



Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 07:47 AM JST

PDB ID : 7WG5
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:

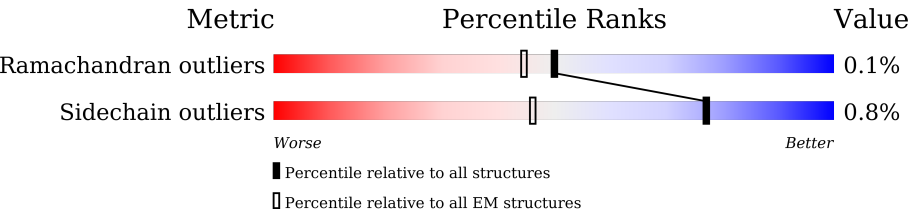
EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

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)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$. 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	98%
1	BA	750	98%
2	AB	734	99%
2	BB	734	99%
3	AC	81	99%
3	BC	81	99%
4	AD	204	69% 31%
4	BD	204	68% 30%
5	AE	143	47% 53%

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Mol	Chain	Length	Quality of chain
5	BE	143	
6	AF	221	
6	BF	221	
7	AG	160	
7	BG	160	
8	AH	145	
8	BH	145	
9	AI	37	
9	BI	37	
10	AJ	44	
10	BJ	44	
11	AK	130	
11	BK	130	
12	AL	219	
12	BL	219	
13	A1	241	
13	B1	241	
14	A3	273	
14	B3	273	
15	A4	251	
16	A6	270	
17	B2	257	
18	B5	256	
19	A	360	
20	B	512	

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Mol	Chain	Length	Quality of chain
21	C	120	
22	D	506	
23	E	101	
24	F	746	
25	G	176	
26	a	461	
27	b	348	
28	c	204	
29	d	161	
30	e	212	
31	f	238	
32	g	190	
33	h	220	
34	i	217	
35	j	255	
36	H	393	
37	I	172	
38	J	158	
39	K	225	
40	L	191	
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 crite-

ria:

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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
45	CLA	BH	201	X	-	-	-
45	CLA	BJ	102	X	-	-	-
45	CLA	BK	201	X	-	-	-
45	CLA	BK	202	X	-	-	-
45	CLA	BK	203	X	-	-	-
45	CLA	BL	304	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-

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 luminal location 1, chloro-
plastic.

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 luminal location 2, chloro-
plastic.

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 luminal location 3, chloro-
plastic.

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 luminal location 4, chloro-
plastic.

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 luminal 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		

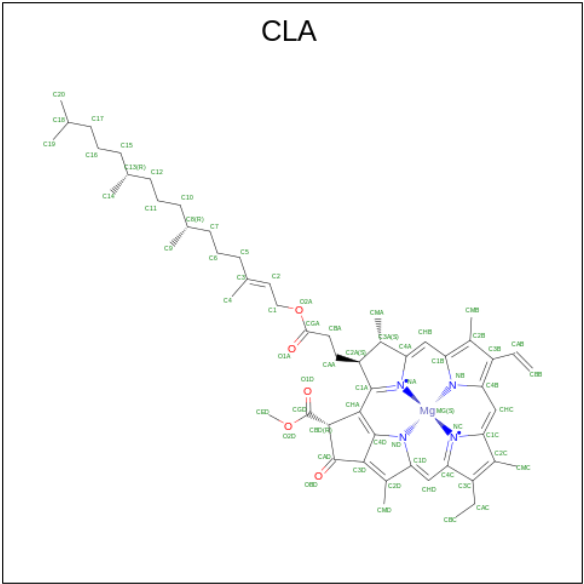
- Molecule 43 is a protein called NdhO.

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 (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



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

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

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

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

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

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

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

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

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

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

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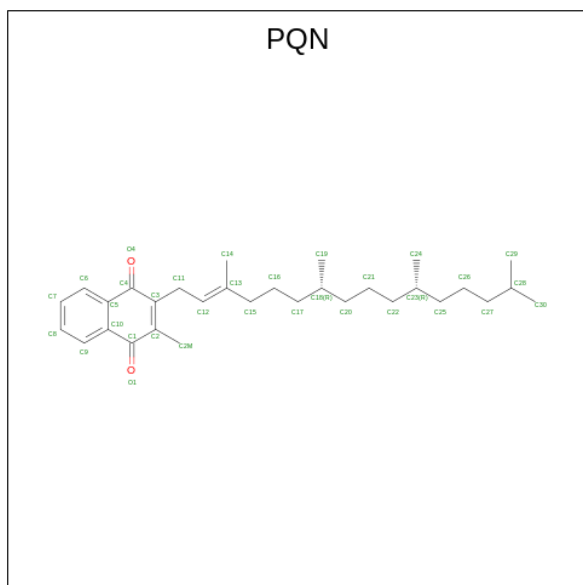
Mol	Chain	Residues	Atoms					AltConf
45	B2	1	Total 43	C 35	Mg 1	N 4	O 3	0
45	B3	1	Total 60	C 50	Mg 1	N 4	O 5	0
45	B3	1	Total 55	C 45	Mg 1	N 4	O 5	0
45	B3	1	Total 42	C 32	Mg 1	N 4	O 5	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 41	C 33	Mg 1	N 4	O 3	0
45	B3	1	Total 45	C 35	Mg 1	N 4	O 5	0
45	B3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

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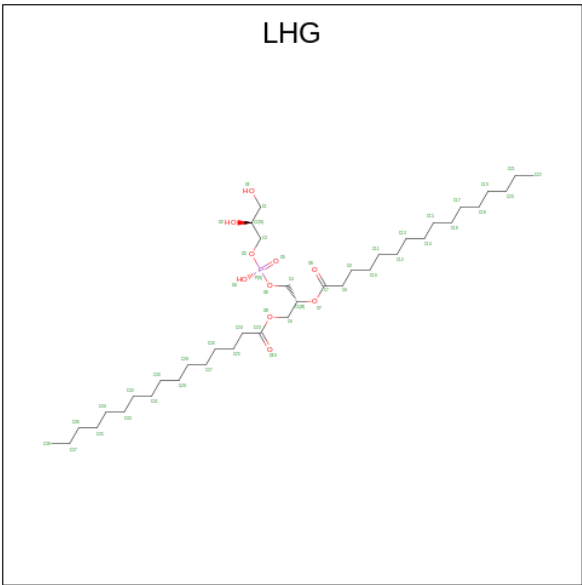
Mol	Chain	Residues	Atoms					AltConf
45	B5	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
45	B5	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
45	B5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 46 is PHYLLOQUINONE (three-letter code: 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 (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$).



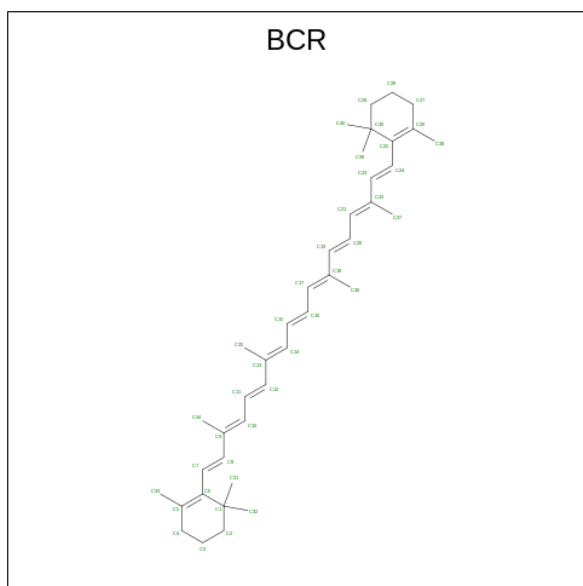
Mol	Chain	Residues	Atoms				AltConf
47	AA	1	Total	C	O	P	0
			49	38	10	1	
47	AJ	1	Total	C	O	P	0
			40	29	10	1	
47	A1	1	Total	C	O	P	0
			38	27	10	1	
47	A1	1	Total	C	O	P	0
			36	25	10	1	
47	A1	1	Total	C	O	P	0
			49	38	10	1	
47	A3	1	Total	C	O	P	0
			36	25	10	1	
47	A3	1	Total	C	O	P	0
			23	12	10	1	
47	A6	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 (three-letter code: 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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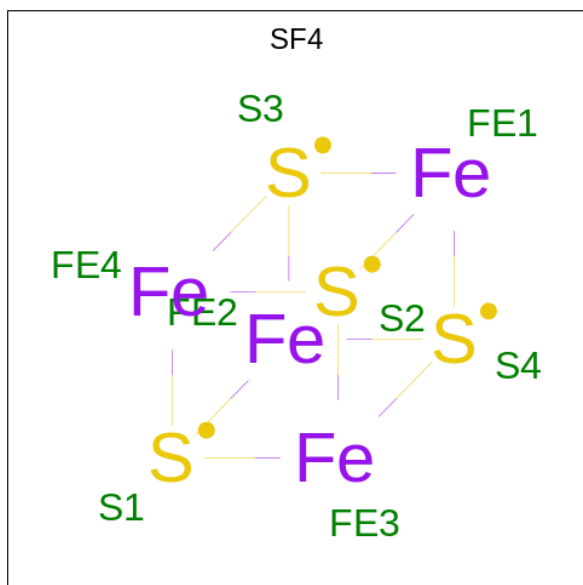
Mol	Chain	Residues	Atoms	AltConf
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BA	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	1	Total C 40 40	0
48	BB	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	0
			40	40	
48	B3	1	Total	C	0
			40	40	
48	B5	1	Total	C	0
			40	40	

- Molecule 49 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



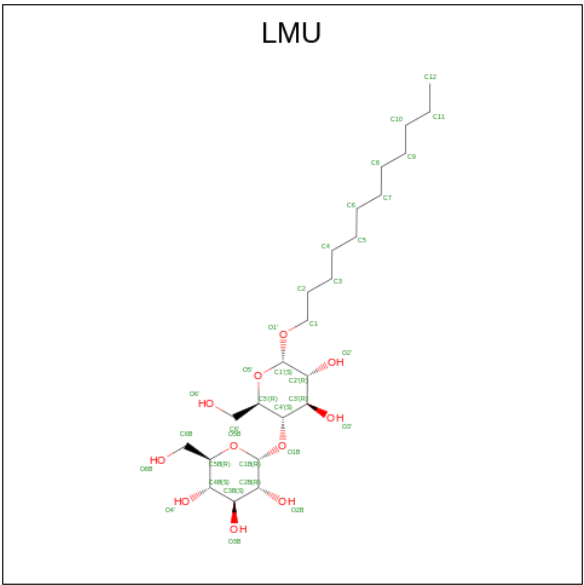
Mol	Chain	Residues	Atoms			AltConf
49	AA	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	AC	1	Total	Fe	S	0
			8	4	4	
49	BA	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	BC	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	
49	I	1	Total	Fe	S	0
			8	4	4	

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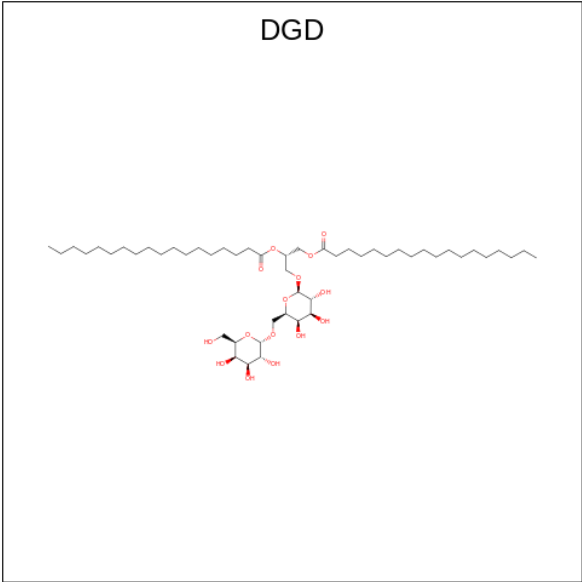
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
49	K	1	8	4	4	0

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



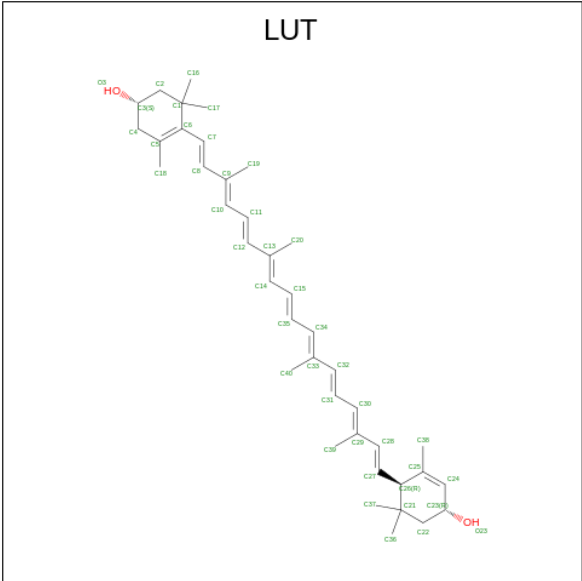
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
50	AA	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AB	1	35	24	11	0
50	AL	1	34	23	11	0
50	BA	1	34	23	11	0
50	BA	1	33	22	11	0
50	BB	1	35	24	11	0

- Molecule 51 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: 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 (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



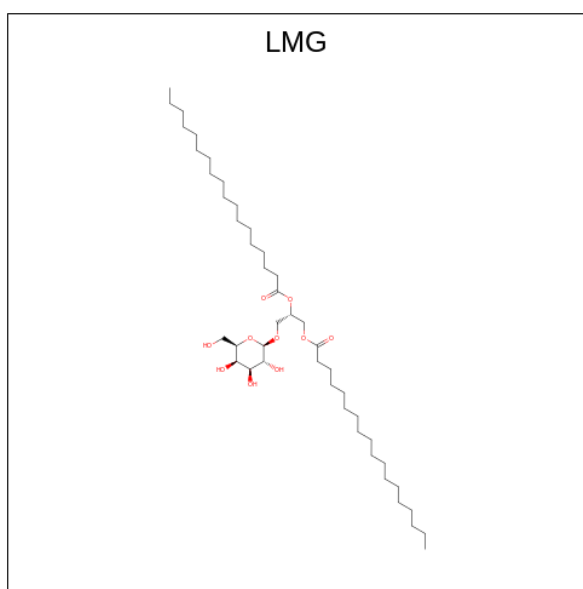
Mol	Chain	Residues	Atoms			AltConf
52	AF	1	Total	C	O	0
			42	40	2	

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

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



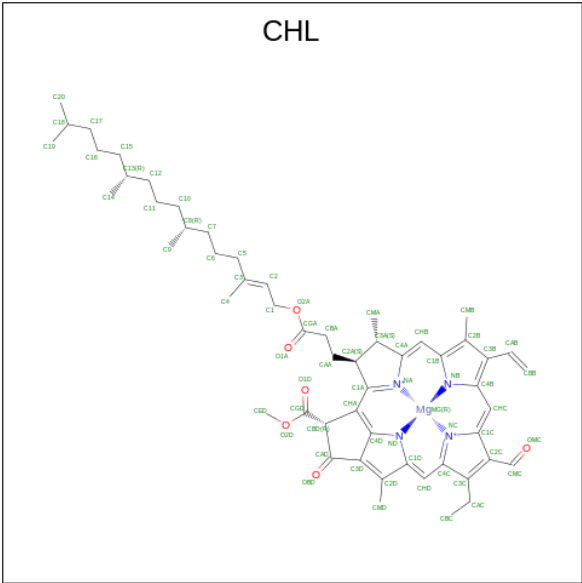
Mol	Chain	Residues	Atoms			AltConf
53	AG	1	Total	C	O	0
			38	28	10	
53	A1	1	Total	C	O	0
			44	34	10	
53	A4	1	Total	C	O	0
			39	29	10	

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

- Molecule 54 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



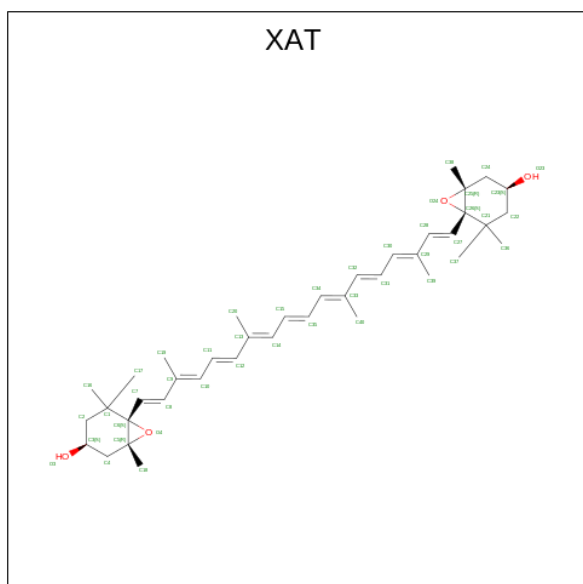
Mol	Chain	Residues	Atoms					AltConf
54	A1	1	Total	C	Mg	N	O	0
			51	40	1	4	6	
54	A1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A3	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
54	A4	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	A4	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
54	A4	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
54	A4	1	Total	C	Mg	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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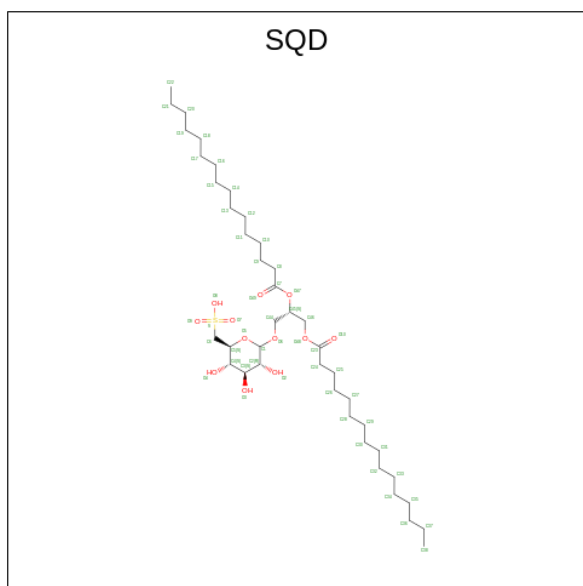
Mol	Chain	Residues	Atoms					AltConf
54	A6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
54	B1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
54	B1	1	Total	C	Mg	N	O	0
			41	32	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			53	42	1	4	6	
54	B2	1	Total	C	Mg	N	O	0
			42	33	1	4	4	
54	B2	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
54	B2	1	Total	C	Mg	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 (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



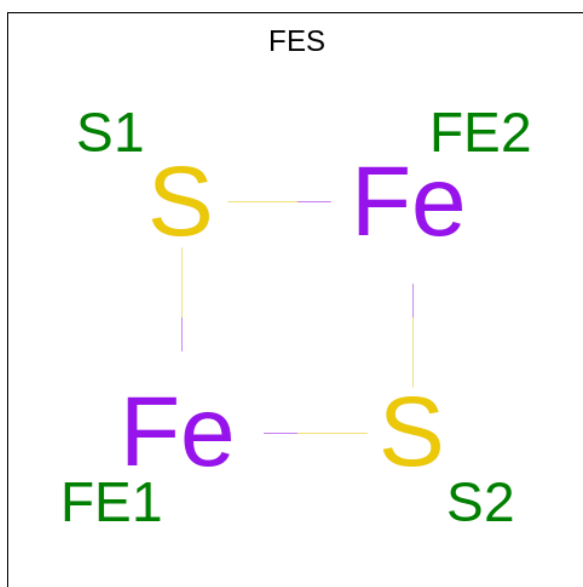
Mol	Chain	Residues	Atoms			AltConf
55	A1	1	Total	C	O	0
			44	40	4	
55	A3	1	Total	C	O	0
			44	40	4	
55	A4	1	Total	C	O	0
			44	40	4	
55	A6	1	Total	C	O	0
			44	40	4	
55	B1	1	Total	C	O	0
			44	40	4	
55	B2	1	Total	C	O	0
			44	40	4	
55	B3	1	Total	C	O	0
			44	40	4	
55	B5	1	Total	C	O	0
			44	40	4	

- Molecule 56 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: 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 (three-letter code: 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.

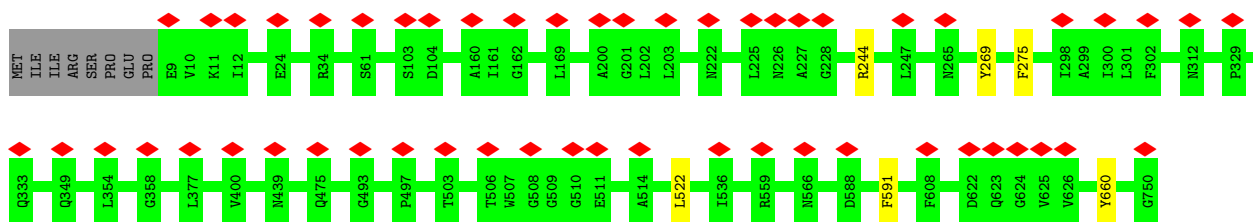
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA:  98%



- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain BA:  98%



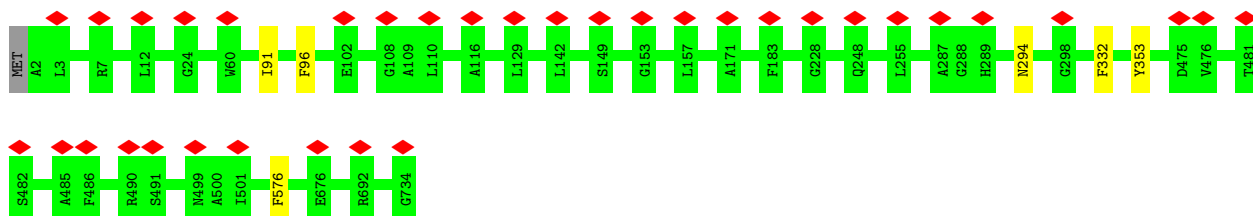
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain AB:  99%



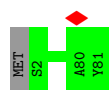
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

Chain BB:  99%



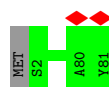
- Molecule 3: Photosystem I iron-sulfur center

Chain AC:  99%



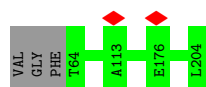
- Molecule 3: Photosystem I iron-sulfur center

Chain BC:  99%




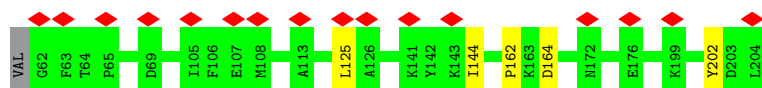
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain AD:  69% 31%



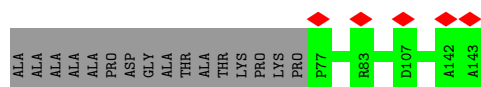
- Molecule 4: Photosystem I reaction center subunit II-2, chloroplastic

Chain BD:  8% 68% 30%



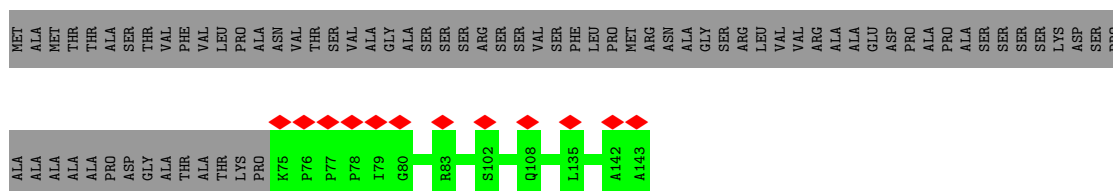
- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

Chain AE:  47% 53%

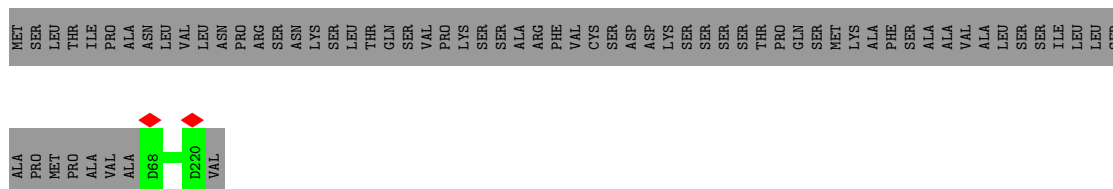


- Molecule 5: Photosystem I reaction center subunit IV A, chloroplastic

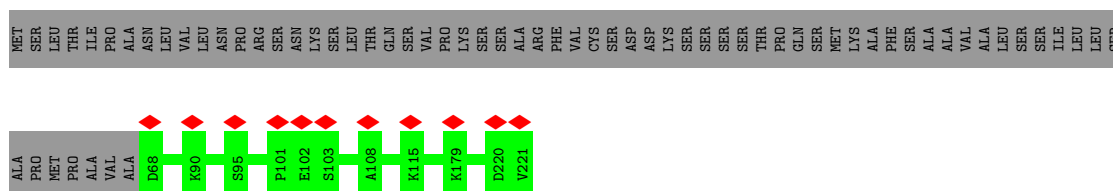
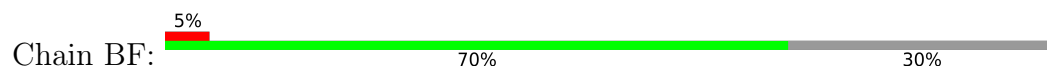
Chain BE:  8% 48% 52%



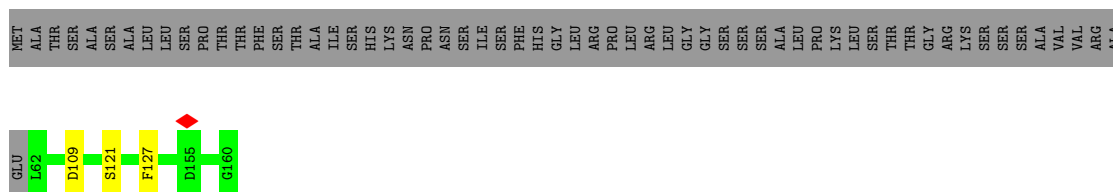
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



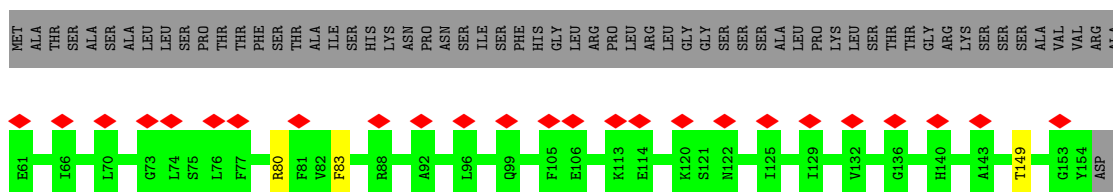
- Molecule 6: Photosystem I reaction center subunit III, chloroplastic



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

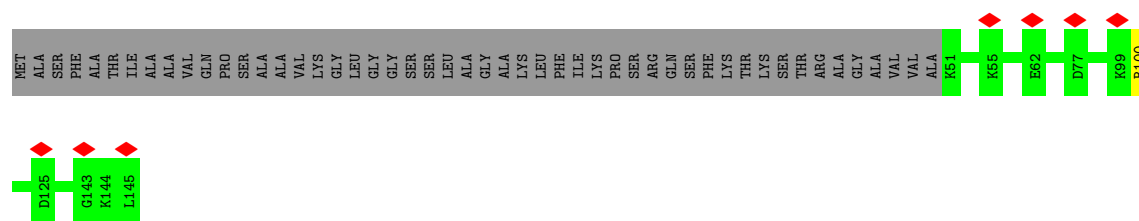


- Molecule 7: Photosystem I reaction center subunit V, chloroplastic

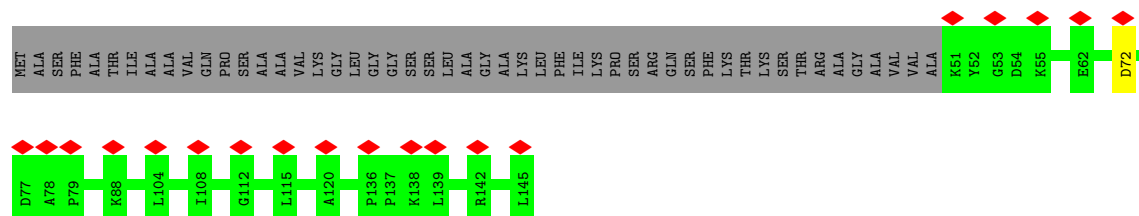


- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic

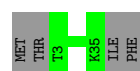
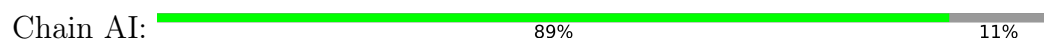




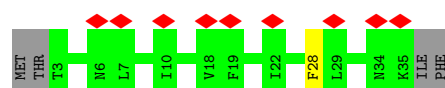
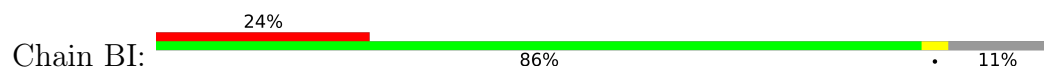
- Molecule 8: Photosystem I reaction center subunit VI-2, chloroplastic



- Molecule 9: Photosystem I reaction center subunit VIII



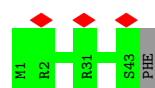
- Molecule 9: Photosystem I reaction center subunit VIII



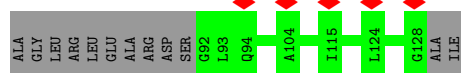
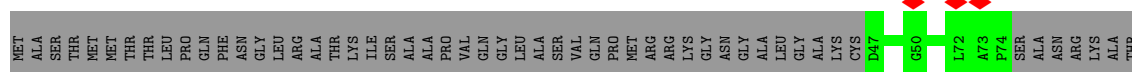
- Molecule 10: Photosystem I reaction center subunit IX



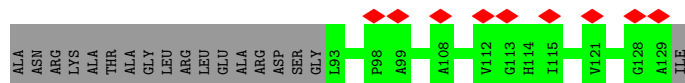
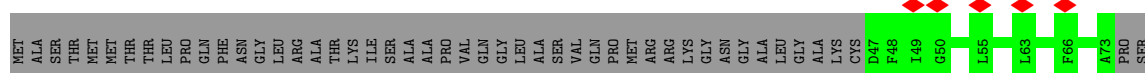
- Molecule 10: Photosystem I reaction center subunit IX



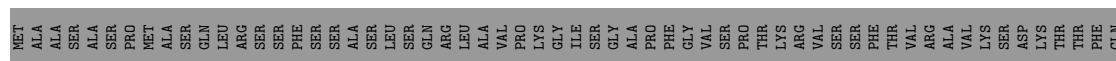
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



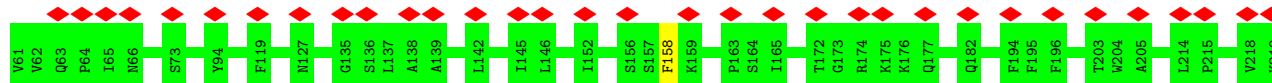
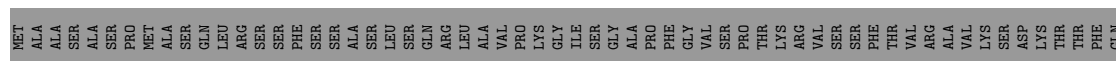
- Molecule 11: Photosystem I reaction center subunit psaK, chloroplastic



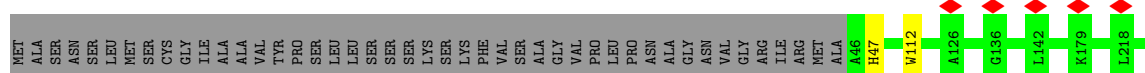
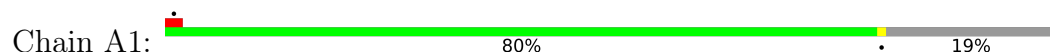
- Molecule 12: Photosystem I reaction center subunit XI, chloroplastic



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

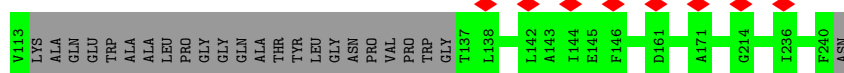
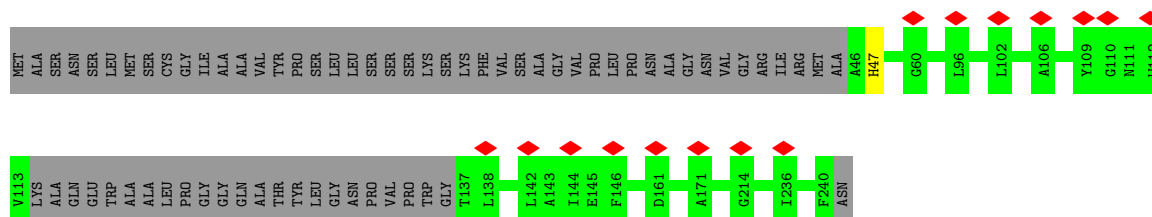
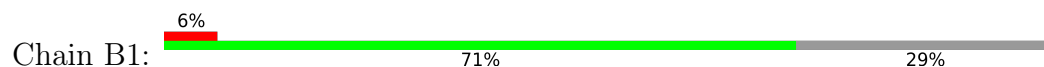


- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic

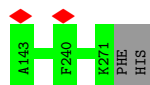
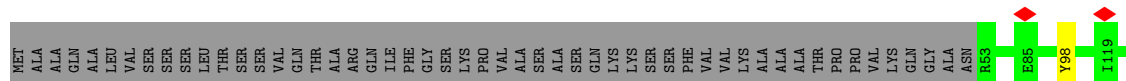
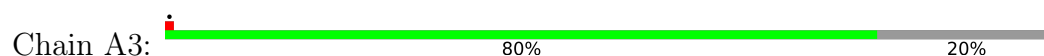




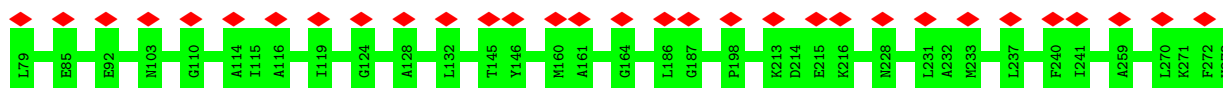
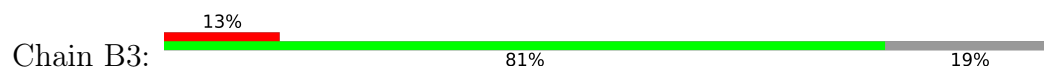
- Molecule 13: Chlorophyll a-b binding protein 6, chloroplastic



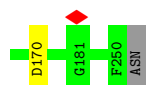
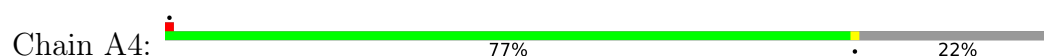
- Molecule 14: Photosystem I chlorophyll a/b-binding protein 3-1, chloroplastic




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

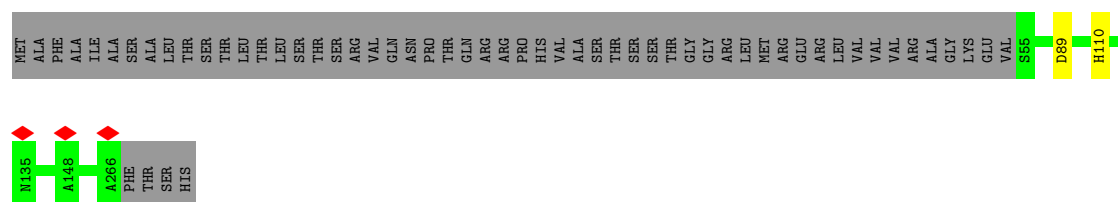


- Molecule 15: Chlorophyll a-b binding protein 4, chloroplastic




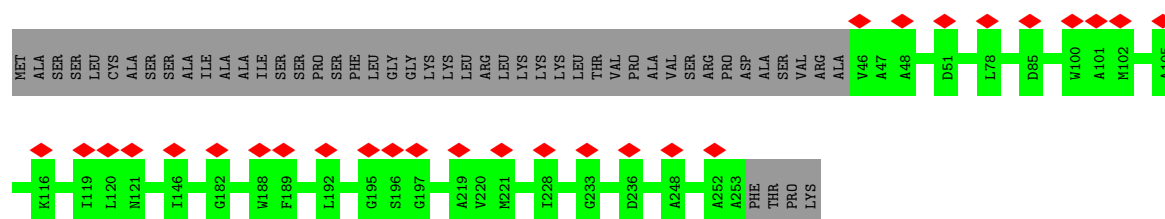
- Molecule 16: Photosystem I chlorophyll a/b-binding protein 6, chloroplastic

Chain A6:  78% 21%




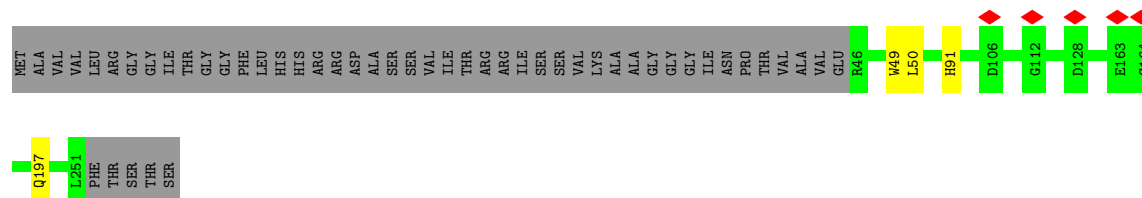
- Molecule 17: Photosystem I chlorophyll a/b-binding protein 2, chloroplastic

Chain B2:  11% 81% 19%




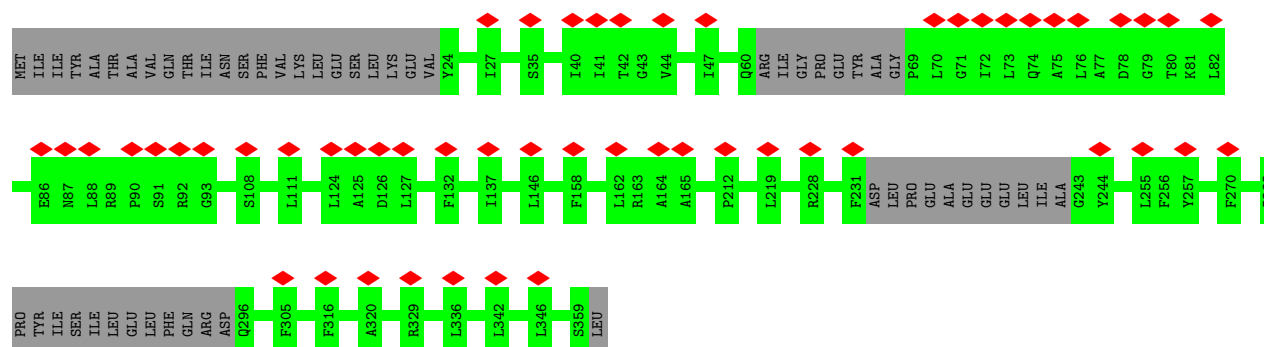
- Molecule 18: Photosystem I chlorophyll a/b-binding protein 5, chloroplastic

Chain B5:  79% 20%



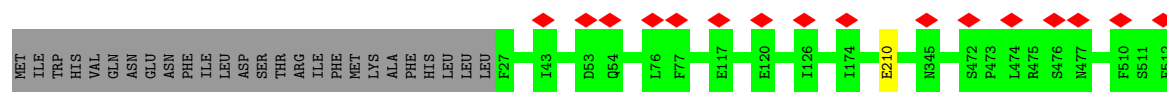
- Molecule 19: NAD(P)H-quinone oxidoreductase subunit 1, chloroplastic

Chain A:  15% 85% 15%

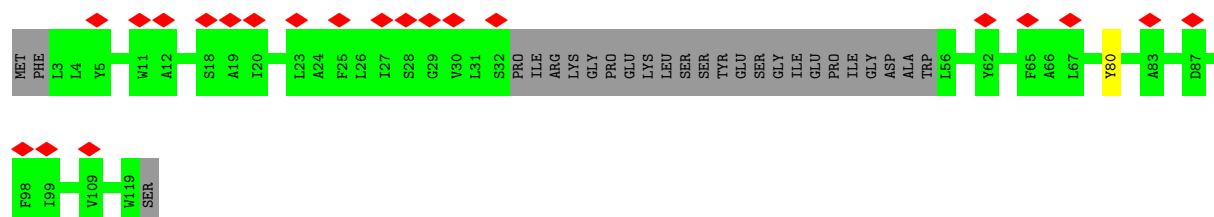
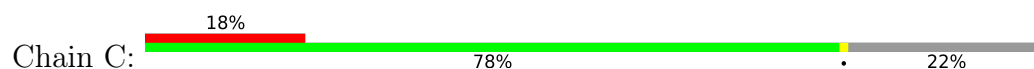


- Molecule 20: NAD(P)H-quinone oxidoreductase subunit 2, chloroplastic

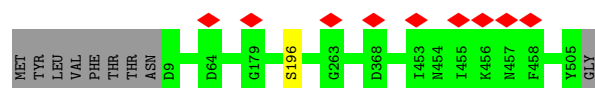
Chain B:  95% 5%



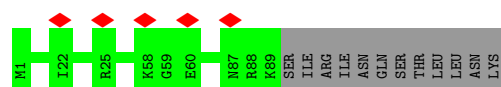
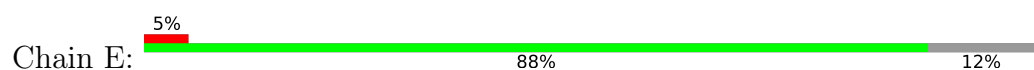
- Molecule 21: NAD(P)H-quinone oxidoreductase subunit 3, chloroplastic



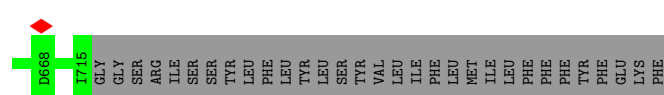
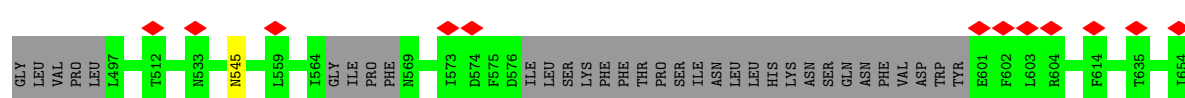
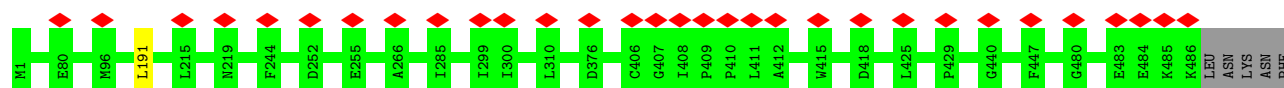
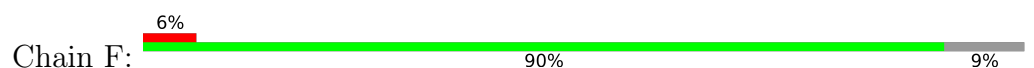
- Molecule 22: NAD(P)H-quinone oxidoreductase chain 4, chloroplastic



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

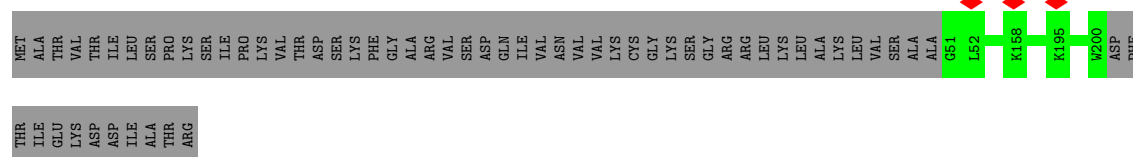


- Molecule 24: NAD(P)H-quinone oxidoreductase subunit 5, chloroplastic

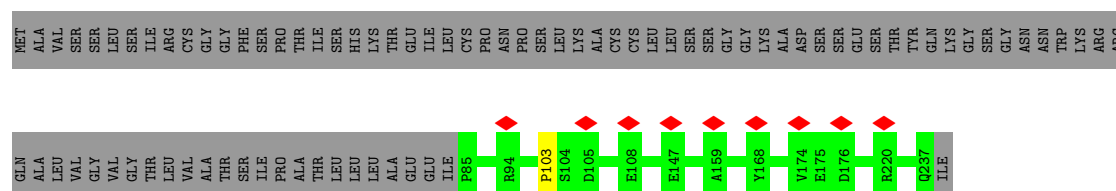


- Molecule 25: NAD(P)H-quinone oxidoreductase subunit 6, chloroplastic

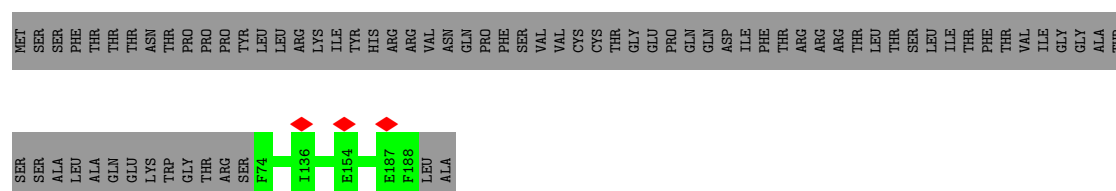




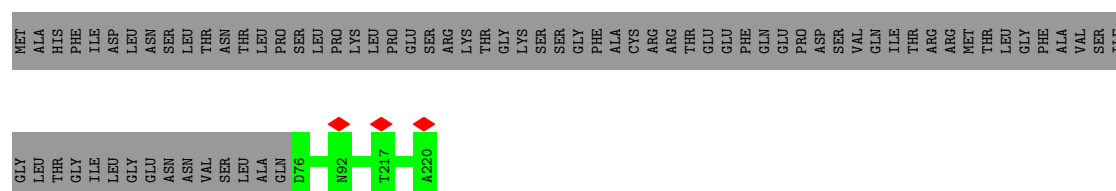
- Molecule 31: Photosynthetic NDH subunit of luminal location 1, chloroplastic



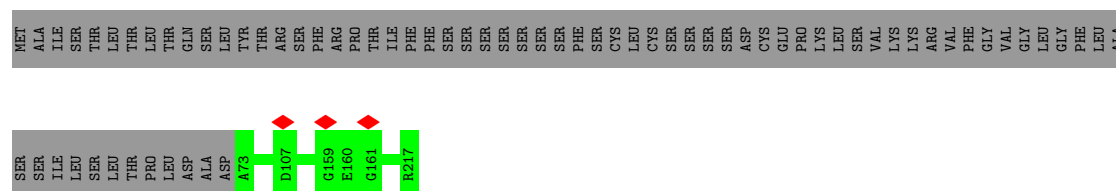
- Molecule 32: Photosynthetic NDH subunit of luminal location 2, chloroplastic



- Molecule 33: Photosynthetic NDH subunit of luminal location 3, chloroplastic

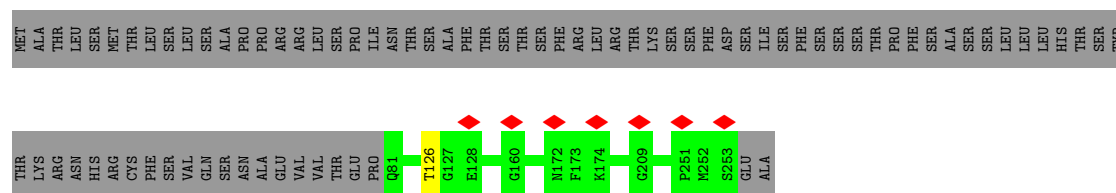


- Molecule 34: Photosynthetic NDH subunit of luminal location 4, chloroplastic

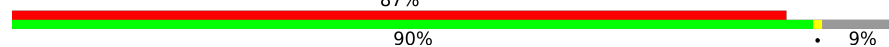


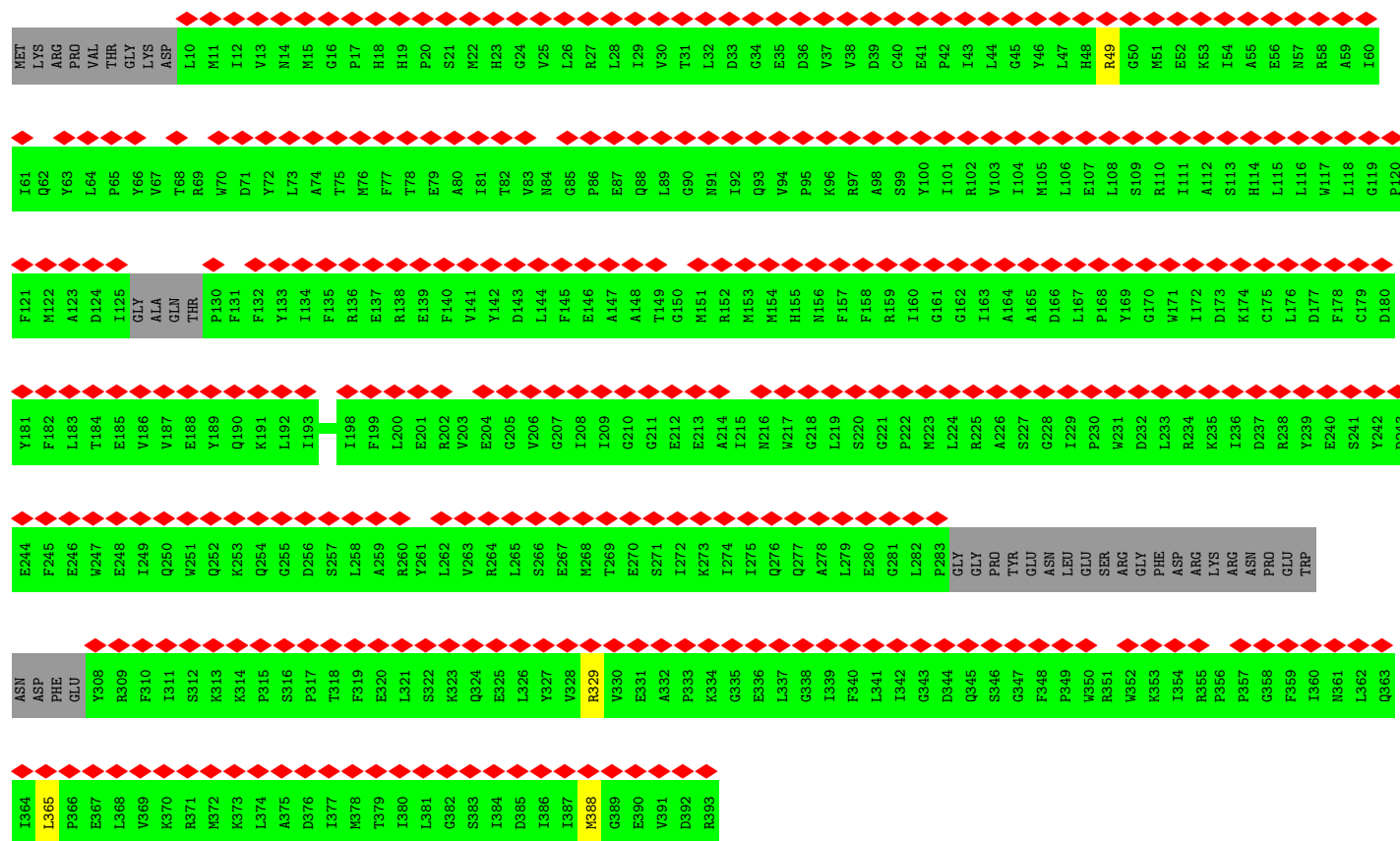
- Molecule 35: Isoform 2 of Photosynthetic NDH subunit of luminal location 5, chloroplastic

Chain j:  67% 32%



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

Chain H:  87% 90% 9%



X1	X2	X3	X4	X5	X6	X7	X8	X9	X10	X11	X12	X13	X14	X15	X16	X17	X18	X19	X20	X21	X22	X23	X24	X25	X26	X27	X28	X29	X30	X31	X32	X33	X34	X35	X36	X37	X38	X39	X40	X41	X42	X43	X44	X45	X46	X47	X48	X49	X50	X51	X52	X53	X54	X55	X56	X57	X58	X59	X60
X61	X62	X63	X64	X65	X66	X67	X68	X69	X70	X71	X72	X73	X74	X75	X76	X77	X78	X79	X80	X81	X82	X83	X84	X85	X86	X87	X88	X89	X90	X91	X92	X93	X94	X95	X96	X97	X103	X110	X111	X112	X113	X114	X120	X121	X122														

4 Experimental information

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 ($e^-/\text{\AA}^2$)	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

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	AA	0.37	0/6037	0.53	0/8236
1	BA	0.36	0/6039	0.54	0/8239
2	AB	0.36	0/6073	0.53	0/8291
2	BB	0.37	0/6065	0.54	0/8281
3	AC	0.37	0/628	0.61	0/852
3	BC	0.38	0/628	0.60	0/852
4	AD	0.31	0/1140	0.58	0/1542
4	BD	0.34	0/1156	0.61	0/1563
5	AE	0.32	0/542	0.50	0/736
5	BE	0.30	0/559	0.50	0/760
6	AF	0.31	0/1243	0.53	0/1677
6	BF	0.31	0/1250	0.55	0/1687
7	AG	0.37	0/791	0.51	0/1072
7	BG	0.32	0/750	0.50	0/1016
8	AH	0.30	0/751	0.52	0/1018
8	BH	0.31	0/751	0.52	0/1018
9	AI	0.30	0/264	0.45	0/359
9	BI	0.37	0/264	0.56	0/359
10	AJ	0.37	0/348	0.58	0/474
10	BJ	0.33	0/354	0.67	0/482
11	AK	0.31	0/456	0.53	0/617
11	BK	0.35	0/449	0.60	0/607
12	AL	0.31	0/1208	0.52	0/1650
12	BL	0.33	0/1218	0.53	0/1663
13	A1	0.31	0/1562	0.51	0/2131
13	B1	0.29	0/1381	0.51	0/1879
14	A3	0.31	0/1726	0.51	0/2347
14	B3	0.31	0/1749	0.51	0/2378
15	A4	0.33	0/1611	0.52	0/2194
16	A6	0.32	0/1732	0.55	0/2363
17	B2	0.29	0/1663	0.53	0/2277
18	B5	0.30	0/1646	0.54	0/2239

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	A	0.31	0/2430	0.60	0/3312
20	B	0.37	0/3872	0.62	0/5263
21	C	0.38	0/802	0.56	0/1094
22	D	0.41	0/4058	0.63	0/5509
23	E	0.33	0/705	0.56	0/952
24	F	0.36	0/5478	0.58	0/7446
25	G	0.31	0/1307	0.62	0/1785
26	a	0.37	0/2708	0.62	0/3668
27	b	0.31	0/2417	0.57	0/3265
28	c	0.33	0/1030	0.62	0/1401
29	d	0.41	0/784	0.59	0/1057
30	e	0.34	0/1241	0.59	0/1685
31	f	0.30	0/1312	0.57	0/1777
32	g	0.28	0/986	0.51	0/1329
33	h	0.32	0/1193	0.59	0/1610
34	i	0.32	0/1124	0.56	0/1523
35	j	0.32	0/1357	0.57	0/1823
36	H	0.28	0/2877	0.55	0/3894
37	I	0.32	0/1256	0.57	0/1701
38	J	0.26	0/1142	0.50	0/1545
39	K	0.32	0/1222	0.57	0/1656
40	L	0.32	0/669	0.58	0/911
41	M	0.34	0/783	0.56	0/1062
42	N	0.41	0/921	0.53	0/1252
43	O	0.35	0/525	0.51	0/705
All	All	0.34	0/94233	0.56	0/128084

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	39
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
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	25	60
19	A	297/360 (82%)	279 (94%)	18 (6%)	0	100	100
20	B	484/512 (94%)	443 (92%)	40 (8%)	1 (0%)	44	75
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%)	37	70
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%)	19	54
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%)	10	41
38	J	153/158 (97%)	134 (88%)	19 (12%)	0	100	100
39	K	161/225 (72%)	137 (85%)	23 (14%)	1 (1%)	22	57
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%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
43	O	69/158 (44%)	62 (90%)	7 (10%)	0	100	100
All	All	11603/14548 (80%)	10637 (92%)	955 (8%)	11 (0%)	50	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 ⓘ

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%)	591 (98%)	9 (2%)	60	74
1	BA	601/610 (98%)	595 (99%)	6 (1%)	73	81
2	AB	598/600 (100%)	591 (99%)	7 (1%)	67	78
2	BB	597/600 (100%)	591 (99%)	6 (1%)	73	81
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%)	120 (100%)	0	100	100
4	BD	121/170 (71%)	118 (98%)	3 (2%)	42	62
5	AE	56/114 (49%)	56 (100%)	0	100	100
5	BE	58/114 (51%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AF	125/185 (68%)	125 (100%)	0	100	100
6	BF	126/185 (68%)	126 (100%)	0	100	100
7	AG	83/133 (62%)	80 (96%)	3 (4%)	30	54
7	BG	79/133 (59%)	76 (96%)	3 (4%)	28	52
8	AH	77/113 (68%)	76 (99%)	1 (1%)	65	76
8	BH	77/113 (68%)	76 (99%)	1 (1%)	65	76
9	AI	29/33 (88%)	29 (100%)	0	100	100
9	BI	29/33 (88%)	28 (97%)	1 (3%)	32	55
10	AJ	37/39 (95%)	37 (100%)	0	100	100
10	BJ	38/39 (97%)	38 (100%)	0	100	100
11	AK	47/95 (50%)	47 (100%)	0	100	100
11	BK	46/95 (48%)	46 (100%)	0	100	100
12	AL	119/174 (68%)	116 (98%)	3 (2%)	42	62
12	BL	120/174 (69%)	119 (99%)	1 (1%)	79	84
13	A1	151/190 (80%)	149 (99%)	2 (1%)	65	76
13	B1	138/190 (73%)	137 (99%)	1 (1%)	81	86
14	A3	168/211 (80%)	167 (99%)	1 (1%)	84	88
14	B3	170/211 (81%)	170 (100%)	0	100	100
15	A4	164/210 (78%)	161 (98%)	3 (2%)	54	71
16	A6	177/226 (78%)	175 (99%)	2 (1%)	70	79
17	B2	165/205 (80%)	165 (100%)	0	100	100
18	B5	166/205 (81%)	163 (98%)	3 (2%)	54	71
19	A	258/312 (83%)	258 (100%)	0	100	100
20	B	420/446 (94%)	420 (100%)	0	100	100
21	C	78/103 (76%)	77 (99%)	1 (1%)	65	76
22	D	430/439 (98%)	429 (100%)	1 (0%)	92	94
23	E	75/87 (86%)	75 (100%)	0	100	100
24	F	561/661 (85%)	559 (100%)	2 (0%)	89	91
25	G	145/154 (94%)	145 (100%)	0	100	100
26	a	288/397 (72%)	286 (99%)	2 (1%)	81	86
27	b	263/297 (89%)	262 (100%)	1 (0%)	89	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
28	c	112/177 (63%)	112 (100%)	0	100	100
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%)	134 (100%)	0	100	100
32	g	104/172 (60%)	104 (100%)	0	100	100
33	h	127/192 (66%)	127 (100%)	0	100	100
34	i	114/180 (63%)	114 (100%)	0	100	100
35	j	143/219 (65%)	142 (99%)	1 (1%)	81	86
36	H	291/342 (85%)	287 (99%)	4 (1%)	62	75
37	I	132/159 (83%)	129 (98%)	3 (2%)	45	64
38	J	87/140 (62%)	85 (98%)	2 (2%)	45	64
39	K	114/205 (56%)	114 (100%)	0	100	100
40	L	66/171 (39%)	66 (100%)	0	100	100
41	M	58/195 (30%)	57 (98%)	1 (2%)	56	72
42	N	49/174 (28%)	48 (98%)	1 (2%)	50	68
43	O	36/138 (26%)	36 (100%)	0	100	100
All	All	9513/12210 (78%)	9438 (99%)	75 (1%)	77	84

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	46	ILE
1	AA	133	ARG
1	AA	141	PHE
1	AA	224	PHE
1	AA	247	LEU
1	AA	275	PHE
1	AA	308	MET
1	AA	505	LEU
1	AA	591	PHE
2	AB	5	PHE
2	AB	96	PHE
2	AB	332	PHE
2	AB	576	PHE
2	AB	577	TYR
2	AB	638	PHE

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Mol	Chain	Res	Type
2	AB	648	TRP
7	AG	109	ASP
7	AG	121	SER
7	AG	127	PHE
8	AH	100	ARG
12	AL	114	PHE
12	AL	126	ARG
12	AL	158	PHE
13	A1	47	HIS
13	A1	112	TRP
14	A3	98	TYR
15	A4	79	PRO
15	A4	136	PHE
15	A4	170	ASP
16	A6	89	ASP
16	A6	110	HIS
1	BA	244	ARG
1	BA	269	TYR
1	BA	275	PHE
1	BA	522	LEU
1	BA	591	PHE
1	BA	660	TYR
2	BB	91	ILE
2	BB	96	PHE
2	BB	294	ASN
2	BB	332	PHE
2	BB	353	TYR
2	BB	576	PHE
4	BD	125	LEU
4	BD	144	ILE
4	BD	202	TYR
7	BG	80	ARG
7	BG	83	PHE
7	BG	149	THR
8	BH	72	ASP
9	BI	28	PHE
12	BL	158	PHE
13	B1	47	HIS
18	B5	50	LEU
18	B5	91	HIS
18	B5	197	GLN
21	C	80	TYR

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Mol	Chain	Res	Type
22	D	196	SER
24	F	191	LEU
24	F	545	ASN
26	a	164	LYS
26	a	221	ARG
27	b	257	ARG
35	j	126	THR
36	H	49	ARG
36	H	329	ARG
36	H	365	LEU
36	H	388	MET
37	I	30	LEU
37	I	67	CYS
37	I	78	LEU
38	J	33	PRO
38	J	52	ARG
41	M	110	GLU
42	N	176	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (70) such sidechains are listed below:

Mol	Chain	Res	Type
1	AA	243	ASN
1	AA	628	HIS
2	AB	452	GLN
6	AF	213	ASN
7	AG	90	ASN
8	AH	86	GLN
8	AH	121	ASN
11	AK	126	ASN
12	AL	66	ASN
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	250	ASN
1	BA	214	GLN
1	BA	713	GLN
2	BB	350	GLN

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Mol	Chain	Res	Type
4	BD	200	GLN
7	BG	99	GLN
7	BG	140	HIS
11	BK	94	GLN
13	B1	208	GLN
14	B3	103	ASN
14	B3	172	GLN
14	B3	183	GLN
14	B3	242	GLN
14	B3	253	ASN
18	B5	197	GLN
18	B5	241	ASN
19	A	128	ASN
19	A	211	GLN
20	B	90	ASN
20	B	222	GLN
20	B	331	GLN
22	D	248	HIS
23	E	54	ASN
23	E	87	ASN
24	F	35	ASN
24	F	71	ASN
24	F	206	GLN
24	F	214	ASN
24	F	644	ASN
25	G	56	HIS
25	G	62	GLN
26	a	129	ASN
26	a	170	ASN
26	a	177	HIS
26	a	209	HIS
26	a	230	ASN
26	a	352	HIS
26	a	400	ASN
27	b	347	ASN
29	d	93	ASN
30	e	164	ASN
30	e	193	ASN
31	f	156	HIS
31	f	179	ASN
31	f	225	GLN
33	h	96	ASN

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Mol	Chain	Res	Type
33	h	162	ASN
33	h	185	ASN
34	i	116	ASN
34	i	198	ASN
35	j	249	GLN
37	I	109	ASN
37	I	133	HIS
38	J	54	GLN

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	AA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.38	9 (11%)
45	CLA	BA	844	47	41,49,73	1.90	5 (12%)	47,84,113	1.43	8 (17%)
45	CLA	B1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.51	6 (11%)
54	CHL	A3	307	-	45,53,74	2.29	16 (35%)	52,89,114	2.69	21 (40%)
45	CLA	AB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.59	14 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	AJ	101	-	41,41,41	0.89	1 (2%)	56,56,56	1.98	16 (28%)
45	CLA	AB	833	-	65,73,73	1.49	9 (13%)	76,113,113	1.18	7 (9%)
54	CHL	A4	305	-	41,49,74	2.25	13 (31%)	51,84,114	2.78	20 (39%)
48	BCR	BA	856	-	41,41,41	0.93	1 (2%)	56,56,56	2.15	17 (30%)
45	CLA	A1	307	-	39,48,73	1.89	9 (23%)	45,82,113	1.74	11 (24%)
45	CLA	A1	312	47	37,46,73	2.01	7 (18%)	46,81,113	1.43	10 (21%)
45	CLA	AA	834	-	65,73,73	1.47	10 (15%)	76,113,113	1.48	14 (18%)
45	CLA	BA	827	-	65,73,73	1.47	6 (9%)	76,113,113	1.23	7 (9%)
45	CLA	AL	303	12	41,49,73	1.91	7 (17%)	47,84,113	1.46	8 (17%)
48	BCR	BB	848	-	41,41,41	0.81	0	56,56,56	2.15	19 (33%)
45	CLA	A3	304	-	41,50,73	1.94	7 (17%)	51,86,113	1.50	9 (17%)
45	CLA	BB	836	-	60,68,73	1.56	8 (13%)	70,107,113	1.38	7 (10%)
52	LUT	A3	316	-	42,43,43	0.84	0	51,60,60	1.78	14 (27%)
47	LHG	A1	320	45	48,48,48	0.93	2 (4%)	51,54,54	0.84	2 (3%)
48	BCR	BA	855	-	41,41,41	0.77	0	56,56,56	2.19	24 (42%)
47	LHG	AJ	104	-	39,39,48	1.06	2 (5%)	42,45,54	0.92	2 (4%)
57	FES	c	301	28	0,4,4	-	-	-	-	-
54	CHL	A6	602	16	51,60,74	2.24	18 (35%)	54,97,114	2.65	26 (48%)
48	BCR	AJ	103	-	41,41,41	0.74	0	56,56,56	2.38	22 (39%)
45	CLA	A4	308	15	54,62,73	1.67	8 (14%)	62,99,113	1.29	9 (14%)
45	CLA	BB	804	-	65,73,73	1.49	9 (13%)	76,113,113	1.27	8 (10%)
45	CLA	AB	832	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	9 (11%)
45	CLA	BA	837	-	51,59,73	1.63	8 (15%)	59,96,113	1.47	7 (11%)
55	XAT	B5	615	-	39,47,47	0.99	2 (5%)	54,74,74	2.41	18 (33%)
45	CLA	BB	816	-	64,72,73	1.51	9 (14%)	75,112,113	1.35	8 (10%)
52	LUT	B2	615	-	42,43,43	0.81	0	51,60,60	1.98	15 (29%)
45	CLA	BB	812	-	65,73,73	1.47	7 (10%)	76,113,113	1.37	10 (13%)
45	CLA	BA	835	-	45,53,73	1.81	7 (15%)	52,89,113	1.43	6 (11%)
45	CLA	AB	805	-	41,49,73	1.81	6 (14%)	47,84,113	1.55	8 (17%)
45	CLA	AA	824	-	53,62,73	1.68	8 (15%)	61,100,113	1.50	11 (18%)
45	CLA	BA	817	-	60,68,73	1.52	6 (10%)	70,107,113	1.37	11 (15%)
48	BCR	AL	302	-	41,41,41	0.78	0	56,56,56	2.22	22 (39%)
45	CLA	B5	613	-	45,53,73	1.80	7 (15%)	52,89,113	1.37	7 (13%)
45	CLA	AB	836	-	42,50,73	1.86	7 (16%)	48,85,113	1.52	7 (14%)
45	CLA	AJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
47	LHG	B1	318	45	41,41,48	1.01	2 (4%)	44,47,54	0.95	2 (4%)
45	CLA	A1	314	-	63,72,73	1.52	8 (12%)	73,112,113	1.30	9 (12%)
45	CLA	BA	832	-	56,64,73	1.59	8 (14%)	65,102,113	1.31	8 (12%)
47	LHG	B1	301	45	37,37,48	1.08	2 (5%)	40,43,54	1.01	3 (7%)
45	CLA	A6	610	16	55,63,73	1.67	9 (16%)	64,101,113	1.33	10 (15%)
49	SF4	K	301	39	0,12,12	-	-	-	-	-
48	BCR	BB	847	-	41,41,41	0.87	1 (2%)	56,56,56	1.93	11 (19%)
45	CLA	A3	309	14	41,49,73	1.88	8 (19%)	47,84,113	1.49	10 (21%)
45	CLA	B5	609	18	54,62,73	1.67	9 (16%)	62,99,113	1.26	8 (12%)
45	CLA	BB	838	-	50,58,73	1.67	7 (14%)	58,95,113	1.50	9 (15%)
45	CLA	BB	839	-	65,73,73	1.49	8 (12%)	76,113,113	1.28	6 (7%)
45	CLA	BA	830	-	65,73,73	1.53	9 (13%)	76,113,113	1.23	8 (10%)
48	BCR	AF	801	-	41,41,41	0.86	1 (2%)	56,56,56	1.56	10 (17%)
45	CLA	AA	816	-	45,53,73	1.82	9 (20%)	52,89,113	1.58	9 (17%)
45	CLA	BA	838	-	55,62,73	1.69	8 (14%)	59,99,113	1.45	11 (18%)
45	CLA	AA	804	-	52,60,73	1.65	8 (15%)	60,97,113	1.54	7 (11%)
45	CLA	A3	305	-	40,49,73	1.90	7 (17%)	45,84,113	1.45	7 (15%)
45	CLA	B3	304	-	40,49,73	1.91	7 (17%)	45,84,113	1.44	7 (15%)
47	LHG	A1	302	-	35,35,48	1.10	2 (5%)	38,41,54	1.04	2 (5%)
45	CLA	B2	609	17	55,63,73	1.66	8 (14%)	64,101,113	1.34	10 (15%)
48	BCR	B5	616	-	41,41,41	0.79	0	56,56,56	2.31	23 (41%)
45	CLA	AB	828	-	65,73,73	1.46	8 (12%)	76,113,113	1.43	8 (10%)
45	CLA	B3	308	14	41,49,73	1.85	8 (19%)	47,84,113	1.45	7 (14%)
45	CLA	AA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.40	12 (15%)
45	CLA	BB	821	-	55,63,73	1.64	8 (14%)	64,101,113	1.14	5 (7%)
48	BCR	BA	850	-	41,41,41	0.78	0	56,56,56	2.09	11 (19%)
45	CLA	AB	817	-	55,63,73	1.63	8 (14%)	64,101,113	1.34	7 (10%)
45	CLA	A3	311	14	43,51,73	1.82	5 (11%)	49,86,113	1.48	7 (14%)
48	BCR	AB	846	-	41,41,41	0.86	0	56,56,56	2.07	16 (28%)
45	CLA	AA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.45	8 (15%)
45	CLA	BB	819	-	59,67,73	1.57	9 (15%)	68,105,113	1.40	9 (13%)
45	CLA	B5	612	18	57,65,73	1.62	8 (14%)	66,103,113	1.28	7 (10%)
54	CHL	B5	606	-	40,48,74	2.31	13 (32%)	50,83,114	2.83	21 (42%)
45	CLA	BB	828	-	62,70,73	1.51	7 (11%)	72,109,113	1.48	11 (15%)
45	CLA	AA	821	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
52	LUT	B3	315	-	42,43,43	0.97	1 (2%)	51,60,60	2.10	17 (33%)
45	CLA	BF	303	-	41,49,73	1.86	6 (14%)	47,84,113	1.47	8 (17%)
53	LMG	AG	202	-	38,38,55	1.14	3 (7%)	46,46,63	1.07	2 (4%)
45	CLA	AA	819	-	65,73,73	1.48	10 (15%)	76,113,113	1.43	9 (11%)
45	CLA	BK	203	-	46,54,73	1.73	6 (13%)	53,90,113	1.54	6 (11%)
45	CLA	AA	838	-	55,63,73	1.61	9 (16%)	64,101,113	1.29	10 (15%)
45	CLA	BA	813	-	65,73,73	1.46	7 (10%)	76,113,113	1.33	8 (10%)
54	CHL	A4	306	-	46,54,74	2.32	17 (36%)	49,90,114	2.85	21 (42%)
45	CLA	BA	804	-	52,60,73	1.66	7 (13%)	60,97,113	1.56	11 (18%)
45	CLA	B5	610	47	42,50,73	1.86	7 (16%)	48,85,113	1.47	7 (14%)
47	LHG	BA	846	45	26,26,48	1.06	2 (7%)	29,32,54	1.00	1 (3%)
45	CLA	BL	304	-	43,51,73	1.78	6 (13%)	49,86,113	1.47	7 (14%)
45	CLA	BA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.45	11 (14%)
45	CLA	AB	821	-	50,58,73	1.70	8 (16%)	58,95,113	1.49	8 (13%)
54	CHL	B1	308	-	40,49,74	2.55	18 (45%)	41,84,114	2.79	17 (41%)
45	CLA	A6	613	16	64,72,73	1.53	8 (12%)	74,111,113	1.28	7 (9%)
45	CLA	AA	839	-	52,60,73	1.66	8 (15%)	60,97,113	1.37	7 (11%)
45	CLA	BA	812	-	54,62,73	1.59	9 (16%)	62,99,113	1.46	8 (12%)
48	BCR	AK	204	-	41,41,41	1.02	3 (7%)	56,56,56	2.06	14 (25%)
45	CLA	AB	814	-	65,73,73	1.49	10 (15%)	76,113,113	1.30	7 (9%)
45	CLA	AB	823	-	65,73,73	1.50	9 (13%)	76,113,113	1.31	9 (11%)
48	BCR	AG	205	-	41,41,41	0.93	0	56,56,56	2.00	18 (32%)
45	CLA	A4	301	15	60,68,73	1.55	9 (15%)	70,107,113	1.33	10 (14%)
45	CLA	AF	802	-	57,65,73	1.58	11 (19%)	66,103,113	1.43	9 (13%)
55	XAT	A3	317	-	39,47,47	0.97	1 (2%)	54,74,74	2.31	19 (35%)
45	CLA	AA	820	-	45,53,73	1.78	8 (17%)	52,89,113	1.46	7 (13%)
48	BCR	BB	849	-	41,41,41	0.90	1 (2%)	56,56,56	1.86	16 (28%)
45	CLA	A6	609	16	45,53,73	1.80	7 (15%)	52,89,113	1.42	7 (13%)
45	CLA	AB	819	-	60,68,73	1.53	9 (15%)	70,107,113	1.64	12 (17%)
45	CLA	BA	826	-	53,61,73	1.62	7 (13%)	61,98,113	1.40	10 (16%)
47	LHG	F	801	-	36,36,48	0.73	1 (2%)	39,42,54	1.22	3 (7%)
48	BCR	AA	845	-	41,41,41	1.03	2 (4%)	56,56,56	1.91	13 (23%)
45	CLA	AF	804	-	41,49,73	1.87	7 (17%)	47,84,113	1.59	8 (17%)
45	CLA	B3	310	14	43,51,73	1.82	5 (11%)	49,86,113	1.44	8 (16%)
51	DGD	AB	851	-	67,67,67	0.80	2 (2%)	81,81,81	0.99	4 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	AA	828	-	65,73,73	1.45	7 (10%)	76,113,113	1.56	9 (11%)
45	CLA	AG	201	-	43,52,73	1.87	7 (16%)	49,88,113	1.48	7 (14%)
55	XAT	A6	616	-	39,47,47	0.98	2 (5%)	54,74,74	2.49	21 (38%)
45	CLA	B2	602	17	65,73,73	1.51	9 (13%)	76,113,113	1.26	10 (13%)
50	LMU	AB	850	-	36,36,36	1.13	2 (5%)	47,47,47	1.08	4 (8%)
54	CHL	A1	308	13	40,49,74	2.48	18 (45%)	41,84,114	2.86	17 (41%)
45	CLA	B3	313	-	37,44,73	1.95	9 (24%)	42,77,113	1.35	7 (16%)
46	PQN	AB	843	-	34,34,34	3.39	11 (32%)	42,45,45	1.83	6 (14%)
46	PQN	BA	843	-	34,34,34	3.47	12 (35%)	42,45,45	1.62	5 (11%)
45	CLA	AB	807	2	65,73,73	1.45	10 (15%)	76,113,113	1.35	8 (10%)
45	CLA	AK	202	-	45,53,73	1.82	6 (13%)	52,89,113	1.41	7 (13%)
45	CLA	AB	831	-	43,51,73	1.84	9 (20%)	49,86,113	1.33	8 (16%)
45	CLA	A3	308	14	45,53,73	1.80	8 (17%)	52,89,113	1.43	8 (15%)
45	CLA	A3	303	14	55,63,73	1.67	9 (16%)	64,101,113	1.46	9 (14%)
54	CHL	B2	607	-	46,54,74	2.33	17 (36%)	49,90,114	2.82	20 (40%)
45	CLA	AA	812	-	54,62,73	1.61	9 (16%)	62,99,113	1.51	8 (12%)
51	DGD	BB	850	-	67,67,67	0.81	2 (2%)	81,81,81	0.98	4 (4%)
56	SQD	e	301	-	33,34,54	1.20	6 (18%)	42,45,65	1.77	10 (23%)
45	CLA	B1	304	13	61,69,73	1.52	7 (11%)	71,108,113	1.39	8 (11%)
45	CLA	A1	316	13	43,51,73	1.89	7 (16%)	54,87,113	1.63	9 (16%)
45	CLA	AB	804	-	65,73,73	1.45	10 (15%)	76,113,113	1.69	15 (19%)
45	CLA	A3	306	14	41,49,73	1.90	7 (17%)	51,84,113	1.67	9 (17%)
45	CLA	BK	202	-	45,53,73	1.81	6 (13%)	52,89,113	1.47	7 (13%)
45	CLA	BB	830	-	65,73,73	1.50	9 (13%)	76,113,113	1.26	8 (10%)
45	CLA	BA	815	-	42,50,73	1.79	8 (19%)	48,85,113	1.51	6 (12%)
48	BCR	BB	803	-	41,41,41	0.85	0	56,56,56	1.99	19 (33%)
45	CLA	A1	311	13	59,67,73	1.57	7 (11%)	69,106,113	1.27	8 (11%)
45	CLA	BB	806	-	41,49,73	1.80	7 (17%)	47,84,113	1.58	9 (19%)
48	BCR	AA	849	-	41,41,41	0.91	2 (4%)	56,56,56	2.12	20 (35%)
45	CLA	BB	810	-	65,73,73	1.50	8 (12%)	76,113,113	1.33	12 (15%)
49	SF4	AA	850	1,2	0,12,12	-	-	-	-	-
45	CLA	B1	306	-	41,49,73	1.86	5 (12%)	47,84,113	1.45	7 (14%)
45	CLA	B2	604	-	43,51,73	1.84	6 (13%)	48,86,113	1.43	7 (14%)
48	BCR	BA	848	-	41,41,41	0.80	0	56,56,56	2.03	17 (30%)
48	BCR	BB	846	-	41,41,41	0.85	1 (2%)	56,56,56	2.14	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A1	305	-	55,63,73	1.63	7 (12%)	64,101,113	1.60	10 (15%)
56	SQD	BJ	104	-	46,47,54	1.28	5 (10%)	55,58,65	4.16	12 (21%)
45	CLA	AA	836	1	45,53,73	1.85	7 (15%)	52,89,113	1.47	8 (15%)
45	CLA	A4	302	15	44,52,73	1.85	8 (18%)	55,88,113	1.61	9 (16%)
47	LHG	BA	845	-	48,48,48	0.88	2 (4%)	51,54,54	0.97	3 (5%)
45	CLA	AH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.36	10 (14%)
52	LUT	B5	614	-	42,43,43	0.83	1 (2%)	51,60,60	1.85	15 (29%)
45	CLA	BB	801	-	65,73,73	1.47	9 (13%)	76,113,113	1.47	13 (17%)
54	CHL	A4	304	-	40,49,74	2.45	16 (40%)	42,84,114	2.82	20 (47%)
45	CLA	BG	201	-	42,50,73	1.85	7 (16%)	48,85,113	1.28	7 (14%)
48	BCR	B2	617	-	41,41,41	0.89	1 (2%)	56,56,56	2.47	23 (41%)
47	LHG	A1	301	45	37,37,48	1.07	2 (5%)	40,43,54	0.97	3 (7%)
45	CLA	AA	815	-	40,49,73	1.79	5 (12%)	44,83,113	1.62	8 (18%)
50	LMU	BB	851	-	36,36,36	1.10	2 (5%)	47,47,47	0.89	0
45	CLA	BB	805	-	65,73,73	1.43	10 (15%)	76,113,113	1.56	12 (15%)
47	LHG	a	501	-	28,28,48	0.89	1 (3%)	31,34,54	1.24	2 (6%)
48	BCR	AB	849	-	41,41,41	0.83	0	56,56,56	2.41	24 (42%)
45	CLA	BA	841	-	65,73,73	1.47	8 (12%)	76,113,113	1.55	11 (14%)
45	CLA	AB	838	-	65,73,73	1.46	7 (10%)	76,113,113	1.34	8 (10%)
54	CHL	B5	607	-	45,53,74	2.37	17 (37%)	49,89,114	2.81	19 (38%)
48	BCR	AA	848	-	41,41,41	0.77	1 (2%)	56,56,56	1.97	16 (28%)
45	CLA	A3	313	-	39,48,73	1.91	7 (17%)	44,83,113	1.46	8 (18%)
45	CLA	AB	816	-	43,51,73	1.80	7 (16%)	49,86,113	1.42	6 (12%)
45	CLA	BB	811	2	65,73,73	1.48	10 (15%)	76,113,113	1.37	9 (11%)
45	CLA	AA	803	-	65,73,73	1.47	10 (15%)	76,113,113	1.36	11 (14%)
45	CLA	A1	304	13	60,68,73	1.52	9 (15%)	69,106,113	1.33	8 (11%)
50	LMU	AB	852	-	36,36,36	1.14	2 (5%)	47,47,47	0.94	1 (2%)
45	CLA	AA	810	-	65,72,73	1.55	9 (13%)	71,111,113	1.29	7 (9%)
48	BCR	A3	318	-	41,41,41	0.98	1 (2%)	56,56,56	2.77	20 (35%)
45	CLA	BA	802	-	65,73,73	1.54	9 (13%)	76,113,113	1.38	6 (7%)
49	SF4	BA	852	1,2	0,12,12	-	-	-	-	-
45	CLA	AB	809	-	65,73,73	1.52	8 (12%)	76,113,113	1.36	10 (13%)
45	CLA	B5	601	18	46,54,73	1.75	8 (17%)	53,90,113	1.37	7 (13%)
48	BCR	BL	305	-	41,41,41	0.78	0	56,56,56	2.22	20 (35%)
48	BCR	BG	203	-	41,41,41	0.91	2 (4%)	56,56,56	6.99	26 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BA	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.47	10 (13%)
45	CLA	BA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.20	6 (7%)
45	CLA	BB	808	2	65,73,73	1.47	9 (13%)	76,113,113	1.33	7 (9%)
45	CLA	AA	801	-	65,73,73	1.50	7 (10%)	76,113,113	1.27	8 (10%)
45	CLA	AB	811	-	65,73,73	1.46	8 (12%)	76,113,113	1.48	10 (13%)
45	CLA	BA	811	-	65,73,73	1.50	8 (12%)	76,113,113	1.28	8 (10%)
45	CLA	BA	821	-	65,73,73	1.50	9 (13%)	76,113,113	1.39	10 (13%)
46	PQN	BB	844	-	34,34,34	3.42	10 (29%)	42,45,45	1.66	8 (19%)
45	CLA	AB	837	-	50,58,73	1.69	9 (18%)	58,95,113	1.51	8 (13%)
53	LMG	B5	617	-	33,33,55	1.18	2 (6%)	41,41,63	1.20	4 (9%)
45	CLA	B3	311	-	53,62,73	1.69	7 (13%)	61,100,113	1.25	6 (9%)
45	CLA	A3	312	-	53,62,73	1.67	7 (13%)	61,100,113	1.39	8 (13%)
45	CLA	A6	603	16	65,73,73	1.51	9 (13%)	76,113,113	1.29	9 (11%)
48	BCR	A4	317	-	41,41,41	0.82	0	56,56,56	2.37	23 (41%)
45	CLA	AB	841	-	65,73,73	1.54	9 (13%)	76,113,113	1.22	6 (7%)
55	XAT	B2	616	-	39,47,47	1.01	1 (2%)	54,74,74	2.30	20 (37%)
52	LUT	A6	615	-	42,43,43	0.90	1 (2%)	51,60,60	1.59	12 (23%)
54	CHL	B2	606	-	43,51,74	2.40	16 (37%)	45,86,114	2.78	17 (37%)
48	BCR	BA	851	-	41,41,41	0.87	1 (2%)	56,56,56	1.99	20 (35%)
45	CLA	BL	302	12	45,53,73	1.85	8 (17%)	52,89,113	1.60	11 (21%)
45	CLA	A6	611	47	38,45,73	2.88	9 (23%)	41,76,113	1.68	9 (21%)
45	CLA	AA	830	-	65,73,73	1.52	9 (13%)	76,113,113	1.31	8 (10%)
45	CLA	BL	303	-	60,68,73	1.58	8 (13%)	70,107,113	1.37	10 (14%)
45	CLA	AB	803	-	65,73,73	1.49	8 (12%)	76,113,113	1.23	7 (9%)
45	CLA	B1	314	-	60,68,73	1.60	7 (11%)	70,107,113	1.24	10 (14%)
50	LMU	AA	851	-	36,36,36	1.16	2 (5%)	47,47,47	1.04	2 (4%)
45	CLA	AA	806	1	65,73,73	1.49	9 (13%)	76,113,113	1.38	8 (10%)
48	BCR	AI	102	-	41,41,41	0.86	0	56,56,56	2.54	18 (32%)
47	LHG	BF	305	-	44,44,48	0.97	2 (4%)	47,50,54	1.09	3 (6%)
45	CLA	AA	826	-	59,67,73	1.56	9 (15%)	68,105,113	1.28	8 (11%)
48	BCR	A6	617	-	41,41,41	0.99	2 (4%)	56,56,56	2.01	16 (28%)
45	CLA	BB	827	-	62,70,73	1.52	8 (12%)	72,109,113	1.27	8 (11%)
55	XAT	A4	316	-	39,47,47	0.95	2 (5%)	54,74,74	2.29	16 (29%)
45	CLA	BA	824	-	55,63,73	1.63	9 (16%)	64,101,113	1.39	8 (12%)
45	CLA	A6	614	-	43,51,73	1.89	6 (13%)	49,86,113	1.47	7 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	A1	313	13	45,53,73	1.78	7 (15%)	52,89,113	1.57	7 (13%)
45	CLA	A6	605	-	43,51,73	1.83	8 (18%)	48,86,113	1.40	7 (14%)
48	BCR	B3	317	-	41,41,41	0.84	0	56,56,56	3.61	28 (50%)
45	CLA	AB	808	-	51,59,73	1.67	9 (17%)	58,95,113	1.45	7 (12%)
45	CLA	A4	312	-	45,53,73	1.81	7 (15%)	52,89,113	1.40	7 (13%)
48	BCR	BL	301	-	41,41,41	0.87	1 (2%)	56,56,56	2.36	14 (25%)
47	LHG	A3	319	45	22,22,48	1.44	2 (9%)	25,28,54	1.27	2 (8%)
45	CLA	BA	820	-	45,53,73	1.73	7 (15%)	52,89,113	1.50	6 (11%)
45	CLA	A6	612	16	44,52,73	1.84	7 (15%)	51,88,113	1.37	6 (11%)
48	BCR	AF	805	-	41,41,41	0.81	0	56,56,56	1.86	14 (25%)
52	LUT	B1	316	-	42,43,43	1.60	8 (19%)	51,60,60	1.51	10 (19%)
52	LUT	AF	806	-	42,43,43	1.03	3 (7%)	51,60,60	1.72	12 (23%)
45	CLA	B3	307	14	45,53,73	1.79	6 (13%)	52,89,113	1.50	8 (15%)
45	CLA	A3	310	47	36,45,73	1.97	6 (16%)	43,79,113	1.48	8 (18%)
45	CLA	AB	802	-	64,72,73	1.60	8 (12%)	79,112,113	1.34	9 (11%)
45	CLA	B3	309	47	39,48,73	1.93	5 (12%)	44,83,113	1.40	7 (15%)
45	CLA	A1	306	-	49,57,73	1.71	7 (14%)	55,93,113	1.45	8 (14%)
48	BCR	BF	304	-	41,41,41	0.87	1 (2%)	56,56,56	1.94	19 (33%)
45	CLA	BA	810	-	65,73,73	1.50	9 (13%)	76,113,113	1.22	7 (9%)
45	CLA	BA	842	-	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
45	CLA	BB	817	-	41,50,73	1.80	7 (17%)	46,85,113	1.48	7 (15%)
49	SF4	BC	102	3	0,12,12	-	-	-	-	-
45	CLA	AA	807	-	50,58,73	1.69	8 (16%)	58,95,113	1.43	6 (10%)
45	CLA	AA	802	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	6 (7%)
45	CLA	AA	813	-	65,73,73	1.47	9 (13%)	76,113,113	1.38	8 (10%)
45	CLA	BF	302	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	BA	816	-	45,53,73	1.81	7 (15%)	52,89,113	1.45	8 (15%)
45	CLA	BB	802	-	65,73,73	1.55	9 (13%)	76,113,113	1.42	8 (10%)
45	CLA	AA	831	-	47,55,73	1.78	9 (19%)	54,91,113	1.43	7 (12%)
45	CLA	AB	815	-	65,73,73	1.46	8 (12%)	76,113,113	1.39	9 (11%)
45	CLA	BB	823	-	45,54,73	1.75	6 (13%)	51,90,113	1.31	8 (15%)
45	CLA	BB	841	-	65,73,73	1.48	9 (13%)	76,113,113	1.30	7 (9%)
45	CLA	A6	601	15	46,54,73	1.73	8 (17%)	53,90,113	1.46	8 (15%)
45	CLA	B3	302	14	55,63,73	1.61	7 (12%)	64,101,113	1.34	8 (12%)
45	CLA	B3	303	-	41,50,73	1.94	7 (17%)	51,86,113	1.55	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BB	832	-	43,51,73	1.83	8 (18%)	49,86,113	1.30	6 (12%)
45	CLA	B5	611	18	40,49,73	1.87	8 (20%)	45,84,113	1.47	7 (15%)
45	CLA	BH	201	-	60,68,73	1.60	7 (11%)	70,107,113	1.29	8 (11%)
48	BCR	BI	101	-	41,41,41	0.92	2 (4%)	56,56,56	2.15	21 (37%)
45	CLA	A4	303	-	43,51,73	1.86	7 (16%)	54,87,113	1.59	9 (16%)
45	CLA	BB	814	-	43,51,73	1.78	6 (13%)	49,86,113	1.48	8 (16%)
45	CLA	AB	829	-	65,73,73	1.50	9 (13%)	76,113,113	1.33	9 (11%)
45	CLA	AA	808	1	65,73,73	1.50	7 (10%)	76,113,113	1.34	9 (11%)
54	CHL	A6	607	-	43,51,74	2.34	16 (37%)	45,86,114	2.83	19 (42%)
45	CLA	AB	810	2	65,73,73	1.48	11 (16%)	76,113,113	1.38	6 (7%)
45	CLA	A3	302	14	60,68,73	1.57	8 (13%)	70,107,113	1.22	9 (12%)
45	CLA	BB	842	-	65,73,73	1.50	9 (13%)	76,113,113	1.30	7 (9%)
45	CLA	AA	823	-	41,49,73	1.93	7 (17%)	47,84,113	1.46	8 (17%)
45	CLA	AA	841	-	65,73,73	1.50	9 (13%)	76,113,113	1.34	8 (10%)
45	CLA	AL	305	-	42,50,73	1.85	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	AA	832	-	56,64,73	1.60	6 (10%)	65,102,113	1.36	10 (15%)
45	CLA	AG	204	7	45,53,73	1.84	7 (15%)	52,89,113	1.46	7 (13%)
45	CLA	B5	604	-	43,51,73	1.91	7 (16%)	54,87,113	1.53	10 (18%)
45	CLA	AA	817	-	60,68,73	1.55	6 (10%)	70,107,113	1.36	9 (12%)
45	CLA	B2	611	17	44,52,73	1.85	7 (15%)	51,88,113	1.42	7 (13%)
45	CLA	BB	815	-	65,73,73	1.47	9 (13%)	76,113,113	1.49	11 (14%)
45	CLA	BA	819	-	65,73,73	1.48	9 (13%)	76,113,113	1.34	9 (11%)
45	CLA	AA	842	-	65,73,73	1.48	8 (12%)	76,113,113	1.41	11 (14%)
48	BCR	BL	306	-	41,41,41	0.88	1 (2%)	56,56,56	11.27	26 (46%)
52	LUT	A4	315	-	42,43,43	0.95	2 (4%)	51,60,60	1.84	15 (29%)
45	CLA	AB	840	-	65,73,73	1.54	9 (13%)	76,113,113	1.25	7 (9%)
45	CLA	BB	807	-	65,73,73	1.49	7 (10%)	76,113,113	1.33	10 (13%)
48	BCR	BA	847	-	41,41,41	0.99	1 (2%)	56,56,56	1.63	11 (19%)
45	CLA	BB	831	-	56,64,73	1.63	9 (16%)	65,102,113	1.38	6 (9%)
45	CLA	AK	203	-	46,54,73	1.78	9 (19%)	53,90,113	1.47	7 (13%)
48	BCR	AB	844	-	41,41,41	0.86	0	56,56,56	2.28	23 (41%)
45	CLA	BA	839	-	51,59,73	1.69	8 (15%)	59,96,113	1.41	8 (13%)
45	CLA	BB	835	-	65,73,73	1.53	9 (13%)	76,113,113	1.14	5 (6%)
45	CLA	B5	608	18	44,52,73	1.86	9 (20%)	51,88,113	1.44	7 (13%)
54	CHL	B1	303	13	49,58,74	2.23	17 (34%)	52,95,114	2.63	22 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
48	BCR	A1	319	-	41,41,41	0.90	1 (2%)	56,56,56	3.13	20 (35%)
45	CLA	AB	842	47	65,73,73	1.46	8 (12%)	76,113,113	1.37	10 (13%)
45	CLA	BB	822	-	41,49,73	1.83	8 (19%)	47,84,113	1.56	7 (14%)
45	CLA	A1	309	-	43,52,73	1.87	6 (13%)	49,88,113	1.42	9 (18%)
52	LUT	A1	317	-	42,43,43	0.94	1 (2%)	51,60,60	1.88	13 (25%)
45	CLA	A4	313	-	50,58,73	1.72	8 (16%)	58,95,113	1.47	10 (17%)
45	CLA	AB	834	-	65,73,73	1.49	9 (13%)	76,113,113	1.23	9 (11%)
45	CLA	AB	827	-	62,70,73	1.50	7 (11%)	72,109,113	1.50	9 (12%)
54	CHL	A4	314	15	40,49,74	2.26	13 (32%)	45,84,114	2.77	17 (37%)
48	BCR	AA	846	-	41,41,41	0.82	0	56,56,56	2.12	21 (37%)
48	BCR	AL	306	-	41,41,41	0.94	1 (2%)	56,56,56	2.01	21 (37%)
45	CLA	BA	829	-	65,73,73	1.49	9 (13%)	76,113,113	1.31	9 (11%)
45	CLA	B3	305	-	41,49,73	1.89	7 (17%)	51,84,113	1.73	11 (21%)
45	CLA	AA	835	-	43,52,73	1.85	8 (18%)	49,88,113	1.47	7 (14%)
54	CHL	B2	601	17	53,61,74	2.20	16 (30%)	57,98,114	2.66	25 (43%)
48	BCR	AB	847	-	41,41,41	0.87	0	56,56,56	2.02	14 (25%)
47	LHG	B3	318	45	22,22,48	1.49	2 (9%)	25,28,54	1.38	2 (8%)
45	CLA	BB	820	-	60,68,73	1.51	7 (11%)	70,107,113	1.62	11 (15%)
45	CLA	BB	840	-	47,55,73	1.71	7 (14%)	54,91,113	1.43	8 (14%)
45	CLA	AB	839	-	47,55,73	1.74	8 (17%)	54,91,113	1.56	7 (12%)
47	LHG	AA	844	-	48,48,48	0.93	2 (4%)	51,54,54	0.89	2 (3%)
45	CLA	B1	311	13	59,67,73	1.59	6 (10%)	69,106,113	1.22	8 (11%)
49	SF4	BC	101	3	0,12,12	-	-	-	-	-
48	BCR	BJ	103	-	41,41,41	0.75	0	56,56,56	2.37	21 (37%)
45	CLA	B2	613	-	43,51,73	1.81	6 (13%)	49,86,113	1.44	8 (16%)
45	CLA	AB	835	-	60,68,73	1.55	8 (13%)	70,107,113	1.37	8 (11%)
48	BCR	BA	849	-	41,41,41	0.84	0	56,56,56	2.01	18 (32%)
49	SF4	I	202	37	0,12,12	-	-	-	-	-
45	CLA	BA	840	-	65,73,73	1.44	8 (12%)	76,113,113	1.33	8 (10%)
55	XAT	B3	316	-	39,47,47	0.97	1 (2%)	54,74,74	2.48	21 (38%)
45	CLA	BA	825	-	65,73,73	1.47	7 (10%)	76,113,113	1.31	6 (7%)
45	CLA	BA	818	-	56,64,73	1.64	8 (14%)	65,102,113	1.32	8 (12%)
45	CLA	AA	840	-	65,73,73	1.51	8 (12%)	76,113,113	1.31	10 (13%)
45	CLA	B1	315	-	37,46,73	2.00	7 (18%)	46,81,113	1.61	9 (19%)
45	CLA	B3	312	-	39,48,73	1.93	6 (15%)	44,83,113	1.40	7 (15%)

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	-	-	-		
47	LHG	B5	618	45	29,29,48	1.17	2 (6%)	32,35,54	1.20	3 (9%)
45	CLA	AB	822	-	47,55,73	1.77	7 (14%)	54,91,113	1.35	7 (12%)
45	CLA	BB	826	-	65,73,73	1.51	10 (15%)	76,113,113	1.30	7 (9%)
50	LMU	AL	301	-	35,35,36	1.23	2 (5%)	46,46,47	1.05	5 (10%)
45	CLA	B2	610	47	38,45,73	2.83	10 (26%)	41,76,113	1.61	9 (21%)
53	LMG	A1	321	-	44,44,55	1.03	2 (4%)	52,52,63	1.19	5 (9%)
45	CLA	AK	201	11	37,43,73	2.45	10 (27%)	45,75,113	1.48	8 (17%)
45	CLA	AB	813	-	43,51,73	1.78	6 (13%)	49,86,113	1.44	8 (16%)
45	CLA	BA	814	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	8 (15%)
45	CLA	B3	314	-	39,48,73	1.87	6 (15%)	44,83,113	1.46	7 (15%)
45	CLA	AA	827	-	65,73,73	1.48	7 (10%)	76,113,113	1.34	8 (10%)
45	CLA	BA	803	-	65,73,73	1.41	7 (10%)	76,113,113	1.37	10 (13%)
45	CLA	AA	822	-	42,50,73	1.86	6 (14%)	48,85,113	1.50	8 (16%)
54	CHL	B2	614	17	43,51,74	2.35	15 (34%)	45,86,114	2.87	19 (42%)
45	CLA	AB	806	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	9 (11%)
47	LHG	A3	301	-	35,35,48	1.09	2 (5%)	38,41,54	1.01	2 (5%)
54	CHL	A6	606	-	42,50,74	2.35	15 (35%)	45,85,114	2.88	20 (44%)
48	BCR	AA	847	-	41,41,41	1.00	2 (4%)	56,56,56	2.28	24 (42%)
45	CLA	B1	307	-	39,48,73	1.94	5 (12%)	45,82,113	1.55	7 (15%)
45	CLA	B1	312	47	37,46,73	1.97	7 (18%)	46,81,113	1.60	9 (19%)
54	CHL	A1	303	13	50,59,74	2.22	15 (30%)	53,96,114	2.68	24 (45%)
45	CLA	A3	314	-	37,44,73	1.97	8 (21%)	42,77,113	1.42	7 (16%)
45	CLA	B1	305	-	54,62,73	1.64	8 (14%)	62,99,113	1.53	10 (16%)
45	CLA	B1	309	-	43,52,73	1.85	7 (16%)	49,88,113	1.44	7 (14%)
45	CLA	BA	808	1	65,73,73	1.49	8 (12%)	76,113,113	1.23	8 (10%)
46	PQN	AA	843	-	34,34,34	3.42	10 (29%)	42,45,45	1.74	8 (19%)
45	CLA	AA	825	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	6 (7%)
45	CLA	A4	307	15	45,53,73	1.85	7 (15%)	52,89,113	1.36	7 (13%)
48	BCR	BJ	101	-	41,41,41	0.89	0	56,56,56	1.70	14 (25%)
45	CLA	BB	809	-	52,60,73	1.69	8 (15%)	60,97,113	1.33	7 (11%)
45	CLA	AF	803	-	42,50,73	1.88	8 (19%)	48,85,113	1.57	8 (16%)
45	CLA	BA	823	-	41,49,73	1.86	6 (14%)	47,84,113	1.49	9 (19%)
45	CLA	B1	310	13	38,47,73	1.99	7 (18%)	47,82,113	1.54	10 (21%)
50	LMU	BA	854	-	34,34,36	1.18	2 (5%)	45,45,47	0.91	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	BK	201	11	37,44,73	2.00	7 (18%)	46,77,113	1.73	9 (19%)
49	SF4	AC	102	3	0,12,12	-	-	-		
45	CLA	BA	807	-	50,58,73	1.70	7 (14%)	58,95,113	1.34	7 (12%)
45	CLA	BA	831	-	47,55,73	1.79	8 (17%)	54,91,113	1.49	10 (18%)
45	CLA	BB	813	-	54,62,73	1.66	8 (14%)	67,100,113	1.50	11 (16%)
54	CHL	B2	605	-	42,50,74	2.37	16 (38%)	45,85,114	2.84	18 (40%)
54	CHL	A6	608	-	50,58,74	2.26	16 (32%)	58,95,114	2.64	21 (36%)
48	BCR	AB	845	-	41,41,41	0.85	1 (2%)	56,56,56	1.93	17 (30%)
45	CLA	AB	818	-	59,67,73	1.58	8 (13%)	68,105,113	1.34	10 (14%)
45	CLA	BG	202	7	45,53,73	1.81	6 (13%)	52,89,113	1.56	7 (13%)
45	CLA	AB	830	-	56,64,73	1.62	9 (16%)	65,102,113	1.39	7 (10%)
45	CLA	BB	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.32	7 (9%)
45	CLA	BA	809	1	50,58,73	1.73	8 (16%)	58,95,113	1.44	10 (17%)
45	CLA	A3	315	-	39,48,73	1.86	6 (15%)	44,83,113	1.42	7 (15%)
45	CLA	BB	843	47	65,73,73	1.52	9 (13%)	76,113,113	1.27	7 (9%)
45	CLA	AB	825	-	65,73,73	1.49	10 (15%)	76,113,113	1.34	9 (11%)
45	CLA	BB	837	-	42,50,73	1.86	5 (11%)	48,85,113	1.45	7 (14%)
45	CLA	BF	301	-	55,63,73	1.58	7 (12%)	62,100,113	1.37	7 (11%)
47	LHG	B2	618	45	34,34,48	1.04	2 (5%)	37,40,54	0.96	2 (5%)
48	BCR	BK	204	-	41,41,41	0.88	1 (2%)	56,56,56	2.14	21 (37%)
50	LMU	AB	853	-	36,36,36	1.13	2 (5%)	47,47,47	1.05	2 (4%)
55	XAT	A1	318	-	39,47,47	0.91	2 (5%)	54,74,74	2.42	24 (44%)
45	CLA	A4	311	-	55,64,73	1.64	7 (12%)	63,102,113	1.31	7 (11%)
45	CLA	B3	301	14	60,68,73	1.58	9 (15%)	70,107,113	1.22	8 (11%)
45	CLA	BB	833	-	43,51,73	1.80	7 (16%)	49,86,113	1.65	8 (16%)
45	CLA	BB	818	-	55,63,73	1.61	8 (14%)	64,101,113	1.33	8 (12%)
45	CLA	AA	829	-	65,73,73	1.46	9 (13%)	76,113,113	1.49	11 (14%)
45	CLA	A1	310	13	40,48,73	1.92	7 (17%)	50,83,113	1.65	10 (20%)
45	CLA	AA	837	-	51,59,73	1.62	7 (13%)	59,96,113	1.59	9 (15%)
45	CLA	B2	608	17	45,53,73	1.80	7 (15%)	52,89,113	1.39	8 (15%)
45	CLA	BA	822	-	42,50,73	1.83	6 (14%)	48,85,113	1.56	7 (14%)
54	CHL	B3	306	-	45,53,74	2.28	16 (35%)	52,89,114	2.69	20 (38%)
47	LHG	B1	302	-	35,35,48	1.09	2 (5%)	38,41,54	0.99	2 (5%)
45	CLA	A4	309	-	42,50,73	1.79	5 (11%)	48,85,113	1.53	7 (14%)
45	CLA	AB	812	-	54,62,73	1.66	8 (14%)	67,100,113	1.52	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
45	CLA	B5	603	-	44,52,73	1.87	7 (15%)	55,88,113	1.58	8 (14%)
45	CLA	AA	809	1	50,58,73	1.77	9 (18%)	58,95,113	1.48	11 (18%)
45	CLA	BJ	102	10	42,50,73	1.84	5 (11%)	48,85,113	1.48	7 (14%)
48	BCR	BB	845	-	41,41,41	0.93	1 (2%)	56,56,56	2.19	18 (32%)
45	CLA	BA	833	-	65,73,73	1.51	7 (10%)	76,113,113	1.30	8 (10%)
49	SF4	I	201	37	0,12,12	-	-	-	-	-
48	BCR	AA	852	-	41,41,41	0.94	2 (4%)	56,56,56	2.19	17 (30%)
48	BCR	AI	101	-	41,41,41	0.92	1 (2%)	56,56,56	2.05	20 (35%)
45	CLA	AA	818	-	59,67,73	1.58	9 (15%)	68,105,113	1.33	8 (11%)
47	LHG	A6	618	45	35,35,48	1.05	2 (5%)	38,41,54	0.97	2 (5%)
45	CLA	AA	811	-	65,73,73	1.49	7 (10%)	76,113,113	1.31	8 (10%)
48	BCR	AB	848	-	41,41,41	0.89	1 (2%)	56,56,56	1.97	18 (32%)
45	CLA	A6	604	-	41,50,73	1.90	6 (14%)	46,85,113	1.60	7 (15%)
45	CLA	AL	304	-	60,68,73	1.57	9 (15%)	70,107,113	1.41	10 (14%)
45	CLA	BA	805	-	65,73,73	1.48	8 (12%)	76,113,113	1.36	9 (11%)
45	CLA	A4	310	15	40,49,73	1.90	8 (20%)	45,84,113	1.47	7 (15%)
53	LMG	A4	318	-	39,39,55	1.00	2 (5%)	47,47,63	1.40	7 (14%)
55	XAT	B1	317	-	39,47,47	0.93	2 (5%)	54,74,74	2.43	18 (33%)
45	CLA	B2	603	-	43,52,73	1.85	7 (16%)	49,88,113	1.58	8 (16%)
45	CLA	B2	612	17	65,73,73	1.52	7 (10%)	76,113,113	1.29	8 (10%)
45	CLA	BB	825	-	45,53,73	1.79	8 (17%)	52,89,113	1.37	6 (11%)
45	CLA	BA	806	1	65,73,73	1.50	8 (12%)	76,113,113	1.33	7 (9%)
45	CLA	AB	826	-	62,70,73	1.52	9 (14%)	72,109,113	1.32	7 (9%)
45	CLA	AB	824	-	43,51,73	1.77	10 (23%)	49,86,113	1.57	8 (16%)
45	CLA	AG	203	-	42,50,73	1.85	6 (14%)	48,85,113	1.44	7 (14%)
45	CLA	BB	834	-	65,73,73	1.51	10 (15%)	76,113,113	1.31	8 (10%)
45	CLA	BA	836	1	45,53,73	1.81	6 (13%)	52,89,113	1.53	8 (15%)
45	CLA	AB	820	-	55,63,73	1.70	8 (14%)	64,101,113	1.28	6 (9%)
45	CLA	BB	824	-	65,73,73	1.48	8 (12%)	76,113,113	1.34	10 (13%)
45	CLA	B5	602	18	60,68,73	1.62	9 (15%)	70,107,113	1.29	6 (8%)
50	LMU	BA	853	-	35,35,36	1.15	2 (5%)	46,46,47	0.93	0
54	CHL	B5	605	-	40,49,74	2.42	17 (42%)	42,84,114	2.80	18 (42%)
45	CLA	A1	315	-	37,46,73	1.99	7 (18%)	46,81,113	1.69	11 (23%)

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	AA	833	-	1/1/15/20	19/37/115/115	-
45	CLA	BA	844	47	1/1/10/20	4/8/86/115	-
45	CLA	B1	313	13	1/1/11/20	5/13/91/115	-
54	CHL	A3	307	-	3/3/16/26	4/13/111/137	-
45	CLA	AB	801	-	1/1/15/20	17/37/115/115	-
48	BCR	AJ	101	-	-	1/29/63/63	0/2/2/2
45	CLA	AB	833	-	1/1/15/20	10/37/115/115	-
54	CHL	A4	305	-	3/3/15/26	0/10/106/137	-
48	BCR	BA	856	-	-	5/29/63/63	0/2/2/2
45	CLA	A1	307	-	1/1/9/20	4/8/82/115	-
45	CLA	A1	312	47	1/1/10/20	0/4/80/115	-
45	CLA	AA	834	-	-	15/37/115/115	-
45	CLA	BA	827	-	1/1/15/20	14/37/115/115	-
45	CLA	AL	303	12	1/1/10/20	5/8/86/115	-
48	BCR	BB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	A3	304	-	1/1/11/20	0/9/85/115	-
45	CLA	BB	836	-	-	11/31/109/115	-
52	LUT	A3	316	-	-	0/29/67/67	0/2/2/2
47	LHG	A1	320	45	-	16/53/53/53	-
48	BCR	BA	855	-	-	4/29/63/63	0/2/2/2
47	LHG	AJ	104	-	-	16/44/44/53	-
57	FES	c	301	28	-	-	0/1/1/1
54	CHL	A6	602	16	3/3/17/26	6/22/120/137	-
48	BCR	AJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	A4	308	15	1/1/12/20	4/24/102/115	-
45	CLA	BB	804	-	1/1/15/20	15/37/115/115	-
45	CLA	AB	832	-	-	7/37/115/115	-
45	CLA	BA	837	-	1/1/12/20	3/21/99/115	-
55	XAT	B5	615	-	-	0/31/93/93	0/4/4/4
45	CLA	BB	816	-	1/1/15/20	15/35/113/115	-
52	LUT	B2	615	-	-	0/29/67/67	0/2/2/2
45	CLA	BB	812	-	1/1/15/20	13/37/115/115	-
45	CLA	BA	835	-	1/1/11/20	6/13/91/115	-
45	CLA	AB	805	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	824	-	1/1/13/20	7/23/101/115	-
45	CLA	BA	817	-	-	9/31/109/115	-
48	BCR	AL	302	-	-	5/29/63/63	0/2/2/2
45	CLA	B5	613	-	1/1/11/20	5/13/91/115	-
45	CLA	AJ	102	10	1/1/10/20	3/10/88/115	-
45	CLA	AB	836	-	-	2/10/88/115	-
47	LHG	B1	318	45	-	12/46/46/53	-
45	CLA	A1	314	-	1/1/15/20	12/35/113/115	-
45	CLA	BA	832	-	-	7/27/105/115	-
47	LHG	B1	301	45	-	7/42/42/53	-
45	CLA	A6	610	16	1/1/13/20	4/25/103/115	-
49	SF4	K	301	39	-	-	0/6/5/5
48	BCR	BB	847	-	-	6/29/63/63	0/2/2/2
45	CLA	A3	309	14	1/1/10/20	3/8/86/115	-
45	CLA	B5	609	18	1/1/12/20	3/24/102/115	-
45	CLA	BB	838	-	1/1/12/20	5/19/97/115	-
45	CLA	BB	839	-	-	8/37/115/115	-
45	CLA	BA	830	-	1/1/15/20	13/37/115/115	-
48	BCR	AF	801	-	-	2/29/63/63	0/2/2/2
45	CLA	AA	816	-	1/1/11/20	6/13/91/115	-
45	CLA	BA	838	-	1/1/12/20	11/25/99/115	-
45	CLA	AA	804	-	-	7/22/100/115	-
45	CLA	A3	305	-	1/1/10/20	4/8/86/115	-
45	CLA	B3	304	-	1/1/10/20	4/8/86/115	-
47	LHG	A1	302	-	-	15/40/40/53	-
45	CLA	B2	609	17	1/1/13/20	6/25/103/115	-
48	BCR	B5	616	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	828	-	1/1/15/20	13/37/115/115	-
45	CLA	B3	308	14	1/1/10/20	3/8/86/115	-
45	CLA	AA	805	-	1/1/15/20	17/37/115/115	-
45	CLA	BB	821	-	1/1/13/20	6/25/103/115	-
48	BCR	BA	850	-	-	3/29/63/63	0/2/2/2
45	CLA	AB	817	-	1/1/13/20	8/25/103/115	-
45	CLA	A3	311	14	1/1/10/20	0/11/89/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	AB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	AA	814	-	1/1/11/20	5/13/91/115	-
45	CLA	BB	819	-	1/1/13/20	12/30/108/115	-
45	CLA	B5	612	18	1/1/13/20	8/28/106/115	-
45	CLA	BB	828	-	1/1/14/20	9/34/112/115	-
45	CLA	AA	821	-	1/1/15/20	15/37/115/115	-
52	LUT	B3	315	-	-	4/29/67/67	0/2/2/2
45	CLA	BF	303	-	1/1/10/20	2/8/86/115	-
53	LMG	AG	202	-	-	5/33/53/70	0/1/1/1
45	CLA	AA	819	-	1/1/15/20	14/37/115/115	-
45	CLA	BK	203	-	1/1/11/20	5/15/93/115	-
45	CLA	AA	838	-	-	6/25/103/115	-
45	CLA	BA	813	-	1/1/15/20	17/37/115/115	-
54	CHL	A4	306	-	3/3/16/26	2/15/113/137	-
45	CLA	BA	804	-	-	5/22/100/115	-
45	CLA	B5	610	47	-	4/10/88/115	-
47	LHG	BA	846	45	-	7/30/30/53	-
45	CLA	BL	304	-	1/1/10/20	5/11/89/115	-
45	CLA	BA	828	-	1/1/15/20	14/37/115/115	-
45	CLA	AB	821	-	1/1/12/20	7/19/97/115	-
54	CHL	B1	308	-	3/3/15/26	0/8/106/137	-
45	CLA	A6	613	16	1/1/14/20	7/35/113/115	-
45	CLA	AA	839	-	-	6/22/100/115	-
45	CLA	BA	812	-	1/1/12/20	5/24/102/115	-
48	BCR	AK	204	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	814	-	1/1/15/20	14/37/115/115	-
45	CLA	AB	823	-	-	19/37/115/115	-
48	BCR	AG	205	-	-	2/29/63/63	0/2/2/2
45	CLA	A4	301	15	1/1/14/20	8/31/109/115	-
45	CLA	AF	802	-	1/1/13/20	10/28/106/115	-
55	XAT	A3	317	-	-	0/31/93/93	0/4/4/4
45	CLA	AA	820	-	1/1/11/20	3/13/91/115	-
48	BCR	BB	849	-	-	2/29/63/63	0/2/2/2
45	CLA	A6	609	16	1/1/11/20	3/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AB	819	-	1/1/14/20	14/31/109/115	-
45	CLA	BA	826	-	-	6/23/101/115	-
47	LHG	F	801	-	-	21/41/41/53	-
48	BCR	AA	845	-	-	2/29/63/63	0/2/2/2
45	CLA	AF	804	-	1/1/10/20	2/8/86/115	-
45	CLA	B3	310	14	1/1/10/20	2/11/89/115	-
51	DGD	AB	851	-	-	21/55/95/95	0/2/2/2
45	CLA	AA	828	-	1/1/15/20	15/37/115/115	-
45	CLA	AG	201	-	1/1/11/20	3/11/89/115	-
55	XAT	A6	616	-	-	0/31/93/93	0/4/4/4
45	CLA	B2	602	17	1/1/15/20	9/37/115/115	-
50	LMU	AB	850	-	-	9/21/61/61	0/2/2/2
54	CHL	A1	308	13	3/3/15/26	2/8/106/137	-
45	CLA	B3	313	-	1/1/8/20	0/0/74/115	-
46	PQN	AB	843	-	-	8/23/43/43	0/2/2/2
46	PQN	BA	843	-	-	8/23/43/43	0/2/2/2
45	CLA	AB	807	2	1/1/15/20	11/37/115/115	-
45	CLA	AK	202	-	1/1/11/20	5/13/91/115	-
45	CLA	AB	831	-	1/1/10/20	3/11/89/115	-
45	CLA	A3	308	14	1/1/11/20	5/13/91/115	-
45	CLA	A3	303	14	1/1/13/20	8/25/103/115	-
54	CHL	B2	607	-	3/3/16/26	4/15/113/137	-
45	CLA	AA	812	-	1/1/12/20	9/24/102/115	-
51	DGD	BB	850	-	-	13/55/95/95	0/2/2/2
56	SQD	e	301	-	-	10/29/49/69	0/1/1/1
45	CLA	B1	304	13	1/1/14/20	7/33/111/115	-
45	CLA	A1	316	13	1/1/11/20	9/11/87/115	-
45	CLA	AB	804	-	1/1/15/20	16/37/115/115	-
45	CLA	A3	306	14	1/1/10/20	0/10/86/115	-
45	CLA	BK	202	-	1/1/11/20	6/13/91/115	-
45	CLA	BB	830	-	1/1/15/20	11/37/115/115	-
45	CLA	BA	815	-	-	4/10/88/115	-
48	BCR	BB	803	-	-	4/29/63/63	0/2/2/2
45	CLA	A1	311	13	1/1/14/20	3/29/107/115	-
45	CLA	BB	806	-	1/1/10/20	2/8/86/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	AA	849	-	-	8/29/63/63	0/2/2/2
45	CLA	BB	810	-	1/1/15/20	15/37/115/115	-
49	SF4	AA	850	1,2	-	-	0/6/5/5
45	CLA	B1	306	-	1/1/10/20	3/8/86/115	-
45	CLA	B2	604	-	1/1/10/20	4/9/88/115	-
48	BCR	BA	848	-	-	4/29/63/63	0/2/2/2
48	BCR	BB	846	-	-	6/29/63/63	0/2/2/2
45	CLA	A1	305	-	1/1/13/20	7/25/103/115	-
56	SQD	BJ	104	-	-	21/42/62/69	0/1/1/1
45	CLA	AA	836	1	-	7/13/91/115	-
45	CLA	A4	302	15	1/1/11/20	5/13/89/115	-
47	LHG	BA	845	-	-	29/53/53/53	-
45	CLA	AH	201	-	1/1/14/20	10/31/109/115	-
52	LUT	B5	614	-	-	1/29/67/67	0/2/2/2
45	CLA	BB	801	-	1/1/15/20	17/37/115/115	-
54	CHL	A4	304	-	3/3/15/26	1/8/106/137	-
45	CLA	BG	201	-	1/1/10/20	7/10/88/115	-
48	BCR	B2	617	-	-	0/29/63/63	0/2/2/2
47	LHG	A1	301	45	-	11/42/42/53	-
45	CLA	AA	815	-	-	3/10/88/115	-
50	LMU	BB	851	-	-	10/21/61/61	0/2/2/2
45	CLA	BB	805	-	1/1/15/20	14/37/115/115	-
47	LHG	a	501	-	-	17/33/33/53	-
48	BCR	AB	849	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	841	-	1/1/15/20	15/37/115/115	-
45	CLA	AB	838	-	-	7/37/115/115	-
54	CHL	B5	607	-	3/3/16/26	5/13/111/137	-
48	BCR	AA	848	-	-	4/29/63/63	0/2/2/2
45	CLA	A3	313	-	-	1/6/84/115	-
45	CLA	AB	816	-	1/1/10/20	4/11/89/115	-
45	CLA	BB	811	2	1/1/15/20	15/37/115/115	-
45	CLA	AA	803	-	1/1/15/20	15/37/115/115	-
45	CLA	A1	304	13	1/1/13/20	11/31/109/115	-
50	LMU	AB	852	-	-	9/21/61/61	0/2/2/2
45	CLA	AA	810	-	1/1/14/20	10/37/111/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	A3	318	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	802	-	1/1/15/20	4/37/115/115	-
49	SF4	BA	852	1,2	-	-	0/6/5/5
45	CLA	AB	809	-	1/1/15/20	16/37/115/115	-
45	CLA	B5	601	18	1/1/11/20	8/15/93/115	-
48	BCR	BL	305	-	-	2/29/63/63	0/2/2/2
48	BCR	BG	203	-	-	6/29/63/63	0/2/2/2
45	CLA	BB	808	2	1/1/15/20	10/37/115/115	-
45	CLA	BA	801	-	1/1/15/20	9/37/115/115	-
45	CLA	BA	834	-	-	11/37/115/115	-
45	CLA	AA	801	-	1/1/15/20	13/37/115/115	-
45	CLA	AB	811	-	1/1/15/20	15/37/115/115	-
45	CLA	BA	811	-	1/1/15/20	14/37/115/115	-
45	CLA	BA	821	-	-	12/37/115/115	-
46	PQN	BB	844	-	-	9/23/43/43	0/2/2/2
45	CLA	AB	837	-	1/1/12/20	7/19/97/115	-
53	LMG	B5	617	-	-	14/28/48/70	0/1/1/1
45	CLA	B3	311	-	1/1/13/20	7/23/101/115	-
45	CLA	A3	312	-	1/1/13/20	11/23/101/115	-
45	CLA	A6	603	16	1/1/15/20	9/37/115/115	-
48	BCR	A4	317	-	-	2/29/63/63	0/2/2/2
45	CLA	AB	841	-	1/1/15/20	7/37/115/115	-
55	XAT	B2	616	-	-	0/31/93/93	0/4/4/4
54	CHL	B2	606	-	3/3/15/26	2/12/110/137	-
52	LUT	A6	615	-	-	0/29/67/67	0/2/2/2
48	BCR	BA	851	-	-	8/29/63/63	0/2/2/2
45	CLA	BL	302	12	-	4/13/91/115	-
45	CLA	A6	611	47	1/1/7/20	6/10/70/115	-
45	CLA	AA	830	-	1/1/15/20	14/37/115/115	-
45	CLA	B1	314	-	1/1/14/20	9/31/109/115	-
45	CLA	AB	803	-	1/1/15/20	17/37/115/115	-
45	CLA	BL	303	-	-	7/31/109/115	-
50	LMU	AA	851	-	-	10/21/61/61	0/2/2/2
45	CLA	AA	806	1	1/1/15/20	13/37/115/115	-
48	BCR	AI	102	-	-	3/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	LHG	BF	305	-	-	18/49/49/53	-
45	CLA	AA	826	-	1/1/13/20	11/30/108/115	-
48	BCR	A6	617	-	-	2/29/63/63	0/2/2/2
45	CLA	BB	827	-	-	8/34/112/115	-
55	XAT	A4	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	824	-	1/1/13/20	8/25/103/115	-
45	CLA	A6	614	-	1/1/10/20	2/11/89/115	-
45	CLA	A1	313	13	1/1/11/20	4/13/91/115	-
45	CLA	A6	605	-	1/1/10/20	1/9/88/115	-
48	BCR	B3	317	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	808	-	-	5/20/98/115	-
45	CLA	A4	312	-	1/1/11/20	4/13/91/115	-
48	BCR	BL	301	-	-	6/29/63/63	0/2/2/2
47	LHG	A3	319	45	-	14/26/26/53	-
45	CLA	BA	820	-	1/1/11/20	4/13/91/115	-
45	CLA	A6	612	16	1/1/11/20	6/11/89/115	-
48	BCR	AF	805	-	-	6/29/63/63	0/2/2/2
52	LUT	B1	316	-	-	14/29/67/67	0/2/2/2
52	LUT	AF	806	-	-	0/29/67/67	0/2/2/2
45	CLA	B3	307	14	1/1/11/20	3/13/91/115	-
45	CLA	A3	310	47	1/1/9/20	0/0/78/115	-
45	CLA	AB	802	-	1/1/15/20	16/37/113/115	-
45	CLA	B3	309	47	1/1/10/20	0/6/84/115	-
45	CLA	A1	306	-	1/1/11/20	9/18/96/115	-
48	BCR	BF	304	-	-	7/29/63/63	0/2/2/2
45	CLA	BA	810	-	1/1/15/20	12/37/115/115	-
45	CLA	BA	842	-	1/1/15/20	13/37/115/115	-
45	CLA	BB	817	-	1/1/10/20	4/9/87/115	-
49	SF4	BC	102	3	-	-	0/6/5/5
45	CLA	AA	807	-	1/1/12/20	4/19/97/115	-
45	CLA	AA	802	-	1/1/15/20	8/37/115/115	-
45	CLA	AA	813	-	1/1/15/20	17/37/115/115	-
45	CLA	BF	302	-	1/1/10/20	3/10/88/115	-
45	CLA	BA	816	-	1/1/11/20	2/13/91/115	-
45	CLA	BB	802	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	831	-	1/1/11/20	7/16/94/115	-
45	CLA	AB	815	-	1/1/15/20	17/37/115/115	-
45	CLA	BB	823	-	1/1/11/20	4/14/92/115	-
45	CLA	BB	841	-	1/1/15/20	7/37/115/115	-
45	CLA	A6	601	15	1/1/11/20	2/15/93/115	-
45	CLA	B3	302	14	1/1/13/20	6/25/103/115	-
45	CLA	B3	303	-	1/1/11/20	2/9/85/115	-
45	CLA	BB	832	-	1/1/10/20	4/11/89/115	-
45	CLA	B5	611	18	1/1/10/20	4/8/86/115	-
45	CLA	BH	201	-	1/1/14/20	11/31/109/115	-
48	BCR	BI	101	-	-	6/29/63/63	0/2/2/2
45	CLA	A4	303	-	1/1/11/20	4/11/87/115	-
45	CLA	BB	814	-	1/1/10/20	1/11/89/115	-
45	CLA	AB	829	-	1/1/15/20	15/37/115/115	-
45	CLA	AA	808	1	1/1/15/20	10/37/115/115	-
54	CHL	A6	607	-	3/3/15/26	2/12/110/137	-
45	CLA	AB	810	2	1/1/15/20	16/37/115/115	-
45	CLA	A3	302	14	1/1/14/20	6/31/109/115	-
45	CLA	BB	842	-	1/1/15/20	9/37/115/115	-
45	CLA	AA	823	-	1/1/10/20	4/8/86/115	-
45	CLA	AA	841	-	-	10/37/115/115	-
45	CLA	AL	305	-	1/1/10/20	5/10/88/115	-
45	CLA	AA	832	-	1/1/13/20	7/27/105/115	-
45	CLA	AG	204	7	1/1/11/20	4/13/91/115	-
45	CLA	B5	604	-	1/1/11/20	3/11/87/115	-
45	CLA	AA	817	-	1/1/14/20	6/31/109/115	-
45	CLA	B2	611	17	1/1/11/20	7/11/89/115	-
45	CLA	BB	815	-	1/1/15/20	20/37/115/115	-
45	CLA	BA	819	-	1/1/15/20	13/37/115/115	-
45	CLA	AA	842	-	1/1/15/20	18/37/115/115	-
48	BCR	BL	306	-	-	15/29/63/63	0/2/2/2
52	LUT	A4	315	-	-	1/29/67/67	0/2/2/2
45	CLA	AB	840	-	1/1/15/20	7/37/115/115	-
45	CLA	BB	807	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	BCR	BA	847	-	-	5/29/63/63	0/2/2/2
45	CLA	BB	831	-	1/1/13/20	8/27/105/115	-
45	CLA	AK	203	-	1/1/11/20	7/15/93/115	-
48	BCR	AB	844	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	839	-	-	6/21/99/115	-
45	CLA	BB	835	-	1/1/15/20	16/37/115/115	-
45	CLA	B5	608	18	1/1/11/20	4/11/89/115	-
54	CHL	B1	303	13	3/3/17/26	3/19/117/137	-
48	BCR	A1	319	-	-	4/29/63/63	0/2/2/2
45	CLA	AB	842	47	1/1/15/20	18/37/115/115	-
45	CLA	BB	822	-	1/1/10/20	2/8/86/115	-
45	CLA	A1	309	-	1/1/11/20	5/11/89/115	-
52	LUT	A1	317	-	-	0/29/67/67	0/2/2/2
45	CLA	A4	313	-	1/1/12/20	9/19/97/115	-
45	CLA	AB	834	-	1/1/15/20	16/37/115/115	-
45	CLA	AB	827	-	1/1/14/20	14/34/112/115	-
54	CHL	A4	314	15	3/3/15/26	0/10/106/137	-
48	BCR	AA	846	-	-	6/29/63/63	0/2/2/2
48	BCR	AL	306	-	-	5/29/63/63	0/2/2/2
45	CLA	BA	829	-	1/1/15/20	11/37/115/115	-
45	CLA	B3	305	-	1/1/10/20	2/10/86/115	-
45	CLA	AA	835	-	1/1/11/20	0/11/89/115	-
54	CHL	B2	601	17	3/3/17/26	9/24/122/137	-
48	BCR	AB	847	-	-	0/29/63/63	0/2/2/2
47	LHG	B3	318	45	-	11/26/26/53	-
45	CLA	BB	820	-	1/1/14/20	12/31/109/115	-
45	CLA	BB	840	-	-	4/16/94/115	-
45	CLA	AB	839	-	1/1/11/20	3/16/94/115	-
47	LHG	AA	844	-	-	18/53/53/53	-
45	CLA	B1	311	13	1/1/14/20	3/29/107/115	-
49	SF4	BC	101	3	-	-	0/6/5/5
48	BCR	BJ	103	-	-	5/29/63/63	0/2/2/2
45	CLA	B2	613	-	1/1/10/20	1/11/89/115	-
45	CLA	AB	835	-	-	7/31/109/115	-
48	BCR	BA	849	-	-	4/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
49	SF4	I	202	37	-	-	0/6/5/5
45	CLA	BA	840	-	1/1/15/20	13/37/115/115	-
55	XAT	B3	316	-	-	0/31/93/93	0/4/4/4
45	CLA	BA	825	-	1/1/15/20	15/37/115/115	-
45	CLA	BA	818	-	-	6/27/105/115	-
45	CLA	AA	840	-	1/1/15/20	14/37/115/115	-
45	CLA	B1	315	-	1/1/10/20	0/4/80/115	-
45	CLA	B3	312	-	1/1/10/20	0/6/84/115	-
49	SF4	AC	101	3	-	-	0/6/5/5
47	LHG	B5	618	45	-	13/34/34/53	-
45	CLA	AB	822	-	1/1/11/20	5/16/94/115	-
45	CLA	BB	826	-	1/1/15/20	10/37/115/115	-
50	LMU	AL	301	-	-	11/20/60/61	0/2/2/2
45	CLA	B2	610	47	1/1/7/20	7/10/70/115	-
53	LMG	A1	321	-	-	17/39/59/70	0/1/1/1
45	CLA	AK	201	11	1/1/8/20	0/2/74/115	-
45	CLA	AB	813	-	1/1/10/20	3/11/89/115	-
45	CLA	BA	814	-	1/1/11/20	6/13/91/115	-
45	CLA	B3	314	-	1/1/10/20	0/6/84/115	-
45	CLA	AA	827	-	1/1/15/20	18/37/115/115	-
45	CLA	BA	803	-	1/1/15/20	18/37/115/115	-
45	CLA	AA	822	-	1/1/10/20	3/10/88/115	-
54	CHL	B2	614	17	3/3/15/26	0/12/110/137	-
45	CLA	AB	806	-	1/1/15/20	15/37/115/115	-
54	CHL	A6	606	-	3/3/15/26	2/10/108/137	-
47	LHG	A3	301	-	-	11/40/40/53	-
48	BCR	AA	847	-	-	13/29/63/63	0/2/2/2
45	CLA	B1	307	-	1/1/9/20	4/8/82/115	-
45	CLA	B1	312	47	1/1/10/20	0/4/80/115	-
54	CHL	A1	303	13	3/3/17/26	4/21/119/137	-
45	CLA	A3	314	-	1/1/8/20	0/0/74/115	-
45	CLA	B1	305	-	1/1/12/20	6/23/101/115	-
45	CLA	B1	309	-	-	2/11/89/115	-
45	CLA	BA	808	1	1/1/15/20	10/37/115/115	-
46	PQN	AA	843	-	-	6/23/43/43	0/2/2/2
45	CLA	AA	825	-	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	A4	307	15	1/1/11/20	1/13/91/115	-
48	BCR	BJ	101	-	-	0/29/63/63	0/2/2/2
45	CLA	BB	809	-	-	5/22/100/115	-
45	CLA	AF	803	-	1/1/10/20	2/10/88/115	-
45	CLA	BA	823	-	1/1/10/20	4/8/86/115	-
45	CLA	B1	310	13	1/1/10/20	3/6/82/115	-
50	LMU	BA	854	-	-	8/19/59/61	0/2/2/2
45	CLA	BK	201	11	1/1/8/20	0/2/74/115	-
49	SF4	AC	102	3	-	-	0/6/5/5
45	CLA	BA	807	-	1/1/12/20	4/19/97/115	-
45	CLA	BA	831	-	1/1/11/20	7/16/94/115	-
45	CLA	BB	813	-	1/1/13/20	4/25/101/115	-
54	CHL	B2	605	-	3/3/15/26	3/10/108/137	-
54	CHL	A6	608	-	3/3/17/26	8/19/117/137	-
48	BCR	AB	845	-	-	6/29/63/63	0/2/2/2
45	CLA	AB	818	-	1/1/13/20	10/30/108/115	-
45	CLA	BG	202	7	1/1/11/20	6/13/91/115	-
45	CLA	AB	830	-	1/1/13/20	10/27/105/115	-
45	CLA	BB	829	-	1/1/15/20	17/37/115/115	-
45	CLA	BA	809	1	-	9/19/97/115	-
45	CLA	A3	315	-	1/1/10/20	0/6/84/115	-
45	CLA	BB	843	47	1/1/15/20	11/37/115/115	-
45	CLA	AB	825	-	1/1/15/20	14/37/115/115	-
45	CLA	BB	837	-	1/1/10/20	4/10/88/115	-
45	CLA	BF	301	-	1/1/12/20	8/24/102/115	-
47	LHG	B2	618	45	-	22/39/39/53	-
48	BCR	BK	204	-	-	1/29/63/63	0/2/2/2
50	LMU	AB	853	-	-	13/21/61/61	0/2/2/2
55	XAT	A1	318	-	-	0/31/93/93	0/4/4/4
45	CLA	A4	311	-	1/1/13/20	7/26/104/115	-
45	CLA	B3	301	14	1/1/14/20	5/31/109/115	-
45	CLA	BB	833	-	-	4/11/89/115	-
45	CLA	BB	818	-	1/1/13/20	8/25/103/115	-
45	CLA	AA	829	-	1/1/15/20	18/37/115/115	-
45	CLA	A1	310	13	1/1/10/20	2/8/84/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	AA	837	-	1/1/12/20	6/21/99/115	-
45	CLA	B2	608	17	1/1/11/20	3/13/91/115	-
45	CLA	BA	822	-	1/1/10/20	8/10/88/115	-
54	CHL	B3	306	-	3/3/16/26	5/13/111/137	-
47	LHG	B1	302	-	-	14/40/40/53	-
45	CLA	A4	309	-	1/1/10/20	3/10/88/115	-
45	CLA	AB	812	-	1/1/13/20	8/25/101/115	-
45	CLA	B5	603	-	1/1/11/20	4/13/89/115	-
45	CLA	AA	809	1	1/1/12/20	5/19/97/115	-
45	CLA	BJ	102	10	1/1/10/20	4/10/88/115	-
48	BCR	BB	845	-	-	4/29/63/63	0/2/2/2
45	CLA	BA	833	-	1/1/15/20	15/37/115/115	-
54	CHL	B5	605	-	3/3/15/26	2/8/106/137	-
49	SF4	I	201	37	-	-	0/6/5/5
48	BCR	AA	852	-	-	5/29/63/63	0/2/2/2
48	BCR	AI	101	-	-	7/29/63/63	0/2/2/2
45	CLA	AA	818	-	-	7/30/108/115	-
47	LHG	A6	618	45	-	17/40/40/53	-
45	CLA	AA	811	-	1/1/15/20	11/37/115/115	-
48	BCR	AB	848	-	-	2/29/63/63	0/2/2/2
45	CLA	A6	604	-	1/1/10/20	2/9/87/115	-
45	CLA	AL	304	-	-	9/31/109/115	-
45	CLA	BA	805	-	1/1/15/20	22/37/115/115	-
45	CLA	A4	310	15	1/1/10/20	5/8/86/115	-
53	LMG	A4	318	-	-	15/34/54/70	0/1/1/1
55	XAT	B1	317	-	-	0/31/93/93	0/4/4/4
45	CLA	B2	603	-	1/1/11/20	4/11/89/115	-
45	CLA	B2	612	17	1/1/15/20	13/37/115/115	-
45	CLA	BB	825	-	1/1/11/20	6/13/91/115	-
45	CLA	BA	806	1	1/1/15/20	18/37/115/115	-
45	CLA	AB	826	-	1/1/14/20	6/34/112/115	-
45	CLA	AB	824	-	1/1/10/20	4/11/89/115	-
45	CLA	AG	203	-	1/1/10/20	3/10/88/115	-
45	CLA	BB	834	-	-	9/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
45	CLA	BA	836	1	-	6/13/91/115	-
45	CLA	AB	820	-	1/1/13/20	8/25/103/115	-
45	CLA	BB	824	-	-	18/37/115/115	-
45	CLA	B5	602	18	-	9/31/109/115	-
50	LMU	BA	853	-	-	9/20/60/61	0/2/2/2
54	CHL	B5	606	-	3/3/15/26	2/8/104/137	-
45	CLA	A1	315	-	1/1/10/20	0/4/80/115	-

All (2732) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	611	CLA	C1A-NA	12.32	1.40	1.29
45	B2	610	CLA	C1A-NA	11.85	1.40	1.29
46	BB	844	PQN	C12-C13	9.75	1.56	1.33
46	AA	843	PQN	C12-C13	9.56	1.55	1.33
46	BA	843	PQN	C12-C13	9.52	1.55	1.33
46	AB	843	PQN	C12-C13	9.36	1.55	1.33
45	AK	201	CLA	C3B-C4B	8.50	1.49	1.39
45	BA	844	CLA	C4B-NB	8.02	1.42	1.35
45	A6	614	CLA	C4B-NB	7.99	1.42	1.35
45	AK	201	CLA	C4B-NB	7.91	1.42	1.35
45	B3	311	CLA	C4B-NB	7.87	1.42	1.35
45	AF	803	CLA	C4B-NB	7.87	1.42	1.35
45	AG	204	CLA	C4B-NB	7.86	1.42	1.35
45	AH	201	CLA	C4B-NB	7.84	1.42	1.35
45	AA	822	CLA	C4B-NB	7.83	1.42	1.35
45	B2	611	CLA	C4B-NB	7.83	1.42	1.35
45	BG	201	CLA	C4B-NB	7.80	1.42	1.35
46	AB	843	PQN	O4-C4	7.78	1.39	1.23
46	AA	843	PQN	O4-C4	7.78	1.39	1.23
45	B1	311	CLA	C4B-NB	7.78	1.42	1.35
45	AA	836	CLA	C4B-NB	7.77	1.42	1.35
45	A4	307	CLA	C4B-NB	7.76	1.42	1.35
45	A4	308	CLA	C4B-NB	7.76	1.42	1.35
45	AB	809	CLA	C4B-NB	7.75	1.42	1.35
45	BF	302	CLA	C4B-NB	7.75	1.42	1.35
45	BH	201	CLA	C4B-NB	7.74	1.42	1.35
45	B2	604	CLA	C4B-NB	7.73	1.42	1.35
45	AK	202	CLA	C4B-NB	7.71	1.42	1.35
45	A1	309	CLA	C4B-NB	7.71	1.42	1.35
45	B5	610	CLA	C4B-NB	7.71	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B3	309	CLA	C4B-NB	7.71	1.42	1.35
45	BA	822	CLA	C4B-NB	7.71	1.42	1.35
46	BA	843	PQN	O4-C4	7.70	1.39	1.23
45	B2	609	CLA	C4B-NB	7.69	1.42	1.35
45	AA	823	CLA	C4B-NB	7.69	1.42	1.35
45	AB	822	CLA	C4B-NB	7.69	1.42	1.35
45	AB	820	CLA	C4B-NB	7.69	1.42	1.35
45	AA	809	CLA	C4B-NB	7.68	1.42	1.35
45	BK	201	CLA	C4B-NB	7.68	1.42	1.35
45	AG	201	CLA	C4B-NB	7.67	1.42	1.35
45	A6	604	CLA	C4B-NB	7.67	1.42	1.35
45	AL	303	CLA	C4B-NB	7.67	1.42	1.35
45	AG	203	CLA	C4B-NB	7.67	1.42	1.35
45	B1	306	CLA	C4B-NB	7.66	1.42	1.35
45	B3	304	CLA	C4B-NB	7.65	1.42	1.35
45	B5	604	CLA	C4B-NB	7.65	1.42	1.35
45	B3	312	CLA	C4B-NB	7.65	1.42	1.35
45	A1	311	CLA	C4B-NB	7.65	1.42	1.35
45	AA	824	CLA	C4B-NB	7.65	1.42	1.35
45	A4	311	CLA	C4B-NB	7.63	1.42	1.35
45	B1	314	CLA	C4B-NB	7.63	1.42	1.35
45	B3	310	CLA	C4B-NB	7.63	1.42	1.35
45	A3	304	CLA	C4B-NB	7.62	1.42	1.35
45	B1	310	CLA	C4B-NB	7.62	1.42	1.35
45	A1	305	CLA	C4B-NB	7.62	1.42	1.35
45	BA	838	CLA	C4B-NB	7.62	1.42	1.35
45	B3	303	CLA	C4B-NB	7.62	1.42	1.35
45	B2	603	CLA	C4B-NB	7.62	1.42	1.35
45	A6	611	CLA	C4B-NB	7.61	1.42	1.35
45	BK	202	CLA	C4B-NB	7.61	1.42	1.35
45	BA	836	CLA	C4B-NB	7.61	1.42	1.35
45	B5	602	CLA	C4B-NB	7.61	1.42	1.35
45	A6	610	CLA	C4B-NB	7.61	1.42	1.35
45	A3	314	CLA	C4B-NB	7.60	1.42	1.35
46	BA	843	PQN	O1-C1	7.60	1.39	1.23
45	A4	310	CLA	C4B-NB	7.60	1.42	1.35
46	BB	844	PQN	O4-C4	7.59	1.39	1.23
46	BB	844	PQN	O1-C1	7.58	1.39	1.23
45	BB	835	CLA	C4B-NB	7.58	1.42	1.35
45	A3	311	CLA	C4B-NB	7.57	1.42	1.35
45	A3	305	CLA	C4B-NB	7.57	1.42	1.35
45	BB	810	CLA	C4B-NB	7.57	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	612	CLA	C4B-NB	7.57	1.42	1.35
45	A3	310	CLA	C4B-NB	7.56	1.42	1.35
45	A6	613	CLA	C4B-NB	7.56	1.42	1.35
45	BL	304	CLA	C4B-NB	7.56	1.41	1.35
45	B1	307	CLA	C4B-NB	7.56	1.41	1.35
45	BL	302	CLA	C4B-NB	7.55	1.41	1.35
45	B5	612	CLA	C4B-NB	7.55	1.41	1.35
45	AJ	102	CLA	C4B-NB	7.55	1.41	1.35
45	B1	309	CLA	C4B-NB	7.55	1.41	1.35
45	B5	609	CLA	C4B-NB	7.55	1.41	1.35
45	AA	831	CLA	C4B-NB	7.55	1.41	1.35
45	A6	612	CLA	C4B-NB	7.54	1.41	1.35
45	B1	315	CLA	C4B-NB	7.54	1.41	1.35
45	BB	843	CLA	C4B-NB	7.54	1.41	1.35
45	AA	808	CLA	C4B-NB	7.54	1.41	1.35
45	BA	809	CLA	C4B-NB	7.53	1.41	1.35
45	A1	310	CLA	C4B-NB	7.53	1.41	1.35
45	BB	802	CLA	C4B-NB	7.53	1.41	1.35
45	A4	313	CLA	C4B-NB	7.53	1.41	1.35
45	A3	303	CLA	C4B-NB	7.52	1.41	1.35
45	BA	823	CLA	C4B-NB	7.52	1.41	1.35
45	AL	305	CLA	C4B-NB	7.51	1.41	1.35
45	BB	837	CLA	C4B-NB	7.51	1.41	1.35
45	BB	833	CLA	C4B-NB	7.51	1.41	1.35
45	B3	305	CLA	C4B-NB	7.51	1.41	1.35
45	AF	804	CLA	C4B-NB	7.50	1.41	1.35
45	B1	305	CLA	C4B-NB	7.50	1.41	1.35
45	B2	613	CLA	C4B-NB	7.50	1.41	1.35
45	BF	303	CLA	C4B-NB	7.50	1.41	1.35
46	AB	843	PQN	O1-C1	7.50	1.39	1.23
45	AA	801	CLA	C4B-NB	7.49	1.41	1.35
45	A4	312	CLA	C4B-NB	7.49	1.41	1.35
45	BJ	102	CLA	C4B-NB	7.49	1.41	1.35
45	AB	830	CLA	C4B-NB	7.48	1.41	1.35
45	AB	840	CLA	C4B-NB	7.48	1.41	1.35
45	A3	306	CLA	C4B-NB	7.48	1.41	1.35
45	AA	810	CLA	C4B-NB	7.48	1.41	1.35
45	B5	608	CLA	C4B-NB	7.48	1.41	1.35
45	AB	802	CLA	C4B-NB	7.48	1.41	1.35
45	AB	836	CLA	C4B-NB	7.47	1.41	1.35
45	A1	306	CLA	C4B-NB	7.47	1.41	1.35
45	A1	315	CLA	C4B-NB	7.47	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BG	202	CLA	C4B-NB	7.47	1.41	1.35
45	B3	301	CLA	C4B-NB	7.47	1.41	1.35
45	B2	610	CLA	C4B-NB	7.47	1.41	1.35
45	BB	839	CLA	C4B-NB	7.45	1.41	1.35
45	B5	603	CLA	C4B-NB	7.45	1.41	1.35
45	B5	613	CLA	C4B-NB	7.44	1.41	1.35
45	AA	816	CLA	C4B-NB	7.44	1.41	1.35
45	A3	312	CLA	C4B-NB	7.42	1.41	1.35
45	A3	313	CLA	C4B-NB	7.42	1.41	1.35
45	BA	827	CLA	C4B-NB	7.42	1.41	1.35
45	BB	831	CLA	C4B-NB	7.41	1.41	1.35
45	AA	811	CLA	C4B-NB	7.41	1.41	1.35
45	B3	314	CLA	C4B-NB	7.41	1.41	1.35
45	BA	811	CLA	C4B-NB	7.40	1.41	1.35
45	AA	833	CLA	C4B-NB	7.40	1.41	1.35
45	BA	831	CLA	C4B-NB	7.40	1.41	1.35
45	BB	823	CLA	C4B-NB	7.39	1.41	1.35
45	BA	802	CLA	C4B-NB	7.39	1.41	1.35
45	A4	309	CLA	C4B-NB	7.39	1.41	1.35
45	BA	801	CLA	C4B-NB	7.39	1.41	1.35
45	AA	817	CLA	C4B-NB	7.39	1.41	1.35
45	BB	836	CLA	C4B-NB	7.39	1.41	1.35
45	BK	203	CLA	C4B-NB	7.39	1.41	1.35
45	BB	813	CLA	C4B-NB	7.38	1.41	1.35
45	AA	827	CLA	C4B-NB	7.38	1.41	1.35
45	BA	833	CLA	C4B-NB	7.38	1.41	1.35
45	AA	830	CLA	C4B-NB	7.38	1.41	1.35
45	BA	806	CLA	C4B-NB	7.38	1.41	1.35
45	A1	312	CLA	C4B-NB	7.38	1.41	1.35
45	A6	609	CLA	C4B-NB	7.38	1.41	1.35
45	BB	838	CLA	C4B-NB	7.37	1.41	1.35
45	BA	807	CLA	C4B-NB	7.37	1.41	1.35
45	BB	824	CLA	C4B-NB	7.37	1.41	1.35
45	BA	814	CLA	C4B-NB	7.36	1.41	1.35
45	BB	822	CLA	C4B-NB	7.36	1.41	1.35
45	A6	605	CLA	C4B-NB	7.36	1.41	1.35
45	AA	815	CLA	C4B-NB	7.36	1.41	1.35
45	AB	803	CLA	C4B-NB	7.35	1.41	1.35
45	AB	837	CLA	C4B-NB	7.35	1.41	1.35
45	A3	309	CLA	C4B-NB	7.35	1.41	1.35
45	BA	842	CLA	C4B-NB	7.35	1.41	1.35
45	AA	821	CLA	C4B-NB	7.35	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	313	CLA	C4B-NB	7.34	1.41	1.35
45	AB	812	CLA	C4B-NB	7.34	1.41	1.35
45	AB	821	CLA	C4B-NB	7.34	1.41	1.35
45	AK	203	CLA	C4B-NB	7.34	1.41	1.35
45	BA	830	CLA	C4B-NB	7.34	1.41	1.35
46	AA	843	PQN	O1-C1	7.34	1.38	1.23
45	BA	804	CLA	C4B-NB	7.34	1.41	1.35
45	B1	313	CLA	C4B-NB	7.34	1.41	1.35
45	BA	835	CLA	C4B-NB	7.33	1.41	1.35
45	BA	828	CLA	C4B-NB	7.33	1.41	1.35
45	A1	307	CLA	C4B-NB	7.32	1.41	1.35
45	AA	825	CLA	C4B-NB	7.32	1.41	1.35
45	BF	301	CLA	C4B-NB	7.32	1.41	1.35
45	AB	834	CLA	C4B-NB	7.32	1.41	1.35
45	A1	316	CLA	C4B-NB	7.31	1.41	1.35
45	B1	312	CLA	C4B-NB	7.31	1.41	1.35
45	AA	835	CLA	C4B-NB	7.31	1.41	1.35
45	AA	820	CLA	C4B-NB	7.31	1.41	1.35
45	B5	611	CLA	C4B-NB	7.30	1.41	1.35
45	AB	841	CLA	C4B-NB	7.30	1.41	1.35
45	AA	814	CLA	C4B-NB	7.30	1.41	1.35
45	BA	816	CLA	C4B-NB	7.30	1.41	1.35
45	B3	302	CLA	C4B-NB	7.30	1.41	1.35
45	BB	807	CLA	C4B-NB	7.30	1.41	1.35
45	B2	608	CLA	C4B-NB	7.29	1.41	1.35
45	BA	817	CLA	C4B-NB	7.29	1.41	1.35
45	B3	308	CLA	C4B-NB	7.28	1.41	1.35
45	A4	303	CLA	C4B-NB	7.28	1.41	1.35
45	A3	302	CLA	C4B-NB	7.28	1.41	1.35
45	BB	828	CLA	C4B-NB	7.28	1.41	1.35
45	B3	307	CLA	C4B-NB	7.28	1.41	1.35
45	A4	302	CLA	C4B-NB	7.27	1.41	1.35
45	AB	831	CLA	C4B-NB	7.27	1.41	1.35
45	BA	818	CLA	C4B-NB	7.27	1.41	1.35
45	BA	810	CLA	C4B-NB	7.27	1.41	1.35
45	BA	824	CLA	C4B-NB	7.26	1.41	1.35
45	BB	826	CLA	C4B-NB	7.26	1.41	1.35
46	AA	843	PQN	C9-C10	7.26	1.51	1.39
45	AA	802	CLA	C4B-NB	7.24	1.41	1.35
45	B2	602	CLA	C4B-NB	7.24	1.41	1.35
45	AA	828	CLA	C4B-NB	7.23	1.41	1.35
45	B3	313	CLA	C4B-NB	7.23	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	816	CLA	C4B-NB	7.22	1.41	1.35
45	BB	812	CLA	C4B-NB	7.21	1.41	1.35
45	A3	308	CLA	C4B-NB	7.21	1.41	1.35
45	BB	840	CLA	C4B-NB	7.21	1.41	1.35
45	AB	823	CLA	C4B-NB	7.21	1.41	1.35
45	BB	816	CLA	C4B-NB	7.20	1.41	1.35
45	AB	838	CLA	C4B-NB	7.20	1.41	1.35
45	BB	827	CLA	C4B-NB	7.20	1.41	1.35
45	AB	835	CLA	C4B-NB	7.19	1.41	1.35
45	BB	842	CLA	C4B-NB	7.18	1.41	1.35
45	A4	301	CLA	C4B-NB	7.18	1.41	1.35
46	BA	843	PQN	C9-C10	7.17	1.51	1.39
45	AB	813	CLA	C4B-NB	7.17	1.41	1.35
45	AA	804	CLA	C4B-NB	7.17	1.41	1.35
45	AB	827	CLA	C4B-NB	7.16	1.41	1.35
45	BA	825	CLA	C4B-NB	7.15	1.41	1.35
45	A1	314	CLA	C4B-NB	7.15	1.41	1.35
45	BL	303	CLA	C4B-NB	7.15	1.41	1.35
45	A6	603	CLA	C4B-NB	7.15	1.41	1.35
45	BB	832	CLA	C4B-NB	7.15	1.41	1.35
45	AA	832	CLA	C4B-NB	7.14	1.41	1.35
45	AB	826	CLA	C4B-NB	7.14	1.41	1.35
45	BB	819	CLA	C4B-NB	7.14	1.41	1.35
45	BA	839	CLA	C4B-NB	7.14	1.41	1.35
45	BB	825	CLA	C4B-NB	7.14	1.41	1.35
45	AB	839	CLA	C4B-NB	7.13	1.41	1.35
45	AB	817	CLA	C4B-NB	7.13	1.41	1.35
45	BB	809	CLA	C4B-NB	7.12	1.41	1.35
45	BB	821	CLA	C4B-NB	7.12	1.41	1.35
45	AA	839	CLA	C4B-NB	7.12	1.41	1.35
45	AA	838	CLA	C4B-NB	7.11	1.41	1.35
45	B1	304	CLA	C4B-NB	7.11	1.41	1.35
45	AA	803	CLA	C4B-NB	7.11	1.41	1.35
45	BB	817	CLA	C4B-NB	7.10	1.41	1.35
45	BB	814	CLA	C4B-NB	7.10	1.41	1.35
45	AB	825	CLA	C4B-NB	7.08	1.41	1.35
45	BB	804	CLA	C4B-NB	7.08	1.41	1.35
45	A3	315	CLA	C4B-NB	7.07	1.41	1.35
45	AA	807	CLA	C4B-NB	7.07	1.41	1.35
45	BA	841	CLA	C4B-NB	7.07	1.41	1.35
45	AA	841	CLA	C4B-NB	7.06	1.41	1.35
46	BA	843	PQN	C6-C5	7.04	1.51	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	806	CLA	C4B-NB	7.04	1.41	1.35
45	BB	818	CLA	C4B-NB	7.03	1.41	1.35
45	BB	834	CLA	C4B-NB	7.03	1.41	1.35
45	AA	842	CLA	C4B-NB	7.03	1.41	1.35
45	AB	806	CLA	C4B-NB	7.03	1.41	1.35
45	BA	826	CLA	C4B-NB	7.02	1.41	1.35
45	BA	832	CLA	C4B-NB	7.02	1.41	1.35
45	AB	832	CLA	C4B-NB	7.02	1.41	1.35
45	AB	805	CLA	C4B-NB	7.01	1.41	1.35
46	BB	844	PQN	C10-C5	-7.00	1.29	1.40
45	AB	815	CLA	C4B-NB	7.00	1.41	1.35
45	BB	841	CLA	C4B-NB	7.00	1.41	1.35
45	AB	828	CLA	C4B-NB	6.99	1.41	1.35
45	AB	818	CLA	C4B-NB	6.98	1.41	1.35
45	AA	826	CLA	C4B-NB	6.98	1.41	1.35
45	B5	601	CLA	C4B-NB	6.98	1.41	1.35
45	BA	813	CLA	C4B-NB	6.97	1.41	1.35
45	AB	819	CLA	C4B-NB	6.97	1.41	1.35
46	AA	843	PQN	C6-C5	6.96	1.51	1.39
45	AA	818	CLA	C4B-NB	6.96	1.41	1.35
45	AB	801	CLA	C4B-NB	6.95	1.41	1.35
45	BA	821	CLA	C4B-NB	6.95	1.41	1.35
45	AA	806	CLA	C4B-NB	6.94	1.41	1.35
45	AB	808	CLA	C4B-NB	6.92	1.41	1.35
45	BA	815	CLA	C4B-NB	6.91	1.41	1.35
45	BB	820	CLA	C4B-NB	6.90	1.41	1.35
45	A1	304	CLA	C4B-NB	6.90	1.41	1.35
45	BA	819	CLA	C4B-NB	6.90	1.41	1.35
45	AB	833	CLA	C4B-NB	6.89	1.41	1.35
45	BA	834	CLA	C4B-NB	6.89	1.41	1.35
45	BB	829	CLA	C4B-NB	6.89	1.41	1.35
45	AA	805	CLA	C4B-NB	6.88	1.41	1.35
45	BB	801	CLA	C4B-NB	6.88	1.41	1.35
46	AB	843	PQN	C6-C5	6.88	1.50	1.39
45	BB	830	CLA	C4B-NB	6.88	1.41	1.35
46	AB	843	PQN	C9-C10	6.88	1.50	1.39
45	BA	808	CLA	C4B-NB	6.87	1.41	1.35
45	BA	820	CLA	C4B-NB	6.87	1.41	1.35
45	AL	304	CLA	C4B-NB	6.87	1.41	1.35
45	BB	811	CLA	C4B-NB	6.87	1.41	1.35
45	BA	837	CLA	C4B-NB	6.86	1.41	1.35
45	BA	805	CLA	C4B-NB	6.84	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	824	CLA	C4B-NB	6.83	1.41	1.35
45	AF	802	CLA	C4B-NB	6.81	1.41	1.35
45	AB	811	CLA	C4B-NB	6.80	1.41	1.35
46	BB	844	PQN	C9-C10	6.80	1.50	1.39
45	AB	829	CLA	C4B-NB	6.80	1.41	1.35
45	AA	840	CLA	C4B-NB	6.80	1.41	1.35
45	AA	813	CLA	C4B-NB	6.79	1.41	1.35
45	AA	834	CLA	C4B-NB	6.78	1.41	1.35
45	BB	808	CLA	C4B-NB	6.78	1.41	1.35
45	AA	812	CLA	C4B-NB	6.77	1.41	1.35
45	AA	837	CLA	C4B-NB	6.75	1.41	1.35
45	AB	842	CLA	C4B-NB	6.73	1.41	1.35
45	A6	601	CLA	C4B-NB	6.73	1.41	1.35
46	BA	843	PQN	C10-C5	-6.69	1.29	1.40
46	AB	843	PQN	C10-C5	-6.68	1.29	1.40
45	AA	819	CLA	C4B-NB	6.65	1.41	1.35
45	AB	814	CLA	C4B-NB	6.64	1.41	1.35
45	BA	803	CLA	C4B-NB	6.64	1.41	1.35
45	BA	812	CLA	C4B-NB	6.61	1.41	1.35
45	BB	815	CLA	C4B-NB	6.60	1.41	1.35
45	AB	807	CLA	C4B-NB	6.58	1.41	1.35
46	AA	843	PQN	C10-C5	-6.56	1.29	1.40
45	BA	829	CLA	C4B-NB	6.55	1.41	1.35
45	AB	810	CLA	C4B-NB	6.49	1.41	1.35
46	BB	844	PQN	C6-C5	6.45	1.50	1.39
45	BA	840	CLA	C4B-NB	6.43	1.40	1.35
45	BB	805	CLA	C4B-NB	6.36	1.40	1.35
45	AB	804	CLA	C4B-NB	6.35	1.40	1.35
45	AA	829	CLA	C4B-NB	5.98	1.40	1.35
54	A4	304	CHL	C3B-C2B	5.84	1.48	1.40
54	B2	614	CHL	C3B-C2B	5.66	1.48	1.40
54	B5	607	CHL	C3B-C2B	5.58	1.48	1.40
54	A6	602	CHL	C3B-C2B	5.58	1.48	1.40
54	A6	608	CHL	C3B-C2B	5.53	1.48	1.40
54	B1	303	CHL	C3B-C2B	5.52	1.48	1.40
54	B1	308	CHL	C3B-C2B	5.51	1.48	1.40
54	B2	601	CHL	C3B-C2B	5.46	1.48	1.40
54	B5	605	CHL	C3B-C2B	5.44	1.47	1.40
54	B2	607	CHL	C3B-C2B	5.42	1.47	1.40
54	B5	606	CHL	C3C-C2C	5.38	1.47	1.36
54	A6	607	CHL	C3B-C2B	5.35	1.47	1.40
54	B1	308	CHL	C2C-C3C	5.26	1.48	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A6	606	CHL	C3B-C2B	5.23	1.47	1.40
54	B2	606	CHL	C3B-C2B	5.23	1.47	1.40
54	B5	606	CHL	O2D-CGD	5.22	1.45	1.33
54	B2	606	CHL	O2D-CGD	5.21	1.45	1.33
54	B2	605	CHL	O2D-CGD	5.21	1.45	1.33
54	B2	605	CHL	C3B-C2B	5.21	1.47	1.40
54	A4	306	CHL	C3B-C2B	5.19	1.47	1.40
54	A4	305	CHL	O2D-CGD	5.18	1.45	1.33
54	A6	607	CHL	O2D-CGD	5.16	1.45	1.33
54	B2	614	CHL	O2D-CGD	5.15	1.45	1.33
54	A6	606	CHL	O2D-CGD	5.13	1.45	1.33
54	A4	314	CHL	C2C-C3C	5.09	1.47	1.36
54	A6	608	CHL	O2D-CGD	5.08	1.45	1.33
54	A4	306	CHL	CHC-C1C	5.08	1.48	1.35
54	A4	304	CHL	C2C-C3C	5.05	1.47	1.37
54	B5	605	CHL	C2C-C3C	5.04	1.47	1.37
54	A1	303	CHL	C2C-C3C	5.03	1.47	1.36
54	B2	601	CHL	C2C-C3C	5.02	1.47	1.36
54	A6	602	CHL	C2C-C3C	5.01	1.47	1.36
56	BJ	104	SQD	O8-S	5.00	1.65	1.47
54	A4	306	CHL	O2D-CGD	5.00	1.45	1.33
54	B1	308	CHL	CHC-C1C	5.00	1.47	1.35
54	B2	605	CHL	C2C-C3C	4.99	1.47	1.37
54	B5	607	CHL	O2D-CGD	4.99	1.45	1.33
54	B2	606	CHL	C2C-C3C	4.98	1.47	1.36
54	B3	306	CHL	O2D-CGD	4.97	1.45	1.33
54	B2	607	CHL	O2D-CGD	4.96	1.45	1.33
54	A3	307	CHL	O2D-CGD	4.95	1.45	1.33
47	B3	318	LHG	O7-C7	4.94	1.46	1.35
54	B2	606	CHL	CHC-C1C	4.93	1.47	1.35
54	A1	308	CHL	C2C-C3C	4.93	1.47	1.36
54	B5	607	CHL	CHC-C1C	4.92	1.47	1.35
54	A1	308	CHL	C3B-C2B	4.91	1.47	1.40
54	A4	305	CHL	C3C-C2C	4.90	1.47	1.36
54	B2	614	CHL	C2C-C3C	4.89	1.47	1.36
54	A1	303	CHL	C3B-C2B	4.89	1.47	1.40
54	B5	607	CHL	C2C-C3C	4.88	1.47	1.37
54	A3	307	CHL	C3B-C2B	4.88	1.47	1.40
54	B2	607	CHL	CHC-C1C	4.84	1.47	1.35
54	A1	303	CHL	CHC-C1C	4.83	1.47	1.35
54	A6	606	CHL	CHC-C1C	4.83	1.47	1.35
54	B2	601	CHL	O2D-CGD	4.83	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B5	605	CHL	CHC-C1C	4.83	1.47	1.35
54	A4	314	CHL	CHC-C1C	4.83	1.47	1.35
54	B2	607	CHL	C2C-C3C	4.80	1.47	1.36
54	A6	607	CHL	C2C-C3C	4.80	1.47	1.36
54	A6	608	CHL	C3C-C2C	4.80	1.46	1.36
54	A6	606	CHL	C2C-C3C	4.77	1.46	1.37
54	B1	303	CHL	C2C-C3C	4.77	1.47	1.36
54	B2	601	CHL	CHC-C1C	4.77	1.47	1.35
54	A1	308	CHL	CHC-C1C	4.76	1.47	1.35
54	A6	608	CHL	CHC-C1C	4.75	1.47	1.35
54	B5	606	CHL	CHC-C1C	4.75	1.47	1.35
54	A4	305	CHL	CHC-C1C	4.75	1.47	1.35
54	B2	605	CHL	CHC-C1C	4.74	1.47	1.35
54	B1	303	CHL	CHC-C1C	4.73	1.47	1.35
47	A3	319	LHG	O7-C7	4.72	1.45	1.35
54	A4	306	CHL	C2C-C3C	4.71	1.46	1.36
54	B2	614	CHL	CHC-C1C	4.71	1.47	1.35
54	A4	304	CHL	CHC-C1C	4.67	1.47	1.35
54	B1	308	CHL	O2D-CGD	4.67	1.45	1.30
54	A6	602	CHL	CHC-C1C	4.66	1.46	1.35
54	A4	314	CHL	O2D-CGD	4.66	1.45	1.30
54	A3	307	CHL	C3C-C2C	4.65	1.46	1.36
54	B3	306	CHL	C3C-C2C	4.65	1.46	1.36
54	B5	605	CHL	O2D-CGD	4.64	1.45	1.30
54	A4	304	CHL	O2D-CGD	4.63	1.45	1.30
54	A1	308	CHL	O2D-CGD	4.63	1.45	1.30
54	A6	607	CHL	CHC-C1C	4.62	1.46	1.35
54	B1	303	CHL	O2D-CGD	4.60	1.45	1.30
54	B3	306	CHL	C3B-C2B	4.57	1.46	1.40
54	A1	303	CHL	O2D-CGD	4.57	1.45	1.30
54	A6	602	CHL	O2D-CGD	4.55	1.45	1.30
54	B3	306	CHL	O2A-CGA	4.51	1.45	1.30
54	B5	607	CHL	O2A-CGA	4.51	1.45	1.30
54	A4	306	CHL	O2A-CGA	4.51	1.45	1.30
54	B2	606	CHL	CHD-C1D	4.50	1.47	1.38
54	B2	601	CHL	O2A-CGA	4.49	1.46	1.33
54	A1	303	CHL	O2A-CGA	4.48	1.46	1.33
54	A3	307	CHL	O2A-CGA	4.47	1.45	1.30
54	B2	607	CHL	O2A-CGA	4.46	1.45	1.30
54	B2	605	CHL	CHD-C1D	4.45	1.47	1.38
54	A6	602	CHL	O2A-CGA	4.45	1.46	1.33
54	A1	303	CHL	C1D-ND	-4.42	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B5	606	CHL	CHD-C1D	4.40	1.46	1.38
54	B5	605	CHL	CHD-C1D	4.40	1.46	1.38
54	B1	308	CHL	CHD-C1D	4.39	1.46	1.38
54	B3	306	CHL	CHD-C1D	4.38	1.46	1.38
53	AG	202	LMG	O7-C10	4.38	1.46	1.34
54	A3	307	CHL	CHC-C1C	4.38	1.46	1.35
54	A1	308	CHL	CHD-C1D	4.38	1.46	1.38
54	A4	314	CHL	CHD-C1D	4.37	1.46	1.38
54	B3	306	CHL	CHC-C1C	4.36	1.46	1.35
54	A1	308	CHL	C3A-C2A	-4.36	1.50	1.54
47	B1	301	LHG	O7-C7	4.34	1.46	1.34
47	AJ	104	LHG	O8-C23	4.29	1.45	1.33
45	A6	611	CLA	CHB-C4A	4.29	1.38	1.34
53	B5	617	LMG	O7-C10	4.29	1.46	1.34
53	AG	202	LMG	O8-C28	4.28	1.45	1.33
54	A4	305	CHL	CHD-C1D	4.28	1.46	1.38
54	A6	608	CHL	O2A-CGA	4.28	1.45	1.33
47	A1	301	LHG	O7-C7	4.27	1.46	1.34
47	A1	302	LHG	O8-C23	4.27	1.45	1.33
54	A6	602	CHL	CHD-C1D	4.27	1.46	1.38
54	A6	608	CHL	CHD-C1D	4.26	1.46	1.38
47	B3	318	LHG	O8-C23	4.26	1.45	1.33
47	AA	844	LHG	O8-C23	4.26	1.45	1.33
47	AJ	104	LHG	O7-C7	4.26	1.46	1.34
47	B1	302	LHG	O7-C7	4.26	1.46	1.34
53	B5	617	LMG	O8-C28	4.25	1.45	1.33
47	A3	301	LHG	O8-C23	4.25	1.45	1.33
47	B1	301	LHG	O8-C23	4.24	1.45	1.33
47	A1	320	LHG	O8-C23	4.24	1.45	1.33
54	A6	607	CHL	CHD-C1D	4.24	1.46	1.38
47	B1	318	LHG	O7-C7	4.23	1.46	1.34
54	A4	304	CHL	CHD-C1D	4.23	1.46	1.38
53	A1	321	LMG	O8-C28	4.22	1.45	1.33
47	B5	618	LHG	O8-C23	4.21	1.45	1.33
54	B1	303	CHL	O2A-CGA	4.20	1.45	1.33
47	B1	302	LHG	O8-C23	4.20	1.45	1.33
53	A1	321	LMG	O7-C10	4.19	1.46	1.34
54	B2	601	CHL	CHD-C1D	4.19	1.46	1.38
56	BJ	104	SQD	O47-C7	4.19	1.46	1.34
54	A3	307	CHL	CHD-C1D	4.18	1.46	1.38
54	A6	606	CHL	CHD-C1D	4.17	1.46	1.38
51	BB	850	DGD	O1G-C1A	4.15	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A1	308	CHL	C1D-ND	-4.14	1.32	1.37
47	B1	318	LHG	O8-C23	4.13	1.45	1.33
47	A1	302	LHG	O7-C7	4.13	1.46	1.34
47	BF	305	LHG	O8-C23	4.12	1.45	1.33
47	A3	301	LHG	O7-C7	4.11	1.45	1.34
54	B2	614	CHL	C1D-ND	-4.10	1.32	1.37
56	BJ	104	SQD	O48-C23	4.10	1.45	1.33
47	BA	846	LHG	O7-C7	4.09	1.45	1.34
47	A1	301	LHG	O8-C23	4.09	1.45	1.33
47	A3	319	LHG	O8-C23	4.09	1.45	1.33
45	B2	610	CLA	CHB-C4A	4.07	1.37	1.34
51	AB	851	DGD	O1G-C1A	4.06	1.45	1.33
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	B2	607	CHL	C1D-ND	-4.03	1.32	1.37
54	B1	303	CHL	CHD-C1D	4.02	1.46	1.38
54	B5	607	CHL	C1D-ND	-4.02	1.32	1.37
54	A4	314	CHL	CHD-C4C	4.02	1.48	1.39
45	AA	823	CLA	C1D-ND	4.02	1.42	1.37
54	A4	304	CHL	C1D-ND	-4.01	1.32	1.37
54	B1	308	CHL	C3A-C2A	-4.01	1.50	1.54
47	A6	618	LHG	O7-C7	4.00	1.45	1.34
54	B2	614	CHL	CHD-C1D	4.00	1.46	1.38
54	A1	303	CHL	CHD-C1D	3.99	1.46	1.38
45	A6	614	CLA	C1D-ND	3.99	1.42	1.37
51	BB	850	DGD	O2G-C1B	3.98	1.45	1.34
47	B2	618	LHG	O8-C23	3.98	1.45	1.33
54	B2	607	CHL	CHD-C1D	3.98	1.46	1.38
54	A4	306	CHL	C1D-ND	-3.97	1.32	1.37
47	A6	618	LHG	O8-C23	3.96	1.44	1.33
47	B5	618	LHG	O7-C7	3.95	1.45	1.34
54	B2	606	CHL	CHD-C4C	3.95	1.48	1.39
45	BA	801	CLA	C1D-ND	3.95	1.42	1.37
54	B2	606	CHL	C1D-ND	-3.94	1.32	1.37
54	B1	303	CHL	C1D-ND	-3.94	1.32	1.37
54	A4	304	CHL	CHD-C4C	3.93	1.48	1.39
54	B5	607	CHL	CHD-C1D	3.93	1.46	1.38
45	BB	837	CLA	C1D-ND	3.92	1.42	1.37
54	B1	308	CHL	CHD-C4C	3.92	1.48	1.39
54	A6	606	CHL	C1D-ND	-3.91	1.33	1.37
45	AB	802	CLA	CAB-C3B	-3.90	1.43	1.51
45	AA	801	CLA	C1D-ND	3.90	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A4	314	CHL	C1D-ND	-3.89	1.33	1.37
53	A4	318	LMG	O8-C28	3.89	1.44	1.33
47	AA	844	LHG	O7-C7	3.89	1.45	1.34
45	BK	201	CLA	C1D-ND	3.89	1.42	1.37
54	A6	608	CHL	C1D-ND	-3.88	1.33	1.37
52	B1	316	LUT	C10-C9	3.88	1.40	1.35
45	BL	302	CLA	C1D-ND	3.88	1.42	1.37
45	AK	201	CLA	C4B-CHC	-3.88	1.36	1.43
45	A3	311	CLA	C1D-ND	3.88	1.42	1.37
45	BA	844	CLA	C1D-ND	3.87	1.42	1.37
45	B1	307	CLA	C1D-ND	3.87	1.42	1.37
54	A6	602	CHL	CHD-C4C	3.86	1.48	1.39
45	A4	302	CLA	C1D-ND	3.85	1.42	1.37
54	B5	605	CHL	CHD-C4C	3.85	1.48	1.39
51	AB	851	DGD	O2G-C1B	3.85	1.45	1.34
45	B3	309	CLA	C1D-ND	3.84	1.42	1.37
54	B5	606	CHL	C1D-ND	-3.84	1.33	1.37
45	BA	836	CLA	C1D-ND	3.84	1.42	1.37
45	A3	313	CLA	C1D-ND	3.84	1.42	1.37
54	A4	305	CHL	CHD-C4C	3.83	1.48	1.39
47	B2	618	LHG	O7-C7	3.83	1.45	1.34
54	B2	605	CHL	CHD-C4C	3.82	1.48	1.39
54	A6	607	CHL	C1D-ND	-3.82	1.33	1.37
45	B1	309	CLA	C1D-ND	3.82	1.42	1.37
54	B3	306	CHL	C1D-ND	-3.82	1.33	1.37
45	AK	201	CLA	C1D-ND	3.82	1.42	1.37
54	B2	601	CHL	CHD-C4C	3.82	1.47	1.39
47	BA	845	LHG	O8-C23	3.82	1.44	1.33
54	B5	605	CHL	C1D-ND	-3.82	1.33	1.37
45	A3	312	CLA	C1D-ND	3.81	1.42	1.37
54	A4	305	CHL	C1D-ND	-3.81	1.33	1.37
45	A1	316	CLA	C1D-ND	3.81	1.42	1.37
54	A6	607	CHL	CHD-C4C	3.80	1.47	1.39
45	AL	304	CLA	C1D-ND	3.80	1.42	1.37
45	A1	305	CLA	C1D-ND	3.80	1.42	1.37
45	AH	201	CLA	C1D-ND	3.80	1.42	1.37
45	A1	312	CLA	CAB-C3B	-3.79	1.43	1.51
45	AB	836	CLA	C1D-ND	3.79	1.42	1.37
45	AF	804	CLA	C1D-ND	3.79	1.42	1.37
45	BB	842	CLA	C1D-ND	3.79	1.42	1.37
45	BG	202	CLA	C1D-ND	3.79	1.42	1.37
45	B3	310	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	313	CLA	C1D-ND	3.78	1.42	1.37
54	B2	614	CHL	CHD-C4C	3.78	1.47	1.39
54	A4	305	CHL	OBD-CAD	3.78	1.29	1.22
45	AG	204	CLA	C1D-ND	3.78	1.42	1.37
45	B3	312	CLA	C1D-ND	3.78	1.42	1.37
45	BL	303	CLA	C1D-ND	3.78	1.42	1.37
54	A1	308	CHL	CHD-C4C	3.77	1.47	1.39
54	B5	606	CHL	CHD-C4C	3.77	1.47	1.39
45	AA	836	CLA	C1D-ND	3.77	1.42	1.37
45	AA	816	CLA	C1D-ND	3.77	1.42	1.37
45	BK	202	CLA	C1D-ND	3.77	1.42	1.37
45	A3	303	CLA	C1D-ND	3.77	1.42	1.37
45	AB	817	CLA	C1D-ND	3.76	1.42	1.37
45	B5	601	CLA	C1D-ND	3.76	1.42	1.37
52	B1	316	LUT	C34-C33	3.76	1.40	1.35
54	B1	308	CHL	C1D-ND	-3.76	1.33	1.37
45	BB	818	CLA	C1D-ND	3.76	1.42	1.37
54	A6	602	CHL	C1D-ND	-3.75	1.33	1.37
45	B1	313	CLA	C1D-ND	3.75	1.42	1.37
54	A4	306	CHL	CHD-C1D	3.75	1.45	1.38
54	A6	608	CHL	CHD-C4C	3.75	1.47	1.39
54	B2	605	CHL	C1D-ND	-3.75	1.33	1.37
45	AA	812	CLA	C1D-ND	3.74	1.42	1.37
45	A6	613	CLA	C1D-ND	3.74	1.42	1.37
45	BA	815	CLA	C1D-ND	3.74	1.42	1.37
45	A1	309	CLA	C1D-ND	3.74	1.42	1.37
54	A1	308	CHL	OBD-CAD	3.74	1.28	1.22
45	A1	307	CLA	C1D-ND	3.74	1.42	1.37
45	B3	313	CLA	C1D-ND	3.74	1.42	1.37
45	B1	306	CLA	C1D-ND	3.74	1.42	1.37
45	AK	203	CLA	C1D-ND	3.73	1.42	1.37
45	BJ	102	CLA	C1D-ND	3.73	1.42	1.37
45	B2	611	CLA	C1D-ND	3.73	1.42	1.37
54	B5	607	CHL	CHD-C4C	3.73	1.47	1.39
54	A3	307	CHL	C1D-ND	-3.73	1.33	1.37
54	B2	614	CHL	OBD-CAD	3.73	1.28	1.22
54	B2	606	CHL	OBD-CAD	3.73	1.28	1.22
45	AK	202	CLA	C1D-ND	3.73	1.42	1.37
45	A3	306	CLA	C1D-ND	3.72	1.42	1.37
45	B2	609	CLA	C1D-ND	3.72	1.42	1.37
54	A6	606	CHL	CHD-C4C	3.72	1.47	1.39
45	BA	832	CLA	C1D-ND	3.72	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B2	601	CHL	C1D-ND	-3.71	1.33	1.37
54	B1	308	CHL	OBD-CAD	3.71	1.28	1.22
54	A1	303	CHL	CHD-C4C	3.71	1.47	1.39
45	A1	306	CLA	C1D-ND	3.71	1.42	1.37
54	A6	607	CHL	OBD-CAD	3.71	1.28	1.22
45	A4	310	CLA	C1D-ND	3.71	1.42	1.37
45	B3	305	CLA	C1D-ND	3.71	1.42	1.37
45	A3	305	CLA	C1D-ND	3.71	1.42	1.37
45	A1	315	CLA	C1D-ND	3.70	1.42	1.37
54	A6	606	CHL	OBD-CAD	3.69	1.28	1.22
45	AG	201	CLA	C1D-ND	3.69	1.42	1.37
45	A4	312	CLA	C1D-ND	3.69	1.42	1.37
45	B5	604	CLA	C1D-ND	3.69	1.42	1.37
45	B1	312	CLA	C1D-ND	3.69	1.42	1.37
45	AB	808	CLA	C1D-ND	3.69	1.42	1.37
54	A4	314	CHL	OBD-CAD	3.69	1.28	1.22
45	B1	305	CLA	C1D-ND	3.69	1.42	1.37
46	BB	844	PQN	C11-C12	3.68	1.56	1.50
45	AJ	102	CLA	C1D-ND	3.68	1.42	1.37
45	BB	836	CLA	C1D-ND	3.68	1.42	1.37
45	AA	822	CLA	C1D-ND	3.68	1.42	1.37
45	BB	820	CLA	C1D-ND	3.67	1.42	1.37
45	B5	613	CLA	C1D-ND	3.67	1.42	1.37
45	AA	832	CLA	C1D-ND	3.67	1.42	1.37
45	A6	605	CLA	C1D-ND	3.67	1.42	1.37
45	AL	305	CLA	C1D-ND	3.67	1.42	1.37
50	AL	301	LMU	O5B-C1B	3.67	1.51	1.41
45	BF	303	CLA	C1D-ND	3.67	1.42	1.37
45	BA	812	CLA	C1D-ND	3.67	1.42	1.37
52	B1	316	LUT	C14-C13	3.66	1.40	1.35
54	B5	606	CHL	OBD-CAD	3.66	1.28	1.22
45	B5	603	CLA	C1D-ND	3.66	1.42	1.37
45	A3	314	CLA	C1D-ND	3.66	1.42	1.37
45	BB	809	CLA	C1D-ND	3.66	1.42	1.37
45	BA	816	CLA	C1D-ND	3.66	1.42	1.37
45	BA	823	CLA	C1D-ND	3.65	1.42	1.37
45	BB	828	CLA	C1D-ND	3.65	1.42	1.37
45	AA	835	CLA	C1D-ND	3.65	1.42	1.37
45	A3	310	CLA	C1D-ND	3.65	1.42	1.37
54	B1	303	CHL	OBD-CAD	3.65	1.28	1.22
45	B5	611	CLA	C1D-ND	3.65	1.42	1.37
54	A4	304	CHL	OBD-CAD	3.65	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	819	CLA	C1D-ND	3.65	1.42	1.37
45	BB	833	CLA	C1D-ND	3.64	1.42	1.37
54	B5	606	CHL	C3D-C2D	3.64	1.49	1.39
45	B3	303	CLA	C1D-ND	3.64	1.42	1.37
54	B2	601	CHL	OBD-CAD	3.64	1.28	1.22
54	A4	306	CHL	CHD-C4C	3.64	1.47	1.39
45	BA	813	CLA	C1D-ND	3.64	1.42	1.37
47	BA	845	LHG	O7-C7	3.64	1.44	1.34
45	A4	308	CLA	C1D-ND	3.64	1.42	1.37
54	A6	602	CHL	OBD-CAD	3.64	1.28	1.22
45	BA	835	CLA	C1D-ND	3.64	1.42	1.37
45	B1	310	CLA	C1D-ND	3.63	1.42	1.37
54	B2	607	CHL	CHD-C4C	3.63	1.47	1.39
45	A3	304	CLA	CAB-C3B	-3.63	1.44	1.51
45	B5	610	CLA	C1D-ND	3.63	1.42	1.37
45	BB	843	CLA	C1D-ND	3.62	1.42	1.37
45	BA	807	CLA	C1D-ND	3.62	1.42	1.37
45	B5	612	CLA	C1D-ND	3.62	1.42	1.37
54	A6	608	CHL	OBD-CAD	3.61	1.28	1.22
45	BA	810	CLA	C1D-ND	3.61	1.42	1.37
45	A4	303	CLA	C1D-ND	3.61	1.42	1.37
45	AA	802	CLA	C4D-ND	-3.61	1.32	1.37
45	AB	841	CLA	C1D-ND	3.60	1.42	1.37
54	B1	308	CHL	C3D-C2D	3.60	1.49	1.39
45	BA	802	CLA	C4D-ND	-3.60	1.32	1.37
45	B2	612	CLA	C1D-ND	3.60	1.42	1.37
45	B1	310	CLA	CAB-C3B	-3.60	1.44	1.51
45	BA	824	CLA	C1D-ND	3.60	1.42	1.37
45	BA	818	CLA	C1D-ND	3.59	1.42	1.37
45	A3	309	CLA	C1D-ND	3.59	1.42	1.37
45	A4	307	CLA	C1D-ND	3.59	1.42	1.37
45	BA	839	CLA	C1D-ND	3.59	1.42	1.37
45	BA	820	CLA	C1D-ND	3.59	1.42	1.37
45	BH	201	CLA	C1D-ND	3.59	1.42	1.37
45	AB	827	CLA	C1D-ND	3.59	1.42	1.37
45	AA	807	CLA	C1D-ND	3.59	1.42	1.37
45	B5	603	CLA	CAB-C3B	-3.58	1.44	1.51
45	A4	303	CLA	CAB-C3B	-3.58	1.44	1.51
45	BA	822	CLA	C1D-ND	3.58	1.42	1.37
45	A1	311	CLA	C1D-ND	3.58	1.42	1.37
45	B3	307	CLA	C1D-ND	3.58	1.42	1.37
54	B3	306	CHL	CHD-C4C	3.58	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A3	304	CLA	C1D-ND	3.58	1.42	1.37
45	BA	834	CLA	C1D-ND	3.58	1.42	1.37
45	B2	604	CLA	C1D-ND	3.58	1.42	1.37
45	BF	302	CLA	C1D-ND	3.57	1.42	1.37
45	A4	302	CLA	CAB-C3B	-3.57	1.44	1.51
45	AA	809	CLA	C1D-ND	3.57	1.42	1.37
45	AA	820	CLA	C1D-ND	3.57	1.42	1.37
45	AB	812	CLA	C1D-ND	3.57	1.42	1.37
45	B5	604	CLA	CAB-C3B	-3.57	1.44	1.51
45	AB	816	CLA	C1D-ND	3.57	1.42	1.37
45	AB	819	CLA	C1D-ND	3.57	1.42	1.37
45	A4	309	CLA	C1D-ND	3.57	1.42	1.37
45	BB	813	CLA	C1D-ND	3.57	1.42	1.37
45	AB	832	CLA	C1D-ND	3.57	1.42	1.37
45	AA	806	CLA	C1D-ND	3.57	1.42	1.37
45	AL	303	CLA	C1D-ND	3.56	1.42	1.37
45	A6	610	CLA	C1D-ND	3.56	1.42	1.37
45	BA	817	CLA	C1D-ND	3.56	1.42	1.37
45	A1	310	CLA	CAB-C3B	-3.56	1.44	1.51
45	BA	821	CLA	C1D-ND	3.55	1.42	1.37
45	B1	311	CLA	C1D-ND	3.55	1.42	1.37
45	AA	828	CLA	C1D-ND	3.55	1.42	1.37
45	B3	303	CLA	CAB-C3B	-3.55	1.44	1.51
45	B2	613	CLA	C1D-ND	3.55	1.42	1.37
45	A6	612	CLA	C1D-ND	3.55	1.42	1.37
45	BK	203	CLA	C1D-ND	3.55	1.42	1.37
45	B5	608	CLA	C1D-ND	3.55	1.42	1.37
45	A1	316	CLA	CAB-C3B	-3.55	1.44	1.51
45	A4	311	CLA	C1D-ND	3.55	1.42	1.37
53	A4	318	LMG	O7-C10	3.54	1.44	1.34
45	B3	302	CLA	C1D-ND	3.54	1.42	1.37
45	A1	312	CLA	C1D-ND	3.54	1.42	1.37
54	B2	605	CHL	OBD-CAD	3.54	1.28	1.22
45	BA	840	CLA	C1D-ND	3.54	1.42	1.37
45	AB	812	CLA	CAB-C3B	-3.54	1.44	1.51
45	AA	803	CLA	C1D-ND	3.54	1.42	1.37
45	B2	603	CLA	C1D-ND	3.54	1.42	1.37
45	B3	311	CLA	C1D-ND	3.54	1.42	1.37
45	BA	814	CLA	C1D-ND	3.53	1.42	1.37
45	AA	827	CLA	C1D-ND	3.53	1.42	1.37
45	A4	313	CLA	C1D-ND	3.53	1.42	1.37
45	BA	837	CLA	C1D-ND	3.53	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	601	CLA	C1D-ND	3.53	1.42	1.37
54	A3	307	CHL	CHD-C4C	3.53	1.47	1.39
45	AB	818	CLA	C1D-ND	3.53	1.42	1.37
45	B5	609	CLA	C1D-ND	3.53	1.42	1.37
45	B3	304	CLA	C1D-ND	3.53	1.42	1.37
54	A4	305	CHL	C3D-C2D	3.52	1.48	1.39
45	AA	813	CLA	C1D-ND	3.52	1.42	1.37
46	BA	843	PQN	C11-C12	3.52	1.55	1.50
45	A6	604	CLA	C1D-ND	3.52	1.42	1.37
45	BB	813	CLA	CAB-C3B	-3.52	1.44	1.51
45	AA	811	CLA	C1D-ND	3.52	1.42	1.37
45	BK	201	CLA	CAB-C3B	-3.52	1.44	1.51
45	AB	842	CLA	C1D-ND	3.52	1.42	1.37
45	AA	839	CLA	C1D-ND	3.52	1.42	1.37
54	B1	303	CHL	CHD-C4C	3.52	1.47	1.39
45	A3	306	CLA	CAB-C3B	-3.52	1.44	1.51
45	BB	808	CLA	C1D-ND	3.52	1.42	1.37
45	AA	807	CLA	C4D-ND	-3.51	1.32	1.37
45	B5	602	CLA	C4D-ND	-3.51	1.32	1.37
45	AA	814	CLA	C1D-ND	3.51	1.42	1.37
45	B1	312	CLA	CAB-C3B	-3.51	1.44	1.51
45	B3	305	CLA	CAB-C3B	-3.51	1.44	1.51
45	A6	611	CLA	CAB-C3B	-3.51	1.44	1.51
45	B1	314	CLA	C1D-ND	3.51	1.42	1.37
45	BA	805	CLA	C1D-ND	3.51	1.42	1.37
45	B1	315	CLA	CAB-C3B	-3.51	1.44	1.51
52	B1	316	LUT	C30-C29	3.50	1.40	1.35
54	A3	307	CHL	OBD-CAD	3.50	1.28	1.22
45	B3	308	CLA	C1D-ND	3.50	1.42	1.37
45	A3	308	CLA	C1D-ND	3.50	1.42	1.37
45	A1	314	CLA	C1D-ND	3.50	1.42	1.37
54	A6	607	CHL	C3D-C2D	3.50	1.48	1.39
45	BB	834	CLA	C1D-ND	3.50	1.42	1.37
45	AA	831	CLA	C1D-ND	3.49	1.42	1.37
54	B5	605	CHL	OBD-CAD	3.49	1.28	1.22
45	AF	803	CLA	C1D-ND	3.49	1.42	1.37
54	A4	314	CHL	C3D-C2D	3.49	1.48	1.39
54	B3	306	CHL	OBD-CAD	3.49	1.28	1.22
45	AB	806	CLA	C1D-ND	3.49	1.42	1.37
50	AL	301	LMU	O5'-C1'	3.48	1.50	1.41
45	AB	837	CLA	C1D-ND	3.48	1.42	1.37
45	A6	609	CLA	C1D-ND	3.48	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A6	606	CHL	C3D-C2D	3.48	1.48	1.39
45	BB	807	CLA	C1D-ND	3.48	1.42	1.37
45	AA	826	CLA	C4D-ND	-3.48	1.32	1.37
45	AA	837	CLA	C1D-ND	3.47	1.42	1.37
45	AB	821	CLA	C1D-ND	3.47	1.42	1.37
45	B3	301	CLA	C1D-ND	3.47	1.42	1.37
45	BA	831	CLA	C1D-ND	3.47	1.42	1.37
45	A1	315	CLA	CAB-C3B	-3.47	1.44	1.51
45	BA	841	CLA	C4D-ND	-3.46	1.32	1.37
45	B2	608	CLA	C1D-ND	3.46	1.42	1.37
54	B2	606	CHL	C3D-C2D	3.46	1.48	1.39
45	BA	830	CLA	C4D-ND	-3.46	1.32	1.37
45	AA	821	CLA	C1D-ND	3.46	1.42	1.37
54	A1	303	CHL	C3D-C2D	3.46	1.48	1.39
54	B5	605	CHL	C3D-C2D	3.46	1.48	1.39
45	B1	315	CLA	C1D-ND	3.46	1.42	1.37
45	AB	811	CLA	C1D-ND	3.45	1.42	1.37
54	A1	308	CHL	C3D-C2D	3.45	1.48	1.39
45	AB	828	CLA	C1D-ND	3.45	1.42	1.37
45	BB	817	CLA	C1D-ND	3.44	1.42	1.37
45	B2	610	CLA	C1D-ND	3.44	1.42	1.37
45	A3	302	CLA	C1D-ND	3.44	1.42	1.37
45	BA	808	CLA	C4D-ND	-3.44	1.33	1.37
54	B2	605	CHL	C3D-C2D	3.44	1.48	1.39
45	BB	802	CLA	C4D-ND	-3.44	1.33	1.37
45	BA	827	CLA	C1D-ND	3.44	1.42	1.37
45	BB	811	CLA	C1D-ND	3.44	1.42	1.37
50	AB	852	LMU	O5B-C1B	3.44	1.50	1.41
45	AA	818	CLA	C1D-ND	3.44	1.42	1.37
45	BB	807	CLA	C4D-ND	-3.44	1.33	1.37
45	AB	802	CLA	C1D-ND	3.43	1.42	1.37
45	A1	310	CLA	C1D-ND	3.43	1.42	1.37
45	BB	821	CLA	C4D-ND	-3.42	1.33	1.37
45	BA	809	CLA	C1D-ND	3.42	1.42	1.37
45	B2	610	CLA	CAB-C3B	-3.42	1.44	1.51
45	BG	201	CLA	C1D-ND	3.42	1.42	1.37
45	BB	821	CLA	C1D-ND	3.41	1.42	1.37
54	B2	607	CHL	OBD-CAD	3.41	1.28	1.22
45	AA	805	CLA	C1D-ND	3.41	1.42	1.37
45	BA	828	CLA	C1D-ND	3.41	1.42	1.37
45	B2	610	CLA	C4D-ND	-3.41	1.33	1.37
50	BA	853	LMU	O5B-C1B	3.41	1.50	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	810	CLA	C1D-ND	3.41	1.42	1.37
45	BA	811	CLA	C1D-ND	3.41	1.42	1.37
45	BB	819	CLA	C1D-ND	3.40	1.42	1.37
45	BA	804	CLA	C1D-ND	3.40	1.42	1.37
45	AG	203	CLA	C1D-ND	3.40	1.42	1.37
45	BB	827	CLA	C1D-ND	3.40	1.42	1.37
54	A4	304	CHL	C3D-C2D	3.40	1.48	1.39
45	BA	808	CLA	C1D-ND	3.40	1.42	1.37
54	A6	608	CHL	C3D-C2D	3.39	1.48	1.39
45	AB	826	CLA	C1D-ND	3.39	1.42	1.37
46	AB	843	PQN	C11-C12	3.39	1.55	1.50
45	B3	314	CLA	C1D-ND	3.39	1.42	1.37
45	BL	304	CLA	C1D-ND	3.39	1.41	1.37
45	AB	811	CLA	C4D-ND	-3.39	1.33	1.37
45	BA	841	CLA	C1D-ND	3.39	1.41	1.37
45	AA	804	CLA	C1D-ND	3.38	1.41	1.37
45	BA	832	CLA	C4D-ND	-3.38	1.33	1.37
45	BA	819	CLA	C1D-ND	3.38	1.41	1.37
45	BA	838	CLA	C4D-ND	-3.38	1.33	1.37
45	A6	603	CLA	C1D-ND	3.37	1.41	1.37
50	AB	853	LMU	O5'-C1'	3.37	1.50	1.41
54	A3	307	CHL	C3D-C2D	3.37	1.48	1.39
45	BA	826	CLA	C4D-ND	-3.37	1.33	1.37
45	AB	833	CLA	C1D-ND	3.37	1.41	1.37
45	BB	827	CLA	C4D-ND	-3.37	1.33	1.37
45	BB	829	CLA	C1D-ND	3.37	1.41	1.37
45	AB	835	CLA	C1D-ND	3.37	1.41	1.37
54	A1	303	CHL	OBD-CAD	3.37	1.28	1.22
45	AB	833	CLA	C4D-ND	-3.37	1.33	1.37
45	BA	830	CLA	C1D-ND	3.37	1.41	1.37
54	B2	614	CHL	C3D-C2D	3.36	1.48	1.39
45	BA	806	CLA	C1D-ND	3.36	1.41	1.37
45	AB	820	CLA	C4D-ND	-3.36	1.33	1.37
45	BA	821	CLA	C4D-ND	-3.36	1.33	1.37
45	AA	842	CLA	C1D-ND	3.36	1.41	1.37
45	AA	829	CLA	C1D-ND	3.36	1.41	1.37
45	BB	812	CLA	C1D-ND	3.36	1.41	1.37
45	BB	822	CLA	C1D-ND	3.36	1.41	1.37
45	BB	816	CLA	C1D-ND	3.36	1.41	1.37
46	AA	843	PQN	C11-C12	3.35	1.55	1.50
45	AB	823	CLA	C1D-ND	3.35	1.41	1.37
45	BA	842	CLA	C1D-ND	3.35	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BF	301	CLA	C1D-ND	3.35	1.41	1.37
45	A4	301	CLA	C4D-ND	-3.35	1.33	1.37
45	BA	825	CLA	C1D-ND	3.34	1.41	1.37
54	B1	303	CHL	C3D-C2D	3.34	1.48	1.39
45	AB	822	CLA	C1D-ND	3.34	1.41	1.37
50	AA	851	LMU	O5'-C1'	3.34	1.50	1.41
45	BA	833	CLA	C1D-ND	3.34	1.41	1.37
45	BA	807	CLA	C4D-ND	-3.34	1.33	1.37
45	BB	806	CLA	C1D-ND	3.34	1.41	1.37
45	BB	840	CLA	C1D-ND	3.34	1.41	1.37
45	AB	805	CLA	C1D-ND	3.34	1.41	1.37
45	AB	814	CLA	C4D-ND	-3.34	1.33	1.37
54	A4	306	CHL	OBD-CAD	3.34	1.28	1.22
50	AB	853	LMU	O5B-C1B	3.33	1.50	1.41
50	BA	854	LMU	O5B-C1B	3.33	1.50	1.41
45	BA	804	CLA	C4D-ND	-3.33	1.33	1.37
45	BA	838	CLA	C1D-ND	3.33	1.41	1.37
54	A6	602	CHL	C3D-C2D	3.33	1.48	1.39
45	AA	824	CLA	C1D-ND	3.32	1.41	1.37
45	BB	802	CLA	C1D-ND	3.32	1.41	1.37
45	BB	825	CLA	C4D-ND	-3.32	1.33	1.37
45	B2	602	CLA	C4D-ND	-3.32	1.33	1.37
45	BL	303	CLA	C4D-ND	-3.32	1.33	1.37
45	AA	841	CLA	C1D-ND	3.32	1.41	1.37
45	B5	602	CLA	C1D-ND	3.32	1.41	1.37
45	BA	802	CLA	C1D-ND	3.31	1.41	1.37
45	BA	840	CLA	C4D-ND	-3.31	1.33	1.37
45	BB	824	CLA	C1D-ND	3.31	1.41	1.37
45	AB	802	CLA	C4D-ND	-3.31	1.33	1.37
54	A4	306	CHL	C3D-C2D	3.31	1.48	1.39
45	AA	817	CLA	C1D-ND	3.31	1.41	1.37
45	B1	307	CLA	CHC-C1C	3.31	1.43	1.35
45	AB	803	CLA	C1D-ND	3.31	1.41	1.37
45	AB	826	CLA	C4D-ND	-3.31	1.33	1.37
45	AB	820	CLA	C1D-ND	3.31	1.41	1.37
45	BB	811	CLA	C4D-ND	-3.30	1.33	1.37
50	BA	854	LMU	O5'-C1'	3.30	1.50	1.41
45	BA	830	CLA	CMB-C2B	-3.30	1.44	1.51
45	BA	826	CLA	C1D-ND	3.30	1.41	1.37
50	AB	850	LMU	O5'-C1'	3.29	1.50	1.41
45	BB	814	CLA	C1D-ND	3.29	1.41	1.37
45	AA	838	CLA	C4D-ND	-3.29	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	829	CLA	C4D-ND	-3.29	1.33	1.37
45	BB	830	CLA	C1D-ND	3.29	1.41	1.37
45	BB	812	CLA	C4D-ND	-3.29	1.33	1.37
45	BB	826	CLA	C4D-ND	-3.29	1.33	1.37
45	AB	813	CLA	C1D-ND	3.29	1.41	1.37
45	AB	814	CLA	C1D-ND	3.29	1.41	1.37
45	AA	813	CLA	C4D-ND	-3.29	1.33	1.37
45	AA	838	CLA	C1D-ND	3.28	1.41	1.37
45	AA	819	CLA	C4D-ND	-3.28	1.33	1.37
45	AA	804	CLA	C4D-ND	-3.28	1.33	1.37
45	BA	819	CLA	C4D-ND	-3.28	1.33	1.37
45	BB	804	CLA	C1D-ND	3.28	1.41	1.37
45	BB	823	CLA	C4D-ND	-3.28	1.33	1.37
45	BB	831	CLA	C4D-ND	-3.28	1.33	1.37
45	BB	824	CLA	C4D-ND	-3.28	1.33	1.37
45	BB	830	CLA	C4D-ND	-3.27	1.33	1.37
45	AB	838	CLA	C4D-ND	-3.27	1.33	1.37
45	BA	805	CLA	C4D-ND	-3.27	1.33	1.37
45	AA	808	CLA	C1D-ND	3.27	1.41	1.37
45	B2	609	CLA	CHC-C1C	3.27	1.43	1.35
45	B1	304	CLA	C4D-ND	-3.27	1.33	1.37
45	A6	603	CLA	C4D-ND	-3.27	1.33	1.37
45	AA	834	CLA	C1D-ND	3.27	1.41	1.37
45	AA	830	CLA	CMB-C2B	-3.27	1.44	1.51
45	BB	843	CLA	CHC-C1C	3.27	1.43	1.35
45	A3	315	CLA	C1D-ND	3.26	1.41	1.37
45	BB	832	CLA	C4D-ND	-3.26	1.33	1.37
45	B3	301	CLA	C4D-ND	-3.26	1.33	1.37
50	BA	853	LMU	O5'-C1'	3.26	1.50	1.41
45	AA	802	CLA	C1D-ND	3.26	1.41	1.37
45	AB	807	CLA	C4D-ND	-3.26	1.33	1.37
45	BA	813	CLA	C4D-ND	-3.26	1.33	1.37
45	BA	812	CLA	C4D-ND	-3.26	1.33	1.37
45	BB	820	CLA	C4D-ND	-3.26	1.33	1.37
45	BB	841	CLA	C4D-ND	-3.26	1.33	1.37
45	AB	810	CLA	C4D-ND	-3.25	1.33	1.37
54	B3	306	CHL	C3D-C2D	3.25	1.48	1.39
45	AA	832	CLA	C4D-ND	-3.25	1.33	1.37
45	A3	302	CLA	C4D-ND	-3.25	1.33	1.37
54	B5	607	CHL	C3D-C2D	3.25	1.48	1.39
45	AK	203	CLA	C4D-ND	-3.25	1.33	1.37
45	BB	825	CLA	C1D-ND	3.25	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	809	CLA	C4D-ND	-3.24	1.33	1.37
45	BB	839	CLA	C4D-ND	-3.24	1.33	1.37
54	B2	601	CHL	C3D-C2D	3.24	1.48	1.39
50	BB	851	LMU	O5B-C1B	3.24	1.50	1.41
45	AB	829	CLA	C1D-ND	3.24	1.41	1.37
45	BB	808	CLA	C4D-ND	-3.24	1.33	1.37
45	B2	602	CLA	C1D-ND	3.24	1.41	1.37
45	AL	304	CLA	C4D-ND	-3.24	1.33	1.37
45	AF	803	CLA	C4D-ND	-3.23	1.33	1.37
45	AB	810	CLA	C1D-ND	3.23	1.41	1.37
45	AB	815	CLA	C4D-ND	-3.23	1.33	1.37
45	B5	603	CLA	C4D-ND	-3.23	1.33	1.37
45	AB	804	CLA	C4D-ND	-3.23	1.33	1.37
45	BF	302	CLA	C4D-ND	-3.23	1.33	1.37
50	BB	851	LMU	O5'-C1'	3.23	1.50	1.41
45	BB	834	CLA	C4D-ND	-3.23	1.33	1.37
45	AB	841	CLA	C4D-ND	-3.23	1.33	1.37
45	A6	604	CLA	C4D-ND	-3.23	1.33	1.37
45	AA	826	CLA	C1D-ND	3.22	1.41	1.37
45	AA	840	CLA	C1D-ND	3.22	1.41	1.37
45	AB	831	CLA	C1D-ND	3.22	1.41	1.37
45	BA	814	CLA	C4D-ND	-3.22	1.33	1.37
45	BB	816	CLA	C4D-ND	-3.22	1.33	1.37
45	B5	601	CLA	C4D-ND	-3.22	1.33	1.37
45	BB	838	CLA	C1D-ND	3.22	1.41	1.37
45	AB	820	CLA	CMB-C2B	-3.22	1.44	1.51
45	A6	604	CLA	CHC-C1C	3.22	1.43	1.35
45	AB	839	CLA	CMD-C2D	-3.21	1.44	1.50
45	AB	825	CLA	C4D-ND	-3.21	1.33	1.37
45	AA	833	CLA	CMB-C2B	-3.21	1.45	1.51
45	AA	833	CLA	C1D-ND	3.21	1.41	1.37
45	AF	802	CLA	CMB-C2B	-3.21	1.45	1.51
45	AB	817	CLA	C4D-ND	-3.21	1.33	1.37
45	AB	801	CLA	C4D-ND	-3.21	1.33	1.37
45	A6	601	CLA	C4D-ND	-3.21	1.33	1.37
45	A3	308	CLA	C4D-ND	-3.20	1.33	1.37
45	AA	825	CLA	C1D-ND	3.20	1.41	1.37
50	AB	852	LMU	O5'-C1'	3.20	1.50	1.41
45	A6	614	CLA	CHC-C1C	3.20	1.43	1.35
45	BB	809	CLA	C4D-ND	-3.20	1.33	1.37
45	AB	840	CLA	C4D-ND	-3.20	1.33	1.37
45	AA	839	CLA	C4D-ND	-3.19	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	824	CLA	C4D-ND	-3.19	1.33	1.37
45	BB	832	CLA	C1D-ND	3.19	1.41	1.37
45	AA	842	CLA	C4D-ND	-3.19	1.33	1.37
45	BB	823	CLA	C1D-ND	3.19	1.41	1.37
45	BB	815	CLA	C1D-ND	3.19	1.41	1.37
45	BB	831	CLA	CMB-C2B	-3.19	1.45	1.51
45	AB	823	CLA	C4D-ND	-3.19	1.33	1.37
45	BA	806	CLA	CHC-C1C	3.19	1.43	1.35
45	AA	810	CLA	C4D-ND	-3.19	1.33	1.37
54	B5	607	CHL	OBD-CAD	3.19	1.28	1.22
45	BG	201	CLA	CHC-C1C	3.19	1.43	1.35
45	AA	830	CLA	C4D-ND	-3.19	1.33	1.37
45	AB	815	CLA	C1D-ND	3.18	1.41	1.37
45	AA	829	CLA	C4D-ND	-3.18	1.33	1.37
45	AA	821	CLA	C4D-ND	-3.18	1.33	1.37
45	AF	802	CLA	C4D-ND	-3.18	1.33	1.37
50	AB	850	LMU	O5B-C1B	3.18	1.49	1.41
50	AA	851	LMU	O5B-C1B	3.18	1.49	1.41
45	A6	609	CLA	C4D-ND	-3.18	1.33	1.37
45	AA	805	CLA	C4D-ND	-3.17	1.33	1.37
45	B5	602	CLA	CHC-C1C	3.17	1.43	1.35
45	AB	829	CLA	CMB-C2B	-3.17	1.45	1.51
45	A6	611	CLA	C4D-ND	-3.17	1.33	1.37
45	AA	834	CLA	C4D-ND	-3.17	1.33	1.37
45	B2	608	CLA	C4D-ND	-3.17	1.33	1.37
45	AA	830	CLA	C1D-ND	3.17	1.41	1.37
45	BA	818	CLA	C4D-ND	-3.17	1.33	1.37
45	BB	815	CLA	C4D-ND	-3.17	1.33	1.37
45	AA	814	CLA	C4D-ND	-3.16	1.33	1.37
45	AB	822	CLA	C4D-ND	-3.16	1.33	1.37
45	BB	819	CLA	C4D-ND	-3.16	1.33	1.37
45	A3	312	CLA	C4D-ND	-3.16	1.33	1.37
45	BB	814	CLA	C4D-ND	-3.16	1.33	1.37
45	BA	824	CLA	C4D-ND	-3.16	1.33	1.37
54	B2	607	CHL	C3D-C2D	3.16	1.47	1.39
45	A1	304	CLA	C1D-ND	3.16	1.41	1.37
45	BA	829	CLA	C1D-ND	3.16	1.41	1.37
45	A6	610	CLA	CHC-C1C	3.16	1.43	1.35
45	AB	841	CLA	C3B-C2B	-3.15	1.36	1.40
45	B5	609	CLA	CHC-C1C	3.15	1.43	1.35
45	AA	829	CLA	CMD-C2D	-3.15	1.44	1.50
45	AA	809	CLA	C4D-ND	-3.15	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	802	CLA	CHC-C1C	3.15	1.43	1.35
45	AB	835	CLA	C4D-ND	-3.15	1.33	1.37
45	A4	313	CLA	C4D-ND	-3.15	1.33	1.37
45	AB	839	CLA	C1D-ND	3.15	1.41	1.37
45	AB	842	CLA	C4D-ND	-3.15	1.33	1.37
45	BB	805	CLA	C4D-ND	-3.14	1.33	1.37
45	A1	310	CLA	C4D-ND	-3.14	1.33	1.37
45	AA	808	CLA	C4D-ND	-3.14	1.33	1.37
45	A3	302	CLA	CHC-C1C	3.14	1.43	1.35
45	B3	308	CLA	C4D-ND	-3.14	1.33	1.37
45	AB	817	CLA	CHC-C1C	3.14	1.43	1.35
45	BB	831	CLA	C1D-ND	3.14	1.41	1.37
45	A1	311	CLA	C4D-ND	-3.13	1.33	1.37
45	AB	830	CLA	CMB-C2B	-3.13	1.45	1.51
45	AA	819	CLA	CMB-C2B	-3.13	1.45	1.51
45	AB	824	CLA	C1D-ND	3.13	1.41	1.37
45	AA	841	CLA	C4D-ND	-3.13	1.33	1.37
45	AB	837	CLA	C4D-ND	-3.13	1.33	1.37
45	AA	827	CLA	CHC-C1C	3.12	1.43	1.35
45	BA	822	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	840	CLA	CMB-C2B	-3.12	1.45	1.51
45	BA	809	CLA	CHC-C1C	3.12	1.43	1.35
45	BA	811	CLA	C4D-ND	-3.12	1.33	1.37
45	A3	315	CLA	CHC-C1C	3.12	1.43	1.35
45	AG	203	CLA	CHC-C1C	3.12	1.43	1.35
45	AA	806	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	816	CLA	C4D-ND	-3.12	1.33	1.37
45	BB	804	CLA	C4D-ND	-3.12	1.33	1.37
45	A4	307	CLA	CHC-C1C	3.12	1.43	1.35
45	AB	826	CLA	CHC-C1C	3.12	1.43	1.35
45	A1	312	CLA	CHC-C1C	3.12	1.43	1.35
45	AA	818	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	814	CLA	CHC-C1C	3.12	1.43	1.35
45	AB	834	CLA	C1D-ND	3.12	1.41	1.37
45	A6	605	CLA	C4D-ND	-3.12	1.33	1.37
45	BB	806	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	808	CLA	C4D-ND	-3.12	1.33	1.37
45	BB	833	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	821	CLA	C4D-ND	-3.12	1.33	1.37
45	AB	832	CLA	C4D-ND	-3.11	1.33	1.37
45	AG	203	CLA	C4D-ND	-3.11	1.33	1.37
45	BB	805	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	840	CLA	C1D-ND	3.11	1.41	1.37
45	AB	825	CLA	CHC-C1C	3.11	1.42	1.35
45	AB	810	CLA	CMB-C2B	-3.11	1.45	1.51
45	AB	819	CLA	C4D-ND	-3.11	1.33	1.37
45	BB	829	CLA	C4D-ND	-3.11	1.33	1.37
45	BA	833	CLA	CMB-C2B	-3.11	1.45	1.51
45	AA	837	CLA	C4D-ND	-3.10	1.33	1.37
56	e	301	SQD	O48-C23	3.10	1.42	1.33
45	AB	834	CLA	C4D-ND	-3.10	1.33	1.37
45	AL	303	CLA	C4D-ND	-3.10	1.33	1.37
45	B1	310	CLA	C4D-ND	-3.10	1.33	1.37
45	AG	201	CLA	C4D-ND	-3.10	1.33	1.37
45	AB	831	CLA	C4D-ND	-3.10	1.33	1.37
45	BA	829	CLA	CMD-C2D	-3.09	1.44	1.50
45	A6	601	CLA	CHC-C1C	3.09	1.42	1.35
45	B5	609	CLA	C4D-ND	-3.09	1.33	1.37
45	AB	807	CLA	C1D-ND	3.09	1.41	1.37
45	BB	810	CLA	C4D-ND	-3.09	1.33	1.37
45	B1	311	CLA	CHC-C1C	3.09	1.42	1.35
45	AB	815	CLA	CHC-C1C	3.09	1.42	1.35
45	BB	835	CLA	C1D-ND	3.09	1.41	1.37
45	BB	841	CLA	C1D-ND	3.09	1.41	1.37
45	BB	836	CLA	C4D-ND	-3.09	1.33	1.37
45	A4	310	CLA	CHC-C1C	3.09	1.42	1.35
45	AB	828	CLA	C4D-ND	-3.09	1.33	1.37
45	B5	612	CLA	C4D-ND	-3.09	1.33	1.37
45	AB	827	CLA	CHC-C1C	3.09	1.42	1.35
45	A3	306	CLA	C4D-ND	-3.09	1.33	1.37
45	B1	312	CLA	C4D-ND	-3.09	1.33	1.37
45	A3	304	CLA	CHC-C1C	3.09	1.42	1.35
45	A1	304	CLA	C4D-ND	-3.08	1.33	1.37
45	BA	803	CLA	C4D-ND	-3.08	1.33	1.37
45	BB	816	CLA	CHC-C1C	3.08	1.42	1.35
45	AB	813	CLA	C4D-ND	-3.08	1.33	1.37
45	AB	830	CLA	C4D-ND	-3.08	1.33	1.37
45	BA	834	CLA	C4D-ND	-3.08	1.33	1.37
45	BB	801	CLA	CMD-C2D	-3.08	1.44	1.50
45	A4	312	CLA	CHC-C1C	3.08	1.42	1.35
45	BA	816	CLA	C4D-ND	-3.08	1.33	1.37
45	AB	809	CLA	C1D-ND	3.07	1.41	1.37
45	BB	807	CLA	CHC-C1C	3.07	1.42	1.35
45	B3	302	CLA	C4D-ND	-3.07	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	838	CLA	C1D-ND	3.07	1.41	1.37
45	AA	831	CLA	C4D-ND	-3.07	1.33	1.37
45	A4	308	CLA	CHC-C1C	3.07	1.42	1.35
45	BA	839	CLA	C4D-ND	-3.07	1.33	1.37
45	A3	309	CLA	CHC-C1C	3.07	1.42	1.35
45	AA	812	CLA	C4D-ND	-3.07	1.33	1.37
45	BA	810	CLA	C4D-ND	-3.07	1.33	1.37
45	B3	307	CLA	C4D-ND	-3.06	1.33	1.37
45	BK	201	CLA	CHC-C1C	3.06	1.42	1.35
45	B5	613	CLA	CHC-C1C	3.06	1.42	1.35
45	B3	313	CLA	C4D-ND	-3.06	1.33	1.37
45	B5	608	CLA	C4D-ND	-3.06	1.33	1.37
45	BA	829	CLA	CHC-C1C	3.06	1.42	1.35
45	B3	303	CLA	CHC-C1C	3.06	1.42	1.35
45	BF	303	CLA	C4D-ND	-3.06	1.33	1.37
45	B5	604	CLA	CHC-C1C	3.06	1.42	1.35
45	BA	835	CLA	C4D-ND	-3.06	1.33	1.37
45	B5	610	CLA	C4D-ND	-3.06	1.33	1.37
45	BK	203	CLA	C4D-ND	-3.06	1.33	1.37
45	B1	314	CLA	C4D-ND	-3.06	1.33	1.37
45	A6	611	CLA	C1D-ND	3.06	1.41	1.37
45	A4	312	CLA	C4D-ND	-3.06	1.33	1.37
45	BA	825	CLA	C4D-ND	-3.05	1.33	1.37
45	BA	827	CLA	C4D-ND	-3.05	1.33	1.37
45	BB	840	CLA	C4D-ND	-3.05	1.33	1.37
45	BK	202	CLA	CHC-C1C	3.05	1.42	1.35
45	B5	608	CLA	CHC-C1C	3.05	1.42	1.35
45	A1	312	CLA	C4D-ND	-3.05	1.33	1.37
45	AG	204	CLA	CHC-C1C	3.05	1.42	1.35
45	BB	826	CLA	CHC-C1C	3.05	1.42	1.35
45	A1	306	CLA	C4D-ND	-3.05	1.33	1.37
45	A3	309	CLA	C4D-ND	-3.05	1.33	1.37
45	BB	835	CLA	C4D-ND	-3.05	1.33	1.37
45	AA	840	CLA	C3B-C2B	-3.05	1.36	1.40
45	BB	821	CLA	CHC-C1C	3.05	1.42	1.35
45	AA	823	CLA	CHC-C1C	3.05	1.42	1.35
45	B2	604	CLA	CHC-C1C	3.05	1.42	1.35
45	AK	201	CLA	CHC-C1C	3.05	1.42	1.35
45	A3	315	CLA	C4D-ND	-3.04	1.33	1.37
45	BB	839	CLA	C1D-ND	3.04	1.41	1.37
45	BA	838	CLA	CAD-C3D	-3.04	1.45	1.50
45	AA	817	CLA	C4D-ND	-3.04	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	603	CLA	C4D-ND	-3.04	1.33	1.37
45	B5	613	CLA	C4D-ND	-3.04	1.33	1.37
45	AB	803	CLA	C4D-ND	-3.04	1.33	1.37
45	B5	604	CLA	C4D-ND	-3.04	1.33	1.37
45	B3	314	CLA	CHC-C1C	3.04	1.42	1.35
45	A3	303	CLA	C4D-ND	-3.04	1.33	1.37
45	AB	818	CLA	CHC-C1C	3.04	1.42	1.35
45	AK	202	CLA	CHC-C1C	3.04	1.42	1.35
45	BA	844	CLA	CHC-C1C	3.04	1.42	1.35
45	A1	314	CLA	C4D-ND	-3.04	1.33	1.37
45	AA	822	CLA	CHC-C1C	3.04	1.42	1.35
45	BA	829	CLA	C4D-ND	-3.04	1.33	1.37
45	BB	818	CLA	C4D-ND	-3.04	1.33	1.37
45	AA	826	CLA	CHC-C1C	3.04	1.42	1.35
45	AF	802	CLA	C1D-ND	3.04	1.41	1.37
45	AB	804	CLA	CHC-C1C	3.04	1.42	1.35
45	A1	309	CLA	CHC-C1C	3.03	1.42	1.35
45	AB	838	CLA	CHC-C1C	3.03	1.42	1.35
45	A3	313	CLA	CHC-C1C	3.03	1.42	1.35
45	AA	824	CLA	C4D-ND	-3.03	1.33	1.37
45	B3	314	CLA	C4D-ND	-3.03	1.33	1.37
45	AA	804	CLA	CHC-C1C	3.03	1.42	1.35
45	AA	806	CLA	CHC-C1C	3.03	1.42	1.35
45	AB	813	CLA	CHC-C1C	3.03	1.42	1.35
45	A3	312	CLA	CHC-C1C	3.03	1.42	1.35
45	BB	842	CLA	C4D-ND	-3.03	1.33	1.37
45	B3	312	CLA	CHC-C1C	3.03	1.42	1.35
45	A1	311	CLA	CHC-C1C	3.03	1.42	1.35
45	BA	831	CLA	C4D-ND	-3.03	1.33	1.37
45	BA	833	CLA	C4D-ND	-3.03	1.33	1.37
45	AB	806	CLA	CHC-C1C	3.03	1.42	1.35
45	BJ	102	CLA	C4D-ND	-3.03	1.33	1.37
45	BB	817	CLA	C4D-ND	-3.02	1.33	1.37
45	AJ	102	CLA	CHC-C1C	3.02	1.42	1.35
45	AA	805	CLA	CHC-C1C	3.02	1.42	1.35
45	A4	311	CLA	C4D-ND	-3.02	1.33	1.37
45	A6	613	CLA	C4D-ND	-3.02	1.33	1.37
45	A4	311	CLA	CHC-C1C	3.02	1.42	1.35
45	AA	821	CLA	CHC-C1C	3.02	1.42	1.35
45	BA	842	CLA	C4D-ND	-3.02	1.33	1.37
45	AL	305	CLA	C4D-ND	-3.02	1.33	1.37
45	B3	301	CLA	CHC-C1C	3.02	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	829	CLA	CHC-C1C	3.02	1.42	1.35
45	B1	309	CLA	CHC-C1C	3.01	1.42	1.35
45	AA	836	CLA	CMB-C2B	-3.01	1.45	1.51
45	BA	831	CLA	CHC-C1C	3.01	1.42	1.35
45	BB	815	CLA	CHC-C1C	3.01	1.42	1.35
45	BB	830	CLA	CMB-C2B	-3.01	1.45	1.51
45	B1	315	CLA	CHC-C1C	3.01	1.42	1.35
45	AA	803	CLA	C4D-ND	-3.01	1.33	1.37
45	BA	820	CLA	C4D-ND	-3.01	1.33	1.37
45	B1	311	CLA	C4D-ND	-3.01	1.33	1.37
45	AA	840	CLA	C4D-ND	-3.01	1.33	1.37
45	BA	814	CLA	CHC-C1C	3.01	1.42	1.35
45	BB	828	CLA	C4D-ND	-3.01	1.33	1.37
45	AB	805	CLA	C4D-ND	-3.01	1.33	1.37
45	B3	305	CLA	CHC-C1C	3.01	1.42	1.35
45	AA	807	CLA	CHC-C1C	3.01	1.42	1.35
45	AB	806	CLA	C4D-ND	-3.01	1.33	1.37
45	BA	827	CLA	CHC-C1C	3.01	1.42	1.35
45	AB	842	CLA	CHC-C1C	3.01	1.42	1.35
45	B2	612	CLA	C4D-ND	-3.00	1.33	1.37
45	B3	311	CLA	CHC-C1C	3.00	1.42	1.35
45	B3	304	CLA	C4D-ND	-3.00	1.33	1.37
45	B1	304	CLA	C1D-ND	3.00	1.41	1.37
45	AA	841	CLA	CHC-C1C	3.00	1.42	1.35
45	B2	613	CLA	C4D-ND	-3.00	1.33	1.37
45	A6	612	CLA	CHC-C1C	3.00	1.42	1.35
45	AA	809	CLA	CHC-C1C	3.00	1.42	1.35
45	AB	828	CLA	CHC-C1C	3.00	1.42	1.35
45	AG	201	CLA	CHC-C1C	3.00	1.42	1.35
45	A3	314	CLA	CHC-C1C	3.00	1.42	1.35
45	AB	827	CLA	C4D-ND	-3.00	1.33	1.37
45	B2	604	CLA	C4D-ND	-3.00	1.33	1.37
45	AA	810	CLA	CAD-C3D	-3.00	1.45	1.50
45	A3	305	CLA	CHC-C1C	2.99	1.42	1.35
45	AA	831	CLA	CHC-C1C	2.99	1.42	1.35
45	A3	306	CLA	CHC-C1C	2.99	1.42	1.35
45	AB	839	CLA	C4D-ND	-2.99	1.33	1.37
45	AA	840	CLA	CHC-C1C	2.99	1.42	1.35
45	BG	201	CLA	C4D-ND	-2.99	1.33	1.37
45	BJ	102	CLA	CHC-C1C	2.99	1.42	1.35
45	BB	843	CLA	C4D-ND	-2.99	1.33	1.37
45	AA	820	CLA	CHC-C1C	2.99	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A4	303	CLA	CHC-C1C	2.99	1.42	1.35
45	A6	603	CLA	CHC-C1C	2.99	1.42	1.35
45	A6	612	CLA	C4D-ND	-2.99	1.33	1.37
45	A1	307	CLA	CHC-C1C	2.99	1.42	1.35
45	BA	837	CLA	C4D-ND	-2.99	1.33	1.37
45	B1	306	CLA	C4D-ND	-2.99	1.33	1.37
45	AB	801	CLA	CMB-C2B	-2.99	1.45	1.51
45	AK	202	CLA	C4D-ND	-2.98	1.33	1.37
45	AB	831	CLA	CHC-C1C	2.98	1.42	1.35
45	A1	316	CLA	C4D-ND	-2.98	1.33	1.37
45	AA	811	CLA	C4D-ND	-2.98	1.33	1.37
45	B3	309	CLA	CHC-C1C	2.98	1.42	1.35
45	AA	808	CLA	CHC-C1C	2.98	1.42	1.35
45	A3	310	CLA	CHC-C1C	2.98	1.42	1.35
45	AB	836	CLA	C4D-ND	-2.98	1.33	1.37
45	A6	611	CLA	CHC-C1C	2.98	1.42	1.35
45	BB	810	CLA	CHC-C1C	2.98	1.42	1.35
45	BL	302	CLA	CHC-C1C	2.98	1.42	1.35
45	B2	612	CLA	CMB-C2B	-2.98	1.45	1.51
45	A1	313	CLA	CHC-C1C	2.98	1.42	1.35
45	AB	803	CLA	CHC-C1C	2.97	1.42	1.35
45	A3	311	CLA	CHC-C1C	2.97	1.42	1.35
45	BB	802	CLA	CHC-C1C	2.97	1.42	1.35
45	BB	832	CLA	CMB-C2B	-2.97	1.45	1.51
45	BA	822	CLA	CHC-C1C	2.97	1.42	1.35
45	B2	611	CLA	CHC-C1C	2.97	1.42	1.35
45	B2	610	CLA	CHC-C1C	2.97	1.42	1.35
45	A4	307	CLA	C4D-ND	-2.97	1.33	1.37
45	BB	819	CLA	CHC-C1C	2.97	1.42	1.35
48	BI	101	BCR	C30-C25	-2.97	1.49	1.53
45	B2	612	CLA	CHC-C1C	2.97	1.42	1.35
45	AA	835	CLA	CHC-C1C	2.97	1.42	1.35
45	BF	301	CLA	C4D-ND	-2.97	1.33	1.37
45	AA	833	CLA	C4D-ND	-2.97	1.33	1.37
45	A3	314	CLA	C4D-ND	-2.97	1.33	1.37
45	B5	603	CLA	CHC-C1C	2.97	1.42	1.35
45	BK	203	CLA	CHC-C1C	2.97	1.42	1.35
45	BA	817	CLA	C4D-ND	-2.97	1.33	1.37
45	AA	824	CLA	CHC-C1C	2.97	1.42	1.35
45	BF	303	CLA	CHC-C1C	2.97	1.42	1.35
45	AL	303	CLA	CMB-C2B	-2.96	1.45	1.51
45	A1	314	CLA	CHC-C1C	2.96	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AF	804	CLA	C4D-ND	-2.96	1.33	1.37
45	AK	203	CLA	CHC-C1C	2.96	1.42	1.35
45	BL	303	CLA	CHC-C1C	2.96	1.42	1.35
45	B2	608	CLA	CHC-C1C	2.96	1.42	1.35
45	B3	305	CLA	C4D-ND	-2.96	1.33	1.37
45	AB	831	CLA	CMB-C2B	-2.96	1.45	1.51
45	B3	308	CLA	CHC-C1C	2.96	1.42	1.35
45	A6	609	CLA	CHC-C1C	2.96	1.42	1.35
45	BA	819	CLA	CMB-C2B	-2.96	1.45	1.51
45	AF	803	CLA	CHC-C1C	2.96	1.42	1.35
45	A1	306	CLA	CHC-C1C	2.96	1.42	1.35
45	A4	301	CLA	CHC-C1C	2.96	1.42	1.35
45	BB	826	CLA	C1D-ND	2.96	1.41	1.37
45	AB	812	CLA	CHC-C1C	2.96	1.42	1.35
45	B2	613	CLA	CHC-C1C	2.96	1.42	1.35
45	BA	813	CLA	CHC-C1C	2.96	1.42	1.35
45	BB	818	CLA	CHC-C1C	2.96	1.42	1.35
45	BB	837	CLA	CHC-C1C	2.96	1.42	1.35
45	BB	839	CLA	CHC-C1C	2.95	1.42	1.35
45	B3	303	CLA	C4D-ND	-2.95	1.33	1.37
45	BA	803	CLA	C1D-ND	2.95	1.41	1.37
45	BA	807	CLA	CHC-C1C	2.95	1.42	1.35
45	BB	813	CLA	C4D-ND	-2.95	1.33	1.37
45	BA	826	CLA	CHC-C1C	2.95	1.42	1.35
45	B1	306	CLA	CHC-C1C	2.95	1.42	1.35
45	AB	818	CLA	C4D-ND	-2.95	1.33	1.37
45	BA	806	CLA	C4D-ND	-2.95	1.33	1.37
45	BB	825	CLA	CHC-C1C	2.95	1.42	1.35
45	AJ	102	CLA	C4D-ND	-2.95	1.33	1.37
45	BB	814	CLA	CHC-C1C	2.95	1.42	1.35
45	B2	602	CLA	CHC-C1C	2.95	1.42	1.35
45	BB	828	CLA	CHC-C1C	2.95	1.42	1.35
45	A4	301	CLA	C1D-ND	2.95	1.41	1.37
45	AF	804	CLA	CHC-C1C	2.95	1.42	1.35
45	A3	310	CLA	C4D-ND	-2.95	1.33	1.37
45	A1	309	CLA	C4D-ND	-2.95	1.33	1.37
45	A3	304	CLA	C4D-ND	-2.95	1.33	1.37
45	BB	822	CLA	C4D-ND	-2.95	1.33	1.37
45	AA	832	CLA	CHC-C1C	2.95	1.42	1.35
45	A1	310	CLA	CHC-C1C	2.95	1.42	1.35
45	BK	202	CLA	C4D-ND	-2.95	1.33	1.37
45	AA	835	CLA	C4D-ND	-2.95	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	316	CLA	CHC-C1C	2.95	1.42	1.35
45	A1	315	CLA	CHC-C1C	2.95	1.42	1.35
45	B5	610	CLA	CHC-C1C	2.94	1.42	1.35
45	AA	827	CLA	C4D-ND	-2.94	1.33	1.37
45	BA	809	CLA	C4D-ND	-2.94	1.33	1.37
45	AA	815	CLA	C2D-C1D	2.94	1.48	1.42
45	A6	614	CLA	C4D-ND	-2.94	1.33	1.37
45	BB	827	CLA	CHC-C1C	2.94	1.42	1.35
45	B2	609	CLA	C4D-ND	-2.94	1.33	1.37
45	B1	314	CLA	CHC-C1C	2.94	1.42	1.35
45	AB	822	CLA	CHC-C1C	2.94	1.42	1.35
45	B5	601	CLA	CHC-C1C	2.94	1.42	1.35
45	BB	841	CLA	CHC-C1C	2.94	1.42	1.35
45	BG	202	CLA	C4D-ND	-2.94	1.33	1.37
45	BA	831	CLA	CMB-C2B	-2.94	1.45	1.51
45	AB	812	CLA	C4D-ND	-2.94	1.33	1.37
45	BA	808	CLA	C3B-C2B	-2.94	1.36	1.40
45	AA	828	CLA	C4D-ND	-2.93	1.33	1.37
45	BA	823	CLA	C4D-ND	-2.93	1.33	1.37
45	AL	304	CLA	CHC-C1C	2.93	1.42	1.35
45	B1	310	CLA	CHC-C1C	2.93	1.42	1.35
45	BB	801	CLA	C4D-ND	-2.93	1.33	1.37
45	AA	829	CLA	CMB-C2B	-2.93	1.45	1.51
45	A6	610	CLA	C4D-ND	-2.93	1.33	1.37
45	BB	838	CLA	C4D-ND	-2.93	1.33	1.37
45	BB	835	CLA	CHC-C1C	2.93	1.42	1.35
45	AB	836	CLA	CMB-C2B	-2.93	1.45	1.51
45	B1	315	CLA	C4D-ND	-2.93	1.33	1.37
45	AA	836	CLA	CHC-C1C	2.93	1.42	1.35
45	AA	817	CLA	CHC-C1C	2.92	1.42	1.35
45	BA	821	CLA	CHC-C1C	2.92	1.42	1.35
45	AB	830	CLA	C1D-ND	2.92	1.41	1.37
45	AB	808	CLA	CHC-C1C	2.92	1.42	1.35
45	BB	813	CLA	CHC-C1C	2.92	1.42	1.35
45	AB	820	CLA	CHC-C1C	2.92	1.42	1.35
45	A4	302	CLA	C4D-ND	-2.92	1.33	1.37
45	AA	820	CLA	C4D-ND	-2.92	1.33	1.37
45	BA	817	CLA	CHC-C1C	2.92	1.42	1.35
45	AH	201	CLA	C4D-ND	-2.92	1.33	1.37
45	AA	825	CLA	C4D-ND	-2.92	1.33	1.37
45	AB	834	CLA	CHC-C1C	2.92	1.42	1.35
45	B1	309	CLA	C4D-ND	-2.91	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B1	313	CLA	CHC-C1C	2.91	1.42	1.35
45	B3	310	CLA	CHC-C1C	2.91	1.42	1.35
45	BA	823	CLA	CHC-C1C	2.91	1.42	1.35
45	BA	828	CLA	C4D-ND	-2.91	1.33	1.37
45	B5	611	CLA	C4D-ND	-2.91	1.33	1.37
45	AA	816	CLA	CHC-C1C	2.91	1.42	1.35
45	BF	302	CLA	CHC-C1C	2.91	1.42	1.35
45	BA	804	CLA	CHC-C1C	2.91	1.42	1.35
45	B1	312	CLA	CHC-C1C	2.91	1.42	1.35
45	B3	311	CLA	C4D-ND	-2.91	1.33	1.37
45	AB	839	CLA	CHC-C1C	2.91	1.42	1.35
45	A6	605	CLA	CHC-C1C	2.91	1.42	1.35
45	BA	815	CLA	C4D-ND	-2.90	1.33	1.37
45	AB	805	CLA	CHC-C1C	2.90	1.42	1.35
45	BL	302	CLA	C3B-C2B	-2.90	1.36	1.40
45	AB	816	CLA	CHC-C1C	2.90	1.42	1.35
45	AA	813	CLA	CHC-C1C	2.90	1.42	1.35
45	B3	304	CLA	CHC-C1C	2.90	1.42	1.35
45	B2	611	CLA	C4D-ND	-2.90	1.33	1.37
45	BB	808	CLA	CHC-C1C	2.90	1.42	1.35
45	BL	304	CLA	CHC-C1C	2.90	1.42	1.35
52	B3	315	LUT	C26-C27	2.90	1.54	1.50
45	BA	825	CLA	CHC-C1C	2.90	1.42	1.35
45	BB	830	CLA	CHC-C1C	2.90	1.42	1.35
45	AL	303	CLA	CHC-C1C	2.90	1.42	1.35
45	A3	303	CLA	CHC-C1C	2.90	1.42	1.35
45	AA	818	CLA	CHC-C1C	2.90	1.42	1.35
45	BB	812	CLA	CHC-C1C	2.90	1.42	1.35
45	AA	810	CLA	CHC-C1C	2.90	1.42	1.35
45	A4	303	CLA	C4D-ND	-2.89	1.33	1.37
45	AB	830	CLA	CMD-C2D	-2.89	1.44	1.50
45	AL	305	CLA	CHC-C1C	2.89	1.42	1.35
45	A4	308	CLA	C4D-ND	-2.89	1.33	1.37
45	BA	805	CLA	CHC-C1C	2.89	1.42	1.35
45	BH	201	CLA	CHC-C1C	2.89	1.42	1.35
45	AA	815	CLA	C4D-ND	-2.89	1.33	1.37
45	AA	816	CLA	C4D-ND	-2.89	1.33	1.37
45	AA	815	CLA	CHC-C1C	2.89	1.42	1.35
45	AB	801	CLA	CHC-C1C	2.89	1.42	1.35
45	B5	612	CLA	CHC-C1C	2.89	1.42	1.35
45	BB	837	CLA	C4D-ND	-2.89	1.33	1.37
45	BA	811	CLA	CHC-C1C	2.89	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	821	CLA	CHC-C1C	2.89	1.42	1.35
45	AB	840	CLA	CHC-C1C	2.88	1.42	1.35
45	AA	829	CLA	C3B-CAB	-2.88	1.42	1.47
45	BA	818	CLA	CHC-C1C	2.88	1.42	1.35
45	BL	304	CLA	C4D-ND	-2.88	1.33	1.37
45	AA	802	CLA	CHC-C1C	2.88	1.42	1.35
45	BA	836	CLA	CHC-C1C	2.88	1.42	1.35
45	BB	832	CLA	CHC-C1C	2.88	1.42	1.35
45	BB	836	CLA	CHC-C1C	2.88	1.42	1.35
45	BB	810	CLA	C1D-ND	2.88	1.41	1.37
45	AA	801	CLA	C4D-ND	-2.88	1.33	1.37
54	B2	606	CHL	MG-NA	-2.88	1.99	2.06
45	B3	313	CLA	CHC-C1C	2.88	1.42	1.35
45	B2	603	CLA	CHC-C1C	2.88	1.42	1.35
45	AA	823	CLA	C4D-ND	-2.88	1.33	1.37
45	BA	835	CLA	CHC-C1C	2.87	1.42	1.35
45	BA	837	CLA	CHC-C1C	2.87	1.42	1.35
45	BB	806	CLA	CHC-C1C	2.87	1.42	1.35
45	AA	811	CLA	CHC-C1C	2.87	1.42	1.35
45	AA	842	CLA	CHC-C1C	2.87	1.42	1.35
45	AA	825	CLA	CMD-C2D	-2.87	1.44	1.50
45	B5	611	CLA	CHC-C1C	2.87	1.42	1.35
45	AB	821	CLA	CMB-C2B	-2.87	1.45	1.51
45	AA	838	CLA	CHC-C1C	2.86	1.42	1.35
45	A1	313	CLA	C4D-ND	-2.86	1.33	1.37
45	BB	835	CLA	C3B-C2B	-2.86	1.36	1.40
45	A6	613	CLA	CHC-C1C	2.86	1.42	1.35
45	AA	840	CLA	CMB-C2B	-2.86	1.45	1.51
45	BB	809	CLA	CHC-C1C	2.86	1.42	1.35
45	AB	819	CLA	CMB-C2B	-2.86	1.45	1.51
45	AH	201	CLA	CHC-C1C	2.85	1.42	1.35
45	BB	840	CLA	CHC-C1C	2.85	1.42	1.35
48	A3	318	BCR	C40-C30	2.85	1.59	1.53
45	BA	801	CLA	C4D-ND	-2.85	1.33	1.37
45	AB	814	CLA	CMB-C2B	-2.85	1.45	1.51
45	B3	310	CLA	C4D-ND	-2.85	1.33	1.37
45	BA	842	CLA	CHC-C1C	2.85	1.42	1.35
45	B3	302	CLA	CHC-C1C	2.85	1.42	1.35
45	A1	315	CLA	C4D-ND	-2.85	1.33	1.37
45	B1	307	CLA	C4D-ND	-2.85	1.33	1.37
45	BA	829	CLA	CMB-C2B	-2.85	1.45	1.51
45	AA	809	CLA	CMB-C2B	-2.85	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	822	CLA	C4D-ND	-2.85	1.33	1.37
45	AA	816	CLA	CMB-C2B	-2.85	1.45	1.51
45	A1	304	CLA	CHC-C1C	2.85	1.42	1.35
45	A4	302	CLA	CHC-C1C	2.85	1.42	1.35
45	A4	310	CLA	C4D-ND	-2.85	1.33	1.37
45	BB	822	CLA	CHC-C1C	2.84	1.42	1.35
54	A4	305	CHL	MG-NA	-2.84	1.99	2.06
45	AA	818	CLA	CMB-C2B	-2.84	1.45	1.51
45	AA	836	CLA	C4D-ND	-2.84	1.33	1.37
45	AL	304	CLA	CMB-C2B	-2.84	1.45	1.51
45	BB	802	CLA	C3B-C2B	-2.84	1.36	1.40
45	AA	821	CLA	CMB-C2B	-2.84	1.45	1.51
45	BB	811	CLA	CHC-C1C	2.84	1.42	1.35
45	AB	811	CLA	CHC-C1C	2.84	1.42	1.35
45	A3	305	CLA	C4D-ND	-2.84	1.33	1.37
45	B3	312	CLA	C4D-ND	-2.84	1.33	1.37
52	B1	316	LUT	C8-C9	-2.84	1.39	1.45
45	AA	802	CLA	CMD-C2D	-2.84	1.44	1.50
45	BA	824	CLA	CHC-C1C	2.84	1.42	1.35
45	AB	829	CLA	CHC-C1C	2.84	1.42	1.35
45	AB	835	CLA	CHC-C1C	2.84	1.42	1.35
45	BG	202	CLA	CHC-C1C	2.83	1.42	1.35
45	BA	819	CLA	CHC-C1C	2.83	1.42	1.35
45	AA	834	CLA	CHC-C1C	2.83	1.42	1.35
45	A3	313	CLA	C4D-ND	-2.83	1.33	1.37
45	A4	309	CLA	C4D-ND	-2.83	1.33	1.37
45	AA	831	CLA	CMB-C2B	-2.83	1.45	1.51
45	BA	838	CLA	CHC-C1C	2.83	1.42	1.35
45	BB	834	CLA	CHC-C1C	2.83	1.42	1.35
45	AA	812	CLA	CHC-C1C	2.83	1.42	1.35
45	BB	801	CLA	CHC-C1C	2.83	1.42	1.35
48	AA	849	BCR	C30-C25	-2.83	1.49	1.53
45	AK	201	CLA	C4D-ND	-2.83	1.33	1.37
45	BB	838	CLA	CHC-C1C	2.83	1.42	1.35
45	AB	841	CLA	CMB-C2B	-2.83	1.45	1.51
45	BA	816	CLA	CHC-C1C	2.83	1.42	1.35
45	BK	201	CLA	C4D-ND	-2.83	1.33	1.37
46	AA	843	PQN	C10-C1	2.83	1.53	1.48
45	BA	841	CLA	CHC-C1C	2.82	1.42	1.35
48	BG	203	BCR	C1-C6	-2.82	1.49	1.53
45	BA	808	CLA	CHC-C1C	2.82	1.42	1.35
45	B1	304	CLA	CHC-C1C	2.82	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B3	309	CLA	C4D-ND	-2.82	1.33	1.37
45	AA	814	CLA	CHC-C1C	2.82	1.42	1.35
45	BA	841	CLA	CMB-C2B	-2.82	1.45	1.51
45	B1	313	CLA	C4D-ND	-2.82	1.33	1.37
45	A4	313	CLA	CHC-C1C	2.81	1.42	1.35
45	BA	835	CLA	CMB-C2B	-2.81	1.45	1.51
45	B1	305	CLA	C4D-ND	-2.81	1.33	1.37
45	BB	817	CLA	CHC-C1C	2.81	1.42	1.35
45	A3	308	CLA	CHC-C1C	2.81	1.42	1.35
45	BA	810	CLA	CHC-C1C	2.81	1.42	1.35
45	A1	307	CLA	C4D-ND	-2.81	1.33	1.37
45	A3	311	CLA	C4D-ND	-2.81	1.33	1.37
45	AA	837	CLA	CHC-C1C	2.81	1.42	1.35
45	BF	301	CLA	CMB-C2B	-2.81	1.45	1.51
45	BA	842	CLA	CMB-C2B	-2.81	1.45	1.51
45	BB	804	CLA	CHC-C1C	2.81	1.42	1.35
45	BA	812	CLA	CHC-C1C	2.81	1.42	1.35
45	AA	842	CLA	CMB-C2B	-2.81	1.45	1.51
45	BA	844	CLA	C4D-ND	-2.80	1.33	1.37
45	AB	833	CLA	CHC-C1C	2.80	1.42	1.35
45	AA	812	CLA	CMB-C2B	-2.80	1.45	1.51
45	BB	820	CLA	CMB-C2B	-2.80	1.45	1.51
45	AF	803	CLA	CMB-C2B	-2.79	1.45	1.51
45	AB	840	CLA	CMD-C2D	-2.79	1.44	1.50
45	A3	303	CLA	CMB-C2B	-2.79	1.45	1.51
45	BA	801	CLA	CHC-C1C	2.79	1.42	1.35
45	BH	201	CLA	C4D-ND	-2.79	1.33	1.37
45	AA	825	CLA	CHC-C1C	2.79	1.42	1.35
45	AB	837	CLA	CMB-C2B	-2.78	1.45	1.51
45	B3	304	CLA	CMB-C2B	-2.78	1.45	1.51
45	AB	836	CLA	CHC-C1C	2.78	1.42	1.35
54	B5	606	CHL	MG-NA	-2.78	1.99	2.06
45	AA	841	CLA	CMC-C2C	-2.78	1.44	1.50
45	BA	815	CLA	CHC-C1C	2.78	1.42	1.35
45	A1	304	CLA	CMB-C2B	-2.78	1.45	1.51
45	BA	833	CLA	CHC-C1C	2.78	1.42	1.35
45	BA	803	CLA	CHC-C1C	2.77	1.42	1.35
45	BA	831	CLA	C3B-C2B	-2.77	1.36	1.40
45	AA	803	CLA	CHC-C1C	2.77	1.42	1.35
45	AB	835	CLA	CMB-C2B	-2.77	1.45	1.51
45	BA	829	CLA	C3B-CAB	-2.77	1.42	1.47
45	BA	818	CLA	CMB-C2B	-2.77	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A3	308	CLA	CMB-C2B	-2.77	1.45	1.51
45	A4	309	CLA	CHC-C1C	2.76	1.42	1.35
45	BA	803	CLA	CMD-C2D	-2.76	1.44	1.50
45	AA	835	CLA	CMB-C2B	-2.76	1.45	1.51
45	AA	819	CLA	CHC-C1C	2.76	1.42	1.35
45	BB	833	CLA	CHC-C1C	2.76	1.42	1.35
45	AA	834	CLA	CMB-C2B	-2.76	1.45	1.51
56	e	301	SQD	O47-C7	2.76	1.42	1.34
45	AB	824	CLA	CHC-C1C	2.76	1.42	1.35
45	AG	204	CLA	CMB-C2B	-2.76	1.45	1.51
45	BA	808	CLA	CMB-C2B	-2.76	1.45	1.51
45	B1	305	CLA	CHC-C1C	2.76	1.42	1.35
45	BB	842	CLA	C3B-C2B	-2.75	1.36	1.40
45	AB	837	CLA	CHC-C1C	2.75	1.42	1.35
45	BL	302	CLA	C4D-ND	-2.75	1.33	1.37
45	AB	809	CLA	CHC-C1C	2.75	1.42	1.35
45	A6	613	CLA	CMB-C2B	-2.75	1.45	1.51
45	BH	201	CLA	CMB-C2B	-2.75	1.45	1.51
45	BA	811	CLA	CMB-C2B	-2.75	1.45	1.51
45	AB	801	CLA	CMD-C2D	-2.75	1.45	1.50
45	AA	839	CLA	CHC-C1C	2.75	1.42	1.35
45	AA	829	CLA	CHC-C1C	2.74	1.42	1.35
45	AB	825	CLA	CMD-C2D	-2.74	1.45	1.50
45	AB	825	CLA	C1D-ND	2.74	1.41	1.37
45	A1	305	CLA	C4D-ND	-2.74	1.33	1.37
45	AB	810	CLA	C3B-C2B	-2.74	1.36	1.40
45	BA	839	CLA	C3B-C2B	-2.74	1.36	1.40
45	BB	824	CLA	CHC-C1C	2.74	1.42	1.35
45	AA	825	CLA	CMB-C2B	-2.74	1.46	1.51
45	AB	832	CLA	CMB-C2B	-2.74	1.46	1.51
45	BB	801	CLA	CMB-C2B	-2.74	1.46	1.51
45	BA	832	CLA	CHC-C1C	2.73	1.42	1.35
45	AA	833	CLA	CHC-C1C	2.73	1.42	1.35
45	B3	307	CLA	CHC-C1C	2.73	1.42	1.35
45	A6	610	CLA	C3B-C2B	-2.73	1.36	1.40
45	BL	303	CLA	CMB-C2B	-2.73	1.46	1.51
48	AA	847	BCR	C8-C9	2.73	1.51	1.45
45	AG	204	CLA	C4D-ND	-2.73	1.33	1.37
45	AA	830	CLA	CHC-C1C	2.72	1.41	1.35
45	AA	801	CLA	CHC-C1C	2.72	1.41	1.35
45	AA	813	CLA	CMB-C2B	-2.72	1.46	1.51
45	AB	805	CLA	CMB-C2B	-2.72	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B5	603	CLA	CMB-C2B	-2.72	1.46	1.51
45	BA	836	CLA	CMB-C2B	-2.72	1.46	1.51
45	AB	824	CLA	CMB-C2B	-2.72	1.46	1.51
54	A1	308	CHL	C4C-C3C	2.72	1.49	1.45
45	BB	834	CLA	C3B-C2B	-2.72	1.36	1.40
45	AB	809	CLA	CMB-C2B	-2.72	1.46	1.51
54	B1	308	CHL	MG-NA	-2.72	1.99	2.06
45	AB	818	CLA	CMB-C2B	-2.72	1.46	1.51
54	B1	308	CHL	C4B-CHC	2.71	1.48	1.41
45	AB	841	CLA	CHC-C1C	2.71	1.41	1.35
45	AB	831	CLA	C3B-C2B	-2.71	1.36	1.40
45	BB	823	CLA	CHC-C1C	2.71	1.41	1.35
45	AA	801	CLA	CMB-C2B	-2.71	1.46	1.51
45	AA	802	CLA	CMB-C2B	-2.71	1.46	1.51
45	AB	829	CLA	CMD-C2D	-2.71	1.45	1.50
45	BA	801	CLA	CMB-C2B	-2.71	1.46	1.51
45	BA	802	CLA	CMB-C2B	-2.71	1.46	1.51
45	BA	836	CLA	C4D-ND	-2.71	1.34	1.37
45	BA	834	CLA	CHC-C1C	2.71	1.41	1.35
45	A6	604	CLA	CMB-C2B	-2.71	1.46	1.51
45	BB	839	CLA	CMB-C2B	-2.70	1.46	1.51
54	B5	605	CHL	C4C-C3C	2.70	1.49	1.44
45	A1	316	CLA	CMB-C2B	-2.70	1.46	1.51
45	BA	839	CLA	CMB-C2B	-2.70	1.46	1.51
45	BA	802	CLA	CMD-C2D	-2.70	1.45	1.50
45	BB	811	CLA	CMB-C2B	-2.70	1.46	1.51
45	AA	811	CLA	CMB-C2B	-2.70	1.46	1.51
45	B1	304	CLA	CMB-C2B	-2.70	1.46	1.51
45	AA	814	CLA	CMB-C2B	-2.69	1.46	1.51
45	A4	307	CLA	CMB-C2B	-2.69	1.46	1.51
45	A3	315	CLA	CMD-C2D	-2.69	1.45	1.50
45	BA	805	CLA	CMB-C2B	-2.69	1.46	1.51
45	AB	814	CLA	C3B-C2B	-2.69	1.36	1.40
45	BA	812	CLA	CMB-C2B	-2.69	1.46	1.51
45	AA	808	CLA	CMB-C2B	-2.69	1.46	1.51
45	B2	608	CLA	CMB-C2B	-2.69	1.46	1.51
45	AA	823	CLA	CMB-C2B	-2.69	1.46	1.51
45	B1	314	CLA	CMB-C2B	-2.68	1.46	1.51
45	AF	802	CLA	C3B-C2B	-2.68	1.36	1.40
45	BB	842	CLA	CMB-C2B	-2.68	1.46	1.51
45	BA	820	CLA	CHC-C1C	2.68	1.41	1.35
46	BA	843	PQN	C5-C4	2.68	1.53	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	805	CLA	CMD-C2D	-2.68	1.45	1.50
45	AB	832	CLA	CHC-C1C	2.68	1.41	1.35
45	AB	823	CLA	CMB-C2B	-2.68	1.46	1.51
45	AA	805	CLA	CMB-C2B	-2.68	1.46	1.51
55	A6	616	XAT	O4-C5	-2.68	1.42	1.46
45	A6	605	CLA	CMB-C2B	-2.68	1.46	1.51
45	BB	821	CLA	CMB-C2B	-2.67	1.46	1.51
45	AB	819	CLA	CHC-C1C	2.67	1.41	1.35
45	BB	841	CLA	CMD-C2D	-2.67	1.45	1.50
45	BB	804	CLA	CMB-C2B	-2.67	1.46	1.51
45	BB	826	CLA	CMD-C2D	-2.67	1.45	1.50
45	AB	813	CLA	CMB-C2B	-2.67	1.46	1.51
45	BA	834	CLA	CMB-C2B	-2.67	1.46	1.51
45	BB	809	CLA	C3B-C2B	-2.67	1.36	1.40
45	AA	840	CLA	C3B-CAB	-2.67	1.42	1.47
45	BB	831	CLA	CMD-C2D	-2.66	1.45	1.50
45	BA	834	CLA	C3B-C2B	-2.66	1.36	1.40
45	BA	828	CLA	CHC-C1C	2.66	1.41	1.35
45	BA	825	CLA	CMD-C2D	-2.66	1.45	1.50
45	AB	803	CLA	CMB-C2B	-2.66	1.46	1.51
45	A1	314	CLA	CMB-C2B	-2.66	1.46	1.51
45	BA	802	CLA	CHC-C1C	2.66	1.41	1.35
54	B2	606	CHL	C4C-C3C	2.66	1.49	1.45
45	BA	821	CLA	CMB-C2B	-2.66	1.46	1.51
45	BA	816	CLA	CMB-C2B	-2.66	1.46	1.51
45	BA	825	CLA	CMB-C2B	-2.65	1.46	1.51
46	AA	843	PQN	C5-C4	2.65	1.53	1.48
45	B5	602	CLA	CMB-C2B	-2.65	1.46	1.51
45	AB	810	CLA	C3B-CAB	-2.65	1.42	1.47
54	A6	607	CHL	C4C-C3C	2.65	1.49	1.45
45	AA	830	CLA	CMC-C2C	-2.65	1.45	1.50
45	BB	836	CLA	CMB-C2B	-2.65	1.46	1.51
45	A1	305	CLA	CHC-C1C	2.65	1.41	1.35
45	BG	202	CLA	CMB-C2B	-2.65	1.46	1.51
45	BB	809	CLA	CMB-C2B	-2.65	1.46	1.51
45	BA	842	CLA	CMD-C2D	-2.64	1.45	1.50
45	B5	608	CLA	CMB-C2B	-2.64	1.46	1.51
45	A6	601	CLA	CMB-C2B	-2.64	1.46	1.51
45	B3	307	CLA	CMB-C2B	-2.64	1.46	1.51
45	BB	826	CLA	CMB-C2B	-2.64	1.46	1.51
45	A6	610	CLA	CMB-C2B	-2.64	1.46	1.51
45	BB	835	CLA	CMD-C2D	-2.64	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	839	CLA	CHC-C1C	2.63	1.41	1.35
45	AB	818	CLA	C3B-C2B	-2.63	1.36	1.40
45	BB	814	CLA	CMB-C2B	-2.63	1.46	1.51
45	BB	832	CLA	C3B-C2B	-2.63	1.36	1.40
45	AL	305	CLA	CMB-C2B	-2.63	1.46	1.51
45	BB	830	CLA	CMD-C2D	-2.63	1.45	1.50
45	AB	807	CLA	CHC-C1C	2.63	1.41	1.35
45	AB	822	CLA	CMB-C2B	-2.63	1.46	1.51
45	AB	807	CLA	CMB-C2B	-2.63	1.46	1.51
45	AB	812	CLA	CMB-C2B	-2.63	1.46	1.51
45	AA	838	CLA	CMB-C2B	-2.63	1.46	1.51
54	A4	304	CHL	MG-NA	-2.62	2.00	2.06
45	A6	603	CLA	CMB-C2B	-2.62	1.46	1.51
45	AB	804	CLA	CMB-C2B	-2.62	1.46	1.51
45	BB	815	CLA	CMB-C2B	-2.62	1.46	1.51
45	AA	828	CLA	CHC-C1C	2.62	1.41	1.35
45	A6	612	CLA	CMB-C2B	-2.62	1.46	1.51
45	B2	602	CLA	CMB-C2B	-2.62	1.46	1.51
45	AA	810	CLA	CMB-C2B	-2.62	1.46	1.51
45	AB	804	CLA	CMD-C2D	-2.62	1.45	1.50
45	AB	820	CLA	C3B-C2B	-2.62	1.36	1.40
46	AB	843	PQN	C5-C4	2.62	1.53	1.48
45	AB	842	CLA	CMB-C2B	-2.62	1.46	1.51
45	A4	313	CLA	CMB-C2B	-2.62	1.46	1.51
45	AG	201	CLA	CMB-C2B	-2.61	1.46	1.51
54	A6	608	CHL	MG-NA	-2.61	2.00	2.06
54	A4	314	CHL	MG-NA	-2.61	2.00	2.06
45	A4	301	CLA	CMB-C2B	-2.61	1.46	1.51
45	BB	820	CLA	CHC-C1C	2.61	1.41	1.35
45	AA	828	CLA	CMB-C2B	-2.61	1.46	1.51
45	AB	808	CLA	CMB-C2B	-2.61	1.46	1.51
45	BB	808	CLA	CMB-C2B	-2.61	1.46	1.51
45	A6	609	CLA	CMB-C2B	-2.60	1.46	1.51
45	A6	601	CLA	CMC-C2C	-2.60	1.45	1.50
45	BB	819	CLA	CMB-C2B	-2.60	1.46	1.51
45	B3	301	CLA	CMB-C2B	-2.60	1.46	1.51
46	BA	843	PQN	C11-C3	2.60	1.55	1.51
45	A3	309	CLA	CMB-C2B	-2.60	1.46	1.51
45	AA	818	CLA	CMD-C2D	-2.60	1.45	1.50
45	AA	841	CLA	CMB-C2B	-2.60	1.46	1.51
45	BA	810	CLA	CMB-C2B	-2.60	1.46	1.51
54	B2	601	CHL	MG-NA	-2.60	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	A6	607	CHL	MG-NA	-2.60	2.00	2.06
45	B5	602	CLA	C3B-C2B	-2.60	1.36	1.40
54	A1	303	CHL	MG-NA	-2.60	2.00	2.06
54	A4	306	CHL	MG-NA	-2.59	2.00	2.06
45	AB	818	CLA	C3B-CAB	-2.59	1.42	1.47
45	BA	824	CLA	CMB-C2B	-2.59	1.46	1.51
45	BB	801	CLA	C1D-ND	2.59	1.41	1.37
47	a	501	LHG	O7-C5	-2.59	1.40	1.46
45	AF	804	CLA	CMB-C2B	-2.59	1.46	1.51
45	BA	840	CLA	CHC-C1C	2.59	1.41	1.35
45	BA	840	CLA	CMB-C2B	-2.58	1.46	1.51
45	AB	811	CLA	CMB-C2B	-2.58	1.46	1.51
45	A3	305	CLA	CMB-C2B	-2.58	1.46	1.51
45	BA	829	CLA	C3B-C2B	-2.58	1.36	1.40
54	B1	308	CHL	C2C-C1C	2.58	1.50	1.44
45	AB	823	CLA	CHC-C1C	2.58	1.41	1.35
45	AB	838	CLA	CMB-C2B	-2.58	1.46	1.51
45	BA	838	CLA	CMB-C2B	-2.58	1.46	1.51
45	B3	311	CLA	CMB-C2B	-2.58	1.46	1.51
45	A4	312	CLA	CMB-C2B	-2.57	1.46	1.51
45	BA	830	CLA	C3B-C2B	-2.57	1.36	1.40
45	BB	842	CLA	CHC-C1C	2.57	1.41	1.35
45	A3	314	CLA	CMB-C2B	-2.57	1.46	1.51
45	B5	612	CLA	CMB-C2B	-2.57	1.46	1.51
45	BA	814	CLA	CMB-C2B	-2.57	1.46	1.51
45	B5	609	CLA	C3B-C2B	-2.57	1.36	1.40
45	AA	840	CLA	CMD-C2D	-2.57	1.45	1.50
45	BB	805	CLA	C1D-ND	2.57	1.40	1.37
45	AA	826	CLA	CMB-C2B	-2.57	1.46	1.51
54	A3	307	CHL	MG-NA	-2.57	2.00	2.06
45	BB	843	CLA	CMB-C2B	-2.56	1.46	1.51
46	BB	844	PQN	C2-C1	2.56	1.53	1.48
45	AB	815	CLA	CMB-C2B	-2.56	1.46	1.51
45	BA	809	CLA	CMB-C2B	-2.56	1.46	1.51
45	BB	838	CLA	CMB-C2B	-2.56	1.46	1.51
45	B5	611	CLA	CMB-C2B	-2.56	1.46	1.51
45	AB	809	CLA	C3B-C2B	-2.56	1.36	1.40
45	BB	802	CLA	CMB-C2B	-2.56	1.46	1.51
54	A1	308	CHL	MG-NA	-2.56	2.00	2.06
54	A6	606	CHL	MG-NA	-2.56	2.00	2.06
45	A1	315	CLA	CMB-C2B	-2.56	1.46	1.51
45	BL	303	CLA	C3B-C2B	-2.55	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AB	832	CLA	C3B-C2B	-2.55	1.36	1.40
45	A4	303	CLA	CMB-C2B	-2.55	1.46	1.51
45	A3	312	CLA	CMB-C2B	-2.55	1.46	1.51
45	AA	817	CLA	CMB-C2B	-2.55	1.46	1.51
45	AA	806	CLA	CMB-C2B	-2.55	1.46	1.51
54	B5	607	CHL	MG-NA	-2.55	2.00	2.06
45	AB	801	CLA	C1D-ND	2.55	1.40	1.37
45	BA	821	CLA	C3B-C2B	-2.55	1.36	1.40
45	AB	828	CLA	CMB-C2B	-2.55	1.46	1.51
45	AB	807	CLA	CMD-C2D	-2.55	1.45	1.50
45	AB	834	CLA	CMB-C2B	-2.55	1.46	1.51
54	B1	308	CHL	C4C-C3C	2.55	1.49	1.45
45	AA	824	CLA	CMB-C2B	-2.55	1.46	1.51
45	BF	302	CLA	CMB-C2B	-2.55	1.46	1.51
45	B5	604	CLA	CMB-C2B	-2.54	1.46	1.51
45	A6	611	CLA	CMD-C2D	-2.54	1.45	1.50
45	BA	804	CLA	CMB-C2B	-2.54	1.46	1.51
45	BB	815	CLA	C3B-C2B	-2.54	1.36	1.40
45	BA	820	CLA	CMB-C2B	-2.54	1.46	1.51
52	B1	316	LUT	C32-C33	-2.54	1.40	1.45
45	BB	822	CLA	CMB-C2B	-2.54	1.46	1.51
54	B2	607	CHL	MG-NA	-2.54	2.00	2.06
54	A6	602	CHL	MG-NA	-2.54	2.00	2.06
45	B3	308	CLA	CMB-C2B	-2.54	1.46	1.51
45	A1	312	CLA	CMB-C2B	-2.53	1.46	1.51
45	BB	813	CLA	CMB-C2B	-2.53	1.46	1.51
45	BB	816	CLA	CMB-C2B	-2.53	1.46	1.51
54	A4	304	CHL	C4C-C3C	2.53	1.49	1.44
45	BB	801	CLA	C3B-C2B	-2.53	1.36	1.40
47	F	801	LHG	O7-C5	-2.53	1.40	1.46
45	B2	611	CLA	CMB-C2B	-2.53	1.46	1.51
54	A6	602	CHL	C4C-C3C	2.53	1.49	1.45
54	A4	314	CHL	C4C-C3C	2.53	1.49	1.45
45	AA	820	CLA	CMB-C2B	-2.53	1.46	1.51
45	AA	815	CLA	CMB-C2B	-2.53	1.46	1.51
45	A1	306	CLA	CMB-C2B	-2.53	1.46	1.51
45	A3	306	CLA	CMB-C2B	-2.53	1.46	1.51
45	B2	613	CLA	CMB-C2B	-2.53	1.46	1.51
45	A1	313	CLA	CMB-C2B	-2.53	1.46	1.51
45	AB	810	CLA	CHC-C1C	2.53	1.41	1.35
45	AA	809	CLA	C3B-C2B	-2.53	1.36	1.40
45	AB	829	CLA	C3B-CAB	-2.53	1.42	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B1	305	CLA	CMB-C2B	-2.53	1.46	1.51
45	A4	308	CLA	CMB-C2B	-2.52	1.46	1.51
54	A6	608	CHL	C4C-C3C	2.52	1.49	1.45
54	B3	306	CHL	MG-NA	-2.52	2.00	2.06
45	AB	823	CLA	C3B-C2B	-2.52	1.36	1.40
45	AA	837	CLA	CMB-C2B	-2.52	1.46	1.51
45	B2	603	CLA	CMB-C2B	-2.52	1.46	1.51
48	BA	851	BCR	C1-C6	-2.52	1.50	1.53
45	AH	201	CLA	CMB-C2B	-2.52	1.46	1.51
45	AB	842	CLA	CMD-C2D	-2.52	1.45	1.50
45	A1	311	CLA	CMC-C2C	-2.52	1.45	1.50
46	BA	843	PQN	C10-C1	2.52	1.53	1.48
54	A4	305	CHL	C4C-C3C	2.52	1.49	1.45
54	B5	607	CHL	C2C-C1C	2.52	1.49	1.44
45	AB	833	CLA	CMB-C2B	-2.52	1.46	1.51
45	B2	604	CLA	CMB-C2B	-2.52	1.46	1.51
52	B1	316	LUT	C28-C29	-2.52	1.40	1.45
45	B5	610	CLA	CMB-C2B	-2.51	1.46	1.51
45	BB	821	CLA	C3B-C2B	-2.51	1.36	1.40
45	AA	839	CLA	CMB-C2B	-2.51	1.46	1.51
45	A4	310	CLA	CMB-C2B	-2.51	1.46	1.51
45	B5	608	CLA	C3B-C2B	-2.51	1.36	1.40
54	B2	614	CHL	MG-NA	-2.51	2.00	2.06
45	B1	304	CLA	CMD-C2D	-2.51	1.45	1.50
45	A4	302	CLA	CMB-C2B	-2.51	1.46	1.51
45	B5	609	CLA	CMB-C2B	-2.51	1.46	1.51
45	BA	830	CLA	CHC-C1C	2.50	1.41	1.35
45	AA	803	CLA	CMB-C2B	-2.50	1.46	1.51
45	AB	825	CLA	CMB-C2B	-2.50	1.46	1.51
45	AA	839	CLA	CMD-C2D	-2.50	1.45	1.50
45	A1	309	CLA	CMB-C2B	-2.50	1.46	1.51
45	A3	303	CLA	C3B-C2B	-2.50	1.36	1.40
45	BB	819	CLA	C3B-C2B	-2.50	1.36	1.40
45	A4	307	CLA	CMD-C2D	-2.50	1.45	1.50
45	BB	824	CLA	CMB-C2B	-2.50	1.46	1.51
45	AA	818	CLA	C3B-CAB	-2.50	1.42	1.47
48	AA	847	BCR	C12-C13	2.50	1.51	1.45
45	AA	829	CLA	C3B-C2B	-2.50	1.36	1.40
45	BB	837	CLA	CMB-C2B	-2.50	1.46	1.51
45	A3	304	CLA	CMB-C2B	-2.49	1.46	1.51
45	BF	301	CLA	CHC-C1C	2.49	1.41	1.35
45	AG	203	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	825	CLA	CMB-C2B	-2.49	1.46	1.51
54	B5	605	CHL	MG-NA	-2.49	2.00	2.06
45	A6	603	CLA	C3B-C2B	-2.49	1.36	1.40
45	BA	831	CLA	C3B-CAB	-2.49	1.42	1.47
45	BB	828	CLA	CMB-C2B	-2.49	1.46	1.51
45	B3	302	CLA	CMB-C2B	-2.49	1.46	1.51
45	BB	835	CLA	CMB-C2B	-2.49	1.46	1.51
54	B2	605	CHL	MG-NA	-2.49	2.00	2.06
54	B1	303	CHL	C2C-C1C	2.49	1.49	1.44
54	B2	605	CHL	C4C-C3C	2.49	1.49	1.44
45	BB	810	CLA	CMD-C2D	-2.49	1.45	1.50
45	BA	808	CLA	C3B-CAB	-2.49	1.42	1.47
45	A3	309	CLA	CMD-C2D	-2.49	1.45	1.50
45	A4	309	CLA	CMB-C2B	-2.49	1.46	1.51
45	B2	609	CLA	CMB-C2B	-2.49	1.46	1.51
45	AB	816	CLA	CMB-C2B	-2.49	1.46	1.51
45	AA	809	CLA	CMD-C2D	-2.49	1.45	1.50
45	B1	310	CLA	CMB-C2B	-2.48	1.46	1.51
45	BA	818	CLA	C3B-C2B	-2.48	1.36	1.40
45	BB	812	CLA	CMB-C2B	-2.48	1.46	1.51
45	A3	302	CLA	CMB-C2B	-2.48	1.46	1.51
45	BB	810	CLA	CMB-C2B	-2.48	1.46	1.51
54	B5	607	CHL	C4B-CHC	2.48	1.47	1.41
45	AA	830	CLA	C3B-C2B	-2.48	1.36	1.40
47	BA	846	LHG	O8-C23	2.48	1.45	1.33
45	BB	841	CLA	CMB-C2B	-2.48	1.46	1.51
45	AA	807	CLA	CMB-C2B	-2.48	1.46	1.51
46	BB	844	PQN	C11-C3	2.48	1.55	1.51
45	B1	313	CLA	CMB-C2B	-2.48	1.46	1.51
54	B1	308	CHL	C4D-CHA	2.48	1.47	1.38
45	BB	833	CLA	CMB-C2B	-2.48	1.46	1.51
45	AB	833	CLA	C3B-C2B	-2.48	1.36	1.40
45	A3	302	CLA	C3B-C2B	-2.48	1.36	1.40
45	AB	824	CLA	CMD-C2D	-2.47	1.45	1.50
54	B5	606	CHL	C4C-C3C	2.47	1.49	1.44
45	AA	827	CLA	CMD-C2D	-2.47	1.45	1.50
45	BA	807	CLA	CMB-C2B	-2.47	1.46	1.51
45	BB	806	CLA	CMB-C2B	-2.47	1.46	1.51
45	AB	829	CLA	C3B-C2B	-2.47	1.36	1.40
45	AB	827	CLA	CMB-C2B	-2.47	1.46	1.51
45	AK	202	CLA	CMB-C2B	-2.47	1.46	1.51
45	B1	315	CLA	CMD-C2D	-2.47	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A3	313	CLA	CMB-C2B	-2.47	1.46	1.51
48	BF	304	BCR	C1-C6	-2.47	1.50	1.53
45	BB	825	CLA	CMD-C2D	-2.47	1.45	1.50
45	A1	305	CLA	CMB-C2B	-2.47	1.46	1.51
45	BA	837	CLA	CMB-C2B	-2.47	1.46	1.51
45	AB	806	CLA	CMB-C2B	-2.46	1.46	1.51
45	BA	806	CLA	CMD-C2D	-2.46	1.45	1.50
45	BJ	102	CLA	CMB-C2B	-2.46	1.46	1.51
54	B2	607	CHL	C4B-CHC	2.46	1.47	1.41
54	B2	606	CHL	C4B-CHC	2.46	1.47	1.41
45	B3	313	CLA	CMB-C2B	-2.46	1.46	1.51
45	B1	315	CLA	CMB-C2B	-2.46	1.46	1.51
45	AF	802	CLA	CMD-C2D	-2.46	1.45	1.50
45	BA	826	CLA	CMB-C2B	-2.46	1.46	1.51
45	B1	309	CLA	CMB-C2B	-2.45	1.46	1.51
45	AA	841	CLA	CMD-C2D	-2.45	1.45	1.50
45	B5	613	CLA	CMB-C2B	-2.45	1.46	1.51
45	BB	827	CLA	CMD-C2D	-2.45	1.45	1.50
45	AA	804	CLA	CMB-C2B	-2.45	1.46	1.51
45	BA	810	CLA	C3B-C2B	-2.45	1.37	1.40
45	B5	601	CLA	CMB-C2B	-2.45	1.46	1.51
54	A6	606	CHL	C4C-C3C	2.45	1.49	1.44
45	B2	610	CLA	CMB-C2B	-2.44	1.46	1.51
54	A4	304	CHL	C4B-CHC	2.44	1.47	1.41
45	A6	609	CLA	CMD-C2D	-2.44	1.45	1.50
45	AB	814	CLA	C3B-CAB	-2.44	1.43	1.47
45	AB	831	CLA	CMD-C2D	-2.44	1.45	1.50
45	A3	310	CLA	CMB-C2B	-2.44	1.46	1.51
45	AB	840	CLA	C3B-C2B	-2.44	1.37	1.40
45	AA	822	CLA	CMB-C2B	-2.44	1.46	1.51
54	B2	606	CHL	C4D-CHA	2.44	1.47	1.38
46	AB	843	PQN	C10-C1	2.44	1.52	1.48
45	AB	804	CLA	C1D-ND	2.44	1.40	1.37
45	BB	810	CLA	CMC-C2C	-2.44	1.45	1.50
45	BB	807	CLA	CMB-C2B	-2.43	1.46	1.51
45	BB	834	CLA	CMC-C2C	-2.43	1.45	1.50
45	B2	602	CLA	C3B-C2B	-2.43	1.37	1.40
54	B2	607	CHL	C2C-C1C	2.43	1.49	1.44
45	B3	305	CLA	CMB-C2B	-2.43	1.46	1.51
45	BB	830	CLA	C3B-C2B	-2.43	1.37	1.40
54	B2	607	CHL	C4C-C3C	2.43	1.49	1.45
45	AA	818	CLA	C3B-C2B	-2.43	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	611	CLA	CMB-C2B	-2.43	1.46	1.51
45	BF	303	CLA	CMB-C2B	-2.43	1.46	1.51
54	B5	606	CHL	C4D-CHA	2.43	1.47	1.38
45	BB	805	CLA	CMB-C2B	-2.42	1.46	1.51
45	AA	831	CLA	C3B-C2B	-2.42	1.37	1.40
45	A1	307	CLA	CMB-C2B	-2.42	1.46	1.51
54	A6	608	CHL	C4D-CHA	2.42	1.47	1.38
45	AJ	102	CLA	CMB-C2B	-2.42	1.46	1.51
45	BB	841	CLA	C3B-CAB	-2.42	1.43	1.47
54	A1	308	CHL	C4B-CHC	2.42	1.47	1.41
45	BB	838	CLA	CMD-C2D	-2.42	1.45	1.50
45	BB	805	CLA	CMC-C2C	-2.42	1.45	1.50
45	BA	802	CLA	C3B-C2B	-2.42	1.37	1.40
54	A4	306	CHL	C4B-CHC	2.42	1.47	1.41
45	AB	830	CLA	CHC-C1C	2.42	1.41	1.35
45	BA	834	CLA	C3B-CAB	-2.42	1.43	1.47
45	A4	308	CLA	C3B-C2B	-2.42	1.37	1.40
45	AB	801	CLA	CMC-C2C	-2.42	1.45	1.50
45	AB	839	CLA	CMB-C2B	-2.42	1.46	1.51
45	AA	834	CLA	C3B-C2B	-2.41	1.37	1.40
45	AL	304	CLA	C3B-C2B	-2.41	1.37	1.40
45	AB	817	CLA	CMB-C2B	-2.41	1.46	1.51
45	B1	314	CLA	C3B-C2B	-2.41	1.37	1.40
45	BA	812	CLA	CMC-C2C	-2.41	1.45	1.50
45	AB	824	CLA	C3B-CAB	-2.41	1.43	1.47
45	A4	311	CLA	CMB-C2B	-2.41	1.46	1.51
45	BA	803	CLA	CMB-C2B	-2.41	1.46	1.51
54	A4	305	CHL	C4D-CHA	2.41	1.47	1.38
54	B2	605	CHL	C2C-C1C	2.41	1.49	1.44
45	BL	302	CLA	CMB-C2B	-2.41	1.46	1.51
45	AB	804	CLA	CMC-C2C	-2.41	1.45	1.50
45	B3	312	CLA	CMB-C2B	-2.41	1.46	1.51
45	BB	840	CLA	CMB-C2B	-2.41	1.46	1.51
52	A4	315	LUT	C8-C9	2.41	1.51	1.45
45	BB	834	CLA	CMD-C2D	-2.40	1.45	1.50
45	BA	823	CLA	CMB-C2B	-2.40	1.46	1.51
45	BB	819	CLA	C3B-CAB	-2.40	1.43	1.47
45	AA	808	CLA	CMD-C2D	-2.40	1.45	1.50
45	A3	308	CLA	CMD-C2D	-2.40	1.45	1.50
45	BB	815	CLA	C3B-CAB	-2.40	1.43	1.47
54	B2	601	CHL	C2C-C1C	2.40	1.49	1.44
54	A4	314	CHL	C4D-CHA	2.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AK	203	CLA	CMB-C2B	-2.40	1.46	1.51
45	BA	827	CLA	CMD-C2D	-2.39	1.45	1.50
45	BA	828	CLA	CMD-C2D	-2.39	1.45	1.50
54	A1	303	CHL	C4D-CHA	2.39	1.46	1.38
45	AB	821	CLA	CMD-C2D	-2.39	1.45	1.50
45	A1	310	CLA	CMB-C2B	-2.39	1.46	1.51
45	BA	809	CLA	CMD-C2D	-2.39	1.45	1.50
45	BA	818	CLA	CMD-C2D	-2.39	1.45	1.50
45	BA	806	CLA	CMB-C2B	-2.39	1.46	1.51
45	A4	301	CLA	C3B-C2B	-2.39	1.37	1.40
45	BA	838	CLA	C3B-C2B	-2.39	1.37	1.40
45	B2	609	CLA	C3B-C2B	-2.39	1.37	1.40
54	B1	303	CHL	C4C-C3C	2.39	1.49	1.45
45	A6	614	CLA	CMB-C2B	-2.39	1.46	1.51
45	AB	834	CLA	C3B-C2B	-2.39	1.37	1.40
45	AB	802	CLA	CMB-C2B	-2.38	1.46	1.51
45	AA	813	CLA	C3B-C2B	-2.38	1.37	1.40
45	BA	806	CLA	C3B-C2B	-2.38	1.37	1.40
45	BB	802	CLA	CMD-C2D	-2.38	1.45	1.50
45	BB	832	CLA	CMD-C2D	-2.38	1.45	1.50
52	AF	806	LUT	C12-C13	2.38	1.51	1.45
45	AB	808	CLA	C3B-C2B	-2.38	1.37	1.40
45	B3	309	CLA	CMB-C2B	-2.38	1.46	1.51
45	A1	304	CLA	CMD-C2D	-2.38	1.45	1.50
46	BA	843	PQN	C2-C1	2.38	1.53	1.48
54	A1	308	CHL	C4D-CHA	2.38	1.46	1.38
45	AF	802	CLA	CHC-C1C	2.38	1.41	1.35
54	A1	303	CHL	C2C-C1C	2.38	1.49	1.44
45	A3	311	CLA	CMB-C2B	-2.38	1.46	1.51
45	BA	841	CLA	CMC-C2C	-2.38	1.45	1.50
45	BB	840	CLA	CMD-C2D	-2.38	1.45	1.50
45	BA	832	CLA	CMB-C2B	-2.38	1.46	1.51
45	BA	820	CLA	CMD-C2D	-2.37	1.45	1.50
45	BK	202	CLA	CMB-C2B	-2.37	1.46	1.51
45	AB	835	CLA	CMD-C2D	-2.37	1.45	1.50
54	B2	601	CHL	C4D-CHA	2.37	1.46	1.38
45	BB	831	CLA	C3B-C2B	-2.37	1.37	1.40
45	BB	818	CLA	CMB-C2B	-2.37	1.46	1.51
45	BB	823	CLA	CMB-C2B	-2.37	1.46	1.51
45	AB	834	CLA	CMD-C2D	-2.37	1.45	1.50
54	A6	607	CHL	C4B-CHC	2.37	1.47	1.41
45	A4	301	CLA	CMC-C2C	-2.37	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	311	CLA	CMB-C2B	-2.37	1.46	1.51
45	BA	806	CLA	CMC-C2C	-2.37	1.45	1.50
45	BA	833	CLA	C3B-C2B	-2.37	1.37	1.40
45	AB	815	CLA	CMD-C2D	-2.37	1.45	1.50
45	AA	802	CLA	C3B-C2B	-2.37	1.37	1.40
54	B2	614	CHL	C4B-CHC	2.37	1.47	1.41
45	AB	842	CLA	C3B-CAB	-2.37	1.43	1.47
45	BA	814	CLA	CMC-C2C	-2.37	1.45	1.50
45	A6	603	CLA	CMD-C2D	-2.37	1.45	1.50
45	AL	303	CLA	C3B-C2B	-2.37	1.37	1.40
45	BL	304	CLA	CMB-C2B	-2.36	1.46	1.51
45	BA	844	CLA	CMB-C2B	-2.36	1.46	1.51
45	BB	810	CLA	C3B-C2B	-2.36	1.37	1.40
45	AA	829	CLA	MG-ND	-2.36	2.01	2.05
45	AA	821	CLA	CMD-C2D	-2.36	1.45	1.50
54	B2	605	CHL	C4D-CHA	2.36	1.46	1.38
45	BB	834	CLA	CMB-C2B	-2.36	1.46	1.51
54	B3	306	CHL	C4C-C3C	2.36	1.49	1.45
45	BB	805	CLA	CMD-C2D	-2.36	1.45	1.50
54	B3	306	CHL	C4D-CHA	2.36	1.46	1.38
45	AA	811	CLA	CMD-C2D	-2.36	1.45	1.50
45	AA	826	CLA	CMD-C2D	-2.36	1.45	1.50
54	A6	607	CHL	C4D-CHA	2.36	1.46	1.38
45	AB	809	CLA	CMD-C2D	-2.36	1.45	1.50
45	AA	828	CLA	CMD-C2D	-2.36	1.45	1.50
45	B1	307	CLA	CMB-C2B	-2.36	1.46	1.51
45	BB	801	CLA	MG-ND	-2.36	2.01	2.05
45	BB	831	CLA	CHC-C1C	2.36	1.41	1.35
45	BB	808	CLA	C3B-C2B	-2.36	1.37	1.40
45	AA	803	CLA	CMC-C2C	-2.35	1.45	1.50
45	BA	816	CLA	C3B-C2B	-2.35	1.37	1.40
54	A6	602	CHL	C1B-CHB	2.35	1.47	1.41
45	BA	809	CLA	C3B-C2B	-2.35	1.37	1.40
45	BB	839	CLA	CMD-C2D	-2.35	1.45	1.50
45	AA	832	CLA	CMB-C2B	-2.35	1.46	1.51
45	B3	303	CLA	CMB-C2B	-2.35	1.46	1.51
54	A1	303	CHL	C4B-CHC	2.35	1.47	1.41
45	AB	820	CLA	CMD-C2D	-2.35	1.45	1.50
45	BA	813	CLA	CMB-C2B	-2.35	1.46	1.51
45	AB	832	CLA	CMD-C2D	-2.35	1.45	1.50
45	A6	603	CLA	C3B-CAB	-2.35	1.43	1.47
45	B5	612	CLA	C3B-C2B	-2.35	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B1	312	CLA	CMB-C2B	-2.35	1.46	1.51
45	B3	307	CLA	CMD-C2D	-2.35	1.45	1.50
45	AA	806	CLA	CMD-C2D	-2.34	1.45	1.50
45	BB	825	CLA	C3B-C2B	-2.34	1.37	1.40
45	AA	814	CLA	C3B-C2B	-2.34	1.37	1.40
45	BA	811	CLA	CMD-C2D	-2.34	1.45	1.50
45	BA	840	CLA	CMD-C2D	-2.34	1.45	1.50
55	B3	316	XAT	O24-C25	-2.34	1.42	1.46
45	A6	603	CLA	CMC-C2C	-2.34	1.45	1.50
45	AB	801	CLA	C3B-C2B	-2.34	1.37	1.40
52	B1	316	LUT	C12-C13	-2.34	1.40	1.45
45	BA	802	CLA	CMC-C2C	-2.34	1.45	1.50
45	A4	307	CLA	C3B-C2B	-2.34	1.37	1.40
45	BB	817	CLA	CMB-C2B	-2.34	1.46	1.51
45	AB	819	CLA	CMD-C2D	-2.34	1.45	1.50
45	BB	814	CLA	CMD-C2D	-2.34	1.45	1.50
45	A3	302	CLA	C3B-CAB	-2.34	1.43	1.47
54	A6	602	CHL	C4D-CHA	2.34	1.46	1.38
45	B5	608	CLA	CMD-C2D	-2.34	1.45	1.50
45	AB	830	CLA	C3B-C2B	-2.34	1.37	1.40
45	BA	815	CLA	CMB-C2B	-2.33	1.46	1.51
45	A3	309	CLA	C3B-C2B	-2.33	1.37	1.40
45	B3	304	CLA	C3B-C2B	-2.33	1.37	1.40
45	B1	306	CLA	CMB-C2B	-2.33	1.46	1.51
54	A3	307	CHL	C4D-CHA	2.33	1.46	1.38
45	AB	831	CLA	C3B-CAB	-2.33	1.43	1.47
45	BK	201	CLA	CMB-C2B	-2.33	1.46	1.51
54	A3	307	CHL	C4C-C3C	2.33	1.49	1.45
54	B1	303	CHL	C4D-CHA	2.33	1.46	1.38
54	B2	614	CHL	C4C-C3C	2.33	1.49	1.45
48	AI	101	BCR	C30-C25	-2.33	1.50	1.53
45	AB	802	CLA	CMD-C2D	-2.33	1.45	1.50
45	AB	826	CLA	CMD-C2D	-2.33	1.45	1.50
45	BB	822	CLA	CMD-C2D	-2.33	1.45	1.50
45	BA	840	CLA	C3B-C2B	-2.33	1.37	1.40
45	AA	814	CLA	C3B-CAB	-2.33	1.43	1.47
45	BA	821	CLA	C3B-CAB	-2.33	1.43	1.47
45	AA	834	CLA	CMC-C2C	-2.32	1.45	1.50
45	AB	825	CLA	CMC-C2C	-2.32	1.45	1.50
45	AF	803	CLA	CMD-C2D	-2.32	1.45	1.50
45	AB	803	CLA	CMD-C2D	-2.32	1.45	1.50
45	A6	610	CLA	CMD-C2D	-2.32	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B2	601	CHL	C4B-CHC	2.32	1.47	1.41
45	B3	314	CLA	CMB-C2B	-2.32	1.46	1.51
45	AA	812	CLA	CMD-C2D	-2.32	1.45	1.50
45	AB	801	CLA	MG-ND	-2.32	2.01	2.05
45	B3	311	CLA	C3B-C2B	-2.32	1.37	1.40
54	A6	606	CHL	C2C-C1C	2.32	1.49	1.44
45	AA	827	CLA	CMB-C2B	-2.32	1.46	1.51
45	BB	816	CLA	C3B-CAB	-2.32	1.43	1.47
45	B2	602	CLA	C3B-CAB	-2.32	1.43	1.47
45	BB	802	CLA	CMC-C2C	-2.32	1.45	1.50
45	BB	804	CLA	C3B-C2B	-2.32	1.37	1.40
45	BB	809	CLA	C3B-CAB	-2.32	1.43	1.47
45	BB	807	CLA	CMC-C2C	-2.32	1.45	1.50
45	B5	601	CLA	C3B-CAB	-2.32	1.43	1.47
54	B1	303	CHL	MG-NA	-2.32	2.00	2.06
45	AA	802	CLA	CMC-C2C	-2.32	1.45	1.50
45	B3	310	CLA	CMB-C2B	-2.31	1.46	1.51
45	BB	843	CLA	C3B-C2B	-2.31	1.37	1.40
54	A4	304	CHL	C2C-C1C	2.31	1.49	1.44
54	A1	303	CHL	C4C-C3C	2.31	1.49	1.45
45	AA	820	CLA	CMD-C2D	-2.31	1.45	1.50
56	e	301	SQD	O2-C2	-2.31	1.37	1.43
45	AA	830	CLA	CMD-C2D	-2.31	1.45	1.50
45	AA	803	CLA	CMD-C2D	-2.31	1.45	1.50
45	B3	314	CLA	CMD-C2D	-2.31	1.45	1.50
48	A6	617	BCR	C8-C9	2.31	1.50	1.45
45	AA	805	CLA	CMD-C2D	-2.31	1.45	1.50
45	AB	809	CLA	CMC-C2C	-2.31	1.45	1.50
45	AB	827	CLA	CMD-C2D	-2.31	1.45	1.50
45	BB	829	CLA	CMB-C2B	-2.31	1.46	1.51
54	A6	606	CHL	C4D-CHA	2.31	1.46	1.38
45	BB	807	CLA	CMD-C2D	-2.31	1.45	1.50
54	A4	306	CHL	C4C-C3C	2.31	1.49	1.45
54	B5	605	CHL	C4D-CHA	2.31	1.46	1.38
54	B1	303	CHL	C4B-CHC	2.31	1.47	1.41
45	AA	838	CLA	C3B-C2B	-2.31	1.37	1.40
45	BF	301	CLA	CMD-C2D	-2.30	1.45	1.50
54	A4	304	CHL	C4D-CHA	2.30	1.46	1.38
45	BA	805	CLA	CMD-C2D	-2.30	1.45	1.50
55	A4	316	XAT	O24-C25	-2.30	1.42	1.46
45	A1	305	CLA	C3B-C2B	-2.30	1.37	1.40
48	AA	849	BCR	C1-C6	-2.30	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B5	608	CLA	C3B-CAB	-2.30	1.43	1.47
45	AB	838	CLA	CMC-C2C	-2.30	1.45	1.50
45	BB	830	CLA	C3B-CAB	-2.30	1.43	1.47
45	B1	311	CLA	CMB-C2B	-2.30	1.46	1.51
45	AA	833	CLA	C3B-C2B	-2.30	1.37	1.40
45	AA	824	CLA	CMD-C2D	-2.30	1.45	1.50
48	BG	203	BCR	C30-C25	-2.30	1.50	1.53
45	A1	304	CLA	C3B-C2B	-2.30	1.37	1.40
54	A4	304	CHL	C1B-CHB	2.30	1.47	1.41
54	B2	606	CHL	C2C-C1C	2.30	1.49	1.44
48	BA	847	BCR	C8-C9	2.30	1.50	1.45
53	AG	202	LMG	O1-C1	2.30	1.44	1.40
45	A3	315	CLA	CMB-C2B	-2.30	1.46	1.51
54	B5	607	CHL	C4D-CHA	2.29	1.46	1.38
45	BB	806	CLA	CMD-C2D	-2.29	1.45	1.50
45	AA	838	CLA	CMD-C2D	-2.29	1.45	1.50
45	AB	818	CLA	CMD-C2D	-2.29	1.45	1.50
45	BB	816	CLA	CMD-C2D	-2.29	1.45	1.50
45	BB	831	CLA	C4B-CHC	-2.29	1.34	1.41
45	BB	805	CLA	C3B-CAB	-2.29	1.43	1.47
45	AB	811	CLA	CMD-C2D	-2.29	1.45	1.50
45	B1	305	CLA	C3B-C2B	-2.29	1.37	1.40
45	AB	815	CLA	C3B-CAB	-2.29	1.43	1.47
45	AB	804	CLA	C3B-CAB	-2.29	1.43	1.47
45	BB	804	CLA	CMC-C2C	-2.29	1.45	1.50
45	AB	824	CLA	C3B-C2B	-2.29	1.37	1.40
45	AB	804	CLA	MG-ND	-2.29	2.01	2.05
54	B2	601	CHL	C4C-C3C	2.29	1.49	1.45
45	AA	814	CLA	CMD-C2D	-2.29	1.46	1.50
45	B2	612	CLA	C3B-C2B	-2.28	1.37	1.40
45	BA	818	CLA	C3B-CAB	-2.28	1.43	1.47
45	BA	805	CLA	C3B-C2B	-2.28	1.37	1.40
45	BA	809	CLA	C3B-CAB	-2.28	1.43	1.47
45	BB	832	CLA	C3B-CAB	-2.28	1.43	1.47
45	BB	811	CLA	CMC-C2C	-2.28	1.46	1.50
54	A1	308	CHL	C2C-C1C	2.28	1.49	1.44
45	AB	810	CLA	CMD-C2D	-2.28	1.46	1.50
45	BA	804	CLA	CMD-C2D	-2.28	1.46	1.50
45	AK	201	CLA	CMB-C2B	-2.28	1.46	1.51
45	AL	305	CLA	CMD-C2D	-2.28	1.46	1.50
45	AA	816	CLA	C3B-C2B	-2.28	1.37	1.40
45	BA	822	CLA	CMB-C2B	-2.28	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	B1	308	CHL	C1B-CHB	2.28	1.47	1.41
45	BH	201	CLA	C3B-C2B	-2.28	1.37	1.40
45	BA	837	CLA	CMD-C2D	-2.28	1.46	1.50
45	AB	804	CLA	C3B-C2B	-2.28	1.37	1.40
45	BB	819	CLA	CMD-C2D	-2.27	1.46	1.50
55	B2	616	XAT	O24-C25	-2.27	1.43	1.46
45	BG	201	CLA	CMB-C2B	-2.27	1.46	1.51
45	AB	842	CLA	C3B-C2B	-2.27	1.37	1.40
45	A6	612	CLA	CMD-C2D	-2.27	1.46	1.50
55	A1	318	XAT	O24-C25	-2.27	1.43	1.46
45	AB	810	CLA	MG-ND	-2.27	2.01	2.05
45	AB	837	CLA	CMC-C2C	-2.27	1.46	1.50
45	BB	824	CLA	CMD-C2D	-2.27	1.46	1.50
45	AA	808	CLA	C3B-C2B	-2.27	1.37	1.40
45	AB	817	CLA	CMD-C2D	-2.27	1.46	1.50
45	A1	314	CLA	C3B-C2B	-2.27	1.37	1.40
45	AB	832	CLA	CMC-C2C	-2.26	1.46	1.50
54	A3	307	CHL	C1C-NC	-2.26	1.34	1.37
45	A4	310	CLA	CMD-C2D	-2.26	1.46	1.50
45	AA	819	CLA	C3B-C2B	-2.26	1.37	1.40
45	B2	608	CLA	CMD-C2D	-2.26	1.46	1.50
45	AB	841	CLA	CMD-C2D	-2.26	1.46	1.50
45	AA	807	CLA	CMC-C2C	-2.26	1.46	1.50
45	AA	823	CLA	CMD-C2D	-2.26	1.46	1.50
54	A1	308	CHL	CMC-C2C	2.26	1.49	1.45
45	AB	814	CLA	CMD-C2D	-2.26	1.46	1.50
45	B5	602	CLA	CMD-C2D	-2.26	1.46	1.50
45	AA	831	CLA	CMD-C2D	-2.26	1.46	1.50
56	BJ	104	SQD	C6-S	-2.25	1.69	1.77
45	BB	804	CLA	CMD-C2D	-2.25	1.46	1.50
45	AB	813	CLA	CMD-C2D	-2.25	1.46	1.50
45	AF	803	CLA	CMC-C2C	-2.25	1.46	1.50
45	AA	805	CLA	C3B-C2B	-2.25	1.37	1.40
45	BA	831	CLA	CMD-C2D	-2.25	1.46	1.50
45	B5	612	CLA	CMC-C2C	-2.25	1.46	1.50
45	AL	305	CLA	CMC-C2C	-2.25	1.46	1.50
45	A4	301	CLA	C3B-CAB	-2.25	1.43	1.47
45	AB	823	CLA	CMD-C2D	-2.25	1.46	1.50
45	AA	806	CLA	C3B-CAB	-2.25	1.43	1.47
45	AB	816	CLA	CMC-C2C	-2.25	1.46	1.50
45	AB	802	CLA	CMC-C2C	-2.25	1.46	1.50
45	BB	828	CLA	CMD-C2D	-2.25	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B5	602	CLA	C3B-CAB	-2.25	1.43	1.47
54	B2	607	CHL	C4D-CHA	2.25	1.46	1.38
45	BA	841	CLA	CMD-C2D	-2.25	1.46	1.50
54	A4	306	CHL	C4D-CHA	2.24	1.46	1.38
45	B3	308	CLA	C3B-C2B	-2.24	1.37	1.40
45	AA	842	CLA	CMD-C2D	-2.24	1.46	1.50
46	BA	843	PQN	C3-C4	2.24	1.52	1.47
48	AK	204	BCR	C12-C13	2.24	1.50	1.45
45	AA	837	CLA	CMD-C2D	-2.24	1.46	1.50
45	BB	818	CLA	C3B-CAB	-2.24	1.43	1.47
45	A4	301	CLA	CMD-C2D	-2.24	1.46	1.50
45	BB	842	CLA	CMD-C2D	-2.24	1.46	1.50
45	B5	603	CLA	CMD-C2D	-2.24	1.46	1.50
45	BA	829	CLA	MG-ND	-2.24	2.01	2.05
45	BA	817	CLA	CMB-C2B	-2.24	1.47	1.51
54	A4	306	CHL	C1B-CHB	2.24	1.47	1.41
54	A6	607	CHL	C2C-C1C	2.23	1.49	1.44
45	BA	834	CLA	CMD-C2D	-2.23	1.46	1.50
45	BA	830	CLA	CMC-C2C	-2.23	1.46	1.50
45	AA	836	CLA	C3B-C2B	-2.23	1.37	1.40
45	AA	804	CLA	CMD-C2D	-2.23	1.46	1.50
45	BA	828	CLA	CMB-C2B	-2.23	1.47	1.51
54	B5	605	CHL	C4B-CHC	2.23	1.47	1.41
54	A6	608	CHL	C4B-CHC	2.23	1.47	1.41
45	AB	830	CLA	CMC-C2C	-2.23	1.46	1.50
45	B3	301	CLA	CMC-C2C	-2.23	1.46	1.50
45	BA	833	CLA	CMD-C2D	-2.23	1.46	1.50
54	B2	614	CHL	C4D-CHA	2.23	1.46	1.38
45	AA	819	CLA	CMD-C2D	-2.23	1.46	1.50
45	AA	834	CLA	CMD-C2D	-2.23	1.46	1.50
45	BB	834	CLA	C3B-CAB	-2.23	1.43	1.47
45	AL	304	CLA	CMD-C2D	-2.23	1.46	1.50
54	B2	605	CHL	C4B-CHC	2.23	1.47	1.41
45	BA	819	CLA	CMC-C2C	-2.23	1.46	1.50
45	AA	812	CLA	C4B-CHC	-2.23	1.34	1.41
48	BL	306	BCR	C1-C6	-2.23	1.50	1.53
45	BB	808	CLA	CMD-C2D	-2.23	1.46	1.50
45	AK	203	CLA	C3B-C2B	-2.22	1.37	1.40
45	AB	807	CLA	CAC-C3C	-2.22	1.45	1.51
45	AA	812	CLA	C3B-C2B	-2.22	1.37	1.40
45	AA	839	CLA	C3B-C2B	-2.22	1.37	1.40
45	AF	802	CLA	C3B-CAB	-2.22	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	314	CLA	CMD-C2D	-2.22	1.46	1.50
45	BA	830	CLA	CMD-C2D	-2.22	1.46	1.50
45	AA	806	CLA	C3B-C2B	-2.22	1.37	1.40
45	BA	819	CLA	C3B-C2B	-2.22	1.37	1.40
54	B5	607	CHL	C1B-CHB	2.22	1.47	1.41
45	BB	823	CLA	CMD-C2D	-2.22	1.46	1.50
54	A3	307	CHL	C4B-CHC	2.22	1.47	1.41
45	AB	834	CLA	CMC-C2C	-2.22	1.46	1.50
45	A4	313	CLA	CMD-C2D	-2.22	1.46	1.50
45	B3	301	CLA	C3B-C2B	-2.22	1.37	1.40
45	AA	835	CLA	C3B-C2B	-2.22	1.37	1.40
45	A4	310	CLA	C3B-C2B	-2.22	1.37	1.40
45	BA	827	CLA	CMB-C2B	-2.22	1.47	1.51
45	B5	611	CLA	C3B-C2B	-2.22	1.37	1.40
45	AB	812	CLA	CMD-C2D	-2.21	1.46	1.50
45	BB	827	CLA	CMB-C2B	-2.21	1.47	1.51
45	BA	802	CLA	C3B-CAB	-2.21	1.43	1.47
45	BB	842	CLA	CMC-C2C	-2.21	1.46	1.50
55	A6	616	XAT	O24-C25	-2.21	1.43	1.46
45	B3	311	CLA	CMD-C2D	-2.21	1.46	1.50
54	B1	308	CHL	CMC-C2C	2.21	1.49	1.45
45	BA	839	CLA	CMD-C2D	-2.21	1.46	1.50
45	AB	836	CLA	CMD-C2D	-2.21	1.46	1.50
45	AB	817	CLA	C3B-CAB	-2.21	1.43	1.47
45	B3	308	CLA	CMD-C2D	-2.21	1.46	1.50
52	A4	315	LUT	C22-C21	-2.21	1.51	1.54
45	AA	823	CLA	C3B-C2B	-2.21	1.37	1.40
45	A3	305	CLA	CMD-C2D	-2.21	1.46	1.50
45	B5	613	CLA	CMD-C2D	-2.21	1.46	1.50
45	A4	302	CLA	CMD-C2D	-2.21	1.46	1.50
48	BB	849	BCR	C19-C18	2.21	1.50	1.45
45	AB	808	CLA	CMC-C2C	-2.21	1.46	1.50
45	A1	307	CLA	CMD-C2D	-2.21	1.46	1.50
45	BA	826	CLA	CMD-C2D	-2.21	1.46	1.50
45	BA	824	CLA	CMC-C2C	-2.21	1.46	1.50
45	BB	805	CLA	MG-ND	-2.20	2.01	2.05
45	AA	817	CLA	CMD-C2D	-2.20	1.46	1.50
45	B2	602	CLA	CMD-C2D	-2.20	1.46	1.50
54	A6	608	CHL	C1B-CHB	2.20	1.47	1.41
45	BA	821	CLA	CMC-C2C	-2.20	1.46	1.50
54	B2	614	CHL	C1B-CHB	2.20	1.47	1.41
55	B1	317	XAT	O24-C25	-2.20	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B5	609	CLA	CMD-C2D	-2.20	1.46	1.50
45	AB	827	CLA	CMC-C2C	-2.20	1.46	1.50
45	AK	203	CLA	CMC-C2C	-2.20	1.46	1.50
45	AB	806	CLA	CMD-C2D	-2.20	1.46	1.50
45	AA	813	CLA	CMC-C2C	-2.20	1.46	1.50
45	BB	817	CLA	CMD-C2D	-2.20	1.46	1.50
45	BA	815	CLA	C3B-CAB	-2.20	1.43	1.47
45	AB	817	CLA	C3B-C2B	-2.20	1.37	1.40
45	A1	316	CLA	CMD-C2D	-2.19	1.46	1.50
45	BA	828	CLA	CMC-C2C	-2.19	1.46	1.50
48	AB	848	BCR	C19-C18	2.19	1.50	1.45
45	BB	805	CLA	C3B-C2B	-2.19	1.37	1.40
45	AB	816	CLA	CMD-C2D	-2.19	1.46	1.50
54	A6	602	CHL	C4B-CHC	2.19	1.47	1.41
45	AB	808	CLA	CMD-C2D	-2.19	1.46	1.50
45	BA	812	CLA	CMD-C2D	-2.19	1.46	1.50
45	B3	302	CLA	C3B-C2B	-2.19	1.37	1.40
54	A4	306	CHL	C2C-C1C	2.19	1.49	1.44
45	A3	305	CLA	C3B-C2B	-2.19	1.37	1.40
45	AB	833	CLA	C3B-CAB	-2.19	1.43	1.47
45	AG	203	CLA	CMD-C2D	-2.19	1.46	1.50
45	A1	307	CLA	C3B-CAB	-2.19	1.43	1.47
45	AL	303	CLA	CMD-C2D	-2.19	1.46	1.50
54	B2	614	CHL	C2C-C1C	2.19	1.49	1.44
45	A1	307	CLA	C3B-C2B	-2.19	1.37	1.40
45	A4	308	CLA	CMD-C2D	-2.19	1.46	1.50
45	A6	610	CLA	C3B-CAB	-2.19	1.43	1.47
54	B5	607	CHL	C3D-C4D	-2.19	1.39	1.44
45	AA	805	CLA	CMC-C2C	-2.19	1.46	1.50
45	A6	604	CLA	CMD-C2D	-2.19	1.46	1.50
45	BB	839	CLA	CMC-C2C	-2.19	1.46	1.50
45	AA	813	CLA	C3B-CAB	-2.18	1.43	1.47
55	B5	615	XAT	O24-C25	-2.18	1.43	1.46
45	AA	841	CLA	C3B-C2B	-2.18	1.37	1.40
45	AA	835	CLA	CMD-C2D	-2.18	1.46	1.50
45	BA	808	CLA	CMD-C2D	-2.18	1.46	1.50
45	A3	303	CLA	CMD-C2D	-2.18	1.46	1.50
45	AB	836	CLA	C3B-C2B	-2.18	1.37	1.40
45	BK	203	CLA	CMB-C2B	-2.18	1.47	1.51
46	AB	843	PQN	C2-C1	2.18	1.52	1.48
45	AB	808	CLA	C3B-CAB	-2.18	1.43	1.47
45	BA	814	CLA	CMD-C2D	-2.18	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	B5	614	LUT	C22-C21	-2.18	1.52	1.54
45	BL	303	CLA	CMD-C2D	-2.18	1.46	1.50
45	AA	803	CLA	C3B-C2B	-2.18	1.37	1.40
48	AA	845	BCR	C8-C9	2.18	1.50	1.45
45	B5	610	CLA	CMD-C2D	-2.18	1.46	1.50
45	AB	825	CLA	MG-ND	-2.18	2.01	2.05
45	AA	801	CLA	C3B-C2B	-2.18	1.37	1.40
45	AB	840	CLA	C3B-CAB	-2.18	1.43	1.47
54	A6	606	CHL	C4B-CHC	2.18	1.47	1.41
45	AA	819	CLA	CMC-C2C	-2.18	1.46	1.50
45	A3	306	CLA	CMD-C2D	-2.18	1.46	1.50
45	AB	838	CLA	CMD-C2D	-2.17	1.46	1.50
45	BB	835	CLA	C3B-CAB	-2.17	1.43	1.47
45	AB	824	CLA	MG-ND	-2.17	2.01	2.05
45	AB	815	CLA	CMC-C2C	-2.17	1.46	1.50
45	AB	841	CLA	CMC-C2C	-2.17	1.46	1.50
45	BB	813	CLA	CMC-C2C	-2.17	1.46	1.50
45	AB	835	CLA	C3B-CAB	-2.17	1.43	1.47
45	AB	832	CLA	C4B-CHC	-2.17	1.35	1.41
45	AB	811	CLA	CMC-C2C	-2.17	1.46	1.50
45	AA	838	CLA	C3B-CAB	-2.17	1.43	1.47
45	BF	302	CLA	CMD-C2D	-2.17	1.46	1.50
54	B3	306	CHL	C4B-CHC	2.17	1.47	1.41
54	A6	602	CHL	C2C-C1C	2.17	1.49	1.44
45	BA	838	CLA	CMD-C2D	-2.17	1.46	1.50
45	BA	811	CLA	C3B-C2B	-2.17	1.37	1.40
45	BG	202	CLA	C3B-C2B	-2.17	1.37	1.40
45	BB	811	CLA	C3B-C2B	-2.17	1.37	1.40
45	AB	814	CLA	CMC-C2C	-2.17	1.46	1.50
45	BA	819	CLA	CMD-C2D	-2.17	1.46	1.50
45	BA	814	CLA	C3B-C2B	-2.17	1.37	1.40
45	BB	843	CLA	CMD-C2D	-2.17	1.46	1.50
45	A4	311	CLA	CMD-C2D	-2.17	1.46	1.50
45	AA	832	CLA	CMD-C2D	-2.16	1.46	1.50
45	A4	303	CLA	CMD-C2D	-2.16	1.46	1.50
45	BA	840	CLA	C3B-CAB	-2.16	1.43	1.47
45	A1	310	CLA	CMD-C2D	-2.16	1.46	1.50
45	AB	810	CLA	C4B-CHC	-2.16	1.35	1.41
45	AG	204	CLA	C3B-C2B	-2.16	1.37	1.40
45	BB	816	CLA	C3B-C2B	-2.16	1.37	1.40
45	A6	613	CLA	CMD-C2D	-2.16	1.46	1.50
45	BB	812	CLA	CMD-C2D	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B2	608	CLA	C3B-C2B	-2.16	1.37	1.40
45	BA	813	CLA	CMC-C2C	-2.16	1.46	1.50
45	BF	302	CLA	CMC-C2C	-2.16	1.46	1.50
45	BA	814	CLA	C3B-CAB	-2.16	1.43	1.47
45	AK	201	CLA	CBD-CAD	2.16	1.56	1.51
45	AL	304	CLA	CMC-C2C	-2.16	1.46	1.50
45	B2	603	CLA	CMD-C2D	-2.16	1.46	1.50
45	B1	309	CLA	CMD-C2D	-2.16	1.46	1.50
45	BB	811	CLA	C3B-CAB	-2.16	1.43	1.47
54	B5	607	CHL	C4C-C3C	2.16	1.48	1.44
45	AF	802	CLA	MG-ND	-2.16	2.01	2.05
45	AB	826	CLA	CMB-C2B	-2.16	1.47	1.51
45	BA	821	CLA	CMD-C2D	-2.16	1.46	1.50
45	BB	820	CLA	C4B-CHC	-2.16	1.35	1.41
54	B2	605	CHL	CMC-C2C	2.15	1.49	1.45
45	A6	614	CLA	CMD-C2D	-2.15	1.46	1.50
54	A6	607	CHL	CMC-C2C	2.15	1.49	1.45
45	BH	201	CLA	CMD-C2D	-2.15	1.46	1.50
45	BA	803	CLA	CMC-C2C	-2.15	1.46	1.50
45	AB	807	CLA	C4B-CHC	-2.15	1.35	1.41
45	BL	304	CLA	CMD-C2D	-2.15	1.46	1.50
45	BA	810	CLA	C3B-CAB	-2.15	1.43	1.47
45	A1	305	CLA	CMD-C2D	-2.15	1.46	1.50
45	AB	839	CLA	C3B-C2B	-2.15	1.37	1.40
45	B3	313	CLA	CBD-CAD	2.15	1.56	1.51
54	A4	305	CHL	C1B-CHB	2.15	1.47	1.41
45	BA	824	CLA	C3B-C2B	-2.15	1.37	1.40
45	AB	837	CLA	C3B-C2B	-2.15	1.37	1.40
45	BG	201	CLA	C3B-C2B	-2.15	1.37	1.40
54	B5	606	CHL	C1B-CHB	2.15	1.47	1.41
45	BB	829	CLA	CMD-C2D	-2.15	1.46	1.50
45	AA	835	CLA	C3B-CAB	-2.15	1.43	1.47
45	AG	201	CLA	CMD-C2D	-2.15	1.46	1.50
56	e	301	SQD	O4-C4	-2.15	1.37	1.43
45	BB	808	CLA	C3B-CAB	-2.15	1.43	1.47
45	AB	841	CLA	C3B-CAB	-2.15	1.43	1.47
45	BA	812	CLA	C4B-CHC	-2.15	1.35	1.41
45	BB	821	CLA	CMD-C2D	-2.15	1.46	1.50
45	AF	804	CLA	CMD-C2D	-2.15	1.46	1.50
45	BB	843	CLA	C3B-CAB	-2.14	1.43	1.47
45	BA	807	CLA	CMC-C2C	-2.14	1.46	1.50
45	AB	832	CLA	C3B-CAB	-2.14	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	813	CLA	CMD-C2D	-2.14	1.46	1.50
54	B5	605	CHL	C1B-CHB	2.14	1.46	1.41
45	BB	811	CLA	CMD-C2D	-2.14	1.46	1.50
46	BB	844	PQN	C10-C1	2.14	1.52	1.48
45	A1	313	CLA	CMD-C2D	-2.14	1.46	1.50
48	A1	319	BCR	C40-C30	2.14	1.58	1.53
45	AH	201	CLA	CMD-C2D	-2.14	1.46	1.50
45	BA	811	CLA	CMC-C2C	-2.14	1.46	1.50
45	BB	825	CLA	C3B-CAB	-2.14	1.43	1.47
45	A1	312	CLA	CMD-C2D	-2.14	1.46	1.50
45	BA	807	CLA	CMD-C2D	-2.14	1.46	1.50
45	BA	839	CLA	C4B-CHC	-2.14	1.35	1.41
45	BA	830	CLA	C4B-CHC	-2.14	1.35	1.41
45	AK	202	CLA	CMD-C2D	-2.14	1.46	1.50
45	B3	313	CLA	C3B-C2B	-2.14	1.37	1.40
45	BA	835	CLA	C3B-CAB	-2.14	1.43	1.47
45	AB	822	CLA	C3B-C2B	-2.14	1.37	1.40
45	BB	822	CLA	CMC-C2C	-2.13	1.46	1.50
45	BB	815	CLA	CMD-C2D	-2.13	1.46	1.50
45	BL	302	CLA	CMD-C2D	-2.13	1.46	1.50
45	BB	821	CLA	C3B-CAB	-2.13	1.43	1.47
45	AL	305	CLA	C3B-C2B	-2.13	1.37	1.40
45	BB	836	CLA	CMD-C2D	-2.13	1.46	1.50
45	B5	609	CLA	CMC-C2C	-2.13	1.46	1.50
45	A4	313	CLA	C3B-C2B	-2.13	1.37	1.40
54	A4	304	CHL	CMC-C2C	2.13	1.49	1.45
45	BB	818	CLA	CMD-C2D	-2.13	1.46	1.50
48	BB	847	BCR	C8-C9	2.13	1.50	1.45
45	BB	813	CLA	CMD-C2D	-2.13	1.46	1.50
45	AA	810	CLA	CMD-C2D	-2.13	1.46	1.50
45	A3	312	CLA	C3B-C2B	-2.13	1.37	1.40
45	AB	822	CLA	CMD-C2D	-2.13	1.46	1.50
45	BA	834	CLA	CMC-C2C	-2.13	1.46	1.50
45	AB	839	CLA	C3B-CAB	-2.13	1.43	1.47
45	B1	314	CLA	CMD-C2D	-2.13	1.46	1.50
45	BB	836	CLA	C3B-C2B	-2.13	1.37	1.40
45	AB	826	CLA	C3B-C2B	-2.13	1.37	1.40
45	BB	840	CLA	C3B-C2B	-2.13	1.37	1.40
45	A6	605	CLA	CMD-C2D	-2.13	1.46	1.50
45	AB	825	CLA	C3B-CAB	-2.13	1.43	1.47
45	AF	802	CLA	CMC-C2C	-2.12	1.46	1.50
54	B5	605	CHL	C2C-C1C	2.12	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BB	818	CLA	C3B-C2B	-2.12	1.37	1.40
45	AA	833	CLA	CMD-C2D	-2.12	1.46	1.50
54	B2	606	CHL	CMC-C2C	2.12	1.49	1.45
45	BA	836	CLA	C3B-C2B	-2.12	1.37	1.40
45	A3	313	CLA	CMD-C2D	-2.12	1.46	1.50
45	A6	601	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	816	CLA	CMC-C2C	-2.12	1.46	1.50
45	AB	833	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	826	CLA	C3B-CAB	-2.12	1.43	1.47
45	B1	310	CLA	CMD-C2D	-2.12	1.46	1.50
45	BA	805	CLA	CMC-C2C	-2.12	1.46	1.50
45	BA	823	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	833	CLA	CMC-C2C	-2.12	1.46	1.50
45	BA	822	CLA	CMD-C2D	-2.12	1.46	1.50
48	AK	204	BCR	C8-C9	2.12	1.50	1.45
45	AK	203	CLA	CMD-C2D	-2.12	1.46	1.50
45	A1	309	CLA	CMD-C2D	-2.12	1.46	1.50
45	BA	801	CLA	CMD-C2D	-2.12	1.46	1.50
45	BB	808	CLA	CMC-C2C	-2.12	1.46	1.50
55	A3	317	XAT	O24-C25	-2.12	1.43	1.46
45	AB	828	CLA	CMD-C2D	-2.12	1.46	1.50
45	AB	807	CLA	C3B-C2B	-2.12	1.37	1.40
45	BB	839	CLA	C3B-C2B	-2.12	1.37	1.40
45	AA	821	CLA	CMC-C2C	-2.12	1.46	1.50
45	BB	826	CLA	C3B-C2B	-2.12	1.37	1.40
45	AA	806	CLA	CMC-C2C	-2.12	1.46	1.50
45	BB	830	CLA	MG-ND	-2.12	2.01	2.05
54	A6	602	CHL	C1D-C2D	2.11	1.49	1.45
45	AB	835	CLA	C3B-C2B	-2.11	1.37	1.40
45	A1	307	CLA	CMC-C2C	-2.11	1.46	1.50
45	BB	826	CLA	MG-ND	-2.11	2.01	2.05
45	AA	838	CLA	CMC-C2C	-2.11	1.46	1.50
45	BB	809	CLA	CMD-C2D	-2.11	1.46	1.50
56	e	301	SQD	O3-C3	-2.11	1.38	1.43
45	BL	303	CLA	C3B-CAB	-2.11	1.43	1.47
45	AA	804	CLA	CMC-C2C	-2.11	1.46	1.50
45	A4	311	CLA	C3B-C2B	-2.11	1.37	1.40
45	AB	824	CLA	CMC-C2C	-2.11	1.46	1.50
45	AB	837	CLA	CMD-C2D	-2.11	1.46	1.50
45	B5	602	CLA	CMC-C2C	-2.11	1.46	1.50
45	BB	829	CLA	C3B-C2B	-2.11	1.37	1.40
45	AA	816	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	B5	612	CLA	CMD-C2D	-2.11	1.46	1.50
45	AH	201	CLA	C3B-C2B	-2.11	1.37	1.40
45	BA	801	CLA	C3B-C2B	-2.11	1.37	1.40
54	B2	607	CHL	C3D-C4D	-2.11	1.39	1.44
45	BG	201	CLA	CMD-C2D	-2.11	1.46	1.50
45	AB	826	CLA	C3B-CAB	-2.10	1.43	1.47
45	AB	825	CLA	C3B-C2B	-2.10	1.37	1.40
45	BA	815	CLA	C3B-C2B	-2.10	1.37	1.40
45	AA	820	CLA	CMC-C2C	-2.10	1.46	1.50
45	A4	302	CLA	CMC-C2C	-2.10	1.46	1.50
45	BA	804	CLA	CMC-C2C	-2.10	1.46	1.50
45	B5	601	CLA	C3B-C2B	-2.10	1.37	1.40
45	AA	809	CLA	C3B-CAB	-2.10	1.43	1.47
45	A3	310	CLA	CMD-C2D	-2.10	1.46	1.50
45	A3	312	CLA	CMC-C2C	-2.10	1.46	1.50
45	BA	826	CLA	C3B-CAB	-2.10	1.43	1.47
54	A1	308	CHL	C1B-CHB	2.10	1.46	1.41
45	AA	816	CLA	C3B-CAB	-2.10	1.43	1.47
45	AA	828	CLA	CMC-C2C	-2.10	1.46	1.50
45	B3	302	CLA	CMD-C2D	-2.10	1.46	1.50
45	AA	827	CLA	CMC-C2C	-2.10	1.46	1.50
54	A4	314	CHL	C1B-CHB	2.10	1.46	1.41
45	B3	313	CLA	C3B-CAB	-2.10	1.43	1.47
45	B1	305	CLA	C4B-CHC	-2.10	1.35	1.41
45	AA	822	CLA	CMD-C2D	-2.10	1.46	1.50
45	AB	821	CLA	CMC-C2C	-2.10	1.46	1.50
45	BK	203	CLA	CMD-C2D	-2.10	1.46	1.50
54	A6	608	CHL	C1C-NC	-2.10	1.34	1.37
45	AA	826	CLA	C3B-C2B	-2.10	1.37	1.40
45	A3	313	CLA	C3B-C2B	-2.10	1.37	1.40
45	BA	835	CLA	C3B-C2B	-2.10	1.37	1.40
45	B5	610	CLA	C3B-C2B	-2.10	1.37	1.40
45	AA	812	CLA	CMC-C2C	-2.10	1.46	1.50
45	BB	835	CLA	CMC-C2C	-2.09	1.46	1.50
48	AA	852	BCR	C12-C13	2.09	1.50	1.45
45	A1	306	CLA	CMD-C2D	-2.09	1.46	1.50
45	A4	312	CLA	CMD-C2D	-2.09	1.46	1.50
45	B2	604	CLA	CMD-C2D	-2.09	1.46	1.50
45	BB	812	CLA	C3B-C2B	-2.09	1.37	1.40
45	AA	811	CLA	C3B-C2B	-2.09	1.37	1.40
54	B3	306	CHL	C1C-NC	-2.09	1.34	1.37
45	BA	816	CLA	C3B-CAB	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A6	605	CLA	C3B-C2B	-2.09	1.37	1.40
45	B2	603	CLA	C3B-C2B	-2.09	1.37	1.40
45	AB	829	CLA	MG-ND	-2.09	2.01	2.05
45	AA	802	CLA	C3B-CAB	-2.09	1.43	1.47
45	A1	313	CLA	CMC-C2C	-2.09	1.46	1.50
45	AA	819	CLA	C4B-CHC	-2.09	1.35	1.41
45	AB	807	CLA	CMC-C2C	-2.09	1.46	1.50
45	A3	302	CLA	CMD-C2D	-2.09	1.46	1.50
56	BJ	104	SQD	O6-C1	2.09	1.43	1.40
48	BL	301	BCR	C8-C9	2.09	1.50	1.45
45	AG	204	CLA	CMD-C2D	-2.09	1.46	1.50
45	B2	602	CLA	CMC-C2C	-2.09	1.46	1.50
45	AA	834	CLA	C3B-CAB	-2.09	1.43	1.47
45	A1	311	CLA	CMD-C2D	-2.09	1.46	1.50
45	AA	803	CLA	C4B-CHC	-2.09	1.35	1.41
45	BB	831	CLA	CMC-C2C	-2.09	1.46	1.50
45	AL	304	CLA	C3B-CAB	-2.09	1.43	1.47
45	B2	609	CLA	CMD-C2D	-2.08	1.46	1.50
45	A6	613	CLA	CMC-C2C	-2.08	1.46	1.50
45	BB	820	CLA	CMD-C2D	-2.08	1.46	1.50
54	B5	605	CHL	C1D-C2D	2.08	1.49	1.45
45	BA	815	CLA	CMD-C2D	-2.08	1.46	1.50
45	BB	815	CLA	MG-ND	-2.08	2.01	2.05
45	AA	813	CLA	CMD-C2D	-2.08	1.46	1.50
45	BB	817	CLA	CMC-C2C	-2.08	1.46	1.50
45	AB	819	CLA	C4B-CHC	-2.08	1.35	1.41
45	B5	609	CLA	C3B-CAB	-2.08	1.43	1.47
48	AB	845	BCR	C8-C9	2.08	1.50	1.45
45	AA	837	CLA	C3B-CAB	-2.08	1.43	1.47
45	BB	829	CLA	C3B-CAB	-2.08	1.43	1.47
45	A3	314	CLA	C3B-C2B	-2.08	1.37	1.40
48	BA	856	BCR	C12-C13	2.08	1.50	1.45
45	AA	842	CLA	C3B-C2B	-2.08	1.37	1.40
45	BA	817	CLA	CMD-C2D	-2.08	1.46	1.50
45	B1	304	CLA	C3B-C2B	-2.08	1.37	1.40
45	AB	828	CLA	CMC-C2C	-2.08	1.46	1.50
45	A3	314	CLA	CMD-C2D	-2.07	1.46	1.50
54	B2	606	CHL	C1B-CHB	2.07	1.46	1.41
45	B3	304	CLA	CMD-C2D	-2.07	1.46	1.50
48	AF	801	BCR	C23-C22	2.07	1.50	1.45
45	BB	824	CLA	C3B-C2B	-2.07	1.37	1.40
45	B2	612	CLA	CMD-C2D	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
52	AF	806	LUT	C8-C9	2.07	1.50	1.45
45	BB	838	CLA	MG-ND	-2.07	2.01	2.05
45	BB	804	CLA	C3B-CAB	-2.07	1.43	1.47
45	AA	810	CLA	C3B-C2B	-2.07	1.37	1.40
45	A6	601	CLA	C3B-C2B	-2.07	1.37	1.40
45	AB	831	CLA	CMC-C2C	-2.07	1.46	1.50
45	A1	315	CLA	CMD-C2D	-2.07	1.46	1.50
54	B2	607	CHL	C1B-CHB	2.07	1.46	1.41
54	A1	308	CHL	C3D-C4D	-2.07	1.39	1.44
45	BB	826	CLA	CMC-C2C	-2.07	1.46	1.50
45	A6	605	CLA	CMC-C2C	-2.07	1.46	1.50
45	BA	841	CLA	C3B-C2B	-2.07	1.37	1.40
45	BA	837	CLA	CMC-C2C	-2.07	1.46	1.50
45	A3	314	CLA	CBD-CAD	2.07	1.56	1.51
45	AA	807	CLA	CMD-C2D	-2.07	1.46	1.50
45	B2	611	CLA	CMD-C2D	-2.07	1.46	1.50
45	B5	611	CLA	CMD-C2D	-2.07	1.46	1.50
45	BL	302	CLA	C3B-CAB	-2.06	1.43	1.47
45	AB	823	CLA	C4B-CHC	-2.06	1.35	1.41
54	B2	601	CHL	CMC-C2C	2.06	1.49	1.45
45	B1	305	CLA	CMD-C2D	-2.06	1.46	1.50
45	BB	833	CLA	CMD-C2D	-2.06	1.46	1.50
45	B3	303	CLA	CMD-C2D	-2.06	1.46	1.50
45	A3	309	CLA	C3B-CAB	-2.06	1.43	1.47
55	B1	317	XAT	O4-C5	-2.06	1.43	1.46
45	AB	821	CLA	C3B-C2B	-2.06	1.37	1.40
45	BA	810	CLA	CMD-C2D	-2.06	1.46	1.50
45	B3	308	CLA	C3B-CAB	-2.06	1.43	1.47
45	AB	819	CLA	CMC-C2C	-2.06	1.46	1.50
52	A6	615	LUT	C22-C21	-2.06	1.52	1.54
45	BA	832	CLA	CMD-C2D	-2.06	1.46	1.50
45	AB	811	CLA	C3B-C2B	-2.06	1.37	1.40
45	BB	811	CLA	MG-ND	-2.06	2.01	2.05
45	AA	801	CLA	CMD-C2D	-2.06	1.46	1.50
45	AA	826	CLA	C3B-CAB	-2.06	1.43	1.47
45	AA	831	CLA	C3B-CAB	-2.06	1.43	1.47
45	BB	802	CLA	MG-ND	-2.06	2.01	2.05
45	AB	826	CLA	CMC-C2C	-2.06	1.46	1.50
45	B3	301	CLA	CMD-C2D	-2.06	1.46	1.50
45	AK	203	CLA	C3B-CAB	-2.06	1.43	1.47
48	AA	845	BCR	C12-C13	2.06	1.50	1.45
45	AB	812	CLA	CMC-C2C	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AG	201	CLA	C3B-C2B	-2.06	1.37	1.40
45	A6	612	CLA	C3B-C2B	-2.06	1.37	1.40
45	BB	842	CLA	C4B-CHC	-2.05	1.35	1.41
55	A4	316	XAT	O4-C5	-2.05	1.43	1.46
45	B1	312	CLA	CMD-C2D	-2.05	1.46	1.50
45	B2	613	CLA	CMD-C2D	-2.05	1.46	1.50
45	B2	610	CLA	CMD-C2D	-2.05	1.46	1.50
54	A4	306	CHL	C3D-C4D	-2.05	1.39	1.44
45	AA	810	CLA	CMC-C2C	-2.05	1.46	1.50
45	A3	304	CLA	CMD-C2D	-2.05	1.46	1.50
45	BK	201	CLA	CBD-CAD	2.05	1.56	1.51
45	AF	802	CLA	C4B-CHC	-2.05	1.35	1.41
45	BB	806	CLA	CMC-C2C	-2.05	1.46	1.50
52	AF	806	LUT	C26-C27	2.05	1.53	1.50
45	B5	601	CLA	CMD-C2D	-2.05	1.46	1.50
45	A4	312	CLA	C3B-C2B	-2.05	1.37	1.40
45	B3	301	CLA	C3B-CAB	-2.05	1.43	1.47
45	AA	826	CLA	CMC-C2C	-2.05	1.46	1.50
45	A4	310	CLA	CMC-C2C	-2.05	1.46	1.50
45	A3	308	CLA	C3B-C2B	-2.05	1.37	1.40
45	BA	824	CLA	CMD-C2D	-2.05	1.46	1.50
45	BB	801	CLA	CMC-C2C	-2.05	1.46	1.50
45	AB	814	CLA	MG-ND	-2.05	2.01	2.05
45	BB	836	CLA	C3B-CAB	-2.05	1.43	1.47
54	A6	607	CHL	C1B-CHB	2.05	1.46	1.41
45	AA	824	CLA	C3B-C2B	-2.05	1.37	1.40
45	B3	305	CLA	CMD-C2D	-2.05	1.46	1.50
54	A4	305	CHL	C4B-CHC	2.05	1.46	1.41
54	B1	308	CHL	C1D-C2D	2.05	1.49	1.45
45	B3	313	CLA	CMD-C2D	-2.05	1.46	1.50
45	BB	824	CLA	CMC-C2C	-2.04	1.46	1.50
54	B5	606	CHL	C4B-CHC	2.04	1.46	1.41
45	BB	827	CLA	C3B-C2B	-2.04	1.37	1.40
45	AA	819	CLA	C3B-CAB	-2.04	1.43	1.47
45	BA	832	CLA	C3B-CAB	-2.04	1.43	1.47
45	AB	830	CLA	C4B-CHC	-2.04	1.35	1.41
45	AB	803	CLA	C3B-C2B	-2.04	1.37	1.40
48	A6	617	BCR	C12-C13	2.04	1.50	1.45
54	A3	307	CHL	C1B-CHB	2.04	1.46	1.41
45	BA	824	CLA	C3B-CAB	-2.04	1.43	1.47
45	B5	613	CLA	C3B-C2B	-2.04	1.37	1.40
45	A3	303	CLA	CMC-C2C	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	AA	818	CLA	CMC-C2C	-2.04	1.46	1.50
45	BB	828	CLA	CMC-C2C	-2.04	1.46	1.50
54	A6	602	CHL	CMC-C2C	2.04	1.49	1.45
45	AA	834	CLA	C4B-CHC	-2.04	1.35	1.41
45	AF	803	CLA	C3B-C2B	-2.04	1.37	1.40
45	A1	304	CLA	C3B-CAB	-2.04	1.43	1.47
45	AF	804	CLA	C3B-C2B	-2.04	1.37	1.40
45	BB	841	CLA	CMC-C2C	-2.04	1.46	1.50
45	AB	819	CLA	C3B-C2B	-2.04	1.37	1.40
45	AK	201	CLA	CMC-C2C	-2.04	1.46	1.50
45	AB	820	CLA	C3B-CAB	-2.04	1.43	1.47
45	AA	842	CLA	C4B-CHC	-2.04	1.35	1.41
45	AA	824	CLA	CMC-C2C	-2.04	1.46	1.50
45	AA	802	CLA	MG-ND	-2.03	2.01	2.05
45	AA	831	CLA	CMC-C2C	-2.03	1.46	1.50
45	A4	313	CLA	CMC-C2C	-2.03	1.46	1.50
54	B1	303	CHL	C1B-CHB	2.03	1.46	1.41
45	BB	822	CLA	C3B-C2B	-2.03	1.37	1.40
45	A6	613	CLA	C3B-C2B	-2.03	1.37	1.40
45	A6	610	CLA	CMC-C2C	-2.03	1.46	1.50
45	B5	611	CLA	CMC-C2C	-2.03	1.46	1.50
52	A1	317	LUT	C22-C21	-2.03	1.52	1.54
45	AA	836	CLA	CMD-C2D	-2.03	1.46	1.50
45	BF	301	CLA	C4B-CHC	-2.03	1.35	1.41
54	A6	606	CHL	CMC-C2C	2.03	1.49	1.45
55	B5	615	XAT	O4-C5	-2.03	1.43	1.46
45	BA	819	CLA	C4B-CHC	-2.03	1.35	1.41
45	A1	306	CLA	CMC-C2C	-2.03	1.46	1.50
45	AB	803	CLA	CMC-C2C	-2.03	1.46	1.50
54	A4	314	CHL	C1D-C2D	2.03	1.49	1.45
54	B2	605	CHL	C1D-C2D	2.03	1.49	1.45
45	A3	308	CLA	C3B-CAB	-2.03	1.43	1.47
45	B1	313	CLA	CMD-C2D	-2.03	1.46	1.50
45	BA	812	CLA	C3B-C2B	-2.03	1.37	1.40
45	A4	308	CLA	CMC-C2C	-2.02	1.46	1.50
48	AA	848	BCR	C1-C6	-2.02	1.51	1.53
45	BK	202	CLA	C3B-C2B	-2.02	1.37	1.40
48	AJ	101	BCR	C23-C22	2.02	1.50	1.45
48	BB	845	BCR	C8-C9	2.02	1.50	1.45
45	BF	302	CLA	C3B-C2B	-2.02	1.37	1.40
48	AA	852	BCR	C23-C22	2.02	1.50	1.45
48	BB	846	BCR	C8-C9	2.02	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	A1	314	CLA	C4B-CHC	-2.02	1.35	1.41
45	BB	841	CLA	C3B-C2B	-2.02	1.37	1.40
45	A1	304	CLA	C4B-CHC	-2.02	1.35	1.41
48	B2	617	BCR	C8-C9	2.02	1.50	1.45
45	B1	313	CLA	C3B-C2B	-2.02	1.37	1.40
54	B3	306	CHL	C3D-C4D	-2.02	1.39	1.44
54	B1	303	CHL	CMC-C2C	2.02	1.49	1.45
45	BB	827	CLA	CMC-C2C	-2.02	1.46	1.50
45	A3	303	CLA	C4B-CHC	-2.02	1.35	1.41
45	BA	842	CLA	C3B-C2B	-2.02	1.37	1.40
45	B2	610	CLA	C1A-CHA	-2.02	1.36	1.40
48	BK	204	BCR	C8-C9	2.02	1.50	1.45
45	AA	807	CLA	C3B-C2B	-2.02	1.37	1.40
45	A6	609	CLA	CMC-C2C	-2.02	1.46	1.50
45	B1	311	CLA	CMD-C2D	-2.02	1.46	1.50
45	B5	604	CLA	CMD-C2D	-2.02	1.46	1.50
54	B5	605	CHL	CMC-C2C	2.02	1.49	1.45
45	AA	803	CLA	C3B-CAB	-2.02	1.43	1.47
48	BI	101	BCR	C1-C6	-2.02	1.51	1.53
45	AA	804	CLA	C3B-CAB	-2.02	1.43	1.47
45	B2	611	CLA	C3B-C2B	-2.02	1.37	1.40
45	B2	609	CLA	C3B-CAB	-2.02	1.43	1.47
45	AK	201	CLA	CMD-C2D	-2.01	1.46	1.50
48	AL	306	BCR	C12-C13	2.01	1.50	1.45
46	AA	843	PQN	C2-C1	2.01	1.52	1.48
45	B3	312	CLA	CMD-C2D	-2.01	1.46	1.50
56	e	301	SQD	O47-C45	-2.01	1.41	1.46
45	AA	809	CLA	CMC-C2C	-2.01	1.46	1.50
45	AA	841	CLA	C3B-CAB	-2.01	1.43	1.47
45	BB	834	CLA	C4B-CHC	-2.01	1.35	1.41
46	AB	843	PQN	C11-C3	2.01	1.54	1.51
45	AA	839	CLA	CMC-C2C	-2.01	1.46	1.50
45	AB	837	CLA	MG-ND	-2.01	2.01	2.05
45	AA	816	CLA	CMC-C2C	-2.01	1.46	1.50
45	BB	819	CLA	CMC-C2C	-2.01	1.46	1.50
45	AB	828	CLA	C3B-CAB	-2.01	1.43	1.47
45	AB	834	CLA	C3B-CAB	-2.01	1.43	1.47
45	AB	810	CLA	CMC-C2C	-2.01	1.46	1.50
45	BA	820	CLA	CMC-C2C	-2.01	1.46	1.50
45	BA	825	CLA	MG-ND	-2.01	2.01	2.05
45	AA	820	CLA	C3B-C2B	-2.01	1.37	1.40
55	A1	318	XAT	O4-C5	-2.01	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	BA	832	CLA	CMC-C2C	-2.01	1.46	1.50
45	BB	843	CLA	CMC-C2C	-2.00	1.46	1.50
45	B5	608	CLA	CMC-C2C	-2.00	1.46	1.50
45	AB	840	CLA	CMC-C2C	-2.00	1.46	1.50
45	AB	833	CLA	C4B-CHC	-2.00	1.35	1.41
45	BB	829	CLA	CMC-C2C	-2.00	1.46	1.50
45	AB	823	CLA	CMC-C2C	-2.00	1.46	1.50
45	AA	814	CLA	CMC-C2C	-2.00	1.46	1.50
45	BF	303	CLA	C3B-C2B	-2.00	1.37	1.40
45	BA	810	CLA	CMC-C2C	-2.00	1.46	1.50
45	B1	309	CLA	C3B-C2B	-2.00	1.37	1.40
48	AK	204	BCR	C19-C18	2.00	1.50	1.45
45	AA	830	CLA	C4B-CHC	-2.00	1.35	1.41
45	BA	837	CLA	MG-ND	-2.00	2.01	2.05

