



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 09:25 PM UTC

PDB ID : 9LZK / pdb_00009lzk
EMDB ID : EMD-63528
Title : The PSI1-IsiA13 complex with double-layered IsiA proteins bound to the monomeric PSI core
Authors : Si, L.; Cao, P.; Li, M.
Deposited on : 2025-02-21
Resolution : 3.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

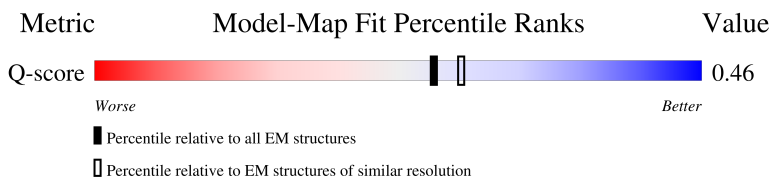
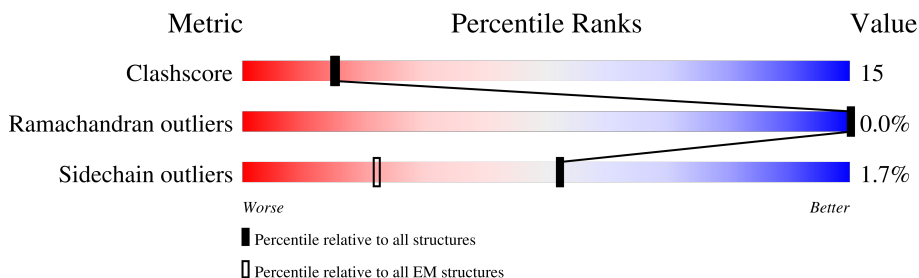
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	1	358	51% 73% 22% 5%
1	2	358	9% 80% 14% 5%
1	3	358	9% 76% 20% .
1	4	358	7% 73% 21% . .

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Mol	Chain	Length	Quality of chain
1	5	358	
1	6	358	
1	a	358	
1	b	358	
1	c	358	
1	d	358	
1	e	358	
1	f	358	
1	g	358	
2	A	755	
3	B	741	
4	C	81	
5	D	139	
6	E	76	
7	F	164	
8	I	38	
9	J	41	
10	K	83	
11	M	31	
12	X	39	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	501	X	-	-	-
13	CLA	1	502	X	-	-	-
13	CLA	1	503	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	1	504	X	-	-	-
13	CLA	1	505	X	-	-	-
13	CLA	1	506	X	-	-	-
13	CLA	1	507	X	-	-	-
13	CLA	1	508	X	-	-	-
13	CLA	1	509	X	-	-	-
13	CLA	1	510	X	-	-	-
13	CLA	1	511	X	-	-	-
13	CLA	1	512	X	-	-	-
13	CLA	1	513	X	-	-	-
13	CLA	1	516	X	-	-	-
13	CLA	1	517	X	-	-	-
13	CLA	1	518	X	-	-	-
13	CLA	1	519	X	-	-	-
13	CLA	2	501	X	-	-	-
13	CLA	2	502	X	-	-	-
13	CLA	2	503	X	-	-	-
13	CLA	2	504	X	-	-	-
13	CLA	2	505	X	-	-	-
13	CLA	2	506	X	-	-	-
13	CLA	2	507	X	-	-	-
13	CLA	2	508	X	-	-	-
13	CLA	2	509	X	-	-	-
13	CLA	2	510	X	-	-	-
13	CLA	2	511	X	-	-	-
13	CLA	2	512	X	-	-	-
13	CLA	2	513	X	-	-	-
13	CLA	2	516	X	-	-	-
13	CLA	2	517	X	-	-	-
13	CLA	2	518	X	-	-	-
13	CLA	2	519	X	-	-	-
13	CLA	3	501	X	-	-	-
13	CLA	3	502	X	-	-	-
13	CLA	3	503	X	-	-	-
13	CLA	3	504	X	-	-	-
13	CLA	3	505	X	-	-	-
13	CLA	3	506	X	-	-	-
13	CLA	3	507	X	-	-	-
13	CLA	3	508	X	-	-	-
13	CLA	3	509	X	-	-	-
13	CLA	3	510	X	-	-	-
13	CLA	3	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	3	512	X	-	-	-
13	CLA	3	513	X	-	-	-
13	CLA	3	516	X	-	-	-
13	CLA	3	517	X	-	-	-
13	CLA	3	518	X	-	-	-
13	CLA	3	519	X	-	-	-
13	CLA	4	501	X	-	-	-
13	CLA	4	503	X	-	-	-
13	CLA	4	504	X	-	-	-
13	CLA	4	505	X	-	-	-
13	CLA	4	506	X	-	-	-
13	CLA	4	507	X	-	-	-
13	CLA	4	508	X	-	-	-
13	CLA	4	509	X	-	-	-
13	CLA	4	510	X	-	-	-
13	CLA	4	512	X	-	-	-
13	CLA	4	513	X	-	-	-
13	CLA	4	516	X	-	-	-
13	CLA	4	517	X	-	-	-
13	CLA	4	518	X	-	-	-
13	CLA	4	519	X	-	-	-
13	CLA	5	501	X	-	-	-
13	CLA	5	502	X	-	-	-
13	CLA	5	503	X	-	-	-
13	CLA	5	504	X	-	-	-
13	CLA	5	505	X	-	-	-
13	CLA	5	506	X	-	-	-
13	CLA	5	507	X	-	-	-
13	CLA	5	508	X	-	-	-
13	CLA	5	509	X	-	-	-
13	CLA	5	510	X	-	-	-
13	CLA	5	511	X	-	-	-
13	CLA	5	512	X	-	-	-
13	CLA	5	513	X	-	-	-
13	CLA	5	516	X	-	-	-
13	CLA	5	517	X	-	-	-
13	CLA	5	518	X	-	-	-
13	CLA	5	519	X	-	-	-
13	CLA	6	501	X	-	-	-
13	CLA	6	502	X	-	-	-
13	CLA	6	503	X	-	-	-
13	CLA	6	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	6	505	X	-	-	-
13	CLA	6	506	X	-	-	-
13	CLA	6	507	X	-	-	-
13	CLA	6	508	X	-	-	-
13	CLA	6	509	X	-	-	-
13	CLA	6	510	X	-	-	-
13	CLA	6	511	X	-	-	-
13	CLA	6	512	X	-	-	-
13	CLA	6	513	X	-	-	-
13	CLA	6	516	X	-	-	-
13	CLA	6	517	X	-	-	-
13	CLA	6	518	X	-	-	-
13	CLA	6	519	X	-	-	-
13	CLA	A	1011	X	-	-	-
13	CLA	A	1013	X	-	-	-
13	CLA	A	1022	X	-	-	-
13	CLA	A	1101	X	-	-	-
13	CLA	A	1102	X	-	-	-
13	CLA	A	1103	X	-	-	-
13	CLA	A	1104	X	-	-	-
13	CLA	A	1105	X	-	-	-
13	CLA	A	1106	X	-	-	-
13	CLA	A	1107	X	-	-	-
13	CLA	A	1108	X	-	-	-
13	CLA	A	1109	X	-	-	-
13	CLA	A	1110	X	-	-	-
13	CLA	A	1111	X	-	-	-
13	CLA	A	1112	X	-	-	-
13	CLA	A	1113	X	-	-	-
13	CLA	A	1114	X	-	-	-
13	CLA	A	1115	X	-	-	-
13	CLA	A	1116	X	-	-	-
13	CLA	A	1117	X	-	-	-
13	CLA	A	1118	X	-	-	-
13	CLA	A	1119	X	-	-	-
13	CLA	A	1120	X	-	-	-
13	CLA	A	1121	X	-	-	-
13	CLA	A	1122	X	-	-	-
13	CLA	A	1123	X	-	-	-
13	CLA	A	1125	X	-	-	-
13	CLA	A	1126	X	-	-	-
13	CLA	A	1127	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	A	1128	X	-	-	-
13	CLA	A	1129	X	-	-	-
13	CLA	A	1130	X	-	-	-
13	CLA	A	1131	X	-	-	-
13	CLA	A	1132	X	-	-	-
13	CLA	A	1133	X	-	-	-
13	CLA	A	1134	X	-	-	-
13	CLA	A	1135	X	-	-	-
13	CLA	A	1136	X	-	-	-
13	CLA	A	1137	X	-	-	-
13	CLA	A	1138	X	-	-	-
13	CLA	A	1139	X	-	-	-
13	CLA	A	1140	X	-	-	-
13	CLA	A	1237	X	-	-	-
13	CLA	A	1801	X	-	-	-
13	CLA	B	1012	X	-	-	-
13	CLA	B	1021	X	-	-	-
13	CLA	B	1023	X	-	-	-
13	CLA	B	1201	X	-	-	-
13	CLA	B	1202	X	-	-	-
13	CLA	B	1203	X	-	-	-
13	CLA	B	1204	X	-	-	-
13	CLA	B	1205	X	-	-	-
13	CLA	B	1206	X	-	-	-
13	CLA	B	1208	X	-	-	-
13	CLA	B	1209	X	-	-	-
13	CLA	B	1210	X	-	-	-
13	CLA	B	1211	X	-	-	-
13	CLA	B	1212	X	-	-	-
13	CLA	B	1213	X	-	-	-
13	CLA	B	1214	X	-	-	-
13	CLA	B	1215	X	-	-	-
13	CLA	B	1216	X	-	-	-
13	CLA	B	1217	X	-	-	-
13	CLA	B	1218	X	-	-	-
13	CLA	B	1219	X	-	-	-
13	CLA	B	1220	X	-	-	-
13	CLA	B	1221	X	-	-	-
13	CLA	B	1222	X	-	-	-
13	CLA	B	1223	X	-	-	-
13	CLA	B	1224	X	-	-	-
13	CLA	B	1225	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	B	1226	X	-	-	-
13	CLA	B	1227	X	-	-	-
13	CLA	B	1228	X	-	-	-
13	CLA	B	1229	X	-	-	-
13	CLA	B	1230	X	-	-	-
13	CLA	B	1231	X	-	-	-
13	CLA	B	1232	X	-	-	-
13	CLA	B	1233	X	-	-	-
13	CLA	B	1234	X	-	-	-
13	CLA	B	1236	X	-	-	-
13	CLA	B	1238	X	-	-	-
13	CLA	F	1301	X	-	-	-
13	CLA	J	1302	X	-	-	-
13	CLA	K	1103	X	-	-	-
13	CLA	K	1401	X	-	-	-
13	CLA	X	1401	X	-	-	-
13	CLA	a	501	X	-	-	-
13	CLA	a	502	X	-	-	-
13	CLA	a	503	X	-	-	-
13	CLA	a	504	X	-	-	-
13	CLA	a	505	X	-	-	-
13	CLA	a	506	X	-	-	-
13	CLA	a	507	X	-	-	-
13	CLA	a	508	X	-	-	-
13	CLA	a	509	X	-	-	-
13	CLA	a	510	X	-	-	-
13	CLA	a	511	X	-	-	-
13	CLA	a	512	X	-	-	-
13	CLA	a	516	X	-	-	-
13	CLA	a	517	X	-	-	-
13	CLA	a	518	X	-	-	-
13	CLA	a	519	X	-	-	-
13	CLA	b	501	X	-	-	-
13	CLA	b	502	X	-	-	-
13	CLA	b	503	X	-	-	-
13	CLA	b	504	X	-	-	-
13	CLA	b	505	X	-	-	-
13	CLA	b	507	X	-	-	-
13	CLA	b	508	X	-	-	-
13	CLA	b	509	X	-	-	-
13	CLA	b	510	X	-	-	-
13	CLA	b	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	b	512	X	-	-	-
13	CLA	b	513	X	-	-	-
13	CLA	b	516	X	-	-	-
13	CLA	b	517	X	-	-	-
13	CLA	b	518	X	-	-	-
13	CLA	b	519	X	-	-	-
13	CLA	c	501	X	-	-	-
13	CLA	c	502	X	-	-	-
13	CLA	c	503	X	-	-	-
13	CLA	c	504	X	-	-	-
13	CLA	c	505	X	-	-	-
13	CLA	c	506	X	-	-	-
13	CLA	c	507	X	-	-	-
13	CLA	c	508	X	-	-	-
13	CLA	c	509	X	-	-	-
13	CLA	c	510	X	-	-	-
13	CLA	c	511	X	-	-	-
13	CLA	c	512	X	-	-	-
13	CLA	c	513	X	-	-	-
13	CLA	c	516	X	-	-	-
13	CLA	c	517	X	-	-	-
13	CLA	c	518	X	-	-	-
13	CLA	c	519	X	-	-	-
13	CLA	d	501	X	-	-	-
13	CLA	d	502	X	-	-	-
13	CLA	d	503	X	-	-	-
13	CLA	d	504	X	-	-	-
13	CLA	d	505	X	-	-	-
13	CLA	d	506	X	-	-	-
13	CLA	d	507	X	-	-	-
13	CLA	d	508	X	-	-	-
13	CLA	d	509	X	-	-	-
13	CLA	d	510	X	-	-	-
13	CLA	d	511	X	-	-	-
13	CLA	d	512	X	-	-	-
13	CLA	d	513	X	-	-	-
13	CLA	d	516	X	-	-	-
13	CLA	d	517	X	-	-	-
13	CLA	d	518	X	-	-	-
13	CLA	d	519	X	-	-	-
13	CLA	e	501	X	-	-	-
13	CLA	e	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	e	503	X	-	-	-
13	CLA	e	504	X	-	-	-
13	CLA	e	505	X	-	-	-
13	CLA	e	506	X	-	-	-
13	CLA	e	507	X	-	-	-
13	CLA	e	508	X	-	-	-
13	CLA	e	509	X	-	-	-
13	CLA	e	510	X	-	-	-
13	CLA	e	511	X	-	-	-
13	CLA	e	512	X	-	-	-
13	CLA	e	513	X	-	-	-
13	CLA	e	516	X	-	-	-
13	CLA	e	517	X	-	-	-
13	CLA	e	518	X	-	-	-
13	CLA	e	519	X	-	-	-
13	CLA	f	501	X	-	-	-
13	CLA	f	502	X	-	-	-
13	CLA	f	503	X	-	-	-
13	CLA	f	504	X	-	-	-
13	CLA	f	505	X	-	-	-
13	CLA	f	507	X	-	-	-
13	CLA	f	508	X	-	-	-
13	CLA	f	509	X	-	-	-
13	CLA	f	510	X	-	-	-
13	CLA	f	511	X	-	-	-
13	CLA	f	512	X	-	-	-
13	CLA	f	513	X	-	-	-
13	CLA	f	516	X	-	-	-
13	CLA	f	517	X	-	-	-
13	CLA	f	518	X	-	-	-
13	CLA	f	519	X	-	-	-
13	CLA	g	501	X	-	-	-
13	CLA	g	502	X	-	-	-
13	CLA	g	503	X	-	-	-
13	CLA	g	504	X	-	-	-
13	CLA	g	505	X	-	-	-
13	CLA	g	506	X	-	-	-
13	CLA	g	507	X	-	-	-
13	CLA	g	508	X	-	-	-
13	CLA	g	509	X	-	-	-
13	CLA	g	510	X	-	-	-
13	CLA	g	511	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
13	CLA	g	512	X	-	-	-
13	CLA	g	513	X	-	-	-
13	CLA	g	516	X	-	-	-
13	CLA	g	517	X	-	-	-
13	CLA	g	518	X	-	-	-
13	CLA	g	519	X	-	-	-

2 Entry composition

There are 20 unique types of molecules in this entry. The entry contains 72827 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 Iron stress-induced chlorophyll-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	3	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	4	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	5	334	Total	C	N	O	S	0	0
			2613	1745	431	433	4		
1	6	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
1	2	339	Total	C	N	O	S	0	0
			2657	1774	437	442	4		
1	1	340	Total	C	N	O	S	0	0
			2665	1780	438	443	4		
1	c	343	Total	C	N	O	S	0	0
			2685	1792	442	447	4		
1	d	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	e	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	f	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
1	g	341	Total	C	N	O	S	0	0
			2673	1784	440	445	4		
1	b	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		
1	a	342	Total	C	N	O	S	0	0
			2680	1789	441	446	4		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	745	Total	C	N	O	S	0	0
			5819	3818	994	981	26		

- Molecule 3 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	739	Total	C	N	O	S	0	0
			5889	3876	987	1005	21		

- Molecule 4 is a protein called Photosystem I iron-sulfur center.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	80	Total	C	N	O	S	0	0
			598	367	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	137	Total	C	N	O	S	0	0
			1068	678	185	202	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	E	69	Total	C	N	O		0	0
			539	342	93	104			

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	141	Total	C	N	O	S	0	0
			1065	680	184	197	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	I	38	Total	C	N	O	S	0	0
			301	208	40	48	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	41	Total	C	N	O	S	0	0
			338	231	51	54	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	60	Total	C	N	O	S	0	0
			437	290	68	78	1		

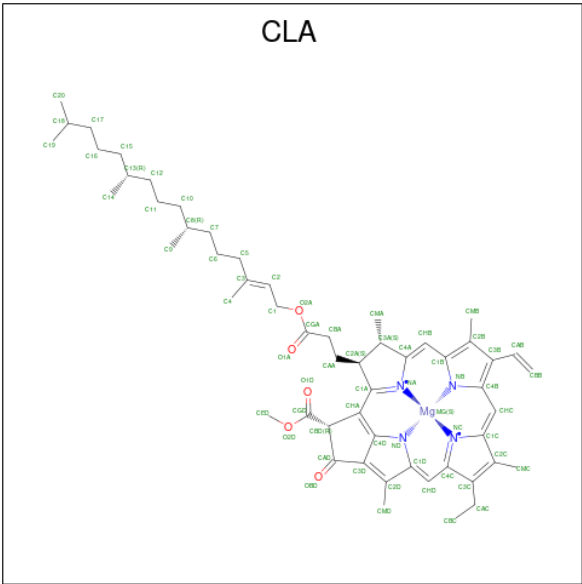
- Molecule 11 is a protein called Photosystem I reaction center subunit XII.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M	31	Total	C	N	O	S	0	0
			241	161	36	43	1		

- Molecule 12 is a protein called Photosystem I 4.8K protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	29	Total	C	N	O		0	0
			232	163	34	35			

- Molecule 13 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	3	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	3	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	3	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	3	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	4	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	4	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	4	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	5	1	Total 64	C 54	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	5	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	5	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	5	1	Total 52	C 42	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	5	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	6	1	Total	C	Mg	N	O	0
			50	40	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	6	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			64	54	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	2	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	1	1	Total	C	Mg	N	O	0
			63	53	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	1	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	1	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	1	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	A	1	Total 51	C 41	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			47	37	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			53	43	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			51	41	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 54	C 44	Mg 1	N 4	O 5	0
13	B	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	B	1	Total 65	C 55	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			58	48	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	F	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	J	1	Total	C	Mg	N	O	0
			44	35	1	3	5	
13	K	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
13	K	1	Total	C	Mg	N	O	0
			55	45	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	X	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	c	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	c	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	c	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	d	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	d	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	d	1	Total 63	C 53	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	d	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	e	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	e	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	e	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	e	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0

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Mol	Chain	Residues	Atoms					AltConf
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	f	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	f	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	g	1	Total 63	C 53	Mg 1	N 4	O 5	0
13	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 60	C 50	Mg 1	N 4	O 5	0
13	g	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 65	C 55	Mg 1	N 4	O 5	0
13	g	1	Total 55	C 45	Mg 1	N 4	O 5	0
13	g	1	Total 52	C 42	Mg 1	N 4	O 5	0
13	g	1	Total 50	C 40	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0
13	g	1	Total 45	C 35	Mg 1	N 4	O 5	0

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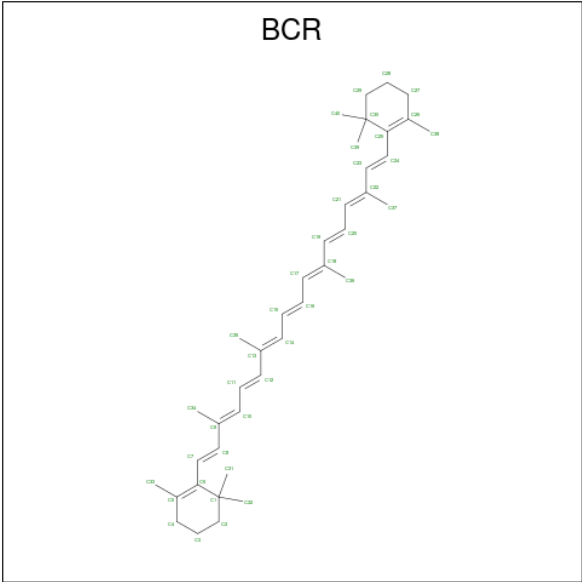
Mol	Chain	Residues	Atoms					AltConf
13	g	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	g	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	b	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
13	a	1	Total	C	Mg	N	O	0
			63	53	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
13	a	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

- Molecule 14 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms		AltConf
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	3	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	4	1	Total	C	0
			40	40	
14	5	1	Total	C	0
			40	40	
14	5	1	Total	C	0
			40	40	
14	5	1	Total	C	0
			40	40	
14	5	1	Total	C	0
			40	40	
14	6	1	Total	C	0
			40	40	
14	6	1	Total	C	0
			40	40	

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Mol	Chain	Residues	Atoms	AltConf
14	6	1	Total C 40 40	0
14	6	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	2	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	1	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	A	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0
14	B	1	Total C 40 40	0

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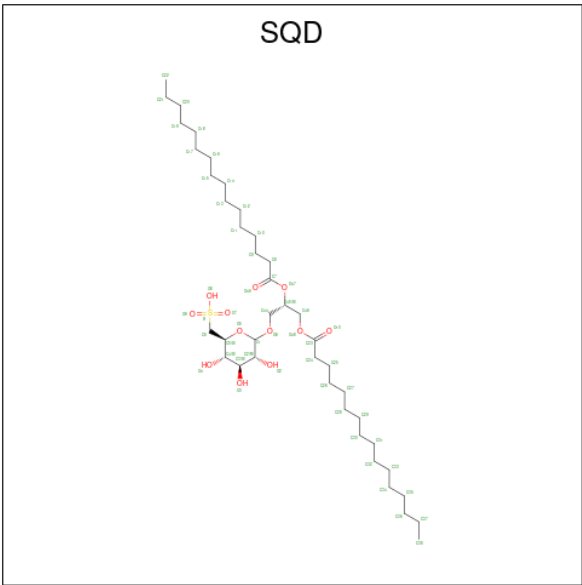
Mol	Chain	Residues	Atoms	AltConf
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	F	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	I	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	J	1	Total C 40 40	0
14	K	1	Total C 40 40	0
14	M	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	c	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	d	1	Total C 40 40	0
14	e	1	Total C 40 40	0
14	e	1	Total C 40 40	0
14	e	1	Total C 40 40	0

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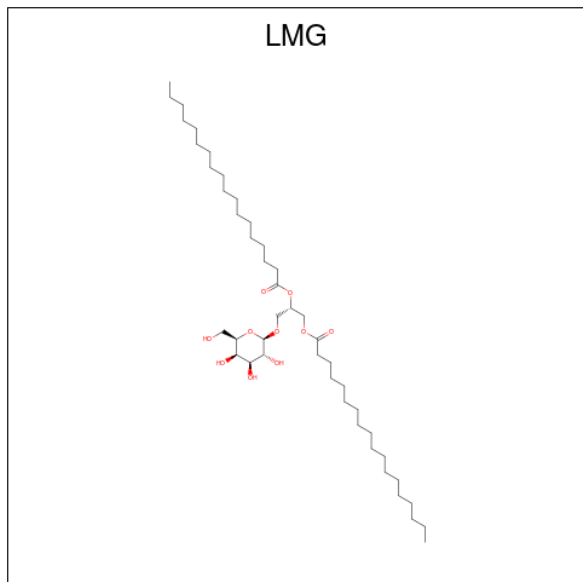
Mol	Chain	Residues	Atoms	AltConf
14	e	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	f	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	g	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	b	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0
14	a	1	Total C 40 40	0

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: C₄₁H₇₈O₁₂S).



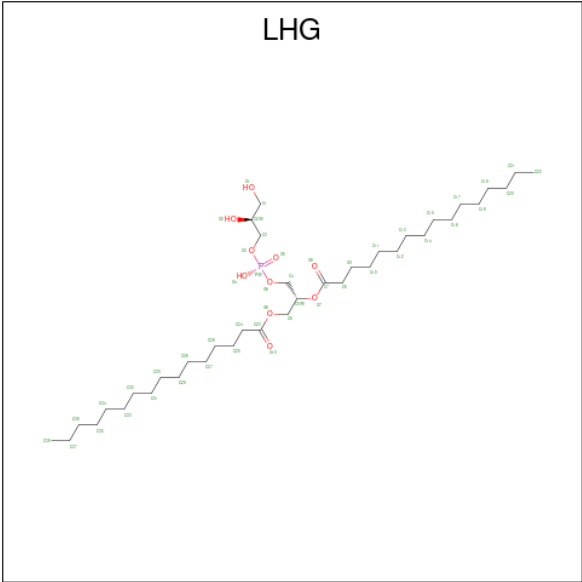
Mol	Chain	Residues	Atoms				AltConf
15	3	1	Total	C	O	S	0
			31	18	12	1	
15	4	1	Total	C	O	S	0
			31	18	12	1	
15	5	1	Total	C	O	S	0
			31	18	12	1	
15	6	1	Total	C	O	S	0
			31	18	12	1	
15	2	1	Total	C	O	S	0
			31	18	12	1	
15	1	1	Total	C	O	S	0
			31	18	12	1	
15	B	1	Total	C	O	S	0
			43	30	12	1	
15	c	1	Total	C	O	S	0
			31	18	12	1	
15	d	1	Total	C	O	S	0
			31	18	12	1	
15	e	1	Total	C	O	S	0
			31	18	12	1	
15	f	1	Total	C	O	S	0
			31	18	12	1	
15	g	1	Total	C	O	S	0
			31	18	12	1	
15	b	1	Total	C	O	S	0
			31	18	12	1	
15	a	1	Total	C	O	S	0
			31	18	12	1	

- Molecule 16 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: $C_{45}H_{86}O_{10}$).



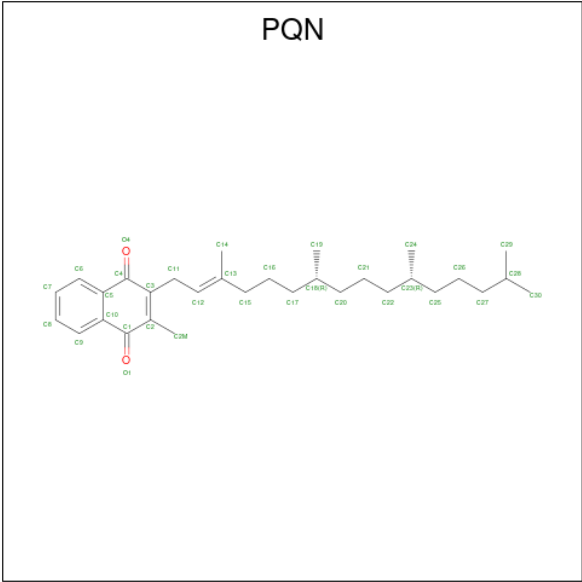
Mol	Chain	Residues	Atoms			AltConf
16	6	1	Total	C	O	0
			38	28	10	
16	2	1	Total	C	O	0
			40	30	10	
16	1	1	Total	C	O	0
			40	30	10	
16	B	1	Total	C	O	0
			55	45	10	
16	J	1	Total	C	O	0
			31	21	10	
16	g	1	Total	C	O	0
			40	30	10	

- Molecule 17 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



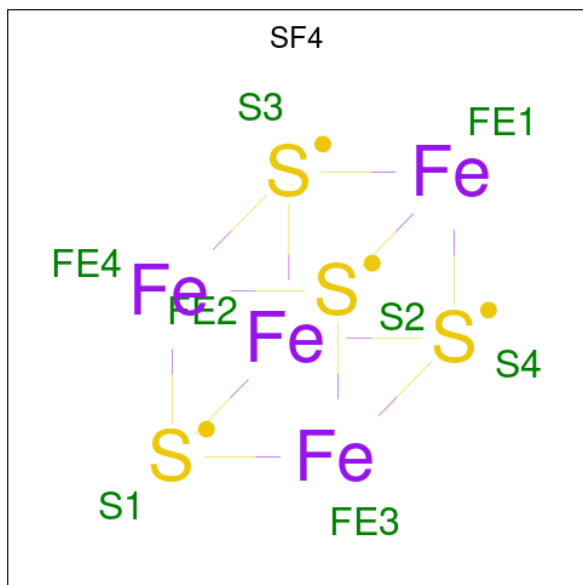
Mol	Chain	Residues	Atoms				AltConf
17	A	1	Total	C	O	P	0
			45	34	10	1	
17	A	1	Total	C	O	P	0
			35	24	10	1	
17	A	1	Total	C	O	P	0
			49	38	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	
17	A	1	Total	C	O	P	0
			41	30	10	1	

- Molecule 18 is PHYLLOQUINONE (CCD ID: PQN) (formula: C₃₁H₄₆O₂).



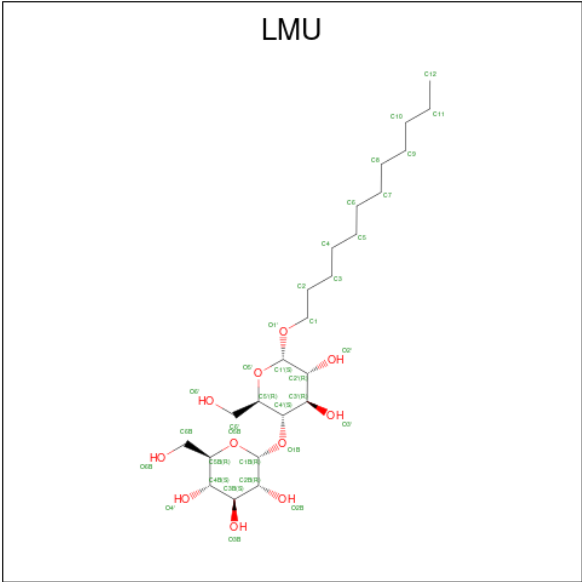
Mol	Chain	Residues	Atoms			AltConf
18	A	1	Total	C	O	0
			33	31	2	
18	B	1	Total	C	O	0
			33	31	2	

- Molecule 19 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 20 is DODECYL-ALPHA-D-MALTOSE (CCD ID: LMU) (formula: $\text{C}_{24}\text{H}_{46}\text{O}_{11}$) (labeled as "Ligand of Interest" by depositor).

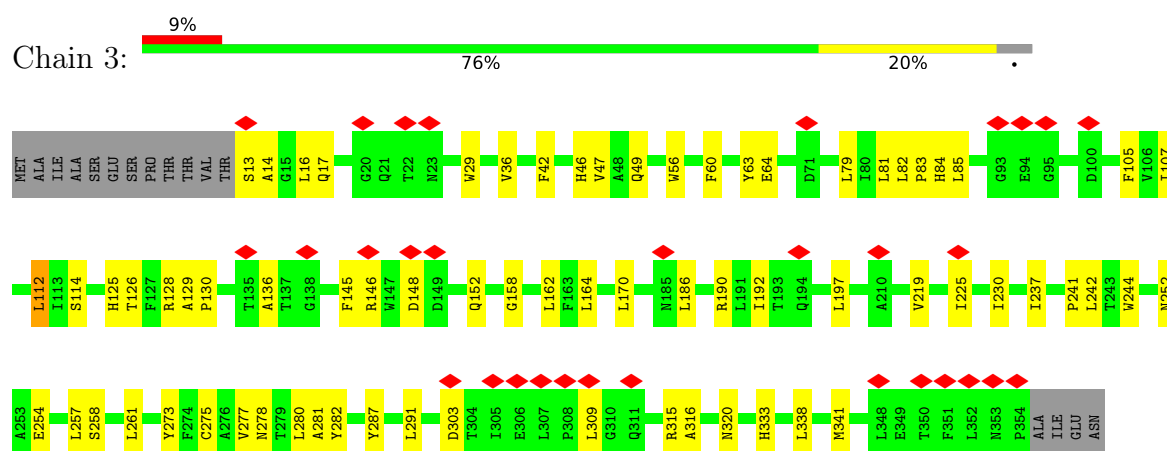


Mol	Chain	Residues	Atoms			AltConf
20	A	1	Total	C	O	0
			24	18	6	
20	A	1	Total	C	O	0
			23	17	6	
20	B	1	Total	C	O	0
			35	24	11	
20	J	1	Total	C	O	0
			22	16	6	

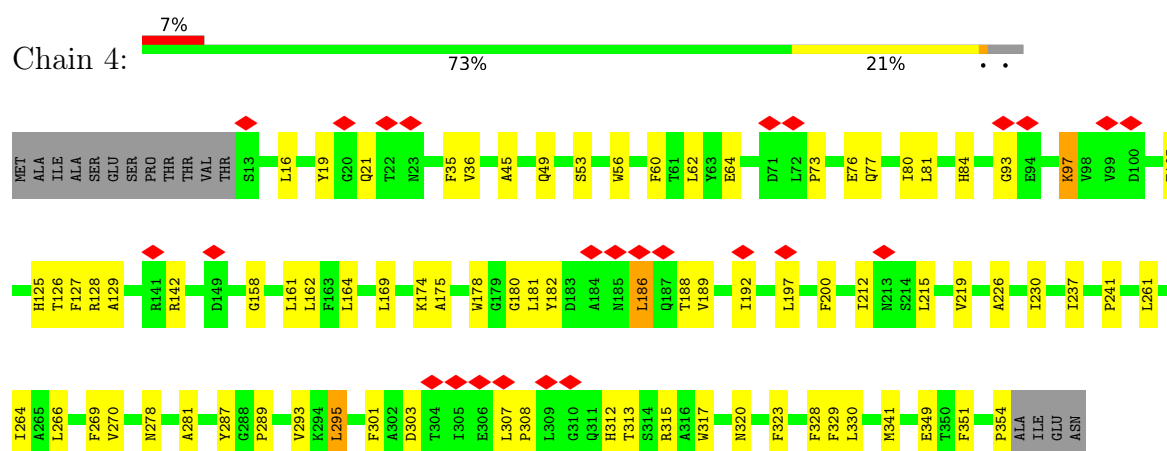
3 Residue-property plots

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.

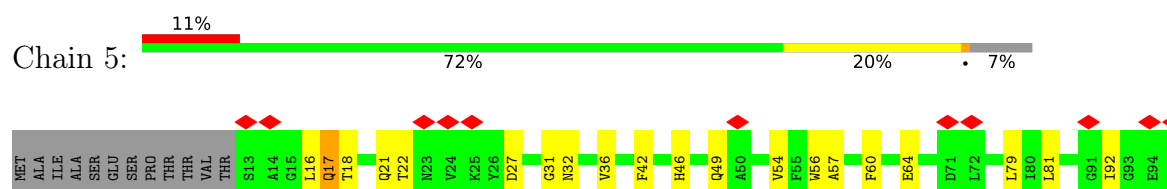
- Molecule 1: Iron stress-induced chlorophyll-binding protein

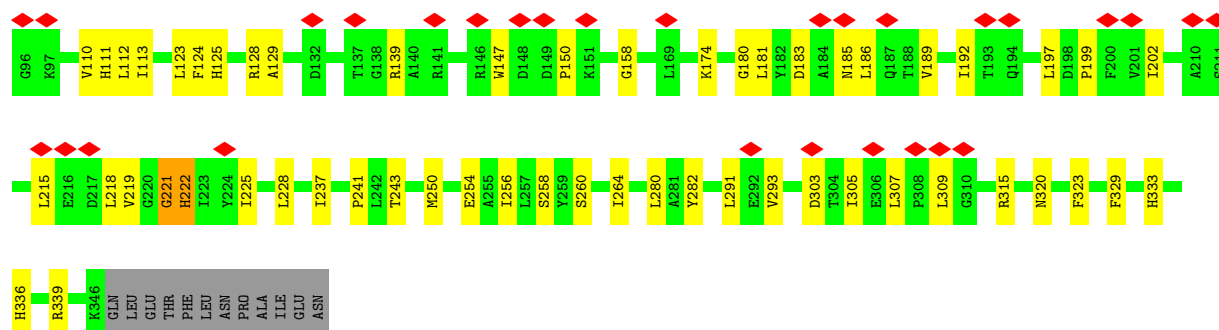


- Molecule 1: Iron stress-induced chlorophyll-binding protein



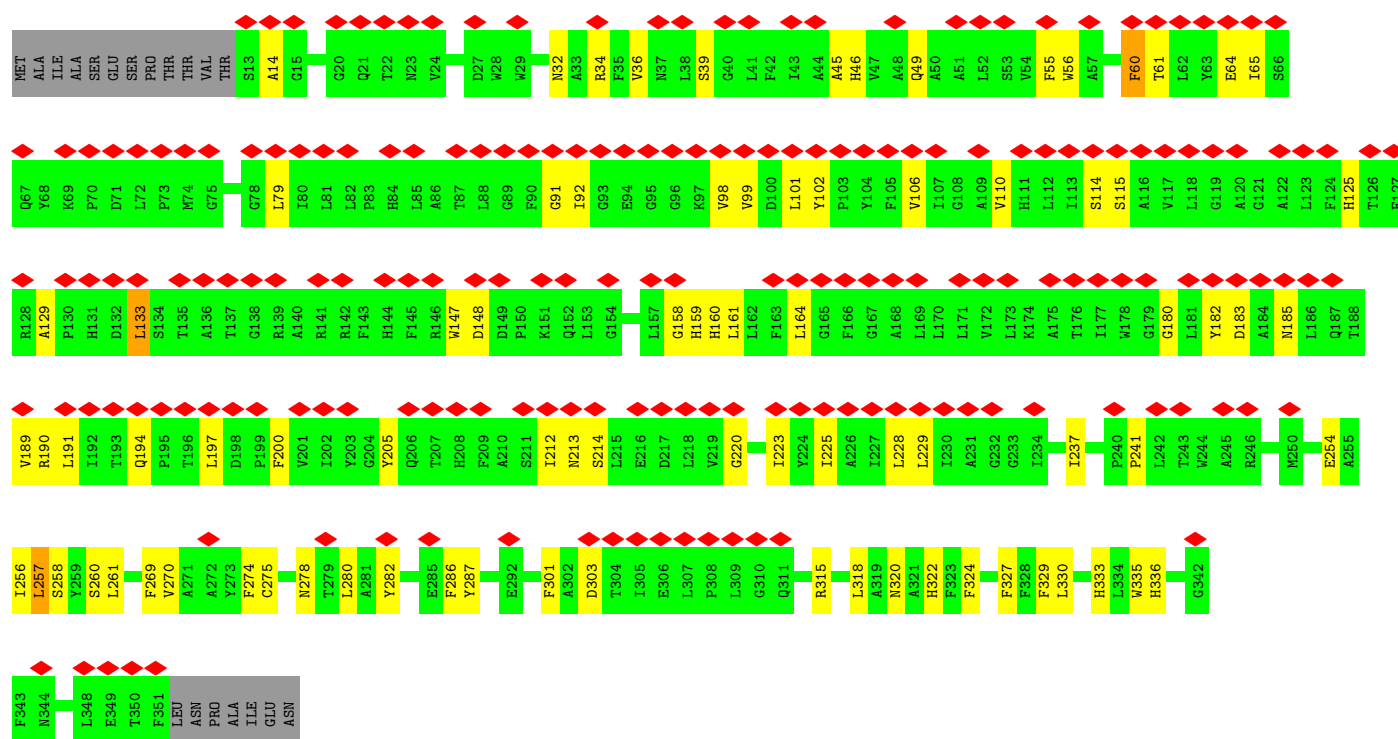
- Molecule 1: Iron stress-induced chlorophyll-binding protein





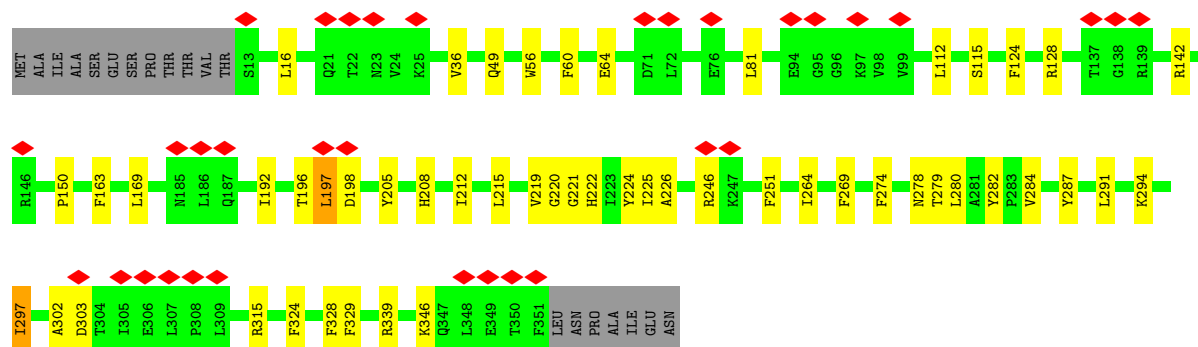
- Molecule 1: Iron stress-induced chlorophyll-binding protein

Chain 6: 53% 71% 23% 5%



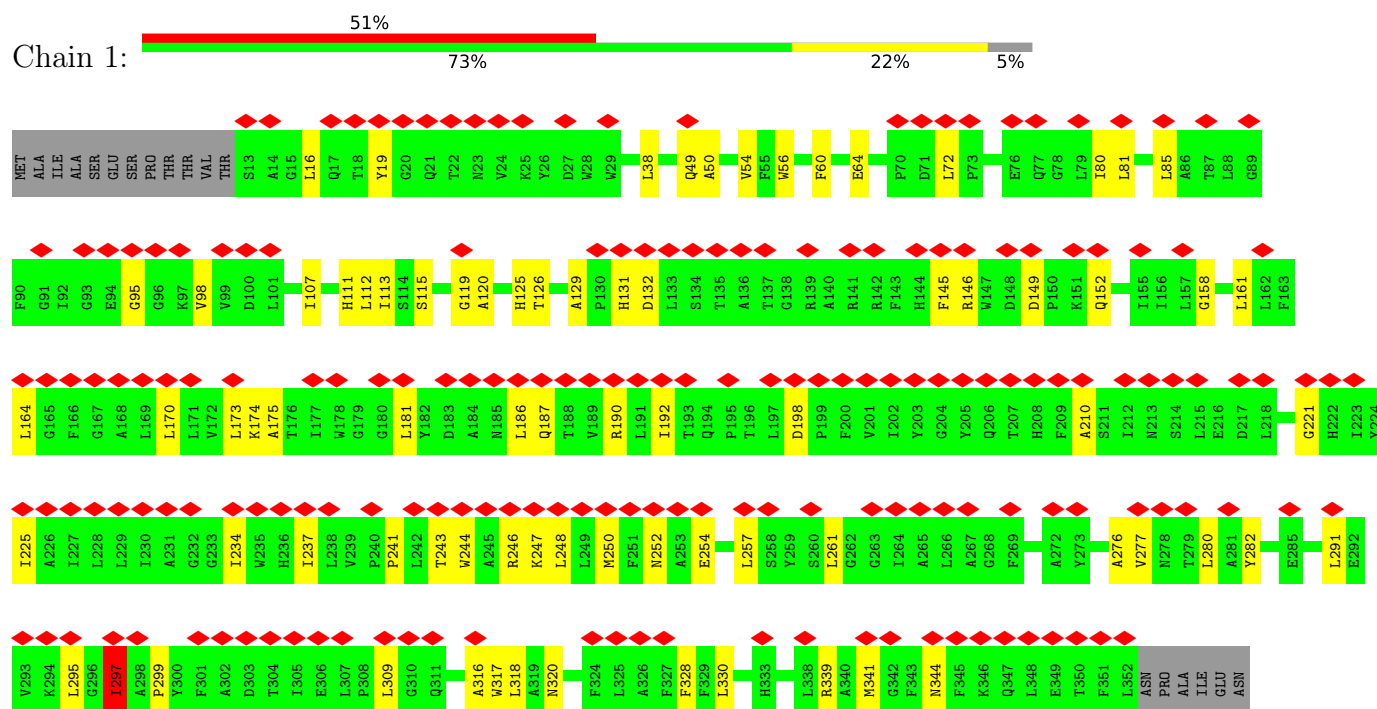
- Molecule 1: Iron stress-induced chlorophyll-binding protein

Chain 2: 9% 80% 14% 5%



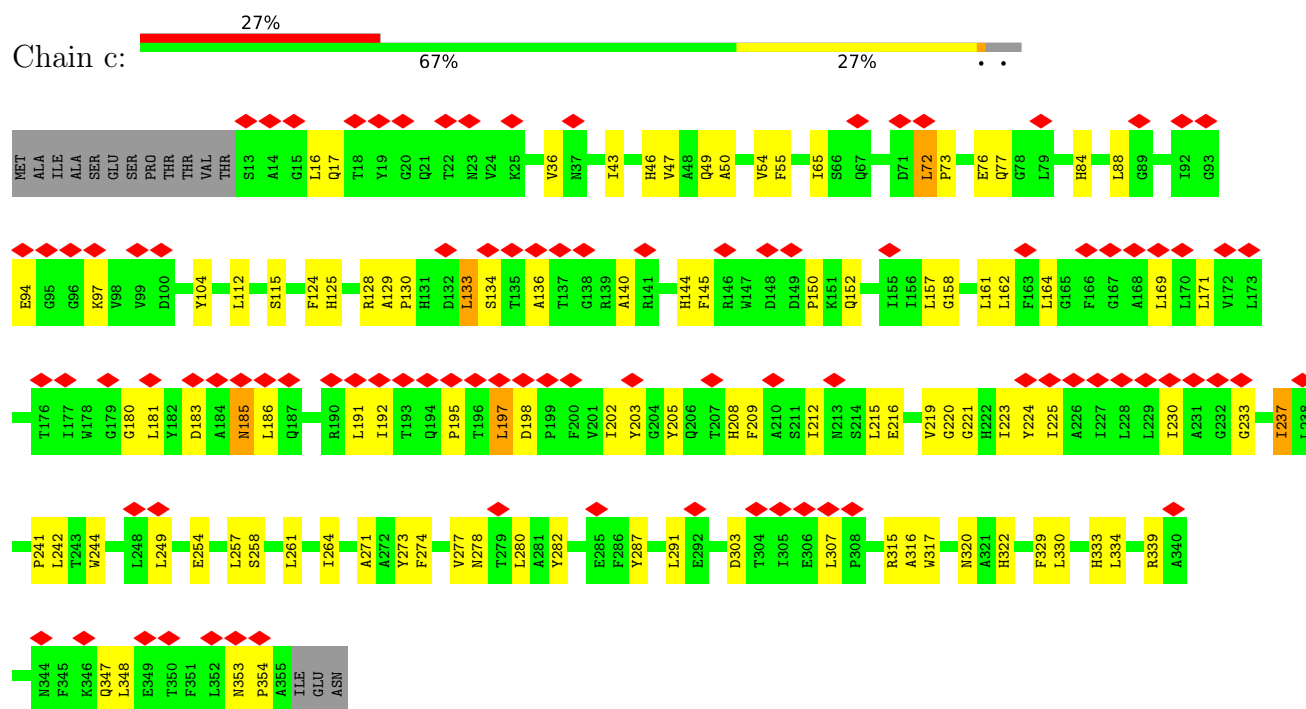
- Molecule 1: Iron stress-induced chlorophyll-binding protein

Chain 1:



- Molecule 1: Iron stress-induced chlorophyll-binding protein

Chain c:



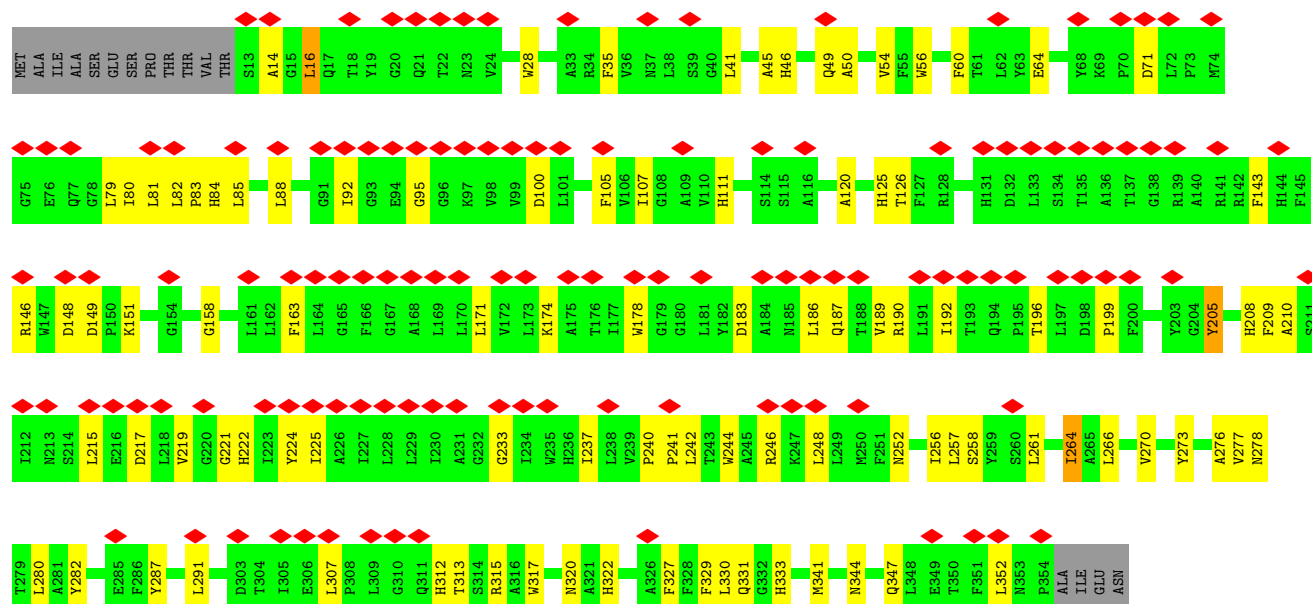
- Molecule 1: Iron stress-induced chlorophyll-binding protein

Chain d:

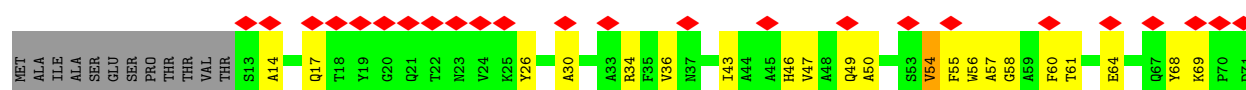


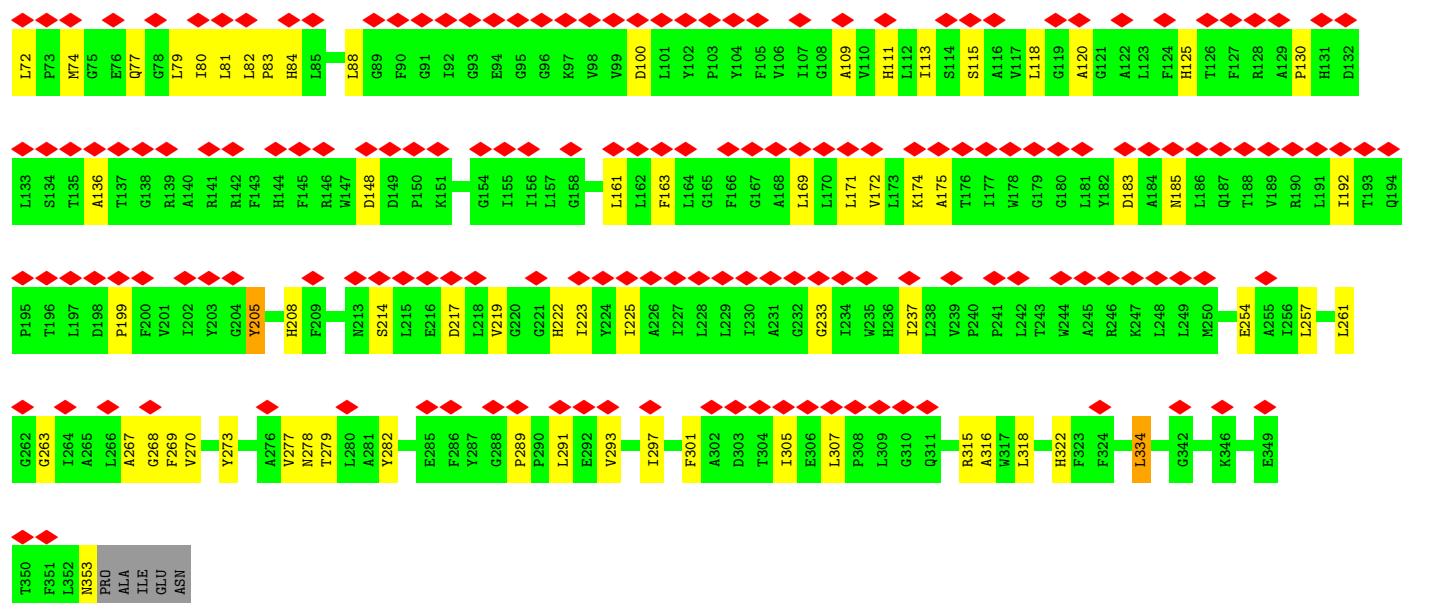


• Molecule 1: Iron stress-induced chlorophyll-binding protein

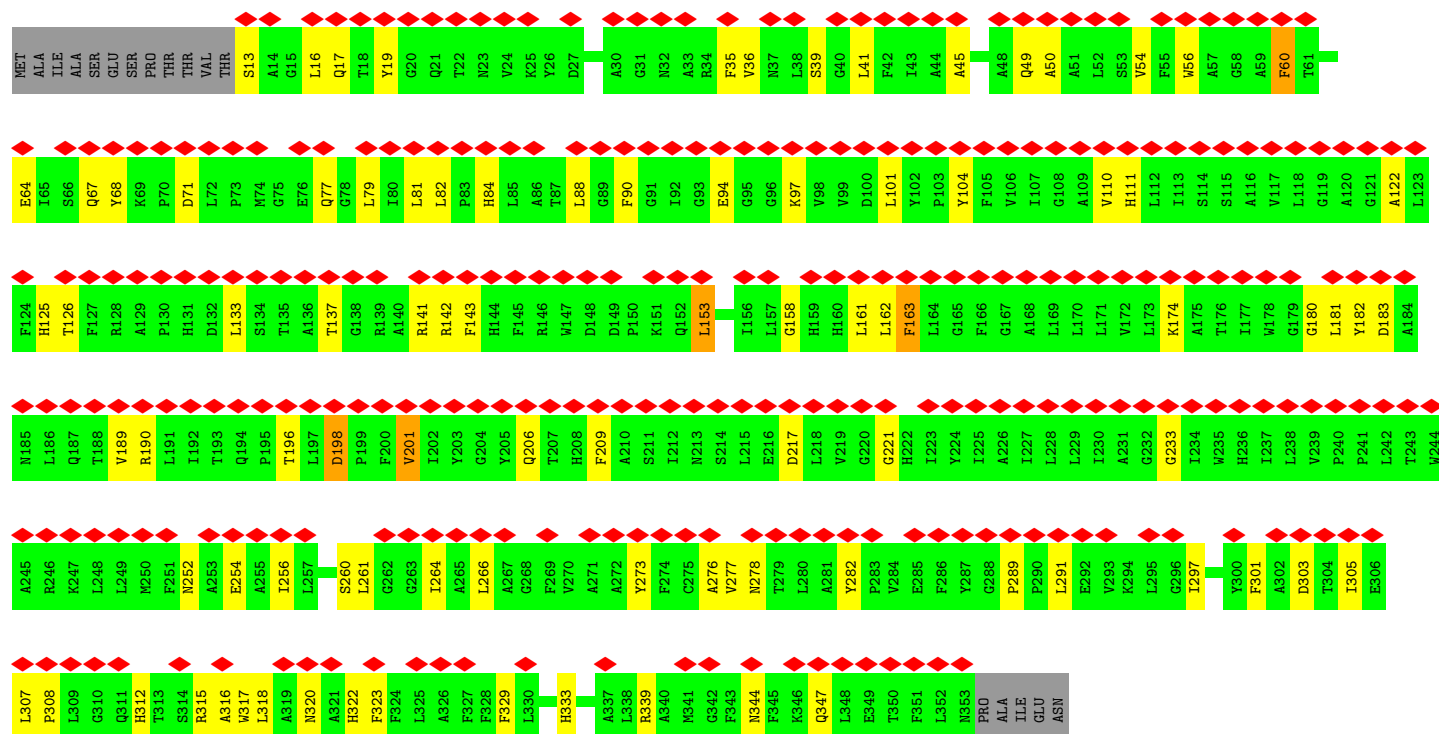
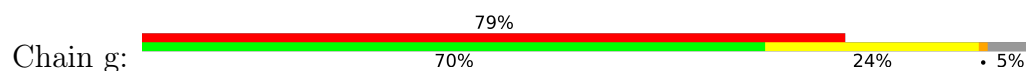


• Molecule 1: Iron stress-induced chlorophyll-binding protein

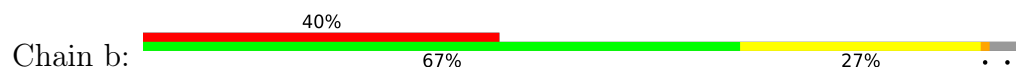


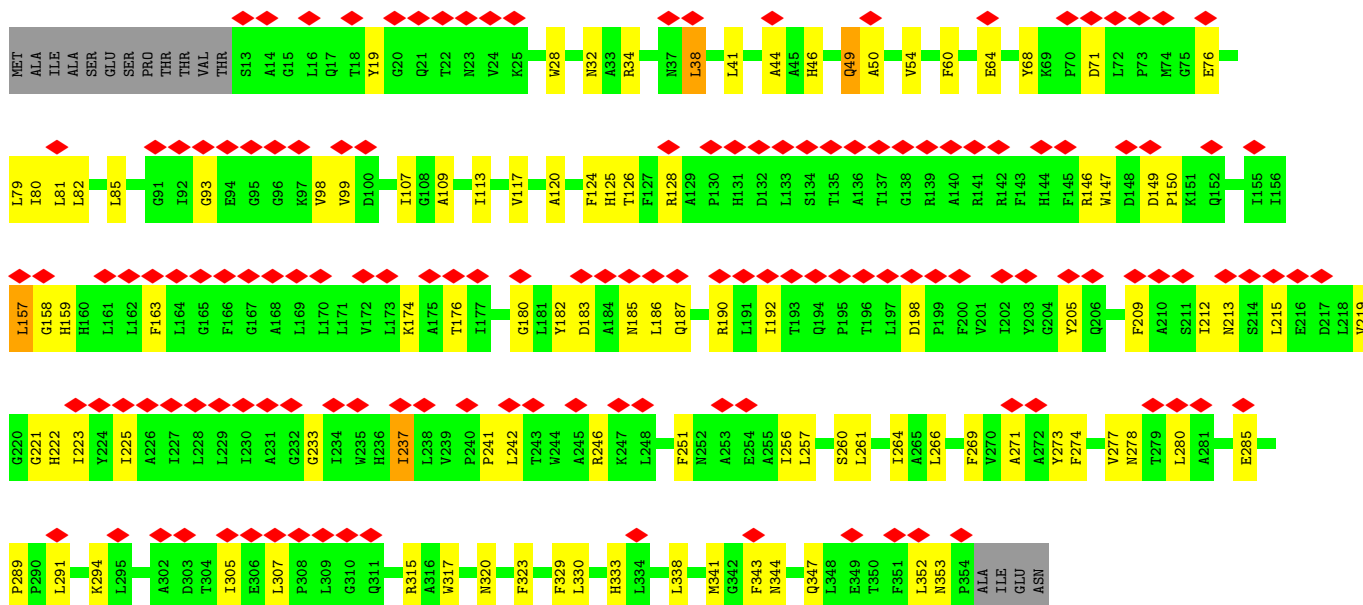


• Molecule 1: Iron stress-induced chlorophyll-binding protein

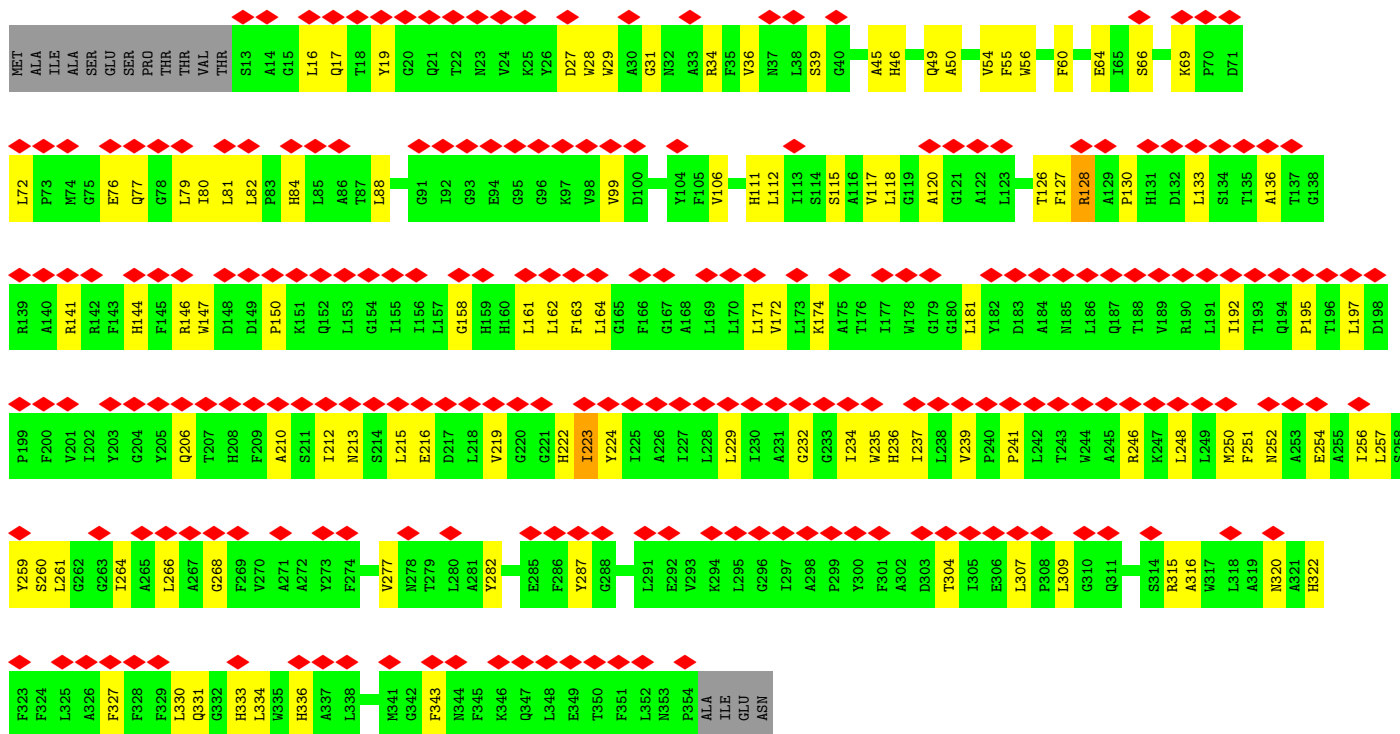


• Molecule 1: Iron stress-induced chlorophyll-binding protein



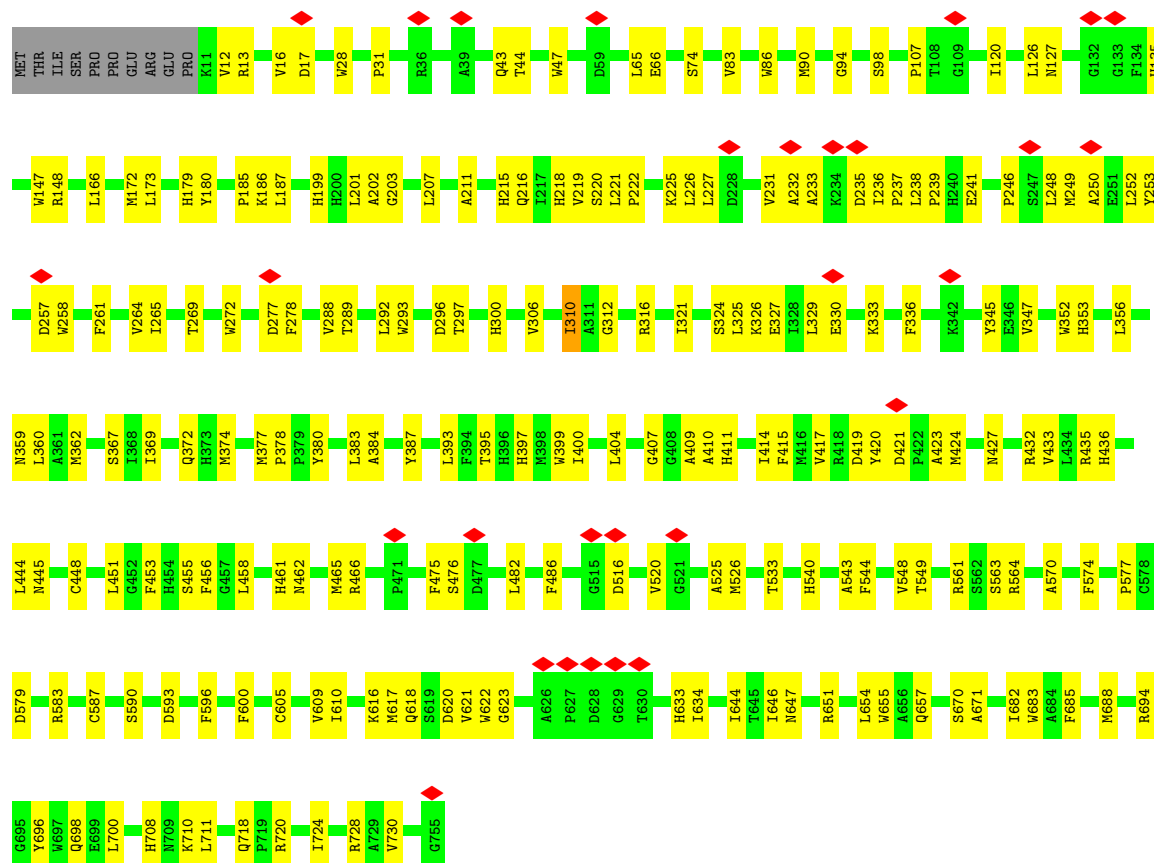


• Molecule 1: Iron stress-induced chlorophyll-binding protein

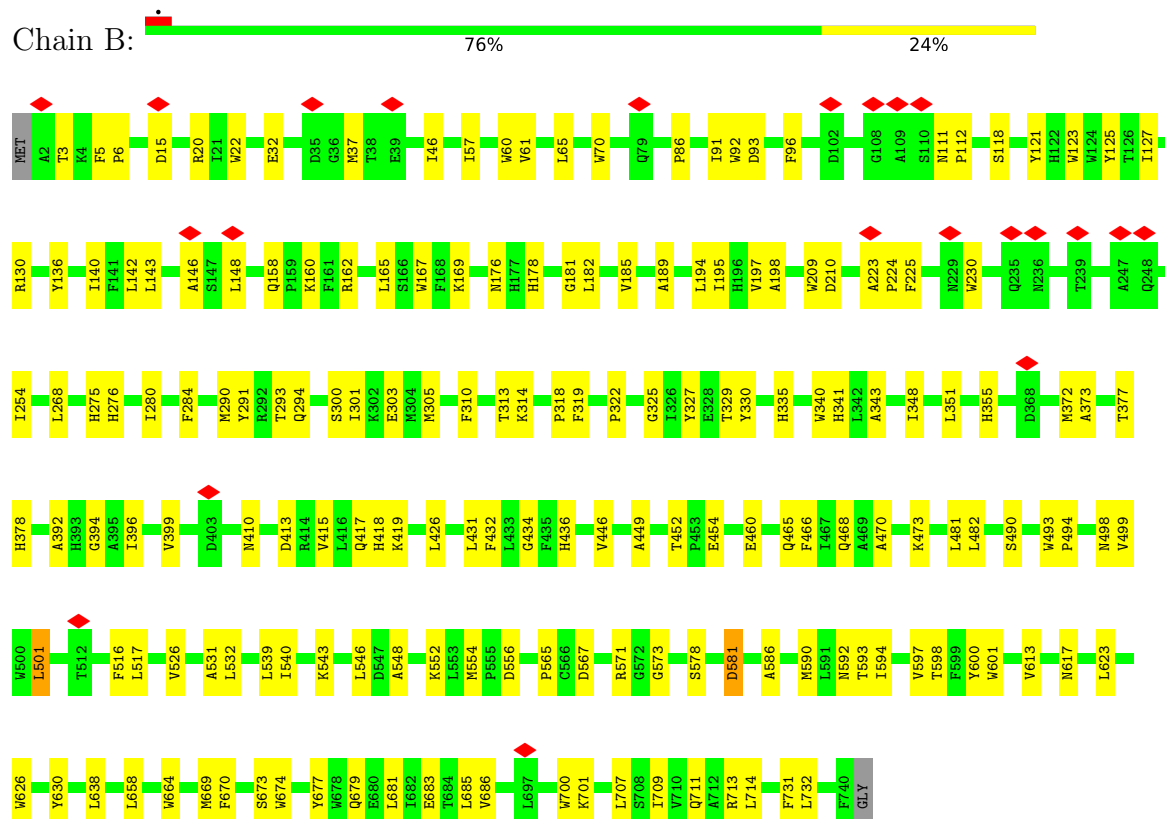


• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A1

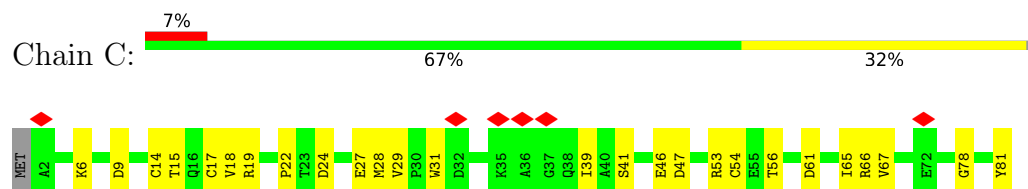




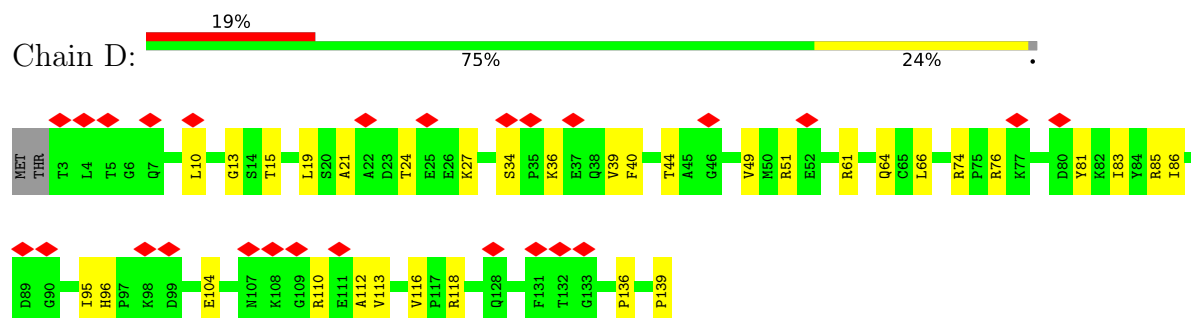
• Molecule 3: Photosystem I P700 chlorophyll a apoprotein A2



