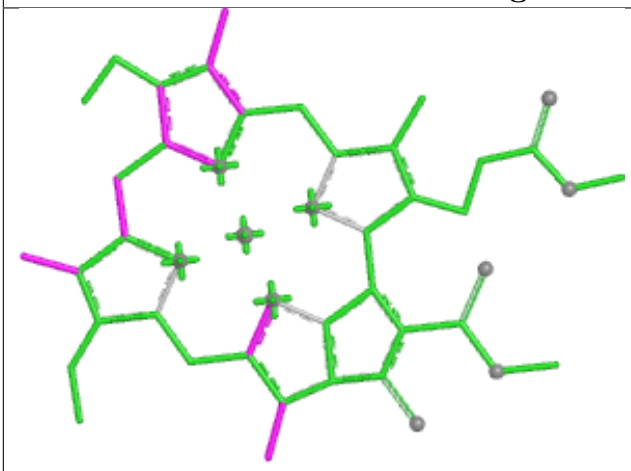
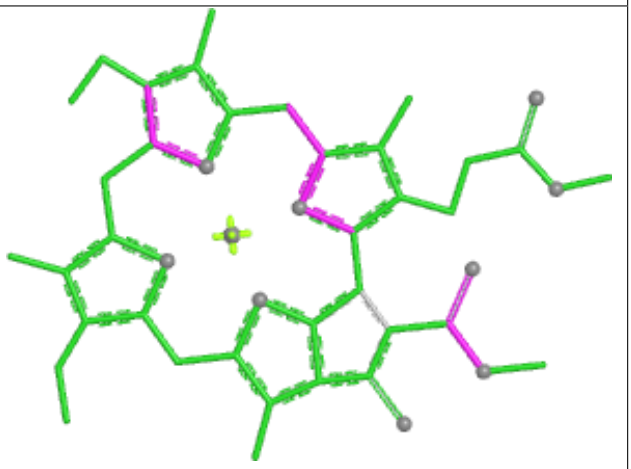
Mol	Chain	Res	Type	Clashes	Symm-Clashes
45	AB	831	CLA	1	0
45	BB	810	CLA	1	0
48	BG	203	BCR	13	0
45	B2	611	CLA	1	0
48	BI	101	BCR	1	0
48	B2	617	BCR	2	0
45	BA	812	CLA	1	0
45	BB	801	CLA	3	0
45	BG	202	CLA	39	0
52	AF	806	LUT	2	0
45	AA	841	CLA	1	0
48	BL	306	BCR	1	0
45	BB	813	CLA	1	0

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.

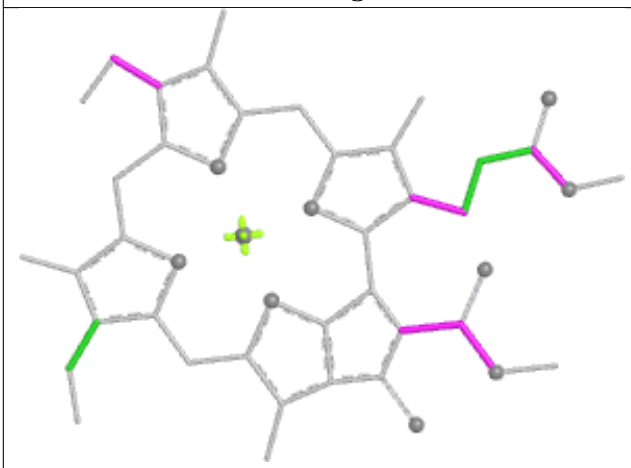
Ligand CLA AK 203



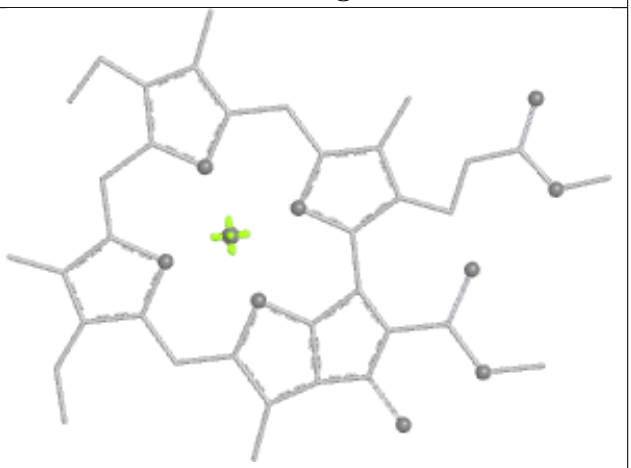
Bond lengths



Bond angles

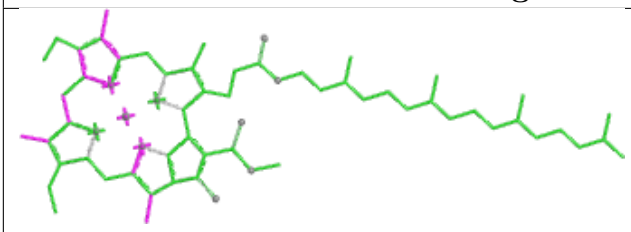


Torsions

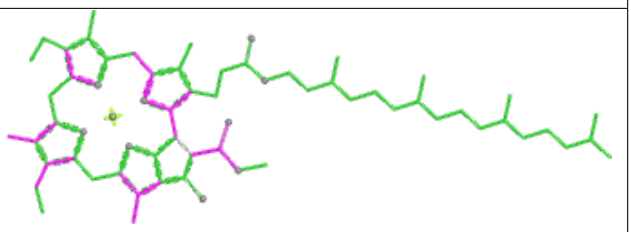


Rings

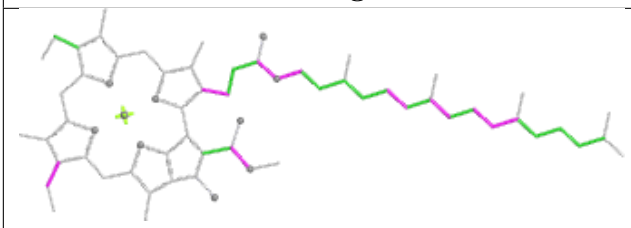
Ligand CLA BB 805



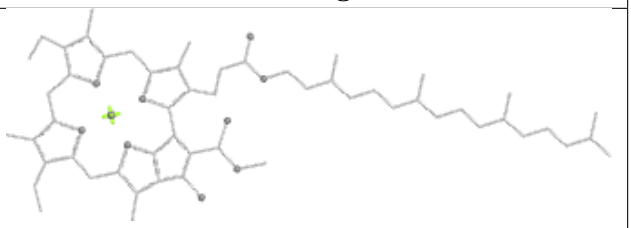
Bond lengths



Bond angles

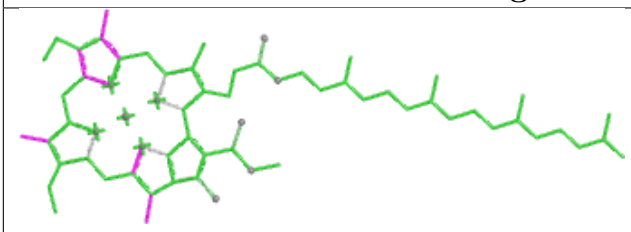


Torsions

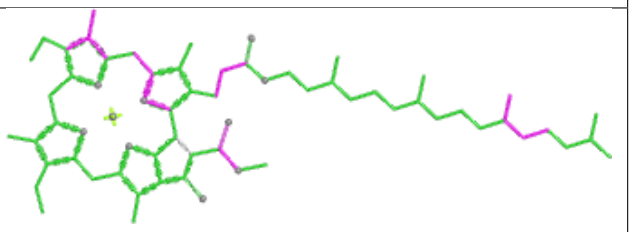


Rings

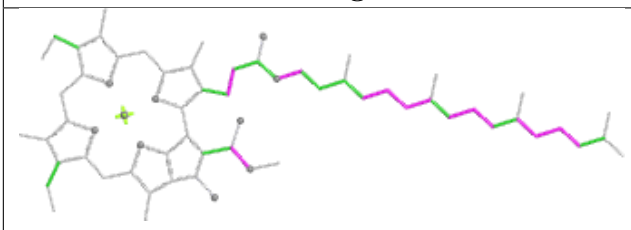
Ligand CLA AA 828



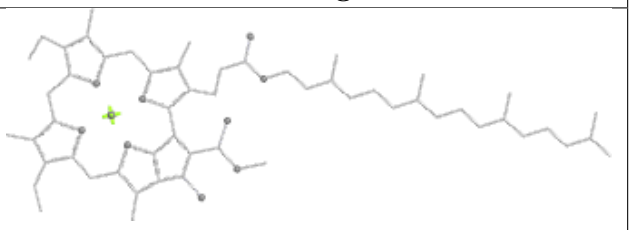
Bond lengths



Bond angles

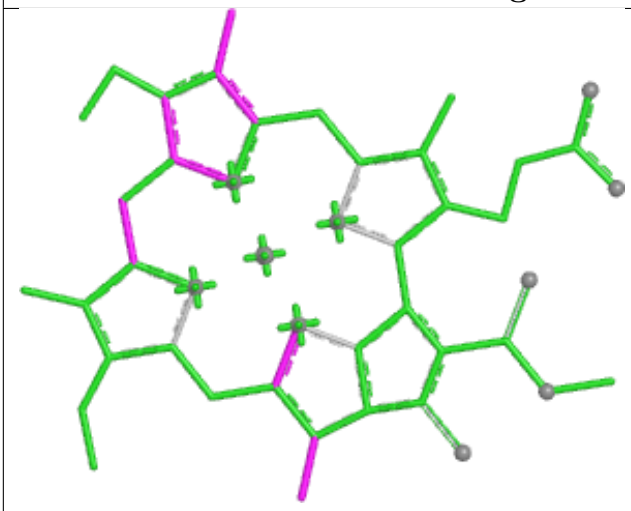


Torsions

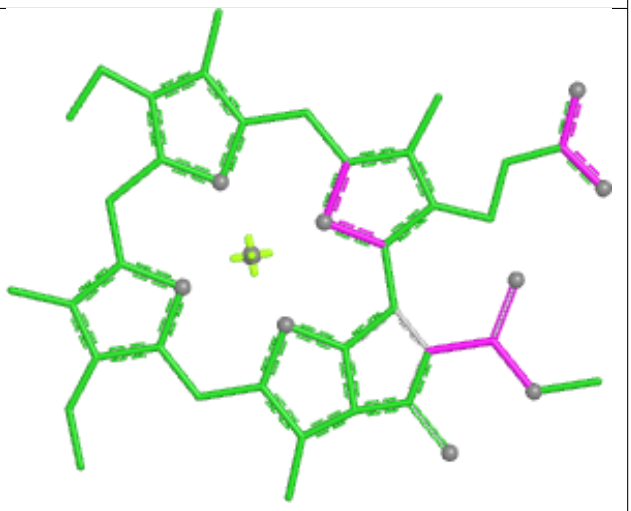


Rings

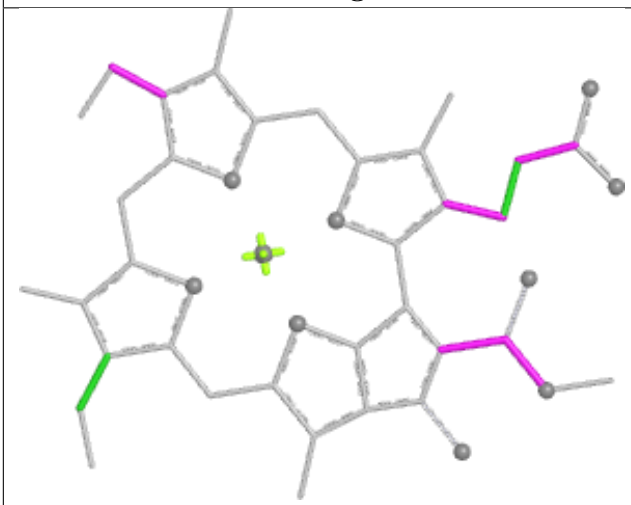
Ligand CLA AK 202



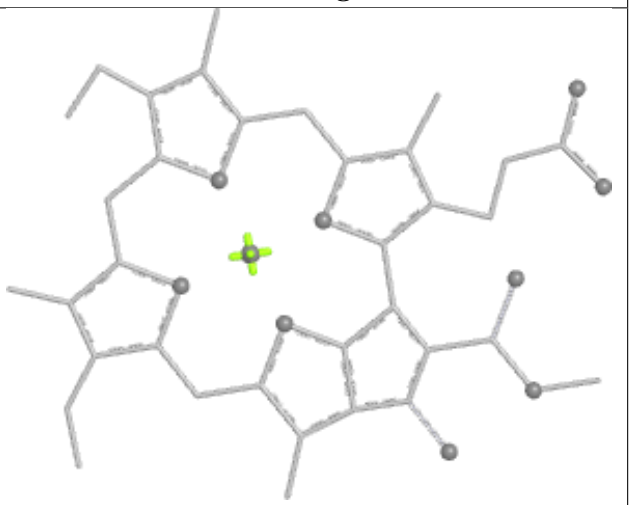
Bond lengths



Bond angles

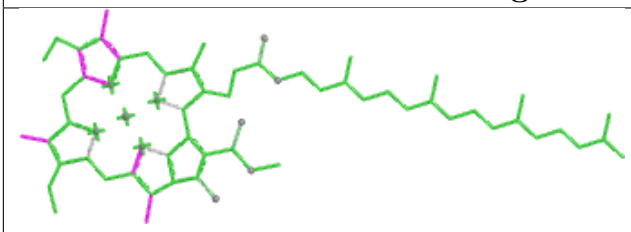


Torsions

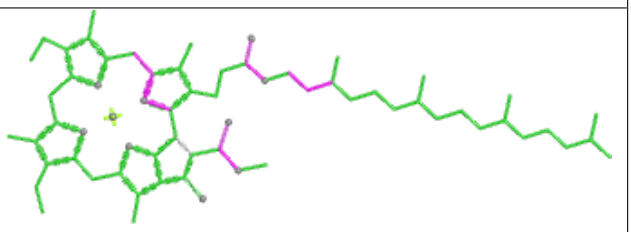


Rings

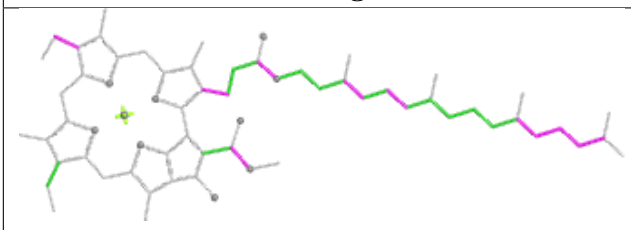
Ligand CLA BA 811



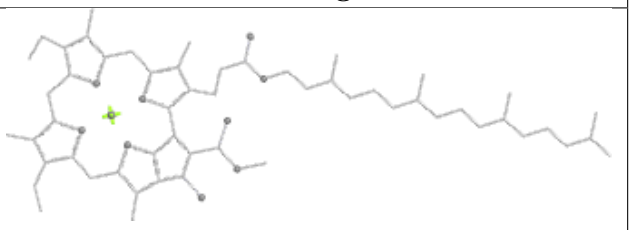
Bond lengths



Bond angles

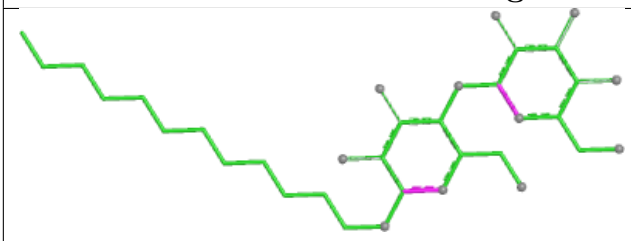


Torsions

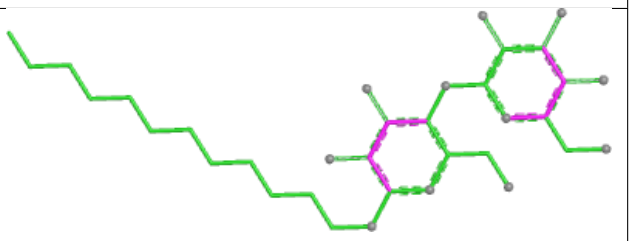


Rings

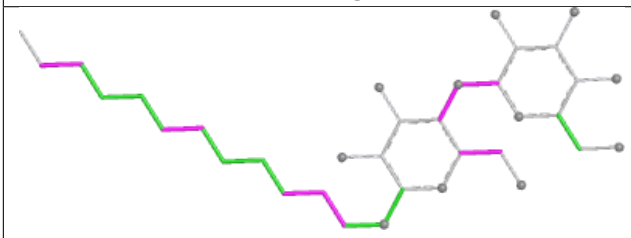
Ligand LMU AB 850



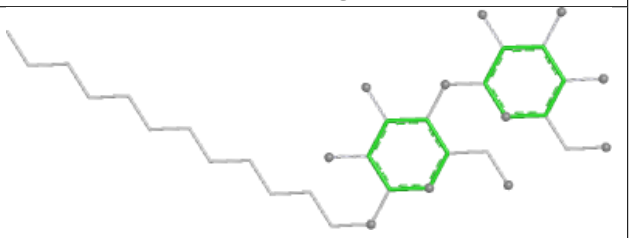
Bond lengths



Bond angles

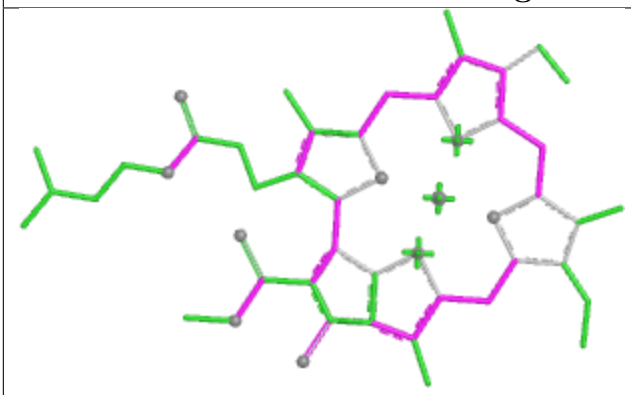


Torsions



Rings

Ligand CHL A6 608



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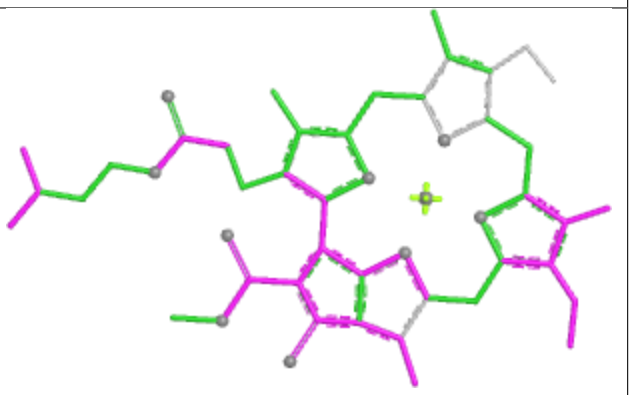
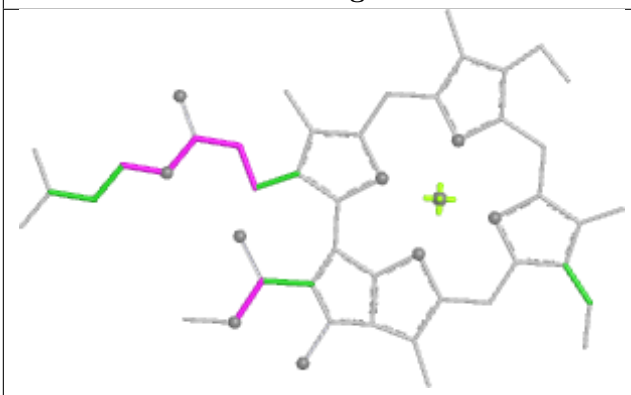
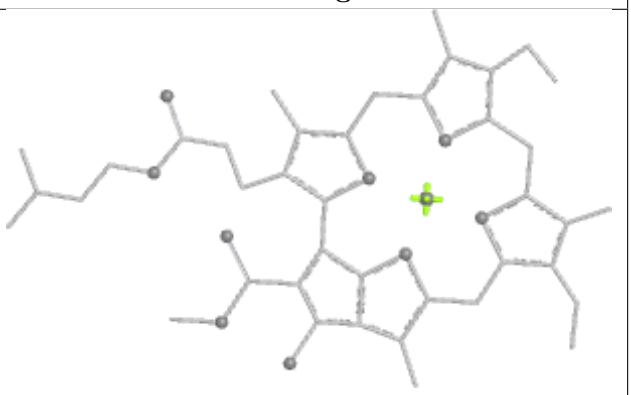


Bond angles

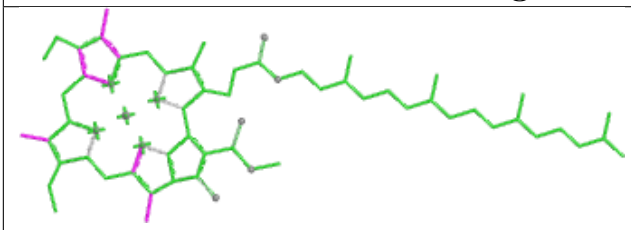


Torsions

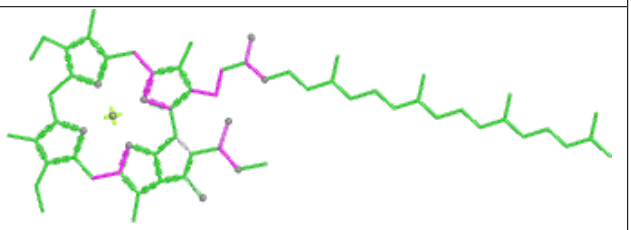


Rings

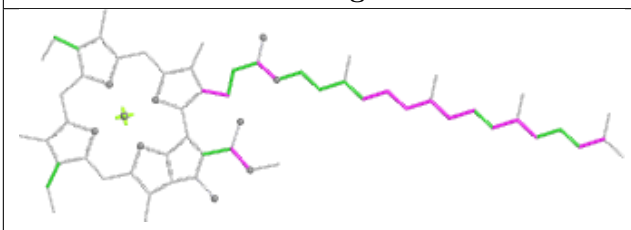
Ligand CLA AB 823



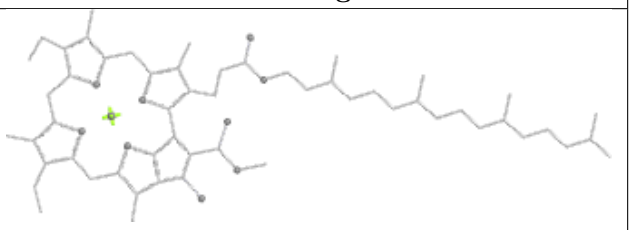
Bond lengths



Bond angles

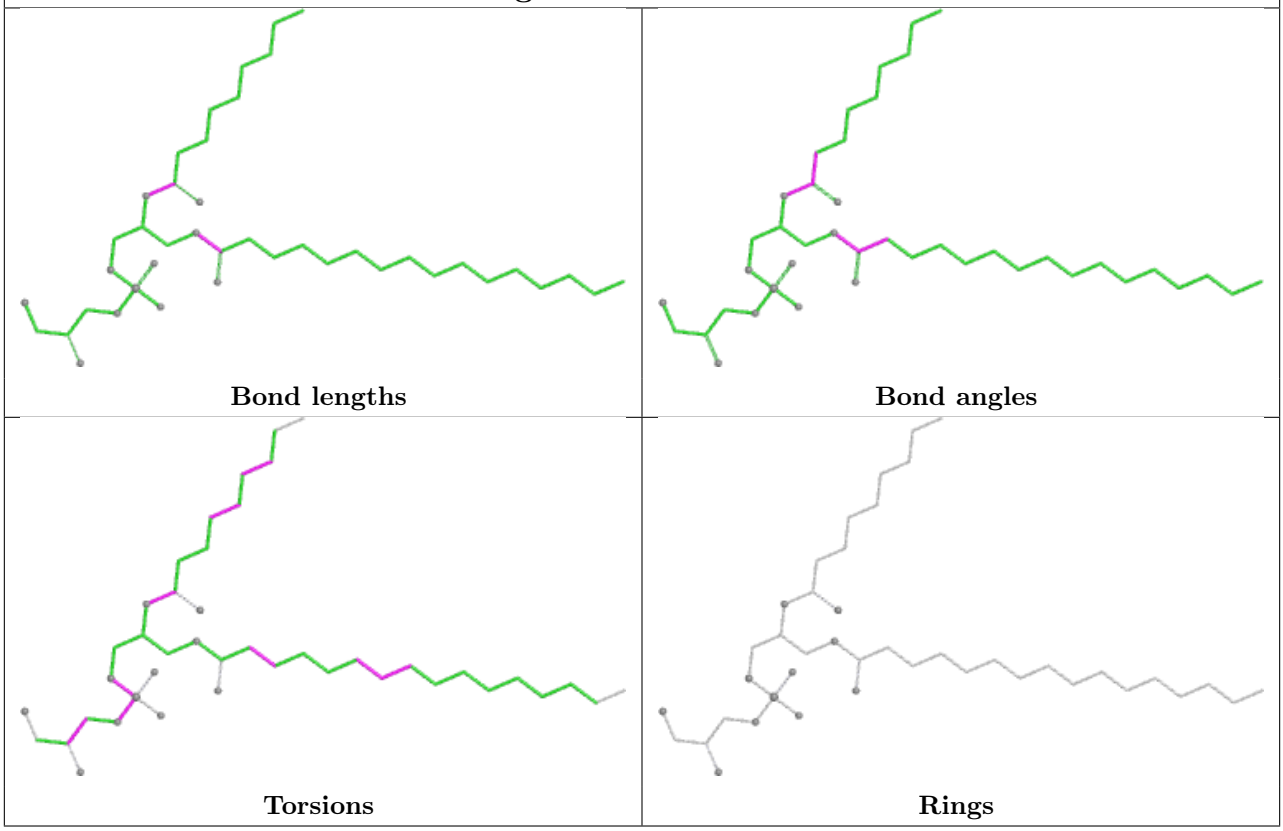


Torsions

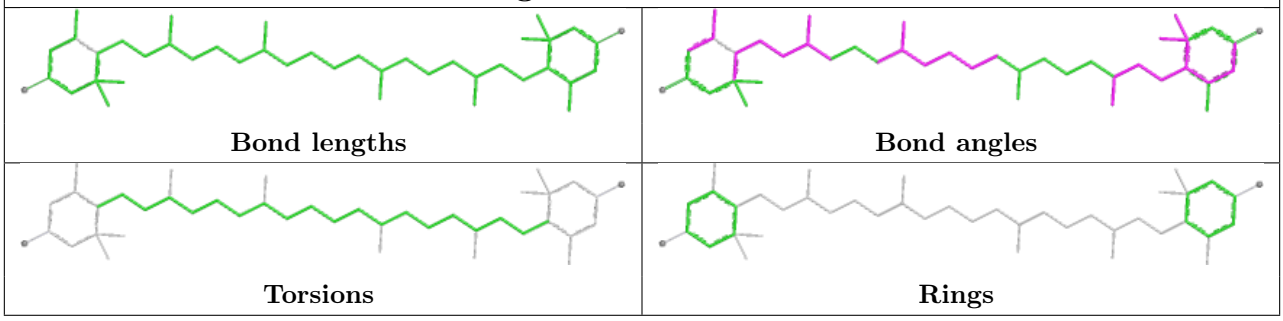


Rings

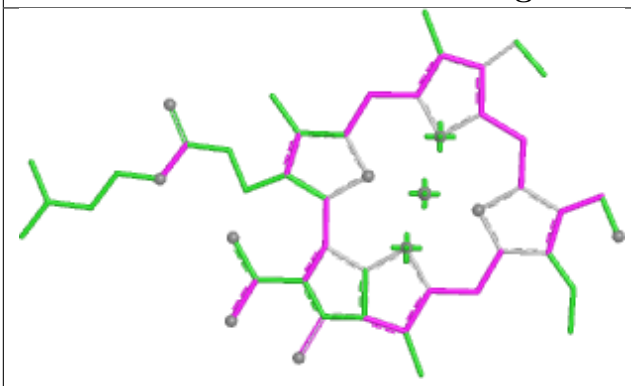
Ligand LHG B1 318



Ligand LUT A3 316



Ligand CHL B1 303



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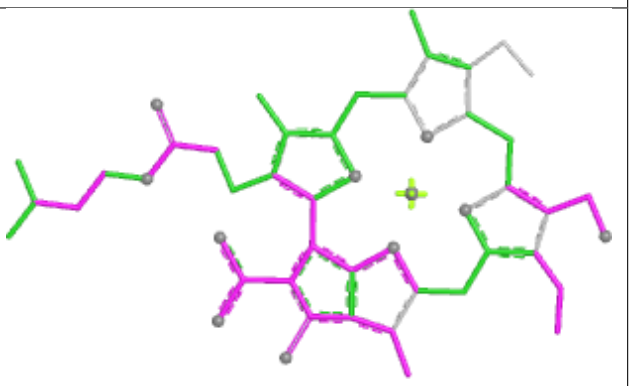
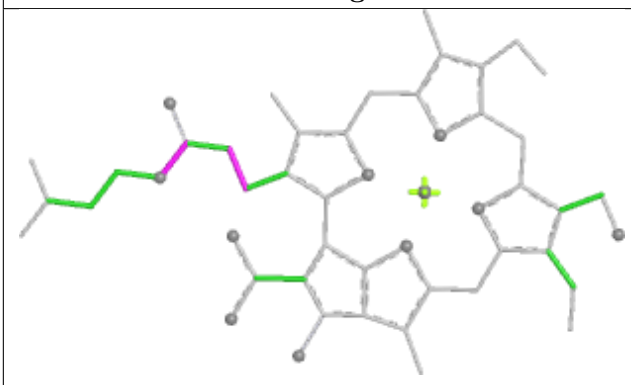
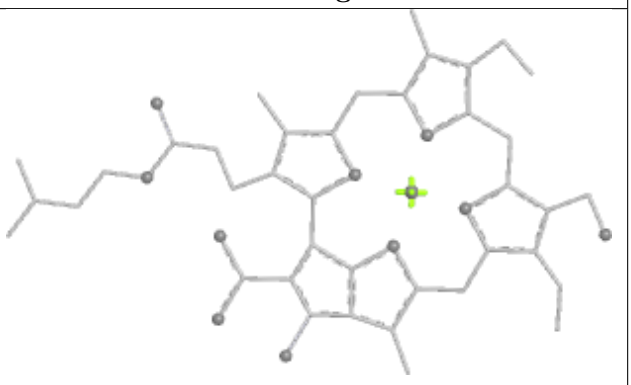


Bond angles

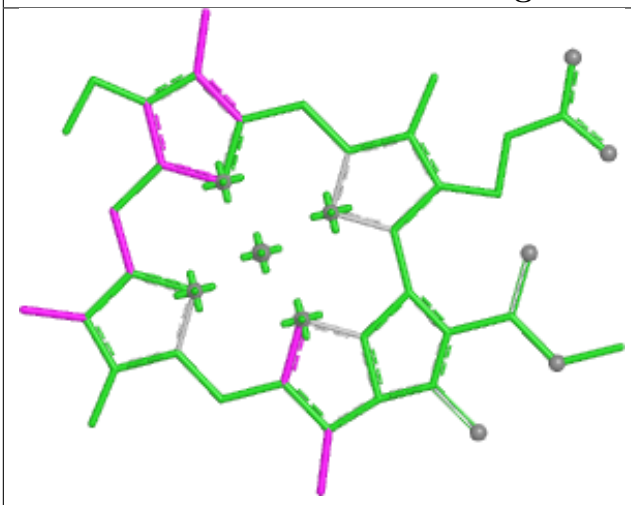


Torsions

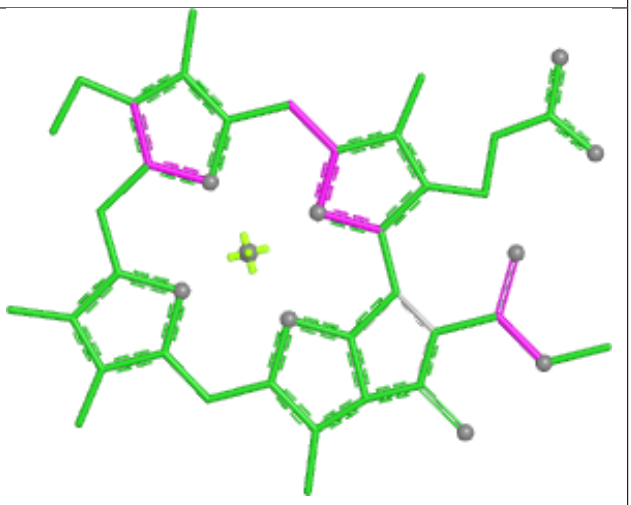


Rings

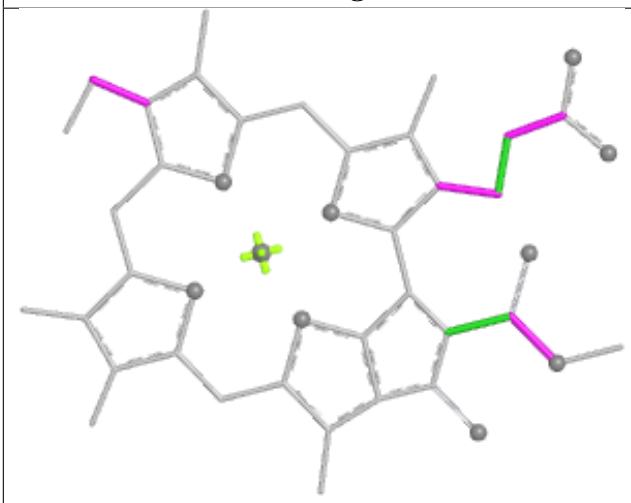
Ligand CLA A6 612



Bond lengths



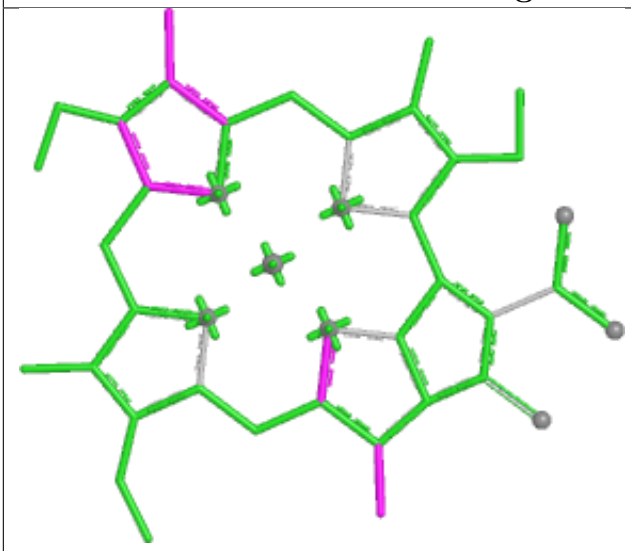
Bond angles



Torsions

Rings

Ligand CLA B3 304



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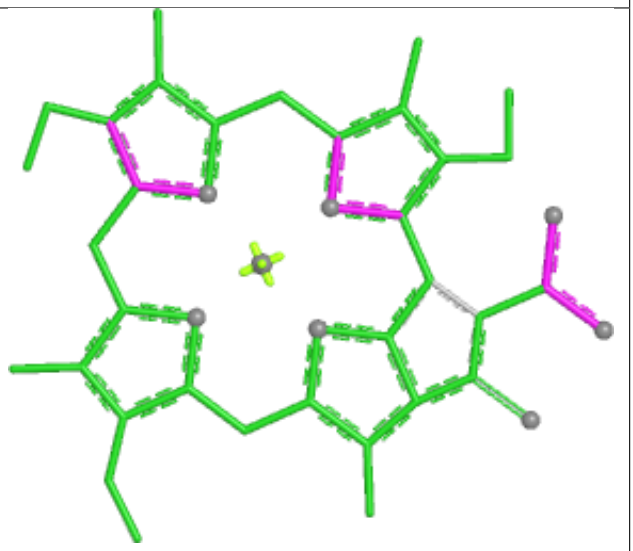
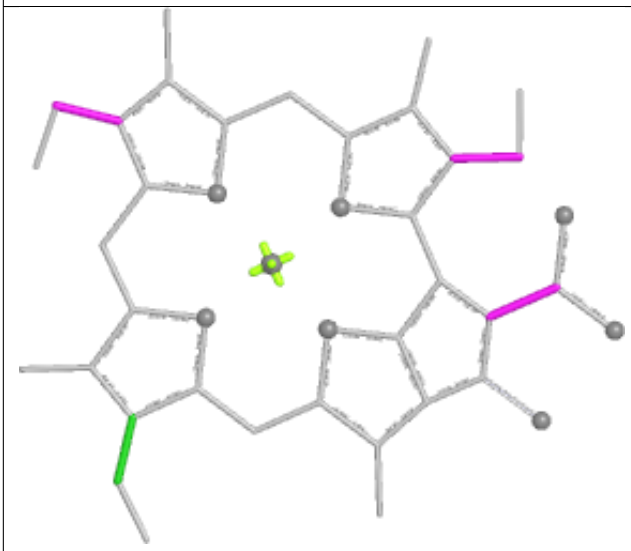


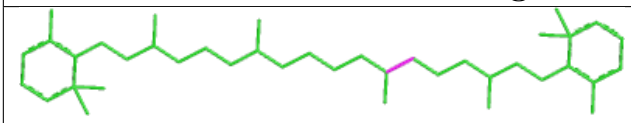
Bond angles



Torsions

Rings

Ligand BCR BB 849



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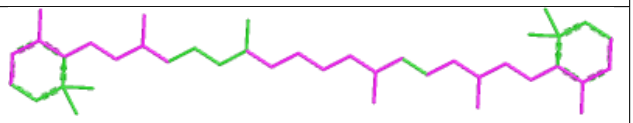
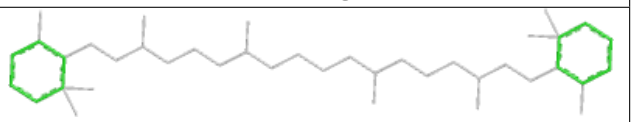


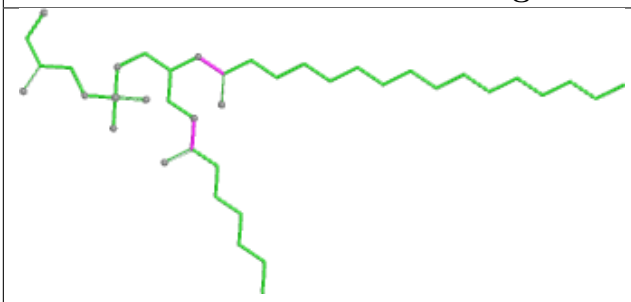
Bond angles

Torsions

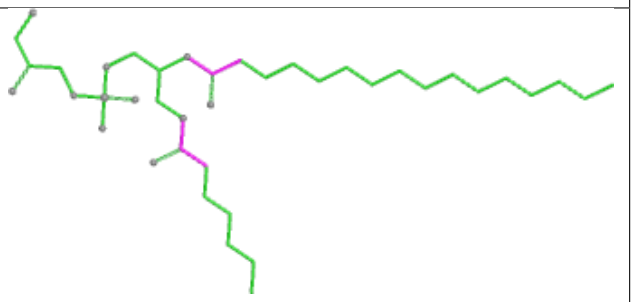


Rings

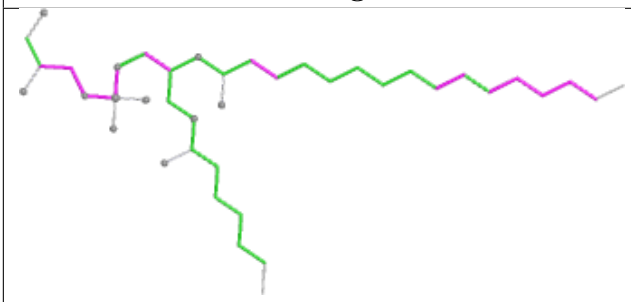
Ligand LHG AJ 104



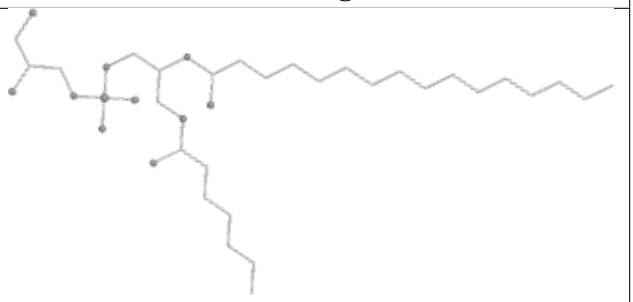
Bond lengths



Bond angles

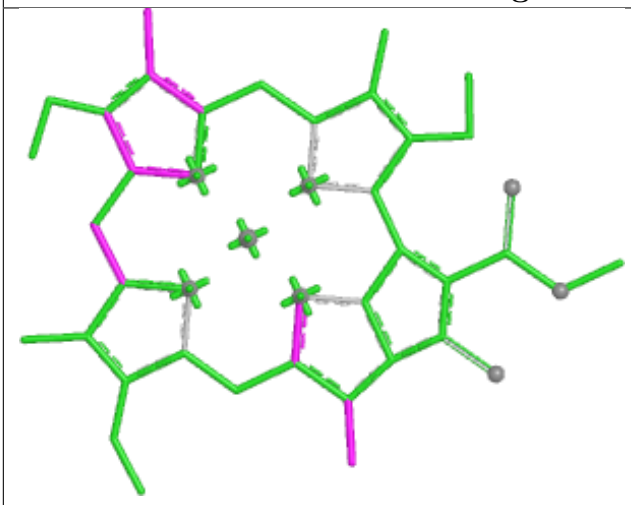


Torsions

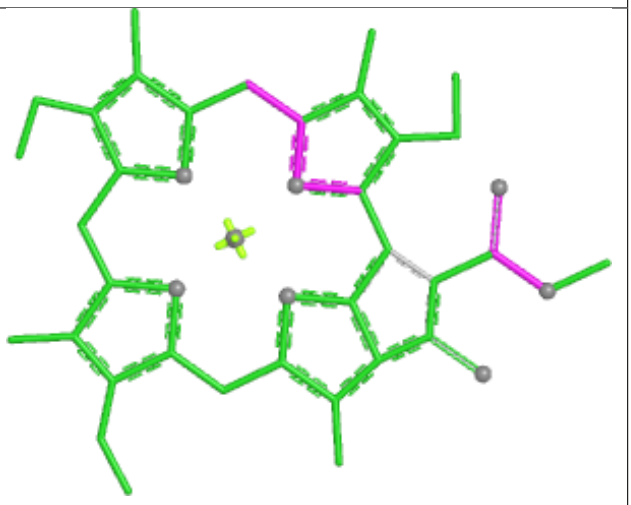


Rings

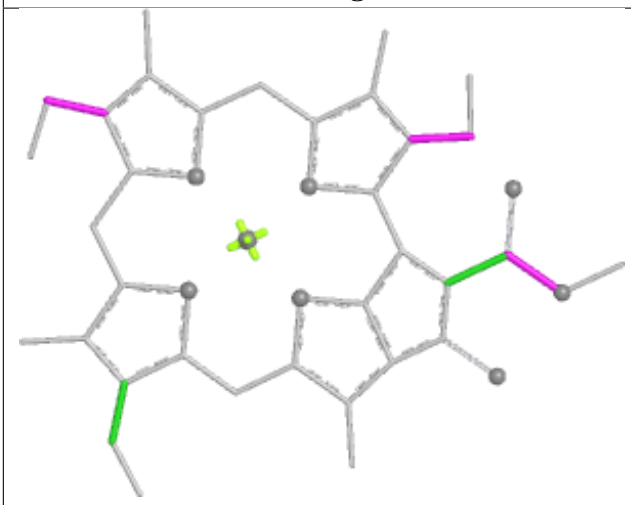
Ligand CLA BB 837



Bond lengths



Bond angles

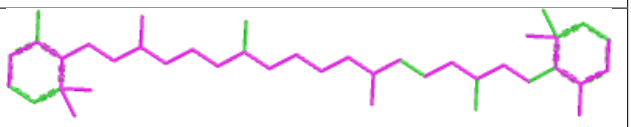


Torsions

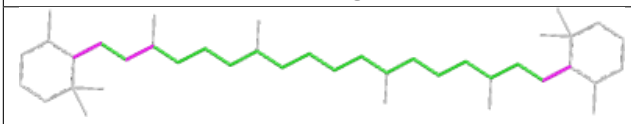
Rings

Ligand BCR AJ 103

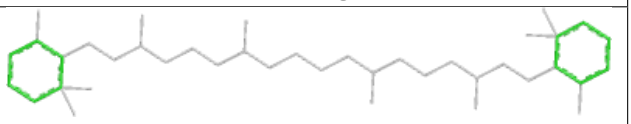
Bond lengths



Bond angles

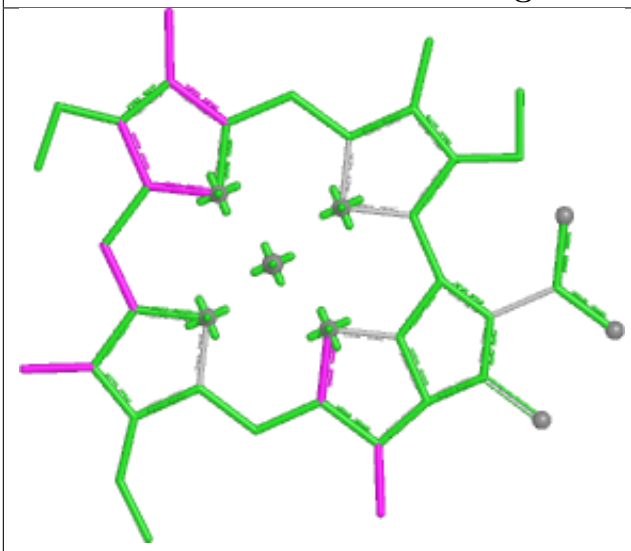


Torsions

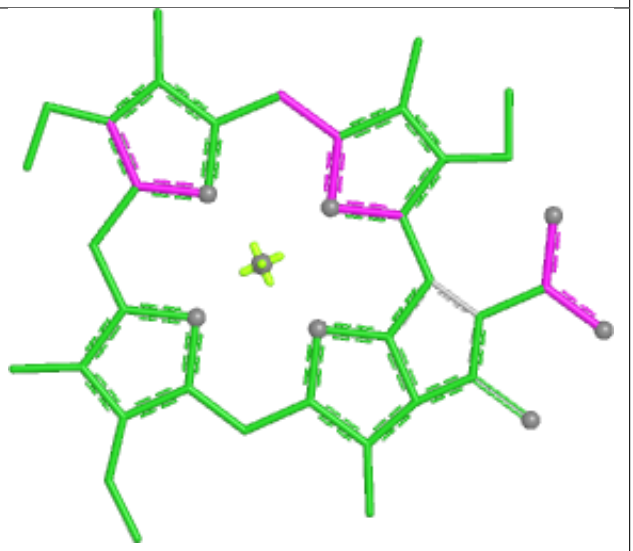


Rings

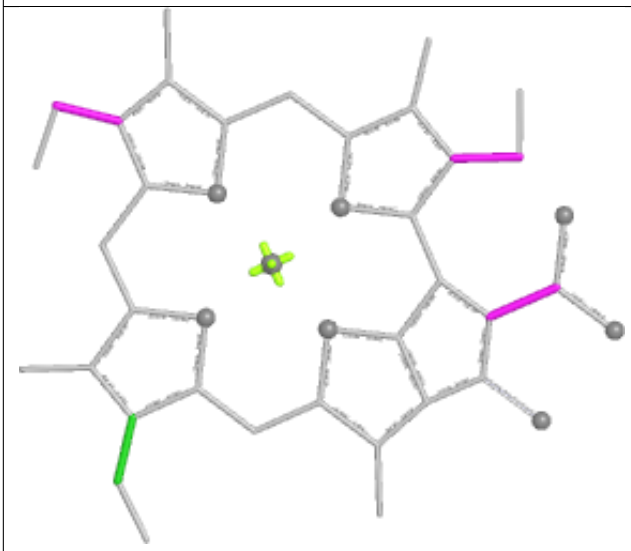
Ligand CLA A4 310



Bond lengths



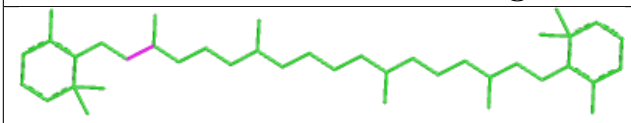
Bond angles



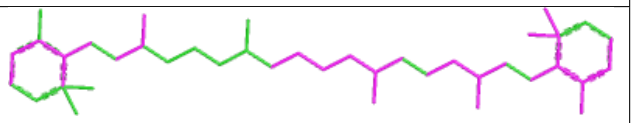
Torsions

Rings

Ligand BCR BK 204

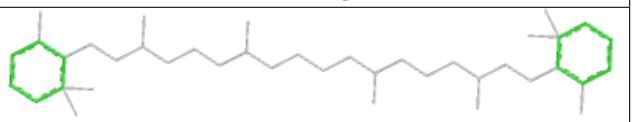


Bond lengths



Bond angles

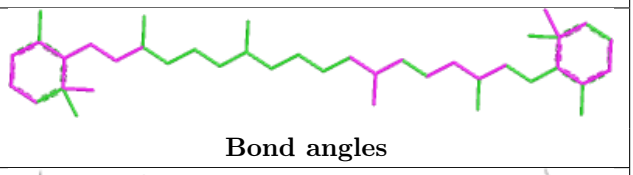
Torsions



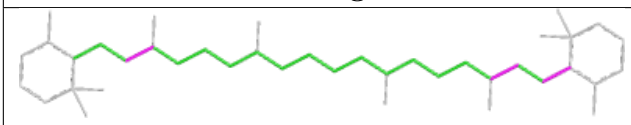
Rings

Ligand BCR AK 204

Bond lengths



Bond angles



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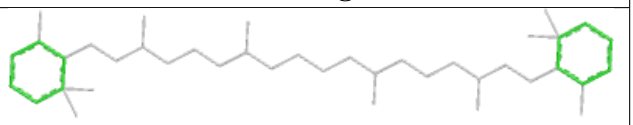
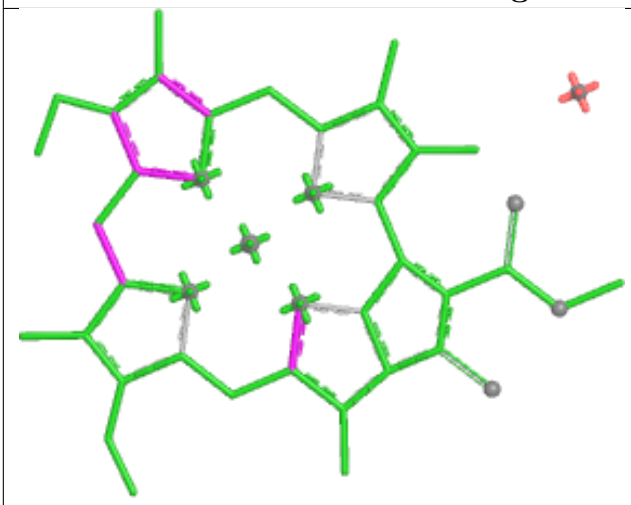


Rings

Ligand CLA BA 844



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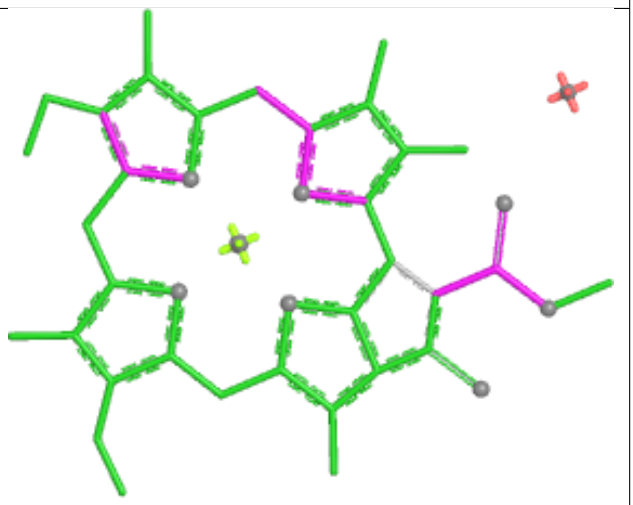
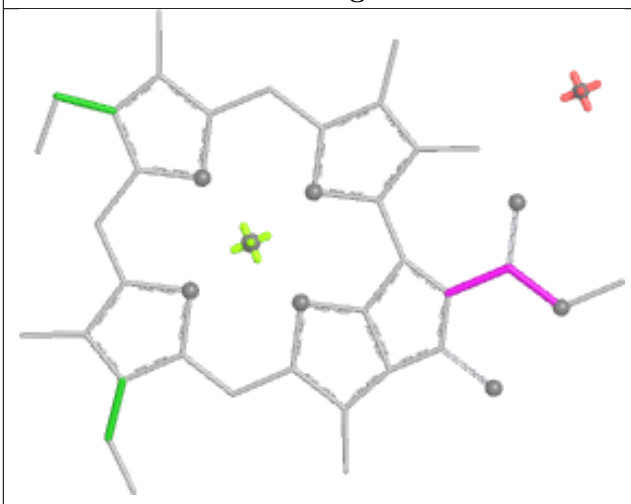
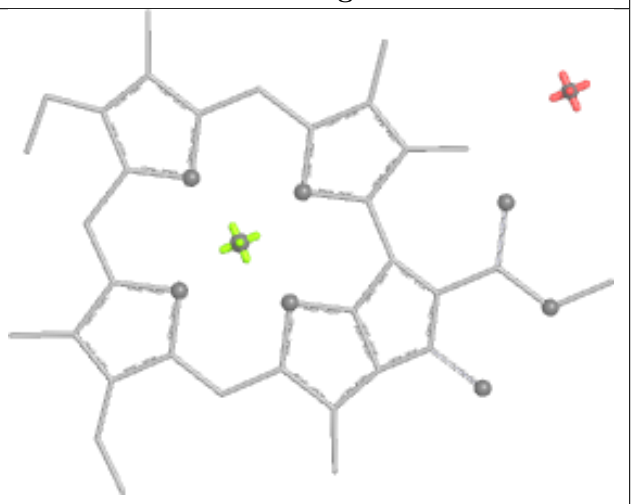


Bond angles

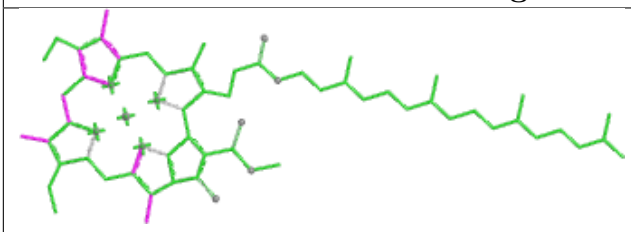


Torsions



Rings

Ligand CLA AA 805



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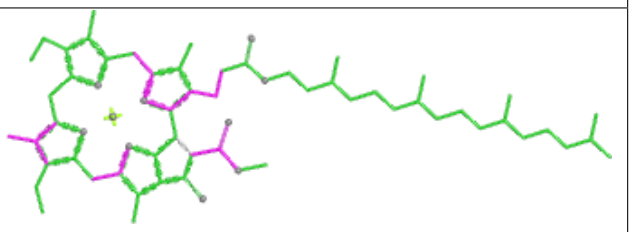
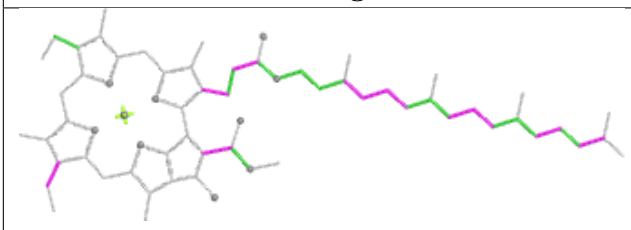
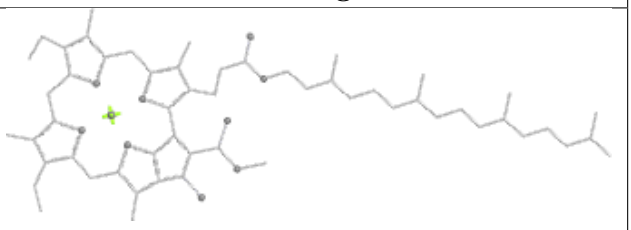


Bond angles

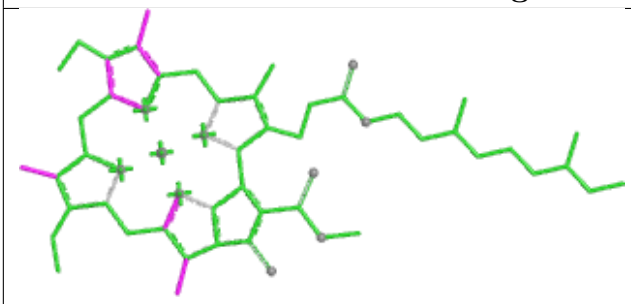


Torsions

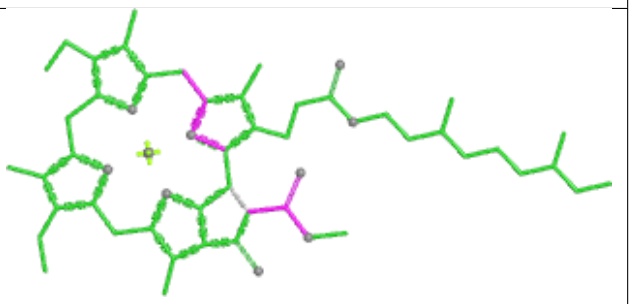


Rings

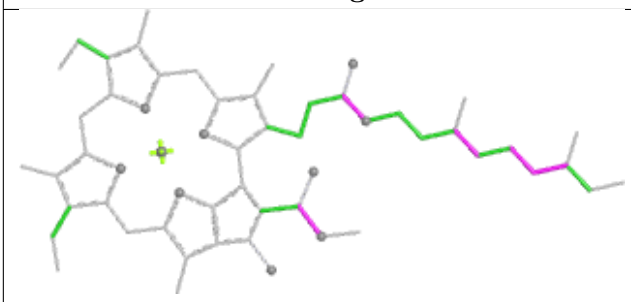
Ligand CLA AB 830



Bond lengths



Bond angles



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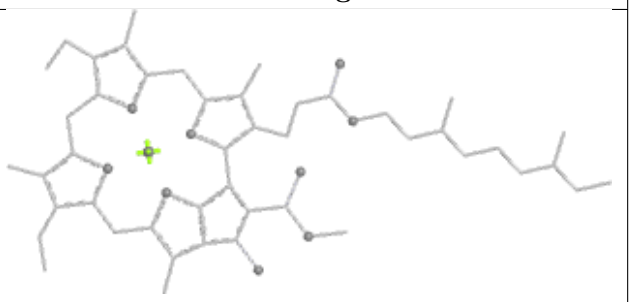
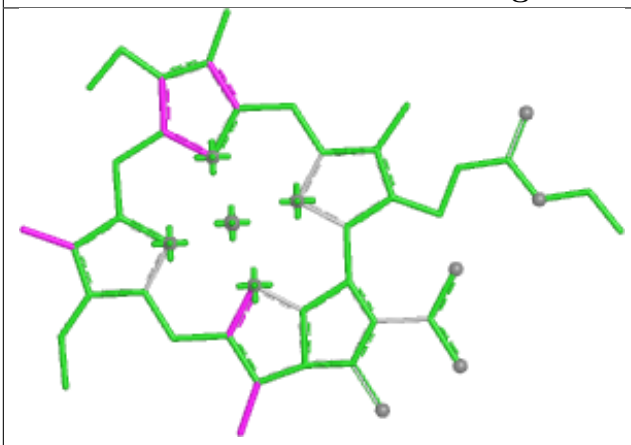


Rings

Ligand CLA BB 823



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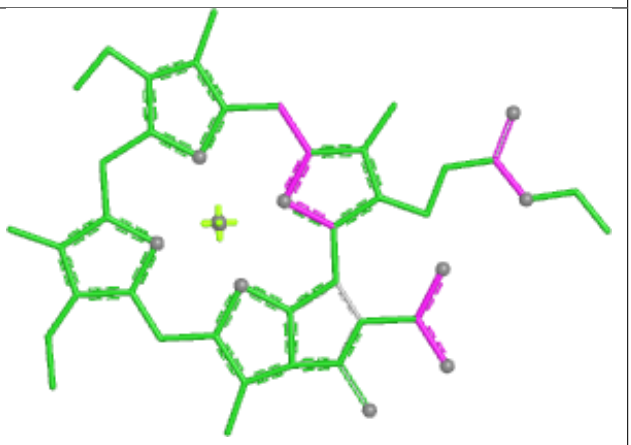
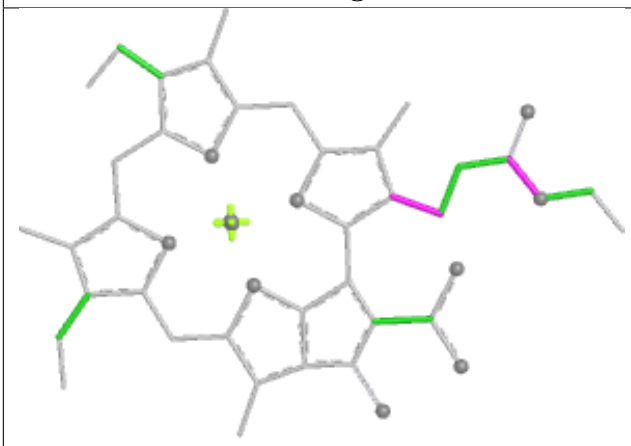
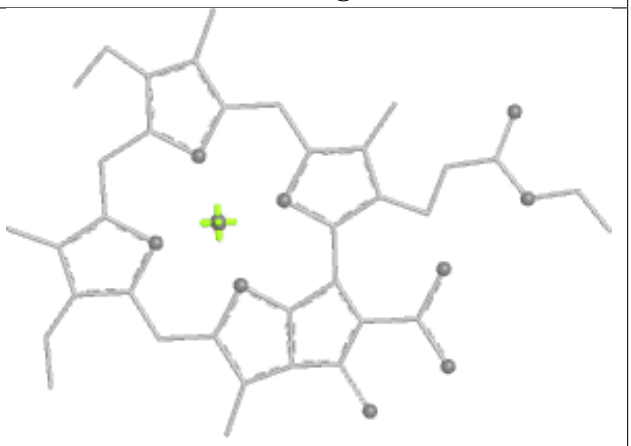


Bond angles



Torsions



Rings

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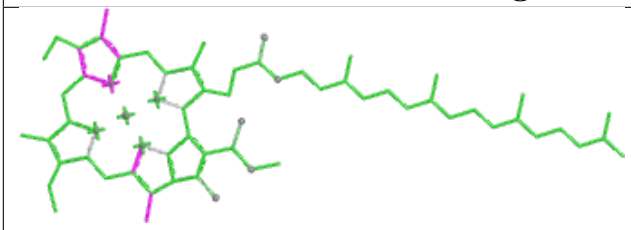

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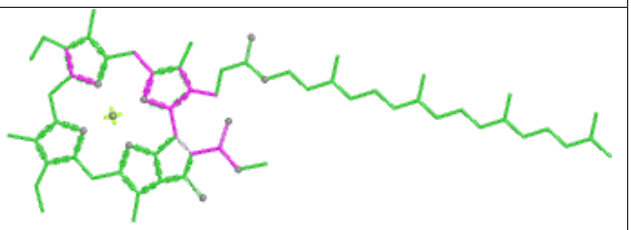
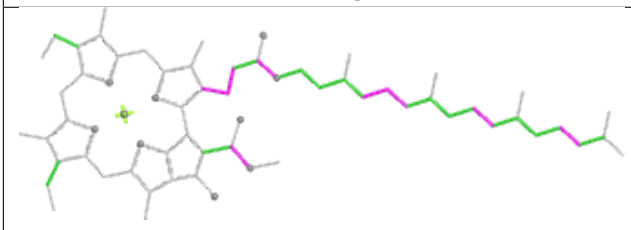


Bond angles



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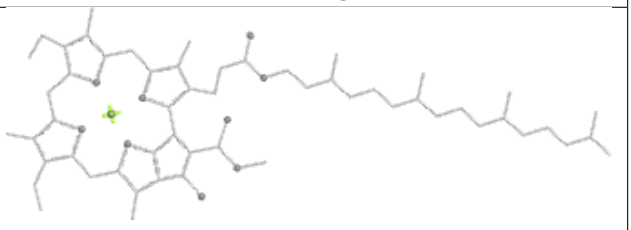
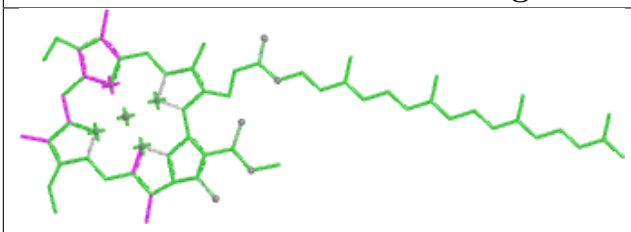
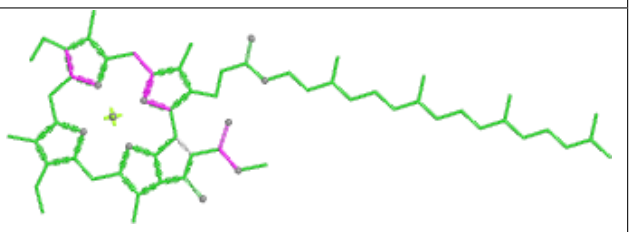


Rings

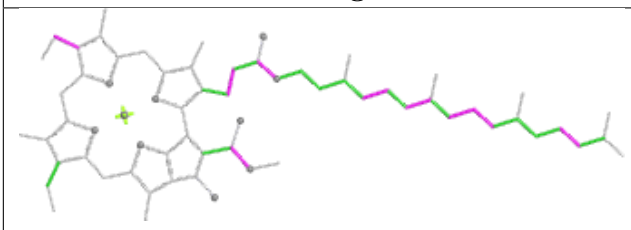
Ligand CLA BB 843



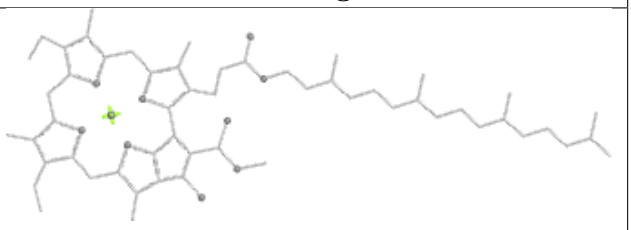
Bond lengths



Bond angles

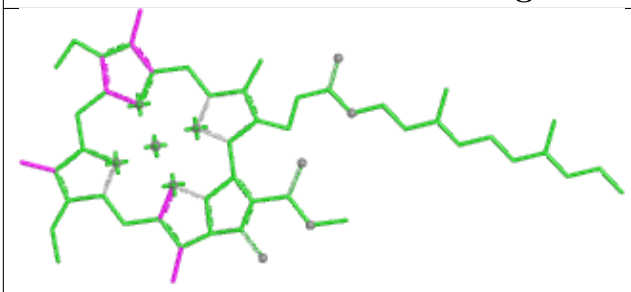


Torsions



Rings

Ligand CLA B5 612



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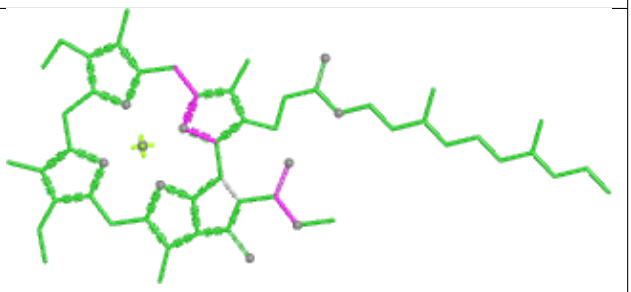
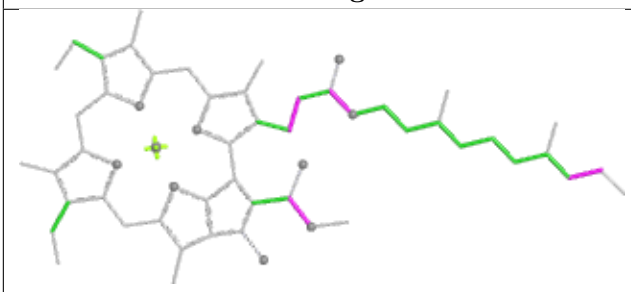
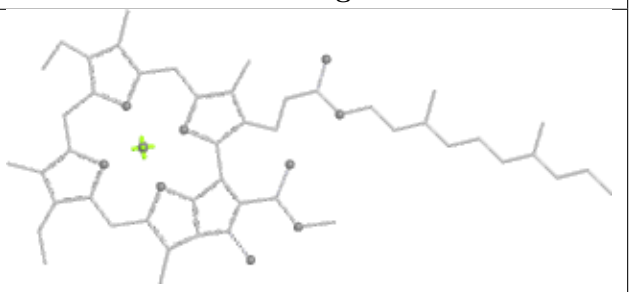


Bond angles

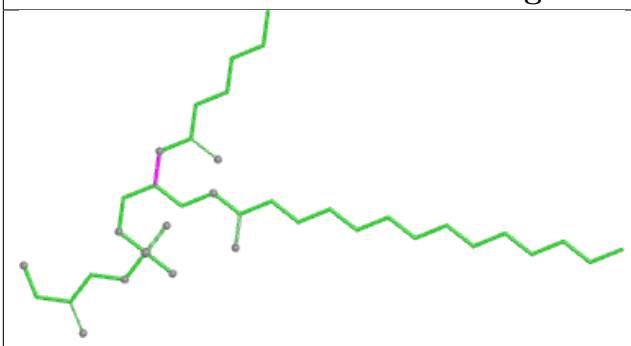


Torsions

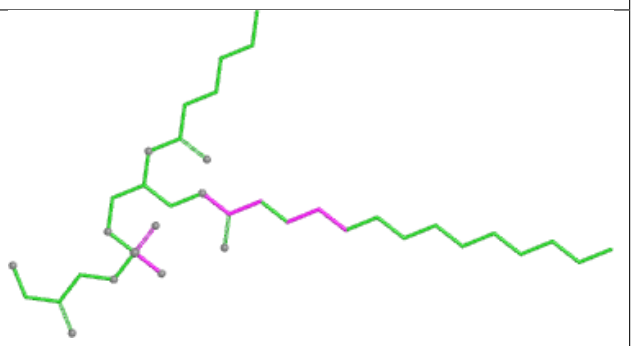


Rings

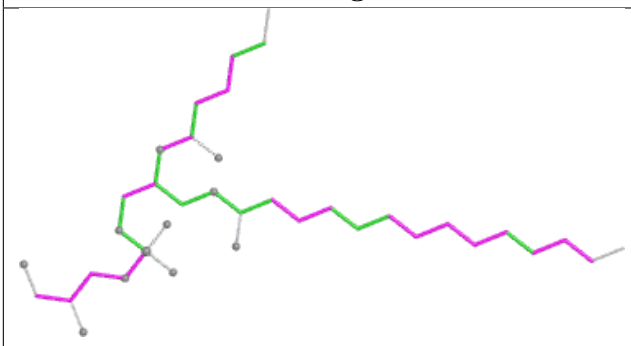
Ligand LHG F 801



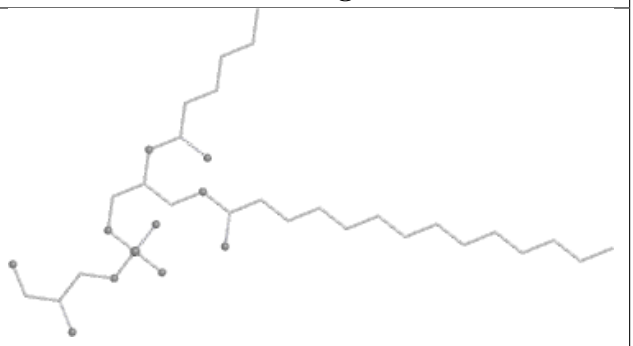
Bond lengths



Bond angles

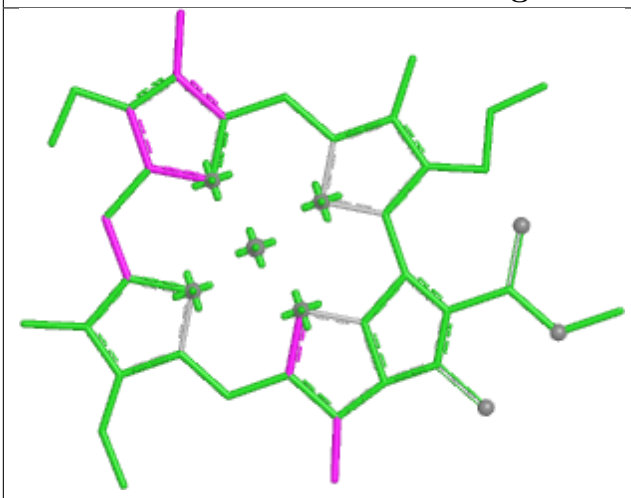


Torsions



Rings

Ligand CLA AB 813



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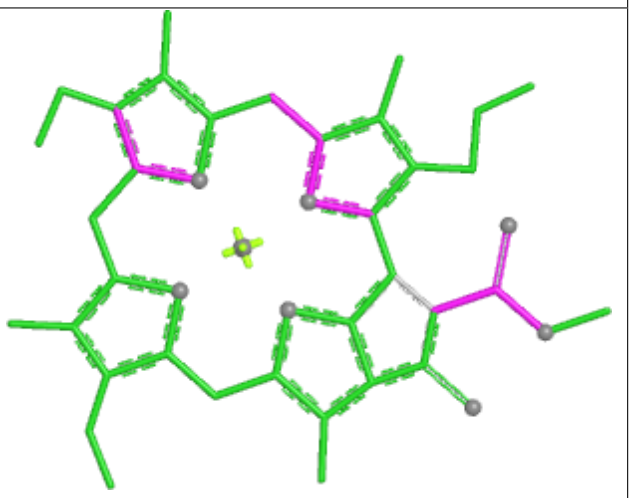
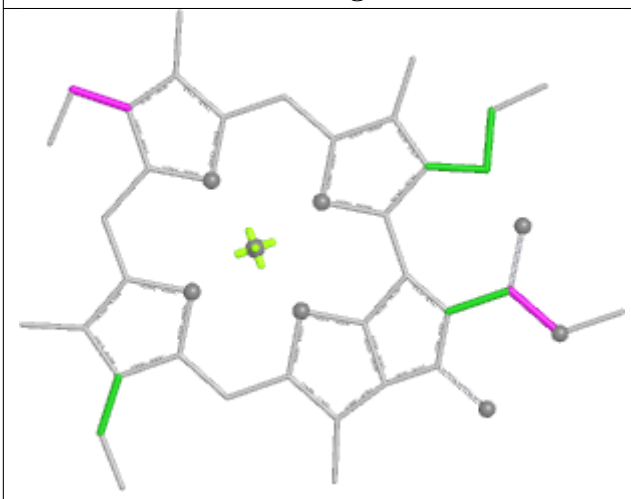
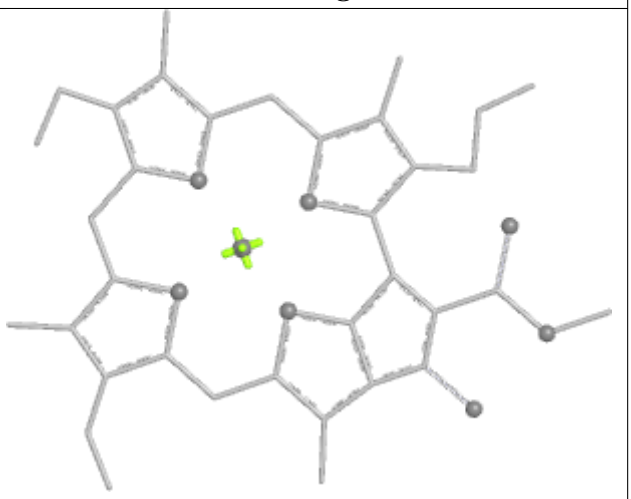


Bond angles

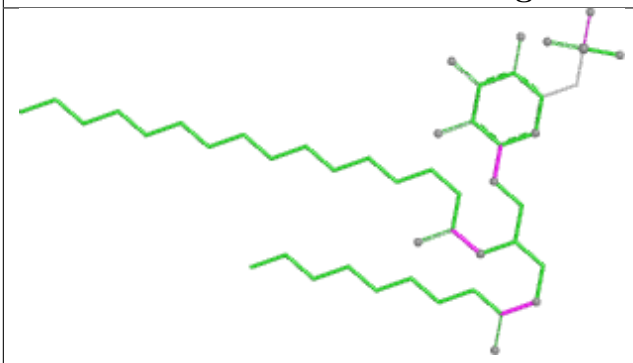


Torsions



Rings

Ligand SQD BJ 104



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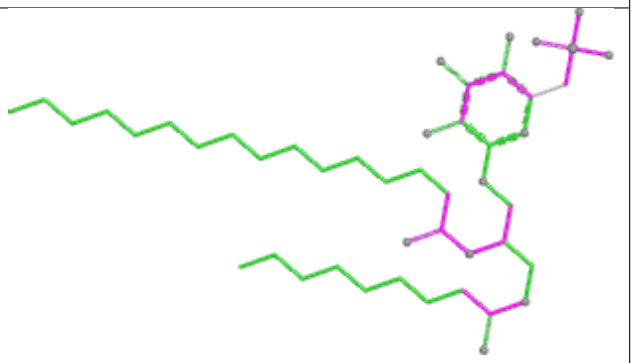
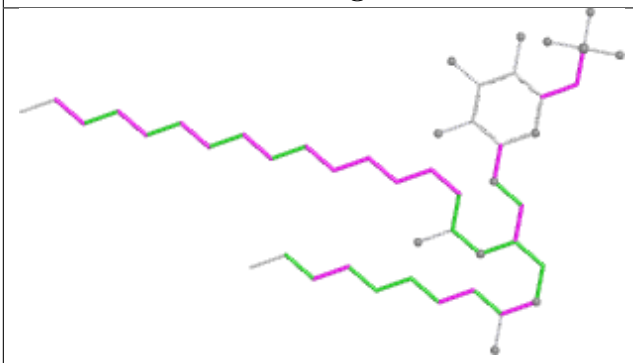
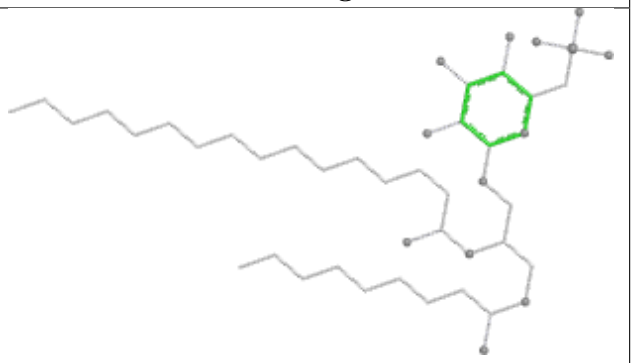


Bond angles

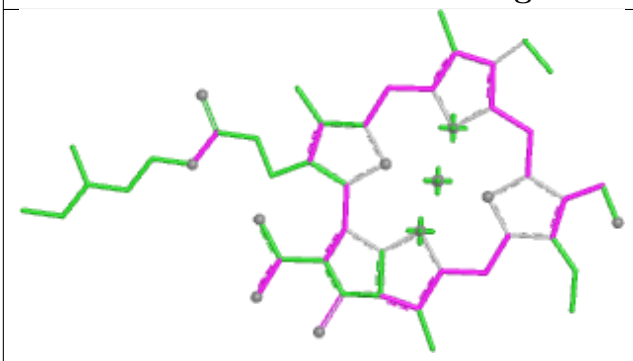


Torsions



Rings

Ligand CHL A1 303



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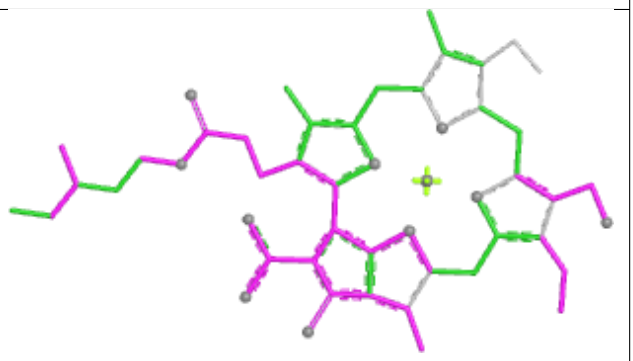
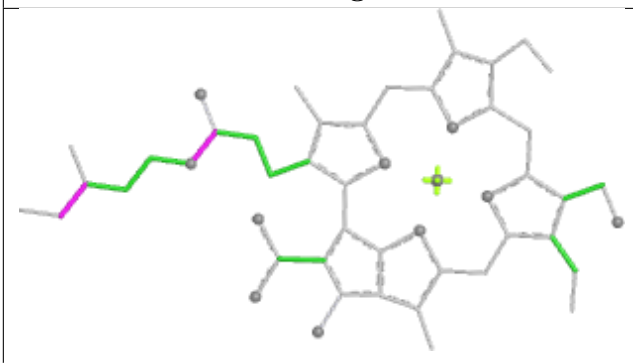
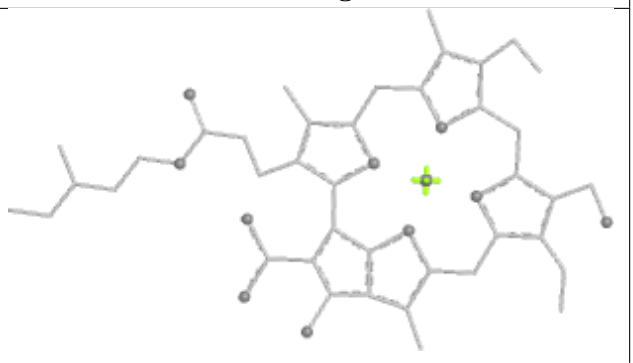


Bond angles

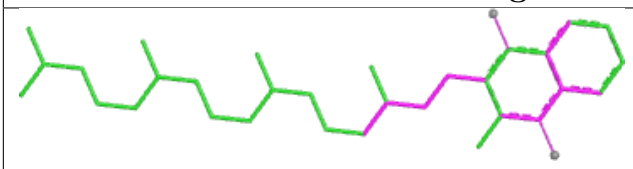


Torsions

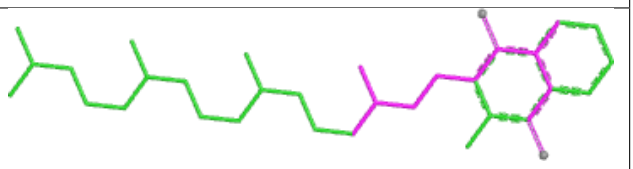


Rings

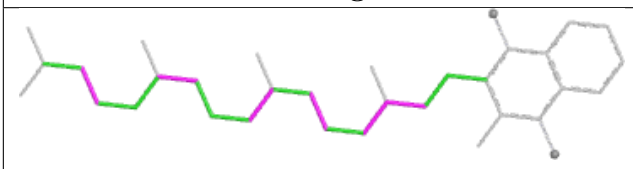
Ligand PQN BB 844



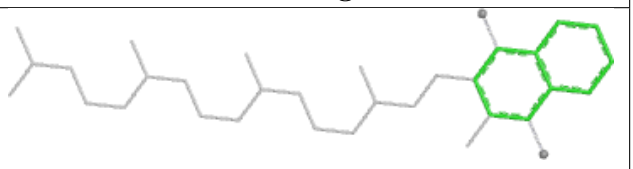
Bond lengths



Bond angles

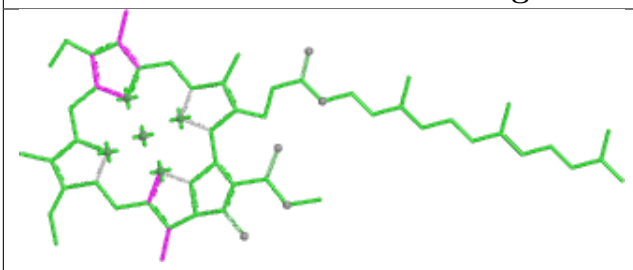


Torsions

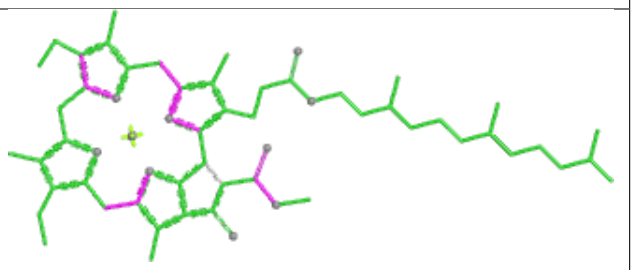


Rings

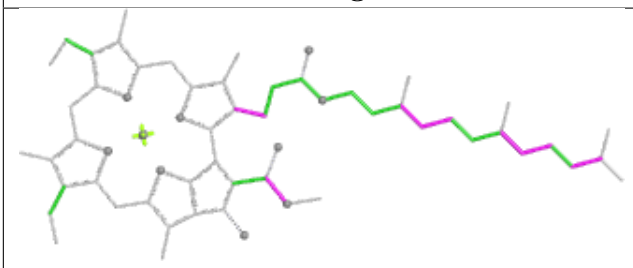
Ligand CLA BB 836



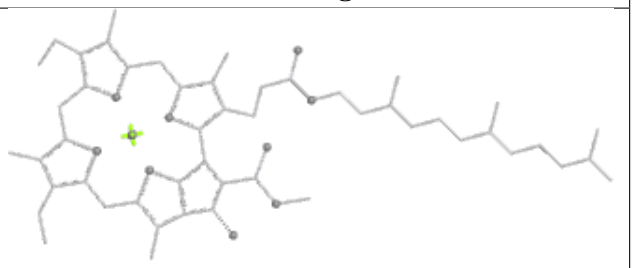
Bond lengths



Bond angles

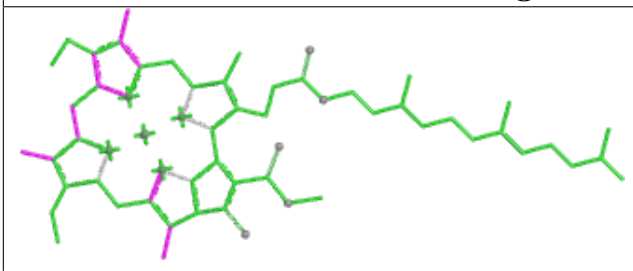


Torsions

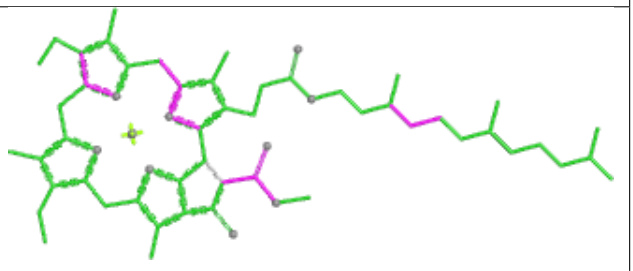


Rings

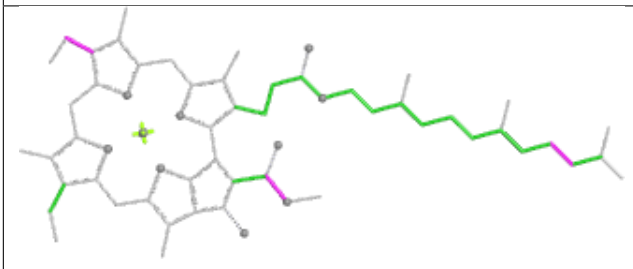
Ligand CLA B3 301



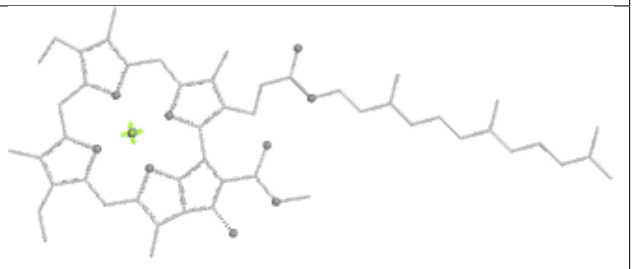
Bond lengths



Bond angles

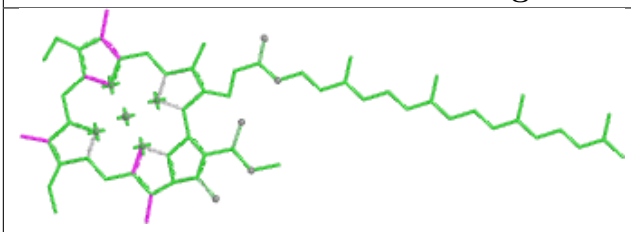


Torsions

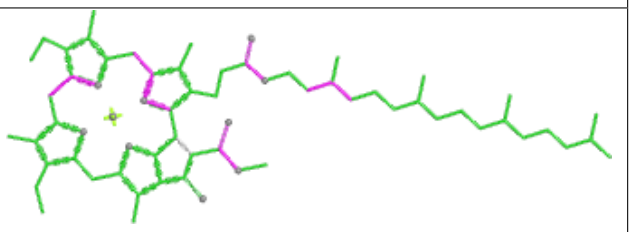


Rings

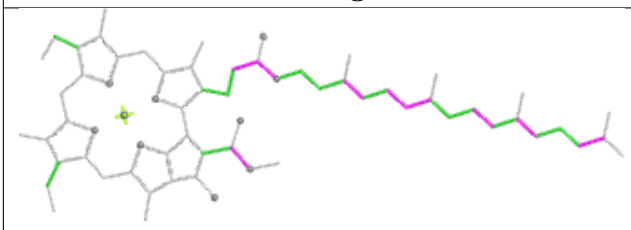
Ligand CLA BB 804



Bond lengths



Bond angles



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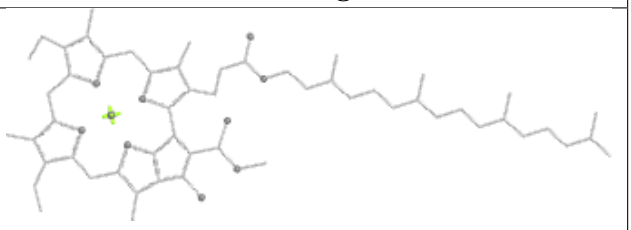
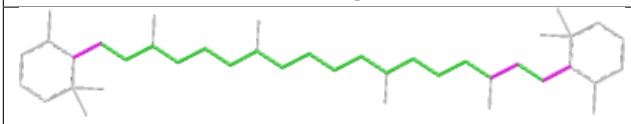


Rings

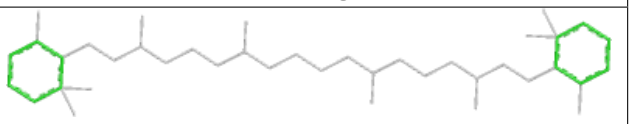
Ligand BCR BA 847

Bond lengths

Bond angles

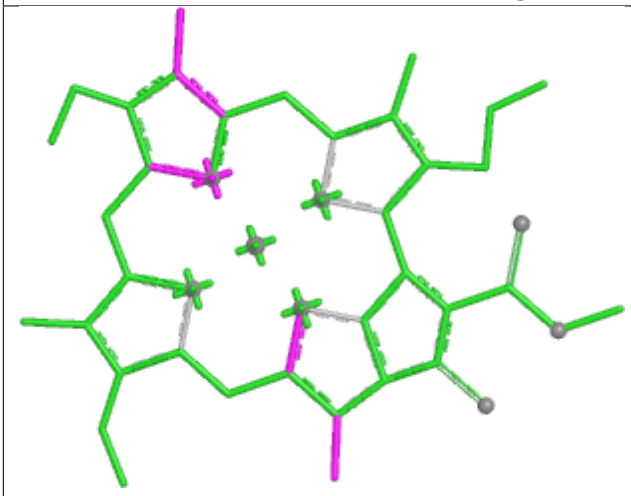


Torsions

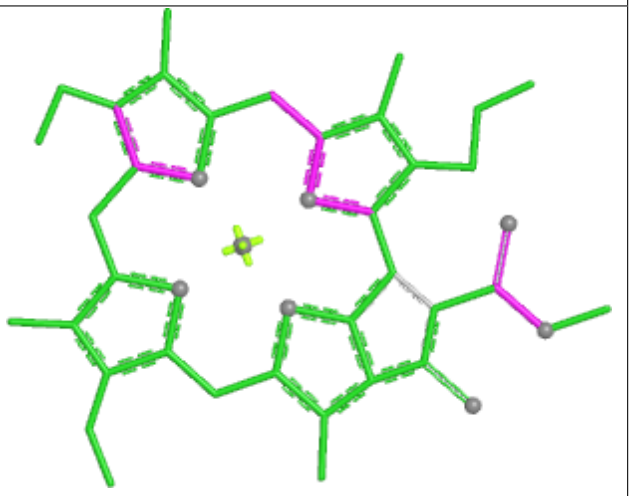


Rings

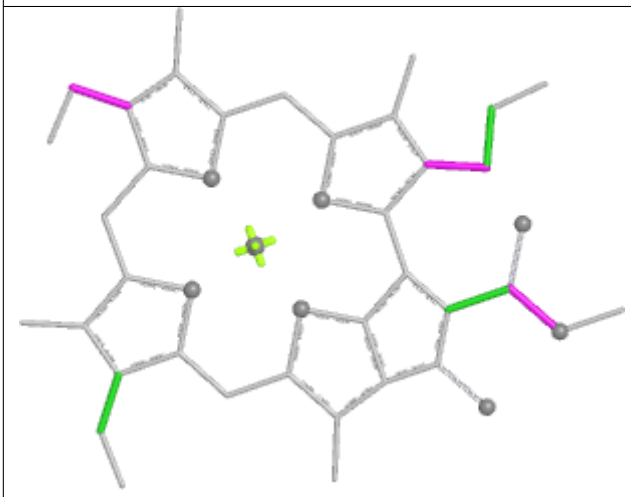
Ligand CLA BB 832



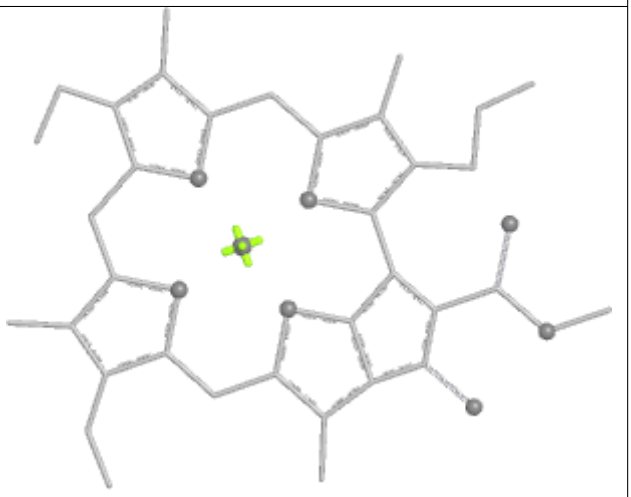
Bond lengths



Bond angles

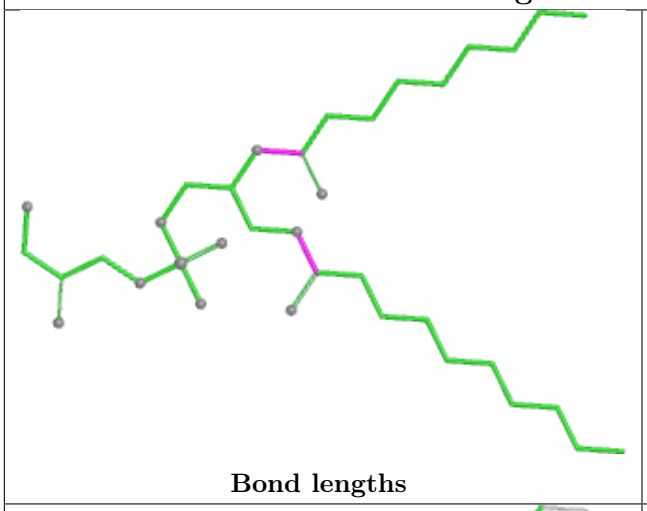


Torsions

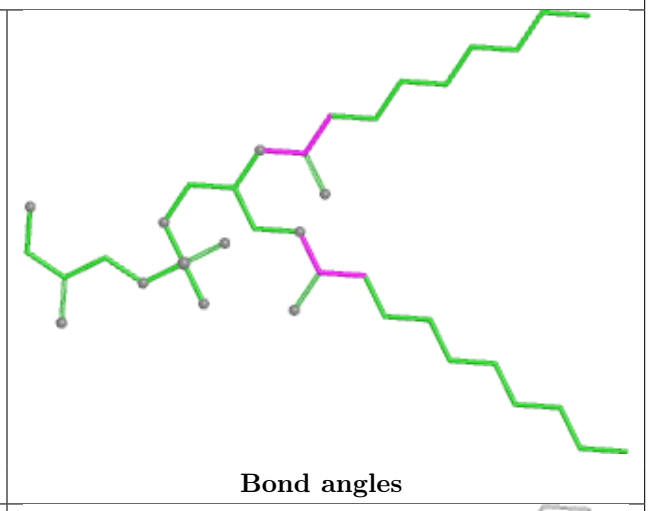


Rings

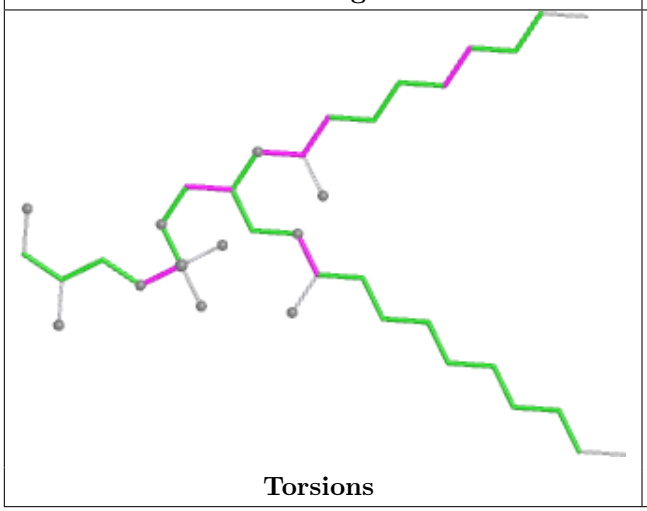
Ligand LHG B1 302



Bond lengths



Bond angles



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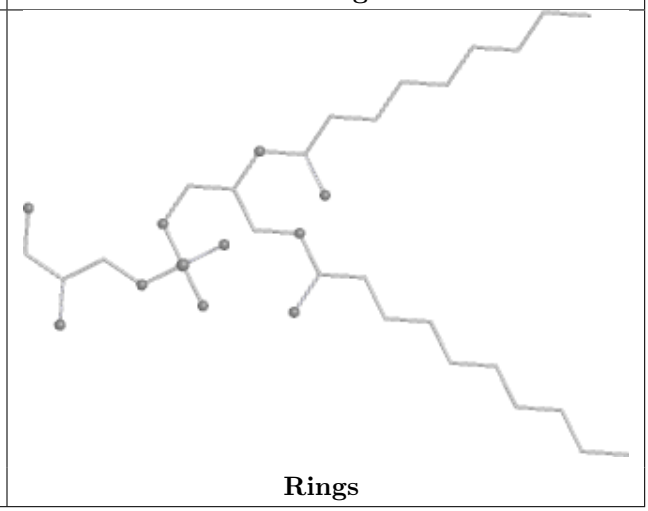
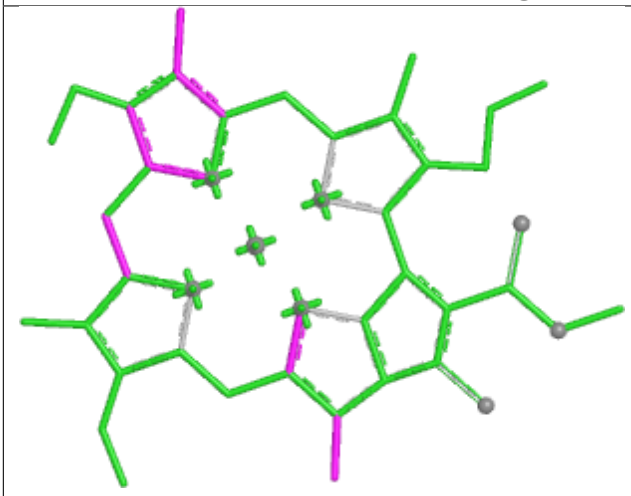
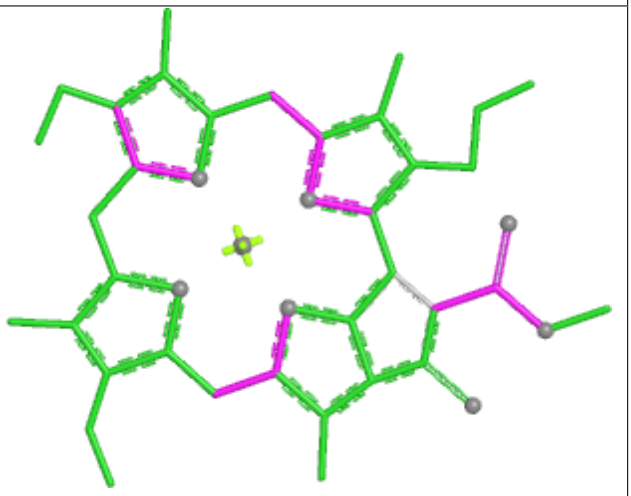
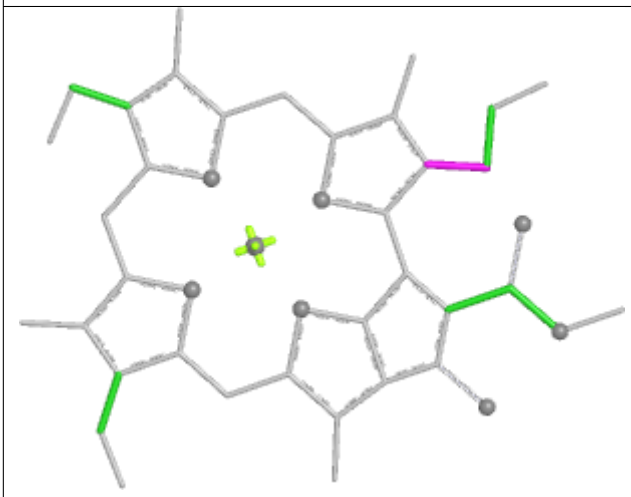
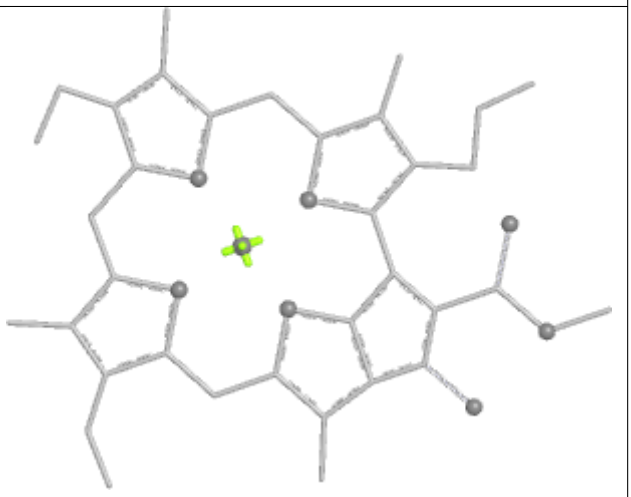
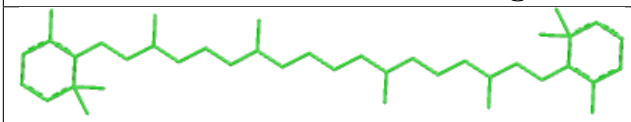
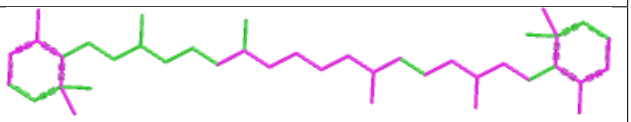
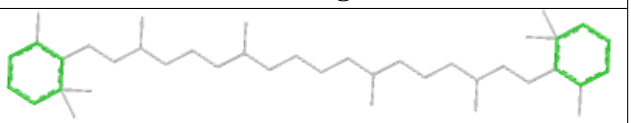
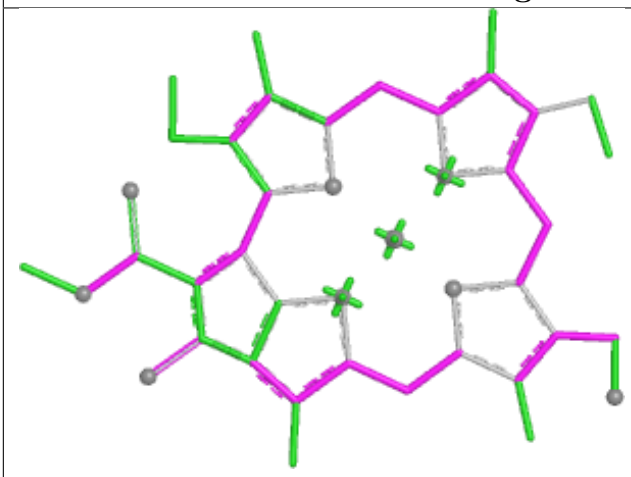


Rings

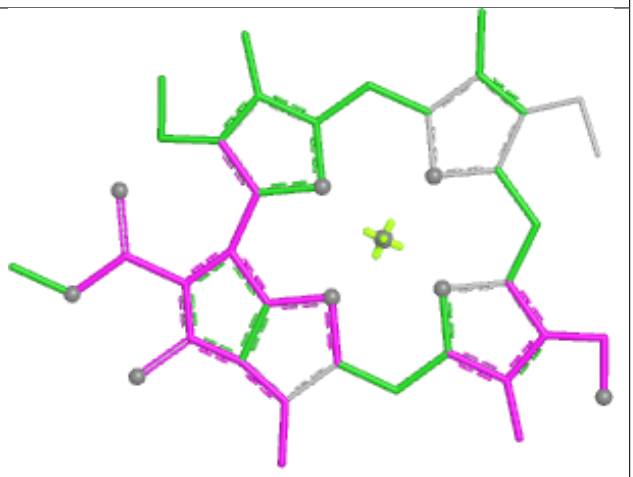
Ligand CLA B2 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR BA 849	
 Bond lengths	 Bond angles
Torsions	 Rings

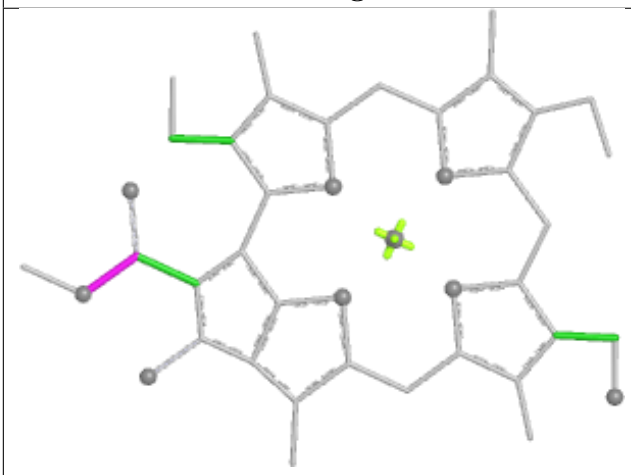
Ligand CHL A6 606



Bond lengths



Bond angles



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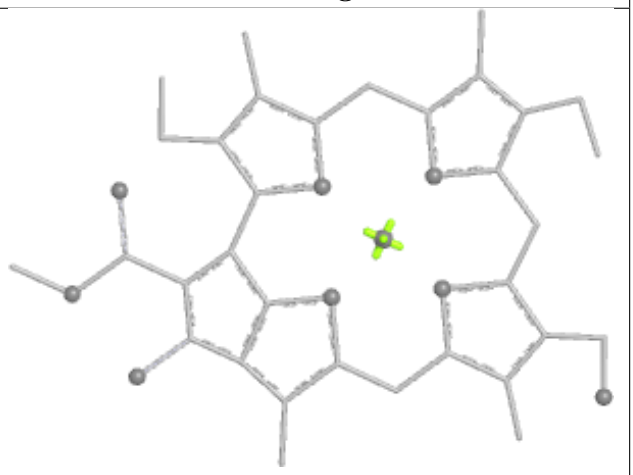
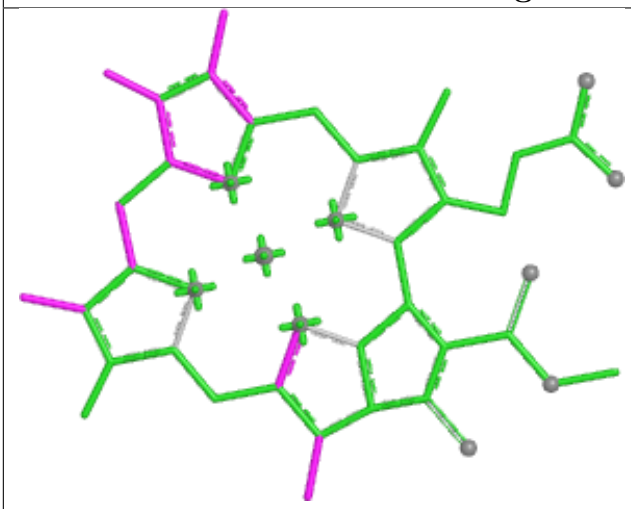


Rings

Ligand CLA A4 303



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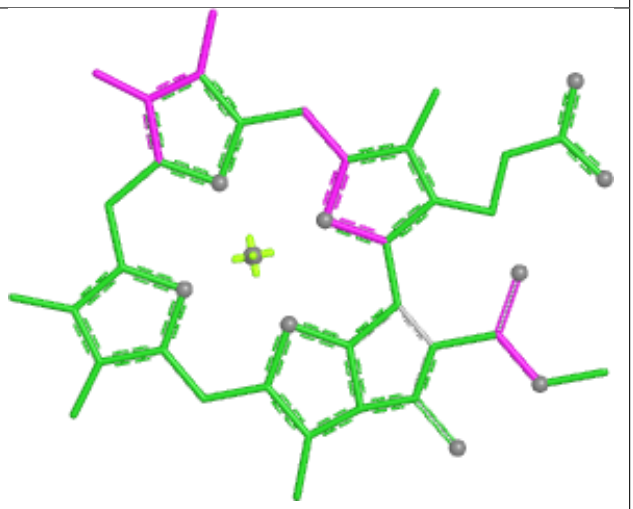
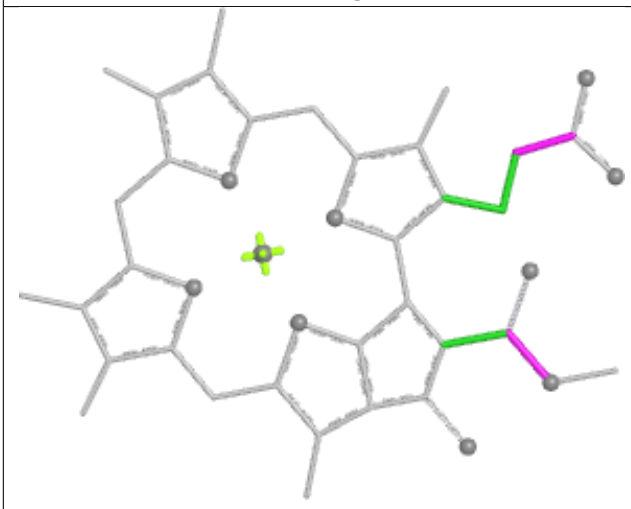


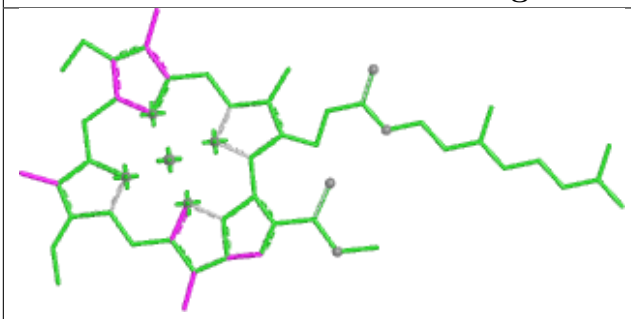
Bond angles



Torsions

Rings

Ligand CLA BA 838



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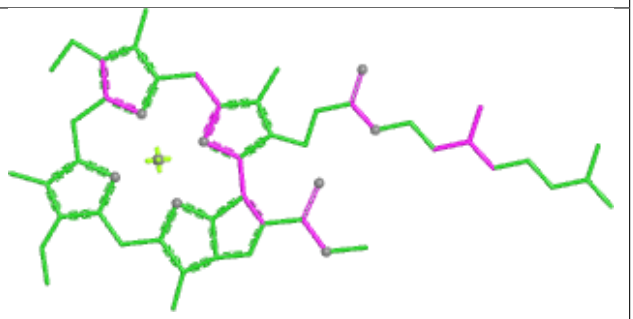

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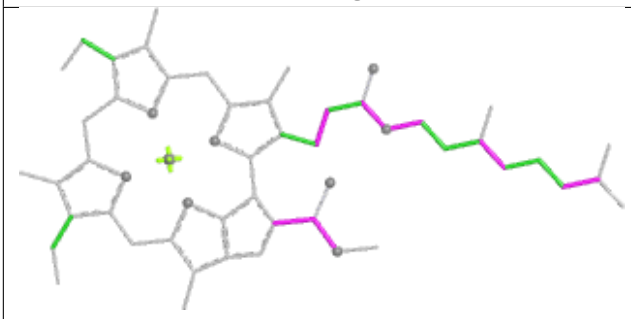

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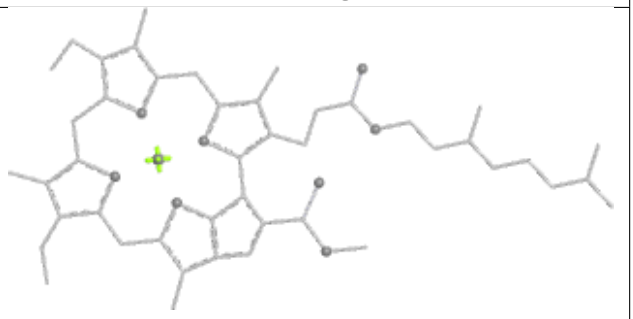
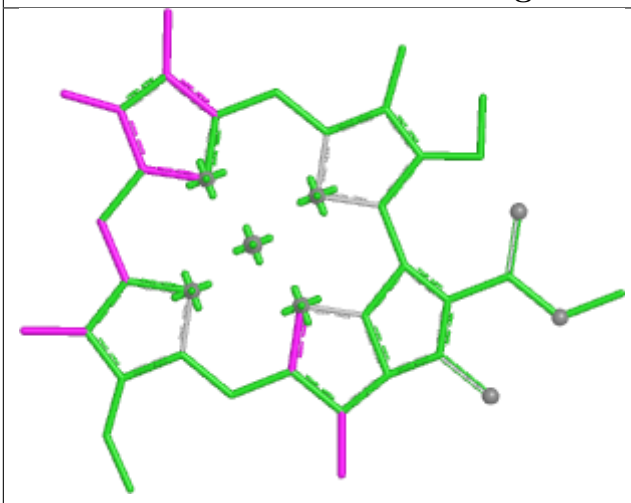


Rings

Ligand CLA A3 306



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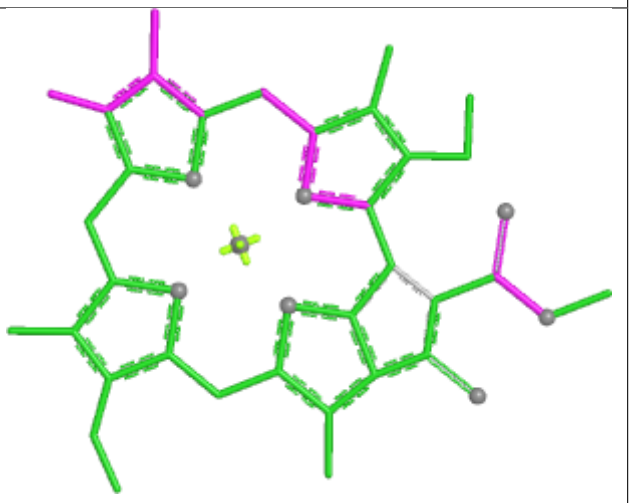
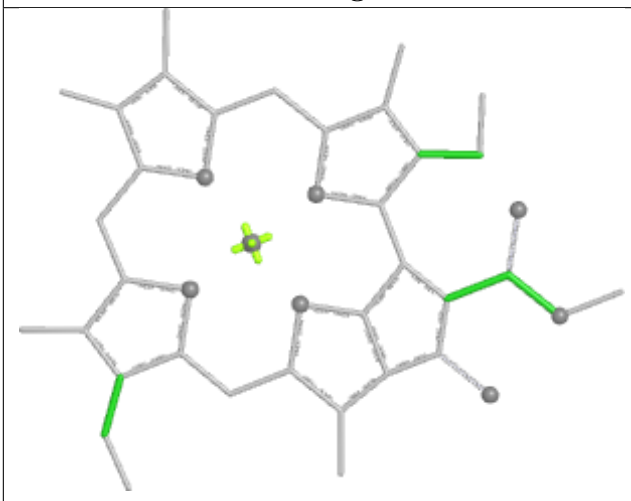


Bond angles



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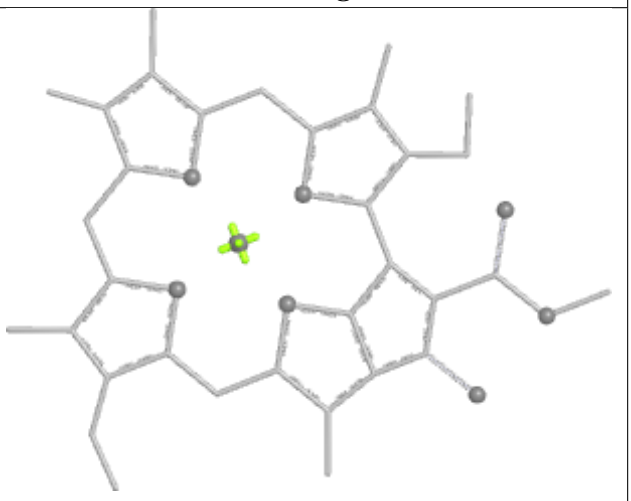
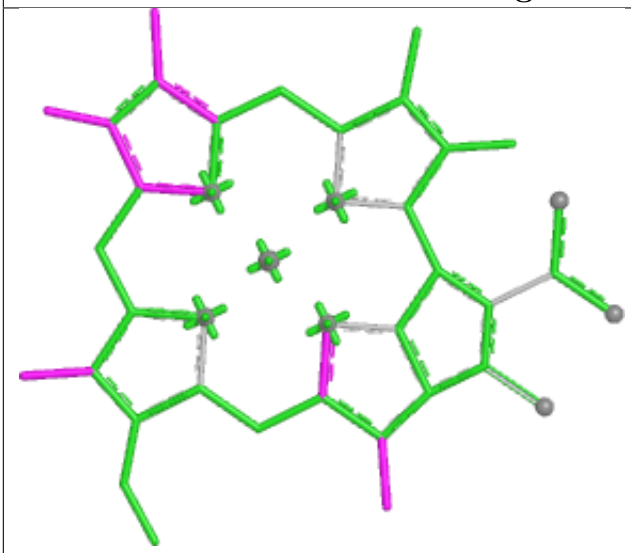


Rings

Ligand CLA B1 310



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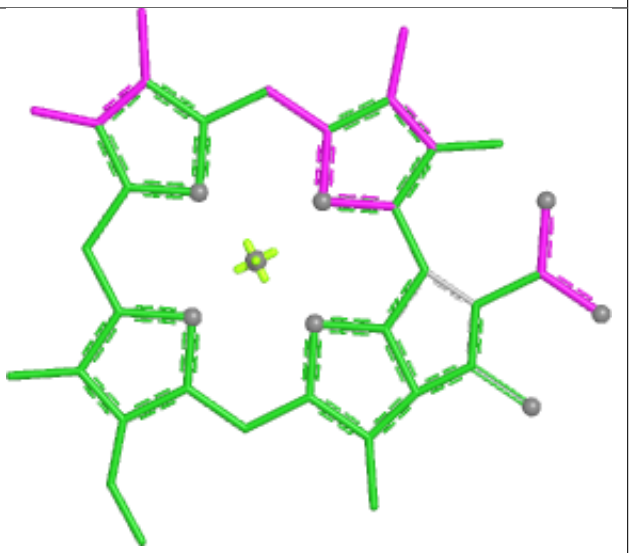
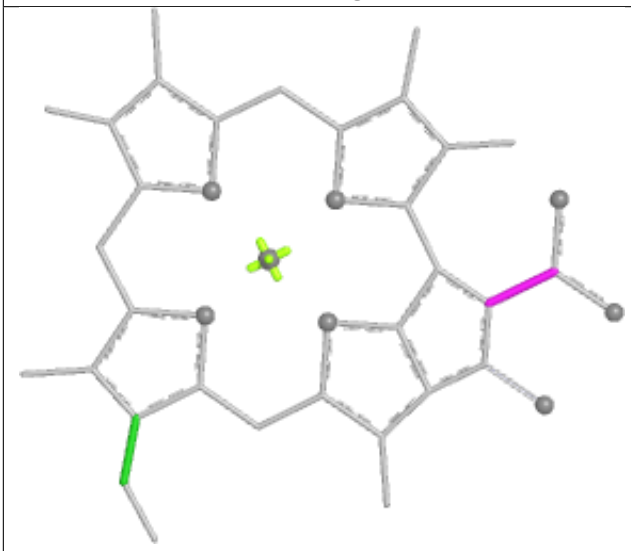
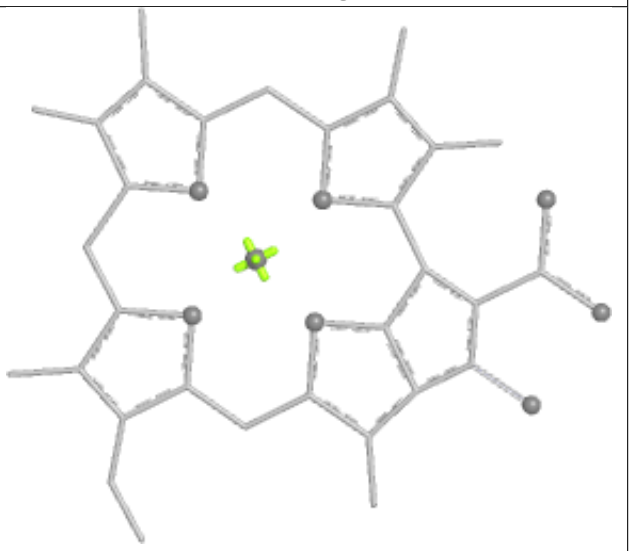


Bond angles

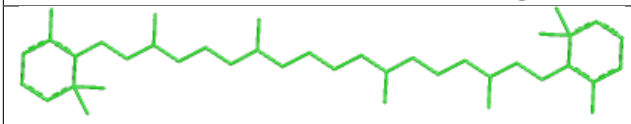


Torsions

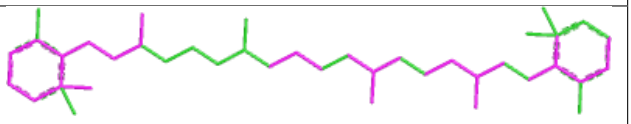


Rings

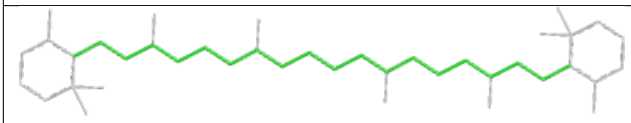
Ligand BCR BJ 101



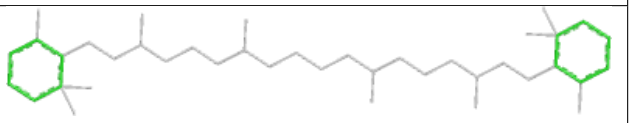
Bond lengths



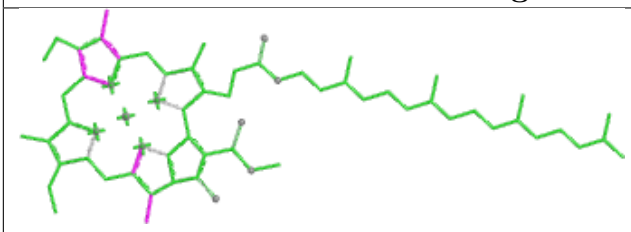
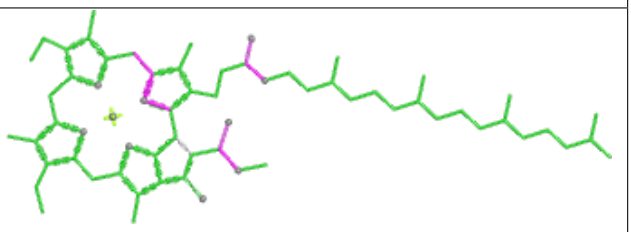
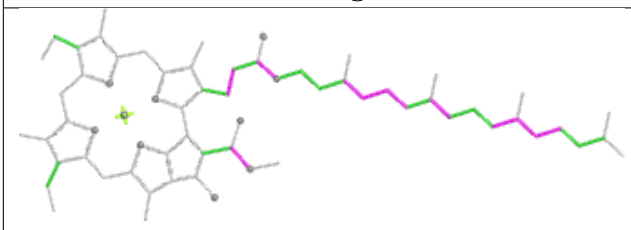
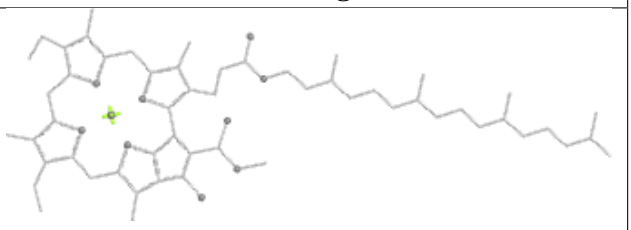
Bond angles

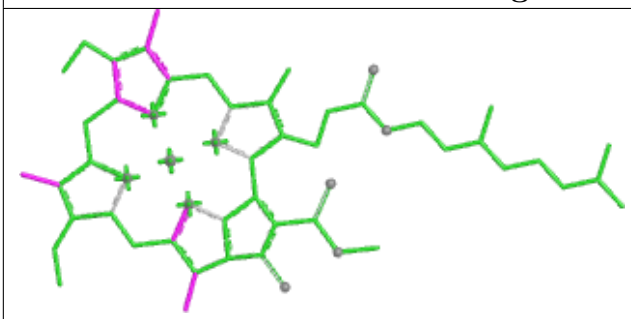
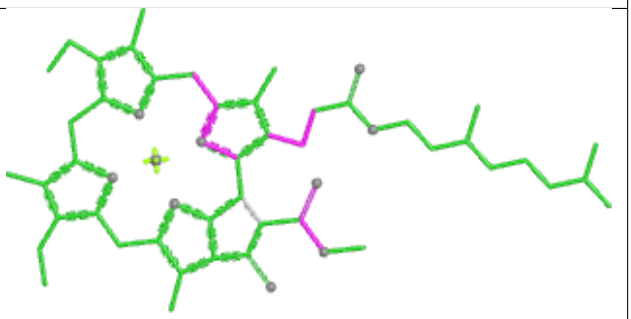
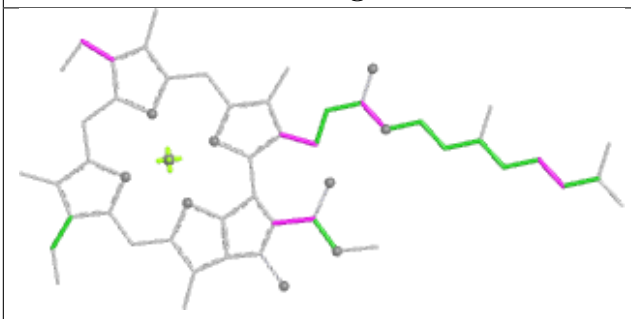
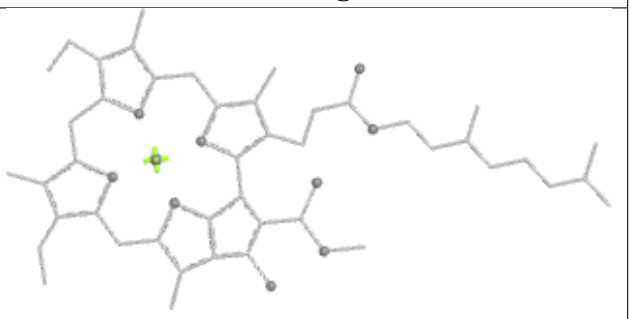


Torsions

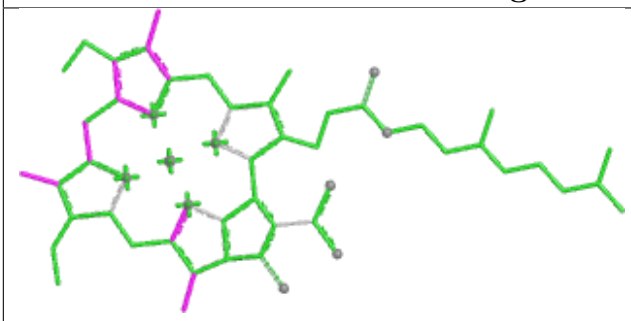


Rings

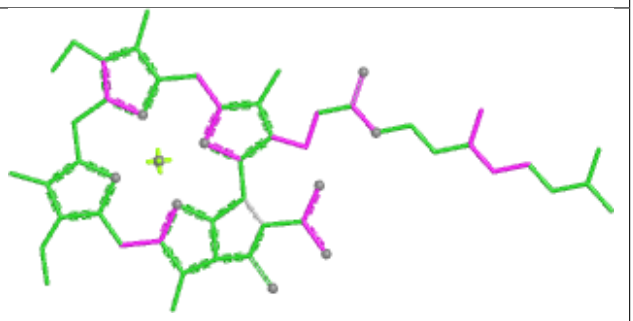
Ligand CLA BA 840	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BA 824	
	
Bond lengths	Bond angles
	
Torsions	Rings

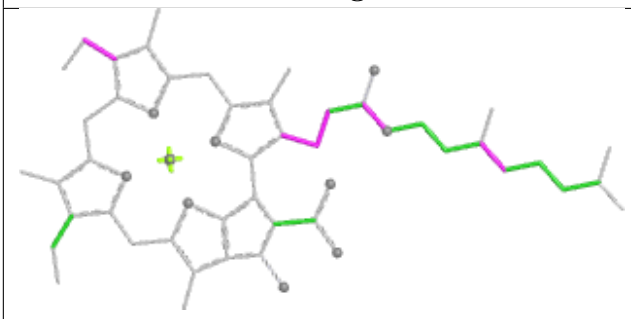
Ligand CLA AA 824



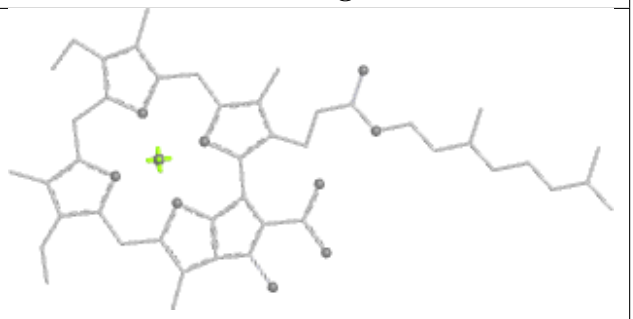
Bond lengths



Bond angles

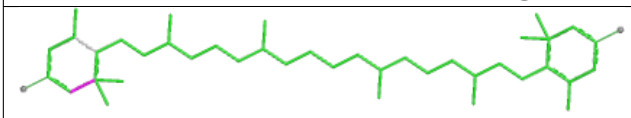


Torsions



Rings

Ligand LUT B5 614



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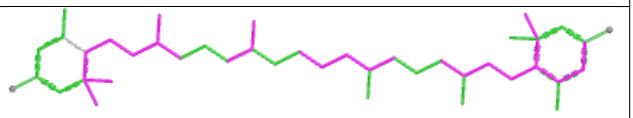
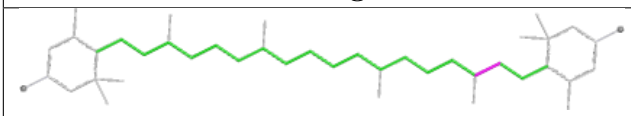
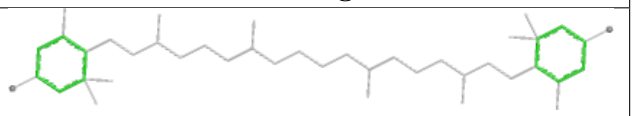


Bond angles

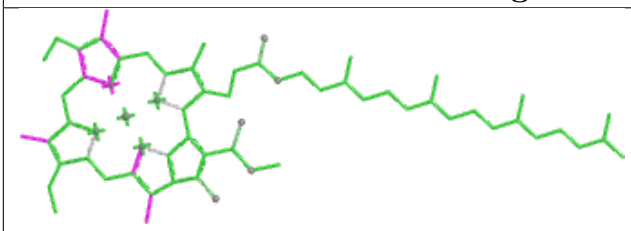


Torsions

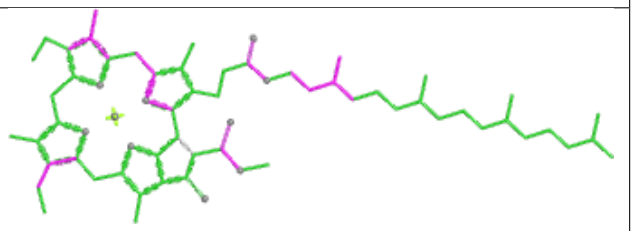


Rings

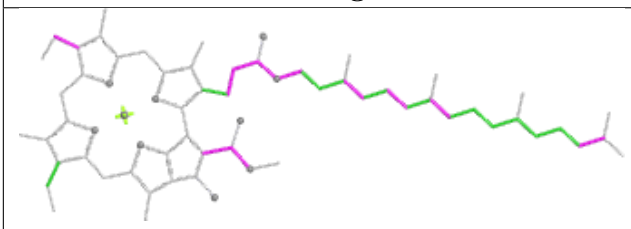
Ligand CLA BA 841



Bond lengths



Bond angles



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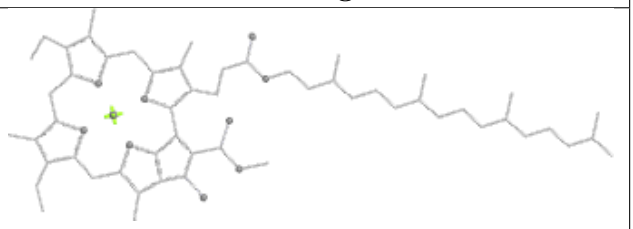
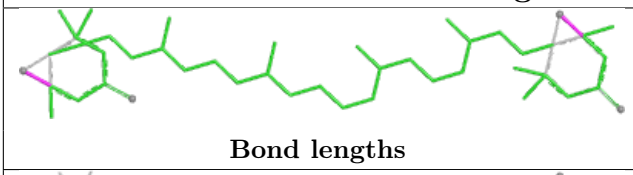


Rings

Ligand XAT A4 316



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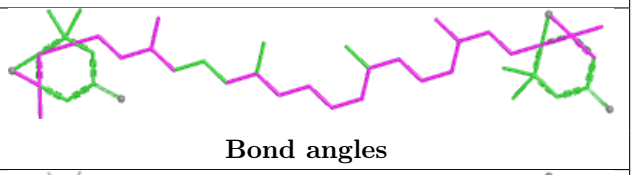
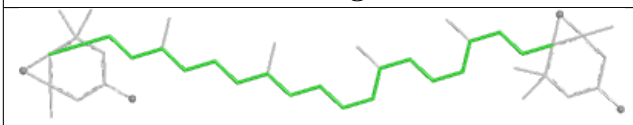


Bond angles



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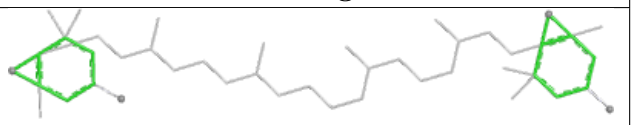
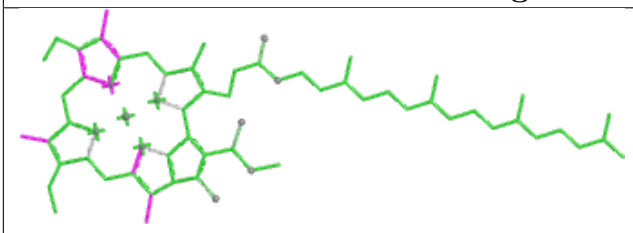


Rings

Ligand CLA BA 802



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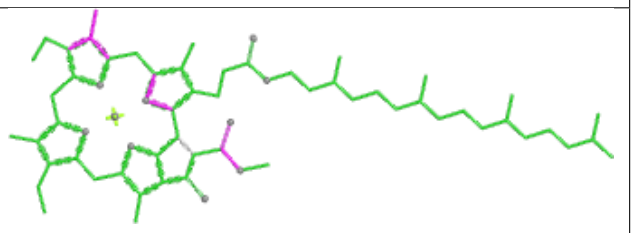
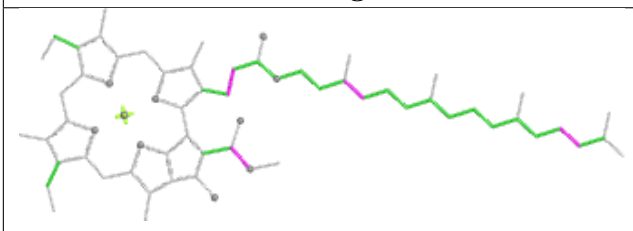


Bond angles



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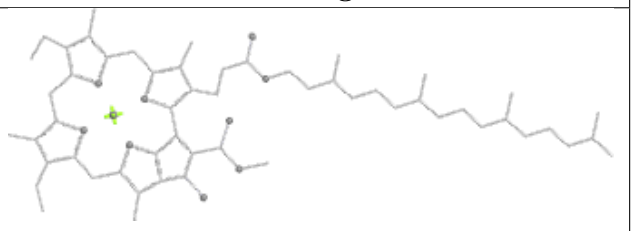
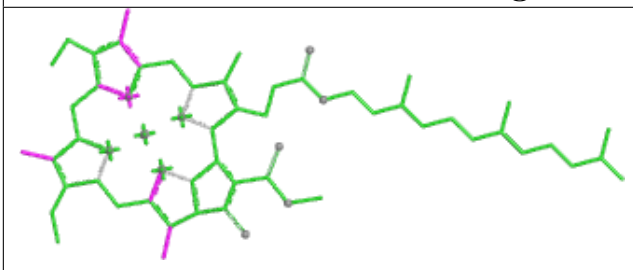


Rings

Ligand CLA AB 819



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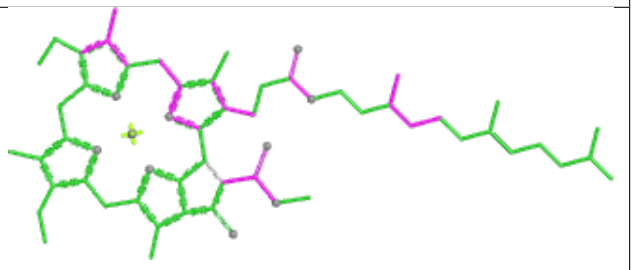

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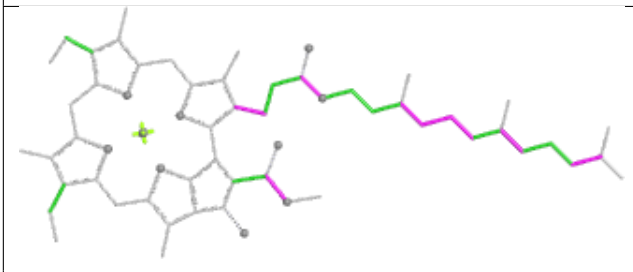

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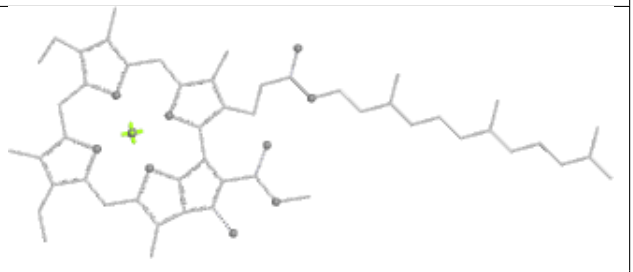
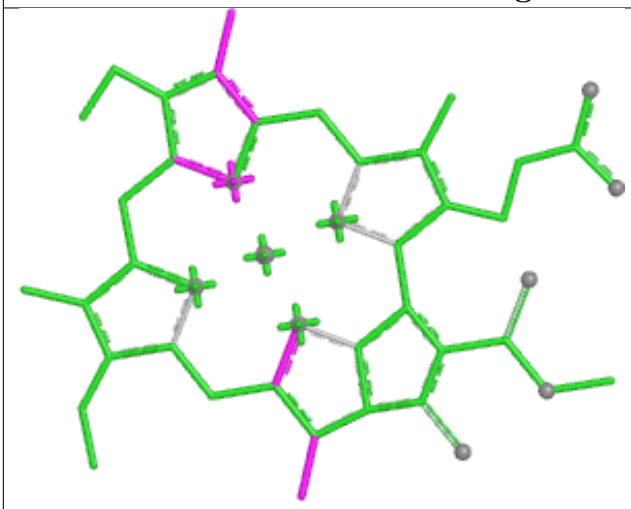