All (4157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BL	306	BCR	C37-C22-C21	-32.50	77.40	122.92
48	BL	306	BCR	C35-C13-C14	-31.52	78.78	122.92
48	BL	306	BCR	C34-C9-C10	-29.92	81.01	122.92
48	BG	203	BCR	C35-C13-C14	-29.72	81.29	122.92
48	BL	306	BCR	C37-C22-C23	-27.87	74.16	118.08
48	BL	306	BCR	C34-C9-C8	-26.08	76.99	118.08
48	BG	203	BCR	C12-C13-C14	25.53	158.12	118.94
48	BG	203	BCR	C35-C13-C12	-25.33	78.17	118.08
48	BL	306	BCR	C8-C9-C10	25.31	157.78	118.94
48	BL	306	BCR	C35-C13-C12	-25.07	78.58	118.08
48	BL	306	BCR	C12-C13-C14	24.99	157.29	118.94
48	BL	306	BCR	C23-C22-C21	21.15	151.40	118.94
56	BJ	104	SQD	O9-S-C6	-20.25	82.88	106.94
48	A1	319	BCR	C40-C30-C25	-13.95	87.67	110.30
48	B3	317	BCR	C40-C30-C25	-12.49	90.04	110.30
56	BJ	104	SQD	O8-S-O9	-12.10	81.70	111.27
48	B3	317	BCR	C39-C30-C25	10.57	127.44	110.30
48	A3	318	BCR	C40-C30-C25	-10.15	93.83	110.30
55	B5	615	XAT	O4-C5-C4	9.81	120.75	113.38
48	AI	102	BCR	C7-C8-C9	-9.80	111.42	126.23
48	BJ	103	BCR	C28-C27-C26	-9.80	96.58	114.08
56	BJ	104	SQD	O8-S-C6	9.79	121.34	105.74
48	A1	319	BCR	C39-C30-C25	9.45	125.63	110.30
48	BG	203	BCR	C7-C8-C9	-9.32	112.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	850	BCR	C28-C27-C26	-9.27	97.53	114.08
55	A4	316	XAT	O4-C5-C4	9.12	120.24	113.38
56	BJ	104	SQD	O7-S-C6	9.11	117.77	106.94
48	B2	617	BCR	C33-C5-C6	9.10	134.74	124.53
48	AJ	103	BCR	C28-C27-C26	-8.86	98.26	114.08
56	BJ	104	SQD	O9-S-O7	-8.81	83.46	113.95
55	A1	318	XAT	O4-C5-C4	8.64	119.87	113.38
55	A6	616	XAT	O4-C5-C4	8.61	119.85	113.38
48	BG	203	BCR	C20-C21-C22	-8.57	115.08	127.31
48	AB	844	BCR	C3-C4-C5	-8.34	99.18	114.08
55	B2	616	XAT	O4-C5-C4	7.96	119.36	113.38
48	B3	317	BCR	C30-C25-C26	-7.95	111.41	122.61
55	A3	317	XAT	O4-C5-C4	7.90	119.31	113.38
55	B1	317	XAT	O4-C5-C4	7.82	119.25	113.38
48	BL	306	BCR	C20-C21-C22	7.77	138.41	127.31
48	BL	306	BCR	C19-C18-C17	7.67	130.72	118.94
48	B3	317	BCR	C24-C23-C22	-7.65	114.67	126.23
54	B2	606	CHL	C4D-CHA-C1A	-7.47	112.16	121.25
54	A6	608	CHL	C4D-CHA-C1A	-7.36	112.29	121.25
48	BB	845	BCR	C3-C4-C5	-7.34	100.96	114.08
54	B2	614	CHL	C4D-CHA-C1A	-7.34	112.31	121.25
54	B2	607	CHL	C4D-CHA-C1A	-7.33	112.33	121.25
54	B5	607	CHL	C4D-CHA-C1A	-7.30	112.37	121.25
54	A1	308	CHL	C4D-CHA-C1A	-7.24	112.43	121.25
54	A4	306	CHL	C4D-CHA-C1A	-7.23	112.46	121.25
54	B1	308	CHL	C4D-CHA-C1A	-7.21	112.47	121.25
54	A4	304	CHL	C4D-CHA-C1A	-7.21	112.47	121.25
54	A6	602	CHL	C4D-CHA-C1A	-7.20	112.49	121.25
54	B2	601	CHL	C4D-CHA-C1A	-7.18	112.51	121.25
54	A1	303	CHL	C4D-CHA-C1A	-7.13	112.57	121.25
48	BL	306	BCR	C20-C19-C18	-7.12	106.43	126.42
54	B1	303	CHL	C4D-CHA-C1A	-7.12	112.59	121.25
55	A1	318	XAT	O24-C25-C24	7.10	118.72	113.38
54	B5	605	CHL	C4D-CHA-C1A	-7.07	112.65	121.25
54	A4	305	CHL	C4D-CHA-C1A	-7.06	112.66	121.25
48	AB	846	BCR	C37-C22-C21	-7.05	113.05	122.92
54	B5	606	CHL	C4D-CHA-C1A	-7.02	112.70	121.25
48	A3	318	BCR	C39-C30-C25	6.97	121.60	110.30
54	A4	314	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
54	A6	607	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
54	A6	606	CHL	C4D-CHA-C1A	-6.96	112.78	121.25
48	B3	317	BCR	C3-C4-C5	-6.94	101.69	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B2	605	CHL	C4D-CHA-C1A	-6.91	112.83	121.25
45	BB	842	CLA	C4A-NA-C1A	6.80	109.77	106.71
54	B3	306	CHL	C4D-CHA-C1A	-6.80	112.97	121.25
56	BJ	104	SQD	O47-C7-C8	6.78	126.11	111.50
48	AK	204	BCR	C28-C27-C26	-6.73	102.06	114.08
45	BB	828	CLA	C4A-NA-C1A	6.70	109.72	106.71
45	AB	811	CLA	C4A-NA-C1A	6.63	109.69	106.71
46	BA	843	PQN	C11-C12-C13	-6.63	115.76	126.79
48	AG	205	BCR	C3-C4-C5	-6.59	102.31	114.08
48	A3	318	BCR	C40-C30-C39	-6.58	88.33	108.53
54	A3	307	CHL	C4D-CHA-C1A	-6.54	113.29	121.25
45	A1	305	CLA	C4A-NA-C1A	6.53	109.64	106.71
48	BB	847	BCR	C37-C22-C21	-6.53	113.77	122.92
55	B3	316	XAT	O24-C25-C38	6.52	122.86	115.06
52	A4	315	LUT	C8-C7-C6	-6.43	109.13	127.20
45	BA	813	CLA	C4A-NA-C1A	6.42	109.59	106.71
48	A1	319	BCR	C40-C30-C39	-6.40	88.87	108.53
48	AA	848	BCR	C28-C27-C26	-6.36	102.72	114.08
48	BA	849	BCR	C28-C27-C26	-6.33	102.77	114.08
48	BL	301	BCR	C8-C7-C6	-6.31	109.48	127.20
48	AB	849	BCR	C24-C23-C22	-6.30	116.71	126.23
45	BB	805	CLA	C4A-NA-C1A	6.30	109.54	106.71
48	AA	845	BCR	C38-C26-C25	-6.30	117.46	124.53
48	BL	301	BCR	C34-C9-C10	-6.30	114.10	122.92
48	A6	617	BCR	C40-C30-C25	-6.28	100.12	110.30
48	AA	852	BCR	C3-C4-C5	-6.27	102.88	114.08
48	AK	204	BCR	C3-C4-C5	-6.27	102.89	114.08
55	B5	615	XAT	O24-C25-C24	6.26	118.09	113.38
45	AB	825	CLA	C4A-NA-C1A	6.25	109.52	106.71
45	AL	305	CLA	C4A-NA-C1A	6.25	109.52	106.71
45	B1	305	CLA	C4A-NA-C1A	6.25	109.51	106.71
48	B5	616	BCR	C28-C27-C26	-6.24	102.93	114.08
45	AA	841	CLA	C4A-NA-C1A	6.24	109.51	106.71
46	AB	843	PQN	C15-C13-C12	-6.22	108.53	121.12
55	B3	316	XAT	O4-C5-C4	6.19	118.03	113.38
45	AB	807	CLA	C4A-NA-C1A	6.17	109.48	106.71
48	A4	317	BCR	C28-C27-C26	-6.16	103.08	114.08
55	B1	317	XAT	O24-C25-C24	6.15	118.00	113.38
45	BB	812	CLA	C4A-NA-C1A	6.13	109.46	106.71
45	AB	804	CLA	CAC-C3C-C4C	6.10	132.73	124.81
55	B3	316	XAT	O4-C5-C18	6.10	122.36	115.06
45	AB	827	CLA	C4A-NA-C1A	6.09	109.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A1	317	LUT	C17-C1-C6	-6.09	100.43	110.30
48	AB	849	BCR	C3-C4-C5	-6.08	103.22	114.08
45	BA	840	CLA	C4A-NA-C1A	6.05	109.43	106.71
45	AA	820	CLA	C4A-NA-C1A	6.04	109.42	106.71
45	AA	813	CLA	C4A-NA-C1A	6.03	109.42	106.71
45	BA	820	CLA	C4A-NA-C1A	6.03	109.42	106.71
52	B2	615	LUT	C3-C4-C5	-6.01	99.88	111.85
45	BG	202	CLA	C4A-NA-C1A	5.99	109.40	106.71
48	BA	856	BCR	C28-C27-C26	-5.98	103.39	114.08
45	AA	828	CLA	CMB-C2B-C1B	-5.98	119.28	128.46
45	B3	305	CLA	C4A-NA-C1A	5.96	109.39	106.71
45	AF	802	CLA	C4A-NA-C1A	5.96	109.38	106.71
48	B2	617	BCR	C28-C27-C26	-5.95	103.46	114.08
45	BB	822	CLA	C4A-NA-C1A	5.94	109.38	106.71
45	AA	837	CLA	C4A-NA-C1A	5.94	109.38	106.71
46	AA	843	PQN	C15-C13-C12	-5.92	109.15	121.12
45	AB	828	CLA	C4A-NA-C1A	5.90	109.36	106.71
45	AA	806	CLA	C4A-NA-C1A	5.90	109.36	106.71
45	AF	803	CLA	C4A-NA-C1A	5.89	109.36	106.71
45	BK	203	CLA	C4A-NA-C1A	5.89	109.35	106.71
54	A6	606	CHL	O2D-CGD-CBD	5.88	121.72	111.27
45	A6	604	CLA	C4A-NA-C1A	5.87	109.34	106.71
48	BA	855	BCR	C3-C4-C5	-5.87	103.60	114.08
45	AB	824	CLA	C4A-NA-C1A	5.84	109.33	106.71
45	BA	806	CLA	C4A-NA-C1A	5.84	109.33	106.71
45	BB	820	CLA	C4A-NA-C1A	5.83	109.33	106.71
48	BI	101	BCR	C38-C26-C25	-5.82	117.99	124.53
48	AB	849	BCR	C37-C22-C23	5.82	127.24	118.08
45	AB	832	CLA	C4A-NA-C1A	5.81	109.32	106.71
52	A3	316	LUT	C17-C1-C6	-5.80	100.88	110.30
48	BG	203	BCR	C8-C9-C10	5.79	127.83	118.94
54	A4	306	CHL	C2C-C3C-C4C	-5.79	102.36	106.49
45	BB	815	CLA	CAC-C3C-C4C	5.79	132.32	124.81
48	AA	849	BCR	C34-C9-C10	-5.78	114.83	122.92
45	AB	839	CLA	C4A-NA-C1A	5.77	109.30	106.71
48	BA	856	BCR	C3-C4-C5	-5.77	103.78	114.08
45	AB	810	CLA	C4A-NA-C1A	5.76	109.30	106.71
48	B5	616	BCR	C1-C6-C5	-5.76	114.50	122.61
48	AL	306	BCR	C38-C26-C25	-5.75	118.07	124.53
45	A1	316	CLA	C4A-NA-C1A	5.73	109.28	106.71
48	BA	848	BCR	C3-C4-C5	-5.73	103.84	114.08
45	BA	812	CLA	C4A-NA-C1A	5.73	109.28	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	833	CLA	C4A-NA-C1A	5.73	109.28	106.71
45	AB	842	CLA	C4A-NA-C1A	5.71	109.28	106.71
45	AB	804	CLA	C4A-NA-C1A	5.71	109.27	106.71
54	B2	601	CHL	CHB-C4A-NA	5.71	132.40	124.51
48	AL	302	BCR	C28-C27-C26	-5.70	103.90	114.08
46	BB	844	PQN	C15-C13-C12	-5.70	109.59	121.12
48	BG	203	BCR	C33-C5-C6	-5.69	118.14	124.53
48	BA	847	BCR	C38-C26-C25	-5.68	118.15	124.53
45	BB	808	CLA	C4A-NA-C1A	5.67	109.26	106.71
45	B5	603	CLA	C4A-NA-C1A	5.67	109.25	106.71
48	B3	317	BCR	C33-C5-C6	-5.66	118.17	124.53
48	BL	306	BCR	C21-C20-C19	5.65	140.85	123.22
45	AA	834	CLA	C4A-NA-C1A	5.65	109.25	106.71
48	BB	848	BCR	C28-C27-C26	-5.64	104.00	114.08
45	BA	822	CLA	C4A-NA-C1A	5.64	109.24	106.71
45	AK	203	CLA	C4A-NA-C1A	5.63	109.24	106.71
48	BG	203	BCR	C24-C23-C22	-5.63	117.73	126.23
45	AA	833	CLA	C4A-NA-C1A	5.63	109.23	106.71
45	AB	841	CLA	C4A-NA-C1A	5.62	109.23	106.71
54	B2	614	CHL	O2D-CGD-CBD	5.61	121.24	111.27
45	AA	808	CLA	C4A-NA-C1A	5.61	109.23	106.71
45	BF	302	CLA	C4A-NA-C1A	5.61	109.23	106.71
48	AB	847	BCR	C38-C26-C25	-5.60	118.24	124.53
45	AA	828	CLA	C4A-NA-C1A	5.60	109.22	106.71
54	A4	304	CHL	CHB-C4A-NA	5.59	132.24	124.51
45	AB	837	CLA	C4A-NA-C1A	5.58	109.22	106.71
45	AA	812	CLA	C4A-NA-C1A	5.58	109.21	106.71
54	B2	607	CHL	C2C-C3C-C4C	-5.58	102.51	106.49
45	BL	302	CLA	C4A-NA-C1A	5.57	109.21	106.71
45	A1	313	CLA	C4A-NA-C1A	5.57	109.21	106.71
45	A4	313	CLA	C4A-NA-C1A	5.56	109.21	106.71
45	BA	837	CLA	C4A-NA-C1A	5.55	109.20	106.71
48	A6	617	BCR	C28-C27-C26	-5.53	104.21	114.08
45	BB	802	CLA	C4A-NA-C1A	5.53	109.19	106.71
45	BB	811	CLA	C4A-NA-C1A	5.52	109.19	106.71
54	B5	607	CHL	C4A-NA-C1A	-5.52	104.22	106.71
45	BB	840	CLA	C4A-NA-C1A	5.52	109.19	106.71
45	AB	830	CLA	C4A-NA-C1A	5.51	109.18	106.71
54	A6	606	CHL	CHB-C4A-NA	5.50	132.12	124.51
45	AA	842	CLA	C4A-NA-C1A	5.50	109.18	106.71
48	BL	306	BCR	C36-C18-C17	-5.49	115.23	122.92
45	AA	810	CLA	C4A-NA-C1A	5.49	109.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A3	318	BCR	C30-C25-C26	-5.49	114.88	122.61
48	BA	855	BCR	C32-C1-C6	-5.49	101.40	110.30
46	AB	843	PQN	C11-C12-C13	-5.48	117.67	126.79
54	B5	607	CHL	CHD-C4C-C3C	-5.48	116.42	124.98
48	A3	318	BCR	C3-C4-C5	-5.48	104.29	114.08
54	A4	305	CHL	CHB-C4A-NA	5.48	132.09	124.51
45	B2	603	CLA	C4A-NA-C1A	5.47	109.17	106.71
45	BA	814	CLA	C4A-NA-C1A	5.46	109.16	106.71
45	AK	201	CLA	C4A-NA-C1A	5.46	109.16	106.71
55	A4	316	XAT	O24-C25-C38	5.46	121.60	115.06
45	AA	814	CLA	C4A-NA-C1A	5.46	109.16	106.71
54	B2	607	CHL	CHB-C4A-NA	5.45	132.05	124.51
48	AI	102	BCR	C8-C7-C6	-5.44	111.92	127.20
54	A4	314	CHL	CHB-C4A-NA	5.44	132.03	124.51
45	A3	306	CLA	C4A-NA-C1A	5.43	109.15	106.71
48	AB	845	BCR	C34-C9-C10	-5.43	115.32	122.92
54	B2	601	CHL	CHD-C4C-C3C	-5.41	116.88	124.84
54	A1	303	CHL	C2C-C3C-C4C	-5.41	102.63	106.49
45	AG	203	CLA	C4A-NA-C1A	5.40	109.13	106.71
48	AA	845	BCR	C23-C24-C25	-5.40	112.04	127.20
48	AK	204	BCR	C32-C1-C6	-5.39	101.55	110.30
45	A6	601	CLA	C4A-NA-C1A	5.39	109.13	106.71
45	BA	833	CLA	C4A-NA-C1A	5.39	109.13	106.71
54	B5	605	CHL	C2C-C3C-C4C	-5.39	102.49	106.49
54	B1	303	CHL	CHD-C4C-C3C	-5.39	116.92	124.84
48	BL	301	BCR	C31-C1-C6	5.39	119.04	110.30
48	AA	847	BCR	C7-C8-C9	-5.38	118.11	126.23
45	AA	839	CLA	C4A-NA-C1A	5.37	109.12	106.71
54	A4	306	CHL	CHD-C4C-C3C	-5.36	116.95	124.84
54	B5	607	CHL	OBD-CAD-C3D	-5.36	115.62	128.52
54	B2	606	CHL	CHB-C4A-NA	5.36	131.92	124.51
48	A4	317	BCR	C32-C1-C6	5.36	118.99	110.30
45	BK	201	CLA	C4A-NA-C1A	5.35	109.11	106.71
45	AB	802	CLA	C4A-NA-C1A	5.35	109.11	106.71
54	A6	607	CHL	CHB-C4A-NA	5.34	131.90	124.51
45	A4	309	CLA	C4A-NA-C1A	5.34	109.11	106.71
54	B2	605	CHL	CHB-C4A-NA	5.34	131.89	124.51
45	BA	805	CLA	C4A-NA-C1A	5.33	109.10	106.71
45	BA	809	CLA	C4A-NA-C1A	5.33	109.10	106.71
45	AG	201	CLA	C4A-NA-C1A	5.33	109.10	106.71
45	BB	843	CLA	C4A-NA-C1A	5.33	109.10	106.71
48	AL	302	BCR	C31-C1-C6	5.33	118.94	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	830	CLA	C4A-NA-C1A	5.32	109.10	106.71
45	AB	814	CLA	C4A-NA-C1A	5.32	109.10	106.71
45	AB	822	CLA	C4A-NA-C1A	5.32	109.10	106.71
48	AB	848	BCR	C23-C24-C25	-5.32	112.27	127.20
54	B3	306	CHL	CHB-C4A-NA	5.32	131.86	124.51
48	B3	317	BCR	C40-C30-C39	-5.31	92.22	108.53
45	BB	826	CLA	C4A-NA-C1A	5.31	109.09	106.71
45	BA	841	CLA	C4-C3-C5	5.31	124.21	115.27
48	BL	301	BCR	C28-C27-C26	-5.31	104.60	114.08
54	B5	606	CHL	CHB-C4A-NA	5.31	131.85	124.51
45	A1	310	CLA	C4A-NA-C1A	5.30	109.09	106.71
54	B5	605	CHL	CHB-C4A-NA	5.30	131.84	124.51
48	AA	847	BCR	C35-C13-C14	-5.30	115.50	122.92
45	AB	821	CLA	C4A-NA-C1A	5.29	109.08	106.71
45	AB	812	CLA	C4A-NA-C1A	5.29	109.08	106.71
45	BB	836	CLA	C4A-NA-C1A	5.29	109.08	106.71
48	B3	317	BCR	C1-C6-C5	-5.29	115.17	122.61
48	AA	847	BCR	C28-C27-C26	-5.29	104.64	114.08
45	BA	839	CLA	C4A-NA-C1A	5.28	109.08	106.71
48	A4	317	BCR	C1-C6-C5	-5.28	115.18	122.61
54	A6	602	CHL	C2C-C3C-C4C	-5.27	102.73	106.49
48	BB	849	BCR	C23-C24-C25	-5.26	112.42	127.20
54	B5	606	CHL	C4C-C3C-C2C	-5.26	102.25	107.07
54	A1	303	CHL	CHD-C4C-C3C	-5.26	117.11	124.84
45	AJ	102	CLA	C4A-NA-C1A	5.26	109.07	106.71
45	BA	819	CLA	C4A-NA-C1A	5.25	109.06	106.71
54	B2	605	CHL	O2D-CGD-CBD	5.25	120.59	111.27
54	A4	304	CHL	C1B-CHB-C4A	-5.25	119.73	130.12
45	BB	804	CLA	C4A-NA-C1A	5.24	109.06	106.71
54	B2	614	CHL	CHB-C4A-NA	5.24	131.76	124.51
54	B2	607	CHL	CHD-C4C-C3C	-5.24	117.14	124.84
45	AA	825	CLA	C4A-NA-C1A	5.24	109.06	106.71
45	BA	824	CLA	C4A-NA-C1A	5.24	109.06	106.71
45	BB	838	CLA	C4A-NA-C1A	5.24	109.06	106.71
48	AI	101	BCR	C38-C26-C25	-5.24	118.65	124.53
45	BA	815	CLA	C4A-NA-C1A	5.24	109.06	106.71
48	AA	847	BCR	C31-C1-C6	5.23	118.78	110.30
54	A4	306	CHL	CHB-C4A-NA	5.23	131.74	124.51
54	B5	606	CHL	C1B-CHB-C4A	-5.23	119.77	130.12
45	BB	813	CLA	C4A-NA-C1A	5.22	109.06	106.71
45	A1	306	CLA	C4A-NA-C1A	5.22	109.05	106.71
54	B1	303	CHL	C2C-C3C-C4C	-5.22	102.77	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B1	308	CHL	C1B-CHB-C4A	-5.22	119.78	130.12
45	BA	817	CLA	C4A-NA-C1A	5.22	109.05	106.71
45	BA	836	CLA	C4A-NA-C1A	5.22	109.05	106.71
45	AA	811	CLA	C4A-NA-C1A	5.22	109.05	106.71
54	A4	306	CHL	OBD-CAD-C3D	-5.21	115.98	128.52
45	AA	822	CLA	C4A-NA-C1A	5.21	109.05	106.71
52	B3	315	LUT	C17-C1-C6	-5.21	101.85	110.30
54	B2	606	CHL	C1B-CHB-C4A	-5.20	119.81	130.12
54	A4	305	CHL	C1B-C2B-C3B	-5.20	102.08	106.92
54	A3	307	CHL	CHD-C4C-C3C	-5.20	117.20	124.84
54	B1	308	CHL	C2C-C3C-C4C	-5.17	102.80	106.49
45	AB	808	CLA	C4A-NA-C1A	5.17	109.03	106.71
45	BF	301	CLA	C4A-NA-C1A	5.17	109.03	106.71
48	BG	203	BCR	C15-C16-C17	-5.17	112.89	123.47
48	BG	203	BCR	C15-C14-C13	-5.17	119.94	127.31
54	A1	308	CHL	C1B-CHB-C4A	-5.15	119.91	130.12
54	A1	308	CHL	CHB-C4A-NA	5.15	131.63	124.51
45	AA	805	CLA	C4A-NA-C1A	5.14	109.02	106.71
55	B3	316	XAT	C18-C5-C6	-5.14	113.65	122.26
45	AF	804	CLA	C4A-NA-C1A	5.14	109.02	106.71
54	A4	314	CHL	C1B-C2B-C3B	-5.13	102.15	106.92
54	B1	303	CHL	CHB-C4A-NA	5.13	131.61	124.51
48	BB	845	BCR	C30-C25-C26	-5.13	115.39	122.61
45	BA	841	CLA	C4A-NA-C1A	5.13	109.01	106.71
55	A3	317	XAT	O24-C25-C38	5.12	121.19	115.06
45	BA	827	CLA	C4A-NA-C1A	5.12	109.01	106.71
45	B5	612	CLA	C4A-NA-C1A	5.11	109.00	106.71
54	B2	614	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
45	AA	804	CLA	C4A-NA-C1A	5.10	109.00	106.71
54	A3	307	CHL	CHB-C4A-NA	5.10	131.57	124.51
54	B3	306	CHL	CHD-C4C-C3C	-5.09	117.35	124.84
45	AB	838	CLA	C4A-NA-C1A	5.09	109.00	106.71
54	B1	308	CHL	CHD-C4C-C3C	-5.09	117.36	124.84
48	BB	803	BCR	C28-C27-C26	-5.09	104.98	114.08
48	AA	846	BCR	C36-C18-C19	5.09	126.10	118.08
45	BA	834	CLA	C4A-NA-C1A	5.09	108.99	106.71
45	BB	839	CLA	C4A-NA-C1A	5.09	108.99	106.71
54	B5	607	CHL	C2C-C3C-C4C	-5.08	102.71	106.49
48	BB	846	BCR	C34-C9-C10	-5.08	115.80	122.92
54	B2	607	CHL	C2A-C1A-CHA	-5.08	114.97	123.86
45	BA	842	CLA	C4A-NA-C1A	5.08	108.99	106.71
48	BB	848	BCR	C3-C4-C5	-5.08	105.00	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A1	303	CHL	OBD-CAD-C3D	-5.08	116.30	128.52
48	B3	317	BCR	C27-C26-C25	-5.08	115.36	122.73
54	A6	606	CHL	C2C-C3C-C4C	-5.08	102.72	106.49
54	A4	305	CHL	C1B-CHB-C4A	-5.07	120.08	130.12
45	AA	827	CLA	C4A-NA-C1A	5.07	108.98	106.71
54	A4	306	CHL	C2A-C1A-CHA	-5.07	115.00	123.86
45	B1	304	CLA	C4A-NA-C1A	5.07	108.98	106.71
45	AA	815	CLA	C4A-NA-C1A	5.06	108.98	106.71
45	B1	313	CLA	C4A-NA-C1A	5.06	108.98	106.71
54	B5	605	CHL	C2A-C1A-CHA	-5.05	115.03	123.86
54	A4	314	CHL	C1B-CHB-C4A	-5.05	120.12	130.12
45	BB	834	CLA	C4A-NA-C1A	5.05	108.97	106.71
45	B5	611	CLA	C4A-NA-C1A	5.04	108.97	106.71
45	B3	304	CLA	C4A-NA-C1A	5.03	108.97	106.71
54	A4	304	CHL	C2A-C1A-CHA	-5.03	115.06	123.86
54	A1	303	CHL	CHB-C4A-NA	5.03	131.46	124.51
45	AA	821	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
54	A1	308	CHL	C2C-C3C-C4C	-5.02	102.91	106.49
48	BB	846	BCR	C30-C25-C26	-5.02	115.55	122.61
45	A3	312	CLA	C4A-NA-C1A	5.02	108.96	106.71
45	BA	804	CLA	C4A-NA-C1A	5.01	108.96	106.71
45	BA	828	CLA	C4A-NA-C1A	5.00	108.96	106.71
48	BF	304	BCR	C28-C27-C26	-5.00	105.14	114.08
54	B2	601	CHL	C2C-C3C-C4C	-4.99	102.93	106.49
48	AJ	103	BCR	C39-C30-C25	-4.99	102.21	110.30
45	A4	302	CLA	C4A-NA-C1A	4.99	108.95	106.71
48	BL	305	BCR	C28-C27-C26	-4.98	105.18	114.08
54	A6	602	CHL	CHB-C4A-NA	4.98	131.40	124.51
45	A6	613	CLA	C4A-NA-C1A	4.97	108.94	106.71
45	BA	825	CLA	C4A-NA-C1A	4.96	108.94	106.71
54	B2	605	CHL	CHD-C4C-C3C	-4.96	117.23	124.98
45	B1	309	CLA	C4A-NA-C1A	4.96	108.94	106.71
54	B1	308	CHL	CHB-C4A-NA	4.96	131.37	124.51
45	AB	819	CLA	C4A-NA-C1A	4.96	108.94	106.71
54	A6	607	CHL	C2C-C3C-C4C	-4.96	102.95	106.49
54	A6	606	CHL	CHD-C4C-C3C	-4.96	117.24	124.98
45	A1	307	CLA	C4A-NA-C1A	4.96	108.93	106.71
48	AI	102	BCR	C27-C26-C25	-4.95	115.54	122.73
54	B2	601	CHL	O2D-CGD-CBD	4.95	120.07	111.27
54	B5	606	CHL	C1B-C2B-C3B	-4.95	102.31	106.92
54	A6	602	CHL	CHD-C4C-C3C	-4.95	117.56	124.84
54	B2	614	CHL	C2A-C1A-CHA	-4.95	115.21	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B2	607	CHL	OBD-CAD-C3D	-4.95	116.62	128.52
54	B3	306	CHL	C1B-CHB-C4A	-4.94	120.33	130.12
45	AG	204	CLA	C4A-NA-C1A	4.94	108.93	106.71
48	AF	805	BCR	C35-C13-C14	-4.94	116.01	122.92
54	A4	305	CHL	O2D-CGD-CBD	4.94	120.04	111.27
45	BB	837	CLA	C4A-NA-C1A	4.93	108.92	106.71
45	AB	813	CLA	C4A-NA-C1A	4.92	108.92	106.71
45	A4	310	CLA	C4A-NA-C1A	4.92	108.92	106.71
45	AB	809	CLA	C4A-NA-C1A	4.92	108.92	106.71
48	B5	616	BCR	C3-C4-C5	-4.92	105.30	114.08
54	A3	307	CHL	OBD-CAD-C3D	-4.91	116.69	128.52
45	AA	821	CLA	C4A-NA-C1A	4.91	108.91	106.71
48	AI	102	BCR	C33-C5-C6	4.90	130.03	124.53
48	BK	204	BCR	C3-C4-C5	-4.90	105.33	114.08
45	BB	831	CLA	C4A-NA-C1A	4.90	108.91	106.71
54	A6	607	CHL	C1B-CHB-C4A	-4.90	120.42	130.12
54	B1	303	CHL	C2A-C1A-CHA	-4.90	115.30	123.86
48	BA	851	BCR	C37-C22-C23	4.90	125.79	118.08
54	A4	305	CHL	CHD-C4C-C3C	-4.89	117.65	124.84
45	BJ	102	CLA	C4A-NA-C1A	4.89	108.91	106.71
54	B2	605	CHL	C1B-CHB-C4A	-4.89	120.43	130.12
54	A4	304	CHL	C2C-C3C-C4C	-4.89	102.86	106.49
45	BA	811	CLA	C4A-NA-C1A	4.89	108.90	106.71
45	BA	802	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
54	A3	307	CHL	C1B-CHB-C4A	-4.88	120.46	130.12
54	A6	606	CHL	C2A-C1A-CHA	-4.88	115.33	123.86
54	A4	304	CHL	CHD-C4C-C3C	-4.87	117.36	124.98
45	BA	808	CLA	C4A-NA-C1A	4.87	108.90	106.71
45	BF	303	CLA	C4A-NA-C1A	4.86	108.89	106.71
45	BB	823	CLA	C4A-NA-C1A	4.86	108.89	106.71
48	AA	852	BCR	C36-C18-C19	4.86	125.73	118.08
45	B3	311	CLA	C4A-NA-C1A	4.85	108.89	106.71
45	AA	817	CLA	C4A-NA-C1A	4.85	108.89	106.71
48	BG	203	BCR	C20-C19-C18	-4.85	112.80	126.42
47	B3	318	LHG	O7-C7-C8	4.85	120.01	111.09
48	AB	847	BCR	C28-C27-C26	-4.85	105.42	114.08
45	AA	828	CLA	CMB-C2B-C3B	4.85	133.75	124.68
45	BB	829	CLA	C4A-NA-C1A	4.84	108.88	106.71
45	A4	311	CLA	C4A-NA-C1A	4.84	108.88	106.71
54	B1	303	CHL	OBD-CAD-C3D	-4.84	116.88	128.52
54	B5	607	CHL	C2A-C1A-CHA	-4.83	115.41	123.86
48	BA	848	BCR	C36-C18-C19	4.83	125.69	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A4	314	CHL	CHD-C4C-C3C	-4.83	117.74	124.84
45	A3	305	CLA	C4A-NA-C1A	4.83	108.88	106.71
54	B5	606	CHL	CHD-C4C-C3C	-4.83	117.44	124.98
48	BL	306	BCR	C15-C14-C13	-4.83	120.42	127.31
54	A6	608	CHL	OBD-CAD-C3D	-4.82	116.91	128.52
45	BB	806	CLA	C4A-NA-C1A	4.82	108.87	106.71
45	AA	816	CLA	C4A-NA-C1A	4.82	108.87	106.71
54	A6	607	CHL	OBD-CAD-C3D	-4.81	116.94	128.52
45	A1	314	CLA	C4A-NA-C1A	4.81	108.87	106.71
45	A3	311	CLA	C4A-NA-C1A	4.81	108.87	106.71
45	AB	801	CLA	C4A-NA-C1A	4.80	108.86	106.71
54	A6	608	CHL	C4A-NA-C1A	-4.80	104.55	106.71
54	A6	602	CHL	C1B-CHB-C4A	-4.80	120.61	130.12
54	A6	606	CHL	C1B-CHB-C4A	-4.80	120.61	130.12
54	B1	308	CHL	OBD-CAD-C3D	-4.80	116.98	128.52
48	AA	852	BCR	C30-C25-C26	-4.80	115.86	122.61
54	A6	608	CHL	CHB-C4A-NA	4.79	131.14	124.51
54	B5	605	CHL	C1B-CHB-C4A	-4.79	120.63	130.12
54	B2	607	CHL	C1B-CHB-C4A	-4.79	120.64	130.12
45	AB	836	CLA	C4A-NA-C1A	4.78	108.85	106.71
54	B5	607	CHL	CHB-C4A-NA	4.77	131.11	124.51
54	B2	601	CHL	C1B-CHB-C4A	-4.77	120.67	130.12
45	BA	834	CLA	C4-C3-C5	4.77	123.29	115.27
54	B2	601	CHL	OBD-CAD-C3D	-4.77	117.05	128.52
54	B2	606	CHL	OBD-CAD-C3D	-4.76	117.06	128.52
54	B3	306	CHL	OBD-CAD-C3D	-4.76	117.06	128.52
54	A6	608	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
54	A4	306	CHL	CAC-C3C-C4C	4.76	130.99	124.81
45	AA	802	CLA	CMB-C2B-C1B	-4.76	121.15	128.46
45	AA	818	CLA	C4A-NA-C1A	4.76	108.84	106.71
48	BB	847	BCR	C34-C9-C10	-4.75	116.26	122.92
54	A4	314	CHL	OBD-CAD-C3D	-4.75	117.08	128.52
56	BJ	104	SQD	C45-O47-C7	-4.75	106.10	117.79
48	BG	203	BCR	C19-C18-C17	4.74	126.21	118.94
54	A1	308	CHL	OBD-CAD-C3D	-4.74	117.12	128.52
45	BB	817	CLA	C4A-NA-C1A	4.74	108.83	106.71
55	A6	616	XAT	O24-C25-C24	4.73	116.94	113.38
54	B5	606	CHL	C1D-ND-C4D	4.73	109.70	106.33
54	A4	306	CHL	C1B-CHB-C4A	-4.73	120.75	130.12
54	A4	305	CHL	OBD-CAD-C3D	-4.72	117.15	128.52
45	BB	820	CLA	C4-C3-C5	4.72	123.21	115.27
54	B2	605	CHL	C2A-C1A-CHA	-4.71	115.62	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A6	602	CHL	OBD-CAD-C3D	-4.71	117.19	128.52
55	A1	318	XAT	C6-C7-C8	-4.71	116.04	125.99
54	A6	607	CHL	CHD-C4C-C3C	-4.71	117.92	124.84
45	AB	803	CLA	C4A-NA-C1A	4.70	108.82	106.71
54	B2	606	CHL	C1D-ND-C4D	4.70	109.67	106.33
48	BB	846	BCR	C27-C26-C25	-4.70	115.91	122.73
48	BA	855	BCR	C37-C22-C23	4.70	125.48	118.08
54	A4	314	CHL	C2C-C3C-C4C	-4.69	103.14	106.49
45	B3	302	CLA	C4A-NA-C1A	4.69	108.82	106.71
45	AA	803	CLA	C4A-NA-C1A	4.69	108.81	106.71
54	B2	614	CHL	OBD-CAD-C3D	-4.69	117.23	128.52
46	BA	843	PQN	C15-C13-C12	-4.69	111.63	121.12
54	A6	602	CHL	C2A-C1A-CHA	-4.69	115.66	123.86
54	B5	606	CHL	OBD-CAD-C3D	-4.69	117.23	128.52
54	A1	308	CHL	C1D-ND-C4D	4.69	109.66	106.33
54	B2	614	CHL	C2C-C3C-C4C	-4.69	103.15	106.49
45	AA	801	CLA	C4A-NA-C1A	4.68	108.81	106.71
54	B2	614	CHL	C1B-CHB-C4A	-4.67	120.87	130.12
45	AB	834	CLA	C4A-NA-C1A	4.67	108.81	106.71
48	AB	846	BCR	C34-C9-C10	-4.66	116.39	122.92
45	BA	821	CLA	C4A-NA-C1A	4.66	108.80	106.71
48	A4	317	BCR	C40-C30-C25	-4.65	102.75	110.30
45	B3	310	CLA	C4A-NA-C1A	4.65	108.80	106.71
54	B2	606	CHL	C2C-C3C-C4C	-4.65	103.18	106.49
54	B2	605	CHL	OBD-CAD-C3D	-4.64	117.35	128.52
54	A6	606	CHL	OBD-CAD-C3D	-4.64	117.36	128.52
45	A3	303	CLA	C4A-NA-C1A	4.64	108.79	106.71
45	AA	835	CLA	C4A-NA-C1A	4.63	108.79	106.71
45	AB	816	CLA	C4A-NA-C1A	4.63	108.79	106.71
55	A6	616	XAT	C6-C7-C8	-4.63	116.21	125.99
48	BJ	103	BCR	C36-C18-C19	4.63	125.37	118.08
45	AA	831	CLA	C4A-NA-C1A	4.63	108.79	106.71
48	A4	317	BCR	C23-C24-C25	-4.62	114.21	127.20
46	AA	843	PQN	C11-C12-C13	-4.61	119.11	126.79
45	A1	315	CLA	C4A-NA-C1A	4.61	108.78	106.71
45	AA	836	CLA	C4A-NA-C1A	4.61	108.78	106.71
45	BB	814	CLA	C4A-NA-C1A	4.61	108.78	106.71
45	B5	601	CLA	C4A-NA-C1A	4.60	108.78	106.71
48	BB	848	BCR	C38-C26-C25	-4.60	119.36	124.53
52	B2	615	LUT	C39-C29-C28	4.60	125.32	118.08
54	A4	314	CHL	C2A-C1A-CHA	-4.60	115.82	123.86
48	AJ	101	BCR	C3-C4-C5	-4.59	105.88	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A1	319	BCR	C29-C30-C25	4.59	117.55	110.48
54	A6	607	CHL	CAC-C3C-C4C	4.59	130.77	124.81
54	A1	308	CHL	CHD-C4C-C3C	-4.59	118.10	124.84
45	A3	304	CLA	C4A-NA-C1A	4.59	108.77	106.71
54	B5	607	CHL	C1B-CHB-C4A	-4.58	121.04	130.12
48	AA	852	BCR	C28-C27-C26	-4.58	105.89	114.08
45	AA	829	CLA	C4A-NA-C1A	4.58	108.76	106.71
54	B5	605	CHL	CHD-C4C-C3C	-4.58	117.83	124.98
45	AA	809	CLA	C4A-NA-C1A	4.58	108.76	106.71
45	BA	818	CLA	C4A-NA-C1A	4.57	108.76	106.71
48	BG	203	BCR	C31-C1-C6	-4.57	102.88	110.30
54	A1	303	CHL	C2A-C1A-CHA	-4.56	115.89	123.86
54	B5	606	CHL	O2D-CGD-CBD	4.56	119.37	111.27
54	A3	307	CHL	C2A-C1A-CHA	-4.55	115.90	123.86
48	BB	848	BCR	C37-C22-C23	4.55	125.25	118.08
45	BA	838	CLA	C4A-NA-C1A	4.55	108.75	106.71
45	A6	603	CLA	C4A-NA-C1A	4.55	108.75	106.71
48	BB	845	BCR	C36-C18-C19	4.55	125.24	118.08
55	B2	616	XAT	O24-C25-C24	4.54	116.79	113.38
54	B2	605	CHL	C4A-NA-C1A	-4.53	104.67	106.71
45	AB	829	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
45	AH	201	CLA	C4A-NA-C1A	4.53	108.74	106.71
45	A3	310	CLA	C4A-NA-C1A	4.52	108.74	106.71
54	A1	303	CHL	C1B-CHB-C4A	-4.52	121.17	130.12
54	A4	304	CHL	OBD-CAD-C3D	-4.51	117.67	128.52
45	A4	303	CLA	C4A-NA-C1A	4.51	108.73	106.71
54	B1	303	CHL	C1B-CHB-C4A	-4.51	121.19	130.12
48	BK	204	BCR	C36-C18-C19	4.50	125.17	118.08
45	AA	840	CLA	C4A-NA-C1A	4.50	108.73	106.71
48	AJ	101	BCR	C34-C9-C8	4.49	125.16	118.08
48	AB	847	BCR	C36-C18-C19	4.49	125.16	118.08
45	AK	202	CLA	C4A-NA-C1A	4.49	108.73	106.71
45	BB	807	CLA	C4A-NA-C1A	4.49	108.73	106.71
48	BG	203	BCR	C34-C9-C10	-4.49	116.63	122.92
48	BJ	101	BCR	C8-C7-C6	-4.48	114.61	127.20
54	B3	306	CHL	C1D-ND-C4D	4.48	109.52	106.33
47	A3	319	LHG	O7-C7-C8	4.48	119.34	111.09
54	B5	607	CHL	O2D-CGD-CBD	4.48	119.23	111.27
55	A6	616	XAT	C18-C5-C6	-4.48	114.76	122.26
45	BB	818	CLA	C4A-NA-C1A	4.48	108.72	106.71
48	A6	617	BCR	C3-C4-C5	-4.48	106.08	114.08
48	B5	616	BCR	C37-C22-C23	4.48	125.13	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B2	612	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
54	A1	308	CHL	C2A-C1A-CHA	-4.47	116.04	123.85
45	B2	611	CLA	C4A-NA-C1A	4.47	108.72	106.71
45	BL	304	CLA	C4A-NA-C1A	4.47	108.72	106.71
54	B2	607	CHL	O2D-CGD-CBD	4.47	119.21	111.27
54	B2	605	CHL	C2C-C3C-C4C	-4.47	103.17	106.49
48	AL	306	BCR	C33-C5-C6	-4.47	119.51	124.53
45	A4	301	CLA	C4A-NA-C1A	4.47	108.71	106.71
45	BK	202	CLA	C4A-NA-C1A	4.46	108.71	106.71
54	A6	607	CHL	O2D-CGD-CBD	4.46	119.19	111.27
54	B5	605	CHL	C4A-NA-C1A	-4.46	104.70	106.71
45	BB	809	CLA	C4A-NA-C1A	4.45	108.71	106.71
45	BB	811	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
54	B3	306	CHL	C2A-C1A-CHA	-4.44	116.09	123.86
54	A6	608	CHL	O2D-CGD-CBD	4.43	119.14	111.27
45	BB	833	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
54	A4	306	CHL	O2D-CGD-CBD	4.43	119.13	111.27
45	BH	201	CLA	C4A-NA-C1A	4.42	108.69	106.71
45	AB	819	CLA	C4-C3-C5	4.42	122.70	115.27
48	AB	848	BCR	C33-C5-C6	-4.42	119.57	124.53
48	AI	101	BCR	C36-C18-C19	4.41	125.03	118.08
48	BF	304	BCR	C35-C13-C14	-4.41	116.74	122.92
45	B3	301	CLA	C4A-NA-C1A	4.41	108.69	106.71
48	BL	305	BCR	C27-C26-C25	-4.41	116.33	122.73
54	A3	307	CHL	O2D-CGD-CBD	4.41	119.10	111.27
54	A4	305	CHL	C1D-ND-C4D	4.41	109.47	106.33
54	B5	605	CHL	OBD-CAD-C3D	-4.41	117.92	128.52
48	AL	302	BCR	C8-C7-C6	-4.40	114.83	127.20
45	BA	832	CLA	C4A-NA-C1A	4.40	108.69	106.71
48	BL	305	BCR	C37-C22-C23	4.40	125.01	118.08
48	AJ	101	BCR	C32-C1-C6	-4.40	103.16	110.30
54	A6	607	CHL	C2A-C1A-CHA	-4.39	116.17	123.86
54	B2	601	CHL	C2A-C1A-CHA	-4.39	116.17	123.86
48	BL	305	BCR	C40-C30-C25	-4.39	103.18	110.30
45	AA	838	CLA	C4A-NA-C1A	4.39	108.68	106.71
45	B3	309	CLA	C4A-NA-C1A	4.39	108.68	106.71
45	AB	819	CLA	CMB-C2B-C1B	-4.38	121.73	128.46
54	B2	606	CHL	CAC-C3C-C4C	4.38	130.49	124.81
45	AB	815	CLA	C4A-NA-C1A	4.38	108.67	106.71
54	A6	608	CHL	CAC-C3C-C4C	4.38	130.49	124.81
45	BA	802	CLA	CMB-C2B-C3B	4.37	132.86	124.68
48	BB	846	BCR	C37-C22-C23	4.37	124.96	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	801	CLA	C4A-NA-C1A	4.37	108.67	106.71
48	BL	305	BCR	C31-C1-C6	4.37	117.38	110.30
48	AA	845	BCR	C32-C1-C6	-4.36	103.22	110.30
48	BL	306	BCR	C15-C16-C17	-4.36	114.55	123.47
45	AB	827	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
45	A3	313	CLA	C4A-NA-C1A	4.35	108.66	106.71
48	BB	849	BCR	C36-C18-C19	4.35	124.93	118.08
45	BA	803	CLA	C4A-NA-C1A	4.35	108.66	106.71
48	BA	856	BCR	C36-C18-C19	4.35	124.92	118.08
54	B2	606	CHL	CHD-C4C-C3C	-4.34	118.46	124.84
45	AA	802	CLA	CMB-C2B-C3B	4.34	132.80	124.68
48	AA	846	BCR	C32-C1-C6	4.33	117.33	110.30
48	AA	846	BCR	C24-C23-C22	-4.33	119.69	126.23
48	AA	846	BCR	C3-C4-C5	-4.33	106.35	114.08
45	B5	604	CLA	C4A-NA-C1A	4.33	108.65	106.71
45	A6	605	CLA	C4A-NA-C1A	4.32	108.65	106.71
45	B1	312	CLA	C4A-NA-C1A	4.32	108.65	106.71
45	A3	308	CLA	C4A-NA-C1A	4.32	108.65	106.71
48	BB	803	BCR	C35-C13-C12	4.32	124.88	118.08
45	B1	306	CLA	C4A-NA-C1A	4.31	108.64	106.71
48	AL	302	BCR	C34-C9-C10	-4.31	116.88	122.92
45	B2	612	CLA	C4A-NA-C1A	4.31	108.64	106.71
54	B1	308	CHL	C1D-ND-C4D	4.31	109.40	106.33
48	AG	205	BCR	C36-C18-C17	-4.30	116.90	122.92
45	A6	613	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
45	B3	313	CLA	C4A-NA-C1A	4.30	108.64	106.71
45	AB	837	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
46	AB	843	PQN	C14-C13-C12	-4.29	112.67	123.68
55	A3	317	XAT	C6-C7-C8	-4.29	116.92	125.99
48	BA	856	BCR	C27-C26-C25	-4.29	116.50	122.73
54	A6	608	CHL	C1D-ND-C4D	4.29	109.38	106.33
48	BA	850	BCR	C37-C22-C23	4.29	124.83	118.08
48	AA	852	BCR	C37-C22-C23	4.28	124.83	118.08
45	AB	823	CLA	C4A-NA-C1A	4.28	108.63	106.71
54	A6	608	CHL	C1B-CHB-C4A	-4.28	121.64	130.12
52	B3	315	LUT	C3-C4-C5	-4.28	103.33	111.85
52	AF	806	LUT	C40-C33-C32	4.28	124.82	118.08
54	B3	306	CHL	O2D-CGD-CBD	4.27	118.86	111.27
48	AJ	103	BCR	C36-C18-C19	4.27	124.81	118.08
45	AA	819	CLA	C4A-NA-C1A	4.27	108.63	106.71
55	A6	616	XAT	C39-C29-C28	4.27	124.80	118.08
48	AB	844	BCR	C34-C9-C8	4.26	124.80	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	815	CLA	CMB-C2B-C1B	-4.26	121.91	128.46
45	AA	829	CLA	C4-C3-C5	4.26	122.44	115.27
48	AJ	103	BCR	C32-C1-C6	-4.26	103.39	110.30
48	AG	205	BCR	C28-C27-C26	-4.26	106.47	114.08
54	A4	314	CHL	C1D-ND-C4D	4.26	109.36	106.33
45	BA	841	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
45	B3	307	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
45	BB	810	CLA	C4A-NA-C1A	4.25	108.62	106.71
48	BG	203	BCR	C36-C18-C17	-4.25	116.97	122.92
48	AF	805	BCR	C37-C22-C23	4.25	124.77	118.08
54	A3	307	CHL	CMC-C2C-C1C	4.25	131.51	125.04
54	A1	308	CHL	CAC-C3C-C4C	4.25	130.32	124.81
48	A1	319	BCR	C1-C6-C5	-4.25	116.63	122.61
48	AL	302	BCR	C38-C26-C25	-4.24	119.76	124.53
48	A4	317	BCR	C3-C4-C5	-4.24	106.51	114.08
45	AB	840	CLA	C4A-NA-C1A	4.24	108.61	106.71
45	B2	604	CLA	C4A-NA-C1A	4.24	108.61	106.71
54	A4	305	CHL	CHC-C1C-NC	4.23	130.62	124.20
55	B2	616	XAT	C6-C7-C8	-4.22	117.06	125.99
45	AB	817	CLA	C4A-NA-C1A	4.22	108.61	106.71
48	AA	848	BCR	C37-C22-C23	4.22	124.72	118.08
48	AF	801	BCR	C37-C22-C23	4.22	124.72	118.08
54	A6	608	CHL	CMC-C2C-C1C	4.22	131.46	125.04
45	AA	824	CLA	C4-C3-C5	4.22	122.36	115.27
55	B1	317	XAT	C18-C5-C6	-4.21	115.20	122.26
48	BB	845	BCR	C27-C26-C25	-4.21	116.62	122.73
45	AA	832	CLA	C4A-NA-C1A	4.20	108.60	106.71
45	AA	825	CLA	CMB-C2B-C1B	-4.20	122.00	128.46
48	BB	846	BCR	C36-C18-C19	4.20	124.70	118.08
48	BL	305	BCR	C36-C18-C19	4.20	124.69	118.08
45	A3	314	CLA	C4A-NA-C1A	4.20	108.59	106.71
48	B5	616	BCR	C30-C25-C26	-4.20	116.70	122.61
45	AA	804	CLA	CMB-C2B-C1B	-4.19	122.02	128.46
48	AJ	101	BCR	C37-C22-C23	4.19	124.68	118.08
52	A6	615	LUT	C8-C7-C6	-4.19	115.43	127.20
48	A6	617	BCR	C37-C22-C23	4.19	124.68	118.08
45	AA	807	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
48	AA	849	BCR	C39-C30-C25	-4.19	103.51	110.30
52	B5	614	LUT	C39-C29-C28	4.19	124.67	118.08
45	A4	312	CLA	C4A-NA-C1A	4.18	108.59	106.71
45	BA	830	CLA	C4A-NA-C1A	4.18	108.58	106.71
48	AA	847	BCR	C1-C6-C5	-4.18	116.73	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AL	302	BCR	C3-C4-C5	-4.18	106.62	114.08
45	AB	805	CLA	CMB-C2B-C1B	-4.17	122.05	128.46
55	A3	317	XAT	C38-C25-C26	-4.17	115.28	122.26
54	A3	307	CHL	C1D-ND-C4D	4.16	109.29	106.33
52	A1	317	LUT	C3-C4-C5	-4.15	103.58	111.85
54	B5	607	CHL	C1D-CHD-C4C	-4.15	117.10	126.06
48	AI	102	BCR	C40-C30-C25	-4.15	103.57	110.30
47	F	801	LHG	O4-P-O5	4.15	132.75	112.24
45	BB	830	CLA	CMB-C2B-C1B	-4.15	122.09	128.46
48	AJ	103	BCR	C31-C1-C6	4.15	117.02	110.30
45	BA	838	CLA	C4-C3-C5	4.14	122.24	115.27
48	A4	317	BCR	C36-C18-C19	4.14	124.60	118.08
48	BA	851	BCR	C34-C9-C10	-4.14	117.13	122.92
45	BK	203	CLA	CMB-C2B-C1B	-4.14	122.11	128.46
45	B3	308	CLA	C4A-NA-C1A	4.13	108.56	106.71
54	B2	607	CHL	C4A-NA-C1A	-4.13	104.85	106.71
54	B2	605	CHL	C1D-ND-C4D	4.13	109.27	106.33
48	BB	845	BCR	C28-C27-C26	-4.13	106.70	114.08
45	AA	802	CLA	C4A-NA-C1A	4.13	108.56	106.71
45	BA	816	CLA	C4A-NA-C1A	4.13	108.56	106.71
45	BA	807	CLA	C4A-NA-C1A	4.12	108.56	106.71
45	BB	824	CLA	C4A-NA-C1A	4.12	108.56	106.71
52	AF	806	LUT	C39-C29-C28	4.11	124.56	118.08
54	A4	305	CHL	C2A-C1A-CHA	-4.11	116.67	123.86
45	BB	805	CLA	CHB-C4A-NA	4.11	130.20	124.51
48	AB	844	BCR	C38-C26-C25	-4.11	119.91	124.53
55	B2	616	XAT	O4-C5-C18	4.11	119.98	115.06
45	AA	837	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
45	B2	604	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
45	BA	822	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
54	B2	607	CHL	CAC-C3C-C4C	4.10	130.13	124.81
45	BB	841	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
45	A1	313	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
54	B5	606	CHL	C1D-CHD-C4C	-4.09	117.23	126.06
45	B3	314	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
54	B5	606	CHL	C2A-C1A-CHA	-4.09	116.71	123.86
48	BB	803	BCR	C36-C18-C19	4.09	124.52	118.08
45	BA	812	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
48	BA	849	BCR	C1-C6-C5	-4.09	116.86	122.61
45	A1	315	CLA	CAB-C3B-C4B	-4.09	122.18	128.46
45	BF	301	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
45	BA	810	CLA	C4A-NA-C1A	4.08	108.54	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AB	847	BCR	C37-C22-C23	4.08	124.51	118.08
47	a	501	LHG	O4-P-O5	4.08	132.42	112.24
45	BB	825	CLA	C4A-NA-C1A	4.08	108.54	106.71
48	BB	848	BCR	C36-C18-C19	4.08	124.51	118.08
48	BI	101	BCR	C33-C5-C6	-4.08	119.95	124.53
45	A4	302	CLA	CAB-C3B-C4B	-4.08	122.19	128.46
48	AA	852	BCR	C27-C26-C25	-4.08	116.81	122.73
48	BI	101	BCR	C36-C18-C19	4.08	124.50	118.08
54	B3	306	CHL	CMC-C2C-C1C	4.07	131.24	125.04
45	AB	821	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
54	A3	307	CHL	C1D-CHD-C4C	-4.07	117.28	126.06
45	AB	840	CLA	CMB-C2B-C1B	-4.07	122.22	128.46
45	BB	828	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
45	BA	802	CLA	C4A-NA-C1A	4.06	108.53	106.71
54	A4	305	CHL	C1D-CHD-C4C	-4.06	117.30	126.06
48	AI	101	BCR	C7-C8-C9	-4.06	120.11	126.23
45	BB	816	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
53	A4	318	LMG	C8-O7-C10	-4.05	107.82	117.79
48	A4	317	BCR	C37-C22-C23	4.05	124.46	118.08
45	BA	804	CLA	CMB-C2B-C1B	-4.05	122.25	128.46
55	A3	317	XAT	O4-C5-C18	4.04	119.90	115.06
55	B1	317	XAT	O24-C25-C38	4.04	119.90	115.06
45	A3	306	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
45	B1	315	CLA	CAB-C3B-C4B	-4.04	122.25	128.46
48	BL	305	BCR	C30-C25-C26	-4.04	116.92	122.61
48	BA	851	BCR	C33-C5-C6	-4.04	119.99	124.53
54	A6	608	CHL	CHC-C1C-NC	4.04	130.33	124.20
47	BF	305	LHG	O7-C7-C8	4.04	120.20	111.50
48	AI	101	BCR	C31-C1-C6	-4.04	103.75	110.30
48	BA	856	BCR	C37-C22-C23	4.03	124.43	118.08
45	A4	303	CLA	CAB-C3B-C4B	-4.03	122.27	128.46
45	AB	805	CLA	C4A-NA-C1A	4.03	108.52	106.71
45	BK	201	CLA	CAB-C3B-C4B	-4.03	122.27	128.46
48	BK	204	BCR	C1-C6-C5	-4.03	116.94	122.61
45	BB	832	CLA	C4A-NA-C1A	4.02	108.52	106.71
48	BA	851	BCR	C1-C6-C5	-4.02	116.95	122.61
54	A6	608	CHL	C2A-C1A-CHA	-4.02	116.83	123.86
54	A6	607	CHL	C1D-ND-C4D	4.02	109.19	106.33
47	A3	301	LHG	O7-C7-C8	4.02	120.16	111.50
55	B3	316	XAT	C38-C25-C26	-4.01	115.53	122.26
45	AA	826	CLA	C4A-NA-C1A	4.01	108.51	106.71
55	A4	316	XAT	C39-C29-C28	4.01	124.40	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B2	614	CHL	C4A-NA-C1A	-4.01	104.91	106.71
54	A1	303	CHL	C1D-CHD-C4C	-4.00	117.42	126.06
54	B2	606	CHL	C1D-CHD-C4C	-4.00	117.42	126.06
54	A6	602	CHL	C4A-NA-C1A	-4.00	104.91	106.71
54	B1	308	CHL	C1D-CHD-C4C	-4.00	117.43	126.06
45	AA	821	CLA	CMB-C2B-C3B	4.00	132.16	124.68
48	AB	847	BCR	C3-C4-C5	-4.00	106.94	114.08
45	B1	311	CLA	C4A-NA-C1A	4.00	108.50	106.71
55	A6	616	XAT	C40-C33-C32	4.00	124.37	118.08
55	B2	616	XAT	O24-C25-C38	4.00	119.84	115.06
45	AB	820	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
48	B3	317	BCR	C40-C30-C29	-3.99	92.93	108.91
45	BA	823	CLA	C4A-NA-C1A	3.99	108.50	106.71
45	A1	316	CLA	CAB-C3B-C4B	-3.99	122.33	128.46
54	B3	306	CHL	C1D-CHD-C4C	-3.99	117.46	126.06
54	A4	306	CHL	C4A-NA-C1A	-3.99	104.91	106.71
48	BG	203	BCR	C33-C5-C4	3.99	121.27	113.62
54	B2	601	CHL	C1D-CHD-C4C	-3.99	117.46	126.06
54	B1	303	CHL	C1D-CHD-C4C	-3.98	117.47	126.06
48	BL	301	BCR	C3-C4-C5	-3.98	106.97	114.08
47	A1	301	LHG	O7-C7-C8	3.98	120.08	111.50
48	AB	849	BCR	C32-C1-C6	-3.98	103.85	110.30
45	A6	612	CLA	C4A-NA-C1A	3.97	108.49	106.71
48	BL	301	BCR	C36-C18-C19	3.97	124.34	118.08
45	B3	305	CLA	CAB-C3B-C4B	-3.97	122.36	128.46
48	AJ	103	BCR	C8-C9-C10	-3.97	112.84	118.94
45	B5	610	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
45	BA	826	CLA	C4A-NA-C1A	3.97	108.49	106.71
54	B3	306	CHL	CHC-C1C-NC	3.97	130.22	124.20
48	AG	205	BCR	C36-C18-C19	3.97	124.33	118.08
45	BA	835	CLA	C4A-NA-C1A	3.96	108.49	106.71
55	A6	616	XAT	O24-C25-C38	3.96	119.80	115.06
48	AB	845	BCR	C37-C22-C23	3.95	124.31	118.08
48	AB	846	BCR	C37-C22-C23	3.95	124.31	118.08
52	A1	317	LUT	C16-C1-C6	3.95	116.71	110.30
45	AB	833	CLA	C4A-NA-C1A	3.95	108.48	106.71
55	B3	316	XAT	C39-C29-C28	3.95	124.30	118.08
55	B1	317	XAT	C20-C13-C12	3.95	124.30	118.08
55	B3	316	XAT	C19-C9-C8	3.95	124.30	118.08
45	BA	828	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
45	BB	841	CLA	CMB-C2B-C3B	3.95	132.06	124.68
53	B5	617	LMG	O7-C10-C11	3.94	120.00	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	844	CLA	C4A-NA-C1A	3.94	108.48	106.71
48	AB	846	BCR	C33-C5-C6	-3.94	120.10	124.53
54	B3	306	CHL	C4A-NA-C1A	-3.94	104.94	106.71
48	A1	319	BCR	C30-C25-C26	-3.94	117.06	122.61
45	AB	835	CLA	C4A-NA-C1A	3.94	108.48	106.71
48	AL	302	BCR	C37-C22-C23	3.94	124.28	118.08
45	A3	306	CLA	CAB-C3B-C4B	-3.93	122.42	128.46
45	AA	807	CLA	C4A-NA-C1A	3.93	108.47	106.71
45	A1	309	CLA	C4A-NA-C1A	3.93	108.47	106.71
54	B2	607	CHL	C1D-CHD-C4C	-3.93	117.58	126.06
48	AI	102	BCR	C28-C27-C26	-3.93	107.06	114.08
45	B1	310	CLA	C4A-NA-C1A	3.93	108.47	106.71
45	B2	613	CLA	C4A-NA-C1A	3.93	108.47	106.71
45	B1	307	CLA	CMB-C2B-C1B	-3.92	122.43	128.46
48	AI	102	BCR	C1-C6-C5	-3.92	117.09	122.61
45	BB	841	CLA	C4A-NA-C1A	3.92	108.47	106.71
48	AA	849	BCR	C36-C18-C17	-3.91	117.44	122.92
48	AA	846	BCR	C38-C26-C25	-3.91	120.14	124.53
55	B1	317	XAT	C39-C29-C28	3.91	124.24	118.08
45	BA	826	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
45	B3	303	CLA	CAB-C3B-C4B	-3.91	122.46	128.46
48	AA	849	BCR	C37-C22-C23	3.91	124.23	118.08
45	BB	806	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
45	AB	815	CLA	CMB-C2B-C3B	3.91	131.99	124.68
48	AB	845	BCR	C36-C18-C19	3.90	124.23	118.08
45	AB	811	CLA	O2D-CGD-O1D	-3.90	116.21	123.84
45	A4	307	CLA	C4A-NA-C1A	3.90	108.46	106.71
48	A3	318	BCR	C40-C30-C29	-3.90	93.31	108.91
54	A3	307	CHL	CHC-C1C-NC	3.90	130.12	124.20
54	B2	606	CHL	O2D-CGD-CBD	3.89	118.19	111.27
45	B1	312	CLA	CAB-C3B-C4B	-3.89	122.48	128.46
54	A6	607	CHL	C1D-CHD-C4C	-3.89	117.67	126.06
45	BA	829	CLA	C4A-NA-C1A	3.89	108.45	106.71
56	e	301	SQD	O7-S-C6	3.89	111.56	106.94
45	AF	804	CLA	CAA-C2A-C3A	-3.89	107.03	116.10
45	BA	831	CLA	C4A-NA-C1A	3.88	108.45	106.71
45	AB	810	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
54	A4	306	CHL	C1D-CHD-C4C	-3.88	117.68	126.06
45	BA	802	CLA	C1B-CHB-C4A	-3.88	122.43	130.12
45	BB	838	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
45	B2	613	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
45	B3	307	CLA	C4A-NA-C1A	3.88	108.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A6	606	CHL	C4A-NA-C1A	-3.88	104.96	106.71
54	B2	606	CHL	C2A-C1A-CHA	-3.88	117.08	123.86
48	B2	617	BCR	C30-C25-C26	-3.88	117.15	122.61
55	B5	615	XAT	C39-C29-C28	3.87	124.18	118.08
52	B1	316	LUT	C19-C9-C10	-3.87	117.50	122.92
54	B1	303	CHL	C1D-ND-C4D	3.87	109.08	106.33
48	A1	319	BCR	C37-C22-C23	3.87	124.17	118.08
45	BB	811	CLA	CMB-C2B-C3B	3.87	131.91	124.68
47	B1	318	LHG	O7-C7-C8	3.87	119.83	111.50
54	A1	303	CHL	C1D-ND-C4D	3.86	109.08	106.33
45	A1	304	CLA	C4A-NA-C1A	3.86	108.44	106.71
48	BK	204	BCR	C30-C25-C26	-3.86	117.18	122.61
45	AB	806	CLA	C4A-NA-C1A	3.86	108.44	106.71
45	A1	310	CLA	CAB-C3B-C4B	-3.86	122.54	128.46
45	A1	311	CLA	CMB-C2B-C1B	-3.85	122.54	128.46
47	A1	302	LHG	O7-C7-C8	3.85	119.80	111.50
45	BB	815	CLA	C4A-NA-C1A	3.85	108.44	106.71
48	BK	204	BCR	C37-C22-C23	3.85	124.14	118.08
45	AB	827	CLA	CMB-C2B-C3B	3.85	131.88	124.68
52	B2	615	LUT	C40-C33-C32	3.85	124.14	118.08
48	BK	204	BCR	C38-C26-C27	3.85	121.00	113.62
45	A4	308	CLA	C4A-NA-C1A	3.84	108.43	106.71
45	BB	814	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
54	B5	607	CHL	CHD-C4C-NC	3.84	130.26	124.20
48	AA	847	BCR	C24-C23-C22	-3.84	120.43	126.23
45	AB	828	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
45	B5	603	CLA	CAB-C3B-C4B	-3.84	122.56	128.46
45	AA	808	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
56	e	301	SQD	O9-S-O7	-3.84	100.67	113.95
46	BB	844	PQN	C11-C12-C13	-3.83	120.41	126.79
52	B1	316	LUT	C15-C35-C34	3.83	131.33	123.47
45	B1	313	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
47	B5	618	LHG	O7-C7-C8	3.83	119.76	111.50
54	A1	308	CHL	C1D-CHD-C4C	-3.83	117.79	126.06
45	B3	303	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
45	AL	303	CLA	C4A-NA-C1A	3.82	108.42	106.71
45	AL	304	CLA	C4A-NA-C1A	3.82	108.42	106.71
54	B1	308	CHL	C2A-C1A-CHA	-3.82	117.18	123.85
48	BB	849	BCR	C3-C4-C5	-3.82	107.25	114.08
51	BB	850	DGD	O2G-C1B-C2B	3.82	119.73	111.50
48	BB	845	BCR	C38-C26-C27	3.82	120.95	113.62
45	B3	305	CLA	CMB-C2B-C1B	-3.82	122.59	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AL	304	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
55	B3	316	XAT	C6-C7-C8	-3.82	117.92	125.99
45	A3	302	CLA	C4A-NA-C1A	3.81	108.42	106.71
45	BB	819	CLA	C4A-NA-C1A	3.81	108.42	106.71
54	B2	605	CHL	C1D-CHD-C4C	-3.81	117.83	126.06
52	B1	316	LUT	C39-C29-C30	-3.81	117.58	122.92
48	AF	805	BCR	C7-C8-C9	-3.81	120.48	126.23
45	AB	835	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
45	AB	836	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
54	B2	614	CHL	C1D-CHD-C4C	-3.81	117.85	126.06
54	A6	607	CHL	C4A-NA-C1A	-3.81	105.00	106.71
48	B2	617	BCR	C23-C24-C25	-3.81	116.51	127.20
54	A1	303	CHL	C4A-NA-C1A	-3.80	105.00	106.71
45	BL	304	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
45	B3	303	CLA	C4A-NA-C1A	3.80	108.42	106.71
52	B3	315	LUT	C21-C26-C27	-3.80	107.90	112.70
45	A6	611	CLA	O2D-CGD-O1D	-3.80	116.41	123.84
45	BB	820	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
45	B2	608	CLA	C4A-NA-C1A	3.79	108.41	106.71
52	B3	315	LUT	C38-C25-C24	-3.79	115.44	123.56
45	BB	802	CLA	C4-C3-C5	3.79	121.65	115.27
54	A6	602	CHL	C1D-ND-C4D	3.79	109.03	106.33
45	BA	837	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
45	A3	315	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
45	AA	837	CLA	CMB-C2B-C3B	3.79	131.76	124.68
54	A4	314	CHL	C1D-CHD-C4C	-3.79	117.89	126.06
54	B5	606	CHL	CHC-C1C-NC	3.78	129.94	124.20
48	BL	301	BCR	C30-C25-C26	-3.78	117.29	122.61
45	AA	816	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
45	AA	819	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
48	BG	203	BCR	C38-C26-C25	-3.78	120.28	124.53
45	BB	813	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
55	B5	615	XAT	O24-C25-C38	3.78	119.58	115.06
51	AB	851	DGD	O2G-C1B-C2B	3.78	119.64	111.50
45	A6	609	CLA	CMB-C2B-C1B	-3.77	122.68	128.46
48	BB	849	BCR	C33-C5-C6	-3.76	120.30	124.53
45	B1	315	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
45	B2	602	CLA	C4A-NA-C1A	3.76	108.40	106.71
54	A3	307	CHL	C4A-NA-C1A	-3.76	105.02	106.71
45	AB	812	CLA	CAB-C3B-C4B	-3.76	122.68	128.46
45	B3	312	CLA	C4A-NA-C1A	3.76	108.40	106.71
54	A6	608	CHL	C1D-CHD-C4C	-3.76	117.95	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B5	610	CLA	C4A-NA-C1A	3.75	108.39	106.71
54	B5	605	CHL	C1D-ND-C4D	3.75	109.00	106.33
54	A6	602	CHL	C1D-CHD-C4C	-3.75	117.97	126.06
54	A6	606	CHL	C1D-CHD-C4C	-3.75	117.97	126.06
54	B2	601	CHL	C1D-ND-C4D	3.75	109.00	106.33
48	BJ	103	BCR	C32-C1-C6	-3.75	104.22	110.30
48	A1	319	BCR	C36-C18-C19	3.75	123.98	118.08
45	AA	826	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
55	A6	616	XAT	C8-C9-C10	-3.74	113.20	118.94
45	A4	303	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
54	B2	601	CHL	CHD-C4C-NC	3.73	130.08	124.20
45	BK	201	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
45	BL	303	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
52	B3	315	LUT	C39-C29-C28	3.73	123.95	118.08
45	AA	802	CLA	C1B-CHB-C4A	-3.73	122.74	130.12
45	A6	609	CLA	C4A-NA-C1A	3.72	108.38	106.71
48	BI	101	BCR	C31-C1-C6	-3.72	104.26	110.30
48	B2	617	BCR	C40-C30-C25	-3.72	104.26	110.30
45	BA	842	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
48	BA	849	BCR	C36-C18-C19	3.72	123.94	118.08
45	BA	825	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
45	B1	310	CLA	CAB-C3B-C4B	-3.72	122.75	128.46
48	BA	851	BCR	C23-C22-C21	-3.72	113.24	118.94
45	A6	611	CLA	CAB-C3B-C4B	-3.72	122.75	128.46
52	B5	614	LUT	C1-C6-C5	-3.72	117.38	122.61
48	BG	203	BCR	C37-C22-C21	-3.72	117.72	122.92
45	A6	614	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
55	B2	616	XAT	C20-C13-C12	3.71	123.93	118.08
54	A4	304	CHL	C1D-ND-C4D	3.71	108.97	106.33
45	AA	804	CLA	CMB-C2B-C3B	3.71	131.62	124.68
45	BL	303	CLA	C4A-NA-C1A	3.71	108.37	106.71
45	B5	604	CLA	CAB-C3B-C4B	-3.71	122.77	128.46
48	B5	616	BCR	C33-C5-C6	-3.70	120.37	124.53
52	B5	614	LUT	C36-C21-C26	3.70	115.16	109.55
45	AB	838	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
48	BA	848	BCR	C34-C9-C8	3.70	123.91	118.08
45	B2	603	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
45	BA	807	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
45	AB	829	CLA	CMB-C2B-C3B	3.70	131.60	124.68
48	BB	803	BCR	C30-C25-C26	-3.70	117.41	122.61
45	BB	816	CLA	CMB-C2B-C3B	3.69	131.59	124.68
45	B5	613	CLA	C4A-NA-C1A	3.69	108.37	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A3	303	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
45	AA	817	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
45	BB	826	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
48	BK	204	BCR	C30-C25-C24	3.69	126.22	115.78
54	A1	303	CHL	O2A-CGA-CBA	3.69	123.48	111.91
48	BL	305	BCR	C32-C1-C6	-3.69	104.32	110.30
48	AJ	103	BCR	C1-C6-C5	-3.69	117.42	122.61
54	B5	607	CHL	C1D-ND-C4D	3.68	108.95	106.33
54	A1	308	CHL	C4A-NA-C1A	-3.68	105.05	106.71
45	B5	604	CLA	CMB-C2B-C1B	-3.68	122.80	128.46
48	B2	617	BCR	C32-C1-C6	-3.68	104.33	110.30
45	BK	203	CLA	CMB-C2B-C3B	3.68	131.56	124.68
54	A6	606	CHL	C1D-ND-C4D	3.68	108.95	106.33
48	BL	301	BCR	C38-C26-C25	-3.68	120.40	124.53
45	AB	839	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
54	A4	304	CHL	C4A-NA-C1A	-3.67	105.06	106.71
45	BB	836	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
55	A3	317	XAT	C39-C29-C28	3.67	123.86	118.08
45	AB	806	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
48	BA	848	BCR	C30-C25-C26	-3.67	117.45	122.61
54	A4	306	CHL	CHD-C4C-NC	3.66	129.97	124.20
48	AB	849	BCR	C23-C22-C21	-3.66	113.32	118.94
45	A6	604	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
48	BA	850	BCR	C30-C25-C26	-3.66	117.45	122.61
48	BA	849	BCR	C38-C26-C25	-3.66	120.42	124.53
45	BA	829	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
54	A4	305	CHL	CAC-C3C-C4C	3.66	129.56	124.81
45	AB	819	CLA	CMB-C2B-C3B	3.66	131.52	124.68
54	A4	304	CHL	C1D-CHD-C4C	-3.66	118.17	126.06
45	BA	821	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
45	BA	831	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
45	AB	826	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
45	BA	836	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
45	B1	315	CLA	C4A-NA-C1A	3.64	108.34	106.71
45	A1	306	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
45	A1	315	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
51	AB	851	DGD	C2G-O2G-C1B	-3.63	108.84	117.79
48	AI	102	BCR	C37-C22-C23	3.63	123.80	118.08
54	B5	605	CHL	C1D-CHD-C4C	-3.63	118.22	126.06
45	AA	829	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
54	B2	614	CHL	CHD-C4C-NC	3.63	129.93	124.20
48	AB	844	BCR	C7-C8-C9	-3.63	120.75	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	803	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
45	A4	309	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
45	B5	602	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
48	BA	848	BCR	C38-C26-C27	3.62	120.58	113.62
45	BB	833	CLA	CMB-C2B-C3B	3.62	131.45	124.68
54	B2	607	CHL	C1D-ND-C4D	3.62	108.91	106.33
45	BA	828	CLA	CMB-C2B-C3B	3.62	131.44	124.68
48	AL	306	BCR	C28-C27-C26	-3.61	107.62	114.08
45	AL	303	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
48	B3	317	BCR	C37-C22-C23	3.61	123.77	118.08
48	A3	318	BCR	C38-C26-C25	-3.61	120.48	124.53
48	B2	617	BCR	C36-C18-C19	3.61	123.76	118.08
48	AL	306	BCR	C38-C26-C27	3.60	120.54	113.62
45	A1	309	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
45	B5	602	CLA	C4A-NA-C1A	3.60	108.33	106.71
48	BG	203	BCR	C10-C11-C12	-3.60	111.97	123.22
45	AB	816	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
48	BL	305	BCR	C30-C25-C24	3.60	125.96	115.78
48	BB	803	BCR	C37-C22-C23	3.60	123.75	118.08
45	AB	826	CLA	CMB-C2B-C3B	3.60	131.41	124.68
48	BA	851	BCR	C33-C5-C4	3.60	120.53	113.62
53	A1	321	LMG	O7-C10-C11	3.60	119.25	111.50
48	AG	205	BCR	C32-C1-C6	-3.60	104.47	110.30
45	AA	807	CLA	CMB-C2B-C3B	3.60	131.41	124.68
45	AB	812	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
48	BB	846	BCR	C8-C7-C6	-3.59	117.12	127.20
45	AB	818	CLA	C4A-NA-C1A	3.59	108.32	106.71
53	A4	318	LMG	C7-O1-C1	-3.59	106.73	113.74
45	AA	811	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
45	A6	614	CLA	C4A-NA-C1A	3.59	108.32	106.71
48	AA	852	BCR	C37-C22-C21	-3.59	117.90	122.92
48	BB	845	BCR	C1-C6-C5	-3.59	117.56	122.61
45	AA	815	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
48	AI	102	BCR	C30-C25-C26	-3.59	117.56	122.61
48	A3	318	BCR	C39-C30-C29	3.58	123.24	108.91
45	A3	308	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
55	B3	316	XAT	C35-C15-C14	-3.58	116.14	123.47
45	BB	813	CLA	CAB-C3B-C4B	-3.58	122.96	128.46
45	B2	610	CLA	CAB-C3B-C4B	-3.58	122.97	128.46
45	A1	311	CLA	C4A-NA-C1A	3.58	108.31	106.71
55	A1	318	XAT	C8-C9-C10	-3.57	113.46	118.94
45	BB	821	CLA	C4A-NA-C1A	3.57	108.31	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B3	314	CLA	C4A-NA-C1A	3.57	108.31	106.71
48	BI	101	BCR	C39-C30-C25	-3.57	104.50	110.30
45	AA	829	CLA	CMB-C2B-C3B	3.57	131.36	124.68
45	A6	611	CLA	O2D-CGD-CBD	3.57	117.61	111.27
48	AA	848	BCR	C36-C18-C19	3.57	123.70	118.08
55	B1	317	XAT	C6-C7-C8	-3.56	118.46	125.99
54	A4	314	CHL	CHD-C4C-NC	3.56	129.82	124.20
45	BB	824	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
45	AB	814	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
45	A3	309	CLA	C4A-NA-C1A	3.56	108.31	106.71
48	BB	846	BCR	C3-C4-C5	-3.56	107.73	114.08
48	AB	848	BCR	C36-C18-C19	3.55	123.67	118.08
55	A3	317	XAT	C19-C9-C8	3.55	123.67	118.08
48	BL	306	BCR	C33-C5-C6	-3.55	120.55	124.53
54	B2	605	CHL	C1C-C2C-C3C	-3.54	104.30	107.11
45	BA	826	CLA	CMB-C2B-C3B	3.54	131.31	124.68
45	BB	835	CLA	C4A-NA-C1A	3.54	108.30	106.71
45	AA	803	CLA	O2D-CGD-O1D	-3.54	116.91	123.84
45	BB	815	CLA	CAC-C3C-C2C	-3.54	121.47	127.53
45	B1	304	CLA	O2D-CGD-O1D	-3.54	116.92	123.84
45	AB	828	CLA	CMB-C2B-C3B	3.54	131.30	124.68
53	A4	318	LMG	O7-C10-C11	3.54	119.12	111.50
45	BJ	102	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
48	A3	318	BCR	C1-C6-C5	-3.53	117.64	122.61
46	AB	843	PQN	C11-C3-C4	-3.53	114.72	118.50
45	B3	307	CLA	CMB-C2B-C3B	3.53	131.29	124.68
45	BB	817	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
45	AB	801	CLA	O2D-CGD-O1D	-3.53	116.94	123.84
48	BB	847	BCR	C8-C9-C10	3.53	124.35	118.94
54	B2	605	CHL	CHD-C4C-NC	3.53	129.76	124.20
45	BB	801	CLA	O2D-CGD-O1D	-3.53	116.95	123.84
45	AB	817	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
45	BA	841	CLA	CMB-C2B-C3B	3.52	131.27	124.68
54	B2	614	CHL	CAC-C3C-C4C	3.52	129.38	124.81
55	B5	615	XAT	C6-C7-C8	-3.52	118.55	125.99
45	AA	816	CLA	O2D-CGD-O1D	-3.52	116.95	123.84
47	BF	305	LHG	C5-O7-C7	-3.52	109.12	117.79
45	B3	314	CLA	CMB-C2B-C3B	3.52	131.26	124.68
45	BA	837	CLA	CMB-C2B-C3B	3.52	131.26	124.68
45	BA	822	CLA	CMB-C2B-C3B	3.52	131.26	124.68
48	BJ	101	BCR	C3-C4-C5	-3.52	107.80	114.08
45	AA	832	CLA	C4-C3-C5	3.52	121.18	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	843	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
45	BA	811	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
45	AB	813	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
54	A3	307	CHL	CHD-C4C-NC	3.51	129.73	124.20
45	AA	829	CLA	C6-C5-C3	3.51	122.65	113.45
46	AB	843	PQN	C12-C11-C3	-3.51	102.59	112.05
45	AB	804	CLA	CAC-C3C-C2C	-3.51	121.53	127.53
45	AA	812	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
54	B1	308	CHL	CHD-C4C-NC	3.50	129.72	124.20
54	B3	306	CHL	CHD-C4C-NC	3.50	129.72	124.20
48	BJ	103	BCR	C39-C30-C25	-3.50	104.62	110.30
48	AB	849	BCR	C16-C15-C14	-3.50	116.31	123.47
45	B5	608	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
45	BA	835	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
48	BI	101	BCR	C38-C26-C27	3.49	120.33	113.62
54	B1	303	CHL	CHD-C4C-NC	3.49	129.71	124.20
48	BJ	103	BCR	C8-C9-C10	-3.49	113.58	118.94
45	A1	307	CLA	CBD-CHA-C1A	3.49	132.61	128.50
45	AA	835	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
48	BA	850	BCR	C36-C18-C19	3.49	123.57	118.08
47	B1	301	LHG	O7-C7-C8	3.49	119.02	111.50
45	BA	844	CLA	CMB-C2B-C1B	-3.49	123.11	128.46
56	e	301	SQD	O8-S-C6	3.48	111.29	105.74
45	AA	830	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
54	B5	605	CHL	CHC-C1C-NC	3.48	129.49	124.20
45	B1	307	CLA	C4A-NA-C1A	3.48	108.27	106.71
45	B2	610	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
45	B2	611	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
52	AF	806	LUT	C15-C35-C34	-3.48	116.34	123.47
56	e	301	SQD	C4-C3-C2	3.48	116.90	110.82
45	BA	829	CLA	CMB-C2B-C3B	3.48	131.19	124.68
48	BA	847	BCR	C30-C25-C26	-3.48	117.72	122.61
48	BA	856	BCR	C30-C25-C26	-3.48	117.72	122.61
48	BA	855	BCR	C24-C23-C22	-3.47	120.98	126.23
46	BB	844	PQN	C11-C3-C4	-3.47	114.78	118.50
45	BA	814	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
45	BA	803	CLA	O2D-CGD-O1D	-3.47	117.05	123.84
45	AA	818	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
52	B3	315	LUT	C40-C33-C32	3.47	123.54	118.08
55	B2	616	XAT	C36-C21-C22	-3.47	102.96	108.98
45	B1	312	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
45	BB	805	CLA	C1B-CHB-C4A	-3.47	123.25	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A3	313	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
54	A1	303	CHL	CHD-C4C-NC	3.46	129.66	124.20
54	B2	607	CHL	CHD-C4C-NC	3.46	129.66	124.20
45	B5	608	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
54	B5	606	CHL	CMC-C2C-C1C	3.46	130.31	125.04
45	A4	301	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
48	A1	319	BCR	C40-C30-C29	-3.46	95.06	108.91
45	AA	836	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
45	BB	801	CLA	CHB-C4A-NA	3.46	129.29	124.51
45	AB	801	CLA	CAA-C2A-C1A	-3.46	100.64	111.97
54	B5	606	CHL	CHD-C4C-NC	3.46	129.65	124.20
45	AB	839	CLA	CMB-C2B-C3B	3.46	131.15	124.68
45	BA	821	CLA	C1B-CHB-C4A	-3.46	123.27	130.12
54	A3	307	CHL	CAC-C3C-C4C	3.46	129.29	124.81
45	BB	834	CLA	O2D-CGD-O1D	-3.45	117.08	123.84
45	BA	834	CLA	O2D-CGD-O1D	-3.45	117.09	123.84
45	AB	835	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
45	A4	310	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
54	A6	606	CHL	CHD-C4C-NC	3.45	129.64	124.20
48	BI	101	BCR	C30-C25-C26	-3.45	117.75	122.61
45	BK	201	CLA	CAA-C2A-C3A	-3.45	108.05	116.10
45	A3	311	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
48	BA	855	BCR	C34-C9-C8	3.45	123.51	118.08
48	AA	849	BCR	C27-C26-C25	-3.45	117.73	122.73
54	A6	602	CHL	CAC-C3C-C4C	3.44	129.28	124.81
48	BA	856	BCR	C37-C22-C21	-3.44	118.10	122.92
48	AB	848	BCR	C15-C16-C17	-3.44	116.43	123.47
48	AA	846	BCR	C15-C16-C17	-3.44	116.43	123.47
45	AA	822	CLA	O2D-CGD-O1D	-3.44	117.12	123.84
48	AB	847	BCR	C23-C24-C25	-3.44	117.55	127.20
48	AA	849	BCR	C38-C26-C27	3.44	120.22	113.62
45	BB	828	CLA	CMB-C2B-C3B	3.43	131.10	124.68
45	AB	804	CLA	CHB-C4A-NA	3.43	129.26	124.51
48	A1	319	BCR	C4-C5-C6	-3.43	117.75	122.73
45	BB	839	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
54	B3	306	CHL	CHC-C1C-C2C	-3.43	117.23	126.72
54	A4	305	CHL	CMC-C2C-C1C	3.43	130.26	125.04
45	AF	802	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
48	BB	847	BCR	C36-C18-C19	3.43	123.48	118.08
54	A4	305	CHL	CHD-C4C-NC	3.43	129.61	124.20
45	AA	824	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
52	A4	315	LUT	C21-C26-C27	-3.43	108.37	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A6	610	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
45	A3	315	CLA	C4A-NA-C1A	3.43	108.25	106.71
45	AB	805	CLA	CMB-C2B-C3B	3.43	131.09	124.68
45	A1	313	CLA	CMB-C2B-C3B	3.43	131.09	124.68
54	B1	303	CHL	C4A-NA-C1A	-3.43	105.17	106.71
45	AA	827	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
45	AB	810	CLA	CMB-C2B-C3B	3.42	131.08	124.68
45	B1	307	CLA	CMB-C2B-C3B	3.42	131.08	124.68
45	A1	312	CLA	C4A-NA-C1A	3.42	108.24	106.71
55	B1	317	XAT	C40-C33-C32	3.42	123.47	118.08
45	AA	813	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
45	B2	612	CLA	CMB-C2B-C3B	3.42	131.07	124.68
56	e	301	SQD	O47-C7-C8	3.42	118.86	111.50
45	BA	812	CLA	CMB-C2B-C3B	3.42	131.07	124.68
53	AG	202	LMG	O7-C10-C11	3.41	118.86	111.50
54	A3	307	CHL	CHC-C1C-C2C	-3.41	117.28	126.72
48	AJ	101	BCR	C8-C7-C6	-3.41	117.61	127.20
45	AA	837	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
45	AB	811	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
54	A6	602	CHL	CHD-C4C-NC	3.41	129.58	124.20
55	A4	316	XAT	C35-C15-C14	-3.41	116.49	123.47
45	AB	823	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
45	A3	304	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
48	BB	848	BCR	C39-C30-C25	-3.41	104.77	110.30
45	AA	840	CLA	C1B-CHB-C4A	-3.41	123.37	130.12
55	B2	616	XAT	C39-C29-C28	3.41	123.44	118.08
45	BA	803	CLA	CMB-C2B-C3B	3.41	131.05	124.68
48	AA	847	BCR	C36-C18-C19	3.40	123.44	118.08
48	BA	851	BCR	C8-C9-C10	3.40	124.16	118.94
48	A6	617	BCR	C23-C24-C25	-3.40	117.65	127.20
45	BA	804	CLA	CMB-C2B-C3B	3.40	131.04	124.68
45	B3	310	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
55	B1	317	XAT	O4-C5-C18	3.40	119.13	115.06
45	B2	609	CLA	C4A-NA-C1A	3.40	108.23	106.71
45	B2	608	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
54	B2	601	CHL	O2A-CGA-CBA	3.39	122.56	111.91
45	B1	305	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
45	A6	611	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
45	AB	835	CLA	CMB-C2B-C3B	3.39	131.02	124.68
45	AA	825	CLA	CMB-C2B-C3B	3.39	131.02	124.68
45	AB	830	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
45	BB	812	CLA	CMB-C2B-C1B	-3.39	123.26	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BF	304	BCR	C30-C25-C26	-3.39	117.84	122.61
54	B3	306	CHL	CAC-C3C-C4C	3.39	129.20	124.81
48	AA	849	BCR	C31-C1-C6	-3.38	104.81	110.30
56	e	301	SQD	O9-S-C6	3.38	110.96	106.94
48	BI	101	BCR	C37-C22-C23	3.38	123.40	118.08
45	A6	610	CLA	C4A-NA-C1A	3.38	108.22	106.71
45	A3	315	CLA	CMB-C2B-C3B	3.38	131.00	124.68
45	A1	311	CLA	CMB-C2B-C3B	3.37	130.99	124.68
48	B2	617	BCR	C33-C5-C4	-3.37	107.14	113.62
52	B3	315	LUT	C19-C9-C8	3.37	123.39	118.08
55	B2	616	XAT	C40-C33-C32	3.37	123.39	118.08
48	AA	848	BCR	C30-C25-C24	3.37	125.31	115.78
45	BB	807	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
45	AB	842	CLA	O2D-CGD-O1D	-3.37	117.25	123.84
48	AA	848	BCR	C38-C26-C25	-3.37	120.75	124.53
45	AA	842	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
48	BA	855	BCR	C16-C15-C14	-3.37	116.58	123.47
45	AA	823	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
45	AB	817	CLA	CMB-C2B-C3B	3.36	130.97	124.68
45	AB	819	CLA	O2D-CGD-O1D	-3.36	117.26	123.84
55	B5	615	XAT	C18-C5-C6	-3.36	116.63	122.26
45	A4	307	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
45	BA	817	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
48	BA	856	BCR	C38-C26-C25	3.36	128.30	124.53
45	AA	826	CLA	CMB-C2B-C3B	3.36	130.96	124.68
45	AB	818	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
48	BL	306	BCR	C38-C26-C25	-3.36	120.76	124.53
55	B5	615	XAT	C36-C21-C22	-3.36	103.15	108.98
45	B5	608	CLA	C4A-NA-C1A	3.36	108.22	106.71
48	AB	844	BCR	C37-C22-C23	3.36	123.36	118.08
48	AI	101	BCR	C37-C22-C23	3.35	123.36	118.08
45	BA	819	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
48	AF	805	BCR	C16-C15-C14	-3.35	116.60	123.47
48	AA	852	BCR	C15-C16-C17	-3.35	116.61	123.47
54	A4	304	CHL	CHD-C4C-NC	3.35	129.49	124.20
45	AA	809	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
45	AB	808	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
45	B5	610	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
45	BG	201	CLA	C4A-NA-C1A	3.35	108.21	106.71
48	AL	306	BCR	C30-C25-C24	3.35	125.25	115.78
48	AL	302	BCR	C2-C1-C6	-3.35	105.33	110.48
45	AB	831	CLA	C4A-NA-C1A	3.35	108.21	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	826	CLA	C1B-CHB-C4A	-3.34	123.49	130.12
46	BB	844	PQN	C14-C13-C12	-3.34	115.10	123.68
45	AG	201	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
47	B1	302	LHG	O7-C7-C8	3.34	118.70	111.50
45	B2	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
45	BB	819	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
56	BJ	104	SQD	O47-C7-O49	-3.34	115.64	123.70
48	AL	302	BCR	C35-C13-C12	3.34	123.33	118.08
47	BA	846	LHG	O7-C7-C8	3.33	118.69	111.50
52	A3	316	LUT	C39-C29-C28	3.33	123.33	118.08
54	A4	306	CHL	CHC-C1C-NC	3.33	129.26	124.20
45	A1	304	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
45	BB	831	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
45	AB	813	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
45	AA	833	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
47	A6	618	LHG	O7-C7-C8	3.33	118.68	111.50
45	B1	309	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
46	BA	843	PQN	C16-C15-C13	-3.33	104.73	113.45
48	AF	801	BCR	C35-C13-C12	3.33	123.32	118.08
45	AA	833	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
48	AB	846	BCR	C36-C18-C19	3.32	123.31	118.08
48	BB	846	BCR	C38-C26-C27	3.32	120.00	113.62
54	A6	602	CHL	O2A-CGA-CBA	3.32	122.33	111.91
45	B5	609	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
45	AB	832	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
55	A3	317	XAT	C26-C27-C28	-3.32	118.98	125.99
48	BJ	101	BCR	C34-C9-C8	3.32	123.31	118.08
45	AB	827	CLA	O2D-CGD-O1D	-3.32	117.35	123.84
55	B1	317	XAT	C38-C25-C26	-3.32	116.70	122.26
45	B5	603	CLA	CMB-C2B-C1B	-3.32	123.37	128.46
48	BG	203	BCR	C11-C10-C9	3.31	132.04	127.31
45	A3	304	CLA	CAB-C3B-C4B	-3.31	123.37	128.46
54	A4	314	CHL	CHC-C1C-NC	3.31	129.23	124.20
48	AB	845	BCR	C8-C7-C6	-3.31	117.91	127.20
45	B2	609	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
48	BA	847	BCR	C38-C26-C27	3.31	119.97	113.62
45	AF	804	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
45	BA	823	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
45	B5	610	CLA	CMB-C2B-C3B	3.31	130.87	124.68
45	AB	818	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
45	BB	830	CLA	CMB-C2B-C3B	3.30	130.86	124.68
45	BA	839	CLA	O2D-CGD-O1D	-3.30	117.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A4	305	CHL	C4C-C3C-C2C	-3.30	102.08	106.90
55	A1	318	XAT	C18-C5-C6	-3.30	116.73	122.26
45	A3	310	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
48	AI	102	BCR	C30-C25-C24	3.30	125.12	115.78
45	B1	304	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
45	BB	806	CLA	CMB-C2B-C3B	3.30	130.85	124.68
52	A1	317	LUT	C8-C7-C6	-3.30	117.94	127.20
45	A3	306	CLA	CMB-C2B-C3B	3.30	131.15	124.69
45	AA	827	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
45	A6	613	CLA	CMB-C2B-C3B	3.30	130.84	124.68
48	BG	203	BCR	C16-C17-C18	3.29	132.01	127.31
45	BA	836	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
48	BB	847	BCR	C33-C5-C6	-3.29	120.83	124.53
45	AB	837	CLA	CMB-C2B-C3B	3.29	130.84	124.68
45	AB	809	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
48	AB	849	BCR	C39-C30-C25	-3.29	104.96	110.30
48	AB	848	BCR	C8-C9-C10	-3.29	113.89	118.94
48	BI	101	BCR	C16-C15-C14	-3.29	116.74	123.47
45	AB	801	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
45	AA	824	CLA	C4A-NA-C1A	3.29	108.18	106.71
45	B2	604	CLA	CMB-C2B-C3B	3.29	130.83	124.68
45	A6	612	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
48	AI	101	BCR	C24-C23-C22	-3.28	121.27	126.23
48	B5	616	BCR	C33-C5-C4	3.28	119.92	113.62
45	A1	314	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
48	AB	844	BCR	C4-C5-C6	-3.28	117.97	122.73
48	BK	204	BCR	C27-C26-C25	-3.28	117.97	122.73
48	BJ	101	BCR	C32-C1-C6	-3.28	104.98	110.30
45	AA	819	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
45	A1	312	CLA	CAB-C3B-C4B	-3.28	123.42	128.46
54	A6	608	CHL	CHD-C4C-NC	3.28	129.37	124.20
45	AA	839	CLA	O2D-CGD-O1D	-3.28	117.43	123.84
45	BG	202	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
45	BB	814	CLA	CMB-C2B-C3B	3.28	130.81	124.68
45	AB	806	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
48	BA	856	BCR	C29-C30-C25	3.27	115.52	110.48
48	AG	205	BCR	C8-C7-C6	-3.27	118.01	127.20
45	AJ	102	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
48	AB	849	BCR	C24-C25-C26	3.27	129.39	121.46
45	B2	609	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
45	BA	821	CLA	CMB-C2B-C3B	3.27	130.80	124.68
45	AA	824	CLA	CHD-C1D-ND	-3.27	121.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AI	101	BCR	C39-C30-C25	-3.27	105.00	110.30
48	AB	845	BCR	C8-C9-C10	3.26	123.95	118.94
48	B3	317	BCR	C33-C5-C4	3.26	119.89	113.62
45	B3	309	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
48	B2	617	BCR	C4-C5-C6	-3.26	117.99	122.73
55	A4	316	XAT	C6-C7-C8	-3.26	119.10	125.99
45	AB	835	CLA	O2D-CGD-O1D	-3.26	117.47	123.84
45	A6	614	CLA	CMB-C2B-C3B	3.26	130.78	124.68
45	BL	303	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
54	B2	606	CHL	CHD-C4C-NC	3.26	129.34	124.20
45	BA	818	CLA	CMB-C2B-C1B	-3.26	123.46	128.46
48	AB	846	BCR	C3-C4-C5	-3.26	108.26	114.08
45	BB	840	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
48	BL	305	BCR	C3-C4-C5	-3.25	108.27	114.08
45	BA	841	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
48	AK	204	BCR	C30-C25-C26	-3.25	118.03	122.61
45	BB	826	CLA	CMB-C2B-C3B	3.25	130.76	124.68
48	AJ	103	BCR	C15-C16-C17	-3.25	116.81	123.47
48	BA	848	BCR	C27-C26-C25	-3.25	118.01	122.73
45	AB	839	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
45	BA	840	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
48	BK	204	BCR	C36-C18-C17	-3.25	118.37	122.92
45	B2	613	CLA	CMB-C2B-C3B	3.25	130.76	124.68
45	A1	307	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
45	B5	613	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
45	AA	806	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
45	BA	828	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
48	A1	319	BCR	C38-C26-C25	-3.25	120.88	124.53
45	BB	816	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
54	B1	303	CHL	CAC-C3C-C4C	3.24	129.02	124.81
45	AF	802	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
45	A4	311	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
45	AB	804	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
45	AB	840	CLA	CMB-C2B-C3B	3.24	130.74	124.68
54	A6	606	CHL	CAC-C3C-C4C	3.24	129.97	125.04
45	BB	829	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
55	A4	316	XAT	C28-C29-C30	-3.24	113.97	118.94
45	AF	803	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
48	AK	204	BCR	C23-C22-C21	3.24	123.91	118.94
45	AA	830	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
45	BK	202	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
45	AA	816	CLA	CMB-C2B-C3B	3.23	130.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	AF	806	LUT	C8-C7-C6	-3.23	118.12	127.20
54	A6	602	CHL	CHC-C1C-NC	3.23	129.10	124.20
45	BA	833	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
45	B1	311	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
48	B3	317	BCR	C28-C29-C30	-3.23	103.05	114.60
48	BB	803	BCR	C16-C15-C14	-3.23	116.86	123.47
55	A4	316	XAT	C38-C25-C26	-3.23	116.85	122.26
45	BB	810	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
54	A4	305	CHL	CHC-C1C-C2C	-3.23	117.79	126.72
48	AA	846	BCR	C36-C18-C17	-3.23	118.40	122.92
45	BA	830	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
55	A6	616	XAT	C15-C35-C34	-3.23	116.86	123.47
45	A4	302	CLA	CAB-C3B-C2B	3.23	131.00	124.69
48	AB	848	BCR	C38-C26-C25	-3.22	120.91	124.53
45	B1	313	CLA	CMB-C2B-C3B	3.22	130.71	124.68
45	A1	315	CLA	CAB-C3B-C2B	3.22	131.00	124.69
54	B2	606	CHL	CHC-C1C-NC	3.22	129.09	124.20
45	BB	816	CLA	C4A-NA-C1A	3.22	108.15	106.71
45	AK	202	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
48	A4	317	BCR	C33-C5-C6	-3.22	120.91	124.53
45	AA	822	CLA	CMB-C2B-C1B	-3.22	123.52	128.46
45	BB	812	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
45	B2	610	CLA	O2D-CGD-CBD	3.22	116.98	111.27
45	BA	818	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
48	BG	203	BCR	C38-C26-C27	3.21	119.79	113.62
45	A6	609	CLA	CMB-C2B-C3B	3.21	130.69	124.68
54	A6	607	CHL	CHC-C1C-NC	3.21	129.08	124.20
48	AA	849	BCR	C28-C27-C26	-3.21	108.34	114.08
45	BB	824	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
54	A6	607	CHL	CHD-C4C-NC	3.21	129.26	124.20
45	AB	806	CLA	CMB-C2B-C3B	3.21	130.68	124.68
45	AA	827	CLA	CAA-CBA-CGA	-3.21	103.88	113.25
50	AA	851	LMU	O5B-C5B-C4B	3.20	115.51	109.69
55	A3	317	XAT	C35-C15-C14	-3.20	116.91	123.47
45	AB	801	CLA	CMD-C2D-C1D	-3.20	119.07	124.71
48	AA	849	BCR	C8-C9-C10	3.20	123.85	118.94
48	BF	304	BCR	C31-C1-C6	-3.20	105.11	110.30
45	AA	836	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
52	B5	614	LUT	C21-C26-C27	-3.20	108.66	112.70
48	AJ	101	BCR	C4-C5-C6	-3.20	118.09	122.73
54	A6	608	CHL	C4C-C3C-C2C	-3.19	102.24	106.90
45	AA	819	CLA	CMB-C2B-C3B	3.19	130.65	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	804	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
45	BB	820	CLA	CMB-C2B-C3B	3.19	130.65	124.68
45	BB	841	CLA	O2D-CGD-O1D	-3.19	117.60	123.84
45	A6	610	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
45	AA	803	CLA	O2D-CGD-CBD	3.19	116.94	111.27
45	AA	811	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
45	B1	314	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
54	B2	614	CHL	C1D-ND-C4D	3.19	108.60	106.33
45	B1	310	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
48	AF	801	BCR	C30-C25-C26	-3.19	118.13	122.61
45	BB	829	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
45	BG	201	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
45	AL	304	CLA	CMB-C2B-C3B	3.18	130.63	124.68
45	AB	840	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
45	B3	303	CLA	CMB-C2B-C3B	3.18	130.92	124.69
45	AA	809	CLA	CAA-C2A-C3A	-3.18	104.06	112.78
48	AB	845	BCR	C3-C4-C5	-3.18	108.40	114.08
45	BL	304	CLA	CMB-C2B-C3B	3.18	130.63	124.68
45	B5	601	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
45	BB	819	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
45	AA	817	CLA	CMB-C2B-C3B	3.18	130.63	124.68
45	AB	823	CLA	CHD-C1D-ND	-3.18	121.53	124.45
45	AB	816	CLA	CMB-C2B-C3B	3.18	130.62	124.68
45	B2	603	CLA	CMB-C2B-C3B	3.18	130.62	124.68
54	A6	608	CHL	CHC-C1C-C2C	-3.17	117.94	126.72
45	AL	305	CLA	CMB-C2B-C1B	-3.17	123.58	128.46
45	AA	824	CLA	CBA-CAA-C2A	3.17	123.23	113.86
45	BB	819	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
56	BJ	104	SQD	C3-C4-C5	3.17	115.90	110.24
45	AA	815	CLA	CMB-C2B-C3B	3.17	130.61	124.68
45	A4	308	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
45	BL	303	CLA	CHD-C1D-ND	-3.17	121.54	124.45
48	BA	849	BCR	C36-C18-C17	-3.17	118.48	122.92
48	BK	204	BCR	C38-C26-C25	-3.17	120.97	124.53
45	B3	305	CLA	CMB-C2B-C3B	3.17	130.89	124.69
45	A3	309	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
45	A4	313	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
45	AB	821	CLA	CMB-C2B-C3B	3.17	130.60	124.68
45	AB	842	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
45	AA	807	CLA	CHD-C1D-ND	-3.16	121.55	124.45
45	BK	201	CLA	CMB-C2B-C3B	3.16	130.88	124.69
45	AB	838	CLA	CMB-C2B-C3B	3.16	130.60	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	819	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
45	AA	829	CLA	C2D-C1D-ND	-3.16	107.77	110.10
45	AB	804	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
45	B3	305	CLA	CAB-C3B-C2B	3.16	130.88	124.69
45	AA	812	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
45	B2	613	CLA	CHD-C1D-ND	-3.16	121.55	124.45
45	AB	836	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
48	B5	616	BCR	C23-C22-C21	-3.16	114.09	118.94
45	AB	812	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
48	AK	204	BCR	C29-C30-C25	3.16	115.34	110.48
45	BB	827	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
45	AA	818	CLA	CMB-C2B-C3B	3.16	130.58	124.68
45	BA	832	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
46	AA	843	PQN	C14-C13-C12	-3.16	115.58	123.68
48	BF	304	BCR	C37-C22-C23	3.15	123.05	118.08
45	BA	834	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
54	A4	304	CHL	C1C-C2C-C3C	-3.15	104.61	107.11
45	AG	204	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
45	AA	815	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
48	BB	803	BCR	C29-C30-C25	3.15	115.33	110.48
55	A1	318	XAT	C40-C33-C32	3.15	123.05	118.08
45	A3	311	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
45	BB	830	CLA	C4A-NA-C1A	3.15	108.12	106.71
45	B3	312	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
45	A1	307	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
48	AA	848	BCR	C33-C5-C6	-3.15	120.99	124.53
45	BK	201	CLA	CAB-C3B-C2B	3.15	130.86	124.69
48	BJ	103	BCR	C1-C6-C5	-3.15	118.18	122.61
48	BF	304	BCR	C16-C15-C14	-3.15	117.02	123.47
48	BA	855	BCR	C8-C9-C10	-3.15	114.11	118.94
45	B2	608	CLA	C1B-CHB-C4A	-3.15	123.89	130.12
45	A1	316	CLA	CAB-C3B-C2B	3.15	130.85	124.69
54	B2	607	CHL	CHC-C1C-NC	3.15	128.98	124.20
45	AB	801	CLA	CHB-C4A-NA	3.15	128.86	124.51
52	B1	316	LUT	C20-C13-C14	-3.15	118.52	122.92
45	A1	316	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
52	A3	316	LUT	C3-C4-C5	-3.14	105.59	111.85
45	BB	817	CLA	CMB-C2B-C3B	3.14	130.56	124.68
45	BB	814	CLA	O2D-CGD-O1D	-3.14	117.69	123.84
45	BK	202	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
54	B1	308	CHL	C4A-NA-C1A	-3.14	105.30	106.71
45	B3	305	CLA	O2D-CGD-O1D	-3.14	117.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	836	CLA	CMB-C2B-C3B	3.14	130.55	124.68
45	BB	809	CLA	O2D-CGD-O1D	-3.14	117.71	123.84
48	AB	849	BCR	C4-C5-C6	-3.13	118.18	122.73
55	B1	317	XAT	C35-C15-C14	-3.13	117.06	123.47
45	BB	838	CLA	CMB-C2B-C3B	3.13	130.54	124.68
45	BA	808	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
45	AB	828	CLA	CHB-C4A-NA	3.13	128.84	124.51
45	AB	806	CLA	CHB-C4A-NA	3.13	128.84	124.51
45	AB	817	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
45	AB	825	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
48	BL	301	BCR	C34-C9-C8	3.13	123.00	118.08
45	AB	808	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
55	B1	317	XAT	C26-C27-C28	-3.13	119.38	125.99
45	BB	825	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
45	BL	304	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
45	AA	823	CLA	C4A-NA-C1A	3.13	108.11	106.71
45	BB	827	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
48	BI	101	BCR	C28-C27-C26	-3.12	108.50	114.08
55	A1	318	XAT	C39-C29-C28	3.12	123.00	118.08
45	B5	612	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
45	BF	301	CLA	CMB-C2B-C3B	3.12	130.52	124.68
48	BA	847	BCR	C37-C22-C23	3.12	123.00	118.08
45	AA	834	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
45	BB	828	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
45	BB	819	CLA	CMB-C2B-C3B	3.12	130.52	124.68
45	A1	310	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
48	AJ	103	BCR	C7-C8-C9	-3.12	121.52	126.23
48	BF	304	BCR	C7-C8-C9	-3.12	121.52	126.23
45	BB	810	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
45	BF	303	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
45	A3	314	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
52	B1	316	LUT	C40-C33-C34	-3.12	118.55	122.92
45	AB	825	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
48	AB	844	BCR	C33-C5-C6	3.12	128.03	124.53
48	BB	848	BCR	C29-C30-C25	3.12	115.28	110.48
45	A4	303	CLA	CAB-C3B-C2B	3.12	130.79	124.69
45	AB	828	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
54	B5	605	CHL	CHD-C4C-NC	3.11	129.11	124.20
45	AB	817	CLA	CHD-C1D-ND	-3.11	121.59	124.45
45	BB	802	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
45	A1	304	CLA	CAC-C3C-C4C	3.11	128.85	124.81
45	BL	303	CLA	CMB-C2B-C3B	3.11	130.50	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	850	BCR	C19-C18-C17	-3.11	114.17	118.94
45	AL	304	CLA	CHD-C1D-ND	-3.11	121.60	124.45
45	B2	602	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
48	BL	301	BCR	C37-C22-C23	3.11	122.97	118.08
45	B3	304	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
45	AA	831	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
45	A6	605	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
45	B3	308	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
45	AB	818	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
48	BA	855	BCR	C39-C30-C25	-3.10	105.26	110.30
54	A1	308	CHL	C1C-C2C-C3C	-3.10	104.65	107.11
45	AB	817	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
54	B5	607	CHL	CHA-C4D-ND	3.10	138.99	132.50
45	BB	802	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
45	A4	303	CLA	CMB-C2B-C3B	3.10	130.76	124.69
45	AA	808	CLA	CMB-C2B-C3B	3.10	130.48	124.68
48	BA	850	BCR	C27-C26-C25	-3.10	118.23	122.73
45	A3	306	CLA	CAB-C3B-C2B	3.10	130.76	124.69
45	BB	829	CLA	CMB-C2B-C3B	3.10	130.47	124.68
45	AA	834	CLA	C4-C3-C5	3.10	120.48	115.27
45	AB	814	CLA	CMB-C2B-C3B	3.10	130.47	124.68
45	BA	829	CLA	C2D-C1D-ND	-3.10	107.82	110.10
45	AB	815	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
45	BB	830	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
45	BA	810	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
48	B5	616	BCR	C23-C24-C25	-3.09	118.52	127.20
45	AB	818	CLA	CHB-C4A-NA	3.09	128.78	124.51
45	BA	807	CLA	CMB-C2B-C3B	3.09	130.46	124.68
45	AA	832	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
48	AA	849	BCR	C2-C3-C4	-3.09	104.48	111.38
45	A4	301	CLA	CMB-C2B-C3B	3.09	130.45	124.68
45	BB	824	CLA	CMB-C2B-C3B	3.09	130.45	124.68
45	AB	839	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
48	AB	844	BCR	C30-C25-C26	-3.09	118.27	122.61
48	A1	319	BCR	C33-C5-C4	3.08	119.54	113.62
51	BB	850	DGD	O1G-C1A-C2A	3.08	121.58	111.91
48	AB	846	BCR	C1-C6-C5	-3.08	118.27	122.61
45	AA	841	CLA	CHB-C4A-NA	3.08	128.78	124.51
48	BB	849	BCR	C15-C16-C17	-3.08	117.16	123.47
52	A6	615	LUT	C8-C9-C10	-3.08	114.21	118.94
45	BA	828	CLA	O2D-CGD-CBD	3.08	116.74	111.27
45	AA	821	CLA	O2D-CGD-O1D	-3.08	117.81	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	824	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
45	A6	603	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
45	BB	818	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
45	A4	312	CLA	CHD-C1D-ND	-3.08	121.62	124.45
45	AA	813	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
45	A4	301	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
45	BB	827	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
45	AA	828	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
45	BF	302	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
45	A4	312	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
45	AA	804	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
45	A6	609	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
45	AB	810	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
52	B3	315	LUT	C15-C35-C34	-3.08	117.17	123.47
45	AB	818	CLA	CMB-C2B-C3B	3.07	130.43	124.68
45	AB	807	CLA	CHD-C1D-ND	-3.07	121.63	124.45
45	BB	827	CLA	C4A-NA-C1A	3.07	108.09	106.71
52	AF	806	LUT	C37-C21-C36	3.07	112.42	107.89
45	BA	817	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
48	BB	849	BCR	C38-C26-C25	-3.07	121.08	124.53
45	BB	829	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
45	BA	806	CLA	CHB-C4A-NA	3.06	128.75	124.51
54	B5	606	CHL	CHC-C1C-C2C	-3.06	118.25	126.72
48	BB	849	BCR	C28-C27-C26	-3.06	108.61	114.08
45	BA	821	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
45	A6	601	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
45	B1	315	CLA	CAB-C3B-C2B	3.06	130.69	124.69
54	A6	608	CHL	CHA-C4D-ND	3.06	138.91	132.50
45	AA	810	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
45	B3	307	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
45	BB	805	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
48	BB	803	BCR	C12-C13-C14	-3.06	114.24	118.94
54	A1	308	CHL	CHD-C4C-NC	3.06	129.03	124.20
45	AA	829	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
45	B1	315	CLA	CMB-C2B-C3B	3.06	130.68	124.69
45	AA	828	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
45	B5	608	CLA	CMB-C2B-C3B	3.06	130.40	124.68
45	BA	841	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
45	AA	842	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
45	BA	824	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
48	AA	852	BCR	C36-C18-C17	-3.05	118.65	122.92
45	BA	844	CLA	O2D-CGD-O1D	-3.05	117.87	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	B2	615	LUT	C17-C1-C6	-3.05	105.35	110.30
45	A6	605	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
45	BH	201	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
45	B5	603	CLA	CAB-C3B-C2B	3.05	130.66	124.69
45	AB	819	CLA	C6-C5-C3	3.05	121.44	113.45
45	AB	829	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
45	A3	313	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
48	AB	846	BCR	C8-C9-C10	3.05	123.61	118.94
54	B2	601	CHL	CHC-C1C-NC	3.05	128.82	124.20
45	BA	814	CLA	CMB-C2B-C3B	3.04	130.38	124.68
48	AF	801	BCR	C37-C22-C21	-3.04	118.66	122.92
45	BA	820	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
45	B2	613	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
45	BA	835	CLA	CMB-C2B-C3B	3.04	130.37	124.68
45	A6	603	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
45	B1	314	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
45	A3	308	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
54	B2	607	CHL	CHA-C4D-ND	3.04	138.86	132.50
45	BB	833	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
45	B2	610	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
45	B3	312	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
46	AA	843	PQN	O1-C1-C2	-3.04	116.31	120.25
45	AB	803	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
45	AA	836	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
55	A4	316	XAT	C26-C27-C28	-3.04	119.57	125.99
45	BB	829	CLA	CHB-C4A-NA	3.04	128.71	124.51
45	B5	602	CLA	CMB-C2B-C3B	3.04	130.36	124.68
45	BA	809	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
45	B3	301	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
45	BL	302	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
45	BA	806	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
45	AB	802	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
48	BJ	103	BCR	C19-C18-C17	-3.03	114.28	118.94
45	BA	820	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
45	AB	809	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
45	B5	613	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
45	BA	842	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
45	BH	201	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
45	A4	309	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
45	BB	813	CLA	CMB-C2B-C3B	3.03	130.62	124.69
45	BB	836	CLA	CHD-C1D-ND	-3.03	121.67	124.45
45	BA	819	CLA	O2D-CGD-O1D	-3.03	117.92	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A4	309	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
45	A1	306	CLA	CMB-C2B-C3B	3.03	130.34	124.68
48	BI	101	BCR	C1-C6-C5	-3.03	118.35	122.61
45	B5	609	CLA	C4A-NA-C1A	3.03	108.07	106.71
48	AF	805	BCR	C36-C18-C19	3.02	122.84	118.08
45	B1	306	CLA	CMB-C2B-C1B	-3.02	123.81	128.46
45	BA	831	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
48	AL	306	BCR	C36-C18-C19	3.02	122.84	118.08
48	AL	306	BCR	C30-C25-C26	-3.02	118.36	122.61
45	AA	817	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
45	AB	804	CLA	CMB-C2B-C3B	3.02	130.33	124.68
45	AA	807	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
45	AB	808	CLA	CMB-C2B-C3B	3.02	130.33	124.68
48	AJ	101	BCR	C37-C22-C21	-3.02	118.69	122.92
45	AA	834	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
45	A1	314	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
45	BA	835	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
52	A4	315	LUT	C39-C29-C28	3.01	122.83	118.08
45	B5	601	CLA	CMB-C2B-C3B	3.01	130.32	124.68
45	B1	310	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
45	BA	811	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
45	BB	836	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
45	BB	822	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
45	A1	305	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
54	B2	614	CHL	C1C-C2C-C3C	-3.01	104.72	107.11
48	AB	844	BCR	C32-C1-C6	-3.01	105.42	110.30
52	B2	615	LUT	C28-C29-C30	-3.01	114.32	118.94
54	A1	308	CHL	CHC-C1C-NC	3.01	128.77	124.20
45	BB	813	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
45	BA	822	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
45	AA	805	CLA	CHD-C1D-ND	-3.01	121.69	124.45
54	A6	606	CHL	CHC-C1C-NC	3.01	128.76	124.20
45	BJ	102	CLA	CMB-C2B-C3B	3.01	130.30	124.68
45	A3	309	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
48	BF	304	BCR	C1-C6-C5	-3.00	118.38	122.61
45	B3	308	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
45	A3	313	CLA	CMB-C2B-C3B	3.00	130.30	124.68
48	BA	855	BCR	C4-C5-C6	-3.00	118.37	122.73
45	BB	818	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
48	AJ	101	BCR	C36-C18-C19	3.00	122.81	118.08
45	AA	806	CLA	CHB-C4A-NA	3.00	128.66	124.51
55	A1	318	XAT	C12-C13-C14	-3.00	114.34	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	825	CLA	CMB-C2B-C3B	3.00	130.29	124.68
45	AB	819	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
45	AL	305	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
45	BB	824	CLA	CHD-C1D-ND	-3.00	121.70	124.45
45	BA	833	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
45	AB	803	CLA	C1B-CHB-C4A	-3.00	124.18	130.12
55	B5	615	XAT	C40-C33-C32	3.00	122.80	118.08
48	AA	848	BCR	C30-C25-C26	-3.00	118.39	122.61
54	B3	306	CHL	CHA-C4D-ND	3.00	138.77	132.50
45	A6	604	CLA	CMB-C2B-C3B	3.00	130.28	124.68
45	A1	310	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
45	A3	308	CLA	CMB-C2B-C3B	2.99	130.28	124.68
45	A3	311	CLA	CMB-C2B-C3B	2.99	130.28	124.68
45	AB	820	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
45	BA	815	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
45	A4	309	CLA	CMB-C2B-C3B	2.99	130.28	124.68
54	B1	303	CHL	CHA-C4D-ND	2.99	138.76	132.50
45	A6	611	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
45	AA	821	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
48	B2	617	BCR	C38-C26-C25	-2.99	121.17	124.53
48	B5	616	BCR	C12-C13-C14	-2.99	114.36	118.94
45	AA	820	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
45	A4	312	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
45	BA	831	CLA	CMB-C2B-C3B	2.99	130.26	124.68
45	BA	839	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
45	AL	304	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
45	B5	604	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
45	AH	201	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
47	BA	845	LHG	O7-C7-C8	2.98	117.93	111.50
54	A6	607	CHL	C1C-C2C-C3C	-2.98	104.75	107.11
45	A3	303	CLA	CMB-C2B-C3B	2.98	130.26	124.68
45	AB	829	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
45	A4	307	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
45	A4	303	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
45	BA	834	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
45	AA	820	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
48	A3	318	BCR	C24-C23-C22	-2.98	121.73	126.23
45	AA	812	CLA	C4-C3-C5	2.98	120.28	115.27
48	BB	847	BCR	C37-C22-C23	2.98	122.77	118.08
45	BB	820	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
45	BB	843	CLA	CMB-C2B-C3B	2.98	130.25	124.68
45	BA	815	CLA	CMB-C2B-C1B	-2.98	123.89	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	848	BCR	C8-C9-C10	-2.97	114.38	118.94
45	BB	809	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
45	AB	842	CLA	CMB-C2B-C3B	2.97	130.24	124.68
45	AA	804	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
45	A3	310	CLA	CBD-CHA-C1A	2.97	132.19	127.43
48	BA	848	BCR	C38-C26-C25	-2.97	121.19	124.53
45	BA	817	CLA	CMB-C2B-C3B	2.97	130.24	124.68
45	BB	841	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
45	B3	303	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
48	BB	803	BCR	C40-C30-C25	-2.97	105.48	110.30
47	AA	844	LHG	O7-C7-C8	2.97	117.90	111.50
45	AA	841	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
54	B1	303	CHL	CHC-C1C-NC	2.97	128.71	124.20
45	AB	811	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
45	AB	812	CLA	CAB-C3B-C2B	2.97	130.50	124.69
45	BA	844	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
48	AI	101	BCR	C38-C26-C27	2.97	119.31	113.62
45	A4	311	CLA	C1B-CHB-C4A	-2.97	124.24	130.12
45	AA	835	CLA	CMB-C2B-C3B	2.97	130.23	124.68
52	A3	316	LUT	C16-C1-C6	2.97	115.11	110.30
45	BA	826	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
45	BB	827	CLA	CMB-C2B-C3B	2.96	130.22	124.68
45	AB	826	CLA	C4A-NA-C1A	2.96	108.04	106.71
45	B2	602	CLA	CAC-C3C-C4C	2.96	128.65	124.81
45	A3	305	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
45	AA	805	CLA	CAA-C2A-C1A	-2.96	102.27	111.97
52	A4	315	LUT	C28-C29-C30	-2.96	114.40	118.94
45	BB	801	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
45	AB	825	CLA	CMB-C2B-C3B	2.96	130.22	124.68
45	AA	818	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
45	B5	601	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
47	B1	301	LHG	O8-C23-C24	2.96	121.19	111.91
45	BF	302	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
45	BB	810	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
45	AA	822	CLA	O2D-CGD-CBD	2.96	116.53	111.27
54	A6	602	CHL	CHA-C4D-ND	2.96	138.69	132.50
54	B2	601	CHL	CHA-C4D-ND	2.96	138.69	132.50
45	B5	602	CLA	CHD-C1D-ND	-2.96	121.74	124.45
45	B1	312	CLA	CAB-C3B-C2B	2.96	130.48	124.69
45	BB	836	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
45	AB	823	CLA	CHB-C4A-NA	2.95	128.60	124.51
54	A4	314	CHL	C4A-NA-C1A	-2.95	105.38	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B5	610	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
51	BB	850	DGD	C2G-O2G-C1B	-2.95	110.52	117.79
45	A1	313	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
45	BA	810	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
45	BB	808	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
54	A4	306	CHL	C1D-ND-C4D	2.95	108.43	106.33
45	A3	302	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
45	AA	834	CLA	CHD-C1D-ND	-2.95	121.74	124.45
45	AB	835	CLA	CHD-C1D-ND	-2.95	121.74	124.45
45	BA	816	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
45	AL	303	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
54	B2	605	CHL	CHA-C4D-ND	2.95	138.67	132.50
48	B2	617	BCR	C37-C22-C23	2.95	122.72	118.08
52	A6	615	LUT	C21-C26-C27	-2.95	108.97	112.70
52	B5	614	LUT	C8-C9-C10	-2.95	114.42	118.94
48	BB	848	BCR	C15-C16-C17	-2.95	117.44	123.47
45	BA	801	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
48	B3	317	BCR	C15-C16-C17	-2.94	117.44	123.47
56	e	301	SQD	O5-C5-C4	2.94	115.04	109.69
48	BA	856	BCR	C15-C16-C17	-2.94	117.44	123.47
45	A1	312	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
45	AB	801	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
45	A6	601	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
54	B2	601	CHL	C1C-C2C-C3C	-2.94	104.78	107.11
55	B3	316	XAT	C36-C21-C22	-2.94	103.87	108.98
45	B1	305	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
48	AA	849	BCR	C30-C25-C26	-2.94	118.47	122.61
45	AA	816	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
45	AB	824	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
48	BB	846	BCR	C37-C22-C21	-2.94	118.81	122.92
45	B2	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
45	A3	312	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
45	BA	832	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
45	AB	826	CLA	CHD-C1D-ND	-2.94	121.75	124.45
45	AA	813	CLA	CMB-C2B-C3B	2.94	130.17	124.68
52	B5	614	LUT	C35-C15-C14	-2.94	117.46	123.47
45	BK	202	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
45	A1	310	CLA	CAB-C3B-C2B	2.93	130.44	124.69
48	AJ	101	BCR	C16-C15-C14	-2.93	117.46	123.47
45	BB	821	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
48	AA	852	BCR	C24-C23-C22	-2.93	121.80	126.23
45	BA	806	CLA	CMB-C2B-C1B	-2.93	123.96	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B2	614	CHL	CHC-C1C-NC	2.93	128.65	124.20
45	A1	307	CLA	CMB-C2B-C3B	2.93	130.16	124.68
45	A6	614	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
48	AB	848	BCR	C28-C27-C26	-2.93	108.84	114.08
45	AB	820	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
48	AL	306	BCR	C37-C22-C21	-2.93	118.82	122.92
45	B2	602	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
54	B2	606	CHL	CHA-C4D-ND	2.93	138.63	132.50
54	A1	303	CHL	CHC-C1C-NC	2.93	128.65	124.20
55	A4	316	XAT	O4-C5-C18	2.93	118.57	115.06
45	BK	202	CLA	CMB-C2B-C3B	2.93	130.16	124.68
45	B2	609	CLA	CMB-C2B-C3B	2.93	130.16	124.68
45	A3	304	CLA	CMB-C2B-C3B	2.93	130.42	124.69
54	A1	308	CHL	CHA-C4D-ND	2.93	138.62	132.50
45	AA	824	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
45	AA	810	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
45	A3	303	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
45	AA	806	CLA	CMB-C2B-C1B	-2.93	123.97	128.46
45	B3	303	CLA	CAB-C3B-C2B	2.93	130.42	124.69
45	BA	817	CLA	CHD-C1D-ND	-2.93	121.77	124.45
45	AA	835	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
45	B1	307	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
55	A6	616	XAT	C20-C13-C12	2.92	122.69	118.08
45	AF	802	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
45	AF	803	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
48	AB	849	BCR	C36-C18-C19	2.92	122.68	118.08
45	AA	809	CLA	CHB-C4A-NA	2.92	128.56	124.51
48	AB	846	BCR	C33-C5-C4	2.92	119.23	113.62
45	A1	306	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
45	BA	825	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
45	A1	315	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
45	B2	610	CLA	CGD-CBD-CAD	2.92	120.19	110.73
48	BA	849	BCR	C3-C4-C5	-2.92	108.86	114.08
45	AA	827	CLA	CMB-C2B-C3B	2.92	130.14	124.68
45	AB	811	CLA	CMB-C2B-C3B	2.92	130.14	124.68
48	AA	847	BCR	C37-C22-C21	-2.92	118.83	122.92
45	A1	309	CLA	CMB-C2B-C3B	2.92	130.14	124.68
48	A4	317	BCR	C15-C16-C17	-2.92	117.50	123.47
45	BA	807	CLA	CHD-C1D-ND	-2.92	121.77	124.45
54	A4	304	CHL	CHC-C1C-NC	2.92	128.63	124.20
54	B5	607	CHL	CHC-C1C-NC	2.92	128.63	124.20
45	BB	837	CLA	CMB-C2B-C1B	-2.92	123.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	838	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
45	BB	807	CLA	CHD-C1D-ND	-2.92	121.78	124.45
52	B3	315	LUT	C8-C9-C10	-2.91	114.47	118.94
48	AI	102	BCR	C4-C5-C6	-2.91	118.50	122.73
45	AA	815	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
45	A4	303	CLA	C1B-CHB-C4A	-2.91	124.34	130.12
45	BB	815	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
55	A6	616	XAT	C12-C13-C14	-2.91	114.47	118.94
52	B3	315	LUT	C37-C21-C22	-2.91	103.92	109.44
45	AB	814	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
45	B3	310	CLA	CMB-C2B-C3B	2.91	130.13	124.68
54	B2	605	CHL	CHC-C1C-NC	2.91	128.62	124.20
48	BK	204	BCR	C28-C27-C26	-2.91	108.88	114.08
48	AA	845	BCR	C37-C22-C23	2.91	122.66	118.08
54	A6	608	CHL	C3A-C2A-C1A	-2.91	96.98	101.34
45	A1	315	CLA	CMB-C2B-C3B	2.91	130.38	124.69
45	BJ	102	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
48	BA	849	BCR	C37-C22-C23	2.91	122.66	118.08
45	AA	811	CLA	CMB-C2B-C3B	2.91	130.12	124.68
45	AA	831	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
45	A4	310	CLA	CMB-C2B-C3B	2.91	130.11	124.68
48	BB	848	BCR	C23-C22-C21	-2.90	114.49	118.94
45	BA	811	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
48	A3	318	BCR	C37-C22-C23	2.90	122.65	118.08
45	B2	609	CLA	CHB-C4A-NA	2.90	128.52	124.51
45	AB	836	CLA	CMB-C2B-C3B	2.90	130.10	124.68
48	AA	846	BCR	C35-C13-C12	2.90	122.65	118.08
54	A3	307	CHL	C4C-C3C-C2C	-2.90	102.67	106.90
45	A1	305	CLA	C5-C3-C2	2.90	126.99	121.12
45	AA	823	CLA	CHD-C1D-ND	-2.90	121.79	124.45
54	B5	605	CHL	CHA-C4D-ND	2.90	138.56	132.50
45	AK	202	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
48	AA	846	BCR	C31-C1-C6	-2.90	105.60	110.30
48	BB	847	BCR	C23-C22-C21	2.90	123.39	118.94
45	BA	812	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
45	B1	311	CLA	CHB-C4A-NA	2.90	128.52	124.51
45	AB	808	CLA	CHD-C1D-ND	-2.90	121.79	124.45
45	BA	824	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
45	AB	812	CLA	CMB-C2B-C3B	2.90	130.36	124.69
45	AB	828	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
45	BA	816	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
45	B1	312	CLA	C1B-CHB-C4A	-2.90	124.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	828	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
45	AJ	102	CLA	CMB-C2B-C3B	2.90	130.10	124.68
45	AK	203	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
45	BA	818	CLA	CMB-C2B-C3B	2.90	130.09	124.68
48	AB	844	BCR	C16-C15-C14	-2.89	117.54	123.47
45	A1	316	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
45	BB	806	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
45	BB	833	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
45	A6	613	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
45	BB	804	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
45	BB	804	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
45	BB	801	CLA	C2D-C1D-ND	-2.89	107.97	110.10
45	B3	301	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
45	AB	820	CLA	C4A-NA-C1A	2.89	108.01	106.71
55	B1	317	XAT	C12-C13-C14	-2.89	114.50	118.94
45	BB	838	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
45	B1	314	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
48	AA	847	BCR	C10-C11-C12	2.89	132.24	123.22
45	BB	813	CLA	CAB-C3B-C2B	2.89	130.35	124.69
45	BA	836	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
45	B2	612	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
48	AJ	101	BCR	C8-C9-C10	-2.89	114.51	118.94
45	AG	203	CLA	CMB-C2B-C1B	-2.89	124.03	128.46
45	BA	823	CLA	CMB-C2B-C3B	2.89	130.08	124.68
47	F	801	LHG	O8-C23-C24	2.89	120.97	111.91
45	B5	604	CLA	CMB-C2B-C3B	2.89	130.34	124.69
45	BA	831	CLA	O2D-CGD-O1D	-2.89	118.20	123.84
45	AB	834	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
48	B2	617	BCR	C38-C26-C27	2.88	119.16	113.62
45	BB	834	CLA	CHB-C4A-NA	2.88	128.50	124.51
45	A3	310	CLA	CMB-C2B-C3B	2.88	130.07	124.68
45	AB	824	CLA	CBA-CAA-C2A	2.88	120.10	114.02
45	B5	604	CLA	CAB-C3B-C2B	2.88	130.34	124.69
45	BA	827	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
48	AA	848	BCR	C23-C22-C21	-2.88	114.52	118.94
48	AA	847	BCR	C32-C1-C6	-2.88	105.62	110.30
54	A4	306	CHL	CHA-C4D-ND	2.88	138.53	132.50
48	BA	848	BCR	C36-C18-C17	-2.88	118.89	122.92
48	B3	317	BCR	C23-C22-C21	-2.88	114.52	118.94
45	BA	805	CLA	CHD-C1D-ND	-2.88	121.81	124.45
50	AA	851	LMU	C3B-C4B-C5B	2.88	115.37	110.24
45	AB	813	CLA	CMB-C2B-C3B	2.88	130.06	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	851	BCR	C31-C1-C6	-2.88	105.63	110.30
45	AA	813	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
45	BA	803	CLA	O2D-CGD-CBD	2.88	116.38	111.27
45	A6	605	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
45	AA	822	CLA	CMB-C2B-C3B	2.88	130.06	124.68
45	BB	806	CLA	O2D-CGD-O1D	-2.88	118.22	123.84
45	AA	809	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
45	AB	805	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
45	B1	315	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
45	BB	834	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
45	BB	840	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
45	BA	813	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
48	AB	844	BCR	C40-C30-C25	-2.87	105.64	110.30
48	BJ	103	BCR	C7-C8-C9	-2.87	121.89	126.23
45	AB	841	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
55	B3	316	XAT	C12-C13-C14	-2.87	114.53	118.94
45	AB	832	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
45	BB	812	CLA	CMB-C2B-C3B	2.87	130.05	124.68
45	BA	829	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
48	A6	617	BCR	C1-C6-C5	-2.87	118.57	122.61
45	BB	801	CLA	CMB-C2B-C1B	-2.87	124.05	128.46
48	BJ	103	BCR	C16-C15-C14	-2.87	117.59	123.47
45	B3	308	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
48	BA	849	BCR	C16-C15-C14	-2.87	117.59	123.47
45	B1	306	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
55	A3	317	XAT	C8-C9-C10	-2.87	114.54	118.94
45	A1	304	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
45	BA	807	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
48	BJ	103	BCR	C15-C16-C17	-2.87	117.60	123.47
45	BA	814	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
45	BA	819	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
45	AA	813	CLA	CHB-C4A-NA	2.86	128.47	124.51
45	BA	815	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
45	B5	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
48	BA	850	BCR	C23-C22-C21	-2.86	114.55	118.94
45	B1	309	CLA	CMB-C2B-C3B	2.86	130.04	124.68
45	BB	801	CLA	CAA-C2A-C1A	-2.86	102.59	111.97
45	AA	826	CLA	C1B-CHB-C4A	-2.86	124.45	130.12
45	B1	312	CLA	CMB-C2B-C3B	2.86	130.29	124.69
52	A1	317	LUT	C28-C29-C30	-2.86	114.55	118.94
48	AA	849	BCR	C20-C21-C22	-2.86	123.23	127.31
45	AB	816	CLA	C1B-CHB-C4A	-2.86	124.45	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	805	CLA	CMC-C2C-C1C	-2.86	120.68	125.04
45	BB	842	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
45	BB	834	CLA	C6-C5-C3	2.86	120.95	113.45
48	BL	305	BCR	C1-C6-C5	-2.86	118.59	122.61
45	AB	802	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
45	AA	823	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
48	A3	318	BCR	C29-C30-C25	2.86	114.88	110.48
45	BB	820	CLA	C6-C5-C3	2.86	120.95	113.45
45	AA	811	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
45	A1	309	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
48	AJ	103	BCR	C34-C9-C8	2.86	122.58	118.08
45	AB	827	CLA	CHB-C4A-NA	2.86	128.46	124.51
45	AA	834	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
45	AB	838	CLA	CHD-C1D-ND	-2.85	121.83	124.45
48	A4	317	BCR	C27-C26-C25	-2.85	118.59	122.73
45	BH	201	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
46	AA	843	PQN	C16-C15-C13	-2.85	105.98	113.45
45	BA	827	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
45	A4	302	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
45	B5	608	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
45	BA	842	CLA	CMB-C2B-C3B	2.85	130.01	124.68
52	B2	615	LUT	C1-C6-C5	-2.85	118.60	122.61
45	A4	311	CLA	CMB-C2B-C3B	2.85	130.00	124.68
55	B2	616	XAT	C38-C25-C26	-2.85	117.49	122.26
45	BB	820	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
45	AA	824	CLA	CMB-C2B-C3B	2.84	130.00	124.68
48	BB	848	BCR	C30-C25-C26	-2.84	118.61	122.61
45	AB	801	CLA	O2D-CGD-CBD	2.84	116.32	111.27
54	A3	307	CHL	CHA-C4D-ND	2.84	138.45	132.50
45	B1	307	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
45	A3	306	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
54	A6	608	CHL	O2A-CGA-CBA	2.84	120.83	111.91
45	AA	804	CLA	CHB-C4A-NA	2.84	128.44	124.51
48	B2	617	BCR	C31-C1-C6	2.84	114.91	110.30
54	B1	303	CHL	C1C-C2C-C3C	-2.84	104.86	107.11
45	B5	604	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
45	AB	834	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
45	A1	312	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
45	AA	801	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
45	AB	808	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
45	A6	610	CLA	CMB-C2B-C3B	2.84	129.99	124.68
45	B5	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B2	603	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
48	BA	849	BCR	C33-C5-C4	2.84	119.07	113.62
45	A1	307	CLA	O2D-CGD-CBD	2.84	116.31	111.27
45	BB	832	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
45	BB	826	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
45	AA	832	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
45	B3	302	CLA	CMB-C2B-C1B	-2.84	124.11	128.46
54	B1	308	CHL	CHC-C1C-NC	2.84	128.50	124.20
45	BL	302	CLA	CHB-C4A-NA	2.83	128.43	124.51
45	BA	835	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
45	A3	310	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
54	A4	314	CHL	CHA-C4D-ND	2.83	138.42	132.50
45	BB	837	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
45	BB	821	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
45	A4	301	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
45	BB	807	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
45	BA	830	CLA	C1B-CHB-C4A	-2.83	124.52	130.12
48	BJ	103	BCR	C30-C25-C26	-2.83	118.63	122.61
48	BF	304	BCR	C33-C5-C6	-2.83	121.36	124.53
45	AA	828	CLA	C14-C13-C15	2.83	121.52	111.29
52	A6	615	LUT	C28-C29-C30	-2.83	114.61	118.94
45	BA	816	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
45	BA	838	CLA	C1B-CHB-C4A	-2.82	124.52	130.12
45	AJ	102	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
45	B5	613	CLA	CHD-C1D-ND	-2.82	121.86	124.45
45	B1	309	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
45	AB	834	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
45	AA	831	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
45	AB	831	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
45	AB	838	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
52	B5	614	LUT	C40-C33-C32	2.82	122.52	118.08
45	AB	825	CLA	CHB-C4A-NA	2.82	128.41	124.51
48	AF	805	BCR	C12-C13-C14	2.82	123.27	118.94
45	BB	826	CLA	CHB-C4A-NA	2.82	128.41	124.51
52	A1	317	LUT	C1-C6-C5	-2.82	118.64	122.61
45	AA	812	CLA	CMB-C2B-C3B	2.82	129.95	124.68
45	BA	811	CLA	CMB-C2B-C3B	2.82	129.95	124.68
45	A6	613	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
54	A6	606	CHL	CHA-C4D-ND	2.82	138.40	132.50
45	A6	610	CLA	CHB-C4A-NA	2.82	128.41	124.51
45	AB	821	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
45	AG	204	CLA	O2D-CGD-O1D	-2.82	118.33	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B5	605	CHL	CAC-C3C-C4C	2.82	129.33	125.04
48	AB	847	BCR	C38-C26-C27	2.82	119.03	113.62
45	B1	311	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
53	A1	321	LMG	C8-O7-C10	-2.82	110.86	117.79
45	A3	312	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
48	AB	847	BCR	C15-C16-C17	-2.82	117.70	123.47
45	BG	202	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
48	BK	204	BCR	C4-C5-C6	-2.82	118.64	122.73
48	B2	617	BCR	C34-C9-C8	2.82	122.51	118.08
48	BG	203	BCR	C23-C22-C21	2.81	123.26	118.94
45	B3	313	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
45	A4	308	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
45	AB	805	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	BL	301	BCR	C36-C18-C17	-2.81	118.98	122.92
45	BB	814	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
54	A3	307	CHL	C2C-C1C-NC	2.81	112.61	109.97
47	a	501	LHG	O8-C23-C24	2.81	120.73	111.91
45	BB	817	CLA	O2D-CGD-O1D	-2.81	117.70	124.09
45	BA	824	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
54	A6	607	CHL	CHA-C4D-ND	2.81	138.38	132.50
45	BB	809	CLA	O2D-CGD-CBD	2.81	116.26	111.27
45	A4	302	CLA	CMB-C2B-C1B	-2.81	124.14	128.46
45	A6	614	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
48	AB	849	BCR	C16-C17-C18	-2.81	123.30	127.31
45	AA	804	CLA	CHD-C1D-ND	-2.81	121.87	124.45
48	AF	801	BCR	C16-C15-C14	-2.81	117.72	123.47
45	BB	837	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
45	A3	306	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
45	AA	806	CLA	CMB-C2B-C3B	2.81	129.93	124.68
45	BA	838	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
45	BB	812	CLA	CAA-C2A-C3A	-2.81	105.09	112.78
48	AA	848	BCR	C7-C8-C9	-2.80	122.00	126.23
45	AB	807	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
54	A4	304	CHL	CHA-C4D-ND	2.80	138.36	132.50
45	AL	305	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
45	A3	304	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
45	A3	309	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
48	B5	616	BCR	C36-C18-C19	2.80	122.49	118.08
45	A3	312	CLA	O2D-CGD-O1D	-2.80	117.73	124.09
45	B3	311	CLA	C1B-CHB-C4A	-2.80	124.57	130.12
47	AJ	104	LHG	O8-C23-C24	2.80	120.69	111.91
45	B5	612	CLA	C1B-CHB-C4A	-2.80	124.57	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	A1	303	CHL	O2A-CGA-O1A	-2.80	116.53	123.59
54	B1	308	CHL	CHA-C4D-ND	2.80	138.35	132.50
45	AB	829	CLA	C2D-C1D-ND	-2.80	108.04	110.10
45	BA	836	CLA	CMB-C2B-C3B	2.80	129.91	124.68
45	B2	612	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
54	A1	303	CHL	CHA-C4D-ND	2.80	138.35	132.50
45	AA	842	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
53	A1	321	LMG	C7-O1-C1	2.79	119.20	113.74
45	A6	603	CLA	CMB-C2B-C3B	2.79	129.90	124.68
52	B3	315	LUT	C32-C33-C34	-2.79	114.66	118.94
45	BA	815	CLA	CMB-C2B-C3B	2.79	129.90	124.68
48	AA	849	BCR	C23-C22-C21	-2.79	114.66	118.94
54	B2	614	CHL	CHA-C4D-ND	2.79	138.34	132.50
45	AB	831	CLA	CMB-C2B-C1B	-2.79	124.17	128.46
45	AA	818	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
45	AB	820	CLA	CMB-C2B-C3B	2.79	129.90	124.68
48	AA	845	BCR	C16-C15-C14	-2.79	117.76	123.47
45	AA	831	CLA	CHD-C1D-ND	-2.79	121.89	124.45
45	BA	844	CLA	CMB-C2B-C3B	2.79	129.90	124.68
45	BA	802	CLA	O2D-CGD-O1D	-2.79	118.38	123.84
45	AB	824	CLA	CMB-C2B-C3B	2.79	129.90	124.68
48	BB	846	BCR	C8-C9-C10	2.79	123.22	118.94
48	BL	301	BCR	C38-C26-C27	2.79	118.97	113.62
45	A3	314	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
45	B2	604	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
52	B2	615	LUT	C15-C35-C34	-2.79	117.76	123.47
45	A1	304	CLA	CMB-C2B-C3B	2.79	129.89	124.68
45	B5	609	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
48	BJ	101	BCR	C37-C22-C23	2.79	122.47	118.08
45	BB	805	CLA	CAC-C3C-C4C	2.79	128.43	124.81
45	BA	804	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
48	AA	846	BCR	C38-C26-C27	2.79	118.97	113.62
45	AB	803	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
45	BA	821	CLA	CHD-C1D-ND	-2.78	121.89	124.45
45	BB	819	CLA	CHB-C4A-NA	2.78	128.36	124.51
48	BB	846	BCR	C28-C27-C26	-2.78	109.11	114.08
45	A6	611	CLA	CAB-C3B-C2B	2.78	130.14	124.69
48	AA	846	BCR	C40-C30-C25	-2.78	105.78	110.30
45	BB	839	CLA	C1B-CHB-C4A	-2.78	124.60	130.12
45	AG	204	CLA	CHB-C4A-NA	2.78	128.36	124.51
48	AK	204	BCR	C36-C18-C17	-2.78	119.02	122.92
48	BK	204	BCR	C37-C22-C21	-2.78	119.02	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	809	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
48	B5	616	BCR	C8-C9-C10	-2.78	114.67	118.94
45	AA	805	CLA	CMB-C2B-C1B	-2.78	124.19	128.46
45	AA	810	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
45	BA	823	CLA	C1B-CHB-C4A	-2.78	124.61	130.12
54	B5	606	CHL	CHA-C4D-ND	2.78	138.32	132.50
48	BJ	103	BCR	C31-C1-C6	2.78	114.81	110.30
45	B2	608	CLA	CMB-C2B-C3B	2.78	129.88	124.68
55	A4	316	XAT	C18-C5-C6	-2.78	117.60	122.26
45	A3	312	CLA	CHD-C1D-ND	-2.78	121.90	124.45
45	A4	309	CLA	CHB-C4A-NA	2.78	128.36	124.51
48	B5	616	BCR	C16-C15-C14	-2.78	117.78	123.47
45	A1	310	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
48	AB	849	BCR	C37-C22-C21	-2.78	119.03	122.92
45	A1	304	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
45	AB	833	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
45	AB	823	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
45	A1	311	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
48	BB	847	BCR	C1-C6-C5	-2.77	118.71	122.61
45	B3	311	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
48	A6	617	BCR	C1-C6-C7	2.77	123.62	115.78
45	A1	315	CLA	O2D-CGD-O1D	-2.77	117.80	124.09
45	A6	603	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
45	AG	201	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
53	AG	202	LMG	O8-C28-C29	2.77	120.60	111.91
45	BB	819	CLA	O2A-CGA-O1A	-2.77	116.61	123.59
45	BA	817	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
48	A3	318	BCR	C36-C18-C19	2.77	122.44	118.08
48	B3	317	BCR	C20-C21-C22	-2.77	123.36	127.31
52	AF	806	LUT	C38-C25-C24	-2.77	117.64	123.56
45	BA	801	CLA	C4A-NA-C1A	2.76	107.95	106.71
45	AB	813	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
45	B5	609	CLA	CHB-C4A-NA	2.76	128.33	124.51
45	A1	305	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
48	AK	204	BCR	C40-C30-C25	-2.76	105.82	110.30
48	B3	317	BCR	C36-C18-C19	2.76	122.43	118.08
55	B3	316	XAT	C26-C27-C28	-2.76	120.15	125.99
54	B1	308	CHL	C1C-C2C-C3C	-2.76	104.92	107.11
48	BK	204	BCR	C34-C9-C8	2.76	122.43	118.08
45	A1	314	CLA	CMB-C2B-C3B	2.76	129.84	124.68
45	AA	809	CLA	C2A-C1A-CHA	2.76	128.69	123.86
52	A1	317	LUT	C39-C29-C28	2.76	122.43	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	823	CLA	CMB-C2B-C3B	2.76	129.84	124.68
45	AA	825	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
45	BA	819	CLA	CMB-C2B-C3B	2.76	129.84	124.68
45	AK	203	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
54	A4	305	CHL	CHA-C4D-ND	2.76	138.27	132.50
48	A4	317	BCR	C1-C6-C7	2.76	123.58	115.78
45	B5	613	CLA	CMB-C2B-C3B	2.76	129.84	124.68
45	B1	310	CLA	CAB-C3B-C2B	2.76	130.09	124.69
45	A4	313	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
54	B3	306	CHL	C4C-C3C-C2C	-2.75	102.88	106.90
47	AJ	104	LHG	O7-C7-C8	2.75	117.44	111.50
45	AB	815	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
45	A3	311	CLA	CHB-C4A-NA	2.75	128.32	124.51
45	BF	303	CLA	CMB-C2B-C3B	2.75	129.83	124.68
45	A6	603	CLA	CHB-C4A-NA	2.75	128.32	124.51
47	B5	618	LHG	C5-O7-C7	-2.75	111.02	117.79
45	AG	201	CLA	CMB-C2B-C3B	2.75	129.83	124.68
48	AI	101	BCR	C16-C15-C14	-2.75	117.84	123.47
47	B3	318	LHG	O8-C23-C24	2.75	120.54	111.91
45	BA	813	CLA	CHB-C4A-NA	2.75	128.32	124.51
52	A6	615	LUT	C1-C6-C5	-2.75	118.74	122.61
52	A4	315	LUT	C37-C21-C22	-2.75	104.23	109.44
54	B3	306	CHL	C2C-C1C-NC	2.75	112.55	109.97
56	e	301	SQD	O6-C1-C2	2.75	112.60	108.30
48	AI	101	BCR	C20-C21-C22	-2.75	123.39	127.31
48	B2	617	BCR	C36-C18-C17	-2.75	119.07	122.92
45	AB	801	CLA	C1-O2A-CGA	2.75	123.65	116.44
45	AB	836	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
54	A4	314	CHL	CAC-C3C-C4C	2.75	128.37	124.81
48	A3	318	BCR	C23-C22-C21	-2.75	114.73	118.94
45	BA	818	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
48	AA	848	BCR	C38-C26-C27	2.75	118.89	113.62
45	BA	820	CLA	CMB-C2B-C3B	2.75	129.81	124.68
45	B3	309	CLA	CMB-C2B-C3B	2.75	129.81	124.68
45	AA	812	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
45	BB	822	CLA	C1B-CHB-C4A	-2.75	124.68	130.12
48	A4	317	BCR	C12-C13-C14	-2.74	114.73	118.94
45	BB	839	CLA	CMB-C2B-C3B	2.74	129.81	124.68
52	B5	614	LUT	C28-C29-C30	-2.74	114.73	118.94
48	AG	205	BCR	C37-C22-C23	2.74	122.40	118.08
55	B1	317	XAT	C36-C21-C22	-2.74	104.22	108.98
45	BA	833	CLA	C1B-CHB-C4A	-2.74	124.69	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	822	CLA	CHB-C4A-NA	2.74	128.30	124.51
45	A6	611	CLA	CMB-C2B-C3B	2.74	130.06	124.69
54	B2	606	CHL	C4A-NA-C1A	-2.74	105.47	106.71
45	BA	809	CLA	CMB-C2B-C3B	2.74	129.81	124.68
45	BA	834	CLA	CMB-C2B-C3B	2.74	129.81	124.68
45	AA	801	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
45	B2	610	CLA	CMB-C2B-C3B	2.74	130.05	124.69
52	B2	615	LUT	C8-C7-C6	-2.74	119.51	127.20
52	A3	316	LUT	C40-C33-C32	2.74	122.39	118.08
45	AK	202	CLA	CMB-C2B-C3B	2.74	129.80	124.68
45	A4	312	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
45	BB	822	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
45	AB	822	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
48	AA	847	BCR	C7-C6-C5	2.74	128.09	121.46
45	B1	305	CLA	CMB-C2B-C3B	2.74	129.80	124.68
45	AB	832	CLA	CMB-C2B-C1B	-2.74	124.26	128.46
45	AA	837	CLA	CHB-C4A-NA	2.74	128.30	124.51
45	AB	821	CLA	C1B-CHB-C4A	-2.73	124.70	130.12
45	AA	809	CLA	CMB-C2B-C3B	2.73	129.79	124.68
45	A1	307	CLA	CAC-C3C-C4C	2.73	128.35	124.81
45	AA	817	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
45	AH	201	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
48	AB	845	BCR	C16-C15-C14	-2.73	117.88	123.47
45	BB	827	CLA	CHD-C1D-ND	-2.73	121.94	124.45
45	BA	836	CLA	O2D-CGD-CBD	2.73	116.12	111.27
45	A3	302	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
45	AA	839	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
45	BA	830	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
48	BI	101	BCR	C32-C1-C6	2.73	114.72	110.30
48	A1	319	BCR	C23-C22-C21	-2.73	114.75	118.94
45	BB	817	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
45	A3	315	CLA	C1B-CHB-C4A	-2.73	124.72	130.12
45	AF	804	CLA	CMB-C2B-C3B	2.73	129.78	124.68
45	AA	834	CLA	CHB-C4A-NA	2.73	128.28	124.51
45	AF	802	CLA	CMB-C2B-C3B	2.73	129.78	124.68
48	AB	848	BCR	C1-C6-C5	-2.73	118.78	122.61
45	B1	310	CLA	CMA-C3A-C2A	-2.72	109.74	116.10
45	BA	842	CLA	C1B-CHB-C4A	-2.72	124.72	130.12
45	AA	814	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
45	BB	818	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
45	AA	812	CLA	CHD-C1D-ND	-2.72	121.95	124.45
45	A3	305	CLA	CHD-C1D-ND	-2.72	121.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AF	801	BCR	C8-C9-C10	-2.72	114.77	118.94
50	AB	853	LMU	C2'-C3'-C4'	2.72	115.89	109.68
48	BF	304	BCR	C34-C9-C8	2.72	122.36	118.08
45	AB	810	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
48	AL	306	BCR	C3-C4-C5	-2.72	109.23	114.08
52	A4	315	LUT	C40-C33-C32	2.72	122.36	118.08
54	A4	314	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
45	A3	305	CLA	C1B-CHB-C4A	-2.72	124.74	130.12
45	B1	313	CLA	O2D-CGD-O1D	-2.72	118.53	123.84
45	AL	303	CLA	CMB-C2B-C3B	2.72	129.76	124.68
45	BG	202	CLA	CMB-C2B-C3B	2.72	129.76	124.68
45	B3	312	CLA	CMB-C2B-C3B	2.71	129.76	124.68
45	BA	801	CLA	C1D-ND-C4D	-2.71	104.41	106.33
45	AA	802	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
48	AB	848	BCR	C8-C7-C6	-2.71	119.59	127.20
45	AK	202	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
45	B5	611	CLA	CHB-C4A-NA	2.71	128.26	124.51
45	BF	303	CLA	CAA-C2A-C3A	-2.71	109.77	116.10
48	BB	848	BCR	C19-C18-C17	-2.71	114.78	118.94
45	BA	824	CLA	CHB-C4A-NA	2.71	128.26	124.51
55	B2	616	XAT	C26-C27-C28	-2.71	120.26	125.99
45	A6	612	CLA	CMB-C2B-C3B	2.71	129.75	124.68
55	A6	616	XAT	C40-C33-C34	-2.71	119.13	122.92
45	B3	310	CLA	CHB-C4A-NA	2.71	128.26	124.51
45	BB	826	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
48	BA	856	BCR	C36-C18-C17	-2.71	119.13	122.92
46	BA	843	PQN	C21-C22-C23	-2.71	107.17	115.92
55	A6	616	XAT	C10-C11-C12	-2.71	114.77	123.22
45	BA	823	CLA	CHD-C1D-ND	-2.71	121.97	124.45
45	AB	809	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
45	BA	805	CLA	CMC-C2C-C1C	-2.71	120.92	125.04
45	BA	840	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
54	A4	306	CHL	C3D-C2D-C1D	-2.71	102.14	105.83
48	AB	845	BCR	C38-C26-C25	2.70	127.56	124.53
45	AA	842	CLA	CMB-C2B-C3B	2.70	129.74	124.68
55	A4	316	XAT	C8-C9-C10	-2.70	114.79	118.94
52	B1	316	LUT	C32-C33-C34	2.70	123.09	118.94
48	AB	845	BCR	C30-C25-C26	-2.70	118.81	122.61
48	BA	848	BCR	C12-C13-C14	-2.70	114.80	118.94
48	AB	849	BCR	C30-C25-C26	-2.70	118.81	122.61
45	BB	824	CLA	CHB-C4A-NA	2.70	128.25	124.51
48	BI	101	BCR	C24-C23-C22	-2.70	122.15	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	855	BCR	C36-C18-C19	2.70	122.33	118.08
48	BA	855	BCR	C12-C13-C14	-2.70	114.80	118.94
48	BL	306	BCR	C7-C8-C9	-2.70	122.16	126.23
45	A6	614	CLA	CHD-C1D-ND	-2.70	121.97	124.45
45	BB	820	CLA	CHD-C1D-ND	-2.70	121.97	124.45
48	BA	850	BCR	C16-C15-C14	-2.70	117.94	123.47
45	A1	314	CLA	O2D-CGD-O1D	-2.70	117.96	124.09
45	A6	603	CLA	CAC-C3C-C4C	2.70	128.31	124.81
55	B5	615	XAT	C39-C29-C30	-2.70	119.14	122.92
45	BA	803	CLA	CAC-C3C-C4C	2.70	128.31	124.81
48	AI	101	BCR	C30-C25-C26	-2.70	118.81	122.61
48	A6	617	BCR	C27-C26-C25	-2.70	118.81	122.73
45	BB	816	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
48	BJ	103	BCR	C3-C4-C5	-2.70	109.26	114.08
45	B2	610	CLA	CAB-C3B-C2B	2.70	129.97	124.69
48	AJ	103	BCR	C3-C4-C5	-2.69	109.27	114.08
54	A6	602	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
45	AA	840	CLA	CHB-C4A-NA	2.69	128.24	124.51
45	A6	605	CLA	CMB-C2B-C3B	2.69	129.72	124.68
45	B5	602	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
45	BA	805	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
45	BL	302	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
48	AB	844	BCR	C8-C9-C10	-2.69	114.81	118.94
48	BL	305	BCR	C38-C26-C27	2.69	118.78	113.62
45	B3	305	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
45	B1	304	CLA	CAC-C3C-C4C	2.69	128.30	124.81
45	AJ	102	CLA	C1B-CHB-C4A	-2.69	124.79	130.12
45	B1	304	CLA	CMB-C2B-C3B	2.69	129.71	124.68
55	A1	318	XAT	O24-C25-C38	2.69	118.28	115.06
45	AB	816	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
45	AF	804	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
45	B2	609	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
45	A3	315	CLA	O2D-CGD-O1D	-2.69	117.99	124.09
48	A6	617	BCR	C2-C3-C4	-2.69	105.37	111.38
45	AB	811	CLA	O1D-CGD-CBD	2.69	129.98	124.48
45	AH	201	CLA	C4-C3-C5	2.69	119.79	115.27
45	AA	805	CLA	O2D-CGD-O1D	-2.69	118.59	123.84
55	B5	615	XAT	C38-C25-C26	-2.69	117.76	122.26
45	A6	611	CLA	CGD-CBD-CAD	2.69	119.43	110.73
50	AB	850	LMU	C3B-C4B-C5B	2.68	115.03	110.24
48	AJ	103	BCR	C7-C6-C5	2.68	127.97	121.46
45	BB	820	CLA	C5-C3-C2	-2.68	115.69	121.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	805	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
48	AB	848	BCR	C37-C22-C23	2.68	122.30	118.08
45	BK	203	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
45	B3	309	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
45	AG	201	CLA	CHD-C1D-ND	-2.68	121.99	124.45
45	A1	311	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
45	AA	805	CLA	CMC-C2C-C1C	-2.68	120.96	125.04
45	BF	303	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
48	AL	306	BCR	C37-C22-C23	2.68	122.30	118.08
45	AL	303	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
45	A1	305	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
45	BB	840	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
46	AA	843	PQN	C12-C11-C3	-2.68	104.82	112.05
45	BA	828	CLA	C11-C10-C8	2.68	124.58	115.92
45	BK	201	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
48	BB	849	BCR	C8-C7-C6	-2.68	119.68	127.20
45	B5	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
45	BB	818	CLA	CMB-C2B-C3B	2.68	129.69	124.68
45	AA	822	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
45	A6	609	CLA	O2D-CGD-O1D	-2.68	118.61	123.84
45	A1	313	CLA	CHB-C4A-NA	2.68	128.21	124.51
48	AB	849	BCR	C23-C24-C25	2.68	134.72	127.20
45	BB	838	CLA	CHB-C4A-NA	2.68	128.21	124.51
48	AA	847	BCR	C35-C13-C12	2.67	122.29	118.08
45	BA	822	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
45	AB	835	CLA	CHB-C4A-NA	2.67	128.21	124.51
45	BB	828	CLA	CHB-C4A-NA	2.67	128.21	124.51
45	AA	832	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
45	BF	301	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
48	BL	301	BCR	C2-C1-C6	-2.67	106.37	110.48
48	B2	617	BCR	C1-C6-C5	-2.67	118.85	122.61
45	BB	802	CLA	O2A-CGA-O1A	-2.67	116.85	123.59
45	BA	801	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
50	AL	301	LMU	O5B-C5B-C4B	2.67	114.54	109.69
45	AF	802	CLA	CHB-C4A-NA	2.67	128.20	124.51
45	AB	840	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
45	AA	840	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
45	A1	309	CLA	O2D-CGD-O1D	-2.67	118.03	124.09
48	B3	317	BCR	C1-C6-C7	2.67	123.33	115.78
45	AA	833	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
48	BF	304	BCR	C38-C26-C25	-2.67	121.53	124.53
52	B2	615	LUT	C8-C9-C10	-2.67	114.85	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A4	310	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
48	BB	848	BCR	C38-C26-C27	2.67	118.74	113.62
52	B5	614	LUT	C3-C4-C5	-2.67	106.54	111.85
45	A6	601	CLA	CMB-C2B-C3B	2.67	129.67	124.68
45	BA	829	CLA	C1B-CHB-C4A	-2.67	124.84	130.12
48	BL	306	BCR	C33-C5-C4	2.66	118.73	113.62
45	AA	823	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	AA	808	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	AA	814	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	BL	303	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	A3	302	CLA	CMB-C2B-C3B	2.66	129.66	124.68
45	B1	307	CLA	CHD-C1D-ND	-2.66	122.01	124.45
45	AA	819	CLA	CHB-C4A-NA	2.66	128.19	124.51
48	BF	304	BCR	C12-C13-C14	2.66	123.03	118.94
45	A3	303	CLA	C5-C3-C2	2.66	126.50	121.12
48	BA	855	BCR	C29-C28-C27	-2.66	105.43	111.38
45	AA	840	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
45	BA	839	CLA	O2D-CGD-CBD	2.66	116.00	111.27
45	B1	309	CLA	O2D-CGD-O1D	-2.66	118.05	124.09
45	A3	314	CLA	CMB-C2B-C3B	2.66	129.66	124.68
48	BJ	103	BCR	C12-C13-C14	-2.66	114.86	118.94
52	B2	615	LUT	C32-C33-C34	-2.66	114.86	118.94
45	B3	310	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
52	B3	315	LUT	C7-C8-C9	-2.66	122.22	126.23
45	A3	309	CLA	CMB-C2B-C3B	2.66	129.65	124.68
47	B2	618	LHG	O7-C7-C8	2.66	117.23	111.50
46	BB	844	PQN	O4-C4-C5	-2.66	117.26	121.56
45	AB	837	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
54	B2	601	CHL	O2A-CGA-O1A	-2.66	116.89	123.59
47	A1	320	LHG	O7-C7-C8	2.66	117.23	111.50
45	AG	203	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
45	A1	315	CLA	CHD-C1D-ND	-2.66	122.01	124.45
45	BA	840	CLA	CHD-C1D-ND	-2.66	122.01	124.45
45	AB	814	CLA	C1B-CHB-C4A	-2.66	124.86	130.12
45	A4	302	CLA	C1B-CHB-C4A	-2.65	124.86	130.12
48	BI	101	BCR	C12-C13-C14	-2.65	114.87	118.94
45	BA	840	CLA	CMB-C2B-C3B	2.65	129.64	124.68
48	BB	848	BCR	C40-C30-C25	-2.65	106.00	110.30
45	AB	826	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
54	B2	606	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
48	AB	848	BCR	C20-C21-C22	-2.65	123.53	127.31
52	B3	315	LUT	C12-C13-C14	-2.65	114.87	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	841	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
45	BA	806	CLA	CMB-C2B-C3B	2.65	129.63	124.68
45	B3	308	CLA	CMB-C2B-C3B	2.65	129.63	124.68
45	BA	821	CLA	C4-C3-C5	2.65	119.73	115.27
45	BB	815	CLA	CBC-CAC-C3C	2.65	119.73	112.43
45	AA	803	CLA	CAC-C3C-C4C	2.65	128.25	124.81
48	AA	848	BCR	C40-C30-C25	-2.65	106.00	110.30
48	BA	849	BCR	C24-C23-C22	-2.65	122.23	126.23
45	AB	842	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
48	BA	855	BCR	C37-C22-C21	-2.64	119.22	122.92
45	BA	823	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
45	BA	820	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
48	B5	616	BCR	C38-C26-C27	2.64	118.69	113.62
45	BL	303	CLA	O2D-CGD-CBD	2.64	115.97	111.27
55	B5	615	XAT	C8-C9-C10	-2.64	114.89	118.94
48	B3	317	BCR	C19-C18-C17	-2.64	114.89	118.94
45	A3	303	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
54	B5	607	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
45	AB	802	CLA	CAB-C3B-C4B	-2.64	124.41	128.46
48	BA	851	BCR	C36-C18-C17	-2.64	119.22	122.92
45	AB	829	CLA	C4A-NA-C1A	2.64	107.89	106.71
45	AA	829	CLA	CHB-C4A-NA	2.64	128.16	124.51
45	BA	840	CLA	CHB-C4A-NA	2.64	128.16	124.51
47	B5	618	LHG	O8-C23-C24	2.64	120.19	111.91
45	B3	314	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
45	BA	831	CLA	CHD-C1D-ND	-2.64	122.03	124.45
45	AB	801	CLA	CMB-C2B-C3B	2.64	129.62	124.68
45	BJ	102	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
48	A6	617	BCR	C23-C22-C21	-2.64	114.89	118.94
45	BB	813	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
45	B2	611	CLA	CMB-C2B-C3B	2.64	129.61	124.68
45	AA	824	CLA	C6-C5-C3	2.64	120.37	113.45
48	BA	847	BCR	C1-C6-C5	-2.64	118.90	122.61
45	BL	304	CLA	C1B-CHB-C4A	-2.64	124.90	130.12
45	B1	310	CLA	CMB-C2B-C3B	2.64	129.85	124.69
45	A3	302	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
45	B5	609	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
48	AJ	103	BCR	C19-C18-C17	-2.63	114.90	118.94
45	BB	823	CLA	CHB-C4A-NA	2.63	128.15	124.51
45	B2	604	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
45	A6	611	CLA	C1A-CHA-C4D	-2.63	122.03	125.72
45	BB	843	CLA	C1B-CHB-C4A	-2.63	124.90	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AB	847	BCR	C39-C30-C25	-2.63	106.03	110.30
45	AA	840	CLA	CMB-C2B-C3B	2.63	129.60	124.68
45	B2	602	CLA	CMB-C2B-C3B	2.63	129.60	124.68
45	AB	822	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
48	AA	846	BCR	C8-C9-C10	-2.63	114.90	118.94
48	AF	805	BCR	C23-C22-C21	-2.63	114.90	118.94
45	BA	801	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
45	AK	201	CLA	CAA-C2A-C3A	-2.63	109.96	116.10
48	BJ	103	BCR	C27-C26-C25	-2.63	118.91	122.73
48	AB	848	BCR	C15-C14-C13	-2.63	123.56	127.31
45	AK	201	CLA	C4B-CHC-C1C	-2.63	125.58	129.64
45	BB	808	CLA	CMB-C2B-C3B	2.63	129.60	124.68
48	BB	847	BCR	C32-C1-C6	-2.63	106.03	110.30
45	A4	311	CLA	O2D-CGD-O1D	-2.63	118.12	124.09
45	AB	830	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
45	AB	824	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
45	AA	824	CLA	O2D-CGD-O1D	-2.63	118.12	124.09
48	BB	845	BCR	C16-C15-C14	-2.63	118.09	123.47
45	B1	306	CLA	CMB-C2B-C3B	2.63	129.59	124.68
45	B1	313	CLA	CHB-C4A-NA	2.63	128.15	124.51
45	A4	307	CLA	CMB-C2B-C3B	2.63	129.59	124.68
45	A3	311	CLA	C1B-CHB-C4A	-2.63	124.92	130.12
45	A4	310	CLA	CHB-C4A-NA	2.63	128.14	124.51
48	BA	851	BCR	C3-C4-C5	-2.62	109.39	114.08
45	B1	305	CLA	C5-C3-C2	2.62	126.43	121.12
45	A1	314	CLA	CHB-C4A-NA	2.62	128.14	124.51
54	A1	303	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
45	B3	310	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
45	B1	311	CLA	CMB-C2B-C1B	-2.62	124.43	128.46
45	A1	311	CLA	CHB-C4A-NA	2.62	128.14	124.51
45	A4	308	CLA	CHB-C4A-NA	2.62	128.14	124.51
45	BA	826	CLA	O2D-CGD-O1D	-2.62	118.71	123.84
45	BB	816	CLA	CHB-C4A-NA	2.62	128.14	124.51
45	BA	808	CLA	O2A-CGA-O1A	-2.62	116.98	123.59
48	AI	102	BCR	C37-C22-C21	-2.62	119.25	122.92
48	AA	847	BCR	C8-C9-C10	-2.62	114.92	118.94
45	AA	842	CLA	CHB-C4A-NA	2.62	128.13	124.51
55	B3	316	XAT	C8-C9-C10	-2.62	114.92	118.94
45	AA	820	CLA	CMB-C2B-C3B	2.62	129.58	124.68
51	AB	851	DGD	O1G-C1A-C2A	2.62	120.13	111.91
45	BA	819	CLA	CHB-C4A-NA	2.62	128.13	124.51
48	AA	846	BCR	C20-C21-C22	-2.62	123.57	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	811	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
55	A6	616	XAT	C39-C29-C30	-2.62	119.26	122.92
52	AF	806	LUT	C1-C6-C5	-2.62	118.93	122.61
45	A6	604	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
45	B5	611	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
45	B2	608	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
45	AA	833	CLA	C4-C3-C2	-2.62	116.96	123.68
45	AL	305	CLA	CHB-C4A-NA	2.62	128.13	124.51
45	BB	809	CLA	CMB-C2B-C3B	2.62	129.57	124.68
48	AA	847	BCR	C3-C4-C5	-2.62	109.41	114.08
45	B1	315	CLA	O2D-CGD-O1D	-2.62	118.15	124.09
45	BA	808	CLA	CHB-C4A-NA	2.62	128.13	124.51
45	BF	303	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
45	BF	302	CLA	CHB-C4A-NA	2.61	128.13	124.51
48	AB	844	BCR	C31-C1-C6	2.61	114.54	110.30
45	AA	835	CLA	O2D-CGD-O1D	-2.61	118.15	124.09
45	AA	808	CLA	CHD-C1D-ND	-2.61	122.05	124.45
45	AB	804	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
45	B5	601	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
45	BA	832	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
45	BA	805	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
45	A1	316	CLA	CHD-C1D-ND	-2.61	122.05	124.45
45	BA	804	CLA	CHD-C1D-ND	-2.61	122.05	124.45
45	A1	313	CLA	C1B-CHB-C4A	-2.61	124.94	130.12
45	AA	828	CLA	CHB-C4A-NA	2.61	128.12	124.51
45	BB	831	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
48	AB	844	BCR	C36-C18-C19	2.61	122.19	118.08
48	BB	803	BCR	C3-C4-C5	-2.61	109.42	114.08
45	AB	801	CLA	CMD-C2D-C3D	2.61	133.62	127.61
45	AA	814	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
45	BA	837	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
48	AI	101	BCR	C36-C18-C17	-2.61	119.27	122.92
54	A6	606	CHL	C1C-C2C-C3C	-2.61	105.05	107.11
47	A1	320	LHG	O8-C23-C24	2.61	120.08	111.91
53	B5	617	LMG	O8-C28-C29	2.61	120.08	111.91
47	B2	618	LHG	O8-C23-C24	2.60	120.08	111.91
45	A3	302	CLA	C6-C5-C3	2.60	120.28	113.45
45	A6	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
45	BB	825	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
45	BB	838	CLA	C1-C2-C3	-2.60	122.54	126.75
45	BB	808	CLA	CHB-C4A-NA	2.60	128.11	124.51
45	AB	808	CLA	O2D-CGD-CBD	2.60	115.89	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AK	201	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
45	B1	306	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
45	AB	806	CLA	CHD-C1D-ND	-2.60	122.06	124.45
45	A3	309	CLA	CHB-C4A-NA	2.60	128.11	124.51
45	A3	313	CLA	O2D-CGD-O1D	-2.60	118.19	124.09
45	A4	302	CLA	CAC-C3C-C4C	2.60	128.18	124.81
45	AF	804	CLA	C1B-CHB-C4A	-2.60	124.97	130.12
45	AB	802	CLA	CHB-C4A-NA	2.60	128.10	124.51
45	B5	603	CLA	CHB-C4A-NA	2.60	128.10	124.51
48	AA	849	BCR	C24-C23-C22	-2.60	122.31	126.23
45	AA	838	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
45	AB	804	CLA	CBC-CAC-C3C	2.59	119.58	112.43
45	AA	801	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
45	B5	612	CLA	CMB-C2B-C3B	2.59	129.53	124.68
45	B3	314	CLA	O2D-CGD-O1D	-2.59	118.20	124.09
45	BB	801	CLA	O1D-CGD-CBD	2.59	129.79	124.48
52	A3	316	LUT	C2-C3-C4	-2.59	106.75	110.30
45	BF	302	CLA	CAA-C2A-C3A	-2.59	107.78	114.26
48	BK	204	BCR	C1-C6-C7	2.59	123.11	115.78
45	AB	809	CLA	O2D-CGD-CBD	2.59	115.87	111.27
45	BA	813	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
45	A1	314	CLA	CHD-C1D-ND	-2.59	122.07	124.45
48	B3	317	BCR	C38-C26-C27	2.59	118.59	113.62
45	A1	316	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
45	AA	827	CLA	CHB-C4A-NA	2.59	128.09	124.51
45	AB	836	CLA	CHD-C1D-ND	-2.59	122.08	124.45
54	A1	303	CHL	C4-C3-C5	2.59	118.94	115.98
45	AB	841	CLA	C1B-CHB-C4A	-2.59	124.99	130.12
45	BL	302	CLA	O2A-CGA-O1A	-2.59	116.85	123.30
48	BA	848	BCR	C15-C16-C17	-2.59	118.18	123.47
45	BA	838	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
45	AA	817	CLA	C4-C3-C2	-2.59	117.05	123.68
45	B1	310	CLA	O2D-CGD-O1D	-2.58	118.22	124.09
54	B2	601	CHL	C4A-NA-C1A	-2.58	105.54	106.71
45	AA	808	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
45	A3	305	CLA	O2D-CGD-O1D	-2.58	118.22	124.09
45	BA	824	CLA	CBA-CAA-C2A	2.58	121.49	113.86
45	A1	310	CLA	CMB-C2B-C3B	2.58	129.75	124.69
45	AB	812	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
45	AA	834	CLA	CMC-C2C-C1C	-2.58	121.11	125.04
45	AB	806	CLA	CMC-C2C-C1C	-2.58	121.11	125.04
45	AG	203	CLA	C1B-CHB-C4A	-2.58	125.00	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AF	801	BCR	C12-C13-C14	-2.58	114.98	118.94
48	BA	851	BCR	C39-C30-C25	-2.58	106.11	110.30
55	A1	318	XAT	C26-C27-C28	-2.58	120.54	125.99
45	B2	613	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
45	B5	603	CLA	CMB-C2B-C3B	2.58	129.74	124.69
45	B3	301	CLA	CMB-C2B-C3B	2.58	129.50	124.68
45	BB	820	CLA	CHB-C4A-NA	2.58	128.08	124.51
45	BB	808	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
48	AA	846	BCR	C30-C25-C26	-2.58	118.98	122.61
45	A3	312	CLA	C4-C3-C5	2.58	119.61	115.27
48	BA	855	BCR	C24-C25-C26	2.58	127.70	121.46
45	BA	812	CLA	O2A-CGA-O1A	-2.58	117.09	123.59
48	BL	305	BCR	C15-C16-C17	-2.58	118.20	123.47
45	AG	204	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
45	AA	803	CLA	CMB-C2B-C1B	-2.58	124.50	128.46
45	AL	304	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
45	BB	810	CLA	CMB-C2B-C3B	2.58	129.50	124.68
45	AB	830	CLA	C1B-CHB-C4A	-2.58	125.02	130.12
45	BA	824	CLA	CMB-C2B-C3B	2.58	129.50	124.68
45	BB	807	CLA	CHB-C4A-NA	2.58	128.07	124.51
45	AB	842	CLA	C6-C5-C3	2.57	120.21	113.45
48	AF	801	BCR	C24-C25-C26	2.57	127.70	121.46
45	A4	312	CLA	CMB-C2B-C3B	2.57	129.49	124.68
48	BL	301	BCR	C8-C9-C10	2.57	122.89	118.94
45	BB	811	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
45	AA	812	CLA	CHB-C4A-NA	2.57	128.07	124.51
52	B1	316	LUT	C35-C15-C14	2.57	128.74	123.47
50	AB	850	LMU	O5B-C5B-C4B	2.57	114.36	109.69
53	A4	318	LMG	O7-C10-O9	-2.57	117.49	123.70
48	AI	101	BCR	C15-C16-C17	-2.57	118.21	123.47
45	AB	811	CLA	CHB-C4A-NA	2.57	128.06	124.51
45	BA	809	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
45	AA	834	CLA	CMB-C2B-C3B	2.57	129.48	124.68
48	AB	847	BCR	C36-C18-C17	-2.57	119.33	122.92
45	B5	611	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
45	BA	828	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
45	A1	307	CLA	CHB-C4A-NA	2.57	128.06	124.51
54	B5	605	CHL	C1C-C2C-C3C	-2.57	105.08	107.11
45	AB	806	CLA	C1B-CHB-C4A	-2.57	125.04	130.12
48	AI	102	BCR	C31-C1-C6	2.56	114.46	110.30
48	AB	849	BCR	C33-C5-C4	2.56	118.54	113.62
45	BA	834	CLA	CHD-C1D-ND	-2.56	122.10	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	849	BCR	C4-C5-C6	-2.56	119.01	122.73
45	BA	814	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
45	AA	815	CLA	CHB-C4A-NA	2.56	128.06	124.51
45	BA	812	CLA	CHB-C4A-NA	2.56	128.06	124.51
45	BB	839	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
45	A6	601	CLA	CHB-C4A-NA	2.56	128.05	124.51
55	B5	615	XAT	C26-C27-C28	-2.56	120.58	125.99
45	AB	819	CLA	CHD-C1D-ND	-2.56	122.10	124.45
45	BG	201	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
45	BB	808	CLA	CHD-C1D-ND	-2.56	122.10	124.45
45	AA	840	CLA	O2A-CGA-O1A	-2.56	117.13	123.59
45	A6	612	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
45	AA	832	CLA	CHD-C1D-ND	-2.56	122.11	124.45
52	A3	316	LUT	C38-C25-C24	-2.56	118.09	123.56
45	A4	313	CLA	CHB-C4A-NA	2.55	128.04	124.51
48	BL	306	BCR	C36-C18-C19	-2.55	114.05	118.08
54	B5	606	CHL	CAC-C3C-C4C	2.55	128.93	125.04
45	BB	831	CLA	C1B-CHB-C4A	-2.55	125.06	130.12
45	BA	808	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
45	AL	304	CLA	CBA-CAA-C2A	2.55	121.39	113.86
48	AJ	103	BCR	C38-C26-C25	-2.55	121.66	124.53
52	B2	615	LUT	C19-C9-C8	2.55	122.10	118.08
45	AB	834	CLA	CHB-C4A-NA	2.55	128.04	124.51
45	B1	312	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
45	B2	603	CLA	O2D-CGD-O1D	-2.55	118.30	124.09
55	B3	316	XAT	C24-C23-C22	-2.55	105.85	110.77
48	AF	805	BCR	C33-C5-C6	-2.55	121.67	124.53
45	A1	306	CLA	C1B-CHB-C4A	-2.55	125.07	130.12
45	BB	817	CLA	CHB-C4A-NA	2.55	128.03	124.51
45	AB	831	CLA	CHD-C1D-ND	-2.55	122.11	124.45
48	B2	617	BCR	C7-C6-C5	2.55	127.63	121.46
45	AB	833	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
45	A1	307	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
55	A3	317	XAT	C36-C21-C22	-2.54	104.57	108.98
45	B1	313	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
48	AB	845	BCR	C19-C18-C17	-2.54	115.04	118.94
45	AA	832	CLA	CMB-C2B-C3B	2.54	129.43	124.68
45	AL	305	CLA	CMB-C2B-C3B	2.54	129.43	124.68
48	BJ	101	BCR	C36-C18-C19	2.54	122.08	118.08
45	AH	201	CLA	CHB-C4A-NA	2.54	128.03	124.51
45	BB	813	CLA	CHB-C4A-NA	2.54	128.03	124.51
52	A1	317	LUT	C37-C21-C36	2.54	111.64	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B1	304	CLA	O1D-CGD-CBD	2.54	129.68	124.48
45	B3	304	CLA	CHD-C1D-ND	-2.54	122.12	124.45
45	BA	808	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
45	B5	611	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
48	BB	849	BCR	C36-C18-C17	-2.54	119.37	122.92
45	AA	813	CLA	O2A-C1-C2	-2.54	101.96	108.64
45	B3	312	CLA	O2D-CGD-O1D	-2.54	118.33	124.09
45	BB	842	CLA	CAC-C3C-C4C	2.54	128.10	124.81
45	BA	813	CLA	CMB-C2B-C3B	2.54	129.43	124.68
45	A1	304	CLA	CHD-C1D-ND	-2.54	122.12	124.45
47	BA	845	LHG	O8-C23-C24	2.53	119.86	111.91
45	BA	807	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
45	BL	302	CLA	CMB-C2B-C1B	-2.53	124.57	128.46
45	AA	819	CLA	CHD-C1D-ND	-2.53	122.13	124.45
48	AA	845	BCR	C34-C9-C10	-2.53	119.38	122.92
45	BA	837	CLA	CHB-C4A-NA	2.53	128.01	124.51
45	BK	203	CLA	CHB-C4A-NA	2.53	128.01	124.51
48	AA	848	BCR	C15-C16-C17	-2.53	118.29	123.47
45	A4	307	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
45	AA	826	CLA	CHD-C1D-ND	-2.53	122.13	124.45
45	A1	310	CLA	CHB-C4A-NA	2.53	128.01	124.51
48	AA	848	BCR	C31-C1-C6	-2.53	106.20	110.30
54	B2	614	CHL	O2D-CGD-O1D	-2.53	118.89	123.84
45	AG	203	CLA	CMB-C2B-C3B	2.53	129.41	124.68
45	B2	612	CLA	CHB-C4A-NA	2.53	128.01	124.51
48	BA	848	BCR	C35-C13-C12	2.53	122.06	118.08
45	A3	304	CLA	CHB-C4A-NA	2.53	128.01	124.51
45	BA	832	CLA	CMB-C2B-C3B	2.53	129.41	124.68
48	BB	845	BCR	C15-C16-C17	-2.53	118.30	123.47
48	BA	855	BCR	C2-C3-C4	-2.53	105.73	111.38
45	AB	811	CLA	C1B-CHB-C4A	-2.53	125.11	130.12
45	B5	609	CLA	CHD-C1D-ND	-2.52	122.13	124.45
45	A4	313	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
48	AL	306	BCR	C1-C6-C5	-2.52	119.06	122.61
48	AF	805	BCR	C29-C28-C27	-2.52	105.74	111.38
48	AI	102	BCR	C2-C3-C4	-2.52	105.74	111.38
45	BL	302	CLA	O1A-CGA-CBA	2.52	131.19	123.08
45	B1	304	CLA	C1B-CHB-C4A	-2.52	125.12	130.12
45	B1	311	CLA	CHD-C1D-ND	-2.52	122.14	124.45
52	A1	317	LUT	C21-C26-C27	-2.52	109.51	112.70
54	B5	607	CHL	C3C-C4C-NC	2.52	113.33	110.57
52	A3	316	LUT	C28-C29-C30	-2.52	115.07	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A4	308	CLA	CMB-C2B-C3B	2.52	129.40	124.68
52	A4	315	LUT	C3-C4-C5	-2.52	106.83	111.85
45	A3	304	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
45	B3	304	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
45	BB	843	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
45	BA	813	CLA	C1B-CHB-C4A	-2.52	125.13	130.12
45	BB	810	CLA	CBA-CAA-C2A	2.52	121.30	113.86
45	AK	203	CLA	CHB-C4A-NA	2.52	128.00	124.51
45	BB	805	CLA	CMB-C2B-C3B	2.52	129.39	124.68
45	A1	305	CLA	CHB-C4A-NA	2.52	127.99	124.51
45	B5	604	CLA	CHD-C1D-ND	-2.52	122.14	124.45
45	AB	831	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
45	B3	311	CLA	O2D-CGD-O1D	-2.52	118.37	124.09
45	AB	832	CLA	CMB-C2B-C3B	2.52	129.39	124.68
45	AF	803	CLA	CHB-C4A-NA	2.52	127.99	124.51
45	A3	302	CLA	CHB-C4A-NA	2.52	127.99	124.51
45	BA	816	CLA	CMB-C2B-C3B	2.52	129.39	124.68
52	AF	806	LUT	C32-C33-C34	-2.52	115.08	118.94
48	AB	844	BCR	C15-C16-C17	-2.52	118.32	123.47
45	BA	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
46	BA	843	PQN	C14-C13-C12	-2.51	117.23	123.68
45	AB	824	CLA	CHB-C4A-NA	2.51	127.99	124.51
45	BA	841	CLA	C5-C3-C2	-2.51	116.03	121.12
45	BB	812	CLA	CHB-C4A-NA	2.51	127.99	124.51
45	AB	838	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
45	BB	805	CLA	CMD-C2D-C3D	2.51	133.40	127.61
45	A3	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
45	B5	608	CLA	CHB-C4A-NA	2.51	127.99	124.51
45	A6	613	CLA	CHD-C1D-ND	-2.51	122.14	124.45
45	BA	844	CLA	CHD-C1D-ND	-2.51	122.14	124.45
54	A6	606	CHL	O1D-CGD-CBD	-2.51	119.34	124.48
45	B1	305	CLA	CHB-C4A-NA	2.51	127.99	124.51
45	BL	303	CLA	CHB-C4A-NA	2.51	127.98	124.51
45	AA	830	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
48	BB	848	BCR	C23-C24-C25	-2.51	120.15	127.20
45	BB	801	CLA	C1-O2A-CGA	2.51	123.03	116.44
45	AB	824	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
45	A4	301	CLA	CHB-C4A-NA	2.51	127.98	124.51
48	AB	848	BCR	C19-C18-C17	-2.51	115.09	118.94
45	AA	838	CLA	CHD-C1D-ND	-2.51	122.15	124.45
45	BA	816	CLA	CAC-C3C-C4C	2.51	128.06	124.81
48	A1	319	BCR	C15-C16-C17	-2.51	118.34	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AL	302	BCR	C19-C18-C17	-2.51	115.09	118.94
45	A6	610	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
45	B5	601	CLA	CHB-C4A-NA	2.51	127.98	124.51
54	A6	606	CHL	O2D-CGD-O1D	-2.51	118.94	123.84
45	AB	810	CLA	CHB-C4A-NA	2.51	127.98	124.51
45	B3	309	CLA	O2D-CGD-O1D	-2.51	118.40	124.09
50	AL	301	LMU	O1B-C4'-C3'	2.51	113.95	107.28
45	BA	839	CLA	CHB-C4A-NA	2.51	127.98	124.51
45	AB	827	CLA	O2D-CGD-CBD	2.50	115.72	111.27
45	BA	810	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
45	AB	807	CLA	CHB-C4A-NA	2.50	127.97	124.51
48	A1	319	BCR	C23-C24-C25	-2.50	120.17	127.20
45	AB	822	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
45	AA	838	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
45	BB	839	CLA	CHD-C1D-ND	-2.50	122.15	124.45
45	BA	809	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
45	AK	203	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
47	B1	302	LHG	O8-C23-C24	2.50	119.76	111.91
45	B1	315	CLA	CMA-C3A-C2A	-2.50	110.26	116.10
45	BA	813	CLA	C4-C3-C5	2.50	119.48	115.27
48	AK	204	BCR	C36-C18-C19	2.50	122.02	118.08
56	e	301	SQD	O48-C23-C24	2.50	119.75	111.91
48	BJ	103	BCR	C7-C6-C5	2.50	127.52	121.46
54	B1	303	CHL	C3C-C4C-NC	2.50	113.37	110.57
48	BB	846	BCR	C36-C18-C17	-2.50	119.42	122.92
45	BA	836	CLA	CHB-C4A-NA	2.50	127.97	124.51
48	AA	845	BCR	C7-C8-C9	-2.50	122.46	126.23
48	BA	855	BCR	C30-C25-C26	-2.50	119.09	122.61
45	BA	831	CLA	CHB-C4A-NA	2.50	127.97	124.51
45	AK	201	CLA	CMB-C2B-C3B	2.50	129.50	124.93
48	BJ	101	BCR	C30-C25-C26	-2.50	119.10	122.61
45	B3	303	CLA	O2D-CGD-O1D	-2.50	118.42	124.09
45	AL	305	CLA	O2D-CGD-CBD	2.50	115.70	111.27
45	BA	817	CLA	CHB-C4A-NA	2.50	127.96	124.51
45	AB	801	CLA	C4-C3-C5	2.50	119.47	115.27
48	B2	617	BCR	C16-C15-C14	-2.50	118.36	123.47
45	BB	834	CLA	C4-C3-C5	-2.49	111.08	115.27
45	BA	819	CLA	CHD-C1D-ND	-2.49	122.16	124.45
48	AB	844	BCR	C24-C23-C22	-2.49	122.47	126.23
45	AH	201	CLA	CAA-C2A-C3A	2.49	119.60	112.78
45	BA	832	CLA	CHB-C4A-NA	2.49	127.96	124.51
48	AL	302	BCR	C8-C9-C10	2.49	122.76	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	818	CLA	CHB-C4A-NA	2.49	127.96	124.51
45	BB	833	CLA	CHB-C4A-NA	2.49	127.95	124.51
45	BA	812	CLA	CHD-C1D-ND	-2.49	122.17	124.45
48	BK	204	BCR	C16-C15-C14	-2.49	118.38	123.47
45	AA	817	CLA	CHB-C4A-NA	2.49	127.95	124.51
45	A1	305	CLA	CMB-C2B-C3B	2.49	129.34	124.68
45	B1	311	CLA	CMB-C2B-C3B	2.49	129.34	124.68
48	BA	855	BCR	C8-C7-C6	-2.49	120.21	127.20
45	AB	812	CLA	CHB-C4A-NA	2.49	127.95	124.51
45	AA	839	CLA	O2D-CGD-CBD	2.49	115.69	111.27
48	AG	205	BCR	C16-C15-C14	-2.49	118.38	123.47
53	A1	321	LMG	O8-C28-C29	2.49	119.71	111.91
45	BA	838	CLA	C4-C3-C2	-2.49	117.30	123.68
45	AB	820	CLA	CHD-C1D-ND	-2.49	122.17	124.45
45	AB	821	CLA	CHD-C1D-ND	-2.49	122.17	124.45
45	BK	203	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
48	AI	101	BCR	C34-C9-C8	2.48	121.99	118.08
45	B3	302	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
45	AL	303	CLA	CHD-C1D-ND	-2.48	122.17	124.45
45	BK	202	CLA	CHD-C1D-ND	-2.48	122.17	124.45
45	BB	812	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
45	BB	832	CLA	O2D-CGD-O1D	-2.48	118.98	123.84
45	BB	832	CLA	CHD-C1D-ND	-2.48	122.17	124.45
45	B3	307	CLA	CHB-C4A-NA	2.48	127.94	124.51
45	AA	820	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
45	AA	807	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
48	BA	849	BCR	C31-C1-C6	-2.48	106.28	110.30
47	BA	845	LHG	C5-O7-C7	-2.48	111.69	117.79
48	BF	304	BCR	C33-C5-C4	2.48	118.38	113.62
45	AB	833	CLA	CHD-C1D-ND	-2.48	122.18	124.45
52	B1	316	LUT	C12-C13-C14	2.48	122.74	118.94
45	BA	827	CLA	CHB-C4A-NA	2.48	127.94	124.51
45	B3	308	CLA	CMA-C3A-C2A	-2.48	110.31	116.10
45	AA	836	CLA	CMB-C2B-C3B	2.48	129.31	124.68
48	AL	302	BCR	C38-C26-C27	2.48	118.38	113.62
45	AB	828	CLA	CHD-C1D-ND	-2.48	122.18	124.45
45	A1	304	CLA	CHB-C4A-NA	2.48	127.94	124.51
45	AA	806	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
48	AK	204	BCR	C27-C26-C25	-2.48	119.14	122.73
45	AB	822	CLA	CHD-C1D-ND	-2.48	122.18	124.45
45	AA	834	CLA	C6-C5-C3	2.48	119.95	113.45
45	AA	837	CLA	O2D-CGD-CBD	2.48	115.67	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	AL	301	LMU	C1B-O5B-C5B	2.48	118.55	113.69
45	AA	831	CLA	CMB-C2B-C3B	2.47	129.31	124.68
45	BB	837	CLA	CMB-C2B-C3B	2.47	129.31	124.68
45	AA	821	CLA	CHD-C1D-ND	-2.47	122.18	124.45
45	BB	834	CLA	CHD-C1D-ND	-2.47	122.18	124.45
45	B5	603	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
48	B5	616	BCR	C15-C16-C17	-2.47	118.41	123.47
45	AA	841	CLA	CMB-C2B-C3B	2.47	129.31	124.68
52	A4	315	LUT	C1-C6-C5	-2.47	119.13	122.61
45	BA	814	CLA	CHB-C4A-NA	2.47	127.93	124.51
48	AF	805	BCR	C19-C18-C17	-2.47	115.15	118.94
48	AI	101	BCR	C12-C13-C14	-2.47	115.15	118.94
48	BB	845	BCR	C36-C18-C17	-2.47	119.46	122.92
48	B5	616	BCR	C1-C6-C7	2.47	122.77	115.78
45	BB	807	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
47	A1	302	LHG	O8-C23-C24	2.47	119.66	111.91
55	A3	317	XAT	C12-C13-C14	-2.47	115.15	118.94
45	A4	310	CLA	O2D-CGD-O1D	-2.47	118.48	124.09
45	AB	819	CLA	CHB-C4A-NA	2.47	127.93	124.51
45	A6	604	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
45	A1	316	CLA	CMB-C2B-C3B	2.47	129.52	124.69
52	B1	316	LUT	C39-C29-C28	2.47	121.97	118.08
45	AA	842	CLA	C4-C3-C5	-2.47	111.12	115.27
45	B3	311	CLA	CHB-C4A-NA	2.47	127.92	124.51
48	BA	851	BCR	C38-C26-C25	-2.47	121.76	124.53
45	B5	608	CLA	CHD-C1D-ND	-2.47	122.19	124.45
45	BA	840	CLA	O2D-CGD-O1D	-2.47	119.02	123.84
45	A4	301	CLA	CAC-C3C-C4C	2.47	128.01	124.81
54	A1	303	CHL	CAC-C3C-C4C	2.47	128.01	124.81
46	AB	843	PQN	C14-C13-C15	-2.47	111.12	115.27
45	B2	612	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
48	A3	318	BCR	C33-C5-C6	-2.46	121.76	124.53
45	B3	303	CLA	CHB-C4A-NA	2.46	127.92	124.51
45	BB	832	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
45	BB	809	CLA	CHD-C1D-ND	-2.46	122.19	124.45
45	AA	810	CLA	CMB-C2B-C3B	2.46	129.28	124.68
45	B1	314	CLA	CMB-C2B-C3B	2.46	129.28	124.68
52	A3	316	LUT	C8-C7-C6	-2.46	120.29	127.20
45	BA	812	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
55	A6	616	XAT	C36-C21-C26	2.46	116.69	110.05
55	A3	317	XAT	C10-C11-C12	-2.46	115.54	123.22
45	A6	610	CLA	C6-C5-C3	2.46	119.91	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BL	304	CLA	O2D-CGD-CBD	2.46	115.64	111.27
45	A3	306	CLA	CHB-C4A-NA	2.46	127.91	124.51
55	B3	316	XAT	C4-C3-C2	-2.46	106.02	110.77
45	AA	831	CLA	CHB-C4A-NA	2.46	127.91	124.51
45	B5	609	CLA	CMB-C2B-C3B	2.46	129.28	124.68
45	BA	837	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
45	AA	833	CLA	CMD-C2D-C3D	2.46	133.27	127.61
45	BB	816	CLA	CHD-C1D-ND	-2.46	122.20	124.45
45	BB	806	CLA	CHB-C4A-NA	2.46	127.91	124.51
45	BG	201	CLA	CHB-C4A-NA	2.46	127.91	124.51
52	AF	806	LUT	C8-C9-C10	-2.45	115.17	118.94
45	AB	815	CLA	CHB-C4A-NA	2.45	127.91	124.51
45	AF	804	CLA	CHB-C4A-NA	2.45	127.91	124.51
45	B3	308	CLA	CHB-C4A-NA	2.45	127.91	124.51
48	AA	852	BCR	C40-C30-C25	-2.45	106.32	110.30
45	AG	201	CLA	O2D-CGD-O1D	-2.45	118.52	124.09
48	AG	205	BCR	C20-C21-C22	-2.45	123.81	127.31
45	BB	804	CLA	CMB-C2B-C1B	-2.45	124.69	128.46
45	AA	815	CLA	O2D-CGD-CBD	2.45	115.63	111.27
45	A1	312	CLA	O2D-CGD-O1D	-2.45	118.52	124.09
45	BB	840	CLA	CMB-C2B-C3B	2.45	129.26	124.68
45	AF	803	CLA	CHD-C1D-ND	-2.45	122.20	124.45
45	BB	805	CLA	CMB-C2B-C1B	-2.45	124.70	128.46
45	AB	827	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
45	AB	834	CLA	CHD-C1D-ND	-2.45	122.20	124.45
48	AL	302	BCR	C23-C22-C21	-2.45	115.18	118.94
48	BB	846	BCR	C12-C13-C14	-2.45	115.18	118.94
48	B2	617	BCR	C29-C30-C25	2.45	114.25	110.48
45	B2	603	CLA	CHD-C1D-ND	-2.45	122.20	124.45
45	AL	304	CLA	CHB-C4A-NA	2.45	127.90	124.51
48	BA	847	BCR	C28-C27-C26	-2.45	109.70	114.08
52	A6	615	LUT	C39-C29-C28	2.45	121.93	118.08
45	AA	841	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
45	A3	304	CLA	CAB-C3B-C2B	2.45	129.48	124.69
56	BJ	104	SQD	O48-C23-C24	2.45	119.59	111.91
48	AL	302	BCR	C30-C25-C26	-2.45	119.17	122.61
48	AJ	101	BCR	C30-C25-C26	-2.45	119.17	122.61
48	AB	848	BCR	C34-C9-C8	2.45	121.93	118.08
45	A3	306	CLA	CHD-C1D-ND	-2.45	122.21	124.45
48	BA	855	BCR	C19-C18-C17	-2.45	115.19	118.94
45	B3	301	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	BJ	102	CLA	CHB-C4A-NA	2.44	127.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BA	811	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	AB	834	CLA	CMB-C2B-C3B	2.44	129.25	124.68
45	A3	305	CLA	CMB-C2B-C3B	2.44	129.25	124.68
45	AB	804	CLA	CMD-C2D-C1D	-2.44	120.41	124.71
48	AA	846	BCR	C1-C6-C5	-2.44	119.17	122.61
45	BB	835	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
45	BA	808	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	BB	806	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	AA	805	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
45	AB	842	CLA	CHB-C4A-NA	2.44	127.89	124.51
45	BA	826	CLA	CHD-C1D-ND	-2.44	122.21	124.45
45	BF	302	CLA	CHD-C1D-ND	-2.44	122.21	124.45
48	BA	855	BCR	C23-C22-C21	-2.44	115.20	118.94
45	AB	817	CLA	CHB-C4A-NA	2.44	127.89	124.51
45	A6	604	CLA	CHB-C4A-NA	2.44	127.89	124.51
45	AA	811	CLA	CHD-C1D-ND	-2.44	122.21	124.45
48	AB	844	BCR	C12-C13-C14	-2.44	115.20	118.94
45	B3	302	CLA	CMB-C2B-C3B	2.44	129.24	124.68
45	BA	834	CLA	CHB-C4A-NA	2.44	127.88	124.51
48	AA	845	BCR	C16-C17-C18	-2.44	123.83	127.31
48	AB	847	BCR	C30-C25-C26	-2.44	119.18	122.61
48	BA	849	BCR	C33-C5-C6	-2.44	121.79	124.53
45	A1	315	CLA	CHB-C4A-NA	2.44	127.88	124.51
45	BA	827	CLA	CMB-C2B-C3B	2.44	129.24	124.68
45	B5	610	CLA	CHD-C1D-ND	-2.44	122.22	124.45
45	AB	831	CLA	CAC-C3C-C4C	2.44	127.97	124.81
45	B5	612	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
45	BB	808	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
45	A3	303	CLA	CAC-C3C-C4C	2.44	127.97	124.81
45	AA	837	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
48	AI	102	BCR	C39-C30-C25	2.43	114.25	110.30
48	AI	101	BCR	C28-C27-C26	-2.43	109.73	114.08
48	AB	849	BCR	C12-C13-C14	-2.43	115.21	118.94
45	B2	608	CLA	CHB-C4A-NA	2.43	127.87	124.51
48	AB	844	BCR	C23-C22-C21	-2.43	115.21	118.94
54	B1	303	CHL	O2A-CGA-O1A	-2.43	117.46	123.59
54	B5	606	CHL	C4A-NA-C1A	-2.43	105.61	106.71
48	A3	318	BCR	C30-C25-C24	2.43	122.64	115.78
48	BB	848	BCR	C32-C1-C6	-2.43	106.36	110.30
45	A1	309	CLA	CHD-C1D-ND	-2.43	122.22	124.45
48	AL	306	BCR	C34-C9-C10	-2.43	119.53	122.92
48	B5	616	BCR	C38-C26-C25	-2.42	121.81	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	842	CLA	CHD-C1D-ND	-2.42	122.23	124.45
48	BG	203	BCR	C39-C30-C25	-2.42	106.37	110.30
45	BA	829	CLA	O2A-CGA-O1A	-2.42	117.48	123.59
48	AA	849	BCR	C12-C13-C14	-2.42	115.23	118.94
48	A4	317	BCR	C38-C26-C27	2.42	118.26	113.62
48	B2	617	BCR	C23-C22-C21	-2.42	115.23	118.94
55	B2	616	XAT	C8-C9-C10	-2.42	115.23	118.94
48	AB	848	BCR	C24-C23-C22	-2.42	122.58	126.23
48	BL	305	BCR	C37-C22-C21	-2.42	119.54	122.92
48	BA	847	BCR	C40-C30-C25	-2.42	106.38	110.30
45	BA	804	CLA	CHB-C4A-NA	2.42	127.85	124.51
45	BA	834	CLA	O2D-CGD-CBD	2.42	115.56	111.27
45	B3	312	CLA	CHD-C1D-ND	-2.42	122.23	124.45
54	A6	606	CHL	OMC-CMC-C2C	-2.42	120.22	125.69
48	BB	846	BCR	C16-C15-C14	-2.41	118.53	123.47
45	A4	308	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
45	BA	809	CLA	CHB-C4A-NA	2.41	127.85	124.51
45	AA	813	CLA	CHD-C1D-ND	-2.41	122.24	124.45
48	AA	852	BCR	C11-C10-C9	-2.41	123.87	127.31
45	BA	816	CLA	CHD-C1D-ND	-2.41	122.24	124.45
45	AA	818	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
45	AB	815	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
45	BA	818	CLA	O2A-CGA-O1A	-2.41	117.50	123.59
45	BB	833	CLA	CHD-C1D-ND	-2.41	122.24	124.45
45	AA	810	CLA	CHB-C4A-NA	2.41	127.85	124.51
52	AF	806	LUT	C39-C29-C30	-2.41	119.55	122.92
48	AA	846	BCR	C37-C22-C23	2.41	121.88	118.08
45	BB	831	CLA	CHD-C1D-ND	-2.41	122.24	124.45
45	B1	307	CLA	CBD-CHA-C1A	2.41	131.34	128.50
52	A4	315	LUT	C8-C9-C10	-2.41	115.25	118.94
45	AK	203	CLA	CMB-C2B-C3B	2.41	129.18	124.68
48	BL	306	BCR	C23-C24-C25	-2.41	120.44	127.20
45	AB	832	CLA	CHB-C4A-NA	2.41	127.84	124.51
45	B3	302	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
45	A4	303	CLA	CHB-C4A-NA	2.41	127.84	124.51
45	B2	611	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
45	A3	312	CLA	CMB-C2B-C3B	2.41	129.18	124.68
55	A3	317	XAT	O24-C25-C24	2.41	115.19	113.38
45	AA	835	CLA	CHB-C4A-NA	2.40	127.84	124.51
45	AB	805	CLA	CHB-C4A-NA	2.40	127.84	124.51
45	BA	824	CLA	CHD-C1D-ND	-2.40	122.25	124.45
48	AA	848	BCR	C19-C18-C17	-2.40	115.25	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AJ	101	BCR	C12-C13-C14	-2.40	115.25	118.94
48	BB	803	BCR	C24-C25-C26	2.40	127.28	121.46
48	BA	847	BCR	C23-C22-C21	-2.40	115.25	118.94
48	AA	846	BCR	C15-C14-C13	-2.40	123.88	127.31
45	A4	311	CLA	CHD-C1D-ND	-2.40	122.25	124.45
48	AA	847	BCR	C37-C22-C23	2.40	121.86	118.08
48	AB	848	BCR	C37-C22-C21	-2.40	119.56	122.92
45	BB	818	CLA	CHD-C1D-ND	-2.40	122.25	124.45
45	AA	801	CLA	C1D-ND-C4D	-2.40	104.63	106.33
45	AA	809	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
45	AA	823	CLA	CAA-C2A-C3A	-2.40	110.50	116.10
48	BB	803	BCR	C29-C28-C27	-2.40	106.02	111.38
48	A6	617	BCR	C36-C18-C19	2.40	121.86	118.08
52	A3	316	LUT	C19-C9-C8	2.40	121.86	118.08
45	A3	304	CLA	CHD-C1D-ND	-2.40	122.25	124.45
45	B3	307	CLA	CHD-C1D-ND	-2.40	122.25	124.45
45	AA	805	CLA	CBA-CAA-C2A	2.40	120.94	113.86
45	B3	307	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
48	BL	306	BCR	C16-C17-C18	2.40	130.73	127.31
45	BB	805	CLA	C2A-C1A-CHA	2.40	128.05	123.86
48	AA	849	BCR	C38-C26-C25	-2.40	121.84	124.53
45	BB	829	CLA	O2A-CGA-O1A	-2.40	117.54	123.59
48	BI	101	BCR	C33-C5-C4	2.40	118.22	113.62
45	AA	821	CLA	CHB-C4A-NA	2.40	127.83	124.51
48	AB	847	BCR	C19-C18-C17	-2.40	115.26	118.94
55	A6	616	XAT	C38-C25-C26	-2.40	118.25	122.26
45	AB	809	CLA	CBA-CAA-C2A	2.40	120.94	113.86
52	B5	614	LUT	C37-C21-C36	2.40	111.42	107.89
45	AA	839	CLA	CHB-C4A-NA	2.40	127.82	124.51
45	A1	312	CLA	CMB-C2B-C3B	2.39	129.38	124.69
45	AA	829	CLA	C5-C3-C2	-2.39	116.27	121.12
45	BB	841	CLA	CHB-C4A-NA	2.39	127.82	124.51
45	B3	302	CLA	C5-C3-C2	2.39	125.96	121.12
45	AA	820	CLA	CHB-C4A-NA	2.39	127.82	124.51
45	AA	830	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
45	AA	814	CLA	CMB-C2B-C3B	2.39	129.16	124.68
45	B3	303	CLA	CHD-C1D-ND	-2.39	122.25	124.45
45	BA	837	CLA	O2A-CGA-O1A	-2.39	117.55	123.59
48	AA	845	BCR	C8-C7-C6	-2.39	120.48	127.20
45	AB	819	CLA	O2D-CGD-CBD	2.39	115.52	111.27
45	BA	816	CLA	CHB-C4A-NA	2.39	127.82	124.51
45	BF	301	CLA	CHB-C4A-NA	2.39	127.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	B1	312	CLA	CHB-C4A-NA	2.39	127.82	124.51
48	BA	851	BCR	C4-C5-C6	-2.39	119.26	122.73
48	B5	616	BCR	C27-C26-C25	-2.39	119.26	122.73
45	AB	839	CLA	O2D-CGD-CBD	2.39	115.52	111.27
45	BA	827	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
45	B1	310	CLA	CHB-C4A-NA	2.39	127.82	124.51
48	AB	845	BCR	C12-C13-C14	-2.39	115.28	118.94
45	AB	803	CLA	CMB-C2B-C3B	2.39	129.15	124.68
45	AB	816	CLA	CHB-C4A-NA	2.39	127.81	124.51
55	B1	317	XAT	C39-C29-C30	-2.39	119.58	122.92
48	A4	317	BCR	C8-C9-C10	-2.39	115.28	118.94
48	AA	847	BCR	C27-C26-C25	-2.39	119.27	122.73
55	B1	317	XAT	C8-C9-C10	-2.39	115.28	118.94
45	AA	803	CLA	CHB-C4A-NA	2.39	127.81	124.51
52	A4	315	LUT	C35-C15-C14	-2.39	118.59	123.47
54	B1	308	CHL	CAC-C3C-C4C	2.39	127.91	124.81
48	B3	317	BCR	C29-C30-C25	2.39	114.15	110.48
45	B3	304	CLA	CMB-C2B-C3B	2.38	129.14	124.68
45	B1	314	CLA	CHD-C1D-ND	-2.38	122.26	124.45
45	AA	819	CLA	CBA-CAA-C2A	2.38	120.90	113.86
45	AB	814	CLA	CHB-C4A-NA	2.38	127.81	124.51
48	BB	845	BCR	C19-C18-C17	-2.38	115.28	118.94
45	A4	312	CLA	CHB-C4A-NA	2.38	127.81	124.51
54	B2	605	CHL	O2D-CGD-O1D	-2.38	119.18	123.84
54	A6	602	CHL	O2A-CGA-O1A	-2.38	117.58	123.59
45	AA	836	CLA	CHB-C4A-NA	2.38	127.80	124.51
45	B3	305	CLA	CHB-C4A-NA	2.38	127.80	124.51
55	A3	317	XAT	C24-C23-C22	-2.38	106.18	110.77
52	B3	315	LUT	C36-C21-C26	2.38	113.15	109.55
45	AG	203	CLA	CHD-C1D-ND	-2.38	122.27	124.45
45	A4	311	CLA	CHB-C4A-NA	2.38	127.80	124.51
48	AA	845	BCR	C11-C10-C9	-2.38	123.92	127.31
48	AB	845	BCR	C15-C16-C17	-2.38	118.60	123.47
45	B5	612	CLA	CHB-C4A-NA	2.38	127.80	124.51
54	A4	306	CHL	CMD-C2D-C1D	2.38	128.90	124.71
45	AB	807	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
45	AB	823	CLA	CMB-C2B-C1B	-2.38	124.81	128.46
45	BA	830	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
45	A3	313	CLA	CHD-C1D-ND	-2.38	122.27	124.45
45	BA	832	CLA	CHD-C1D-ND	-2.38	122.27	124.45
45	BA	838	CLA	O2A-CGA-O1A	-2.38	117.59	123.59
48	BA	851	BCR	C30-C25-C26	-2.38	119.27	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AB	849	BCR	C8-C9-C10	-2.38	115.30	118.94
45	AA	805	CLA	CMB-C2B-C3B	2.38	129.12	124.68
45	AA	827	CLA	O2D-CGD-CBD	2.37	115.49	111.27
48	BL	305	BCR	C19-C18-C17	-2.37	115.30	118.94
45	A1	306	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
45	BB	807	CLA	CMB-C2B-C3B	2.37	129.12	124.68
45	AB	825	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
48	BJ	101	BCR	C2-C1-C6	2.37	114.13	110.48
54	A6	602	CHL	C4-C3-C5	2.37	119.26	115.27
48	AF	801	BCR	C36-C18-C19	2.37	121.81	118.08
45	A4	302	CLA	CMB-C2B-C3B	2.37	129.33	124.69
54	A1	303	CHL	C3C-C4C-NC	2.37	113.23	110.57
45	A6	605	CLA	CHB-C4A-NA	2.37	127.79	124.51
45	BA	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
45	B1	305	CLA	CBC-CAC-C3C	-2.37	105.90	112.43
45	B2	612	CLA	CHD-C1D-ND	-2.37	122.28	124.45
45	BK	202	CLA	CHB-C4A-NA	2.37	127.79	124.51
45	B3	301	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
47	B1	318	LHG	O8-C23-C24	2.37	119.33	111.91
48	BF	304	BCR	C11-C10-C9	-2.36	123.94	127.31
45	B2	609	CLA	C4-C3-C5	2.36	119.25	115.27
55	B2	616	XAT	C35-C15-C14	-2.36	118.63	123.47
54	A6	602	CHL	O2D-CGD-O1D	-2.36	118.72	124.09
45	BB	814	CLA	CHB-C4A-NA	2.36	127.78	124.51
45	AF	803	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
45	AA	835	CLA	CHD-C1D-ND	-2.36	122.28	124.45
45	AG	204	CLA	CMB-C2B-C3B	2.36	129.10	124.68
48	A1	319	BCR	C8-C9-C10	-2.36	115.31	118.94
45	BA	820	CLA	CHB-C4A-NA	2.36	127.78	124.51
48	BA	850	BCR	C38-C26-C27	2.36	118.15	113.62
48	A6	617	BCR	C29-C30-C25	2.36	114.11	110.48
48	AB	849	BCR	C29-C28-C27	-2.36	106.10	111.38
53	B5	617	LMG	C6-C5-C4	-2.36	107.47	113.00
48	A6	617	BCR	C8-C9-C10	-2.36	115.32	118.94
45	BA	828	CLA	CHB-C4A-NA	2.36	127.78	124.51
45	BB	814	CLA	CHD-C1D-ND	-2.36	122.29	124.45
45	BA	821	CLA	CHB-C4A-NA	2.36	127.77	124.51
48	BB	845	BCR	C16-C17-C18	-2.36	123.94	127.31
45	BA	815	CLA	CHB-C4A-NA	2.36	127.77	124.51
45	AF	803	CLA	CMB-C2B-C3B	2.36	129.09	124.68
45	AA	806	CLA	O2D-CGD-CBD	2.36	115.46	111.27
45	BB	801	CLA	CMB-C2B-C3B	2.36	129.09	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	829	CLA	CBA-CAA-C2A	2.36	120.82	113.86
54	A4	304	CHL	C3C-C4C-NC	2.36	113.14	110.57
48	BB	849	BCR	C15-C14-C13	-2.36	123.95	127.31
48	AB	845	BCR	C24-C25-C26	2.36	127.17	121.46
45	AK	201	CLA	CHD-C1D-ND	-2.35	122.29	124.45
48	AI	101	BCR	C11-C10-C9	-2.35	123.95	127.31
55	A6	616	XAT	C36-C21-C22	-2.35	104.89	108.98
48	AB	849	BCR	C29-C30-C25	2.35	114.10	110.48
45	A3	314	CLA	CHD-C1D-ND	-2.35	122.29	124.45
45	B3	304	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
45	AA	826	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
48	B5	616	BCR	C29-C30-C25	2.35	114.10	110.48
45	AA	830	CLA	CMB-C2B-C3B	2.35	129.08	124.68
55	B1	317	XAT	C32-C33-C34	-2.35	115.33	118.94
55	B5	615	XAT	C4-C3-C2	-2.35	106.23	110.77
48	AB	849	BCR	C2-C3-C4	-2.35	106.13	111.38
54	B2	607	CHL	C3C-C4C-NC	2.35	113.21	110.57
48	BB	848	BCR	C2-C1-C6	2.35	114.10	110.48
45	BA	811	CLA	CHB-C4A-NA	2.35	127.76	124.51
45	BA	818	CLA	CHB-C4A-NA	2.35	127.76	124.51
48	BA	856	BCR	C40-C30-C25	-2.35	106.49	110.30
45	A6	609	CLA	CHB-C4A-NA	2.35	127.76	124.51
47	AA	844	LHG	O8-C23-C24	2.35	119.27	111.91
45	A1	307	CLA	CHD-C1D-ND	-2.35	122.30	124.45
54	B2	606	CHL	CED-O2D-CGD	2.35	121.24	115.94
48	AA	852	BCR	C32-C1-C6	-2.35	106.49	110.30
45	BB	815	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
45	A3	312	CLA	CHB-C4A-NA	2.35	127.75	124.51
55	A1	318	XAT	C36-C21-C22	-2.34	104.91	108.98
45	A1	307	CLA	C2A-C1A-CHA	2.34	126.35	122.71
45	B3	305	CLA	CAA-C2A-C3A	-2.34	108.40	114.26
45	BF	303	CLA	CHB-C4A-NA	2.34	127.75	124.51
45	AA	803	CLA	C1-C2-C3	-2.34	121.99	126.04
55	B2	616	XAT	C32-C33-C34	-2.34	115.34	118.94
48	AJ	103	BCR	C16-C15-C14	-2.34	118.67	123.47
45	B1	306	CLA	CAA-C2A-C3A	-2.34	110.63	116.10
55	A1	318	XAT	C10-C11-C12	-2.34	115.91	123.22
45	BL	302	CLA	CBA-CAA-C2A	2.34	120.78	113.86
45	AA	803	CLA	CMB-C2B-C3B	2.34	129.06	124.68
45	BA	808	CLA	CMB-C2B-C3B	2.34	129.06	124.68
45	AB	818	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
48	BB	803	BCR	C8-C9-C10	-2.34	115.35	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	842	CLA	O2D-CGD-CBD	2.34	115.43	111.27
48	BB	803	BCR	C19-C18-C17	-2.34	115.35	118.94
45	BB	842	CLA	CHB-C4A-NA	2.34	127.75	124.51
45	B2	602	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
45	AB	821	CLA	CHB-C4A-NA	2.34	127.75	124.51
52	A1	317	LUT	C35-C15-C14	-2.34	118.68	123.47
54	A6	606	CHL	C3C-C4C-NC	2.34	113.12	110.57
52	A1	317	LUT	C8-C9-C10	-2.34	115.36	118.94
45	BF	302	CLA	CMB-C2B-C3B	2.34	129.05	124.68
48	AJ	103	BCR	C10-C11-C12	-2.34	115.92	123.22
48	AA	852	BCR	C29-C30-C25	2.34	114.08	110.48
48	A6	617	BCR	C4-C5-C6	-2.34	119.34	122.73
45	BB	807	CLA	CMC-C2C-C1C	-2.34	121.48	125.04
45	BB	840	CLA	O2D-CGD-CBD	2.33	115.42	111.27
55	B3	316	XAT	C10-C11-C12	-2.33	115.93	123.22
45	B2	609	CLA	C6-C5-C3	2.33	119.58	113.45
45	AA	817	CLA	CHD-C1D-ND	-2.33	122.31	124.45
48	AJ	101	BCR	C16-C17-C18	-2.33	123.98	127.31
45	BA	831	CLA	CAC-C3C-C4C	2.33	127.84	124.81
45	BB	835	CLA	CHD-C1D-ND	-2.33	122.31	124.45
45	BB	837	CLA	CHD-C1D-ND	-2.33	122.31	124.45
45	BG	201	CLA	O1D-CGD-CBD	2.33	129.26	124.48
48	A4	317	BCR	C19-C18-C17	-2.33	115.36	118.94
45	AA	824	CLA	CHB-C4A-NA	2.33	127.74	124.51
48	BI	101	BCR	C3-C4-C5	-2.33	109.92	114.08
48	AB	845	BCR	C37-C22-C21	-2.33	119.66	122.92
45	B1	305	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
45	B1	309	CLA	CHB-C4A-NA	2.33	127.73	124.51
54	A6	602	CHL	CMD-C2D-C1D	2.33	128.82	124.71
45	AB	833	CLA	CHB-C4A-NA	2.33	127.73	124.51
48	BB	848	BCR	C1-C6-C5	-2.33	119.33	122.61
48	AA	847	BCR	C11-C12-C13	2.33	132.96	126.42
48	BJ	103	BCR	C10-C11-C12	-2.33	115.95	123.22
45	AB	833	CLA	O2A-C1-C2	-2.33	102.52	108.64
55	A3	317	XAT	C4-C3-C2	-2.33	106.28	110.77
48	AB	845	BCR	C40-C30-C25	-2.33	106.53	110.30
48	B3	317	BCR	C24-C25-C26	2.33	127.10	121.46
45	BA	823	CLA	CHB-C4A-NA	2.33	127.73	124.51
48	AB	849	BCR	C2-C1-C6	2.33	114.06	110.48
55	B3	316	XAT	C36-C21-C26	2.33	116.33	110.05
45	AA	832	CLA	CHB-C4A-NA	2.33	127.73	124.51
45	BB	806	CLA	CAA-C2A-C3A	-2.33	110.67	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AB	846	BCR	C23-C22-C21	2.33	122.51	118.94
45	BA	805	CLA	CHB-C4A-NA	2.32	127.73	124.51
45	BF	301	CLA	C6-C5-C3	2.32	119.55	113.45
45	AA	838	CLA	C5-C3-C2	2.32	125.82	121.12
48	BB	846	BCR	C40-C30-C25	-2.32	106.53	110.30
45	BB	830	CLA	CBA-CAA-C2A	2.32	120.72	113.86
48	BA	848	BCR	C28-C27-C26	-2.32	109.93	114.08
48	B2	617	BCR	C8-C9-C10	-2.32	115.38	118.94
54	A4	304	CHL	O2D-CGD-O1D	-2.32	118.82	124.09
45	BL	304	CLA	CHB-C4A-NA	2.32	127.72	124.51
45	AB	841	CLA	O2A-CGA-O1A	-2.32	117.73	123.59
45	BG	202	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
45	B2	602	CLA	C1-C2-C3	-2.32	122.03	126.04
45	A1	310	CLA	CAA-C2A-C3A	-2.32	110.69	116.10
45	A6	613	CLA	CHB-C4A-NA	2.32	127.72	124.51
45	BA	804	CLA	O2D-CGD-CBD	2.32	115.39	111.27
48	BA	849	BCR	C38-C26-C27	2.32	118.07	113.62
45	AA	814	CLA	O2A-CGA-O1A	-2.32	117.52	123.30
48	BA	848	BCR	C19-C18-C17	-2.32	115.38	118.94
55	B2	616	XAT	C19-C9-C8	2.32	121.73	118.08
45	AA	841	CLA	CHD-C1D-ND	-2.32	122.32	124.45
45	B1	309	CLA	CHD-C1D-ND	-2.32	122.32	124.45
45	AA	811	CLA	CHB-C4A-NA	2.32	127.72	124.51
45	BL	302	CLA	CMB-C2B-C3B	2.32	129.01	124.68
45	AG	201	CLA	CHB-C4A-NA	2.32	127.71	124.51
45	BA	803	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
45	A6	601	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
45	AF	803	CLA	CAA-C2A-C3A	-2.31	108.48	114.26
52	A6	615	LUT	C37-C21-C22	-2.31	105.05	109.44
52	B3	315	LUT	C28-C29-C30	-2.31	115.39	118.94
45	B3	301	CLA	CHB-C4A-NA	2.31	127.71	124.51
45	BK	201	CLA	CHB-C4A-NA	2.31	127.71	124.51
48	B5	616	BCR	C21-C20-C19	-2.31	116.00	123.22
48	AG	205	BCR	C2-C1-C6	2.31	114.04	110.48
45	A1	305	CLA	CBC-CAC-C3C	-2.31	106.06	112.43
48	AB	849	BCR	C7-C8-C9	-2.31	122.74	126.23
48	AA	847	BCR	C15-C16-C17	-2.31	118.74	123.47
52	A4	315	LUT	C38-C25-C24	-2.31	118.61	123.56
48	B3	317	BCR	C39-C30-C29	2.31	118.15	108.91
45	BA	821	CLA	C7-C6-C5	-2.31	107.08	113.36
48	BB	803	BCR	C16-C17-C18	-2.31	124.01	127.31
48	BI	101	BCR	C36-C18-C17	-2.31	119.69	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A4	317	BCR	C2-C1-C6	-2.31	106.92	110.48
55	A1	318	XAT	C20-C13-C12	2.31	121.72	118.08
45	AH	201	CLA	CBA-CAA-C2A	2.31	120.68	113.86
45	A6	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
45	AB	823	CLA	CBA-CAA-C2A	2.31	120.68	113.86
45	BB	801	CLA	O2A-C1-C2	-2.31	102.57	108.64
45	AA	816	CLA	CHD-C1D-ND	-2.31	122.33	124.45
45	A1	306	CLA	CHD-C1D-ND	-2.31	122.33	124.45
45	AB	838	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
52	A3	316	LUT	C15-C35-C34	-2.31	118.75	123.47
45	BB	812	CLA	O1D-CGD-CBD	2.31	129.20	124.48
45	AB	827	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
48	BB	849	BCR	C37-C22-C23	2.31	121.71	118.08
52	B1	316	LUT	C19-C9-C8	2.31	121.71	118.08
45	B1	305	CLA	C4-C3-C2	-2.30	117.77	123.68
50	AB	852	LMU	C1B-O1B-C4'	-2.30	112.26	117.96
45	A3	310	CLA	CHB-C4A-NA	2.30	127.70	124.51
53	A1	321	LMG	O4-C4-C3	-2.30	105.03	110.35
45	AA	808	CLA	CHB-C4A-NA	2.30	127.69	124.51
45	AA	836	CLA	CHD-C1D-ND	-2.30	122.34	124.45
54	B2	607	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
45	BA	806	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
45	A4	307	CLA	CHD-C1D-ND	-2.30	122.34	124.45
45	B3	313	CLA	CHB-C4A-NA	2.30	127.69	124.51
45	BB	823	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
48	BA	847	BCR	C36-C18-C17	-2.30	119.70	122.92
45	AA	836	CLA	O2D-CGD-CBD	2.30	115.36	111.27
54	A1	303	CHL	C1-O2A-CGA	2.30	122.48	116.44
45	A3	308	CLA	CHB-C4A-NA	2.30	127.69	124.51
48	AK	204	BCR	C2-C3-C4	-2.30	106.24	111.38
45	AK	201	CLA	CHB-C4A-NA	2.30	127.69	124.51
48	B2	617	BCR	C27-C26-C25	-2.30	119.39	122.73
45	A1	310	CLA	CMA-C3A-C2A	-2.30	110.74	116.10
45	BB	838	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
52	A4	315	LUT	C19-C9-C8	2.30	121.70	118.08
48	AI	101	BCR	C16-C17-C18	-2.30	124.03	127.31
45	BB	810	CLA	CHB-C4A-NA	2.30	127.69	124.51
48	A6	617	BCR	C15-C16-C17	-2.30	118.77	123.47
45	AA	839	CLA	CMB-C2B-C1B	-2.30	124.94	128.46
48	BA	848	BCR	C16-C15-C14	-2.30	118.77	123.47
50	AB	850	LMU	C1'-C2'-C3'	2.29	114.77	110.00
48	BL	306	BCR	C3-C4-C5	-2.29	109.98	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	841	CLA	CBA-CAA-C2A	2.29	120.63	113.86
45	AA	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
45	BB	828	CLA	O2D-CGD-CBD	2.29	115.34	111.27
45	AG	203	CLA	CHB-C4A-NA	2.29	127.68	124.51
45	A1	305	CLA	O2A-C1-C2	-2.29	102.61	108.64
45	BB	807	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
48	AB	849	BCR	C21-C20-C19	-2.29	116.07	123.22
45	BB	834	CLA	O2D-CGD-CBD	2.29	115.34	111.27
45	AB	809	CLA	C11-C10-C8	-2.29	108.52	115.92
48	BA	856	BCR	C24-C23-C22	-2.29	122.78	126.23
45	A3	314	CLA	CHB-C4A-NA	2.29	127.68	124.51
48	BJ	103	BCR	C34-C9-C8	2.29	121.68	118.08
55	A6	616	XAT	C19-C9-C8	2.29	121.68	118.08
55	B3	316	XAT	C16-C1-C2	-2.29	105.01	108.98
45	BB	825	CLA	CHD-C1D-ND	-2.29	122.35	124.45
48	AA	847	BCR	C29-C30-C25	2.29	114.00	110.48
45	BG	201	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
55	A6	616	XAT	C24-C23-C22	-2.29	106.36	110.77
48	AB	847	BCR	C37-C22-C21	-2.29	119.72	122.92
54	B1	303	CHL	O2A-CGA-CBA	2.29	119.08	111.91
45	BA	829	CLA	O2D-CGD-CBD	2.29	115.33	111.27
45	AG	204	CLA	CHD-C1D-ND	-2.29	122.35	124.45
48	AI	102	BCR	C38-C26-C25	2.29	127.09	124.53
45	BA	826	CLA	C5-C3-C2	2.28	125.74	121.12
48	AK	204	BCR	C7-C8-C9	-2.28	122.78	126.23
55	A4	316	XAT	C35-C34-C33	-2.28	124.05	127.31
45	AB	809	CLA	CHB-C4A-NA	2.28	127.67	124.51
45	AA	829	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
48	AB	845	BCR	C7-C8-C9	-2.28	122.78	126.23
45	AB	804	CLA	CMD-C2D-C3D	2.28	132.87	127.61
45	BF	303	CLA	CHD-C1D-ND	-2.28	122.36	124.45
48	BA	849	BCR	C40-C30-C25	-2.28	106.60	110.30
45	BB	821	CLA	CHB-C4A-NA	2.28	127.67	124.51
45	BB	836	CLA	CHB-C4A-NA	2.28	127.67	124.51
45	AB	809	CLA	C5-C3-C2	2.28	125.73	121.12
45	BF	302	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
48	BA	847	BCR	C16-C15-C14	-2.28	118.80	123.47
48	BL	305	BCR	C23-C22-C21	-2.28	115.44	118.94
45	BB	830	CLA	C2D-C1D-ND	-2.28	108.42	110.10
48	BI	101	BCR	C16-C17-C18	-2.28	124.06	127.31
55	A1	318	XAT	C35-C15-C14	-2.28	118.81	123.47
48	BB	845	BCR	C20-C21-C22	-2.28	124.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	842	CLA	CHD-C1D-ND	-2.28	122.36	124.45
45	AA	833	CLA	CHB-C4A-NA	2.28	127.66	124.51
45	B3	305	CLA	CHD-C1D-ND	-2.28	122.36	124.45
45	AA	805	CLA	CHB-C4A-NA	2.28	127.66	124.51
45	AB	826	CLA	CHB-C4A-NA	2.28	127.66	124.51
45	A6	614	CLA	CHB-C4A-NA	2.28	127.66	124.51
54	B2	601	CHL	O2D-CGD-O1D	-2.28	119.39	123.84
54	B2	601	CHL	C6-C5-C3	-2.28	110.90	114.62
54	B5	605	CHL	C3C-C4C-NC	2.28	113.06	110.57
45	BL	303	CLA	CBA-CAA-C2A	2.28	120.58	113.86
45	BB	823	CLA	CMB-C2B-C1B	-2.28	124.97	128.46
48	BB	848	BCR	C21-C20-C19	-2.28	116.12	123.22
45	A1	309	CLA	CHB-C4A-NA	2.28	127.66	124.51
45	AA	833	CLA	CMB-C2B-C3B	2.27	128.93	124.68
48	BJ	103	BCR	C37-C22-C23	2.27	121.66	118.08
48	B5	616	BCR	C19-C18-C17	-2.27	115.45	118.94
45	B5	613	CLA	CHB-C4A-NA	2.27	127.66	124.51
47	B1	301	LHG	O8-C23-O10	-2.27	117.86	123.59
45	A4	301	CLA	O2D-CGD-CBD	2.27	115.31	111.27
45	B2	604	CLA	CHD-C1D-ND	-2.27	122.37	124.45
50	AB	850	LMU	C2'-C3'-C4'	2.27	114.87	109.68
45	BB	804	CLA	CHB-C4A-NA	2.27	127.65	124.51
48	BJ	101	BCR	C30-C25-C24	2.27	122.20	115.78
48	AL	302	BCR	C2-C3-C4	-2.27	106.30	111.38
45	A1	305	CLA	C4-C3-C2	-2.27	117.85	123.68
46	AA	843	PQN	C17-C16-C15	-2.27	107.19	113.36
45	BA	804	CLA	O2A-CGA-O1A	-2.27	117.86	123.59
48	BA	847	BCR	C36-C18-C19	2.27	121.65	118.08
45	A1	312	CLA	CAB-C3B-C2B	2.27	129.13	124.69
54	A4	305	CHL	C4A-NA-C1A	-2.27	105.69	106.71
45	BA	803	CLA	C2D-C1D-ND	-2.27	108.43	110.10
45	AJ	102	CLA	CHB-C4A-NA	2.27	127.65	124.51
54	B2	601	CHL	CMD-C2D-C1D	2.27	128.71	124.71
45	BB	805	CLA	CMD-C2D-C1D	-2.27	120.72	124.71
45	BA	821	CLA	O2D-CGD-CBD	2.27	115.30	111.27
45	B5	611	CLA	CAA-C2A-C3A	-2.27	108.60	114.26
45	AA	822	CLA	CHB-C4A-NA	2.27	127.64	124.51
45	BB	804	CLA	C5-C3-C2	-2.27	116.53	121.12
45	BB	813	CLA	C5-C3-C2	2.26	125.70	121.12
45	BA	814	CLA	CHD-C1D-ND	-2.26	122.37	124.45
51	AB	851	DGD	O2G-C1B-O1B	-2.26	118.23	123.70
45	AB	828	CLA	O2A-CGA-O1A	-2.26	117.88	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	828	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
48	BB	845	BCR	C37-C22-C23	2.26	121.64	118.08
48	AG	205	BCR	C40-C30-C25	-2.26	106.63	110.30
54	B1	303	CHL	O2D-CGD-O1D	-2.26	118.95	124.09
48	AA	846	BCR	C19-C18-C17	-2.26	115.47	118.94
45	A4	302	CLA	CHB-C4A-NA	2.26	127.64	124.51
45	BB	810	CLA	O2D-CGD-CBD	2.26	115.29	111.27
54	A4	304	CHL	CAC-C3C-C4C	2.26	128.48	125.04
45	BA	810	CLA	CMB-C2B-C3B	2.26	128.91	124.68
45	BA	803	CLA	C1-C2-C3	-2.26	122.13	126.04
45	A1	312	CLA	CAA-C2A-C3A	-2.26	110.82	116.10
52	B5	614	LUT	C12-C13-C14	-2.26	115.47	118.94
54	B2	601	CHL	C3D-C2D-C1D	-2.26	102.75	105.83
48	AB	844	BCR	C35-C13-C12	2.26	121.64	118.08
45	AA	802	CLA	C2D-C1D-ND	-2.26	108.44	110.10
45	A3	302	CLA	CHD-C1D-ND	-2.26	122.38	124.45
54	B2	614	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
52	B2	615	LUT	C12-C13-C14	-2.26	115.48	118.94
45	A4	309	CLA	O2D-CGD-CBD	2.26	115.28	111.27
45	A6	601	CLA	CHD-C1D-ND	-2.26	122.38	124.45
45	AB	812	CLA	C5-C3-C2	2.26	125.68	121.12
45	BA	826	CLA	CHB-C4A-NA	2.26	127.63	124.51
55	B2	616	XAT	C18-C5-C6	-2.26	118.48	122.26
45	AA	808	CLA	O2D-CGD-CBD	2.25	115.28	111.27
45	BL	302	CLA	C3A-C2A-C1A	2.25	104.72	101.34
47	A3	319	LHG	O8-C23-C24	2.25	118.98	111.91
48	BK	204	BCR	C20-C21-C22	-2.25	124.09	127.31
45	BB	843	CLA	CHB-C4A-NA	2.25	127.63	124.51
48	A4	317	BCR	C21-C20-C19	-2.25	116.19	123.22
48	B3	317	BCR	C12-C13-C14	-2.25	115.48	118.94
45	A3	308	CLA	O2D-CGD-O1D	-2.25	119.44	123.84
55	A1	318	XAT	C19-C9-C8	2.25	121.62	118.08
45	BB	824	CLA	CBA-CAA-C2A	2.25	120.51	113.86
45	AB	811	CLA	C2A-C1A-CHA	2.25	127.79	123.86
45	B5	604	CLA	CHB-C4A-NA	2.25	127.62	124.51
45	BH	201	CLA	CMB-C2B-C3B	2.25	128.89	124.68
52	A1	317	LUT	C37-C21-C22	-2.25	105.17	109.44
45	B2	602	CLA	CHD-C1D-ND	-2.25	122.39	124.45
45	BB	842	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
54	B5	606	CHL	CED-O2D-CGD	2.25	121.02	115.94
45	BL	302	CLA	CHD-C1D-ND	-2.25	122.39	124.45
48	AI	102	BCR	C15-C16-C17	-2.25	118.87	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	816	CLA	CHB-C4A-NA	2.25	127.62	124.51
45	A3	313	CLA	CHB-C4A-NA	2.25	127.62	124.51
55	A1	318	XAT	C36-C21-C26	2.25	116.11	110.05
45	BA	817	CLA	C5-C3-C2	2.25	125.66	121.12
45	A4	307	CLA	CHB-C4A-NA	2.25	127.62	124.51
45	BH	201	CLA	CHB-C4A-NA	2.25	127.62	124.51
45	BB	802	CLA	C7-C6-C5	-2.25	107.26	113.36
48	BA	856	BCR	C29-C28-C27	-2.25	106.36	111.38
47	BF	305	LHG	O8-C23-C24	2.25	118.95	111.91
48	AL	306	BCR	C35-C13-C12	2.24	121.61	118.08
45	BB	811	CLA	CHB-C4A-NA	2.24	127.62	124.51
45	BB	832	CLA	CHB-C4A-NA	2.24	127.62	124.51
45	B2	613	CLA	CHB-C4A-NA	2.24	127.62	124.51
48	AJ	103	BCR	C24-C23-C22	-2.24	122.85	126.23
45	BA	805	CLA	CMC-C2C-C3C	2.24	132.20	126.12
45	A4	313	CLA	CMB-C2B-C3B	2.24	128.87	124.68
45	AB	809	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
48	BB	849	BCR	C20-C21-C22	-2.24	124.11	127.31
55	B2	616	XAT	C24-C23-C22	-2.24	106.45	110.77
45	BB	830	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
45	AA	819	CLA	O2D-CGD-CBD	2.24	115.25	111.27
48	BB	849	BCR	C8-C9-C10	-2.24	115.50	118.94
45	AA	833	CLA	CMD-C2D-C1D	-2.24	120.77	124.71
45	BA	803	CLA	CHB-C4A-NA	2.24	127.61	124.51
55	A3	317	XAT	O4-C5-C6	-2.24	57.11	58.96
45	B3	313	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
45	BA	813	CLA	CHD-C1D-ND	-2.24	122.40	124.45
47	A3	301	LHG	O8-C23-C24	2.24	118.92	111.91
54	A4	306	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
54	B2	605	CHL	C3C-C4C-NC	2.24	113.01	110.57
45	AA	827	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
48	BJ	101	BCR	C16-C15-C14	-2.24	118.89	123.47
48	AJ	101	BCR	C2-C3-C4	-2.24	106.38	111.38
45	AB	841	CLA	CAC-C3C-C4C	2.24	127.71	124.81
45	BJ	102	CLA	CHD-C1D-ND	-2.24	122.40	124.45
48	AI	101	BCR	C32-C1-C6	2.23	113.92	110.30
48	BL	305	BCR	C8-C9-C10	-2.23	115.51	118.94
45	A3	311	CLA	O2D-CGD-CBD	2.23	115.24	111.27
48	AL	306	BCR	C20-C21-C22	-2.23	124.12	127.31
45	BB	802	CLA	O2D-CGD-CBD	2.23	115.24	111.27
45	A6	612	CLA	CHB-C4A-NA	2.23	127.60	124.51
45	AA	834	CLA	CBC-CAC-C3C	2.23	118.58	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AB	807	CLA	C3C-C4C-NC	-2.23	108.07	110.57
45	AA	840	CLA	CHD-C1D-ND	-2.23	122.40	124.45
48	AB	845	BCR	C32-C1-C6	-2.23	106.68	110.30
45	AA	809	CLA	CHA-C1A-NA	-2.23	121.29	126.40
45	AB	837	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
48	AI	102	BCR	C36-C18-C19	2.23	121.59	118.08
45	AB	829	CLA	CHB-C4A-NA	2.23	127.60	124.51
45	AB	802	CLA	O2D-CGD-CBD	2.23	115.23	111.27
45	BA	828	CLA	C6-C7-C8	-2.23	108.71	115.92
45	AB	831	CLA	CMB-C2B-C3B	2.23	128.85	124.68
54	A3	307	CHL	C3C-C4C-NC	2.23	113.07	110.57
45	BB	824	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
45	A3	309	CLA	CMA-C3A-C2A	-2.23	110.90	116.10
54	A4	306	CHL	C3C-C4C-NC	2.23	113.07	110.57
45	AB	827	CLA	CAA-C2A-C3A	-2.23	106.68	112.78
45	A6	601	CLA	CMC-C2C-C1C	-2.23	121.65	125.04
45	AB	832	CLA	O2A-CGA-O1A	-2.23	117.98	123.59
55	A1	318	XAT	C31-C30-C29	-2.22	124.14	127.31
45	AB	830	CLA	CMB-C2B-C3B	2.22	128.84	124.68
45	A3	315	CLA	CHB-C4A-NA	2.22	127.59	124.51
45	BB	840	CLA	CHB-C4A-NA	2.22	127.59	124.51
54	A4	306	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
54	B2	607	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
45	BB	804	CLA	CMB-C2B-C3B	2.22	128.84	124.68
45	AA	803	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
45	BB	828	CLA	C2A-C1A-CHA	2.22	127.75	123.86
48	BF	304	BCR	C8-C9-C10	-2.22	115.53	118.94
48	AA	848	BCR	C24-C25-C26	-2.22	116.08	121.46
52	A1	317	LUT	C38-C25-C24	-2.22	118.81	123.56
45	AA	821	CLA	O2D-CGD-CBD	2.22	115.21	111.27
45	AB	818	CLA	CHD-C1D-ND	-2.22	122.42	124.45
48	A1	319	BCR	C3-C4-C5	-2.22	110.12	114.08
45	BB	822	CLA	CMB-C2B-C3B	2.22	128.83	124.68
45	A3	313	CLA	CAA-C2A-C3A	-2.22	110.92	116.10
54	A1	303	CHL	O2D-CGD-O1D	-2.22	119.06	124.09
54	B5	607	CHL	C3D-C2D-C1D	-2.22	102.81	105.83
48	A4	317	BCR	C23-C22-C21	-2.22	115.54	118.94
48	BB	846	BCR	C33-C5-C6	-2.22	122.04	124.53
45	AB	814	CLA	CHD-C1D-ND	-2.22	122.42	124.45
45	AB	839	CLA	CHB-C4A-NA	2.22	127.58	124.51
45	AB	802	CLA	C4-C3-C5	2.21	119.00	115.27
54	A4	306	CHL	O2A-CGA-CBA	2.21	121.14	114.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	A3	316	LUT	C1-C6-C5	-2.21	119.50	122.61
45	AK	203	CLA	CHD-C1D-ND	-2.21	122.42	124.45
45	BA	841	CLA	CHD-C1D-ND	-2.21	122.42	124.45
52	B2	615	LUT	C30-C31-C32	-2.21	116.31	123.22
45	BB	840	CLA	CHD-C1D-ND	-2.21	122.42	124.45
48	AJ	101	BCR	C1-C6-C5	-2.21	119.50	122.61
45	A4	313	CLA	CHD-C1D-ND	-2.21	122.42	124.45
52	AF	806	LUT	C37-C21-C22	-2.21	105.25	109.44
48	A3	318	BCR	C20-C21-C22	-2.21	124.16	127.31
45	BB	807	CLA	CBA-CAA-C2A	2.21	120.39	113.86
45	AA	814	CLA	O2D-CGD-CBD	2.21	115.20	111.27
55	B5	615	XAT	C40-C33-C34	-2.21	119.83	122.92
48	BA	850	BCR	C21-C20-C19	-2.21	116.32	123.22
45	AL	303	CLA	CMA-C3A-C2A	-2.21	110.94	116.10
52	A6	615	LUT	C3-C4-C5	-2.21	107.45	111.85
45	BB	835	CLA	CHB-C4A-NA	2.21	127.57	124.51
45	B2	602	CLA	CHB-C4A-NA	2.21	127.57	124.51
45	A3	315	CLA	CAA-C2A-C3A	-2.21	110.94	116.10
48	AL	306	BCR	C29-C30-C25	-2.21	107.08	110.48
48	AL	306	BCR	C11-C10-C9	-2.21	124.16	127.31
45	BB	802	CLA	CHB-C4A-NA	2.21	127.56	124.51
45	A1	315	CLA	CAA-C2A-C3A	-2.21	110.95	116.10
48	BA	849	BCR	C12-C13-C14	-2.21	115.56	118.94
52	B5	614	LUT	C16-C1-C6	2.21	113.88	110.30
48	AF	805	BCR	C11-C10-C9	-2.21	124.16	127.31
45	B5	611	CLA	CMB-C2B-C3B	2.21	128.81	124.68
52	A6	615	LUT	C15-C35-C34	-2.21	118.95	123.47
45	BB	823	CLA	O2D-CGD-O1D	-2.21	119.08	124.09
48	AA	846	BCR	C28-C27-C26	-2.21	110.14	114.08
48	BJ	101	BCR	C28-C27-C26	-2.21	110.14	114.08
55	B5	615	XAT	C24-C23-C22	-2.21	106.51	110.77
48	BL	305	BCR	C12-C13-C14	-2.20	115.56	118.94
45	BB	815	CLA	C7-C6-C5	2.20	119.34	113.36
45	BB	817	CLA	CAC-C3C-C4C	2.20	127.67	124.81
48	BG	203	BCR	C21-C20-C19	2.20	130.09	123.22
48	AB	844	BCR	C15-C14-C13	-2.20	124.17	127.31
45	AA	838	CLA	CMB-C2B-C3B	2.20	128.80	124.68
45	AA	806	CLA	CHD-C1D-ND	-2.20	122.43	124.45
45	AK	202	CLA	CHD-C1D-ND	-2.20	122.43	124.45
45	AB	804	CLA	CMC-C2C-C1C	-2.20	121.69	125.04
55	B3	316	XAT	C39-C29-C30	-2.20	119.84	122.92
45	AL	303	CLA	CHB-C4A-NA	2.20	127.56	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	818	CLA	CAA-C2A-C3A	2.20	118.80	112.78
45	BB	830	CLA	CHB-C4A-NA	2.20	127.56	124.51
55	A4	316	XAT	C12-C13-C14	-2.20	115.57	118.94
45	AB	802	CLA	CHD-C1D-ND	-2.20	122.43	124.45
45	B3	312	CLA	CHB-C4A-NA	2.20	127.55	124.51
54	A6	602	CHL	C3B-C4B-NB	2.20	112.05	109.21
48	AK	204	BCR	C20-C21-C22	-2.20	124.17	127.31
55	A4	316	XAT	C32-C33-C34	-2.20	115.57	118.94
54	A6	608	CHL	O2D-CGD-O1D	-2.20	119.54	123.84
45	A1	312	CLA	CHB-C4A-NA	2.20	127.55	124.51
45	AA	834	CLA	O2D-CGD-CBD	2.20	115.17	111.27
45	A6	603	CLA	O1D-CGD-CBD	2.20	128.98	124.48
45	BB	815	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
45	A3	309	CLA	CHD-C1D-ND	-2.20	122.44	124.45
45	BB	810	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
45	B1	304	CLA	CHB-C4A-NA	2.20	127.55	124.51
48	BF	304	BCR	C3-C4-C5	-2.20	110.16	114.08
45	AA	817	CLA	C5-C3-C2	2.19	125.56	121.12
54	A4	304	CHL	C3B-C4B-NB	2.19	112.05	109.21
53	B5	617	LMG	O6-C5-C4	2.19	113.68	109.69
45	BB	814	CLA	O2D-CGD-CBD	2.19	115.17	111.27
53	A4	318	LMG	C13-C12-C11	-2.19	105.31	113.19
45	BA	839	CLA	C1-C2-C3	-2.19	122.25	126.04
55	A4	316	XAT	C19-C9-C8	2.19	121.53	118.08
46	BB	844	PQN	O1-C1-C10	-2.19	118.01	121.56
48	BA	848	BCR	C40-C30-C25	-2.19	106.74	110.30
50	AL	301	LMU	O5B-C1B-C2B	2.19	114.98	110.35
45	A3	309	CLA	C2D-C1D-ND	-2.19	108.49	110.10
55	A1	318	XAT	C37-C21-C36	-2.19	104.14	107.37
53	A4	318	LMG	O8-C28-C29	2.19	118.78	111.91
45	AH	201	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
45	AB	824	CLA	CAA-C2A-C1A	2.19	119.14	111.97
45	BA	838	CLA	CHD-C1D-ND	-2.19	122.45	124.45
45	B3	313	CLA	CMB-C2B-C3B	2.18	128.77	124.68
45	BB	810	CLA	C5-C3-C2	2.18	125.54	121.12
45	BH	201	CLA	CAC-C3C-C4C	2.18	127.64	124.81
48	BG	203	BCR	C28-C27-C26	-2.18	110.18	114.08
45	AB	825	CLA	O2D-CGD-CBD	2.18	115.15	111.27
45	AB	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
54	A4	314	CHL	O2D-CGD-O1D	-2.18	119.13	124.09
45	BB	819	CLA	CHD-C1D-ND	-2.18	122.45	124.45
48	BB	847	BCR	C15-C16-C17	-2.18	119.01	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AA	805	CLA	CMC-C2C-C3C	2.18	132.03	126.12
45	AB	831	CLA	CHB-C4A-NA	2.18	127.53	124.51
45	BB	813	CLA	CHD-C1D-ND	-2.18	122.45	124.45
53	A4	318	LMG	O1-C1-C2	2.18	111.70	108.30
45	BB	838	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
48	AG	205	BCR	C34-C9-C8	2.18	121.51	118.08
45	BB	823	CLA	CHD-C1D-ND	-2.18	122.45	124.45
52	A3	316	LUT	C32-C33-C34	-2.18	115.60	118.94
45	AB	804	CLA	CHD-C4C-C3C	2.18	128.04	124.84
48	B5	616	BCR	C4-C5-C6	-2.18	119.57	122.73
45	B2	603	CLA	O2A-CGA-O1A	-2.18	117.88	123.30
55	A6	616	XAT	C26-C27-C28	-2.18	121.39	125.99
45	B2	604	CLA	CHB-C4A-NA	2.18	127.52	124.51
48	AA	852	BCR	C19-C18-C17	-2.18	115.60	118.94
50	BA	854	LMU	C1-O1'-C1'	2.18	117.45	113.84
45	BA	839	CLA	CHD-C1D-ND	-2.18	122.45	124.45
54	B2	601	CHL	C3C-C4C-NC	2.17	113.01	110.57
45	BA	801	CLA	CMB-C2B-C3B	2.17	128.75	124.68
45	B2	608	CLA	CHD-C1D-ND	-2.17	122.46	124.45
48	AL	302	BCR	C1-C6-C7	2.17	121.93	115.78
48	AL	302	BCR	C16-C15-C14	-2.17	119.02	123.47
45	AB	837	CLA	CHA-C1A-NA	-2.17	121.42	126.40
48	AA	845	BCR	C36-C18-C17	-2.17	119.88	122.92
54	B2	607	CHL	CMD-C2D-C1D	2.17	128.54	124.71
45	BB	828	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
48	A3	318	BCR	C33-C5-C4	2.17	117.79	113.62
55	B2	616	XAT	C4-C3-C2	-2.17	106.58	110.77
45	BB	841	CLA	O2D-CGD-CBD	2.17	115.13	111.27
45	AF	804	CLA	CHD-C1D-ND	-2.17	122.46	124.45
45	A3	308	CLA	O1D-CGD-CBD	2.17	128.92	124.48
52	A6	615	LUT	C17-C1-C6	-2.17	106.78	110.30
45	AB	834	CLA	CAC-C3C-C4C	2.17	127.62	124.81
45	B1	312	CLA	CHD-C1D-ND	-2.17	122.46	124.45
45	AA	842	CLA	CAA-CBA-CGA	-2.17	106.92	113.25
45	AB	823	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
55	A1	318	XAT	C28-C29-C30	-2.17	115.61	118.94
48	BB	846	BCR	C7-C8-C9	-2.17	122.96	126.23
45	AB	813	CLA	CHB-C4A-NA	2.17	127.51	124.51
45	BB	837	CLA	CHB-C4A-NA	2.17	127.51	124.51
45	B5	612	CLA	CHD-C1D-ND	-2.17	122.46	124.45
45	AB	822	CLA	CHB-C4A-NA	2.17	127.51	124.51
45	BB	804	CLA	O2A-CGA-O1A	-2.17	118.13	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	AH	201	CLA	CMB-C2B-C1B	-2.17	125.14	128.46
45	AB	842	CLA	C3A-C2A-C1A	2.17	104.58	101.34
48	AA	847	BCR	C29-C28-C27	-2.17	106.54	111.38
48	AA	846	BCR	C37-C22-C21	-2.16	119.89	122.92
47	F	801	LHG	C27-C26-C25	-2.16	103.44	114.42
45	AB	829	CLA	O2D-CGD-CBD	2.16	115.11	111.27
48	AL	302	BCR	C7-C6-C5	-2.16	116.22	121.46
45	AB	830	CLA	O1D-CGD-CBD	2.16	128.91	124.48
45	B1	315	CLA	CHB-C4A-NA	2.16	127.50	124.51
45	AA	816	CLA	CAC-C3C-C4C	2.16	127.61	124.81
45	BB	838	CLA	CHA-C1A-NA	-2.16	121.45	126.40
54	A6	602	CHL	CBA-CAA-C2A	2.16	120.24	113.86
45	B1	314	CLA	CAC-C3C-C4C	2.16	127.61	124.81
45	BA	842	CLA	CHB-C4A-NA	2.16	127.50	124.51
45	BB	810	CLA	CMD-C2D-C3D	2.16	132.58	127.61
46	BB	844	PQN	C12-C11-C3	-2.16	106.22	112.05
48	AJ	103	BCR	C30-C25-C26	-2.16	119.57	122.61
52	A6	615	LUT	C40-C33-C32	2.16	121.48	118.08
45	AA	808	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
45	AB	840	CLA	C2D-C1D-ND	-2.16	108.51	110.10
45	B2	603	CLA	CBC-CAC-C3C	-2.16	106.48	112.43
45	BA	811	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
45	AA	830	CLA	O1D-CGD-CBD	2.16	128.90	124.48
45	BA	810	CLA	CAC-C3C-C4C	2.15	127.61	124.81
45	AB	805	CLA	CMA-C3A-C2A	-2.15	111.07	116.10
48	AB	846	BCR	C12-C13-C14	-2.15	115.64	118.94
45	A3	302	CLA	O1D-CGD-CBD	2.15	128.89	124.48
52	A3	316	LUT	C35-C15-C14	-2.15	119.06	123.47
45	BB	835	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
45	A6	605	CLA	CHD-C1D-ND	-2.15	122.47	124.45
45	BA	809	CLA	O1D-CGD-CBD	2.15	128.89	124.48
45	BA	823	CLA	CAA-C2A-C3A	-2.15	111.07	116.10
45	A4	301	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
45	A1	314	CLA	CBC-CAC-C3C	2.15	118.37	112.43
48	BJ	101	BCR	C2-C3-C4	-2.15	106.57	111.38
45	AA	809	CLA	CHD-C1D-ND	-2.15	122.48	124.45
45	B3	309	CLA	CHB-C4A-NA	2.15	127.49	124.51
55	A4	316	XAT	C10-C11-C12	-2.15	116.50	123.22
45	A1	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
45	B1	311	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
45	AB	836	CLA	CHB-C4A-NA	2.15	127.49	124.51
48	AB	844	BCR	C20-C21-C22	-2.15	124.24	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BA	851	BCR	C19-C18-C17	2.15	122.24	118.94
48	BA	850	BCR	C12-C13-C14	-2.15	115.64	118.94
45	BB	824	CLA	O2A-CGA-O1A	-2.15	118.17	123.59
48	AF	805	BCR	C28-C27-C26	-2.15	110.24	114.08
45	AJ	102	CLA	CHD-C1D-ND	-2.15	122.48	124.45
45	BA	819	CLA	CBA-CAA-C2A	2.15	120.20	113.86
45	AB	822	CLA	CMB-C2B-C3B	2.15	128.69	124.68
45	AB	812	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
48	BA	851	BCR	C12-C13-C14	-2.15	115.65	118.94
45	B3	302	CLA	CAC-C3C-C4C	2.15	127.59	124.81
45	BF	301	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
48	AA	846	BCR	C2-C3-C4	-2.14	106.58	111.38
54	B3	306	CHL	C1C-C2C-C3C	-2.14	104.70	106.96
45	BA	844	CLA	CHB-C4A-NA	2.14	127.47	124.51
54	B5	605	CHL	CHC-C1C-C2C	-2.14	118.34	126.11
52	A6	615	LUT	C19-C9-C8	2.14	121.45	118.08
45	AA	809	CLA	O1D-CGD-CBD	2.14	128.87	124.48
48	AB	848	BCR	C38-C26-C27	2.14	117.73	113.62
48	AB	844	BCR	C1-C6-C5	-2.14	119.60	122.61
52	B5	614	LUT	C8-C7-C6	-2.14	121.19	127.20
45	AB	834	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
48	AB	846	BCR	C24-C23-C22	-2.14	123.00	126.23
45	AA	834	CLA	C7-C6-C5	-2.14	107.55	113.36
48	AB	844	BCR	C16-C17-C18	-2.14	124.26	127.31
45	AB	818	CLA	O2D-CGD-CBD	2.14	115.07	111.27
52	A4	315	LUT	C37-C21-C26	2.14	112.78	109.55
48	AA	849	BCR	C19-C18-C17	2.14	122.22	118.94
48	AB	846	BCR	C24-C25-C26	2.14	126.64	121.46
45	A1	311	CLA	CHD-C1D-ND	-2.14	122.49	124.45
48	AJ	103	BCR	C38-C26-C27	2.14	117.72	113.62
48	AA	852	BCR	C20-C21-C22	-2.14	124.26	127.31
45	AB	807	CLA	CMB-C2B-C3B	2.14	128.68	124.68
54	A4	304	CHL	CMB-C2B-C3B	2.14	128.67	124.68
47	A1	301	LHG	O8-C23-C24	2.14	118.61	111.91
45	AA	842	CLA	O2D-CGD-CBD	2.14	115.06	111.27
55	A1	318	XAT	C24-C23-C22	-2.13	106.65	110.77
45	B1	314	CLA	CMC-C2C-C1C	-2.13	121.79	125.04
54	B5	607	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
48	BA	855	BCR	C23-C24-C25	2.13	133.19	127.20
45	AA	816	CLA	O2D-CGD-CBD	2.13	115.06	111.27
45	BA	833	CLA	CHB-C4A-NA	2.13	127.46	124.51
48	BA	851	BCR	C21-C20-C19	-2.13	116.56	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B2	601	CHL	O2A-C1-C2	2.13	114.24	108.64
45	BA	840	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
48	AG	205	BCR	C29-C30-C25	2.13	113.76	110.48
45	B3	314	CLA	CHB-C4A-NA	2.13	127.46	124.51
48	B3	317	BCR	C2-C1-C6	-2.13	107.20	110.48
45	B1	306	CLA	CHD-C1D-ND	-2.13	122.50	124.45
54	B5	606	CHL	C3C-C4C-NC	2.13	112.90	110.57
55	A3	317	XAT	C28-C29-C30	-2.13	115.67	118.94
47	A1	301	LHG	O8-C23-O10	-2.13	118.22	123.59
45	B3	311	CLA	CMB-C2B-C3B	2.13	128.66	124.68
45	BA	817	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
45	A1	316	CLA	CHB-C4A-NA	2.13	127.46	124.51
45	BA	829	CLA	CHB-C4A-NA	2.13	127.46	124.51
45	BB	842	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
45	BA	817	CLA	C4-C3-C2	-2.13	118.22	123.68
45	AB	825	CLA	C1-O2A-CGA	2.13	122.03	116.44
45	BA	835	CLA	CHB-C4A-NA	2.13	127.46	124.51
48	BB	849	BCR	C19-C18-C17	-2.13	115.67	118.94
54	A6	602	CHL	C1-C2-C3	-2.13	122.36	126.04
45	AB	825	CLA	CMA-C3A-C4A	-2.13	106.06	111.77
48	BB	849	BCR	C37-C22-C21	-2.13	119.94	122.92
54	A1	308	CHL	O2D-CGD-O1D	-2.13	119.26	124.09
48	AA	849	BCR	C16-C15-C14	-2.13	119.12	123.47
45	BA	834	CLA	C5-C3-C2	-2.13	116.82	121.12
55	B5	615	XAT	C36-C21-C26	2.13	115.78	110.05
45	AH	201	CLA	CHD-C1D-ND	-2.13	122.50	124.45
45	AA	805	CLA	O1D-CGD-CBD	2.12	128.83	124.48
52	B3	315	LUT	C30-C31-C32	-2.12	116.59	123.22
48	AA	847	BCR	C12-C13-C14	2.12	122.20	118.94
45	BB	842	CLA	CHD-C1D-ND	-2.12	122.50	124.45
45	B1	305	CLA	CHD-C1D-ND	-2.12	122.50	124.45
45	B5	610	CLA	CHB-C4A-NA	2.12	127.45	124.51
48	AA	852	BCR	C38-C26-C25	2.12	126.91	124.53
45	AF	802	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
45	B2	609	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
48	BB	845	BCR	C12-C13-C14	-2.12	115.68	118.94
48	AL	302	BCR	C23-C24-C25	-2.12	121.24	127.20
45	BB	815	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
45	BB	828	CLA	CAA-CBA-CGA	-2.12	107.05	113.25
48	AI	101	BCR	C19-C18-C17	-2.12	115.69	118.94
45	BA	841	CLA	CAC-C3C-C4C	2.12	127.56	124.81
48	AG	205	BCR	C16-C17-C18	-2.12	124.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BI	101	BCR	C20-C21-C22	-2.12	124.29	127.31
55	B5	615	XAT	O4-C5-C18	2.12	117.59	115.06
45	B3	309	CLA	CHD-C1D-ND	-2.12	122.51	124.45
54	A4	305	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
45	BB	815	CLA	CHB-C4A-NA	2.12	127.44	124.51
48	AL	306	BCR	C16-C15-C14	-2.12	119.14	123.47
45	AA	837	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
45	AA	838	CLA	O2A-CGA-O1A	-2.11	118.25	123.59
45	A4	303	CLA	CHD-C1D-ND	-2.11	122.51	124.45
48	B3	317	BCR	C8-C9-C10	-2.11	115.70	118.94
48	BA	855	BCR	C20-C21-C22	-2.11	124.29	127.31
45	A1	306	CLA	CHB-C4A-NA	2.11	127.44	124.51
48	BJ	103	BCR	C35-C13-C14	2.11	125.88	122.92
45	B2	611	CLA	CHB-C4A-NA	2.11	127.43	124.51
45	B1	314	CLA	CHB-C4A-NA	2.11	127.43	124.51
48	AA	845	BCR	C20-C21-C22	-2.11	124.30	127.31
48	BL	306	BCR	C1-C6-C5	-2.11	119.64	122.61
45	AA	829	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
45	AB	837	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
45	AB	840	CLA	CHB-C4A-NA	2.11	127.43	124.51
54	A3	307	CHL	C3D-C2D-C1D	-2.11	102.95	105.83
45	AB	813	CLA	O2D-CGD-CBD	2.11	115.02	111.27
45	AB	815	CLA	C16-C15-C13	2.11	122.74	115.92
55	A1	318	XAT	C17-C1-C16	-2.11	104.26	107.37
45	BL	303	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
45	AA	834	CLA	CMC-C2C-C3C	2.11	131.84	126.12
48	AF	805	BCR	C40-C30-C25	-2.11	106.88	110.30
45	BA	831	CLA	O1D-CGD-CBD	2.11	128.80	124.48
55	A1	318	XAT	C35-C34-C33	-2.11	124.30	127.31
45	AB	806	CLA	CMC-C2C-C3C	2.11	131.84	126.12
54	B5	605	CHL	O2D-CGD-O1D	-2.11	119.30	124.09
48	AA	845	BCR	C36-C18-C19	2.11	121.40	118.08
45	AB	805	CLA	CHD-C1D-ND	-2.11	122.52	124.45
45	AB	830	CLA	CHB-C4A-NA	2.11	127.42	124.51
45	AB	802	CLA	CMB-C2B-C3B	2.11	128.81	124.69
45	BG	202	CLA	CHD-C1D-ND	-2.11	122.52	124.45
55	B2	616	XAT	C12-C13-C14	-2.11	115.71	118.94
48	BB	803	BCR	C10-C11-C12	-2.11	116.65	123.22
45	BA	807	CLA	CHB-C4A-NA	2.10	127.42	124.51
54	B3	306	CHL	C3C-C4C-NC	2.10	112.93	110.57
45	A6	604	CLA	CHD-C1D-ND	-2.10	122.52	124.45
48	AB	848	BCR	C3-C4-C5	-2.10	110.32	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	B5	606	CHL	O2D-CGD-O1D	-2.10	119.73	123.84
45	AB	837	CLA	CHB-C4A-NA	2.10	127.42	124.51
54	B1	308	CHL	O2D-CGD-O1D	-2.10	119.32	124.09
48	AL	306	BCR	C29-C28-C27	-2.10	106.68	111.38
45	A6	610	CLA	CHD-C1D-ND	-2.10	122.52	124.45
48	BA	851	BCR	C24-C23-C22	-2.10	123.06	126.23
52	B3	315	LUT	C11-C10-C9	-2.10	124.31	127.31
48	BB	845	BCR	C23-C22-C21	-2.10	115.72	118.94
45	AA	814	CLA	CHB-C4A-NA	2.10	127.41	124.51
45	B2	611	CLA	CHD-C1D-ND	-2.10	122.53	124.45
48	A4	317	BCR	C37-C22-C21	-2.10	119.99	122.92
45	BB	801	CLA	CMD-C2D-C1D	-2.10	121.02	124.71
45	BA	805	CLA	CMB-C2B-C3B	2.10	128.60	124.68
45	BA	831	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
45	B1	314	CLA	C4A-NA-C1A	2.10	107.65	106.71
45	BA	819	CLA	O2D-CGD-CBD	2.10	114.99	111.27
45	A4	310	CLA	CHD-C1D-ND	-2.09	122.53	124.45
55	A3	317	XAT	C38-C25-C24	2.09	116.64	114.28
48	AG	205	BCR	C1-C6-C5	-2.09	119.66	122.61
45	BG	201	CLA	CMB-C2B-C3B	2.09	128.60	124.68
45	AA	826	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
45	AA	803	CLA	CAA-CBA-CGA	-2.09	107.13	113.25
54	A6	608	CHL	C5-C3-C4	2.09	119.23	114.60
48	BL	305	BCR	C16-C15-C14	-2.09	119.19	123.47
45	AL	304	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
45	AA	840	CLA	C1-C2-C3	-2.09	122.42	126.04
45	BA	822	CLA	CHD-C1D-ND	-2.09	122.53	124.45
48	BL	305	BCR	C36-C18-C17	-2.09	119.99	122.92
45	AB	823	CLA	CMB-C2B-C3B	2.09	128.59	124.68
48	AB	846	BCR	C16-C15-C14	-2.09	119.19	123.47
45	BB	812	CLA	C2A-C1A-CHA	2.09	127.52	123.86
47	A6	618	LHG	O8-C23-C24	2.09	118.47	111.91
45	BA	826	CLA	C1-C2-C3	-2.09	122.42	126.04
45	BB	805	CLA	O2D-CGD-CBD	2.09	114.98	111.27
48	A3	318	BCR	C28-C27-C26	-2.09	110.34	114.08
45	BA	841	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
48	BB	803	BCR	C23-C22-C21	-2.09	115.73	118.94
48	AL	306	BCR	C24-C25-C26	-2.09	116.40	121.46
45	AA	815	CLA	CHD-C1D-ND	-2.09	122.50	124.52
52	A4	315	LUT	C36-C21-C26	2.09	112.71	109.55
45	BB	815	CLA	CMB-C2B-C3B	2.09	128.59	124.68
45	AB	807	CLA	CAA-C2A-C1A	-2.09	105.13	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	806	CLA	CAC-C3C-C4C	2.09	127.52	124.81
45	AL	305	CLA	CHD-C1D-ND	-2.09	122.53	124.45
45	AA	842	CLA	CAC-C3C-C4C	2.09	127.52	124.81
54	B2	601	CHL	CAC-C3C-C4C	2.09	127.52	124.81
54	B5	607	CHL	O2D-CGD-O1D	-2.09	119.76	123.84
45	A3	314	CLA	CAA-C2A-C3A	-2.09	111.23	116.10
45	BK	201	CLA	CHD-C1D-ND	-2.09	122.54	124.45
45	AA	828	CLA	C16-C15-C13	2.08	122.66	115.92
45	BA	822	CLA	CHB-C4A-NA	2.08	127.39	124.51
45	A4	308	CLA	C1D-ND-C4D	-2.08	104.85	106.33
54	B2	605	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
45	AB	804	CLA	C2A-C1A-CHA	2.08	127.50	123.86
45	BA	842	CLA	CAA-CBA-CGA	-2.08	107.17	113.25
45	BB	831	CLA	CMB-C2B-C3B	2.08	128.57	124.68
45	AB	801	CLA	C2A-C1A-CHA	2.08	127.50	123.86
45	AA	832	CLA	O2D-CGD-CBD	2.08	114.97	111.27
54	A4	305	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
45	AF	802	CLA	CMD-C2D-C3D	2.08	132.40	127.61
48	A3	318	BCR	C15-C16-C17	-2.08	119.21	123.47
45	BB	827	CLA	CHB-C4A-NA	2.08	127.39	124.51
48	AJ	101	BCR	C19-C18-C17	-2.08	115.75	118.94
48	AK	204	BCR	C8-C7-C6	-2.08	121.36	127.20
45	BA	838	CLA	CHB-C4A-NA	2.08	127.39	124.51
54	A6	607	CHL	CED-O2D-CGD	2.08	120.64	115.94
45	AB	804	CLA	O2D-CGD-CBD	2.08	114.96	111.27
54	B1	303	CHL	C1-C2-C3	-2.08	123.39	126.75
50	BA	854	LMU	C1B-O1B-C4'	-2.08	112.82	117.96
45	BB	811	CLA	CAA-C2A-C3A	-2.08	107.09	112.78
45	A3	303	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
48	AA	849	BCR	C15-C16-C17	-2.08	119.22	123.47
45	AA	838	CLA	CHB-C4A-NA	2.08	127.38	124.51
45	BA	832	CLA	O2D-CGD-CBD	2.08	114.96	111.27
45	BA	809	CLA	CHD-C1D-ND	-2.08	122.55	124.45
45	B3	314	CLA	CAA-C2A-C3A	-2.07	111.26	116.10
48	BK	204	BCR	C40-C30-C39	2.07	114.90	108.53
48	B5	616	BCR	C10-C11-C12	-2.07	116.74	123.22
48	BF	304	BCR	C23-C22-C21	-2.07	115.76	118.94
55	A1	318	XAT	C38-C25-C26	-2.07	118.78	122.26
45	AB	819	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
45	B2	608	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
48	A1	319	BCR	C12-C13-C14	-2.07	115.76	118.94
45	B3	313	CLA	CAA-C2A-C3A	-2.07	111.26	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	A4	313	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
45	AK	202	CLA	O2A-CGA-O1A	-2.07	118.13	123.30
45	BA	838	CLA	CMB-C2B-C3B	2.07	128.56	124.68
45	AA	838	CLA	O2D-CGD-CBD	2.07	114.95	111.27
48	BB	845	BCR	C32-C1-C6	-2.07	106.94	110.30
48	BA	849	BCR	C16-C17-C18	-2.07	124.35	127.31
55	B3	316	XAT	C32-C33-C34	-2.07	115.76	118.94
48	AL	302	BCR	C20-C21-C22	-2.07	124.35	127.31
48	A1	319	BCR	C20-C21-C22	-2.07	124.35	127.31
54	B2	601	CHL	C4-C3-C5	2.07	118.75	115.27
45	BB	818	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
48	BA	856	BCR	C20-C21-C22	-2.07	124.36	127.31
45	BB	816	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
54	A6	602	CHL	C3D-C2D-C1D	-2.07	103.01	105.83
45	BA	830	CLA	CHD-C1D-ND	-2.07	122.55	124.45
45	AA	830	CLA	CHB-C4A-NA	2.07	127.37	124.51
48	AB	847	BCR	C23-C22-C21	-2.07	115.77	118.94
48	BB	847	BCR	C29-C30-C25	2.07	113.66	110.48
45	AB	818	CLA	CAC-C3C-C4C	2.07	127.49	124.81
48	BI	101	BCR	C23-C22-C21	-2.07	115.77	118.94
45	AB	811	CLA	CHA-C1A-NA	-2.06	121.67	126.40
54	A4	304	CHL	CMA-C3A-C4A	-2.06	106.22	111.77
45	B2	609	CLA	CHD-C1D-ND	-2.06	122.56	124.45
45	B5	601	CLA	CHD-C1D-ND	-2.06	122.56	124.45
54	B1	308	CHL	C3C-C4C-NC	2.06	112.89	110.57
48	AB	849	BCR	C8-C7-C6	-2.06	121.41	127.20
55	A1	318	XAT	O4-C5-C18	2.06	117.53	115.06
45	A1	311	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
45	A1	314	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
45	AB	819	CLA	CAA-C2A-C3A	2.06	118.43	112.78
48	BB	846	BCR	C15-C16-C17	-2.06	119.25	123.47
48	AJ	103	BCR	C20-C21-C22	-2.06	124.37	127.31
48	BL	306	BCR	C28-C27-C26	-2.06	110.40	114.08
45	A3	309	CLA	CAA-C2A-C3A	-2.06	111.29	116.10
54	A6	602	CHL	CAA-C2A-C3A	2.06	118.42	112.78
48	AA	847	BCR	C34-C9-C8	2.06	121.32	118.08
52	B2	615	LUT	C35-C15-C14	-2.06	119.25	123.47
45	BA	830	CLA	CMB-C2B-C3B	2.06	128.53	124.68
45	AB	801	CLA	C3A-C2A-C1A	2.06	104.42	101.34
48	BB	803	BCR	C36-C18-C17	-2.06	120.04	122.92
54	A6	607	CHL	CHC-C1C-C2C	-2.06	118.64	126.11
48	A4	317	BCR	C36-C18-C17	-2.06	120.04	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	AG	205	BCR	C29-C28-C27	-2.06	106.78	111.38
56	e	301	SQD	C1-O5-C5	2.06	117.73	113.69
45	BA	818	CLA	CHD-C1D-ND	-2.06	122.56	124.45
48	AA	849	BCR	C34-C9-C8	2.06	121.32	118.08
50	AL	301	LMU	C1-O1'-C1'	2.06	117.25	113.84
45	BB	801	CLA	C3C-C4C-NC	-2.06	108.26	110.57
48	BJ	101	BCR	C19-C18-C17	-2.06	115.79	118.94
48	BA	856	BCR	C24-C25-C26	2.06	126.44	121.46
48	BA	849	BCR	C20-C21-C22	-2.06	124.38	127.31
45	A6	610	CLA	CBA-CAA-C2A	2.06	119.93	113.86
45	BA	802	CLA	C2D-C1D-ND	-2.05	108.59	110.10
45	B3	310	CLA	C2A-C1A-CHA	2.05	127.45	123.86
45	AB	821	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
45	BA	833	CLA	C4-C3-C2	-2.05	118.42	123.68
45	B3	310	CLA	CHA-C1A-NA	-2.05	121.70	126.40
45	AA	821	CLA	C7-C6-C5	-2.05	107.79	113.36
48	BA	848	BCR	C37-C22-C23	2.05	121.31	118.08
48	BB	849	BCR	C34-C9-C8	2.05	121.31	118.08
45	AB	832	CLA	CMC-C2C-C3C	2.05	131.68	126.12
48	AJ	103	BCR	C12-C13-C14	-2.05	115.80	118.94
48	AL	306	BCR	C12-C13-C14	-2.05	115.80	118.94
52	A4	315	LUT	C12-C13-C14	-2.05	115.80	118.94
45	BA	826	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
45	BB	811	CLA	CHD-C1D-ND	-2.05	122.57	124.45
45	BB	828	CLA	CHA-C1A-NA	-2.05	121.71	126.40
48	BA	855	BCR	C10-C11-C12	-2.05	116.83	123.22
48	BI	101	BCR	C19-C18-C17	-2.05	115.80	118.94
48	B2	617	BCR	C16-C17-C18	-2.05	124.39	127.31
48	AA	848	BCR	C1-C6-C5	-2.05	119.73	122.61
45	BB	812	CLA	CHD-C1D-ND	-2.05	122.57	124.45
48	BB	845	BCR	C31-C1-C6	2.05	113.62	110.30
48	AL	302	BCR	C12-C13-C14	-2.05	115.80	118.94
45	BA	804	CLA	C5-C3-C2	2.04	125.25	121.12
45	AB	833	CLA	C4-C3-C5	2.04	118.71	115.27
45	B3	302	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
45	AA	826	CLA	CHB-C4A-NA	2.04	127.34	124.51
48	A4	317	BCR	C35-C13-C12	2.04	121.30	118.08
54	A1	303	CHL	C3D-C2D-C1D	-2.04	103.04	105.83
45	BA	817	CLA	O2D-CGD-CBD	2.04	114.90	111.27
45	BA	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
55	B3	316	XAT	C28-C29-C30	-2.04	115.81	118.94
45	B3	305	CLA	C3A-C2A-C1A	2.04	104.40	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	A6	617	BCR	C30-C25-C26	-2.04	119.74	122.61
48	BA	851	BCR	C24-C25-C26	2.04	126.41	121.46
48	BJ	103	BCR	C16-C17-C18	-2.04	124.40	127.31
45	BA	828	CLA	C14-C13-C15	2.04	118.68	111.29
48	A1	319	BCR	C36-C18-C17	-2.04	120.07	122.92
56	BJ	104	SQD	C4-C3-C2	2.04	114.38	110.82
52	B5	614	LUT	C7-C8-C9	-2.04	123.16	126.23
54	B1	303	CHL	C5-C3-C4	2.04	119.10	114.60
45	BB	823	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
45	AA	825	CLA	C2D-C1D-ND	-2.04	108.60	110.10
45	AK	201	CLA	CMA-C3A-C2A	-2.04	111.34	116.10
45	BA	825	CLA	C6-C5-C3	2.04	118.79	113.45
45	BA	827	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
45	BA	814	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
54	A1	308	CHL	C3C-C4C-NC	2.04	112.85	110.57
48	BB	848	BCR	C2-C3-C4	-2.04	106.83	111.38
55	B2	616	XAT	O4-C5-C6	-2.04	57.27	58.96
45	A1	309	CLA	CAC-C3C-C4C	2.04	127.45	124.81
48	BA	855	BCR	C29-C30-C25	2.04	113.61	110.48
45	BG	202	CLA	CHB-C4A-NA	2.03	127.33	124.51
45	BA	833	CLA	C5-C3-C2	2.03	125.23	121.12
48	BB	803	BCR	C2-C3-C4	-2.03	106.83	111.38
45	A4	308	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
45	AA	824	CLA	CAA-C2A-C3A	2.03	118.34	112.78
46	BB	844	PQN	C6-C5-C10	2.03	121.52	119.26
48	AG	205	BCR	C37-C22-C21	-2.03	120.08	122.92
48	BA	855	BCR	C35-C13-C12	2.03	121.28	118.08
45	AA	801	CLA	O1D-CGD-CBD	2.03	128.64	124.48
45	AA	839	CLA	CHD-C1D-ND	-2.03	122.59	124.45
45	BH	201	CLA	CED-O2D-CGD	2.03	120.53	115.94
54	B1	303	CHL	OMC-CMC-C2C	-2.03	121.10	125.69
45	BB	813	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
45	AA	832	CLA	C5-C3-C2	-2.03	117.01	121.12
45	BB	819	CLA	C6-C5-C3	2.03	118.78	113.45
50	AB	853	LMU	O5B-C5B-C4B	2.03	113.38	109.69
45	B3	313	CLA	CHD-C1D-ND	-2.03	122.59	124.45
56	BJ	104	SQD	O47-C45-C44	2.03	115.75	108.40
52	B5	614	LUT	C38-C25-C24	-2.03	119.22	123.56
45	A1	313	CLA	O2A-CGA-O1A	-2.03	118.24	123.30
45	A4	313	CLA	O2D-CGD-CBD	2.03	114.87	111.27
55	B1	317	XAT	C35-C34-C33	-2.03	124.42	127.31
48	AB	846	BCR	C32-C1-C6	-2.03	107.01	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	BF	304	BCR	C20-C21-C22	-2.03	124.42	127.31
54	A6	602	CHL	C3C-C4C-NC	2.03	112.84	110.57
45	B2	602	CLA	O1D-CGD-CBD	2.03	128.63	124.48
45	AB	832	CLA	CMC-C2C-C1C	-2.03	121.95	125.04
45	A1	315	CLA	CMA-C3A-C2A	-2.03	111.37	116.10
45	BB	825	CLA	CHB-C4A-NA	2.03	127.31	124.51
45	B2	610	CLA	CHD-C1D-ND	-2.03	122.59	124.45
45	BB	826	CLA	C1-O2A-CGA	2.03	121.76	116.44
45	BB	827	CLA	O1D-CGD-CBD	2.03	128.63	124.48
45	BB	810	CLA	CMD-C2D-C1D	-2.03	121.14	124.71
48	BK	204	BCR	C15-C16-C17	-2.02	119.33	123.47
48	AL	306	BCR	C34-C9-C8	2.02	121.27	118.08
45	BB	822	CLA	CMA-C3A-C2A	-2.02	111.37	116.10
45	BA	825	CLA	C5-C3-C2	2.02	125.21	121.12
48	AA	847	BCR	C16-C15-C14	-2.02	119.33	123.47
45	AB	803	CLA	O1D-CGD-CBD	2.02	128.62	124.48
45	BA	844	CLA	O2D-CGD-CBD	2.02	114.86	111.27
45	BA	806	CLA	CHD-C1D-ND	-2.02	122.59	124.45
45	AA	825	CLA	CBA-CAA-C2A	-2.02	107.89	113.86
45	A6	610	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
45	BB	825	CLA	CAA-C2A-C3A	2.02	118.31	112.78
45	BA	804	CLA	C6-C5-C3	2.02	117.93	114.62
48	AJ	103	BCR	C27-C26-C25	-2.02	119.80	122.73
45	AA	822	CLA	CHD-C1D-ND	-2.02	122.60	124.45
45	BB	823	CLA	CMB-C2B-C3B	2.02	128.46	124.68
45	AA	840	CLA	C2D-C1D-ND	-2.02	108.61	110.10
45	A3	310	CLA	CAA-C2A-C3A	-2.02	111.38	116.10
48	BA	856	BCR	C7-C8-C9	-2.02	123.18	126.23
45	AA	811	CLA	O1D-CGD-CBD	2.02	128.62	124.48
45	AA	828	CLA	CAA-CBA-CGA	-2.02	107.36	113.25
45	A4	313	CLA	CBA-CAA-C2A	2.02	119.82	113.86
45	AA	823	CLA	CHB-C4A-NA	2.02	127.30	124.51
45	AB	803	CLA	CHB-C4A-NA	2.02	127.30	124.51
45	BB	820	CLA	CAA-C2A-C3A	2.02	118.30	112.78
54	A1	303	CHL	CBA-CAA-C2A	2.02	119.81	113.86
45	A4	301	CLA	CHD-C1D-ND	-2.02	122.60	124.45
54	A1	303	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
55	B5	615	XAT	C15-C35-C34	-2.02	119.35	123.47
45	AA	803	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
45	BB	843	CLA	CHD-C1D-ND	-2.01	122.60	124.45
48	BK	204	BCR	C24-C25-C26	-2.01	116.58	121.46
45	AB	835	CLA	CAA-C2A-C3A	-2.01	107.26	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
52	AF	806	LUT	C40-C33-C34	-2.01	120.10	122.92
54	A3	307	CHL	C1C-C2C-C3C	-2.01	104.84	106.96
45	AA	837	CLA	C2A-C1A-CHA	2.01	127.38	123.86
45	B3	307	CLA	O1D-CGD-CBD	2.01	128.60	124.48
48	B3	317	BCR	C30-C25-C24	2.01	121.47	115.78
54	B2	607	CHL	OMC-CMC-C2C	-2.01	121.14	125.69
45	B3	301	CLA	O1D-CGD-CBD	2.01	128.60	124.48
45	BB	821	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
45	A3	303	CLA	CHD-C1D-ND	-2.01	122.61	124.45
45	A3	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
48	B3	317	BCR	C28-C27-C26	-2.01	110.48	114.08
45	BA	839	CLA	CAA-CBA-CGA	-2.01	107.38	113.25
48	BA	851	BCR	C32-C1-C6	2.01	113.56	110.30
55	A6	616	XAT	C35-C34-C33	-2.01	124.44	127.31
45	B5	604	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
48	BF	304	BCR	C29-C28-C27	-2.01	106.88	111.38
54	B2	614	CHL	C3D-C2D-C1D	-2.01	103.09	105.83
48	AG	205	BCR	C33-C5-C6	-2.01	122.27	124.53
48	AF	801	BCR	C39-C30-C25	-2.01	107.04	110.30
45	BA	823	CLA	CMA-C3A-C2A	-2.01	111.41	116.10
45	AA	820	CLA	O2A-CGA-O1A	-2.01	118.29	123.30
48	BJ	101	BCR	C20-C21-C22	-2.01	124.44	127.31
52	B2	615	LUT	C38-C25-C24	-2.01	119.26	123.56
45	B1	310	CLA	CHD-C1D-ND	-2.01	122.61	124.45
45	BB	811	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
45	BA	809	CLA	CAA-C2A-C1A	2.01	118.56	111.97
45	AF	802	CLA	O1D-CGD-CBD	2.01	128.59	124.48
45	A4	308	CLA	CHD-C1D-ND	-2.01	122.61	124.45
45	A1	309	CLA	O2A-CGA-O1A	-2.01	118.30	123.30
45	BA	833	CLA	CMB-C2B-C3B	2.01	128.43	124.68
48	AA	847	BCR	C19-C18-C17	-2.01	115.86	118.94
45	B2	613	CLA	O2D-CGD-CBD	2.01	114.83	111.27
48	BK	204	BCR	C16-C17-C18	-2.01	124.45	127.31
45	AL	304	CLA	CHD-C1D-C2D	2.01	129.69	125.48
45	AB	812	CLA	CHD-C1D-ND	-2.01	122.61	124.45
45	BA	830	CLA	O1D-CGD-CBD	2.01	128.59	124.48
45	AB	812	CLA	C4-C3-C2	-2.01	118.53	123.68
51	BB	850	DGD	O1G-C1A-O1A	-2.01	118.53	123.59
54	A6	607	CHL	C3D-C2D-C1D	-2.01	103.09	105.83
45	AB	841	CLA	CHD-C1D-ND	-2.01	122.61	124.45
48	AF	805	BCR	C24-C25-C26	2.01	126.32	121.46
48	AB	846	BCR	C15-C16-C17	-2.00	119.37	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	BB	833	CLA	CMC-C2C-C1C	-2.00	121.99	125.04
45	A6	609	CLA	O2A-CGA-O1A	-2.00	118.30	123.30
46	AA	843	PQN	C21-C22-C23	-2.00	109.44	115.92
45	AB	815	CLA	CHD-C1D-ND	-2.00	122.61	124.45
48	A4	317	BCR	C34-C9-C8	2.00	121.23	118.08
48	BB	846	BCR	C19-C18-C17	-2.00	115.87	118.94
45	B5	609	CLA	CBA-CAA-C2A	2.00	119.78	113.86
45	BA	836	CLA	CHD-C1D-ND	-2.00	122.61	124.45
45	B1	314	CLA	C2D-C1D-ND	-2.00	108.63	110.10
45	AA	801	CLA	CBA-CAA-C2A	-2.00	107.95	113.86
45	B3	304	CLA	CHB-C4A-NA	2.00	127.28	124.51
45	A3	308	CLA	CHD-C1D-ND	-2.00	122.61	124.45
45	AB	838	CLA	CHB-C4A-NA	2.00	127.28	124.51
45	BA	838	CLA	O2D-CGD-CBD	2.00	114.83	111.49
45	AA	810	CLA	CHD-C1D-ND	-2.00	122.62	124.45
48	AL	302	BCR	C15-C16-C17	-2.00	119.38	123.47
45	AA	801	CLA	CMB-C2B-C3B	2.00	128.42	124.68