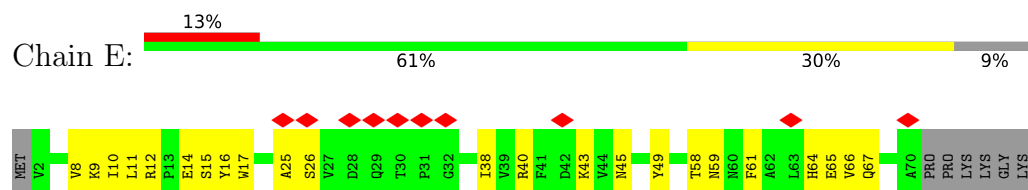
- Molecule 4: Photosystem I iron-sulfur center



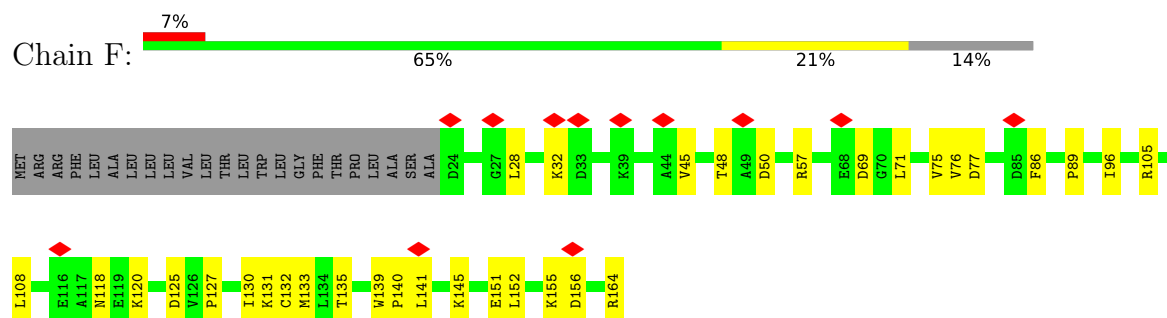
- Molecule 5: Photosystem I reaction center subunit II



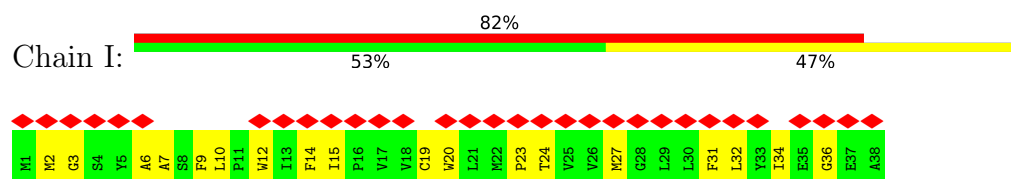
- Molecule 6: Photosystem I reaction center subunit IV



- Molecule 7: Photosystem I reaction center subunit III



- Molecule 8: Photosystem I reaction center subunit VIII



- Molecule 9: Photosystem I reaction center subunit IX

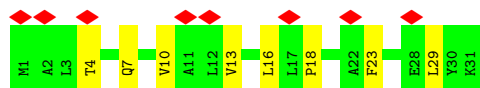
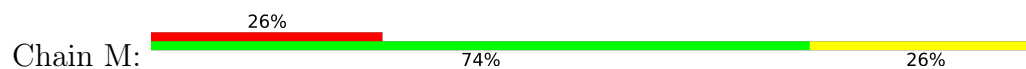




- Molecule 10: Photosystem I reaction center subunit PsaK



- Molecule 11: Photosystem I reaction center subunit XII



- Molecule 12: Photosystem I 4.8K protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	55670	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.055	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	350.0, 350.0, 350.0	wwPDB
Map dimensions	350, 350, 350	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.18	0/2754	0.31	1/3760 (0.0%)
1	2	0.15	0/2746	0.28	1/3749 (0.0%)
1	3	0.14	0/2770	0.26	0/3783
1	4	0.14	0/2770	0.26	0/3783
1	5	0.14	0/2701	0.53	3/3688 (0.1%)
1	6	0.13	0/2746	0.27	0/3749
1	a	0.14	0/2770	0.31	0/3783
1	b	0.17	0/2770	0.31	0/3783
1	c	0.15	0/2775	0.31	0/3790
1	d	0.23	1/2770 (0.0%)	0.32	2/3783 (0.1%)
1	e	0.16	0/2770	0.31	0/3783
1	f	0.21	1/2762 (0.0%)	0.31	1/3771 (0.0%)
1	g	0.16	0/2762	0.30	0/3771
2	A	0.25	0/6019	0.30	0/8209
3	B	0.23	0/6107	0.28	0/8345
4	C	0.22	0/608	0.34	0/824
5	D	0.24	0/1094	0.39	1/1482 (0.1%)
6	E	0.18	0/551	0.23	0/750
7	F	0.19	0/1087	0.30	0/1476
8	I	0.21	0/312	0.54	0/425
9	J	0.23	0/350	0.30	0/477
10	K	0.24	0/446	0.38	0/610
11	M	0.45	0/244	0.89	2/332 (0.6%)
12	X	0.22	0/241	0.30	0/330
All	All	0.19	2/52925 (0.0%)	0.32	11/72236 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	199	PRO	N-CD	-9.69	1.34	1.47
1	f	199	PRO	N-CD	-8.07	1.36	1.47