Rings

Ligand CLA A3 308



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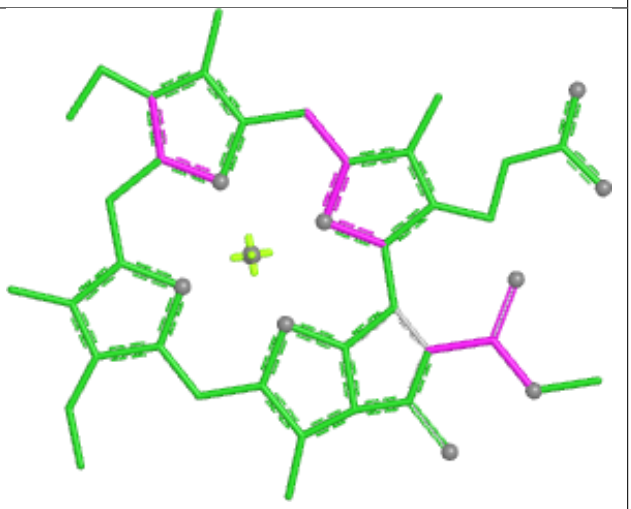

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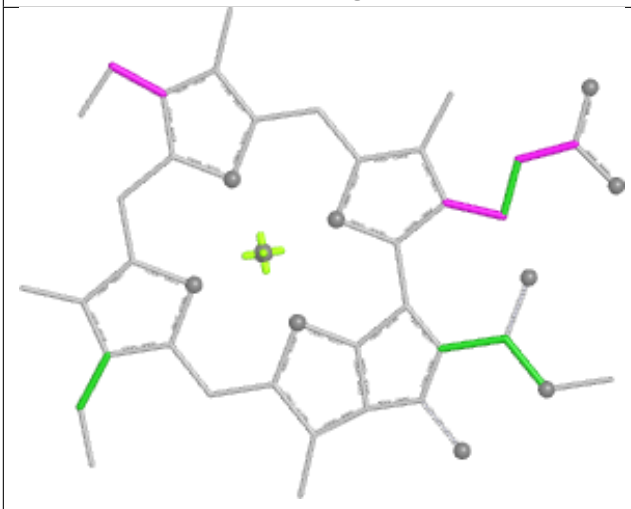
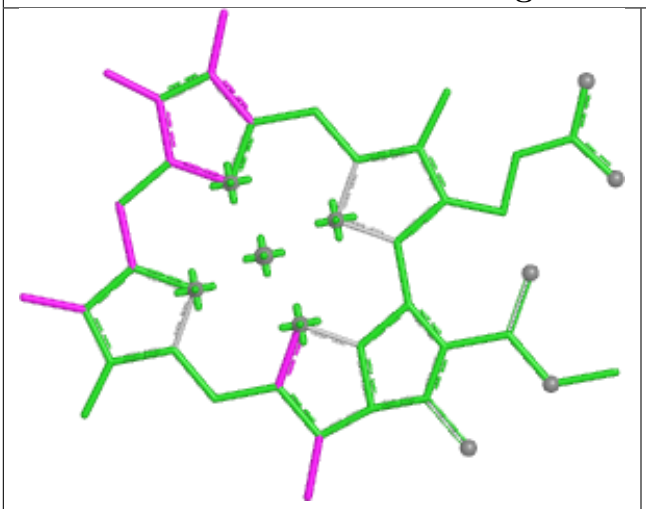


Torsions

Rings

Ligand CLA B5 604



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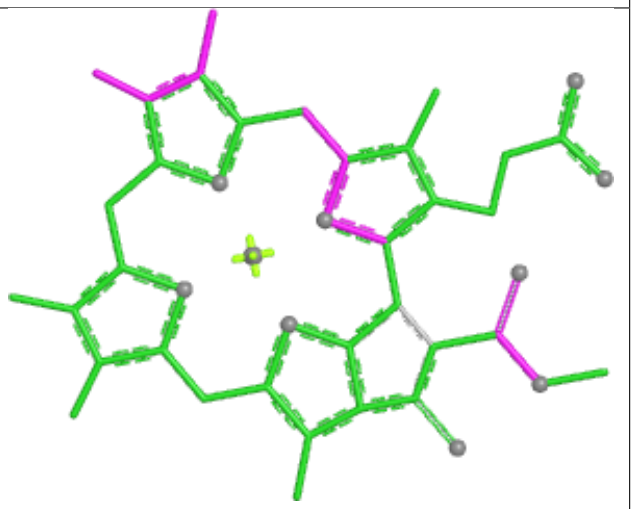

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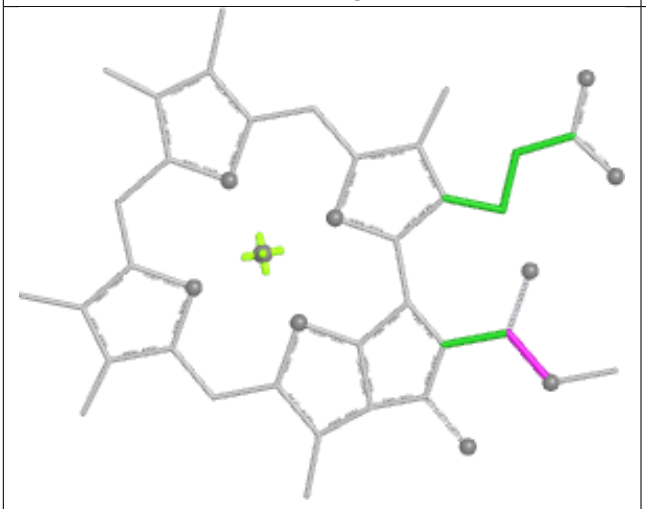
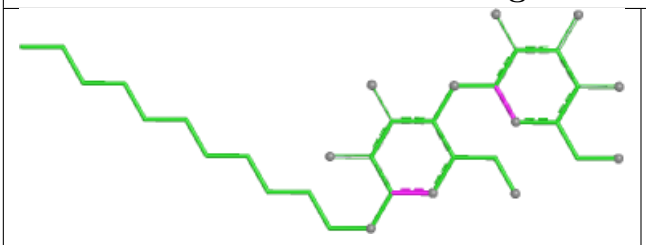


Torsions

Rings

Ligand LMU AL 301



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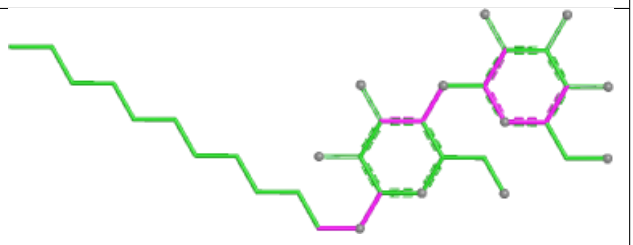

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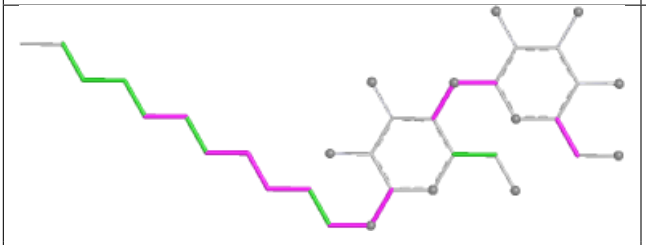

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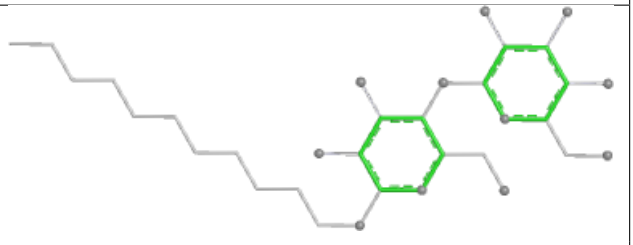
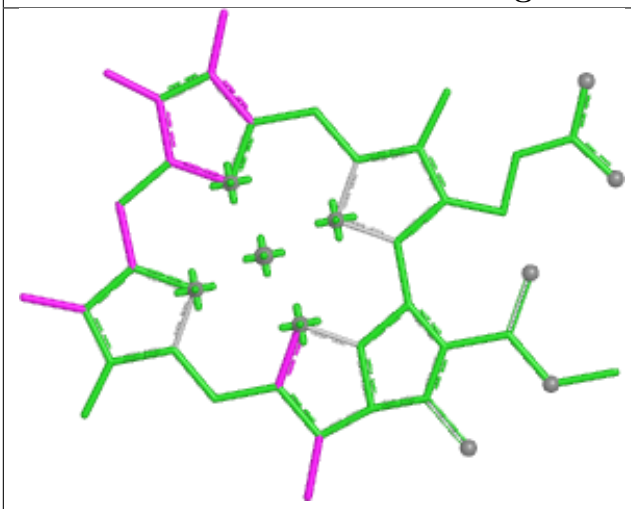


Rings

Ligand CLA A1 316



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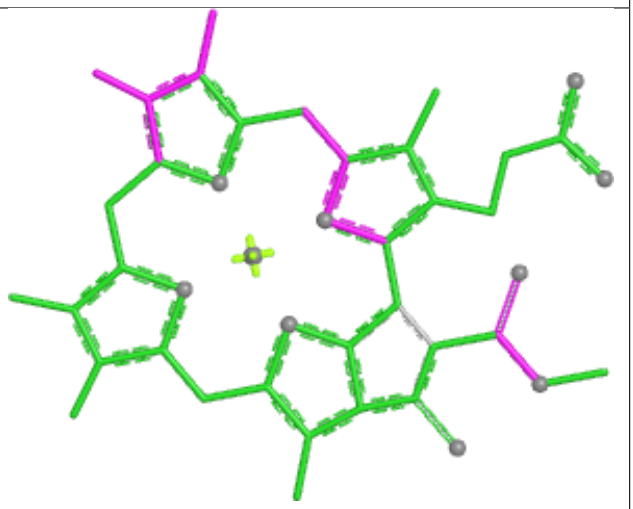
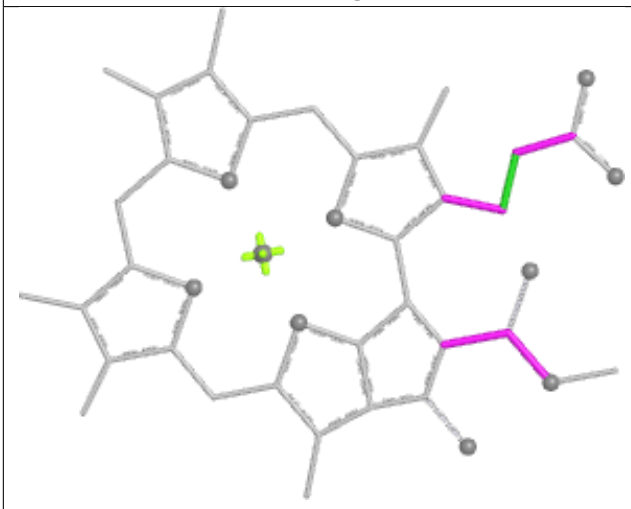


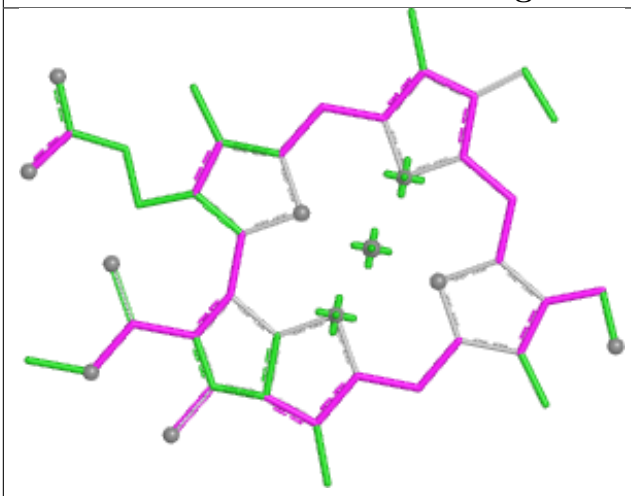
Bond angles



Torsions

Rings

Ligand CHL B5 607



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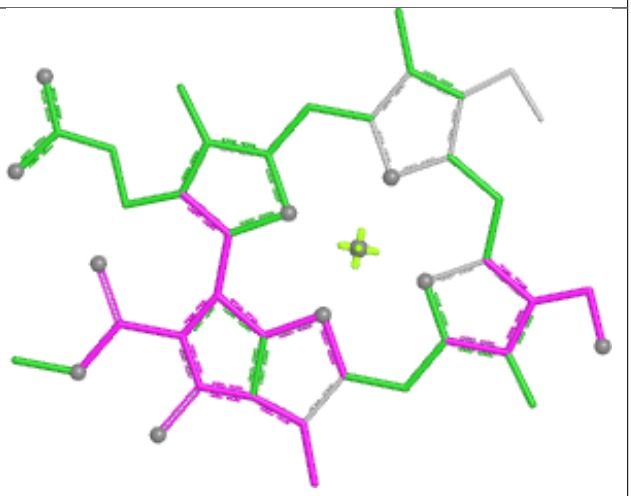

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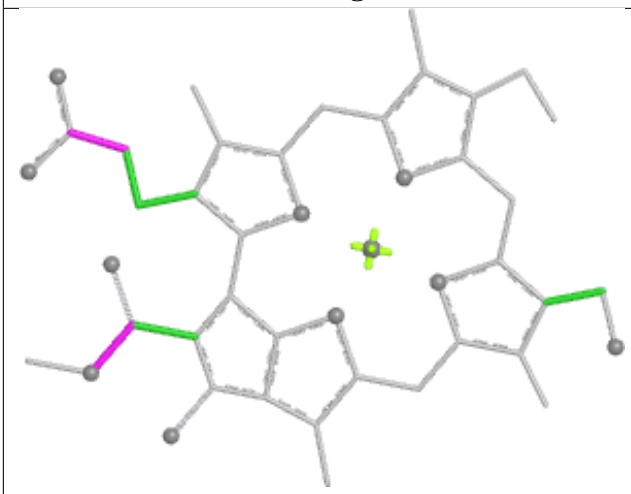
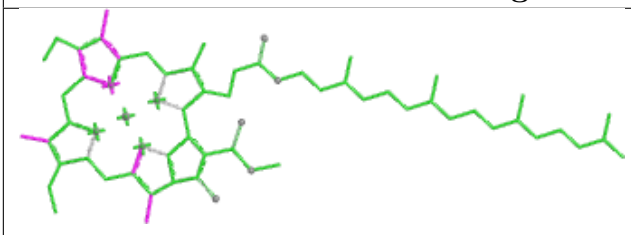


Torsions

Rings

Ligand CLA BA 842



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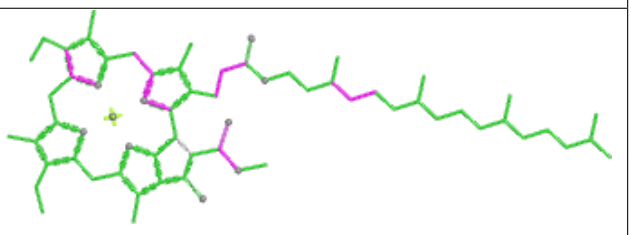
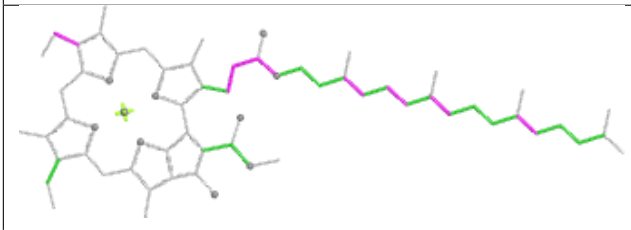
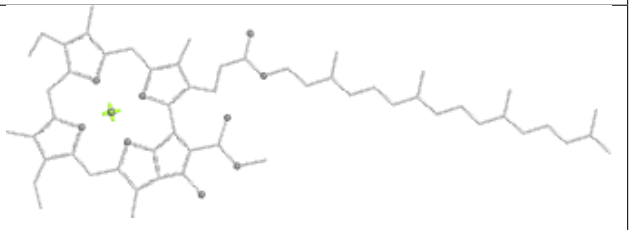


Bond angles

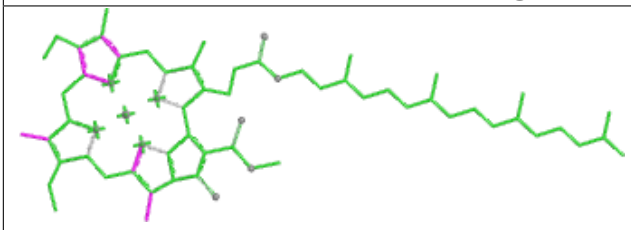


Torsions



Rings

Ligand CLA BA 828



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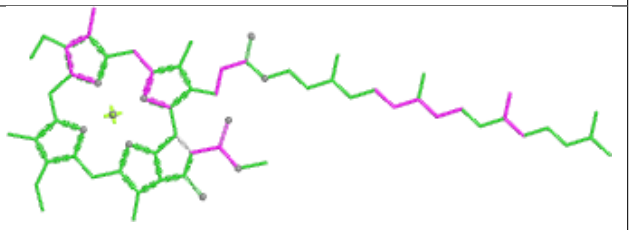
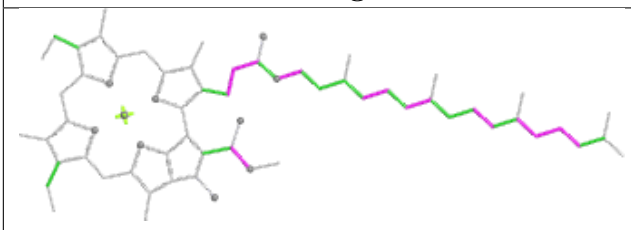
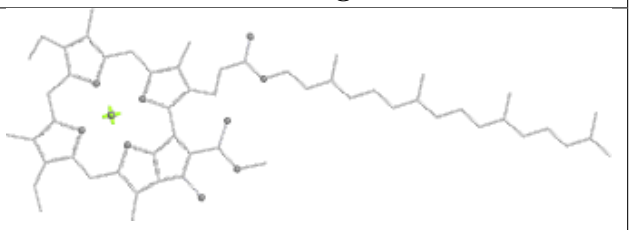


Bond angles

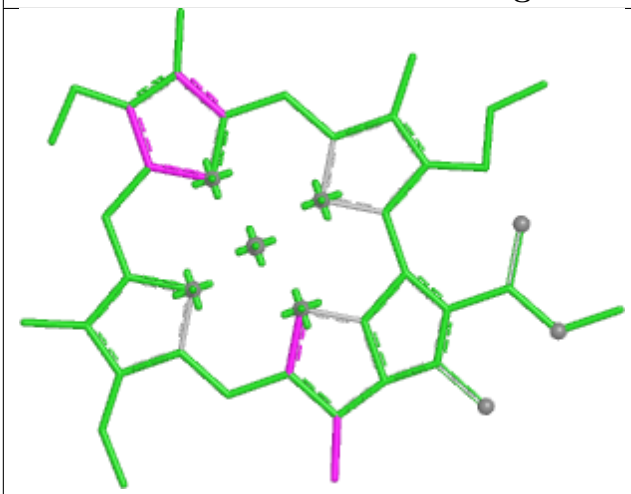


Torsions

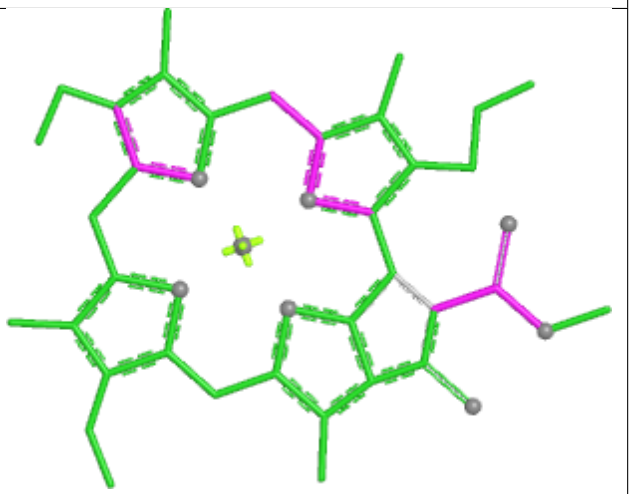


Rings

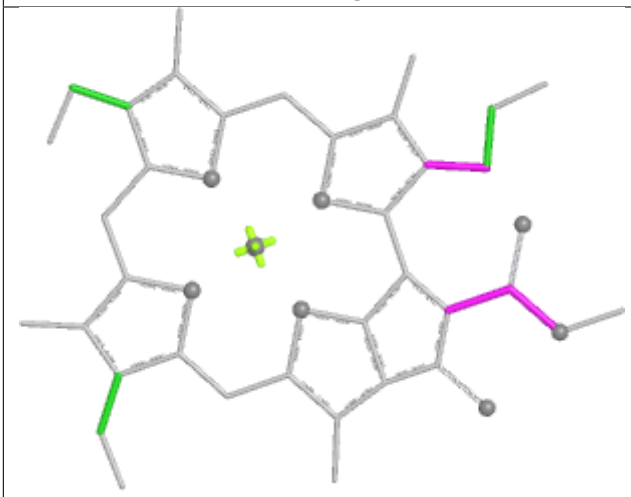
Ligand CLA BL 304



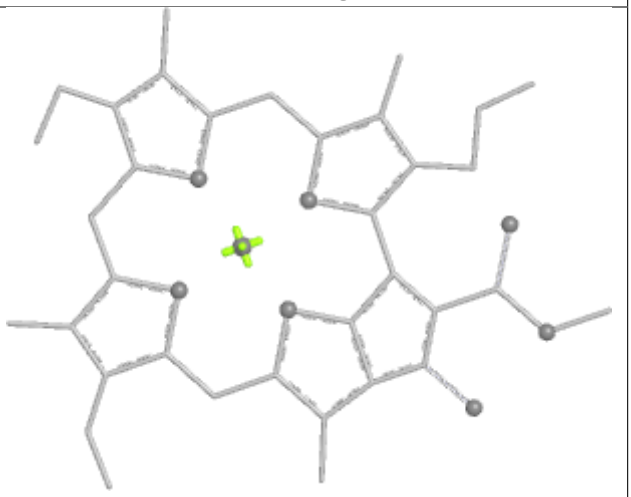
Bond lengths



Bond angles

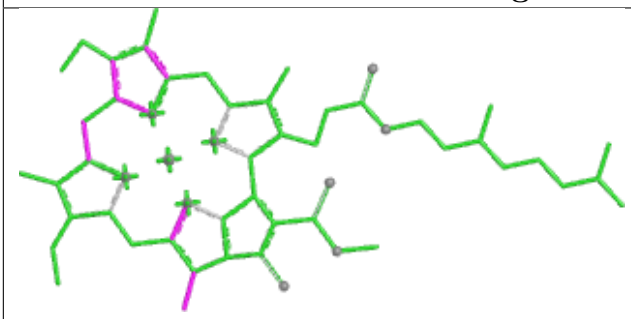


Torsions

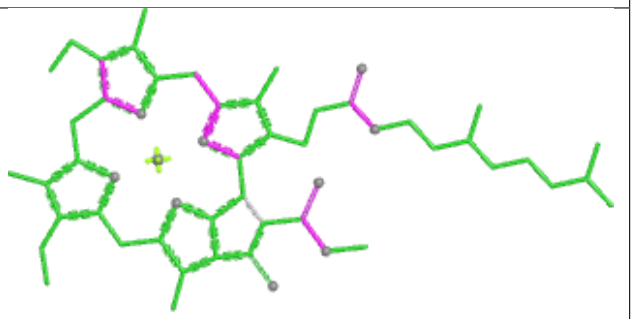


Rings

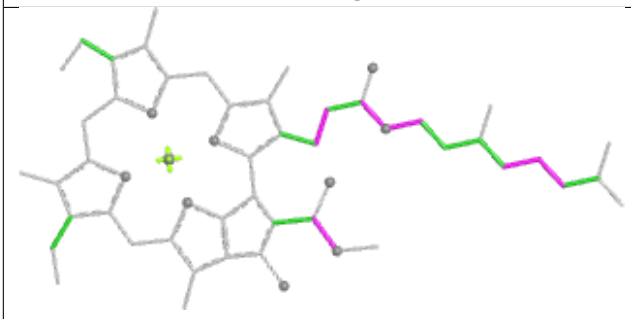
Ligand CLA BB 818



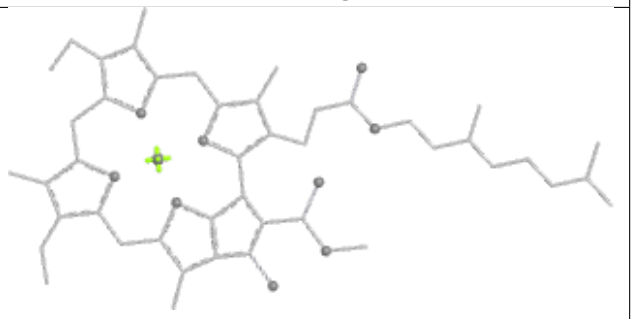
Bond lengths



Bond angles

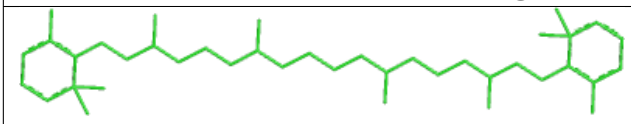


Torsions



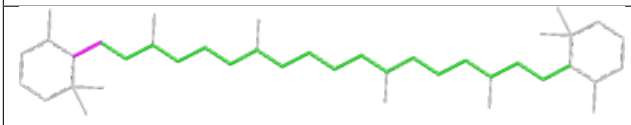
Rings

Ligand BCR BL 305

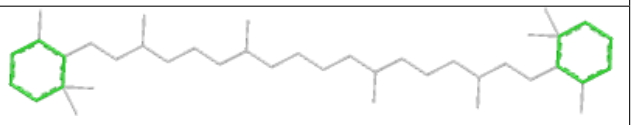


Bond lengths

Bond angles

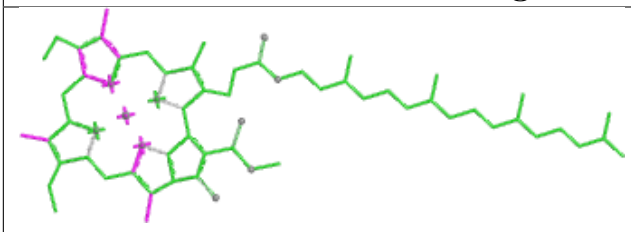


Torsions

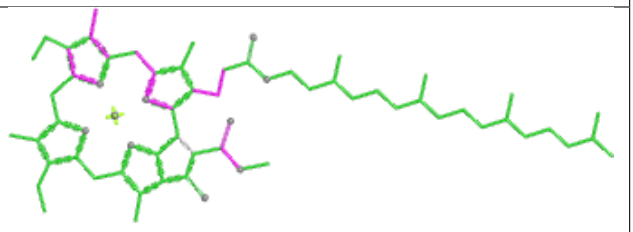


Rings

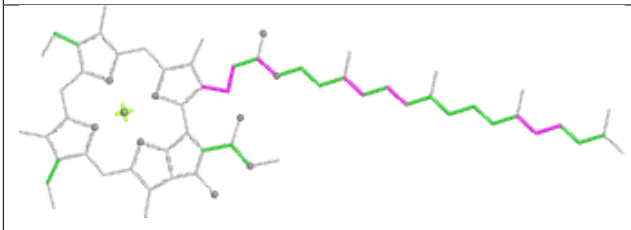
Ligand CLA BB 830



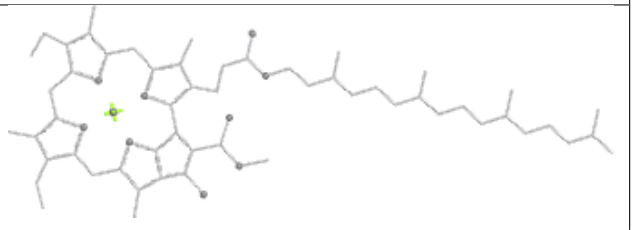
Bond lengths



Bond angles

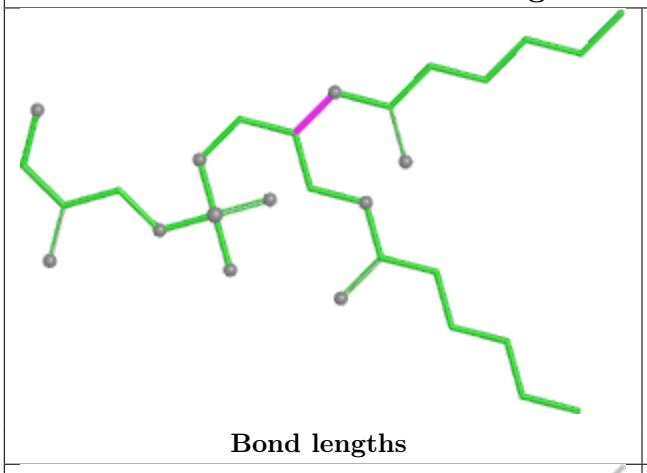


Torsions



Rings

Ligand LHG a 501



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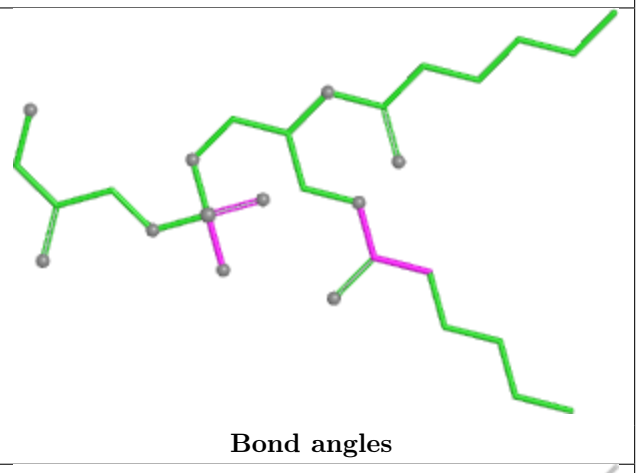
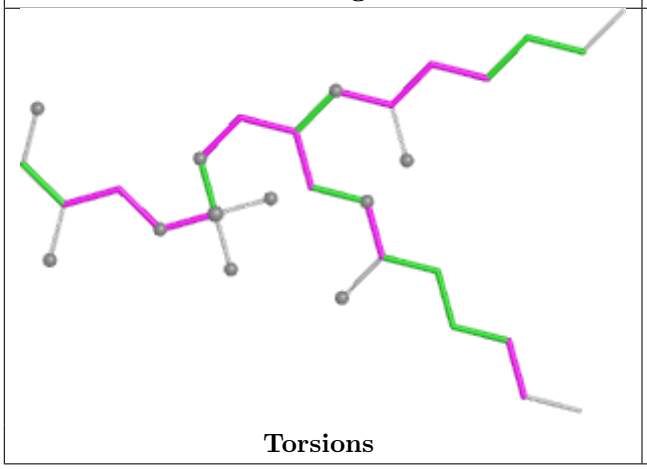
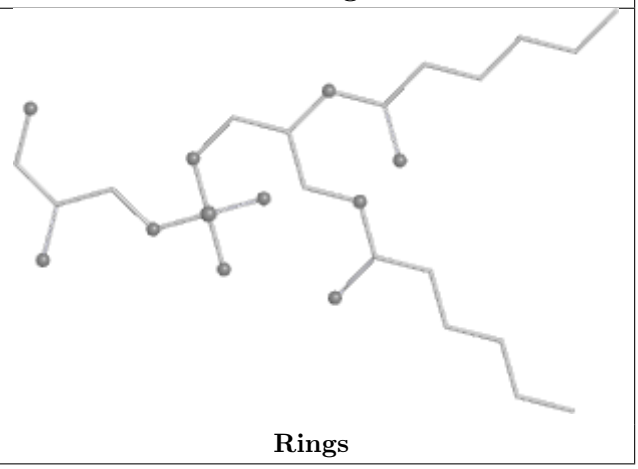


Bond angles

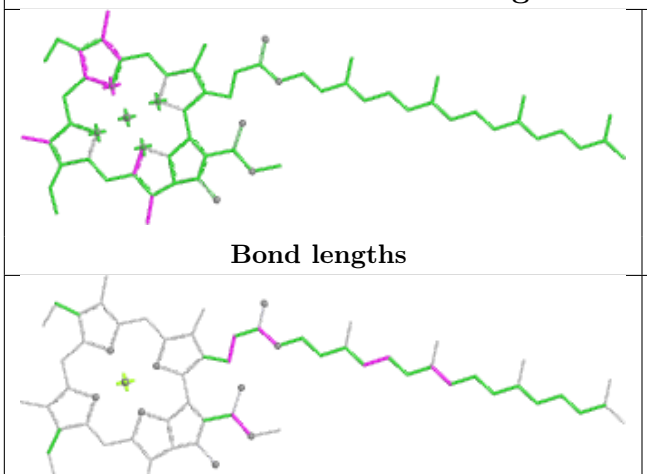


Torsions

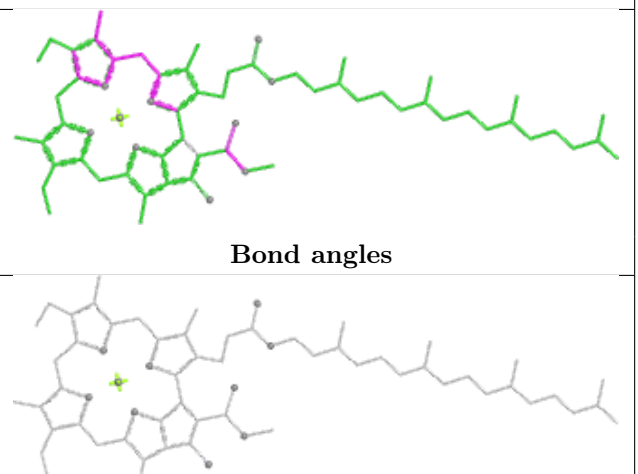


Rings

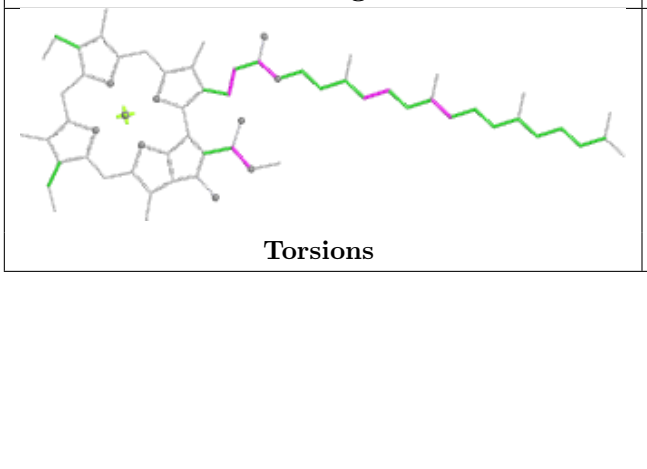
Ligand CLA AB 840



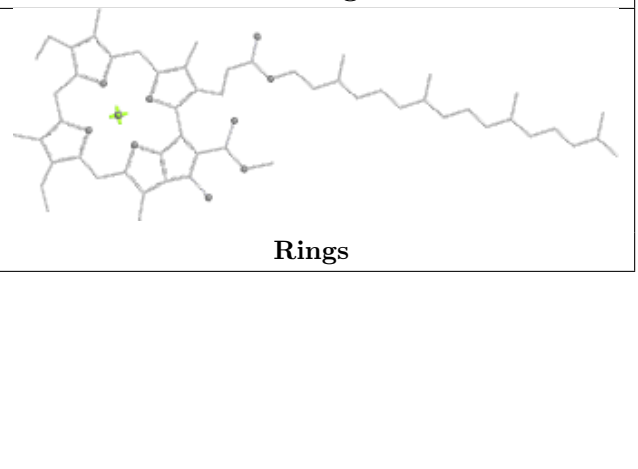
Bond lengths



Bond angles



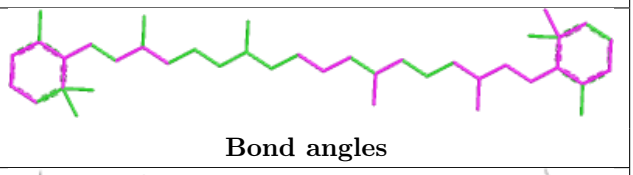
Torsions



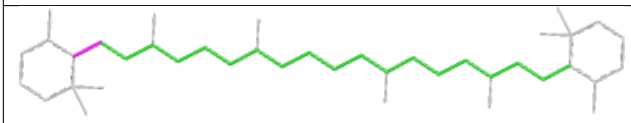
Rings

Ligand BCR A6 617

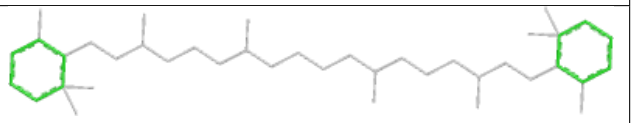
Bond lengths



Bond angles

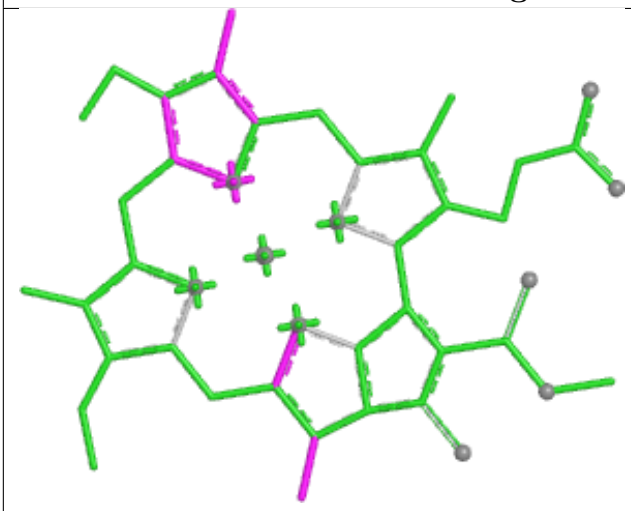


Torsions



Rings

Ligand CLA AA 836



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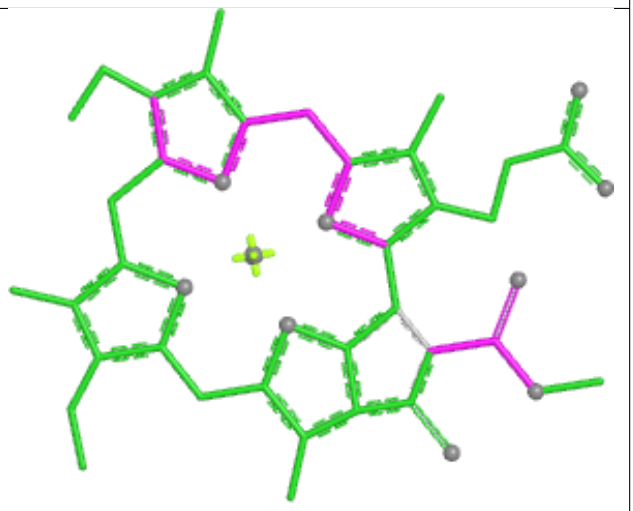
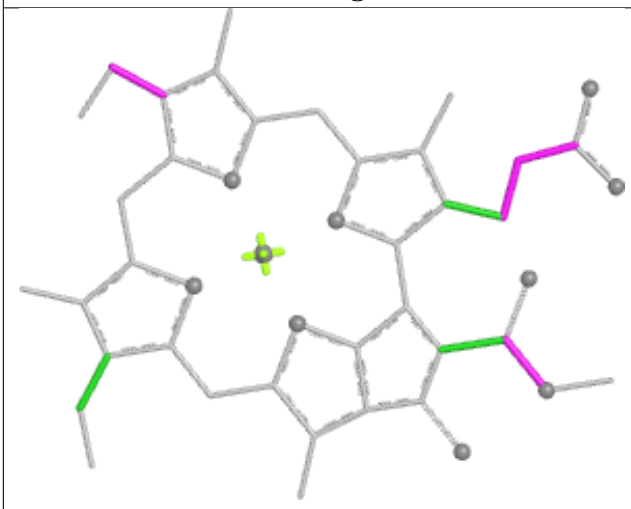


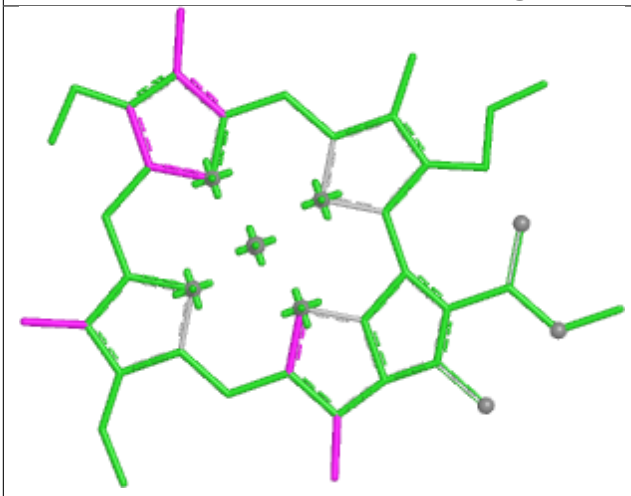
Bond angles



Torsions

Rings

Ligand CLA AB 816



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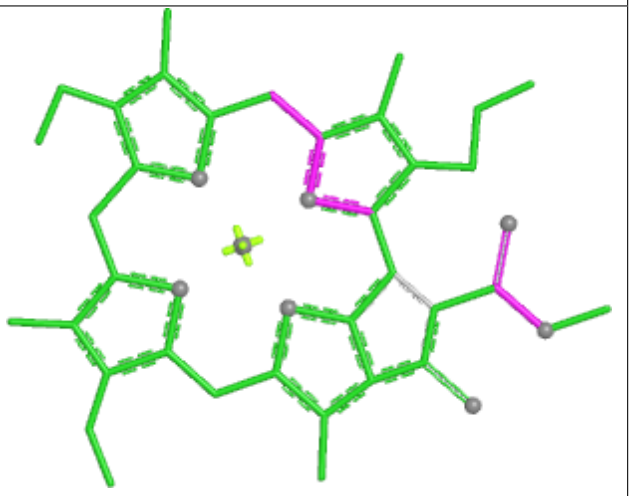
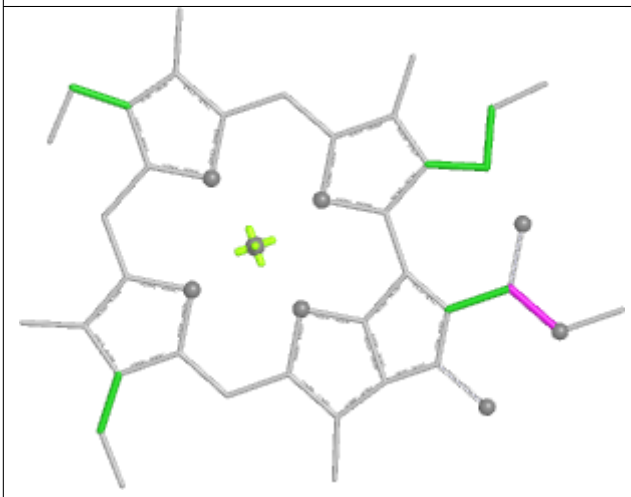


Bond angles



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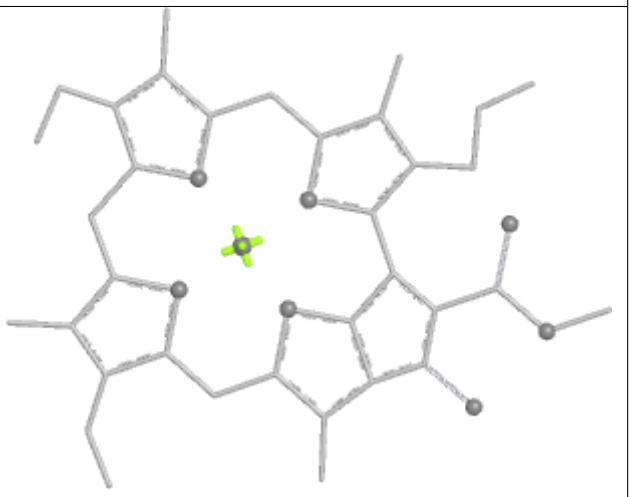
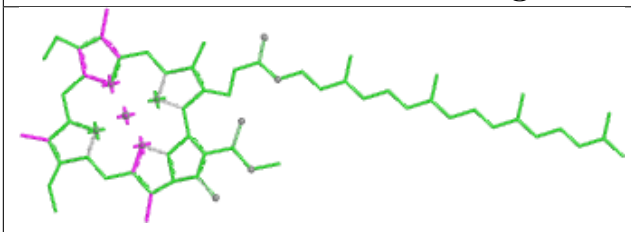
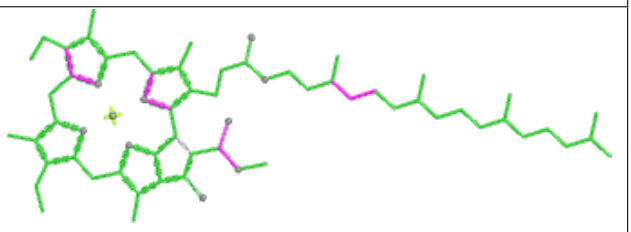


Rings

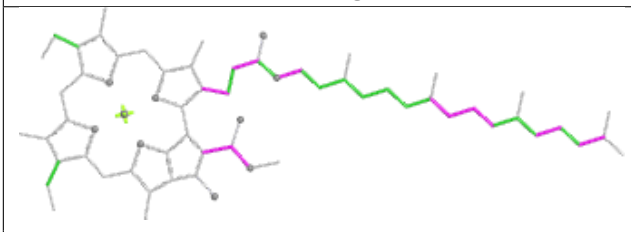
Ligand CLA BA 825



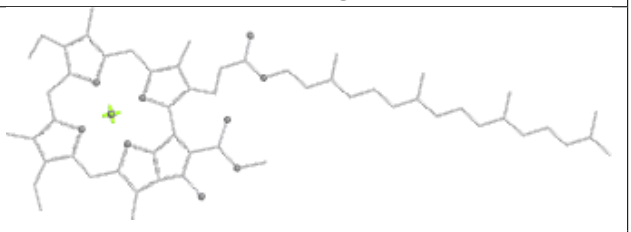
Bond lengths



Bond angles

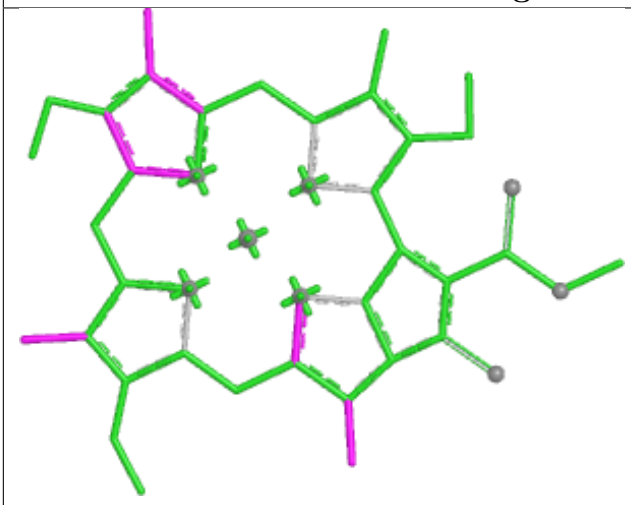


Torsions



Rings

Ligand CLA AL 305



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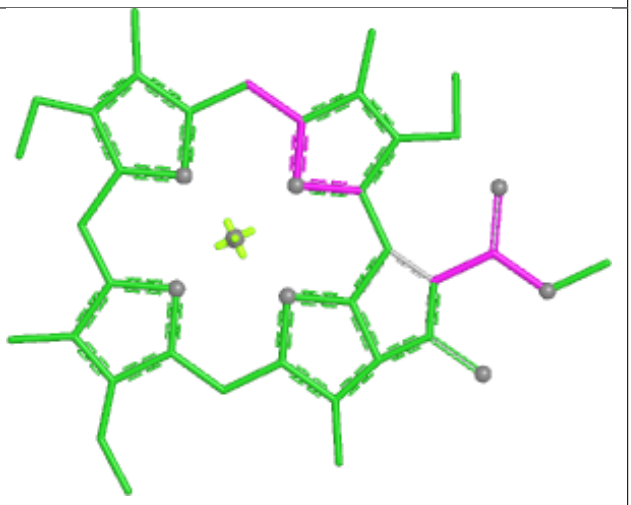
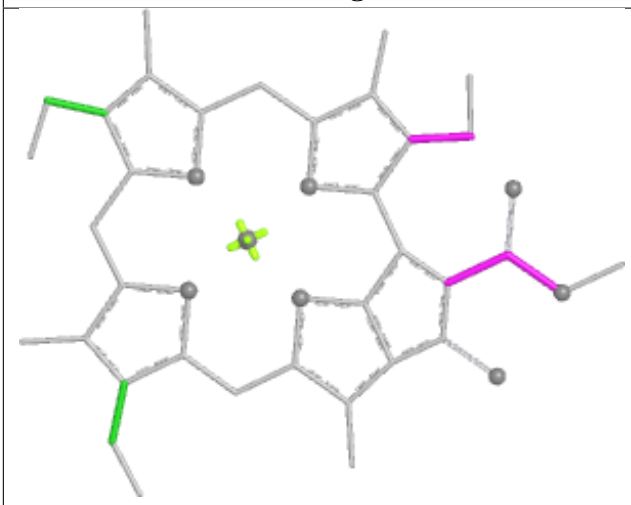


Bond angles

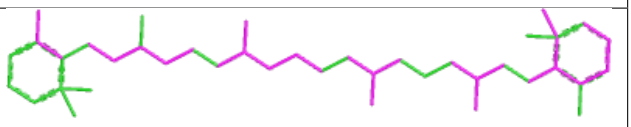


Torsions

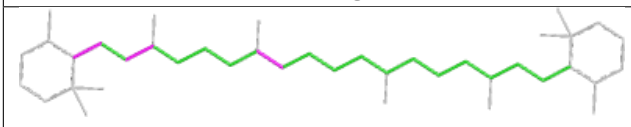
Rings

Ligand BCR AF 805

Bond lengths



Bond angles



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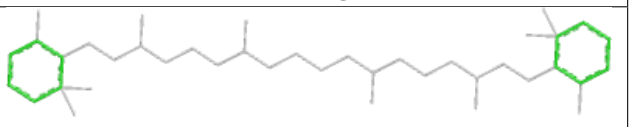
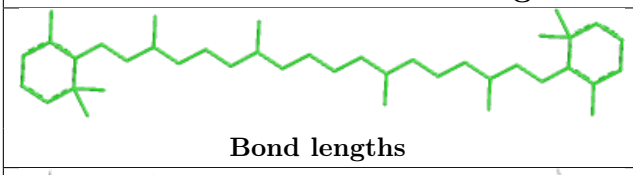


Rings

Ligand BCR B5 616



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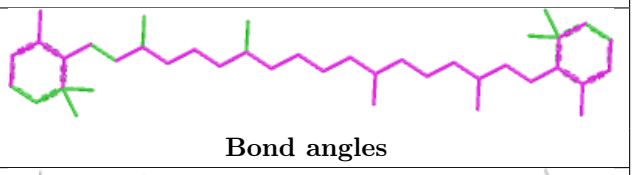
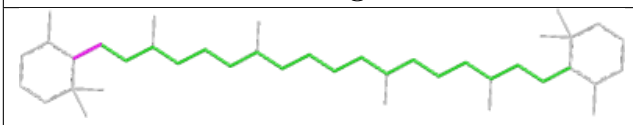


Bond angles



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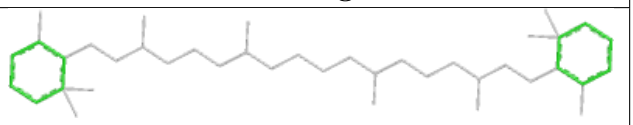
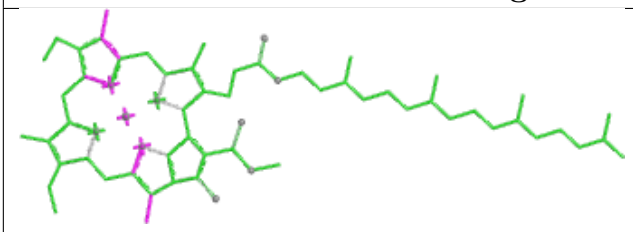


Rings

Ligand CLA AA 829



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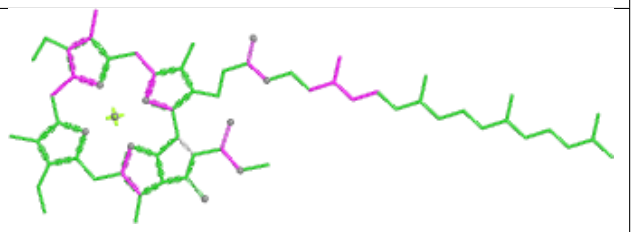
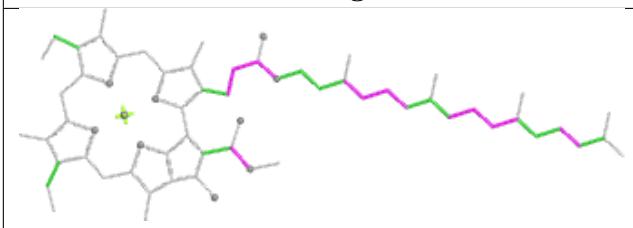
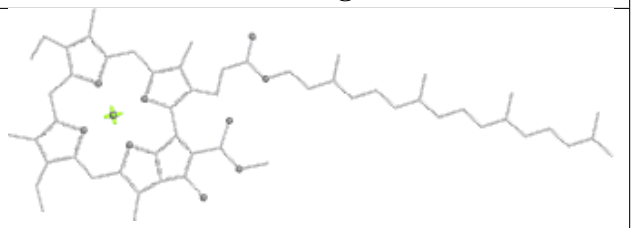


Bond angles

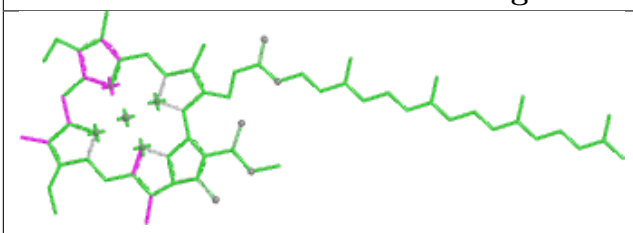


Torsions

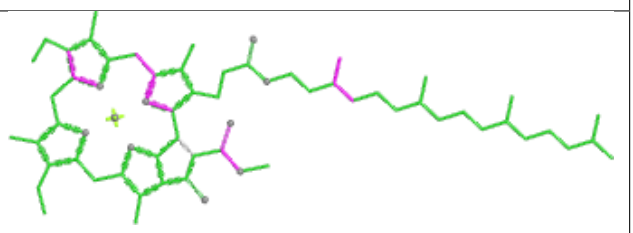


Rings

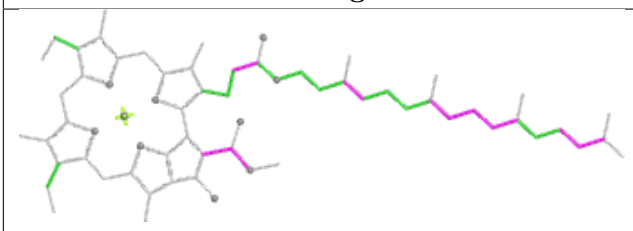
Ligand CLA BA 813



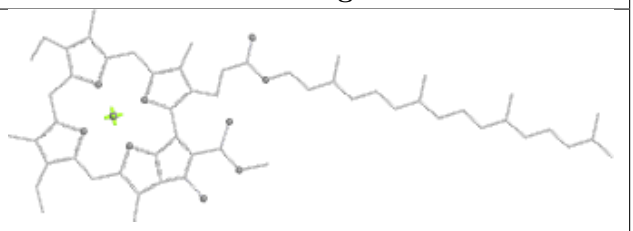
Bond lengths



Bond angles

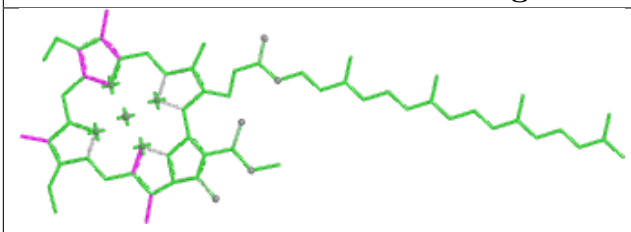


Torsions

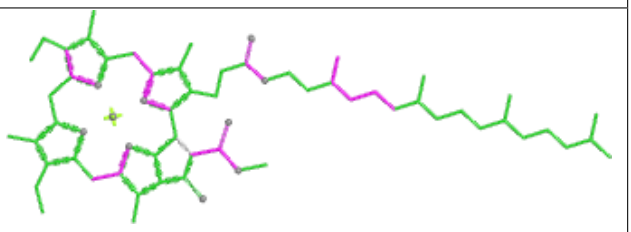


Rings

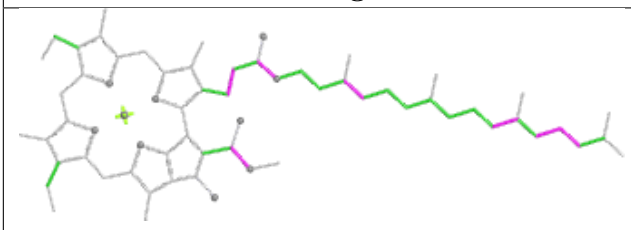
Ligand CLA BA 821



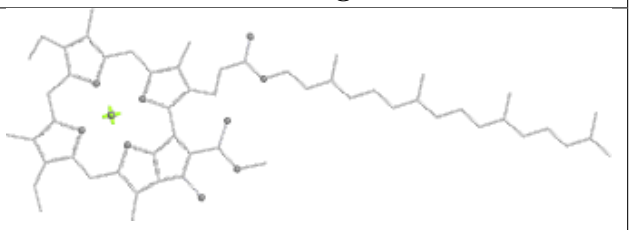
Bond lengths



Bond angles

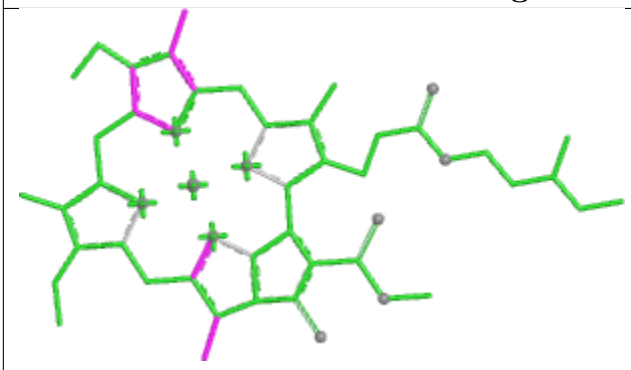


Torsions

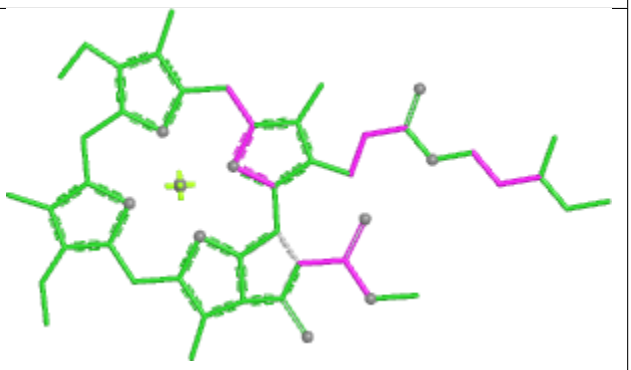


Rings

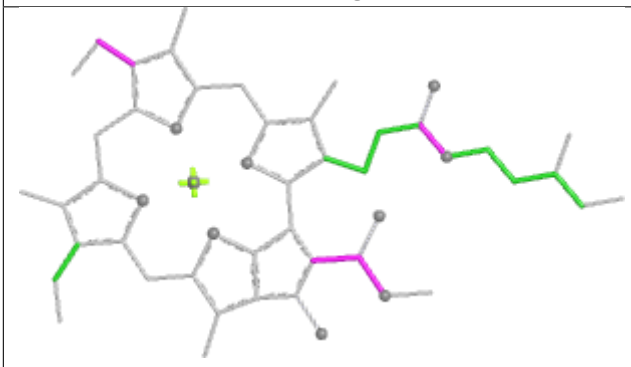
Ligand CLA BA 839



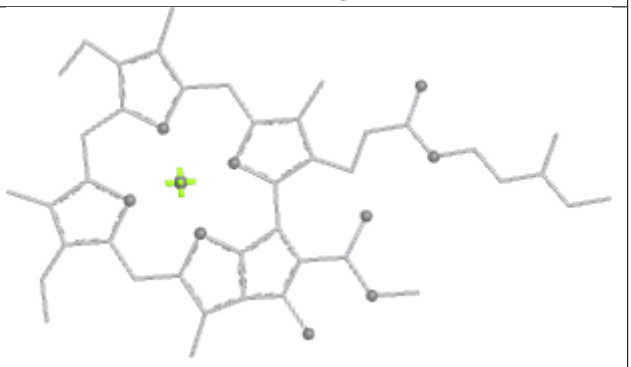
Bond lengths



Bond angles

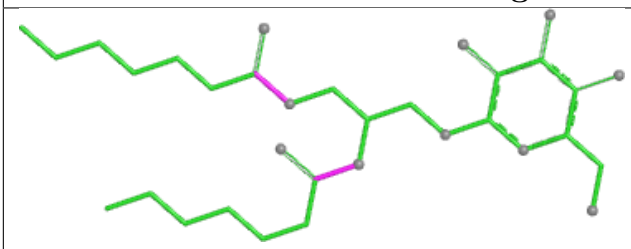


Torsions

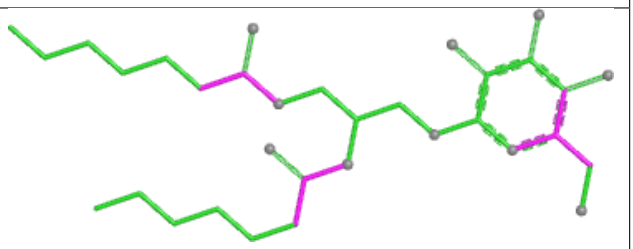


Rings

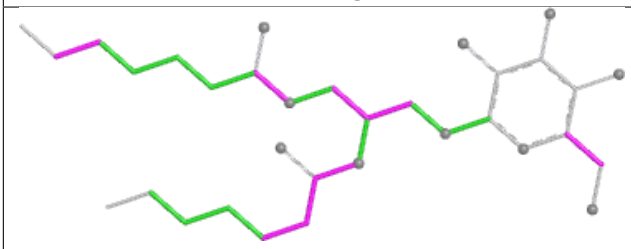
Ligand LMG B5 617



Bond lengths



Bond angles



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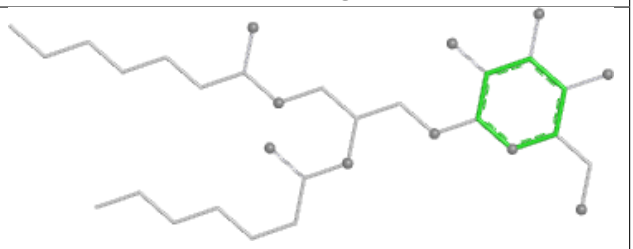
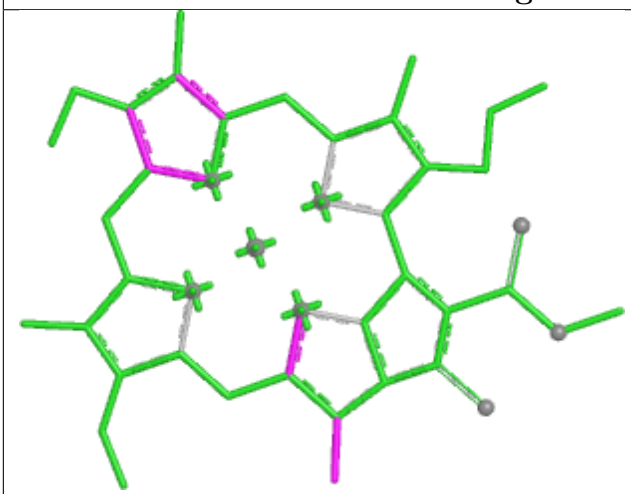


Rings

Ligand CLA B3 310



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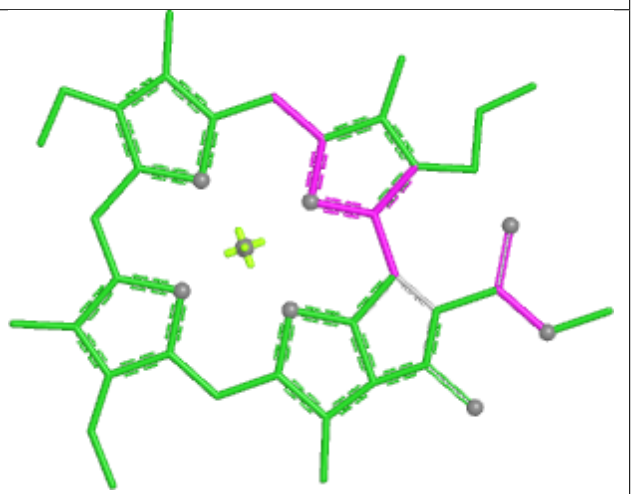
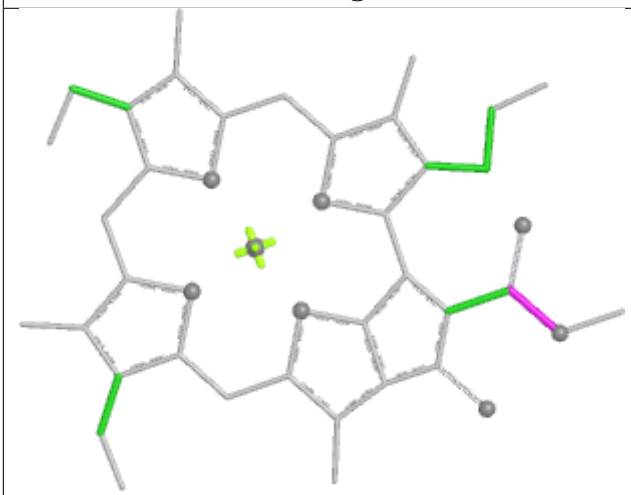


Bond angles



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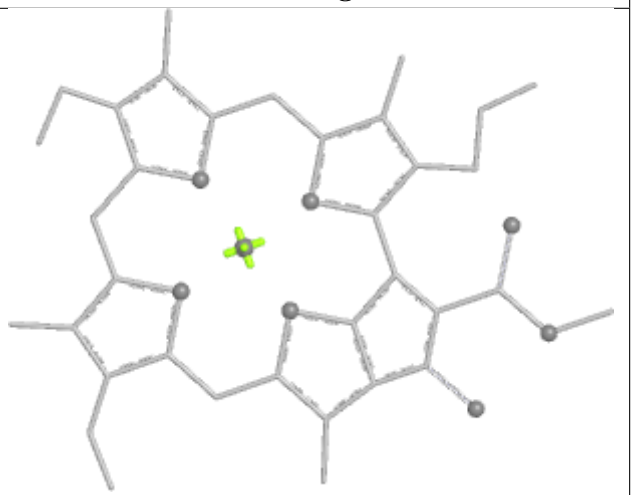
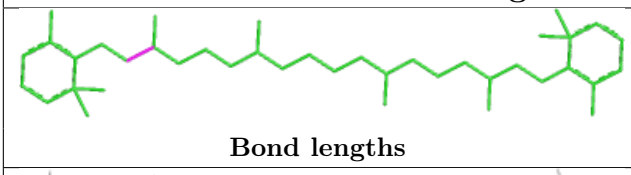


Rings

Ligand BCR AB 845



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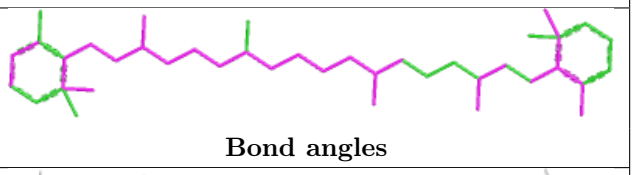
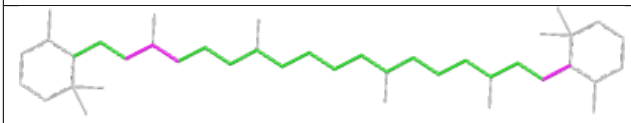


Bond angles



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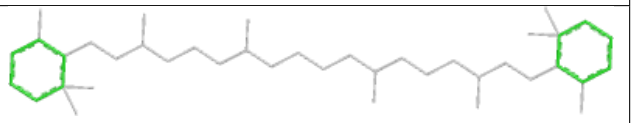
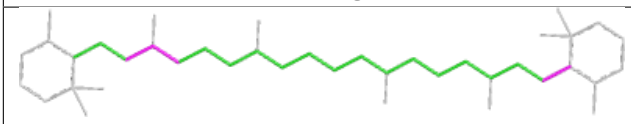


Rings

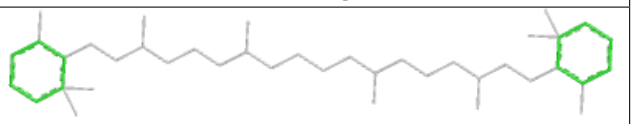
Ligand BCR BB 846

Bond lengths

Bond angles

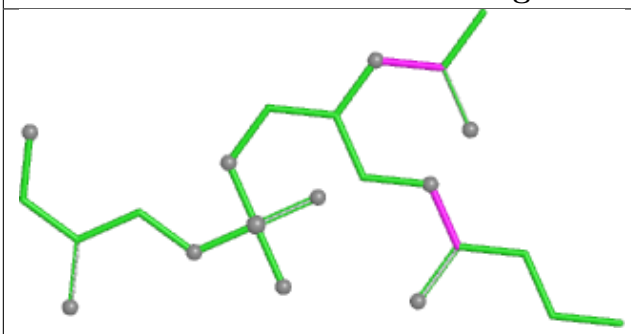


Torsions

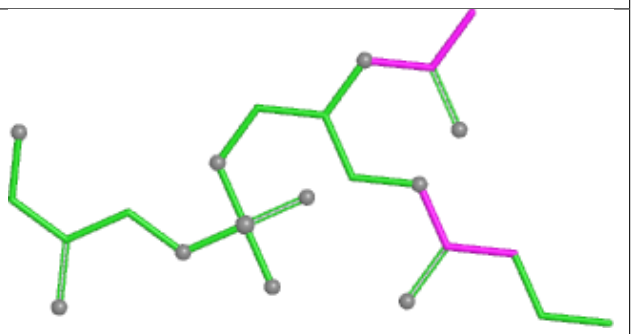


Rings

Ligand LHG A3 319



Bond lengths



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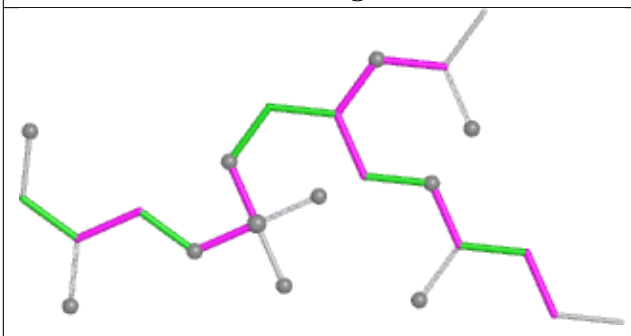

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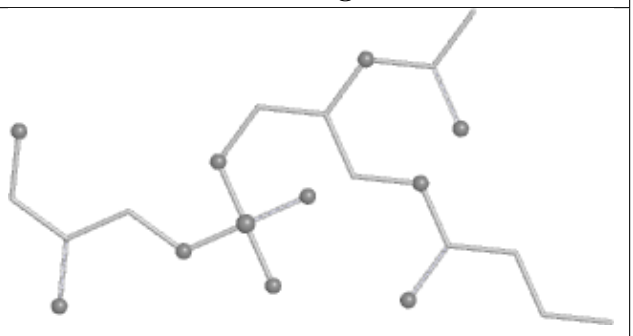
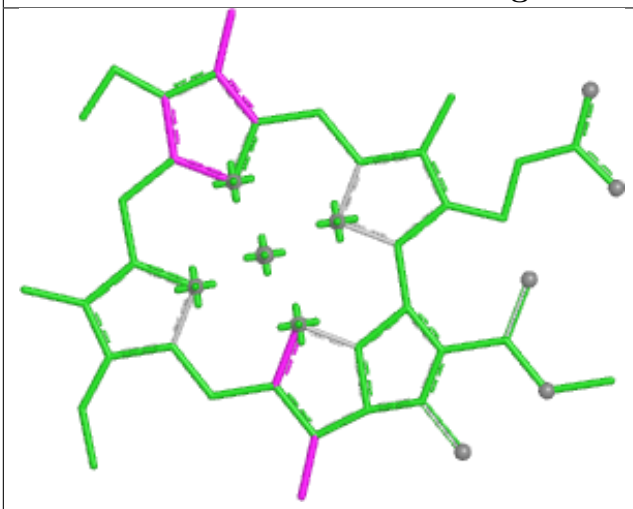


Rings

Ligand CLA BA 835



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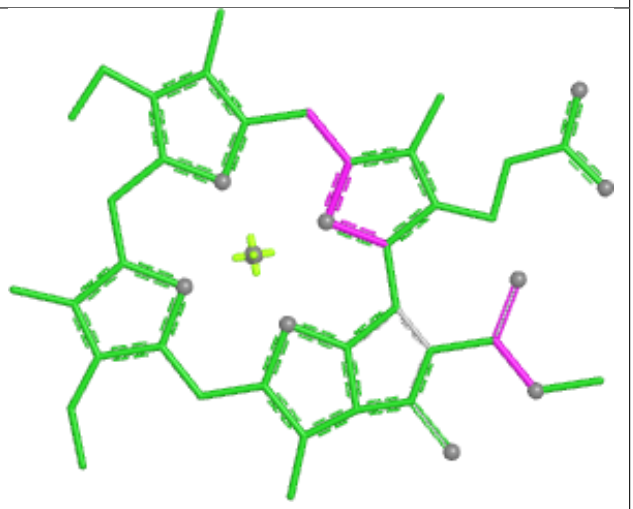
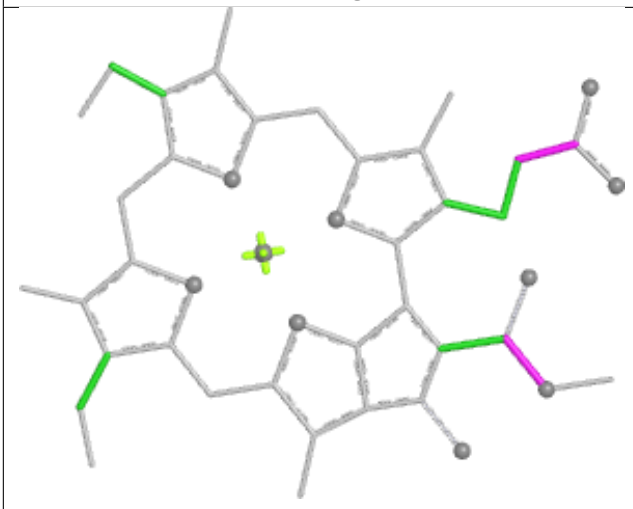


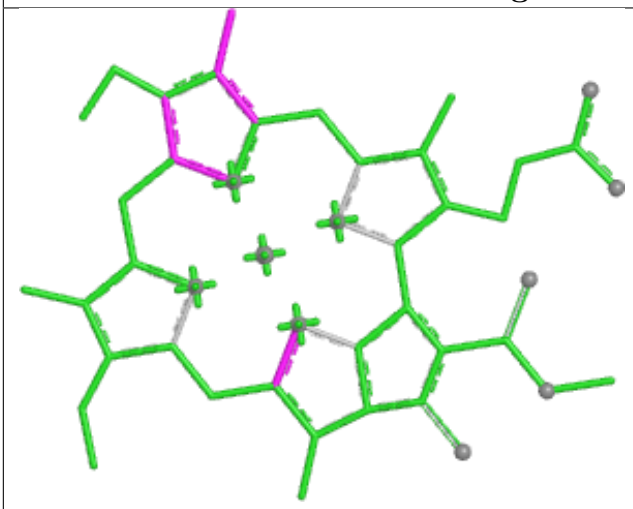
Bond angles



Torsions

Rings

Ligand CLA BA 836



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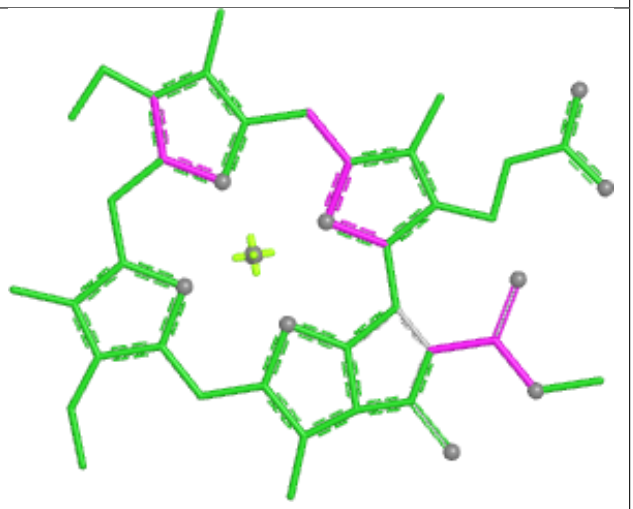
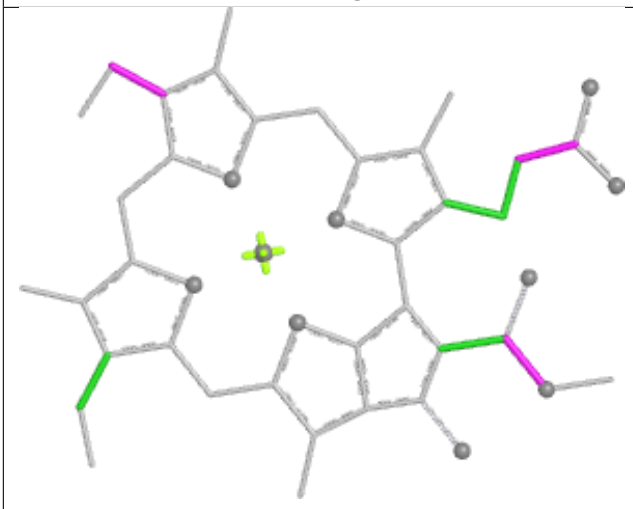


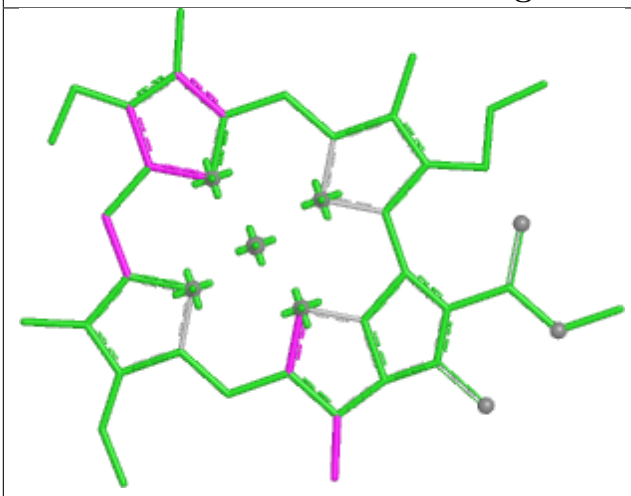
Bond angles



Torsions

Rings

Ligand CLA A6 614



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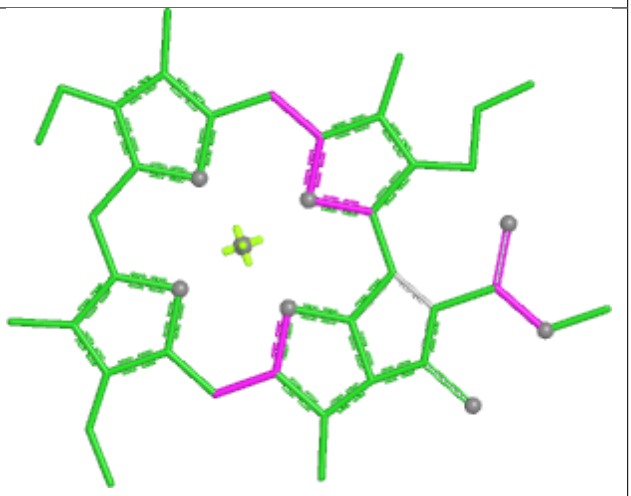
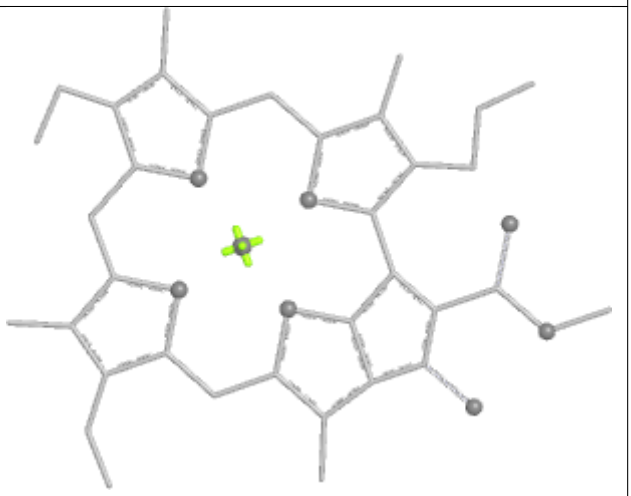


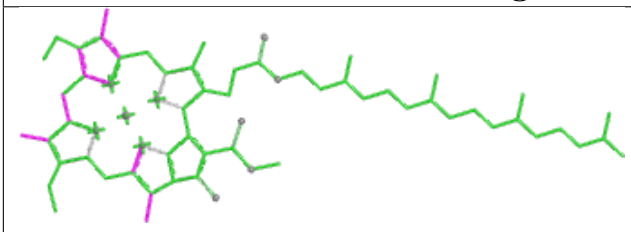
Bond angles

Torsions



Rings

Ligand CLA AB 828



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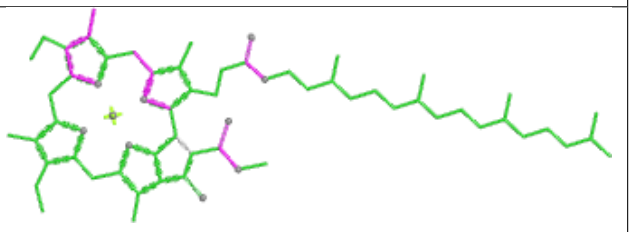
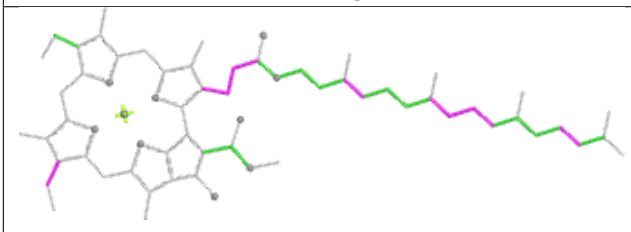
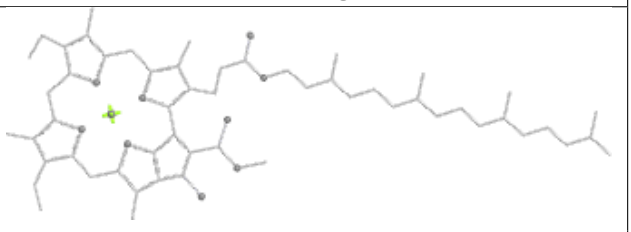


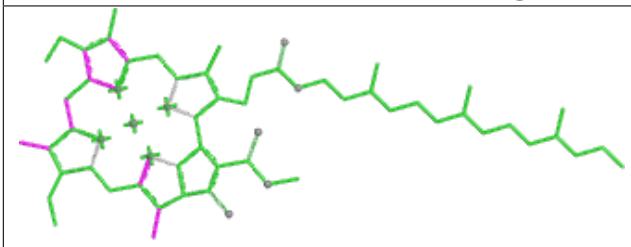
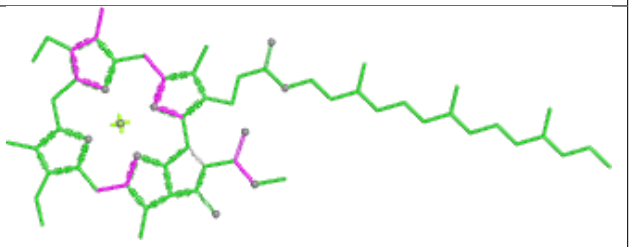
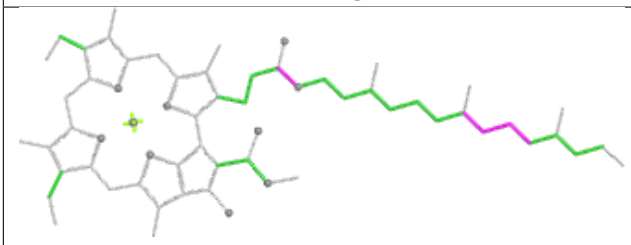
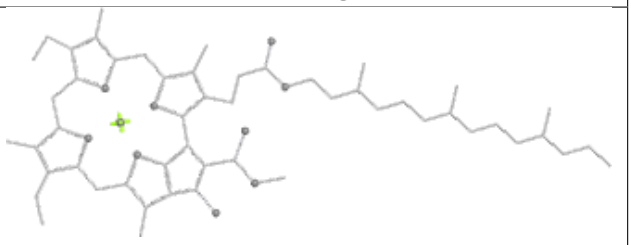
Bond angles

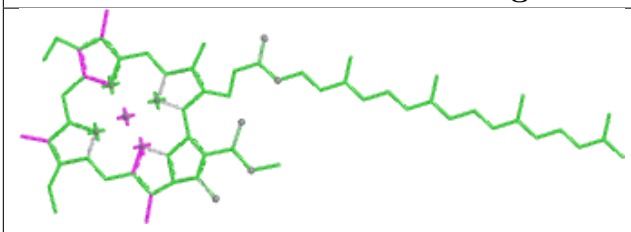
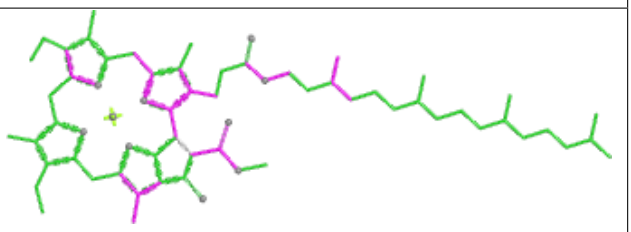
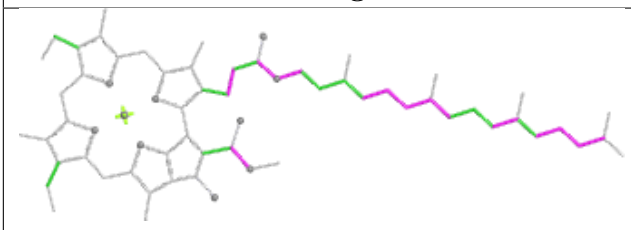
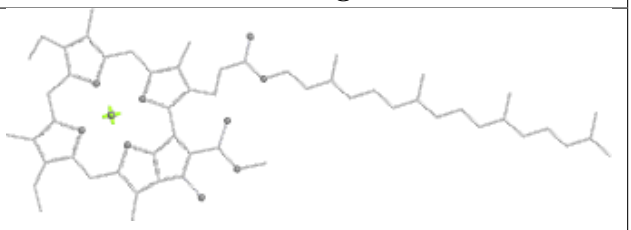


Torsions

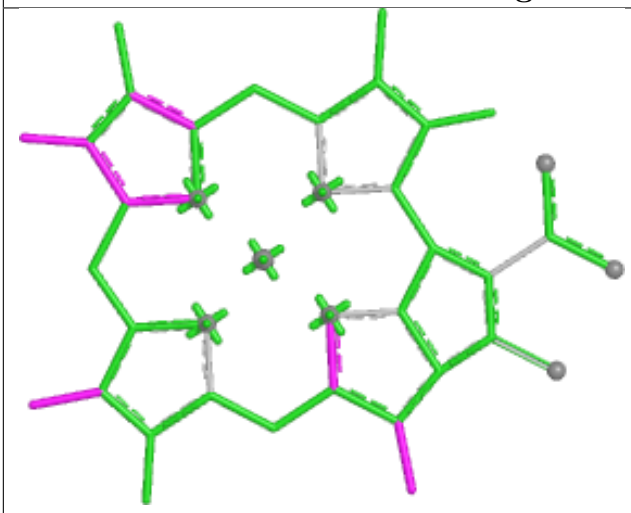


Rings

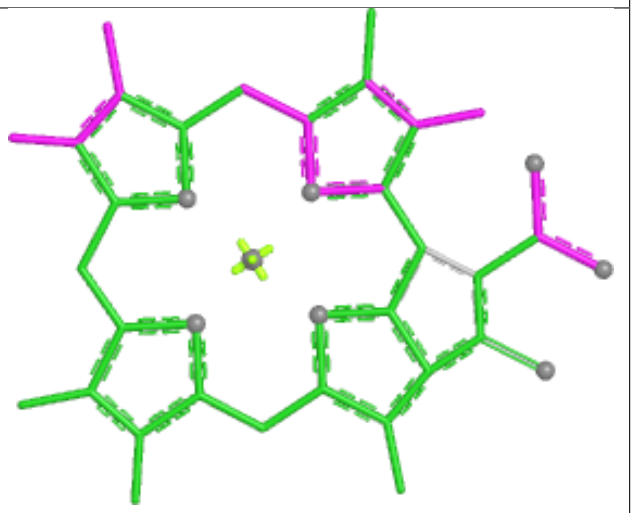
Ligand CLA AB 826	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AB 801	
	
Bond lengths	Bond angles
	
Torsions	Rings

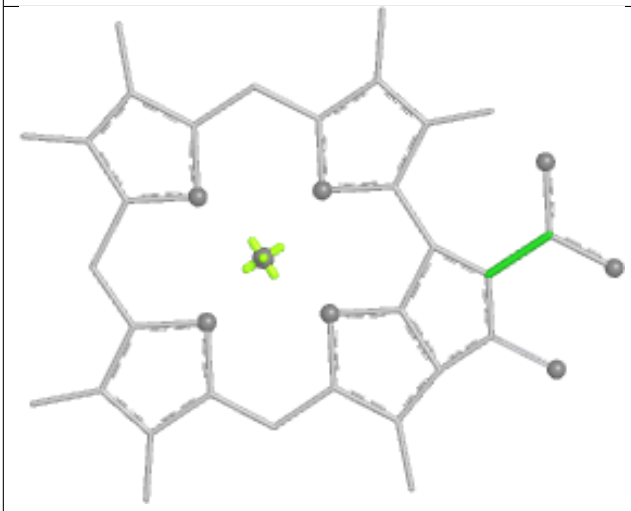
Ligand CLA B1 312



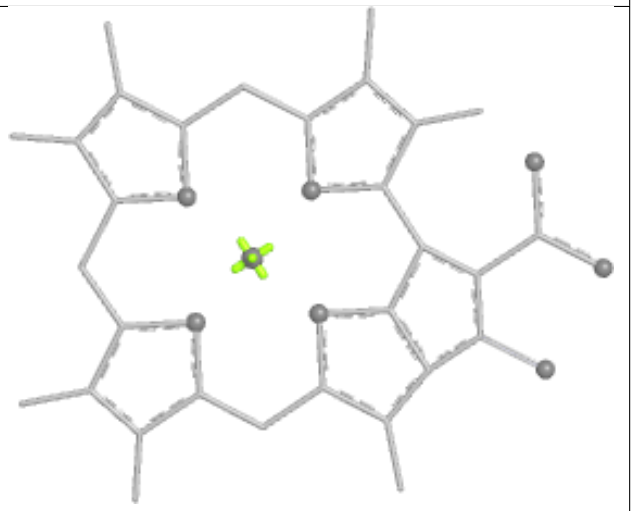
Bond lengths



Bond angles

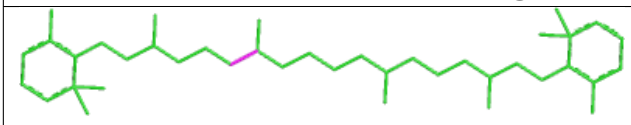


Torsions



Rings

Ligand BCR AL 306



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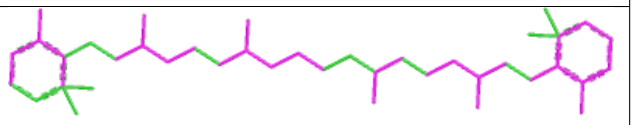
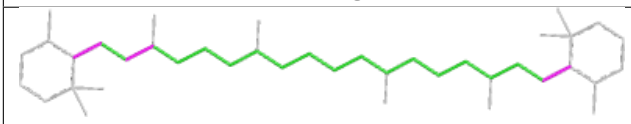
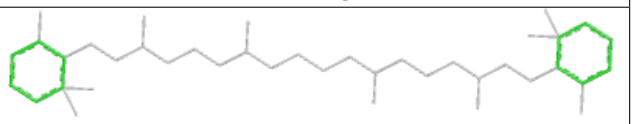


Bond angles

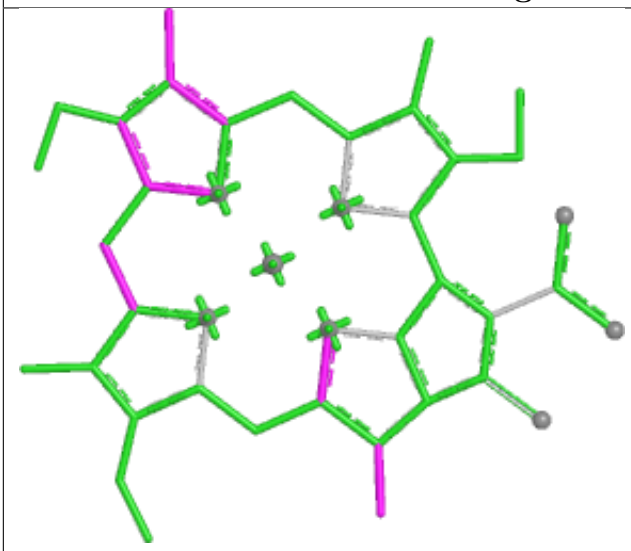


Torsions

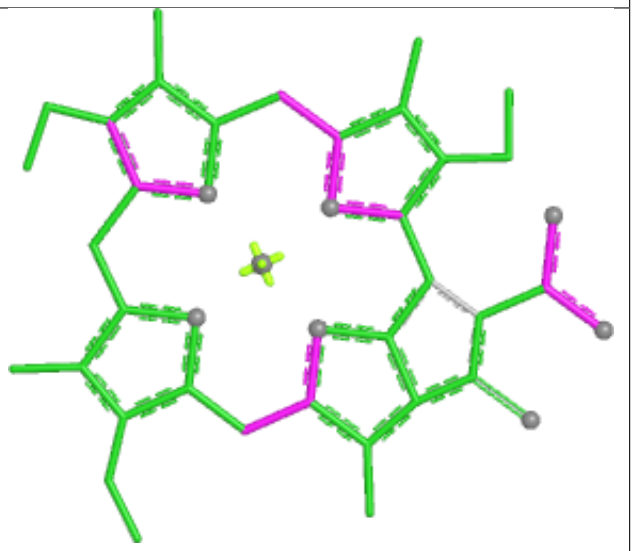


Rings

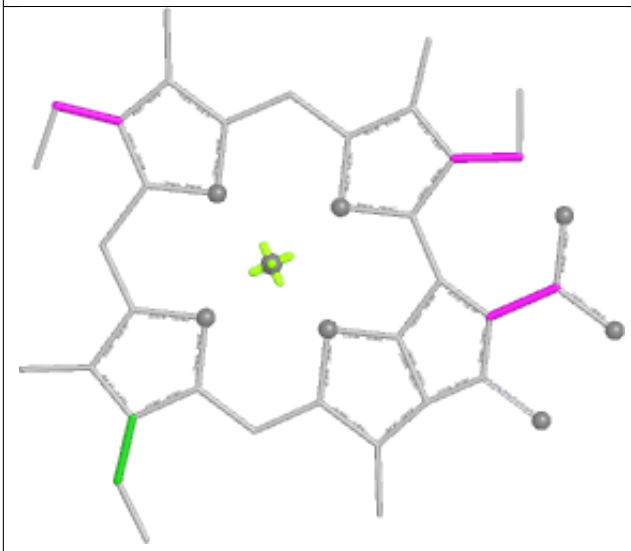
Ligand CLA A3 305



Bond lengths



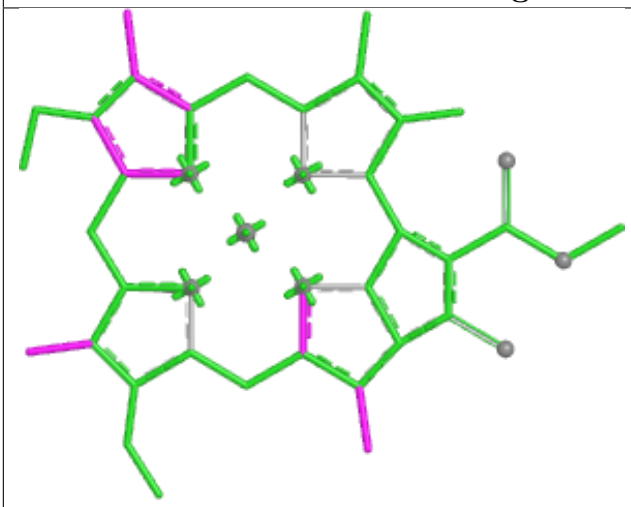
Bond angles



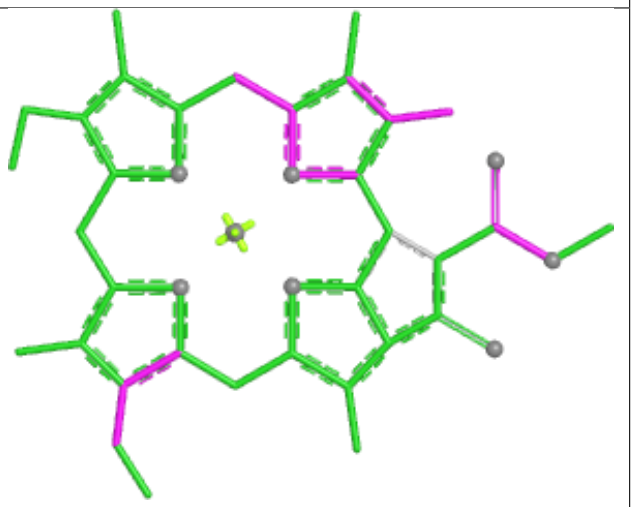
Torsions

Rings

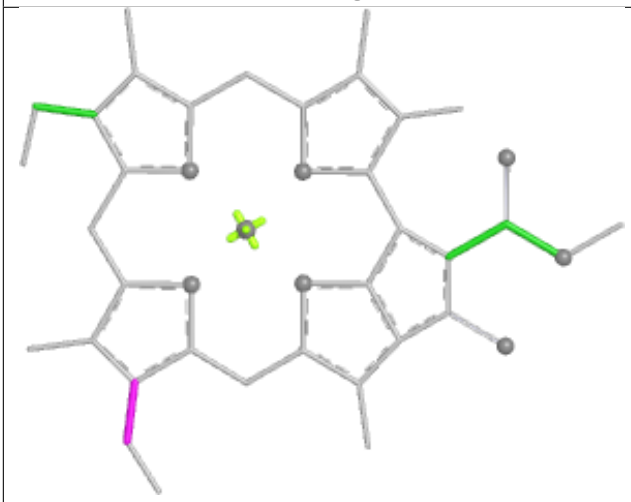
Ligand CLA BB 806



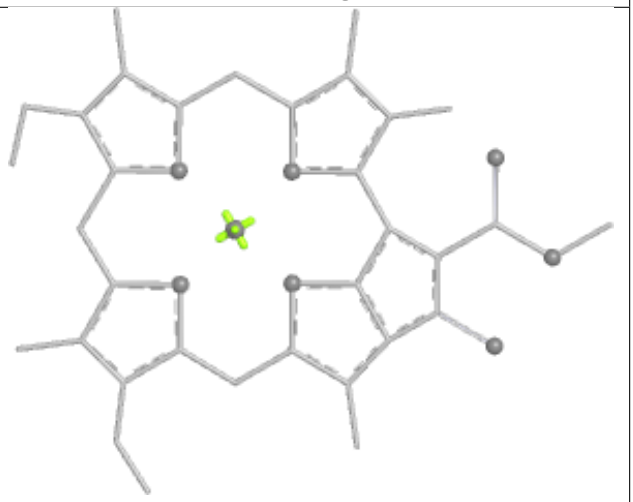
Bond lengths



Bond angles

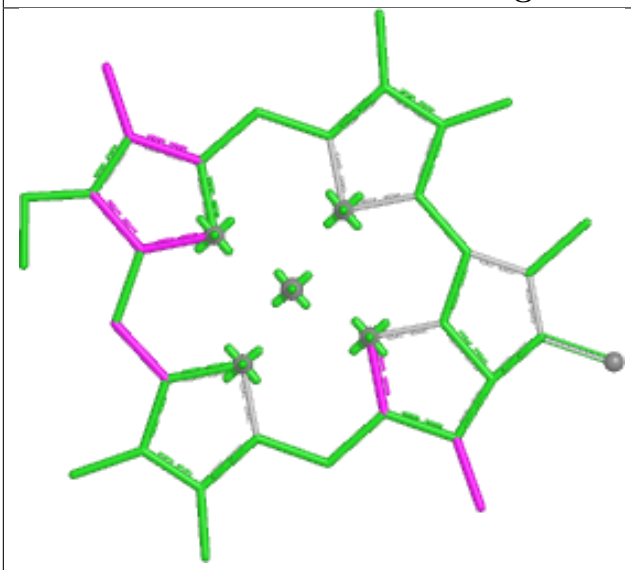


Torsions

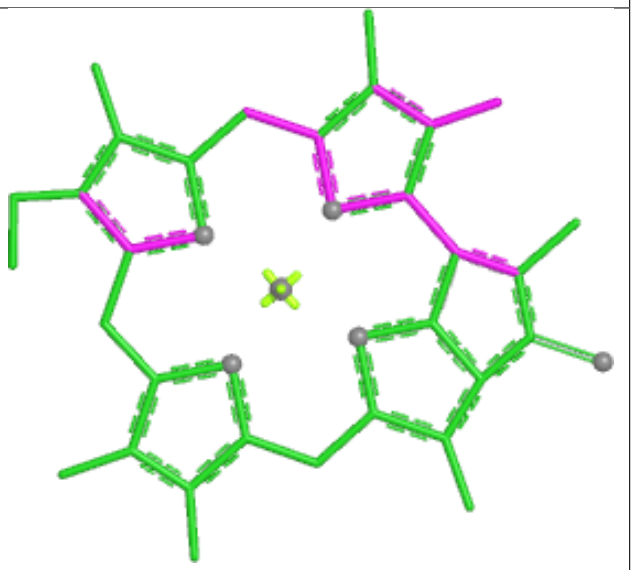


Rings

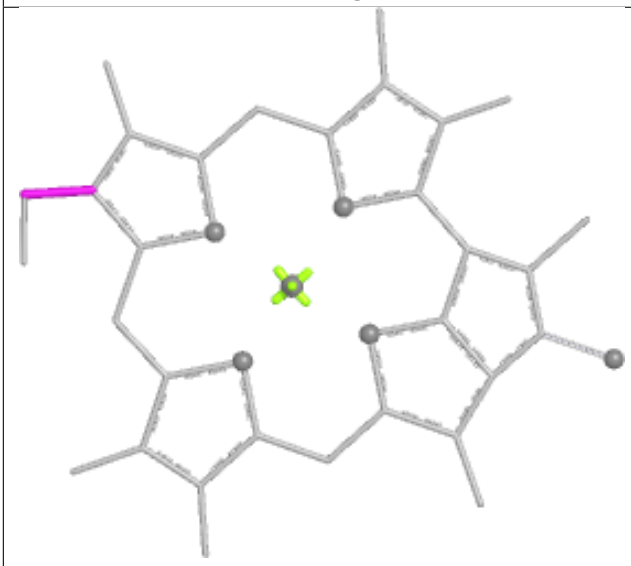
Ligand CLA A3 310



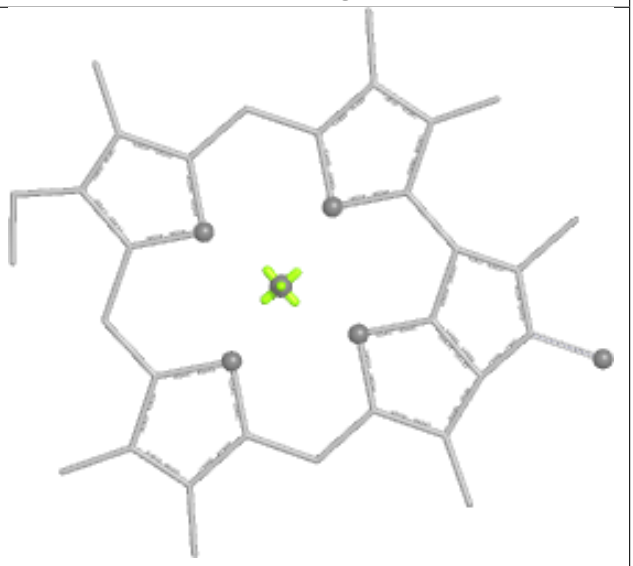
Bond lengths



Bond angles

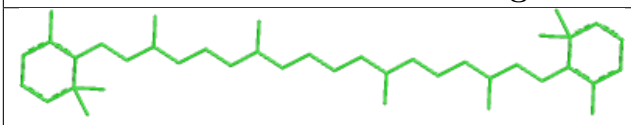


Torsions



Rings

Ligand BCR BB 803



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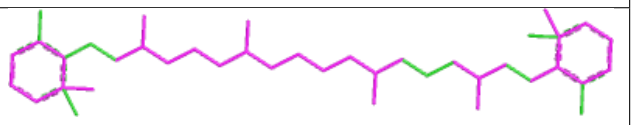
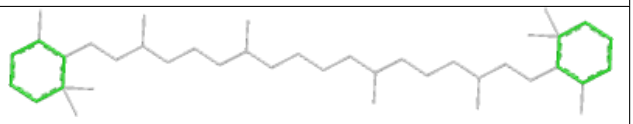


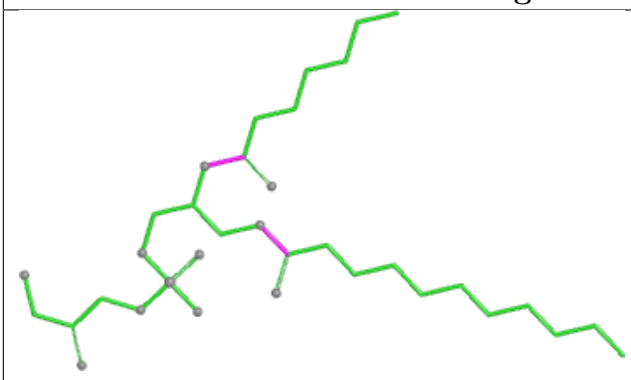
Bond angles

Torsions



Rings

Ligand LHG B2 618



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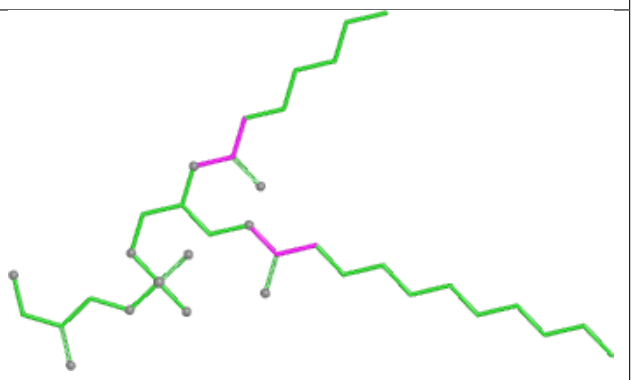
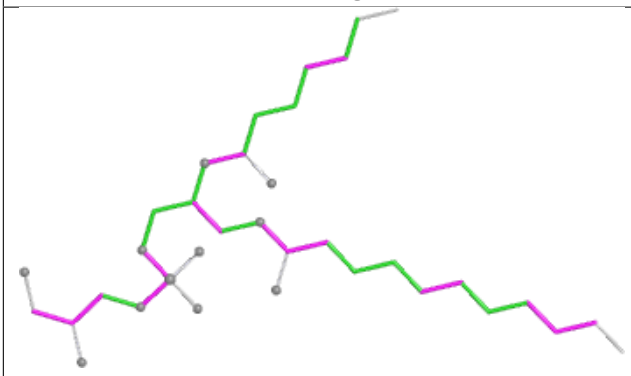
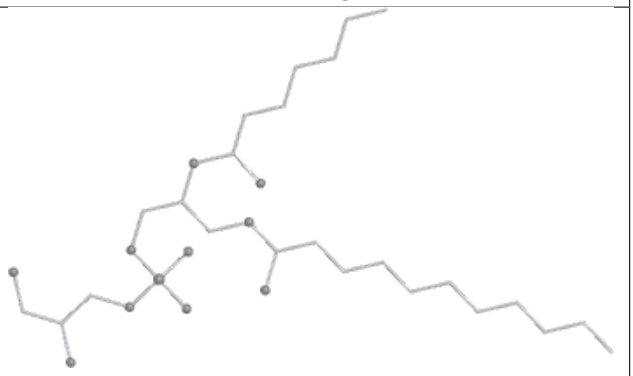


Bond angles

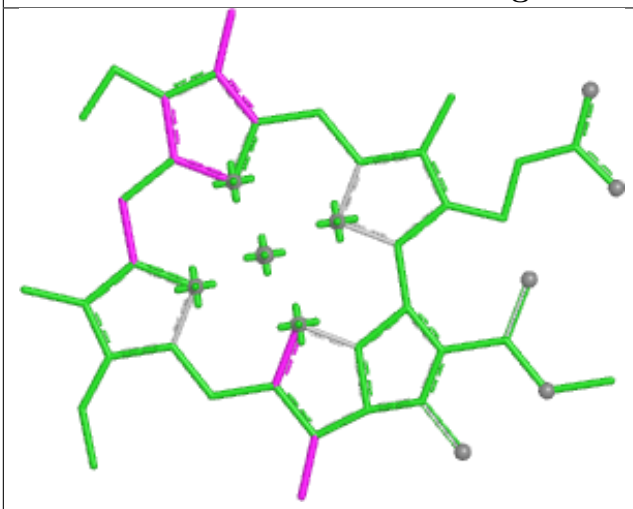


Torsions



Rings

Ligand CLA BB 825



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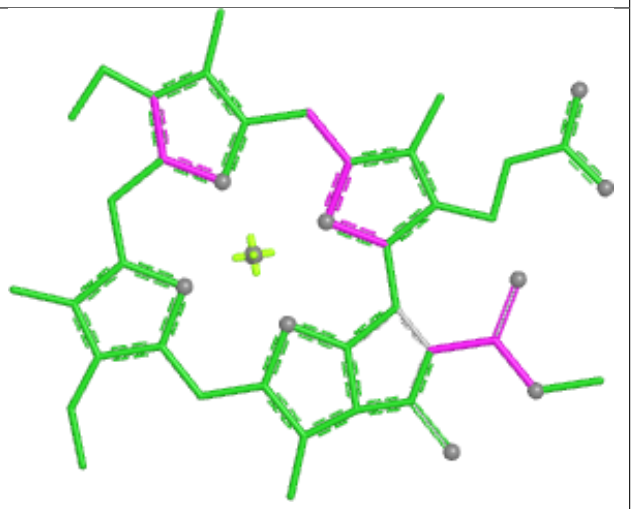
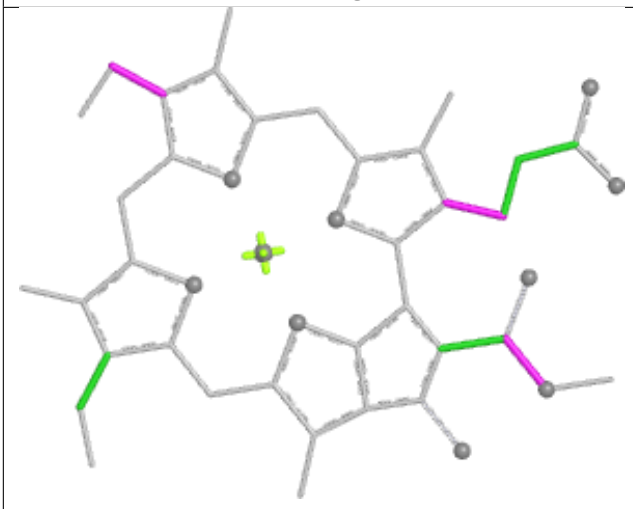


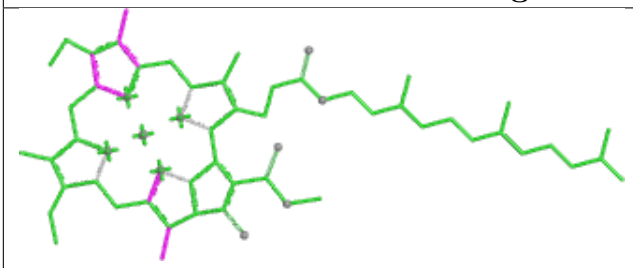
Bond angles



Torsions

Rings

Ligand CLA AB 835



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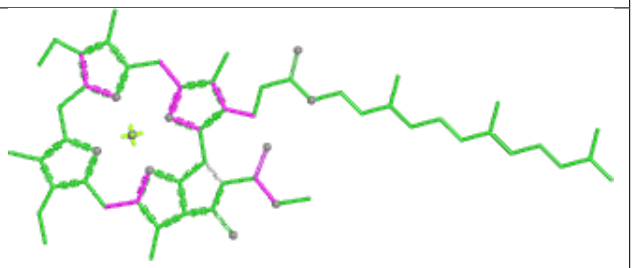
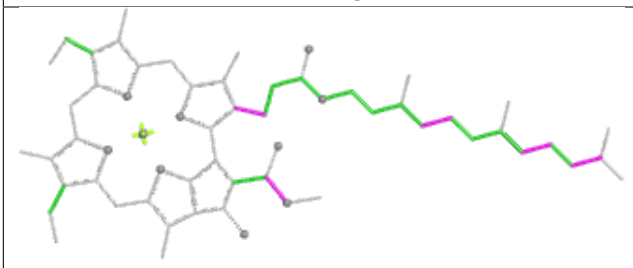


Bond angles



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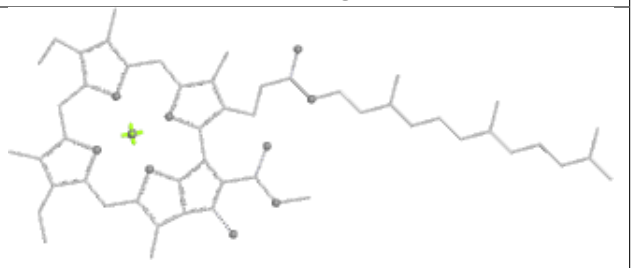
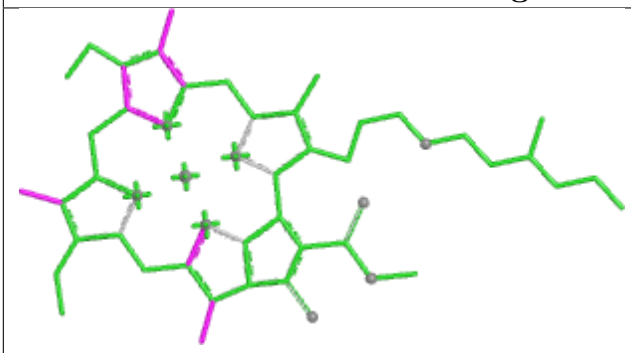


Rings

Ligand CLA AB 808



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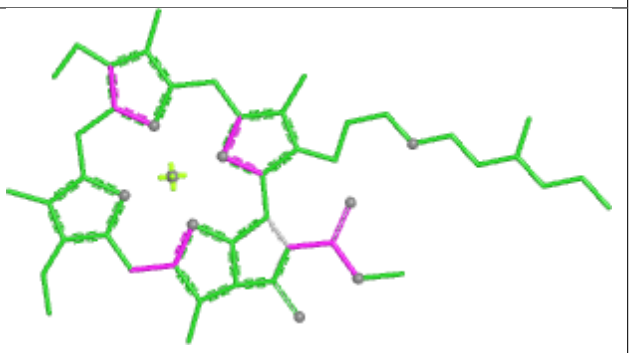
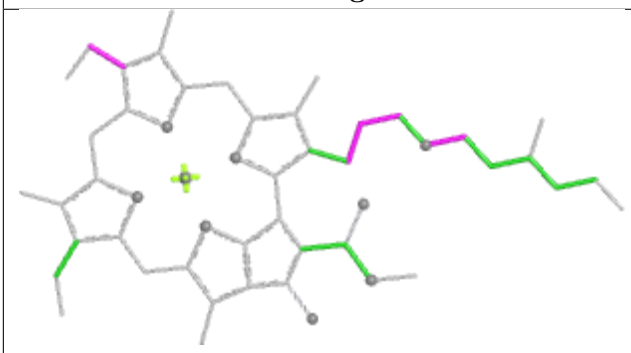


Bond angles



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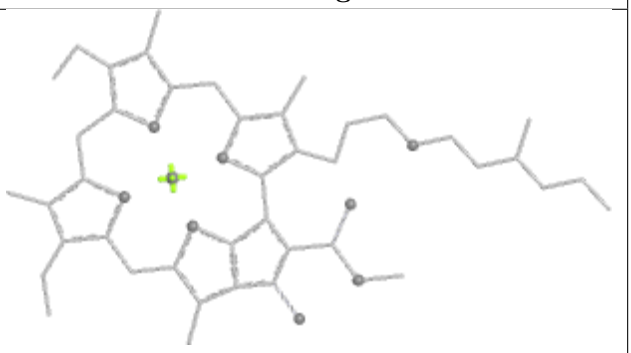
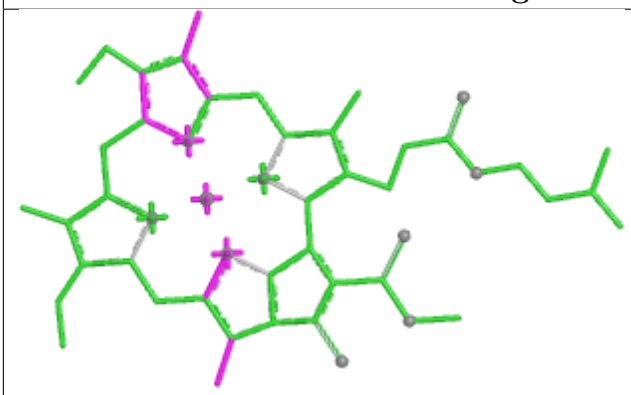
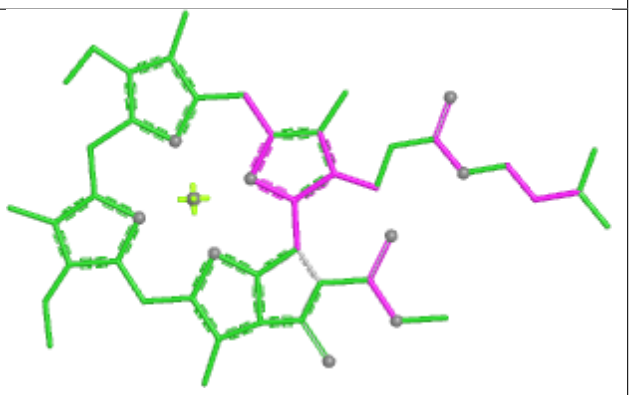


Rings

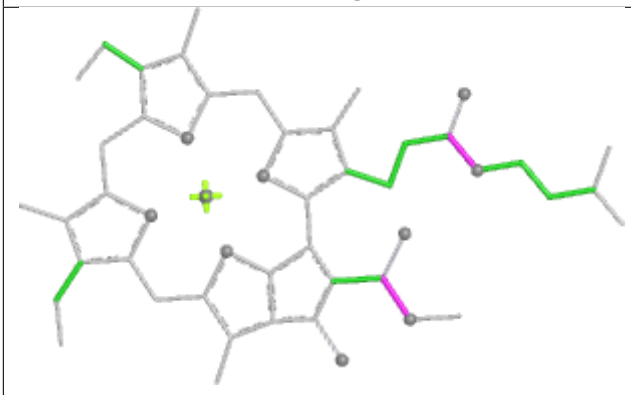
Ligand CLA BB 838



Bond lengths



Bond angles



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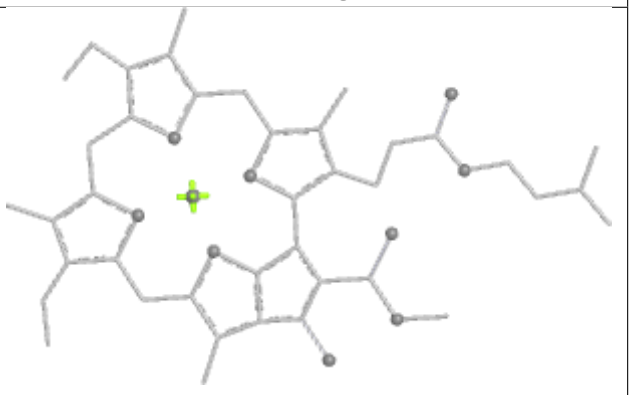
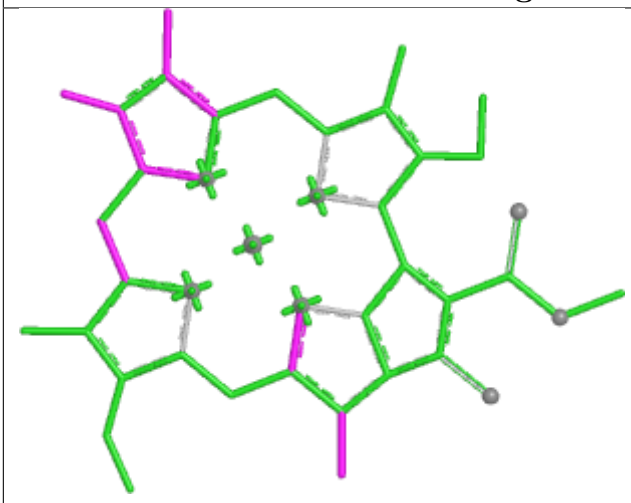


Rings

Ligand CLA B3 305



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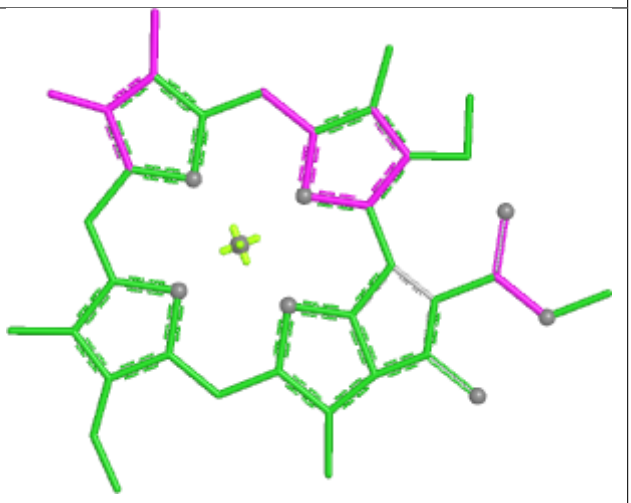
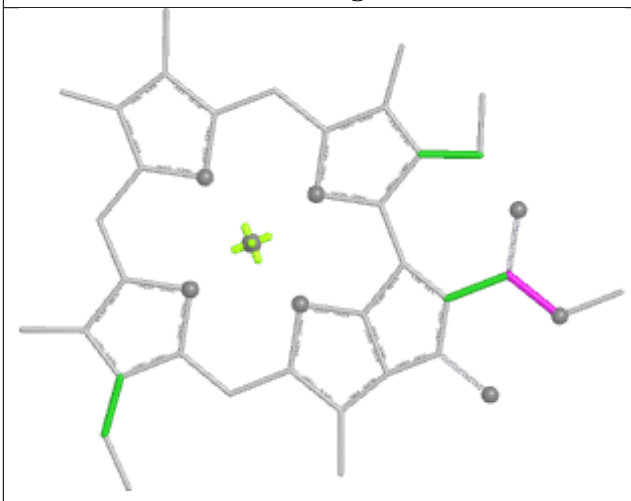
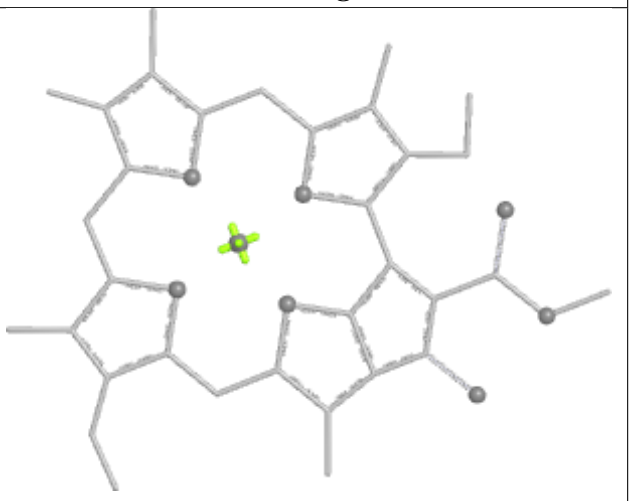


Bond angles

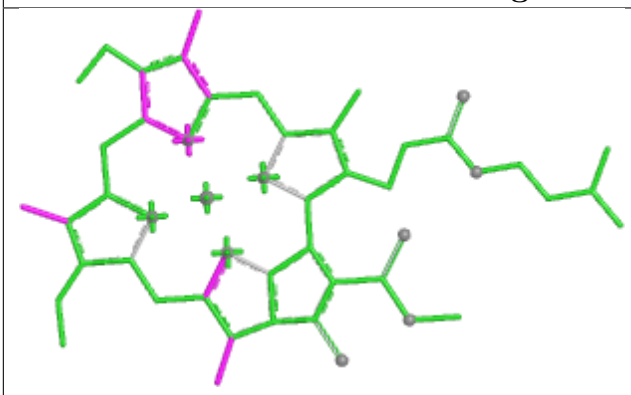


Torsions



Rings

Ligand CLA AB 821



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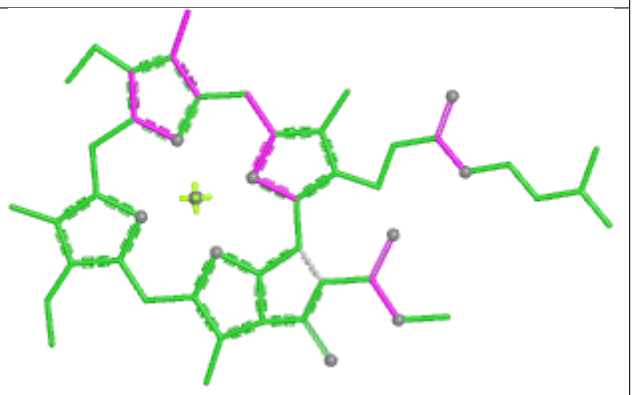
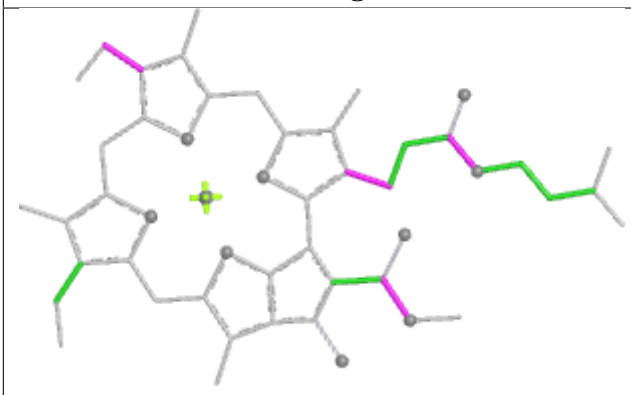


Bond angles



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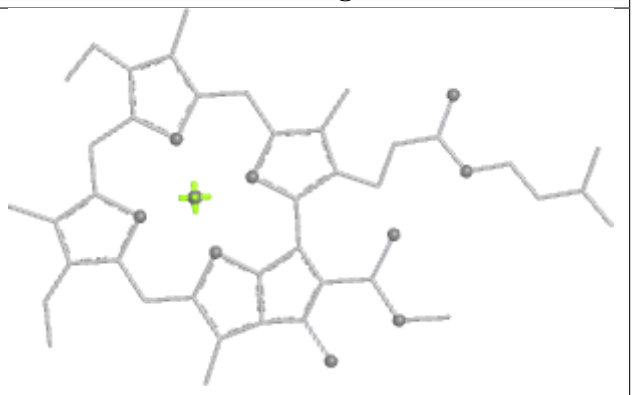
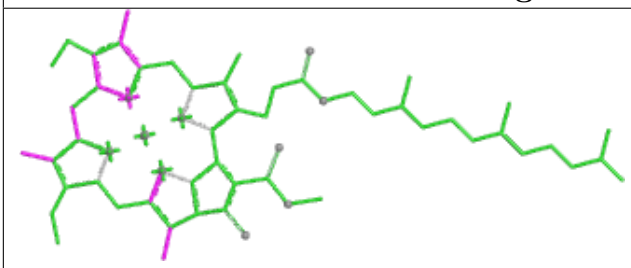


Rings

Ligand CLA B5 602



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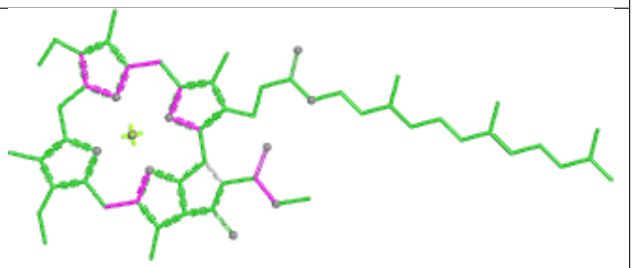
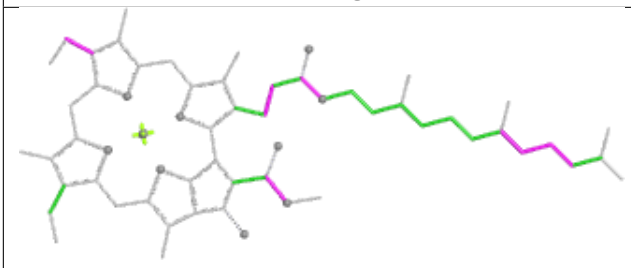


Bond angles



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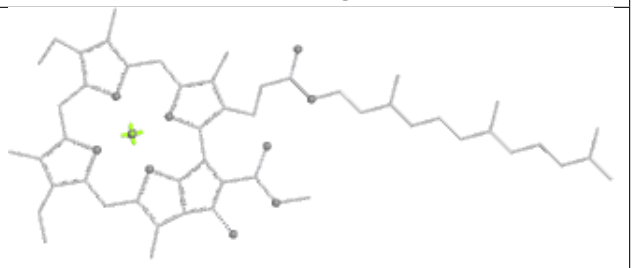
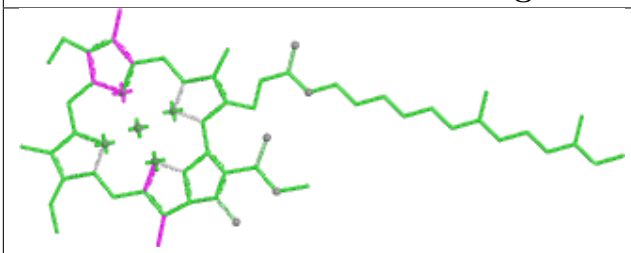


Rings

Ligand CLA A1 304



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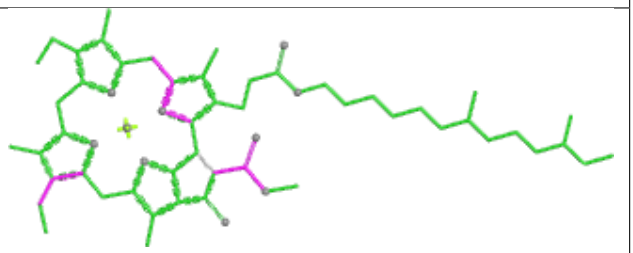

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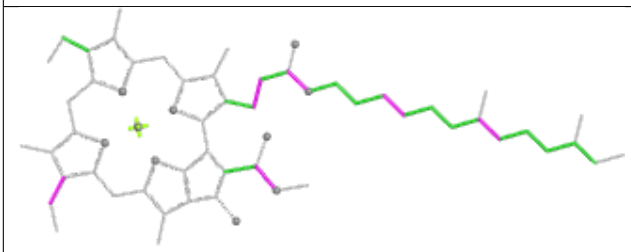

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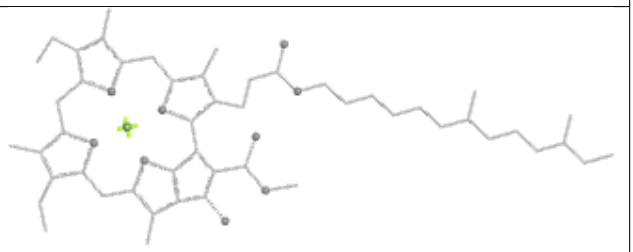
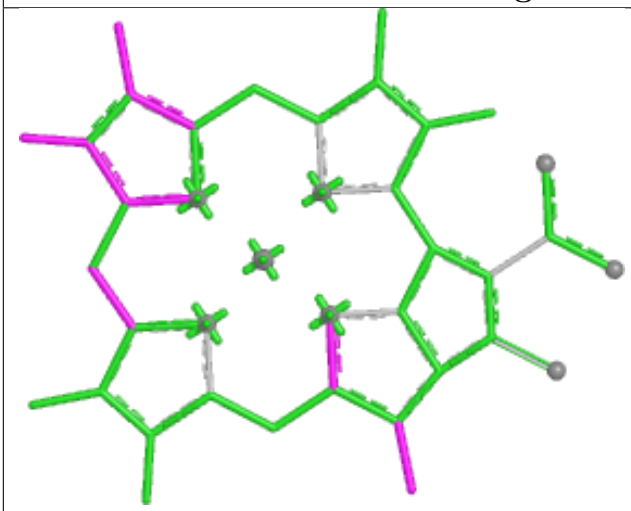


Rings

Ligand CLA A1 312



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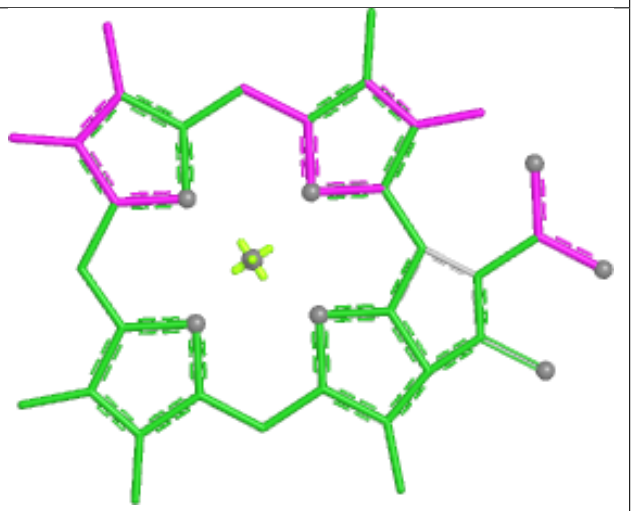
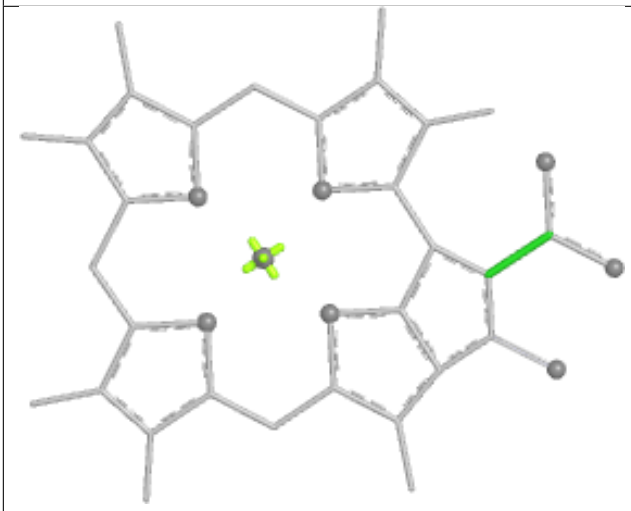
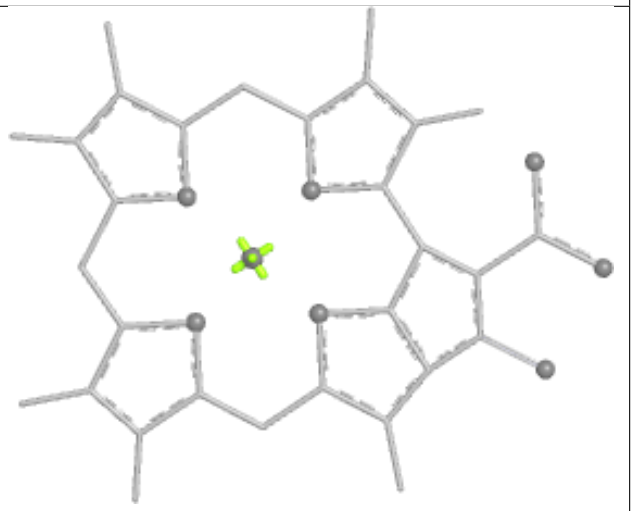


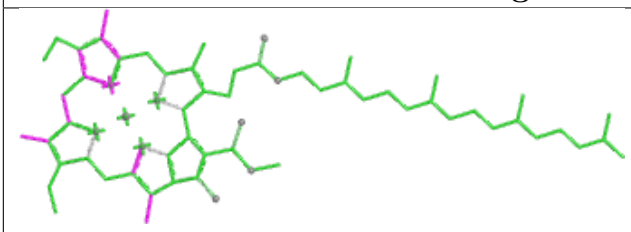
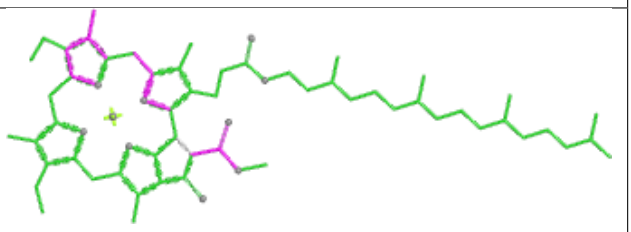
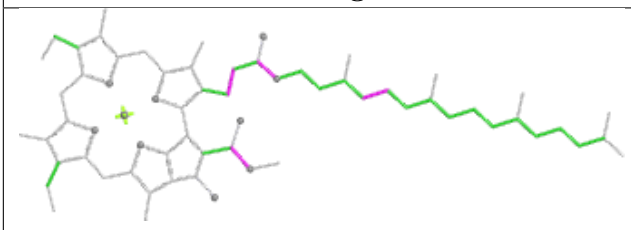
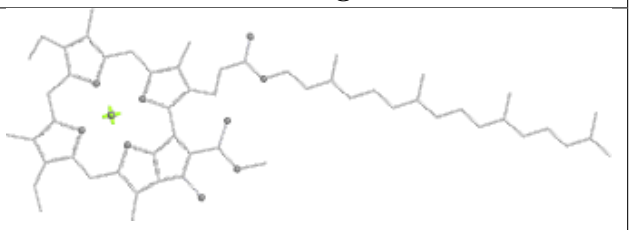
Bond angles

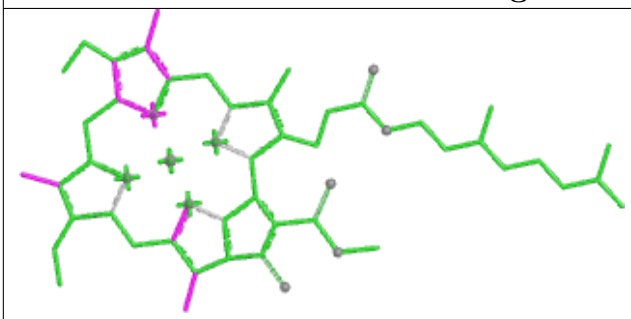
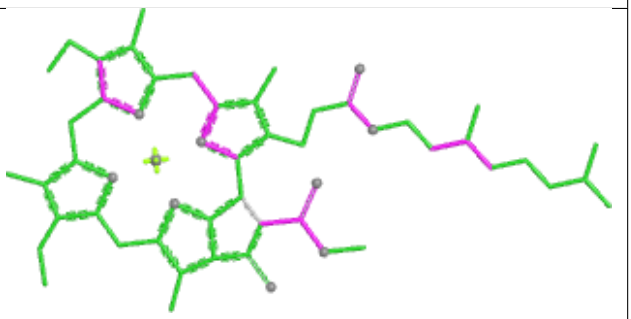
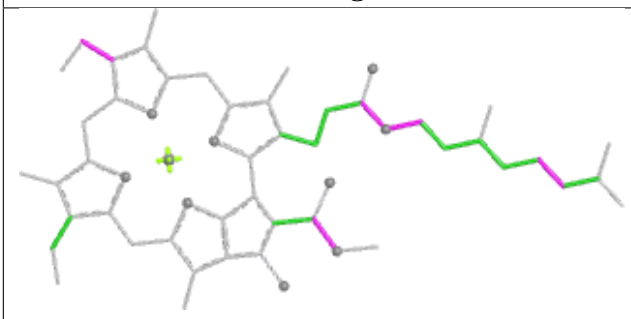
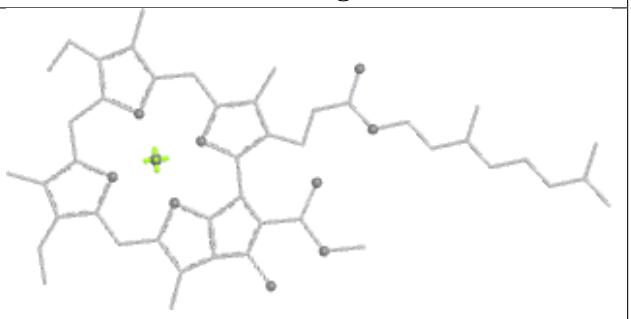