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

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Mol	Chain	Res	Type	Atom
45	AA	825	CLA	ND
45	AA	826	CLA	ND
45	AA	827	CLA	ND
45	AA	828	CLA	ND
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

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Mol	Chain	Res	Type	Atom
45	AB	833	CLA	ND
45	AB	834	CLA	ND
45	AB	837	CLA	ND
45	AB	839	CLA	ND
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

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Mol	Chain	Res	Type	Atom
45	A3	314	CLA	ND
45	A3	315	CLA	ND
45	A4	301	CLA	ND
45	A4	302	CLA	ND
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

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Mol	Chain	Res	Type	Atom
45	BA	828	CLA	ND
45	BA	829	CLA	ND
45	BA	830	CLA	ND
45	BA	831	CLA	ND
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

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Mol	Chain	Res	Type	Atom
45	BB	838	CLA	ND
45	BB	841	CLA	ND
45	BB	842	CLA	ND
45	BB	843	CLA	ND
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

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Mol	Chain	Res	Type	Atom
45	B3	310	CLA	ND
45	B3	311	CLA	ND
45	B3	312	CLA	ND
45	B3	313	CLA	ND
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	NA
54	A1	303	CHL	NC
54	A1	303	CHL	ND
54	A1	308	CHL	NA
54	A1	308	CHL	NC
54	A1	308	CHL	ND
54	A3	307	CHL	NA
54	A3	307	CHL	NC
54	A3	307	CHL	ND
54	A4	304	CHL	NA
54	A4	304	CHL	NC
54	A4	304	CHL	ND
54	A4	305	CHL	NA
54	A4	305	CHL	NC
54	A4	305	CHL	ND
54	A4	306	CHL	NA
54	A4	306	CHL	NC
54	A4	306	CHL	ND
54	A4	314	CHL	NA
54	A4	314	CHL	NC
54	A4	314	CHL	ND
54	A6	602	CHL	NA
54	A6	602	CHL	NC
54	A6	602	CHL	ND
54	A6	606	CHL	NA
54	A6	606	CHL	NC
54	A6	606	CHL	ND
54	A6	607	CHL	NA
54	A6	607	CHL	NC

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Mol	Chain	Res	Type	Atom
54	A6	607	CHL	ND
54	A6	608	CHL	NA
54	A6	608	CHL	NC
54	A6	608	CHL	ND
54	B1	303	CHL	NA
54	B1	303	CHL	NC
54	B1	303	CHL	ND
54	B1	308	CHL	NA
54	B1	308	CHL	NC
54	B1	308	CHL	ND
54	B2	601	CHL	NA
54	B2	601	CHL	NC
54	B2	601	CHL	ND
54	B2	605	CHL	NA
54	B2	605	CHL	NC
54	B2	605	CHL	ND
54	B2	606	CHL	NA
54	B2	606	CHL	NC
54	B2	606	CHL	ND
54	B2	607	CHL	NA
54	B2	607	CHL	NC
54	B2	607	CHL	ND
54	B2	614	CHL	NA
54	B2	614	CHL	NC
54	B2	614	CHL	ND
54	B3	306	CHL	NA
54	B3	306	CHL	NC
54	B3	306	CHL	ND
54	B5	605	CHL	NA
54	B5	605	CHL	NC
54	B5	605	CHL	ND
54	B5	606	CHL	NA
54	B5	606	CHL	NC
54	B5	606	CHL	ND
54	B5	607	CHL	NA
54	B5	607	CHL	NC
54	B5	607	CHL	ND

All (3005) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
45	AA	801	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	AA	802	CLA	CBD-CGD-O2D-CED
45	AA	804	CLA	C1A-C2A-CAA-CBA
45	AA	804	CLA	C3A-C2A-CAA-CBA
45	AA	805	CLA	CHA-CBD-CGD-O1D
45	AA	805	CLA	CHA-CBD-CGD-O2D
45	AA	813	CLA	CHA-CBD-CGD-O1D
45	AA	813	CLA	CHA-CBD-CGD-O2D
45	AA	813	CLA	CAD-CBD-CGD-O1D
45	AA	814	CLA	CHA-CBD-CGD-O1D
45	AA	816	CLA	CHA-CBD-CGD-O1D
45	AA	816	CLA	CHA-CBD-CGD-O2D
45	AA	816	CLA	CAD-CBD-CGD-O1D
45	AA	818	CLA	C3A-C2A-CAA-CBA
45	AA	819	CLA	C3A-C2A-CAA-CBA
45	AA	822	CLA	C1A-C2A-CAA-CBA
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	829	CLA	CHA-CBD-CGD-O1D
45	AA	829	CLA	C2-C3-C5-C6
45	AA	829	CLA	C4-C3-C5-C6
45	AA	831	CLA	C1A-C2A-CAA-CBA
45	AA	831	CLA	C3A-C2A-CAA-CBA
45	AA	832	CLA	C2-C3-C5-C6
45	AA	832	CLA	C4-C3-C5-C6
45	AA	833	CLA	CHA-CBD-CGD-O1D
45	AA	833	CLA	CHA-CBD-CGD-O2D
45	AA	833	CLA	CAD-CBD-CGD-O1D
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	842	CLA	C2A-CAA-CBA-CGA
45	AB	802	CLA	C2-C3-C5-C6
45	AB	802	CLA	C4-C3-C5-C6
45	AB	803	CLA	CHA-CBD-CGD-O1D
45	AB	803	CLA	CHA-CBD-CGD-O2D
45	AB	804	CLA	C1A-C2A-CAA-CBA
45	AB	804	CLA	C3A-C2A-CAA-CBA
45	AB	804	CLA	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
45	AB	804	CLA	C4C-C3C-CAC-CBC
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	CHA-CBD-CGD-O1D
45	AB	806	CLA	CHA-CBD-CGD-O2D
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	808	CLA	CHA-CBD-CGD-O1D
45	AB	808	CLA	CHA-CBD-CGD-O2D
45	AB	809	CLA	C1A-C2A-CAA-CBA
45	AB	809	CLA	C3A-C2A-CAA-CBA
45	AB	810	CLA	C2A-CAA-CBA-CGA
45	AB	810	CLA	CBD-CGD-O2D-CED
45	AB	811	CLA	C1A-C2A-CAA-CBA
45	AB	811	CLA	CHA-CBD-CGD-O1D
45	AB	811	CLA	CHA-CBD-CGD-O2D
45	AB	811	CLA	CAD-CBD-CGD-O1D
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	819	CLA	C3A-C2A-CAA-CBA
45	AB	819	CLA	C4-C3-C5-C6
45	AB	824	CLA	C1A-C2A-CAA-CBA
45	AB	824	CLA	C3A-C2A-CAA-CBA
45	AB	824	CLA	CHA-CBD-CGD-O1D
45	AB	828	CLA	C1A-C2A-CAA-CBA
45	AB	829	CLA	C1A-C2A-CAA-CBA
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
45	AF	804	CLA	CHA-CBD-CGD-O1D

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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	CBD-CGD-O2D-CED
45	AJ	102	CLA	C1A-C2A-CAA-CBA
45	AJ	102	CLA	CHA-CBD-CGD-O1D
45	AJ	102	CLA	CHA-CBD-CGD-O2D
45	AK	203	CLA	C1A-C2A-CAA-CBA
45	AK	203	CLA	CBA-CGA-O2A-C1
45	AK	203	CLA	CBD-CGD-O2D-CED
45	AL	303	CLA	CHA-CBD-CGD-O1D
45	AL	303	CLA	CHA-CBD-CGD-O2D
45	AL	305	CLA	C1A-C2A-CAA-CBA
45	AL	305	CLA	CHA-CBD-CGD-O2D
45	A1	306	CLA	CHA-CBD-CGD-O1D
45	A1	306	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	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	309	CLA	CBD-CGD-O2D-CED
45	A4	301	CLA	CHA-CBD-CGD-O1D
45	A4	301	CLA	CHA-CBD-CGD-O2D
45	A4	302	CLA	CBD-CGD-O2D-CED
45	A4	303	CLA	CBD-CGD-O2D-CED
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	312	CLA	CBD-CGD-O2D-CED
45	A4	313	CLA	C1A-C2A-CAA-CBA
45	A4	313	CLA	CBD-CGD-O2D-CED
45	A6	609	CLA	C1A-C2A-CAA-CBA
45	A6	609	CLA	C3A-C2A-CAA-CBA
45	A6	611	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	A6	611	CLA	CHA-CBD-CGD-O2D
45	A6	611	CLA	CAD-CBD-CGD-O1D
45	BA	801	CLA	CBD-CGD-O2D-CED
45	BA	802	CLA	CBD-CGD-O2D-CED
45	BA	804	CLA	C1A-C2A-CAA-CBA
45	BA	804	CLA	C3A-C2A-CAA-CBA
45	BA	809	CLA	C1A-C2A-CAA-CBA
45	BA	813	CLA	CHA-CBD-CGD-O1D
45	BA	813	CLA	CHA-CBD-CGD-O2D
45	BA	814	CLA	CHA-CBD-CGD-O1D
45	BA	818	CLA	C1A-C2A-CAA-CBA
45	BA	818	CLA	C3A-C2A-CAA-CBA
45	BA	819	CLA	C3A-C2A-CAA-CBA
45	BA	819	CLA	CHA-CBD-CGD-O1D
45	BA	819	CLA	CHA-CBD-CGD-O2D
45	BA	821	CLA	CBD-CGD-O2D-CED
45	BA	822	CLA	C1A-C2A-CAA-CBA
45	BA	822	CLA	CAD-CBD-CGD-O1D
45	BA	822	CLA	CAD-CBD-CGD-O2D
45	BA	823	CLA	CHA-CBD-CGD-O1D
45	BA	823	CLA	CHA-CBD-CGD-O2D
45	BA	824	CLA	C1A-C2A-CAA-CBA
45	BA	824	CLA	C3A-C2A-CAA-CBA
45	BA	827	CLA	C6-C7-C8-C9
45	BA	828	CLA	CBD-CGD-O2D-CED
45	BA	833	CLA	CHA-CBD-CGD-O1D
45	BA	833	CLA	CHA-CBD-CGD-O2D
45	BA	833	CLA	CAD-CBD-CGD-O1D
45	BA	833	CLA	CBD-CGD-O2D-CED
45	BA	834	CLA	C4-C3-C5-C6
45	BA	835	CLA	CBD-CGD-O2D-CED
45	BA	840	CLA	CBD-CGD-O2D-CED
45	BA	841	CLA	CHA-CBD-CGD-O1D
45	BA	841	CLA	CHA-CBD-CGD-O2D
45	BA	841	CLA	C2-C3-C5-C6
45	BA	841	CLA	C4-C3-C5-C6
45	BA	844	CLA	CBD-CGD-O2D-CED
45	BB	802	CLA	CHA-CBD-CGD-O1D
45	BB	802	CLA	CHA-CBD-CGD-O2D
45	BB	802	CLA	C2-C3-C5-C6
45	BB	802	CLA	C4-C3-C5-C6
45	BB	804	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	BB	804	CLA	CHA-CBD-CGD-O2D
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	809	CLA	CHA-CBD-CGD-O1D
45	BB	809	CLA	CHA-CBD-CGD-O2D
45	BB	810	CLA	C1A-C2A-CAA-CBA
45	BB	811	CLA	CBD-CGD-O2D-CED
45	BB	812	CLA	C1A-C2A-CAA-CBA
45	BB	812	CLA	C2A-CAA-CBA-CGA
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	CHA-CBD-CGD-O1D
45	BB	816	CLA	CHA-CBD-CGD-O2D
45	BB	816	CLA	CBD-CGD-O2D-CED
45	BB	818	CLA	CBD-CGD-O2D-CED
45	BB	820	CLA	C3A-C2A-CAA-CBA
45	BB	820	CLA	C4-C3-C5-C6
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	825	CLA	CHA-CBD-CGD-O1D
45	BB	825	CLA	CHA-CBD-CGD-O2D
45	BB	830	CLA	C1A-C2A-CAA-CBA
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	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

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Mol	Chain	Res	Type	Atoms
45	BJ	102	CLA	CHA-CBD-CGD-O1D
45	BJ	102	CLA	CHA-CBD-CGD-O2D
45	BL	303	CLA	C1A-C2A-CAA-CBA
45	B1	307	CLA	CHA-CBD-CGD-O1D
45	B1	307	CLA	CHA-CBD-CGD-O2D
45	B1	307	CLA	CBD-CGD-O2D-CED
45	B1	311	CLA	CBD-CGD-O2D-CED
45	B2	603	CLA	CHA-CBD-CGD-O2D
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	304	CLA	C1A-C2A-CAA-CBA
45	B3	304	CLA	C3A-C2A-CAA-CBA
45	B5	601	CLA	CHA-CBD-CGD-O1D
45	B5	601	CLA	CHA-CBD-CGD-O2D
45	B5	601	CLA	CAD-CBD-CGD-O1D
45	B5	604	CLA	CBD-CGD-O2D-CED
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
45	B5	612	CLA	CHA-CBD-CGD-O1D
45	B5	612	CLA	CHA-CBD-CGD-O2D
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-O3
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	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
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	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
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	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-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-O5
47	B2	618	LHG	O7-C5-C6-O8
47	B3	318	LHG	C4-O6-P-O4
47	B5	618	LHG	C3-O3-P-O5
47	B5	618	LHG	C8-C7-O7-C5
47	F	801	LHG	C1-C2-C3-O3
47	F	801	LHG	O6-C4-C5-O7
47	a	501	LHG	C1-C2-C3-O3
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	C7-C8-C9-C34
48	AA	847	BCR	C21-C22-C23-C24
48	AA	847	BCR	C37-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

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Mol	Chain	Res	Type	Atoms
48	AB	848	BCR	C21-C22-C23-C24
48	AB	848	BCR	C37-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	AF	805	BCR	C7-C8-C9-C34
48	AI	101	BCR	C7-C8-C9-C10
48	AI	101	BCR	C7-C8-C9-C34
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
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	C7-C8-C9-C34
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

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Mol	Chain	Res	Type	Atoms
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	BL	306	BCR	C23-C24-C25-C30
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
50	AL	301	LMU	C2'-C1'-O1'-C1
50	BA	853	LMU	C2-C1-O1'-C1'
50	BA	854	LMU	C2'-C1'-O1'-C1
50	BA	854	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	A4	315	LUT	C1-C6-C7-C8
52	B1	316	LUT	C1-C6-C7-C8
52	B1	316	LUT	C10-C11-C12-C13
52	B1	316	LUT	C11-C12-C13-C14
52	B1	316	LUT	C11-C12-C13-C20
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	A3	307	CHL	CBD-CGD-O2D-CED
54	A6	602	CHL	C1A-C2A-CAA-CBA
54	A6	607	CHL	CBD-CGD-O2D-CED
54	B2	601	CHL	CHA-CBD-CGD-O1D
54	B2	601	CHL	CHA-CBD-CGD-O2D
54	B2	601	CHL	CAD-CBD-CGD-O1D
54	B2	601	CHL	C3-C5-C6-C7
54	B3	306	CHL	CBD-CGD-O2D-CED
56	BJ	104	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
56	BJ	104	SQD	C5-C6-S-O7
56	e	301	SQD	O5-C5-C6-S
45	BB	815	CLA	C2C-C3C-CAC-CBC
47	A3	319	LHG	C8-C7-O7-C5
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	BB	805	CLA	C2C-C3C-CAC-CBC
47	B3	318	LHG	C8-C7-O7-C5
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
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	AB	837	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	BB	843	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

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Mol	Chain	Res	Type	Atoms
54	B2	607	CHL	CBD-CGD-O2D-CED
54	B5	607	CHL	CBD-CGD-O2D-CED
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	AA	834	CLA	C4C-C3C-CAC-CBC
45	AA	814	CLA	O1D-CGD-O2D-CED
45	AA	833	CLA	O1D-CGD-O2D-CED
45	AB	801	CLA	O1D-CGD-O2D-CED
45	AG	203	CLA	O1D-CGD-O2D-CED
45	BA	814	CLA	O1D-CGD-O2D-CED
45	BA	844	CLA	O1D-CGD-O2D-CED
45	BB	804	CLA	O1D-CGD-O2D-CED
45	B1	311	CLA	O1D-CGD-O2D-CED
45	B5	604	CLA	O1D-CGD-O2D-CED
45	B5	609	CLA	O1D-CGD-O2D-CED
45	B5	610	CLA	O1D-CGD-O2D-CED
54	A3	307	CHL	O1D-CGD-O2D-CED
54	A4	306	CHL	O1D-CGD-O2D-CED
54	B5	607	CHL	O1D-CGD-O2D-CED
45	BK	203	CLA	CBA-CGA-O2A-C1
45	AA	834	CLA	C2C-C3C-CAC-CBC
45	AA	801	CLA	O1D-CGD-O2D-CED
45	AA	811	CLA	O1D-CGD-O2D-CED
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	A1	313	CLA	O1D-CGD-O2D-CED
45	A3	309	CLA	O1D-CGD-O2D-CED
45	A4	302	CLA	O1D-CGD-O2D-CED
45	A4	313	CLA	O1D-CGD-O2D-CED
45	BA	833	CLA	O1D-CGD-O2D-CED
45	BB	826	CLA	O1D-CGD-O2D-CED
45	BB	836	CLA	O1D-CGD-O2D-CED
45	BF	303	CLA	O1D-CGD-O2D-CED
45	BG	201	CLA	O1D-CGD-O2D-CED
45	B1	307	CLA	O1D-CGD-O2D-CED
54	A6	608	CHL	O1D-CGD-O2D-CED
54	B3	306	CHL	O1D-CGD-O2D-CED
45	BA	832	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
47	B1	302	LHG	C24-C23-O8-C6
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
45	BA	831	CLA	CBD-CGD-O2D-CED
45	BA	836	CLA	CBD-CGD-O2D-CED
45	BB	822	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
45	B5	612	CLA	CBD-CGD-O2D-CED
54	B2	605	CHL	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

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Mol	Chain	Res	Type	Atoms
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	828	CLA	O1D-CGD-O2D-CED
45	A1	306	CLA	O1D-CGD-O2D-CED
45	A4	312	CLA	O1D-CGD-O2D-CED
45	BA	835	CLA	O1D-CGD-O2D-CED
45	BB	838	CLA	O1D-CGD-O2D-CED
54	A6	607	CHL	O1D-CGD-O2D-CED
45	AB	834	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
50	AL	301	LMU	O5B-C1B-O1B-C4'
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
45	AA	815	CLA	O1D-CGD-O2D-CED
45	AB	810	CLA	O1D-CGD-O2D-CED
45	BA	811	CLA	O1D-CGD-O2D-CED
45	BB	815	CLA	O1D-CGD-O2D-CED
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	AA	833	CLA	O1A-CGA-O2A-C1
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
45	BA	828	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
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	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	AB	822	CLA	O1D-CGD-O2D-CED
45	B3	302	CLA	O1D-CGD-O2D-CED
45	AA	832	CLA	CBD-CGD-O2D-CED
45	AK	203	CLA	O1A-CGA-O2A-C1
45	AA	812	CLA	C4-C3-C5-C6
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	817	CLA	C2A-CAA-CBA-CGA
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	BA	805	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	829	CLA	C2A-CAA-CBA-CGA
45	BA	842	CLA	C2A-CAA-CBA-CGA
45	BB	811	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
45	BB	841	CLA	C2A-CAA-CBA-CGA
45	AB	811	CLA	O1A-CGA-O2A-C1
47	A3	319	LHG	O9-C7-O7-C5
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
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
50	AB	852	LMU	O5'-C5'-C6'-O6'
47	B3	318	LHG	O9-C7-O7-C5
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
46	AB	843	PQN	C11-C12-C13-C14
46	BA	843	PQN	C11-C12-C13-C14
45	AA	812	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
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	AA	813	CLA	O1D-CGD-O2D-CED
45	BB	812	CLA	O1D-CGD-O2D-CED
45	BF	302	CLA	O1D-CGD-O2D-CED
45	BK	203	CLA	O1D-CGD-O2D-CED
45	B3	308	CLA	O1D-CGD-O2D-CED
53	A4	318	LMG	O9-C10-O7-C8
51	AB	851	DGD	C4E-C5E-C6E-O5E
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
45	BB	828	CLA	O1A-CGA-O2A-C1
56	e	301	SQD	O10-C23-O48-C46
48	BL	306	BCR	C19-C20-C21-C22
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

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Mol	Chain	Res	Type	Atoms
45	B5	613	CLA	CBD-CGD-O2D-CED
45	AA	842	CLA	O1D-CGD-O2D-CED
45	AB	823	CLA	O1D-CGD-O2D-CED
45	BB	834	CLA	O1D-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	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	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
50	AB	850	LMU	O5'-C5'-C6'-O6'
50	AB	852	LMU	C4'-C5'-C6'-O6'
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	A6	603	CLA	O1D-CGD-O2D-CED
45	AL	303	CLA	CBD-CGD-O2D-CED
45	BA	839	CLA	CBD-CGD-O2D-CED
50	AA	851	LMU	O5B-C5B-C6B-O6B
47	A3	319	LHG	O10-C23-O8-C6
50	AB	853	LMU	O5'-C5'-C6'-O6'
50	AB	850	LMU	C4'-C5'-C6'-O6'
45	BA	820	CLA	O1D-CGD-O2D-CED
45	BB	843	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	BB	815	CLA	C5-C6-C7-C8
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	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	A4	308	CLA	O1D-CGD-O2D-CED
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
51	AB	851	DGD	O6E-C5E-C6E-O5E
45	AA	824	CLA	C4-C3-C5-C6
45	BA	838	CLA	C4-C3-C5-C6
45	AA	824	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	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	AA	838	CLA	O1A-CGA-O2A-C1
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	AL	301	LMU	O5'-C1'-O1'-C1
51	AB	851	DGD	O6D-C1D-O3G-C3G
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

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Mol	Chain	Res	Type	Atoms
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	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	826	CLA	O1A-CGA-O2A-C1
45	BB	805	CLA	C4C-C3C-CAC-CBC
45	AA	821	CLA	O1D-CGD-O2D-CED
45	BB	839	CLA	O1D-CGD-O2D-CED
45	B3	301	CLA	O1D-CGD-O2D-CED
45	BA	823	CLA	O1D-CGD-O2D-CED
47	B2	618	LHG	C1-C2-C3-O3
56	e	301	SQD	O49-C7-O47-C45
50	AB	853	LMU	C4'-C5'-C6'-O6'
45	AB	815	CLA	O1A-CGA-O2A-C1
45	AB	832	CLA	O1A-CGA-O2A-C1
45	BB	802	CLA	O1A-CGA-O2A-C1
45	BB	807	CLA	O1A-CGA-O2A-C1
45	BF	301	CLA	O1A-CGA-O2A-C1
45	AA	813	CLA	C3-C5-C6-C7
45	AB	838	CLA	O1D-CGD-O2D-CED
45	BA	813	CLA	O1D-CGD-O2D-CED
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

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Mol	Chain	Res	Type	Atoms
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	BA	834	CLA	C5-C6-C7-C8
46	BA	843	PQN	C18-C20-C21-C22
50	AL	301	LMU	C5'-C4'-O1B-C1B
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
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
50	AA	851	LMU	C2'-C1'-O1'-C1
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
45	AA	812	CLA	C2-C3-C5-C6
45	AA	821	CLA	C11-C10-C8-C9
45	AA	825	CLA	C11-C12-C13-C14
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

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Mol	Chain	Res	Type	Atoms
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
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
45	BB	842	CLA	CBD-CGD-O2D-CED
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	B5	601	CLA	C2A-CAA-CBA-CGA
48	AA	845	BCR	C7-C8-C9-C34
48	AA	846	BCR	C37-C22-C23-C24
48	AA	847	BCR	C11-C12-C13-C35
48	AB	845	BCR	C7-C8-C9-C34
48	AK	204	BCR	C37-C22-C23-C24
48	BA	849	BCR	C37-C22-C23-C24
48	BB	849	BCR	C37-C22-C23-C24
48	BL	306	BCR	C11-C12-C13-C35
48	AK	204	BCR	C21-C22-C23-C24
48	B3	317	BCR	C21-C22-C23-C24
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	BA	828	CLA	C13-C15-C16-C17
45	BA	808	CLA	CBD-CGD-O2D-CED
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	AA	803	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
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	AB	835	CLA	C8-C10-C11-C12
45	AB	838	CLA	C15-C16-C17-C18
45	BA	811	CLA	C15-C16-C17-C18
45	BA	819	CLA	C13-C15-C16-C17
45	BA	827	CLA	C10-C11-C12-C13
45	BA	829	CLA	C10-C11-C12-C13
45	BB	808	CLA	C10-C11-C12-C13
45	BB	816	CLA	C10-C11-C12-C13
45	BB	816	CLA	C13-C15-C16-C17
45	BB	826	CLA	C8-C10-C11-C12
45	BB	826	CLA	C13-C15-C16-C17
45	B3	301	CLA	C10-C11-C12-C13
45	BA	831	CLA	C2-C1-O2A-CGA
56	BJ	104	SQD	C23-C24-C25-C26
45	AB	802	CLA	O1D-CGD-O2D-CED
45	AB	820	CLA	O1D-CGD-O2D-CED
50	AB	850	LMU	O5B-C1B-O1B-C4'
45	AB	833	CLA	CBD-CGD-O2D-CED
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	803	CLA	C10-C11-C12-C13
45	AB	806	CLA	C13-C15-C16-C17
45	AB	815	CLA	C8-C10-C11-C12
45	A6	603	CLA	C13-C15-C16-C17
45	A6	613	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
46	AB	843	PQN	C15-C16-C17-C18
46	BB	844	PQN	C25-C26-C27-C28
45	AA	826	CLA	O1D-CGD-O2D-CED
45	AL	305	CLA	O1D-CGD-O2D-CED
45	BA	817	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
45	BA	825	CLA	O1D-CGD-O2D-CED
47	F	801	LHG	O1-C1-C2-O2
47	B5	618	LHG	C23-C24-C25-C26
47	F	801	LHG	C7-C8-C9-C10
53	A1	321	LMG	C10-C11-C12-C13
53	A1	321	LMG	C28-C29-C30-C31
53	B5	617	LMG	C10-C11-C12-C13
56	BJ	104	SQD	C7-C8-C9-C10
45	BA	822	CLA	CBD-CGD-O2D-CED
45	AA	805	CLA	C8-C10-C11-C12
45	AA	810	CLA	C13-C15-C16-C17
45	AA	840	CLA	C5-C6-C7-C8
45	AB	802	CLA	C15-C16-C17-C18
45	BB	826	CLA	C10-C11-C12-C13
46	BB	844	PQN	C15-C16-C17-C18
45	AH	201	CLA	CBA-CGA-O2A-C1
45	B2	609	CLA	CBA-CGA-O2A-C1
50	AL	301	LMU	O5B-C5B-C6B-O6B
53	B5	617	LMG	O6-C5-C6-O5
45	AA	825	CLA	C2-C1-O2A-CGA
45	BB	805	CLA	C2-C1-O2A-CGA
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	A3	302	CLA	C10-C11-C12-C13
45	BA	825	CLA	C10-C11-C12-C13
45	BA	825	CLA	C13-C15-C16-C17
45	BB	839	CLA	C15-C16-C17-C18
45	BL	303	CLA	C5-C6-C7-C8
46	AA	843	PQN	C25-C26-C27-C28
46	AB	843	PQN	C25-C26-C27-C28
47	F	801	LHG	C23-C24-C25-C26
54	A6	606	CHL	CBD-CGD-O2D-CED
45	B5	612	CLA	C8-C10-C11-C12
45	BB	801	CLA	C10-C11-C12-C13
46	BA	843	PQN	C23-C25-C26-C27
45	B3	310	CLA	O1D-CGD-O2D-CED
45	AA	806	CLA	C11-C12-C13-C15
45	AB	826	CLA	C11-C10-C8-C7
45	BA	842	CLA	C12-C13-C15-C16
45	BB	824	CLA	C11-C12-C13-C15
46	BA	843	PQN	C21-C22-C23-C25

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Mol	Chain	Res	Type	Atoms
46	BB	844	PQN	C21-C22-C23-C25
45	AB	827	CLA	C3-C5-C6-C7
45	BB	828	CLA	C3-C5-C6-C7
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
45	BB	830	CLA	O1A-CGA-O2A-C1
47	A1	302	LHG	O10-C23-O8-C6
50	AB	852	LMU	O1'-C1-C2-C3
45	AA	808	CLA	C2A-CAA-CBA-CGA
45	AG	201	CLA	C2A-CAA-CBA-CGA
45	A3	312	CLA	C2A-CAA-CBA-CGA
45	A6	601	CLA	C2A-CAA-CBA-CGA
45	BA	802	CLA	C2A-CAA-CBA-CGA
45	BA	808	CLA	C2A-CAA-CBA-CGA
54	A6	602	CHL	C2A-CAA-CBA-CGA
54	B3	306	CHL	C2A-CAA-CBA-CGA
45	BA	815	CLA	O1D-CGD-O2D-CED
45	BB	822	CLA	O1D-CGD-O2D-CED
45	B5	612	CLA	O1D-CGD-O2D-CED
54	B2	606	CHL	O1D-CGD-O2D-CED
45	AA	805	CLA	C13-C15-C16-C17
45	AA	827	CLA	C10-C11-C12-C13
45	AB	807	CLA	C13-C15-C16-C17
45	BA	830	CLA	C13-C15-C16-C17
45	AA	839	CLA	O1A-CGA-O2A-C1
45	AB	822	CLA	O1A-CGA-O2A-C1
45	BB	839	CLA	O1A-CGA-O2A-C1
54	A6	602	CHL	O1A-CGA-O2A-C1
45	BA	809	CLA	CBD-CGD-O2D-CED
45	BA	829	CLA	C8-C10-C11-C12
45	BA	801	CLA	C3-C5-C6-C7
46	AA	843	PQN	C13-C15-C16-C17
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

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Mol	Chain	Res	Type	Atoms
45	AB	832	CLA	C13-C15-C16-C17
45	AB	834	CLA	C15-C16-C17-C18
45	BA	810	CLA	C5-C6-C7-C8
45	BA	840	CLA	C5-C6-C7-C8
45	BB	827	CLA	C8-C10-C11-C12
45	BB	835	CLA	C8-C10-C11-C12
45	BB	839	CLA	C5-C6-C7-C8
46	AA	843	PQN	C20-C21-C22-C23
45	AA	830	CLA	CBA-CGA-O2A-C1
45	BB	827	CLA	CBA-CGA-O2A-C1
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	815	CLA	O1A-CGA-O2A-C1
45	BB	835	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
50	AB	850	LMU	O1'-C1-C2-C3
45	A6	614	CLA	O1D-CGD-O2D-CED
45	AA	828	CLA	C8-C10-C11-C12
45	BA	803	CLA	C5-C6-C7-C8
45	BA	803	CLA	C13-C15-C16-C17
45	BA	810	CLA	C13-C15-C16-C17
45	BA	819	CLA	C10-C11-C12-C13
45	BA	833	CLA	C15-C16-C17-C18
45	BB	829	CLA	C10-C11-C12-C13
45	BB	831	CLA	C5-C6-C7-C8
45	BB	843	CLA	C8-C10-C11-C12
45	BB	802	CLA	CBD-CGD-O2D-CED
45	AB	808	CLA	CAA-CBA-CGA-O2A
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	C5-C6-C7-C8
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	BB	828	CLA	C10-C11-C12-C13
45	BB	836	CLA	C8-C10-C11-C12
47	A1	302	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
47	A1	302	LHG	C4-O6-P-O3
47	A6	618	LHG	C3-O3-P-O6
47	A6	618	LHG	C4-O6-P-O3
47	BF	305	LHG	C3-O3-P-O6
47	B2	618	LHG	C4-O6-P-O3
47	B3	318	LHG	C4-O6-P-O3
47	B5	618	LHG	C4-O6-P-O3
47	a	501	LHG	C3-O3-P-O6
45	AB	801	CLA	C3-C5-C6-C7
45	AA	803	CLA	CBA-CGA-O2A-C1
45	A4	308	CLA	CBA-CGA-O2A-C1
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	AA	838	CLA	O1D-CGD-O2D-CED
45	AB	825	CLA	O1D-CGD-O2D-CED
45	AA	832	CLA	O1D-CGD-O2D-CED
47	AJ	104	LHG	C1-C2-C3-O3
45	AB	815	CLA	C13-C15-C16-C17
45	AA	824	CLA	C2A-CAA-CBA-CGA
45	BA	817	CLA	C2A-CAA-CBA-CGA
45	BA	841	CLA	C2A-CAA-CBA-CGA
45	B2	612	CLA	C2A-CAA-CBA-CGA
45	AA	806	CLA	C16-C17-C18-C19
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	C13-C15-C16-C17
45	AA	806	CLA	C13-C15-C16-C17
45	AA	830	CLA	C8-C10-C11-C12
45	BA	821	CLA	C13-C15-C16-C17
45	BA	828	CLA	C15-C16-C17-C18
45	AB	805	CLA	O1D-CGD-O2D-CED
47	BA	845	LHG	C8-C7-O7-C5
45	BA	821	CLA	C15-C16-C17-C18
45	A6	613	CLA	C2A-CAA-CBA-CGA
50	BA	853	LMU	O5B-C5B-C6B-O6B
52	B1	316	LUT	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
52	B1	316	LUT	C39-C29-C30-C31
47	AJ	104	LHG	C18-C19-C20-C21
47	A1	320	LHG	C11-C12-C13-C14
47	BA	845	LHG	C14-C15-C16-C17
53	A4	318	LMG	C12-C13-C14-C15
45	AB	826	CLA	O1A-CGA-O2A-C1
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	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	801	CLA	CBA-CGA-O2A-C1
45	BA	812	CLA	CBA-CGA-O2A-C1
47	B1	318	LHG	C28-C29-C30-C31
51	AB	851	DGD	CAA-CBA-CCA-CDA
45	AA	812	CLA	O1D-CGD-O2D-CED
45	B2	602	CLA	O1D-CGD-O2D-CED
54	B5	606	CHL	O1D-CGD-O2D-CED
47	BA	845	LHG	O9-C7-O7-C5
47	F	801	LHG	O9-C7-O7-C5
56	BJ	104	SQD	C10-C11-C12-C13
56	BJ	104	SQD	C13-C14-C15-C16
45	B2	610	CLA	O1D-CGD-O2D-CED
53	A4	318	LMG	C13-C14-C15-C16
45	AA	825	CLA	C15-C16-C17-C18
45	AB	832	CLA	C8-C10-C11-C12
47	A1	320	LHG	C33-C34-C35-C36
47	BF	305	LHG	C27-C28-C29-C30
56	BJ	104	SQD	C9-C10-C11-C12
45	AA	801	CLA	C3-C5-C6-C7
45	BA	803	CLA	O1D-CGD-O2D-CED
45	B2	612	CLA	O1D-CGD-O2D-CED
52	B1	316	LUT	C11-C10-C9-C8
52	B1	316	LUT	C28-C29-C30-C31
56	BJ	104	SQD	C2-C1-O6-C44
56	e	301	SQD	C2-C1-O6-C44
45	AA	809	CLA	CBA-CGA-O2A-C1
45	AB	806	CLA	CBA-CGA-O2A-C1
45	A1	305	CLA	CBA-CGA-O2A-C1
47	A1	301	LHG	C24-C25-C26-C27
50	BB	851	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
53	A4	318	LMG	C29-C30-C31-C32
45	AA	828	CLA	C15-C16-C17-C18
45	AA	833	CLA	C13-C15-C16-C17
45	BB	839	CLA	C8-C10-C11-C12
45	A4	313	CLA	O1A-CGA-O2A-C1
45	BB	818	CLA	O1A-CGA-O2A-C1
45	AA	819	CLA	C16-C17-C18-C19
45	AA	819	CLA	C16-C17-C18-C20
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	AA	819	CLA	O1D-CGD-O2D-CED
45	AA	840	CLA	O1D-CGD-O2D-CED
50	BB	851	LMU	O5'-C5'-C6'-O6'
46	AA	843	PQN	C11-C12-C13-C14
47	AA	844	LHG	C10-C11-C12-C13
47	BF	305	LHG	C11-C10-C9-C8
50	AL	301	LMU	C3'-C4'-O1B-C1B
51	AB	851	DGD	C3A-C4A-C5A-C6A
45	AA	819	CLA	C11-C12-C13-C14
45	AB	803	CLA	C11-C10-C8-C9
45	AB	811	CLA	C14-C13-C15-C16
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	BA	825	CLA	C11-C10-C8-C9
45	BA	829	CLA	C14-C13-C15-C16
45	B2	612	CLA	C14-C13-C15-C16
45	BA	838	CLA	O1D-CGD-O2D-CED
45	BB	824	CLA	O1D-CGD-O2D-CED
45	B1	313	CLA	O1D-CGD-O2D-CED
47	F	801	LHG	C30-C31-C32-C33
50	AA	851	LMU	C4-C5-C6-C7
50	BA	853	LMU	C5-C6-C7-C8
51	BB	850	DGD	CAA-CBA-CCA-CDA
56	BJ	104	SQD	C11-C12-C13-C14
45	AA	817	CLA	C10-C11-C12-C13
54	B2	601	CHL	C2A-CAA-CBA-CGA
45	B2	609	CLA	O1A-CGA-O2A-C1
48	BL	306	BCR	C7-C8-C9-C34
47	AA	844	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
47	A3	301	LHG	O1-C1-C2-C3
47	B2	618	LHG	O1-C1-C2-C3
47	F	801	LHG	O1-C1-C2-C3
48	BL	306	BCR	C21-C22-C23-C24
45	AA	827	CLA	C3-C5-C6-C7
47	A6	618	LHG	C8-C7-O7-C5
47	BF	305	LHG	C30-C31-C32-C33
47	AJ	104	LHG	C7-C8-C9-C10
45	BB	829	CLA	O1D-CGD-O2D-CED
45	B5	613	CLA	O1D-CGD-O2D-CED
47	BA	845	LHG	C25-C26-C27-C28
47	B1	318	LHG	C11-C12-C13-C14
45	BB	824	CLA	O1A-CGA-O2A-C1
45	AB	810	CLA	C16-C17-C18-C20
45	AB	812	CLA	C6-C7-C8-C9
45	AB	817	CLA	C6-C7-C8-C9
45	BA	813	CLA	C16-C17-C18-C19
45	BA	825	CLA	C16-C17-C18-C20
56	BJ	104	SQD	O5-C1-O6-C44
45	A6	603	CLA	C10-C11-C12-C13
45	BA	802	CLA	C15-C16-C17-C18
45	BB	824	CLA	C8-C10-C11-C12
50	AA	851	LMU	C3-C4-C5-C6
50	AB	852	LMU	C11-C10-C9-C8
51	AB	851	DGD	C9B-CAB-CBB-CCB
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	B1	304	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	CCA-CDA-CEA-CFA
45	AA	829	CLA	C5-C6-C7-C8
45	BB	843	CLA	C15-C16-C17-C18
50	BA	853	LMU	O5B-C1B-O1B-C4'
45	BA	830	CLA	O1A-CGA-O2A-C1
45	BB	827	CLA	O1A-CGA-O2A-C1
47	BF	305	LHG	C11-C12-C13-C14
45	BB	843	CLA	C3-C5-C6-C7
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	BB	821	CLA	O1D-CGD-O2D-CED
45	AA	803	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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
50	BB	851	LMU	C2-C1-O1'-C1'
45	AB	840	CLA	O1D-CGD-O2D-CED
45	BA	807	CLA	O1D-CGD-O2D-CED
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	808	CLA	C16-C17-C18-C19
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	A4	301	CLA	C11-C12-C13-C14
45	BA	825	CLA	C16-C17-C18-C19
45	BB	835	CLA	C16-C17-C18-C20
45	BB	836	CLA	C11-C12-C13-C14
45	BB	836	CLA	C11-C12-C13-C15
45	AB	814	CLA	O1D-CGD-O2D-CED
45	B3	305	CLA	O1D-CGD-O2D-CED
50	AB	853	LMU	O5B-C5B-C6B-O6B
45	AB	821	CLA	CBD-CGD-O2D-CED
47	BA	845	LHG	C29-C30-C31-C32
45	AB	804	CLA	C5-C6-C7-C8
45	BA	842	CLA	C4-C3-C5-C6
46	AB	843	PQN	C14-C13-C15-C16
46	BB	844	PQN	C14-C13-C15-C16
45	AA	831	CLA	CBA-CGA-O2A-C1
45	BA	842	CLA	C2-C3-C5-C6
47	B2	618	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
56	e	301	SQD	C8-C7-O47-C45
47	AA	844	LHG	C33-C34-C35-C36
45	A1	305	CLA	O1A-CGA-O2A-C1
45	AA	805	CLA	C16-C17-C18-C19
45	BB	807	CLA	C16-C17-C18-C20
50	AB	850	LMU	C1-C2-C3-C4
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
47	A6	618	LHG	O9-C7-O7-C5
45	AB	804	CLA	C2-C1-O2A-CGA
45	BA	841	CLA	C2-C1-O2A-CGA
47	BA	845	LHG	C32-C33-C34-C35
45	AB	821	CLA	O1A-CGA-O2A-C1
45	BA	812	CLA	O1A-CGA-O2A-C1
45	BB	842	CLA	O1A-CGA-O2A-C1
45	BA	806	CLA	C16-C17-C18-C20
45	BB	804	CLA	C16-C17-C18-C20
45	AA	811	CLA	C3-C5-C6-C7
45	AB	811	CLA	C3-C5-C6-C7
48	AA	846	BCR	C5-C6-C7-C8
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	AG	205	BCR	C23-C24-C25-C26
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

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Mol	Chain	Res	Type	Atoms
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	848	BCR	C5-C6-C7-C8
48	BA	850	BCR	C5-C6-C7-C8
48	BA	850	BCR	C23-C24-C25-C30
48	BA	851	BCR	C1-C6-C7-C8
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	803	BCR	C5-C6-C7-C8
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	BB	848	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	BL	306	BCR	C5-C6-C7-C8
48	BL	306	BCR	C23-C24-C25-C26
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
52	B1	316	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
50	AL	301	LMU	C2-C3-C4-C5
45	BB	835	CLA	O1D-CGD-O2D-CED
45	BA	805	CLA	CBA-CGA-O2A-C1
45	BB	840	CLA	CBA-CGA-O2A-C1
45	AA	827	CLA	C8-C10-C11-C12
45	BA	833	CLA	C5-C6-C7-C8
45	AA	804	CLA	O1A-CGA-O2A-C1
45	BB	831	CLA	O1A-CGA-O2A-C1
47	A1	301	LHG	C7-C8-C9-C10
47	A1	301	LHG	C23-C24-C25-C26
45	BB	811	CLA	C13-C15-C16-C17
45	AB	819	CLA	O1D-CGD-O2D-CED
47	F	801	LHG	C27-C28-C29-C30
45	AA	827	CLA	C4-C3-C5-C6
45	AB	815	CLA	C4-C3-C5-C6
45	AA	811	CLA	C12-C13-C15-C16
45	AA	813	CLA	C6-C7-C8-C10
45	AA	821	CLA	C2-C3-C5-C6
45	AA	827	CLA	C2-C3-C5-C6
45	AB	815	CLA	C2-C3-C5-C6
45	AB	823	CLA	C11-C12-C13-C15
45	AB	834	CLA	C11-C12-C13-C15
45	AB	842	CLA	C12-C13-C15-C16
45	A4	311	CLA	C6-C7-C8-C10
45	BA	801	CLA	C12-C13-C15-C16
45	BA	806	CLA	C2-C3-C5-C6
45	BA	806	CLA	C12-C13-C15-C16
45	BA	808	CLA	C11-C12-C13-C15
45	BA	810	CLA	C6-C7-C8-C10
45	BA	821	CLA	C11-C12-C13-C15
45	BA	829	CLA	C11-C10-C8-C7
45	BA	829	CLA	C12-C13-C15-C16
45	BB	815	CLA	C6-C7-C8-C10
45	BB	828	CLA	C11-C10-C8-C7
45	BB	828	CLA	C11-C12-C13-C15
45	BB	835	CLA	C11-C12-C13-C15
45	B2	612	CLA	C12-C13-C15-C16
46	AB	843	PQN	C21-C22-C23-C25
45	AA	803	CLA	C3-C5-C6-C7
45	AA	831	CLA	O1A-CGA-O2A-C1
47	F	801	LHG	C32-C33-C34-C35
45	AB	802	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	AB	806	CLA	C8-C10-C11-C12
45	BA	810	CLA	C10-C11-C12-C13
45	AL	304	CLA	C11-C12-C13-C14
47	B2	618	LHG	O9-C7-O7-C5
53	B5	617	LMG	O9-C10-O7-C8
56	e	301	SQD	C7-C8-C9-C10
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	839	CLA	O1D-CGD-O2D-CED
45	B2	602	CLA	C13-C15-C16-C17
47	B1	318	LHG	C9-C10-C11-C12
50	AB	850	LMU	C3'-C4'-O1B-C1B
51	BB	850	DGD	CDA-CEA-CFA-CGA
45	AB	842	CLA	O1D-CGD-O2D-CED
45	AL	303	CLA	O1D-CGD-O2D-CED
45	BA	830	CLA	C5-C6-C7-C8
45	B2	612	CLA	C8-C10-C11-C12
47	BA	845	LHG	C15-C16-C17-C18
50	AB	850	LMU	C5'-C4'-O1B-C1B
53	AG	202	LMG	C11-C12-C13-C14
50	BB	851	LMU	O5B-C1B-O1B-C4'
45	AB	835	CLA	CBD-CGD-O2D-CED
45	BB	820	CLA	CBD-CGD-O2D-CED
45	BB	821	CLA	CBA-CGA-O2A-C1
54	B2	601	CHL	CBA-CGA-O2A-C1
45	A3	312	CLA	C6-C7-C8-C9
45	BA	805	CLA	C16-C17-C18-C19
56	e	301	SQD	O5-C1-O6-C44
45	BB	834	CLA	C5-C6-C7-C8
45	B1	314	CLA	C8-C10-C11-C12
47	A3	301	LHG	C11-C10-C9-C8
50	AB	850	LMU	C5-C6-C7-C8
53	AG	202	LMG	C10-C11-C12-C13
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
48	AA	847	BCR	C10-C11-C12-C13
47	AJ	104	LHG	C14-C15-C16-C17
45	BB	808	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
45	BB	829	CLA	C15-C16-C17-C18
47	AA	844	LHG	O9-C7-O7-C5
45	AB	809	CLA	C3-C5-C6-C7
53	AG	202	LMG	C30-C31-C32-C33
50	AB	853	LMU	C2'-C1'-O1'-C1
47	a	501	LHG	O7-C5-C6-O8
45	AA	805	CLA	C16-C17-C18-C20
45	AA	806	CLA	C16-C17-C18-C20
45	BA	838	CLA	C6-C7-C8-C10
45	B3	311	CLA	C6-C7-C8-C9
45	AA	821	CLA	C4-C3-C5-C6
45	AA	834	CLA	C4-C3-C5-C6
45	BA	806	CLA	C4-C3-C5-C6
47	BA	845	LHG	C23-C24-C25-C26
45	AA	826	CLA	C2-C3-C5-C6
45	AA	834	CLA	C2-C3-C5-C6
47	A1	320	LHG	C30-C31-C32-C33
45	AA	803	CLA	C11-C12-C13-C14
45	AA	811	CLA	C14-C13-C15-C16
45	AB	826	CLA	C11-C10-C8-C9
45	A1	304	CLA	C11-C10-C8-C9
45	A4	301	CLA	C11-C10-C8-C9
45	A4	311	CLA	C6-C7-C8-C9
45	BA	808	CLA	C11-C12-C13-C14
45	BA	810	CLA	C6-C7-C8-C9
45	BA	813	CLA	C11-C10-C8-C9
45	BA	842	CLA	C14-C13-C15-C16
45	BB	811	CLA	C14-C13-C15-C16
45	BB	815	CLA	C6-C7-C8-C9
45	BB	824	CLA	C11-C12-C13-C14
45	BB	826	CLA	C14-C13-C15-C16
45	BB	835	CLA	C11-C12-C13-C14
45	B5	602	CLA	C11-C10-C8-C9
46	BA	843	PQN	C21-C22-C23-C24
47	A6	618	LHG	C9-C10-C11-C12
56	BJ	104	SQD	C11-C10-C9-C8
45	AB	802	CLA	C3-C5-C6-C7
45	AL	304	CLA	C3-C5-C6-C7
45	A1	314	CLA	C2A-CAA-CBA-CGA
45	BB	818	CLA	C2A-CAA-CBA-CGA
45	BB	830	CLA	C2A-CAA-CBA-CGA
54	A6	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
50	AB	852	LMU	C5-C6-C7-C8
48	AA	848	BCR	C7-C8-C9-C34
45	BA	811	CLA	C13-C15-C16-C17
45	A1	314	CLA	C2C-C3C-CAC-CBC
48	AI	101	BCR	C21-C22-C23-C24
48	A1	319	BCR	C21-C22-C23-C24
45	BA	805	CLA	O1A-CGA-O2A-C1
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	801	CLA	C16-C17-C18-C19
45	AB	815	CLA	C16-C17-C18-C20
45	AB	823	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
45	BA	805	CLA	C16-C17-C18-C20
45	BA	813	CLA	C16-C17-C18-C20
47	B1	302	LHG	C8-C7-O7-C5
47	BA	845	LHG	C10-C11-C12-C13
45	BB	801	CLA	C5-C6-C7-C8
45	BB	811	CLA	C10-C11-C12-C13
45	AA	810	CLA	CAD-CBD-CGD-O2D
45	A6	611	CLA	CMA-C3A-C4A-CHB
45	B2	610	CLA	CMA-C3A-C4A-CHB
45	AB	817	CLA	C3-C5-C6-C7
47	BA	845	LHG	C34-C35-C36-C37
45	BB	840	CLA	O1A-CGA-O2A-C1
45	AA	803	CLA	C5-C6-C7-C8
45	AA	803	CLA	C10-C11-C12-C13
45	AA	829	CLA	C15-C16-C17-C18
47	F	801	LHG	O6-C4-C5-C6
47	A1	301	LHG	C30-C31-C32-C33
51	AB	851	DGD	C9A-CAA-CBA-CCA
45	BA	809	CLA	CBA-CGA-O2A-C1
47	B1	318	LHG	O9-C7-O7-C5
45	BA	811	CLA	C4-C3-C5-C6
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	812	CLA	C5-C6-C7-C8
50	AB	852	LMU	C4-C5-C6-C7
51	AB	851	DGD	CCA-CDA-CEA-CFA
45	AB	803	CLA	C16-C17-C18-C20
45	BA	801	CLA	C16-C17-C18-C19
45	B2	602	CLA	C16-C17-C18-C19
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
45	BB	806	CLA	C2C-C3C-CAC-CBC
45	A6	604	CLA	C2A-CAA-CBA-CGA
45	BA	828	CLA	C10-C11-C12-C13
53	B5	617	LMG	C31-C32-C33-C34
56	BJ	104	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
45	BA	806	CLA	C10-C11-C12-C13
45	BA	809	CLA	O1A-CGA-O2A-C1
45	BB	821	CLA	O1A-CGA-O2A-C1
47	A1	320	LHG	C8-C7-O7-C5
45	BA	808	CLA	O1D-CGD-O2D-CED
45	AB	808	CLA	C2A-CAA-CBA-CGA
45	B1	305	CLA	C2A-CAA-CBA-CGA
45	AA	805	CLA	C4-C3-C5-C6
45	AA	826	CLA	C4-C3-C5-C6
45	AB	809	CLA	C4-C3-C5-C6
45	AB	842	CLA	C4-C3-C5-C6
45	BB	819	CLA	C4-C3-C5-C6
45	BB	836	CLA	C4-C3-C5-C6
45	BF	301	CLA	C4-C3-C5-C6
45	BB	836	CLA	C2-C3-C5-C6
45	BA	811	CLA	C16-C17-C18-C19
47	B5	618	LHG	C24-C23-O8-C6
45	AL	304	CLA	C8-C10-C11-C12
45	BA	813	CLA	C15-C16-C17-C18
45	BB	830	CLA	C5-C6-C7-C8
56	BJ	104	SQD	C19-C20-C21-C22
45	AB	829	CLA	C2A-CAA-CBA-CGA
45	A1	314	CLA	C15-C16-C17-C18
45	BA	806	CLA	C5-C6-C7-C8
45	BH	201	CLA	C10-C11-C12-C13
45	AB	801	CLA	C2-C1-O2A-CGA
45	BB	807	CLA	C2-C1-O2A-CGA
47	a	501	LHG	C25-C26-C27-C28
45	BA	822	CLA	O1D-CGD-O2D-CED
47	B2	618	LHG	C9-C10-C11-C12
51	AB	851	DGD	CCB-CDB-CEB-CFB
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	BB	842	CLA	O1D-CGD-O2D-CED
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	838	CLA	C6-C7-C8-C9
45	B3	311	CLA	C6-C7-C8-C10
45	AB	802	CLA	C8-C10-C11-C12
45	A1	314	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
45	BA	809	CLA	O1D-CGD-O2D-CED
45	BB	825	CLA	CBD-CGD-O2D-CED
45	AB	826	CLA	C10-C11-C12-C13
47	A3	301	LHG	O7-C5-C6-O8
51	BB	850	DGD	O1G-C1G-C2G-O2G
53	A4	318	LMG	O1-C7-C8-O7
47	BF	305	LHG	C10-C11-C12-C13
47	B1	302	LHG	O9-C7-O7-C5
45	AB	801	CLA	C5-C6-C7-C8
54	A6	606	CHL	O1D-CGD-O2D-CED
51	AB	851	DGD	CDA-CEA-CFA-CGA
45	AB	808	CLA	C2-C1-O2A-CGA
45	A6	613	CLA	C2-C1-O2A-CGA
45	AA	804	CLA	C4-C3-C5-C6
45	AB	833	CLA	C4-C3-C5-C6
45	AA	801	CLA	C12-C13-C15-C16
45	AA	803	CLA	C11-C12-C13-C15
45	AA	805	CLA	C2-C3-C5-C6
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	AA	829	CLA	C11-C12-C13-C15
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	815	CLA	C11-C10-C8-C7
45	AB	815	CLA	C12-C13-C15-C16
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	AB	842	CLA	C2-C3-C5-C6
45	A1	304	CLA	C11-C10-C8-C7
45	A4	301	CLA	C11-C10-C8-C7
45	A6	603	CLA	C11-C12-C13-C15
45	BA	811	CLA	C2-C3-C5-C6
45	BA	813	CLA	C11-C10-C8-C7
45	BA	819	CLA	C11-C12-C13-C15
45	BA	828	CLA	C6-C7-C8-C10
45	BA	828	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
45	BB	802	CLA	C6-C7-C8-C10
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	BF	301	CLA	C2-C3-C5-C6
45	BL	303	CLA	C11-C10-C8-C7
45	B5	602	CLA	C11-C10-C8-C7
46	AB	843	PQN	C17-C18-C20-C21
45	BB	819	CLA	CAA-CBA-CGA-O2A
54	B2	601	CHL	O1A-CGA-O2A-C1
45	AA	803	CLA	C11-C10-C8-C9
45	AA	808	CLA	C11-C12-C13-C14
45	AA	813	CLA	C11-C10-C8-C9
45	AA	813	CLA	C11-C12-C13-C14
45	AA	821	CLA	C11-C12-C13-C14
45	AA	825	CLA	C11-C10-C8-C9
45	AA	827	CLA	C14-C13-C15-C16
45	AA	828	CLA	C6-C7-C8-C9
45	AA	830	CLA	C14-C13-C15-C16
45	AA	842	CLA	C11-C10-C8-C9
45	AB	802	CLA	C14-C13-C15-C16
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	810	CLA	C11-C10-C8-C9
45	AB	814	CLA	C6-C7-C8-C9
45	AB	825	CLA	C14-C13-C15-C16
45	AB	834	CLA	C11-C12-C13-C14
45	BA	803	CLA	C11-C10-C8-C9
45	BA	819	CLA	C6-C7-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	807	CLA	C11-C12-C13-C14
45	BB	811	CLA	C6-C7-C8-C9
45	BB	811	CLA	C11-C10-C8-C9
45	BB	819	CLA	C6-C7-C8-C9
45	BB	826	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
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	BB	843	CLA	C6-C7-C8-C9
45	BL	303	CLA	C11-C10-C8-C9
45	B1	314	CLA	C6-C7-C8-C9
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
45	A4	311	CLA	C2A-CAA-CBA-CGA
48	A3	318	BCR	C37-C22-C23-C24
45	AB	828	CLA	C10-C11-C12-C13
45	B2	602	CLA	C16-C17-C18-C20
48	AJ	103	BCR	C7-C8-C9-C10
48	BA	855	BCR	C21-C22-C23-C24
48	BI	101	BCR	C21-C22-C23-C24
45	AA	840	CLA	C3-C5-C6-C7
45	AB	833	CLA	O1D-CGD-O2D-CED
45	AB	829	CLA	C5-C6-C7-C8
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
50	AA	851	LMU	C7-C8-C9-C10
45	B2	612	CLA	C10-C11-C12-C13
45	BA	826	CLA	C5-C6-C7-C8
45	BB	819	CLA	C11-C12-C13-C14
45	BB	833	CLA	C2A-CAA-CBA-CGA
45	BA	811	CLA	C16-C17-C18-C20
47	A1	320	LHG	O6-C4-C5-C6
45	AA	841	CLA	CBA-CGA-O2A-C1
45	AA	805	CLA	C10-C11-C12-C13
45	AF	802	CLA	C4-C3-C5-C6
45	AA	804	CLA	C2-C3-C5-C6
45	AB	809	CLA	C2-C3-C5-C6
45	AB	833	CLA	C2-C3-C5-C6
47	A1	320	LHG	O9-C7-O7-C5
51	AB	851	DGD	C4A-C5A-C6A-C7A
45	BB	824	CLA	C16-C17-C18-C20
45	AB	817	CLA	C5-C6-C7-C8
45	AB	830	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	AA	824	CLA	CBA-CGA-O2A-C1
45	AB	820	CLA	CBA-CGA-O2A-C1
45	BB	810	CLA	CBA-CGA-O2A-C1
47	B2	618	LHG	O8-C23-C24-C25
47	a	501	LHG	C2-C3-O3-P
45	BB	801	CLA	O1A-CGA-O2A-C1
45	AA	805	CLA	C3A-C2A-CAA-CBA
45	AB	810	CLA	C3A-C2A-CAA-CBA
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	BH	201	CLA	C3A-C2A-CAA-CBA
54	A6	602	CHL	C3A-C2A-CAA-CBA
45	BA	811	CLA	C5-C6-C7-C8
50	AB	853	LMU	C2-C1-O1'-C1'
50	BA	854	LMU	C2-C1-O1'-C1'
50	AB	850	LMU	C9-C10-C11-C12
45	BB	820	CLA	O1D-CGD-O2D-CED
45	A3	303	CLA	C6-C7-C8-C10
45	BB	835	CLA	C16-C17-C18-C19
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	C4-C5-C6-O8
51	AB	851	DGD	C1G-C2G-C3G-O3G
56	BJ	104	SQD	O6-C44-C45-C46
47	AA	844	LHG	C23-C24-C25-C26
45	AB	809	CLA	O1A-CGA-O2A-C1
47	B5	618	LHG	O10-C23-O8-C6
47	B1	302	LHG	C10-C11-C12-C13
45	BA	830	CLA	O2A-C1-C2-C3
51	BB	850	DGD	O6E-C5E-C6E-O5E
45	BB	829	CLA	CAA-CBA-CGA-O2A
45	BA	801	CLA	C16-C17-C18-C20
45	BB	819	CLA	C2-C3-C5-C6
45	BA	805	CLA	C15-C16-C17-C18
47	A3	319	LHG	C4-O6-P-O3
47	B1	302	LHG	C4-O6-P-O3
45	AA	801	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	BJ	102	CLA	O1D-CGD-O2D-CED
45	BB	818	CLA	C3-C5-C6-C7
47	A3	301	LHG	O1-C1-C2-O2
45	AA	811	CLA	C13-C15-C16-C17
47	A1	320	LHG	C34-C35-C36-C37
47	A1	320	LHG	O6-C4-C5-O7
45	AA	825	CLA	O1A-CGA-O2A-C1
45	AB	840	CLA	O1A-CGA-O2A-C1
45	AA	801	CLA	C16-C17-C18-C20
45	AB	819	CLA	C11-C12-C13-C15
47	F	801	LHG	C29-C30-C31-C32
51	BB	850	DGD	CAB-CBB-CCB-CDB
45	BB	802	CLA	O1D-CGD-O2D-CED
47	B1	318	LHG	O2-C2-C3-O3
51	AB	851	DGD	C4B-C5B-C6B-C7B
50	BA	854	LMU	C1-C2-C3-C4
45	A6	610	CLA	O1A-CGA-O2A-C1
54	A6	608	CHL	O1A-CGA-O2A-C1
45	AB	821	CLA	O1D-CGD-O2D-CED
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	834	CLA	CBA-CGA-O2A-C1
45	BA	801	CLA	CAA-CBA-CGA-O2A
47	A1	320	LHG	C7-C8-C9-C10
45	BB	824	CLA	C16-C17-C18-C19
45	BA	819	CLA	C5-C6-C7-C8
45	A4	301	CLA	CBD-CGD-O2D-CED
47	BF	305	LHG	C1-C2-C3-O3
45	AA	833	CLA	C2-C1-O2A-CGA
45	AB	829	CLA	C2-C1-O2A-CGA
45	BB	816	CLA	C2-C1-O2A-CGA
54	A6	608	CHL	C2-C1-O2A-CGA
45	AF	802	CLA	C2-C3-C5-C6
45	AA	819	CLA	C6-C7-C8-C9
45	AB	803	CLA	C6-C7-C8-C9
45	AB	810	CLA	C11-C12-C13-C14
45	AB	819	CLA	C11-C10-C8-C9
45	AB	827	CLA	C11-C12-C13-C14
45	AB	830	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
45	BB	810	CLA	C11-C10-C8-C9
45	BB	820	CLA	C11-C10-C8-C9
45	AA	816	CLA	CBD-CGD-O2D-CED
47	F	801	LHG	C33-C34-C35-C36
53	A1	321	LMG	C11-C12-C13-C14
45	AB	818	CLA	C8-C10-C11-C12
45	AB	833	CLA	C10-C11-C12-C13
45	BA	805	CLA	C10-C11-C12-C13
45	BB	812	CLA	C15-C16-C17-C18
47	A6	618	LHG	C5-C4-O6-P
47	B3	318	LHG	C5-C4-O6-P
50	AA	851	LMU	C1-C2-C3-C4
45	BB	829	CLA	C2C-C3C-CAC-CBC
47	A1	320	LHG	C11-C10-C9-C8
51	AB	851	DGD	C7A-C8A-C9A-CAA
45	BB	819	CLA	C2A-CAA-CBA-CGA
54	B1	303	CHL	C2A-CAA-CBA-CGA
45	AA	808	CLA	C16-C17-C18-C20
45	AB	815	CLA	C16-C17-C18-C19
45	BB	834	CLA	C3-C5-C6-C7
48	AA	847	BCR	C23-C24-C25-C30
48	AA	852	BCR	C1-C6-C7-C8
48	AI	101	BCR	C5-C6-C7-C8
48	AI	102	BCR	C1-C6-C7-C8
48	AJ	103	BCR	C23-C24-C25-C30
48	BF	304	BCR	C23-C24-C25-C30
45	AA	802	CLA	C15-C16-C17-C18
45	B1	314	CLA	C2C-C3C-CAC-CBC
48	BG	203	BCR	C11-C12-C13-C35
45	AB	831	CLA	O1D-CGD-O2D-CED
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	AB	803	CLA	C16-C17-C18-C19
45	AB	814	CLA	C15-C16-C17-C18
45	BA	818	CLA	O1A-CGA-O2A-C1
45	BA	839	CLA	O1A-CGA-O2A-C1
47	AJ	104	LHG	O6-C4-C5-C6
47	B3	318	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
47	a	501	LHG	O6-C4-C5-C6
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	819	CLA	C11-C12-C13-C15
45	AA	821	CLA	C6-C7-C8-C10
45	AA	827	CLA	C6-C7-C8-C10
45	AA	828	CLA	C12-C13-C15-C16
45	AA	830	CLA	C12-C13-C15-C16
45	AA	842	CLA	C11-C10-C8-C7
45	AB	801	CLA	C6-C7-C8-C10
45	AB	801	CLA	C11-C10-C8-C7
45	AB	802	CLA	C6-C7-C8-C10
45	AB	803	CLA	C11-C10-C8-C7
45	AB	807	CLA	C12-C13-C15-C16
45	AB	809	CLA	C6-C7-C8-C10
45	AB	810	CLA	C11-C10-C8-C7
45	AB	814	CLA	C6-C7-C8-C10
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	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	830	CLA	C12-C13-C15-C16
45	BA	840	CLA	C11-C10-C8-C7
45	BA	841	CLA	C11-C10-C8-C7
45	BA	842	CLA	C11-C10-C8-C7
45	BB	804	CLA	C6-C7-C8-C10
45	BB	807	CLA	C11-C12-C13-C15
45	BB	815	CLA	C11-C12-C13-C15
45	BB	816	CLA	C11-C10-C8-C7
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	304	CLA	C11-C12-C13-C15
45	B1	314	CLA	C6-C7-C8-C10
46	BB	844	PQN	C17-C18-C20-C21

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Mol	Chain	Res	Type	Atoms
51	AB	851	DGD	C5A-C6A-C7A-C8A
45	A6	612	CLA	CBD-CGD-O2D-CED
45	AB	801	CLA	C16-C17-C18-C19
45	A3	303	CLA	C6-C7-C8-C9
50	AL	301	LMU	C1-C2-C3-C4
53	A4	318	LMG	C29-C28-O8-C9
47	A1	301	LHG	C11-C12-C13-C14
45	AA	830	CLA	C5-C6-C7-C8
45	AB	819	CLA	C5-C6-C7-C8
45	AB	826	CLA	C8-C10-C11-C12
45	AA	841	CLA	O1A-CGA-O2A-C1
45	AA	830	CLA	C10-C11-C12-C13
45	AA	840	CLA	CBA-CGA-O2A-C1
45	A1	304	CLA	CBA-CGA-O2A-C1
50	AL	301	LMU	C3-C4-C5-C6
47	AA	844	LHG	C25-C26-C27-C28
50	AL	301	LMU	C5-C6-C7-C8
47	AA	844	LHG	C31-C32-C33-C34
47	A6	618	LHG	C26-C27-C28-C29
45	AA	804	CLA	CAD-CBD-CGD-O2D
45	AA	806	CLA	CAD-CBD-CGD-O2D
45	AA	807	CLA	CAD-CBD-CGD-O2D
45	AA	815	CLA	CAD-CBD-CGD-O2D
45	AA	816	CLA	CAD-CBD-CGD-O2D
45	AA	825	CLA	CAD-CBD-CGD-O2D
45	AA	833	CLA	CAD-CBD-CGD-O2D
45	AA	841	CLA	CAD-CBD-CGD-O2D
45	AB	810	CLA	CAD-CBD-CGD-O2D
45	AB	811	CLA	CAD-CBD-CGD-O2D
45	AB	813	CLA	CAD-CBD-CGD-O2D
45	AB	815	CLA	CAD-CBD-CGD-O2D
45	AB	816	CLA	CAD-CBD-CGD-O2D
45	AB	817	CLA	CAD-CBD-CGD-O2D
45	AB	823	CLA	CAD-CBD-CGD-O2D
45	AB	828	CLA	CAD-CBD-CGD-O2D
45	AB	833	CLA	CAD-CBD-CGD-O2D
45	AG	203	CLA	CAD-CBD-CGD-O2D
45	AH	201	CLA	CAD-CBD-CGD-O2D
45	A1	311	CLA	CAD-CBD-CGD-O2D
45	A6	610	CLA	CAD-CBD-CGD-O2D
45	BA	817	CLA	CAD-CBD-CGD-O2D
45	BA	818	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
45	BA	833	CLA	CAD-CBD-CGD-O2D
45	BA	836	CLA	CAD-CBD-CGD-O2D
45	BB	821	CLA	CAD-CBD-CGD-O2D
45	BB	824	CLA	CAD-CBD-CGD-O2D
45	BB	832	CLA	CAD-CBD-CGD-O2D
45	BB	833	CLA	CAD-CBD-CGD-O2D
45	BB	835	CLA	CAD-CBD-CGD-O2D
45	BF	302	CLA	CAD-CBD-CGD-O2D
45	B1	306	CLA	CAD-CBD-CGD-O2D
45	B1	313	CLA	CAD-CBD-CGD-O2D
45	B3	301	CLA	CAD-CBD-CGD-O2D
45	B3	307	CLA	CAD-CBD-CGD-O2D
45	B5	601	CLA	CAD-CBD-CGD-O2D
45	B5	609	CLA	CAD-CBD-CGD-O2D
47	A3	319	LHG	C6-C5-O7-C7
54	B2	601	CHL	CAD-CBD-CGD-O2D
45	AA	834	CLA	C5-C6-C7-C8
45	AH	201	CLA	C5-C6-C7-C8
45	BB	801	CLA	C13-C15-C16-C17
45	AB	842	CLA	C16-C17-C18-C19
45	BB	801	CLA	CBD-CGD-O2D-CED
45	BB	810	CLA	O1A-CGA-O2A-C1
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	AA	805	CLA	C2C-C3C-CAC-CBC
47	BA	845	LHG	C12-C13-C14-C15
53	A1	321	LMG	C30-C31-C32-C33
45	BB	821	CLA	C5-C6-C7-C8
47	AA	844	LHG	C30-C31-C32-C33
45	A1	304	CLA	O1A-CGA-O2A-C1
45	AA	808	CLA	CHA-CBD-CGD-O1D
45	AA	808	CLA	CHA-CBD-CGD-O2D
45	AA	814	CLA	CHA-CBD-CGD-O2D
45	AA	829	CLA	CHA-CBD-CGD-O2D
45	AA	834	CLA	CHA-CBD-CGD-O1D
45	AA	834	CLA	CHA-CBD-CGD-O2D
45	AA	836	CLA	CHA-CBD-CGD-O1D
45	AA	836	CLA	CHA-CBD-CGD-O2D
45	AA	839	CLA	CHA-CBD-CGD-O1D
45	AA	839	CLA	CHA-CBD-CGD-O2D
45	AB	802	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	AB	802	CLA	CHA-CBD-CGD-O2D
45	AB	809	CLA	CHA-CBD-CGD-O1D
45	AB	809	CLA	CHA-CBD-CGD-O2D
45	AB	814	CLA	CHA-CBD-CGD-O1D
45	AB	821	CLA	CHA-CBD-CGD-O1D
45	AB	824	CLA	CHA-CBD-CGD-O2D
45	AB	825	CLA	CHA-CBD-CGD-O1D
45	AB	825	CLA	CHA-CBD-CGD-O2D
45	AB	827	CLA	CHA-CBD-CGD-O1D
45	AB	827	CLA	CHA-CBD-CGD-O2D
45	AB	837	CLA	CHA-CBD-CGD-O1D
45	AB	842	CLA	CHA-CBD-CGD-O1D
45	AB	842	CLA	CHA-CBD-CGD-O2D
45	AF	804	CLA	CHA-CBD-CGD-O2D
45	AL	305	CLA	CHA-CBD-CGD-O1D
45	A1	305	CLA	CHA-CBD-CGD-O1D
45	A1	305	CLA	CHA-CBD-CGD-O2D
45	A1	316	CLA	CHA-CBD-CGD-O1D
45	A1	316	CLA	CHA-CBD-CGD-O2D
45	BA	803	CLA	CHA-CBD-CGD-O1D
45	BA	803	CLA	CHA-CBD-CGD-O2D
45	BA	805	CLA	CHA-CBD-CGD-O1D
45	BA	805	CLA	CHA-CBD-CGD-O2D
45	BA	814	CLA	CHA-CBD-CGD-O2D
45	BA	815	CLA	CHA-CBD-CGD-O1D
45	BA	815	CLA	CHA-CBD-CGD-O2D
45	BA	820	CLA	CHA-CBD-CGD-O1D
45	BA	824	CLA	CHA-CBD-CGD-O1D
45	BA	824	CLA	CHA-CBD-CGD-O2D
45	BA	831	CLA	CHA-CBD-CGD-O1D
45	BA	831	CLA	CHA-CBD-CGD-O2D
45	BA	834	CLA	CHA-CBD-CGD-O1D
45	BA	834	CLA	CHA-CBD-CGD-O2D
45	BA	844	CLA	CHA-CBD-CGD-O1D
45	BA	844	CLA	CHA-CBD-CGD-O2D
45	BB	810	CLA	CHA-CBD-CGD-O1D
45	BB	810	CLA	CHA-CBD-CGD-O2D
45	BB	815	CLA	CHA-CBD-CGD-O1D
45	BB	815	CLA	CHA-CBD-CGD-O2D
45	BB	840	CLA	CHA-CBD-CGD-O1D
45	BB	840	CLA	CHA-CBD-CGD-O2D
45	BG	201	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	BG	201	CLA	CHA-CBD-CGD-O2D
45	BK	202	CLA	CHA-CBD-CGD-O1D
45	BK	202	CLA	CHA-CBD-CGD-O2D
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	B2	610	CLA	CHA-CBD-CGD-O1D
45	B3	301	CLA	CHA-CBD-CGD-O1D
45	AA	829	CLA	O1A-CGA-O2A-C1
45	AB	820	CLA	O1A-CGA-O2A-C1
45	BA	841	CLA	O1A-CGA-O2A-C1
45	BB	834	CLA	O1A-CGA-O2A-C1
45	B5	602	CLA	O1A-CGA-O2A-C1
47	A1	302	LHG	C10-C11-C12-C13
45	AB	835	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	C9B-CAB-CBB-CCB
47	A6	618	LHG	O7-C5-C6-O8
53	B5	617	LMG	O1-C7-C8-O7
45	AA	805	CLA	C5-C6-C7-C8
45	AA	824	CLA	O1A-CGA-O2A-C1
45	AA	829	CLA	CAA-CBA-CGA-O2A
47	A1	320	LHG	C25-C26-C27-C28
47	B2	618	LHG	C29-C30-C31-C32
45	AB	828	CLA	C4-C3-C5-C6
45	B3	311	CLA	C4-C3-C5-C6
45	B3	311	CLA	C2-C3-C5-C6
45	BB	841	CLA	O1D-CGD-O2D-CED
45	BB	838	CLA	CBA-CGA-O2A-C1
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	814	CLA	C11-C12-C13-C14
45	AB	818	CLA	C6-C7-C8-C9
45	AB	828	CLA	C11-C10-C8-C9
45	A6	613	CLA	CBA-CGA-O2A-C1
45	AB	823	CLA	C5-C6-C7-C8
46	AA	843	PQN	C18-C20-C21-C22
50	AA	851	LMU	C4'-C5'-C6'-O6'
45	BB	801	CLA	C2A-CAA-CBA-CGA
45	BB	810	CLA	C2A-CAA-CBA-CGA
51	AB	851	DGD	C8B-C9B-CAB-CBB
48	AI	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
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
47	AJ	104	LHG	C16-C17-C18-C19
50	BA	853	LMU	C3'-C4'-O1B-C1B
45	BB	802	CLA	C3-C5-C6-C7
53	A1	321	LMG	C33-C34-C35-C36
45	AA	830	CLA	C1A-C2A-CAA-CBA
45	AB	810	CLA	C1A-C2A-CAA-CBA
45	AB	841	CLA	C1A-C2A-CAA-CBA
45	A3	308	CLA	C1A-C2A-CAA-CBA
45	A4	310	CLA	CHA-CBD-CGD-O2D
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	B1	310	CLA	CHA-CBD-CGD-O2D
45	B3	303	CLA	CHA-CBD-CGD-O2D
54	B5	605	CHL	CHA-CBD-CGD-O2D
45	BB	820	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	BA	838	CLA	C2-C1-O2A-CGA
45	BA	803	CLA	CBA-CGA-O2A-C1
45	B3	311	CLA	CBA-CGA-O2A-C1
47	A1	320	LHG	C3-O3-P-O6
47	A3	301	LHG	C3-O3-P-O6
47	BA	845	LHG	C35-C36-C37-C38
47	F	801	LHG	C11-C10-C9-C8
45	BB	824	CLA	C5-C6-C7-C8
47	AJ	104	LHG	C2-C3-O3-P
47	F	801	LHG	C2-C3-O3-P
47	A6	618	LHG	C29-C30-C31-C32
50	AB	853	LMU	C3'-C4'-O1B-C1B
53	A4	318	LMG	O10-C28-O8-C9
47	AA	844	LHG	C4-O6-P-O4
47	A1	301	LHG	C3-O3-P-O4
47	A1	302	LHG	C3-O3-P-O5
47	A1	302	LHG	C4-O6-P-O4
47	A1	302	LHG	C4-O6-P-O5
47	A6	618	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
47	BF	305	LHG	C3-O3-P-O4
47	B1	318	LHG	C3-O3-P-O4
47	B2	618	LHG	C4-O6-P-O4
47	B5	618	LHG	C4-O6-P-O5
47	F	801	LHG	C3-O3-P-O4
47	a	501	LHG	C3-O3-P-O5
47	A1	302	LHG	C7-C8-C9-C10
45	BA	803	CLA	C8-C10-C11-C12
45	BB	835	CLA	C10-C11-C12-C13
45	AA	813	CLA	CBA-CGA-O2A-C1
47	BF	305	LHG	C13-C14-C15-C16
47	F	801	LHG	C24-C25-C26-C27
45	BA	803	CLA	O1A-CGA-O2A-C1
45	AA	817	CLA	C5-C6-C7-C8
47	a	501	LHG	C7-C8-C9-C10
45	BB	801	CLA	C3-C5-C6-C7
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	837	CLA	C2-C3-C5-C6
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	AL	303	CLA	CAD-CBD-CGD-O1D
45	A1	305	CLA	CAD-CBD-CGD-O1D
45	A1	316	CLA	CAD-CBD-CGD-O1D
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	831	CLA	CAD-CBD-CGD-O1D
45	BA	841	CLA	CAD-CBD-CGD-O1D
45	BB	815	CLA	CAD-CBD-CGD-O1D
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
56	BJ	104	SQD	C5-C6-S-O9
45	AA	818	CLA	CAA-CBA-CGA-O2A
45	AB	828	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	B3	311	CLA	O1A-CGA-O2A-C1
45	BB	819	CLA	C3-C5-C6-C7
45	AA	816	CLA	O1D-CGD-O2D-CED
47	BA	845	LHG	C11-C12-C13-C14
47	BF	305	LHG	C14-C15-C16-C17
45	AA	811	CLA	C6-C7-C8-C10
45	AA	830	CLA	C11-C10-C8-C7
45	AA	840	CLA	C11-C10-C8-C7
45	AA	841	CLA	C11-C10-C8-C7
45	AB	814	CLA	C11-C12-C13-C15
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	828	CLA	C11-C10-C8-C7
45	AB	829	CLA	C12-C13-C15-C16
45	A3	308	CLA	C3A-C2A-CAA-CBA
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	804	CLA	C12-C13-C15-C16
45	BB	808	CLA	C12-C13-C15-C16
45	BB	810	CLA	C6-C7-C8-C10
45	BB	830	CLA	C12-C13-C15-C16
45	B3	304	CLA	CAD-CBD-CGD-O2D
45	AB	804	CLA	C15-C16-C17-C18
45	AB	829	CLA	C13-C15-C16-C17
45	AA	813	CLA	O1A-CGA-O2A-C1
50	AL	301	LMU	C2-C1-O1'-C1'
45	AB	833	CLA	CAA-CBA-CGA-O2A
50	AA	851	LMU	C4B-C5B-C6B-O6B
45	B3	311	CLA	C2A-CAA-CBA-CGA
47	AA	844	LHG	C35-C36-C37-C38
50	BA	853	LMU	C5'-C4'-O1B-C1B
45	BA	818	CLA	CAA-CBA-CGA-O2A
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	838	CLA	O1A-CGA-O2A-C1
56	BJ	104	SQD	O6-C44-C45-O47
45	BB	819	CLA	O2A-C1-C2-C3
45	BA	817	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
45	BB	812	CLA	C3-C5-C6-C7
47	AA	844	LHG	C29-C30-C31-C32
47	BA	845	LHG	C31-C32-C33-C34
45	BB	841	CLA	O1A-CGA-O2A-C1
45	A6	612	CLA	O1D-CGD-O2D-CED
45	AA	826	CLA	C8-C10-C11-C12
45	BB	808	CLA	C5-C6-C7-C8
45	AA	842	CLA	C4-C3-C5-C6
45	BB	829	CLA	C4-C3-C5-C6
46	AA	843	PQN	C14-C13-C15-C16
45	AB	837	CLA	CBA-CGA-O2A-C1
45	BB	841	CLA	CBA-CGA-O2A-C1
51	AB	851	DGD	CBB-CCB-CDB-CEB
45	AB	810	CLA	C8-C10-C11-C12
45	AB	828	CLA	C15-C16-C17-C18
45	AA	810	CLA	C6-C7-C8-C9
45	AB	801	CLA	C11-C10-C8-C9
45	AB	809	CLA	C6-C7-C8-C9
45	AB	809	CLA	C11-C10-C8-C9
45	AB	825	CLA	C6-C7-C8-C9
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	804	CLA	C6-C7-C8-C9
45	BB	805	CLA	C11-C12-C13-C14
45	BB	810	CLA	C6-C7-C8-C9
45	BB	815	CLA	C11-C12-C13-C14
45	BB	816	CLA	C11-C10-C8-C9
45	B1	304	CLA	C11-C12-C13-C14
45	AA	840	CLA	O1A-CGA-O2A-C1
45	BA	841	CLA	C16-C17-C18-C19
45	AB	837	CLA	O1A-CGA-O2A-C1
45	AB	818	CLA	C10-C11-C12-C13
48	BA	855	BCR	C37-C22-C23-C24
47	BF	305	LHG	C24-C25-C26-C27
47	B1	301	LHG	C28-C29-C30-C31
48	AA	852	BCR	C21-C22-C23-C24
48	BA	856	BCR	C21-C22-C23-C24
45	BA	829	CLA	CAA-CBA-CGA-O2A
45	BA	805	CLA	C2C-C3C-CAC-CBC
45	BB	806	CLA	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
47	AA	844	LHG	C32-C33-C34-C35
45	AA	838	CLA	C5-C6-C7-C8
45	A1	306	CLA	C1-C2-C3-C4
45	AA	813	CLA	C2A-CAA-CBA-CGA
45	AB	809	CLA	C2A-CAA-CBA-CGA
45	AB	817	CLA	C2A-CAA-CBA-CGA
45	BK	202	CLA	C2A-CAA-CBA-CGA
47	A1	302	LHG	O9-C7-O7-C5
45	BB	805	CLA	C5-C6-C7-C8
45	AA	834	CLA	C2-C1-O2A-CGA
45	AA	838	CLA	C2-C1-O2A-CGA
45	AB	812	CLA	C2-C1-O2A-CGA
45	AB	815	CLA	C2-C1-O2A-CGA
45	AB	818	CLA	C2-C1-O2A-CGA
45	BA	806	CLA	C2-C1-O2A-CGA
45	BA	829	CLA	C2-C1-O2A-CGA
45	AB	828	CLA	C2C-C3C-CAC-CBC
45	AB	818	CLA	CAA-CBA-CGA-O2A
45	A3	312	CLA	O1A-CGA-O2A-C1
45	BA	840	CLA	C3-C5-C6-C7
45	A6	611	CLA	CMA-C3A-C4A-NA
47	BA	845	LHG	C11-C10-C9-C8
50	BA	854	LMU	C6-C7-C8-C9
50	AB	853	LMU	C5'-C4'-O1B-C1B
45	AB	829	CLA	C4-C3-C5-C6
48	AA	846	BCR	C1-C6-C7-C8
45	A4	301	CLA	O1D-CGD-O2D-CED
50	BA	853	LMU	C3-C4-C5-C6
50	AB	853	LMU	C3-C4-C5-C6
45	AB	819	CLA	C11-C12-C13-C14
50	AB	853	LMU	O5'-C1'-O1'-C1
45	A1	304	CLA	C2-C3-C5-C6
45	AB	818	CLA	C5-C6-C7-C8
45	AB	806	CLA	C2C-C3C-CAC-CBC
47	AA	844	LHG	C3-O3-P-O6
47	AJ	104	LHG	C3-O3-P-O6
47	BA	845	LHG	C3-O3-P-O6
47	BF	305	LHG	C4-O6-P-O3
47	B5	618	LHG	C3-O3-P-O6
47	F	801	LHG	C3-O3-P-O6
45	AA	826	CLA	C10-C11-C12-C13
47	AJ	104	LHG	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
51	BB	850	DGD	O1G-C1G-C2G-C3G
53	A4	318	LMG	O1-C7-C8-C9
45	A3	312	CLA	C4-C3-C5-C6
50	BA	853	LMU	C11-C10-C9-C8
45	AA	821	CLA	C11-C12-C13-C15
45	AA	842	CLA	C12-C13-C15-C16
45	AB	811	CLA	C12-C13-C15-C16
45	BA	825	CLA	C11-C10-C8-C7
45	BB	810	CLA	C11-C10-C8-C7
47	BA	845	LHG	C9-C10-C11-C12
45	AA	811	CLA	C6-C7-C8-C9
45	AA	829	CLA	C11-C12-C13-C14
45	AA	830	CLA	C11-C10-C8-C9
45	AB	815	CLA	C11-C10-C8-C9
45	AB	823	CLA	C14-C13-C15-C16
45	A1	314	CLA	C14-C13-C15-C16
45	BB	802	CLA	C6-C7-C8-C9
45	BB	808	CLA	C14-C13-C15-C16
46	BB	844	PQN	C21-C22-C23-C24
52	B1	316	LUT	C9-C10-C11-C12
50	BB	851	LMU	C3-C4-C5-C6
45	AB	838	CLA	C8-C10-C11-C12
47	A1	302	LHG	C23-C24-C25-C26
45	AA	826	CLA	C11-C12-C13-C14
45	BA	830	CLA	C16-C17-C18-C20
50	AA	851	LMU	C2-C3-C4-C5
45	AA	842	CLA	C10-C11-C12-C13
45	AB	814	CLA	C5-C6-C7-C8
45	BA	840	CLA	C13-C15-C16-C17
52	B3	315	LUT	C7-C8-C9-C10
45	BA	826	CLA	CBD-CGD-O2D-CED
45	BA	821	CLA	C4-C3-C5-C6
45	AA	842	CLA	C2-C3-C5-C6
45	A3	312	CLA	CBA-CGA-O2A-C1
53	B5	617	LMG	C29-C28-O8-C9
45	BA	806	CLA	CBD-CGD-O2D-CED
53	A1	321	LMG	C31-C32-C33-C34
50	AB	853	LMU	C5-C6-C7-C8
54	A6	602	CHL	C3-C5-C6-C7
45	BB	811	CLA	CBA-CGA-O2A-C1
45	BB	805	CLA	C10-C11-C12-C13
45	A3	312	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
45	BB	843	CLA	C10-C11-C12-C13
47	A1	320	LHG	C15-C16-C17-C18
50	BB	851	LMU	C4B-C5B-C6B-O6B
45	AA	802	CLA	C4-C3-C5-C6
45	AH	201	CLA	C2-C1-O2A-CGA
45	BA	828	CLA	C2-C1-O2A-CGA
45	BB	818	CLA	C2-C1-O2A-CGA
45	AA	833	CLA	C8-C10-C11-C12
45	AB	842	CLA	C10-C11-C12-C13
45	BA	838	CLA	C2A-CAA-CBA-CGA
47	a	501	LHG	C5-C4-O6-P
51	AB	851	DGD	CBA-CCA-CDA-CEA
45	AA	809	CLA	C3A-C2A-CAA-CBA
45	AB	811	CLA	C3A-C2A-CAA-CBA
45	BB	834	CLA	CAA-CBA-CGA-O2A
45	A1	309	CLA	CAA-CBA-CGA-O2A
45	BK	202	CLA	CAA-CBA-CGA-O2A
45	AA	806	CLA	C4-C3-C5-C6
45	BB	830	CLA	C4-C3-C5-C6
47	B1	301	LHG	C11-C10-C9-C8
45	BB	832	CLA	CBD-CGD-O2D-CED
45	AB	803	CLA	C11-C12-C13-C14
45	BA	805	CLA	C11-C12-C13-C14
45	BA	830	CLA	C11-C10-C8-C9
45	BB	802	CLA	C11-C10-C8-C9
45	B2	602	CLA	C11-C10-C8-C9
45	BA	830	CLA	C16-C17-C18-C19
45	B2	602	CLA	C8-C10-C11-C12
45	BB	829	CLA	CBA-CGA-O2A-C1
47	A3	319	LHG	C1-C2-C3-O3
47	B3	318	LHG	C1-C2-C3-O3
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

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Mol	Chain	Res	Type	Atoms
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
53	A4	318	LMG	C7-C8-C9-O8
45	BB	843	CLA	C2A-CAA-CBA-CGA
50	BA	854	LMU	C3'-C4'-O1B-C1B
45	B2	612	CLA	C16-C17-C18-C20
45	AB	804	CLA	O2A-C1-C2-C3
45	BK	202	CLA	CAA-CBA-CGA-O1A
46	BA	843	PQN	C20-C21-C22-C23
51	BB	850	DGD	C9A-CAA-CBA-CCA
48	BJ	103	BCR	C7-C8-C9-C10
45	A3	308	CLA	CAA-CBA-CGA-O1A
45	BA	806	CLA	C15-C16-C17-C18
45	AB	830	CLA	C4-C3-C5-C6
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
56	BJ	104	SQD	C27-C28-C29-C30
45	AA	833	CLA	C11-C12-C13-C15
45	AB	827	CLA	C11-C10-C8-C7
45	AB	827	CLA	C11-C12-C13-C15
45	AB	840	CLA	C11-C10-C8-C7
45	BA	803	CLA	C11-C12-C13-C15
45	BA	805	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

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Mol	Chain	Res	Type	Atoms
45	BB	842	CLA	C6-C7-C8-C10
45	BA	813	CLA	C8-C10-C11-C12
45	B5	613	CLA	CAA-CBA-CGA-O1A
47	B1	318	LHG	C4-O6-P-O3
47	A1	302	LHG	C27-C28-C29-C30
45	BH	201	CLA	CBA-CGA-O2A-C1
45	A1	309	CLA	CAA-CBA-CGA-O1A
45	BG	202	CLA	CAA-CBA-CGA-O1A
54	B5	607	CHL	CAA-CBA-CGA-O1A
45	AA	808	CLA	C15-C16-C17-C18
45	BH	201	CLA	C11-C12-C13-C14
45	AB	818	CLA	C3-C5-C6-C7
45	BB	827	CLA	C3-C5-C6-C7
45	AA	806	CLA	C2A-CAA-CBA-CGA
45	AB	828	CLA	C2A-CAA-CBA-CGA
45	BA	831	CLA	C2A-CAA-CBA-CGA
45	BB	839	CLA	C2A-CAA-CBA-CGA
45	B5	612	CLA	C2A-CAA-CBA-CGA
45	AB	841	CLA	C5-C6-C7-C8
45	BA	813	CLA	C10-C11-C12-C13
45	BB	818	CLA	C5-C6-C7-C8
45	BF	301	CLA	C5-C6-C7-C8
45	B1	311	CLA	C5-C6-C7-C8
45	A6	612	CLA	CAA-CBA-CGA-O2A
47	A3	319	LHG	C23-C24-C25-C26
47	A1	302	LHG	C8-C7-O7-C5
45	BA	824	CLA	C5-C6-C7-C8
45	BG	202	CLA	CAA-CBA-CGA-O2A
54	B5	607	CHL	CAA-CBA-CGA-O2A
53	B5	617	LMG	O10-C28-O8-C9
45	AB	802	CLA	C10-C11-C12-C13
45	AB	828	CLA	C2-C3-C5-C6
45	AB	829	CLA	C2-C3-C5-C6
45	A4	311	CLA	C2-C3-C5-C6
45	BB	831	CLA	C2-C3-C5-C6
45	B2	608	CLA	CAA-CBA-CGA-O2A
45	BB	827	CLA	C5-C6-C7-C8
45	BB	829	CLA	O1A-CGA-O2A-C1
45	AB	842	CLA	C3-C5-C6-C7
50	BB	851	LMU	C3'-C4'-O1B-C1B
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	812	CLA	C10-C11-C12-C13
45	BA	836	CLA	CAA-CBA-CGA-O1A
53	A4	318	LMG	O7-C8-C9-O8
47	B2	618	LHG	O10-C23-C24-C25
45	A6	612	CLA	CAA-CBA-CGA-O1A
45	BB	827	CLA	C13-C15-C16-C17
45	BB	811	CLA	O1A-CGA-O2A-C1
45	BH	201	CLA	O1A-CGA-O2A-C1
45	AG	204	CLA	CAA-CBA-CGA-O2A
45	B5	613	CLA	CAA-CBA-CGA-O2A
50	AB	852	LMU	C4B-C5B-C6B-O6B
45	AB	813	CLA	O1D-CGD-O2D-CED
45	AB	803	CLA	C4-C3-C5-C6
45	BA	826	CLA	O1D-CGD-O2D-CED
45	AA	806	CLA	C2-C3-C5-C6
45	A3	312	CLA	C2-C3-C5-C6
45	A3	308	CLA	CAA-CBA-CGA-O2A
45	AA	821	CLA	C13-C15-C16-C17
45	BA	806	CLA	O1D-CGD-O2D-CED
45	AK	202	CLA	CAA-CBA-CGA-O1A
54	A1	303	CHL	C4-C3-C5-C6
45	BA	841	CLA	C5-C6-C7-C8
45	AA	809	CLA	C2A-CAA-CBA-CGA
45	AB	842	CLA	C2A-CAA-CBA-CGA
47	B2	618	LHG	C26-C27-C28-C29
56	BJ	104	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
48	AG	205	BCR	C23-C24-C25-C30
48	AL	302	BCR	C23-C24-C25-C26
48	BA	847	BCR	C1-C6-C7-C8
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	BL	301	BCR	C23-C24-C25-C30
52	B3	315	LUT	C5-C6-C7-C8
45	BB	832	CLA	O1D-CGD-O2D-CED
45	B2	608	CLA	CAA-CBA-CGA-O1A
54	A3	307	CHL	CAA-CBA-CGA-O2A
45	BA	808	CLA	C5-C6-C7-C8
45	A4	311	CLA	C4-C3-C5-C6
45	BA	805	CLA	C4-C3-C5-C6
45	BA	840	CLA	C4-C3-C5-C6
52	B5	614	LUT	C7-C8-C9-C10
45	AA	828	CLA	C5-C6-C7-C8
45	AA	802	CLA	C2-C3-C5-C6
45	BB	829	CLA	C2-C3-C5-C6
45	A6	610	CLA	C3-C5-C6-C7
45	A1	316	CLA	CAA-CBA-CGA-O2A
45	BA	836	CLA	CAA-CBA-CGA-O2A
45	AA	801	CLA	CAA-CBA-CGA-O1A
45	AB	809	CLA	C16-C17-C18-C19
47	F	801	LHG	C28-C29-C30-C31
45	BA	825	CLA	C8-C10-C11-C12
47	BA	845	LHG	O6-C4-C5-O7
47	B1	301	LHG	O6-C4-C5-O7
45	AG	204	CLA	CAA-CBA-CGA-O1A
54	B2	607	CHL	CAA-CBA-CGA-O2A
45	AA	810	CLA	CAD-CBD-CGD-O1D
45	A6	603	CLA	C2A-CAA-CBA-CGA
45	BB	829	CLA	C2A-CAA-CBA-CGA
53	A1	321	LMG	C34-C35-C36-C37
45	BB	810	CLA	C3-C5-C6-C7
45	B2	611	CLA	CAA-CBA-CGA-O2A
50	AB	853	LMU	O5B-C1B-O1B-C4'
47	B1	301	LHG	O6-C4-C5-C6
47	B1	302	LHG	O6-C4-C5-C6
45	BB	816	CLA	C4-C3-C5-C6
45	BB	827	CLA	C4-C3-C5-C6
54	B2	601	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
45	BB	819	CLA	CAA-CBA-CGA-O1A
45	AB	809	CLA	C11-C10-C8-C7
45	AB	830	CLA	C2-C3-C5-C6
45	A1	314	CLA	C6-C7-C8-C10
45	BA	806	CLA	C11-C12-C13-C15
45	BA	813	CLA	C11-C12-C13-C15
45	BA	821	CLA	C2-C3-C5-C6
45	BB	801	CLA	C12-C13-C15-C16
45	BB	811	CLA	C12-C13-C15-C16
45	BB	830	CLA	C2-C3-C5-C6
45	BB	834	CLA	C11-C12-C13-C15
45	BB	801	CLA	C8-C10-C11-C12
45	BB	830	CLA	C13-C15-C16-C17
47	B2	618	LHG	O1-C1-C2-O2
45	AB	813	CLA	CBD-CGD-O2D-CED
50	BB	851	LMU	C2B-C1B-O1B-C4'
47	A3	319	LHG	O7-C5-C6-O8
53	B5	617	LMG	C4-C5-C6-O5
45	B1	304	CLA	CBA-CGA-O2A-C1
45	BB	802	CLA	C15-C16-C17-C18
45	BA	835	CLA	CAA-CBA-CGA-O2A
54	A6	608	CHL	CAA-CBA-CGA-O2A
45	AB	801	CLA	O1A-CGA-O2A-C1
45	AB	825	CLA	C8-C10-C11-C12
45	B1	309	CLA	CAA-CBA-CGA-O2A
45	AA	833	CLA	CAA-CBA-CGA-O2A
45	BA	832	CLA	O1D-CGD-O2D-CED
45	AB	827	CLA	C4-C3-C5-C6
45	BA	813	CLA	C4-C3-C5-C6
45	BB	804	CLA	C4-C3-C5-C6
45	AA	821	CLA	C10-C11-C12-C13
47	BA	845	LHG	C19-C20-C21-C22
56	e	301	SQD	C25-C26-C27-C28
45	AA	836	CLA	CAA-CBA-CGA-O2A
45	AA	818	CLA	C10-C11-C12-C13
47	A3	301	LHG	O7-C7-C8-C9
53	B5	617	LMG	O7-C10-C11-C12
45	AA	821	CLA	C6-C7-C8-C9
45	AA	833	CLA	C11-C12-C13-C14
45	AA	842	CLA	C14-C13-C15-C16
45	AB	801	CLA	C11-C12-C13-C14
45	AL	304	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
45	A3	302	CLA	C6-C7-C8-C9
45	BA	811	CLA	C14-C13-C15-C16
45	BA	827	CLA	C11-C10-C8-C9
45	BA	828	CLA	C6-C7-C8-C9
45	BB	808	CLA	C11-C10-C8-C9
45	BB	828	CLA	C11-C10-C8-C9
45	A1	304	CLA	C4C-C3C-CAC-CBC
45	A4	302	CLA	CAA-CBA-CGA-O2A
45	A4	303	CLA	CAA-CBA-CGA-O1A
45	B2	603	CLA	CAA-CBA-CGA-O1A
50	BA	853	LMU	C2B-C1B-O1B-C4'
45	AA	841	CLA	C3A-C2A-CAA-CBA
45	BA	827	CLA	C3A-C2A-CAA-CBA
45	B5	608	CLA	C3A-C2A-CAA-CBA
53	A4	318	LMG	O7-C10-C11-C12
45	BA	832	CLA	CBD-CGD-O2D-CED
45	AA	813	CLA	CAD-CBD-CGD-O2D
45	AA	818	CLA	CAD-CBD-CGD-O2D
45	AA	821	CLA	CAD-CBD-CGD-O2D
45	AA	826	CLA	CAD-CBD-CGD-O2D
45	AA	842	CLA	CAD-CBD-CGD-O2D
45	AB	820	CLA	CAD-CBD-CGD-O2D
45	AB	821	CLA	CAD-CBD-CGD-O2D
45	AB	822	CLA	CAD-CBD-CGD-O2D
45	AB	834	CLA	CAD-CBD-CGD-O2D
45	AF	802	CLA	CAD-CBD-CGD-O2D
45	A1	304	CLA	CAD-CBD-CGD-O2D
45	A1	307	CLA	CAD-CBD-CGD-O2D
45	A3	308	CLA	CAD-CBD-CGD-O2D
45	A3	309	CLA	CAD-CBD-CGD-O2D
45	A4	309	CLA	CAD-CBD-CGD-O2D
45	A4	312	CLA	CAD-CBD-CGD-O2D
45	A4	313	CLA	CAD-CBD-CGD-O2D
45	A6	601	CLA	CAD-CBD-CGD-O2D
45	A6	603	CLA	CAD-CBD-CGD-O2D
45	A6	611	CLA	CAD-CBD-CGD-O2D
45	BA	804	CLA	CAD-CBD-CGD-O2D
45	BA	807	CLA	CAD-CBD-CGD-O2D
45	BA	809	CLA	CAD-CBD-CGD-O2D
45	BA	826	CLA	CAD-CBD-CGD-O2D
45	BA	830	CLA	CAD-CBD-CGD-O2D
45	BA	832	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
45	BA	837	CLA	CAD-CBD-CGD-O2D
45	BB	814	CLA	CAD-CBD-CGD-O2D
45	BB	831	CLA	CAD-CBD-CGD-O2D
45	BB	837	CLA	CAD-CBD-CGD-O2D
45	BB	838	CLA	CAD-CBD-CGD-O2D
45	BB	841	CLA	CAD-CBD-CGD-O2D
45	BK	203	CLA	CAD-CBD-CGD-O2D
45	B1	314	CLA	CAD-CBD-CGD-O2D
45	B2	604	CLA	CAD-CBD-CGD-O2D
45	B2	608	CLA	CAD-CBD-CGD-O2D
45	B2	609	CLA	CAD-CBD-CGD-O2D
45	B3	308	CLA	CAD-CBD-CGD-O2D
47	A6	618	LHG	C4-C5-O7-C7
45	A1	304	CLA	C2A-CAA-CBA-CGA
45	B1	313	CLA	CAA-CBA-CGA-O2A
50	BB	851	LMU	C5'-C4'-O1B-C1B
45	AA	834	CLA	CAA-CBA-CGA-O2A
47	B2	618	LHG	C30-C31-C32-C33
45	B2	609	CLA	C4-C3-C5-C6
54	B2	607	CHL	CAA-CBA-CGA-O1A
45	BB	829	CLA	CAA-CBA-CGA-O1A
45	BA	805	CLA	C2-C3-C5-C6
45	BB	810	CLA	C2-C3-C5-C6
45	BB	815	CLA	CAA-CBA-CGA-O2A
47	B1	301	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
47	A6	618	LHG	C4-C5-C6-O8
53	A1	321	LMG	C7-C8-C9-O8
53	B5	617	LMG	C7-C8-C9-O8
45	A1	316	CLA	CAA-CBA-CGA-O1A
45	B2	611	CLA	CAA-CBA-CGA-O1A
45	B5	603	CLA	CAA-CBA-CGA-O2A
54	A3	307	CHL	CAA-CBA-CGA-O1A
45	B1	304	CLA	O1A-CGA-O2A-C1
47	BA	846	LHG	O6-C4-C5-O7
47	B1	302	LHG	O6-C4-C5-O7
45	A3	302	CLA	C8-C10-C11-C12
45	BA	833	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	BA	835	CLA	CAA-CBA-CGA-O1A
54	B3	306	CHL	CAA-CBA-CGA-O1A
54	B3	306	CHL	CAA-CBA-CGA-O2A
45	AA	803	CLA	O2A-C1-C2-C3
45	AA	827	CLA	O2A-C1-C2-C3
45	AA	830	CLA	O2A-C1-C2-C3
45	AA	839	CLA	O2A-C1-C2-C3
45	AA	842	CLA	O2A-C1-C2-C3
45	AB	834	CLA	O2A-C1-C2-C3
45	A4	313	CLA	O2A-C1-C2-C3
45	BA	803	CLA	O2A-C1-C2-C3
45	BA	839	CLA	O2A-C1-C2-C3
45	BB	801	CLA	O2A-C1-C2-C3
45	BB	802	CLA	O2A-C1-C2-C3
45	BB	805	CLA	O2A-C1-C2-C3
45	BB	835	CLA	O2A-C1-C2-C3
50	AB	853	LMU	C2-C3-C4-C5
51	BB	850	DGD	CEA-CFA-CGA-CHA
45	AA	829	CLA	C2A-CAA-CBA-CGA
45	BA	806	CLA	CAA-CBA-CGA-O2A
47	B5	618	LHG	O7-C7-C8-C9
45	B3	307	CLA	CAA-CBA-CGA-O2A
45	BH	201	CLA	C11-C12-C13-C15
46	BA	843	PQN	C26-C27-C28-C29
45	AA	803	CLA	CHA-CBD-CGD-O1D
45	AA	803	CLA	CHA-CBD-CGD-O2D
45	AA	820	CLA	CHA-CBD-CGD-O1D
45	AA	822	CLA	CHA-CBD-CGD-O2D
45	AA	823	CLA	CHA-CBD-CGD-O1D
45	AA	823	CLA	CHA-CBD-CGD-O2D
45	AA	827	CLA	CHA-CBD-CGD-O1D
45	AA	831	CLA	CHA-CBD-CGD-O2D
45	AA	840	CLA	CHA-CBD-CGD-O1D
45	AA	840	CLA	CHA-CBD-CGD-O2D
45	AB	814	CLA	CHA-CBD-CGD-O2D
45	AB	816	CLA	CHA-CBD-CGD-O2D
45	AB	837	CLA	CHA-CBD-CGD-O2D
45	AK	202	CLA	CHA-CBD-CGD-O1D
45	AK	203	CLA	CHA-CBD-CGD-O1D
45	AL	304	CLA	CHA-CBD-CGD-O2D
45	A1	307	CLA	CHA-CBD-CGD-O1D
45	A4	302	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
45	BA	808	CLA	CHA-CBD-CGD-O1D
45	BA	808	CLA	CHA-CBD-CGD-O2D
45	BA	810	CLA	CHA-CBD-CGD-O1D
45	BA	816	CLA	CHA-CBD-CGD-O1D
45	BA	816	CLA	CHA-CBD-CGD-O2D
45	BA	820	CLA	CHA-CBD-CGD-O2D
45	BA	822	CLA	CHA-CBD-CGD-O1D
45	BA	822	CLA	CHA-CBD-CGD-O2D
45	BA	825	CLA	CHA-CBD-CGD-O1D
45	BA	827	CLA	CHA-CBD-CGD-O1D
45	BA	835	CLA	CHA-CBD-CGD-O1D
45	BA	835	CLA	CHA-CBD-CGD-O2D
45	BA	839	CLA	CHA-CBD-CGD-O2D
45	BA	842	CLA	CHA-CBD-CGD-O1D
45	BA	842	CLA	CHA-CBD-CGD-O2D
45	BB	807	CLA	CHA-CBD-CGD-O1D
45	BB	812	CLA	CHA-CBD-CGD-O1D
45	BB	826	CLA	CHA-CBD-CGD-O1D
45	BG	202	CLA	CHA-CBD-CGD-O2D
45	B1	304	CLA	CHA-CBD-CGD-O2D
45	B1	305	CLA	CHA-CBD-CGD-O2D
45	B2	610	CLA	CHA-CBD-CGD-O2D
45	B5	603	CLA	CHA-CBD-CGD-O1D
45	B5	603	CLA	CHA-CBD-CGD-O2D
45	A4	302	CLA	CAA-CBA-CGA-O1A
45	B1	313	CLA	CAA-CBA-CGA-O1A
45	B3	307	CLA	CAA-CBA-CGA-O1A
45	B5	603	CLA	CAA-CBA-CGA-O1A
45	BB	831	CLA	C4-C3-C5-C6
47	A1	302	LHG	O8-C23-C24-C25
47	AA	844	LHG	O6-C4-C5-C6
47	A1	301	LHG	O6-C4-C5-C6
47	BA	845	LHG	C30-C31-C32-C33
45	AA	827	CLA	CAA-CBA-CGA-O2A
45	AB	806	CLA	CAA-CBA-CGA-O2A
45	AB	834	CLA	CAA-CBA-CGA-O2A
45	BA	825	CLA	CAA-CBA-CGA-O2A
45	BA	834	CLA	CAA-CBA-CGA-O2A
47	B1	302	LHG	O7-C7-C8-C9
45	BB	804	CLA	C5-C6-C7-C8
45	BB	828	CLA	C5-C6-C7-C8
45	A4	303	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
45	A6	605	CLA	O1D-CGD-O2D-CED
45	BA	812	CLA	CAA-CBA-CGA-O2A
45	BA	828	CLA	CAA-CBA-CGA-O2A
47	BA	845	LHG	O8-C23-C24-C25
53	A1	321	LMG	O8-C28-C29-C30
47	BA	845	LHG	C17-C18-C19-C20
45	AB	801	CLA	C2A-CAA-CBA-CGA
45	AA	836	CLA	CAA-CBA-CGA-O1A
45	A1	313	CLA	CAA-CBA-CGA-O2A
45	BA	817	CLA	CAA-CBA-CGA-O2A
45	BB	801	CLA	CAA-CBA-CGA-O2A
45	AA	801	CLA	C11-C10-C8-C7
45	AB	810	CLA	C11-C12-C13-C15
45	AB	827	CLA	C2-C3-C5-C6
45	BA	805	CLA	C6-C7-C8-C10
45	BB	842	CLA	C11-C10-C8-C7
45	B2	612	CLA	C16-C17-C18-C19
45	B1	309	CLA	CAA-CBA-CGA-O1A
45	AA	801	CLA	C11-C10-C8-C9
45	AA	801	CLA	C14-C13-C15-C16
45	AA	806	CLA	C11-C12-C13-C14
45	AA	813	CLA	C6-C7-C8-C9
45	AA	841	CLA	C11-C10-C8-C9
45	BA	801	CLA	C14-C13-C15-C16
45	BA	803	CLA	C11-C12-C13-C14
45	BA	805	CLA	C6-C7-C8-C9
45	BB	816	CLA	C11-C12-C13-C14
46	AB	843	PQN	C21-C22-C23-C24
45	AG	201	CLA	CAA-CBA-CGA-O2A
45	B2	603	CLA	CAA-CBA-CGA-O2A
45	B5	608	CLA	CAA-CBA-CGA-O2A
45	BB	811	CLA	C5-C6-C7-C8
45	BA	801	CLA	CAA-CBA-CGA-O1A
56	BJ	104	SQD	C4-C5-C6-S
50	BA	854	LMU	C5'-C4'-O1B-C1B
47	AJ	104	LHG	C17-C18-C19-C20
47	F	801	LHG	C8-C7-O7-C5
45	AK	202	CLA	CAA-CBA-CGA-O2A
45	BB	809	CLA	C2A-CAA-CBA-CGA
45	BB	824	CLA	C2A-CAA-CBA-CGA
45	B5	602	CLA	C2A-CAA-CBA-CGA
45	BB	815	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
53	B5	617	LMG	O9-C10-C11-C12
47	AA	844	LHG	C12-C13-C14-C15
47	BF	305	LHG	C32-C33-C34-C35
45	BB	815	CLA	C2-C3-C5-C6
50	BA	854	LMU	C4-C5-C6-C7
48	BF	304	BCR	C7-C8-C9-C10
45	AA	802	CLA	C1A-C2A-CAA-CBA
45	AA	827	CLA	C1A-C2A-CAA-CBA
45	AA	829	CLA	C1A-C2A-CAA-CBA
45	AB	803	CLA	C1A-C2A-CAA-CBA
45	AB	823	CLA	C1A-C2A-CAA-CBA
45	A4	307	CLA	C1A-C2A-CAA-CBA
45	BA	814	CLA	C1A-C2A-CAA-CBA
45	BB	817	CLA	C1A-C2A-CAA-CBA
45	BB	817	CLA	CHA-CBD-CGD-O2D
45	BL	302	CLA	C1A-C2A-CAA-CBA
45	B2	604	CLA	C1A-C2A-CAA-CBA
45	B5	608	CLA	C1A-C2A-CAA-CBA
54	A1	303	CHL	C1A-C2A-CAA-CBA
54	A1	308	CHL	CHA-CBD-CGD-O2D
54	A4	304	CHL	CHA-CBD-CGD-O2D
54	B5	607	CHL	C1A-C2A-CAA-CBA
47	a	501	LHG	O7-C7-C8-C9
45	AB	820	CLA	C2-C1-O2A-CGA
47	B1	318	LHG	C27-C28-C29-C30
45	A3	302	CLA	C5-C6-C7-C8
45	BB	829	CLA	C13-C15-C16-C17
45	AA	807	CLA	O1D-CGD-O2D-CED
45	AA	833	CLA	CAA-CBA-CGA-O1A
45	BA	833	CLA	CAA-CBA-CGA-O1A
47	B5	618	LHG	O9-C7-C8-C9
54	A6	608	CHL	CAA-CBA-CGA-O1A
45	AB	842	CLA	C5-C6-C7-C8
45	AA	807	CLA	CBD-CGD-O2D-CED
45	BA	838	CLA	CAD-CBD-CGD-O2D
45	BA	829	CLA	C5-C6-C7-C8
45	BB	835	CLA	C15-C16-C17-C18
45	AA	818	CLA	O1A-CGA-O2A-C1
45	BB	835	CLA	CAA-CBA-CGA-O2A
45	AA	834	CLA	C15-C16-C17-C18
45	AB	806	CLA	CAA-CBA-CGA-O1A
45	BA	812	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
46	BB	844	PQN	C12-C13-C15-C16
45	A6	609	CLA	CAA-CBA-CGA-O2A
47	AJ	104	LHG	C3-O3-P-O5
47	A3	319	LHG	C4-O6-P-O5
47	B1	302	LHG	C4-O6-P-O5
45	AB	842	CLA	C16-C17-C18-C20
45	BA	829	CLA	C16-C17-C18-C20
45	AA	834	CLA	CAA-CBA-CGA-O1A
45	BA	806	CLA	CAA-CBA-CGA-O1A
47	BA	845	LHG	O10-C23-C24-C25
45	BB	804	CLA	CAA-CBA-CGA-O2A
48	AA	849	BCR	C1-C6-C7-C8
48	AI	101	BCR	C23-C24-C25-C30
48	AL	306	BCR	C23-C24-C25-C26
48	AL	306	BCR	C23-C24-C25-C30
48	BA	847	BCR	C23-C24-C25-C30
48	BK	204	BCR	C5-C6-C7-C8
45	AK	202	CLA	O1D-CGD-O2D-CED
45	BA	817	CLA	CAA-CBA-CGA-O1A
47	B1	302	LHG	O9-C7-C8-C9
53	A4	318	LMG	O9-C10-C11-C12
45	AA	805	CLA	CAA-CBA-CGA-O2A
47	A6	618	LHG	O8-C23-C24-C25
53	A4	318	LMG	O8-C28-C29-C30
47	B1	318	LHG	C23-C24-C25-C26
45	AA	840	CLA	C2A-CAA-CBA-CGA
45	AB	825	CLA	C2A-CAA-CBA-CGA
45	BB	815	CLA	C2A-CAA-CBA-CGA
45	AB	828	CLA	C8-C10-C11-C12
45	A1	313	CLA	CAA-CBA-CGA-O1A
45	BA	842	CLA	CAA-CBA-CGA-O2A
45	B2	602	CLA	CAA-CBA-CGA-O2A
45	BB	801	CLA	O1D-CGD-O2D-CED
51	BB	850	DGD	C1B-C2B-C3B-C4B
45	AB	834	CLA	CAA-CBA-CGA-O1A
45	BA	834	CLA	CAA-CBA-CGA-O1A
45	AA	818	CLA	CBA-CGA-O2A-C1
45	B5	608	CLA	CAA-CBA-CGA-O1A
45	AA	811	CLA	CAD-CBD-CGD-O1D
45	AA	827	CLA	CAD-CBD-CGD-O1D
45	AA	830	CLA	CAD-CBD-CGD-O1D
45	AA	840	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
45	AB	831	CLA	CAD-CBD-CGD-O1D
45	BA	803	CLA	CAD-CBD-CGD-O1D
45	BA	810	CLA	CAD-CBD-CGD-O1D
45	BA	827	CLA	CAD-CBD-CGD-O1D
45	BA	836	CLA	CAD-CBD-CGD-O1D
45	BB	807	CLA	CAD-CBD-CGD-O1D
45	BB	812	CLA	CAD-CBD-CGD-O1D
45	BG	202	CLA	CAD-CBD-CGD-O1D
45	BH	201	CLA	CAD-CBD-CGD-O1D
45	B2	610	CLA	CAD-CBD-CGD-O1D
45	B2	612	CLA	CAD-CBD-CGD-O1D
54	B2	605	CHL	CAD-CBD-CGD-O1D
56	BJ	104	SQD	O5-C5-C6-S
53	A1	321	LMG	O10-C28-C29-C30
45	BA	809	CLA	CAA-CBA-CGA-O2A
45	B5	601	CLA	CAA-CBA-CGA-O2A
45	AB	825	CLA	C11-C10-C8-C9
45	AB	827	CLA	C11-C10-C8-C9
45	A1	304	CLA	C6-C7-C8-C9
45	BA	813	CLA	C11-C12-C13-C14
45	BB	801	CLA	C14-C13-C15-C16
45	BB	824	CLA	C14-C13-C15-C16
45	BA	825	CLA	CAA-CBA-CGA-O1A
45	BA	828	CLA	CAA-CBA-CGA-O1A
45	AA	806	CLA	C3-C5-C6-C7
45	AB	819	CLA	C3-C5-C6-C7
45	AB	810	CLA	CAA-CBA-CGA-O2A
45	BA	813	CLA	CAA-CBA-CGA-O2A
53	A1	321	LMG	O7-C10-C11-C12
45	B5	602	CLA	C10-C11-C12-C13
45	AG	201	CLA	CAA-CBA-CGA-O1A
45	AA	828	CLA	C2A-CAA-CBA-CGA
45	B2	611	CLA	C2A-CAA-CBA-CGA
45	AB	807	CLA	CAA-CBA-CGA-O2A
45	AB	829	CLA	CAA-CBA-CGA-O2A
45	BB	842	CLA	C15-C16-C17-C18
56	e	301	SQD	C24-C25-C26-C27
45	AA	805	CLA	C6-C7-C8-C10
45	AA	840	CLA	C12-C13-C15-C16
45	AB	804	CLA	C11-C12-C13-C15
45	AB	823	CLA	C3A-C2A-CAA-CBA
45	AB	825	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
45	AB	835	CLA	C3A-C2A-CAA-CBA
45	A1	309	CLA	CHA-CBD-CGD-O1D
45	A3	305	CLA	CAD-CBD-CGD-O2D
45	A3	312	CLA	CHA-CBD-CGD-O1D
45	A3	313	CLA	CHA-CBD-CGD-O1D
45	A4	310	CLA	CHA-CBD-CGD-O1D
45	A4	310	CLA	CAD-CBD-CGD-O2D
45	A6	604	CLA	CAD-CBD-CGD-O2D
45	BB	805	CLA	C11-C10-C8-C7
45	BB	810	CLA	C11-C12-C13-C15
45	BB	812	CLA	C3A-C2A-CAA-CBA
45	BB	817	CLA	CHA-CBD-CGD-O1D
45	BB	817	CLA	CAD-CBD-CGD-O2D
45	B1	310	CLA	CHA-CBD-CGD-O1D
45	B1	310	CLA	CAD-CBD-CGD-O2D
45	B2	603	CLA	CHA-CBD-CGD-O1D
45	B3	303	CLA	CAD-CBD-CGD-O2D
45	B5	611	CLA	CAD-CBD-CGD-O2D
47	A1	301	LHG	O6-C4-C5-O7
54	A1	308	CHL	CAD-CBD-CGD-O2D
54	B5	605	CHL	CHA-CBD-CGD-O1D
47	A1	302	LHG	O10-C23-C24-C25
45	BL	302	CLA	CAA-CBA-CGA-O1A
45	AA	817	CLA	O1D-CGD-O2D-CED
45	AA	812	CLA	CAA-CBA-CGA-O2A
45	AA	828	CLA	CAA-CBA-CGA-O2A
45	AA	841	CLA	CAA-CBA-CGA-O2A
45	AA	842	CLA	CAA-CBA-CGA-O2A
45	AB	801	CLA	CAA-CBA-CGA-O2A
45	BB	809	CLA	CAA-CBA-CGA-O2A
47	B5	618	LHG	O8-C23-C24-C25
47	a	501	LHG	O8-C23-C24-C25
45	AB	809	CLA	C15-C16-C17-C18
45	AA	827	CLA	CAA-CBA-CGA-O1A
45	A3	312	CLA	CAA-CBA-CGA-O1A
45	BA	813	CLA	CAA-CBA-CGA-O1A
45	BB	809	CLA	CAA-CBA-CGA-O1A
47	B5	618	LHG	O10-C23-C24-C25
45	BL	302	CLA	CAA-CBA-CGA-O2A
45	AA	809	CLA	CAA-CBA-CGA-O2A
45	A3	312	CLA	CAA-CBA-CGA-O2A
45	BA	821	CLA	CAA-CBA-CGA-O2A

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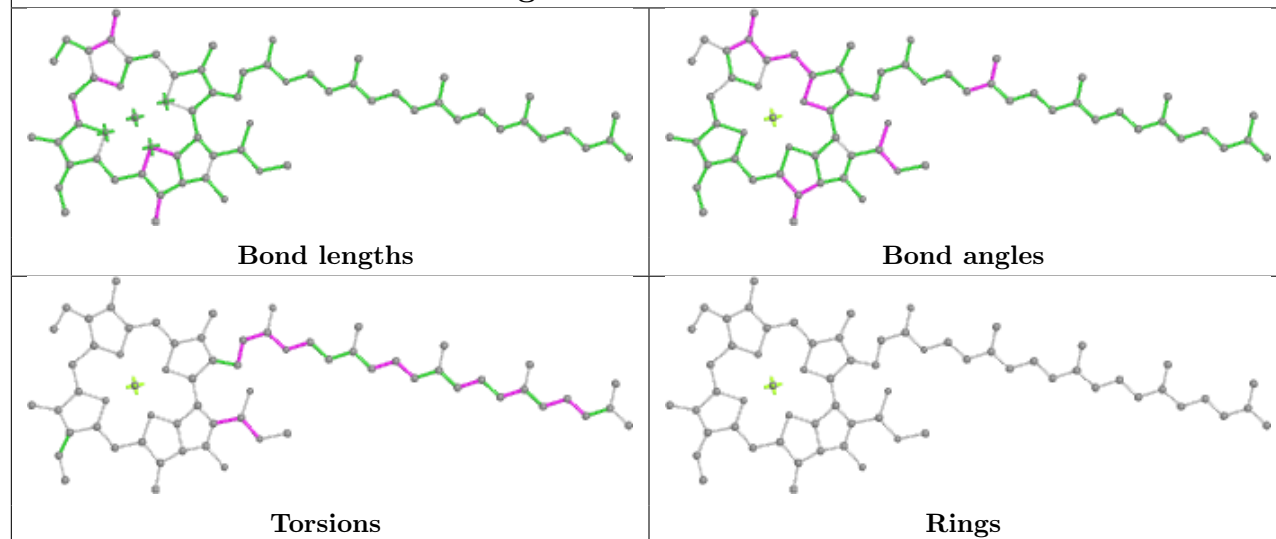
Mol	Chain	Res	Type	Atoms
47	BA	846	LHG	O7-C7-C8-C9
45	AA	802	CLA	C8-C10-C11-C12
45	AA	842	CLA	C8-C10-C11-C12
45	AB	832	CLA	C10-C11-C12-C13
45	B5	602	CLA	C8-C10-C11-C12
47	A1	301	LHG	O9-C7-O7-C5
45	AA	812	CLA	CAA-CBA-CGA-O1A
45	AB	807	CLA	CAA-CBA-CGA-O1A
45	AB	810	CLA	CAA-CBA-CGA-O1A
45	BA	809	CLA	CAA-CBA-CGA-O1A
45	BB	801	CLA	CAA-CBA-CGA-O1A
45	BB	835	CLA	CAA-CBA-CGA-O1A
45	AA	819	CLA	C5-C6-C7-C8
45	BB	802	CLA	C13-C15-C16-C17
45	BB	811	CLA	C15-C16-C17-C18
50	AB	853	LMU	C2B-C1B-O1B-C4'
47	BA	845	LHG	O7-C7-C8-C9
45	AB	830	CLA	C2A-CAA-CBA-CGA
53	A1	321	LMG	C14-C15-C16-C17
45	BB	810	CLA	C4-C3-C5-C6
47	AA	844	LHG	O7-C7-C8-C9
45	B5	604	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

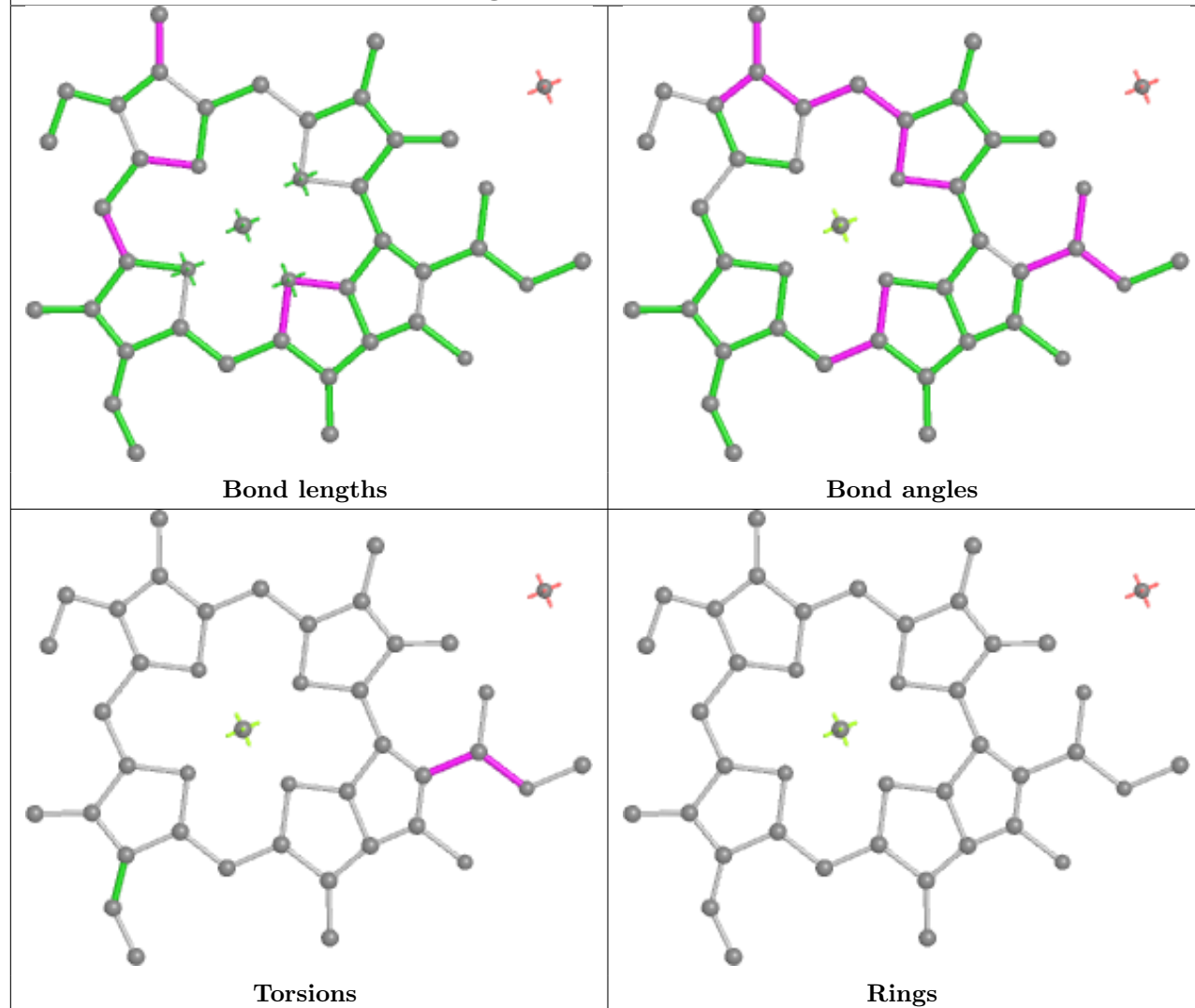
No monomer is involved in short contacts.