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	5	222	HIS	N-CA-CB	18.73	142.14	110.49
1	5	221	GLY	N-CA-C	-18.32	79.75	112.54
11	M	18	PRO	CA-N-CD	-11.80	95.48	112.00
11	M	18	PRO	N-CD-CG	-6.88	92.88	103.20
1	5	222	HIS	N-CA-C	-6.43	97.10	110.80
1	d	199	PRO	CA-N-CD	6.22	120.71	112.00
1	d	199	PRO	N-CA-CB	-5.66	97.28	103.39
1	1	297	ILE	CA-C-O	-5.29	115.44	120.95
5	D	44	THR	CA-C-O	-5.28	115.26	121.07
1	2	198	ASP	CA-CB-CG	5.28	117.88	112.60
1	f	199	PRO	CA-N-CD	5.12	119.16	112.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	2665	0	2652	69	0
1	2	2657	0	2641	46	0
1	3	2680	0	2665	67	0
1	4	2680	0	2665	65	0
1	5	2613	0	2600	57	0
1	6	2657	0	2641	64	0
1	a	2680	0	2665	91	0
1	b	2680	0	2665	86	0
1	c	2685	0	2670	81	0
1	d	2680	0	2665	79	0
1	e	2680	0	2665	80	0
1	f	2673	0	2658	81	0
1	g	2673	0	2658	83	0
2	A	5819	0	5684	190	0
3	B	5889	0	5646	162	0
4	C	598	0	578	26	0
5	D	1068	0	1067	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	E	539	0	525	16	0
7	F	1065	0	1074	40	0
8	I	301	0	306	19	0
9	J	338	0	347	10	0
10	K	437	0	451	12	0
11	M	241	0	264	7	0
12	X	232	0	220	4	0
13	1	945	0	881	48	0
13	2	936	0	867	46	0
13	3	945	0	881	47	0
13	4	924	0	848	42	0
13	5	956	0	900	50	0
13	6	914	0	832	59	0
13	A	2681	0	2703	185	0
13	B	2443	0	2455	161	0
13	F	45	0	33	1	0
13	J	89	0	66	1	0
13	K	96	0	78	4	0
13	X	45	0	33	2	0
13	a	925	0	849	64	0
13	b	945	0	881	51	0
13	c	933	0	861	70	0
13	d	945	0	880	48	0
13	e	935	0	865	53	0
13	f	938	0	871	68	0
13	g	942	0	875	54	0
14	1	160	0	224	22	0
14	2	160	0	224	17	0
14	3	160	0	224	20	0
14	4	160	0	224	14	0
14	5	160	0	224	22	0
14	6	160	0	224	18	0
14	A	200	0	280	31	0
14	B	240	0	336	25	0
14	F	120	0	168	14	0
14	I	120	0	167	16	0
14	J	80	0	112	8	0
14	K	40	0	56	6	0
14	M	40	0	56	3	0
14	a	160	0	224	27	0
14	b	160	0	224	22	0
14	c	160	0	224	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	d	160	0	224	18	0
14	e	160	0	224	20	0
14	f	160	0	224	22	0
14	g	160	0	223	24	0
15	1	31	0	26	0	0
15	2	31	0	26	3	0
15	3	31	0	26	0	0
15	4	31	0	26	7	0
15	5	31	0	26	2	0
15	6	31	0	26	2	0
15	B	43	0	50	2	0
15	a	31	0	26	0	0
15	b	31	0	26	0	0
15	c	31	0	26	0	0
15	d	31	0	26	0	0
15	e	31	0	26	0	0
15	f	31	0	26	0	0
15	g	31	0	26	1	0
16	1	40	0	50	0	0
16	2	40	0	50	1	0
16	6	38	0	46	2	0
16	B	55	0	86	5	0
16	J	31	0	32	0	0
16	g	40	0	50	1	0
17	A	211	0	281	21	0
18	A	33	0	46	2	0
18	B	33	0	46	4	0
19	A	8	0	0	1	0
19	C	16	0	0	2	0
20	A	47	0	65	3	0
20	B	35	0	46	1	0
20	J	22	0	28	10	0
All	All	72827	0	72631	2153	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (2153) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:309:LEU:HD21	2:A:250:ALA:CB	1.62	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:309:LEU:HD21	2:A:250:ALA:HB2	1.22	1.12
1:3:29:TRP:CE2	20:J:5105:LMU:H31	1.88	1.08
1:d:197:LEU:O	1:d:198:ASP:OD1	1.83	0.96
1:1:309:LEU:CD2	2:A:250:ALA:HB2	1.94	0.96
14:2:521:BCR:HC22	17:A:5005:LHG:HC41	1.49	0.93
13:5:513:CLA:H61	14:5:523:BCR:H272	1.53	0.91
1:1:309:LEU:HD21	2:A:250:ALA:HB3	1.51	0.89
1:1:309:LEU:CD2	2:A:250:ALA:CB	2.49	0.88
13:a:513:CLA:NA	14:a:523:BCR:H282	1.90	0.86
13:6:508:CLA:HMB3	13:6:509:CLA:NC	1.90	0.86
13:c:501:CLA:HBB2	13:c:507:CLA:H92	1.57	0.85
1:f:322:HIS:NE2	13:f:502:CLA:ND	2.25	0.84
14:A:4011:BCR:H362	13:B:1012:CLA:H2	1.58	0.84
2:A:179:HIS:HE1	13:A:1108:CLA:NC	1.76	0.83
1:3:29:TRP:CG	20:J:5105:LMU:H51	2.14	0.83
1:b:341:MET:HE3	1:a:128:ARG:HG2	1.62	0.82
13:a:503:CLA:H151	13:a:510:CLA:HBB2	1.62	0.82
15:4:822:SQD:C24	7:F:141:LEU:HD11	2.08	0.81
1:2:294:LYS:HE2	17:A:5005:LHG:O1	1.80	0.81
13:A:1237:CLA:H101	14:I:4019:BCR:H21C	1.61	0.81
1:6:60:PHE:HE2	13:6:504:CLA:NC	1.79	0.81
1:d:261:LEU:HD21	13:d:508:CLA:HAB	1.62	0.81
1:4:161:LEU:HD21	13:4:506:CLA:HAB	1.63	0.81
13:A:1102:CLA:H2	13:A:1109:CLA:H92	1.62	0.81
13:A:1013:CLA:HBB1	13:B:1012:CLA:C4B	2.10	0.80
1:5:218:LEU:O	1:5:221:GLY:O	2.00	0.80
1:g:161:LEU:HD21	13:g:506:CLA:HAB	1.63	0.79
13:A:1127:CLA:H2	14:A:4003:BCR:H392	1.65	0.78
4:C:46:GLU:OE1	4:C:46:GLU:N	2.17	0.77
13:a:502:CLA:H122	13:a:503:CLA:H3A	1.65	0.77
13:2:502:CLA:HBB2	13:2:510:CLA:H151	1.63	0.77
13:b:508:CLA:H72	14:b:521:BCR:H23C	1.67	0.77
1:5:27:ASP:OD2	3:B:313:THR:OG1	2.03	0.76
1:f:270:VAL:HG21	13:f:501:CLA:H92	1.67	0.76
13:5:503:CLA:H172	13:5:510:CLA:HBB2	1.68	0.76
1:f:47:VAL:HG22	13:f:512:CLA:HED1	1.66	0.76
1:e:45:ALA:HB2	13:e:511:CLA:HMA1	1.67	0.76
13:A:1125:CLA:HBA1	14:A:4008:BCR:H19C	1.69	0.75
1:4:354:PRO:HG2	7:F:132:CYS:SG	2.27	0.75
1:f:125:HIS:CE1	13:f:513:CLA:NA	2.54	0.75
3:B:300:SER:HB3	3:B:303:GLU:OE1	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:718:GLN:NE2	6:E:43:LYS:HB2	2.01	0.74
1:5:215:LEU:HG	1:5:280:LEU:HD11	1.70	0.74
1:1:161:LEU:HD21	13:1:506:CLA:HAB	1.68	0.74
14:A:4002:BCR:H362	14:A:4003:BCR:H10C	1.69	0.74
1:b:192:ILE:HG21	1:b:219:VAL:HG11	1.70	0.74
13:e:518:CLA:H72	13:e:519:CLA:ND	2.03	0.74
13:f:501:CLA:H202	13:f:507:CLA:HBB1	1.69	0.73
1:6:32:ASN:OD1	13:6:511:CLA:NC	2.21	0.73
13:d:503:CLA:H152	13:d:510:CLA:HBB2	1.70	0.73
1:d:287:TYR:HB3	1:d:315:ARG:HB2	1.71	0.73
13:3:505:CLA:H51	14:3:524:BCR:H342	1.71	0.73
13:d:517:CLA:NC	14:d:524:BCR:H19C	2.02	0.73
3:B:32:GLU:OE2	3:B:335:HIS:NE2	2.22	0.73
1:4:349:GLU:OE2	7:F:145:LYS:HE3	1.88	0.73
13:A:1139:CLA:H72	9:J:14:LEU:HD13	1.69	0.73
1:2:282:TYR:O	1:2:315:ARG:NH2	2.21	0.72
1:g:110:VAL:HG13	14:g:523:BCR:H12C	1.71	0.72
1:e:126:THR:HG21	14:e:522:BCR:H271	1.72	0.72
1:2:212:ILE:HG12	1:2:278:ASN:HD21	1.55	0.72
1:6:161:LEU:HD21	13:6:506:CLA:HAB	1.71	0.72
1:3:29:TRP:CD2	20:J:5105:LMU:H31	2.24	0.72
3:B:554:MET:HE1	3:B:567:ASP:HB2	1.70	0.72
13:g:511:CLA:HBA1	14:g:522:BCR:H281	1.71	0.72
1:b:278:ASN:O	1:b:315:ARG:NH2	2.23	0.72
13:b:501:CLA:HBB2	13:b:507:CLA:H92	1.72	0.72
13:2:503:CLA:H151	13:2:510:CLA:HBB2	1.72	0.72
4:C:81:TYR:HB3	5:D:19:LEU:HD22	1.72	0.72
1:f:278:ASN:O	1:f:315:ARG:NH2	2.22	0.72
4:C:67:VAL:HG11	19:C:3002:SF4:S2	2.29	0.71
4:C:24:ASP:OD2	5:D:96:HIS:ND1	2.22	0.71
1:d:282:TYR:O	1:d:315:ARG:NH2	2.20	0.71
13:d:518:CLA:H43	13:d:519:CLA:C1B	2.18	0.71
13:B:1206:CLA:HHB	13:B:1207:CLA:HBB1	1.71	0.71
13:B:1216:CLA:H2A	13:B:1216:CLA:HED3	1.71	0.71
13:A:1104:CLA:HED1	13:A:1128:CLA:H2	1.72	0.71
1:f:125:HIS:HE1	13:f:513:CLA:NA	1.89	0.71
13:A:1101:CLA:HMA2	13:A:1106:CLA:H201	1.73	0.70
5:D:10:LEU:HG	5:D:51:ARG:HE	1.56	0.70
1:a:72:LEU:HB3	1:a:77:GLN:HE21	1.56	0.70
1:3:29:TRP:HZ2	20:J:5105:LMU:H3'	1.56	0.70
3:B:355:HIS:ND1	13:B:1214:CLA:OBD	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:90:MET:HE1	13:A:1106:CLA:HMA2	1.74	0.70
3:B:351:LEU:HD11	3:B:355:HIS:CE1	2.27	0.70
1:2:291:LEU:HD22	1:2:303:ASP:HA	1.74	0.70
2:A:120:ILE:HB	14:J:4013:BCR:H322	1.72	0.70
8:I:23:PRO:O	8:I:27:MET:HG2	1.91	0.70
13:f:506:CLA:HBB2	13:f:507:CLA:H62	1.74	0.70
14:a:522:BCR:H281	13:a:511:CLA:HBA1	1.74	0.69
1:3:192:ILE:HG13	1:3:219:VAL:HG21	1.74	0.69
1:6:225:ILE:HG12	13:6:501:CLA:HAB	1.74	0.69
1:1:261:LEU:HD21	13:1:508:CLA:HAB	1.74	0.69
13:c:517:CLA:NC	14:c:524:BCR:H19C	2.06	0.69
13:A:1134:CLA:H43	13:K:1401:CLA:H43	1.74	0.69
1:6:64:GLU:HB3	1:6:79:LEU:HD23	1.75	0.69
13:2:501:CLA:HMB2	14:2:524:BCR:H23C	1.73	0.69
2:A:647:ASN:OD1	2:A:651:ARG:NH1	2.26	0.69
1:a:232:GLY:O	1:a:236:HIS:ND1	2.19	0.69
1:3:29:TRP:CZ2	20:J:5105:LMU:H3'	2.28	0.69
1:c:181:LEU:HB2	1:c:215:LEU:HD21	1.75	0.69
14:d:522:BCR:HC8	13:e:505:CLA:H193	1.75	0.69
13:5:503:CLA:H193	13:5:510:CLA:HAB	1.75	0.68
1:d:73:PRO:HB2	1:d:76:GLU:HG2	1.74	0.68
2:A:172:MET:HE1	13:A:1111:CLA:H92	1.75	0.68
1:f:74:MET:HA	1:f:77:GLN:HE21	1.58	0.68
14:2:521:BCR:C2	17:A:5005:LHG:HC41	2.21	0.68
13:A:1022:CLA:C4B	13:B:1023:CLA:HBB1	2.23	0.68
7:F:48:THR:HG22	7:F:50:ASP:H	1.58	0.68
13:B:1216:CLA:HBB1	13:B:1221:CLA:H93	1.75	0.68
13:3:503:CLA:H162	13:3:510:CLA:HBB2	1.75	0.68
1:4:349:GLU:OE2	7:F:145:LYS:CE	2.42	0.68
1:c:133:LEU:HD12	1:c:140:ALA:HB1	1.76	0.68
1:e:282:TYR:O	1:e:315:ARG:NH2	2.27	0.68
1:g:322:HIS:NE2	13:g:502:CLA:ND	2.42	0.68
1:4:35:PHE:HZ	13:4:509:CLA:HAB	1.59	0.68
1:2:294:LYS:CD	17:A:5005:LHG:O1	2.41	0.68
1:6:324:PHE:HD2	14:6:521:BCR:H10C	1.58	0.68
1:5:18:THR:OG1	1:5:21:GLN:O	2.11	0.68
13:A:1013:CLA:H111	14:A:4011:BCR:H23C	1.75	0.68
1:g:261:LEU:HD11	13:g:508:CLA:HAB	1.76	0.68
2:A:31:PRO:HB2	2:A:47:TRP:HH2	1.59	0.67
2:A:202:ALA:HB1	13:A:1118:CLA:HBC3	1.76	0.67
1:a:49:GLN:HB2	13:a:509:CLA:HMB1	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:c:522:BCR:H351	13:d:505:CLA:HBB2	1.75	0.67
1:f:43:ILE:HD11	13:f:512:CLA:HBC3	1.74	0.67
15:4:822:SQD:H242	7:F:141:LEU:HD11	1.76	0.67
1:2:246:ARG:HA	1:2:251:PHE:HE1	1.60	0.67
3:B:92:TRP:CD1	8:I:15:ILE:HG21	2.30	0.67
10:K:54:PHE:CD2	10:K:58:GLU:HG3	2.30	0.67
1:e:320:ASN:HB3	14:e:521:BCR:HC8	1.76	0.67
13:g:505:CLA:H51	14:g:524:BCR:H342	1.75	0.67
14:3:522:BCR:HC22	1:4:293:VAL:HG11	1.76	0.67
13:6:501:CLA:HMB1	14:6:524:BCR:H23C	1.75	0.67
1:c:261:LEU:HD21	13:c:508:CLA:HAB	1.76	0.67
1:f:113:ILE:HD12	14:f:523:BCR:H10C	1.76	0.67
1:a:49:GLN:HE21	13:a:509:CLA:HHB	1.60	0.67
13:e:517:CLA:NC	14:e:524:BCR:H19C	2.10	0.67
13:3:501:CLA:HMB1	14:3:524:BCR:H23C	1.76	0.67
1:6:14:ALA:HB2	1:6:148:ASP:HB2	1.76	0.67
1:b:289:PRO:HG3	1:b:305:ILE:HD13	1.77	0.67
1:4:351:PHE:O	7:F:135:THR:HG21	1.95	0.66
2:A:593:ASP:OD2	2:A:728:ARG:NH1	2.27	0.66
1:b:158:GLY:HA3	1:b:237:ILE:HG23	1.77	0.66
4:C:31:TRP:CE3	4:C:39:ILE:HB	2.31	0.66
1:g:307:LEU:HD12	1:g:308:PRO:HD2	1.76	0.66
1:2:192:ILE:HG13	1:2:219:VAL:HG21	1.78	0.66
3:B:176:ASN:ND2	3:B:291:TYR:O	2.27	0.66
1:a:88:LEU:O	1:a:174:LYS:NZ	2.24	0.66
1:g:143:PHE:HD2	13:g:513:CLA:H3A	1.59	0.66
13:1:508:CLA:H93	14:1:521:BCR:H19C	1.77	0.66
8:I:20:TRP:O	8:I:24:THR:HG23	1.96	0.66
3:B:460:GLU:HG3	7:F:28:LEU:HD11	1.78	0.66
1:5:254:GLU:OE2	1:5:339:ARG:NH1	2.29	0.66
13:B:1222:CLA:HMA1	14:B:4010:BCR:H14C	1.78	0.66
13:2:519:CLA:CBC	17:A:5005:LHG:H142	2.26	0.66
3:B:419:LYS:HB2	3:B:546:LEU:HD13	1.77	0.66
1:4:174:LYS:HA	1:4:178:TRP:HB2	1.78	0.66
1:2:294:LYS:CE	17:A:5005:LHG:O1	2.43	0.66
13:f:505:CLA:H51	14:f:524:BCR:H342	1.78	0.66
1:1:316:ALA:O	1:1:320:ASN:ND2	2.27	0.65
1:5:17:GLN:NE2	1:5:339:ARG:O	2.30	0.65
4:C:61:ASP:O	6:E:59:ASN:ND2	2.28	0.65
13:d:503:CLA:H41	13:d:503:CLA:H101	1.77	0.65
1:4:181:LEU:HD13	13:4:501:CLA:HED1	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:505:CLA:HBA1	1:1:120:ALA:HB1	1.79	0.65
1:3:241:PRO:HA	13:3:506:CLA:HED3	1.78	0.65
1:f:125:HIS:NE2	13:f:513:CLA:NB	2.44	0.65
1:1:64:GLU:HG3	1:1:81:LEU:HB2	1.79	0.65
3:B:5:PHE:CD2	3:B:6:PRO:HD3	2.31	0.65
1:g:320:ASN:HB3	14:g:521:BCR:HC8	1.78	0.65
13:B:1201:CLA:H3A	11:M:29:LEU:HD13	1.79	0.65
4:C:15:THR:HA	4:C:28:MET:HE2	1.78	0.65
1:d:160:HIS:NE2	13:d:512:CLA:NA	2.44	0.65
13:3:508:CLA:H2A	13:3:508:CLA:HED3	1.78	0.65
1:5:125:HIS:HA	1:5:129:ALA:HB3	1.78	0.65
1:2:324:PHE:HZ	17:A:5005:LHG:H102	1.62	0.65
2:A:411:HIS:HE1	13:A:1128:CLA:NA	1.95	0.65
1:e:192:ILE:HG13	1:e:219:VAL:HG21	1.78	0.65
2:A:222:PRO:HG3	2:A:249:MET:HE1	1.80	0.64
13:4:511:CLA:HMB1	14:4:522:BCR:H382	1.79	0.64
1:6:49:GLN:HG2	13:6:509:CLA:HHB	1.78	0.64
1:g:88:LEU:HD11	13:g:503:CLA:HAA2	1.77	0.64
13:B:1229:CLA:H191	13:B:1235:CLA:H13	1.80	0.64
1:g:94:GLU:O	1:g:97:LYS:NZ	2.30	0.64
1:3:29:TRP:CZ3	7:F:127:PRO:HB3	2.32	0.64
2:A:173:LEU:HD21	13:A:1107:CLA:H191	1.78	0.64
1:b:261:LEU:HD21	13:b:508:CLA:HAB	1.78	0.64
2:A:590:SER:OG	2:A:593:ASP:OD1	2.15	0.64
1:3:29:TRP:CB	20:J:5105:LMU:H51	2.27	0.64
1:1:244:TRP:HA	1:1:247:LYS:HE2	1.78	0.64
14:F:4014:BCR:HC22	14:F:4015:BCR:H363	1.80	0.64
13:e:501:CLA:HMB2	14:e:524:BCR:H23C	1.80	0.64
1:e:264:ILE:HG12	13:e:507:CLA:HBA2	1.79	0.64
14:3:522:BCR:HC7	1:4:323:PHE:HE1	1.64	0.63
3:B:319:PHE:HB2	13:B:1220:CLA:HMA1	1.80	0.63
8:I:7:ALA:HB1	8:I:10:LEU:HG	1.80	0.63
1:c:221:GLY:HA3	14:c:524:BCR:H402	1.79	0.63
2:A:269:THR:HB	10:K:11:TRP:HB2	1.81	0.63
2:A:670:SER:HB2	3:B:449:ALA:HB1	1.80	0.63
1:c:334:LEU:HD21	13:c:505:CLA:HMB2	1.79	0.63
1:b:221:GLY:HA3	14:b:524:BCR:H402	1.80	0.63
1:a:163:PHE:HZ	13:a:516:CLA:HBC2	1.63	0.63
1:4:49:GLN:NE2	1:4:53:SER:OG	2.32	0.63
1:6:45:ALA:HB2	13:6:511:CLA:HMA1	1.79	0.63
3:B:454:GLU:OE2	7:F:57:ARG:NH1	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:669:MET:O	3:B:673:SER:OG	2.13	0.63
1:3:282:TYR:O	1:3:315:ARG:NH2	2.30	0.63
13:3:501:CLA:H202	13:3:507:CLA:HBB1	1.80	0.63
13:A:1119:CLA:H102	14:A:4008:BCR:H10C	1.80	0.63
1:g:339:ARG:NH1	15:g:822:SQD:O9	2.32	0.63
1:a:79:LEU:HD13	1:a:82:LEU:HD12	1.80	0.63
13:A:1101:CLA:HBB1	14:J:4013:BCR:H271	1.79	0.63
1:g:88:LEU:HD13	13:g:502:CLA:H143	1.80	0.63
8:I:2:MET:HE3	8:I:12:TRP:CZ2	2.33	0.63
1:1:225:ILE:HG12	13:1:501:CLA:HAB	1.80	0.63
1:c:273:TYR:HB2	14:b:522:BCR:HC41	1.81	0.63
1:d:16:LEU:HD13	1:d:36:VAL:HG21	1.81	0.63
1:g:125:HIS:HE1	13:g:513:CLA:NA	1.97	0.63
1:a:46:HIS:HD2	13:a:509:CLA:H141	1.63	0.63
2:A:482:LEU:HB2	2:A:533:THR:HG23	1.81	0.62
1:a:282:TYR:O	1:a:315:ARG:NH2	2.31	0.62
13:B:1222:CLA:H122	13:B:1232:CLA:HBB2	1.81	0.62
1:d:258:SER:O	1:d:333:HIS:ND1	2.27	0.62
1:g:45:ALA:HB2	13:g:511:CLA:HMA1	1.81	0.62
1:g:49:GLN:HG2	13:g:509:CLA:HHB	1.81	0.62
1:a:248:LEU:HD13	14:a:524:BCR:HC42	1.81	0.62
2:A:579:ASP:OD2	2:A:583:ARG:NH2	2.26	0.62
3:B:531:ALA:HB2	13:B:1235:CLA:HMA1	1.80	0.62
1:4:241:PRO:HA	13:4:506:CLA:HED3	1.82	0.62
1:b:49:GLN:HG3	13:b:509:CLA:HMB3	1.81	0.62
1:3:49:GLN:HG2	13:3:509:CLA:HHB	1.82	0.62
1:1:339:ARG:HH12	13:1:508:CLA:HED2	1.65	0.62
3:B:677:TYR:OH	13:B:1023:CLA:OBD	2.15	0.62
1:5:16:LEU:HD13	1:5:36:VAL:HG21	1.80	0.62
13:6:503:CLA:H193	13:6:510:CLA:HAB	1.82	0.62
1:1:309:LEU:HB3	2:A:257:ASP:O	2.00	0.61
1:4:60:PHE:HE1	13:5:519:CLA:HAA2	1.65	0.61
13:A:1123:CLA:HBA1	13:A:1127:CLA:H18	1.81	0.61
13:A:1013:CLA:H3A	13:A:1013:CLA:O2A	2.00	0.61
1:f:84:HIS:HE1	1:f:318:LEU:HD11	1.65	0.61
1:b:46:HIS:HD2	13:b:509:CLA:H141	1.64	0.61
1:3:84:HIS:NE2	13:3:502:CLA:O1D	2.29	0.61
1:6:125:HIS:HA	1:6:129:ALA:HB3	1.80	0.61
13:2:518:CLA:H71	13:2:519:CLA:ND	2.14	0.61
1:1:299:PRO:HG2	13:1:519:CLA:C1B	2.30	0.61
1:d:60:PHE:O	1:d:64:GLU:HG2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:241:PRO:O	1:e:246:ARG:NH2	2.33	0.61
2:A:353:HIS:HD2	2:A:411:HIS:HD1	1.47	0.61
4:C:41:SER:HB2	5:D:113:VAL:H	1.65	0.61
13:e:511:CLA:HBA1	14:e:522:BCR:H281	1.80	0.61
13:B:1203:CLA:H162	13:B:1225:CLA:HBB2	1.83	0.61
2:A:451:LEU:HB3	2:A:544:PHE:HB2	1.81	0.61
2:A:718:GLN:HE21	6:E:43:LYS:HB2	1.65	0.61
13:3:508:CLA:H42	14:3:521:BCR:H272	1.83	0.61
1:3:341:MET:HE1	1:2:124:PHE:HA	1.82	0.61
15:4:822:SQD:C26	7:F:141:LEU:HD11	2.30	0.61
13:g:508:CLA:H42	14:g:521:BCR:H272	1.82	0.61
2:A:232:ALA:O	2:A:235:ASP:N	2.27	0.60
13:A:1128:CLA:H42	17:A:5001:LHG:H241	1.83	0.60
7:F:57:ARG:NE	9:J:35:ASP:OD2	2.27	0.60
13:g:501:CLA:HMB2	14:g:524:BCR:H23C	1.83	0.60
13:2:505:CLA:H43	14:2:524:BCR:HC7	1.82	0.60
13:1:503:CLA:H41	13:1:503:CLA:H101	1.83	0.60
6:E:12:ARG:HD3	6:E:14:GLU:OE2	2.00	0.60
10:K:12:THR:HG22	10:K:13:PRO:HD2	1.83	0.60
1:f:291:LEU:HD21	1:f:316:ALA:HA	1.83	0.60
13:b:501:CLA:H202	13:b:507:CLA:HBB1	1.81	0.60
1:a:192:ILE:HD11	1:a:215:LEU:HD23	1.82	0.60
5:D:61:ARG:HB2	5:D:64:GLN:HG3	1.83	0.60
1:g:221:GLY:HA3	14:g:524:BCR:H402	1.82	0.60
1:c:181:LEU:HD13	13:c:501:CLA:HED1	1.83	0.60
1:a:60:PHE:O	1:a:64:GLU:HG2	2.02	0.60
3:B:417:GLN:O	7:F:164:ARG:NH2	2.34	0.60
1:d:221:GLY:HA3	14:d:524:BCR:H402	1.84	0.60
13:5:501:CLA:H122	13:5:507:CLA:H8	1.83	0.60
3:B:554:MET:HE2	4:C:66:ARG:HH22	1.67	0.60
10:K:73:VAL:HA	13:K:1401:CLA:HBB1	1.83	0.60
1:g:206:GLN:HB2	13:g:517:CLA:HMD2	1.83	0.60
1:c:150:PRO:HB2	1:c:241:PRO:HD2	1.82	0.60
1:g:174:LYS:NZ	1:g:180:GLY:O	2.33	0.60
1:3:316:ALA:O	1:3:320:ASN:ND2	2.29	0.60
13:1:502:CLA:HMB2	13:1:504:CLA:HAB	1.83	0.60
2:A:207:LEU:HD22	14:A:4002:BCR:H361	1.83	0.60
1:e:322:HIS:HD2	13:e:502:CLA:HED2	1.67	0.60
1:3:164:LEU:HD21	13:3:509:CLA:H61	1.82	0.60
1:1:80:ILE:HG13	1:1:81:LEU:HD22	1.84	0.60
1:1:210:ALA:HB1	1:1:277:VAL:HG21	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1238:CLA:H51	13:B:1239:CLA:H121	1.83	0.60
13:4:509:CLA:HBD	13:4:509:CLA:H121	1.83	0.60
13:6:510:CLA:H2	13:6:510:CLA:HMA1	1.84	0.60
1:a:162:LEU:HD21	1:a:234:ILE:HG13	1.84	0.60
13:6:507:CLA:H112	14:6:524:BCR:H362	1.84	0.59
1:c:282:TYR:O	1:c:315:ARG:NH2	2.34	0.59
1:e:49:GLN:HG2	13:e:509:CLA:HBB	1.82	0.59
3:B:5:PHE:HB2	8:I:34:ILE:HA	1.84	0.59
3:B:581:ASP:OD1	3:B:713:ARG:NH1	2.35	0.59
13:f:513:CLA:C4B	14:f:523:BCR:H383	2.31	0.59
14:f:522:BCR:HC7	1:g:323:PHE:HE1	1.66	0.59
13:b:517:CLA:NC	14:b:524:BCR:H19C	2.17	0.59
13:A:1022:CLA:H121	13:B:1207:CLA:HBC3	1.84	0.59
9:J:21:ILE:HA	13:J:1302:CLA:HBB2	1.85	0.59
1:b:241:PRO:HA	13:b:506:CLA:HED3	1.83	0.59
1:6:254:GLU:OE1	1:6:336:HIS:ND1	2.32	0.59
1:f:214:SER:HB3	1:f:217:ASP:HB2	1.83	0.59
1:g:77:GLN:HB2	1:g:79:LEU:HD13	1.82	0.59
1:g:125:HIS:NE2	13:g:513:CLA:NB	2.51	0.59
13:b:503:CLA:H151	13:b:510:CLA:HBB2	1.83	0.59
13:1:508:CLA:H72	14:1:521:BCR:H21C	1.84	0.59
13:B:1202:CLA:H2	13:B:1202:CLA:HAA2	1.85	0.59
2:A:435:ARG:NH1	5:D:13:GLY:O	2.29	0.59
2:A:458:LEU:O	2:A:462:ASN:ND2	2.34	0.59
13:A:1101:CLA:HBB2	13:A:1109:CLA:H72	1.84	0.59
3:B:592:ASN:HB2	13:B:1012:CLA:HBC2	1.84	0.59
1:f:50:ALA:O	1:f:54:VAL:HG22	2.03	0.59
15:4:822:SQD:H241	7:F:141:LEU:HD11	1.85	0.59
1:d:320:ASN:HB3	14:d:521:BCR:HC8	1.84	0.59
1:e:92:ILE:HD11	1:e:189:VAL:HG23	1.84	0.59
13:6:502:CLA:HMB2	13:6:504:CLA:HAB	1.85	0.59
2:A:688:MET:HB2	13:A:1013:CLA:C1C	2.33	0.59
7:F:131:LYS:O	7:F:135:THR:HG23	2.02	0.59
1:c:192:ILE:HD12	1:c:216:GLU:HG2	1.85	0.59
1:f:291:LEU:HD13	1:f:315:ARG:HD3	1.84	0.59
1:5:228:LEU:HD12	13:5:506:CLA:HBC1	1.85	0.58
2:A:694:ARG:NH1	3:B:573:GLY:O	2.36	0.58
1:1:186:LEU:HD22	1:1:190:ARG:HD2	1.85	0.58
4:C:24:ASP:HB2	5:D:66:LEU:HD21	1.84	0.58
13:c:510:CLA:H2	13:c:510:CLA:H2A	1.86	0.58
1:d:80:ILE:HG13	1:d:81:LEU:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:159:HIS:CG	13:b:512:CLA:HAB	2.37	0.58
1:a:172:VAL:HG21	1:a:223:ILE:HG23	1.85	0.58
13:a:501:CLA:H162	13:a:507:CLA:H122	1.84	0.58
1:1:125:HIS:HA	1:1:129:ALA:HB3	1.84	0.58
13:B:1223:CLA:H13	14:B:4010:BCR:H351	1.84	0.58
13:c:501:CLA:HMB2	14:c:524:BCR:H23C	1.85	0.58
1:d:36:VAL:HG22	13:d:509:CLA:HAC2	1.85	0.58
13:f:501:CLA:HBB2	13:f:507:CLA:H92	1.84	0.58
1:g:64:GLU:HB3	1:g:79:LEU:HG	1.86	0.58
2:A:325:LEU:HD13	13:A:1123:CLA:HAC2	1.85	0.58
1:c:112:LEU:HD22	14:c:522:BCR:H12C	1.84	0.58
13:3:511:CLA:HBA1	14:3:522:BCR:H281	1.86	0.58
13:4:503:CLA:H151	13:4:510:CLA:HBB2	1.86	0.58
15:4:822:SQD:C26	7:F:141:LEU:CD1	2.82	0.58
1:5:219:VAL:C	1:5:221:GLY:O	2.45	0.58
2:A:420:TYR:HD2	2:A:561:ARG:HH11	1.49	0.58
2:A:696:TYR:OH	13:A:1013:CLA:OBD	2.22	0.58
3:B:340:TRP:HE1	13:B:1221:CLA:C2B	2.16	0.58
13:B:1023:CLA:H143	14:B:4017:BCR:H362	1.84	0.58
14:B:4009:BCR:H383	14:B:4010:BCR:H23C	1.84	0.58
1:g:289:PRO:HG3	1:g:305:ILE:HG13	1.85	0.58
1:5:199:PRO:HG3	1:f:297:ILE:HB	1.86	0.58
1:2:112:LEU:O	1:2:115:SER:OG	2.21	0.58
5:D:10:LEU:HB2	5:D:49:VAL:HB	1.85	0.58
3:B:670:PHE:HA	18:B:2002:PQN:H9	1.85	0.58
4:C:17:CYS:HB3	19:C:3003:SF4:S4	2.43	0.58
1:b:60:PHE:O	1:b:64:GLU:HG2	2.04	0.58
1:1:16:LEU:HD23	1:1:254:GLU:HB2	1.86	0.58
11:M:7:GLN:HA	11:M:10:VAL:HG12	1.85	0.58
1:f:77:GLN:HG3	1:f:79:LEU:HG	1.85	0.58
2:A:700:LEU:HD21	13:A:1013:CLA:HED2	1.85	0.58
1:c:197:LEU:HD13	1:c:223:ILE:HD11	1.84	0.58
3:B:70:TRP:NE1	8:I:6:ALA:O	2.32	0.57
13:d:501:CLA:HMB2	14:d:524:BCR:H23C	1.86	0.57
4:C:19:ARG:HG3	5:D:104:GLU:HG2	1.86	0.57
13:c:502:CLA:HBA2	13:c:503:CLA:H161	1.86	0.57
13:d:518:CLA:O2A	13:d:518:CLA:H3A	2.04	0.57
1:3:291:LEU:HD22	1:3:303:ASP:HA	1.87	0.57
13:3:505:CLA:HBC2	14:3:524:BCR:H341	1.86	0.57
13:2:501:CLA:HBB2	13:2:507:CLA:H92	1.85	0.57
13:B:1012:CLA:HMA3	13:B:1021:CLA:H202	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:329:PHE:HA	13:4:508:CLA:HMC2	1.87	0.57
3:B:373:ALA:HB1	3:B:732:LEU:HD11	1.84	0.57
1:d:241:PRO:HA	13:d:506:CLA:HED3	1.84	0.57
13:b:509:CLA:H162	13:b:512:CLA:HMD2	1.87	0.57
1:2:36:VAL:HG23	13:2:509:CLA:HAC2	1.85	0.57
1:c:225:ILE:HD13	14:c:524:BCR:H372	1.86	0.57
1:f:125:HIS:HE1	13:f:513:CLA:C1A	2.17	0.57
1:g:143:PHE:CD2	13:g:513:CLA:H3A	2.39	0.57
13:a:502:CLA:H11	13:a:503:CLA:H161	1.87	0.57
1:1:175:ALA:HB1	1:1:192:ILE:HD13	1.86	0.57
2:A:310:ILE:HG12	10:K:68:LEU:HD11	1.86	0.57
1:e:60:PHE:O	1:e:64:GLU:HG2	2.04	0.57
1:5:282:TYR:O	1:5:315:ARG:NH2	2.35	0.57
13:A:1129:CLA:HAB	13:A:1137:CLA:HBB2	1.87	0.57
13:B:1012:CLA:O1A	13:B:1012:CLA:H3A	2.04	0.57
14:I:4018:BCR:H383	14:I:4020:BCR:H353	1.86	0.57
1:c:169:LEU:HD11	1:c:230:ILE:HD11	1.86	0.57
13:6:519:CLA:HED2	13:6:519:CLA:H2A	1.87	0.57
1:2:225:ILE:HD11	13:2:507:CLA:H93	1.87	0.57
13:A:1103:CLA:H172	14:A:4002:BCR:H10C	1.84	0.57
13:B:1204:CLA:H2	14:I:4018:BCR:HC42	1.87	0.57
1:d:192:ILE:HG21	1:d:219:VAL:HG11	1.86	0.57
1:6:180:GLY:HA3	1:6:191:LEU:HA	1.86	0.56
13:c:505:CLA:H61	1:b:117:VAL:HG22	1.87	0.56
1:b:212:ILE:HG23	1:b:280:LEU:HB3	1.86	0.56
14:4:522:BCR:HC22	1:5:293:VAL:HG21	1.86	0.56
2:A:233:ALA:HA	2:A:236:ILE:HB	1.85	0.56
1:f:26:TYR:O	1:f:34:ARG:NH2	2.37	0.56
13:f:501:CLA:H71	13:f:507:CLA:H41	1.87	0.56
1:g:125:HIS:CE1	13:g:513:CLA:NA	2.73	0.56
1:b:49:GLN:HG3	13:b:509:CLA:CMB	2.35	0.56
1:3:64:GLU:HB3	1:3:82:LEU:HG	1.86	0.56
3:B:167:TRP:CZ2	13:B:1208:CLA:HHB	2.41	0.56
5:D:40:PHE:HA	5:D:76:ARG:HH22	1.70	0.56
8:I:34:ILE:HD11	14:I:4019:BCR:H333	1.86	0.56
1:c:130:PRO:HG3	1:c:136:ALA:HB2	1.87	0.56
1:e:221:GLY:HA3	14:e:524:BCR:H402	1.88	0.56
13:e:501:CLA:C4D	13:e:503:CLA:H2	2.36	0.56
1:3:128:ARG:HB2	1:4:341:MET:HE2	1.87	0.56
1:2:264:ILE:HG12	13:2:502:CLA:HAC1	1.87	0.56
13:A:1119:CLA:H143	13:A:1122:CLA:H91	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:130:PRO:HG3	1:a:136:ALA:HB2	1.87	0.56
1:d:197:LEU:O	1:d:198:ASP:CG	2.48	0.56
13:f:513:CLA:C1C	14:f:523:BCR:H383	2.29	0.56
1:g:264:ILE:HG12	13:g:502:CLA:HAC1	1.88	0.56
1:4:36:VAL:HG22	13:4:509:CLA:HAC2	1.87	0.56
13:6:502:CLA:HAA1	13:6:503:CLA:H11	1.86	0.56
13:d:501:CLA:H18	13:d:507:CLA:H122	1.87	0.56
1:e:276:ALA:HA	1:e:291:LEU:HD12	1.87	0.56
1:f:36:VAL:HG22	13:f:509:CLA:HAC2	1.87	0.56
13:a:513:CLA:C4A	14:a:523:BCR:H282	2.35	0.56
13:4:501:CLA:H151	13:4:507:CLA:H8	1.88	0.56
15:4:822:SQD:H242	7:F:141:LEU:CD1	2.35	0.56
1:2:329:PHE:HA	13:2:508:CLA:HMC2	1.88	0.56
13:B:1205:CLA:H102	13:B:1205:CLA:H2	1.88	0.56
1:6:60:PHE:HE2	13:6:504:CLA:C4C	2.18	0.56
2:A:583:ARG:HG2	4:C:78:GLY:HA3	1.87	0.56
5:D:39:VAL:HA	5:D:49:VAL:HA	1.88	0.56
13:f:505:CLA:HBC2	14:f:524:BCR:H341	1.87	0.56
1:a:334:LEU:HD21	13:a:505:CLA:HMB2	1.87	0.56
1:1:170:LEU:HD23	1:1:173:LEU:HD12	1.88	0.56
2:A:253:TYR:HB3	2:A:277:ASP:HB3	1.86	0.56
13:c:518:CLA:HBB1	13:c:519:CLA:HAC2	1.87	0.56
1:d:163:PHE:CE1	13:d:512:CLA:HHB	2.40	0.56
13:a:503:CLA:H152	13:a:509:CLA:H42	1.88	0.56
1:6:228:LEU:HD21	13:6:517:CLA:HED1	1.88	0.56
13:a:502:CLA:HBD	13:a:503:CLA:H43	1.88	0.56
1:c:125:HIS:HA	1:c:129:ALA:HB3	1.87	0.55
13:c:503:CLA:H101	13:c:503:CLA:H41	1.86	0.55
1:e:120:ALA:HB1	13:f:505:CLA:H11	1.87	0.55
1:f:161:LEU:HD21	13:f:506:CLA:HAB	1.86	0.55
3:B:15:ASP:HB3	3:B:20:ARG:HB3	1.88	0.55
1:f:257:LEU:HD22	13:f:509:CLA:HBC3	1.89	0.55
1:a:163:PHE:CE2	13:a:512:CLA:HHB	2.41	0.55
1:5:192:ILE:HG13	1:5:219:VAL:HG21	1.86	0.55
1:6:303:ASP:OD1	1:6:303:ASP:N	2.40	0.55
3:B:415:VAL:HG11	14:B:4009:BCR:H271	1.87	0.55
1:e:258:SER:O	1:e:333:HIS:ND1	2.28	0.55
13:e:502:CLA:HBD	13:e:503:CLA:H43	1.88	0.55
1:b:185:ASN:ND2	1:b:213:ASN:O	2.39	0.55
3:B:118:SER:HA	13:B:1224:CLA:HMA2	1.89	0.55
1:3:13:SER:OG	1:3:14:ALA:N	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:194:GLN:NE2	1:g:67:GLN:OE1	2.29	0.55
13:1:501:CLA:H151	13:1:507:CLA:H72	1.89	0.55
2:A:543:ALA:HB2	13:A:1136:CLA:HMA1	1.88	0.55
3:B:526:VAL:HG21	3:B:600:TYR:HB2	1.88	0.55
3:B:669:MET:HB2	13:B:1023:CLA:C1C	2.36	0.55
13:B:1204:CLA:H2	14:I:4018:BCR:C4	2.36	0.55
7:F:75:VAL:HG12	7:F:77:ASP:OD1	2.05	0.55
1:d:303:ASP:OD1	1:d:303:ASP:N	2.40	0.55
1:g:122:ALA:O	1:g:126:THR:OG1	2.18	0.55
13:3:506:CLA:HBC3	13:3:507:CLA:H143	1.89	0.55
1:2:339:ARG:NH2	15:2:822:SQD:O9	2.40	0.55
1:1:164:LEU:HD21	13:1:507:CLA:H43	1.89	0.55
2:A:409:ALA:HB2	14:A:4008:BCR:H323	1.89	0.55
13:5:510:CLA:H2A	13:5:510:CLA:H12	1.89	0.55
1:1:174:LYS:HG3	13:1:502:CLA:H141	1.89	0.55
13:1:501:CLA:HMB2	14:1:524:BCR:H23C	1.88	0.55
3:B:378:HIS:HE1	13:B:1224:CLA:ND	2.05	0.55
13:B:1204:CLA:HHB	13:B:1205:CLA:HMB3	1.88	0.55
1:2:324:PHE:CZ	17:A:5005:LHG:H102	2.42	0.55
3:B:209:TRP:NE1	13:B:1211:CLA:O1A	2.39	0.55
13:B:1238:CLA:HAB	18:B:2002:PQN:H162	1.88	0.55
13:a:513:CLA:C4B	14:a:523:BCR:H272	2.25	0.55
1:4:278:ASN:O	1:4:315:ARG:NH1	2.40	0.55
3:B:301:ILE:O	3:B:305:MET:HG2	2.06	0.55
1:b:352:LEU:HD23	1:b:353:ASN:HB3	1.88	0.55
1:4:16:LEU:HD11	1:4:36:VAL:HG21	1.89	0.55
2:A:718:GLN:OE1	6:E:16:TYR:OH	2.25	0.55
13:c:511:CLA:H51	1:d:348:LEU:HD12	1.89	0.55
1:2:302:ALA:HB2	17:A:5005:LHG:HC11	1.89	0.54
1:1:145:PHE:HA	1:1:152:GLN:HG2	1.89	0.54
2:A:264:VAL:HG11	14:K:4001:BCR:HC21	1.88	0.54
1:e:278:ASN:O	1:e:315:ARG:NH2	2.39	0.54
1:f:88:LEU:HB3	1:f:174:LYS:HE3	1.89	0.54
13:f:501:CLA:H111	13:f:507:CLA:H51	1.89	0.54
13:6:502:CLA:H142	13:6:503:CLA:HHB	1.89	0.54
1:c:316:ALA:O	1:c:320:ASN:ND2	2.39	0.54
1:5:320:ASN:HB3	14:5:521:BCR:HC8	1.89	0.54
1:c:43:ILE:HD11	13:c:512:CLA:HBC3	1.89	0.54
14:d:522:BCR:HC42	1:e:273:TYR:HB2	1.88	0.54
1:b:330:LEU:HD11	13:b:505:CLA:HHC	1.88	0.54
1:4:192:ILE:HD11	1:4:215:LEU:HG	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:215:LEU:HG	1:2:280:LEU:HD11	1.89	0.54
1:1:250:MET:HE2	1:1:252:ASN:HD21	1.71	0.54
13:A:1119:CLA:H72	13:A:1122:CLA:H92	1.87	0.54
1:d:279:THR:HG23	1:d:284:VAL:HG23	1.90	0.54
2:A:359:ASN:ND2	13:A:1103:CLA:OBD	2.37	0.54
13:A:1105:CLA:OBD	20:A:1848:LMU:O2'	2.24	0.54
13:A:1011:CLA:C1A	13:B:1021:CLA:HAB	2.37	0.54
1:e:248:LEU:HD21	14:e:524:BCR:HC21	1.89	0.54
1:g:84:HIS:NE2	13:g:502:CLA:O1D	2.38	0.54
1:3:278:ASN:ND2	1:3:281:ALA:H	2.05	0.54
1:6:212:ILE:HG22	1:6:278:ASN:HD21	1.72	0.54
13:c:502:CLA:H42	13:c:503:CLA:H122	1.87	0.54
1:g:110:VAL:HG22	14:g:523:BCR:H10C	1.90	0.54
1:g:278:ASN:O	1:g:315:ARG:NH2	2.40	0.54
13:g:503:CLA:H172	13:g:510:CLA:HBB2	1.89	0.54
1:b:19:TYR:OH	1:b:343:PHE:O	2.21	0.54
1:b:341:MET:HE1	13:b:505:CLA:HAA1	1.90	0.54
1:a:76:GLU:HG3	1:a:307:LEU:HD22	1.89	0.54
1:6:185:ASN:ND2	1:6:213:ASN:O	2.41	0.54
13:f:511:CLA:H52	14:f:522:BCR:H282	1.88	0.54
1:g:60:PHE:HB3	1:g:81:LEU:HD21	1.90	0.54
1:b:185:ASN:OD1	1:b:186:LEU:N	2.40	0.54
1:3:186:LEU:HD12	1:3:190:ARG:HD3	1.88	0.54
9:J:26:LEU:HD13	14:J:4012:BCR:HC7	1.90	0.54
1:c:242:LEU:HD12	1:c:244:TRP:HE1	1.73	0.54
1:d:88:LEU:HB3	1:d:174:LYS:HE3	1.89	0.54
1:e:79:LEU:HD13	1:e:82:LEU:HD12	1.90	0.54
1:f:261:LEU:HD23	13:f:509:CLA:HED1	1.90	0.54
1:f:289:PRO:HG3	1:f:305:ILE:HB	1.90	0.54
1:4:158:GLY:HA3	1:4:237:ILE:HG13	1.89	0.54
1:4:351:PHE:O	7:F:135:THR:CG2	2.54	0.54
13:5:506:CLA:HAB	13:5:507:CLA:HED2	1.89	0.54
14:1:523:BCR:H382	13:1:513:CLA:C1C	2.28	0.54
2:A:65:LEU:HB3	2:A:187:LEU:HD11	1.89	0.54
2:A:216:GLN:HA	2:A:220:SER:HB2	1.89	0.54
6:E:8:VAL:HB	6:E:66:VAL:HB	1.90	0.54
13:f:505:CLA:H52	14:f:524:BCR:H331	1.89	0.54
1:a:219:VAL:O	1:a:223:ILE:HG12	2.08	0.54
1:1:282:TYR:OH	13:1:502:CLA:O1D	2.25	0.54
17:A:5005:LHG:H292	17:A:5004:LHG:H281	1.90	0.54
13:A:1119:CLA:H122	14:A:4008:BCR:HC8	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:473:LYS:NZ	3:B:516:PHE:O	2.35	0.54
9:J:20:THR:HG23	14:J:4013:BCR:H351	1.90	0.54
1:e:85:LEU:HD22	1:e:107:ILE:HD13	1.89	0.54
1:5:225:ILE:HG12	13:5:501:CLA:HAB	1.88	0.53
2:A:246:PRO:O	2:A:250:ALA:N	2.41	0.53
2:A:421:ASP:HB2	2:A:424:MET:HE2	1.90	0.53
13:B:1225:CLA:H12	14:B:4005:BCR:H393	1.89	0.53
1:g:322:HIS:NE2	13:g:502:CLA:C4D	2.70	0.53
13:b:502:CLA:HBB2	13:b:510:CLA:H192	1.90	0.53
1:a:336:HIS:HE1	13:a:508:CLA:NC	2.06	0.53
14:1:523:BCR:H282	13:1:513:CLA:H11	1.90	0.53
2:A:352:TRP:HB3	13:A:1103:CLA:HAC1	1.90	0.53
2:A:432:ARG:HG2	2:A:435:ARG:HH21	1.73	0.53
13:A:1122:CLA:HHB	13:A:1801:CLA:HAB	1.91	0.53
14:A:4007:BCR:H403	17:A:5002:LHG:H302	1.90	0.53
1:d:215:LEU:HG	1:d:280:LEU:HD11	1.89	0.53
13:4:518:CLA:C2	13:4:518:CLA:H3A	2.38	0.53
3:B:92:TRP:CH2	8:I:12:TRP:HA	2.43	0.53
13:B:1223:CLA:HBA1	14:B:4010:BCR:H10C	1.89	0.53
1:e:95:GLY:HA2	1:e:187:GLN:HB3	1.91	0.53
1:f:175:ALA:HB1	1:f:192:ILE:HD13	1.89	0.53
1:6:282:TYR:O	1:6:315:ARG:NH2	2.35	0.53
2:A:618:GLN:OE1	2:A:657:GLN:NE2	2.41	0.53
3:B:679:GLN:O	3:B:683:GLU:HG3	2.08	0.53
1:a:322:HIS:CD2	13:a:502:CLA:ND	2.76	0.53
13:5:510:CLA:H51	13:5:510:CLA:HMA3	1.91	0.53
2:A:120:ILE:HD13	14:J:4013:BCR:H313	1.90	0.53
1:f:84:HIS:CE1	1:f:318:LEU:HD11	2.42	0.53
13:a:501:CLA:H152	13:a:507:CLA:HMB3	1.90	0.53
2:A:16:VAL:HG12	2:A:185:PRO:HA	1.89	0.53
1:a:241:PRO:HA	13:a:506:CLA:HED3	1.89	0.53
13:5:513:CLA:H61	14:5:523:BCR:C27	2.34	0.53
2:A:219:VAL:HG13	2:A:239:PRO:HB3	1.91	0.53
2:A:310:ILE:HD11	10:K:68:LEU:HD21	1.91	0.53
2:A:400:ILE:HG23	13:A:1104:CLA:H143	1.90	0.53
2:A:711:LEU:HD21	13:B:1228:CLA:H3A	1.91	0.53
13:A:1119:CLA:H61	14:A:4007:BCR:H352	1.90	0.53
3:B:195:ILE:HD12	3:B:254:ILE:HB	1.90	0.53
1:c:278:ASN:O	1:c:315:ARG:NH1	2.36	0.53
1:d:49:GLN:HG2	13:d:509:CLA:HHB	1.90	0.53
1:f:64:GLU:HB3	1:f:79:LEU:HD22	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:501:CLA:O2D	13:a:501:CLA:H2A	2.09	0.53
2:A:654:LEU:HD11	13:A:1011:CLA:H72	1.91	0.53
13:A:1126:CLA:O1D	13:A:1127:CLA:HHB	2.09	0.53
5:D:34:SER:OG	5:D:36:LYS:O	2.25	0.53
13:B:1204:CLA:H42	13:B:1204:CLA:C1D	2.38	0.53
1:3:60:PHE:HE1	13:4:519:CLA:HBA1	1.74	0.53
1:4:64:GLU:HG3	1:4:81:LEU:HB2	1.91	0.53
1:e:287:TYR:HB3	1:e:315:ARG:HB2	1.91	0.53
1:a:316:ALA:O	1:a:320:ASN:ND2	2.39	0.53
1:5:258:SER:O	1:5:333:HIS:ND1	2.39	0.52
1:5:339:ARG:NH2	15:5:822:SQD:O9	2.39	0.52
13:B:1234:CLA:H13	12:X:23:LEU:HD22	1.90	0.52
1:c:164:LEU:HD21	13:c:509:CLA:H61	1.90	0.52
1:c:183:ASP:OD1	1:c:185:ASN:ND2	2.42	0.52
1:d:264:ILE:HG12	13:d:502:CLA:HAC1	1.91	0.52
1:2:328:PHE:HE1	13:2:518:CLA:HAB	1.75	0.52
1:1:241:PRO:HA	13:1:506:CLA:HED3	1.91	0.52
1:c:353:ASN:HB2	1:c:354:PRO:HD3	1.91	0.52
13:d:517:CLA:C4C	14:d:524:BCR:H19C	2.38	0.52
1:g:261:LEU:HB3	1:g:333:HIS:HB2	1.90	0.52
1:2:49:GLN:HG2	13:2:509:CLA:HHB	1.91	0.52
3:B:92:TRP:N	13:B:1206:CLA:O1D	2.41	0.52
3:B:290:MET:HE1	13:B:1216:CLA:C3D	2.39	0.52
1:c:339:ARG:HH22	13:c:508:CLA:HED2	1.73	0.52
1:f:278:ASN:OD1	1:f:279:THR:N	2.42	0.52
1:a:39:SER:HB3	1:a:133:LEU:HB2	1.91	0.52
1:5:64:GLU:OE1	1:5:79:LEU:HA	2.10	0.52
1:5:110:VAL:HG22	14:5:523:BCR:H10C	1.91	0.52
13:A:1124:CLA:HAB	14:A:4008:BCR:H311	1.92	0.52
3:B:60:TRP:NE1	13:B:1224:CLA:OBD	2.43	0.52
6:E:40:ARG:HG3	6:E:58:THR:HG22	1.91	0.52
1:e:143:PHE:CE1	13:e:513:CLA:HBA1	2.44	0.52
1:f:270:VAL:HG11	13:f:501:CLA:H61	1.91	0.52
1:g:143:PHE:HE1	13:g:512:CLA:HBB1	1.75	0.52
13:b:503:CLA:H172	13:b:510:CLA:HBB2	1.91	0.52
1:a:54:VAL:HG13	1:a:115:SER:HB3	1.90	0.52
13:4:505:CLA:HBC2	14:4:524:BCR:H341	1.91	0.52
2:A:577:PRO:HB3	2:A:724:ILE:HB	1.91	0.52
2:A:671:ALA:HA	13:A:1107:CLA:HBC1	1.91	0.52
1:c:49:GLN:HG2	13:c:509:CLA:HHB	1.90	0.52
1:c:203:TYR:OH	13:c:517:CLA:O2A	2.22	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:505:CLA:HAB	13:a:505:CLA:H101	1.92	0.52
13:a:508:CLA:H93	14:a:521:BCR:H21C	1.91	0.52
2:A:461:HIS:HE1	13:A:1132:CLA:NA	2.03	0.52
13:A:1237:CLA:H161	14:I:4020:BCR:H14C	1.92	0.52
13:B:1234:CLA:HMB1	13:B:1234:CLA:HBB1	1.92	0.52
5:D:83:ILE:HB	5:D:96:HIS:HB3	1.91	0.52
1:a:49:GLN:OE1	13:a:510:CLA:NC	2.42	0.52
1:4:261:LEU:HD21	13:4:508:CLA:HAB	1.92	0.52
1:6:301:PHE:H	1:6:320:ASN:HD21	1.56	0.52
5:D:74:ARG:NE	5:D:81:TYR:OH	2.42	0.52
1:c:50:ALA:O	1:c:54:VAL:HG23	2.10	0.52
1:e:71:ASP:N	1:e:71:ASP:OD1	2.43	0.52
1:f:172:VAL:HG23	1:f:219:VAL:HG13	1.90	0.52
1:g:60:PHE:O	1:g:64:GLU:HG2	2.09	0.52
1:3:341:MET:SD	13:3:505:CLA:HMA2	2.49	0.52
1:4:287:TYR:HB3	1:4:315:ARG:HB2	1.92	0.52
1:1:38:LEU:HD22	1:1:131:HIS:HB3	1.91	0.52
1:1:95:GLY:HA2	1:1:187:GLN:HB3	1.92	0.52
1:1:234:ILE:HG12	13:1:516:CLA:HAB	1.91	0.52
3:B:127:ILE:HG22	13:B:1215:CLA:HED2	1.92	0.52
3:B:182:LEU:HD13	13:B:1210:CLA:HHB	1.92	0.52
3:B:601:TRP:HB2	13:B:1234:CLA:HMC1	1.91	0.52
13:b:502:CLA:HBD	13:b:503:CLA:H43	1.91	0.52
1:3:64:GLU:HG3	1:3:79:LEU:HD22	1.91	0.52
1:5:303:ASP:N	1:5:303:ASP:OD1	2.43	0.52
13:2:506:CLA:HAB	13:2:507:CLA:HED2	1.91	0.52
2:A:445:ASN:HD22	3:B:681:LEU:HD11	1.75	0.52
2:A:694:ARG:HD3	3:B:573:GLY:HA3	1.91	0.52
13:A:1119:CLA:HBC3	13:A:1125:CLA:H18	1.91	0.52
3:B:210:ASP:N	3:B:210:ASP:OD1	2.41	0.52
3:B:394:GLY:HA3	14:B:4010:BCR:H382	1.92	0.52
3:B:498:ASN:HB3	3:B:501:LEU:HB2	1.92	0.52
3:B:554:MET:HE2	4:C:66:ARG:NH2	2.25	0.52
13:B:1205:CLA:HAB	13:B:1206:CLA:CGA	2.39	0.52
1:e:282:TYR:HB2	1:e:315:ARG:HH21	1.75	0.52
13:3:505:CLA:HBD	13:3:505:CLA:HBA1	1.92	0.52
16:2:5104:LMG:H381	13:2:503:CLA:HBB1	1.92	0.52
2:A:74:SER:OG	2:A:180:TYR:HB2	2.10	0.52
13:B:1204:CLA:H43	8:I:14:PHE:CE2	2.44	0.52
8:I:20:TRP:CZ2	14:I:4020:BCR:HC42	2.45	0.52
1:c:322:HIS:NE2	13:c:502:CLA:ND	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:183:ASP:OD1	1:f:185:ASN:ND2	2.42	0.52
1:a:261:LEU:HD21	13:a:508:CLA:HAB	1.90	0.52
13:3:511:CLA:HMB1	14:3:522:BCR:H382	1.92	0.51
1:4:60:PHE:O	1:4:64:GLU:HG2	2.10	0.51
1:1:49:GLN:HG2	13:1:509:CLA:HHB	1.92	0.51
2:A:293:TRP:HB2	2:A:296:ASP:HB2	1.92	0.51
3:B:181:GLY:HA3	13:B:1210:CLA:HBB1	1.91	0.51
13:d:508:CLA:HBC3	13:d:510:CLA:H92	1.91	0.51
13:f:505:CLA:H111	13:f:517:CLA:HBB2	1.92	0.51
13:a:517:CLA:HBC3	14:a:524:BCR:H21C	1.92	0.51
1:3:287:TYR:HB3	1:3:315:ARG:HB2	1.92	0.51
1:5:241:PRO:HA	13:5:506:CLA:HED3	1.91	0.51
2:A:374:MET:HE1	2:A:393:LEU:HD13	1.91	0.51
13:A:1138:CLA:H2	13:B:1229:CLA:H42	1.91	0.51
1:g:312:HIS:HB2	1:g:317:TRP:CD1	2.45	0.51
1:5:60:PHE:O	1:5:64:GLU:HG3	2.10	0.51
2:A:227:LEU:HD21	2:A:233:ALA:HB2	1.92	0.51
13:B:1023:CLA:CGA	13:B:1023:CLA:H3A	2.41	0.51
13:B:1223:CLA:HMA3	14:B:4010:BCR:HC41	1.92	0.51
1:f:60:PHE:O	1:f:64:GLU:HG2	2.11	0.51
13:f:511:CLA:HBA1	14:f:522:BCR:H281	1.92	0.51
1:a:80:ILE:O	1:a:84:HIS:ND1	2.42	0.51
13:a:517:CLA:HED2	13:a:517:CLA:H2A	1.92	0.51
1:3:16:LEU:HD22	1:3:254:GLU:HG2	1.92	0.51
1:3:85:LEU:HD22	1:3:107:ILE:HD13	1.93	0.51
1:5:264:ILE:HG12	13:5:502:CLA:HAC1	1.93	0.51
2:A:377:MET:SD	13:A:1116:CLA:HBD	2.50	0.51
13:A:1105:CLA:HMB3	13:A:1106:CLA:HHB	1.93	0.51
3:B:343:ALA:HB2	14:B:4010:BCR:H372	1.91	0.51
13:B:1023:CLA:HHH	13:B:1023:CLA:HBC2	1.92	0.51
13:B:1023:CLA:H142	14:I:4018:BCR:H271	1.91	0.51
13:B:1224:CLA:HBC3	16:B:5002:LMG:H442	1.90	0.51
13:B:1236:CLA:HBC2	13:X:1401:CLA:HBC3	1.93	0.51
1:c:202:ILE:HG13	1:c:224:TYR:CD2	2.46	0.51
1:f:100:ASP:OD1	1:f:100:ASP:N	2.43	0.51
1:b:150:PRO:HB2	1:b:241:PRO:HG2	1.90	0.51
13:A:1120:CLA:C1D	14:K:4001:BCR:H382	2.40	0.51
1:d:160:HIS:CE1	13:d:512:CLA:ND	2.79	0.51
1:4:162:LEU:HD23	1:4:230:ILE:HA	1.93	0.51
1:5:183:ASP:HB3	1:5:186:LEU:HB2	1.91	0.51
1:1:38:LEU:HD23	1:1:132:ASP:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1119:CLA:H193	13:A:1122:CLA:HAC2	1.93	0.51
13:3:502:CLA:H12	13:3:503:CLA:H42	1.92	0.51
1:e:60:PHE:HE1	13:f:519:CLA:HBA2	1.75	0.51
1:a:192:ILE:HG23	1:a:216:GLU:HG3	1.93	0.51
13:6:509:CLA:HBB1	13:6:510:CLA:HAA2	1.92	0.51
2:A:587:CYS:SG	3:B:674:TRP:HB3	2.51	0.51
2:A:617:MET:HE3	2:A:622:TRP:CE2	2.46	0.51
1:d:14:ALA:HB1	1:d:147:TRP:HB2	1.93	0.51
1:e:261:LEU:HB3	1:e:333:HIS:HB2	1.92	0.51
1:g:17:GLN:H	1:g:254:GLU:HG3	1.75	0.51
1:g:71:ASP:OD1	1:g:71:ASP:N	2.44	0.51
1:b:109:ALA:O	1:b:113:ILE:HG12	2.11	0.51
1:3:146:ARG:HH21	1:3:148:ASP:HB3	1.76	0.51
1:3:275:CYS:O	1:3:315:ARG:NH1	2.43	0.51
1:5:150:PRO:HB2	1:5:241:PRO:HD2	1.91	0.51
1:1:112:LEU:O	1:1:115:SER:OG	2.27	0.51
14:A:4002:BCR:H383	14:K:4001:BCR:H10C	1.93	0.51
13:X:1401:CLA:H3A	13:X:1401:CLA:O2A	2.11	0.51
1:e:264:ILE:HG13	13:e:509:CLA:HED3	1.92	0.51
1:g:16:LEU:HG	1:g:36:VAL:HG11	1.93	0.51
1:b:261:LEU:HD23	1:b:264:ILE:HD11	1.91	0.51
1:b:338:LEU:HA	1:b:341:MET:HB2	1.92	0.51
1:3:13:SER:O	1:3:252:ASN:ND2	2.42	0.51
1:6:183:ASP:OD2	1:6:190:ARG:NH1	2.44	0.51
10:K:16:GLY:O	10:K:20:ILE:HG13	2.11	0.51
1:g:329:PHE:HE1	13:g:510:CLA:H101	1.76	0.51
13:g:505:CLA:HMC1	13:g:505:CLA:H122	1.93	0.51
1:5:260:SER:HB3	13:5:507:CLA:HAA1	1.92	0.50
1:4:125:HIS:HA	1:4:129:ALA:HB3	1.94	0.50
1:5:31:GLY:HA3	13:5:511:CLA:HMD2	1.92	0.50
14:2:521:BCR:C3	17:A:5005:LHG:HC41	2.41	0.50
3:B:310:PHE:HE1	13:B:1219:CLA:H12	1.76	0.50
3:B:554:MET:HE1	3:B:567:ASP:CB	2.41	0.50
14:b:523:BCR:H271	13:b:513:CLA:H11	1.92	0.50
13:a:501:CLA:H143	14:a:524:BCR:H353	1.94	0.50
13:a:506:CLA:HBB2	13:a:507:CLA:H52	1.92	0.50
1:3:130:PRO:HG3	1:3:136:ALA:HB2	1.93	0.50
1:5:329:PHE:HA	13:5:508:CLA:HMC2	1.93	0.50
2:A:127:ASN:HB3	2:A:135:HIS:HB3	1.93	0.50
3:B:446:VAL:HG21	13:B:1230:CLA:HAC2	1.94	0.50
1:b:174:LYS:NZ	1:b:180:GLY:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:102:TYR:HD2	16:6:5104:LMG:HC1	1.75	0.50
1:1:309:LEU:HD11	2:A:250:ALA:HB1	1.94	0.50
13:A:1139:CLA:HMC2	14:F:4014:BCR:H381	1.94	0.50
1:f:69:LYS:HD2	1:f:72:LEU:HD12	1.93	0.50
1:f:172:VAL:HG21	1:f:223:ILE:HB	1.92	0.50
1:g:39:SER:HB2	1:g:133:LEU:HB2	1.93	0.50
13:g:502:CLA:HBB1	13:g:504:CLA:HAB	1.93	0.50
1:1:60:PHE:O	1:1:64:GLU:HG2	2.12	0.50
1:c:47:VAL:HG22	13:c:513:CLA:HAB	1.94	0.50
13:e:517:CLA:C4C	14:e:524:BCR:H19C	2.41	0.50
1:f:322:HIS:NE2	13:f:502:CLA:C4D	2.74	0.50
14:g:522:BCR:HC41	14:g:523:BCR:HC42	1.92	0.50
1:a:36:VAL:HG22	13:a:509:CLA:HAC2	1.94	0.50
1:a:248:LEU:HB3	14:a:524:BCR:HC32	1.94	0.50
3:B:65:LEU:HD11	14:B:4006:BCR:H281	1.93	0.50
13:B:1212:CLA:H2A	13:B:1212:CLA:CED	2.42	0.50
1:c:76:GLU:OE1	1:c:307:LEU:HD21	2.11	0.50
1:c:219:VAL:O	1:c:223:ILE:HG23	2.11	0.50
1:e:54:VAL:HG13	1:e:111:HIS:ND1	2.27	0.50
1:e:84:HIS:NE2	13:e:502:CLA:O1D	2.33	0.50
13:g:507:CLA:HED3	13:g:509:CLA:H8	1.94	0.50
1:a:45:ALA:HB2	13:a:511:CLA:HMA1	1.93	0.50
1:3:29:TRP:CD2	20:J:5105:LMU:H51	2.46	0.50
13:5:501:CLA:HMB2	14:5:524:BCR:H23C	1.93	0.50
1:6:225:ILE:HD13	14:6:524:BCR:H372	1.93	0.50
2:A:166:LEU:HD11	13:A:1105:CLA:HAC1	1.94	0.50
3:B:468:GLN:NE2	3:B:517:LEU:O	2.45	0.50
1:e:35:PHE:HB2	1:e:41:LEU:HB3	1.93	0.50
1:b:205:TYR:OH	1:b:212:ILE:HB	2.12	0.50
1:3:303:ASP:OD1	1:3:303:ASP:N	2.42	0.50
1:6:322:HIS:NE2	13:6:502:CLA:ND	2.60	0.50
1:g:221:GLY:C	14:g:524:BCR:H383	2.37	0.50
1:3:273:TYR:HB2	14:2:522:BCR:HC41	1.93	0.50
13:3:502:CLA:HBD	13:3:503:CLA:H43	1.94	0.50
1:4:93:GLY:N	1:4:97:LYS:O	2.44	0.50
1:5:243:THR:HG23	1:f:353:ASN:HB2	1.93	0.50
2:A:380:TYR:OH	13:A:1127:CLA:OBD	2.26	0.50
3:B:426:LEU:HD13	3:B:539:LEU:HA	1.94	0.50
1:d:228:LEU:HD22	13:d:506:CLA:HBC1	1.94	0.50
1:e:327:PHE:O	1:e:331:GLN:HG2	2.12	0.50
13:e:501:CLA:H121	14:e:524:BCR:H15C	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:510:CLA:CAD	13:e:511:CLA:HAB	2.42	0.50
1:f:80:ILE:C	1:f:83:PRO:HD2	2.37	0.50
13:A:1139:CLA:H121	7:F:130:ILE:HD11	1.94	0.49
7:F:69:ASP:OD1	7:F:69:ASP:N	2.45	0.49
1:c:46:HIS:HD2	13:c:509:CLA:H141	1.77	0.49
1:g:81:LEU:H	1:g:81:LEU:HD22	1.76	0.49
1:g:282:TYR:O	1:g:315:ARG:NH2	2.45	0.49
13:5:501:CLA:H152	13:5:507:CLA:HMB2	1.94	0.49
5:D:118:ARG:NH2	5:D:136:PRO:O	2.44	0.49
13:c:501:CLA:H111	13:c:507:CLA:H8	1.94	0.49
1:d:74:MET:HE2	1:d:82:LEU:HB3	1.94	0.49
1:e:163:PHE:CE2	13:e:512:CLA:HHB	2.47	0.49
1:a:69:LYS:O	1:a:77:GLN:NE2	2.45	0.49
3:B:123:TRP:CH2	13:B:1225:CLA:H2	2.47	0.49
13:c:505:CLA:H2	14:c:524:BCR:H331	1.93	0.49
1:d:28:TRP:HA	13:d:511:CLA:HMD3	1.93	0.49
14:d:523:BCR:H323	1:e:209:PHE:HE1	1.78	0.49
1:5:174:LYS:NZ	1:5:180:GLY:O	2.45	0.49
1:5:225:ILE:HD13	14:5:524:BCR:H372	1.94	0.49
13:5:502:CLA:HAA1	13:5:503:CLA:H11	1.94	0.49
1:2:287:TYR:HB2	1:2:315:ARG:HH21	1.77	0.49
2:A:94:GLY:O	2:A:98:SER:OG	2.23	0.49
2:A:300:HIS:HE2	13:A:1117:CLA:C2B	2.25	0.49
2:A:623:GLY:HA3	2:A:633:HIS:HA	1.94	0.49
3:B:142:LEU:HG	14:B:4006:BCR:H382	1.93	0.49
3:B:305:MET:HG3	3:B:327:TYR:HB2	1.94	0.49
5:D:116:VAL:HG12	5:D:118:ARG:HG2	1.93	0.49
1:6:205:TYR:CD1	14:6:524:BCR:H391	2.47	0.49
1:2:16:LEU:HG	1:2:36:VAL:HG21	1.94	0.49
1:2:297:ILE:HG12	17:A:5004:LHG:H251	1.94	0.49
2:A:12:VAL:HG21	13:A:1110:CLA:HAA2	1.93	0.49
13:A:1113:CLA:H12	14:K:4001:BCR:HC32	1.94	0.49
3:B:60:TRP:HB2	13:B:1205:CLA:H193	1.94	0.49
3:B:565:PRO:HB3	3:B:709:ILE:HB	1.94	0.49
13:B:1205:CLA:O1A	13:B:1224:CLA:HBD	2.12	0.49
1:d:41:LEU:HB3	13:d:511:CLA:HMA1	1.94	0.49
1:e:56:TRP:CH2	1:e:81:LEU:HD21	2.48	0.49
1:f:14:ALA:HB2	1:f:148:ASP:HB2	1.94	0.49
1:a:287:TYR:HB3	1:a:315:ARG:HB2	1.93	0.49
1:1:276:ALA:HB1	1:1:291:LEU:HB2	1.94	0.49
1:c:287:TYR:HB3	1:c:315:ARG:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:e:502:CLA:H52	13:e:512:CLA:H42	1.95	0.49
1:f:269:PHE:HB3	13:f:505:CLA:H18	1.95	0.49
13:f:508:CLA:H93	14:f:521:BCR:H21C	1.93	0.49
13:g:518:CLA:H72	13:g:518:CLA:HMA1	1.95	0.49
1:b:182:TYR:OH	1:b:285:GLU:OE2	2.28	0.49
1:b:338:LEU:HD12	13:b:518:CLA:HMD1	1.94	0.49
13:5:505:CLA:CMD	13:5:507:CLA:HAB	2.43	0.49
1:6:327:PHE:CE1	13:6:519:CLA:HAB	2.48	0.49
1:2:279:THR:HG23	1:2:284:VAL:HG23	1.95	0.49
13:A:1117:CLA:H8	13:A:1117:CLA:HAB	1.94	0.49
13:A:1133:CLA:H202	14:A:4007:BCR:H21C	1.95	0.49
3:B:351:LEU:HG	13:B:1215:CLA:H41	1.95	0.49
1:g:252:ASN:O	1:g:256:ILE:HG12	2.12	0.49
1:a:27:ASP:OD1	1:a:28:TRP:N	2.42	0.49
1:a:112:LEU:HD13	14:a:522:BCR:H10C	1.95	0.49
1:a:320:ASN:HB3	14:a:521:BCR:HC8	1.94	0.49
1:3:105:PHE:HZ	14:3:522:BCR:HC31	1.77	0.49
13:4:509:CLA:H141	13:4:512:CLA:HMD3	1.95	0.49
1:6:261:LEU:HD21	13:6:508:CLA:HAB	1.94	0.49
13:A:1111:CLA:H122	14:A:4003:BCR:H353	1.94	0.49
13:A:1138:CLA:H203	13:A:1139:CLA:H62	1.95	0.49
3:B:590:MET:O	3:B:594:ILE:HG12	2.13	0.49
1:a:56:TRP:CH2	1:a:81:LEU:HD21	2.48	0.49
1:4:73:PRO:HG2	1:4:76:GLU:HG2	1.94	0.49
13:4:501:CLA:H143	14:4:524:BCR:H353	1.93	0.49
1:2:196:THR:HG22	1:2:220:GLY:HA3	1.95	0.49
2:A:44:THR:OG1	2:A:720:ARG:HG3	2.12	0.49
3:B:86:PRO:HB3	3:B:121:TYR:CG	2.48	0.49
3:B:111:ASN:HB3	8:I:3:GLY:HA2	1.95	0.49
7:F:45:VAL:O	7:F:57:ARG:NH2	2.38	0.49
12:X:18:PHE:CD1	12:X:18:PHE:C	2.91	0.49
1:c:36:VAL:HG22	13:c:509:CLA:HAC2	1.94	0.49
13:b:518:CLA:H3A	13:b:518:CLA:O2A	2.13	0.49
1:a:17:GLN:H	1:a:254:GLU:HG3	1.78	0.49
1:3:125:HIS:HA	1:3:129:ALA:HB3	1.95	0.49
1:6:39:SER:HB2	1:6:133:LEU:HB2	1.95	0.49
13:6:501:CLA:H203	13:6:507:CLA:H111	1.95	0.49
1:2:287:TYR:HB3	1:2:315:ARG:HB2	1.95	0.49
2:A:86:TRP:HA	13:A:1105:CLA:HBB2	1.94	0.49
2:A:250:ALA:HA	2:A:258:TRP:CD1	2.47	0.49
3:B:415:VAL:HA	3:B:418:HIS:CE1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:578:SER:N	3:B:581:ASP:OD2	2.44	0.49
3:B:638:LEU:HD22	3:B:731:PHE:HA	1.95	0.49
14:d:523:BCR:H323	1:e:209:PHE:CE1	2.48	0.49
1:g:64:GLU:HB2	1:g:82:LEU:HD23	1.95	0.49
1:3:56:TRP:CZ3	1:3:81:LEU:HD21	2.48	0.48
1:1:299:PRO:HG2	13:1:519:CLA:CHB	2.42	0.48
13:1:510:CLA:H72	13:1:510:CLA:H112	1.48	0.48
2:A:238:LEU:H	2:A:241:GLU:CD	2.20	0.48
2:A:423:ALA:HA	5:D:39:VAL:HG11	1.94	0.48
13:A:1105:CLA:HBA2	20:A:1848:LMU:H61	1.95	0.48
3:B:348:ILE:HA	3:B:351:LEU:HB3	1.95	0.48
3:B:419:LYS:HD2	3:B:546:LEU:HB3	1.94	0.48
1:c:220:GLY:O	1:c:223:ILE:HG12	2.13	0.48
13:f:502:CLA:HBD	13:f:503:CLA:H43	1.95	0.48
1:b:344:ASN:O	1:b:347:GLN:HG2	2.13	0.48
2:A:83:VAL:HG11	13:A:1103:CLA:H72	1.95	0.48
13:A:1022:CLA:HED2	13:A:1011:CLA:H92	1.95	0.48
13:B:1239:CLA:HBC2	18:B:2002:PQN:H172	1.95	0.48
10:K:7:PRO:HD3	10:K:79:TYR:CE1	2.48	0.48
11:M:13:VAL:HA	11:M:16:LEU:HD12	1.95	0.48
1:g:162:LEU:HD11	13:g:516:CLA:HBB1	1.95	0.48
13:b:517:CLA:C4C	14:b:524:BCR:H19C	2.43	0.48
1:5:54:VAL:HG12	1:5:111:HIS:O	2.14	0.48
13:B:1023:CLA:HED3	14:B:4017:BCR:H401	1.95	0.48
12:X:21:VAL:O	12:X:25:ALA:N	2.41	0.48
1:f:222:HIS:O	1:f:225:ILE:HG22	2.13	0.48
1:3:29:TRP:CE2	20:J:5105:LMU:C3	2.80	0.48
2:A:221:LEU:HD13	2:A:278:PHE:HB2	1.95	0.48
2:A:427:ASN:OD1	2:A:432:ARG:NH1	2.42	0.48
2:A:448:CYS:HB3	2:A:548:VAL:HG22	1.95	0.48
13:A:1139:CLA:H91	13:A:1139:CLA:H111	1.63	0.48
1:d:80:ILE:O	1:d:84:HIS:ND1	2.34	0.48
1:e:199:PRO:HA	1:e:224:TYR:HE2	1.78	0.48
1:f:57:ALA:HB3	1:f:111:HIS:HD1	1.79	0.48
1:b:205:TYR:CZ	1:b:209:PHE:HA	2.49	0.48
1:a:106:VAL:HG22	14:a:523:BCR:HC22	1.95	0.48
1:1:295:LEU:HD12	1:1:299:PRO:HB3	1.96	0.48
13:B:1229:CLA:HBB2	14:F:4014:BCR:HC41	1.95	0.48
14:c:524:BCR:H15C	14:c:524:BCR:H351	1.68	0.48
13:b:512:CLA:H3A	13:b:512:CLA:HBA1	1.46	0.48
1:4:349:GLU:OE2	7:F:145:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:5:510:CLA:H2	14:5:521:BCR:H383	1.96	0.48
1:f:291:LEU:HD23	1:f:301:PHE:HB2	1.96	0.48
1:2:169:LEU:HG	1:2:226:ALA:HB1	1.96	0.48
2:A:646:ILE:HG21	13:A:1022:CLA:HBA2	1.94	0.48
3:B:57:ILE:O	3:B:61:VAL:HG23	2.13	0.48
1:d:137:THR:HA	1:d:141:ARG:HB2	1.96	0.48
1:e:257:LEU:HD22	13:e:509:CLA:HBC3	1.95	0.48
13:e:505:CLA:H62	13:e:505:CLA:H41	1.52	0.48
13:f:518:CLA:H42	13:f:518:CLA:HHB	1.96	0.48
1:g:50:ALA:O	1:g:54:VAL:HG23	2.13	0.48
13:A:1102:CLA:H141	13:A:1102:CLA:H162	1.70	0.48
17:A:5002:LHG:O9	17:A:5002:LHG:O2	2.32	0.48
3:B:454:GLU:HA	7:F:71:LEU:HD22	1.94	0.48
13:d:501:CLA:H172	13:d:507:CLA:HMB3	1.96	0.48
1:e:344:ASN:HB3	1:e:347:GLN:HG3	1.96	0.48
1:f:322:HIS:CD2	13:f:502:CLA:ND	2.81	0.48
1:f:322:HIS:CE1	13:f:502:CLA:NA	2.81	0.48
1:g:49:GLN:HG2	13:g:509:CLA:HMA3	1.95	0.48
1:4:264:ILE:HG12	13:4:502:CLA:HAC1	1.95	0.48
1:6:60:PHE:O	1:6:64:GLU:HG2	2.13	0.48
2:A:94:GLY:HA3	2:A:147:TRP:CH2	2.49	0.48
2:A:288:VAL:HG23	2:A:289:THR:HG23	1.95	0.48
2:A:297:THR:HG23	13:A:1117:CLA:HMA3	1.96	0.48
3:B:348:ILE:HD13	13:B:1221:CLA:H43	1.96	0.48
3:B:436:HIS:HB2	14:F:4015:BCR:HC42	1.96	0.48
13:B:1209:CLA:HBC2	20:B:1843:LMU:H72	1.96	0.48
13:c:510:CLA:CAD	13:c:511:CLA:HAB	2.44	0.48
13:b:505:CLA:H52	1:a:117:VAL:HG23	1.95	0.48
13:a:503:CLA:H93	13:a:507:CLA:H42	1.96	0.48
13:a:509:CLA:H92	13:a:509:CLA:H62	1.75	0.48
1:5:158:GLY:HA3	1:5:237:ILE:HG13	1.96	0.48
13:5:508:CLA:H93	14:5:521:BCR:H21C	1.96	0.48
1:2:142:ARG:NE	13:2:516:CLA:O2A	2.46	0.48
13:A:1125:CLA:CGA	14:A:4008:BCR:H17C	2.44	0.48
1:d:77:GLN:HG3	1:d:79:LEU:HG	1.95	0.48
1:e:313:THR:HG22	1:e:315:ARG:H	1.78	0.48
1:b:260:SER:O	1:b:264:ILE:HG12	2.14	0.48
1:3:126:THR:HG21	14:3:522:BCR:H271	1.96	0.47
1:4:142:ARG:NH1	13:4:516:CLA:O2A	2.47	0.47
1:5:113:ILE:HG22	14:5:523:BCR:H14C	1.94	0.47
1:2:222:HIS:HA	1:2:225:ILE:HG22	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:A:1117:CLA:HBA2	13:A:1117:CLA:H3A	1.50	0.47
3:B:123:TRP:O	3:B:127:ILE:HG23	2.13	0.47
3:B:125:TYR:O	3:B:130:ARG:NH1	2.40	0.47
13:c:512:CLA:HBA1	13:c:512:CLA:H3A	1.39	0.47
1:d:150:PRO:HB2	1:d:241:PRO:HG2	1.96	0.47
1:a:147:TRP:HE3	1:a:256:ILE:HD12	1.79	0.47
1:5:329:PHE:HE1	13:5:510:CLA:H112	1.78	0.47
2:A:12:VAL:HG23	2:A:13:ARG:H	1.80	0.47
2:A:292:LEU:HD13	13:A:1116:CLA:HMA2	1.95	0.47
13:A:1127:CLA:H122	14:A:4003:BCR:H383	1.95	0.47
13:A:1132:CLA:HED2	13:A:1132:CLA:H2A	1.95	0.47
13:B:1023:CLA:H52	13:B:1023:CLA:HMB1	1.96	0.47
11:M:4:THR:OG1	11:M:7:GLN:HG2	2.14	0.47
13:c:511:CLA:HMB1	14:c:522:BCR:H382	1.95	0.47
1:e:80:ILE:O	1:e:84:HIS:ND1	2.47	0.47
1:f:263:GLY:HA3	13:f:507:CLA:HMA1	1.95	0.47
1:a:282:TYR:OH	13:a:502:CLA:O1D	2.31	0.47
13:a:518:CLA:HBB1	13:a:519:CLA:HMC2	1.96	0.47
13:5:503:CLA:H41	13:5:503:CLA:H62	1.62	0.47
1:d:17:GLN:H	1:d:254:GLU:HG3	1.79	0.47
13:f:501:CLA:C1B	13:f:501:CLA:H2	2.44	0.47
1:g:266:LEU:HG	13:g:501:CLA:H91	1.96	0.47
1:2:269:PHE:HB3	13:2:505:CLA:H193	1.95	0.47
13:1:508:CLA:H2	13:1:510:CLA:H12	1.97	0.47
2:A:362:MET:HE3	2:A:362:MET:HA	1.95	0.47
2:A:378:PRO:HG2	2:A:384:ALA:HB2	1.95	0.47
2:A:433:VAL:HA	2:A:436:HIS:CE1	2.48	0.47
2:A:710:LYS:NZ	7:F:156:ASP:OD1	2.43	0.47
3:B:613:VAL:HG12	3:B:617:ASN:OD1	2.14	0.47
5:D:27:LYS:HB2	5:D:86:ILE:HB	1.95	0.47
1:d:269:PHE:CD2	13:d:505:CLA:H151	2.49	0.47
1:f:54:VAL:HG21	1:f:118:LEU:HD12	1.96	0.47
13:f:518:CLA:C2	13:f:518:CLA:H3A	2.45	0.47
13:b:501:CLA:HMD1	13:b:502:CLA:H93	1.97	0.47
1:5:42:PHE:O	1:5:46:HIS:ND1	2.46	0.47
1:c:212:ILE:HB	1:c:278:ASN:HD21	1.79	0.47
1:c:322:HIS:CD2	13:c:502:CLA:ND	2.83	0.47
1:g:16:LEU:HD22	1:g:254:GLU:HG2	1.96	0.47
1:g:163:PHE:CE2	13:g:512:CLA:HHB	2.49	0.47
13:a:510:CLA:H151	13:a:510:CLA:H111	1.58	0.47
1:1:126:THR:HG21	14:1:522:BCR:H271	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:181:LEU:HD13	13:1:501:CLA:HED1	1.97	0.47
2:A:399:TRP:HB3	13:A:1126:CLA:HMC3	1.96	0.47
13:A:1103:CLA:H11	13:A:1103:CLA:HBA2	1.58	0.47
13:c:502:CLA:HBD	13:c:503:CLA:H43	1.96	0.47
13:c:517:CLA:C4C	14:c:524:BCR:H19C	2.45	0.47
1:d:249:LEU:HD11	13:d:506:CLA:HBA1	1.96	0.47
13:f:513:CLA:CHC	14:f:523:BCR:H383	2.45	0.47
1:a:212:ILE:HD12	14:a:524:BCR:H292	1.96	0.47
1:5:49:GLN:HG2	13:5:509:CLA:HHB	1.96	0.47
13:6:505:CLA:H41	13:6:505:CLA:H62	1.73	0.47
14:6:524:BCR:H351	14:6:524:BCR:H15C	1.76	0.47
13:1:518:CLA:H3A	13:1:518:CLA:O2A	2.15	0.47
2:A:239:PRO:HG2	13:A:1112:CLA:OBD	2.15	0.47
2:A:710:LYS:HG2	13:B:1228:CLA:HMA2	1.97	0.47
13:A:1134:CLA:CHA	13:A:1134:CLA:HBA1	2.45	0.47
13:A:1140:CLA:H41	13:A:1140:CLA:H62	1.63	0.47
3:B:194:LEU:HA	3:B:198:ALA:HB3	1.96	0.47
13:B:1012:CLA:HMB1	13:B:1012:CLA:HBB1	1.97	0.47
13:c:505:CLA:H51	14:c:524:BCR:H342	1.96	0.47
13:e:509:CLA:H3A	13:e:509:CLA:HBA1	1.51	0.47
1:g:273:TYR:O	1:g:277:VAL:HG22	2.15	0.47
13:g:505:CLA:H2	14:g:524:BCR:H331	1.96	0.47
1:b:291:LEU:HD21	1:b:315:ARG:HB3	1.97	0.47
1:a:80:ILE:HG23	13:a:504:CLA:HMA1	1.96	0.47
1:4:56:TRP:O	1:4:60:PHE:HB2	2.14	0.47
13:5:501:CLA:H18	13:5:507:CLA:HMB2	1.97	0.47
1:6:212:ILE:HG13	1:6:214:SER:H	1.80	0.47
13:6:511:CLA:HBA1	14:6:522:BCR:H271	1.95	0.47
13:B:1201:CLA:HMC2	13:B:1203:CLA:HED2	1.96	0.47
4:C:54:CYS:HB3	4:C:65:ILE:HD13	1.97	0.47
1:c:134:SER:HB3	1:c:144:HIS:CD2	2.50	0.47
1:d:334:LEU:HD21	13:d:505:CLA:HMB2	1.96	0.47
13:e:505:CLA:H193	13:e:505:CLA:H162	1.70	0.47
2:A:66:GLU:HB2	2:A:187:LEU:HB2	1.97	0.47
2:A:380:TYR:HB2	2:A:383:LEU:HB2	1.96	0.47
13:A:1115:CLA:CHD	13:A:1116:CLA:HBB2	2.45	0.47
1:c:258:SER:O	1:c:333:HIS:ND1	2.47	0.47
1:e:49:GLN:NE2	1:e:49:GLN:O	2.48	0.47
1:e:158:GLY:HA3	1:e:237:ILE:HG13	1.97	0.47
13:e:508:CLA:HMA1	13:e:509:CLA:HBC2	1.96	0.47
1:b:71:ASP:OD1	1:b:71:ASP:N	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:80:ILE:HG13	1:b:81:LEU:HD22	1.96	0.47
1:b:163:PHE:CE2	13:b:512:CLA:HHB	2.50	0.47
13:b:503:CLA:H41	13:b:503:CLA:H62	1.58	0.47
13:b:518:CLA:H62	13:b:518:CLA:HMA1	1.97	0.47
1:a:260:SER:OG	13:a:509:CLA:O2D	2.33	0.47
1:6:159:HIS:CE1	13:6:512:CLA:HAB	2.51	0.47
2:A:329:LEU:HD12	2:A:345:TYR:HB2	1.96	0.47
14:A:4002:BCR:H341	14:A:4002:BCR:H11C	1.73	0.47
3:B:160:LYS:N	15:B:1852:SQD:O8	2.41	0.47
13:3:510:CLA:HED2	13:3:510:CLA:H52	1.97	0.46
1:4:175:ALA:HA	1:4:180:GLY:HA2	1.97	0.46
13:4:519:CLA:HBA2	13:4:519:CLA:H3A	1.48	0.46
1:6:159:HIS:CG	13:6:512:CLA:HAB	2.50	0.46
13:2:511:CLA:HBA1	14:2:522:BCR:H281	1.97	0.46
13:1:502:CLA:HBD	13:1:503:CLA:H43	1.97	0.46
13:A:1122:CLA:H13	13:A:1122:CLA:H102	1.79	0.46
13:A:1237:CLA:H111	14:I:4019:BCR:H392	1.95	0.46
4:C:22:PRO:HD3	4:C:53:ARG:HD2	1.97	0.46
7:F:76:VAL:HG12	7:F:86:PHE:HB2	1.98	0.46
14:c:522:BCR:C35	13:d:505:CLA:HBB2	2.44	0.46
14:d:524:BCR:H351	14:d:524:BCR:H15C	1.70	0.46
13:e:513:CLA:C2B	14:e:523:BCR:H292	2.45	0.46
1:f:49:GLN:HG2	13:f:509:CLA:HHB	1.96	0.46
1:g:35:PHE:HB2	1:g:41:LEU:HB3	1.96	0.46
1:b:242:LEU:O	1:b:246:ARG:HG3	2.15	0.46
13:4:503:CLA:H193	13:4:510:CLA:HAB	1.96	0.46
13:1:501:CLA:H91	13:1:501:CLA:H112	1.77	0.46
2:A:199:HIS:O	2:A:203:GLY:N	2.47	0.46
2:A:207:LEU:HG	13:A:1118:CLA:HBC1	1.97	0.46
2:A:353:HIS:CD2	2:A:411:HIS:HD1	2.30	0.46
1:c:158:GLY:HA2	1:c:233:GLY:HA2	1.96	0.46
1:c:195:PRO:HB3	1:c:219:VAL:HG12	1.96	0.46
14:e:523:BCR:H15C	14:e:523:BCR:H351	1.79	0.46
1:a:158:GLY:HA3	1:a:237:ILE:HG13	1.97	0.46
13:3:505:CLA:HMB1	13:3:505:CLA:HBB1	1.97	0.46
1:4:182:TYR:HA	1:4:189:VAL:HA	1.97	0.46
14:5:522:BCR:H332	13:6:505:CLA:H193	1.97	0.46
1:6:46:HIS:NE2	13:6:509:CLA:NB	2.63	0.46
13:6:508:CLA:HBB1	13:6:510:CLA:H3A	1.97	0.46
15:6:822:SQD:O49	15:6:822:SQD:H442	2.14	0.46
13:A:1140:CLA:H172	9:J:19:MET:SD	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:A:4008:BCR:H15C	14:A:4008:BCR:H351	1.76	0.46
3:B:552:LYS:NZ	6:E:15:SER:O	2.39	0.46