Torsions

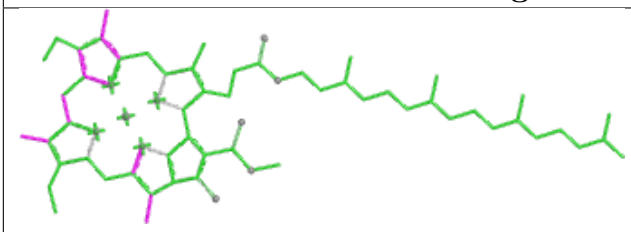


Rings

Ligand CLA BB 841	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 838	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BA 806



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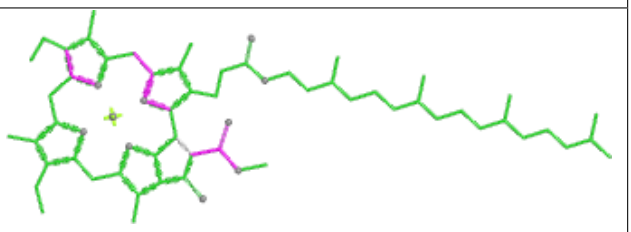

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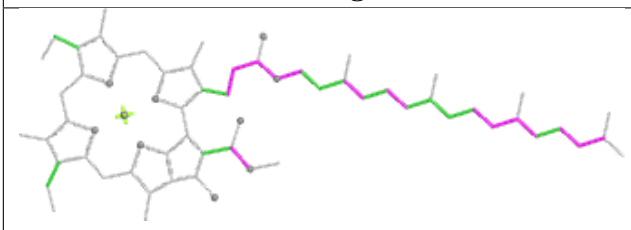
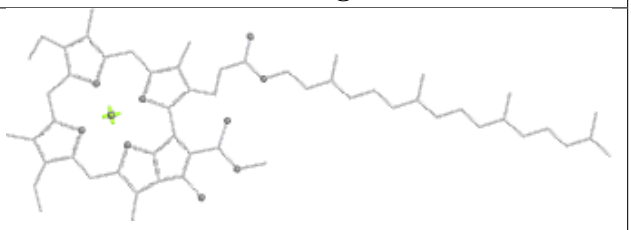
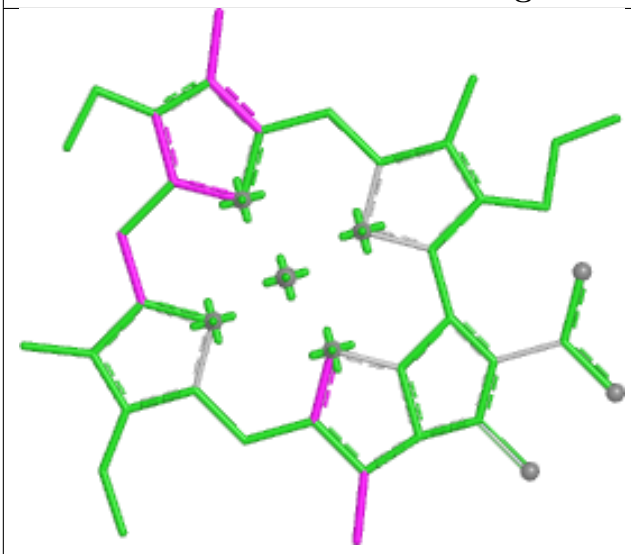


Torsions



Rings

Ligand CLA A6 604



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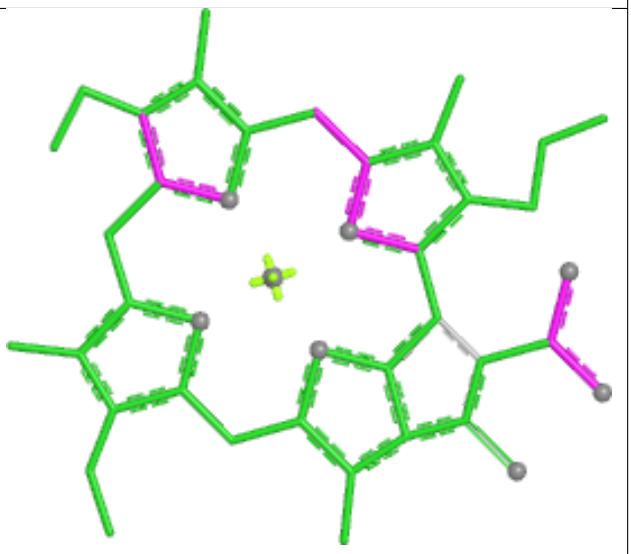

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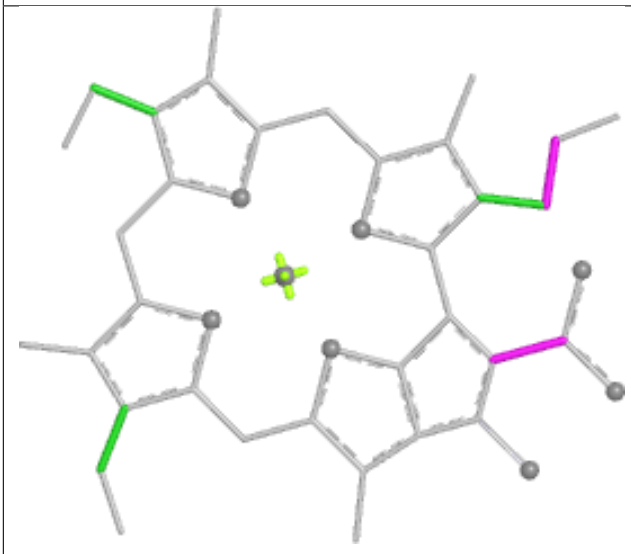

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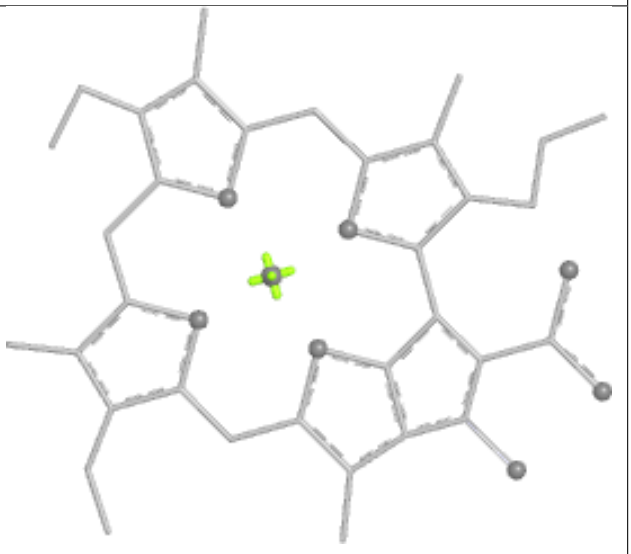
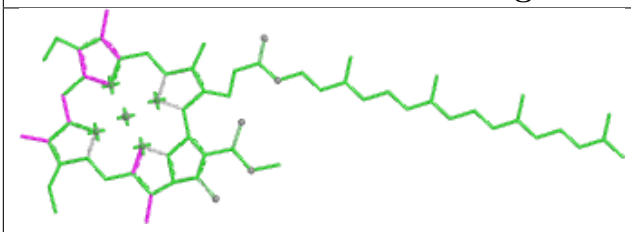


Rings

Ligand CLA A6 603



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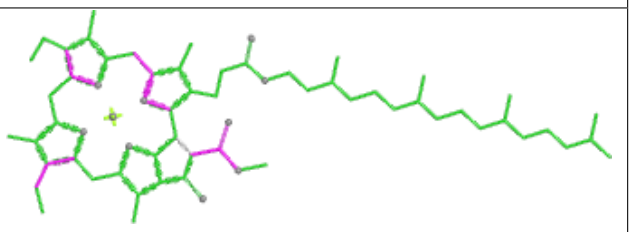
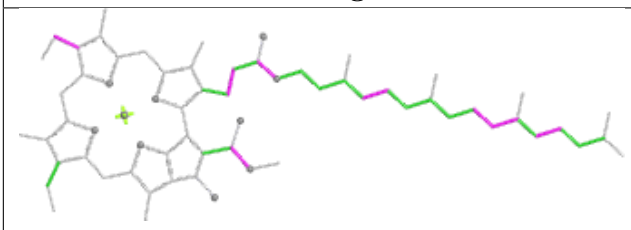


Bond angles



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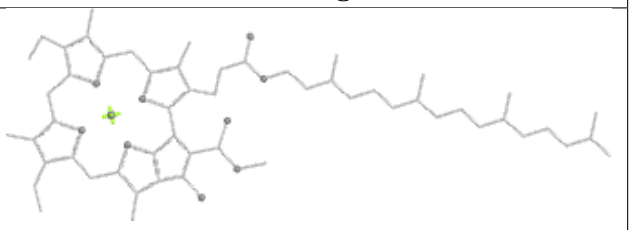
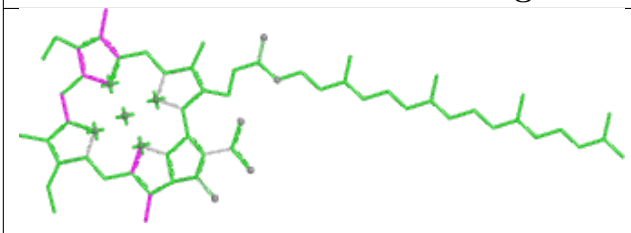


Rings

Ligand CLA A1 314



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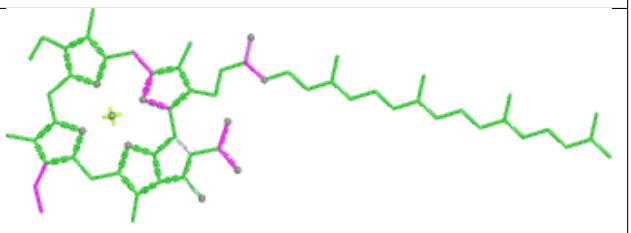
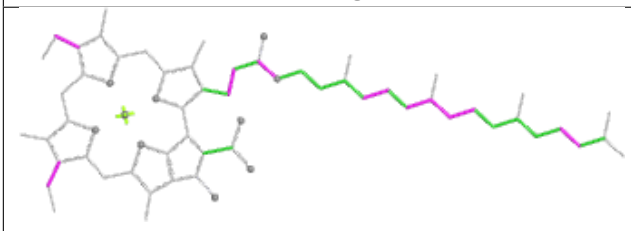


Bond angles



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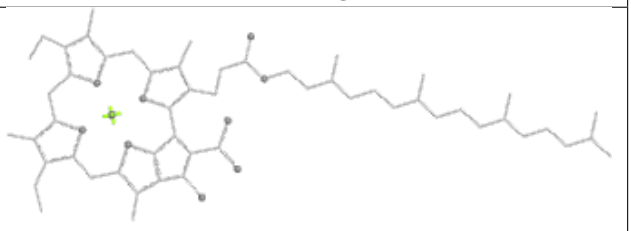
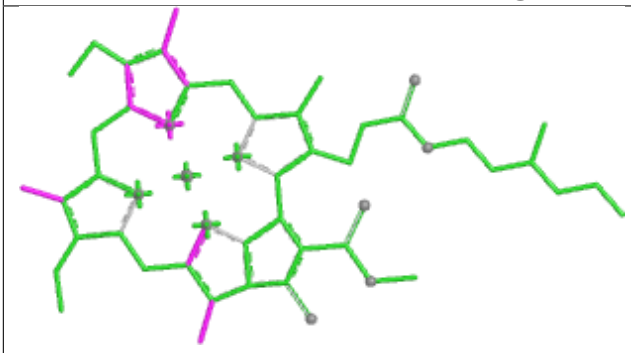


Rings

Ligand CLA BB 809



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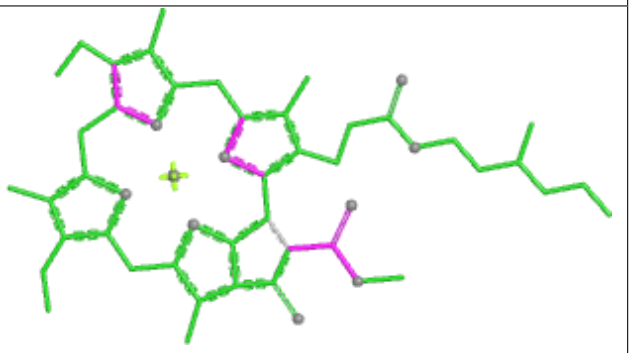
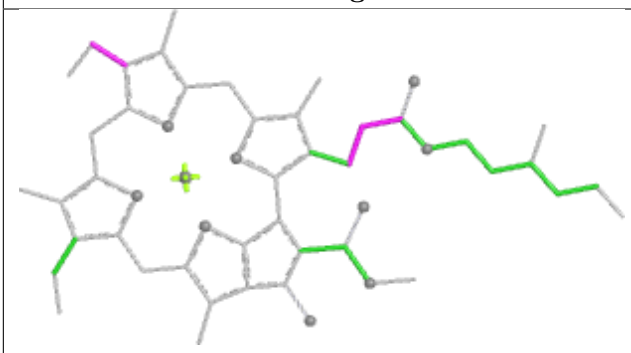


Bond angles



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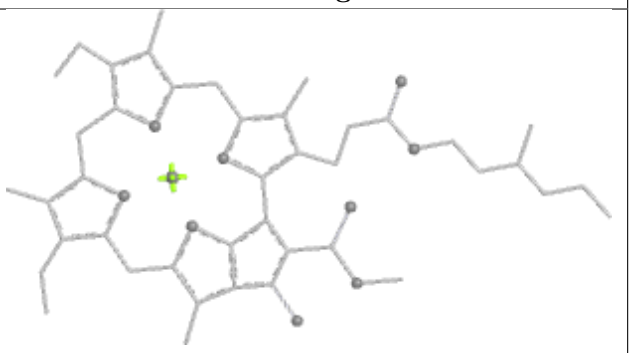
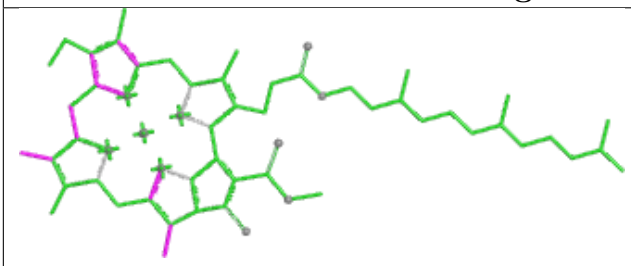


Rings

Ligand CLA A1 311



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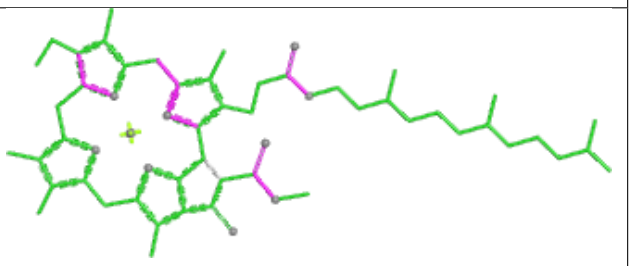

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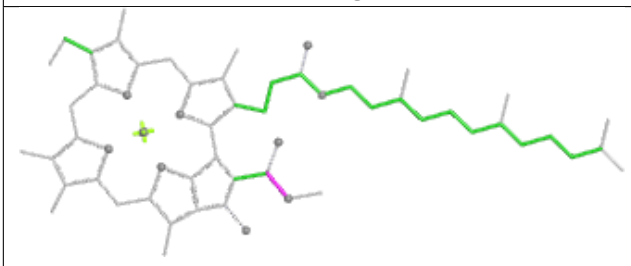

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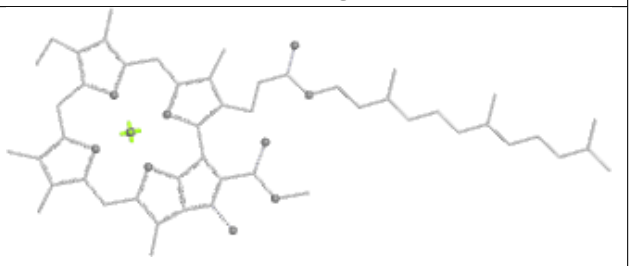
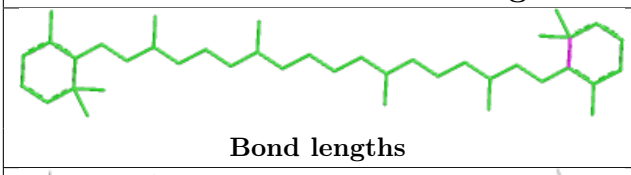


Rings

Ligand BCR AB 844



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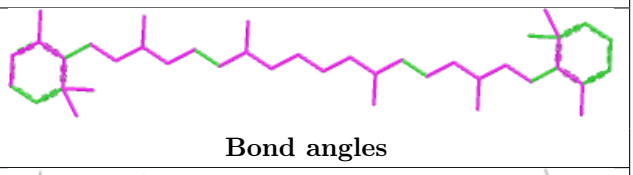
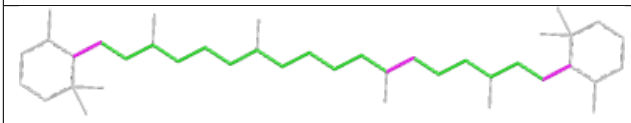


Bond angles



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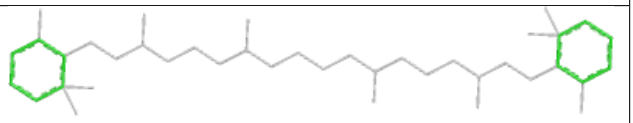
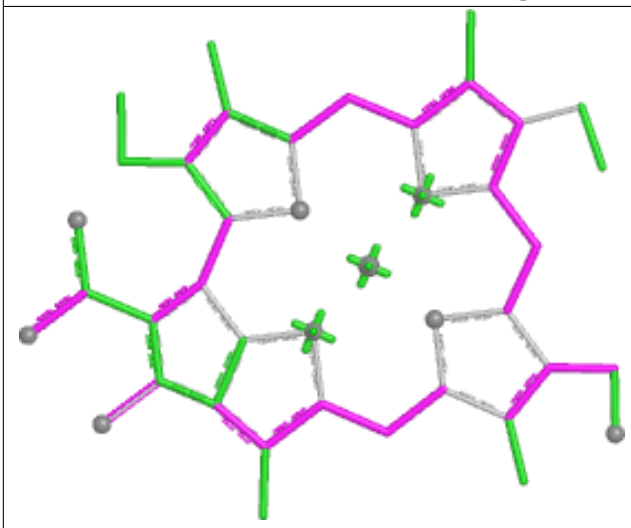


Rings

Ligand CHL A4 304



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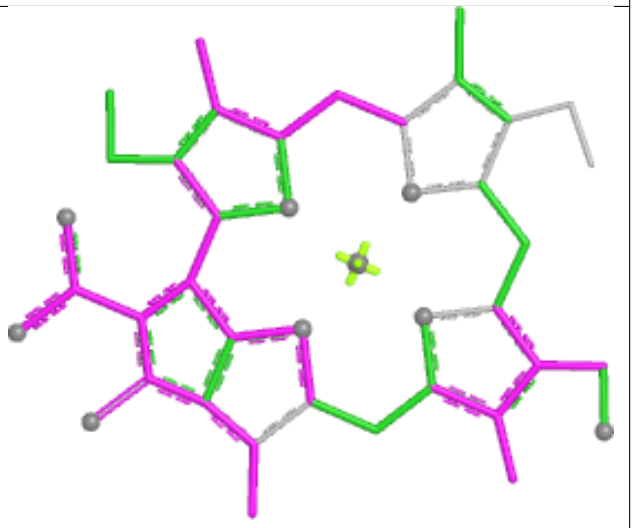
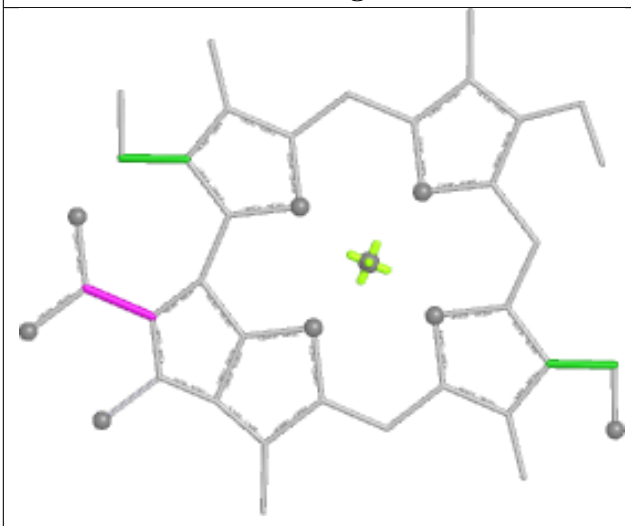


Bond angles



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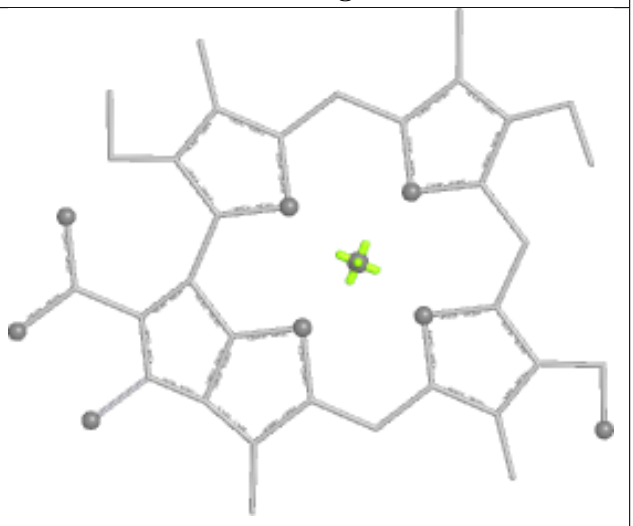
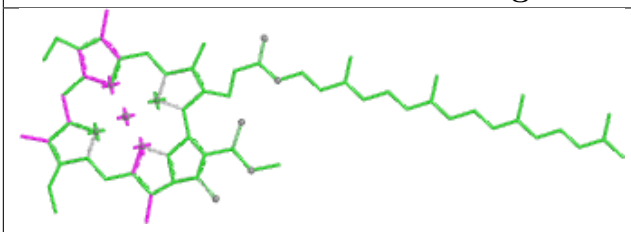


Rings

Ligand CLA BB 826



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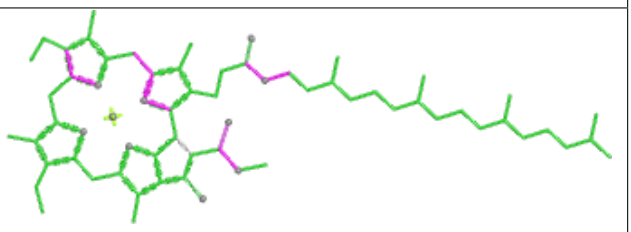
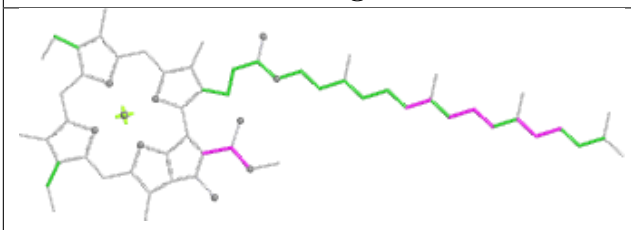


Bond angles



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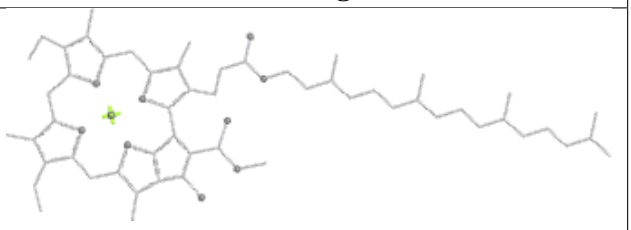
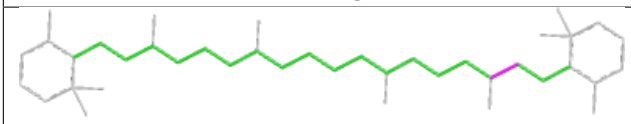


Rings

Ligand BCR AB 848

Bond lengths

Bond angles



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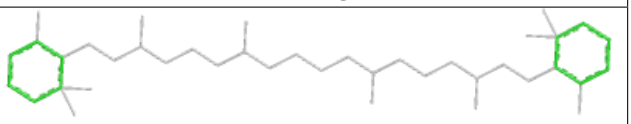
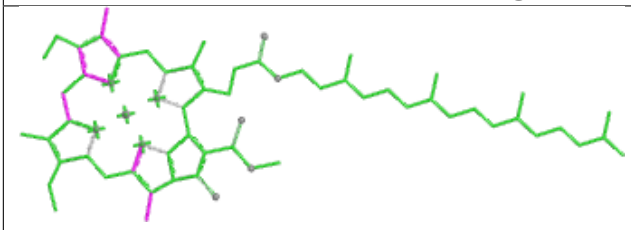
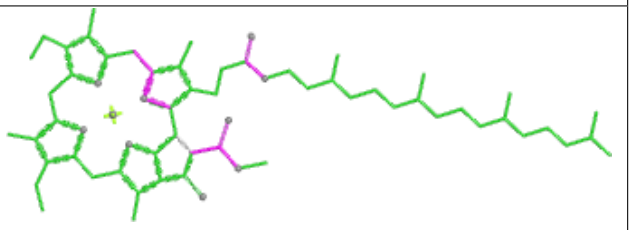


Rings

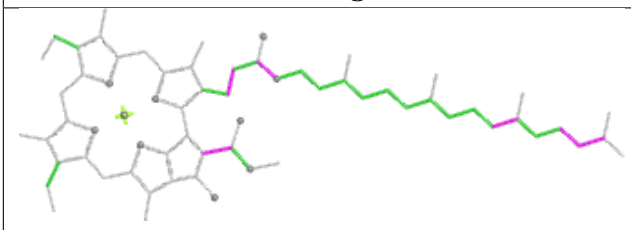
Ligand CLA AA 808



Bond lengths



Bond angles



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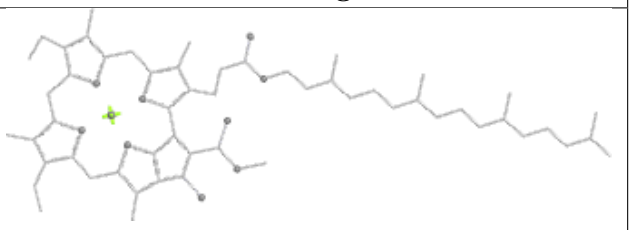
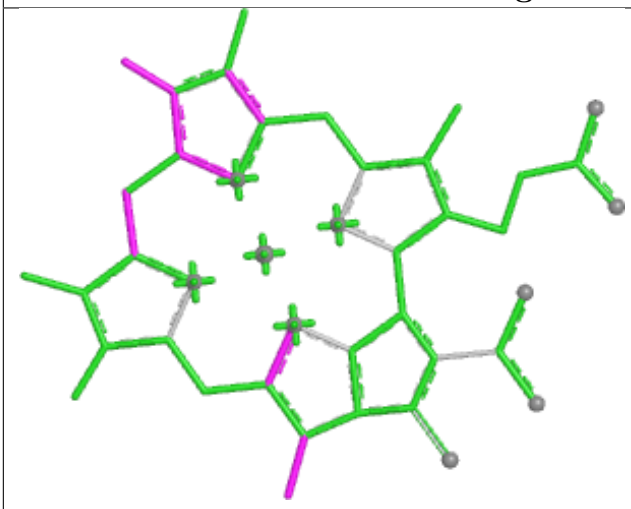


Rings

Ligand CLA B3 303



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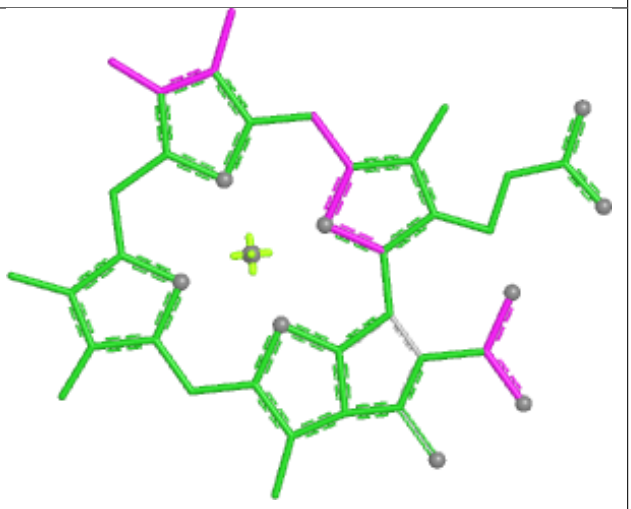
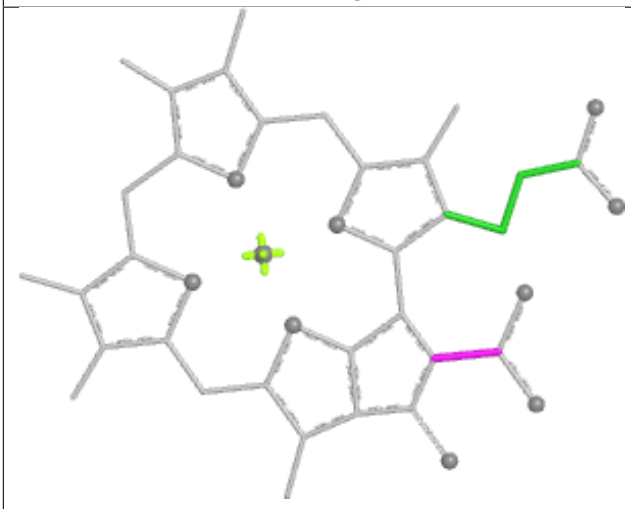


Bond angles



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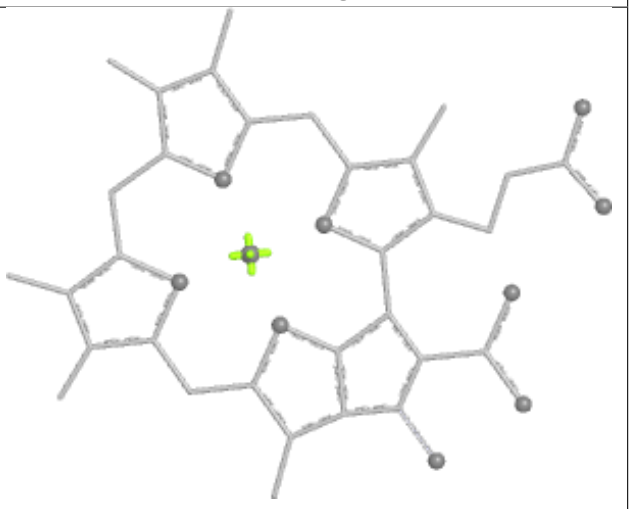
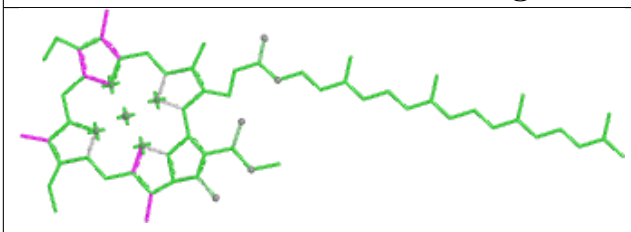
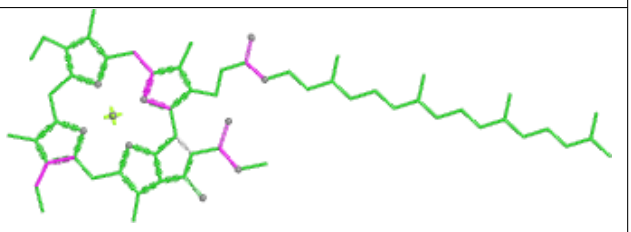


Rings

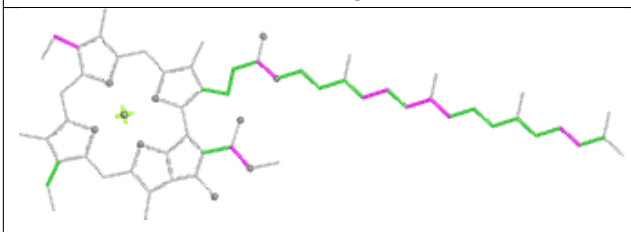
Ligand CLA BB 842



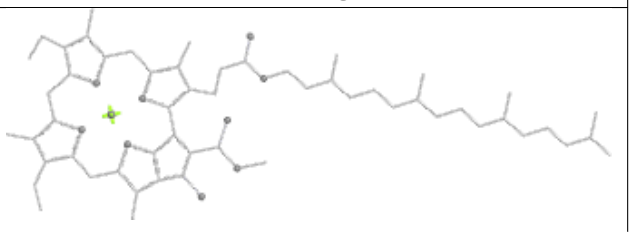
Bond lengths



Bond angles

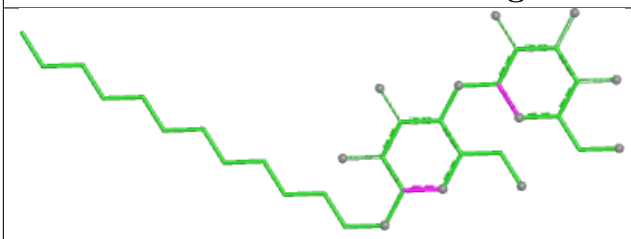


Torsions

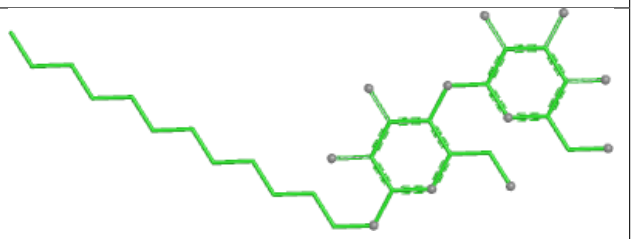


Rings

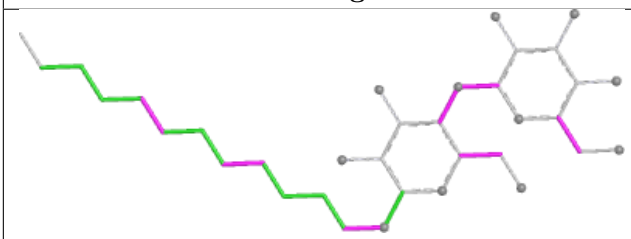
Ligand LMU BB 851



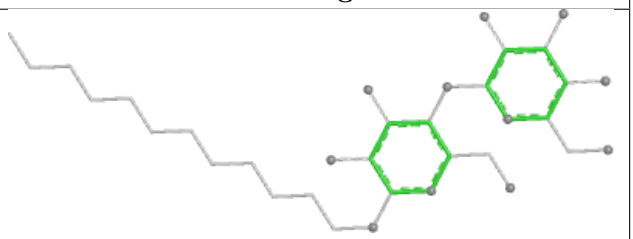
Bond lengths



Bond angles

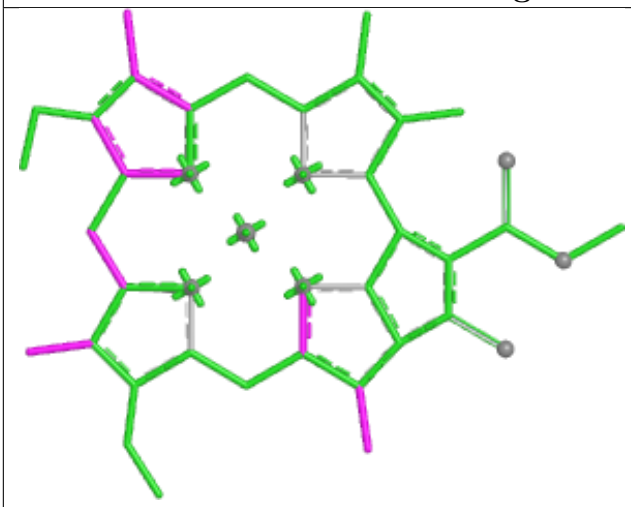


Torsions

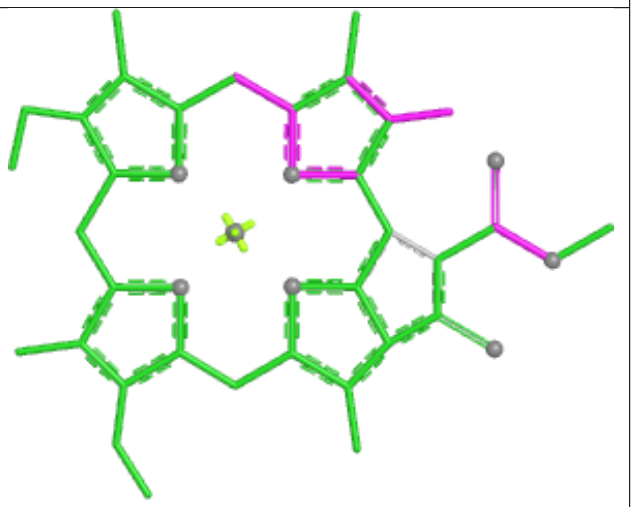


Rings

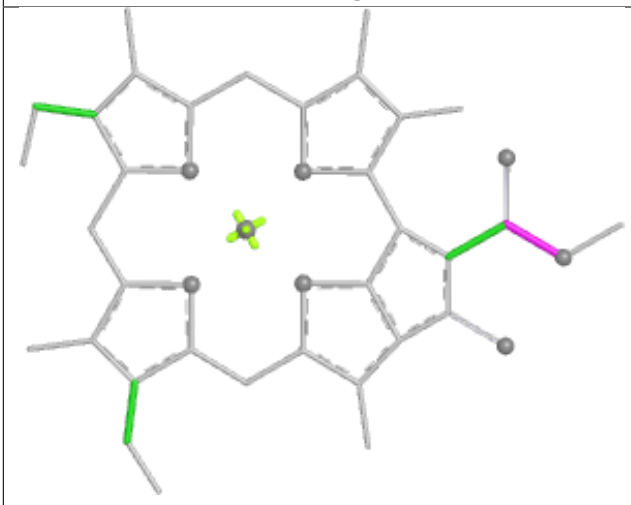
Ligand CLA BF 303



Bond lengths



Bond angles



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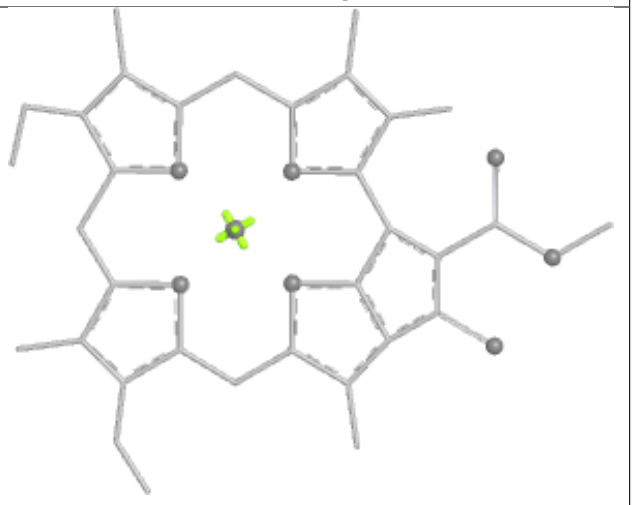
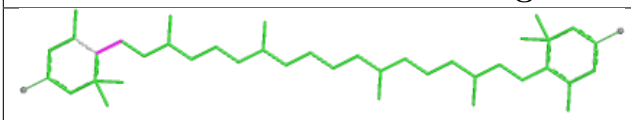


Rings

Ligand LUT B3 315



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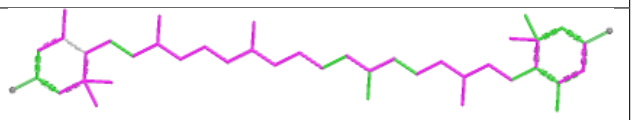
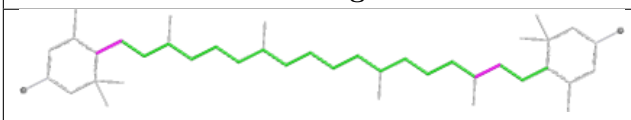
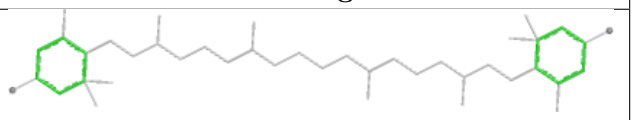


Bond angles

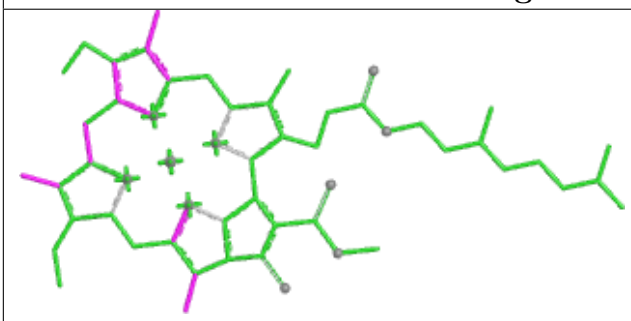


Torsions



Rings

Ligand CLA A6 610



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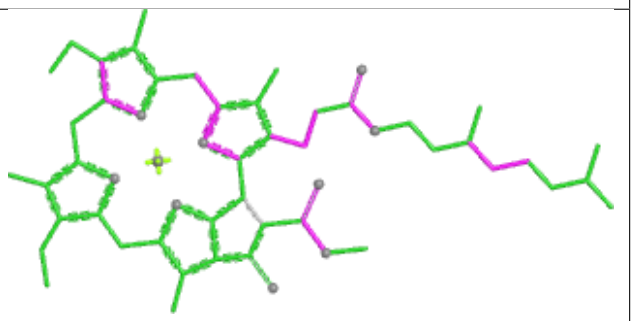
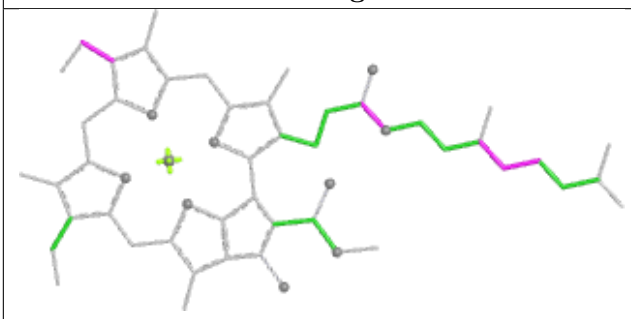
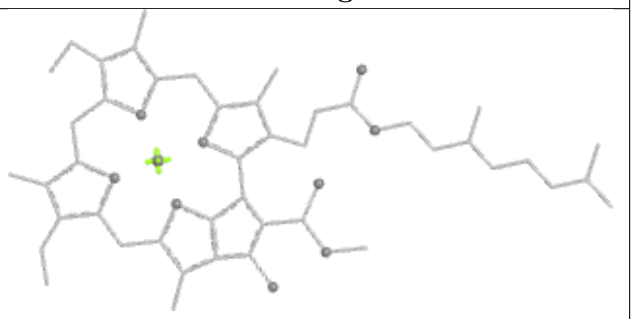


Bond angles

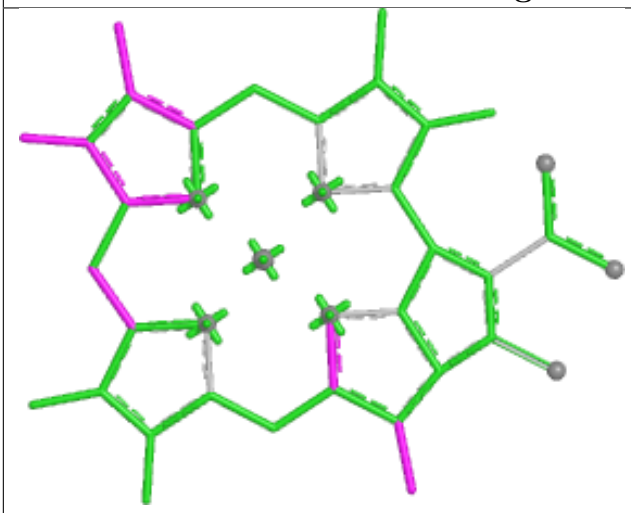


Torsions

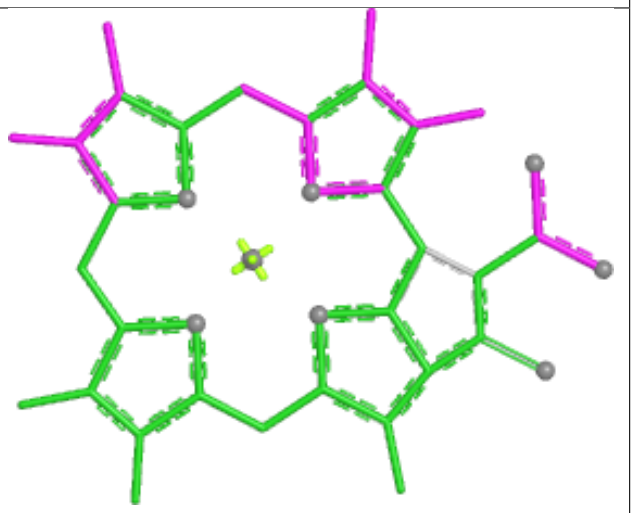


Rings

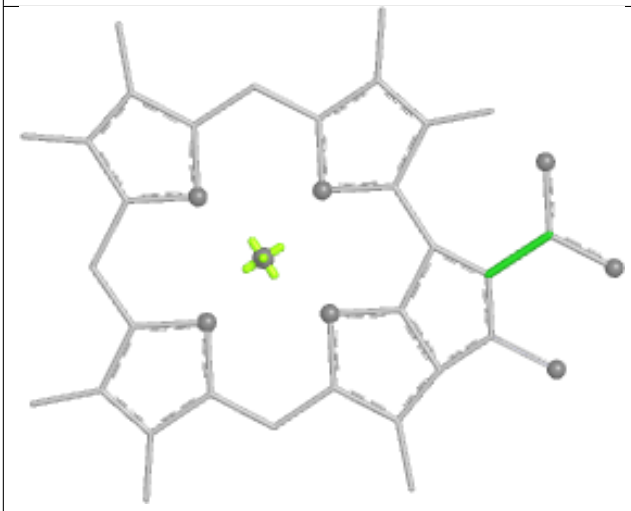
Ligand CLA A1 315



Bond lengths



Bond angles



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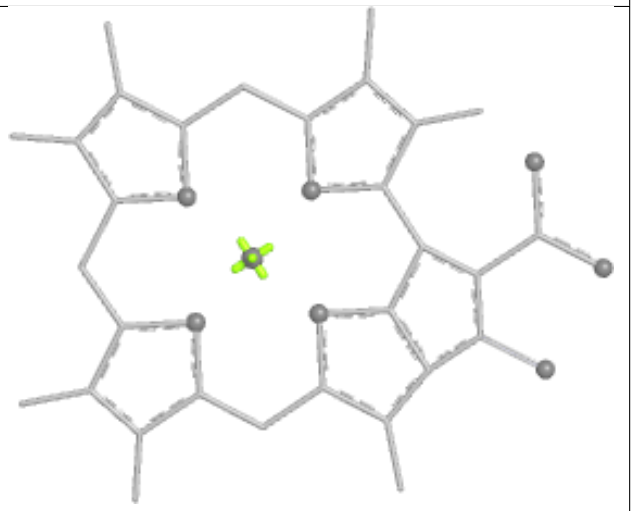
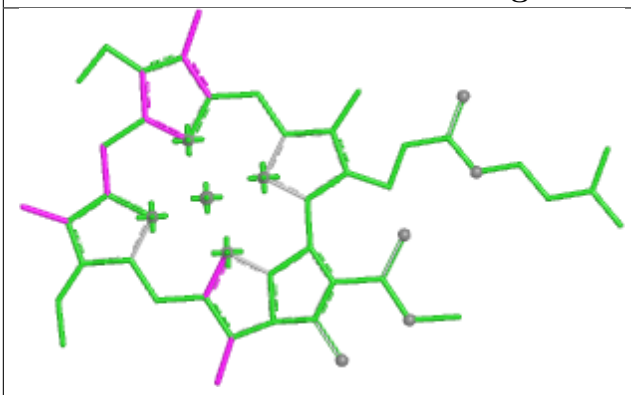


Rings

Ligand CLA BA 807



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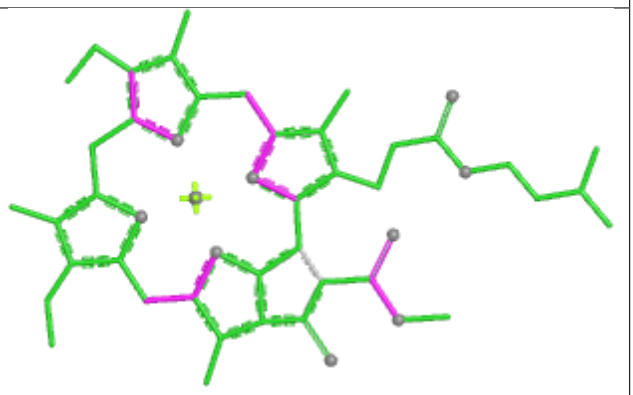
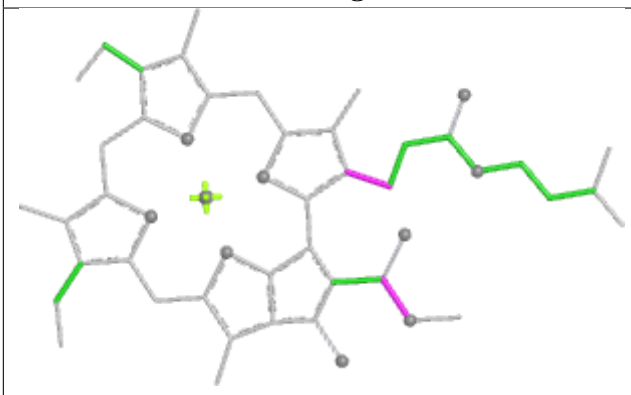


Bond angles



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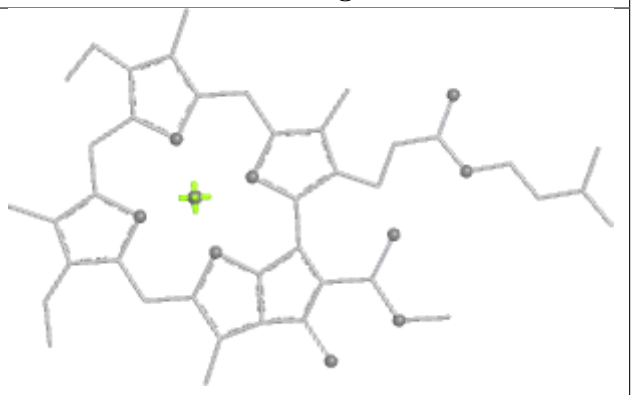
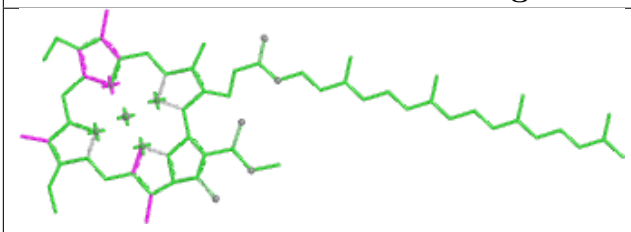
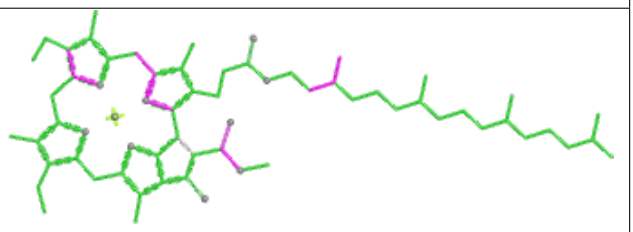


Rings

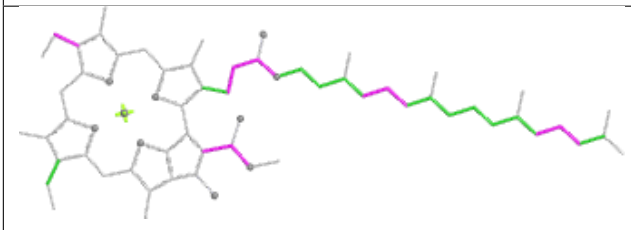
Ligand CLA BA 833



Bond lengths



Bond angles



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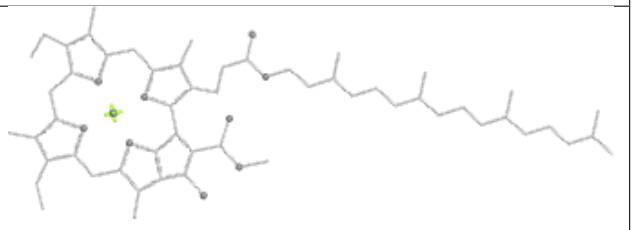
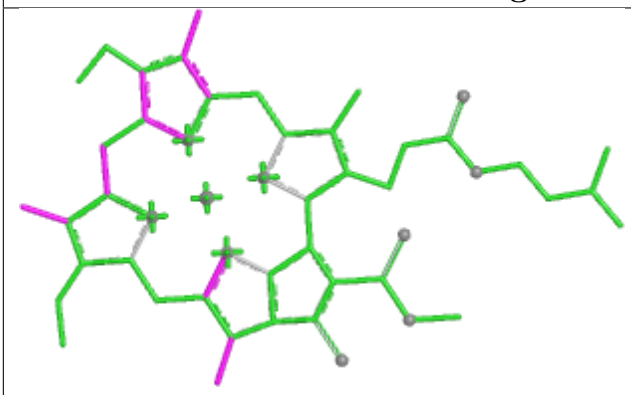


Rings

Ligand CLA AA 807



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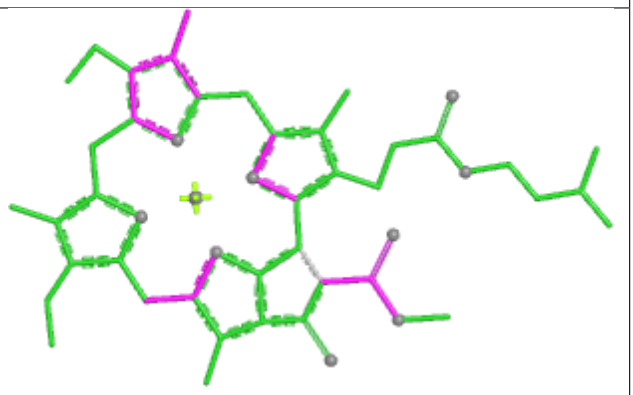
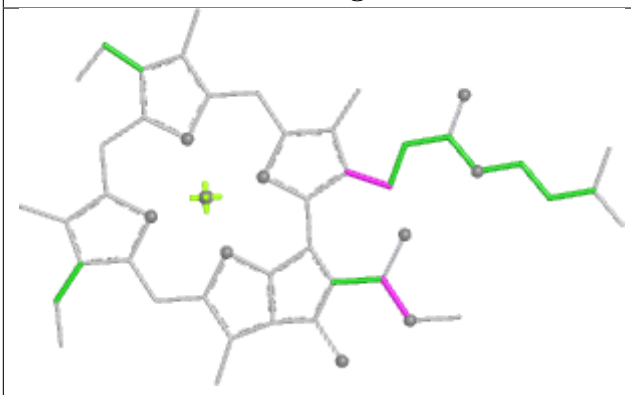


Bond angles



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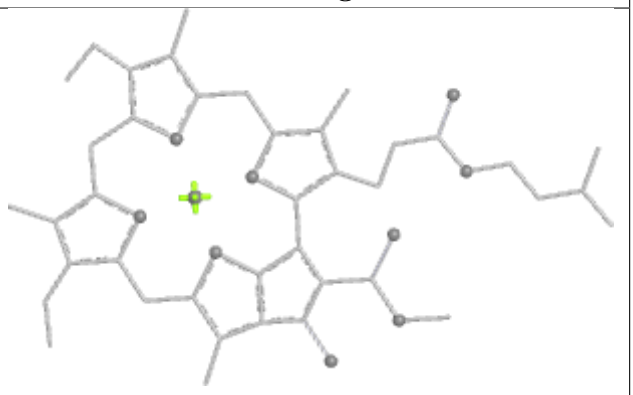
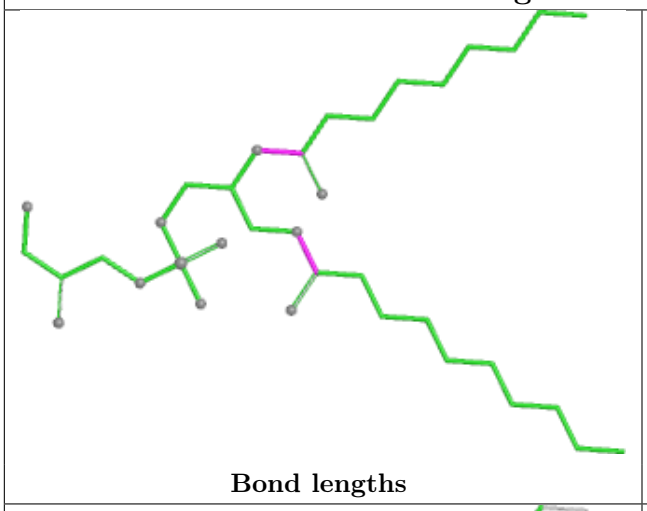


Rings

Ligand LHG A3 301



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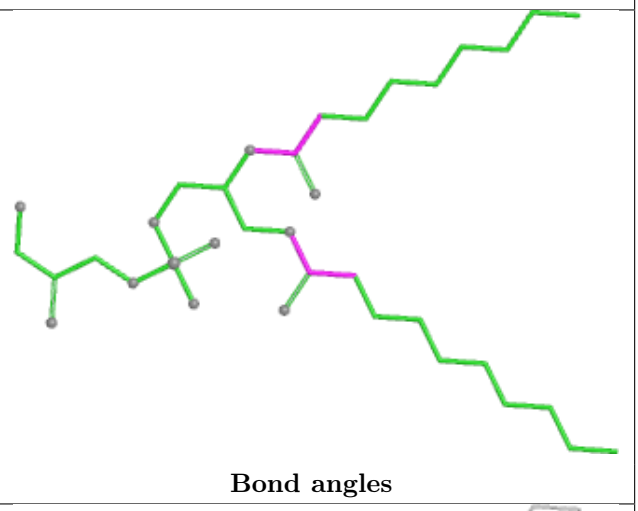
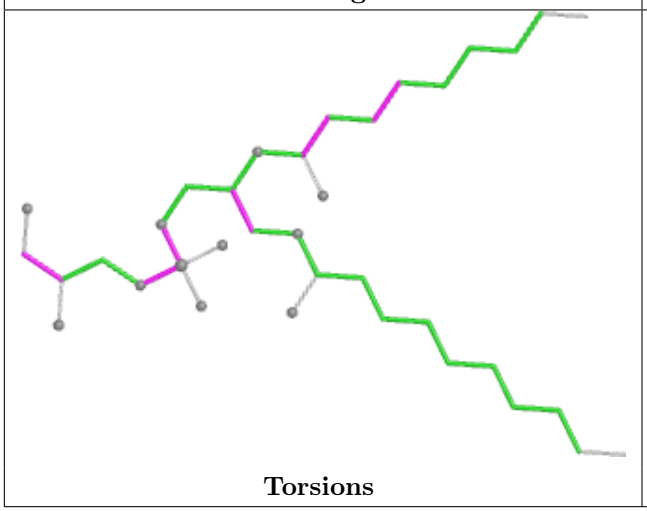
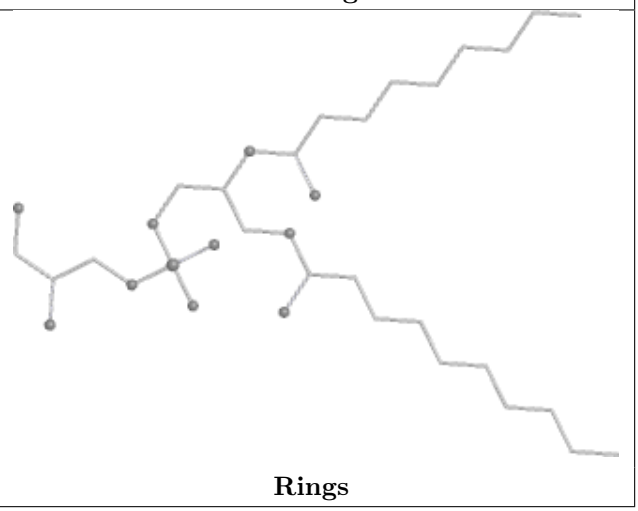


Bond angles

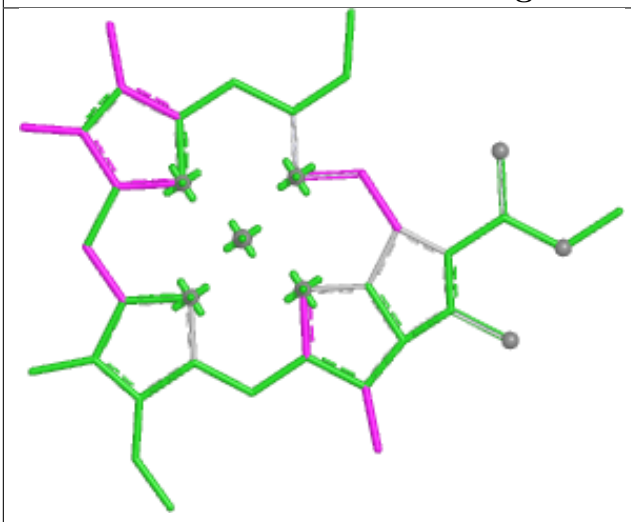


Torsions



Rings

Ligand CLA B2 610



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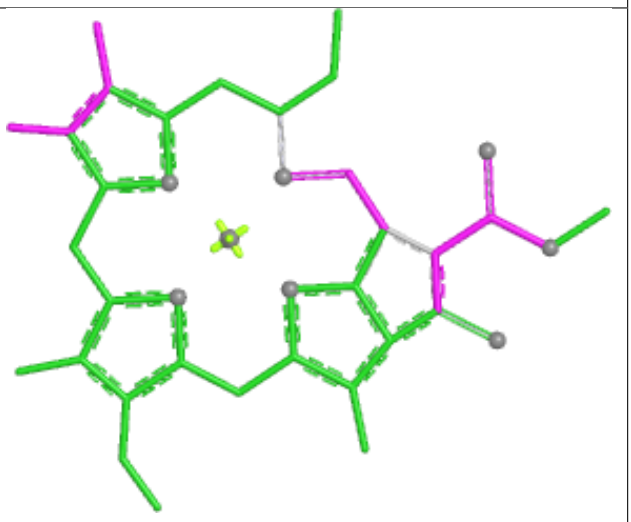
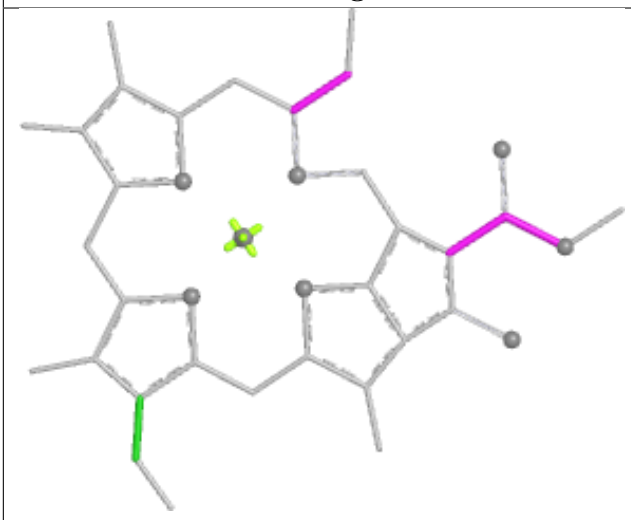


Bond angles



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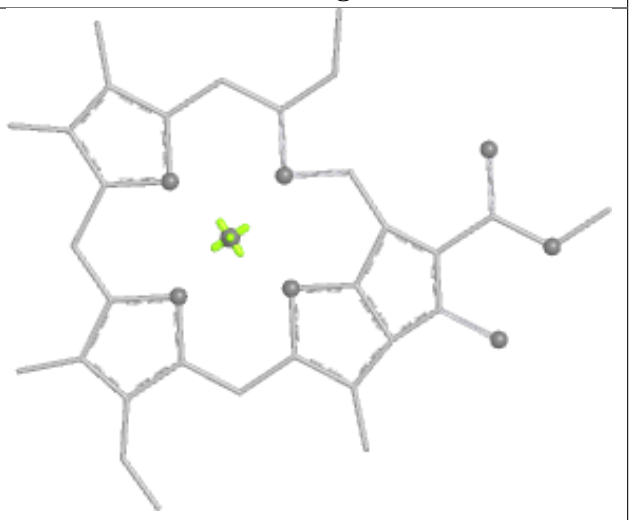
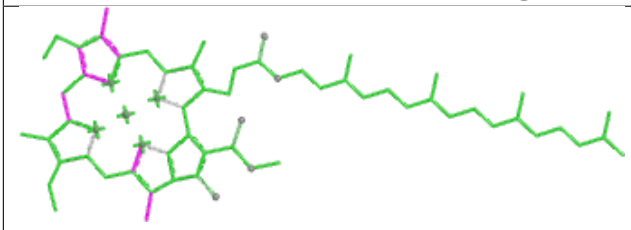


Rings

Ligand CLA B2 612



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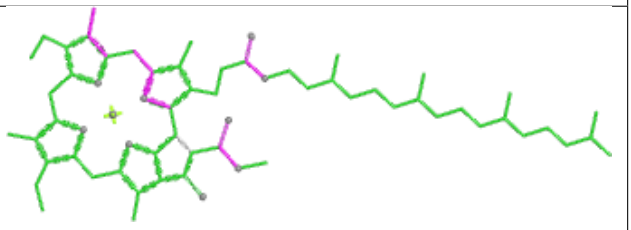
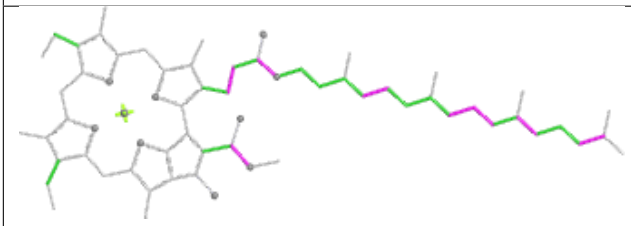
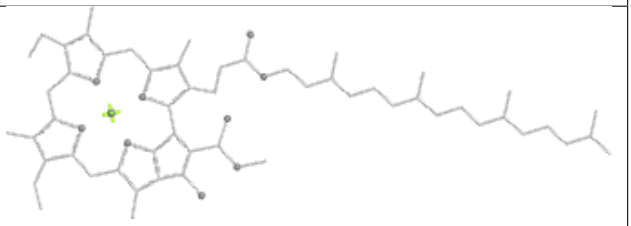


Bond angles

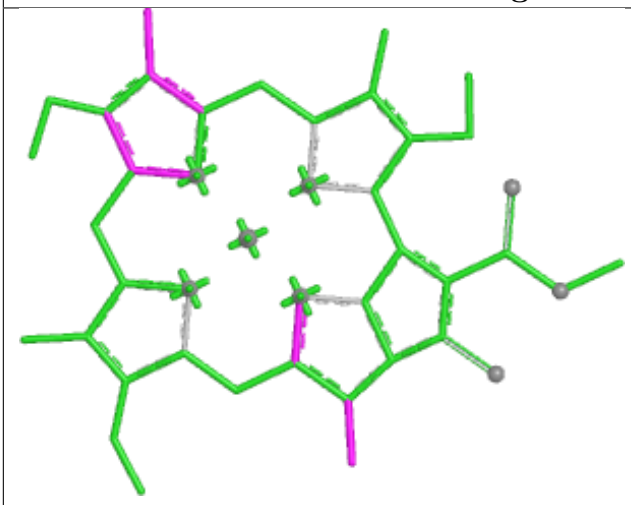


Torsions



Rings

Ligand CLA AB 836



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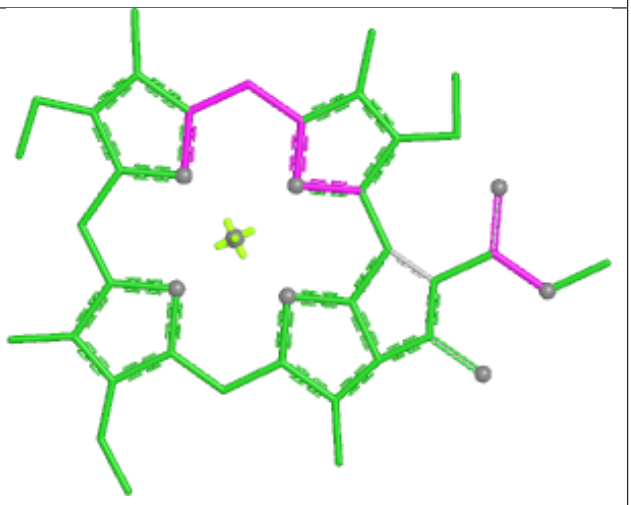
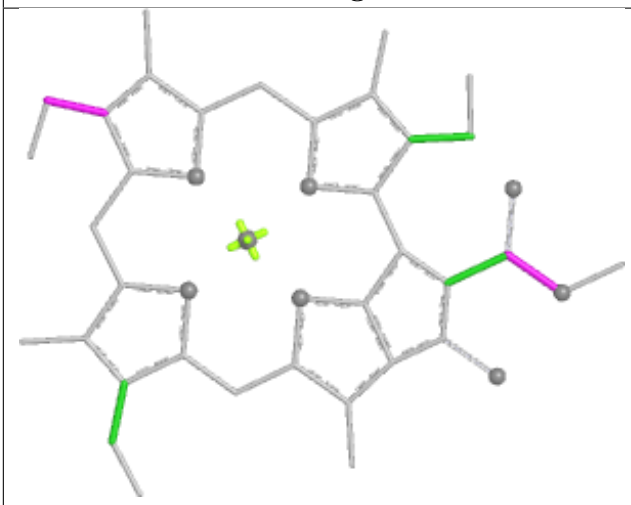


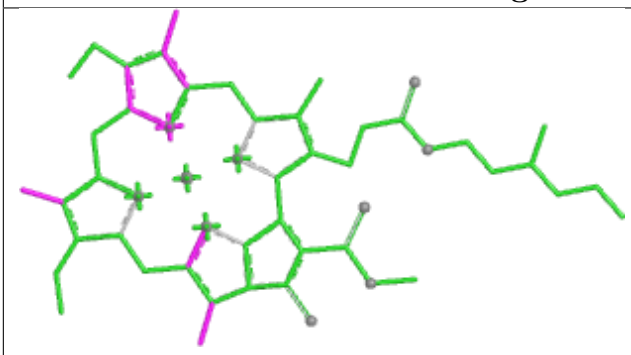
Bond angles



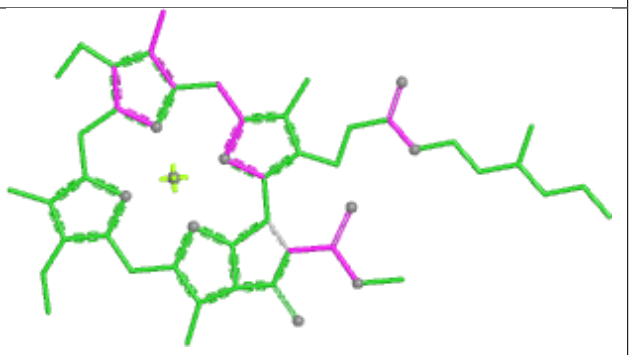
Torsions

Rings

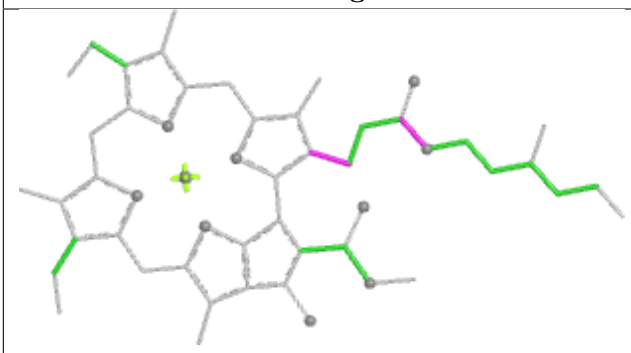
Ligand CLA BA 804



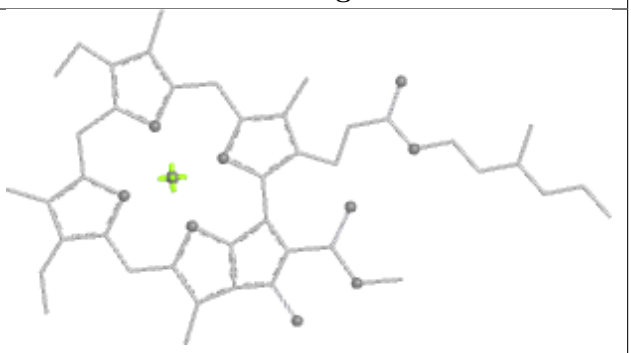
Bond lengths



Bond angles

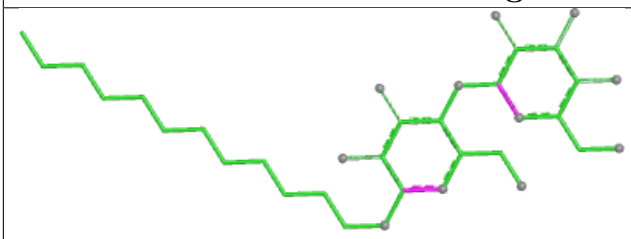


Torsions



Rings

Ligand LMU AA 851



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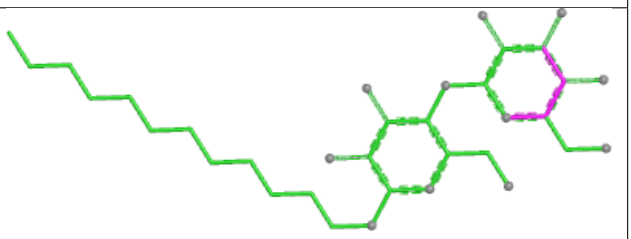
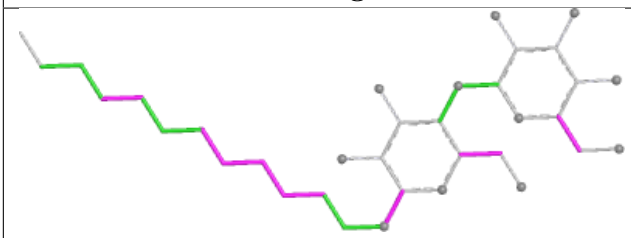
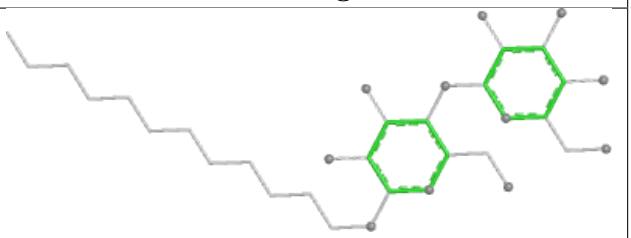


Bond angles

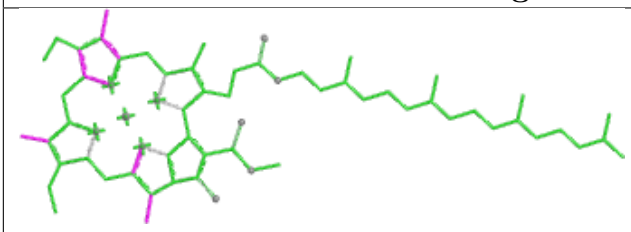


Torsions

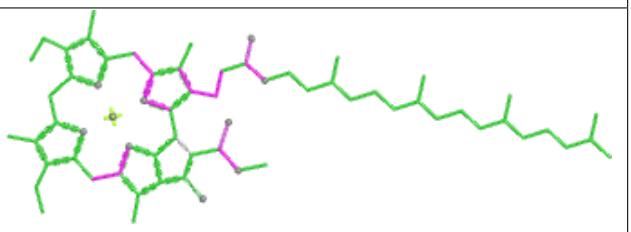


Rings

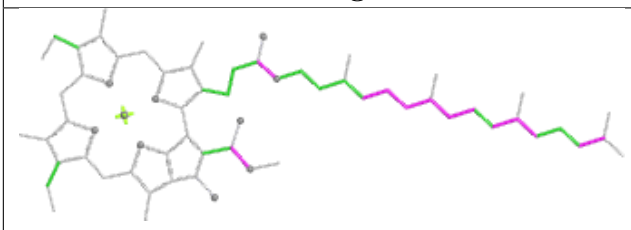
Ligand CLA BB 824



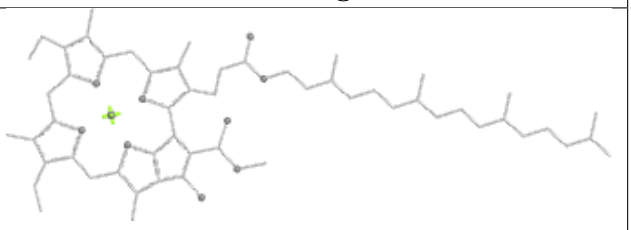
Bond lengths



Bond angles

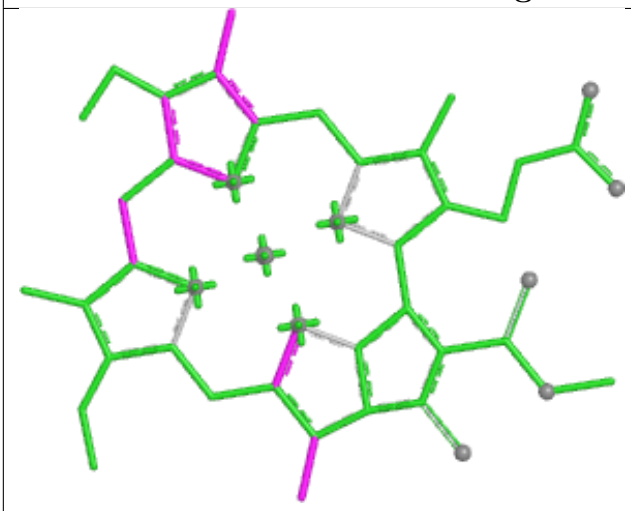


Torsions

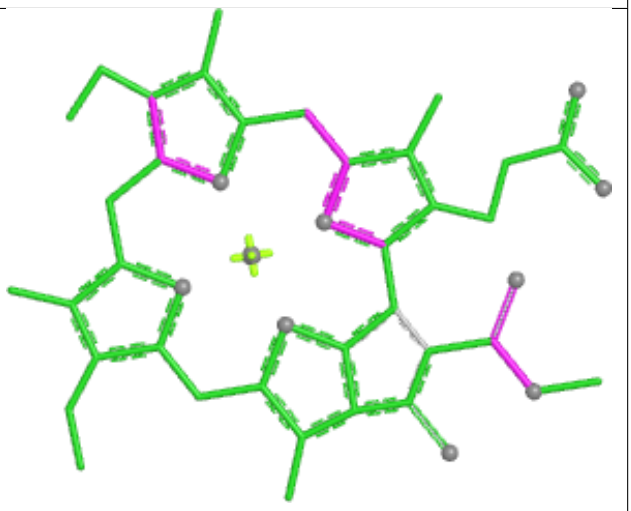


Rings

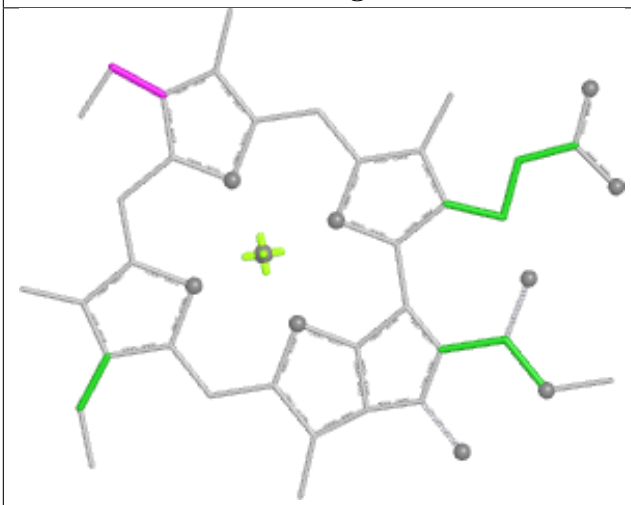
Ligand CLA A4 307



Bond lengths



Bond angles



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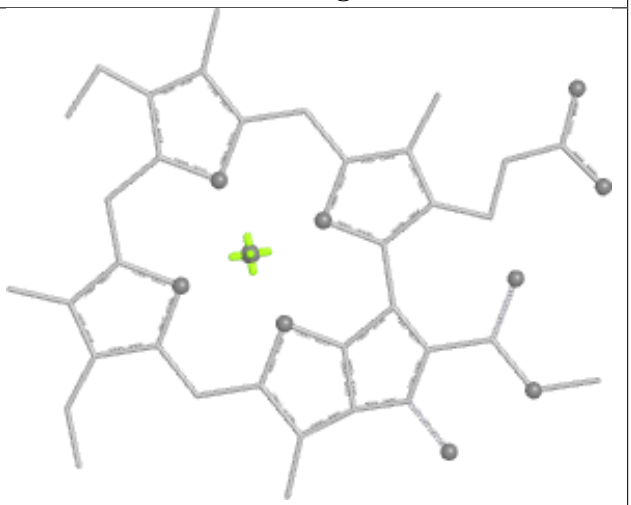
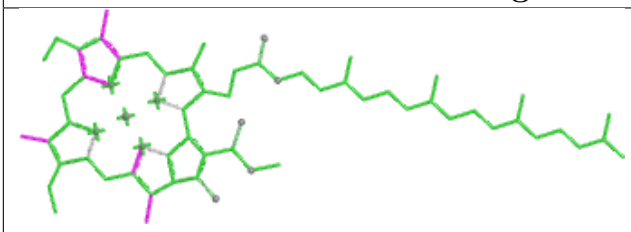


Rings

Ligand CLA BB 835



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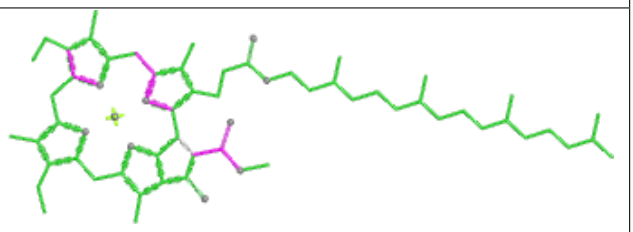
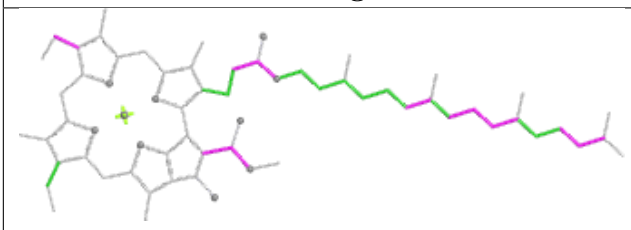
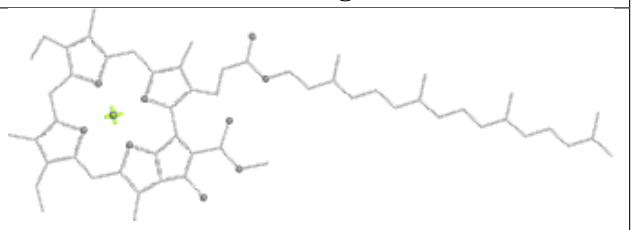


Bond angles

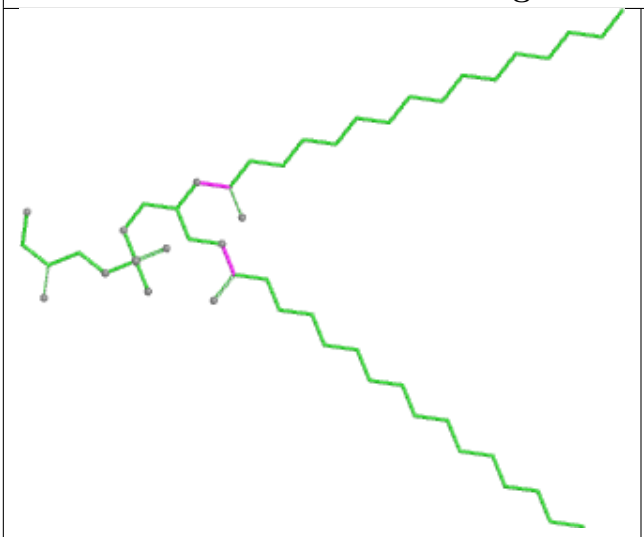


Torsions



Rings

Ligand LHG A1 320



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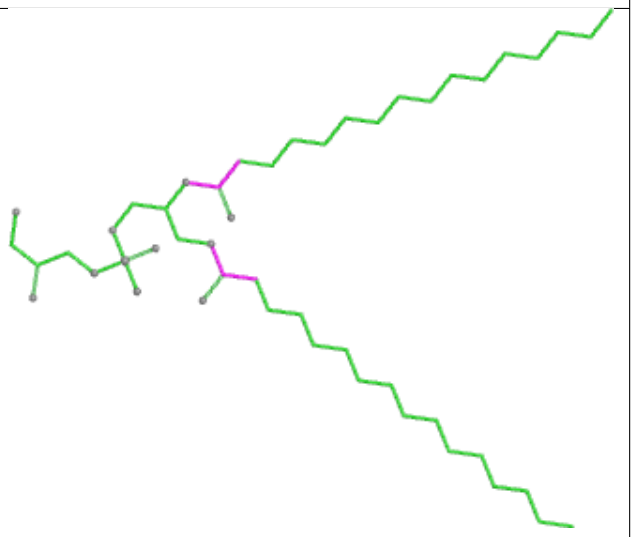
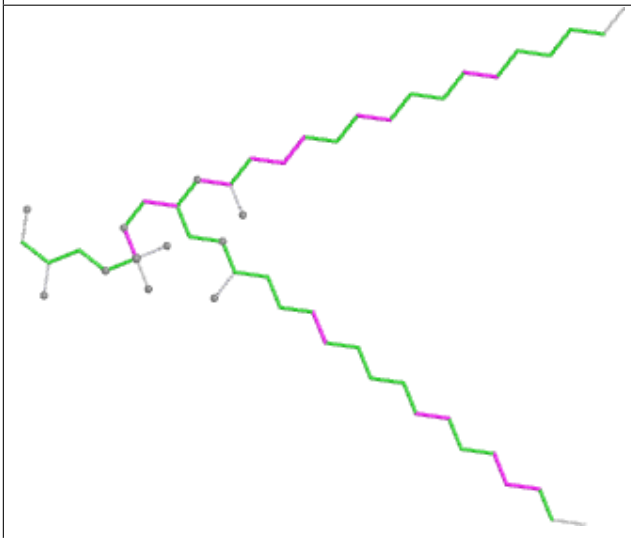
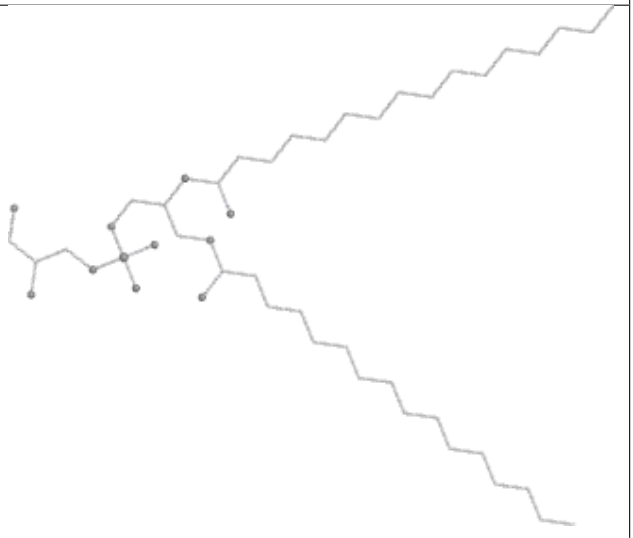


Bond angles

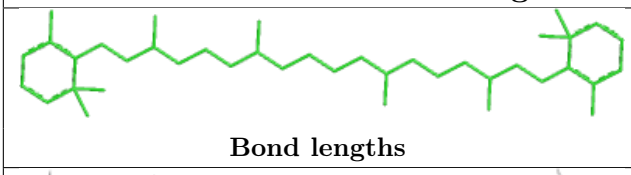


Torsions



Rings

Ligand BCR AL 302



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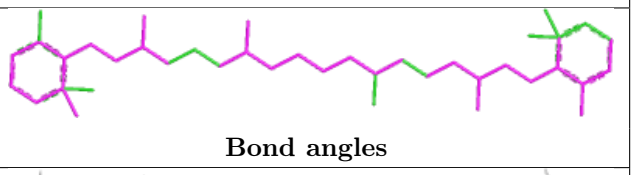
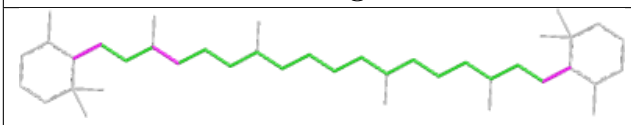


Bond angles



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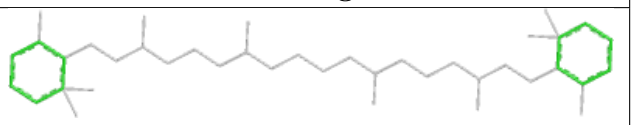
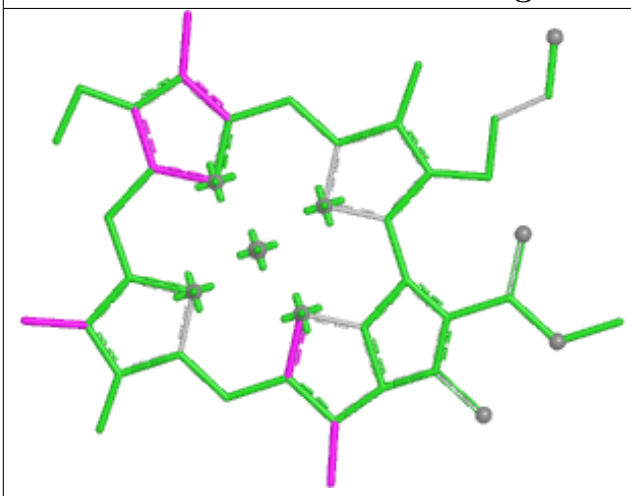


Rings

Ligand CLA A6 605



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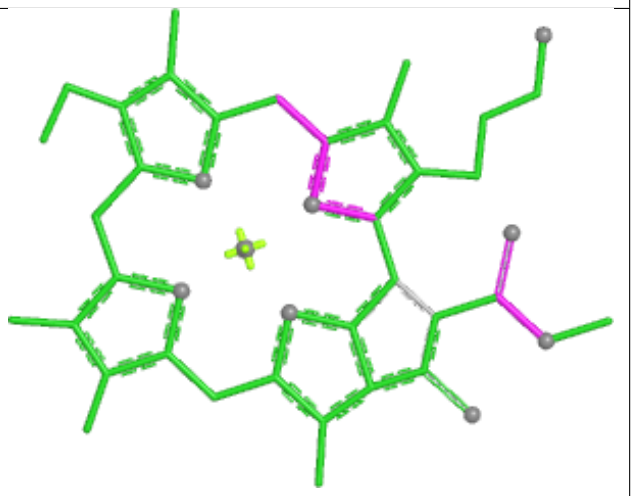
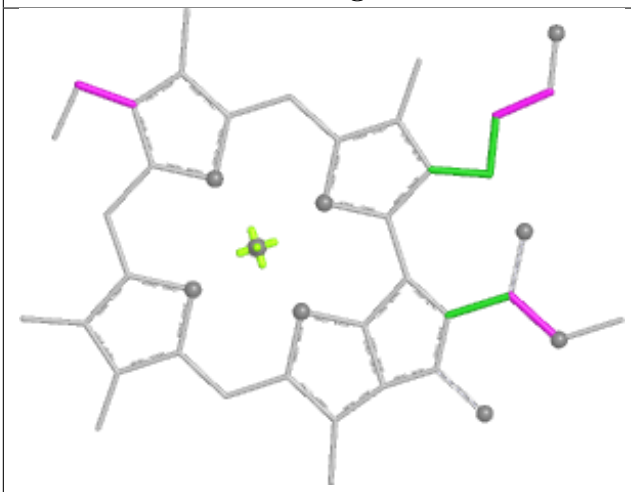


Bond angles



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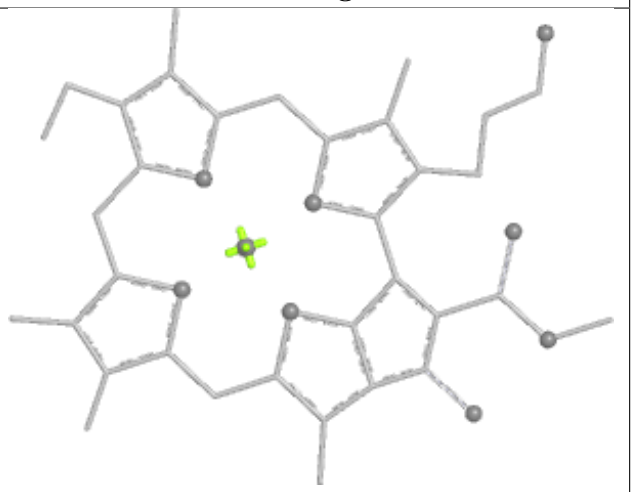
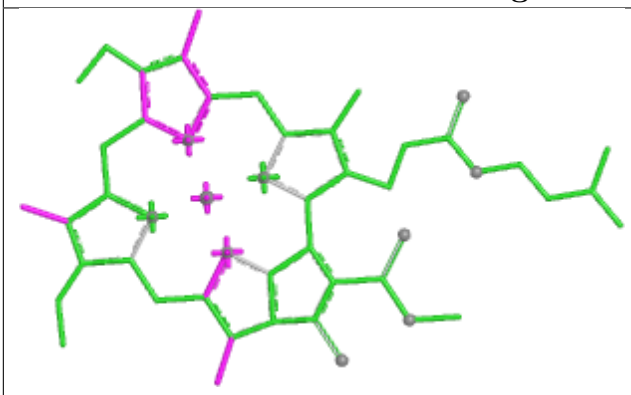


Rings

Ligand CLA AB 837



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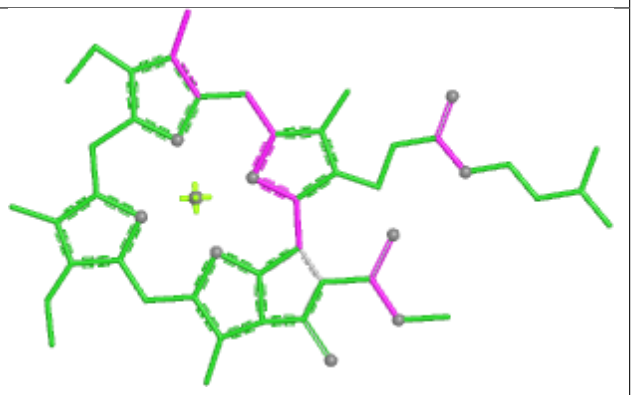
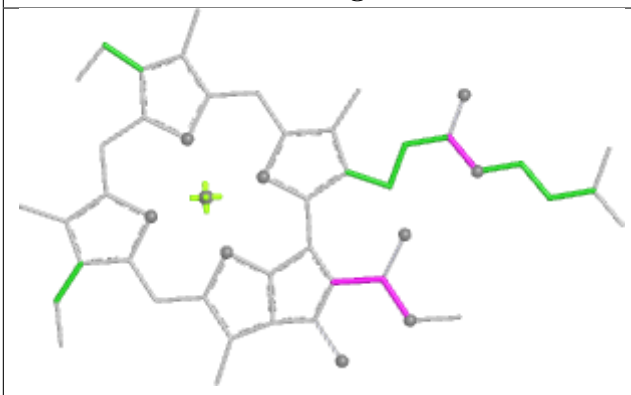


Bond angles



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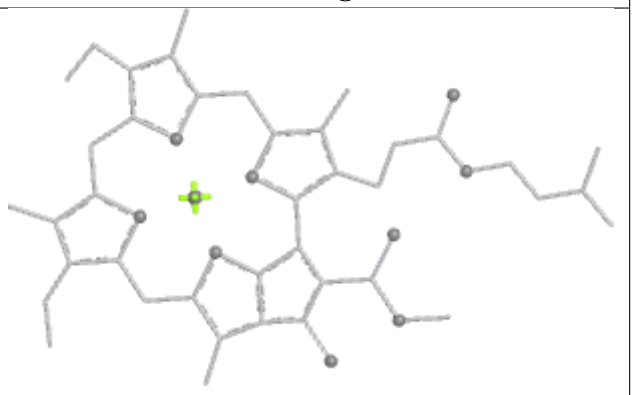
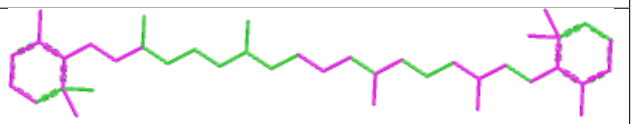


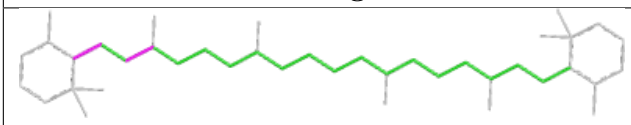
Rings

Ligand BCR AI 102

Bond lengths



Bond angles



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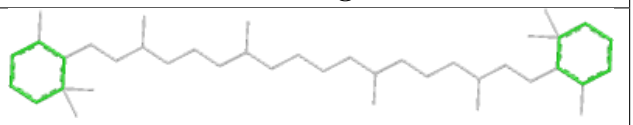
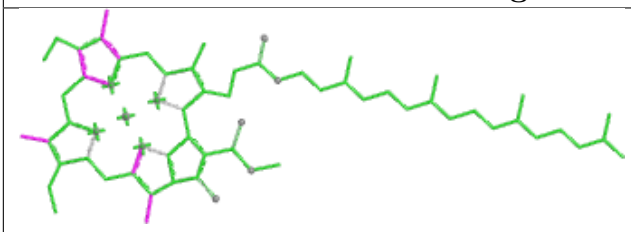


Rings

Ligand CLA AA 803



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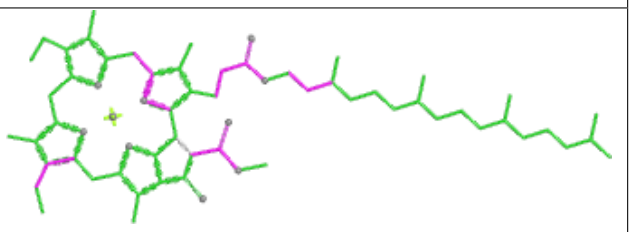
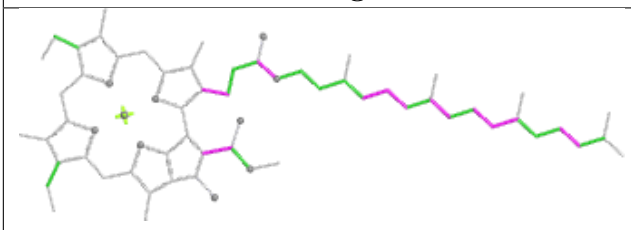


Bond angles



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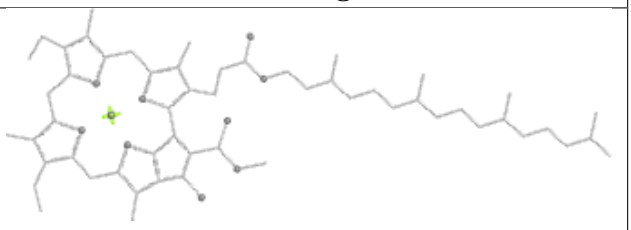
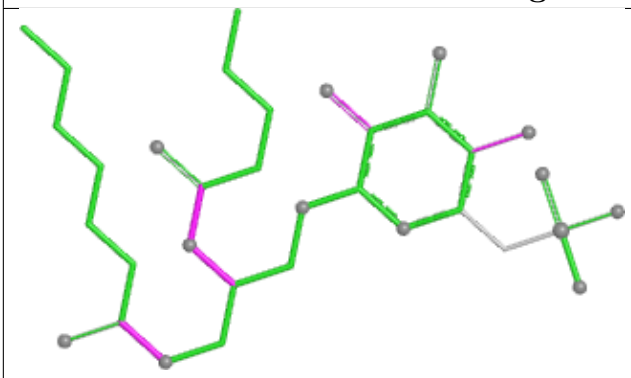


Rings

Ligand SQD e 301



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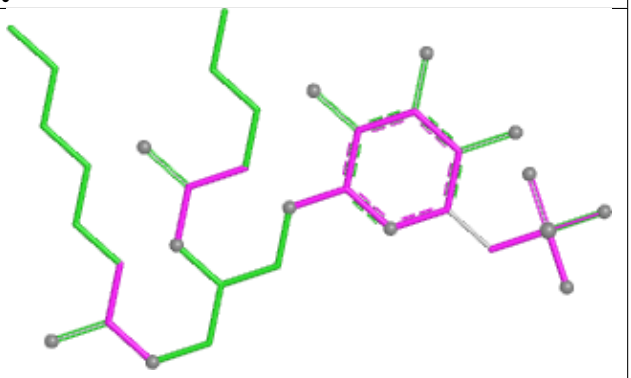
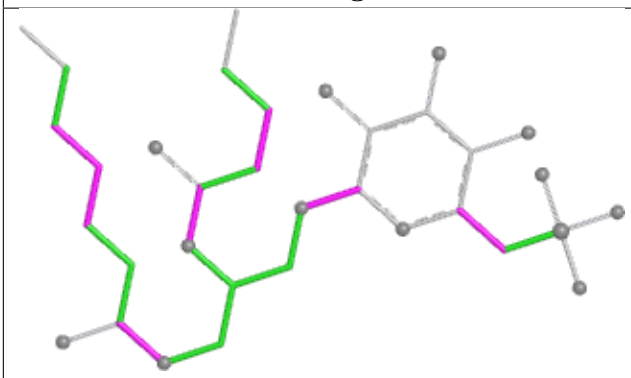
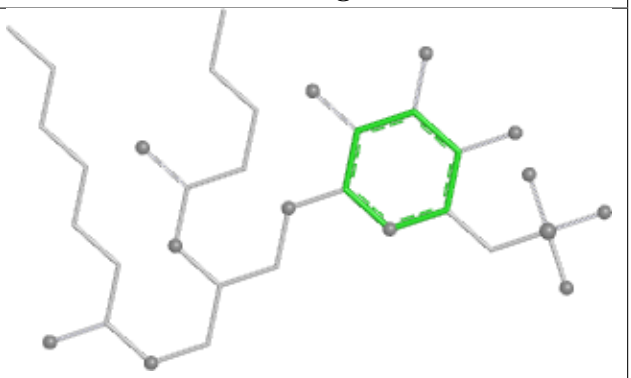


Bond angles

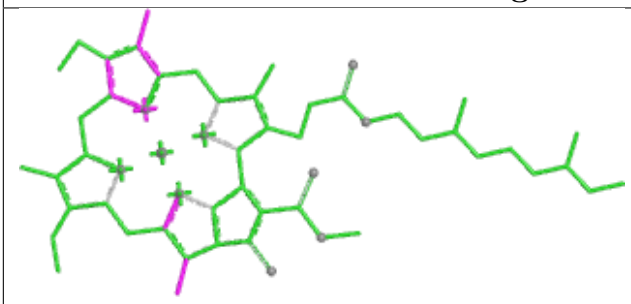


Torsions



Rings

Ligand CLA BA 818



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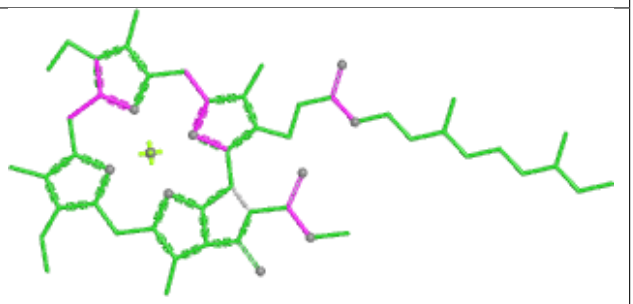
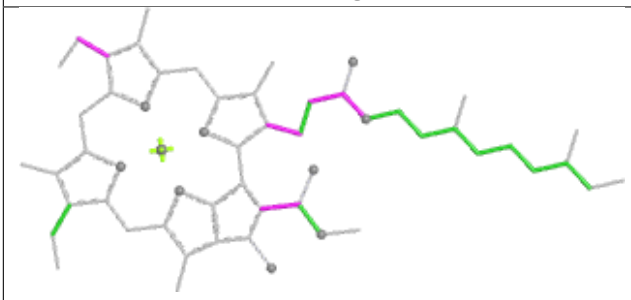


Bond angles



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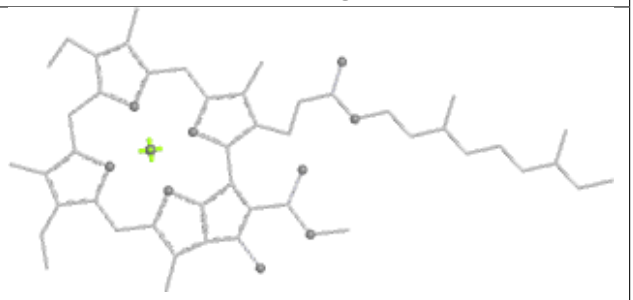
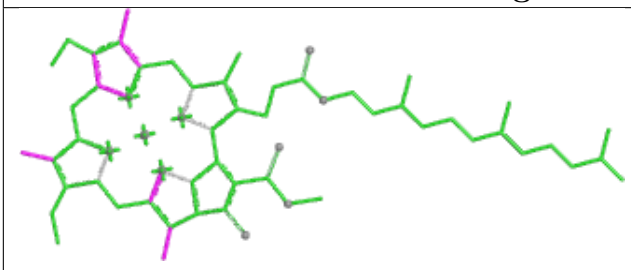
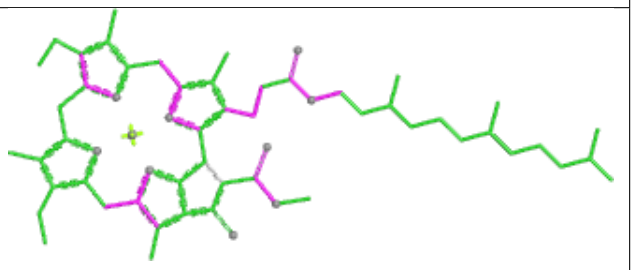


Rings

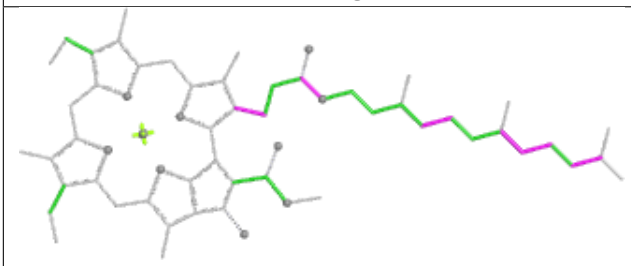
Ligand CLA AL 304



Bond lengths



Bond angles



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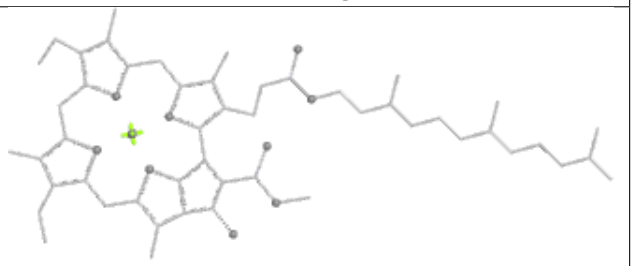
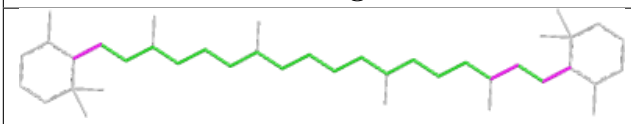


Rings

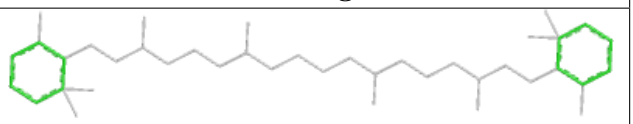
Ligand BCR BA 856

Bond lengths

Bond angles

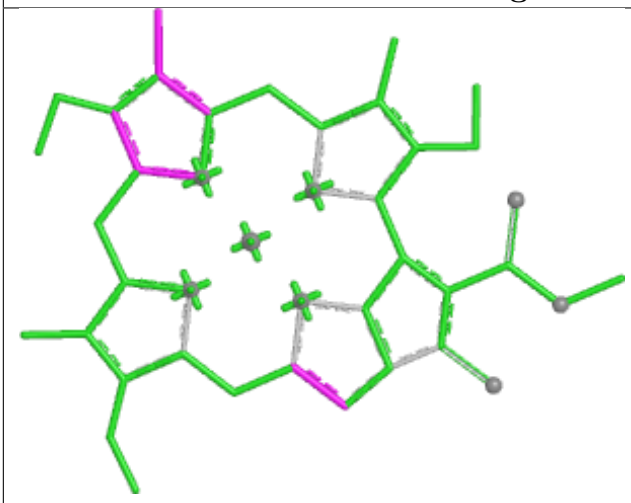


Torsions

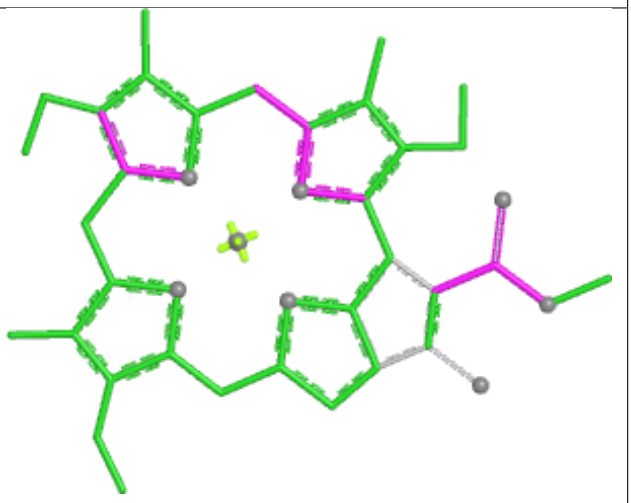


Rings

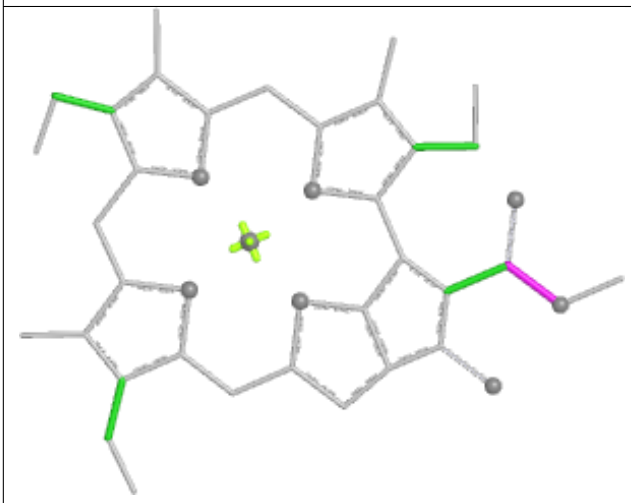
Ligand CLA AA 815



Bond lengths



Bond angles



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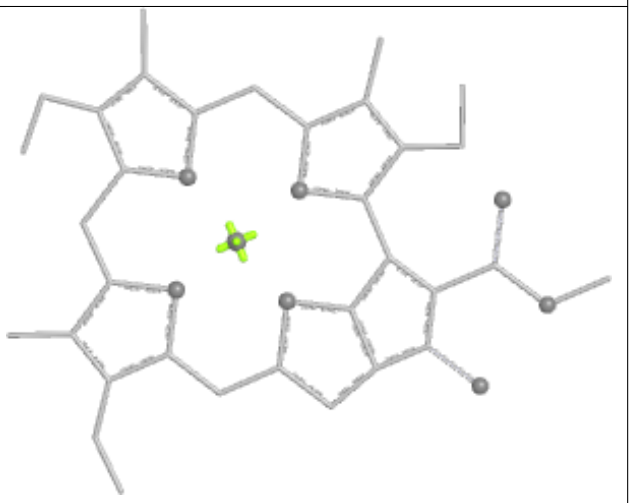
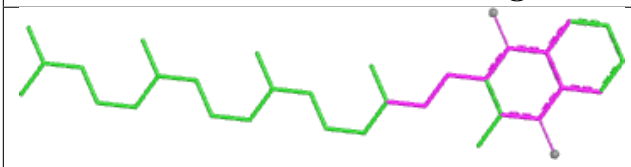
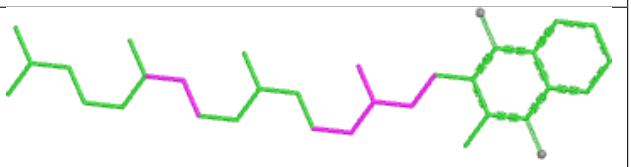


Rings

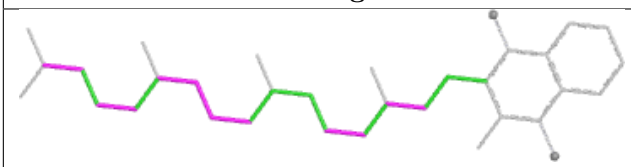
Ligand PQN BA 843



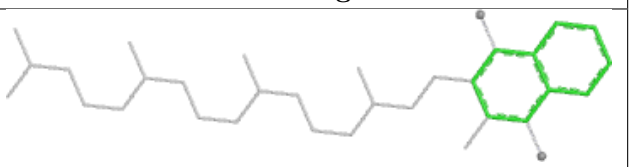
Bond lengths



Bond angles

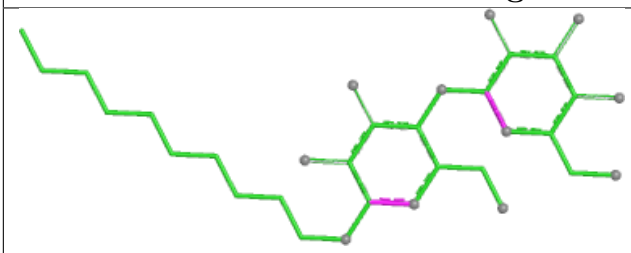


Torsions

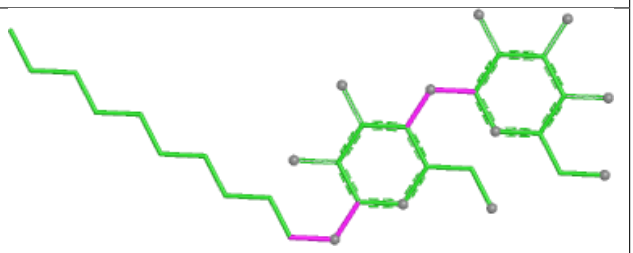


Rings

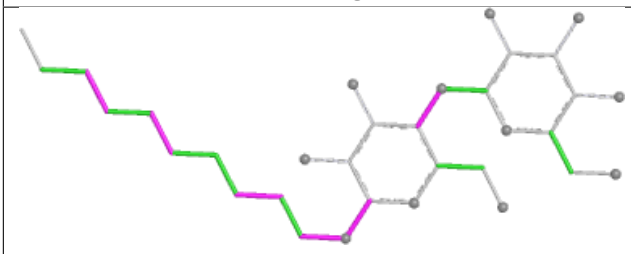
Ligand LMU BA 854



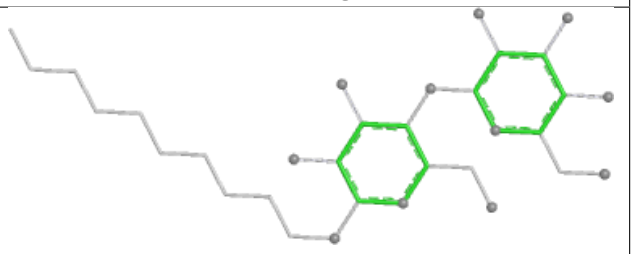
Bond lengths



Bond angles

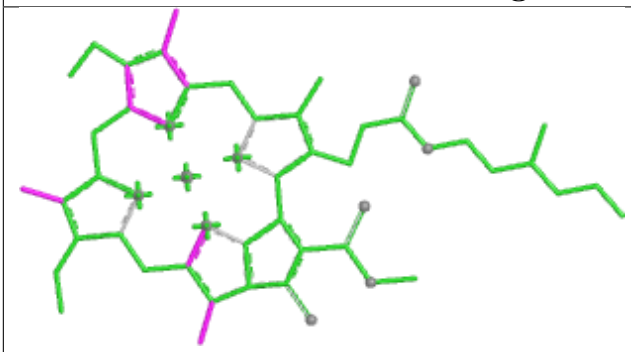


Torsions



Rings

Ligand CLA AA 839



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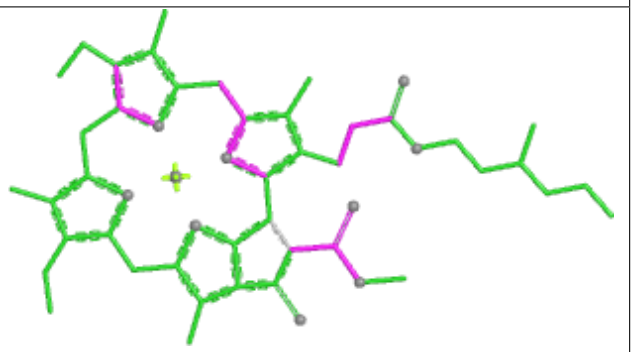
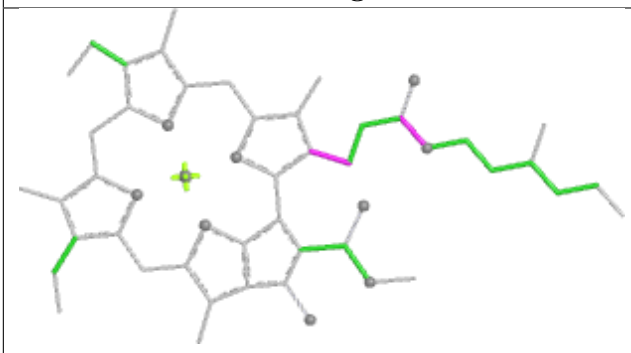
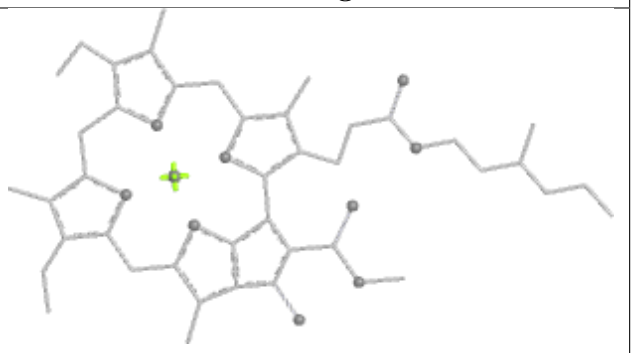


Bond angles

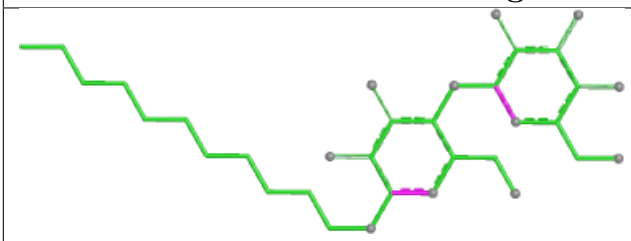


Torsions



Rings

Ligand LMU BA 853



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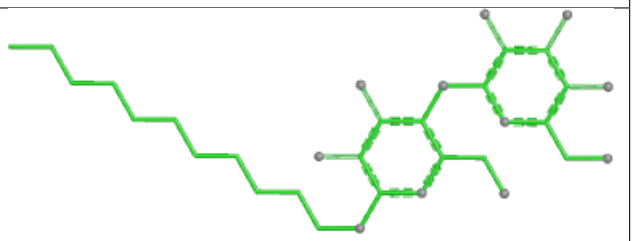
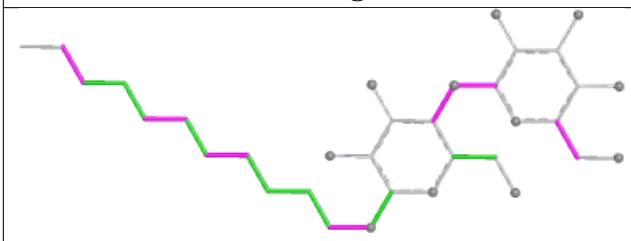


Bond angles



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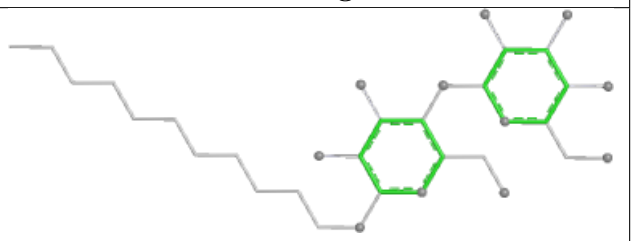
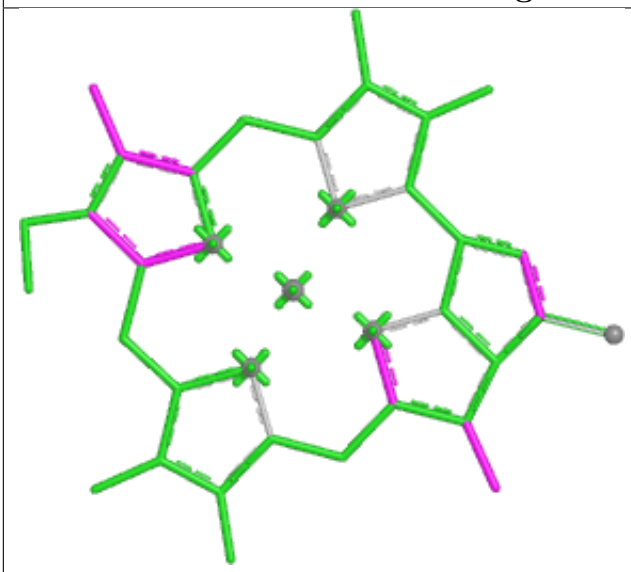


Rings

Ligand CLA B3 313



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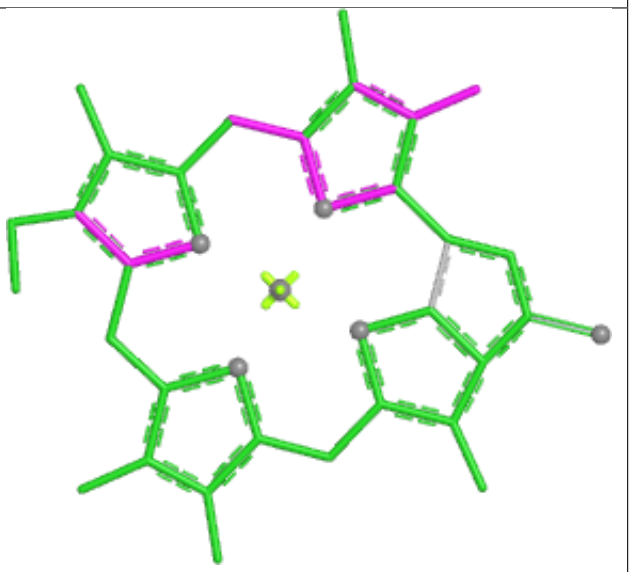
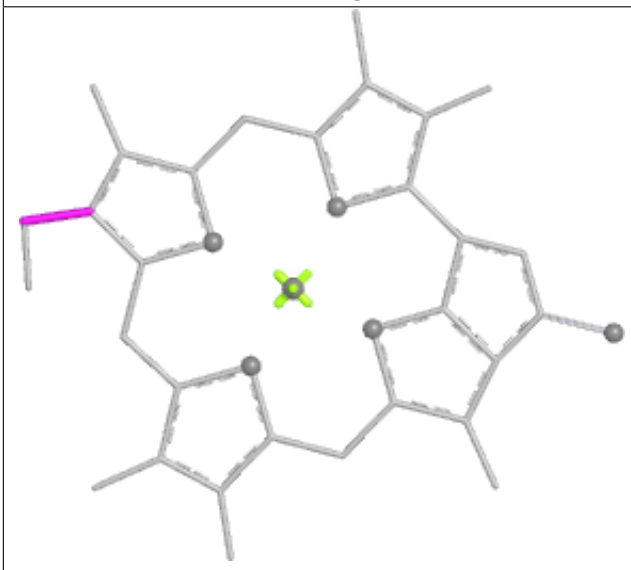


Bond angles



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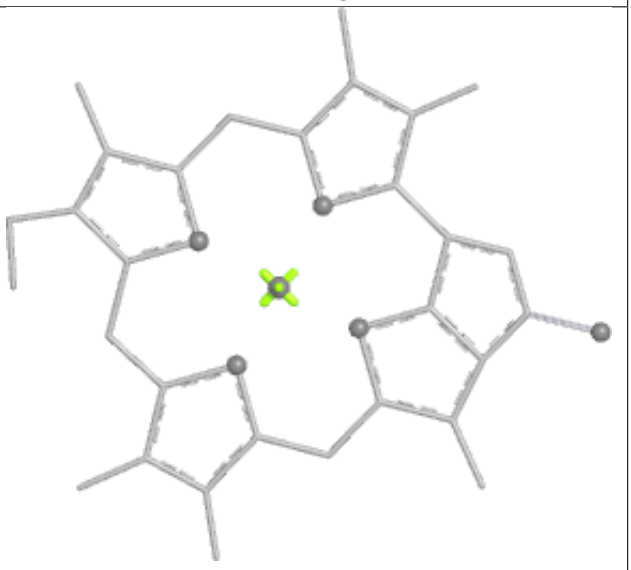
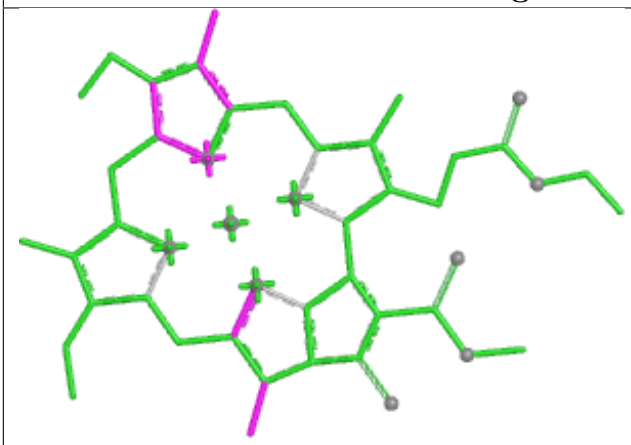


Rings

Ligand CLA BB 840



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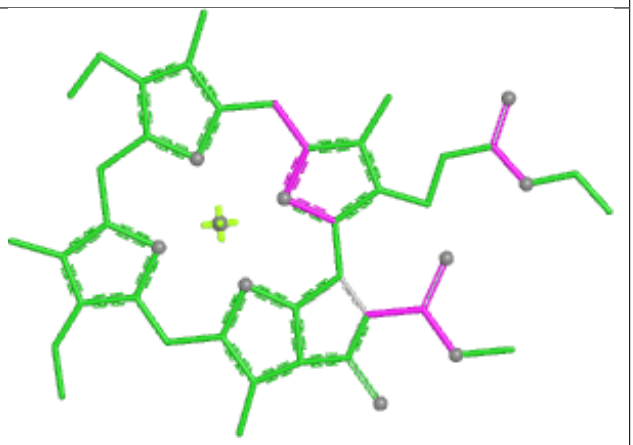
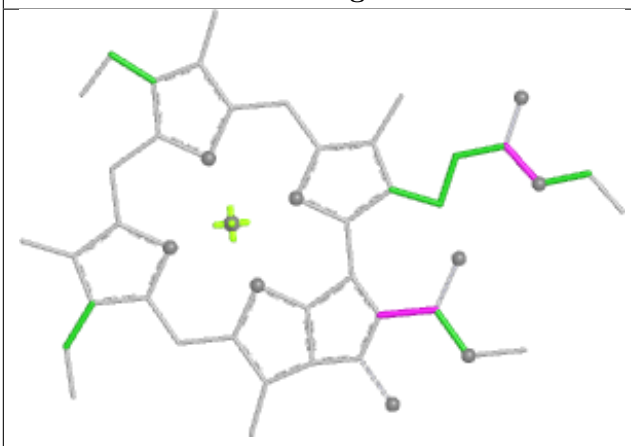


Bond angles



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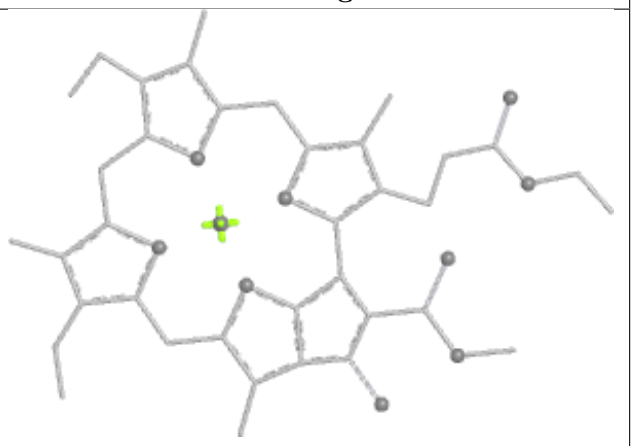
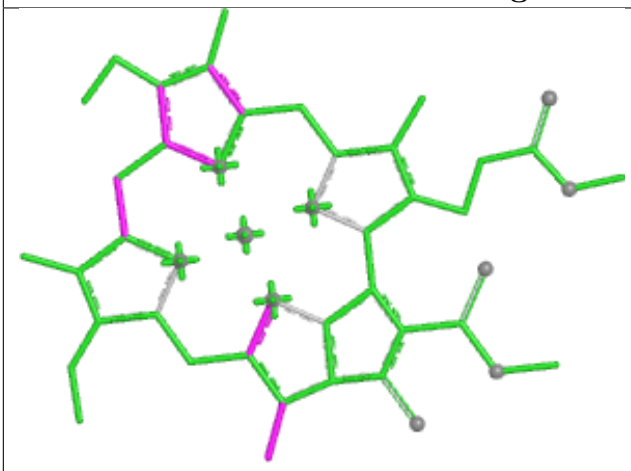


Rings

Ligand CLA BK 203



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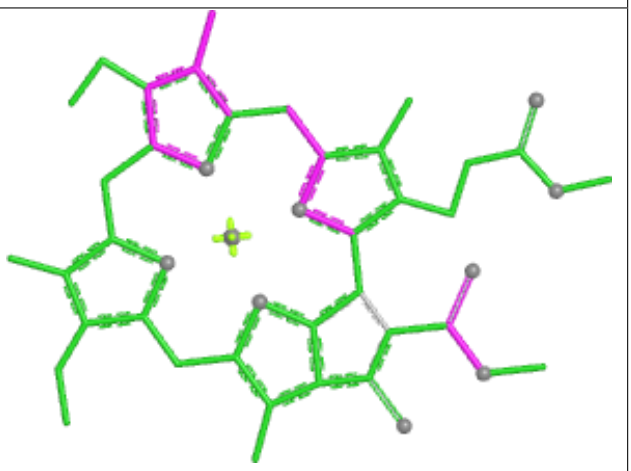
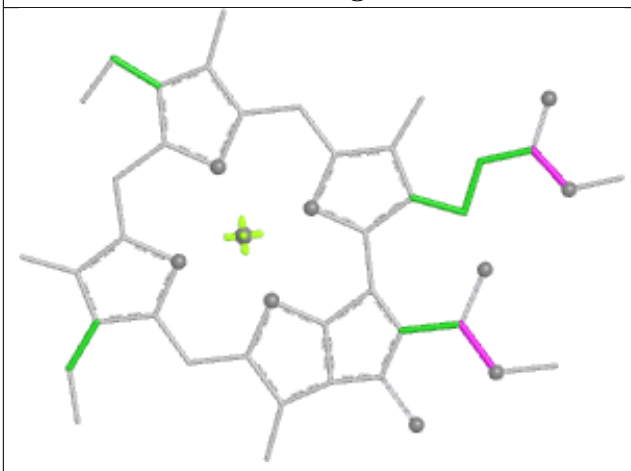
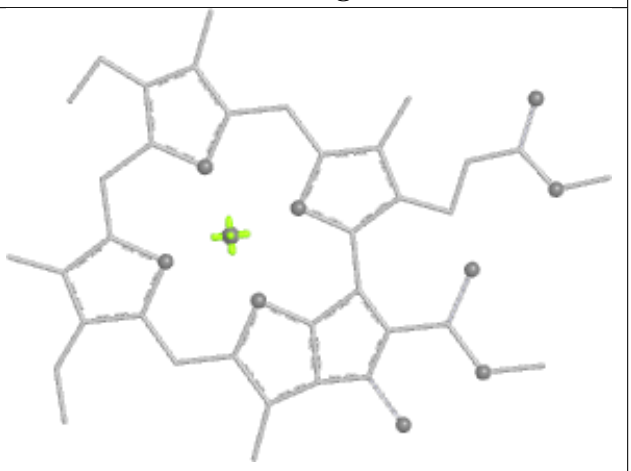


Bond angles

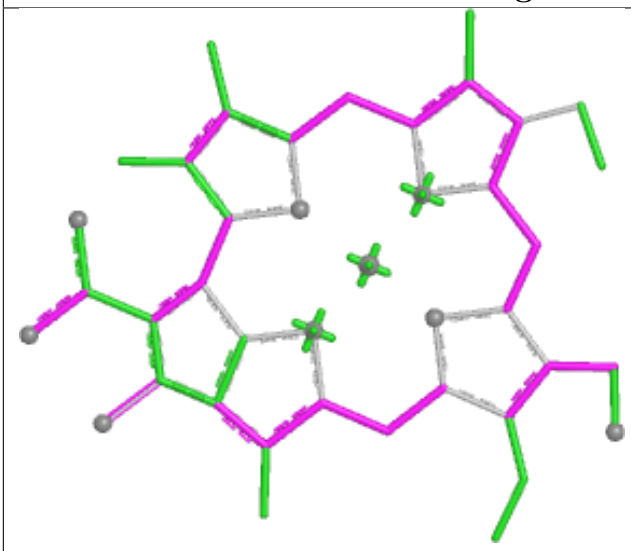


Torsions

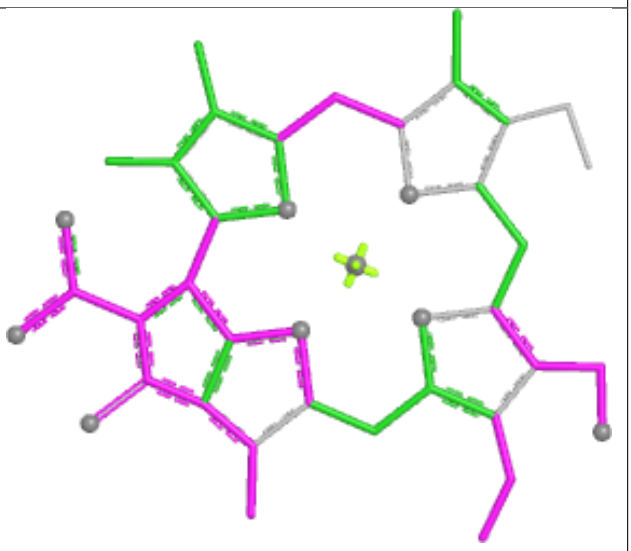


Rings

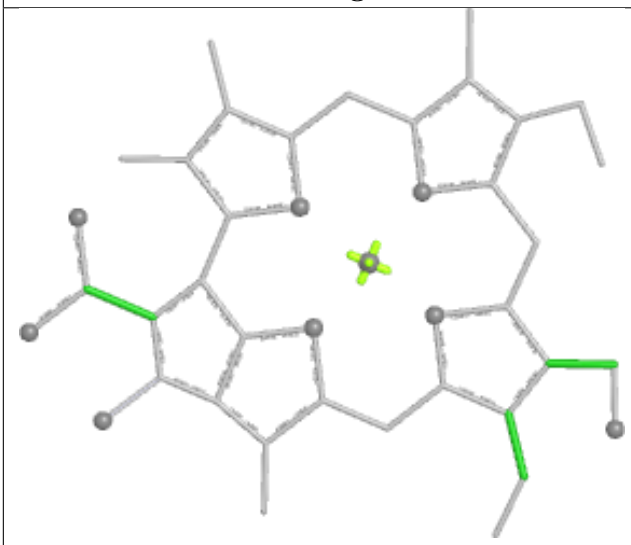
Ligand CHL B1 308



Bond lengths

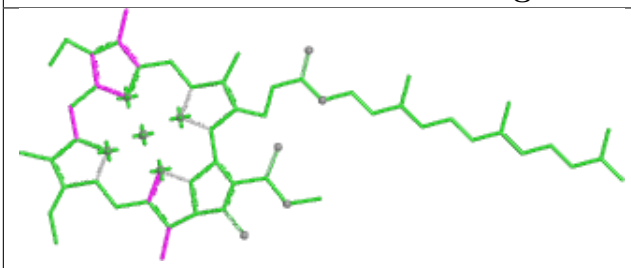
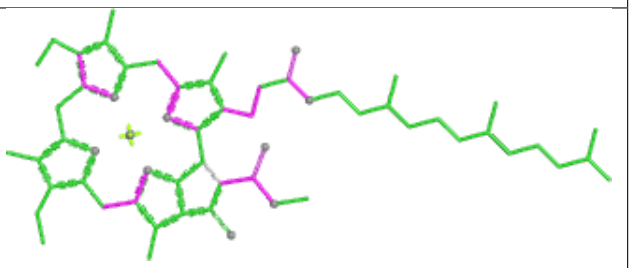
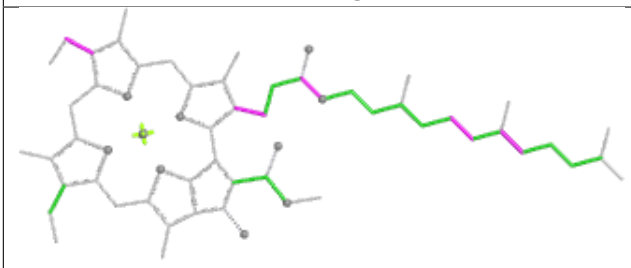
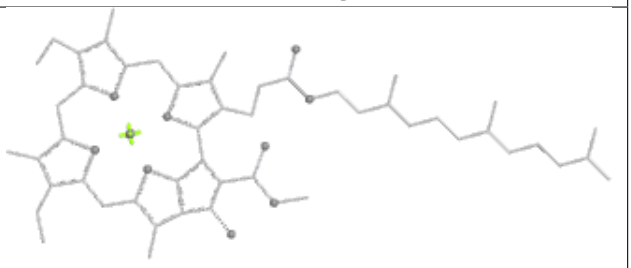


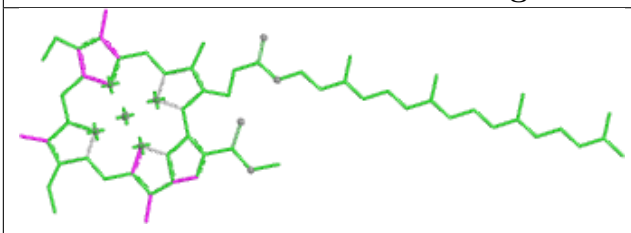
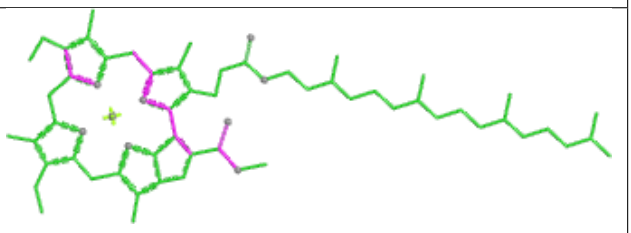
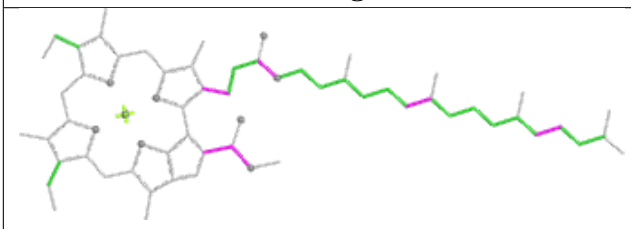
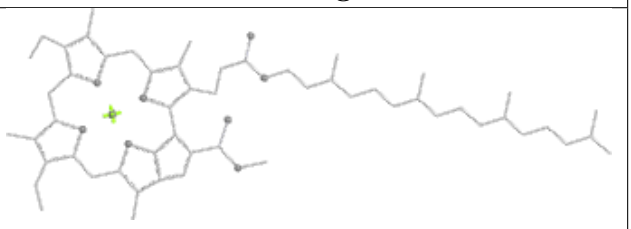
Bond angles