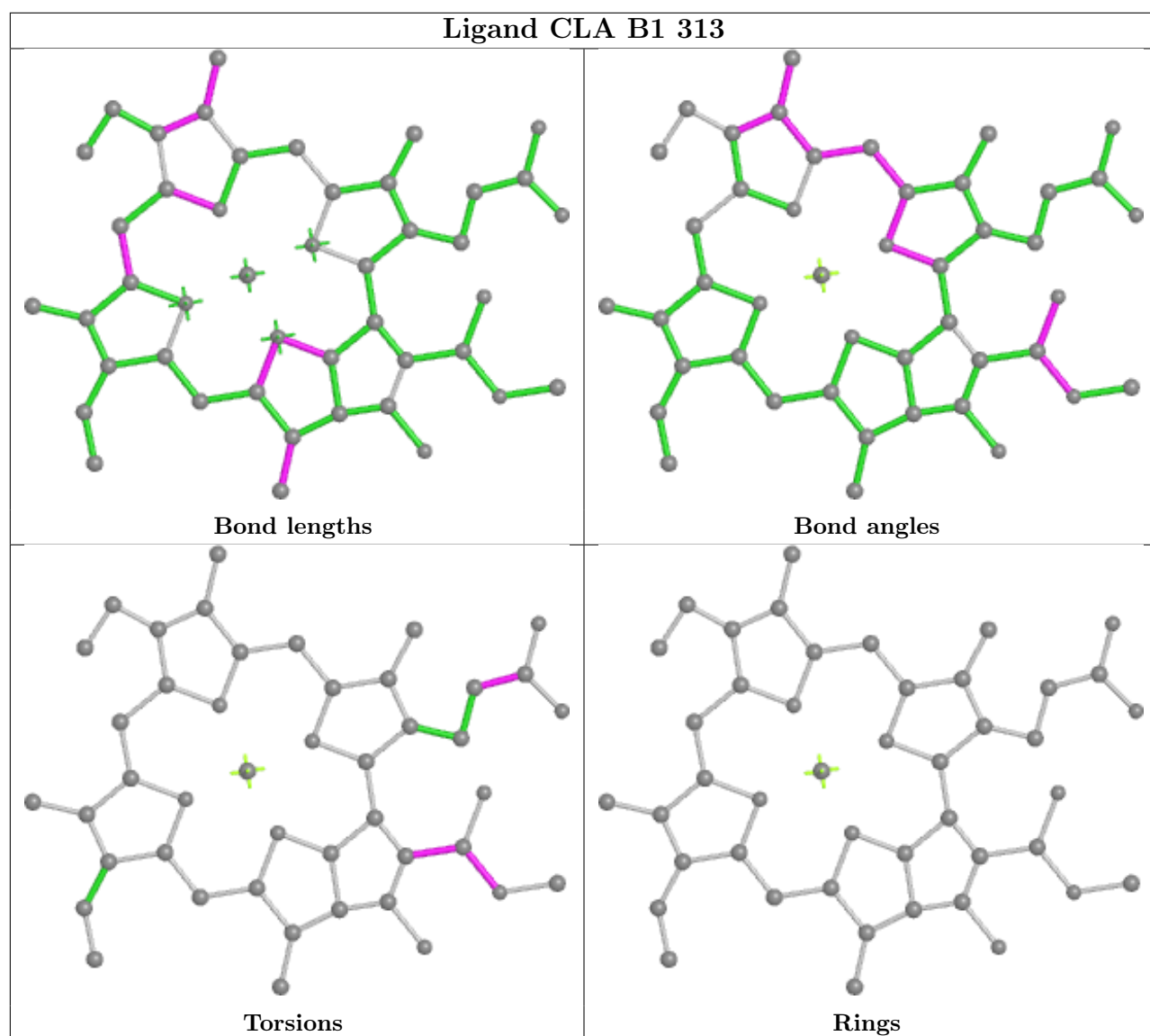
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 AA 833

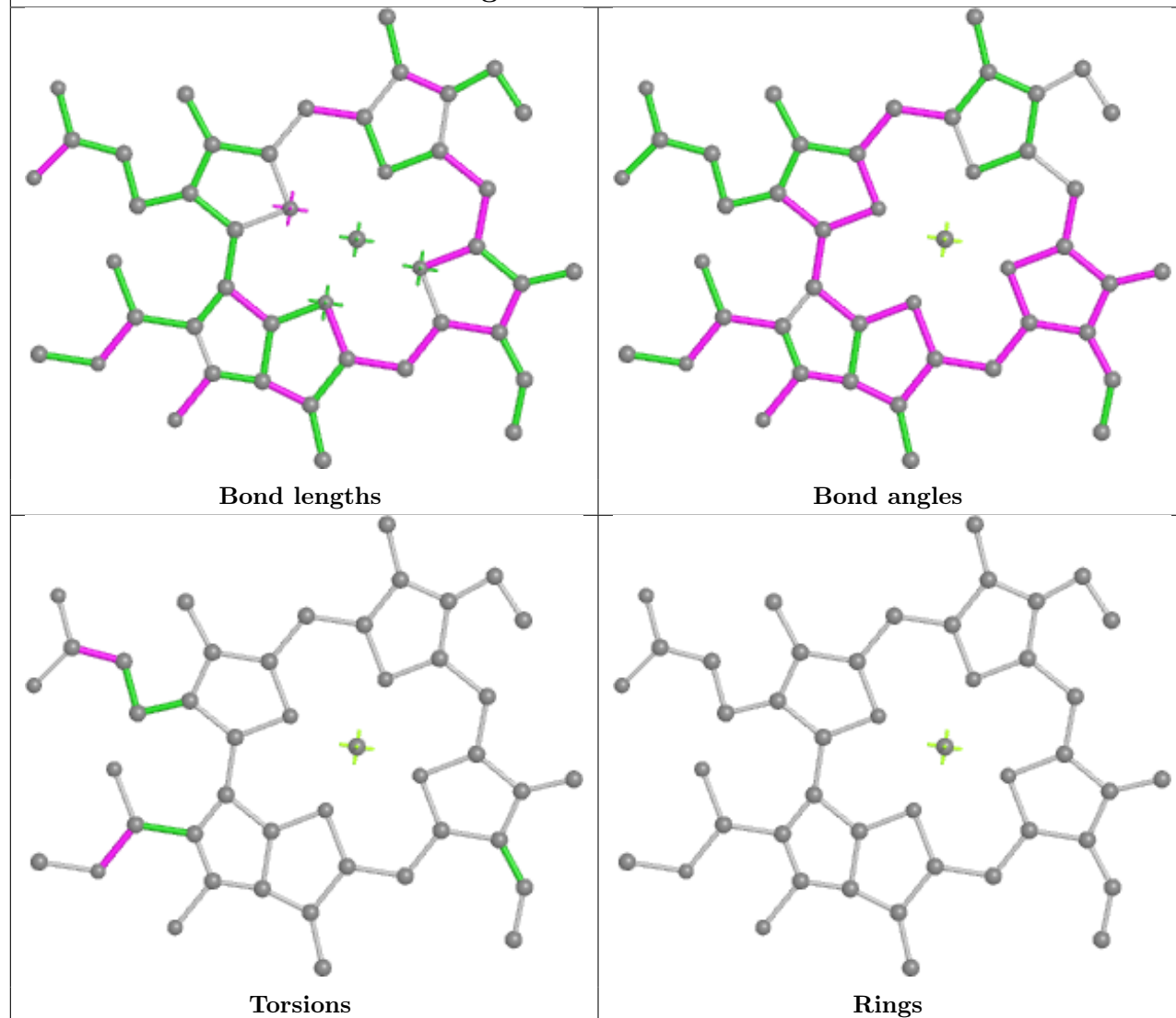


Ligand CLA BA 844

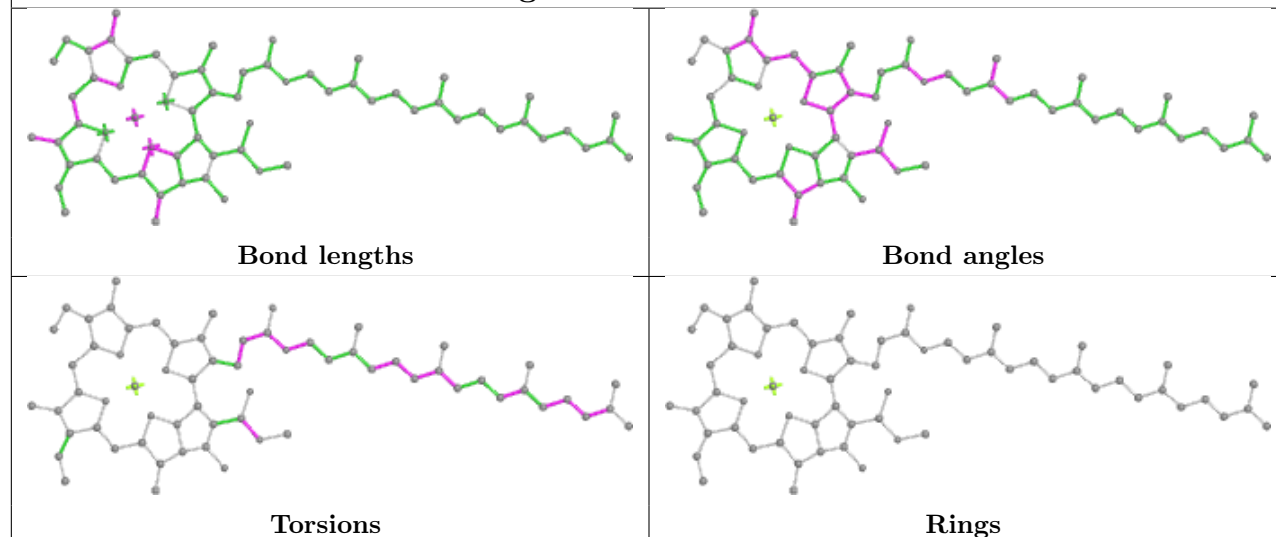


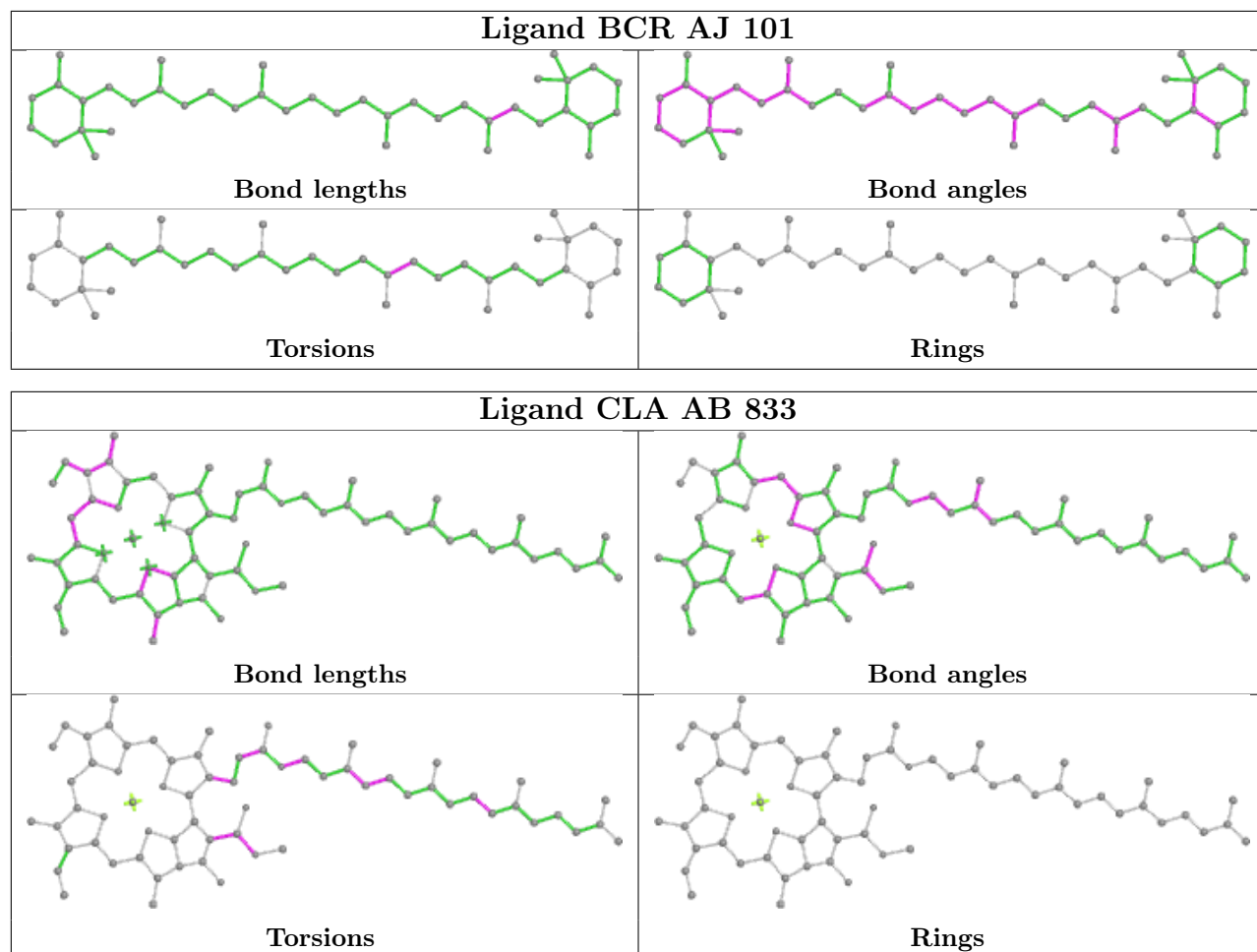


Ligand CHL A3 307

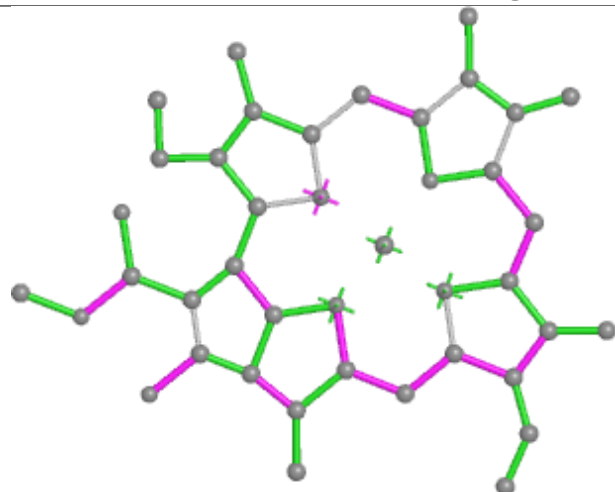


Ligand CLA AB 801

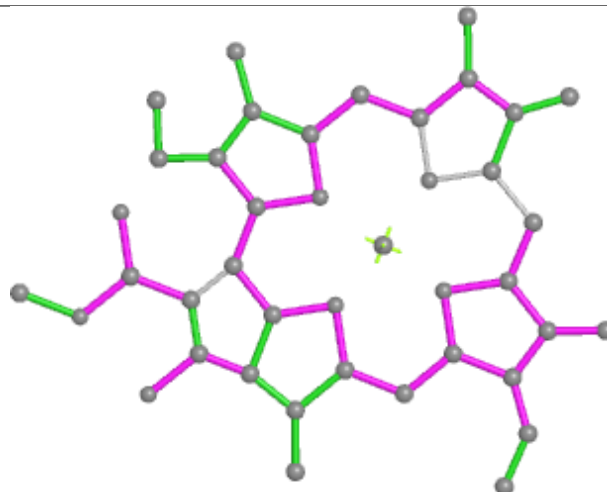




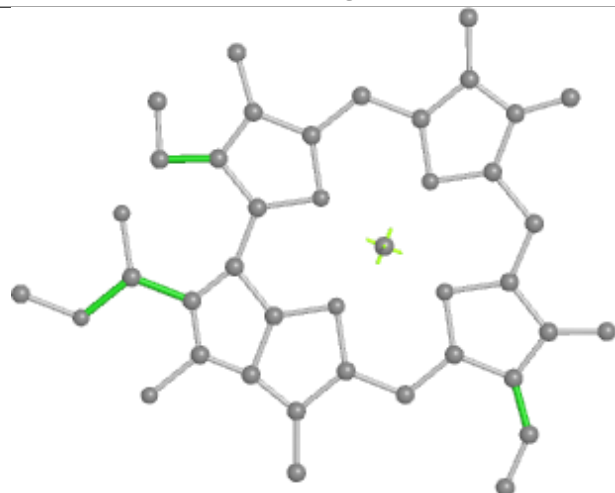
Ligand CHL A4 305



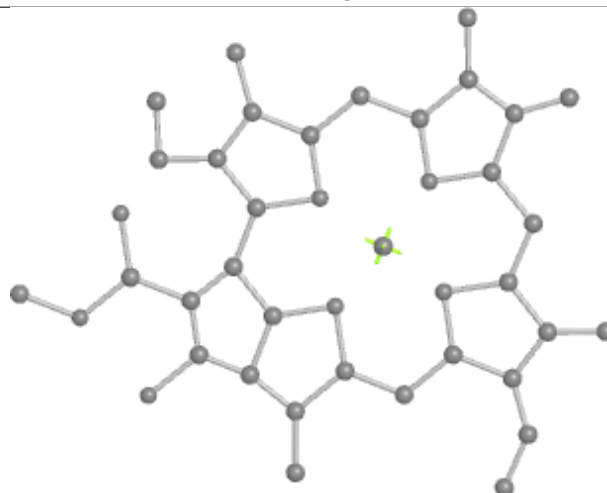
Bond lengths



Bond angles

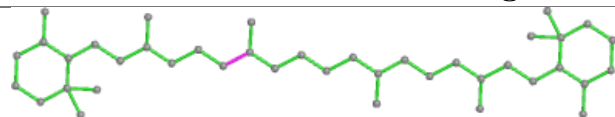


Torsions

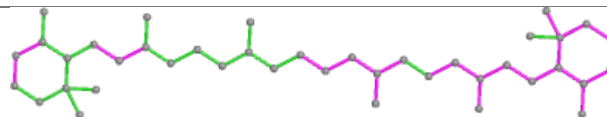


Rings

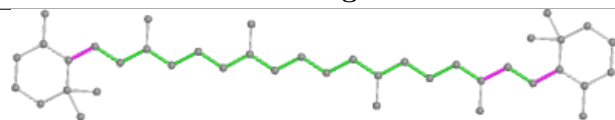
Ligand BCR BA 856



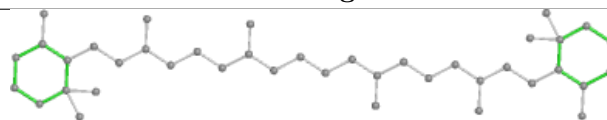
Bond lengths



Bond angles

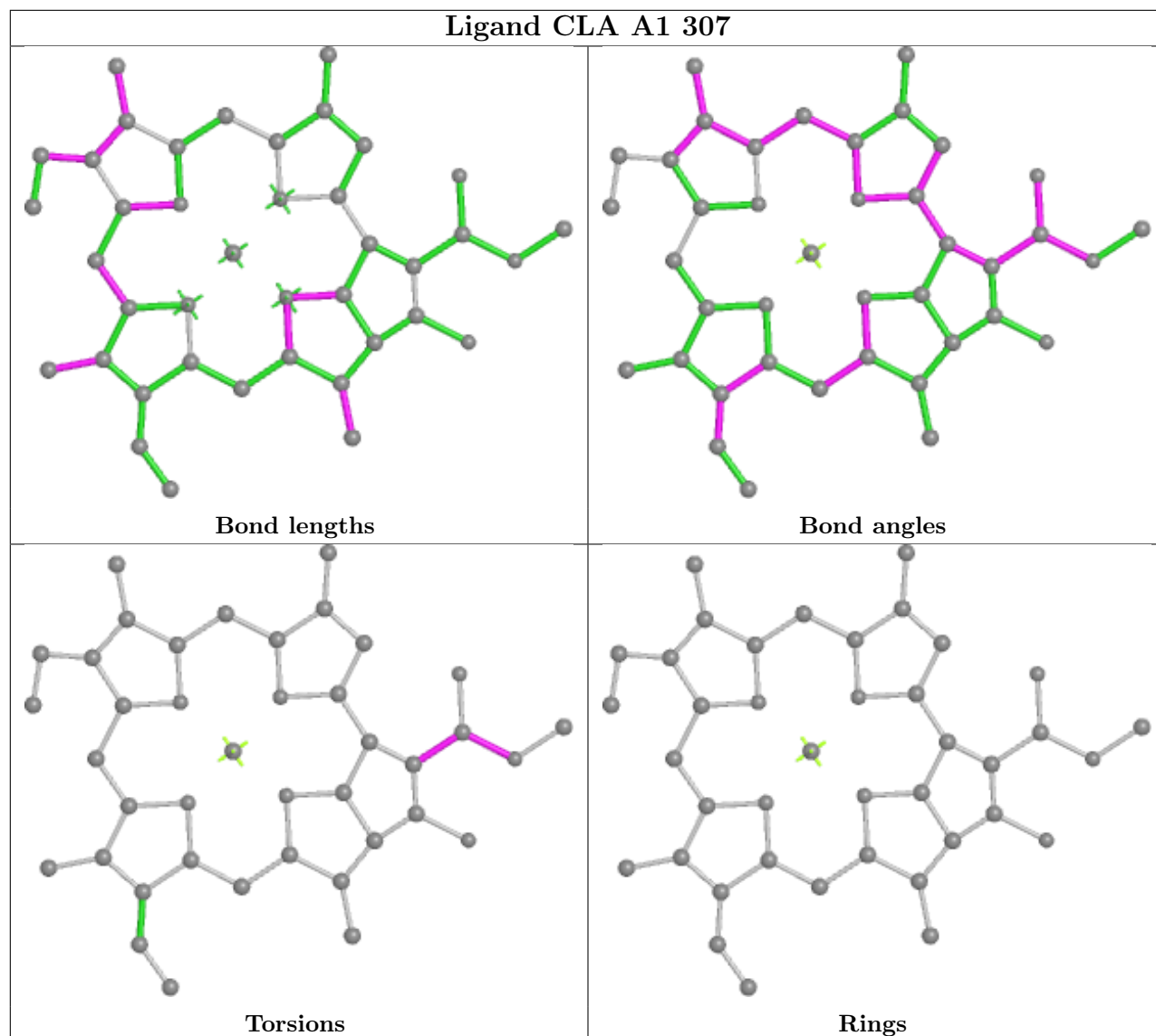


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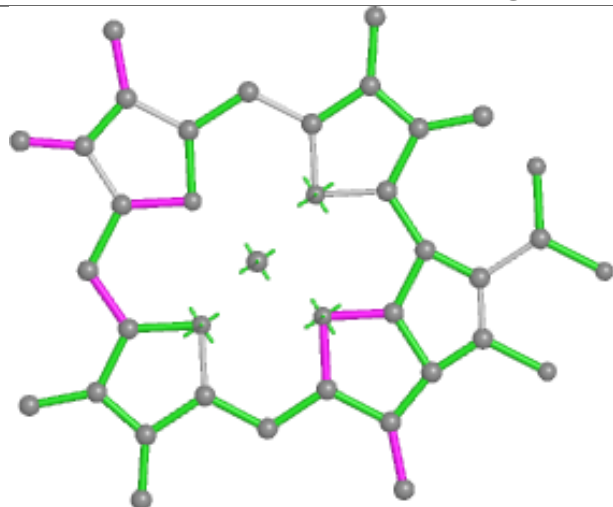


Rings

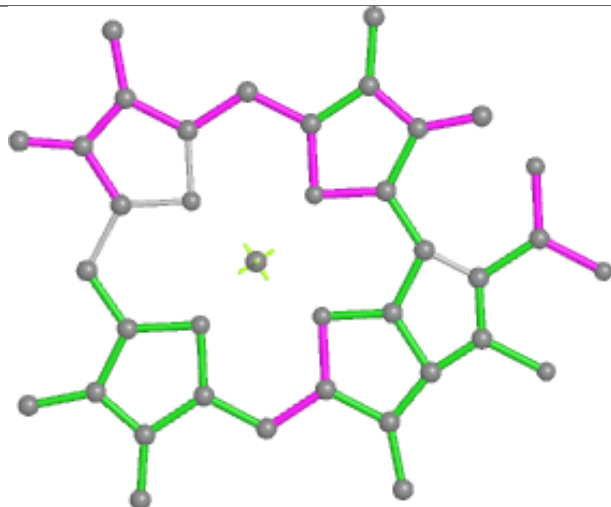
Ligand CLA A1 307



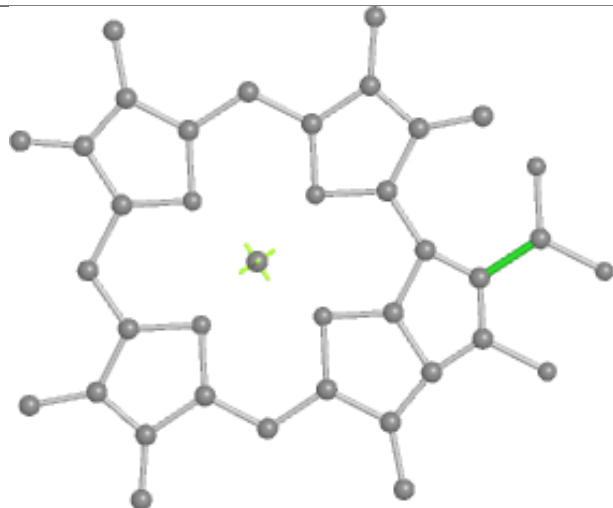
Ligand CLA A1 312



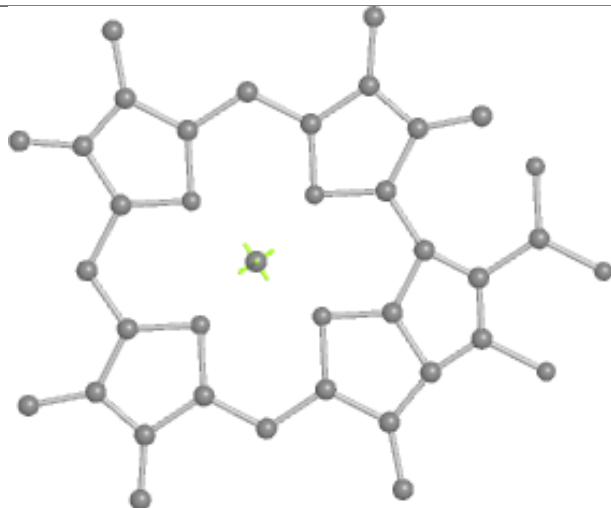
Bond lengths



Bond angles

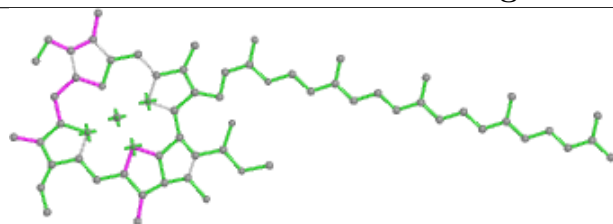


Torsions

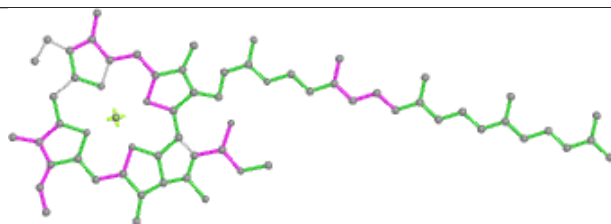


Rings

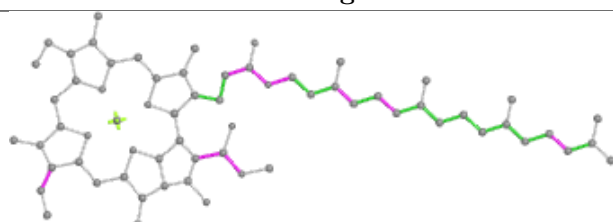
Ligand CLA AA 834



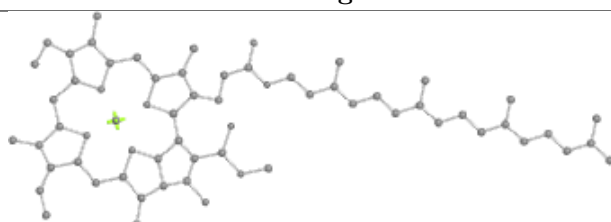
Bond lengths



Bond angles

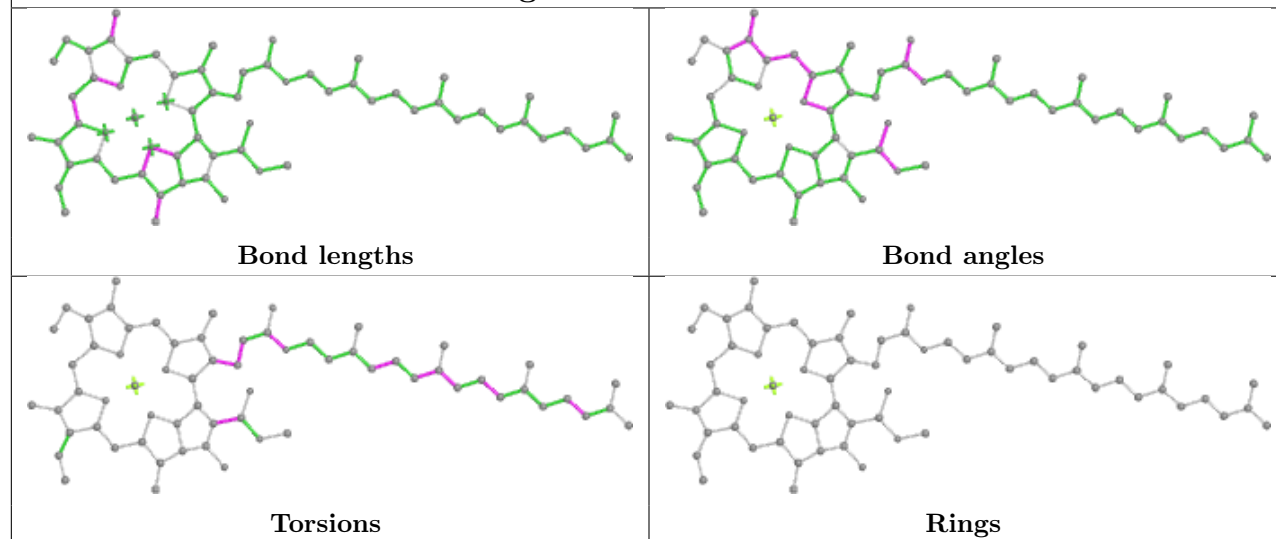


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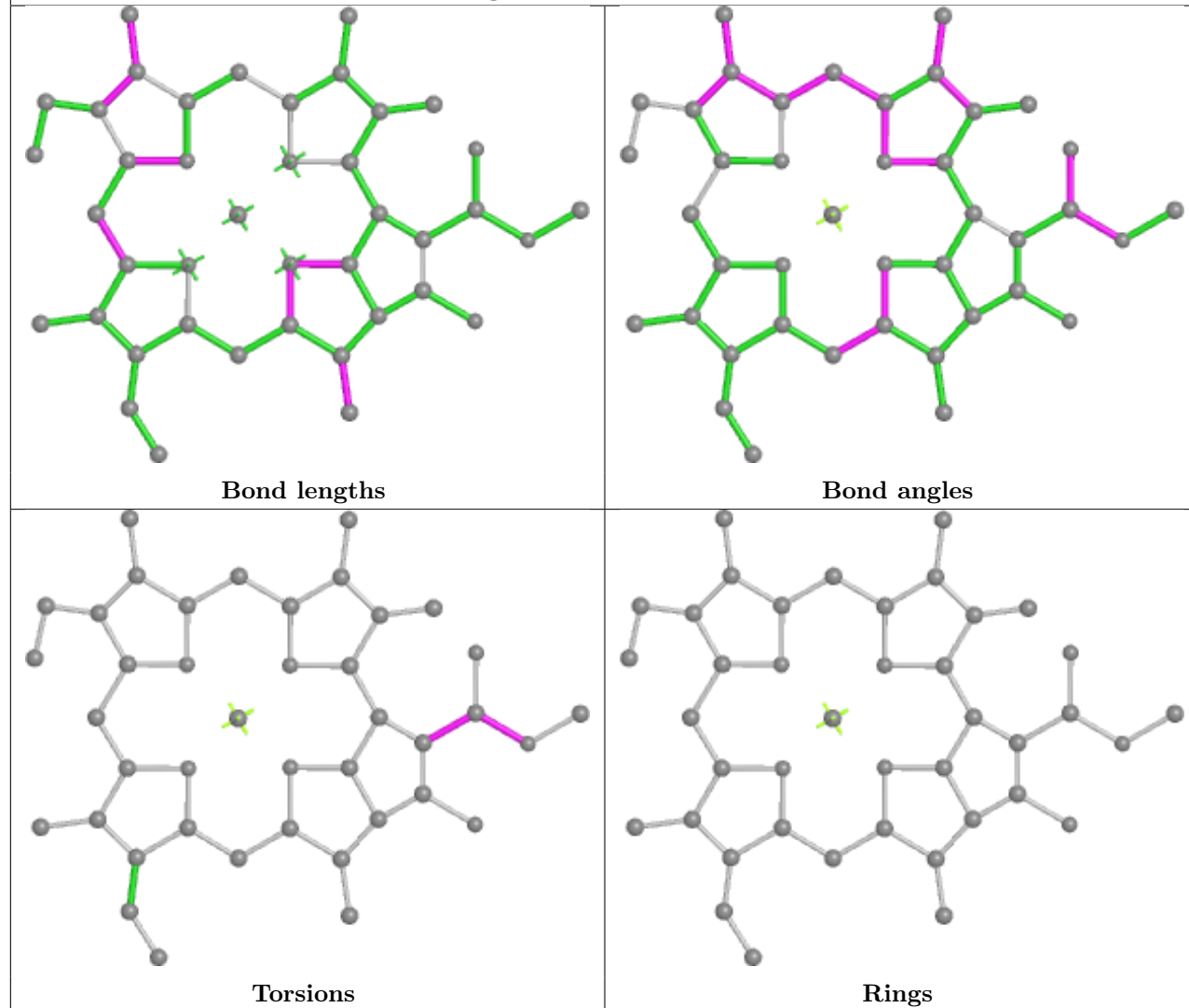


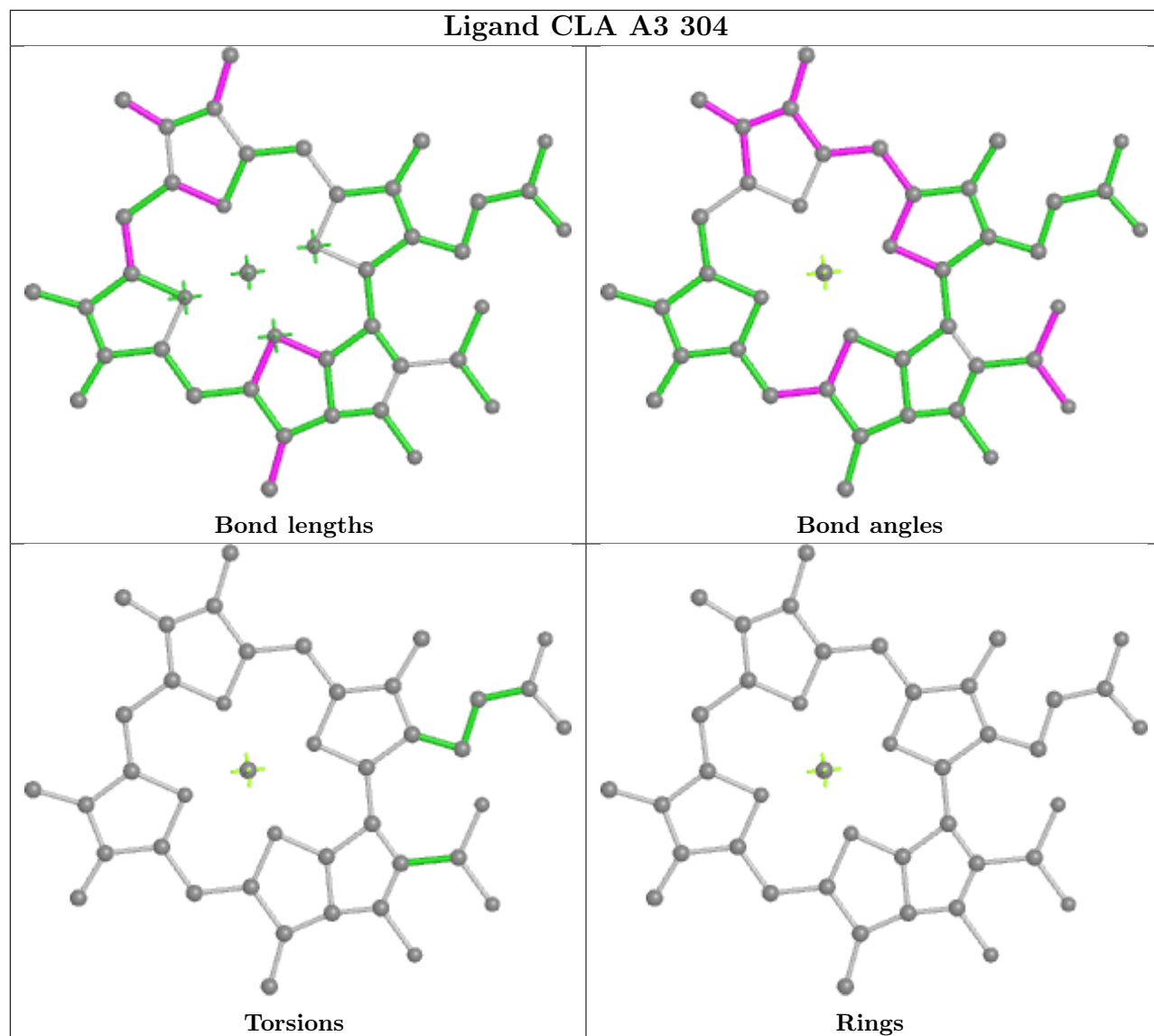
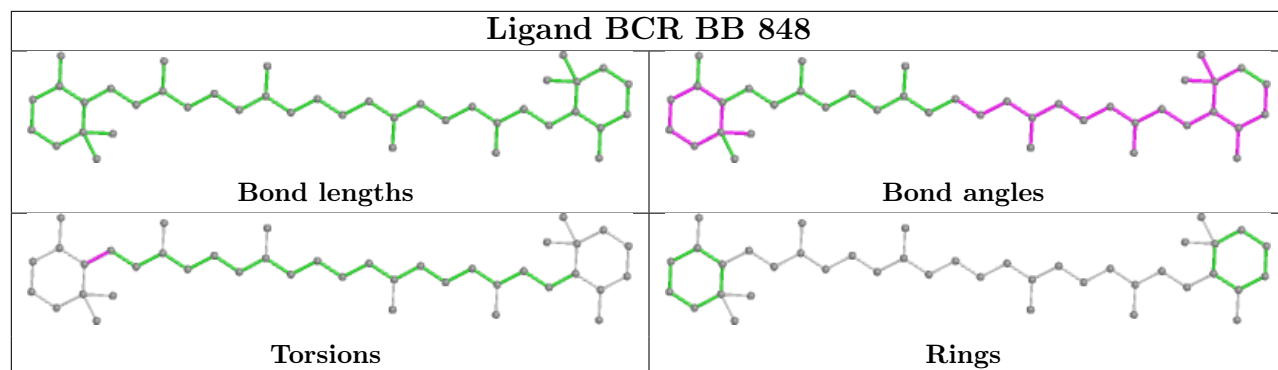
Rings

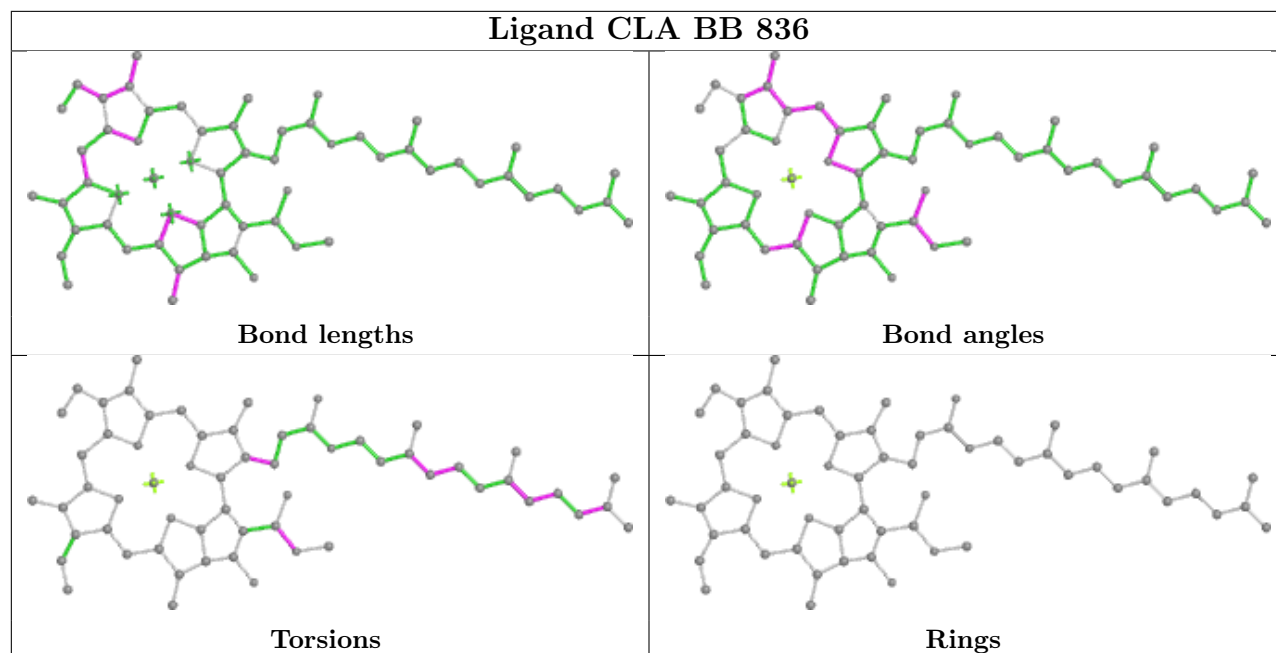
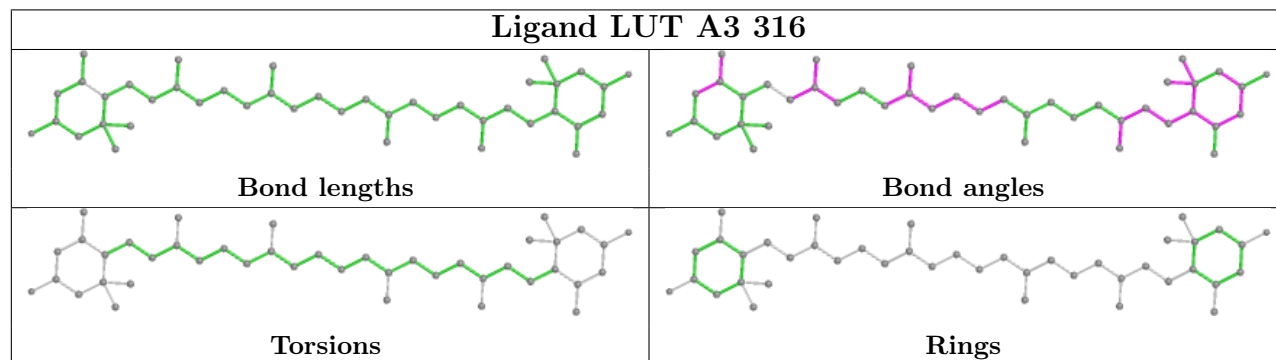
Ligand CLA BA 827

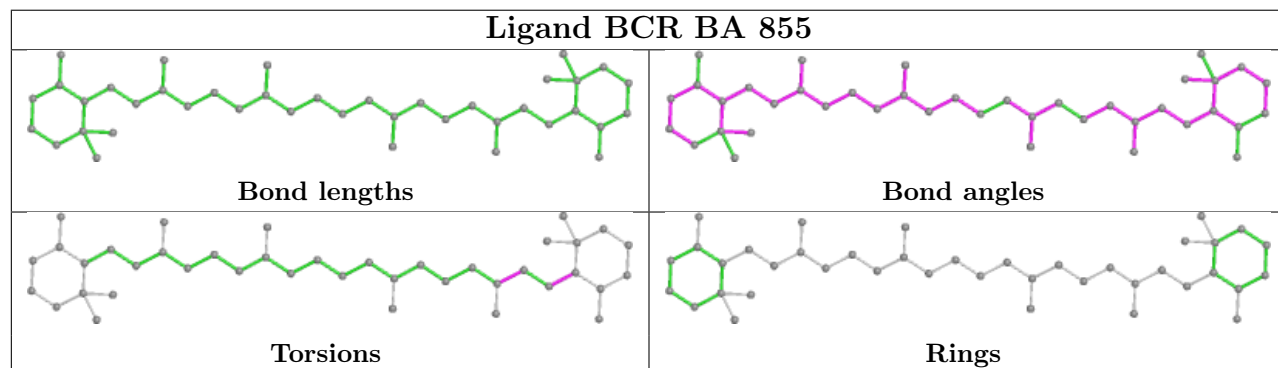
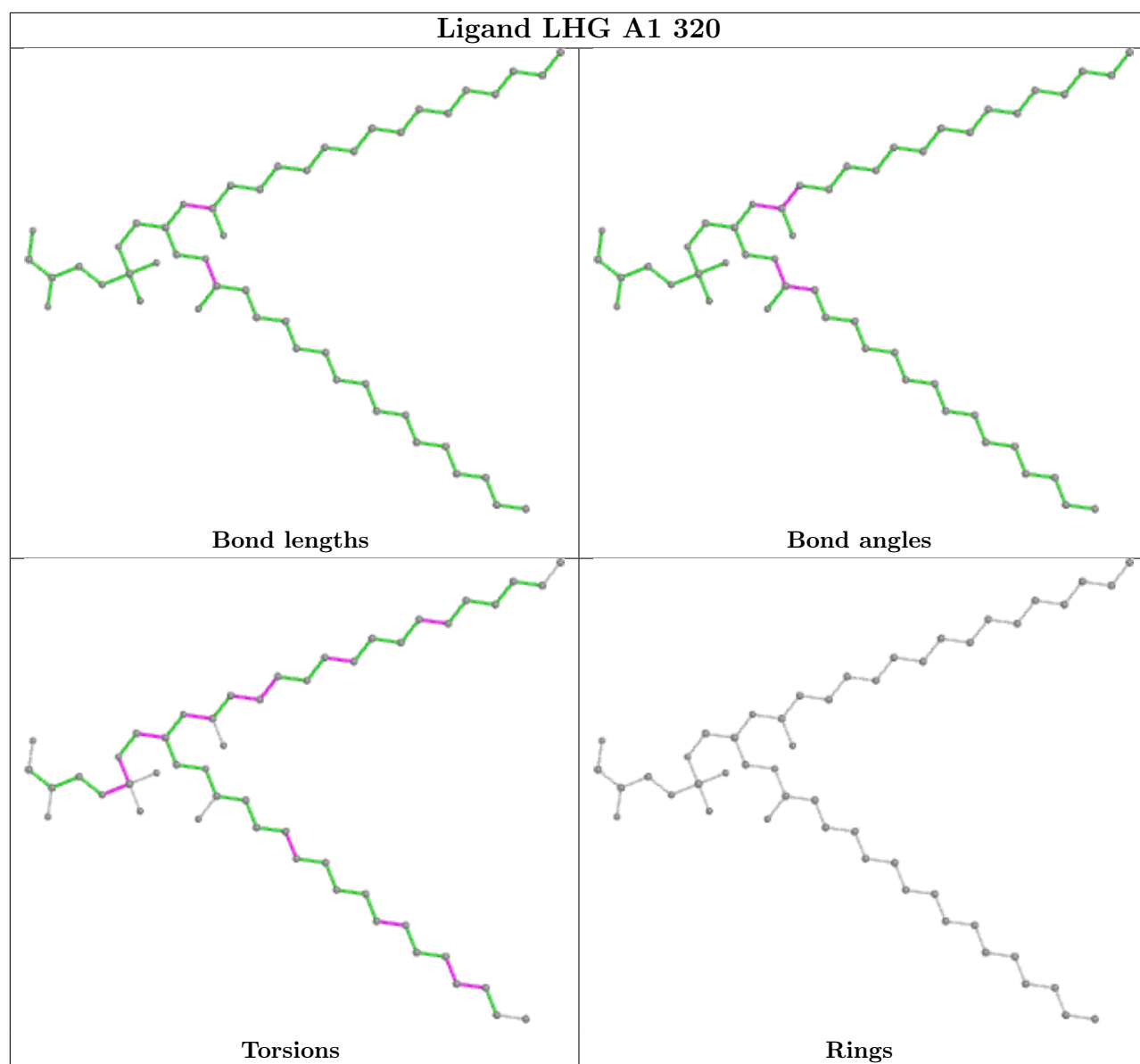


Ligand CLA AL 303

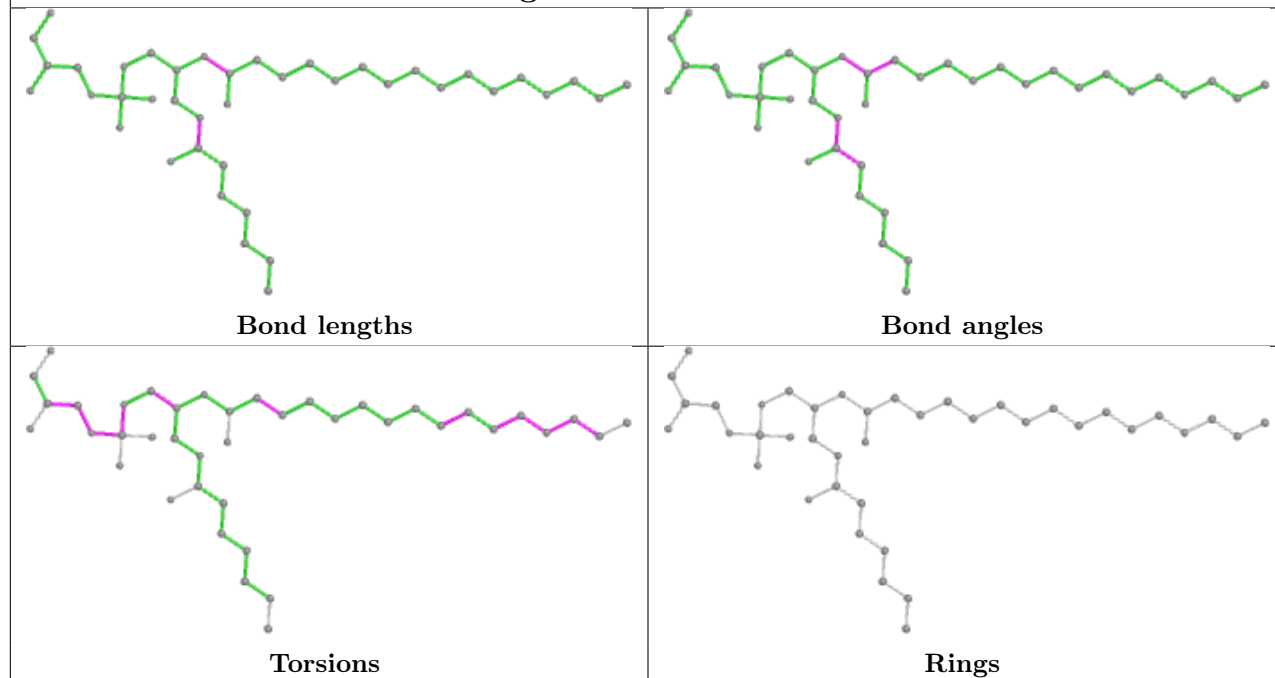




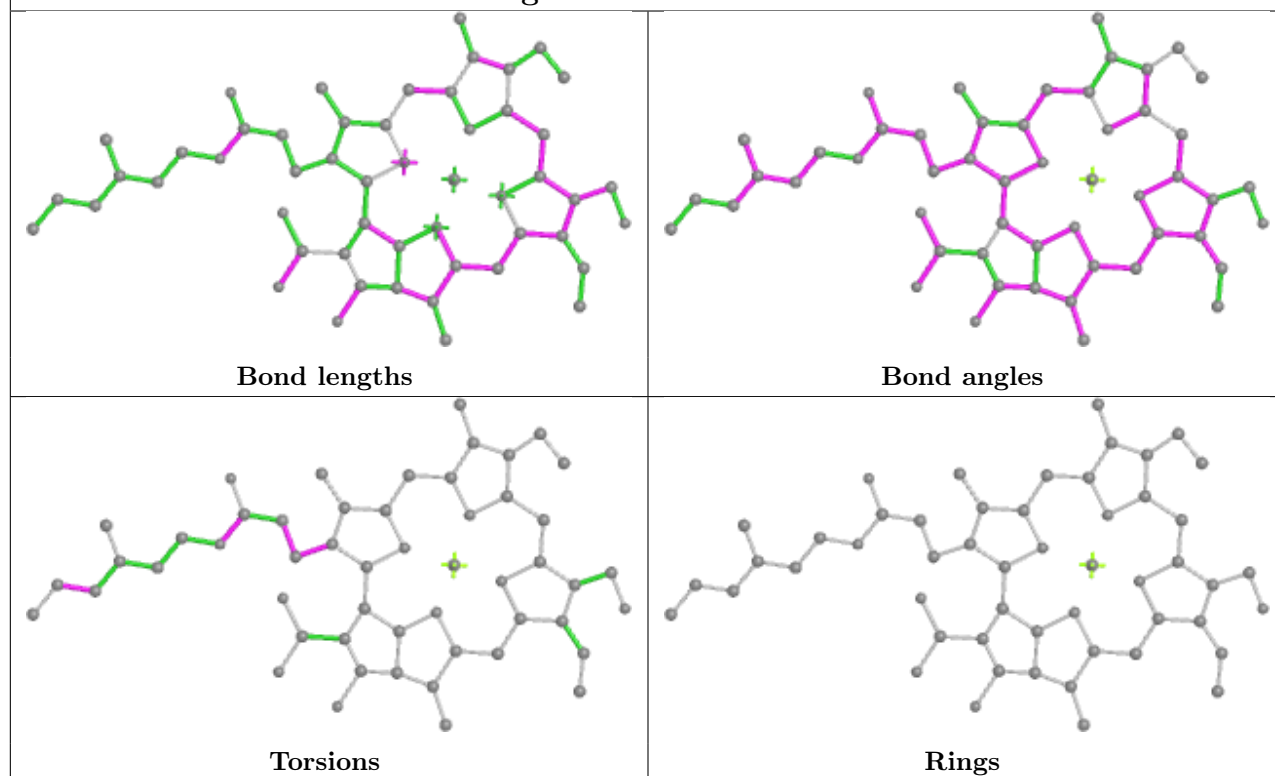
Ligand CLA BB 836**Ligand LUT A3 316**



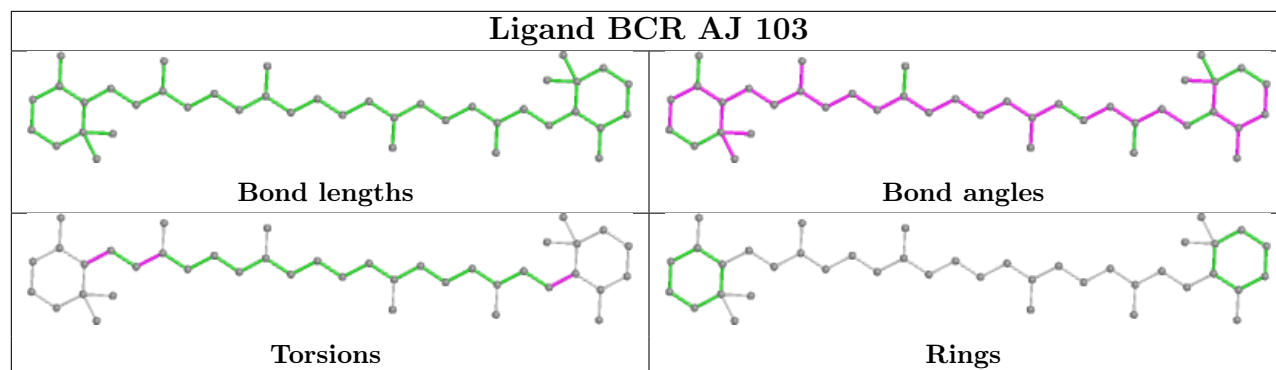
Ligand LHG AJ 104



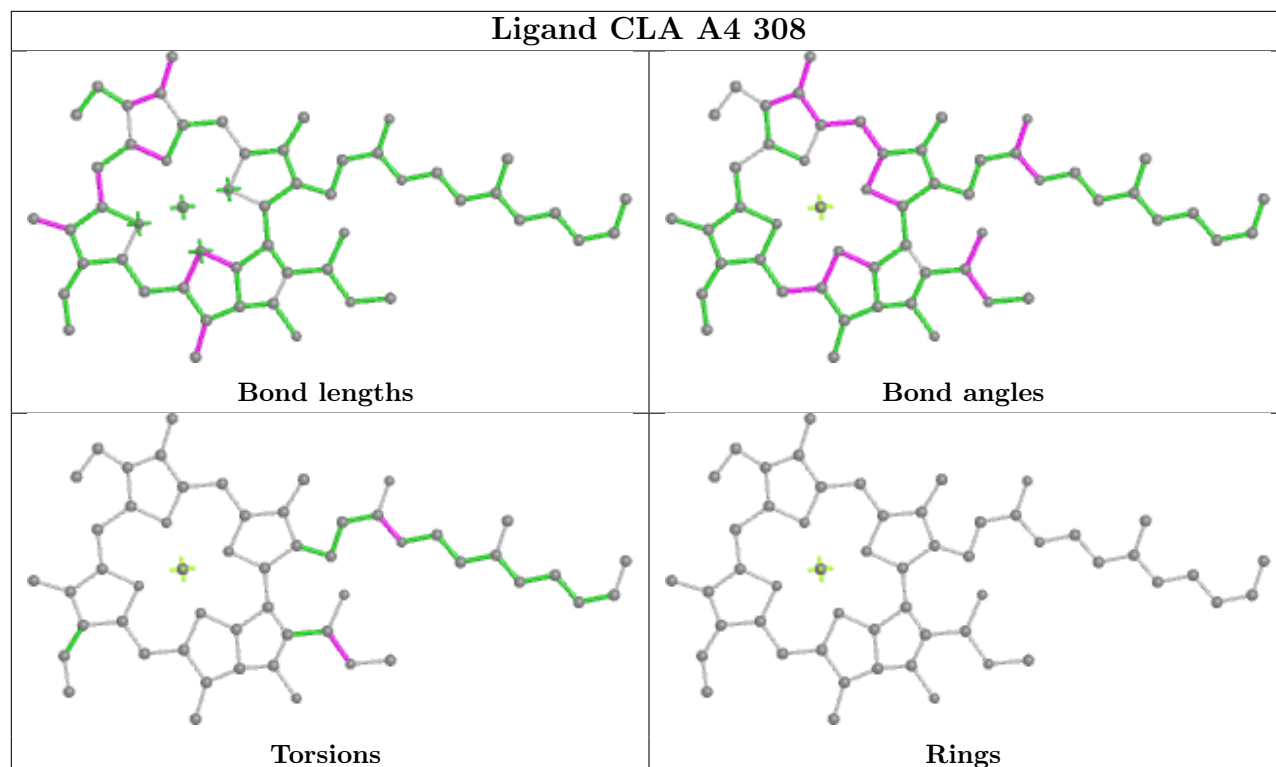
Ligand CHL A6 602



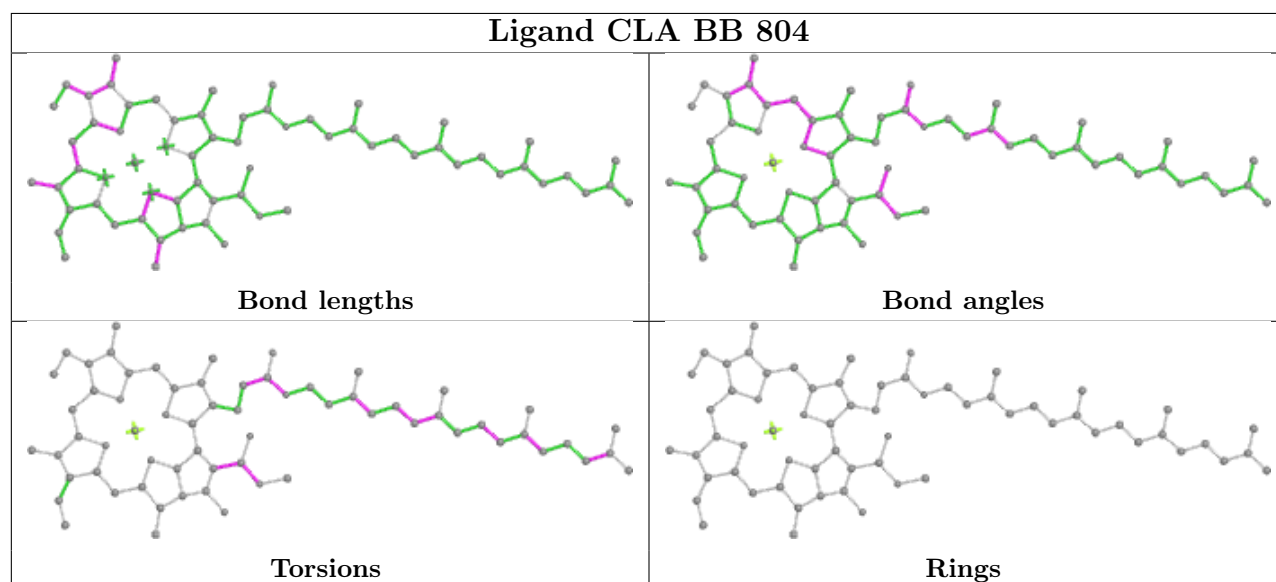
Ligand BCR AJ 103



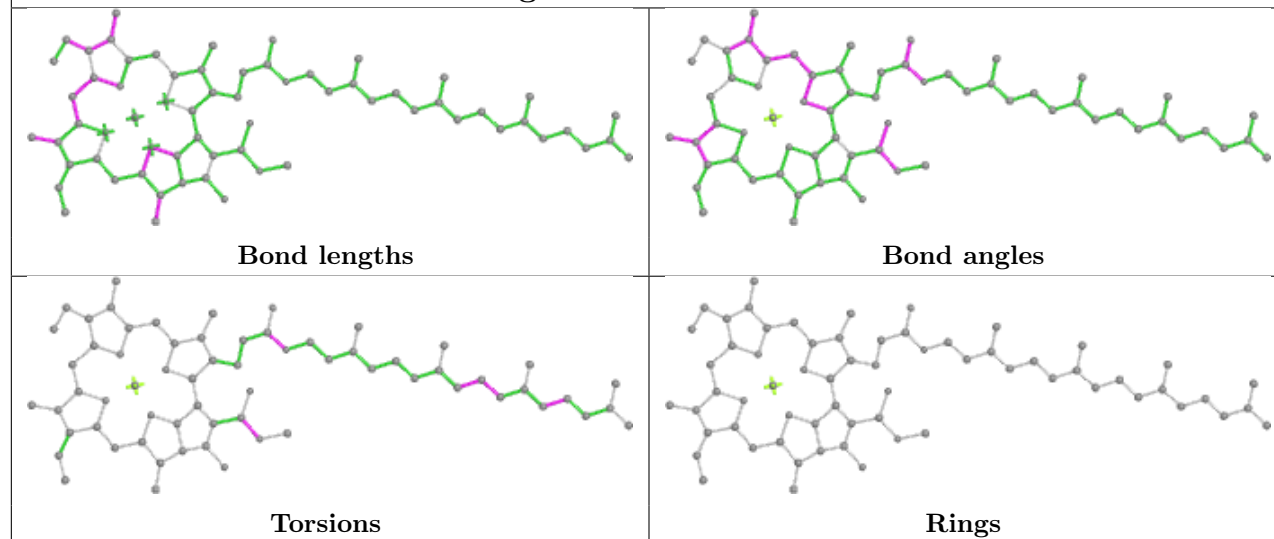
Ligand CLA A4 308



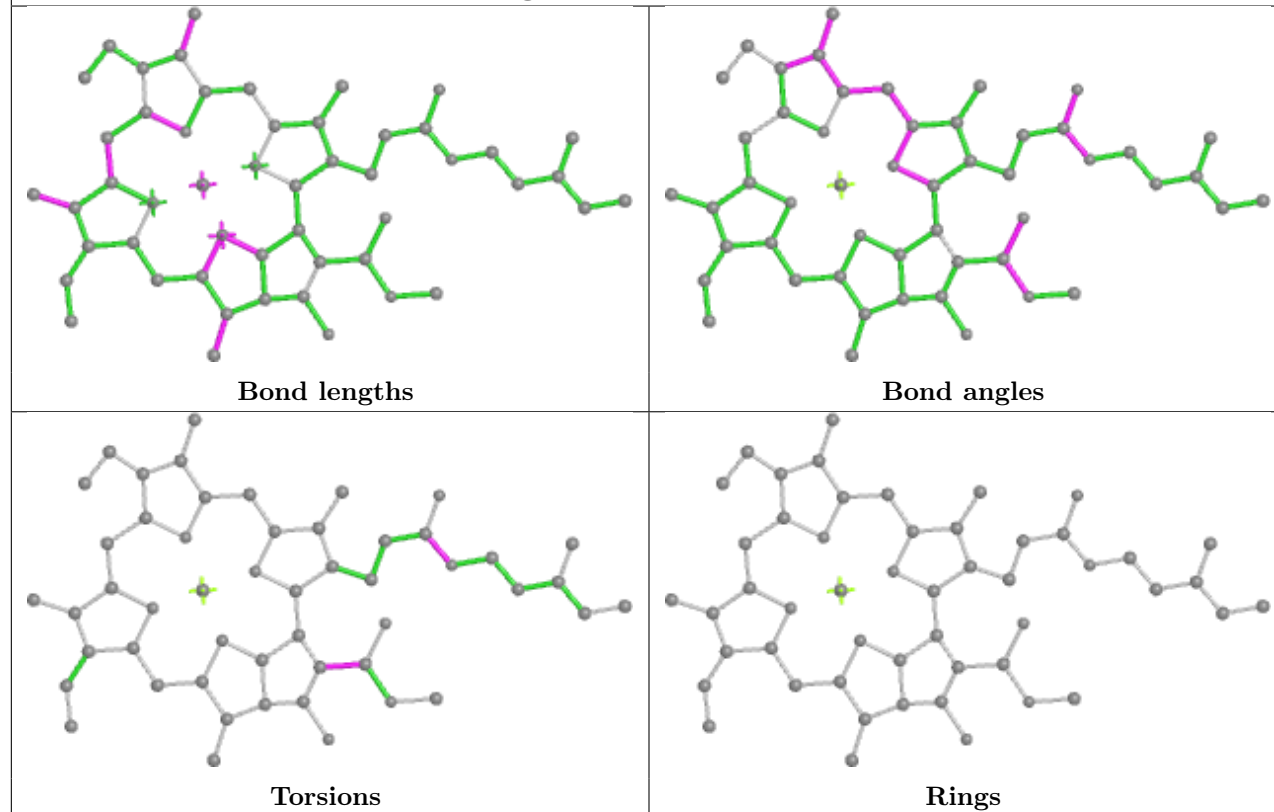
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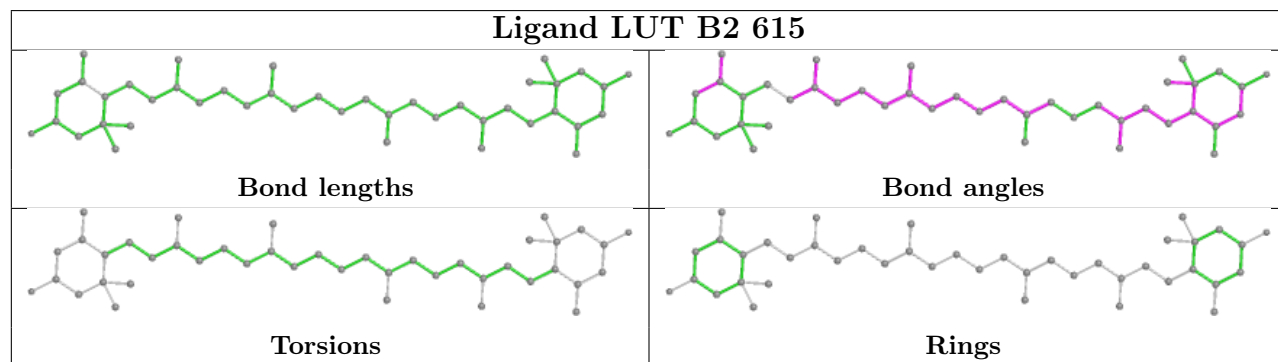
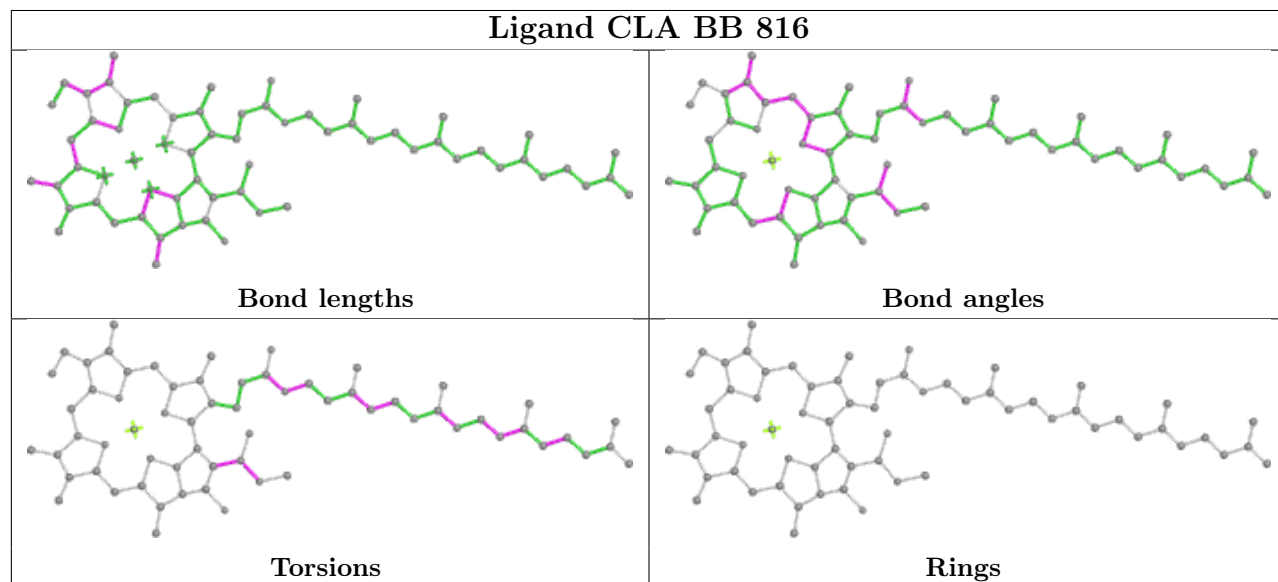
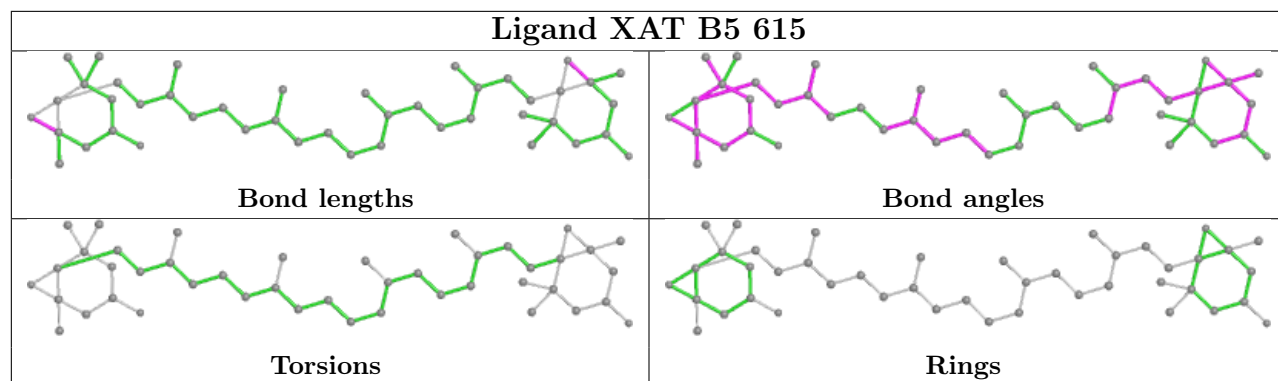


Ligand CLA AB 832

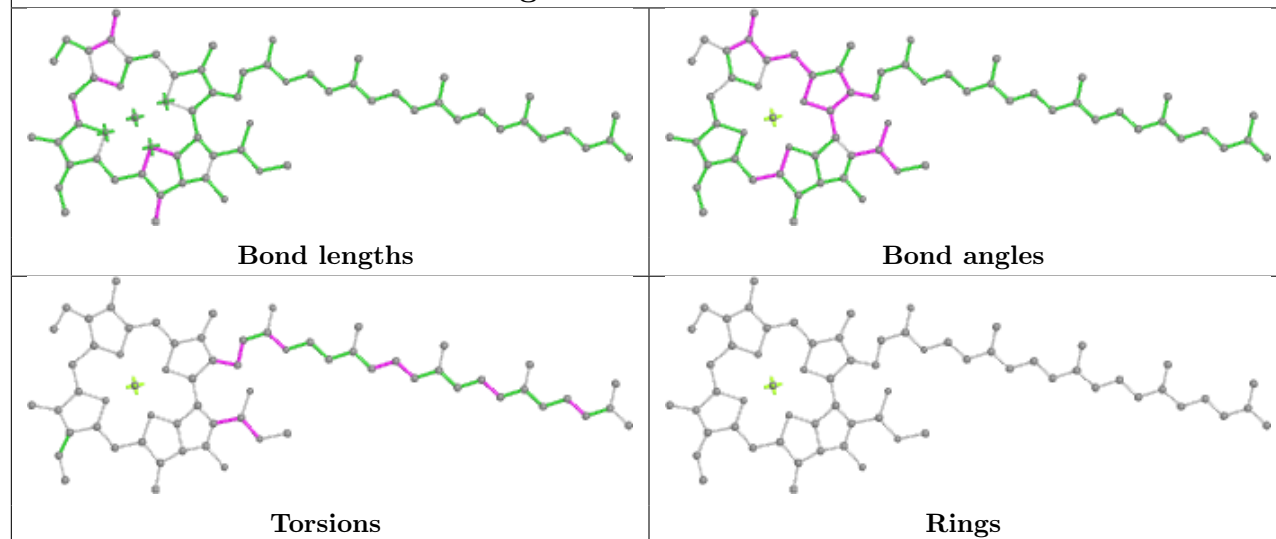


Ligand CLA BA 837

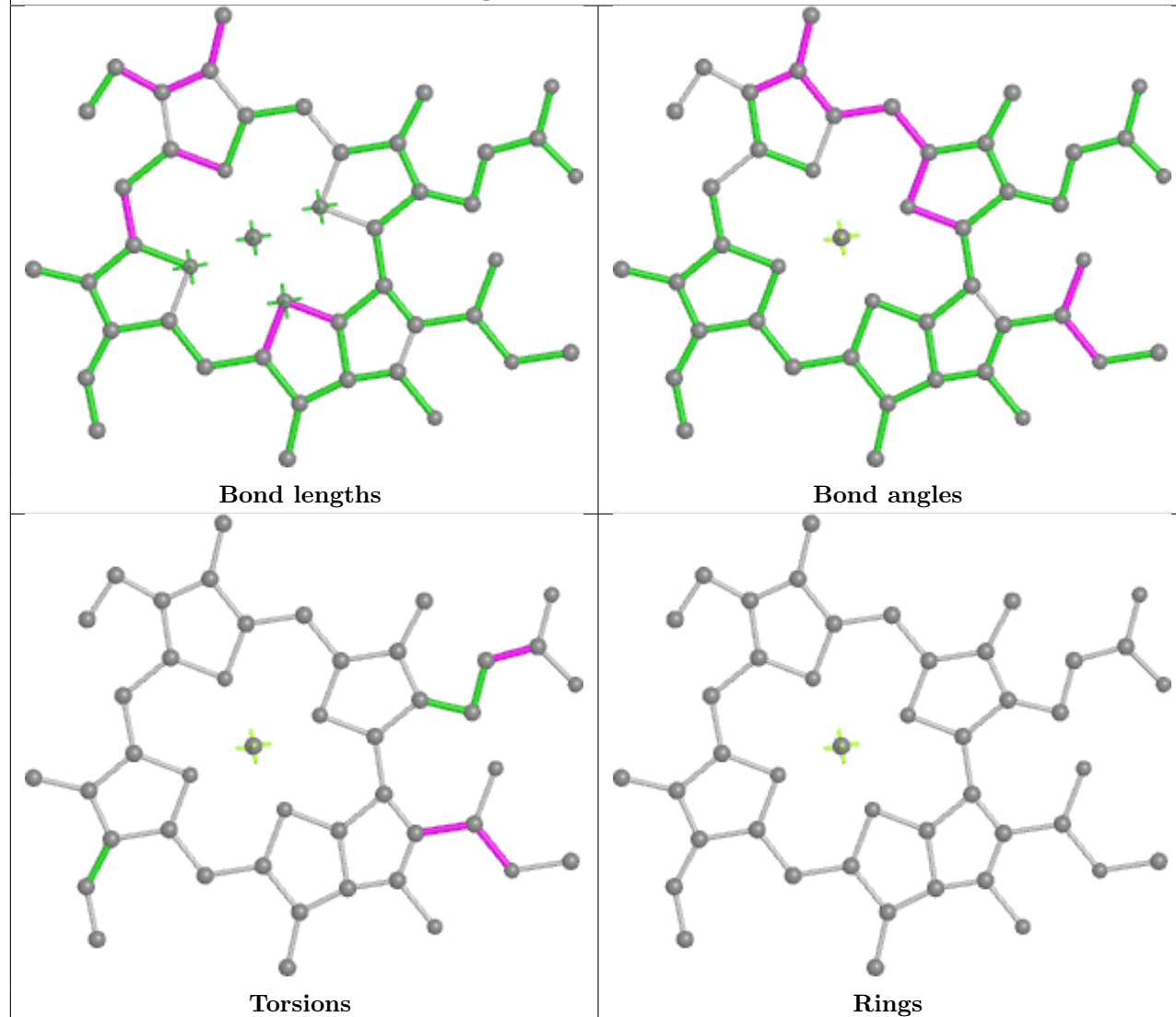




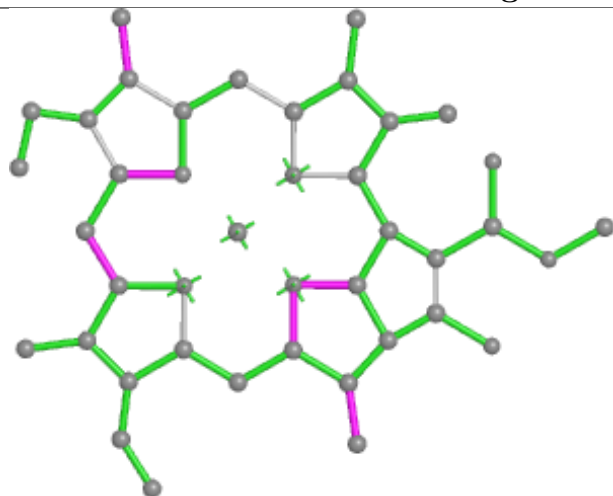
Ligand CLA BB 812



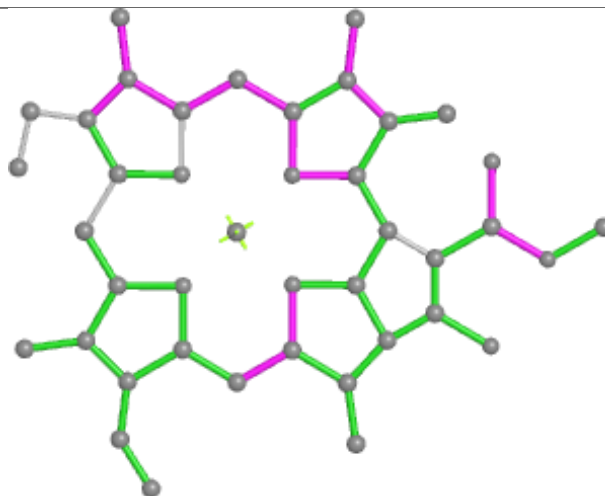
Ligand CLA BA 835



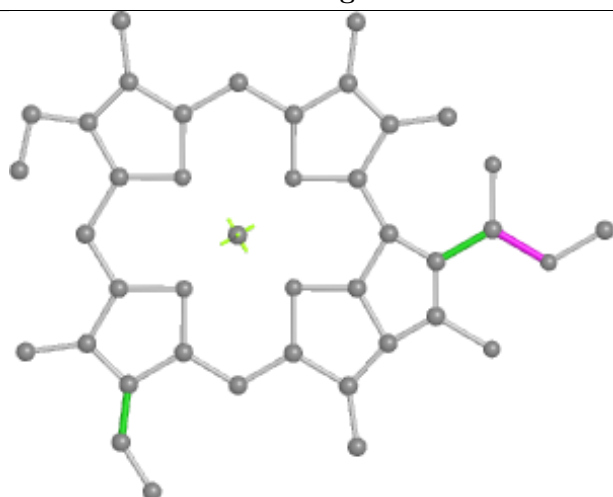
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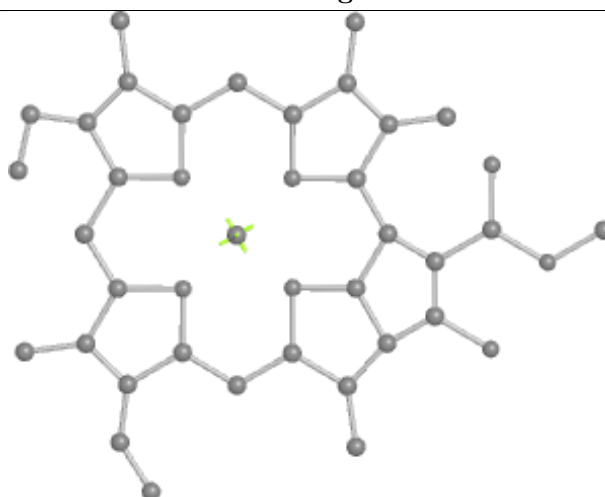
Bond lengths



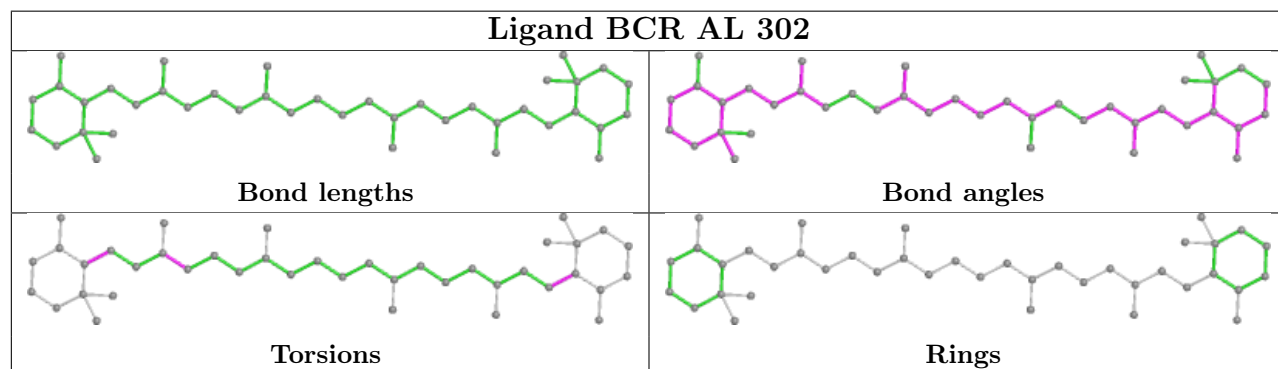
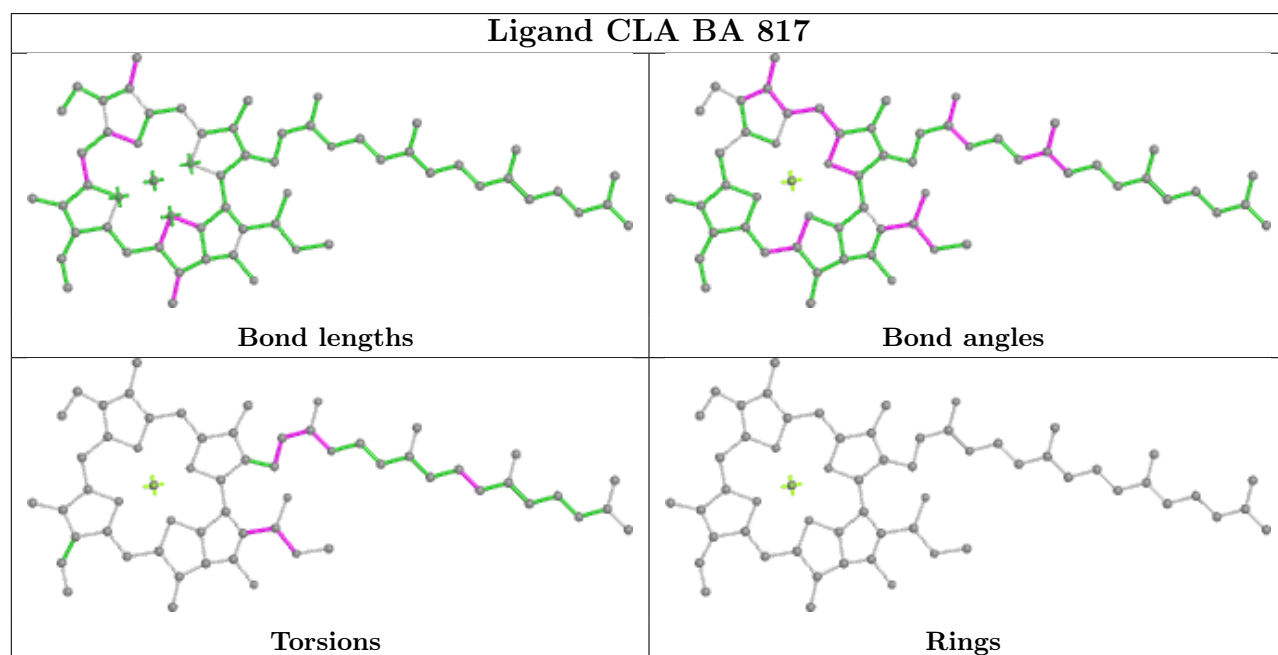
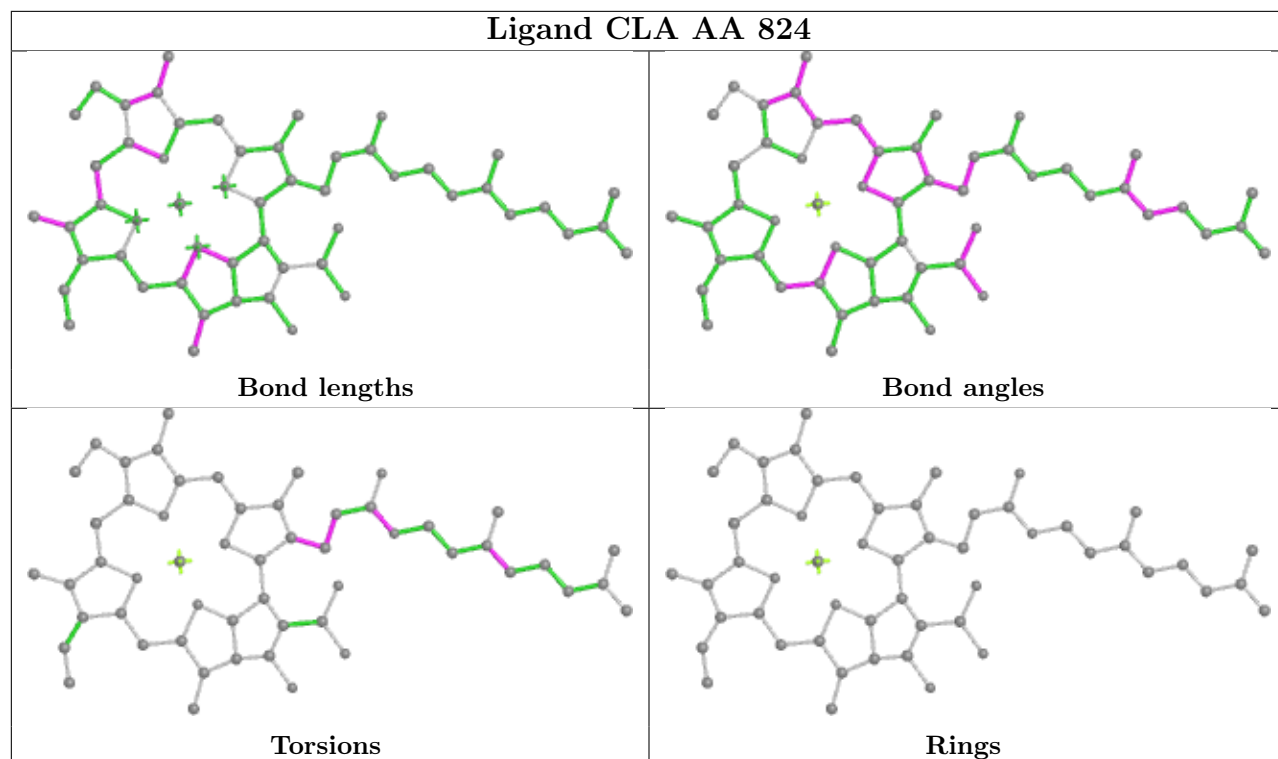
Bond angles

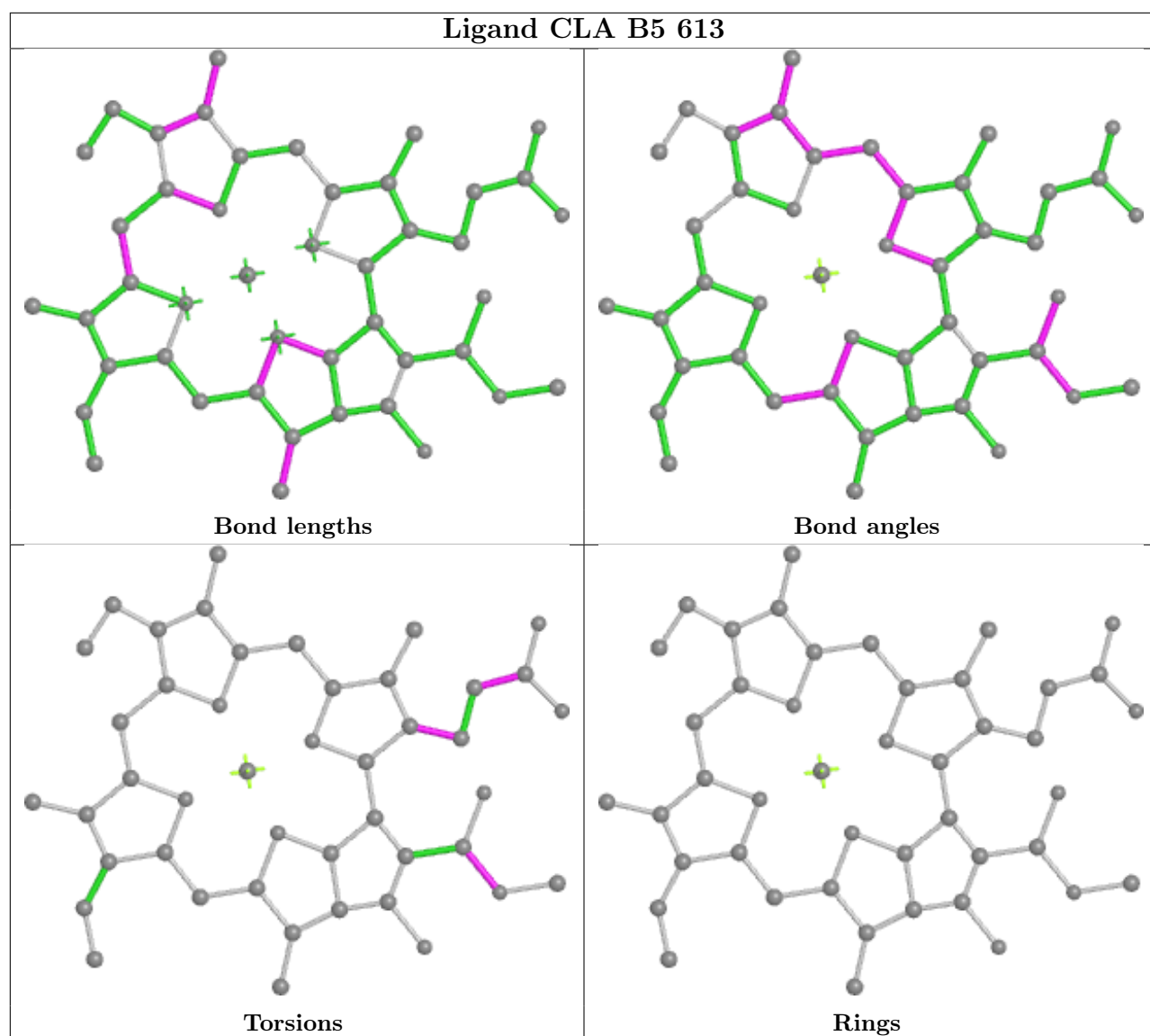


Torsions

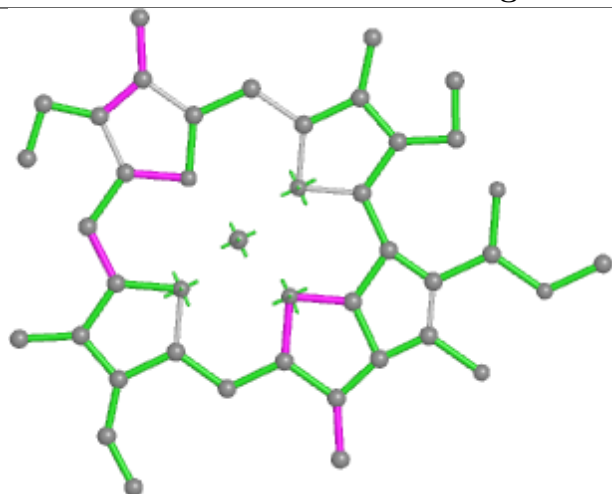


Rings

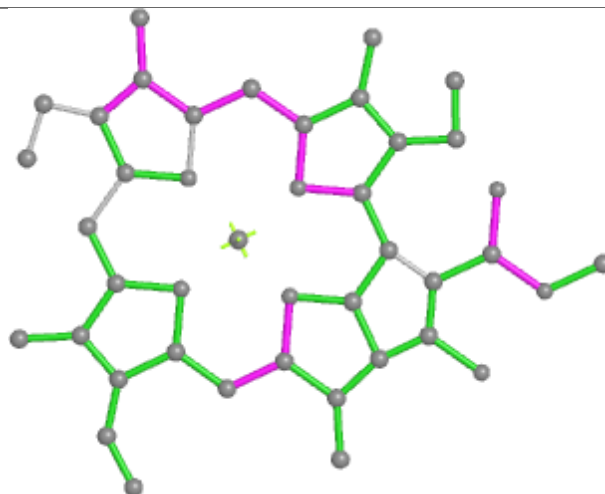




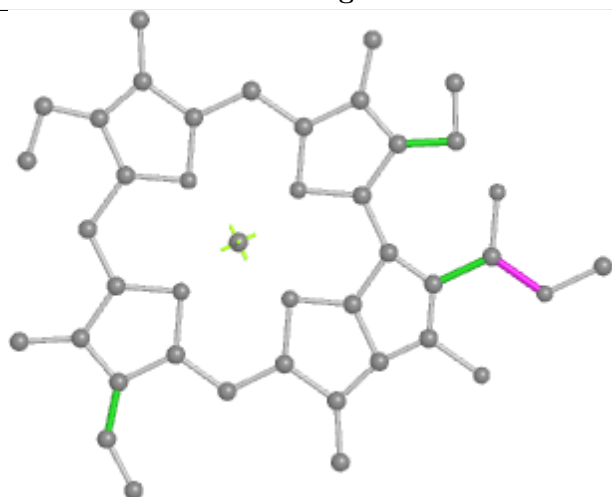
Ligand CLA AB 836



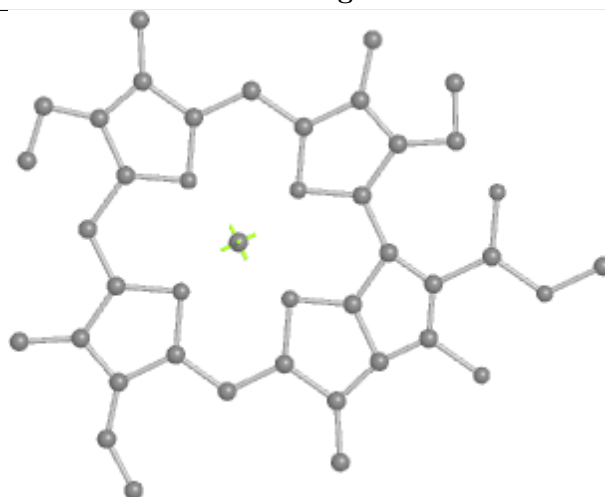
Bond lengths



Bond angles

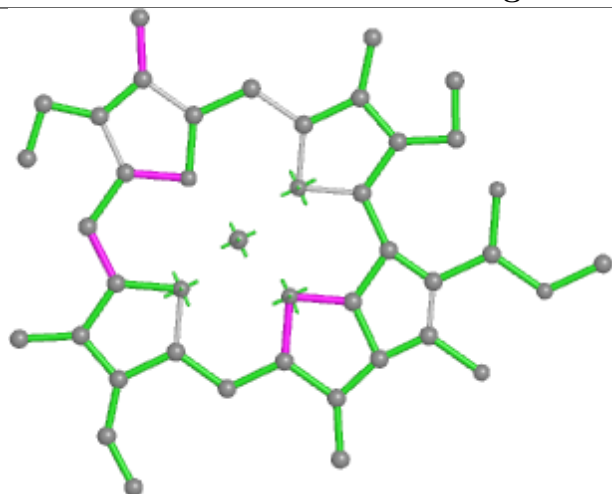


Torsions

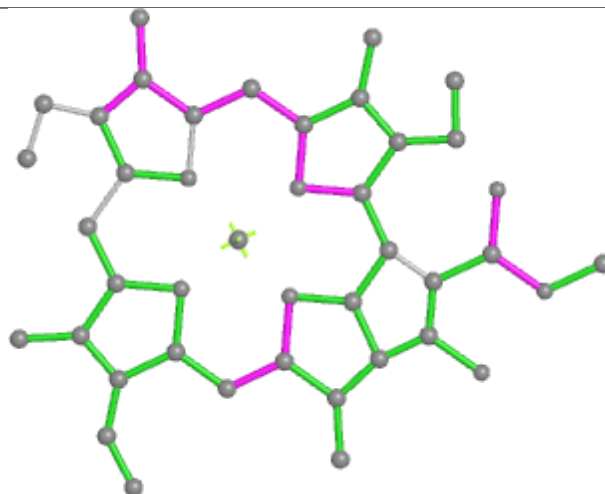


Rings

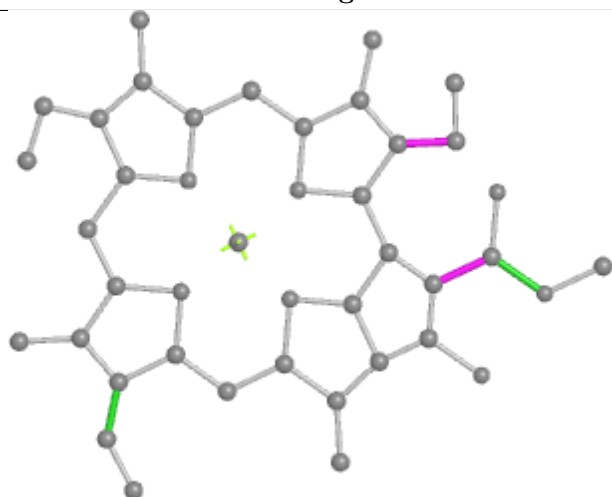
Ligand CLA AJ 102



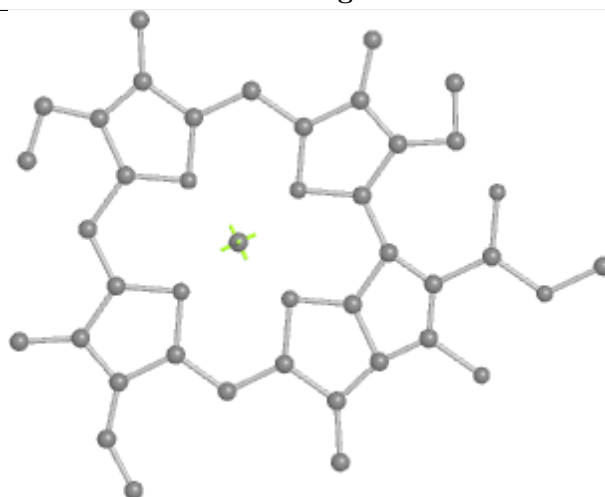
Bond lengths



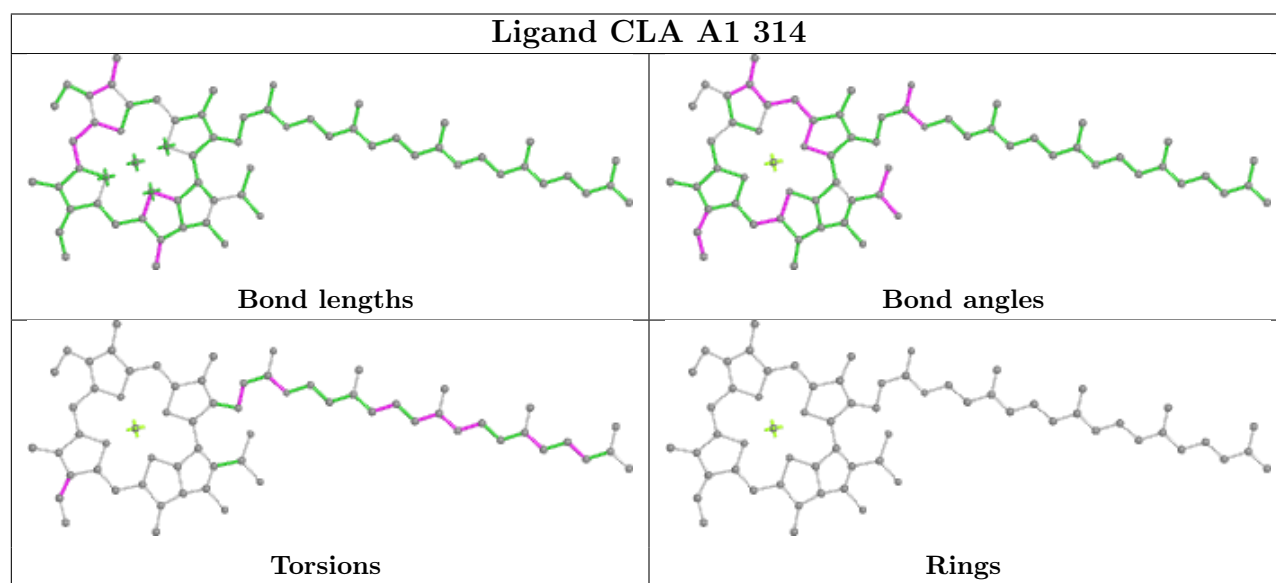
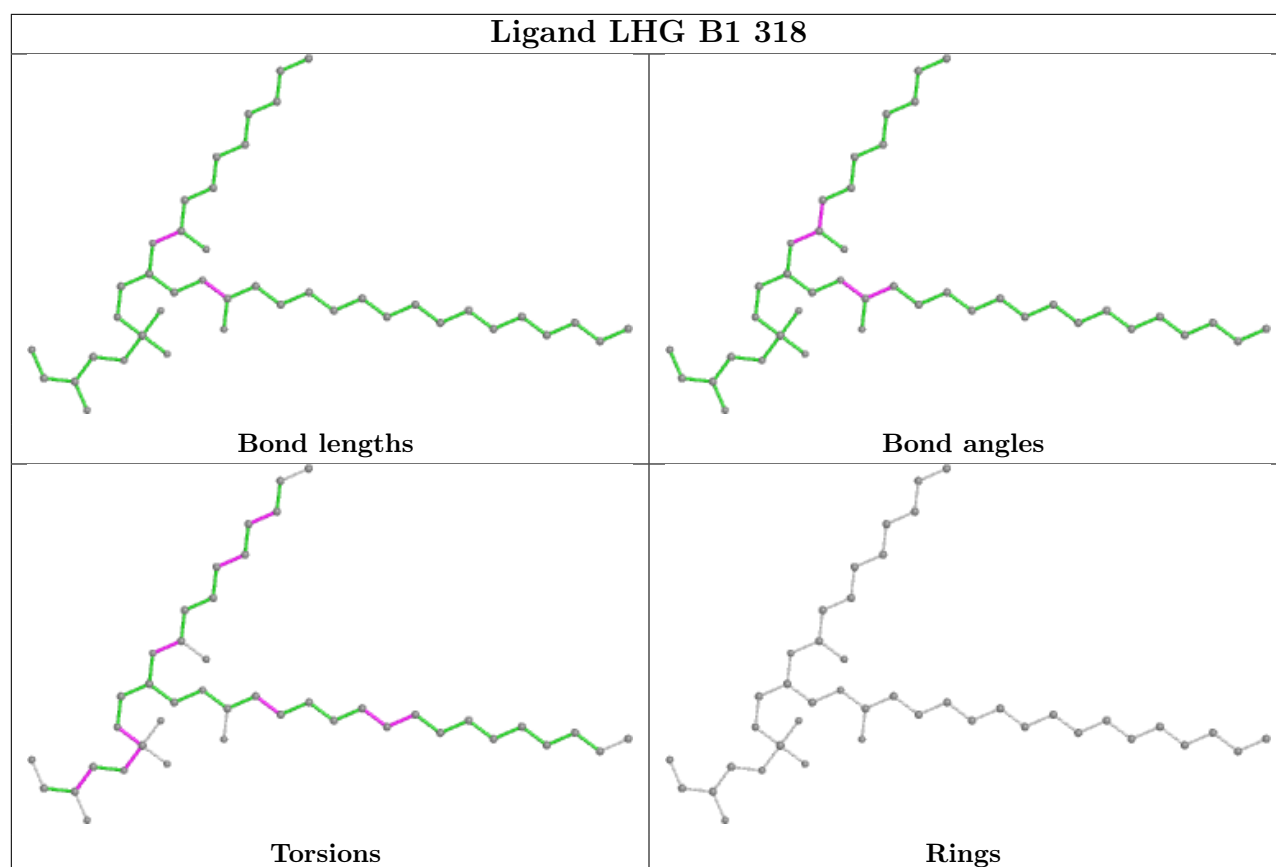
Bond angles

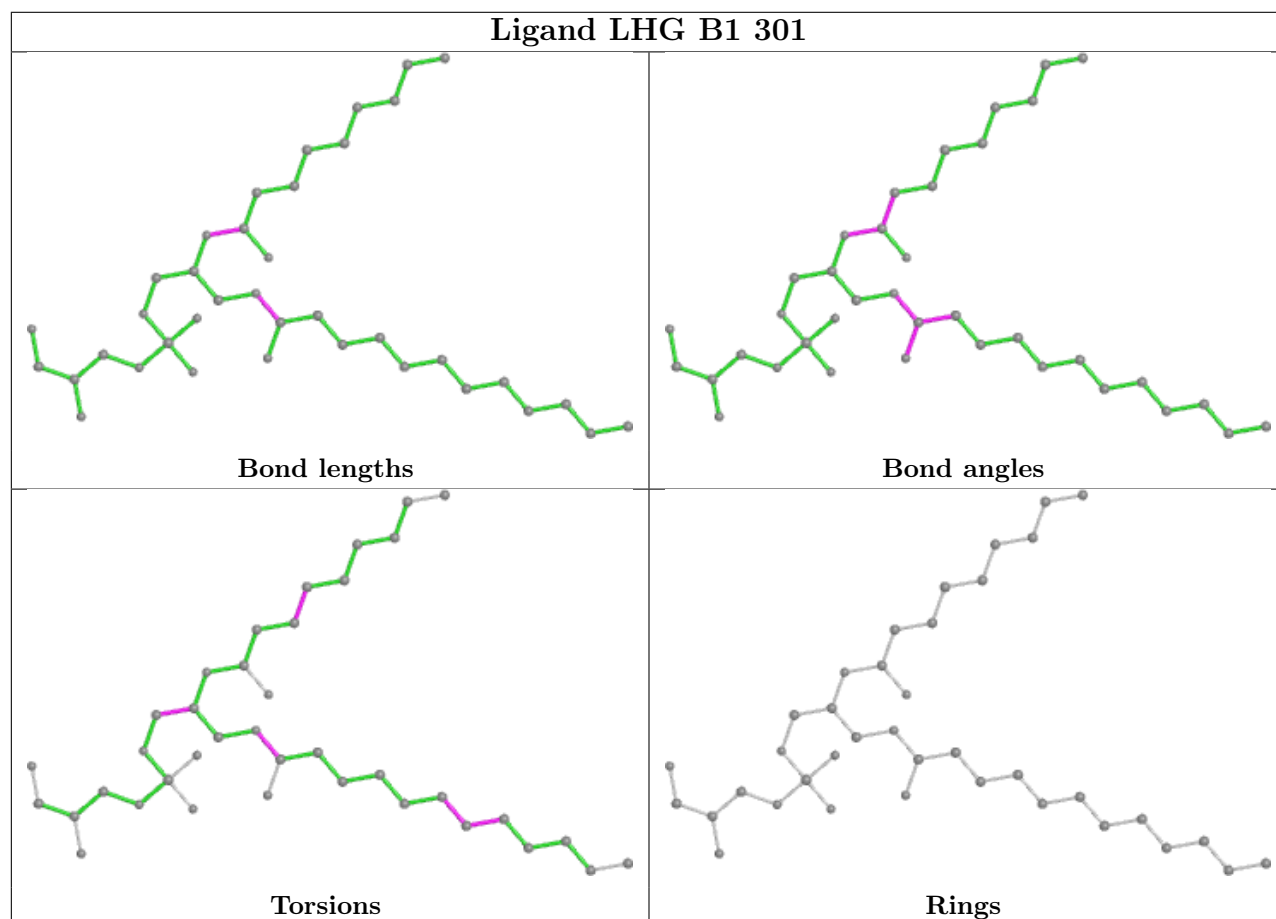
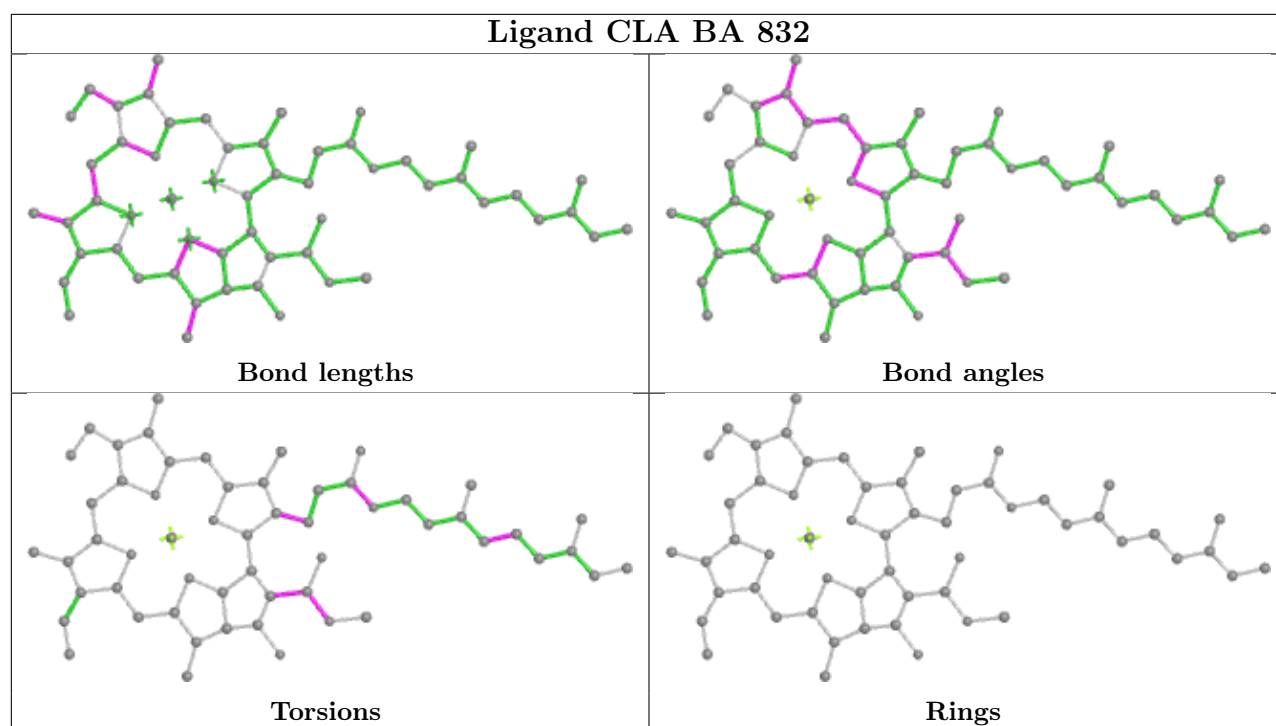


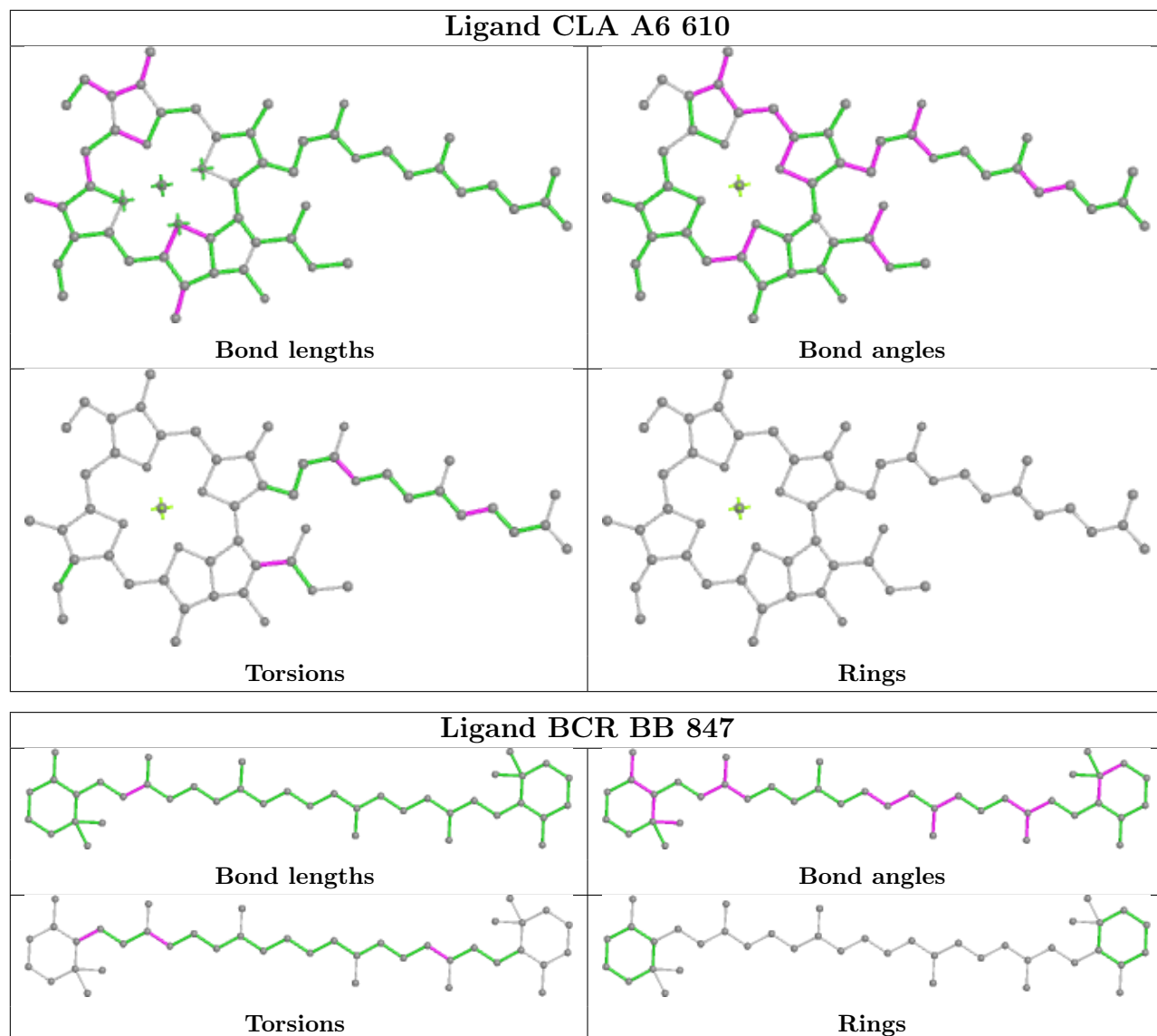
Torsions



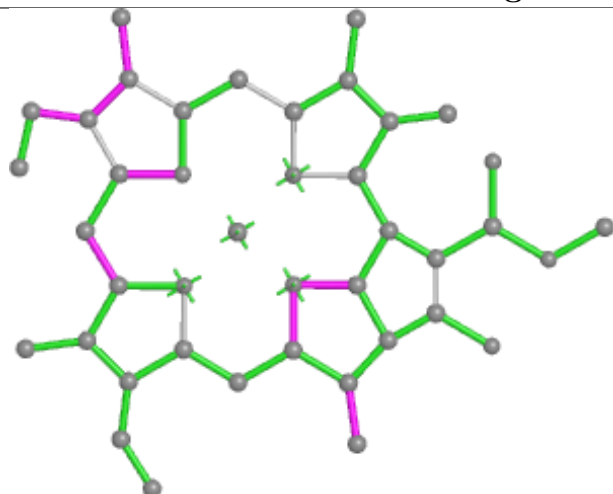
Rings



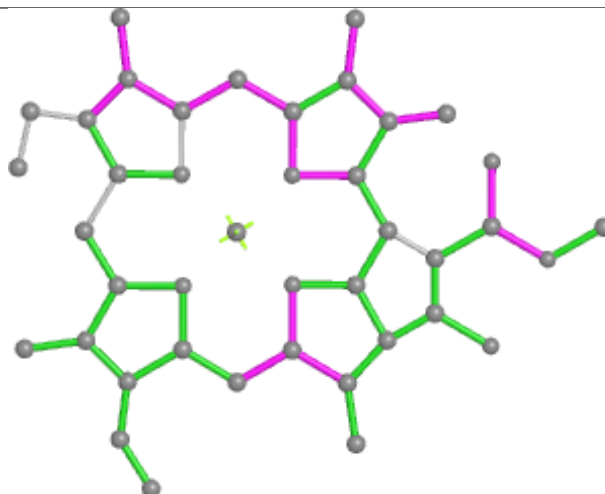




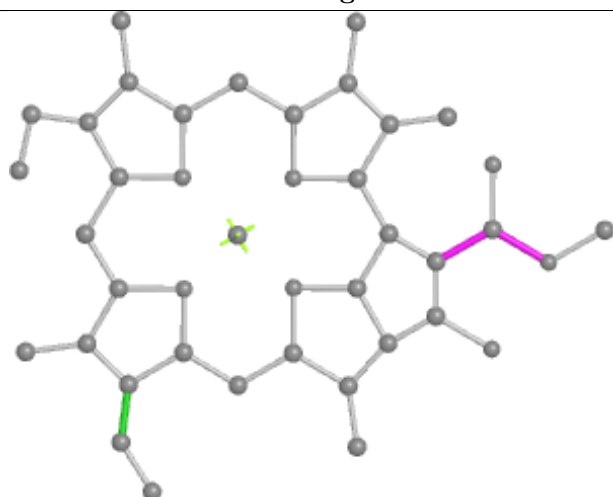
Ligand CLA A3 309



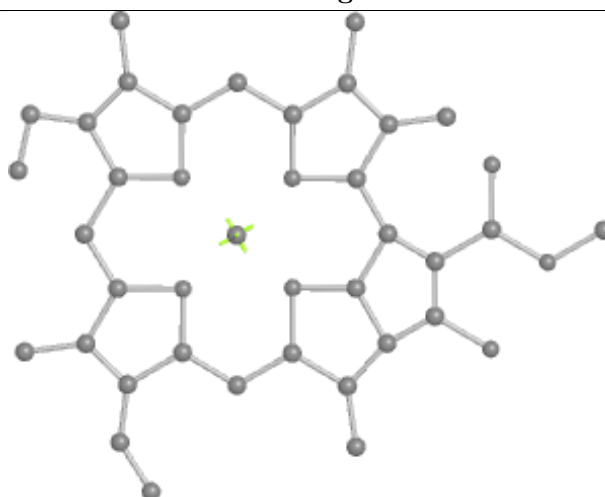
Bond lengths



Bond angles

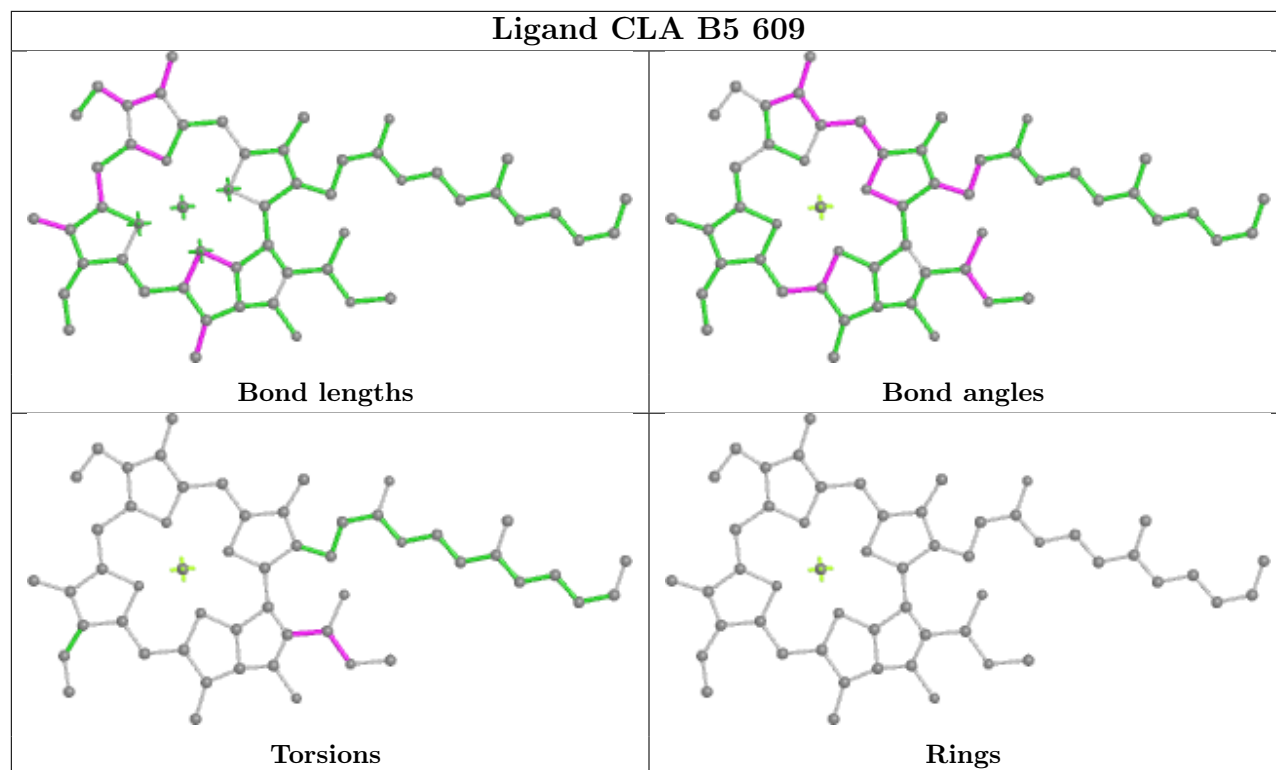


Torsions

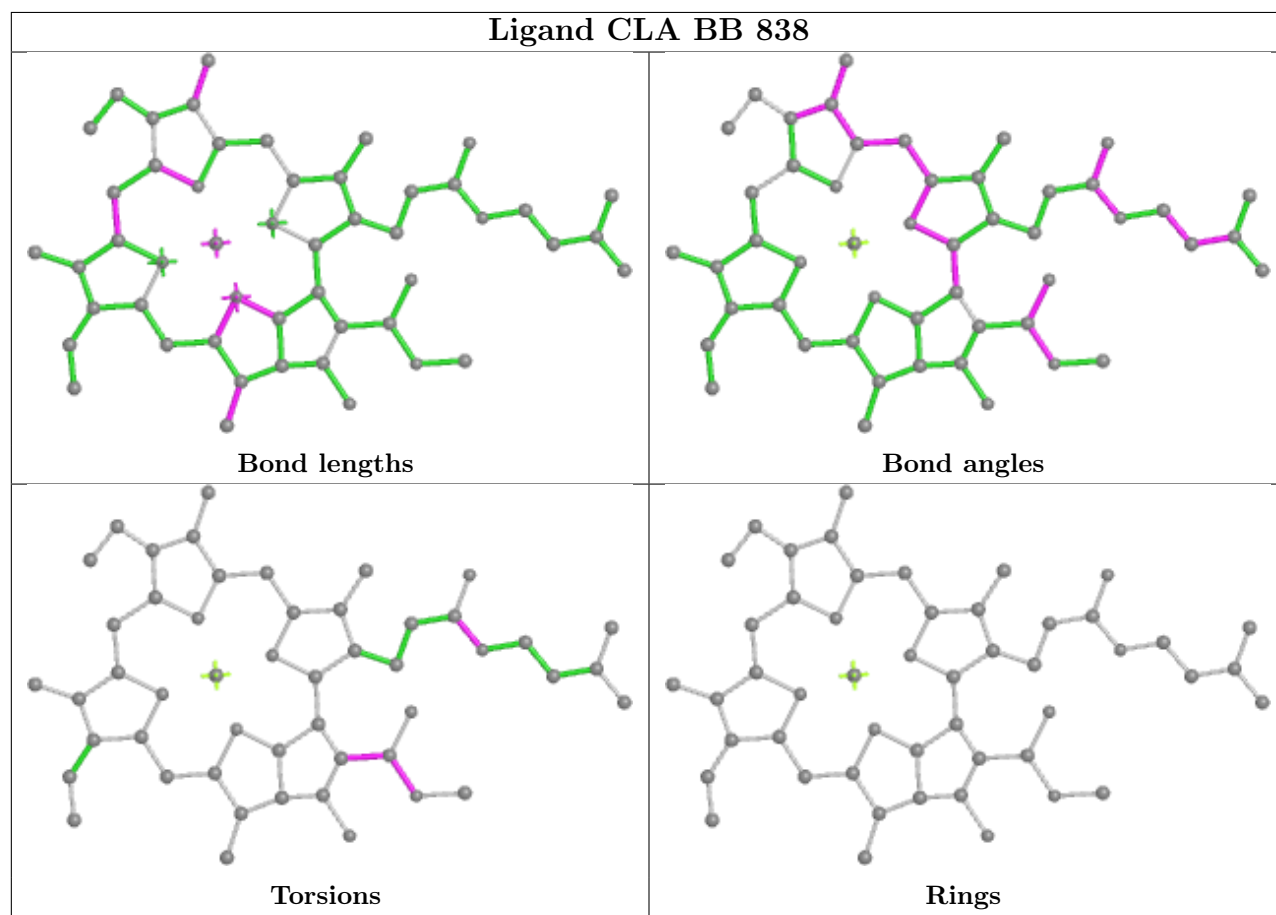


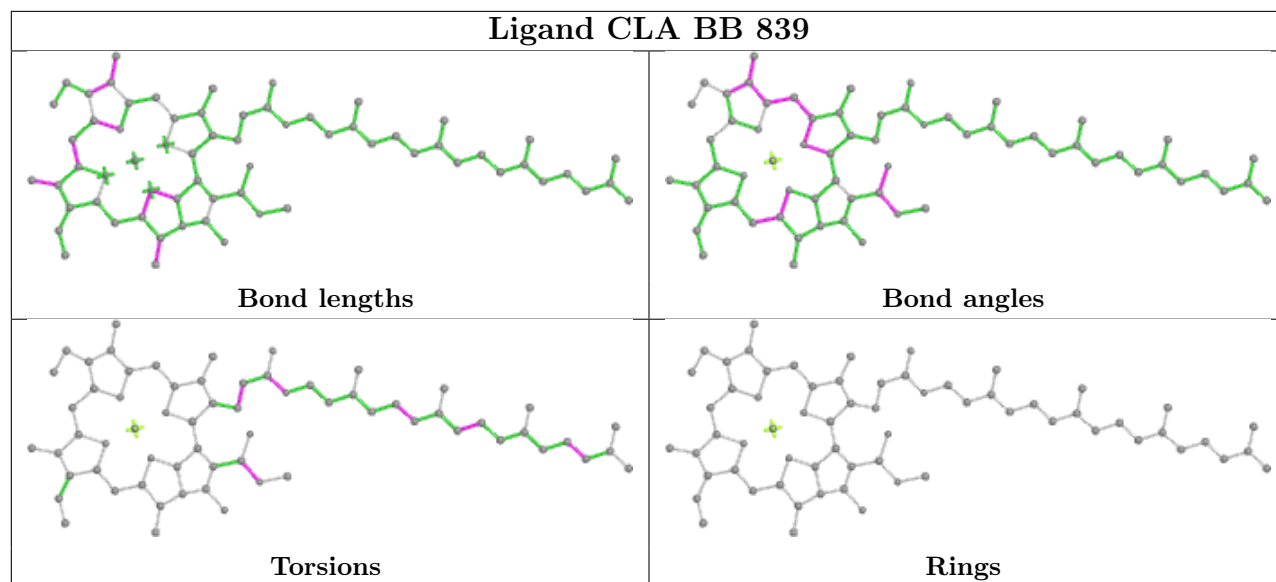
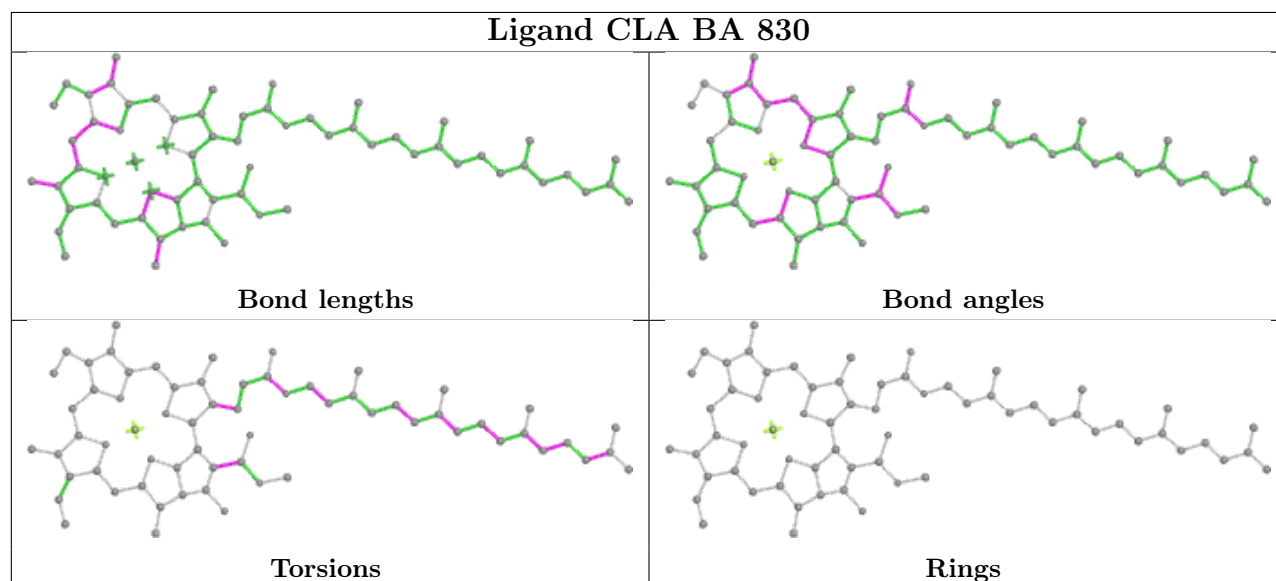
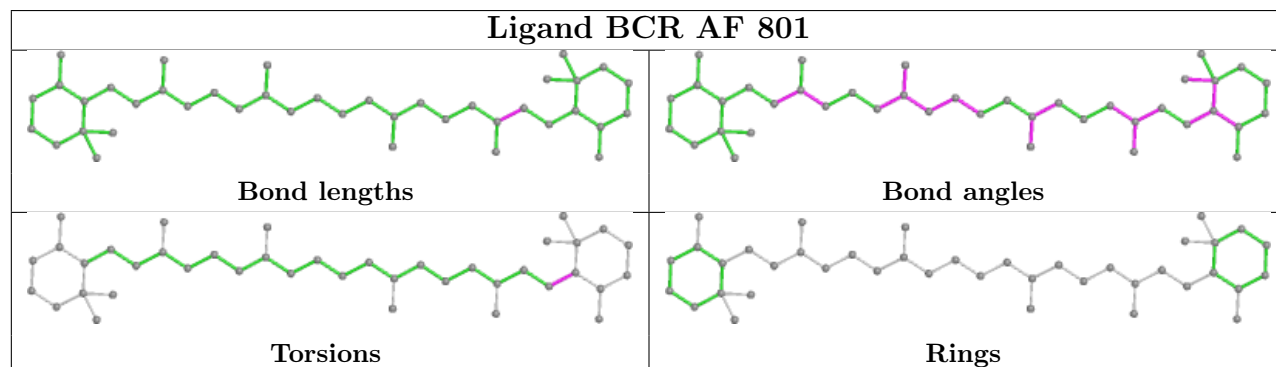
Rings

Ligand CLA B5 609

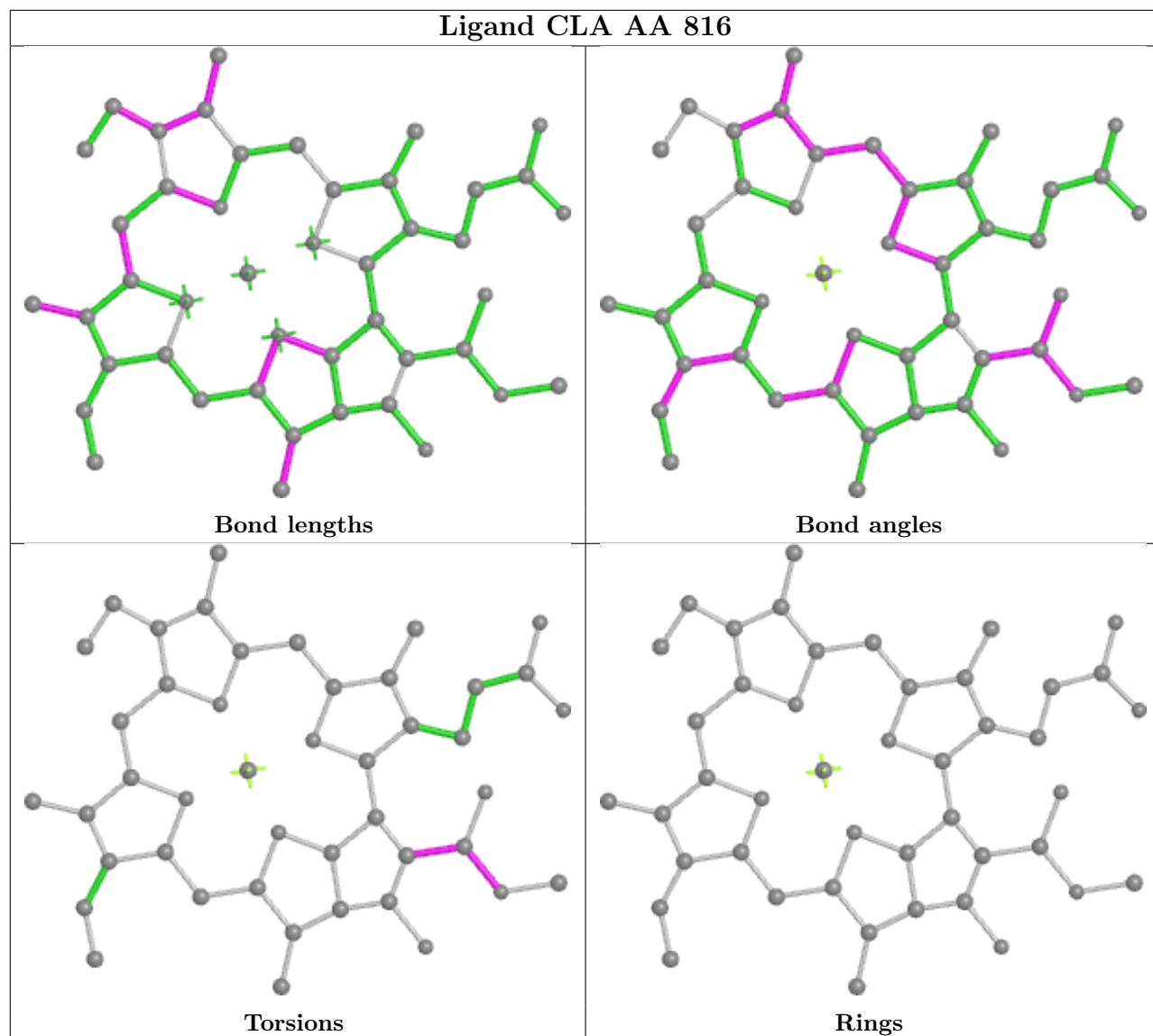


Ligand CLA BB 838

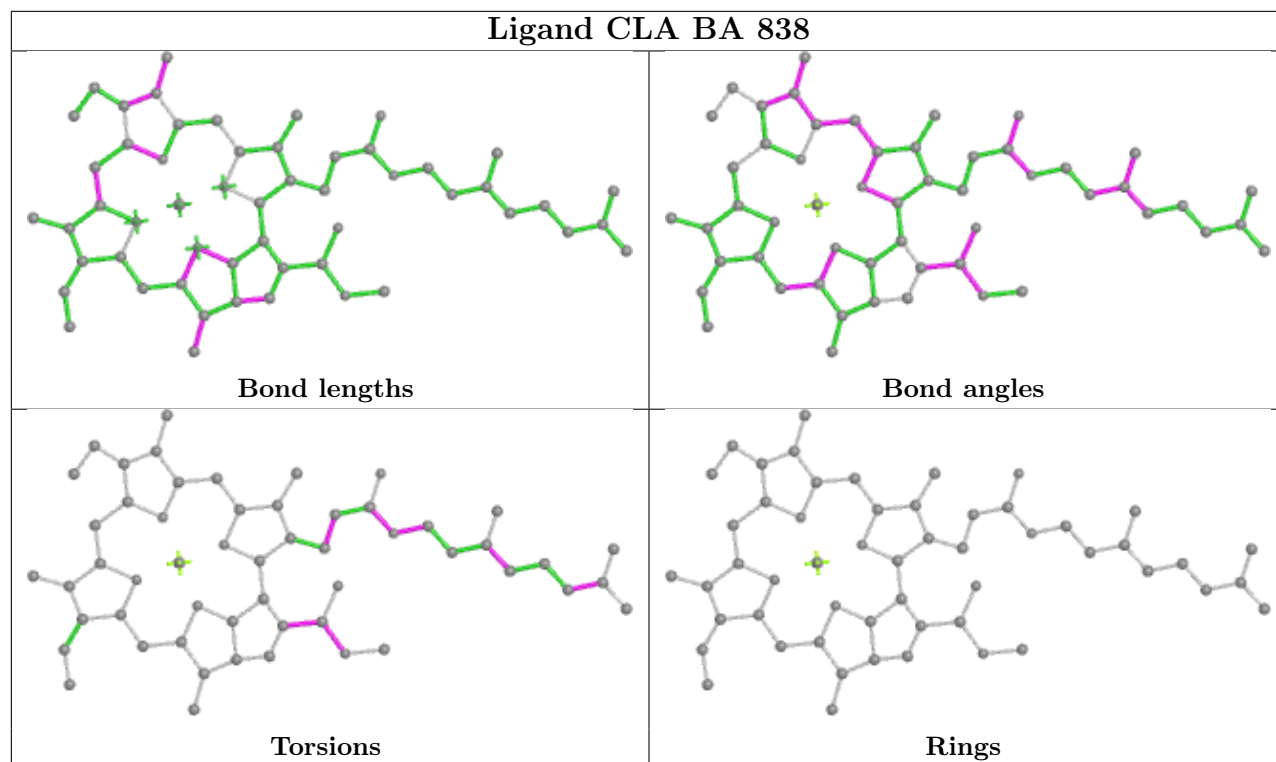


Ligand CLA BB 839**Ligand CLA BA 830****Ligand BCR AF 801**

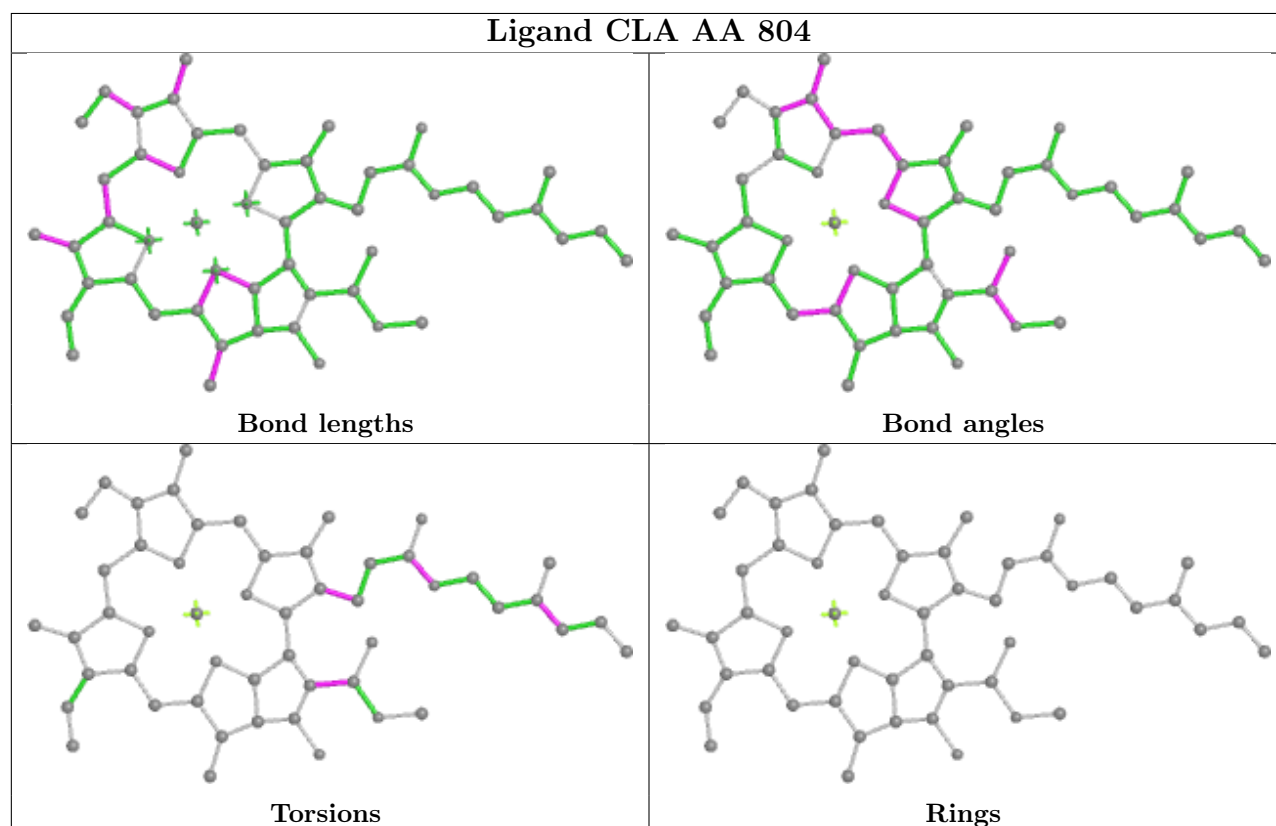
Ligand CLA AA 816



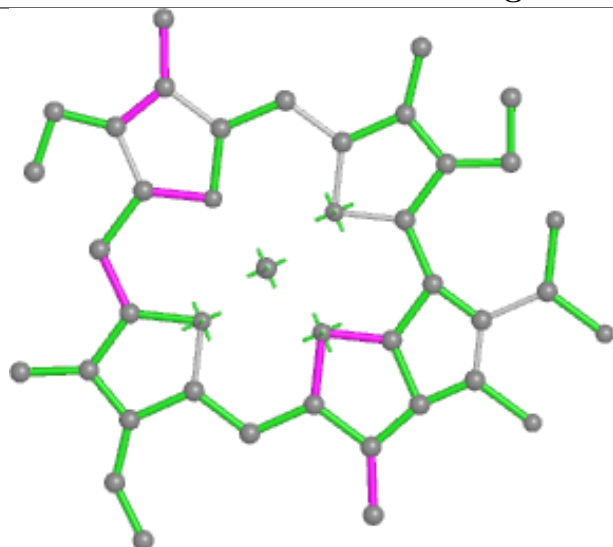
Ligand CLA BA 838



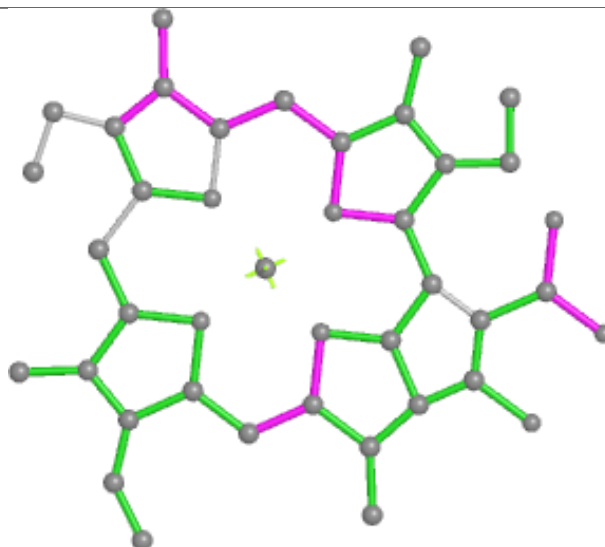
Ligand CLA AA 804



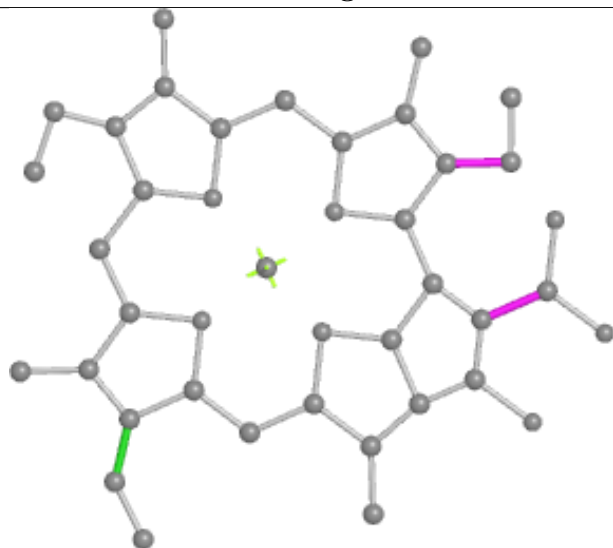
Ligand CLA A3 305



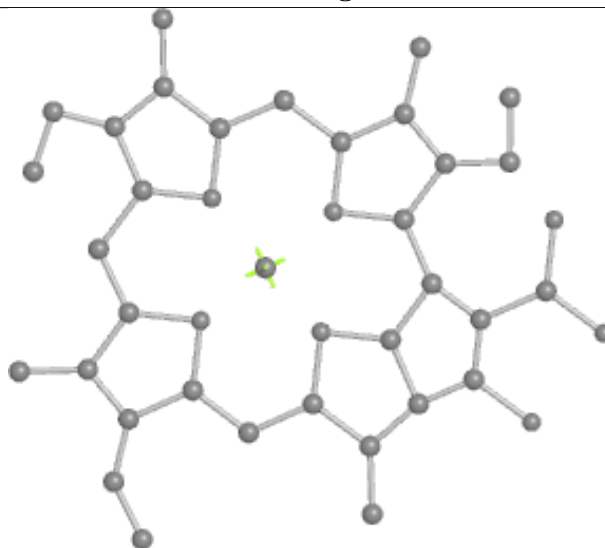
Bond lengths



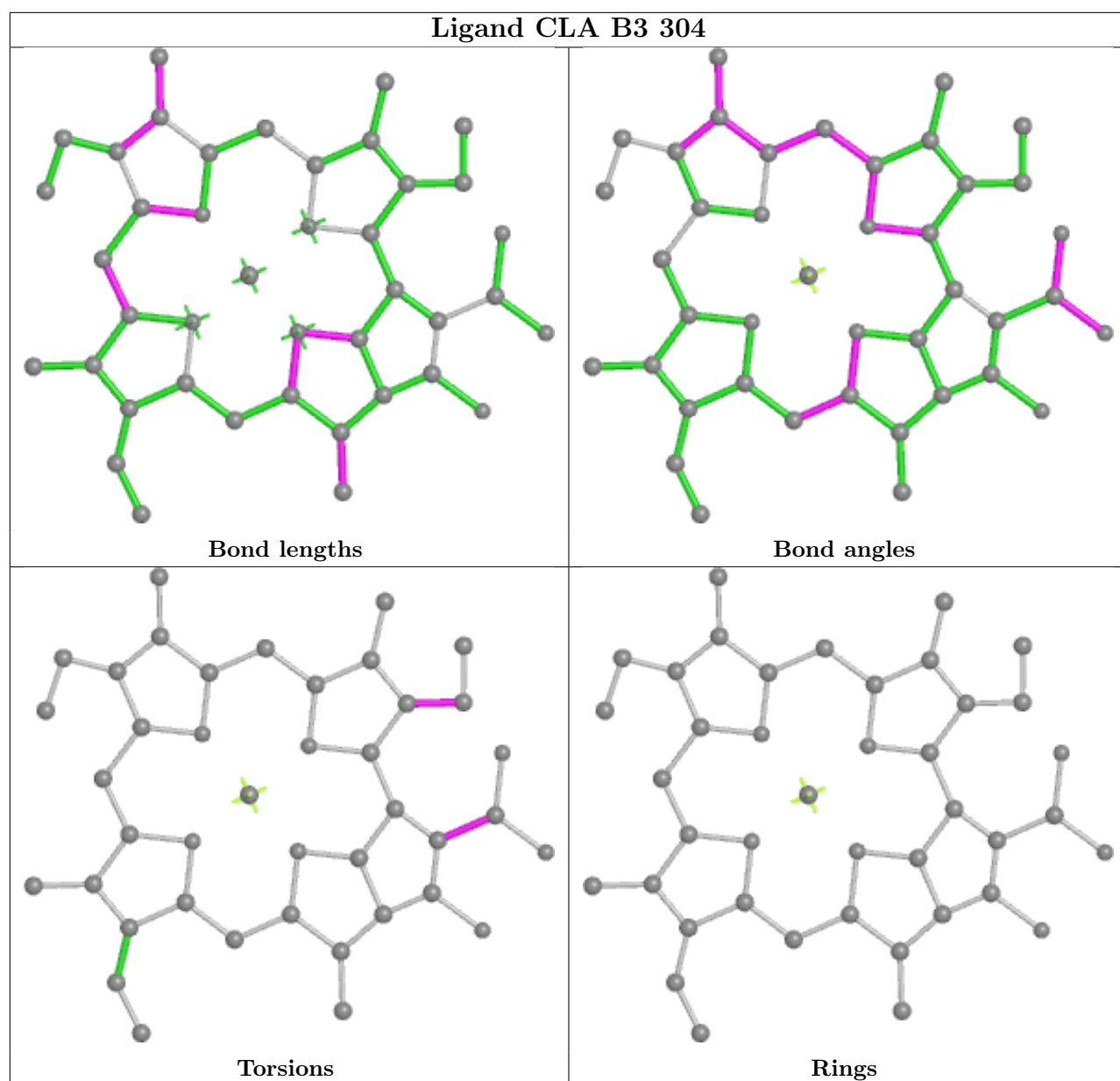
Bond angles

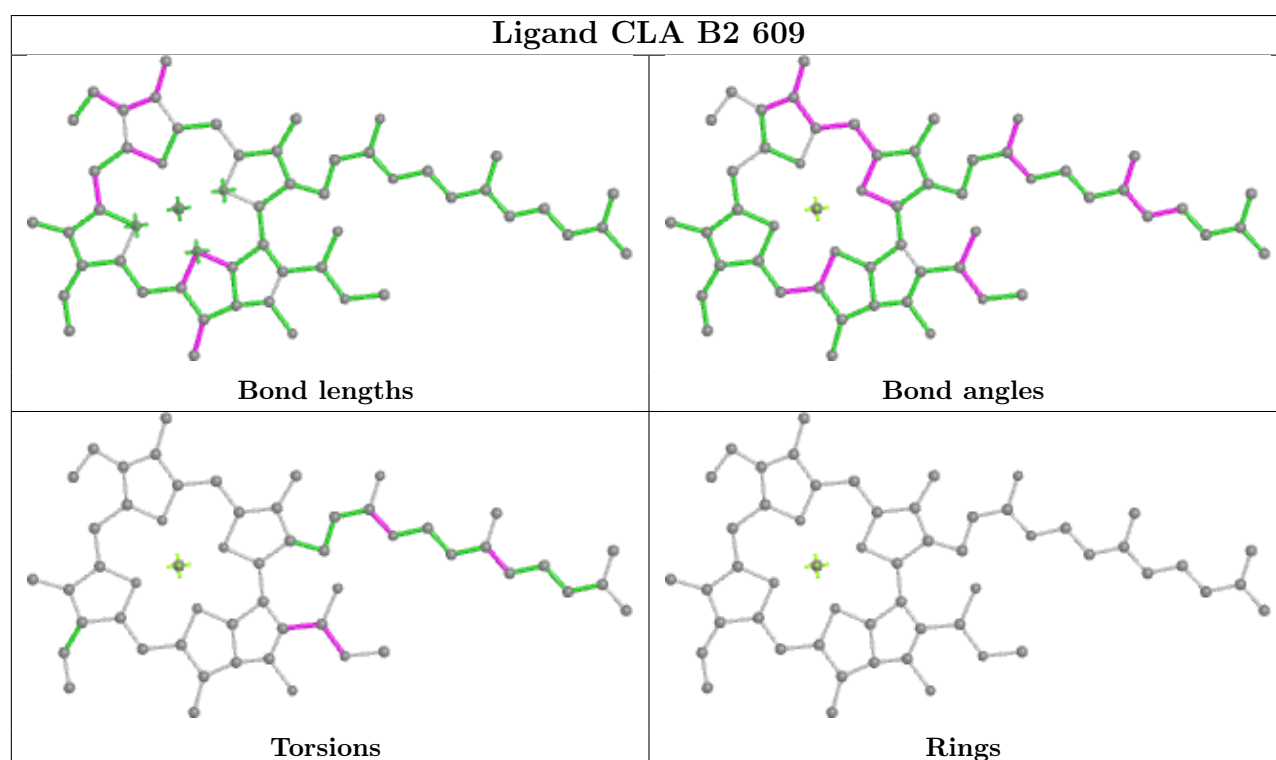
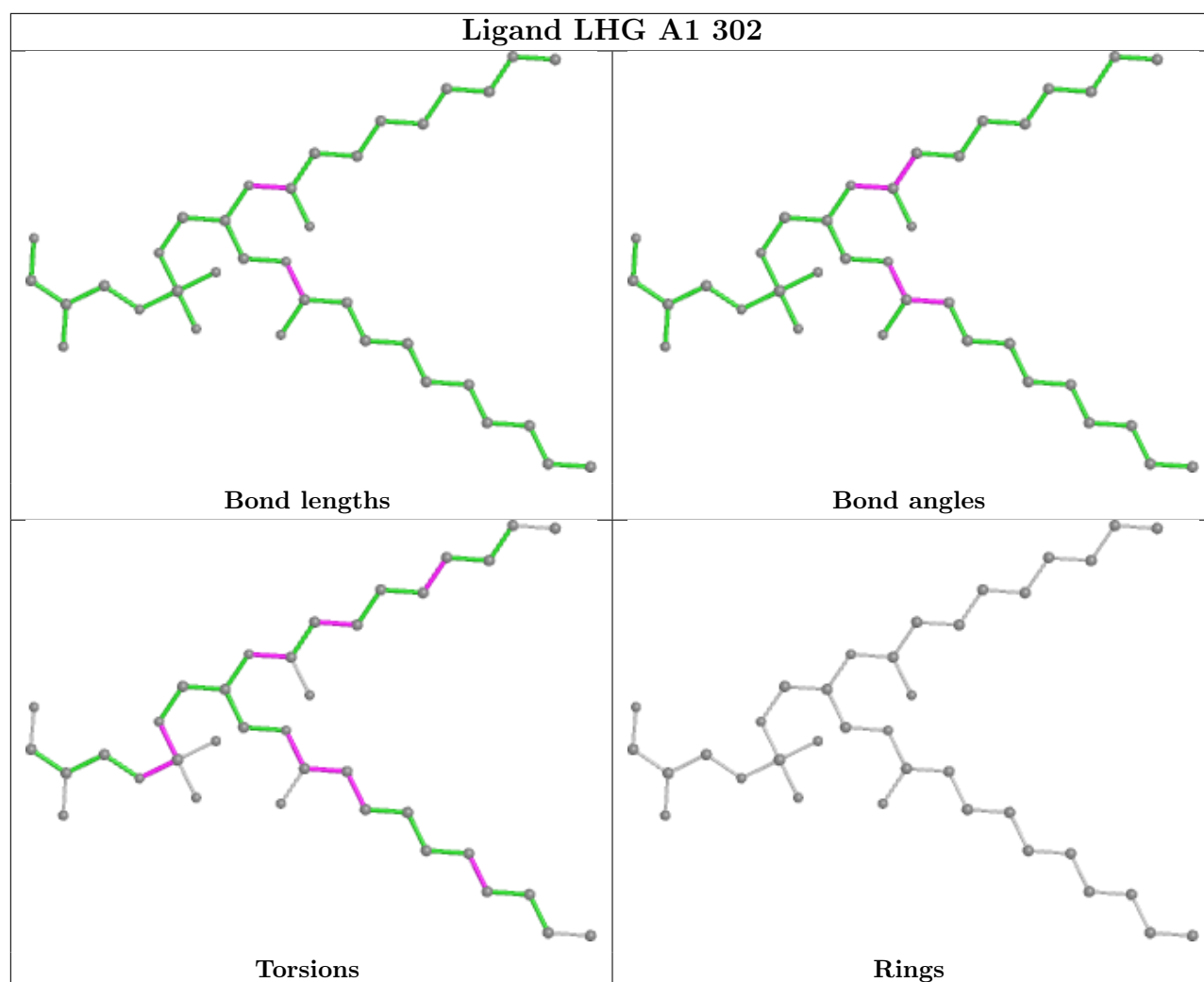