3:B:554:MET:HE3	3:B:571:ARG:NH2	2.30	0.46
13:B:1238:CLA:H41	13:B:1238:CLA:H62	1.70	0.46
14:B:4010:BCR:H351	14:B:4010:BCR:H15C	1.65	0.46
13:c:518:CLA:H92	13:c:518:CLA:H61	1.74	0.46
1:e:183:ASP:O	1:e:187:GLN:N	2.47	0.46
13:g:518:CLA:H42	13:g:518:CLA:HHB	1.97	0.46
1:b:34:ARG:NH1	13:b:511:CLA:OBD	2.42	0.46
1:a:76:GLU:OE1	1:a:76:GLU:N	2.48	0.46
1:5:139:ARG:NH1	1:5:139:ARG:HA	2.29	0.46
1:6:110:VAL:HG11	16:6:5104:LMG:H342	1.97	0.46
14:6:523:BCR:H351	14:6:523:BCR:H15C	1.77	0.46
1:1:85:LEU:HD22	1:1:107:ILE:HD13	1.97	0.46
13:1:507:CLA:H142	14:1:524:BCR:H16C	1.96	0.46
13:A:1103:CLA:H161	14:A:4002:BCR:HC8	1.98	0.46
13:A:1106:CLA:HBA2	13:A:1106:CLA:H3A	1.45	0.46
13:A:1127:CLA:HBA2	14:A:4003:BCR:H391	1.98	0.46
13:A:1138:CLA:HAA2	13:B:1228:CLA:HMB2	1.96	0.46
3:B:91:ILE:HB	3:B:112:PRO:HB2	1.98	0.46
3:B:432:PHE:CE1	14:F:4015:BCR:HC41	2.50	0.46
3:B:664:TRP:CZ3	13:B:1021:CLA:HHB	2.51	0.46
13:B:1214:CLA:H91	13:B:1214:CLA:H111	1.72	0.46
4:C:29:VAL:HG12	5:D:110:ARG:HB3	1.96	0.46
6:E:64:HIS:ND1	6:E:65:GLU:HG3	2.30	0.46
1:c:73:PRO:HB2	1:c:76:GLU:HG2	1.97	0.46
14:c:522:BCR:H351	14:c:522:BCR:H15C	1.77	0.46
1:d:278:ASN:O	1:d:315:ARG:NH1	2.49	0.46
13:f:510:CLA:H192	13:f:510:CLA:H162	1.80	0.46
13:a:502:CLA:H12	13:a:503:CLA:H42	1.97	0.46
13:5:512:CLA:HBA1	13:5:512:CLA:H3A	1.38	0.46
1:6:254:GLU:CD	1:6:336:HIS:HD1	2.22	0.46
2:A:698:GLN:HE22	2:A:720:ARG:HA	1.81	0.46
13:A:1106:CLA:H71	13:A:1128:CLA:H172	1.97	0.46
13:A:1128:CLA:HBB1	13:A:1128:CLA:HMB3	1.98	0.46
13:A:1139:CLA:H91	13:A:1139:CLA:H143	1.97	0.46
3:B:123:TRP:HH2	13:B:1225:CLA:H2	1.80	0.46
3:B:578:SER:HG	3:B:581:ASP:CG	2.23	0.46
3:B:623:LEU:HD12	13:B:1012:CLA:H12	1.98	0.46
13:B:1023:CLA:H92	13:B:1023:CLA:H62	1.77	0.46
7:F:77:ASP:OD1	7:F:77:ASP:N	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:d:344:ASN:O	1:d:347:GLN:HB3	2.16	0.46
13:e:509:CLA:HED2	13:e:509:CLA:H2A	1.98	0.46
13:a:505:CLA:H43	14:a:524:BCR:H321	1.98	0.46
1:3:29:TRP:CZ2	20:J:5105:LMU:H31	2.44	0.46
1:3:49:GLN:NE2	1:3:49:GLN:O	2.48	0.46
13:6:509:CLA:H141	13:6:512:CLA:HMD3	1.98	0.46
1:2:303:ASP:N	1:2:303:ASP:OD1	2.47	0.46
2:A:683:TRP:HZ3	13:B:1012:CLA:HMD3	1.80	0.46
13:A:1119:CLA:H92	13:A:1123:CLA:HMB2	1.96	0.46
13:A:1130:CLA:HBB1	13:A:1237:CLA:HAA2	1.97	0.46
3:B:482:LEU:HA	3:B:490:SER:HB2	1.98	0.46
1:g:182:TYR:HA	1:g:189:VAL:HA	1.98	0.46
13:g:503:CLA:H62	13:g:503:CLA:H41	1.57	0.46
14:g:523:BCR:H15C	14:g:523:BCR:H351	1.74	0.46
1:b:266:LEU:HD13	13:b:505:CLA:H122	1.97	0.46
1:b:271:ALA:HA	13:b:501:CLA:H11	1.97	0.46
13:3:504:CLA:H2	13:3:504:CLA:H61	1.66	0.46
1:5:250:MET:HE3	1:5:250:MET:HB2	1.77	0.46
1:1:221:GLY:HA3	14:1:524:BCR:H402	1.98	0.46
13:1:518:CLA:HBB1	13:1:519:CLA:HAC2	1.97	0.46
13:A:1140:CLA:HBA2	13:A:1140:CLA:C4A	2.45	0.46
3:B:46:ILE:HG21	13:B:1202:CLA:H191	1.97	0.46
13:B:1227:CLA:HAB	13:B:1236:CLA:HBB2	1.97	0.46
11:M:16:LEU:HD11	14:M:4021:BCR:H373	1.98	0.46
1:d:128:ARG:HB2	1:e:341:MET:HE2	1.97	0.46
13:e:518:CLA:H3A	13:e:518:CLA:O2A	2.16	0.46
1:f:58:GLY:O	1:f:61:THR:OG1	2.28	0.46
13:f:517:CLA:NA	14:f:524:BCR:H16C	2.30	0.46
13:g:501:CLA:H152	13:g:507:CLA:HMB3	1.98	0.46
14:g:522:BCR:H351	14:g:522:BCR:H15C	1.68	0.46
1:b:158:GLY:HA2	1:b:233:GLY:HA2	1.97	0.46
1:3:145:PHE:HA	1:3:152:GLN:HG2	1.97	0.46
13:5:501:CLA:H121	13:5:501:CLA:H161	1.81	0.46
14:5:521:BCR:H393	15:5:822:SQD:H252	1.98	0.46
1:6:61:THR:O	1:6:65:ILE:HG13	2.16	0.46
13:6:503:CLA:H41	13:6:503:CLA:H62	1.54	0.46
13:6:506:CLA:HMC1	13:6:507:CLA:H102	1.97	0.46
13:B:1214:CLA:H93	13:B:1231:CLA:HBA1	1.96	0.46
10:K:19:VAL:HG22	10:K:70:ALA:HB1	1.97	0.46
1:c:258:SER:OG	1:c:333:HIS:ND1	2.47	0.46
1:3:47:VAL:HG22	13:3:512:CLA:HED1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:5:320:ASN:HD22	14:5:521:BCR:H332	1.81	0.46
1:6:257:LEU:HD12	13:6:509:CLA:HBC3	1.97	0.46
2:A:369:ILE:HD12	13:A:1125:CLA:H42	1.96	0.46
2:A:451:LEU:O	2:A:455:SER:OG	2.19	0.46
2:A:685:PHE:HZ	13:A:1140:CLA:HBC2	1.80	0.46
2:A:696:TYR:CE1	3:B:543:LYS:HD2	2.51	0.46
13:A:1131:CLA:H102	13:B:1238:CLA:H52	1.98	0.46
7:F:108:LEU:HD12	7:F:108:LEU:HA	1.81	0.46
14:e:524:BCR:H15C	14:e:524:BCR:H351	1.77	0.46
1:3:83:PRO:HB2	1:3:287:TYR:CZ	2.51	0.46
1:4:341:MET:SD	13:4:505:CLA:HMA2	2.56	0.46
13:B:1224:CLA:HBC3	16:B:5002:LMG:H421	1.98	0.46
13:B:1224:CLA:HBA2	13:B:1224:CLA:H3A	1.54	0.46
1:c:54:VAL:HB	1:c:115:SER:HB2	1.98	0.46
1:c:183:ASP:HB3	1:c:186:LEU:HB2	1.97	0.46
1:c:241:PRO:HA	13:c:506:CLA:HED3	1.98	0.46
1:d:113:ILE:HD11	13:e:505:CLA:H192	1.98	0.46
13:d:501:CLA:H151	13:d:507:CLA:H8	1.98	0.46
1:b:190:ARG:NH1	1:b:215:LEU:HD12	2.30	0.46
13:a:510:CLA:H2A	13:a:510:CLA:H2	1.97	0.46
13:4:507:CLA:H112	14:4:524:BCR:H362	1.97	0.45
13:6:505:CLA:H142	13:6:505:CLA:H112	1.73	0.45
1:1:297:ILE:HD13	1:1:297:ILE:HA	1.82	0.45
1:1:309:LEU:CG	2:A:250:ALA:CB	2.95	0.45
2:A:330:GLU:O	2:A:333:LYS:HE3	2.16	0.45
2:A:411:HIS:HE1	13:A:1128:CLA:C4A	2.29	0.45
13:A:1123:CLA:H143	13:A:1123:CLA:H111	1.73	0.45
14:A:4003:BCR:H20C	14:A:4003:BCR:H361	1.79	0.45
7:F:105:ARG:NH2	7:F:152:LEU:O	2.48	0.45
1:c:209:PHE:HE1	14:b:523:BCR:H323	1.81	0.45
13:c:502:CLA:H91	13:c:502:CLA:H111	1.75	0.45
1:d:85:LEU:HD22	1:d:107:ILE:HD13	1.97	0.45
1:d:124:PHE:HB2	13:e:505:CLA:HAA2	1.98	0.45
13:e:501:CLA:C3D	13:e:503:CLA:H2	2.46	0.45
1:f:49:GLN:HG2	13:f:509:CLA:HMA3	1.97	0.45
1:g:137:THR:HA	1:g:141:ARG:HB2	1.96	0.45
1:g:289:PRO:CG	1:g:305:ILE:HG13	2.45	0.45
1:g:303:ASP:OD1	1:g:303:ASP:N	2.38	0.45
13:a:501:CLA:H92	13:a:501:CLA:H62	1.76	0.45
1:3:112:LEU:HD22	14:3:522:BCR:H12C	1.99	0.45
13:3:510:CLA:H41	13:3:510:CLA:H61	1.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:501:CLA:H143	13:4:501:CLA:H161	1.81	0.45
14:5:522:BCR:H15C	14:5:522:BCR:H351	1.77	0.45
1:2:56:TRP:CZ3	1:2:81:LEU:HD21	2.51	0.45
1:1:54:VAL:HG13	1:1:111:HIS:HD2	1.80	0.45
13:A:1115:CLA:H62	13:A:1115:CLA:H41	1.44	0.45
13:A:1126:CLA:H3A	13:A:1126:CLA:HBA2	1.70	0.45
3:B:373:ALA:HA	3:B:601:TRP:CZ3	2.50	0.45
13:B:1231:CLA:HAB	13:B:1234:CLA:HED2	1.97	0.45
1:c:291:LEU:HD21	1:c:316:ALA:HB2	1.98	0.45
14:c:522:BCR:HC7	13:d:505:CLA:H162	1.97	0.45
13:e:502:CLA:H92	13:e:502:CLA:H61	1.73	0.45
1:f:169:LEU:HA	1:f:172:VAL:HG12	1.98	0.45
13:4:510:CLA:H41	13:4:510:CLA:H61	1.48	0.45
14:4:523:BCR:H11C	14:4:523:BCR:H341	1.82	0.45
1:5:282:TYR:OH	13:5:502:CLA:O1D	2.32	0.45
1:6:241:PRO:HA	13:6:506:CLA:HED3	1.98	0.45
2:A:215:HIS:HB2	13:A:1112:CLA:CHC	2.47	0.45
13:A:1138:CLA:H91	18:A:2001:PQN:H293	1.98	0.45
3:B:158:GLN:O	3:B:162:ARG:HG3	2.17	0.45
3:B:318:PRO:HB2	13:B:1220:CLA:HMA3	1.98	0.45
3:B:493:TRP:N	3:B:494:PRO:HD2	2.31	0.45
14:B:4006:BCR:H371	14:B:4006:BCR:H24C	1.70	0.45
14:B:4010:BCR:H11C	14:B:4010:BCR:H341	1.81	0.45
5:D:21:ALA:HA	5:D:24:THR:HG22	1.98	0.45
1:f:55:PHE:HB2	1:f:115:SER:OG	2.17	0.45
1:5:309:LEU:HA	1:5:309:LEU:HD23	1.74	0.45
13:6:508:CLA:H72	14:6:521:BCR:H21C	1.99	0.45
2:A:356:LEU:O	2:A:360:LEU:HB2	2.17	0.45
14:A:4007:BCR:H11C	14:A:4007:BCR:H341	1.81	0.45
3:B:142:LEU:O	3:B:146:ALA:N	2.44	0.45
13:B:1213:CLA:HBC1	13:B:1214:CLA:H172	1.99	0.45
1:c:225:ILE:HD11	13:c:507:CLA:H93	1.98	0.45
1:d:341:MET:HE3	13:d:505:CLA:H2A	1.99	0.45
14:f:522:BCR:H11C	14:f:522:BCR:H341	1.63	0.45
1:a:128:ARG:HD3	1:a:128:ARG:HA	1.59	0.45
13:3:510:CLA:H121	13:3:510:CLA:H161	1.68	0.45
14:3:521:BCR:H11C	14:3:521:BCR:H341	1.83	0.45
13:4:502:CLA:H92	13:4:502:CLA:H61	1.70	0.45
13:4:502:CLA:HBA2	13:4:503:CLA:H171	1.99	0.45
13:5:505:CLA:H12	14:5:524:BCR:H312	1.99	0.45
13:6:516:CLA:H3A	13:6:516:CLA:HBA1	1.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:2:518:CLA:HHB	13:2:518:CLA:H42	1.98	0.45
13:1:504:CLA:H41	13:1:504:CLA:H62	1.45	0.45
3:B:394:GLY:HA2	14:B:4010:BCR:H393	1.99	0.45
10:K:83:LEU:HD23	10:K:83:LEU:OXT	2.16	0.45
1:d:125:HIS:HA	1:d:129:ALA:HB3	1.98	0.45
14:d:522:BCR:H15C	14:d:522:BCR:H351	1.72	0.45
1:e:49:GLN:HG2	13:e:509:CLA:HMA3	1.97	0.45
1:e:205:TYR:HA	1:e:208:HIS:CE1	2.51	0.45
1:e:242:LEU:HD12	1:e:244:TRP:HE1	1.81	0.45
1:e:264:ILE:HD13	1:e:264:ILE:HA	1.89	0.45
1:f:120:ALA:HB1	13:g:505:CLA:H11	1.98	0.45
1:b:273:TYR:O	1:b:277:VAL:HG22	2.17	0.45
1:a:50:ALA:O	1:a:54:VAL:HG12	2.17	0.45
13:a:502:CLA:HBB2	13:a:510:CLA:H162	1.99	0.45
1:4:192:ILE:HD12	1:4:219:VAL:HG21	1.99	0.45
1:2:60:PHE:O	1:2:64:GLU:HG2	2.17	0.45
14:2:521:BCR:H24C	14:2:521:BCR:H371	1.80	0.45
13:A:1101:CLA:H42	13:A:1106:CLA:H202	1.98	0.45
13:B:1222:CLA:HED2	13:B:1223:CLA:HBD	1.98	0.45
13:e:513:CLA:NB	14:e:523:BCR:H272	2.32	0.45
1:f:30:ALA:HB1	13:f:508:CLA:HAA1	1.99	0.45
1:g:68:TYR:HB2	1:g:79:LEU:HD21	1.98	0.45
1:b:257:LEU:HD22	13:b:509:CLA:HBC3	1.99	0.45
1:4:169:LEU:HG	1:4:226:ALA:HB1	1.99	0.45
13:5:501:CLA:H92	13:5:501:CLA:H62	1.83	0.45
13:5:508:CLA:H72	14:5:521:BCR:H23C	1.97	0.45
13:6:503:CLA:H172	13:6:510:CLA:HBB2	1.98	0.45
13:6:509:CLA:H3A	13:6:509:CLA:HBA1	1.52	0.45
1:1:158:GLY:HA3	1:1:237:ILE:HG13	1.99	0.45
14:1:524:BCR:H15C	14:1:524:BCR:H351	1.65	0.45
2:A:237:PRO:HB3	2:A:241:GLU:OE1	2.16	0.45
14:A:4003:BCR:H341	14:A:4003:BCR:H11C	1.78	0.45
13:B:1225:CLA:H142	13:B:1225:CLA:H111	1.72	0.45
8:I:2:MET:HE3	8:I:12:TRP:CE2	2.52	0.45
1:c:233:GLY:O	1:c:237:ILE:HG13	2.17	0.45
13:c:510:CLA:H52	13:c:510:CLA:H8	1.77	0.45
13:d:503:CLA:H41	13:d:503:CLA:H62	1.63	0.45
1:e:312:HIS:HB2	1:e:317:TRP:NE1	2.31	0.45
1:e:330:LEU:HD11	13:e:505:CLA:HHC	1.98	0.45
1:g:101:LEU:HD23	1:g:104:TYR:HD2	1.82	0.45
1:b:124:PHE:CE2	1:b:128:ARG:HG2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:a:508:CLA:H71	13:a:510:CLA:HED2	1.98	0.45
1:4:19:TYR:O	1:4:21:GLN:NE2	2.50	0.45
1:4:105:PHE:CE2	14:4:523:BCR:HC31	2.52	0.45
13:2:518:CLA:H92	13:2:518:CLA:HMB3	1.99	0.45
1:1:309:LEU:CB	2:A:257:ASP:O	2.64	0.45
2:A:237:PRO:HG2	2:A:248:LEU:HD21	1.99	0.45
13:A:1124:CLA:H93	13:A:1137:CLA:H62	1.98	0.45
13:A:1131:CLA:H151	18:B:2002:PQN:H191	1.98	0.45
3:B:460:GLU:OE1	3:B:465:GLN:NE2	2.47	0.45
13:B:1203:CLA:H72	13:B:1203:CLA:H111	1.50	0.45
6:E:26:SER:HB3	6:E:38:ILE:HD12	1.99	0.45
1:g:344:ASN:O	1:g:347:GLN:HG2	2.16	0.45
14:g:523:BCR:H11C	14:g:523:BCR:H341	1.72	0.45
14:b:521:BCR:H15C	14:b:521:BCR:H351	1.77	0.45
1:a:54:VAL:HG11	1:a:118:LEU:HD12	1.98	0.45
13:3:501:CLA:H152	13:3:507:CLA:HMA1	1.99	0.45
1:6:55:PHE:HB2	1:6:115:SER:OG	2.17	0.45
13:6:510:CLA:CAD	13:6:511:CLA:HAB	2.47	0.45
14:2:521:BCR:HC22	17:A:5005:LHG:C4	2.32	0.45
2:A:728:ARG:NH2	19:A:3001:SF4:S4	2.90	0.45
13:A:1118:CLA:H61	13:A:1118:CLA:H41	1.60	0.45
17:A:5003:LHG:H132	17:A:5003:LHG:H102	1.69	0.45
13:B:1205:CLA:H143	13:B:1205:CLA:H161	1.77	0.45
1:d:145:PHE:HA	1:d:152:GLN:HG2	1.97	0.45
1:f:54:VAL:HG23	1:f:115:SER:HB2	1.99	0.45
1:f:307:LEU:HD23	1:f:307:LEU:H	1.82	0.45
13:3:511:CLA:H12	13:3:511:CLA:H52	1.77	0.45
1:6:329:PHE:HA	13:6:508:CLA:HMC2	1.99	0.45
13:2:505:CLA:H111	13:2:505:CLA:H93	1.79	0.45
2:A:347:VAL:HG23	2:A:424:MET:HG2	1.99	0.45
2:A:395:THR:HG23	2:A:610:ILE:HG21	1.98	0.45
13:A:1107:CLA:O1A	14:J:4013:BCR:H14C	2.17	0.45
13:A:1113:CLA:CAB	14:K:4001:BCR:H333	2.48	0.45
14:B:4009:BCR:H11C	14:B:4009:BCR:H341	1.87	0.45
13:c:510:CLA:H112	13:c:510:CLA:H72	1.75	0.45
1:d:164:LEU:HD11	13:d:509:CLA:H61	1.98	0.45
1:e:80:ILE:C	1:e:83:PRO:HD2	2.41	0.45
1:e:151:LYS:HD3	1:e:240:PRO:HB3	1.99	0.45
1:b:50:ALA:O	1:b:54:VAL:HG23	2.17	0.45
1:b:109:ALA:HB1	14:b:522:BCR:H322	1.99	0.45
1:a:171:LEU:HD22	13:a:501:CLA:C1D	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:503:CLA:H72	13:4:503:CLA:H112	1.88	0.44
14:1:522:BCR:H15C	14:1:522:BCR:H351	1.76	0.44
2:A:520:VAL:HG23	2:A:525:ALA:HB2	1.99	0.44
3:B:526:VAL:HG11	3:B:600:TYR:CD1	2.52	0.44
13:B:1202:CLA:H3A	13:B:1202:CLA:HBA1	1.32	0.44
7:F:139:TRP:CD1	7:F:140:PRO:HD3	2.52	0.44
14:J:4012:BCR:H11C	14:J:4012:BCR:H341	1.72	0.44
1:c:329:PHE:HA	13:c:508:CLA:HMC1	1.99	0.44
1:3:42:PHE:O	1:3:46:HIS:ND1	2.47	0.44
14:3:524:BCR:H15C	14:3:524:BCR:H351	1.70	0.44
2:A:202:ALA:HB2	2:A:312:GLY:HA3	2.00	0.44
13:A:1116:CLA:HBA2	13:A:1116:CLA:H3A	1.58	0.44
3:B:593:THR:O	3:B:597:VAL:HG23	2.17	0.44
1:c:257:LEU:HD22	13:c:509:CLA:HBC3	1.98	0.44
1:d:236:HIS:HE1	13:d:506:CLA:NC	2.15	0.44
1:e:329:PHE:HA	13:e:508:CLA:HMC1	1.98	0.44
13:e:501:CLA:H2	13:e:501:CLA:C1B	2.48	0.44
1:f:49:GLN:HG2	13:f:509:CLA:H3A	1.99	0.44
1:g:183:ASP:HB2	1:g:190:ARG:HD2	1.98	0.44
13:g:502:CLA:H122	13:g:503:CLA:H3A	1.98	0.44
14:b:522:BCR:H11C	14:b:522:BCR:H341	1.83	0.44
1:a:19:TYR:OH	1:a:343:PHE:O	2.33	0.44
14:a:521:BCR:H11C	14:a:521:BCR:H341	1.70	0.44
1:4:49:GLN:HG2	13:4:509:CLA:HMA3	1.99	0.44
1:6:158:GLY:HA3	1:6:237:ILE:HG13	1.98	0.44
1:6:220:GLY:O	1:6:223:ILE:HG22	2.17	0.44
3:B:197:VAL:HG21	13:B:1211:CLA:C1D	2.47	0.44
15:B:1852:SQD:H312	15:B:1852:SQD:H281	1.82	0.44
1:e:174:LYS:HD2	1:e:178:TRP:O	2.17	0.44
1:e:330:LEU:HD11	13:e:505:CLA:CHC	2.47	0.44
1:b:93:GLY:HA3	1:b:99:VAL:HG23	1.99	0.44
1:a:72:LEU:O	1:a:77:GLN:NE2	2.50	0.44
13:3:503:CLA:H62	13:3:503:CLA:H41	1.65	0.44
1:5:291:LEU:HD22	1:5:303:ASP:HA	2.00	0.44
1:6:200:PHE:CE2	14:g:521:BCR:HC7	2.52	0.44
13:6:519:CLA:HBA1	13:6:519:CLA:H3A	1.72	0.44
13:2:512:CLA:HBA1	13:2:512:CLA:H3A	1.55	0.44
1:1:56:TRP:O	1:1:60:PHE:HB2	2.17	0.44
13:1:519:CLA:H3A	13:1:519:CLA:HBA2	1.66	0.44
2:A:616:LYS:NZ	2:A:620:ASP:OD2	2.38	0.44
13:A:1139:CLA:H93	13:A:1139:CLA:H61	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:140:ILE:HD13	3:B:143:LEU:HD12	1.99	0.44
13:B:1217:CLA:HBA2	13:B:1217:CLA:H3A	1.46	0.44
13:B:1231:CLA:H62	13:B:1231:CLA:H2	1.50	0.44
1:c:65:ILE:HD11	1:c:104:TYR:HB2	1.99	0.44
1:f:46:HIS:CD2	13:f:512:CLA:HMD3	2.52	0.44
1:f:171:LEU:HD22	13:f:501:CLA:C1D	2.47	0.44
1:b:225:ILE:HD11	13:b:507:CLA:H93	2.00	0.44
1:a:216:GLU:OE1	1:a:216:GLU:N	2.37	0.44
13:3:505:CLA:H11	13:2:513:CLA:HAC2	1.98	0.44
14:3:521:BCR:H20C	14:3:521:BCR:H361	1.86	0.44
13:5:504:CLA:HMC1	13:5:510:CLA:HBC2	1.99	0.44
13:6:508:CLA:HBC3	13:6:510:CLA:H61	2.00	0.44
13:6:510:CLA:H62	13:6:510:CLA:H41	1.67	0.44
1:1:299:PRO:HG2	13:1:519:CLA:NB	2.32	0.44
2:A:404:LEU:HD21	13:A:1104:CLA:H142	1.98	0.44
13:A:1137:CLA:O2D	13:A:1137:CLA:H2A	2.17	0.44
3:B:276:HIS:HE2	13:B:1215:CLA:C2B	2.31	0.44
13:c:505:CLA:H142	13:c:505:CLA:H112	1.80	0.44
1:f:171:LEU:HD22	13:f:501:CLA:C2D	2.47	0.44
1:a:54:VAL:HG23	1:a:111:HIS:CD2	2.52	0.44
1:a:264:ILE:HG12	13:a:502:CLA:HAC1	1.98	0.44
13:5:513:CLA:C1B	14:5:523:BCR:H292	2.48	0.44
1:6:160:HIS:NE2	13:6:512:CLA:ND	2.65	0.44
1:1:19:TYR:CZ	1:1:344:ASN:HA	2.52	0.44
2:A:272:TRP:CH2	13:A:1115:CLA:HBB1	2.52	0.44
3:B:189:ALA:HA	13:B:1212:CLA:HBB2	1.99	0.44
3:B:431:LEU:HB3	13:B:1229:CLA:HED2	2.00	0.44
6:E:10:ILE:H	6:E:10:ILE:HG12	1.65	0.44
1:d:273:TYR:O	1:d:277:VAL:HG22	2.18	0.44
13:f:509:CLA:H3A	13:f:509:CLA:HBA1	1.76	0.44
13:b:505:CLA:H192	14:a:522:BCR:H323	2.00	0.44
1:3:338:LEU:HD22	13:3:518:CLA:HMD3	1.98	0.44
1:5:219:VAL:O	1:5:221:GLY:O	2.35	0.44
2:A:292:LEU:N	2:A:378:PRO:O	2.50	0.44
2:A:708:HIS:HE1	13:A:1138:CLA:C4D	2.31	0.44
3:B:197:VAL:HG11	13:B:1211:CLA:HED3	2.00	0.44
3:B:686:VAL:HG11	4:C:81:TYR:CG	2.53	0.44
3:B:707:LEU:HD22	3:B:711:GLN:NE2	2.33	0.44
7:F:151:GLU:OE1	7:F:151:GLU:N	2.48	0.44
9:J:39:HIS:HD1	9:J:41:LEU:H	1.66	0.44
1:d:49:GLN:HG2	13:d:509:CLA:HMA3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:f:273:TYR:O	1:f:277:VAL:HG22	2.17	0.44
13:g:501:CLA:H141	13:g:507:CLA:HMB3	1.97	0.44
1:a:161:LEU:HD21	13:a:506:CLA:CHC	2.47	0.44
13:3:509:CLA:H143	13:3:509:CLA:CHA	2.48	0.44
13:5:505:CLA:HMB1	13:5:505:CLA:HBB1	2.00	0.44
13:2:501:CLA:H202	13:2:507:CLA:HMB1	2.00	0.44
1:1:54:VAL:HG12	1:1:111:HIS:O	2.17	0.44
3:B:413:ASP:O	3:B:417:GLN:HG2	2.18	0.44
13:B:1201:CLA:H72	11:M:23:PHE:HD1	1.83	0.44
13:B:1202:CLA:H111	13:B:1202:CLA:H142	1.75	0.44
1:d:18:THR:HB	1:d:21:GLN:O	2.17	0.44
14:d:521:BCR:H371	14:d:521:BCR:H24C	1.78	0.44
13:f:502:CLA:H62	13:f:502:CLA:H41	1.46	0.44
14:f:521:BCR:H15C	14:f:521:BCR:H351	1.86	0.44
1:g:79:LEU:HD23	1:g:82:LEU:HB2	2.00	0.44
1:g:196:THR:OG1	1:g:217:ASP:HA	2.18	0.44
1:b:125:HIS:CE1	13:b:513:CLA:NA	2.86	0.44
1:b:147:TRP:HE3	1:b:256:ILE:HD12	1.83	0.44
1:3:158:GLY:HA3	1:3:237:ILE:HG13	2.00	0.44
13:3:501:CLA:C4D	13:3:503:CLA:H2	2.48	0.44
13:3:513:CLA:HMC1	14:3:523:BCR:H372	2.00	0.44
1:4:289:PRO:HD2	1:4:313:THR:HG21	2.00	0.44
1:5:56:TRP:CZ3	1:5:81:LEU:HD21	2.53	0.44
1:6:147:TRP:HE3	1:6:256:ILE:HD12	1.82	0.44
14:6:521:BCR:H351	14:6:521:BCR:H15C	1.75	0.44
13:1:503:CLA:H162	13:1:510:CLA:HBB2	2.00	0.44
13:A:1105:CLA:HBB1	13:A:1105:CLA:HMB1	2.00	0.44
13:A:1107:CLA:H202	13:A:1107:CLA:H162	1.80	0.44
13:A:1139:CLA:H93	7:F:133:MET:HE1	2.00	0.44
13:A:1237:CLA:H142	13:A:1237:CLA:H112	1.79	0.44
3:B:526:VAL:HG23	13:B:1021:CLA:H141	2.00	0.44
13:B:1012:CLA:H93	13:B:1012:CLA:H62	1.70	0.44
13:B:1216:CLA:H2A	13:B:1216:CLA:CED	2.46	0.44
5:D:85:ARG:NH1	5:D:95:ILE:HG21	2.33	0.44
1:c:291:LEU:HD23	1:c:303:ASP:N	2.33	0.44
13:c:510:CLA:H43	14:c:521:BCR:H383	2.00	0.44
1:d:113:ILE:HG12	13:e:505:CLA:H161	2.00	0.44
1:d:242:LEU:HD22	1:d:244:TRP:HE1	1.82	0.44
13:e:510:CLA:H112	13:e:510:CLA:H72	1.74	0.44
1:f:267:ALA:HA	13:f:501:CLA:H72	2.00	0.44
13:g:505:CLA:HBC2	14:g:524:BCR:H341	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:205:TYR:CE2	14:b:524:BCR:H391	2.53	0.44
1:5:32:ASN:ND2	13:5:510:CLA:O1A	2.47	0.43
14:2:523:BCR:H11C	14:2:523:BCR:H341	1.87	0.43
13:1:501:CLA:H121	13:1:501:CLA:H161	1.66	0.43
2:A:201:LEU:HD23	2:A:201:LEU:HA	1.87	0.43
2:A:516:ASP:OD1	2:A:516:ASP:N	2.51	0.43
2:A:549:THR:HG21	13:A:1124:CLA:HAC2	2.00	0.43
3:B:466:PHE:O	3:B:470:ALA:N	2.46	0.43
3:B:686:VAL:HG13	3:B:700:TRP:CH2	2.53	0.43
13:B:1227:CLA:HBA2	13:B:1227:CLA:H3A	1.37	0.43
1:c:330:LEU:HD11	13:c:505:CLA:CHC	2.48	0.43
1:e:100:ASP:N	1:e:100:ASP:OD1	2.50	0.43
14:e:524:BCR:H11C	14:e:524:BCR:H341	1.74	0.43
1:f:49:GLN:O	1:f:49:GLN:NE2	2.51	0.43
1:g:19:TYR:CZ	1:g:344:ASN:HA	2.53	0.43
14:g:521:BCR:H11C	14:g:521:BCR:H341	1.76	0.43
1:b:246:ARG:HG2	1:b:251:PHE:HE2	1.83	0.43
1:b:323:PHE:CD1	14:a:522:BCR:H333	2.53	0.43
14:b:523:BCR:H24C	14:b:523:BCR:H371	1.87	0.43
1:a:241:PRO:O	1:a:246:ARG:NH2	2.51	0.43
1:a:257:LEU:HD22	13:a:509:CLA:HBC3	1.99	0.43
1:a:266:LEU:HD12	1:a:266:LEU:HA	1.88	0.43
14:a:523:BCR:H11C	14:a:523:BCR:H341	1.86	0.43
1:3:29:TRP:NE1	20:J:5105:LMU:H31	2.30	0.43
13:3:502:CLA:H61	13:3:502:CLA:H92	1.84	0.43
14:4:521:BCR:H15C	14:4:521:BCR:H351	1.79	0.43
13:6:508:CLA:C2D	14:6:521:BCR:H382	2.48	0.43
13:2:509:CLA:H161	13:2:509:CLA:H192	1.73	0.43
2:A:417:VAL:HG11	2:A:574:PHE:N	2.33	0.43
2:A:461:HIS:HE1	13:A:1132:CLA:C1A	2.31	0.43
3:B:452:THR:O	3:B:452:THR:OG1	2.30	0.43
3:B:701:LYS:HE3	3:B:701:LYS:HB2	1.88	0.43
13:B:1221:CLA:H61	13:B:1221:CLA:H41	1.53	0.43
13:B:1223:CLA:H112	13:B:1223:CLA:H72	1.92	0.43
13:B:1225:CLA:H3A	13:B:1225:CLA:HBA2	1.51	0.43
14:I:4018:BCR:H15C	14:I:4018:BCR:H351	1.68	0.43
1:c:72:LEU:HD22	1:c:77:GLN:HG3	2.00	0.43
1:d:14:ALA:HB2	1:d:148:ASP:CG	2.43	0.43
1:d:195:PRO:HB3	1:d:219:VAL:HG13	1.99	0.43
13:d:504:CLA:H61	13:d:504:CLA:H41	1.83	0.43
1:e:171:LEU:HD23	1:e:222:HIS:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:215:LEU:HG	1:e:280:LEU:HD11	2.00	0.43
1:e:270:VAL:HG21	13:e:501:CLA:H92	2.00	0.43
13:f:517:CLA:C4A	14:f:524:BCR:H16C	2.48	0.43
1:g:282:TYR:HB2	1:g:315:ARG:HH21	1.83	0.43
1:g:297:ILE:O	13:g:519:CLA:NC	2.51	0.43
14:3:523:BCR:H15C	14:3:523:BCR:H351	1.74	0.43
1:6:98:VAL:HG11	1:6:101:LEU:HD23	2.00	0.43
1:6:287:TYR:HB3	1:6:315:ARG:HB2	1.99	0.43
2:A:415:PHE:CD1	2:A:419:ASP:HB2	2.54	0.43
13:A:1129:CLA:HBA1	13:A:1129:CLA:H3A	1.81	0.43
13:B:1229:CLA:HBB1	13:B:1229:CLA:HHC	2.00	0.43
6:E:9:LYS:HB3	6:E:67:GLN:HG3	2.00	0.43
6:E:59:ASN:HB3	6:E:61:PHE:CE2	2.53	0.43
1:c:171:LEU:HD22	13:c:501:CLA:C1D	2.47	0.43
13:c:505:CLA:HBC1	14:c:524:BCR:H353	2.00	0.43
1:d:246:ARG:HA	1:d:251:PHE:HE1	1.83	0.43
13:d:501:CLA:H143	13:d:501:CLA:H161	1.83	0.43
1:e:186:LEU:HD12	1:e:190:ARG:HE	1.83	0.43
1:g:56:TRP:O	1:g:60:PHE:HB2	2.18	0.43
13:g:512:CLA:HBB1	13:g:512:CLA:HHC	2.00	0.43
14:b:521:BCR:H371	14:b:521:BCR:H24C	1.81	0.43
1:3:242:LEU:HB2	1:3:244:TRP:CD1	2.52	0.43
13:4:505:CLA:H93	13:4:505:CLA:H111	1.73	0.43
13:2:502:CLA:H12	13:2:503:CLA:H43	1.99	0.43
1:1:146:ARG:HB3	1:1:149:ASP:HB2	1.99	0.43
1:1:243:THR:HA	1:1:246:ARG:HD3	2.01	0.43
3:B:22:TRP:HE1	13:B:1238:CLA:CBB	2.31	0.43
3:B:185:VAL:O	3:B:189:ALA:N	2.42	0.43
4:C:18:VAL:HG11	4:C:28:MET:HG2	2.01	0.43
13:c:518:CLA:H61	13:c:518:CLA:H41	1.78	0.43
13:c:518:CLA:CBB	13:c:519:CLA:HAC2	2.48	0.43
1:d:221:GLY:C	14:d:524:BCR:H383	2.44	0.43
1:e:252:ASN:O	1:e:256:ILE:HG12	2.18	0.43
13:e:519:CLA:HBA1	13:e:519:CLA:H3A	1.56	0.43
14:e:522:BCR:H15C	14:e:522:BCR:H351	1.71	0.43
13:g:511:CLA:H52	14:g:522:BCR:H282	1.99	0.43
1:b:246:ARG:HG2	1:b:251:PHE:CE2	2.53	0.43
1:b:320:ASN:HB3	14:b:521:BCR:HC8	1.99	0.43
13:4:509:CLA:H142	13:4:509:CLA:H111	1.82	0.43
13:5:502:CLA:H92	13:5:502:CLA:H61	1.73	0.43
13:5:509:CLA:HBA1	13:5:509:CLA:H3A	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:6:106:VAL:HG22	14:6:523:BCR:H313	2.00	0.43
1:6:258:SER:O	1:6:333:HIS:ND1	2.44	0.43
14:6:523:BCR:H361	14:6:523:BCR:H20C	1.82	0.43
13:2:501:CLA:H162	13:2:507:CLA:H111	1.99	0.43
13:1:503:CLA:H41	13:1:503:CLA:H62	1.74	0.43
13:1:506:CLA:HBA2	13:1:506:CLA:H3A	1.41	0.43
13:A:1125:CLA:H111	13:A:1125:CLA:H152	1.75	0.43
3:B:148:LEU:HD12	3:B:148:LEU:HA	1.86	0.43
3:B:165:LEU:HD11	3:B:169:LYS:HE2	2.00	0.43
3:B:556:ASP:OD1	4:C:66:ARG:NH2	2.50	0.43
13:B:1201:CLA:H92	13:B:1201:CLA:H62	1.79	0.43
13:B:1231:CLA:HBA2	13:B:1231:CLA:H3A	1.69	0.43
7:F:96:ILE:HG23	13:F:1301:CLA:HAA1	2.00	0.43
8:I:9:PHE:O	8:I:12:TRP:HB2	2.17	0.43
1:g:56:TRP:HB2	13:g:510:CLA:HAC2	1.99	0.43
1:g:291:LEU:HD11	1:g:316:ALA:HA	2.00	0.43
1:b:32:ASN:HB3	13:b:509:CLA:HAB	2.00	0.43
14:a:521:BCR:H15C	14:a:521:BCR:H351	1.76	0.43
1:4:307:LEU:HD23	1:4:308:PRO:HD2	1.99	0.43
15:4:822:SQD:C26	7:F:141:LEU:HD13	2.49	0.43
1:6:56:TRP:HB2	13:6:510:CLA:HAC2	1.99	0.43
14:6:523:BCR:H11C	14:6:523:BCR:H341	1.74	0.43
4:C:29:VAL:HG21	5:D:112:ALA:HB2	2.00	0.43
13:c:508:CLA:H62	13:c:508:CLA:H93	1.76	0.43
1:d:35:PHE:HA	1:d:38:LEU:HD12	2.00	0.43
1:d:158:GLY:HA2	1:d:233:GLY:HA2	1.99	0.43
1:d:161:LEU:HD21	13:d:506:CLA:HAB	2.01	0.43
13:e:505:CLA:HBA2	13:e:505:CLA:H11	1.64	0.43
1:g:158:GLY:HA2	1:g:233:GLY:HA2	1.99	0.43
1:g:276:ALA:HA	1:g:291:LEU:HD12	2.00	0.43
13:g:503:CLA:H122	13:g:503:CLA:H8	1.68	0.43
1:b:113:ILE:O	1:b:117:VAL:HG23	2.19	0.43
1:a:31:GLY:O	1:a:34:ARG:HG2	2.18	0.43
1:a:195:PRO:HA	1:a:216:GLU:HB3	2.00	0.43
13:a:513:CLA:CHC	14:a:523:BCR:H23C	2.49	0.43
1:4:169:LEU:HD23	1:4:169:LEU:HA	1.87	0.43
14:4:521:BCR:H11C	14:4:521:BCR:H341	1.82	0.43
13:5:508:CLA:H93	14:5:521:BCR:H19C	2.01	0.43
13:6:503:CLA:H91	13:6:503:CLA:H112	1.80	0.43
13:2:502:CLA:H61	13:2:502:CLA:H92	1.78	0.43
1:1:170:LEU:HD23	1:1:170:LEU:HA	1.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:564:ARG:NH2	5:D:15:THR:O	2.52	0.43
13:A:1106:CLA:CHC	13:A:1107:CLA:HMD2	2.49	0.43
3:B:223:ALA:HB3	3:B:224:PRO:HD3	1.99	0.43
3:B:322:PRO:HB2	3:B:410:ASN:HA	2.01	0.43
3:B:554:MET:HE3	3:B:571:ARG:HH22	1.83	0.43
7:F:120:LYS:HD3	7:F:125:ASP:HB2	2.01	0.43
1:d:50:ALA:O	1:d:54:VAL:HG23	2.19	0.43
1:d:157:LEU:HD21	13:d:506:CLA:C1B	2.49	0.43
1:e:50:ALA:O	1:e:54:VAL:HG23	2.18	0.43
1:f:88:LEU:HD13	13:f:502:CLA:H142	2.01	0.43
1:b:146:ARG:HB3	1:b:149:ASP:HB2	2.00	0.43
13:b:505:CLA:HBA1	1:a:120:ALA:O	2.19	0.43
1:4:80:ILE:O	1:4:84:HIS:ND1	2.41	0.43
14:6:522:BCR:H15C	14:6:522:BCR:H351	1.61	0.43
14:2:523:BCR:H15C	14:2:523:BCR:H351	1.77	0.43
1:1:257:LEU:HD22	13:1:509:CLA:HBC3	2.01	0.43
13:1:512:CLA:H3A	13:1:512:CLA:HBA1	1.44	0.43
2:A:107:PRO:HG3	2:A:148:ARG:HH12	1.84	0.43
2:A:261:PHE:O	2:A:265:ILE:HG12	2.19	0.43
13:A:1108:CLA:HBD	20:A:1849:LMU:H21	2.01	0.43
13:A:1126:CLA:H41	13:A:1126:CLA:H61	1.66	0.43
13:A:1139:CLA:H61	13:A:1139:CLA:H41	1.77	0.43
3:B:3:THR:HG21	3:B:20:ARG:CZ	2.49	0.43
13:B:1213:CLA:H61	13:B:1213:CLA:H2	1.64	0.43
13:B:1229:CLA:H3A	14:F:4014:BCR:C14	2.49	0.43
14:F:4015:BCR:H20C	14:F:4015:BCR:H361	1.86	0.43
1:d:271:ALA:HB2	13:d:501:CLA:H43	2.00	0.43
1:d:289:PRO:HG3	1:d:305:ILE:HD13	2.01	0.43
13:d:505:CLA:H11	13:d:505:CLA:HBA2	1.73	0.43
13:e:512:CLA:O2D	13:e:513:CLA:HBB2	2.19	0.43
14:e:521:BCR:H351	14:e:521:BCR:H15C	1.78	0.43
13:a:502:CLA:HAB	13:a:510:CLA:H141	2.01	0.43
1:3:162:LEU:HD23	1:3:230:ILE:HA	2.01	0.43
1:3:261:LEU:HD11	13:3:508:CLA:HAB	2.00	0.43
13:3:505:CLA:HBA2	1:2:124:PHE:HD2	1.84	0.43
1:5:147:TRP:HE3	1:5:256:ILE:HD12	1.83	0.43
1:6:91:GLY:O	1:6:99:VAL:HG22	2.18	0.43
1:2:215:LEU:HD23	1:2:215:LEU:HA	1.91	0.43
2:A:444:LEU:HB2	13:A:1137:CLA:HBB1	2.00	0.43
13:A:1125:CLA:HED2	13:A:1137:CLA:H42	2.00	0.43
14:M:4021:BCR:H11C	14:M:4021:BCR:H341	1.93	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:17:GLN:H	1:c:254:GLU:HG3	1.84	0.43
13:c:505:CLA:H92	13:c:505:CLA:H62	1.78	0.43
13:f:519:CLA:HED2	13:f:519:CLA:H2A	2.00	0.43
1:b:330:LEU:HD11	13:b:505:CLA:CHC	2.49	0.43
1:a:164:LEU:HD21	13:a:509:CLA:H72	2.01	0.43
1:a:259:TYR:HB3	13:a:507:CLA:C4B	2.48	0.43
1:4:278:ASN:OD1	1:4:281:ALA:N	2.49	0.43
13:5:518:CLA:H3A	13:5:518:CLA:O2A	2.19	0.43
13:6:510:CLA:HBB1	13:6:510:CLA:HMB1	2.01	0.43
13:2:518:CLA:H3A	13:2:518:CLA:O2A	2.19	0.43
14:2:524:BCR:H15C	14:2:524:BCR:H351	1.80	0.43
2:A:466:ARG:NH2	2:A:644:ILE:HD11	2.34	0.43
2:A:486:PHE:HB3	13:A:1135:CLA:H11	2.00	0.43
13:A:1138:CLA:H8	13:A:1138:CLA:HMC2	2.00	0.43
14:A:4002:BCR:H361	14:A:4002:BCR:H20C	1.82	0.43
3:B:330:TYR:OH	3:B:341:HIS:NE2	2.49	0.43
3:B:417:GLN:OE1	7:F:164:ARG:HG2	2.19	0.43
3:B:540:ILE:HB	3:B:586:ALA:HB2	2.01	0.43
13:B:1228:CLA:HAC1	13:B:1236:CLA:HBC3	2.01	0.43
4:C:56:THR:HG21	6:E:49:TYR:HD1	1.82	0.43
14:F:4015:BCR:H15C	14:F:4015:BCR:H351	1.73	0.43
14:I:4019:BCR:H15C	14:I:4019:BCR:H351	1.74	0.43
1:c:16:LEU:HD22	1:c:254:GLU:HG2	2.00	0.43
1:c:322:HIS:NE2	13:c:502:CLA:C4D	2.82	0.43
14:c:522:BCR:H333	1:d:323:PHE:CD1	2.53	0.43
14:f:522:BCR:H24C	14:f:522:BCR:H371	1.89	0.43
13:3:505:CLA:H92	13:3:505:CLA:H61	1.79	0.42
1:6:182:TYR:HA	1:6:189:VAL:HA	2.01	0.42
13:2:505:CLA:H122	1:1:113:ILE:HG23	2.00	0.42
13:2:516:CLA:H3A	1:b:352:LEU:HD21	2.00	0.42
1:1:221:GLY:C	14:1:524:BCR:H383	2.44	0.42
2:A:617:MET:HA	2:A:621:VAL:HB	2.01	0.42
2:A:682:ILE:HD13	2:A:682:ILE:HA	1.87	0.42
13:A:1022:CLA:HMB3	13:A:1022:CLA:HBB1	2.01	0.42
13:A:1115:CLA:H11	13:K:1401:CLA:HED1	2.01	0.42
13:A:1136:CLA:H52	13:A:1136:CLA:H8	1.88	0.42
3:B:167:TRP:CZ2	13:B:1210:CLA:HAC2	2.54	0.42
13:B:1214:CLA:H62	13:B:1214:CLA:H101	1.80	0.42
13:c:509:CLA:H192	13:c:509:CLA:H161	1.86	0.42
14:c:521:BCR:H11C	14:c:521:BCR:H341	1.89	0.42
14:c:523:BCR:H15C	14:c:523:BCR:H351	1.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:510:CLA:H61	13:f:510:CLA:H41	1.51	0.42
13:g:502:CLA:HAA1	13:g:503:CLA:H11	2.00	0.42
1:b:68:TYR:HD1	1:b:79:LEU:HD11	1.84	0.42
1:b:85:LEU:HD22	1:b:107:ILE:HD13	2.00	0.42
1:a:206:GLN:HB3	13:a:517:CLA:HMD2	2.00	0.42
13:3:508:CLA:H52	13:3:510:CLA:HED3	2.01	0.42
1:4:164:LEU:HD12	13:4:507:CLA:HED3	1.99	0.42
13:5:505:CLA:H141	13:5:505:CLA:H161	1.89	0.42
1:2:150:PRO:HG3	1:2:246:ARG:HH11	1.84	0.42
2:A:465:MET:HA	2:A:465:MET:HE2	2.01	0.42
3:B:378:HIS:HE2	13:B:1225:CLA:C2B	2.31	0.42
3:B:626:TRP:O	3:B:630:TYR:HB3	2.18	0.42
14:c:522:BCR:H11C	14:c:522:BCR:H341	1.60	0.42
1:d:243:THR:HA	1:d:246:ARG:HD3	2.01	0.42
1:d:285:GLU:H	1:d:285:GLU:CD	2.27	0.42
14:d:522:BCR:H341	14:d:522:BCR:H11C	1.75	0.42
1:f:64:GLU:O	1:f:68:TYR:N	2.52	0.42
1:f:282:TYR:O	1:f:315:ARG:NH2	2.52	0.42
14:g:521:BCR:H20C	14:g:521:BCR:H361	1.84	0.42
1:b:269:PHE:HB3	13:b:505:CLA:H193	1.99	0.42
1:a:333:HIS:NE2	13:a:505:CLA:NB	2.66	0.42
13:5:519:CLA:HBA1	13:5:519:CLA:H3A	1.89	0.42
14:5:522:BCR:C35	13:6:505:CLA:HBB2	2.49	0.42
1:2:346:LYS:HA	15:2:822:SQD:H81	2.01	0.42
13:2:517:CLA:HBA1	13:2:517:CLA:H3A	1.64	0.42
2:A:17:ASP:OD1	2:A:186:LYS:HD3	2.20	0.42
2:A:43:GLN:HA	7:F:118:ASN:HD22	1.84	0.42
2:A:360:LEU:HD23	2:A:407:GLY:C	2.45	0.42
2:A:453:PHE:CE2	13:B:1023:CLA:H12	2.54	0.42
13:A:1102:CLA:H62	13:A:1107:CLA:H203	2.00	0.42
13:A:1138:CLA:O1A	13:B:1229:CLA:HED3	2.19	0.42
18:A:2001:PQN:H193	14:F:4014:BCR:H23C	2.01	0.42
3:B:454:GLU:H	3:B:454:GLU:CD	2.26	0.42
13:B:1217:CLA:H12	13:B:1217:CLA:H52	1.74	0.42
13:c:505:CLA:H11	1:b:120:ALA:HB1	2.00	0.42
1:g:209:PHE:CE2	13:g:517:CLA:HHD	2.53	0.42
1:b:233:GLY:O	1:b:237:ILE:HG12	2.19	0.42
1:b:317:TRP:HZ3	14:b:521:BCR:H342	1.84	0.42
1:a:150:PRO:HB3	1:a:251:PHE:CE2	2.54	0.42
1:2:163:PHE:CE1	13:2:512:CLA:HHB	2.54	0.42
1:1:317:TRP:CZ2	13:1:504:CLA:HBA1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:1:502:CLA:H12	13:1:503:CLA:H42	2.02	0.42
13:1:502:CLA:H92	13:1:502:CLA:H61	1.75	0.42
13:c:507:CLA:H3A	13:c:507:CLA:HBA1	1.77	0.42
14:c:521:BCR:H20C	14:c:521:BCR:H361	1.87	0.42
1:f:163:PHE:CE2	13:f:512:CLA:HHB	2.55	0.42
1:f:205:TYR:HA	1:f:208:HIS:CE1	2.54	0.42
14:g:524:BCR:H351	14:g:524:BCR:H15C	1.70	0.42
1:b:38:LEU:CD1	1:b:41:LEU:HB2	2.49	0.42
1:b:157:LEU:HD13	1:b:157:LEU:HA	1.92	0.42
13:3:501:CLA:H92	13:3:501:CLA:H62	1.91	0.42
13:3:518:CLA:H3A	13:3:518:CLA:O2A	2.19	0.42
1:4:293:VAL:HG22	1:4:301:PHE:CE1	2.54	0.42
13:4:509:CLA:HMB1	13:4:509:CLA:HBB1	2.02	0.42
13:5:503:CLA:H62	13:5:503:CLA:H102	1.67	0.42
13:5:513:CLA:HBB1	14:5:523:BCR:C40	2.50	0.42
1:6:114:SER:HB3	14:6:523:BCR:H14C	2.01	0.42
13:2:509:CLA:H93	13:2:509:CLA:H62	1.77	0.42
2:A:316:ARG:HH11	2:A:324:SER:HB2	1.85	0.42
13:A:1013:CLA:H143	13:A:1140:CLA:H101	2.01	0.42
13:B:1206:CLA:H141	13:B:1206:CLA:H162	1.79	0.42
13:B:1215:CLA:HBA2	13:B:1215:CLA:H3A	1.53	0.42
13:B:1226:CLA:H143	16:B:5002:LMG:H231	2.02	0.42
1:c:317:TRP:CZ2	13:c:504:CLA:HBA1	2.54	0.42
1:c:348:LEU:HD13	13:b:511:CLA:H41	2.01	0.42
13:c:508:CLA:HMA1	13:c:509:CLA:HBC2	2.01	0.42
1:d:38:LEU:HD22	1:d:131:HIS:HB3	2.02	0.42
1:g:153:LEU:HD22	13:g:507:CLA:HAC1	2.02	0.42
13:g:503:CLA:H62	13:g:503:CLA:H102	1.56	0.42
13:b:510:CLA:CAD	13:b:511:CLA:HAB	2.49	0.42
14:3:522:BCR:C35	13:4:505:CLA:HBB2	2.49	0.42
1:4:320:ASN:HB3	14:4:521:BCR:HC8	2.02	0.42
1:6:260:SER:OG	13:6:509:CLA:O2D	2.37	0.42
1:1:115:SER:O	1:1:119:GLY:N	2.45	0.42
2:A:226:LEU:O	2:A:231:VAL:HG23	2.20	0.42
2:A:296:ASP:HB3	13:A:1116:CLA:HMA1	2.01	0.42
3:B:392:ALA:O	3:B:396:ILE:HG13	2.19	0.42
3:B:434:GLY:HA2	3:B:532:LEU:HD22	2.02	0.42
13:B:1204:CLA:H43	8:I:14:PHE:CD2	2.54	0.42
14:B:4004:BCR:H20C	14:B:4004:BCR:H361	1.88	0.42
7:F:86:PHE:C	7:F:89:PRO:HD2	2.45	0.42
14:F:4014:BCR:H15C	14:F:4014:BCR:H351	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:c:145:PHE:HA	1:c:152:GLN:HG2	2.01	0.42
1:c:273:TYR:O	1:c:277:VAL:HG22	2.20	0.42
13:c:509:CLA:H122	13:c:509:CLA:H8	1.90	0.42
1:d:156:ILE:HD13	1:d:156:ILE:N	2.35	0.42
13:e:510:CLA:H61	13:e:510:CLA:H41	1.75	0.42
1:f:109:ALA:HB1	14:f:523:BCR:H333	2.02	0.42
1:b:79:LEU:HD13	1:b:82:LEU:HD12	2.01	0.42
14:b:524:BCR:H351	14:b:524:BCR:H15C	1.75	0.42
1:3:170:LEU:HD23	1:3:170:LEU:HA	1.90	0.42
13:4:507:CLA:H92	13:4:507:CLA:H61	1.89	0.42
13:5:510:CLA:HMB1	13:5:510:CLA:HBB1	2.01	0.42
13:1:509:CLA:H141	13:1:509:CLA:H161	1.73	0.42
14:1:524:BCR:H361	14:1:524:BCR:H20C	1.84	0.42
3:B:399:VAL:HG23	3:B:548:ALA:HB1	2.01	0.42
12:X:11:PRO:HB2	12:X:12:THR:H	1.70	0.42
1:c:124:PHE:CE1	1:c:128:ARG:HG2	2.55	0.42
14:c:524:BCR:H11C	14:c:524:BCR:H341	1.80	0.42
1:e:14:ALA:HB2	1:e:148:ASP:HB2	2.02	0.42
1:e:146:ARG:HG2	1:e:149:ASP:H	1.85	0.42
1:e:273:TYR:O	1:e:277:VAL:HG22	2.19	0.42
13:f:505:CLA:H2	14:f:524:BCR:H331	2.02	0.42
13:f:507:CLA:CAD	13:f:509:CLA:H152	2.50	0.42
1:b:271:ALA:HB2	13:b:501:CLA:H43	2.02	0.42
1:a:29:TRP:O	13:a:508:CLA:H11	2.20	0.42
1:a:55:PHE:HB2	1:a:115:SER:HB2	2.01	0.42
1:a:141:ARG:HH22	1:a:146:ARG:HH12	1.67	0.42
1:1:248:LEU:HD21	14:1:524:BCR:HC21	2.02	0.42
2:A:367:SER:OG	2:A:397:HIS:O	2.34	0.42
13:A:1107:CLA:H71	13:A:1107:CLA:H112	1.59	0.42
14:A:4008:BCR:H11C	14:A:4008:BCR:H341	1.88	0.42
13:B:1225:CLA:H41	13:B:1225:CLA:H61	1.89	0.42
14:F:4015:BCR:H24C	14:F:4015:BCR:H371	1.83	0.42
14:I:4018:BCR:H11C	14:I:4018:BCR:H341	1.75	0.42
9:J:8:LEU:HA	9:J:13:VAL:HG11	2.01	0.42
9:J:31:ARG:HD3	14:J:4013:BCR:H312	2.00	0.42
1:c:205:TYR:HA	1:c:208:HIS:CE1	2.55	0.42
13:c:511:CLA:HBB1	13:c:511:CLA:HMB3	2.02	0.42
14:d:523:BCR:H15C	14:d:523:BCR:H351	1.68	0.42
1:e:105:PHE:HE1	14:e:522:BCR:HC21	1.85	0.42
1:f:57:ALA:HB2	13:f:503:CLA:C2D	2.49	0.42
1:f:130:PRO:HG3	1:f:136:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:501:CLA:HBB2	13:g:507:CLA:H93	2.01	0.42
14:g:523:BCR:H371	14:g:523:BCR:H24C	1.82	0.42
13:b:503:CLA:H62	13:b:503:CLA:H101	1.82	0.42
1:3:16:LEU:HA	1:3:254:GLU:HG2	2.02	0.42
1:4:200:PHE:CE2	14:d:521:BCR:HC7	2.55	0.42
13:4:505:CLA:H92	13:4:505:CLA:H61	1.77	0.42
14:4:524:BCR:H341	14:4:524:BCR:H11C	1.84	0.42
14:5:524:BCR:H15C	14:5:524:BCR:H351	1.87	0.42
13:6:501:CLA:H201	13:6:506:CLA:C4B	2.50	0.42
1:2:294:LYS:HD3	17:A:5005:LHG:O1	2.16	0.42
1:1:318:LEU:HD23	1:1:318:LEU:HA	1.89	0.42
13:1:501:CLA:H162	13:1:507:CLA:H111	2.00	0.42
14:1:521:BCR:H15C	14:1:521:BCR:H351	1.73	0.42
2:A:321:ILE:H	2:A:321:ILE:HG12	1.70	0.42
2:A:352:TRP:CE2	13:A:1123:CLA:H18	2.55	0.42
2:A:445:ASN:CG	3:B:685:LEU:HD21	2.45	0.42
2:A:525:ALA:O	2:A:526:MET:HE2	2.20	0.42
13:A:1103:CLA:H161	13:A:1103:CLA:H143	1.76	0.42
3:B:280:ILE:O	3:B:284:PHE:HD1	2.03	0.42
13:B:1211:CLA:HBB1	13:B:1211:CLA:HMB3	2.02	0.42
14:B:4017:BCR:H15C	14:B:4017:BCR:H351	1.85	0.42
1:c:47:VAL:CG2	13:c:513:CLA:HAB	2.50	0.42
1:c:264:ILE:HG12	13:c:502:CLA:HAC1	2.00	0.42
1:d:152:GLN:O	1:d:156:ILE:HG12	2.20	0.42
1:d:158:GLY:HA3	1:d:237:ILE:HG13	2.02	0.42
1:e:196:THR:OG1	1:e:217:ASP:HA	2.19	0.42
1:f:17:GLN:H	1:f:254:GLU:HG3	1.83	0.42
14:f:523:BCR:H11C	14:f:523:BCR:H341	1.84	0.42
1:g:142:ARG:HD3	1:g:142:ARG:HA	1.92	0.42
1:b:183:ASP:O	1:b:187:GLN:N	2.53	0.42
13:b:503:CLA:H112	13:b:503:CLA:H91	1.76	0.42
13:b:507:CLA:H61	13:b:507:CLA:H41	1.91	0.42
1:a:126:THR:HG21	14:a:522:BCR:H271	2.02	0.42
1:4:77:GLN:H	1:4:77:GLN:HG2	1.65	0.42
13:4:502:CLA:HBD	13:4:503:CLA:H42	2.00	0.42
1:6:92:ILE:HD13	1:6:286:PHE:CZ	2.55	0.42
1:6:270:VAL:O	1:6:274:PHE:N	2.40	0.42
13:2:510:CLA:H111	13:2:510:CLA:H52	2.01	0.42
1:1:50:ALA:O	1:1:54:VAL:HG23	2.20	0.42
2:A:600:PHE:HB2	13:B:1023:CLA:HBC3	2.02	0.42
13:A:1106:CLA:H111	13:A:1109:CLA:H191	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:B:1232:CLA:HBA1	13:B:1232:CLA:H3A	1.88	0.42
14:B:4009:BCR:H15C	14:B:4009:BCR:H351	1.73	0.42
4:C:14:CYS:O	4:C:15:THR:OG1	2.31	0.42
1:d:57:ALA:HB1	13:d:503:CLA:HED3	2.02	0.42
13:d:510:CLA:H71	14:d:521:BCR:H19C	2.01	0.42
1:e:28:TRP:HA	13:e:511:CLA:HMD3	2.00	0.42
14:f:523:BCR:H351	14:f:523:BCR:H15C	1.66	0.42
1:3:36:VAL:HG22	13:3:509:CLA:HAC2	2.01	0.41
1:5:254:GLU:CD	1:5:336:HIS:HD1	2.28	0.41
13:2:510:CLA:H142	13:2:510:CLA:H112	1.70	0.41
1:1:330:LEU:HD21	13:1:505:CLA:HAB	2.02	0.41
2:A:655:TRP:CD1	13:B:1021:CLA:HBC1	2.55	0.41
13:A:1104:CLA:H71	13:A:1104:CLA:H112	1.70	0.41
13:A:1134:CLA:HBA2	13:K:1401:CLA:HBD	2.00	0.41
3:B:93:ASP:HB3	3:B:96:PHE:CD1	2.56	0.41
3:B:178:HIS:CD2	13:B:1210:CLA:NB	2.88	0.41
3:B:714:LEU:HD11	16:B:5002:LMG:H351	2.01	0.41
5:D:118:ARG:HH12	5:D:139:PRO:HA	1.85	0.41
6:E:17:TRP:CZ2	6:E:45:ASN:HB3	2.55	0.41
1:c:209:PHE:CE1	14:b:523:BCR:H323	2.54	0.41
1:d:169:LEU:O	1:d:173:LEU:HG	2.20	0.41
1:d:320:ASN:ND2	14:d:521:BCR:HC41	2.34	0.41
1:e:54:VAL:HG12	1:e:111:HIS:O	2.20	0.41
1:f:268:GLY:HA3	13:f:502:CLA:HBC3	2.02	0.41
1:f:334:LEU:HD11	13:f:505:CLA:HMB2	2.02	0.41
13:g:501:CLA:H62	13:g:501:CLA:H41	1.92	0.41
1:b:44:ALA:HB1	1:b:126:THR:OG1	2.20	0.41
1:a:164:LEU:HB3	1:a:229:LEU:HD23	2.02	0.41
1:3:63:TYR:HB2	1:4:295:LEU:HD23	2.02	0.41
1:4:269:PHE:HE2	1:4:330:LEU:HD22	1.86	0.41
1:4:328:PHE:O	13:4:508:CLA:HAC1	2.20	0.41
13:6:508:CLA:HMB3	13:6:509:CLA:C1C	2.50	0.41
13:2:501:CLA:H143	13:2:501:CLA:H161	1.82	0.41
14:1:522:BCR:H20C	14:1:522:BCR:H361	1.91	0.41
14:A:4011:BCR:H24C	13:B:1230:CLA:HMC1	2.02	0.41
13:B:1206:CLA:H18	13:B:1206:CLA:H151	1.78	0.41
13:B:1209:CLA:O2D	13:B:1209:CLA:H2A	2.21	0.41
13:B:1225:CLA:H43	14:B:4005:BCR:H24C	2.01	0.41
13:B:1226:CLA:H92	13:B:1226:CLA:H61	1.81	0.41
4:C:6:LYS:HE2	5:D:116:VAL:HG22	2.01	0.41
1:c:271:ALA:HB2	13:c:501:CLA:H43	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:g:503:CLA:H143	13:g:503:CLA:H111	1.80	0.41
14:g:521:BCR:H371	14:g:521:BCR:H24C	1.81	0.41
1:b:28:TRP:HZ3	13:b:511:CLA:HBC1	1.85	0.41
1:b:274:PHE:HD1	1:b:278:ASN:HD22	1.66	0.41
1:b:333:HIS:NE2	13:b:505:CLA:NC	2.68	0.41
14:a:522:BCR:H24C	14:a:522:BCR:H371	1.91	0.41
1:5:123:LEU:HD12	13:6:505:CLA:HHB	2.02	0.41
13:2:510:CLA:H192	13:2:510:CLA:H162	1.78	0.41
2:A:218:HIS:HE1	13:A:1113:CLA:ND	2.16	0.41
2:A:561:ARG:HH21	2:A:570:ALA:HB1	1.86	0.41
3:B:225:PHE:HA	3:B:230:TRP:CD1	2.55	0.41
13:c:501:CLA:H172	13:c:507:CLA:HMB2	2.02	0.41
14:c:521:BCR:H24C	14:c:521:BCR:H371	1.76	0.41
13:d:503:CLA:H101	13:d:503:CLA:H62	1.80	0.41
1:e:210:ALA:HB1	1:e:277:VAL:HG21	2.02	0.41
13:e:503:CLA:H102	13:e:503:CLA:H13	1.73	0.41
13:f:507:CLA:H51	13:f:507:CLA:H8	1.95	0.41
1:b:294:LYS:HG2	1:a:66:SER:OG	2.19	0.41
13:a:508:CLA:HMA1	13:a:509:CLA:HBC2	2.02	0.41
1:3:261:LEU:HD11	13:3:508:CLA:CAB	2.50	0.41
14:3:522:BCR:H24C	14:3:522:BCR:H371	1.87	0.41
1:6:34:ARG:NH1	13:6:511:CLA:OBD	2.50	0.41
1:2:197:LEU:O	1:2:224:TYR:OH	2.39	0.41
13:2:503:CLA:H41	13:2:503:CLA:H62	1.46	0.41
13:1:509:CLA:H62	13:1:509:CLA:H2	1.84	0.41
2:A:410:ALA:O	2:A:414:ILE:HG13	2.20	0.41
2:A:462:ASN:OD1	2:A:475:PHE:N	2.49	0.41
2:A:476:SER:HB3	2:A:644:ILE:HD12	2.01	0.41
13:A:1119:CLA:CMD	13:A:1120:CLA:HAB	2.50	0.41
13:A:1122:CLA:HBB1	17:A:5003:LHG:HC42	2.02	0.41
3:B:182:LEU:HD21	13:B:1210:CLA:H12	2.03	0.41
13:B:1023:CLA:H122	14:I:4018:BCR:H281	2.02	0.41
13:B:1206:CLA:H91	13:B:1239:CLA:H12	2.02	0.41
7:F:32:LYS:H	7:F:32:LYS:HG2	1.70	0.41
7:F:155:LYS:H	7:F:155:LYS:HG2	1.66	0.41
1:c:273:TYR:CZ	1:c:277:VAL:HG21	2.54	0.41
1:e:171:LEU:HD22	13:e:501:CLA:C1D	2.51	0.41
1:e:266:LEU:O	1:e:270:VAL:HG23	2.21	0.41
13:f:503:CLA:H142	13:f:503:CLA:H111	1.83	0.41
13:a:512:CLA:H62	13:a:512:CLA:H41	1.79	0.41
14:3:522:BCR:H15C	14:3:522:BCR:H351	1.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:4:45:ALA:HB2	13:4:511:CLA:HMA1	2.02	0.41
1:4:128:ARG:HD2	1:4:128:ARG:HA	1.83	0.41
1:5:57:ALA:HB2	13:5:503:CLA:C2D	2.50	0.41
2:A:28:TRP:HZ2	13:A:1102:CLA:H11	1.86	0.41
2:A:436:HIS:CE1	13:A:1129:CLA:ND	2.88	0.41
2:A:730:VAL:HG22	13:A:1140:CLA:CAD	2.51	0.41
13:A:1101:CLA:H93	13:A:1106:CLA:H18	2.03	0.41
13:A:1119:CLA:H112	14:A:4007:BCR:C10	2.50	0.41
13:A:1011:CLA:NA	13:B:1021:CLA:HAB	2.35	0.41
3:B:268:LEU:HD13	13:B:1214:CLA:H2A	2.02	0.41
3:B:314:LYS:HE2	3:B:314:LYS:HB2	1.91	0.41
13:B:1023:CLA:H192	14:B:4017:BCR:H353	2.03	0.41
13:B:1203:CLA:H3A	13:B:1203:CLA:HBA1	1.43	0.41
13:c:511:CLA:H12	13:c:511:CLA:H52	1.69	0.41
1:d:270:VAL:HG22	13:d:505:CLA:H201	2.03	0.41
1:e:16:LEU:HD22	1:e:16:LEU:HA	1.85	0.41
1:e:291:LEU:HD11	1:e:315:ARG:HG2	2.02	0.41
1:f:233:GLY:O	1:f:237:ILE:HG13	2.21	0.41
14:g:524:BCR:H341	14:g:524:BCR:H11C	1.78	0.41
14:b:523:BCR:H15C	14:b:523:BCR:H351	1.65	0.41
13:b:505:CLA:HBB2	14:a:522:BCR:H351	2.03	0.41
1:3:258:SER:O	1:3:333:HIS:ND1	2.52	0.41
1:4:303:ASP:OD1	1:4:303:ASP:N	2.50	0.41
1:5:124:PHE:CE2	1:5:128:ARG:HG2	2.55	0.41
14:5:521:BCR:H351	14:5:521:BCR:H15C	1.80	0.41
1:6:282:TYR:HD2	1:6:287:TYR:CE2	2.38	0.41
2:A:28:TRP:CZ2	13:A:1102:CLA:H11	2.56	0.41
2:A:225:LYS:HD3	2:A:252:LEU:HD13	2.01	0.41
13:A:1013:CLA:O1A	3:B:434:GLY:HA3	2.20	0.41
13:A:1104:CLA:H161	13:A:1104:CLA:H193	1.80	0.41
13:B:1203:CLA:H51	16:B:5002:LMG:H352	2.03	0.41
13:B:1223:CLA:HBD	13:B:1223:CLA:HAA2	2.03	0.41
13:B:1233:CLA:O2D	13:B:1233:CLA:H2A	2.21	0.41
14:F:4016:BCR:H24C	14:F:4016:BCR:H371	1.93	0.41
14:F:4016:BCR:H341	14:F:4016:BCR:H11C	1.75	0.41
14:f:524:BCR:H15C	14:f:524:BCR:H351	1.81	0.41
1:g:90:PHE:CE2	1:g:174:LYS:HD2	2.56	0.41
1:g:198:ASP:O	1:g:201:VAL:HG12	2.20	0.41
1:g:260:SER:HB2	13:g:507:CLA:HAA1	2.02	0.41
1:b:76:GLU:OE1	1:b:307:LEU:HD21	2.20	0.41
1:b:109:ALA:HB1	14:b:523:BCR:H333	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:b:126:THR:HG21	14:b:522:BCR:H271	2.01	0.41
1:a:16:LEU:HG	1:a:36:VAL:HG21	2.02	0.41
1:a:133:LEU:HB3	1:a:144:HIS:HB2	2.02	0.41
1:a:224:TYR:HD1	1:a:224:TYR:HA	1.81	0.41
13:a:507:CLA:OBD	13:a:509:CLA:H122	2.20	0.41
1:3:17:GLN:H	1:3:254:GLU:HG3	1.84	0.41
13:3:508:CLA:HMD3	13:3:518:CLA:HBC1	2.01	0.41
1:4:62:LEU:HD22	1:4:105:PHE:HD1	1.84	0.41
1:5:183:ASP:CG	1:5:215:LEU:HD11	2.46	0.41
13:5:518:CLA:HMA1	13:5:518:CLA:H61	2.03	0.41
1:6:275:CYS:HA	1:6:282:TYR:CD1	2.56	0.41
13:6:510:CLA:H111	13:6:510:CLA:H72	1.92	0.41
13:2:505:CLA:HBB2	14:1:522:BCR:C35	2.50	0.41
1:1:309:LEU:HD11	2:A:250:ALA:CB	2.50	0.41
14:A:4008:BCR:H361	14:A:4008:BCR:H20C	1.82	0.41
13:B:1221:CLA:HBA1	13:B:1221:CLA:H3A	1.67	0.41
13:B:1239:CLA:O1D	13:B:1239:CLA:H2A	2.21	0.41
8:I:9:PHE:HA	8:I:12:TRP:CD1	2.56	0.41
1:c:94:GLU:O	1:c:97:LYS:HG2	2.20	0.41
1:e:158:GLY:HA2	1:e:233:GLY:HA2	2.03	0.41
13:e:503:CLA:H41	13:e:503:CLA:H62	1.72	0.41
14:e:523:BCR:H20C	14:e:523:BCR:H361	1.78	0.41
14:f:523:BCR:H371	14:f:523:BCR:H24C	1.77	0.41
1:b:343:PHE:HB2	1:a:127:PHE:CD1	2.56	0.41
13:3:512:CLA:O2D	13:3:513:CLA:HBB2	2.21	0.41
1:5:181:LEU:HD13	13:5:501:CLA:HED1	2.02	0.41
14:6:521:BCR:H20C	14:6:521:BCR:H361	1.81	0.41
13:2:502:CLA:HAB	13:2:510:CLA:H141	2.03	0.41
13:2:507:CLA:H112	14:2:524:BCR:H362	2.01	0.41
14:1:524:BCR:H341	14:1:524:BCR:H11C	1.68	0.41
2:A:623:GLY:HA2	2:A:634:ILE:HG13	2.03	0.41
13:A:1011:CLA:HED2	13:A:1011:CLA:HBD	1.75	0.41
1:c:180:GLY:HA3	1:c:191:LEU:HA	2.03	0.41
1:c:303:ASP:N	1:c:303:ASP:OD1	2.38	0.41
1:e:307:LEU:HD23	1:e:307:LEU:HA	1.95	0.41
13:e:505:CLA:H112	13:e:505:CLA:H142	1.87	0.41
1:f:120:ALA:O	13:g:505:CLA:HBA1	2.21	0.41
1:b:176:THR:HG22	1:b:192:ILE:HB	2.02	0.41
13:b:509:CLA:H91	13:b:509:CLA:H111	1.75	0.41
1:a:72:LEU:HD23	1:a:77:GLN:HG3	2.03	0.41
1:a:192:ILE:HG13	1:a:219:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:212:ILE:HG12	1:a:213:ASN:H	1.86	0.41
14:a:522:BCR:H11C	14:a:522:BCR:H341	1.67	0.41
13:a:507:CLA:H3A	13:a:507:CLA:HBA1	1.84	0.41
1:3:114:SER:HB2	14:3:523:BCR:H363	2.03	0.41
1:3:273:TYR:O	1:3:277:VAL:HG22	2.21	0.41
1:3:275:CYS:HA	1:3:282:TYR:CD1	2.55	0.41
13:3:506:CLA:HMB3	13:3:507:CLA:C4A	2.46	0.41
1:4:126:THR:OG1	1:4:127:PHE:N	2.53	0.41
13:4:511:CLA:HBA1	14:4:522:BCR:H281	2.02	0.41
13:6:510:CLA:H192	13:6:510:CLA:H162	1.78	0.41
1:2:128:ARG:HA	1:2:128:ARG:HD2	1.74	0.41
13:2:511:CLA:H92	13:2:511:CLA:H62	1.90	0.41
14:2:521:BCR:H11C	14:2:521:BCR:H341	1.85	0.41
1:1:318:LEU:HD21	13:1:502:CLA:HMA3	2.03	0.41
1:1:328:PHE:HE2	14:1:521:BCR:H363	1.86	0.41
1:1:341:MET:HE1	13:1:505:CLA:H2A	2.03	0.41
13:1:502:CLA:HBB2	13:1:510:CLA:H141	2.02	0.41
14:1:521:BCR:H11C	14:1:521:BCR:H341	1.89	0.41
2:A:83:VAL:HG21	13:A:1103:CLA:H43	2.03	0.41
2:A:325:LEU:HD23	2:A:325:LEU:HA	1.92	0.41
2:A:372:GLN:HG2	13:A:1125:CLA:HMD1	2.03	0.41
2:A:393:LEU:HD23	2:A:393:LEU:HA	1.90	0.41
2:A:432:ARG:NE	13:A:1129:CLA:OBD	2.45	0.41
17:A:5005:LHG:H321	17:A:5005:LHG:H352	1.69	0.41
13:A:1101:CLA:CGA	13:A:1140:CLA:H43	2.50	0.41
13:A:1101:CLA:H62	13:A:1101:CLA:H102	1.81	0.41
13:A:1102:CLA:H112	13:A:1102:CLA:H91	1.83	0.41
13:A:1122:CLA:H41	13:A:1122:CLA:H61	1.54	0.41
13:A:1134:CLA:H2A	13:A:1134:CLA:O2D	2.21	0.41
13:A:1011:CLA:H102	13:A:1011:CLA:H62	1.73	0.41
3:B:136:TYR:OH	11:M:10:VAL:HG13	2.21	0.41
13:B:1223:CLA:H122	14:B:4009:BCR:H20C	2.02	0.41
13:B:1238:CLA:H202	13:B:1238:CLA:H162	1.75	0.41
8:I:27:MET:O	8:I:31:PHE:N	2.49	0.41
1:c:157:LEU:HD21	13:c:506:CLA:C1B	2.51	0.41
1:c:212:ILE:HD12	1:c:274:PHE:HZ	1.86	0.41
1:d:171:LEU:HD23	1:d:222:HIS:CD2	2.56	0.41
1:d:268:GLY:HA2	13:d:502:CLA:HMD3	2.01	0.41
13:e:505:CLA:H93	13:e:505:CLA:H61	1.91	0.41
1:f:56:TRP:CH2	1:f:81:LEU:HD21	2.55	0.41
13:f:507:CLA:OBD	13:f:509:CLA:H152	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:f:509:CLA:H151	13:f:509:CLA:CAD	2.50	0.41
14:a:524:BCR:H11C	14:a:524:BCR:H341	1.81	0.41
1:4:186:LEU:HD23	1:4:188:THR:HG22	2.03	0.41
1:6:269:PHE:HE2	1:6:330:LEU:HD22	1.85	0.41
1:6:318:LEU:HD23	1:6:318:LEU:HA	1.79	0.41
14:6:524:BCR:H11C	14:6:524:BCR:H341	1.85	0.41
13:2:508:CLA:OBD	15:2:822:SQD:H462	2.21	0.41
14:1:523:BCR:H20C	14:1:523:BCR:H361	1.92	0.41
2:A:324:SER:HB3	2:A:327:GLU:HG3	2.02	0.41
2:A:387:TYR:CE1	2:A:622:TRP:CD1	3.09	0.41
3:B:284:PHE:HE2	13:B:1216:CLA:HAB	1.86	0.41
3:B:293:THR:OG1	3:B:294:GLN:N	2.53	0.41
3:B:494:PRO:HB3	13:B:1233:CLA:C2D	2.51	0.41
4:C:47:ASP:OD1	5:D:85:ARG:NH2	2.54	0.41
13:c:513:CLA:C1C	14:c:523:BCR:H383	2.51	0.41
14:c:522:BCR:H20C	14:c:522:BCR:H361	1.86	0.41
13:d:503:CLA:H142	13:d:503:CLA:H111	1.91	0.41
13:d:504:CLA:H61	13:d:504:CLA:H93	1.73	0.41
1:e:46:HIS:HD2	13:e:509:CLA:H141	1.86	0.41
13:e:503:CLA:H62	13:e:503:CLA:H101	1.61	0.41
1:f:64:GLU:HB2	1:f:82:LEU:HD23	2.03	0.41
1:f:293:VAL:HG12	1:f:301:PHE:CD1	2.56	0.41
1:g:13:SER:O	1:g:252:ASN:ND2	2.54	0.41
13:b:511:CLA:HBA1	14:b:522:BCR:H281	2.03	0.41
1:3:60:PHE:HA	1:3:63:TYR:HB3	2.02	0.40
1:3:242:LEU:HD12	1:3:244:TRP:HE1	1.86	0.40
13:3:503:CLA:H62	13:3:503:CLA:H101	1.73	0.40
13:3:509:CLA:H192	13:3:509:CLA:H161	1.75	0.40
14:5:522:BCR:H24C	14:5:522:BCR:H371	1.91	0.40
1:1:299:PRO:HD2	13:1:519:CLA:C4B	2.44	0.40
14:1:523:BCR:H11C	14:1:523:BCR:H341	1.84	0.40
2:A:336:PHE:HB2	17:A:5003:LHG:HC41	2.02	0.40
13:A:1022:CLA:H42	3:B:658:LEU:HB2	2.02	0.40
13:A:1137:CLA:H51	13:A:1137:CLA:H12	1.79	0.40
3:B:372:MET:HE2	3:B:372:MET:HA	2.03	0.40
8:I:32:LEU:O	8:I:36:GLY:N	2.55	0.40
14:I:4018:BCR:H20C	14:I:4018:BCR:H361	1.88	0.40
10:K:15:VAL:CG2	10:K:83:LEU:HD21	2.51	0.40
10:K:26:ALA:O	10:K:30:GLY:N	2.44	0.40
13:c:513:CLA:HED2	13:c:513:CLA:HBD	1.96	0.40
1:e:105:PHE:CE1	1:f:293:VAL:HG21	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:e:125:HIS:HE1	13:e:513:CLA:NA	2.19	0.40
13:f:509:CLA:H141	13:f:512:CLA:HMD3	2.02	0.40
1:g:318:LEU:HD21	13:g:502:CLA:HED3	2.03	0.40
14:g:521:BCR:H15C	14:g:521:BCR:H351	1.76	0.40
1:b:222:HIS:HA	1:b:225:ILE:HG22	2.03	0.40
1:a:235:TRP:CD1	1:a:239:VAL:HB	2.56	0.40
1:a:250:MET:HE2	1:a:250:MET:HB2	1.86	0.40
1:a:327:PHE:O	1:a:331:GLN:HG2	2.21	0.40
13:a:501:CLA:HMD2	13:a:502:CLA:H101	2.03	0.40
13:a:510:CLA:H43	14:a:521:BCR:H383	2.02	0.40
1:3:225:ILE:HD13	1:3:225:ILE:HA	1.93	0.40
1:4:266:LEU:O	1:4:270:VAL:HG23	2.22	0.40
14:4:522:BCR:HC7	1:5:323:PHE:HE1	1.87	0.40
13:5:506:CLA:HBA1	13:5:507:CLA:HBB1	2.03	0.40
13:5:509:CLA:H192	13:5:509:CLA:H161	1.81	0.40
1:6:164:LEU:HB3	1:6:229:LEU:HD13	2.02	0.40
1:6:335:TRP:HH2	15:6:822:SQD:H45	1.85	0.40
1:2:60:PHE:HB3	1:2:81:LEU:HD12	2.03	0.40
2:A:126:LEU:HD11	13:A:1107:CLA:HBC3	2.02	0.40
2:A:456:PHE:CE1	13:A:1022:CLA:HHB	2.56	0.40
2:A:540:HIS:HE1	13:A:1136:CLA:ND	2.18	0.40
2:A:563:SER:OG	2:A:564:ARG:N	2.54	0.40
2:A:593:ASP:HA	2:A:596:PHE:HB3	2.04	0.40
13:A:1013:CLA:O1A	3:B:532:LEU:HD11	2.21	0.40
13:A:1133:CLA:H91	13:A:1133:CLA:H111	1.89	0.40
14:A:4007:BCR:H15C	14:A:4007:BCR:H351	1.76	0.40
3:B:20:ARG:NH2	8:I:34:ILE:O	2.43	0.40
3:B:275:HIS:HE1	13:B:1213:CLA:ND	2.18	0.40
4:C:27:GLU:HG3	5:D:110:ARG:HD3	2.03	0.40
14:I:4018:BCR:H23C	14:I:4018:BCR:H382	2.03	0.40
1:c:161:LEU:HD21	13:c:506:CLA:CAB	2.51	0.40
13:c:505:CLA:H11	13:c:505:CLA:HBA2	1.73	0.40
1:d:206:GLN:HG2	13:d:517:CLA:C1D	2.50	0.40
13:d:502:CLA:H61	13:d:502:CLA:H92	1.74	0.40
14:e:522:BCR:H11C	14:e:522:BCR:H341	1.81	0.40
1:a:172:VAL:HG11	1:a:223:ILE:HG23	2.03	0.40
1:3:257:LEU:HD22	13:3:509:CLA:HBC3	2.04	0.40
1:3:341:MET:HE2	1:2:128:ARG:HB2	2.02	0.40
1:4:97:LYS:HE3	1:4:97:LYS:HB3	1.90	0.40
1:4:164:LEU:HD21	13:4:509:CLA:H52	2.03	0.40
1:4:312:HIS:HB2	1:4:317:TRP:NE1	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:4:512:CLA:HBA1	13:4:512:CLA:H3A	1.68	0.40
14:4:521:BCR:H24C	14:4:521:BCR:H371	1.86	0.40
1:5:215:LEU:HD12	1:5:215:LEU:H	1.86	0.40
1:2:205:TYR:HA	1:2:208:HIS:CE1	2.57	0.40
13:2:503:CLA:H41	13:2:503:CLA:H102	2.03	0.40
14:2:521:BCR:H20C	14:2:521:BCR:H361	1.92	0.40
2:A:444:LEU:HB2	13:A:1137:CLA:CBB	2.52	0.40
13:A:1022:CLA:H192	14:B:4017:BCR:H343	2.03	0.40
13:A:1104:CLA:H41	13:A:1128:CLA:H92	2.03	0.40
13:A:1124:CLA:H12	13:A:1136:CLA:HAA2	2.03	0.40
13:A:1138:CLA:H8	13:A:1138:CLA:H121	1.93	0.40
13:B:1012:CLA:H2A	13:B:1012:CLA:O1D	2.22	0.40
13:B:1222:CLA:HBA2	13:B:1222:CLA:H3A	1.80	0.40
5:D:10:LEU:HG	5:D:51:ARG:NE	2.29	0.40
14:F:4015:BCR:H391	9:J:33:TYR:CD1	2.57	0.40
1:c:55:PHE:HB2	1:c:115:SER:OG	2.21	0.40
13:c:513:CLA:HBB1	14:c:523:BCR:C40	2.51	0.40
13:f:511:CLA:HBB1	13:f:511:CLA:HMB1	2.03	0.40
1:g:49:GLN:O	1:g:49:GLN:NE2	2.54	0.40
1:g:291:LEU:HD13	1:g:301:PHE:HB2	2.01	0.40
1:b:113:ILE:HG21	14:b:523:BCR:H12C	2.04	0.40
13:b:505:CLA:H61	1:a:117:VAL:HA	2.03	0.40
1:a:210:ALA:HB1	1:a:277:VAL:HG11	2.03	0.40
1:a:235:TRP:CD1	1:a:235:TRP:C	2.98	0.40
13:a:501:CLA:C4D	13:a:503:CLA:H2	2.51	0.40
14:a:523:BCR:H15C	14:a:523:BCR:H351	1.79	0.40
14:1:522:BCR:H24C	14:1:522:BCR:H371	1.93	0.40
2:A:326:LYS:O	2:A:330:GLU:HG2	2.21	0.40
13:A:1138:CLA:H93	13:A:1138:CLA:H61	1.72	0.40
13:A:1237:CLA:H152	13:B:1238:CLA:H102	2.03	0.40
3:B:268:LEU:HD13	13:B:1214:CLA:HMA2	2.04	0.40
3:B:319:PHE:O	3:B:319:PHE:CD1	2.74	0.40
3:B:377:THR:HG23	3:B:598:THR:HG21	2.04	0.40
3:B:481:LEU:O	3:B:482:LEU:HB2	2.21	0.40
6:E:25:ALA:N	6:E:38:ILE:O	2.49	0.40
14:I:4020:BCR:H20C	14:I:4020:BCR:H361	1.93	0.40
14:M:4021:BCR:H20C	14:M:4021:BCR:H361	1.79	0.40
1:c:88:LEU:HD11	13:c:503:CLA:HAA2	2.03	0.40
14:e:522:BCR:H24C	14:e:522:BCR:H371	1.91	0.40
13:f:504:CLA:H62	13:f:504:CLA:H41	1.78	0.40
1:b:329:PHE:HA	13:b:508:CLA:HMC1	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:268:GLY:HA2	13:a:502:CLA:HMD2	2.04	0.40
13:a:510:CLA:HBB1	13:a:510:CLA:HMB3	2.04	0.40
1:4:49:GLN:HG2	13:4:509:CLA:HHB	2.03	0.40
1:5:305:ILE:HG23	1:5:307:LEU:HG	2.03	0.40
1:6:36:VAL:HG12	13:6:509:CLA:HMC1	2.03	0.40
13:6:508:CLA:HMA1	13:6:509:CLA:HBC2	2.03	0.40
1:2:221:GLY:HA3	14:2:524:BCR:H402	2.03	0.40
14:2:521:BCR:H351	14:2:521:BCR:H15C	1.78	0.40
2:A:211:ALA:O	13:A:1112:CLA:HMC3	2.22	0.40
2:A:306:VAL:HG12	2:A:310:ILE:HD12	2.03	0.40
2:A:605:CYS:O	2:A:609:VAL:HG23	2.21	0.40
13:A:1123:CLA:HBD	13:A:1123:CLA:HAA2	2.04	0.40
3:B:37:MET:HE2	3:B:37:MET:HB2	1.89	0.40
3:B:325:GLY:O	3:B:329:THR:HG23	2.21	0.40
13:B:1228:CLA:H92	13:B:1228:CLA:H62	1.89	0.40
14:K:4001:BCR:H341	14:K:4001:BCR:H11C	1.80	0.40
1:c:249:LEU:HD11	13:c:506:CLA:O1A	2.21	0.40
13:c:509:CLA:H142	13:c:509:CLA:H112	1.79	0.40
1:g:110:VAL:HG11	16:g:5104:LMG:H362	2.02	0.40
1:b:190:ARG:HH12	1:b:215:LEU:HB2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	338/358 (94%)	334 (99%)	4 (1%)	0	100	100
1	2	337/358 (94%)	334 (99%)	3 (1%)	0	100	100
1	3	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	4	340/358 (95%)	333 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	5	332/358 (93%)	325 (98%)	6 (2%)	1 (0%)	36	67
1	6	337/358 (94%)	332 (98%)	5 (2%)	0	100	100
1	a	340/358 (95%)	335 (98%)	5 (2%)	0	100	100
1	b	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	c	341/358 (95%)	332 (97%)	9 (3%)	0	100	100
1	d	340/358 (95%)	334 (98%)	6 (2%)	0	100	100
1	e	340/358 (95%)	336 (99%)	4 (1%)	0	100	100
1	f	339/358 (95%)	333 (98%)	6 (2%)	0	100	100
1	g	339/358 (95%)	336 (99%)	3 (1%)	0	100	100
2	A	724/755 (96%)	694 (96%)	30 (4%)	0	100	100
3	B	687/741 (93%)	666 (97%)	21 (3%)	0	100	100
4	C	78/81 (96%)	76 (97%)	2 (3%)	0	100	100
5	D	135/139 (97%)	129 (96%)	6 (4%)	0	100	100
6	E	67/76 (88%)	65 (97%)	2 (3%)	0	100	100
7	F	139/164 (85%)	135 (97%)	4 (3%)	0	100	100
8	I	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
9	J	39/41 (95%)	39 (100%)	0	0	100	100
10	K	56/83 (68%)	56 (100%)	0	0	100	100
11	M	29/31 (94%)	26 (90%)	3 (10%)	0	100	100
12	X	27/39 (69%)	27 (100%)	0	0	100	100
All	All	6420/6842 (94%)	6284 (98%)	135 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	5	222	HIS