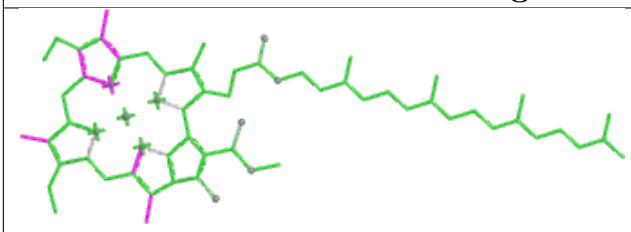
Torsions

Rings

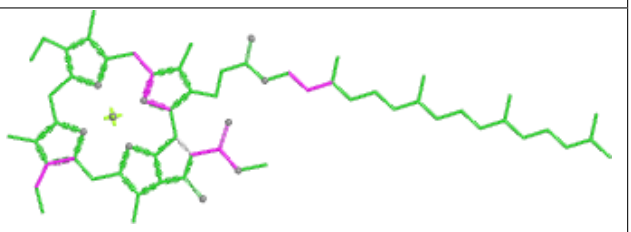
Ligand CLA BL 303	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AA 810	
	
Bond lengths	Bond angles
	
Torsions	Rings

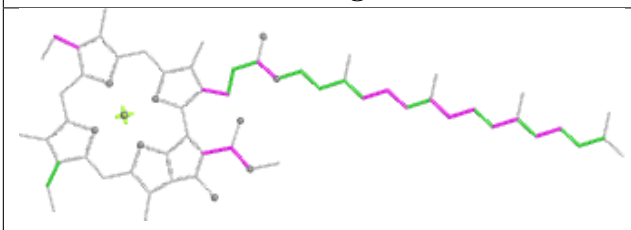
Ligand CLA BA 803



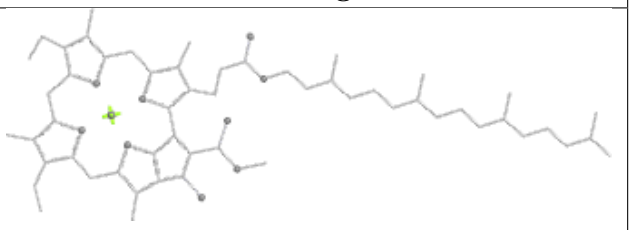
Bond lengths



Bond angles



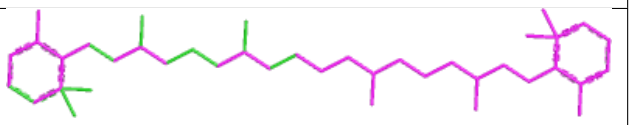
Torsions



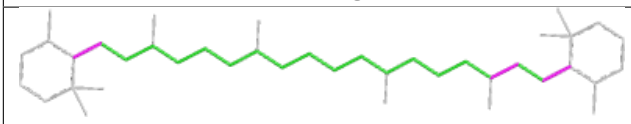
Rings

Ligand BCR B3 317

Bond lengths



Bond angles



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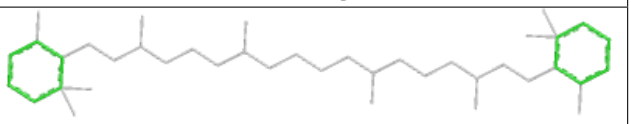
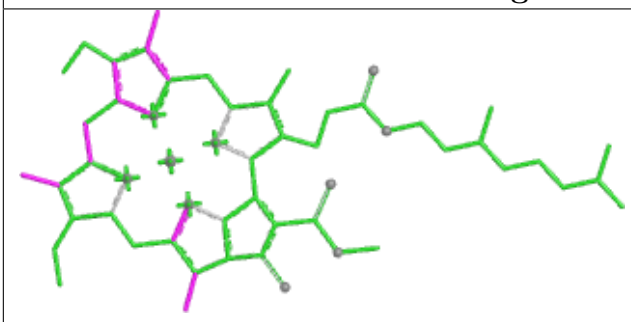
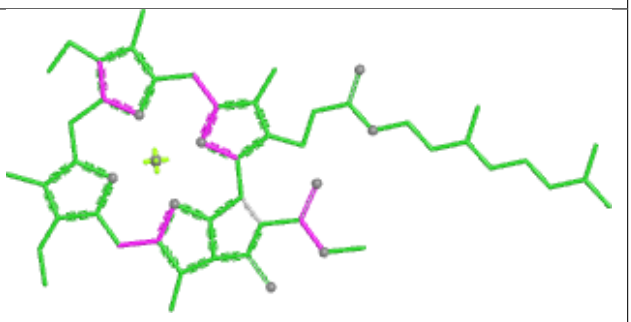


Rings

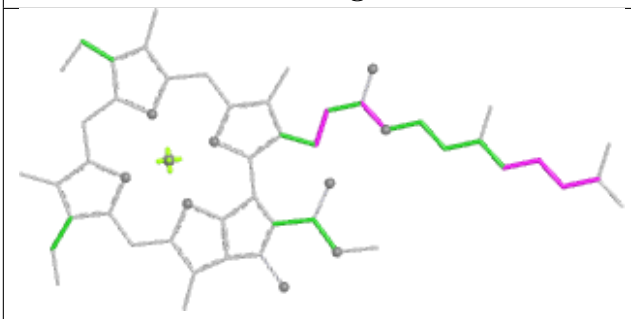
Ligand CLA AB 817



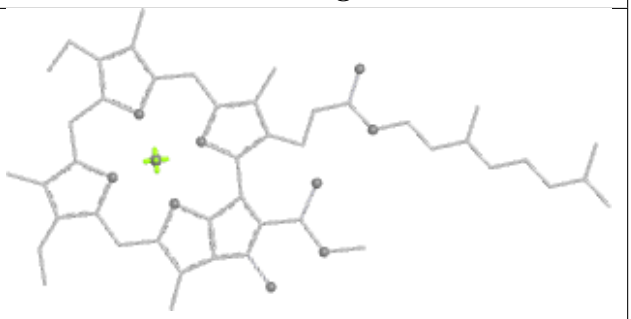
Bond lengths



Bond angles

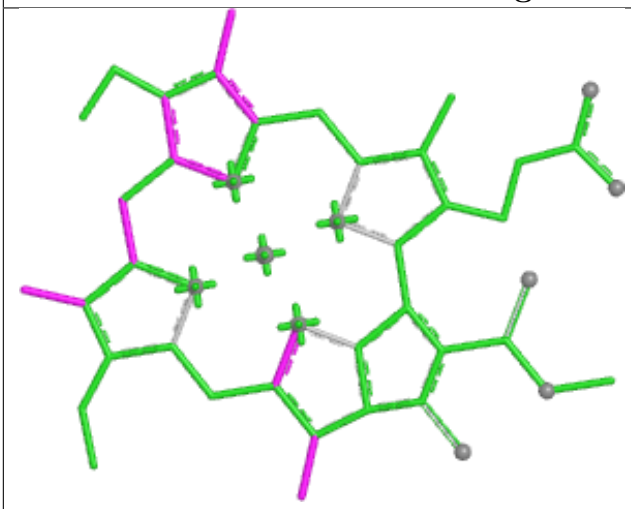


Torsions



Rings

Ligand CLA A1 313



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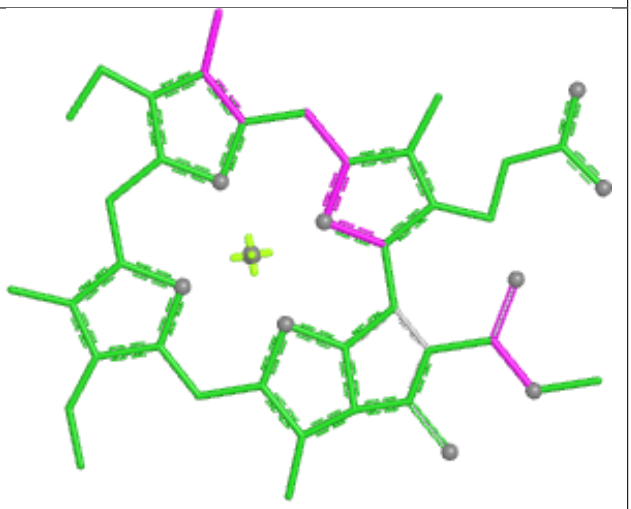
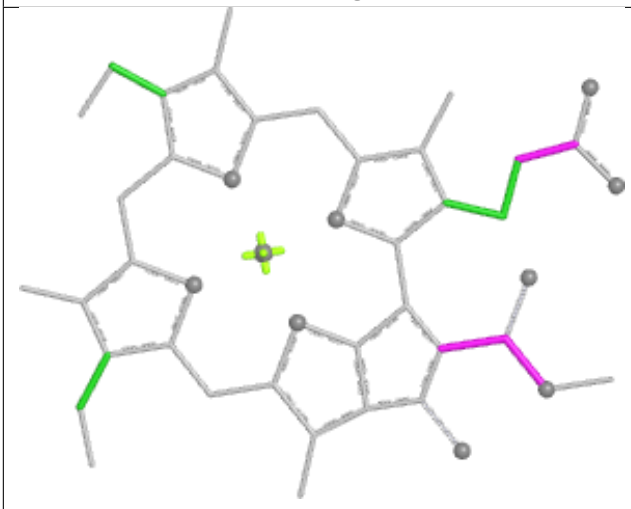


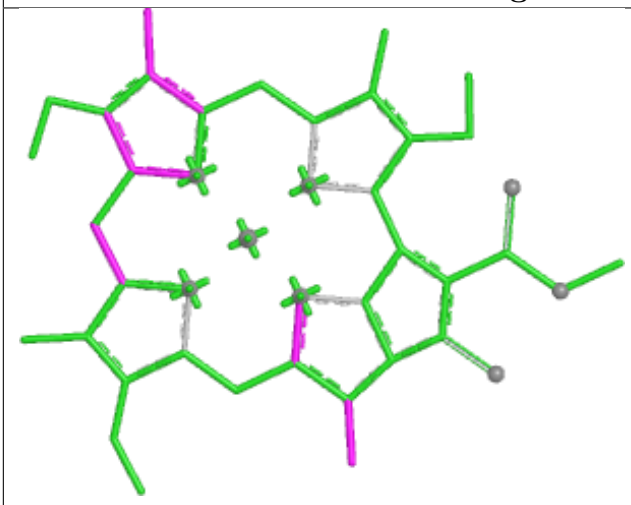
Bond angles



Torsions

Rings

Ligand CLA AG 203



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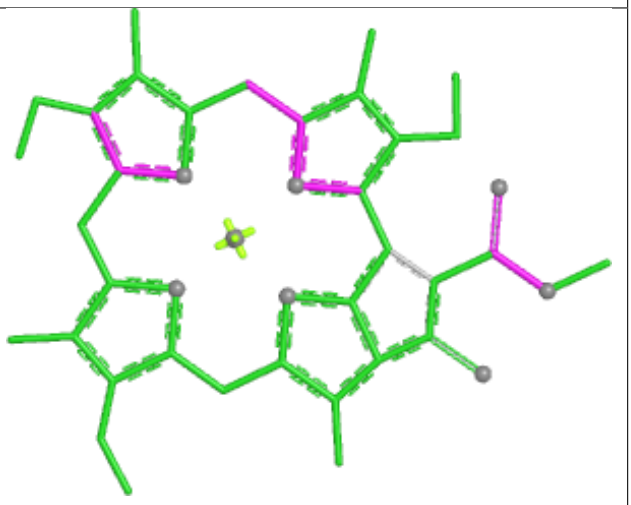
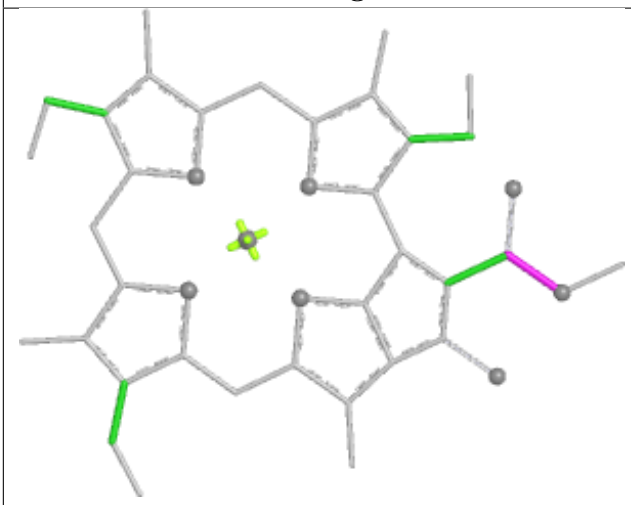


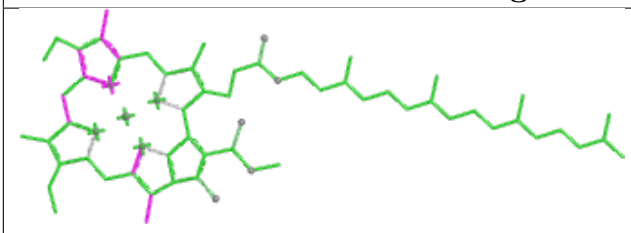
Bond angles



Torsions

Rings

Ligand CLA AA 840



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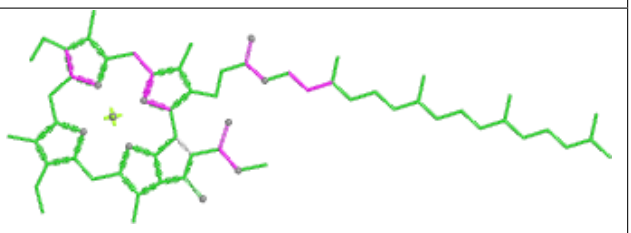
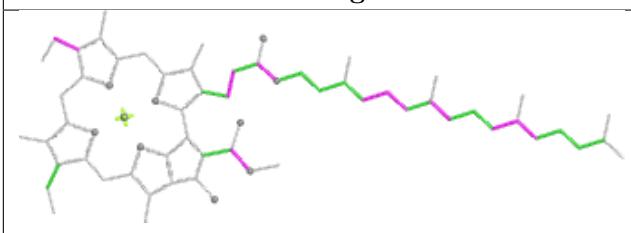
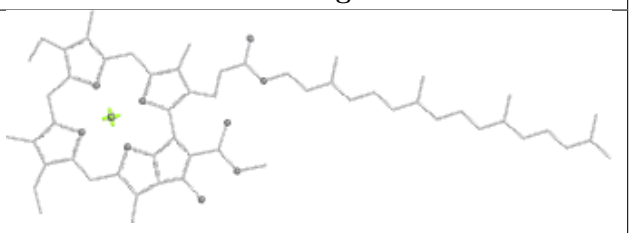


Bond angles

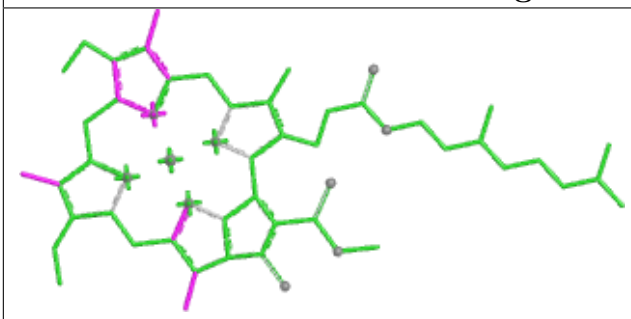


Torsions

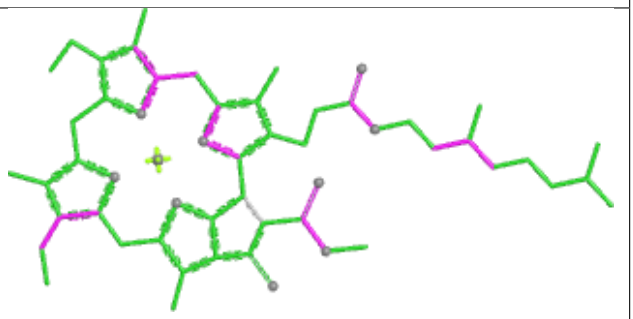


Rings

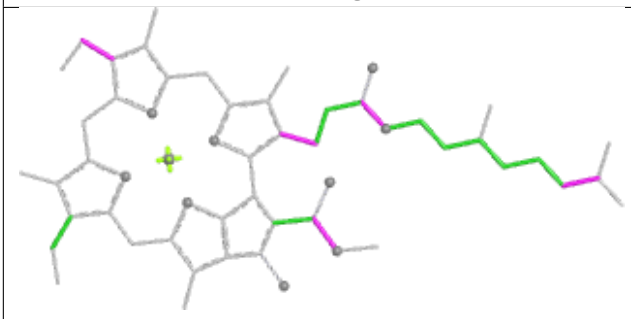
Ligand CLA A3 303



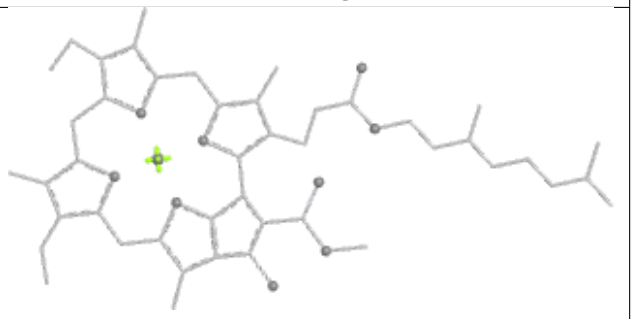
Bond lengths



Bond angles

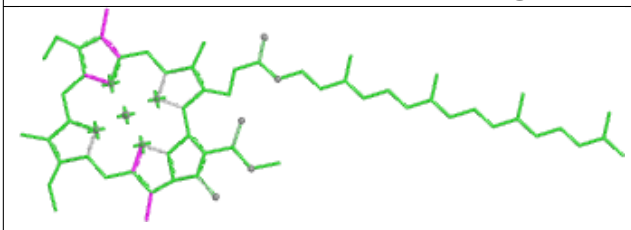


Torsions

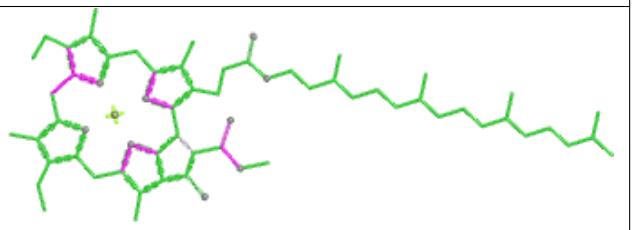


Rings

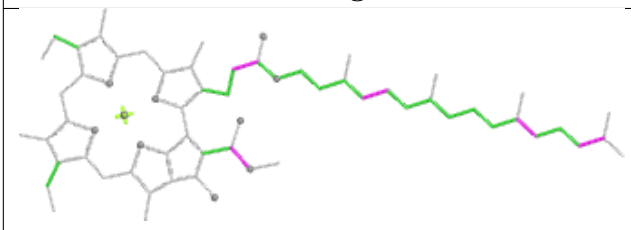
Ligand CLA BA 801



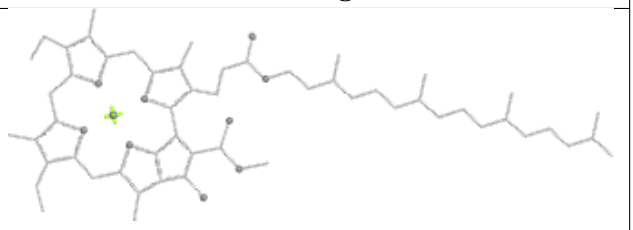
Bond lengths



Bond angles

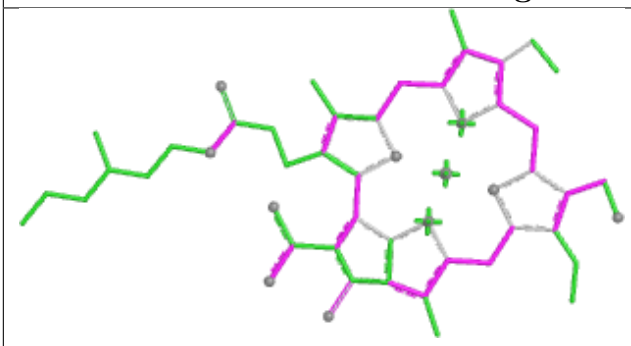


Torsions



Rings

Ligand CHL A6 602



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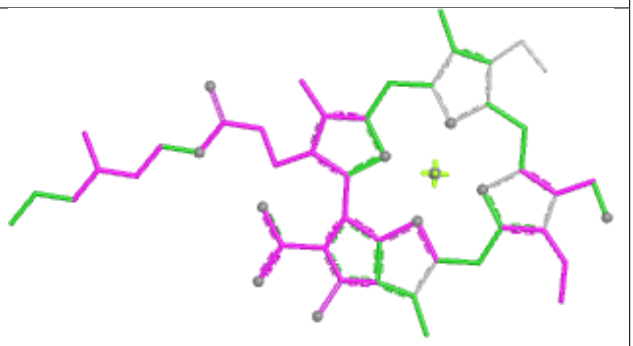
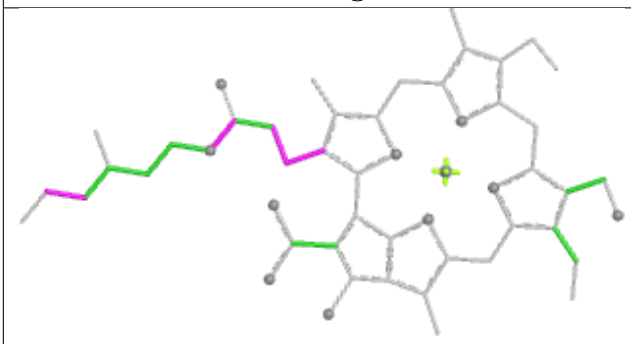


Bond angles



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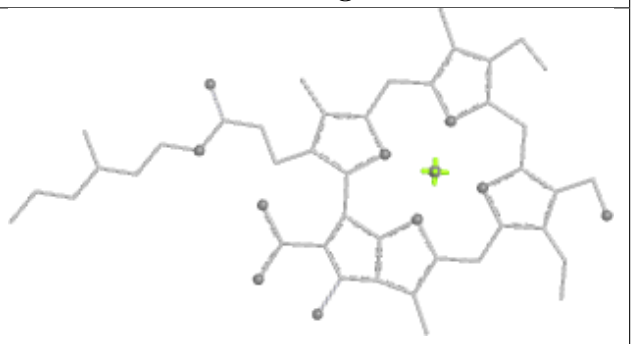
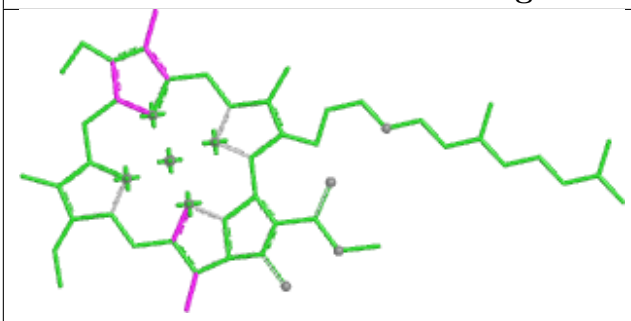


Rings

Ligand CLA B1 305



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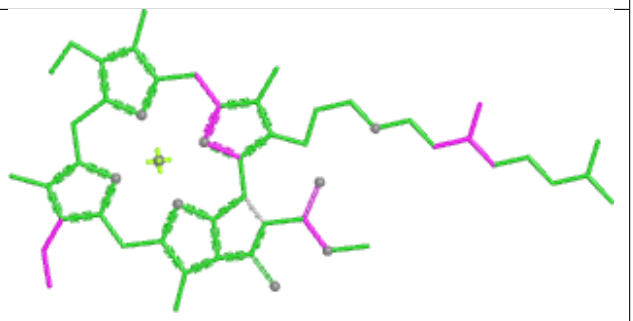
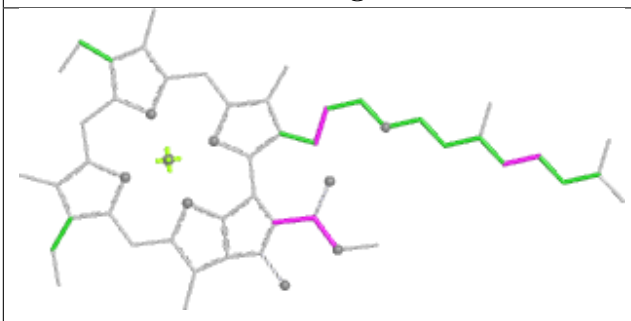
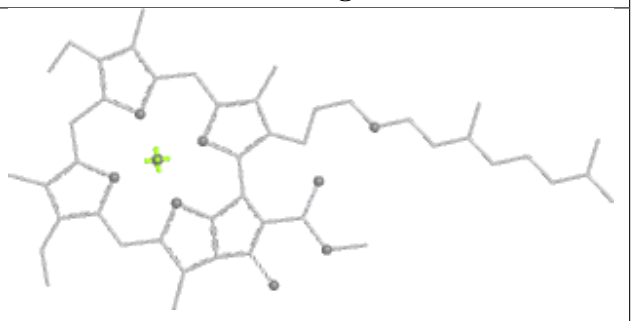


Bond angles

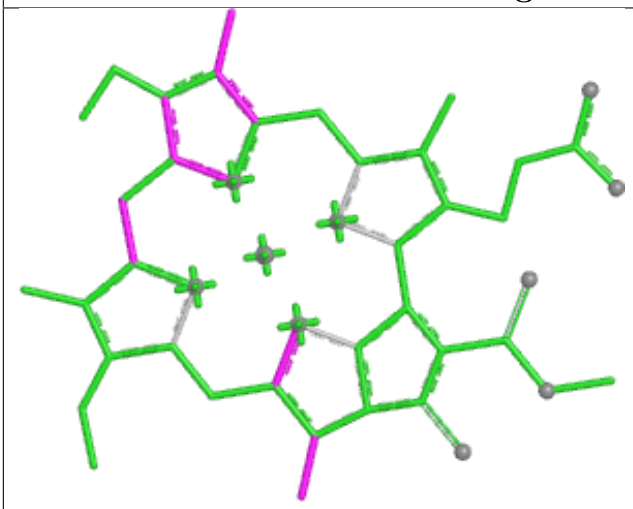


Torsions



Rings

Ligand CLA B5 613



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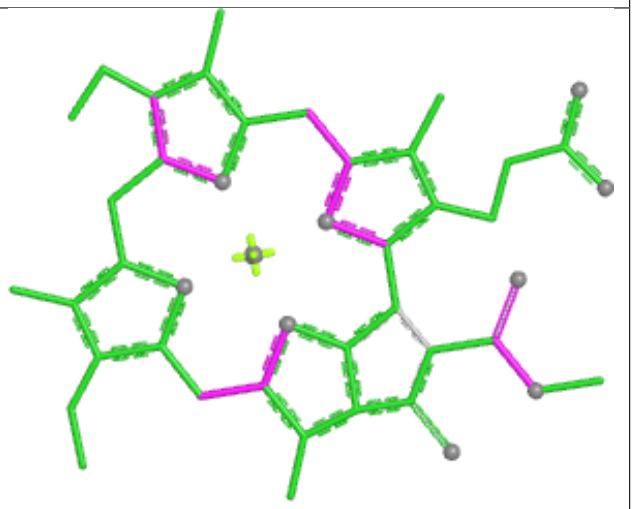
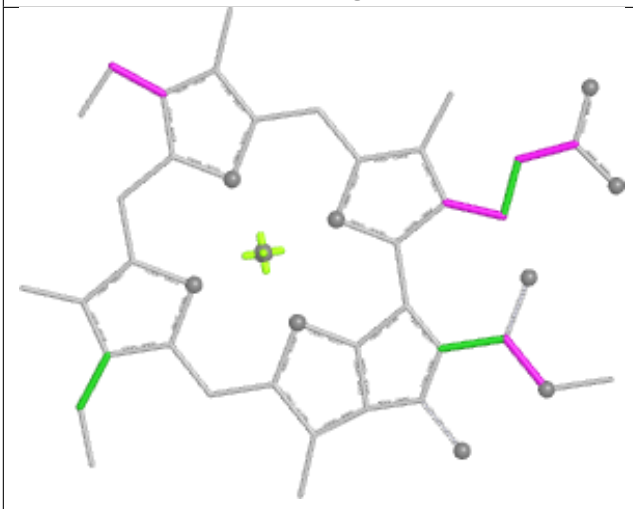


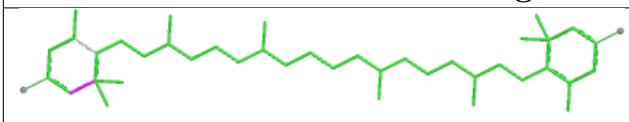
Bond angles



Torsions

Rings

Ligand LUT A6 615



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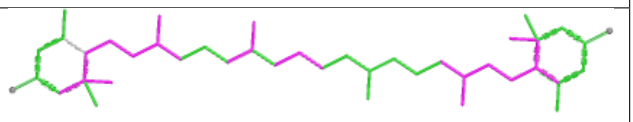
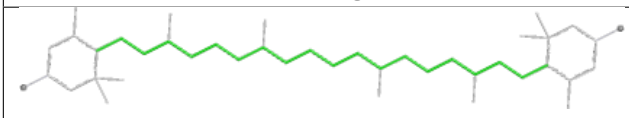
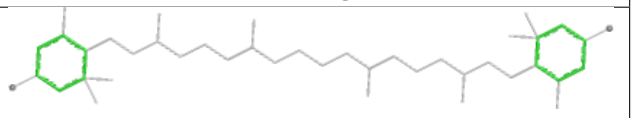


Bond angles

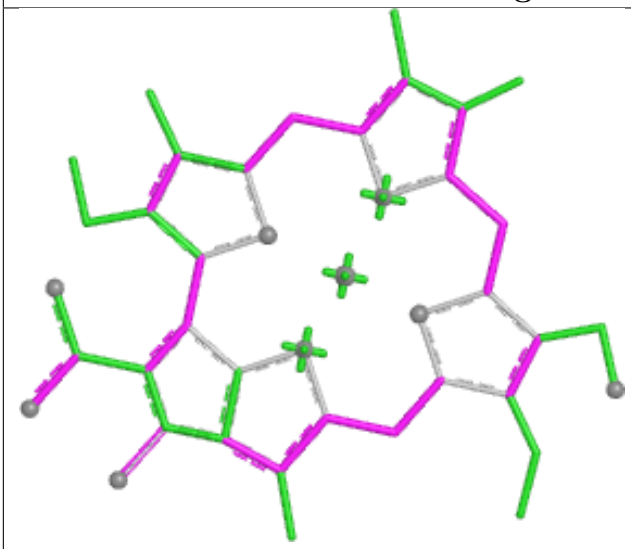


Torsions



Rings

Ligand CHL A4 314



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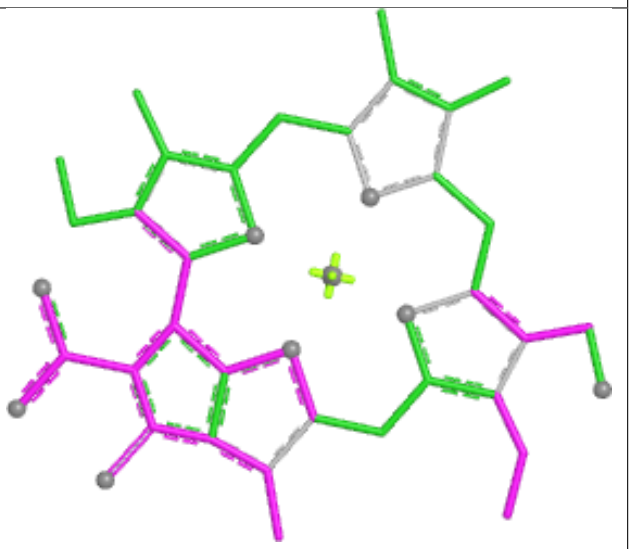
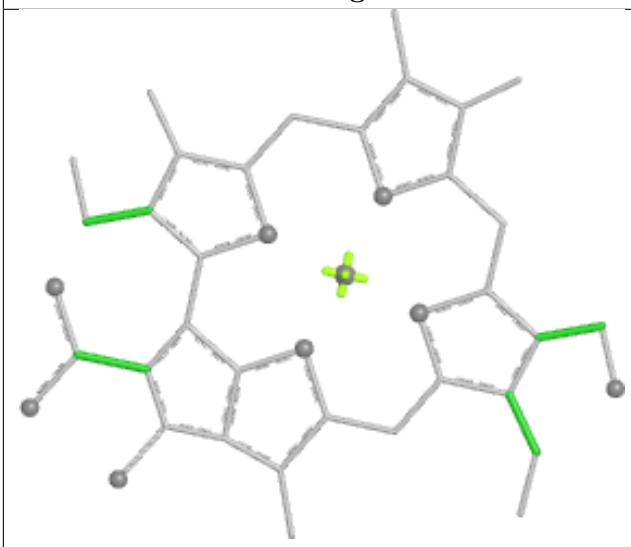


Bond angles



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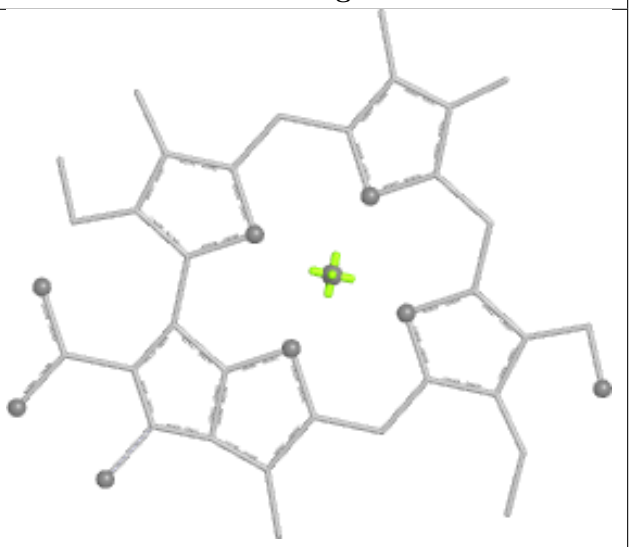
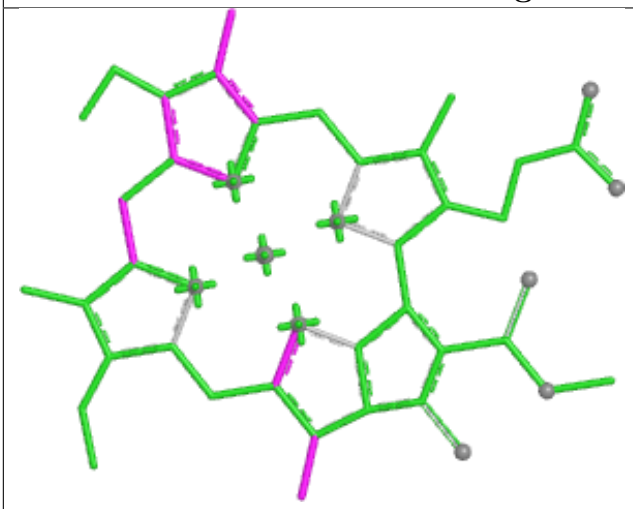


Rings

Ligand CLA A4 312



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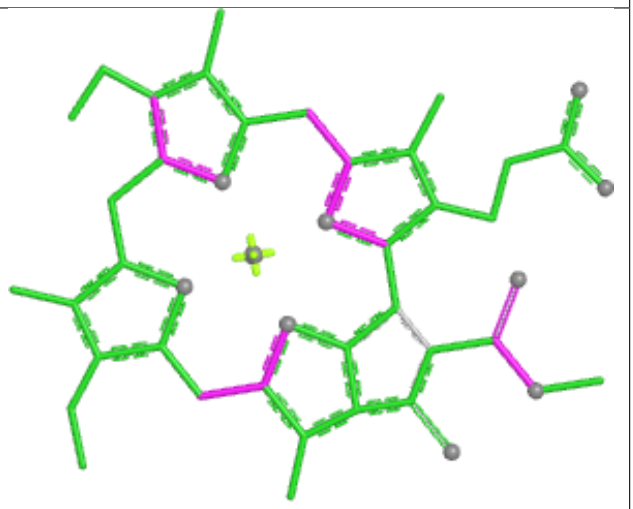
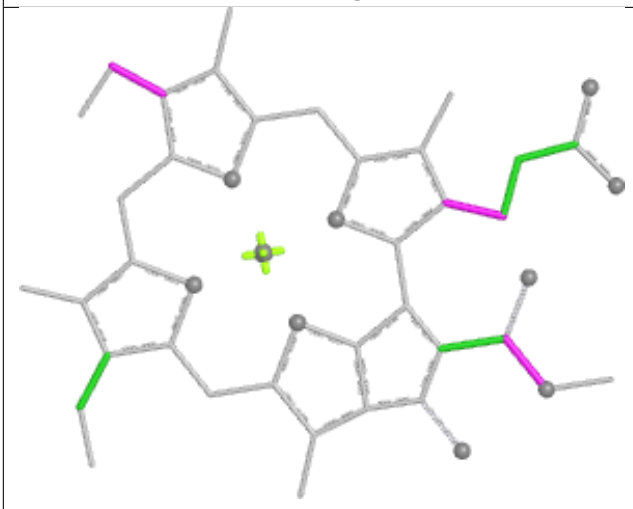


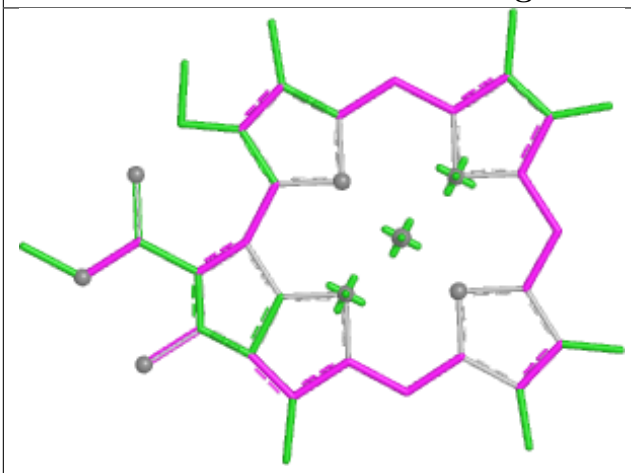
Bond angles



Torsions

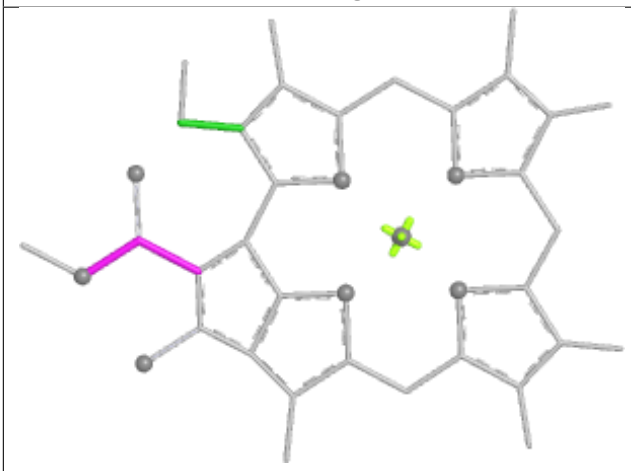
Rings

Ligand CHL B5 606



Bond lengths

Bond angles



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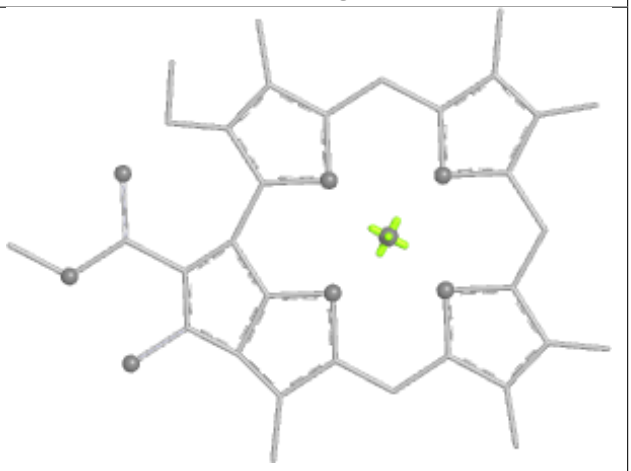
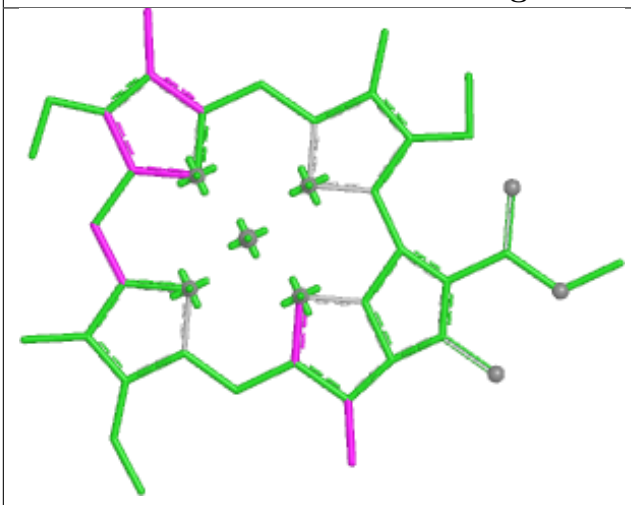


Rings

Ligand CLA AA 822



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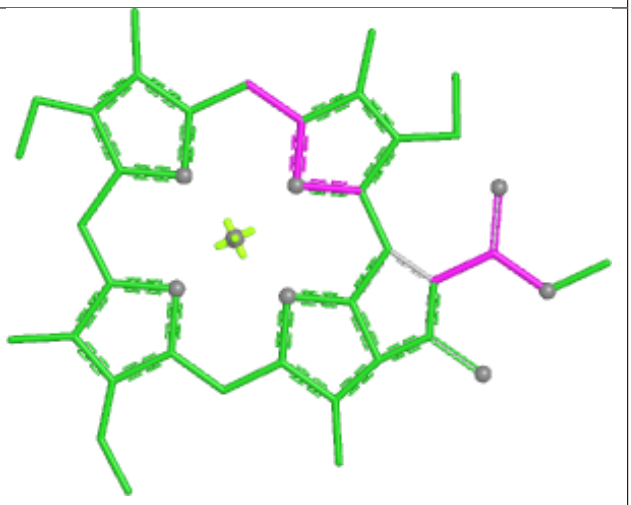
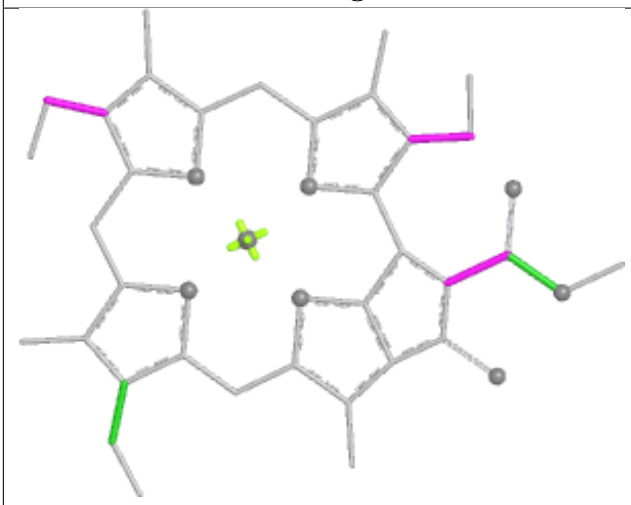


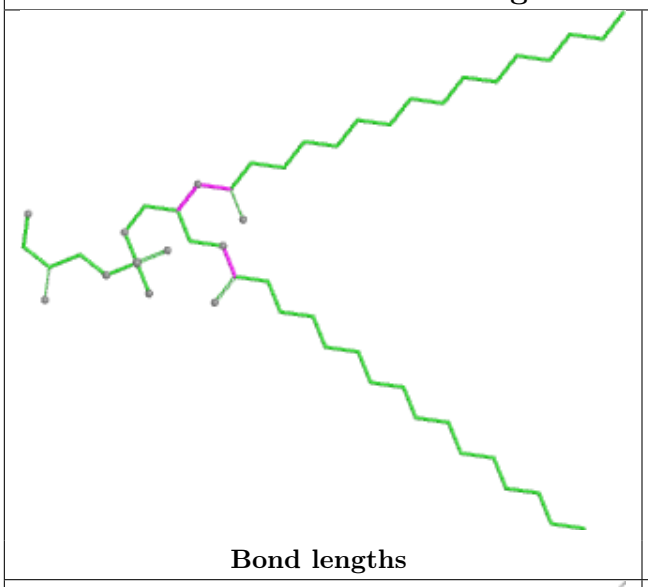
Bond angles



Torsions

Rings

Ligand LHG BA 845



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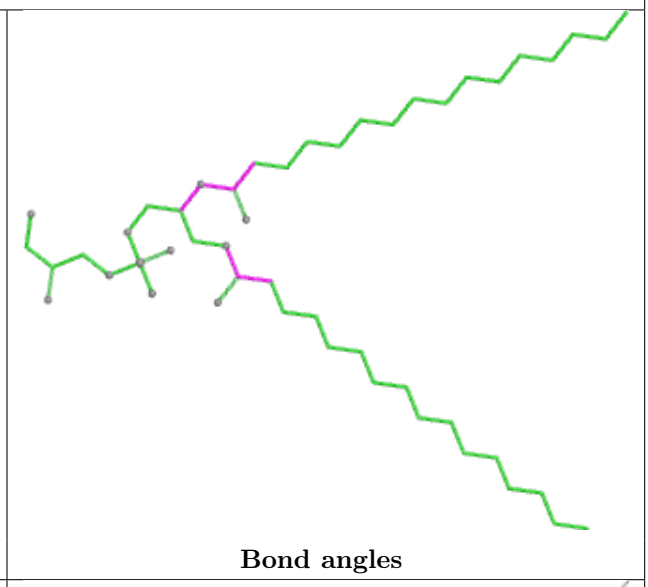
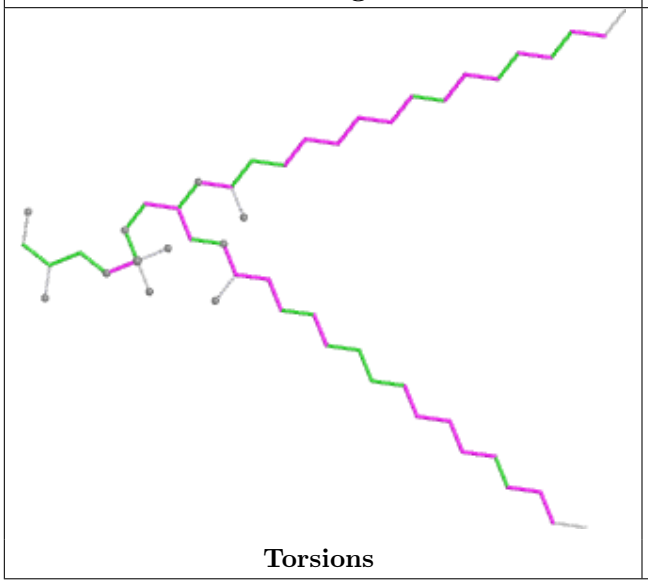
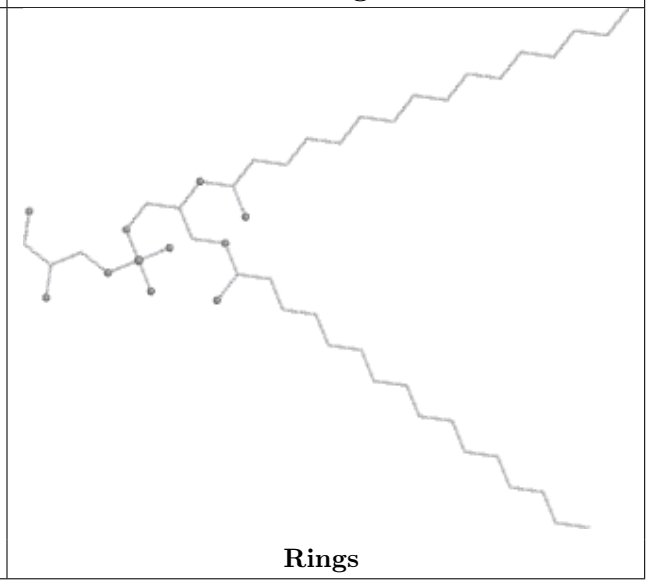


Bond angles

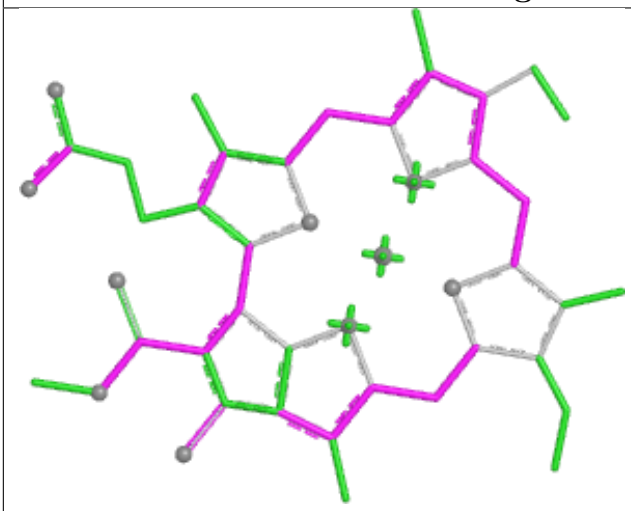


Torsions



Rings

Ligand CHL A3 307



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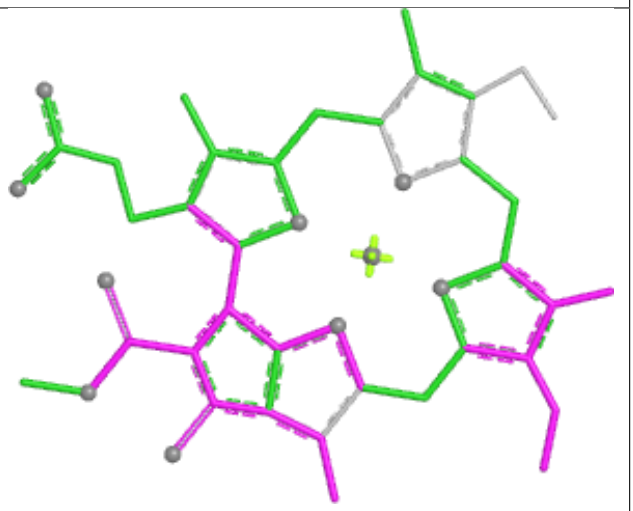
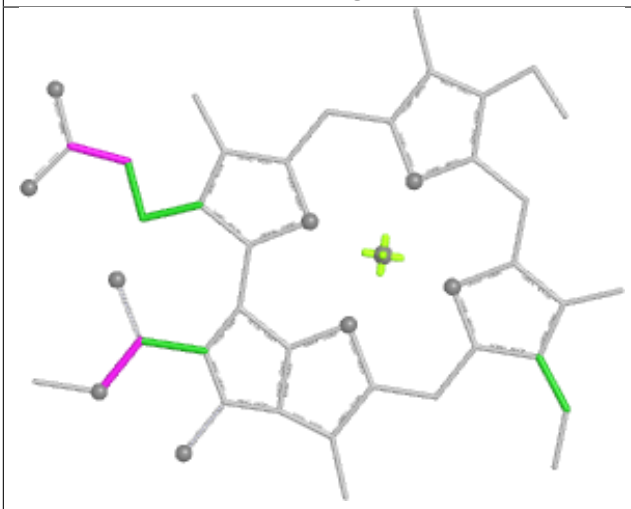


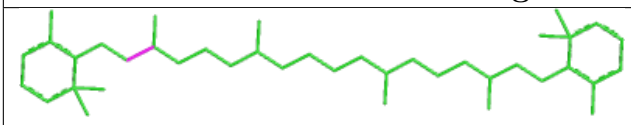
Bond angles



Torsions

Rings

Ligand BCR BL 301



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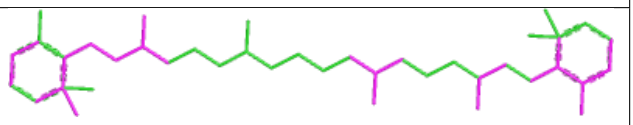
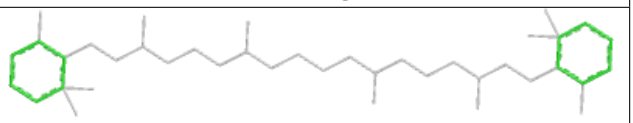


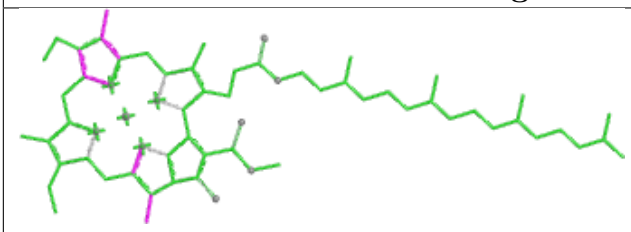
Bond angles

Torsions

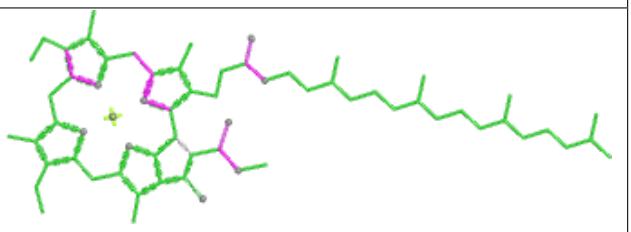


Rings

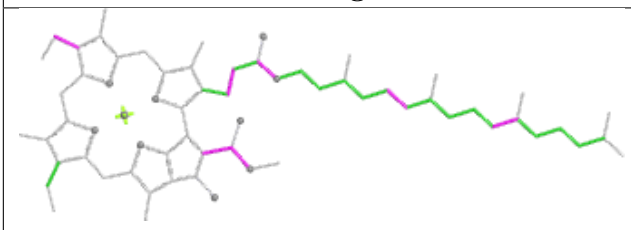
Ligand CLA BA 808



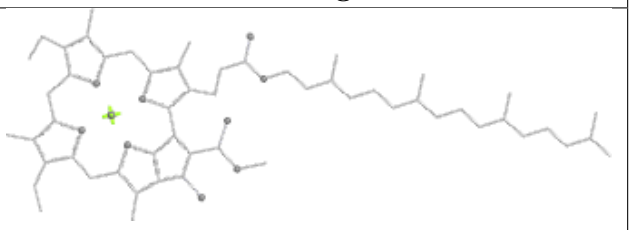
Bond lengths



Bond angles

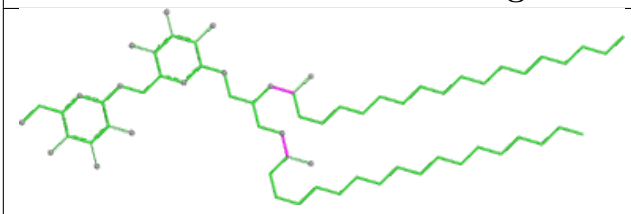


Torsions

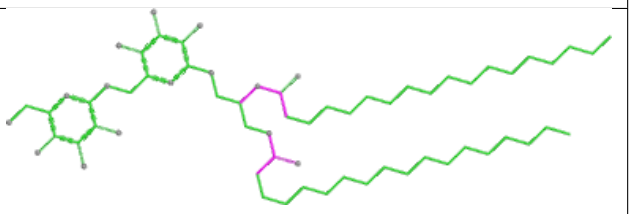


Rings

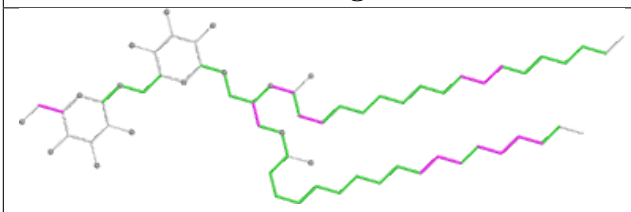
Ligand DGD BB 850



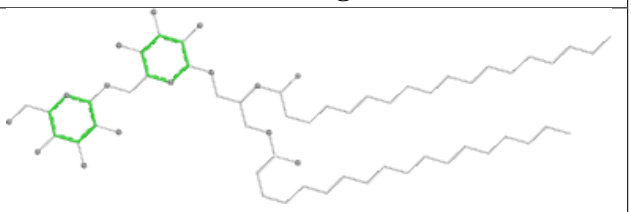
Bond lengths



Bond angles

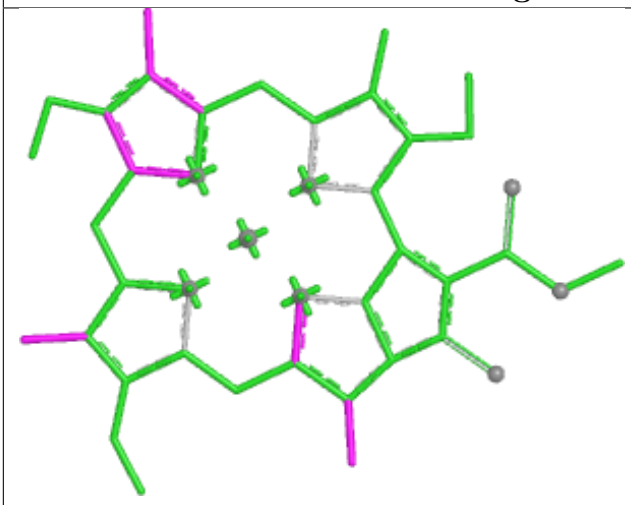


Torsions

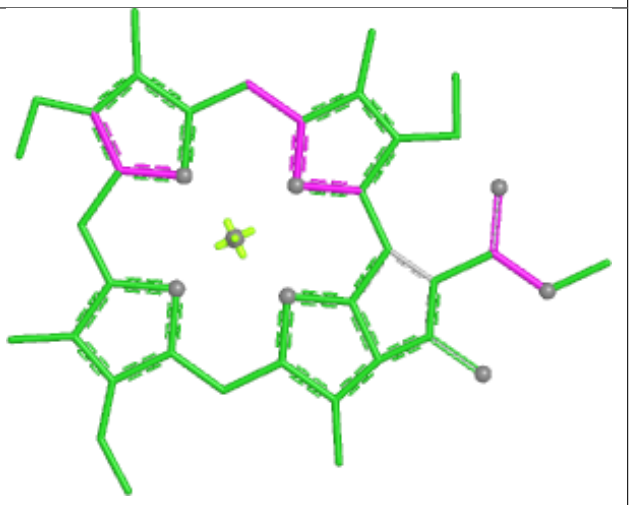


Rings

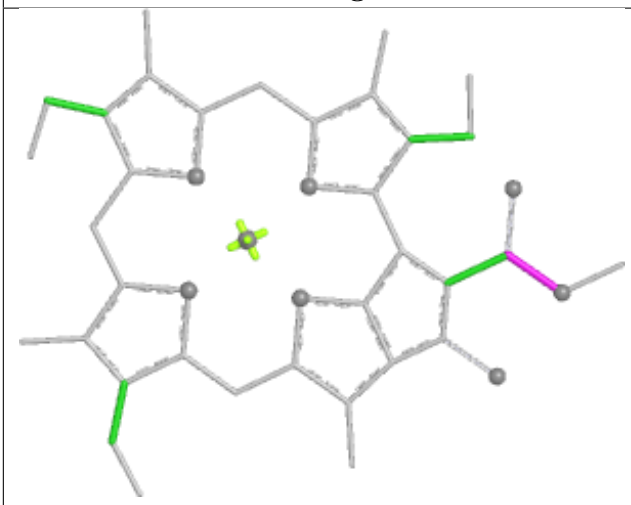
Ligand CLA BF 302



Bond lengths



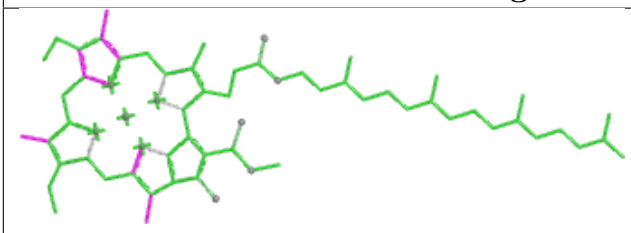
Bond angles



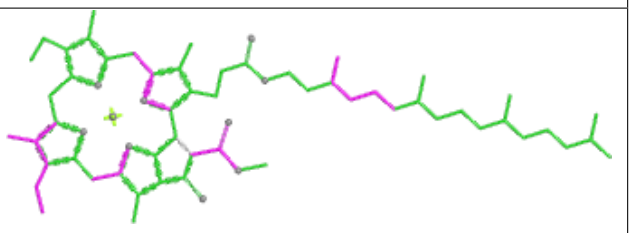
Torsions

Rings

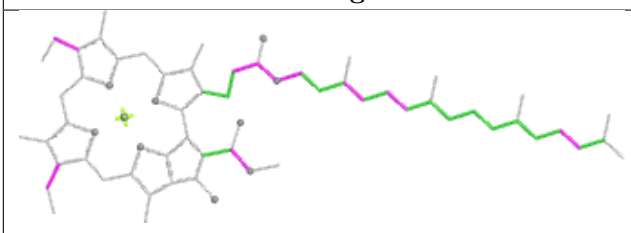
Ligand CLA AA 834



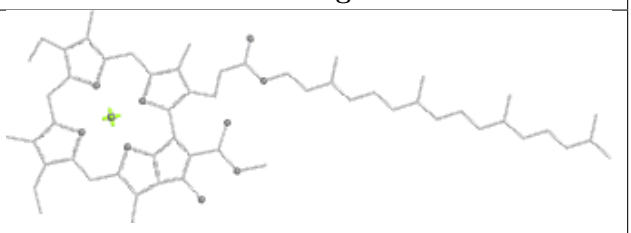
Bond lengths



Bond angles

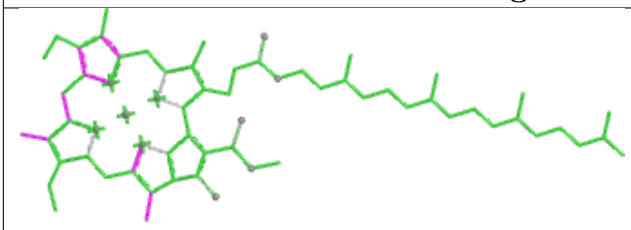


Torsions

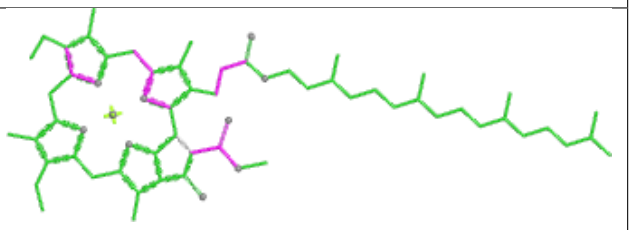


Rings

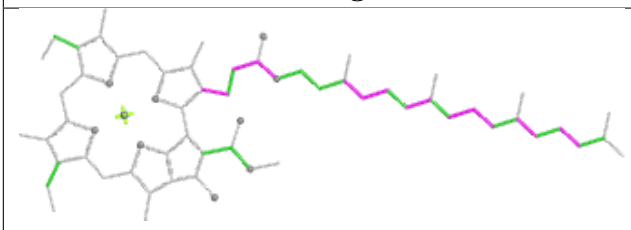
Ligand CLA AA 827



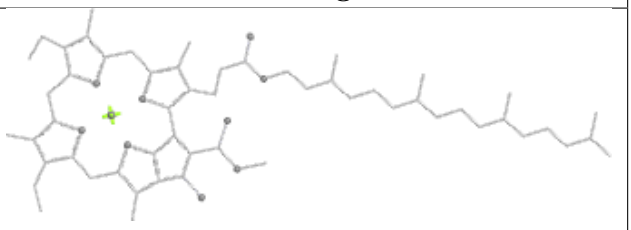
Bond lengths



Bond angles

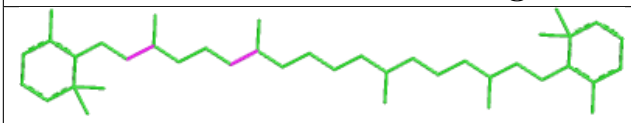


Torsions



Rings

Ligand BCR AA 847



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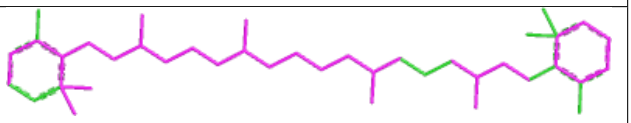
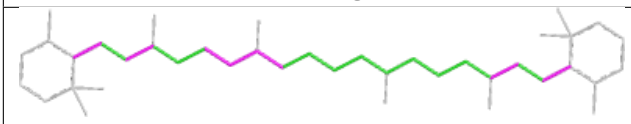
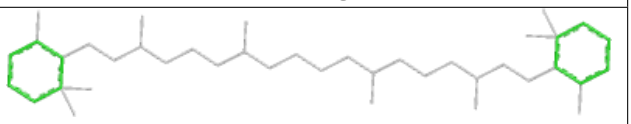


Bond angles

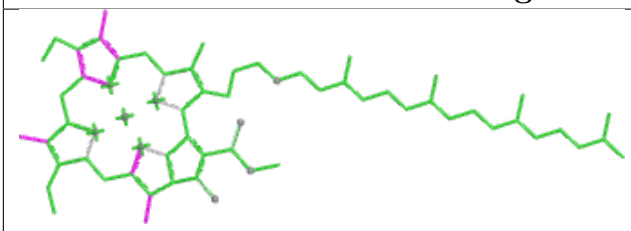


Torsions



Rings

Ligand CLA A6 613



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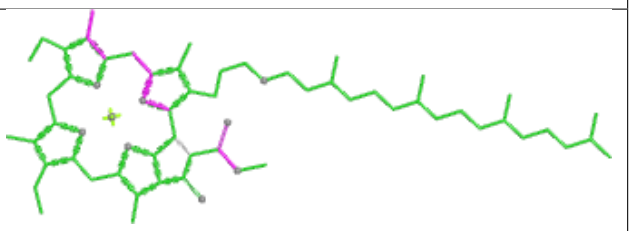
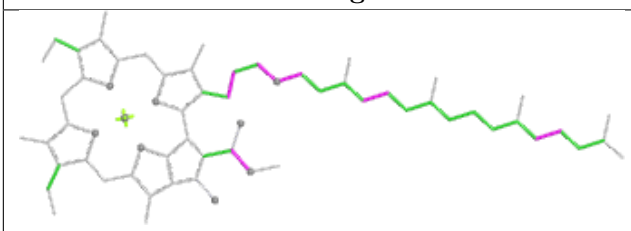
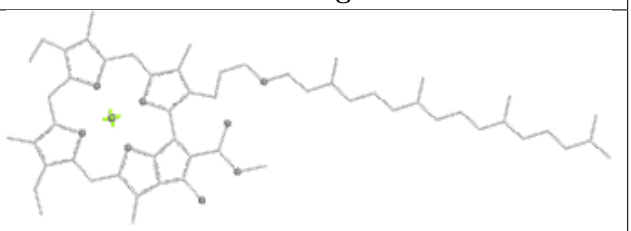


Bond angles

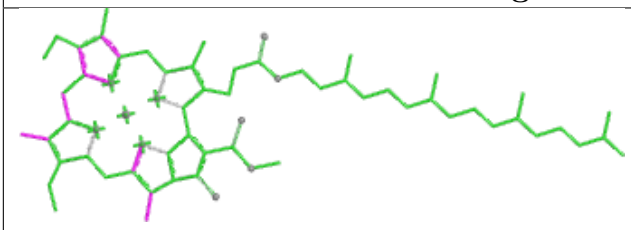


Torsions



Rings

Ligand CLA BB 829



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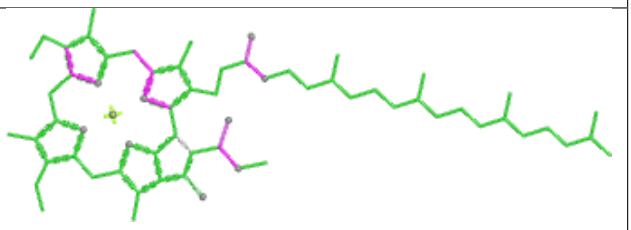
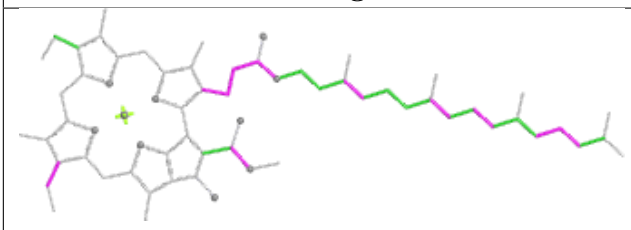


Bond angles



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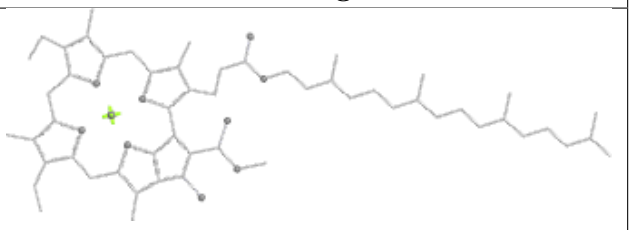
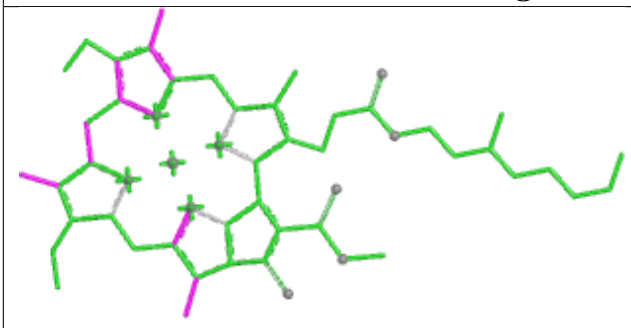


Rings

Ligand CLA A4 308



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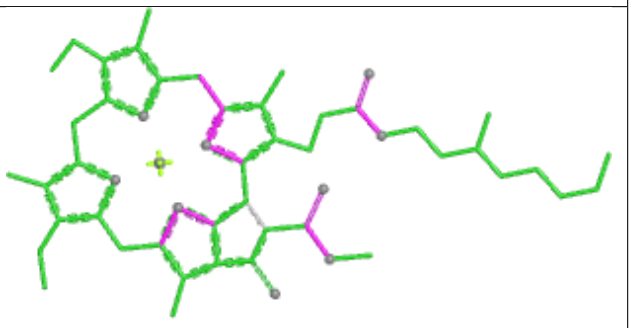
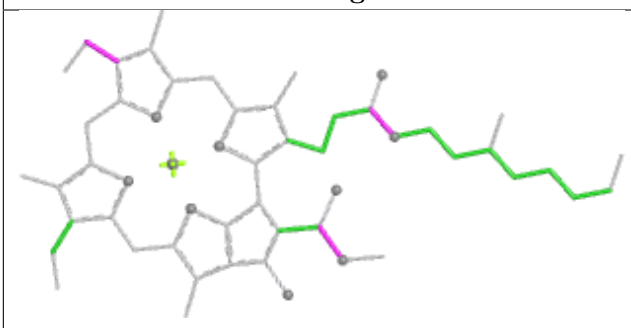


Bond angles



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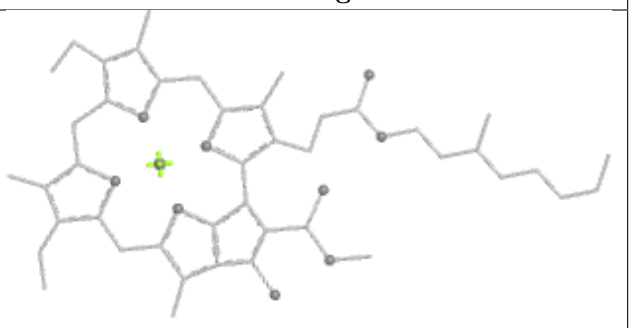
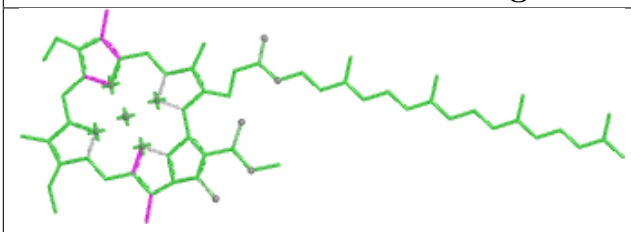


Rings

Ligand CLA AA 801



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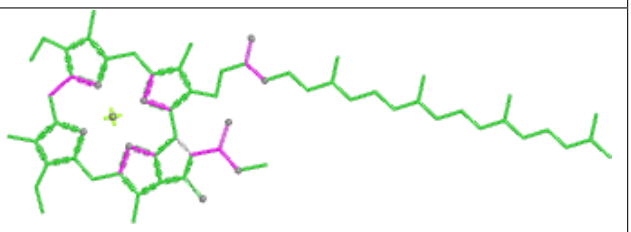
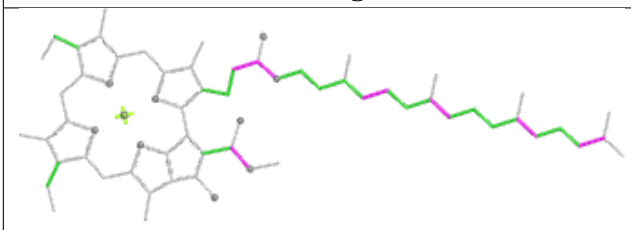


Bond angles



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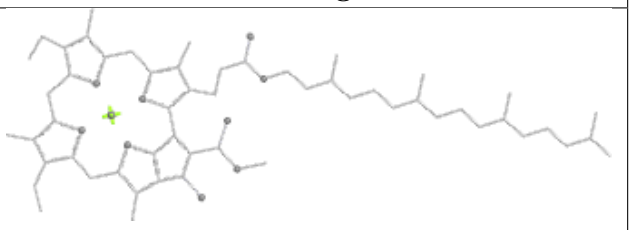
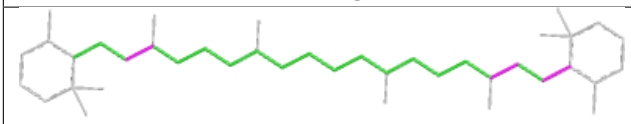


Rings

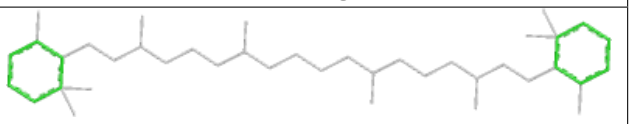
Ligand BCR AB 849

Bond lengths

Bond angles

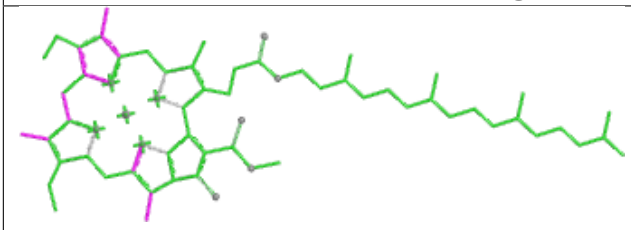


Torsions

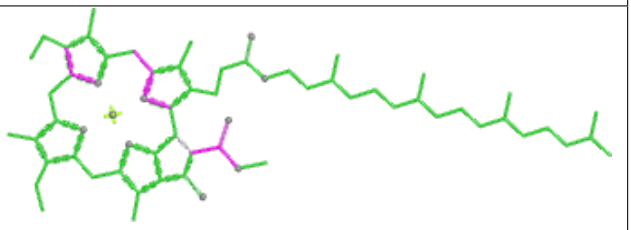


Rings

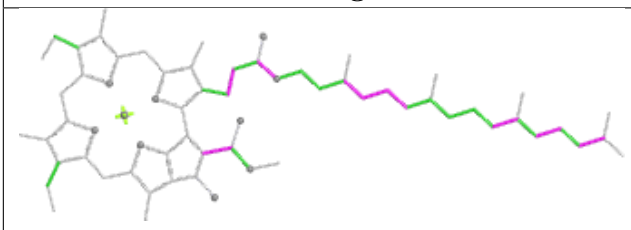
Ligand CLA AA 806



Bond lengths



Bond angles



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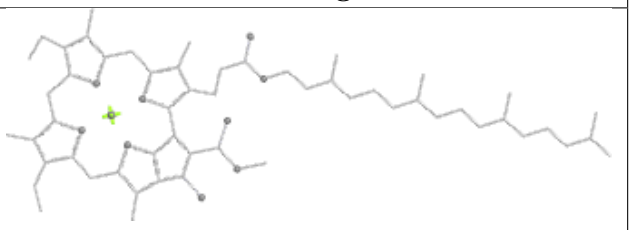
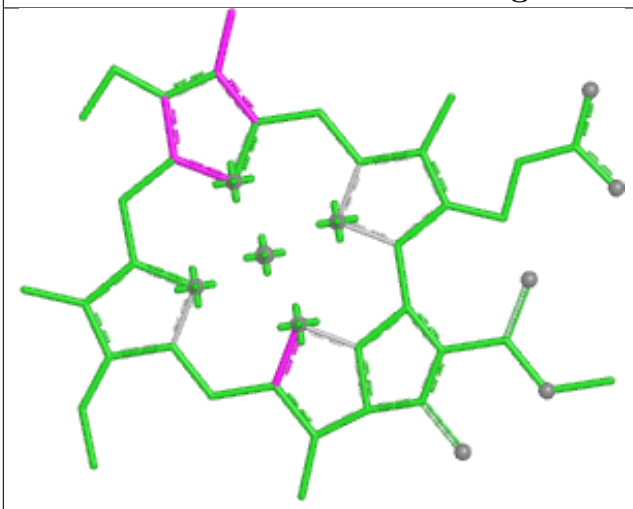


Rings

Ligand CLA BA 816



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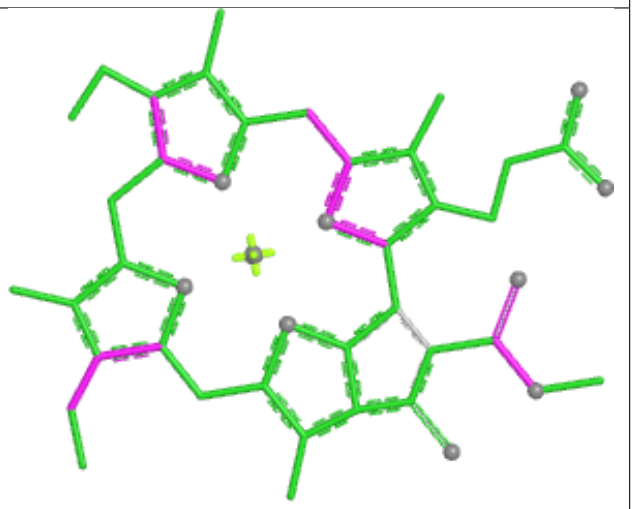
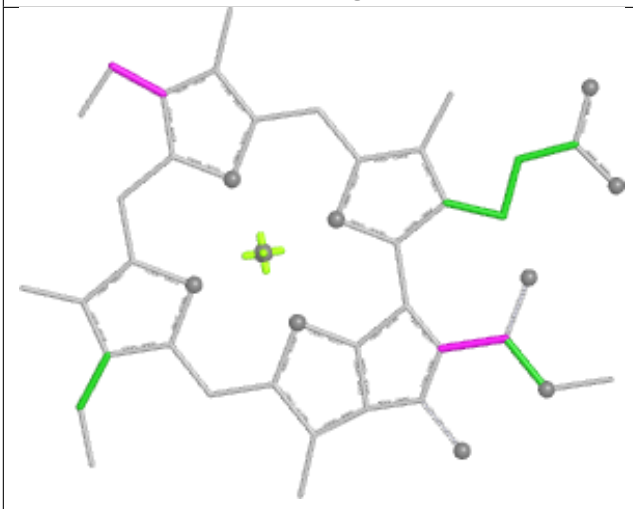


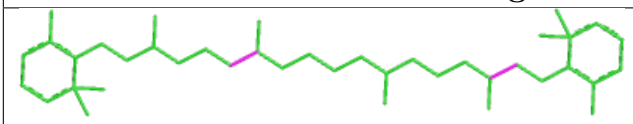
Bond angles



Torsions

Rings

Ligand BCR AA 852



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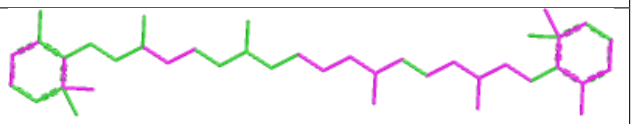
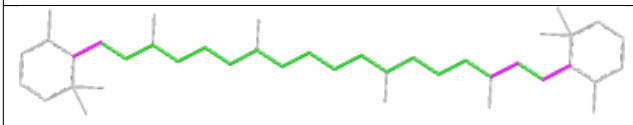
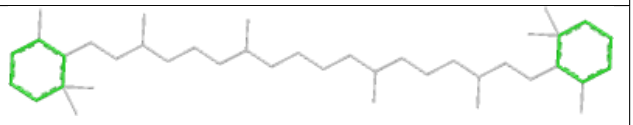


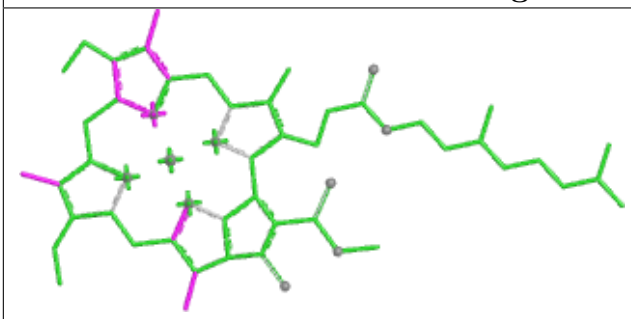
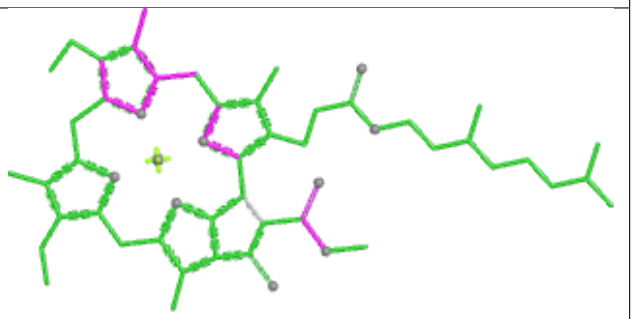
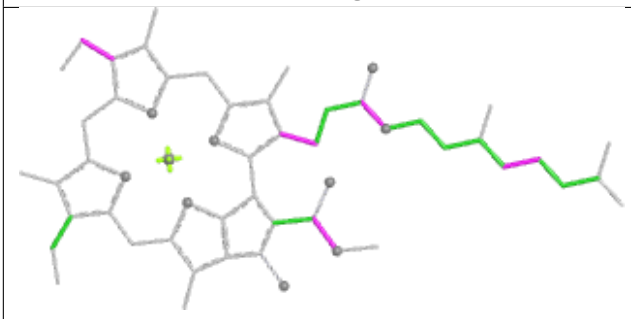
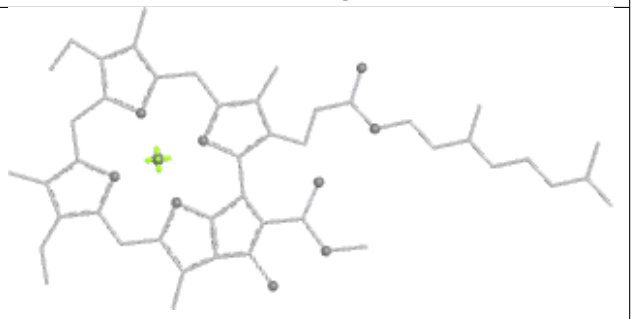
Bond angles



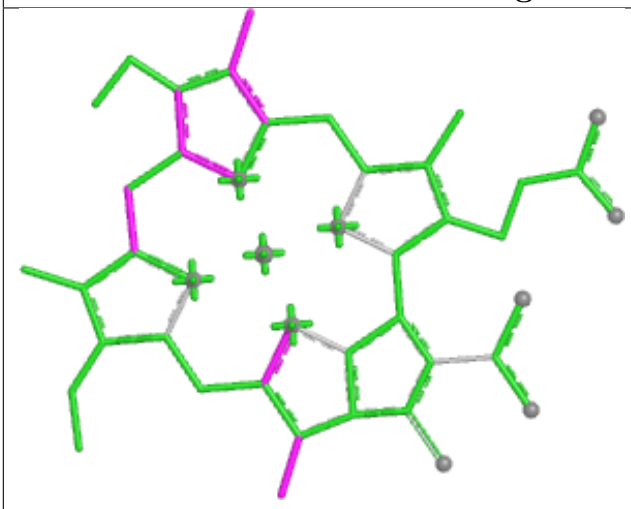
Torsions



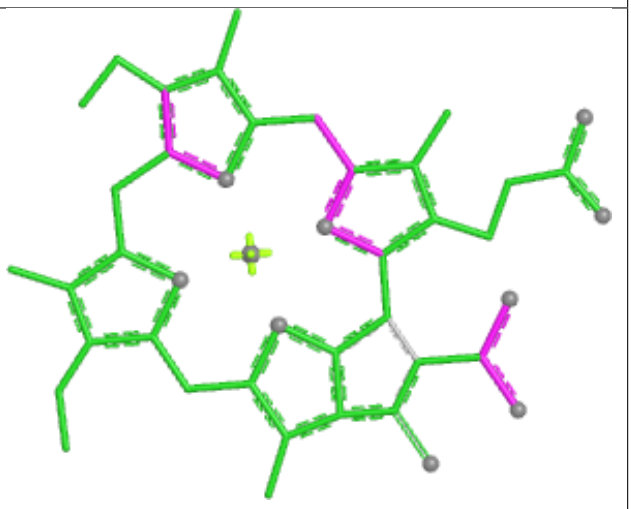
Rings

Ligand CLA AB 820	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

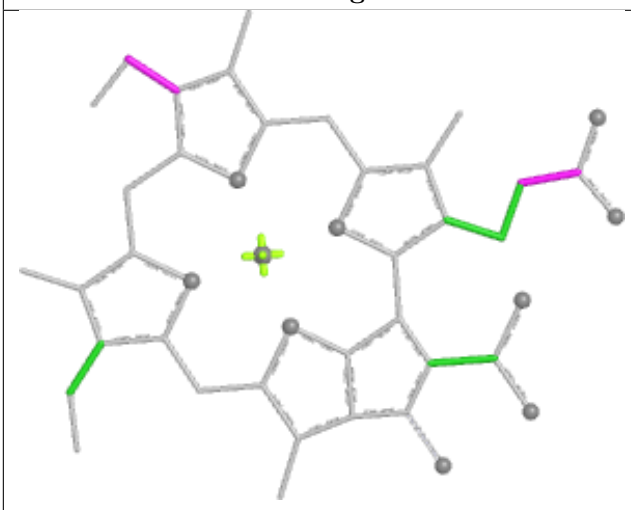
Ligand CLA B1 309



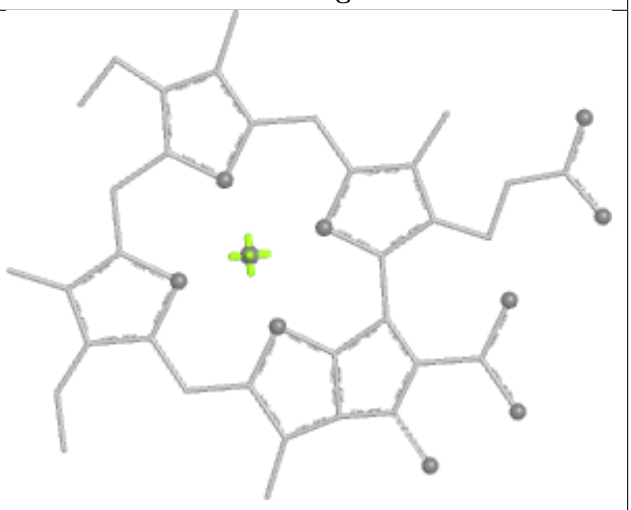
Bond lengths



Bond angles

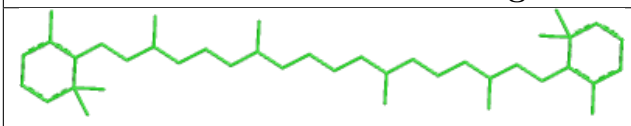


Torsions

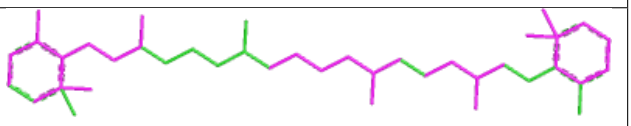


Rings

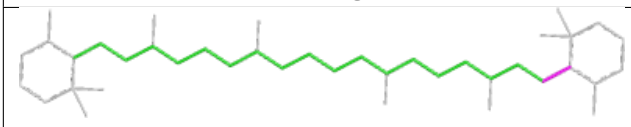
Ligand BCR AG 205



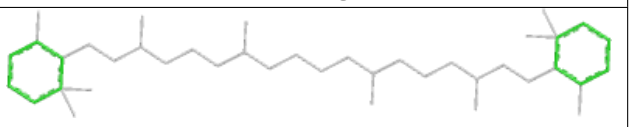
Bond lengths



Bond angles

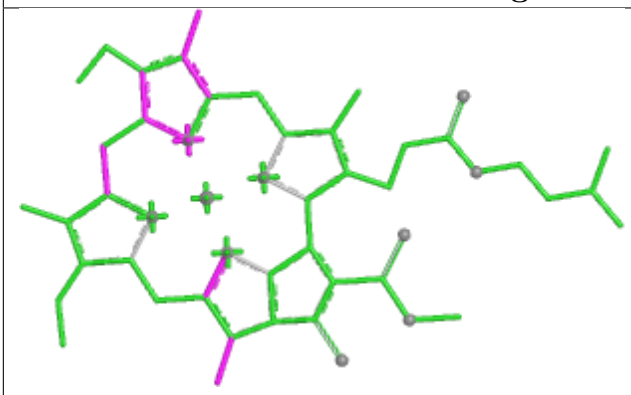


Torsions

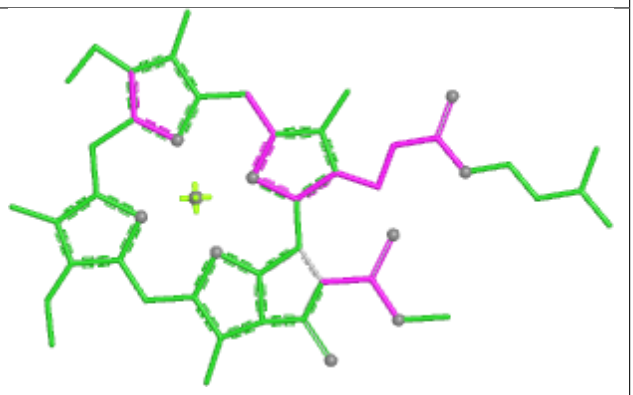


Rings

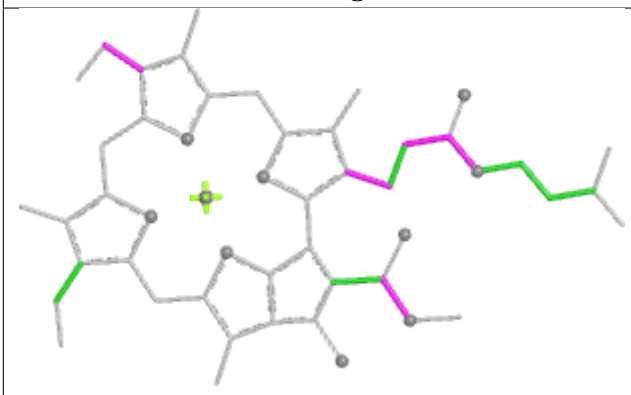
Ligand CLA BA 809



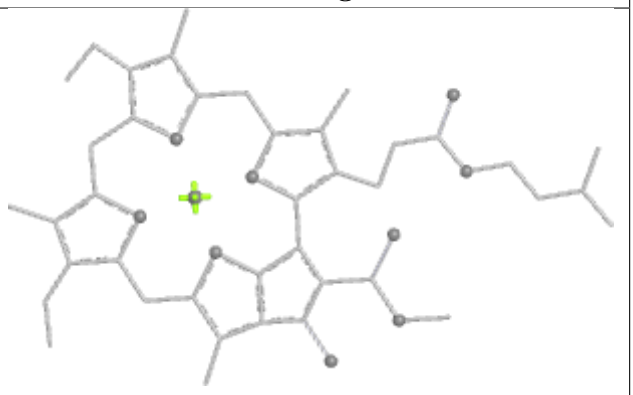
Bond lengths



Bond angles

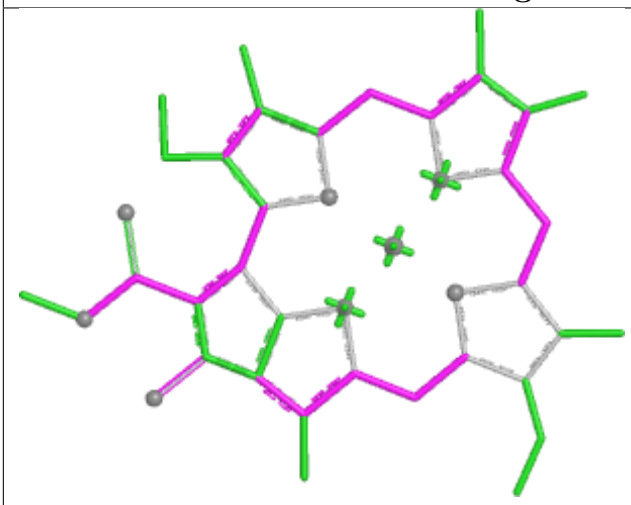


Torsions



Rings

Ligand CHL A4 305



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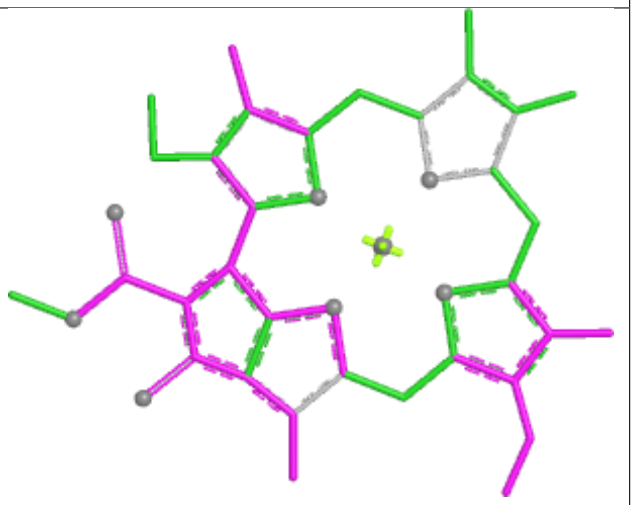
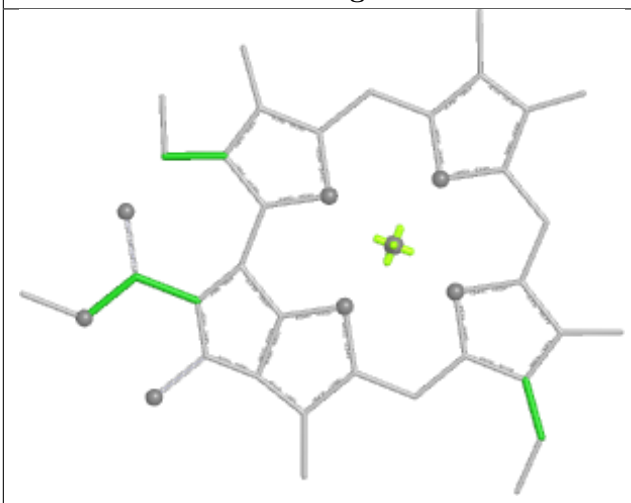
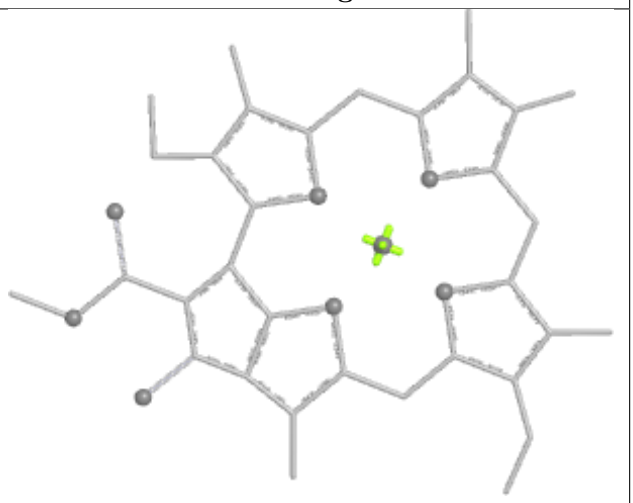


Bond angles

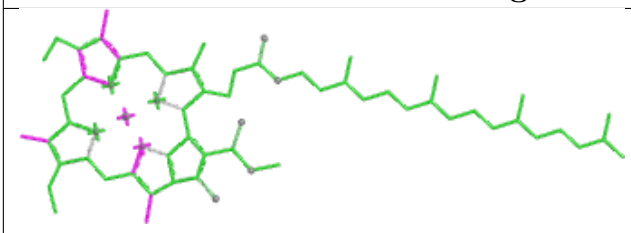


Torsions



Rings

Ligand CLA AA 802



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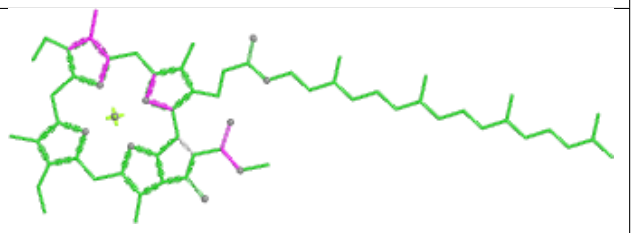
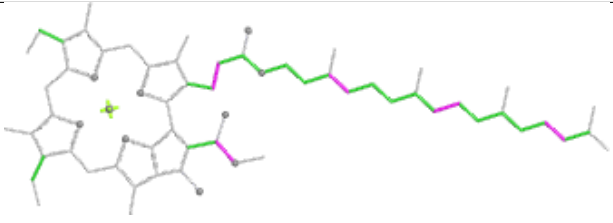


Bond angles



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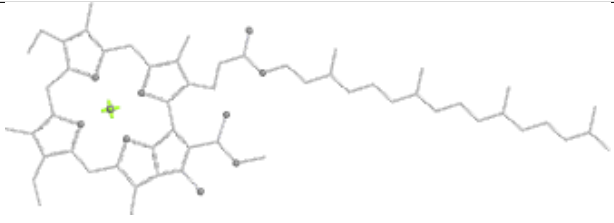
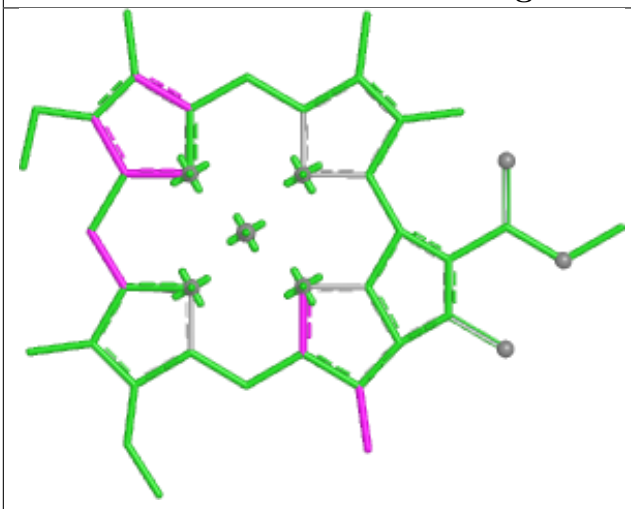


Rings

Ligand CLA B1 306



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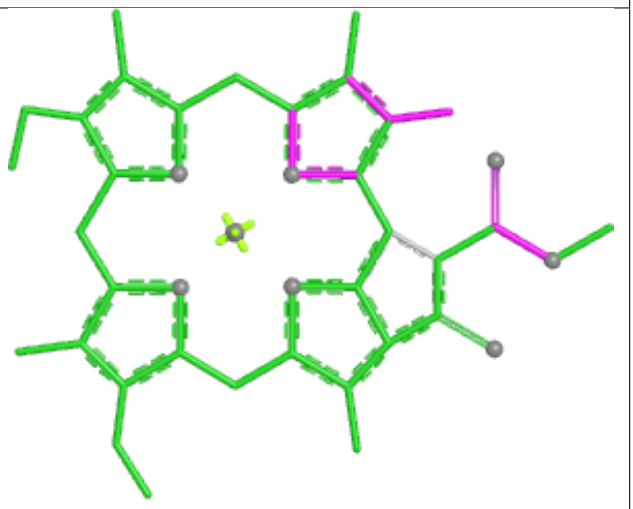
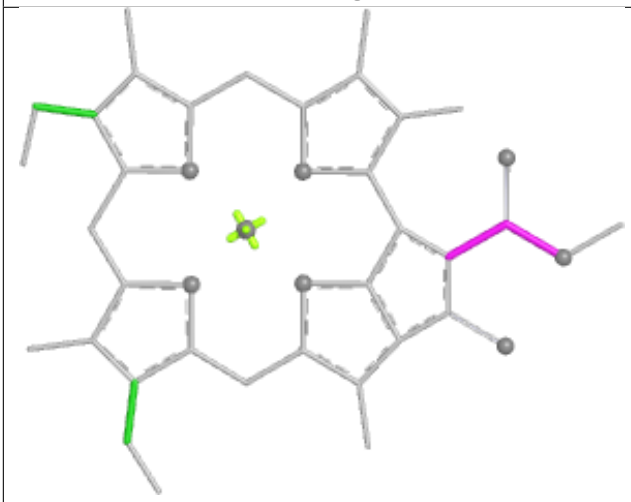


Bond angles



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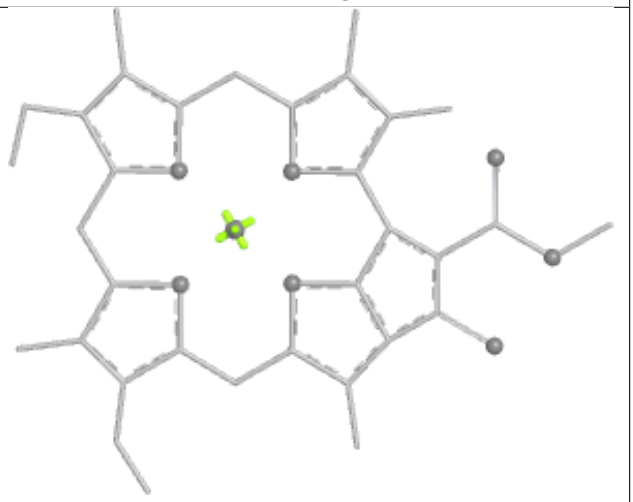
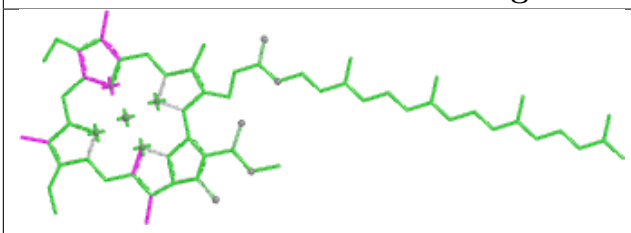


Rings

Ligand CLA AB 841



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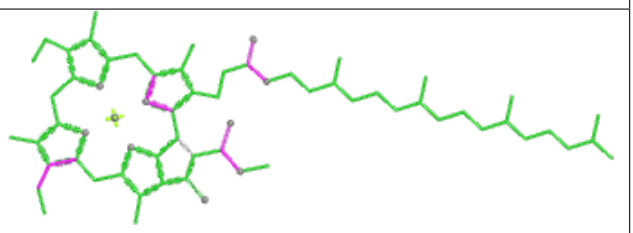
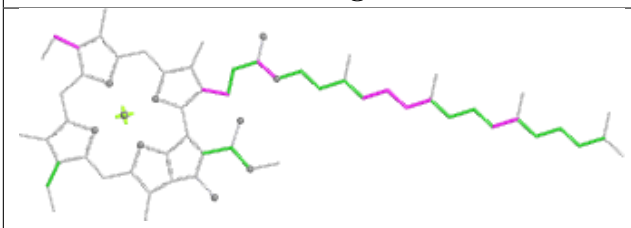


Bond angles



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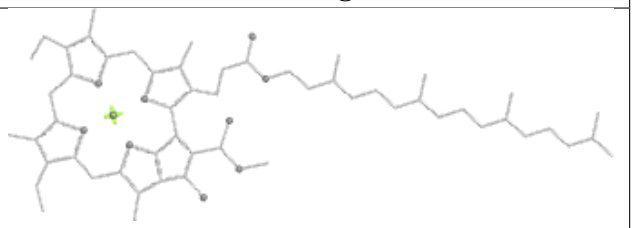
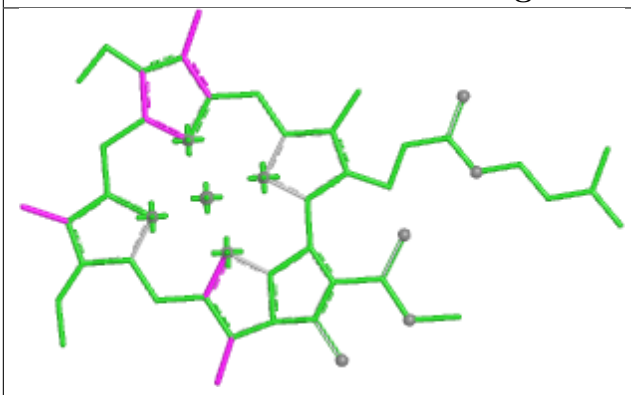


Rings

Ligand CLA A4 313



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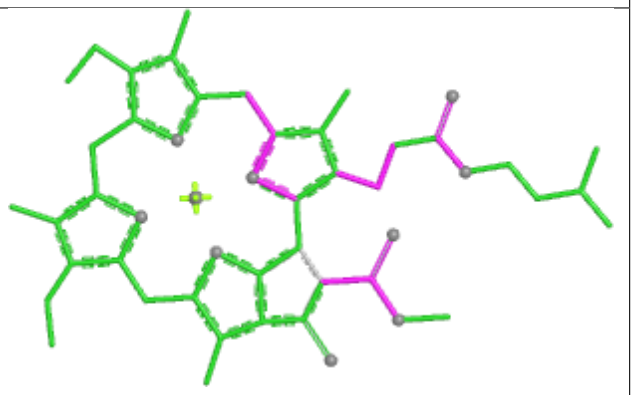
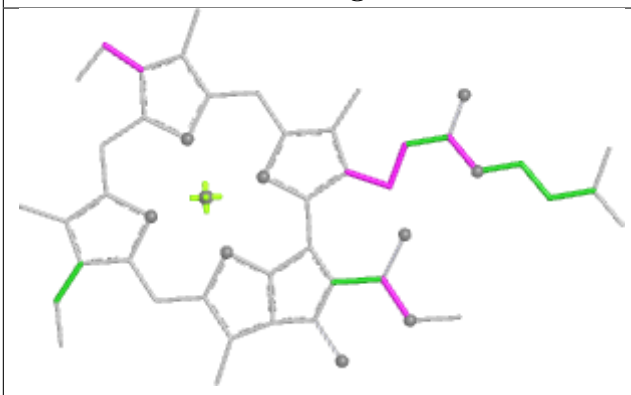


Bond angles



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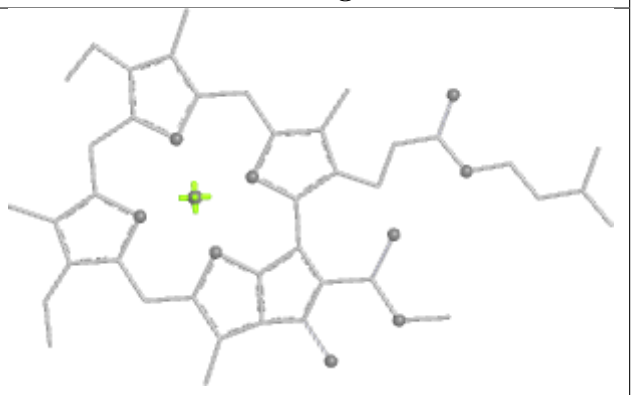
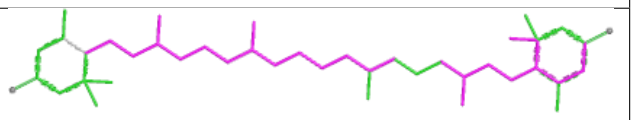


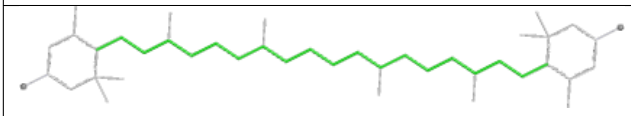
Rings

Ligand LUT B2 615

Bond lengths



Bond angles



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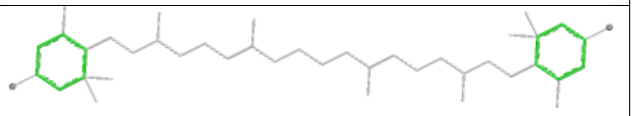
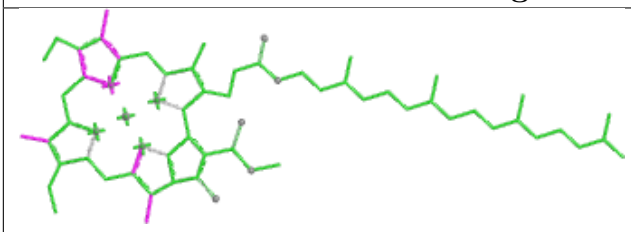


Rings

Ligand CLA BA 819



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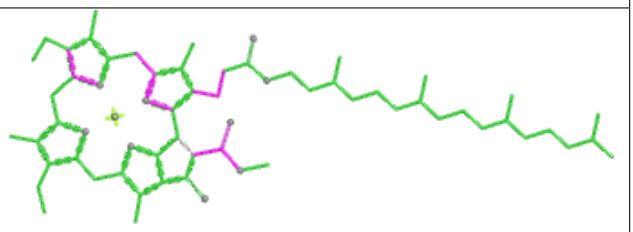
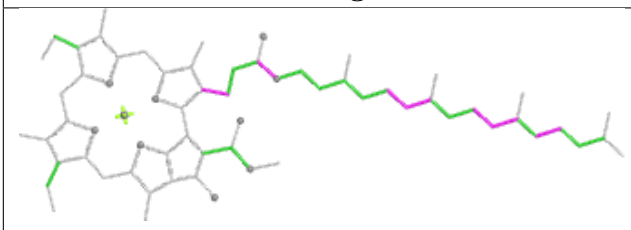


Bond angles



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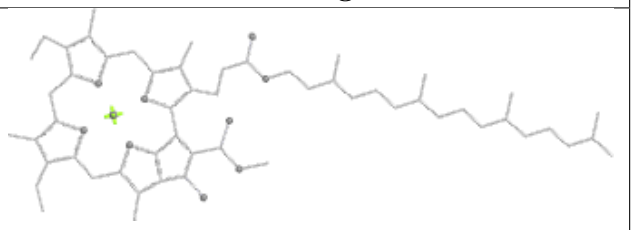
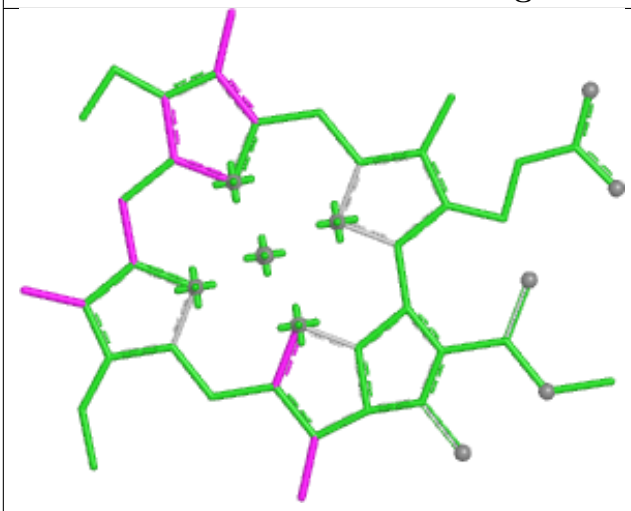


Rings

Ligand CLA A6 609



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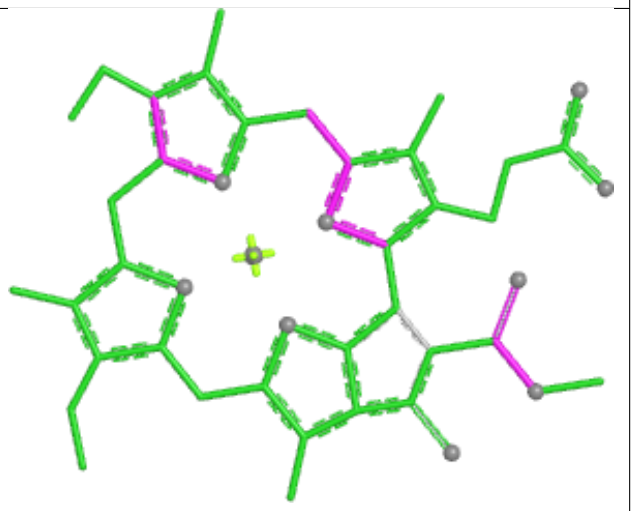
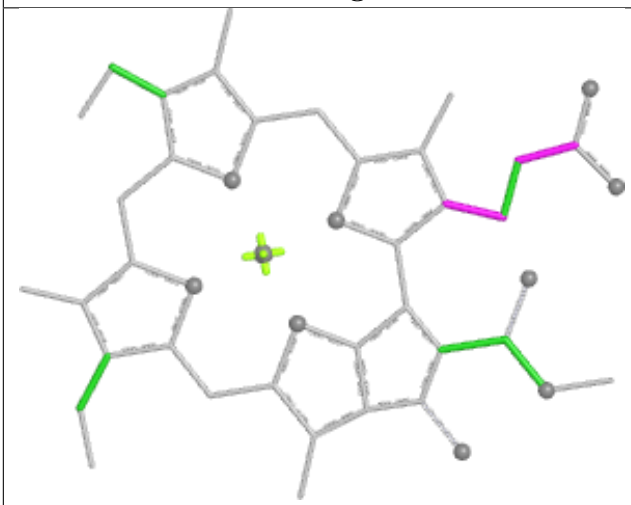


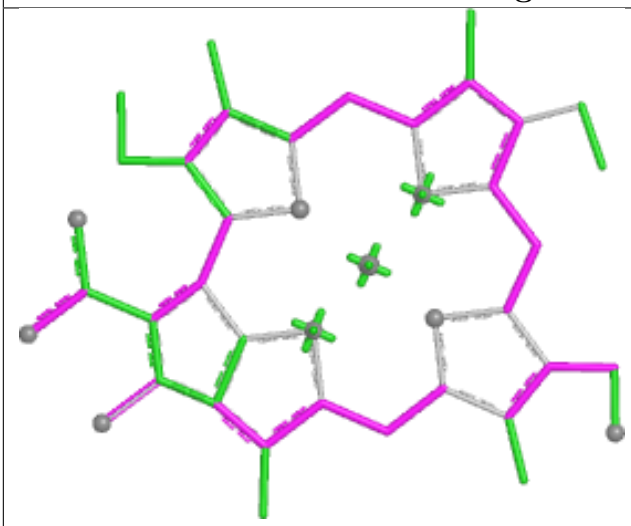
Bond angles



Torsions

Rings

Ligand CHL B5 605



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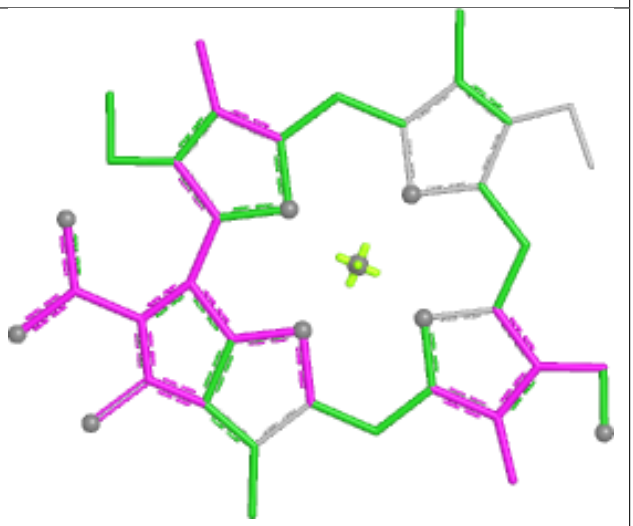
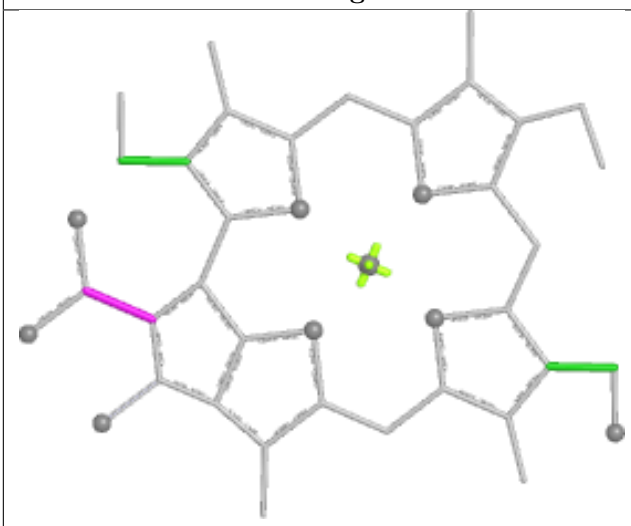


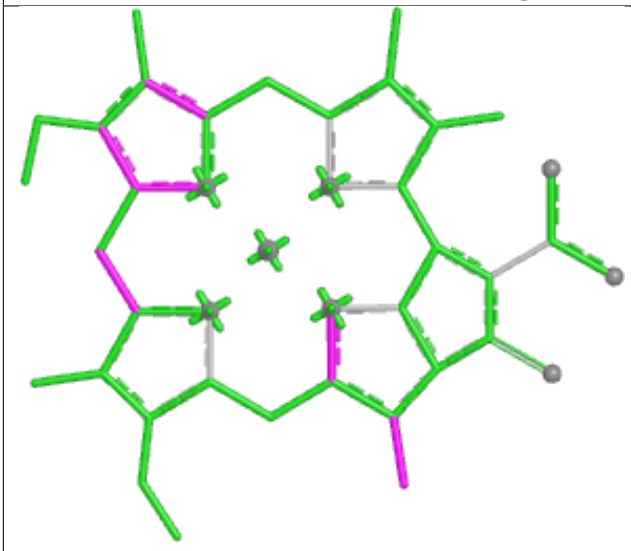
Bond angles



Torsions

Rings

Ligand CLA B3 314



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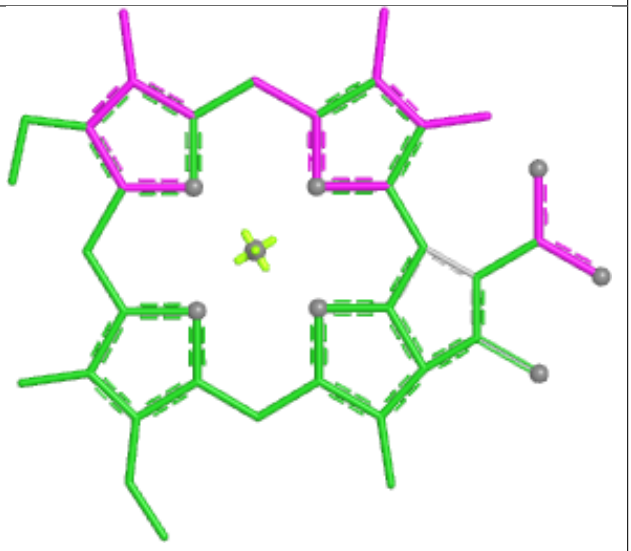
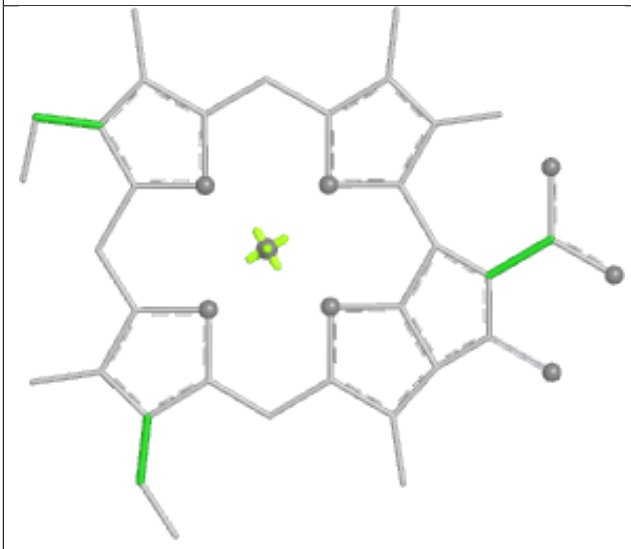
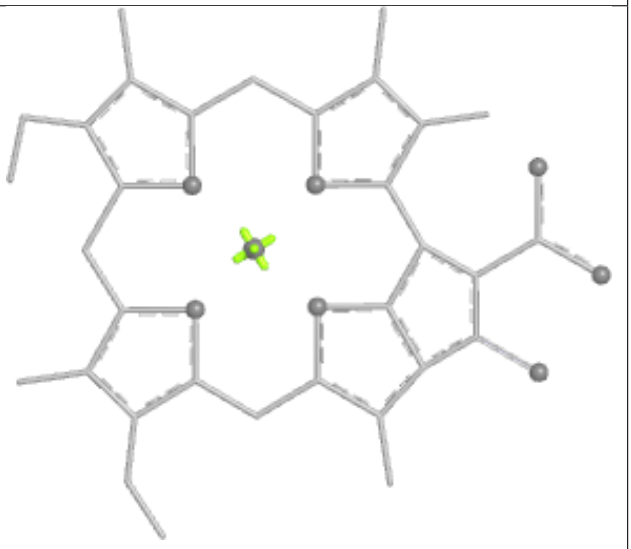


Bond angles

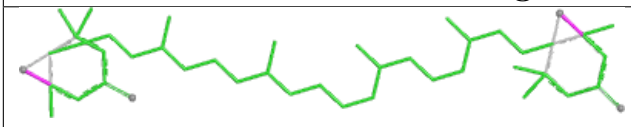


Torsions



Rings

Ligand XAT A1 318



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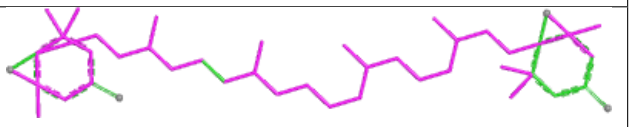
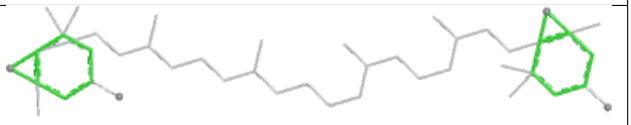
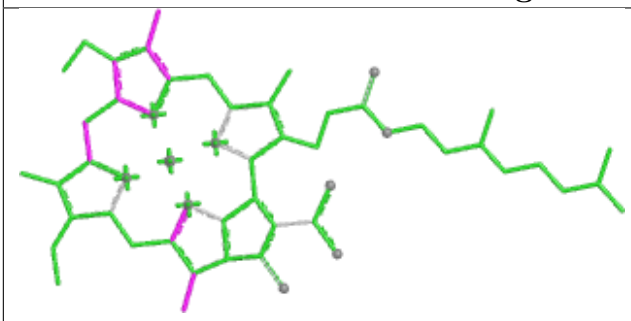
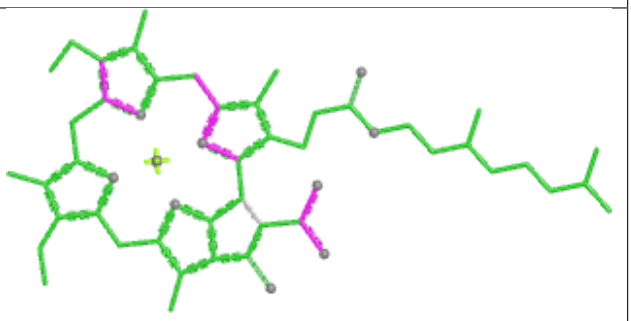
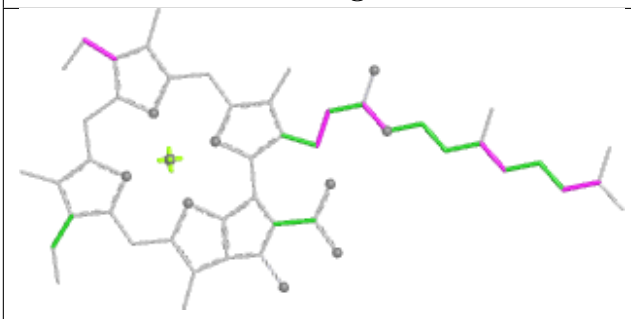
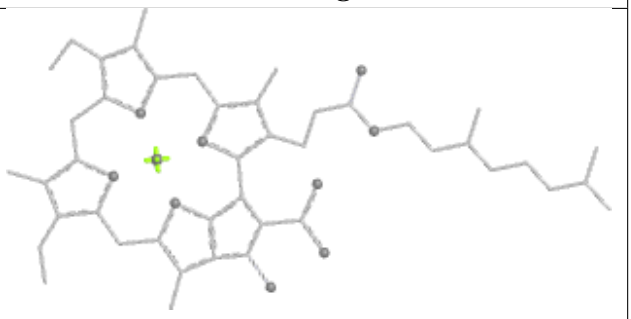


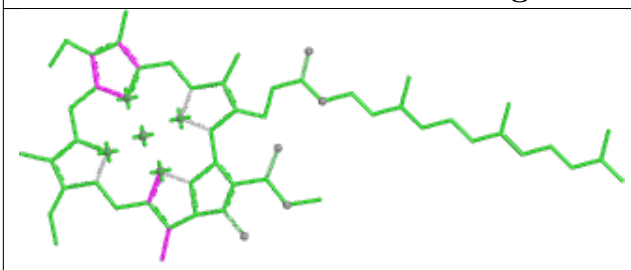
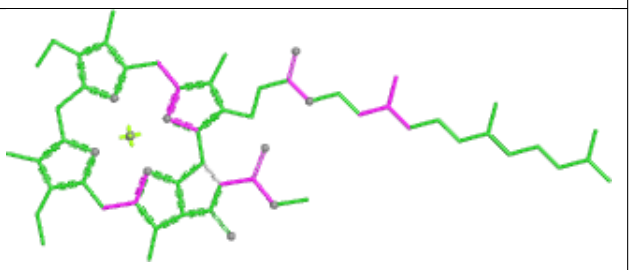
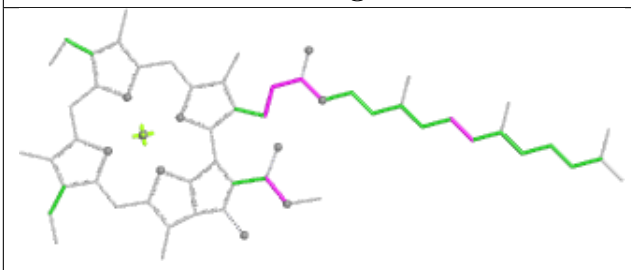
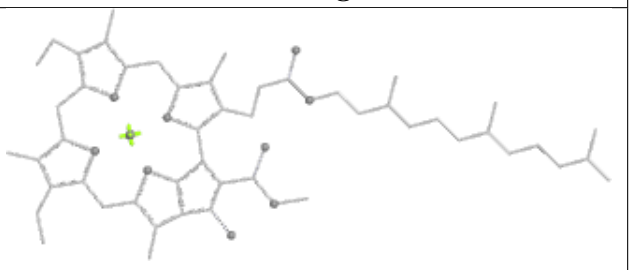
Bond angles

Torsions

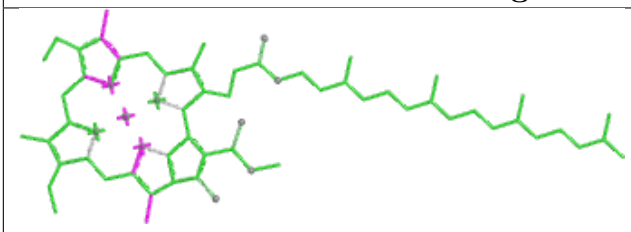


Rings

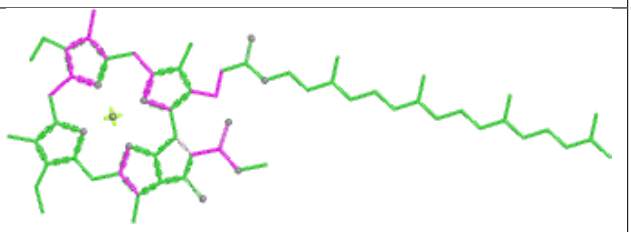
Ligand CLA B3 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA BA 817	
	
Bond lengths	Bond angles
	
Torsions	Rings

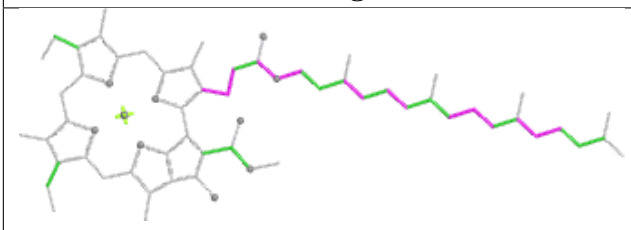
Ligand CLA AB 829



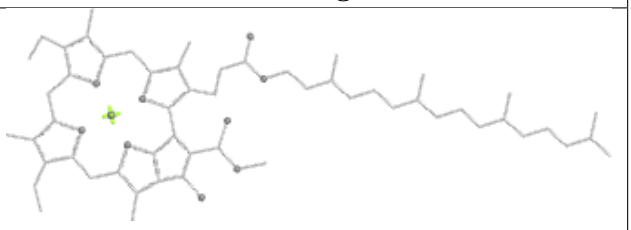
Bond lengths



Bond angles

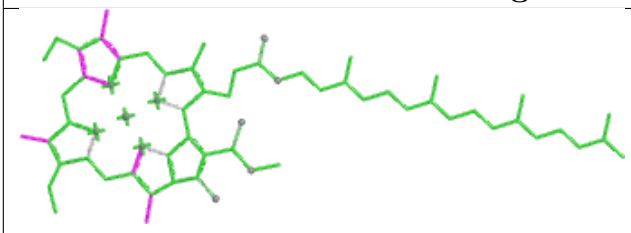


Torsions

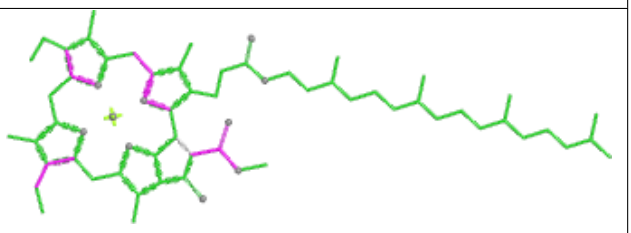


Rings

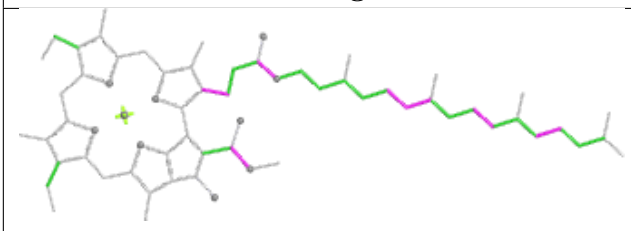
Ligand CLA BA 810



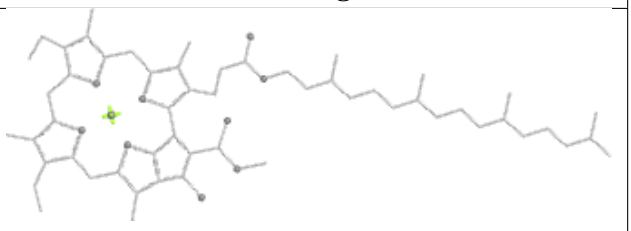
Bond lengths



Bond angles

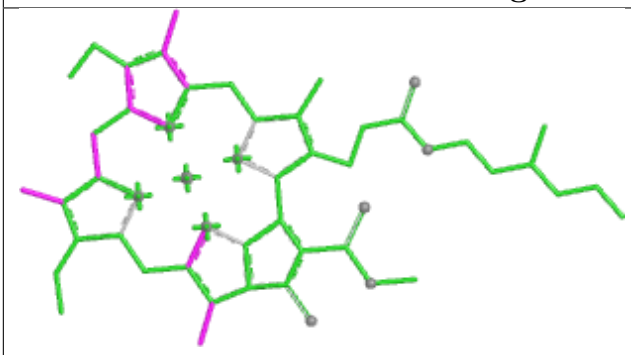


Torsions

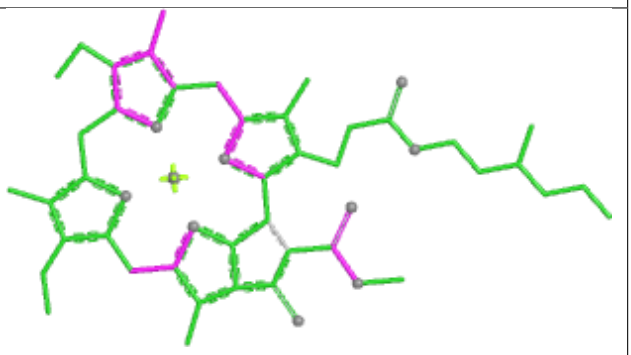


Rings

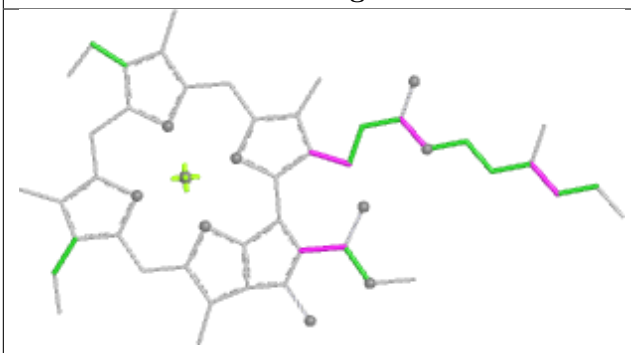
Ligand CLA AA 804



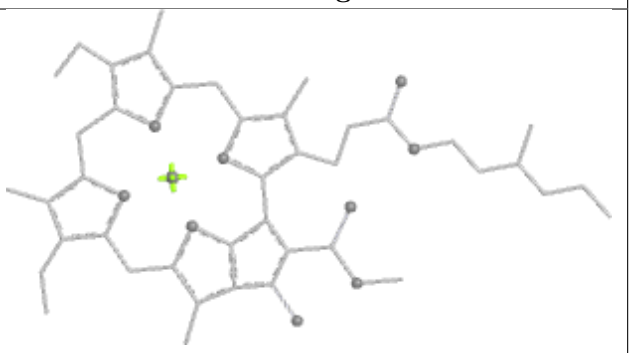
Bond lengths



Bond angles

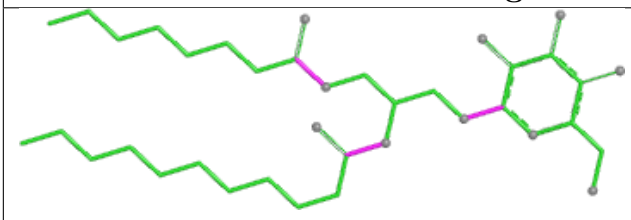


Torsions



Rings

Ligand LMG AG 202



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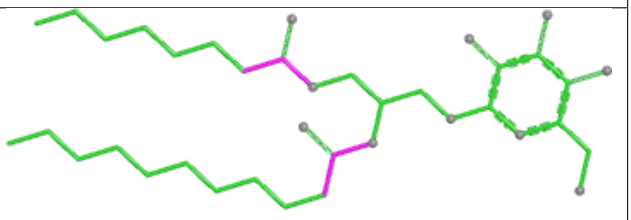
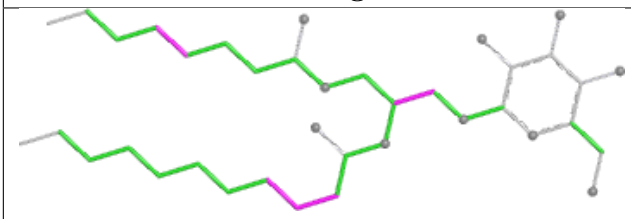
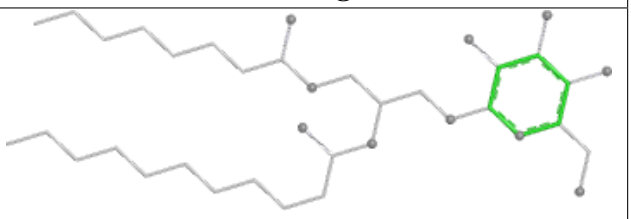