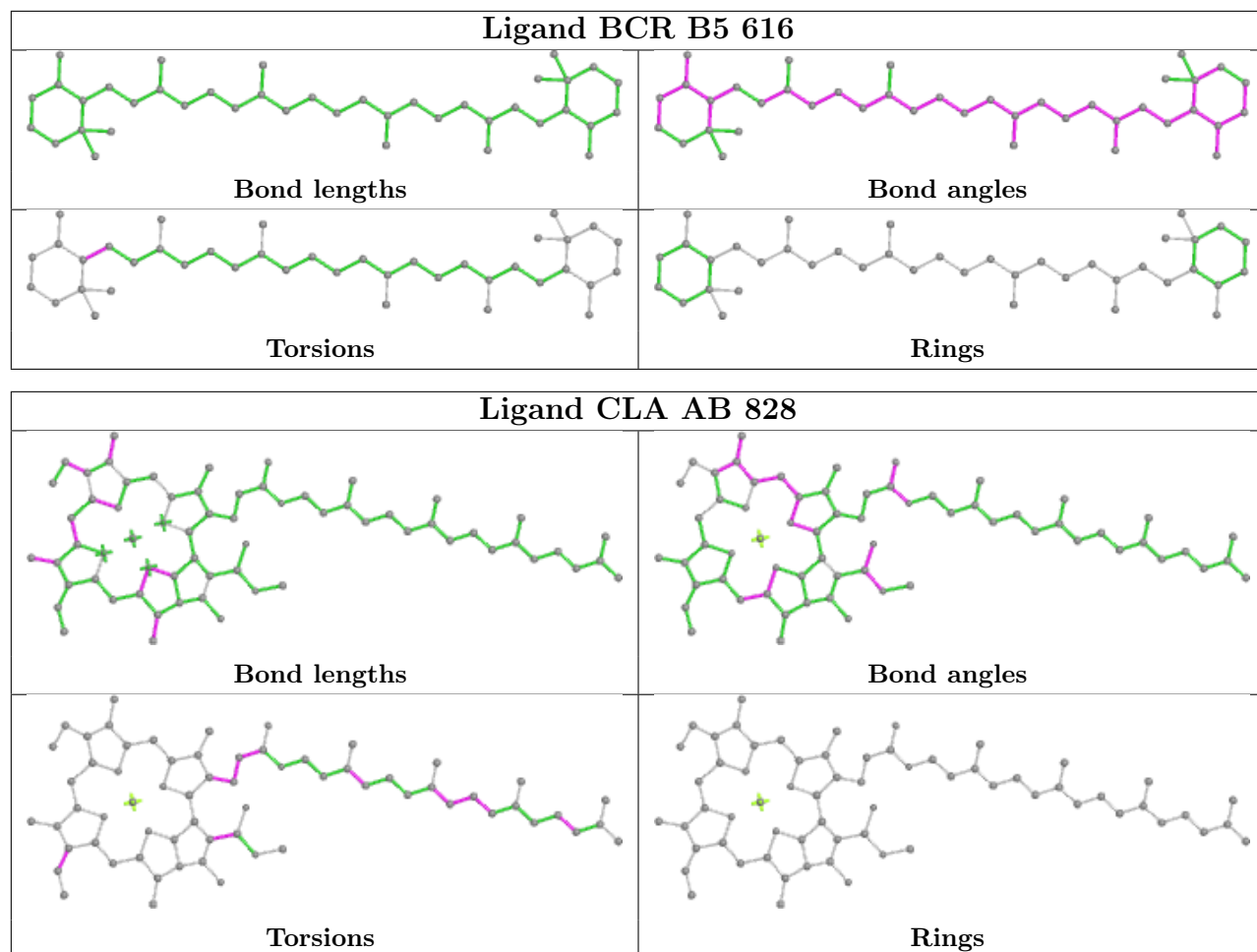
Torsions



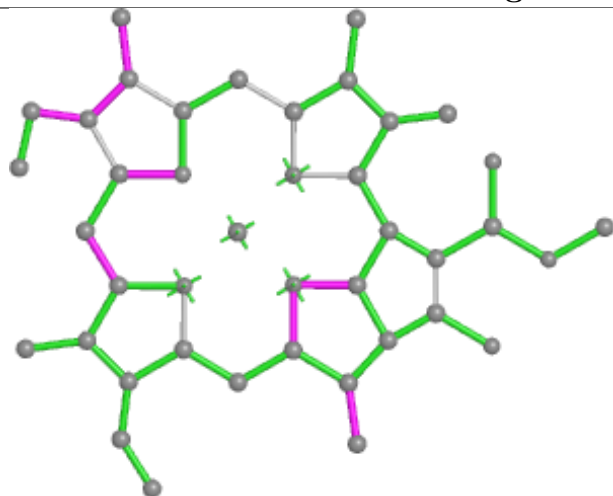
Rings



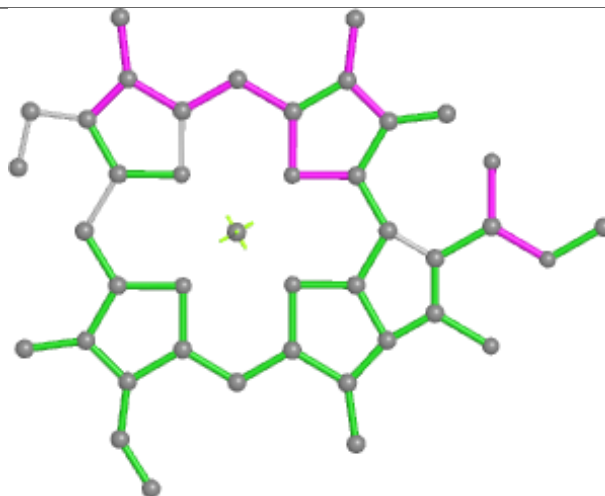




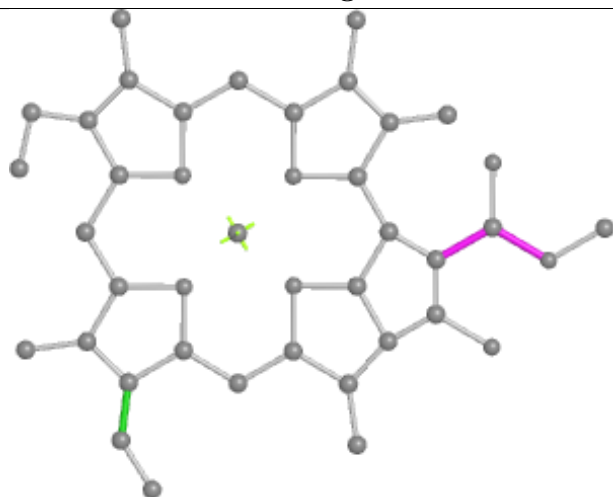
Ligand CLA B3 308



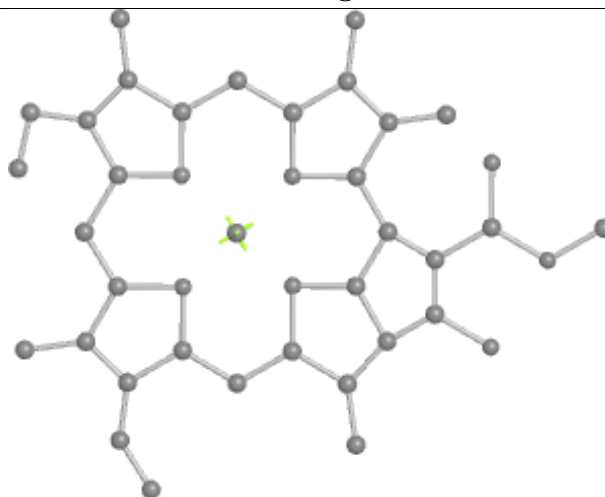
Bond lengths



Bond angles

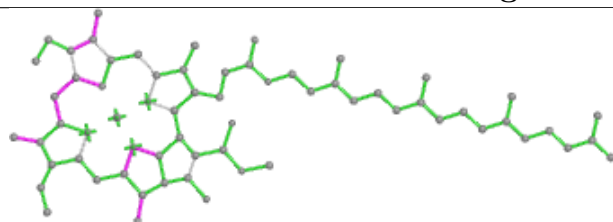


Torsions

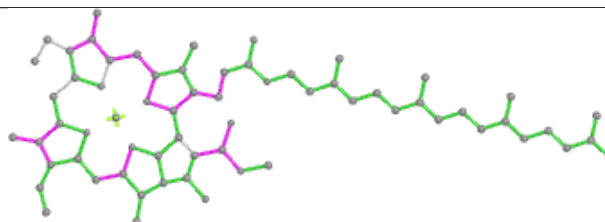


Rings

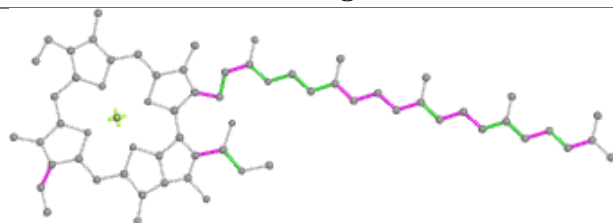
Ligand CLA AA 805



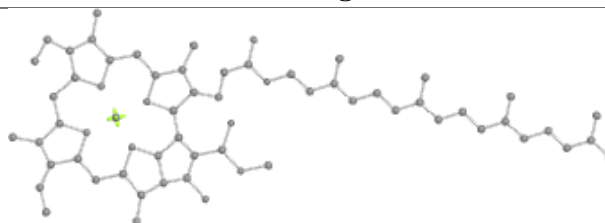
Bond lengths



Bond angles

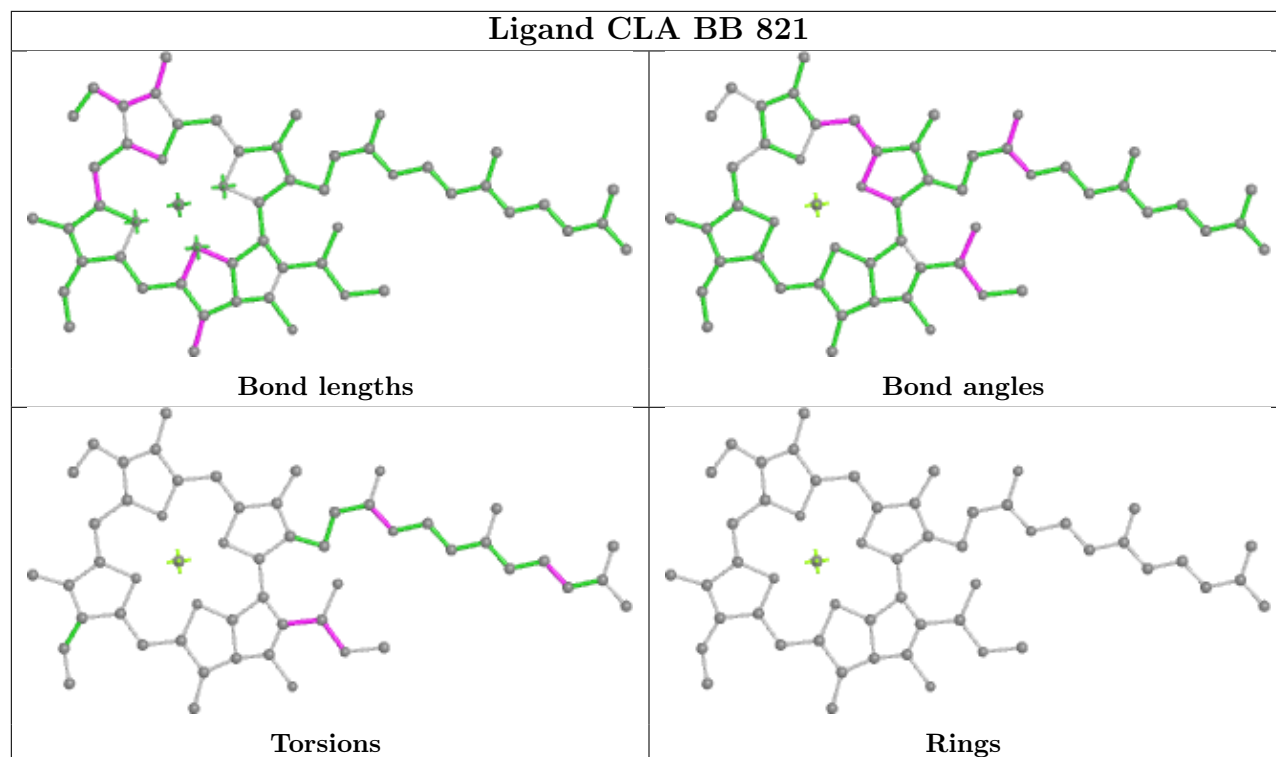


Torsions

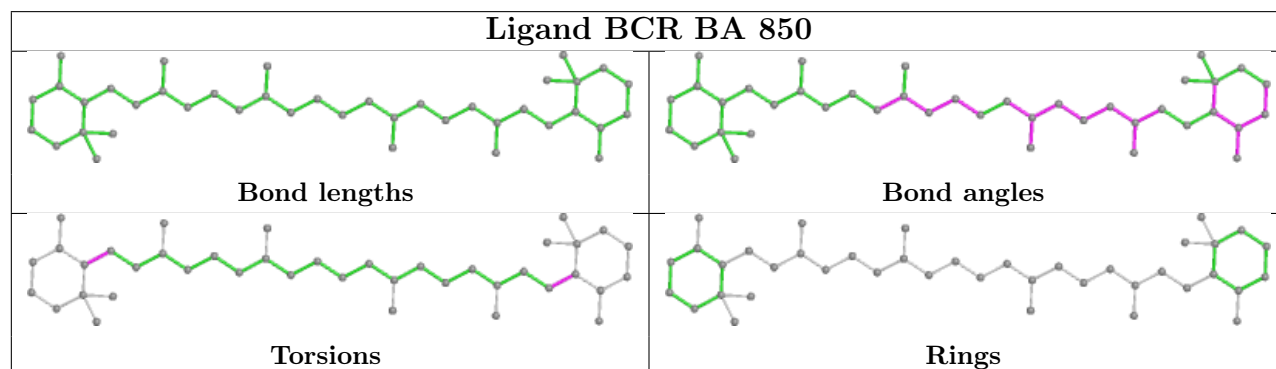


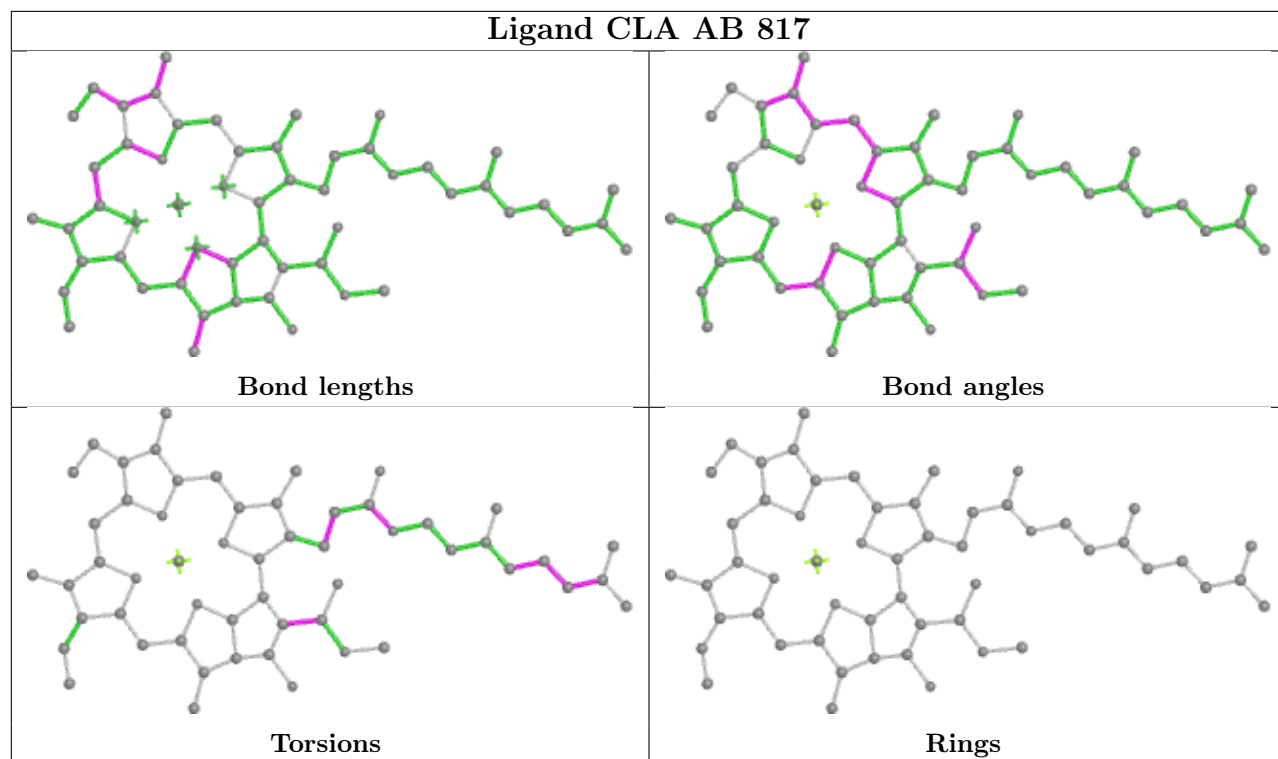
Rings

Ligand CLA BB 821

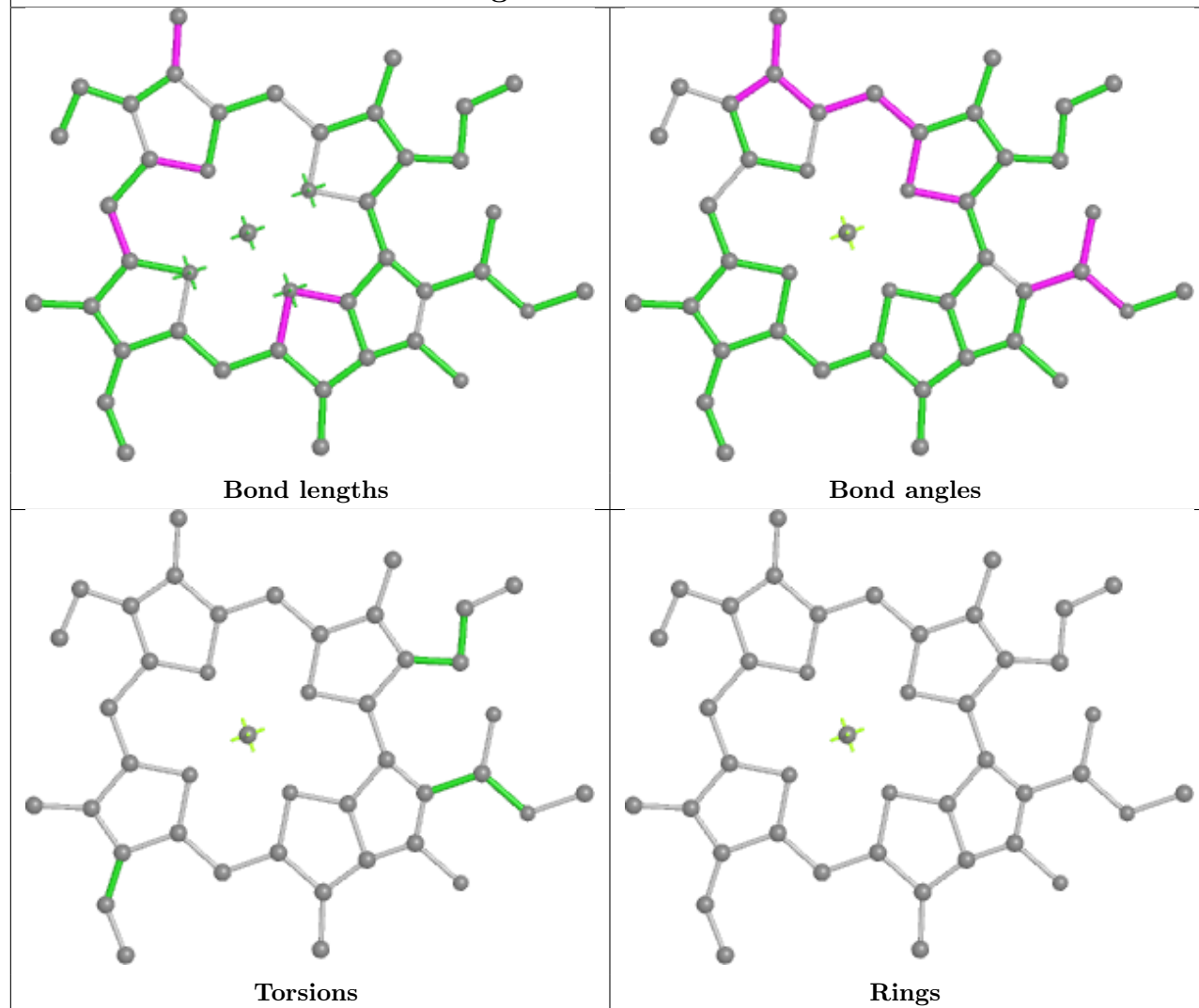


Ligand BCR BA 850

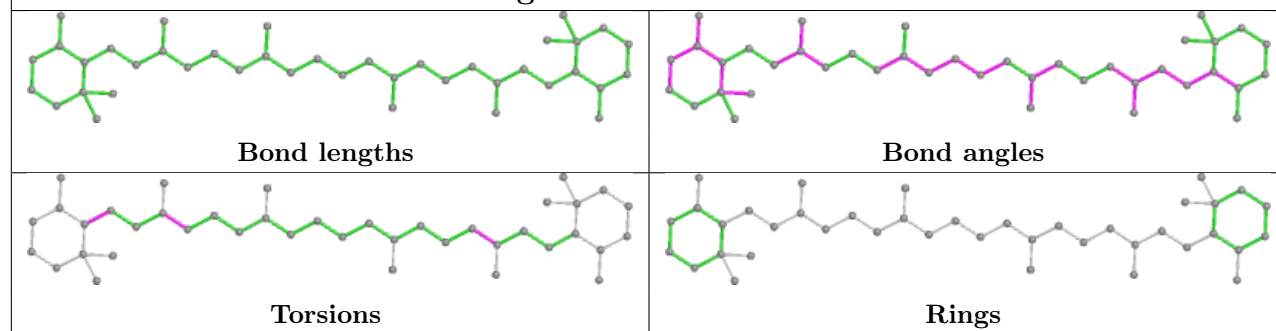




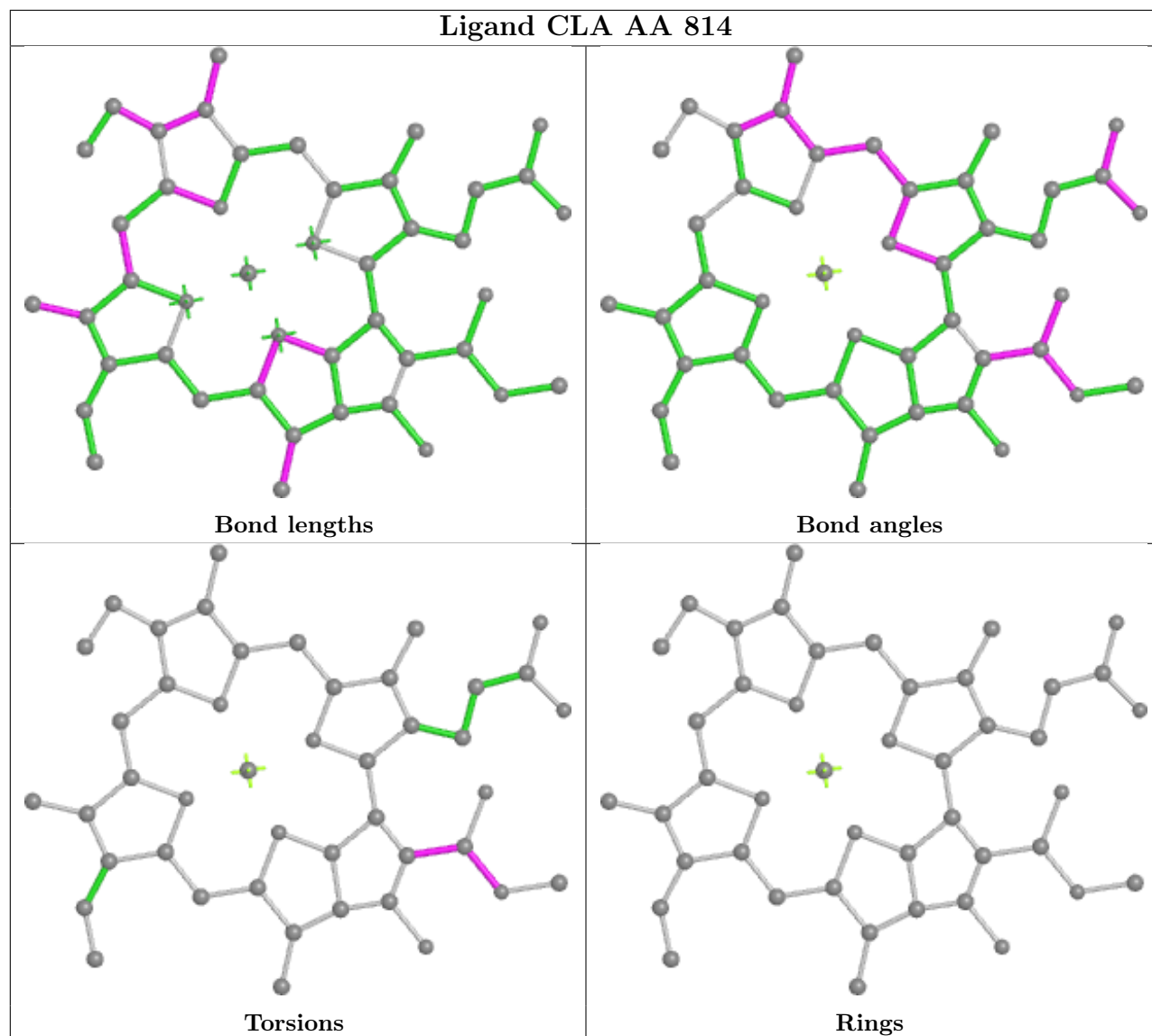
Ligand CLA A3 311



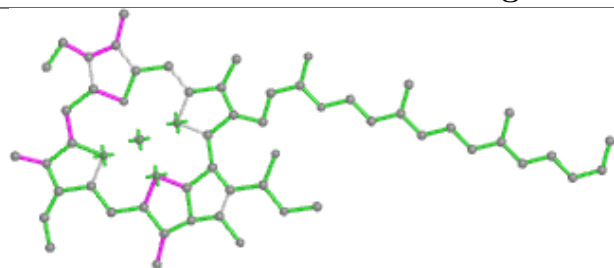
Ligand BCR AB 846



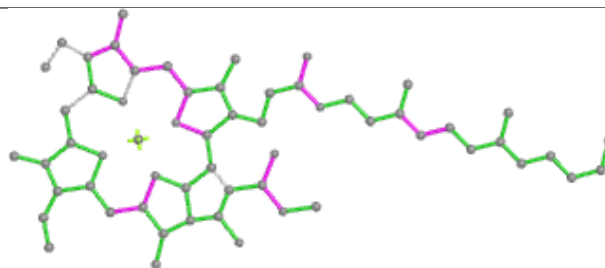
Ligand CLA AA 814



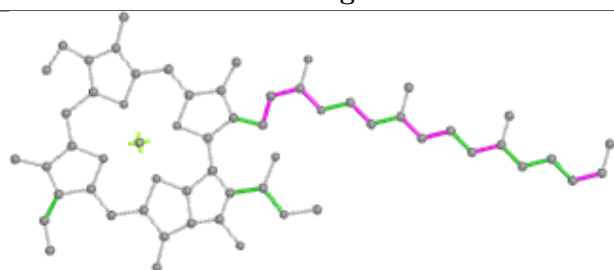
Ligand CLA BB 819



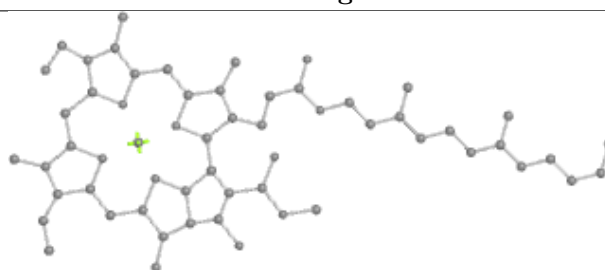
Bond lengths



Bond angles

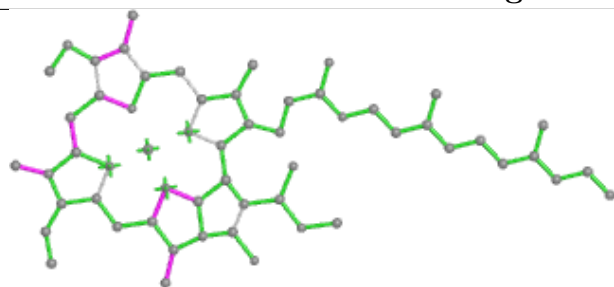


Torsions

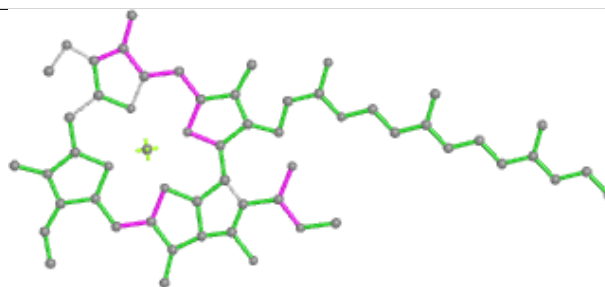


Rings

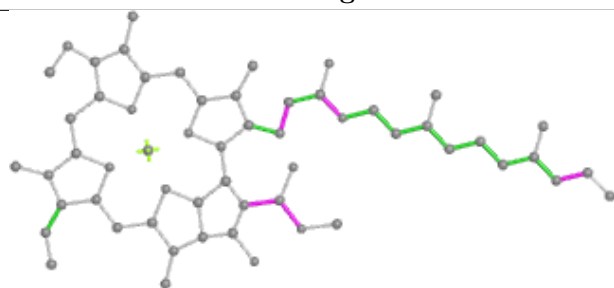
Ligand CLA B5 612



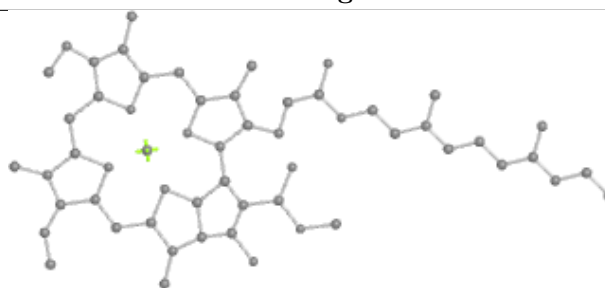
Bond lengths



Bond angles

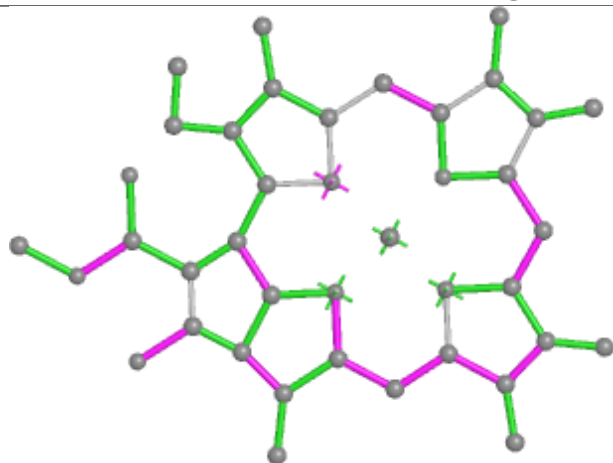


Torsions

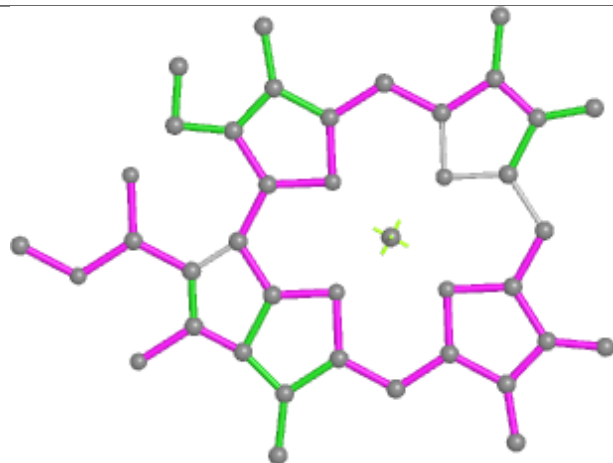


Rings

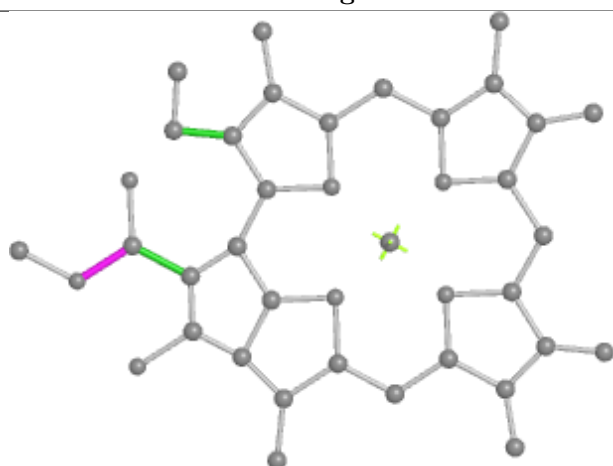
Ligand CHL B5 606



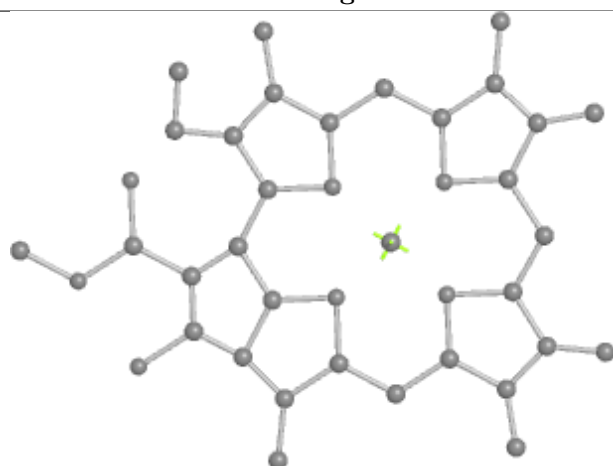
Bond lengths



Bond angles

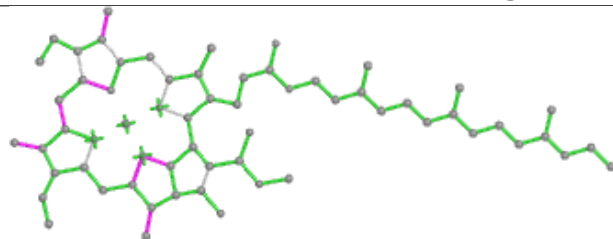


Torsions

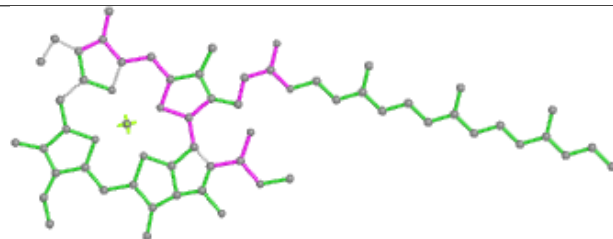


Rings

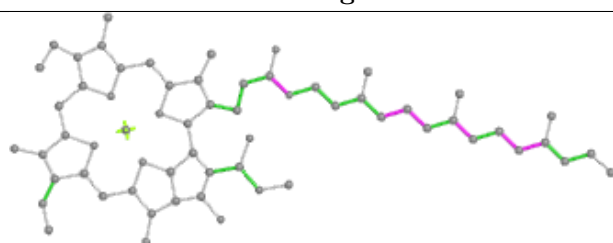
Ligand CLA BB 828



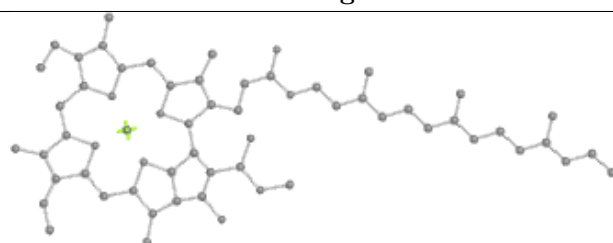
Bond lengths



Bond angles

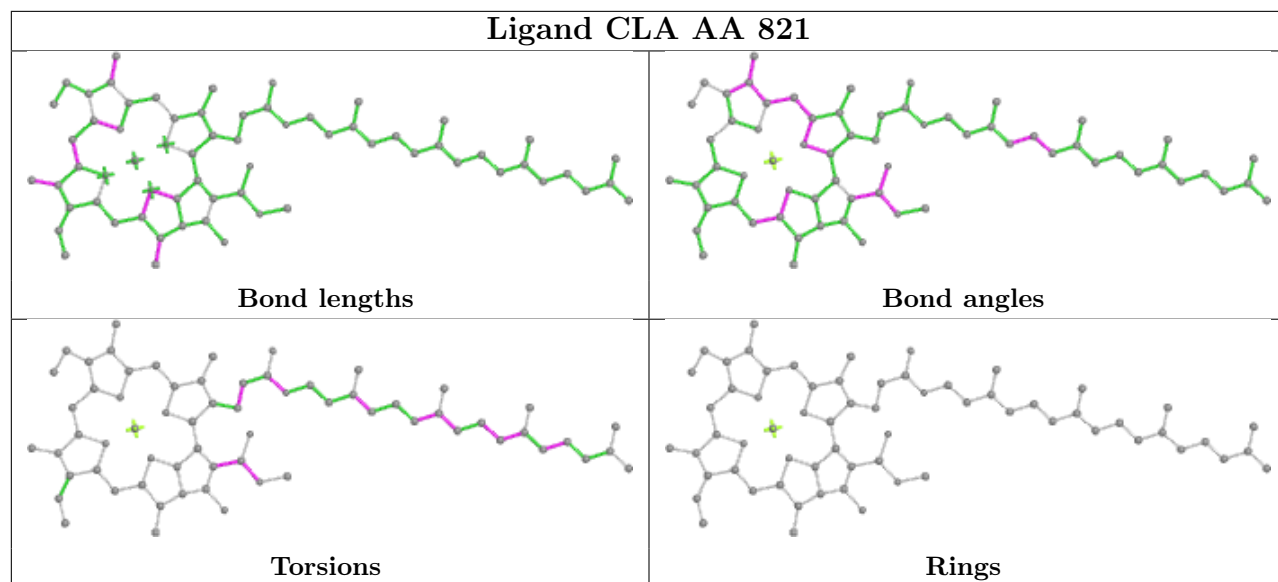


Torsions

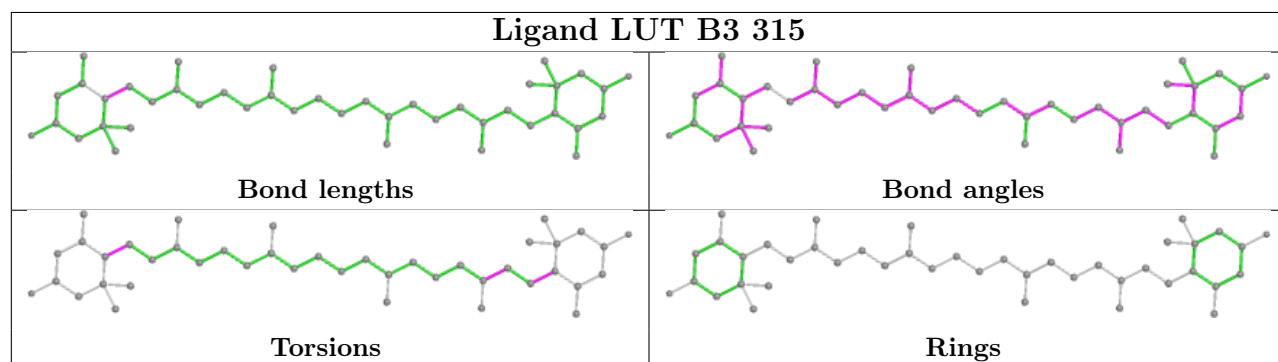


Rings

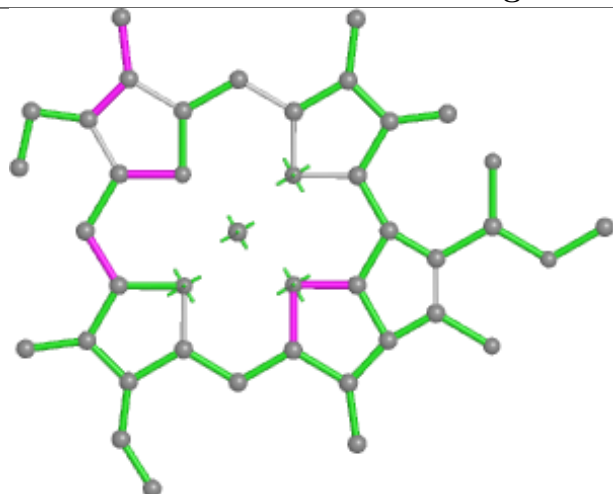
Ligand CLA AA 821



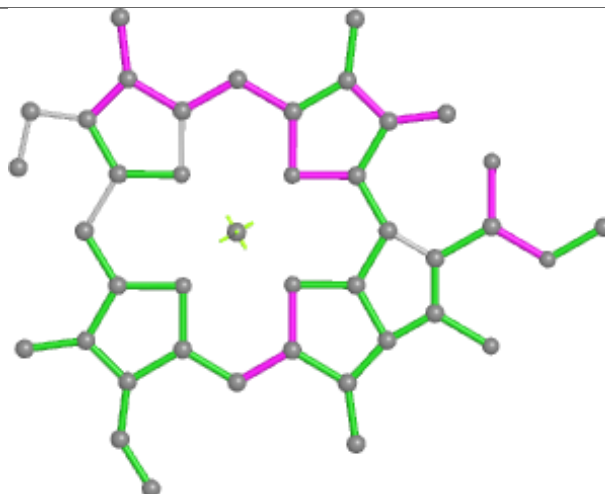
Ligand LUT B3 315



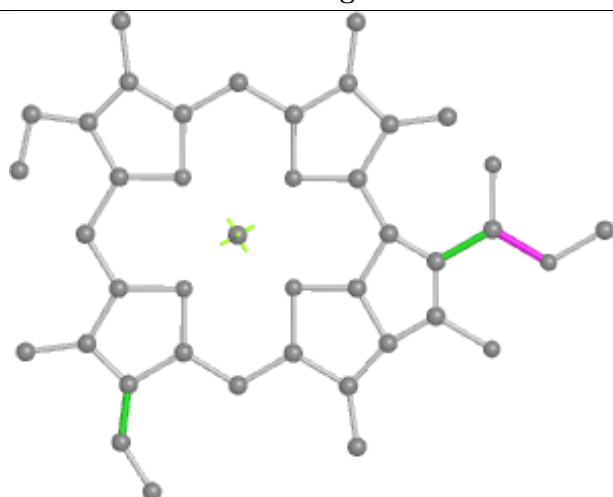
Ligand CLA BF 303



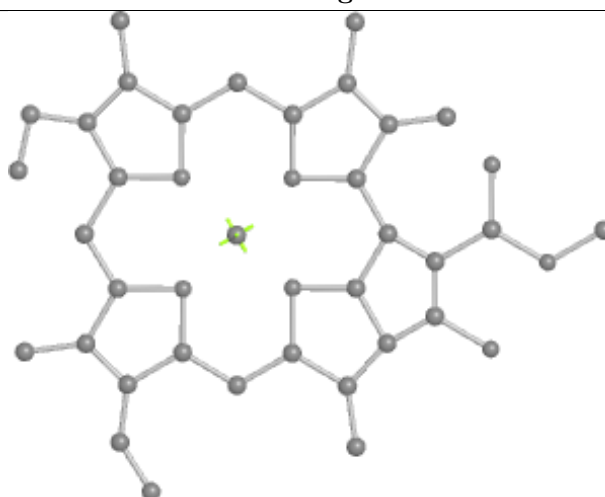
Bond lengths



Bond angles

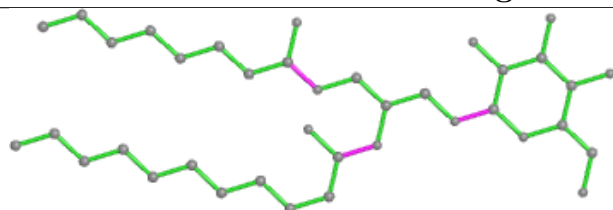


Torsions

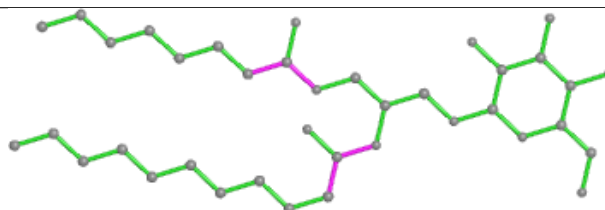


Rings

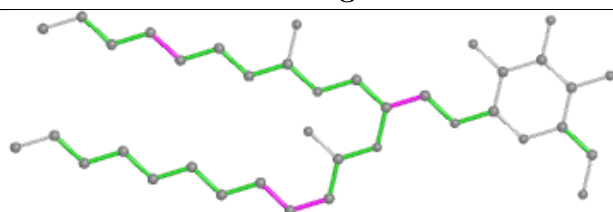
Ligand LMG AG 202



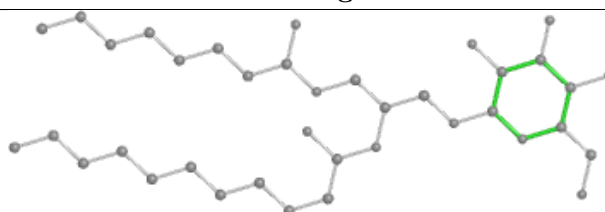
Bond lengths



Bond angles

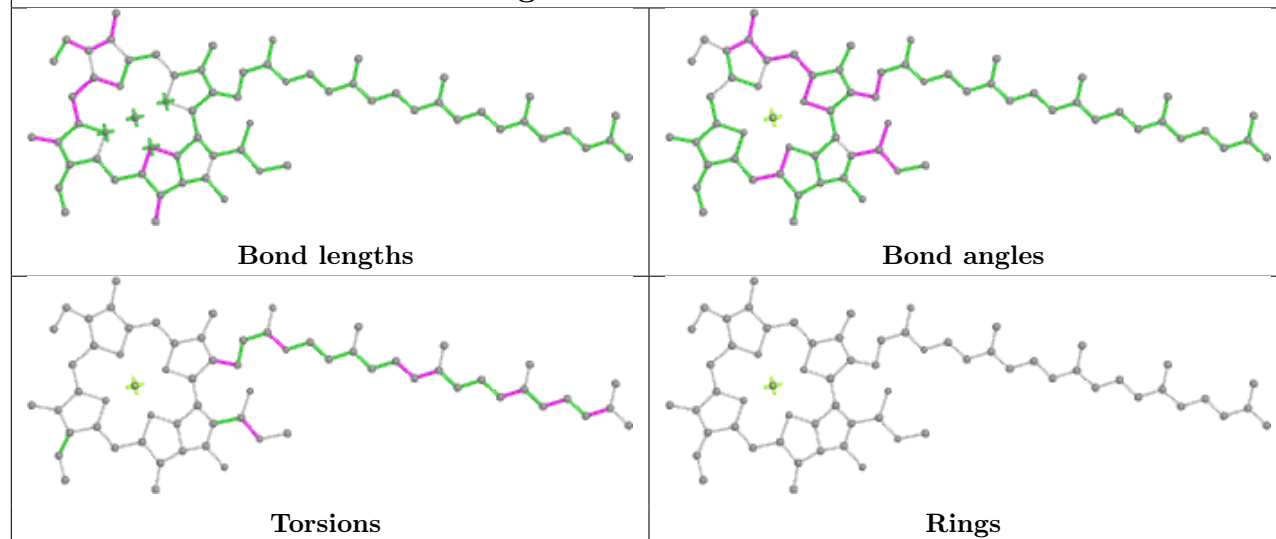


Torsions

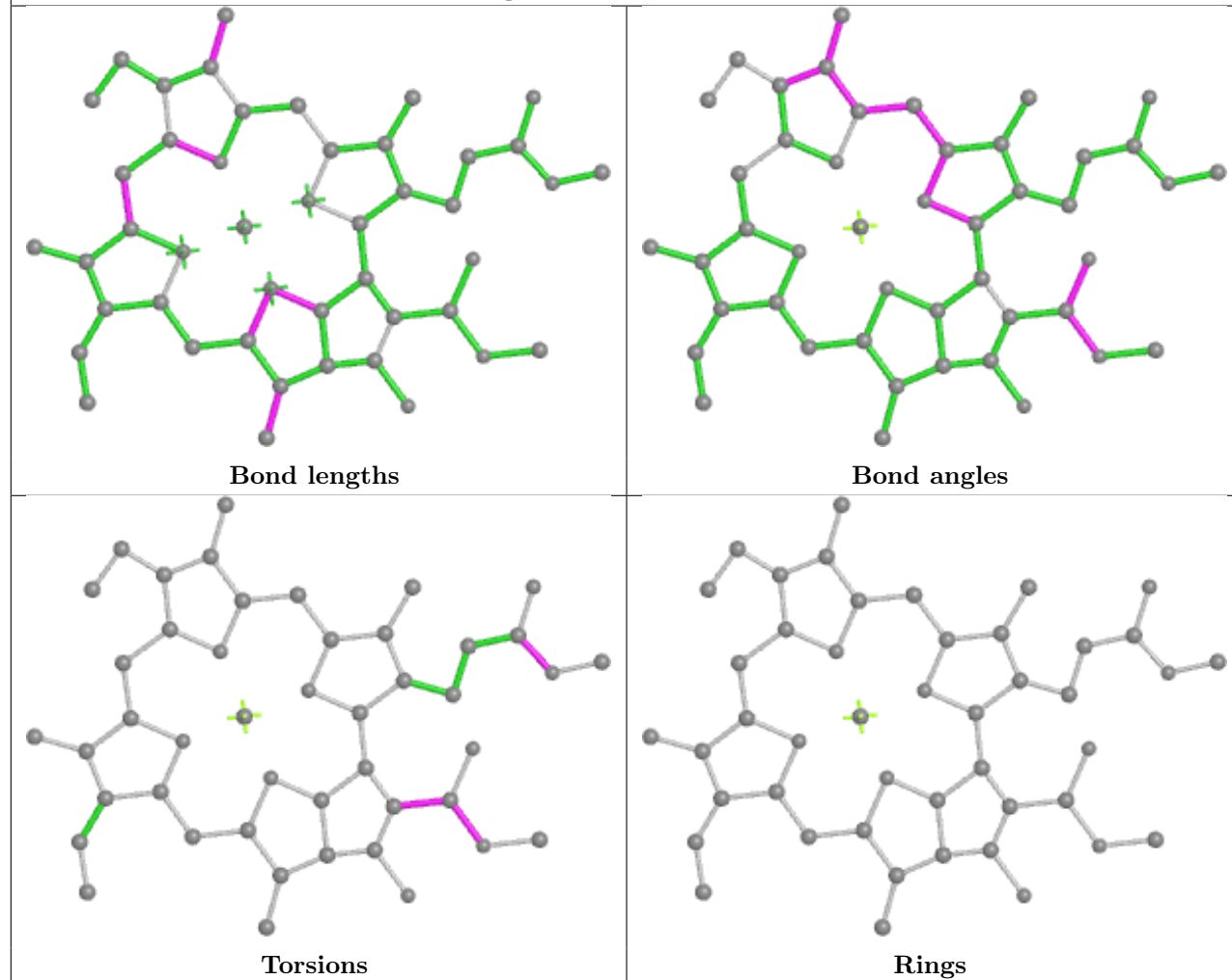


Rings

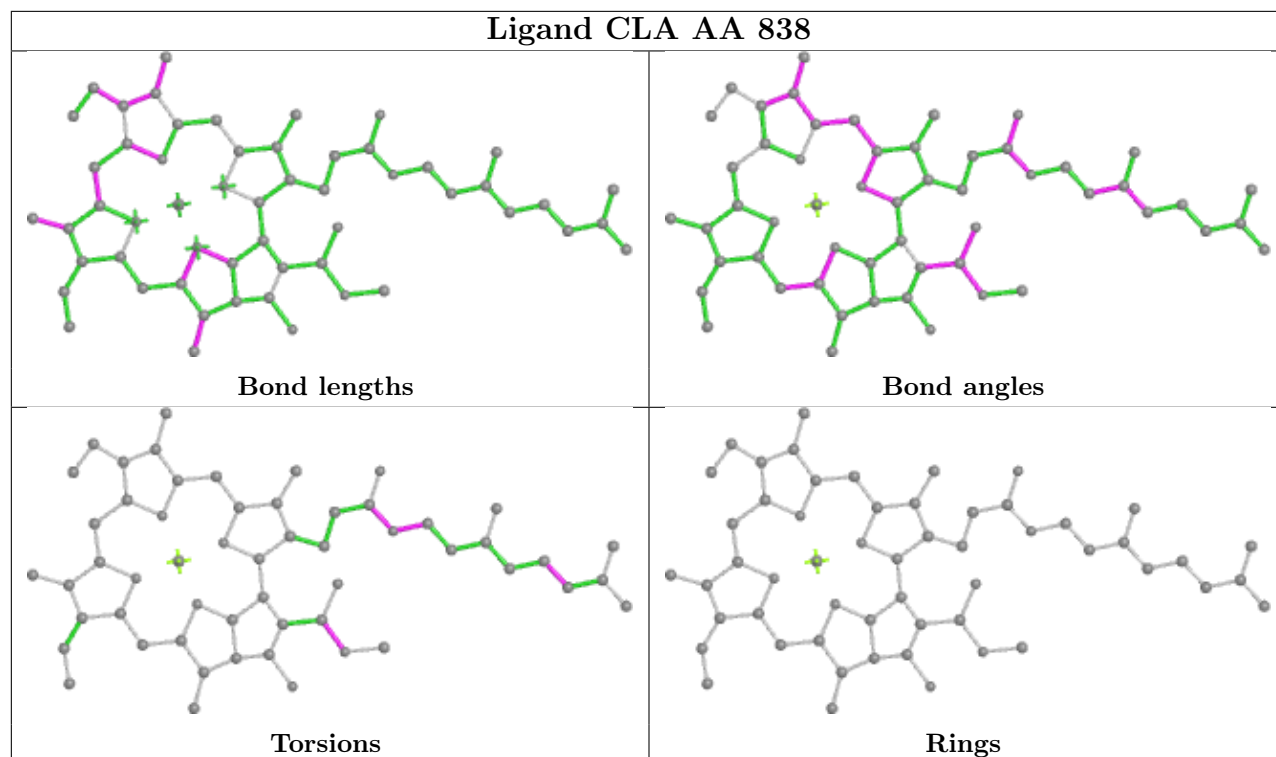
Ligand CLA AA 819



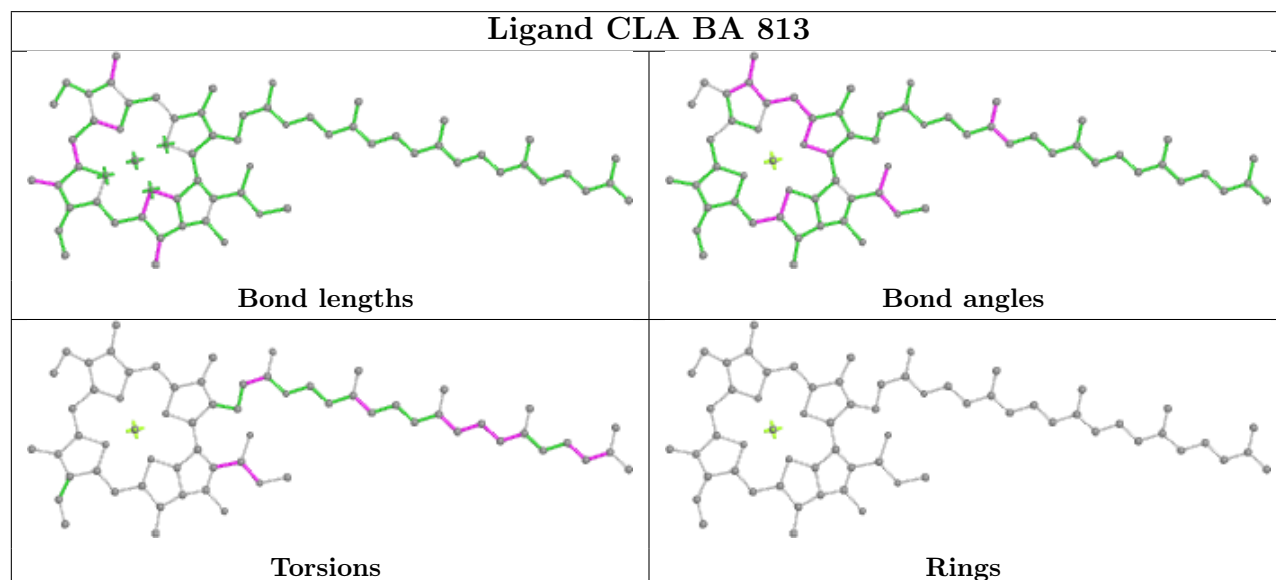
Ligand CLA BK 203



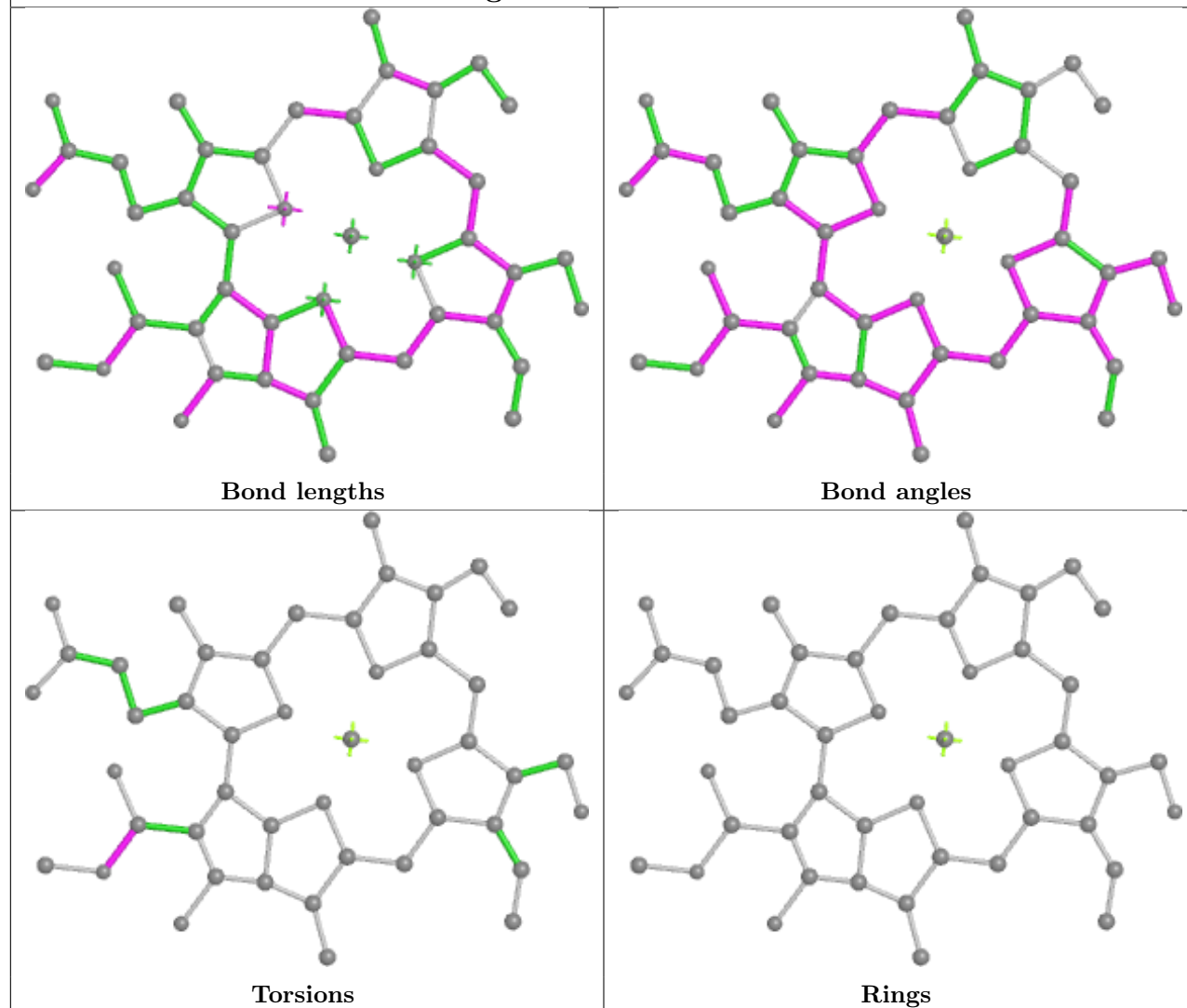
Ligand CLA AA 838

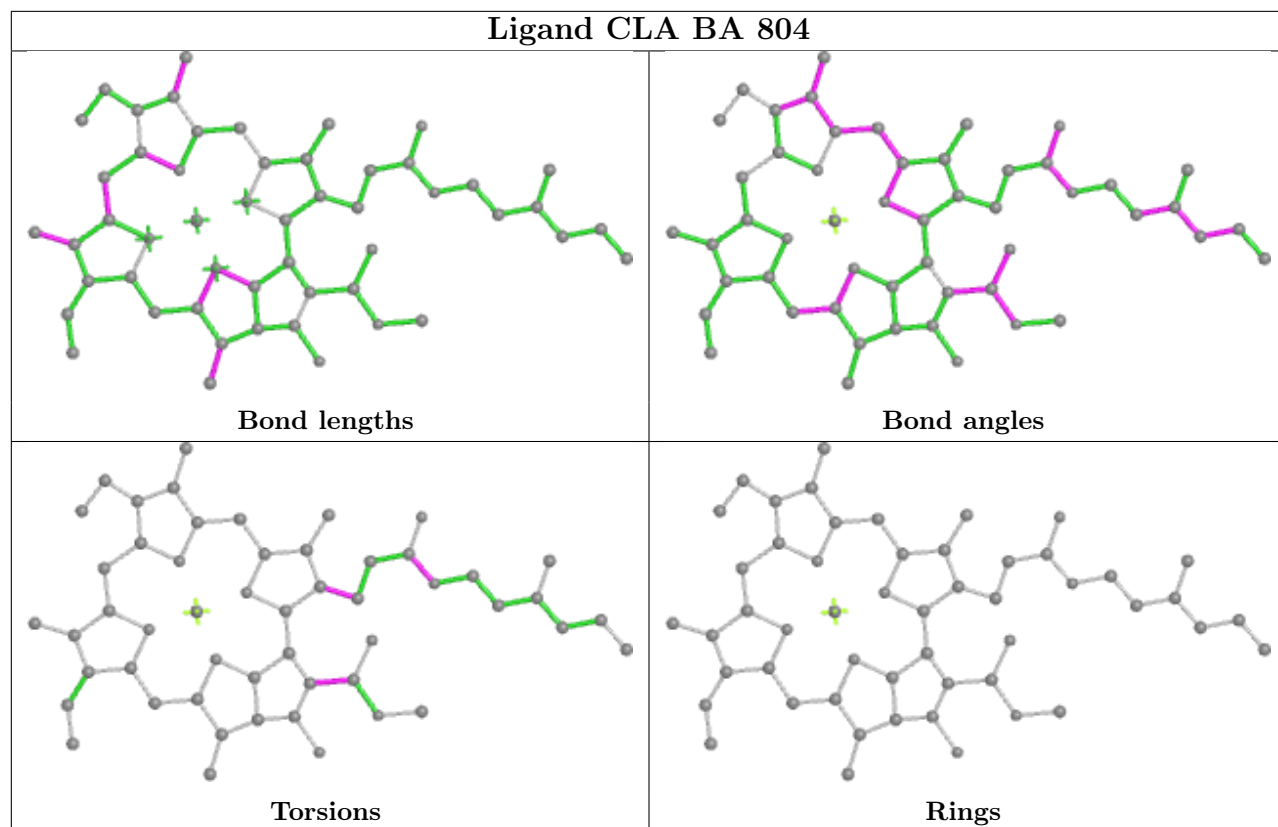


Ligand CLA BA 813

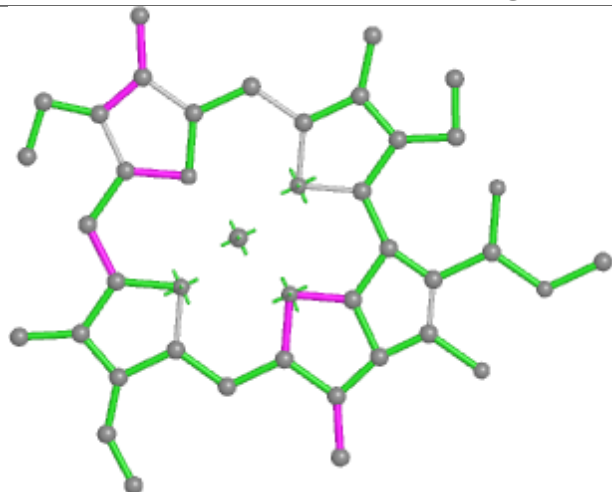


Ligand CHL A4 306

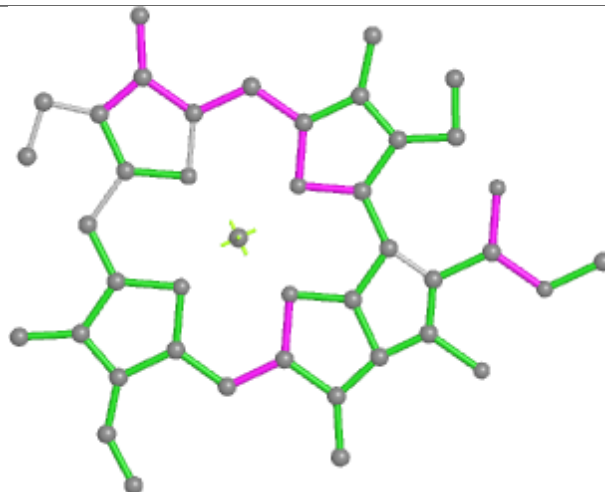




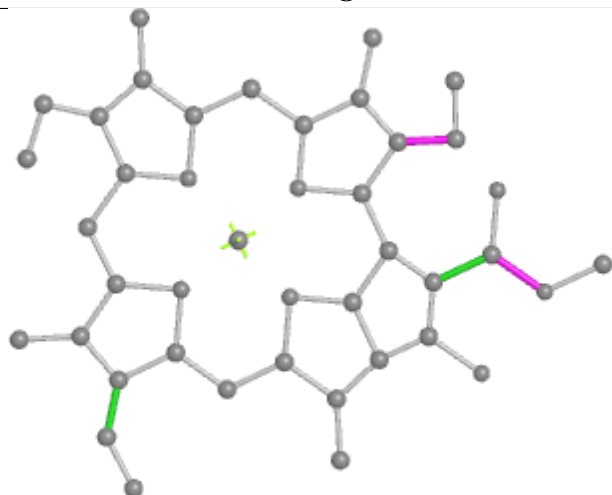
Ligand CLA B5 610



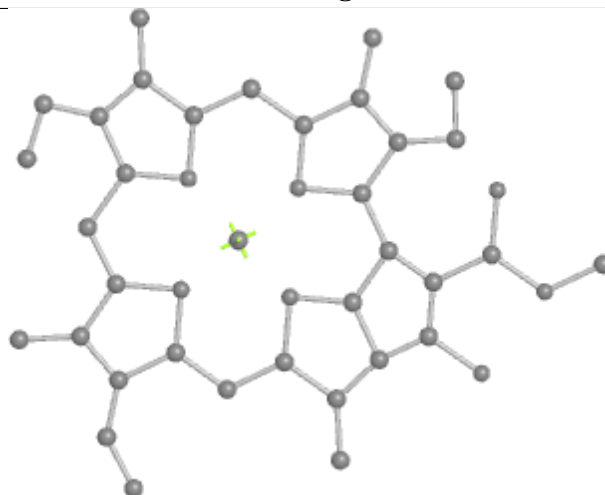
Bond lengths



Bond angles

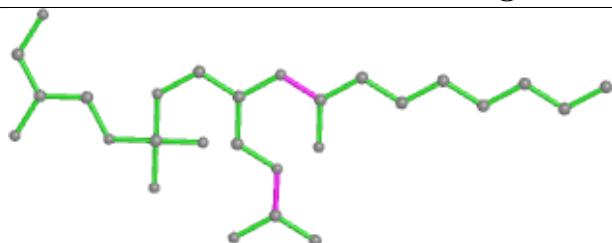


Torsions

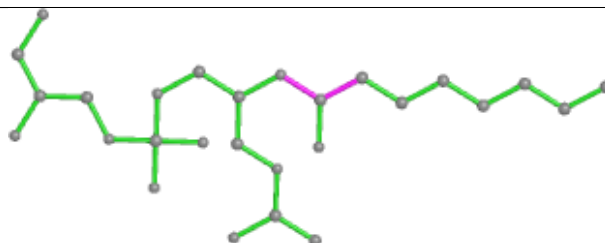


Rings

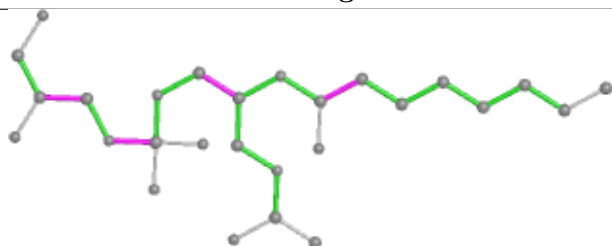
Ligand LHG BA 846



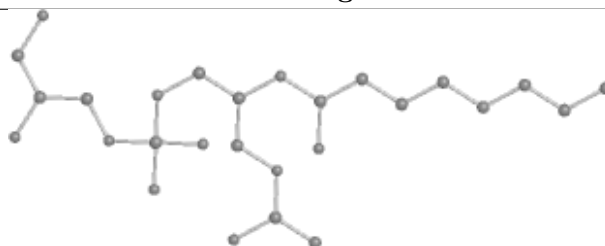
Bond lengths



Bond angles

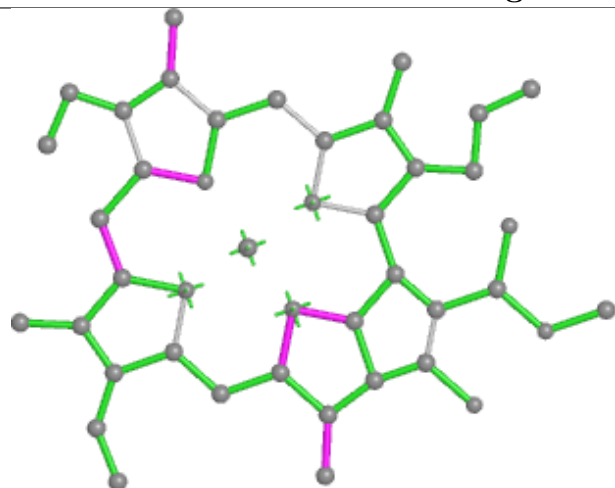


Torsions

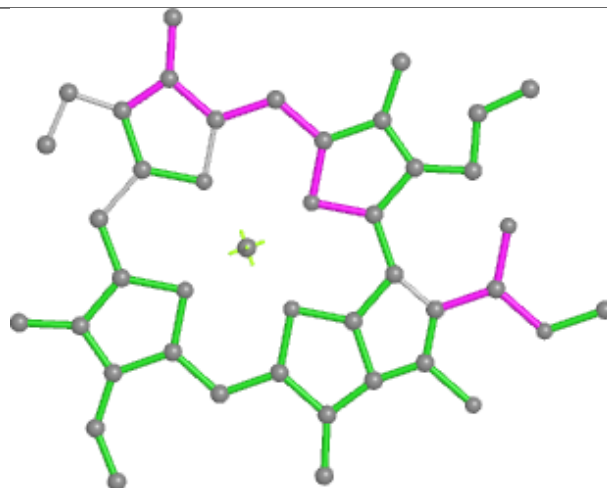


Rings

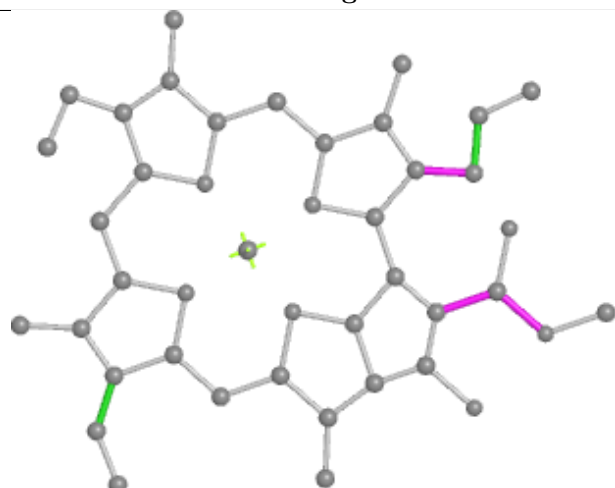
Ligand CLA BL 304



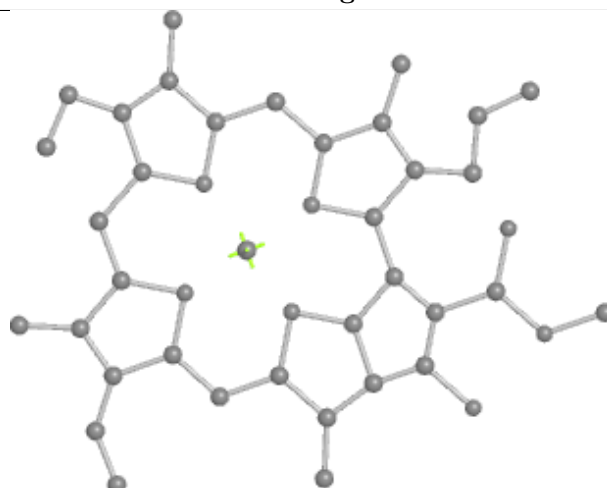
Bond lengths



Bond angles

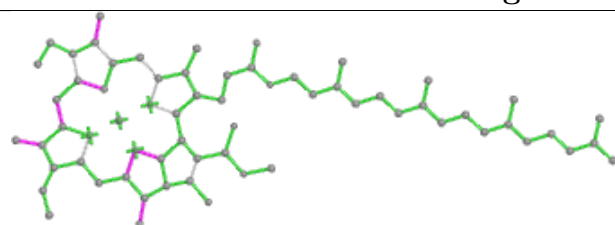


Torsions

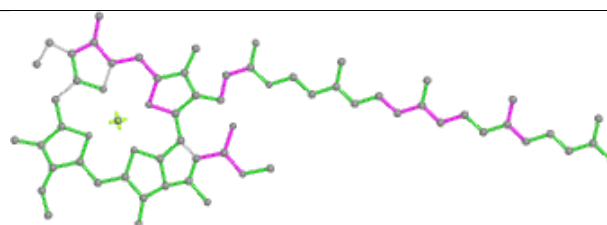


Rings

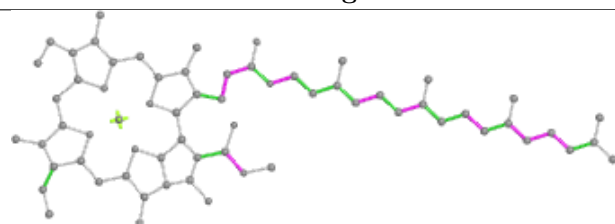
Ligand CLA BA 828



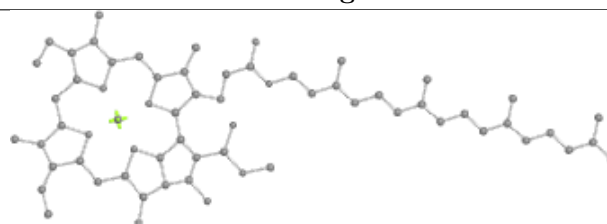
Bond lengths



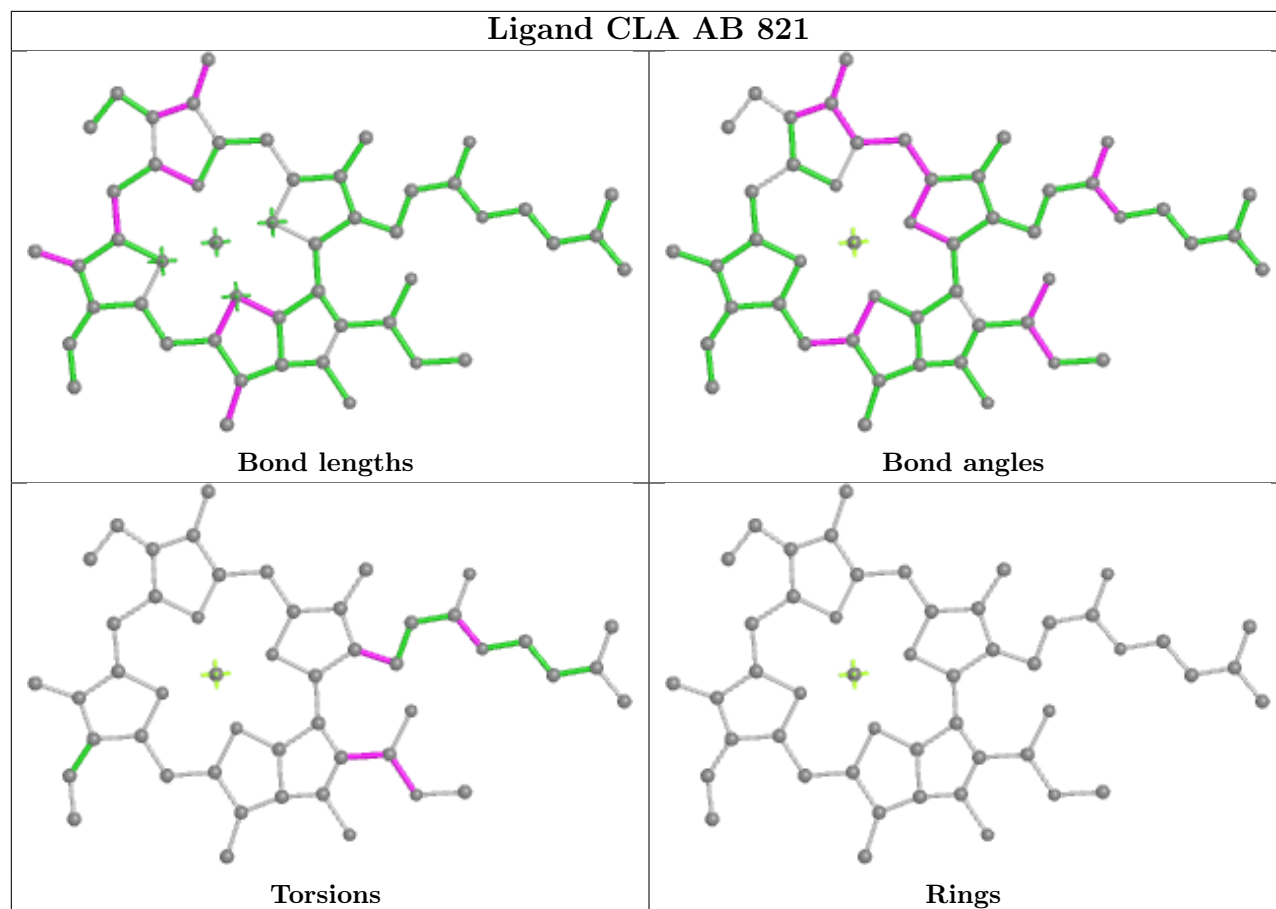
Bond angles



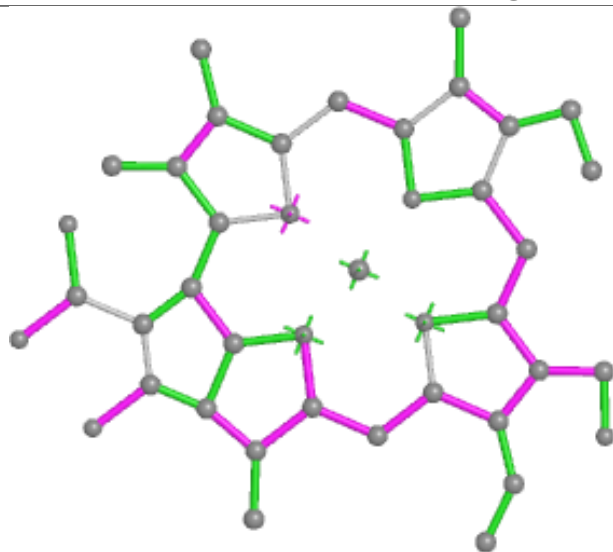
Torsions



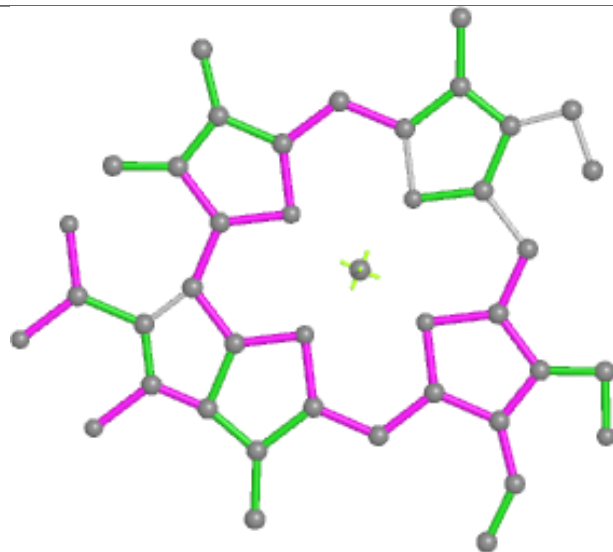
Rings



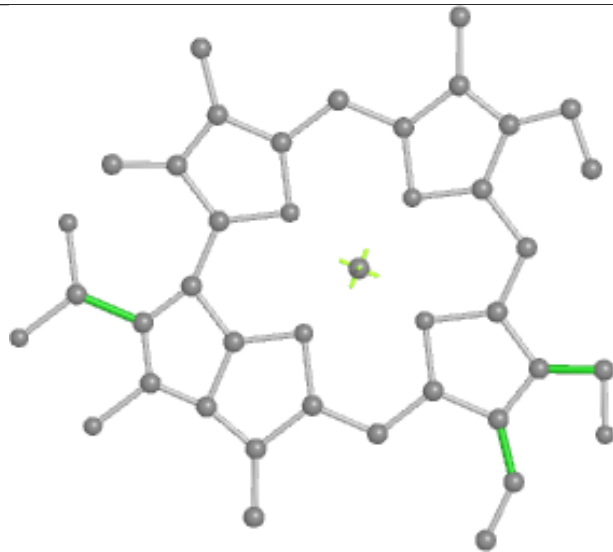
Ligand CHL B1 308



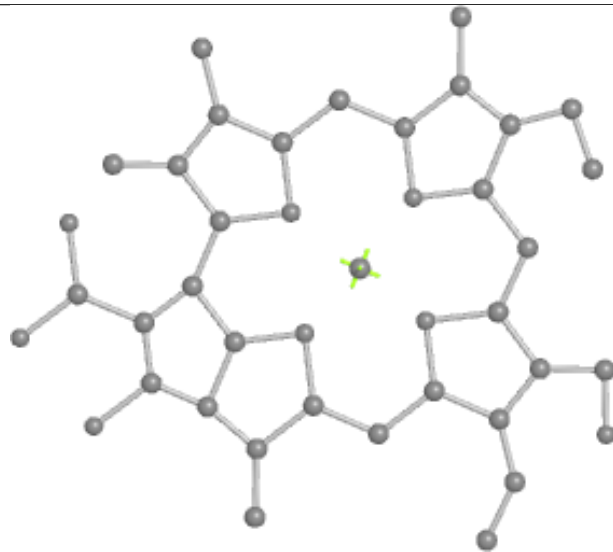
Bond lengths



Bond angles

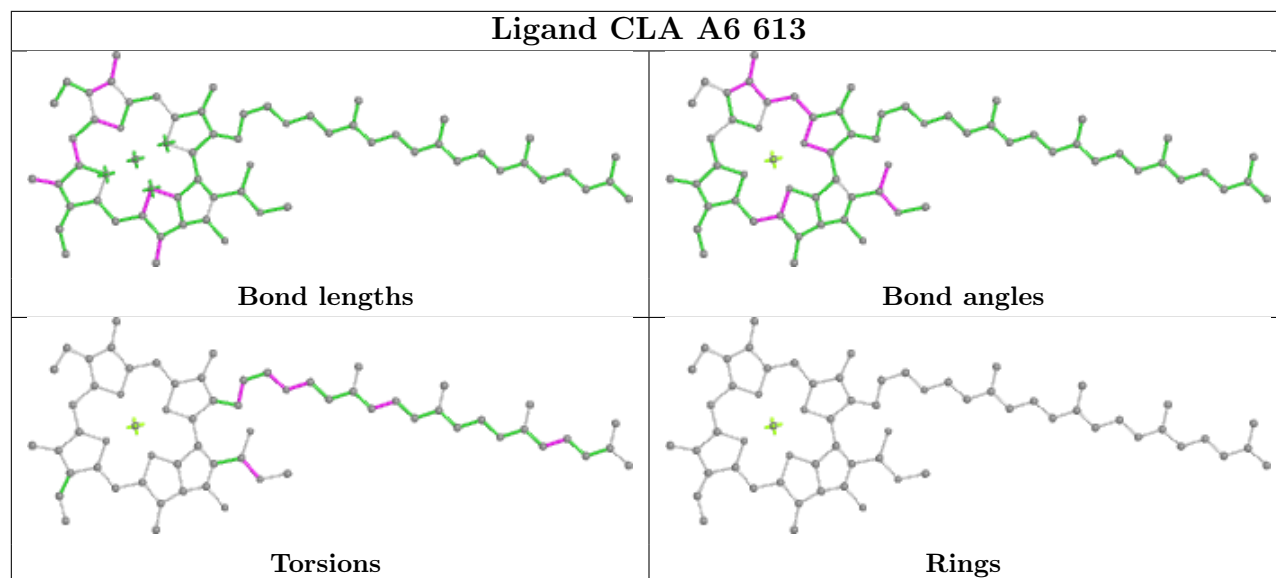


Torsions

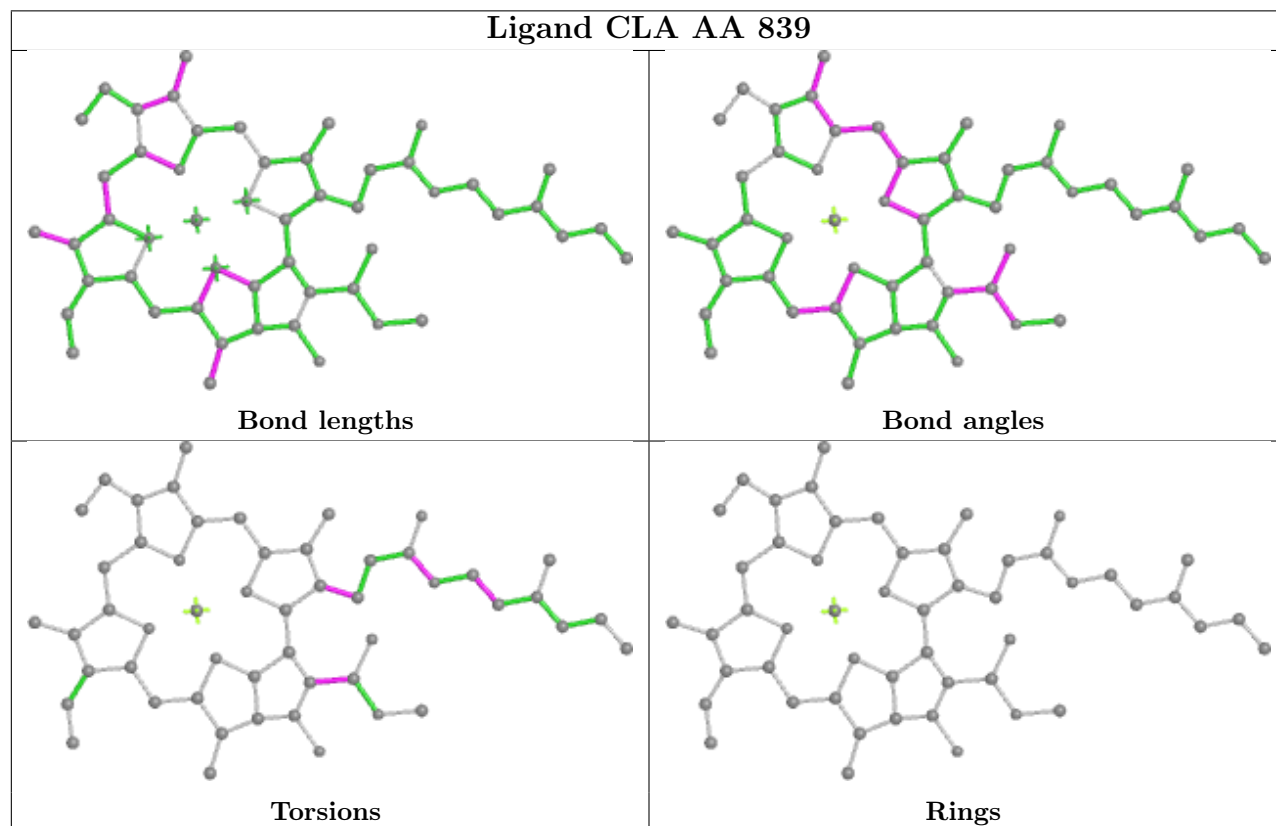


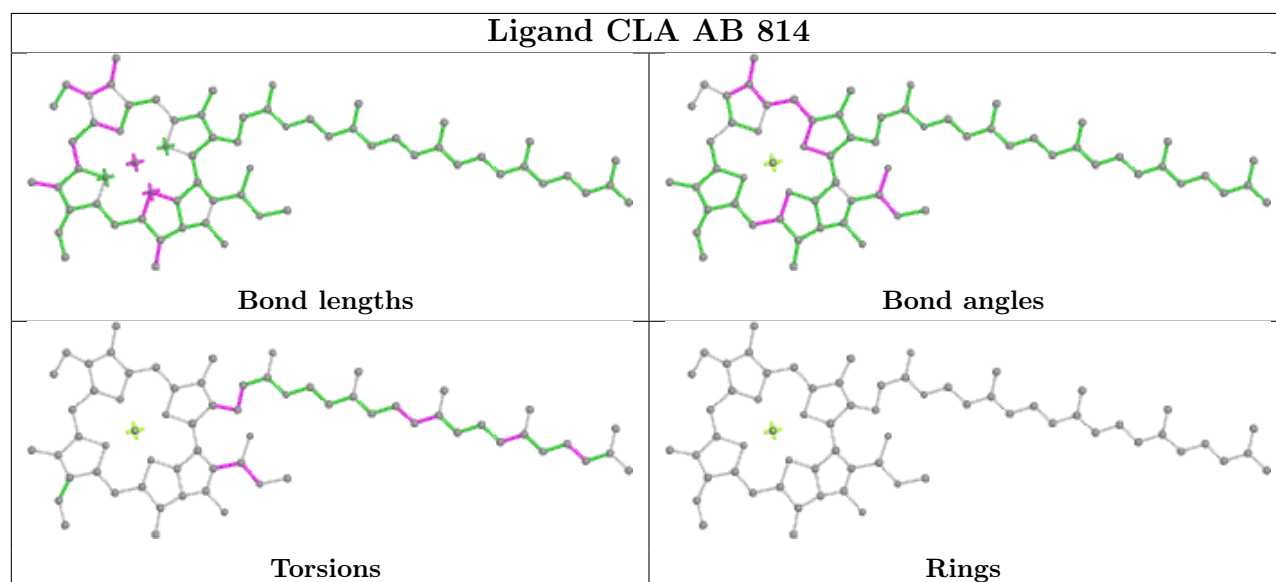
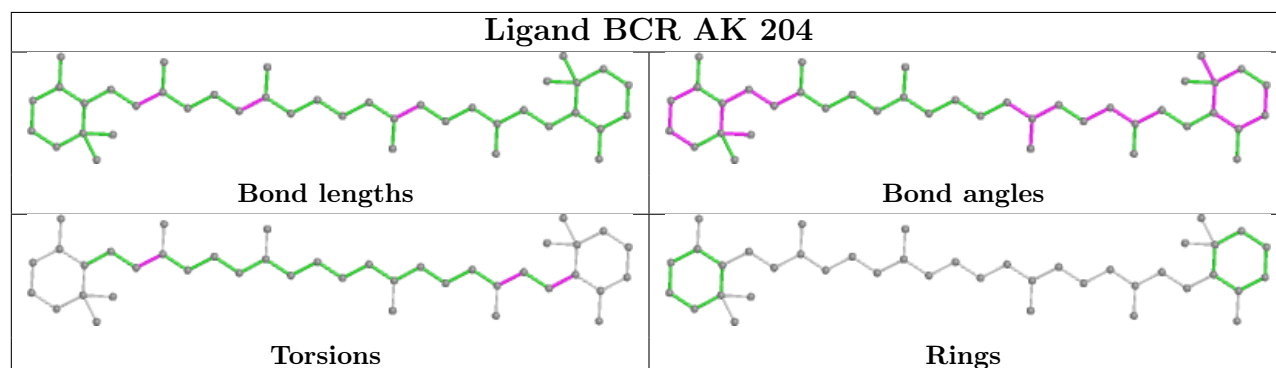
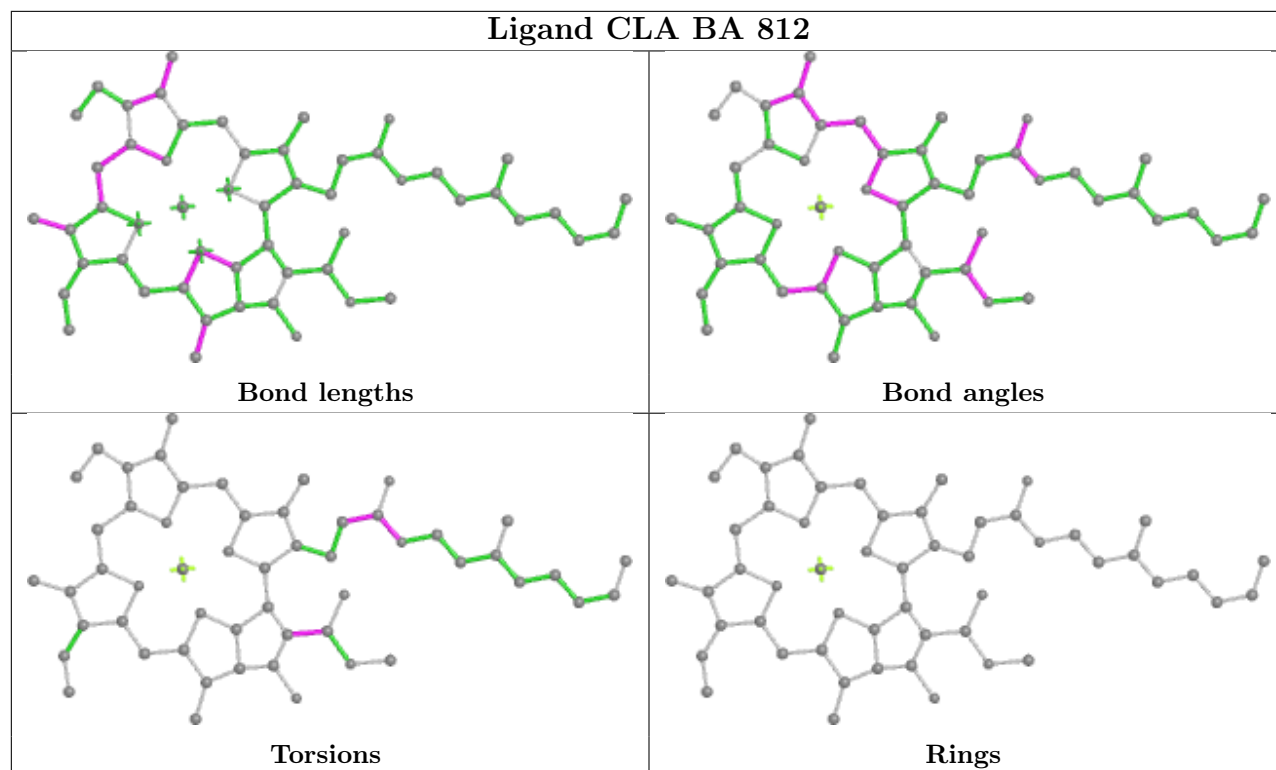
Rings

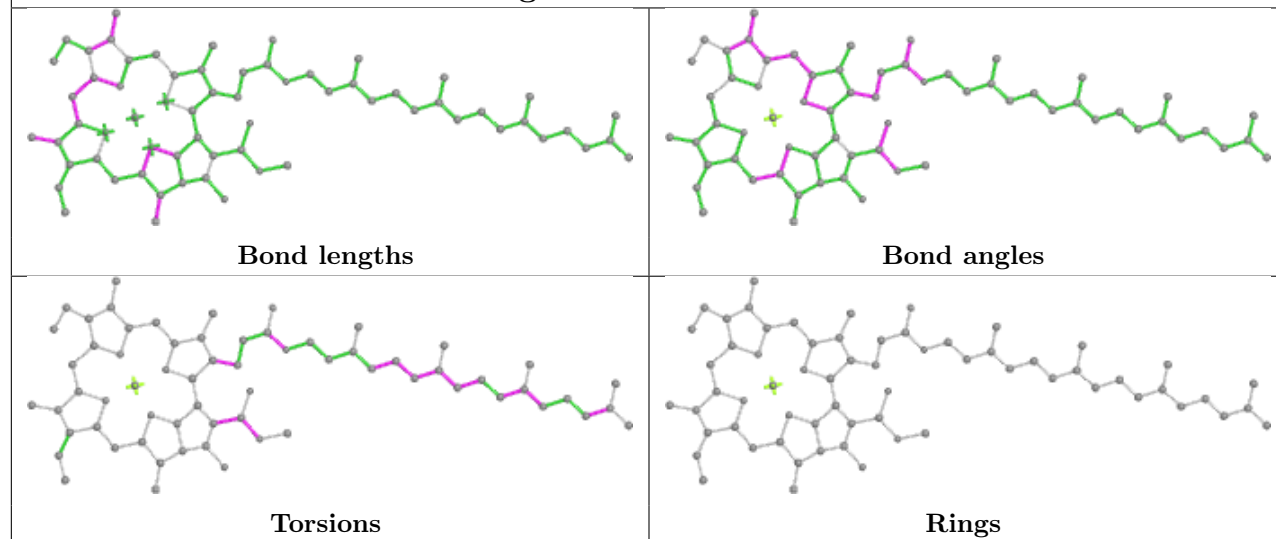
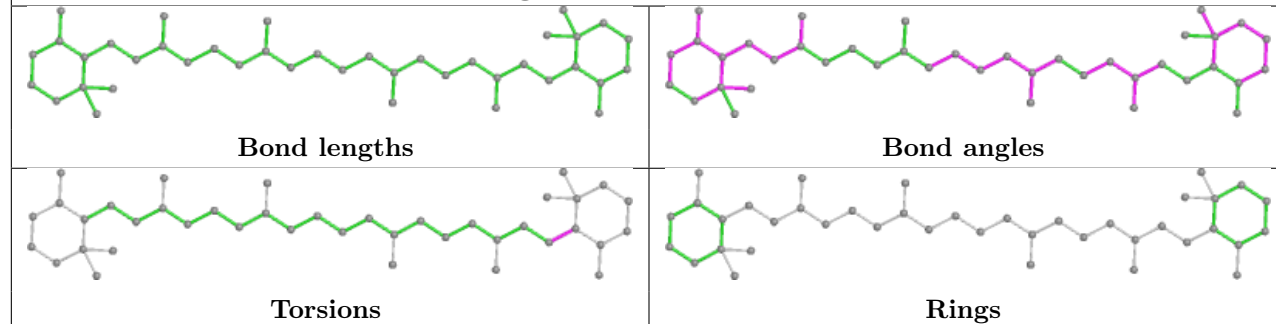
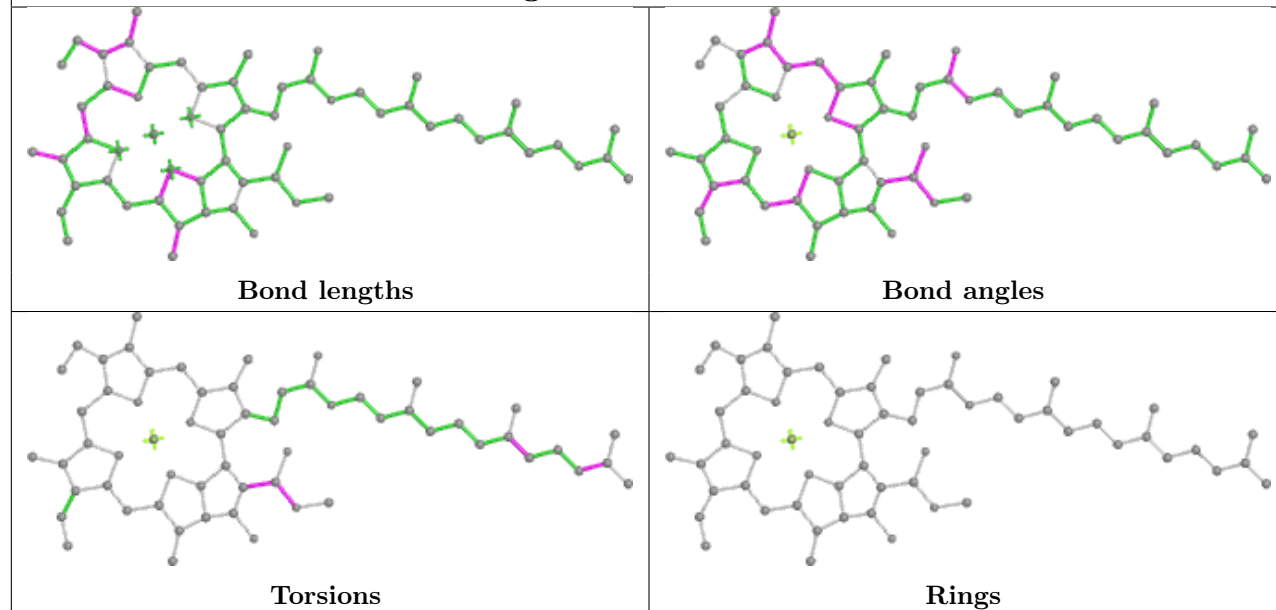
Ligand CLA A6 613

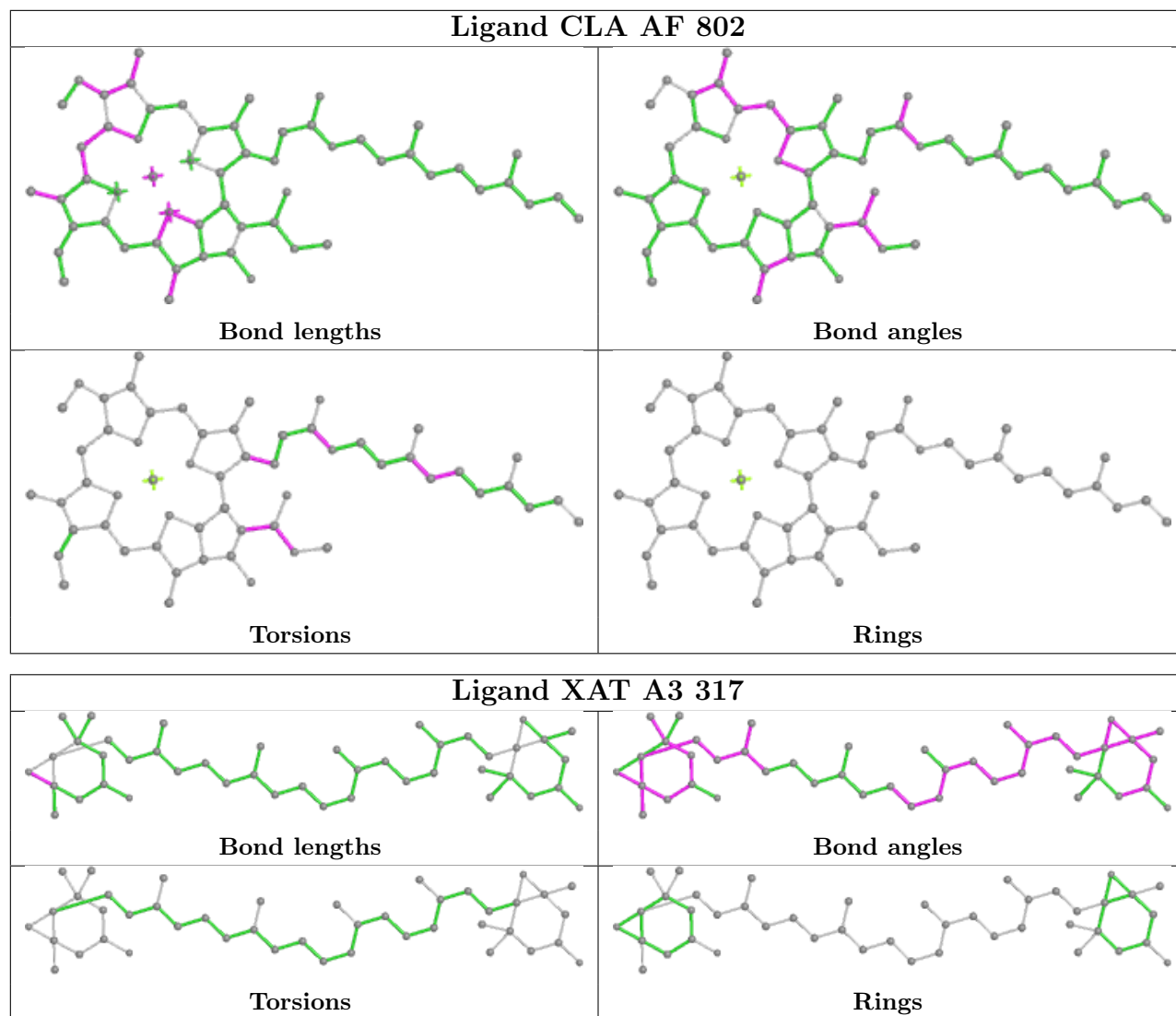


Ligand CLA AA 839

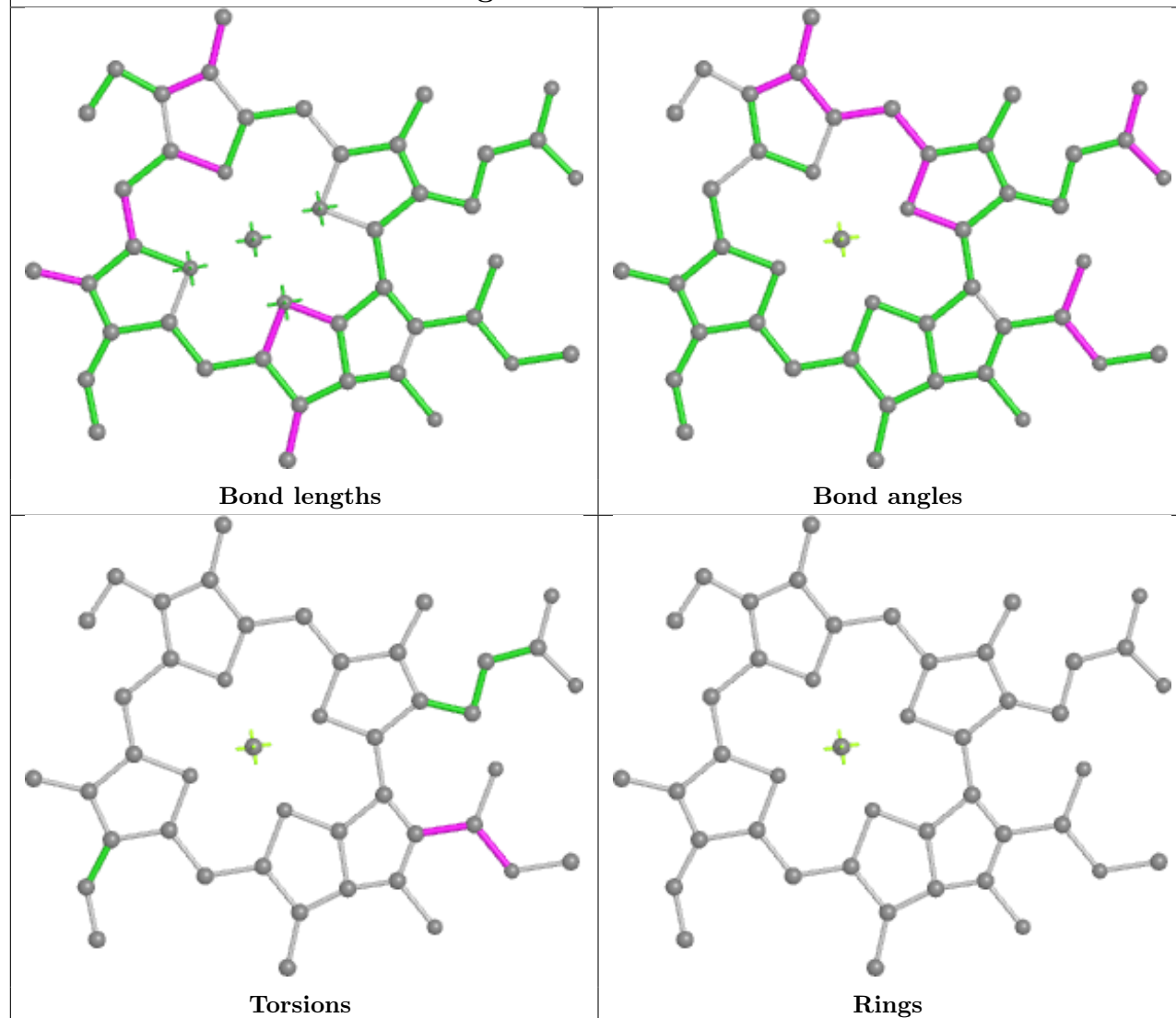




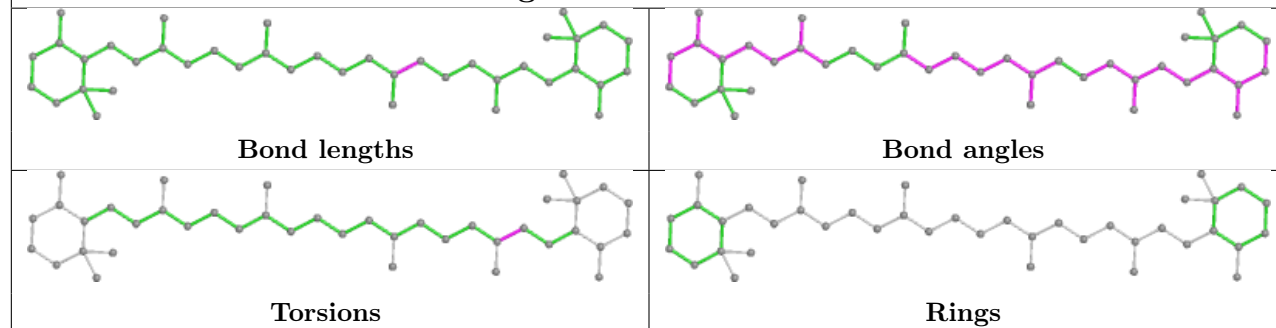
Ligand CLA AB 823**Ligand BCR AG 205****Ligand CLA A4 301**



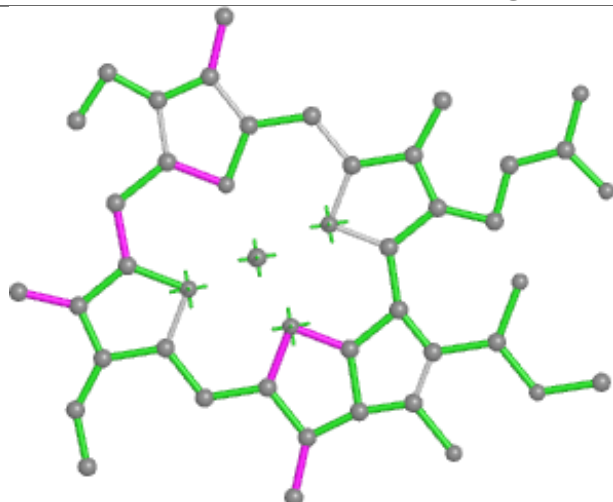
Ligand CLA AA 820



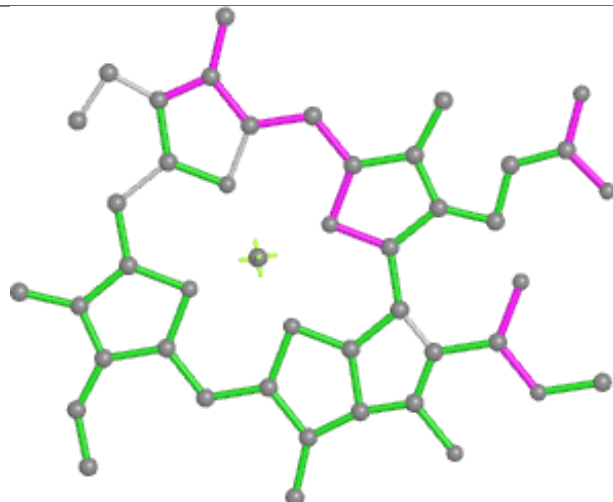
Ligand BCR BB 849



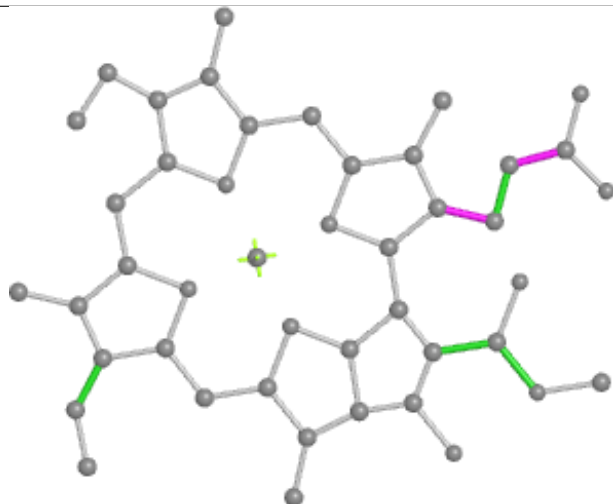
Ligand CLA A6 609



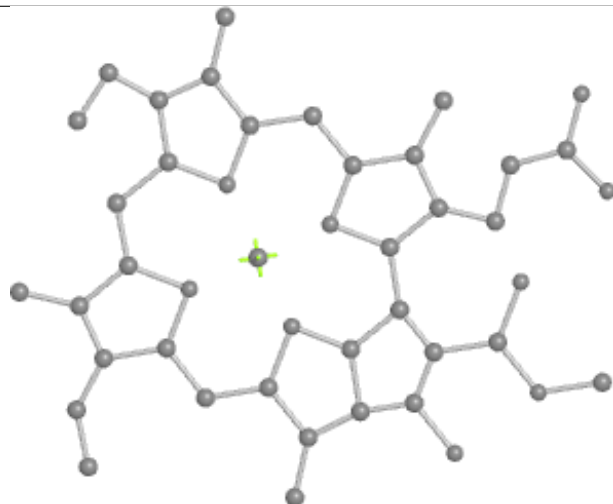
Bond lengths



Bond angles

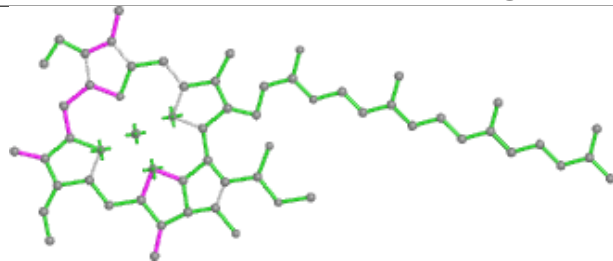


Torsions

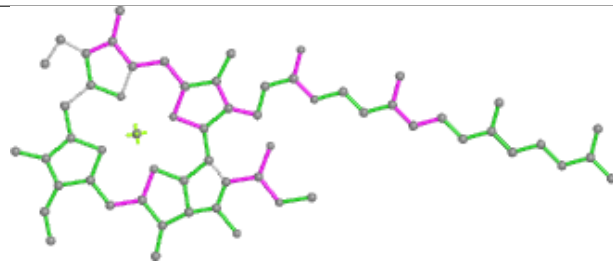


Rings

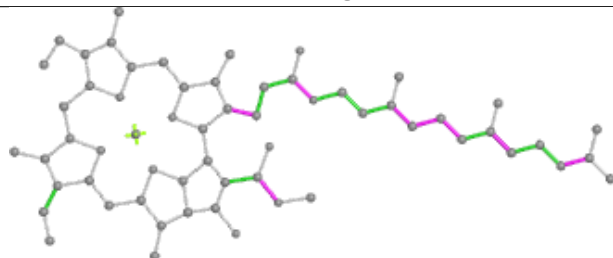
Ligand CLA AB 819



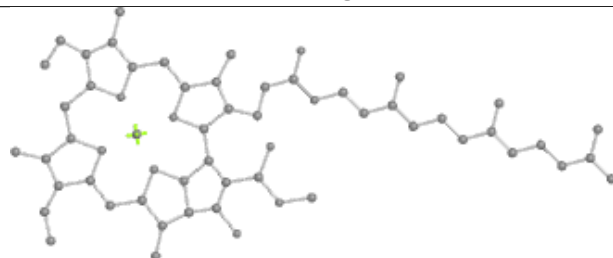
Bond lengths



Bond angles

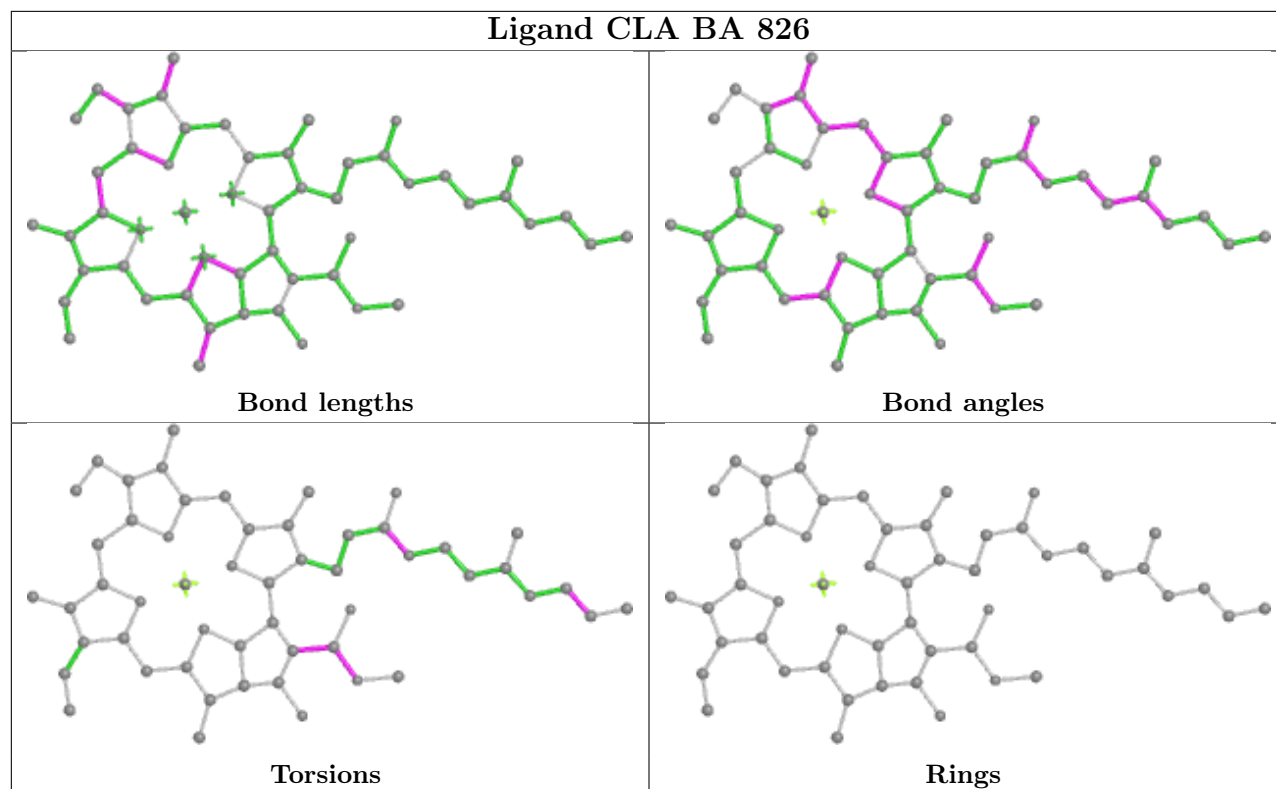


Torsions

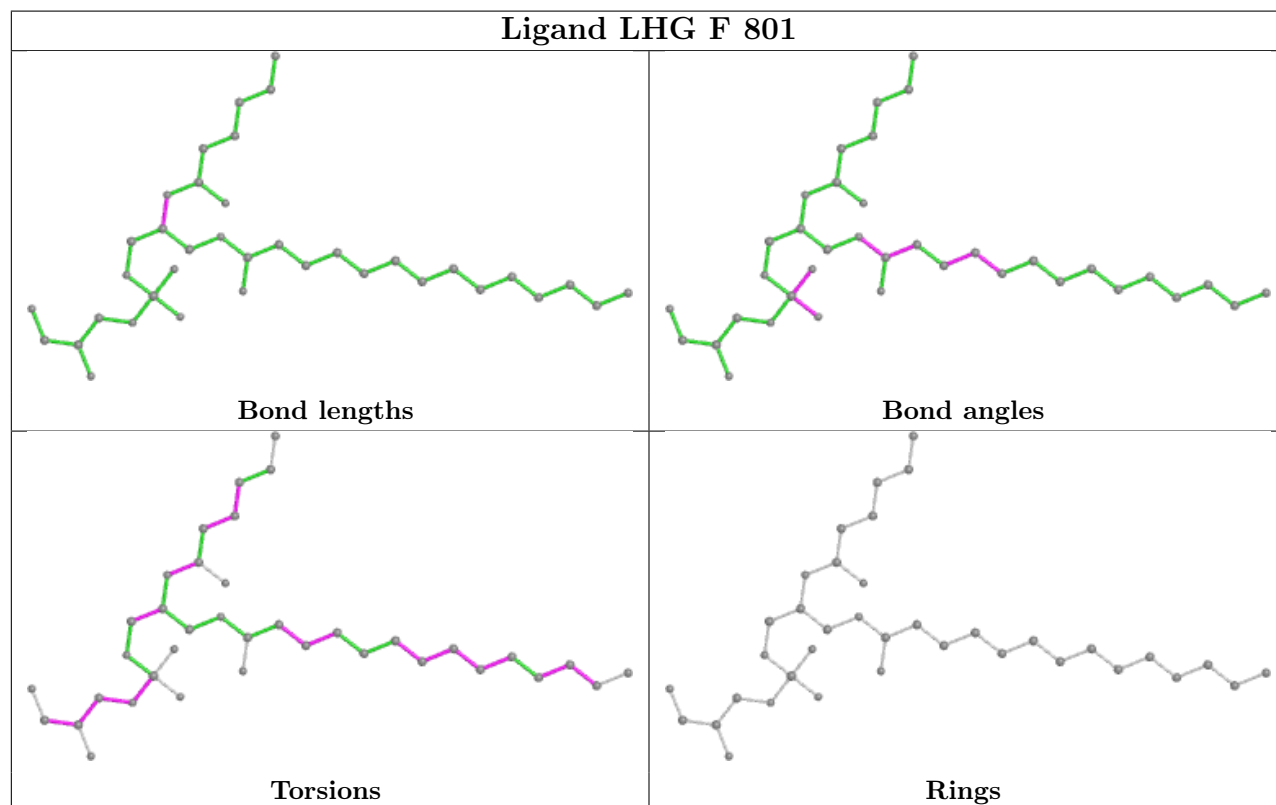


Rings

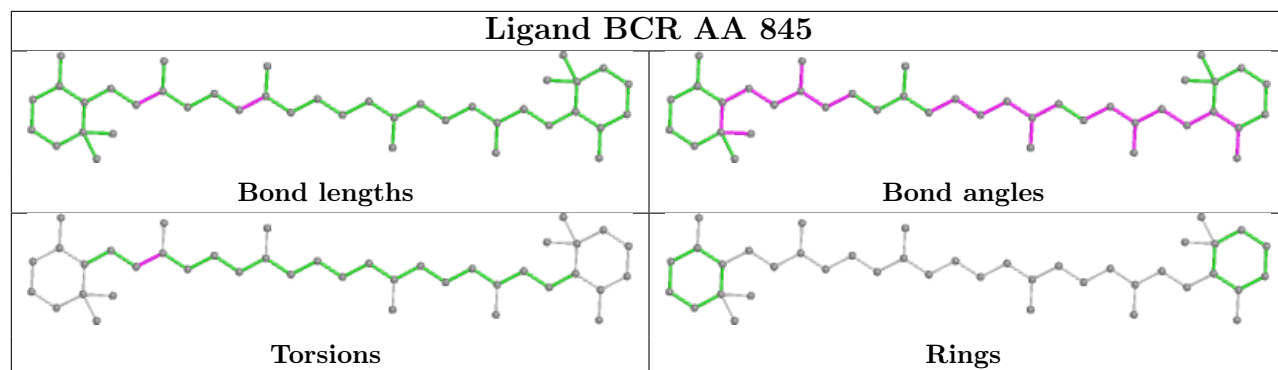
Ligand CLA BA 826



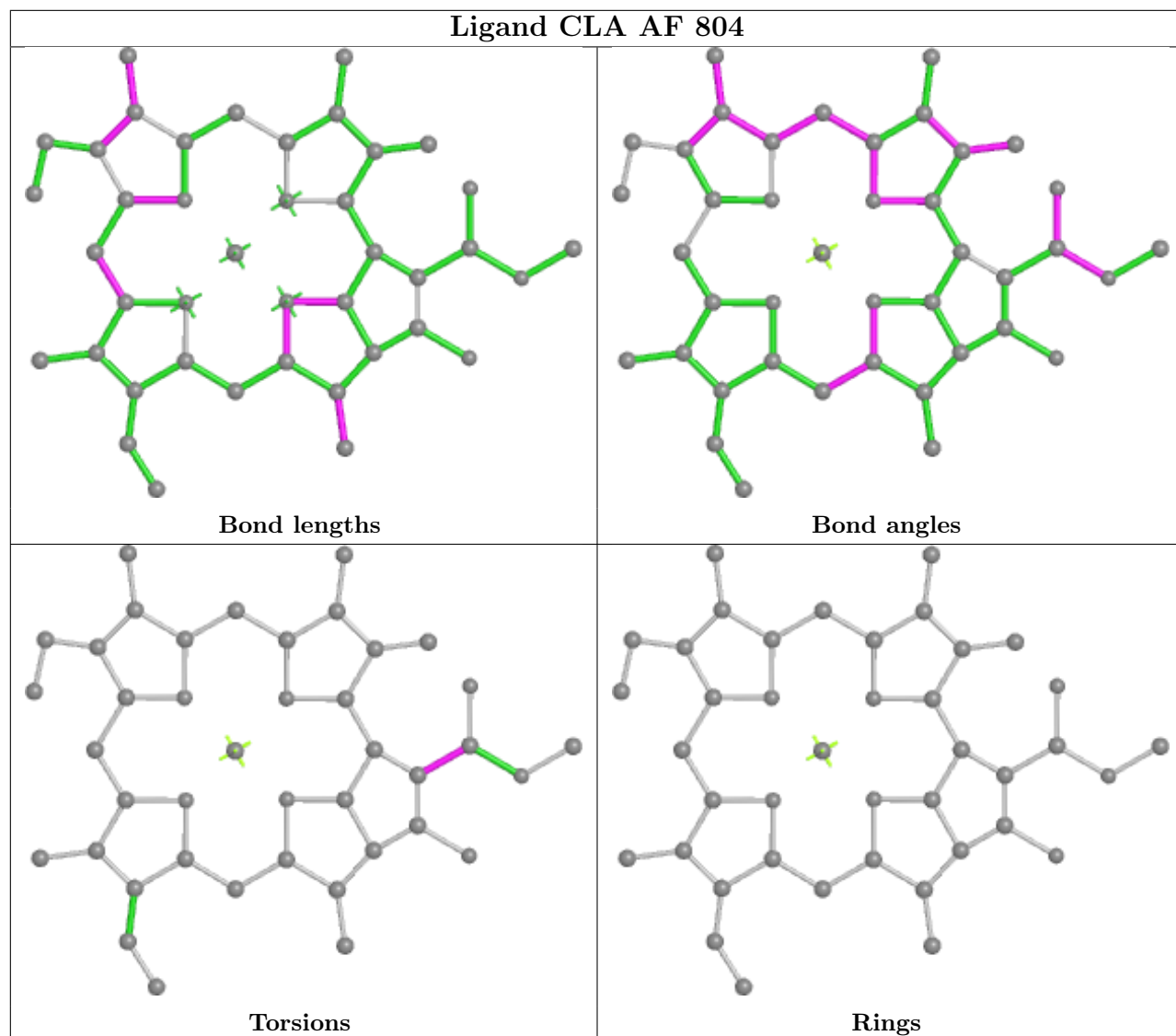
Ligand LHG F 801



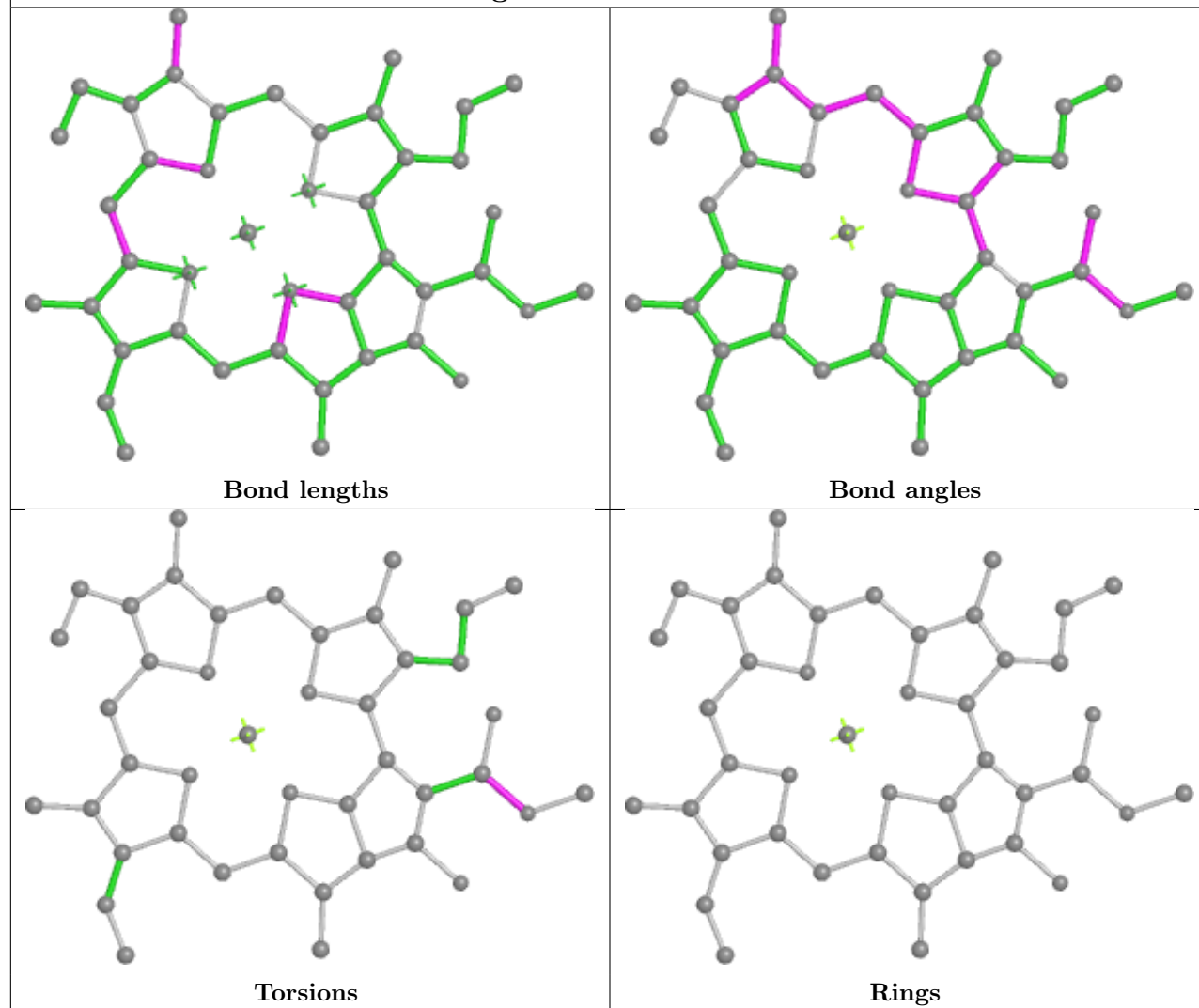
Ligand BCR AA 845



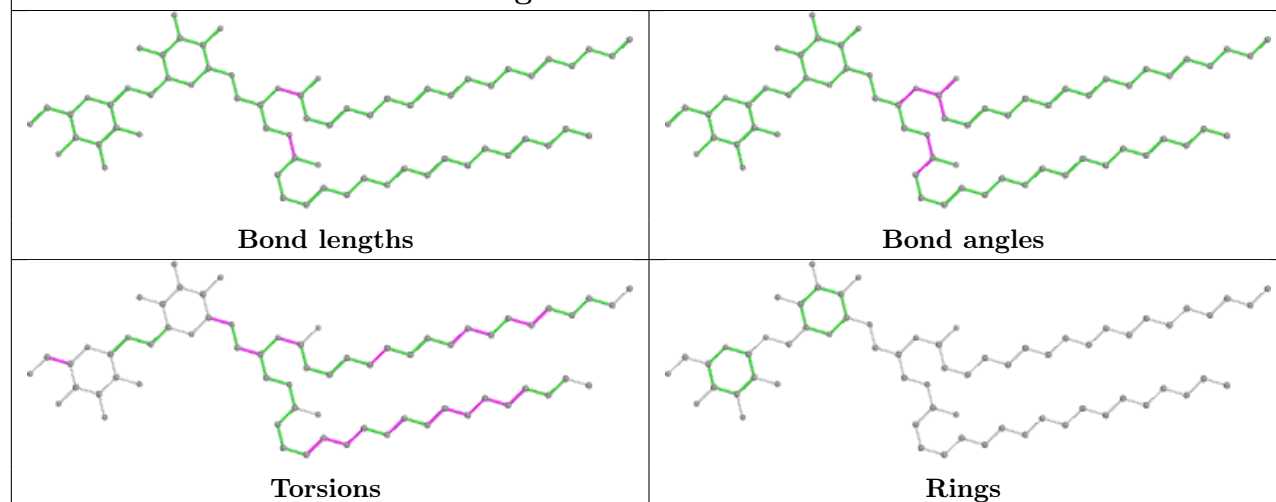
Ligand CLA AF 804



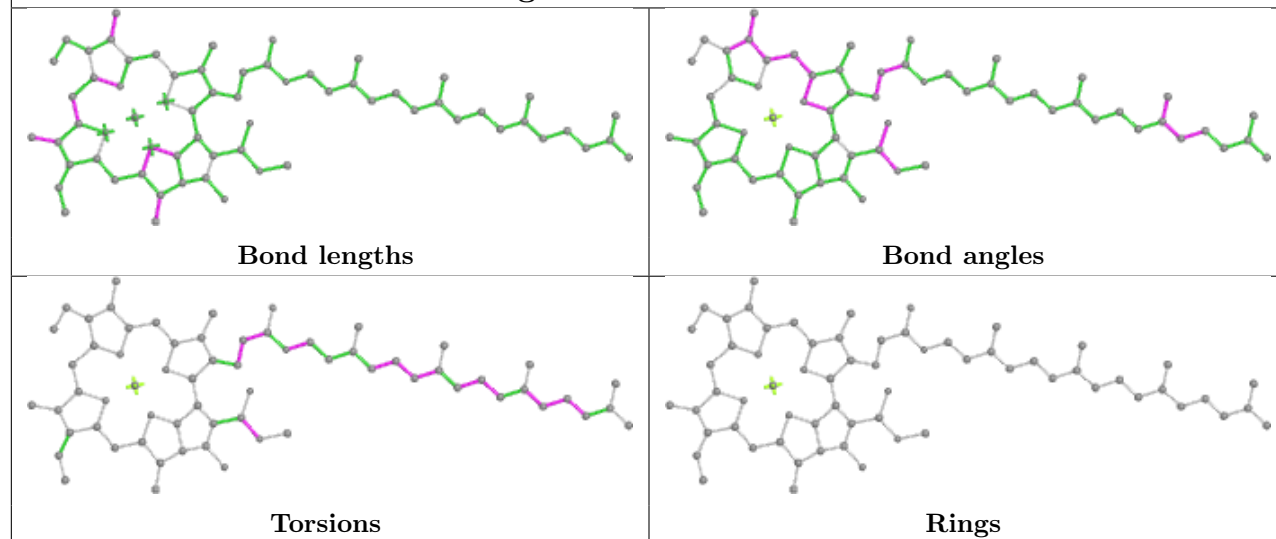
Ligand CLA B3 310



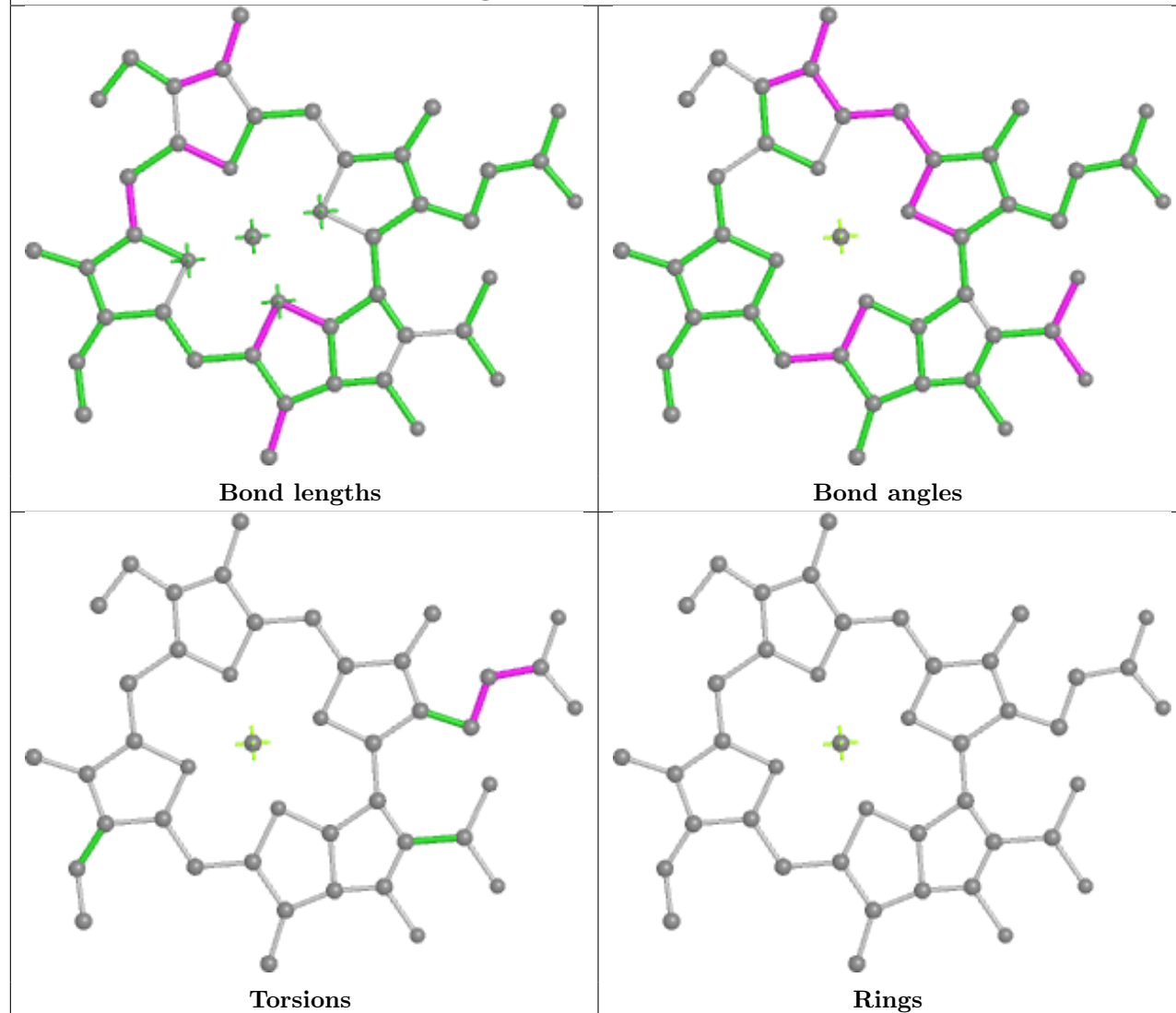
Ligand DGD AB 851

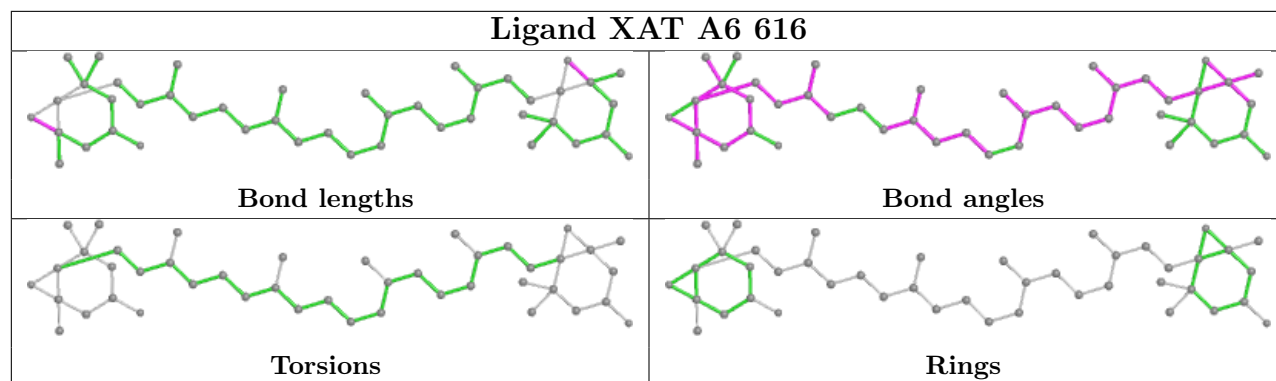
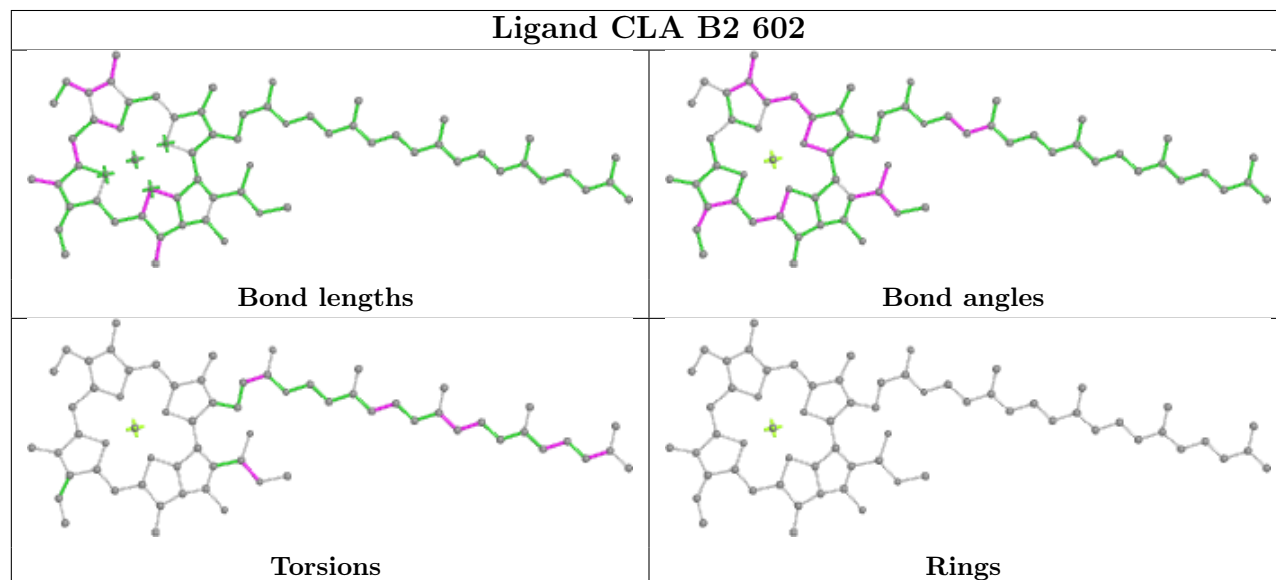
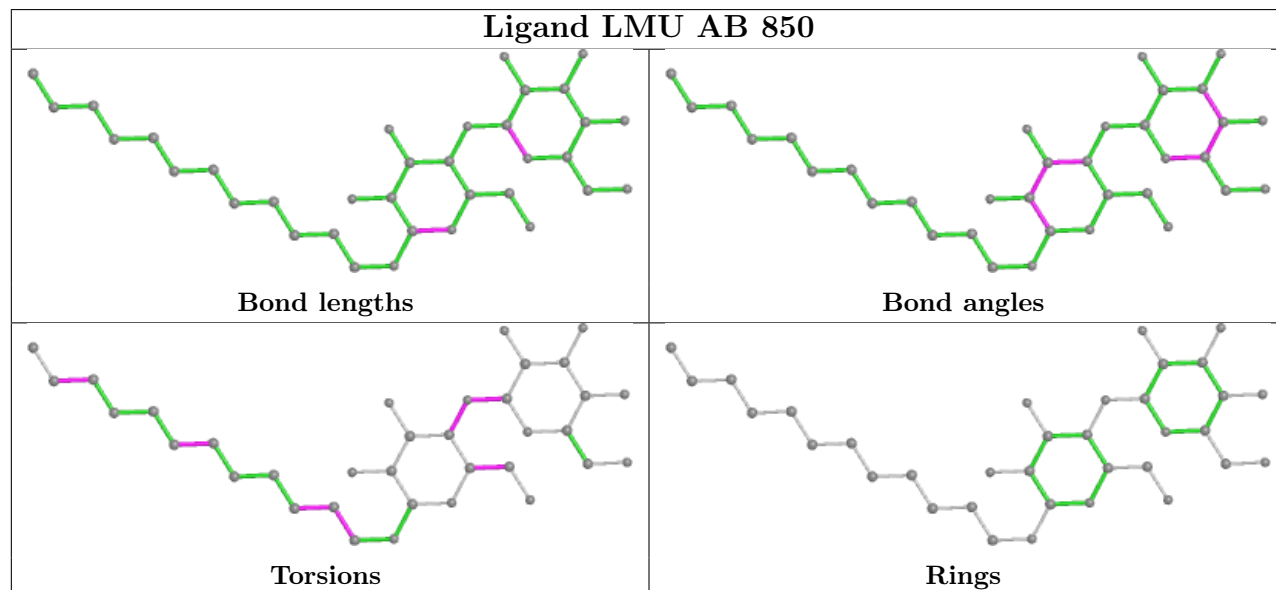


Ligand CLA AA 828

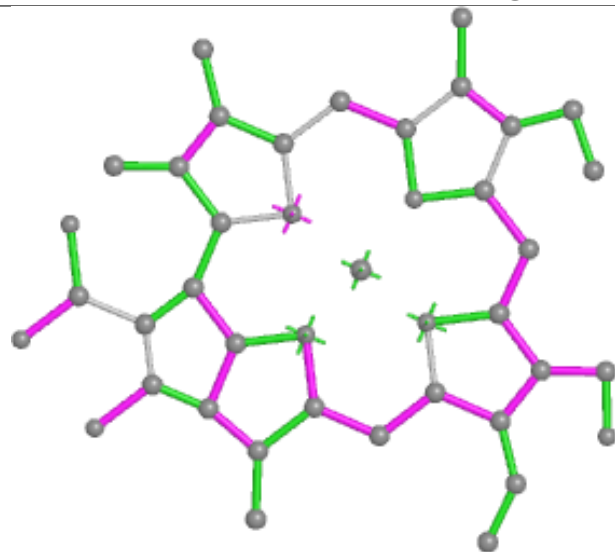


Ligand CLA AG 201

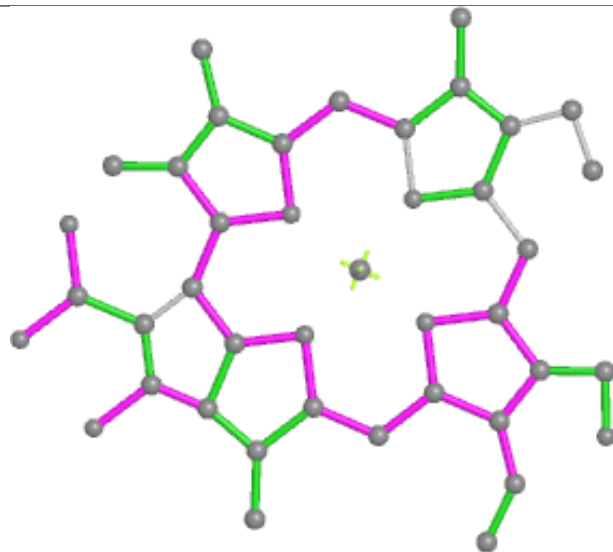


Ligand XAT A6 616**Ligand CLA B2 602****Ligand LMU AB 850**

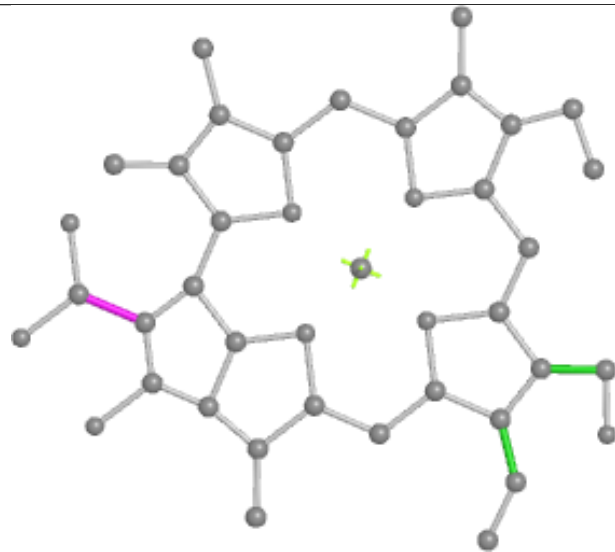
Ligand CHL A1 308



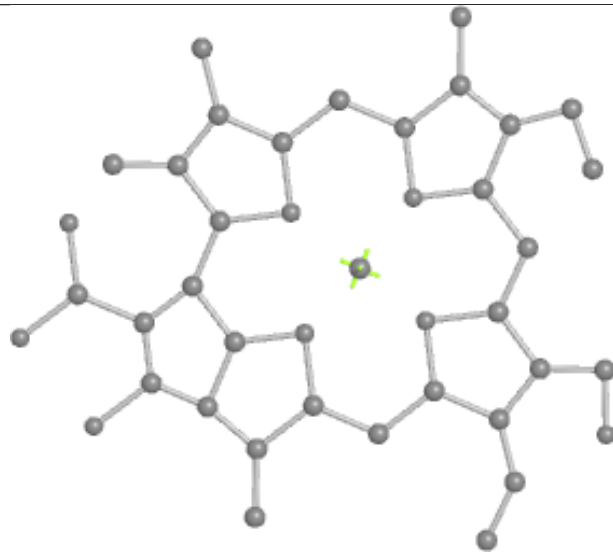
Bond lengths



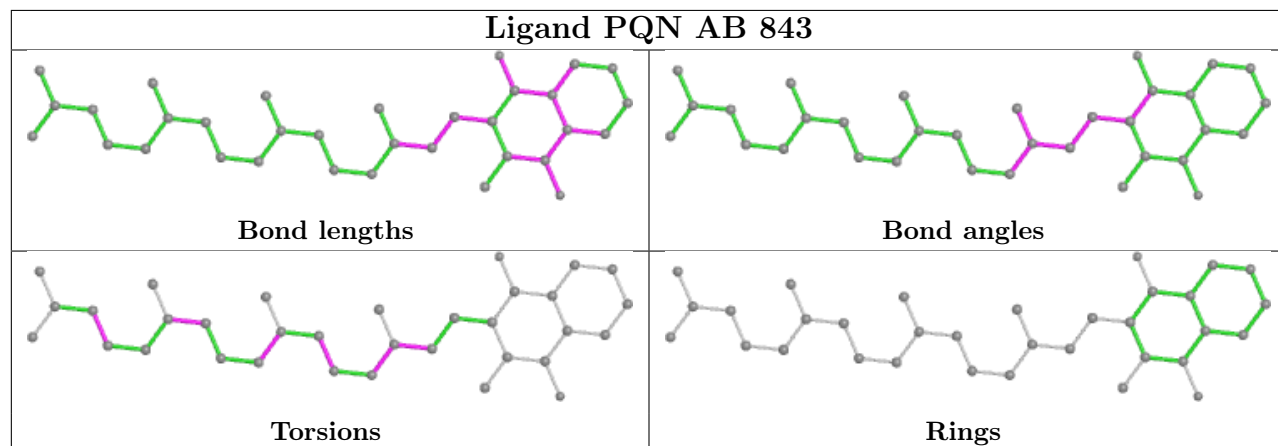
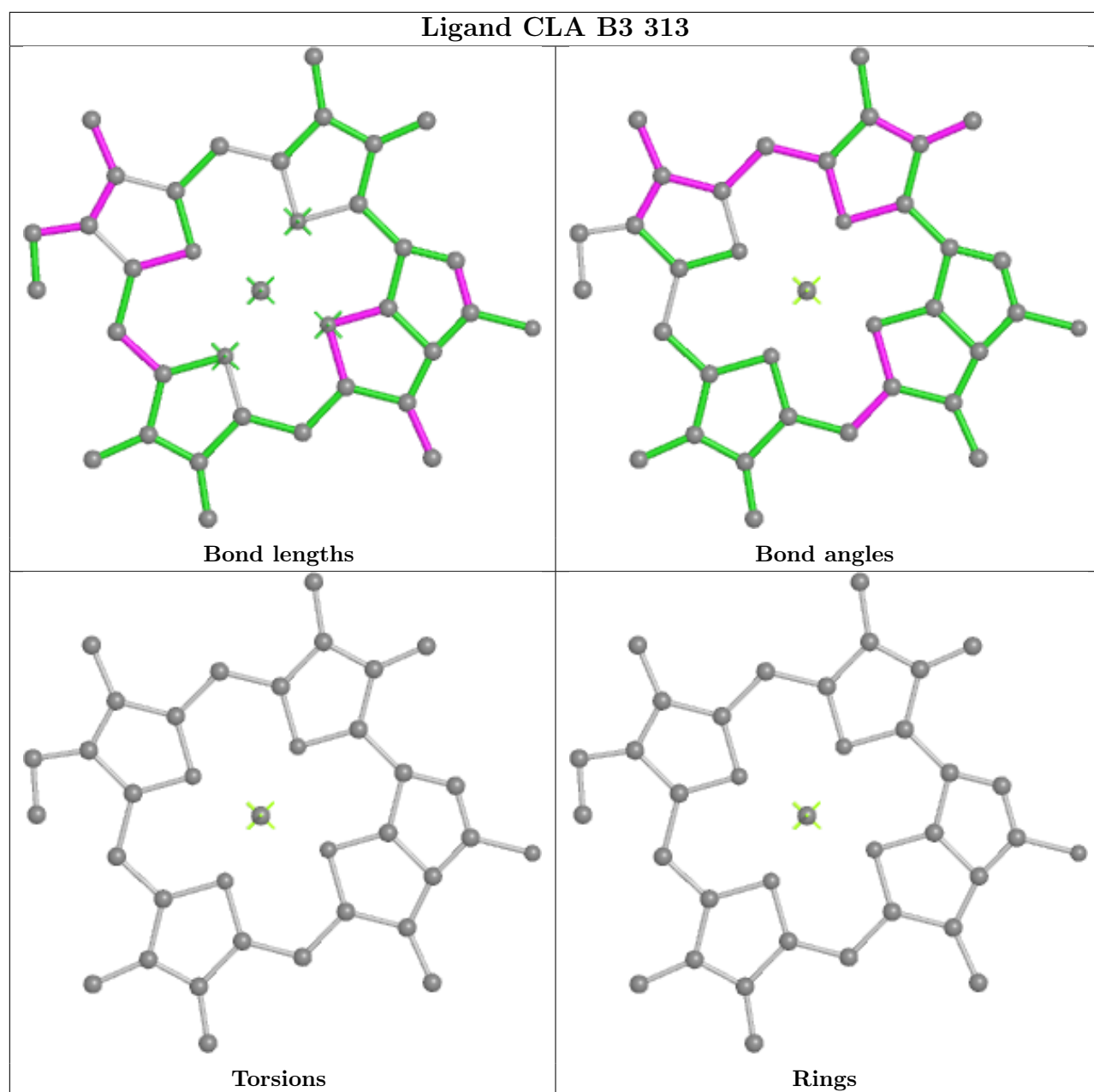
Bond angles

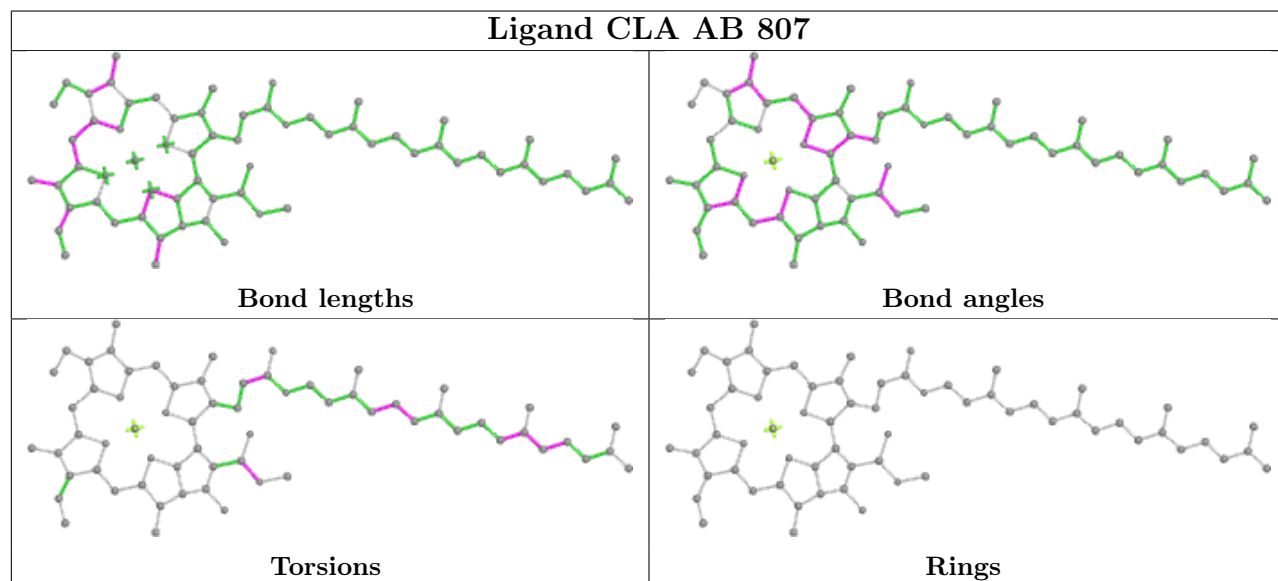
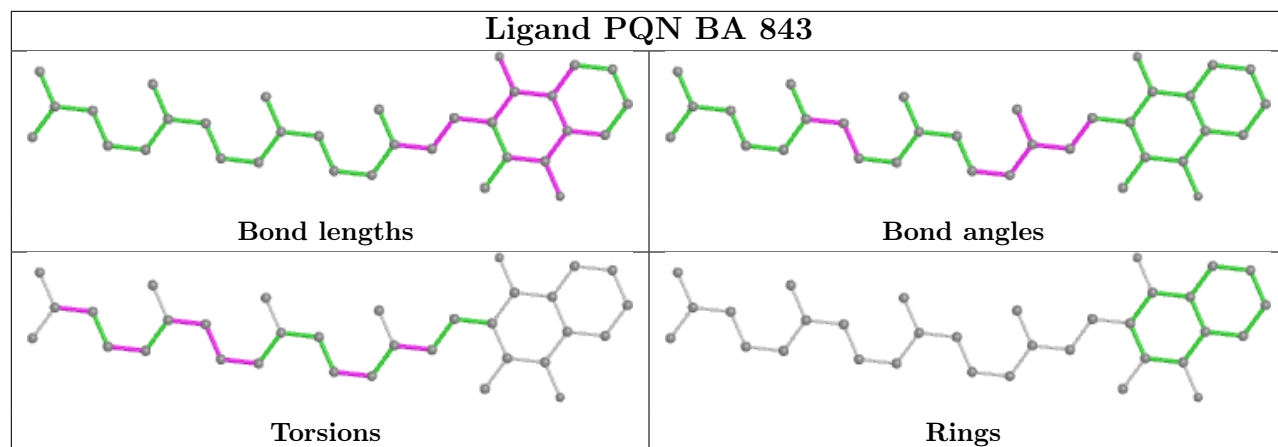


Torsions

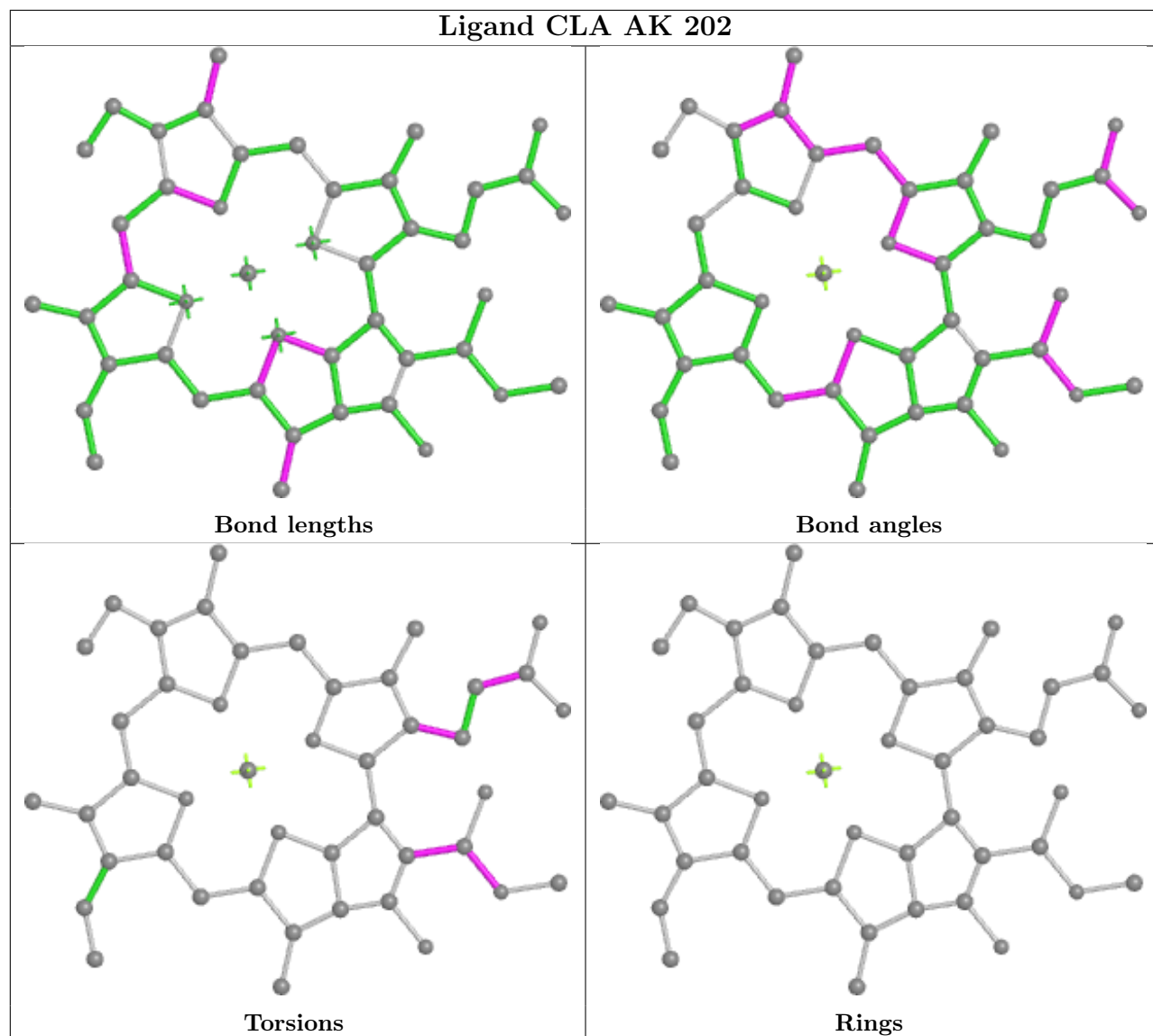


Rings

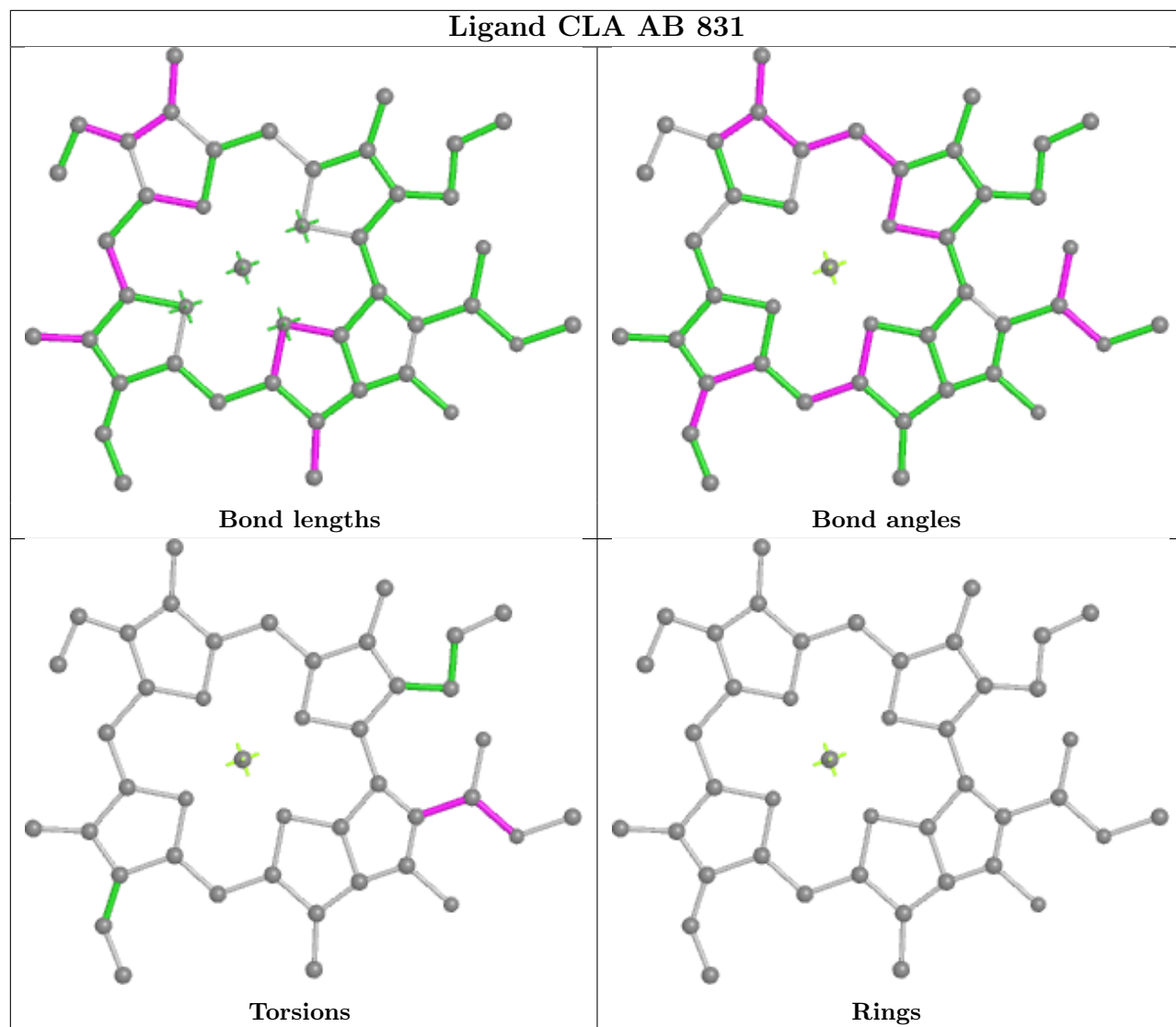


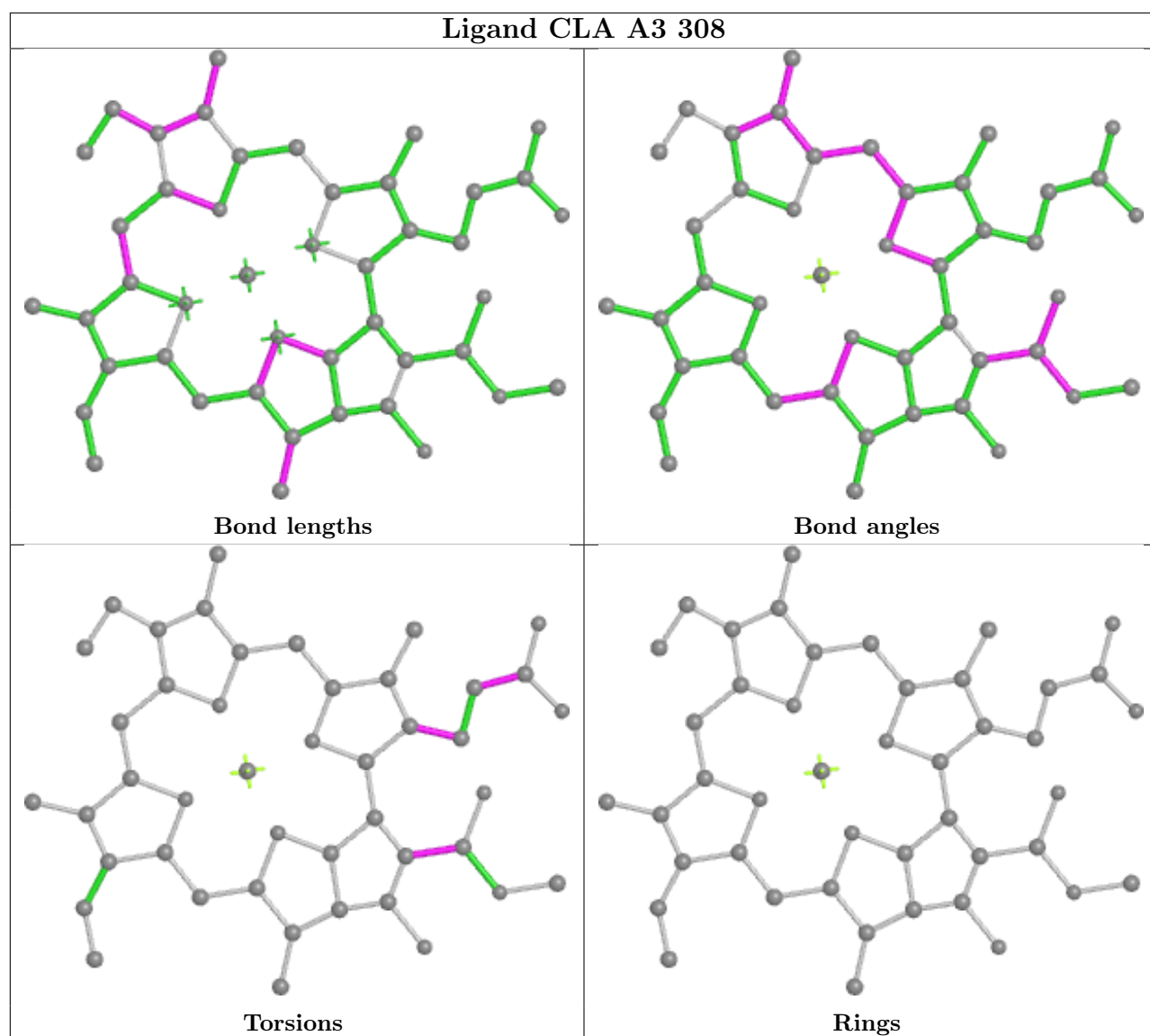


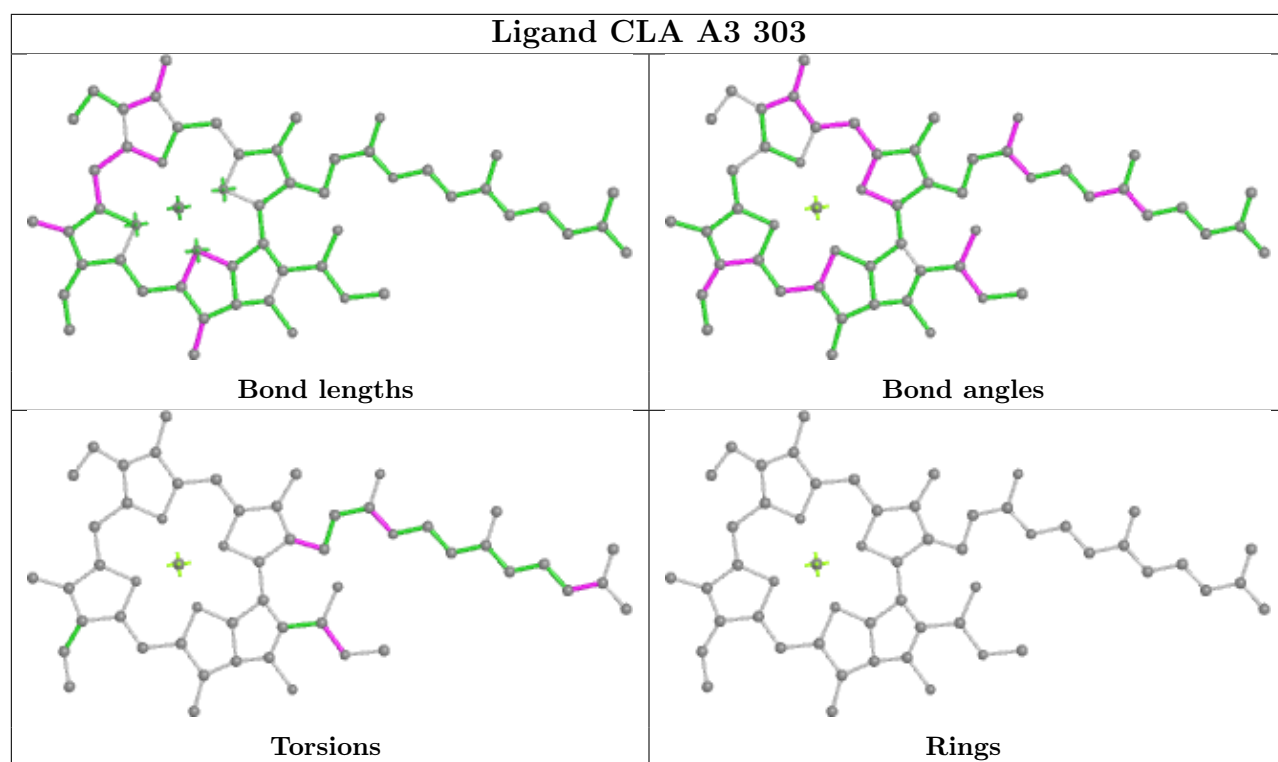
Ligand CLA AK 202

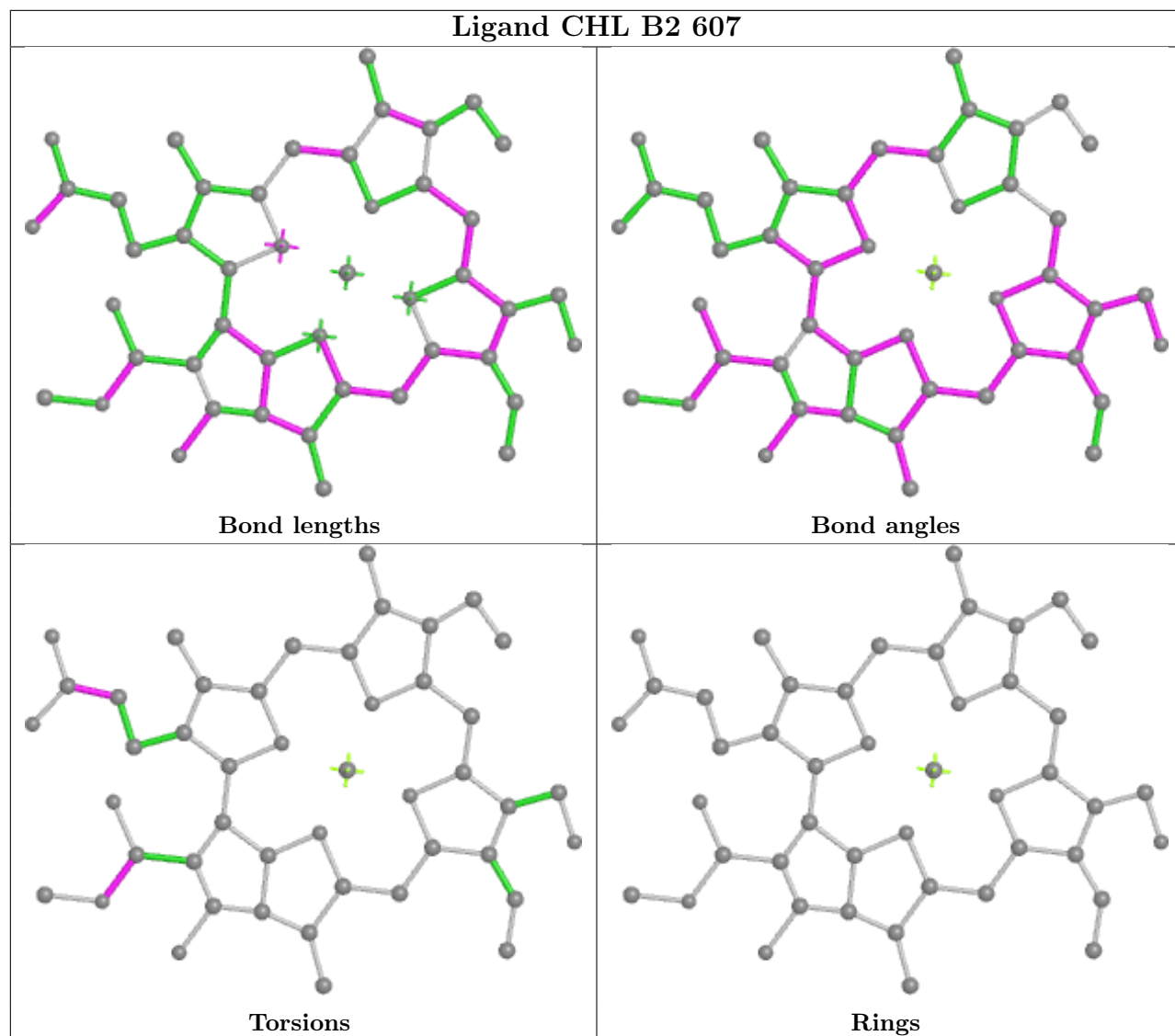


Ligand CLA AB 831

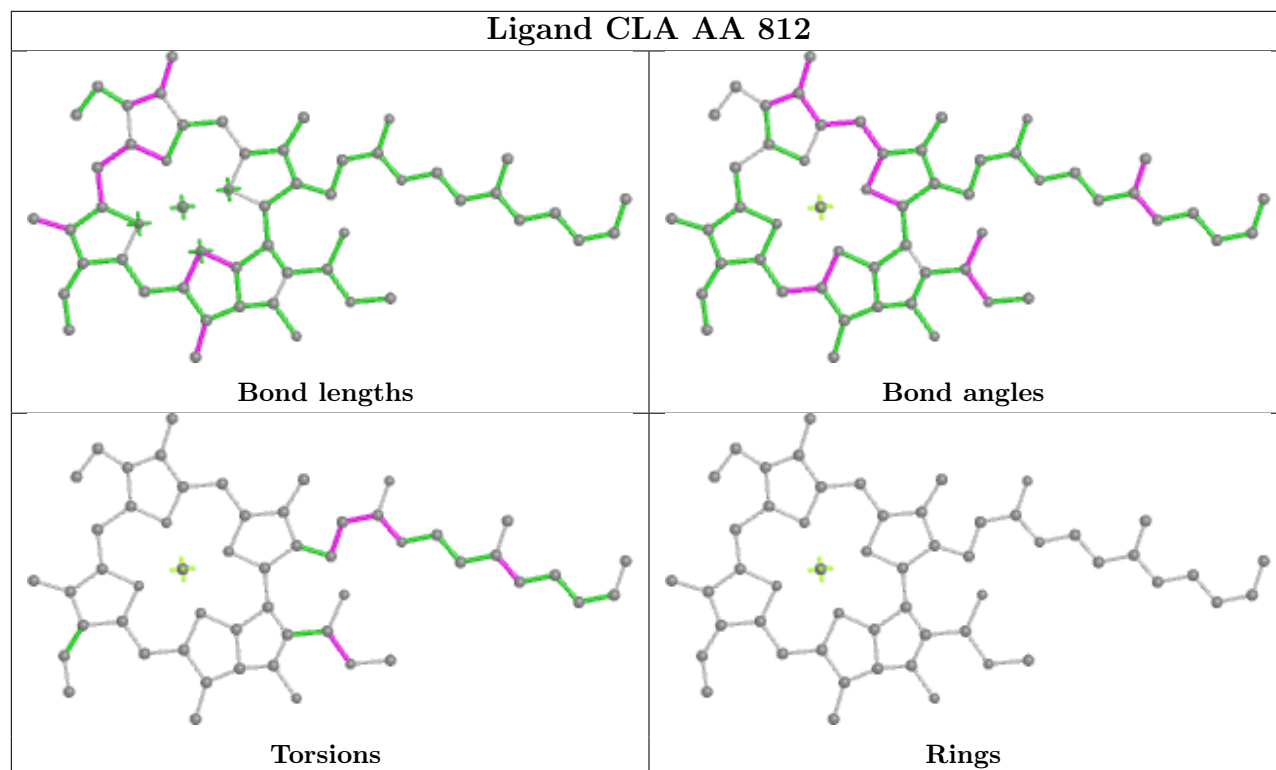




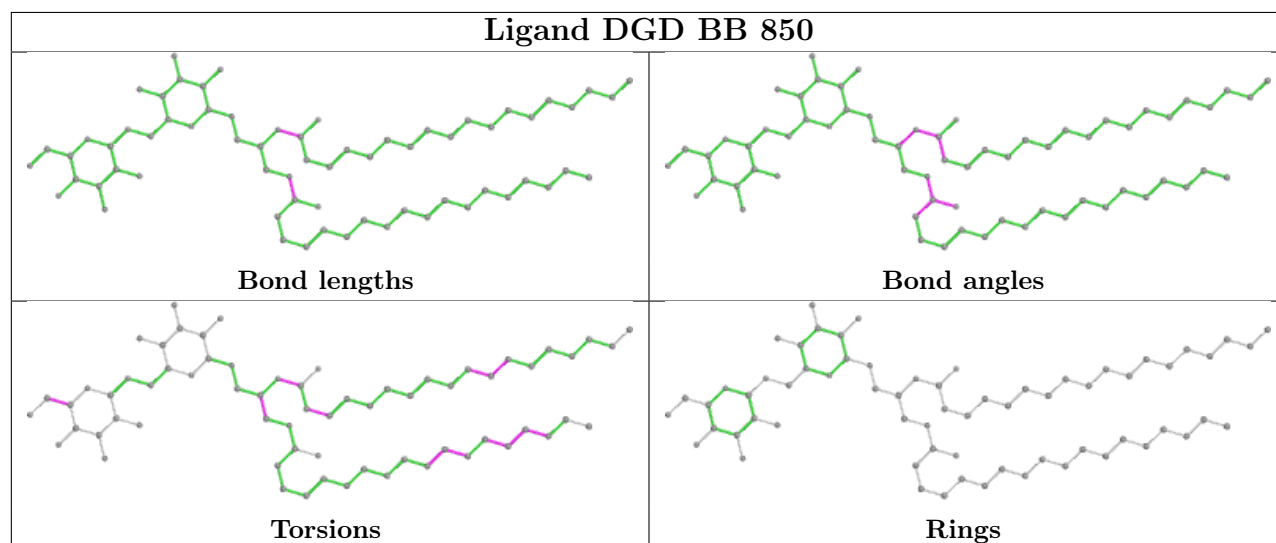


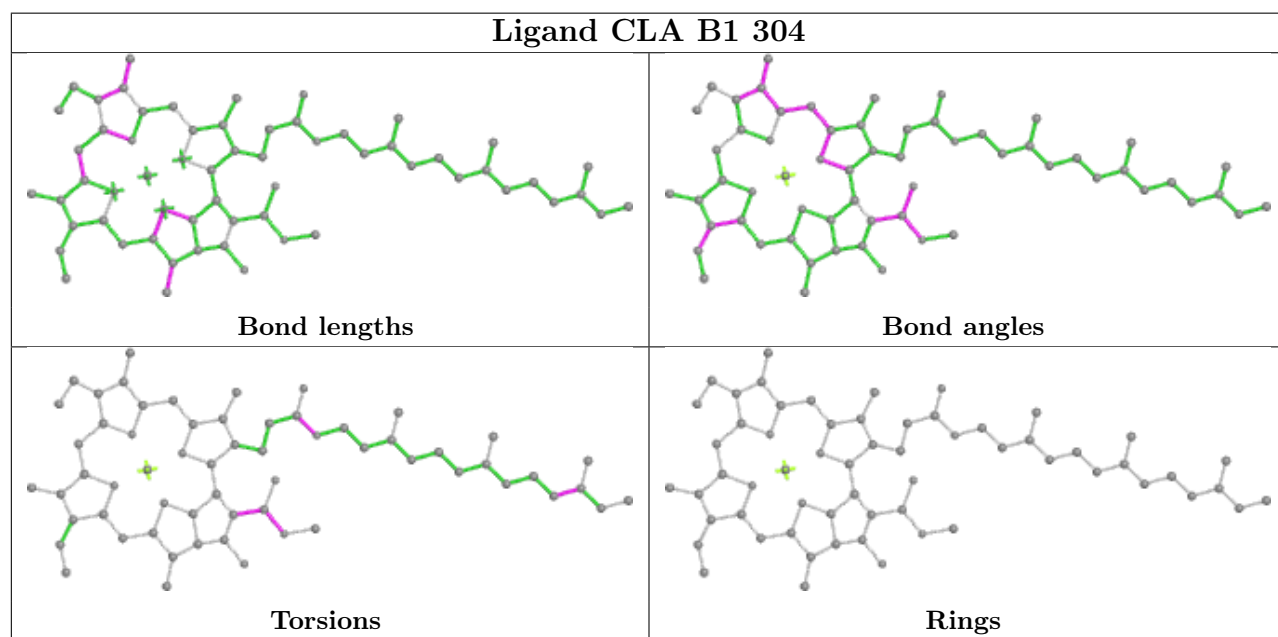
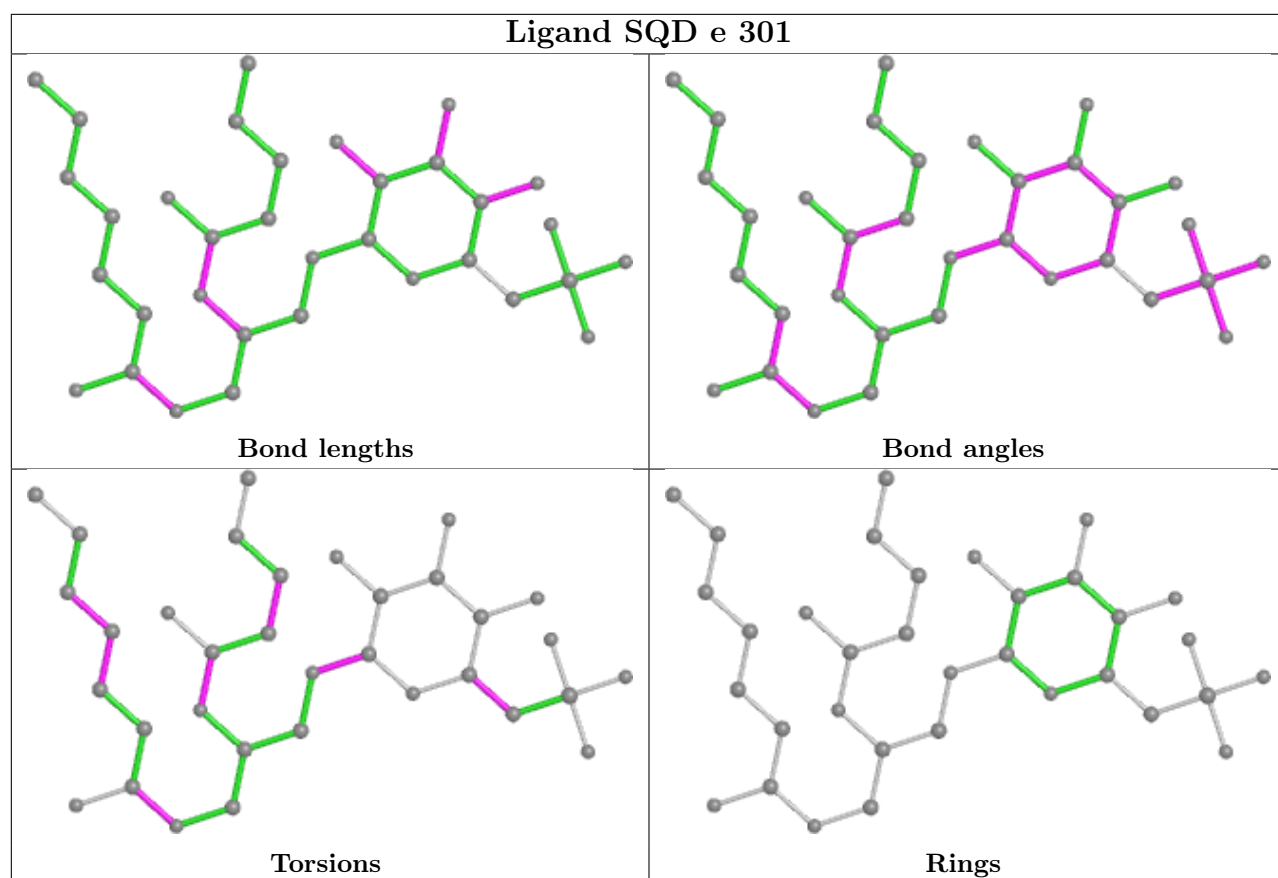


Ligand CLA AA 812

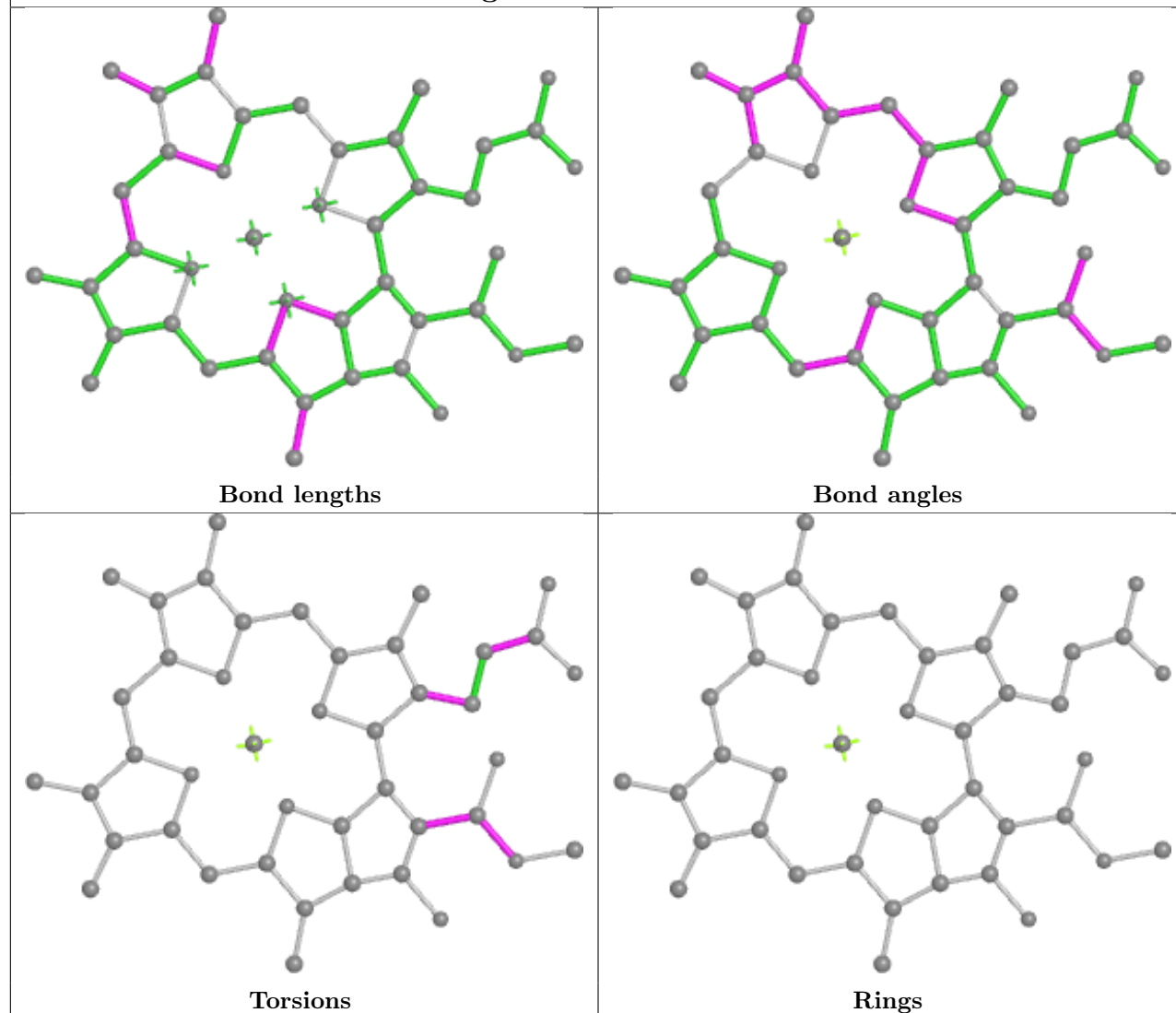


Ligand DGD BB 850

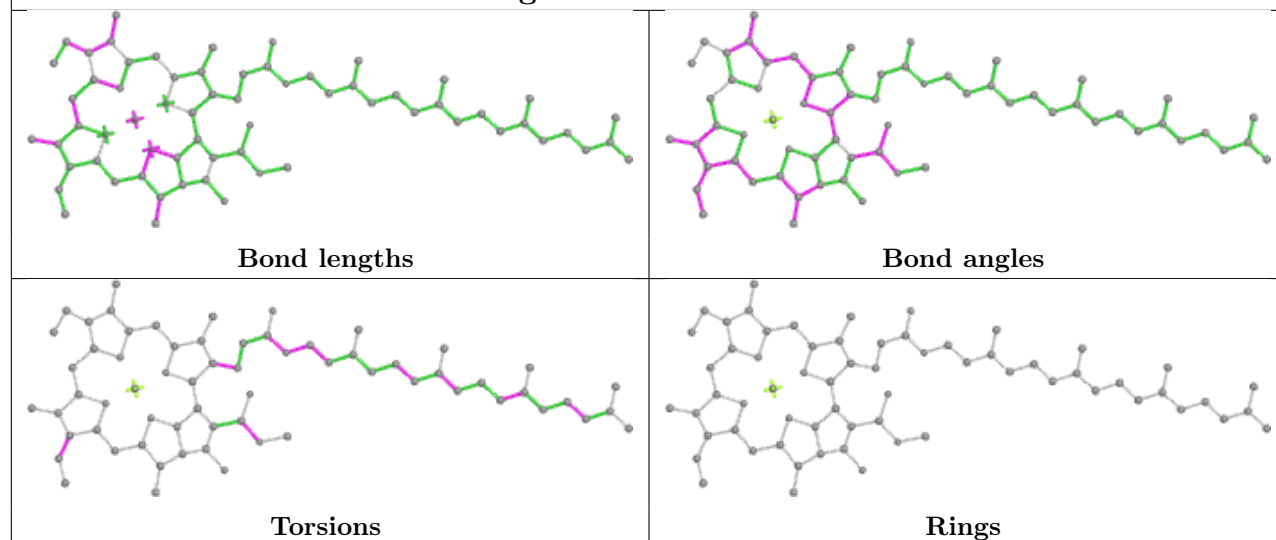




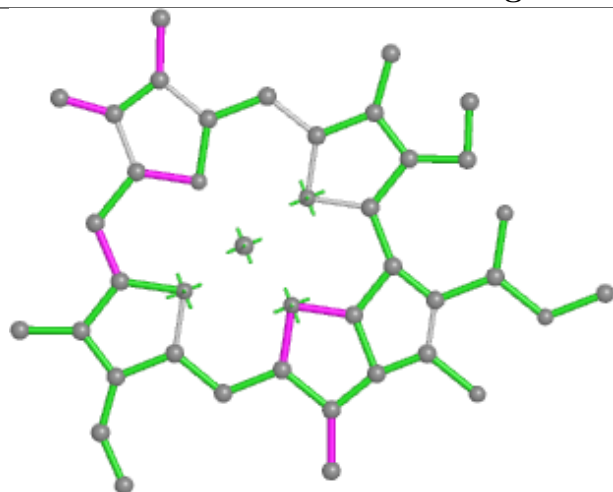
Ligand CLA A1 316



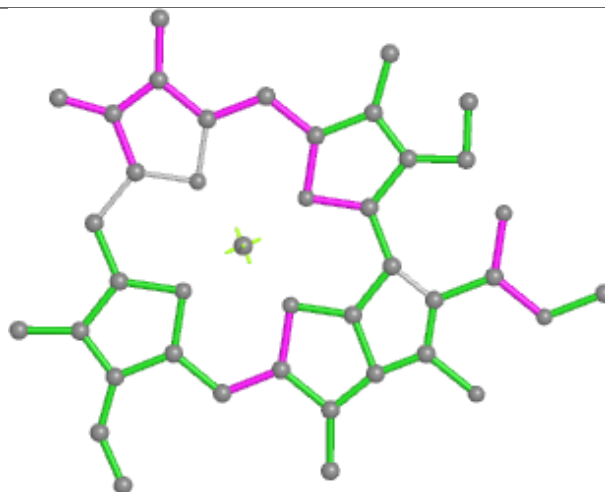
Ligand CLA AB 804



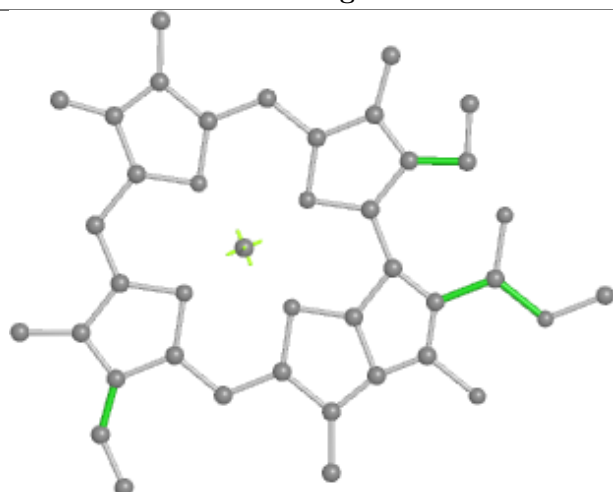
Ligand CLA A3 306



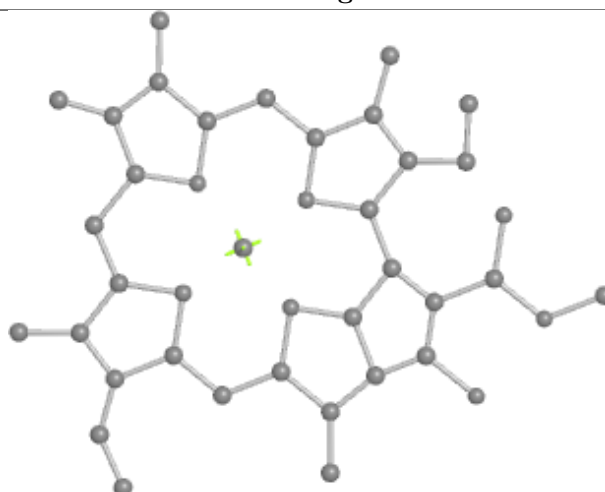
Bond lengths



Bond angles

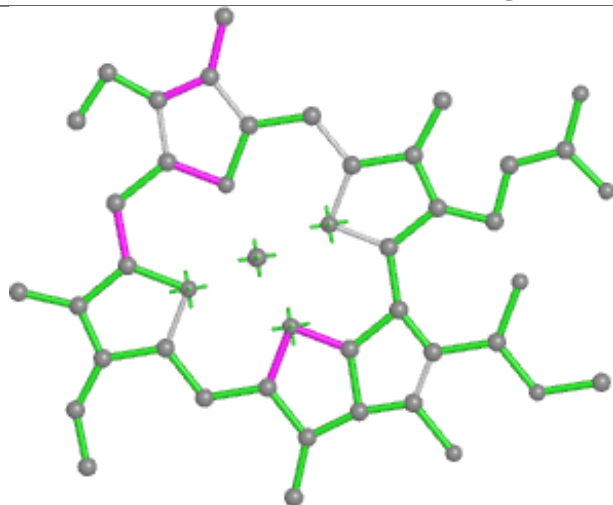


Torsions

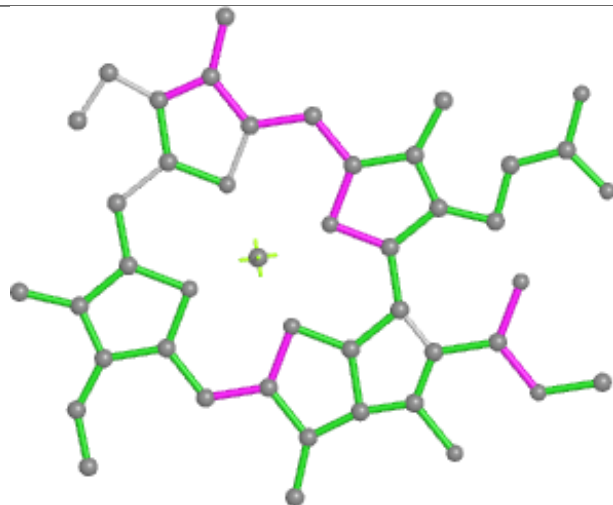


Rings

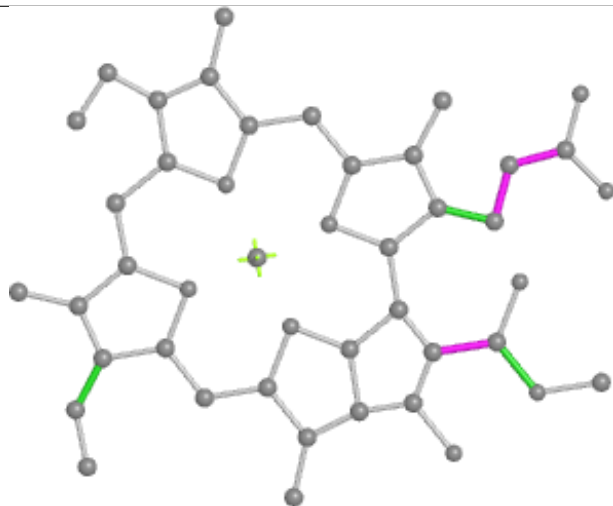
Ligand CLA BK 202



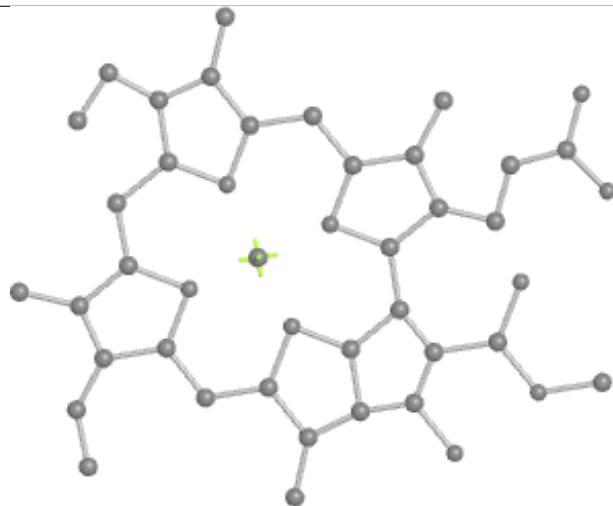
Bond lengths



Bond angles

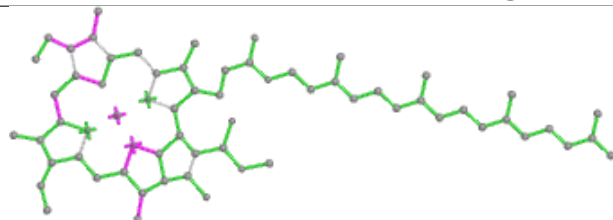


Torsions

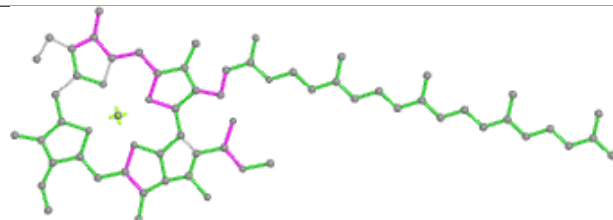


Rings

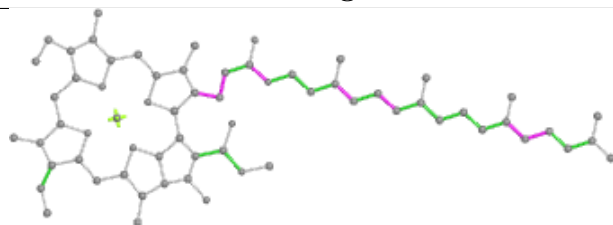
Ligand CLA BB 830



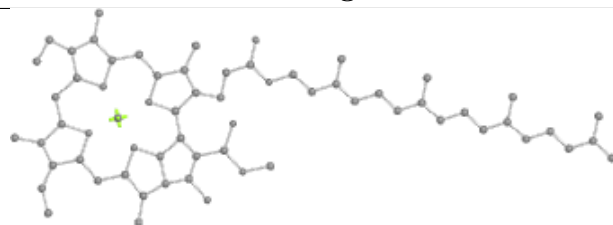
Bond lengths



Bond angles

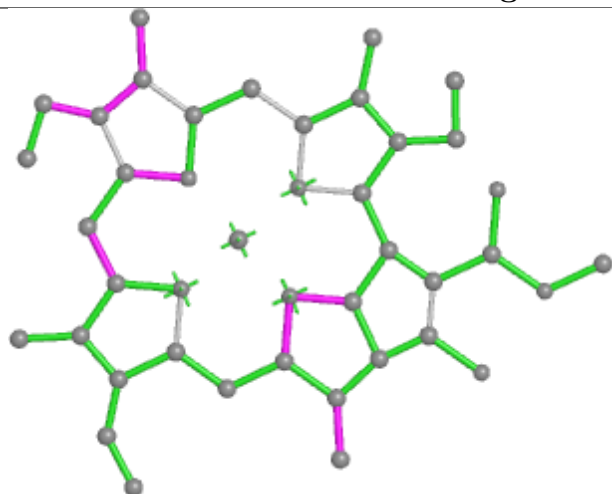


Torsions

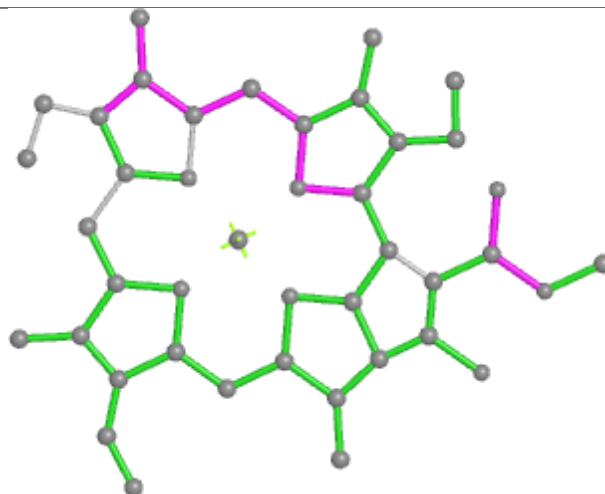


Rings

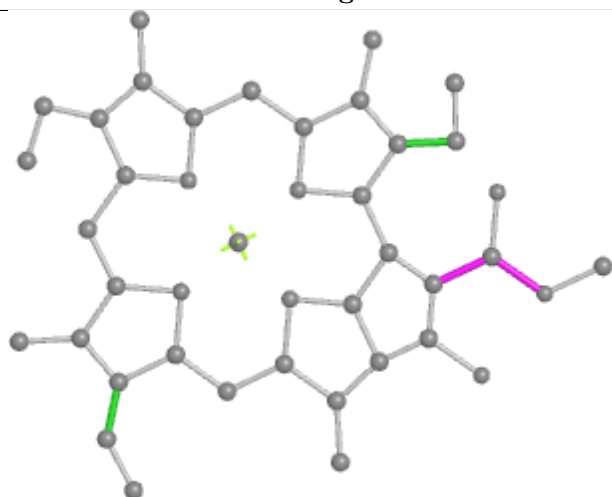
Ligand CLA BA 815



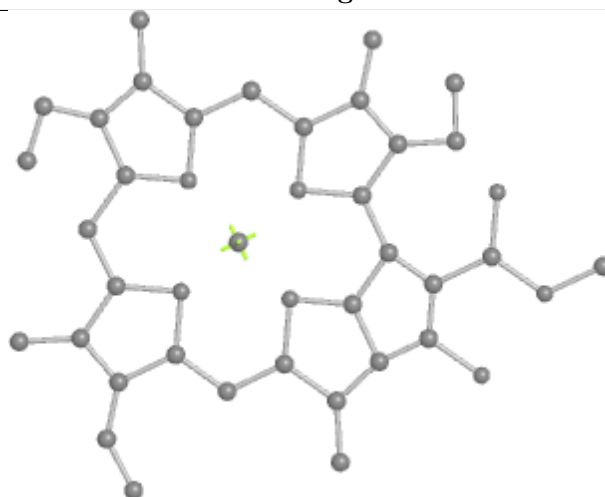
Bond lengths



Bond angles

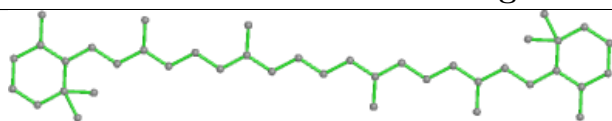


Torsions

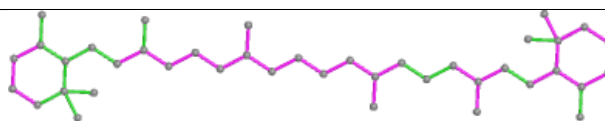


Rings

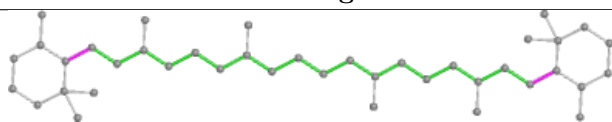
Ligand BCR BB 803



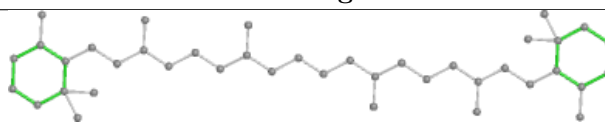
Bond lengths



Bond angles

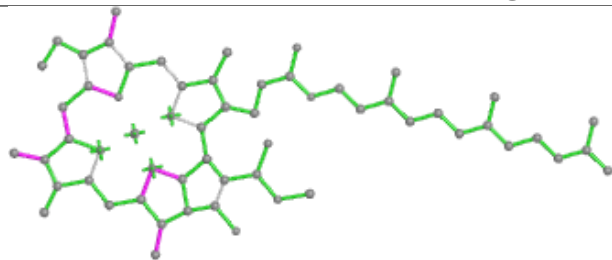


Torsions

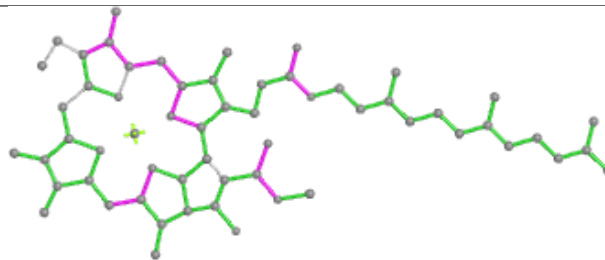


Rings

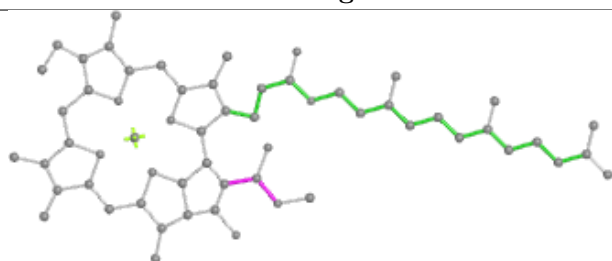
Ligand CLA A1 311



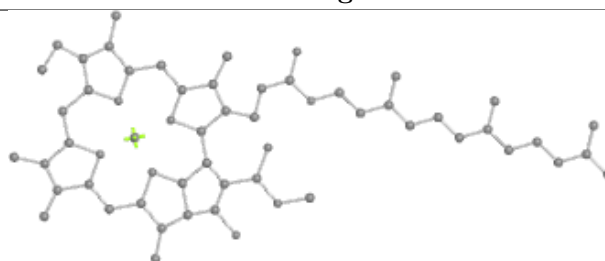
Bond lengths



Bond angles

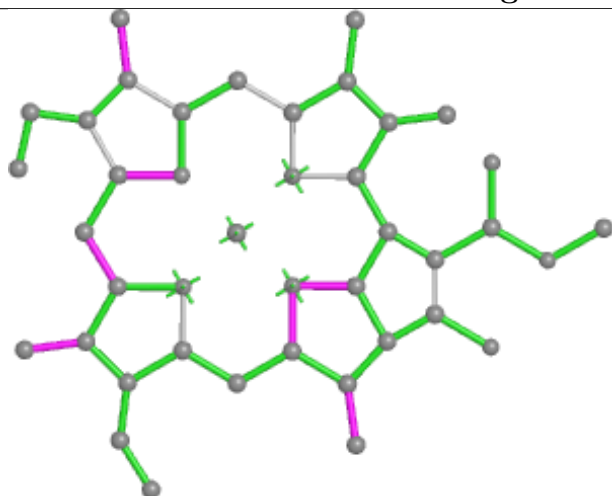


Torsions

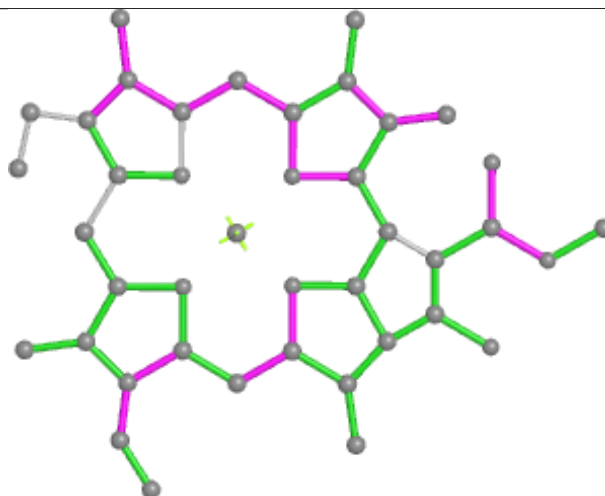


Rings

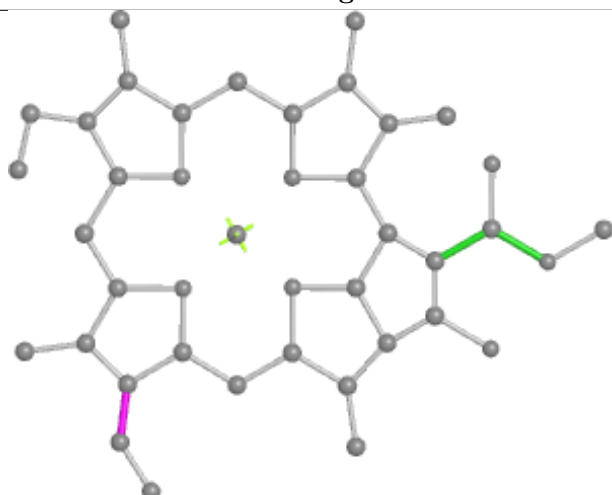
Ligand CLA BB 806



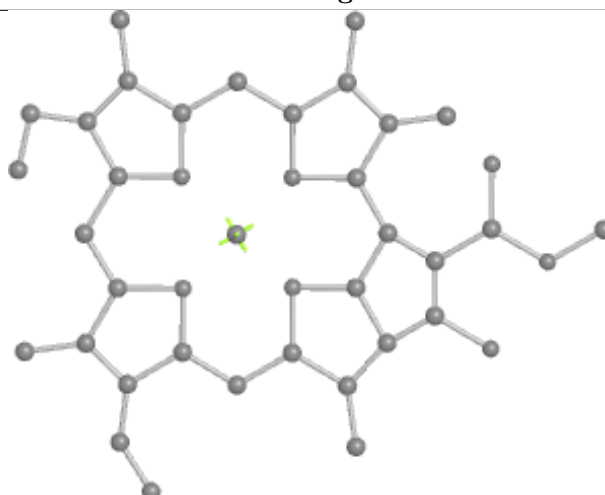
Bond lengths



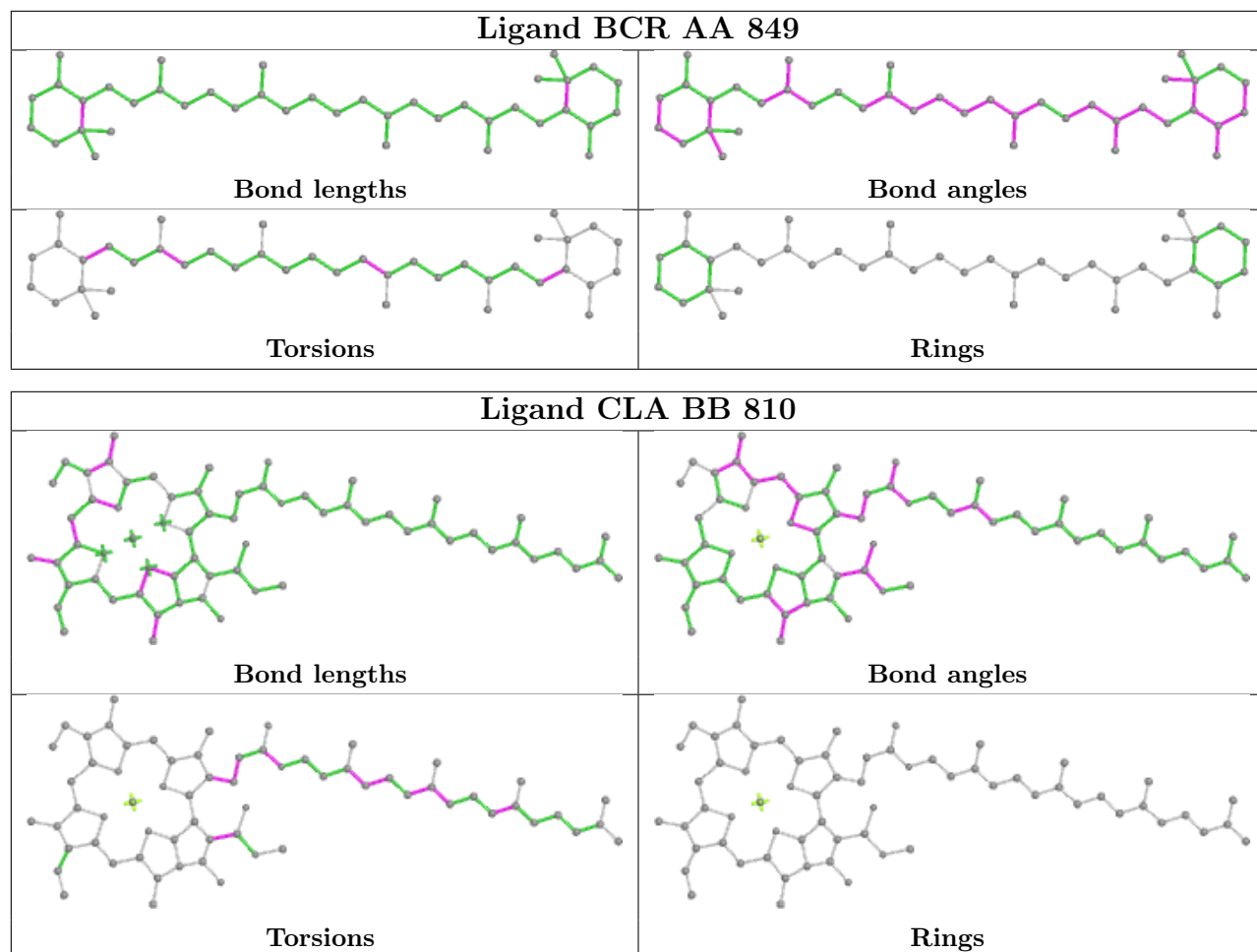
Bond angles

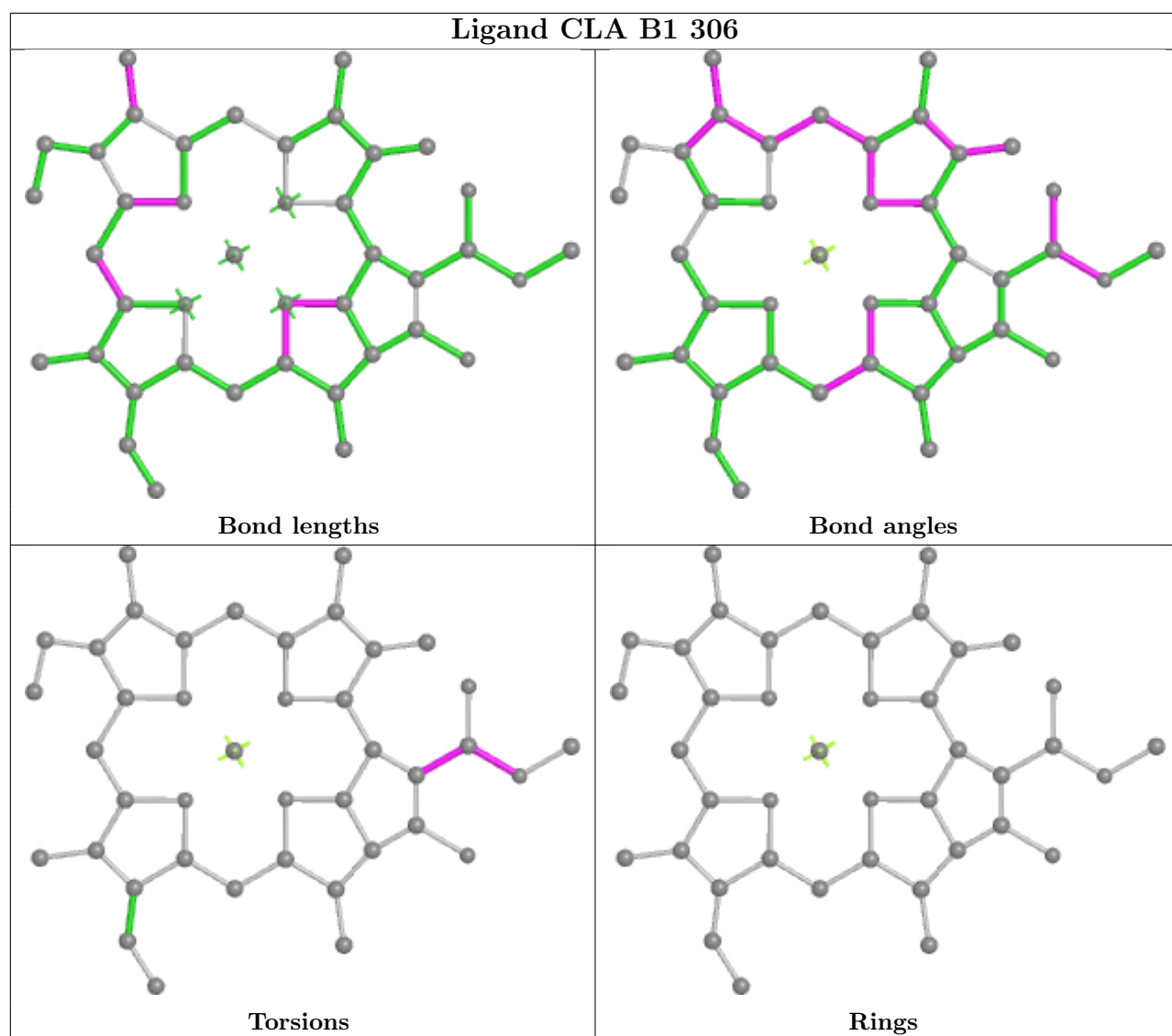


Torsions

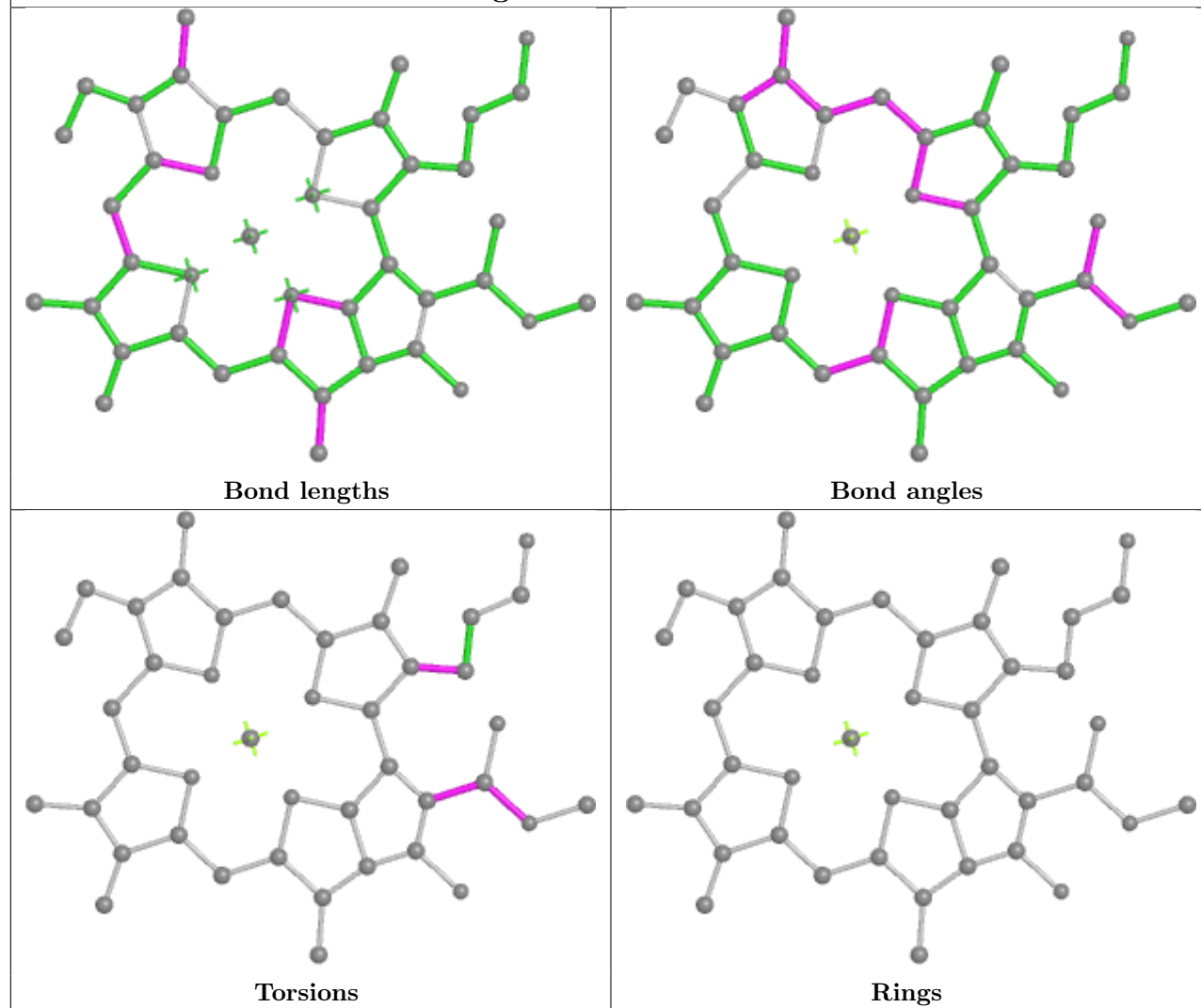


Rings

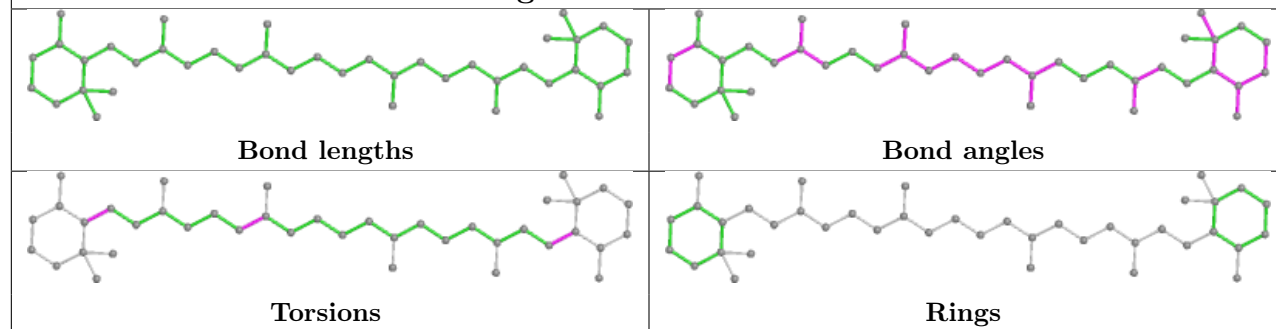


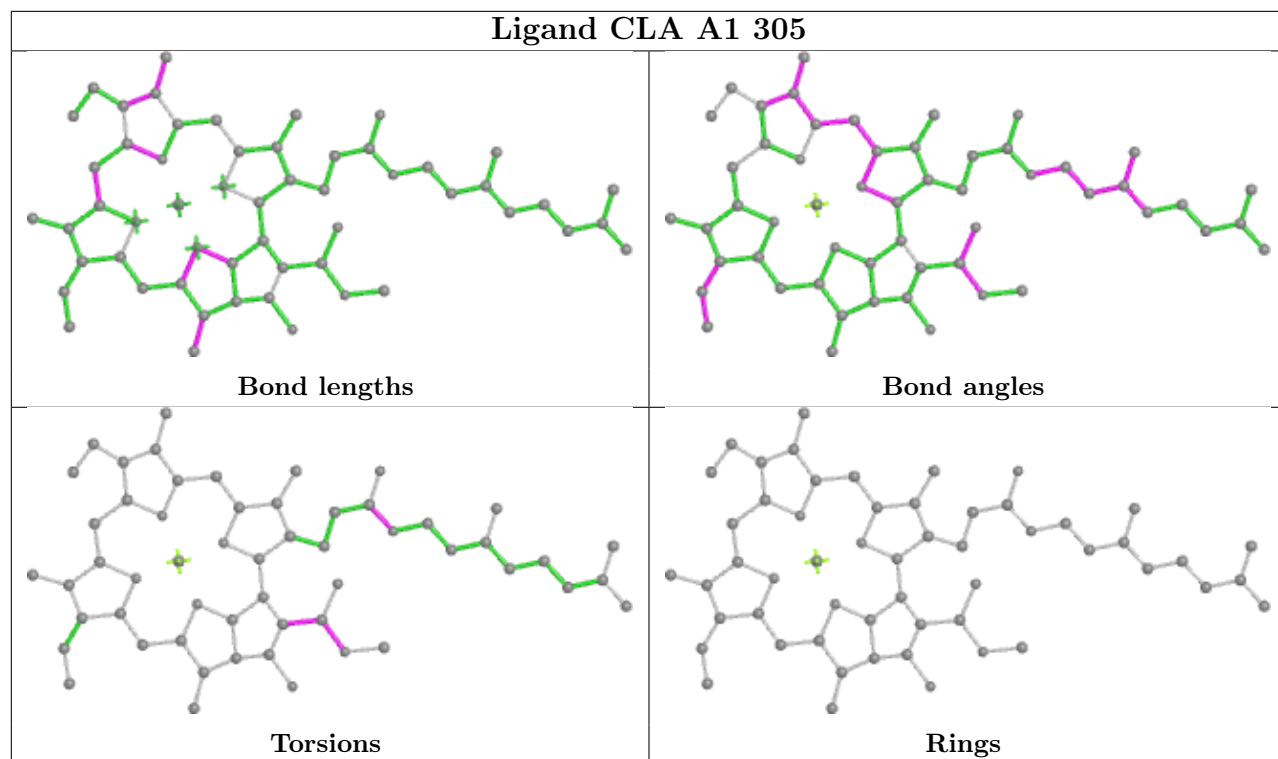
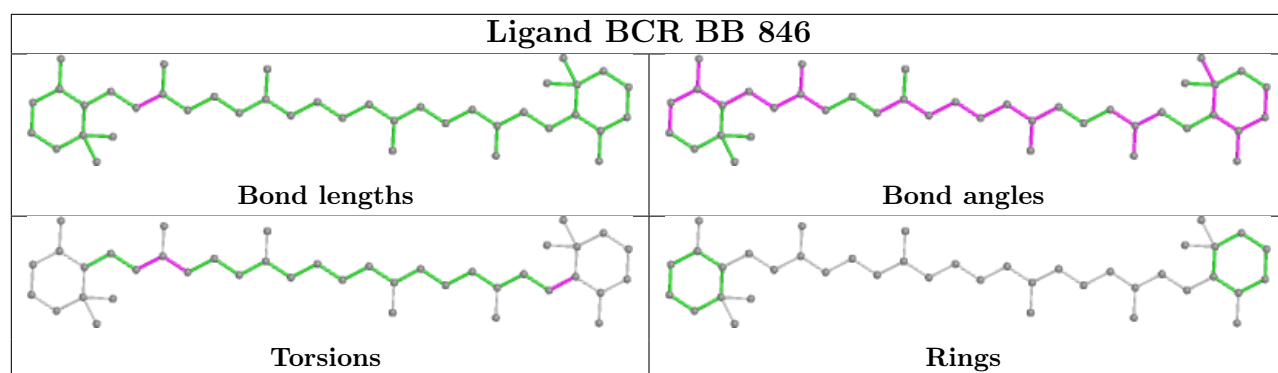


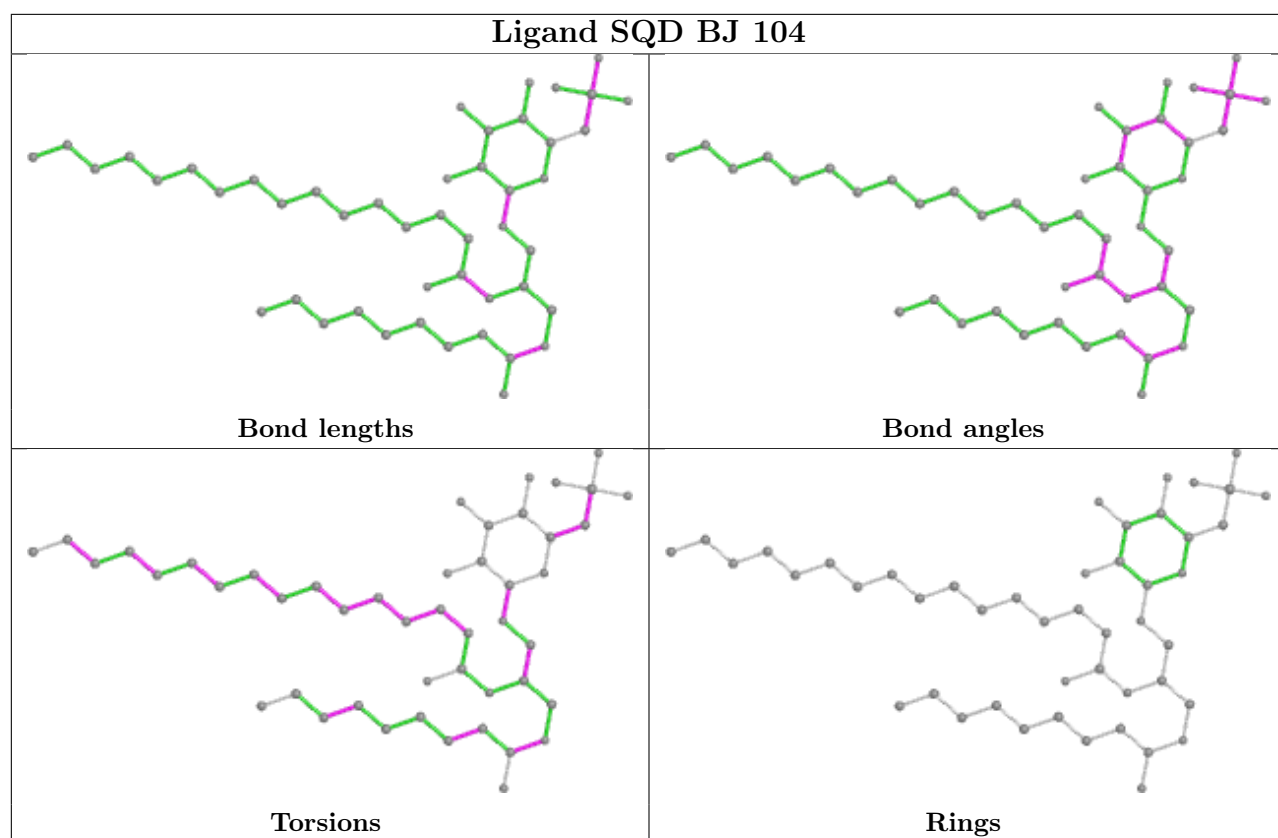
Ligand CLA B2 604



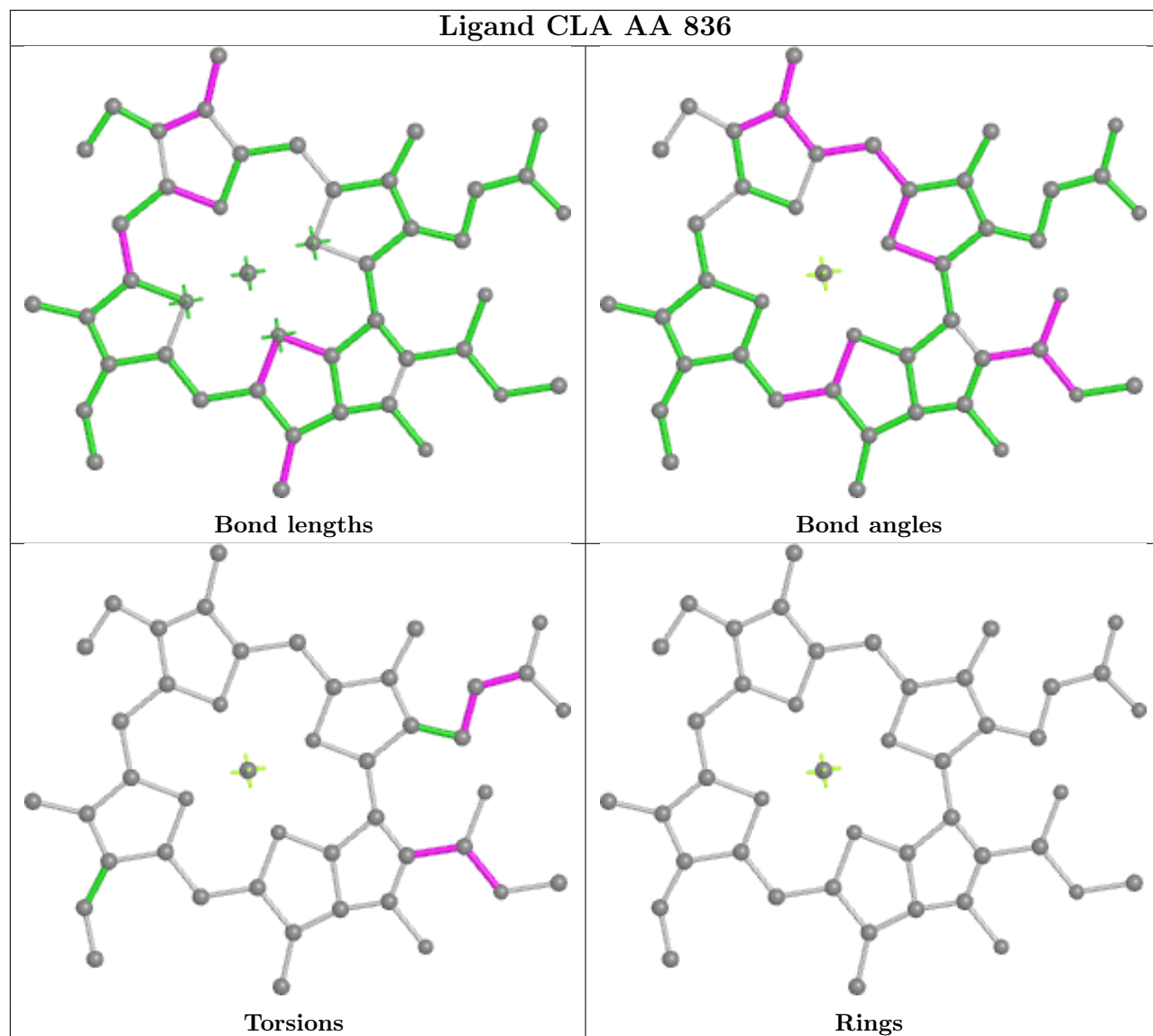
Ligand BCR BA 848

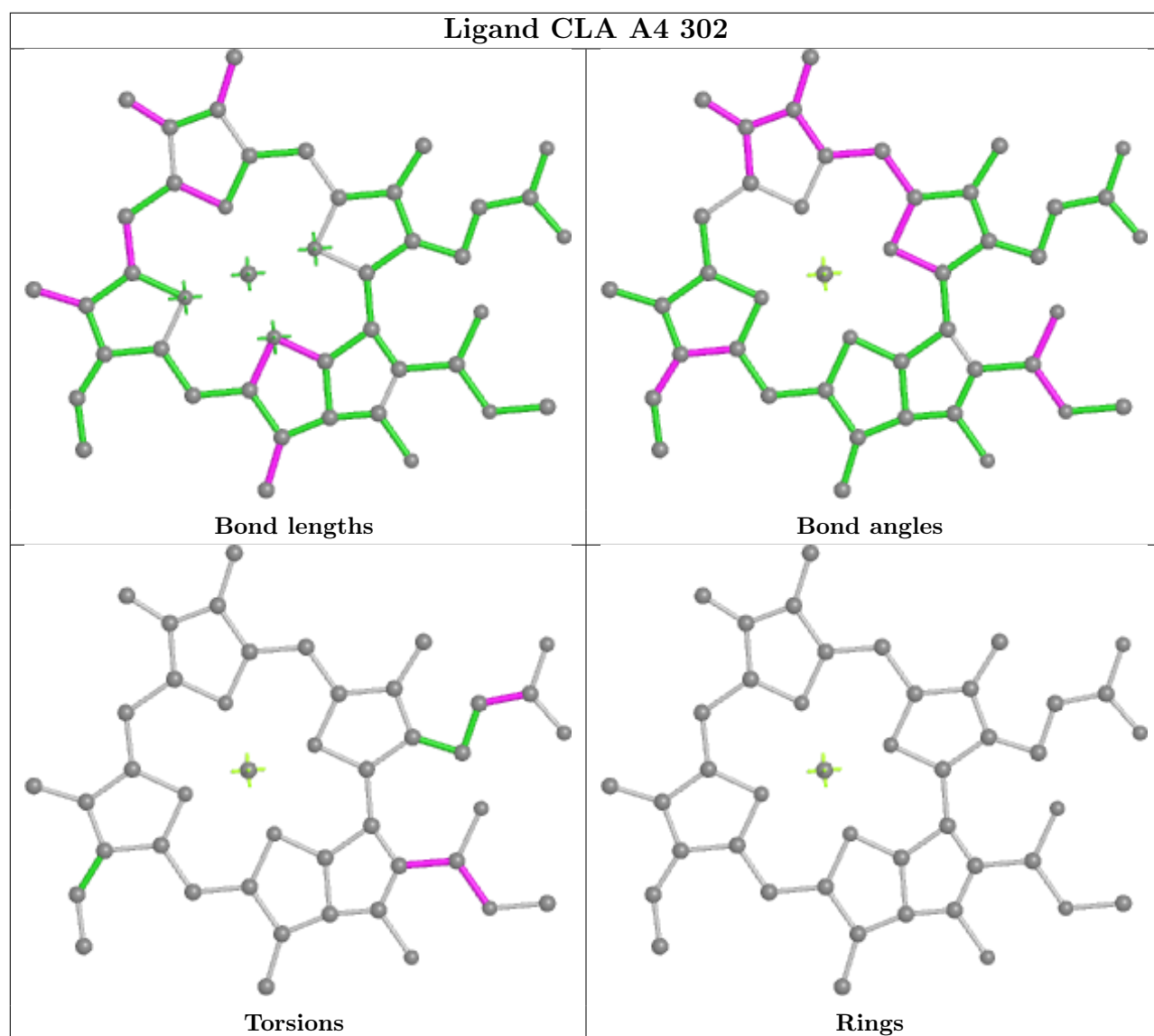


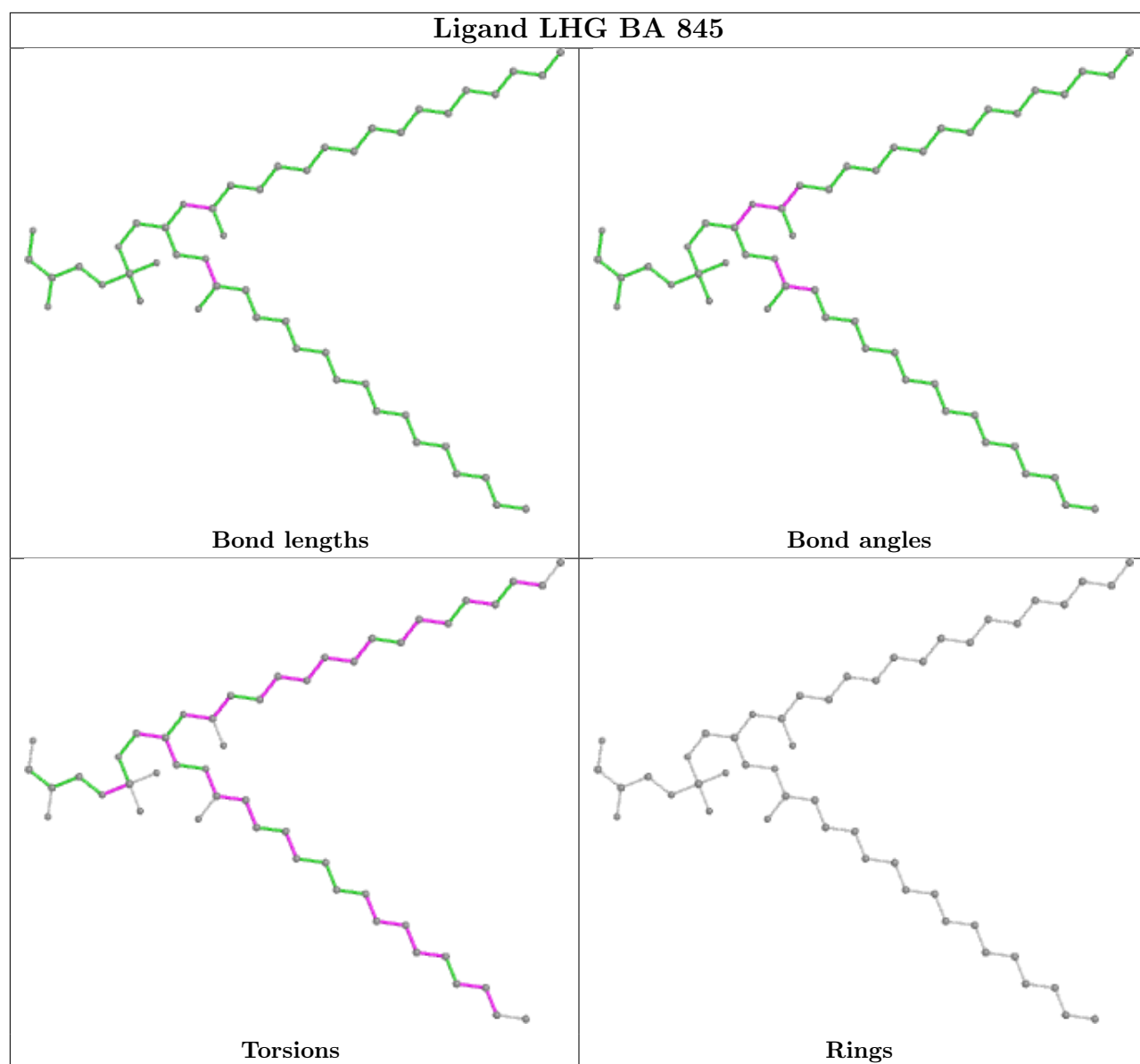




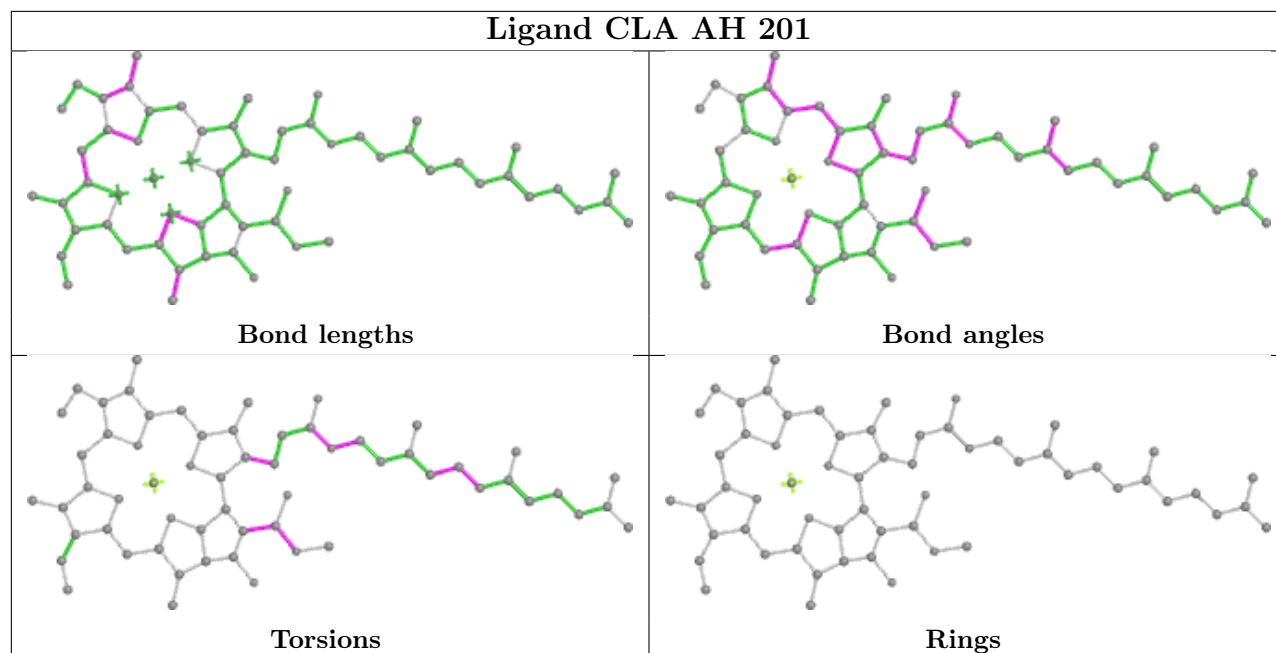
Ligand CLA AA 836



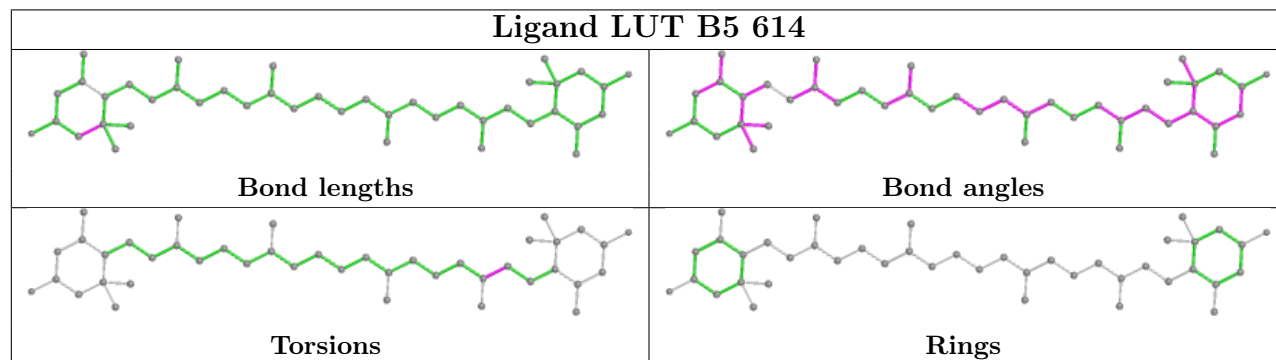




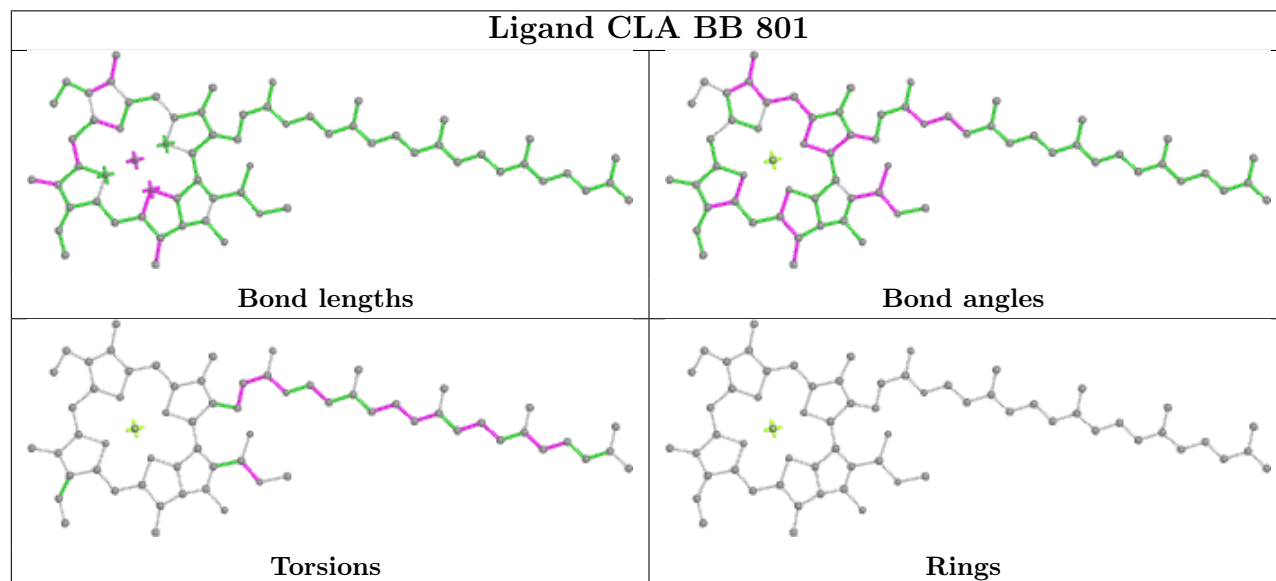
Ligand CLA AH 201

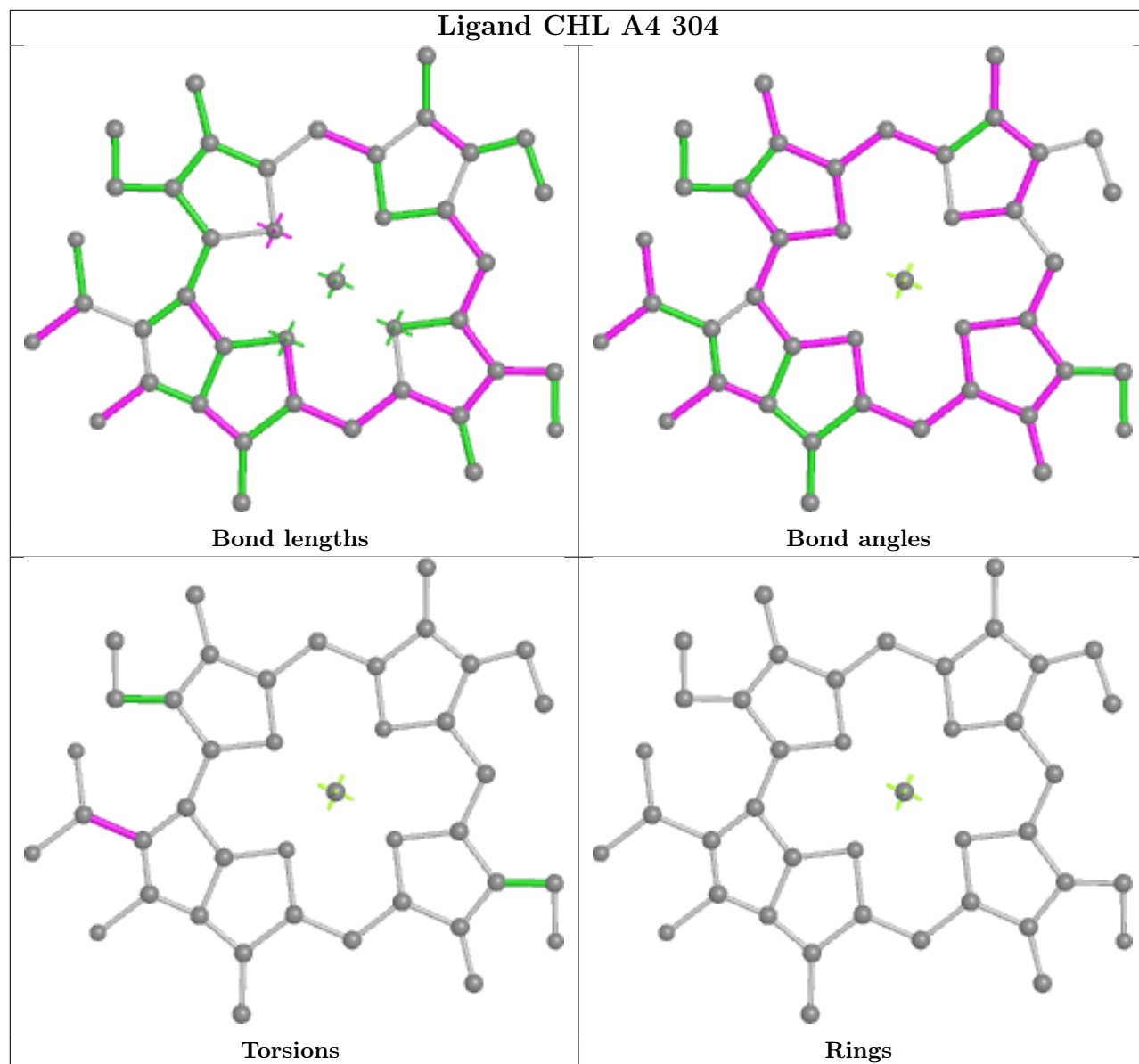


Ligand LUT B5 614

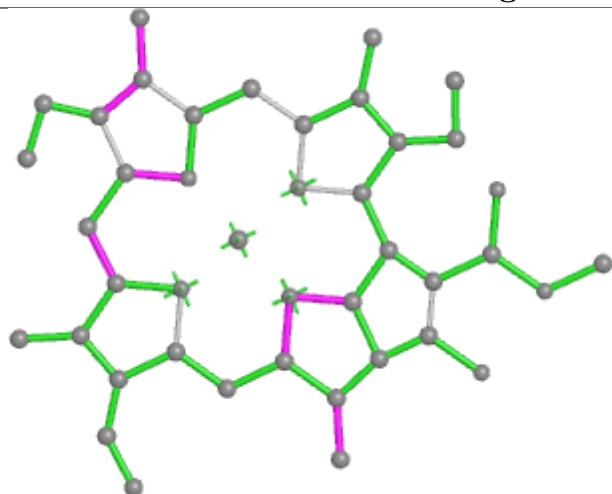


Ligand CLA BB 801

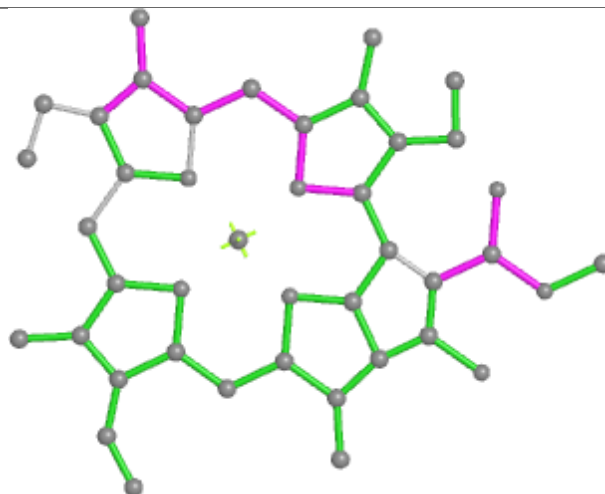




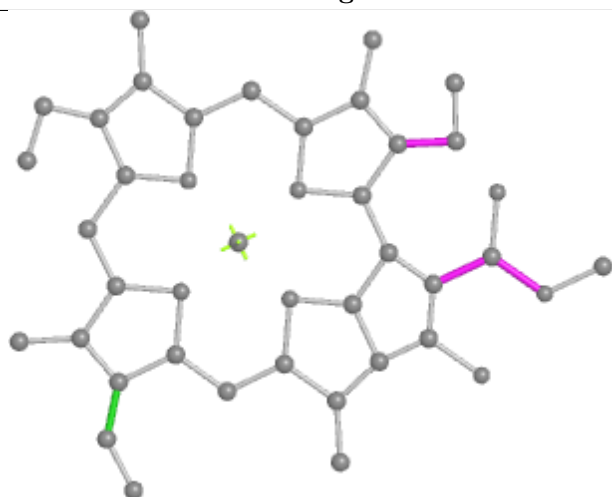
Ligand CLA BG 201



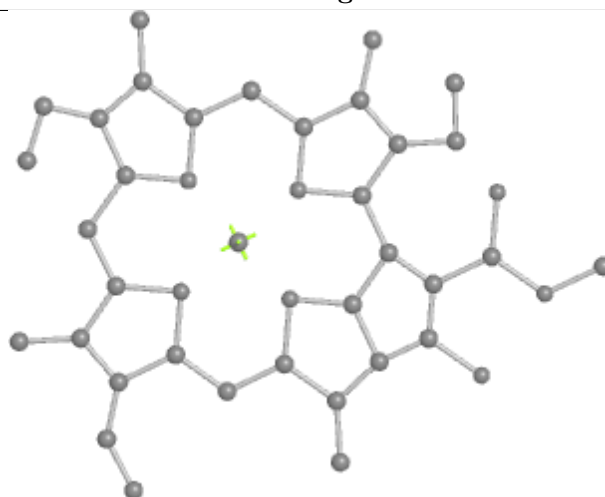
Bond lengths



Bond angles

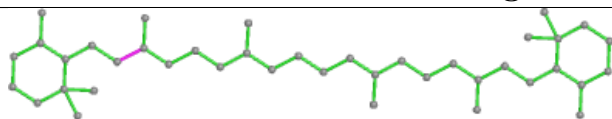


Torsions

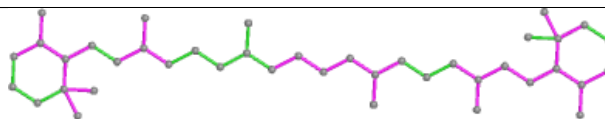


Rings

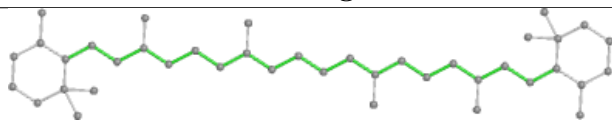
Ligand BCR B2 617



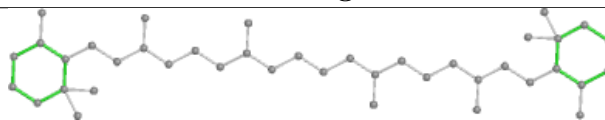
Bond lengths



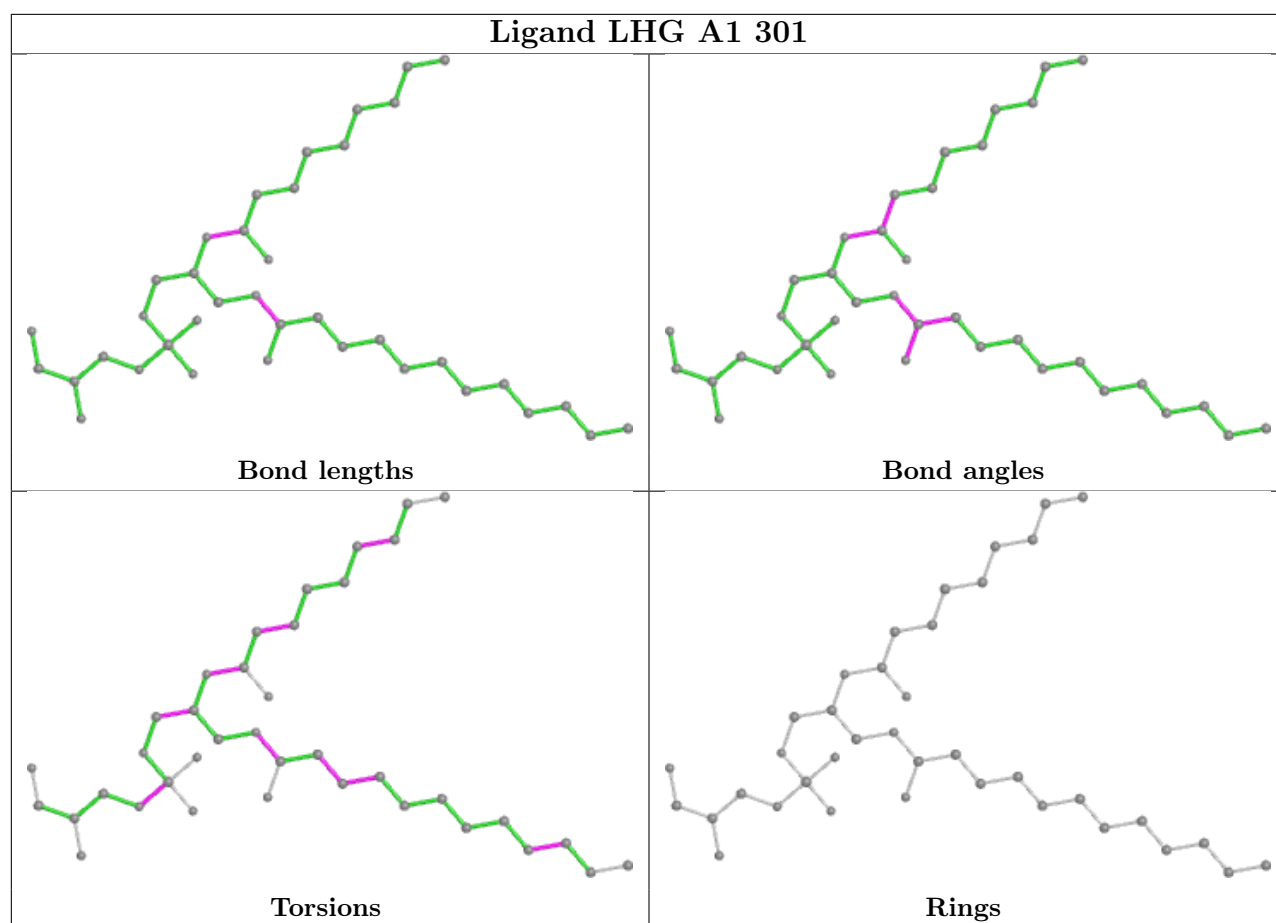
Bond angles



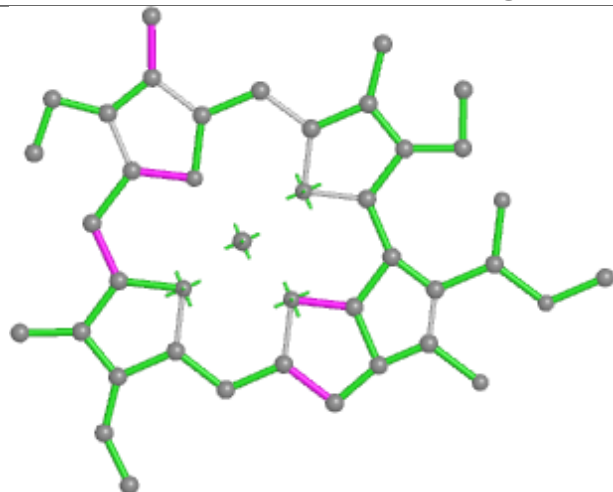
Torsions



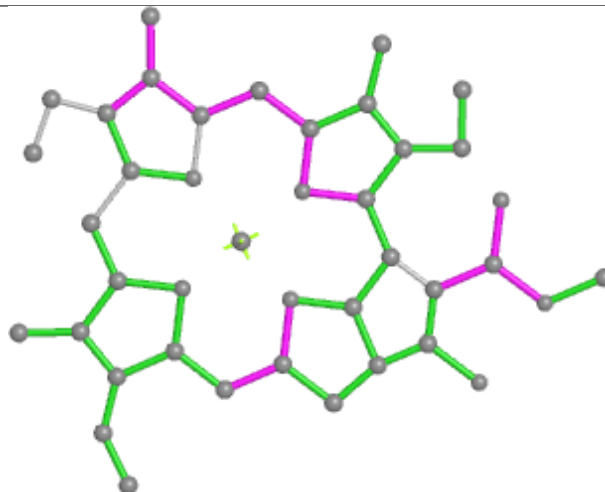
Rings



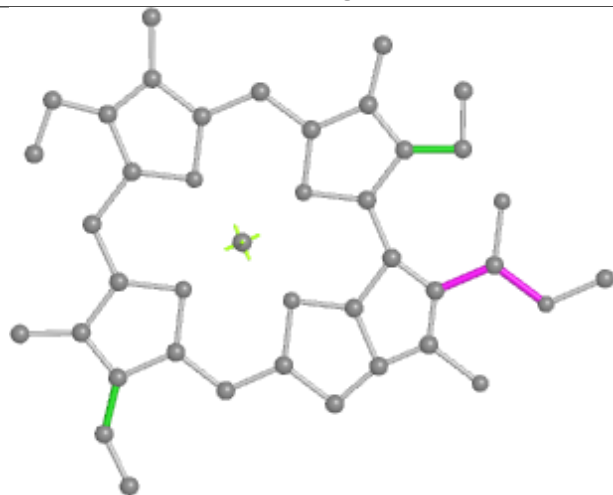
Ligand CLA AA 815



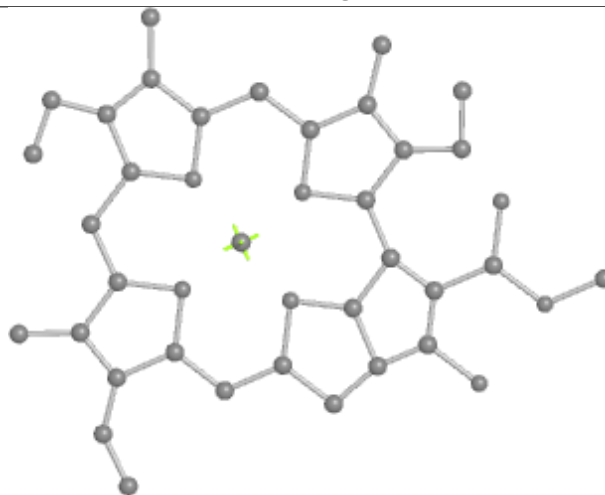
Bond lengths



Bond angles

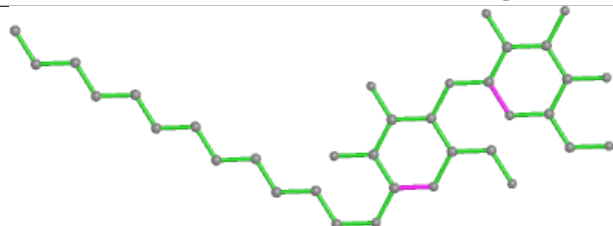


Torsions

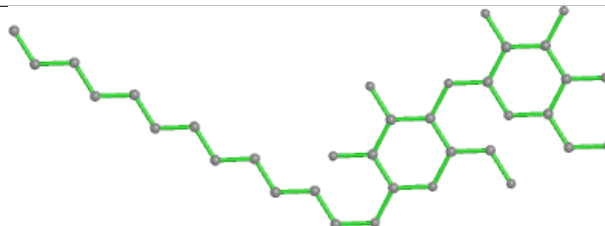


Rings

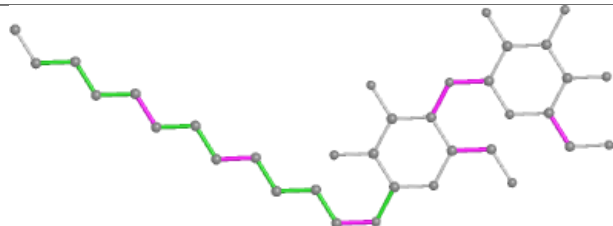
Ligand LMU BB 851



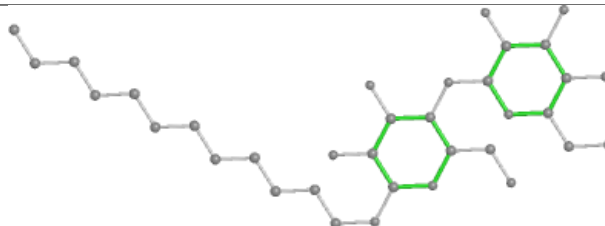
Bond lengths



Bond angles

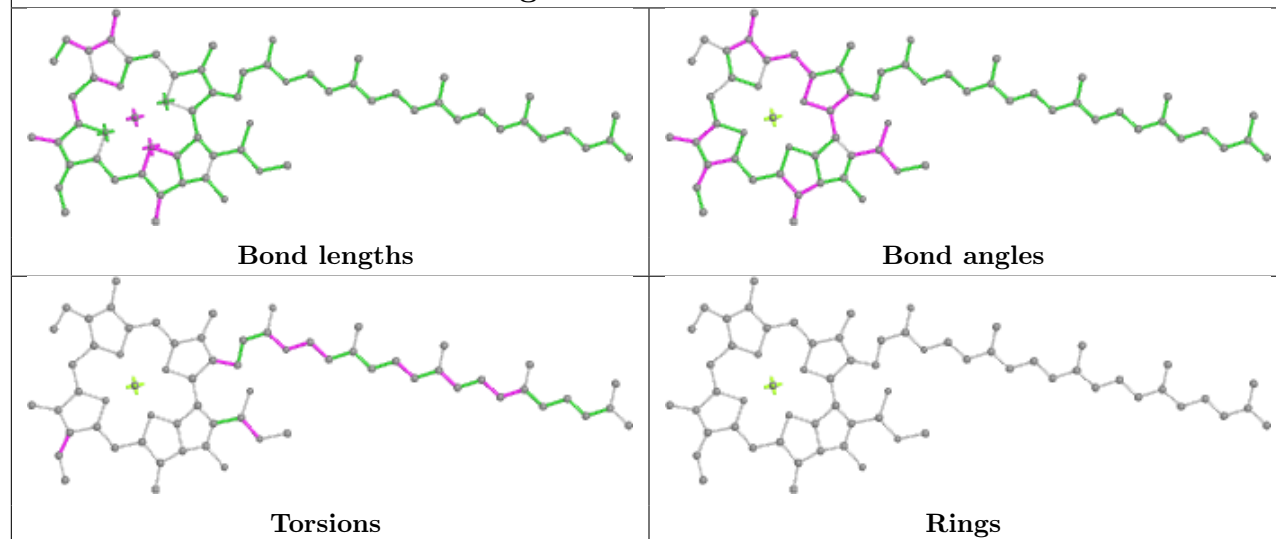


Torsions

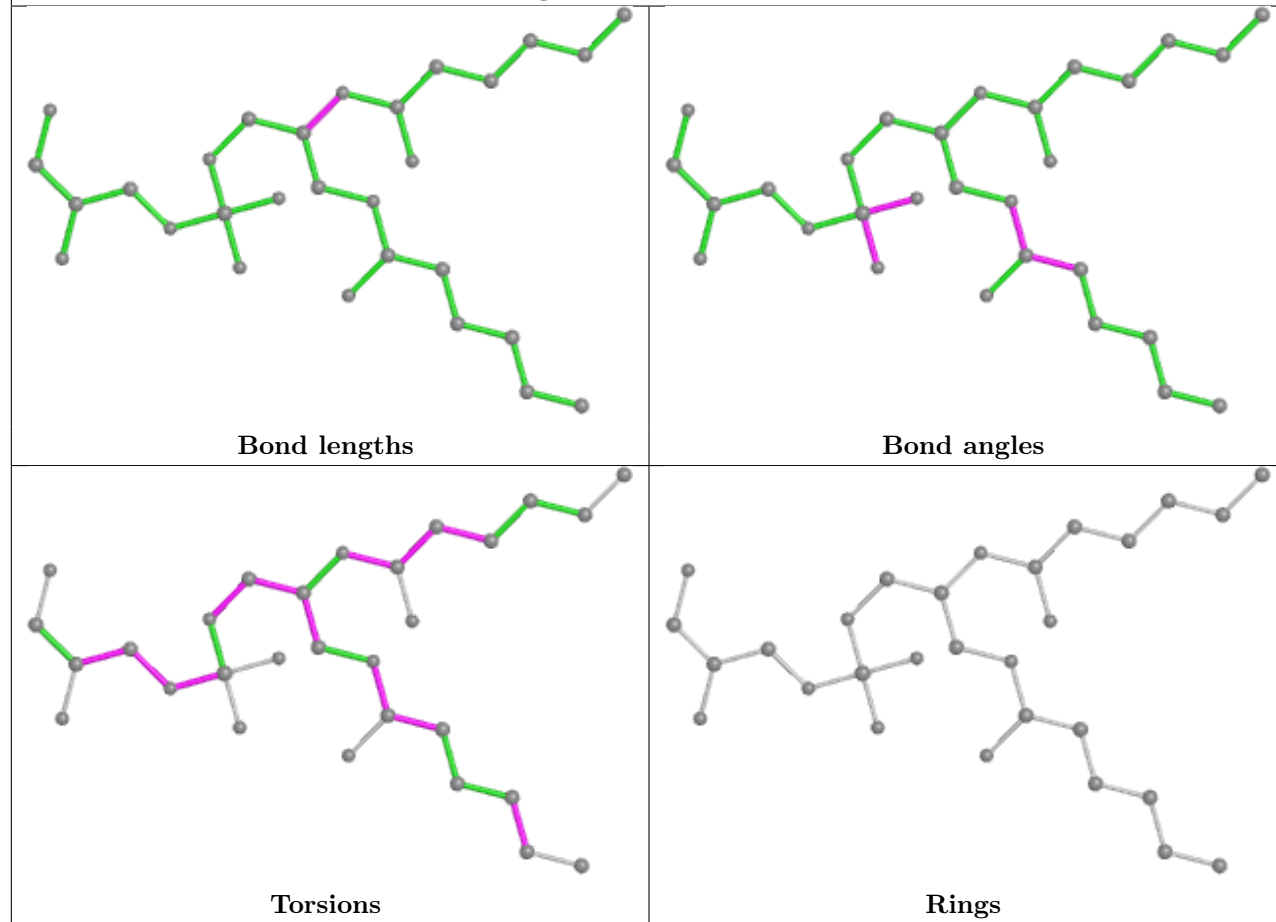


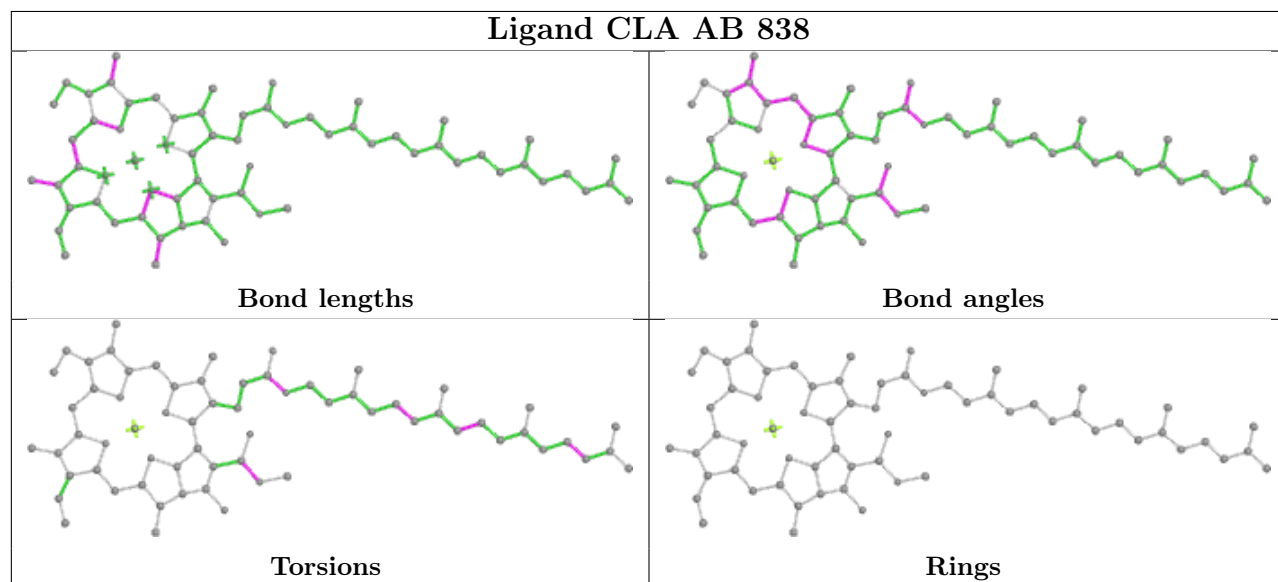
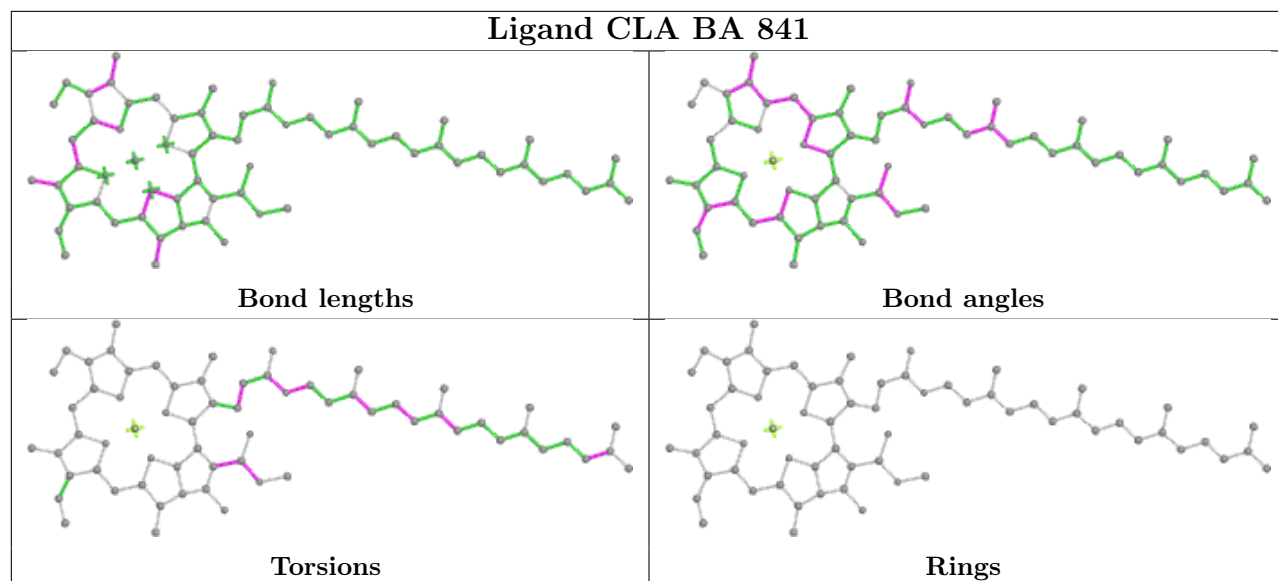
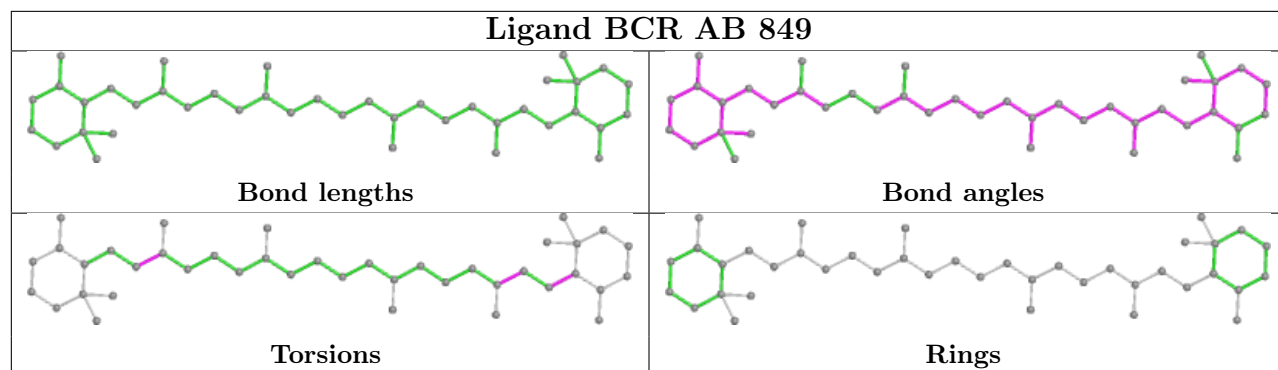
Rings