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	1	264/279 (95%)	259 (98%)	5 (2%)	50	68
1	2	263/279 (94%)	260 (99%)	3 (1%)	65	74
1	3	266/279 (95%)	262 (98%)	4 (2%)	57	71
1	4	266/279 (95%)	261 (98%)	5 (2%)	50	68
1	5	258/279 (92%)	250 (97%)	8 (3%)	35	59
1	6	263/279 (94%)	258 (98%)	5 (2%)	50	68
1	a	266/279 (95%)	256 (96%)	10 (4%)	29	55
1	b	266/279 (95%)	259 (97%)	7 (3%)	40	62
1	c	266/279 (95%)	256 (96%)	10 (4%)	29	55
1	d	266/279 (95%)	261 (98%)	5 (2%)	50	68
1	e	266/279 (95%)	260 (98%)	6 (2%)	44	64
1	f	265/279 (95%)	262 (99%)	3 (1%)	65	74
1	g	265/279 (95%)	258 (97%)	7 (3%)	40	62
2	A	593/603 (98%)	592 (100%)	1 (0%)	87	85
3	B	597/598 (100%)	594 (100%)	3 (0%)	81	80
4	C	67/68 (98%)	66 (98%)	1 (2%)	57	71
5	D	114/116 (98%)	114 (100%)	0	100	100
6	E	59/65 (91%)	58 (98%)	1 (2%)	53	70
7	F	109/128 (85%)	109 (100%)	0	100	100
8	I	32/32 (100%)	31 (97%)	1 (3%)	35	59
9	J	36/36 (100%)	36 (100%)	0	100	100
10	K	45/61 (74%)	43 (96%)	2 (4%)	25	51
11	M	26/26 (100%)	26 (100%)	0	100	100
12	X	20/31 (64%)	20 (100%)	0	100	100
All	All	5138/5391 (95%)	5051 (98%)	87 (2%)	52	70

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	3	112	LEU
1	3	197	LEU
1	3	280	LEU
1	3	309	LEU
1	4	97	LYS
1	4	186	LEU

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Mol	Chain	Res	Type
1	4	197	LEU
1	4	212	ILE
1	4	295	LEU
1	5	17	GLN
1	5	22	THR
1	5	92	ILE
1	5	112	LEU
1	5	185	ASN
1	5	189	VAL
1	5	197	LEU
1	5	202	ILE
1	6	60	PHE
1	6	133	LEU
1	6	197	LEU
1	6	257	LEU
1	6	280	LEU
1	2	197	LEU
1	2	274	PHE
1	2	297	ILE
1	1	72	LEU
1	1	98	VAL
1	1	198	ASP
1	1	280	LEU
1	1	297	ILE
2	A	310	ILE
3	B	499	VAL
3	B	501	LEU
3	B	581	ASP
4	C	9	ASP
6	E	11	LEU
8	I	19	CYS
10	K	6	LEU
10	K	54	PHE
1	c	72	LEU
1	c	84	HIS
1	c	133	LEU
1	c	162	LEU
1	c	185	ASN
1	c	197	LEU
1	c	198	ASP
1	c	237	ILE
1	c	280	LEU

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Mol	Chain	Res	Type
1	c	347	GLN
1	d	16	LEU
1	d	133	LEU
1	d	205	TYR
1	d	225	ILE
1	d	348	LEU
1	e	16	LEU
1	e	88	LEU
1	e	205	TYR
1	e	225	ILE
1	e	264	ILE
1	e	352	LEU
1	f	54	VAL
1	f	205	TYR
1	f	334	LEU
1	g	60	PHE
1	g	111	HIS
1	g	153	LEU
1	g	163	PHE
1	g	181	LEU
1	g	198	ASP
1	g	201	VAL
1	b	38	LEU
1	b	49	GLN
1	b	98	VAL
1	b	157	LEU
1	b	198	ASP
1	b	223	ILE
1	b	237	ILE
1	a	99	VAL
1	a	128	ARG
1	a	181	LEU
1	a	197	LEU
1	a	222	HIS
1	a	223	ILE
1	a	252	ASN
1	a	304	THR
1	a	309	LEU
1	a	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	3	37	ASN
1	3	67	GLN
1	3	111	HIS
1	3	131	HIS
1	3	144	HIS
1	4	21	GLN
1	4	37	ASN
1	4	49	GLN
1	4	185	ASN
1	4	208	HIS
1	5	17	GLN
1	5	49	GLN
1	6	49	GLN
1	6	125	HIS
1	6	187	GLN
1	6	222	HIS
1	2	208	HIS
1	1	49	GLN
1	1	125	HIS
1	1	131	HIS
1	1	208	HIS
1	1	252	ASN
1	1	336	HIS
1	1	347	GLN
2	A	192	ASN
2	A	224	ASN
2	A	445	ASN
2	A	481	GLN
2	A	571	ASN
2	A	657	GLN
2	A	698	GLN
2	A	718	GLN
3	B	14	GLN
3	B	34	HIS
3	B	79	GLN
3	B	83	ASN
3	B	95	GLN
3	B	106	GLN
3	B	158	GLN
3	B	354	GLN
3	B	649	ASN
3	B	711	GLN
6	E	19	ASN

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Mol	Chain	Res	Type
7	F	113	ASN
9	J	30	ASN
1	c	187	GLN
1	c	208	HIS
1	d	46	HIS
1	d	111	HIS
1	d	131	HIS
1	d	206	GLN
1	d	344	ASN
1	e	46	HIS
1	e	49	GLN
1	e	111	HIS
1	e	208	HIS
1	e	312	HIS
1	e	353	ASN
1	f	46	HIS
1	f	49	GLN
1	f	111	HIS
1	f	144	HIS
1	f	160	HIS
1	f	185	ASN
1	f	222	HIS
1	f	336	HIS
1	g	77	GLN
1	g	111	HIS
1	g	131	HIS
1	g	159	HIS
1	g	206	GLN
1	g	312	HIS
1	g	344	ASN
1	b	46	HIS
1	b	131	HIS
1	b	144	HIS
1	b	152	GLN
1	b	312	HIS
1	a	46	HIS
1	a	49	GLN
1	a	77	GLN
1	a	131	HIS
1	a	208	HIS
1	a	222	HIS
1	a	331	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