Bond angles

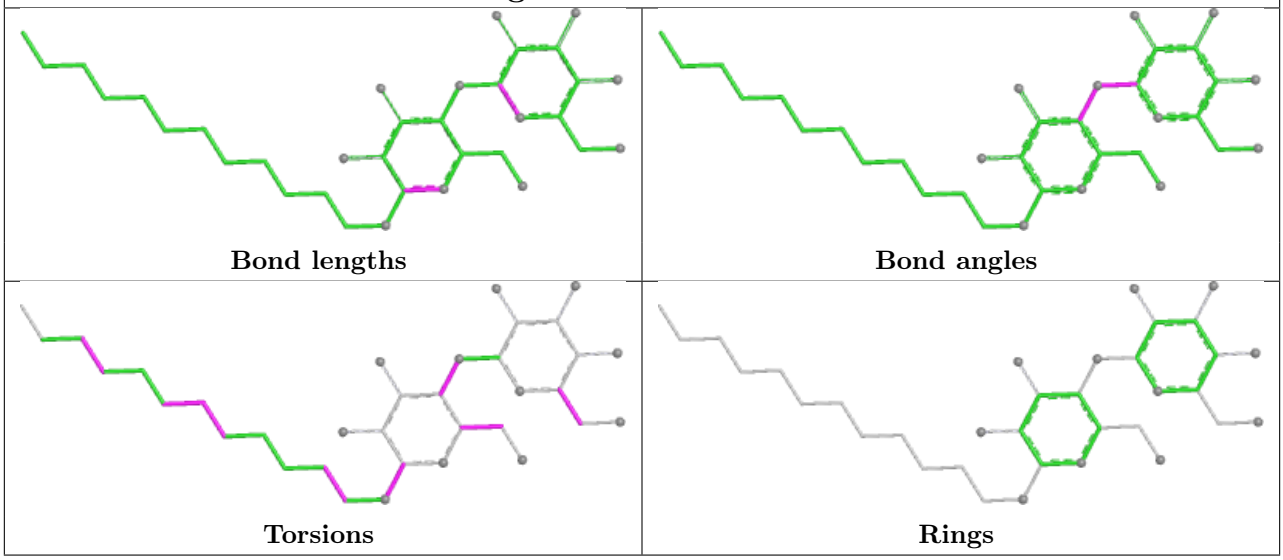


Torsions

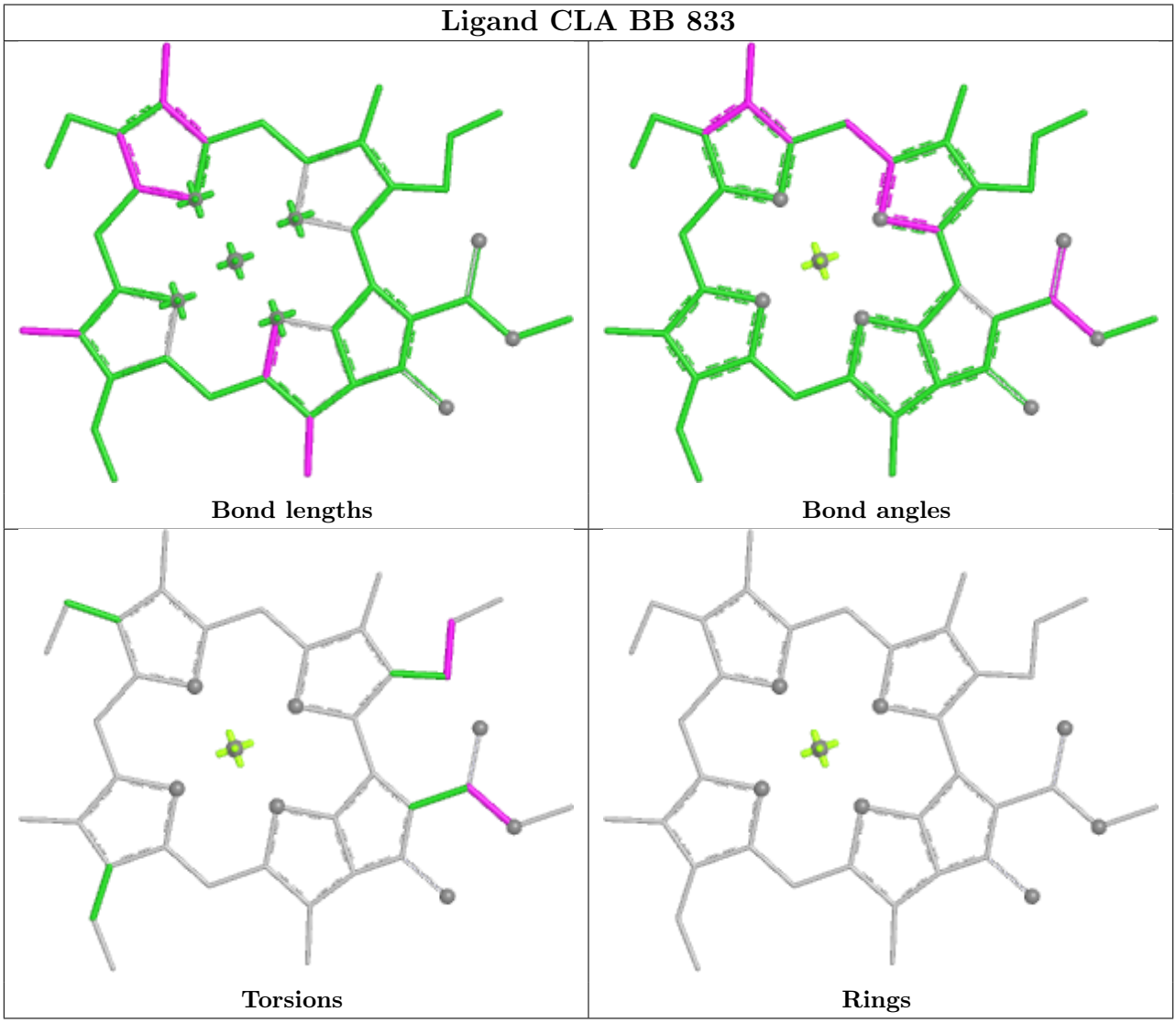


Rings

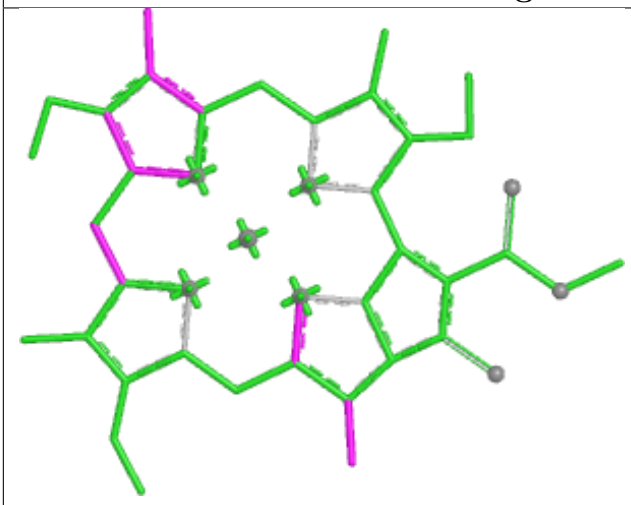
Ligand LMU AB 852



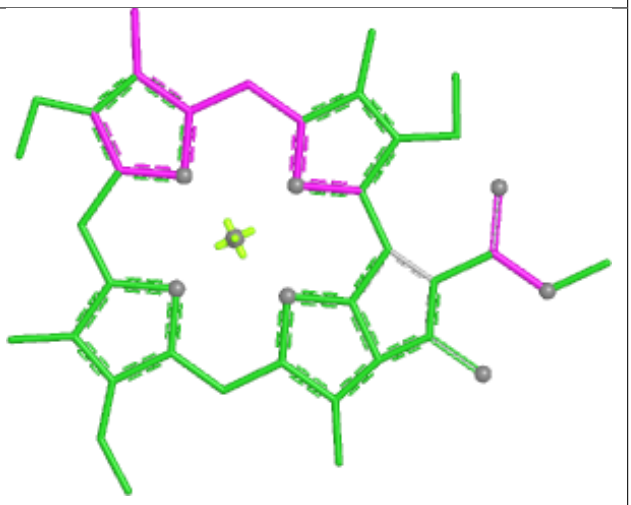
Ligand CLA BB 833



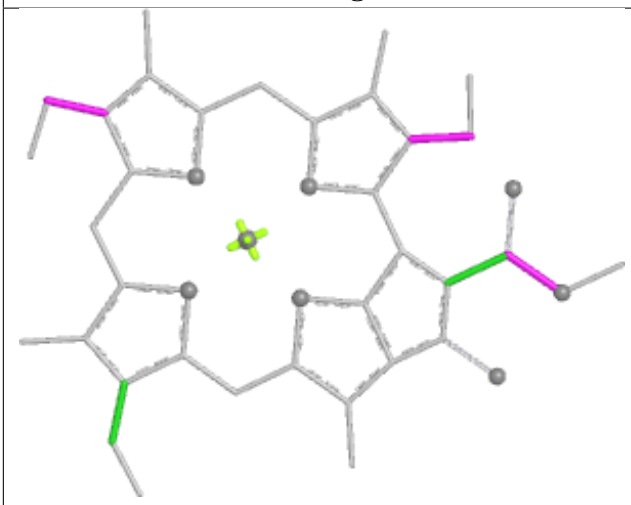
Ligand CLA B5 610



Bond lengths



Bond angles

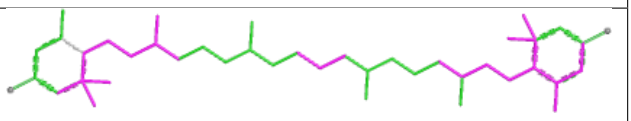


Torsions

Rings

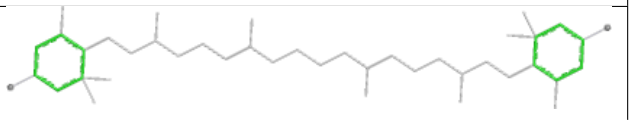
Ligand LUT A1 317

Bond lengths



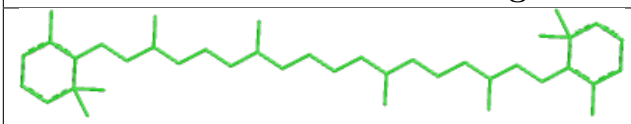
Bond angles

Torsions



Rings

Ligand BCR AB 847



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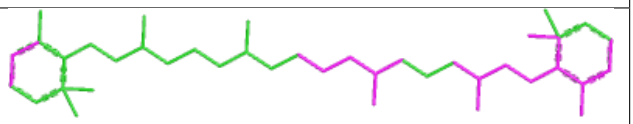
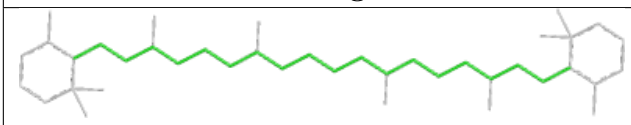


Bond angles



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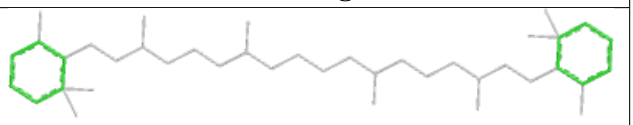
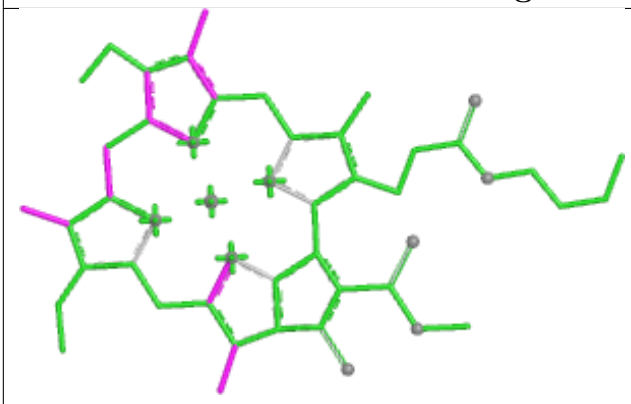
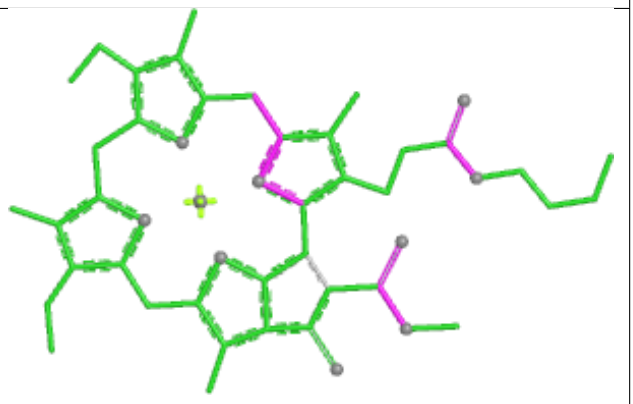


Rings

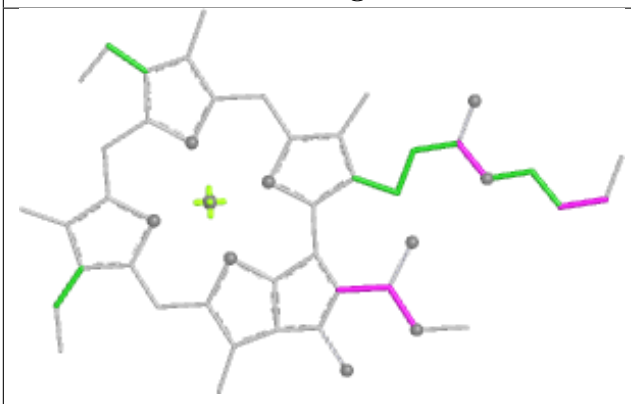
Ligand CLA A1 306



Bond lengths



Bond angles



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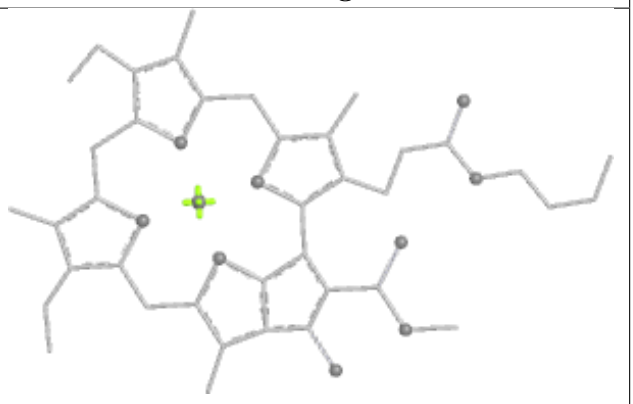
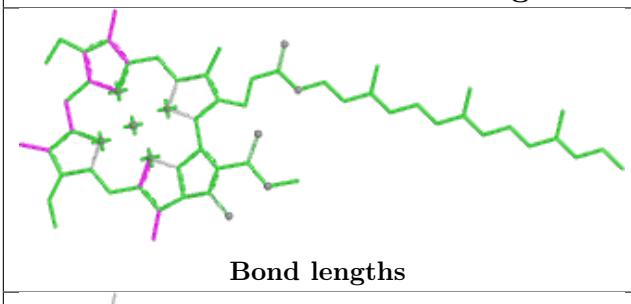


Rings

Ligand CLA BB 828



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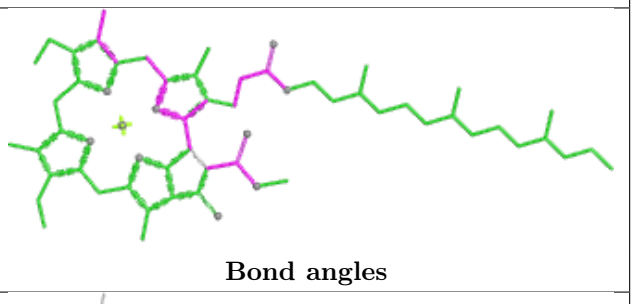
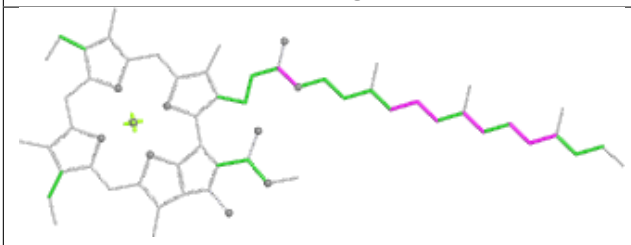


Bond angles



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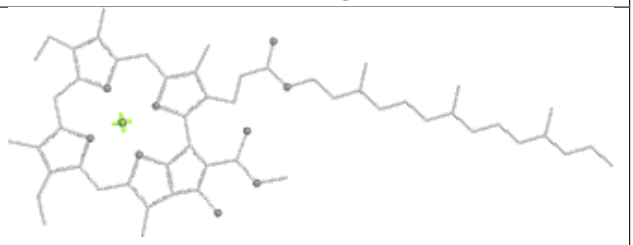
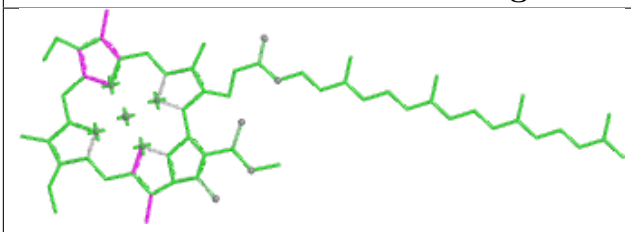
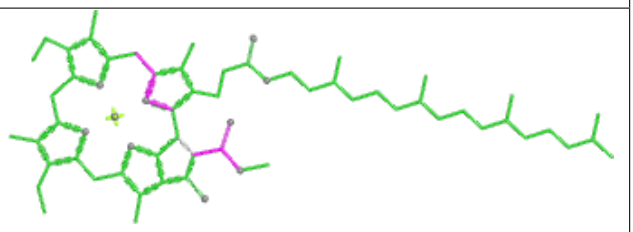


Rings

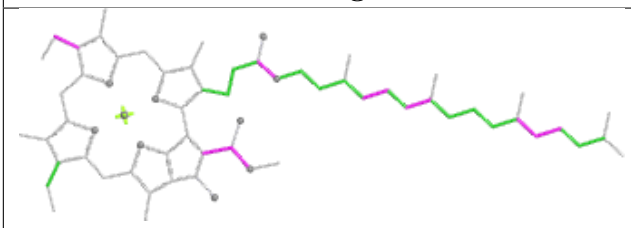
Ligand CLA AA 811



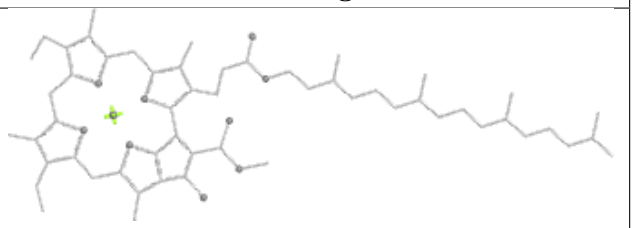
Bond lengths



Bond angles

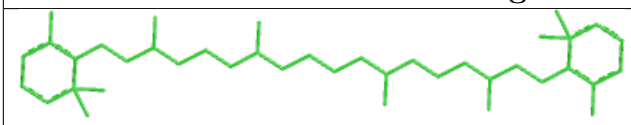


Torsions



Rings

Ligand BCR BA 855



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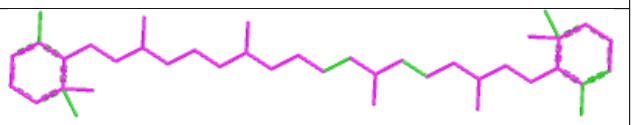
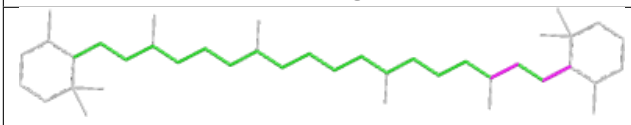


Bond angles



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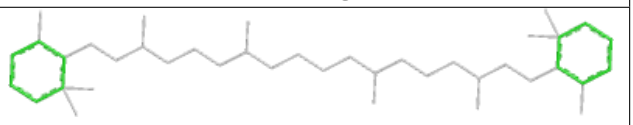
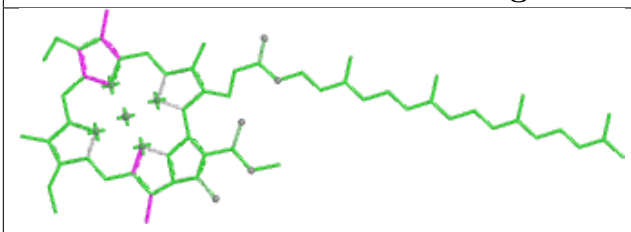


Rings

Ligand CLA AA 842



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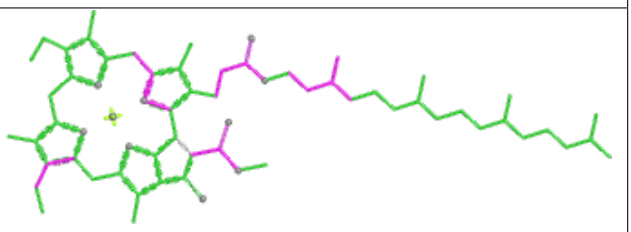
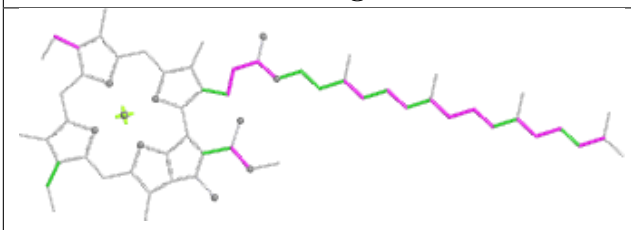


Bond angles



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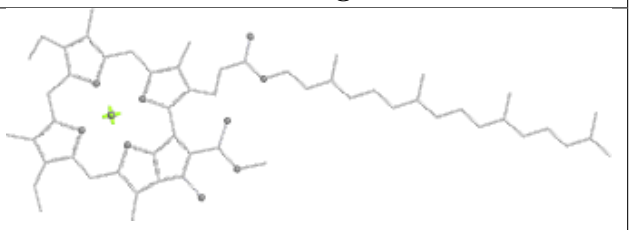
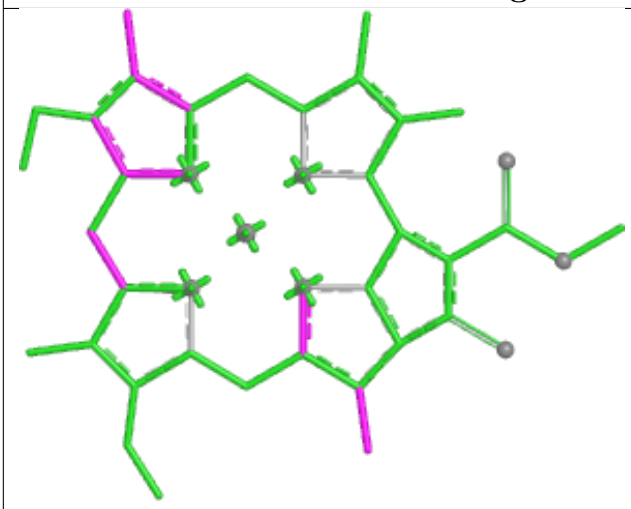


Rings

Ligand CLA AA 823



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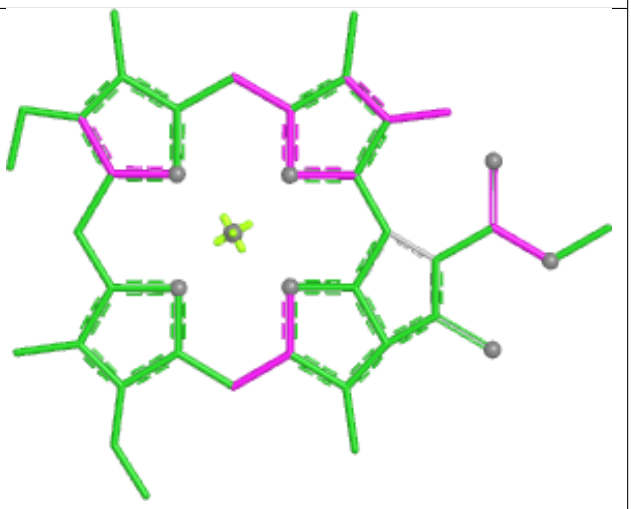
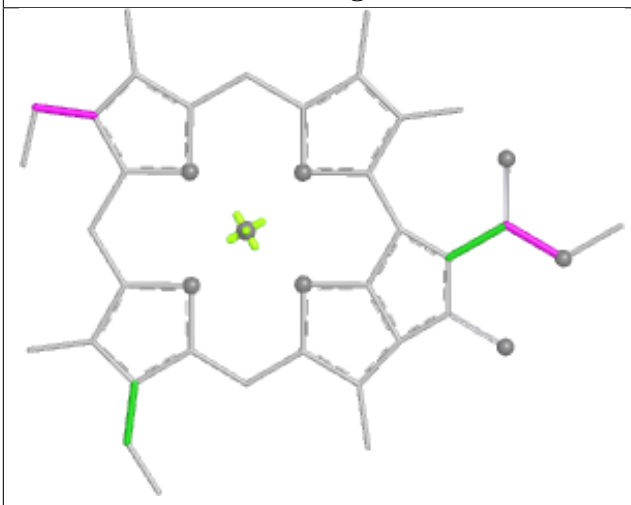
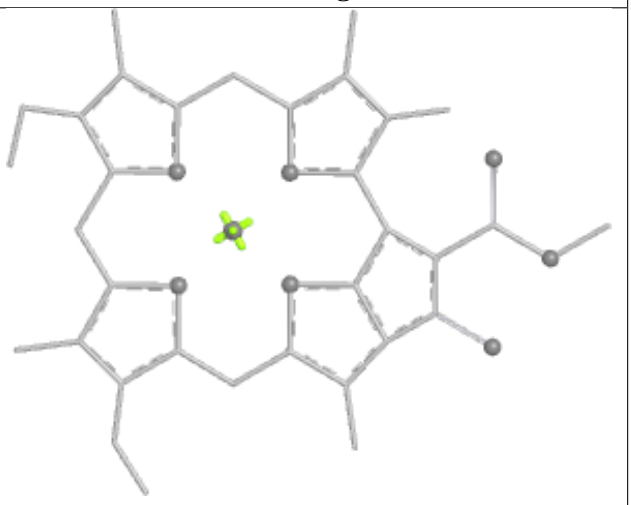


Bond angles

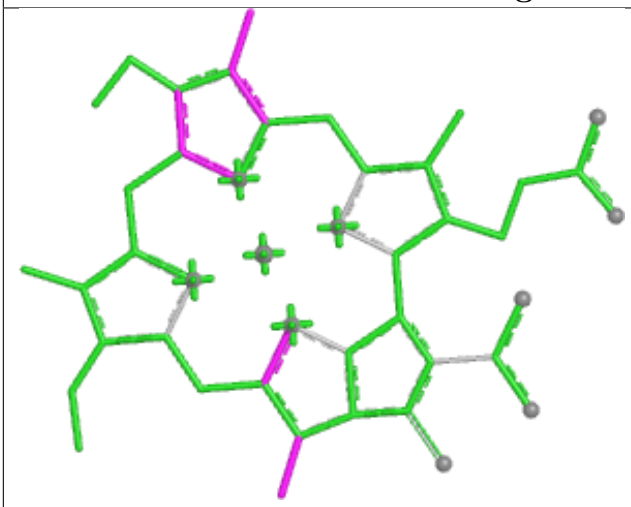


Torsions

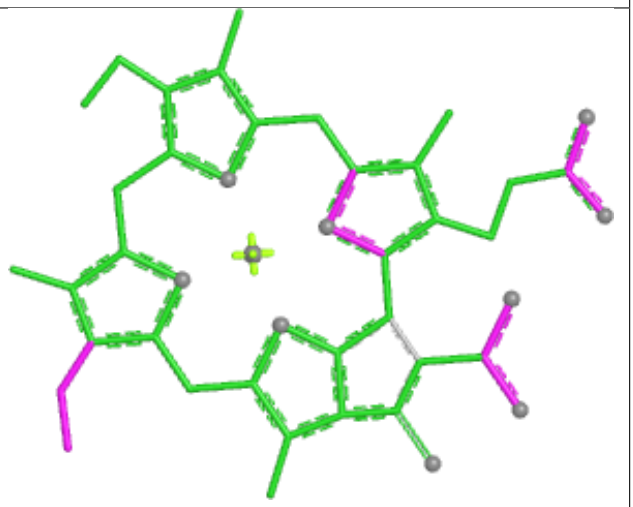


Rings

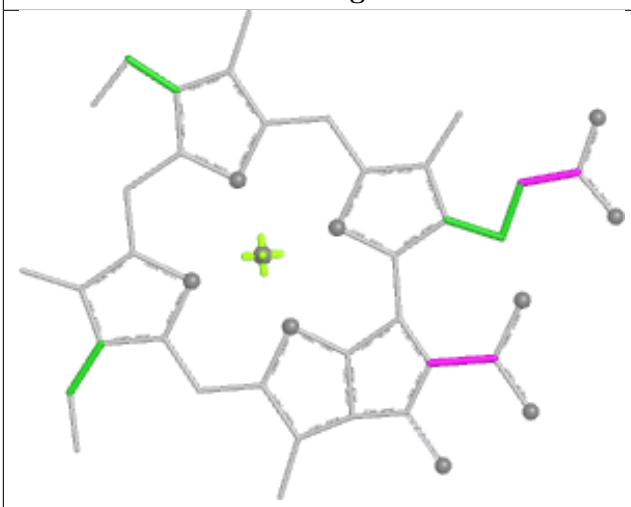
Ligand CLA B2 603



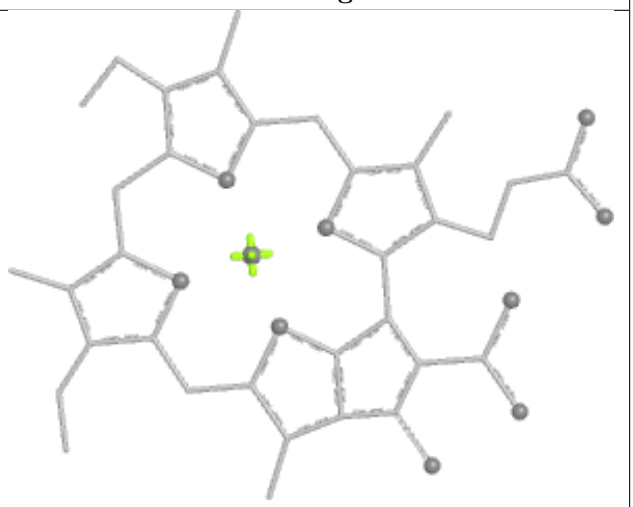
Bond lengths



Bond angles

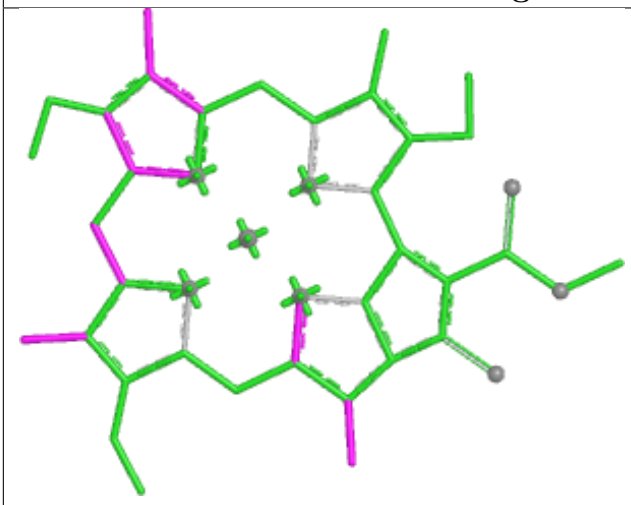


Torsions

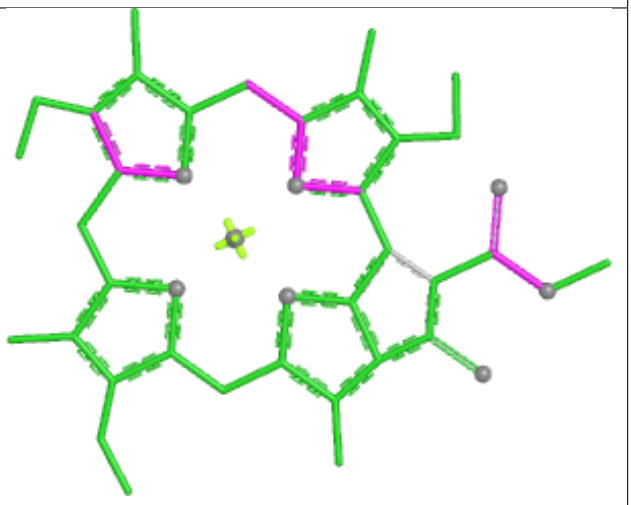


Rings

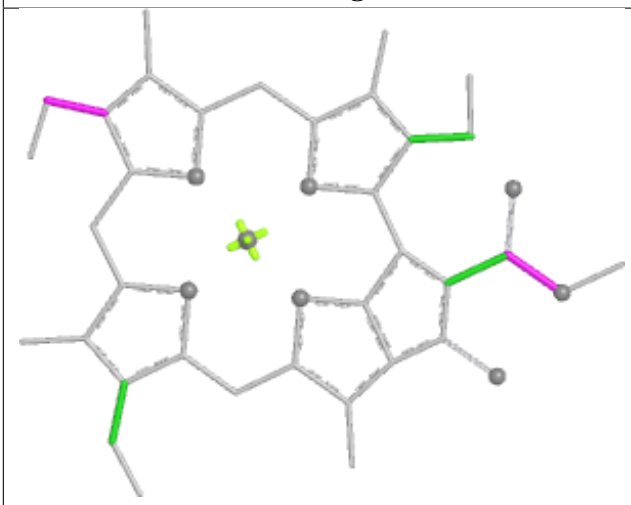
Ligand CLA AF 803



Bond lengths



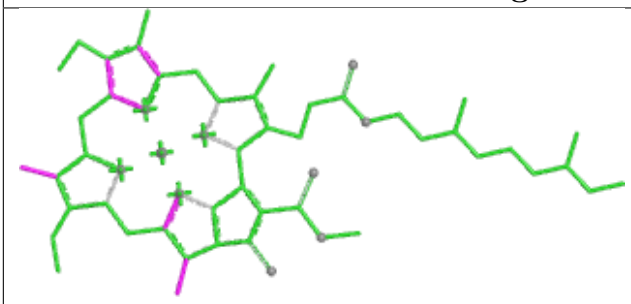
Bond angles



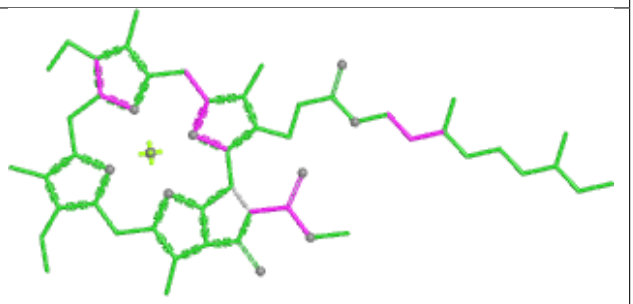
Torsions

Rings

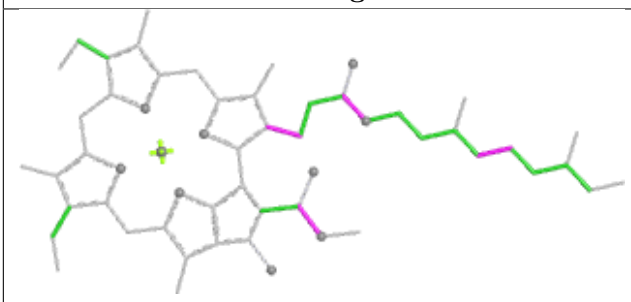
Ligand CLA BA 832



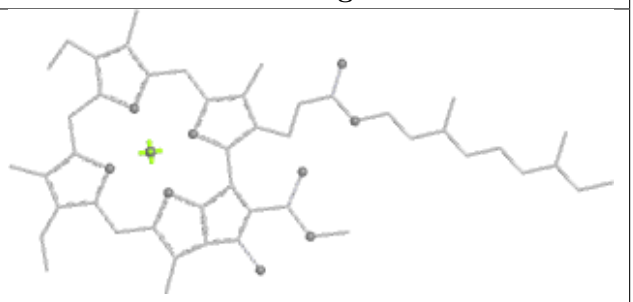
Bond lengths



Bond angles

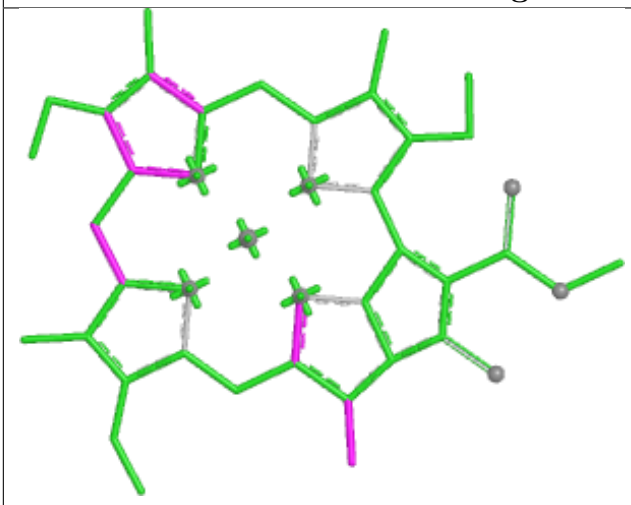


Torsions

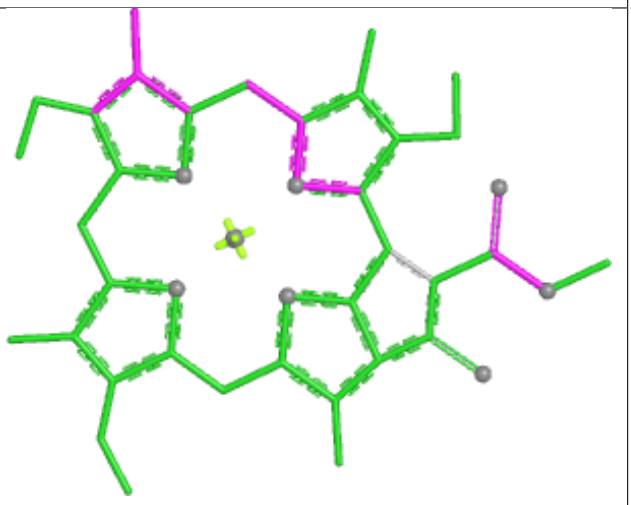


Rings

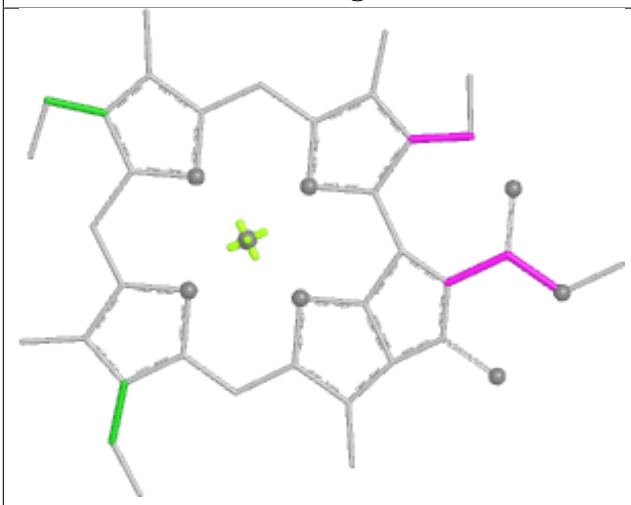
Ligand CLA BA 822



Bond lengths



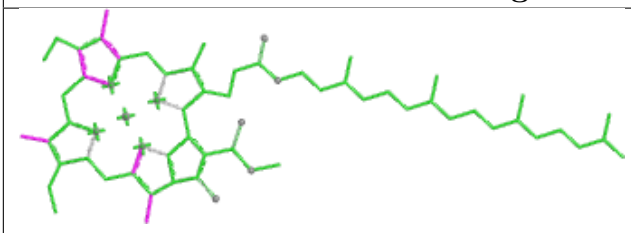
Bond angles



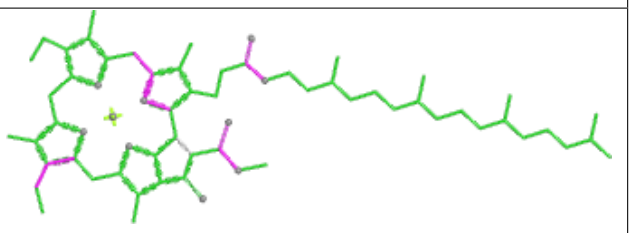
Torsions

Rings

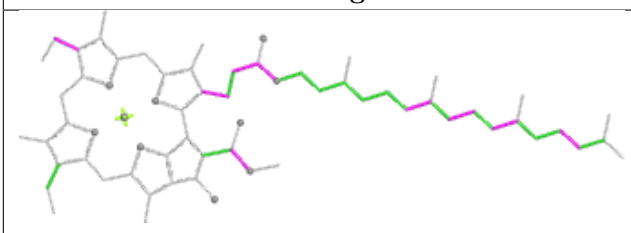
Ligand CLA AB 834



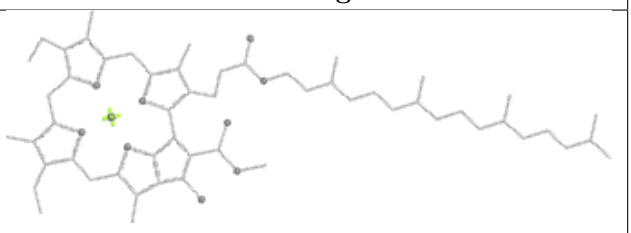
Bond lengths



Bond angles

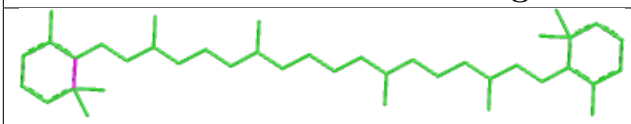


Torsions



Rings

Ligand BCR BF 304



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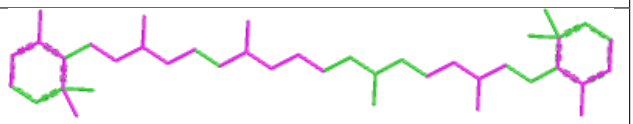
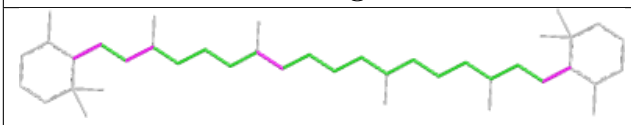
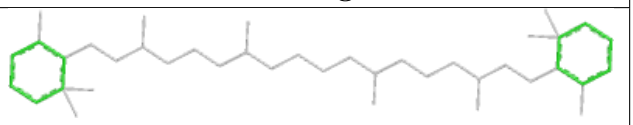


Bond angles

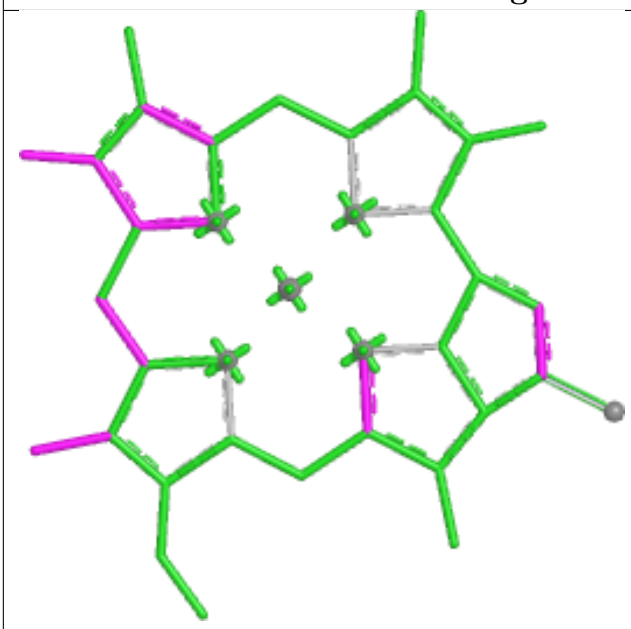


Torsions

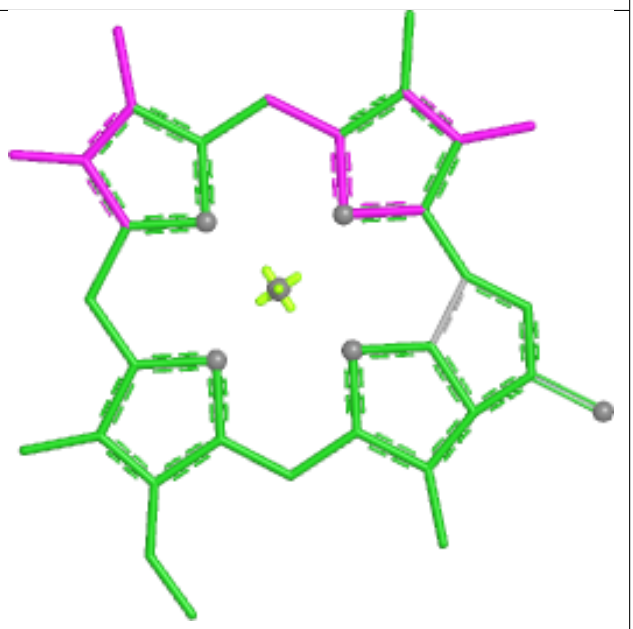


Rings

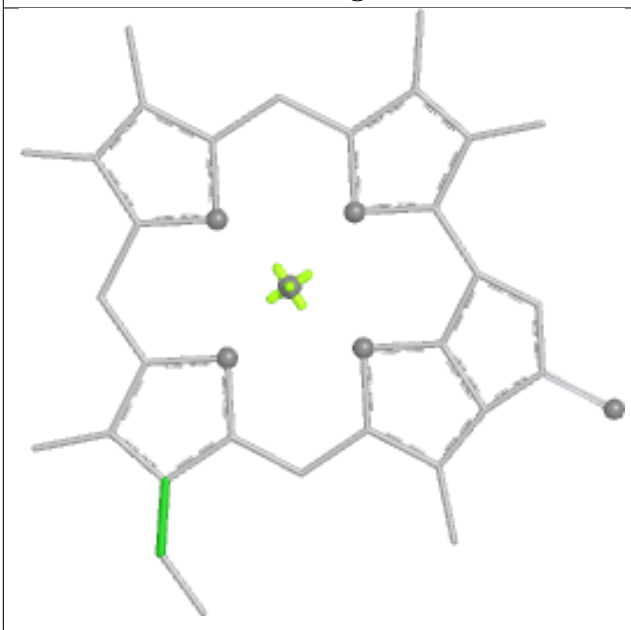
Ligand CLA BK 201



Bond lengths



Bond angles



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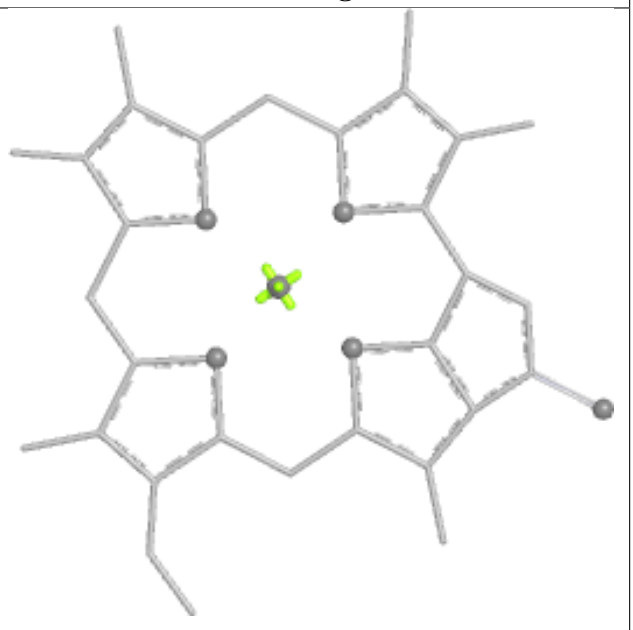
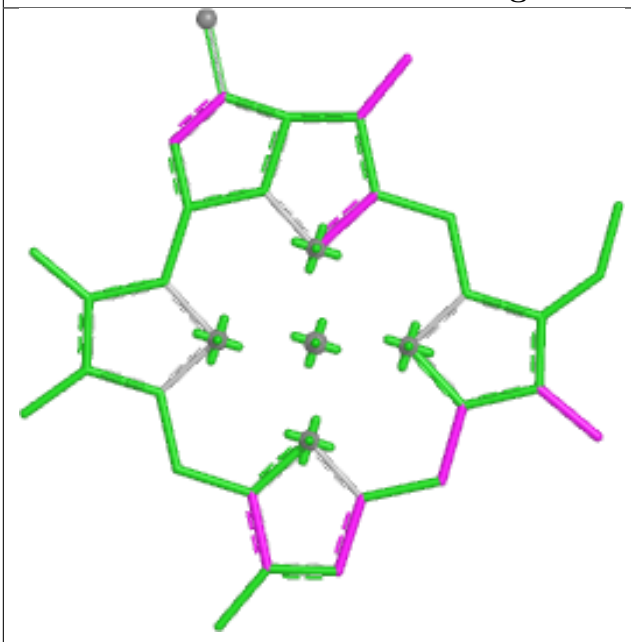


Rings

Ligand CLA AK 201



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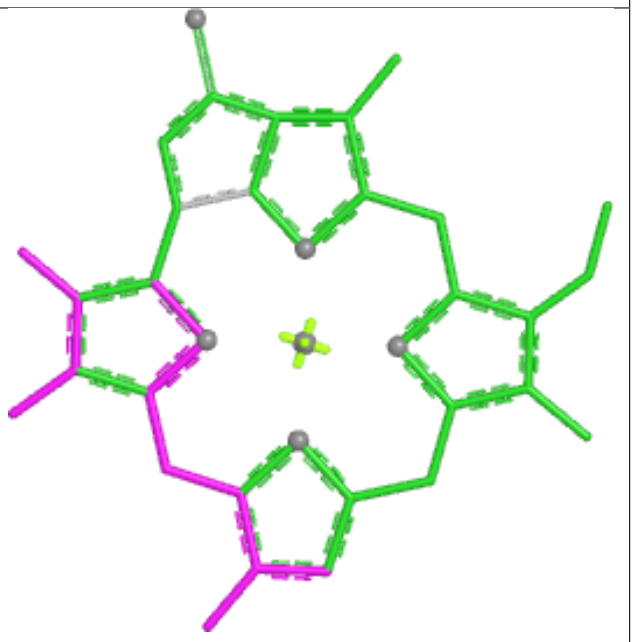
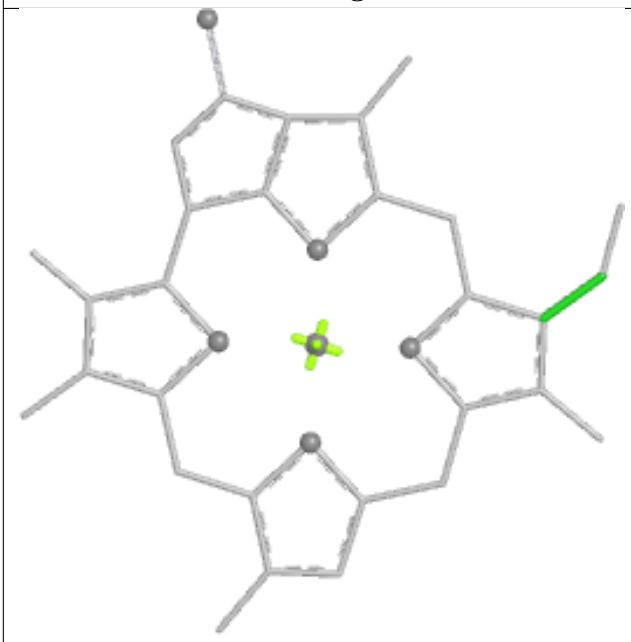
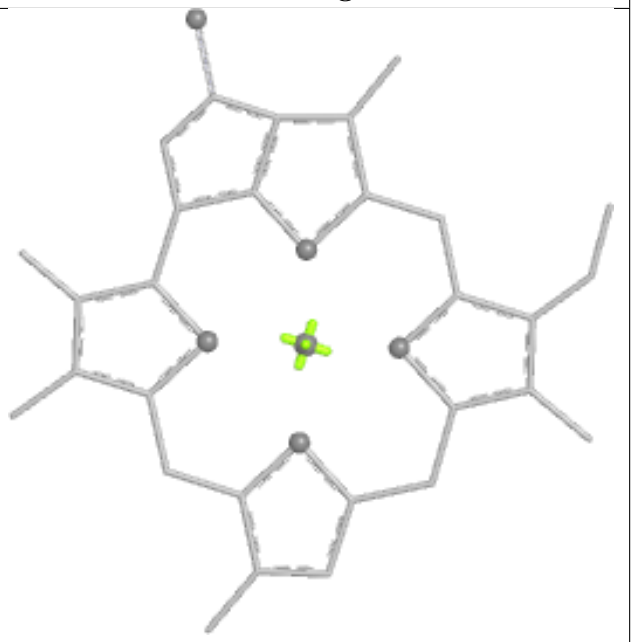


Bond angles

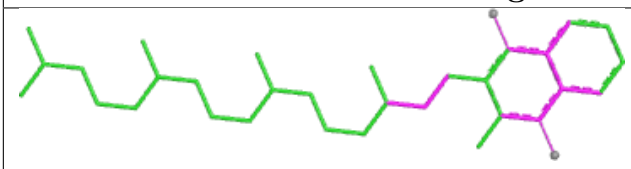


Torsions



Rings

Ligand PQN AA 843



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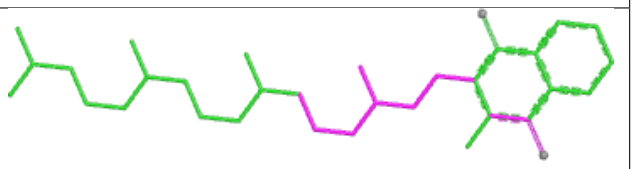
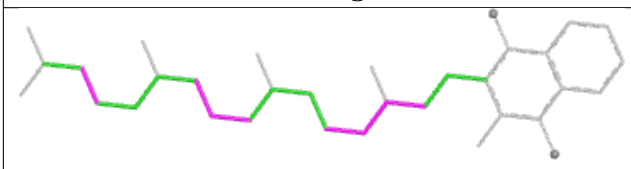


Bond angles



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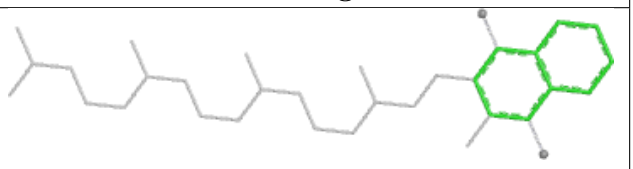
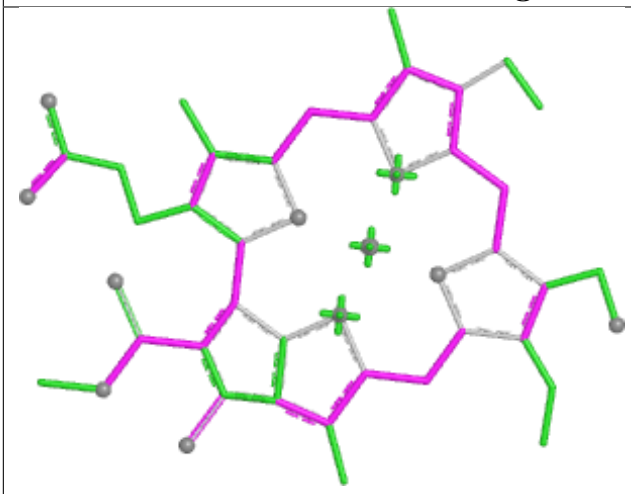


Rings

Ligand CHL A4 306



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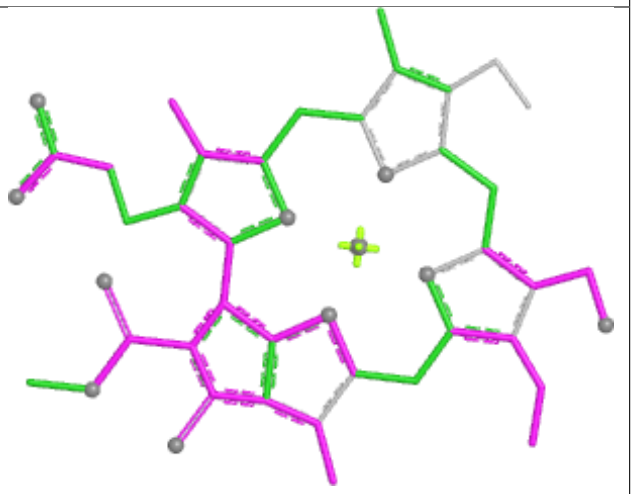
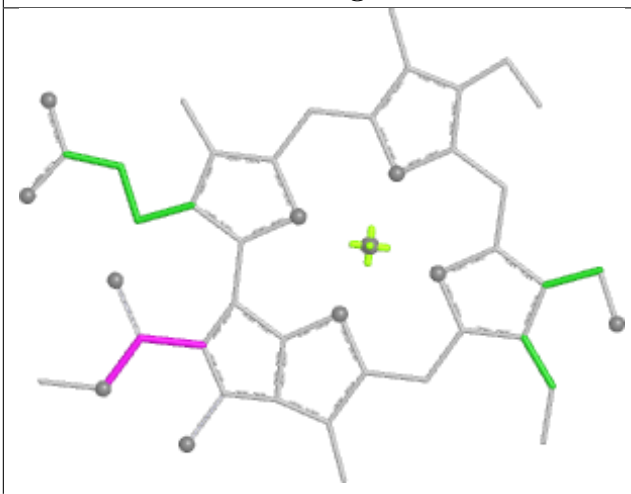
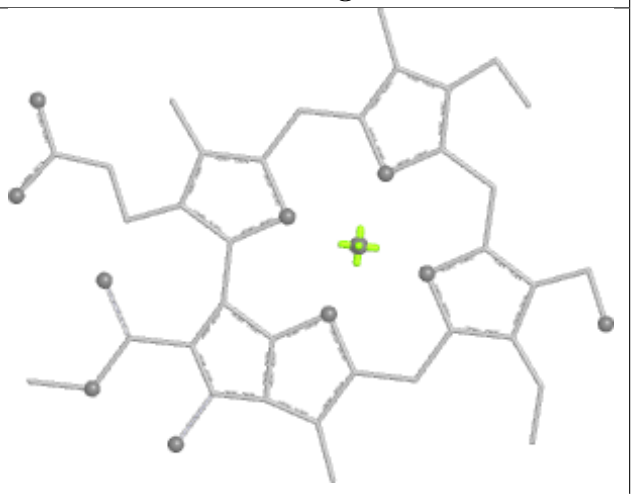


Bond angles

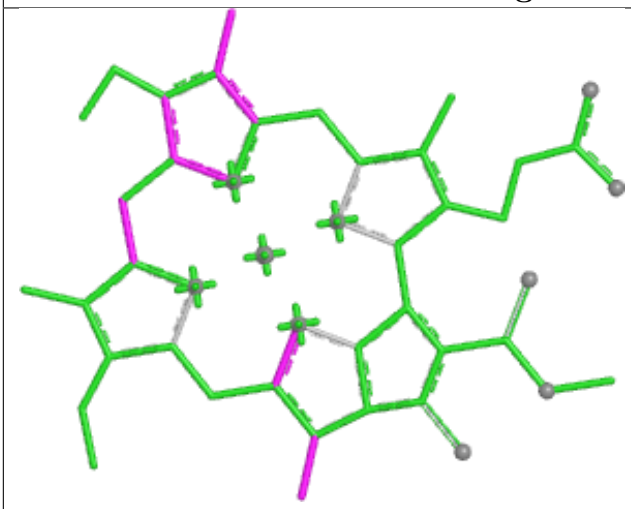


Torsions

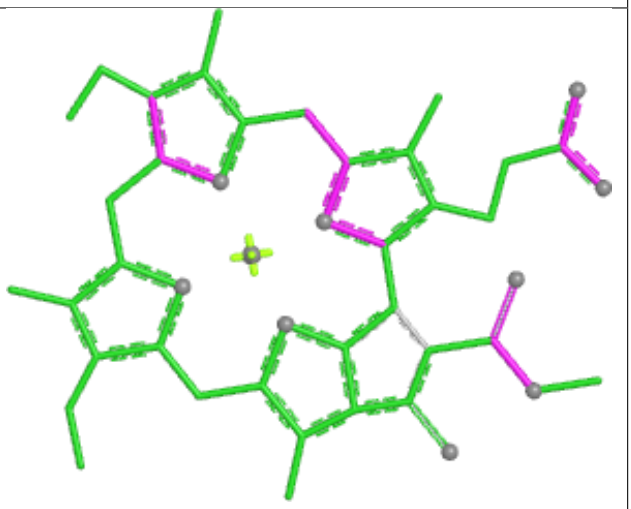


Rings

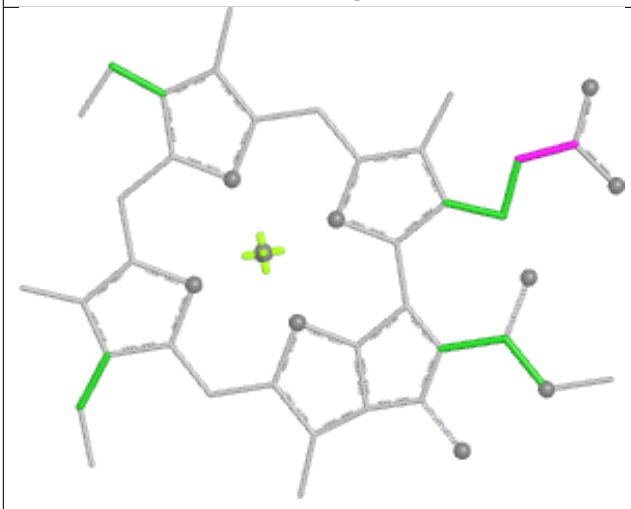
Ligand CLA B2 608



Bond lengths



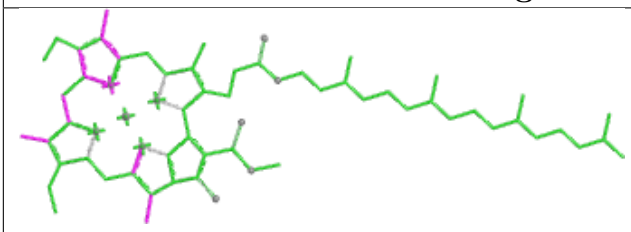
Bond angles



Torsions

Rings

Ligand CLA B2 602



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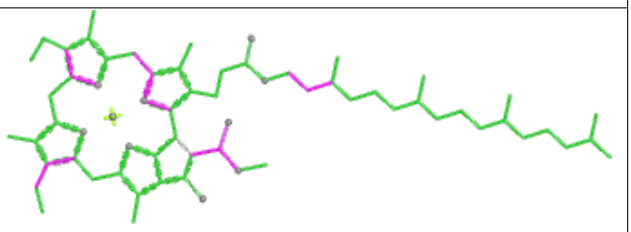
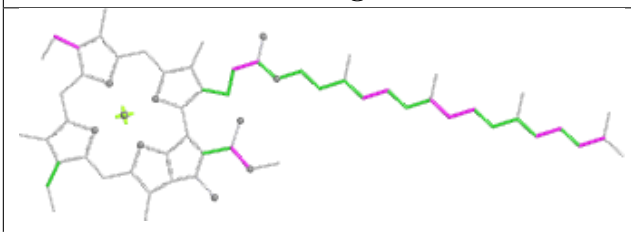
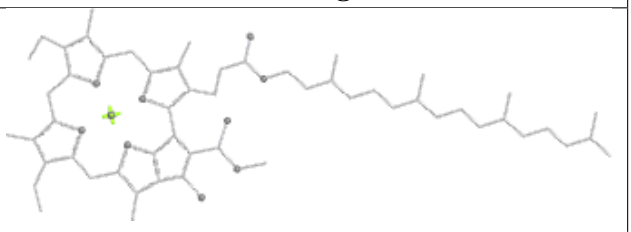


Bond angles

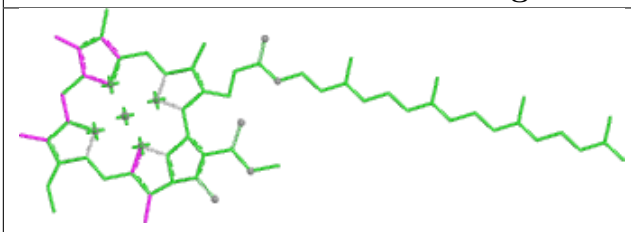


Torsions



Rings

Ligand CLA AB 802



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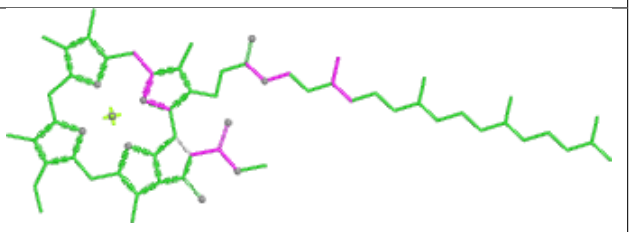
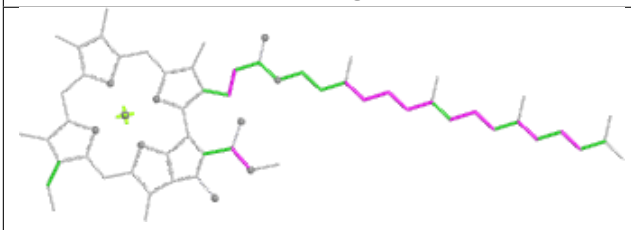
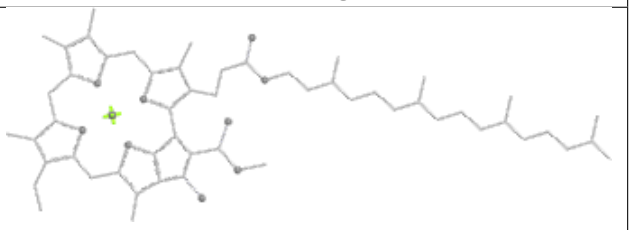


Bond angles

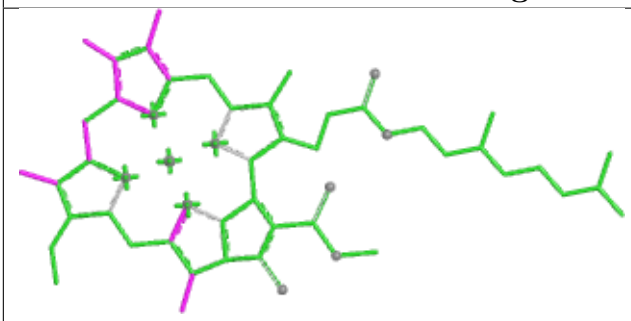


Torsions

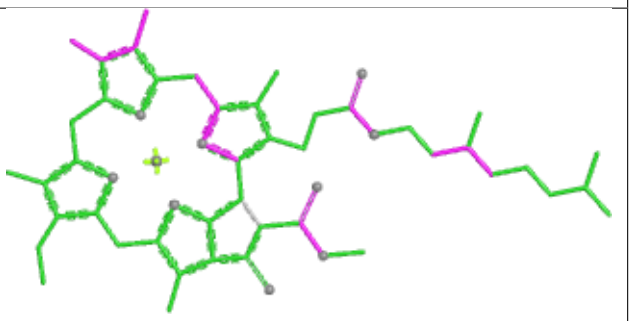


Rings

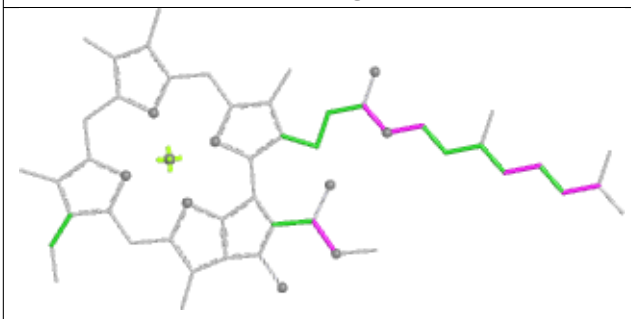
Ligand CLA AB 812



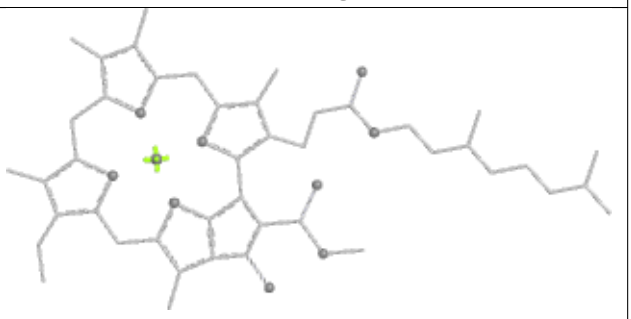
Bond lengths



Bond angles

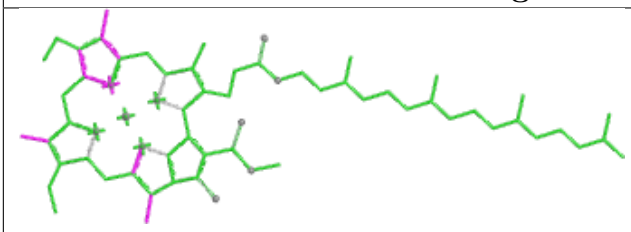


Torsions

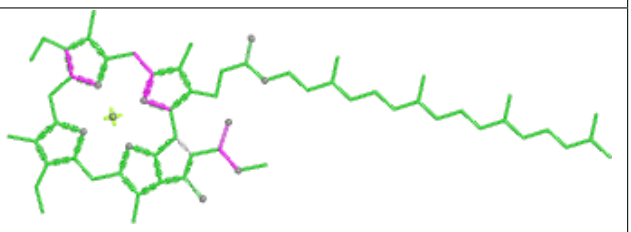


Rings

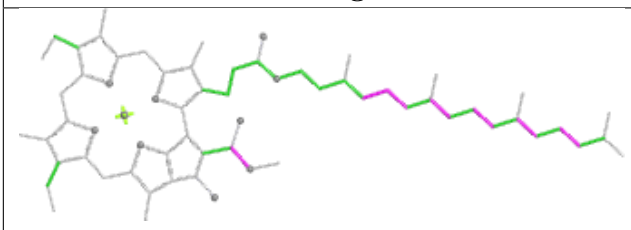
Ligand CLA BB 808



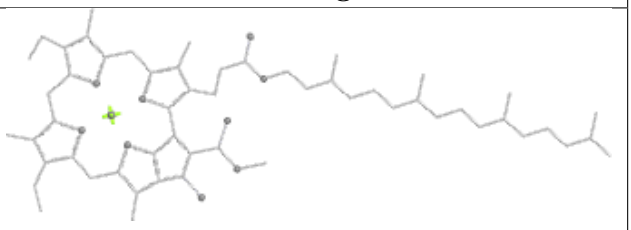
Bond lengths



Bond angles

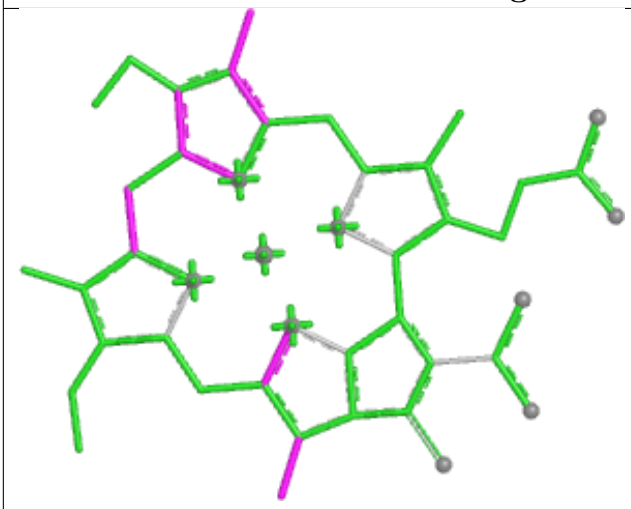


Torsions



Rings

Ligand CLA AG 201



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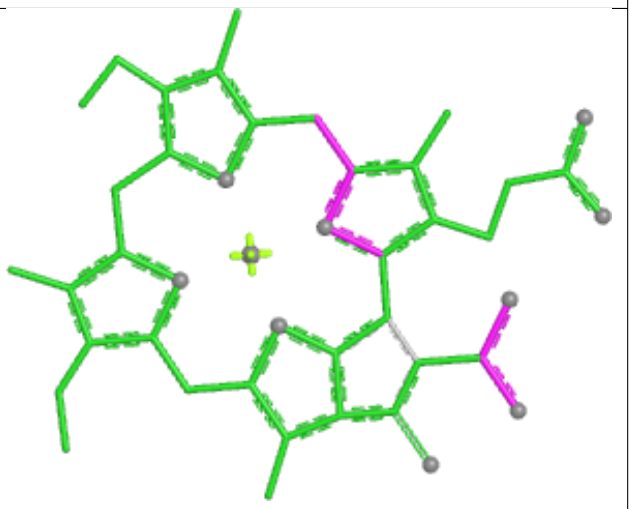
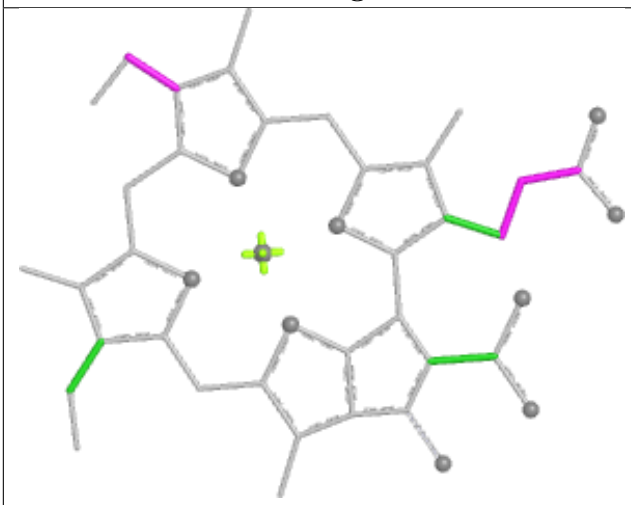
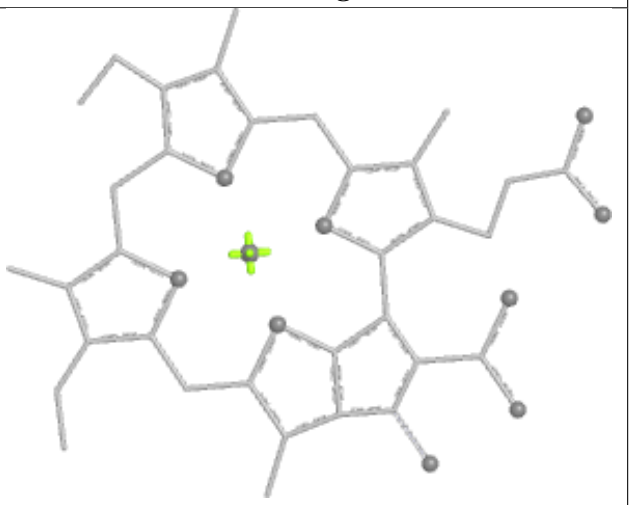


Bond angles

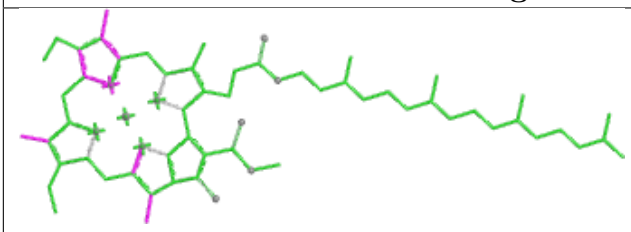


Torsions

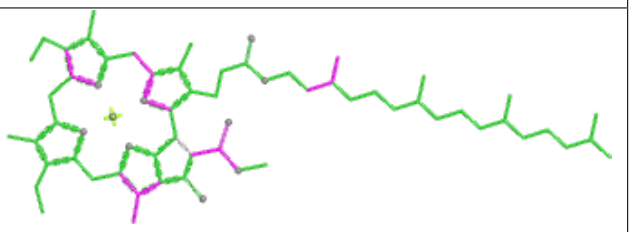


Rings

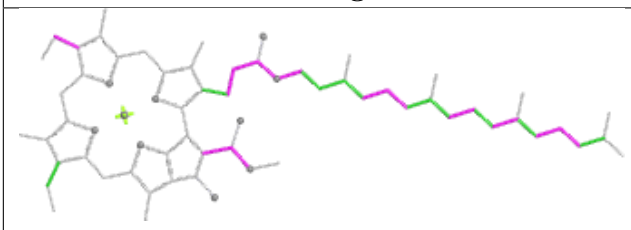
Ligand CLA AA 833



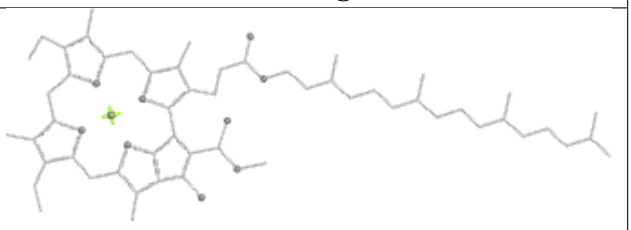
Bond lengths



Bond angles

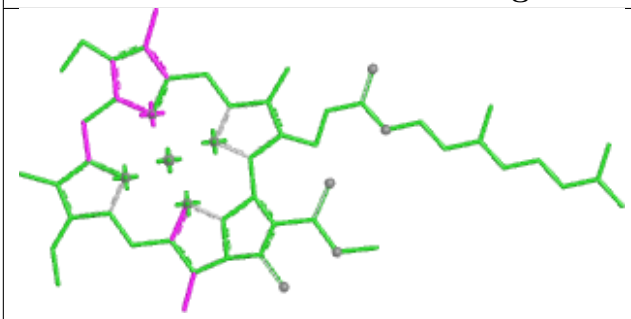


Torsions

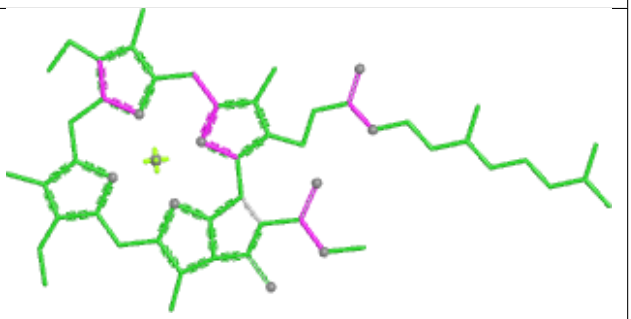


Rings

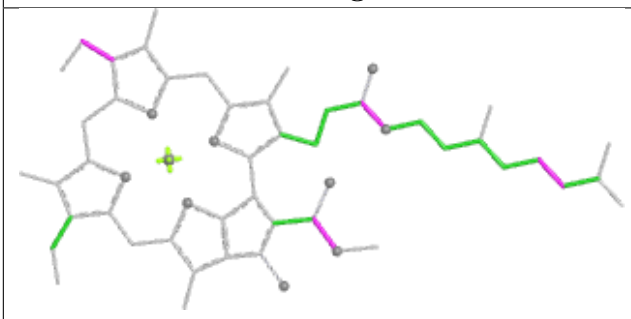
Ligand CLA BB 821



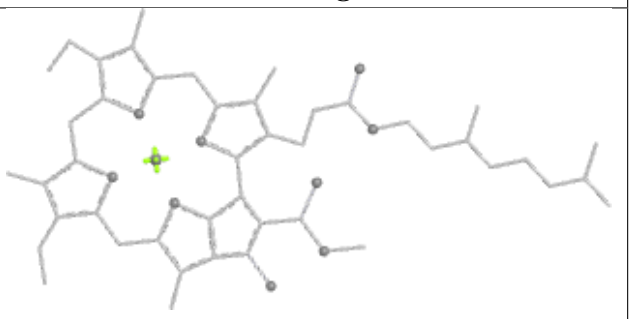
Bond lengths



Bond angles

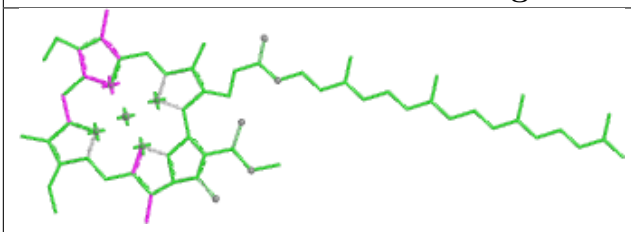


Torsions

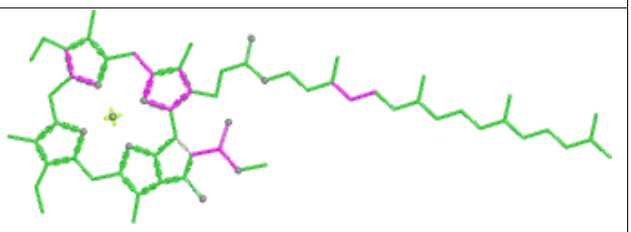


Rings

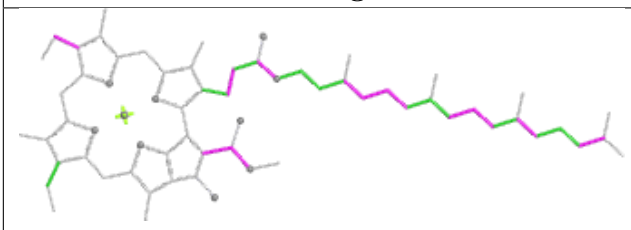
Ligand CLA AB 842



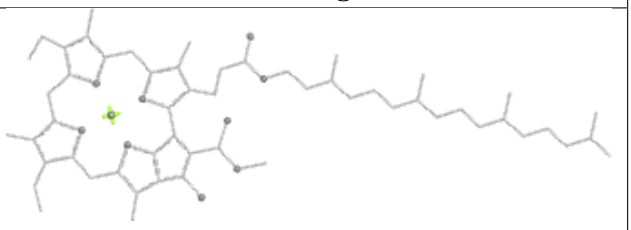
Bond lengths



Bond angles

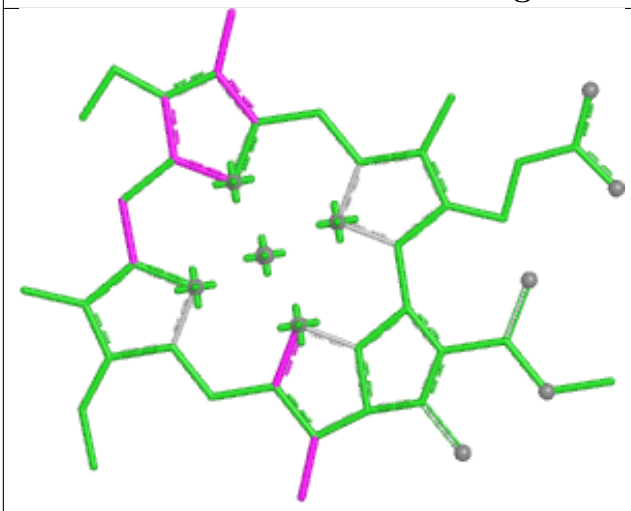


Torsions

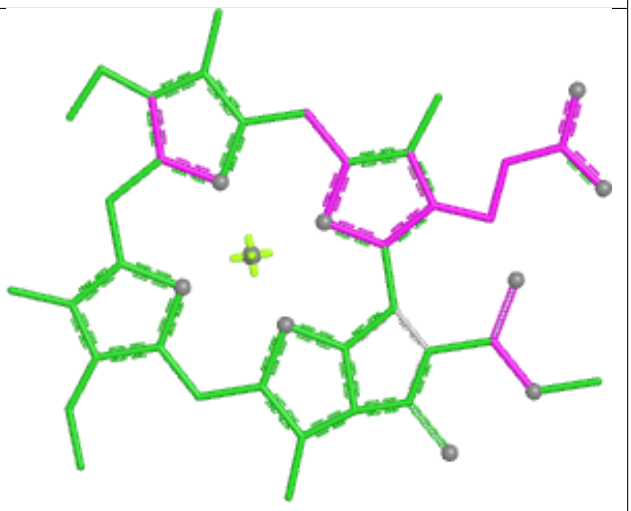


Rings

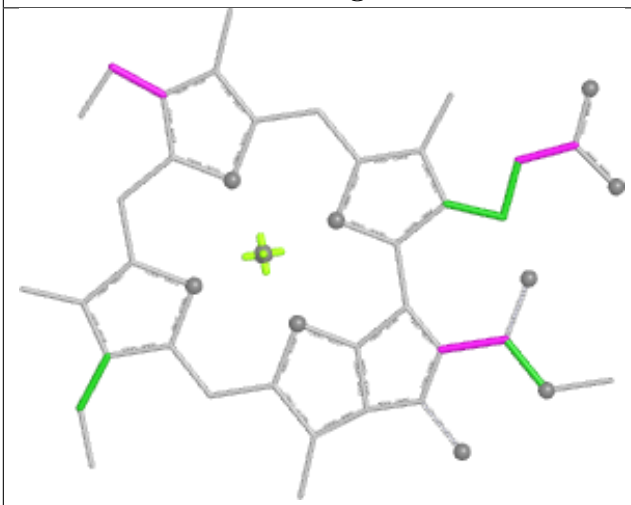
Ligand CLA BL 302



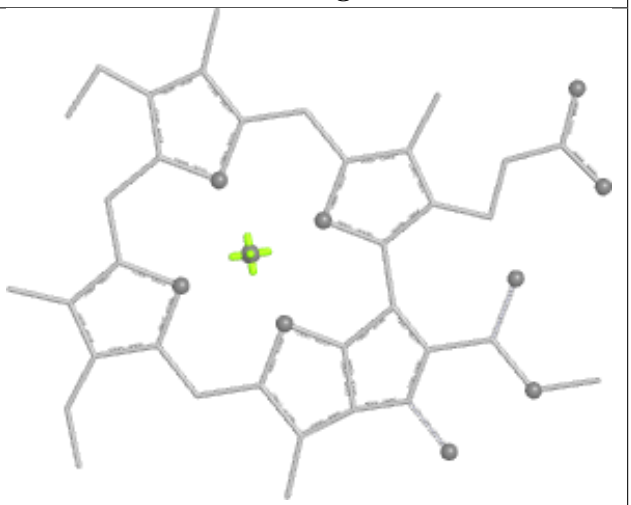
Bond lengths



Bond angles

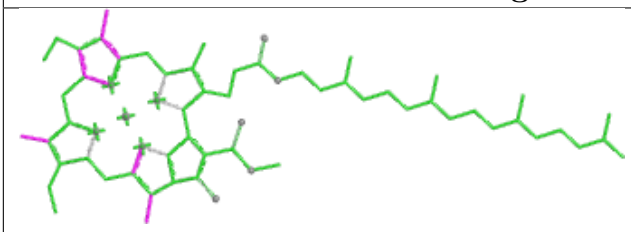


Torsions

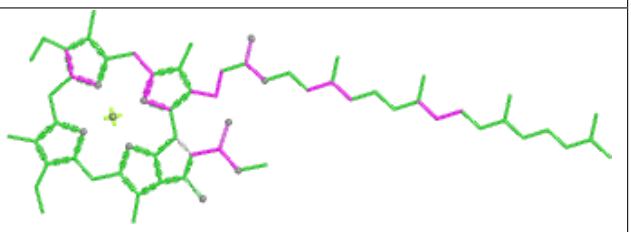


Rings

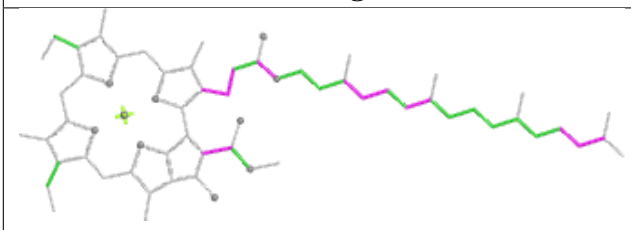
Ligand CLA AB 809



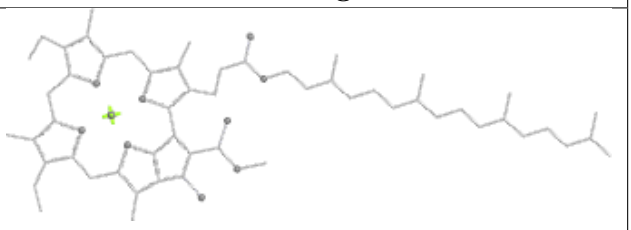
Bond lengths



Bond angles

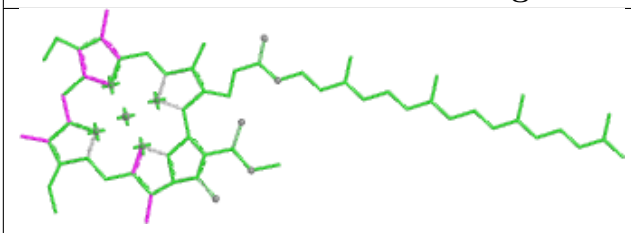


Torsions



Rings

Ligand CLA BB 807



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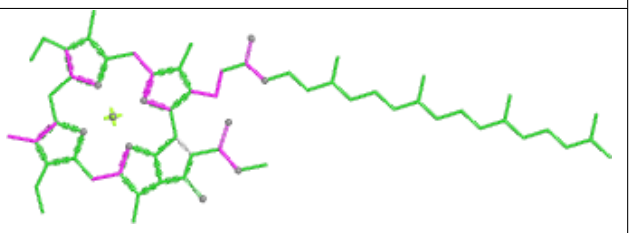
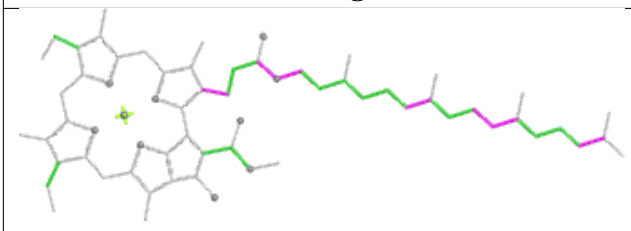


Bond angles



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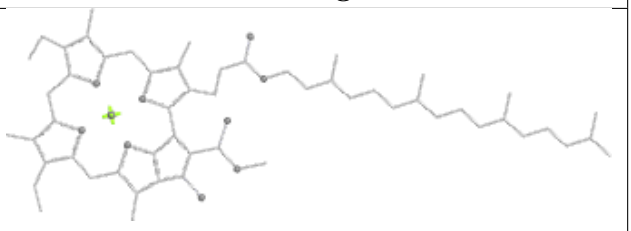
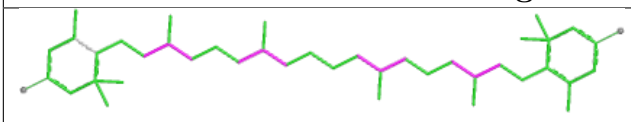


Rings

Ligand LUT B1 316



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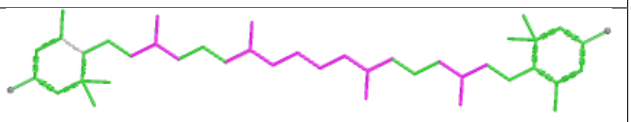
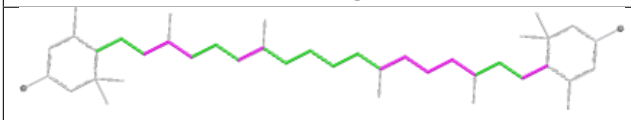
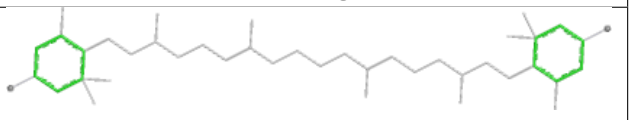


Bond angles

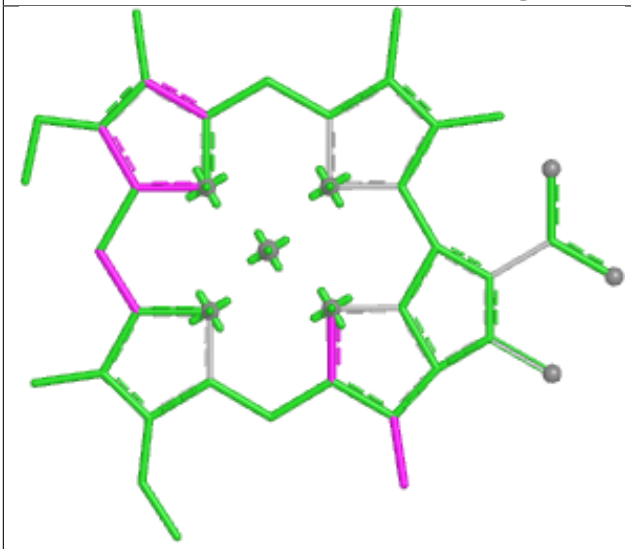


Torsions

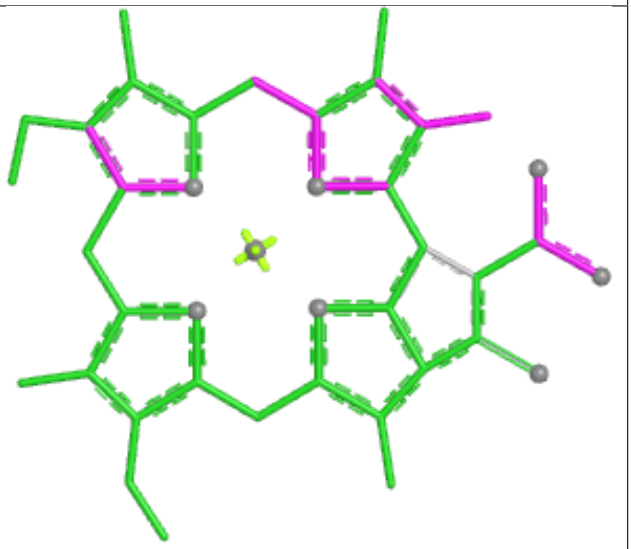


Rings

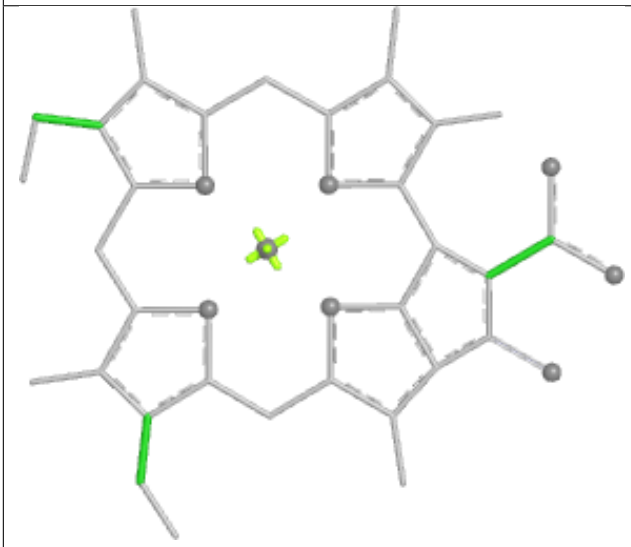
Ligand CLA A3 315



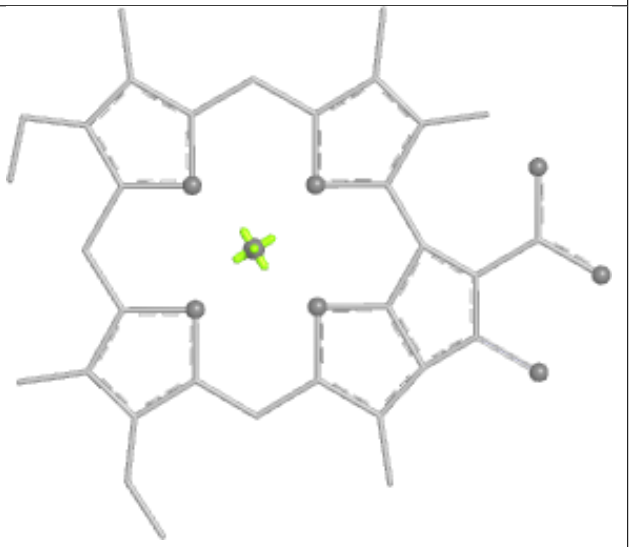
Bond lengths



Bond angles

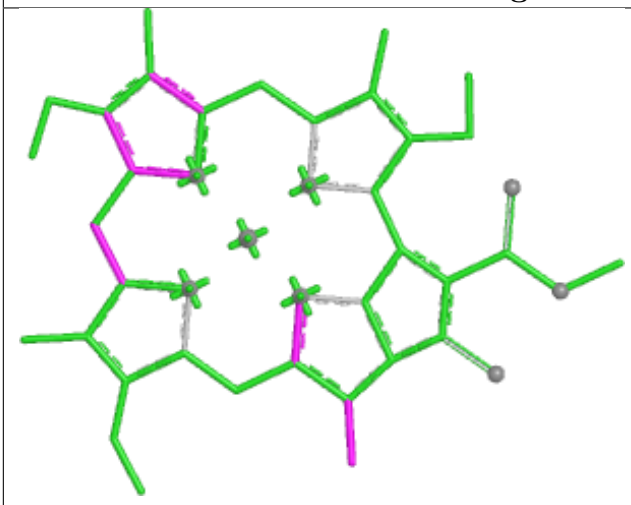


Torsions

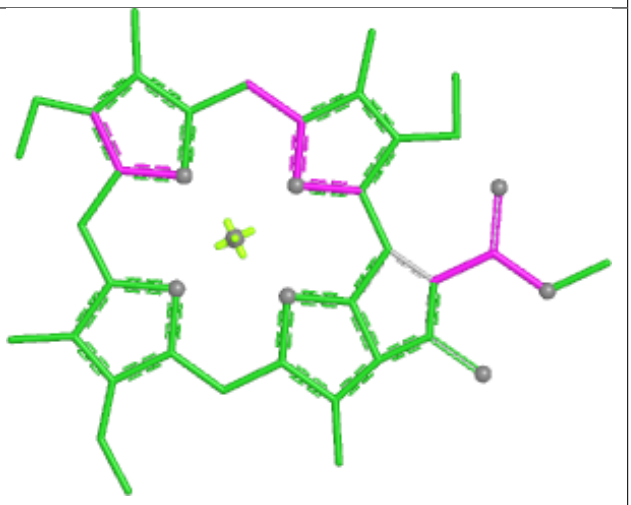


Rings

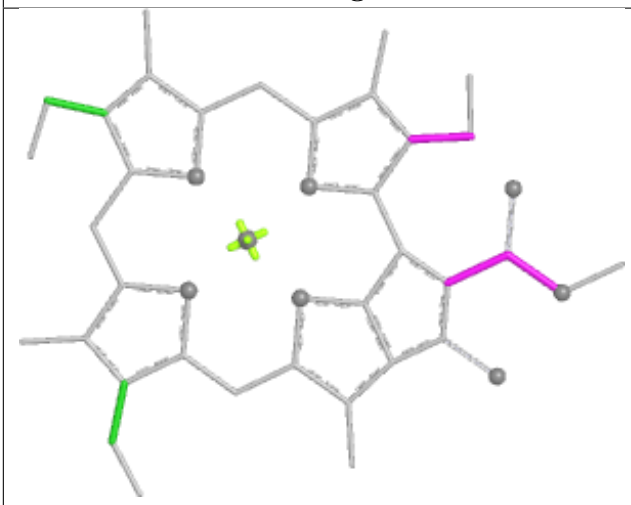
Ligand CLA BG 201



Bond lengths



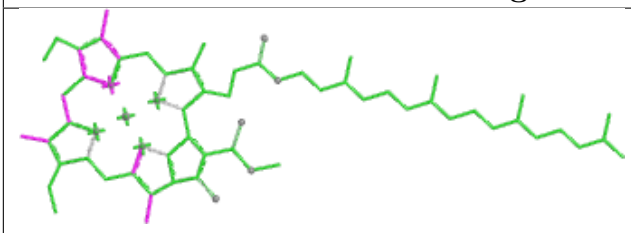
Bond angles



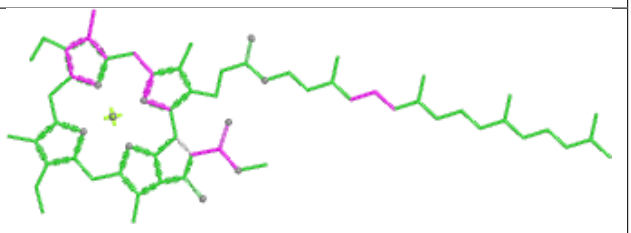
Torsions

Rings

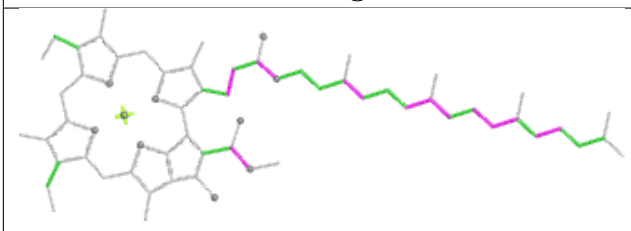
Ligand CLA AA 821



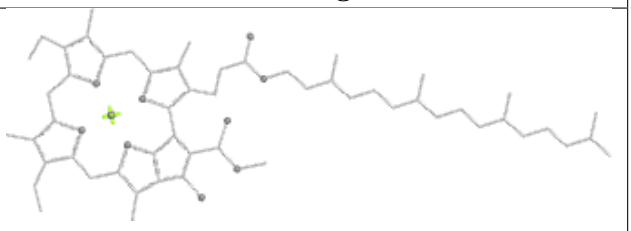
Bond lengths



Bond angles

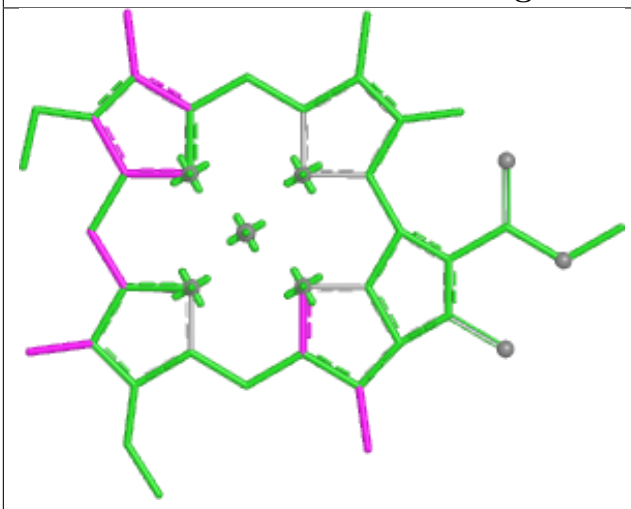


Torsions



Rings

Ligand CLA A3 309



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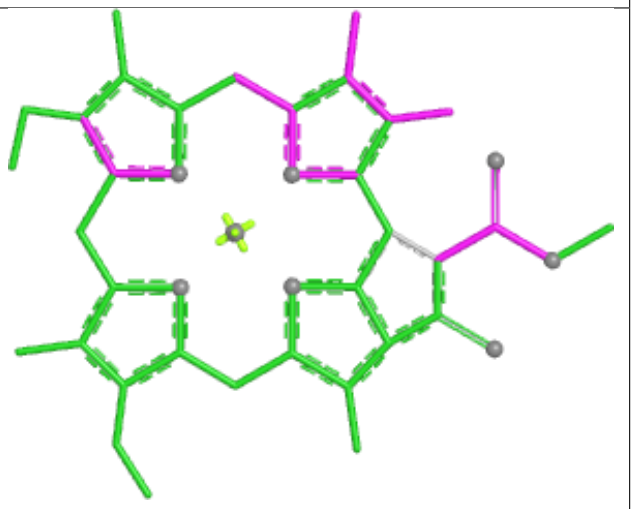
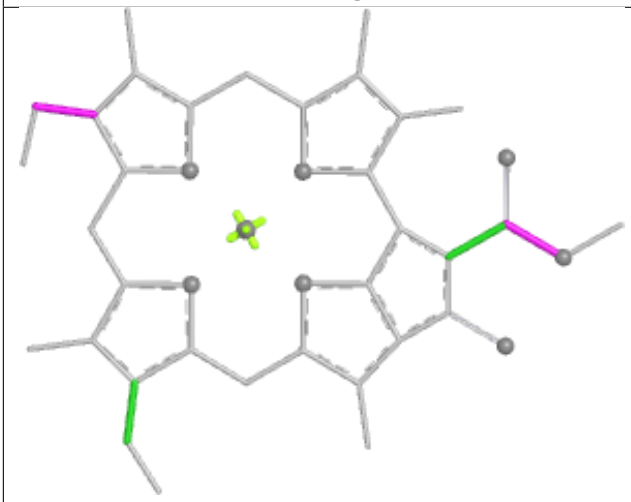


Bond angles



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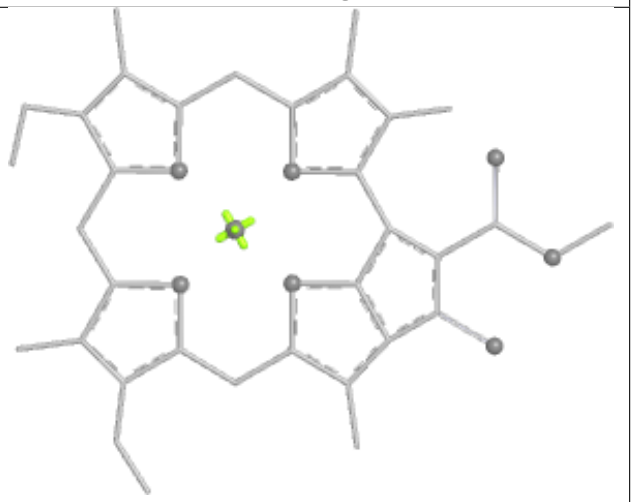
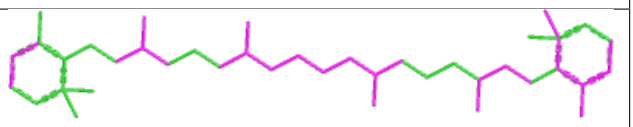


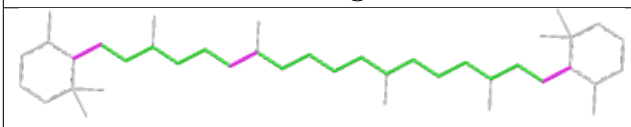
Rings

Ligand BCR BA 848

Bond lengths



Bond angles



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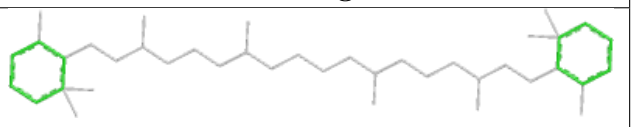
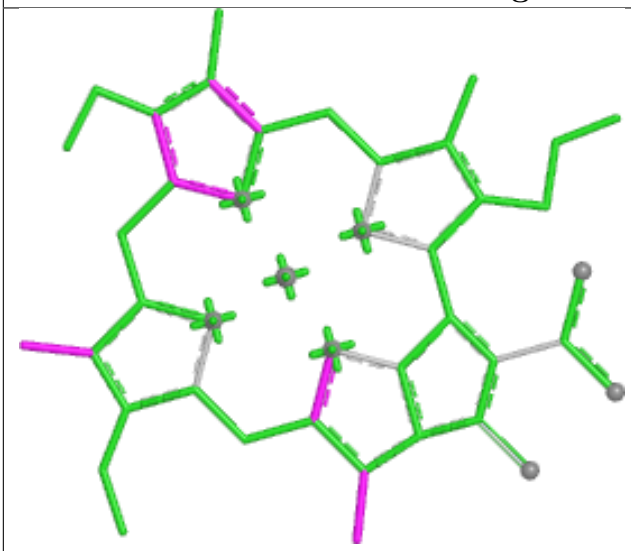
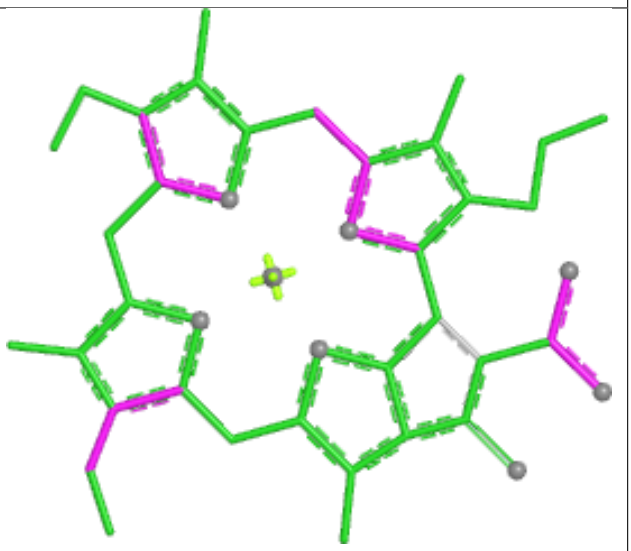


Rings

Ligand CLA BB 817



Bond lengths

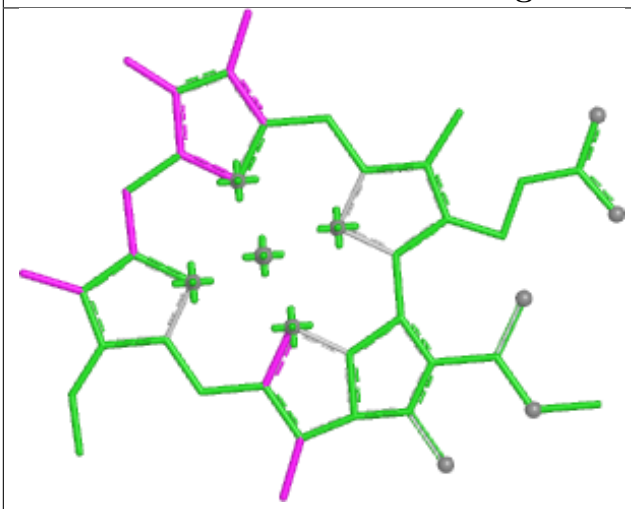


Bond angles

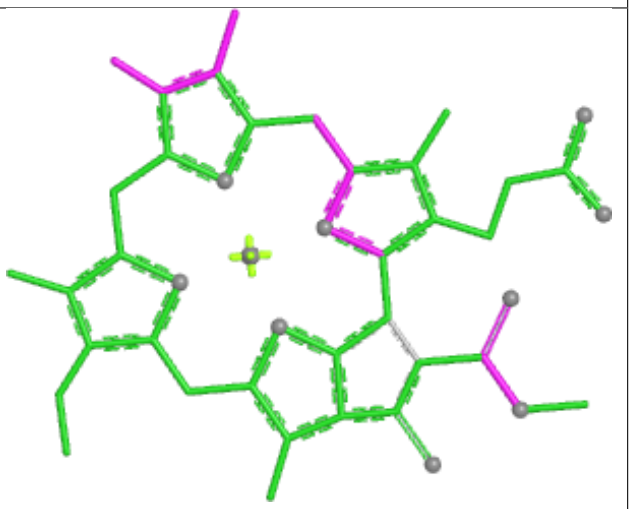
Torsions

Rings

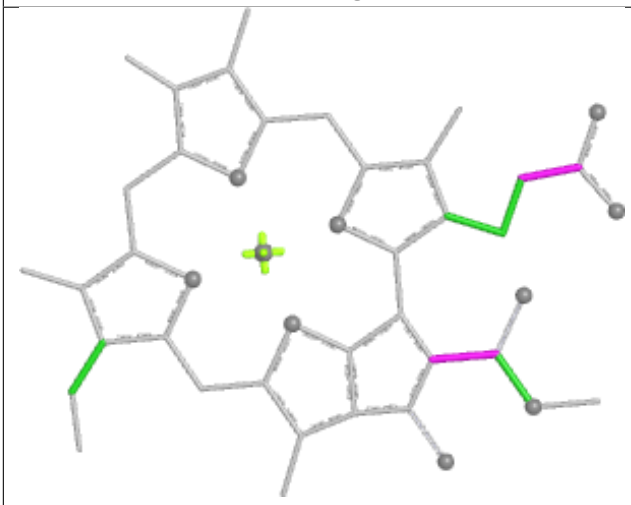
Ligand CLA B5 603



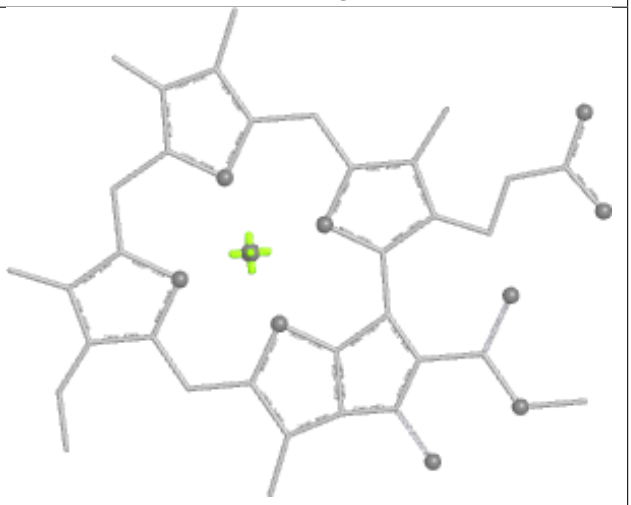
Bond lengths



Bond angles

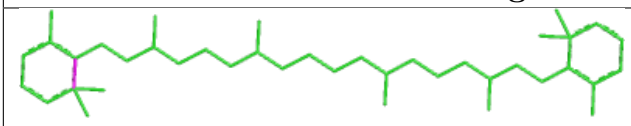


Torsions

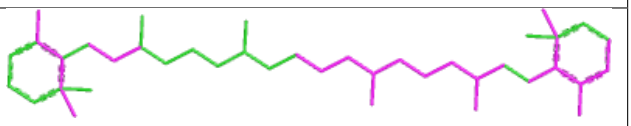


Rings

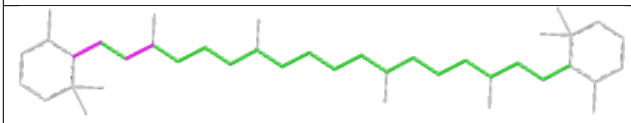
Ligand BCR AA 848



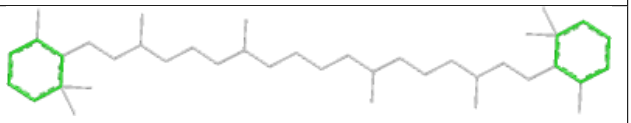
Bond lengths



Bond angles

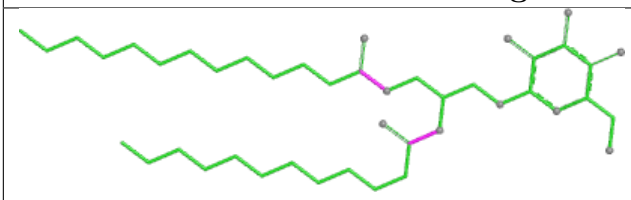


Torsions

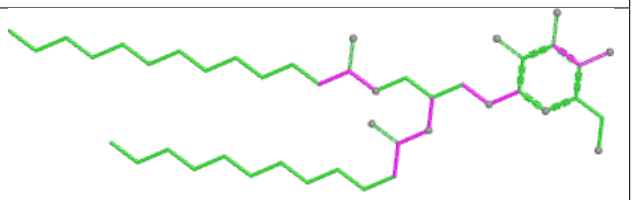


Rings

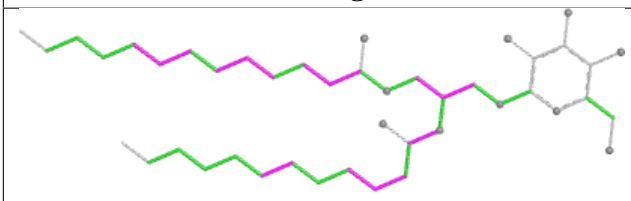
Ligand LMG A1 321



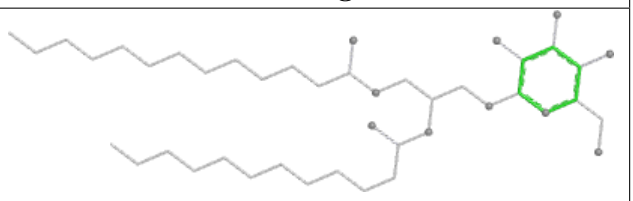
Bond lengths



Bond angles

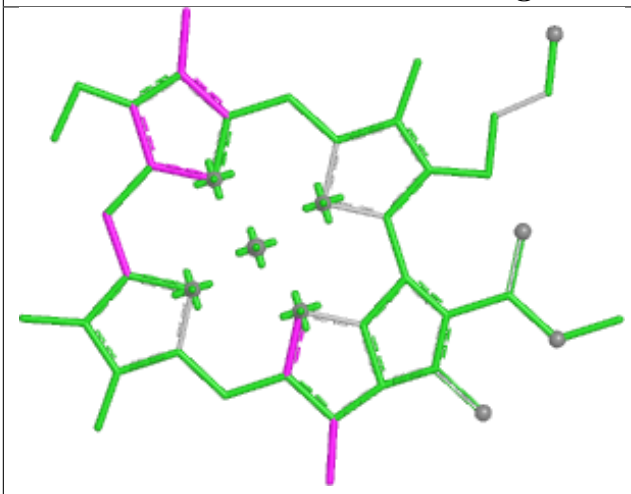


Torsions

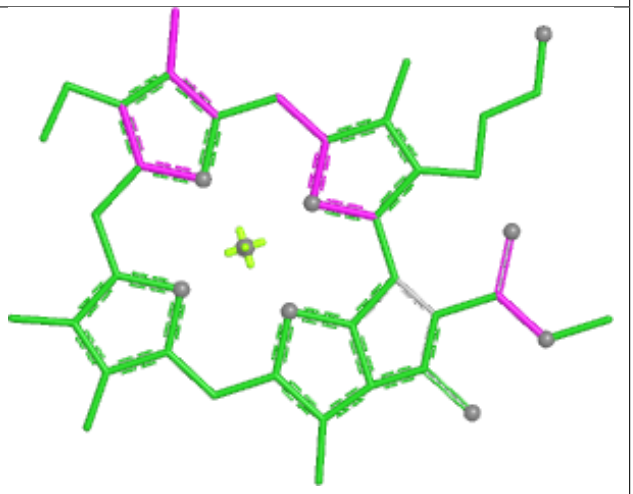


Rings

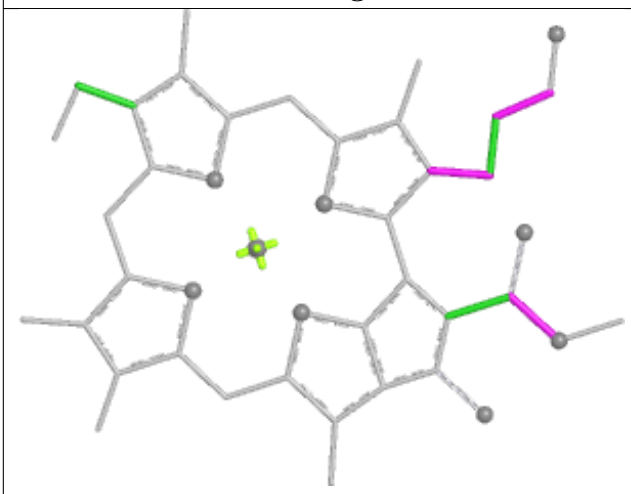
Ligand CLA B2 604



Bond lengths



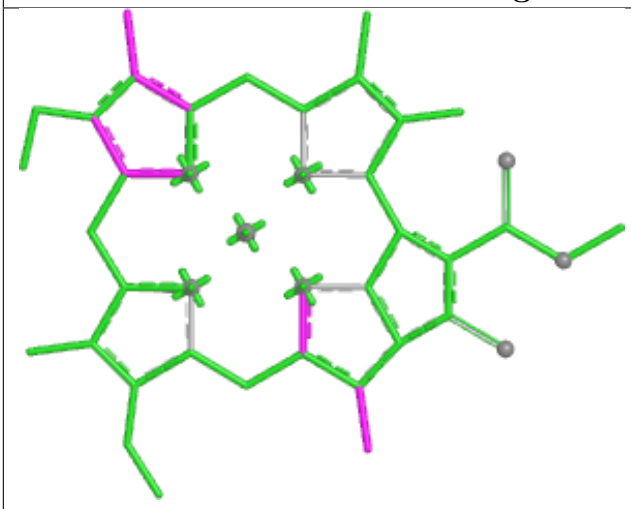
Bond angles



Torsions

Rings

Ligand CLA AL 303



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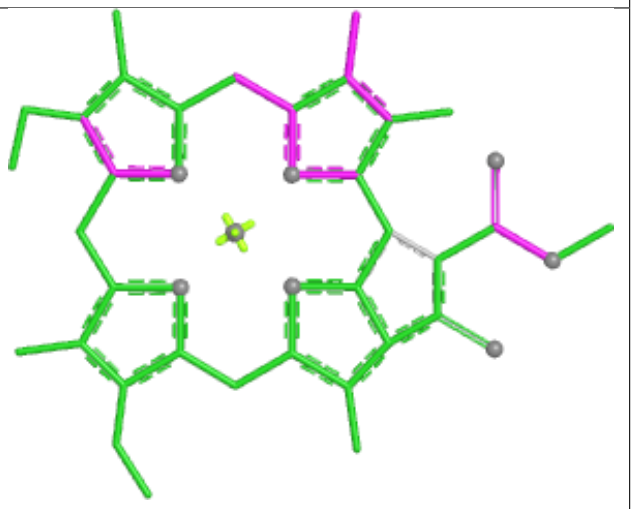
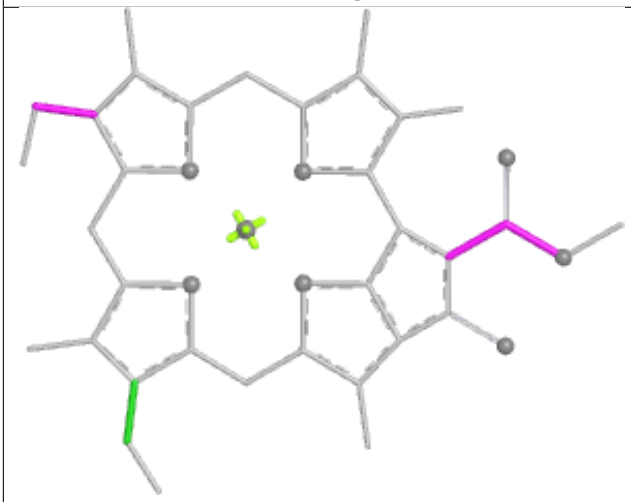
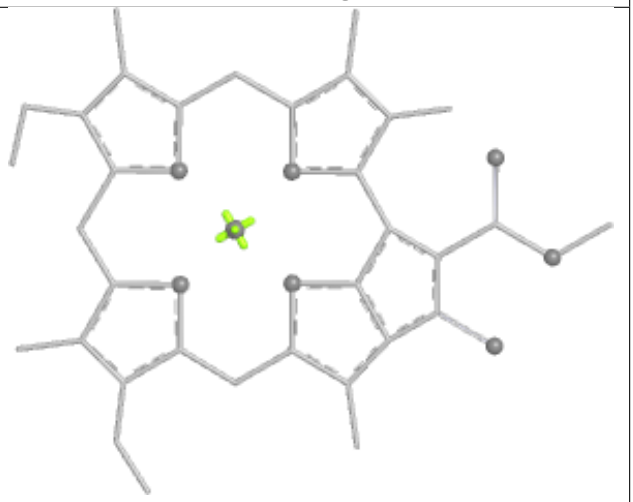


Bond angles

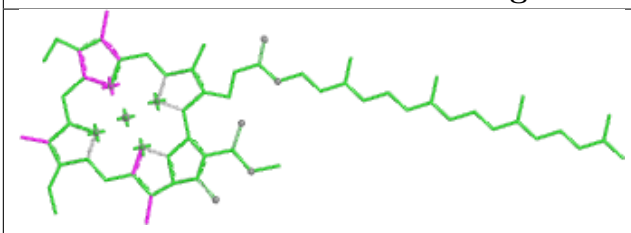


Torsions

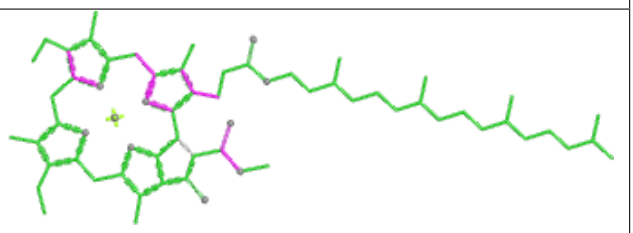


Rings

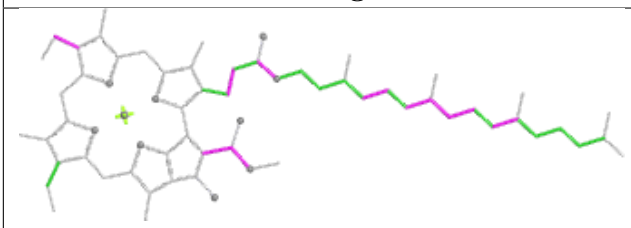
Ligand CLA AA 813



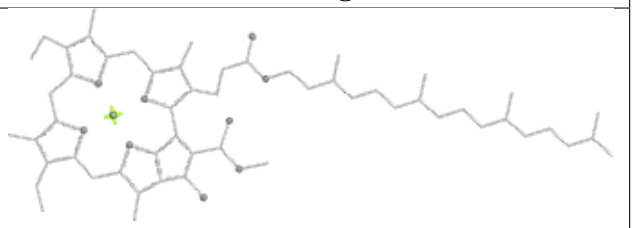
Bond lengths



Bond angles

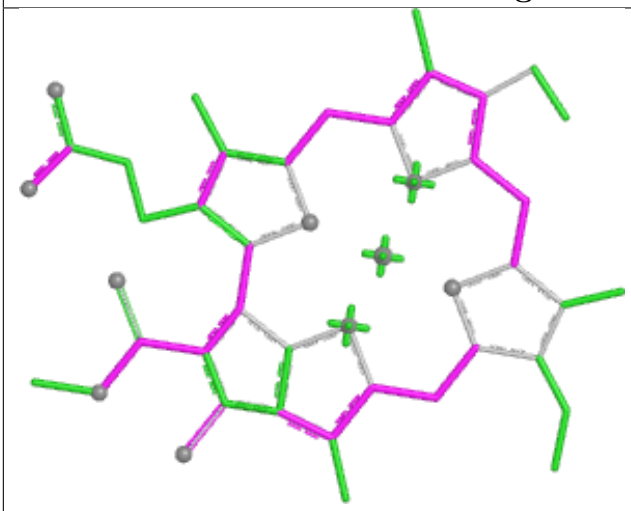


Torsions

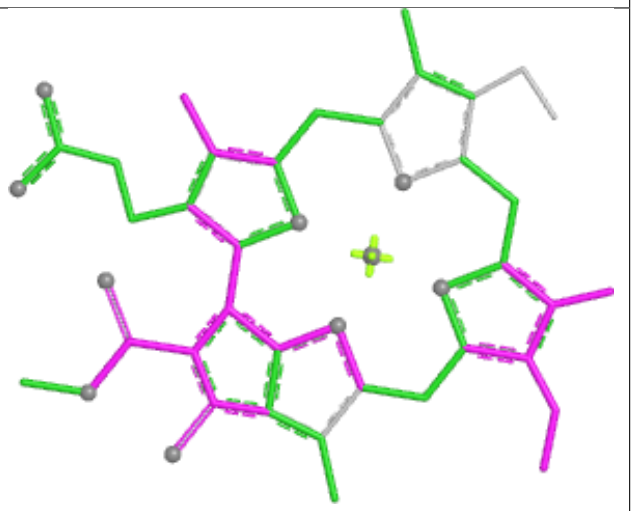


Rings

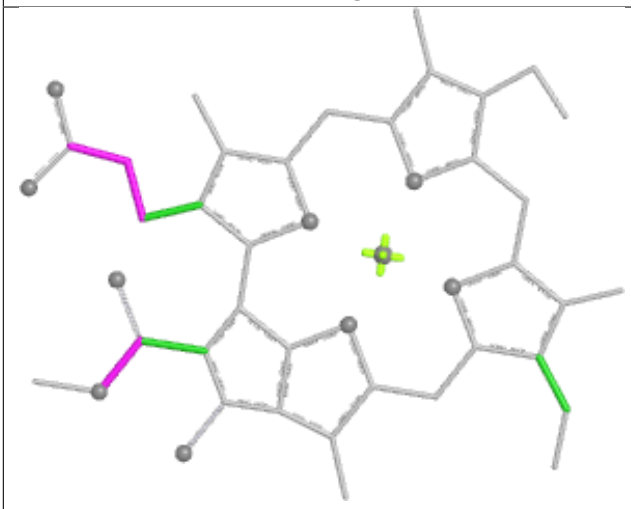
Ligand CHL B3 306



Bond lengths

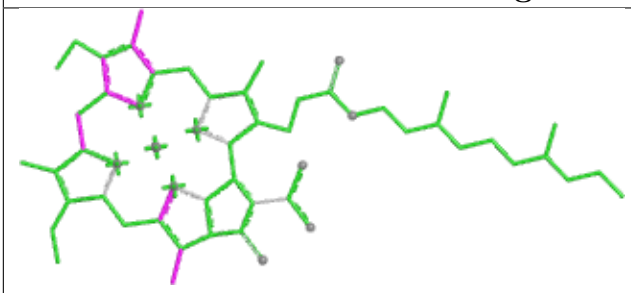
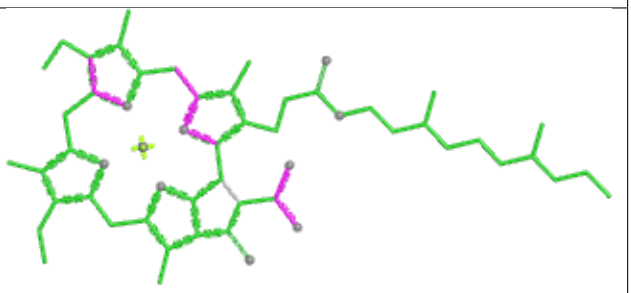
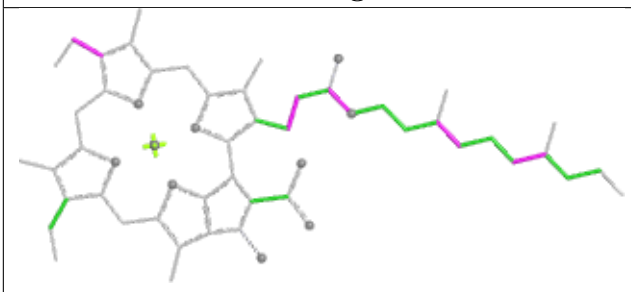
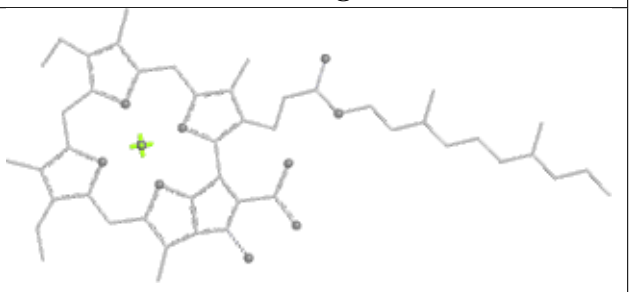


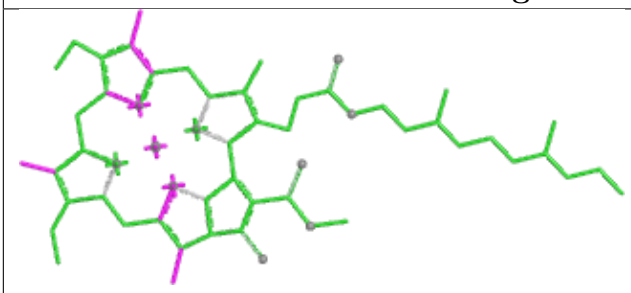
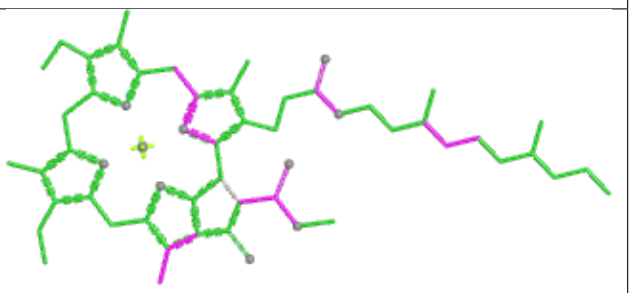
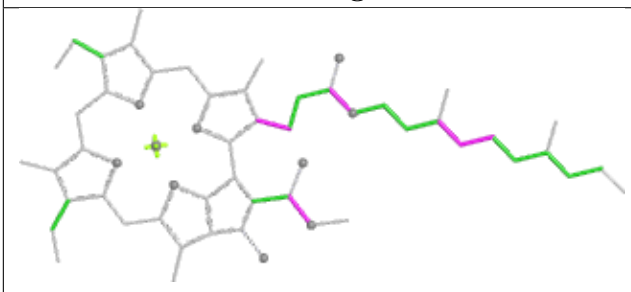
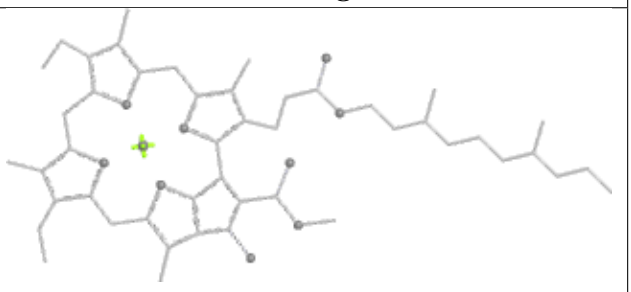
Bond angles



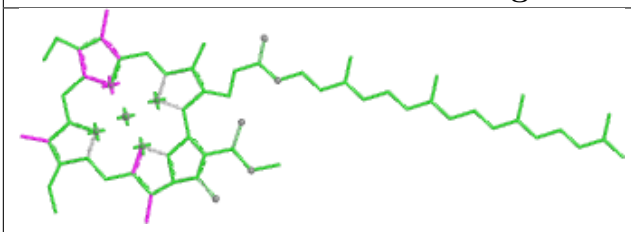
Torsions

Rings

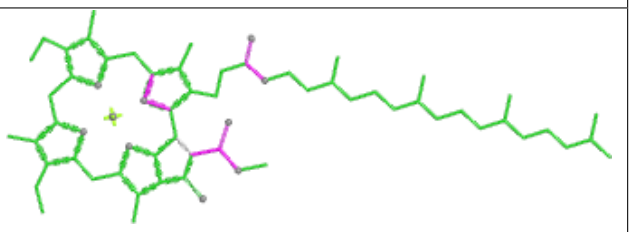
Ligand CLA A4 311	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA AF 802	
	
Bond lengths	Bond angles
	
Torsions	Rings

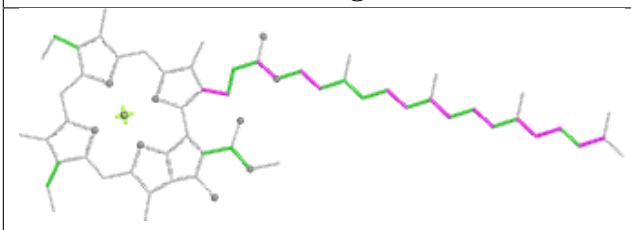
Ligand CLA BA 830



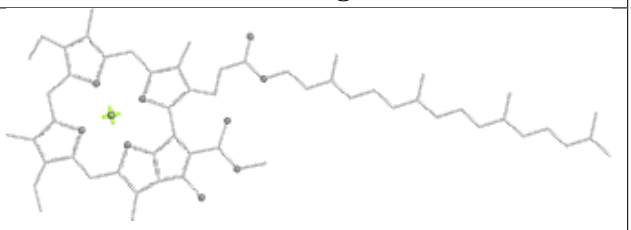
Bond lengths



Bond angles

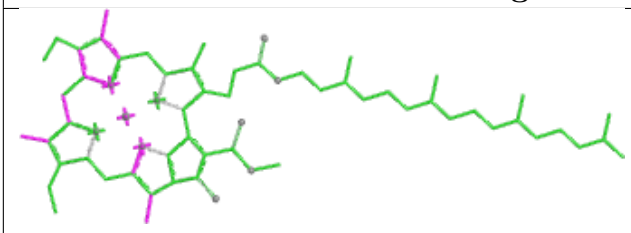


Torsions

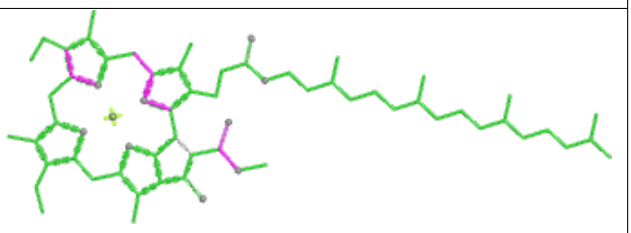


Rings

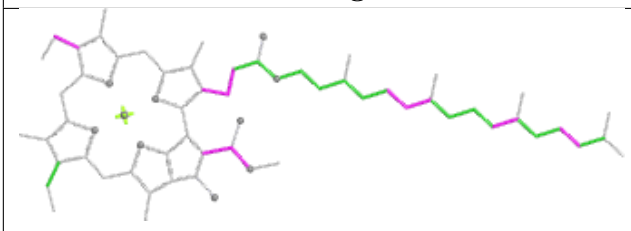
Ligand CLA AB 814



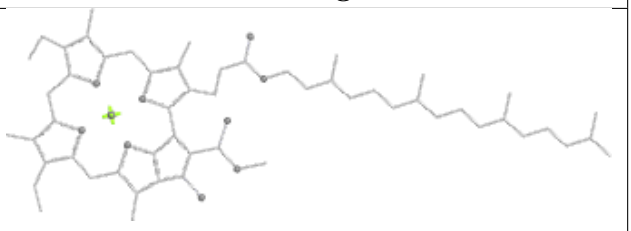
Bond lengths



Bond angles

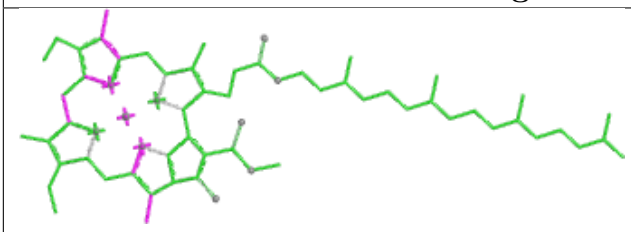


Torsions

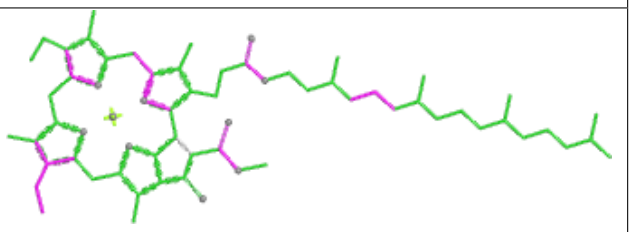


Rings

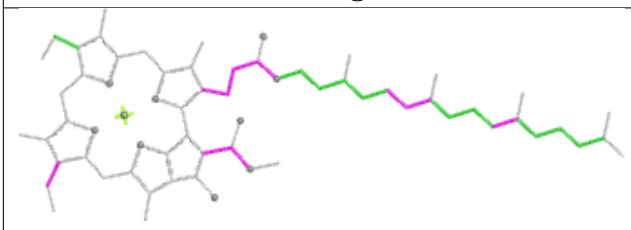
Ligand CLA BB 815



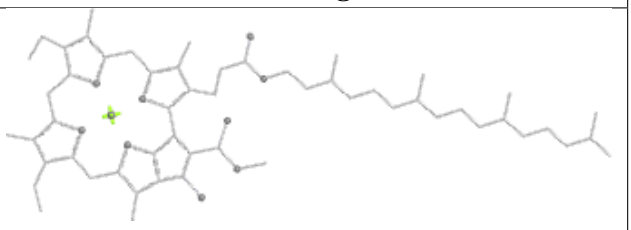
Bond lengths



Bond angles

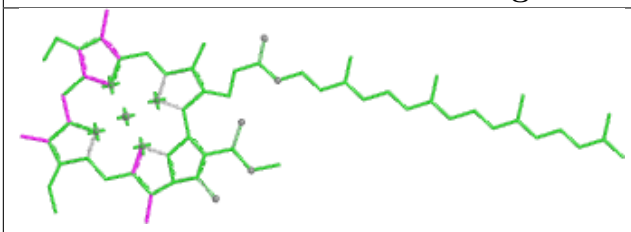


Torsions

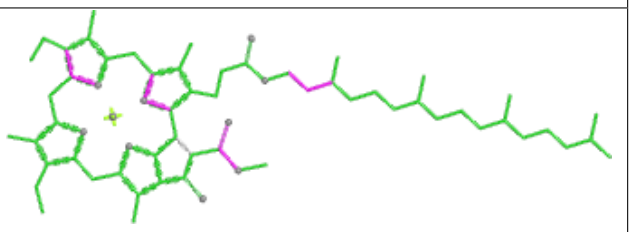


Rings

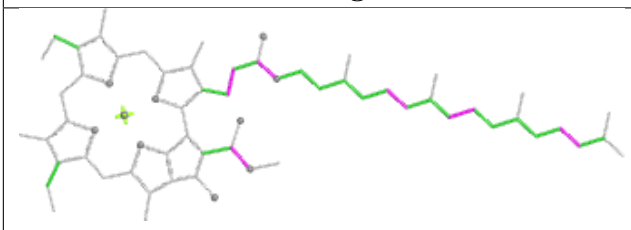
Ligand CLA BB 839



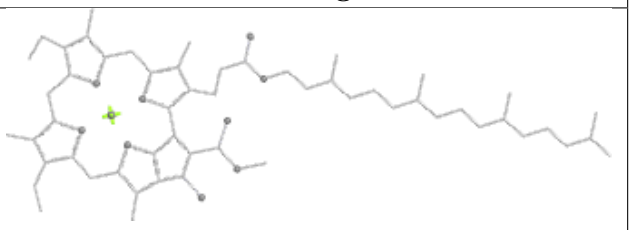
Bond lengths



Bond angles



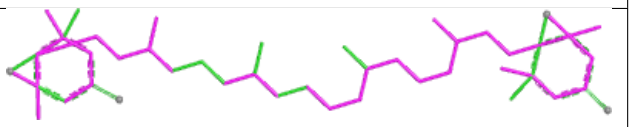
Torsions



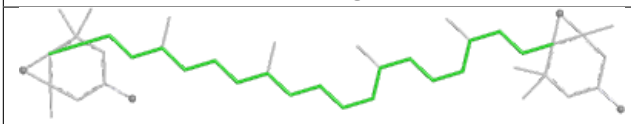
Rings

Ligand XAT B3 316

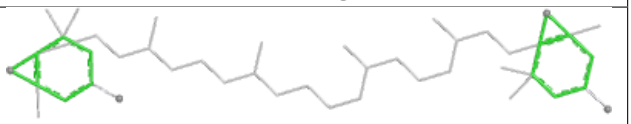
Bond lengths



Bond angles

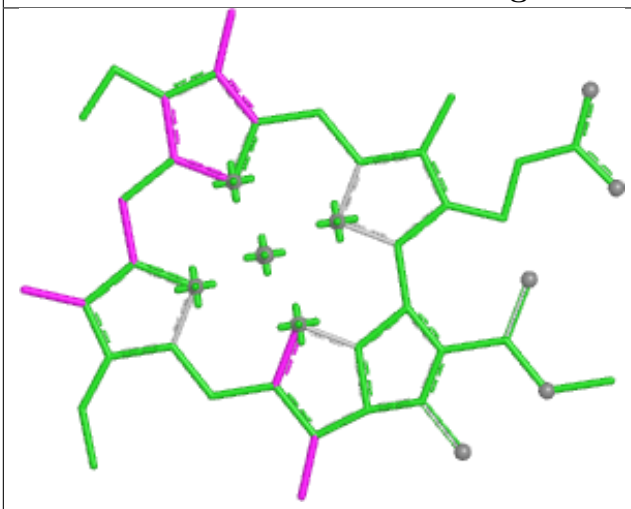


Torsions



Rings

Ligand CLA AG 204



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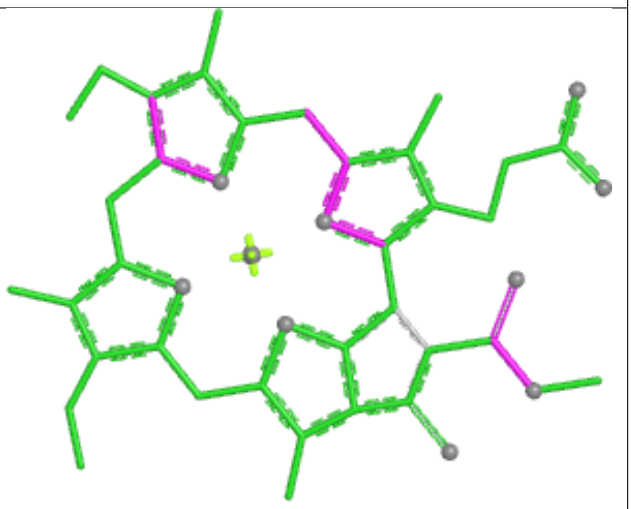
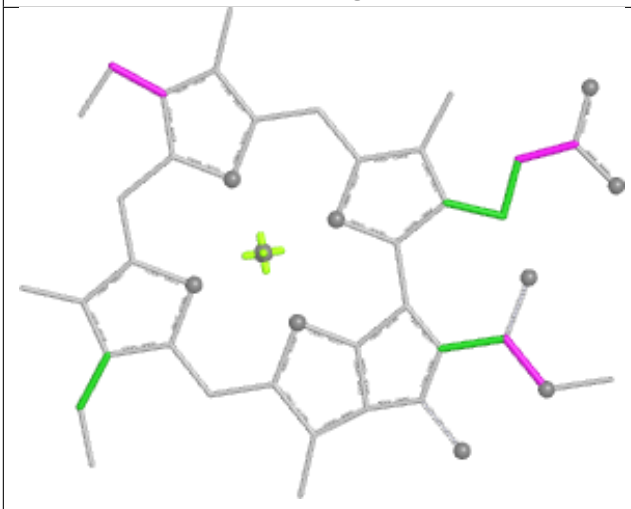