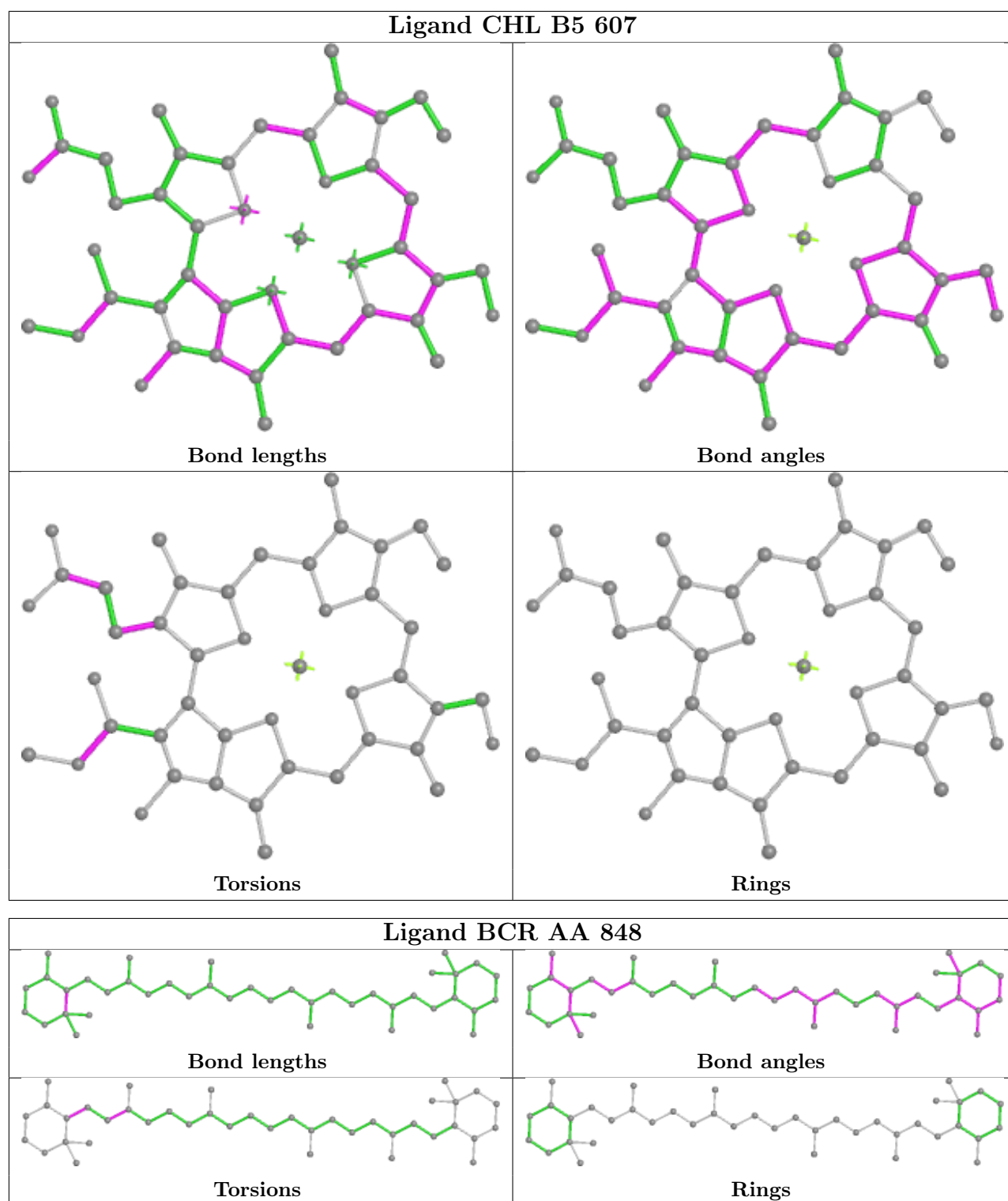
Ligand CLA BB 805

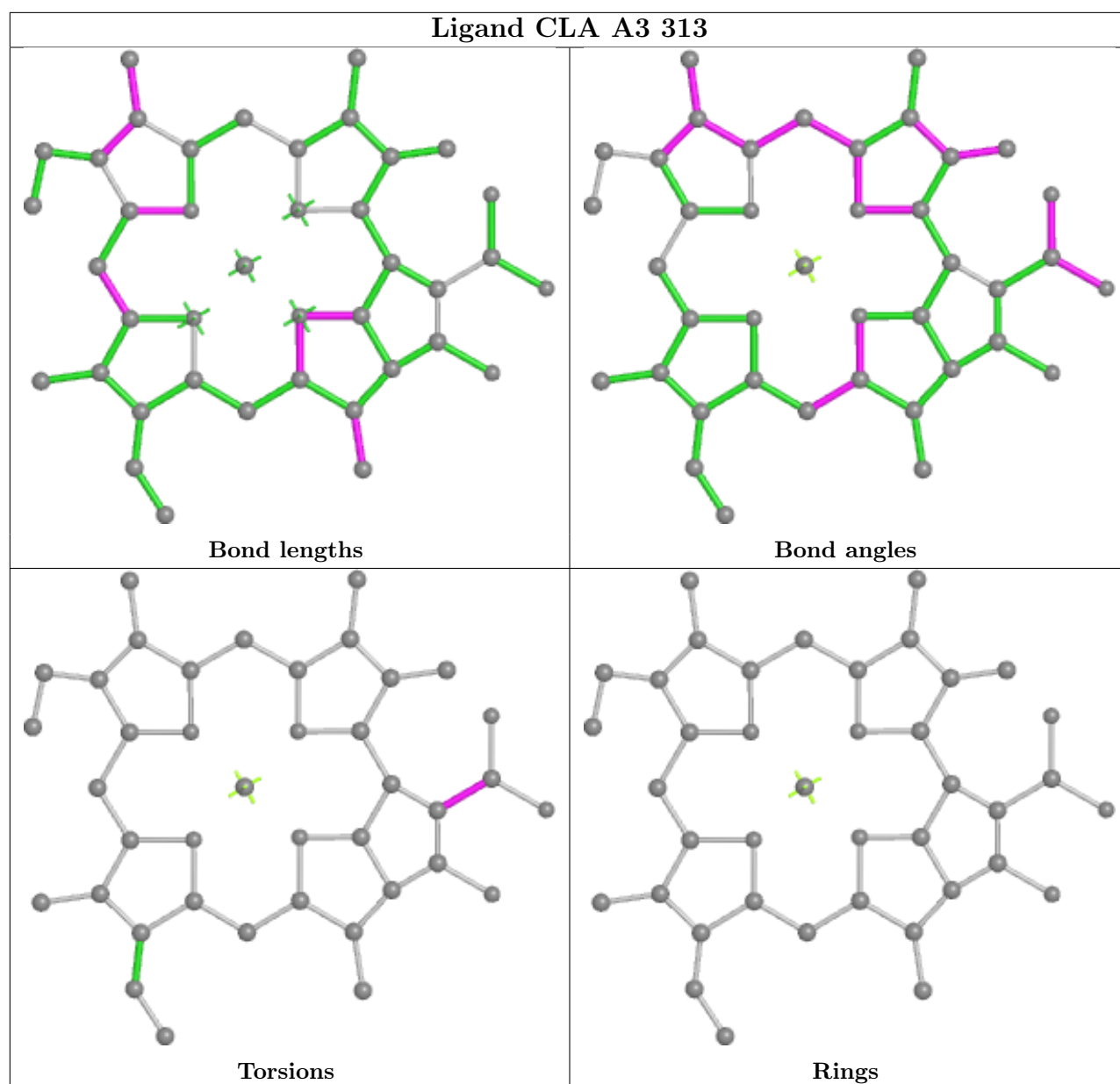


Ligand LHG a 501

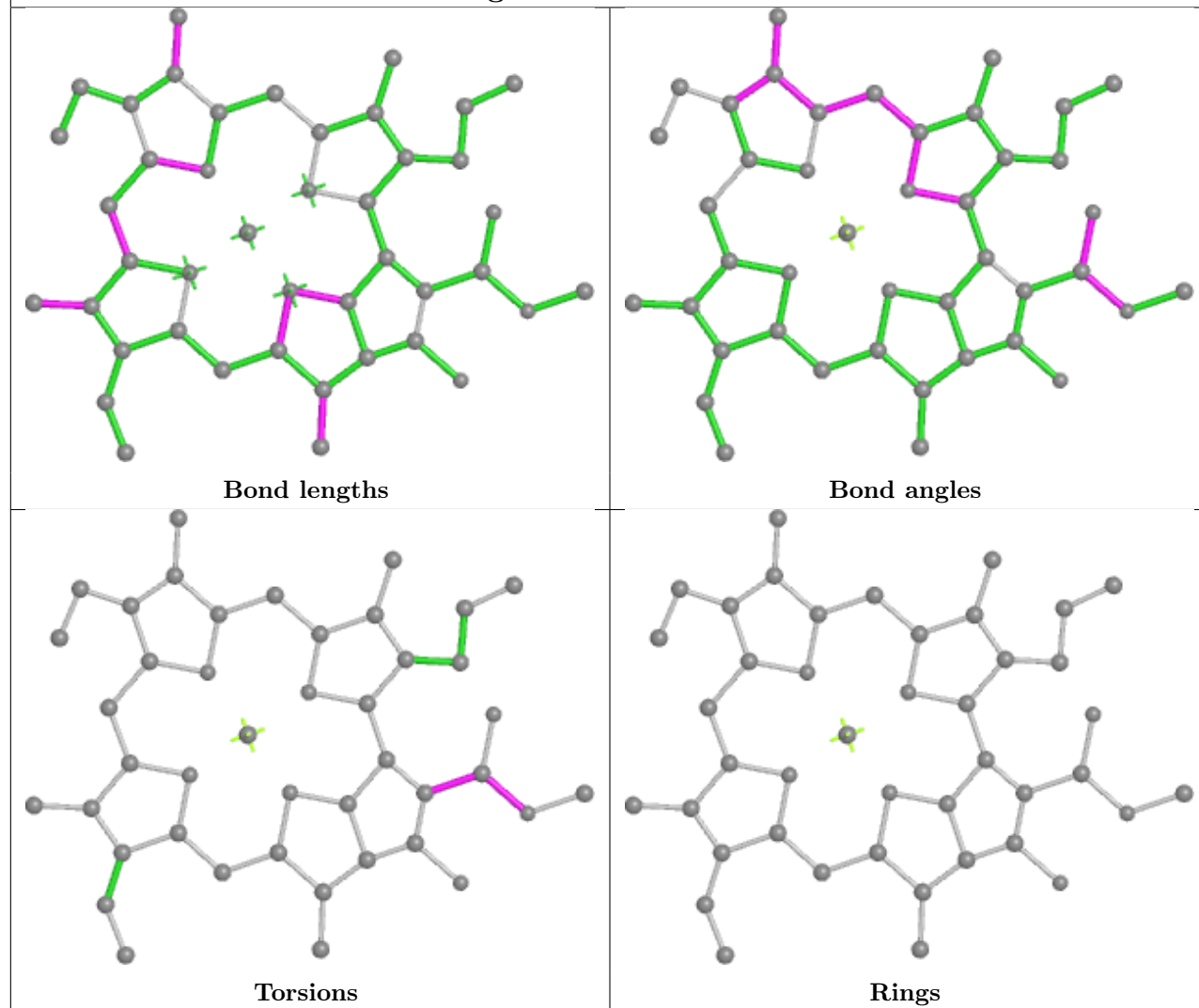




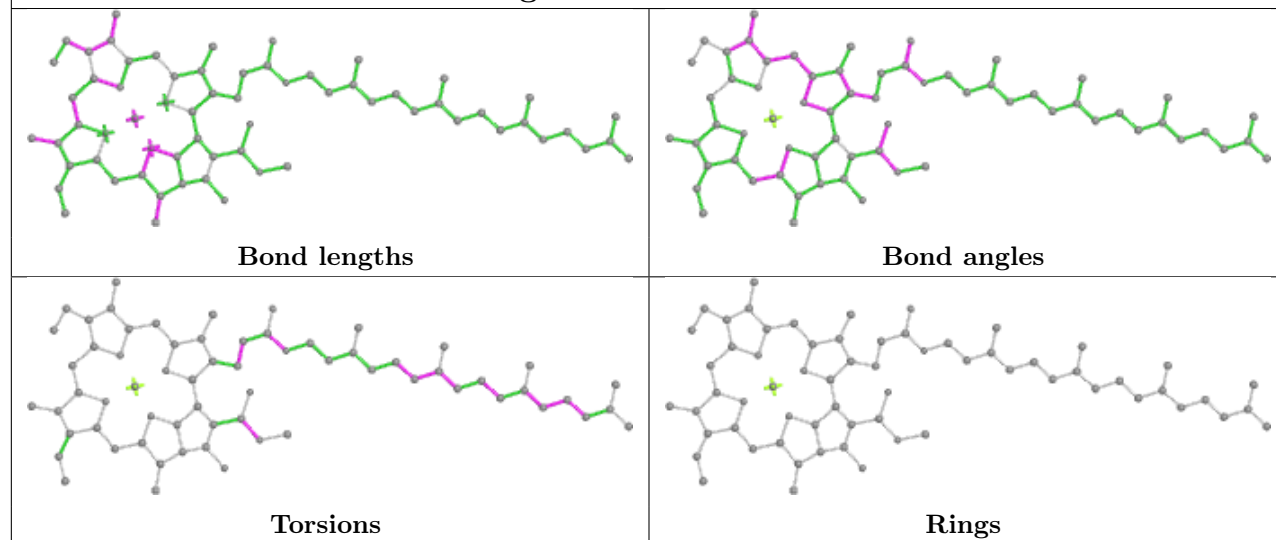




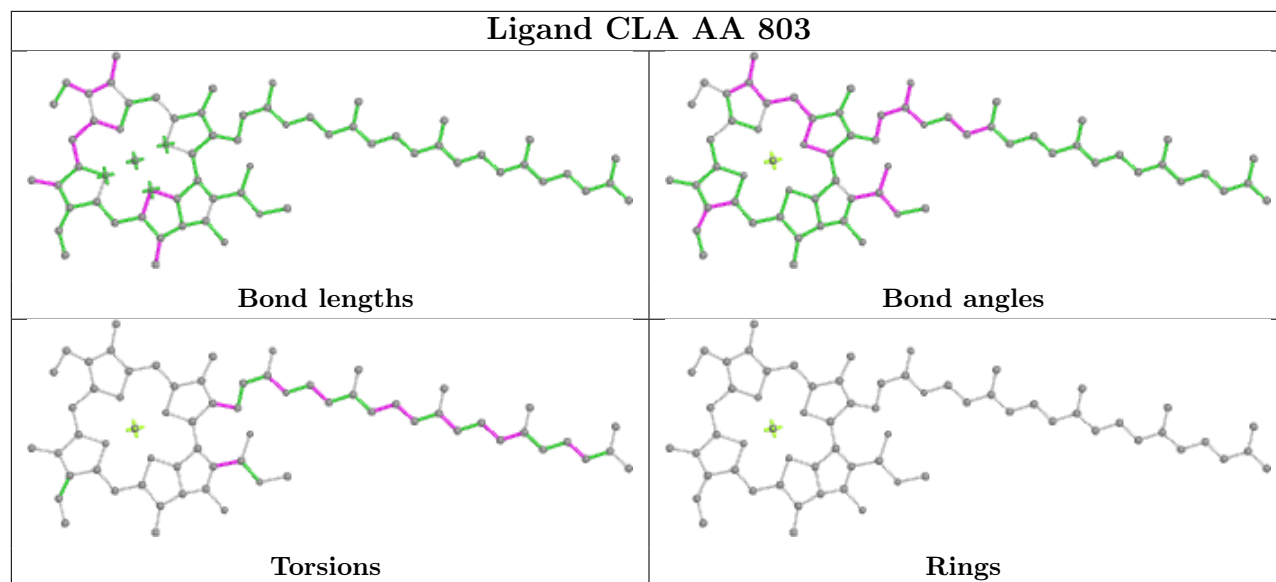
Ligand CLA AB 816



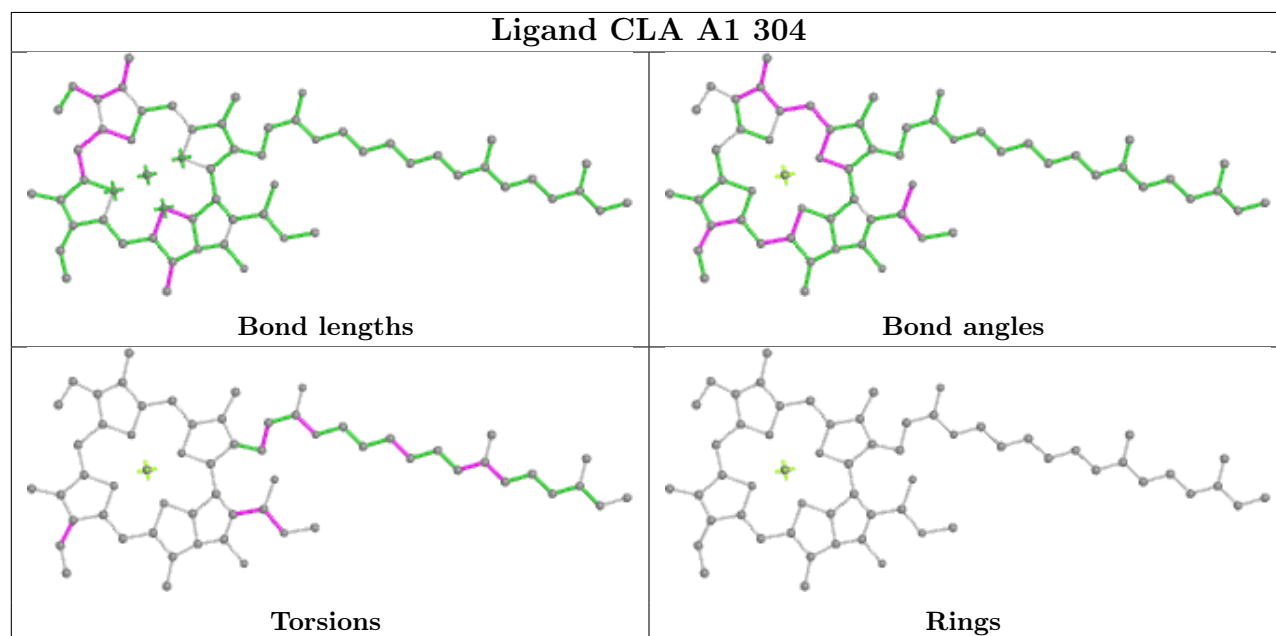
Ligand CLA BB 811

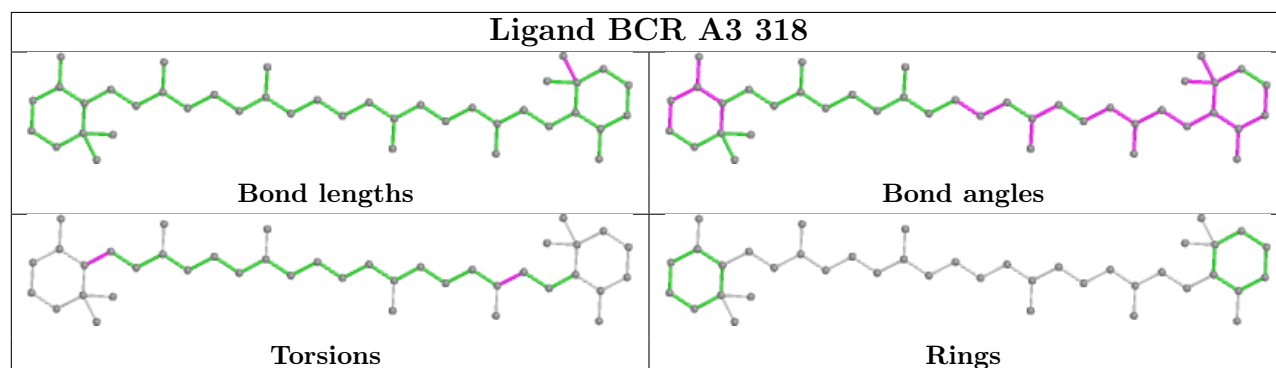
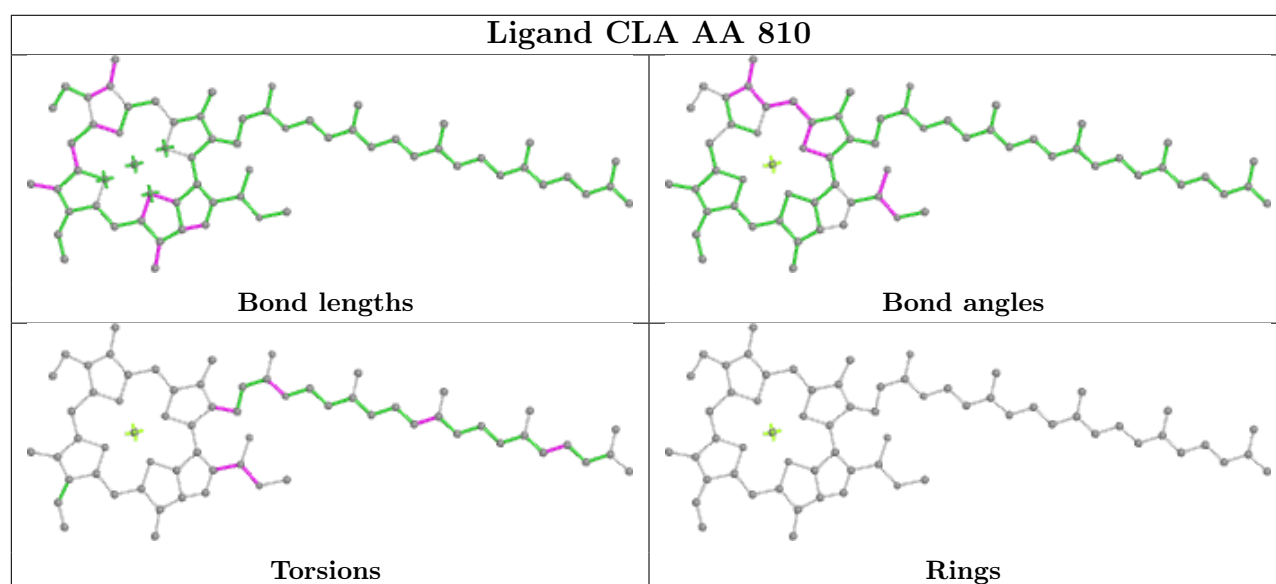
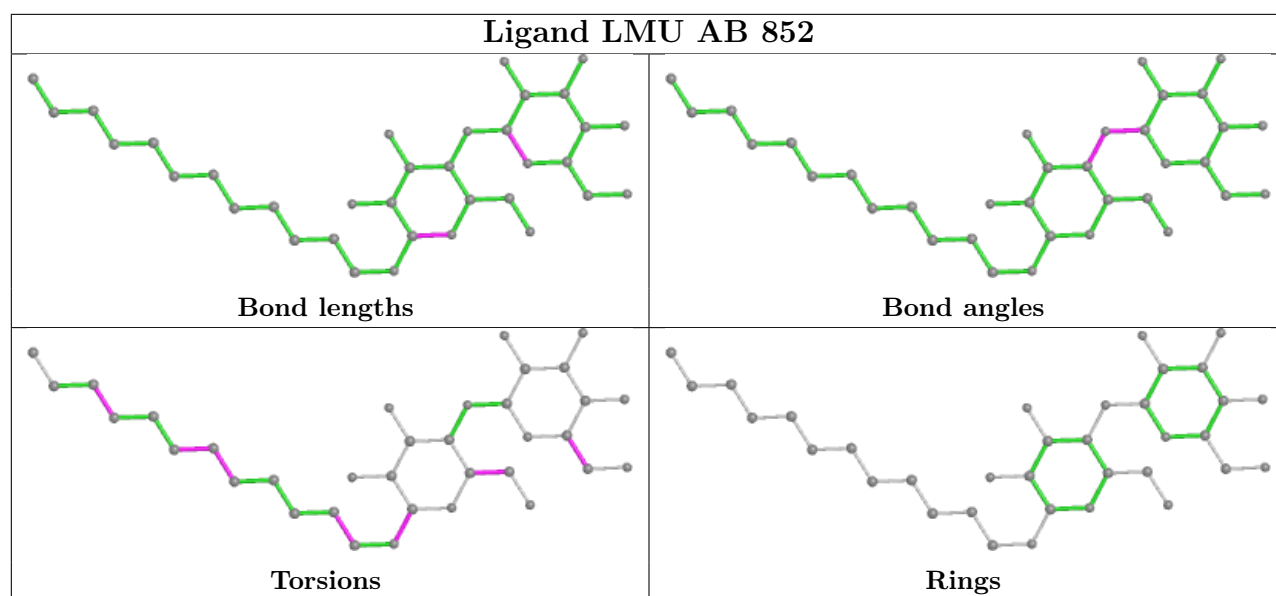


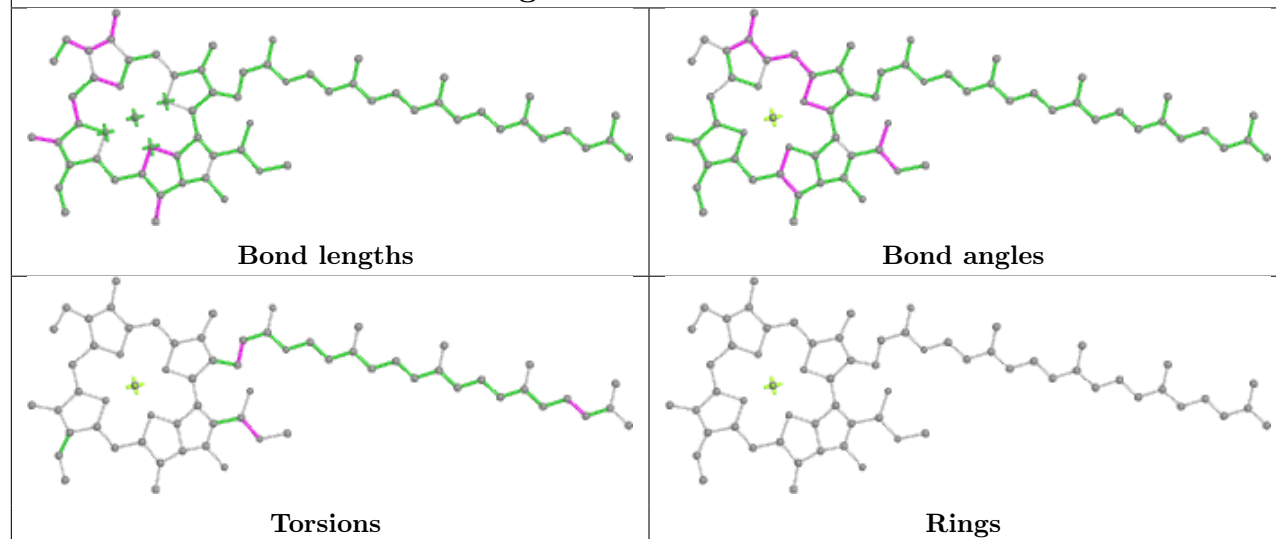
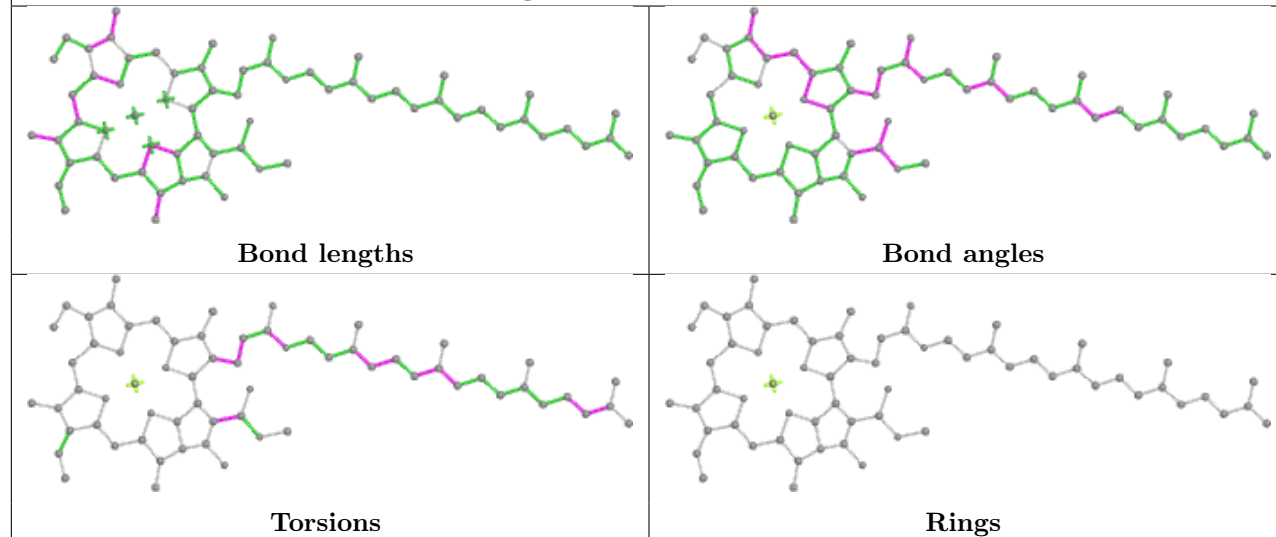
Ligand CLA AA 803



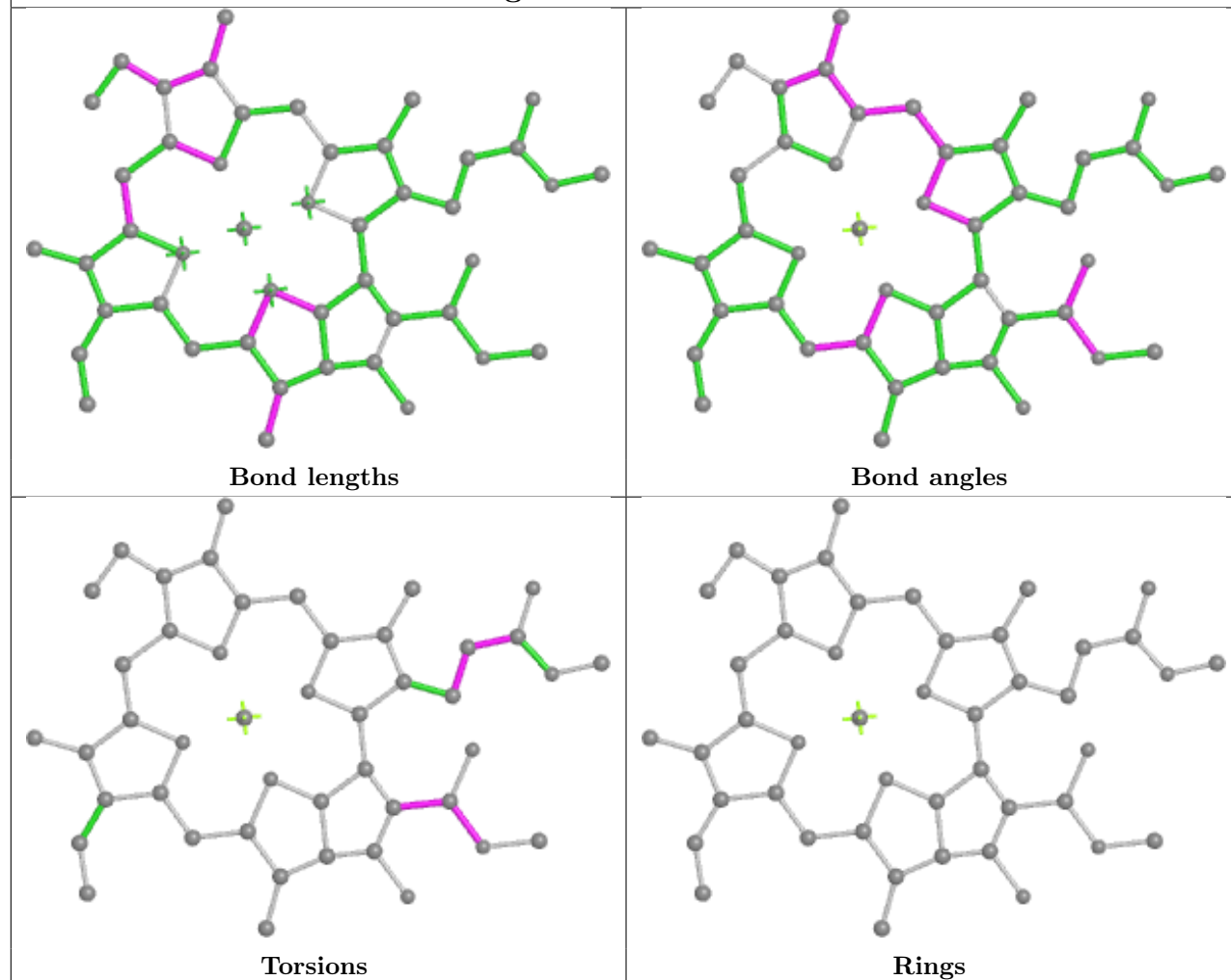
Ligand CLA A1 304



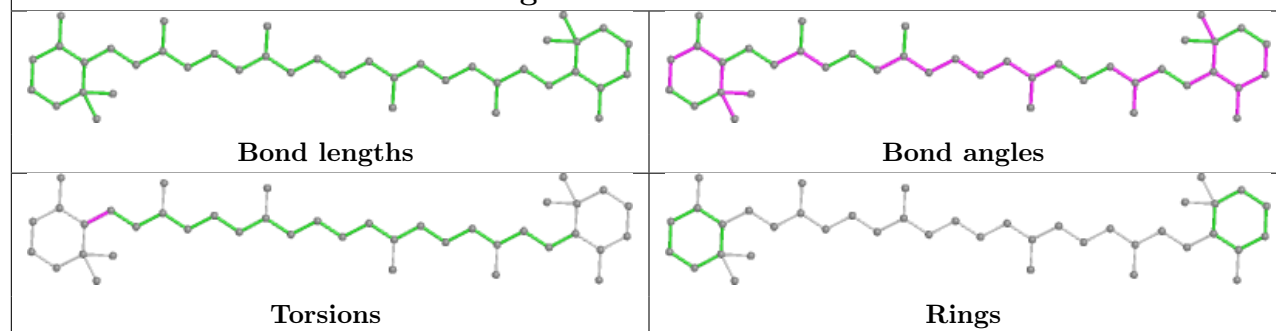


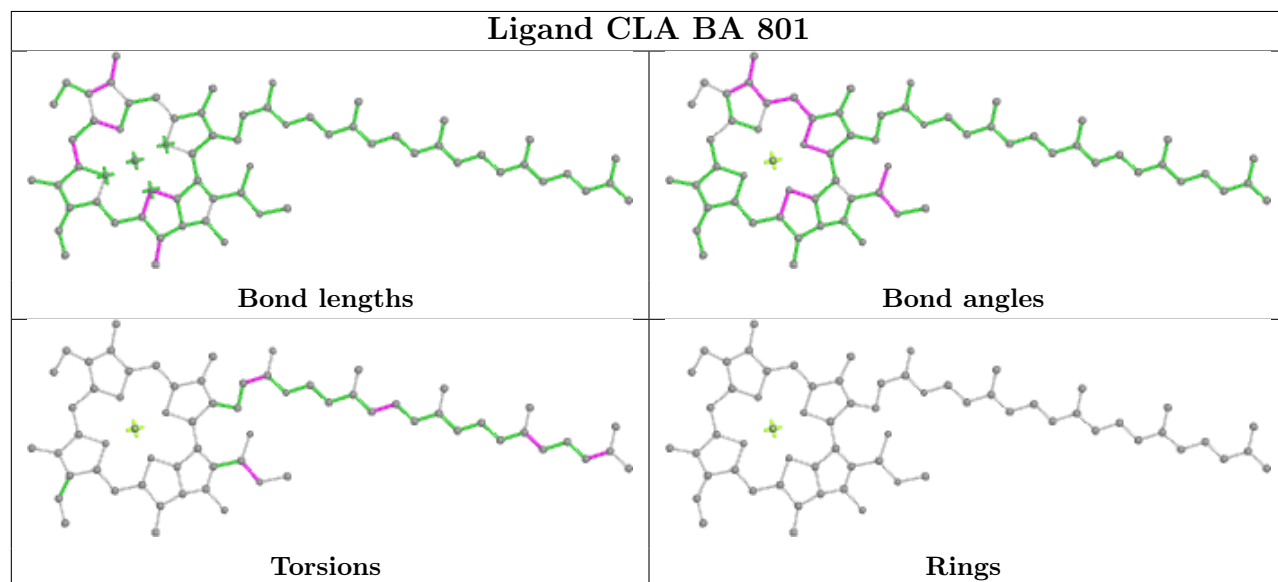
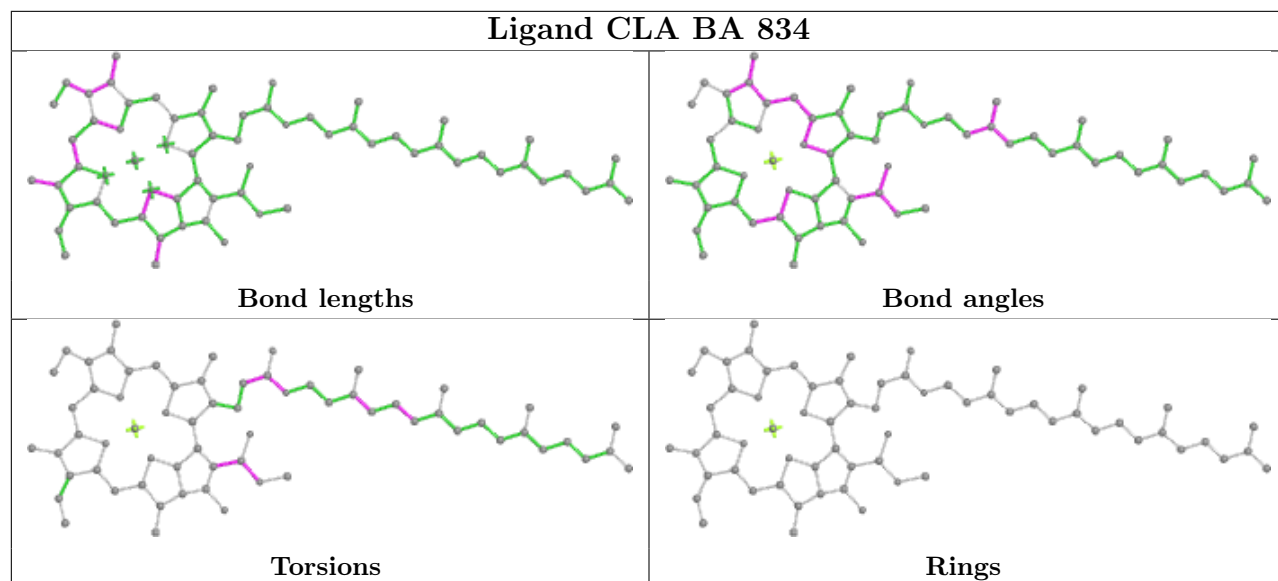
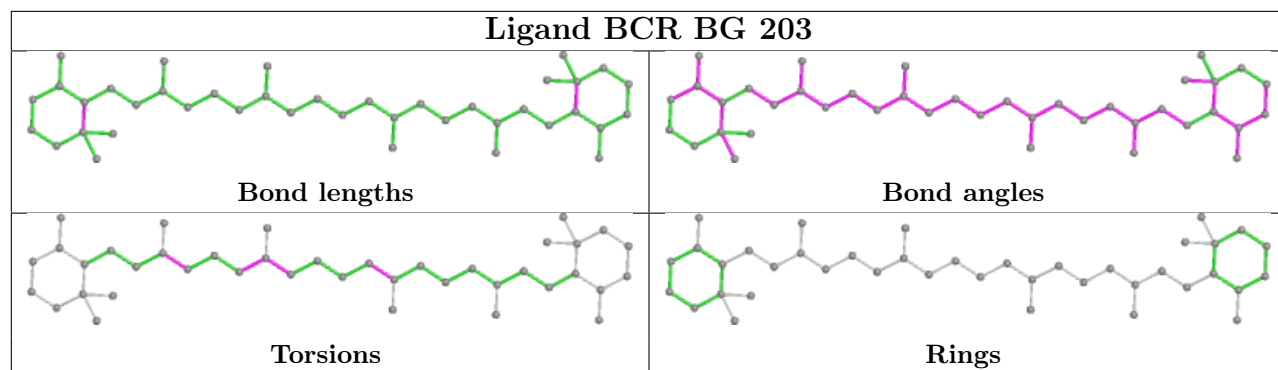
Ligand CLA BA 802**Ligand CLA AB 809**

Ligand CLA B5 601

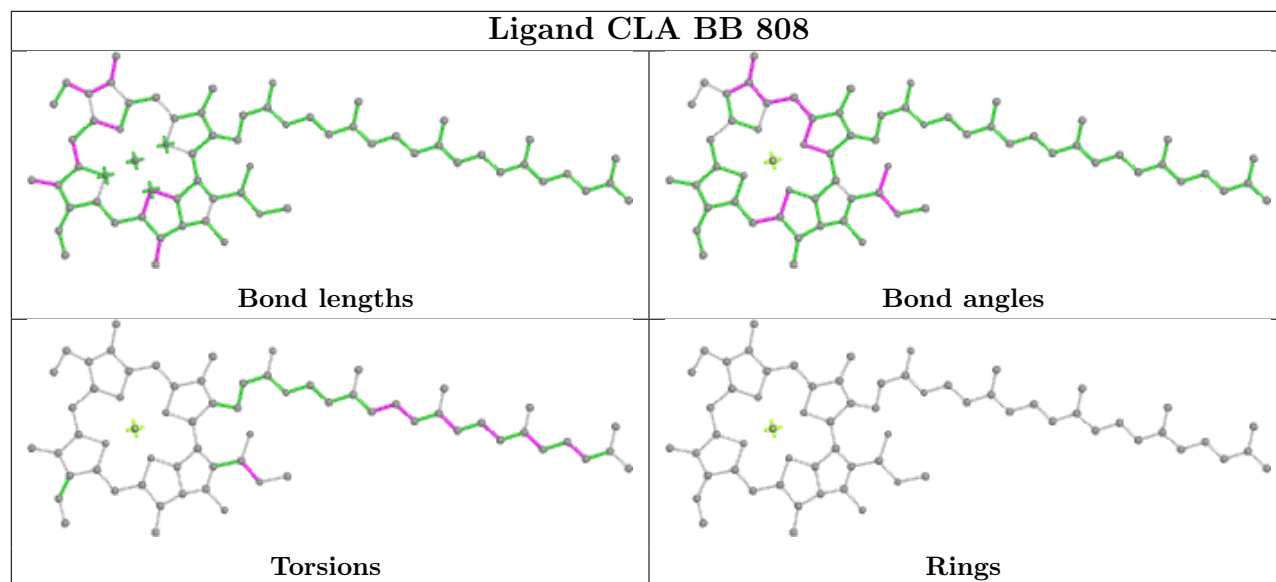


Ligand BCR BL 305

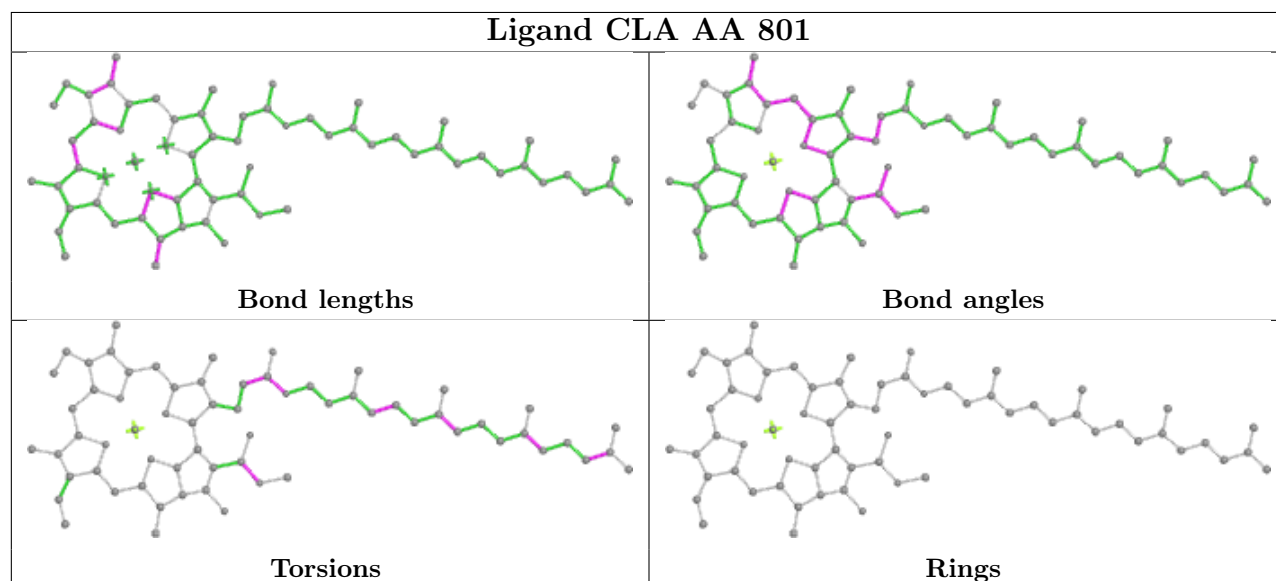




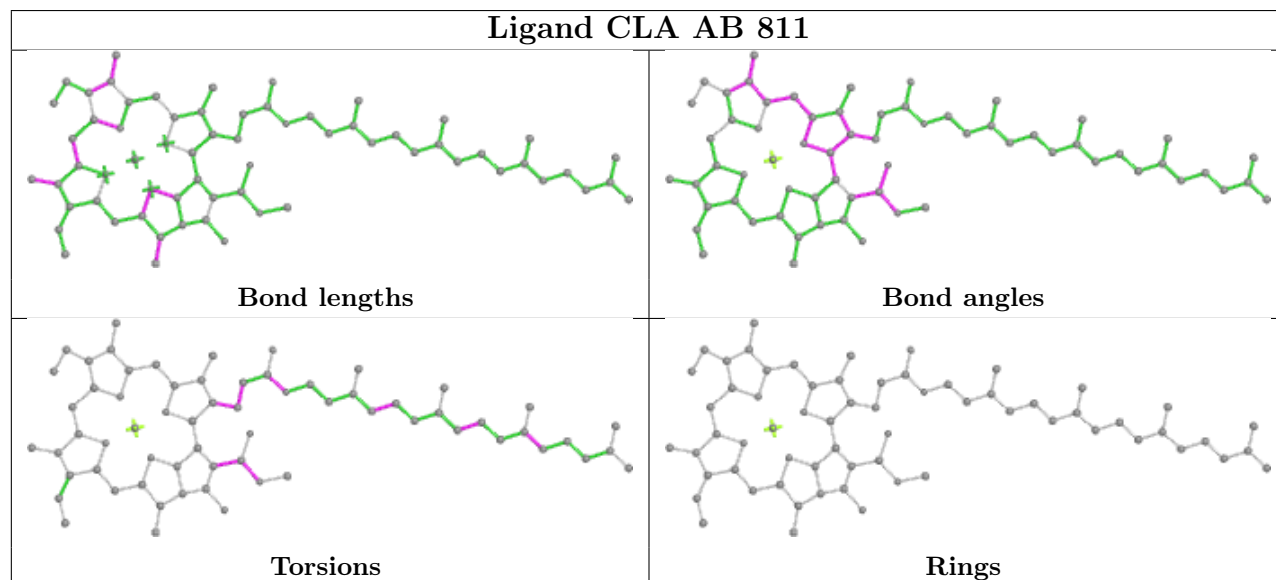
Ligand CLA BB 808



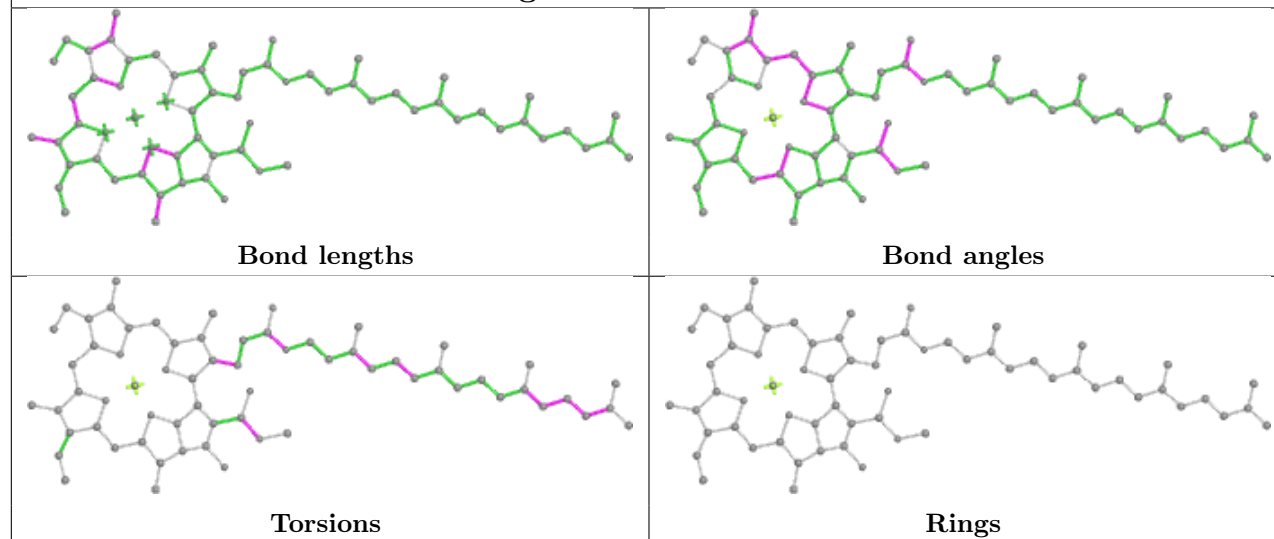
Ligand CLA AA 801



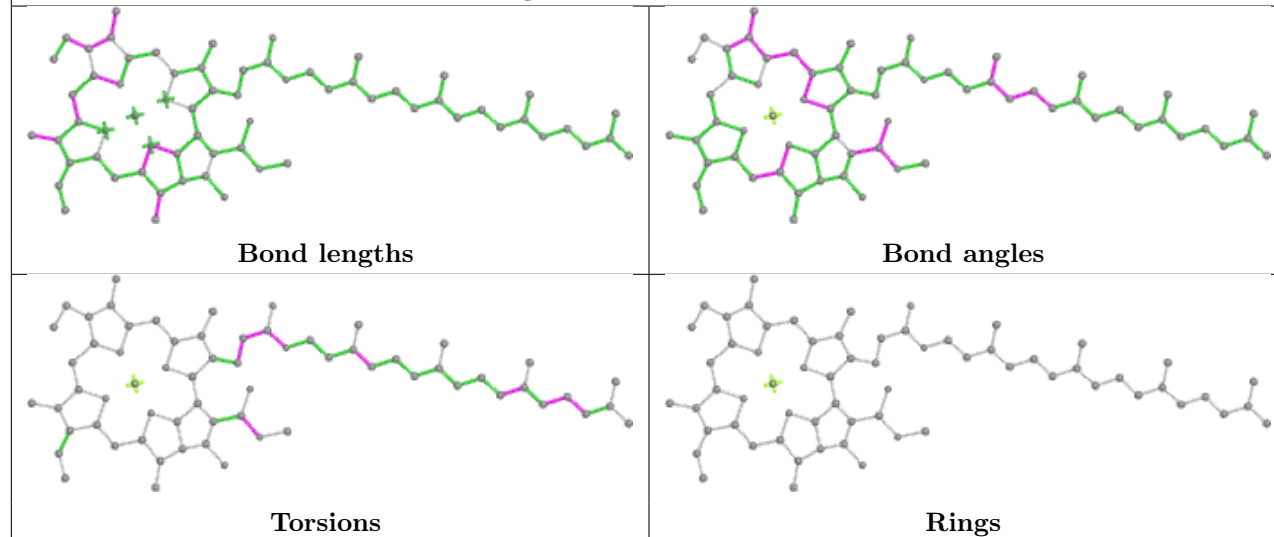
Ligand CLA AB 811



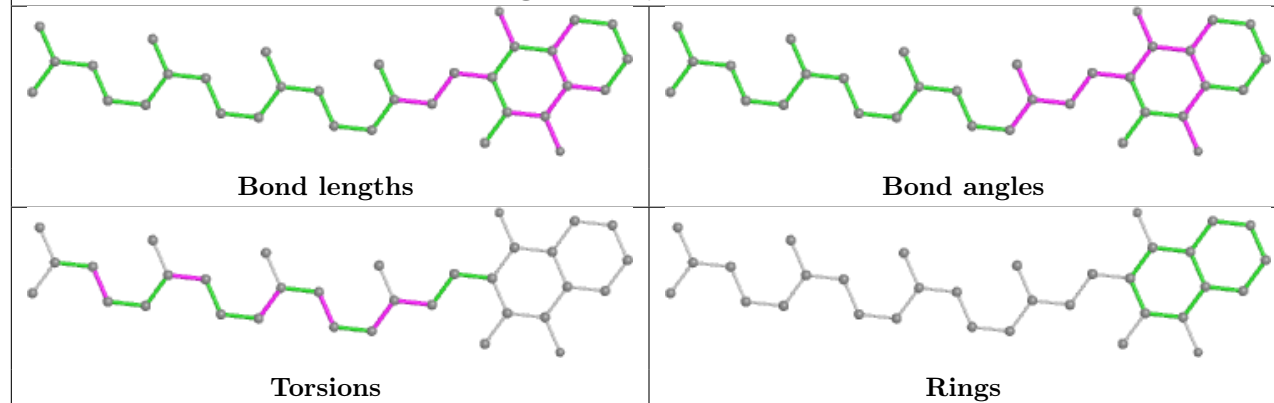
Ligand CLA BA 811



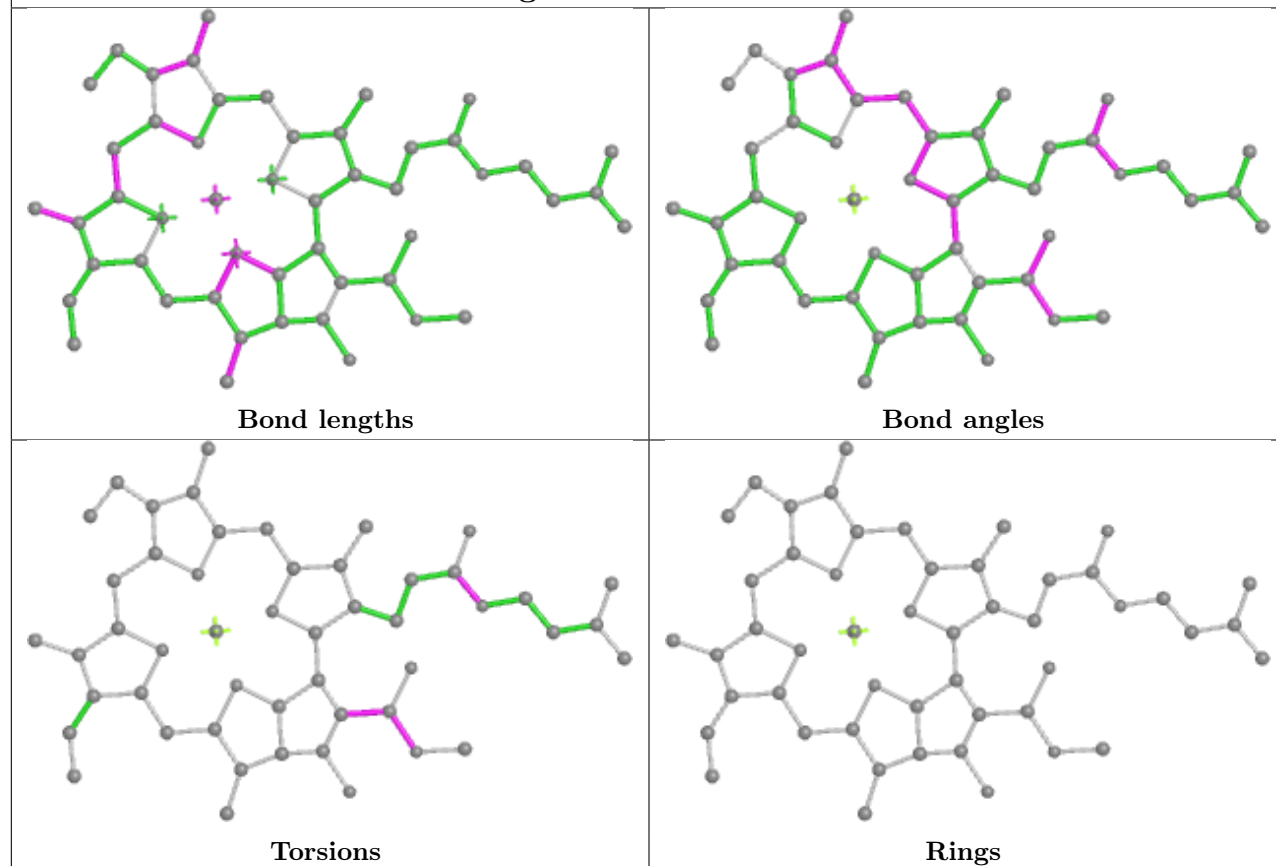
Ligand CLA BA 821



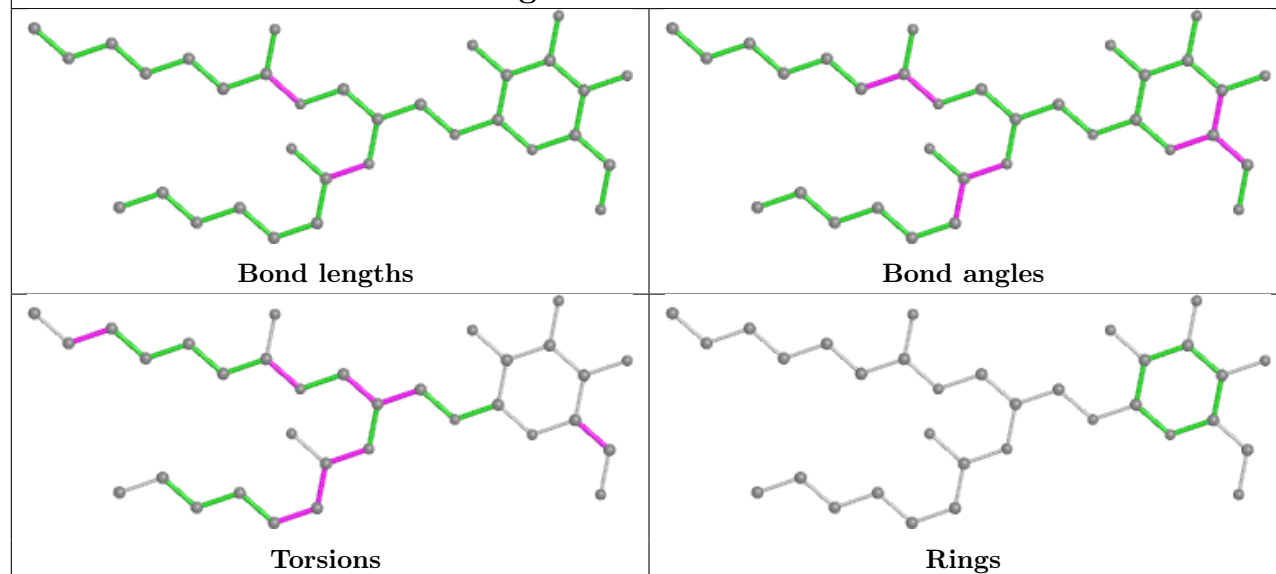
Ligand PQN BB 844

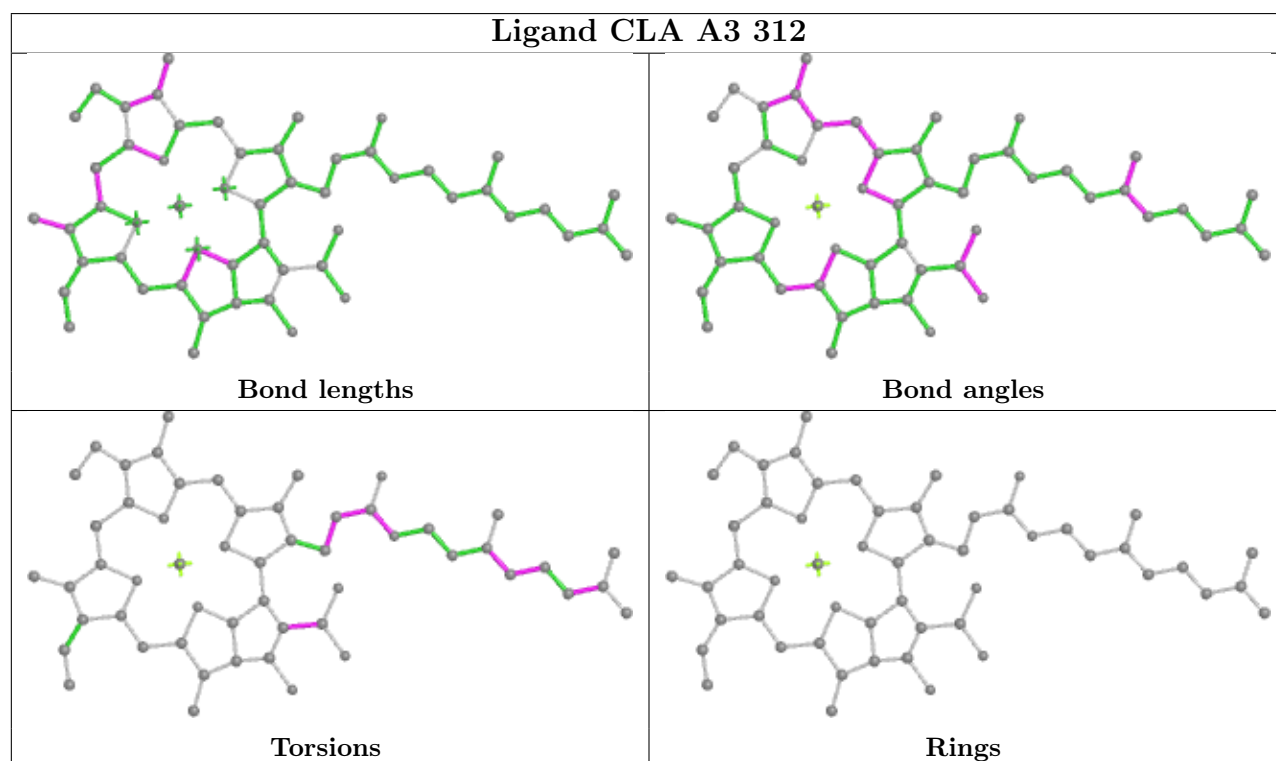
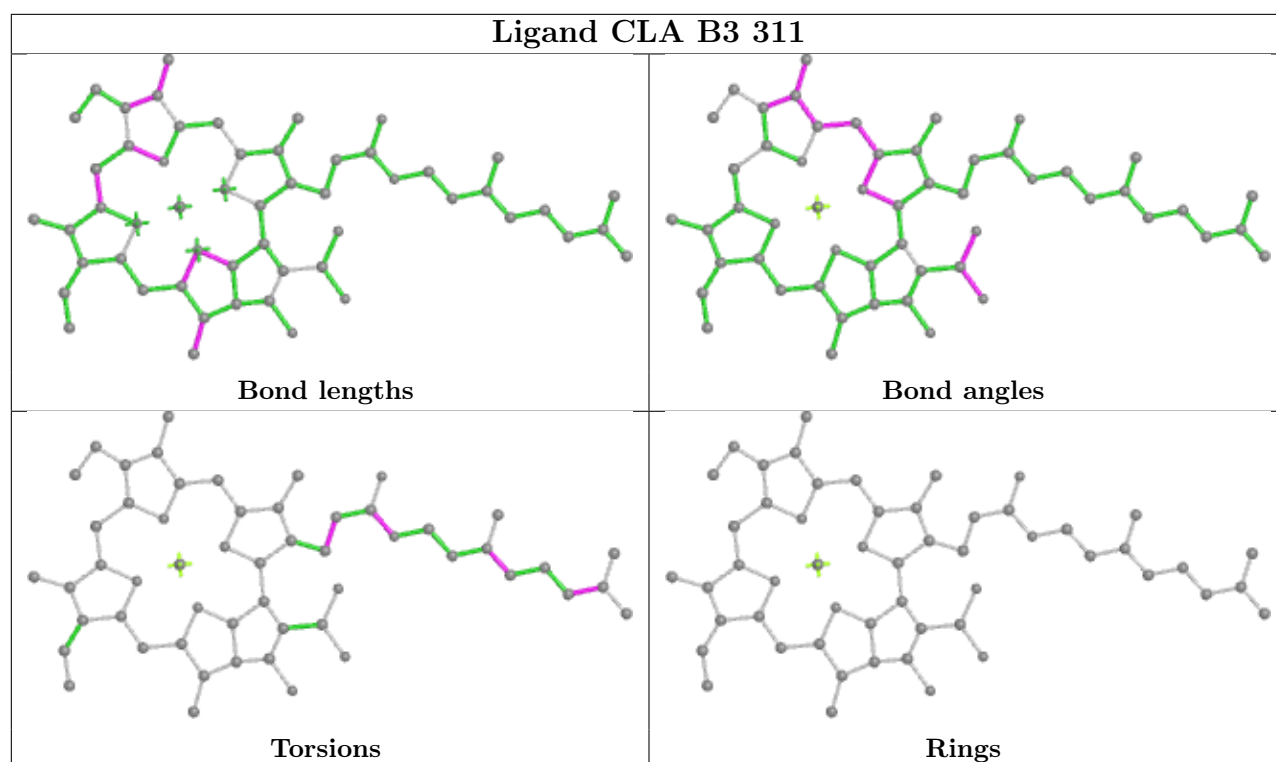


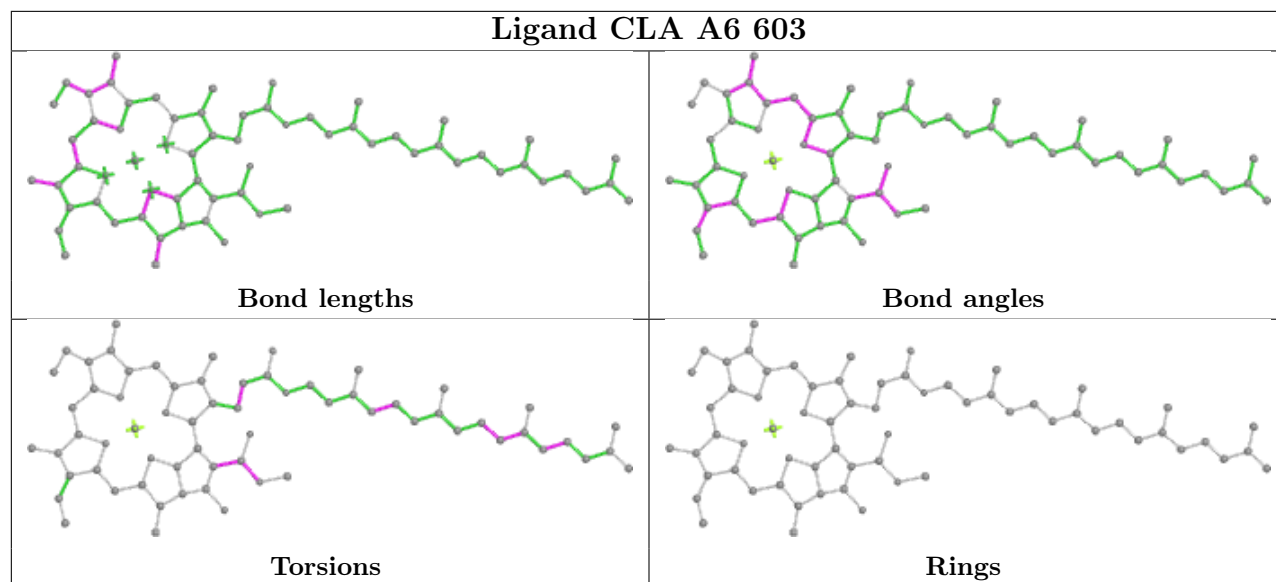
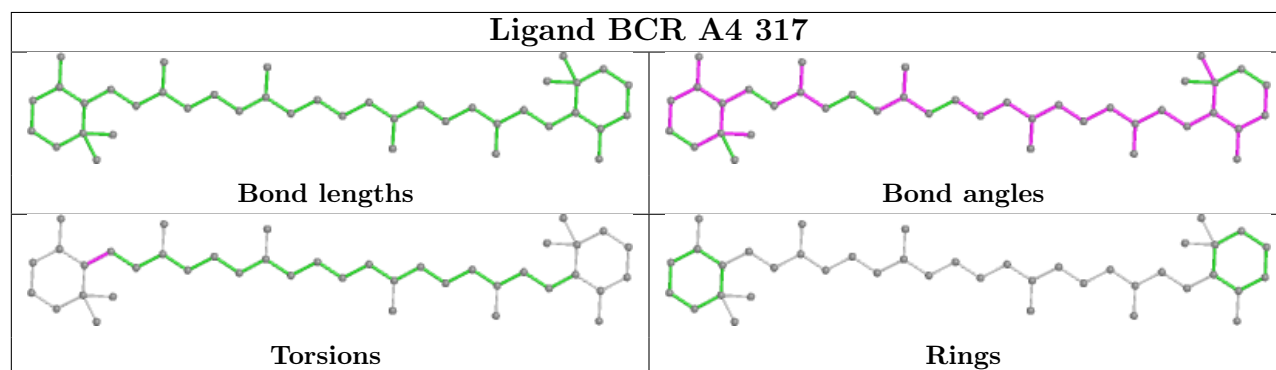
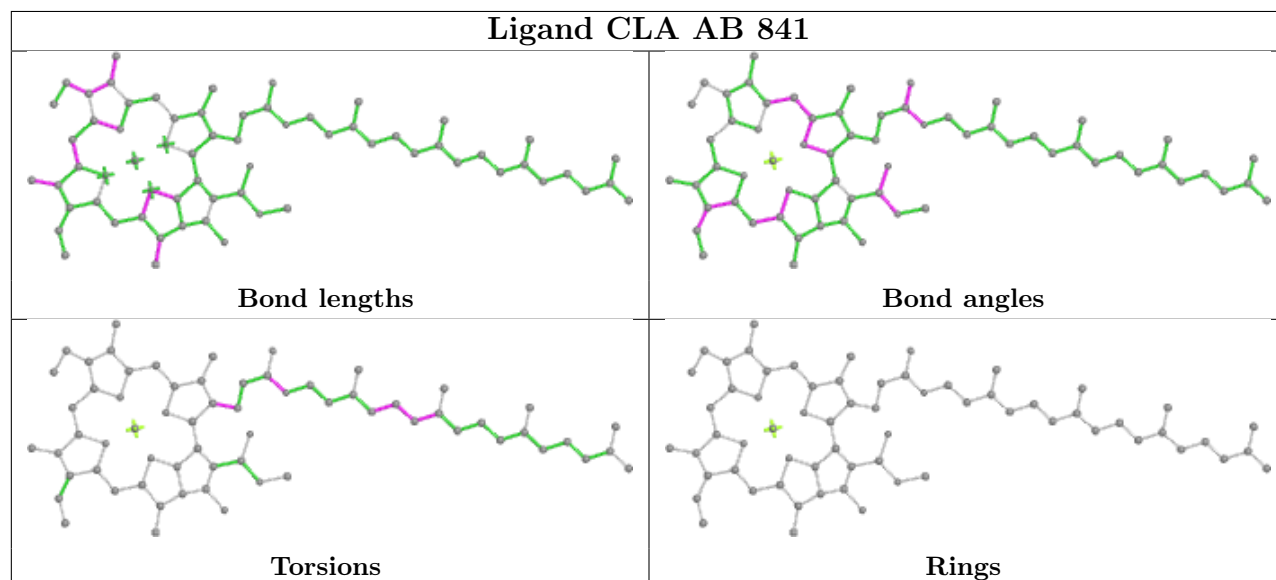
Ligand CLA AB 837

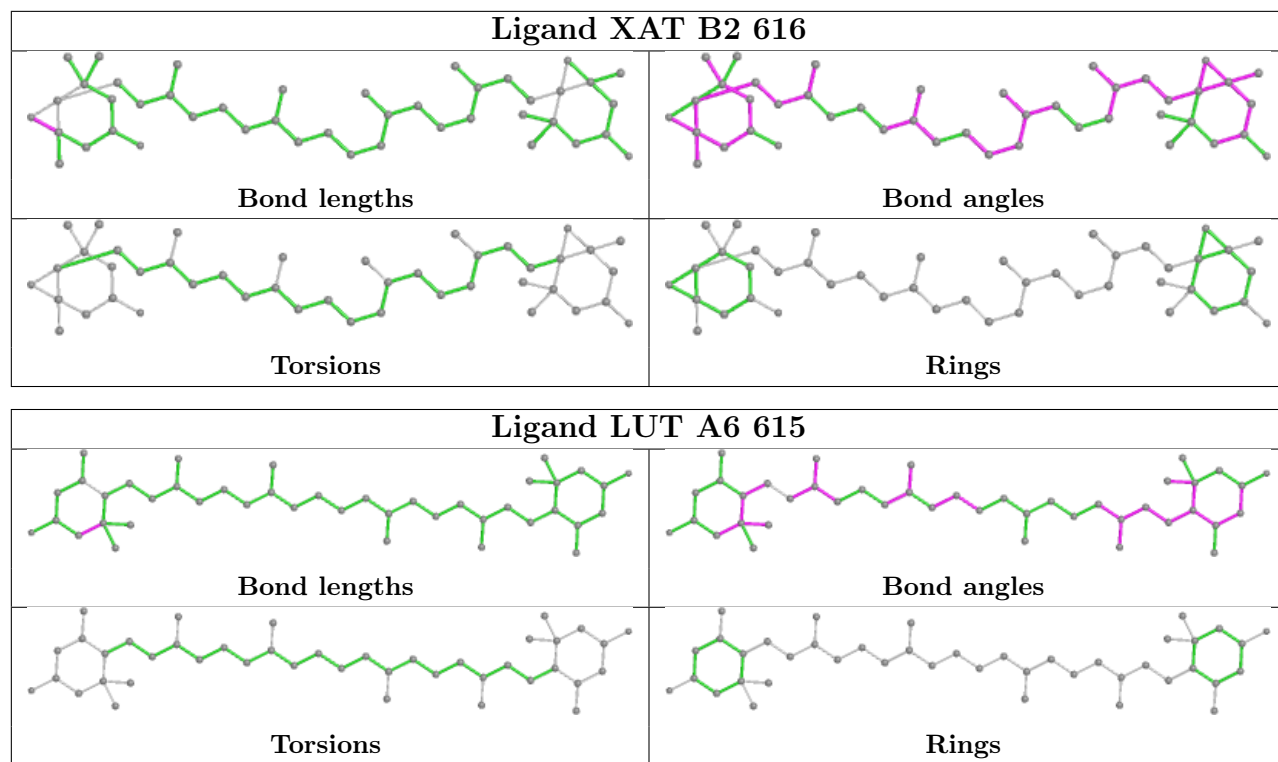


Ligand LMG B5 617

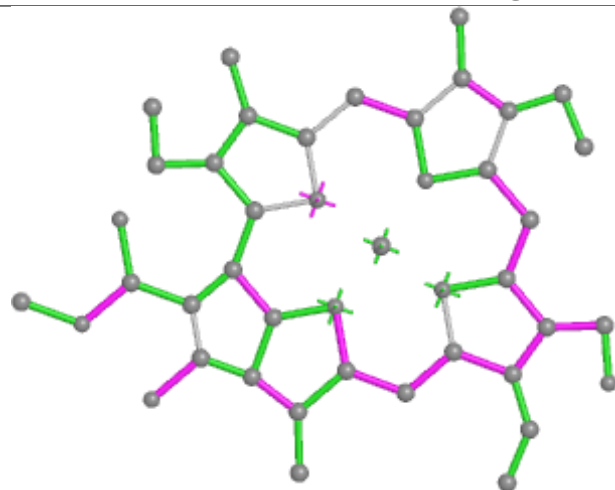




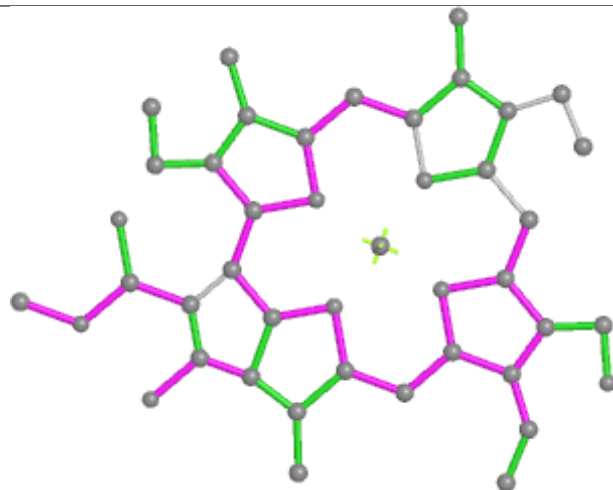
Ligand CLA A6 603**Ligand BCR A4 317****Ligand CLA AB 841**



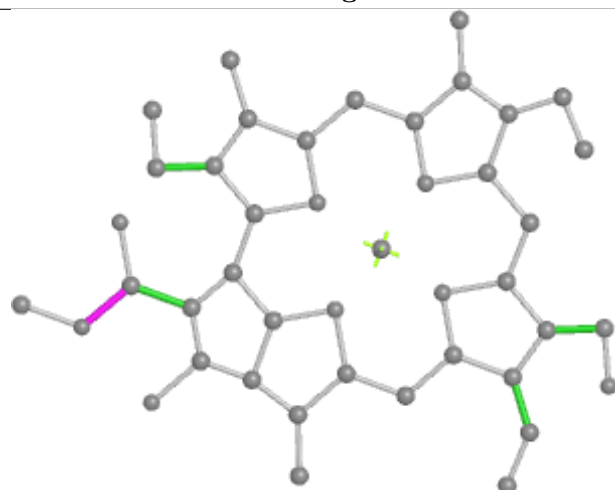
Ligand CHL B2 606



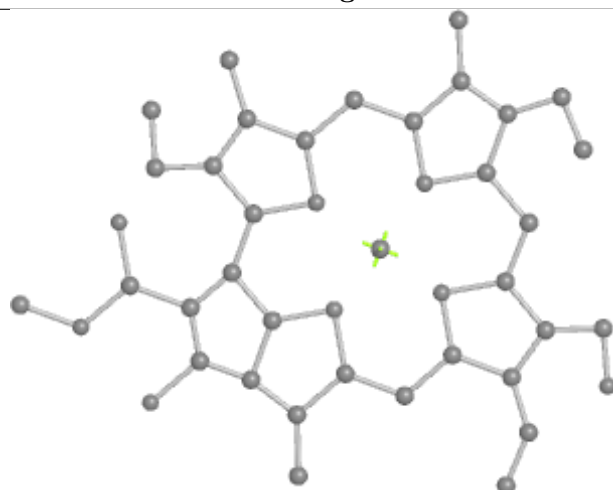
Bond lengths



Bond angles

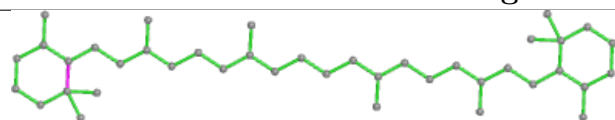


Torsions

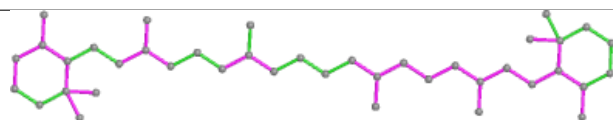


Rings

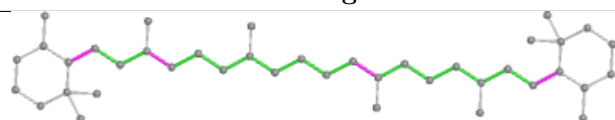
Ligand BCR BA 851



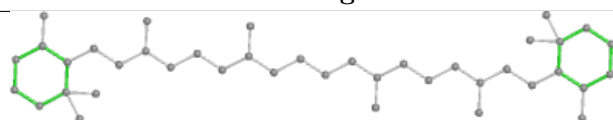
Bond lengths



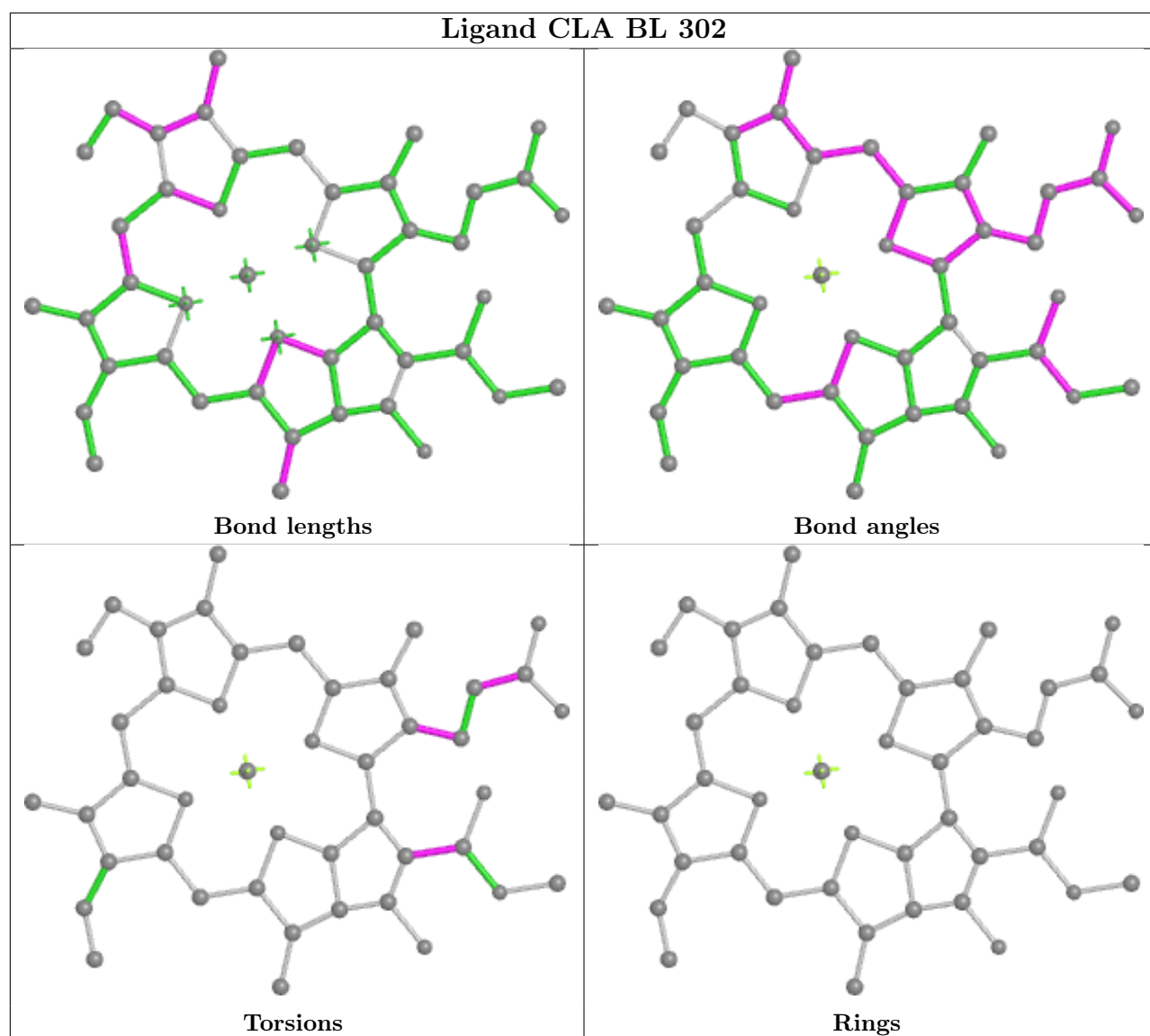
Bond angles



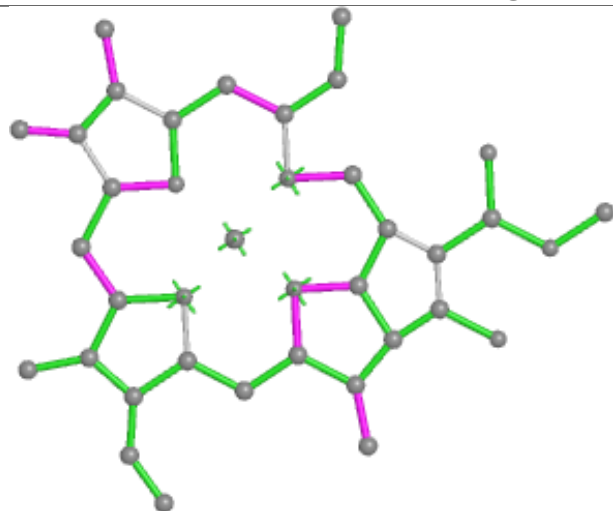
Torsions



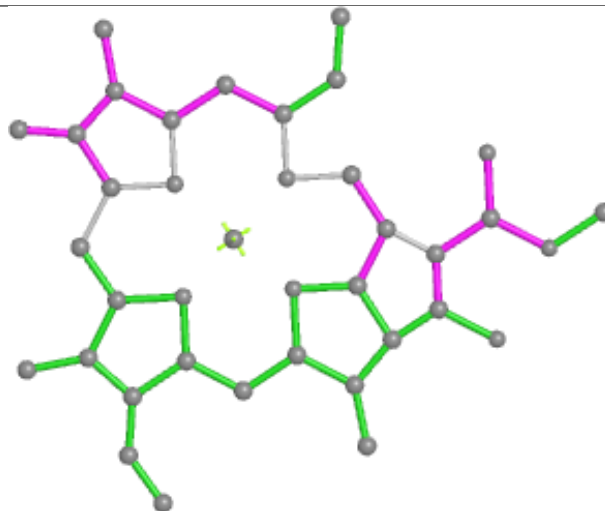
Rings



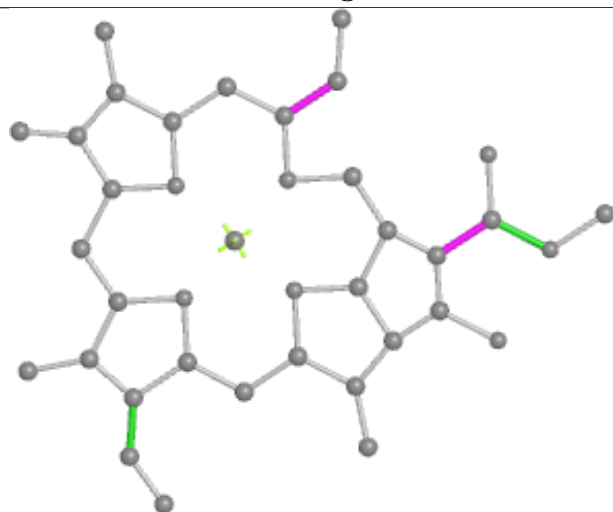
Ligand CLA A6 611



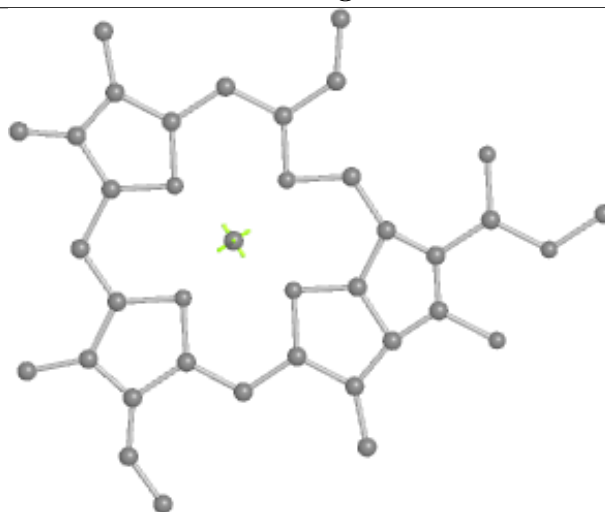
Bond lengths



Bond angles

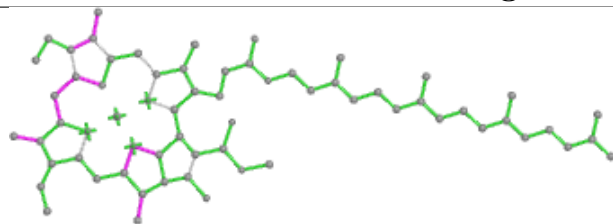


Torsions

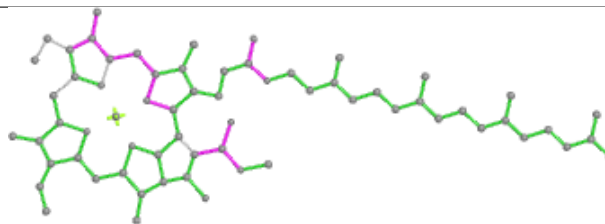


Rings

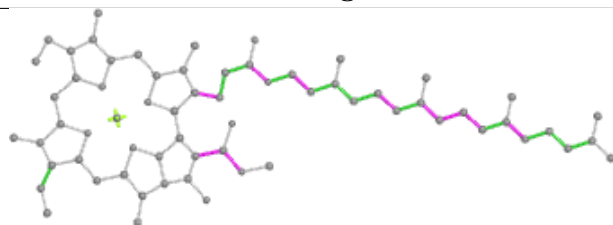
Ligand CLA AA 830



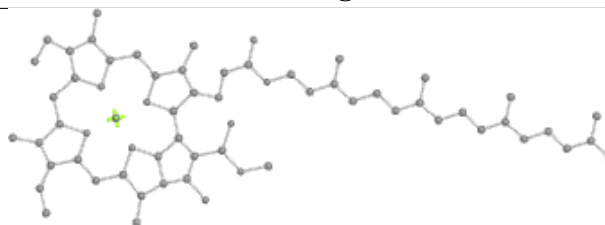
Bond lengths



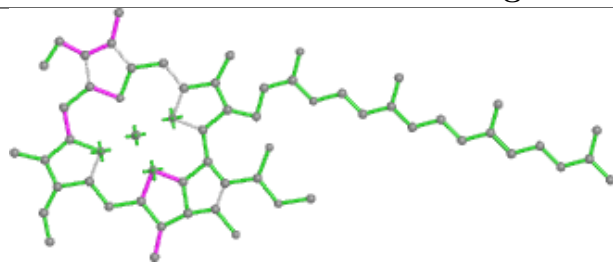
Bond angles



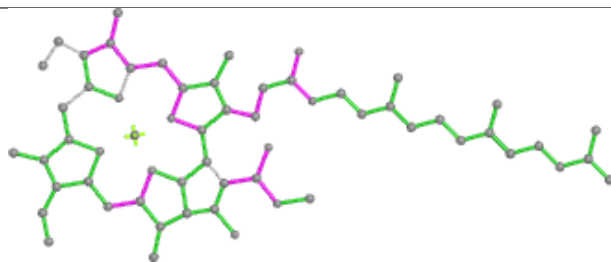
Torsions



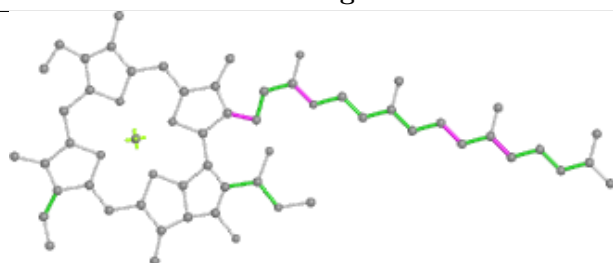
Rings

Ligand CLA BL 303

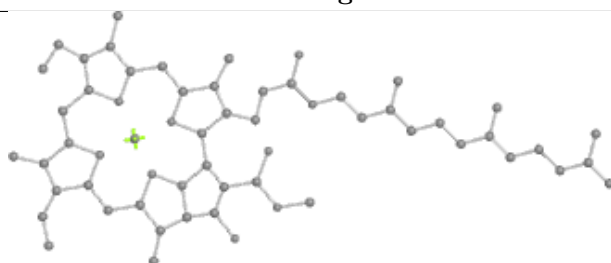
Bond lengths



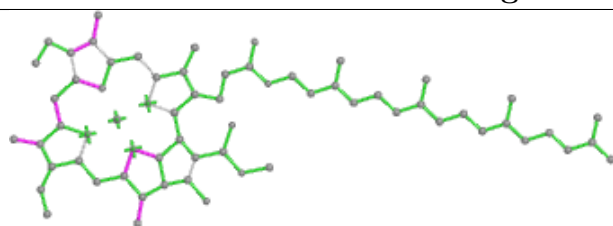
Bond angles



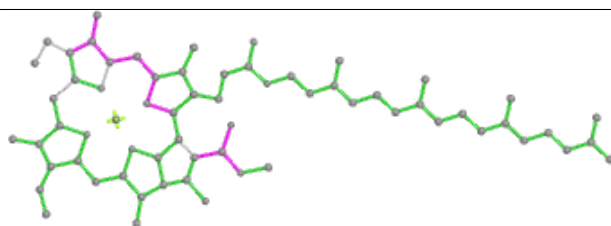
Torsions



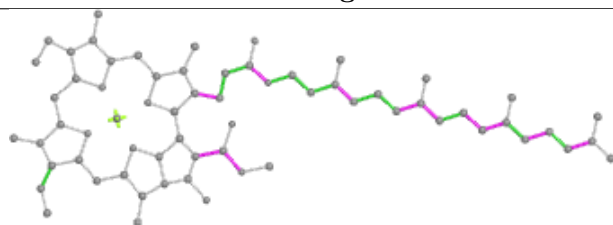
Rings

Ligand CLA AB 803

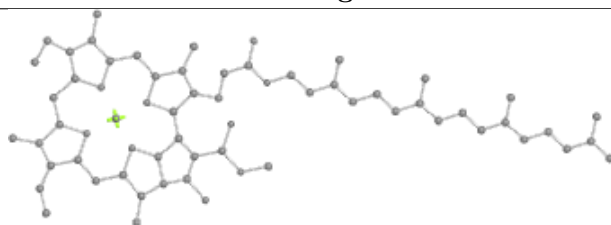
Bond lengths



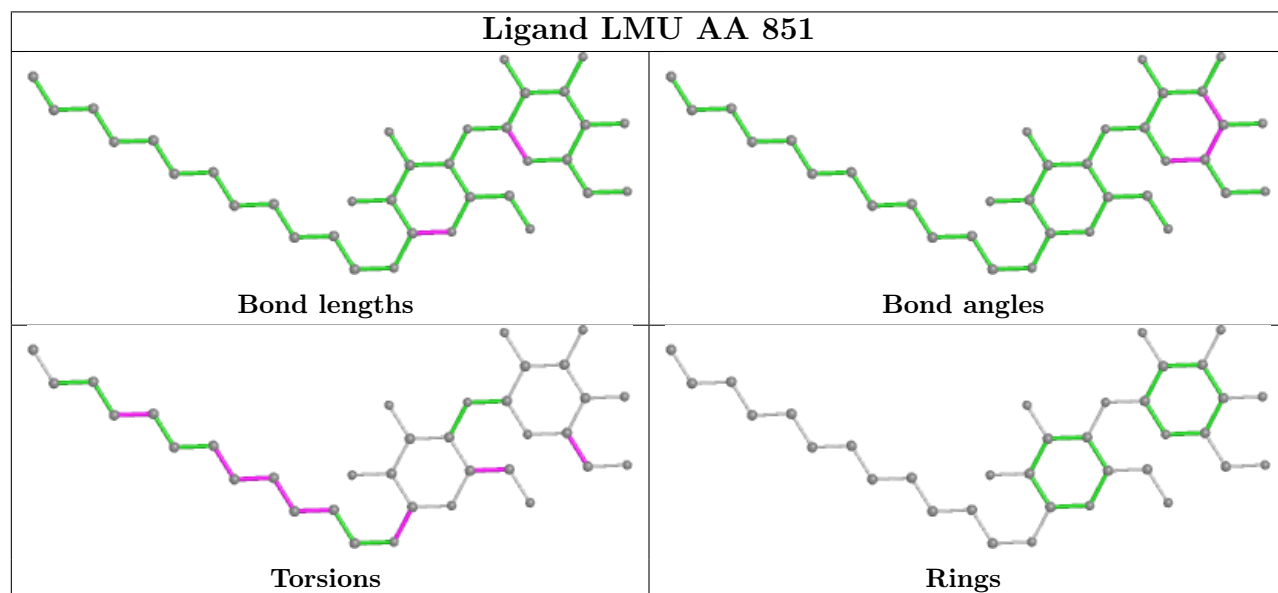
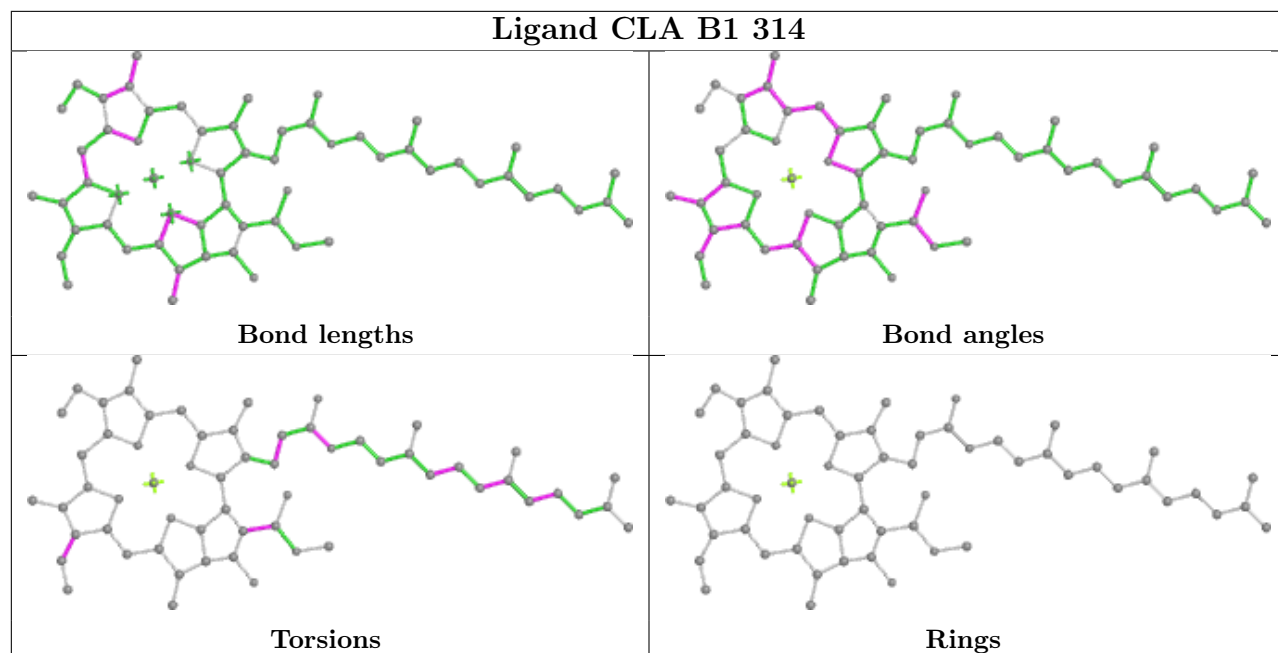
Bond angles

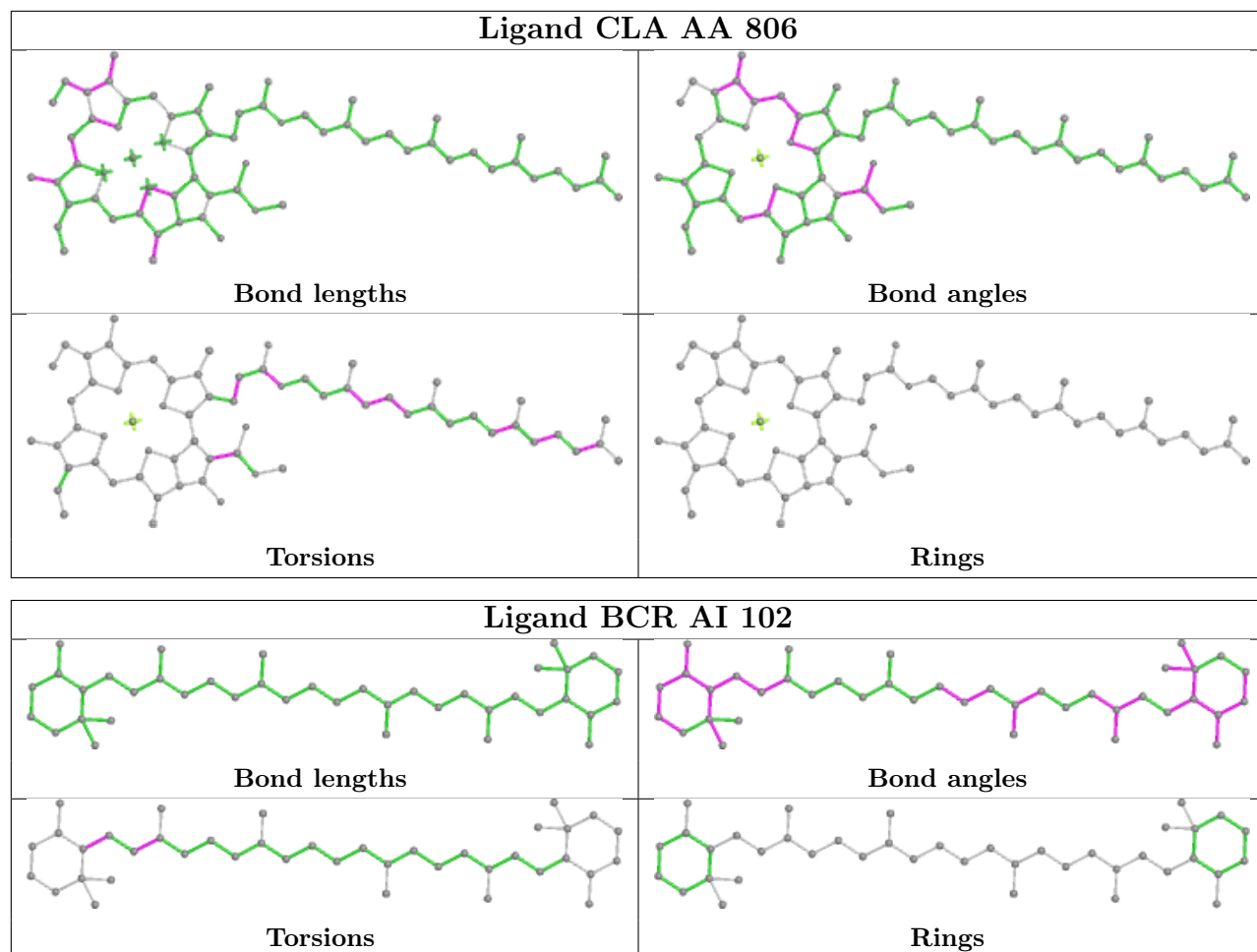


Torsions

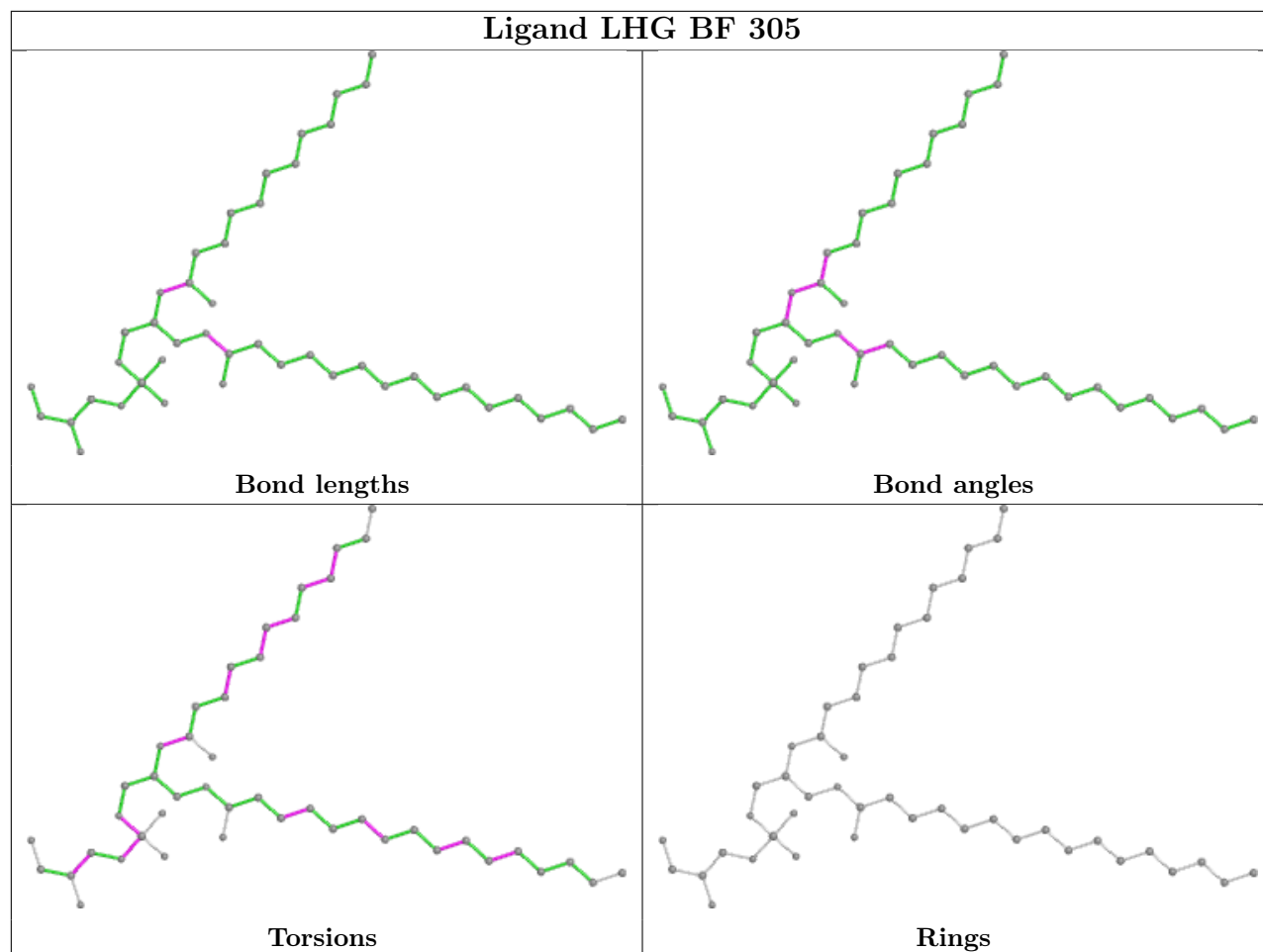


Rings

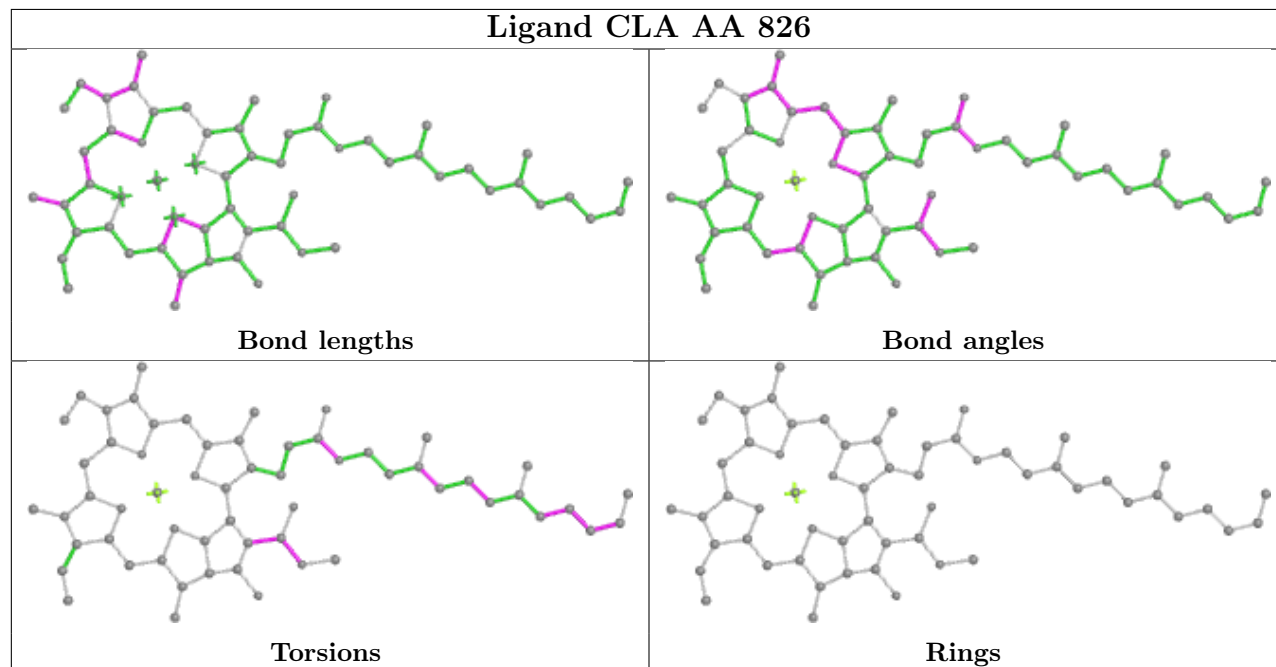


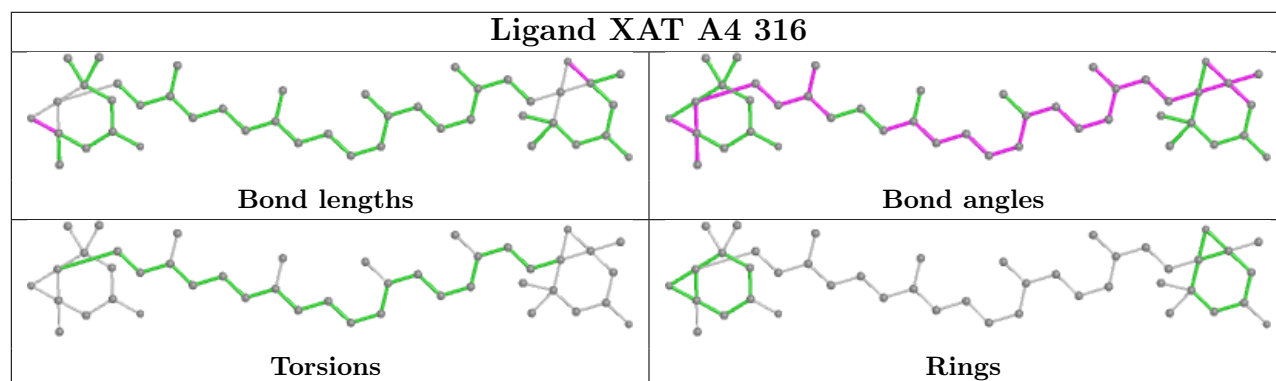
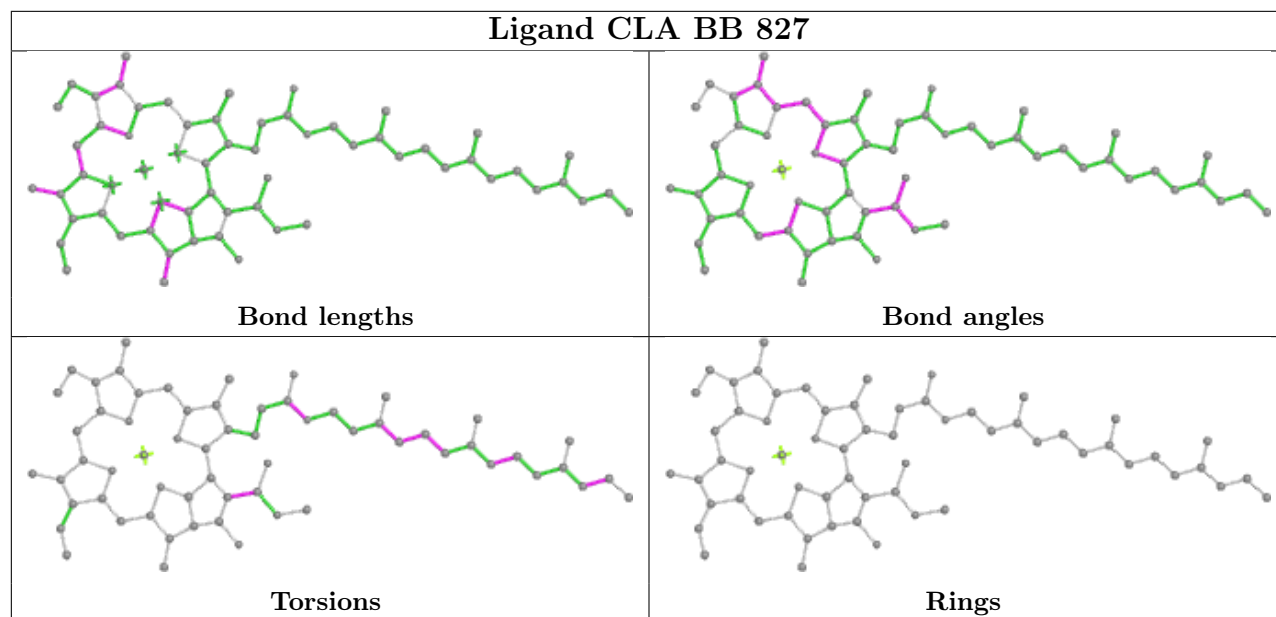
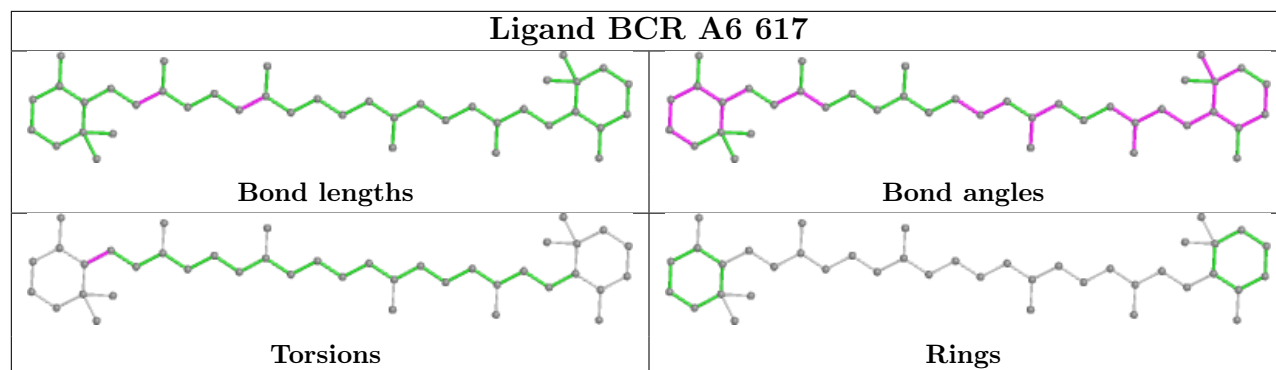