420 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	$\# Z > 2$
13	CLA	1	504	-	59,63,73	1.27	8 (13%)	70,101,113	1.16	4 (5%)
14	BCR	f	523	-	41,41,41	0.72	0	56,56,56	1.89	12 (21%)
13	CLA	5	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.25	7 (10%)
13	CLA	a	509	1	69,73,73	1.19	6 (8%)	82,113,113	1.19	4 (4%)
13	CLA	6	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.19	5 (6%)
13	CLA	5	501	1	69,73,73	1.17	7 (10%)	82,113,113	1.09	3 (3%)
18	PQN	B	2002	-	34,34,34	0.48	0	43,45,45	0.75	1 (2%)
13	CLA	3	505	1	69,73,73	1.15	6 (8%)	82,113,113	1.16	8 (9%)
13	CLA	B	1239	3	69,73,73	1.16	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	A	1105	2	55,59,73	1.29	7 (12%)	64,96,113	1.29	6 (9%)
13	CLA	4	508	1	59,63,73	1.25	7 (11%)	70,101,113	1.19	4 (5%)
13	CLA	c	506	1	49,53,73	1.39	5 (10%)	58,89,113	1.29	4 (6%)
13	CLA	2	501	1	69,73,73	1.17	8 (11%)	82,113,113	1.11	5 (6%)
14	BCR	I	4020	-	41,41,41	0.75	1 (2%)	56,56,56	2.13	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1201	3	61,65,73	1.22	7 (11%)	72,103,113	1.17	7 (9%)
13	CLA	g	503	1	67,71,73	1.20	6 (8%)	79,110,113	1.16	6 (7%)
13	CLA	B	1204	-	64,68,73	1.21	7 (10%)	76,107,113	1.19	3 (3%)
13	CLA	a	503	1	67,71,73	1.20	7 (10%)	79,110,113	1.16	5 (6%)
17	LHG	A	5005	-	44,44,48	0.97	2 (4%)	47,50,54	1.07	3 (6%)
13	CLA	K	1401	-	59,63,73	1.27	8 (13%)	70,101,113	1.20	6 (8%)
14	BCR	a	524	-	41,41,41	0.71	0	56,56,56	2.08	18 (32%)
13	CLA	d	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.18	5 (7%)
13	CLA	A	1129	2	54,58,73	1.28	8 (14%)	64,95,113	1.21	6 (9%)
13	CLA	A	1113	2	53,57,73	1.28	7 (13%)	61,93,113	1.30	6 (9%)
13	CLA	6	504	-	49,53,73	1.39	6 (12%)	58,89,113	1.24	5 (8%)
13	CLA	e	508	1	59,63,73	1.25	8 (13%)	70,101,113	1.20	5 (7%)
13	CLA	f	502	1	64,68,73	1.21	8 (12%)	76,107,113	1.27	6 (7%)
14	BCR	e	524	-	41,41,41	0.70	0	56,56,56	2.21	17 (30%)
13	CLA	d	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.15	3 (5%)
13	CLA	d	504	-	59,63,73	1.25	7 (11%)	70,101,113	1.18	5 (7%)
13	CLA	f	504	-	59,63,73	1.27	6 (10%)	70,101,113	1.13	3 (4%)
13	CLA	f	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	c	503	1	67,71,73	1.19	6 (8%)	79,110,113	1.12	4 (5%)
13	CLA	e	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.24	5 (7%)
14	BCR	c	524	-	41,41,41	0.70	0	56,56,56	2.18	18 (32%)
14	BCR	g	523	-	41,41,41	0.69	0	56,56,56	2.13	16 (28%)
17	LHG	A	5002	-	40,40,48	0.99	2 (5%)	43,46,54	1.14	4 (9%)
13	CLA	c	508	1	59,63,73	1.24	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	1	507	-	64,68,73	1.21	6 (9%)	76,107,113	1.14	4 (5%)
14	BCR	d	521	-	41,41,41	0.68	0	56,56,56	2.07	15 (26%)
13	CLA	1	519	-	49,53,73	1.40	5 (10%)	58,89,113	1.12	2 (3%)
13	CLA	1	503	1	67,71,73	1.18	6 (8%)	79,110,113	1.10	4 (5%)
13	CLA	2	512	1	56,60,73	1.29	7 (12%)	65,97,113	1.44	9 (13%)
13	CLA	1	508	1	59,63,73	1.26	7 (11%)	70,101,113	1.13	4 (5%)
13	CLA	4	507	-	64,68,73	1.21	6 (9%)	76,107,113	1.17	5 (6%)
13	CLA	b	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.22	4 (6%)
13	CLA	A	1136	2	69,73,73	1.15	8 (11%)	82,113,113	1.11	6 (7%)
13	CLA	c	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.14	5 (8%)
13	CLA	a	516	1	49,53,73	1.38	5 (10%)	58,89,113	1.25	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	512	1	56,60,73	1.31	7 (12%)	65,97,113	1.20	5 (7%)
13	CLA	5	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.23	6 (9%)
13	CLA	A	1115	-	64,68,73	1.21	7 (10%)	76,107,113	1.13	4 (5%)
13	CLA	A	1123	-	69,73,73	1.16	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	B	1228	3	59,63,73	1.23	8 (13%)	70,101,113	1.22	7 (10%)
15	SQD	b	822	-	29,31,54	1.49	3 (10%)	39,42,65	1.17	3 (7%)
13	CLA	1	513	1	54,58,73	1.33	8 (14%)	64,95,113	1.26	6 (9%)
13	CLA	e	516	1	49,53,73	1.39	6 (12%)	58,89,113	1.20	4 (6%)
13	CLA	A	1125	2	69,73,73	1.15	8 (11%)	82,113,113	1.23	6 (7%)
13	CLA	a	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.17	7 (8%)
13	CLA	B	1231	3	59,63,73	1.26	8 (13%)	70,101,113	1.18	6 (8%)
13	CLA	B	1220	3	54,58,73	1.29	8 (14%)	64,95,113	1.28	6 (9%)
13	CLA	g	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.19	5 (6%)
13	CLA	g	506	1	49,53,73	1.38	7 (14%)	58,89,113	1.24	5 (8%)
14	BCR	A	4007	-	41,41,41	0.72	1 (2%)	56,56,56	2.01	16 (28%)
13	CLA	4	513	1	54,58,73	1.32	8 (14%)	64,95,113	1.25	6 (9%)
13	CLA	g	504	-	59,63,73	1.28	6 (10%)	70,101,113	1.19	6 (8%)
13	CLA	d	509	1	69,73,73	1.17	6 (8%)	82,113,113	1.20	6 (7%)
13	CLA	c	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.14	5 (6%)
13	CLA	A	1118	2	64,68,73	1.20	7 (10%)	76,107,113	1.20	5 (6%)
13	CLA	2	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	f	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.22	5 (6%)
13	CLA	2	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.19	6 (8%)
13	CLA	b	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.20	4 (5%)
14	BCR	1	521	-	41,41,41	0.65	0	56,56,56	2.06	15 (26%)
13	CLA	f	510	1	69,73,73	1.18	5 (7%)	82,113,113	1.15	5 (6%)
13	CLA	A	1128	2	69,73,73	1.14	7 (10%)	82,113,113	1.13	6 (7%)
13	CLA	4	510	1	69,73,73	1.17	8 (11%)	82,113,113	1.25	10 (12%)
13	CLA	e	503	1	67,71,73	1.20	7 (10%)	79,110,113	1.14	4 (5%)
13	CLA	A	1133	2	69,73,73	1.16	8 (11%)	82,113,113	1.15	8 (9%)
13	CLA	b	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.15	4 (5%)
13	CLA	4	506	1	49,53,73	1.36	6 (12%)	58,89,113	1.26	4 (6%)
13	CLA	A	1112	2	51,55,73	1.32	8 (15%)	60,91,113	1.27	5 (8%)
13	CLA	1	505	1	69,73,73	1.17	7 (10%)	82,113,113	1.12	5 (6%)
14	BCR	4	521	-	41,41,41	0.66	0	56,56,56	2.05	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1202	3	69,73,73	1.14	8 (11%)	82,113,113	1.17	7 (8%)
13	CLA	B	1219	-	55,60,73	1.36	7 (12%)	57,93,113	1.35	7 (12%)
13	CLA	e	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.27	5 (7%)
13	CLA	d	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.30	5 (7%)
13	CLA	A	1121	2	55,59,73	1.29	6 (10%)	64,96,113	1.22	4 (6%)
13	CLA	B	1225	3	69,73,73	1.15	8 (11%)	82,113,113	1.15	6 (7%)
14	BCR	5	524	-	41,41,41	0.72	0	56,56,56	2.01	14 (25%)
15	SQD	B	1852	-	41,43,54	1.24	3 (7%)	51,54,65	1.12	4 (7%)
13	CLA	1	501	1	69,73,73	1.17	6 (8%)	82,113,113	1.09	5 (6%)
13	CLA	g	509	1	69,73,73	1.18	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	3	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.29	4 (6%)
13	CLA	A	1022	-	69,73,73	1.15	8 (11%)	82,113,113	1.12	5 (6%)
13	CLA	e	511	1	49,53,73	1.39	7 (14%)	58,89,113	1.31	6 (10%)
13	CLA	A	1127	2	69,73,73	1.15	8 (11%)	82,113,113	1.18	7 (8%)
13	CLA	B	1218	3	64,68,73	1.20	9 (14%)	76,107,113	1.15	5 (6%)
13	CLA	d	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.13	5 (6%)
14	BCR	f	521	-	41,41,41	0.66	0	56,56,56	1.78	12 (21%)
13	CLA	A	1102	13,2	69,73,73	1.15	8 (11%)	82,113,113	1.17	6 (7%)
13	CLA	A	1011	2	69,73,73	1.16	6 (8%)	82,113,113	1.16	7 (8%)
13	CLA	f	513	1	54,58,73	1.32	6 (11%)	64,95,113	1.32	8 (12%)
16	LMG	2	5104	-	40,40,55	1.06	2 (5%)	48,48,63	1.08	4 (8%)
13	CLA	K	1103	10	45,49,73	1.41	6 (13%)	54,83,113	1.19	2 (3%)
13	CLA	6	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.27	3 (5%)
13	CLA	f	508	1	59,63,73	1.27	8 (13%)	70,101,113	1.19	4 (5%)
13	CLA	B	1235	3	69,73,73	1.15	8 (11%)	82,113,113	1.17	6 (7%)
13	CLA	1	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.17	5 (7%)
13	CLA	A	1013	-	69,73,73	1.15	7 (10%)	82,113,113	1.17	7 (8%)
13	CLA	B	1021	3	69,73,73	1.15	6 (8%)	82,113,113	1.13	7 (8%)
13	CLA	d	510	1	69,73,73	1.18	7 (10%)	82,113,113	1.16	6 (7%)
13	CLA	d	516	1	49,53,73	1.39	6 (12%)	58,89,113	1.21	4 (6%)
13	CLA	b	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.22	3 (4%)
14	BCR	B	4005	-	41,41,41	0.74	0	56,56,56	2.01	15 (26%)
13	CLA	a	511	1	49,53,73	1.39	7 (14%)	58,89,113	1.25	4 (6%)
13	CLA	A	1106	2	69,73,73	1.13	7 (10%)	82,113,113	1.19	6 (7%)
13	CLA	g	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.26	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	e	509	1	69,73,73	1.18	6 (8%)	82,113,113	1.20	6 (7%)
13	CLA	5	506	1	49,53,73	1.38	6 (12%)	58,89,113	1.27	4 (6%)
13	CLA	a	504	-	59,63,73	1.27	8 (13%)	70,101,113	1.18	5 (7%)
13	CLA	5	517	-	49,53,73	1.39	6 (12%)	58,89,113	1.18	4 (6%)
13	CLA	B	1229	3	69,73,73	1.17	8 (11%)	82,113,113	1.17	7 (8%)
13	CLA	B	1215	3	64,68,73	1.19	8 (12%)	76,107,113	1.24	4 (5%)
13	CLA	B	1232	-	49,53,73	1.39	7 (14%)	58,89,113	1.27	5 (8%)
13	CLA	J	1302	9	49,53,73	1.35	7 (14%)	58,89,113	1.27	5 (8%)
14	BCR	5	523	-	41,41,41	0.96	2 (4%)	56,56,56	2.61	22 (39%)
13	CLA	a	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.25	5 (6%)
14	BCR	g	521	-	41,41,41	0.65	0	56,56,56	2.13	15 (26%)
14	BCR	3	522	-	41,41,41	0.72	1 (2%)	56,56,56	2.12	18 (32%)
13	CLA	a	518	1	49,53,73	1.39	6 (12%)	58,89,113	1.33	3 (5%)
13	CLA	3	501	1	69,73,73	1.16	6 (8%)	82,113,113	1.17	6 (7%)
13	CLA	A	1107	2	69,73,73	1.15	6 (8%)	82,113,113	1.16	7 (8%)
13	CLA	6	503	1	68,72,73	1.18	6 (8%)	80,111,113	1.14	5 (6%)
13	CLA	F	1301	-	49,53,73	1.37	8 (16%)	58,89,113	1.32	6 (10%)
15	SQD	e	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.18	2 (5%)
13	CLA	6	517	-	49,53,73	1.41	7 (14%)	58,89,113	1.18	5 (8%)
14	BCR	2	523	-	41,41,41	0.72	1 (2%)	56,56,56	1.91	17 (30%)
14	BCR	f	524	-	41,41,41	0.67	0	56,56,56	2.28	15 (26%)
13	CLA	b	501	1	69,73,73	1.18	8 (11%)	82,113,113	1.11	4 (4%)
13	CLA	1	516	1	49,53,73	1.40	6 (12%)	58,89,113	1.23	3 (5%)
13	CLA	c	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	4	511	1	49,53,73	1.44	8 (16%)	58,89,113	1.34	7 (12%)
13	CLA	A	1801	17	49,53,73	1.39	7 (14%)	58,89,113	1.26	3 (5%)
13	CLA	B	1221	3	64,68,73	1.17	7 (10%)	76,107,113	1.20	7 (9%)
13	CLA	c	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.23	6 (7%)
13	CLA	g	519	1	49,53,73	1.38	5 (10%)	58,89,113	1.24	4 (6%)
13	CLA	A	1139	-	64,68,73	1.20	8 (12%)	76,107,113	1.11	5 (6%)
14	BCR	b	524	-	41,41,41	0.73	1 (2%)	56,56,56	2.10	18 (32%)
13	CLA	b	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.21	6 (8%)
14	BCR	2	524	-	41,41,41	0.69	0	56,56,56	2.01	16 (28%)
14	BCR	B	4017	-	41,41,41	0.74	0	56,56,56	2.18	17 (30%)
13	CLA	6	518	1	54,58,73	1.32	7 (12%)	64,95,113	1.21	5 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	4	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	3	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.27	7 (10%)
13	CLA	6	513	1	54,58,73	1.32	6 (11%)	64,95,113	1.23	5 (7%)
13	CLA	5	504	-	59,63,73	1.26	7 (11%)	70,101,113	1.18	4 (5%)
14	BCR	I	4018	-	41,41,41	0.79	2 (4%)	56,56,56	2.14	15 (26%)
13	CLA	B	1207	-	69,73,73	1.18	6 (8%)	82,113,113	1.20	5 (6%)
13	CLA	f	503	1	67,71,73	1.21	7 (10%)	79,110,113	1.09	4 (5%)
13	CLA	a	507	-	64,68,73	1.22	7 (10%)	76,107,113	1.13	4 (5%)
13	CLA	c	516	1	49,53,73	1.36	6 (12%)	58,89,113	1.22	4 (6%)
13	CLA	B	1234	3	64,68,73	1.19	9 (14%)	76,107,113	1.24	8 (10%)
13	CLA	B	1012	-	69,73,73	1.15	8 (11%)	82,113,113	1.23	8 (9%)
15	SQD	d	822	-	29,31,54	1.51	3 (10%)	39,42,65	1.24	4 (10%)
13	CLA	A	1134	2	59,63,73	1.23	6 (10%)	70,101,113	1.21	6 (8%)
13	CLA	f	511	1	59,63,73	1.28	7 (11%)	70,101,113	1.24	7 (10%)
19	SF4	C	3002	4	0,12,12	-	-	-	-	-
15	SQD	3	822	-	29,31,54	1.48	3 (10%)	39,42,65	1.14	3 (7%)
13	CLA	2	510	1	69,73,73	1.17	7 (10%)	82,113,113	1.17	4 (4%)
13	CLA	2	516	1	49,53,73	1.38	7 (14%)	58,89,113	1.21	4 (6%)
13	CLA	e	517	-	49,53,73	1.39	7 (14%)	58,89,113	1.12	3 (5%)
17	LHG	A	5003	13	40,40,48	1.01	2 (5%)	43,46,54	1.05	3 (6%)
14	BCR	B	4010	-	41,41,41	0.77	1 (2%)	56,56,56	2.12	18 (32%)
14	BCR	5	522	-	41,41,41	0.69	0	56,56,56	2.16	17 (30%)
13	CLA	g	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.17	5 (7%)
13	CLA	c	510	1	69,73,73	1.16	6 (8%)	82,113,113	1.16	5 (6%)
13	CLA	g	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.10	6 (7%)
13	CLA	b	504	-	59,63,73	1.27	7 (11%)	70,101,113	1.17	3 (4%)
13	CLA	4	512	1	49,53,73	1.40	8 (16%)	58,89,113	1.28	4 (6%)
13	CLA	6	512	1	49,53,73	1.39	7 (14%)	58,89,113	1.28	4 (6%)
13	CLA	2	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.19	6 (8%)
14	BCR	3	524	-	41,41,41	0.66	0	56,56,56	2.03	16 (28%)
13	CLA	6	510	1	69,73,73	1.18	6 (8%)	82,113,113	1.19	6 (7%)
14	BCR	2	522	-	41,41,41	0.71	0	56,56,56	2.04	19 (33%)
16	LMG	J	5104	-	31,31,55	1.17	2 (6%)	39,39,63	1.16	4 (10%)
13	CLA	A	1116	2	64,68,73	1.21	8 (12%)	76,107,113	1.22	6 (7%)
13	CLA	5	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
14	BCR	c	523	-	41,41,41	0.69	0	56,56,56	1.88	19 (33%)
13	CLA	A	1140	2	69,73,73	1.15	7 (10%)	82,113,113	1.19	8 (9%)
13	CLA	d	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.12	4 (5%)
17	LHG	A	5004	-	34,34,48	1.09	2 (5%)	37,40,54	1.15	5 (13%)
14	BCR	d	522	-	41,41,41	0.67	0	56,56,56	2.20	19 (33%)
14	BCR	e	521	-	41,41,41	0.64	0	56,56,56	2.04	13 (23%)
13	CLA	3	513	1	54,58,73	1.31	8 (14%)	64,95,113	1.24	5 (7%)
15	SQD	2	822	-	29,31,54	1.45	3 (10%)	39,42,65	1.30	5 (12%)
13	CLA	B	1213	3	69,73,73	1.14	8 (11%)	82,113,113	1.14	6 (7%)
13	CLA	d	508	1	59,63,73	1.25	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	4	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.20	5 (6%)
13	CLA	6	509	1	69,73,73	1.17	8 (11%)	82,113,113	1.09	5 (6%)
13	CLA	1	517	-	49,53,73	1.40	6 (12%)	58,89,113	1.25	3 (5%)
13	CLA	B	1205	3	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
14	BCR	b	523	-	41,41,41	0.68	0	56,56,56	2.03	13 (23%)
13	CLA	f	509	1	69,73,73	1.18	7 (10%)	82,113,113	1.16	5 (6%)
20	LMU	J	5105	-	22,22,36	1.10	1 (4%)	27,27,47	0.83	1 (3%)
13	CLA	B	1227	3	56,60,73	1.28	7 (12%)	65,97,113	1.21	6 (9%)
13	CLA	e	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.24	3 (5%)
13	CLA	6	501	1	69,73,73	1.16	8 (11%)	82,113,113	1.13	5 (6%)
14	BCR	1	522	-	41,41,41	0.67	0	56,56,56	1.98	18 (32%)
13	CLA	c	518	1	59,63,73	1.26	6 (10%)	70,101,113	1.29	7 (10%)
13	CLA	B	1208	3	59,63,73	1.23	6 (10%)	70,101,113	1.19	6 (8%)
13	CLA	A	1138	2	69,73,73	1.14	7 (10%)	82,113,113	1.16	6 (7%)
16	LMG	1	5104	-	40,40,55	1.05	2 (5%)	48,48,63	1.03	2 (4%)
13	CLA	g	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.15	5 (6%)
13	CLA	J	1303	9	41,50,73	2.04	10 (24%)	44,79,113	1.39	7 (15%)
13	CLA	a	506	1	49,53,73	1.37	7 (14%)	58,89,113	1.27	5 (8%)
13	CLA	d	507	-	64,68,73	1.23	6 (9%)	76,107,113	1.16	4 (5%)
13	CLA	2	504	-	49,53,73	1.39	7 (14%)	58,89,113	1.25	3 (5%)
14	BCR	a	523	-	41,41,41	0.71	1 (2%)	56,56,56	2.20	20 (35%)
13	CLA	1	510	1	69,73,73	1.19	7 (10%)	82,113,113	1.15	5 (6%)
15	SQD	g	822	-	29,31,54	1.47	3 (10%)	39,42,65	1.22	2 (5%)
13	CLA	B	1209	3	56,60,73	1.28	7 (12%)	65,97,113	1.27	7 (10%)
14	BCR	e	523	-	41,41,41	0.67	0	56,56,56	2.02	19 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	B	1224	3	64,68,73	1.18	7 (10%)	76,107,113	1.25	7 (9%)
13	CLA	6	505	1	69,73,73	1.16	7 (10%)	82,113,113	1.12	5 (6%)
13	CLA	6	506	1	49,53,73	1.38	7 (14%)	58,89,113	1.28	4 (6%)
13	CLA	B	1223	3	69,73,73	1.14	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	b	508	1	59,63,73	1.27	8 (13%)	70,101,113	1.15	3 (4%)
13	CLA	4	517	-	49,53,73	1.38	5 (10%)	58,89,113	1.18	3 (5%)
13	CLA	5	516	1	49,53,73	1.39	7 (14%)	58,89,113	1.18	4 (6%)
13	CLA	A	1111	2	64,68,73	1.20	7 (10%)	76,107,113	1.26	7 (9%)
17	LHG	A	5001	-	48,48,48	0.91	2 (4%)	51,54,54	1.11	4 (7%)
14	BCR	F	4014	-	41,41,41	0.76	1 (2%)	56,56,56	2.20	15 (26%)
13	CLA	f	517	-	49,53,73	1.38	7 (14%)	58,89,113	1.17	4 (6%)
15	SQD	c	822	-	29,31,54	1.49	3 (10%)	39,42,65	1.16	3 (7%)
13	CLA	3	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.22	3 (5%)
13	CLA	A	1110	2	58,62,73	1.27	8 (13%)	68,99,113	1.19	4 (5%)
19	SF4	C	3003	4	0,12,12	-	-	-	-	-
15	SQD	4	822	-	29,31,54	1.46	3 (10%)	39,42,65	1.15	3 (7%)
15	SQD	6	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.29	3 (7%)
13	CLA	e	501	1	69,73,73	1.18	7 (10%)	82,113,113	1.12	6 (7%)
13	CLA	e	513	1	54,58,73	1.31	7 (12%)	64,95,113	1.22	7 (10%)
14	BCR	3	523	-	41,41,41	0.71	0	56,56,56	1.91	15 (26%)
13	CLA	a	513	1	54,58,73	1.35	8 (14%)	64,95,113	1.26	5 (7%)
13	CLA	A	1237	-	69,73,73	1.17	8 (11%)	82,113,113	1.16	6 (7%)
13	CLA	A	1119	-	69,73,73	1.14	7 (10%)	82,113,113	1.16	7 (8%)
13	CLA	f	506	1	49,53,73	1.39	7 (14%)	58,89,113	1.30	5 (8%)
13	CLA	B	1226	3	69,73,73	1.15	7 (10%)	82,113,113	1.20	5 (6%)
13	CLA	2	513	1	49,53,73	1.38	8 (16%)	58,89,113	1.26	4 (6%)
14	BCR	a	521	-	41,41,41	0.66	0	56,56,56	2.11	14 (25%)
13	CLA	5	518	1	59,63,73	1.26	6 (10%)	70,101,113	1.19	4 (5%)
13	CLA	d	503	1	67,71,73	1.19	7 (10%)	79,110,113	1.17	6 (7%)
13	CLA	A	1126	2	69,73,73	1.15	7 (10%)	82,113,113	1.28	7 (8%)
13	CLA	d	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.28	3 (5%)
13	CLA	B	1210	3	69,73,73	1.15	7 (10%)	82,113,113	1.22	6 (7%)
13	CLA	5	505	1	69,73,73	1.16	5 (7%)	82,113,113	1.15	7 (8%)
13	CLA	b	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.19	4 (5%)
13	CLA	3	510	1	69,73,73	1.17	8 (11%)	82,113,113	1.21	7 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	508	1	59,63,73	1.26	7 (11%)	70,101,113	1.18	4 (5%)
13	CLA	e	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.13	6 (7%)
13	CLA	a	505	1	69,73,73	1.18	6 (8%)	82,113,113	1.13	4 (4%)
14	BCR	M	4021	-	41,41,41	0.66	0	56,56,56	2.09	17 (30%)
16	LMG	g	5104	-	40,40,55	1.06	2 (5%)	48,48,63	1.05	3 (6%)
13	CLA	4	501	1	69,73,73	1.17	8 (11%)	82,113,113	1.12	6 (7%)
14	BCR	4	523	-	41,41,41	0.68	0	56,56,56	1.99	16 (28%)
13	CLA	X	1401	12	49,53,73	1.38	8 (16%)	58,89,113	1.29	5 (8%)
13	CLA	6	508	1	59,63,73	1.25	7 (11%)	70,101,113	1.16	3 (4%)
13	CLA	A	1124	-	64,68,73	1.19	7 (10%)	76,107,113	1.19	7 (9%)
15	SQD	f	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.13	3 (7%)
13	CLA	c	519	1	49,53,73	1.39	8 (16%)	58,89,113	1.23	4 (6%)
14	BCR	1	524	-	41,41,41	0.70	0	56,56,56	2.23	16 (28%)
18	PQN	A	2001	-	34,34,34	0.42	0	43,45,45	0.64	1 (2%)
13	CLA	3	504	-	59,63,73	1.26	8 (13%)	70,101,113	1.15	4 (5%)
13	CLA	1	506	1	49,53,73	1.37	6 (12%)	58,89,113	1.26	4 (6%)
14	BCR	J	4013	-	41,41,41	0.75	1 (2%)	56,56,56	2.21	16 (28%)
13	CLA	b	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.22	9 (10%)
13	CLA	A	1131	2	69,73,73	1.15	6 (8%)	82,113,113	1.18	6 (7%)
13	CLA	c	504	-	54,58,73	1.31	6 (11%)	64,95,113	1.24	5 (7%)
13	CLA	B	1023	-	69,73,73	1.15	7 (10%)	82,113,113	1.18	8 (9%)
14	BCR	b	521	-	41,41,41	0.67	0	56,56,56	2.05	16 (28%)
13	CLA	g	516	1	49,53,73	1.39	5 (10%)	58,89,113	1.19	5 (8%)
13	CLA	4	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.21	5 (6%)
13	CLA	B	1206	3	69,73,73	1.15	8 (11%)	82,113,113	1.23	5 (6%)
13	CLA	B	1212	3	49,53,73	1.35	7 (14%)	58,89,113	1.26	4 (6%)
19	SF4	A	3001	3,2	0,12,12	-	-	-	-	-
13	CLA	4	504	-	49,53,73	1.38	7 (14%)	58,89,113	1.22	3 (5%)
13	CLA	A	1104	2	69,73,73	1.14	8 (11%)	82,113,113	1.21	7 (8%)
13	CLA	4	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.16	6 (8%)
13	CLA	B	1236	3	54,58,73	1.28	7 (12%)	64,95,113	1.33	7 (10%)
13	CLA	6	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.21	3 (5%)
13	CLA	3	506	1	49,53,73	1.37	7 (14%)	58,89,113	1.30	7 (12%)
13	CLA	A	1108	2	49,53,73	1.34	6 (12%)	58,89,113	1.26	3 (5%)
13	CLA	b	517	-	49,53,73	1.42	7 (14%)	58,89,113	1.11	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	f	501	1	69,73,73	1.19	7 (10%)	82,113,113	1.11	6 (7%)
14	BCR	d	523	-	41,41,41	0.70	0	56,56,56	1.96	12 (21%)
13	CLA	3	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.20	6 (7%)
13	CLA	4	516	1	49,53,73	1.38	7 (14%)	58,89,113	1.24	4 (6%)
13	CLA	2	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.16	5 (7%)
13	CLA	3	507	-	64,68,73	1.21	8 (12%)	76,107,113	1.20	4 (5%)
13	CLA	2	503	1	68,72,73	1.18	8 (11%)	80,111,113	1.17	5 (6%)
13	CLA	3	512	1	56,60,73	1.30	7 (12%)	65,97,113	1.24	6 (9%)
13	CLA	b	519	1	49,53,73	1.38	7 (14%)	58,89,113	1.28	5 (8%)
13	CLA	g	510	1	69,73,73	1.17	6 (8%)	82,113,113	1.13	3 (3%)
14	BCR	f	522	-	41,41,41	0.73	0	56,56,56	2.20	15 (26%)
13	CLA	5	509	1	69,73,73	1.17	8 (11%)	82,113,113	1.20	4 (4%)
14	BCR	4	522	-	41,41,41	0.68	0	56,56,56	2.05	18 (32%)
13	CLA	a	519	-	49,53,73	1.39	6 (12%)	58,89,113	1.26	3 (5%)
13	CLA	f	505	1	69,73,73	1.16	8 (11%)	82,113,113	1.22	6 (7%)
13	CLA	A	1132	2	69,73,73	1.16	5 (7%)	82,113,113	1.16	5 (6%)
13	CLA	3	509	1	69,73,73	1.17	7 (10%)	82,113,113	1.23	6 (7%)
13	CLA	B	1222	-	64,68,73	1.19	8 (12%)	76,107,113	1.21	8 (10%)
13	CLA	d	513	1	54,58,73	1.31	8 (14%)	64,95,113	1.24	5 (7%)
20	LMU	A	1848	-	24,24,36	1.05	1 (4%)	29,29,47	0.78	0
13	CLA	B	1203	3	69,73,73	1.15	9 (13%)	82,113,113	1.19	4 (4%)
13	CLA	1	512	1	56,60,73	1.28	6 (10%)	65,97,113	1.42	6 (9%)
13	CLA	6	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.17	5 (6%)
13	CLA	2	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.22	6 (7%)
14	BCR	1	523	-	41,41,41	0.72	1 (2%)	56,56,56	1.93	16 (28%)
13	CLA	A	1135	2	55,59,73	1.28	7 (12%)	64,96,113	1.27	6 (9%)
13	CLA	A	1114	-	49,53,73	1.37	6 (12%)	58,89,113	1.36	3 (5%)
14	BCR	J	4012	-	41,41,41	0.75	0	56,56,56	2.14	18 (32%)
13	CLA	A	1122	2	64,68,73	1.19	8 (12%)	76,107,113	1.18	6 (7%)
20	LMU	B	1843	-	36,36,36	1.16	2 (5%)	47,47,47	0.96	1 (2%)
13	CLA	B	1238	-	69,73,73	1.14	7 (10%)	82,113,113	1.11	4 (4%)
14	BCR	B	4004	-	41,41,41	0.68	0	56,56,56	2.07	17 (30%)
14	BCR	3	521	-	41,41,41	0.68	0	56,56,56	1.96	11 (19%)
13	CLA	c	513	1	54,58,73	1.32	7 (12%)	64,95,113	1.22	6 (9%)
13	CLA	d	505	1	69,73,73	1.16	6 (8%)	82,113,113	1.14	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	LMU	A	1849	-	23,23,36	1.08	1 (4%)	28,28,47	0.80	0
13	CLA	B	1214	3	69,73,73	1.15	8 (11%)	82,113,113	1.18	6 (7%)
13	CLA	A	1117	2	69,73,73	1.17	7 (10%)	82,113,113	1.19	7 (8%)
14	BCR	g	522	-	41,41,41	0.68	0	56,56,56	2.16	15 (26%)
13	CLA	1	502	1	64,68,73	1.21	7 (10%)	76,107,113	1.15	5 (6%)
13	CLA	1	518	1	59,63,73	1.28	7 (11%)	70,101,113	1.14	4 (5%)
13	CLA	A	1137	2	59,63,73	1.23	7 (11%)	70,101,113	1.24	7 (10%)
13	CLA	A	1120	2	57,61,73	1.28	8 (14%)	67,98,113	1.20	4 (5%)
13	CLA	2	506	1	49,53,73	1.39	8 (16%)	58,89,113	1.27	4 (6%)
13	CLA	3	503	1	67,71,73	1.18	7 (10%)	79,110,113	1.21	7 (8%)
13	CLA	f	512	1	49,53,73	1.39	6 (12%)	58,89,113	1.29	3 (5%)
13	CLA	3	517	-	49,53,73	1.39	8 (16%)	58,89,113	1.30	4 (6%)
14	BCR	6	521	-	41,41,41	0.67	0	56,56,56	2.14	16 (28%)
14	BCR	I	4019	-	41,41,41	0.71	0	56,56,56	1.84	10 (17%)
14	BCR	c	521	-	41,41,41	0.65	0	56,56,56	1.98	15 (26%)
14	BCR	b	522	-	41,41,41	0.70	0	56,56,56	2.03	17 (30%)
14	BCR	B	4009	-	41,41,41	0.73	0	56,56,56	2.14	20 (35%)
13	CLA	5	510	1	69,73,73	1.17	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	c	505	1	69,73,73	1.18	7 (10%)	82,113,113	1.18	6 (7%)
13	CLA	4	519	1	54,58,73	1.30	7 (12%)	64,95,113	1.26	7 (10%)
13	CLA	b	513	1	54,58,73	1.31	7 (12%)	64,95,113	1.26	6 (9%)
13	CLA	d	502	1	64,68,73	1.22	7 (10%)	76,107,113	1.17	5 (6%)
13	CLA	f	519	1	49,53,73	1.39	7 (14%)	58,89,113	1.24	5 (8%)
14	BCR	A	4002	-	41,41,41	0.77	1 (2%)	56,56,56	2.13	14 (25%)
15	SQD	a	822	-	29,31,54	1.50	3 (10%)	39,42,65	1.12	2 (5%)
13	CLA	2	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.18	6 (7%)
14	BCR	F	4016	-	41,41,41	0.71	0	56,56,56	1.98	13 (23%)
13	CLA	c	501	1	69,73,73	1.17	7 (10%)	82,113,113	1.11	5 (6%)
13	CLA	3	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.15	5 (7%)
13	CLA	5	507	-	64,68,73	1.22	6 (9%)	76,107,113	1.15	5 (6%)
13	CLA	1	509	1	69,73,73	1.17	7 (10%)	82,113,113	1.18	5 (6%)
13	CLA	a	517	-	49,53,73	1.41	6 (12%)	58,89,113	1.19	3 (5%)
15	SQD	1	822	-	29,31,54	1.51	3 (10%)	39,42,65	1.12	4 (10%)
13	CLA	B	1217	3	59,63,73	1.26	7 (11%)	70,101,113	1.22	4 (5%)
13	CLA	A	1101	2	64,68,73	1.20	8 (12%)	76,107,113	1.23	6 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	a	501	1	69,73,73	1.17	6 (8%)	82,113,113	1.16	6 (7%)
13	CLA	2	509	1	69,73,73	1.16	7 (10%)	82,113,113	1.22	6 (7%)
14	BCR	6	523	-	41,41,41	0.67	0	56,56,56	2.05	15 (26%)
14	BCR	A	4008	-	41,41,41	0.78	1 (2%)	56,56,56	2.16	17 (30%)
13	CLA	b	505	1	69,73,73	1.18	8 (11%)	82,113,113	1.24	6 (7%)
14	BCR	A	4011	-	41,41,41	0.76	1 (2%)	56,56,56	2.19	16 (28%)
13	CLA	5	513	1	59,63,73	1.27	6 (10%)	70,101,113	1.17	5 (7%)
14	BCR	B	4006	-	41,41,41	0.73	0	56,56,56	2.15	15 (26%)
13	CLA	A	1130	2	59,63,73	1.24	7 (11%)	70,101,113	1.26	8 (11%)
14	BCR	4	524	-	41,41,41	0.69	0	56,56,56	2.20	16 (28%)
14	BCR	6	524	-	41,41,41	0.67	0	56,56,56	2.10	16 (28%)
13	CLA	c	511	1	59,63,73	1.27	7 (11%)	70,101,113	1.28	7 (10%)
13	CLA	3	518	1	59,63,73	1.26	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	g	507	-	64,68,73	1.23	7 (10%)	76,107,113	1.14	5 (6%)
13	CLA	f	516	1	49,53,73	1.38	6 (12%)	58,89,113	1.23	3 (5%)
14	BCR	2	521	-	41,41,41	0.67	0	56,56,56	2.07	17 (30%)
13	CLA	g	512	1	56,60,73	1.30	6 (10%)	65,97,113	1.22	4 (6%)
13	CLA	d	506	1	49,53,73	1.38	6 (12%)	58,89,113	1.27	4 (6%)
14	BCR	d	524	-	41,41,41	0.69	0	56,56,56	2.18	19 (33%)
13	CLA	B	1216	-	64,68,73	1.21	8 (12%)	76,107,113	1.17	6 (7%)
13	CLA	g	508	1	56,60,73	1.30	7 (12%)	65,97,113	1.20	3 (4%)
14	BCR	g	524	-	41,41,41	0.70	0	56,56,56	2.06	15 (26%)
13	CLA	5	519	1	54,58,73	1.32	7 (12%)	64,95,113	1.29	5 (7%)
13	CLA	5	503	1	68,72,73	1.18	6 (8%)	80,111,113	1.17	5 (6%)
14	BCR	a	522	-	41,41,41	0.71	1 (2%)	56,56,56	2.26	18 (32%)
13	CLA	e	510	1	69,73,73	1.18	6 (8%)	82,113,113	1.17	5 (6%)
14	BCR	5	521	-	41,41,41	0.69	0	56,56,56	2.01	14 (25%)
13	CLA	e	502	1	64,68,73	1.23	7 (10%)	76,107,113	1.28	4 (5%)
13	CLA	5	508	1	59,63,73	1.26	8 (13%)	70,101,113	1.16	5 (7%)
13	CLA	e	506	1	49,53,73	1.39	7 (14%)	58,89,113	1.29	5 (8%)
13	CLA	e	504	-	59,63,73	1.27	7 (11%)	70,101,113	1.21	5 (7%)
14	BCR	A	4003	-	41,41,41	0.75	1 (2%)	56,56,56	2.11	15 (26%)
14	BCR	e	522	-	41,41,41	0.70	0	56,56,56	2.06	16 (28%)
13	CLA	2	519	1	54,58,73	1.32	6 (11%)	64,95,113	1.24	4 (6%)
13	CLA	g	513	1	54,58,73	1.34	6 (11%)	64,95,113	1.26	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	CLA	2	517	-	49,53,73	1.39	8 (16%)	58,89,113	1.18	4 (6%)
13	CLA	B	1230	3	62,66,73	1.21	7 (11%)	73,104,113	1.21	5 (6%)
13	CLA	B	1233	-	49,53,73	1.38	7 (14%)	58,89,113	1.30	3 (5%)
13	CLA	4	503	1	68,72,73	1.18	7 (10%)	80,111,113	1.21	6 (7%)
15	SQD	5	822	-	29,31,54	1.47	3 (10%)	39,42,65	1.18	3 (7%)
14	BCR	F	4015	-	41,41,41	0.75	1 (2%)	56,56,56	2.10	17 (30%)
13	CLA	g	518	1	59,63,73	1.27	7 (11%)	70,101,113	1.20	5 (7%)
13	CLA	b	503	1	67,71,73	1.19	7 (10%)	79,110,113	1.16	4 (5%)
13	CLA	b	509	1	69,73,73	1.21	7 (10%)	82,113,113	1.21	5 (6%)
13	CLA	A	1109	13,2	69,73,73	1.14	7 (10%)	82,113,113	1.13	5 (6%)
13	CLA	6	511	1	49,53,73	1.40	7 (14%)	58,89,113	1.26	5 (8%)
13	CLA	e	507	-	64,68,73	1.21	7 (10%)	76,107,113	1.22	3 (3%)
14	BCR	c	522	-	41,41,41	0.71	0	56,56,56	2.31	18 (32%)
14	BCR	K	4001	-	41,41,41	0.72	0	56,56,56	1.93	16 (28%)
13	CLA	A	1103	2	69,73,73	1.15	7 (10%)	82,113,113	1.27	4 (4%)
14	BCR	6	522	-	41,41,41	0.70	0	56,56,56	2.22	16 (28%)
13	CLA	B	1211	3	69,73,73	1.17	8 (11%)	82,113,113	1.16	7 (8%)
13	CLA	b	506	1	49,53,73	1.49	9 (18%)	58,89,113	1.74	12 (20%)
16	LMG	6	5104	-	38,38,55	1.07	2 (5%)	46,46,63	1.09	3 (6%)
16	LMG	B	5002	-	55,55,55	0.88	2 (3%)	63,63,63	0.94	2 (3%)
13	CLA	c	512	1	49,53,73	1.40	7 (14%)	58,89,113	1.31	4 (6%)

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
13	CLA	1	504	-	1/1/13/20	15/27/103/115	-
14	BCR	f	523	-	-	3/29/63/63	0/2/2/2
13	CLA	5	511	1	1/1/13/20	10/27/103/115	-
13	CLA	a	509	1	1/1/15/20	11/39/115/115	-
13	CLA	6	502	1	1/1/14/20	12/33/109/115	-
13	CLA	5	501	1	1/1/15/20	11/39/115/115	-
18	PQN	B	2002	-	-	10/23/43/43	0/2/2/2
13	CLA	3	505	1	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1239	3	-	13/39/115/115	-
13	CLA	A	1105	2	1/1/12/20	2/23/99/115	-
13	CLA	4	508	1	1/1/13/20	4/27/103/115	-
13	CLA	c	506	1	1/1/11/20	4/15/91/115	-
13	CLA	2	501	1	1/1/15/20	13/39/115/115	-
14	BCR	I	4020	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1201	3	1/1/13/20	9/30/106/115	-
13	CLA	g	503	1	1/1/14/20	14/37/113/115	-
13	CLA	B	1204	-	1/1/14/20	4/33/109/115	-
13	CLA	a	503	1	1/1/14/20	10/37/113/115	-
17	LHG	A	5005	-	-	15/49/49/53	-
13	CLA	K	1401	-	1/1/13/20	8/27/103/115	-
14	BCR	a	524	-	-	3/29/63/63	0/2/2/2
13	CLA	d	511	1	1/1/13/20	12/27/103/115	-
13	CLA	A	1129	2	1/1/12/20	4/21/97/115	-
13	CLA	A	1113	2	1/1/11/20	6/20/96/115	-
13	CLA	6	504	-	1/1/11/20	4/15/91/115	-
13	CLA	e	508	1	1/1/13/20	5/27/103/115	-
13	CLA	f	502	1	1/1/14/20	11/33/109/115	-
14	BCR	e	524	-	-	3/29/63/63	0/2/2/2
13	CLA	d	517	-	1/1/11/20	6/15/91/115	-
13	CLA	d	504	-	1/1/13/20	9/27/103/115	-
13	CLA	f	504	-	1/1/13/20	11/27/103/115	-
13	CLA	f	518	1	1/1/13/20	15/27/103/115	-
13	CLA	c	503	1	1/1/14/20	13/37/113/115	-
13	CLA	e	518	1	1/1/13/20	15/27/103/115	-
14	BCR	c	524	-	-	4/29/63/63	0/2/2/2
14	BCR	g	523	-	-	4/29/63/63	0/2/2/2
17	LHG	A	5002	-	-	17/45/45/53	-
13	CLA	c	508	1	1/1/13/20	8/27/103/115	-
13	CLA	1	507	-	1/1/14/20	9/33/109/115	-
14	BCR	d	521	-	-	6/29/63/63	0/2/2/2
13	CLA	1	519	-	1/1/11/20	7/15/91/115	-
13	CLA	1	503	1	1/1/14/20	16/37/113/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	2	512	1	1/1/12/20	10/24/100/115	-
13	CLA	1	508	1	1/1/13/20	3/27/103/115	-
13	CLA	4	507	-	1/1/14/20	7/33/109/115	-
13	CLA	b	516	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1136	2	1/1/15/20	12/39/115/115	-
13	CLA	c	517	-	1/1/11/20	6/15/91/115	-
13	CLA	a	516	1	1/1/11/20	5/15/91/115	-
13	CLA	a	512	1	1/1/12/20	9/24/100/115	-
13	CLA	5	512	1	1/1/12/20	3/24/100/115	-
13	CLA	A	1115	-	1/1/14/20	18/33/109/115	-
13	CLA	A	1123	-	1/1/15/20	6/39/115/115	-
13	CLA	B	1228	3	1/1/13/20	6/27/103/115	-
15	SQD	b	822	-	-	6/26/46/69	0/1/1/1
13	CLA	1	513	1	1/1/12/20	8/21/97/115	-
13	CLA	e	516	1	1/1/11/20	9/15/91/115	-
13	CLA	A	1125	2	1/1/15/20	15/39/115/115	-
13	CLA	a	510	1	1/1/15/20	14/39/115/115	-
13	CLA	B	1231	3	1/1/13/20	12/27/103/115	-
13	CLA	B	1220	3	1/1/12/20	0/21/97/115	-
13	CLA	g	502	1	1/1/14/20	15/33/109/115	-
13	CLA	g	506	1	1/1/11/20	7/15/91/115	-
14	BCR	A	4007	-	-	2/29/63/63	0/2/2/2
13	CLA	4	513	1	1/1/12/20	2/21/97/115	-
13	CLA	g	504	-	1/1/13/20	8/27/103/115	-
13	CLA	d	509	1	1/1/15/20	8/39/115/115	-
13	CLA	c	507	-	1/1/14/20	10/33/109/115	-
13	CLA	A	1118	2	1/1/14/20	16/33/109/115	-
13	CLA	2	505	1	1/1/15/20	16/39/115/115	-
13	CLA	f	507	-	1/1/14/20	13/33/109/115	-
13	CLA	2	511	1	1/1/13/20	4/27/103/115	-
13	CLA	b	502	1	1/1/14/20	12/33/109/115	-
14	BCR	1	521	-	-	7/29/63/63	0/2/2/2
13	CLA	f	510	1	1/1/15/20	13/39/115/115	-
13	CLA	A	1128	2	1/1/15/20	6/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	4	510	1	1/1/15/20	16/39/115/115	-
13	CLA	e	503	1	1/1/14/20	11/37/113/115	-
13	CLA	A	1133	2	1/1/15/20	9/39/115/115	-
13	CLA	b	518	1	1/1/13/20	11/27/103/115	-
13	CLA	4	506	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1112	2	1/1/11/20	8/18/94/115	-
13	CLA	1	505	1	1/1/15/20	18/39/115/115	-
14	BCR	4	521	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1202	3	1/1/15/20	21/39/115/115	-
13	CLA	B	1219	-	1/1/13/20	8/28/95/115	-
13	CLA	e	512	1	1/1/12/20	7/24/100/115	-
13	CLA	d	512	1	1/1/12/20	6/24/100/115	-
13	CLA	A	1121	2	1/1/12/20	7/23/99/115	-
13	CLA	B	1225	3	1/1/15/20	12/39/115/115	-
14	BCR	5	524	-	-	7/29/63/63	0/2/2/2
15	SQD	B	1852	-	-	4/38/58/69	0/1/1/1
13	CLA	1	501	1	1/1/15/20	14/39/115/115	-
13	CLA	g	509	1	1/1/15/20	15/39/115/115	-
13	CLA	3	519	1	1/1/11/20	4/15/91/115	-
13	CLA	A	1022	-	1/1/15/20	11/39/115/115	-
13	CLA	e	511	1	1/1/11/20	5/15/91/115	-
13	CLA	A	1127	2	1/1/15/20	11/39/115/115	-
13	CLA	B	1218	3	1/1/14/20	14/33/109/115	-
13	CLA	d	501	1	1/1/15/20	13/39/115/115	-
14	BCR	f	521	-	-	6/29/63/63	0/2/2/2
13	CLA	A	1102	13,2	1/1/15/20	7/39/115/115	-
13	CLA	A	1011	2	1/1/15/20	12/39/115/115	-
13	CLA	f	513	1	1/1/12/20	3/21/97/115	-
16	LMG	2	5104	-	-	4/35/55/70	0/1/1/1
13	CLA	K	1103	10	1/1/9/20	6/9/81/115	-
13	CLA	6	519	1	1/1/11/20	5/15/91/115	-
13	CLA	f	508	1	1/1/13/20	3/27/103/115	-
13	CLA	B	1235	3	-	9/39/115/115	-
13	CLA	1	511	1	1/1/13/20	6/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1013	-	1/1/15/20	13/39/115/115	-
13	CLA	B	1021	3	1/1/15/20	17/39/115/115	-
13	CLA	d	510	1	1/1/15/20	9/39/115/115	-
13	CLA	d	516	1	1/1/11/20	6/15/91/115	-
13	CLA	b	512	1	1/1/12/20	12/24/100/115	-
14	BCR	B	4005	-	-	2/29/63/63	0/2/2/2
13	CLA	a	511	1	1/1/11/20	9/15/91/115	-
13	CLA	A	1106	2	1/1/15/20	20/39/115/115	-
13	CLA	g	517	-	1/1/11/20	8/15/91/115	-
13	CLA	e	509	1	1/1/15/20	9/39/115/115	-
13	CLA	5	506	1	1/1/11/20	6/15/91/115	-
13	CLA	a	504	-	1/1/13/20	6/27/103/115	-
13	CLA	5	517	-	1/1/11/20	6/15/91/115	-
13	CLA	B	1229	3	1/1/15/20	13/39/115/115	-
13	CLA	B	1215	3	1/1/14/20	7/33/109/115	-
13	CLA	B	1232	-	1/1/11/20	9/15/91/115	-
13	CLA	J	1302	9	1/1/11/20	6/15/91/115	-
14	BCR	5	523	-	-	12/29/63/63	0/2/2/2
13	CLA	a	502	1	1/1/14/20	9/33/109/115	-
14	BCR	g	521	-	-	4/29/63/63	0/2/2/2
14	BCR	3	522	-	-	2/29/63/63	0/2/2/2
13	CLA	a	518	1	1/1/11/20	4/15/91/115	-
13	CLA	3	501	1	1/1/15/20	10/39/115/115	-
13	CLA	A	1107	2	1/1/15/20	14/39/115/115	-
13	CLA	6	503	1	1/1/14/20	18/38/114/115	-
13	CLA	F	1301	-	1/1/11/20	6/15/91/115	-
15	SQD	e	822	-	-	4/26/46/69	0/1/1/1
13	CLA	6	517	-	1/1/11/20	8/15/91/115	-
14	BCR	2	523	-	-	2/29/63/63	0/2/2/2
14	BCR	f	524	-	-	4/29/63/63	0/2/2/2
13	CLA	b	501	1	1/1/15/20	9/39/115/115	-
13	CLA	1	516	1	1/1/11/20	6/15/91/115	-
13	CLA	c	509	1	1/1/15/20	10/39/115/115	-
13	CLA	4	511	1	-	3/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1801	17	1/1/11/20	8/15/91/115	-
13	CLA	B	1221	3	1/1/14/20	12/33/109/115	-
13	CLA	c	502	1	1/1/14/20	15/33/109/115	-
13	CLA	g	519	1	1/1/11/20	7/15/91/115	-
13	CLA	A	1139	-	1/1/14/20	12/33/109/115	-
14	BCR	b	524	-	-	6/29/63/63	0/2/2/2
13	CLA	b	511	1	1/1/13/20	3/27/103/115	-
14	BCR	2	524	-	-	3/29/63/63	0/2/2/2
14	BCR	B	4017	-	-	2/29/63/63	0/2/2/2
13	CLA	6	518	1	1/1/12/20	7/21/97/115	-
13	CLA	4	505	1	1/1/15/20	18/39/115/115	-
13	CLA	3	511	1	1/1/13/20	7/27/103/115	-
13	CLA	6	513	1	1/1/12/20	7/21/97/115	-
13	CLA	5	504	-	1/1/13/20	11/27/103/115	-
14	BCR	I	4018	-	-	6/29/63/63	0/2/2/2
13	CLA	B	1207	-	-	12/39/115/115	-
13	CLA	f	503	1	1/1/14/20	15/37/113/115	-
13	CLA	a	507	-	1/1/14/20	6/33/109/115	-
13	CLA	c	516	1	1/1/11/20	6/15/91/115	-
13	CLA	B	1234	3	1/1/14/20	7/33/109/115	-
13	CLA	B	1012	-	1/1/15/20	16/39/115/115	-
15	SQD	d	822	-	-	7/26/46/69	0/1/1/1
13	CLA	A	1134	2	1/1/13/20	11/27/103/115	-
13	CLA	f	511	1	1/1/13/20	6/27/103/115	-
19	SF4	C	3002	4	-	-	0/6/5/5
15	SQD	3	822	-	-	4/26/46/69	0/1/1/1
13	CLA	2	510	1	1/1/15/20	20/39/115/115	-
13	CLA	2	516	1	1/1/11/20	6/15/91/115	-
13	CLA	e	517	-	1/1/11/20	7/15/91/115	-
17	LHG	A	5003	13	-	10/45/45/53	-
14	BCR	B	4010	-	-	2/29/63/63	0/2/2/2
14	BCR	5	522	-	-	5/29/63/63	0/2/2/2
13	CLA	g	511	1	1/1/13/20	11/27/103/115	-
13	CLA	c	510	1	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	g	501	1	1/1/15/20	14/39/115/115	-
13	CLA	b	504	-	1/1/13/20	15/27/103/115	-
13	CLA	4	512	1	1/1/11/20	3/15/91/115	-
13	CLA	6	512	1	1/1/11/20	9/15/91/115	-
13	CLA	2	518	1	1/1/13/20	10/27/103/115	-
14	BCR	3	524	-	-	2/29/63/63	0/2/2/2
13	CLA	6	510	1	1/1/15/20	15/39/115/115	-
14	BCR	2	522	-	-	6/29/63/63	0/2/2/2
16	LMG	J	5104	-	-	5/26/46/70	0/1/1/1
13	CLA	A	1116	2	1/1/14/20	16/33/109/115	-
13	CLA	5	502	1	1/1/14/20	11/33/109/115	-
14	BCR	c	523	-	-	2/29/63/63	0/2/2/2
13	CLA	A	1140	2	1/1/15/20	10/39/115/115	-
13	CLA	d	518	1	1/1/13/20	9/27/103/115	-
17	LHG	A	5004	-	-	15/39/39/53	-
14	BCR	d	522	-	-	4/29/63/63	0/2/2/2
14	BCR	e	521	-	-	5/29/63/63	0/2/2/2
13	CLA	3	513	1	1/1/12/20	3/21/97/115	-
15	SQD	2	822	-	-	5/26/46/69	0/1/1/1
13	CLA	B	1213	3	1/1/15/20	15/39/115/115	-
13	CLA	d	508	1	1/1/13/20	5/27/103/115	-
13	CLA	4	509	1	1/1/15/20	7/39/115/115	-
13	CLA	6	509	1	1/1/15/20	15/39/115/115	-
13	CLA	1	517	-	1/1/11/20	8/15/91/115	-
13	CLA	B	1205	3	1/1/15/20	8/39/115/115	-
14	BCR	b	523	-	-	3/29/63/63	0/2/2/2
13	CLA	f	509	1	1/1/15/20	8/39/115/115	-
20	LMU	J	5105	-	-	8/13/33/61	0/1/1/2
13	CLA	B	1227	3	1/1/12/20	10/24/100/115	-
13	CLA	e	519	1	1/1/11/20	7/15/91/115	-
13	CLA	6	501	1	1/1/15/20	13/39/115/115	-
14	BCR	1	522	-	-	5/29/63/63	0/2/2/2
13	CLA	c	518	1	1/1/13/20	12/27/103/115	-
13	CLA	B	1208	3	1/1/13/20	0/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1138	2	1/1/15/20	13/39/115/115	-
16	LMG	1	5104	-	-	4/35/55/70	0/1/1/1
13	CLA	g	505	1	1/1/15/20	10/39/115/115	-
13	CLA	a	506	1	1/1/11/20	5/15/91/115	-
13	CLA	J	1303	9	-	10/27/77/115	-
13	CLA	d	507	-	1/1/14/20	4/33/109/115	-
13	CLA	2	504	-	1/1/11/20	5/15/91/115	-
14	BCR	a	523	-	-	5/29/63/63	0/2/2/2
13	CLA	1	510	1	1/1/15/20	10/39/115/115	-
15	SQD	g	822	-	-	7/26/46/69	0/1/1/1
13	CLA	B	1209	3	1/1/12/20	10/24/100/115	-
14	BCR	e	523	-	-	2/29/63/63	0/2/2/2
13	CLA	B	1224	3	1/1/14/20	14/33/109/115	-
13	CLA	6	505	1	1/1/15/20	18/39/115/115	-
13	CLA	6	506	1	1/1/11/20	5/15/91/115	-
13	CLA	B	1223	3	1/1/15/20	9/39/115/115	-
13	CLA	b	508	1	1/1/13/20	7/27/103/115	-
13	CLA	4	517	-	1/1/11/20	6/15/91/115	-
13	CLA	5	516	1	1/1/11/20	11/15/91/115	-
13	CLA	A	1111	2	1/1/14/20	10/33/109/115	-
17	LHG	A	5001	-	-	8/53/53/53	-
14	BCR	F	4014	-	-	6/29/63/63	0/2/2/2
13	CLA	f	517	-	1/1/11/20	7/15/91/115	-
15	SQD	c	822	-	-	4/26/46/69	0/1/1/1
13	CLA	3	516	1	1/1/11/20	8/15/91/115	-
13	CLA	A	1110	2	1/1/12/20	7/26/102/115	-
19	SF4	C	3003	4	-	-	0/6/5/5
15	SQD	4	822	-	-	5/26/46/69	0/1/1/1
15	SQD	6	822	-	-	8/26/46/69	0/1/1/1
13	CLA	e	501	1	1/1/15/20	13/39/115/115	-
13	CLA	e	513	1	1/1/12/20	3/21/97/115	-
14	BCR	3	523	-	-	9/29/63/63	0/2/2/2
13	CLA	a	513	1	-	7/21/97/115	-
13	CLA	A	1237	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	A	1119	-	1/1/15/20	12/39/115/115	-
13	CLA	f	506	1	-	2/15/91/115	-
13	CLA	B	1226	3	1/1/15/20	12/39/115/115	-
13	CLA	2	513	1	1/1/11/20	6/15/91/115	-
14	BCR	a	521	-	-	6/29/63/63	0/2/2/2
13	CLA	5	518	1	1/1/13/20	6/27/103/115	-
13	CLA	d	503	1	1/1/14/20	17/37/113/115	-
13	CLA	A	1126	2	1/1/15/20	20/39/115/115	-
13	CLA	d	519	1	1/1/11/20	5/15/91/115	-
13	CLA	B	1210	3	1/1/15/20	16/39/115/115	-
13	CLA	5	505	1	1/1/15/20	11/39/115/115	-
13	CLA	b	507	-	1/1/14/20	6/33/109/115	-
13	CLA	3	510	1	1/1/15/20	16/39/115/115	-
13	CLA	a	508	1	1/1/13/20	6/27/103/115	-
13	CLA	e	505	1	1/1/15/20	15/39/115/115	-
13	CLA	a	505	1	1/1/15/20	15/39/115/115	-
14	BCR	M	4021	-	-	7/29/63/63	0/2/2/2
16	LMG	g	5104	-	-	3/35/55/70	0/1/1/1
13	CLA	4	501	1	1/1/15/20	14/39/115/115	-
14	BCR	4	523	-	-	4/29/63/63	0/2/2/2
13	CLA	X	1401	12	1/1/11/20	3/15/91/115	-
13	CLA	6	508	1	1/1/13/20	8/27/103/115	-
13	CLA	A	1124	-	-	3/33/109/115	-
15	SQD	f	822	-	-	9/26/46/69	0/1/1/1
13	CLA	c	519	1	1/1/11/20	4/15/91/115	-
14	BCR	1	524	-	-	0/29/63/63	0/2/2/2
18	PQN	A	2001	-	-	10/23/43/43	0/2/2/2
13	CLA	3	504	-	1/1/13/20	6/27/103/115	-
13	CLA	1	506	1	1/1/11/20	7/15/91/115	-
14	BCR	J	4013	-	-	5/29/63/63	0/2/2/2
13	CLA	b	510	1	1/1/15/20	14/39/115/115	-
13	CLA	A	1131	2	1/1/15/20	9/39/115/115	-
13	CLA	c	504	-	1/1/12/20	6/21/97/115	-
13	CLA	B	1023	-	1/1/15/20	8/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	b	521	-	-	7/29/63/63	0/2/2/2
13	CLA	g	516	1	1/1/11/20	11/15/91/115	-
13	CLA	4	502	1	-	8/33/109/115	-
13	CLA	B	1206	3	1/1/15/20	13/39/115/115	-
13	CLA	B	1212	3	1/1/11/20	3/15/91/115	-
19	SF4	A	3001	3,2	-	-	0/6/5/5
13	CLA	4	504	-	1/1/11/20	2/15/91/115	-
13	CLA	A	1104	2	1/1/15/20	8/39/115/115	-
13	CLA	4	518	1	1/1/13/20	11/27/103/115	-
13	CLA	B	1236	3	1/1/12/20	3/21/97/115	-
13	CLA	6	516	1	1/1/11/20	9/15/91/115	-
13	CLA	3	506	1	1/1/11/20	4/15/91/115	-
13	CLA	A	1108	2	1/1/11/20	4/15/91/115	-
13	CLA	b	517	-	1/1/11/20	6/15/91/115	-
13	CLA	f	501	1	1/1/15/20	17/39/115/115	-
14	BCR	d	523	-	-	4/29/63/63	0/2/2/2
13	CLA	3	502	1	1/1/14/20	11/33/109/115	-
13	CLA	4	516	1	1/1/11/20	3/15/91/115	-
13	CLA	2	508	1	1/1/13/20	2/27/103/115	-
13	CLA	3	507	-	1/1/14/20	8/33/109/115	-
13	CLA	2	503	1	1/1/14/20	14/38/114/115	-
13	CLA	3	512	1	1/1/12/20	4/24/100/115	-
13	CLA	b	519	1	1/1/11/20	5/15/91/115	-
13	CLA	g	510	1	1/1/15/20	9/39/115/115	-
14	BCR	f	522	-	-	4/29/63/63	0/2/2/2
13	CLA	5	509	1	1/1/15/20	13/39/115/115	-
14	BCR	4	522	-	-	2/29/63/63	0/2/2/2
13	CLA	a	519	-	1/1/11/20	4/15/91/115	-
13	CLA	f	505	1	1/1/15/20	11/39/115/115	-
13	CLA	A	1132	2	1/1/15/20	12/39/115/115	-
13	CLA	3	509	1	1/1/15/20	11/39/115/115	-
13	CLA	B	1222	-	1/1/14/20	6/33/109/115	-
13	CLA	d	513	1	1/1/12/20	2/21/97/115	-
20	LMU	A	1848	-	-	11/15/35/61	0/1/1/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	B	1203	3	1/1/15/20	20/39/115/115	-
13	CLA	1	512	1	1/1/12/20	7/24/100/115	-
13	CLA	6	507	-	1/1/14/20	4/33/109/115	-
13	CLA	2	502	1	1/1/14/20	14/33/109/115	-
14	BCR	1	523	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1135	2	1/1/12/20	7/23/99/115	-
13	CLA	A	1114	-	1/1/11/20	4/15/91/115	-
14	BCR	J	4012	-	-	4/29/63/63	0/2/2/2
13	CLA	A	1122	2	1/1/14/20	8/33/109/115	-
20	LMU	B	1843	-	-	13/21/61/61	0/2/2/2
13	CLA	B	1238	-	1/1/15/20	12/39/115/115	-
14	BCR	B	4004	-	-	7/29/63/63	0/2/2/2
14	BCR	3	521	-	-	4/29/63/63	0/2/2/2
13	CLA	c	513	1	1/1/12/20	7/21/97/115	-
13	CLA	d	505	1	1/1/15/20	15/39/115/115	-
20	LMU	A	1849	-	-	11/14/34/61	0/1/1/2
13	CLA	B	1214	3	1/1/15/20	18/39/115/115	-
13	CLA	A	1117	2	1/1/15/20	12/39/115/115	-
14	BCR	g	522	-	-	4/29/63/63	0/2/2/2
13	CLA	1	502	1	1/1/14/20	12/33/109/115	-
13	CLA	1	518	1	1/1/13/20	15/27/103/115	-
13	CLA	A	1137	2	1/1/13/20	11/27/103/115	-
13	CLA	A	1120	2	1/1/12/20	7/25/101/115	-
13	CLA	2	506	1	1/1/11/20	6/15/91/115	-
13	CLA	3	503	1	1/1/14/20	10/37/113/115	-
13	CLA	f	512	1	1/1/11/20	10/15/91/115	-
13	CLA	3	517	-	1/1/11/20	5/15/91/115	-
14	BCR	6	521	-	-	4/29/63/63	0/2/2/2
14	BCR	I	4019	-	-	4/29/63/63	0/2/2/2
14	BCR	c	521	-	-	3/29/63/63	0/2/2/2
14	BCR	b	522	-	-	7/29/63/63	0/2/2/2
14	BCR	B	4009	-	-	6/29/63/63	0/2/2/2
13	CLA	5	510	1	1/1/15/20	13/39/115/115	-
13	CLA	c	505	1	1/1/15/20	10/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	CLA	4	519	1	1/1/12/20	7/21/97/115	-
13	CLA	b	513	1	1/1/12/20	6/21/97/115	-
13	CLA	d	502	1	1/1/14/20	13/33/109/115	-
13	CLA	f	519	1	1/1/11/20	8/15/91/115	-
14	BCR	A	4002	-	-	4/29/63/63	0/2/2/2
15	SQD	a	822	-	-	4/26/46/69	0/1/1/1
13	CLA	2	507	-	1/1/14/20	8/33/109/115	-
14	BCR	F	4016	-	-	2/29/63/63	0/2/2/2
13	CLA	c	501	1	1/1/15/20	11/39/115/115	-
13	CLA	3	508	1	1/1/13/20	5/27/103/115	-
13	CLA	5	507	-	1/1/14/20	11/33/109/115	-
13	CLA	1	509	1	1/1/15/20	10/39/115/115	-
13	CLA	a	517	-	1/1/11/20	8/15/91/115	-
15	SQD	1	822	-	-	5/26/46/69	0/1/1/1
13	CLA	B	1217	3	1/1/13/20	12/27/103/115	-
13	CLA	A	1101	2	1/1/14/20	10/33/109/115	-
13	CLA	a	501	1	1/1/15/20	11/39/115/115	-
13	CLA	2	509	1	1/1/15/20	11/39/115/115	-
14	BCR	6	523	-	-	2/29/63/63	0/2/2/2
14	BCR	A	4008	-	-	2/29/63/63	0/2/2/2
13	CLA	b	505	1	1/1/15/20	13/39/115/115	-
14	BCR	A	4011	-	-	8/29/63/63	0/2/2/2
13	CLA	5	513	1	1/1/13/20	3/27/103/115	-
14	BCR	B	4006	-	-	8/29/63/63	0/2/2/2
13	CLA	A	1130	2	1/1/13/20	5/27/103/115	-
14	BCR	4	524	-	-	4/29/63/63	0/2/2/2
14	BCR	6	524	-	-	3/29/63/63	0/2/2/2
13	CLA	c	511	1	1/1/13/20	6/27/103/115	-
13	CLA	3	518	1	1/1/13/20	11/27/103/115	-
13	CLA	g	507	-	1/1/14/20	7/33/109/115	-
13	CLA	f	516	1	1/1/11/20	7/15/91/115	-
14	BCR	2	521	-	-	6/29/63/63	0/2/2/2
13	CLA	g	512	1	1/1/12/20	3/24/100/115	-
13	CLA	d	506	1	1/1/11/20	9/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	BCR	d	524	-	-	7/29/63/63	0/2/2/2
13	CLA	B	1216	-	1/1/14/20	12/33/109/115	-
13	CLA	g	508	1	1/1/12/20	1/24/100/115	-
14	BCR	g	524	-	-	0/29/63/63	0/2/2/2
13	CLA	5	519	1	1/1/12/20	6/21/97/115	-
13	CLA	5	503	1	1/1/14/20	18/38/114/115	-
14	BCR	a	522	-	-	5/29/63/63	0/2/2/2
13	CLA	e	510	1	1/1/15/20	10/39/115/115	-
14	BCR	5	521	-	-	6/29/63/63	0/2/2/2
13	CLA	e	502	1	1/1/14/20	15/33/109/115	-
13	CLA	5	508	1	1/1/13/20	5/27/103/115	-
13	CLA	e	506	1	1/1/11/20	9/15/91/115	-
13	CLA	e	504	-	1/1/13/20	14/27/103/115	-
14	BCR	A	4003	-	-	4/29/63/63	0/2/2/2
14	BCR	e	522	-	-	4/29/63/63	0/2/2/2
13	CLA	2	519	1	1/1/12/20	5/21/97/115	-
13	CLA	g	513	1	1/1/12/20	5/21/97/115	-
13	CLA	2	517	-	1/1/11/20	10/15/91/115	-
13	CLA	B	1230	3	1/1/13/20	13/31/107/115	-
13	CLA	B	1233	-	1/1/11/20	0/15/91/115	-
13	CLA	4	503	1	1/1/14/20	10/38/114/115	-
15	SQD	5	822	-	-	5/26/46/69	0/1/1/1
14	BCR	F	4015	-	-	2/29/63/63	0/2/2/2
13	CLA	g	518	1	1/1/13/20	12/27/103/115	-
13	CLA	b	503	1	1/1/14/20	12/37/113/115	-
13	CLA	b	509	1	1/1/15/20	12/39/115/115	-
13	CLA	A	1109	13,2	1/1/15/20	11/39/115/115	-
13	CLA	6	511	1	1/1/11/20	5/15/91/115	-
13	CLA	e	507	-	1/1/14/20	7/33/109/115	-
14	BCR	c	522	-	-	2/29/63/63	0/2/2/2
14	BCR	K	4001	-	-	0/29/63/63	0/2/2/2
13	CLA	A	1103	2	1/1/15/20	16/39/115/115	-
14	BCR	6	522	-	-	5/29/63/63	0/2/2/2
13	CLA	B	1211	3	1/1/15/20	12/39/115/115	-
13	CLA	b	506	1	-	6/15/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	LMG	6	5104	-	-	4/33/53/70	0/1/1/1
16	LMG	B	5002	-	-	11/50/70/70	0/1/1/1
13	CLA	c	512	1	1/1/11/20	5/15/91/115	-