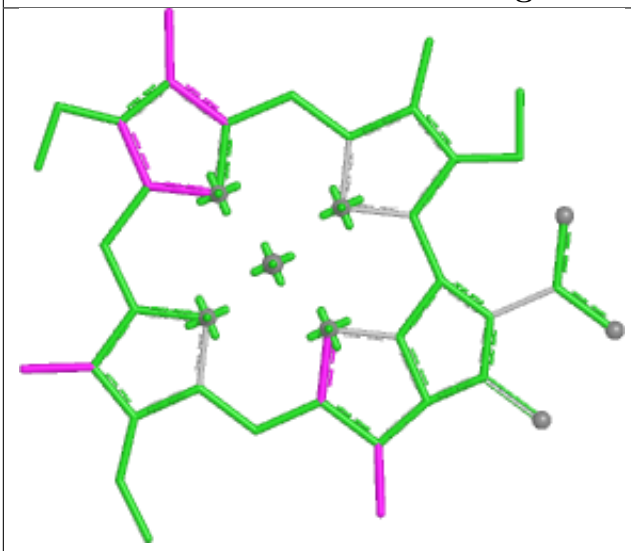
Bond angles



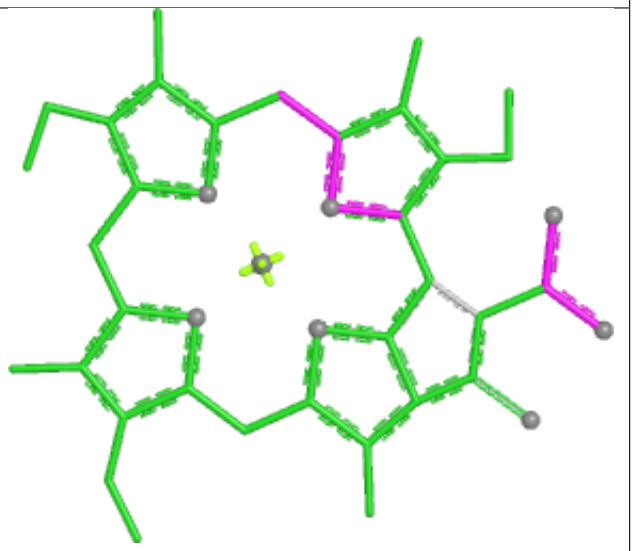
Torsions

Rings

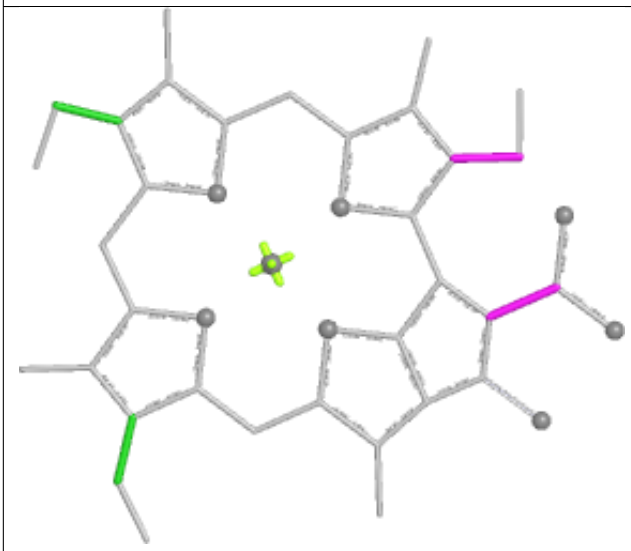
Ligand CLA B5 611



Bond lengths



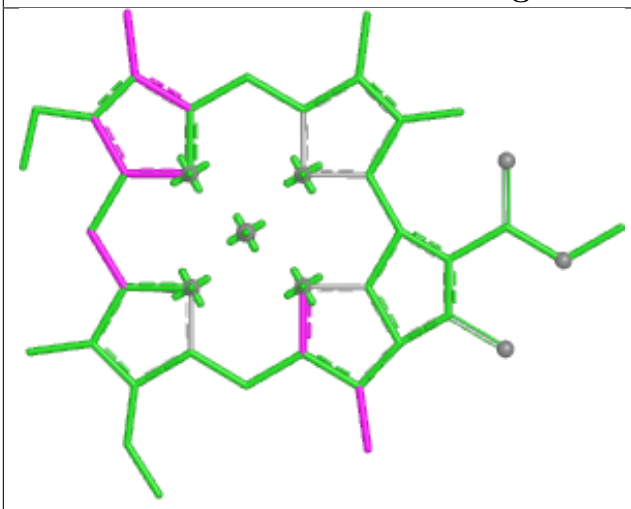
Bond angles



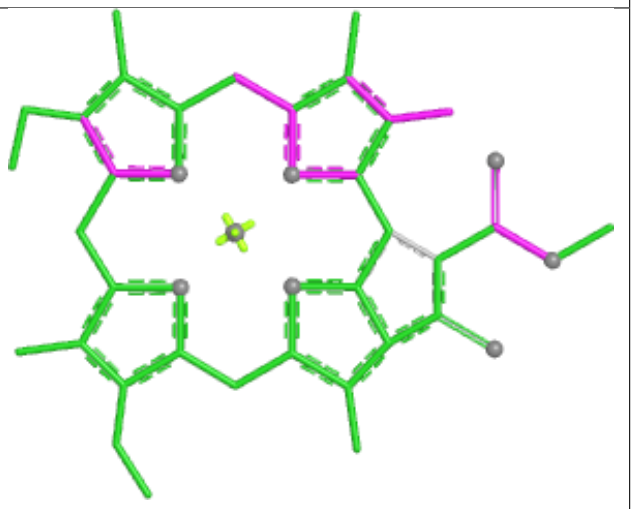
Torsions

Rings

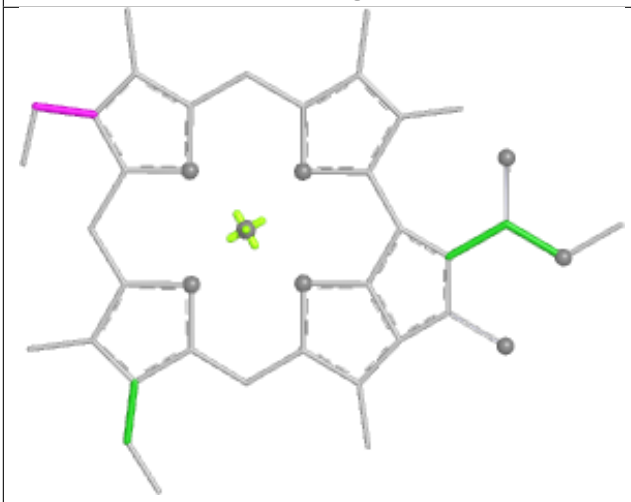
Ligand CLA AF 804



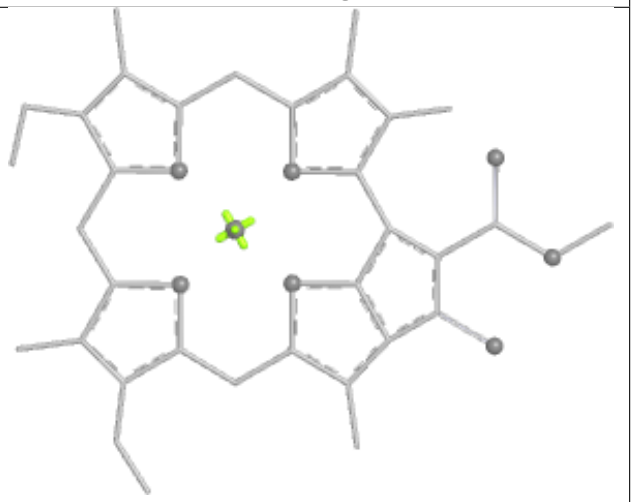
Bond lengths



Bond angles

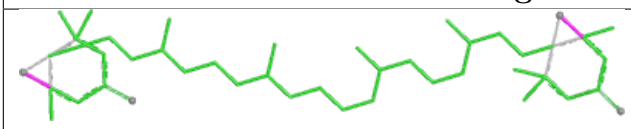


Torsions

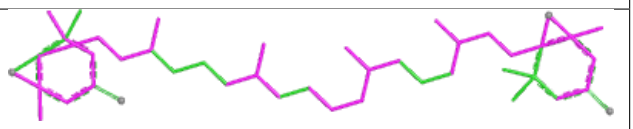


Rings

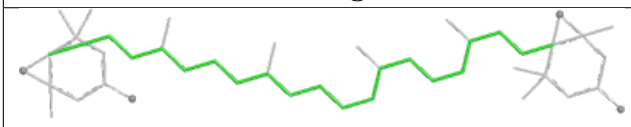
Ligand XAT B2 616



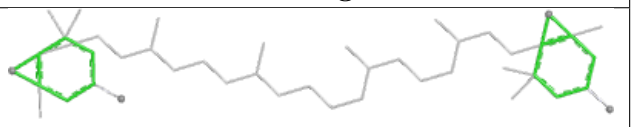
Bond lengths



Bond angles

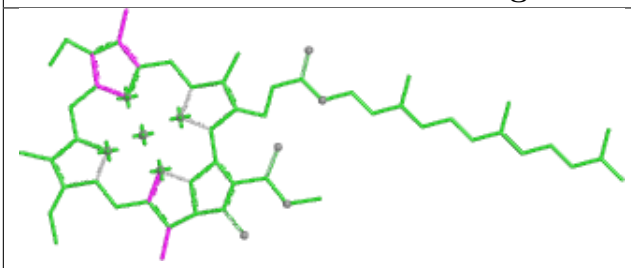


Torsions

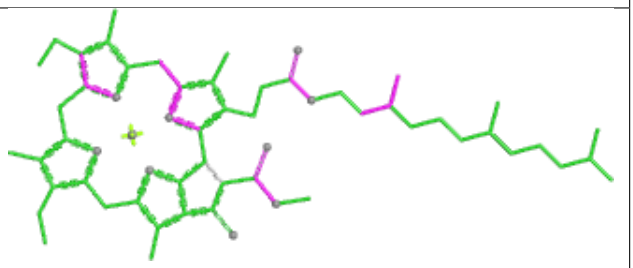


Rings

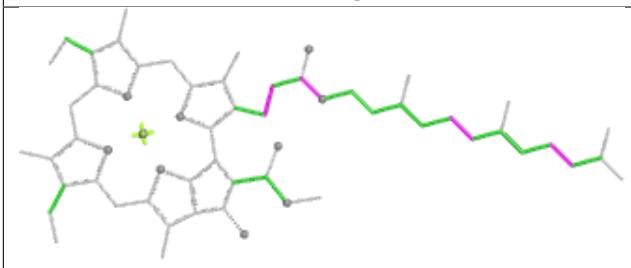
Ligand CLA AA 817



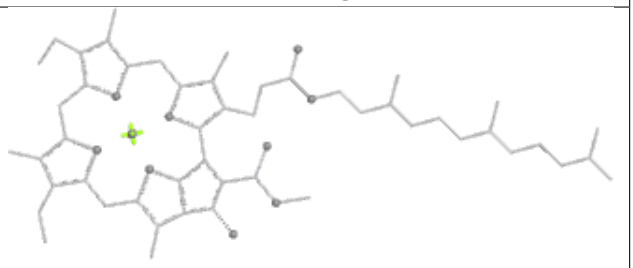
Bond lengths



Bond angles

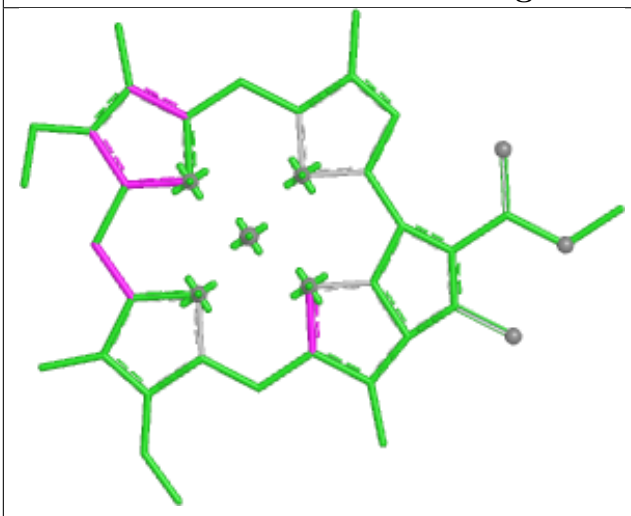


Torsions

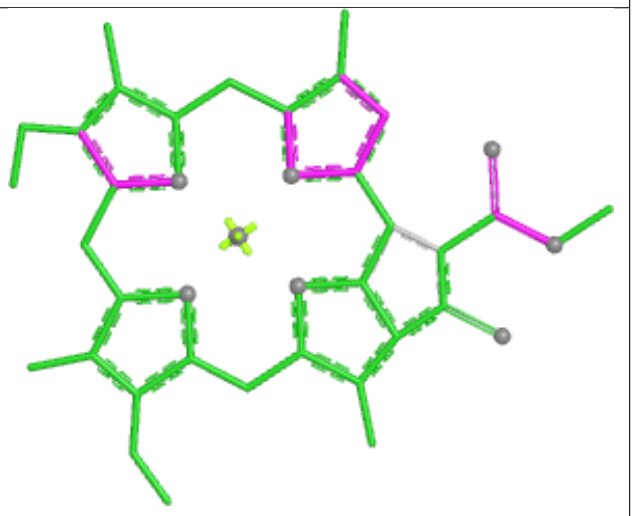


Rings

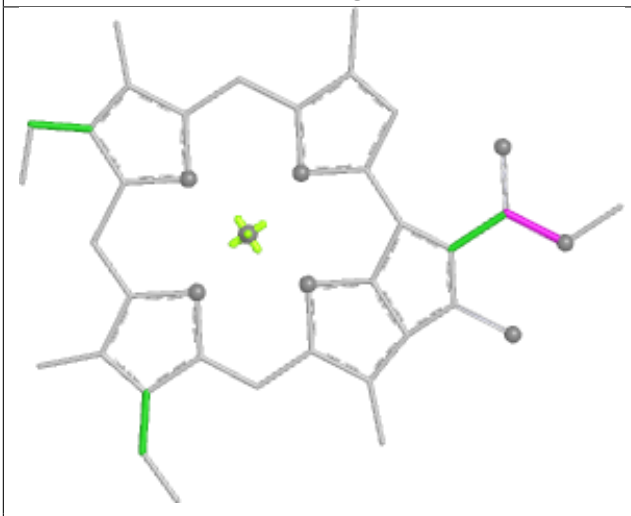
Ligand CLA B1 307



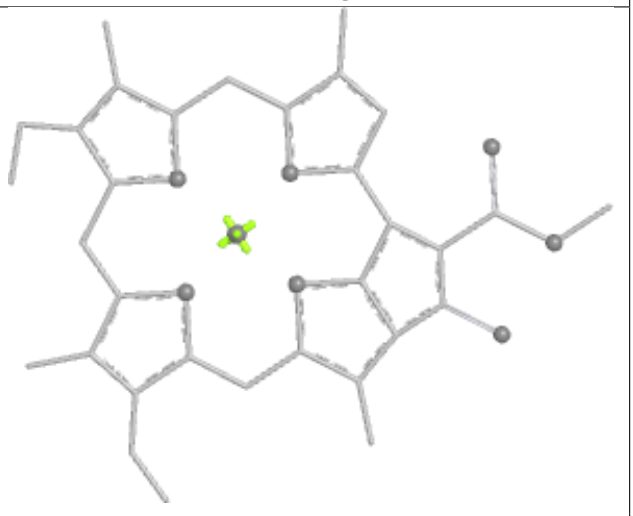
Bond lengths



Bond angles

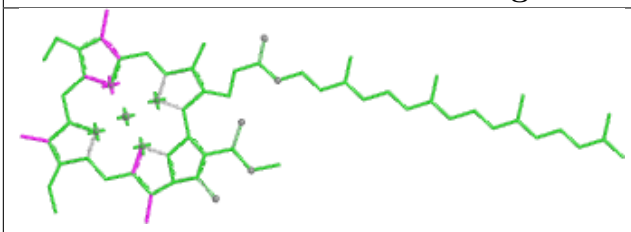


Torsions

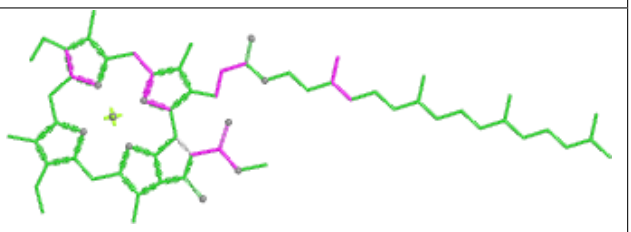


Rings

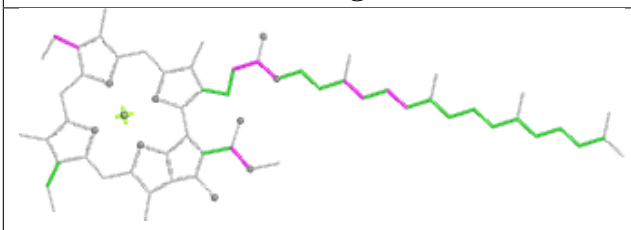
Ligand CLA BA 834



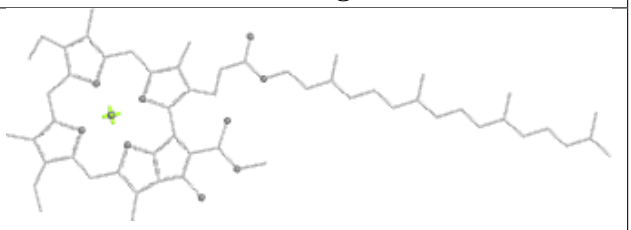
Bond lengths



Bond angles



Torsions

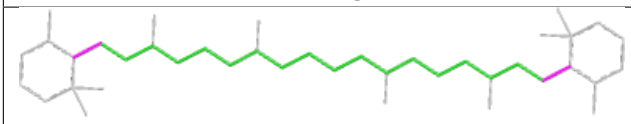


Rings

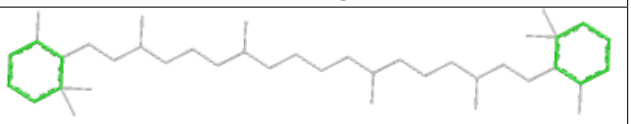
Ligand BCR BB 845

Bond lengths

Bond angles

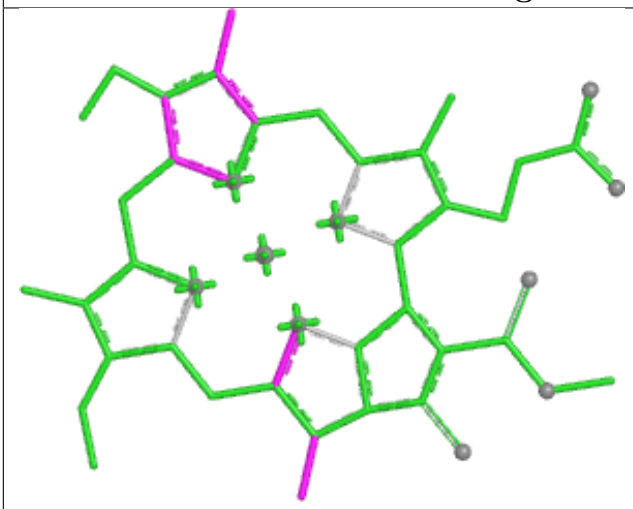


Torsions

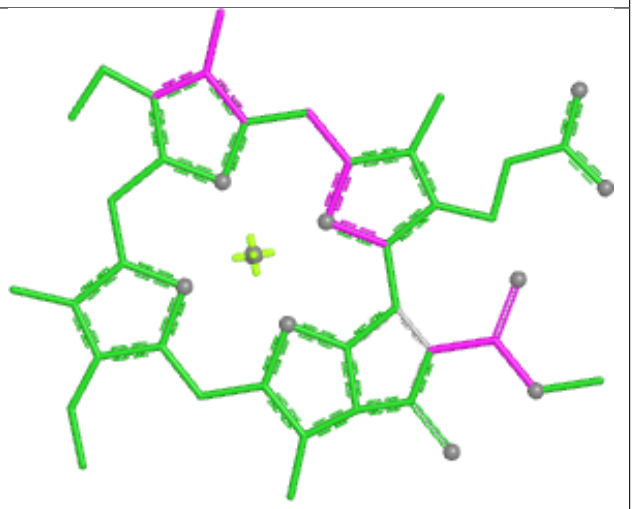


Rings

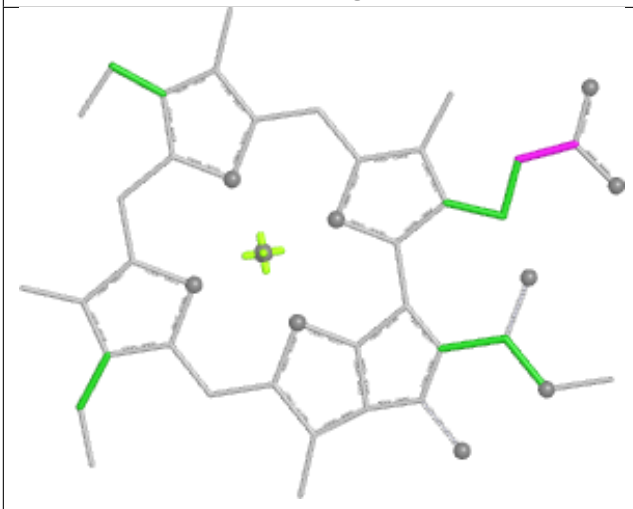
Ligand CLA B3 307



Bond lengths



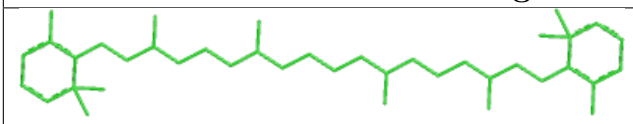
Bond angles



Torsions

Rings

Ligand BCR A4 317



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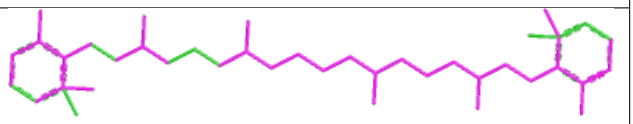
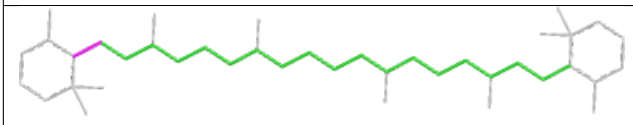
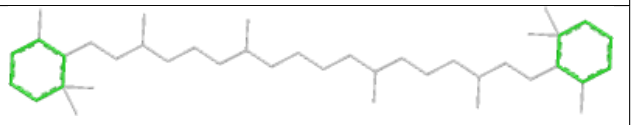


Bond angles

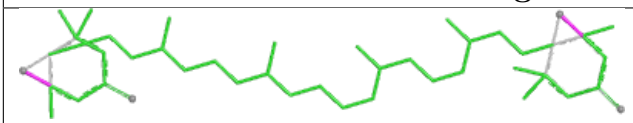


Torsions



Rings

Ligand XAT A3 317



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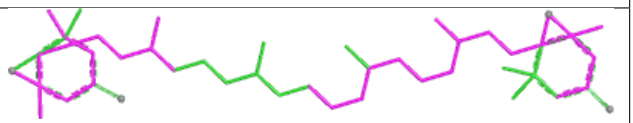
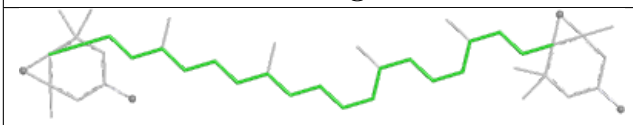
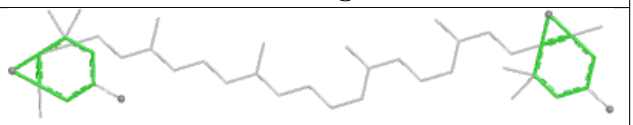


Bond angles

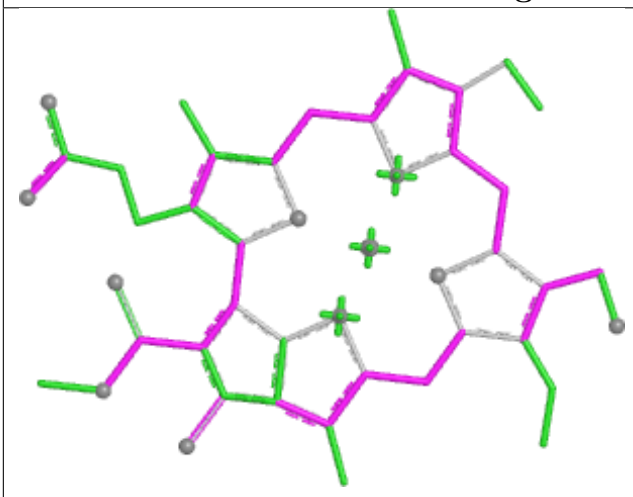


Torsions

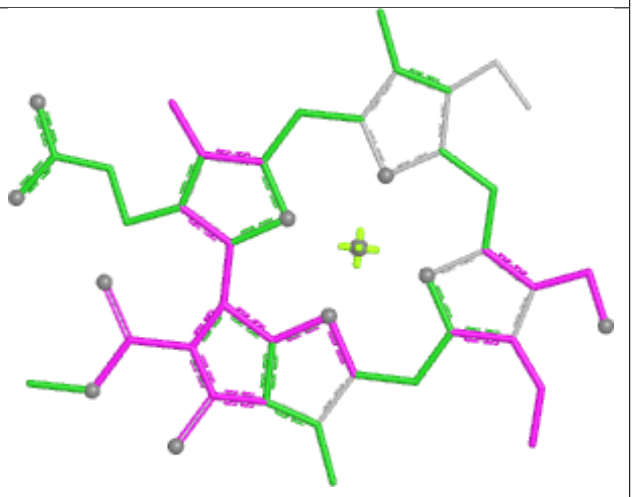


Rings

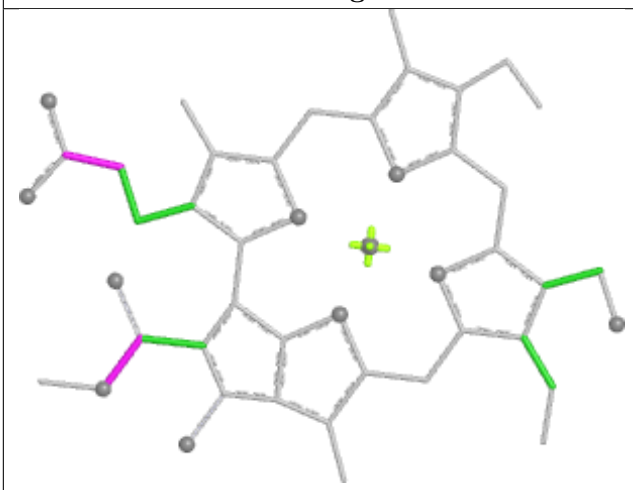
Ligand CHL B2 607



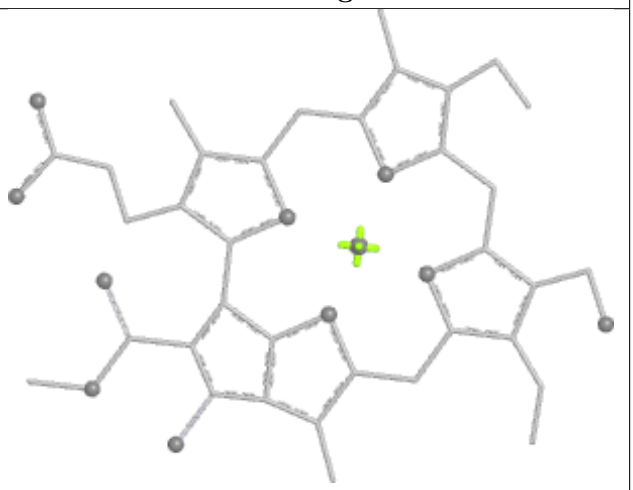
Bond lengths



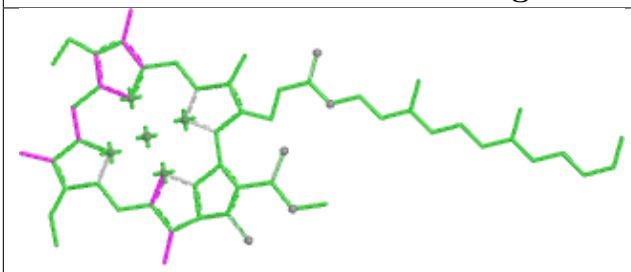
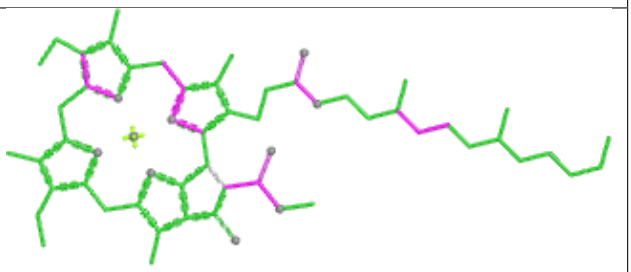
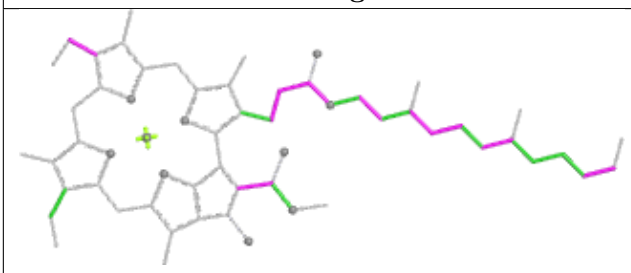
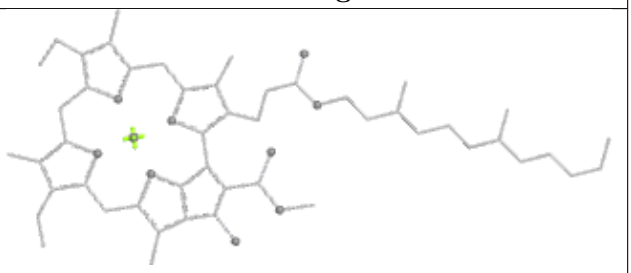
Bond angles

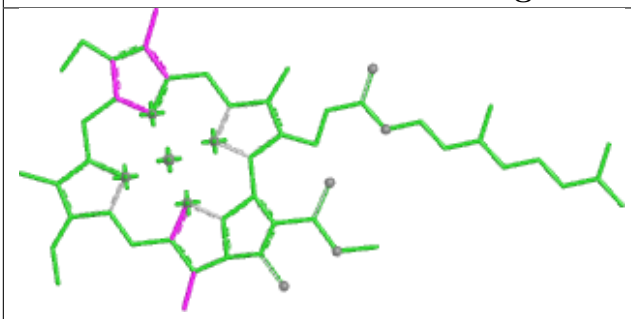
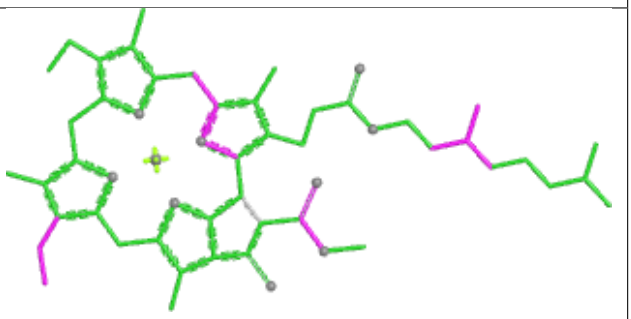
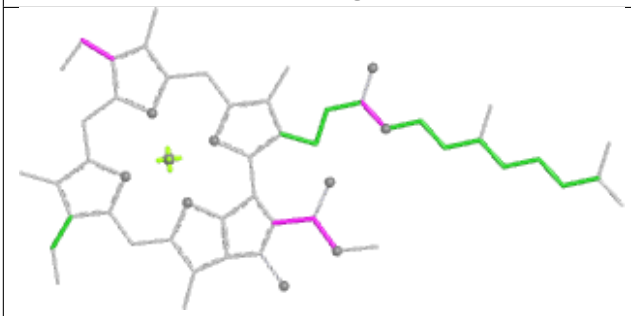
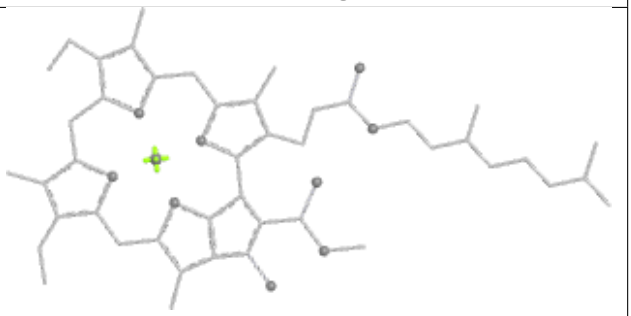


Torsions

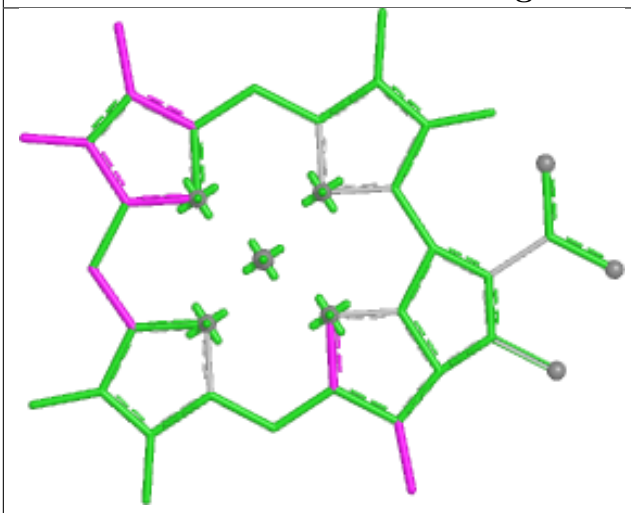


Rings

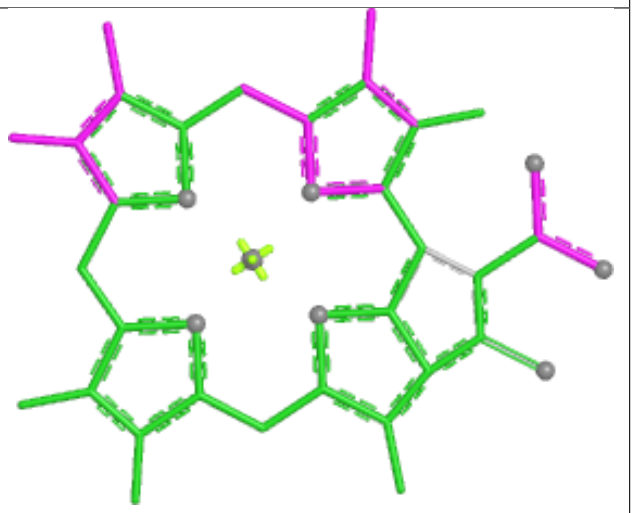
Ligand CLA BB 819	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA A1 305	
	
Bond lengths	Bond angles
	
Torsions	Rings

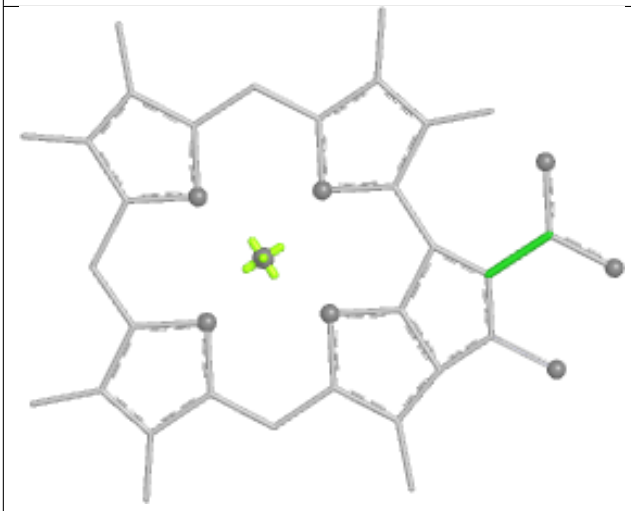
Ligand CLA B1 315



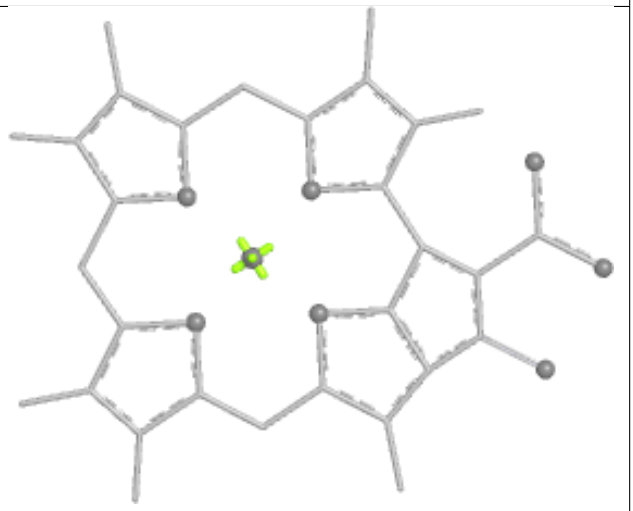
Bond lengths



Bond angles

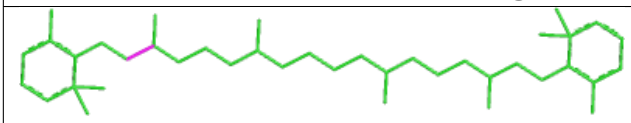


Torsions



Rings

Ligand BCR BB 847



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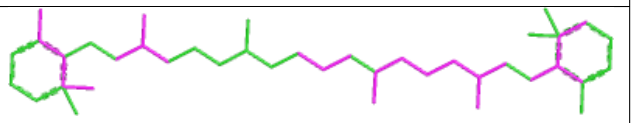
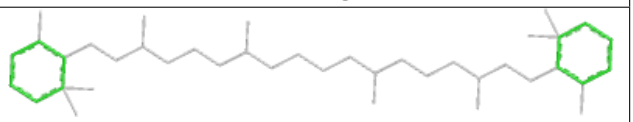


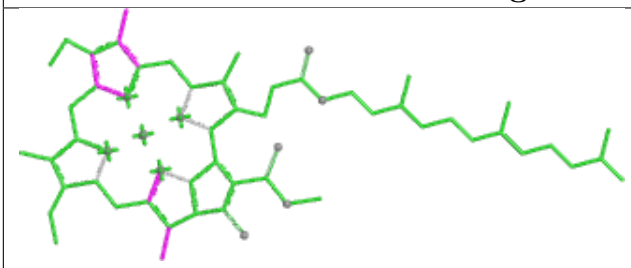
Bond angles

Torsions

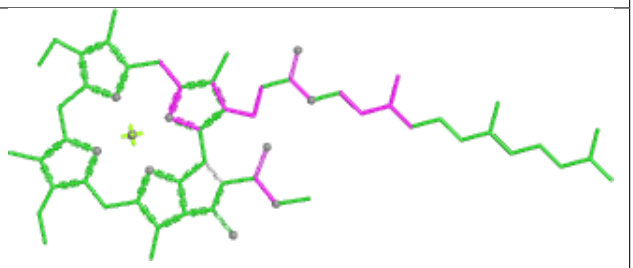


Rings

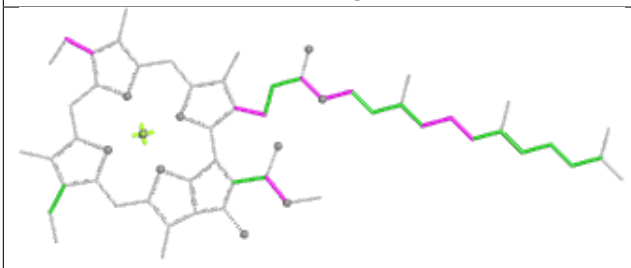
Ligand CLA AH 201



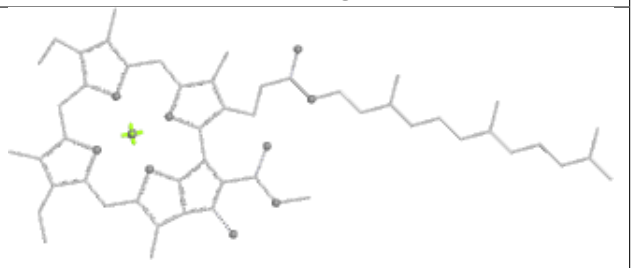
Bond lengths



Bond angles

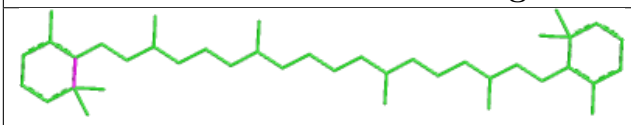


Torsions

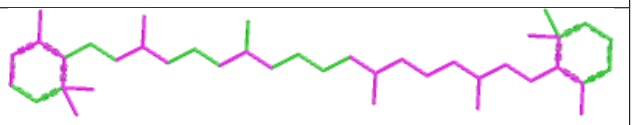


Rings

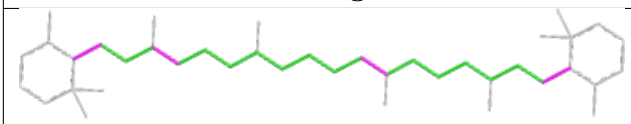
Ligand BCR BA 851



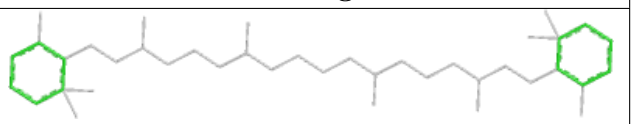
Bond lengths



Bond angles

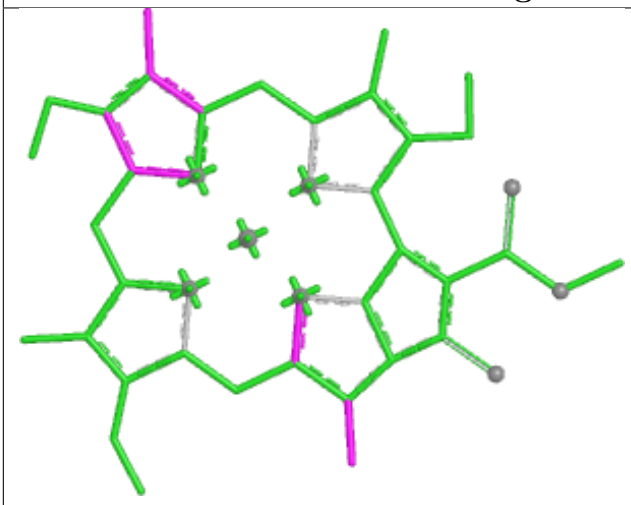


Torsions

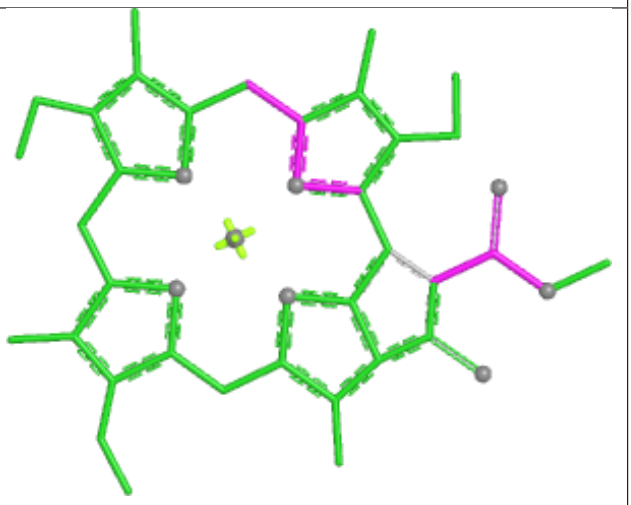


Rings

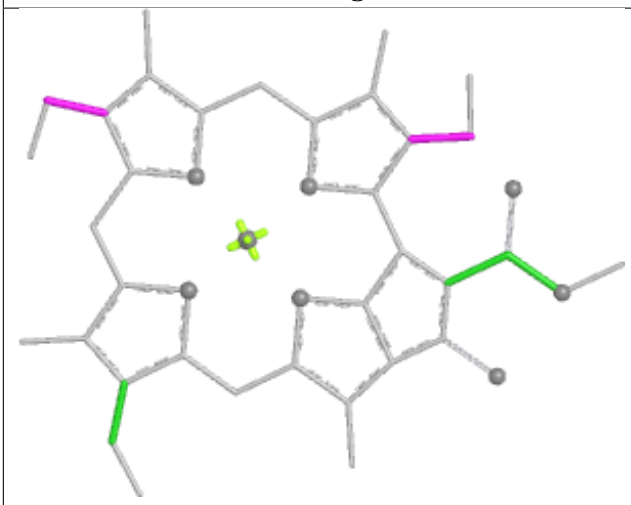
Ligand CLA A4 309



Bond lengths



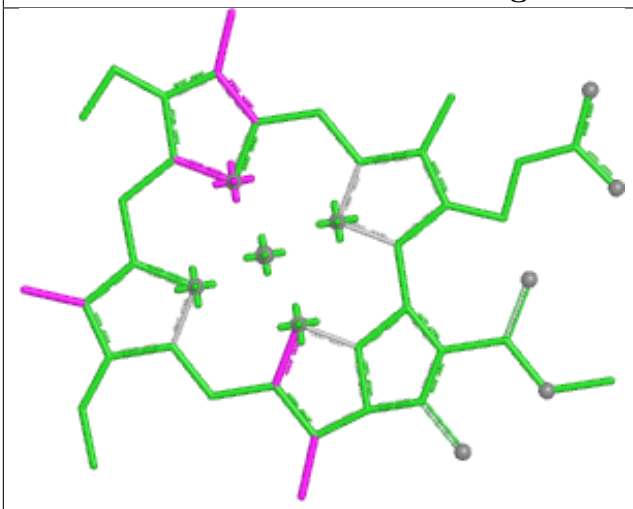
Bond angles



Torsions

Rings

Ligand CLA AA 814



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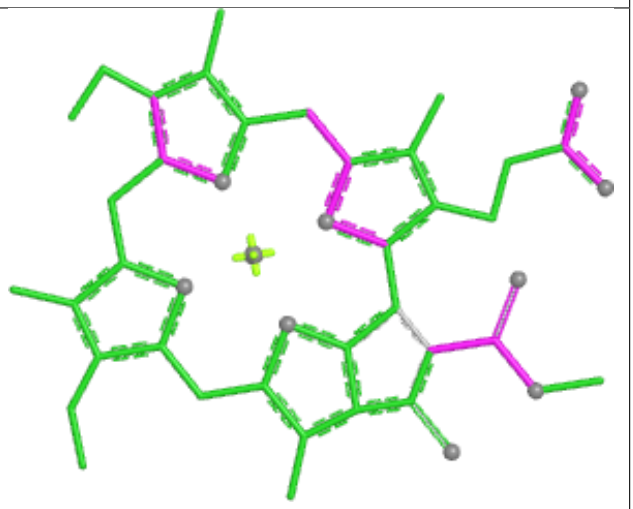
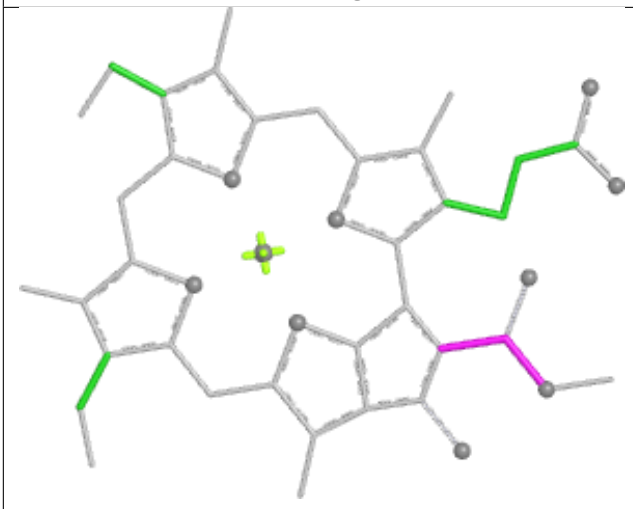


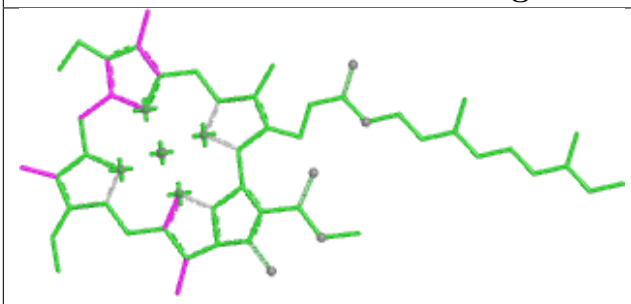
Bond angles



Torsions

Rings

Ligand CLA BB 831



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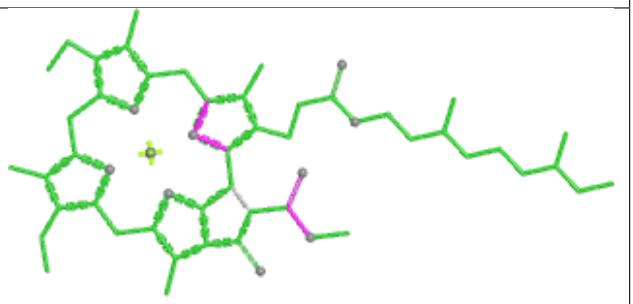
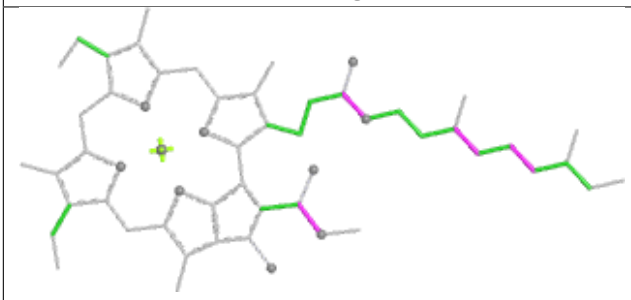
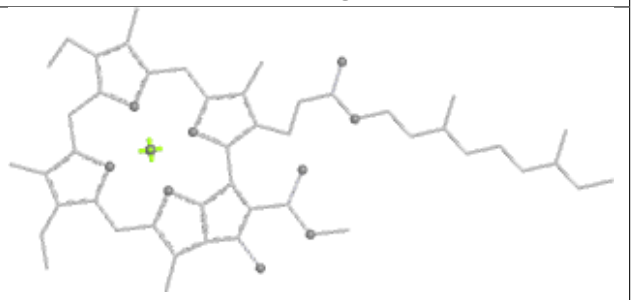


Bond angles

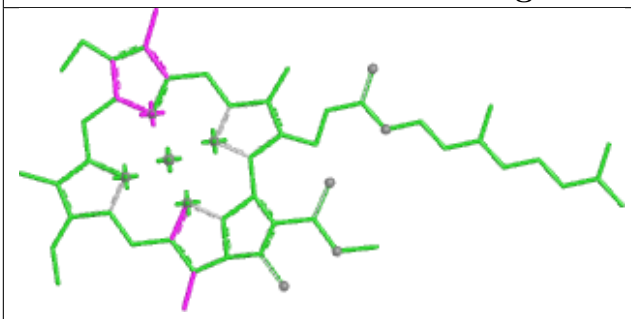


Torsions



Rings

Ligand CLA B3 302



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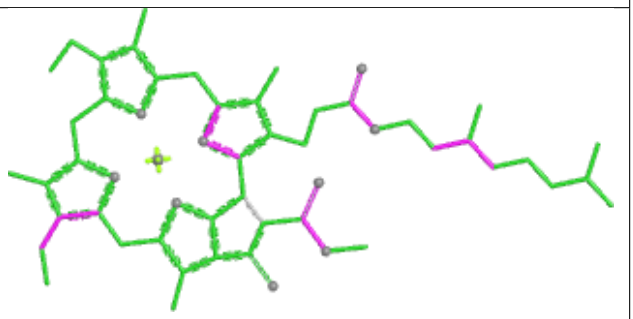
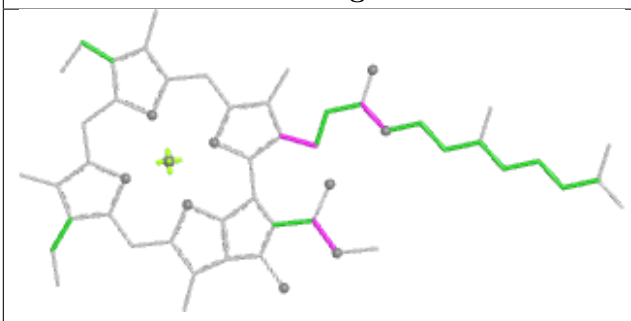
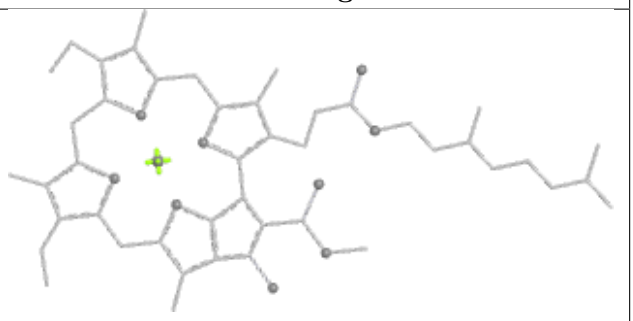


Bond angles

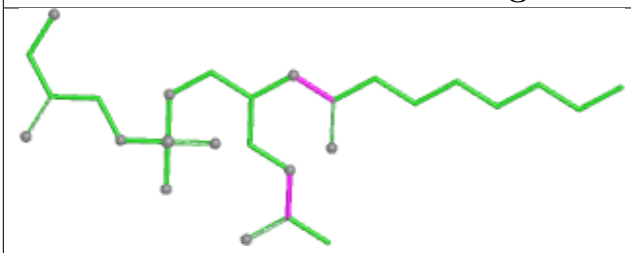


Torsions



Rings

Ligand LHG BA 846



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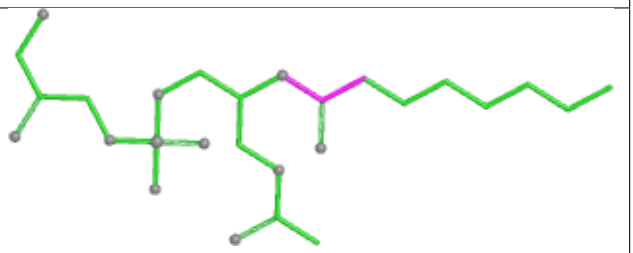
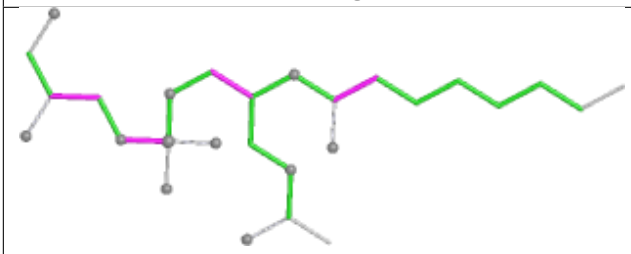
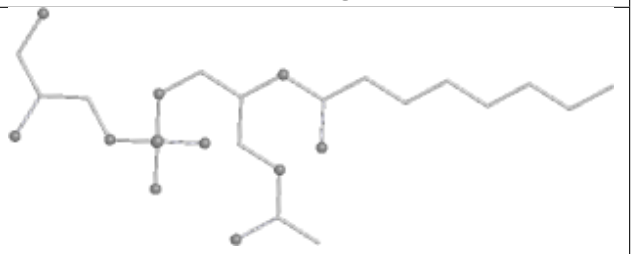


Bond angles

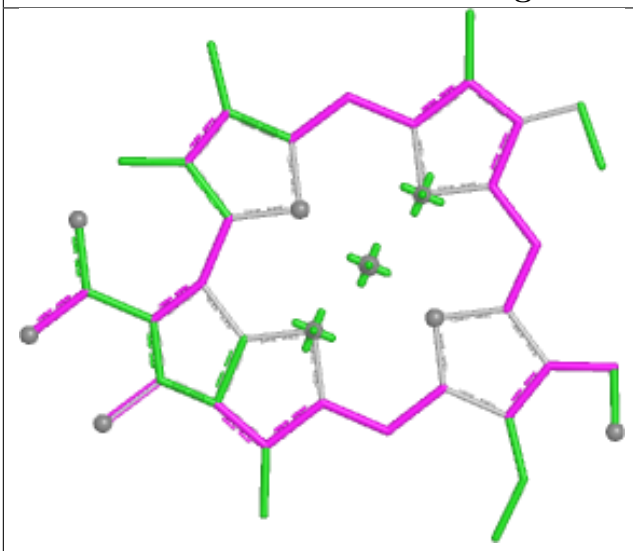


Torsions



Rings

Ligand CHL A1 308



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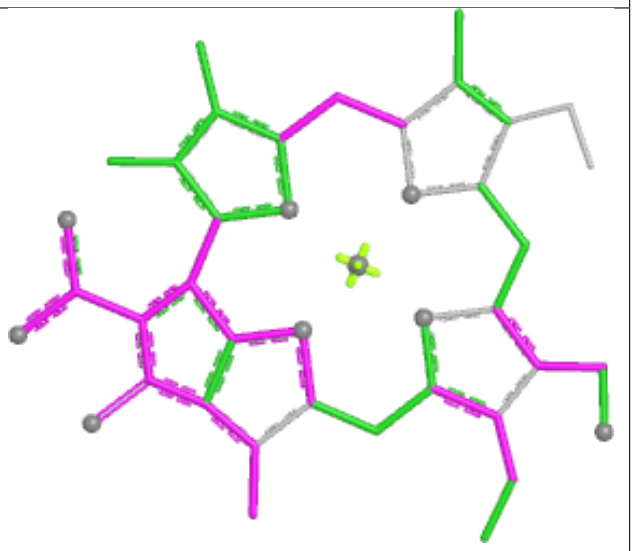
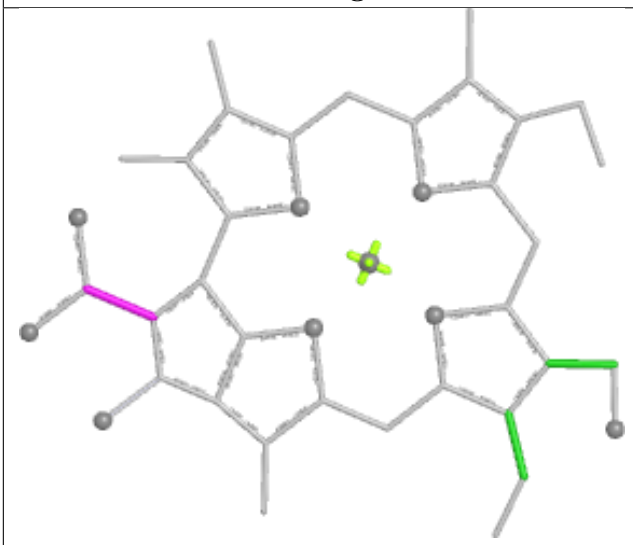


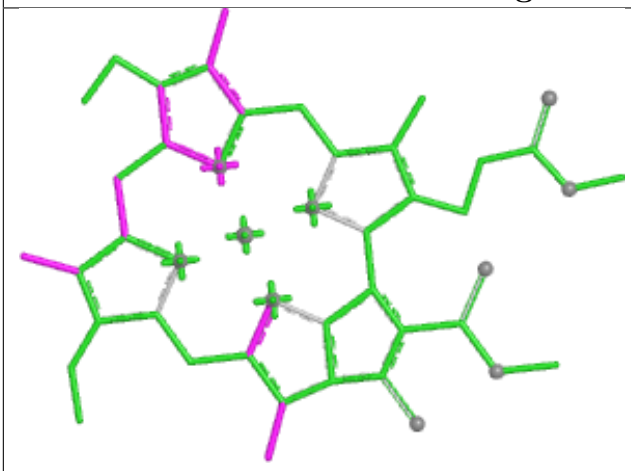
Bond angles



Torsions

Rings

Ligand CLA B5 601



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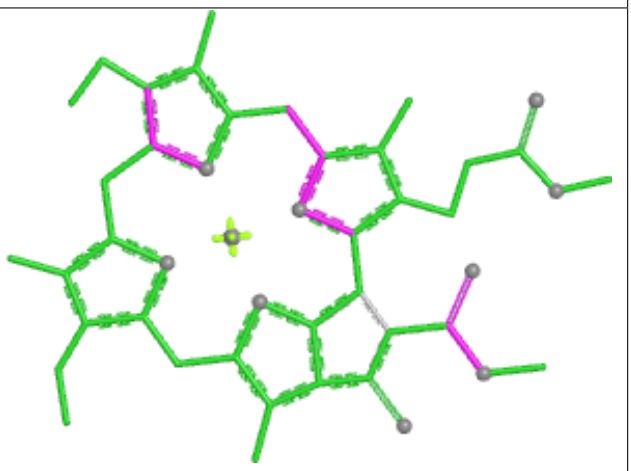
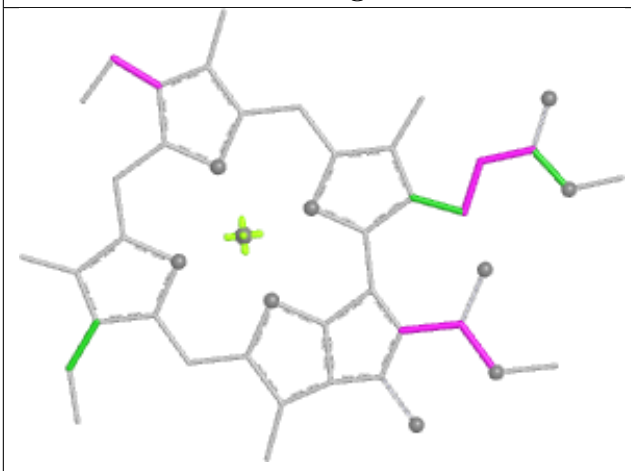
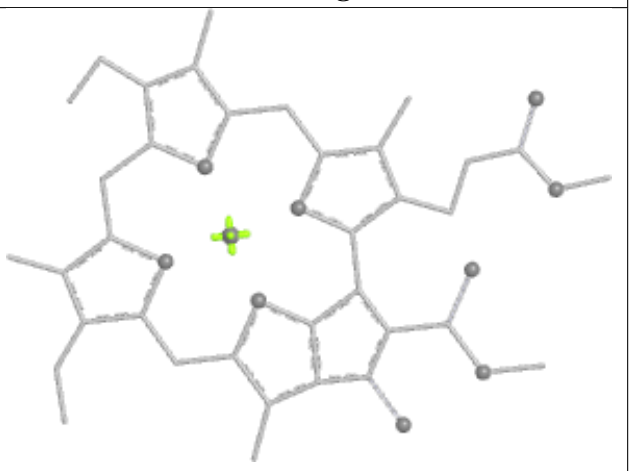


Bond angles

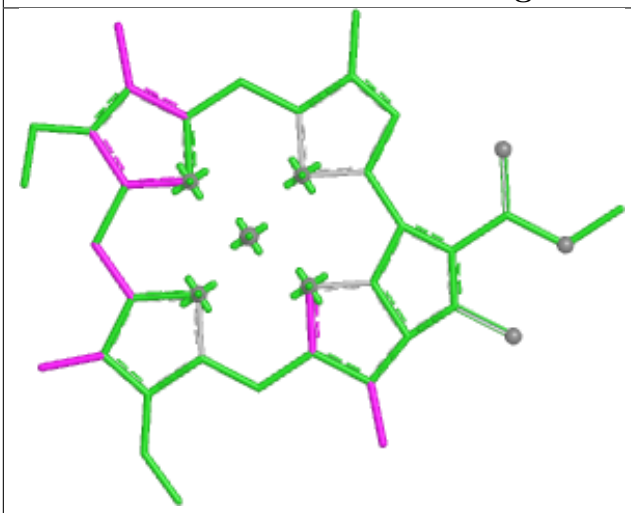


Torsions

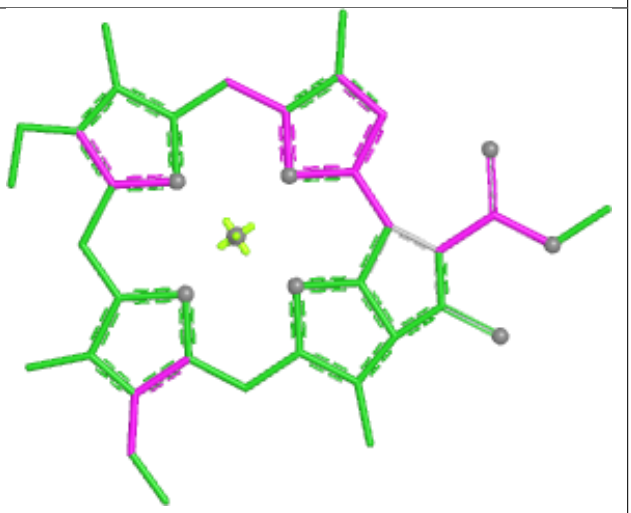


Rings

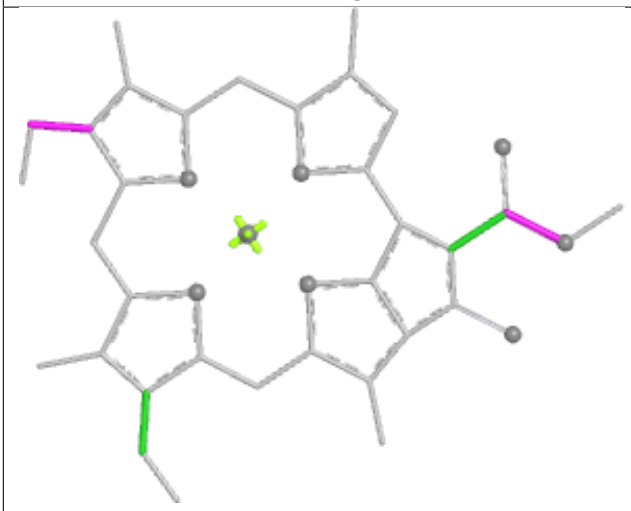
Ligand CLA A1 307



Bond lengths



Bond angles



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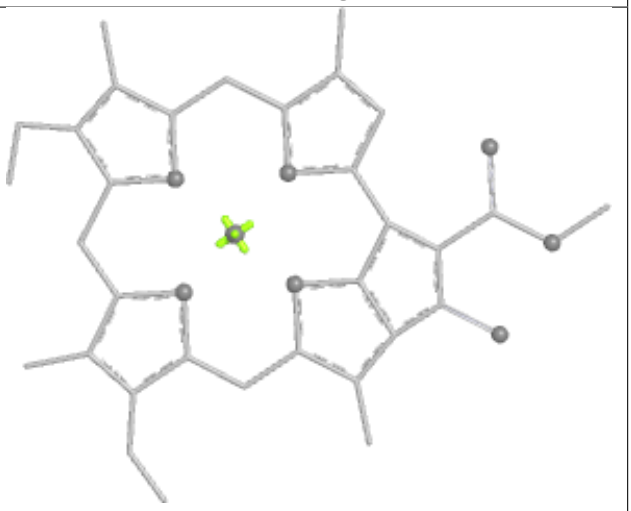
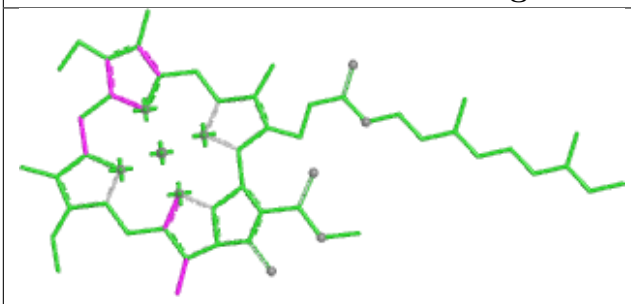


Rings

Ligand CLA AA 832



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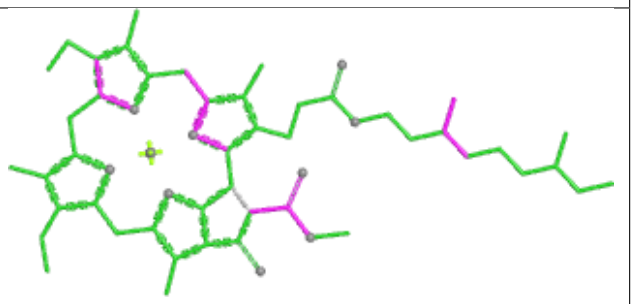
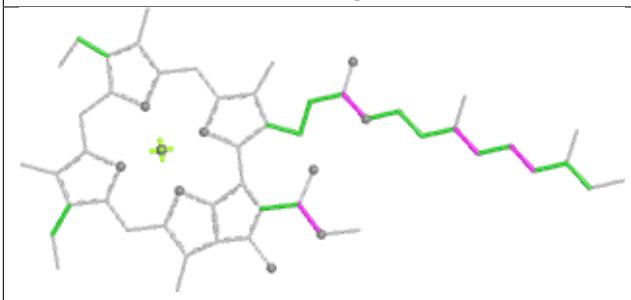
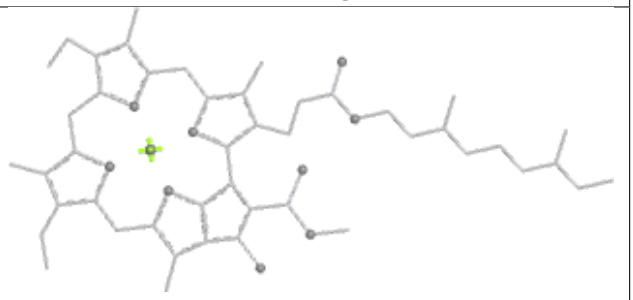


Bond angles

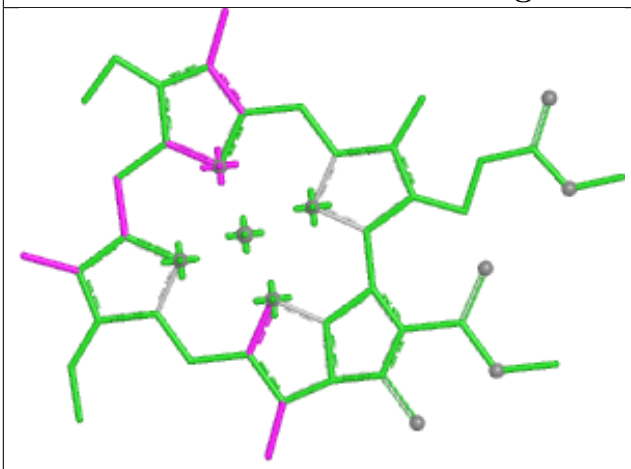


Torsions

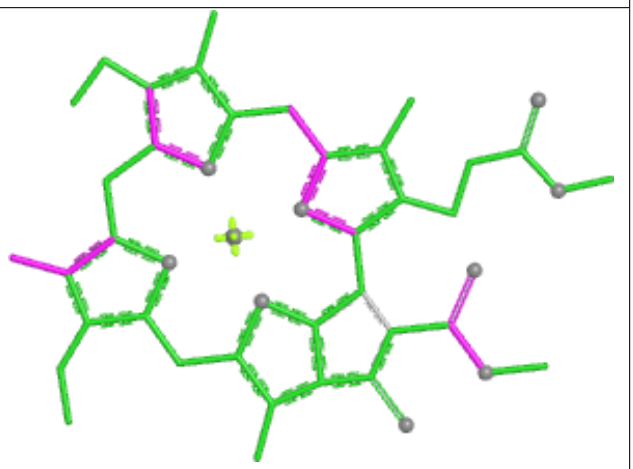


Rings

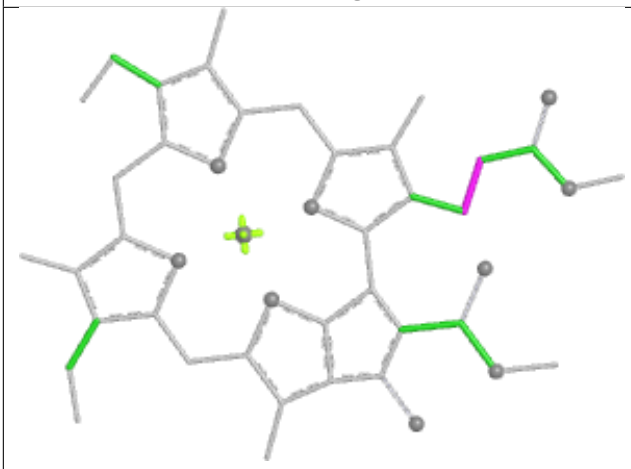
Ligand CLA A6 601



Bond lengths



Bond angles



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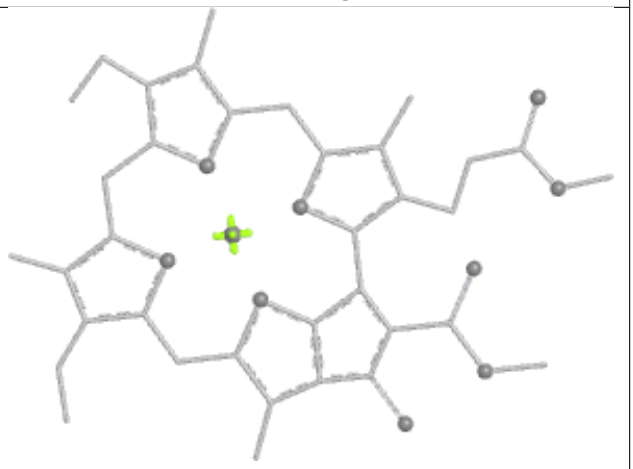
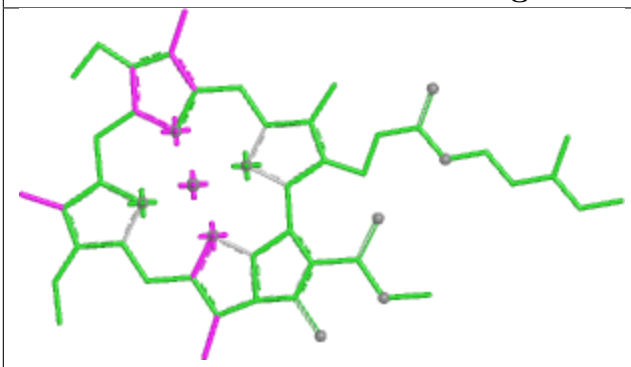


Rings

Ligand CLA BA 837



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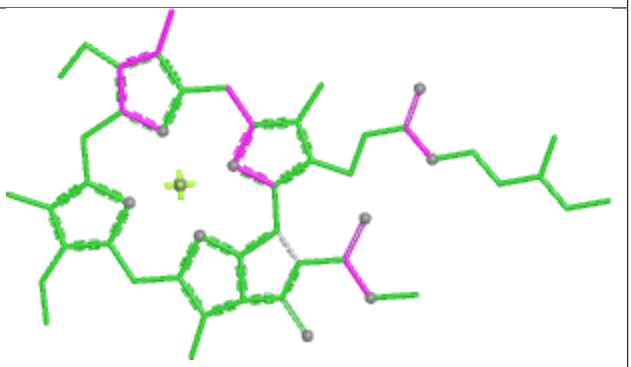
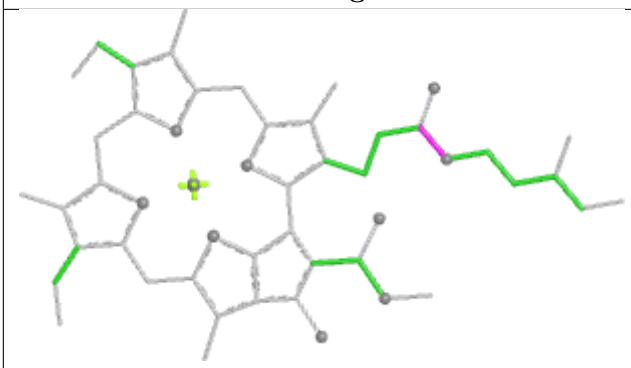


Bond angles



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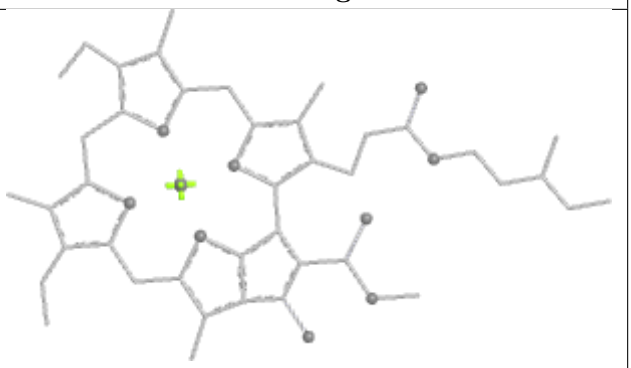
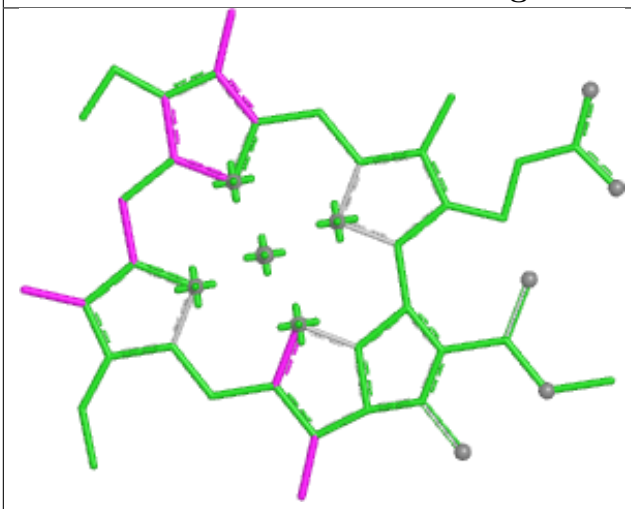


Rings

Ligand CLA AA 820



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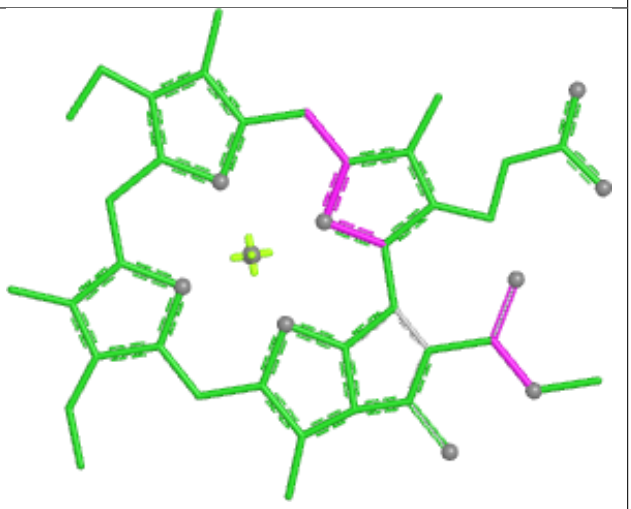
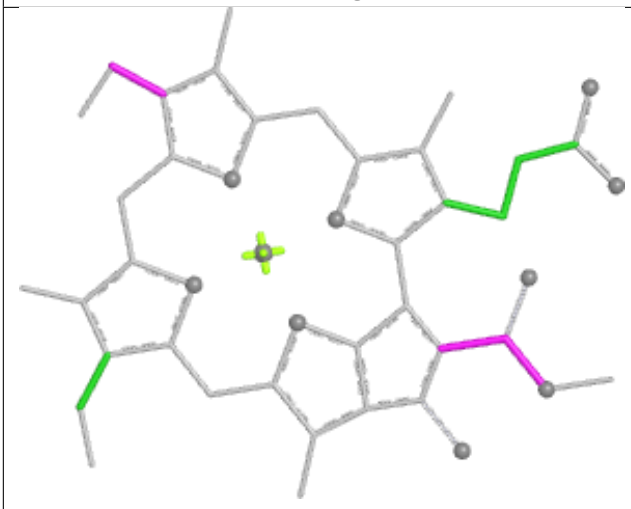


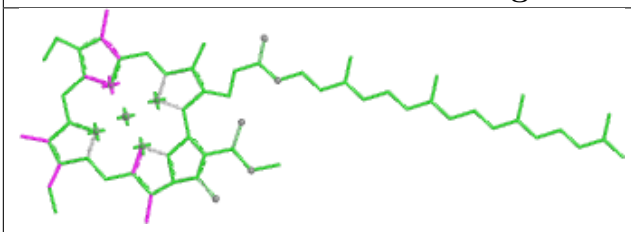
Bond angles



Torsions

Rings

Ligand CLA AB 807



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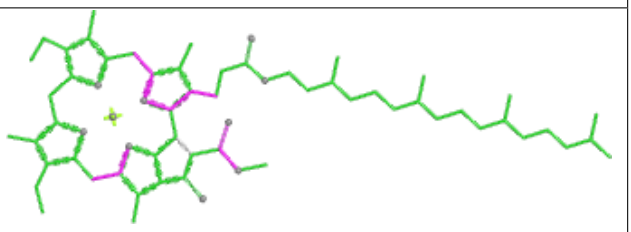
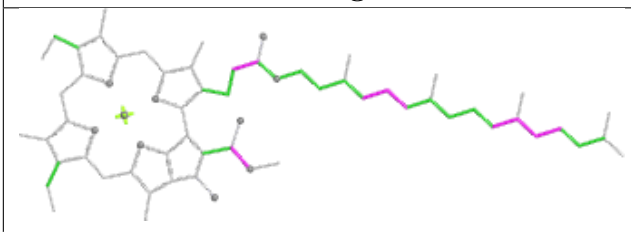
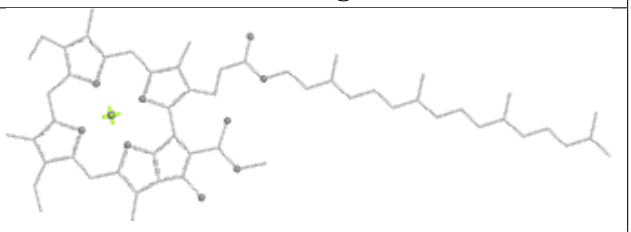


Bond angles

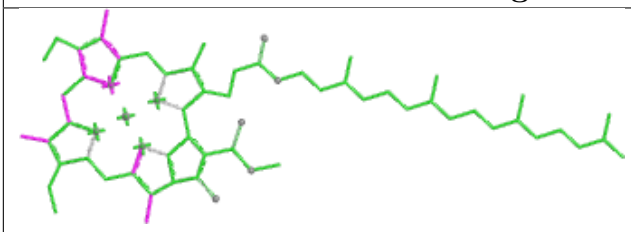


Torsions

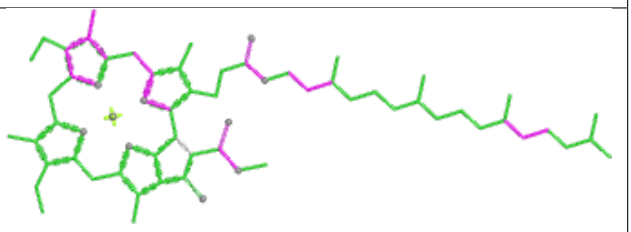


Rings

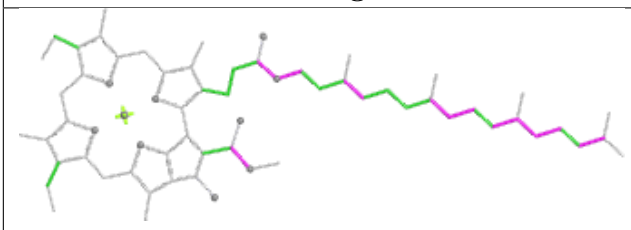
Ligand CLA AB 815



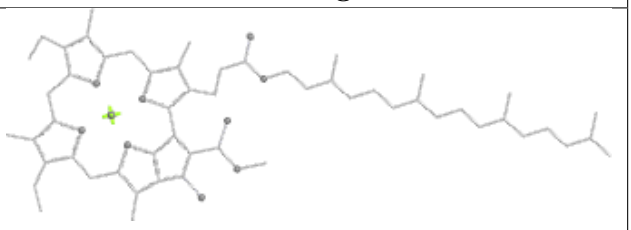
Bond lengths



Bond angles

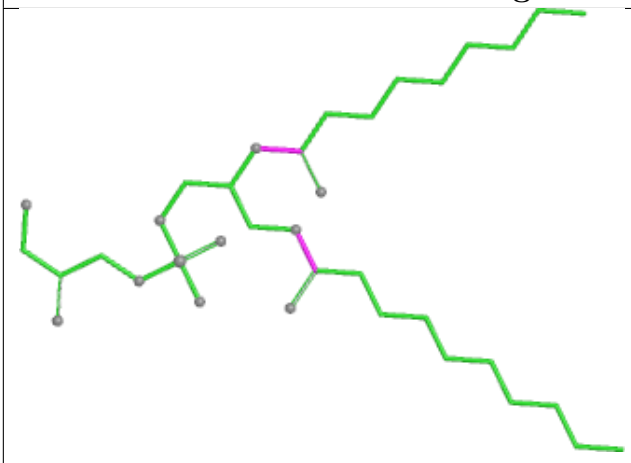


Torsions



Rings

Ligand LHG A1 302



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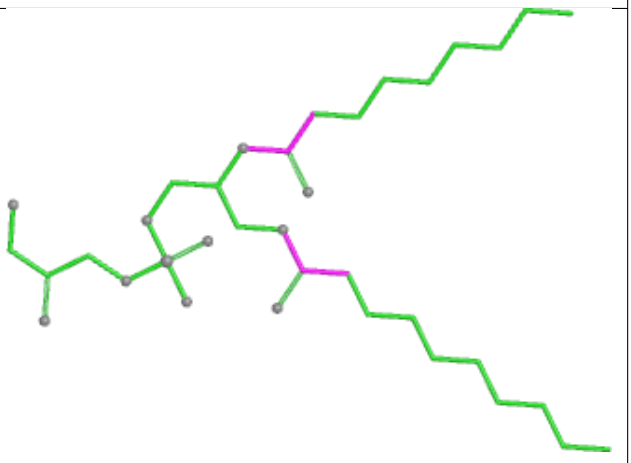
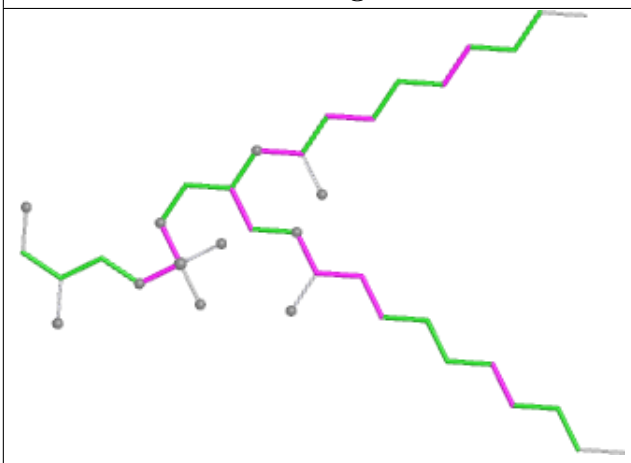
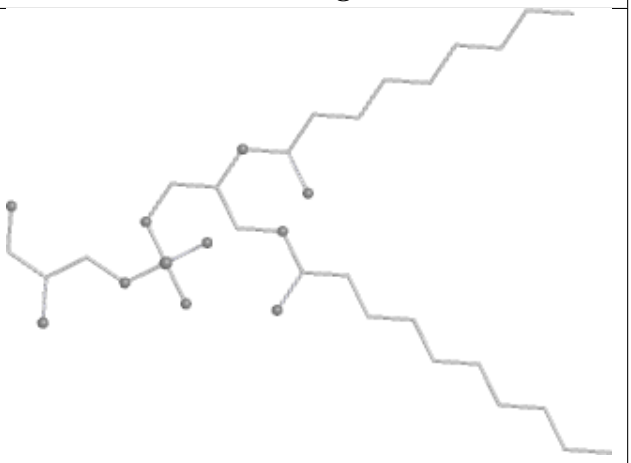


Bond angles

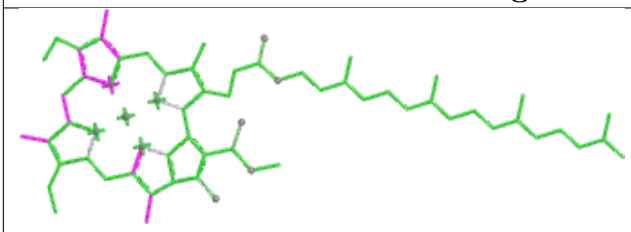


Torsions

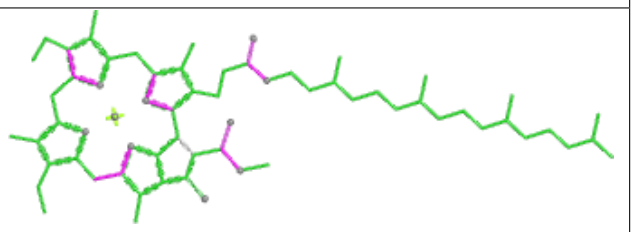


Rings

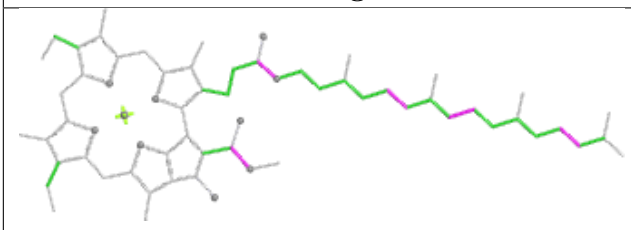
Ligand CLA AB 838



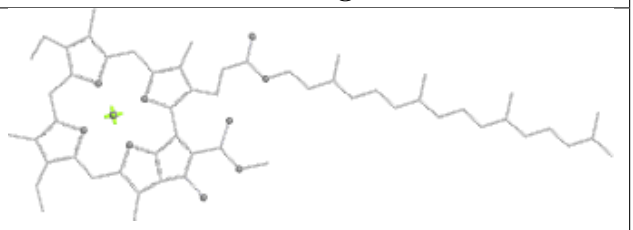
Bond lengths



Bond angles



Torsions

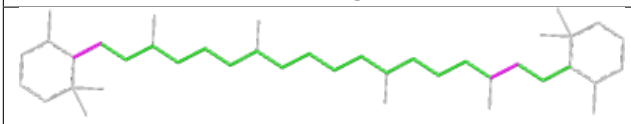


Rings

Ligand BCR A1 319

Bond lengths

Bond angles



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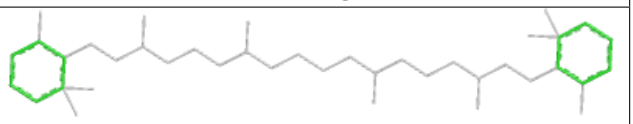
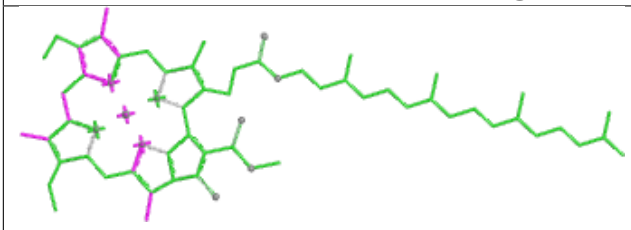
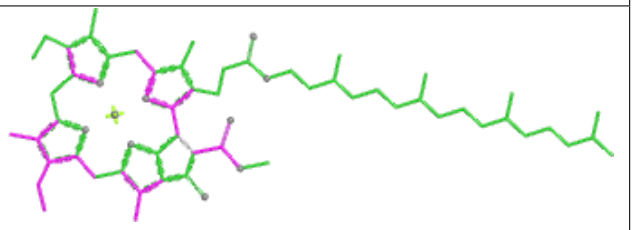


Rings

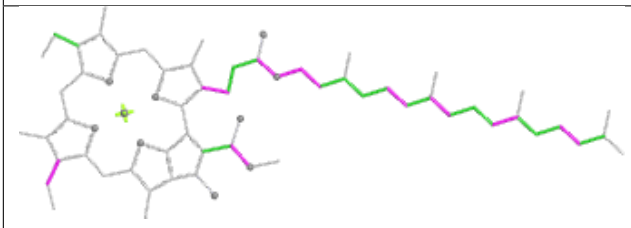
Ligand CLA AB 804



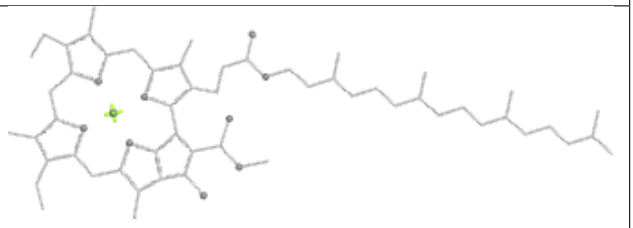
Bond lengths



Bond angles

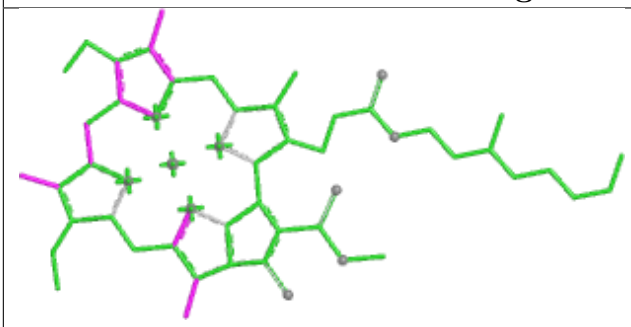


Torsions



Rings

Ligand CLA B5 609



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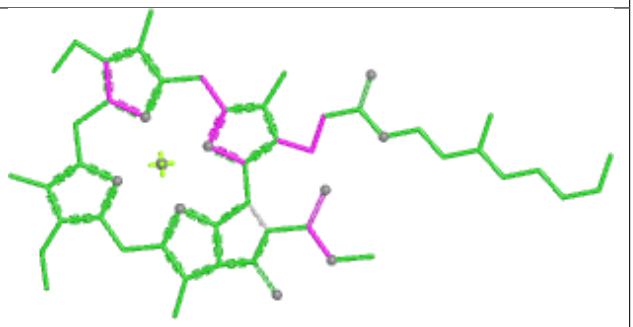
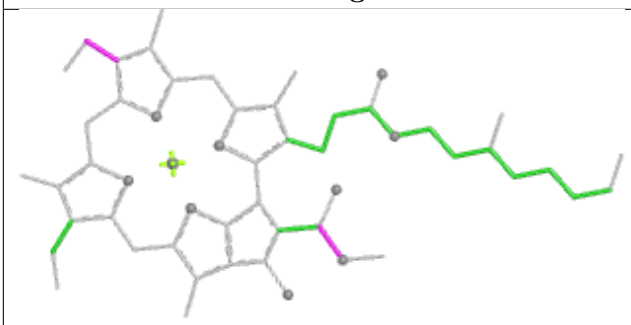
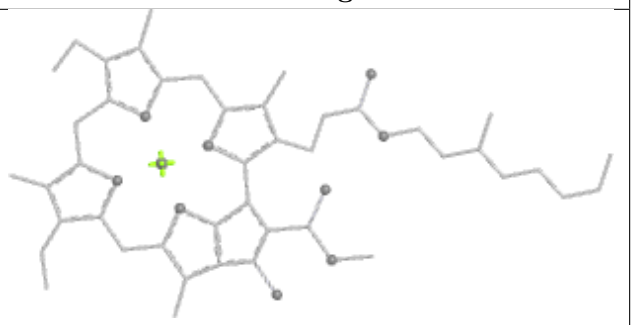


Bond angles



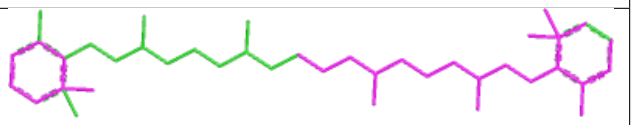
Torsions



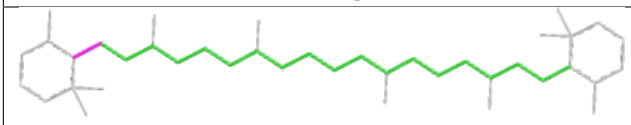
Rings

Ligand BCR BB 848

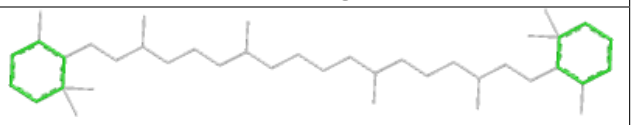
Bond lengths



Bond angles

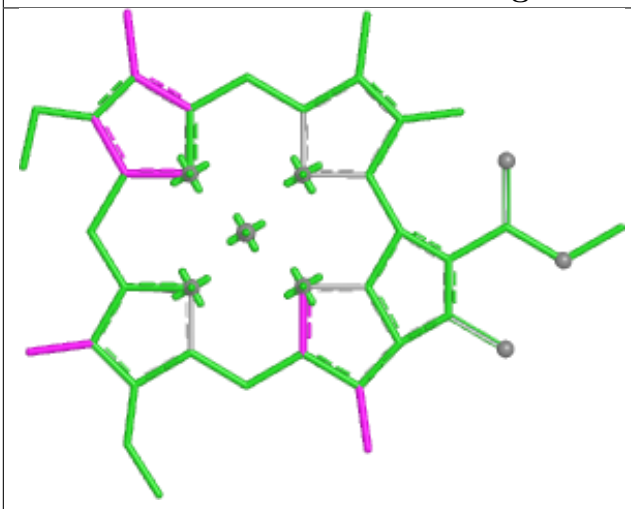


Torsions

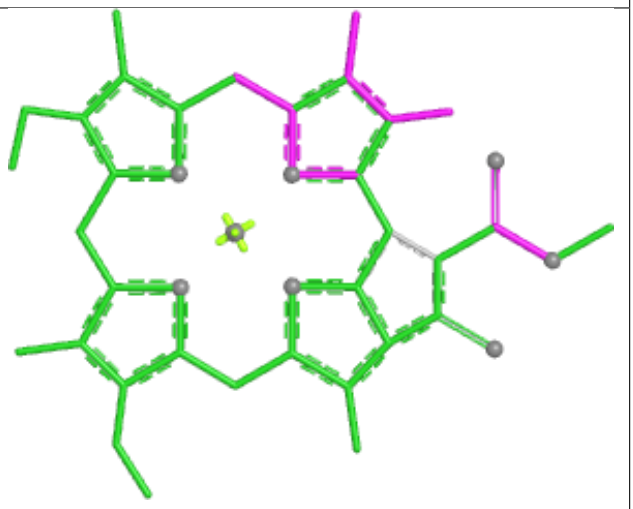


Rings

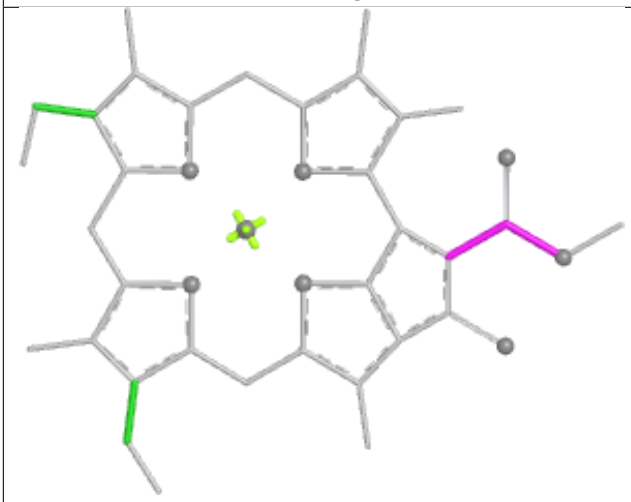
Ligand CLA BB 822



Bond lengths



Bond angles



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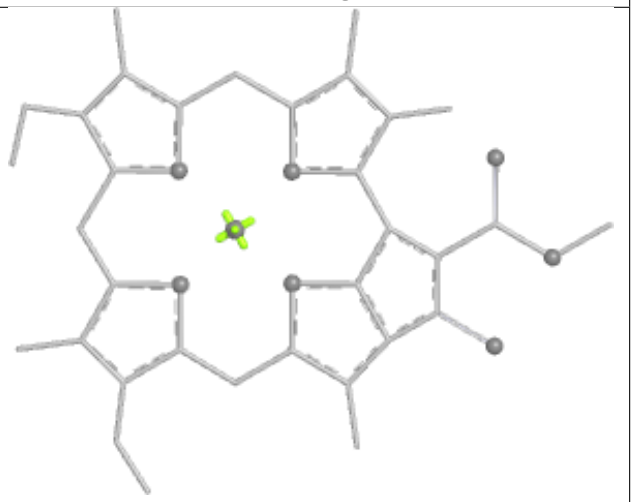
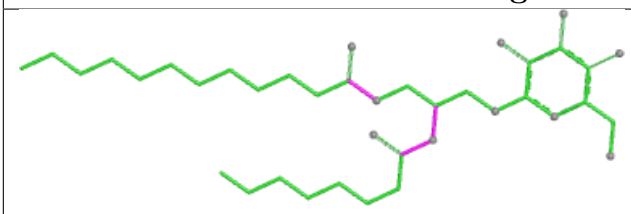


Rings

Ligand LMG A4 318



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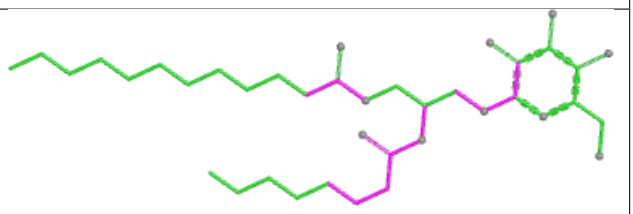
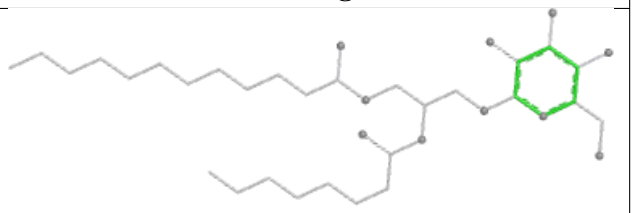


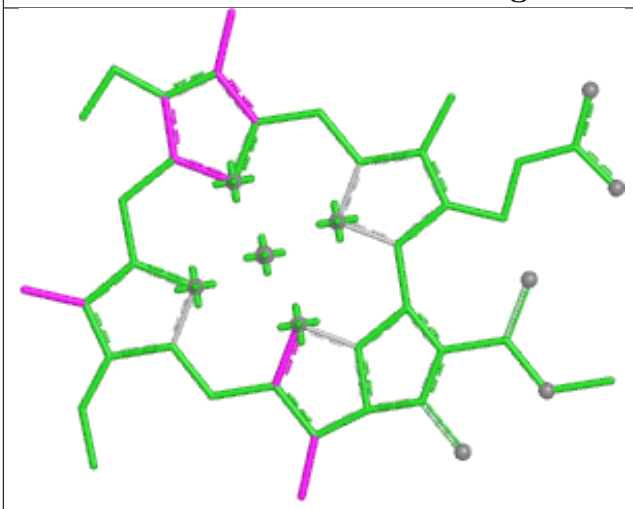
Bond angles

Torsions



Rings

Ligand CLA AA 816



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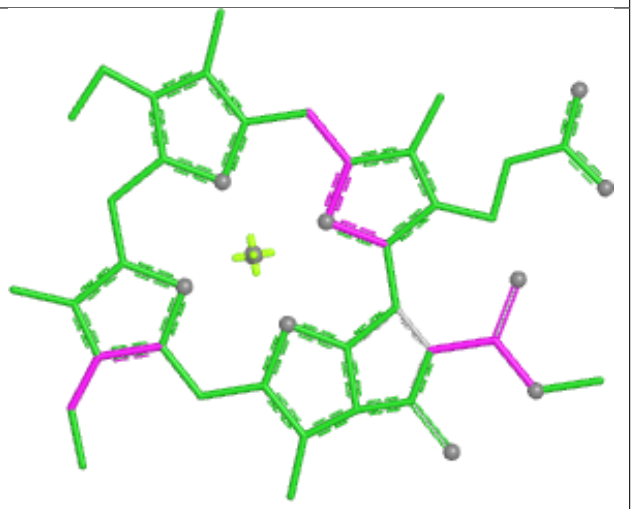
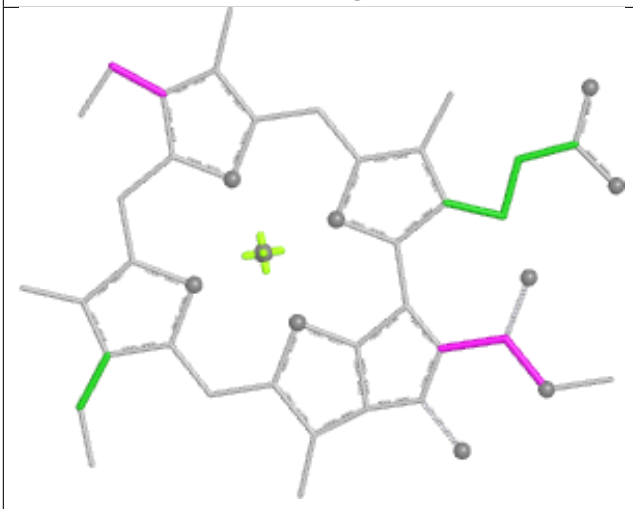


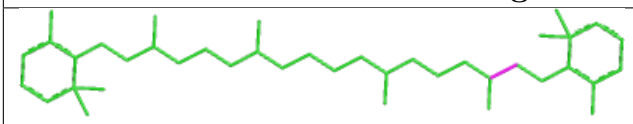
Bond angles



Torsions

Rings

Ligand BCR AF 801



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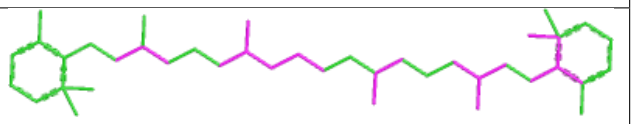
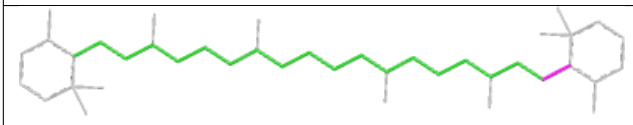
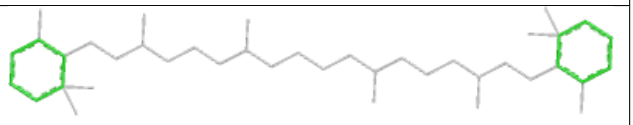


Bond angles

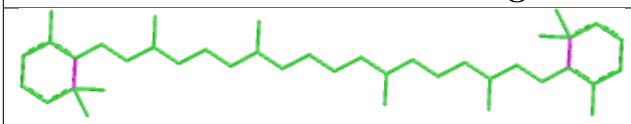


Torsions

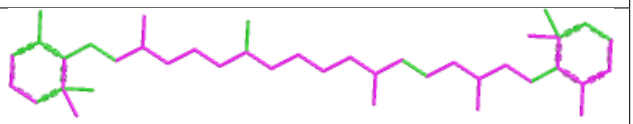


Rings

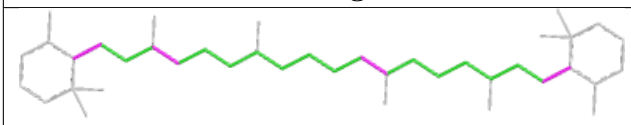
Ligand BCR AA 849



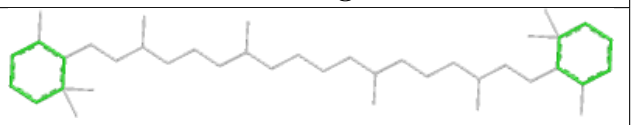
Bond lengths



Bond angles

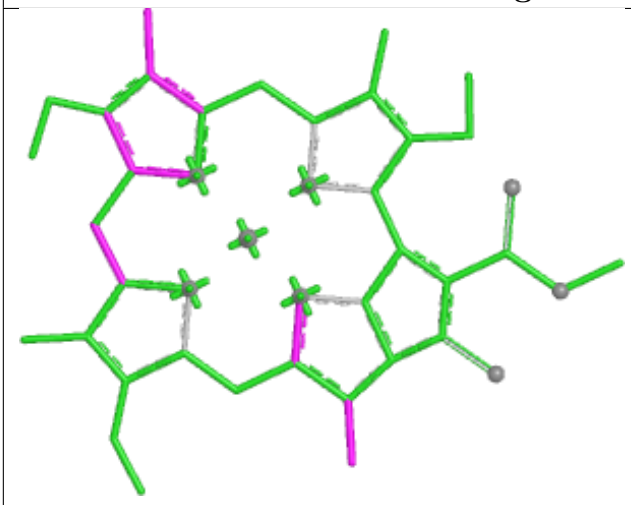


Torsions



Rings

Ligand CLA AJ 102



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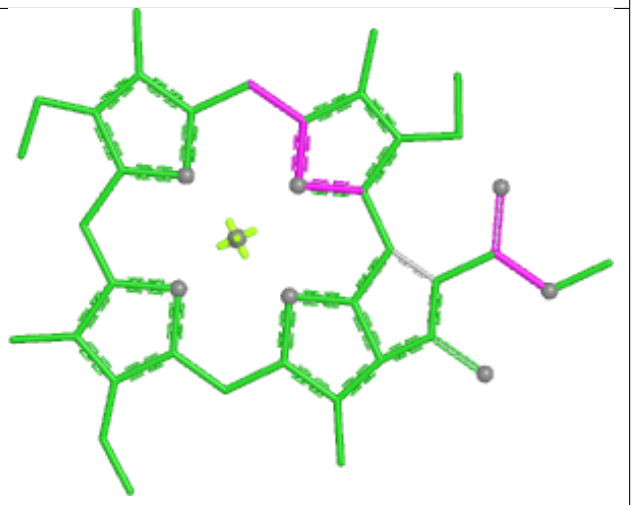
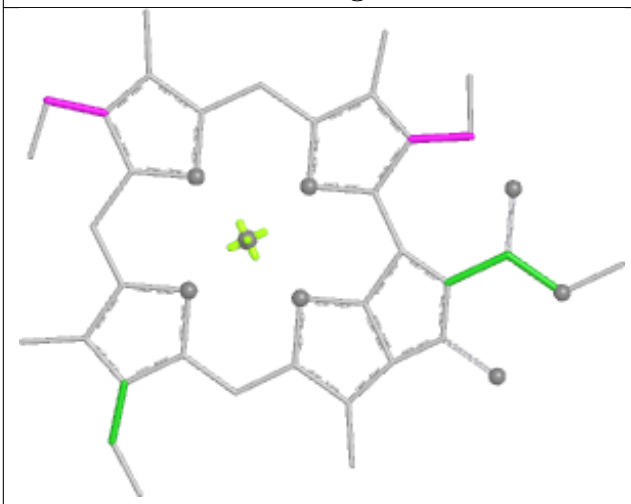


Bond angles



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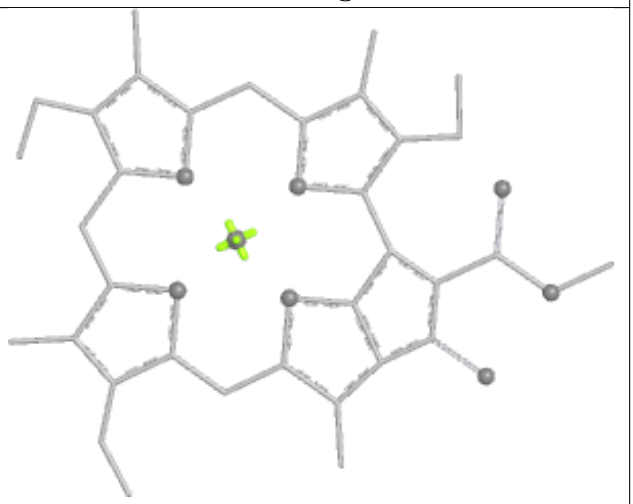
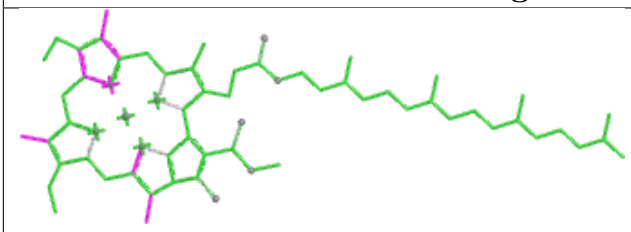


Rings

Ligand CLA AB 811



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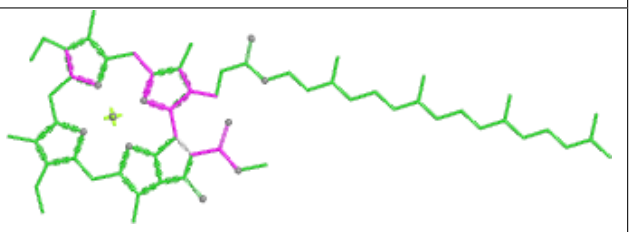
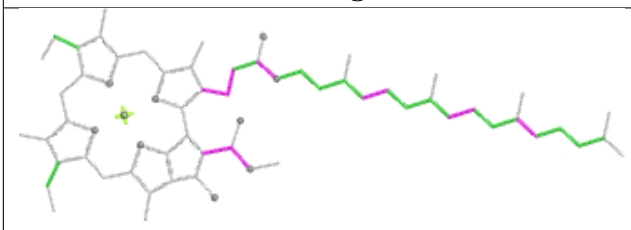


Bond angles



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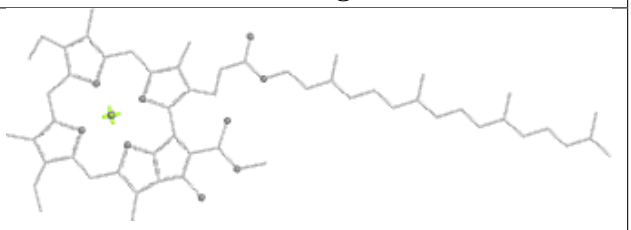
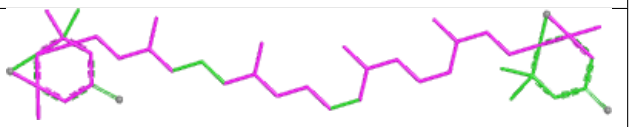


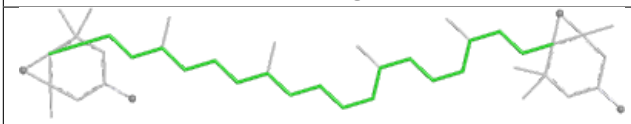
Rings

Ligand XAT A6 616

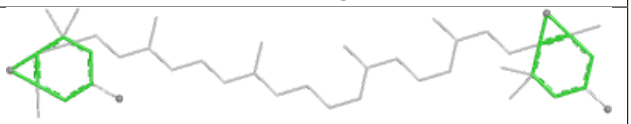
Bond lengths



Bond angles

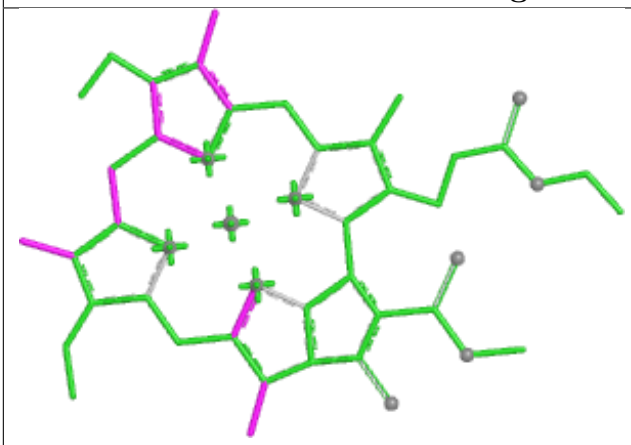


Torsions

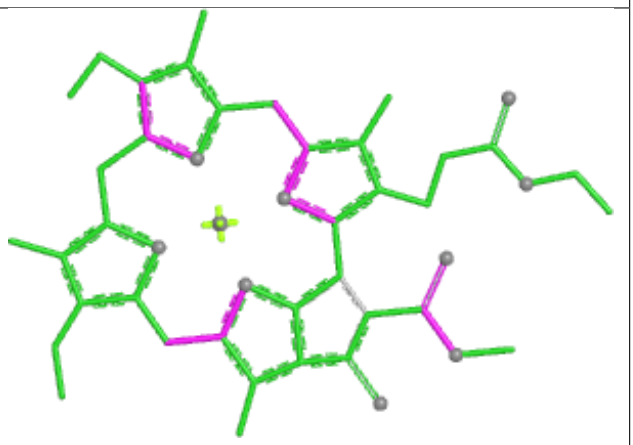


Rings

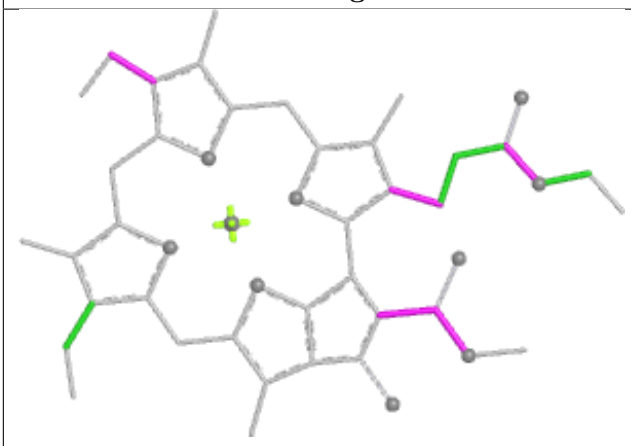
Ligand CLA AA 831



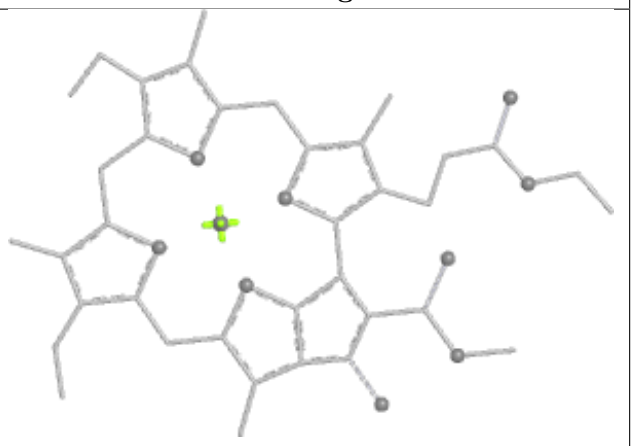
Bond lengths



Bond angles

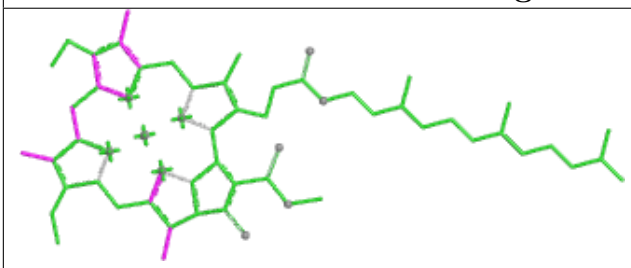


Torsions

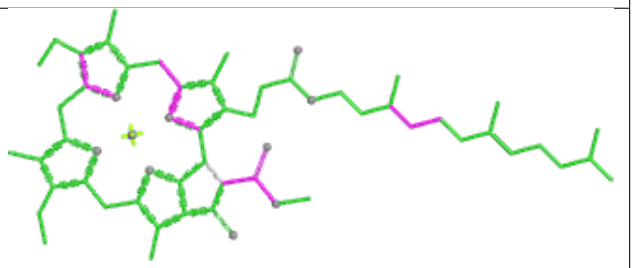


Rings

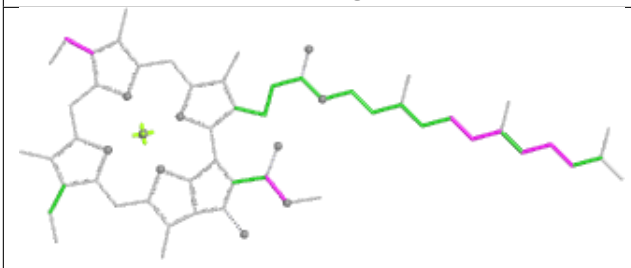
Ligand CLA A3 302



Bond lengths



Bond angles



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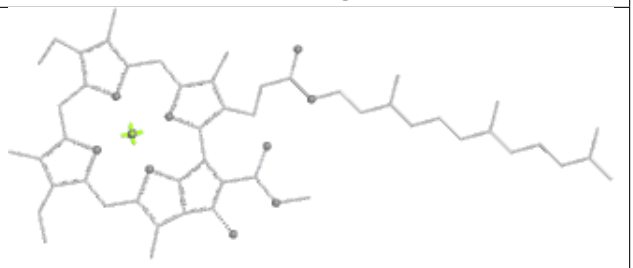
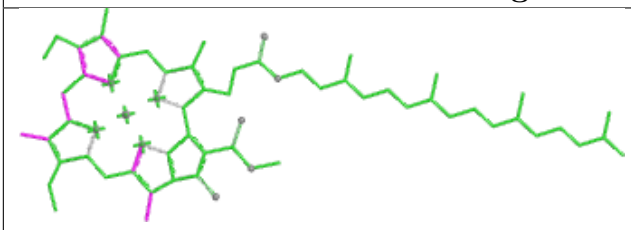
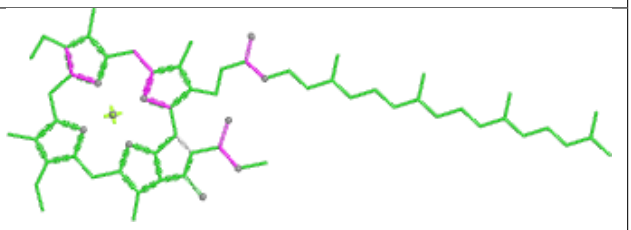


Rings

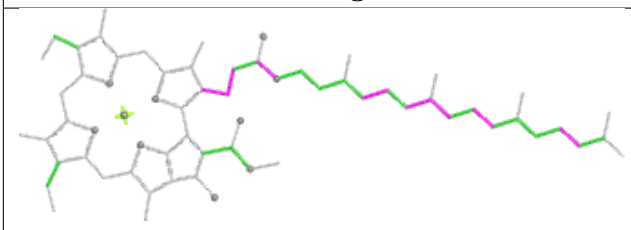
Ligand CLA BA 827



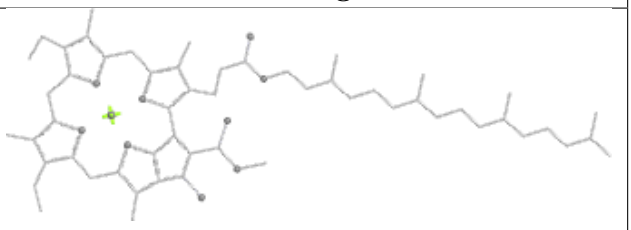
Bond lengths



Bond angles

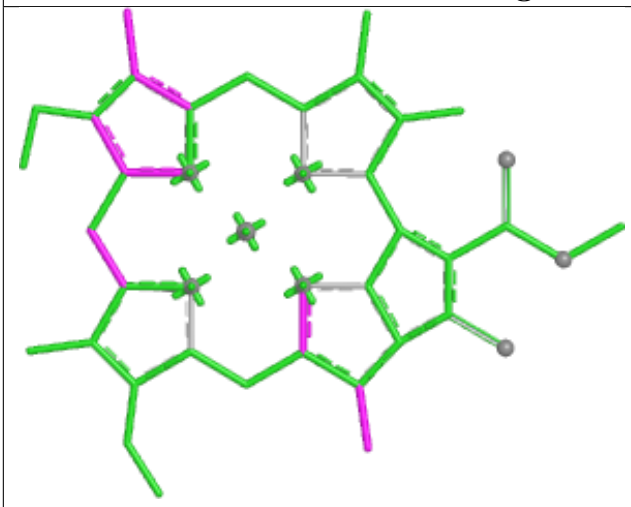


Torsions

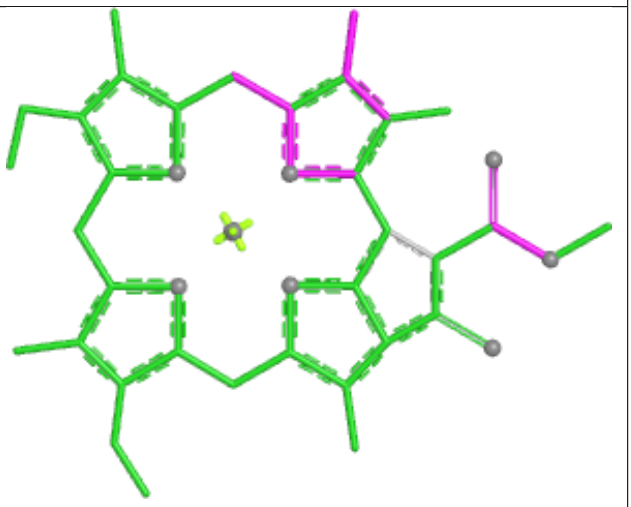


Rings

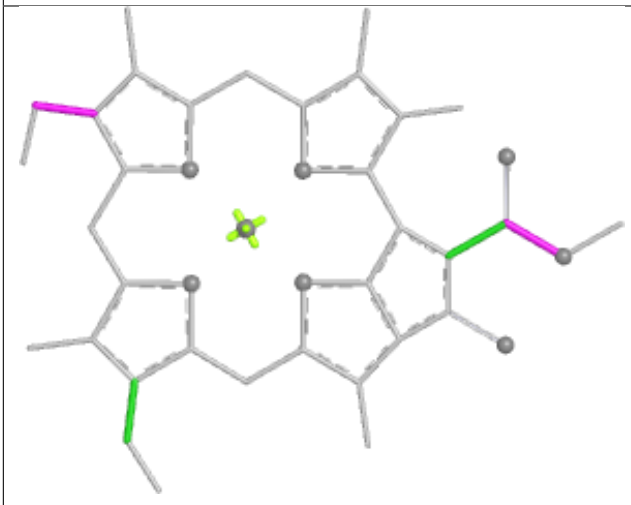
Ligand CLA B3 308



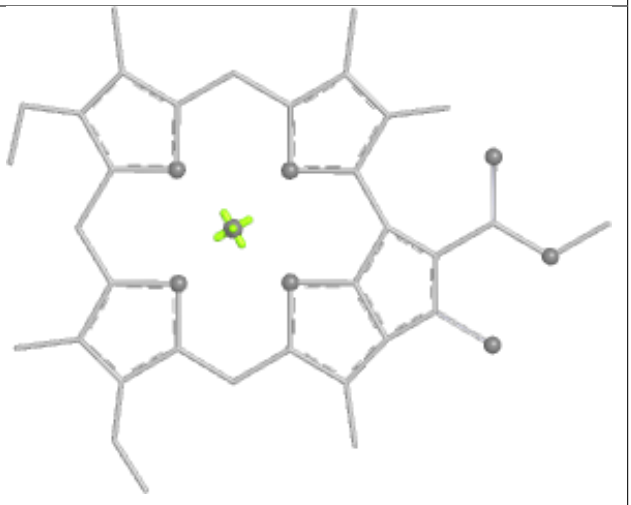
Bond lengths



Bond angles

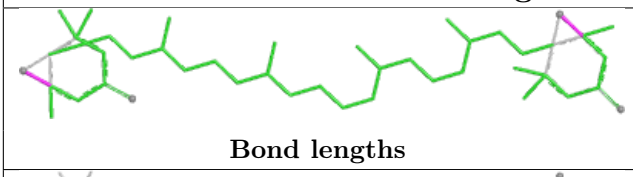


Torsions



Rings

Ligand XAT B1 317



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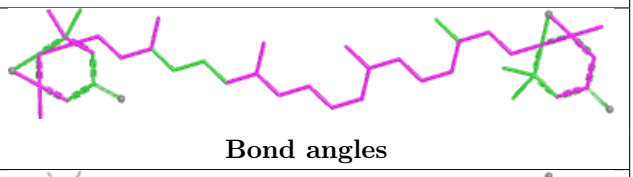
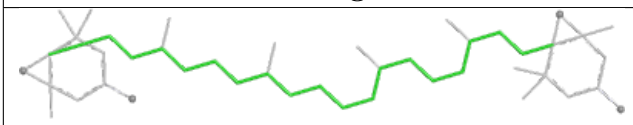
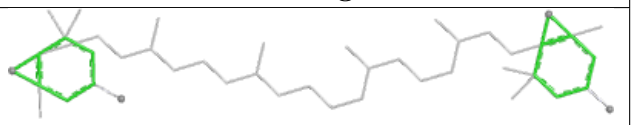


Bond angles

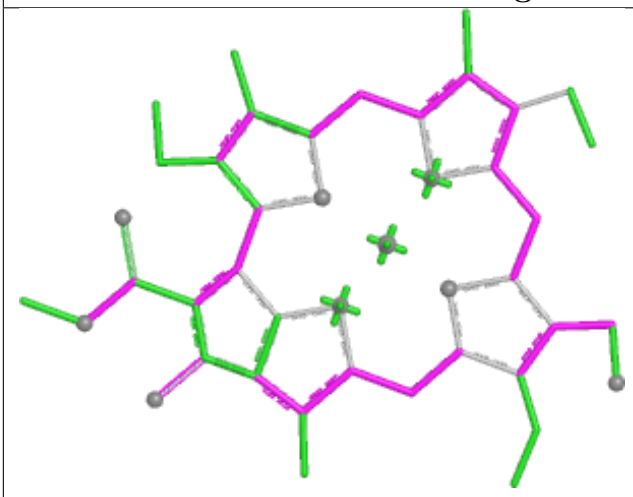


Torsions



Rings

Ligand CHL A6 607



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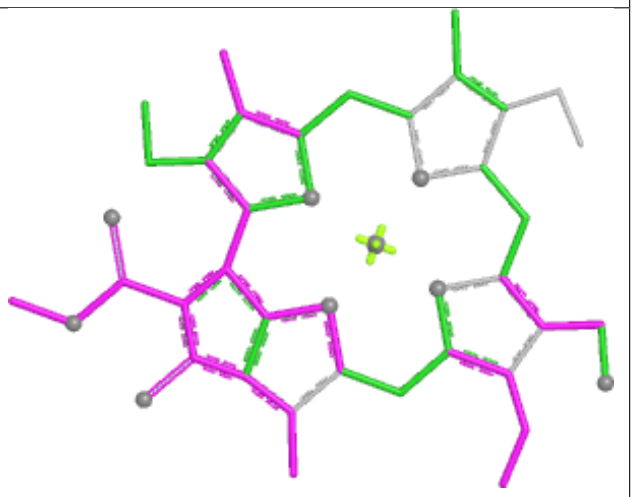
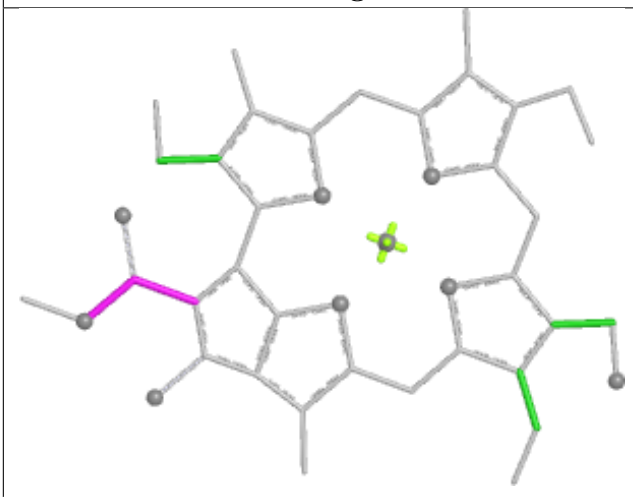
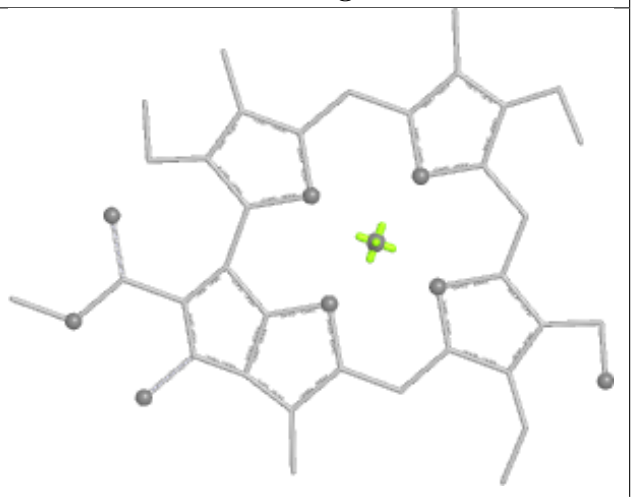


Bond angles

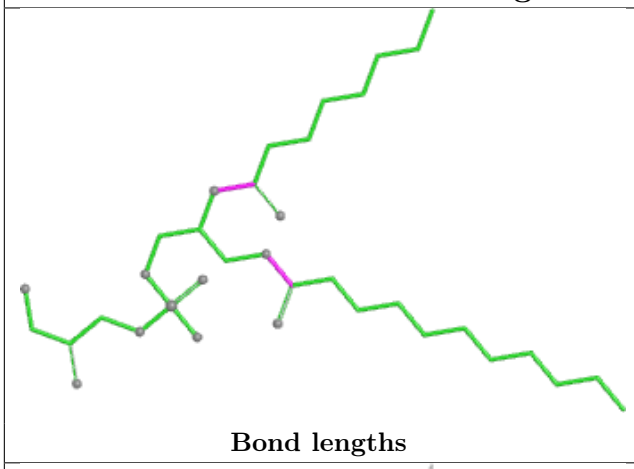


Torsions



Rings

Ligand LHG A6 618



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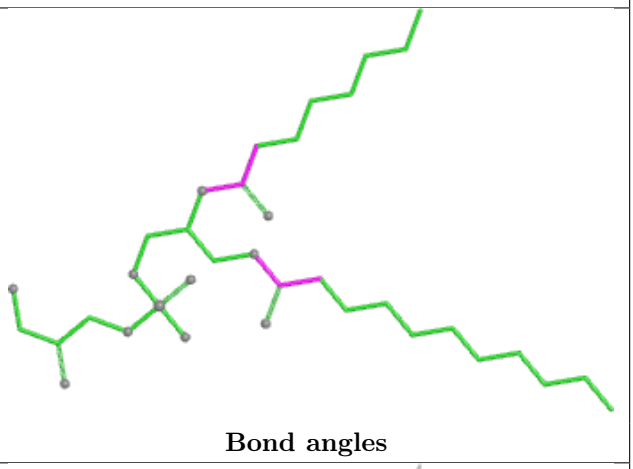
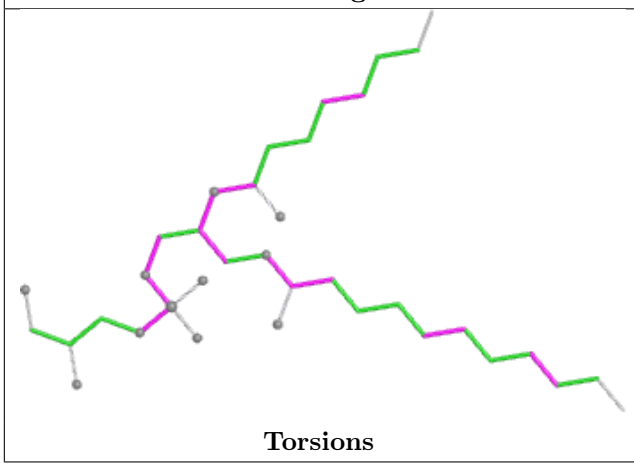


Bond angles



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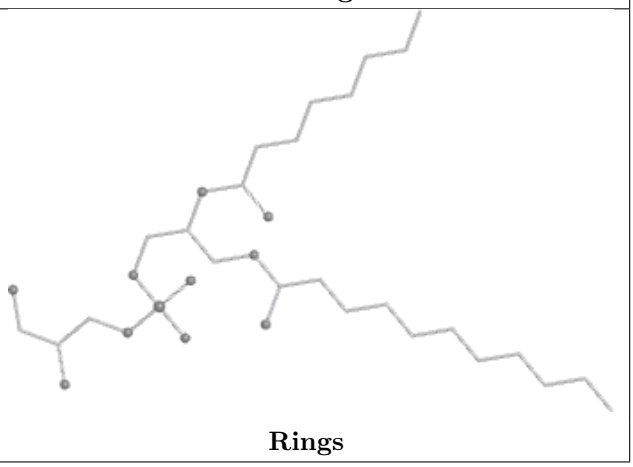
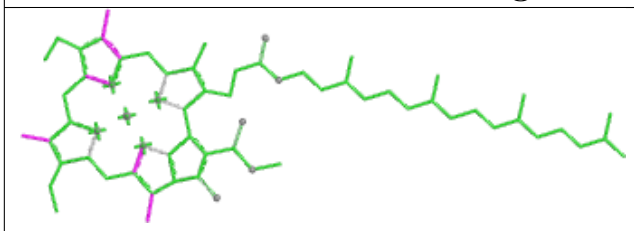


Rings

Ligand CLA AB 832



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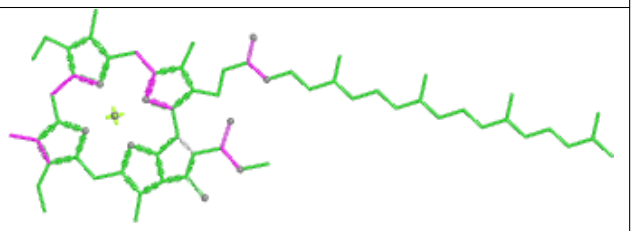
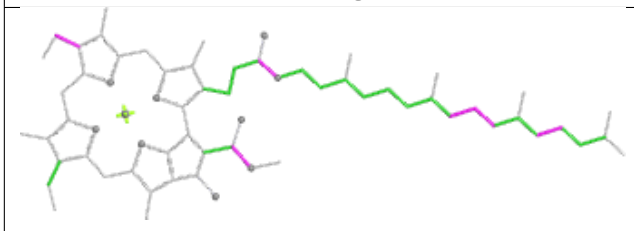


Bond angles



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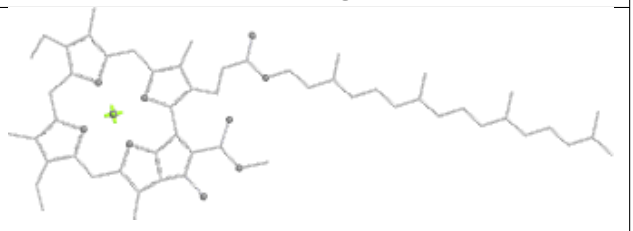
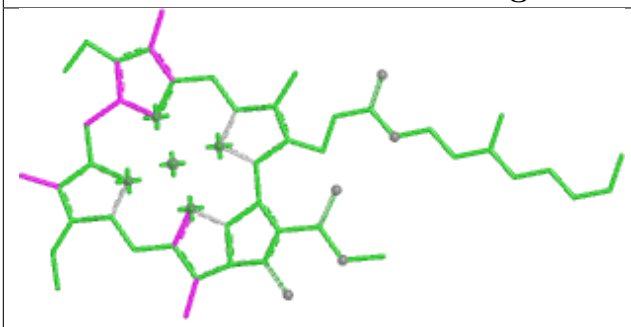


Rings

Ligand CLA AA 812



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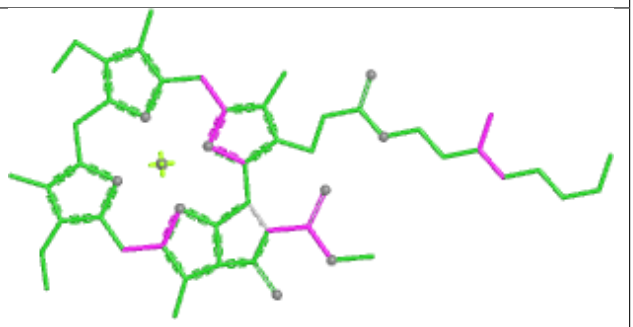
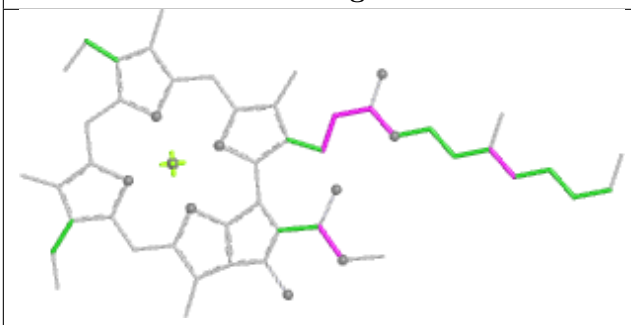