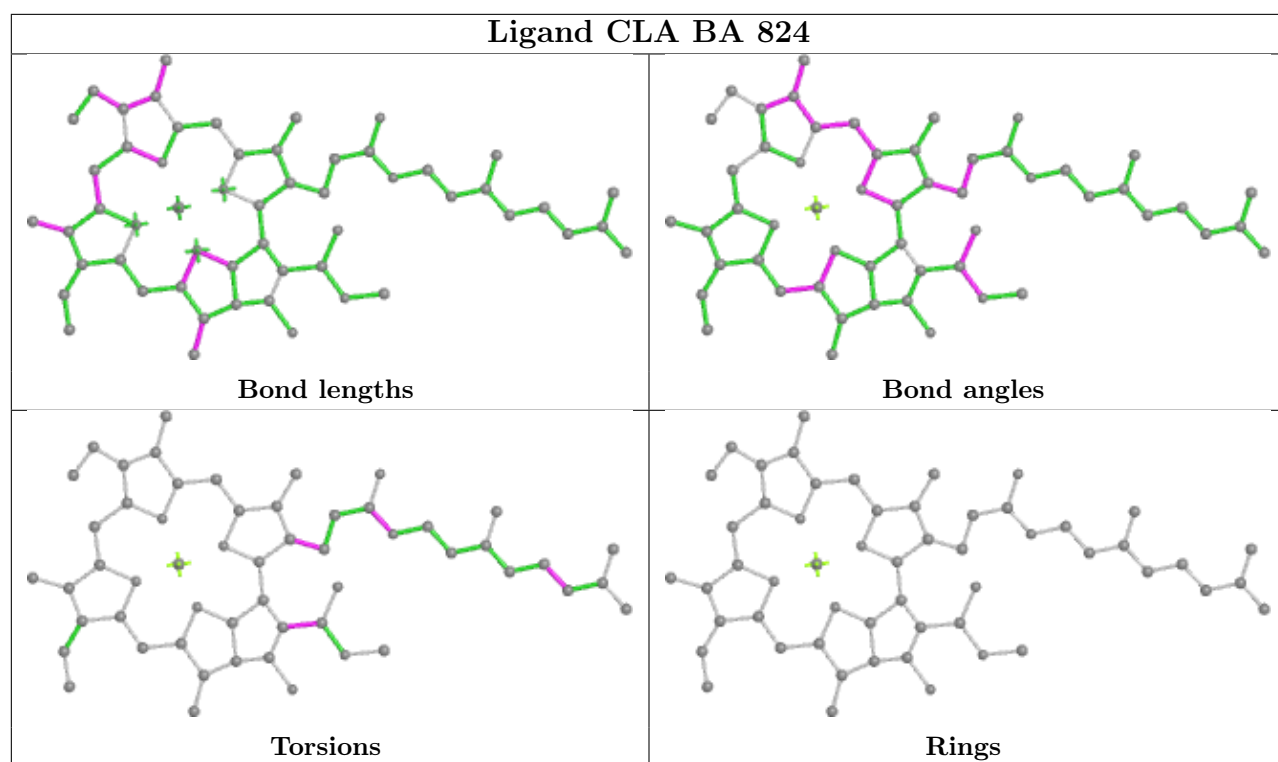
Ligand LHG BF 305

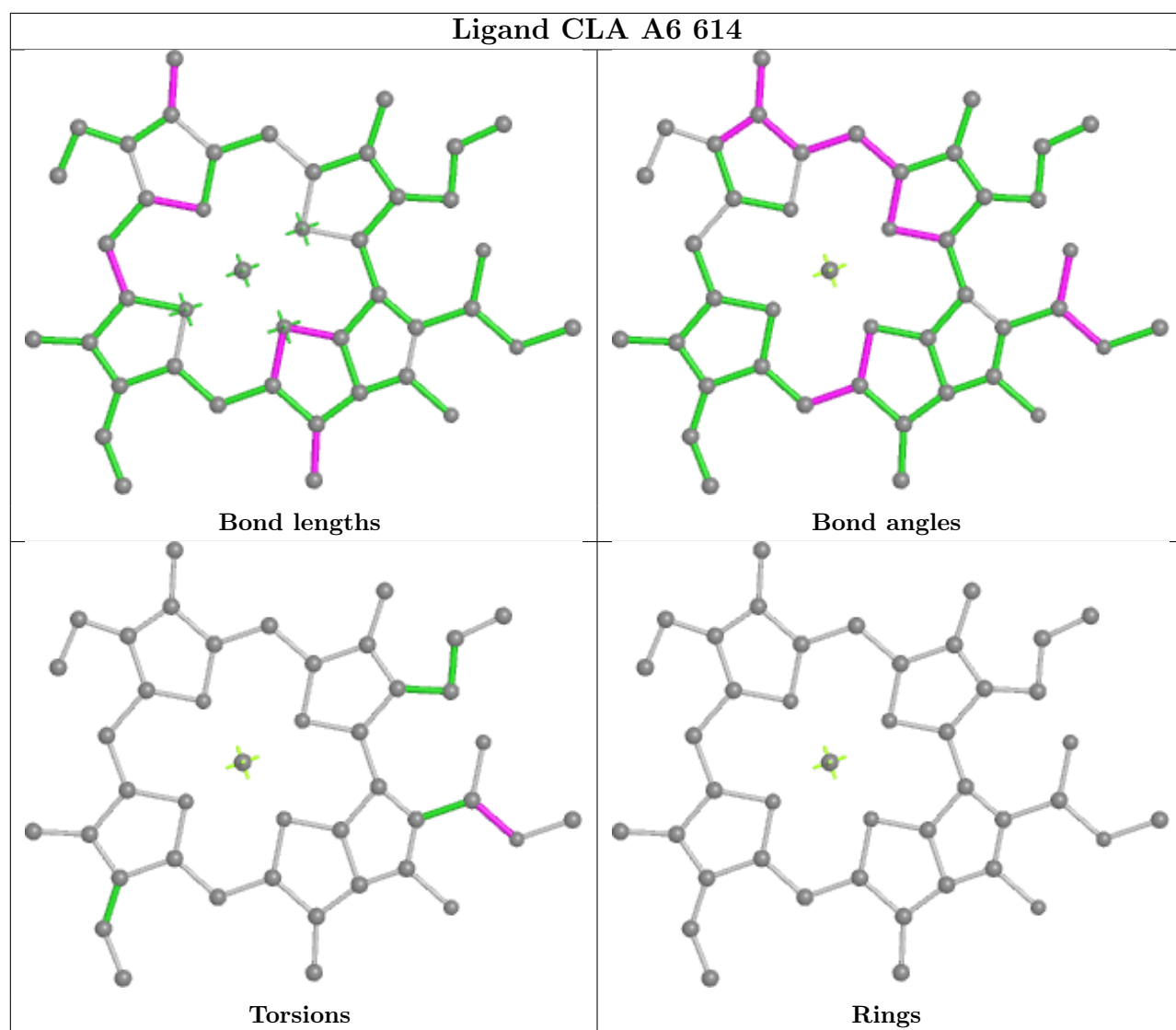


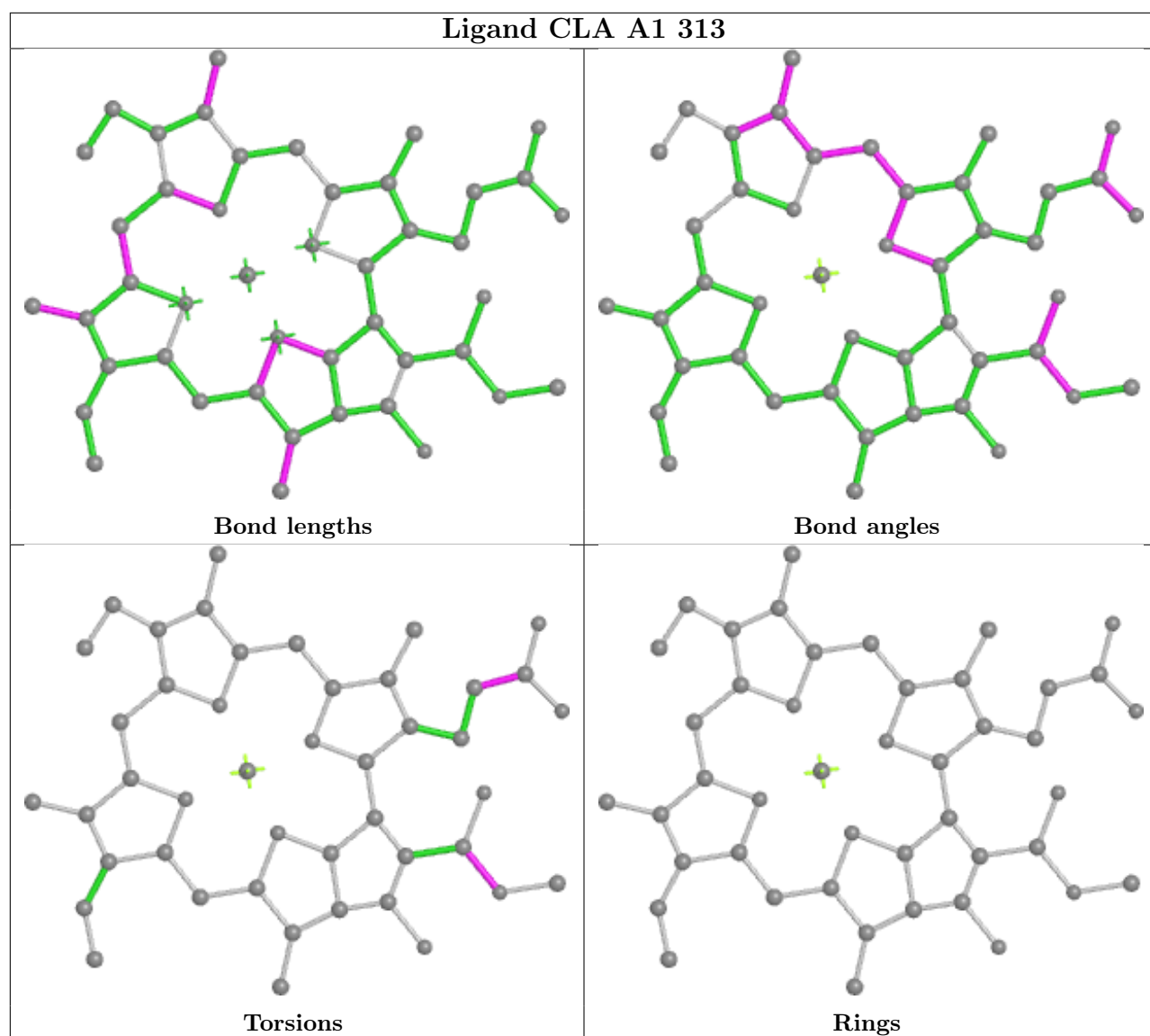
Ligand CLA AA 826



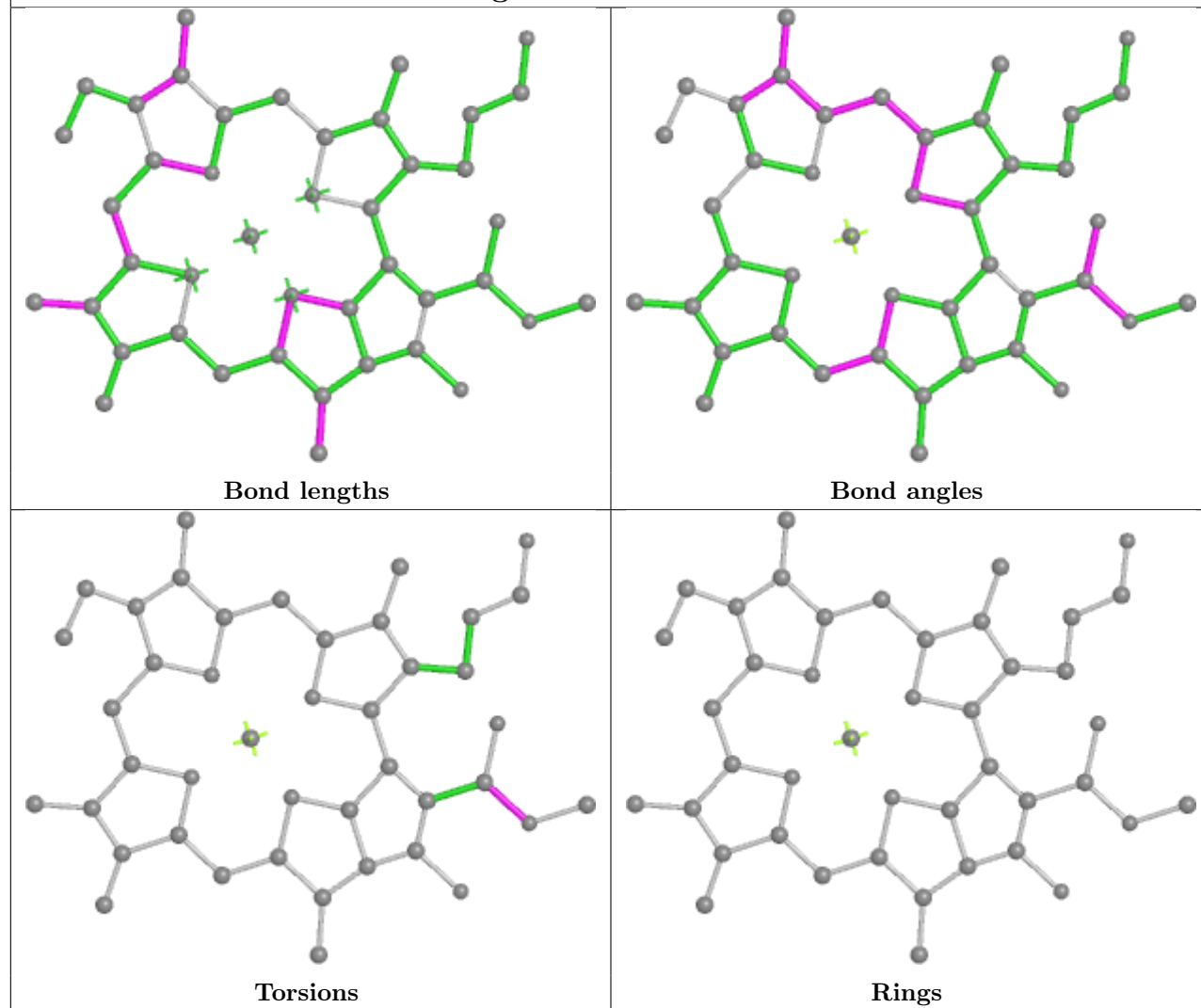




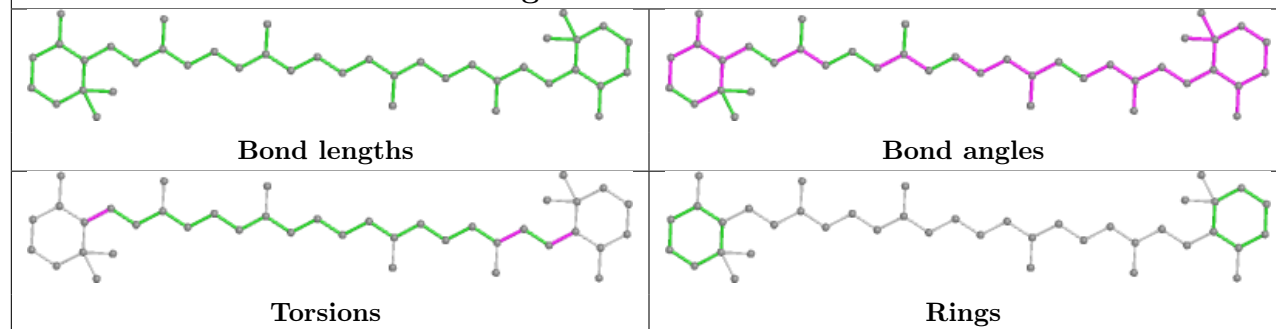


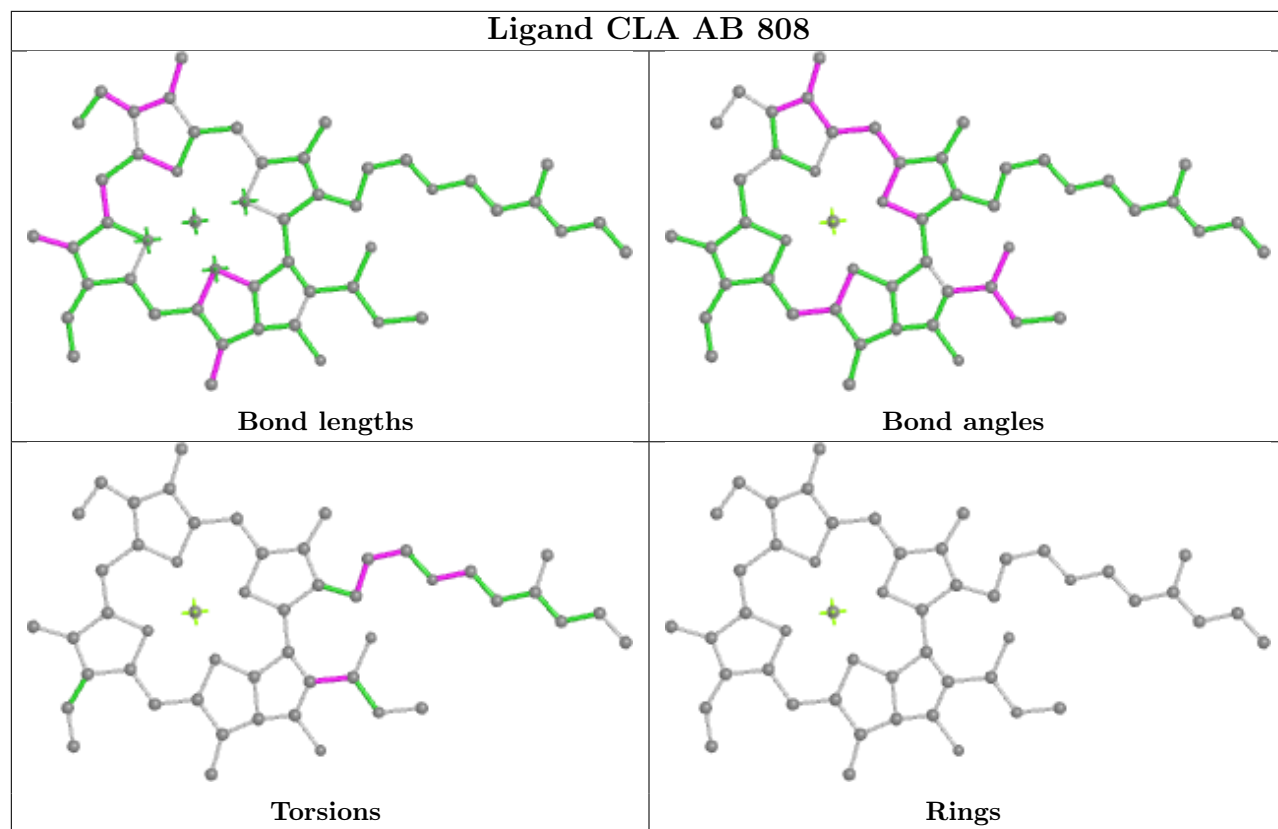


Ligand CLA A6 605

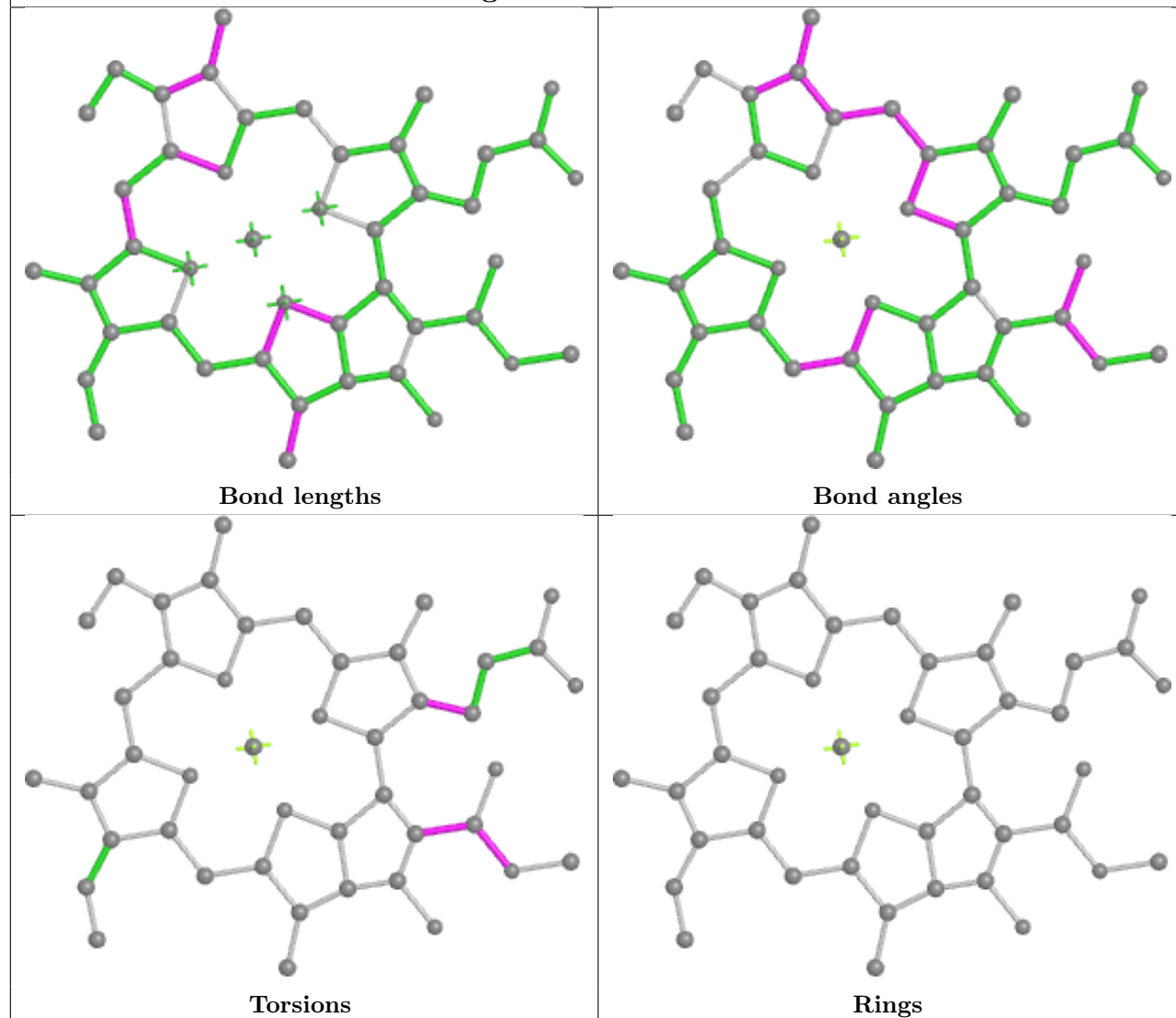


Ligand BCR B3 317

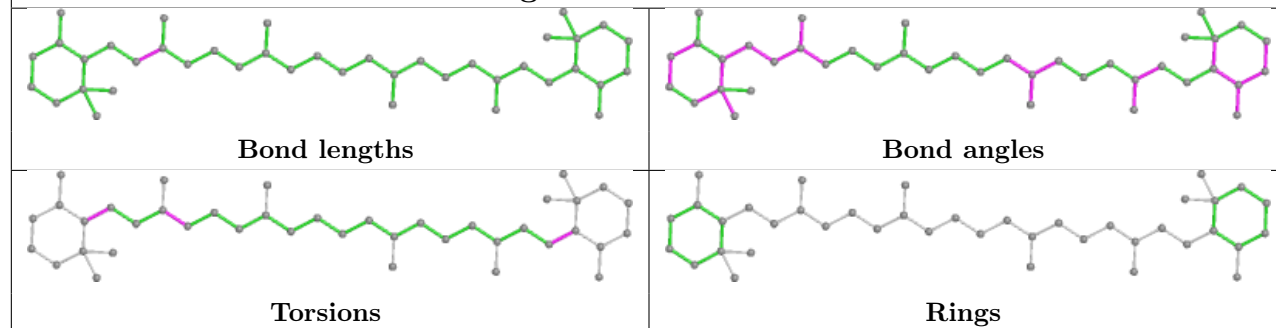


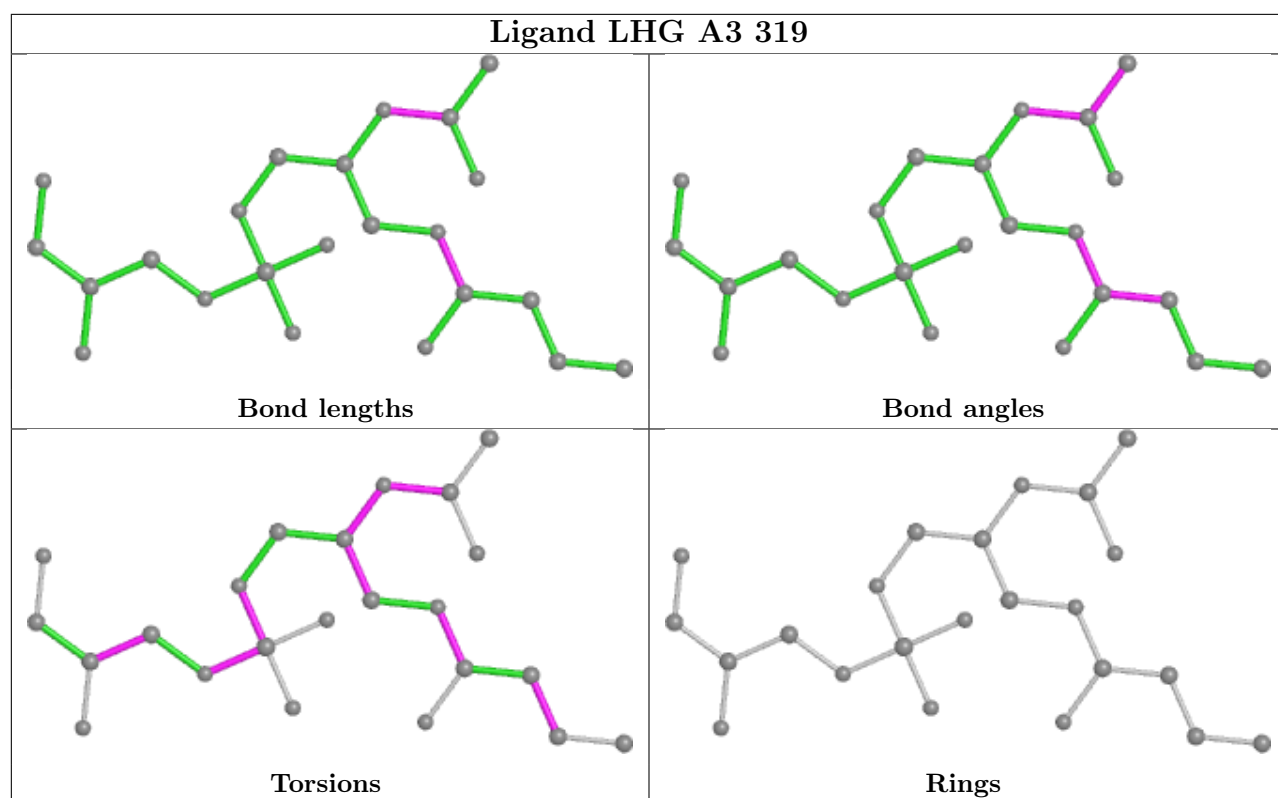


Ligand CLA A4 312

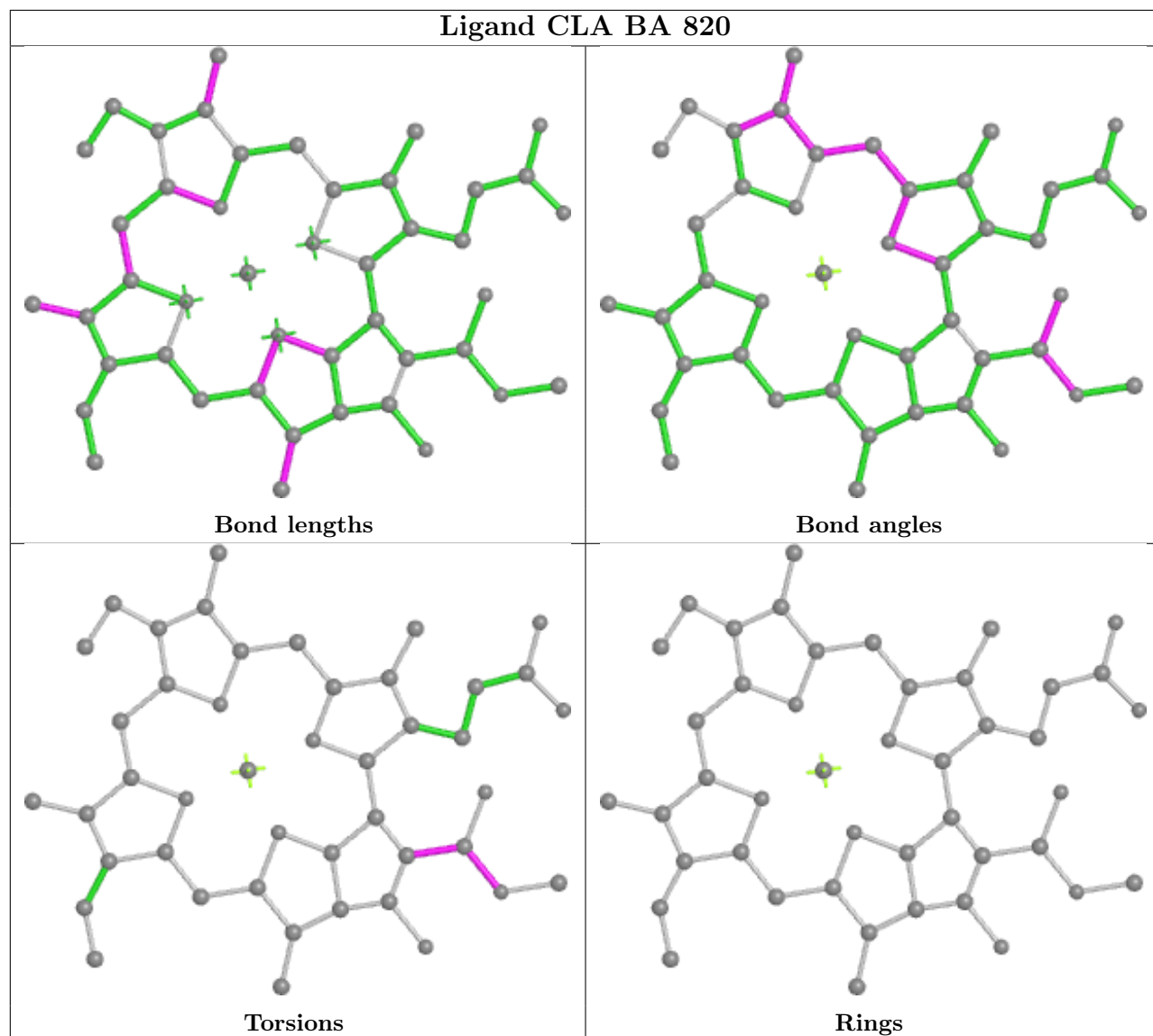


Ligand BCR BL 301

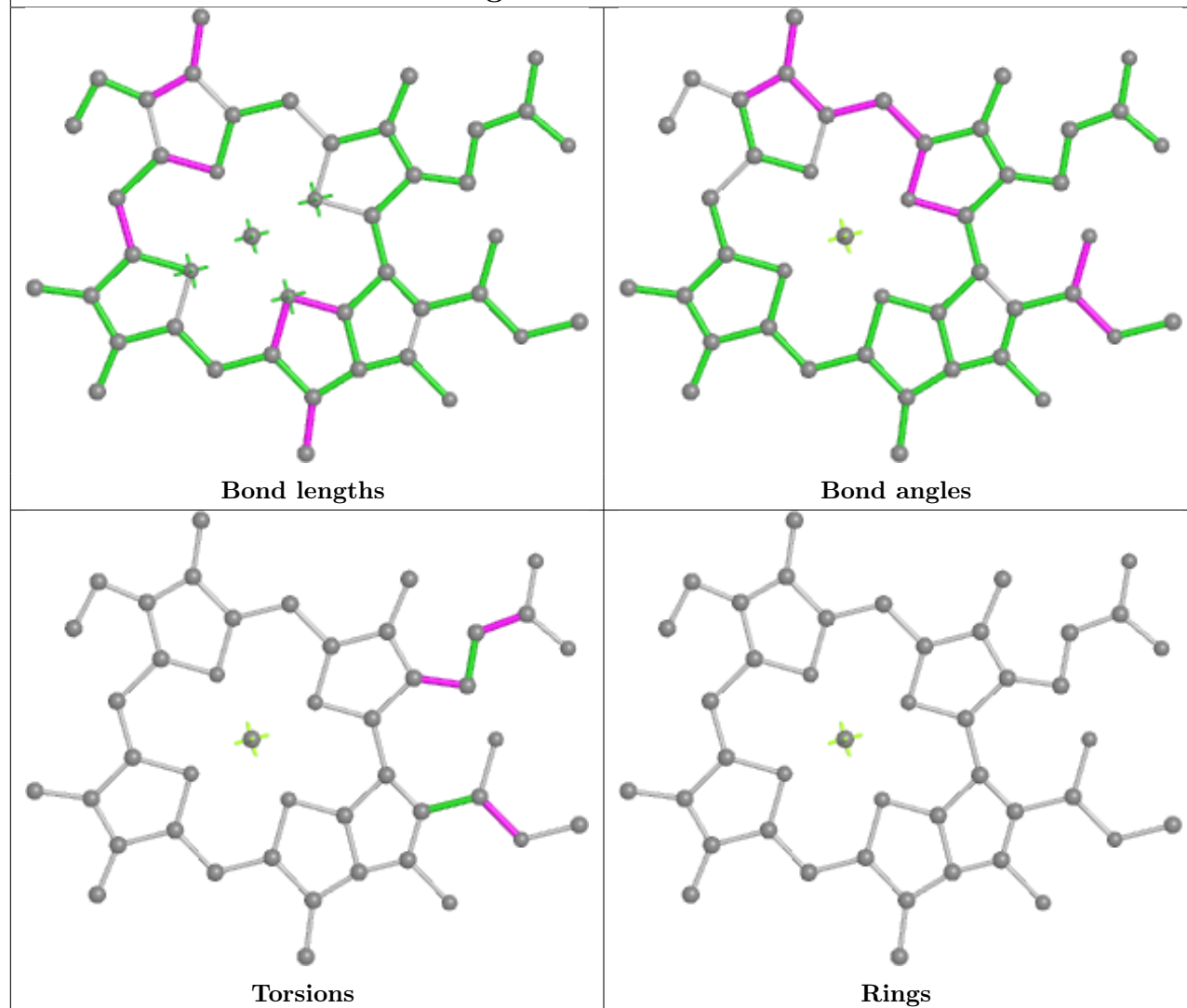




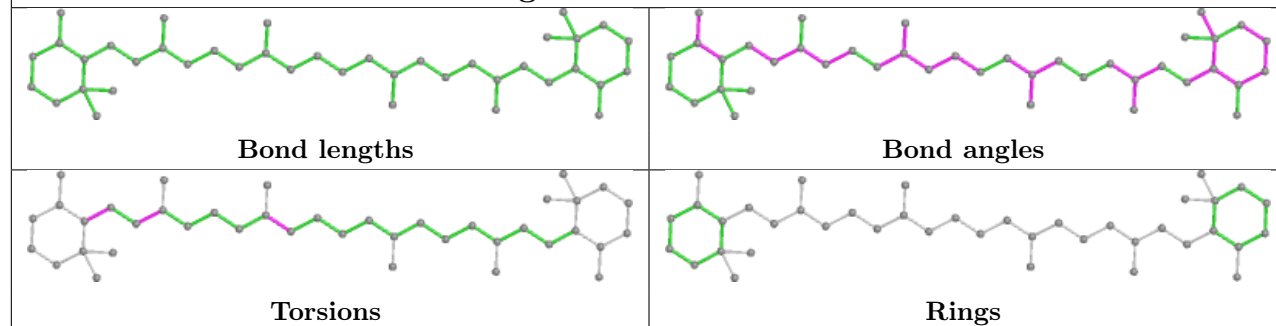
Ligand CLA BA 820

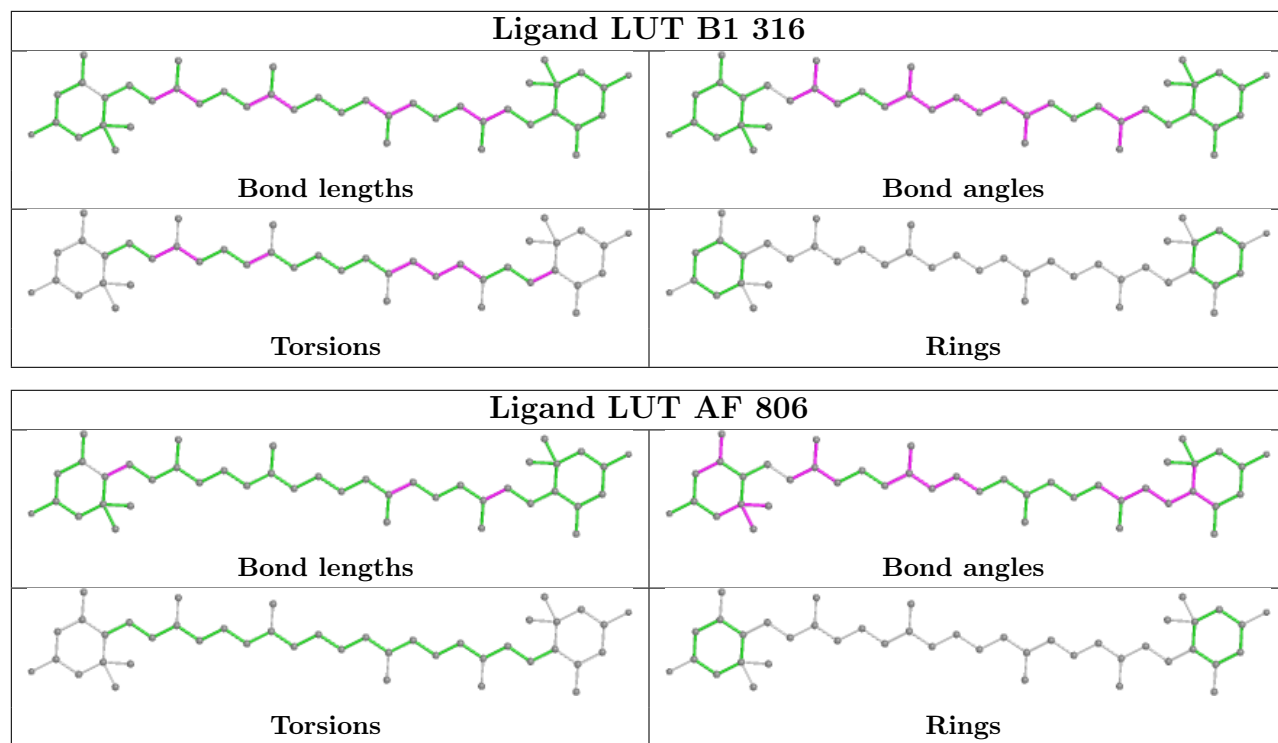


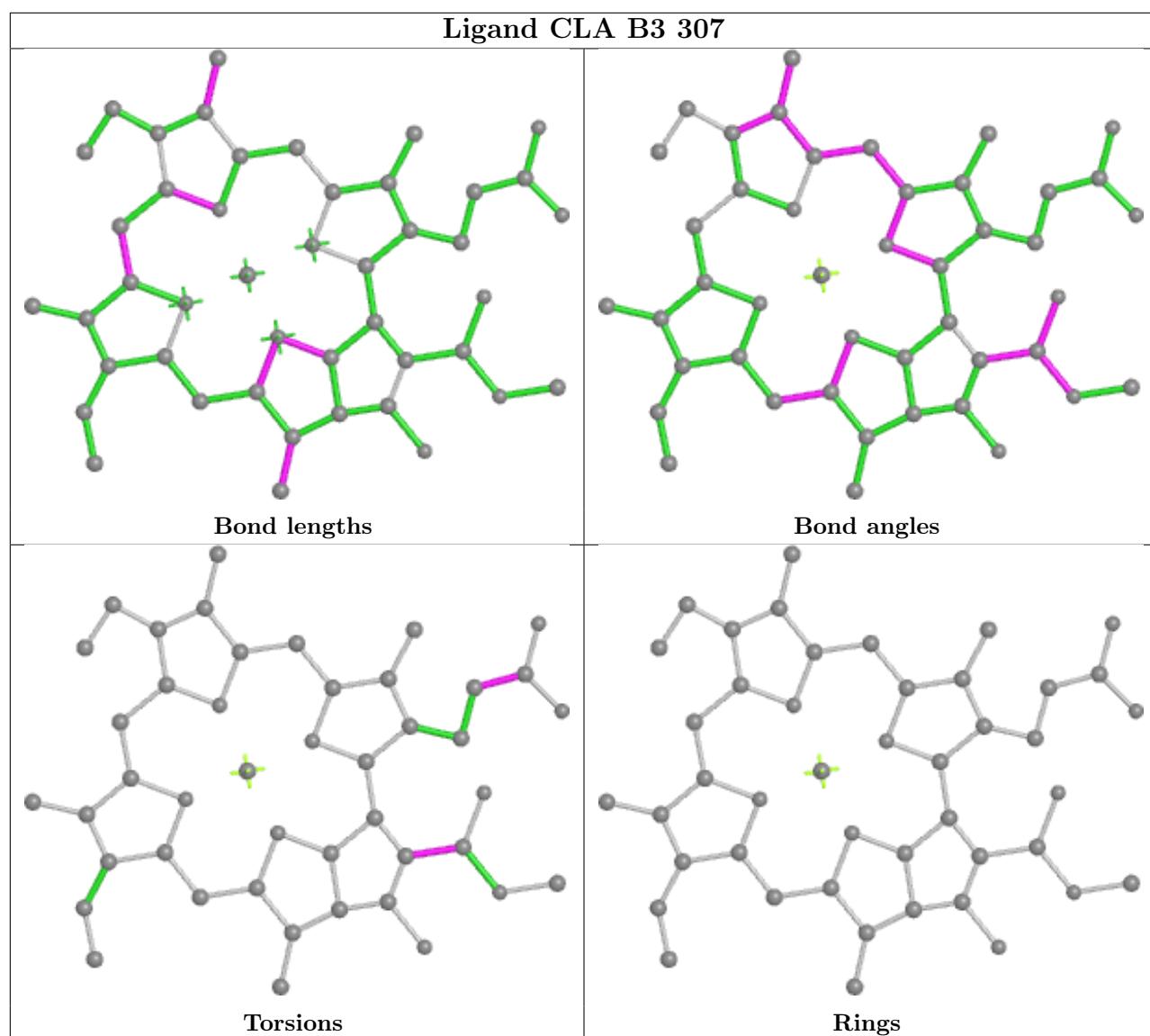
Ligand CLA A6 612



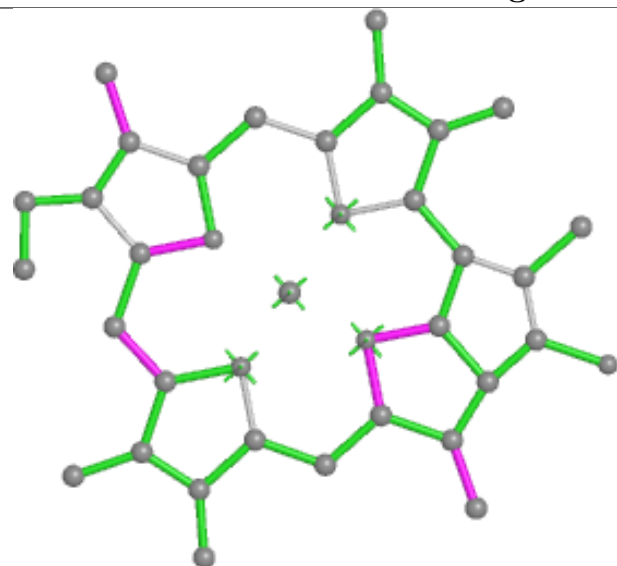
Ligand BCR AF 805



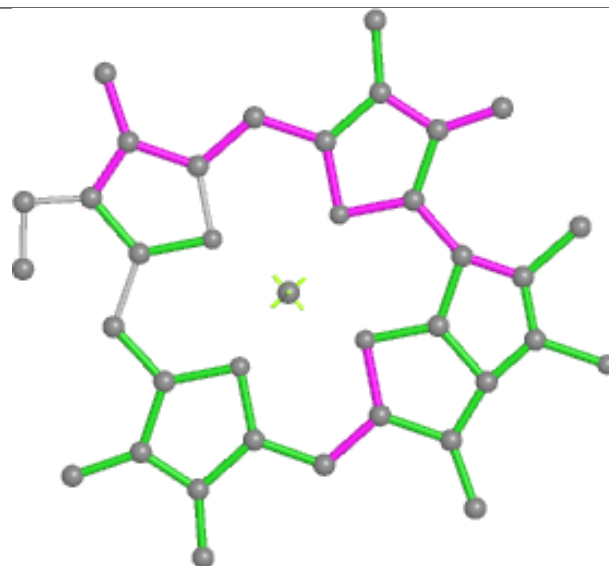




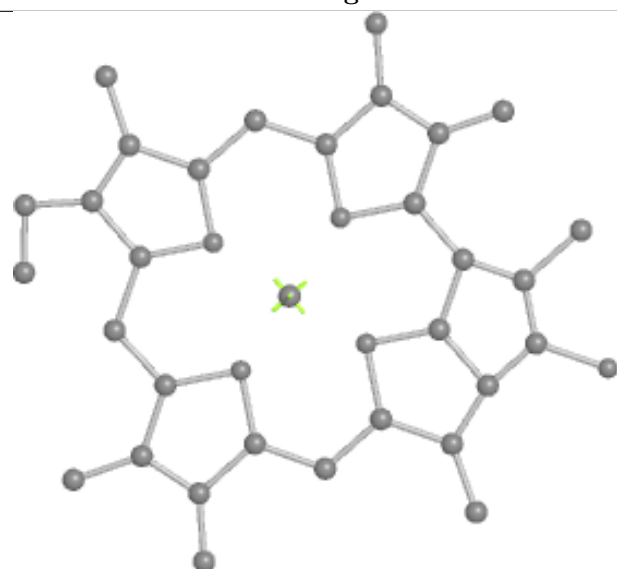
Ligand CLA A3 310



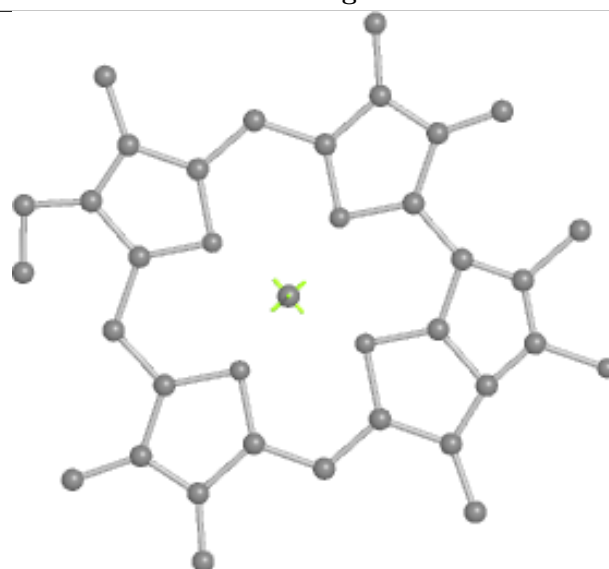
Bond lengths



Bond angles

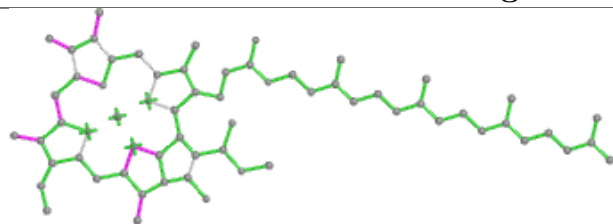


Torsions

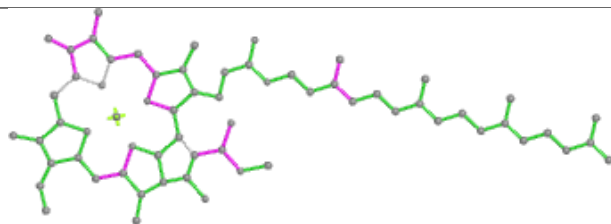


Rings

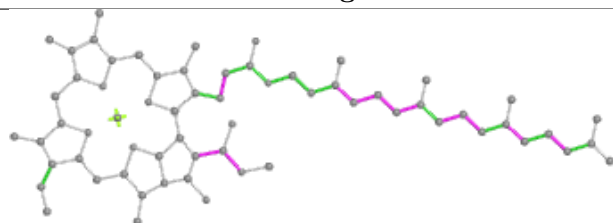
Ligand CLA AB 802



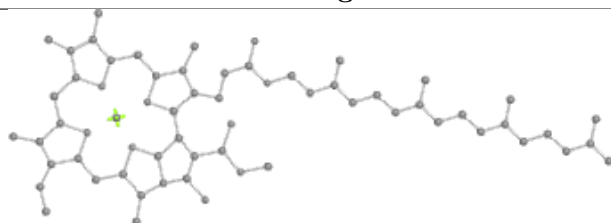
Bond lengths



Bond angles

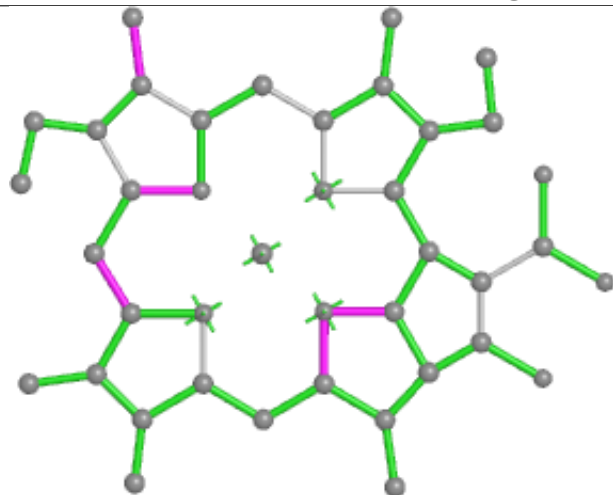


Torsions

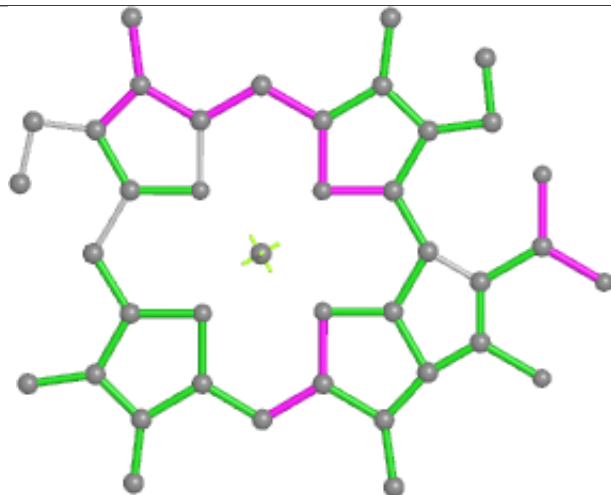


Rings

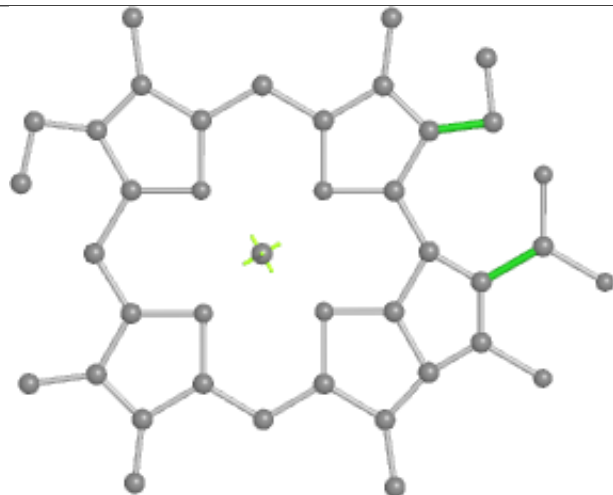
Ligand CLA B3 309



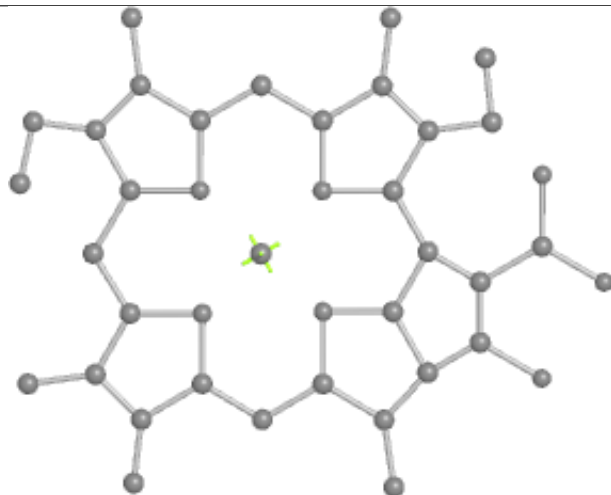
Bond lengths



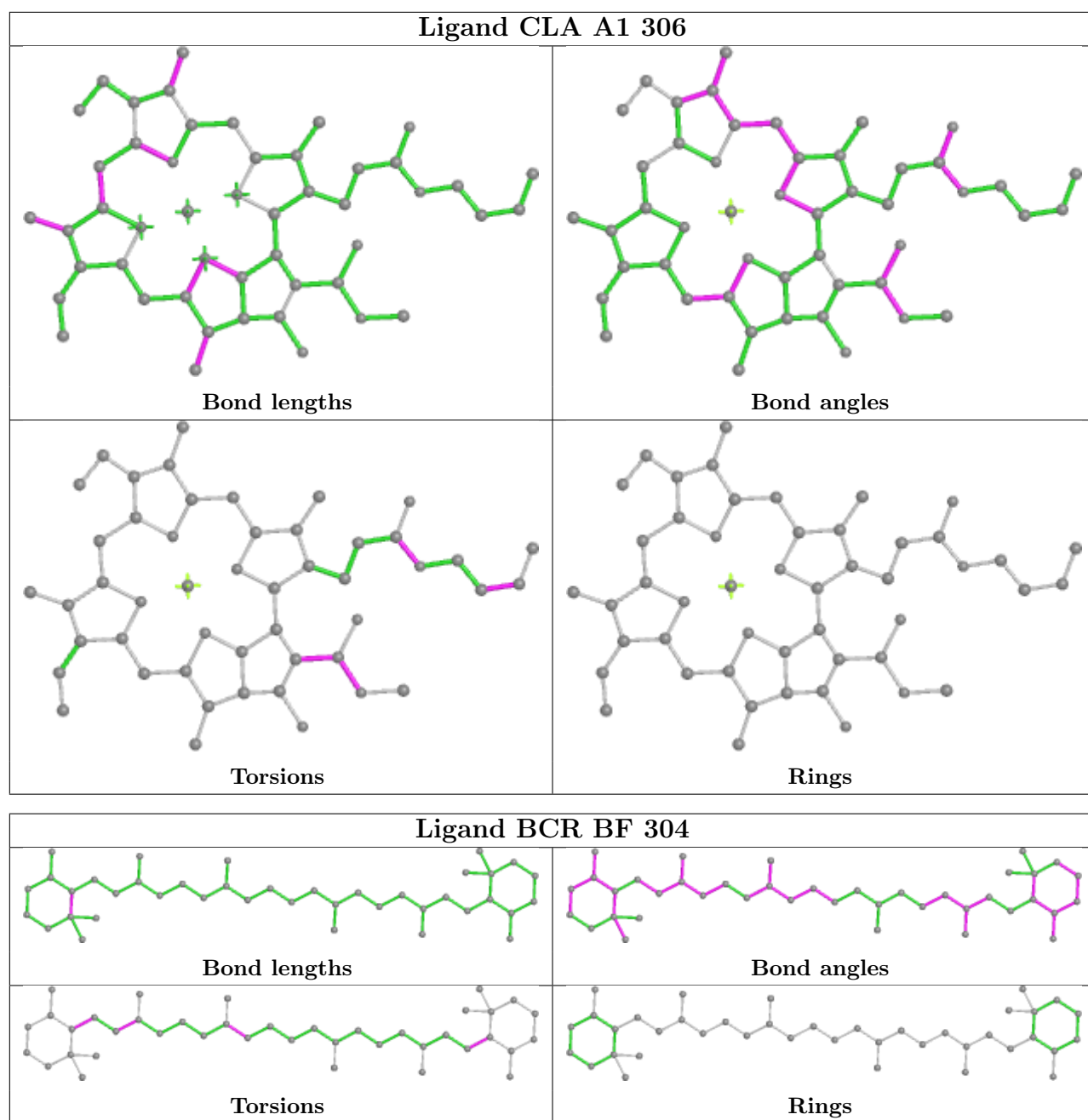
Bond angles



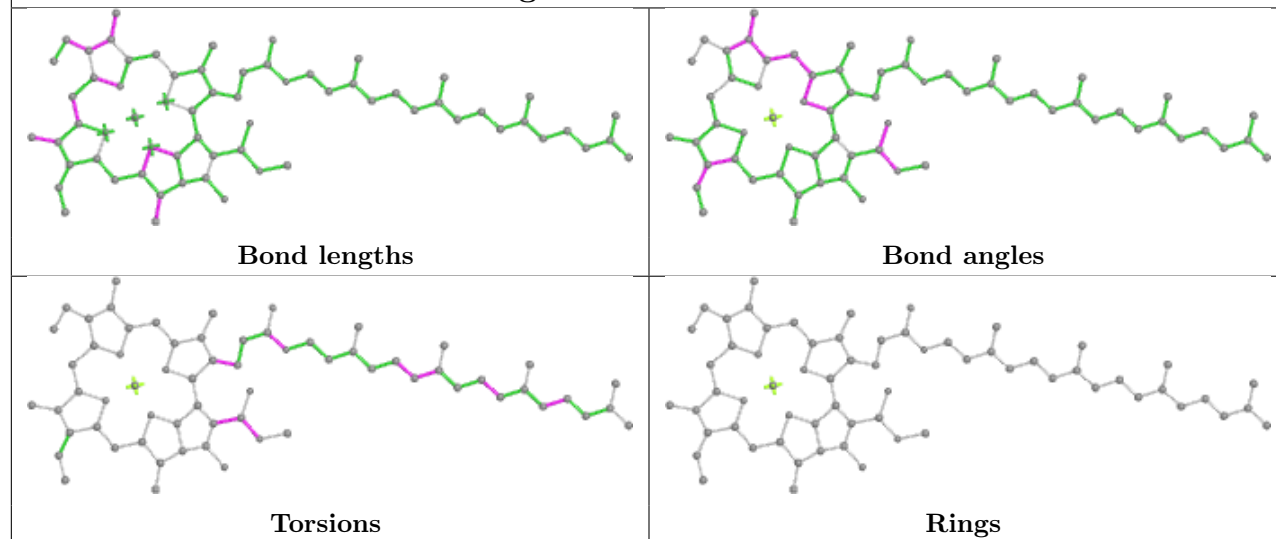
Torsions



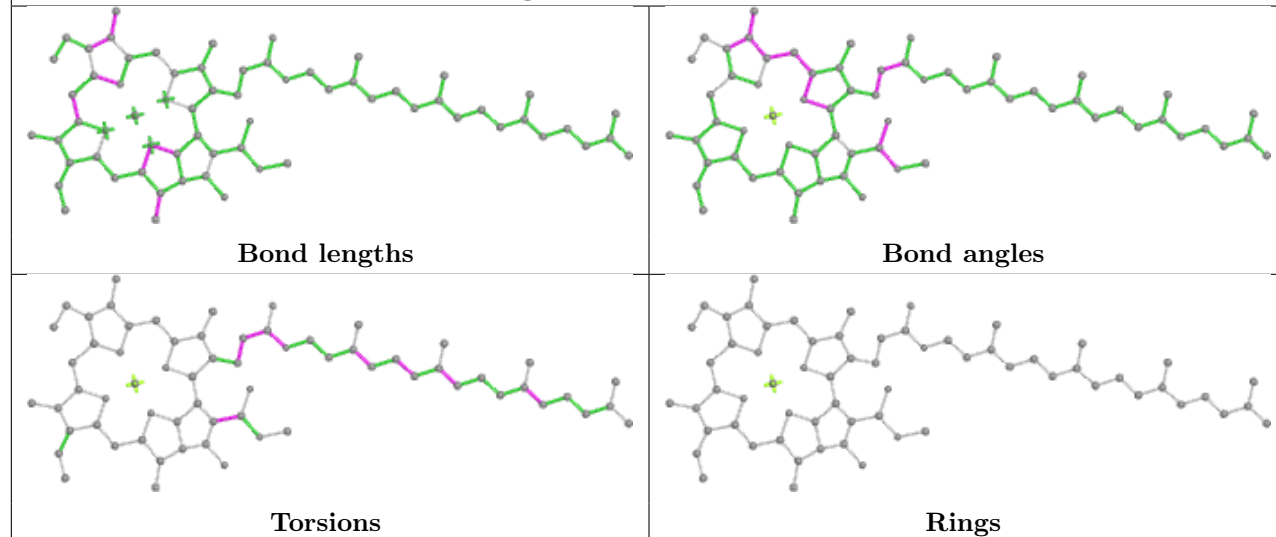
Rings



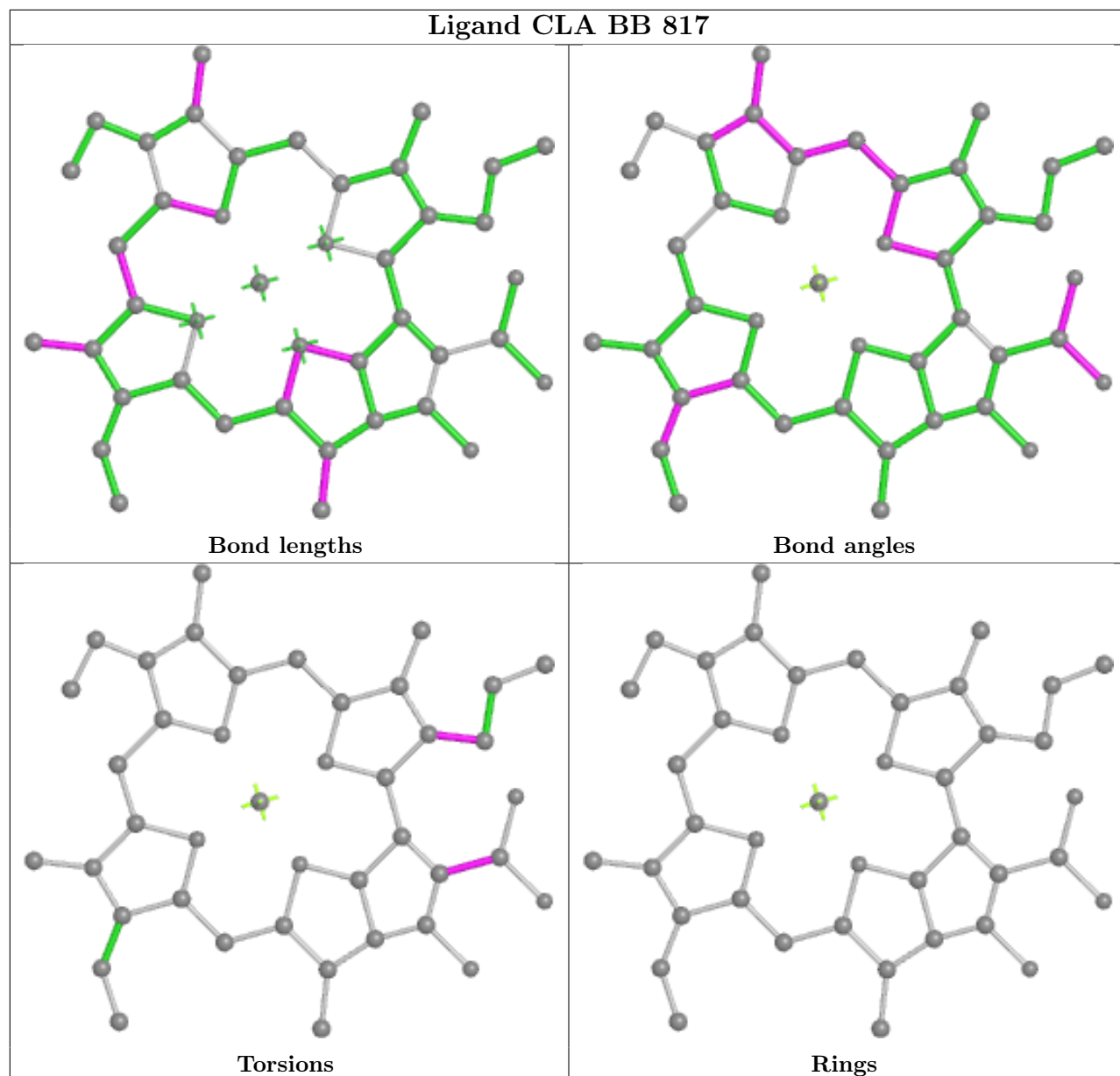
Ligand CLA BA 810



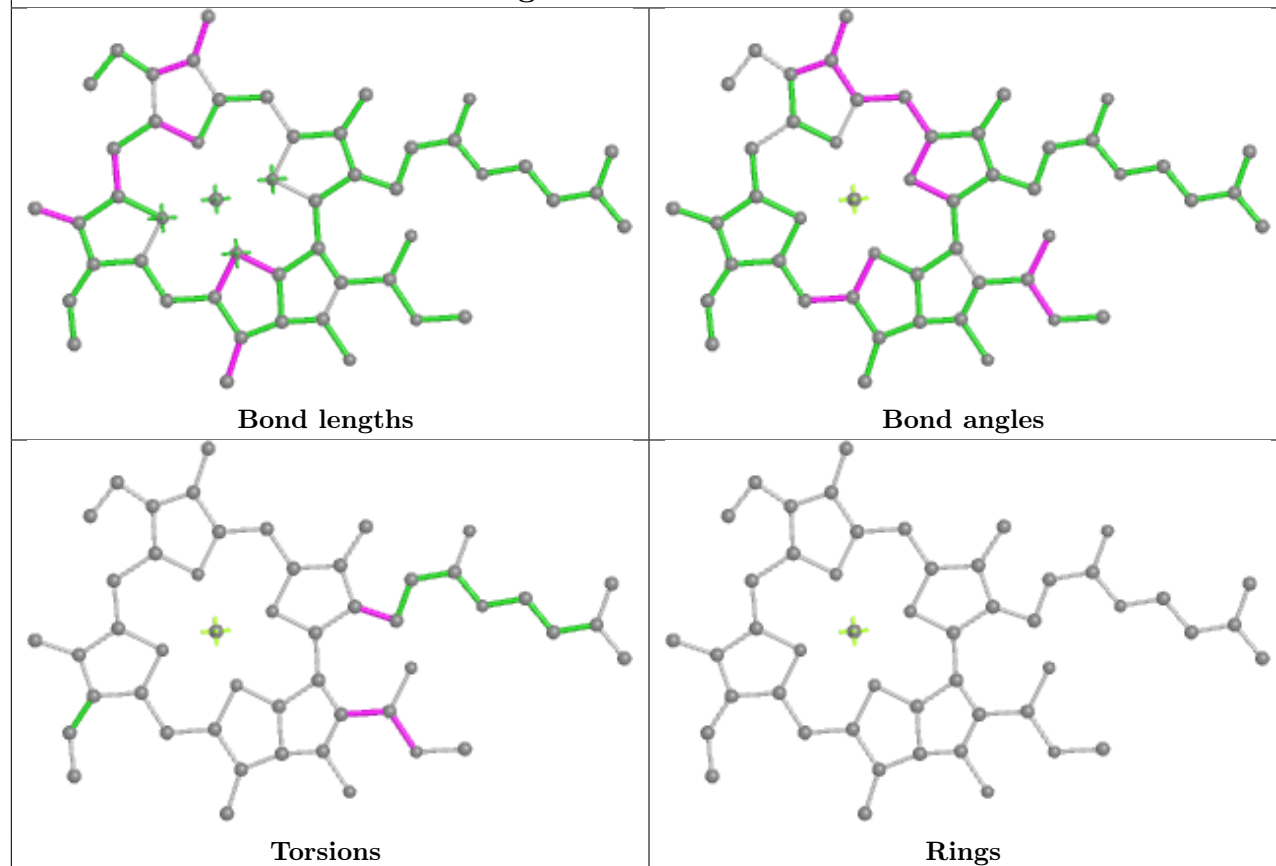
Ligand CLA BA 842



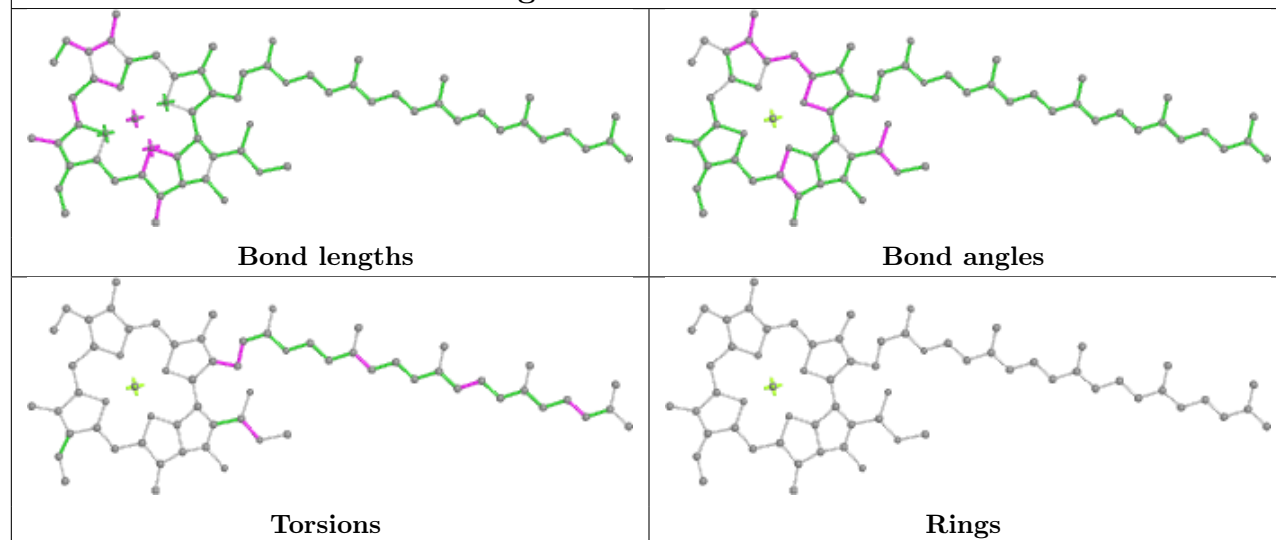
Ligand CLA BB 817



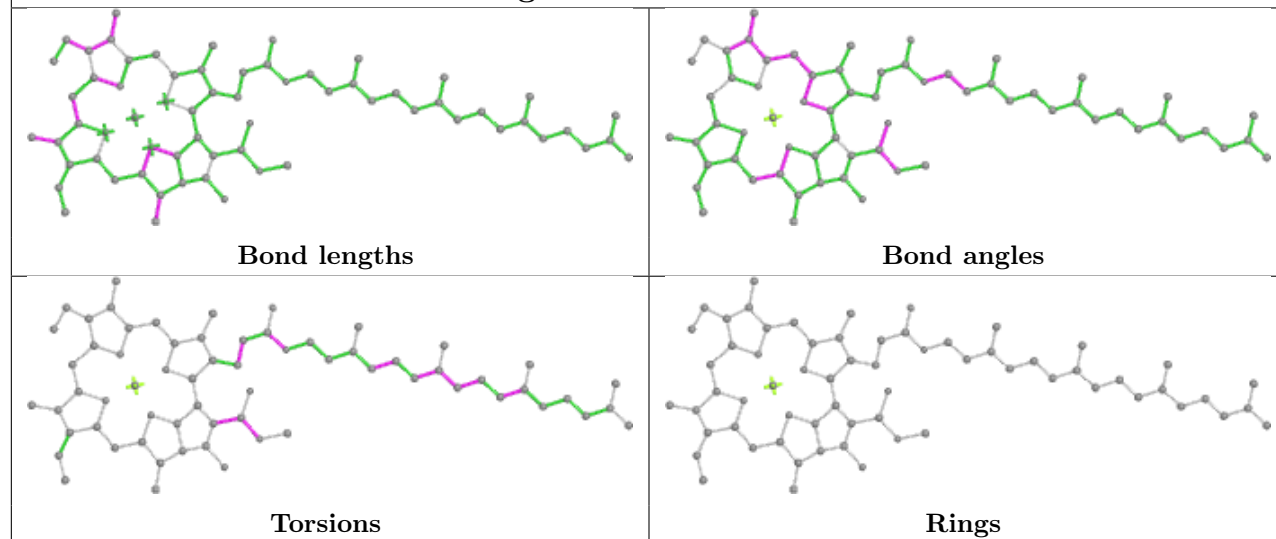
Ligand CLA AA 807



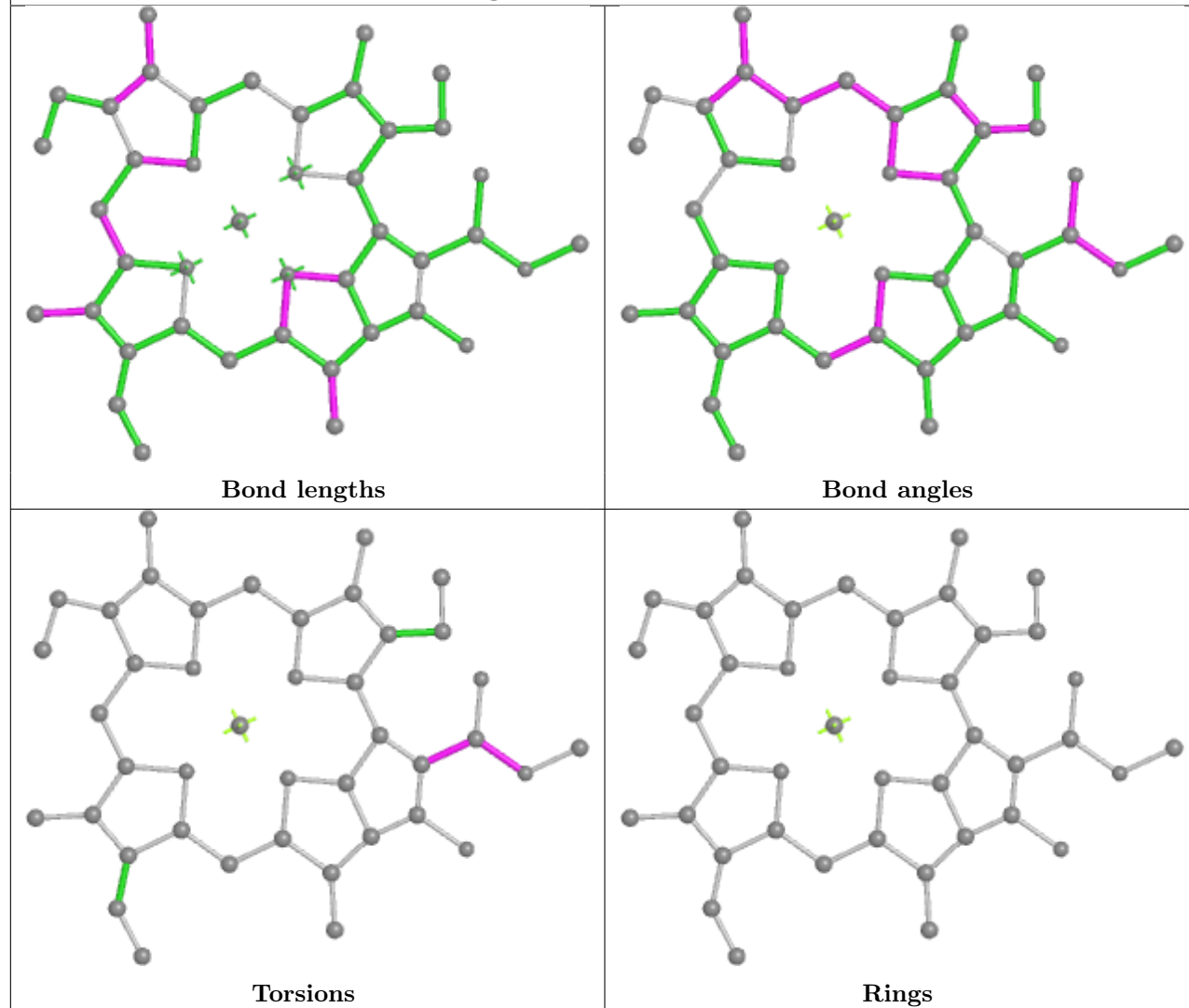
Ligand CLA AA 802



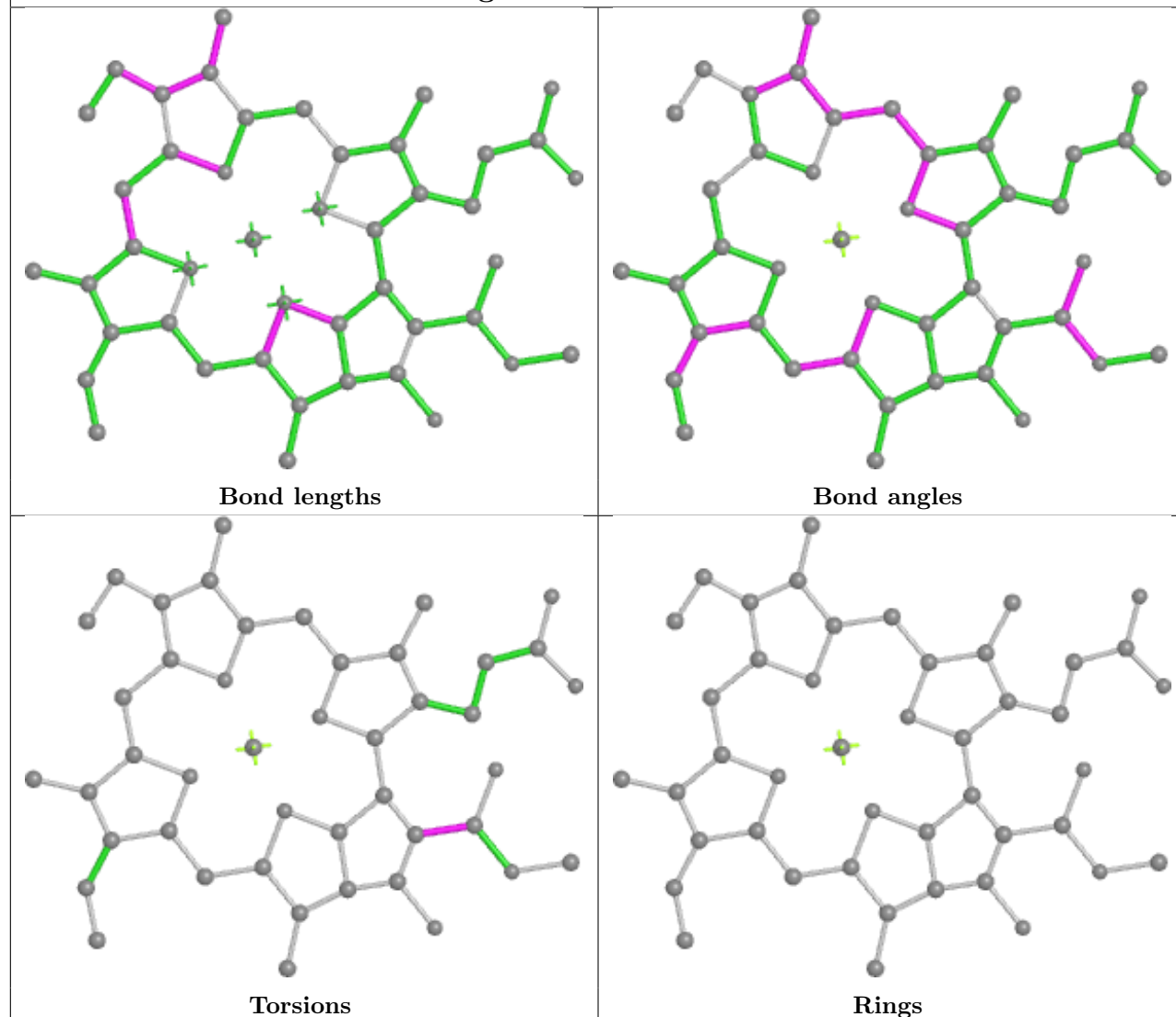
Ligand CLA AA 813



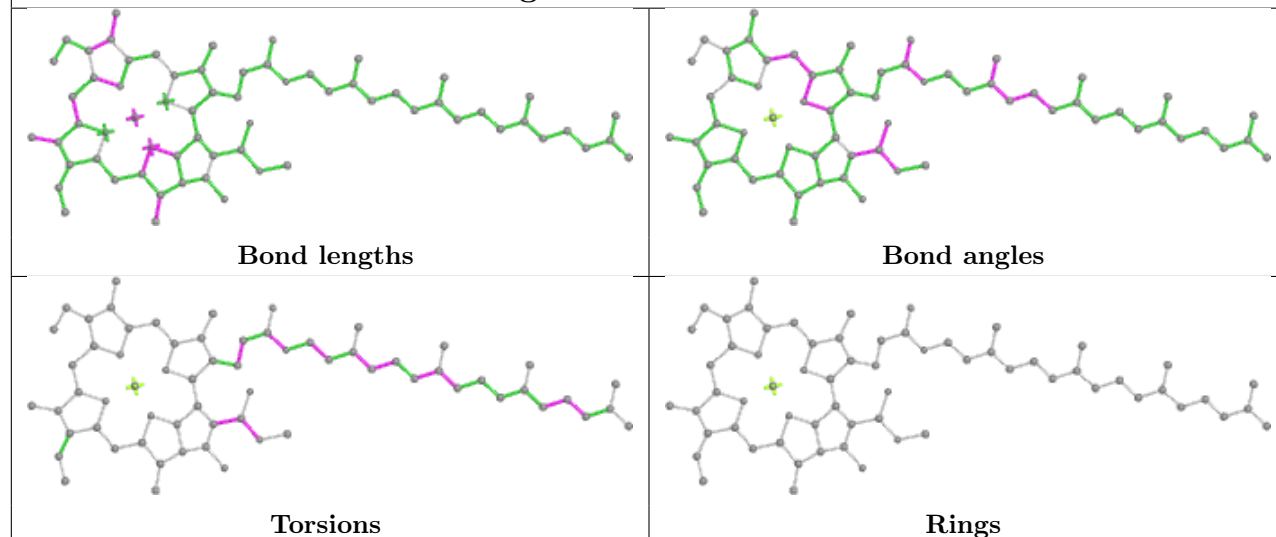
Ligand CLA BF 302



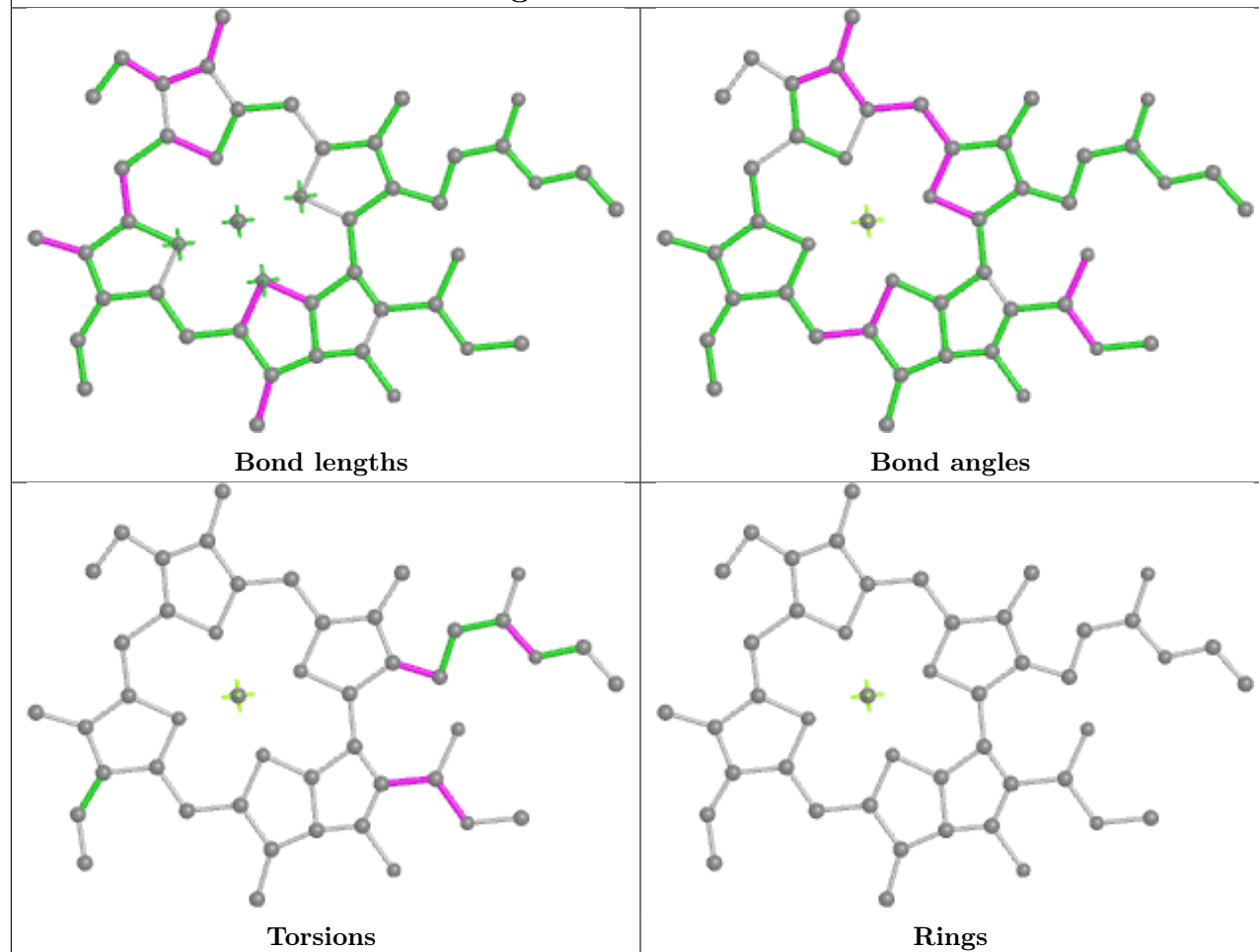
Ligand CLA BA 816



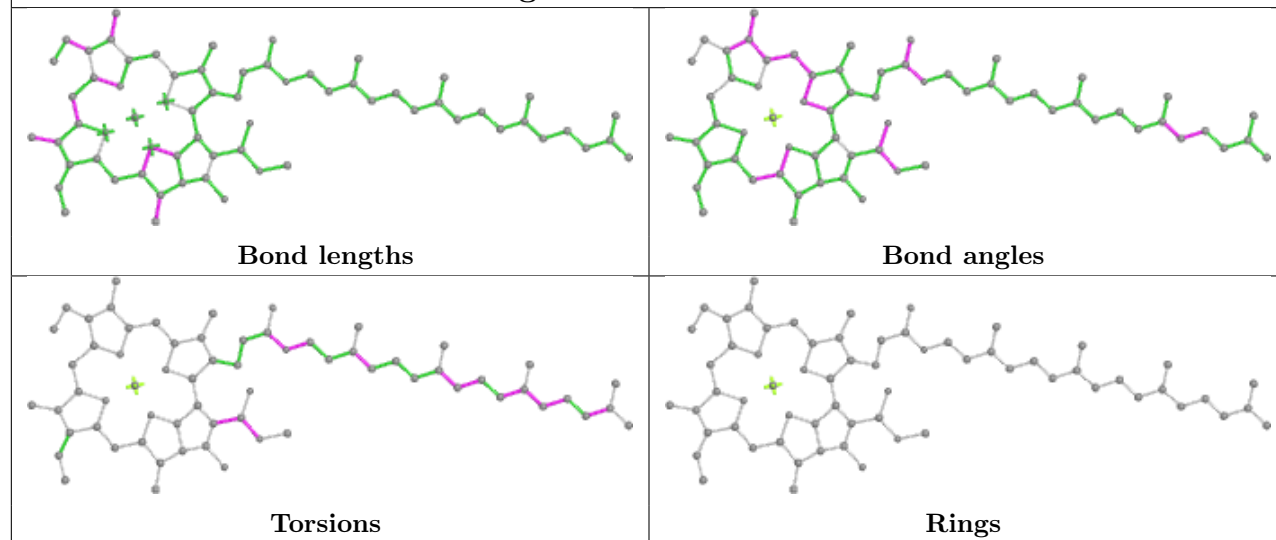
Ligand CLA BB 802



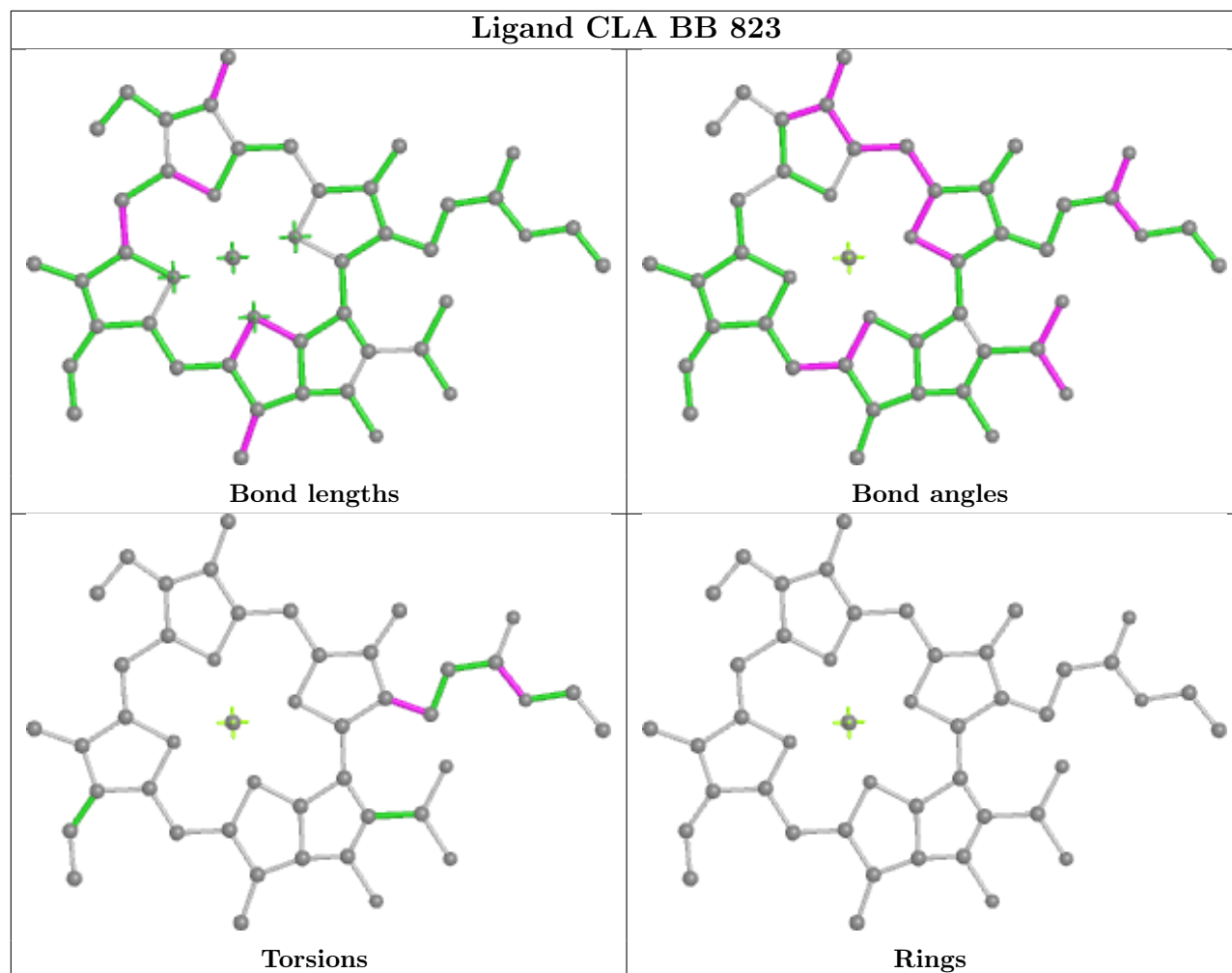
Ligand CLA AA 831



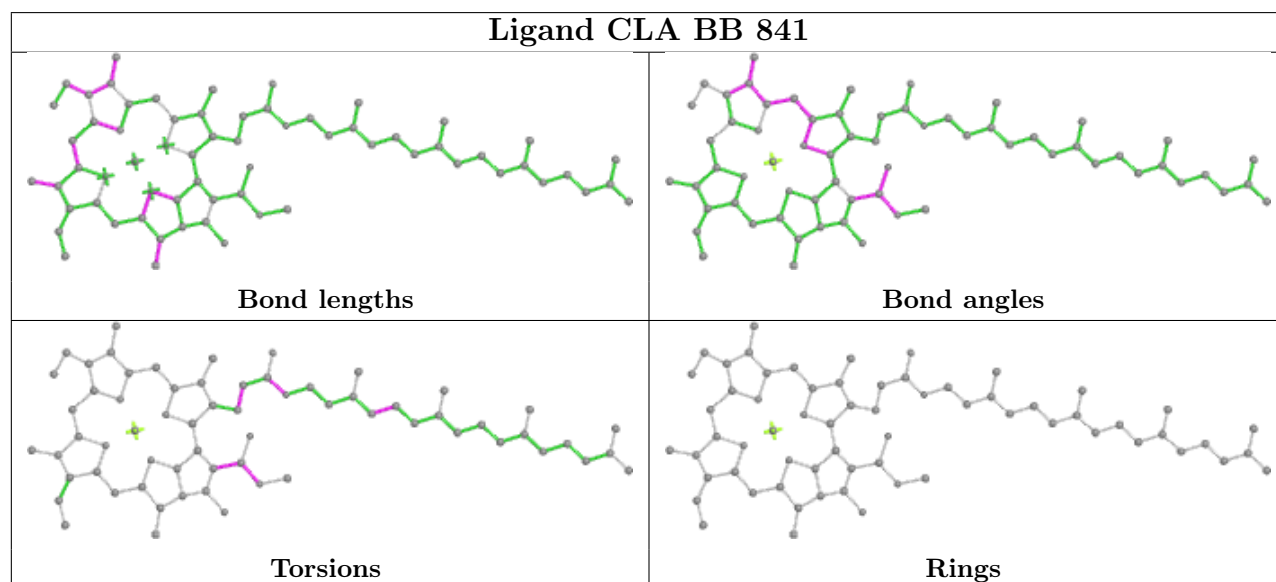
Ligand CLA AB 815



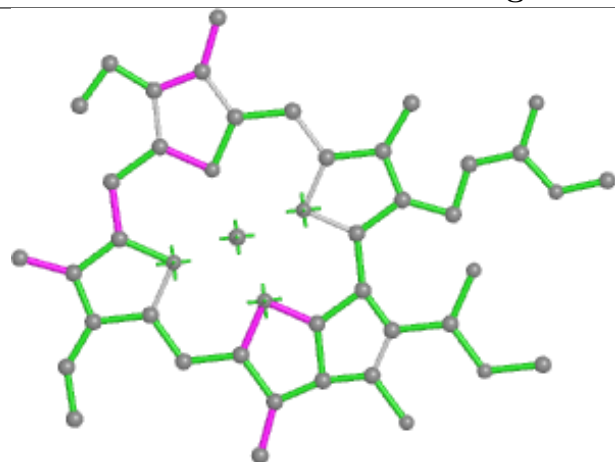
Ligand CLA BB 823



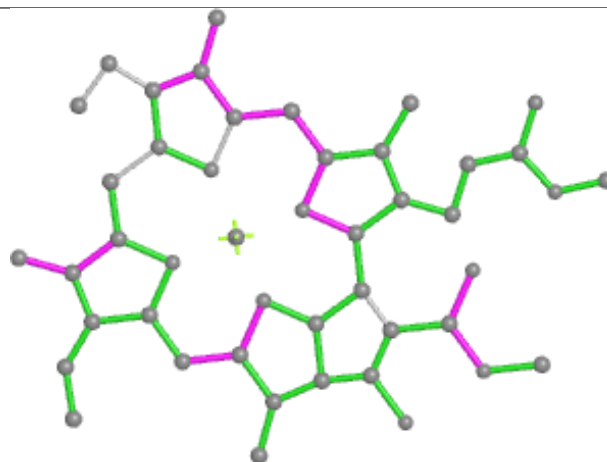
Ligand CLA BB 841



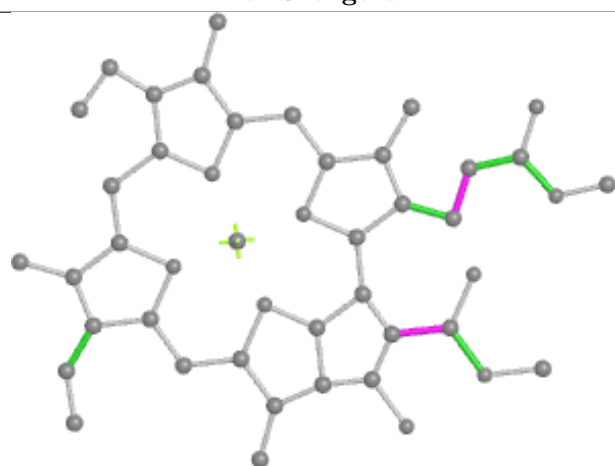
Ligand CLA A6 601



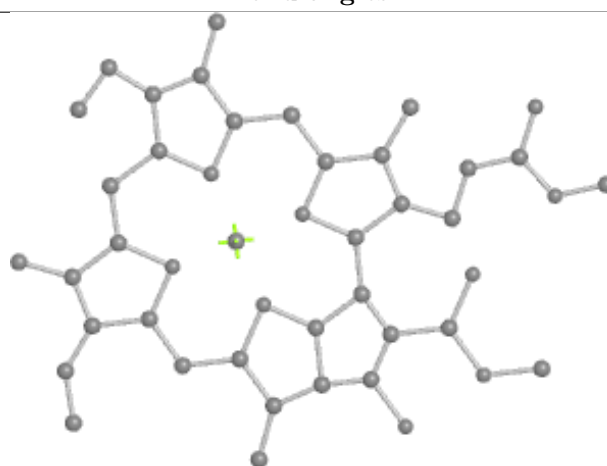
Bond lengths



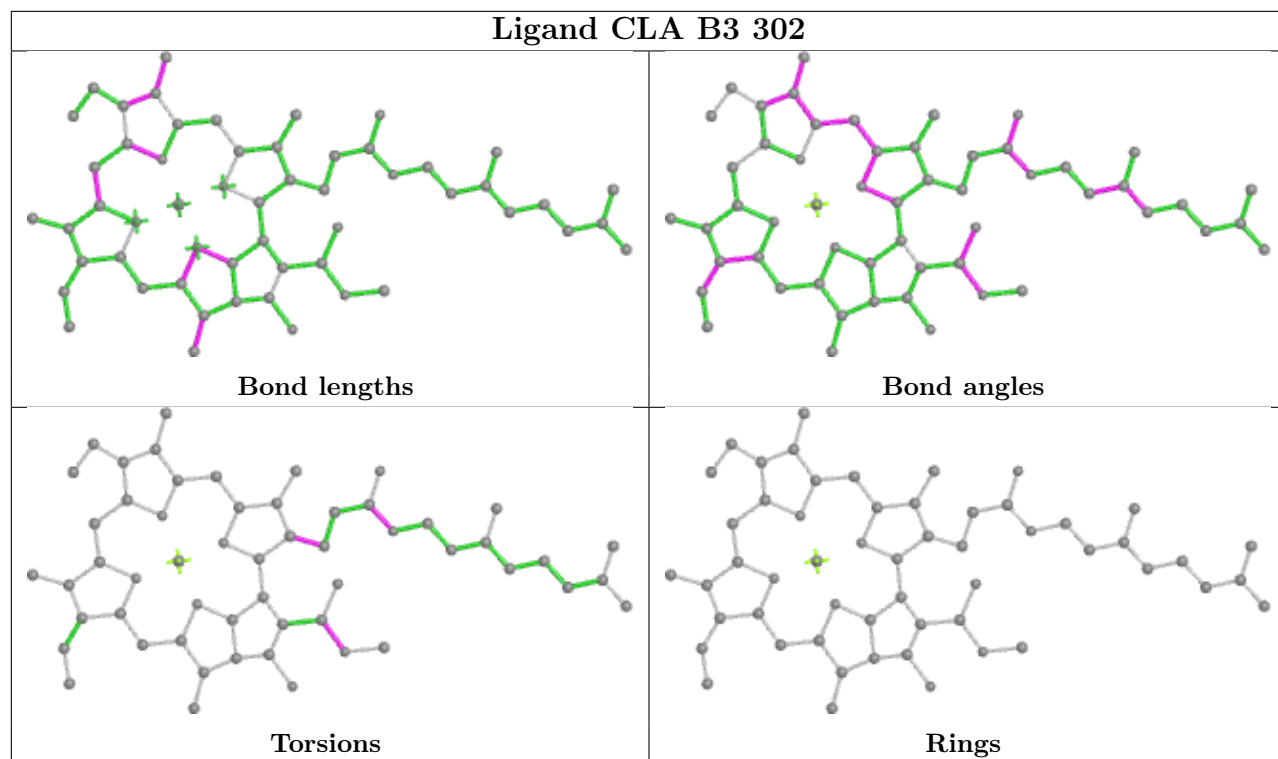
Bond angles



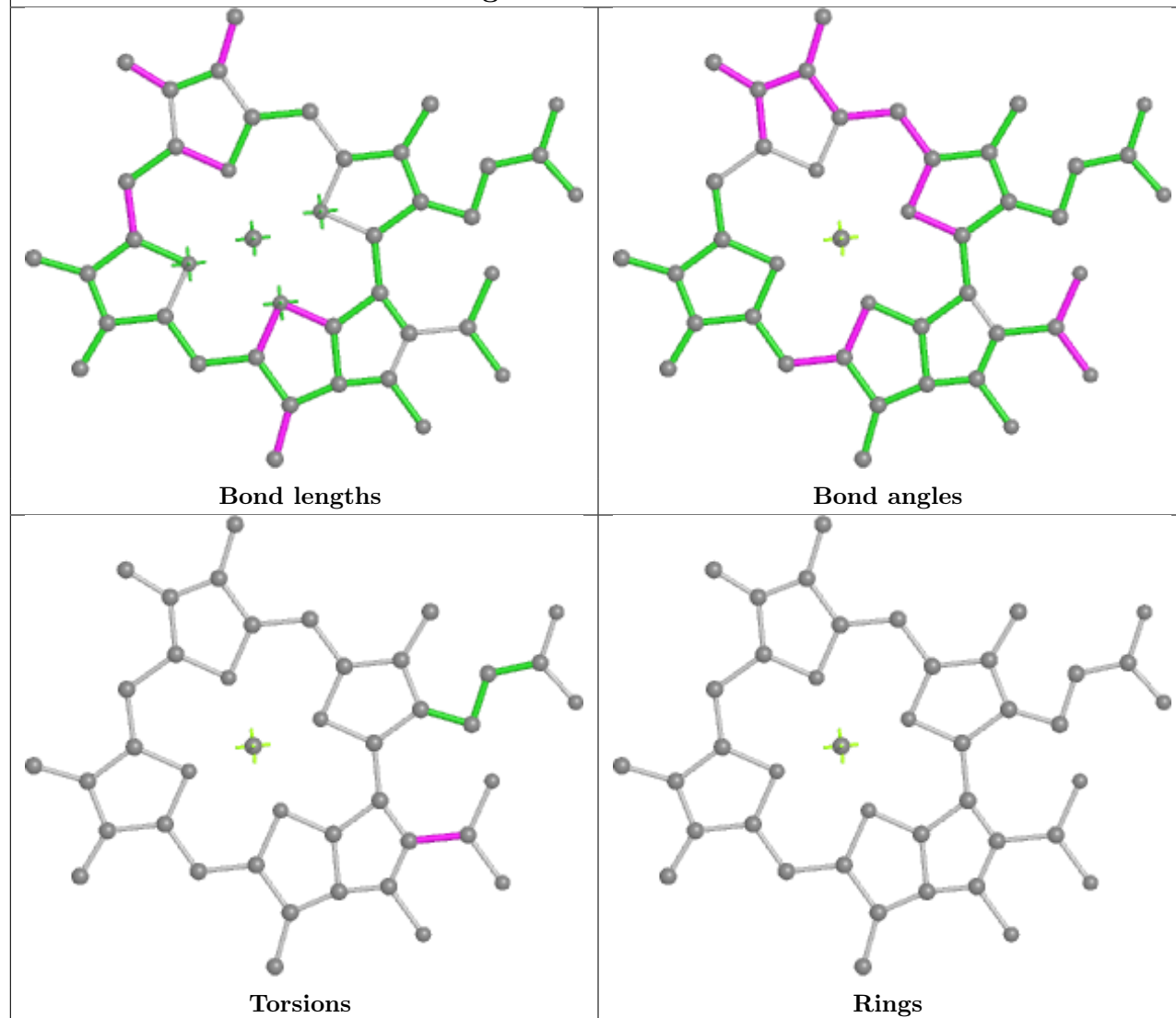
Torsions



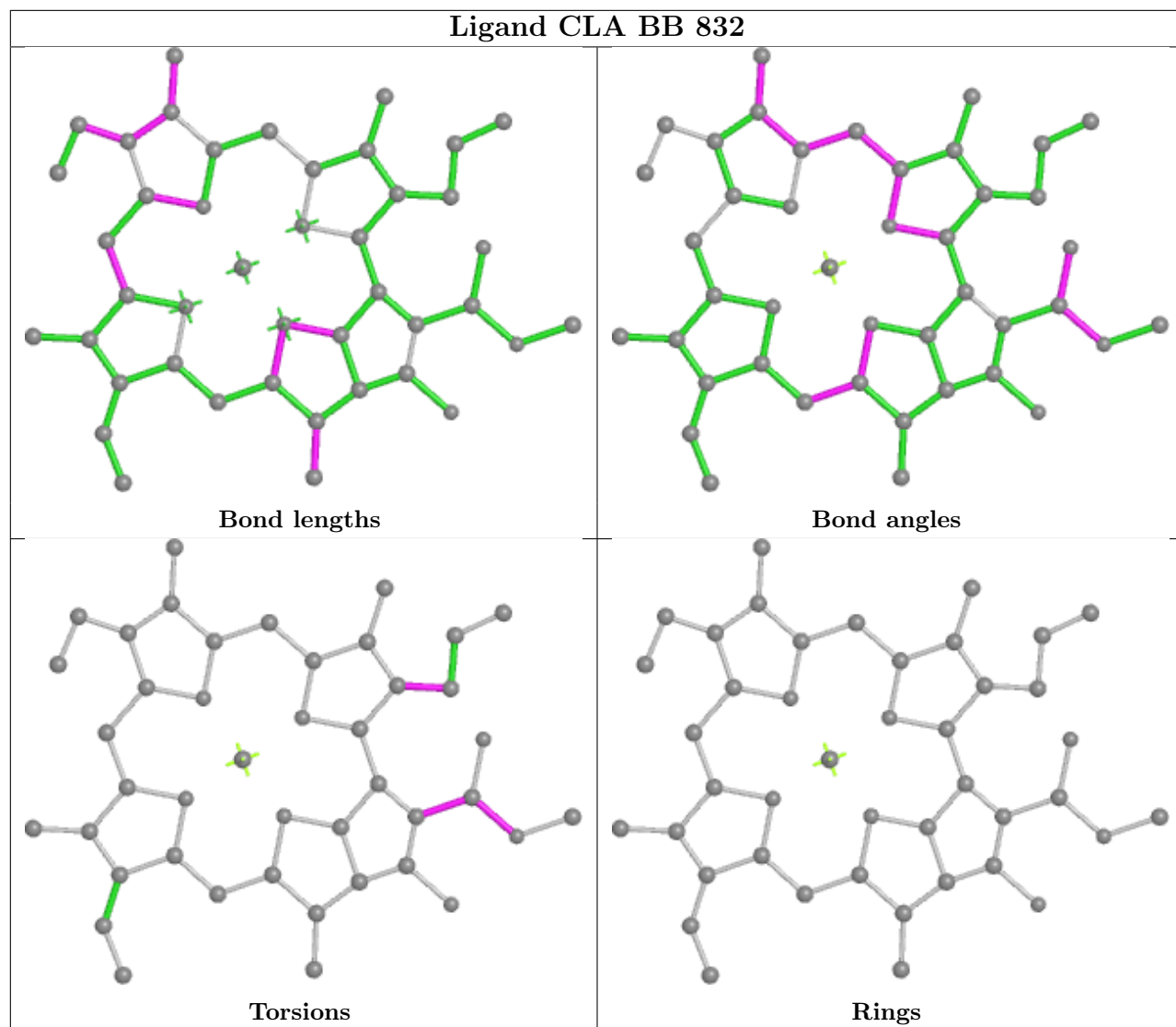
Rings

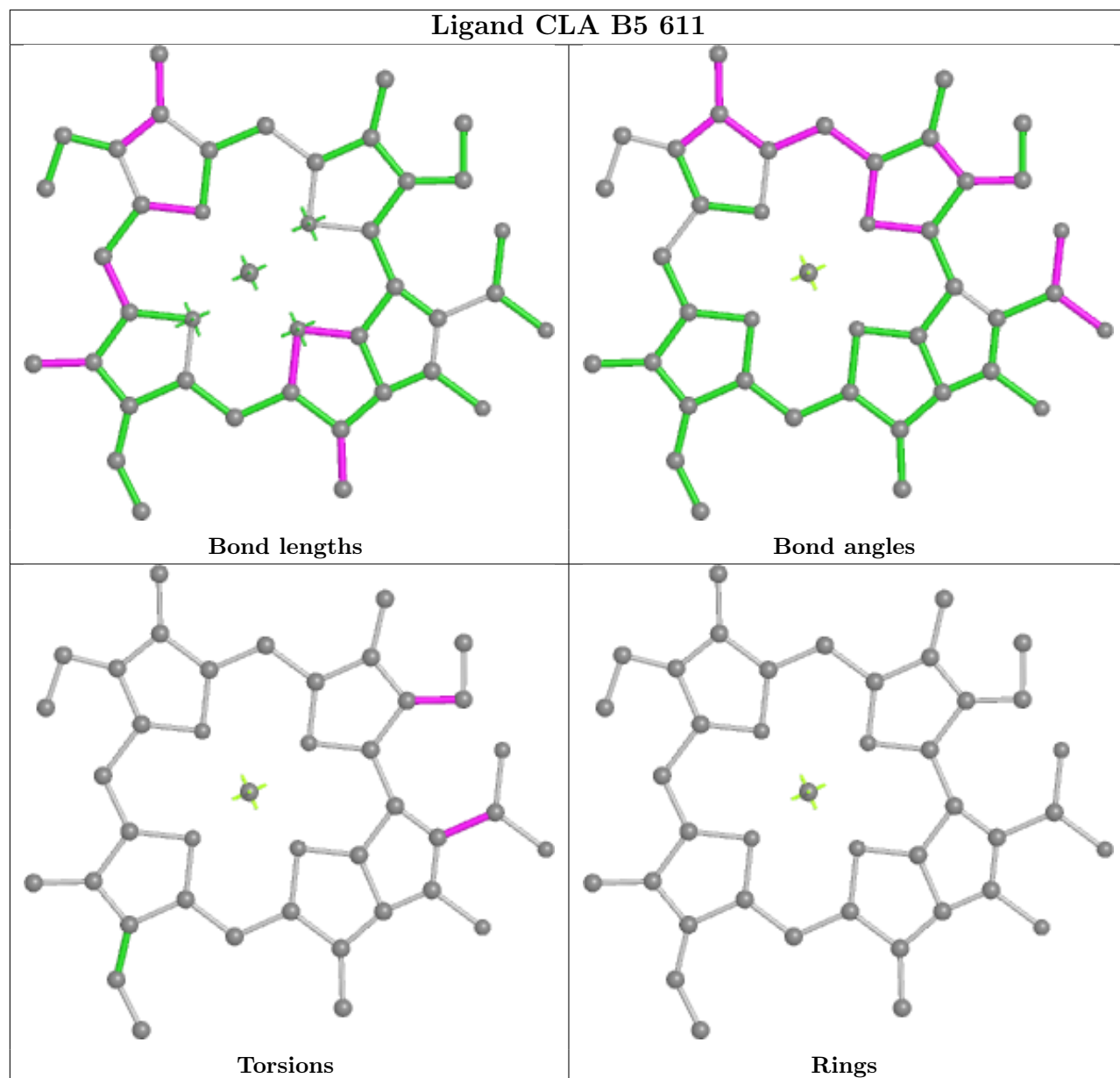


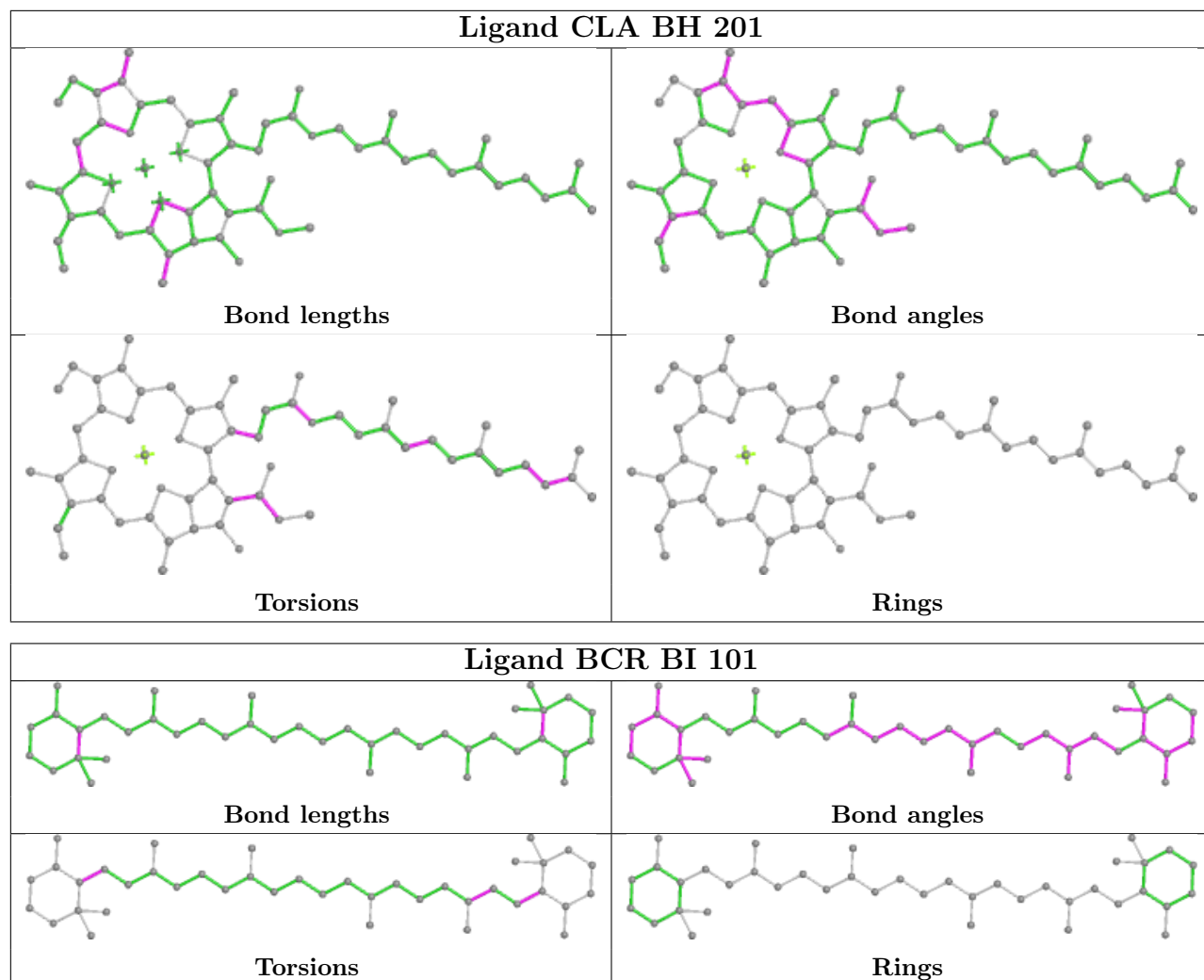
Ligand CLA B3 303

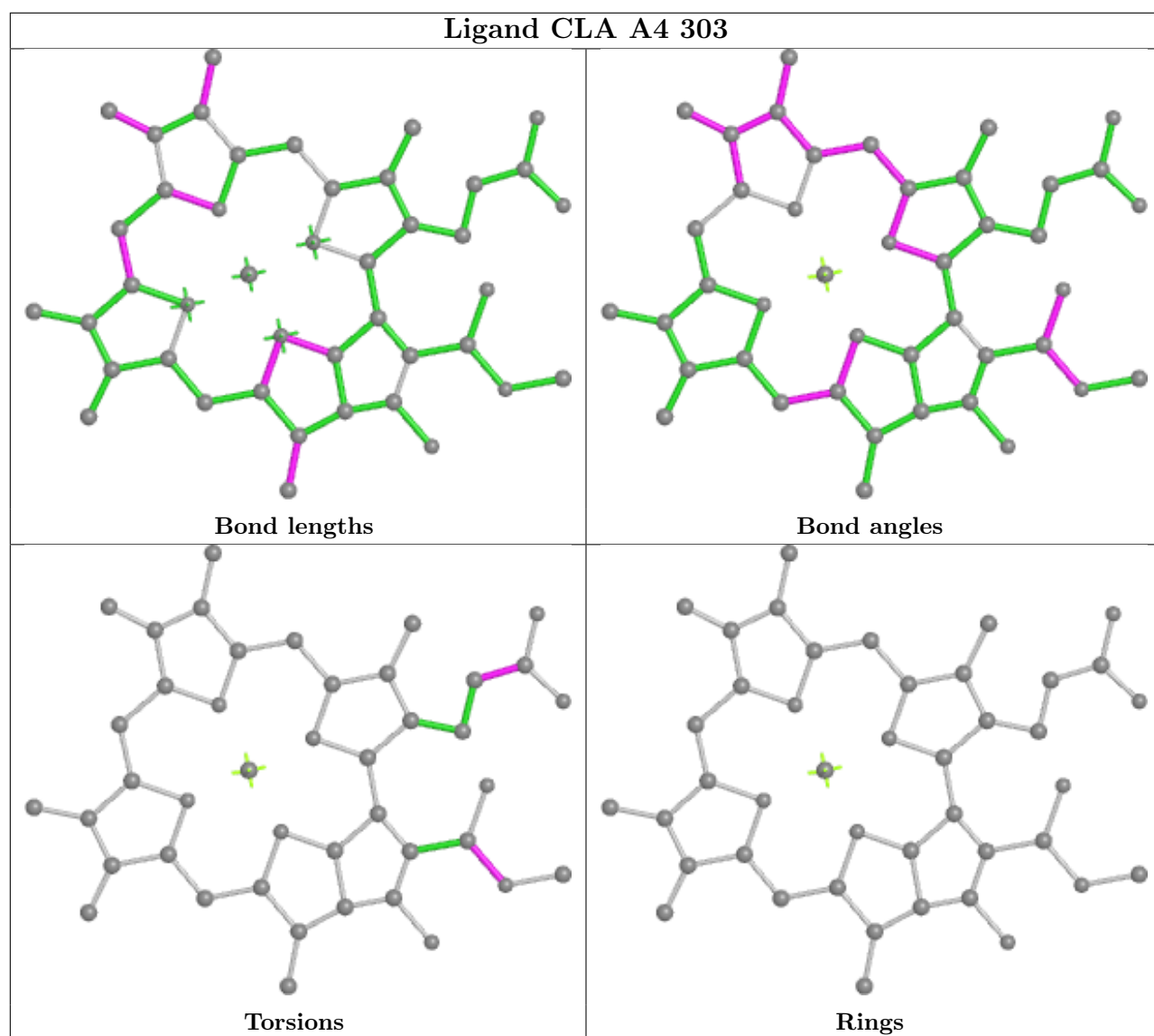


Ligand CLA BB 832

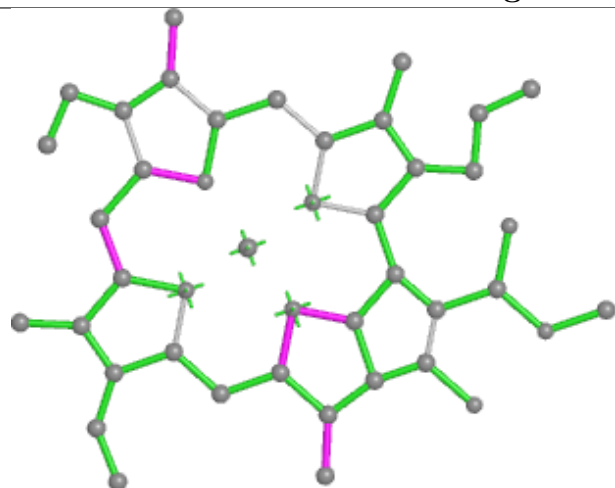




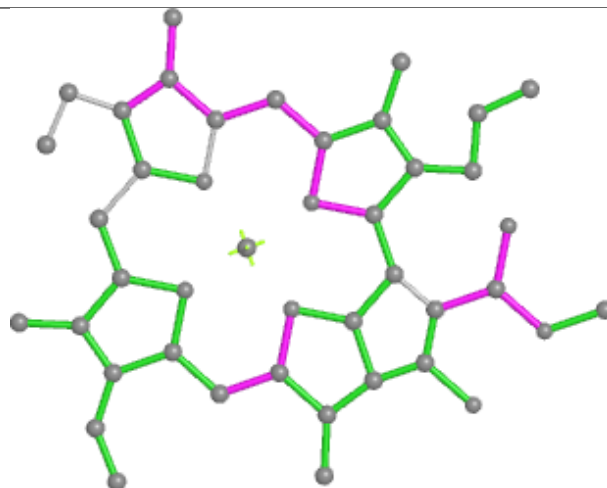




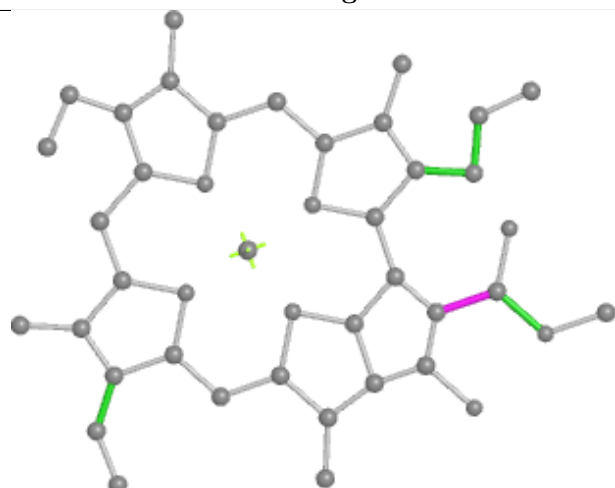
Ligand CLA BB 814



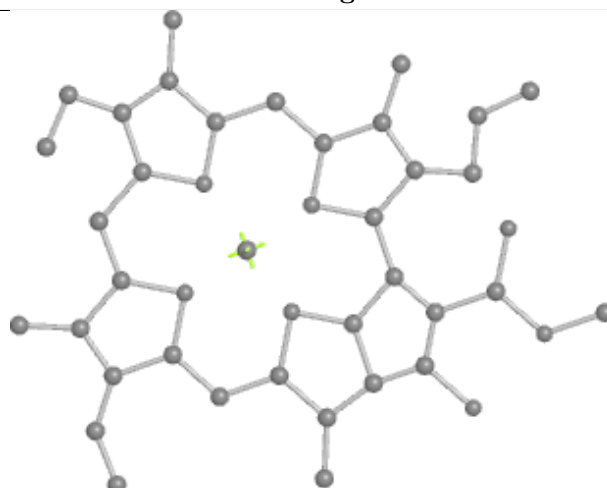
Bond lengths



Bond angles

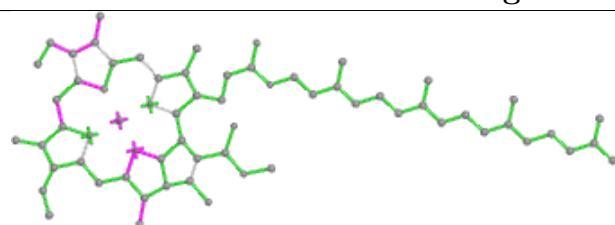


Torsions

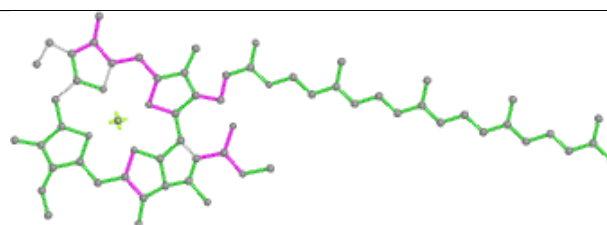


Rings

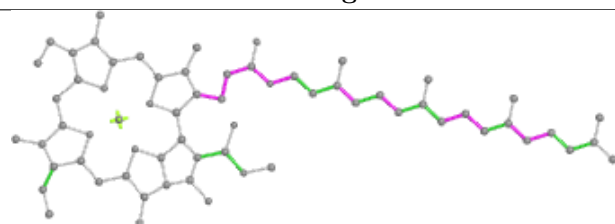
Ligand CLA AB 829



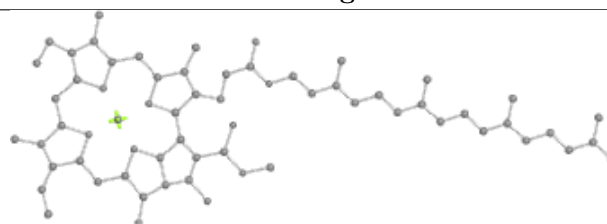
Bond lengths



Bond angles

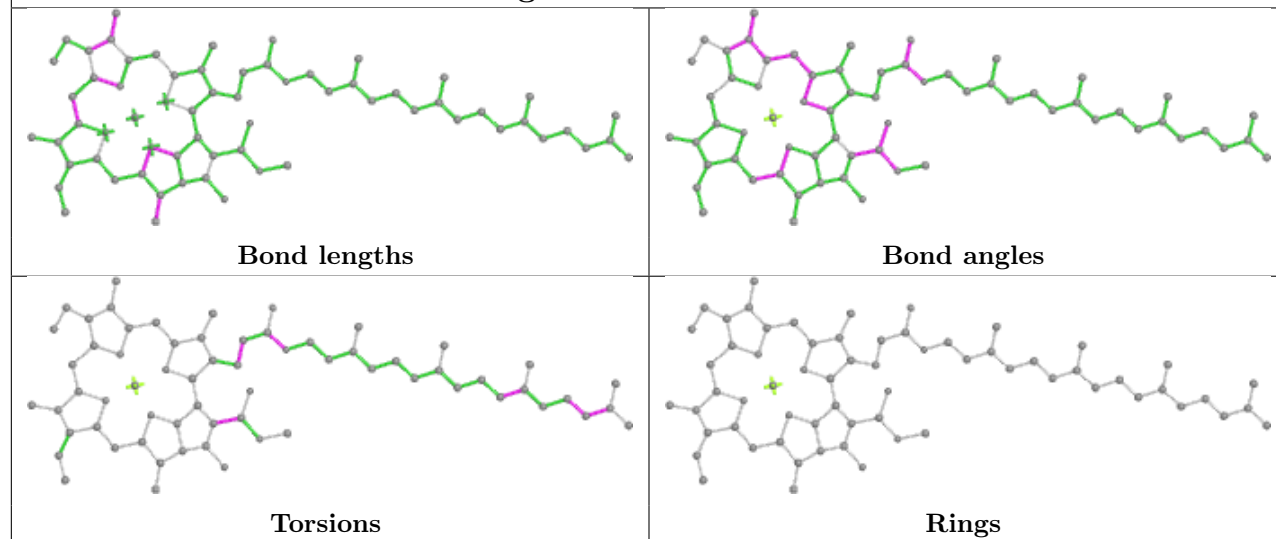


Torsions

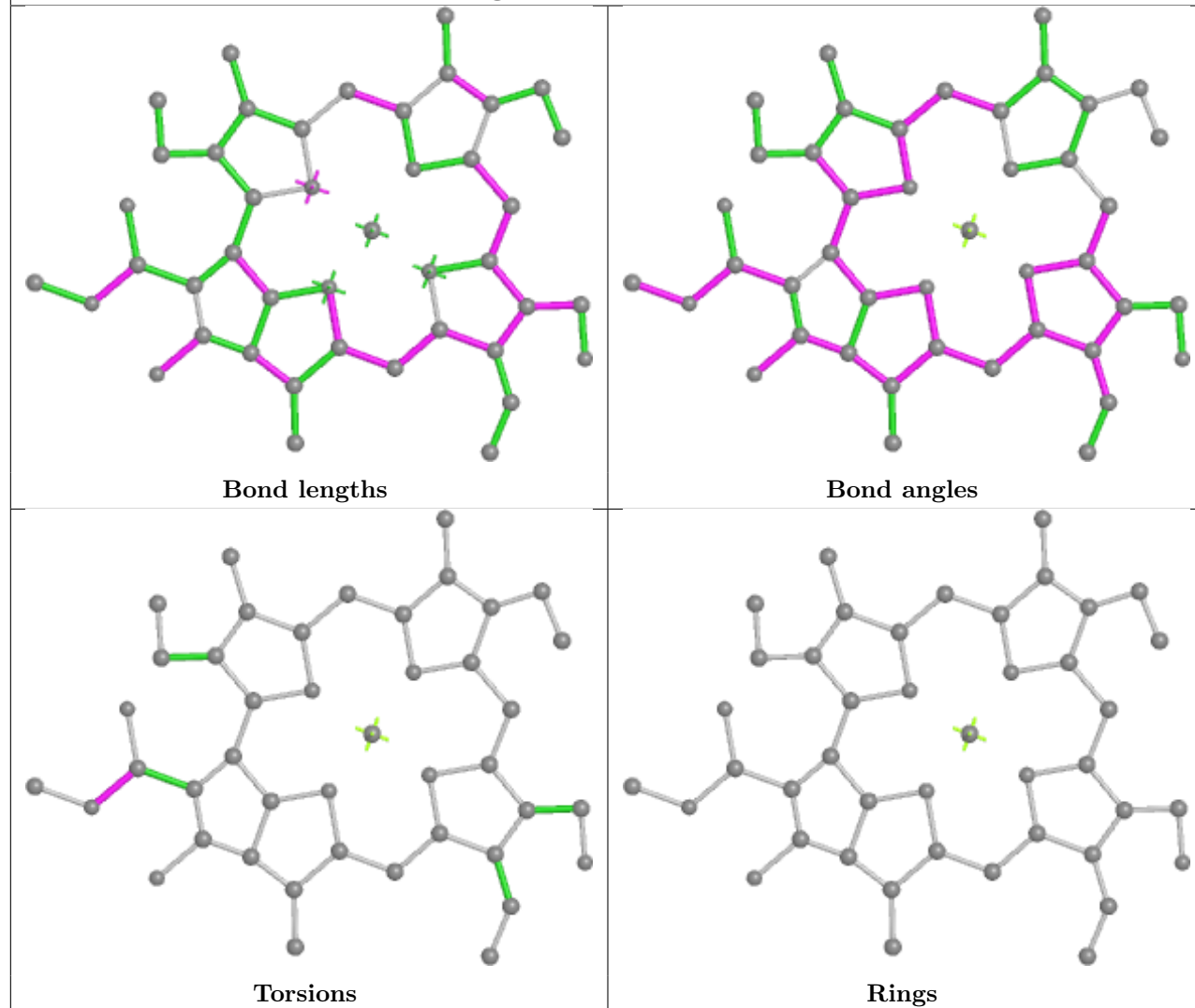


Rings

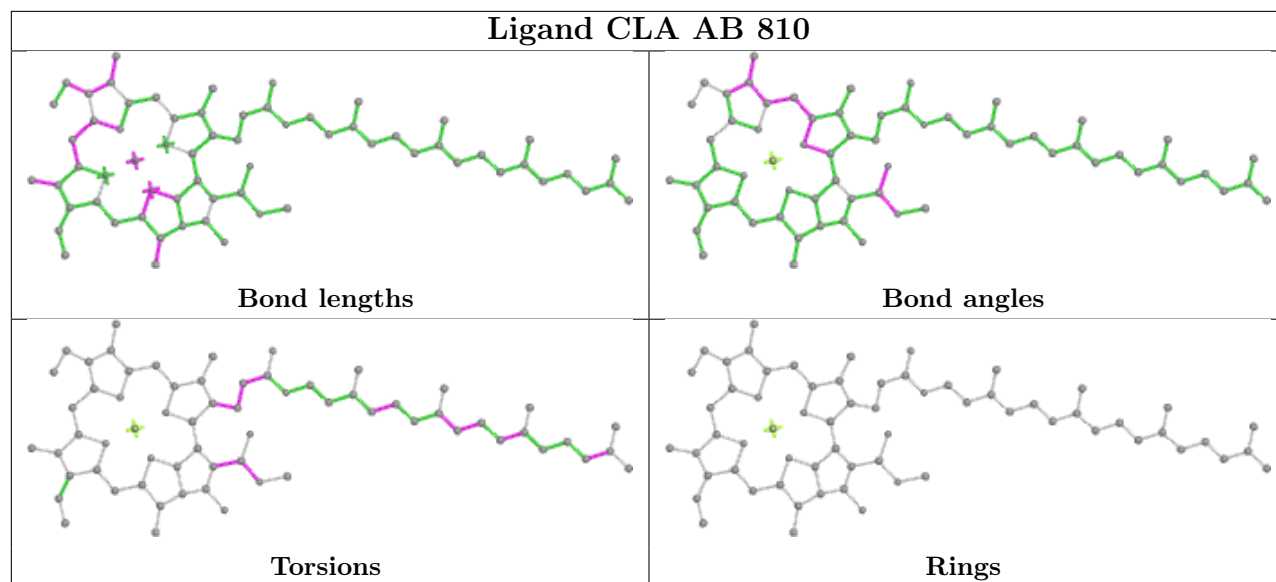
Ligand CLA AA 808



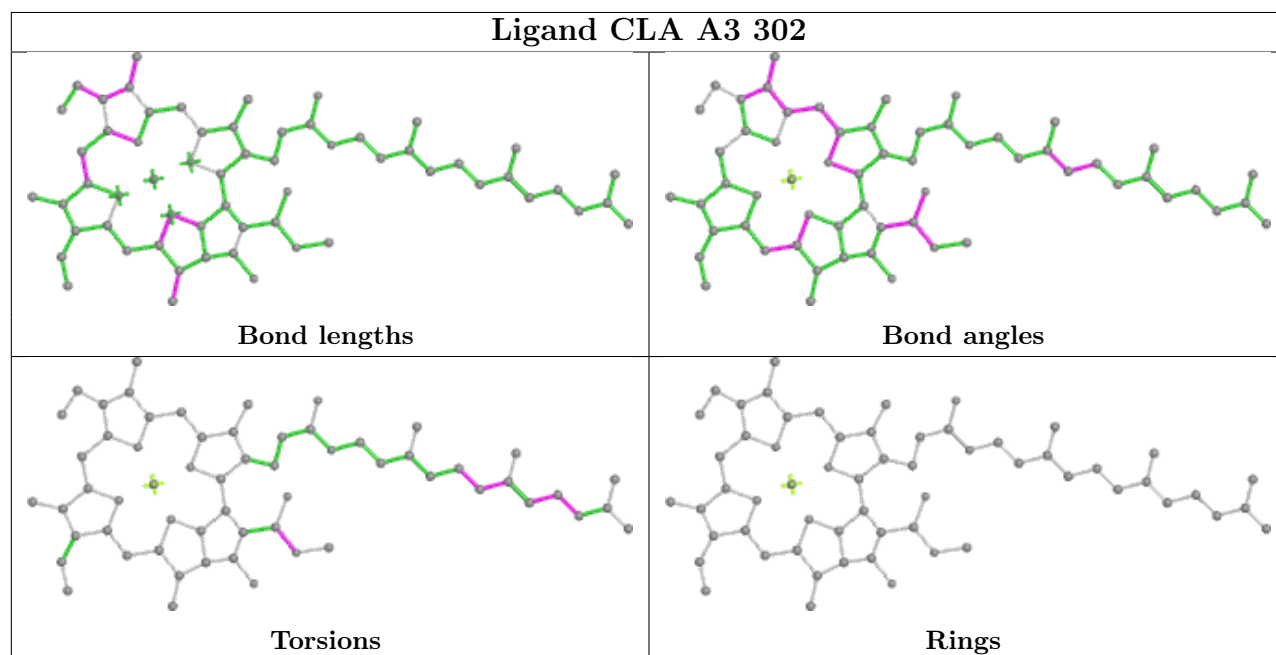
Ligand CHL A6 607



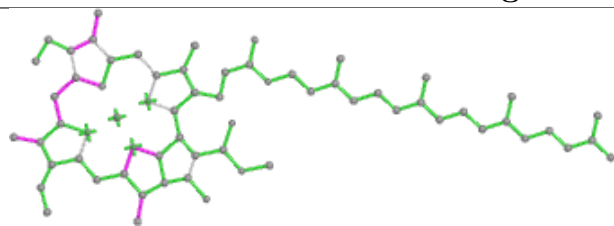
Ligand CLA AB 810



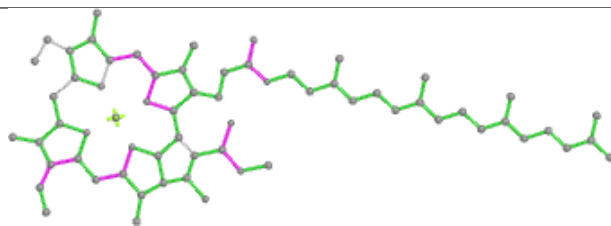
Ligand CLA A3 302



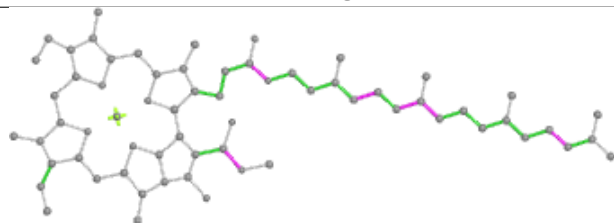
Ligand CLA BB 842



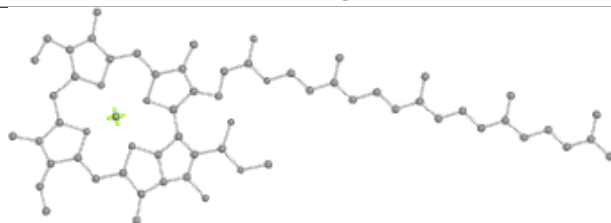
Bond lengths



Bond angles

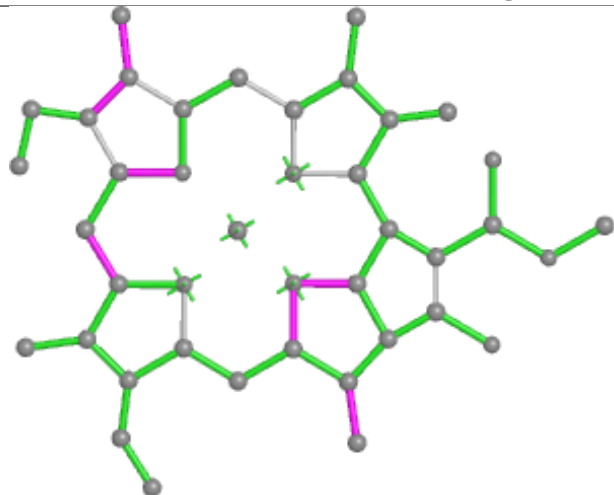


Torsions

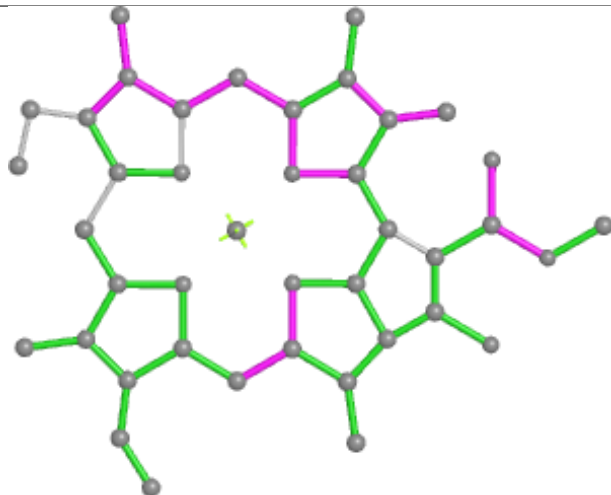


Rings

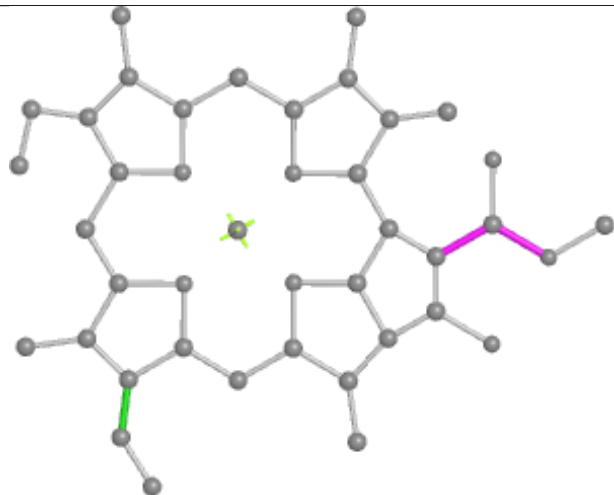
Ligand CLA AA 823



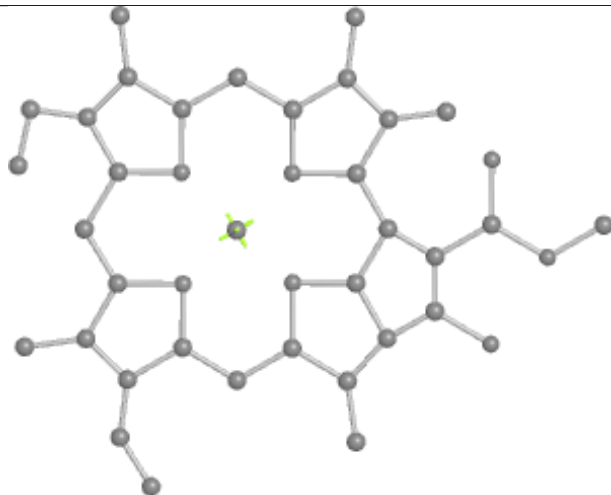
Bond lengths



Bond angles

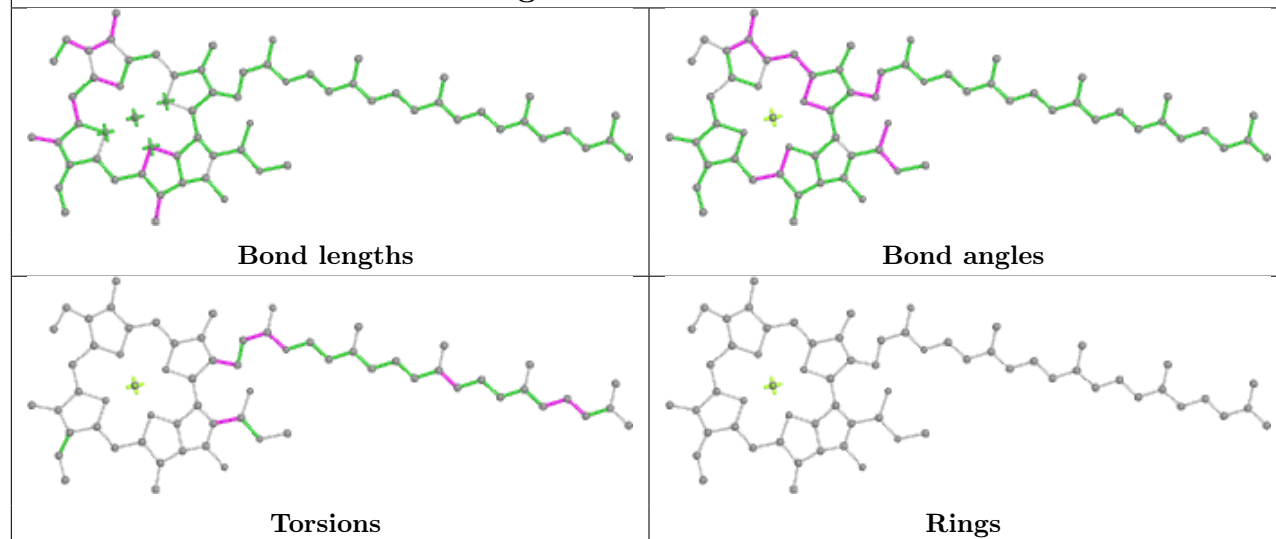


Torsions

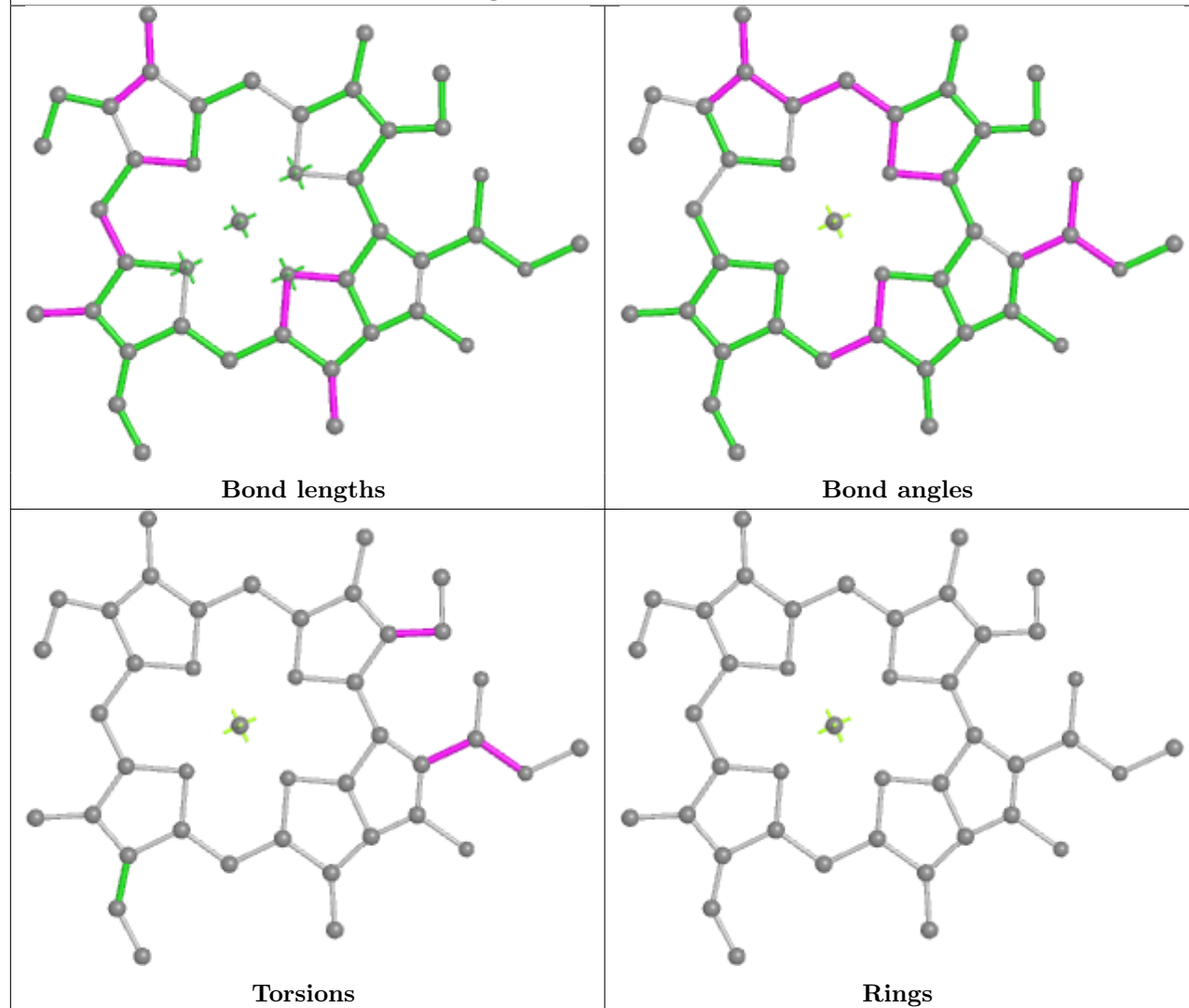


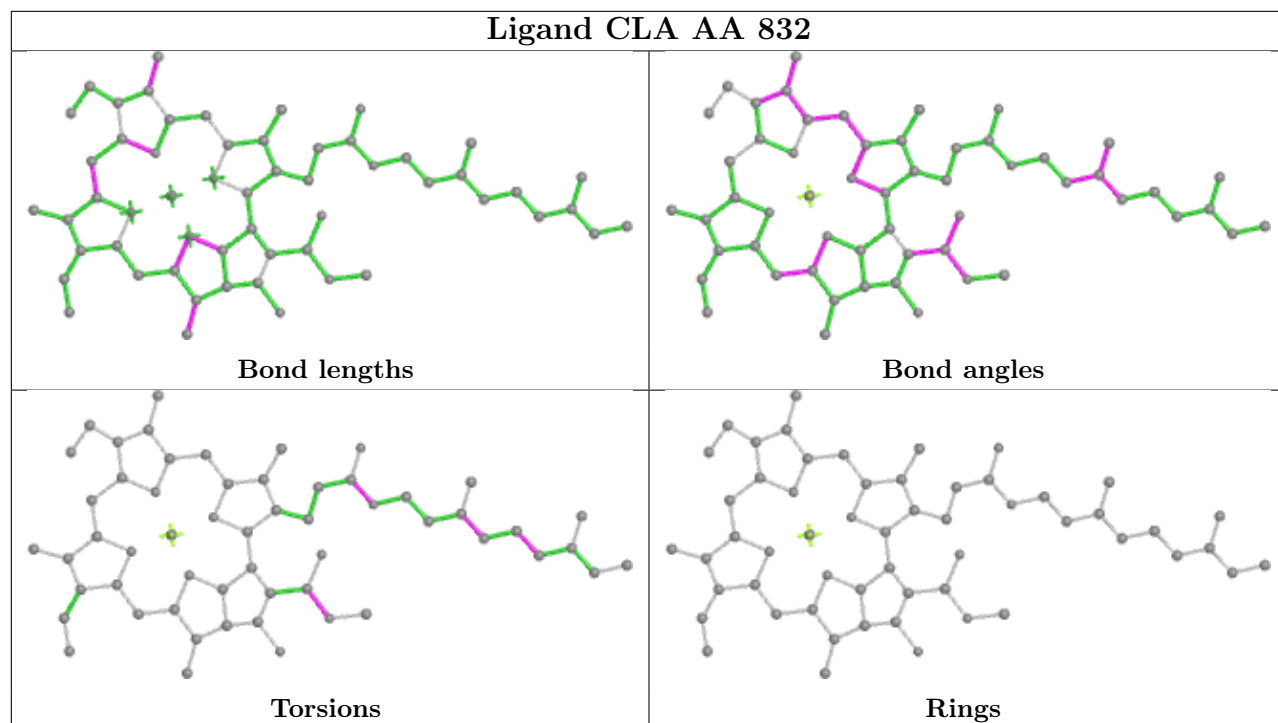
Rings

Ligand CLA AA 841

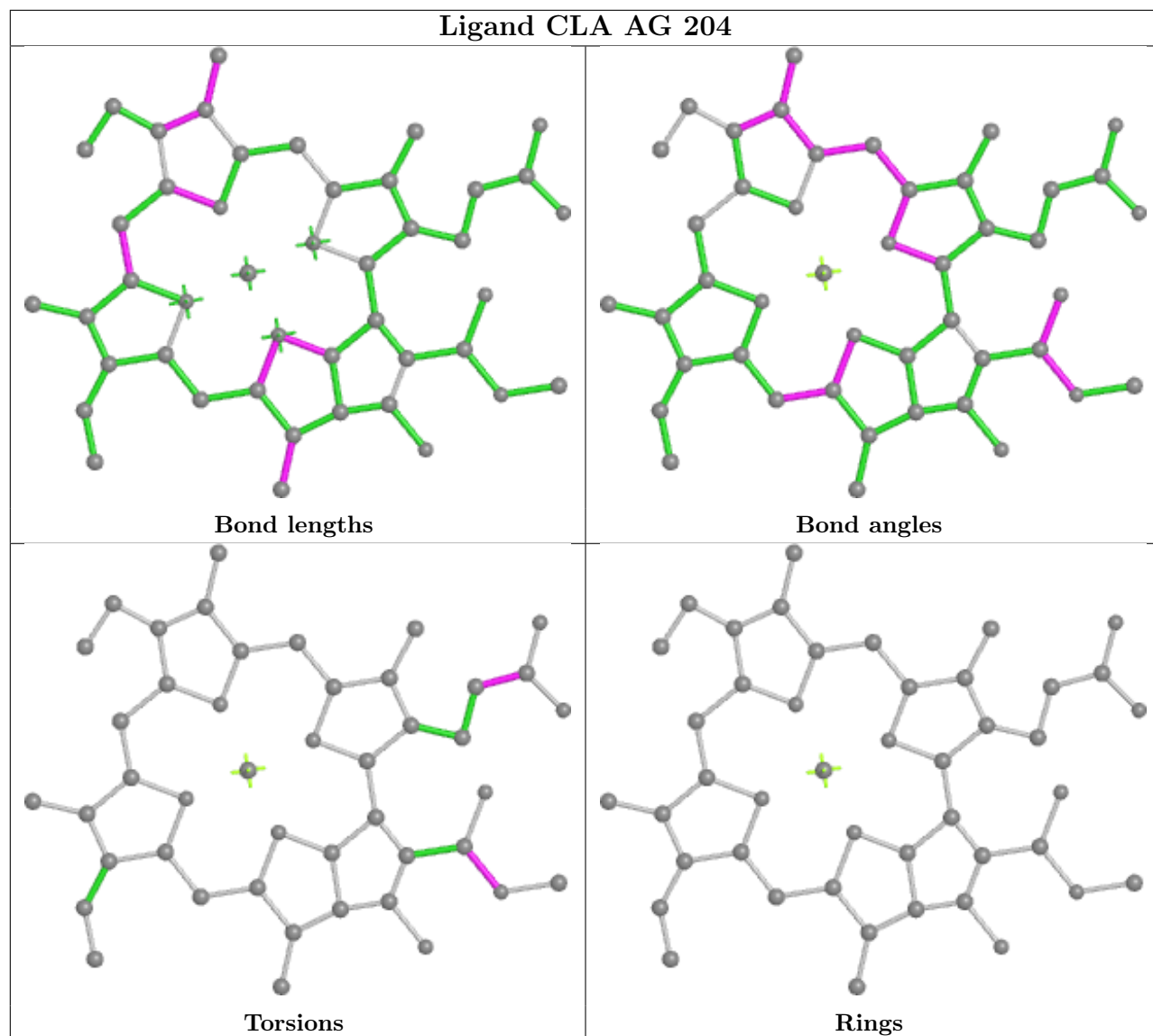


Ligand CLA AL 305

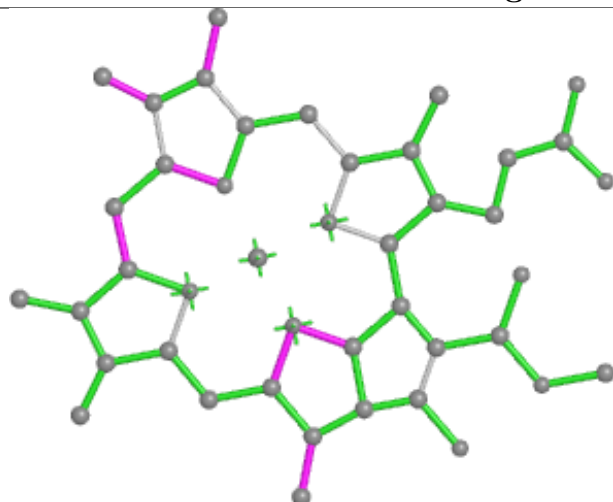




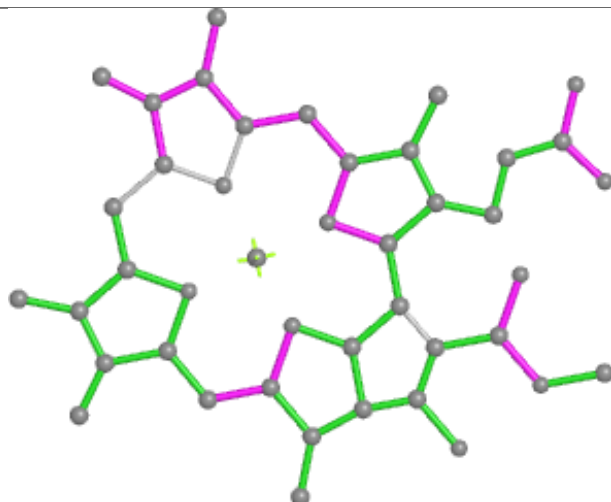
Ligand CLA AG 204



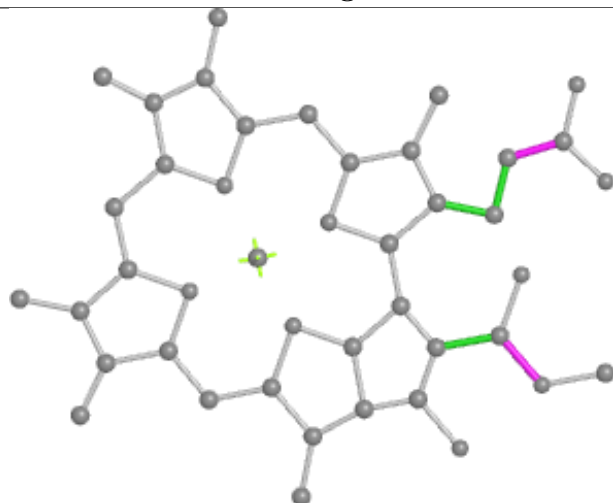
Ligand CLA B5 604



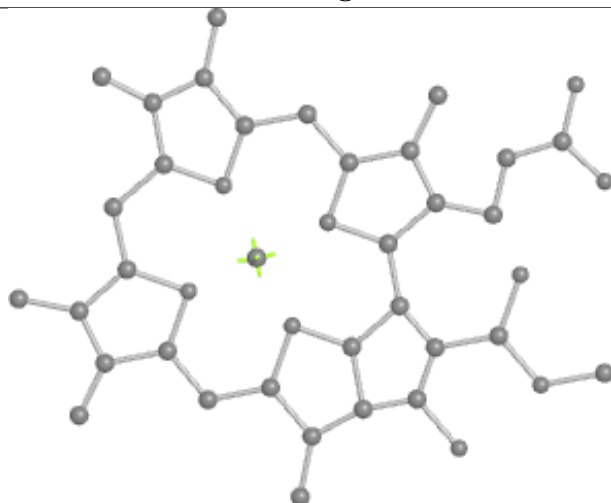
Bond lengths



Bond angles

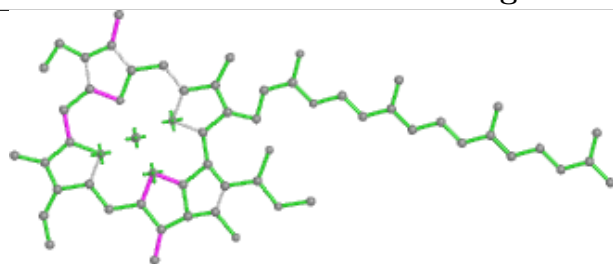


Torsions

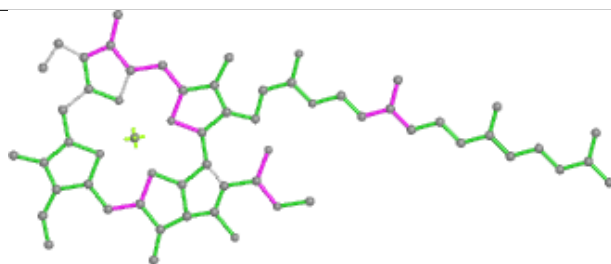


Rings

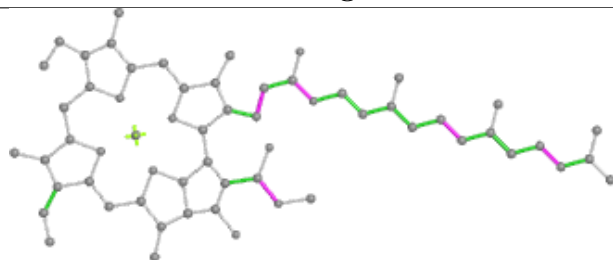
Ligand CLA AA 817



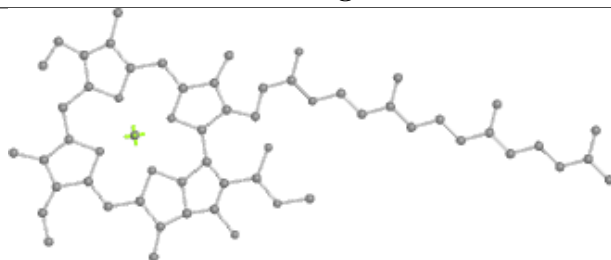
Bond lengths



Bond angles

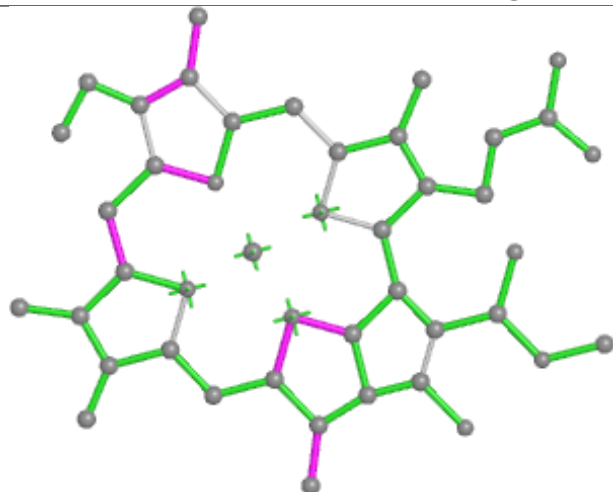


Torsions

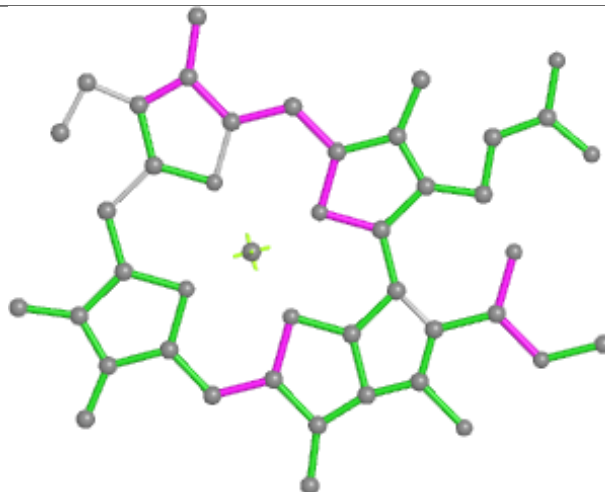


Rings

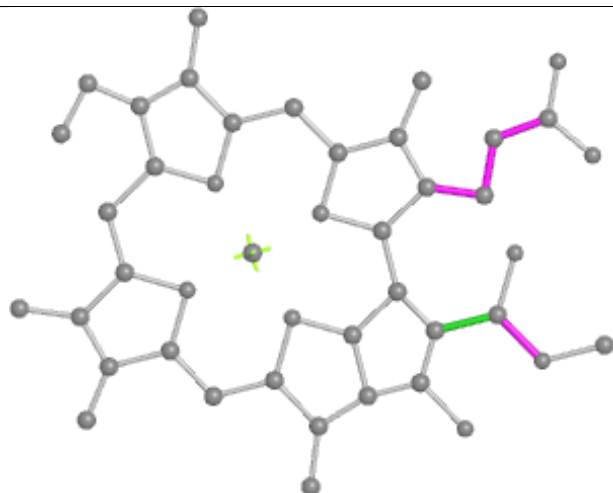
Ligand CLA B2 611



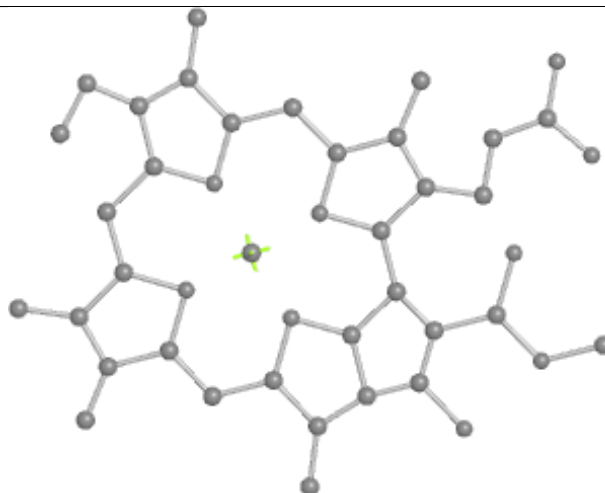
Bond lengths



Bond angles

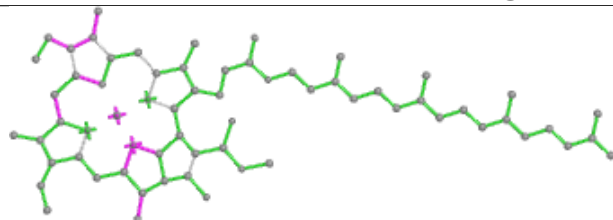


Torsions

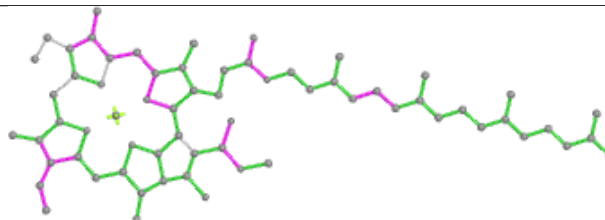


Rings

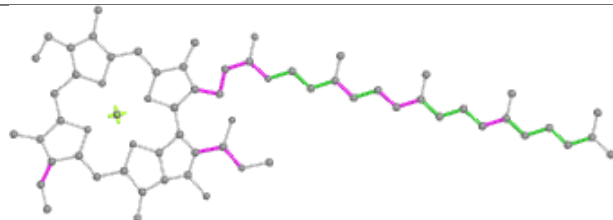
Ligand CLA BB 815



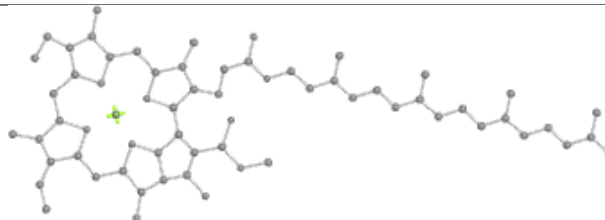
Bond lengths



Bond angles

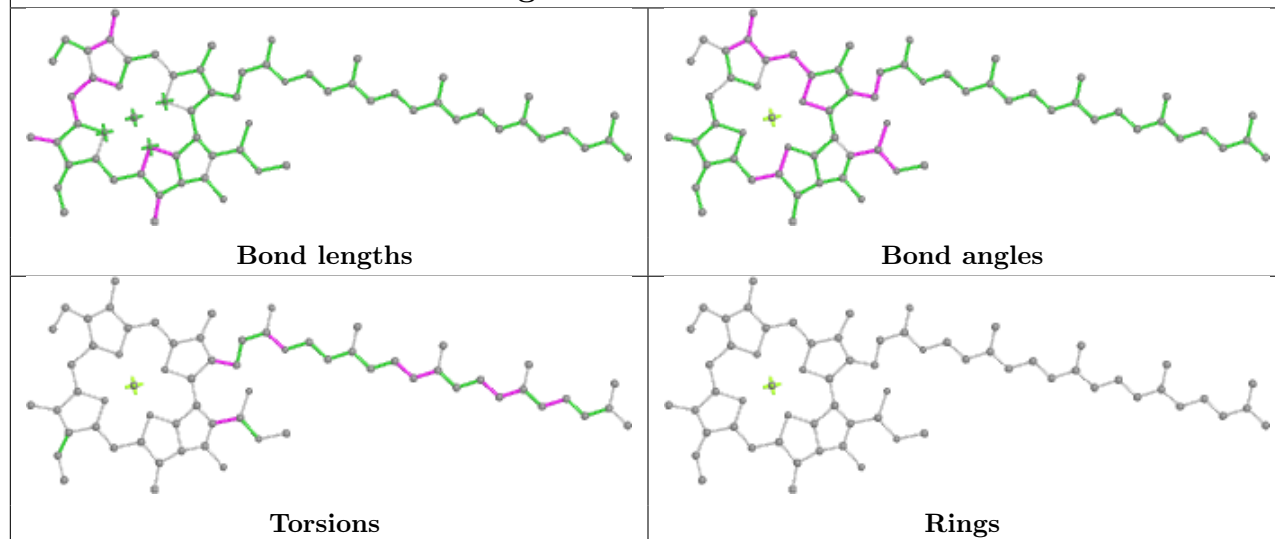


Torsions

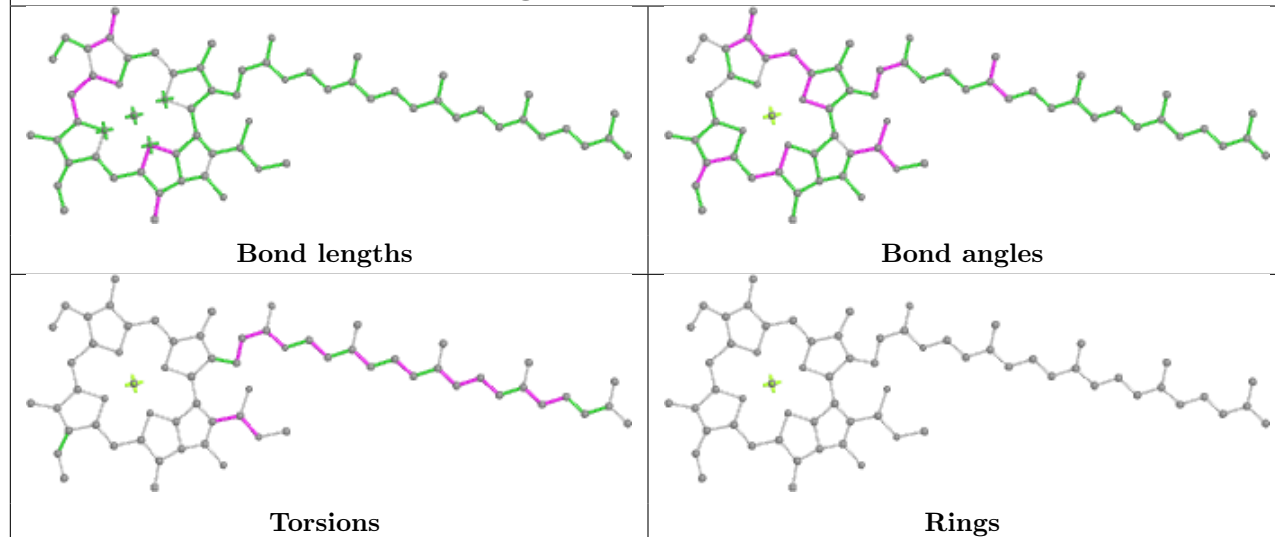


Rings

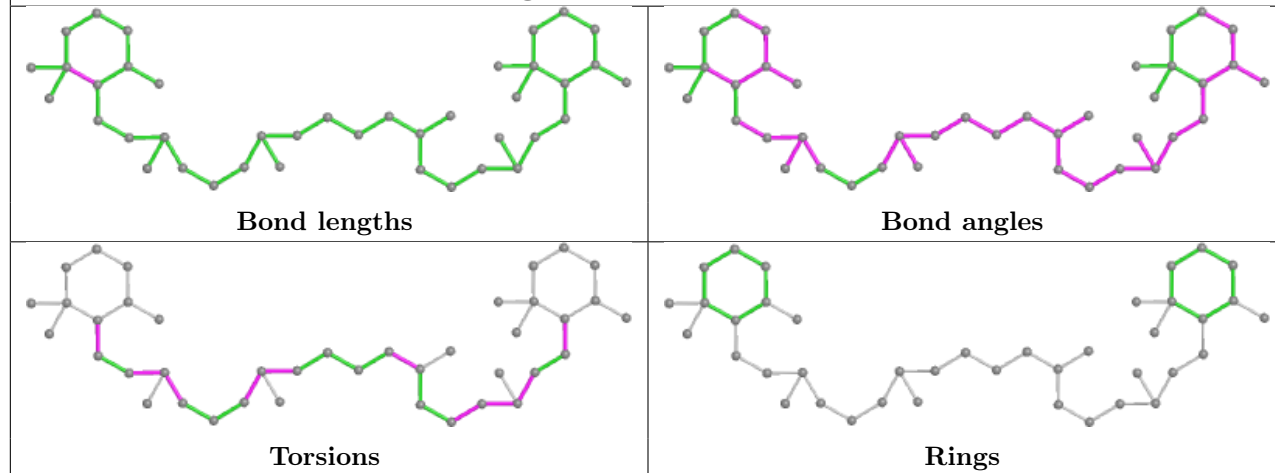
Ligand CLA BA 819

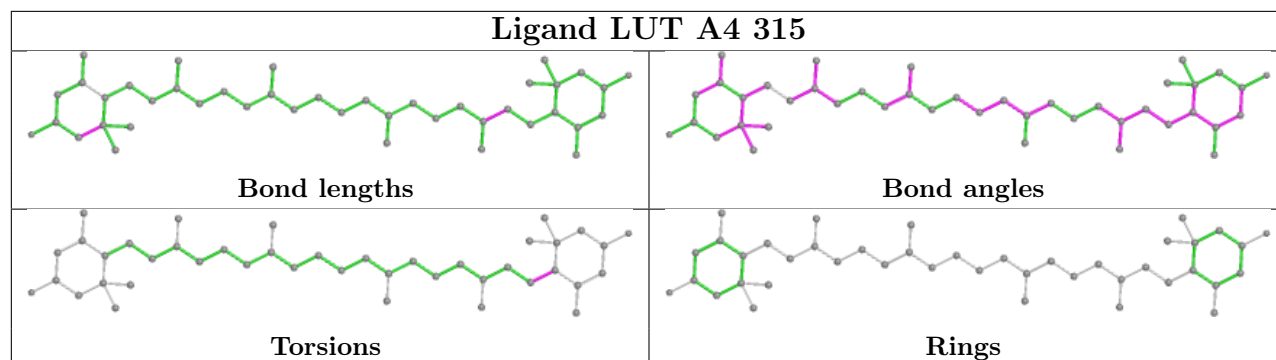
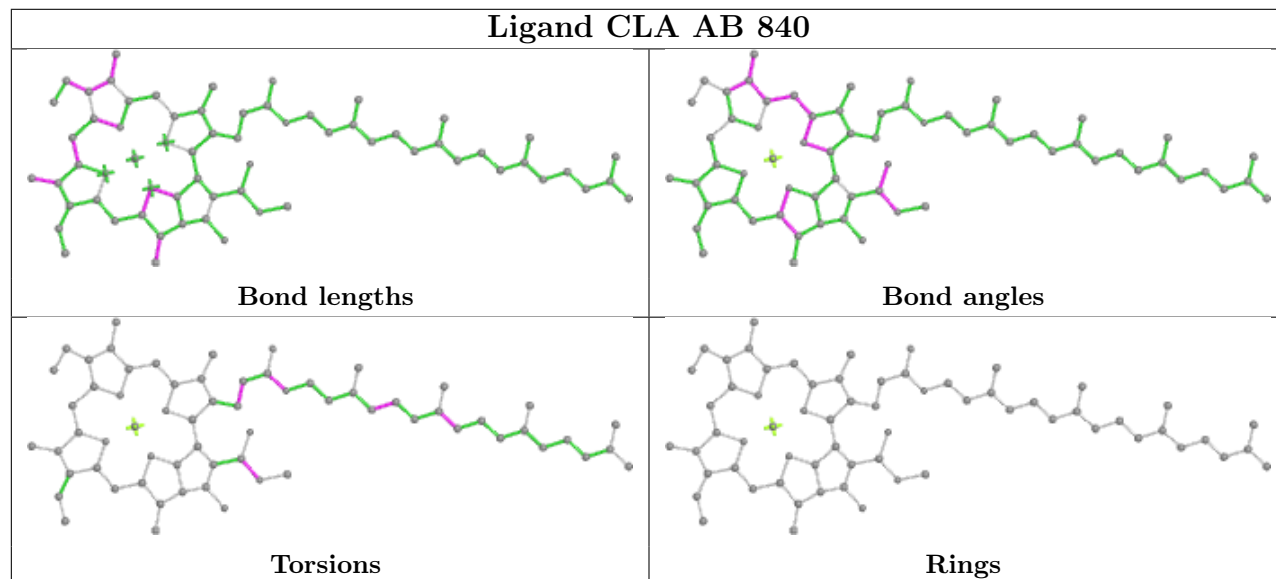
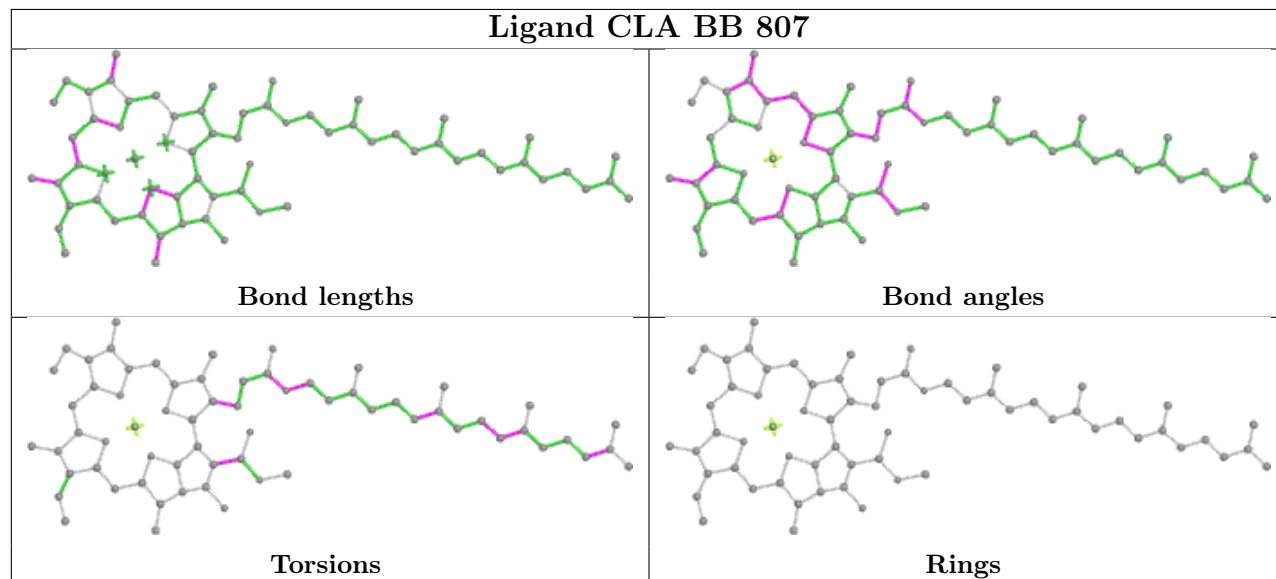


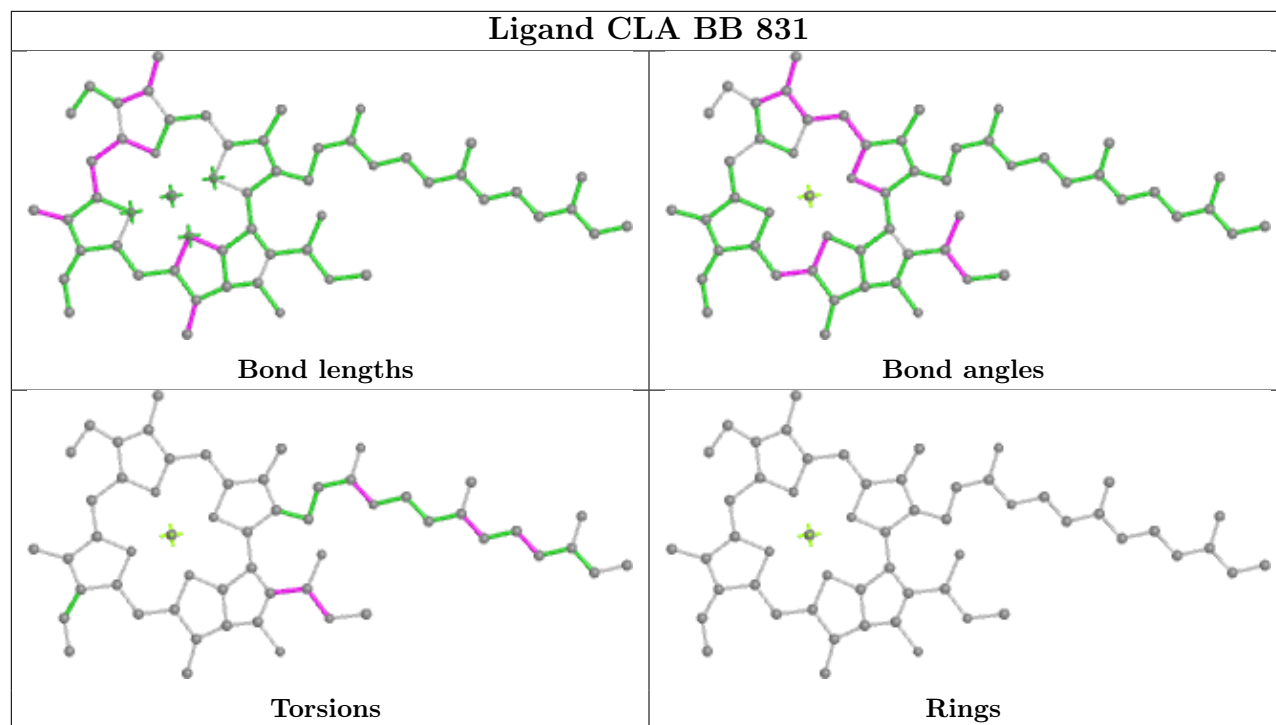
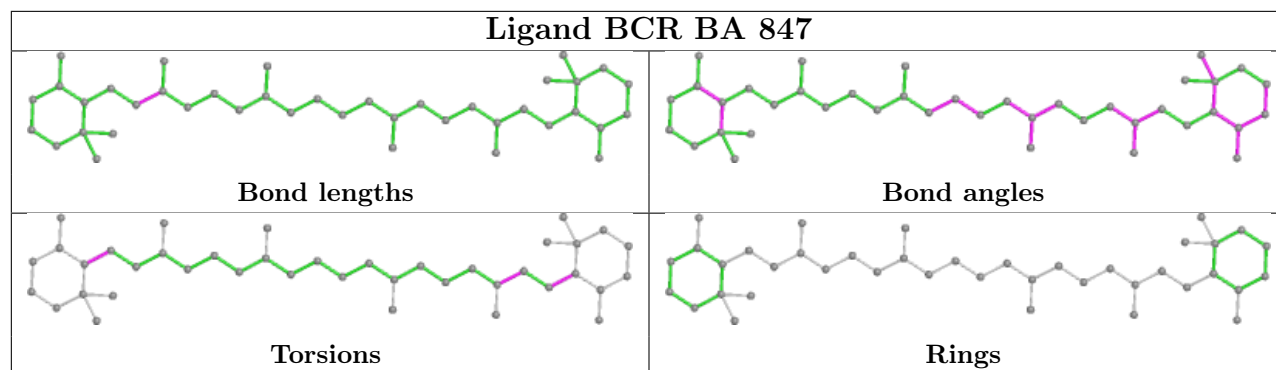
Ligand CLA AA 842



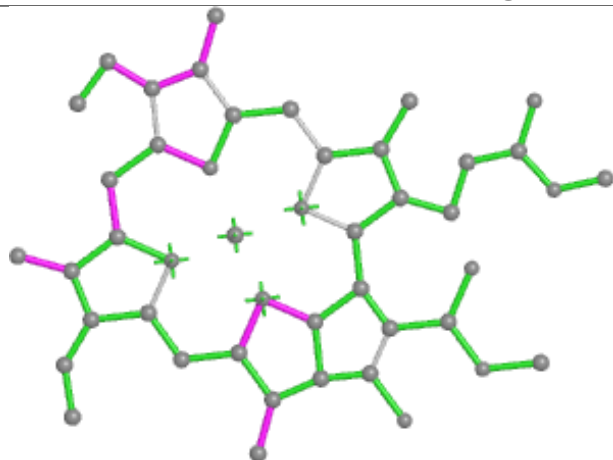
Ligand BCR BL 306



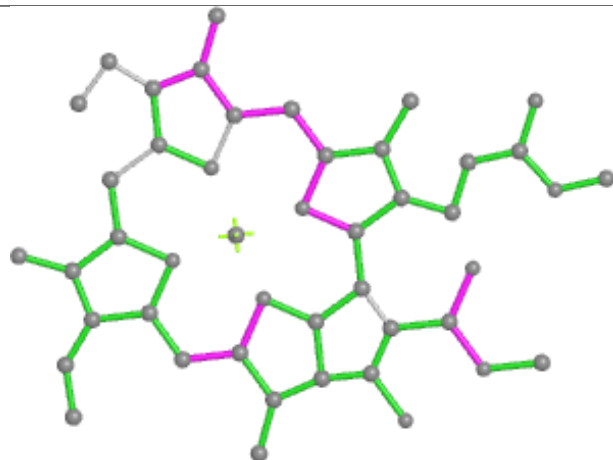
Ligand LUT A4 315**Ligand CLA AB 840****Ligand CLA BB 807**



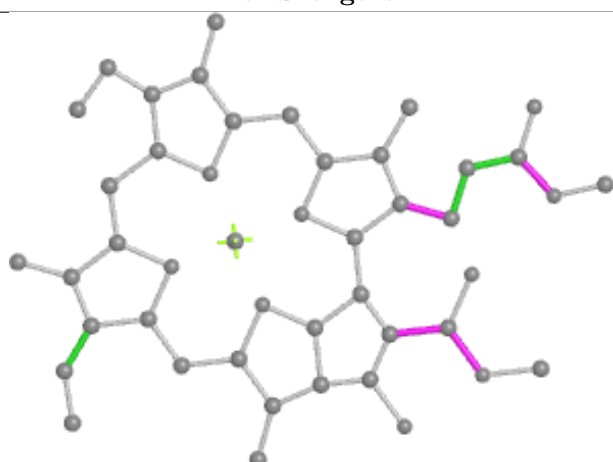
Ligand CLA AK 203



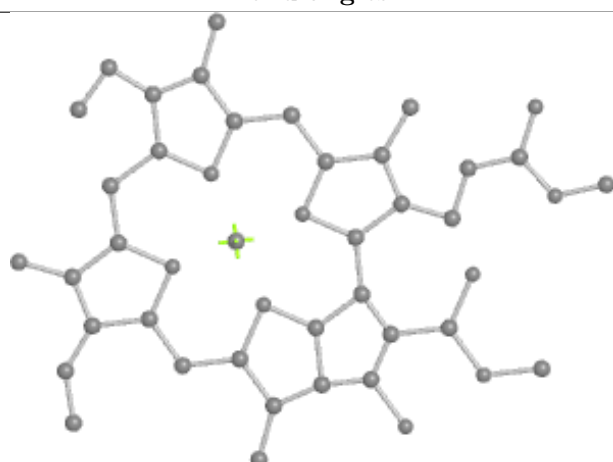
Bond lengths



Bond angles

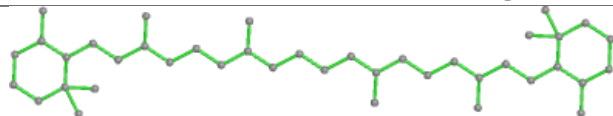


Torsions

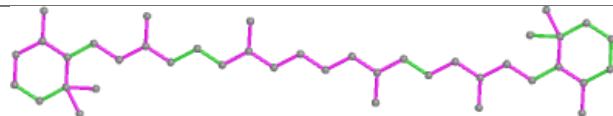


Rings

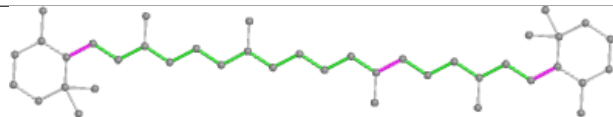
Ligand BCR AB 844



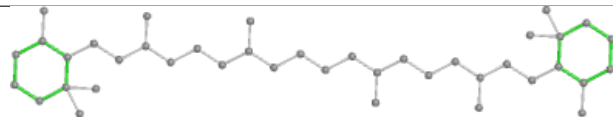
Bond lengths



Bond angles

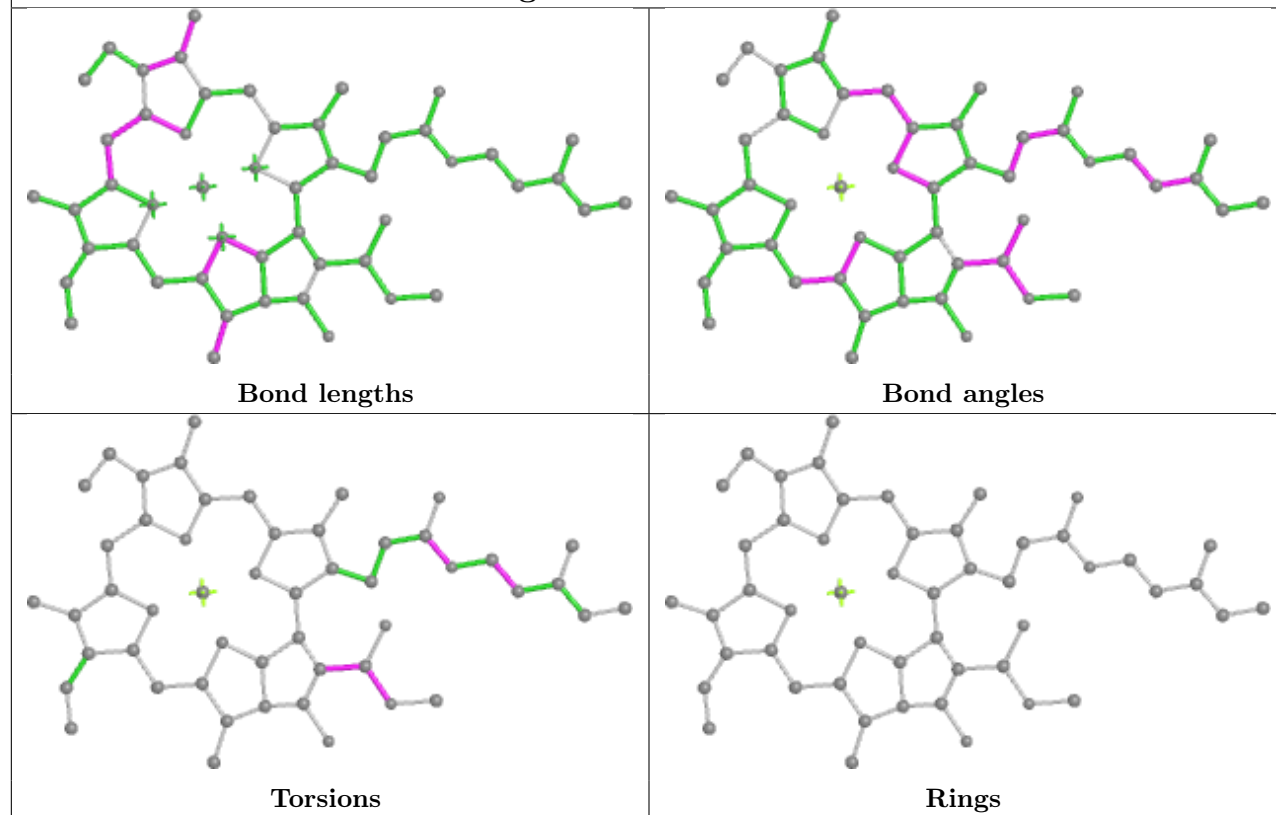


Torsions

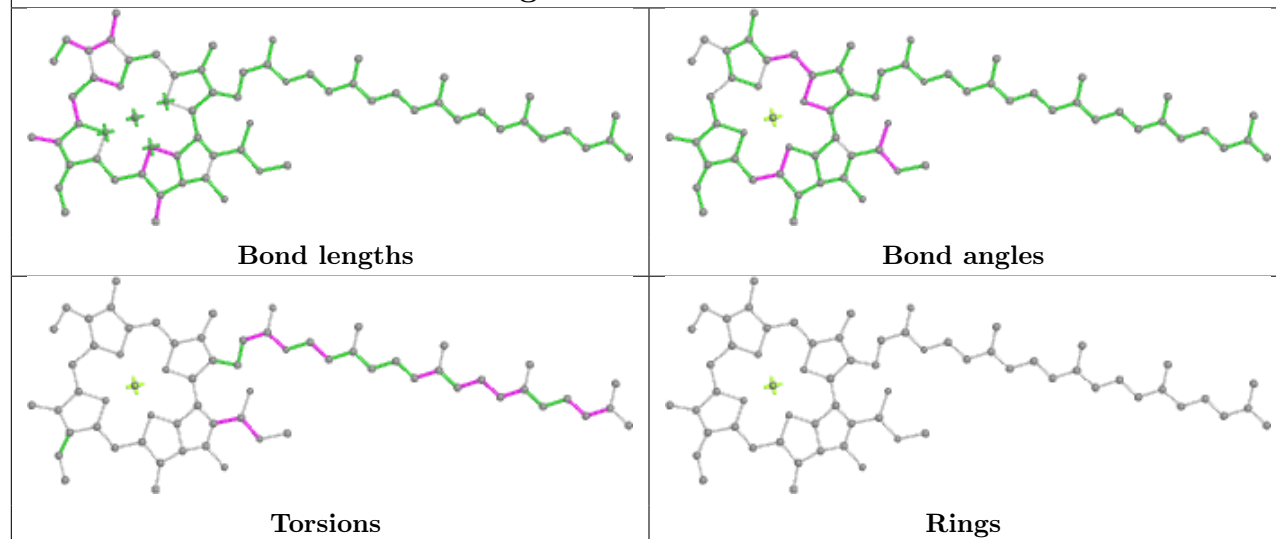


Rings

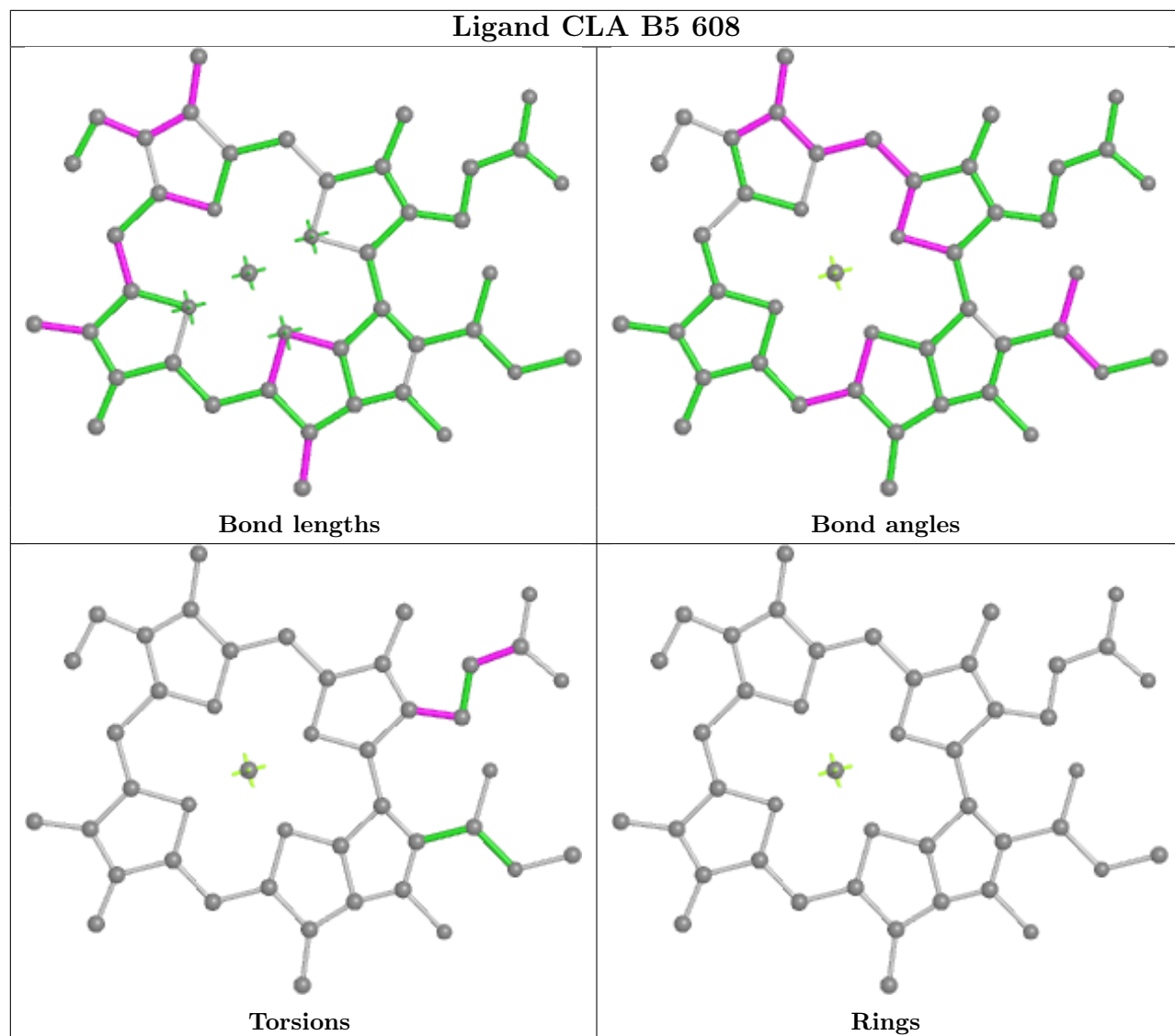
Ligand CLA BA 839

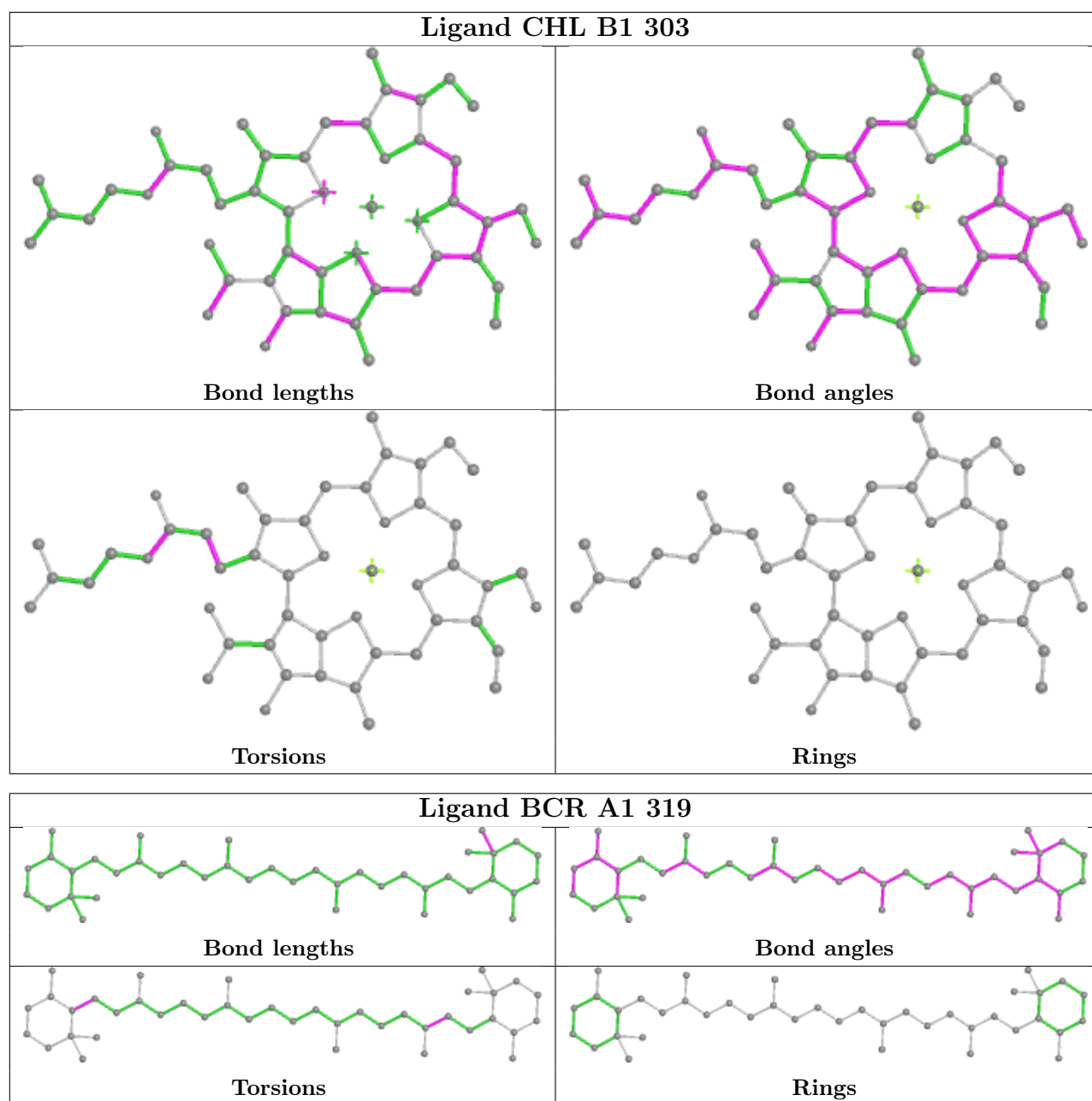


Ligand CLA BB 835

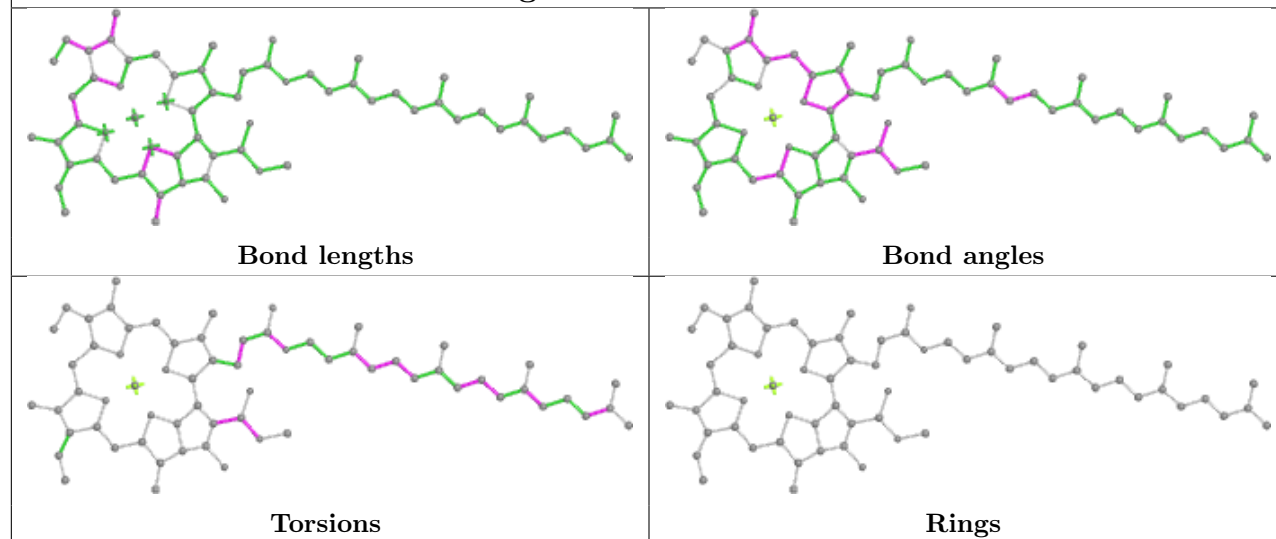


Ligand CLA B5 608

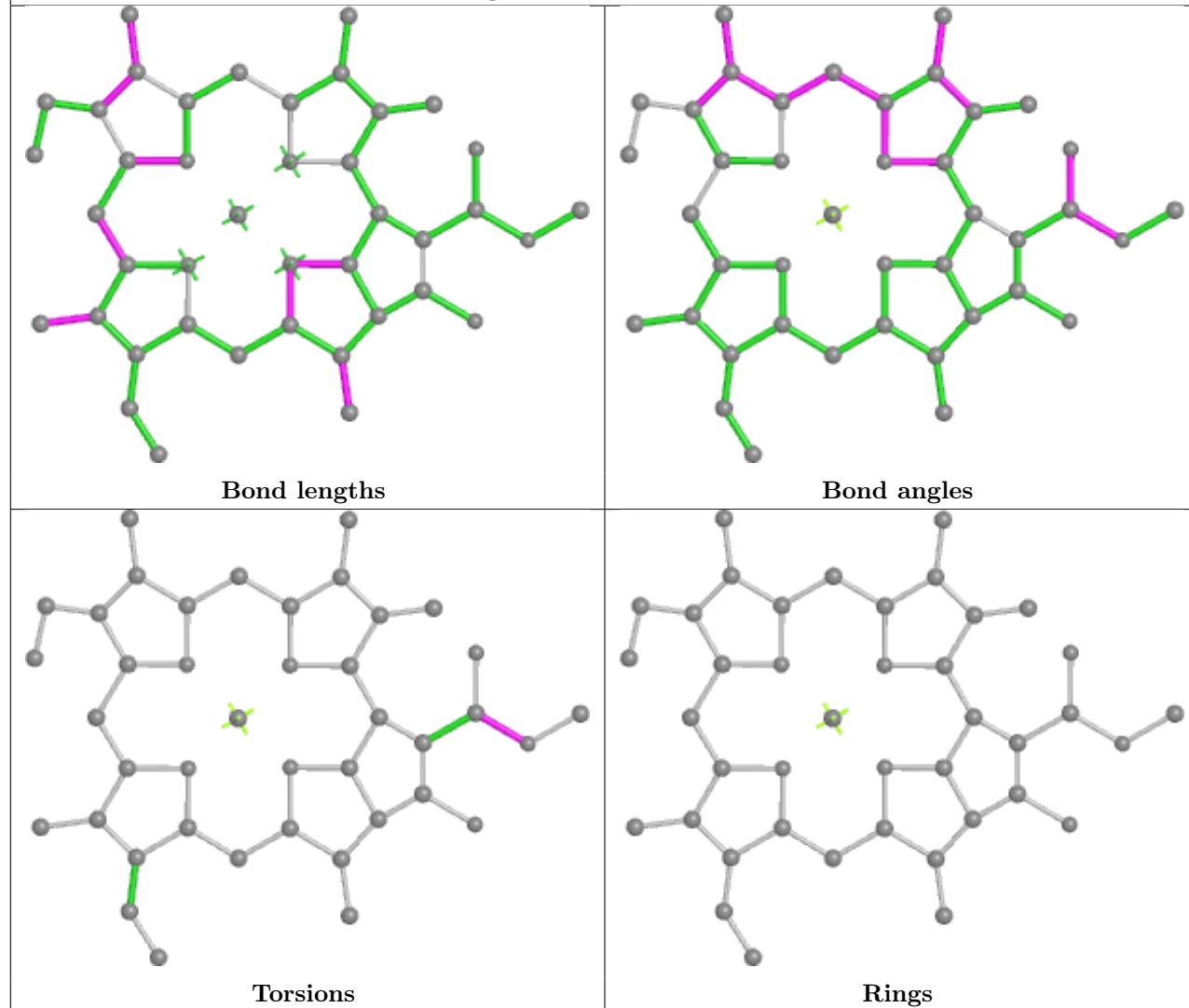




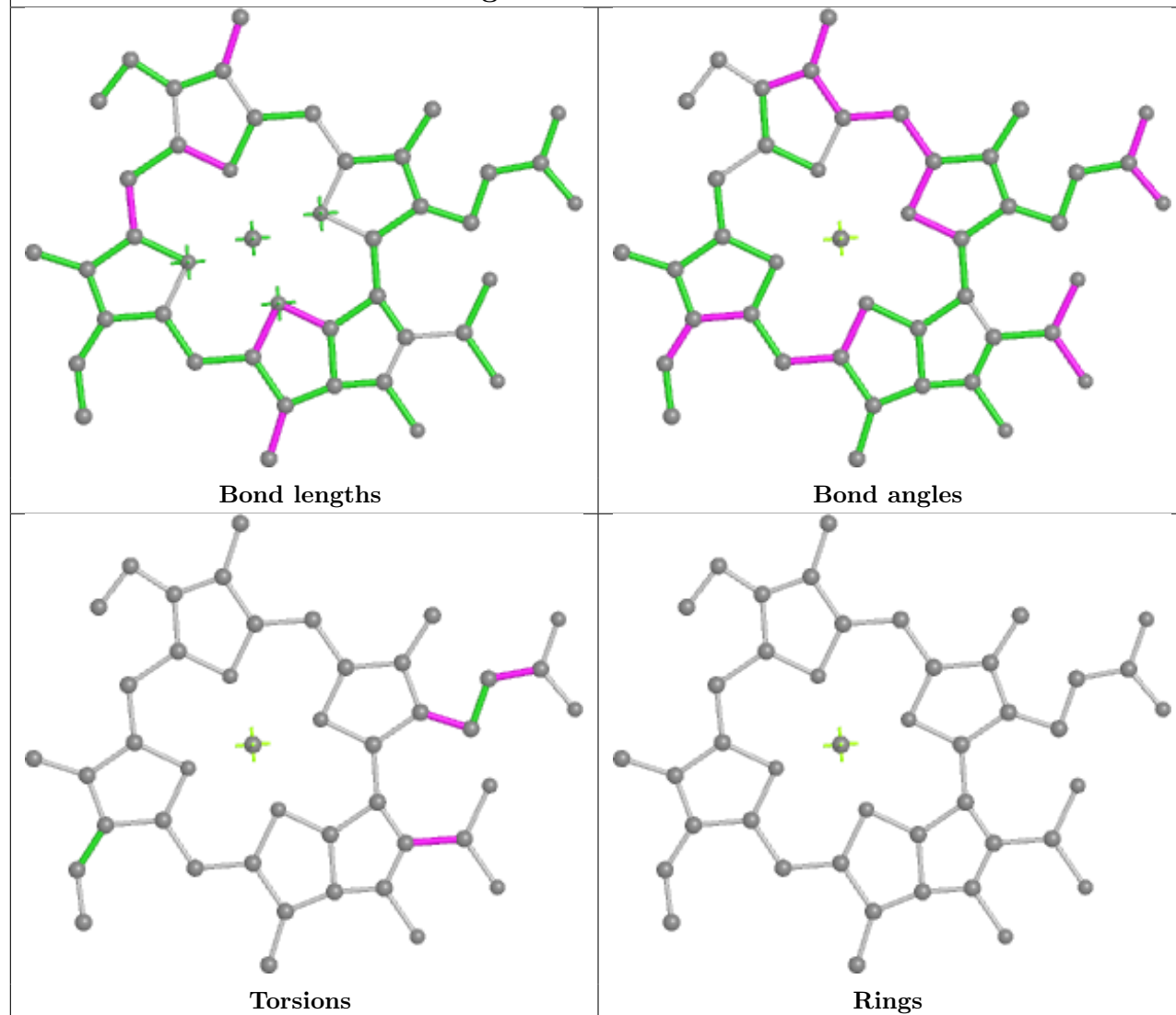
Ligand CLA AB 842



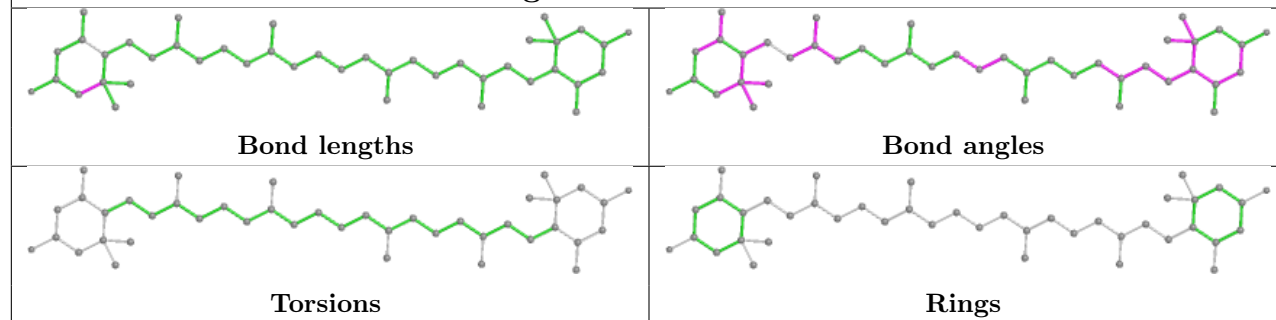
Ligand CLA BB 822



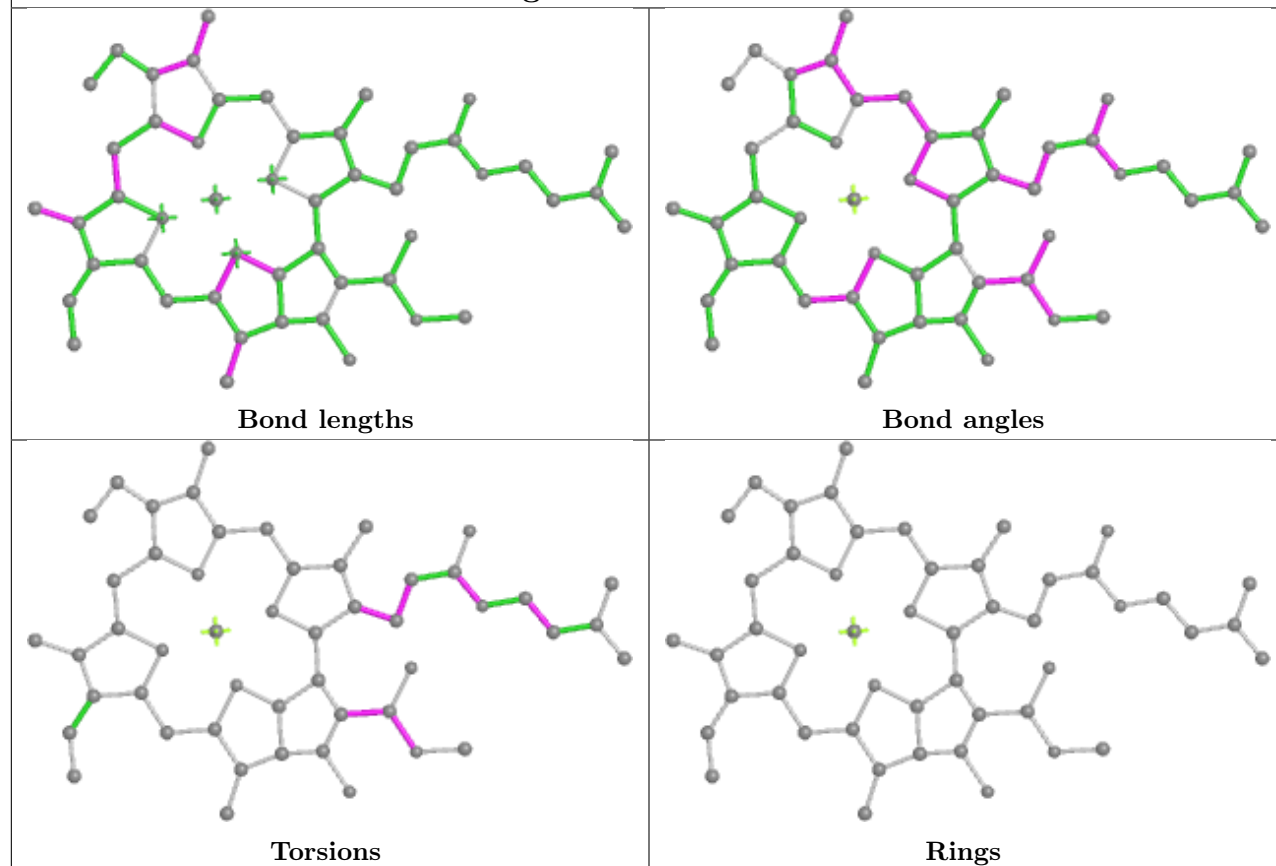
Ligand CLA A1 309



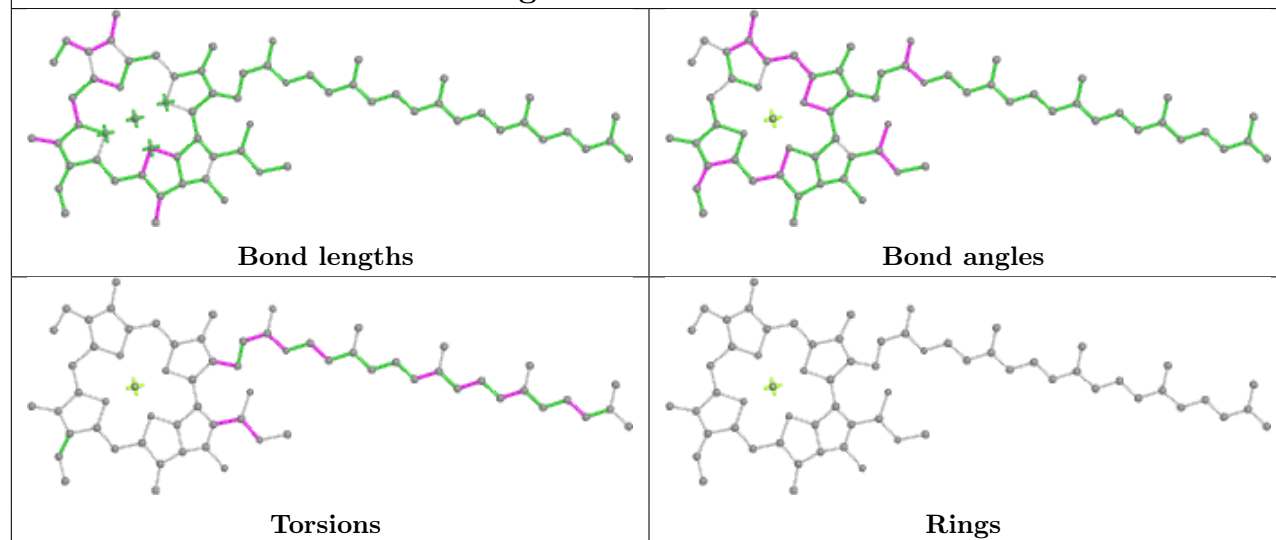
Ligand LUT A1 317

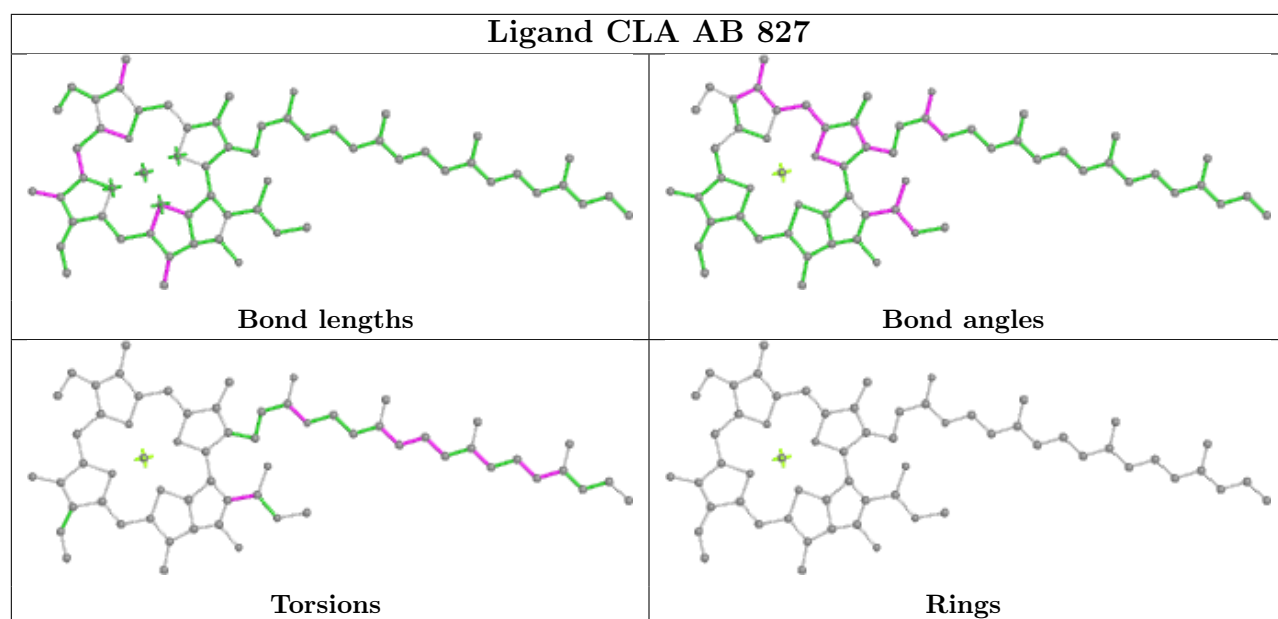


Ligand CLA A4 313

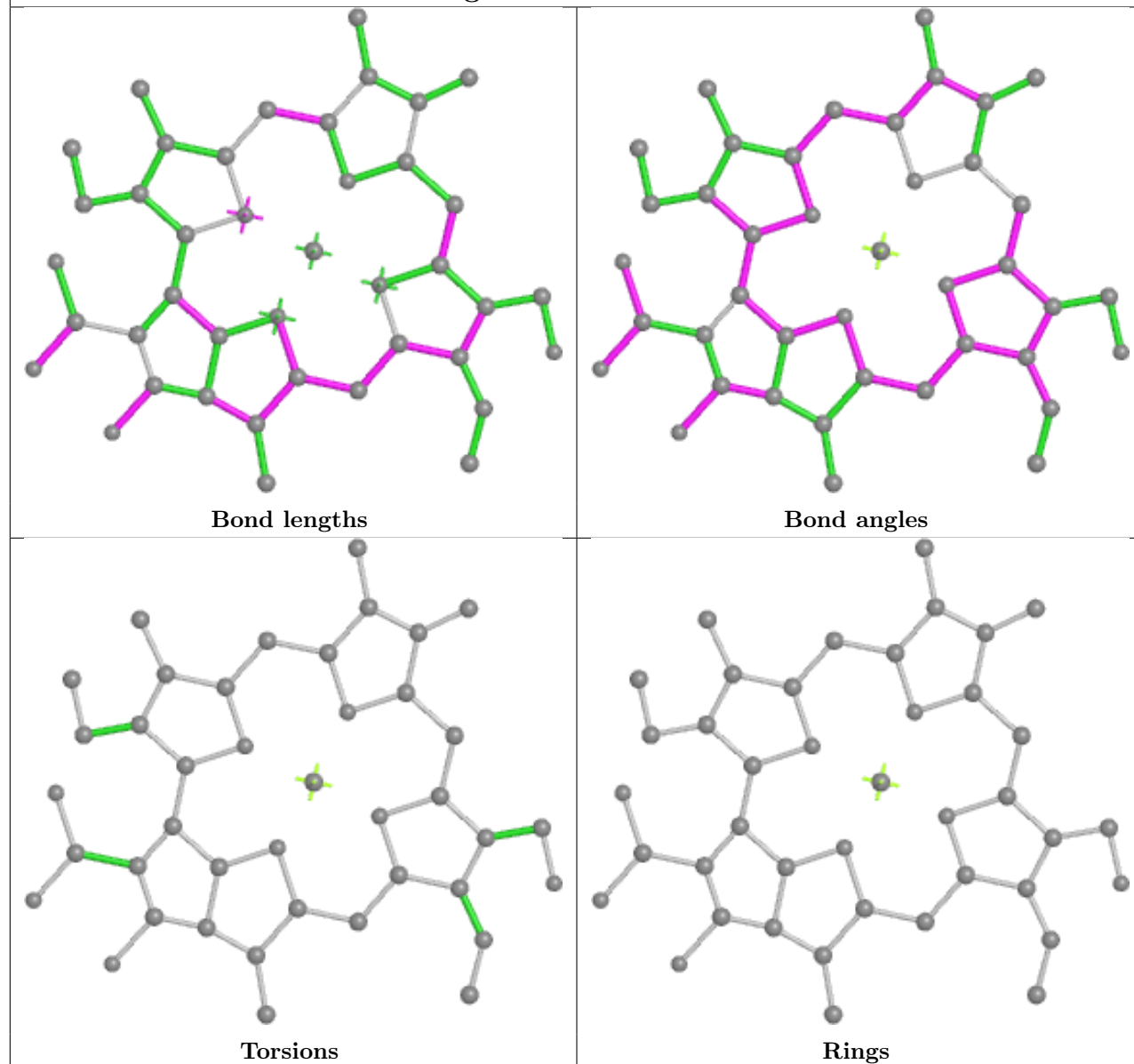


Ligand CLA AB 834

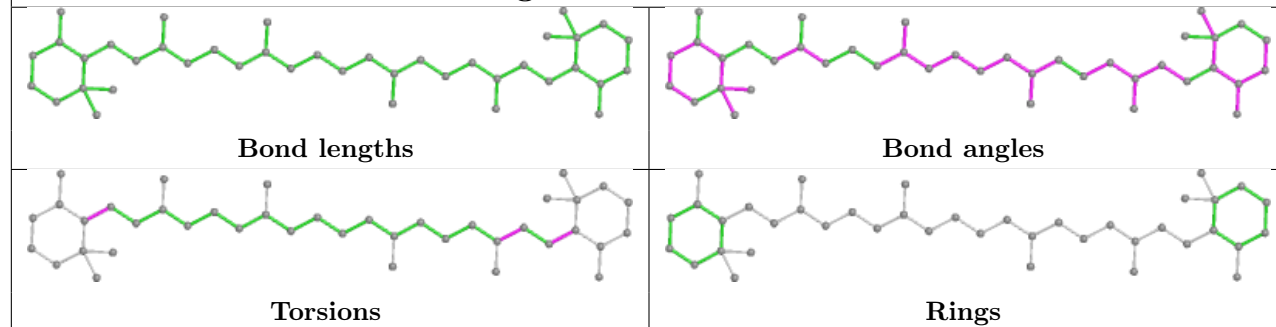


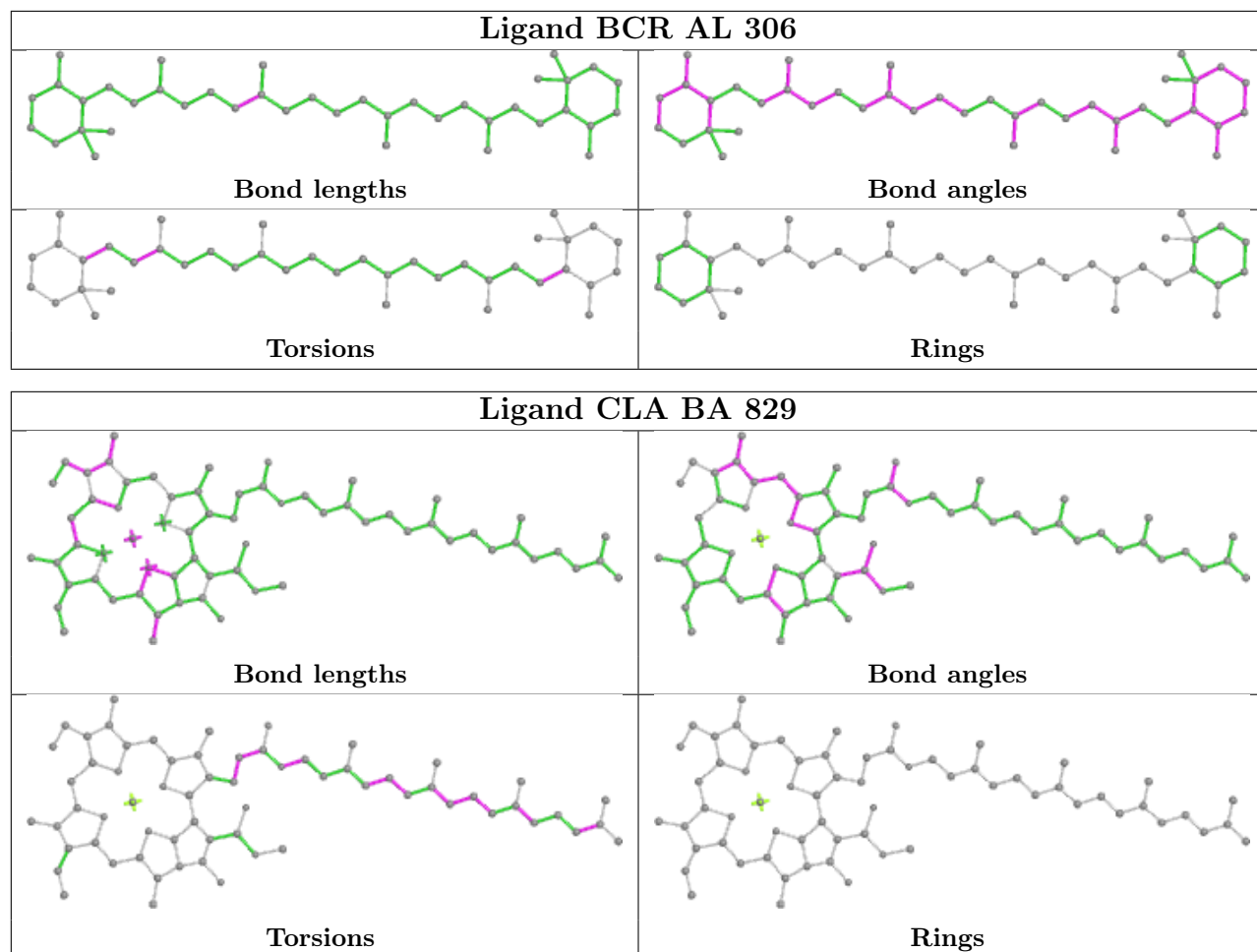


Ligand CHL A4 314

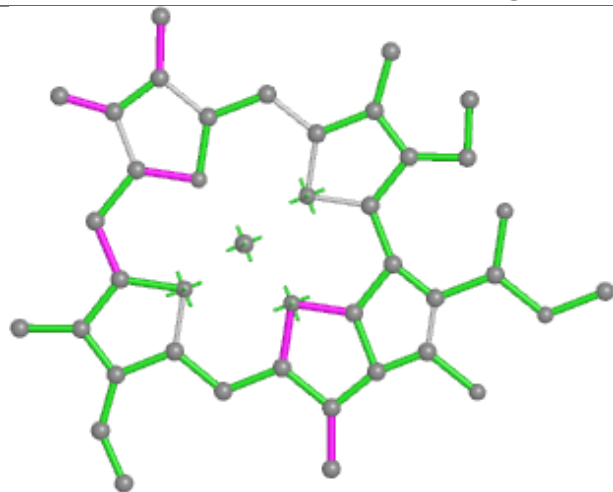


Ligand BCR AA 846

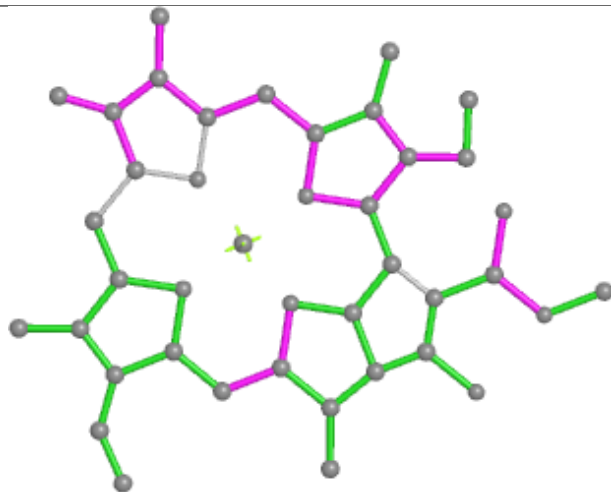




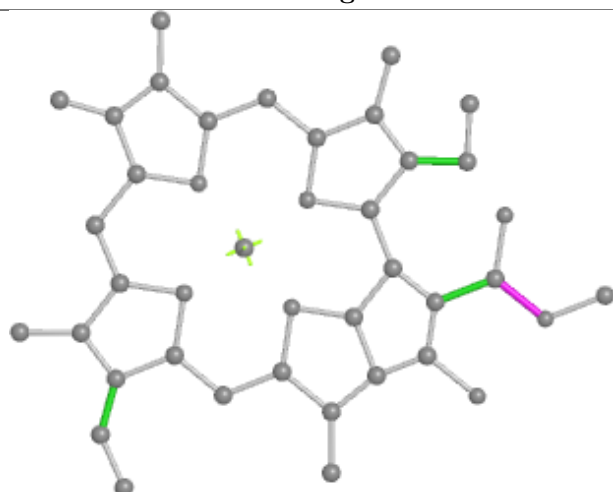
Ligand CLA B3 305



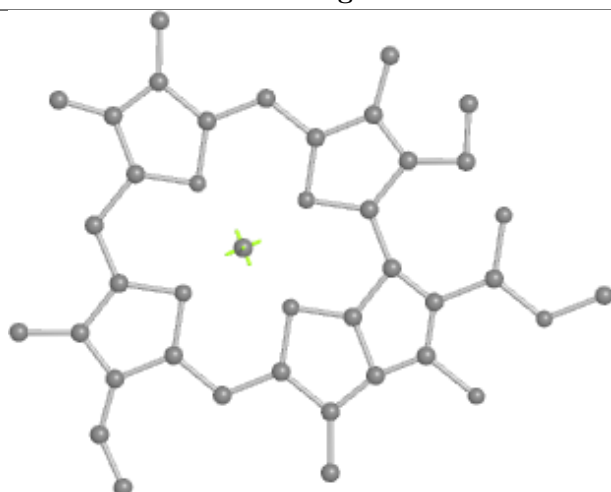
Bond lengths



Bond angles

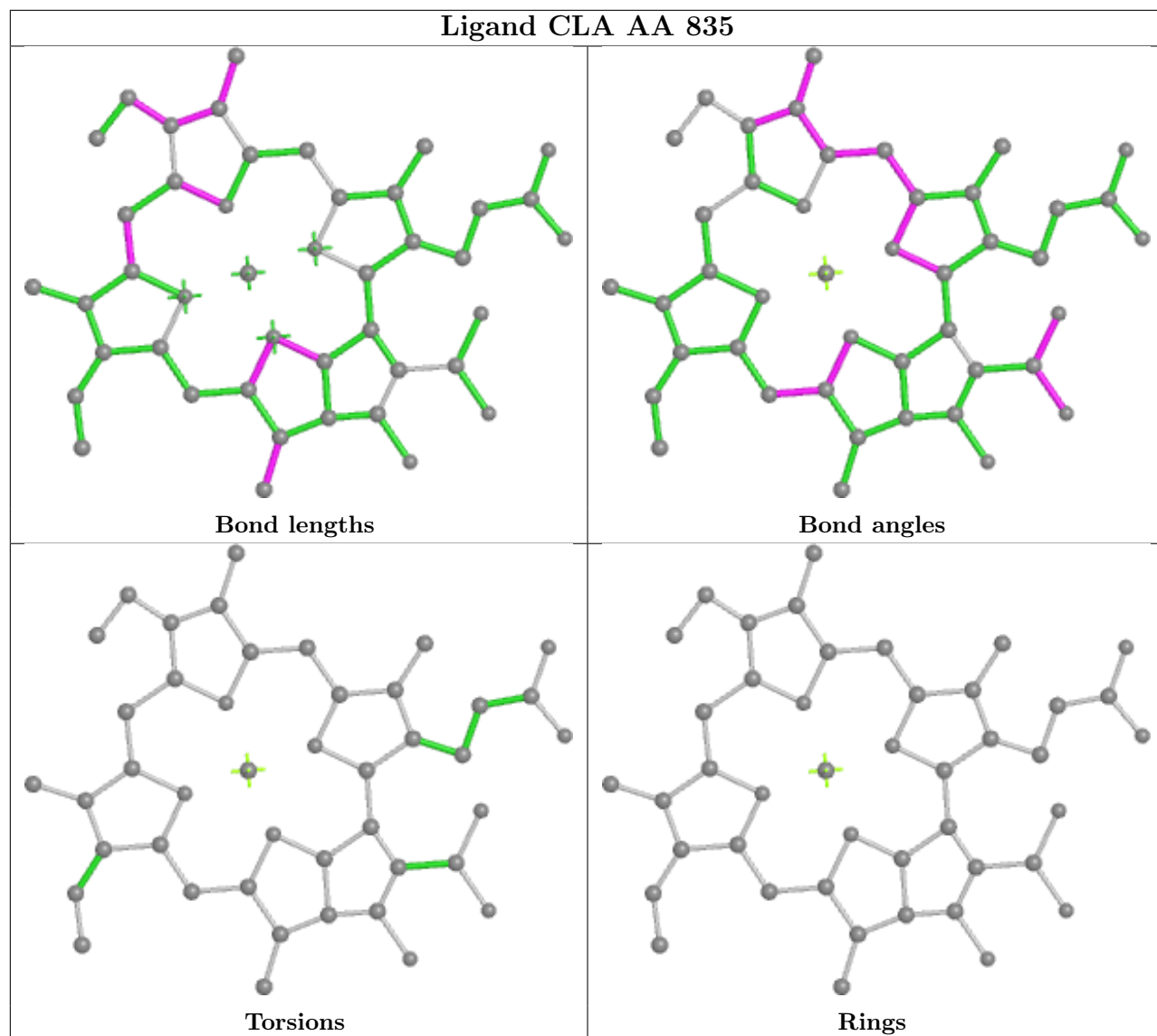


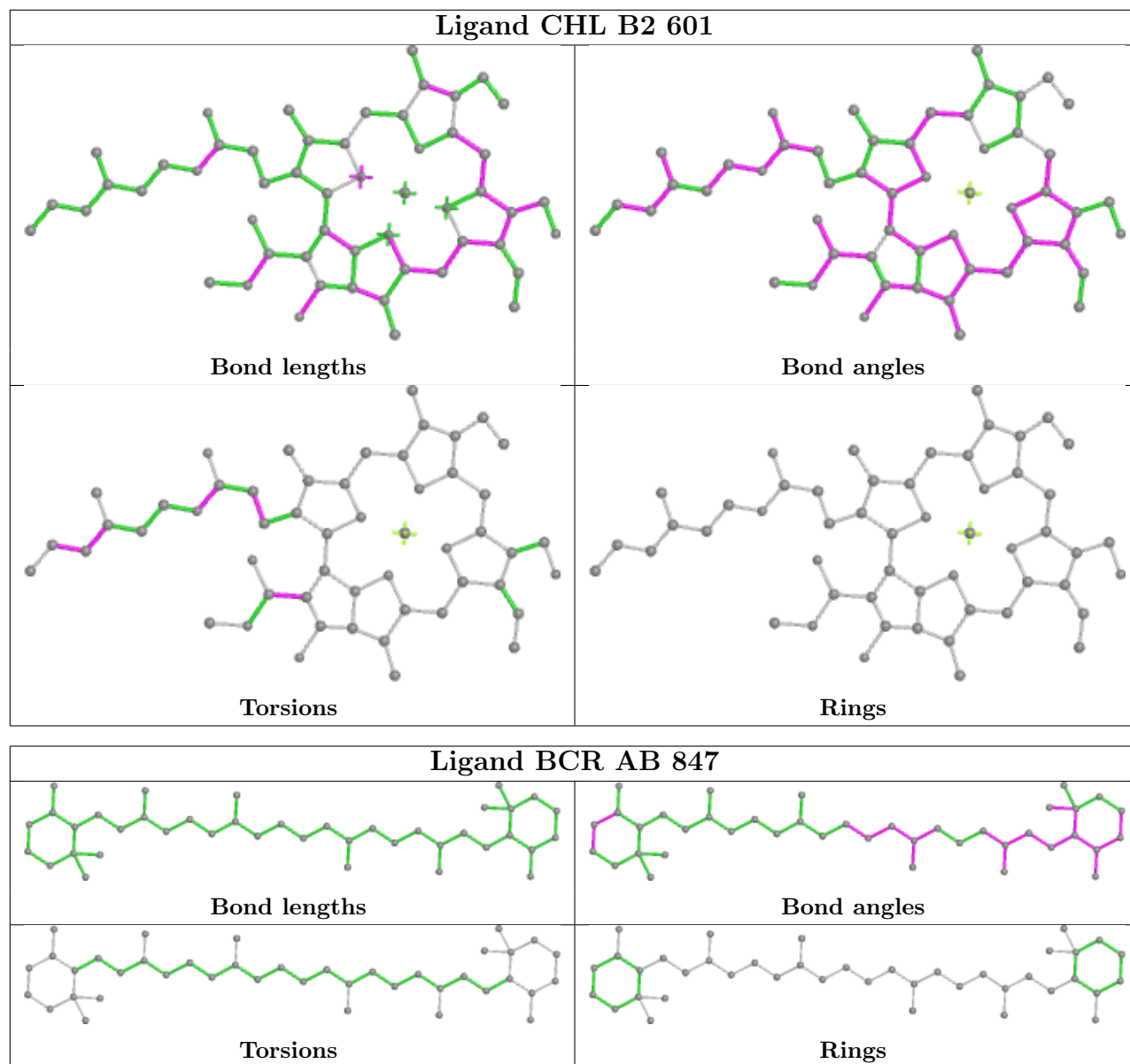
Torsions

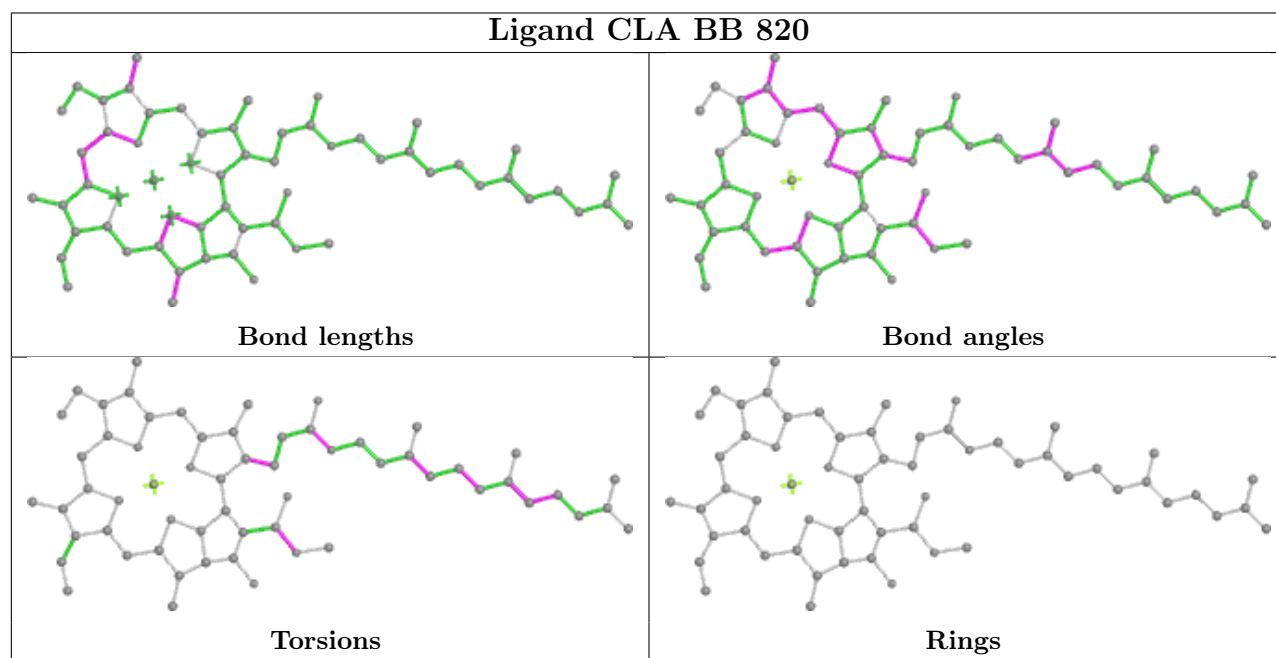
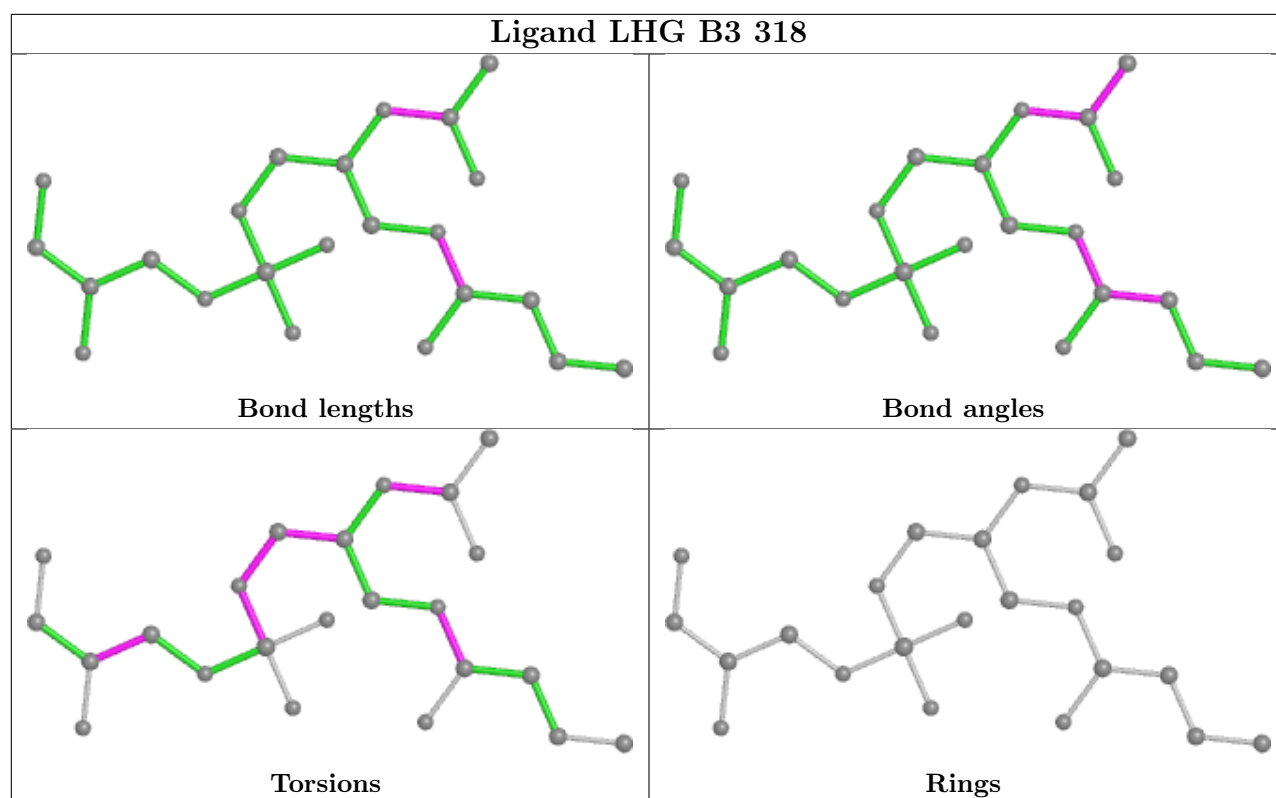


Rings

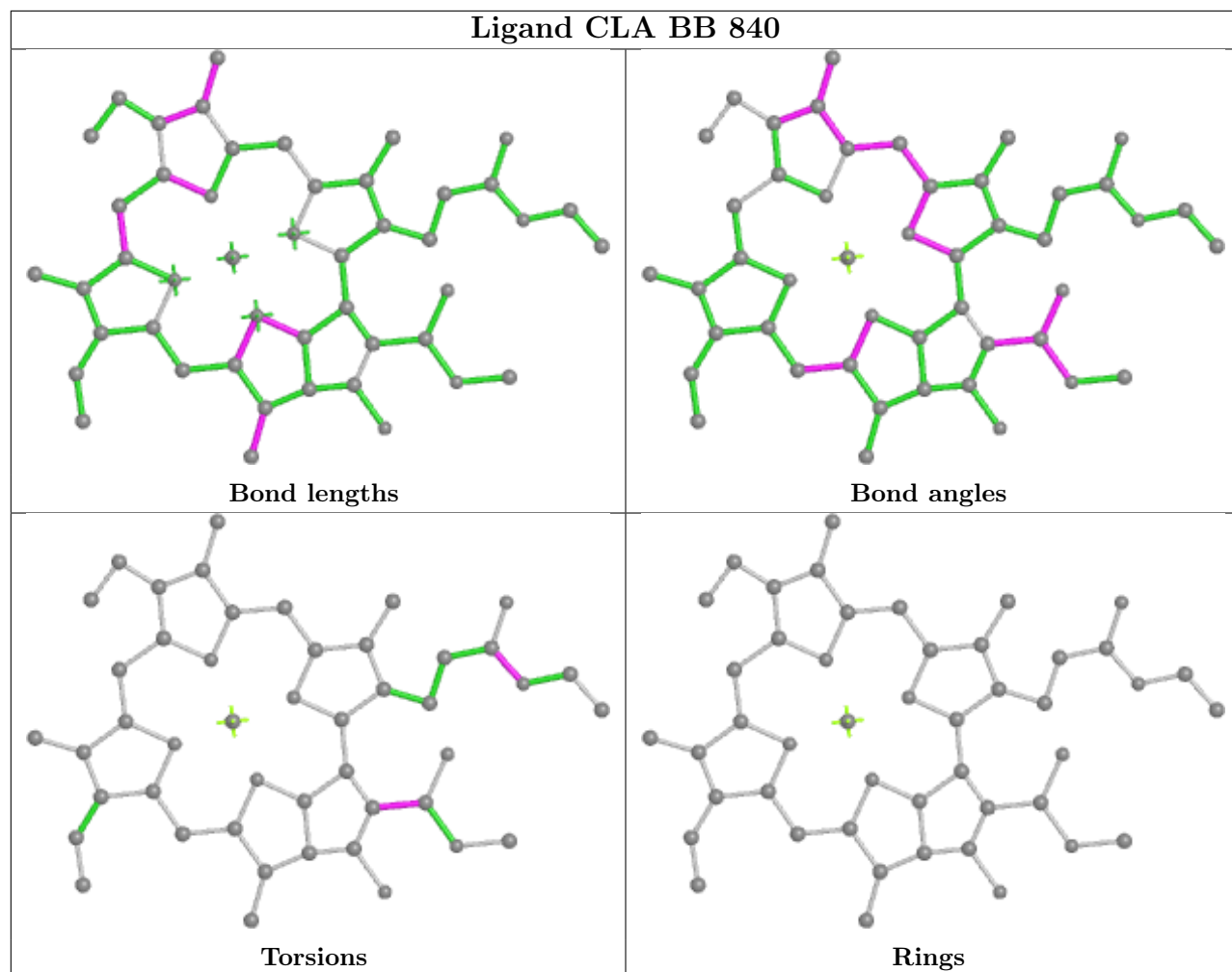
Ligand CLA AA 835



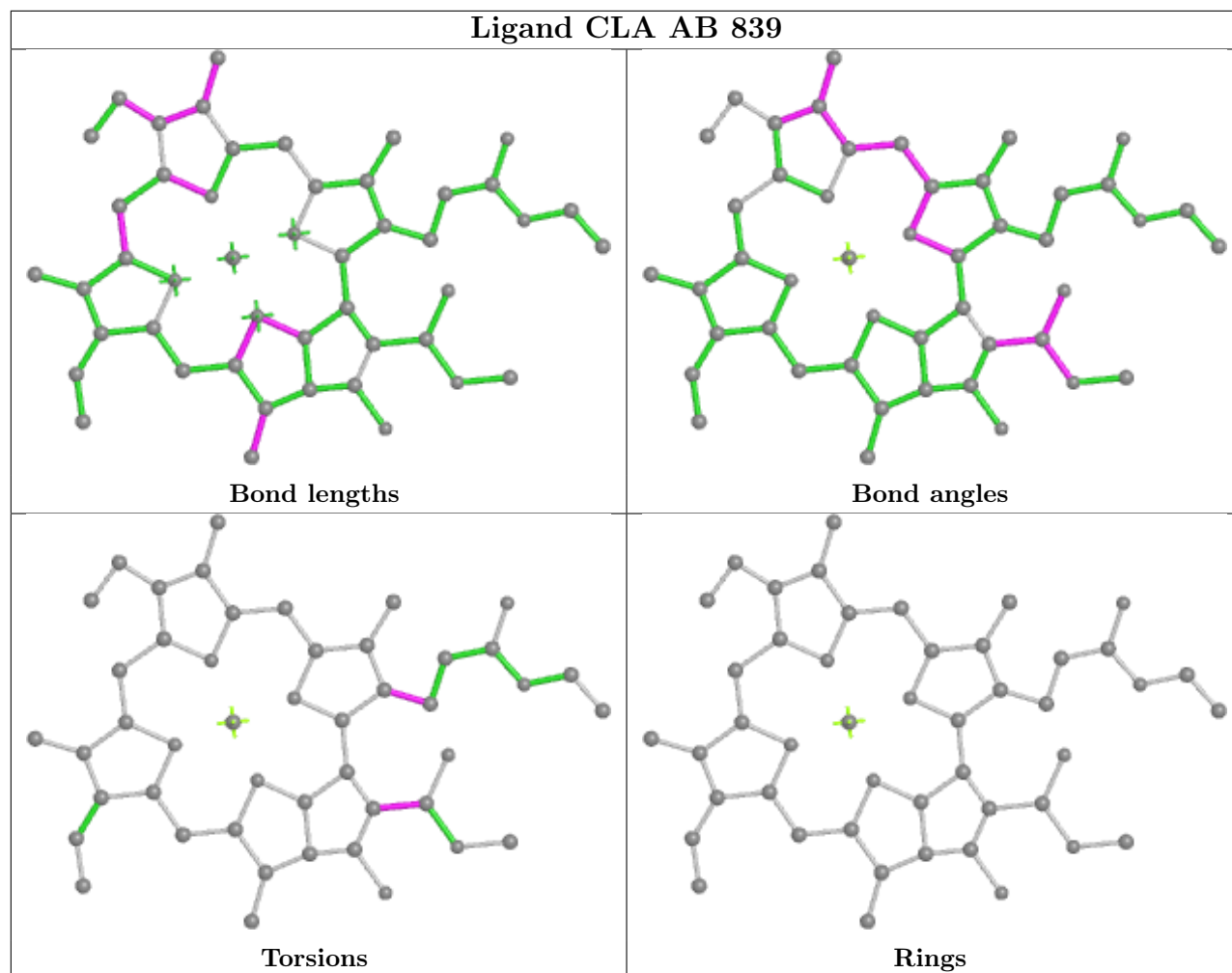


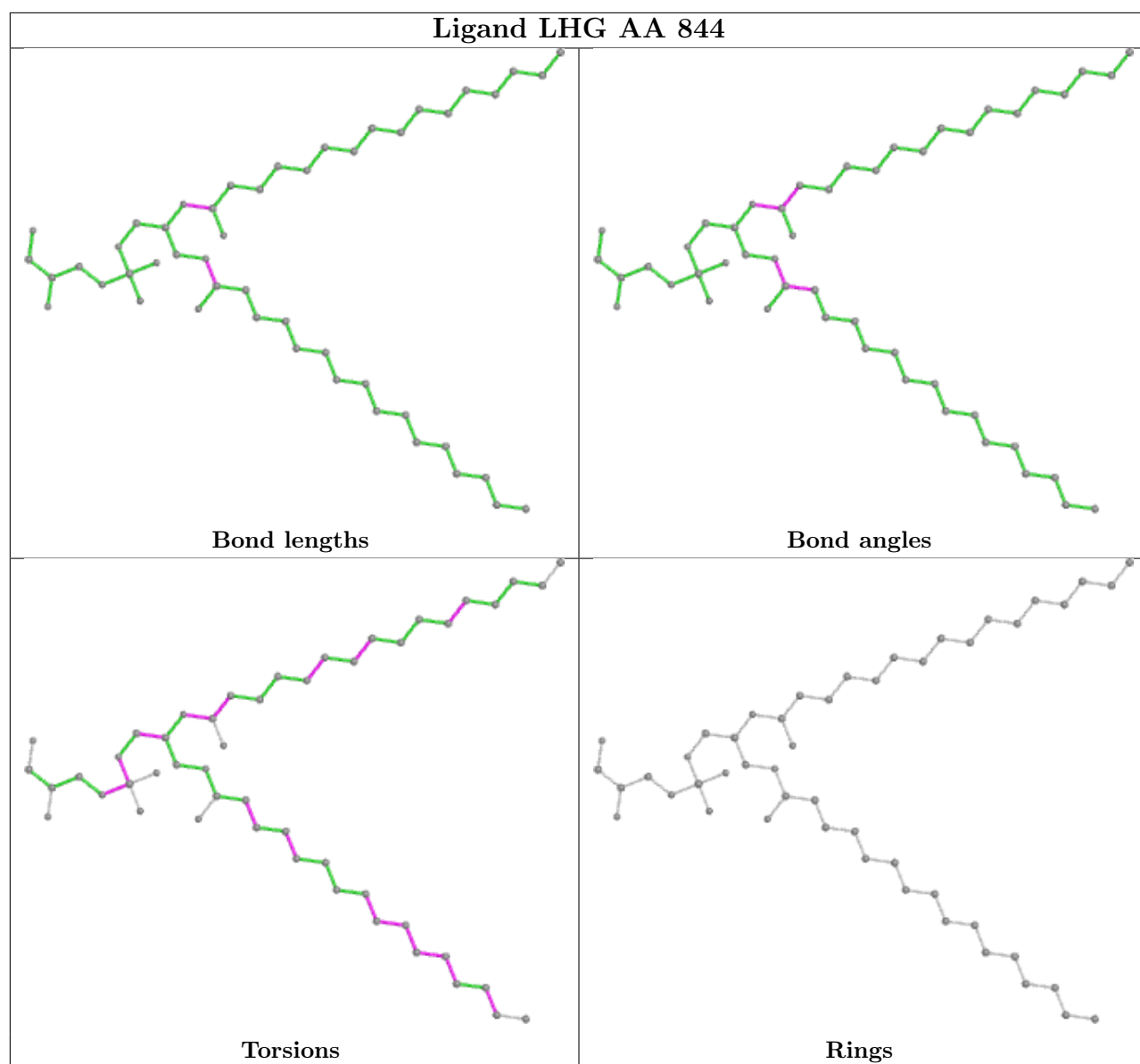


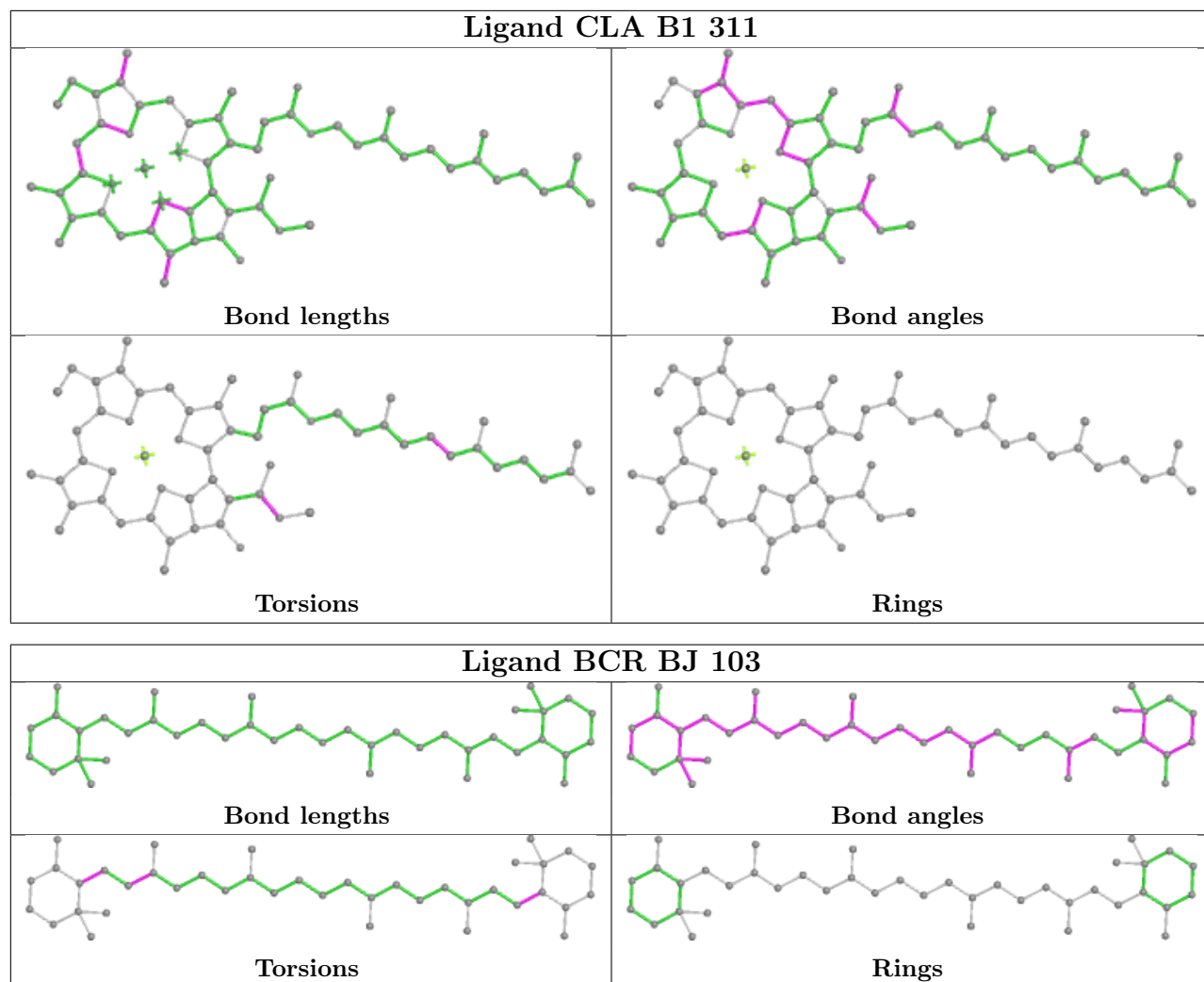
Ligand CLA BB 840



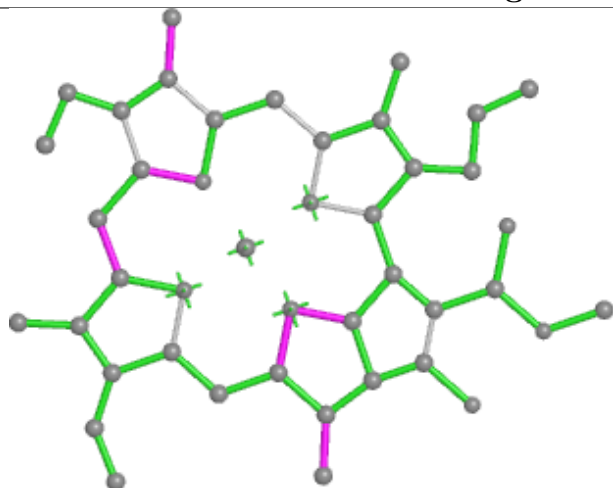
Ligand CLA AB 839



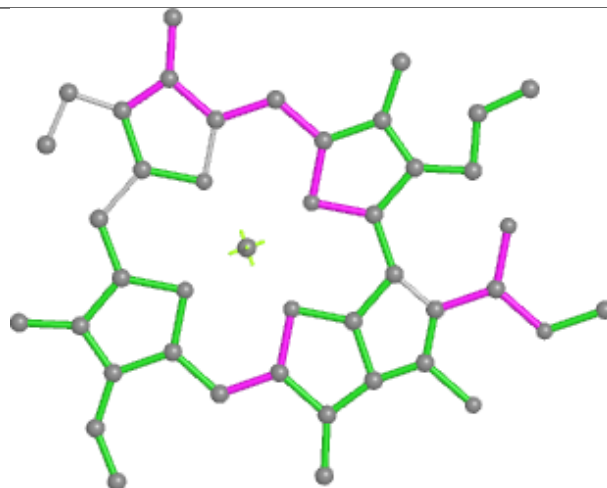




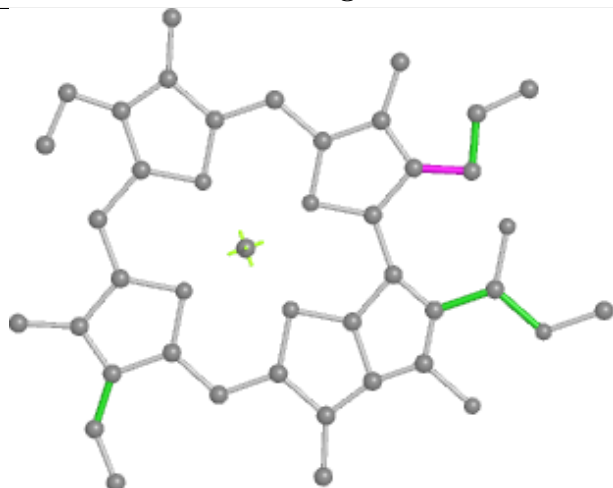
Ligand CLA B2 613



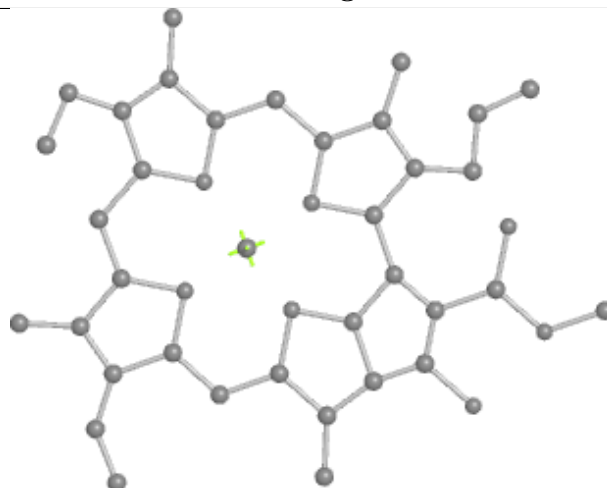
Bond lengths



Bond angles

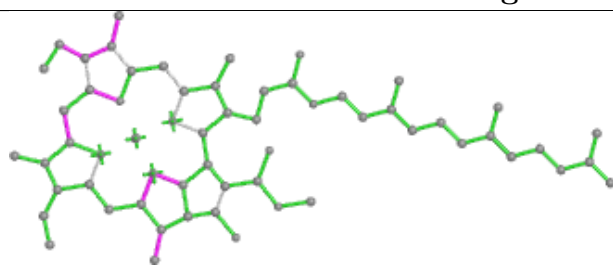


Torsions

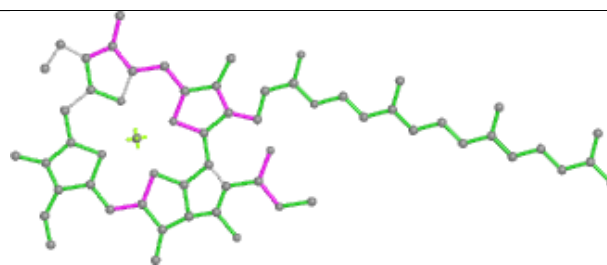


Rings

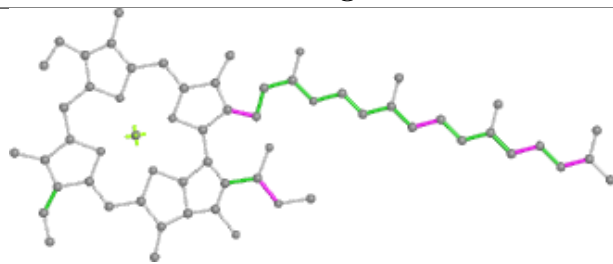
Ligand CLA AB 835



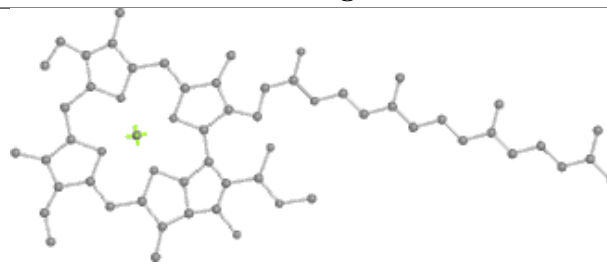
Bond lengths



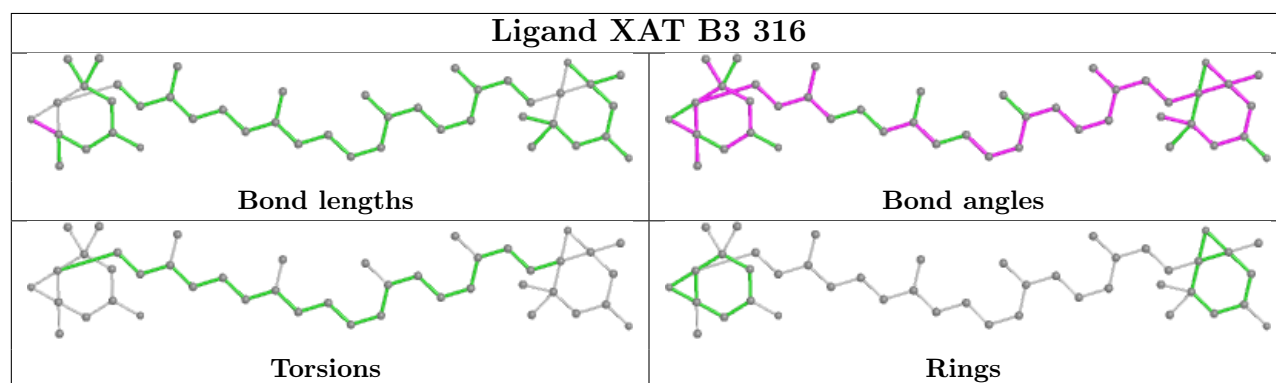
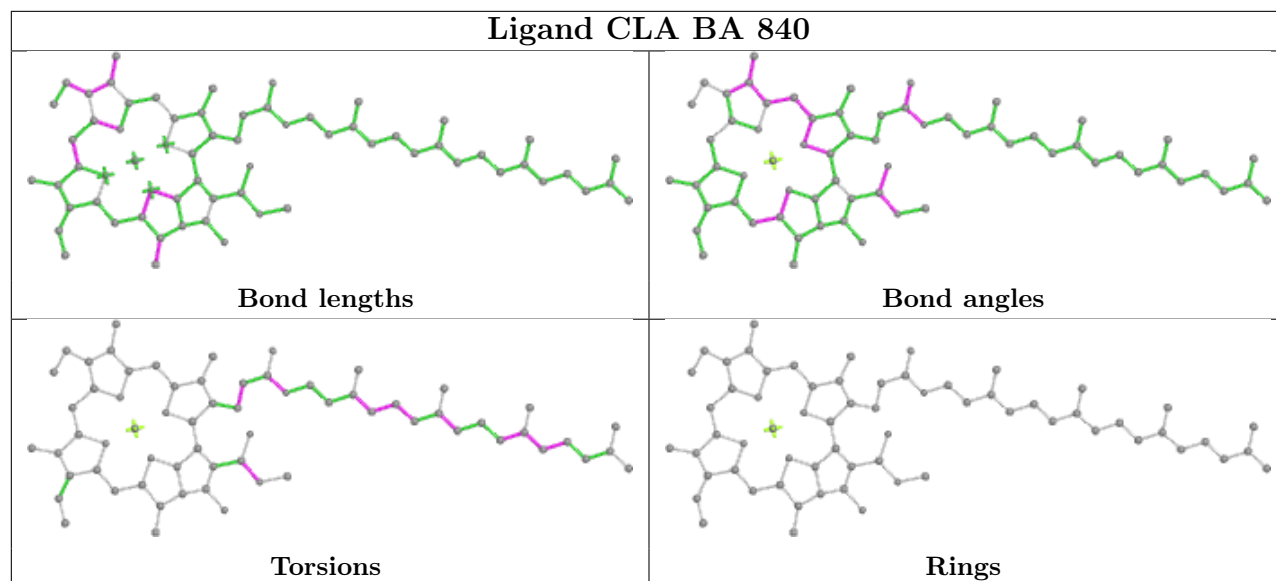
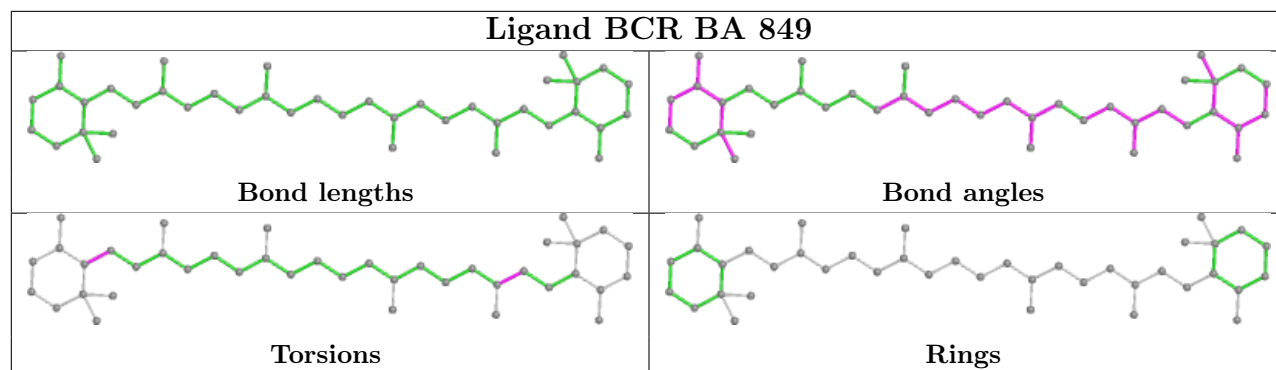
Bond angles



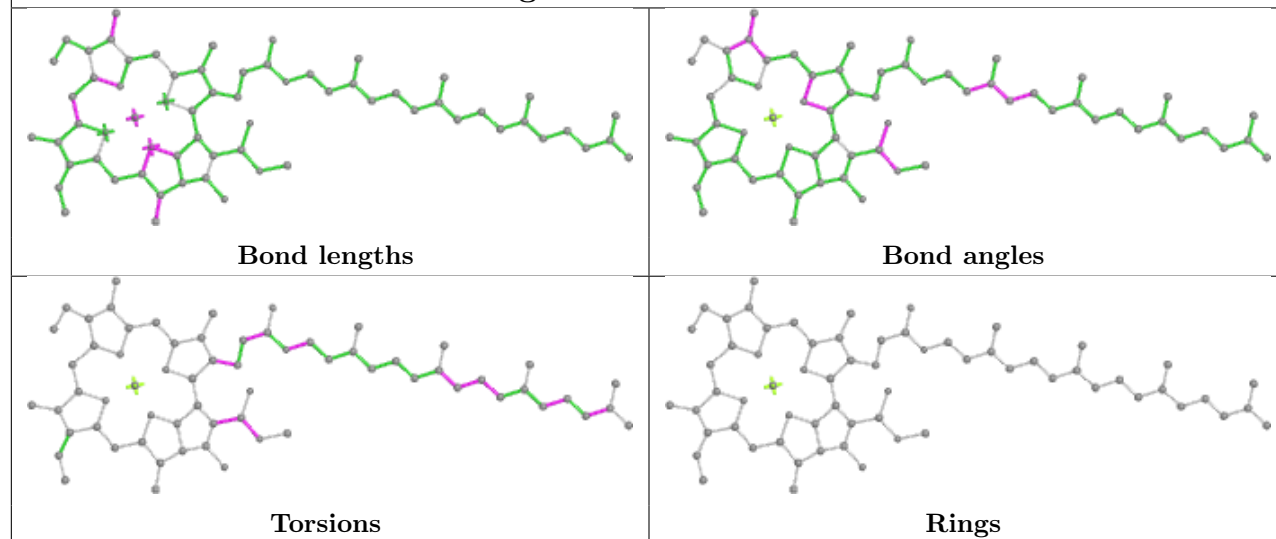
Torsions



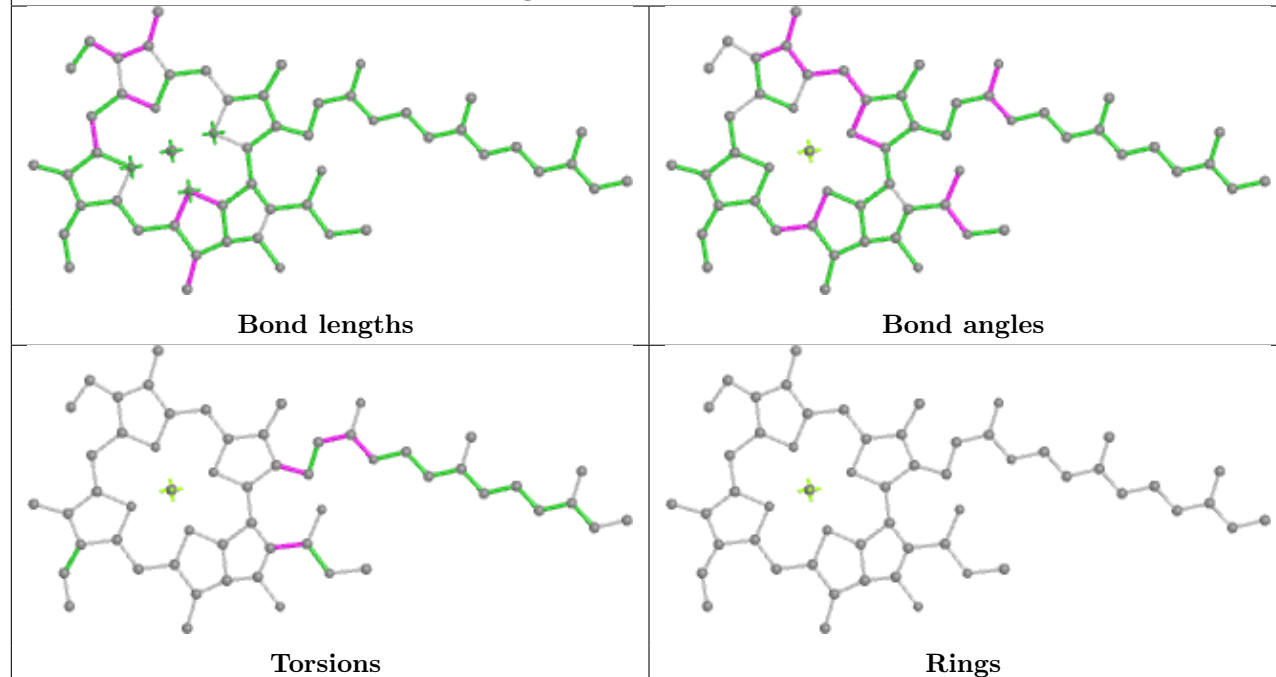
Rings



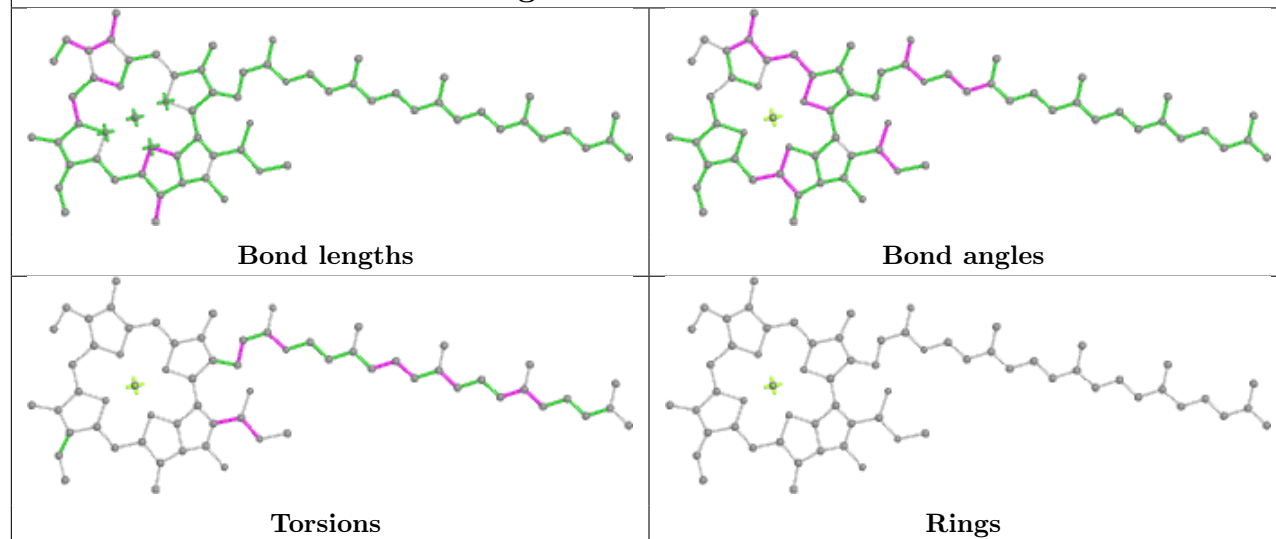
Ligand CLA BA 825



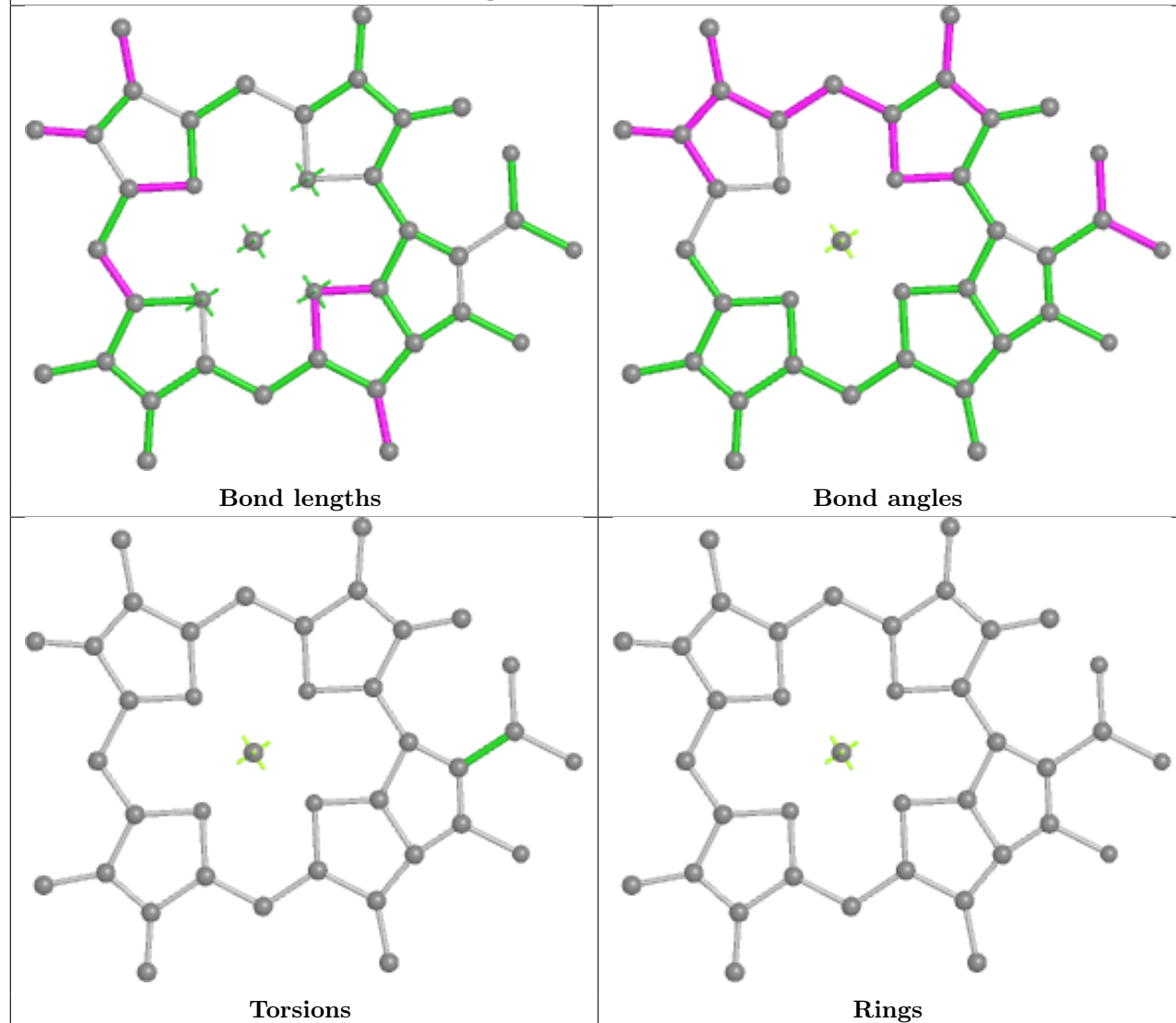
Ligand CLA BA 818

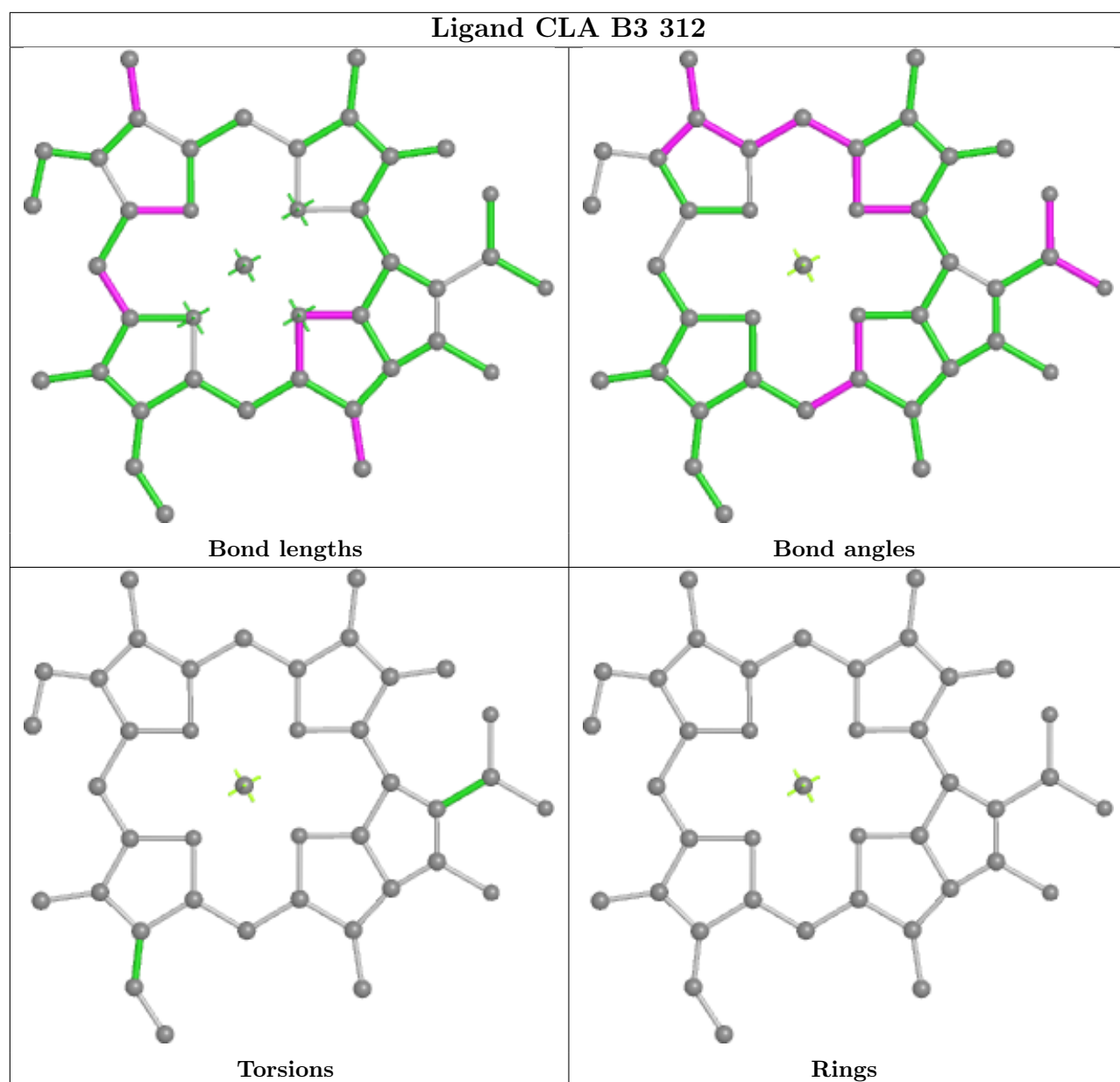


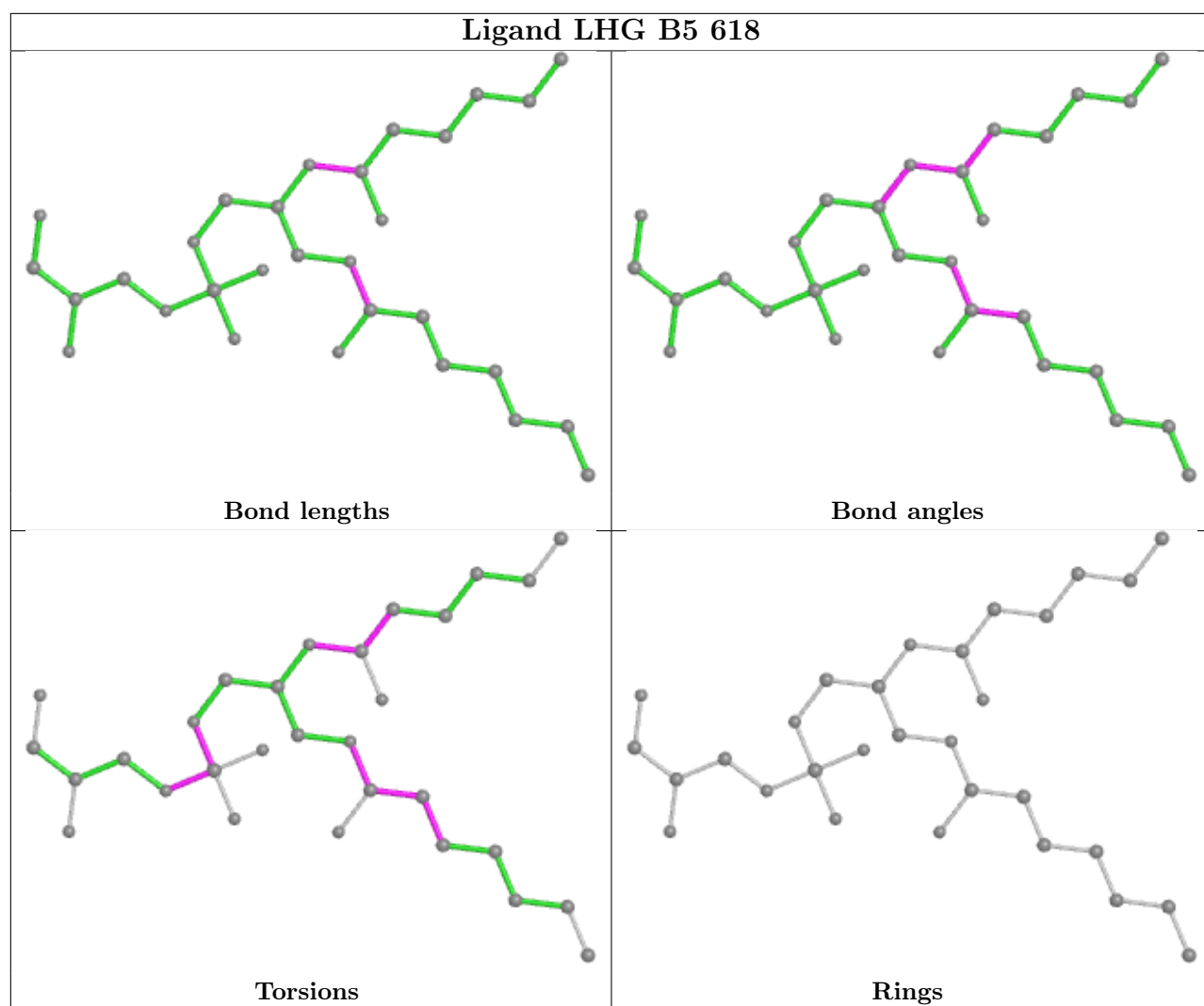
Ligand CLA AA 840



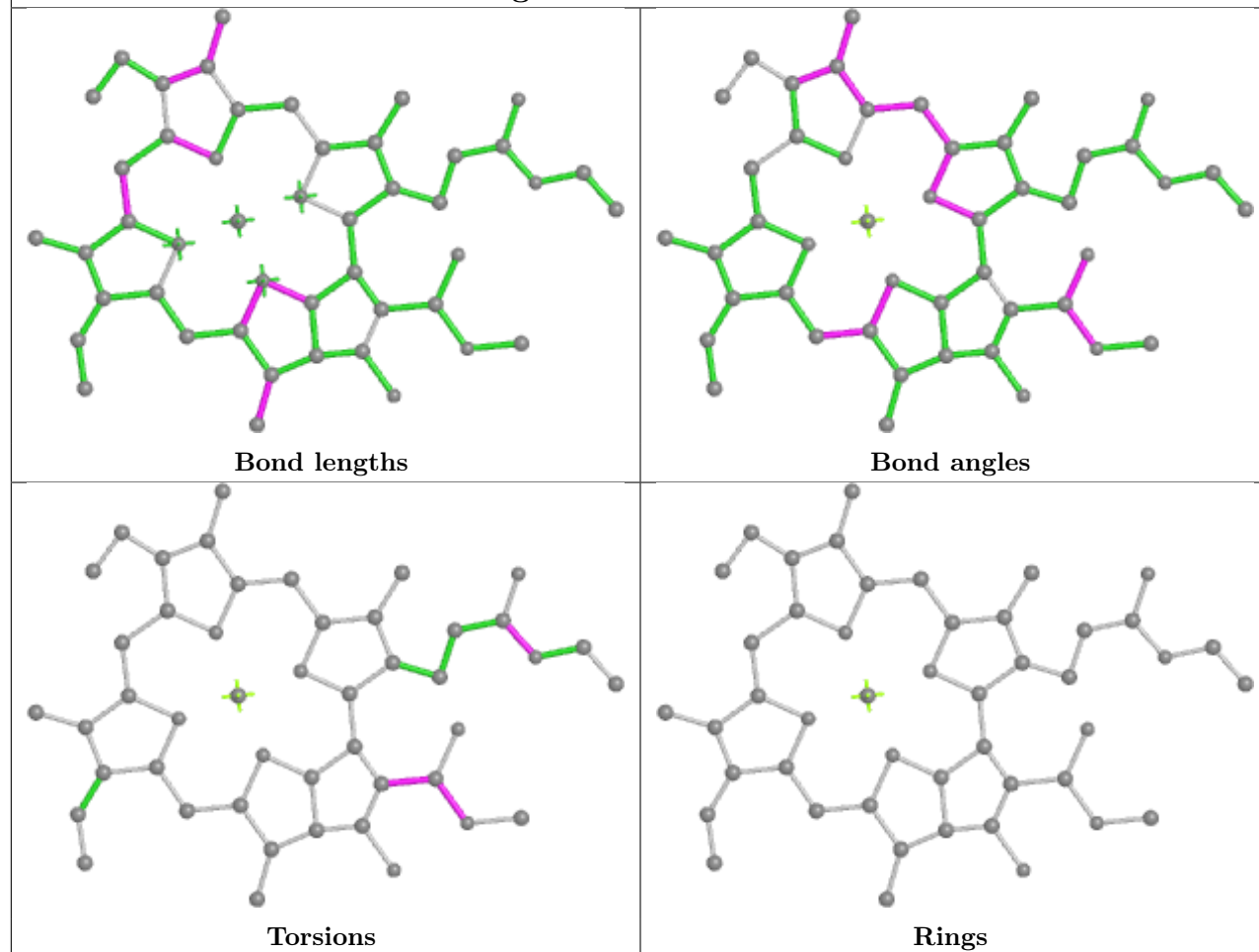
Ligand CLA B1 315



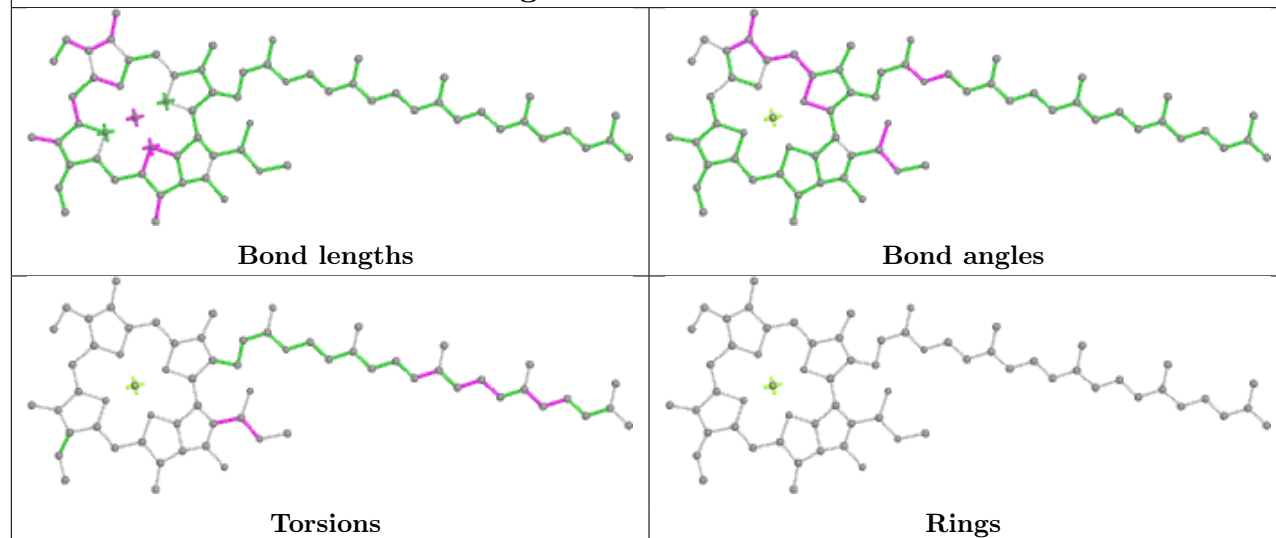




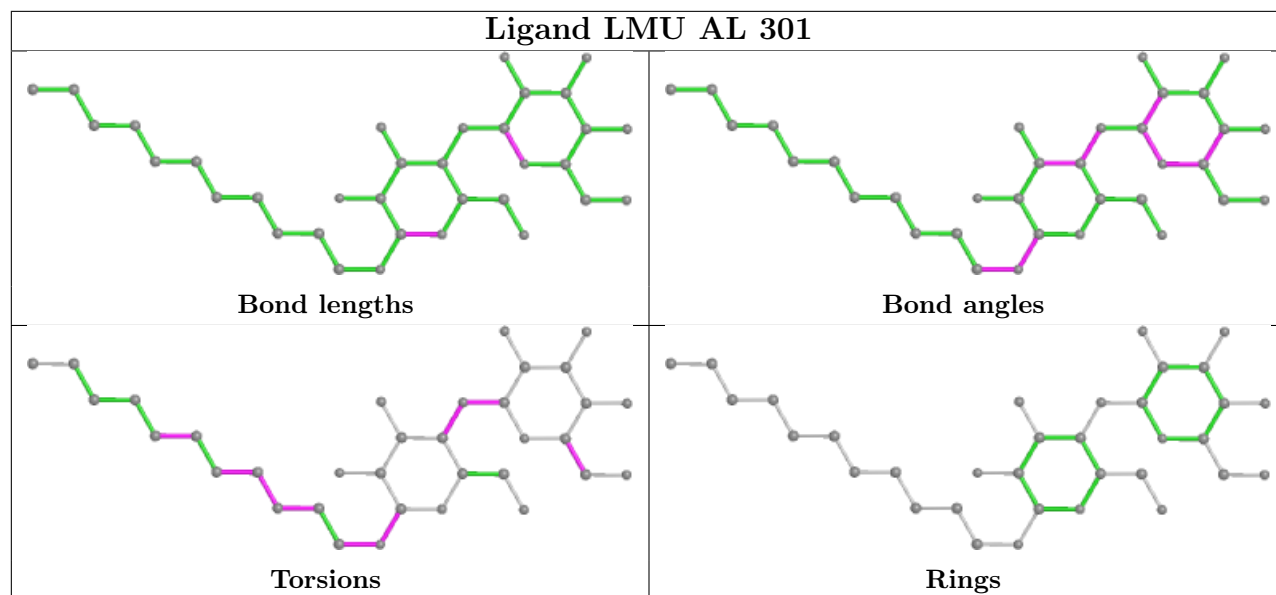
Ligand CLA AB 822



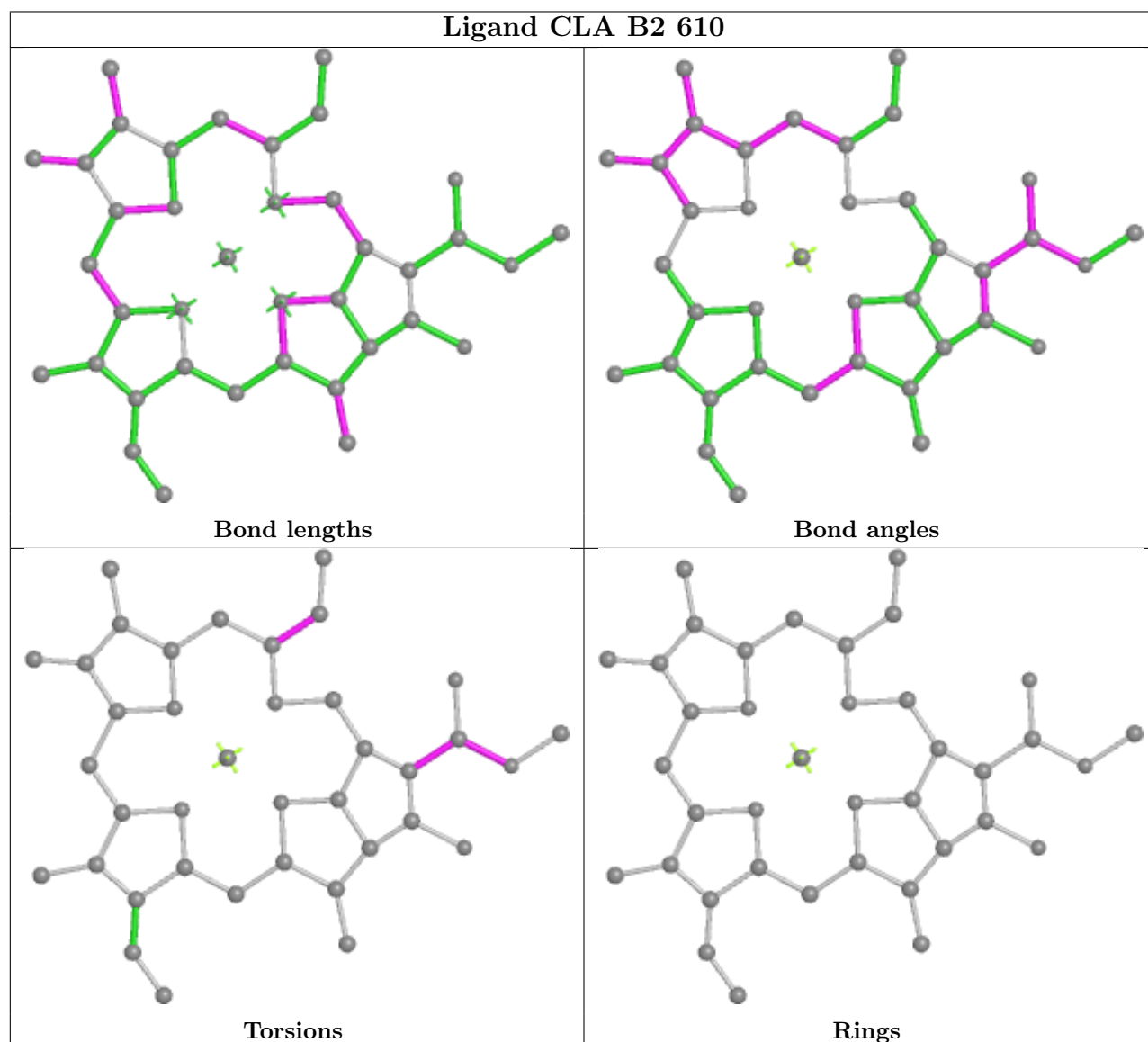
Ligand CLA BB 826

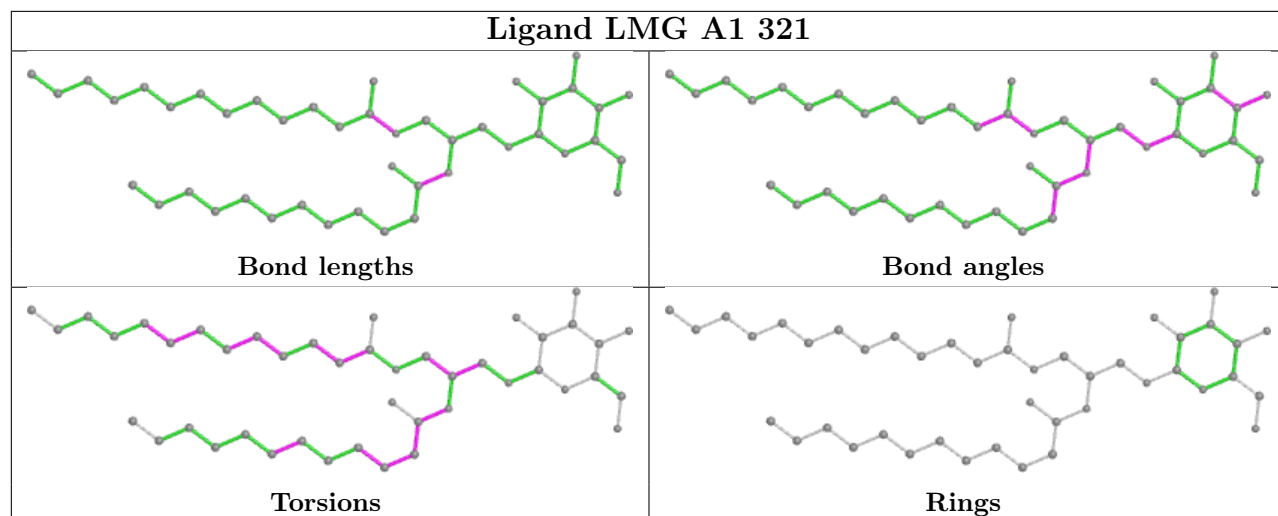


Ligand LMU AL 301

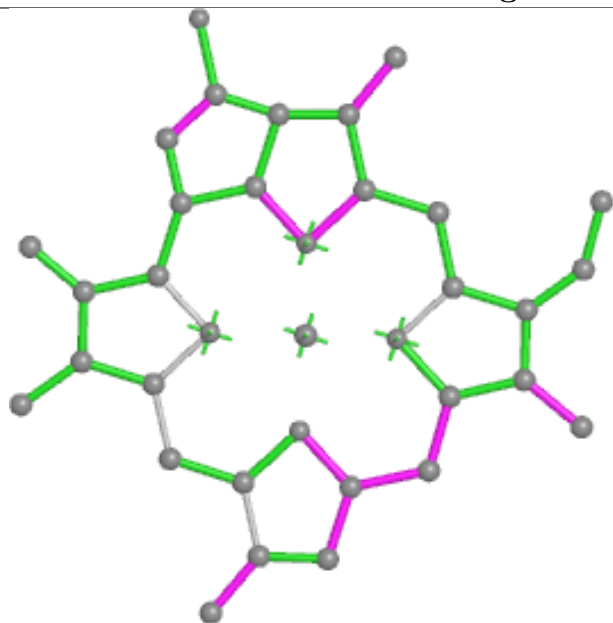


Ligand CLA B2 610

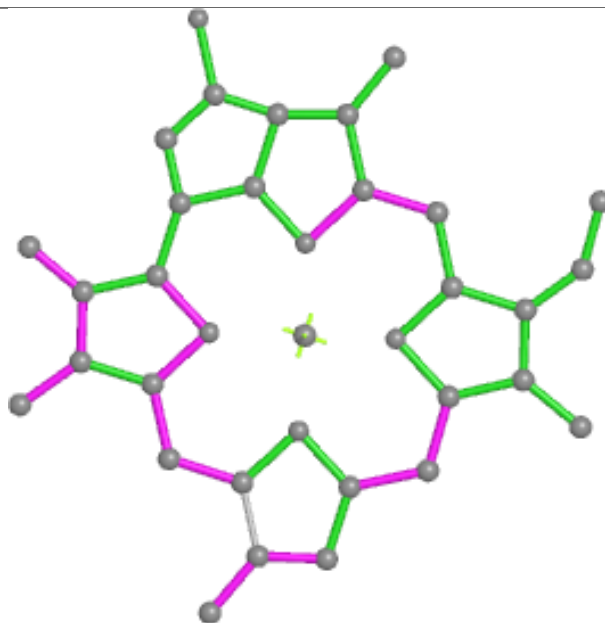




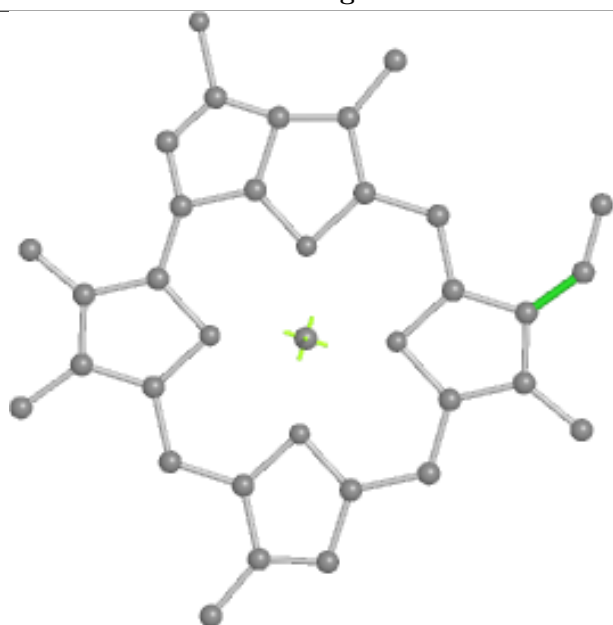
Ligand CLA AK 201



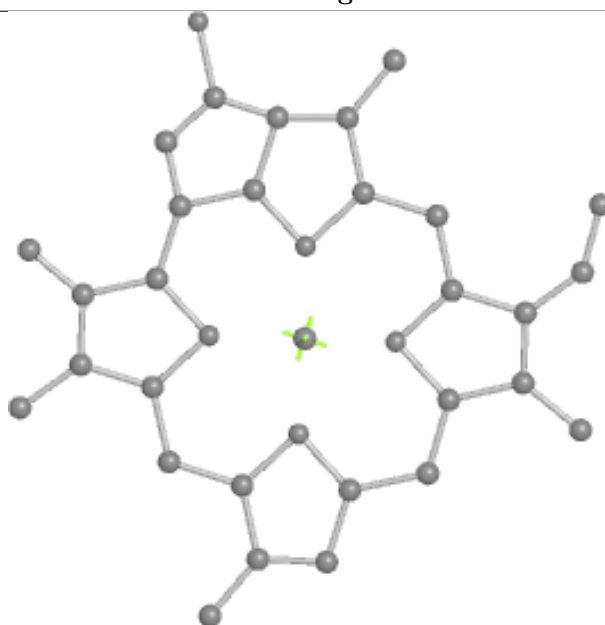
Bond lengths



Bond angles

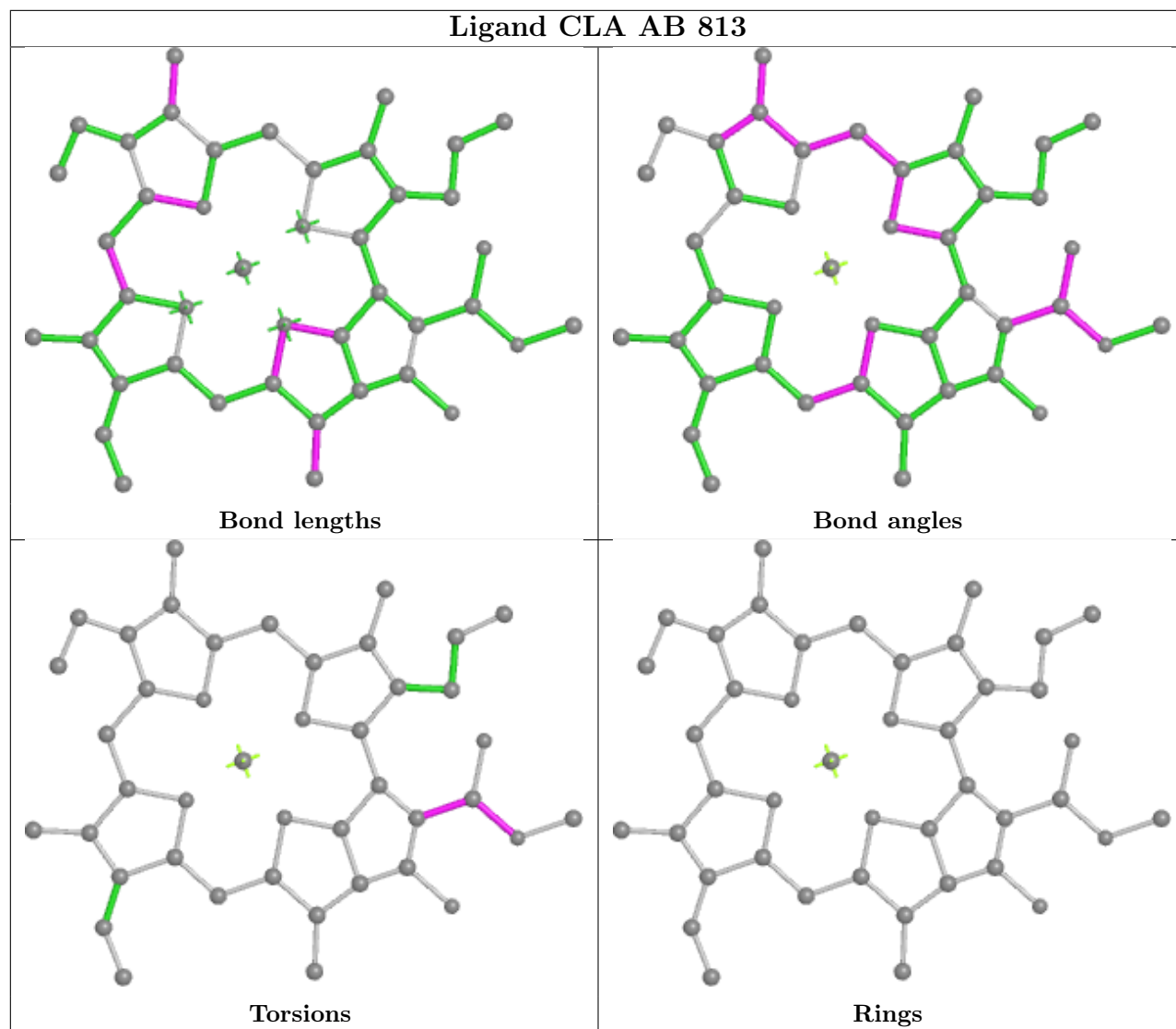


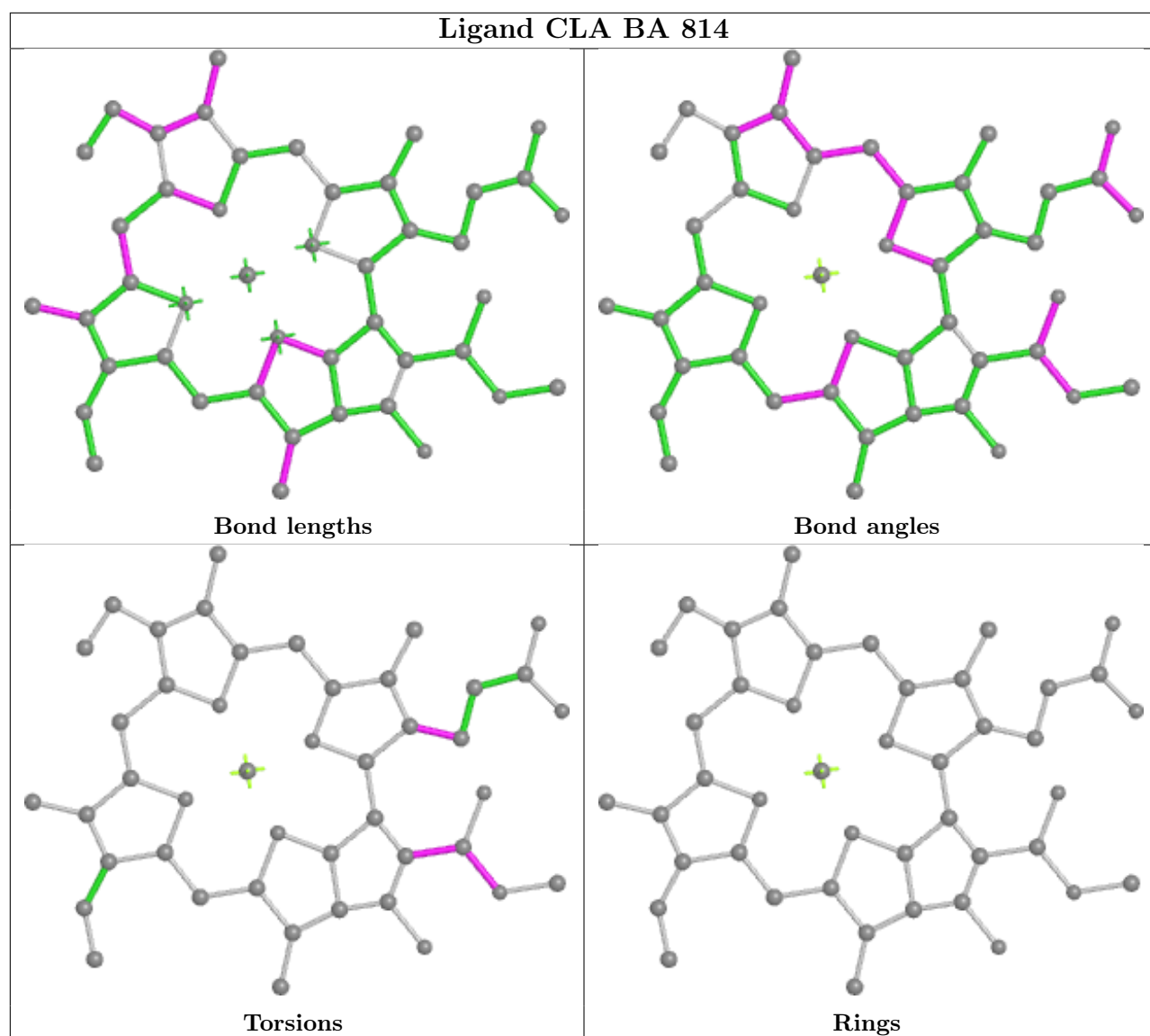
Torsions

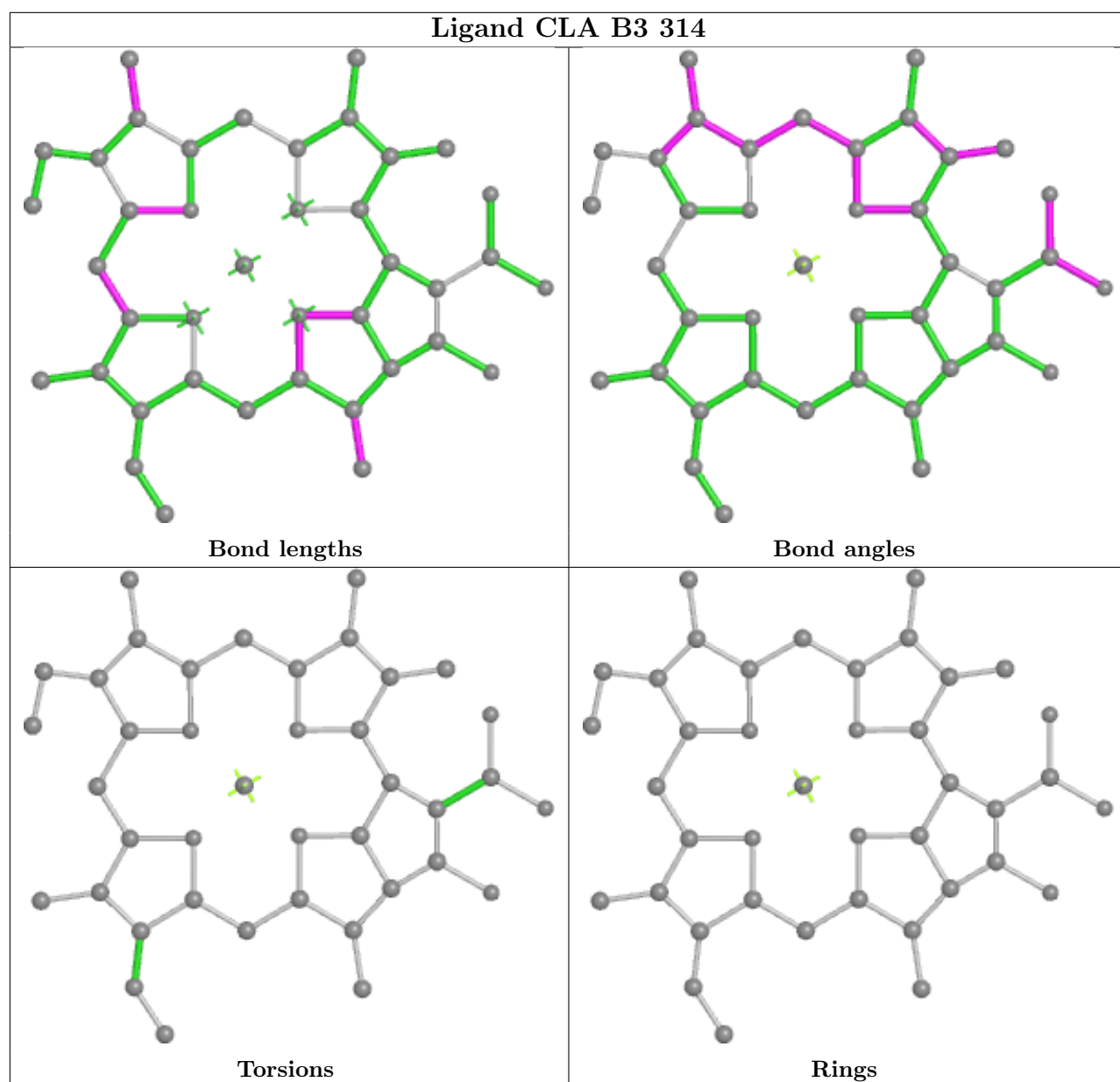


Rings

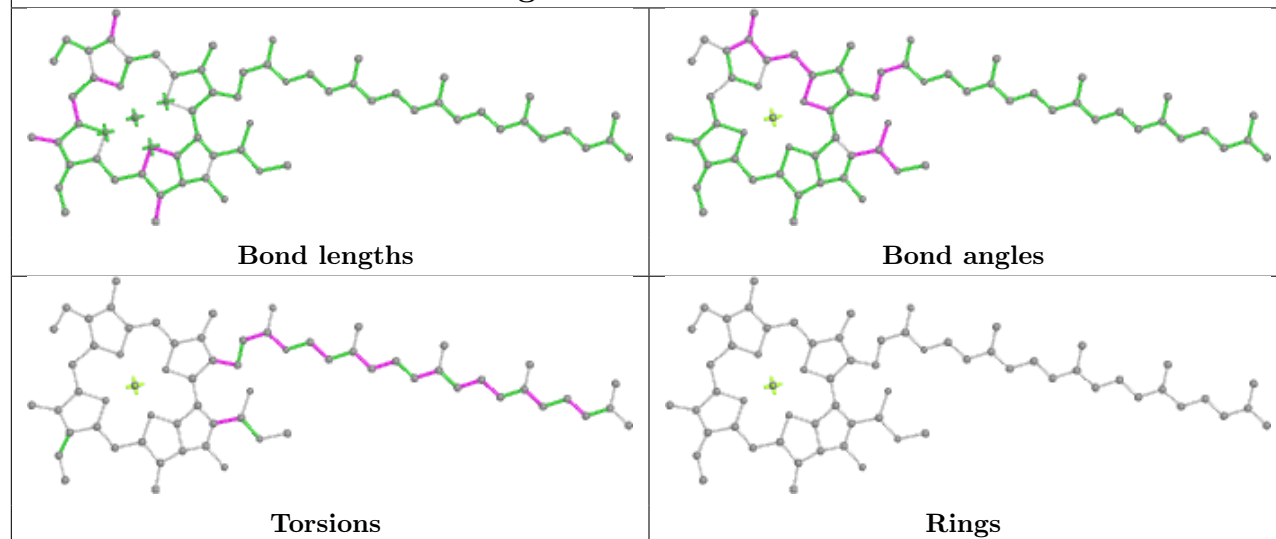
Ligand CLA AB 813



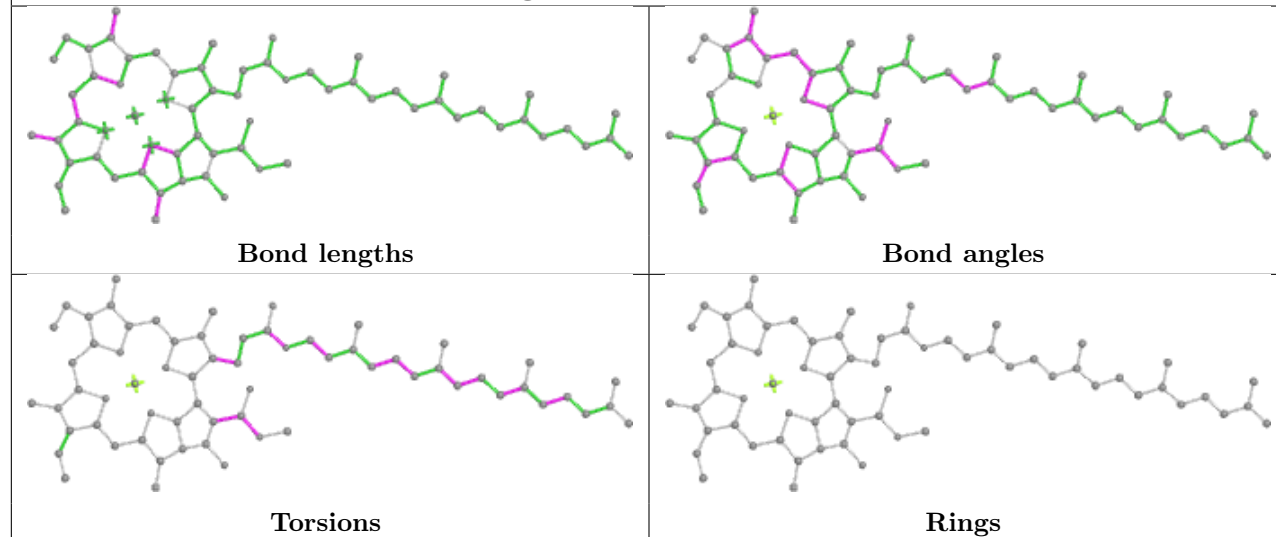




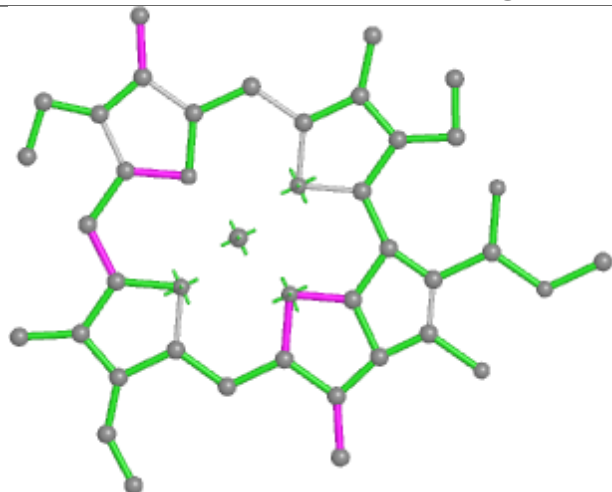
Ligand CLA AA 827



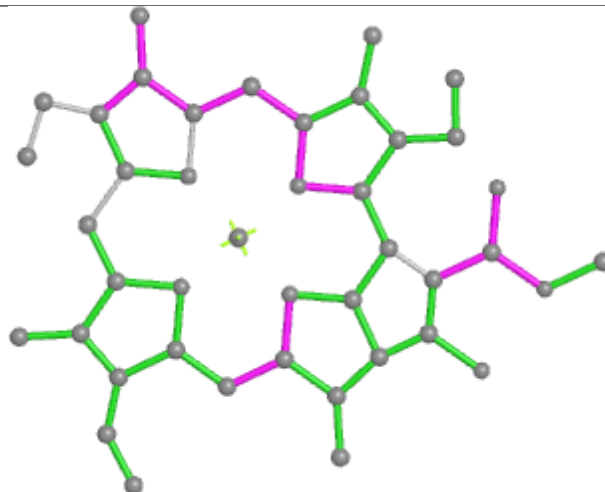
Ligand CLA BA 803



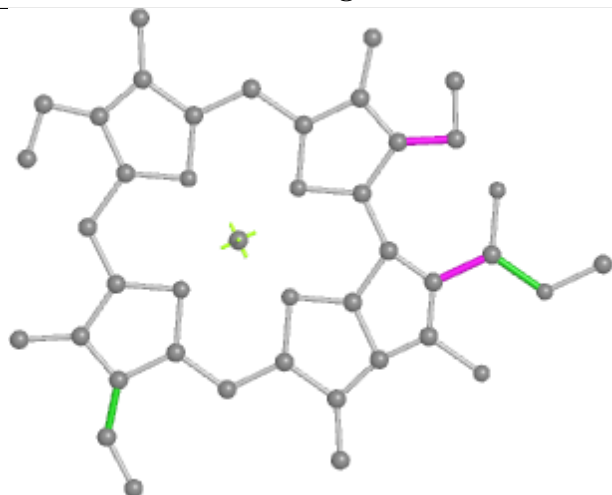
Ligand CLA AA 822



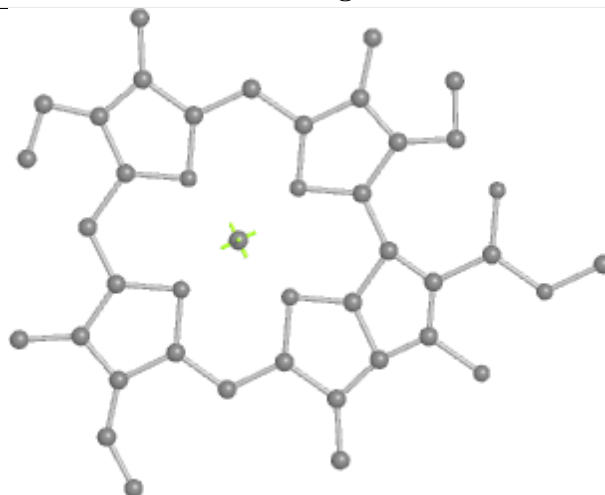
Bond lengths



Bond angles

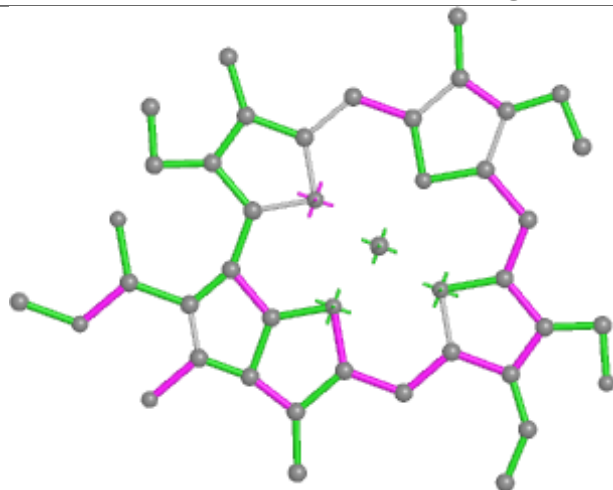


Torsions

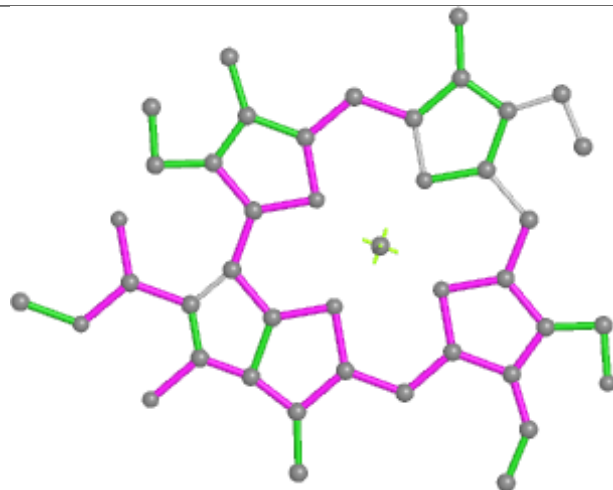


Rings

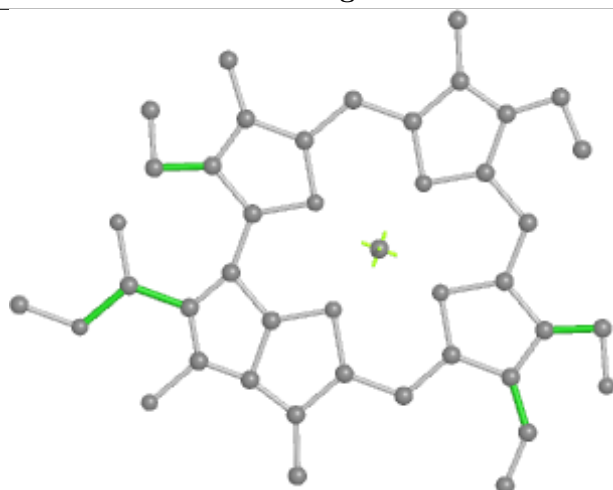
Ligand CHL B2 614



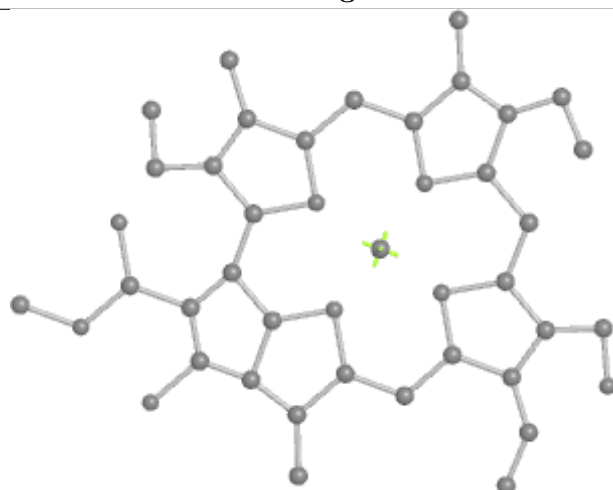
Bond lengths



Bond angles

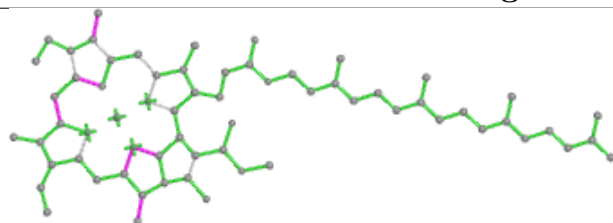


Torsions

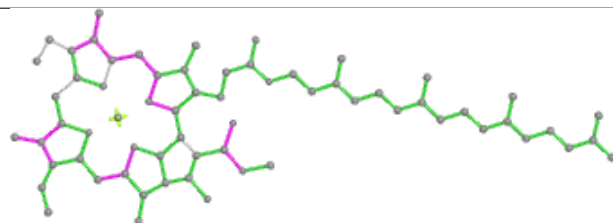


Rings

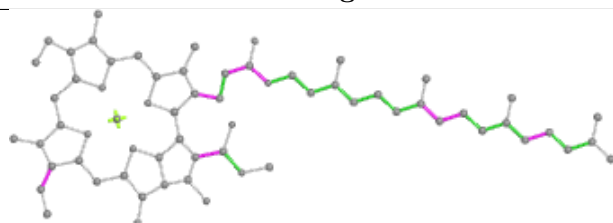
Ligand CLA AB 806



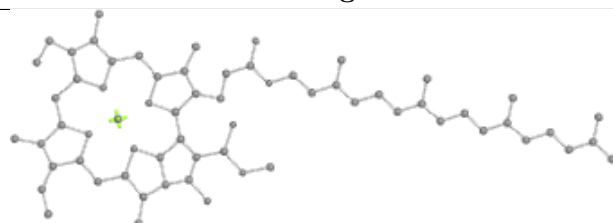
Bond lengths



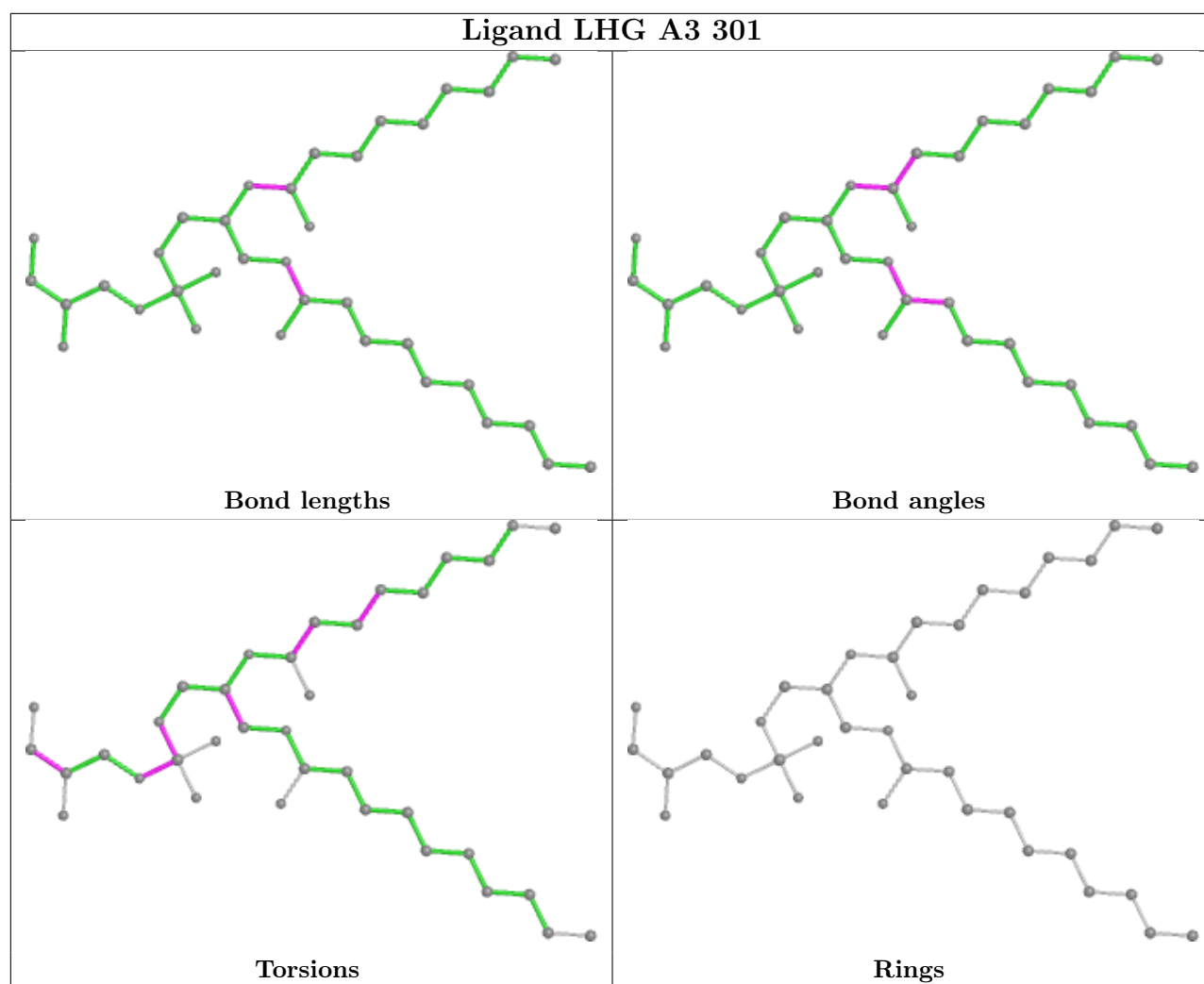
Bond angles



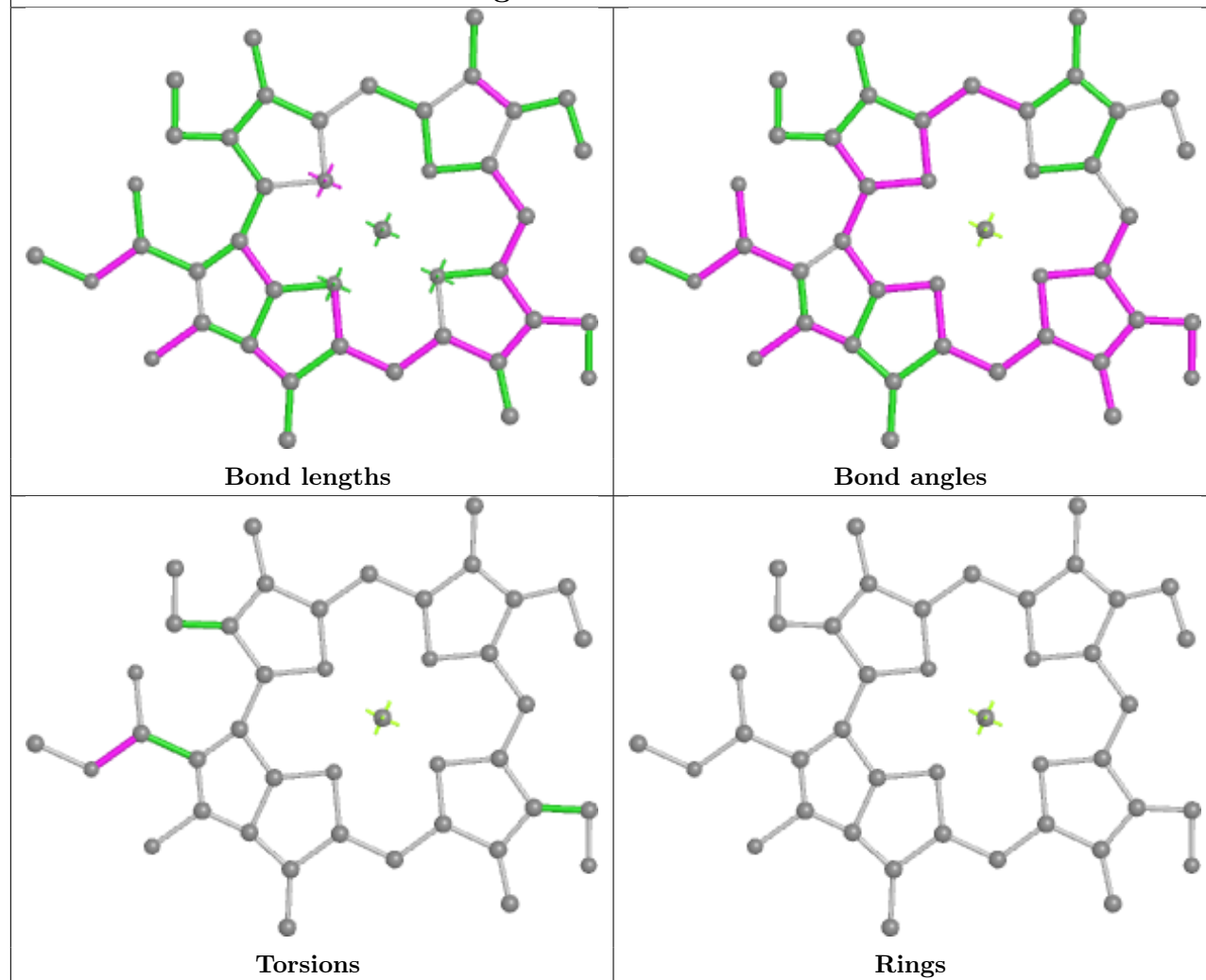
Torsions



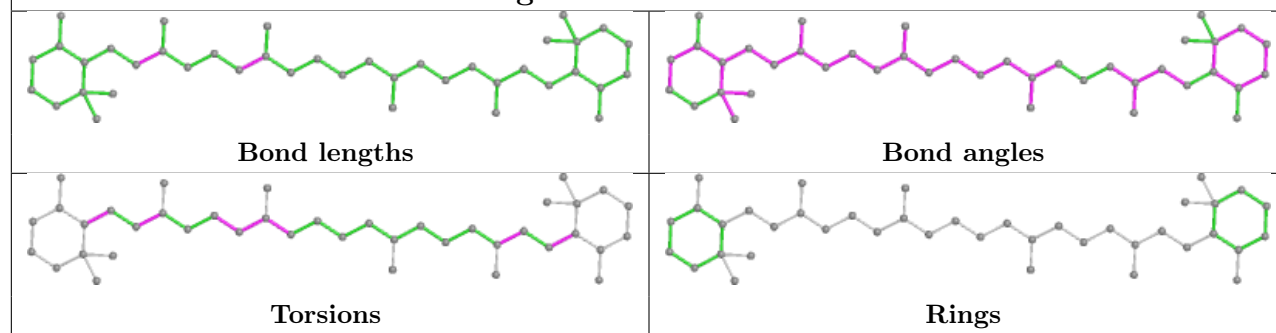
Rings



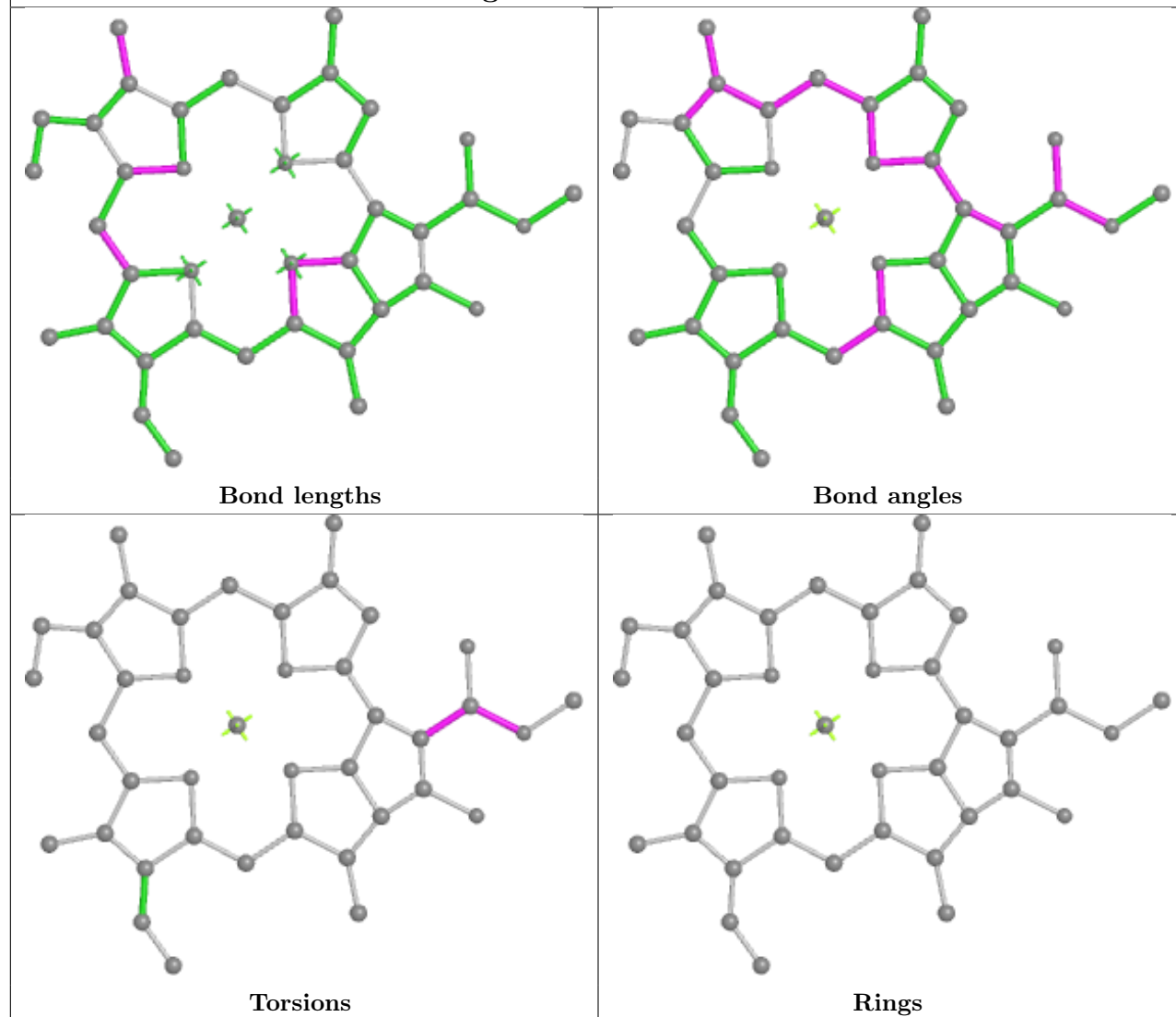
Ligand CHL A6 606



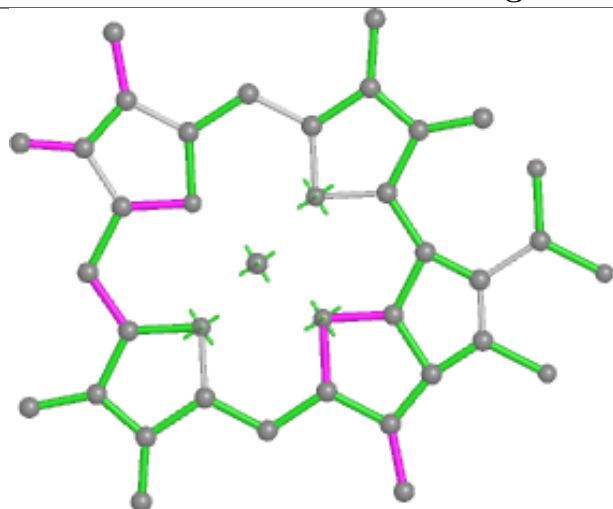
Ligand BCR AA 847



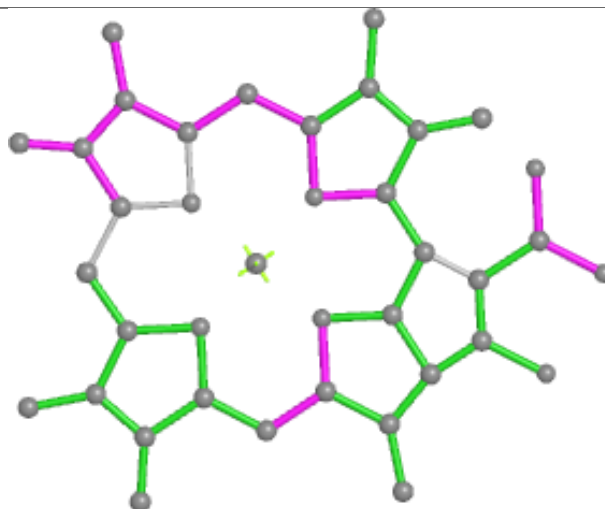
Ligand CLA B1 307



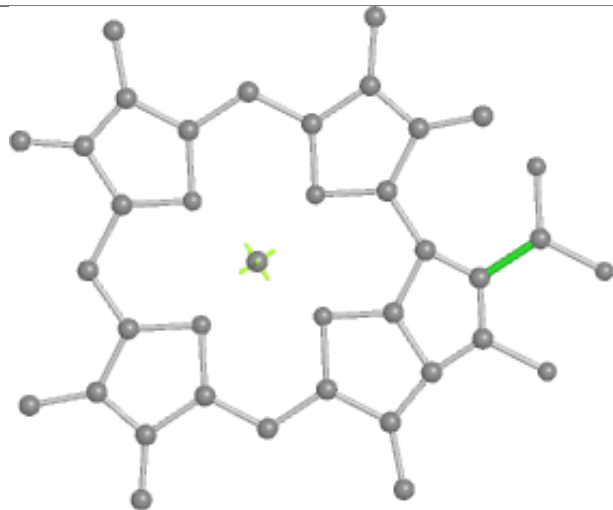
Ligand CLA B1 312



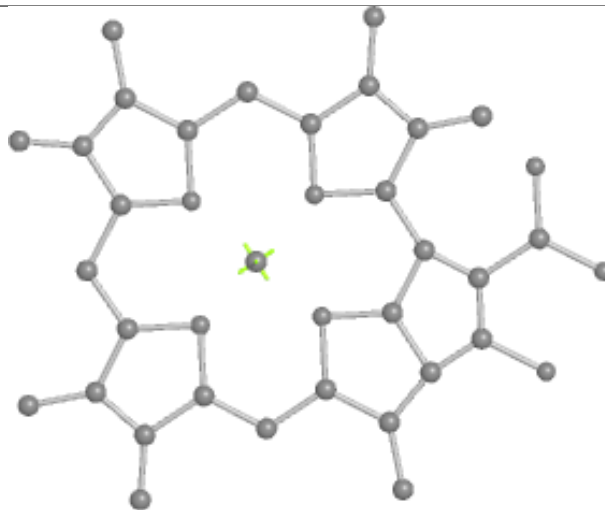
Bond lengths



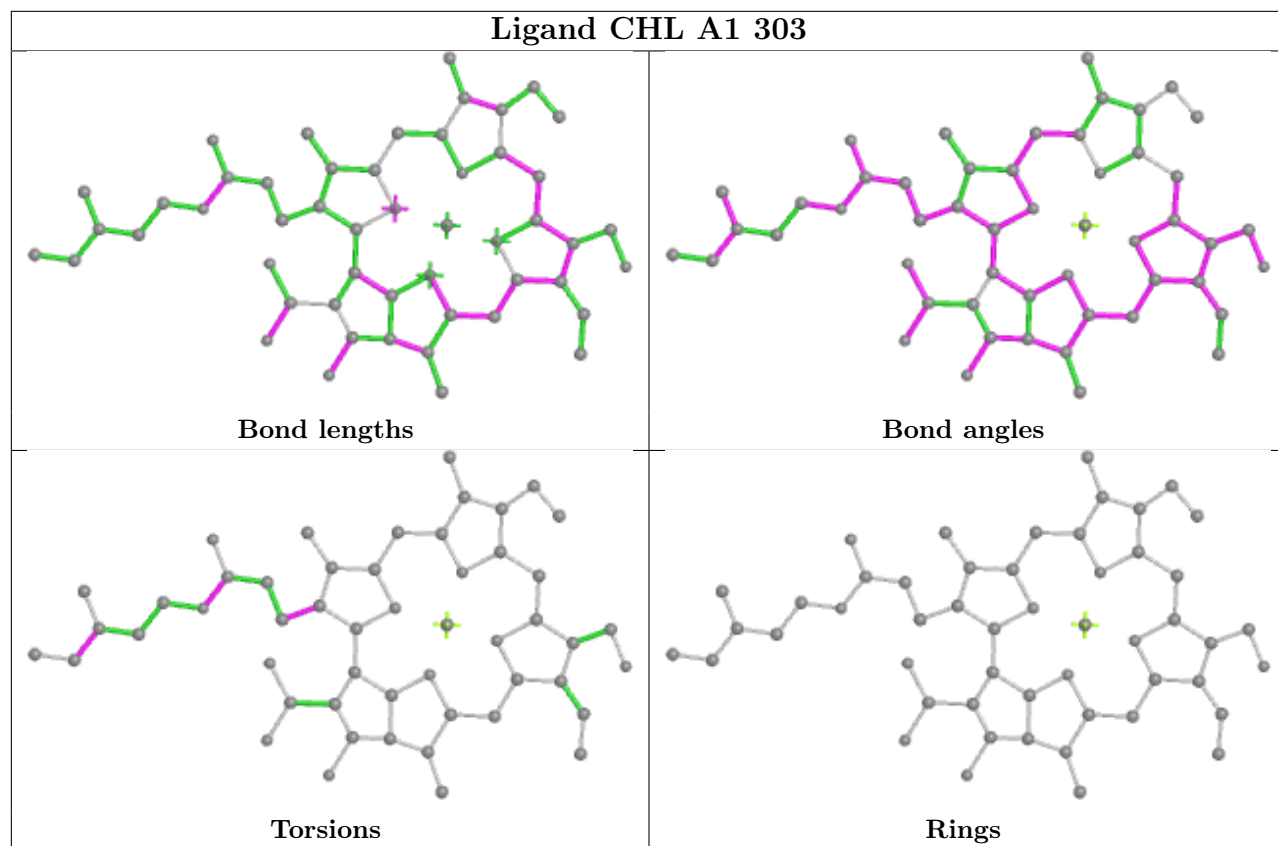
Bond angles



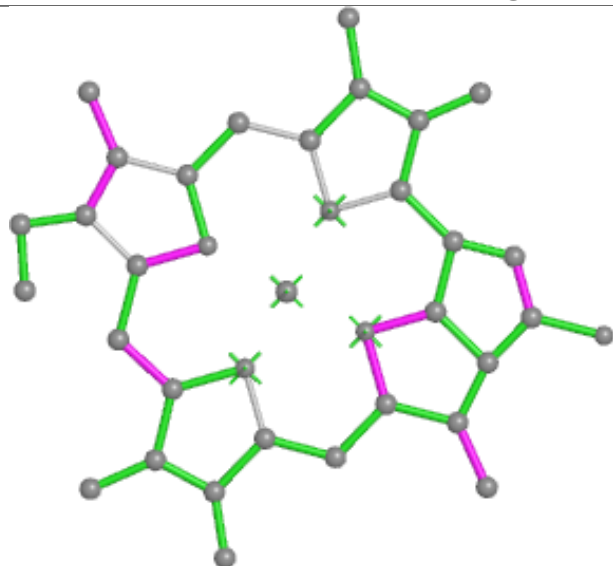
Torsions



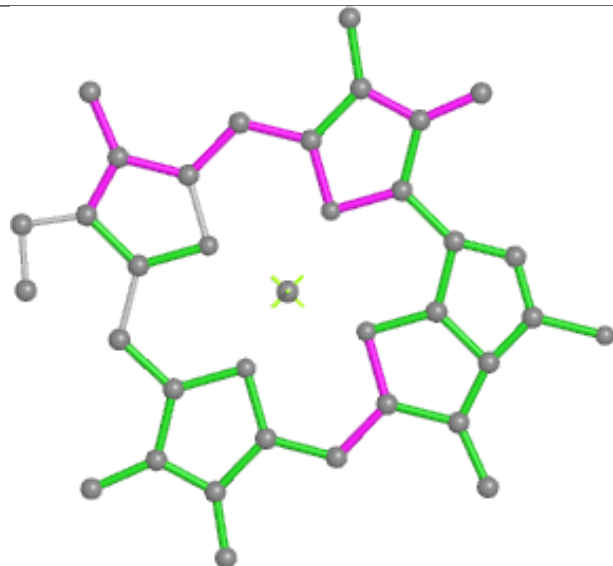
Rings



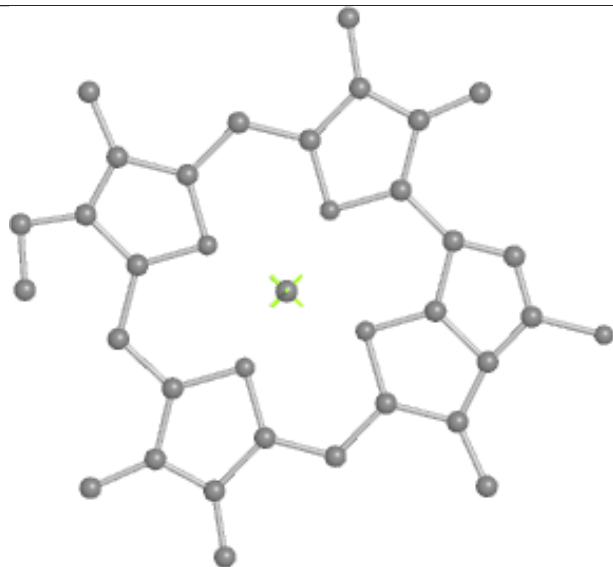
Ligand CLA A3 314



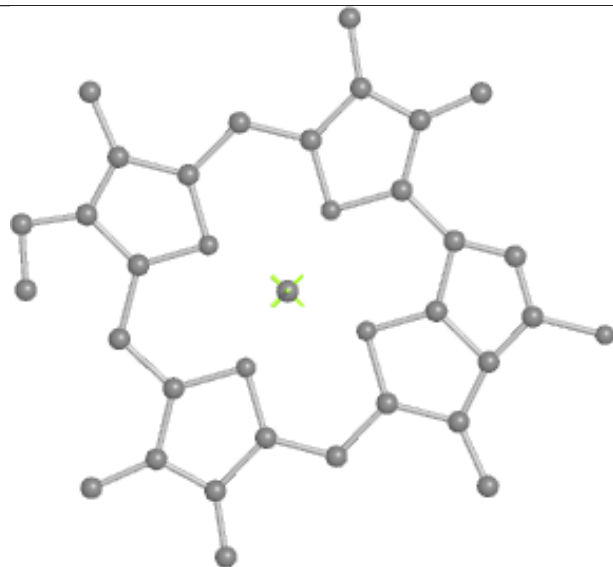
Bond lengths



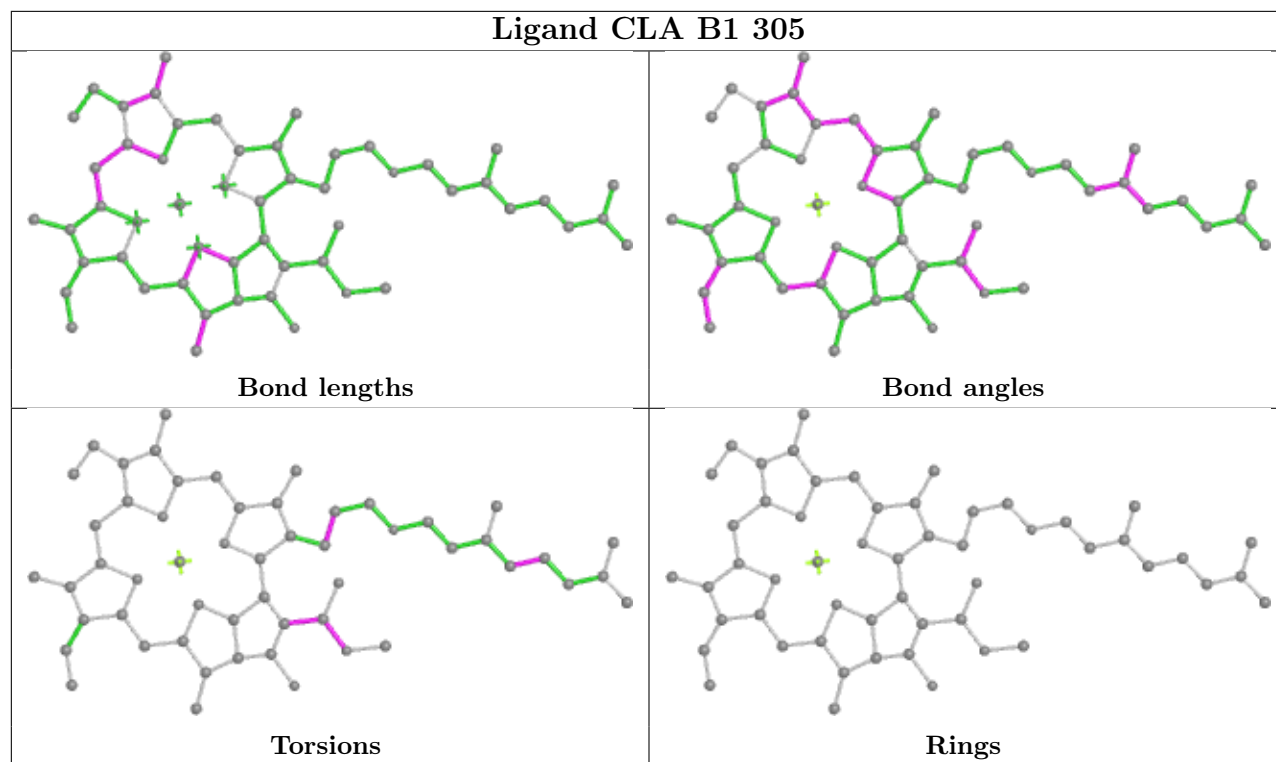
Bond angles



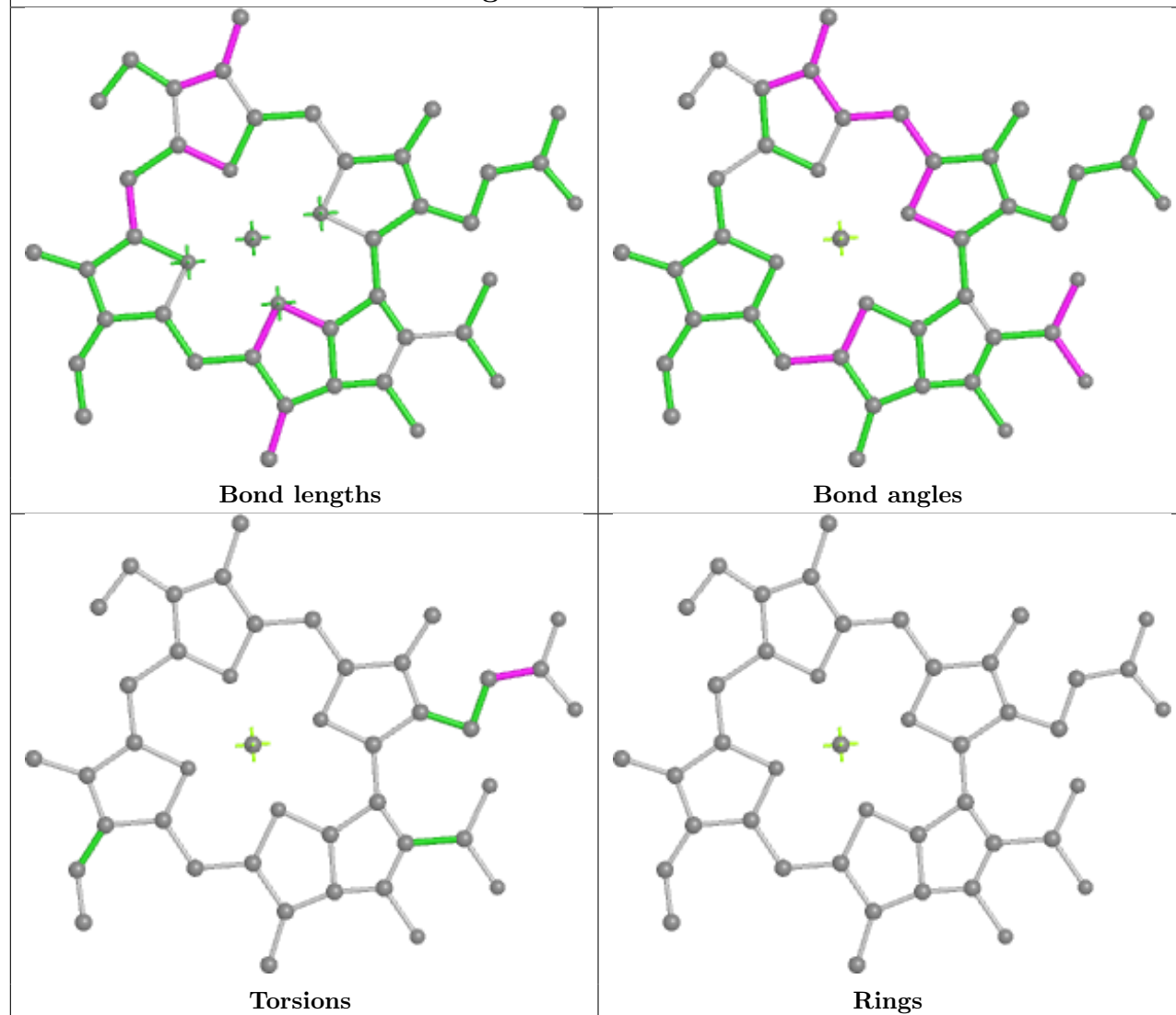
Torsions



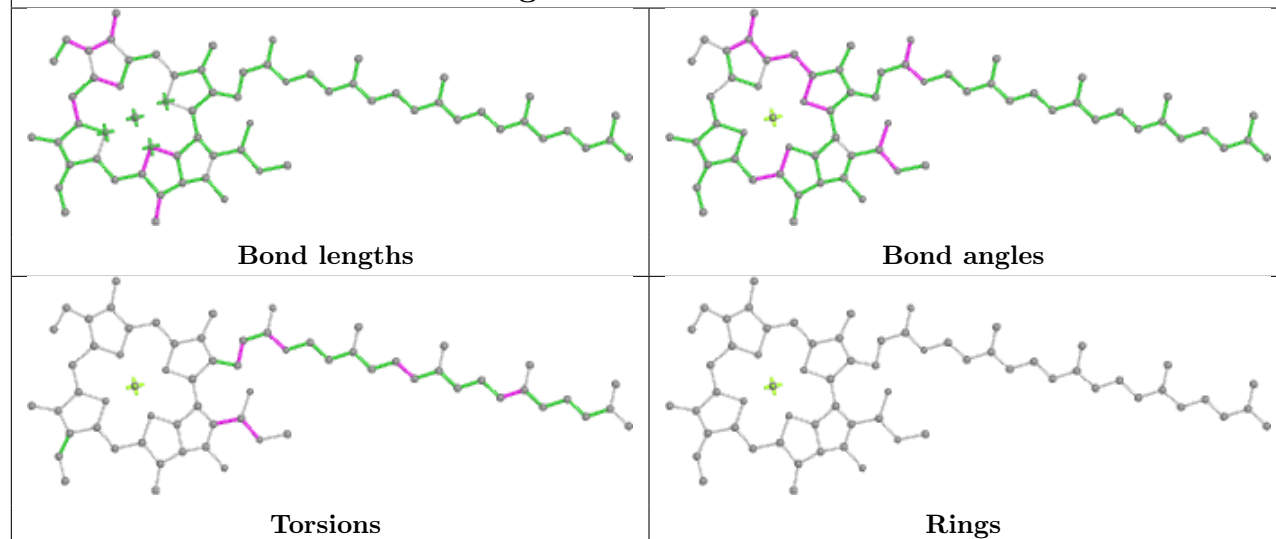
Rings

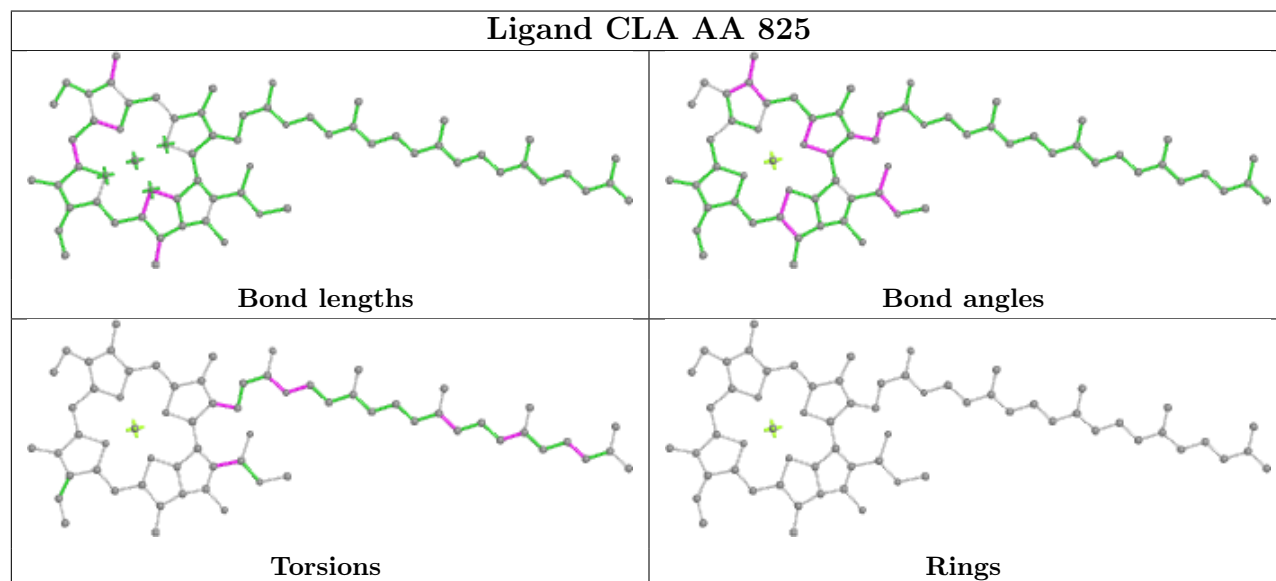
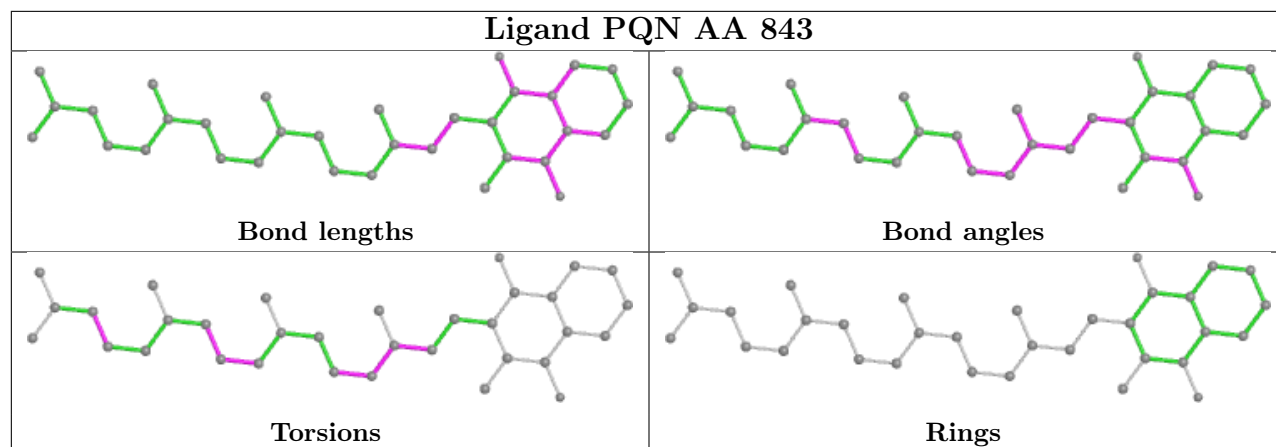