All (2268) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1303	CLA	CHD-C1D	6.88	1.38	1.33
13	J	1303	CLA	C4C-CHD	-6.22	1.40	1.50
15	d	822	SQD	O8-S	4.61	1.64	1.47
15	1	822	SQD	O8-S	4.47	1.64	1.47
15	6	822	SQD	O47-C7	4.46	1.46	1.34
15	B	1852	SQD	O8-S	4.46	1.64	1.47
15	f	822	SQD	O47-C7	4.45	1.46	1.34
15	b	822	SQD	O47-C7	4.44	1.46	1.34
15	6	822	SQD	O8-S	4.43	1.63	1.47
15	a	822	SQD	O8-S	4.43	1.63	1.47
15	4	822	SQD	O8-S	4.43	1.63	1.47
15	c	822	SQD	O8-S	4.42	1.63	1.47
15	d	822	SQD	O47-C7	4.42	1.46	1.34
15	b	822	SQD	O8-S	4.42	1.63	1.47
15	g	822	SQD	O8-S	4.42	1.63	1.47
15	c	822	SQD	O47-C7	4.42	1.46	1.34
15	e	822	SQD	O47-C7	4.42	1.46	1.34
15	1	822	SQD	O47-C7	4.42	1.46	1.34
15	3	822	SQD	O8-S	4.41	1.63	1.47
15	e	822	SQD	O8-S	4.41	1.63	1.47
15	f	822	SQD	O8-S	4.40	1.63	1.47
15	2	822	SQD	O8-S	4.40	1.63	1.47
15	a	822	SQD	O47-C7	4.40	1.46	1.34
15	5	822	SQD	O8-S	4.38	1.63	1.47
15	B	1852	SQD	O48-C23	4.33	1.46	1.33
16	g	5104	LMG	O8-C28	4.32	1.45	1.33
16	2	5104	LMG	O8-C28	4.32	1.45	1.33
15	3	822	SQD	O47-C7	4.32	1.46	1.34
15	e	822	SQD	O48-C23	4.29	1.45	1.33
15	6	822	SQD	O48-C23	4.28	1.45	1.33
15	1	822	SQD	O48-C23	4.27	1.45	1.33
15	f	822	SQD	O48-C23	4.26	1.45	1.33
16	6	5104	LMG	O8-C28	4.25	1.45	1.33
15	5	822	SQD	O47-C7	4.25	1.46	1.34
17	A	5005	LHG	O8-C23	4.24	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	g	822	SQD	O48-C23	4.24	1.45	1.33
15	a	822	SQD	O48-C23	4.23	1.45	1.33
16	J	5104	LMG	O8-C28	4.23	1.45	1.33
15	5	822	SQD	O48-C23	4.23	1.45	1.33
16	1	5104	LMG	O8-C28	4.22	1.45	1.33
15	c	822	SQD	O48-C23	4.22	1.45	1.33
15	b	822	SQD	O48-C23	4.21	1.45	1.33
15	3	822	SQD	O48-C23	4.21	1.45	1.33
15	d	822	SQD	O48-C23	4.20	1.45	1.33
15	4	822	SQD	O48-C23	4.19	1.45	1.33
15	2	822	SQD	O48-C23	4.19	1.45	1.33
17	A	5001	LHG	O8-C23	4.19	1.45	1.33
15	g	822	SQD	O47-C7	4.19	1.46	1.34
17	A	5003	LHG	O8-C23	4.17	1.45	1.33
16	B	5002	LMG	O8-C28	4.13	1.45	1.33
17	A	5004	LHG	O7-C7	4.12	1.45	1.34
16	g	5104	LMG	O7-C10	4.11	1.45	1.34
17	A	5002	LHG	O8-C23	4.10	1.45	1.33
16	2	5104	LMG	O7-C10	4.10	1.45	1.34
17	A	5004	LHG	O8-C23	4.10	1.45	1.33
16	1	5104	LMG	O7-C10	4.08	1.45	1.34
16	J	5104	LMG	O7-C10	4.07	1.45	1.34
16	6	5104	LMG	O7-C10	4.06	1.45	1.34
15	4	822	SQD	O47-C7	4.05	1.45	1.34
17	A	5005	LHG	O7-C7	4.00	1.45	1.34
17	A	5003	LHG	O7-C7	3.98	1.45	1.34
17	A	5002	LHG	O7-C7	3.97	1.45	1.34
13	b	517	CLA	C1D-ND	3.97	1.43	1.37
13	J	1303	CLA	CHC-C4B	-3.97	1.36	1.44
15	B	1852	SQD	O47-C7	3.95	1.45	1.34
15	2	822	SQD	O47-C7	3.93	1.45	1.34
13	B	1219	CLA	C1D-ND	3.91	1.43	1.37
16	B	5002	LMG	O7-C10	3.90	1.45	1.34
13	b	506	CLA	CMB-C2B	-3.90	1.42	1.50
13	c	517	CLA	C1D-ND	3.82	1.42	1.37
13	6	517	CLA	C1D-ND	3.80	1.42	1.37
13	d	517	CLA	C1D-ND	3.80	1.42	1.37
17	A	5001	LHG	O7-C7	3.79	1.45	1.34
13	e	517	CLA	C1D-ND	3.74	1.42	1.37
13	f	503	CLA	C1D-ND	3.73	1.42	1.37
13	a	509	CLA	C1D-ND	3.73	1.42	1.37
13	g	516	CLA	C1D-ND	3.71	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	510	CLA	C1D-ND	3.71	1.42	1.37
13	a	513	CLA	C1D-ND	3.70	1.42	1.37
13	a	519	CLA	C1D-ND	3.69	1.42	1.37
13	g	503	CLA	C1D-ND	3.68	1.42	1.37
13	6	507	CLA	C1D-ND	3.67	1.42	1.37
13	g	513	CLA	C1D-ND	3.67	1.42	1.37
13	f	513	CLA	C1D-ND	3.67	1.42	1.37
13	e	503	CLA	C1D-ND	3.67	1.42	1.37
13	6	510	CLA	C1D-ND	3.67	1.42	1.37
13	1	519	CLA	C1D-ND	3.66	1.42	1.37
13	a	503	CLA	C1D-ND	3.66	1.42	1.37
13	6	504	CLA	C1D-ND	3.66	1.42	1.37
13	c	506	CLA	C1D-ND	3.66	1.42	1.37
13	a	518	CLA	C1D-ND	3.66	1.42	1.37
13	6	508	CLA	C1D-ND	3.65	1.42	1.37
13	f	509	CLA	C1D-ND	3.65	1.42	1.37
13	1	517	CLA	C1D-ND	3.65	1.42	1.37
13	f	518	CLA	C1D-ND	3.64	1.42	1.37
13	c	503	CLA	C1D-ND	3.64	1.42	1.37
13	g	504	CLA	C1D-ND	3.64	1.42	1.37
13	g	510	CLA	C1D-ND	3.64	1.42	1.37
13	2	517	CLA	C1D-ND	3.64	1.42	1.37
13	1	518	CLA	C1D-ND	3.63	1.42	1.37
13	d	513	CLA	C1D-ND	3.63	1.42	1.37
13	6	519	CLA	C1D-ND	3.63	1.42	1.37
13	d	503	CLA	C1D-ND	3.63	1.42	1.37
13	6	502	CLA	C1D-ND	3.62	1.42	1.37
13	g	517	CLA	C1D-ND	3.62	1.42	1.37
13	5	517	CLA	C1D-ND	3.62	1.42	1.37
13	b	509	CLA	C1D-ND	3.62	1.42	1.37
13	f	517	CLA	C1D-ND	3.62	1.42	1.37
13	B	1207	CLA	C1D-ND	3.62	1.42	1.37
13	1	504	CLA	C1D-ND	3.61	1.42	1.37
13	5	503	CLA	C1D-ND	3.61	1.42	1.37
13	5	511	CLA	C1D-ND	3.61	1.42	1.37
13	e	510	CLA	C1D-ND	3.61	1.42	1.37
13	e	519	CLA	C1D-ND	3.61	1.42	1.37
13	f	501	CLA	C1D-ND	3.61	1.42	1.37
13	f	510	CLA	C1D-ND	3.60	1.42	1.37
13	a	510	CLA	C1D-ND	3.60	1.42	1.37
13	4	517	CLA	C1D-ND	3.60	1.42	1.37
13	2	519	CLA	C1D-ND	3.60	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	511	CLA	C1D-ND	3.60	1.42	1.37
13	3	511	CLA	C1D-ND	3.60	1.42	1.37
13	d	507	CLA	C1D-ND	3.60	1.42	1.37
13	g	501	CLA	C1D-ND	3.59	1.42	1.37
13	e	513	CLA	C1D-ND	3.59	1.42	1.37
13	a	517	CLA	C1D-ND	3.58	1.42	1.37
13	2	506	CLA	C1D-ND	3.58	1.42	1.37
13	5	504	CLA	C1D-ND	3.58	1.42	1.37
13	2	508	CLA	C1D-ND	3.58	1.42	1.37
13	B	1233	CLA	C1D-ND	3.58	1.42	1.37
13	2	511	CLA	C1D-ND	3.58	1.42	1.37
13	e	506	CLA	C1D-ND	3.58	1.42	1.37
13	6	516	CLA	C1D-ND	3.58	1.42	1.37
13	a	505	CLA	C1D-ND	3.58	1.42	1.37
13	6	513	CLA	C1D-ND	3.58	1.42	1.37
13	f	516	CLA	C1D-ND	3.58	1.42	1.37
13	1	511	CLA	C1D-ND	3.57	1.42	1.37
13	6	511	CLA	C1D-ND	3.57	1.42	1.37
13	1	516	CLA	C1D-ND	3.57	1.42	1.37
13	b	503	CLA	C1D-ND	3.57	1.42	1.37
13	d	509	CLA	C1D-ND	3.57	1.42	1.37
13	e	504	CLA	C1D-ND	3.57	1.42	1.37
13	4	513	CLA	C1D-ND	3.56	1.42	1.37
13	2	510	CLA	C1D-ND	3.56	1.42	1.37
13	d	519	CLA	C1D-ND	3.56	1.42	1.37
13	f	506	CLA	C1D-ND	3.56	1.42	1.37
13	5	510	CLA	C1D-ND	3.56	1.42	1.37
13	e	509	CLA	C1D-ND	3.56	1.42	1.37
13	e	516	CLA	C1D-ND	3.55	1.42	1.37
13	3	517	CLA	C1D-ND	3.55	1.42	1.37
13	e	502	CLA	C1D-ND	3.55	1.42	1.37
13	5	506	CLA	C1D-ND	3.55	1.42	1.37
13	g	509	CLA	C1D-ND	3.55	1.42	1.37
13	5	519	CLA	C1D-ND	3.55	1.42	1.37
13	A	1801	CLA	C1D-ND	3.55	1.42	1.37
13	1	509	CLA	C1D-ND	3.55	1.42	1.37
13	e	507	CLA	C1D-ND	3.55	1.42	1.37
13	g	507	CLA	C1D-ND	3.55	1.42	1.37
13	4	512	CLA	C1D-ND	3.54	1.42	1.37
13	4	502	CLA	C1D-ND	3.54	1.42	1.37
13	3	506	CLA	C1D-ND	3.54	1.42	1.37
13	d	510	CLA	C1D-ND	3.54	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	511	CLA	C1D-ND	3.54	1.42	1.37
13	3	516	CLA	C1D-ND	3.54	1.42	1.37
13	g	505	CLA	C1D-ND	3.54	1.42	1.37
13	c	501	CLA	C1D-ND	3.54	1.42	1.37
13	4	501	CLA	C1D-ND	3.54	1.42	1.37
13	f	504	CLA	C1D-ND	3.54	1.42	1.37
13	A	1011	CLA	C1D-ND	3.53	1.42	1.37
13	6	518	CLA	C1D-ND	3.53	1.42	1.37
13	f	511	CLA	C1D-ND	3.53	1.42	1.37
13	g	511	CLA	C1D-ND	3.53	1.42	1.37
13	4	503	CLA	C1D-ND	3.53	1.42	1.37
13	d	516	CLA	C1D-ND	3.53	1.42	1.37
13	1	507	CLA	C1D-ND	3.53	1.42	1.37
13	e	501	CLA	C1D-ND	3.53	1.42	1.37
13	b	504	CLA	C1D-ND	3.53	1.42	1.37
13	2	513	CLA	C1D-ND	3.53	1.42	1.37
13	a	502	CLA	C1D-ND	3.52	1.42	1.37
13	f	519	CLA	C1D-ND	3.52	1.42	1.37
13	b	513	CLA	C1D-ND	3.52	1.42	1.37
13	1	503	CLA	C1D-ND	3.52	1.42	1.37
13	K	1103	CLA	C1D-ND	3.52	1.42	1.37
13	g	518	CLA	C1D-ND	3.52	1.42	1.37
13	B	1209	CLA	C1D-ND	3.52	1.42	1.37
13	c	502	CLA	C1D-ND	3.52	1.42	1.37
13	5	509	CLA	C1D-ND	3.52	1.42	1.37
13	5	507	CLA	C1D-ND	3.51	1.42	1.37
13	1	519	CLA	C4B-NB	3.51	1.42	1.37
13	d	501	CLA	C1D-ND	3.51	1.42	1.37
13	5	508	CLA	C1D-ND	3.51	1.42	1.37
13	c	505	CLA	C1D-ND	3.51	1.42	1.37
13	b	507	CLA	C1D-ND	3.51	1.42	1.37
13	B	1204	CLA	C1D-ND	3.51	1.42	1.37
13	d	506	CLA	C1D-ND	3.51	1.42	1.37
13	b	519	CLA	C1D-ND	3.51	1.42	1.37
13	3	510	CLA	C1D-ND	3.51	1.42	1.37
13	5	513	CLA	C1D-ND	3.51	1.42	1.37
13	6	506	CLA	C1D-ND	3.51	1.42	1.37
13	4	516	CLA	C1D-ND	3.51	1.42	1.37
13	g	502	CLA	C1D-ND	3.51	1.42	1.37
13	b	517	CLA	C4B-NB	3.50	1.42	1.37
13	f	508	CLA	C1D-ND	3.50	1.42	1.37
13	2	516	CLA	C1D-ND	3.50	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	507	CLA	C1D-ND	3.50	1.42	1.37
13	1	508	CLA	C1D-ND	3.50	1.42	1.37
13	3	519	CLA	C1D-ND	3.50	1.42	1.37
13	2	518	CLA	C1D-ND	3.50	1.42	1.37
13	4	507	CLA	C1D-ND	3.49	1.42	1.37
13	e	518	CLA	C1D-ND	3.49	1.42	1.37
13	6	509	CLA	C1D-ND	3.49	1.42	1.37
13	a	517	CLA	C4B-NB	3.49	1.42	1.37
13	c	513	CLA	C1D-ND	3.49	1.42	1.37
13	6	501	CLA	C1D-ND	3.49	1.42	1.37
13	B	1236	CLA	C1D-ND	3.49	1.42	1.37
13	b	502	CLA	C1D-ND	3.49	1.42	1.37
13	6	517	CLA	C4B-NB	3.49	1.42	1.37
13	b	511	CLA	C1D-ND	3.49	1.42	1.37
13	1	501	CLA	C1D-ND	3.48	1.42	1.37
13	3	518	CLA	C1D-ND	3.48	1.42	1.37
13	3	509	CLA	C1D-ND	3.48	1.42	1.37
13	f	507	CLA	C1D-ND	3.48	1.42	1.37
13	3	501	CLA	C1D-ND	3.48	1.42	1.37
13	A	1132	CLA	C1D-ND	3.48	1.42	1.37
13	4	504	CLA	C1D-ND	3.48	1.42	1.37
13	e	505	CLA	C1D-ND	3.48	1.42	1.37
13	B	1220	CLA	C1D-ND	3.47	1.42	1.37
13	g	508	CLA	C1D-ND	3.47	1.42	1.37
13	2	504	CLA	C1D-ND	3.47	1.42	1.37
13	c	518	CLA	C1D-ND	3.47	1.42	1.37
13	3	508	CLA	C1D-ND	3.47	1.42	1.37
13	a	504	CLA	C1D-ND	3.47	1.42	1.37
13	2	507	CLA	C1D-ND	3.47	1.42	1.37
13	b	501	CLA	C1D-ND	3.47	1.42	1.37
13	g	519	CLA	C1D-ND	3.47	1.42	1.37
13	1	502	CLA	C1D-ND	3.47	1.42	1.37
13	e	508	CLA	C1D-ND	3.47	1.42	1.37
13	a	507	CLA	C1D-ND	3.47	1.42	1.37
13	6	503	CLA	C1D-ND	3.46	1.42	1.37
13	c	509	CLA	C1D-ND	3.46	1.42	1.37
13	b	508	CLA	C1D-ND	3.46	1.42	1.37
13	a	506	CLA	C1D-ND	3.46	1.42	1.37
13	f	501	CLA	C4B-NB	3.46	1.42	1.37
13	b	505	CLA	C1D-ND	3.46	1.42	1.37
13	c	504	CLA	C1D-ND	3.46	1.42	1.37
13	c	511	CLA	C1D-ND	3.46	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	501	CLA	C1D-ND	3.45	1.42	1.37
13	5	516	CLA	C1D-ND	3.45	1.42	1.37
13	b	516	CLA	C1D-ND	3.45	1.42	1.37
13	5	518	CLA	C1D-ND	3.45	1.42	1.37
13	c	519	CLA	C1D-ND	3.45	1.42	1.37
13	5	501	CLA	C1D-ND	3.45	1.42	1.37
13	a	501	CLA	C4B-NB	3.45	1.42	1.37
13	a	501	CLA	C1D-ND	3.45	1.42	1.37
13	4	509	CLA	C1D-ND	3.45	1.42	1.37
13	3	507	CLA	C1D-ND	3.44	1.42	1.37
13	B	1232	CLA	C1D-ND	3.44	1.42	1.37
13	3	512	CLA	C1D-ND	3.44	1.42	1.37
13	3	504	CLA	C1D-ND	3.44	1.42	1.37
13	4	508	CLA	C1D-ND	3.44	1.42	1.37
13	6	512	CLA	C1D-ND	3.43	1.42	1.37
13	e	517	CLA	C4B-NB	3.43	1.42	1.37
13	1	505	CLA	C1D-ND	3.43	1.42	1.37
13	B	1201	CLA	C1D-ND	3.43	1.42	1.37
13	c	517	CLA	C4B-NB	3.43	1.42	1.37
13	3	513	CLA	C1D-ND	3.43	1.42	1.37
13	3	503	CLA	C1D-ND	3.43	1.42	1.37
13	B	1223	CLA	C1D-ND	3.43	1.42	1.37
13	e	511	CLA	C1D-ND	3.43	1.42	1.37
13	c	512	CLA	C1D-ND	3.43	1.42	1.37
13	4	505	CLA	C1D-ND	3.43	1.42	1.37
13	5	505	CLA	C1D-ND	3.43	1.42	1.37
13	2	503	CLA	C1D-ND	3.43	1.42	1.37
13	a	516	CLA	C1D-ND	3.42	1.42	1.37
13	1	506	CLA	C1D-ND	3.42	1.42	1.37
13	e	501	CLA	C4B-NB	3.42	1.42	1.37
13	A	1121	CLA	C1D-ND	3.42	1.42	1.37
13	g	512	CLA	C4B-NB	3.42	1.42	1.37
13	4	518	CLA	C1D-ND	3.42	1.42	1.37
13	X	1401	CLA	C1D-ND	3.42	1.42	1.37
13	b	501	CLA	C4B-NB	3.42	1.42	1.37
13	K	1401	CLA	C1D-ND	3.42	1.42	1.37
13	c	510	CLA	C1D-ND	3.42	1.42	1.37
13	1	517	CLA	C4B-NB	3.41	1.42	1.37
13	g	506	CLA	C1D-ND	3.41	1.42	1.37
13	d	518	CLA	C1D-ND	3.41	1.42	1.37
13	2	502	CLA	C1D-ND	3.41	1.42	1.37
13	2	503	CLA	C4B-NB	3.41	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	513	CLA	C1D-ND	3.41	1.42	1.37
13	d	504	CLA	C1D-ND	3.41	1.42	1.37
13	d	508	CLA	C1D-ND	3.41	1.42	1.37
13	f	518	CLA	C4B-NB	3.41	1.42	1.37
13	5	502	CLA	C1D-ND	3.41	1.42	1.37
13	f	502	CLA	C1D-ND	3.40	1.42	1.37
13	2	509	CLA	C1D-ND	3.40	1.42	1.37
13	A	1116	CLA	C1D-ND	3.40	1.42	1.37
13	6	505	CLA	C1D-ND	3.40	1.42	1.37
13	A	1131	CLA	C1D-ND	3.39	1.42	1.37
13	a	508	CLA	C1D-ND	3.39	1.42	1.37
13	1	516	CLA	C4B-NB	3.39	1.42	1.37
13	A	1118	CLA	C1D-ND	3.39	1.42	1.37
13	A	1115	CLA	C1D-ND	3.39	1.42	1.37
13	B	1234	CLA	C1D-ND	3.39	1.42	1.37
13	K	1103	CLA	C4B-NB	3.39	1.42	1.37
13	4	506	CLA	C1D-ND	3.39	1.42	1.37
13	B	1210	CLA	C1D-ND	3.38	1.42	1.37
13	d	502	CLA	C1D-ND	3.38	1.42	1.37
13	3	502	CLA	C1D-ND	3.38	1.42	1.37
13	f	503	CLA	C4B-NB	3.38	1.42	1.37
13	A	1105	CLA	C1D-ND	3.38	1.42	1.37
13	B	1219	CLA	C4B-NB	3.38	1.42	1.37
13	a	504	CLA	C4B-NB	3.38	1.42	1.37
13	a	512	CLA	C4B-NB	3.38	1.42	1.37
13	5	512	CLA	C4B-NB	3.38	1.42	1.37
13	5	512	CLA	C1D-ND	3.38	1.42	1.37
13	b	512	CLA	C1D-ND	3.38	1.42	1.37
13	5	517	CLA	C4B-NB	3.38	1.42	1.37
13	A	1108	CLA	C1D-ND	3.37	1.42	1.37
13	e	502	CLA	C4B-NB	3.37	1.42	1.37
13	A	1133	CLA	C1D-ND	3.37	1.42	1.37
13	f	512	CLA	C4B-NB	3.37	1.42	1.37
13	B	1239	CLA	C1D-ND	3.37	1.42	1.37
13	d	512	CLA	C1D-ND	3.37	1.42	1.37
13	c	506	CLA	C4B-NB	3.36	1.42	1.37
13	B	1218	CLA	C1D-ND	3.36	1.42	1.37
13	e	519	CLA	C4B-NB	3.36	1.42	1.37
13	5	501	CLA	C4B-NB	3.36	1.42	1.37
13	B	1213	CLA	C1D-ND	3.36	1.42	1.37
13	g	507	CLA	C4B-NB	3.36	1.42	1.37
13	d	510	CLA	C4B-NB	3.36	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	518	CLA	C4B-NB	3.36	1.42	1.37
13	B	1231	CLA	C4B-NB	3.36	1.42	1.37
13	d	517	CLA	C4B-NB	3.36	1.42	1.37
13	a	513	CLA	C4B-NB	3.35	1.42	1.37
13	A	1120	CLA	C1D-ND	3.35	1.42	1.37
13	B	1216	CLA	C1D-ND	3.35	1.42	1.37
13	B	1012	CLA	C1D-ND	3.35	1.42	1.37
13	d	501	CLA	C4B-NB	3.35	1.42	1.37
13	b	518	CLA	C1D-ND	3.34	1.42	1.37
13	4	510	CLA	C1D-ND	3.34	1.42	1.37
13	c	508	CLA	C1D-ND	3.34	1.42	1.37
13	B	1205	CLA	C1D-ND	3.34	1.42	1.37
13	B	1208	CLA	C1D-ND	3.34	1.42	1.37
13	6	511	CLA	C4B-NB	3.34	1.42	1.37
13	2	504	CLA	C4B-NB	3.34	1.42	1.37
13	g	501	CLA	C4B-NB	3.34	1.42	1.37
13	4	519	CLA	C1D-ND	3.34	1.42	1.37
13	d	507	CLA	C4B-NB	3.34	1.42	1.37
20	B	1843	LMU	O5'-C1'	3.33	1.50	1.41
13	6	512	CLA	C4B-NB	3.33	1.42	1.37
13	3	505	CLA	C1D-ND	3.33	1.42	1.37
13	2	506	CLA	C4B-NB	3.33	1.42	1.37
13	g	504	CLA	C4B-NB	3.33	1.42	1.37
13	A	1134	CLA	C1D-ND	3.33	1.42	1.37
13	A	1124	CLA	C1D-ND	3.32	1.42	1.37
13	e	512	CLA	C4B-NB	3.32	1.42	1.37
13	1	513	CLA	C4B-NB	3.32	1.42	1.37
13	4	512	CLA	C4B-NB	3.32	1.42	1.37
13	b	510	CLA	C1D-ND	3.32	1.42	1.37
13	F	1301	CLA	C1D-ND	3.32	1.42	1.37
13	c	507	CLA	C4B-NB	3.32	1.42	1.37
13	f	504	CLA	C4B-NB	3.32	1.42	1.37
13	1	518	CLA	C4B-NB	3.32	1.42	1.37
13	g	519	CLA	C4B-NB	3.32	1.42	1.37
13	B	1211	CLA	C1D-ND	3.32	1.42	1.37
13	6	503	CLA	C4B-NB	3.32	1.42	1.37
13	c	512	CLA	C4B-NB	3.32	1.42	1.37
13	5	516	CLA	C4B-NB	3.31	1.42	1.37
13	A	1111	CLA	C1D-ND	3.31	1.42	1.37
13	f	510	CLA	C4B-NB	3.31	1.42	1.37
13	1	504	CLA	C4B-NB	3.31	1.42	1.37
13	3	517	CLA	C4B-NB	3.31	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	512	CLA	C1D-ND	3.31	1.42	1.37
13	d	505	CLA	C1D-ND	3.31	1.42	1.37
13	B	1217	CLA	C1D-ND	3.31	1.42	1.37
13	e	512	CLA	C1D-ND	3.31	1.42	1.37
13	l	508	CLA	C4B-NB	3.31	1.42	1.37
13	a	519	CLA	C4B-NB	3.31	1.42	1.37
13	A	1102	CLA	C1D-ND	3.31	1.42	1.37
13	A	1135	CLA	C1D-ND	3.30	1.42	1.37
13	g	508	CLA	C4B-NB	3.30	1.42	1.37
13	B	1212	CLA	C1D-ND	3.30	1.42	1.37
13	e	503	CLA	C4B-NB	3.30	1.42	1.37
13	f	506	CLA	C4B-NB	3.30	1.42	1.37
13	d	518	CLA	C4B-NB	3.30	1.42	1.37
13	g	503	CLA	C4B-NB	3.30	1.42	1.37
13	g	516	CLA	C4B-NB	3.30	1.42	1.37
13	b	518	CLA	C4B-NB	3.29	1.42	1.37
13	a	516	CLA	C4B-NB	3.29	1.42	1.37
13	2	517	CLA	C4B-NB	3.29	1.42	1.37
13	A	1237	CLA	C1D-ND	3.29	1.42	1.37
13	g	506	CLA	C4B-NB	3.29	1.42	1.37
13	A	1113	CLA	C1D-ND	3.29	1.42	1.37
13	B	1227	CLA	C1D-ND	3.29	1.42	1.37
13	b	509	CLA	C4B-NB	3.29	1.42	1.37
13	e	516	CLA	C4B-NB	3.29	1.42	1.37
13	2	505	CLA	C1D-ND	3.29	1.42	1.37
13	2	519	CLA	C4B-NB	3.28	1.42	1.37
13	f	517	CLA	C4B-NB	3.28	1.42	1.37
13	B	1203	CLA	C1D-ND	3.28	1.42	1.37
13	d	516	CLA	C4B-NB	3.28	1.42	1.37
13	g	517	CLA	C4B-NB	3.28	1.42	1.37
13	f	519	CLA	C4B-NB	3.28	1.42	1.37
13	l	501	CLA	C4B-NB	3.28	1.42	1.37
13	A	1110	CLA	C1D-ND	3.28	1.42	1.37
13	e	506	CLA	C4B-NB	3.28	1.42	1.37
13	f	505	CLA	C1D-ND	3.28	1.42	1.37
13	l	510	CLA	C4B-NB	3.28	1.42	1.37
13	A	1139	CLA	C4B-NB	3.28	1.42	1.37
13	5	507	CLA	C4B-NB	3.28	1.42	1.37
13	d	506	CLA	C4B-NB	3.27	1.42	1.37
13	A	1106	CLA	C1D-ND	3.27	1.42	1.37
13	B	1224	CLA	C1D-ND	3.27	1.42	1.37
13	b	503	CLA	C4B-NB	3.27	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	507	CLA	C4B-NB	3.27	1.42	1.37
13	5	513	CLA	C4B-NB	3.27	1.42	1.37
13	g	513	CLA	C4B-NB	3.27	1.42	1.37
13	A	1022	CLA	C1D-ND	3.27	1.42	1.37
13	2	501	CLA	C4B-NB	3.27	1.42	1.37
13	3	516	CLA	C4B-NB	3.27	1.42	1.37
20	B	1843	LMU	O5B-C1B	3.26	1.50	1.41
13	5	504	CLA	C4B-NB	3.26	1.42	1.37
13	1	511	CLA	C4B-NB	3.26	1.42	1.37
13	g	512	CLA	C1D-ND	3.26	1.42	1.37
13	J	1302	CLA	C1D-ND	3.26	1.42	1.37
13	c	519	CLA	C4B-NB	3.26	1.42	1.37
13	b	504	CLA	C4B-NB	3.26	1.42	1.37
13	1	503	CLA	C4B-NB	3.26	1.42	1.37
13	A	1103	CLA	C1D-ND	3.26	1.42	1.37
13	e	504	CLA	C4B-NB	3.26	1.42	1.37
13	5	506	CLA	C4B-NB	3.26	1.42	1.37
13	A	1130	CLA	C1D-ND	3.26	1.42	1.37
13	4	511	CLA	C4B-NB	3.26	1.42	1.37
13	B	1226	CLA	C1D-ND	3.26	1.42	1.37
13	4	517	CLA	C4B-NB	3.25	1.42	1.37
13	B	1228	CLA	C1D-ND	3.25	1.42	1.37
13	e	510	CLA	C4B-NB	3.25	1.42	1.37
13	A	1101	CLA	C1D-ND	3.25	1.42	1.37
13	b	506	CLA	C1D-ND	3.25	1.42	1.37
13	6	501	CLA	C4B-NB	3.25	1.42	1.37
13	B	1229	CLA	C4B-NB	3.25	1.42	1.37
13	g	510	CLA	C4B-NB	3.25	1.42	1.37
13	A	1123	CLA	C1D-ND	3.25	1.42	1.37
13	3	519	CLA	C4B-NB	3.25	1.42	1.37
13	c	513	CLA	C4B-NB	3.25	1.42	1.37
13	2	511	CLA	C4B-NB	3.25	1.42	1.37
13	b	508	CLA	C4B-NB	3.25	1.42	1.37
13	b	519	CLA	C4B-NB	3.24	1.42	1.37
13	6	516	CLA	C4B-NB	3.24	1.42	1.37
13	1	509	CLA	C4B-NB	3.24	1.42	1.37
13	c	501	CLA	C4B-NB	3.24	1.42	1.37
13	c	503	CLA	C4B-NB	3.24	1.42	1.37
13	4	516	CLA	C4B-NB	3.24	1.42	1.37
13	c	504	CLA	C4B-NB	3.24	1.42	1.37
13	b	511	CLA	C4B-NB	3.24	1.42	1.37
13	5	519	CLA	C4B-NB	3.24	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	519	CLA	C4B-NB	3.24	1.42	1.37
13	B	1235	CLA	C1D-ND	3.23	1.42	1.37
20	A	1849	LMU	O5'-C1'	3.23	1.50	1.41
13	b	516	CLA	C4B-NB	3.23	1.42	1.37
13	A	1101	CLA	C4B-NB	3.23	1.42	1.37
13	a	510	CLA	C4B-NB	3.23	1.42	1.37
13	a	511	CLA	C4B-NB	3.23	1.42	1.37
13	g	511	CLA	C4B-NB	3.23	1.42	1.37
13	a	503	CLA	C4B-NB	3.23	1.42	1.37
13	4	511	CLA	C1D-ND	3.23	1.42	1.37
20	A	1848	LMU	O5'-C1'	3.23	1.50	1.41
13	2	516	CLA	C4B-NB	3.23	1.42	1.37
13	e	518	CLA	C4B-NB	3.22	1.42	1.37
13	A	1112	CLA	C1D-ND	3.22	1.42	1.37
13	4	518	CLA	C4B-NB	3.22	1.42	1.37
13	A	1125	CLA	C1D-ND	3.22	1.42	1.37
13	6	518	CLA	C4B-NB	3.22	1.42	1.37
13	f	516	CLA	C4B-NB	3.22	1.42	1.37
13	a	518	CLA	C4B-NB	3.22	1.42	1.37
13	3	501	CLA	C4B-NB	3.22	1.42	1.37
13	6	504	CLA	C4B-NB	3.22	1.42	1.37
13	B	1229	CLA	C1D-ND	3.22	1.42	1.37
13	d	511	CLA	C4B-NB	3.21	1.42	1.37
13	b	513	CLA	C4B-NB	3.21	1.42	1.37
13	3	512	CLA	C4B-NB	3.21	1.42	1.37
13	a	502	CLA	C4B-NB	3.21	1.42	1.37
13	A	1114	CLA	C1D-ND	3.21	1.42	1.37
13	6	513	CLA	C4B-NB	3.21	1.42	1.37
13	f	508	CLA	C4B-NB	3.21	1.42	1.37
13	5	503	CLA	C4B-NB	3.21	1.42	1.37
13	A	1117	CLA	C1D-ND	3.21	1.42	1.37
13	d	519	CLA	C4B-NB	3.21	1.42	1.37
13	A	1136	CLA	C1D-ND	3.20	1.42	1.37
13	A	1237	CLA	C4B-NB	3.20	1.42	1.37
13	B	1204	CLA	C4B-NB	3.20	1.42	1.37
13	4	519	CLA	C4B-NB	3.20	1.42	1.37
13	B	1215	CLA	C1D-ND	3.20	1.42	1.37
13	6	506	CLA	C4B-NB	3.20	1.42	1.37
13	5	518	CLA	C4B-NB	3.20	1.42	1.37
13	1	505	CLA	C4B-NB	3.20	1.42	1.37
13	A	1140	CLA	C1D-ND	3.20	1.42	1.37
13	6	508	CLA	C1B-C2B	3.19	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	510	CLA	C4B-NB	3.19	1.42	1.37
13	2	507	CLA	C4B-NB	3.19	1.42	1.37
13	e	511	CLA	C4B-NB	3.19	1.42	1.37
13	c	516	CLA	C1D-ND	3.19	1.42	1.37
13	3	504	CLA	C4B-NB	3.19	1.42	1.37
13	4	508	CLA	C4B-NB	3.18	1.42	1.37
13	d	502	CLA	C4B-NB	3.18	1.42	1.37
13	1	506	CLA	C4B-NB	3.18	1.42	1.37
13	3	513	CLA	C4B-NB	3.18	1.42	1.37
13	5	510	CLA	C4B-NB	3.18	1.42	1.37
13	1	502	CLA	C4B-NB	3.18	1.42	1.37
13	3	508	CLA	C4B-NB	3.17	1.42	1.37
13	6	509	CLA	C4B-NB	3.17	1.42	1.37
13	4	501	CLA	C4B-NB	3.17	1.42	1.37
13	B	1238	CLA	C1D-ND	3.17	1.42	1.37
13	g	505	CLA	C4B-NB	3.17	1.42	1.37
13	4	513	CLA	C4B-NB	3.17	1.42	1.37
13	2	518	CLA	C4B-NB	3.17	1.42	1.37
13	A	1109	CLA	C1D-ND	3.17	1.42	1.37
13	c	510	CLA	C4B-NB	3.17	1.42	1.37
13	B	1239	CLA	C4B-NB	3.17	1.42	1.37
13	e	508	CLA	C4B-NB	3.17	1.42	1.37
13	B	1021	CLA	C1D-ND	3.17	1.42	1.37
13	d	504	CLA	C4B-NB	3.17	1.42	1.37
13	B	1214	CLA	C1D-ND	3.17	1.42	1.37
13	e	505	CLA	C4B-NB	3.16	1.42	1.37
13	a	508	CLA	C4B-NB	3.16	1.42	1.37
13	d	508	CLA	C4B-NB	3.16	1.42	1.37
13	b	507	CLA	C4B-NB	3.16	1.42	1.37
20	J	5105	LMU	O5'-C1'	3.16	1.50	1.41
13	4	504	CLA	C4B-NB	3.16	1.42	1.37
13	d	503	CLA	C4B-NB	3.16	1.42	1.37
13	3	518	CLA	C4B-NB	3.16	1.42	1.37
13	B	1232	CLA	C4B-NB	3.16	1.42	1.37
13	B	1230	CLA	C4B-NB	3.16	1.42	1.37
13	6	508	CLA	C4B-NB	3.16	1.42	1.37
13	f	511	CLA	C4B-NB	3.16	1.42	1.37
13	6	502	CLA	C4B-NB	3.15	1.42	1.37
13	6	507	CLA	C4B-NB	3.15	1.42	1.37
13	f	509	CLA	C4B-NB	3.15	1.42	1.37
13	1	512	CLA	C1D-ND	3.15	1.42	1.37
13	3	502	CLA	C4B-NB	3.15	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1202	CLA	C1D-ND	3.15	1.42	1.37
13	f	502	CLA	C4B-NB	3.15	1.42	1.37
13	f	512	CLA	C1D-ND	3.15	1.42	1.37
13	3	503	CLA	C4B-NB	3.15	1.42	1.37
13	f	507	CLA	C4B-NB	3.15	1.42	1.37
13	d	513	CLA	C4B-NB	3.14	1.42	1.37
13	A	1119	CLA	C1D-ND	3.14	1.42	1.37
13	A	1140	CLA	C4B-NB	3.14	1.42	1.37
13	4	507	CLA	C4B-NB	3.14	1.42	1.37
13	a	506	CLA	C4B-NB	3.14	1.42	1.37
13	3	511	CLA	C4B-NB	3.14	1.42	1.37
13	B	1217	CLA	C4B-NB	3.14	1.42	1.37
13	4	505	CLA	C4B-NB	3.14	1.42	1.37
13	B	1206	CLA	C1D-ND	3.14	1.42	1.37
13	A	1128	CLA	C1D-ND	3.14	1.42	1.37
13	b	502	CLA	C4B-NB	3.14	1.42	1.37
13	2	502	CLA	C4B-NB	3.14	1.42	1.37
13	X	1401	CLA	C4B-NB	3.14	1.42	1.37
13	1	507	CLA	C4B-NB	3.13	1.42	1.37
13	J	1303	CLA	C1C-CHC	3.13	1.42	1.33
13	B	1230	CLA	C1D-ND	3.13	1.42	1.37
13	d	512	CLA	C4B-NB	3.13	1.42	1.37
13	2	513	CLA	C4B-NB	3.13	1.42	1.37
13	A	1137	CLA	C1D-ND	3.13	1.42	1.37
13	A	1118	CLA	C4B-NB	3.12	1.42	1.37
13	2	510	CLA	C4B-NB	3.12	1.42	1.37
13	c	502	CLA	C4B-NB	3.12	1.42	1.37
13	A	1114	CLA	C4B-NB	3.12	1.42	1.37
13	4	503	CLA	C4B-NB	3.12	1.42	1.37
13	A	1126	CLA	C1D-ND	3.12	1.42	1.37
13	A	1104	CLA	C1D-ND	3.12	1.42	1.37
13	B	1225	CLA	C1D-ND	3.12	1.42	1.37
13	2	508	CLA	C4B-NB	3.11	1.42	1.37
13	5	508	CLA	C4B-NB	3.11	1.41	1.37
13	B	1218	CLA	C4B-NB	3.11	1.41	1.37
13	e	513	CLA	C4B-NB	3.11	1.41	1.37
13	a	505	CLA	C4B-NB	3.11	1.41	1.37
13	2	505	CLA	C4B-NB	3.11	1.41	1.37
13	B	1222	CLA	C1D-ND	3.11	1.41	1.37
13	c	505	CLA	C4B-NB	3.11	1.41	1.37
13	A	1129	CLA	C1D-ND	3.11	1.41	1.37
13	6	505	CLA	C4B-NB	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	511	CLA	C4B-NB	3.10	1.41	1.37
13	c	511	CLA	C4B-NB	3.10	1.41	1.37
13	A	1122	CLA	C1D-ND	3.10	1.41	1.37
13	A	1133	CLA	C4B-NB	3.09	1.41	1.37
13	d	505	CLA	C4B-NB	3.09	1.41	1.37
13	A	1115	CLA	C4B-NB	3.09	1.41	1.37
13	b	512	CLA	C4B-NB	3.09	1.41	1.37
13	B	1231	CLA	C1D-ND	3.09	1.41	1.37
13	A	1110	CLA	C4B-NB	3.09	1.41	1.37
13	A	1121	CLA	C4B-NB	3.08	1.41	1.37
13	3	510	CLA	C4B-NB	3.08	1.41	1.37
13	A	1136	CLA	C4B-NB	3.08	1.41	1.37
13	B	1221	CLA	C1D-ND	3.08	1.41	1.37
13	K	1401	CLA	C4B-NB	3.08	1.41	1.37
13	b	509	CLA	C1B-C2B	3.07	1.50	1.43
13	g	509	CLA	C4B-NB	3.07	1.41	1.37
13	A	1137	CLA	C4B-NB	3.07	1.41	1.37
13	4	502	CLA	C4B-NB	3.06	1.41	1.37
13	e	509	CLA	C4B-NB	3.06	1.41	1.37
13	c	508	CLA	C4B-NB	3.06	1.41	1.37
13	A	1134	CLA	C4B-NB	3.06	1.41	1.37
13	A	1139	CLA	C1D-ND	3.05	1.41	1.37
13	A	1108	CLA	C4B-NB	3.05	1.41	1.37
13	2	509	CLA	C4B-NB	3.05	1.41	1.37
13	3	507	CLA	C4B-NB	3.05	1.41	1.37
13	J	1302	CLA	C4B-NB	3.05	1.41	1.37
13	5	509	CLA	C4B-NB	3.05	1.41	1.37
13	3	509	CLA	C4B-NB	3.05	1.41	1.37
13	A	1109	CLA	C4B-NB	3.05	1.41	1.37
13	4	509	CLA	C4B-NB	3.05	1.41	1.37
13	B	1207	CLA	C4B-NB	3.05	1.41	1.37
13	3	506	CLA	C4B-NB	3.05	1.41	1.37
13	B	1209	CLA	C4B-NB	3.05	1.41	1.37
13	A	1129	CLA	C4B-NB	3.04	1.41	1.37
13	B	1222	CLA	C4B-NB	3.04	1.41	1.37
13	3	505	CLA	C4B-NB	3.04	1.41	1.37
13	B	1201	CLA	C4B-NB	3.04	1.41	1.37
13	A	1107	CLA	C1D-ND	3.04	1.41	1.37
13	4	506	CLA	C4B-NB	3.03	1.41	1.37
13	B	1211	CLA	C4B-NB	3.03	1.41	1.37
13	f	513	CLA	C4B-NB	3.03	1.41	1.37
13	F	1301	CLA	C4B-NB	3.03	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1235	CLA	C4B-NB	3.03	1.41	1.37
13	d	509	CLA	C4B-NB	3.03	1.41	1.37
13	A	1138	CLA	C4B-NB	3.02	1.41	1.37
13	b	505	CLA	C4B-NB	3.02	1.41	1.37
13	A	1116	CLA	C4B-NB	3.02	1.41	1.37
13	B	1213	CLA	C4B-NB	3.02	1.41	1.37
13	c	518	CLA	C4B-NB	3.02	1.41	1.37
13	A	1801	CLA	C4B-NB	3.02	1.41	1.37
13	a	509	CLA	C4B-NB	3.01	1.41	1.37
13	e	507	CLA	C4B-NB	3.01	1.41	1.37
13	A	1138	CLA	C1D-ND	3.01	1.41	1.37
13	5	502	CLA	C4B-NB	3.01	1.41	1.37
13	A	1013	CLA	C4B-NB	3.00	1.41	1.37
13	4	510	CLA	C4B-NB	3.00	1.41	1.37
13	g	502	CLA	C4B-NB	3.00	1.41	1.37
13	A	1120	CLA	C4B-NB	3.00	1.41	1.37
13	2	512	CLA	C4B-NB	3.00	1.41	1.37
13	A	1102	CLA	C4B-NB	3.00	1.41	1.37
13	B	1214	CLA	C4B-NB	3.00	1.41	1.37
13	B	1212	CLA	C4B-NB	3.00	1.41	1.37
13	c	509	CLA	C4B-NB	2.99	1.41	1.37
13	B	1012	CLA	C4B-NB	2.99	1.41	1.37
13	A	1130	CLA	C4B-NB	2.98	1.41	1.37
13	A	1117	CLA	C4B-NB	2.97	1.41	1.37
13	5	505	CLA	C4B-NB	2.97	1.41	1.37
13	A	1127	CLA	C1D-ND	2.97	1.41	1.37
13	b	510	CLA	C4B-NB	2.96	1.41	1.37
13	B	1238	CLA	C4B-NB	2.96	1.41	1.37
13	B	1219	CLA	C3C-C2C	2.96	1.39	1.33
13	B	1223	CLA	C4B-NB	2.96	1.41	1.37
13	B	1216	CLA	C4B-NB	2.95	1.41	1.37
13	B	1226	CLA	C4B-NB	2.95	1.41	1.37
13	B	1205	CLA	C4B-NB	2.95	1.41	1.37
13	c	516	CLA	C4B-NB	2.95	1.41	1.37
13	B	1203	CLA	C4B-NB	2.94	1.41	1.37
13	B	1023	CLA	C1D-ND	2.94	1.41	1.37
13	A	1131	CLA	C4B-NB	2.93	1.41	1.37
13	B	1225	CLA	C4B-NB	2.93	1.41	1.37
13	4	511	CLA	CMB-C2B	-2.93	1.44	1.50
13	B	1023	CLA	C4B-NB	2.93	1.41	1.37
13	A	1123	CLA	C4B-NB	2.92	1.41	1.37
13	A	1128	CLA	C4B-NB	2.92	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	509	CLA	C1B-C2B	2.91	1.50	1.43
13	B	1228	CLA	C4B-NB	2.90	1.41	1.37
13	B	1233	CLA	C4B-NB	2.90	1.41	1.37
13	A	1122	CLA	C4B-NB	2.90	1.41	1.37
13	A	1112	CLA	C4B-NB	2.89	1.41	1.37
13	B	1215	CLA	C4B-NB	2.89	1.41	1.37
13	A	1105	CLA	C4B-NB	2.89	1.41	1.37
13	2	512	CLA	C1D-ND	2.88	1.41	1.37
13	B	1227	CLA	C4B-NB	2.88	1.41	1.37
13	B	1208	CLA	C4B-NB	2.87	1.41	1.37
13	B	1236	CLA	C4B-NB	2.86	1.41	1.37
13	A	1119	CLA	C4B-NB	2.86	1.41	1.37
13	A	1107	CLA	C4B-NB	2.85	1.41	1.37
13	b	506	CLA	C4B-NB	2.85	1.41	1.37
13	A	1132	CLA	C4B-NB	2.83	1.41	1.37
13	A	1127	CLA	C4B-NB	2.83	1.41	1.37
13	1	512	CLA	C4B-NB	2.82	1.41	1.37
13	f	505	CLA	C4B-NB	2.82	1.41	1.37
13	f	504	CLA	C1B-C2B	2.82	1.49	1.43
13	c	519	CLA	C1B-C2B	2.82	1.49	1.43
13	B	1221	CLA	C4B-NB	2.81	1.41	1.37
13	g	510	CLA	C1B-C2B	2.81	1.49	1.43
13	A	1124	CLA	C4B-NB	2.81	1.41	1.37
13	A	1106	CLA	C4B-NB	2.81	1.41	1.37
13	A	1104	CLA	C4B-NB	2.80	1.41	1.37
13	1	516	CLA	C1B-C2B	2.80	1.49	1.43
13	a	502	CLA	C1B-C2B	2.80	1.49	1.43
13	A	1801	CLA	C1B-C2B	2.80	1.49	1.43
13	B	1224	CLA	C4B-NB	2.79	1.41	1.37
13	b	519	CLA	C1B-C2B	2.79	1.49	1.43
13	B	1021	CLA	C4B-NB	2.79	1.41	1.37
13	g	516	CLA	C1B-C2B	2.79	1.49	1.43
13	b	512	CLA	C1B-C2B	2.78	1.49	1.43
13	1	510	CLA	C1B-C2B	2.78	1.49	1.43
13	4	504	CLA	C1B-C2B	2.78	1.49	1.43
13	f	510	CLA	C1B-C2B	2.77	1.49	1.43
13	A	1113	CLA	C4B-NB	2.77	1.41	1.37
13	6	506	CLA	C1B-C2B	2.77	1.49	1.43
13	3	502	CLA	C1B-C2B	2.77	1.49	1.43
13	e	510	CLA	C1B-C2B	2.77	1.49	1.43
13	d	502	CLA	C1B-C2B	2.77	1.49	1.43
13	g	519	CLA	C1B-C2B	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	507	CLA	C1B-C2B	2.77	1.49	1.43
13	a	516	CLA	C1B-C2B	2.77	1.49	1.43
13	2	509	CLA	C1B-C2B	2.76	1.49	1.43
13	3	518	CLA	C1B-C2B	2.76	1.49	1.43
13	d	507	CLA	C1B-C2B	2.76	1.49	1.43
13	6	513	CLA	C1B-C2B	2.76	1.49	1.43
13	1	512	CLA	C1B-C2B	2.76	1.49	1.43
13	d	518	CLA	C1B-C2B	2.76	1.49	1.43
13	g	507	CLA	C1B-C2B	2.76	1.49	1.43
13	a	505	CLA	C1B-C2B	2.76	1.49	1.43
13	5	505	CLA	C1B-C2B	2.76	1.49	1.43
13	A	1125	CLA	C4B-NB	2.76	1.41	1.37
13	e	504	CLA	C1B-C2B	2.76	1.49	1.43
13	a	503	CLA	C1B-C2B	2.76	1.49	1.43
13	1	504	CLA	C1B-C2B	2.75	1.49	1.43
13	A	1121	CLA	C1B-C2B	2.75	1.49	1.43
13	a	518	CLA	C1B-C2B	2.75	1.49	1.43
13	2	502	CLA	C1B-C2B	2.75	1.49	1.43
13	f	502	CLA	C1B-C2B	2.75	1.49	1.43
13	B	1220	CLA	C4B-NB	2.75	1.41	1.37
13	2	516	CLA	C1B-C2B	2.75	1.49	1.43
13	a	519	CLA	C1B-C2B	2.75	1.49	1.43
13	e	502	CLA	C1B-C2B	2.75	1.49	1.43
13	d	512	CLA	C1B-C2B	2.74	1.49	1.43
13	b	504	CLA	C1B-C2B	2.74	1.49	1.43
13	6	518	CLA	C1B-C2B	2.74	1.49	1.43
13	b	511	CLA	C1B-C2B	2.74	1.49	1.43
13	1	517	CLA	C1B-C2B	2.74	1.49	1.43
13	b	506	CLA	MG-NB	-2.74	2.00	2.05
13	a	504	CLA	C1B-C2B	2.74	1.49	1.43
13	f	512	CLA	C1B-C2B	2.74	1.49	1.43
13	d	511	CLA	C1B-C2B	2.74	1.49	1.43
13	e	507	CLA	C1B-C2B	2.74	1.49	1.43
13	5	502	CLA	C1B-C2B	2.74	1.49	1.43
13	e	516	CLA	C1B-C2B	2.74	1.49	1.43
13	B	1206	CLA	C4B-NB	2.74	1.41	1.37
13	6	507	CLA	C1B-C2B	2.74	1.49	1.43
13	2	510	CLA	C1B-C2B	2.74	1.49	1.43
13	1	505	CLA	C1B-C2B	2.74	1.49	1.43
13	4	502	CLA	C1B-C2B	2.73	1.49	1.43
13	6	502	CLA	C1B-C2B	2.73	1.49	1.43
13	1	518	CLA	C1B-C2B	2.73	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1219	CLA	C1B-C2B	2.73	1.49	1.43
13	5	509	CLA	C1B-C2B	2.73	1.49	1.43
13	a	517	CLA	C1B-C2B	2.73	1.49	1.43
13	5	519	CLA	C1B-C2B	2.73	1.49	1.43
13	b	513	CLA	C1B-C2B	2.73	1.49	1.43
13	A	1111	CLA	C4B-NB	2.73	1.41	1.37
13	A	1022	CLA	C4B-NB	2.73	1.41	1.37
13	c	518	CLA	C1B-C2B	2.73	1.49	1.43
13	a	508	CLA	C1B-C2B	2.73	1.49	1.43
13	f	517	CLA	C1B-C2B	2.72	1.49	1.43
13	b	502	CLA	C1B-C2B	2.72	1.49	1.43
13	5	518	CLA	C1B-C2B	2.72	1.49	1.43
13	1	501	CLA	C1B-C2B	2.72	1.49	1.43
13	e	509	CLA	C1B-C2B	2.72	1.49	1.43
13	f	516	CLA	C1B-C2B	2.72	1.49	1.43
13	B	1219	CLA	CHC-C1C	2.72	1.41	1.36
13	d	513	CLA	C1B-C2B	2.72	1.49	1.43
13	c	513	CLA	C1B-C2B	2.72	1.49	1.43
13	d	503	CLA	C1B-C2B	2.72	1.49	1.43
13	4	513	CLA	C1B-C2B	2.72	1.49	1.43
13	4	517	CLA	C1B-C2B	2.72	1.49	1.43
13	d	509	CLA	C1B-C2B	2.72	1.49	1.43
13	g	518	CLA	C1B-C2B	2.72	1.49	1.43
13	g	513	CLA	C1B-C2B	2.72	1.49	1.43
13	A	1135	CLA	C4B-NB	2.72	1.41	1.37
13	c	511	CLA	C1B-C2B	2.72	1.49	1.43
13	B	1202	CLA	C4B-NB	2.71	1.41	1.37
13	d	519	CLA	C1B-C2B	2.71	1.49	1.43
13	c	509	CLA	C1B-C2B	2.71	1.49	1.43
13	e	503	CLA	C1B-C2B	2.71	1.49	1.43
13	e	517	CLA	C1B-C2B	2.71	1.49	1.43
13	g	517	CLA	C1B-C2B	2.71	1.49	1.43
13	5	511	CLA	C1B-C2B	2.71	1.49	1.43
13	6	509	CLA	C1B-C2B	2.71	1.49	1.43
13	f	503	CLA	C1B-C2B	2.71	1.49	1.43
13	6	503	CLA	C1B-C2B	2.71	1.49	1.43
13	A	1013	CLA	C1D-ND	2.71	1.41	1.37
13	g	503	CLA	C1B-C2B	2.71	1.49	1.43
13	2	504	CLA	C1B-C2B	2.71	1.49	1.43
13	c	502	CLA	C1B-C2B	2.71	1.49	1.43
13	g	509	CLA	C1B-C2B	2.70	1.49	1.43
13	6	510	CLA	C1B-C2B	2.70	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	504	CLA	C1B-C2B	2.70	1.49	1.43
13	3	507	CLA	C1B-C2B	2.70	1.49	1.43
13	c	512	CLA	C1B-C2B	2.70	1.49	1.43
13	b	501	CLA	C1B-C2B	2.70	1.49	1.43
13	a	511	CLA	C1B-C2B	2.70	1.49	1.43
13	c	506	CLA	C1B-C2B	2.70	1.49	1.43
13	B	1210	CLA	C4B-NB	2.70	1.41	1.37
13	5	512	CLA	C1B-C2B	2.70	1.49	1.43
13	A	1107	CLA	C1B-C2B	2.70	1.49	1.43
13	d	517	CLA	C1B-C2B	2.70	1.49	1.43
13	b	516	CLA	C1B-C2B	2.70	1.49	1.43
13	g	501	CLA	C1B-C2B	2.69	1.49	1.43
13	b	517	CLA	C1B-C2B	2.69	1.49	1.43
13	2	518	CLA	C1B-C2B	2.69	1.49	1.43
13	b	507	CLA	C1B-C2B	2.69	1.49	1.43
13	c	505	CLA	C1B-C2B	2.69	1.49	1.43
13	A	1118	CLA	C1B-C2B	2.69	1.49	1.43
13	2	503	CLA	C1B-C2B	2.69	1.49	1.43
13	6	517	CLA	C1B-C2B	2.69	1.49	1.43
13	5	507	CLA	C1B-C2B	2.69	1.49	1.43
13	d	501	CLA	C1B-C2B	2.69	1.49	1.43
13	f	513	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1126	CLA	C4B-NB	2.68	1.41	1.37
13	g	504	CLA	C1B-C2B	2.68	1.49	1.43
13	e	508	CLA	C1B-C2B	2.68	1.49	1.43
13	A	1103	CLA	C1B-C2B	2.68	1.49	1.43
13	1	506	CLA	C1B-C2B	2.68	1.49	1.43
13	6	519	CLA	C1B-C2B	2.68	1.49	1.43
13	4	516	CLA	C1B-C2B	2.68	1.49	1.43
13	6	516	CLA	C1B-C2B	2.68	1.49	1.43
13	d	516	CLA	C1B-C2B	2.68	1.49	1.43
13	5	516	CLA	C1B-C2B	2.68	1.49	1.43
13	B	1204	CLA	C1B-C2B	2.67	1.49	1.43
13	B	1234	CLA	C4B-NB	2.67	1.41	1.37
13	3	511	CLA	C1B-C2B	2.67	1.49	1.43
13	e	513	CLA	C1B-C2B	2.67	1.49	1.43
13	F	1301	CLA	C1B-C2B	2.67	1.49	1.43
13	5	506	CLA	C1B-C2B	2.67	1.49	1.43
13	b	506	CLA	C1B-NB	-2.67	1.34	1.37
13	b	518	CLA	C1B-C2B	2.67	1.49	1.43
13	6	511	CLA	C1B-C2B	2.67	1.49	1.43
13	a	506	CLA	C1B-C2B	2.67	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	510	CLA	C1B-C2B	2.67	1.49	1.43
13	5	513	CLA	C1B-C2B	2.67	1.49	1.43
13	2	505	CLA	C1B-C2B	2.66	1.49	1.43
13	a	507	CLA	C1B-C2B	2.66	1.49	1.43
13	4	519	CLA	C1B-C2B	2.66	1.49	1.43
13	2	506	CLA	C1B-C2B	2.66	1.49	1.43
13	c	507	CLA	C1B-C2B	2.66	1.49	1.43
13	3	519	CLA	C1B-C2B	2.66	1.49	1.43
13	4	507	CLA	C1B-C2B	2.66	1.49	1.43
13	1	502	CLA	C1B-C2B	2.66	1.49	1.43
13	e	518	CLA	C1B-C2B	2.66	1.49	1.43
13	A	1011	CLA	C4B-NB	2.66	1.41	1.37
13	A	1126	CLA	CMC-C2C	-2.66	1.45	1.50
13	f	518	CLA	C1B-C2B	2.66	1.49	1.43
13	2	511	CLA	C1B-C2B	2.66	1.49	1.43
13	1	509	CLA	C1B-C2B	2.66	1.49	1.43
13	3	503	CLA	C1B-C2B	2.66	1.49	1.43
13	6	505	CLA	C1B-C2B	2.66	1.49	1.43
13	1	513	CLA	C1B-C2B	2.66	1.49	1.43
13	e	512	CLA	C1B-C2B	2.66	1.49	1.43
13	a	510	CLA	C1B-C2B	2.66	1.49	1.43
13	e	519	CLA	C1B-C2B	2.66	1.49	1.43
13	g	508	CLA	C1B-C2B	2.66	1.49	1.43
13	5	501	CLA	C1B-C2B	2.65	1.49	1.43
13	d	504	CLA	C1B-C2B	2.65	1.49	1.43
13	g	502	CLA	C1B-C2B	2.65	1.49	1.43
13	B	1209	CLA	C1B-C2B	2.65	1.49	1.43
13	b	503	CLA	C1B-C2B	2.65	1.49	1.43
13	5	517	CLA	C1B-C2B	2.65	1.49	1.43
13	1	519	CLA	C1B-C2B	2.65	1.49	1.43
13	4	518	CLA	C1B-C2B	2.65	1.49	1.43
13	f	507	CLA	C1B-C2B	2.65	1.49	1.43
13	1	508	CLA	C1B-C2B	2.65	1.49	1.43
13	c	503	CLA	C1B-C2B	2.65	1.49	1.43
13	c	517	CLA	C1B-C2B	2.65	1.49	1.43
13	c	508	CLA	C1B-C2B	2.65	1.49	1.43
13	e	505	CLA	C1B-C2B	2.65	1.49	1.43
13	a	513	CLA	C1B-C2B	2.65	1.49	1.43
13	4	501	CLA	C1B-C2B	2.65	1.49	1.43
13	A	1117	CLA	CMB-C2B	-2.65	1.45	1.50
13	4	503	CLA	C1B-C2B	2.65	1.49	1.43
13	1	503	CLA	C1B-C2B	2.64	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	512	CLA	C1B-C2B	2.64	1.49	1.43
13	e	511	CLA	C1B-C2B	2.64	1.49	1.43
13	3	509	CLA	C1B-C2B	2.64	1.49	1.43
13	g	505	CLA	C1B-C2B	2.64	1.49	1.43
13	3	516	CLA	C1B-C2B	2.64	1.49	1.43
13	6	501	CLA	C1B-C2B	2.64	1.49	1.43
13	5	503	CLA	C1B-C2B	2.63	1.49	1.43
13	d	506	CLA	C1B-C2B	2.63	1.49	1.43
13	a	501	CLA	C1B-C2B	2.63	1.49	1.43
13	a	512	CLA	C1B-C2B	2.63	1.49	1.43
13	f	501	CLA	C1B-C2B	2.63	1.49	1.43
13	g	511	CLA	C1B-C2B	2.63	1.49	1.43
13	4	509	CLA	C1B-C2B	2.63	1.49	1.43
13	6	512	CLA	C1B-C2B	2.63	1.49	1.43
13	3	517	CLA	C1B-C2B	2.63	1.49	1.43
13	c	504	CLA	C1B-C2B	2.63	1.49	1.43
13	2	517	CLA	C1B-C2B	2.62	1.49	1.43
13	3	505	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1217	CLA	C1B-C2B	2.62	1.49	1.43
13	B	1203	CLA	C1B-C2B	2.62	1.49	1.43
13	2	508	CLA	C1B-C2B	2.62	1.49	1.43
13	c	501	CLA	C1B-C2B	2.62	1.49	1.43
13	3	506	CLA	C1B-C2B	2.62	1.49	1.43
13	d	505	CLA	C1B-C2B	2.62	1.49	1.43
13	4	505	CLA	C1B-C2B	2.61	1.49	1.43
13	2	519	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1110	CLA	C1B-C2B	2.61	1.49	1.43
13	B	1231	CLA	C1B-C2B	2.61	1.49	1.43
13	2	513	CLA	C1B-C2B	2.61	1.49	1.43
13	3	513	CLA	C1B-C2B	2.61	1.49	1.43
13	B	1218	CLA	C1B-C2B	2.61	1.49	1.43
13	g	512	CLA	C1B-C2B	2.61	1.49	1.43
13	4	506	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1111	CLA	C1B-C2B	2.61	1.49	1.43
13	b	508	CLA	C1B-C2B	2.61	1.49	1.43
13	4	508	CLA	C1B-C2B	2.61	1.49	1.43
13	2	501	CLA	C1B-C2B	2.61	1.49	1.43
13	c	510	CLA	C1B-C2B	2.61	1.49	1.43
13	A	1125	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1135	CLA	C1B-C2B	2.60	1.49	1.43
13	f	519	CLA	C1B-C2B	2.60	1.49	1.43
13	f	509	CLA	C1B-C2B	2.60	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1103	CLA	C4B-NB	2.60	1.41	1.37
13	d	508	CLA	C1B-C2B	2.60	1.49	1.43
13	A	1011	CLA	C1B-C2B	2.59	1.49	1.43
13	6	504	CLA	C1B-C2B	2.59	1.49	1.43
13	f	511	CLA	C1B-C2B	2.59	1.49	1.43
13	A	1132	CLA	C1B-C2B	2.59	1.49	1.43
13	B	1023	CLA	C1B-C2B	2.59	1.49	1.43
13	1	511	CLA	C1B-C2B	2.59	1.49	1.43
14	5	523	BCR	C30-C25	-2.59	1.50	1.53
13	5	504	CLA	C1B-C2B	2.59	1.49	1.43
13	4	512	CLA	C1B-C2B	2.59	1.49	1.43
13	d	510	CLA	C1B-C2B	2.59	1.49	1.43
13	B	1208	CLA	C1B-C2B	2.59	1.49	1.43
13	3	510	CLA	C1B-C2B	2.58	1.49	1.43
13	5	508	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1223	CLA	C1B-C2B	2.58	1.49	1.43
13	B	1238	CLA	C1B-C2B	2.58	1.49	1.43
13	A	1114	CLA	C1B-C2B	2.57	1.49	1.43
13	B	1021	CLA	C1B-C2B	2.57	1.49	1.43
13	c	516	CLA	C1B-C2B	2.57	1.49	1.43
13	B	1210	CLA	C1B-C2B	2.57	1.49	1.43
13	2	507	CLA	C1B-C2B	2.57	1.49	1.43
13	B	1212	CLA	C1B-C2B	2.57	1.49	1.43
13	4	511	CLA	C3B-C4B	2.56	1.50	1.42
14	I	4018	BCR	C1-C6	-2.56	1.50	1.53
13	A	1130	CLA	C1B-C2B	2.56	1.49	1.43
13	b	510	CLA	C1B-C2B	2.56	1.49	1.43
13	B	1211	CLA	C1B-C2B	2.56	1.49	1.43
13	e	501	CLA	C1B-C2B	2.56	1.49	1.43
13	3	508	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1227	CLA	C1B-C2B	2.55	1.49	1.43
13	X	1401	CLA	C1B-C2B	2.55	1.49	1.43
13	A	1134	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1233	CLA	C1B-C2B	2.55	1.49	1.43
13	A	1115	CLA	C1B-C2B	2.55	1.49	1.43
13	B	1207	CLA	C1B-C2B	2.54	1.49	1.43
13	K	1103	CLA	C1B-C2B	2.54	1.49	1.43
13	f	506	CLA	C1B-C2B	2.54	1.49	1.43
13	f	508	CLA	C1B-C2B	2.54	1.49	1.43
13	A	1108	CLA	C1B-C2B	2.54	1.49	1.43
13	3	501	CLA	C1B-C2B	2.54	1.49	1.43
13	g	512	CLA	C3B-C4B	2.53	1.50	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1131	CLA	C1B-C2B	2.53	1.49	1.43
13	2	512	CLA	C1B-C2B	2.53	1.49	1.43
13	g	506	CLA	C1B-C2B	2.53	1.49	1.43
13	A	1237	CLA	C1B-C2B	2.52	1.49	1.43
13	B	1229	CLA	C3B-C4B	2.52	1.50	1.42
13	A	1136	CLA	C1B-C2B	2.52	1.49	1.43
13	A	1104	CLA	C1B-C2B	2.52	1.49	1.43
13	f	505	CLA	C1B-C2B	2.52	1.49	1.43
13	B	1201	CLA	C1B-C2B	2.52	1.49	1.43
13	A	1126	CLA	C1B-C2B	2.52	1.49	1.43
13	e	506	CLA	C1B-C2B	2.51	1.49	1.43
13	B	1220	CLA	C1B-C2B	2.51	1.49	1.43
13	J	1302	CLA	C1B-C2B	2.50	1.49	1.43
13	A	1124	CLA	C1B-C2B	2.50	1.49	1.43
13	A	1102	CLA	C1B-C2B	2.50	1.49	1.43
13	A	1112	CLA	C1B-C2B	2.50	1.49	1.43
13	A	1122	CLA	C1B-C2B	2.50	1.49	1.43
13	B	1236	CLA	C1B-C2B	2.49	1.49	1.43
13	b	509	CLA	CMB-C2B	-2.49	1.45	1.50
13	A	1013	CLA	CMD-C2D	-2.49	1.45	1.50
13	A	1105	CLA	C1B-C2B	2.49	1.49	1.43
13	B	1215	CLA	CMB-C2B	-2.49	1.45	1.50
13	A	1013	CLA	CMB-C2B	-2.49	1.45	1.50
13	B	1232	CLA	C1B-C2B	2.49	1.49	1.43
13	A	1123	CLA	C1B-C2B	2.48	1.49	1.43
13	B	1228	CLA	C1B-C2B	2.48	1.49	1.43
13	4	510	CLA	C1B-C2B	2.48	1.49	1.43
13	A	1138	CLA	C1B-C2B	2.48	1.48	1.43
13	J	1303	CLA	C4D-ND	-2.48	1.34	1.37
13	b	506	CLA	MG-ND	-2.48	2.00	2.05
13	4	512	CLA	C3B-C4B	2.48	1.49	1.42
13	A	1120	CLA	C1B-C2B	2.47	1.48	1.43
13	A	1116	CLA	C1B-C2B	2.47	1.48	1.43
13	b	505	CLA	C1B-C2B	2.47	1.48	1.43
13	A	1128	CLA	C1B-C2B	2.46	1.48	1.43
13	B	1239	CLA	C1B-C2B	2.46	1.48	1.43
13	B	1206	CLA	C1B-C2B	2.46	1.48	1.43
13	K	1401	CLA	C1B-C2B	2.46	1.48	1.43
13	B	1226	CLA	C1B-C2B	2.45	1.48	1.43
13	A	1139	CLA	C1B-C2B	2.45	1.48	1.43
13	B	1235	CLA	C1B-C2B	2.45	1.48	1.43
13	A	1125	CLA	CMC-C2C	-2.45	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1129	CLA	C1B-C2B	2.45	1.48	1.43
13	B	1023	CLA	CMC-C2C	-2.44	1.45	1.50
13	A	1128	CLA	CMB-C2B	-2.44	1.45	1.50
13	B	1222	CLA	C1B-C2B	2.44	1.48	1.43
13	c	506	CLA	C3B-C4B	2.44	1.49	1.42
13	A	1106	CLA	C1B-C2B	2.44	1.48	1.43
13	B	1202	CLA	C1B-C2B	2.44	1.48	1.43
13	J	1303	CLA	C1B-C2B	2.44	1.48	1.43
13	A	1127	CLA	C1B-C2B	2.44	1.48	1.43
13	a	512	CLA	C3B-C4B	2.44	1.49	1.42
13	B	1225	CLA	CMD-C2D	-2.43	1.45	1.50
13	g	501	CLA	C3B-C4B	2.43	1.49	1.42
13	a	501	CLA	C3B-C4B	2.43	1.49	1.42
13	2	512	CLA	CMB-C2B	-2.43	1.45	1.50
13	f	519	CLA	C3B-C4B	2.42	1.49	1.42
13	b	510	CLA	C3B-C4B	2.42	1.49	1.42
13	4	511	CLA	CMD-C2D	-2.42	1.45	1.50
13	B	1213	CLA	C1B-C2B	2.42	1.48	1.43
13	2	503	CLA	C3B-C4B	2.41	1.49	1.42
13	B	1221	CLA	C1B-C2B	2.41	1.48	1.43
13	e	512	CLA	C3B-C4B	2.41	1.49	1.42
13	f	501	CLA	C3B-C4B	2.40	1.49	1.42
13	A	1137	CLA	C1B-C2B	2.40	1.48	1.43
13	e	506	CLA	C3B-C4B	2.40	1.49	1.42
13	e	505	CLA	CMD-C2D	-2.40	1.45	1.50
13	b	506	CLA	CMC-C2C	-2.40	1.45	1.50
13	A	1107	CLA	CMD-C2D	-2.40	1.45	1.50
13	A	1237	CLA	C3B-C4B	2.40	1.49	1.42
13	g	503	CLA	C3B-C4B	2.40	1.49	1.42
13	A	1113	CLA	C1B-C2B	2.39	1.48	1.43
13	3	506	CLA	C3B-C4B	2.39	1.49	1.42
13	3	510	CLA	C3B-C4B	2.39	1.49	1.42
14	A	4003	BCR	C30-C25	-2.39	1.50	1.53
13	A	1109	CLA	C1B-C2B	2.39	1.48	1.43
13	A	1119	CLA	C1B-C2B	2.39	1.48	1.43
13	B	1012	CLA	CHC-C1C	2.39	1.43	1.38
13	X	1401	CLA	C3B-C4B	2.39	1.49	1.42
13	f	513	CLA	CHC-C1C	2.39	1.43	1.38
13	4	510	CLA	C3B-C4B	2.39	1.49	1.42
13	B	1225	CLA	C1B-C2B	2.39	1.48	1.43
13	A	1135	CLA	CMD-C2D	-2.39	1.45	1.50
13	2	501	CLA	C3B-C4B	2.39	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	517	CLA	C3B-C4B	2.39	1.49	1.42
13	A	1126	CLA	CMD-C2D	-2.38	1.45	1.50
13	2	517	CLA	C3B-C4B	2.38	1.49	1.42
13	A	1101	CLA	C3B-C4B	2.38	1.49	1.42
13	6	504	CLA	C3B-C4B	2.38	1.49	1.42
13	f	511	CLA	C3B-C4B	2.38	1.49	1.42
13	A	1101	CLA	C1B-C2B	2.38	1.48	1.43
13	A	1013	CLA	C1B-C2B	2.38	1.48	1.43
13	5	506	CLA	C3B-C4B	2.38	1.49	1.42
13	g	516	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1226	CLA	CMB-C2B	-2.37	1.45	1.50
13	g	504	CLA	C3B-C4B	2.37	1.49	1.42
13	1	519	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1229	CLA	C1B-C2B	2.37	1.48	1.43
13	b	508	CLA	C3B-C4B	2.37	1.49	1.42
13	5	512	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1230	CLA	CMB-C2B	-2.37	1.45	1.50
13	A	1127	CLA	CMD-C2D	-2.37	1.45	1.50
13	A	1114	CLA	CMB-C2B	-2.37	1.45	1.50
13	B	1216	CLA	CMB-C2B	-2.37	1.45	1.50
13	2	519	CLA	C3B-C4B	2.37	1.49	1.42
13	e	501	CLA	C3B-C4B	2.37	1.49	1.42
13	B	1214	CLA	C1B-C2B	2.37	1.48	1.43
13	B	1235	CLA	C3B-C4B	2.36	1.49	1.42
13	A	1140	CLA	C3B-C4B	2.36	1.49	1.42
13	g	519	CLA	C3B-C4B	2.36	1.49	1.42
13	2	512	CLA	CMD-C2D	-2.36	1.45	1.50
13	A	1013	CLA	CMC-C2C	-2.36	1.45	1.50
13	B	1021	CLA	CMD-C2D	-2.36	1.45	1.50
13	B	1230	CLA	C1B-C2B	2.36	1.48	1.43
13	d	501	CLA	C3B-C4B	2.36	1.49	1.42
13	6	512	CLA	C3B-C4B	2.36	1.49	1.42
13	3	512	CLA	C3B-C4B	2.36	1.49	1.42
13	c	517	CLA	C3B-C4B	2.36	1.49	1.42
13	d	508	CLA	C3B-C4B	2.36	1.49	1.42
13	4	519	CLA	C3B-C4B	2.36	1.49	1.42
13	a	504	CLA	C3B-C4B	2.35	1.49	1.42
13	a	510	CLA	C3B-C4B	2.35	1.49	1.42
13	B	1205	CLA	CMD-C2D	-2.35	1.45	1.50
13	6	510	CLA	C3B-C4B	2.35	1.49	1.42
13	B	1239	CLA	CMB-C2B	-2.35	1.46	1.50
13	6	508	CLA	CMC-C2C	-2.35	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	505	CLA	CMD-C2D	-2.35	1.46	1.50
13	a	517	CLA	C3B-C4B	2.35	1.49	1.42
13	B	1224	CLA	CMB-C2B	-2.35	1.46	1.50
13	5	513	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1023	CLA	CMD-C2D	-2.34	1.46	1.50
13	5	517	CLA	C3B-C4B	2.34	1.49	1.42
13	f	518	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1215	CLA	C1B-C2B	2.34	1.48	1.43
13	B	1205	CLA	C1B-C2B	2.34	1.48	1.43
13	2	512	CLA	C3B-C4B	2.34	1.49	1.42
13	e	516	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1234	CLA	CMD-C2D	-2.34	1.46	1.50
13	A	1111	CLA	CMD-C2D	-2.34	1.46	1.50
13	c	508	CLA	C3B-C4B	2.34	1.49	1.42
13	B	1207	CLA	C3B-C4B	2.33	1.49	1.42
13	g	505	CLA	C3B-C4B	2.33	1.49	1.42
13	A	1123	CLA	CMD-C2D	-2.33	1.46	1.50
13	B	1238	CLA	CMD-C2D	-2.33	1.46	1.50
13	f	508	CLA	C3B-C4B	2.33	1.49	1.42
13	A	1110	CLA	CMB-C2B	-2.33	1.46	1.50
13	c	501	CLA	C3B-C4B	2.33	1.49	1.42
13	g	506	CLA	C3B-C4B	2.33	1.49	1.42
13	f	512	CLA	C3B-C4B	2.33	1.49	1.42
13	1	508	CLA	C3B-C4B	2.33	1.49	1.42
13	1	517	CLA	C3B-C4B	2.33	1.49	1.42
13	A	1118	CLA	C3B-C4B	2.33	1.49	1.42
13	d	516	CLA	C3B-C4B	2.33	1.49	1.42
13	c	504	CLA	C3B-C4B	2.33	1.49	1.42
13	1	505	CLA	C3B-C4B	2.33	1.49	1.42
13	B	1236	CLA	C3B-C4B	2.32	1.49	1.42
13	1	512	CLA	CMD-C2D	-2.32	1.46	1.50
13	6	517	CLA	C3B-C4B	2.32	1.49	1.42
13	2	506	CLA	C3B-C4B	2.32	1.49	1.42
13	g	513	CLA	C3B-C4B	2.32	1.49	1.42
13	2	513	CLA	C3B-C4B	2.32	1.49	1.42
13	b	517	CLA	C3B-C4B	2.32	1.49	1.42
13	1	516	CLA	C3B-C4B	2.32	1.49	1.42
13	b	516	CLA	C3B-C4B	2.32	1.49	1.42
13	5	510	CLA	C3B-C4B	2.32	1.49	1.42
13	c	511	CLA	C3B-C4B	2.32	1.49	1.42
13	1	506	CLA	C3B-C4B	2.32	1.49	1.42
13	1	511	CLA	C3B-C4B	2.31	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	516	CLA	C3B-C4B	2.31	1.49	1.42
13	d	511	CLA	C3B-C4B	2.31	1.49	1.42
13	A	1101	CLA	CMD-C2D	-2.31	1.46	1.50
13	d	506	CLA	C3B-C4B	2.31	1.49	1.42
13	3	505	CLA	CMD-C2D	-2.31	1.46	1.50
13	A	1011	CLA	CMD-C2D	-2.31	1.46	1.50
13	d	503	CLA	C3B-C4B	2.31	1.49	1.42
13	a	513	CLA	CHC-C1C	2.31	1.43	1.38
13	3	502	CLA	CMB-C2B	-2.31	1.46	1.50
13	B	1225	CLA	CMB-C2B	-2.31	1.46	1.50
13	c	505	CLA	C3B-C4B	2.31	1.49	1.42
13	f	503	CLA	C3B-C4B	2.31	1.49	1.42
13	K	1401	CLA	CMD-C2D	-2.31	1.46	1.50
13	A	1137	CLA	C3B-C4B	2.31	1.49	1.42
13	a	505	CLA	C3B-C4B	2.31	1.49	1.42
13	6	519	CLA	C3B-C4B	2.31	1.49	1.42
13	5	511	CLA	C3B-C4B	2.31	1.49	1.42
13	b	501	CLA	C3B-C4B	2.31	1.49	1.42
13	e	504	CLA	C3B-C4B	2.30	1.49	1.42
13	5	508	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1127	CLA	CMB-C2B	-2.30	1.46	1.50
13	c	502	CLA	CMD-C2D	-2.30	1.46	1.50
13	5	519	CLA	C3B-C4B	2.30	1.49	1.42
13	B	1226	CLA	CMD-C2D	-2.30	1.46	1.50
13	A	1111	CLA	CMC-C2C	-2.30	1.46	1.50
13	B	1012	CLA	C1B-C2B	2.30	1.48	1.43
13	d	504	CLA	C3B-C4B	2.30	1.49	1.42
13	B	1206	CLA	CMB-C2B	-2.30	1.46	1.50
13	3	511	CLA	C3B-C4B	2.30	1.49	1.42
13	b	504	CLA	C3B-C4B	2.30	1.49	1.42
13	6	506	CLA	C3B-C4B	2.30	1.49	1.42
13	e	508	CLA	C3B-C4B	2.30	1.49	1.42
13	1	513	CLA	C3B-C4B	2.30	1.49	1.42
13	d	518	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1104	CLA	CMD-C2D	-2.30	1.46	1.50
13	c	519	CLA	C3B-C4B	2.30	1.49	1.42
13	2	508	CLA	C3B-C4B	2.30	1.49	1.42
13	B	1220	CLA	C3B-C4B	2.30	1.49	1.42
13	a	511	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1119	CLA	C3B-C4B	2.30	1.49	1.42
13	A	1140	CLA	CMB-C2B	-2.29	1.46	1.50
13	6	513	CLA	C3B-C4B	2.29	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1231	CLA	C3B-C4B	2.29	1.49	1.42
13	a	503	CLA	C3B-C4B	2.29	1.49	1.42
13	e	505	CLA	C3B-C4B	2.29	1.49	1.42
13	B	1214	CLA	CMB-C2B	-2.29	1.46	1.50
13	4	506	CLA	C3B-C4B	2.29	1.49	1.42
13	d	505	CLA	C3B-C4B	2.29	1.49	1.42
13	g	511	CLA	C3B-C4B	2.29	1.49	1.42
13	B	1227	CLA	CMD-C2D	-2.29	1.46	1.50
13	A	1120	CLA	CMD-C2D	-2.29	1.46	1.50
13	A	1133	CLA	C1B-C2B	2.29	1.48	1.43
13	c	510	CLA	C3B-C4B	2.29	1.49	1.42
13	4	516	CLA	C3B-C4B	2.29	1.49	1.42
13	A	1109	CLA	CMB-C2B	-2.29	1.46	1.50
13	A	1117	CLA	CMD-C2D	-2.29	1.46	1.50
13	c	516	CLA	CMD-C2D	-2.29	1.46	1.50
13	5	503	CLA	C3B-C4B	2.29	1.49	1.42
13	g	505	CLA	CHC-C1C	2.29	1.43	1.38
13	f	517	CLA	C3B-C4B	2.29	1.49	1.42
13	b	505	CLA	C3B-C4B	2.29	1.49	1.42
13	f	506	CLA	C3B-C4B	2.29	1.49	1.42
13	2	504	CLA	C3B-C4B	2.29	1.49	1.42
13	B	1232	CLA	CMD-C2D	-2.29	1.46	1.50
13	B	1222	CLA	CMD-C2D	-2.29	1.46	1.50
13	B	1223	CLA	CMC-C2C	-2.29	1.46	1.50
13	e	510	CLA	C3B-C4B	2.28	1.49	1.42
13	c	512	CLA	C3B-C4B	2.28	1.49	1.42
13	e	503	CLA	C3B-C4B	2.28	1.49	1.42
13	e	511	CLA	C3B-C4B	2.28	1.49	1.42
13	a	519	CLA	C3B-C4B	2.28	1.49	1.42
13	6	508	CLA	C3B-C4B	2.28	1.49	1.42
13	a	516	CLA	C3B-C4B	2.28	1.49	1.42
13	4	517	CLA	C3B-C4B	2.28	1.49	1.42
13	1	503	CLA	C3B-C4B	2.28	1.49	1.42
13	5	516	CLA	C3B-C4B	2.28	1.49	1.42
13	d	510	CLA	C3B-C4B	2.28	1.49	1.42
13	c	518	CLA	C3B-C4B	2.28	1.49	1.42
13	B	1202	CLA	CMD-C2D	-2.28	1.46	1.50
13	g	517	CLA	C3B-C4B	2.28	1.49	1.42
13	5	505	CLA	CMD-C2D	-2.28	1.46	1.50
13	B	1234	CLA	C1B-C2B	2.28	1.48	1.43
13	B	1205	CLA	C3B-C4B	2.28	1.49	1.42
14	A	4011	BCR	C1-C6	-2.28	1.50	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	506	CLA	C3B-C4B	2.28	1.49	1.42
13	b	510	CLA	CHC-C1C	2.28	1.43	1.38
13	g	508	CLA	C3B-C4B	2.28	1.49	1.42
13	a	513	CLA	C3B-C4B	2.28	1.49	1.42
13	6	505	CLA	CMD-C2D	-2.28	1.46	1.50
13	A	1139	CLA	C3B-C4B	2.28	1.49	1.42
13	f	502	CLA	C3B-C4B	2.28	1.49	1.42
13	A	1115	CLA	C3B-C4B	2.28	1.49	1.42
13	6	511	CLA	C3B-C4B	2.28	1.49	1.42
13	d	505	CLA	CMD-C2D	-2.28	1.46	1.50
13	A	1120	CLA	C3B-C4B	2.28	1.49	1.42
13	c	516	CLA	C3B-C4B	2.28	1.49	1.42
13	a	508	CLA	CMD-C2D	-2.27	1.46	1.50
13	B	1235	CLA	CMC-C2C	-2.27	1.46	1.50
13	g	513	CLA	CHC-C1C	2.27	1.43	1.38
13	A	1136	CLA	C3B-C4B	2.27	1.49	1.42
14	B	4010	BCR	C30-C25	-2.27	1.50	1.53
13	A	1117	CLA	C3B-C4B	2.27	1.49	1.42
13	A	1133	CLA	C3B-C4B	2.27	1.49	1.42
13	f	509	CLA	C3B-C4B	2.27	1.49	1.42
13	B	1210	CLA	CMC-C2C	-2.27	1.46	1.50
13	f	513	CLA	C3B-C4B	2.27	1.49	1.42
13	A	1130	CLA	C3B-C4B	2.27	1.49	1.42
13	K	1103	CLA	C3B-C4B	2.27	1.49	1.42
13	B	1224	CLA	C1B-C2B	2.27	1.48	1.43
13	B	1231	CLA	CMB-C2B	-2.27	1.46	1.50
13	3	503	CLA	C3B-C4B	2.27	1.49	1.42
13	B	1214	CLA	CMC-C2C	-2.27	1.46	1.50
13	3	513	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1108	CLA	CMB-C2B	-2.26	1.46	1.50
13	A	1123	CLA	CMB-C2B	-2.26	1.46	1.50
13	g	505	CLA	CMD-C2D	-2.26	1.46	1.50
13	K	1401	CLA	CMB-C2B	-2.26	1.46	1.50
13	2	516	CLA	C3B-C4B	2.26	1.49	1.42
13	b	505	CLA	CMD-C2D	-2.26	1.46	1.50
13	1	510	CLA	C3B-C4B	2.26	1.49	1.42
13	e	513	CLA	C3B-C4B	2.26	1.49	1.42
13	6	501	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1107	CLA	CMC-C2C	-2.26	1.46	1.50
13	A	1138	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1110	CLA	C3B-C4B	2.26	1.49	1.42
13	4	502	CLA	CMB-C2B	-2.26	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	507	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1103	CLA	CMD-C2D	-2.26	1.46	1.50
13	a	507	CLA	C3B-C4B	2.26	1.49	1.42
13	1	509	CLA	C3B-C4B	2.26	1.49	1.42
13	6	503	CLA	C3B-C4B	2.26	1.49	1.42
13	A	1124	CLA	CMB-C2B	-2.26	1.46	1.50
13	J	1303	CLA	C4C-C3C	-2.25	1.46	1.52
13	f	507	CLA	C3B-C4B	2.25	1.49	1.42
13	B	1211	CLA	CMD-C2D	-2.25	1.46	1.50
13	d	502	CLA	CMD-C2D	-2.25	1.46	1.50
13	4	503	CLA	C3B-C4B	2.25	1.49	1.42
13	f	508	CLA	CMB-C2B	-2.25	1.46	1.50
13	2	505	CLA	CMD-C2D	-2.25	1.46	1.50
13	5	501	CLA	C3B-C4B	2.25	1.49	1.42
13	2	511	CLA	CMB-C2B	-2.25	1.46	1.50
13	b	510	CLA	CMD-C2D	-2.25	1.46	1.50
13	J	1302	CLA	C3B-C4B	2.25	1.49	1.42
13	e	517	CLA	C3B-C4B	2.25	1.49	1.42
13	6	516	CLA	C3B-C4B	2.25	1.49	1.42
13	b	519	CLA	C3B-C4B	2.25	1.49	1.42
13	B	1227	CLA	CMB-C2B	-2.25	1.46	1.50
13	d	511	CLA	CMD-C2D	-2.25	1.46	1.50
13	d	512	CLA	C3B-C4B	2.25	1.49	1.42
13	4	519	CLA	CHC-C1C	2.25	1.43	1.38
13	A	1130	CLA	CMD-C2D	-2.25	1.46	1.50
13	A	1140	CLA	C1B-C2B	2.25	1.48	1.43
13	3	519	CLA	C3B-C4B	2.25	1.49	1.42
13	2	502	CLA	CMD-C2D	-2.25	1.46	1.50
13	4	513	CLA	C3B-C4B	2.25	1.49	1.42
13	2	507	CLA	C3B-C4B	2.25	1.49	1.42
13	3	508	CLA	CMD-C2D	-2.24	1.46	1.50
13	e	502	CLA	CMB-C2B	-2.24	1.46	1.50
13	2	502	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	1022	CLA	C1B-C2B	2.24	1.48	1.43
13	3	508	CLA	C3B-C4B	2.24	1.49	1.42
13	3	506	CLA	CHC-C1C	2.24	1.43	1.38
13	B	1216	CLA	C1B-C2B	2.24	1.48	1.43
13	g	510	CLA	C3B-C4B	2.24	1.49	1.42
13	2	510	CLA	C3B-C4B	2.24	1.49	1.42
13	4	510	CLA	CHC-C1C	2.24	1.43	1.38
13	4	505	CLA	CMD-C2D	-2.24	1.46	1.50
13	A	1119	CLA	CMB-C2B	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	502	CLA	CMB-C2B	-2.24	1.46	1.50
13	4	501	CLA	C3B-C4B	2.24	1.49	1.42
13	B	1234	CLA	CMC-C2C	-2.24	1.46	1.50
13	3	504	CLA	C3B-C4B	2.24	1.49	1.42
13	c	513	CLA	C3B-C4B	2.24	1.49	1.42
13	2	518	CLA	C3B-C4B	2.24	1.49	1.42
13	B	1208	CLA	CMD-C2D	-2.24	1.46	1.50
13	B	1239	CLA	CMD-C2D	-2.24	1.46	1.50
13	A	1116	CLA	C3B-C4B	2.24	1.49	1.42
13	A	1126	CLA	C3B-C4B	2.24	1.49	1.42
14	J	4013	BCR	C30-C25	-2.24	1.50	1.53
13	B	1232	CLA	CMB-C2B	-2.24	1.46	1.50
13	B	1211	CLA	CMB-C2B	-2.24	1.46	1.50
13	A	1140	CLA	CMD-C2D	-2.24	1.46	1.50
13	B	1219	CLA	CMB-C2B	-2.24	1.46	1.50
13	B	1228	CLA	CMD-C2D	-2.24	1.46	1.50
13	B	1215	CLA	CMD-C2D	-2.24	1.46	1.50
13	5	505	CLA	C3B-C4B	2.24	1.49	1.42
13	K	1401	CLA	C3B-C4B	2.24	1.49	1.42
13	d	519	CLA	C3B-C4B	2.24	1.49	1.42
13	b	513	CLA	C3B-C4B	2.24	1.49	1.42
13	A	1116	CLA	CMD-C2D	-2.23	1.46	1.50
13	4	518	CLA	C3B-C4B	2.23	1.49	1.42
13	A	1129	CLA	C3B-C4B	2.23	1.49	1.42
13	6	506	CLA	CHC-C1C	2.23	1.43	1.38
13	B	1012	CLA	CMD-C2D	-2.23	1.46	1.50
13	6	502	CLA	CMB-C2B	-2.23	1.46	1.50
13	A	1115	CLA	CMB-C2B	-2.23	1.46	1.50
13	A	1137	CLA	CMD-C2D	-2.23	1.46	1.50
13	1	501	CLA	C3B-C4B	2.23	1.49	1.42
13	1	507	CLA	C3B-C4B	2.23	1.49	1.42
13	B	1021	CLA	CMC-C2C	-2.23	1.46	1.50
13	1	502	CLA	C3B-C4B	2.23	1.49	1.42
13	c	502	CLA	C3B-C4B	2.23	1.49	1.42
13	B	1205	CLA	CMB-C2B	-2.23	1.46	1.50
13	e	506	CLA	CMB-C2B	-2.23	1.46	1.50
13	3	509	CLA	C3B-C4B	2.23	1.49	1.42
13	4	505	CLA	C3B-C4B	2.23	1.49	1.42
13	1	518	CLA	C3B-C4B	2.23	1.49	1.42
13	d	517	CLA	C3B-C4B	2.23	1.49	1.42
13	e	518	CLA	C3B-C4B	2.23	1.49	1.42
13	5	504	CLA	C3B-C4B	2.23	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1116	CLA	CMB-C2B	-2.23	1.46	1.50
13	6	509	CLA	C3B-C4B	2.23	1.49	1.42
13	B	1211	CLA	C3B-C4B	2.23	1.49	1.42
13	A	1111	CLA	C3B-C4B	2.23	1.49	1.42
13	e	519	CLA	C3B-C4B	2.23	1.49	1.42
13	f	516	CLA	C3B-C4B	2.23	1.49	1.42
13	A	1112	CLA	CMD-C2D	-2.23	1.46	1.50
13	A	1131	CLA	CMD-C2D	-2.23	1.46	1.50
13	A	1135	CLA	CMB-C2B	-2.23	1.46	1.50
13	B	1023	CLA	CMB-C2B	-2.23	1.46	1.50
13	B	1209	CLA	CMD-C2D	-2.23	1.46	1.50
13	B	1233	CLA	C3B-C4B	2.23	1.49	1.42
13	f	505	CLA	MG-NB	-2.23	2.01	2.05
13	2	511	CLA	C3B-C4B	2.23	1.49	1.42
13	1	513	CLA	CHC-C1C	2.22	1.42	1.38
13	4	511	CLA	CHC-C1C	2.22	1.42	1.38
13	A	1109	CLA	CMC-C2C	-2.22	1.46	1.50
13	B	1234	CLA	C3B-C4B	2.22	1.49	1.42
13	f	519	CLA	CHC-C1C	2.22	1.42	1.38
13	5	508	CLA	CMB-C2B	-2.22	1.46	1.50
13	1	504	CLA	C3B-C4B	2.22	1.49	1.42
13	A	1106	CLA	CMD-C2D	-2.22	1.46	1.50
13	B	1201	CLA	C3B-C4B	2.22	1.49	1.42
13	c	503	CLA	C3B-C4B	2.22	1.49	1.42
13	f	504	CLA	C3B-C4B	2.22	1.49	1.42
13	A	1121	CLA	CMD-C2D	-2.22	1.46	1.50
13	B	1210	CLA	C3B-C4B	2.22	1.49	1.42
13	A	1105	CLA	CMB-C2B	-2.22	1.46	1.50
13	B	1206	CLA	CMD-C2D	-2.22	1.46	1.50
13	4	508	CLA	C3B-C4B	2.22	1.49	1.42
13	B	1222	CLA	C3B-C4B	2.22	1.49	1.42
13	F	1301	CLA	CMB-C2B	-2.22	1.46	1.50
13	A	1120	CLA	CHC-C1C	2.22	1.42	1.38
13	A	1113	CLA	CMD-C2D	-2.22	1.46	1.50
13	A	1127	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1022	CLA	CMB-C2B	-2.21	1.46	1.50
13	c	511	CLA	CMD-C2D	-2.21	1.46	1.50
13	g	519	CLA	CHC-C1C	2.21	1.42	1.38
13	4	509	CLA	C3B-C4B	2.21	1.49	1.42
13	5	507	CLA	C3B-C4B	2.21	1.49	1.42
13	g	518	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1118	CLA	CMB-C2B	-2.21	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	g	508	CLA	CMD-C2D	-2.21	1.46	1.50
13	A	1139	CLA	CMB-C2B	-2.21	1.46	1.50
13	A	1022	CLA	CMD-C2D	-2.21	1.46	1.50
13	A	1109	CLA	CMD-C2D	-2.21	1.46	1.50
13	B	1221	CLA	CMB-C2B	-2.21	1.46	1.50
13	b	507	CLA	C3B-C4B	2.21	1.49	1.42
13	1	512	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1132	CLA	CMB-C2B	-2.21	1.46	1.50
13	b	503	CLA	C3B-C4B	2.21	1.49	1.42
13	B	1230	CLA	CMC-C2C	-2.21	1.46	1.50
13	A	1102	CLA	CHC-C1C	2.21	1.42	1.38
13	1	505	CLA	CMD-C2D	-2.21	1.46	1.50
13	3	501	CLA	C3B-C4B	2.21	1.49	1.42
13	3	505	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1121	CLA	C3B-C4B	2.21	1.49	1.42
13	A	1125	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	1131	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	1237	CLA	CMD-C2D	-2.20	1.46	1.50
13	d	504	CLA	CHC-C1C	2.20	1.42	1.38
13	B	1223	CLA	CMD-C2D	-2.20	1.46	1.50
13	a	518	CLA	C3B-C4B	2.20	1.49	1.42
13	B	1229	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	1801	CLA	C3B-C4B	2.20	1.49	1.42
13	A	1237	CLA	CMC-C2C	-2.20	1.46	1.50
13	B	1229	CLA	CMC-C2C	-2.20	1.46	1.50
13	B	1238	CLA	C3B-C4B	2.20	1.49	1.42
13	b	502	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	1011	CLA	CMB-C2B	-2.20	1.46	1.50
13	B	1210	CLA	CMB-C2B	-2.20	1.46	1.50
13	B	1229	CLA	CMD-C2D	-2.20	1.46	1.50
13	B	1230	CLA	CMD-C2D	-2.20	1.46	1.50
13	B	1236	CLA	CMB-C2B	-2.20	1.46	1.50
13	A	1124	CLA	C3B-C4B	2.20	1.49	1.42
13	b	511	CLA	C3B-C4B	2.20	1.49	1.42
13	B	1217	CLA	C3B-C4B	2.20	1.49	1.42
13	B	1231	CLA	CMD-C2D	-2.20	1.46	1.50
13	6	518	CLA	C3B-C4B	2.20	1.49	1.42
13	c	511	CLA	CMB-C2B	-2.20	1.46	1.50
13	B	1225	CLA	C3B-C4B	2.20	1.49	1.42
13	A	1101	CLA	CMB-C2B	-2.20	1.46	1.50
13	b	511	CLA	CMD-C2D	-2.20	1.46	1.50
13	A	1801	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	502	CLA	C3B-C4B	2.19	1.49	1.42
13	b	501	CLA	CMD-C2D	-2.19	1.46	1.50
13	3	507	CLA	C3B-C4B	2.19	1.49	1.42
13	d	502	CLA	C3B-C4B	2.19	1.49	1.42
13	1	513	CLA	CMB-C2B	-2.19	1.46	1.50
13	B	1208	CLA	C3B-C4B	2.19	1.49	1.42
13	B	1213	CLA	C3B-C4B	2.19	1.49	1.42
13	J	1303	CLA	C3B-C4B	2.19	1.49	1.42
13	4	508	CLA	CMB-C2B	-2.19	1.46	1.50
13	a	502	CLA	C3B-C4B	2.19	1.49	1.42
13	B	1218	CLA	CMD-C2D	-2.19	1.46	1.50
13	f	502	CLA	CMD-C2D	-2.19	1.46	1.50
14	I	4020	BCR	C1-C6	-2.19	1.51	1.53
13	2	509	CLA	C3B-C4B	2.19	1.49	1.42
13	B	1217	CLA	CMB-C2B	-2.19	1.46	1.50
13	a	502	CLA	CMC-C2C	-2.19	1.46	1.50
13	b	518	CLA	C3B-C4B	2.19	1.49	1.42
13	6	505	CLA	C3B-C4B	2.19	1.49	1.42
13	f	511	CLA	CHC-C1C	2.19	1.42	1.38
13	B	1216	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1117	CLA	C1B-C2B	2.19	1.48	1.43
13	f	510	CLA	C3B-C4B	2.19	1.49	1.42
13	b	508	CLA	CMB-C2B	-2.19	1.46	1.50
13	e	507	CLA	C3B-C4B	2.19	1.49	1.42
13	d	507	CLA	C3B-C4B	2.19	1.49	1.42
13	A	1022	CLA	C3B-C4B	2.19	1.49	1.42
13	g	509	CLA	C3B-C4B	2.19	1.49	1.42
13	4	518	CLA	CMD-C2D	-2.19	1.46	1.50
13	A	1119	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1122	CLA	CMC-C2C	-2.18	1.46	1.50
13	B	1220	CLA	CMD-C2D	-2.18	1.46	1.50
13	J	1303	CLA	CMB-C2B	-2.18	1.46	1.50
13	2	506	CLA	CHC-C1C	2.18	1.42	1.38
13	c	506	CLA	CHC-C1C	2.18	1.42	1.38
13	B	1012	CLA	C3B-C4B	2.18	1.49	1.42
13	4	507	CLA	C3B-C4B	2.18	1.49	1.42
13	A	1128	CLA	CMD-C2D	-2.18	1.46	1.50
13	b	508	CLA	CMD-C2D	-2.18	1.46	1.50
13	c	519	CLA	CHC-C1C	2.18	1.42	1.38
13	6	502	CLA	CMC-C2C	-2.18	1.46	1.50
13	A	1109	CLA	C3B-C4B	2.18	1.49	1.42
14	A	4008	BCR	C30-C25	-2.18	1.51	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	2	505	CLA	C3B-C4B	2.18	1.49	1.42
13	A	1122	CLA	CMB-C2B	-2.18	1.46	1.50
13	a	517	CLA	CHC-C1C	2.18	1.42	1.38
13	e	511	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	508	CLA	C3B-C4B	2.18	1.49	1.42
13	3	502	CLA	CMD-C2D	-2.18	1.46	1.50
13	A	1102	CLA	C3B-C4B	2.18	1.49	1.42
13	2	501	CLA	CMC-C2C	-2.18	1.46	1.50
13	5	502	CLA	CMC-C2C	-2.18	1.46	1.50
13	c	513	CLA	CMD-C2D	-2.18	1.46	1.50
13	a	501	CLA	CMD-C2D	-2.18	1.46	1.50
13	B	1214	CLA	C3B-C4B	2.18	1.49	1.42
13	A	1139	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1012	CLA	CMB-C2B	-2.17	1.46	1.50
13	B	1211	CLA	CMC-C2C	-2.17	1.46	1.50
13	d	506	CLA	CHC-C1C	2.17	1.42	1.38
13	3	518	CLA	C3B-C4B	2.17	1.49	1.42
13	4	504	CLA	C3B-C4B	2.17	1.49	1.42
13	e	506	CLA	CHC-C1C	2.17	1.42	1.38
13	6	502	CLA	C3B-C4B	2.17	1.49	1.42
13	e	509	CLA	C3B-C4B	2.17	1.49	1.42
13	5	502	CLA	CMB-C2B	-2.17	1.46	1.50
13	B	1204	CLA	CMD-C2D	-2.17	1.46	1.50
13	5	503	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1209	CLA	CMB-C2B	-2.17	1.46	1.50
13	a	506	CLA	CHC-C1C	2.17	1.42	1.38
13	5	502	CLA	CMD-C2D	-2.17	1.46	1.50
13	6	518	CLA	CMD-C2D	-2.17	1.46	1.50
13	A	1120	CLA	CMB-C2B	-2.17	1.46	1.50
13	A	1011	CLA	CMC-C2C	-2.17	1.46	1.50
13	A	1117	CLA	MG-NB	-2.17	2.01	2.05
13	3	509	CLA	CMD-C2D	-2.17	1.46	1.50
13	e	512	CLA	CMD-C2D	-2.17	1.46	1.50
13	5	506	CLA	CHC-C1C	2.17	1.42	1.38
13	2	501	CLA	CMD-C2D	-2.17	1.46	1.50
13	d	511	CLA	CMB-C2B	-2.17	1.46	1.50
13	e	501	CLA	CMD-C2D	-2.17	1.46	1.50
13	a	510	CLA	CHC-C1C	2.17	1.42	1.38
13	A	1112	CLA	CMC-C2C	-2.17	1.46	1.50
13	A	1013	CLA	C3B-C4B	2.17	1.49	1.42
13	A	1237	CLA	CHC-C1C	2.17	1.42	1.38
13	g	504	CLA	CHC-C1C	2.17	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1103	CLA	CMC-C2C	-2.17	1.46	1.50
13	B	1234	CLA	CMB-C2B	-2.17	1.46	1.50
13	6	511	CLA	CHC-C1C	2.17	1.42	1.38
13	B	1219	CLA	C3B-C4B	2.17	1.49	1.42
13	1	502	CLA	CMD-C2D	-2.17	1.46	1.50
13	B	1217	CLA	CMD-C2D	-2.17	1.46	1.50
13	5	509	CLA	C3B-C4B	2.17	1.49	1.42
13	B	1201	CLA	CMB-C2B	-2.17	1.46	1.50
13	B	1205	CLA	CMC-C2C	-2.17	1.46	1.50
13	g	511	CLA	CMD-C2D	-2.17	1.46	1.50
13	2	518	CLA	CMD-C2D	-2.17	1.46	1.50
13	6	507	CLA	C3B-C4B	2.16	1.49	1.42
13	B	1228	CLA	C3B-C4B	2.16	1.49	1.42
13	b	506	CLA	CHC-C4B	-2.16	1.34	1.39
13	A	1137	CLA	CMB-C2B	-2.16	1.46	1.50
13	4	510	CLA	CMD-C2D	-2.16	1.46	1.50
13	B	1224	CLA	CMD-C2D	-2.16	1.46	1.50
13	a	505	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	1022	CLA	CHC-C1C	2.16	1.42	1.38
13	A	1113	CLA	C3B-C4B	2.16	1.49	1.42
13	g	502	CLA	C3B-C4B	2.16	1.49	1.42
13	A	1022	CLA	CMC-C2C	-2.16	1.46	1.50
13	A	1801	CLA	CMC-C2C	-2.16	1.46	1.50
13	B	1221	CLA	CMC-C2C	-2.16	1.46	1.50
13	B	1227	CLA	CMC-C2C	-2.16	1.46	1.50
13	c	504	CLA	CHC-C1C	2.16	1.42	1.38
13	X	1401	CLA	CMD-C2D	-2.16	1.46	1.50
13	B	1204	CLA	C3B-C4B	2.16	1.49	1.42
13	3	510	CLA	CHC-C1C	2.16	1.42	1.38
13	A	1118	CLA	CMD-C2D	-2.16	1.46	1.50
13	A	1125	CLA	C3B-C4B	2.16	1.49	1.42
13	B	1220	CLA	CMC-C2C	-2.16	1.46	1.50
13	c	507	CLA	C3B-C4B	2.16	1.49	1.42
13	B	1210	CLA	CMD-C2D	-2.16	1.46	1.50
13	e	518	CLA	CMD-C2D	-2.16	1.46	1.50
13	b	502	CLA	CMC-C2C	-2.16	1.46	1.50
13	f	505	CLA	C3B-C4B	2.16	1.49	1.42
13	4	508	CLA	CMD-C2D	-2.16	1.46	1.50
13	3	513	CLA	CHC-C1C	2.16	1.42	1.38
13	a	503	CLA	CHC-C1C	2.16	1.42	1.38
13	5	513	CLA	CHC-C1C	2.16	1.42	1.38
13	A	1136	CLA	CMB-C2B	-2.16	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	c	505	CLA	CMD-C2D	-2.16	1.46	1.50
14	5	523	BCR	C40-C30	-2.16	1.49	1.53
13	A	1119	CLA	CMC-C2C	-2.16	1.46	1.50
13	A	1129	CLA	CMB-C2B	-2.16	1.46	1.50
13	A	1138	CLA	CMD-C2D	-2.16	1.46	1.50
13	g	512	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	1115	CLA	CMC-C2C	-2.15	1.46	1.50
13	A	1115	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	1201	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	1124	CLA	CMD-C2D	-2.15	1.46	1.50
13	b	509	CLA	CMD-C2D	-2.15	1.46	1.50
13	A	1133	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1212	CLA	C3B-C4B	2.15	1.49	1.42
13	B	1213	CLA	CMB-C2B	-2.15	1.46	1.50
13	f	506	CLA	CHC-C1C	2.15	1.42	1.38
13	3	502	CLA	CMC-C2C	-2.15	1.46	1.50
13	B	1216	CLA	CMC-C2C	-2.15	1.46	1.50
13	c	511	CLA	CHC-C1C	2.15	1.42	1.38
13	B	1233	CLA	CMD-C2D	-2.15	1.46	1.50
13	g	509	CLA	CMB-C2B	-2.15	1.46	1.50
13	4	511	CLA	MG-NB	-2.15	2.01	2.05
13	4	512	CLA	CMD-C2D	-2.15	1.46	1.50
13	B	1203	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	1238	CLA	CMC-C2C	-2.15	1.46	1.50
13	B	1202	CLA	C3B-C4B	2.15	1.49	1.42
13	B	1239	CLA	C3B-C4B	2.15	1.49	1.42
13	b	507	CLA	CHC-C1C	2.15	1.42	1.38
13	b	512	CLA	C3B-C4B	2.15	1.49	1.42
13	1	511	CLA	CHC-C1C	2.15	1.42	1.38
13	e	509	CLA	CMD-C2D	-2.15	1.46	1.50
13	b	502	CLA	CMB-C2B	-2.15	1.46	1.50
13	4	516	CLA	CHC-C1C	2.15	1.42	1.38
13	A	1101	CLA	CMC-C2C	-2.15	1.46	1.50
13	A	1125	CLA	CMB-C2B	-2.15	1.46	1.50
13	g	502	CLA	CMB-C2B	-2.15	1.46	1.50
13	d	517	CLA	CMC-C2C	-2.15	1.46	1.50
13	g	507	CLA	CMD-C2D	-2.15	1.46	1.50
13	d	508	CLA	CHC-C1C	2.15	1.42	1.38
13	A	1121	CLA	CMB-C2B	-2.15	1.46	1.50
13	B	1012	CLA	CMC-C2C	-2.15	1.46	1.50
13	5	511	CLA	CMD-C2D	-2.15	1.46	1.50
13	d	509	CLA	C3B-C4B	2.14	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	d	513	CLA	C3B-C4B	2.14	1.49	1.42
13	3	510	CLA	CMD-C2D	-2.14	1.46	1.50
13	f	502	CLA	CMC-C2C	-2.14	1.46	1.50
13	A	1122	CLA	C3B-C4B	2.14	1.49	1.42
13	B	1222	CLA	CMB-C2B	-2.14	1.46	1.50
13	2	513	CLA	CHC-C1C	2.14	1.42	1.38
13	4	509	CLA	CMC-C2C	-2.14	1.46	1.50
13	J	1302	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1202	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	1133	CLA	CMC-C2C	-2.14	1.46	1.50
13	b	502	CLA	C3B-C4B	2.14	1.49	1.42
13	5	518	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1203	CLA	CMC-C2C	-2.14	1.46	1.50
13	5	511	CLA	CHC-C1C	2.14	1.42	1.38
13	2	503	CLA	CHC-C1C	2.14	1.42	1.38
13	a	506	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	1134	CLA	C3B-C4B	2.14	1.49	1.42
13	3	508	CLA	CMB-C2B	-2.14	1.46	1.50
13	d	512	CLA	CMB-C2B	-2.14	1.46	1.50
13	A	1123	CLA	C3B-C4B	2.14	1.49	1.42
13	d	519	CLA	CHC-C1C	2.14	1.42	1.38
13	f	506	CLA	CMB-C2B	-2.14	1.46	1.50
13	f	508	CLA	CMD-C2D	-2.14	1.46	1.50
13	g	517	CLA	CMD-C2D	-2.14	1.46	1.50
13	a	512	CLA	CMD-C2D	-2.14	1.46	1.50
13	c	513	CLA	CMB-C2B	-2.14	1.46	1.50
13	J	1303	CLA	CMD-C2D	-2.14	1.46	1.50
13	d	501	CLA	CMD-C2D	-2.14	1.46	1.50
13	A	1129	CLA	CMD-C2D	-2.14	1.46	1.50
13	c	508	CLA	CMC-C2C	-2.14	1.46	1.50
13	b	511	CLA	CMB-C2B	-2.14	1.46	1.50
13	3	501	CLA	CMD-C2D	-2.14	1.46	1.50
13	2	508	CLA	CMC-C2C	-2.14	1.46	1.50
13	B	1236	CLA	CMD-C2D	-2.14	1.46	1.50
13	B	1233	CLA	CMB-C2B	-2.14	1.46	1.50
13	B	1203	CLA	C3B-C4B	2.14	1.49	1.42
13	b	512	CLA	CMD-C2D	-2.14	1.46	1.50
13	4	506	CLA	CHC-C1C	2.14	1.42	1.38
13	a	501	CLA	CHC-C1C	2.14	1.42	1.38
13	A	1105	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	1134	CLA	CMB-C2B	-2.13	1.46	1.50
13	K	1103	CLA	CMD-C2D	-2.13	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	1	512	CLA	CMB-C2B	-2.13	1.46	1.50
13	B	1232	CLA	C3B-C4B	2.13	1.49	1.42
13	B	1235	CLA	CMD-C2D	-2.13	1.46	1.50
13	c	512	CLA	CMB-C2B	-2.13	1.46	1.50
13	a	509	CLA	CMB-C2B	-2.13	1.46	1.50
13	3	511	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1102	CLA	CMC-C2C	-2.13	1.46	1.50
13	B	1213	CLA	CMD-C2D	-2.13	1.46	1.50
13	5	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	d	508	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1235	CLA	CMB-C2B	-2.13	1.46	1.50
13	e	505	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1221	CLA	C3B-C4B	2.13	1.48	1.42
13	a	511	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1206	CLA	CMC-C2C	-2.13	1.46	1.50
13	c	512	CLA	CMD-C2D	-2.13	1.46	1.50
13	d	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	a	511	CLA	CMB-C2B	-2.13	1.46	1.50
13	A	1135	CLA	C3B-C4B	2.13	1.48	1.42
13	2	505	CLA	CHC-C1C	2.13	1.42	1.38
13	e	501	CLA	CHC-C1C	2.13	1.42	1.38
13	6	512	CLA	CMD-C2D	-2.13	1.46	1.50
13	A	1116	CLA	CMC-C2C	-2.13	1.46	1.50
13	a	506	CLA	CMD-C2D	-2.13	1.46	1.50
13	c	509	CLA	C3B-C4B	2.13	1.48	1.42
13	A	1126	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1228	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1237	CLA	CMB-C2B	-2.13	1.46	1.50
13	A	1112	CLA	C3B-C4B	2.13	1.48	1.42
13	c	502	CLA	CMB-C2B	-2.13	1.46	1.50
13	c	502	CLA	CMC-C2C	-2.13	1.46	1.50
13	f	511	CLA	CMD-C2D	-2.13	1.46	1.50
13	2	509	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1203	CLA	CMD-C2D	-2.13	1.46	1.50
13	B	1216	CLA	CHC-C1C	2.13	1.42	1.38
13	B	1229	CLA	CHC-C1C	2.13	1.42	1.38
13	A	1103	CLA	CMB-C2B	-2.13	1.46	1.50
13	A	1106	CLA	CMB-C2B	-2.13	1.46	1.50
13	a	511	CLA	CHC-C1C	2.13	1.42	1.38
13	4	501	CLA	CMD-C2D	-2.13	1.46	1.50
14	a	523	BCR	C30-C25	-2.13	1.51	1.53
13	2	519	CLA	CHC-C1C	2.12	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1228	CLA	CMB-C2B	-2.12	1.46	1.50
13	A	1132	CLA	CMD-C2D	-2.12	1.46	1.50
13	f	512	CLA	CMD-C2D	-2.12	1.46	1.50
13	5	501	CLA	CMD-C2D	-2.12	1.46	1.50
13	6	510	CLA	CHC-C1C	2.12	1.42	1.38
13	3	518	CLA	CMD-C2D	-2.12	1.46	1.50
13	F	1301	CLA	CMC-C2C	-2.12	1.46	1.50
13	a	516	CLA	CHC-C1C	2.12	1.42	1.38
13	B	1201	CLA	CMC-C2C	-2.12	1.46	1.50
13	c	518	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1239	CLA	CMC-C2C	-2.12	1.46	1.50
13	c	519	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1216	CLA	C3B-C4B	2.12	1.48	1.42
13	f	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	e	511	CLA	CHC-C1C	2.12	1.42	1.38
13	A	1136	CLA	CMD-C2D	-2.12	1.46	1.50
13	B	1207	CLA	CMB-C2B	-2.12	1.46	1.50
13	d	512	CLA	CMD-C2D	-2.12	1.46	1.50
13	g	501	CLA	CMD-C2D	-2.12	1.46	1.50
13	A	1110	CLA	CMC-C2C	-2.12	1.46	1.50
13	B	1226	CLA	CMC-C2C	-2.12	1.46	1.50
13	B	1209	CLA	C3B-C4B	2.12	1.48	1.42
13	A	1114	CLA	C3B-C4B	2.12	1.48	1.42
13	6	508	CLA	CHC-C1C	2.12	1.42	1.38
13	3	518	CLA	CMB-C2B	-2.12	1.46	1.50
13	3	511	CLA	CMB-C2B	-2.12	1.46	1.50
13	d	501	CLA	CMB-C2B	-2.12	1.46	1.50
13	5	516	CLA	CHC-C1C	2.12	1.42	1.38
13	5	518	CLA	C3B-C4B	2.11	1.48	1.42
13	3	507	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1212	CLA	CMD-C2D	-2.11	1.46	1.50
13	b	508	CLA	CMC-C2C	-2.11	1.46	1.50
13	B	1222	CLA	CHC-C1C	2.11	1.42	1.38
13	f	505	CLA	CHC-C1C	2.11	1.42	1.38
13	4	503	CLA	CHC-C1C	2.11	1.42	1.38
13	c	509	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	502	CLA	CMD-C2D	-2.11	1.46	1.50
13	5	519	CLA	CHC-C1C	2.11	1.42	1.38
13	a	504	CLA	CHC-C1C	2.11	1.42	1.38
13	e	501	CLA	CMB-C2B	-2.11	1.46	1.50
13	d	510	CLA	CHC-C1C	2.11	1.42	1.38
13	3	504	CLA	CMD-C2D	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	5	501	CLA	CMC-C2C	-2.11	1.46	1.50
13	g	512	CLA	CMB-C2B	-2.11	1.46	1.50
13	d	503	CLA	CHC-C1C	2.11	1.42	1.38
14	3	522	BCR	C30-C25	-2.11	1.51	1.53
13	3	519	CLA	CHC-C1C	2.11	1.42	1.38
13	b	501	CLA	CMB-C2B	-2.11	1.46	1.50
13	1	508	CLA	CHC-C1C	2.11	1.42	1.38
13	2	501	CLA	CMB-C2B	-2.11	1.46	1.50
13	d	518	CLA	CMD-C2D	-2.11	1.46	1.50
13	6	516	CLA	CHC-C1C	2.11	1.42	1.38
13	B	1218	CLA	C3B-C4B	2.11	1.48	1.42
13	4	502	CLA	CMC-C2C	-2.11	1.46	1.50
13	2	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	B	1220	CLA	CMB-C2B	-2.11	1.46	1.50
13	B	1207	CLA	CMD-C2D	-2.11	1.46	1.50
13	e	508	CLA	CMB-C2B	-2.11	1.46	1.50
13	f	511	CLA	CMB-C2B	-2.11	1.46	1.50
13	a	505	CLA	CHC-C1C	2.11	1.42	1.38
13	b	505	CLA	MG-NB	-2.11	2.01	2.05
13	e	513	CLA	CHC-C1C	2.11	1.42	1.38
13	4	503	CLA	CMD-C2D	-2.11	1.46	1.50
13	5	506	CLA	CMD-C2D	-2.11	1.46	1.50
13	6	504	CLA	CHC-C1C	2.11	1.42	1.38
13	5	512	CLA	CMD-C2D	-2.11	1.46	1.50
13	4	505	CLA	CHC-C1C	2.11	1.42	1.38
13	5	516	CLA	CMD-C2D	-2.11	1.46	1.50
13	5	518	CLA	CMB-C2B	-2.11	1.46	1.50
13	6	510	CLA	CMD-C2D	-2.11	1.46	1.50
13	B	1224	CLA	CMC-C2C	-2.11	1.46	1.50
13	b	504	CLA	CMD-C2D	-2.11	1.46	1.50
13	6	504	CLA	CMD-C2D	-2.11	1.46	1.50
13	A	1133	CLA	CMD-C2D	-2.11	1.46	1.50
13	d	508	CLA	CMB-C2B	-2.11	1.46	1.50
13	X	1401	CLA	CHC-C1C	2.10	1.42	1.38
13	A	1127	CLA	CMC-C2C	-2.10	1.46	1.50
13	4	507	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	1222	CLA	CMC-C2C	-2.10	1.46	1.50
13	1	513	CLA	CMC-C2C	-2.10	1.46	1.50
13	A	1801	CLA	CMB-C2B	-2.10	1.46	1.50
13	B	1232	CLA	CMC-C2C	-2.10	1.46	1.50
13	1	501	CLA	CMD-C2D	-2.10	1.46	1.50
13	1	508	CLA	CMB-C2B	-2.10	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	J	1302	CLA	CMB-C2B	-2.10	1.46	1.50
13	b	516	CLA	CMD-C2D	-2.10	1.46	1.50
13	3	513	CLA	CMC-C2C	-2.10	1.46	1.50
13	F	1301	CLA	CMD-C2D	-2.10	1.46	1.50
13	a	507	CLA	CHC-C1C	2.10	1.42	1.38
13	3	512	CLA	CMD-C2D	-2.10	1.46	1.50
13	5	504	CLA	CMD-C2D	-2.10	1.46	1.50
13	d	507	CLA	CMD-C2D	-2.10	1.46	1.50
13	e	507	CLA	CMC-C2C	-2.10	1.46	1.50
13	e	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	1023	CLA	C3B-C4B	2.10	1.48	1.42
13	B	1230	CLA	C3B-C4B	2.10	1.48	1.42
13	4	502	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	1214	CLA	CMD-C2D	-2.10	1.46	1.50
13	B	1231	CLA	CMC-C2C	-2.10	1.46	1.50
13	5	508	CLA	CMC-C2C	-2.10	1.46	1.50
13	2	508	CLA	CMD-C2D	-2.10	1.46	1.50
13	3	517	CLA	CHC-C1C	2.10	1.42	1.38
13	5	511	CLA	CMB-C2B	-2.10	1.46	1.50
13	B	1228	CLA	CMC-C2C	-2.10	1.46	1.50
13	3	502	CLA	C3B-C4B	2.10	1.48	1.42
13	B	1223	CLA	C3B-C4B	2.10	1.48	1.42
13	1	504	CLA	CMB-C2B	-2.10	1.46	1.50
13	e	510	CLA	CHC-C1C	2.10	1.42	1.38
13	b	503	CLA	CHC-C1C	2.10	1.42	1.38
13	6	509	CLA	CMC-C2C	-2.10	1.46	1.50
13	A	1106	CLA	CMC-C2C	-2.10	1.46	1.50
13	e	504	CLA	CMD-C2D	-2.10	1.46	1.50
13	A	1136	CLA	CMC-C2C	-2.10	1.46	1.50
13	B	1202	CLA	CMC-C2C	-2.10	1.46	1.50
13	6	511	CLA	CMB-C2B	-2.10	1.46	1.50
13	5	512	CLA	CMB-C2B	-2.09	1.46	1.50
13	3	503	CLA	CHC-C1C	2.09	1.42	1.38
13	1	502	CLA	CHC-C1C	2.09	1.42	1.38
13	b	508	CLA	CHC-C1C	2.09	1.42	1.38
13	f	501	CLA	CMB-C2B	-2.09	1.46	1.50
13	5	503	CLA	CHC-C1C	2.09	1.42	1.38
13	e	503	CLA	CHC-C1C	2.09	1.42	1.38
13	f	502	CLA	CHC-C1C	2.09	1.42	1.38
13	2	507	CLA	CHC-C1C	2.09	1.42	1.38
13	2	513	CLA	CMD-C2D	-2.09	1.46	1.50
13	c	508	CLA	CMD-C2D	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	a	502	CLA	CMB-C2B	-2.09	1.46	1.50
13	A	1122	CLA	CMD-C2D	-2.09	1.46	1.50
13	6	501	CLA	CHC-C1C	2.09	1.42	1.38
13	d	504	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	1125	CLA	CHC-C1C	2.09	1.42	1.38
13	A	1133	CLA	CMB-C2B	-2.09	1.46	1.50
13	A	1114	CLA	CMD-C2D	-2.09	1.46	1.50
13	e	518	CLA	CMB-C2B	-2.09	1.46	1.50
13	a	502	CLA	CMD-C2D	-2.09	1.46	1.50
13	B	1224	CLA	C3B-C4B	2.09	1.48	1.42
13	B	1021	CLA	CMB-C2B	-2.09	1.46	1.50
13	5	508	CLA	CMD-C2D	-2.09	1.46	1.50
13	5	509	CLA	CMC-C2C	-2.09	1.46	1.50
13	6	518	CLA	CMB-C2B	-2.09	1.46	1.50
13	A	1138	CLA	CMB-C2B	-2.09	1.46	1.50
13	e	502	CLA	C3B-C4B	2.09	1.48	1.42
13	2	502	CLA	C3B-C4B	2.09	1.48	1.42
13	d	516	CLA	CMD-C2D	-2.09	1.46	1.50
13	e	508	CLA	CMC-C2C	-2.09	1.46	1.50
13	2	510	CLA	CMD-C2D	-2.09	1.46	1.50
13	1	503	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	1139	CLA	CMC-C2C	-2.09	1.46	1.50
13	5	507	CLA	CMB-C2B	-2.09	1.46	1.50
13	A	1128	CLA	CMC-C2C	-2.09	1.46	1.50
13	f	506	CLA	CMD-C2D	-2.09	1.46	1.50
13	a	517	CLA	CMD-C2D	-2.09	1.46	1.50
13	4	504	CLA	CMD-C2D	-2.09	1.46	1.50
13	6	502	CLA	CMD-C2D	-2.09	1.46	1.50
13	A	1102	CLA	CMD-C2D	-2.09	1.46	1.50
13	e	516	CLA	CMD-C2D	-2.08	1.46	1.50
13	b	512	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	508	CLA	CHC-C1C	2.08	1.42	1.38
13	6	517	CLA	CHC-C1C	2.08	1.42	1.38
13	1	511	CLA	CMD-C2D	-2.08	1.46	1.50
13	d	517	CLA	CMD-C2D	-2.08	1.46	1.50
13	g	502	CLA	CMD-C2D	-2.08	1.46	1.50
13	2	510	CLA	CHC-C1C	2.08	1.42	1.38
13	1	509	CLA	CHC-C1C	2.08	1.42	1.38
13	3	506	CLA	CMC-C2C	-2.08	1.46	1.50
13	A	1120	CLA	CMC-C2C	-2.08	1.46	1.50
13	a	507	CLA	CMD-C2D	-2.08	1.46	1.50
13	a	509	CLA	CMD-C2D	-2.08	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	513	CLA	CHC-C1C	2.08	1.42	1.38
13	B	1215	CLA	CMC-C2C	-2.08	1.46	1.50
13	g	506	CLA	CHC-C1C	2.08	1.42	1.38
13	3	508	CLA	CMC-C2C	-2.08	1.46	1.50
13	B	1212	CLA	CMB-C2B	-2.08	1.46	1.50
13	c	508	CLA	CMB-C2B	-2.08	1.46	1.50
13	1	505	CLA	CHC-C1C	2.08	1.42	1.38
13	2	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	d	502	CLA	CMC-C2C	-2.08	1.46	1.50
13	A	1131	CLA	C3B-C4B	2.08	1.48	1.42
13	g	507	CLA	CMB-C2B	-2.08	1.46	1.50
13	2	504	CLA	CMC-C2C	-2.08	1.46	1.50
13	5	512	CLA	CHC-C1C	2.08	1.42	1.38
13	1	507	CLA	CHC-C1C	2.08	1.42	1.38
13	2	502	CLA	CMC-C2C	-2.08	1.46	1.50
13	2	516	CLA	CMD-C2D	-2.08	1.46	1.50
13	f	507	CLA	CHC-C1C	2.08	1.42	1.38
13	3	519	CLA	CMD-C2D	-2.08	1.46	1.50
13	c	501	CLA	CMB-C2B	-2.08	1.46	1.50
13	2	511	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1108	CLA	C3B-C4B	2.08	1.48	1.42
13	d	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	b	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	B	1204	CLA	CMB-C2B	-2.08	1.46	1.50
13	c	503	CLA	CMB-C2B	-2.08	1.46	1.50
13	e	509	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	509	CLA	CMB-C2B	-2.08	1.46	1.50
13	d	503	CLA	CMD-C2D	-2.08	1.46	1.50
13	1	506	CLA	CHC-C1C	2.08	1.42	1.38
13	3	512	CLA	CMB-C2B	-2.08	1.46	1.50
13	4	518	CLA	CMB-C2B	-2.08	1.46	1.50
13	1	511	CLA	CMB-C2B	-2.08	1.46	1.50
13	g	518	CLA	CHC-C1C	2.08	1.42	1.38
13	d	516	CLA	CMB-C2B	-2.08	1.46	1.50
13	e	516	CLA	CHC-C1C	2.08	1.42	1.38
13	A	1123	CLA	CMC-C2C	-2.08	1.46	1.50
13	g	506	CLA	CMB-C2B	-2.08	1.46	1.50
13	5	510	CLA	CMD-C2D	-2.07	1.46	1.50
13	2	507	CLA	CMD-C2D	-2.07	1.46	1.50
13	b	519	CLA	CMD-C2D	-2.07	1.46	1.50
13	X	1401	CLA	CMB-C2B	-2.07	1.46	1.50
13	a	513	CLA	CMB-C2B	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	1137	CLA	CHC-C1C	2.07	1.42	1.38
13	b	516	CLA	CHC-C1C	2.07	1.42	1.38
13	g	504	CLA	CMD-C2D	-2.07	1.46	1.50
13	1	519	CLA	CHC-C1C	2.07	1.42	1.38
13	A	1112	CLA	CHC-C1C	2.07	1.42	1.38
13	d	518	CLA	CHC-C1C	2.07	1.42	1.38
13	4	519	CLA	CMD-C2D	-2.07	1.46	1.50
13	5	513	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	509	CLA	CMC-C2C	-2.07	1.46	1.50
13	a	507	CLA	CMB-C2B	-2.07	1.46	1.50
13	5	510	CLA	CHC-C1C	2.07	1.42	1.38
13	A	1134	CLA	CMD-C2D	-2.07	1.46	1.50
13	a	512	CLA	CMB-C2B	-2.07	1.46	1.50
13	4	513	CLA	CHC-C1C	2.07	1.42	1.38
13	B	1203	CLA	CHC-C1C	2.07	1.42	1.38
13	d	505	CLA	CHC-C1C	2.07	1.42	1.38
13	4	510	CLA	CMC-C2C	-2.07	1.46	1.50
13	5	504	CLA	CMC-C2C	-2.07	1.46	1.50
13	1	507	CLA	CMD-C2D	-2.07	1.46	1.50
13	g	508	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	512	CLA	MG-NB	-2.07	2.01	2.05
13	2	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	g	510	CLA	CMD-C2D	-2.07	1.46	1.50
13	4	502	CLA	C3B-C4B	2.07	1.48	1.42
14	A	4002	BCR	C1-C6	-2.07	1.51	1.53
13	6	506	CLA	CMC-C2C	-2.07	1.46	1.50
13	1	513	CLA	CMD-C2D	-2.07	1.46	1.50
13	c	501	CLA	CMD-C2D	-2.07	1.46	1.50
13	A	1105	CLA	C3B-C4B	2.07	1.48	1.42
13	f	501	CLA	CMD-C2D	-2.07	1.46	1.50
13	6	518	CLA	CHC-C1C	2.07	1.42	1.38
13	2	516	CLA	CHC-C1C	2.07	1.42	1.38
13	c	505	CLA	CHC-C1C	2.07	1.42	1.38
13	3	504	CLA	CMC-C2C	-2.07	1.46	1.50
13	2	513	CLA	CMB-C2B	-2.07	1.46	1.50
13	6	505	CLA	CHC-C1C	2.07	1.42	1.38
13	2	508	CLA	CHC-C1C	2.07	1.42	1.38
13	4	509	CLA	CMB-C2B	-2.07	1.46	1.50
13	g	518	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	511	CLA	CMB-C2B	-2.07	1.46	1.50
13	B	1204	CLA	CMC-C2C	-2.07	1.46	1.50
13	d	511	CLA	CHC-C1C	2.07	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1218	CLA	CMB-C2B	-2.07	1.46	1.50
13	f	501	CLA	CHC-C1C	2.07	1.42	1.38
13	6	503	CLA	CMD-C2D	-2.07	1.46	1.50
13	d	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	b	505	CLA	CHC-C1C	2.07	1.42	1.38
13	2	506	CLA	CMB-C2B	-2.07	1.46	1.50
13	1	510	CLA	CMB-C2B	-2.07	1.46	1.50
13	B	1234	CLA	CHC-C1C	2.07	1.42	1.38
13	4	503	CLA	CMB-C2B	-2.07	1.46	1.50
13	f	519	CLA	CMB-C2B	-2.07	1.46	1.50
13	1	510	CLA	CHC-C1C	2.07	1.42	1.38
14	F	4014	BCR	C30-C25	-2.07	1.51	1.53
13	5	517	CLA	CMD-C2D	-2.07	1.46	1.50
13	e	517	CLA	CMC-C2C	-2.07	1.46	1.50
13	6	519	CLA	CHC-C1C	2.07	1.42	1.38
13	1	517	CLA	CHC-C1C	2.06	1.42	1.38
13	f	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	5	504	CLA	CMB-C2B	-2.06	1.46	1.50
13	B	1236	CLA	CMC-C2C	-2.06	1.46	1.50
13	X	1401	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	1140	CLA	CMC-C2C	-2.06	1.46	1.50
13	e	519	CLA	CMB-C2B	-2.06	1.46	1.50
13	4	509	CLA	CHC-C1C	2.06	1.42	1.38
13	c	509	CLA	CMC-C2C	-2.06	1.46	1.50
13	g	511	CLA	CMB-C2B	-2.06	1.46	1.50
14	F	4015	BCR	C30-C25	-2.06	1.51	1.53
13	g	511	CLA	CHC-C1C	2.06	1.42	1.38
13	6	505	CLA	CMB-C2B	-2.06	1.46	1.50
13	2	519	CLA	CMB-C2B	-2.06	1.46	1.50
13	c	519	CLA	CMB-C2B	-2.06	1.46	1.50
13	3	506	CLA	CMD-C2D	-2.06	1.46	1.50
13	c	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	d	513	CLA	CMC-C2C	-2.06	1.46	1.50
13	A	1128	CLA	C3B-C4B	2.06	1.48	1.42
13	b	517	CLA	MG-NA	2.06	2.11	2.06
13	3	519	CLA	CMB-C2B	-2.06	1.46	1.50
13	d	501	CLA	CMC-C2C	-2.06	1.46	1.50
13	c	513	CLA	CHC-C1C	2.06	1.42	1.38
13	g	501	CLA	CHC-C1C	2.06	1.42	1.38
13	b	504	CLA	CMB-C2B	-2.06	1.46	1.50
13	B	1220	CLA	CHC-C1C	2.06	1.42	1.38
13	1	509	CLA	CMD-C2D	-2.06	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1225	CLA	CMC-C2C	-2.06	1.46	1.50
13	f	503	CLA	CMB-C2B	-2.06	1.46	1.50
13	1	501	CLA	CHC-C1C	2.06	1.42	1.38
13	3	501	CLA	CMB-C2B	-2.06	1.46	1.50
13	e	513	CLA	CMD-C2D	-2.06	1.46	1.50
13	5	501	CLA	CHC-C1C	2.06	1.42	1.38
13	B	1209	CLA	CMC-C2C	-2.06	1.46	1.50
13	e	512	CLA	CMB-C2B	-2.06	1.46	1.50
13	B	1215	CLA	C3B-C4B	2.06	1.48	1.42
13	3	509	CLA	CMC-C2C	-2.06	1.46	1.50
13	3	517	CLA	CMD-C2D	-2.06	1.46	1.50
13	2	504	CLA	CMD-C2D	-2.06	1.46	1.50
13	B	1213	CLA	CMC-C2C	-2.06	1.46	1.50
13	g	503	CLA	CMB-C2B	-2.06	1.46	1.50
13	3	504	CLA	CMB-C2B	-2.06	1.46	1.50
13	4	504	CLA	CMB-C2B	-2.06	1.46	1.50
13	2	509	CLA	CMB-C2B	-2.06	1.46	1.50
13	b	507	CLA	CMD-C2D	-2.06	1.46	1.50
13	6	509	CLA	CHC-C1C	2.06	1.42	1.38
13	g	516	CLA	CHC-C1C	2.06	1.42	1.38
13	A	1104	CLA	CMC-C2C	-2.06	1.46	1.50
13	e	519	CLA	CMD-C2D	-2.06	1.46	1.50
13	2	513	CLA	CMC-C2C	-2.06	1.46	1.50
13	c	501	CLA	CHC-C1C	2.06	1.42	1.38
13	c	507	CLA	CMB-C2B	-2.06	1.46	1.50
13	c	509	CLA	CMB-C2B	-2.06	1.46	1.50
13	f	504	CLA	CMD-C2D	-2.06	1.46	1.50
13	f	509	CLA	CMD-C2D	-2.06	1.46	1.50
13	A	1116	CLA	CHC-C1C	2.06	1.42	1.38
13	g	502	CLA	CMC-C2C	-2.05	1.46	1.50
13	3	516	CLA	CMB-C2B	-2.05	1.46	1.50
13	A	1113	CLA	CMC-C2C	-2.05	1.46	1.50
13	g	508	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	513	CLA	CMC-C2C	-2.05	1.46	1.50
13	f	507	CLA	CMD-C2D	-2.05	1.46	1.50
13	B	1221	CLA	MG-NB	-2.05	2.01	2.05
13	A	1104	CLA	C3B-C4B	2.05	1.48	1.42
13	B	1203	CLA	MG-NB	-2.05	2.01	2.05
13	3	511	CLA	CMD-C2D	-2.05	1.46	1.50
13	4	516	CLA	CMD-C2D	-2.05	1.46	1.50
13	d	508	CLA	CMC-C2C	-2.05	1.46	1.50
13	c	510	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	503	CLA	CMD-C2D	-2.05	1.46	1.50
13	g	513	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	518	CLA	CMB-C2B	-2.05	1.46	1.50
13	4	517	CLA	CHC-C1C	2.05	1.42	1.38
13	1	504	CLA	CHC-C1C	2.05	1.42	1.38
13	A	1104	CLA	CHC-C1C	2.05	1.42	1.38
14	1	523	BCR	C30-C25	-2.05	1.51	1.53
14	A	4007	BCR	C1-C6	-2.05	1.51	1.53
13	A	1129	CLA	CMC-C2C	-2.05	1.46	1.50
13	e	517	CLA	CMB-C2B	-2.05	1.46	1.50
13	4	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	6	519	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1110	CLA	CMD-C2D	-2.05	1.46	1.50
13	e	517	CLA	CMD-C2D	-2.05	1.46	1.50
13	b	509	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	518	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	509	CLA	C3B-C4B	2.05	1.48	1.42
13	d	513	CLA	CHC-C1C	2.05	1.42	1.38
13	d	510	CLA	CMD-C2D	-2.05	1.46	1.50
13	c	507	CLA	CHC-C1C	2.05	1.42	1.38
13	3	507	CLA	CMB-C2B	-2.05	1.46	1.50
13	2	506	CLA	CMD-C2D	-2.05	1.46	1.50
13	g	503	CLA	CHC-C1C	2.05	1.42	1.38
13	6	507	CLA	CMD-C2D	-2.05	1.46	1.50
13	2	516	CLA	CMB-C2B	-2.05	1.46	1.50
13	d	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	518	CLA	CMD-C2D	-2.05	1.46	1.50
13	3	504	CLA	CHC-C1C	2.05	1.42	1.38
13	2	517	CLA	CHC-C1C	2.05	1.42	1.38
13	A	1136	CLA	CHC-C1C	2.05	1.42	1.38
13	e	518	CLA	CHC-C1C	2.05	1.42	1.38
13	4	504	CLA	CMC-C2C	-2.05	1.46	1.50
13	4	508	CLA	CMC-C2C	-2.05	1.46	1.50
13	2	517	CLA	CMB-C2B	-2.05	1.46	1.50
13	b	513	CLA	CMD-C2D	-2.05	1.46	1.50
13	K	1401	CLA	CHC-C1C	2.05	1.42	1.38
13	e	519	CLA	CHC-C1C	2.05	1.42	1.38
14	b	524	BCR	C1-C6	-2.05	1.51	1.53
13	4	513	CLA	CMB-C2B	-2.05	1.46	1.50
13	A	1135	CLA	CMC-C2C	-2.05	1.46	1.50
13	b	503	CLA	CMD-C2D	-2.05	1.46	1.50
13	a	508	CLA	CHC-C1C	2.05	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	509	CLA	CMB-C2B	-2.05	1.46	1.50
13	4	501	CLA	CMB-C2B	-2.05	1.46	1.50
13	b	517	CLA	CMD-C2D	-2.05	1.46	1.50
13	A	1130	CLA	CMB-C2B	-2.05	1.46	1.50
13	e	507	CLA	CMD-C2D	-2.05	1.46	1.50
13	f	502	CLA	CMB-C2B	-2.05	1.46	1.50
13	a	508	CLA	CMB-C2B	-2.05	1.46	1.50
13	6	509	CLA	CMB-C2B	-2.04	1.46	1.50
13	b	506	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	519	CLA	CHC-C1C	2.04	1.42	1.38
13	d	518	CLA	CMB-C2B	-2.04	1.46	1.50
13	d	519	CLA	CMD-C2D	-2.04	1.46	1.50
13	4	501	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	516	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	1122	CLA	CHC-C1C	2.04	1.42	1.38
13	c	508	CLA	CHC-C1C	2.04	1.42	1.38
13	6	506	CLA	CMD-C2D	-2.04	1.46	1.50
13	b	509	CLA	C3B-C4B	2.04	1.48	1.42
13	b	511	CLA	CHC-C1C	2.04	1.42	1.38
13	e	504	CLA	CMB-C2B	-2.04	1.46	1.50
13	A	1103	CLA	C3B-C4B	2.04	1.48	1.42
13	b	513	CLA	CHC-C1C	2.04	1.42	1.38
13	3	513	CLA	CMD-C2D	-2.04	1.46	1.50
13	3	517	CLA	CMC-C2C	-2.04	1.46	1.50
13	A	1102	CLA	CMB-C2B	-2.04	1.46	1.50
13	B	1233	CLA	CMC-C2C	-2.04	1.46	1.50
13	e	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	e	513	CLA	CMC-C2C	-2.04	1.46	1.50
13	a	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	B	1227	CLA	C3B-C4B	2.04	1.48	1.42
13	6	513	CLA	CMD-C2D	-2.04	1.46	1.50
13	1	510	CLA	CMD-C2D	-2.04	1.46	1.50
13	f	509	CLA	CHC-C1C	2.04	1.42	1.38
13	a	512	CLA	CHC-C1C	2.04	1.42	1.38
13	6	501	CLA	CMB-C2B	-2.04	1.46	1.50
13	d	519	CLA	CMB-C2B	-2.04	1.46	1.50
13	f	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	2	518	CLA	CHC-C1C	2.04	1.42	1.38
13	3	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	4	519	CLA	CMB-C2B	-2.04	1.46	1.50
13	5	516	CLA	CMB-C2B	-2.04	1.46	1.50
13	6	508	CLA	CMD-C2D	-2.04	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1235	CLA	CHC-C1C	2.04	1.42	1.38
13	6	501	CLA	CMC-C2C	-2.04	1.46	1.50
13	g	517	CLA	CMB-C2B	-2.04	1.46	1.50
13	1	518	CLA	CMD-C2D	-2.04	1.46	1.50
13	4	501	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1112	CLA	CMB-C2B	-2.04	1.46	1.50
13	B	1226	CLA	C3B-C4B	2.04	1.48	1.42
13	f	508	CLA	CHC-C1C	2.04	1.42	1.38
13	1	502	CLA	CMB-C2B	-2.04	1.46	1.50
13	b	504	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1138	CLA	CMC-C2C	-2.04	1.46	1.50
14	2	523	BCR	C1-C6	-2.04	1.51	1.53
13	b	501	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1104	CLA	CMB-C2B	-2.04	1.46	1.50
13	f	508	CLA	CMC-C2C	-2.04	1.46	1.50
13	1	504	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	1118	CLA	CMC-C2C	-2.04	1.46	1.50
13	c	504	CLA	CMD-C2D	-2.04	1.46	1.50
13	A	1111	CLA	CMB-C2B	-2.04	1.46	1.50
13	2	504	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1129	CLA	CHC-C1C	2.04	1.42	1.38
13	A	1106	CLA	C3B-C4B	2.04	1.48	1.42
13	B	1218	CLA	CMC-C2C	-2.04	1.46	1.50
13	5	519	CLA	CMB-C2B	-2.03	1.46	1.50
13	6	511	CLA	CMD-C2D	-2.03	1.46	1.50
13	A	1107	CLA	C3B-C4B	2.03	1.48	1.42
13	4	513	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	518	CLA	CMB-C2B	-2.03	1.46	1.50
13	4	513	CLA	CMD-C2D	-2.03	1.46	1.50
13	1	506	CLA	CMD-C2D	-2.03	1.46	1.50
13	d	504	CLA	CMB-C2B	-2.03	1.46	1.50
13	6	512	CLA	CMB-C2B	-2.03	1.46	1.50
13	d	507	CLA	CMB-C2B	-2.03	1.46	1.50
13	1	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	A	1108	CLA	CMD-C2D	-2.03	1.46	1.50
13	B	1223	CLA	CMB-C2B	-2.03	1.46	1.50
13	B	1202	CLA	CHC-C1C	2.03	1.42	1.38
13	c	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	d	517	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	504	CLA	CMB-C2B	-2.03	1.46	1.50
13	1	518	CLA	CHC-C1C	2.03	1.42	1.38
13	f	510	CLA	CHC-C1C	2.03	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	507	CLA	CMC-C2C	-2.03	1.46	1.50
13	A	1123	CLA	MG-NB	-2.03	2.01	2.05
13	e	503	CLA	CMD-C2D	-2.03	1.46	1.50
13	2	517	CLA	CMC-C2C	-2.03	1.46	1.50
13	g	506	CLA	CMD-C2D	-2.03	1.46	1.50
13	b	501	CLA	CMC-C2C	-2.03	1.46	1.50
13	c	503	CLA	CHC-C1C	2.03	1.42	1.38
13	a	519	CLA	CHC-C1C	2.03	1.42	1.38
13	f	516	CLA	CMD-C2D	-2.03	1.46	1.50
13	4	516	CLA	CMB-C2B	-2.03	1.46	1.50
13	d	506	CLA	CMC-C2C	-2.03	1.46	1.50
13	f	512	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	518	CLA	CMD-C2D	-2.03	1.46	1.50
13	g	501	CLA	CMB-C2B	-2.03	1.46	1.50
13	A	1105	CLA	CMC-C2C	-2.03	1.46	1.50
13	f	513	CLA	CMC-C2C	-2.03	1.46	1.50
13	c	518	CLA	CMB-C2B	-2.03	1.46	1.50
13	e	506	CLA	CMD-C2D	-2.03	1.46	1.50
13	F	1301	CLA	MG-NB	-2.03	2.01	2.05
13	B	1238	CLA	CMB-C2B	-2.03	1.46	1.50
13	f	503	CLA	CHC-C1C	2.03	1.42	1.38
13	b	513	CLA	CMC-C2C	-2.03	1.46	1.50
13	3	503	CLA	CMB-C2B	-2.03	1.46	1.50
13	2	511	CLA	CMD-C2D	-2.03	1.46	1.50
13	1	518	CLA	CMB-C2B	-2.03	1.46	1.50
13	4	512	CLA	CHC-C1C	2.03	1.42	1.38
13	1	516	CLA	CHC-C1C	2.03	1.42	1.38
13	A	1113	CLA	CMB-C2B	-2.02	1.46	1.50
13	c	517	CLA	CMC-C2C	-2.02	1.46	1.50
13	B	1213	CLA	CHC-C1C	2.02	1.42	1.38
13	a	504	CLA	CMB-C2B	-2.02	1.46	1.50
13	A	1101	CLA	CHC-C1C	2.02	1.42	1.38
13	6	517	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	1208	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	1212	CLA	CMC-C2C	-2.02	1.46	1.50
13	g	509	CLA	CMD-C2D	-2.02	1.46	1.50
13	4	518	CLA	CHC-C1C	2.02	1.42	1.38
13	B	1215	CLA	MG-NB	-2.02	2.01	2.05
13	6	507	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	505	CLA	CHC-C1C	2.02	1.42	1.38
13	4	512	CLA	CMB-C2B	-2.02	1.46	1.50
13	1	503	CLA	CHC-C1C	2.02	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	3	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	2	510	CLA	CMC-C2C	-2.02	1.46	1.50
13	1	505	CLA	CMB-C2B	-2.02	1.46	1.50
13	c	519	CLA	CMC-C2C	-2.02	1.46	1.50
13	B	1211	CLA	CHC-C1C	2.02	1.42	1.38
13	f	518	CLA	CHC-C1C	2.02	1.42	1.38
13	5	517	CLA	CMB-C2B	-2.02	1.46	1.50
13	B	1217	CLA	CMC-C2C	-2.02	1.46	1.50
13	J	1302	CLA	CMC-C2C	-2.02	1.46	1.50
13	d	509	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	508	CLA	CHC-C1C	2.02	1.42	1.38
13	6	512	CLA	CHC-C1C	2.02	1.42	1.38
13	5	510	CLA	CMB-C2B	-2.02	1.46	1.50
13	e	502	CLA	CMC-C2C	-2.02	1.46	1.50
13	2	503	CLA	CMD-C2D	-2.02	1.46	1.50
13	B	1218	CLA	MG-NB	-2.02	2.01	2.05
14	I	4018	BCR	C30-C25	-2.02	1.51	1.53
13	6	501	CLA	CMD-C2D	-2.02	1.46	1.50
13	6	509	CLA	CMD-C2D	-2.02	1.46	1.50
13	f	509	CLA	CMB-C2B	-2.02	1.46	1.50
13	a	513	CLA	CMD-C2D	-2.02	1.46	1.50
13	A	1139	CLA	CHC-C1C	2.02	1.42	1.38
13	4	511	CLA	C1B-C2B	2.02	1.47	1.43
13	e	503	CLA	CMB-C2B	-2.02	1.46	1.50
13	3	516	CLA	CMD-C2D	-2.02	1.46	1.50
13	1	509	CLA	CMB-C2B	-2.02	1.46	1.50
13	K	1103	CLA	CMC-C2C	-2.02	1.46	1.50
13	c	512	CLA	C3D-C4D	2.02	1.48	1.44
13	1	508	CLA	CMC-C2C	-2.02	1.46	1.50
13	a	503	CLA	CMB-C2B	-2.01	1.46	1.50
13	a	504	CLA	CMD-C2D	-2.01	1.46	1.50
13	A	1110	CLA	CHC-C1C	2.01	1.42	1.38
13	3	512	CLA	CHC-C1C	2.01	1.42	1.38
13	6	516	CLA	CMB-C2B	-2.01	1.46	1.50
14	a	522	BCR	C30-C25	-2.01	1.51	1.53
13	B	1225	CLA	CHC-C1C	2.01	1.42	1.38
13	e	508	CLA	CHC-C1C	2.01	1.42	1.38
13	d	513	CLA	CMB-C2B	-2.01	1.46	1.50
13	e	507	CLA	CHC-C1C	2.01	1.42	1.38
13	1	504	CLA	CMC-C2C	-2.01	1.46	1.50
13	g	510	CLA	CHC-C1C	2.01	1.42	1.38
13	2	506	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	f	516	CLA	CMB-C2B	-2.01	1.46	1.50
13	d	512	CLA	CHC-C1C	2.01	1.42	1.38
13	2	503	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	1124	CLA	CMC-C2C	-2.01	1.46	1.50
13	b	517	CLA	CMB-C2B	-2.01	1.46	1.50
13	a	519	CLA	CMD-C2D	-2.01	1.46	1.50
13	3	518	CLA	CHC-C1C	2.01	1.42	1.38
13	3	513	CLA	CMB-C2B	-2.01	1.46	1.50
13	c	507	CLA	CMD-C2D	-2.01	1.46	1.50
13	A	1130	CLA	CHC-C1C	2.01	1.42	1.38
13	B	1234	CLA	MG-NB	-2.01	2.01	2.05
13	2	507	CLA	CMB-C2B	-2.01	1.46	1.50
13	b	519	CLA	CMB-C2B	-2.01	1.46	1.50
13	5	507	CLA	CMD-C2D	-2.01	1.46	1.50
13	6	519	CLA	CMB-C2B	-2.01	1.46	1.50
13	g	507	CLA	CHC-C1C	2.01	1.42	1.38
13	K	1401	CLA	CMC-C2C	-2.01	1.46	1.50
13	A	1127	CLA	CHC-C1C	2.01	1.42	1.38
13	4	512	CLA	CMC-C2C	-2.01	1.46	1.50
13	a	503	CLA	CMD-C2D	-2.01	1.46	1.50
13	e	504	CLA	CHC-C1C	2.01	1.42	1.38
13	B	1206	CLA	C3B-C4B	2.01	1.48	1.42
13	F	1301	CLA	C3B-C4B	2.01	1.48	1.42
13	5	519	CLA	CMD-C2D	-2.01	1.46	1.50
13	4	507	CLA	CMC-C2C	-2.01	1.46	1.50
13	6	517	CLA	CMD-C2D	-2.01	1.46	1.50
13	5	509	CLA	CHC-C1C	2.01	1.42	1.38
13	6	503	CLA	CHC-C1C	2.00	1.42	1.38
13	a	518	CLA	CHC-C1C	2.00	1.42	1.38
13	a	504	CLA	CMC-C2C	-2.00	1.46	1.50
13	4	510	CLA	MG-NB	-2.00	2.01	2.05
13	2	501	CLA	CHC-C1C	2.00	1.42	1.38
13	B	1214	CLA	CHC-C1C	2.00	1.42	1.38
13	B	1218	CLA	CHC-C1C	2.00	1.42	1.38
13	3	510	CLA	CMC-C2C	-2.00	1.46	1.50
13	c	510	CLA	CMD-C2D	-2.00	1.46	1.50
13	c	516	CLA	CMB-C2B	-2.00	1.46	1.50
13	f	503	CLA	CMD-C2D	-2.00	1.46	1.50
13	f	505	CLA	CMC-C2C	-2.00	1.46	1.50
13	f	519	CLA	CMD-C2D	-2.00	1.46	1.50
13	b	505	CLA	CMB-C2B	-2.00	1.46	1.50
13	b	518	CLA	CHC-C1C	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	1206	CLA	MG-NB	-2.00	2.01	2.05
13	2	508	CLA	CMB-C2B	-2.00	1.46	1.50
13	b	507	CLA	CMB-C2B	-2.00	1.46	1.50
13	3	507	CLA	CHC-C1C	2.00	1.42	1.38
13	f	517	CLA	CHC-C1C	2.00	1.42	1.38
13	c	505	CLA	CMC-C2C	-2.00	1.46	1.50
13	B	1231	CLA	CHC-C1C	2.00	1.42	1.38