Bond angles



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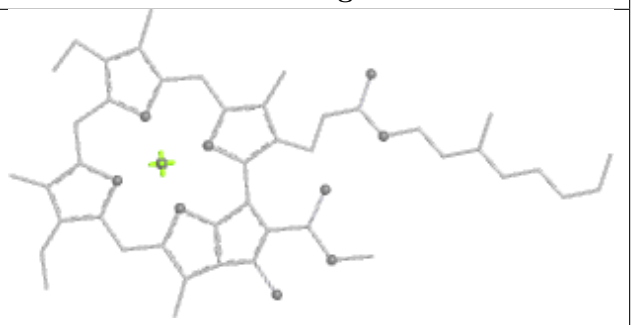
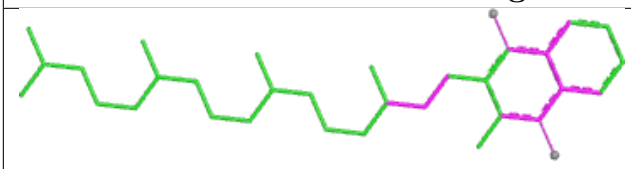


Rings

Ligand PQN AB 843



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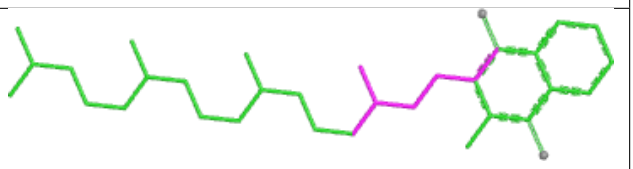
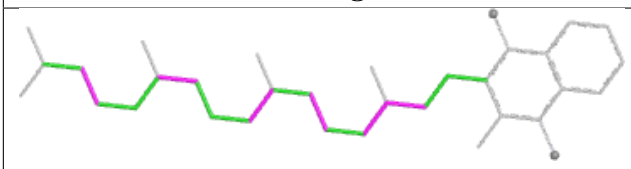


Bond angles



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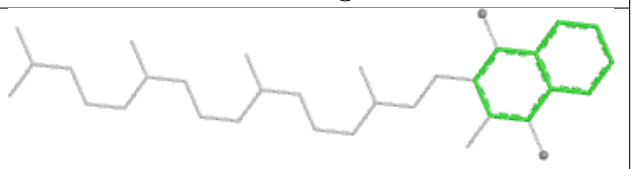
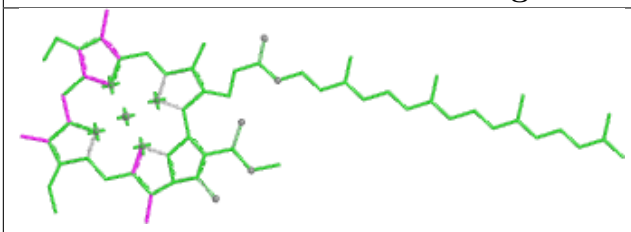
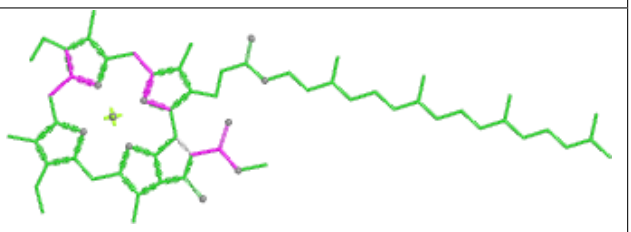


Rings

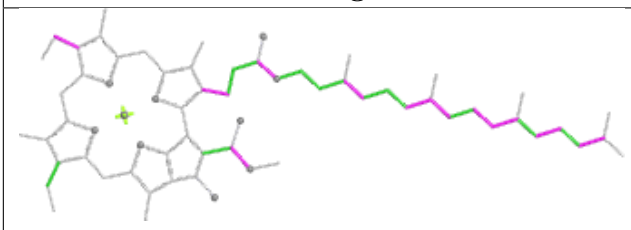
Ligand CLA AB 803



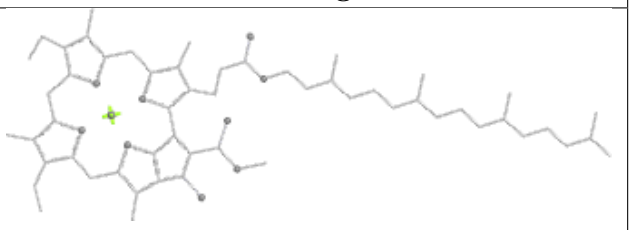
Bond lengths



Bond angles



Torsions



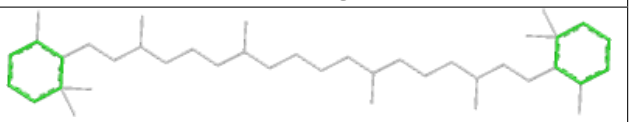
Rings

Ligand BCR BJ 103

Bond lengths

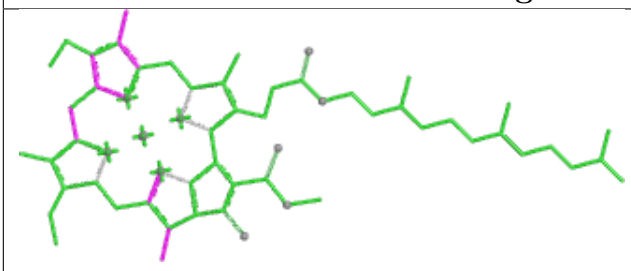
Bond angles

Torsions



Rings

Ligand CLA B1 314



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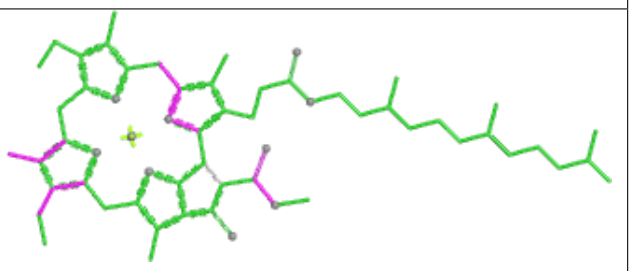
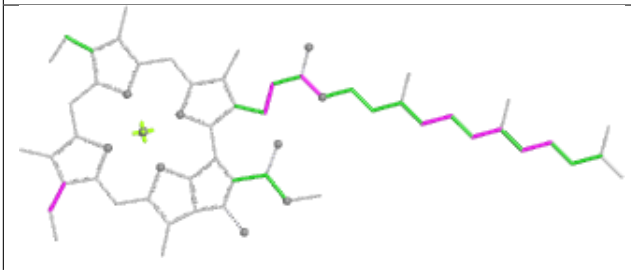


Bond angles



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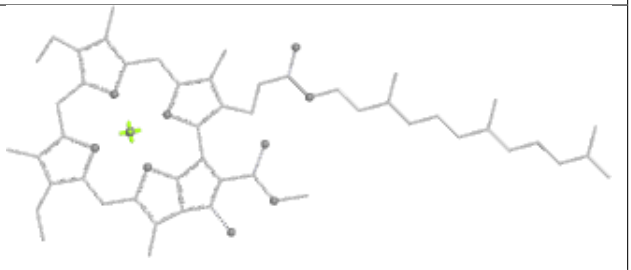
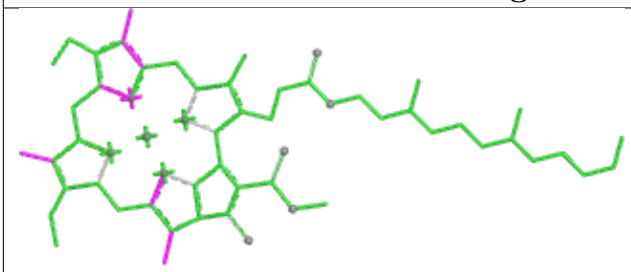
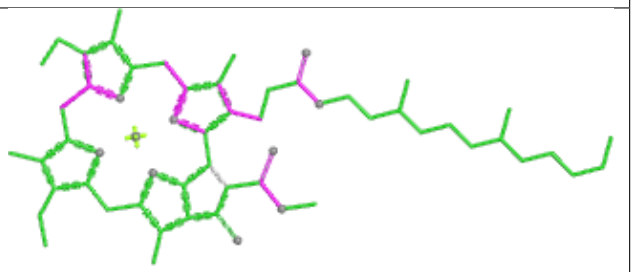
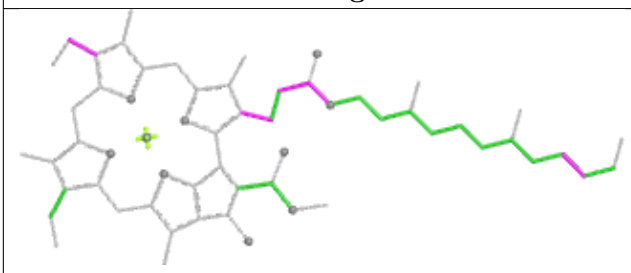
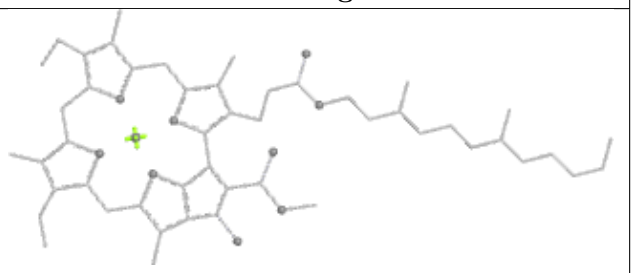
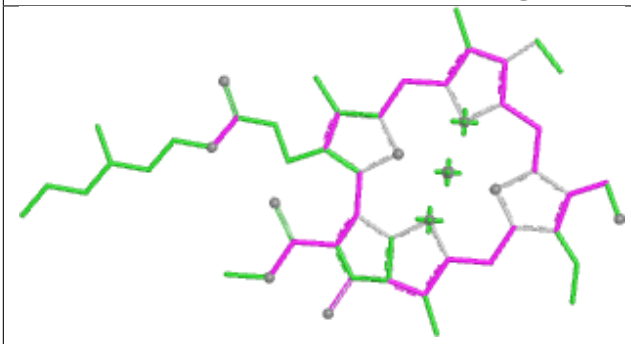
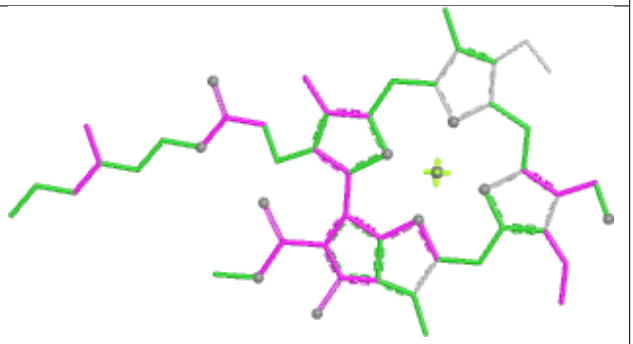
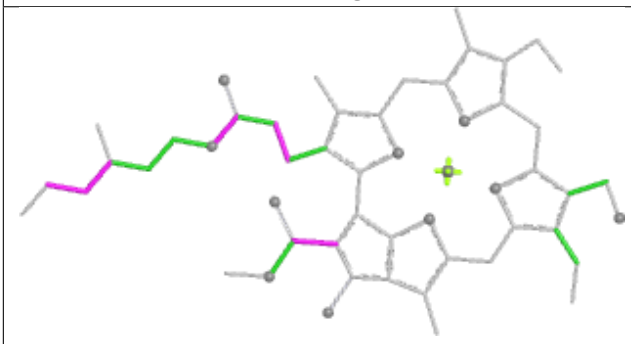
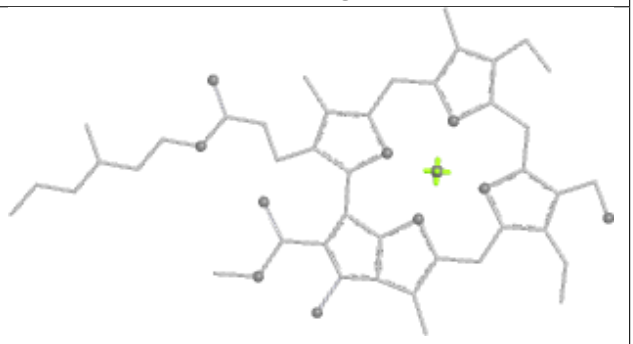
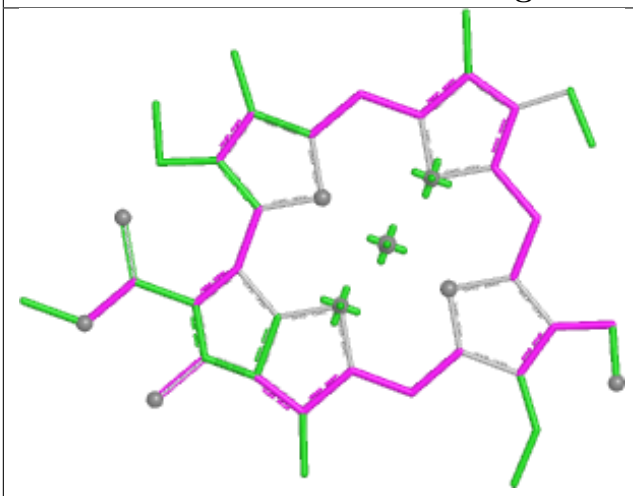


Rings

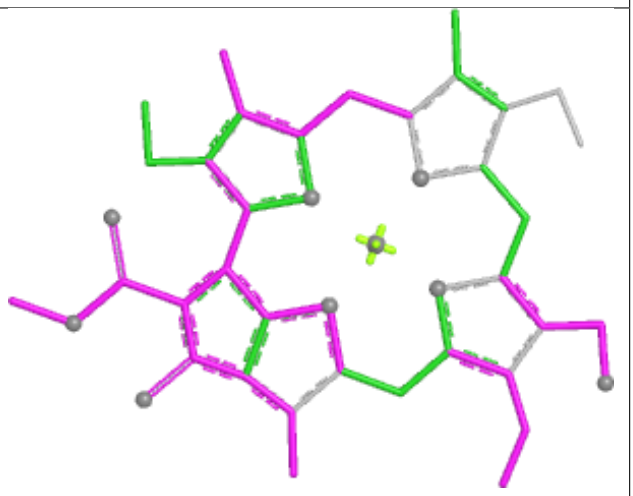
Ligand CLA AA 818	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL B2 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

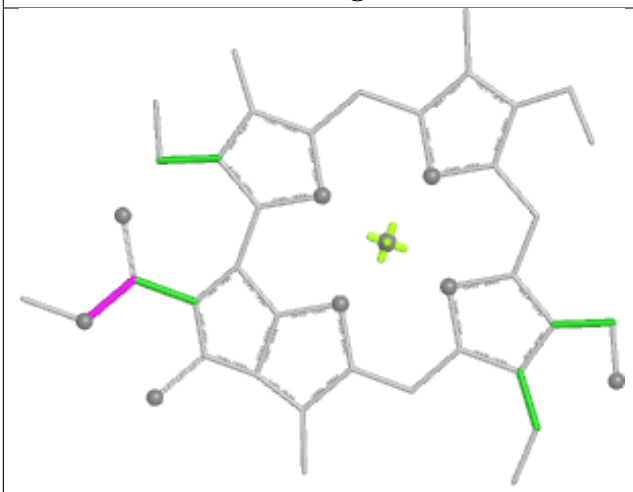
Ligand CHL B2 606



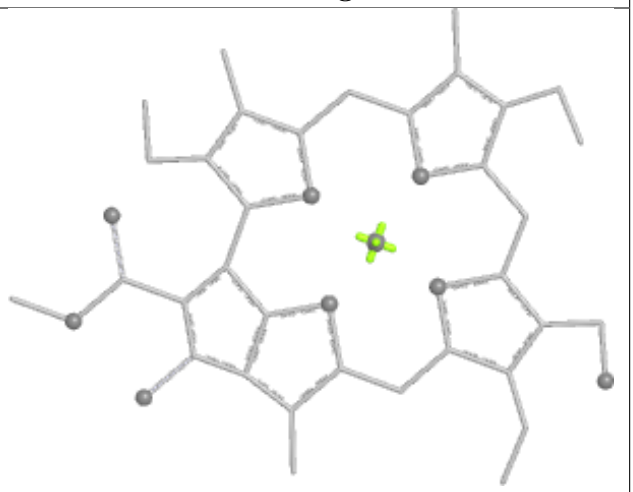
Bond lengths



Bond angles

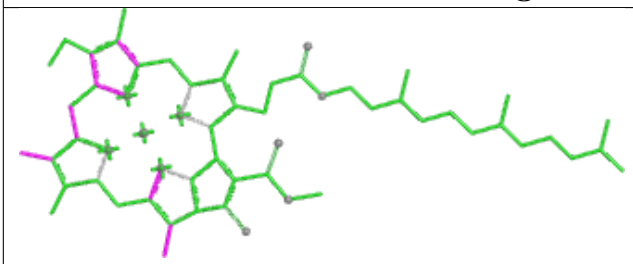


Torsions



Rings

Ligand CLA B1 311



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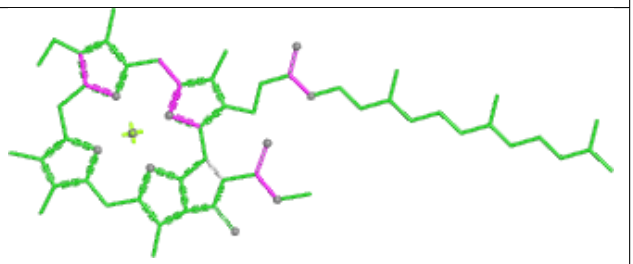
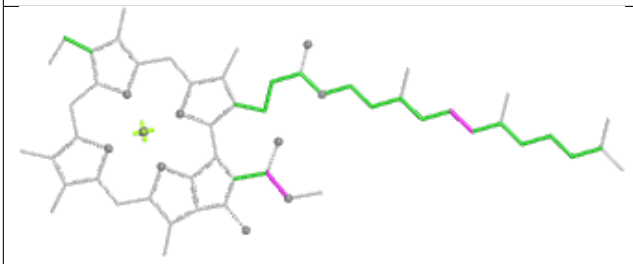


Bond angles



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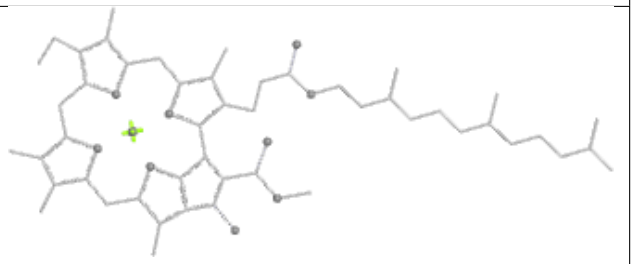
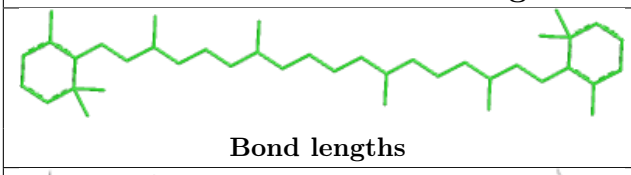


Rings

Ligand BCR BA 850



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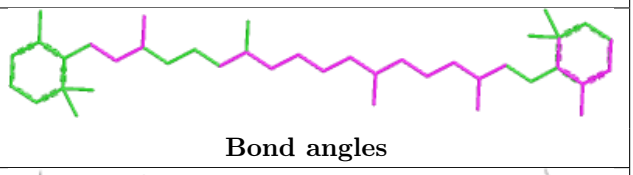

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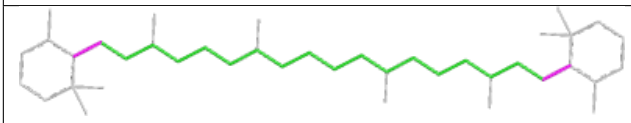
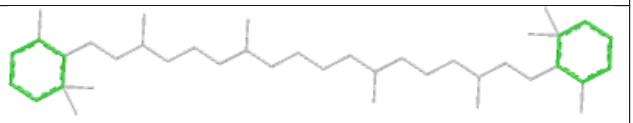
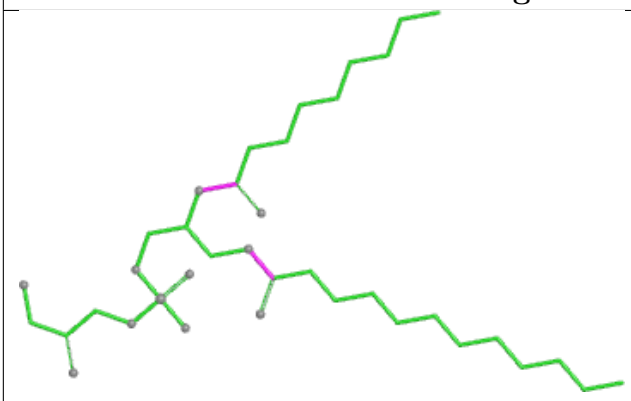


Torsions



Rings

Ligand LHG A1 301



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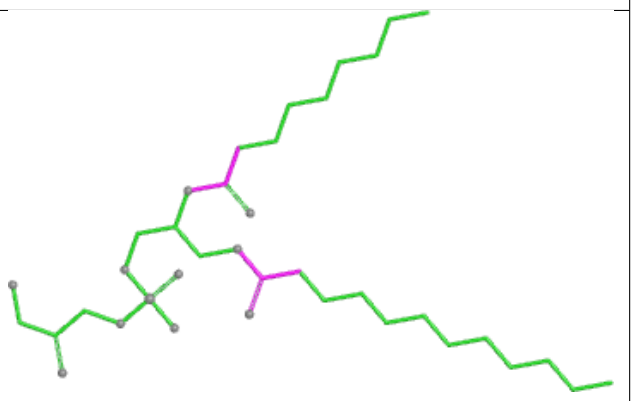

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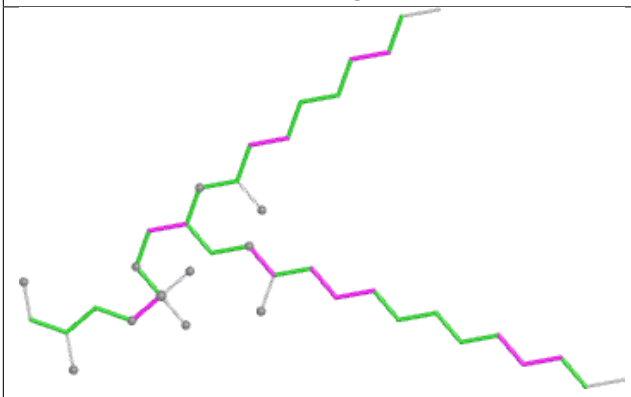

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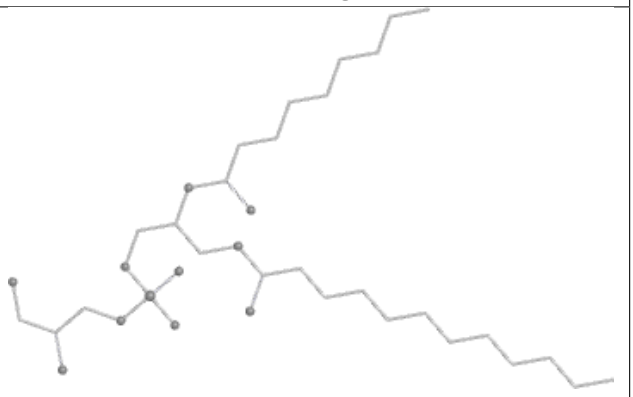
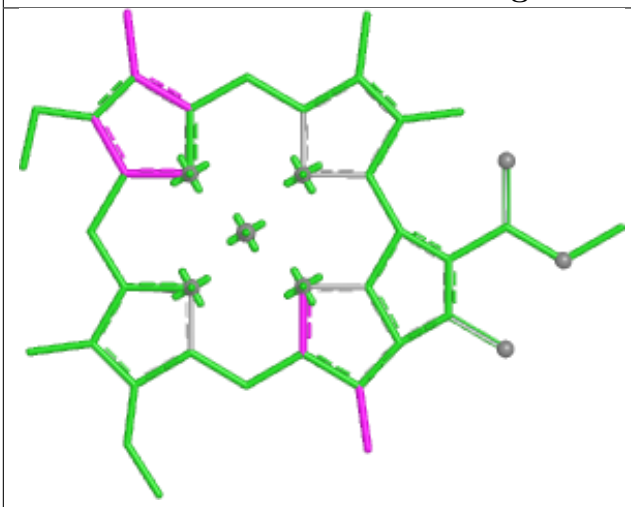


Rings

Ligand CLA AB 805



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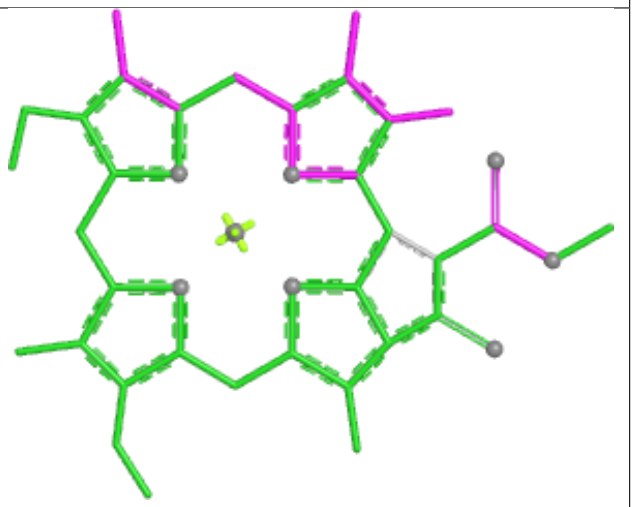
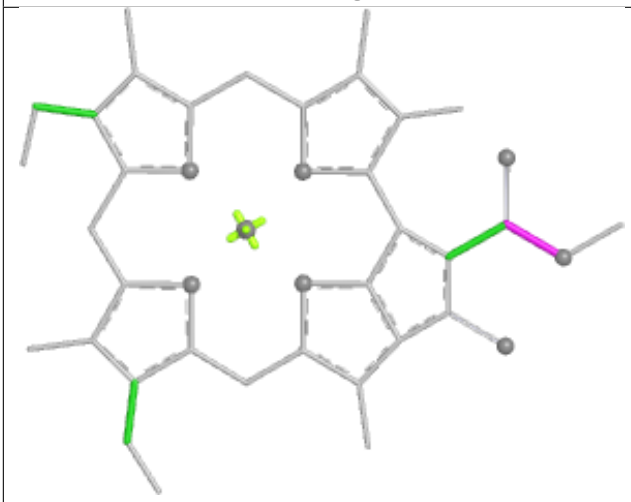


Bond angles



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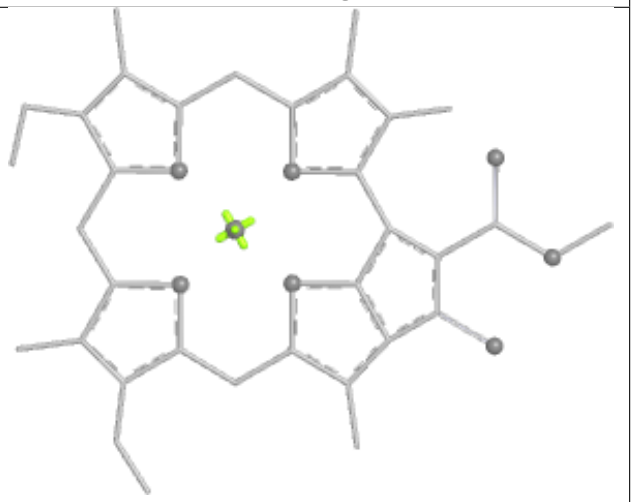
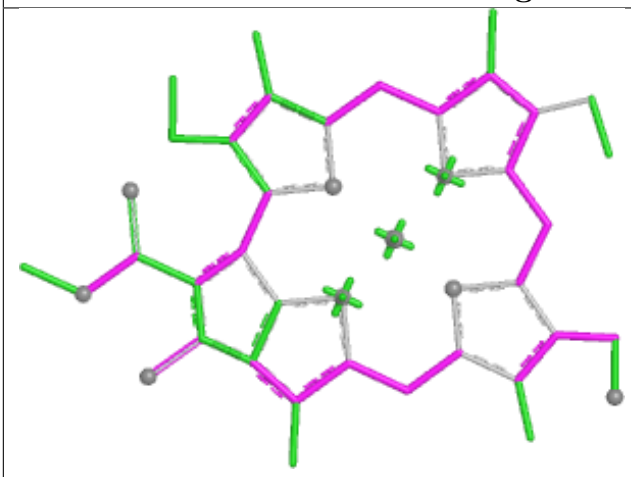


Rings

Ligand CHL B2 605



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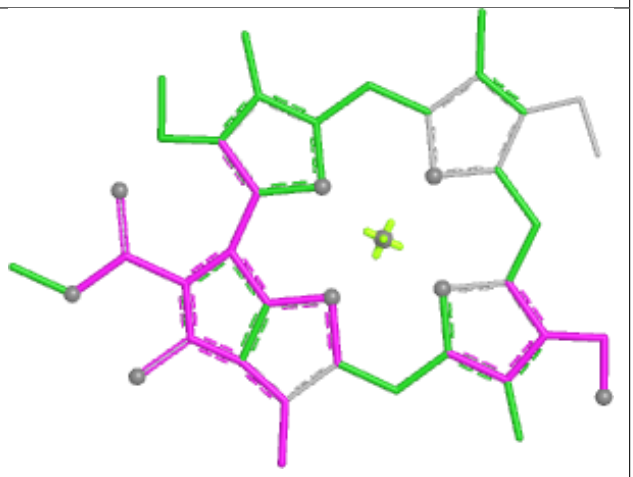
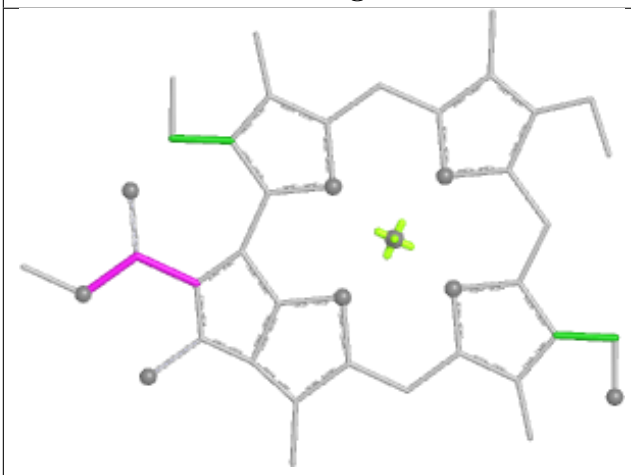


Bond angles



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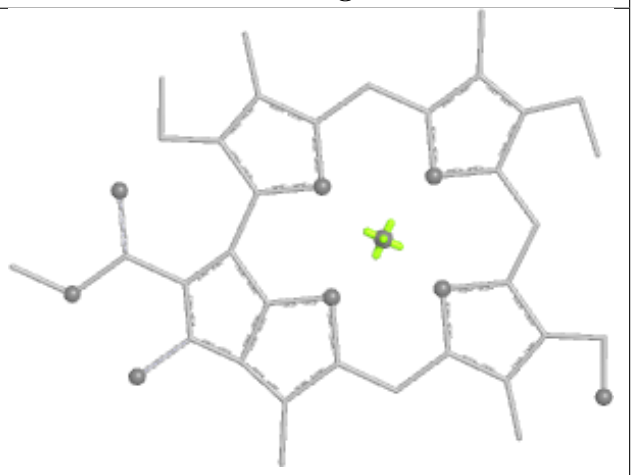
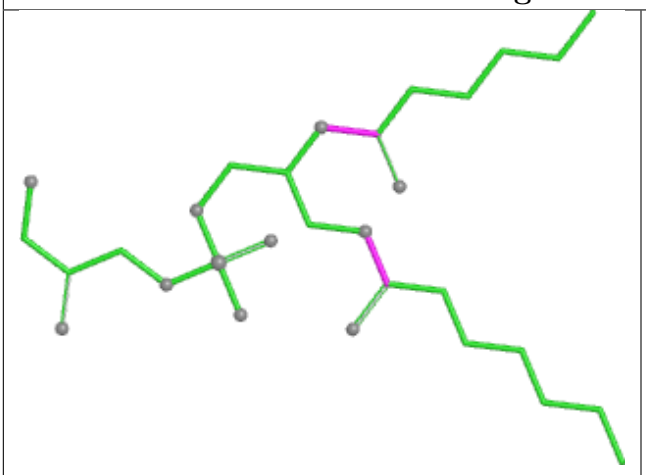


Rings

Ligand LHG B5 618



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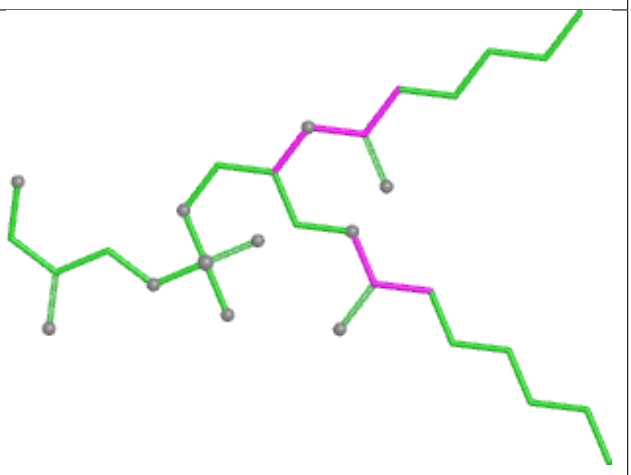

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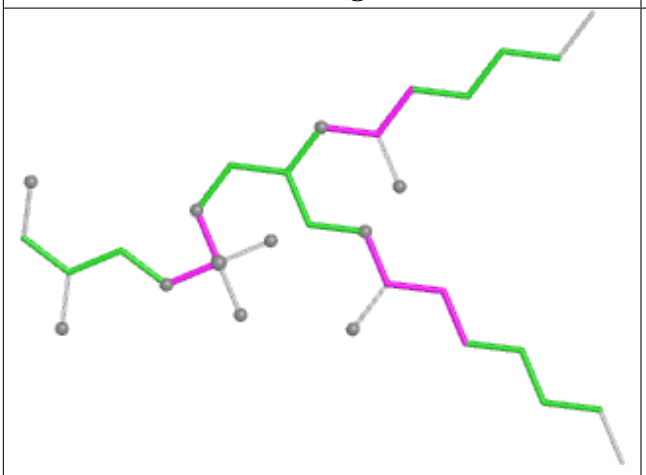

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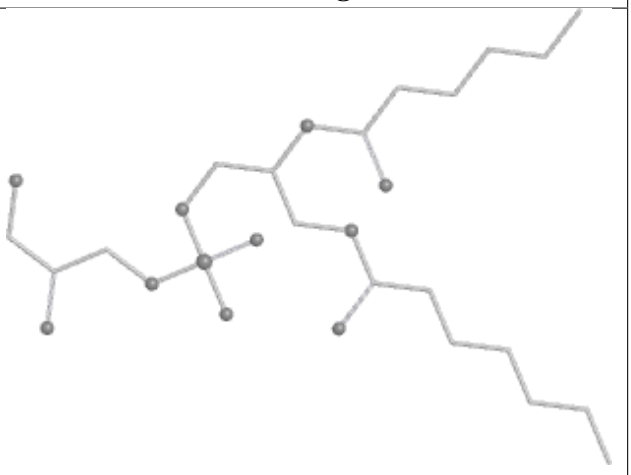
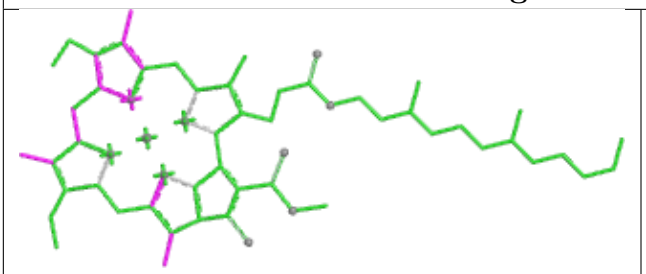


Rings

Ligand CLA AA 826



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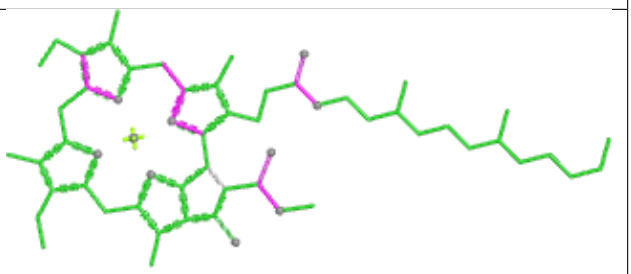
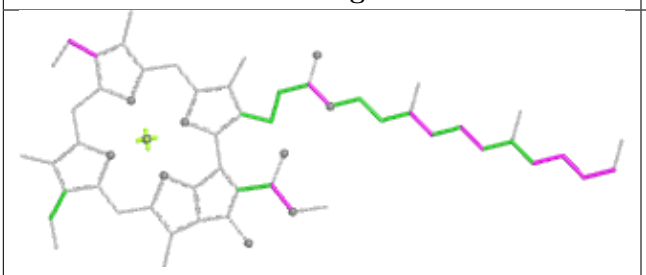


Bond angles



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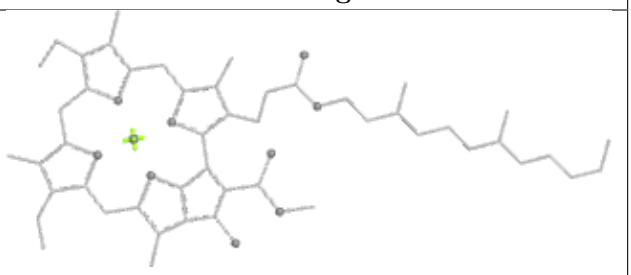
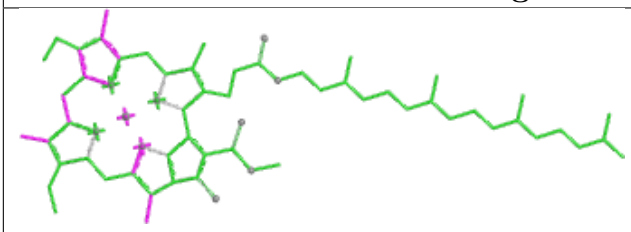


Rings

Ligand CLA BB 802



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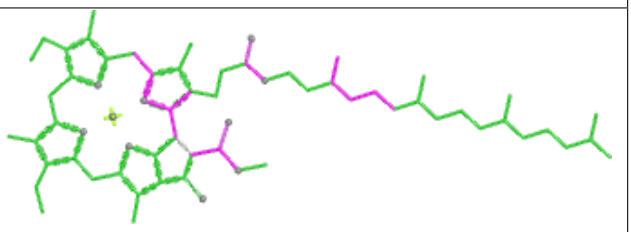

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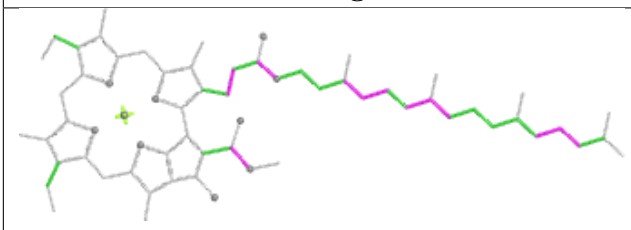

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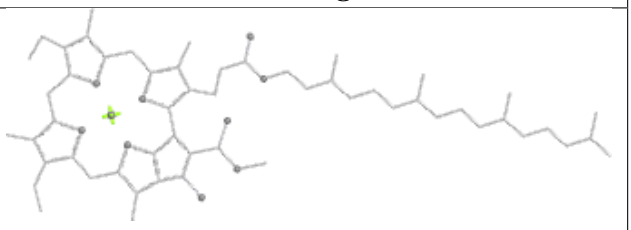
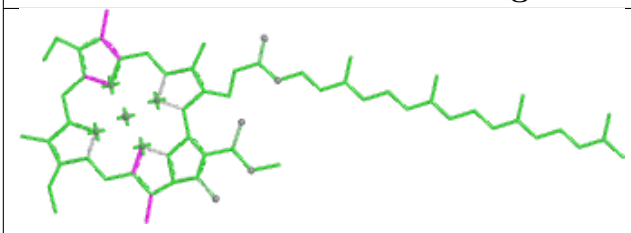


Rings

Ligand CLA AB 833



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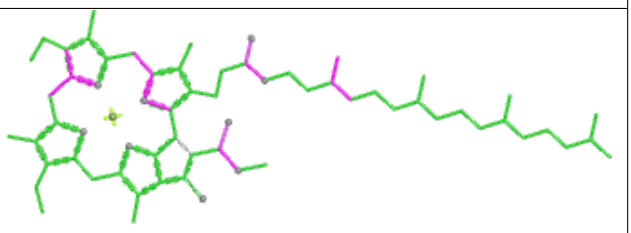
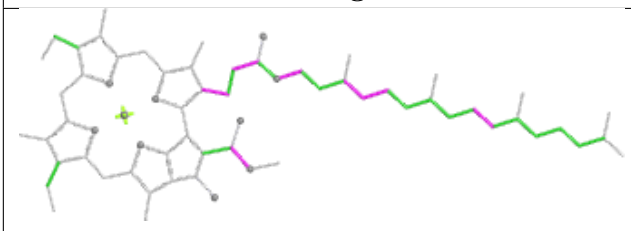


Bond angles



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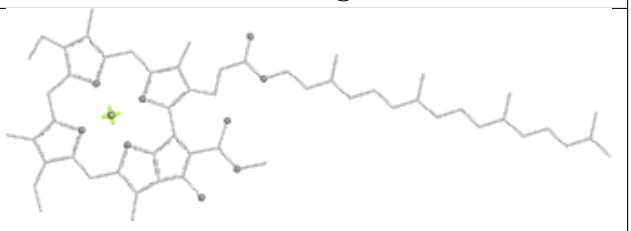
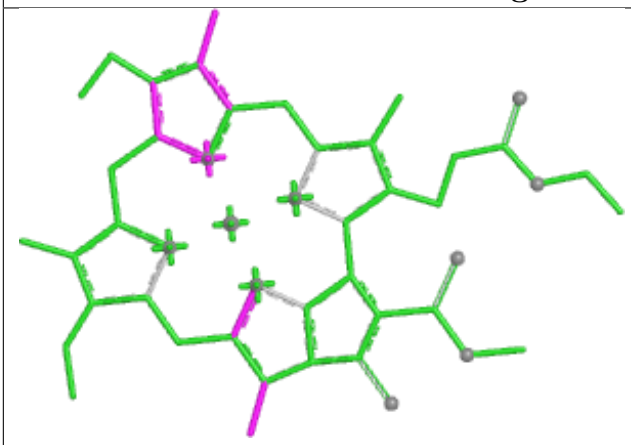


Rings

Ligand CLA AB 839



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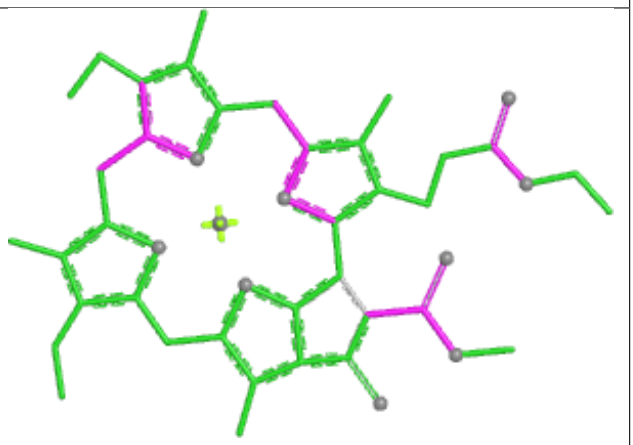
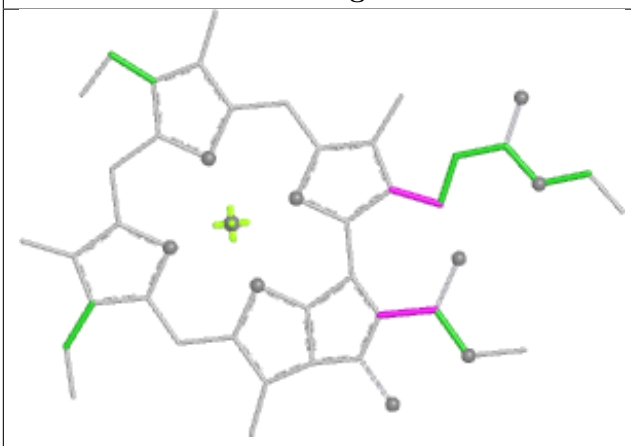


Bond angles



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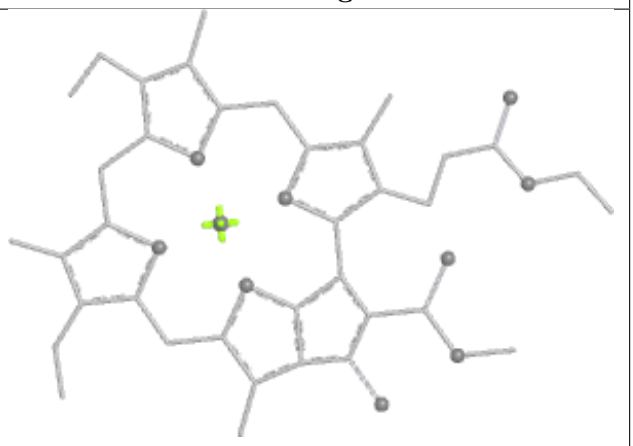
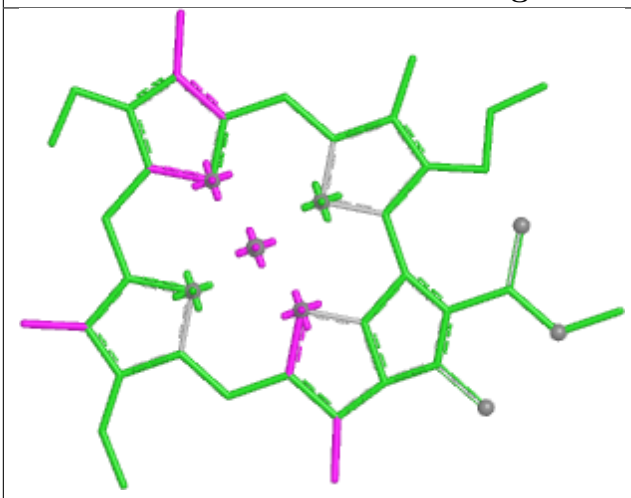


Rings

Ligand CLA AB 824



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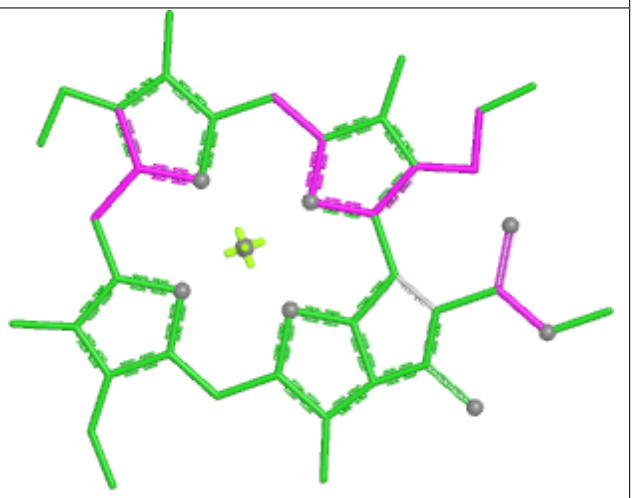

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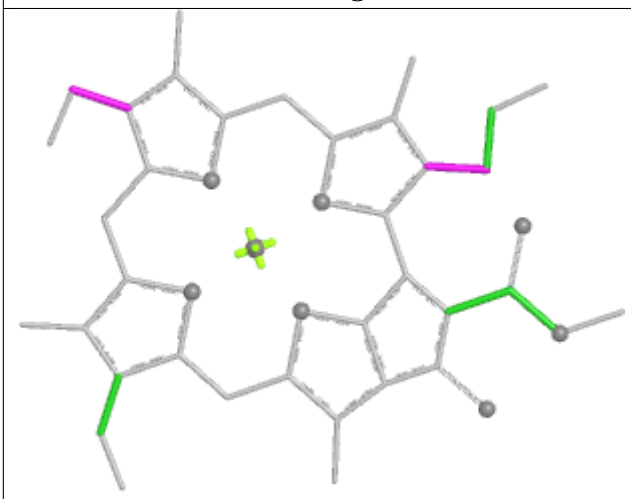

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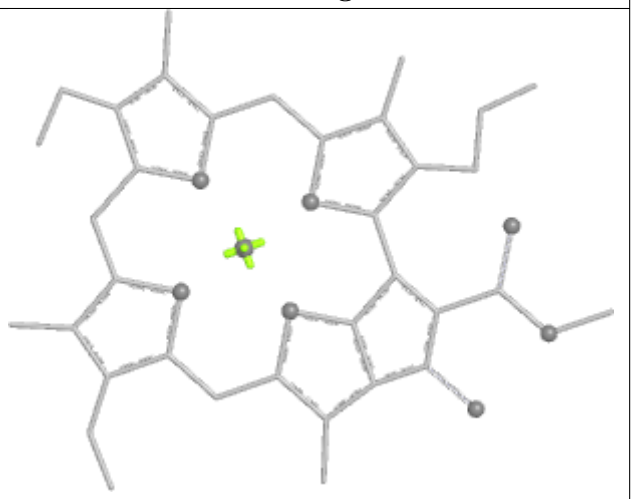
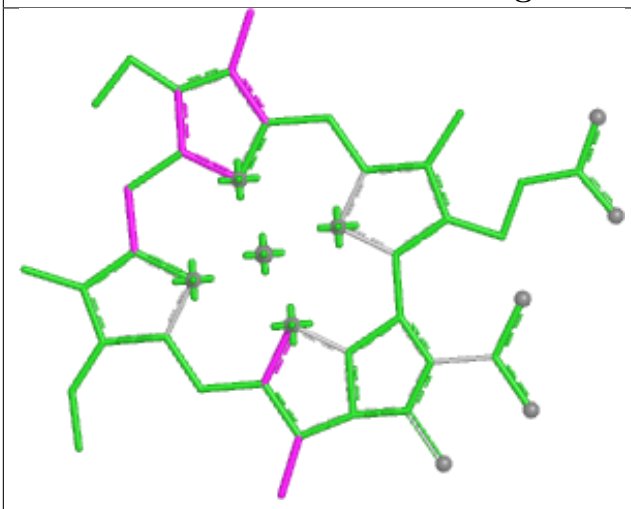


Rings

Ligand CLA A1 309



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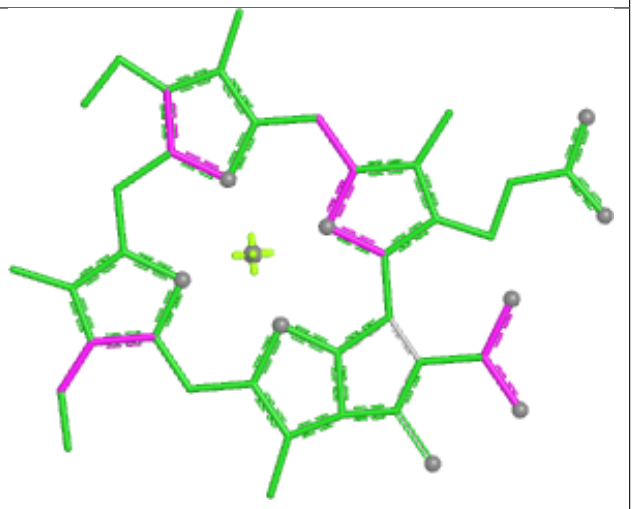

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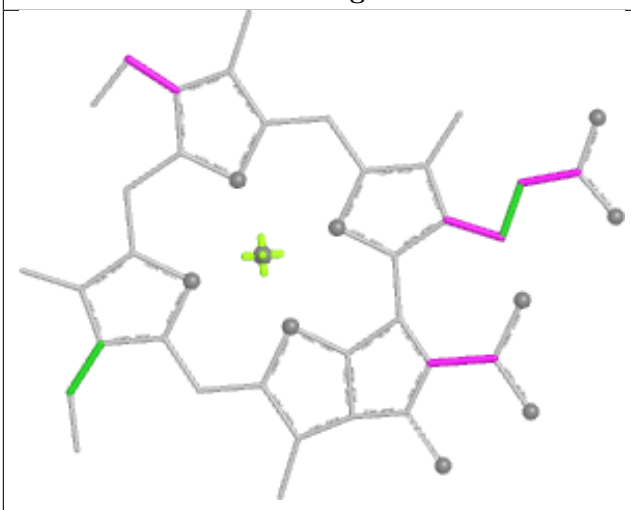

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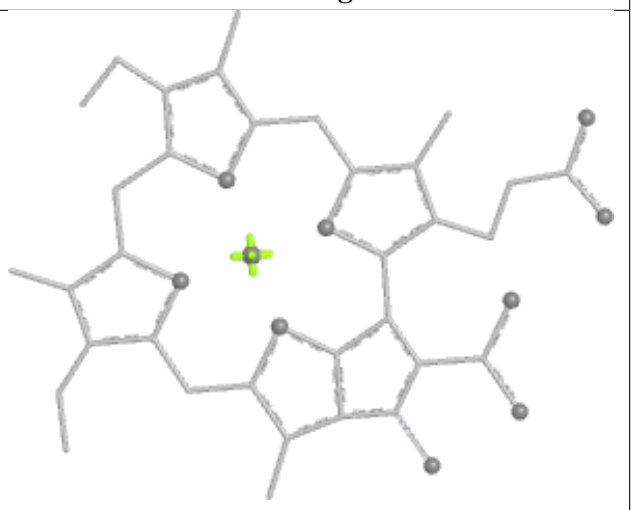
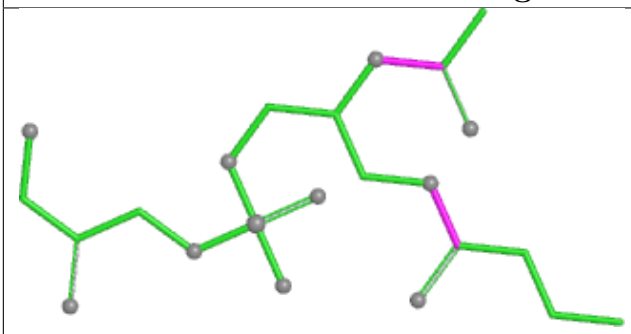


Rings

Ligand LHG B3 318



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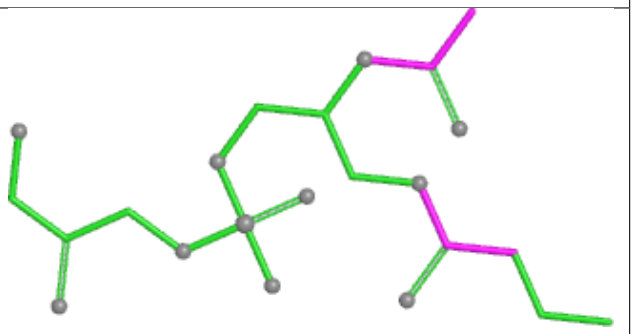
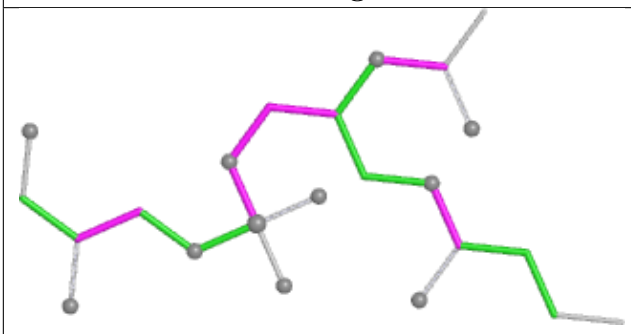
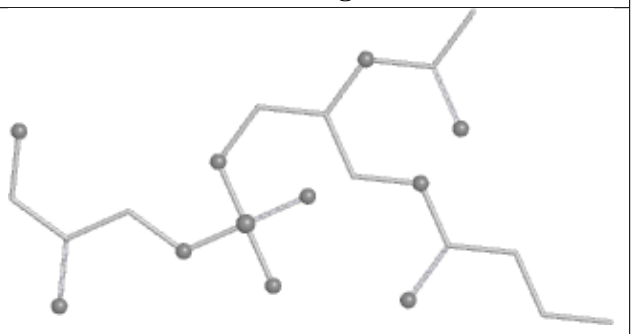


Bond angles

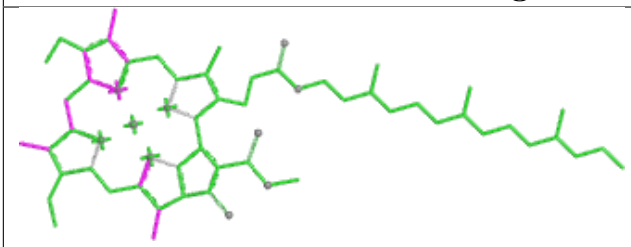


Torsions



Rings

Ligand CLA AB 827



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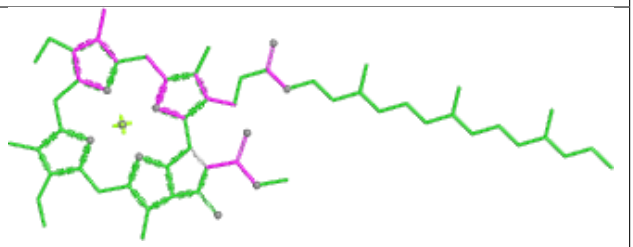
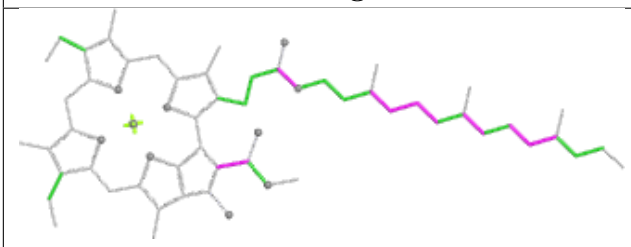
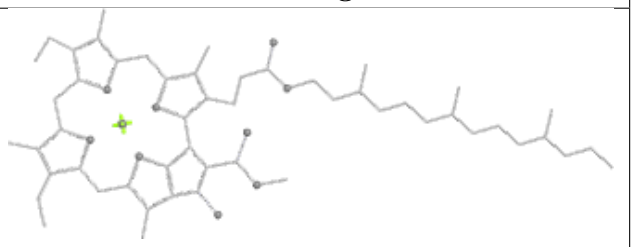


Bond angles

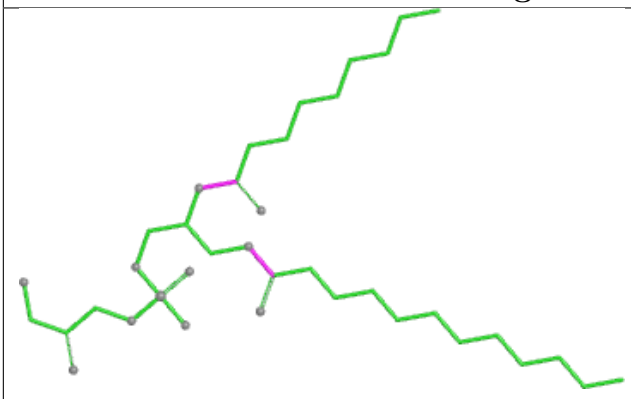


Torsions



Rings

Ligand LHG B1 301



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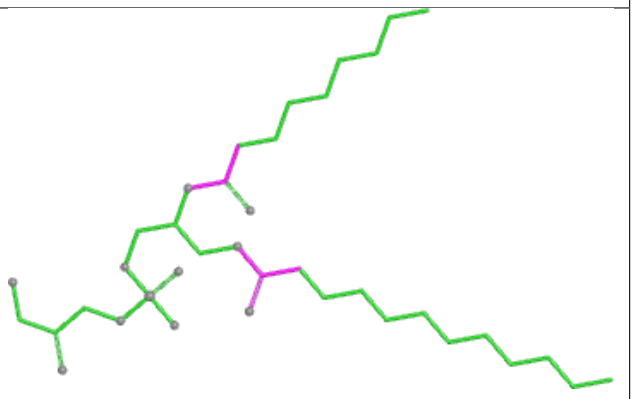
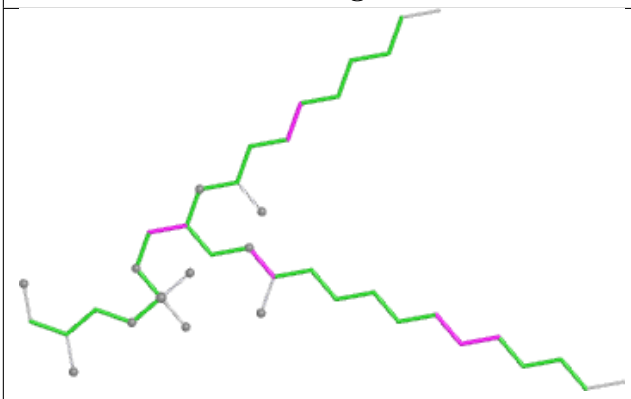
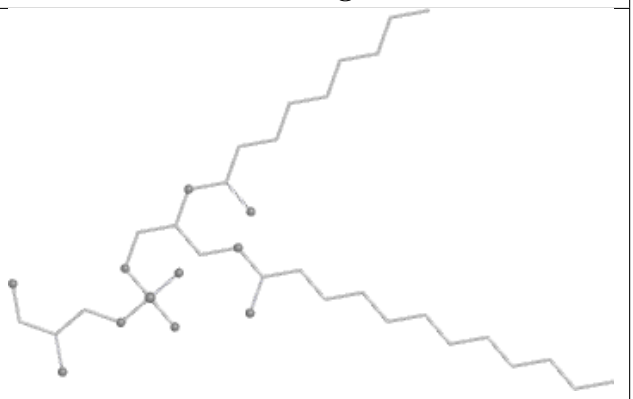


Bond angles

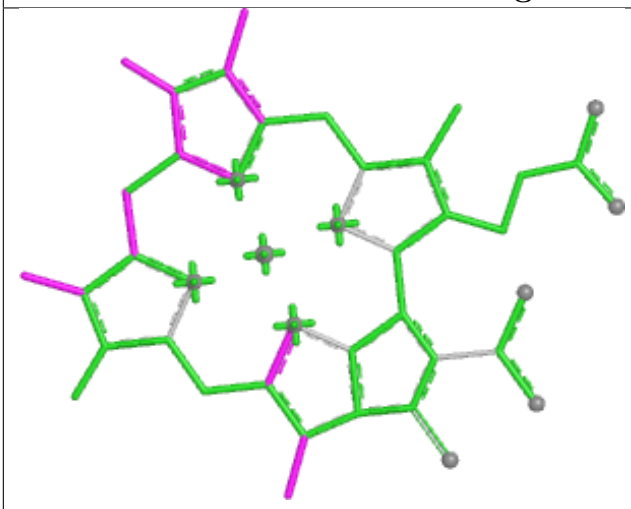


Torsions

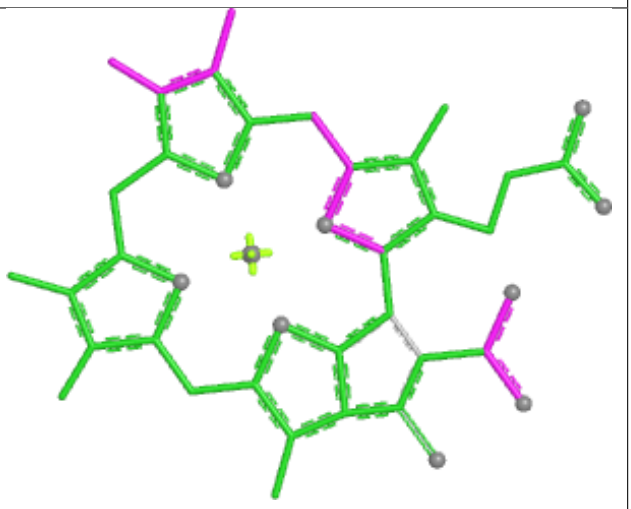


Rings

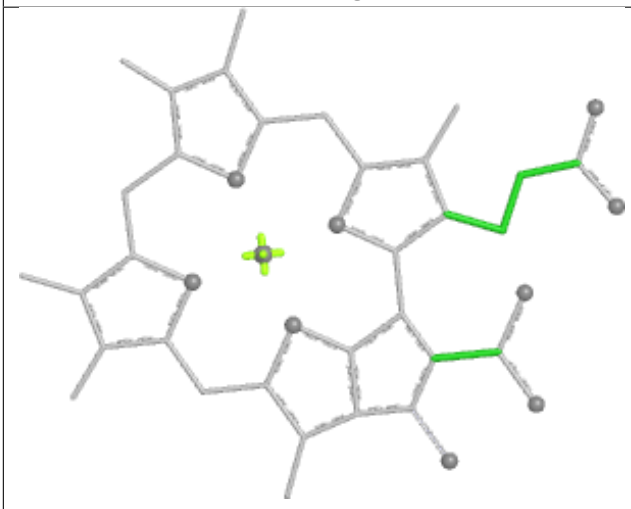
Ligand CLA A3 304



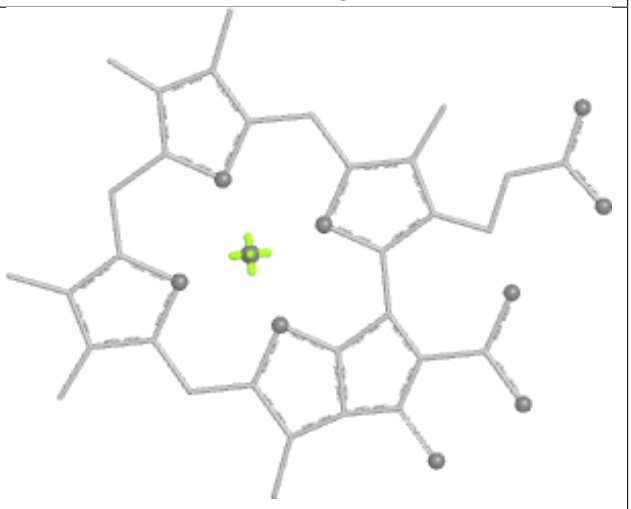
Bond lengths



Bond angles

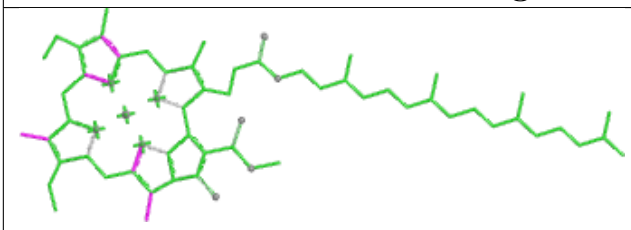


Torsions

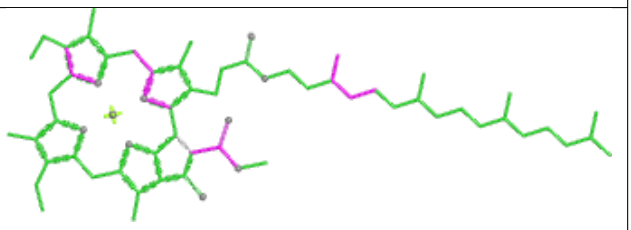


Rings

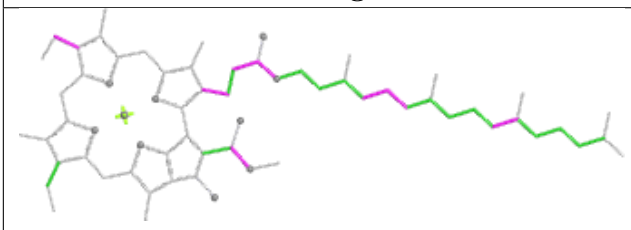
Ligand CLA BB 834



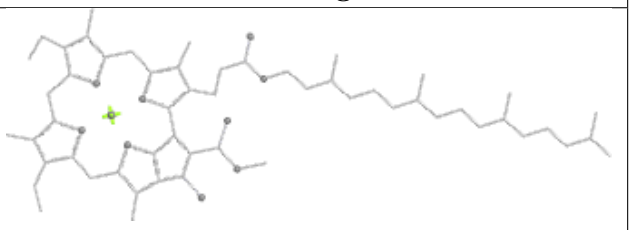
Bond lengths



Bond angles

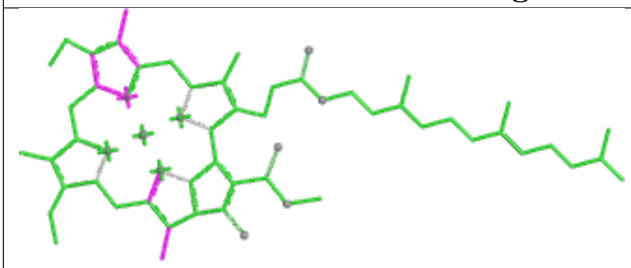


Torsions

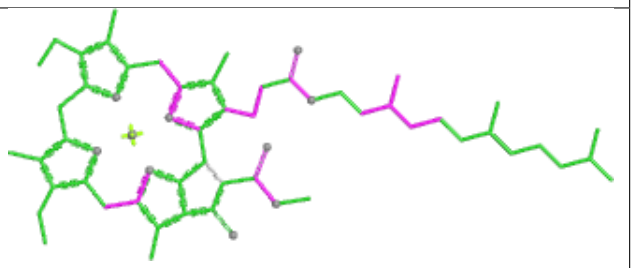


Rings

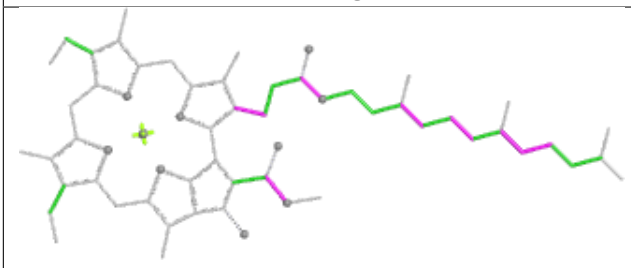
Ligand CLA BB 820



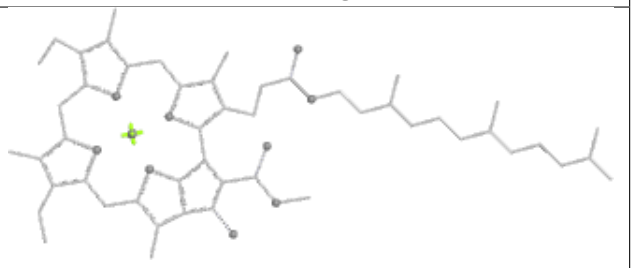
Bond lengths



Bond angles

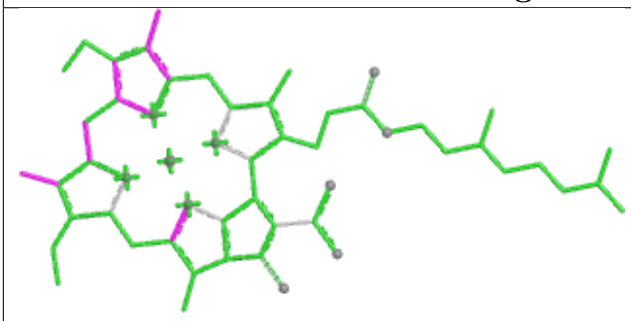


Torsions



Rings

Ligand CLA A3 312



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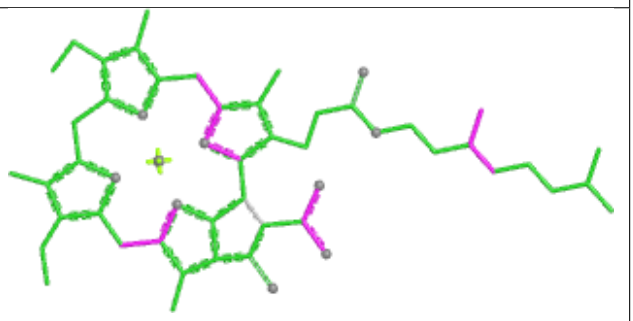
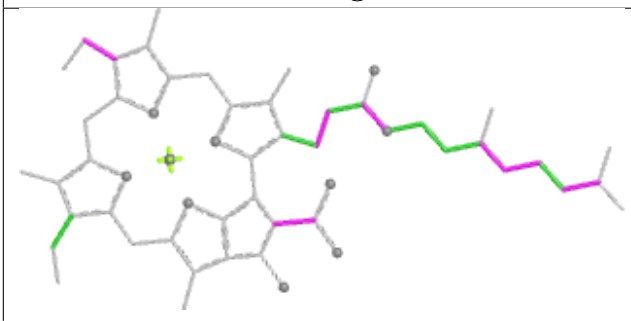


Bond angles



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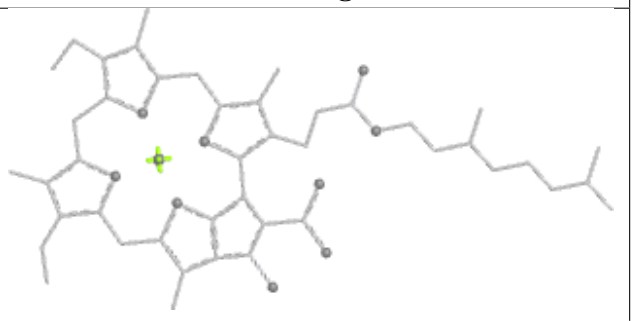
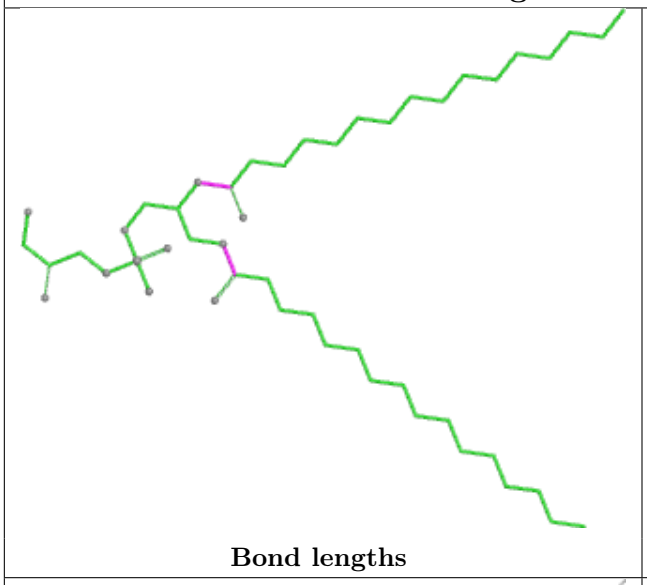


Rings

Ligand LHG AA 844



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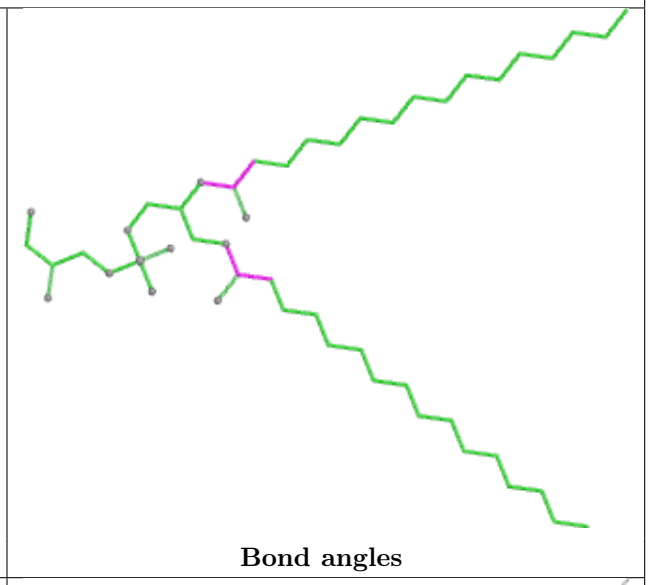
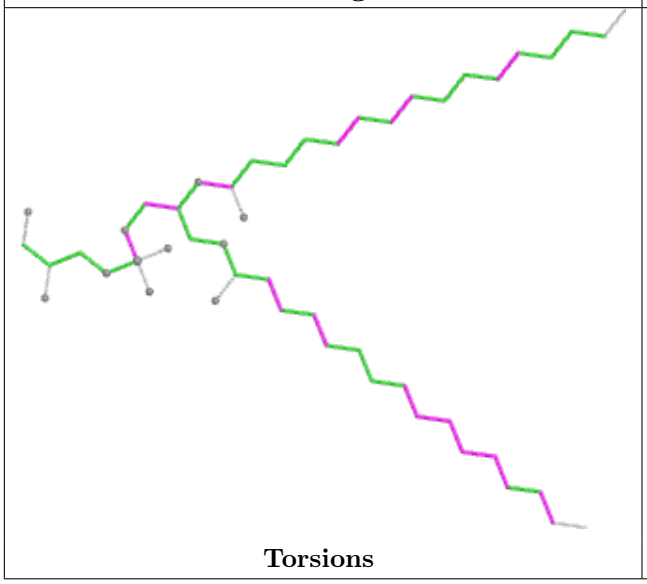


Bond angles



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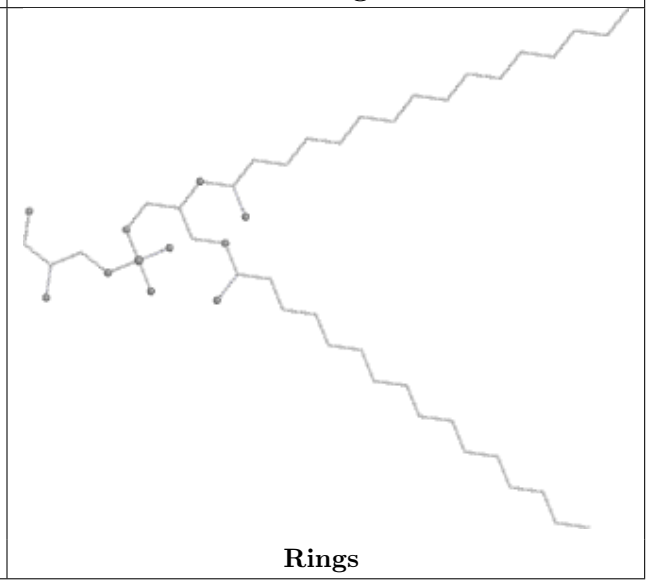
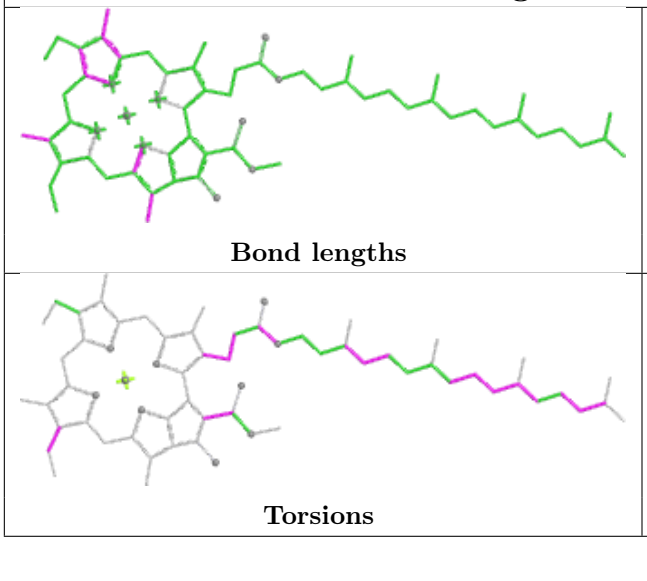


Rings

Ligand CLA BA 805



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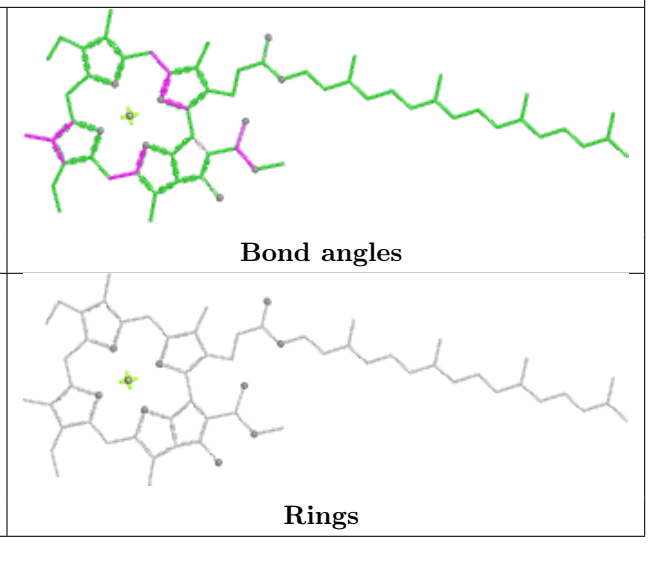
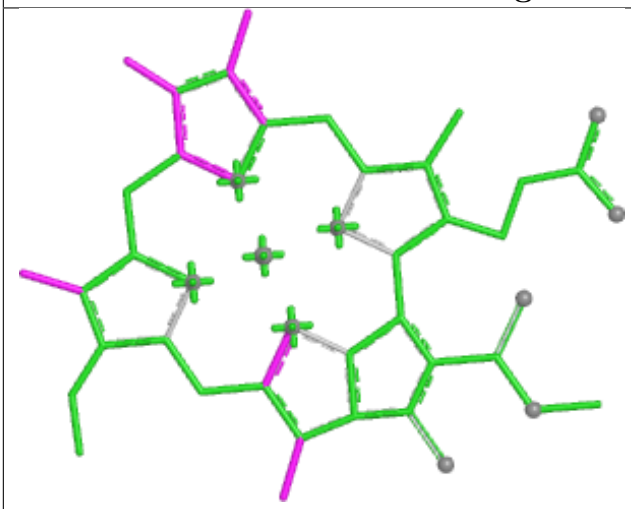


Bond angles

Torsions

Rings

Ligand CLA A4 302



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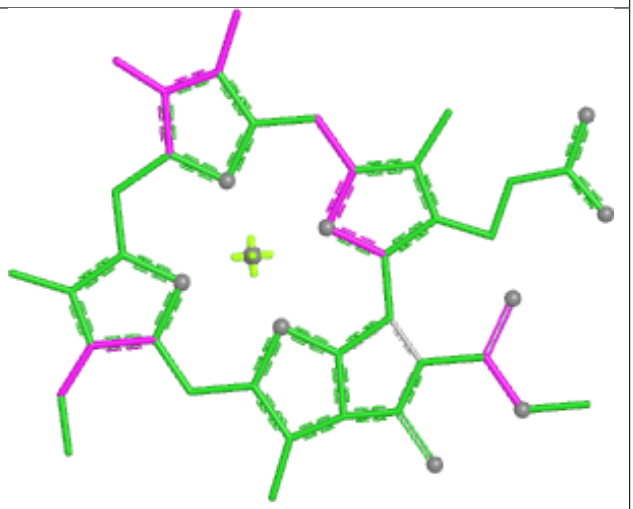
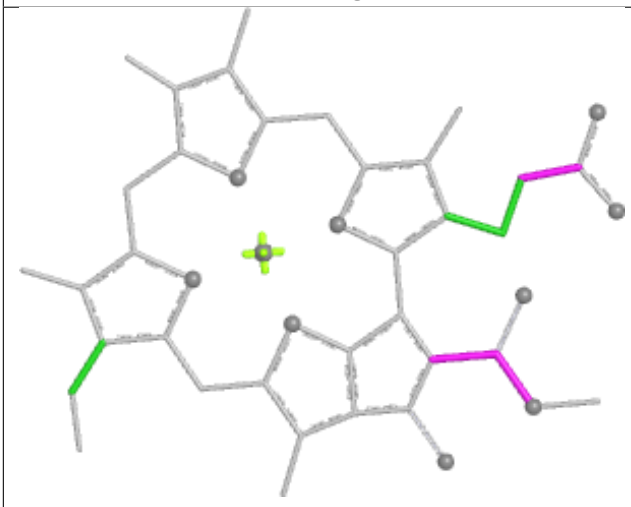


Bond angles



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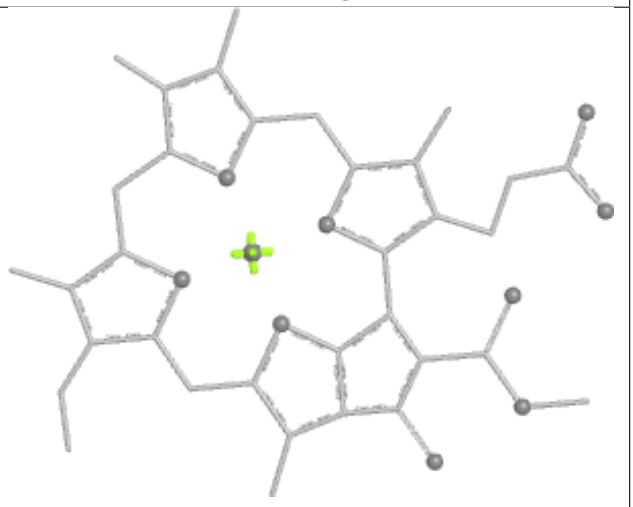
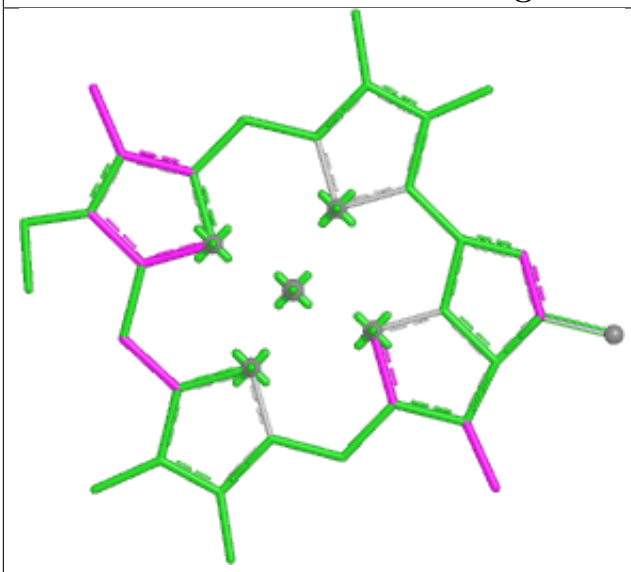


Rings

Ligand CLA A3 314



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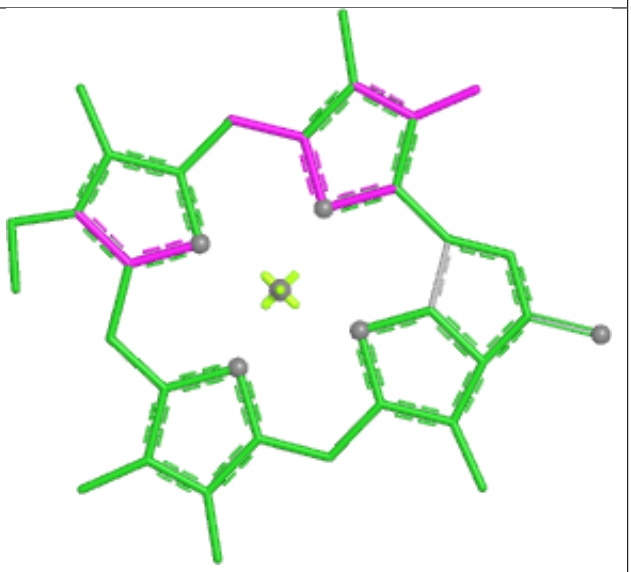
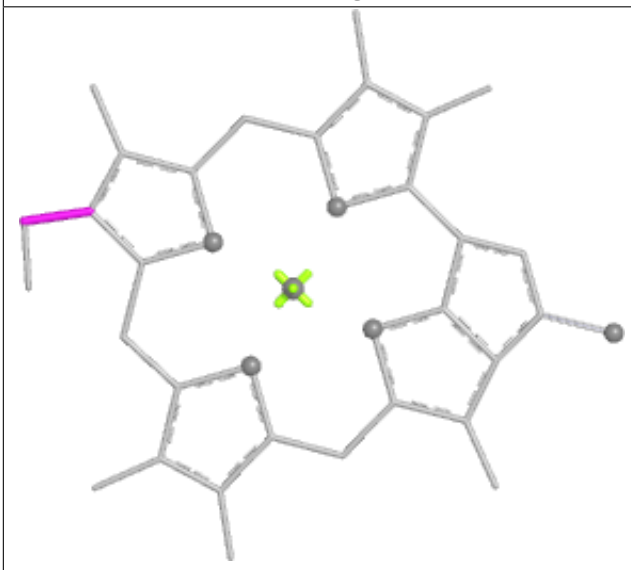
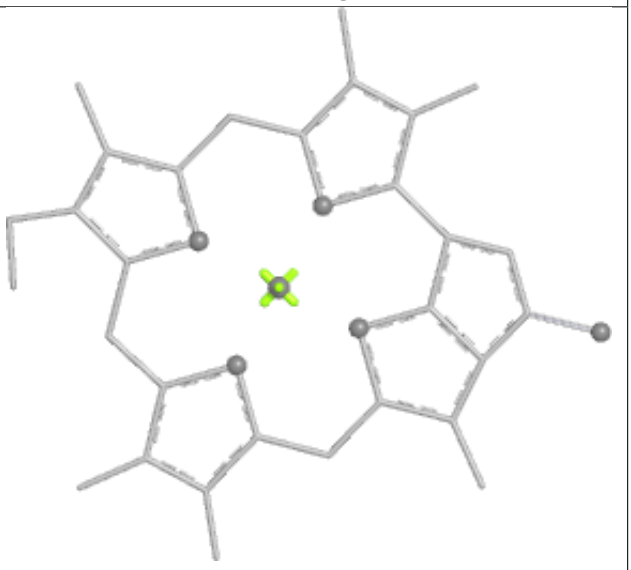


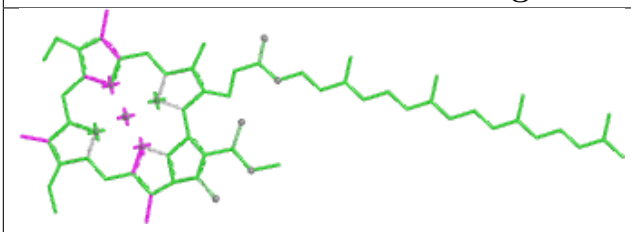
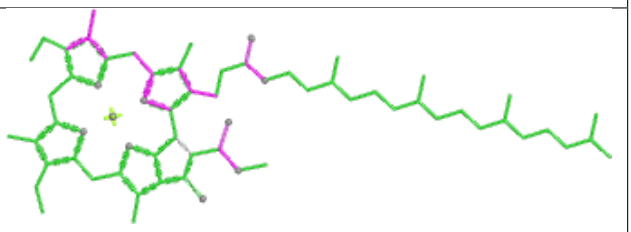
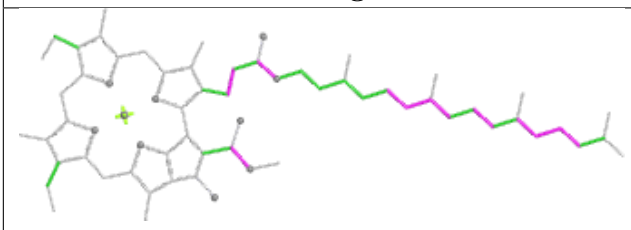
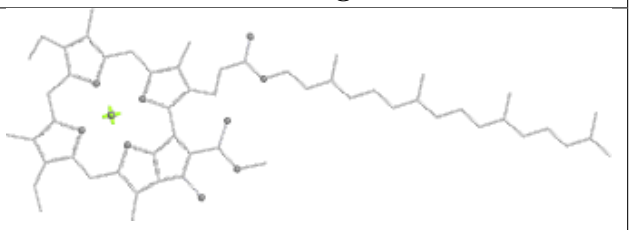
Bond angles

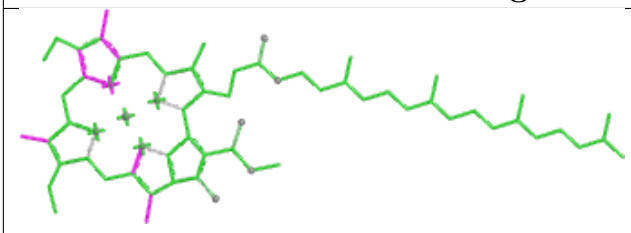
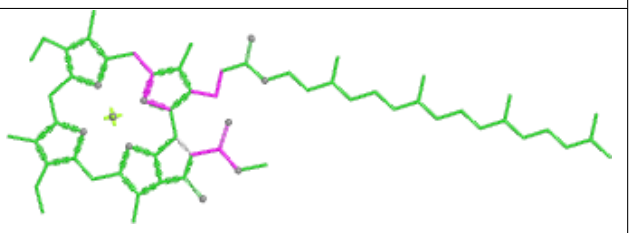
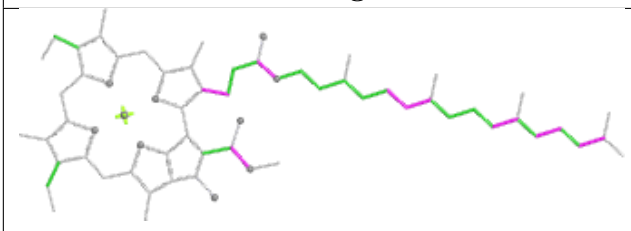
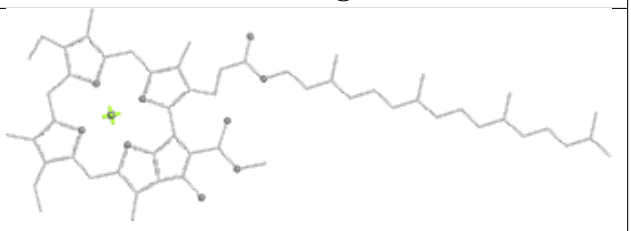


Torsions

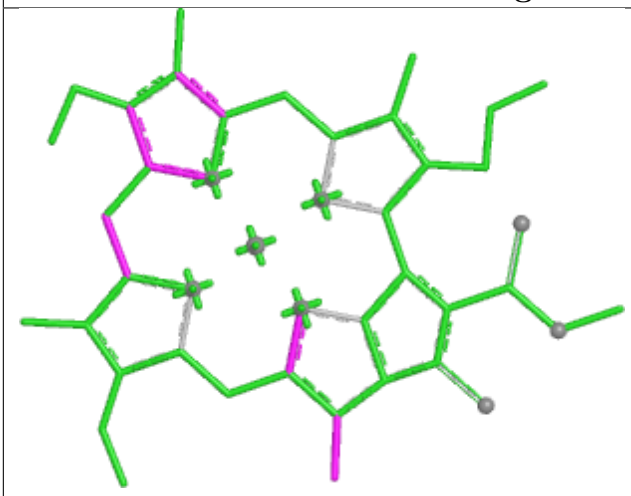


Rings

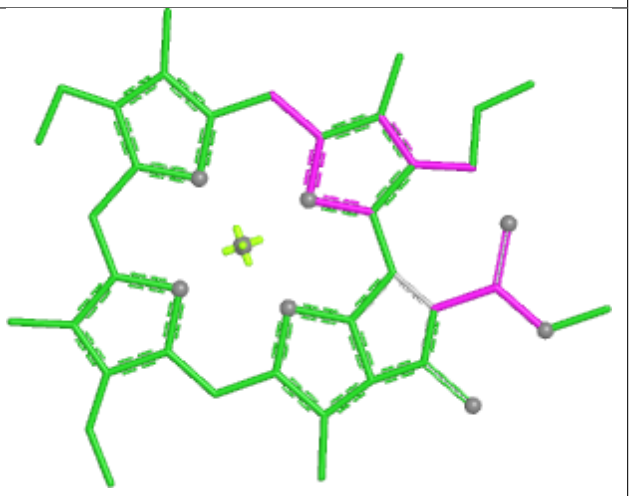
Ligand CLA BB 811	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA AA 819	
 Bond lengths	 Bond angles
 Torsions	 Rings

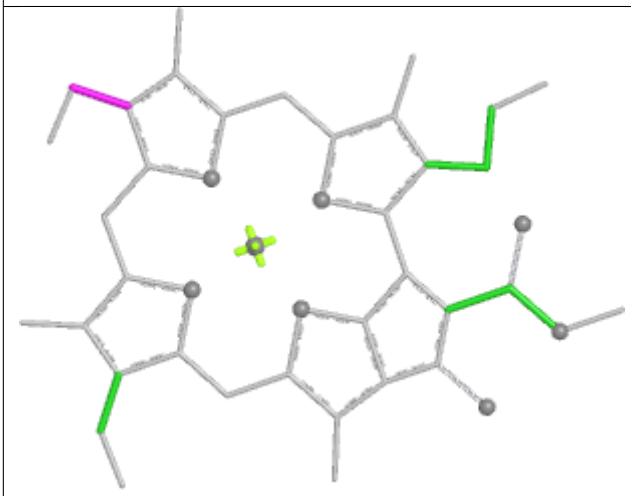
Ligand CLA A3 311



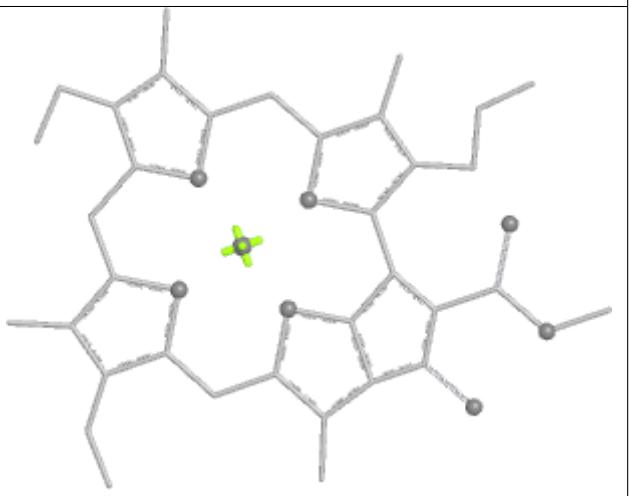
Bond lengths



Bond angles

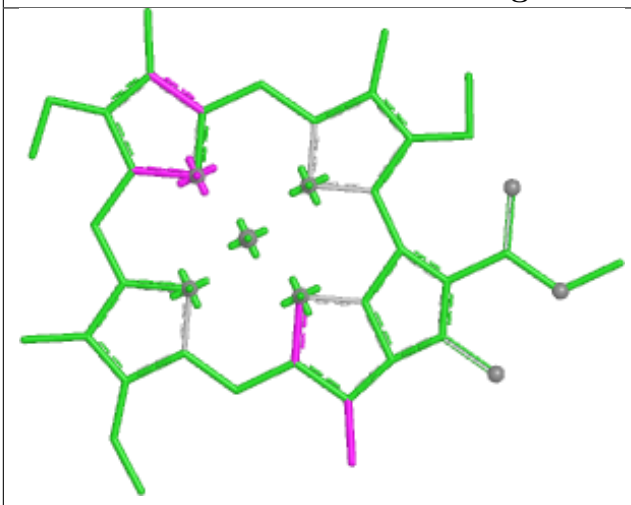


Torsions



Rings

Ligand CLA BA 815



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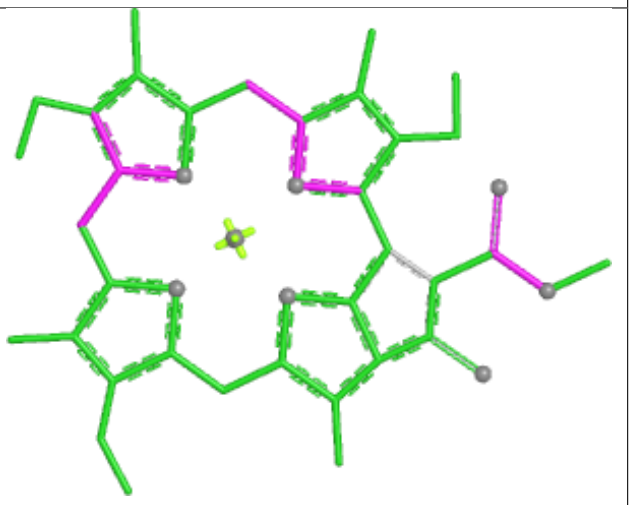
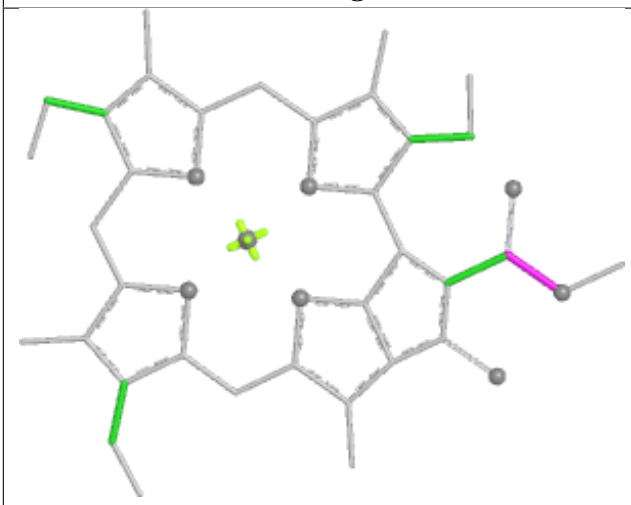


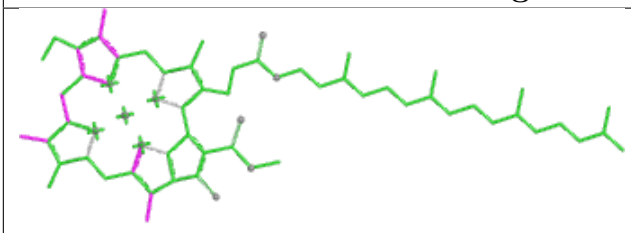
Bond angles



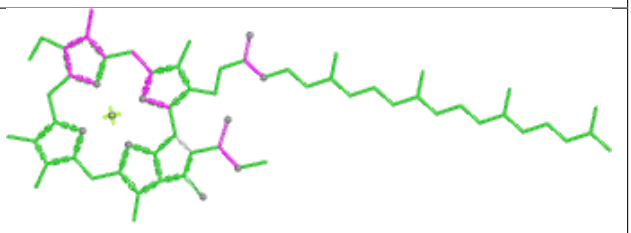
Torsions

Rings

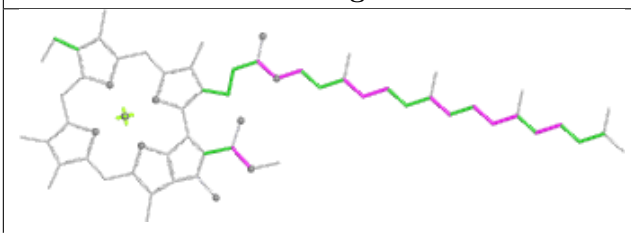
Ligand CLA BB 816



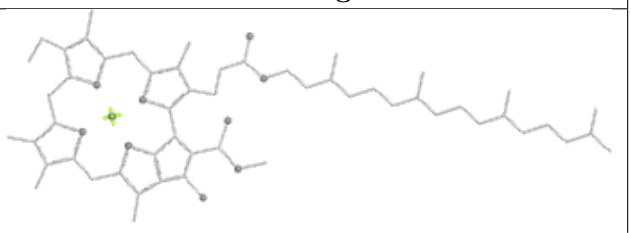
Bond lengths



Bond angles

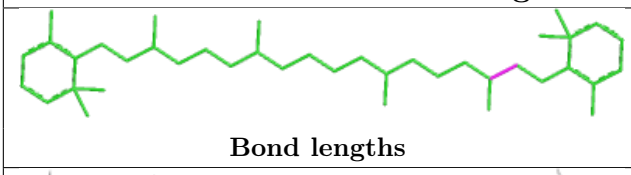


Torsions

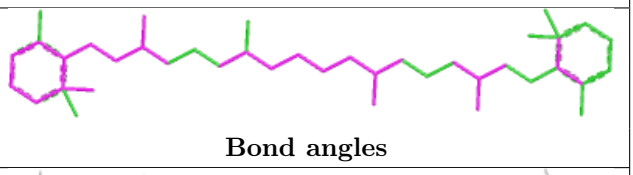


Rings

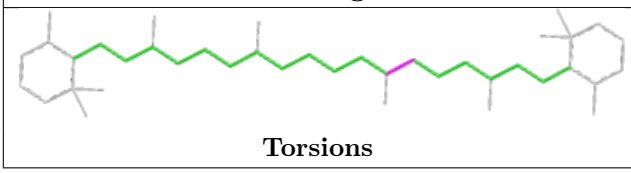
Ligand BCR AJ 101



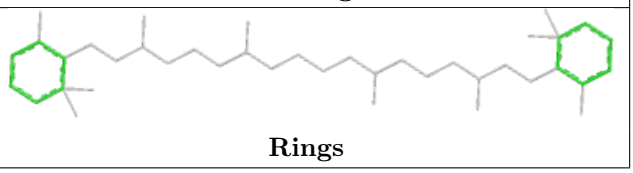
Bond lengths



Bond angles

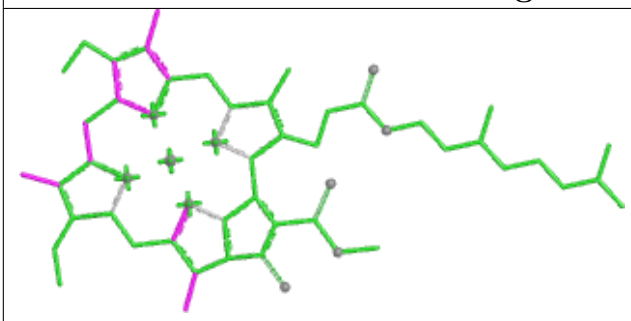


Torsions

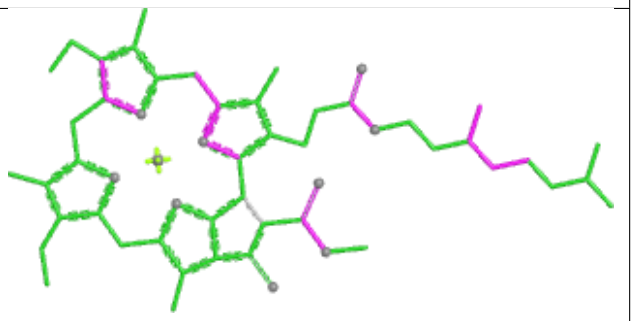


Rings

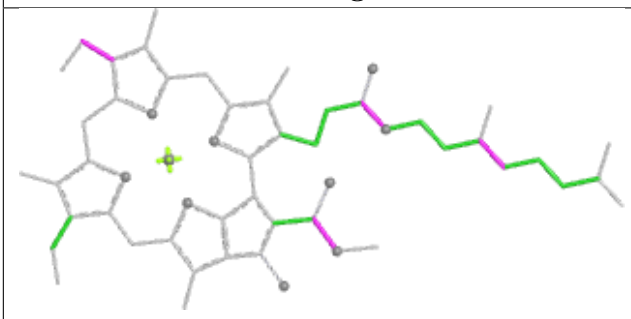
Ligand CLA B2 609



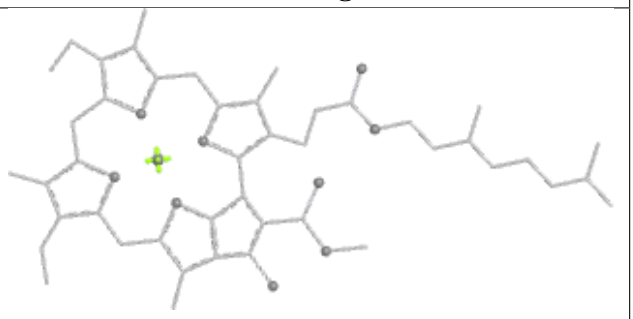
Bond lengths



Bond angles

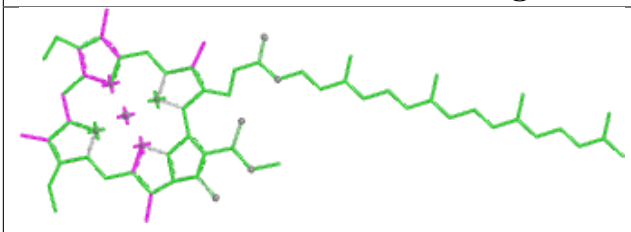


Torsions

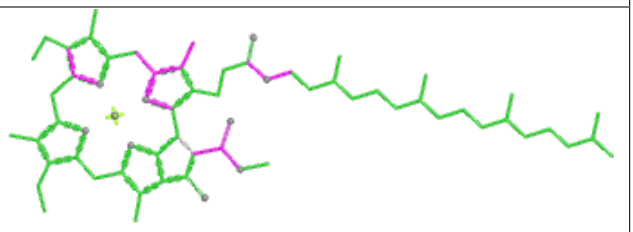


Rings

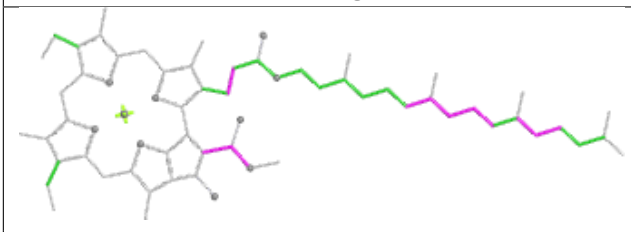
Ligand CLA AB 825



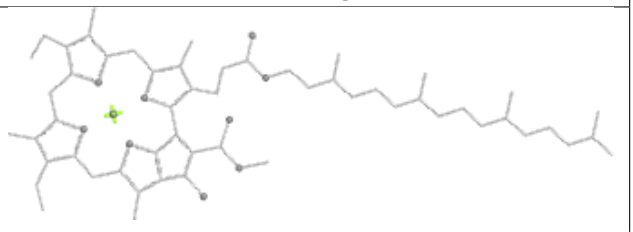
Bond lengths



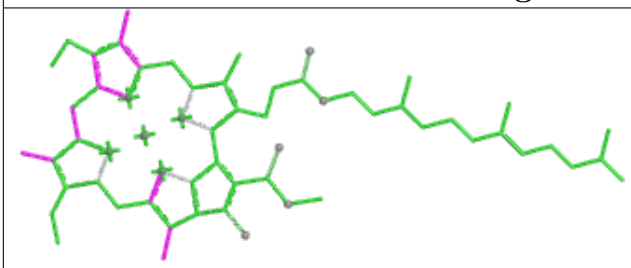
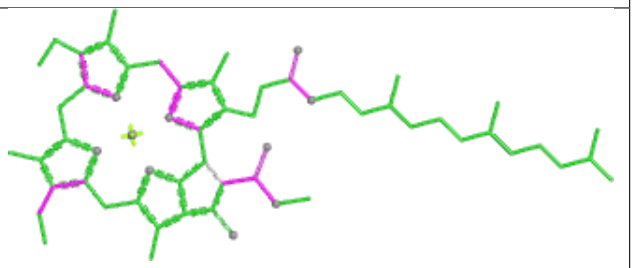
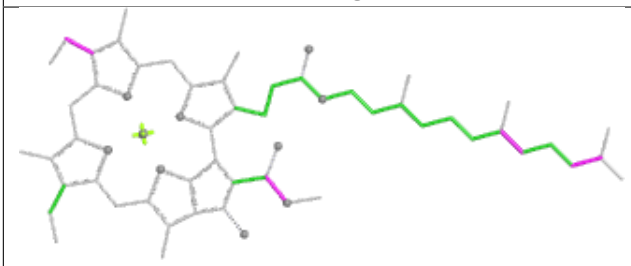
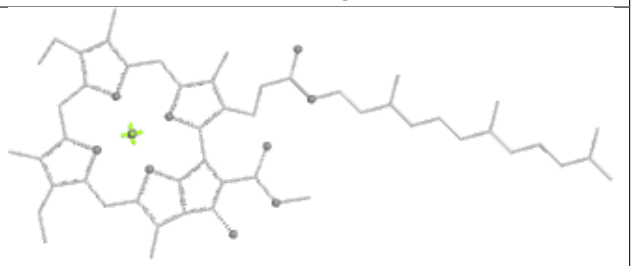
Bond angles



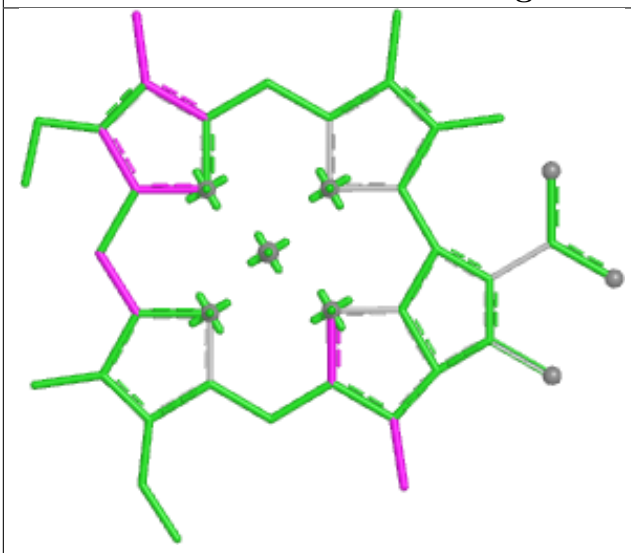
Torsions



Rings

Ligand CLA A4 301	
	
Bond lengths	**Bond angles**
	
Torsions	**Rings**

Ligand CLA B3 312



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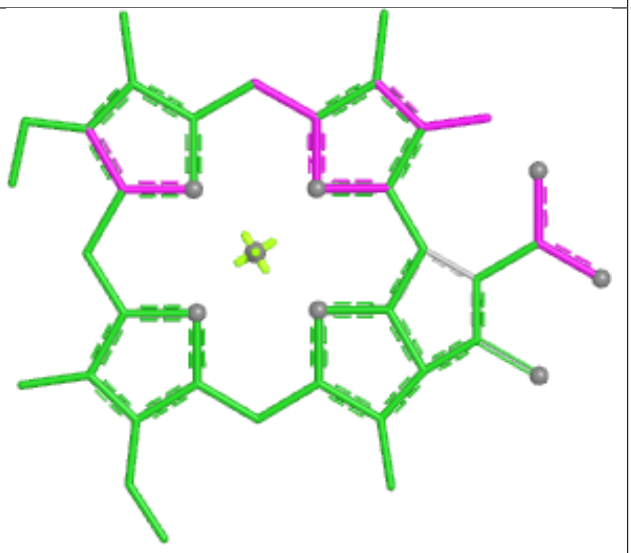
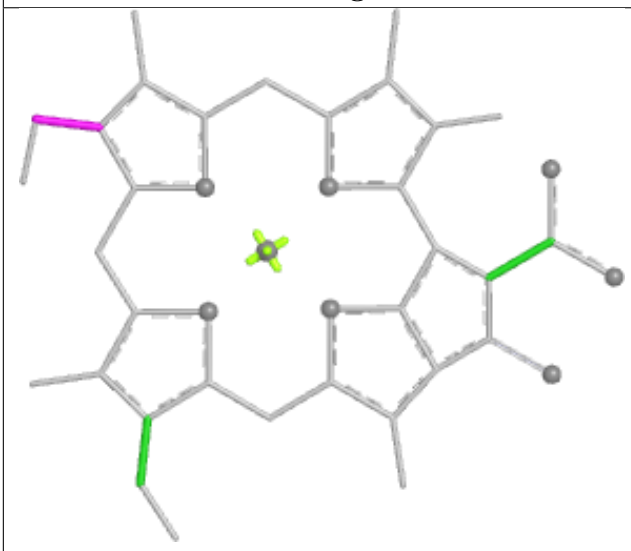


Bond angles



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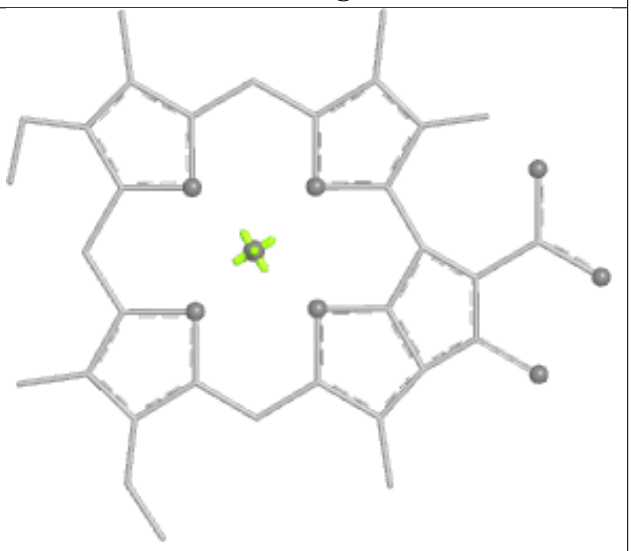
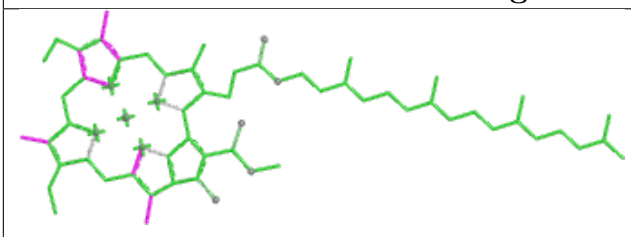


Rings

Ligand CLA AA 830



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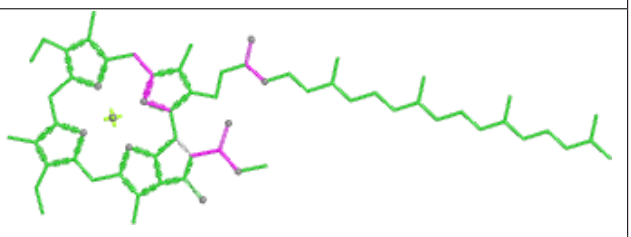
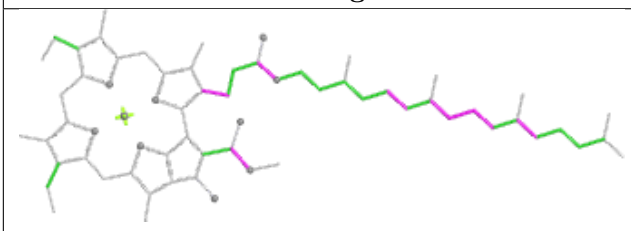
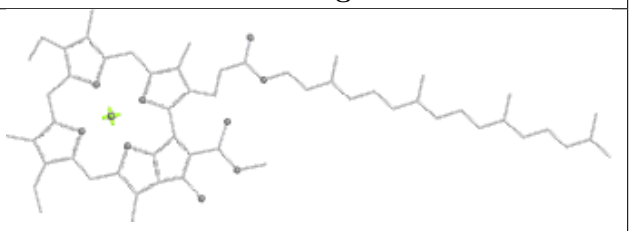


Bond angles

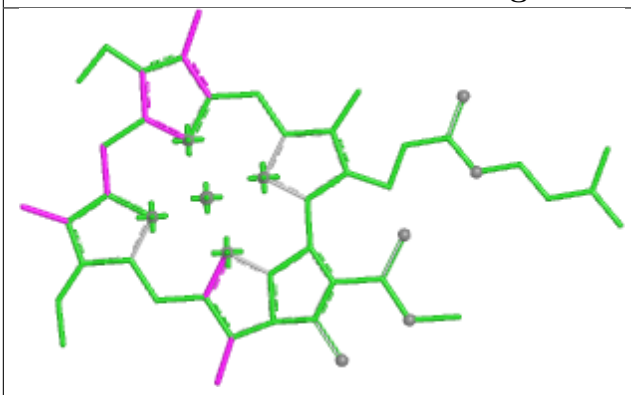


Torsions



Rings

Ligand CLA AA 809



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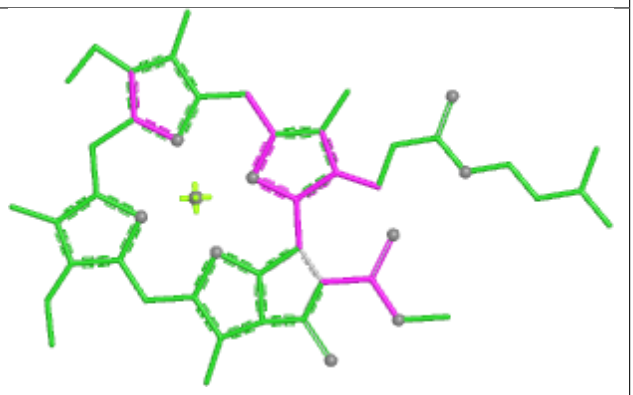
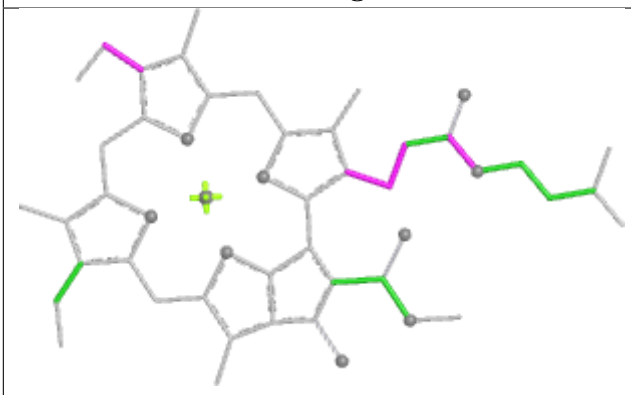
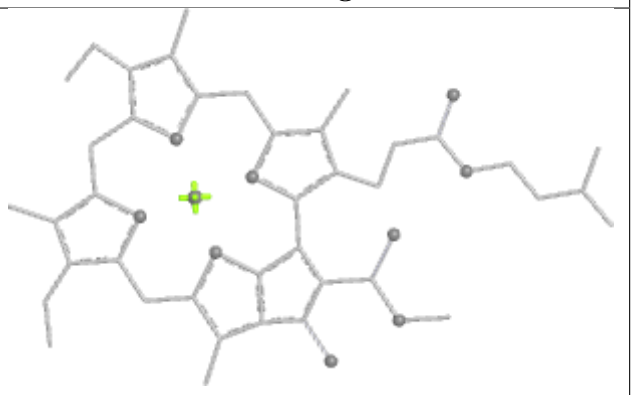


Bond angles

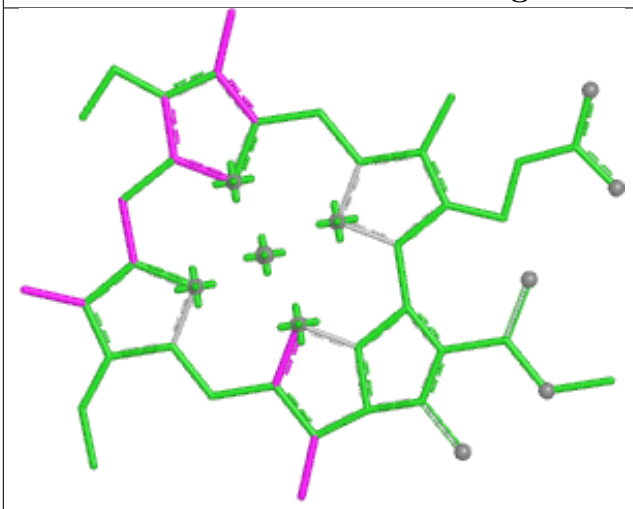


Torsions

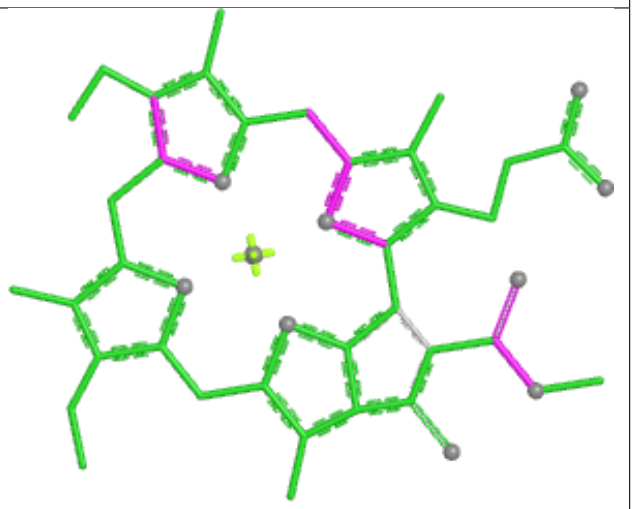


Rings

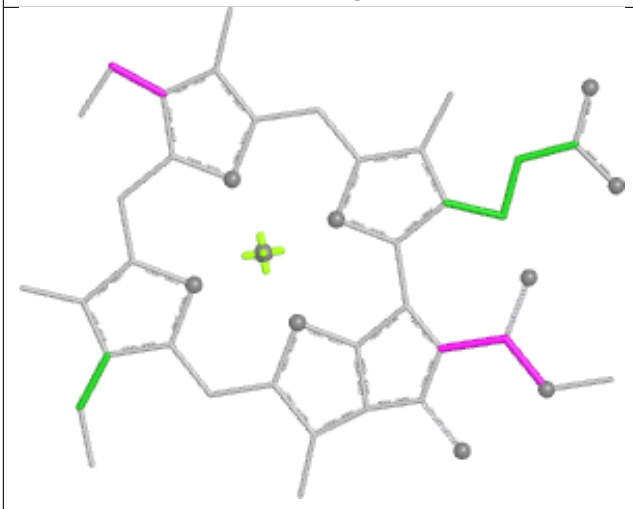
Ligand CLA BA 814



Bond lengths



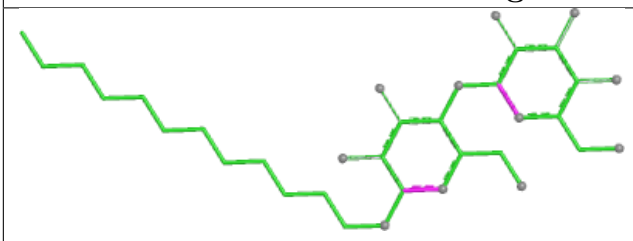
Bond angles



Torsions

Rings

Ligand LMU AB 853



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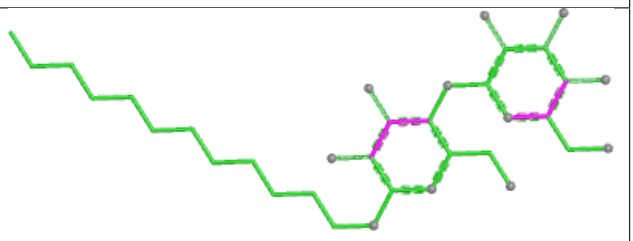
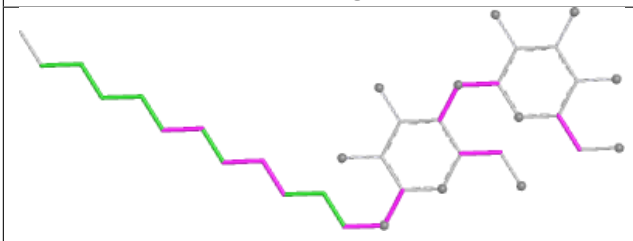


Bond angles



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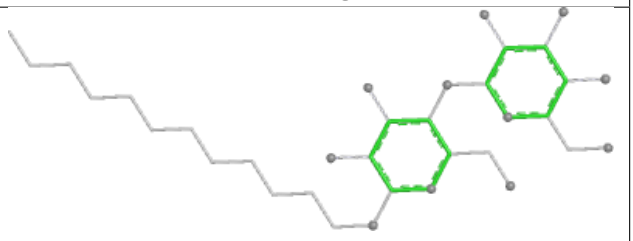
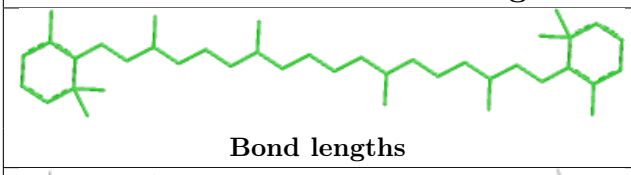


Rings

Ligand BCR AB 846



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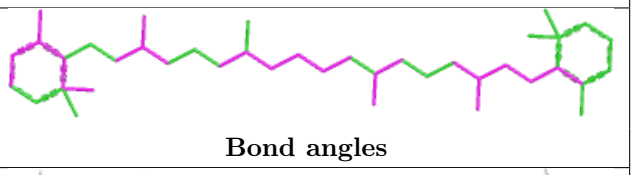
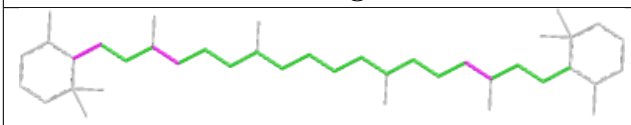


Bond angles



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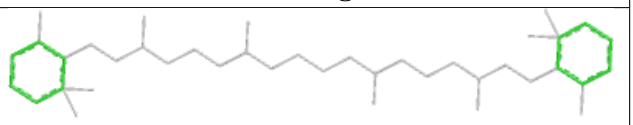
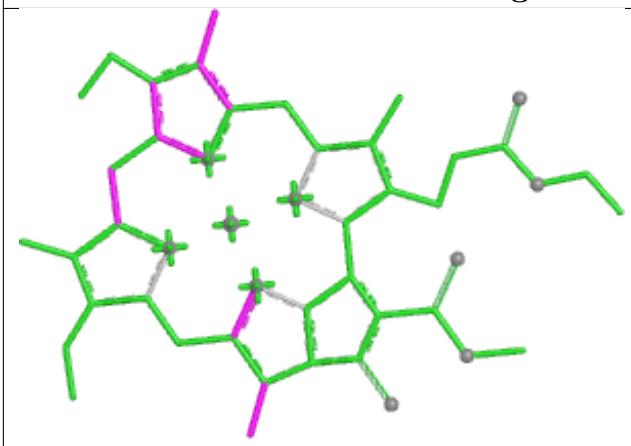


Rings

Ligand CLA AB 822



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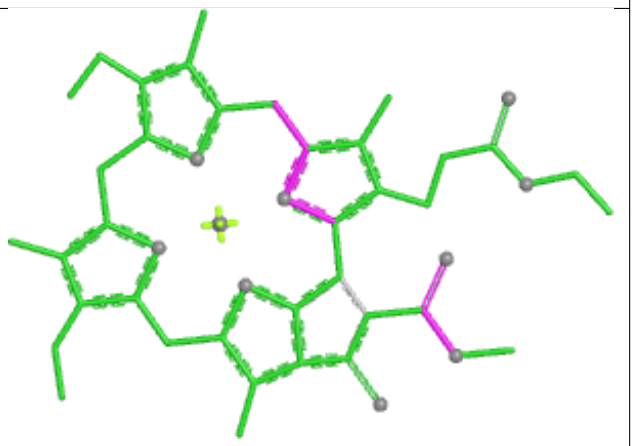
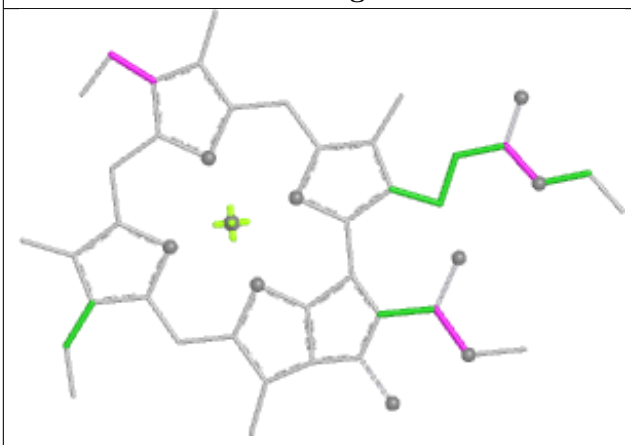


Bond angles



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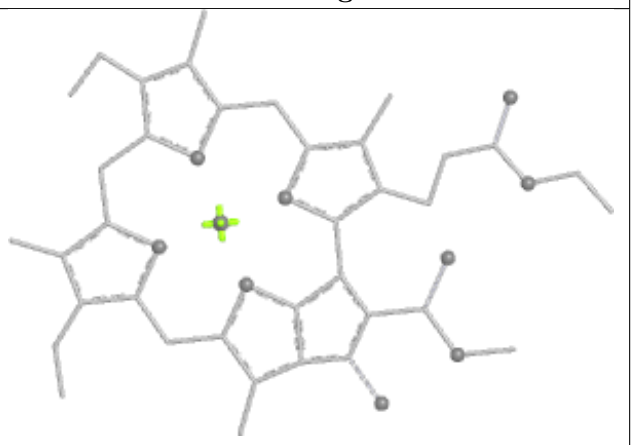
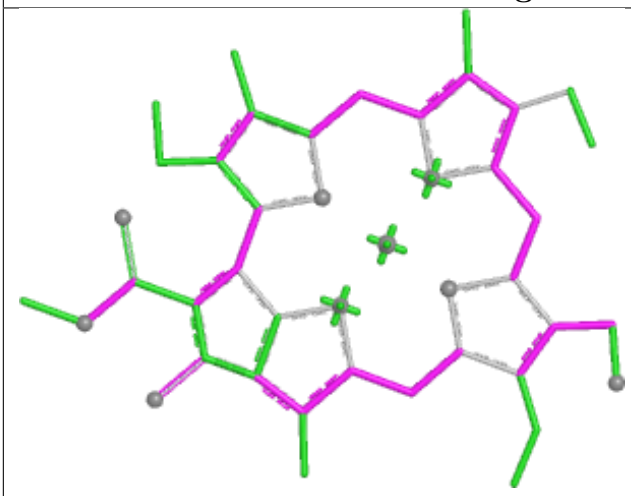


Rings

Ligand CHL B2 614



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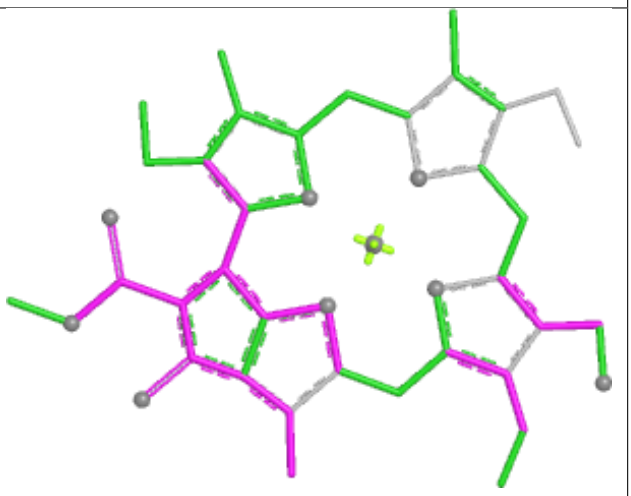
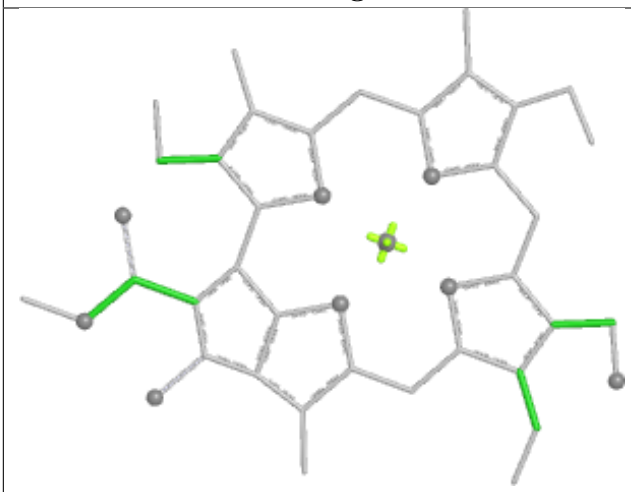


Bond angles



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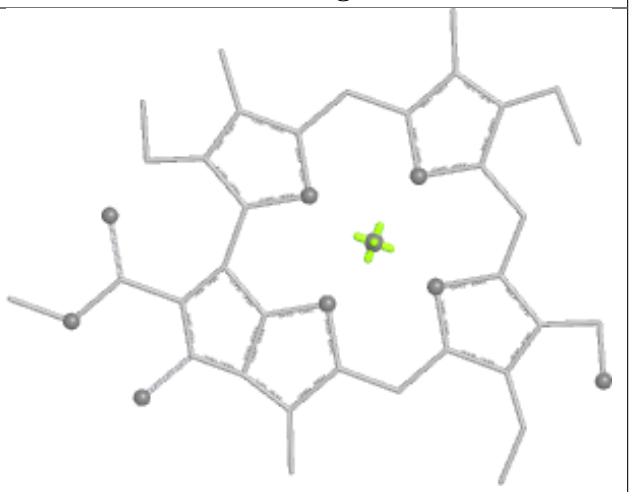
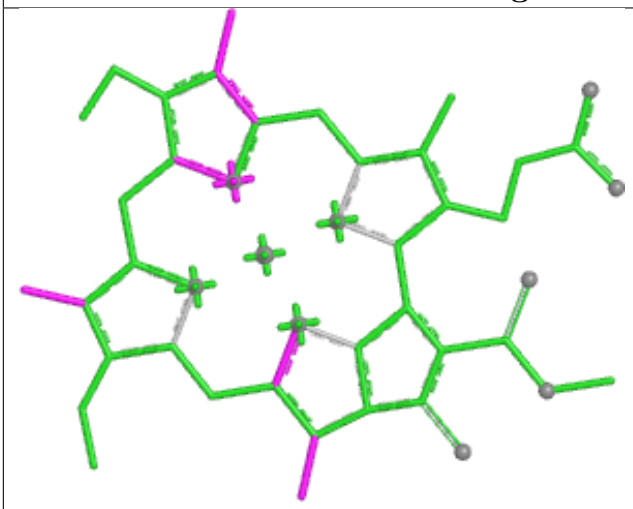


Rings

Ligand CLA BA 820



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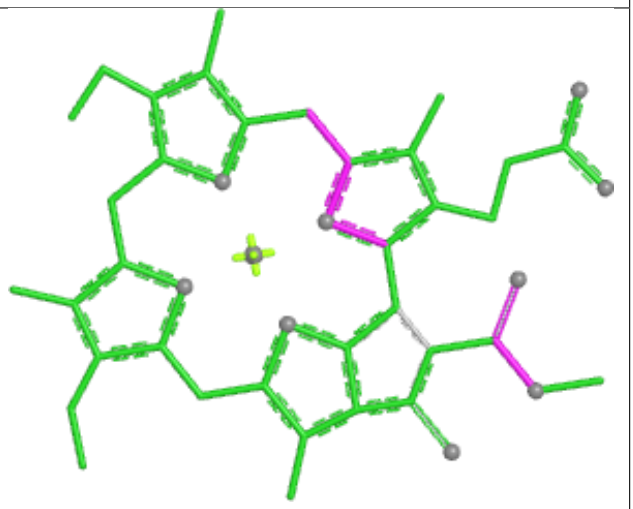
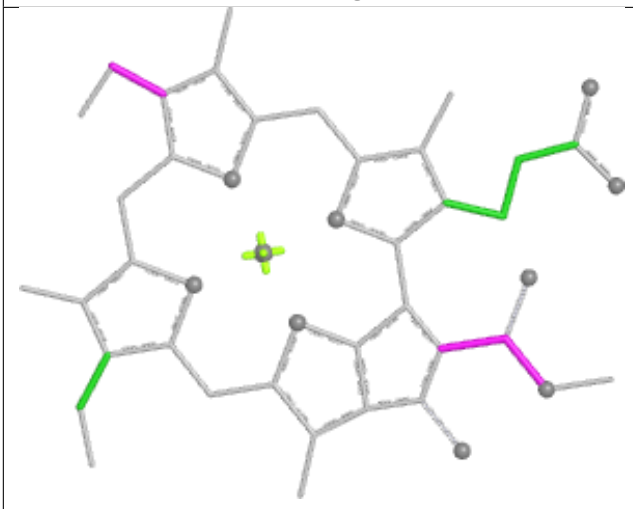