Ligand CLA B1 309

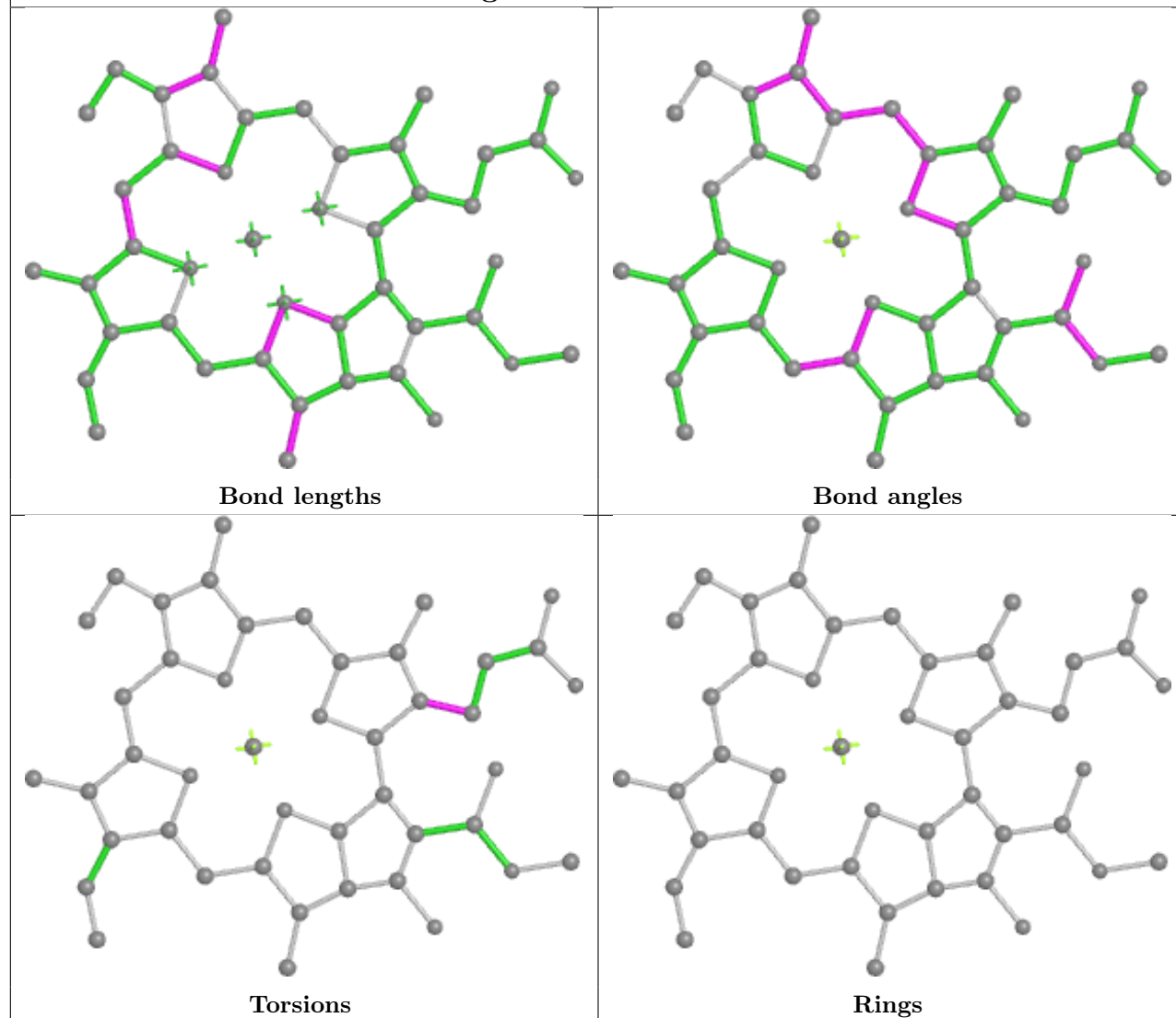


Ligand CLA BA 808

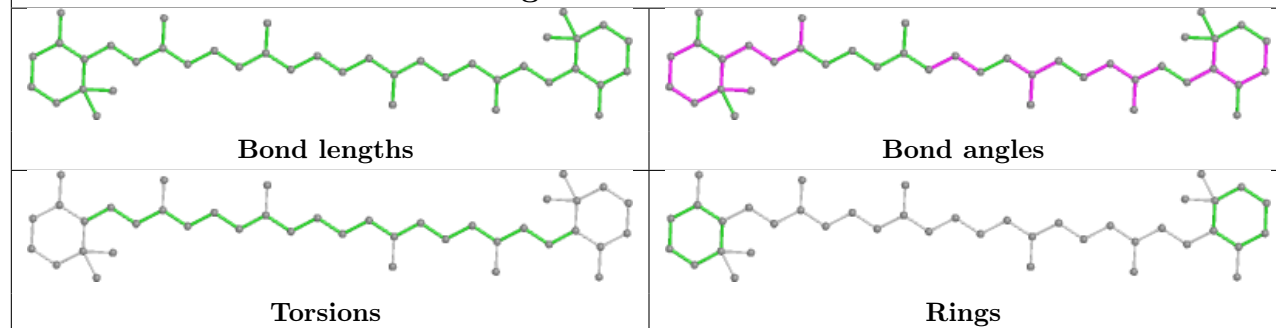


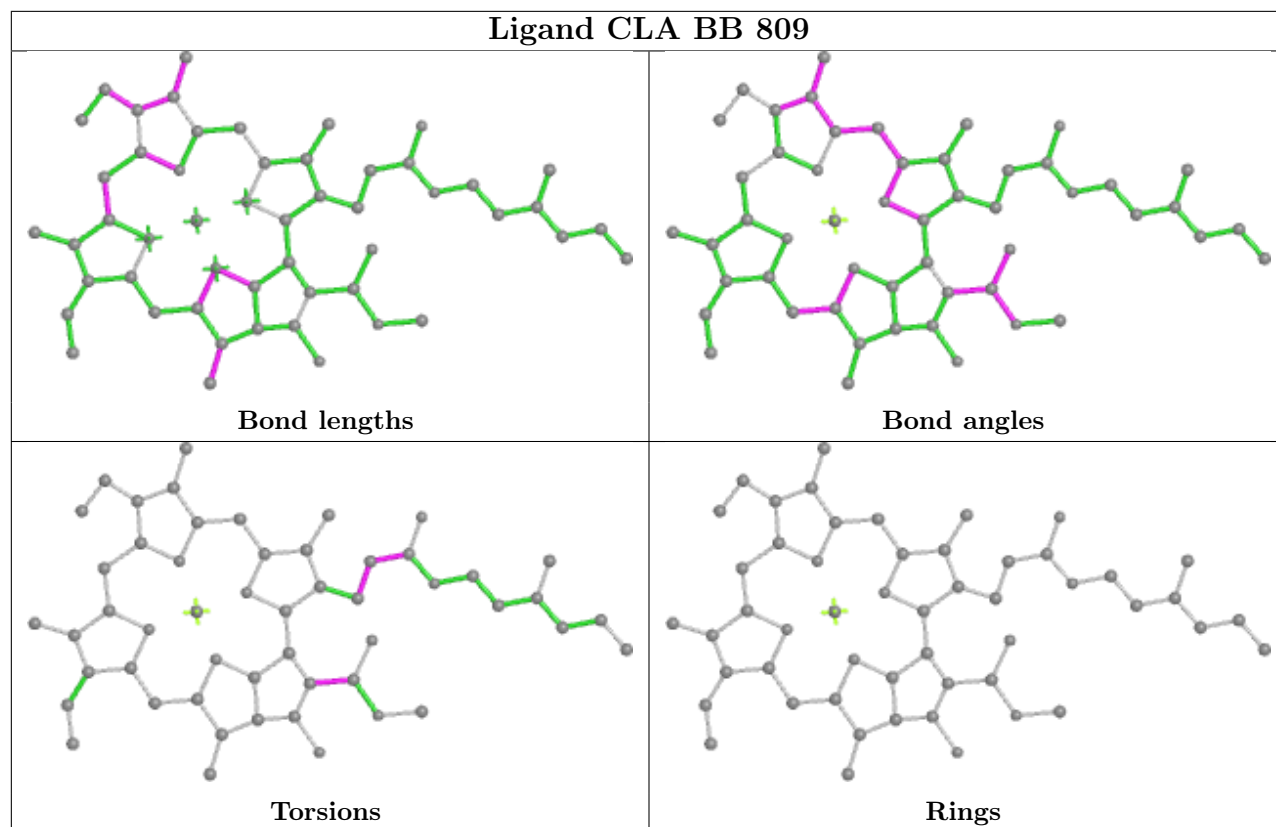


Ligand CLA A4 307

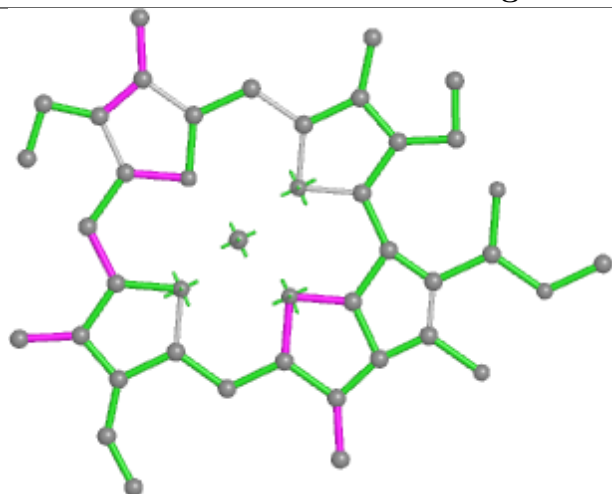


Ligand BCR BJ 101

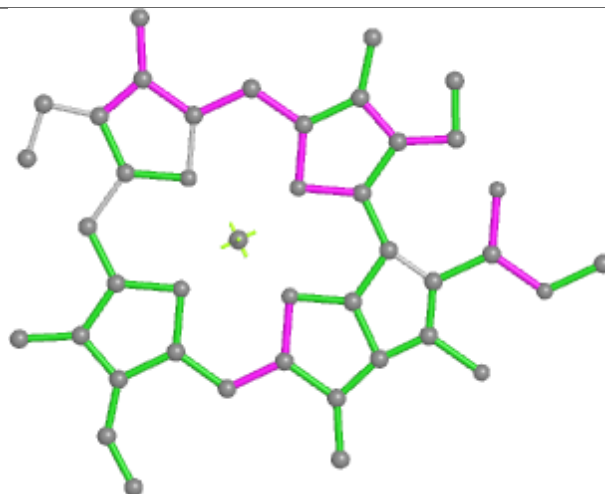




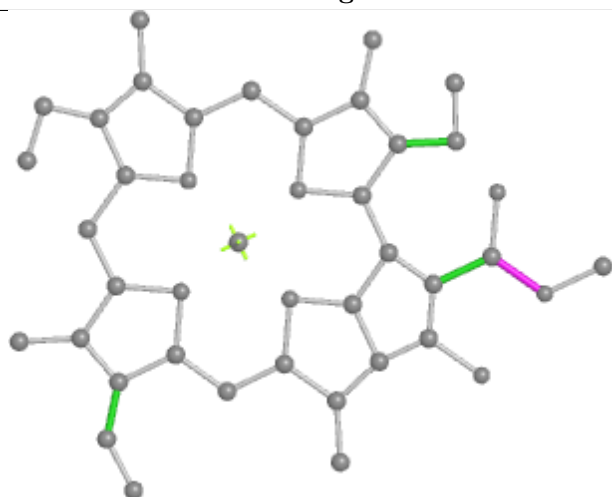
Ligand CLA AF 803



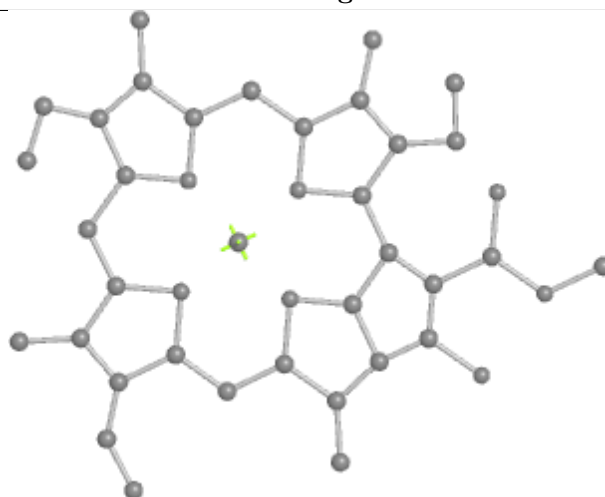
Bond lengths



Bond angles

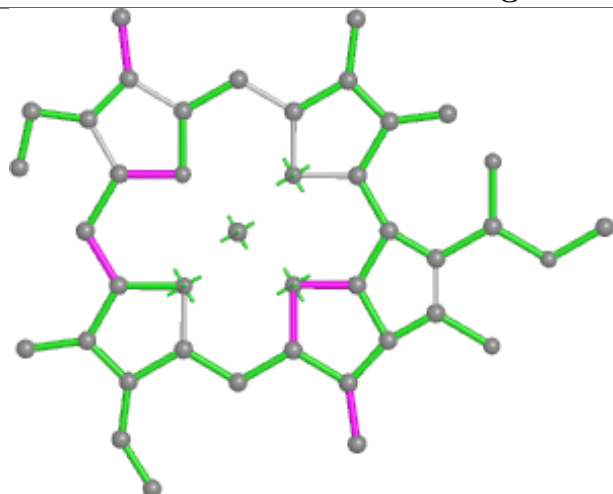


Torsions

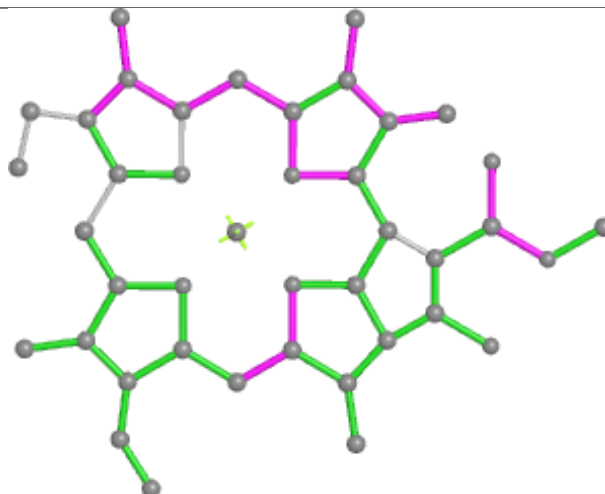


Rings

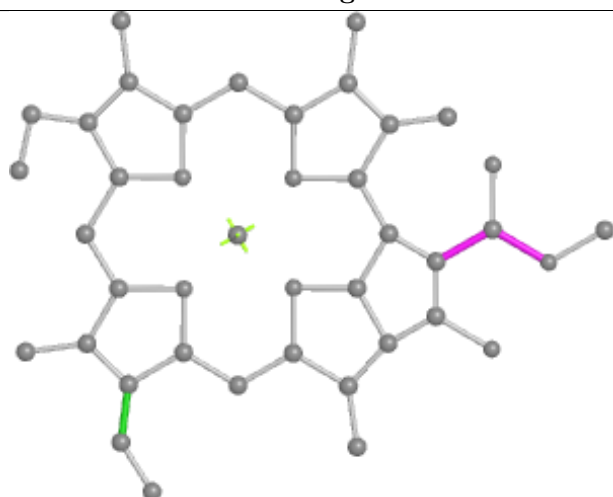
Ligand CLA BA 823



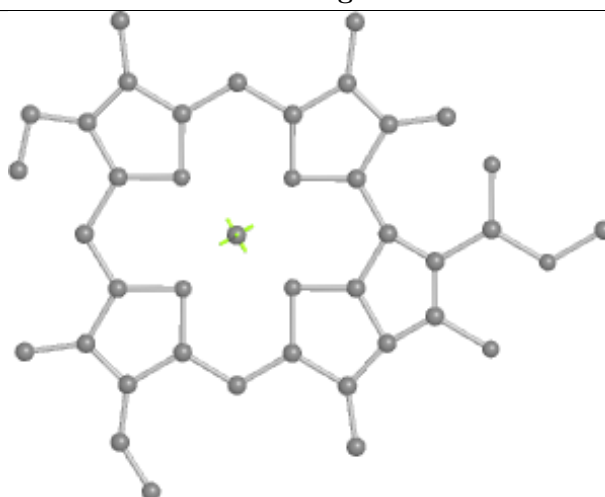
Bond lengths



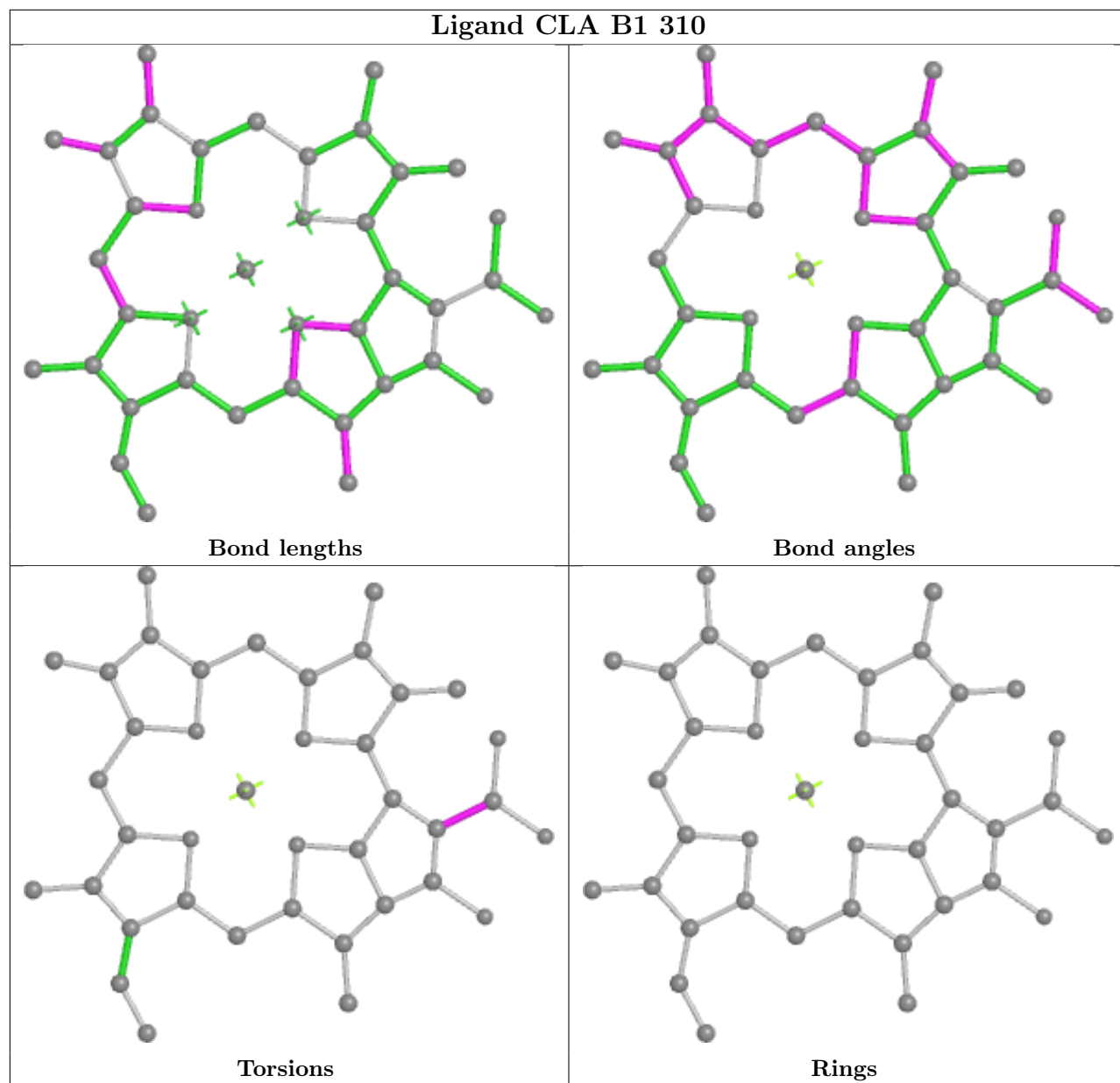
Bond angles

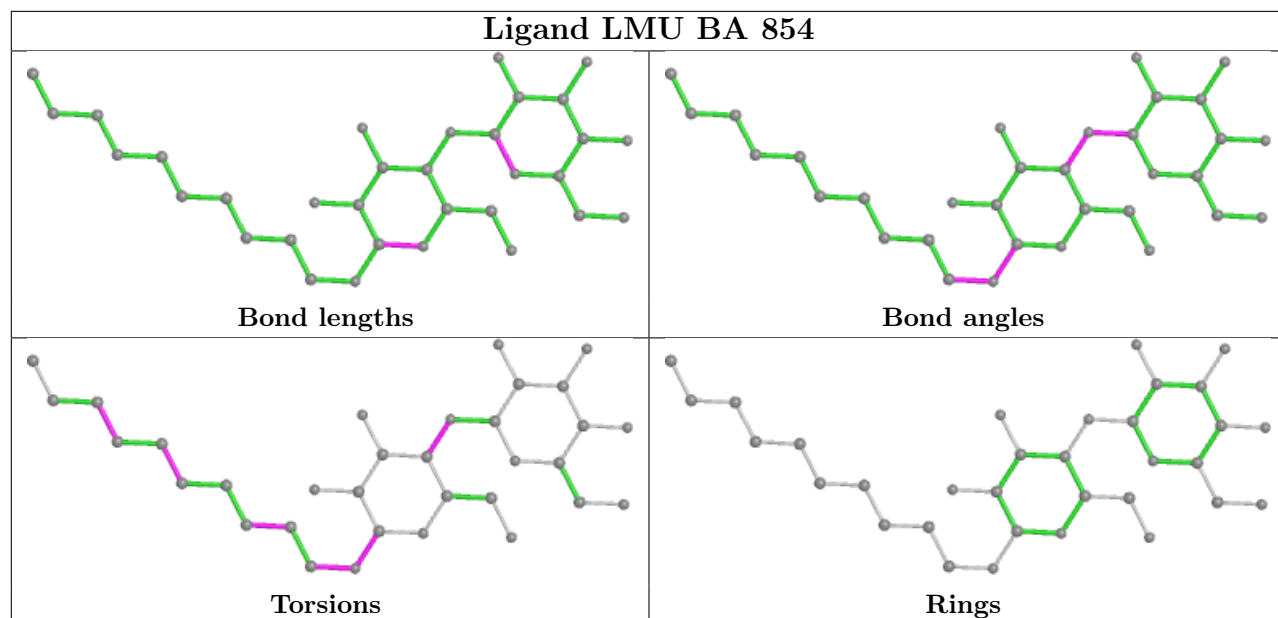


Torsions

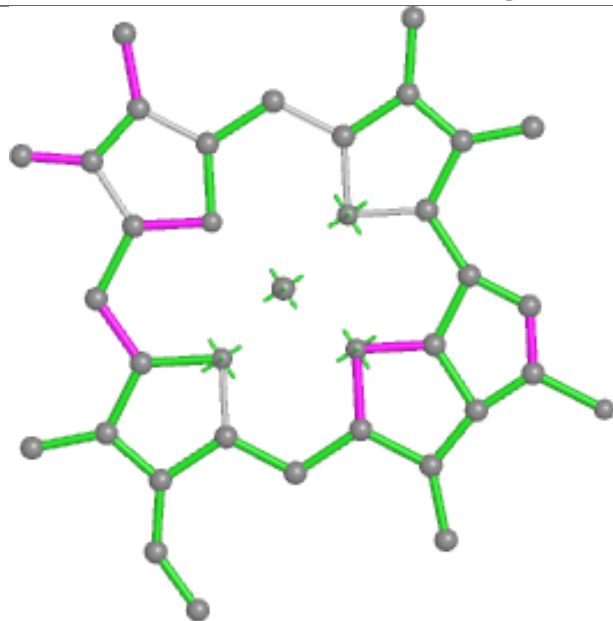


Rings

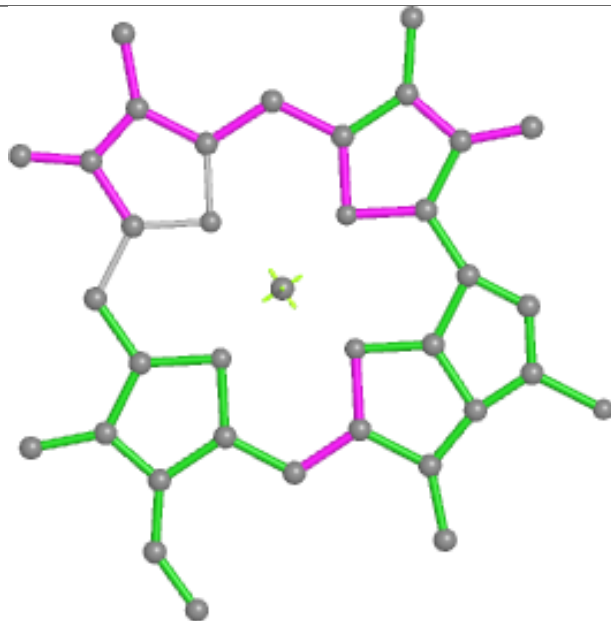




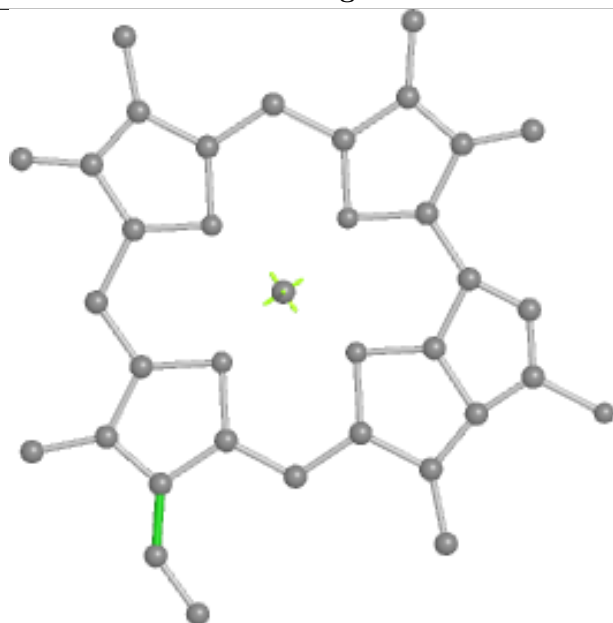
Ligand CLA BK 201



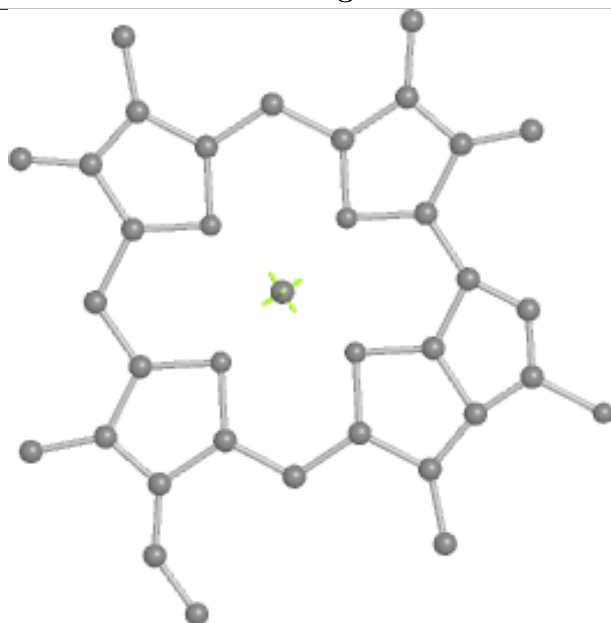
Bond lengths



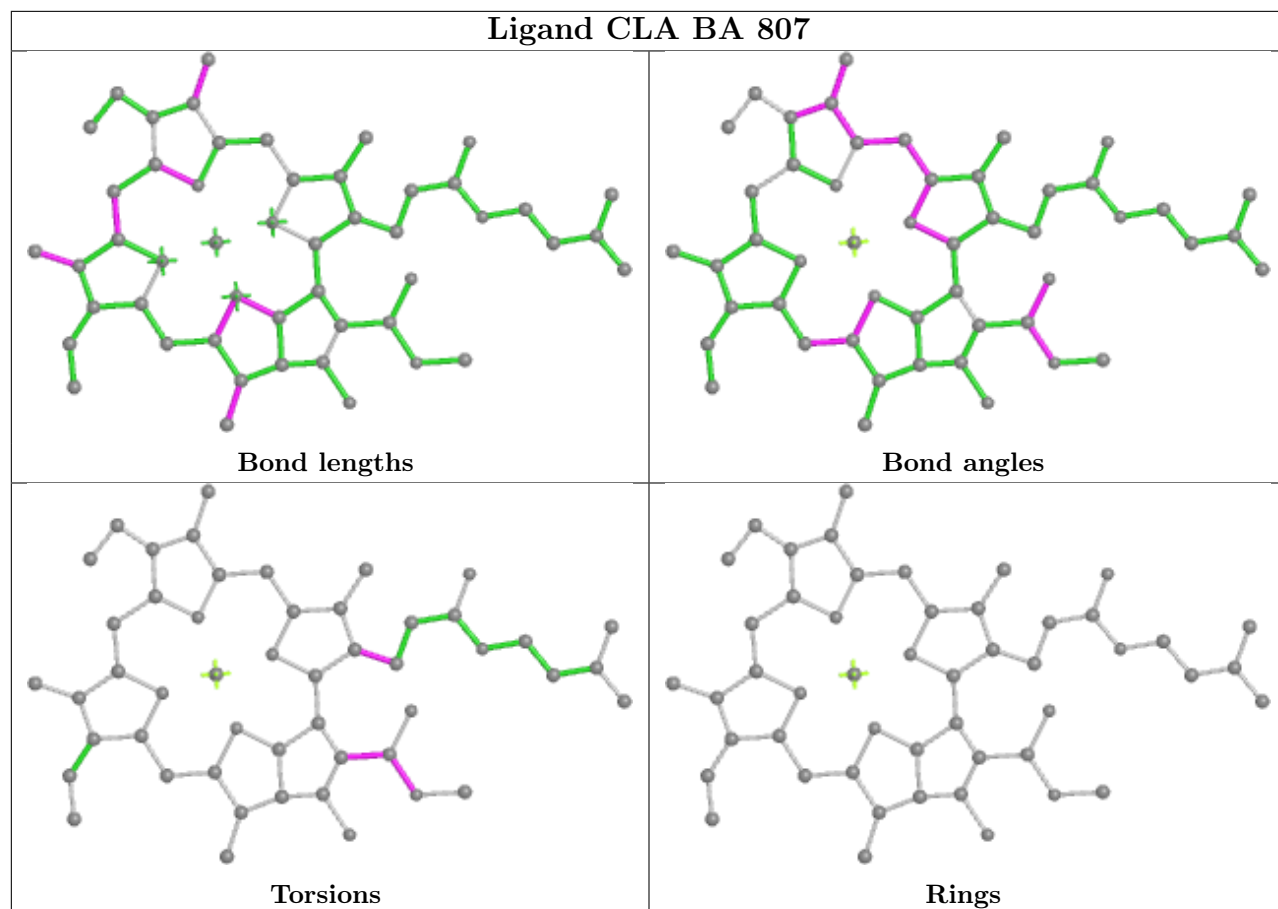
Bond angles



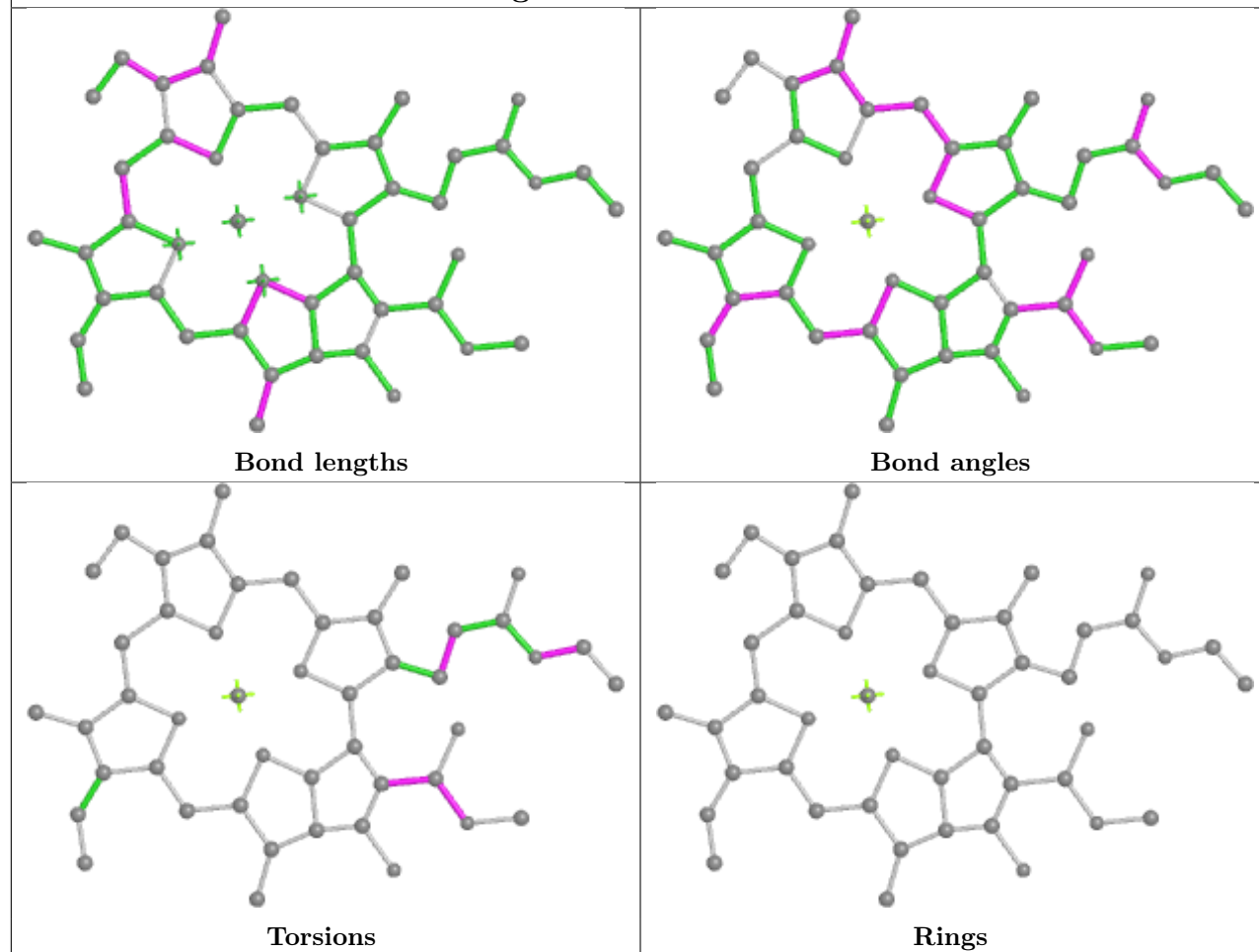
Torsions



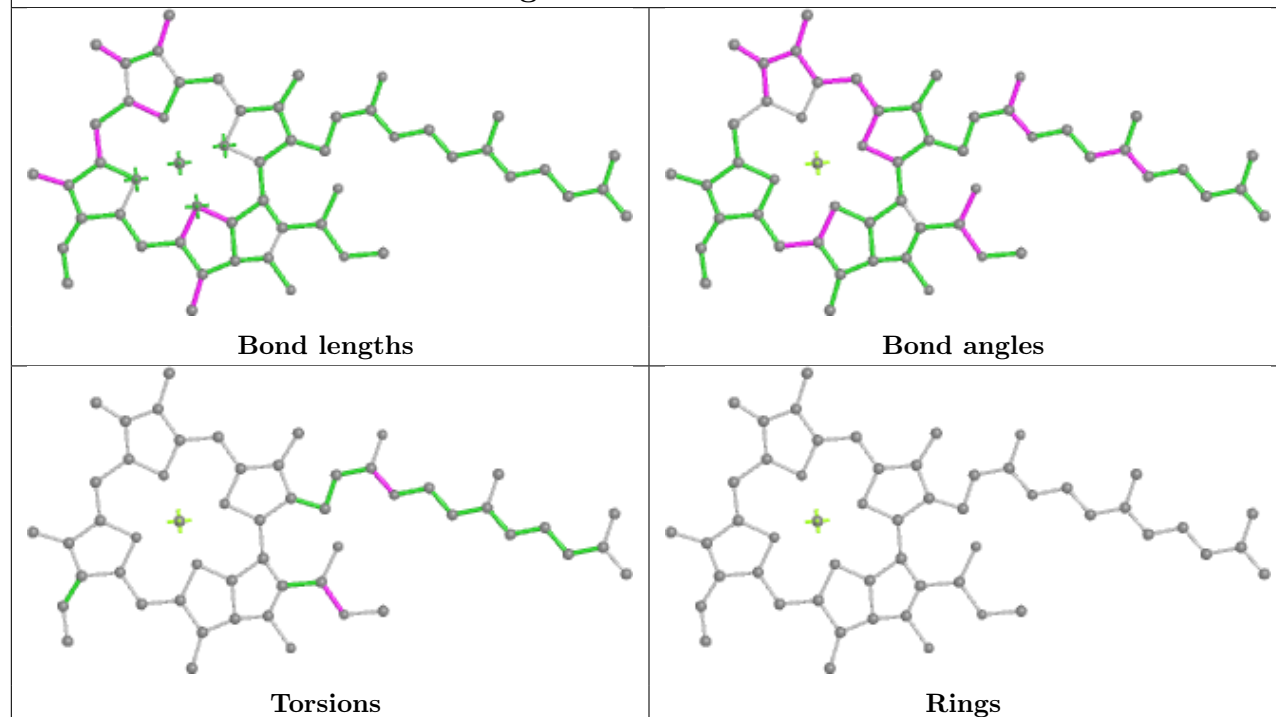
Rings

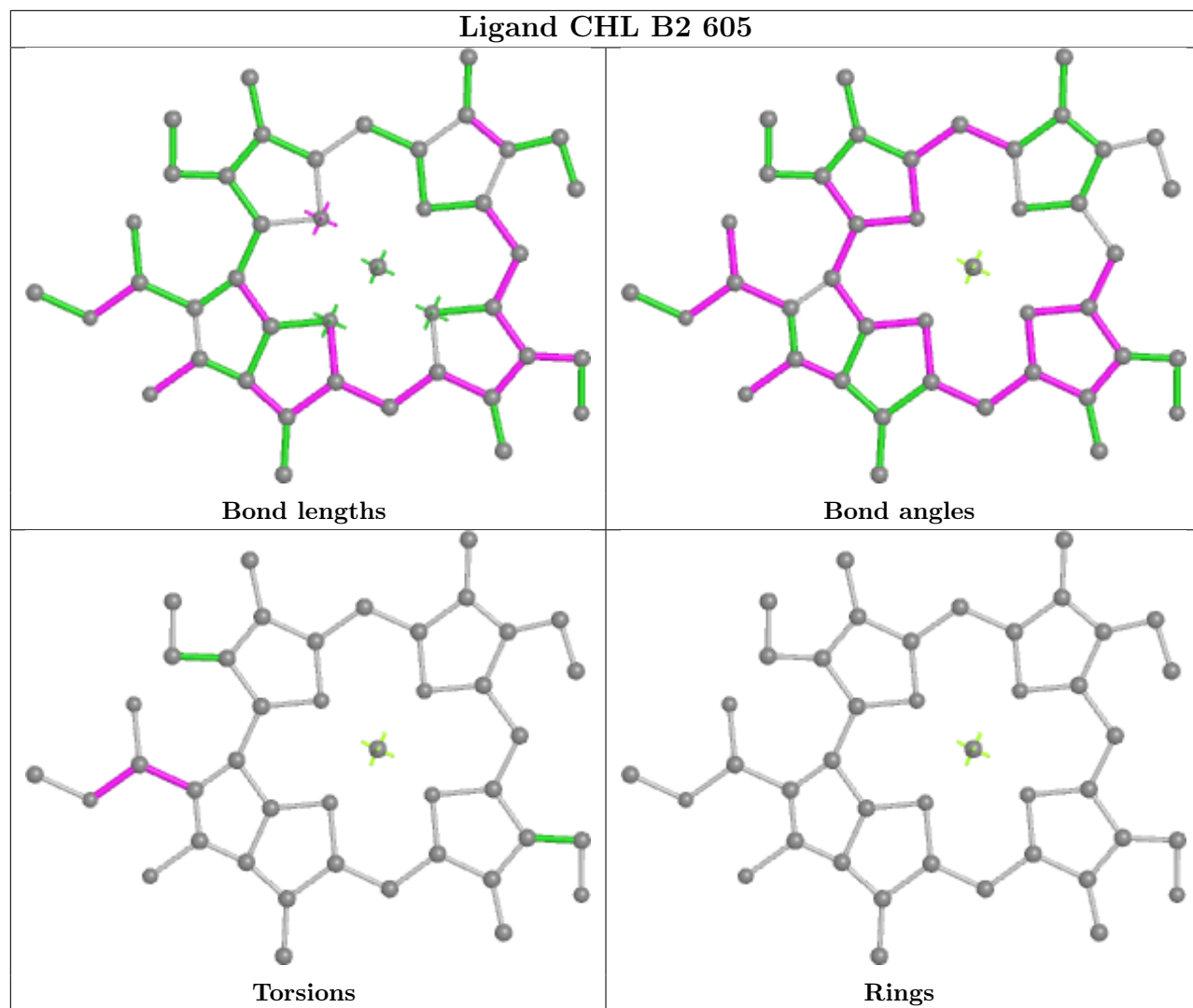


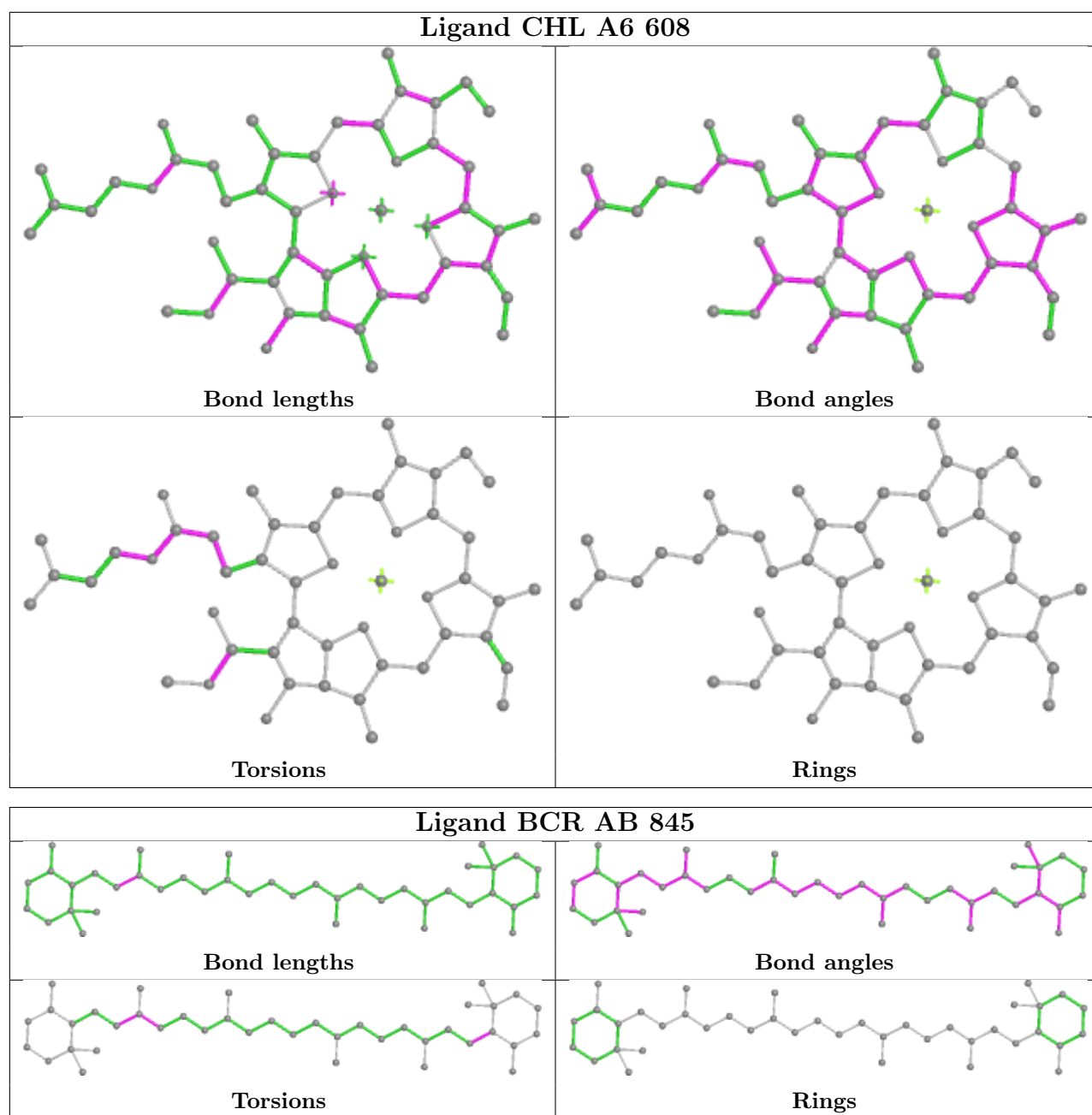
Ligand CLA BA 831

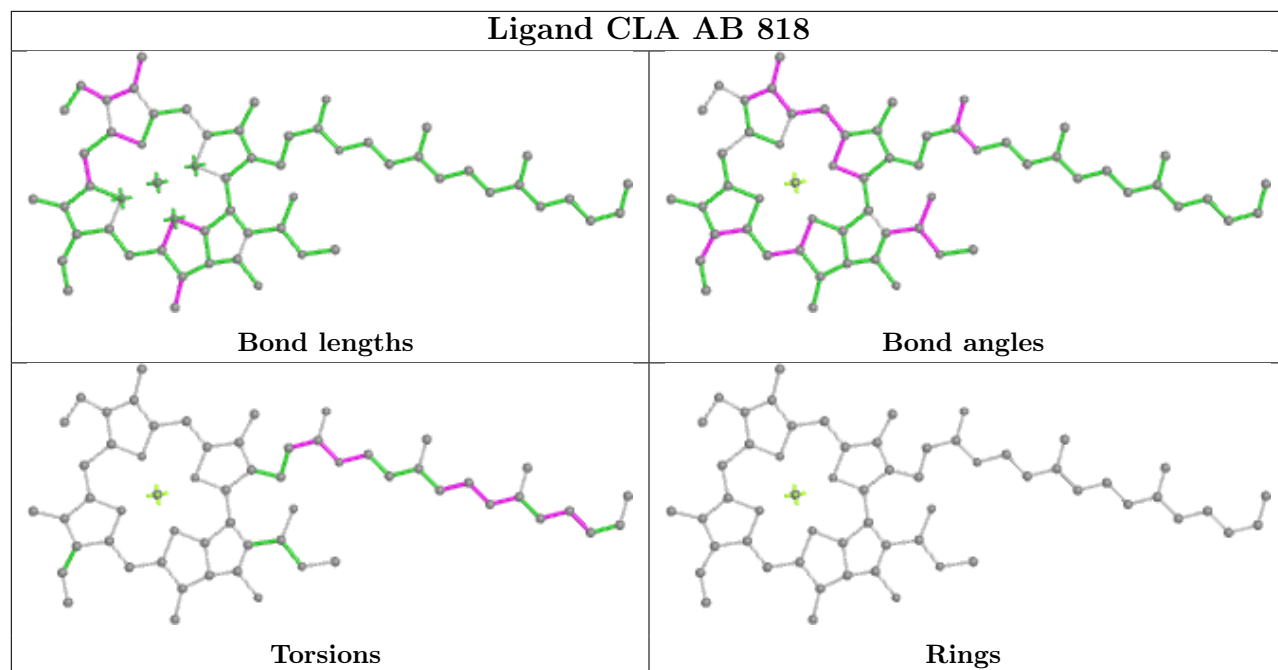


Ligand CLA BB 813

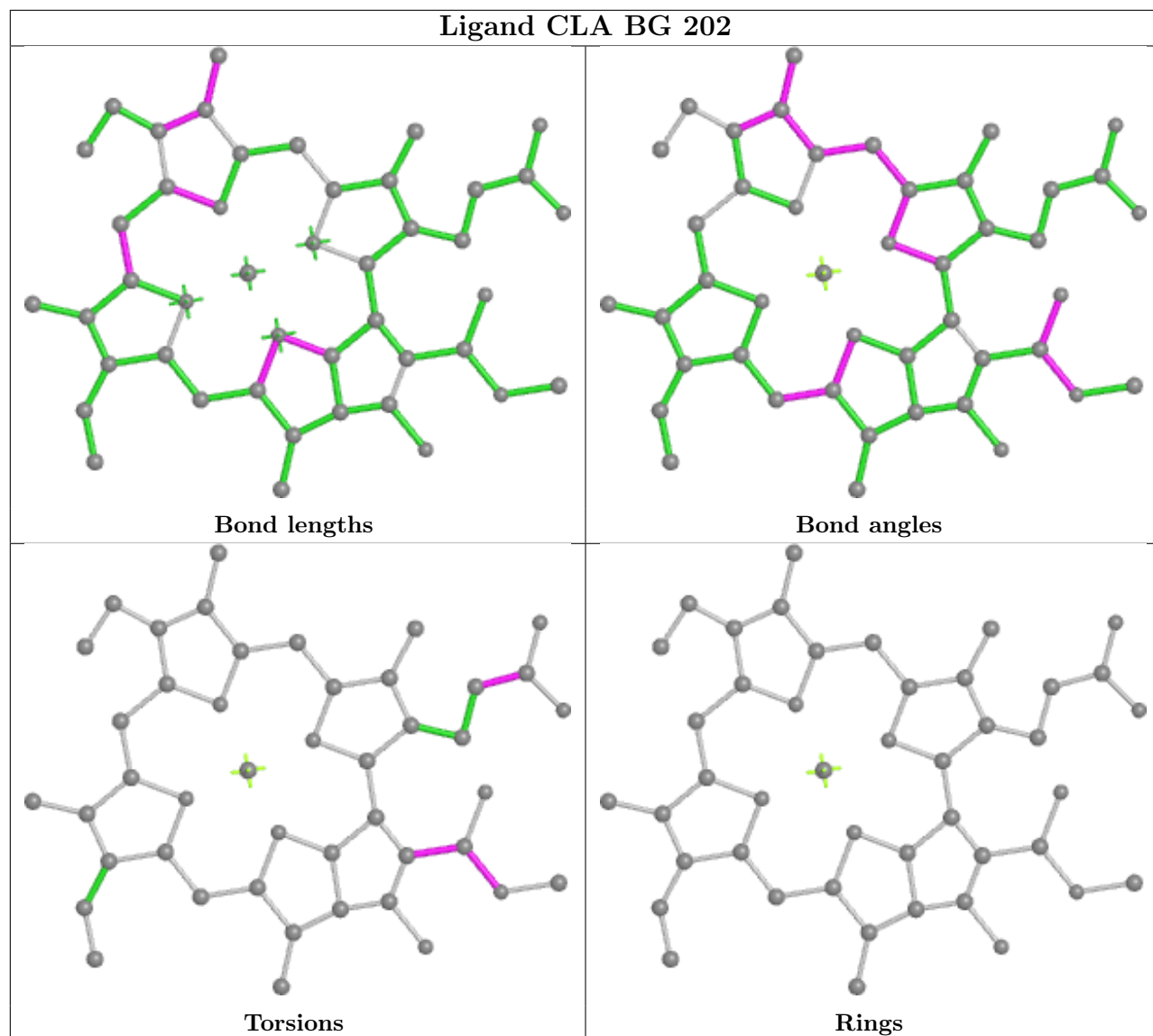




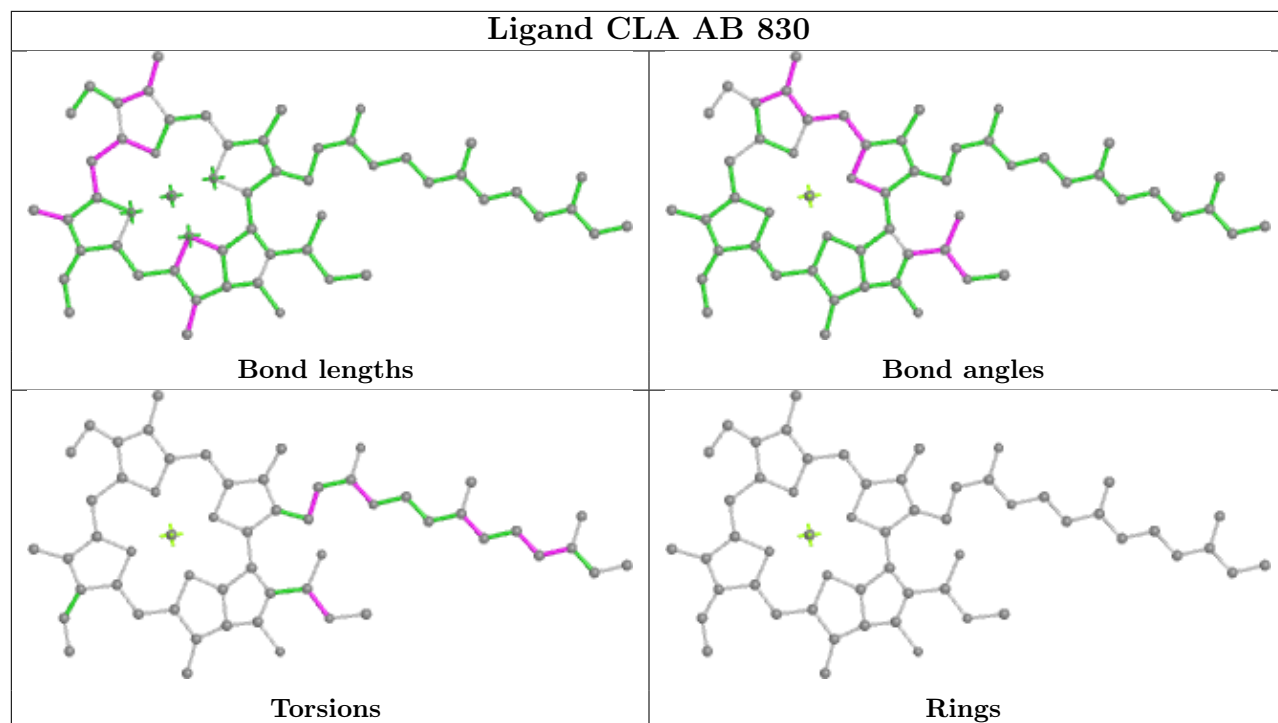




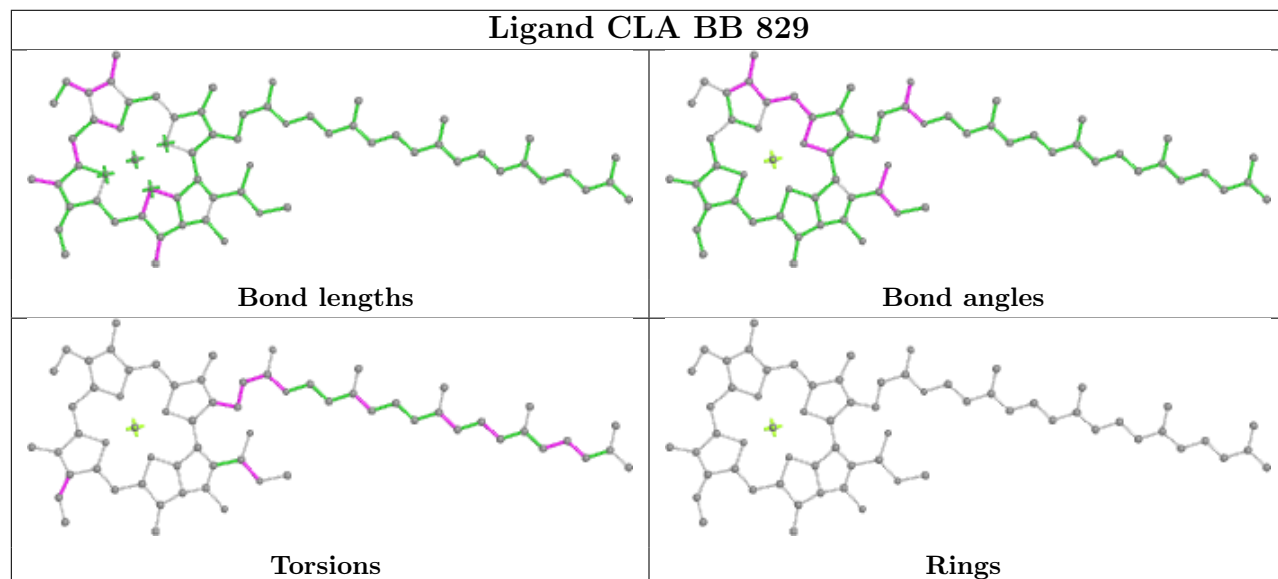
Ligand CLA BG 202



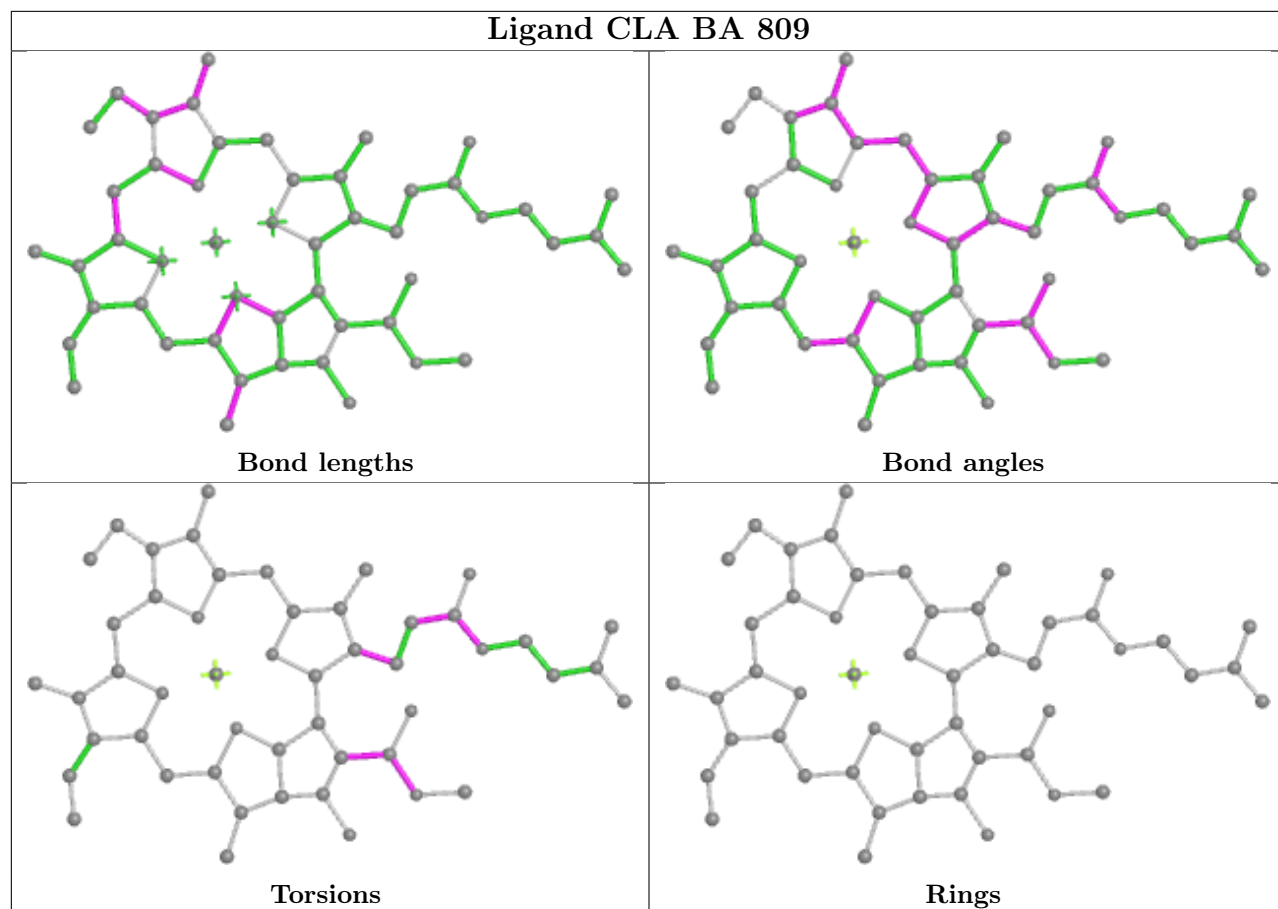
Ligand CLA AB 830

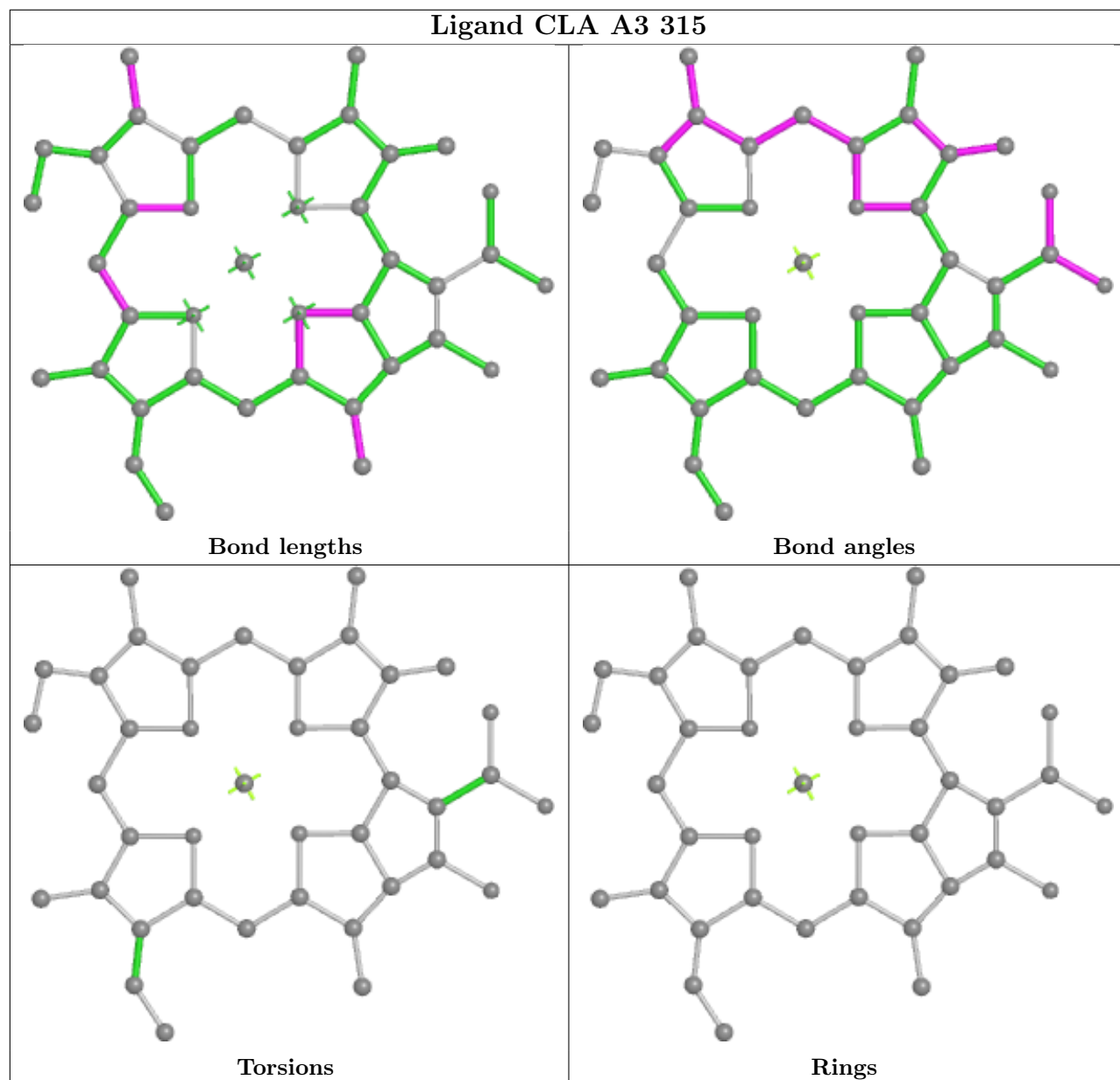


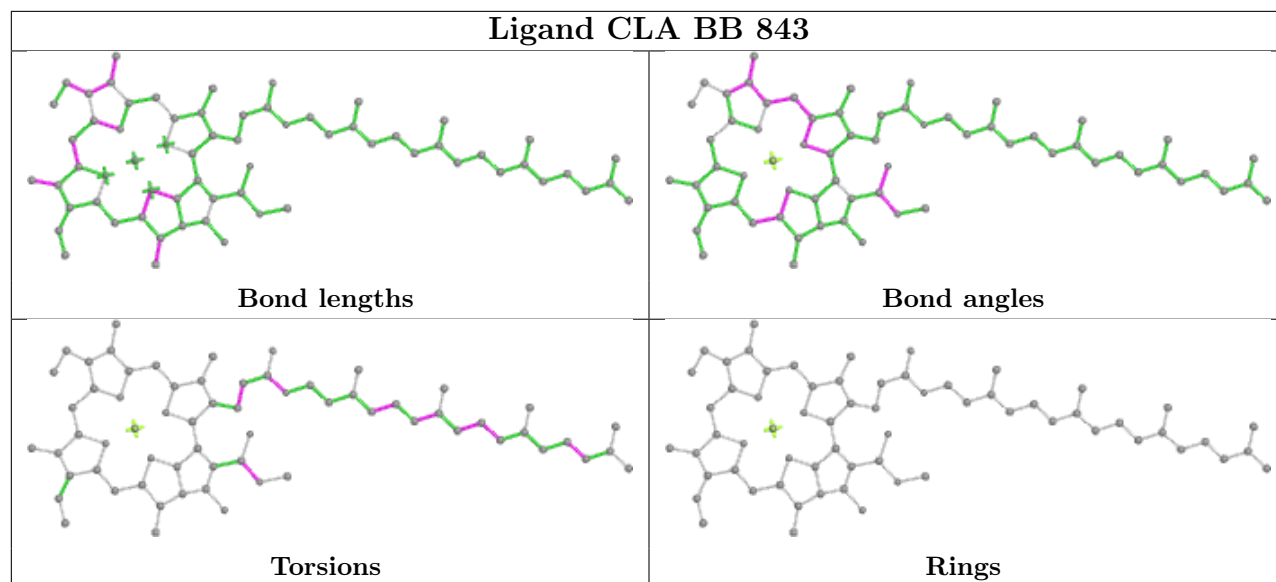
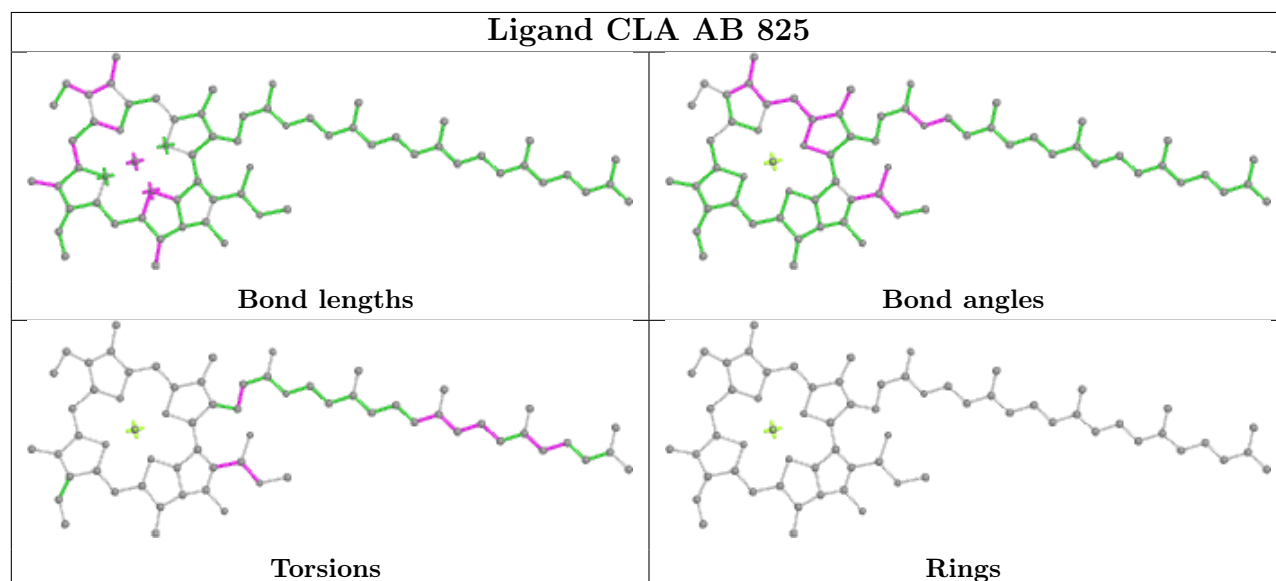
Ligand CLA BB 829



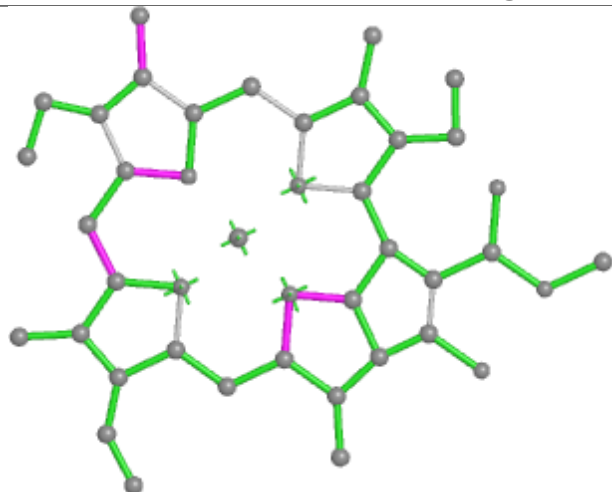
Ligand CLA BA 809



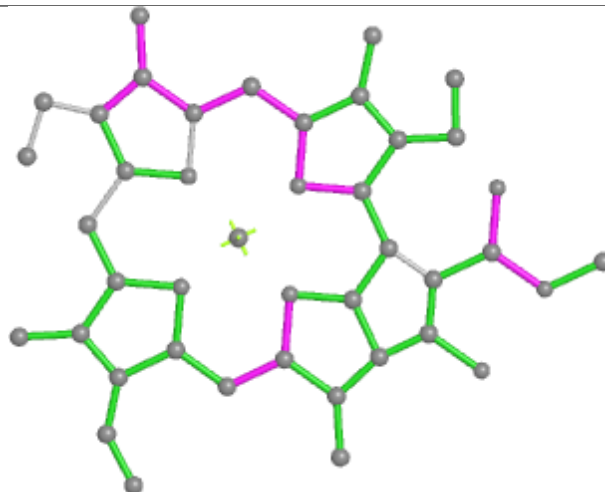


Ligand CLA BB 843**Ligand CLA AB 825**

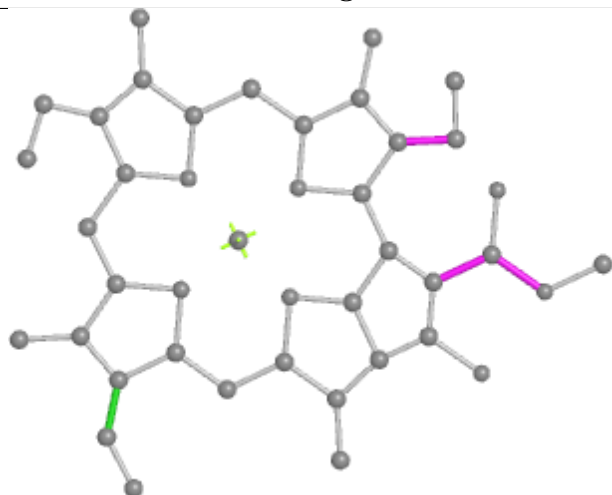
Ligand CLA BB 837



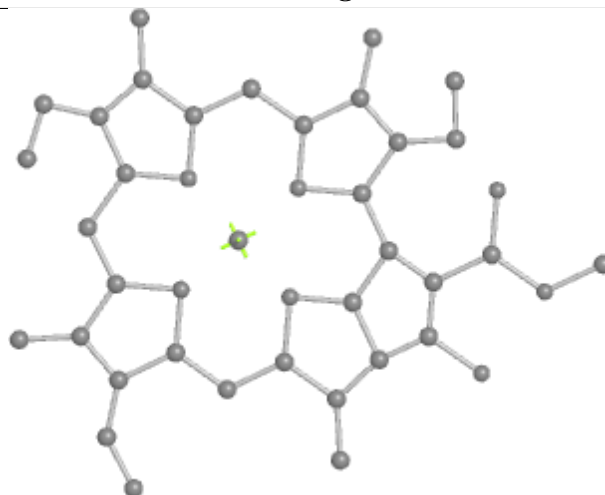
Bond lengths



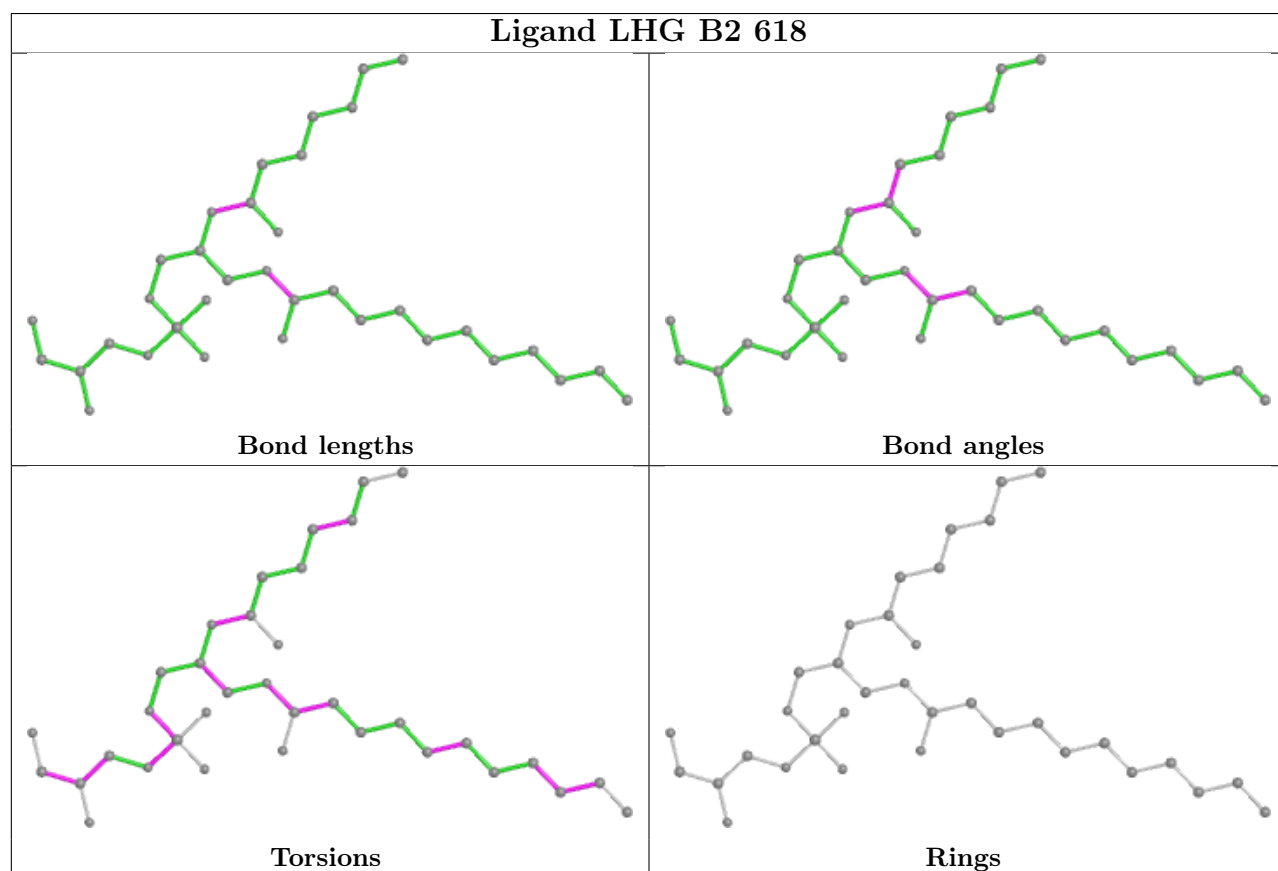
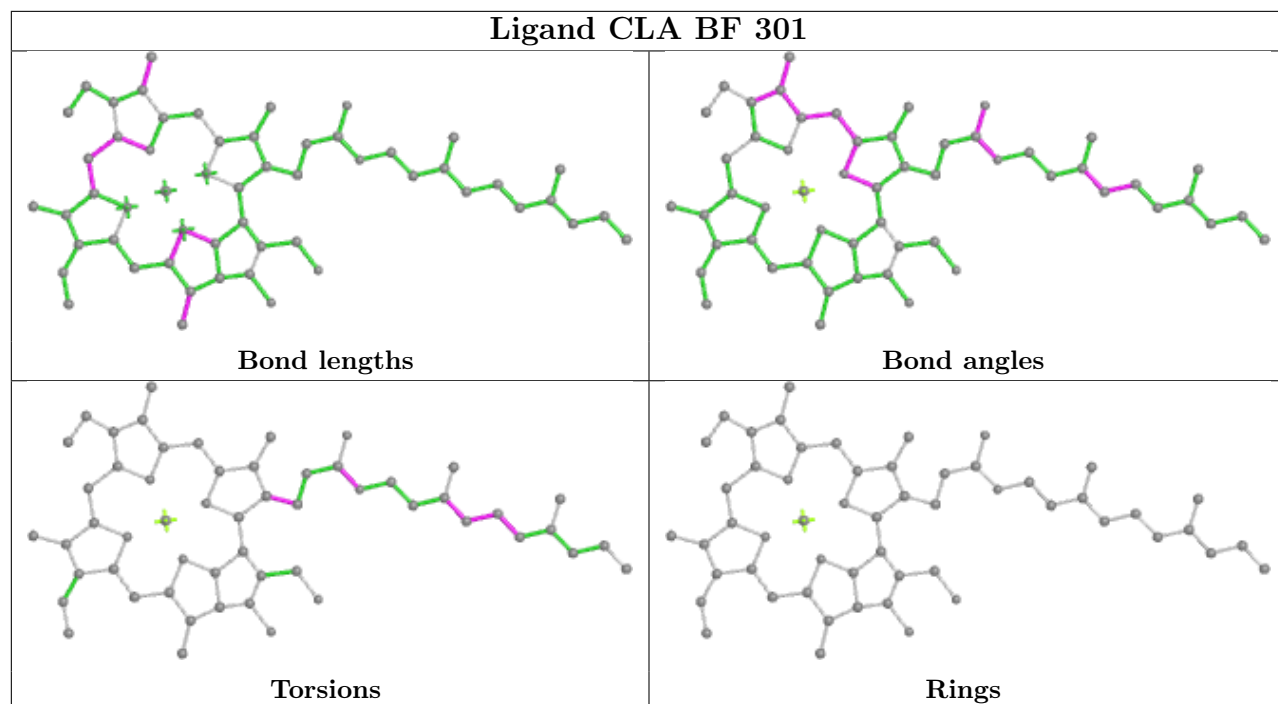
Bond angles



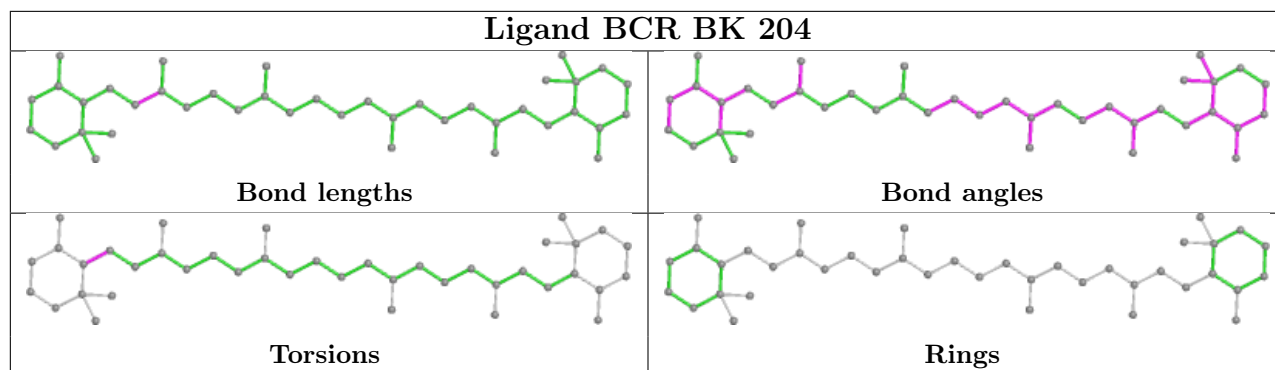
Torsions



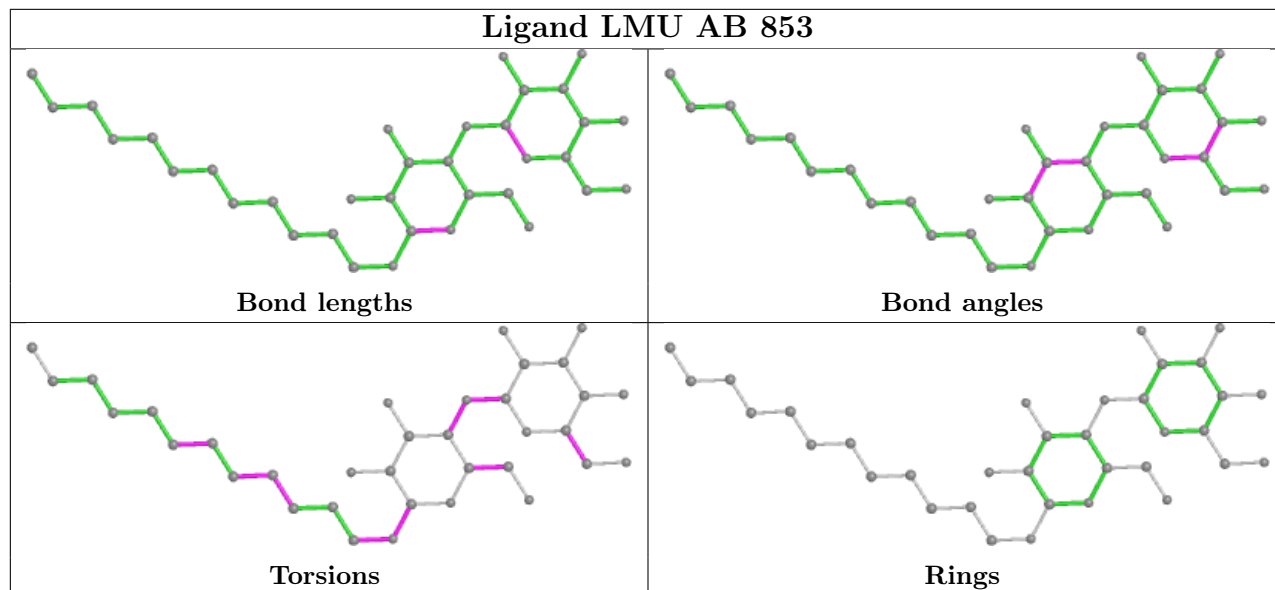
Rings



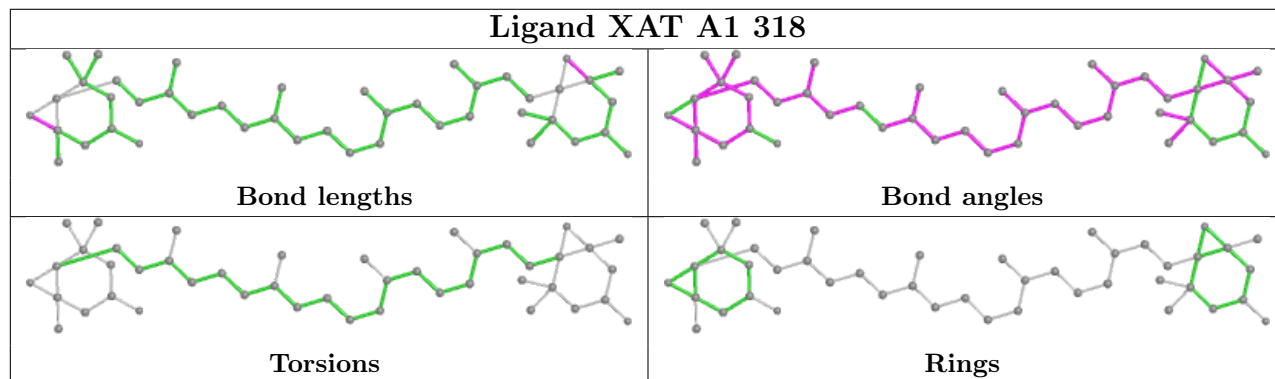
Ligand BCR BK 204



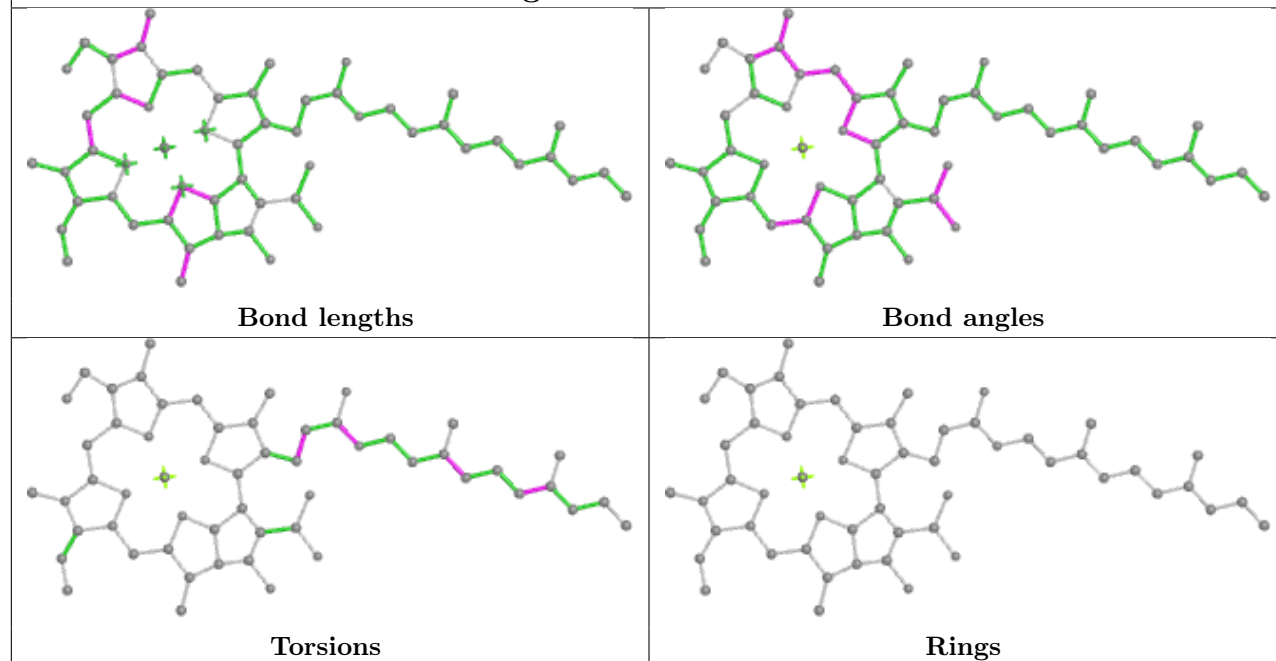
Ligand LMU AB 853



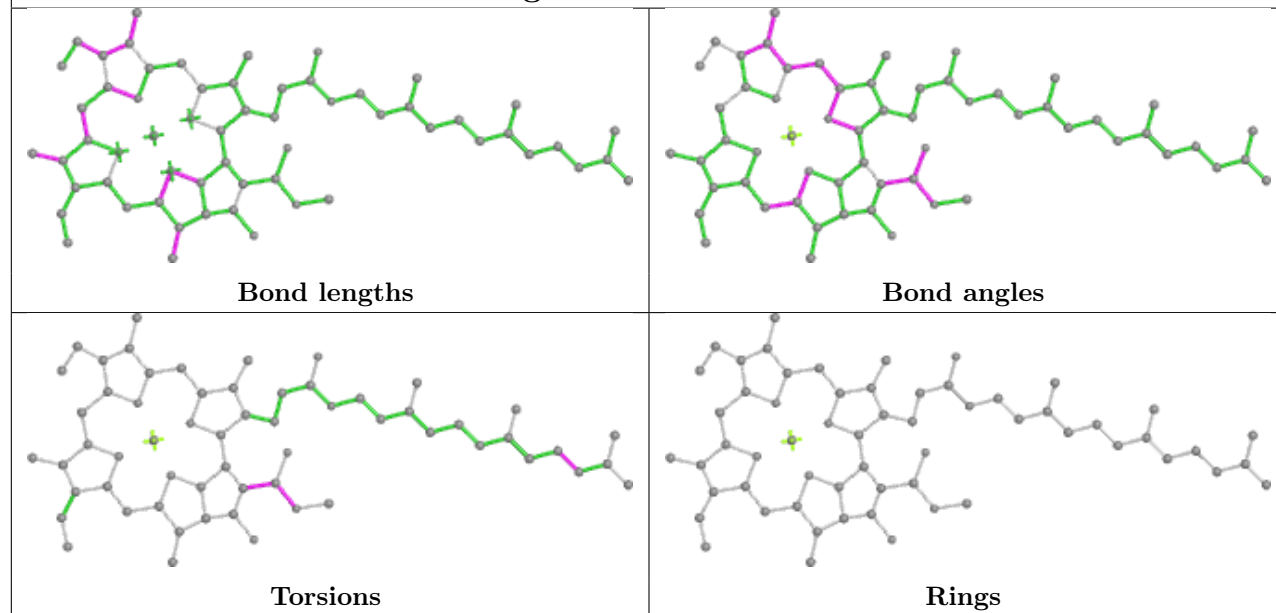
Ligand XAT A1 318



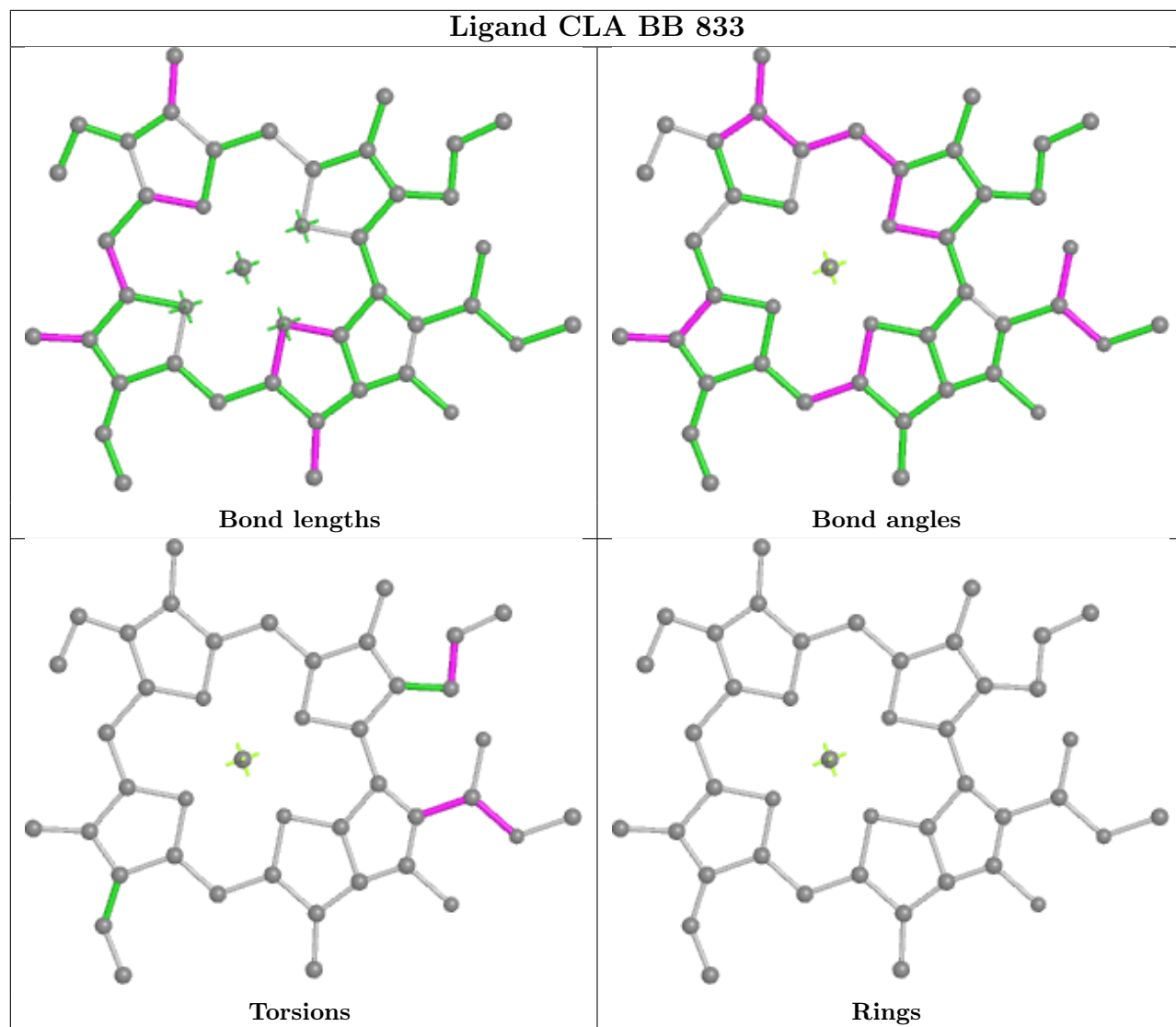
Ligand CLA A4 311



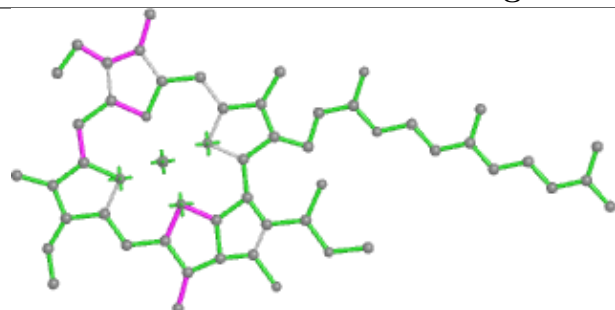
Ligand CLA B3 301



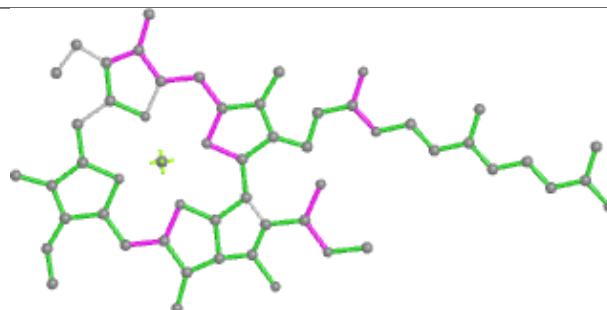
Ligand CLA BB 833



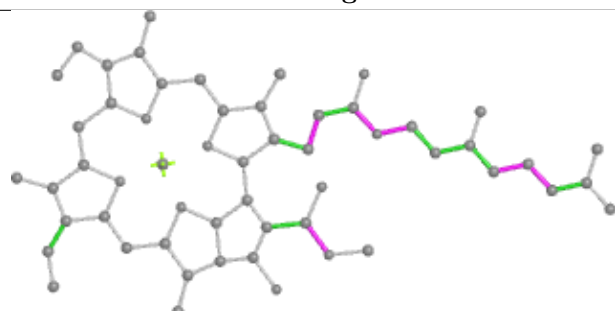
Ligand CLA BB 818



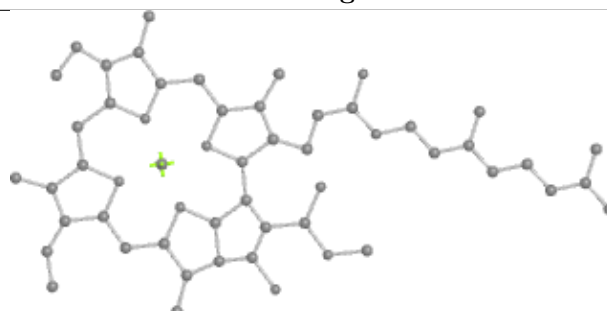
Bond lengths



Bond angles

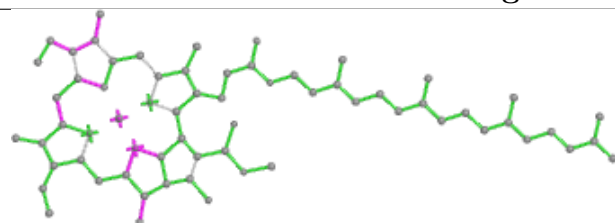


Torsions

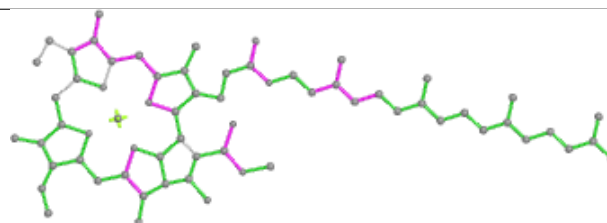


Rings

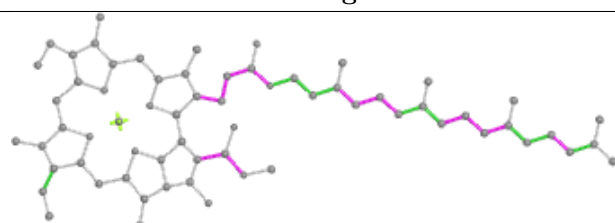
Ligand CLA AA 829



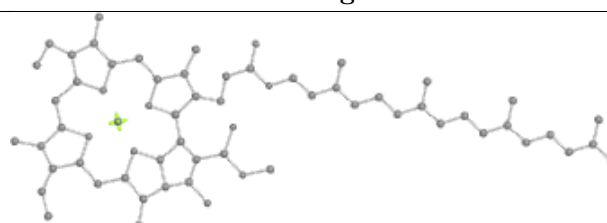
Bond lengths



Bond angles

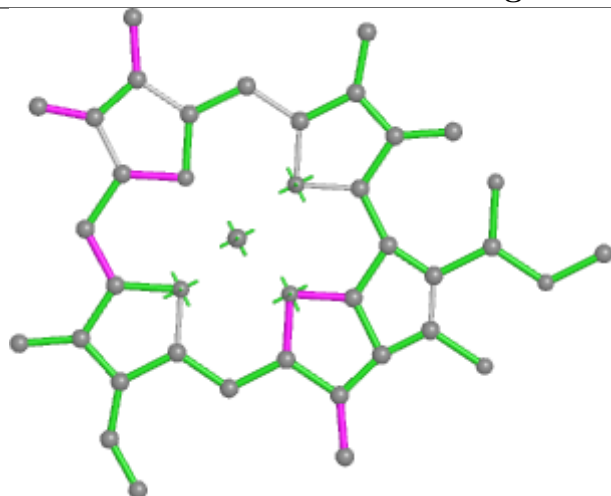


Torsions

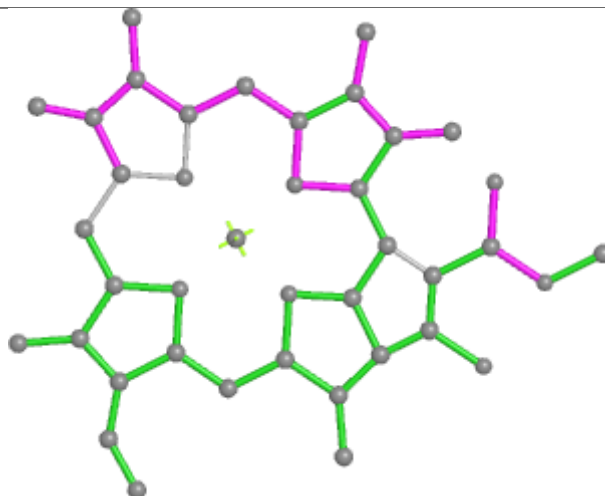


Rings

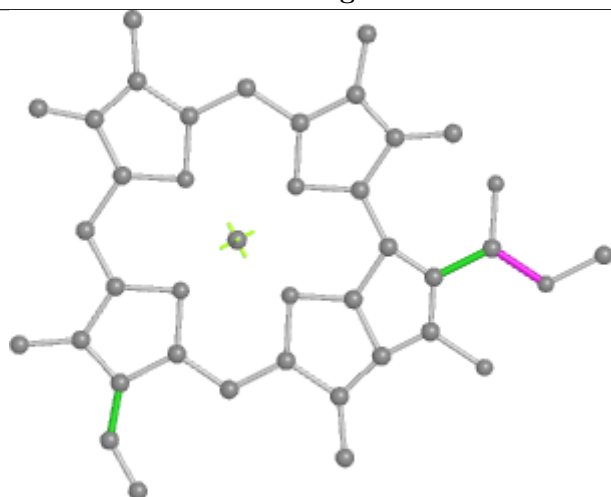
Ligand CLA A1 310



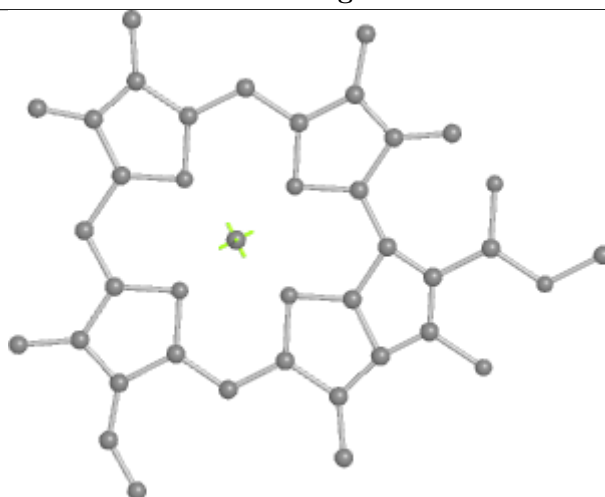
Bond lengths



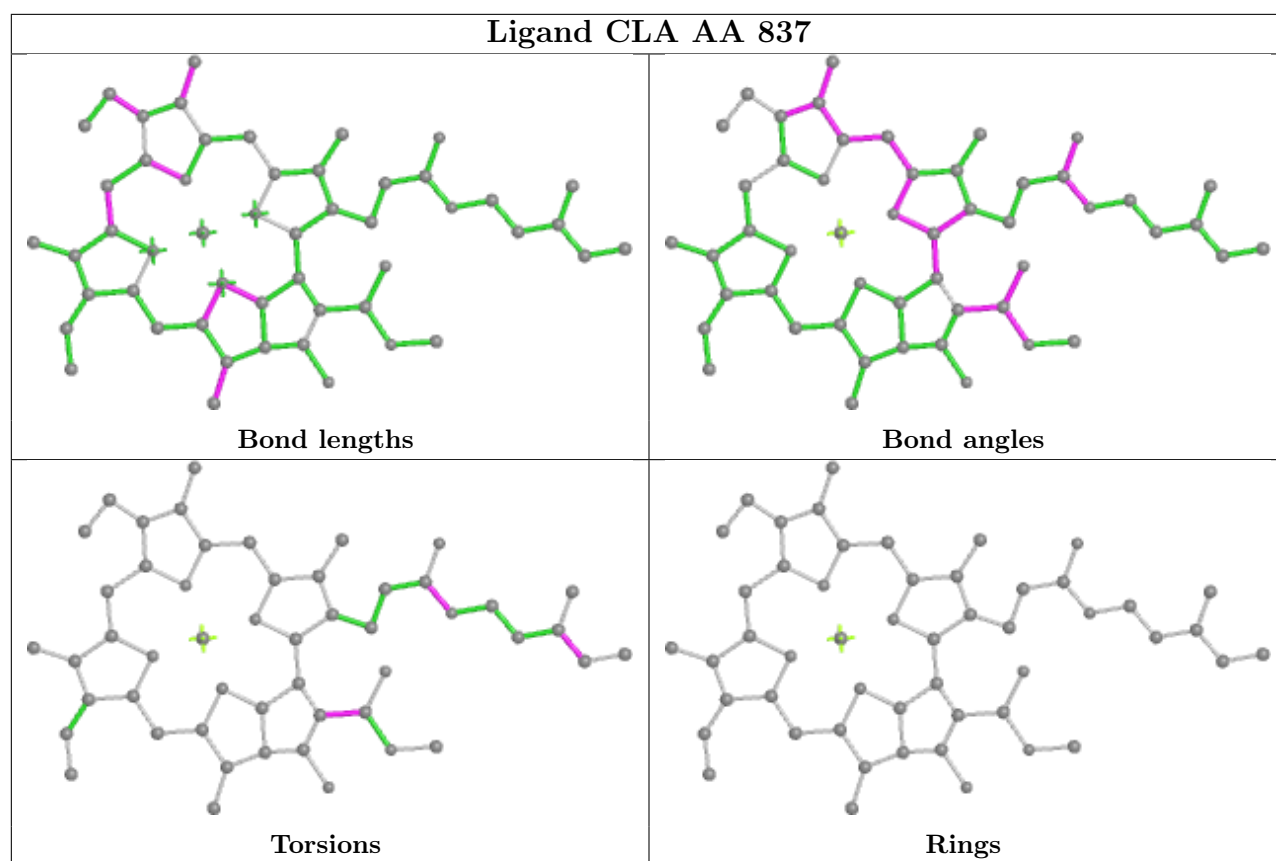
Bond angles

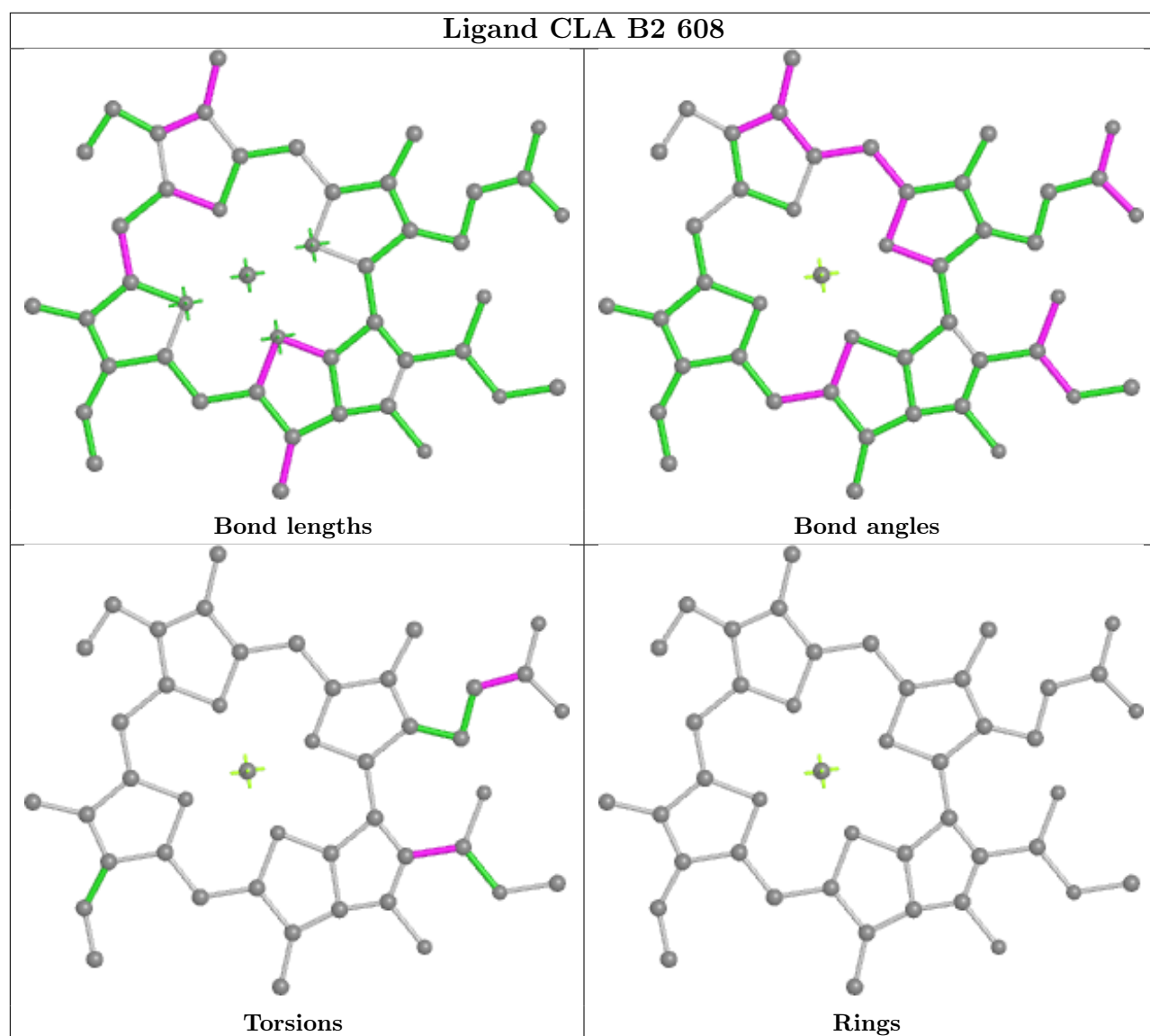


Torsions

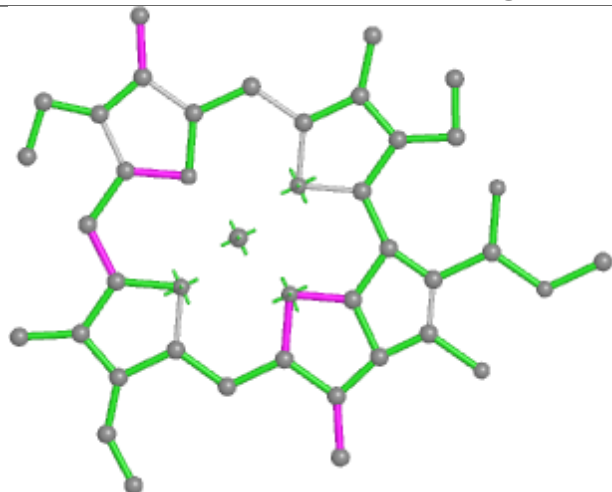


Rings

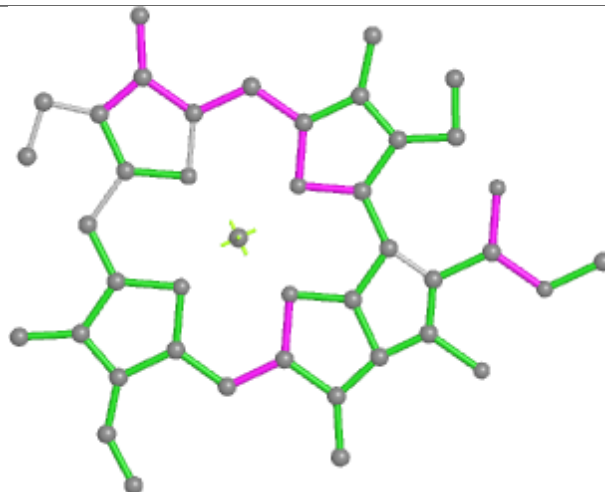




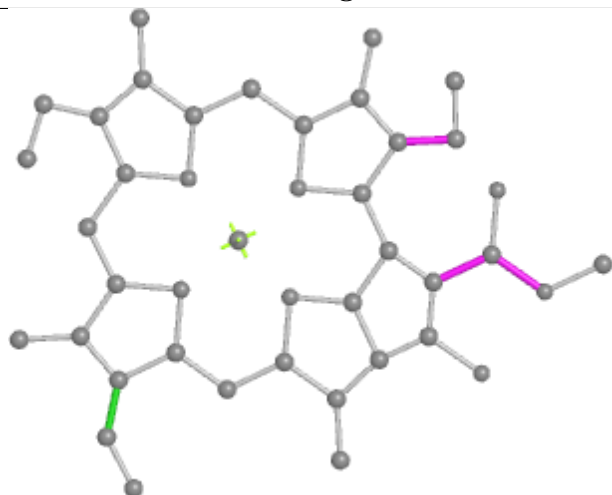
Ligand CLA BA 822



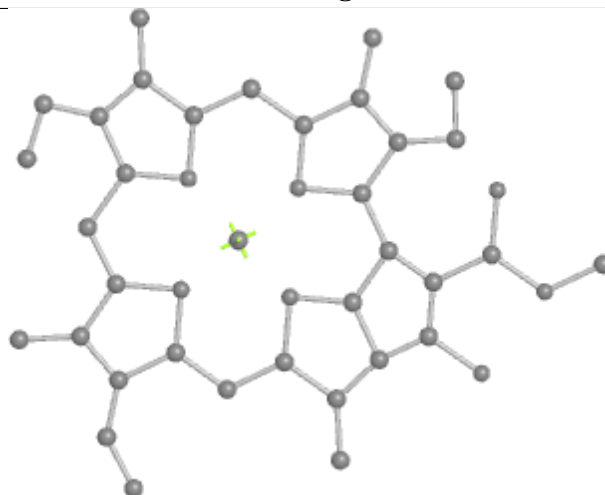
Bond lengths



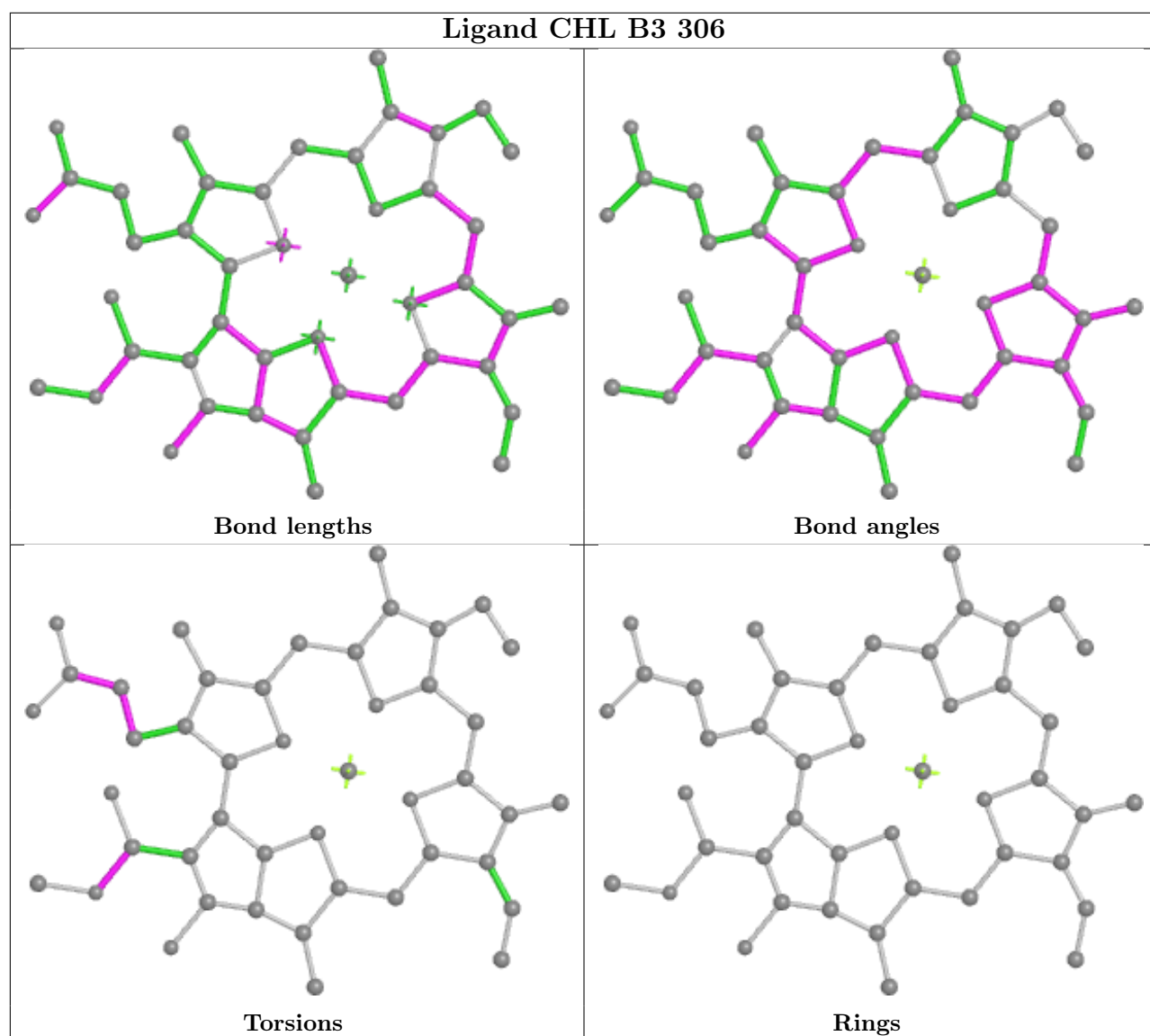
Bond angles

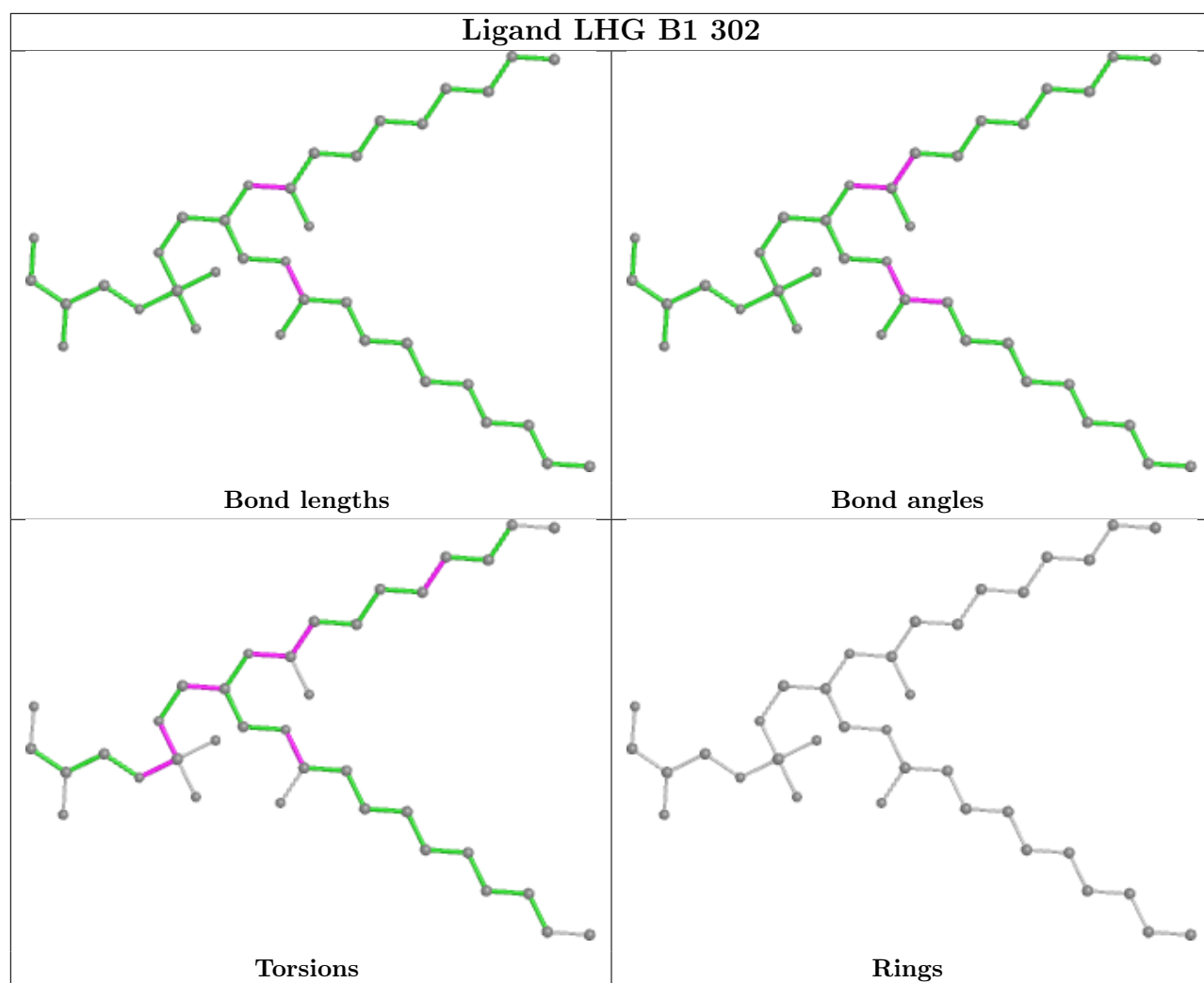


Torsions

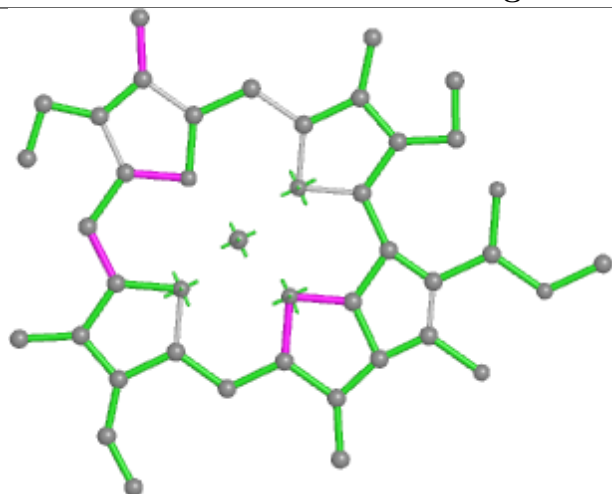


Rings

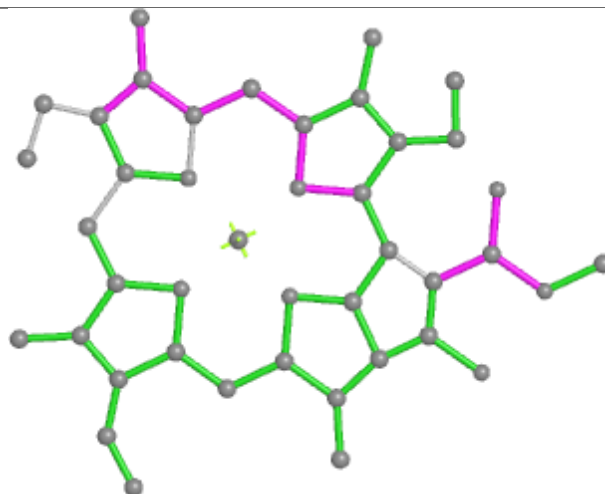




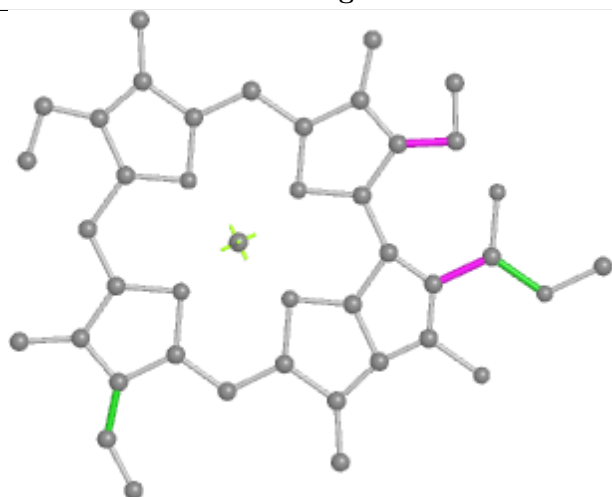
Ligand CLA A4 309



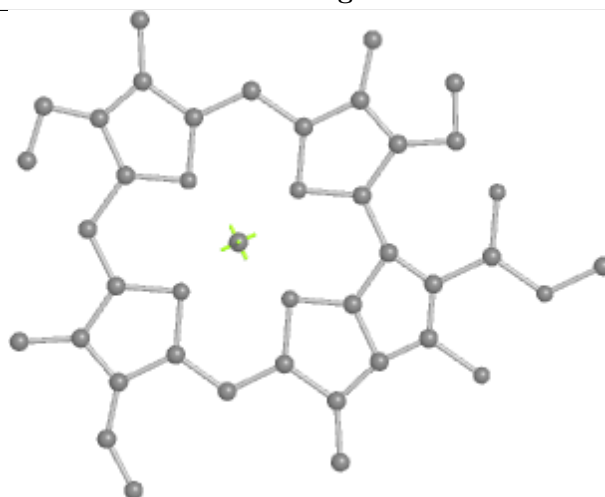
Bond lengths



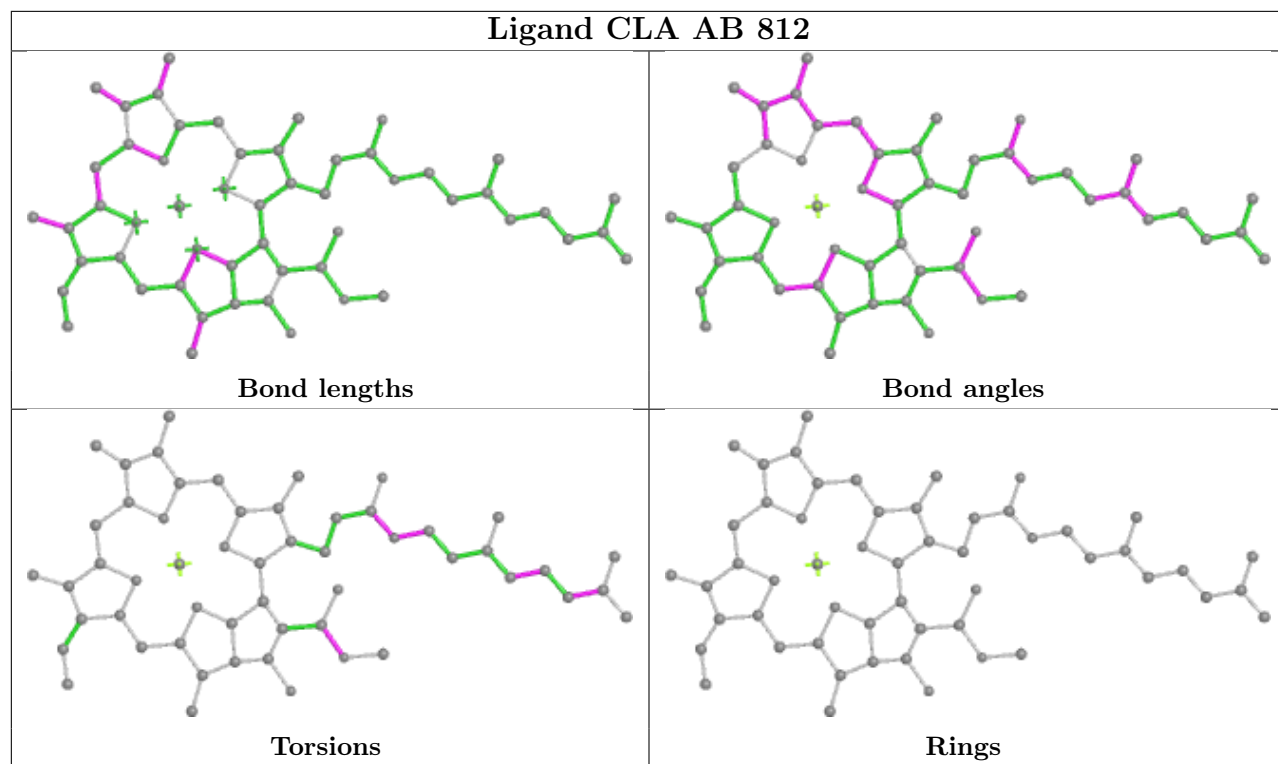
Bond angles

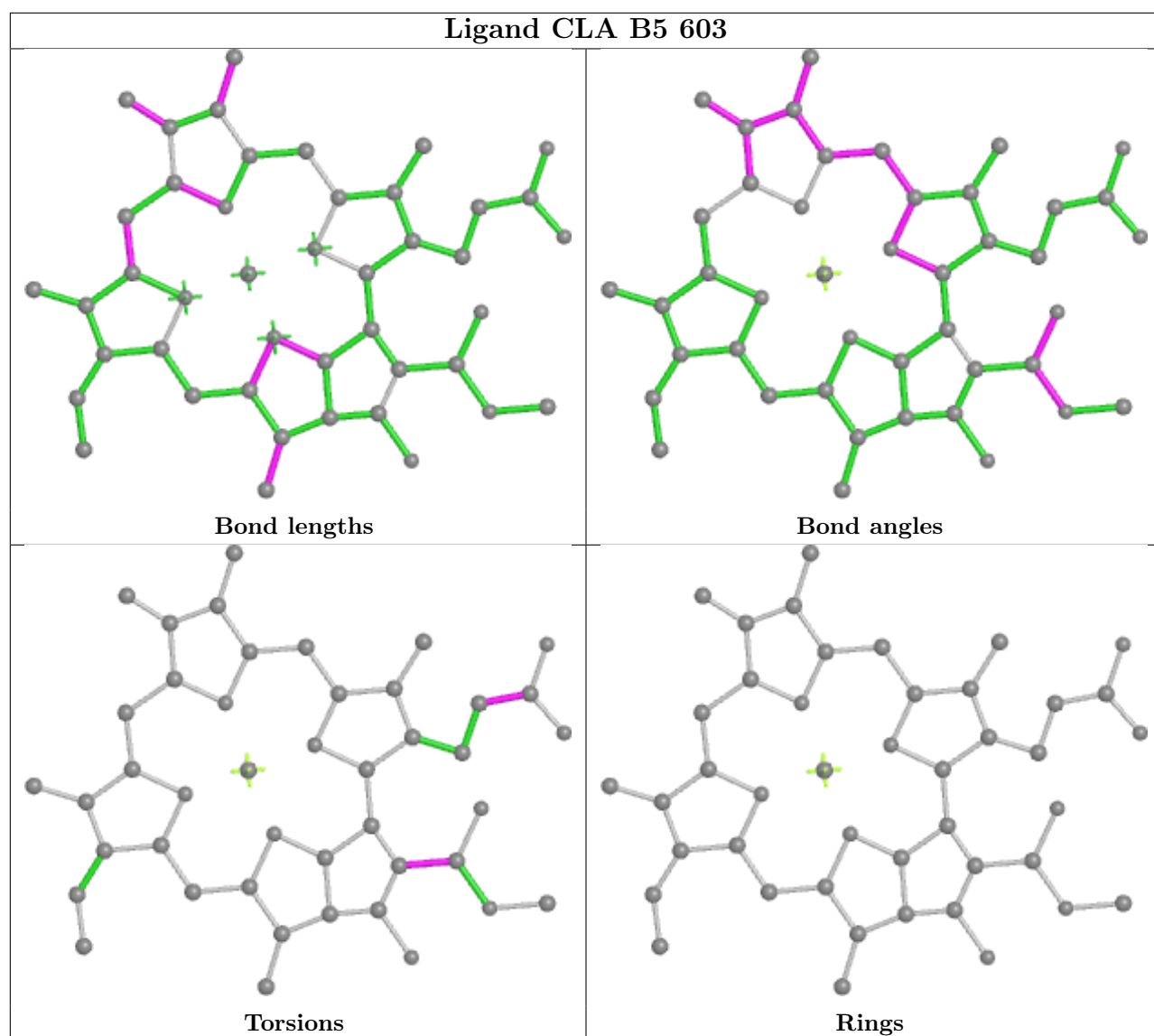


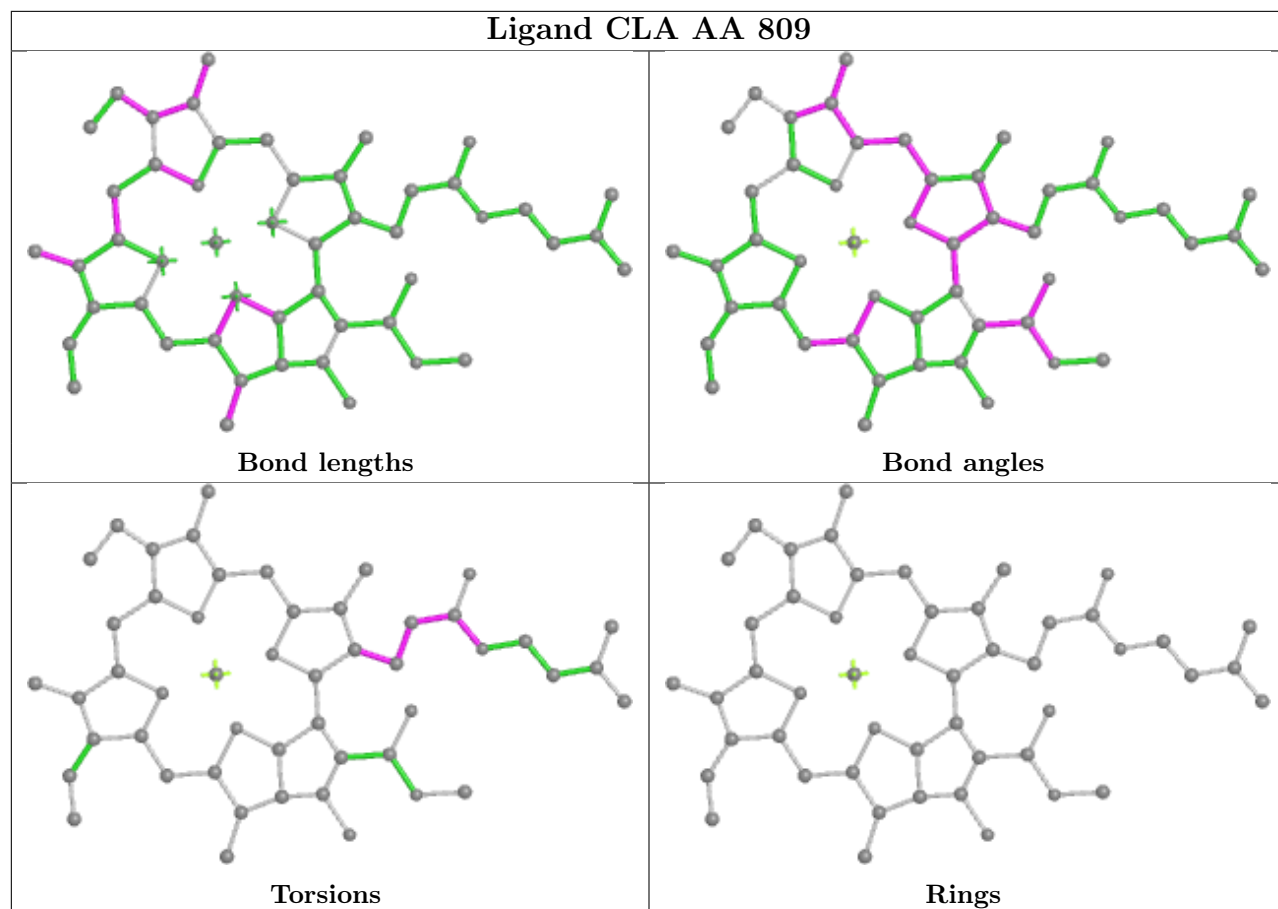
Torsions



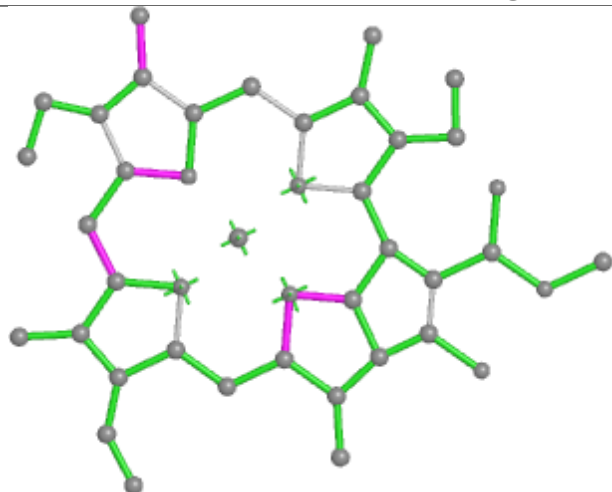
Rings



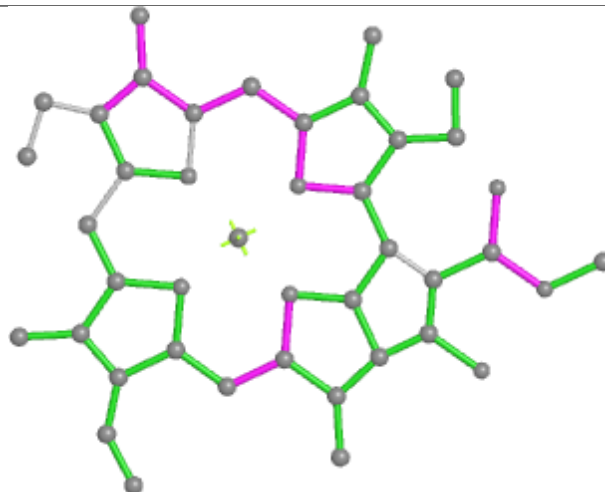




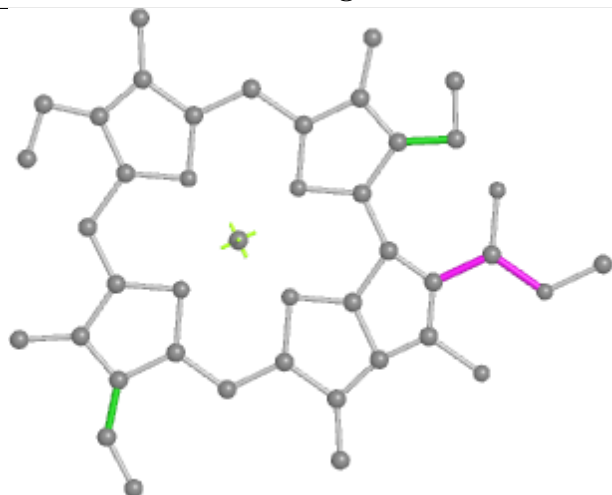
Ligand CLA BJ 102



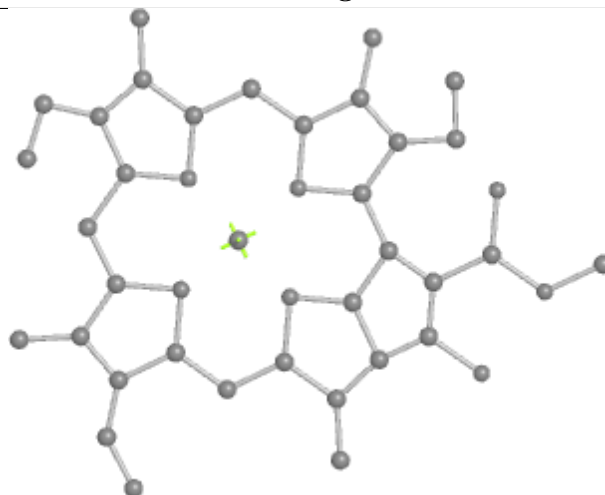
Bond lengths



Bond angles

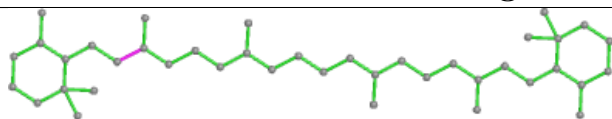


Torsions

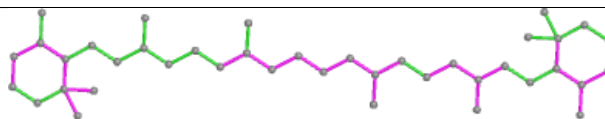


Rings

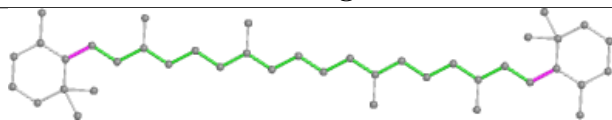
Ligand BCR BB 845



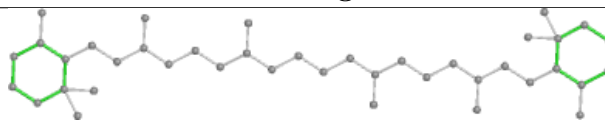
Bond lengths



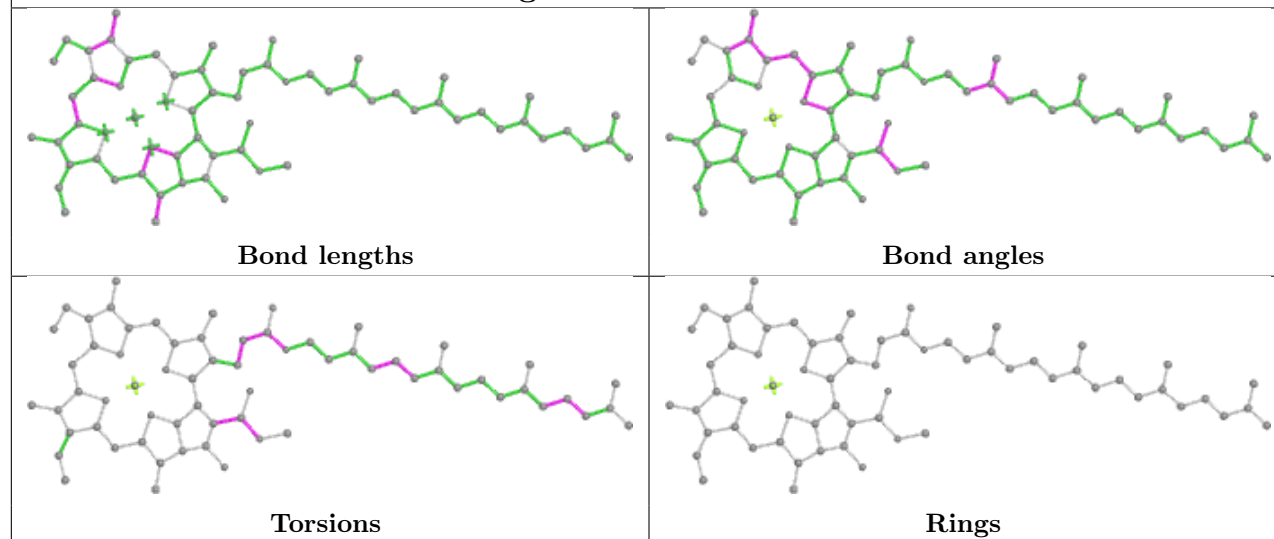
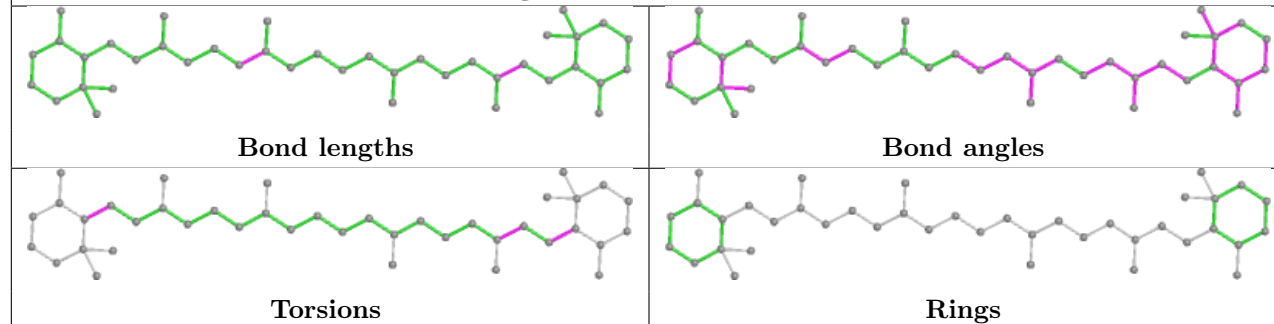
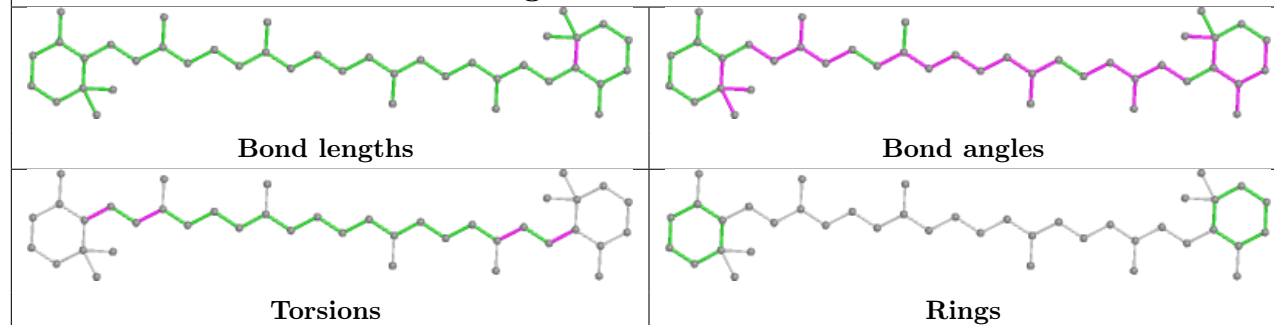
Bond angles



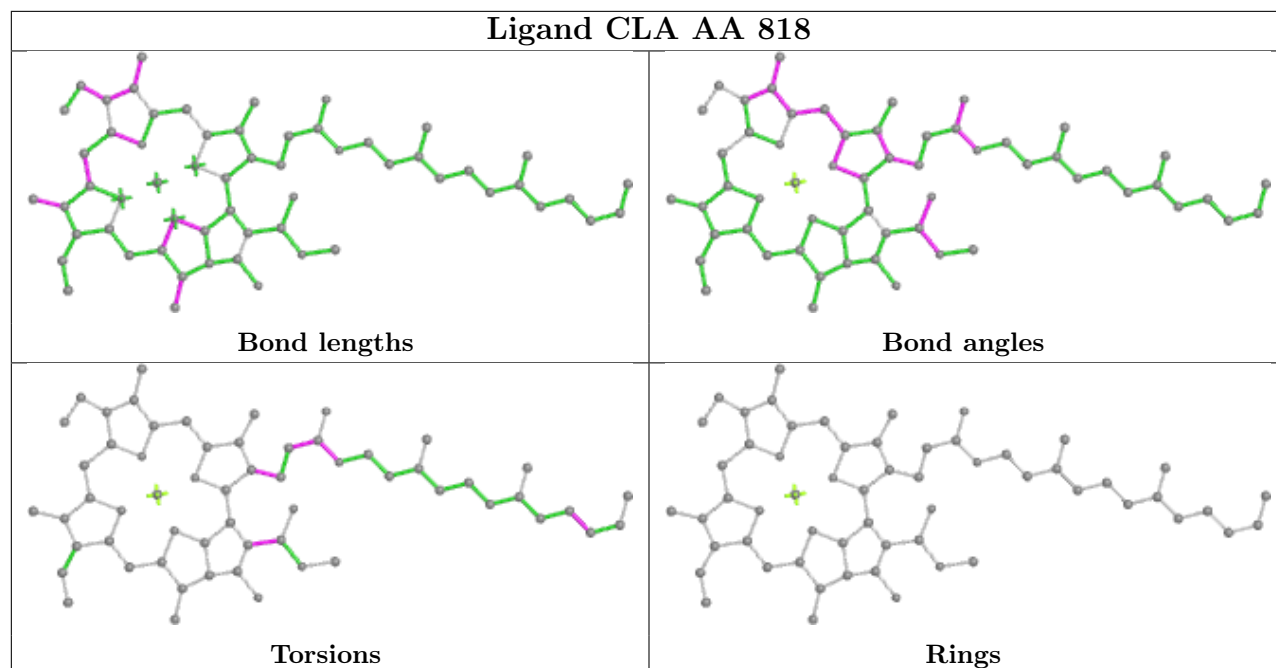
Torsions



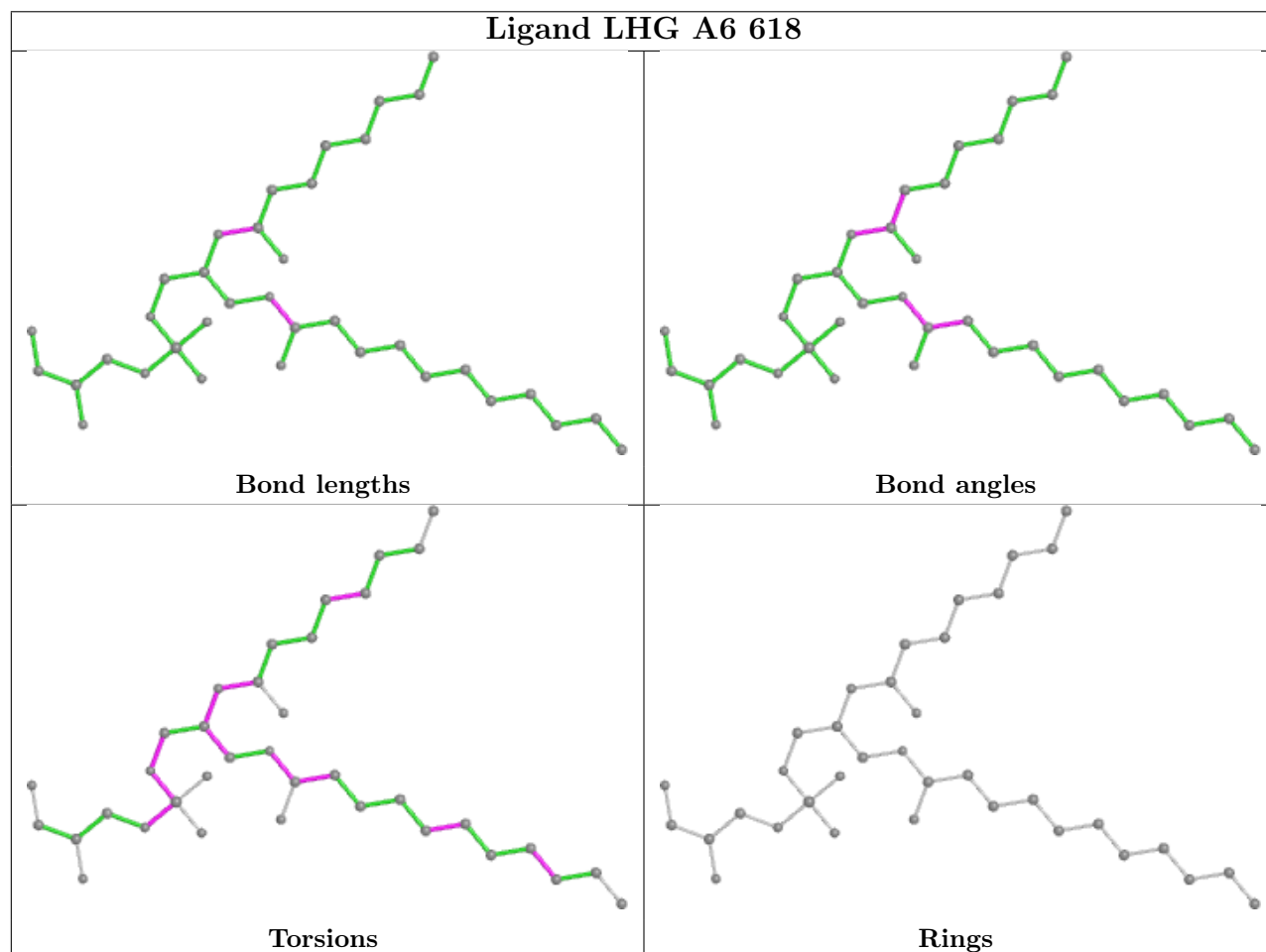
Rings

Ligand CLA BA 833**Ligand BCR AA 852****Ligand BCR AI 101**

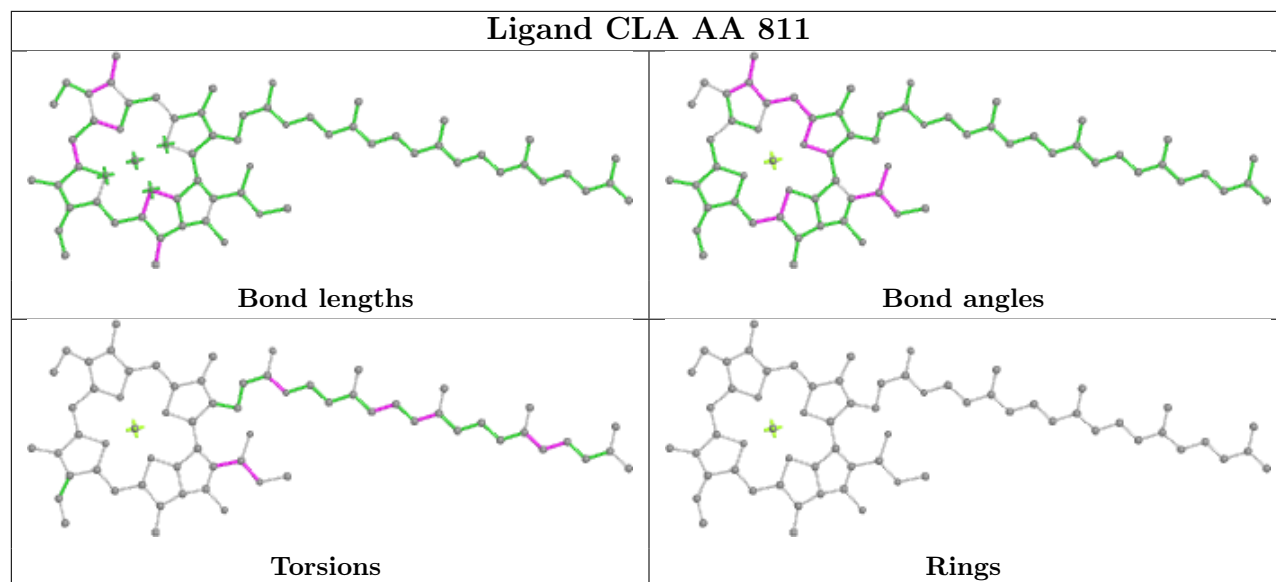
Ligand CLA AA 818



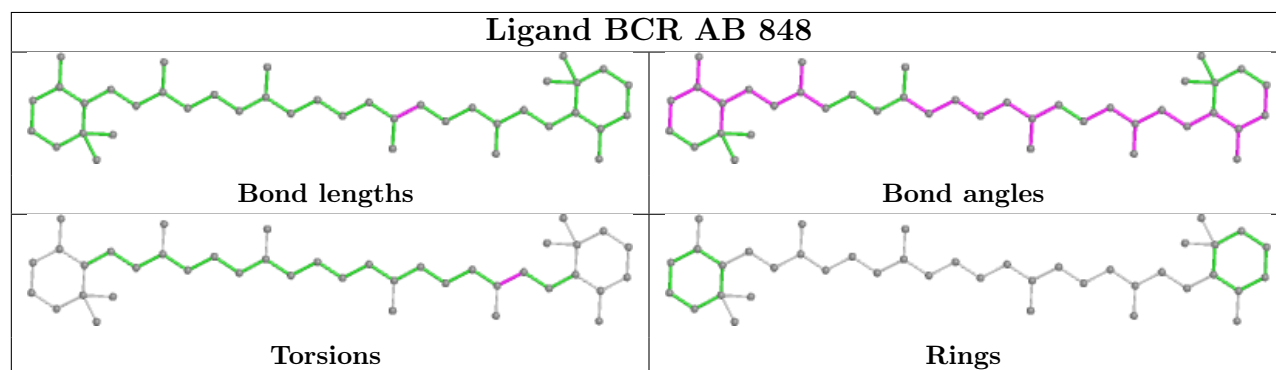
Ligand LHG A6 618

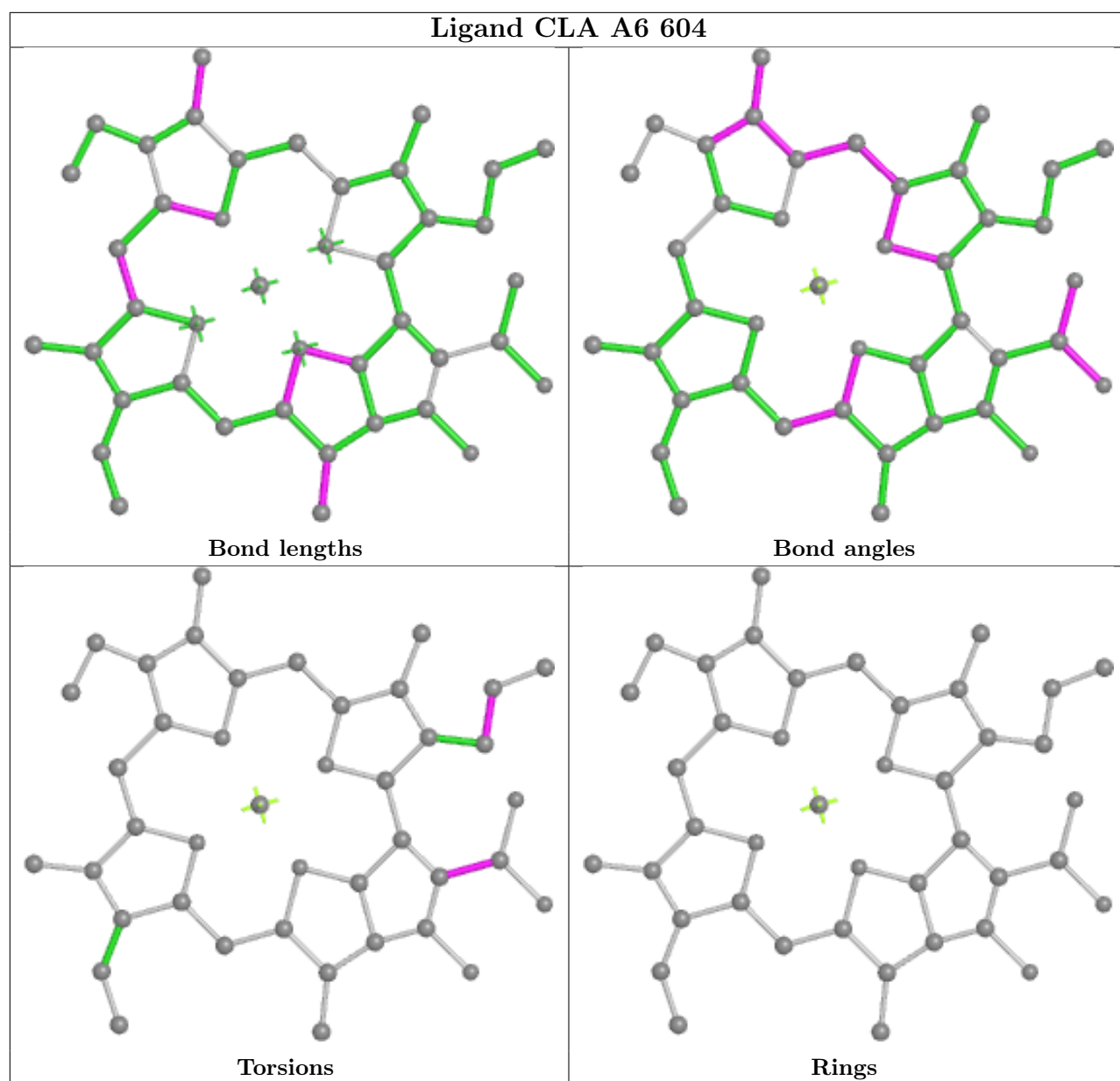


Ligand CLA AA 811

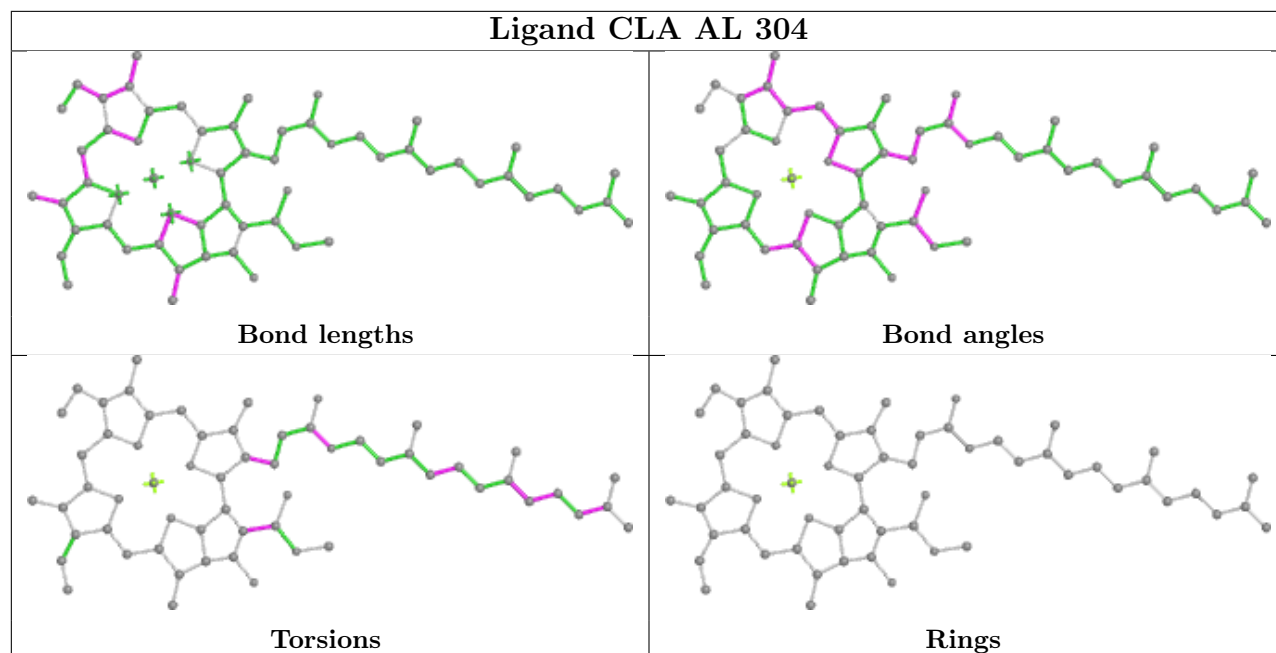


Ligand BCR AB 848

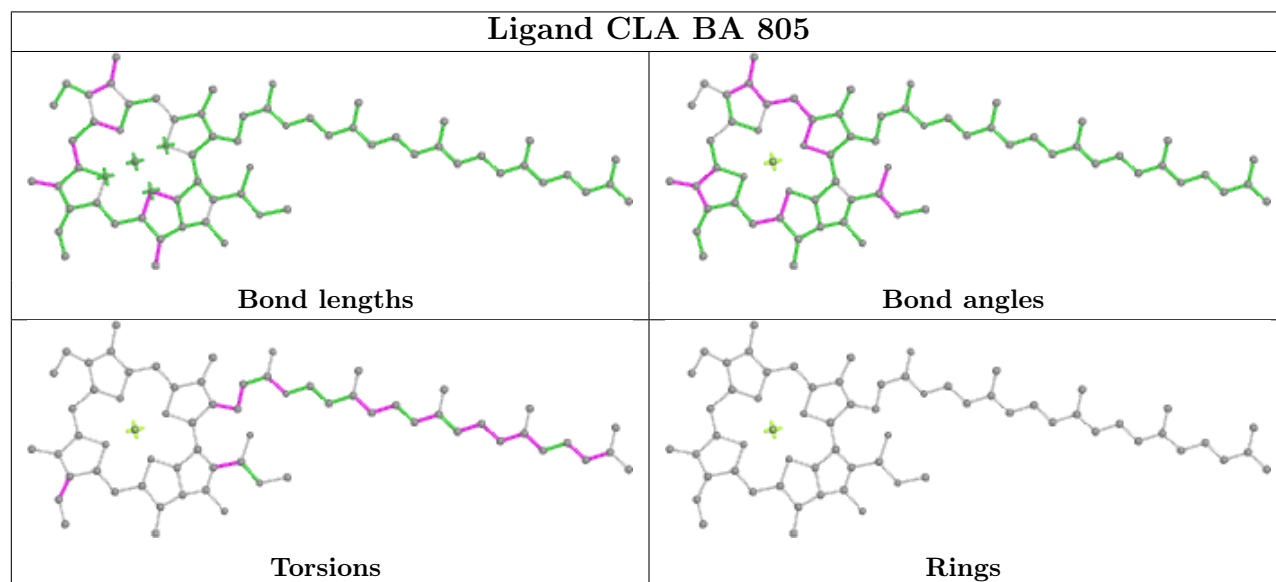




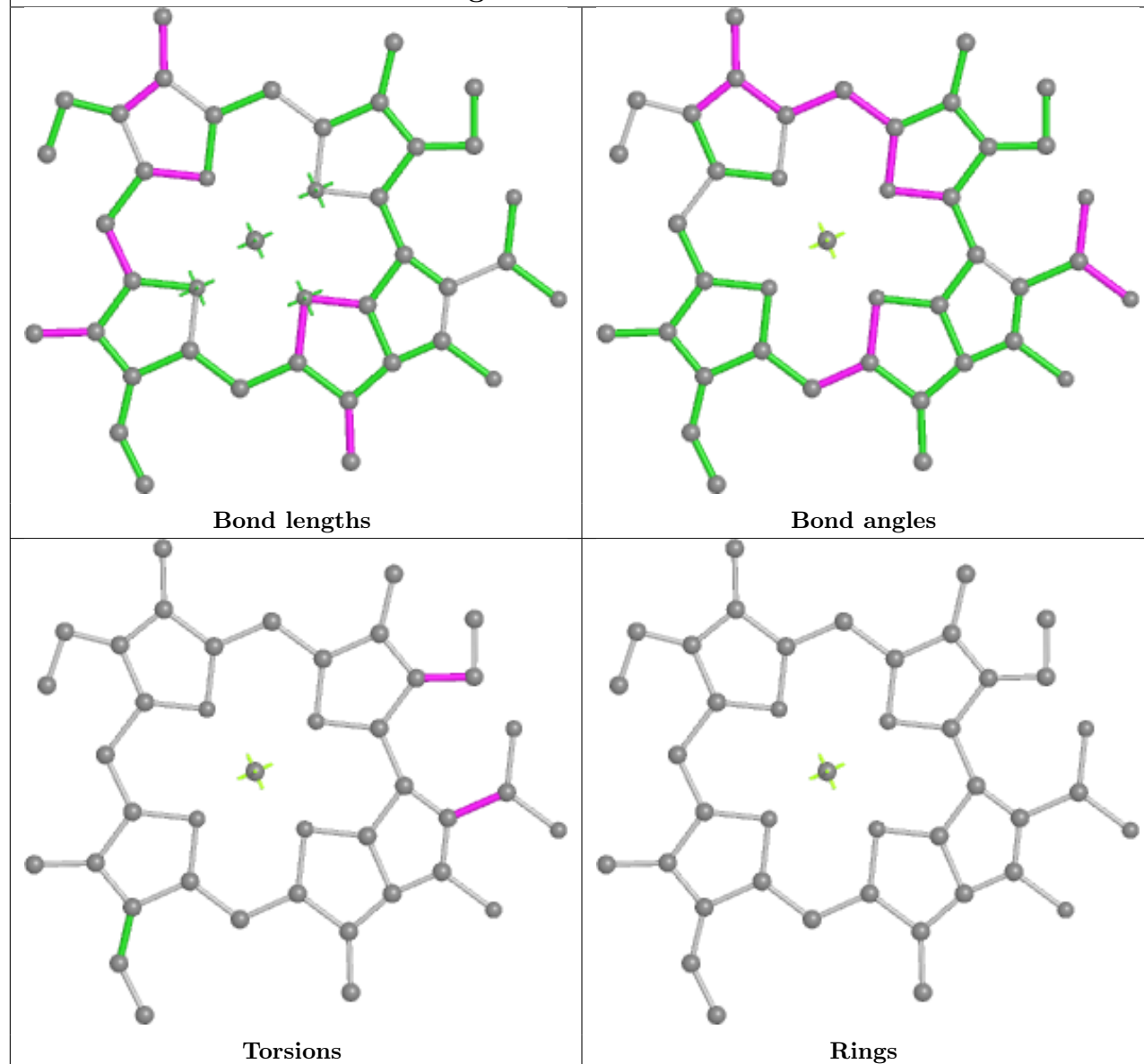
Ligand CLA AL 304



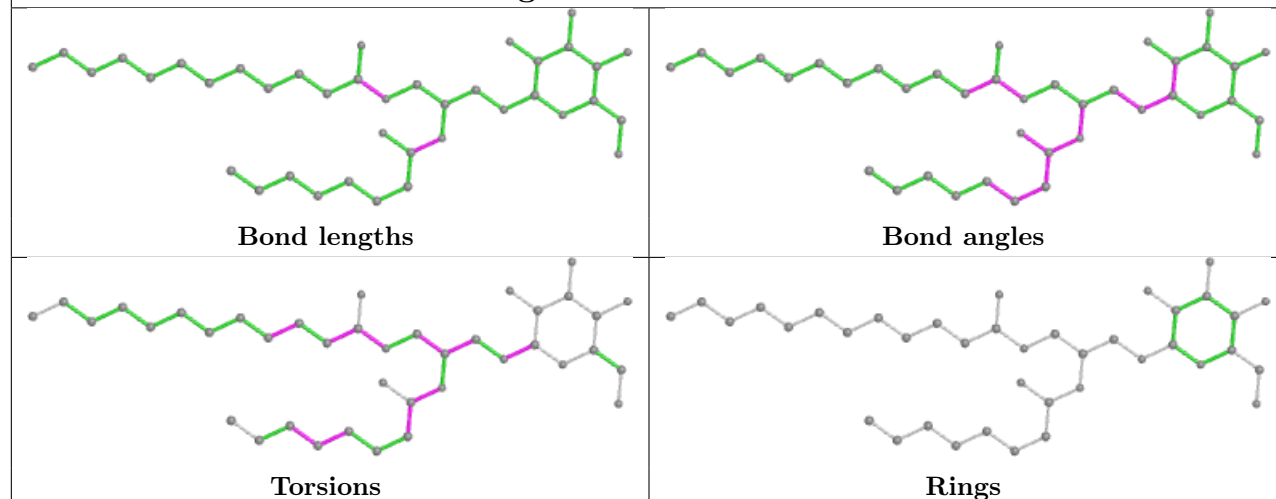
Ligand CLA BA 805



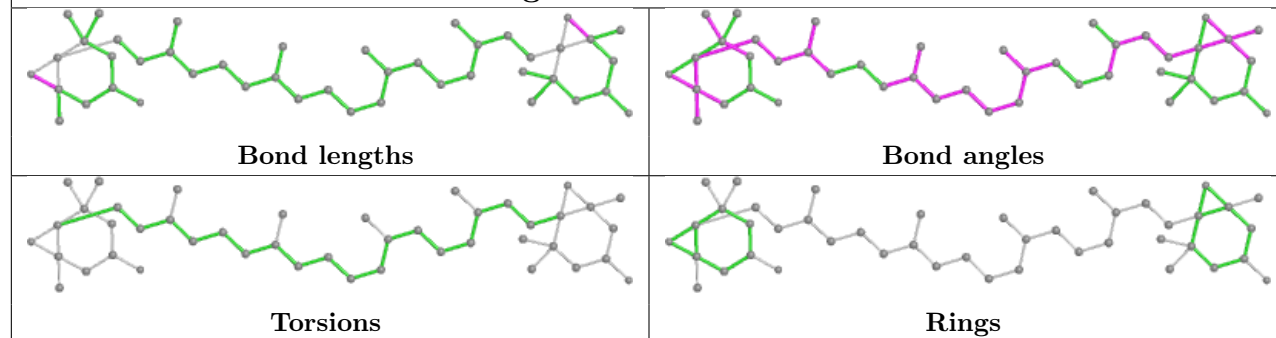
Ligand CLA A4 310



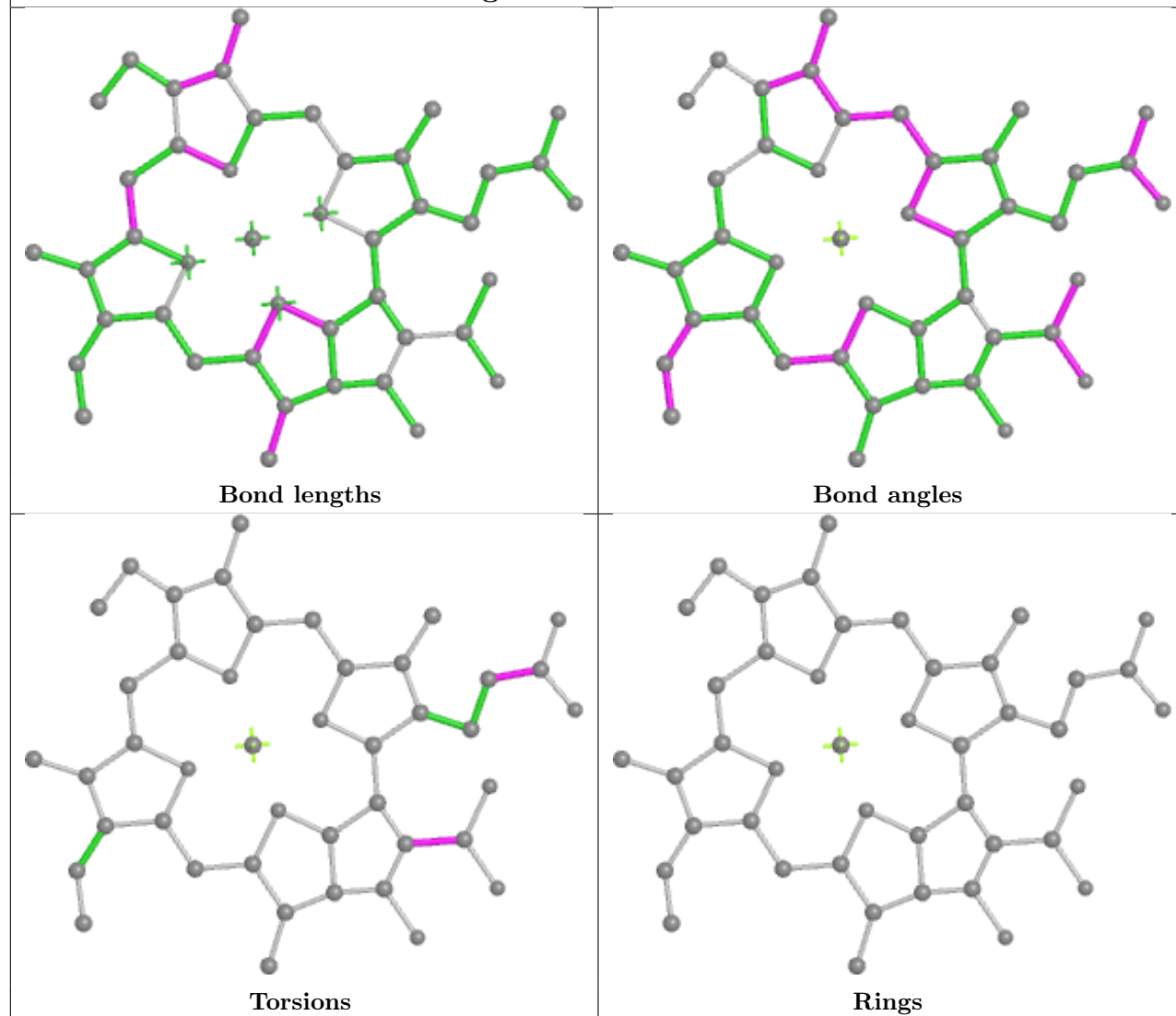
Ligand LMG A4 318



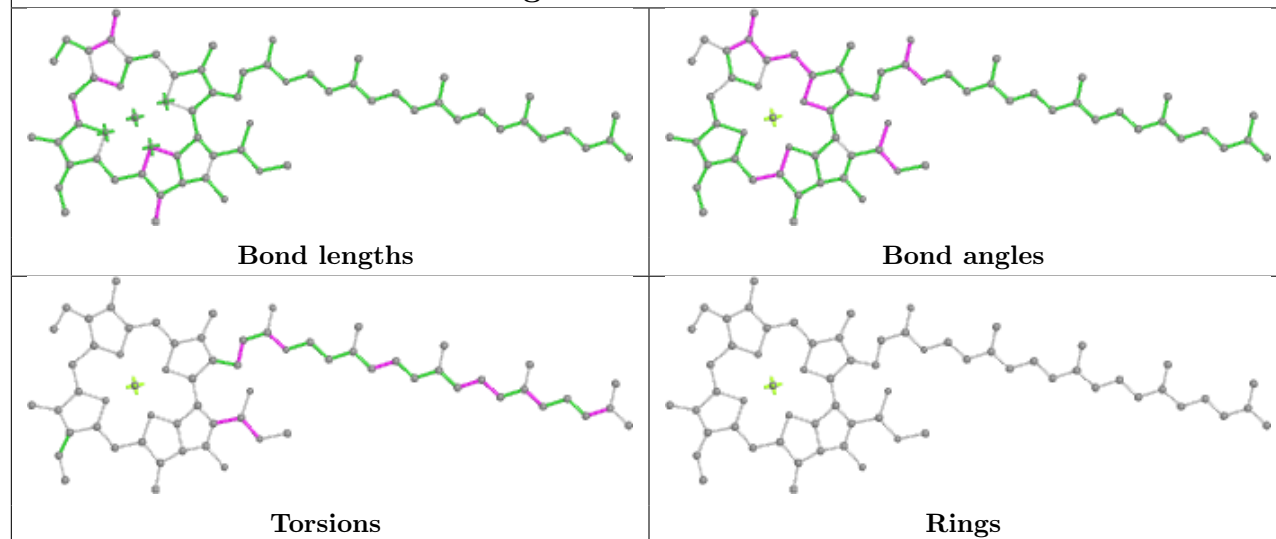
Ligand XAT B1 317



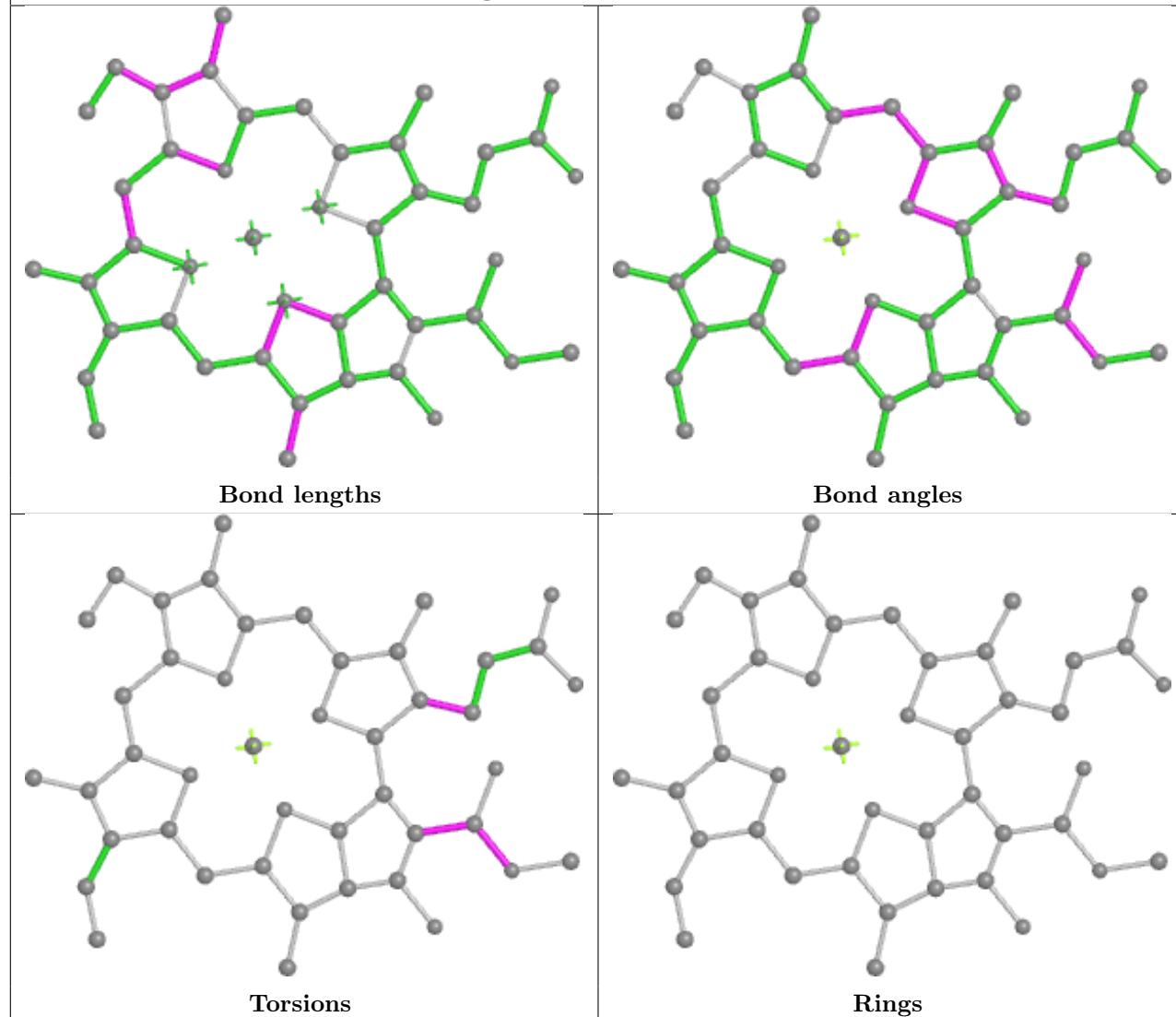
Ligand CLA B2 603



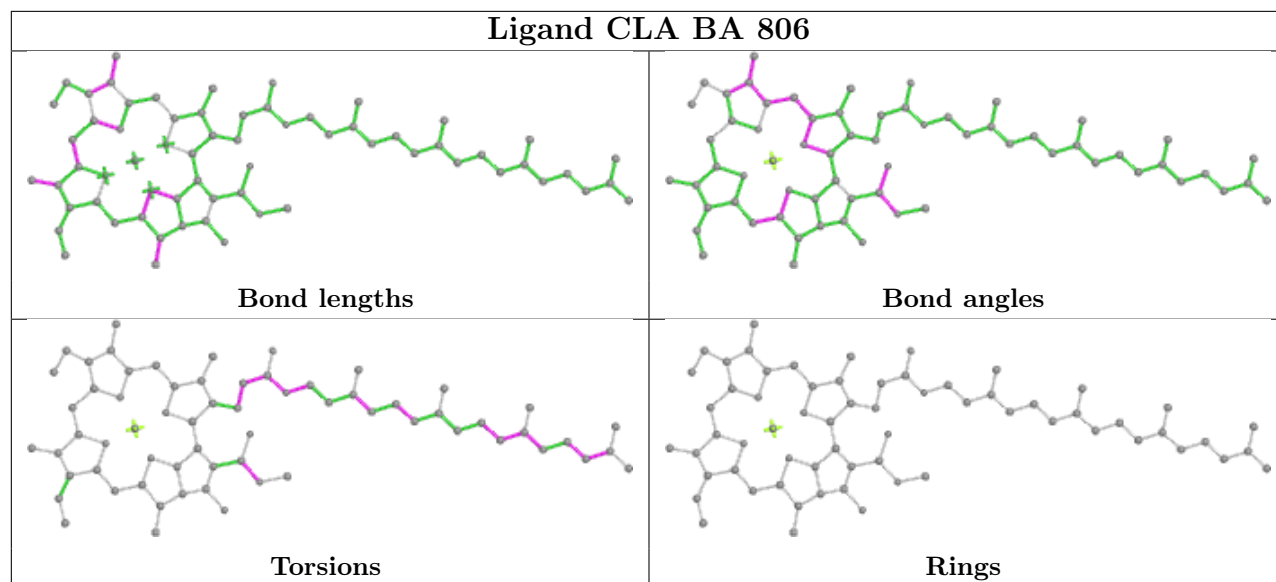
Ligand CLA B2 612



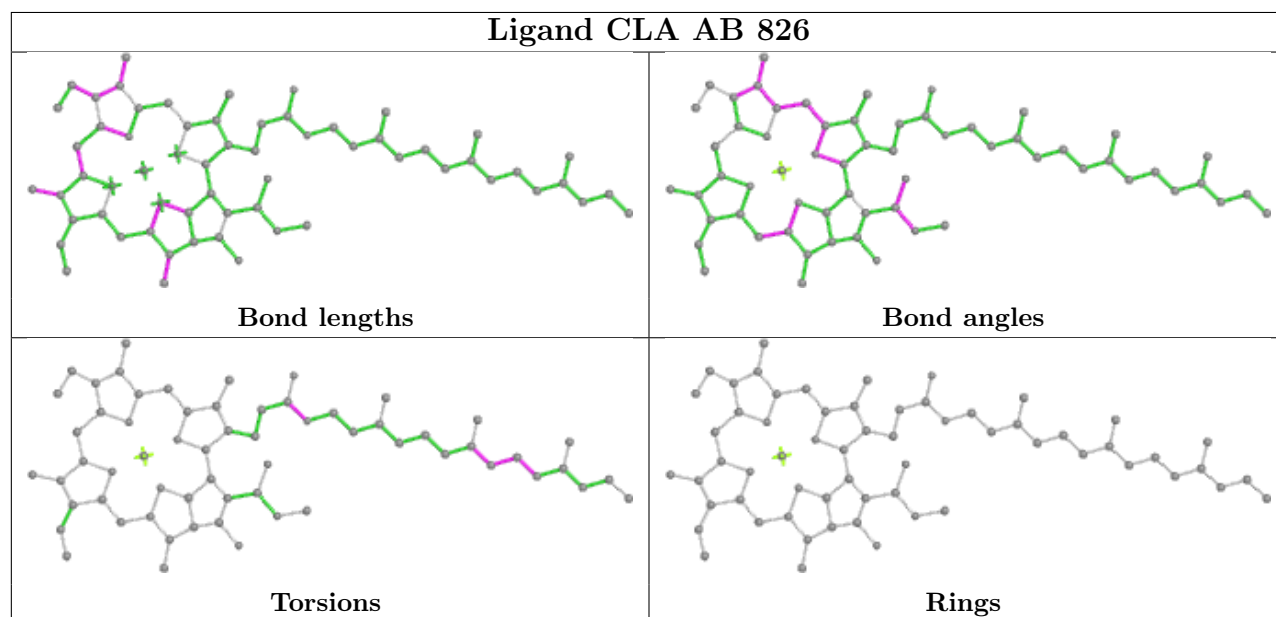
Ligand CLA BB 825

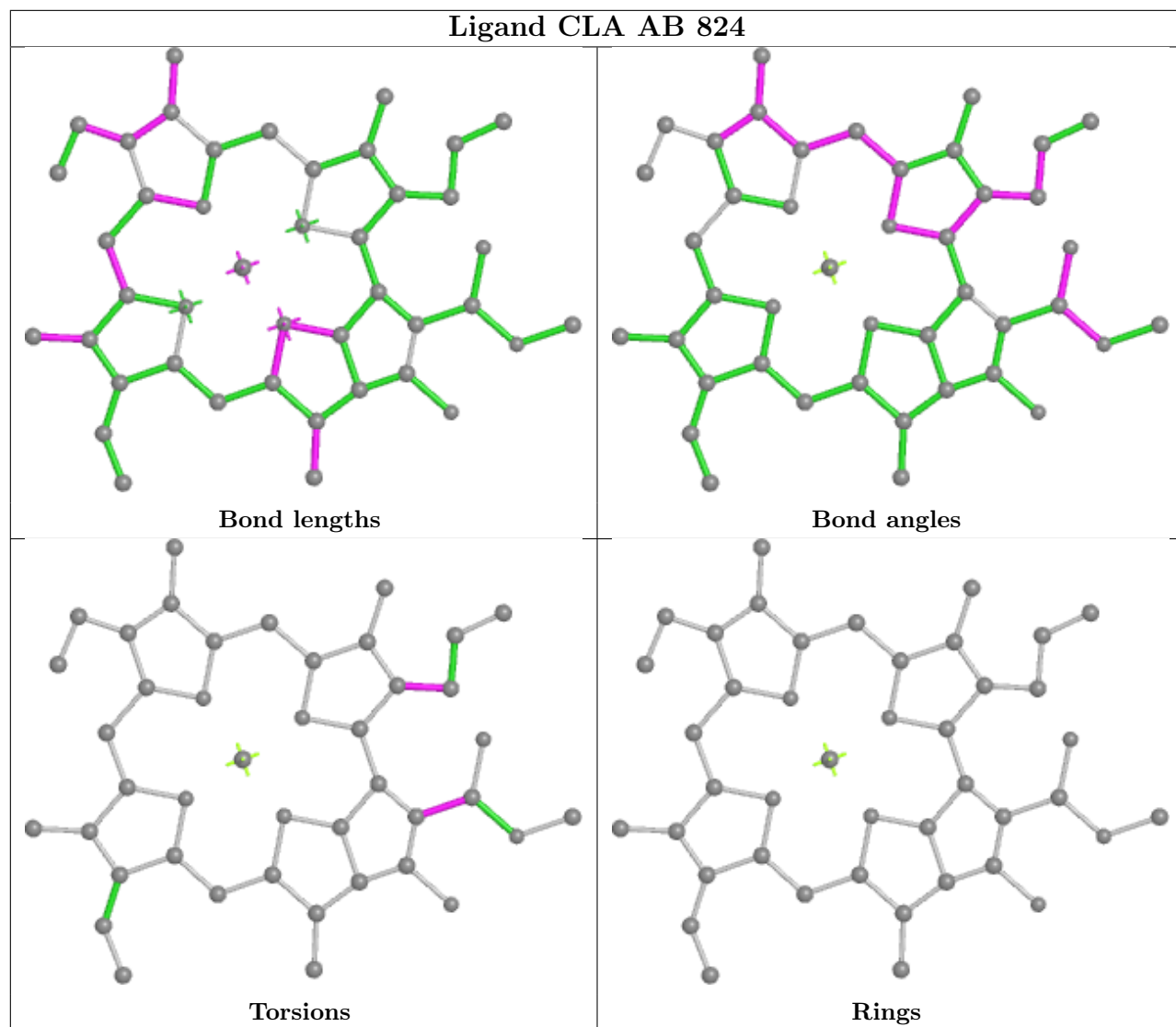


Ligand CLA BA 806

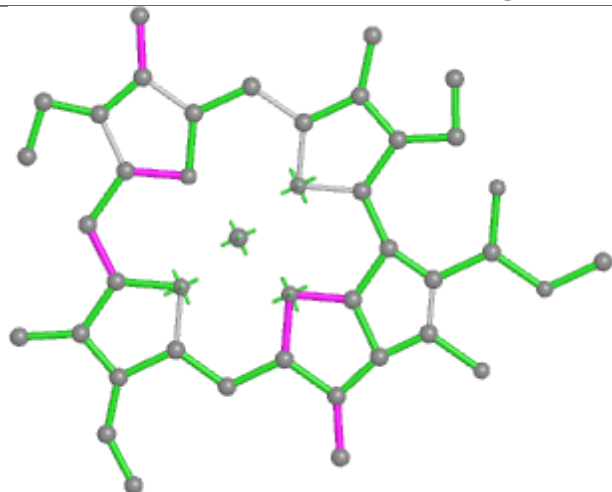


Ligand CLA AB 826

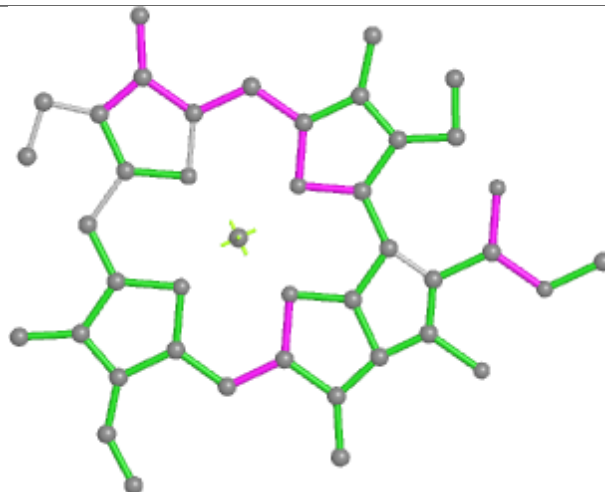




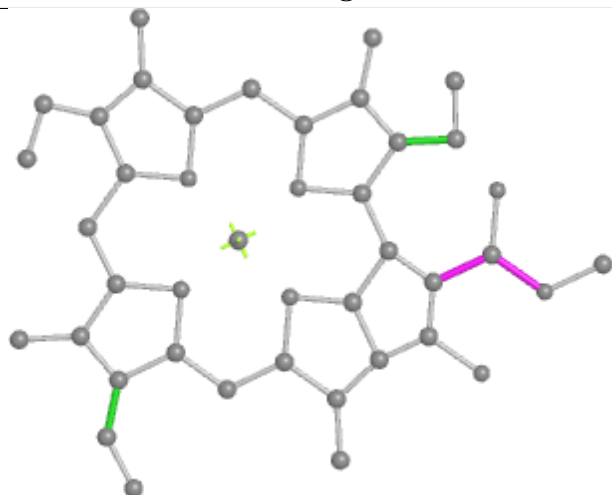
Ligand CLA AG 203



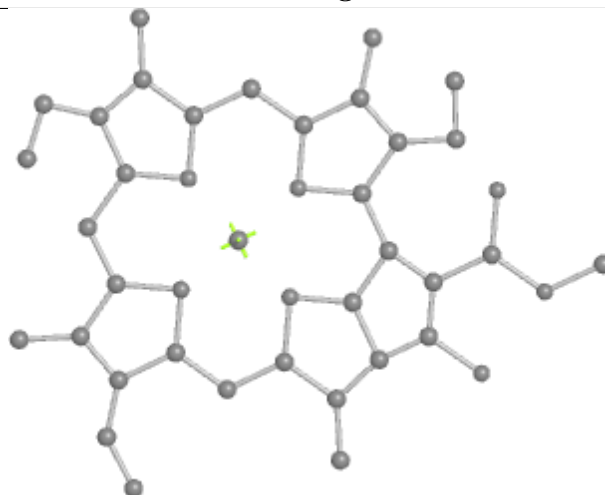
Bond lengths



Bond angles

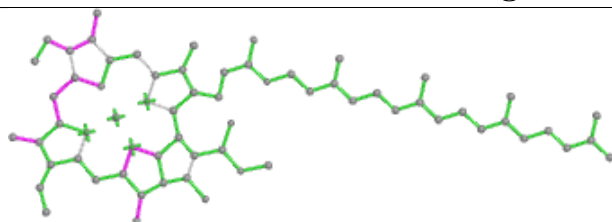


Torsions

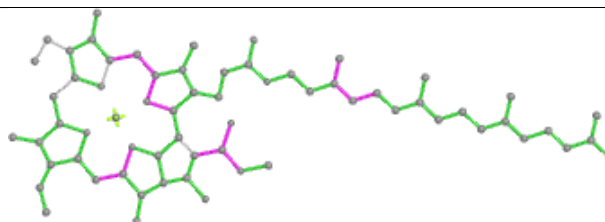


Rings

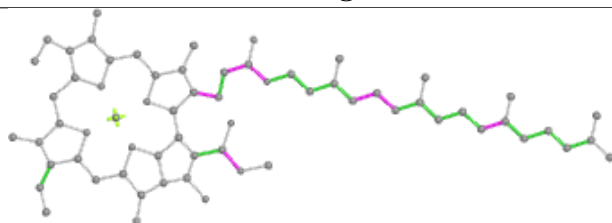
Ligand CLA BB 834



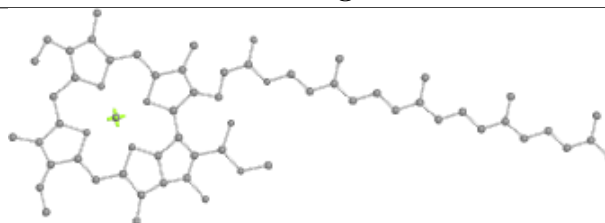
Bond lengths



Bond angles

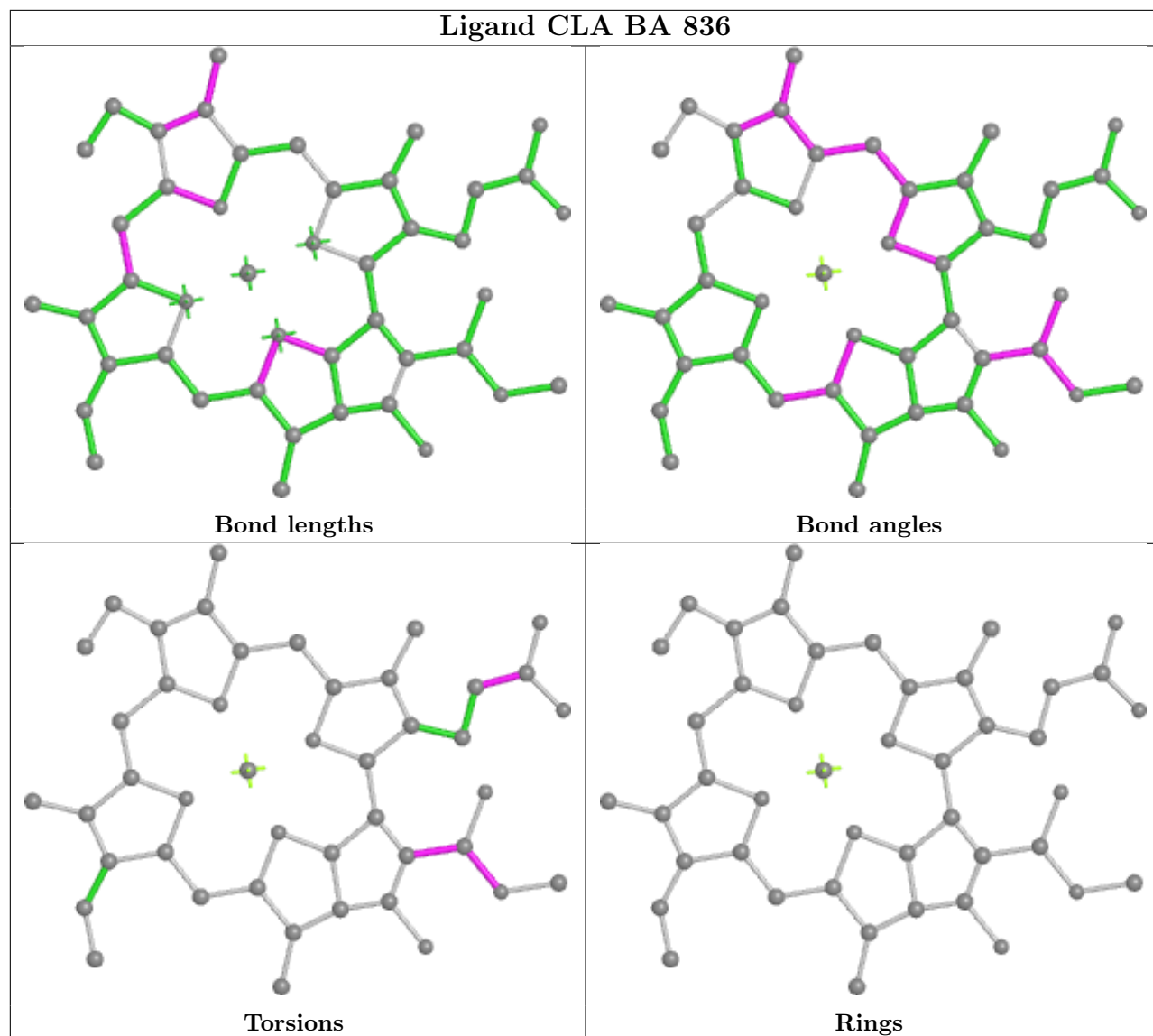


Torsions

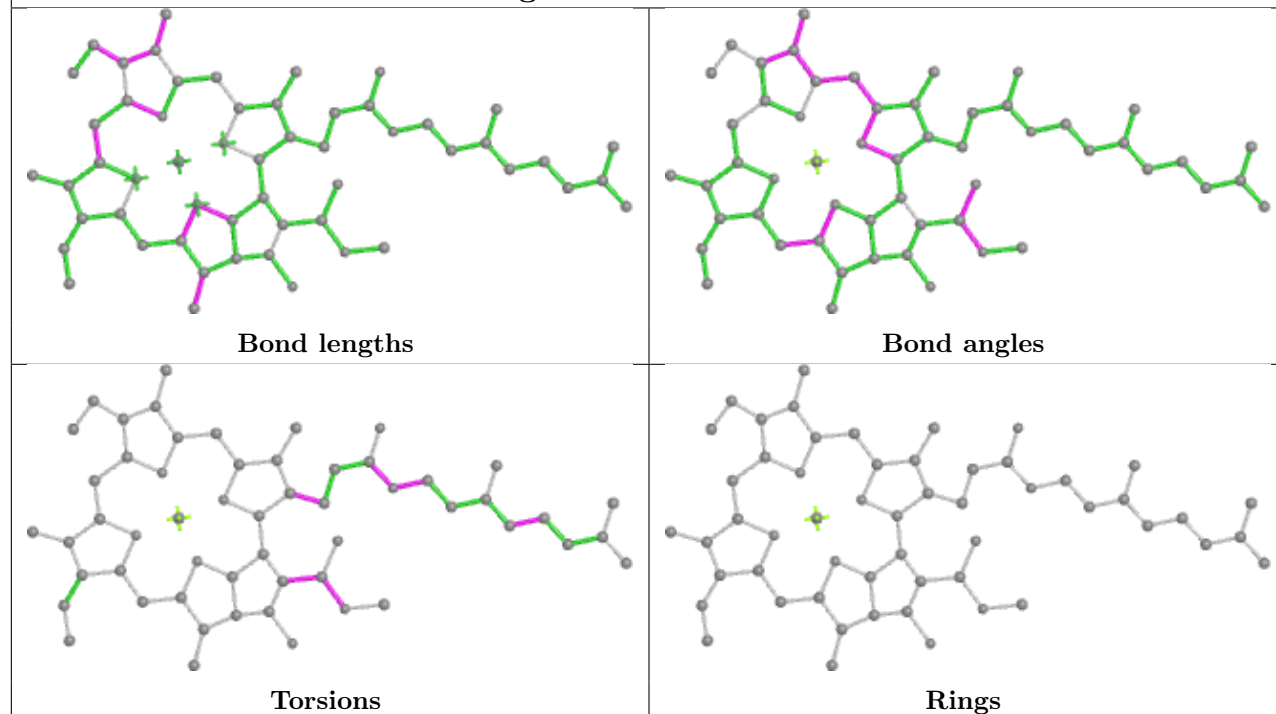


Rings

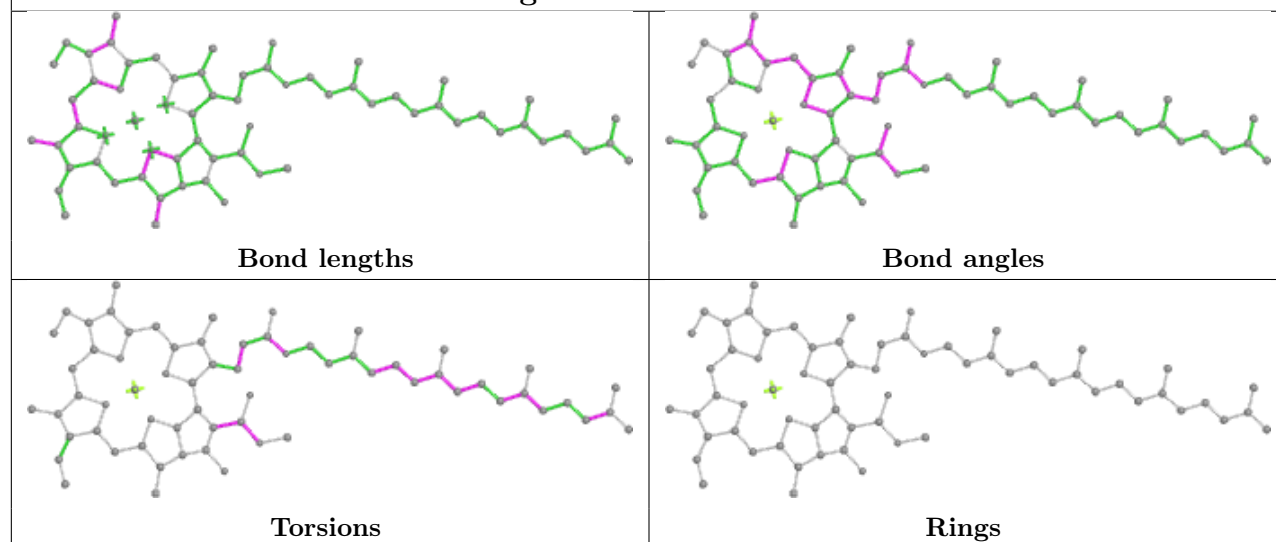
Ligand CLA BA 836



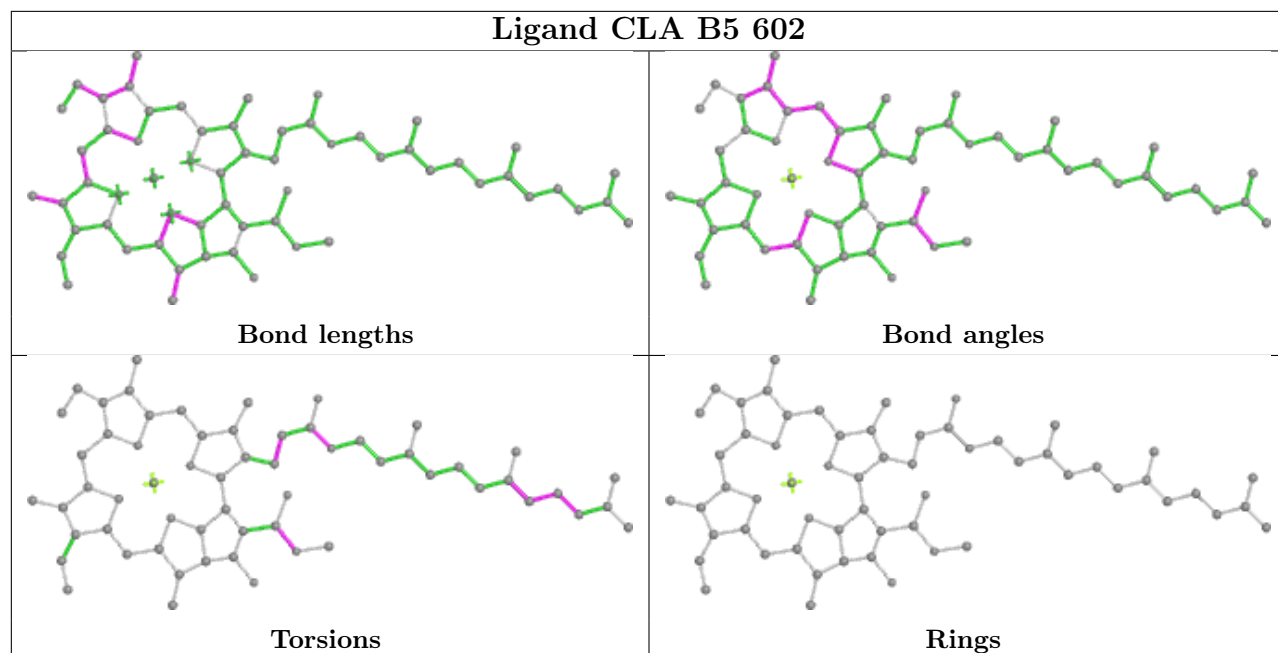
Ligand CLA AB 820



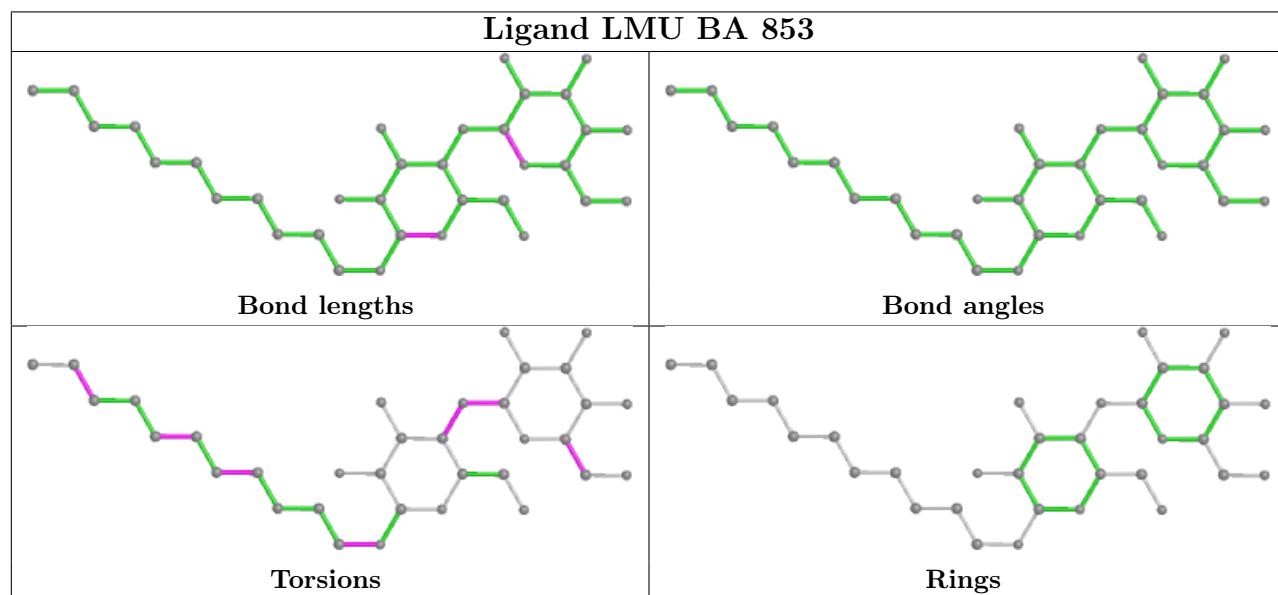
Ligand CLA BB 824

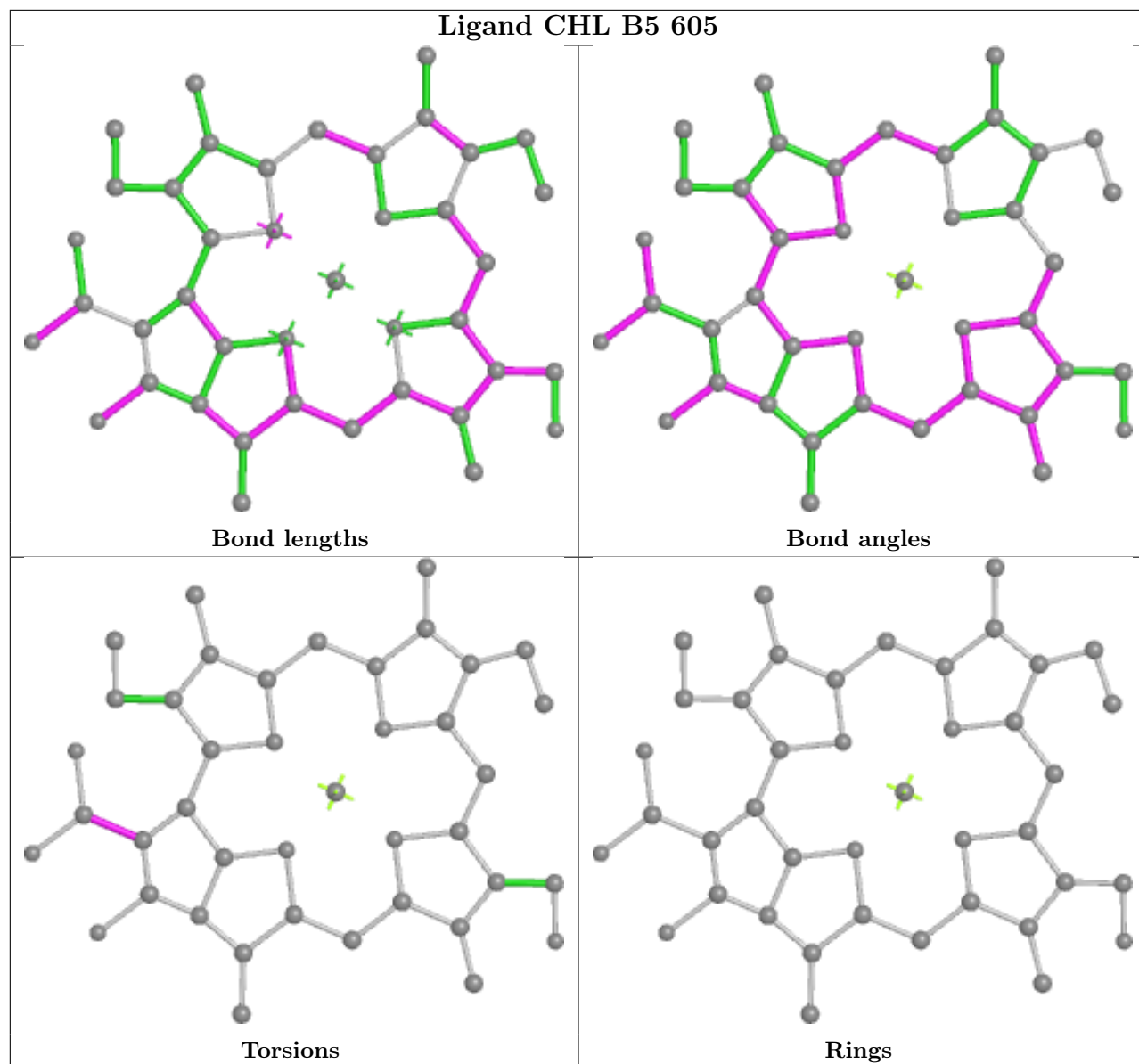


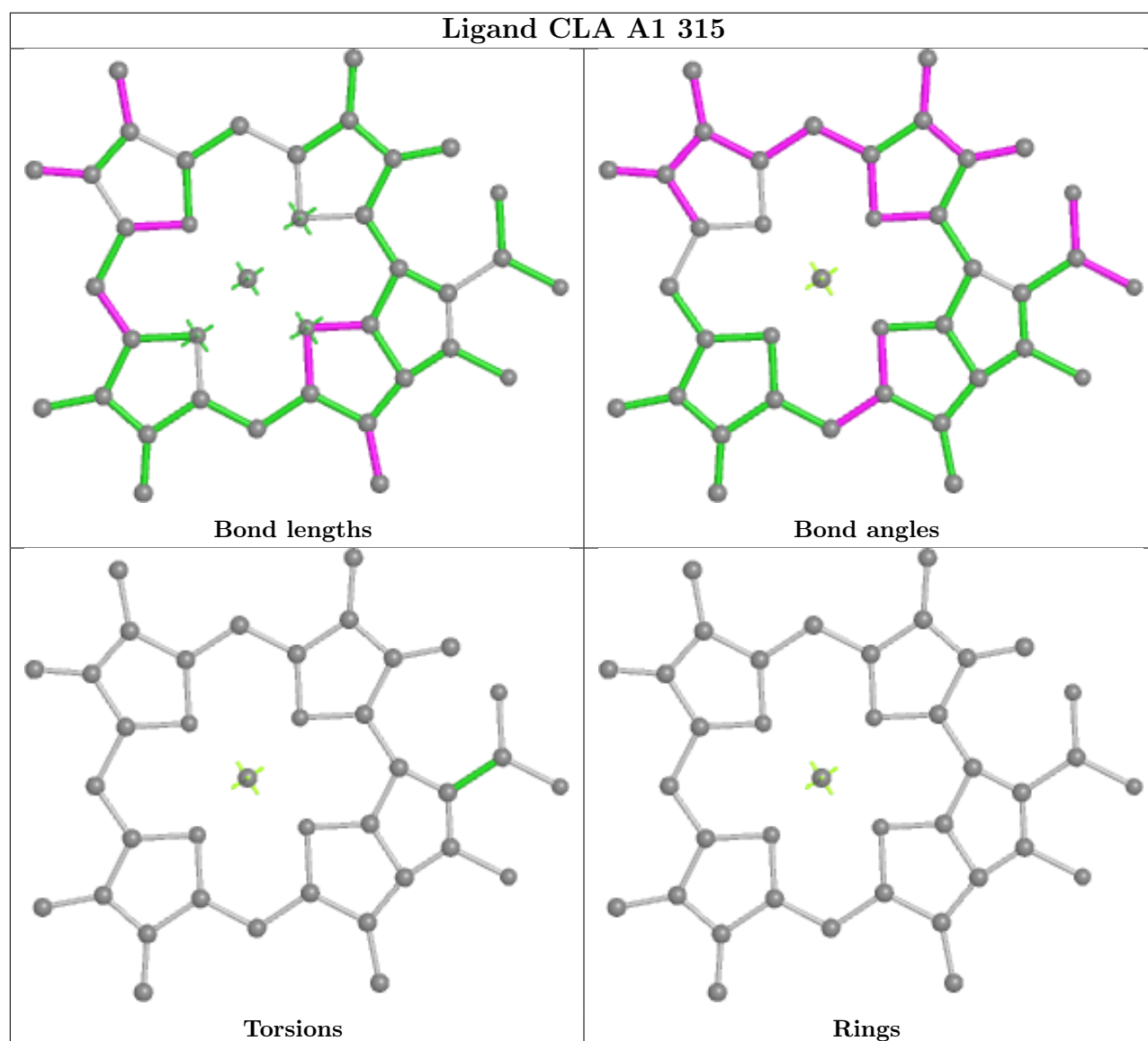
Ligand CLA B5 602



Ligand LMU BA 853







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.

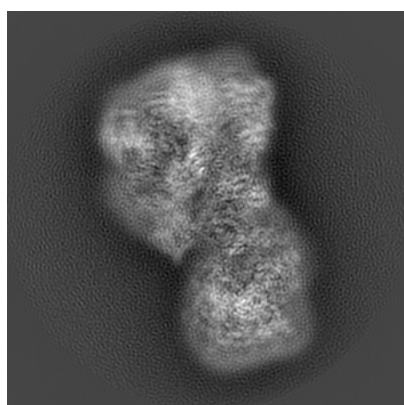
6 Map visualisation [i](#)

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.

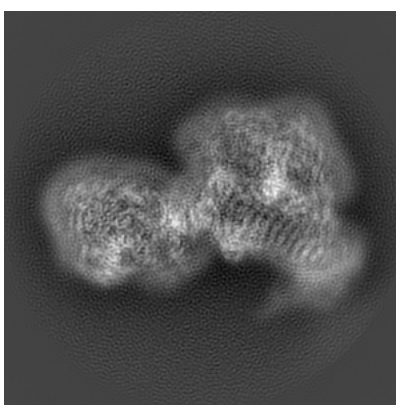
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

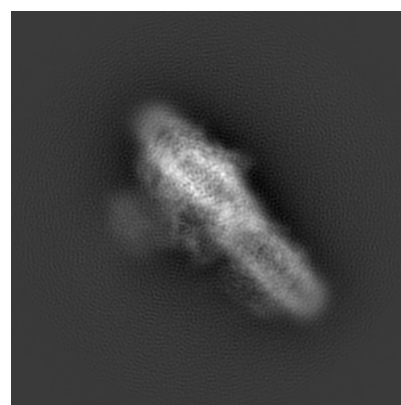
6.1.1 Primary map



X



Y

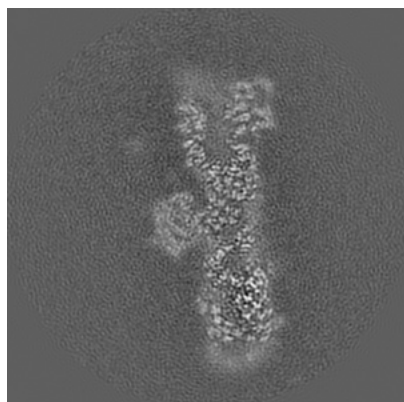


Z

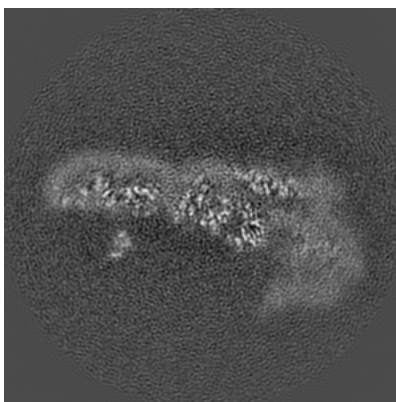
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

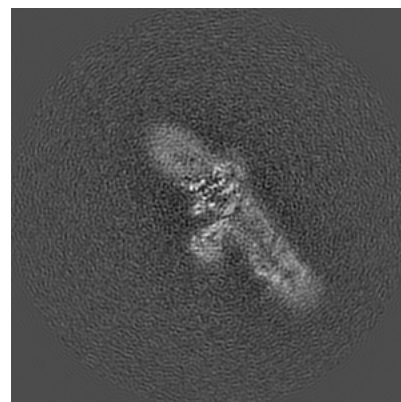
6.2.1 Primary map



X Index: 200



Y Index: 200

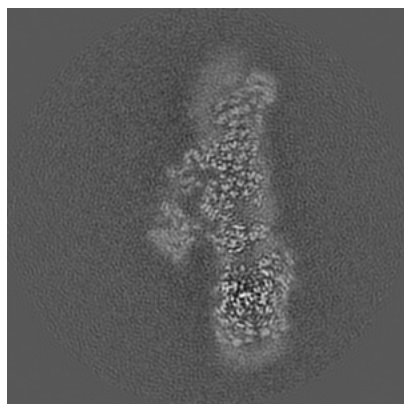


Z Index: 200

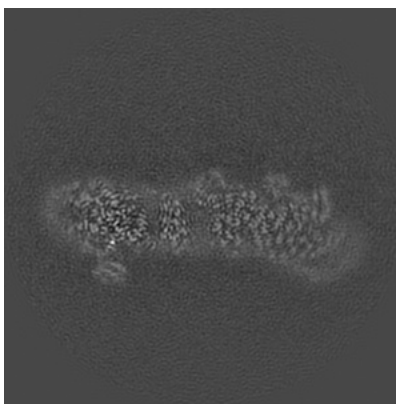
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

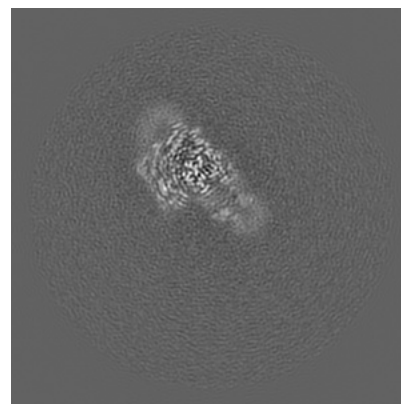
6.3.1 Primary map



X Index: 185



Y Index: 235

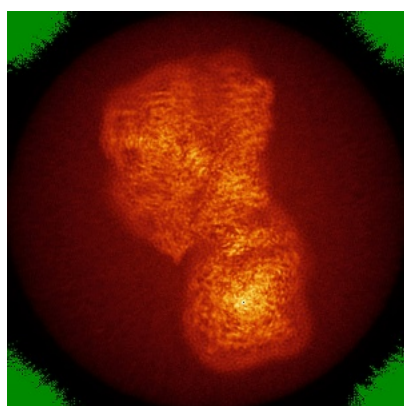


Z Index: 112

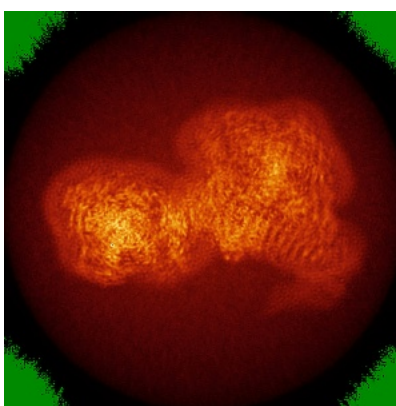
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

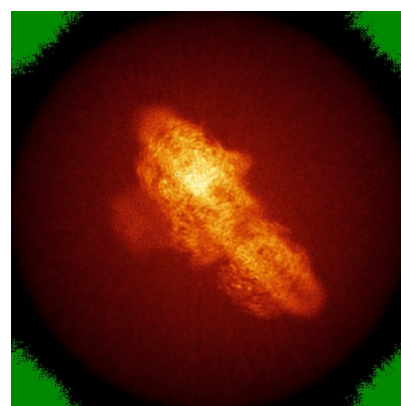
6.4.1 Primary map



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.

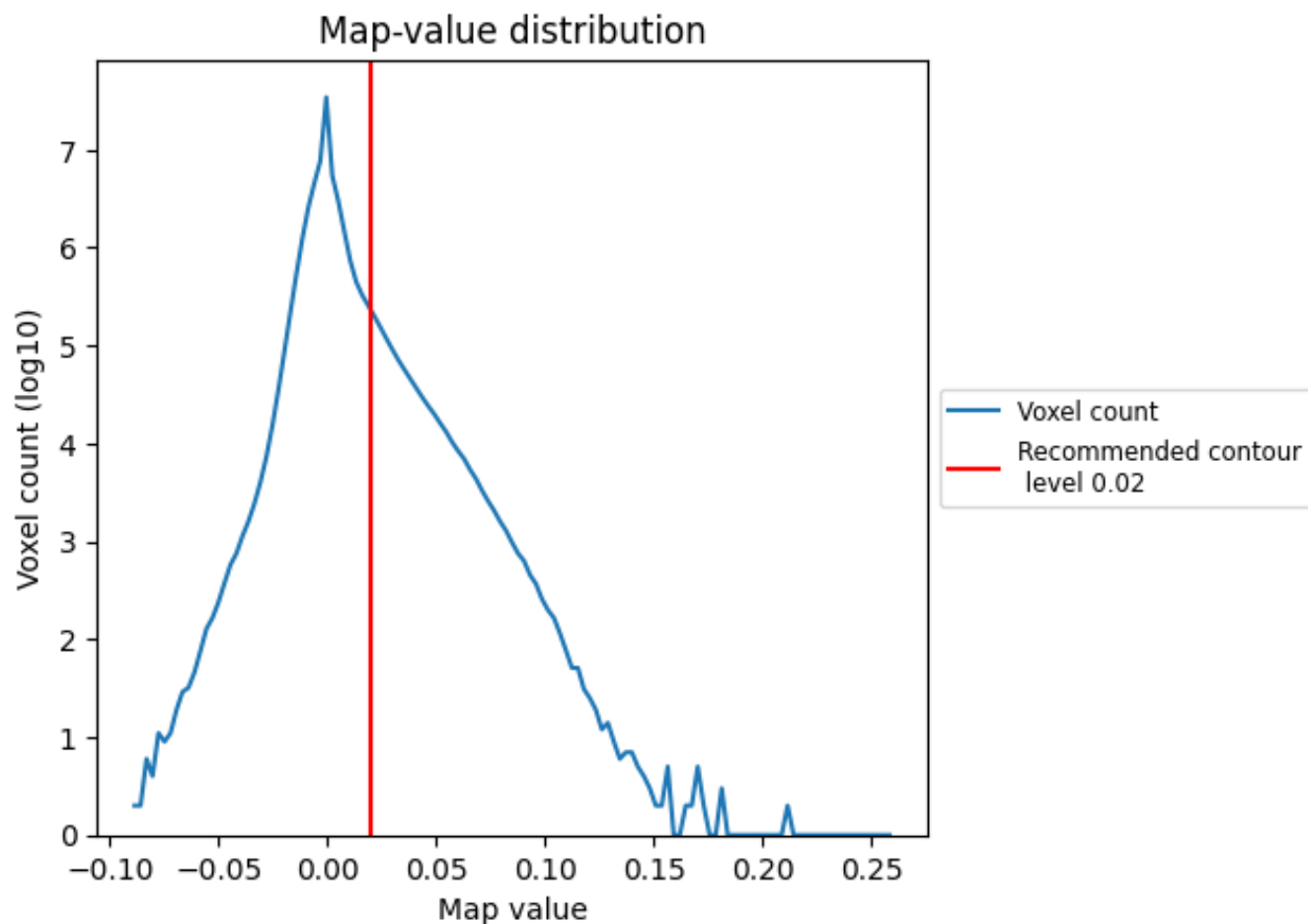
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

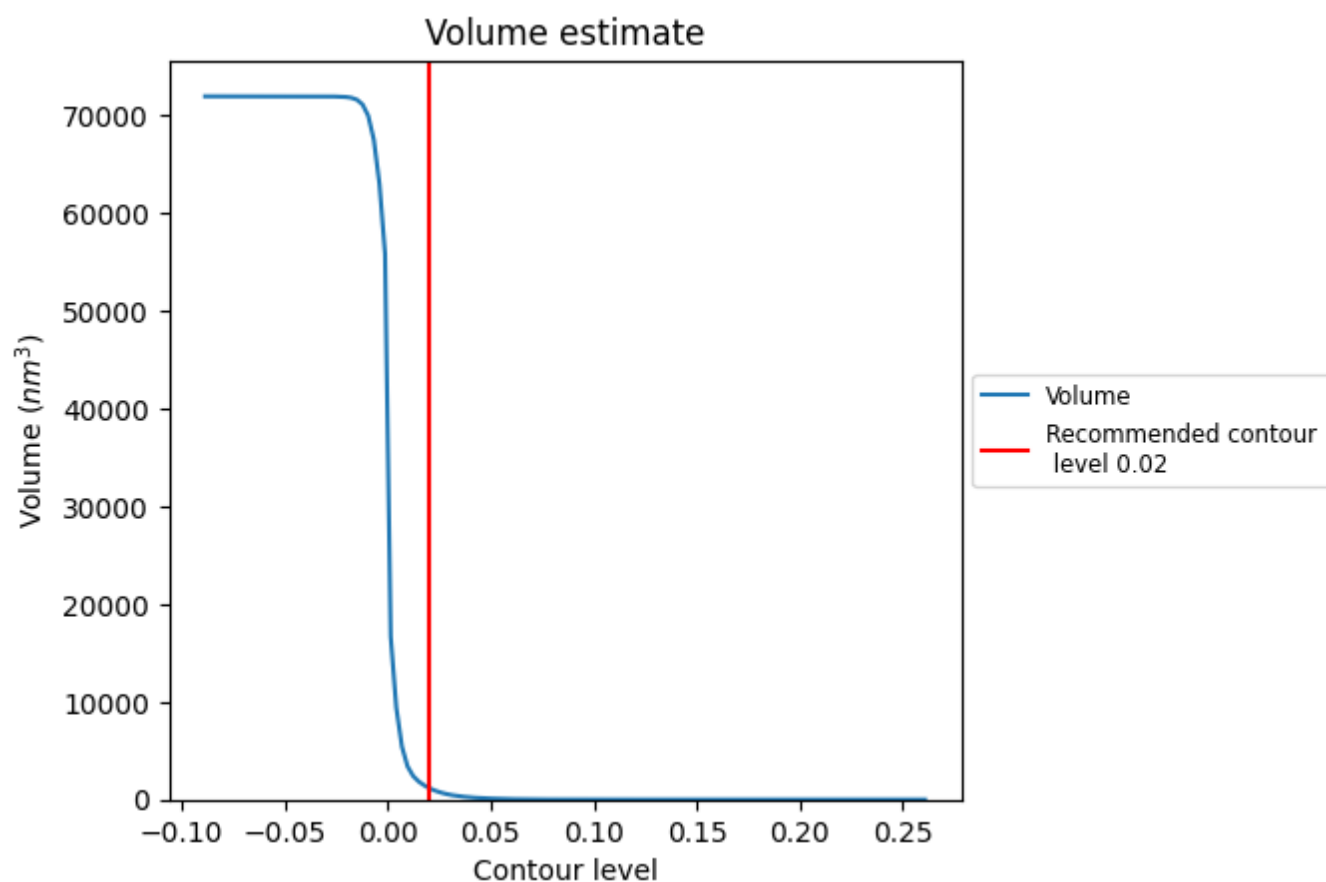
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

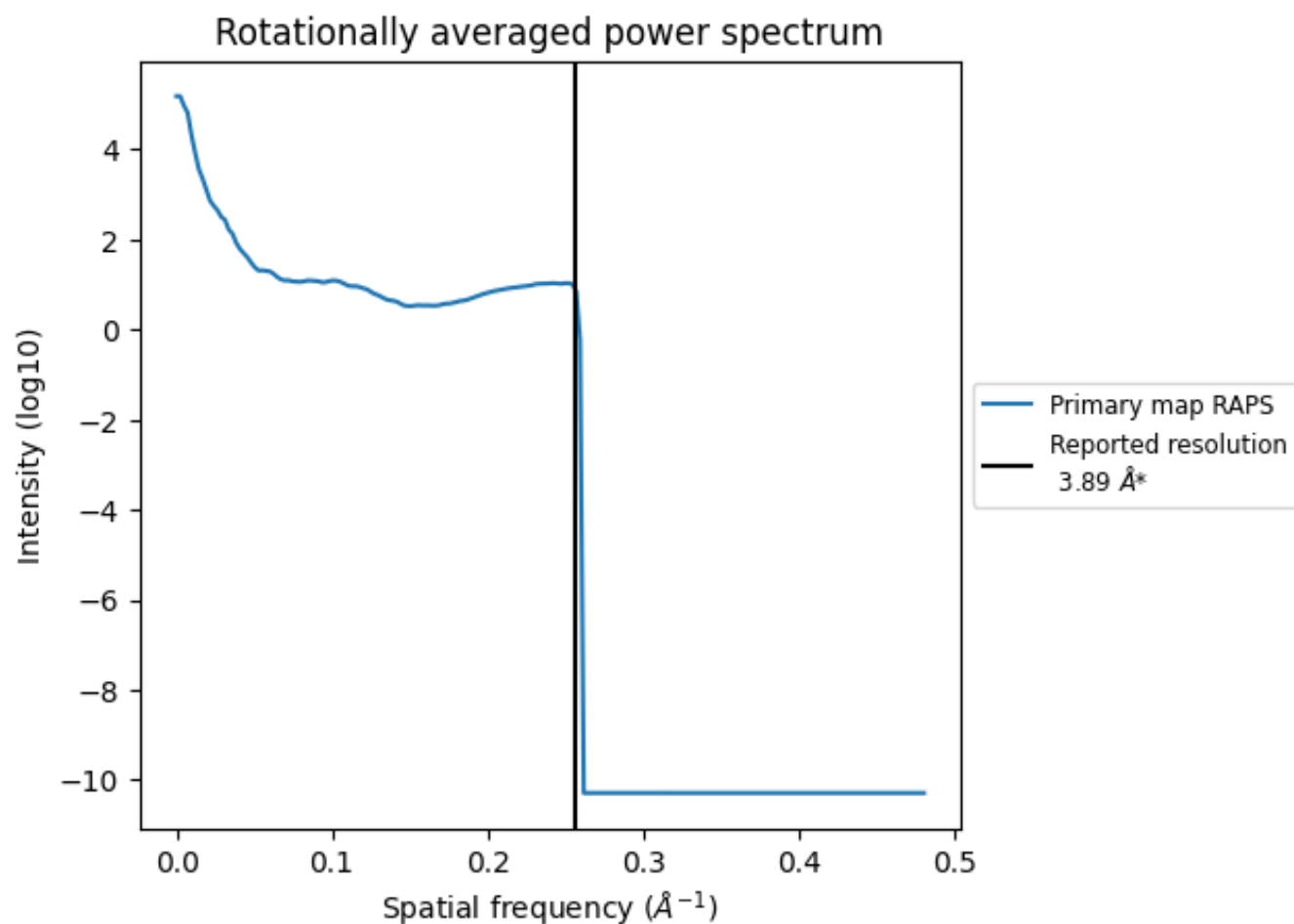
7.2 Volume estimate [i](#)



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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.257 Å⁻¹

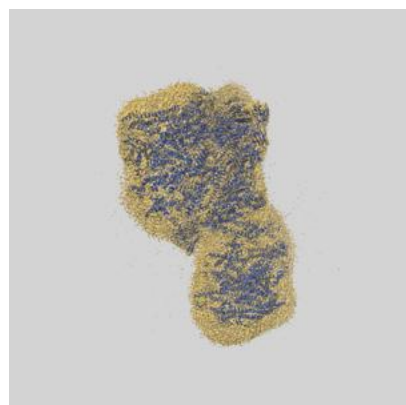
8 Fourier-Shell correlation ⓘ

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

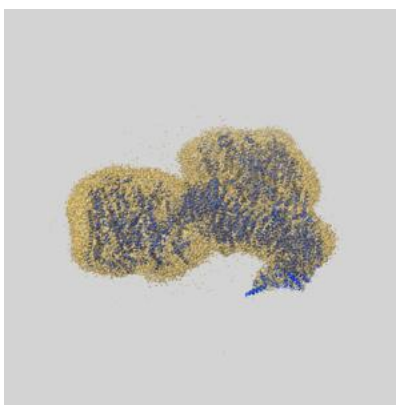
9 Map-model fit [i](#)

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](#).

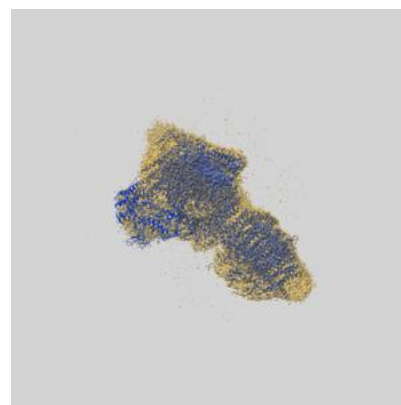
9.1 Map-model overlay [i](#)



X



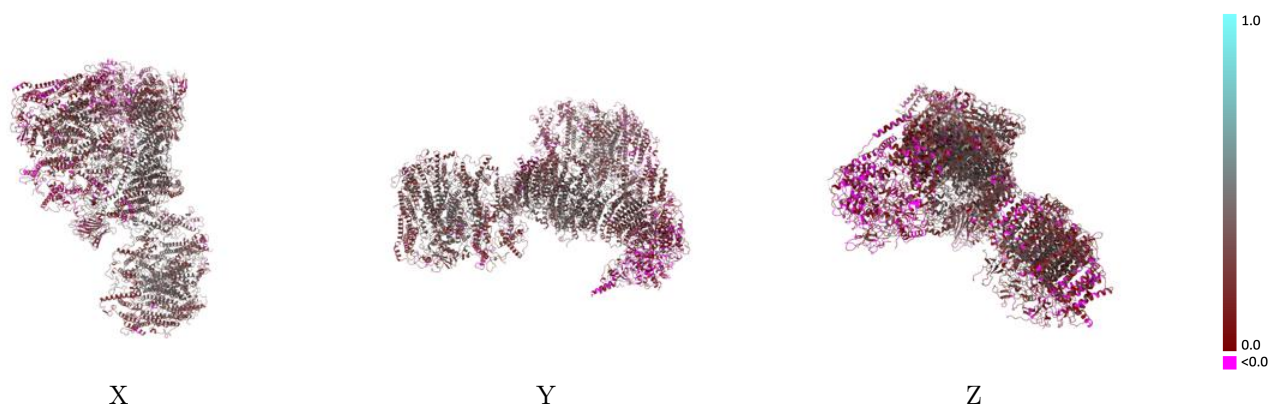
Y



Z

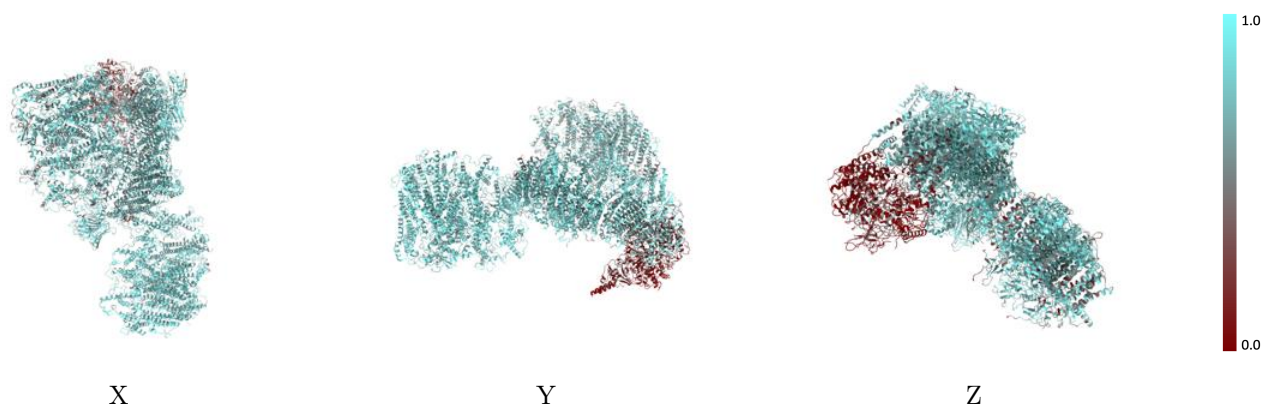
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



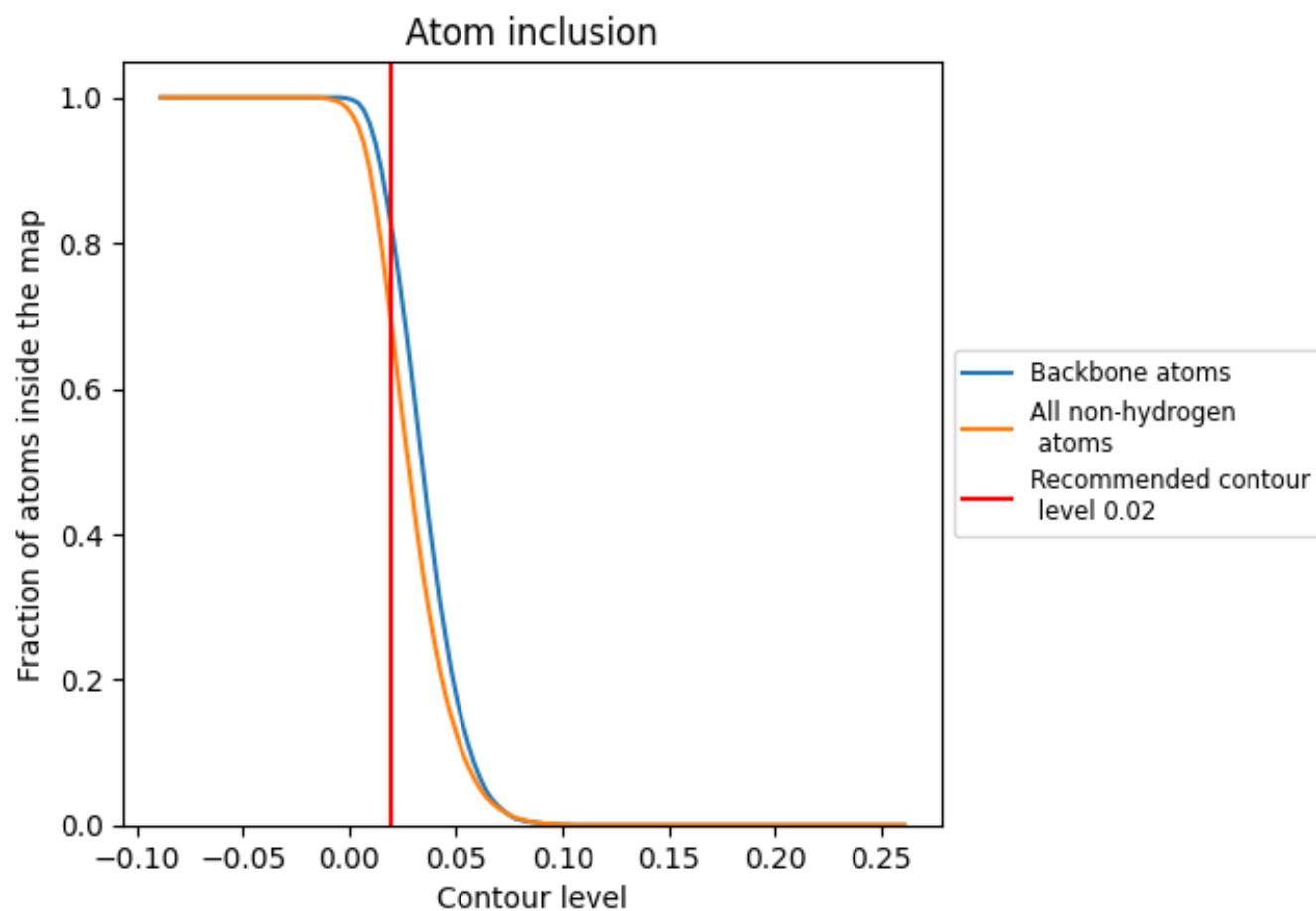
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



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 ⓘ



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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Continued from previous page...

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