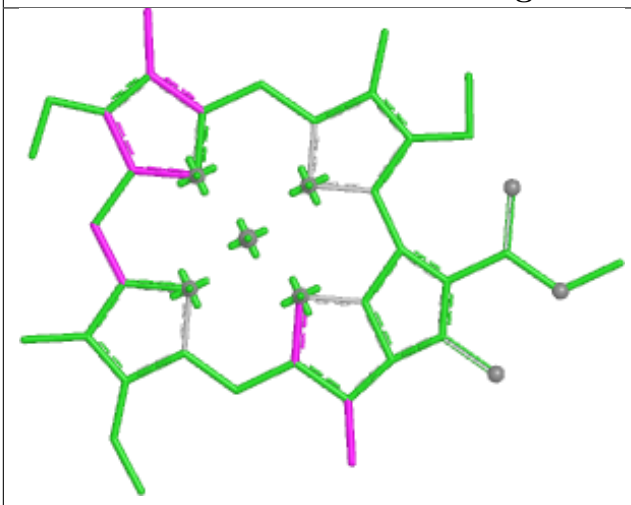
Bond angles



Torsions

Rings

Ligand CLA BJ 102



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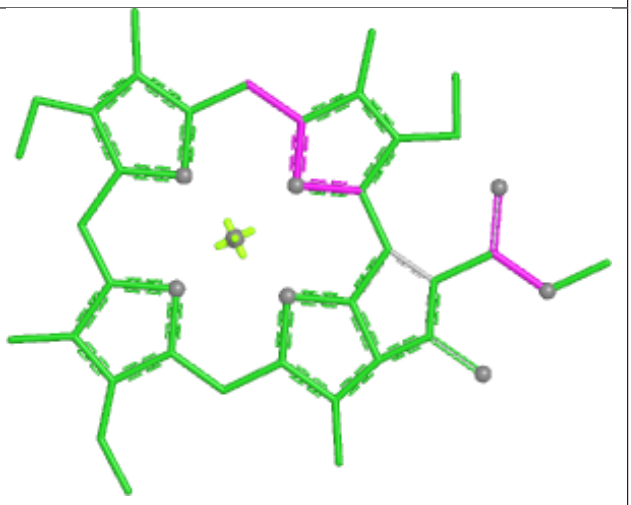
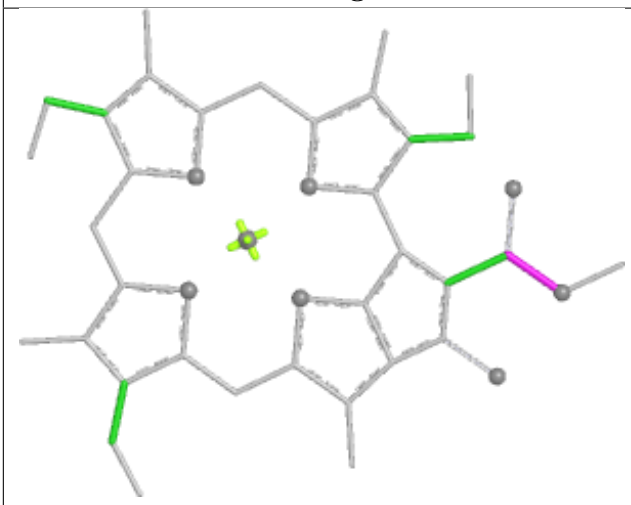


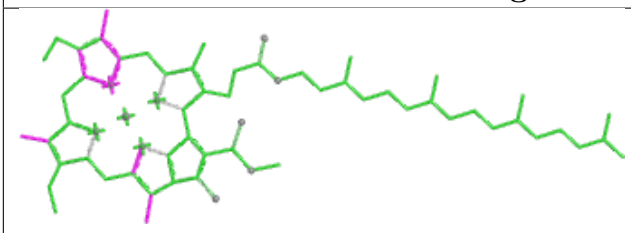
Bond angles



Torsions

Rings

Ligand CLA AA 825



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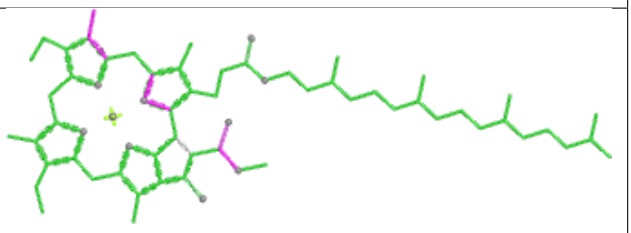
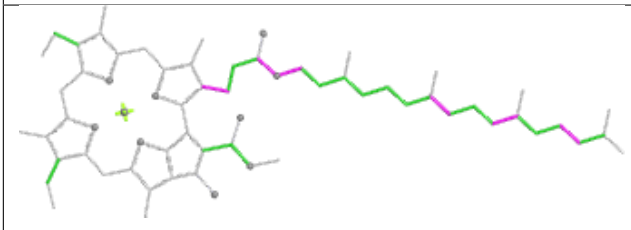


Bond angles



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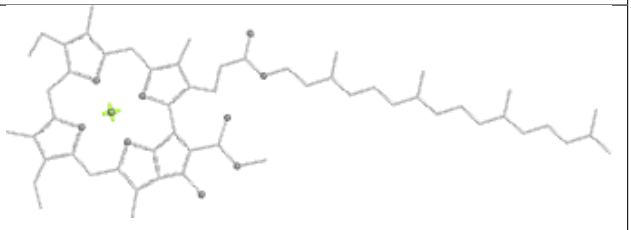
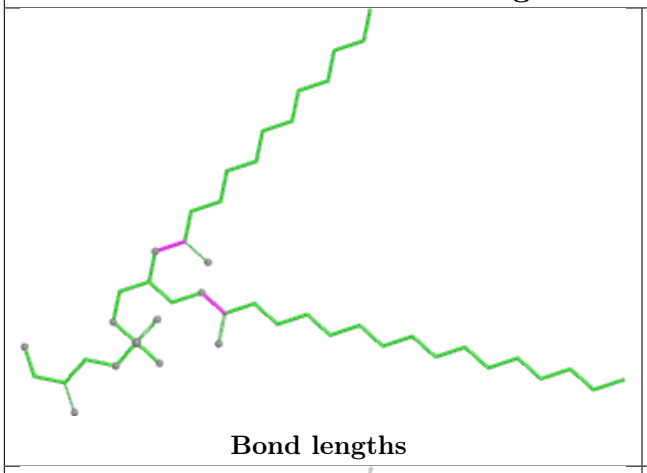


Rings

Ligand LHG BF 305



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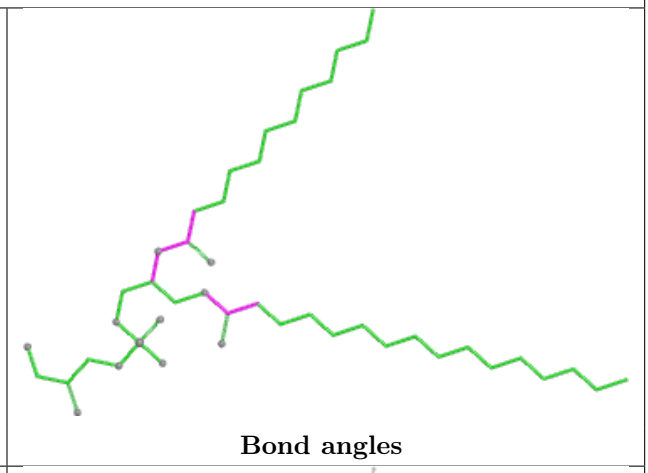
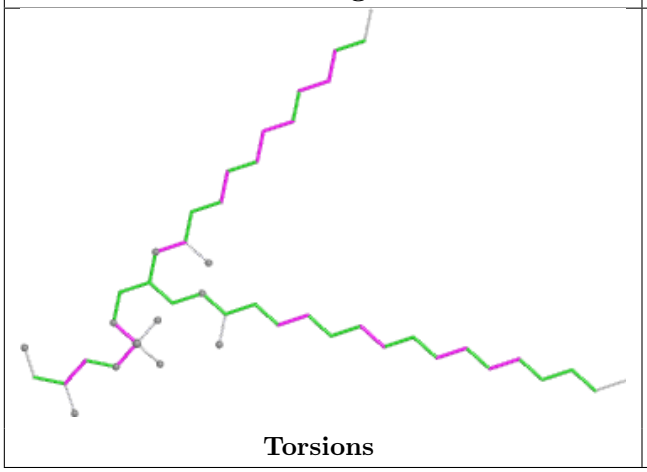


Bond angles



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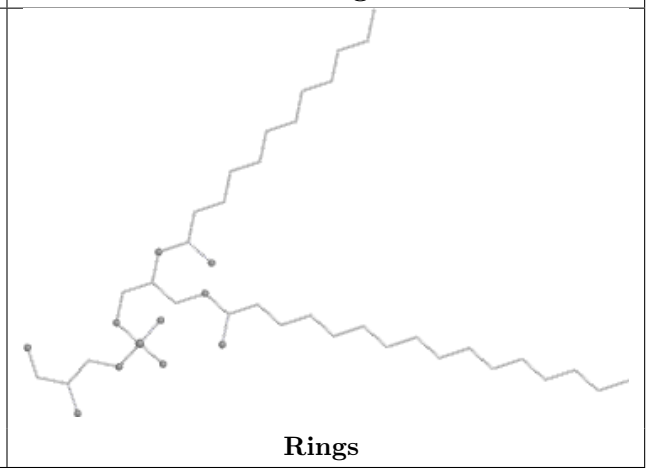
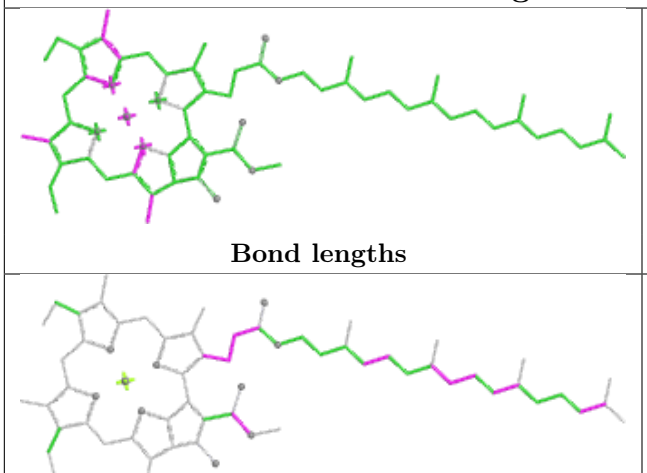
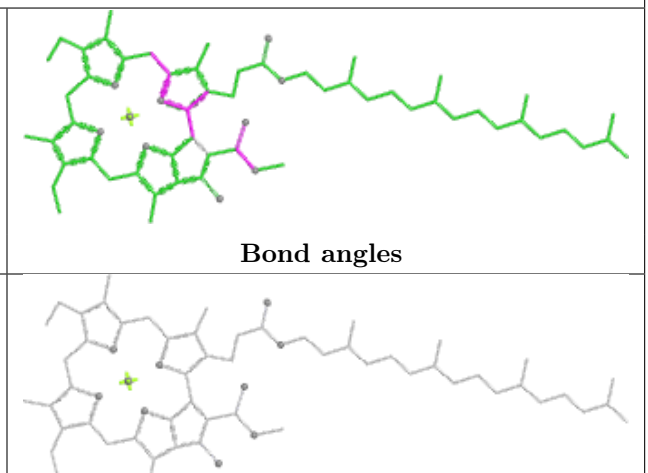


Rings

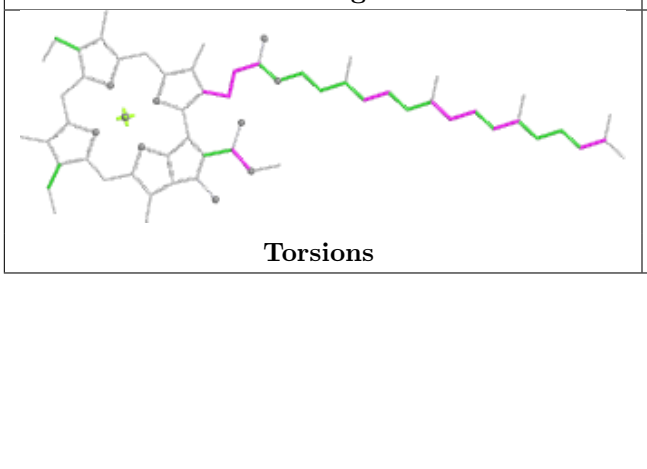
Ligand CLA AB 810



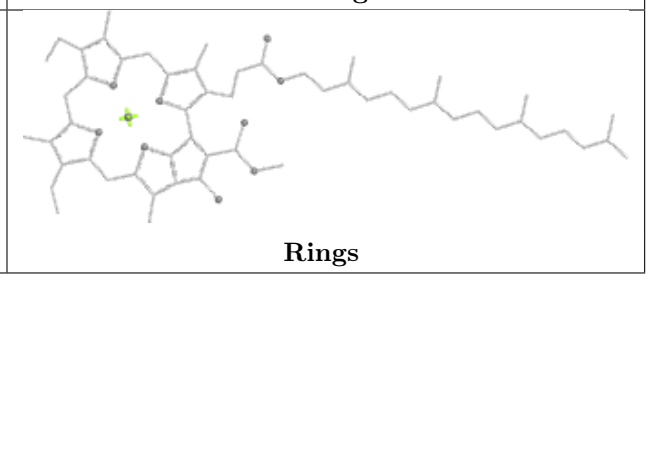
Bond lengths



Bond angles

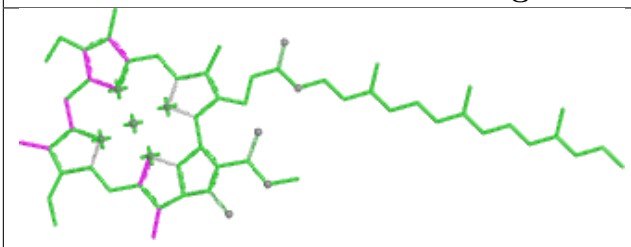


Torsions

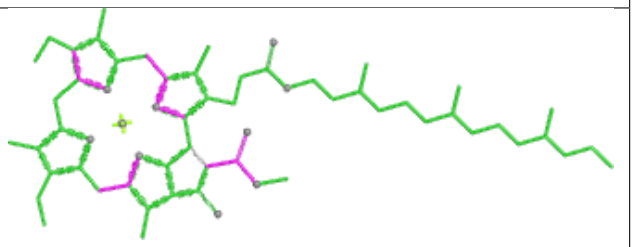


Rings

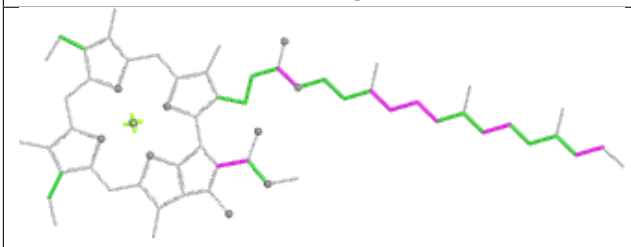
Ligand CLA BB 827



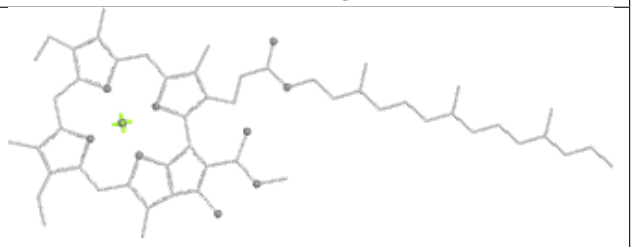
Bond lengths



Bond angles

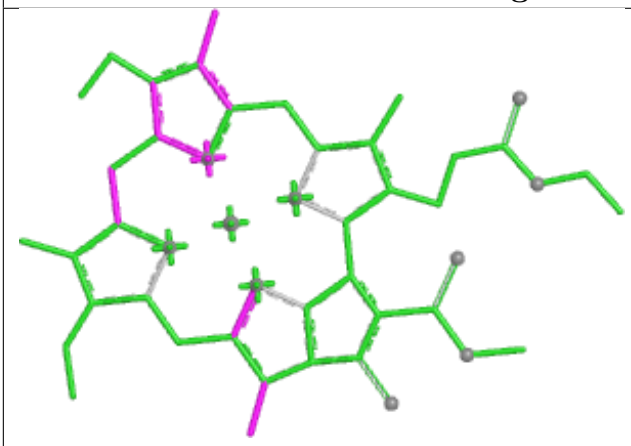


Torsions

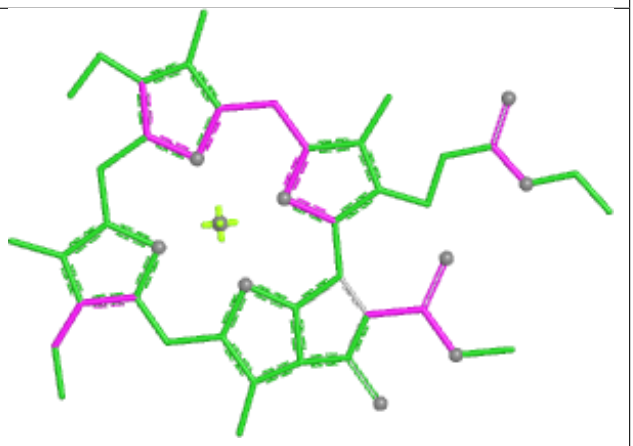


Rings

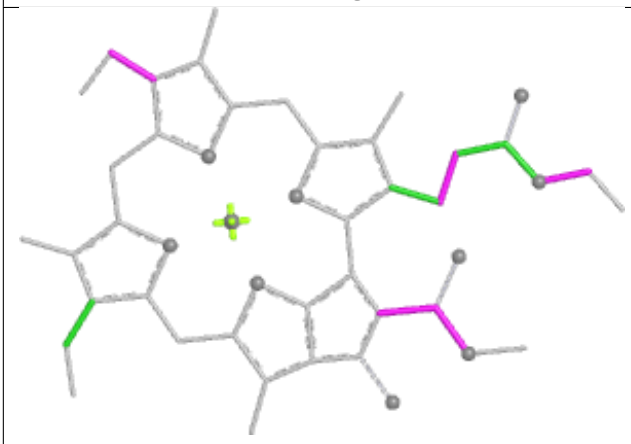
Ligand CLA BA 831



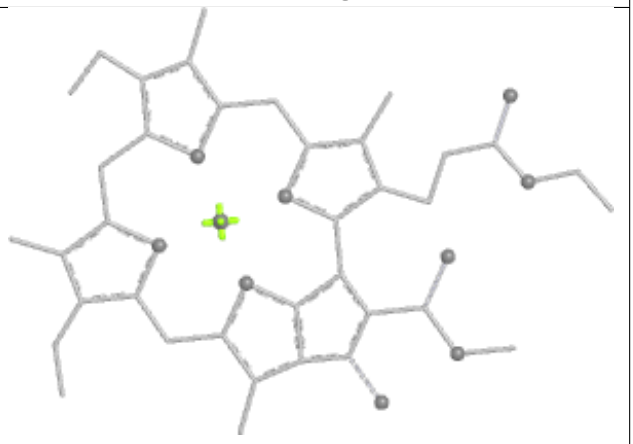
Bond lengths



Bond angles

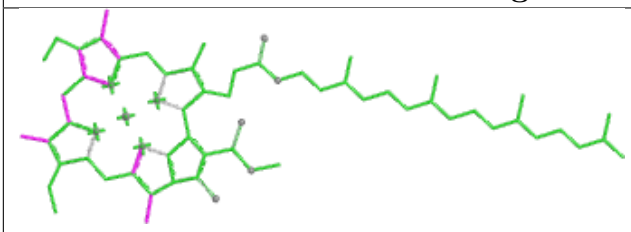


Torsions

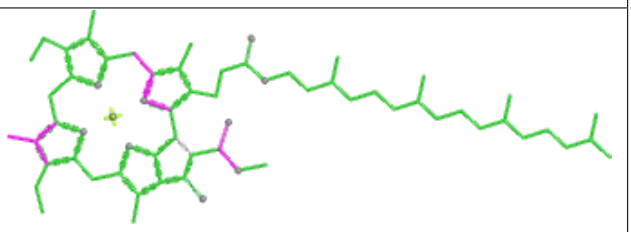


Rings

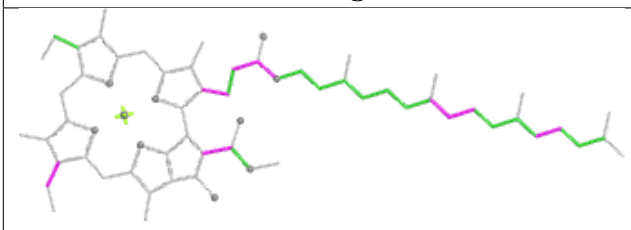
Ligand CLA AB 806



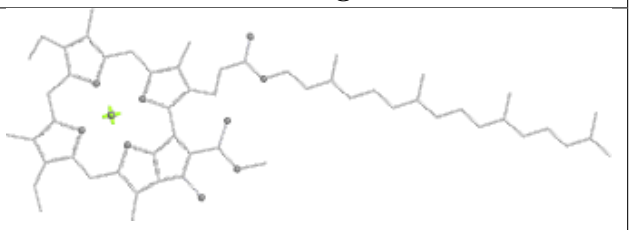
Bond lengths



Bond angles

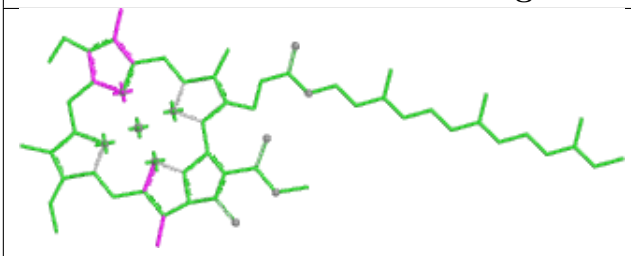


Torsions

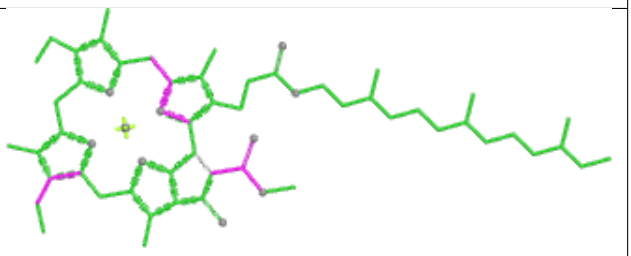


Rings

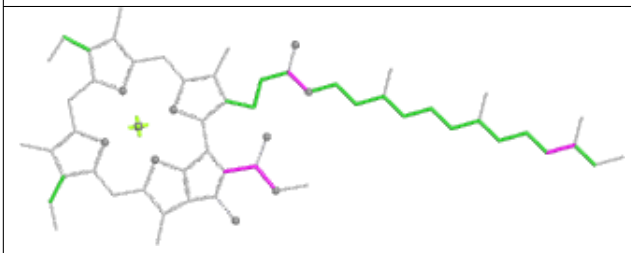
Ligand CLA B1 304



Bond lengths



Bond angles



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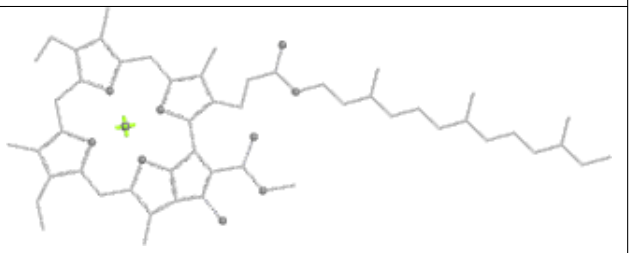
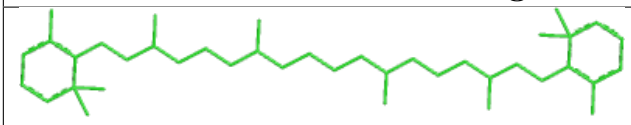


Rings

Ligand BCR AA 846



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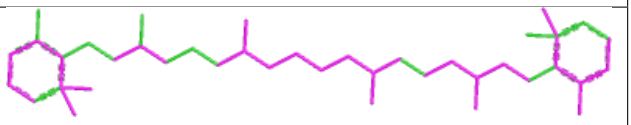
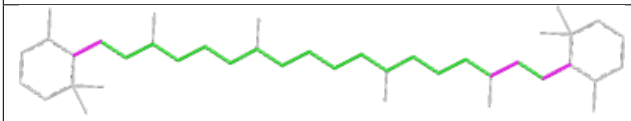


Bond angles



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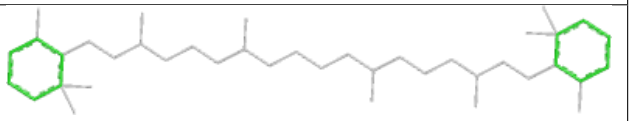
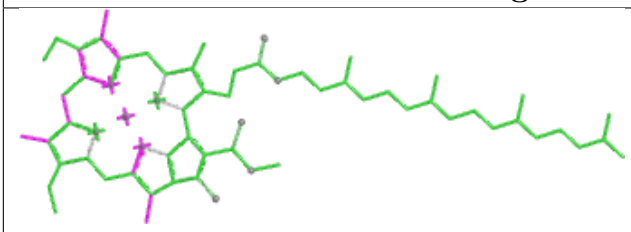
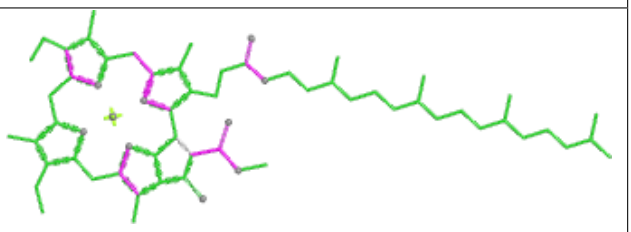


Rings

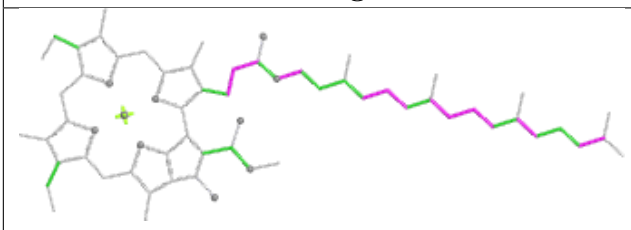
Ligand CLA BA 829



Bond lengths



Bond angles



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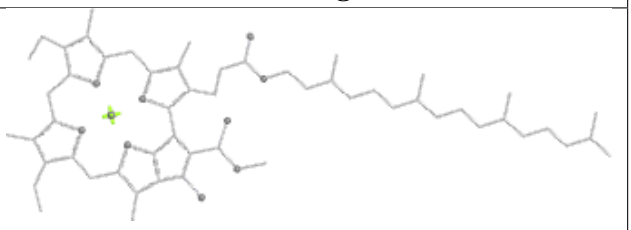
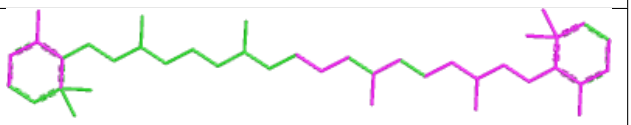


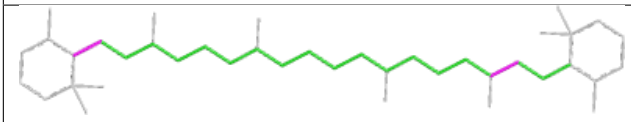
Rings

Ligand BCR A3 318

Bond lengths



Bond angles



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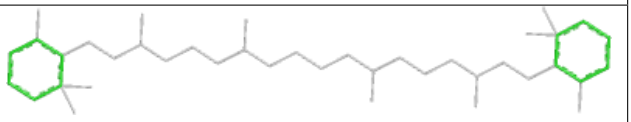
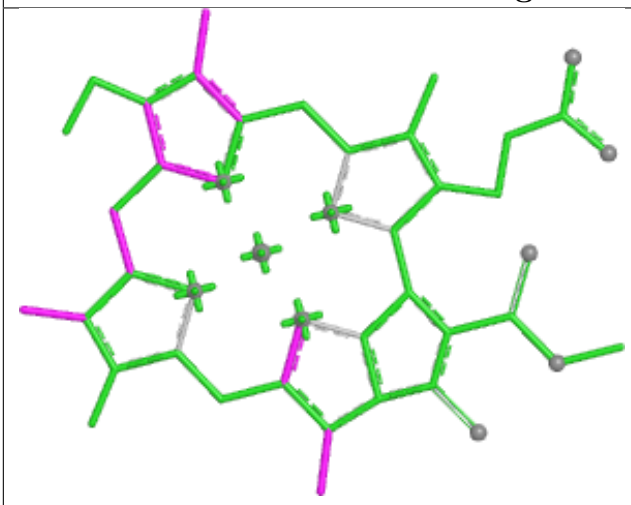
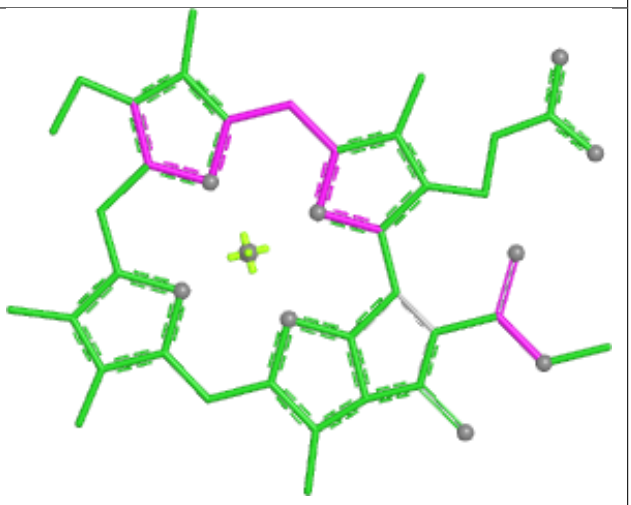


Rings

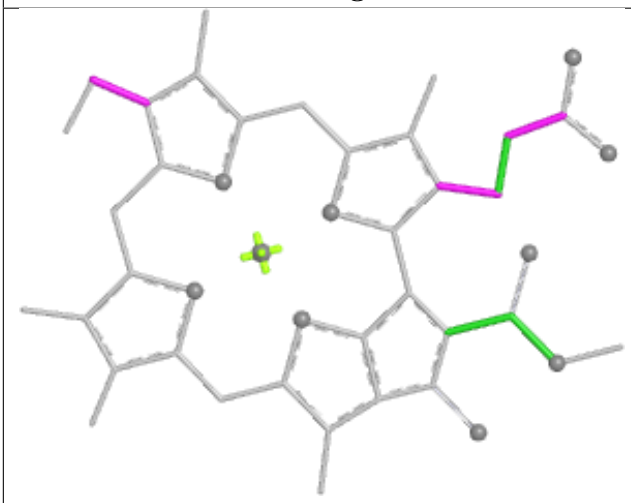
Ligand CLA B5 608



Bond lengths



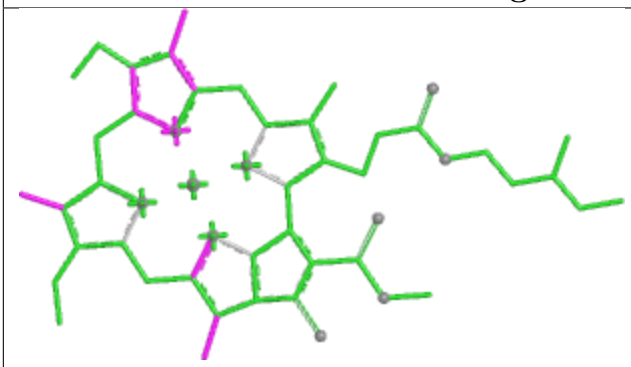
Bond angles



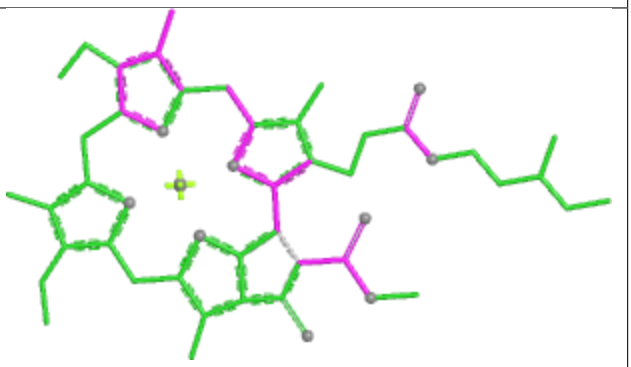
Torsions

Rings

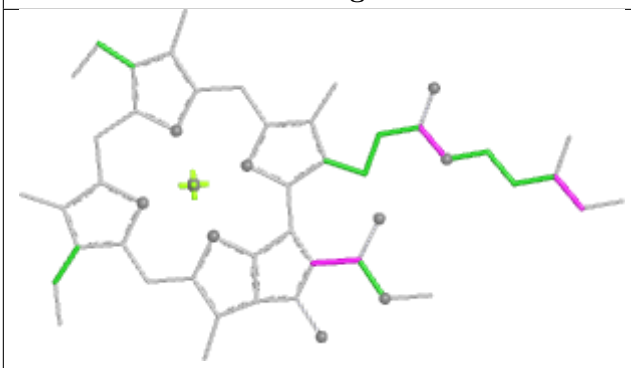
Ligand CLA AA 837



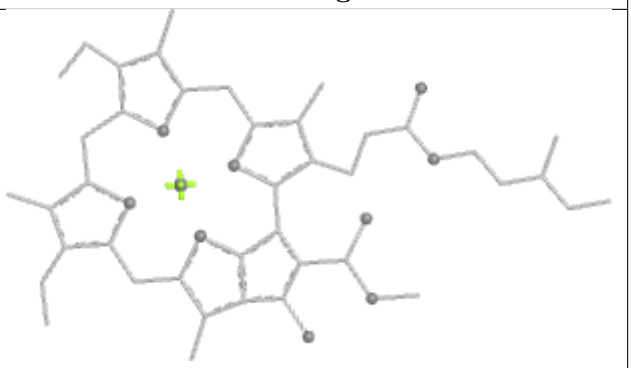
Bond lengths



Bond angles

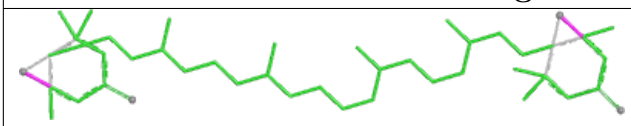


Torsions

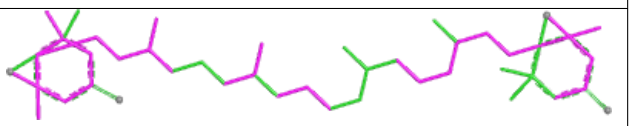


Rings

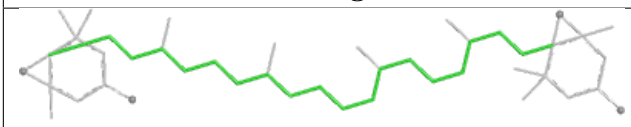
Ligand XAT B5 615



Bond lengths



Bond angles



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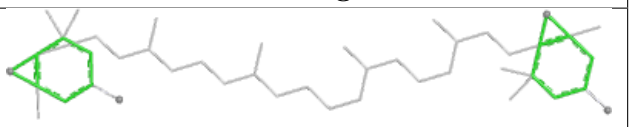
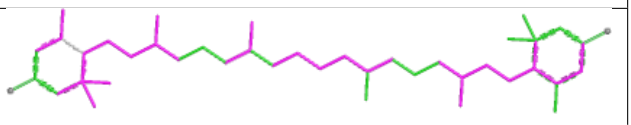


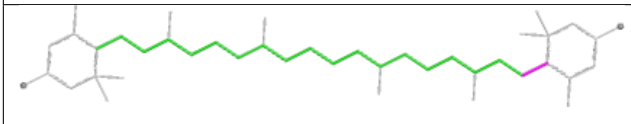
Rings

Ligand LUT A4 315

Bond lengths



Bond angles



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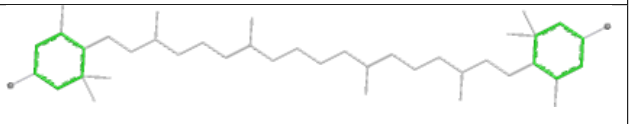
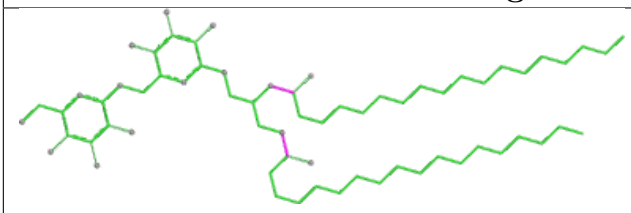
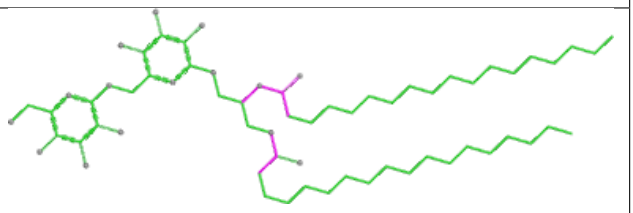


Rings

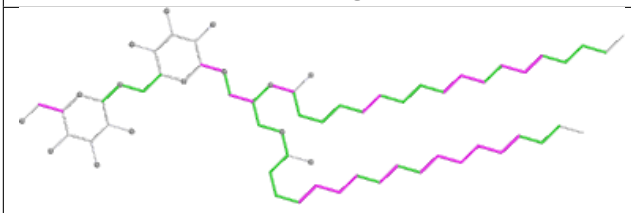
Ligand DGD AB 851



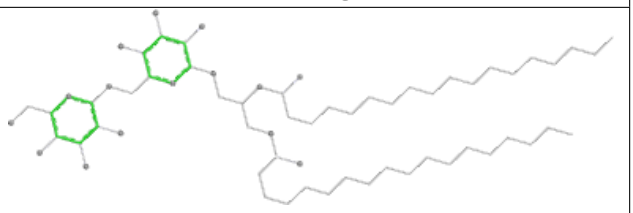
Bond lengths



Bond angles

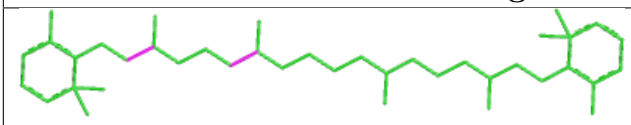


Torsions

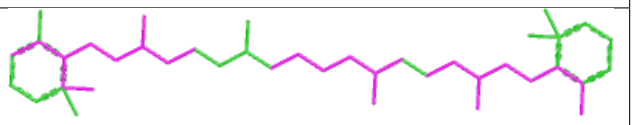


Rings

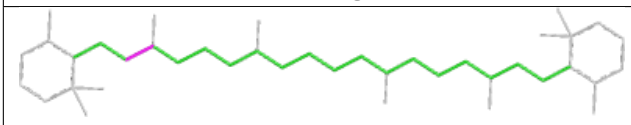
Ligand BCR AA 845



Bond lengths



Bond angles



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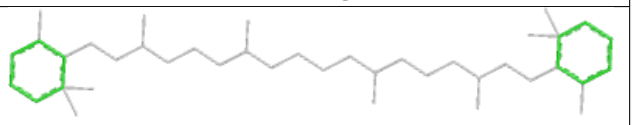
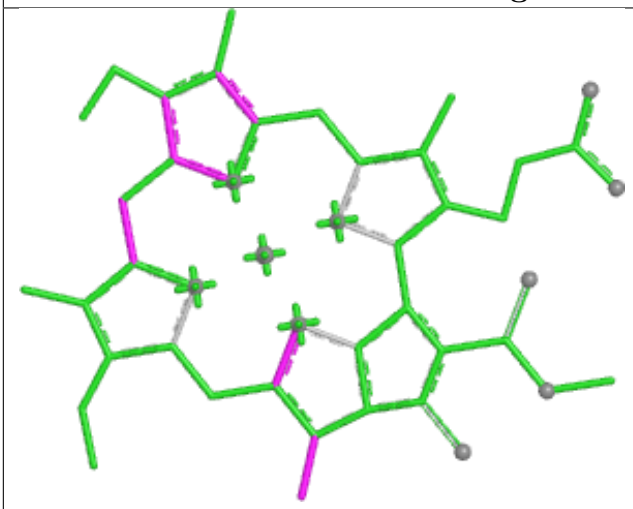
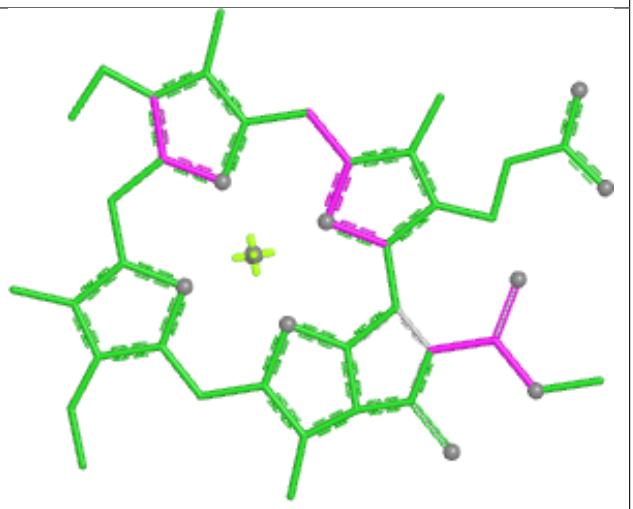


Rings

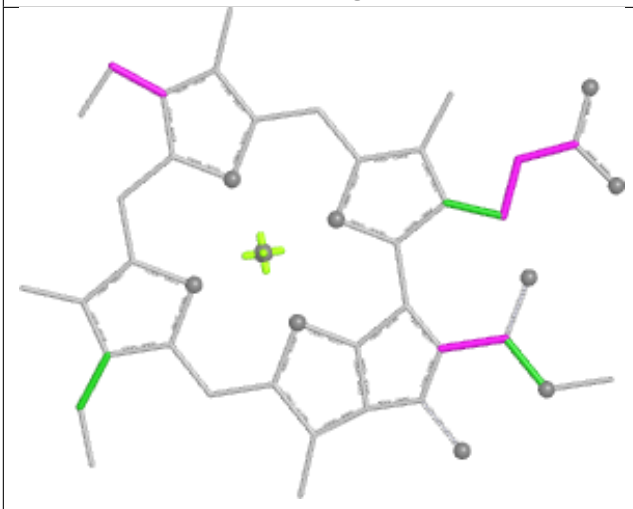
Ligand CLA BK 202



Bond lengths



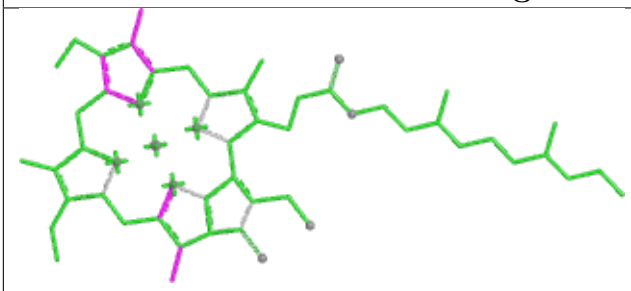
Bond angles



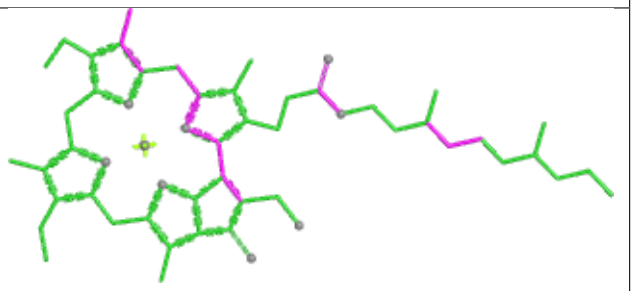
Torsions

Rings

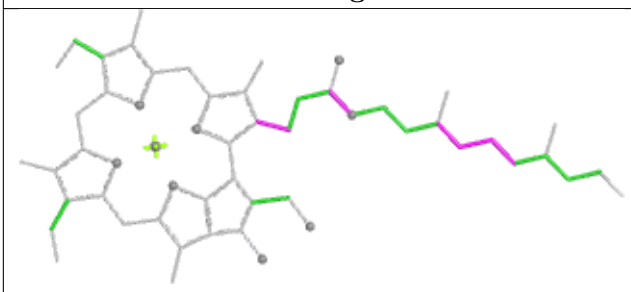
Ligand CLA BF 301



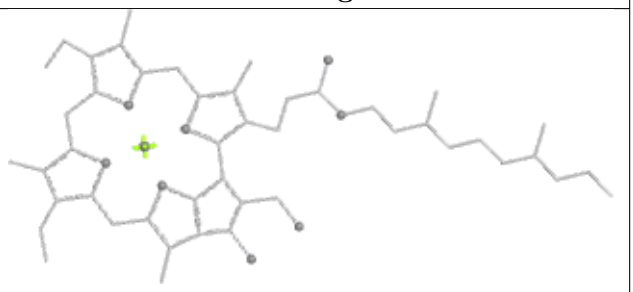
Bond lengths



Bond angles

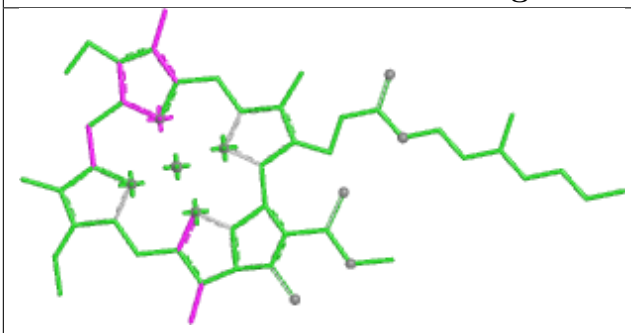


Torsions

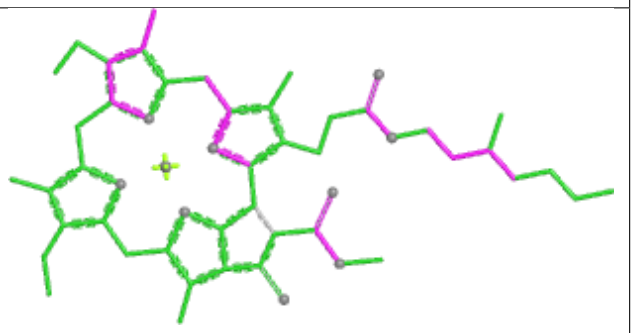


Rings

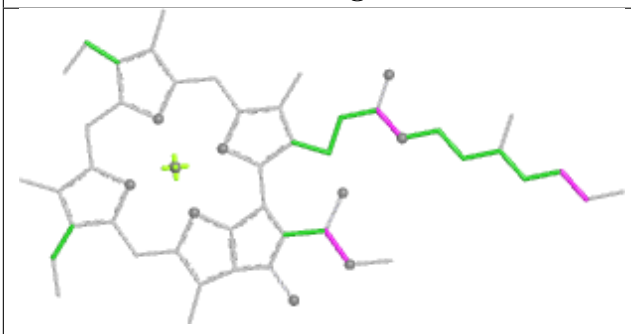
Ligand CLA BA 826



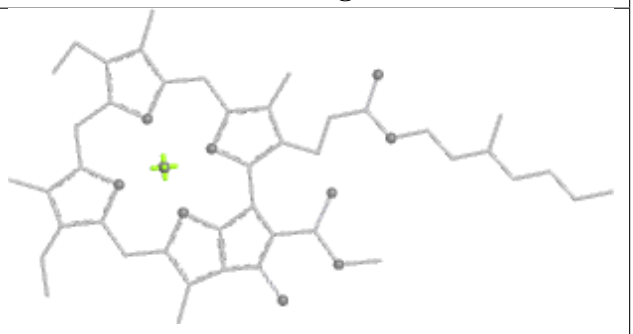
Bond lengths



Bond angles

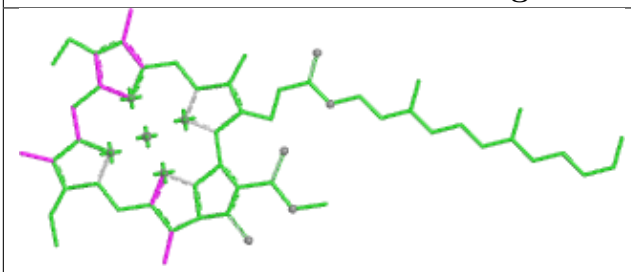


Torsions



Rings

Ligand CLA AB 818



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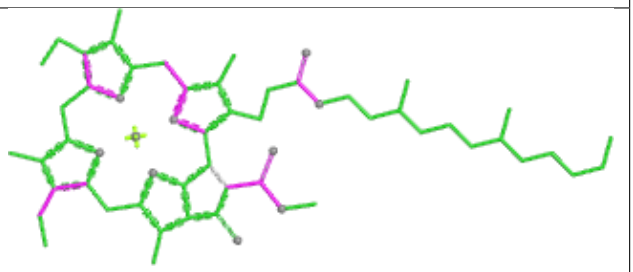
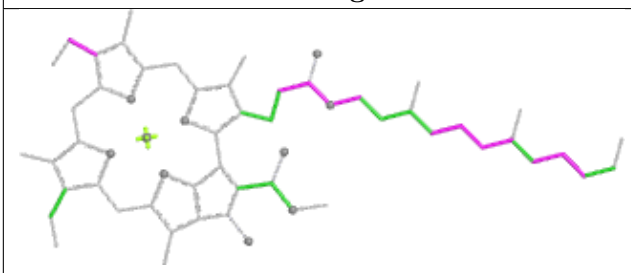
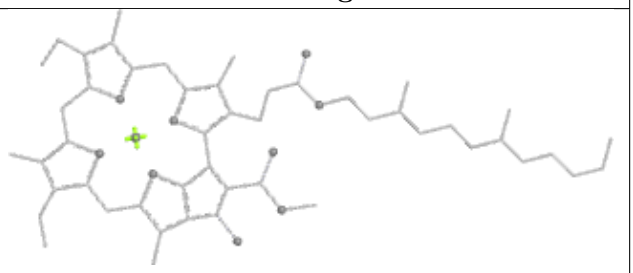


Bond angles

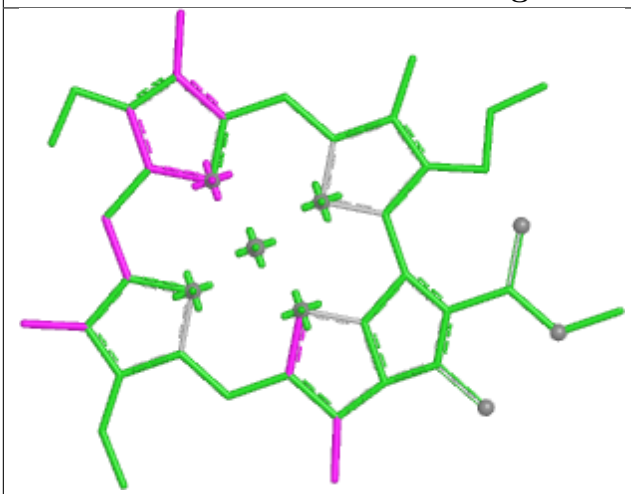


Torsions

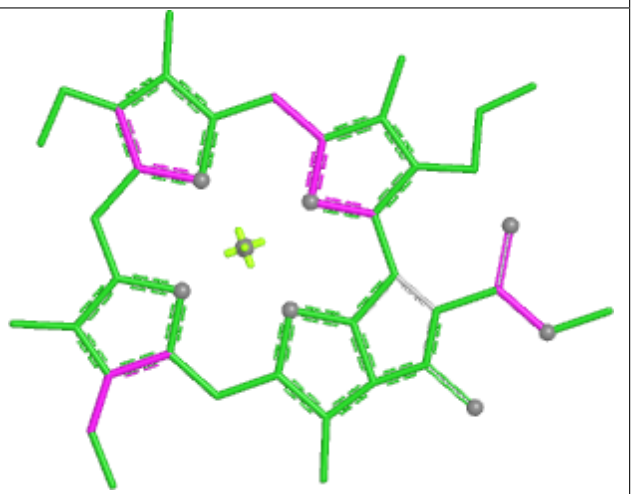


Rings

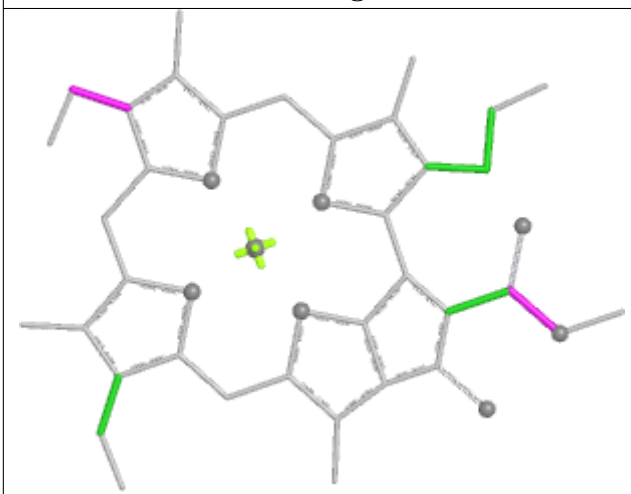
Ligand CLA AB 831



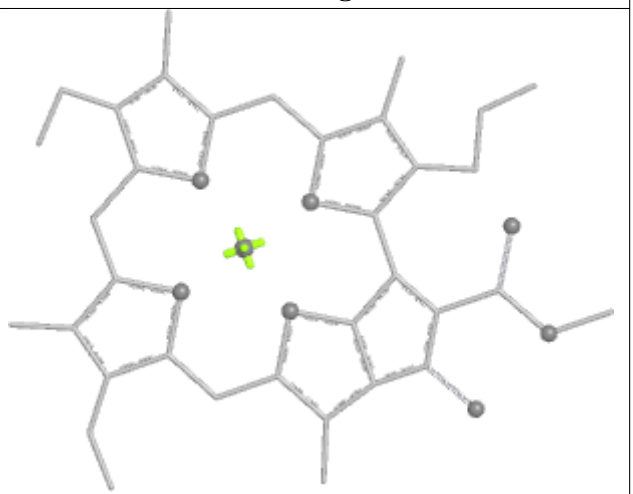
Bond lengths



Bond angles

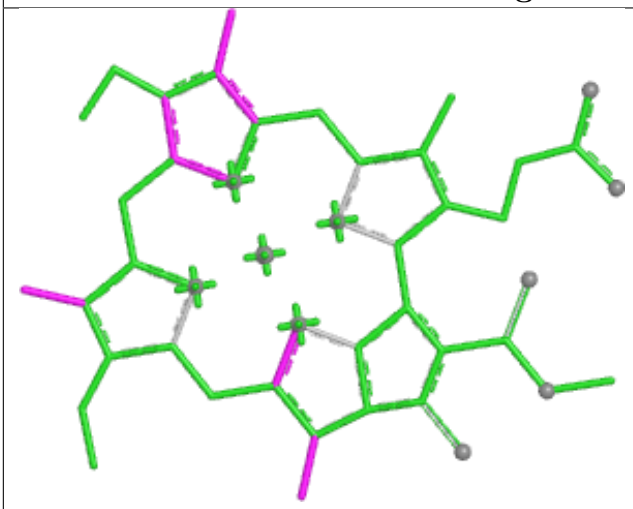


Torsions



Rings

Ligand CLA B1 313



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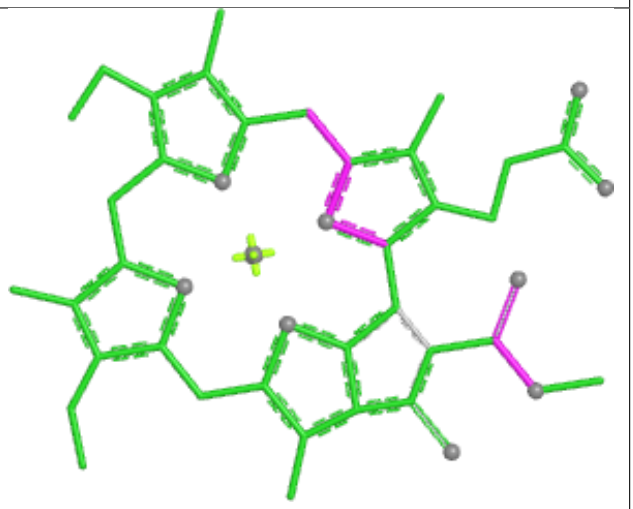
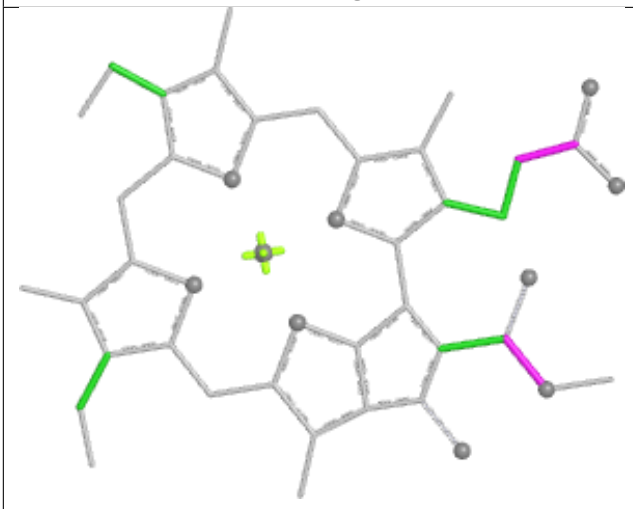


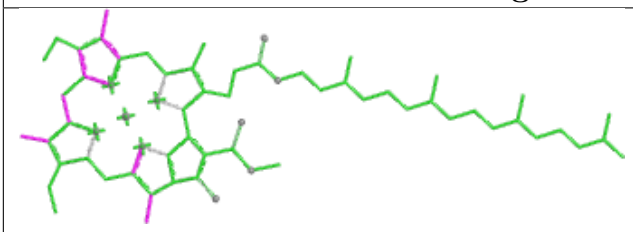
Bond angles



Torsions

Rings

Ligand CLA BB 810



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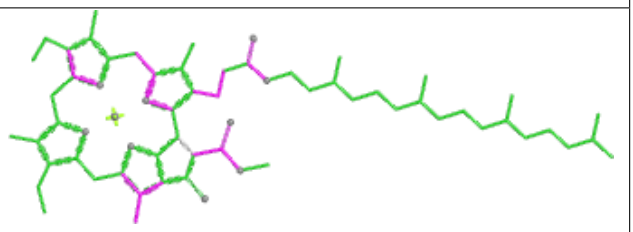
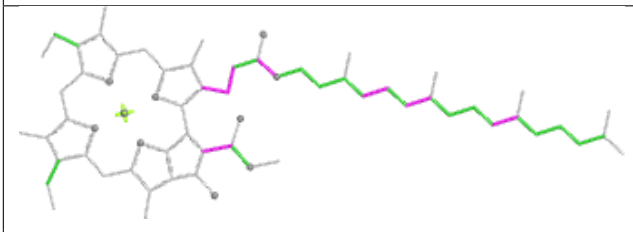
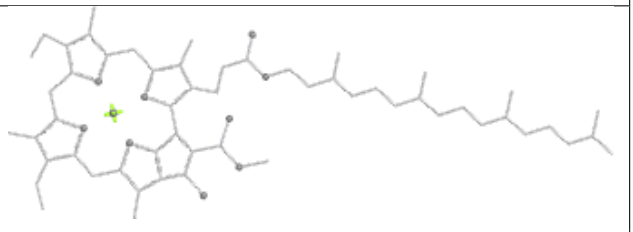


Bond angles

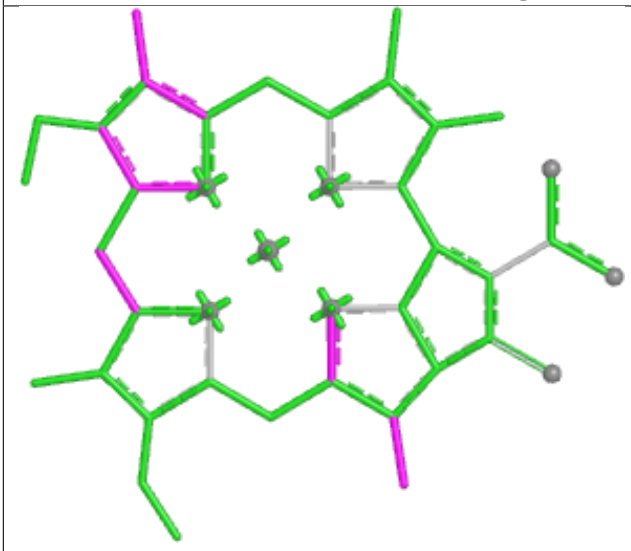


Torsions



Rings

Ligand CLA A3 313



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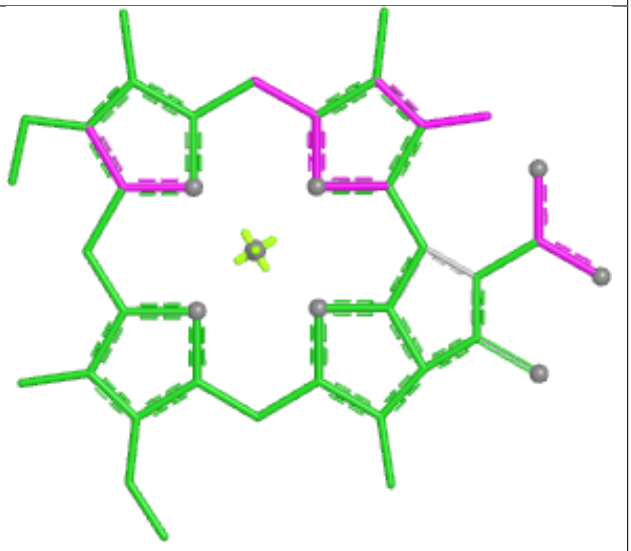
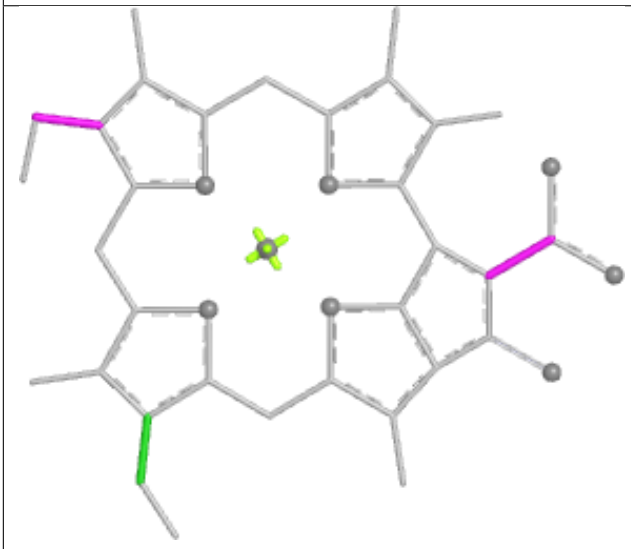


Bond angles



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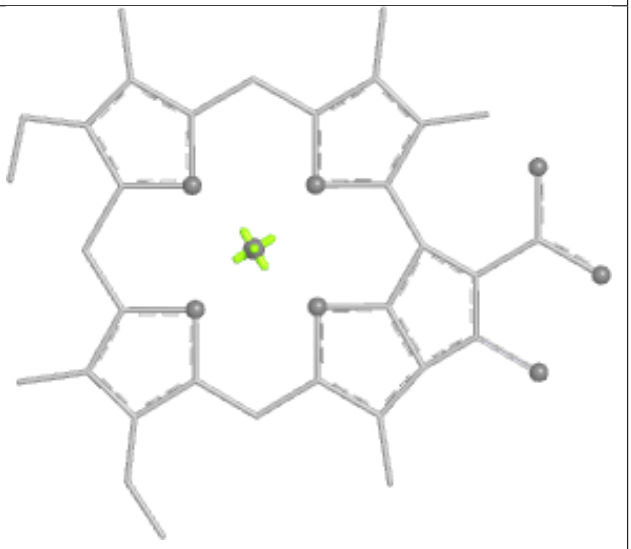
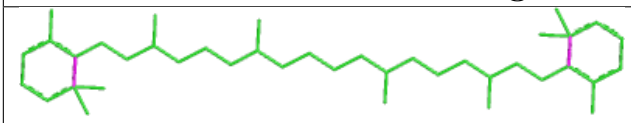


Rings

Ligand BCR BG 203



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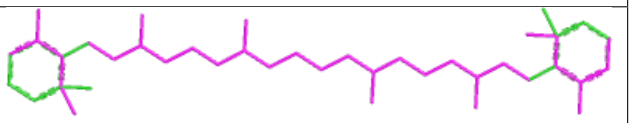
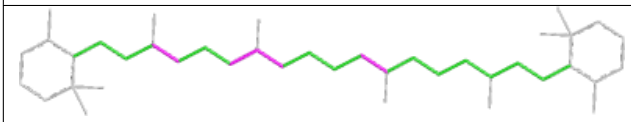
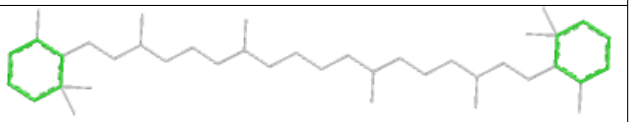


Bond angles

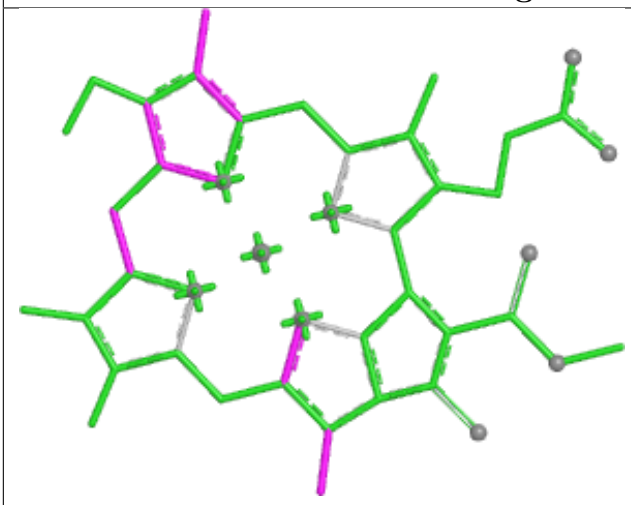


Torsions

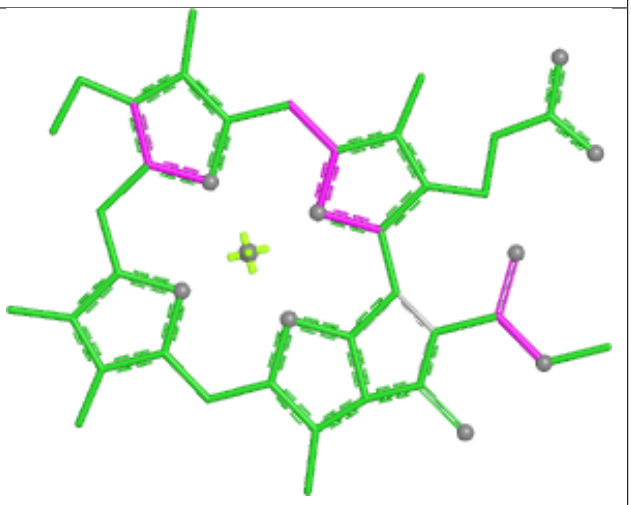


Rings

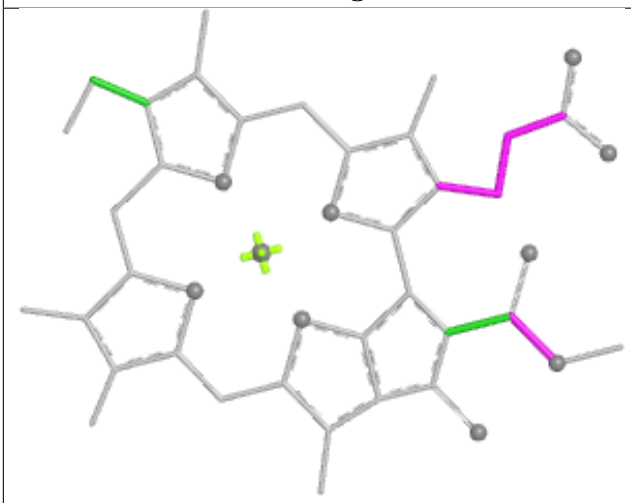
Ligand CLA B2 611



Bond lengths



Bond angles

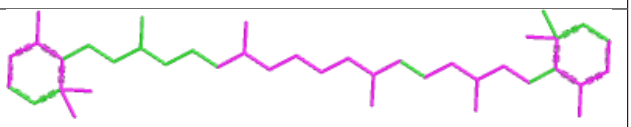


Torsions

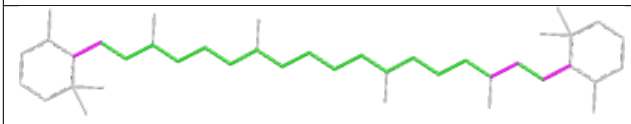
Rings

Ligand BCR BI 101

Bond lengths



Bond angles



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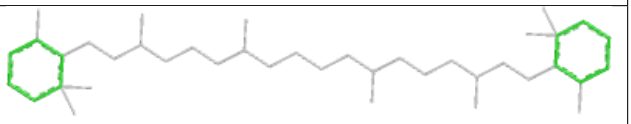
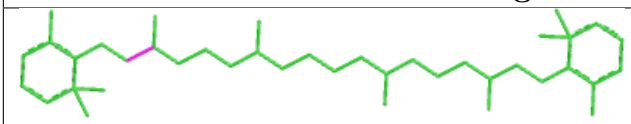


Rings

Ligand BCR B2 617



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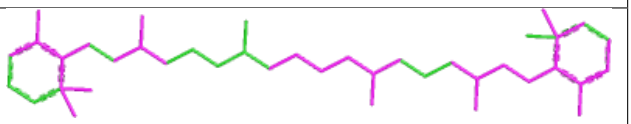
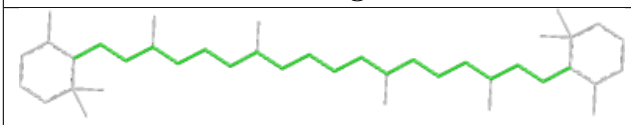


Bond angles



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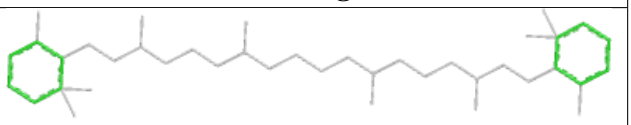
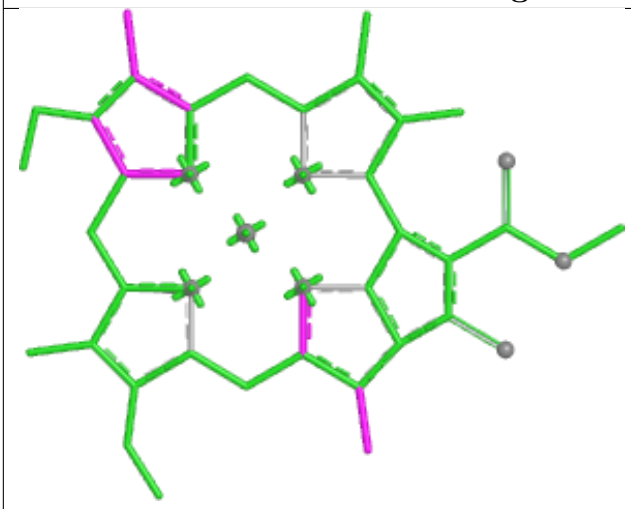


Rings

Ligand CLA BA 823



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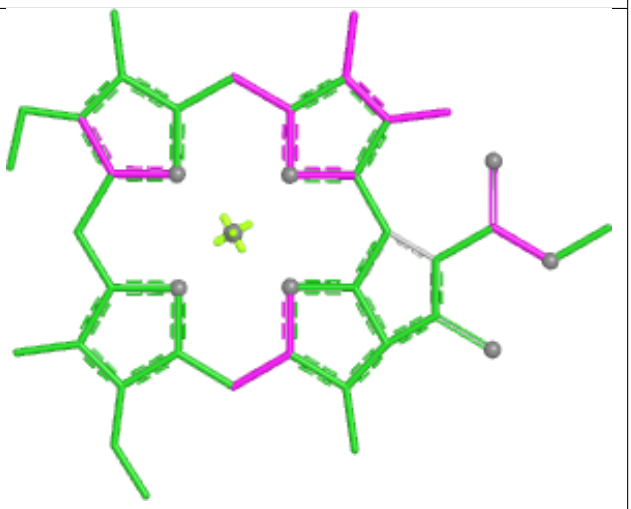
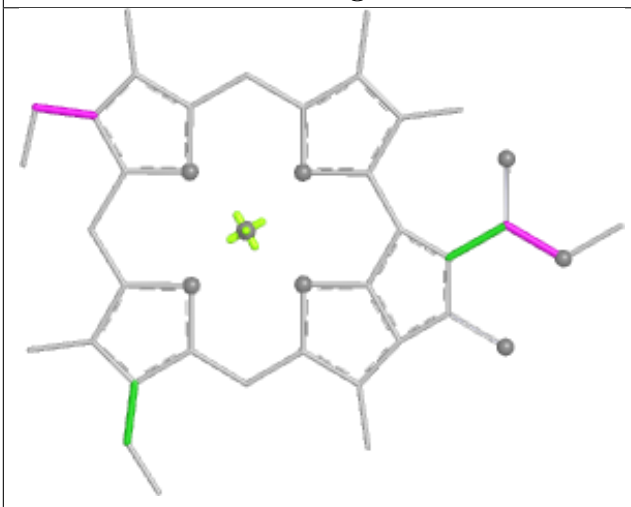


Bond angles



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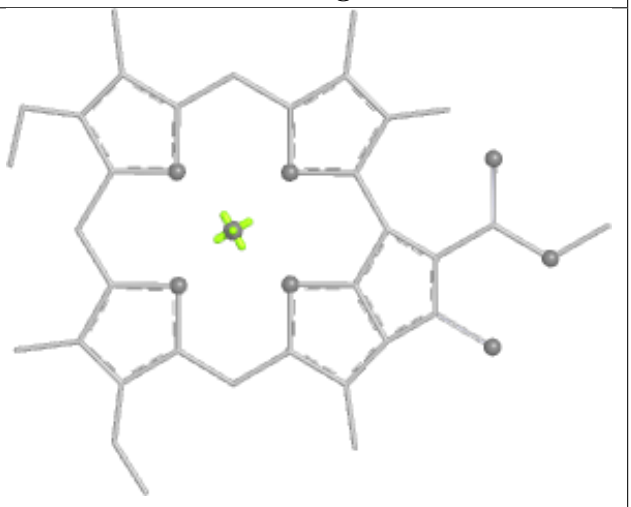
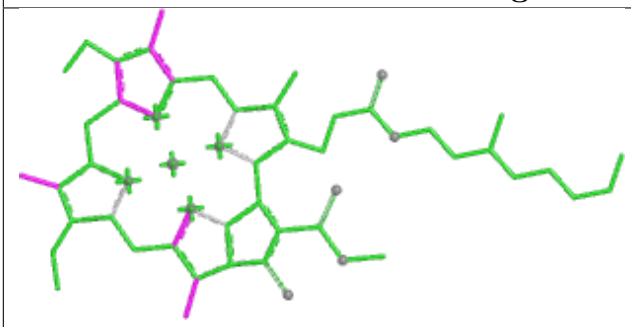


Rings

Ligand CLA BA 812



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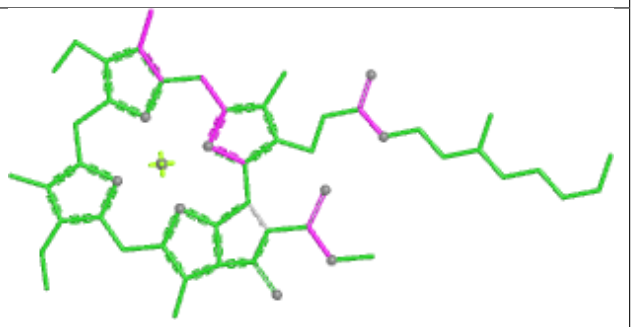
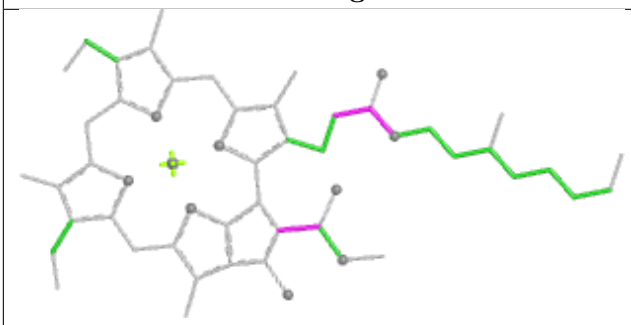
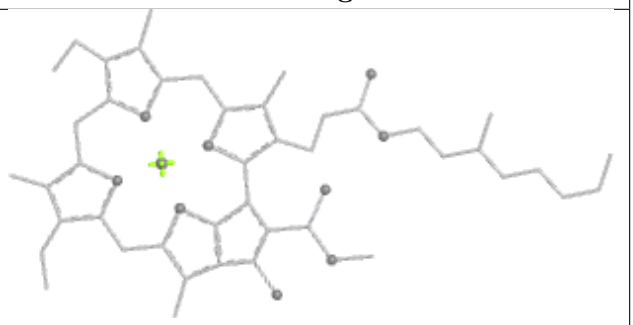


Bond angles

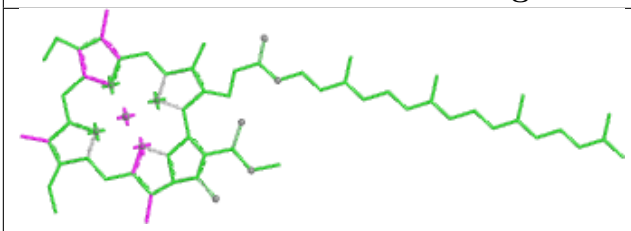


Torsions



Rings

Ligand CLA BB 801



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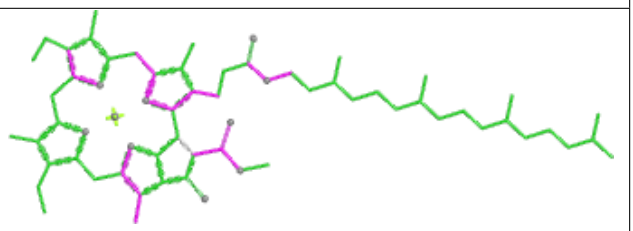
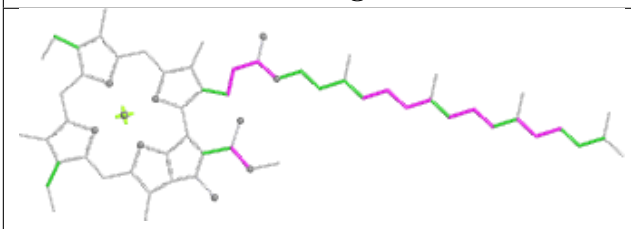
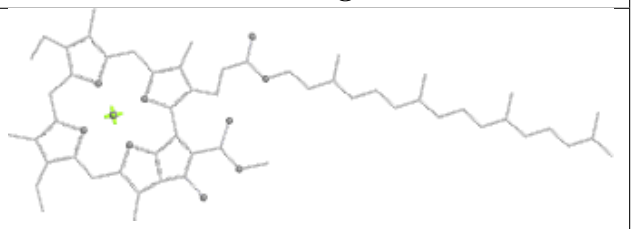


Bond angles

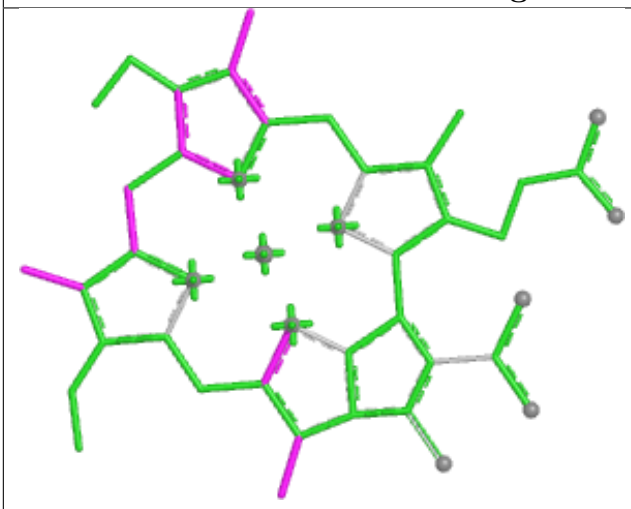


Torsions

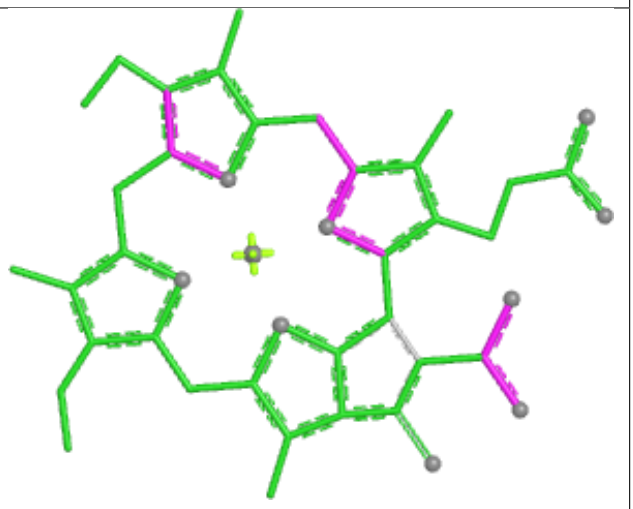


Rings

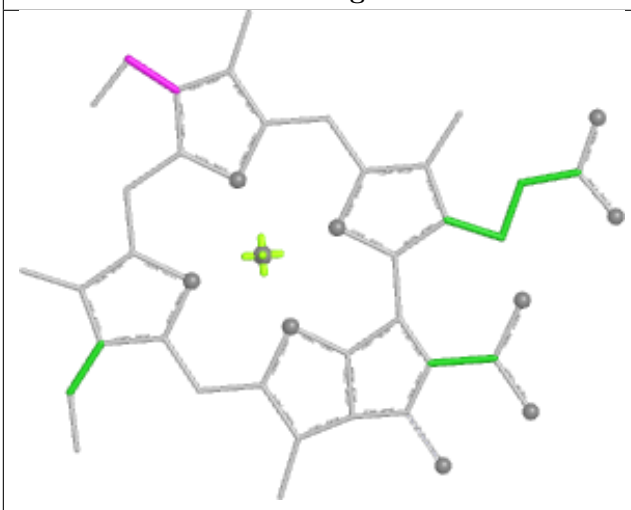
Ligand CLA AA 835



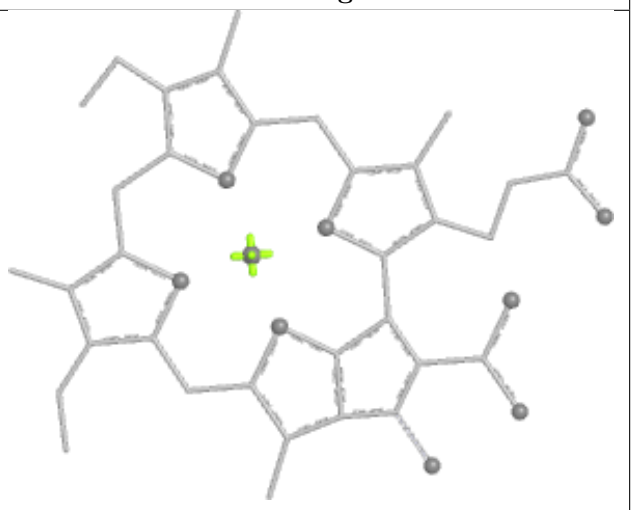
Bond lengths



Bond angles

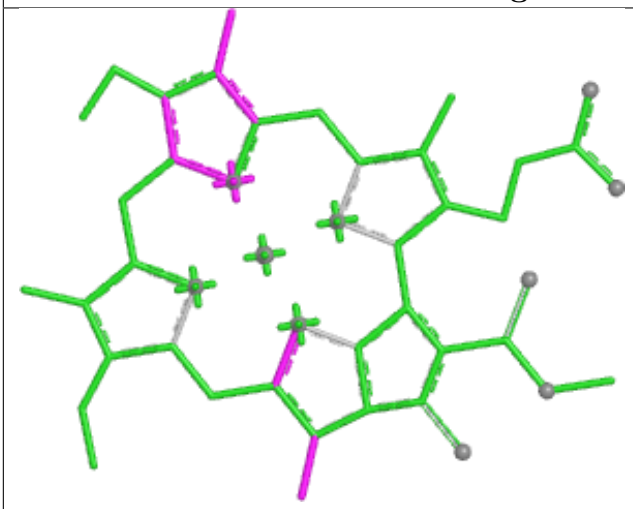


Torsions

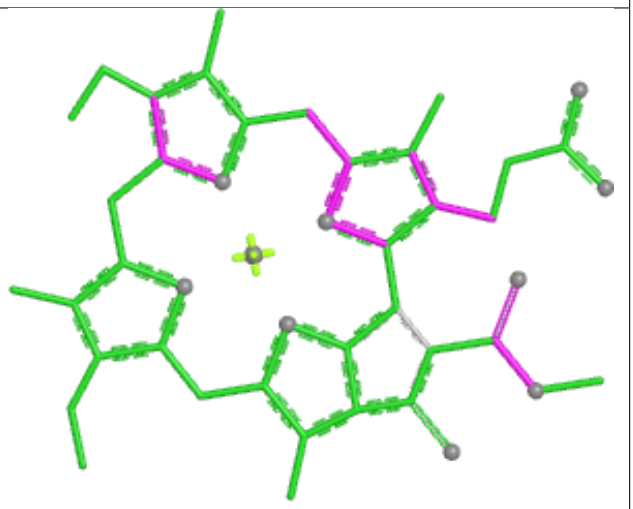


Rings

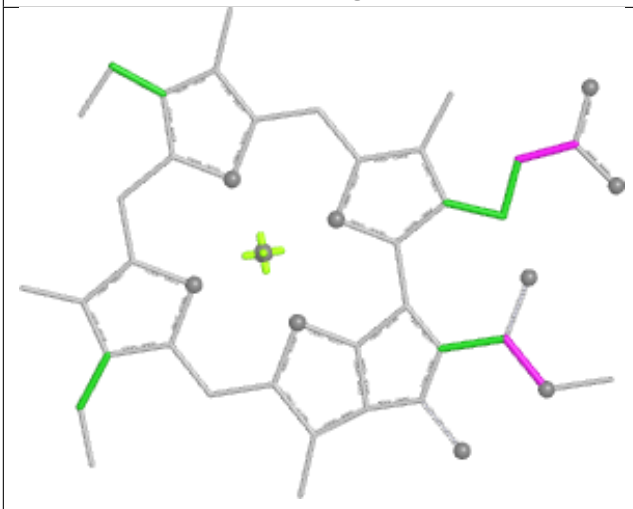
Ligand CLA BG 202



Bond lengths



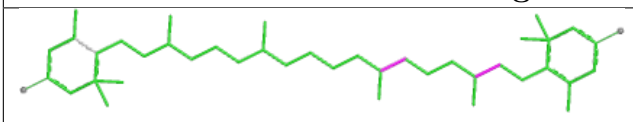
Bond angles



Torsions

Rings

Ligand LUT AF 806



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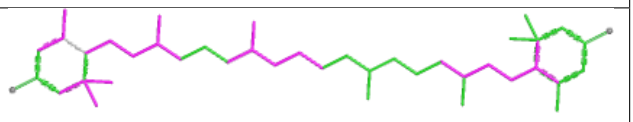
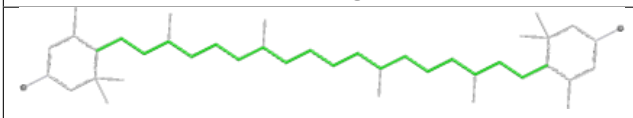
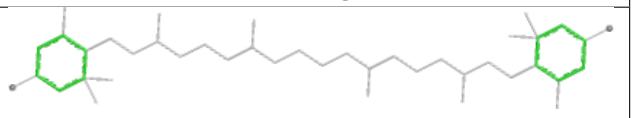


Bond angles

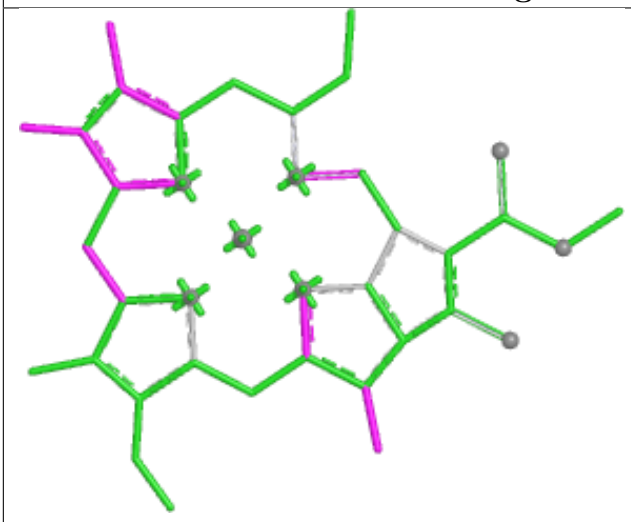


Torsions

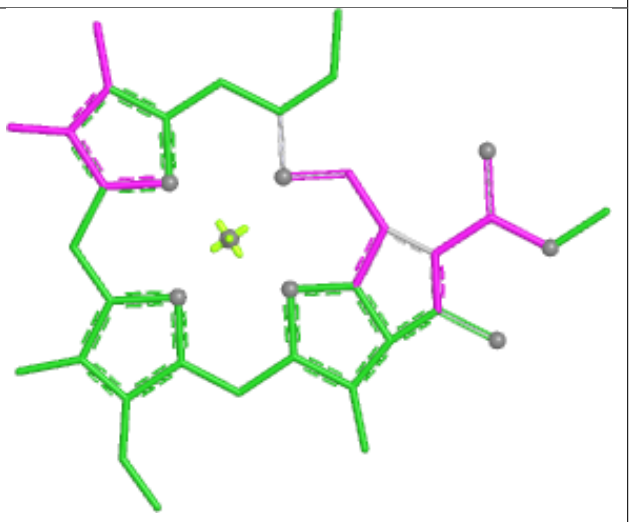


Rings

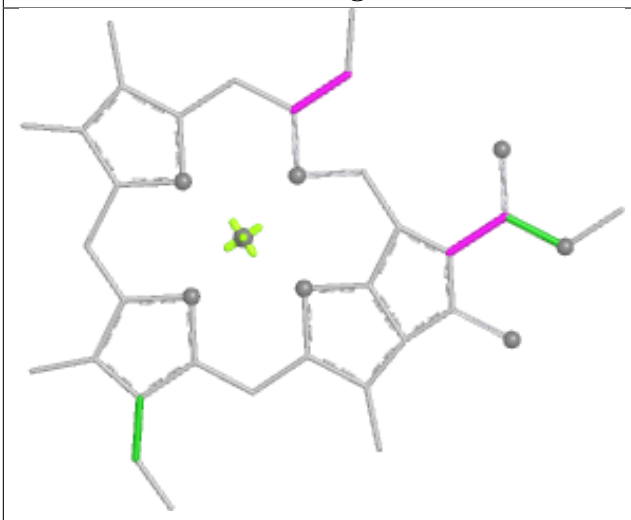
Ligand CLA A6 611



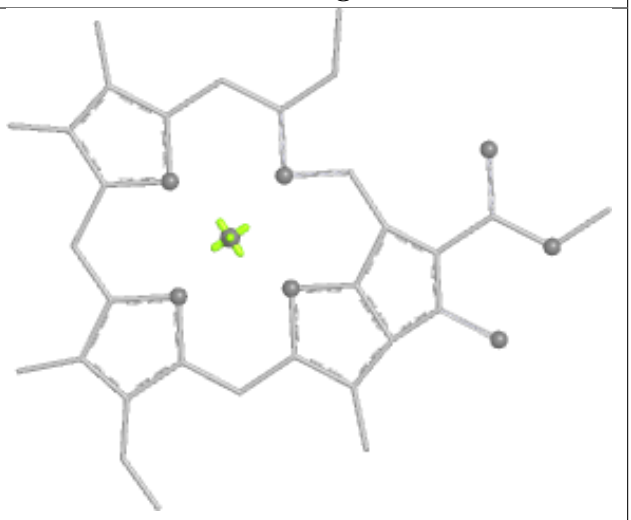
Bond lengths



Bond angles

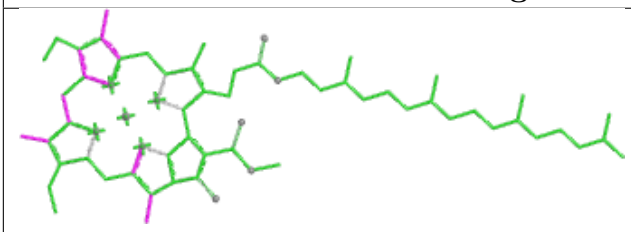


Torsions

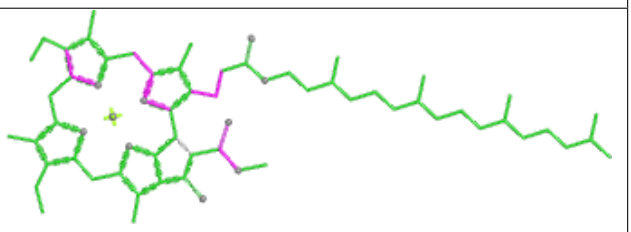


Rings

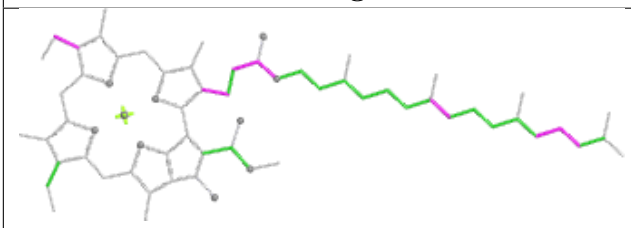
Ligand CLA AA 841



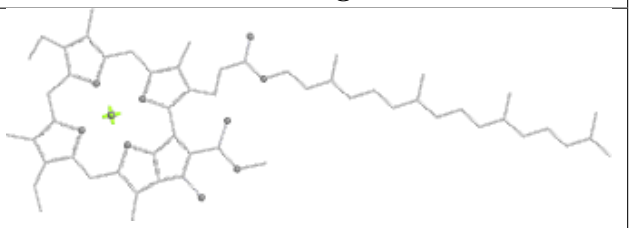
Bond lengths



Bond angles

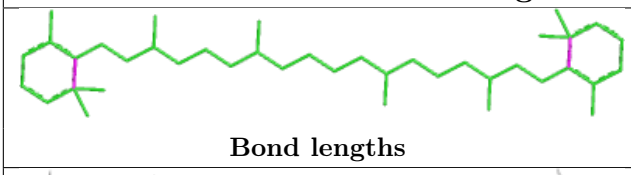


Torsions

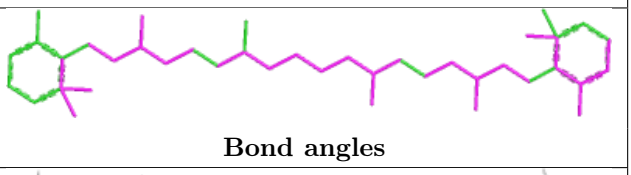


Rings

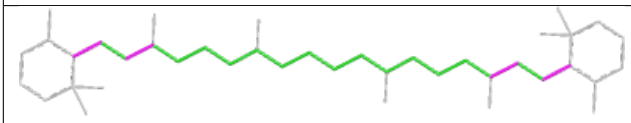
Ligand BCR AI 101



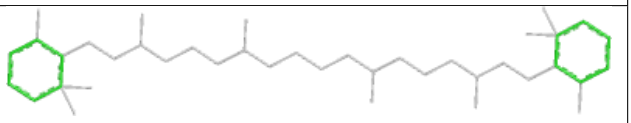
Bond lengths



Bond angles



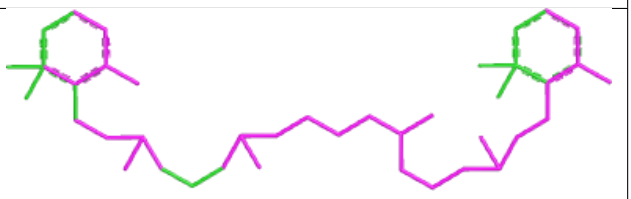
Torsions



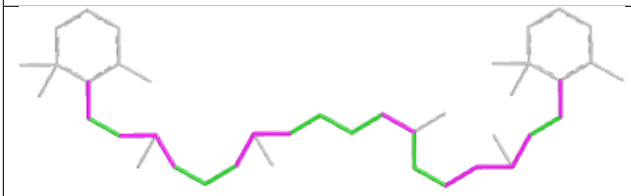
Rings

Ligand BCR BL 306

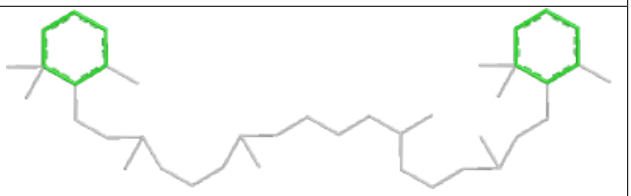
Bond lengths



Bond angles

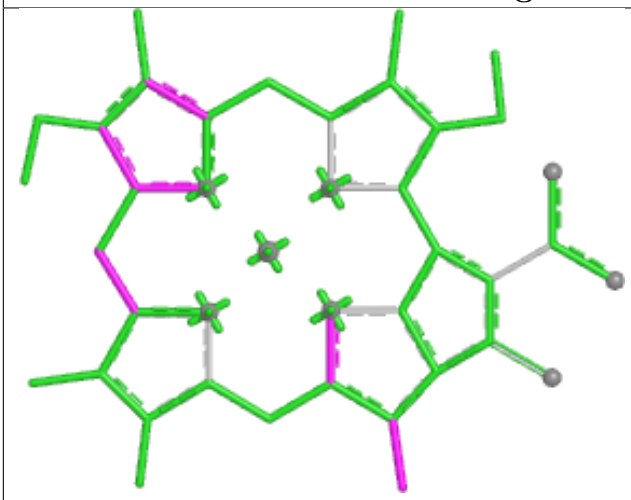


Torsions

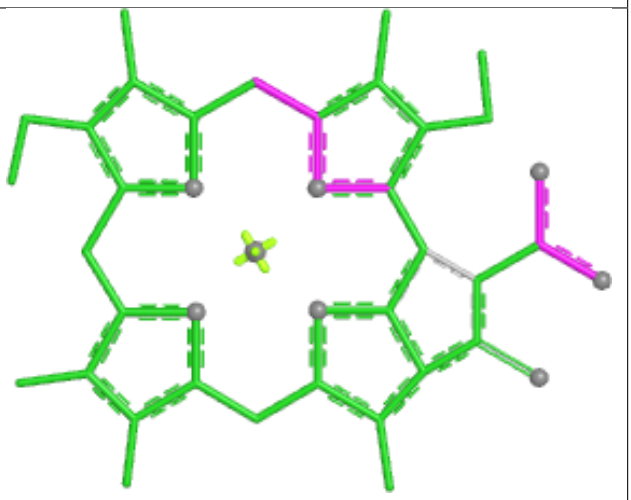


Rings

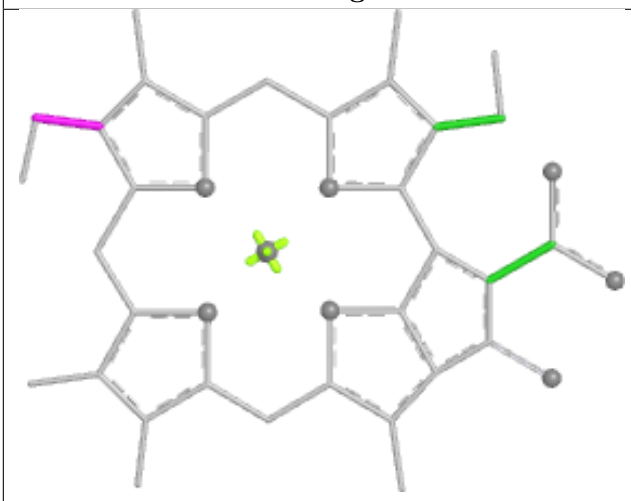
Ligand CLA B3 309



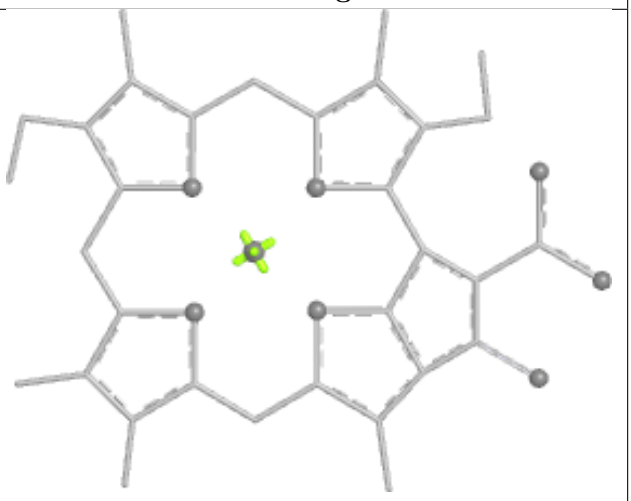
Bond lengths



Bond angles

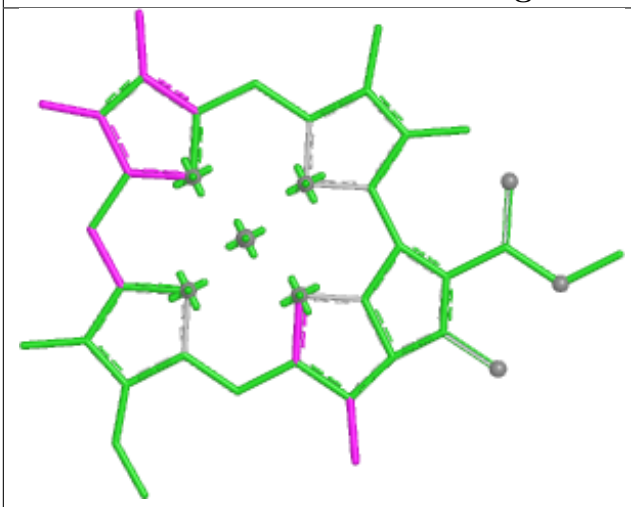


Torsions

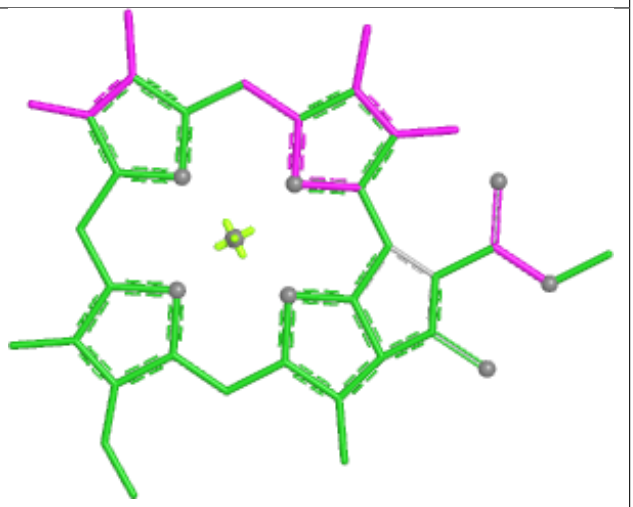


Rings

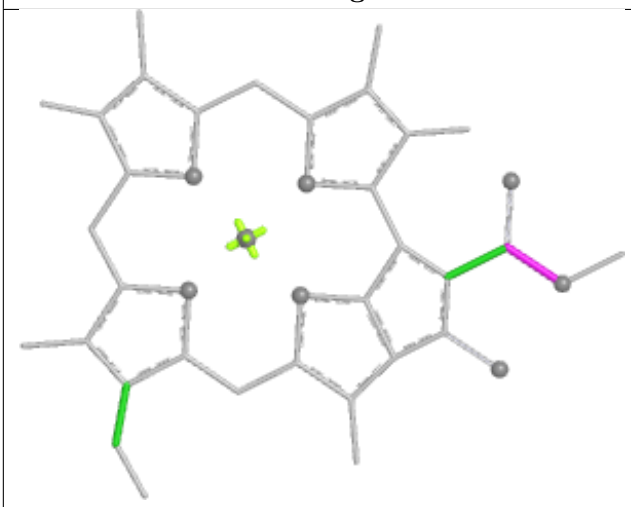
Ligand CLA A1 310



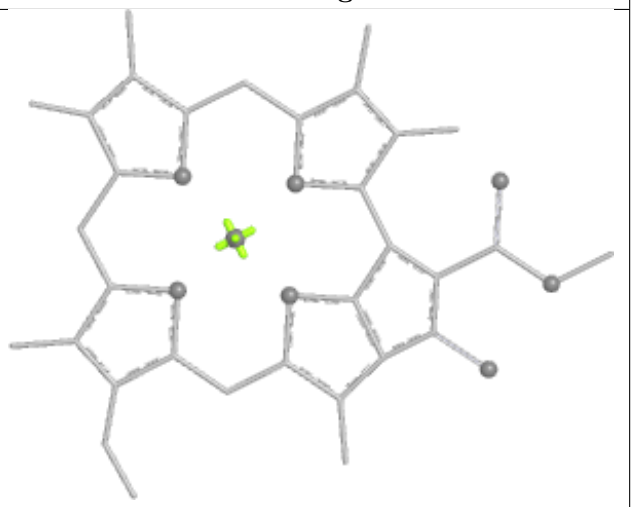
Bond lengths



Bond angles

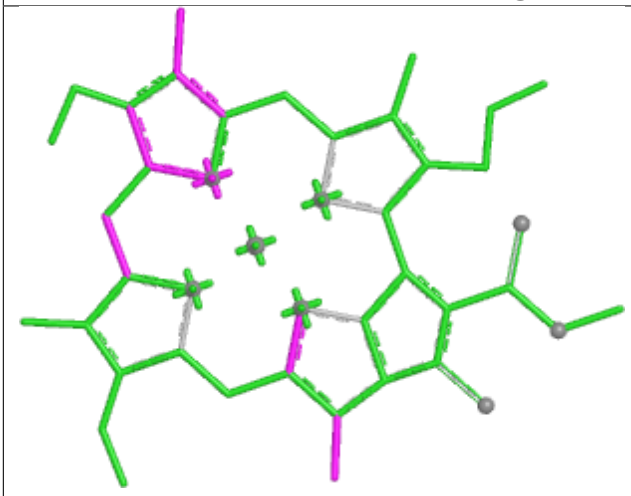


Torsions

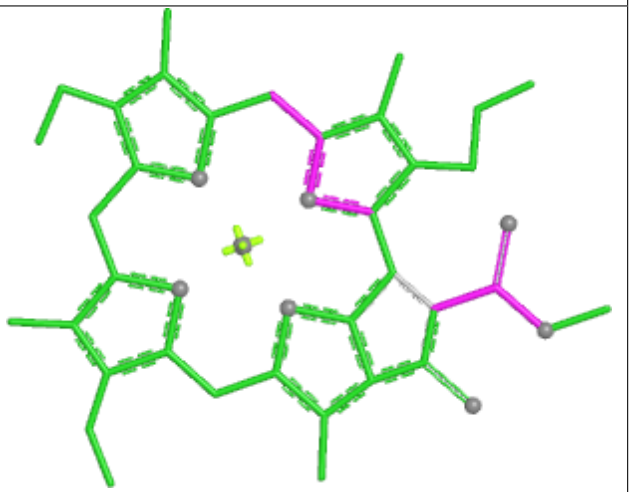


Rings

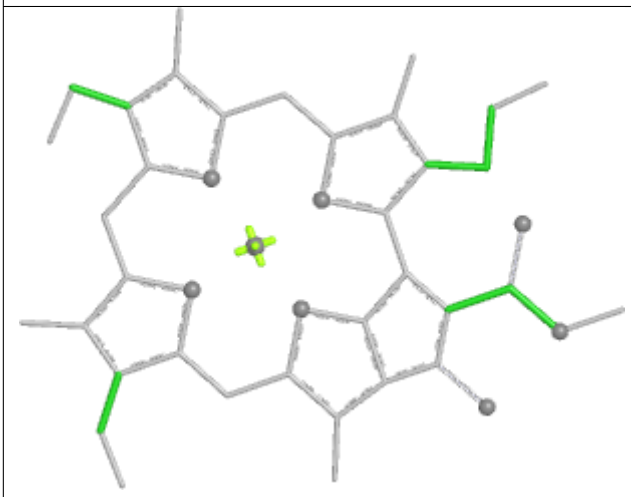
Ligand CLA BB 814



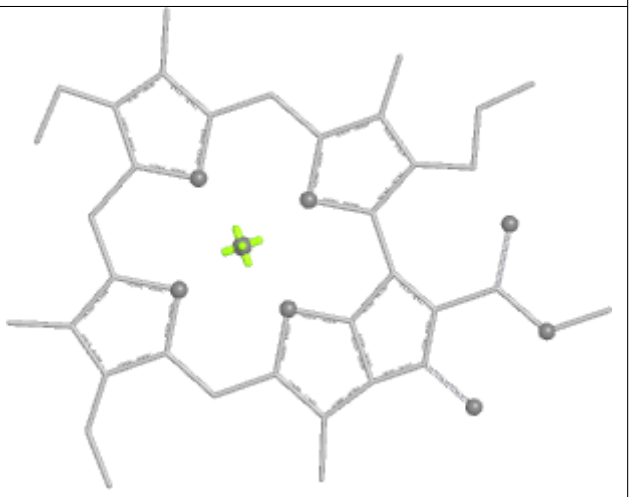
Bond lengths



Bond angles

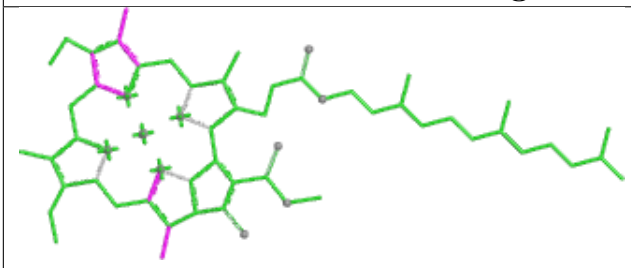


Torsions

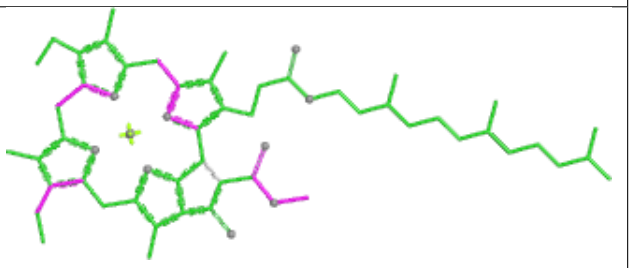


Rings

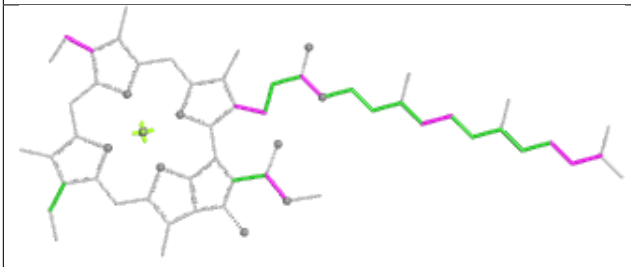
Ligand CLA BH 201



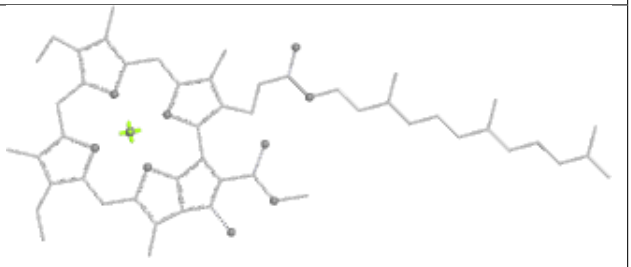
Bond lengths



Bond angles

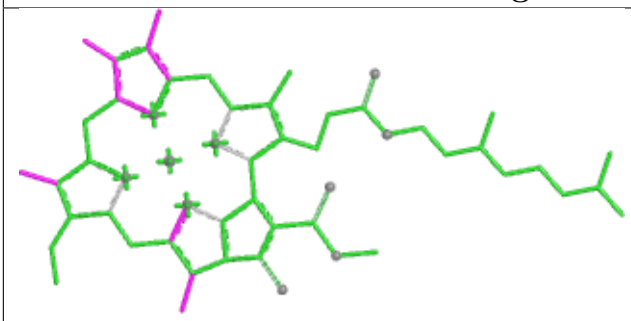


Torsions

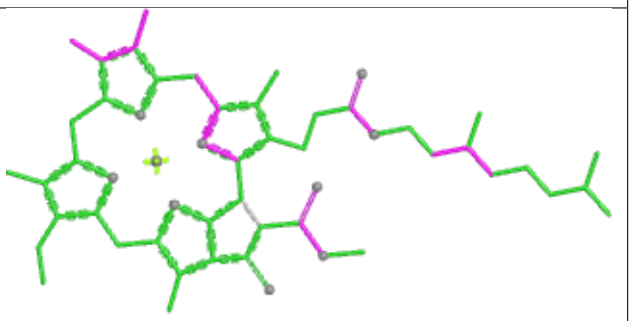


Rings

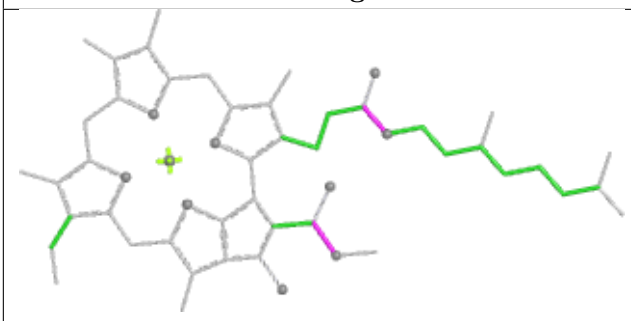
Ligand CLA BB 813



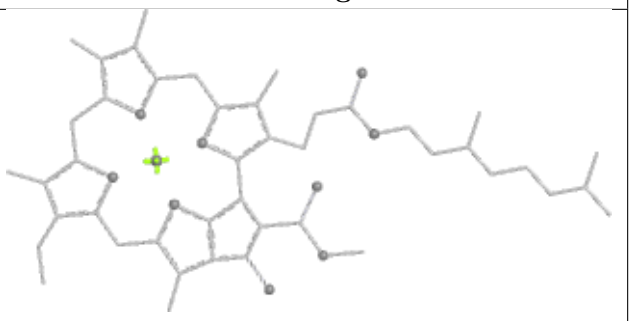
Bond lengths



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.

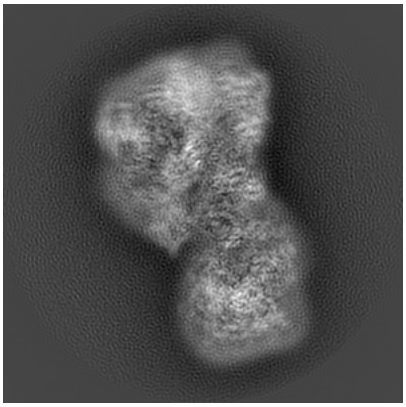
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32477. These allow visual inspection of the internal detail of the map and identification of artifacts.

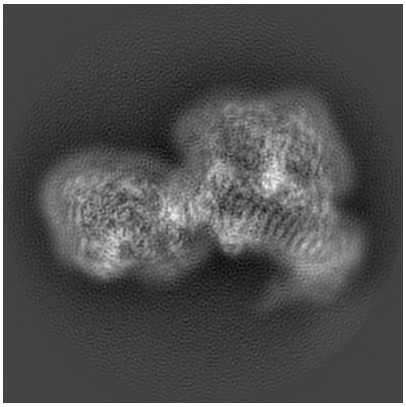
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

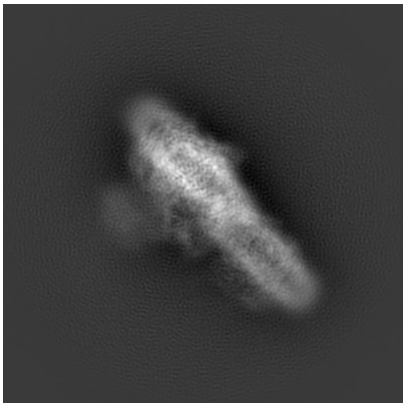
6.1.1 Primary map



X



Y

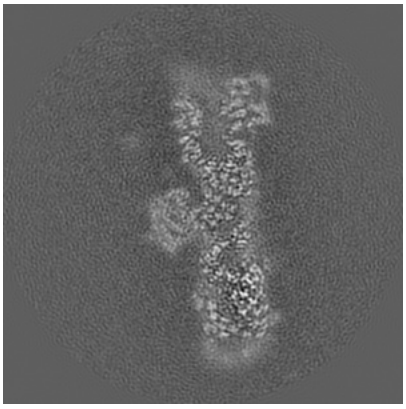


Z

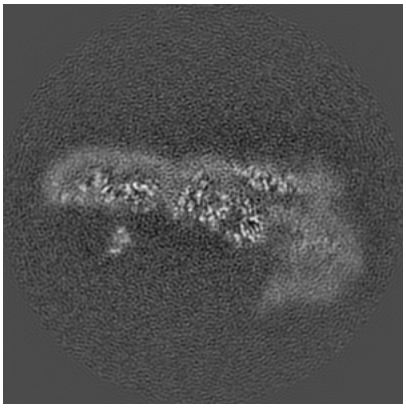
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 200



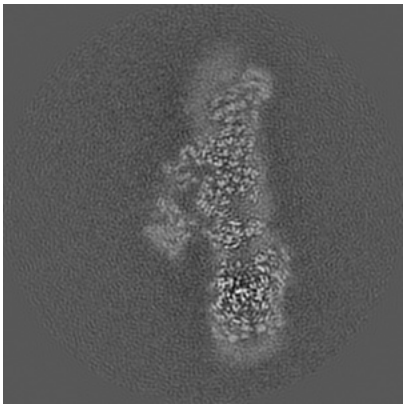
Y Index: 200

Z Index: 200

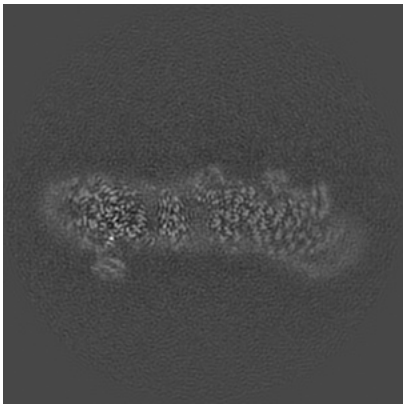
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

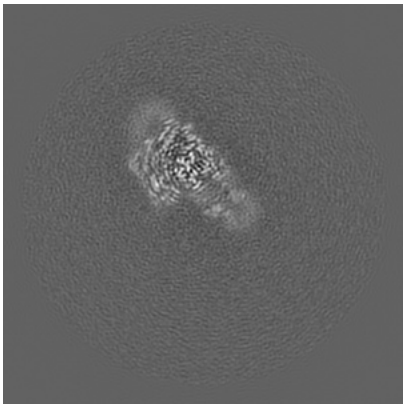
6.3.1 Primary map



X Index: 185



Y Index: 235

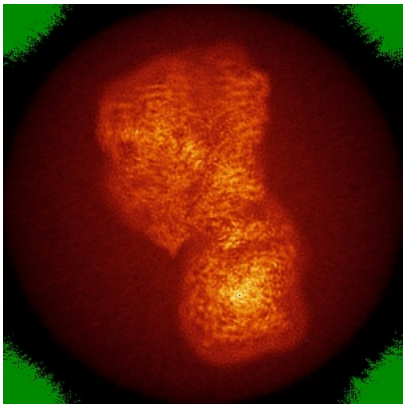


Z Index: 112

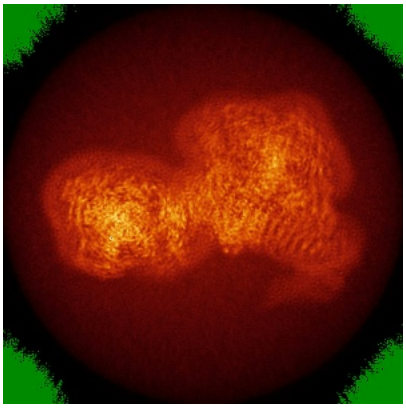
The images above show the largest variance slices of the map in three orthogonal directions.

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

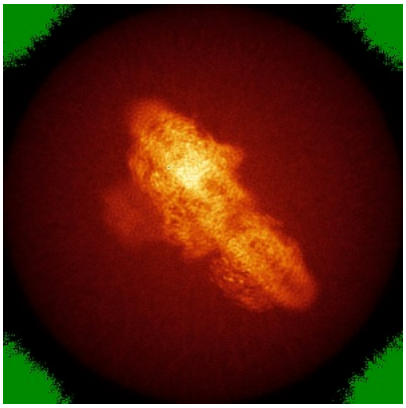
6.4.1 Primary map



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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

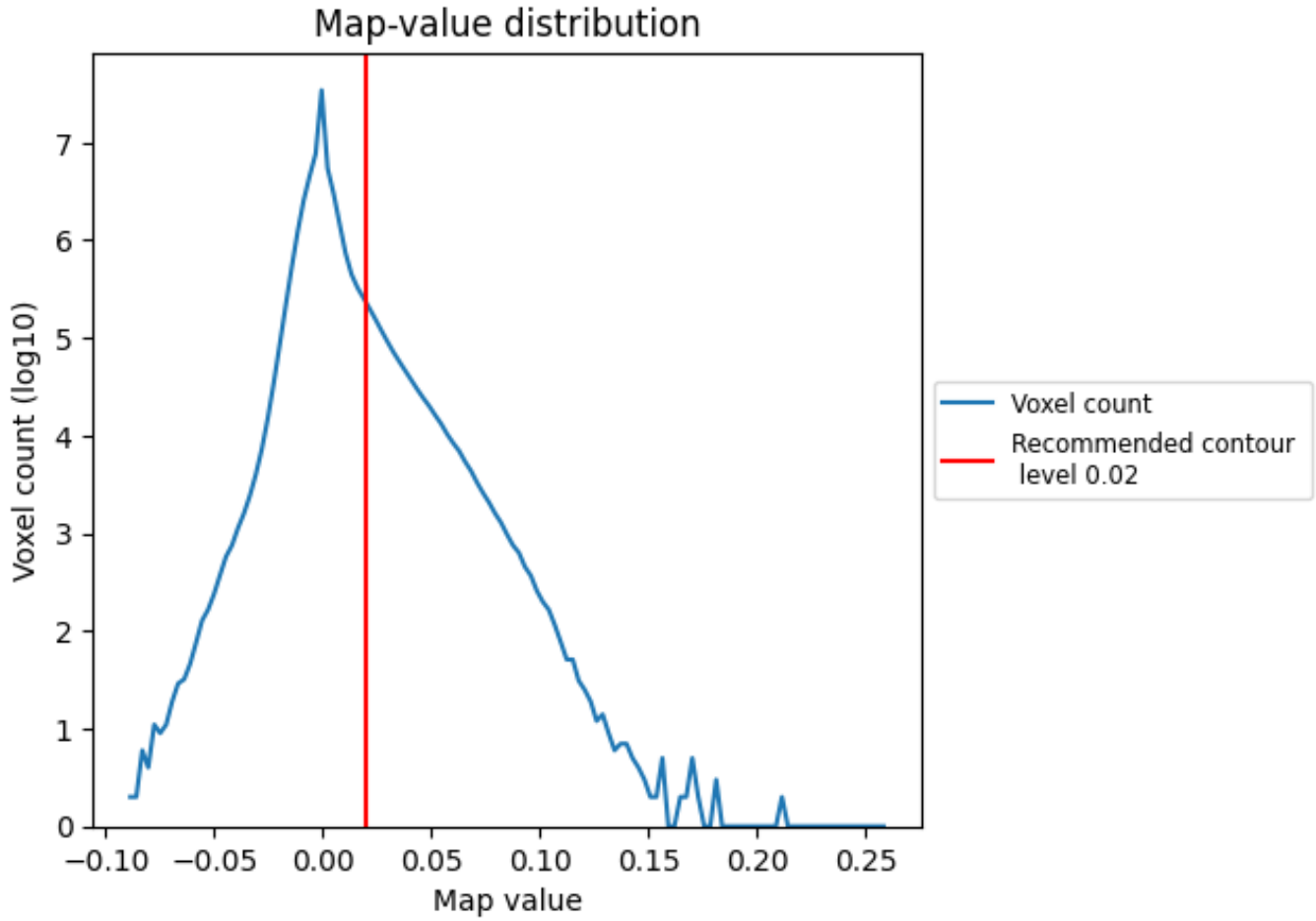
6.6 Mask visualisation (i)

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

7 Map analysis

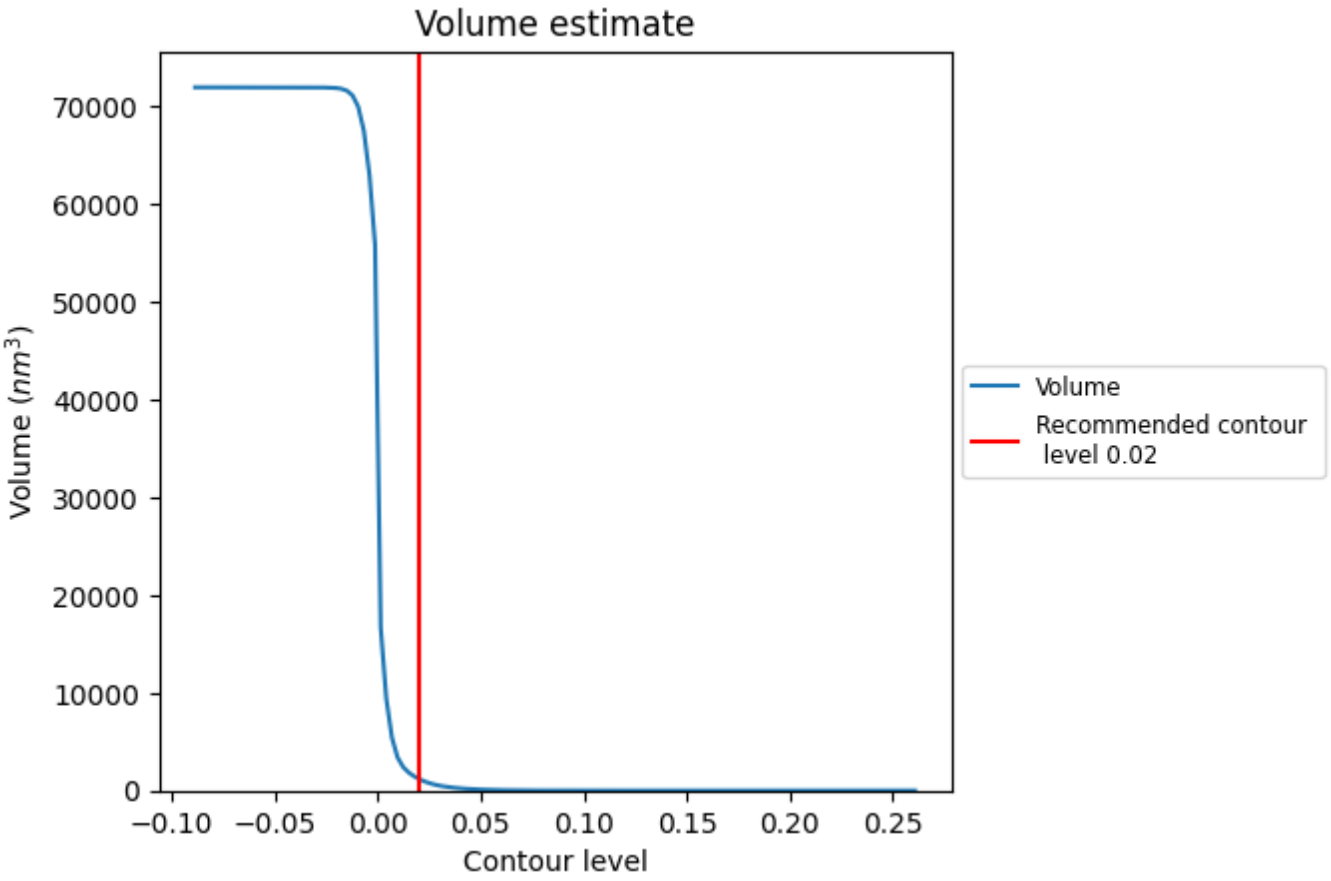
This section contains the results of statistical analysis of the map.

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.

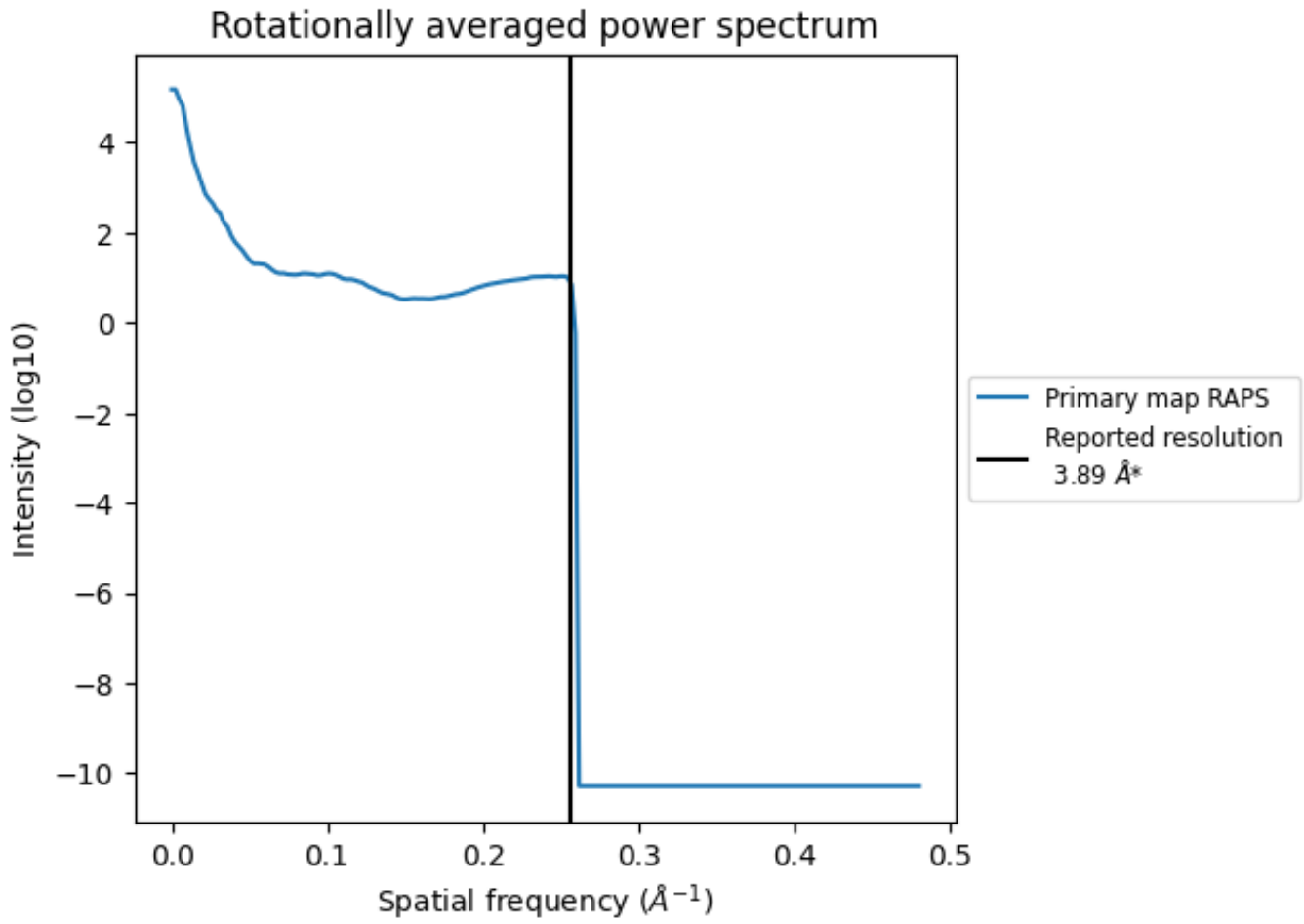
7.2 Volume estimate



The volume at the recommended contour level is 1193 nm^3; this corresponds to an approximate mass of 1078 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 0.257 Å^{-1}

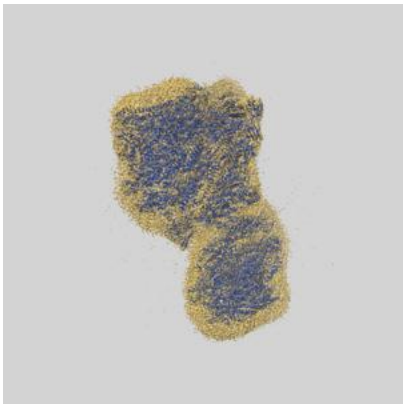
8 Fourier-Shell correlation

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

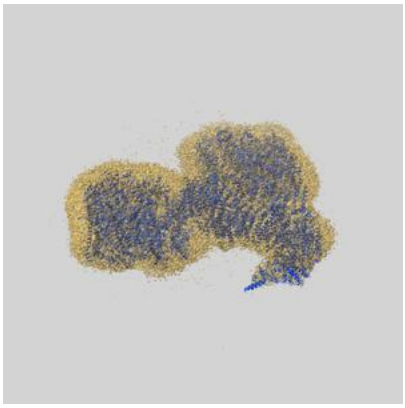
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32477 and PDB model 7WG5. Per-residue inclusion information can be found in section 3 on page 46.

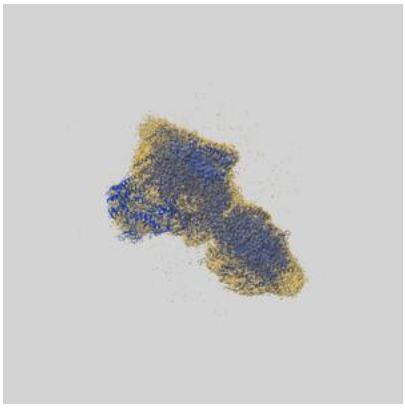
9.1 Map-model overlay



X



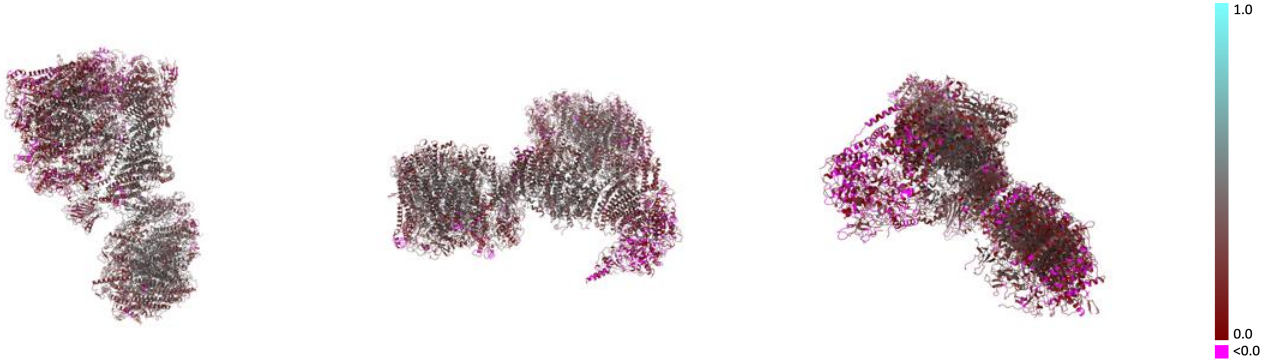
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

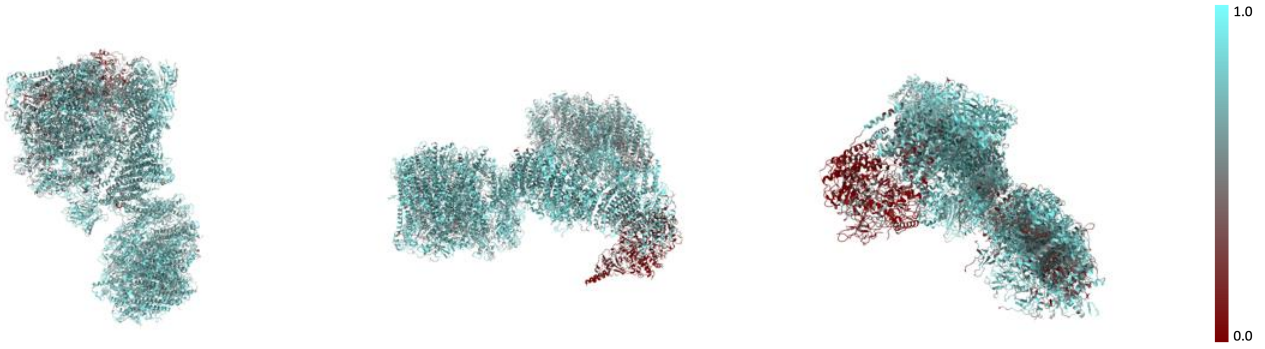
9.2 Q-score mapped to coordinate model



X Y Z

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

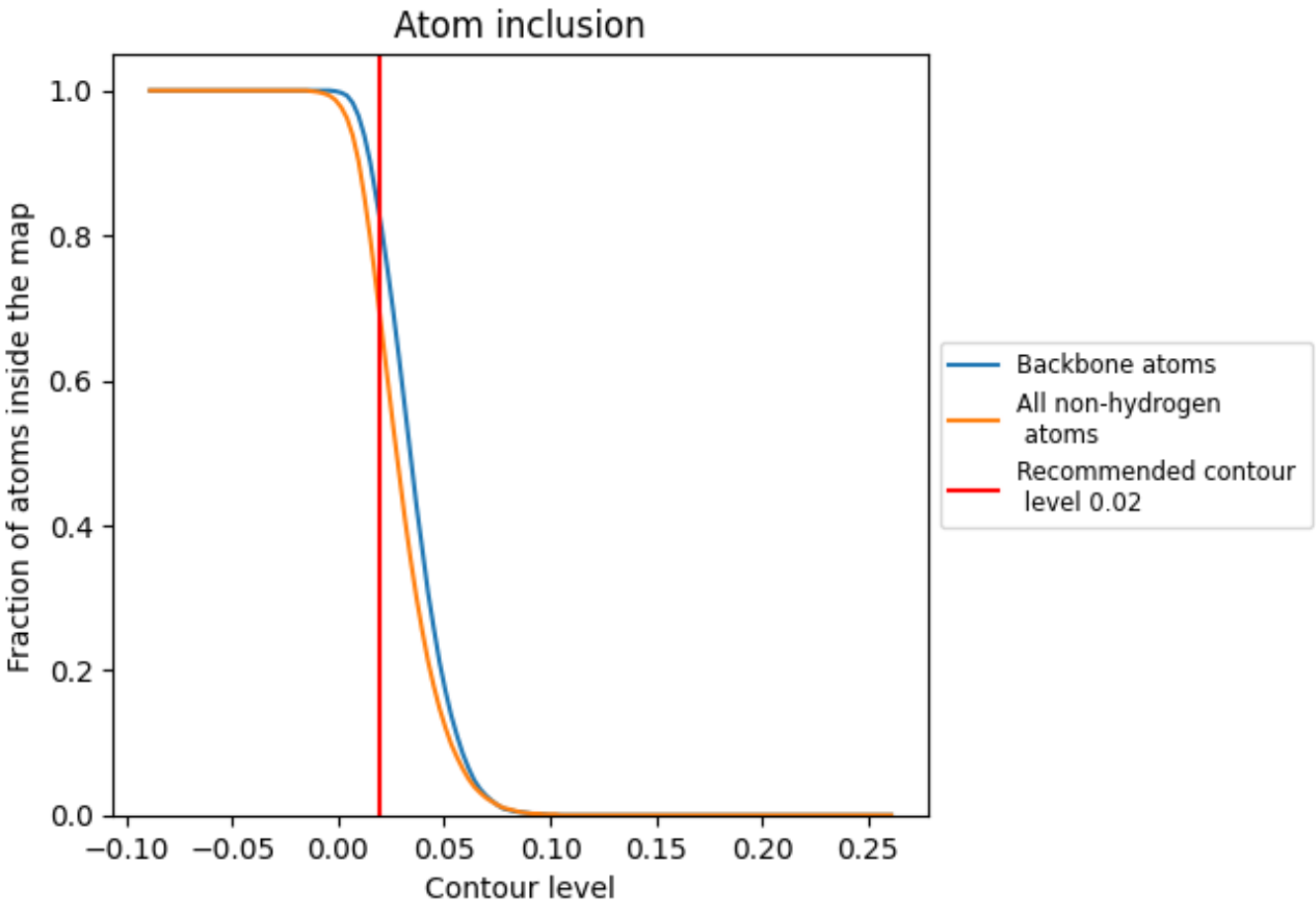
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 68% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.2780
A	0.6080	0.1850
A1	0.7370	0.2670
A3	0.7700	0.2850
A4	0.7720	0.3150
A6	0.7980	0.3780
AA	0.7720	0.3600
AB	0.7770	0.3740
AC	0.8600	0.3480
AD	0.7990	0.3020
AE	0.7820	0.3420
AF	0.8030	0.3850
AG	0.7630	0.2510
AH	0.7180	0.1970
AI	0.6970	0.2870
AJ	0.7650	0.3900
AK	0.6720	0.1590
AL	0.7300	0.2350
B	0.7500	0.3510
B1	0.6830	0.2740
B2	0.6620	0.1940
B3	0.6670	0.1720
B5	0.7600	0.3430
BA	0.6660	0.2590
BB	0.6890	0.2790
BC	0.7820	0.2570
BD	0.6810	0.1900
BE	0.6530	0.2750
BF	0.7310	0.3310
BG	0.5700	0.1030
BH	0.6430	0.1250
BI	0.5080	0.1090
BJ	0.6880	0.3150
BK	0.5580	0.0830
BL	0.5590	0.1090

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Chain	Atom inclusion	Q-score
C	0.5990	0.2350
D	0.7970	0.4030
E	0.7000	0.3040
F	0.7410	0.3140
G	0.6920	0.2930
H	0.0960	0.0450
I	0.2630	0.0770
J	0.1660	0.0950
K	0.2170	0.1070
L	0.5280	0.1300
M	0.1140	0.0580
N	0.1750	0.1100
O	0.1100	0.1230
T	0.2430	0.0880
a	0.7990	0.3570
b	0.7730	0.2460
c	0.7430	0.3020
d	0.8280	0.3790
e	0.7900	0.3720
f	0.7530	0.2040
g	0.7560	0.2360
h	0.8010	0.3240
i	0.7870	0.3360
j	0.7610	0.3130