All (2876) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	523	BCR	C30-C25-C26	-8.71	110.74	122.64
14	F	4014	BCR	C24-C23-C22	-7.36	115.35	126.23
14	B	4017	BCR	C24-C23-C22	-7.34	115.37	126.23
14	4	524	BCR	C16-C17-C18	-7.34	116.98	127.28
13	1	512	CLA	C4A-NA-C1A	7.20	109.96	106.68
14	c	522	BCR	C11-C10-C9	-7.02	117.43	127.28
14	6	524	BCR	C16-C17-C18	-7.01	117.44	127.28
13	2	512	CLA	C4A-NA-C1A	6.84	109.80	106.68
14	6	522	BCR	C15-C14-C13	-6.77	117.79	127.28
14	f	524	BCR	C16-C17-C18	-6.76	117.80	127.28
13	e	502	CLA	C4A-NA-C1A	6.60	109.69	106.68
14	c	524	BCR	C15-C14-C13	-6.50	118.16	127.28
14	B	4006	BCR	C11-C10-C9	-6.42	118.28	127.28
14	B	4010	BCR	C15-C14-C13	-6.37	118.34	127.28
14	f	522	BCR	C11-C10-C9	-6.34	118.39	127.28
14	J	4013	BCR	C15-C14-C13	-6.29	118.46	127.28
14	A	4002	BCR	C16-C17-C18	-6.22	118.56	127.28
14	a	522	BCR	C11-C10-C9	-6.22	118.56	127.28
14	e	524	BCR	C16-C17-C18	-6.17	118.62	127.28
14	e	524	BCR	C15-C14-C13	-6.15	118.66	127.28
14	b	523	BCR	C15-C14-C13	-6.13	118.68	127.28
14	1	524	BCR	C15-C14-C13	-6.13	118.68	127.28
14	a	523	BCR	C28-C27-C26	-6.12	103.14	114.06
13	d	512	CLA	C4A-NA-C1A	6.11	109.47	106.68
14	M	4021	BCR	C16-C17-C18	-6.10	118.72	127.28
14	F	4014	BCR	C20-C21-C22	-6.09	118.74	127.28
13	A	1126	CLA	C4A-NA-C1A	6.05	109.44	106.68
13	a	502	CLA	C4A-NA-C1A	6.05	109.44	106.68
14	F	4014	BCR	C16-C17-C18	-6.04	118.81	127.28
14	A	4011	BCR	C7-C8-C9	-6.01	117.34	126.23
14	2	524	BCR	C16-C17-C18	-6.01	118.85	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	524	BCR	C15-C14-C13	-6.00	118.86	127.28
14	A	4008	BCR	C20-C21-C22	-5.99	118.88	127.28
14	d	524	BCR	C16-C17-C18	-5.98	118.89	127.28
14	d	522	BCR	C15-C14-C13	-5.98	118.89	127.28
13	f	502	CLA	C4A-NA-C1A	5.98	109.41	106.68
13	B	1206	CLA	C4A-NA-C1A	5.93	109.39	106.68
14	A	4011	BCR	C16-C17-C18	-5.92	118.97	127.28
14	J	4013	BCR	C16-C17-C18	-5.89	119.02	127.28
13	A	1114	CLA	C4A-NA-C1A	5.89	109.37	106.68
13	b	502	CLA	C4A-NA-C1A	5.85	109.35	106.68
13	5	502	CLA	C4A-NA-C1A	5.85	109.35	106.68
14	d	523	BCR	C15-C14-C13	-5.84	119.09	127.28
14	d	524	BCR	C15-C14-C13	-5.83	119.11	127.28
13	b	509	CLA	C4A-NA-C1A	5.82	109.33	106.68
13	2	502	CLA	C4A-NA-C1A	5.79	109.32	106.68
13	A	1103	CLA	C4A-NA-C1A	5.78	109.31	106.68
14	A	4008	BCR	C24-C23-C22	-5.76	117.72	126.23
14	f	523	BCR	C15-C14-C13	-5.75	119.22	127.28
13	4	502	CLA	C4A-NA-C1A	5.71	109.29	106.68
13	B	1203	CLA	C4A-NA-C1A	5.70	109.28	106.68
14	5	522	BCR	C11-C10-C9	-5.70	119.29	127.28
13	c	511	CLA	C4A-NA-C1A	5.69	109.27	106.68
13	A	1104	CLA	C4A-NA-C1A	5.68	109.27	106.68
14	I	4018	BCR	C15-C14-C13	-5.67	119.33	127.28
14	1	524	BCR	C11-C10-C9	-5.66	119.34	127.28
14	g	522	BCR	C15-C14-C13	-5.65	119.35	127.28
14	5	523	BCR	C38-C26-C27	5.65	125.64	113.60
14	c	524	BCR	C16-C17-C18	-5.64	119.37	127.28
14	6	522	BCR	C11-C10-C9	-5.62	119.40	127.28
13	2	509	CLA	C4A-NA-C1A	5.61	109.24	106.68
13	a	509	CLA	C4A-NA-C1A	5.60	109.24	106.68
14	B	4004	BCR	C20-C21-C22	-5.59	119.44	127.28
14	d	522	BCR	C11-C10-C9	-5.59	119.44	127.28
14	5	523	BCR	C7-C8-C9	-5.57	117.99	126.23
14	5	523	BCR	C27-C26-C25	-5.57	115.17	122.70
13	b	507	CLA	C4A-NA-C1A	5.56	109.21	106.68
13	f	505	CLA	C4A-NA-C1A	5.55	109.21	106.68
13	c	502	CLA	C4A-NA-C1A	5.55	109.21	106.68
13	a	505	CLA	C4A-NA-C1A	5.54	109.21	106.68
14	a	522	BCR	C15-C14-C13	-5.54	119.51	127.28
13	a	518	CLA	C4A-NA-C1A	5.53	109.20	106.68
13	4	507	CLA	C4A-NA-C1A	5.52	109.20	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	505	CLA	C4A-NA-C1A	5.52	109.20	106.68
14	F	4016	BCR	C15-C14-C13	-5.51	119.55	127.28
14	a	524	BCR	C15-C14-C13	-5.50	119.56	127.28
13	e	509	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	B	4009	BCR	C20-C21-C22	-5.50	119.57	127.28
13	B	1204	CLA	C4A-NA-C1A	5.50	109.19	106.68
14	B	4017	BCR	C16-C17-C18	-5.49	119.58	127.28
14	e	522	BCR	C15-C14-C13	-5.49	119.58	127.28
13	g	507	CLA	C4A-NA-C1A	5.48	109.18	106.68
13	d	502	CLA	C4A-NA-C1A	5.46	109.17	106.68
14	c	522	BCR	C16-C17-C18	-5.46	119.62	127.28
13	3	509	CLA	C4A-NA-C1A	5.45	109.17	106.68
13	d	509	CLA	C4A-NA-C1A	5.45	109.17	106.68
14	3	524	BCR	C15-C14-C13	-5.45	119.64	127.28
13	3	502	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	B	1217	CLA	C4A-NA-C1A	5.44	109.16	106.68
14	g	524	BCR	C15-C14-C13	-5.44	119.64	127.28
13	f	513	CLA	C4A-NA-C1A	5.44	109.16	106.68
13	c	509	CLA	C4A-NA-C1A	5.43	109.16	106.68
13	A	1125	CLA	C4A-NA-C1A	5.42	109.15	106.68
13	B	1223	CLA	C4A-NA-C1A	5.41	109.15	106.68
14	g	524	BCR	C16-C17-C18	-5.41	119.70	127.28
13	g	513	CLA	C4A-NA-C1A	5.41	109.14	106.68
13	F	1301	CLA	C4A-NA-C1A	5.40	109.14	106.68
14	B	4006	BCR	C24-C23-C22	-5.38	118.27	126.23
13	c	518	CLA	C4A-NA-C1A	5.38	109.14	106.68
13	3	517	CLA	C4A-NA-C1A	5.38	109.13	106.68
13	3	511	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	A	1111	CLA	C4A-NA-C1A	5.37	109.13	106.68
13	e	507	CLA	C4A-NA-C1A	5.37	109.13	106.68
14	B	4004	BCR	C16-C17-C18	-5.37	119.75	127.28
13	3	519	CLA	C4A-NA-C1A	5.36	109.13	106.68
13	d	507	CLA	C4A-NA-C1A	5.36	109.13	106.68
13	f	510	CLA	C4A-NA-C1A	5.35	109.12	106.68
14	A	4011	BCR	C20-C21-C22	-5.35	119.78	127.28
13	2	510	CLA	C4A-NA-C1A	5.35	109.12	106.68
14	a	521	BCR	C11-C10-C9	-5.34	119.79	127.28
13	2	503	CLA	C4A-NA-C1A	5.34	109.11	106.68
13	e	510	CLA	C4A-NA-C1A	5.34	109.11	106.68
14	4	524	BCR	C20-C21-C22	-5.33	119.80	127.28
13	1	509	CLA	C4A-NA-C1A	5.33	109.11	106.68
13	b	506	CLA	CMB-C2B-C1B	-5.33	117.31	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	507	CLA	C4A-NA-C1A	5.33	109.11	106.68
13	5	519	CLA	C4A-NA-C1A	5.32	109.11	106.68
13	A	1118	CLA	C4A-NA-C1A	5.32	109.11	106.68
14	A	4007	BCR	C33-C5-C6	-5.31	118.69	124.48
14	d	523	BCR	C7-C8-C9	-5.31	118.38	126.23
13	B	1214	CLA	C4A-NA-C1A	5.31	109.10	106.68
14	a	521	BCR	C16-C17-C18	-5.31	119.84	127.28
13	5	510	CLA	C4A-NA-C1A	5.30	109.10	106.68
14	I	4018	BCR	C24-C23-C22	-5.30	118.39	126.23
13	5	512	CLA	C4A-NA-C1A	5.29	109.09	106.68
13	g	518	CLA	C4A-NA-C1A	5.29	109.09	106.68
13	6	502	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	1	521	BCR	C15-C14-C13	-5.28	119.87	127.28
13	6	507	CLA	C4A-NA-C1A	5.28	109.09	106.68
13	B	1207	CLA	C4A-NA-C1A	5.28	109.09	106.68
14	A	4003	BCR	C15-C14-C13	-5.28	119.88	127.28
13	B	1215	CLA	C4A-NA-C1A	5.27	109.08	106.68
14	e	524	BCR	C11-C10-C9	-5.26	119.89	127.28
13	a	503	CLA	C4A-NA-C1A	5.26	109.08	106.68
14	6	521	BCR	C16-C17-C18	-5.26	119.90	127.28
13	6	508	CLA	C4A-NA-C1A	5.26	109.08	106.68
13	e	504	CLA	C4A-NA-C1A	5.26	109.08	106.68
13	A	1107	CLA	C4A-NA-C1A	5.25	109.07	106.68
14	K	4001	BCR	C20-C21-C22	-5.25	119.92	127.28
13	c	512	CLA	C4A-NA-C1A	5.25	109.07	106.68
13	e	518	CLA	C4A-NA-C1A	5.24	109.07	106.68
13	5	509	CLA	C4A-NA-C1A	5.23	109.07	106.68
13	A	1116	CLA	C4A-NA-C1A	5.23	109.07	106.68
14	f	522	BCR	C7-C8-C9	-5.23	118.50	126.23
13	B	1236	CLA	C4A-NA-C1A	5.23	109.06	106.68
13	2	506	CLA	C4A-NA-C1A	5.23	109.06	106.68
14	4	523	BCR	C15-C14-C13	-5.22	119.96	127.28
13	B	1210	CLA	C4A-NA-C1A	5.22	109.06	106.68
13	4	509	CLA	C4A-NA-C1A	5.22	109.06	106.68
14	g	522	BCR	C11-C10-C9	-5.21	119.97	127.28
13	A	1121	CLA	C4A-NA-C1A	5.21	109.06	106.68
13	5	511	CLA	C4A-NA-C1A	5.20	109.05	106.68
13	1	510	CLA	C4A-NA-C1A	5.19	109.05	106.68
13	g	510	CLA	C4A-NA-C1A	5.19	109.05	106.68
13	1	507	CLA	C4A-NA-C1A	5.19	109.05	106.68
14	f	524	BCR	C24-C23-C22	-5.18	118.57	126.23
13	3	503	CLA	C4A-NA-C1A	5.18	109.04	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	507	CLA	C4A-NA-C1A	5.18	109.04	106.68
14	e	523	BCR	C16-C17-C18	-5.17	120.02	127.28
14	B	4017	BCR	C20-C21-C22	-5.16	120.04	127.28
13	4	503	CLA	C4A-NA-C1A	5.16	109.03	106.68
13	d	510	CLA	C4A-NA-C1A	5.16	109.03	106.68
14	b	524	BCR	C15-C14-C13	-5.15	120.05	127.28
13	6	519	CLA	C4A-NA-C1A	5.15	109.03	106.68
13	d	519	CLA	C4A-NA-C1A	5.15	109.03	106.68
14	6	523	BCR	C16-C17-C18	-5.15	120.06	127.28
14	I	4018	BCR	C7-C8-C9	-5.14	118.63	126.23
13	b	511	CLA	C4A-NA-C1A	5.14	109.02	106.68
14	a	522	BCR	C33-C5-C6	-5.14	118.88	124.48
14	M	4021	BCR	C24-C23-C22	-5.14	118.64	126.23
13	a	513	CLA	C4A-NA-C1A	5.14	109.02	106.68
13	A	1113	CLA	C4A-NA-C1A	5.13	109.02	106.68
13	6	506	CLA	C4A-NA-C1A	5.13	109.02	106.68
13	6	512	CLA	C4A-NA-C1A	5.12	109.02	106.68
13	A	1130	CLA	C4A-NA-C1A	5.12	109.02	106.68
14	a	523	BCR	C16-C17-C18	-5.12	120.10	127.28
13	A	1110	CLA	C4A-NA-C1A	5.11	109.01	106.68
14	g	523	BCR	C15-C14-C13	-5.11	120.11	127.28
13	6	510	CLA	C4A-NA-C1A	5.11	109.01	106.68
13	e	512	CLA	C4A-NA-C1A	5.10	109.00	106.68
14	a	522	BCR	C16-C17-C18	-5.10	120.13	127.28
13	1	517	CLA	C4A-NA-C1A	5.09	109.00	106.68
14	b	523	BCR	C7-C8-C9	-5.09	118.71	126.23
14	5	522	BCR	C15-C14-C13	-5.07	120.17	127.28
13	2	507	CLA	C4A-NA-C1A	5.07	108.99	106.68
13	g	517	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	g	521	BCR	C11-C10-C9	-5.06	120.19	127.28
13	A	1105	CLA	C4A-NA-C1A	5.06	108.99	106.68
14	g	523	BCR	C11-C10-C9	-5.05	120.19	127.28
14	1	524	BCR	C20-C21-C22	-5.05	120.19	127.28
13	A	1101	CLA	C4A-NA-C1A	5.05	108.98	106.68
13	5	506	CLA	C4A-NA-C1A	5.04	108.98	106.68
13	K	1401	CLA	C4A-NA-C1A	5.03	108.97	106.68
14	c	522	BCR	C15-C14-C13	-5.03	120.23	127.28
14	3	522	BCR	C15-C14-C13	-5.03	120.23	127.28
13	3	512	CLA	C4A-NA-C1A	5.02	108.97	106.68
14	3	522	BCR	C11-C10-C9	-5.02	120.24	127.28
13	f	506	CLA	C4A-NA-C1A	5.02	108.97	106.68
13	e	511	CLA	C4A-NA-C1A	5.02	108.97	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	e	522	BCR	C11-C10-C9	-5.01	120.25	127.28
13	A	1801	CLA	C4A-NA-C1A	5.01	108.97	106.68
13	c	505	CLA	C4A-NA-C1A	5.01	108.96	106.68
13	5	518	CLA	C4A-NA-C1A	5.01	108.96	106.68
14	3	523	BCR	C15-C14-C13	-5.00	120.26	127.28
13	6	503	CLA	C4A-NA-C1A	5.00	108.96	106.68
13	b	503	CLA	C4A-NA-C1A	5.00	108.96	106.68
13	d	506	CLA	C4A-NA-C1A	4.99	108.95	106.68
14	J	4012	BCR	C11-C10-C9	-4.98	120.29	127.28
14	5	523	BCR	C38-C26-C25	-4.98	119.05	124.48
13	b	504	CLA	C4A-NA-C1A	4.98	108.95	106.68
14	B	4006	BCR	C15-C14-C13	-4.98	120.30	127.28
13	4	508	CLA	C4A-NA-C1A	4.97	108.95	106.68
13	A	1237	CLA	C4A-NA-C1A	4.96	108.94	106.68
14	5	522	BCR	C7-C8-C9	-4.96	118.90	126.23
13	f	518	CLA	C4A-NA-C1A	4.95	108.94	106.68
13	5	505	CLA	C4A-NA-C1A	4.95	108.94	106.68
13	b	518	CLA	C4A-NA-C1A	4.95	108.94	106.68
13	2	505	CLA	C4A-NA-C1A	4.94	108.93	106.68
13	4	512	CLA	C4A-NA-C1A	4.94	108.93	106.68
14	5	524	BCR	C7-C8-C9	-4.93	118.94	126.23
14	c	521	BCR	C15-C14-C13	-4.93	120.36	127.28
13	J	1302	CLA	C4A-NA-C1A	4.93	108.93	106.68
13	b	512	CLA	C4A-NA-C1A	4.93	108.93	106.68
14	c	523	BCR	C15-C14-C13	-4.93	120.36	127.28
14	1	522	BCR	C15-C14-C13	-4.93	120.37	127.28
14	f	522	BCR	C33-C5-C6	-4.93	119.11	124.48
13	g	509	CLA	C4A-NA-C1A	4.92	108.92	106.68
13	a	501	CLA	C4A-NA-C1A	4.92	108.92	106.68
13	A	1123	CLA	C4A-NA-C1A	4.92	108.92	106.68
13	c	506	CLA	C4A-NA-C1A	4.91	108.92	106.68
14	M	4021	BCR	C20-C21-C22	-4.91	120.39	127.28
14	I	4020	BCR	C15-C14-C13	-4.91	120.40	127.28
13	6	511	CLA	C4A-NA-C1A	4.91	108.92	106.68
13	g	519	CLA	C4A-NA-C1A	4.90	108.91	106.68
13	6	518	CLA	C4A-NA-C1A	4.89	108.91	106.68
13	c	507	CLA	C4A-NA-C1A	4.89	108.91	106.68
14	B	4017	BCR	C33-C5-C6	-4.89	119.15	124.48
13	B	1233	CLA	C4A-NA-C1A	4.88	108.91	106.68
13	a	510	CLA	C4A-NA-C1A	4.88	108.91	106.68
14	J	4012	BCR	C7-C8-C9	-4.88	119.01	126.23
13	B	1212	CLA	C4A-NA-C1A	4.88	108.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	6	521	BCR	C15-C14-C13	-4.88	120.44	127.28
13	a	516	CLA	C4A-NA-C1A	4.88	108.90	106.68
14	b	522	BCR	C11-C10-C9	-4.88	120.44	127.28
13	f	509	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	b	521	BCR	C15-C14-C13	-4.87	120.44	127.28
13	e	519	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	2	522	BCR	C15-C14-C13	-4.87	120.45	127.28
13	3	518	CLA	C4A-NA-C1A	4.87	108.90	106.68
13	X	1401	CLA	C4A-NA-C1A	4.87	108.90	106.68
14	g	521	BCR	C16-C17-C18	-4.87	120.45	127.28
13	6	513	CLA	C4A-NA-C1A	4.86	108.90	106.68
14	B	4005	BCR	C24-C23-C22	-4.86	119.04	126.23
14	A	4008	BCR	C16-C17-C18	-4.86	120.47	127.28
13	3	504	CLA	C4A-NA-C1A	4.86	108.89	106.68
14	J	4012	BCR	C16-C17-C18	-4.86	120.47	127.28
14	2	524	BCR	C11-C10-C9	-4.85	120.47	127.28
14	d	522	BCR	C7-C8-C9	-4.85	119.06	126.23
14	F	4015	BCR	C15-C14-C13	-4.85	120.48	127.28
13	a	504	CLA	C4A-NA-C1A	4.85	108.89	106.68
14	B	4006	BCR	C16-C17-C18	-4.85	120.48	127.28
13	d	503	CLA	C4A-NA-C1A	4.84	108.89	106.68
13	A	1131	CLA	C4A-NA-C1A	4.84	108.89	106.68
14	b	522	BCR	C15-C14-C13	-4.84	120.49	127.28
13	4	510	CLA	C4A-NA-C1A	4.84	108.89	106.68
13	b	510	CLA	C4A-NA-C1A	4.84	108.89	106.68
13	a	519	CLA	C4A-NA-C1A	4.84	108.89	106.68
14	6	521	BCR	C11-C10-C9	-4.83	120.50	127.28
14	6	523	BCR	C11-C10-C9	-4.83	120.50	127.28
13	3	510	CLA	C4A-NA-C1A	4.83	108.88	106.68
13	a	508	CLA	C4A-NA-C1A	4.83	108.88	106.68
13	3	506	CLA	C4A-NA-C1A	4.83	108.88	106.68
13	b	519	CLA	C4A-NA-C1A	4.83	108.88	106.68
14	b	524	BCR	C16-C17-C18	-4.83	120.51	127.28
13	4	504	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	B	4005	BCR	C15-C14-C13	-4.82	120.51	127.28
14	g	521	BCR	C7-C8-C9	-4.82	119.10	126.23
14	2	521	BCR	C16-C17-C18	-4.82	120.52	127.28
13	d	504	CLA	C4A-NA-C1A	4.82	108.88	106.68
14	B	4009	BCR	C15-C14-C13	-4.82	120.52	127.28
14	5	521	BCR	C16-C17-C18	-4.82	120.53	127.28
13	1	502	CLA	C4A-NA-C1A	4.81	108.88	106.68
13	4	505	CLA	C4A-NA-C1A	4.81	108.87	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	e	523	BCR	C24-C23-C22	-4.81	119.12	126.23
13	A	1134	CLA	C4A-NA-C1A	4.80	108.87	106.68
13	g	502	CLA	C4A-NA-C1A	4.80	108.87	106.68
14	B	4009	BCR	C24-C23-C22	-4.80	119.13	126.23
13	A	1137	CLA	C4A-NA-C1A	4.80	108.87	106.68
13	c	503	CLA	C4A-NA-C1A	4.80	108.87	106.68
14	1	521	BCR	C20-C21-C22	-4.80	120.55	127.28
13	5	504	CLA	C4A-NA-C1A	4.79	108.87	106.68
13	1	513	CLA	C4A-NA-C1A	4.79	108.87	106.68
13	g	511	CLA	C4A-NA-C1A	4.79	108.86	106.68
14	5	524	BCR	C16-C17-C18	-4.79	120.56	127.28
14	A	4003	BCR	C11-C10-C9	-4.79	120.57	127.28
13	c	504	CLA	C4A-NA-C1A	4.78	108.86	106.68
14	A	4008	BCR	C15-C14-C13	-4.78	120.57	127.28
13	B	1213	CLA	C4A-NA-C1A	4.78	108.86	106.68
13	B	1239	CLA	C4A-NA-C1A	4.77	108.86	106.68
13	a	506	CLA	C4A-NA-C1A	4.77	108.86	106.68
14	d	524	BCR	C11-C10-C9	-4.77	120.59	127.28
13	2	504	CLA	C4A-NA-C1A	4.77	108.85	106.68
13	B	1209	CLA	C4A-NA-C1A	4.77	108.85	106.68
13	B	1235	CLA	C4A-NA-C1A	4.77	108.85	106.68
13	g	503	CLA	C4A-NA-C1A	4.77	108.85	106.68
14	a	521	BCR	C7-C8-C9	-4.76	119.19	126.23
14	6	521	BCR	C20-C21-C22	-4.76	120.60	127.28
14	F	4016	BCR	C11-C10-C9	-4.76	120.60	127.28
13	d	511	CLA	C4A-NA-C1A	4.76	108.85	106.68
13	c	510	CLA	C4A-NA-C1A	4.75	108.85	106.68
13	e	508	CLA	C4A-NA-C1A	4.75	108.85	106.68
14	B	4004	BCR	C24-C23-C22	-4.75	119.20	126.23
13	B	1226	CLA	C4A-NA-C1A	4.75	108.85	106.68
14	e	522	BCR	C33-C5-C6	-4.75	119.30	124.48
14	e	522	BCR	C7-C8-C9	-4.75	119.21	126.23
13	a	507	CLA	C4A-NA-C1A	4.75	108.84	106.68
13	1	506	CLA	C4A-NA-C1A	4.74	108.84	106.68
13	K	1103	CLA	C4A-NA-C1A	4.74	108.84	106.68
13	5	503	CLA	C4A-NA-C1A	4.74	108.84	106.68
13	A	1115	CLA	C4A-NA-C1A	4.74	108.84	106.68
13	A	1120	CLA	C4A-NA-C1A	4.73	108.84	106.68
13	2	518	CLA	C4A-NA-C1A	4.73	108.84	106.68
13	d	501	CLA	C4A-NA-C1A	4.73	108.84	106.68
13	2	511	CLA	C4A-NA-C1A	4.73	108.84	106.68
13	g	512	CLA	C4A-NA-C1A	4.73	108.83	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	524	BCR	C20-C21-C22	-4.73	120.65	127.28
14	d	521	BCR	C15-C14-C13	-4.72	120.66	127.28
14	a	522	BCR	C7-C8-C9	-4.72	119.25	126.23
13	1	516	CLA	C4A-NA-C1A	4.71	108.83	106.68
14	6	524	BCR	C15-C14-C13	-4.70	120.68	127.28
13	f	516	CLA	C4A-NA-C1A	4.70	108.82	106.68
13	1	504	CLA	C4A-NA-C1A	4.70	108.82	106.68
13	f	507	CLA	C4A-NA-C1A	4.70	108.82	106.68
13	e	503	CLA	C4A-NA-C1A	4.70	108.82	106.68
14	B	4010	BCR	C24-C23-C22	-4.69	119.30	126.23
14	A	4002	BCR	C11-C10-C9	-4.69	120.70	127.28
14	F	4015	BCR	C7-C8-C9	-4.69	119.30	126.23
13	3	513	CLA	C4A-NA-C1A	4.69	108.82	106.68
14	4	521	BCR	C16-C17-C18	-4.69	120.71	127.28
14	6	523	BCR	C20-C21-C22	-4.69	120.71	127.28
13	B	1231	CLA	C4A-NA-C1A	4.68	108.82	106.68
13	A	1106	CLA	C4A-NA-C1A	4.68	108.81	106.68
14	B	4009	BCR	C33-C5-C6	-4.68	119.38	124.48
14	F	4015	BCR	C11-C10-C9	-4.68	120.72	127.28
13	f	512	CLA	C4A-NA-C1A	4.67	108.81	106.68
13	A	1122	CLA	C4A-NA-C1A	4.67	108.81	106.68
13	A	1138	CLA	C4A-NA-C1A	4.67	108.81	106.68
13	2	519	CLA	C4A-NA-C1A	4.66	108.81	106.68
14	d	521	BCR	C11-C10-C9	-4.66	120.74	127.28
13	A	1119	CLA	C4A-NA-C1A	4.66	108.80	106.68
14	J	4013	BCR	C38-C26-C25	-4.65	119.41	124.48
13	d	513	CLA	C4A-NA-C1A	4.64	108.80	106.68
14	1	524	BCR	C7-C8-C9	-4.64	119.36	126.23
14	2	524	BCR	C15-C14-C13	-4.64	120.77	127.28
13	B	1220	CLA	C4A-NA-C1A	4.64	108.80	106.68
13	f	508	CLA	C4A-NA-C1A	4.64	108.80	106.68
13	A	1140	CLA	C4A-NA-C1A	4.64	108.79	106.68
13	c	519	CLA	C4A-NA-C1A	4.64	108.79	106.68
14	4	522	BCR	C15-C14-C13	-4.63	120.79	127.28
13	f	504	CLA	C4A-NA-C1A	4.63	108.79	106.68
13	f	511	CLA	C4A-NA-C1A	4.63	108.79	106.68
14	b	523	BCR	C11-C10-C9	-4.63	120.79	127.28
13	A	1112	CLA	C4A-NA-C1A	4.62	108.79	106.68
13	A	1132	CLA	C4A-NA-C1A	4.62	108.79	106.68
13	B	1227	CLA	C4A-NA-C1A	4.62	108.79	106.68
14	A	4002	BCR	C33-C5-C6	-4.62	119.44	124.48
14	3	524	BCR	C16-C17-C18	-4.62	120.80	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	J	4013	BCR	C16-C15-C14	-4.62	114.06	123.52
13	B	1232	CLA	C4A-NA-C1A	4.61	108.78	106.68
13	A	1135	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	A	4003	BCR	C7-C8-C9	-4.60	119.43	126.23
14	2	524	BCR	C33-C5-C6	-4.60	119.47	124.48
13	1	505	CLA	C4A-NA-C1A	4.60	108.78	106.68
14	a	521	BCR	C15-C14-C13	-4.59	120.84	127.28
14	3	524	BCR	C3-C4-C5	-4.59	105.88	114.06
13	4	513	CLA	C4A-NA-C1A	4.59	108.77	106.68
14	g	524	BCR	C11-C10-C9	-4.58	120.85	127.28
14	d	521	BCR	C20-C21-C22	-4.58	120.86	127.28
14	4	523	BCR	C16-C17-C18	-4.58	120.86	127.28
14	I	4019	BCR	C24-C23-C22	-4.57	119.47	126.23
13	a	511	CLA	C4A-NA-C1A	4.56	108.76	106.68
14	e	521	BCR	C16-C17-C18	-4.56	120.88	127.28
13	4	506	CLA	C4A-NA-C1A	4.56	108.76	106.68
13	B	1211	CLA	C4A-NA-C1A	4.55	108.75	106.68
14	f	524	BCR	C28-C27-C26	-4.55	105.94	114.06
13	5	501	CLA	C4A-NA-C1A	4.54	108.75	106.68
13	1	518	CLA	C4A-NA-C1A	4.54	108.75	106.68
13	B	1218	CLA	C4A-NA-C1A	4.54	108.75	106.68
13	5	513	CLA	C4A-NA-C1A	4.54	108.75	106.68
14	1	522	BCR	C11-C10-C9	-4.53	120.92	127.28
14	2	522	BCR	C11-C10-C9	-4.53	120.92	127.28
13	d	518	CLA	C4A-NA-C1A	4.53	108.75	106.68
13	3	501	CLA	C4A-NA-C1A	4.53	108.74	106.68
14	J	4012	BCR	C15-C14-C13	-4.52	120.93	127.28
13	2	513	CLA	C4A-NA-C1A	4.52	108.74	106.68
13	2	516	CLA	C4A-NA-C1A	4.52	108.74	106.68
13	B	1228	CLA	C4A-NA-C1A	4.52	108.74	106.68
14	I	4019	BCR	C15-C14-C13	-4.52	120.94	127.28
14	b	521	BCR	C20-C21-C22	-4.51	120.95	127.28
14	I	4018	BCR	C20-C21-C22	-4.51	120.95	127.28
13	A	1124	CLA	C4A-NA-C1A	4.51	108.74	106.68
14	A	4007	BCR	C15-C14-C13	-4.51	120.95	127.28
14	e	521	BCR	C11-C10-C9	-4.51	120.95	127.28
14	a	523	BCR	C15-C14-C13	-4.51	120.95	127.28
13	1	511	CLA	C4A-NA-C1A	4.50	108.73	106.68
14	c	521	BCR	C20-C21-C22	-4.50	120.96	127.28
14	B	4004	BCR	C15-C14-C13	-4.50	120.96	127.28
14	g	521	BCR	C15-C14-C13	-4.50	120.97	127.28
14	f	521	BCR	C16-C17-C18	-4.50	120.97	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1224	CLA	C4A-NA-C1A	4.50	108.73	106.68
13	f	501	CLA	C4A-NA-C1A	4.50	108.73	106.68
14	A	4002	BCR	C38-C26-C25	-4.49	119.58	124.48
14	f	522	BCR	C16-C17-C18	-4.49	120.98	127.28
13	g	508	CLA	C4A-NA-C1A	4.49	108.73	106.68
13	B	1222	CLA	C4A-NA-C1A	4.49	108.73	106.68
14	g	523	BCR	C16-C17-C18	-4.49	120.99	127.28
13	4	518	CLA	C4A-NA-C1A	4.48	108.72	106.68
13	B	1238	CLA	C4A-NA-C1A	4.48	108.72	106.68
14	5	523	BCR	C15-C14-C13	-4.48	120.99	127.28
14	3	523	BCR	C24-C23-C22	-4.48	119.61	126.23
14	6	523	BCR	C24-C23-C22	-4.47	119.62	126.23
14	c	524	BCR	C11-C10-C9	-4.47	121.01	127.28
13	B	1202	CLA	C4A-NA-C1A	4.47	108.72	106.68
13	B	1219	CLA	CMC-C2C-C1C	4.47	123.94	115.22
13	b	516	CLA	C4A-NA-C1A	4.46	108.72	106.68
13	4	516	CLA	C4A-NA-C1A	4.46	108.71	106.68
13	A	1108	CLA	C4A-NA-C1A	4.46	108.71	106.68
13	b	501	CLA	C4A-NA-C1A	4.46	108.71	106.68
14	4	524	BCR	C7-C8-C9	-4.46	119.64	126.23
14	4	521	BCR	C7-C8-C9	-4.45	119.65	126.23
13	B	1234	CLA	C4A-NA-C1A	4.45	108.71	106.68
13	4	519	CLA	C4A-NA-C1A	4.45	108.71	106.68
14	6	523	BCR	C15-C14-C13	-4.44	121.05	127.28
14	1	523	BCR	C15-C14-C13	-4.44	121.05	127.28
14	2	523	BCR	C15-C14-C13	-4.44	121.05	127.28
13	2	501	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	c	524	BCR	C7-C8-C9	-4.44	119.67	126.23
13	A	1128	CLA	C4A-NA-C1A	4.44	108.70	106.68
13	a	512	CLA	C4A-NA-C1A	4.44	108.70	106.68
14	4	524	BCR	C24-C23-C22	-4.44	119.67	126.23
13	b	513	CLA	C4A-NA-C1A	4.43	108.70	106.68
13	c	513	CLA	C4A-NA-C1A	4.43	108.70	106.68
14	d	521	BCR	C33-C5-C6	-4.42	119.66	124.48
13	b	506	CLA	C4A-NA-C1A	4.42	108.70	106.68
14	5	523	BCR	C16-C17-C18	-4.42	121.08	127.28
13	B	1229	CLA	C4A-NA-C1A	4.42	108.69	106.68
14	I	4018	BCR	C11-C10-C9	-4.41	121.09	127.28
14	e	521	BCR	C15-C14-C13	-4.41	121.09	127.28
13	A	1127	CLA	C4A-NA-C1A	4.41	108.69	106.68
14	d	521	BCR	C24-C23-C22	-4.40	119.72	126.23
13	d	508	CLA	C4A-NA-C1A	4.40	108.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	517	CLA	C4A-NA-C1A	4.39	108.68	106.68
14	e	524	BCR	C33-C5-C6	-4.39	119.69	124.48
13	g	505	CLA	C4A-NA-C1A	4.39	108.68	106.68
13	B	1225	CLA	C4A-NA-C1A	4.39	108.68	106.68
14	d	522	BCR	C33-C5-C6	-4.39	119.70	124.48
13	3	516	CLA	C4A-NA-C1A	4.39	108.68	106.68
14	g	521	BCR	C20-C21-C22	-4.39	121.13	127.28
14	a	524	BCR	C16-C17-C18	-4.38	121.13	127.28
13	e	513	CLA	C4A-NA-C1A	4.38	108.68	106.68
14	2	521	BCR	C11-C10-C9	-4.38	121.14	127.28
14	g	521	BCR	C33-C5-C6	-4.37	119.71	124.48
14	b	521	BCR	C7-C8-C9	-4.37	119.77	126.23
14	3	521	BCR	C33-C5-C6	-4.37	119.72	124.48
13	e	505	CLA	C4A-NA-C1A	4.37	108.67	106.68
13	g	504	CLA	C4A-NA-C1A	4.37	108.67	106.68
14	g	523	BCR	C7-C8-C9	-4.37	119.78	126.23
13	c	501	CLA	C4A-NA-C1A	4.36	108.67	106.68
13	6	516	CLA	C4A-NA-C1A	4.36	108.67	106.68
13	A	1109	CLA	C4A-NA-C1A	4.36	108.67	106.68
13	e	506	CLA	C4A-NA-C1A	4.36	108.67	106.68
13	B	1221	CLA	C4A-NA-C1A	4.35	108.67	106.68
14	g	522	BCR	C7-C8-C9	-4.35	119.80	126.23
14	B	4010	BCR	C11-C10-C9	-4.35	121.18	127.28
14	A	4003	BCR	C20-C21-C22	-4.35	121.18	127.28
14	g	523	BCR	C33-C5-C6	-4.35	119.74	124.48
13	g	501	CLA	C4A-NA-C1A	4.34	108.66	106.68
13	4	501	CLA	C4A-NA-C1A	4.33	108.65	106.68
14	c	522	BCR	C33-C5-C6	-4.32	119.77	124.48
14	e	523	BCR	C15-C14-C13	-4.32	121.22	127.28
14	f	522	BCR	C15-C14-C13	-4.32	121.22	127.28
14	a	524	BCR	C11-C10-C9	-4.31	121.24	127.28
14	a	521	BCR	C33-C5-C6	-4.31	119.78	124.48
14	I	4020	BCR	C20-C21-C22	-4.30	121.25	127.28
13	g	506	CLA	C4A-NA-C1A	4.30	108.64	106.68
14	b	524	BCR	C11-C10-C9	-4.30	121.25	127.28
14	4	524	BCR	C11-C10-C9	-4.30	121.25	127.28
13	B	1205	CLA	C4A-NA-C1A	4.30	108.64	106.68
15	g	822	SQD	O47-C7-C8	4.29	120.77	111.48
14	4	521	BCR	C20-C21-C22	-4.29	121.26	127.28
14	F	4016	BCR	C7-C8-C9	-4.29	119.89	126.23
14	4	521	BCR	C15-C14-C13	-4.29	121.26	127.28
14	A	4002	BCR	C7-C8-C9	-4.29	119.89	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4004	BCR	C33-C5-C6	-4.29	119.81	124.48
13	d	516	CLA	C4A-NA-C1A	4.29	108.63	106.68
14	d	521	BCR	C16-C17-C18	-4.28	121.27	127.28
14	c	523	BCR	C16-C17-C18	-4.28	121.27	127.28
14	5	522	BCR	C16-C17-C18	-4.28	121.28	127.28
14	6	521	BCR	C7-C8-C9	-4.28	119.91	126.23
14	4	522	BCR	C11-C10-C9	-4.28	121.28	127.28
14	F	4015	BCR	C16-C17-C18	-4.28	121.28	127.28
14	g	523	BCR	C24-C23-C22	-4.27	119.91	126.23
14	6	524	BCR	C11-C10-C9	-4.27	121.29	127.28
14	3	521	BCR	C11-C10-C9	-4.27	121.29	127.28
14	2	521	BCR	C15-C14-C13	-4.27	121.29	127.28
13	6	509	CLA	C4A-NA-C1A	4.27	108.62	106.68
14	3	523	BCR	C11-C10-C9	-4.26	121.30	127.28
14	1	524	BCR	C16-C17-C18	-4.26	121.30	127.28
14	f	524	BCR	C33-C5-C6	-4.26	119.84	124.48
14	J	4012	BCR	C3-C4-C5	-4.25	106.47	114.06
14	d	523	BCR	C11-C10-C9	-4.25	121.31	127.28
14	5	521	BCR	C7-C8-C9	-4.25	119.94	126.23
14	6	522	BCR	C20-C21-C22	-4.25	121.32	127.28
14	A	4007	BCR	C7-C8-C9	-4.25	119.95	126.23
14	K	4001	BCR	C11-C10-C9	-4.25	121.32	127.28
14	g	524	BCR	C20-C21-C22	-4.25	121.32	127.28
13	3	508	CLA	C4A-NA-C1A	4.25	108.62	106.68
14	I	4020	BCR	C24-C23-C22	-4.25	119.95	126.23
14	c	524	BCR	C33-C5-C6	-4.24	119.85	124.48
13	4	511	CLA	C4A-NA-C1A	4.24	108.61	106.68
14	F	4015	BCR	C24-C23-C22	-4.24	119.96	126.23
14	6	521	BCR	C33-C5-C6	-4.23	119.86	124.48
14	e	521	BCR	C20-C21-C22	-4.23	121.34	127.28
13	B	1012	CLA	C4A-NA-C1A	4.23	108.61	106.68
14	2	523	BCR	C7-C8-C9	-4.22	119.99	126.23
13	3	505	CLA	C4A-NA-C1A	4.22	108.60	106.68
17	A	5001	LHG	O7-C7-C8	4.21	120.60	111.48
14	A	4007	BCR	C38-C26-C25	-4.21	119.89	124.48
14	e	524	BCR	C7-C8-C9	-4.21	120.00	126.23
13	c	508	CLA	C4A-NA-C1A	4.21	108.60	106.68
13	1	503	CLA	C4A-NA-C1A	4.20	108.59	106.68
14	f	523	BCR	C11-C10-C9	-4.20	121.39	127.28
14	a	524	BCR	C20-C21-C22	-4.20	121.39	127.28
13	A	1011	CLA	C4A-NA-C1A	4.20	108.59	106.68
14	f	521	BCR	C3-C4-C5	-4.20	106.57	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	c	521	BCR	C24-C23-C22	-4.19	120.03	126.23
14	6	522	BCR	C33-C5-C6	-4.19	119.91	124.48
13	f	519	CLA	C4A-NA-C1A	4.19	108.59	106.68
14	I	4019	BCR	C38-C26-C25	-4.19	119.92	124.48
14	5	521	BCR	C15-C14-C13	-4.18	121.41	127.28
14	f	524	BCR	C11-C10-C9	-4.18	121.42	127.28
14	A	4011	BCR	C28-C27-C26	-4.17	106.61	114.06
14	g	522	BCR	C16-C17-C18	-4.17	121.43	127.28
14	3	521	BCR	C15-C14-C13	-4.17	121.43	127.28
13	1	508	CLA	C4A-NA-C1A	4.17	108.58	106.68
14	a	523	BCR	C33-C5-C6	-4.16	119.94	124.48
14	3	521	BCR	C16-C17-C18	-4.16	121.45	127.28
14	g	523	BCR	C28-C27-C26	-4.15	106.65	114.06
16	2	5104	LMG	O7-C10-C11	4.14	120.45	111.48
14	f	523	BCR	C24-C23-C22	-4.14	120.11	126.23
14	f	524	BCR	C15-C14-C13	-4.14	121.48	127.28
13	5	508	CLA	C4A-NA-C1A	4.13	108.56	106.68
13	e	501	CLA	C4A-NA-C1A	4.13	108.56	106.68
14	4	521	BCR	C11-C10-C9	-4.13	121.48	127.28
14	e	523	BCR	C33-C5-C6	-4.13	119.98	124.48
14	3	522	BCR	C33-C5-C6	-4.13	119.98	124.48
13	6	501	CLA	C4A-NA-C1A	4.13	108.56	106.68
13	A	1102	CLA	C4A-NA-C1A	4.13	108.56	106.68
14	5	524	BCR	C21-C20-C19	-4.13	111.24	123.20
14	6	523	BCR	C7-C8-C9	-4.12	120.14	126.23
14	B	4009	BCR	C16-C17-C18	-4.11	121.51	127.28
14	3	522	BCR	C16-C17-C18	-4.11	121.52	127.28
13	2	508	CLA	C4A-NA-C1A	4.11	108.55	106.68
16	J	5104	LMG	O7-C10-C11	4.11	120.37	111.48
14	2	523	BCR	C20-C21-C22	-4.11	121.52	127.28
14	2	521	BCR	C28-C27-C26	-4.10	106.74	114.06
13	1	501	CLA	C4A-NA-C1A	4.10	108.55	106.68
14	B	4010	BCR	C38-C26-C25	-4.10	120.01	124.48
14	1	521	BCR	C11-C10-C9	-4.10	121.52	127.28
16	g	5104	LMG	O7-C10-C11	4.10	120.35	111.48
14	g	523	BCR	C20-C21-C22	-4.10	121.53	127.28
14	f	521	BCR	C11-C10-C9	-4.09	121.54	127.28
14	F	4015	BCR	C20-C21-C22	-4.09	121.54	127.28
13	f	503	CLA	C4A-NA-C1A	4.09	108.54	106.68
13	b	508	CLA	C4A-NA-C1A	4.09	108.54	106.68
14	6	522	BCR	C38-C26-C25	-4.08	120.03	124.48
13	g	516	CLA	C4A-NA-C1A	4.08	108.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	522	BCR	C7-C8-C9	-4.07	120.21	126.23
14	1	524	BCR	C33-C5-C6	-4.07	120.04	124.48
14	6	522	BCR	C24-C23-C22	-4.07	120.21	126.23
14	c	522	BCR	C28-C27-C26	-4.07	106.80	114.06
13	B	1012	CLA	O2D-CGD-O1D	-4.06	115.94	123.85
13	d	505	CLA	C4A-NA-C1A	4.06	108.53	106.68
14	I	4020	BCR	C16-C17-C18	-4.06	121.59	127.28
13	A	1022	CLA	C4A-NA-C1A	4.06	108.53	106.68
13	e	516	CLA	C4A-NA-C1A	4.05	108.53	106.68
14	I	4020	BCR	C38-C26-C25	-4.05	120.06	124.48
17	A	5004	LHG	O7-C7-C8	4.04	120.23	111.48
14	2	521	BCR	C24-C23-C22	-4.04	120.25	126.23
14	e	521	BCR	C7-C8-C9	-4.04	120.25	126.23
14	3	524	BCR	C7-C8-C9	-4.04	120.25	126.23
14	d	521	BCR	C7-C8-C9	-4.04	120.26	126.23
13	c	516	CLA	C4A-NA-C1A	4.04	108.52	106.68
14	g	524	BCR	C33-C5-C6	-4.04	120.08	124.48
13	5	517	CLA	C4A-NA-C1A	4.04	108.52	106.68
14	6	523	BCR	C33-C5-C6	-4.03	120.08	124.48
14	1	523	BCR	C16-C17-C18	-4.03	121.63	127.28
14	c	521	BCR	C11-C10-C9	-4.03	121.63	127.28
14	f	524	BCR	C7-C8-C9	-4.03	120.28	126.23
14	4	522	BCR	C16-C17-C18	-4.03	121.63	127.28
14	3	521	BCR	C7-C8-C9	-4.02	120.28	126.23
14	I	4018	BCR	C16-C17-C18	-4.02	121.64	127.28
14	B	4005	BCR	C11-C10-C9	-4.02	121.64	127.28
14	A	4002	BCR	C15-C14-C13	-4.02	121.64	127.28
14	a	521	BCR	C20-C21-C22	-4.02	121.64	127.28
13	B	1201	CLA	C4A-NA-C1A	4.02	108.51	106.68
14	6	521	BCR	C24-C23-C22	-4.02	120.30	126.23
13	A	1129	CLA	C4A-NA-C1A	4.01	108.51	106.68
14	4	521	BCR	C33-C5-C6	-4.01	120.11	124.48
13	A	1139	CLA	C4A-NA-C1A	4.00	108.50	106.68
14	6	522	BCR	C16-C17-C18	-4.00	121.67	127.28
14	b	521	BCR	C11-C10-C9	-4.00	121.67	127.28
13	B	1208	CLA	C4A-NA-C1A	4.00	108.50	106.68
14	g	522	BCR	C20-C21-C22	-4.00	121.67	127.28
14	5	521	BCR	C11-C10-C9	-3.99	121.68	127.28
13	5	516	CLA	C4A-NA-C1A	3.99	108.50	106.68
14	b	522	BCR	C33-C5-C6	-3.98	120.14	124.48
14	I	4019	BCR	C16-C17-C18	-3.98	121.70	127.28
14	d	522	BCR	C28-C27-C26	-3.97	106.97	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4010	BCR	C20-C21-C22	-3.97	121.71	127.28
14	B	4006	BCR	C7-C8-C9	-3.97	120.36	126.23
14	A	4007	BCR	C11-C10-C9	-3.97	121.72	127.28
14	4	523	BCR	C11-C10-C9	-3.96	121.72	127.28
14	3	524	BCR	C11-C10-C9	-3.96	121.72	127.28
13	B	1023	CLA	C4A-NA-C1A	3.96	108.49	106.68
14	2	522	BCR	C7-C8-C9	-3.96	120.38	126.23
14	K	4001	BCR	C15-C14-C13	-3.96	121.73	127.28
13	6	504	CLA	C4A-NA-C1A	3.95	108.48	106.68
14	F	4016	BCR	C20-C21-C22	-3.95	121.74	127.28
14	I	4020	BCR	C8-C7-C6	-3.95	116.45	127.00
17	A	5002	LHG	O7-C7-C8	3.94	120.01	111.48
14	F	4016	BCR	C16-C17-C18	-3.94	121.75	127.28
14	B	4005	BCR	C16-C17-C18	-3.94	121.76	127.28
14	b	521	BCR	C33-C5-C6	-3.93	120.19	124.48
14	a	524	BCR	C24-C23-C22	-3.93	120.42	126.23
14	1	521	BCR	C24-C23-C22	-3.93	120.42	126.23
14	2	521	BCR	C7-C8-C9	-3.92	120.43	126.23
14	e	521	BCR	C33-C5-C6	-3.92	120.21	124.48
14	f	523	BCR	C20-C21-C22	-3.91	121.79	127.28
14	d	522	BCR	C24-C23-C22	-3.91	120.44	126.23
14	J	4013	BCR	C33-C5-C6	-3.91	120.22	124.48
14	3	521	BCR	C20-C21-C22	-3.91	121.80	127.28
14	K	4001	BCR	C7-C8-C9	-3.91	120.45	126.23
14	B	4006	BCR	C33-C5-C6	-3.91	120.22	124.48
14	g	522	BCR	C33-C5-C6	-3.90	120.23	124.48
13	4	517	CLA	C4A-NA-C1A	3.89	108.45	106.68
14	1	523	BCR	C33-C5-C6	-3.88	120.25	124.48
14	1	521	BCR	C16-C17-C18	-3.88	121.84	127.28
13	6	505	CLA	C4A-NA-C1A	3.88	108.45	106.68
14	b	521	BCR	C16-C17-C18	-3.88	121.84	127.28
14	F	4015	BCR	C38-C26-C25	-3.88	120.25	124.48
13	6	517	CLA	C4A-NA-C1A	3.88	108.45	106.68
14	a	521	BCR	C24-C23-C22	-3.87	120.51	126.23
14	c	521	BCR	C16-C17-C18	-3.86	121.86	127.28
16	6	5104	LMG	O7-C10-C11	3.86	119.83	111.48
14	1	521	BCR	C7-C8-C9	-3.85	120.53	126.23
13	A	1117	CLA	C4A-NA-C1A	3.85	108.44	106.68
14	e	523	BCR	C20-C21-C22	-3.85	121.88	127.28
13	f	517	CLA	C4A-NA-C1A	3.85	108.43	106.68
15	6	822	SQD	O47-C7-C8	3.84	119.79	111.48
14	2	522	BCR	C33-C5-C6	-3.84	120.30	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	524	BCR	C38-C26-C25	-3.83	120.30	124.48
14	A	4008	BCR	C33-C5-C6	-3.83	120.31	124.48
14	A	4011	BCR	C38-C26-C25	-3.82	120.32	124.48
14	A	4007	BCR	C16-C17-C18	-3.80	121.94	127.28
14	4	522	BCR	C3-C4-C5	-3.80	107.28	114.06
17	A	5005	LHG	O7-C7-C8	3.80	119.70	111.48
13	B	1021	CLA	C4A-NA-C1A	3.80	108.41	106.68
14	4	521	BCR	C28-C27-C26	-3.80	107.29	114.06
14	d	524	BCR	C20-C21-C22	-3.79	121.96	127.28
14	a	523	BCR	C38-C26-C25	-3.79	120.35	124.48
14	B	4005	BCR	C20-C21-C22	-3.79	121.97	127.28
14	b	521	BCR	C24-C23-C22	-3.78	120.64	126.23
13	A	1136	CLA	C4A-NA-C1A	3.78	108.41	106.68
14	A	4003	BCR	C33-C5-C6	-3.78	120.36	124.48
14	g	522	BCR	C38-C26-C25	-3.78	120.36	124.48
14	F	4014	BCR	C16-C15-C14	-3.78	115.79	123.52
14	5	523	BCR	C39-C30-C25	3.78	116.16	110.24
15	d	822	SQD	O47-C7-C8	3.77	119.64	111.48
16	1	5104	LMG	O7-C10-C11	3.77	119.64	111.48
13	2	517	CLA	C4A-NA-C1A	3.77	108.40	106.68
14	J	4012	BCR	C28-C27-C26	-3.76	107.35	114.06
14	f	521	BCR	C7-C8-C9	-3.76	120.67	126.23
14	2	523	BCR	C24-C23-C22	-3.76	120.68	126.23
14	K	4001	BCR	C28-C27-C26	-3.76	107.36	114.06
14	1	521	BCR	C33-C5-C6	-3.75	120.39	124.48
14	1	523	BCR	C11-C10-C9	-3.74	122.03	127.28
14	b	523	BCR	C20-C21-C22	-3.74	122.03	127.28
14	F	4016	BCR	C33-C5-C6	-3.74	120.40	124.48
14	4	524	BCR	C15-C14-C13	-3.74	122.03	127.28
14	I	4019	BCR	C20-C21-C22	-3.74	122.04	127.28
14	6	522	BCR	C7-C8-C9	-3.74	120.71	126.23
14	2	521	BCR	C33-C5-C6	-3.74	120.41	124.48
14	6	524	BCR	C7-C8-C9	-3.73	120.72	126.23
14	5	522	BCR	C33-C5-C6	-3.73	120.41	124.48
14	5	521	BCR	C20-C21-C22	-3.73	122.05	127.28
14	a	523	BCR	C11-C10-C9	-3.73	122.05	127.28
14	B	4010	BCR	C16-C17-C18	-3.73	122.05	127.28
14	d	522	BCR	C20-C21-C22	-3.72	122.06	127.28
14	I	4020	BCR	C1-C6-C5	-3.72	117.55	122.64
14	A	4002	BCR	C20-C21-C22	-3.72	122.06	127.28
14	A	4003	BCR	C24-C23-C22	-3.71	120.74	126.23
14	4	521	BCR	C24-C23-C22	-3.71	120.75	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	d	524	BCR	C3-C4-C5	-3.71	107.44	114.06
14	c	524	BCR	C20-C21-C22	-3.71	122.08	127.28
14	c	522	BCR	C20-C21-C22	-3.71	122.08	127.28
14	b	523	BCR	C24-C23-C22	-3.71	120.75	126.23
13	B	1230	CLA	C4A-NA-C1A	3.70	108.37	106.68
13	B	1209	CLA	O2D-CGD-O1D	-3.70	116.64	123.85
14	4	524	BCR	C33-C5-C6	-3.69	120.45	124.48
14	g	522	BCR	C3-C4-C5	-3.69	107.48	114.06
14	5	521	BCR	C33-C5-C6	-3.68	120.47	124.48
14	1	522	BCR	C33-C5-C6	-3.67	120.48	124.48
14	b	523	BCR	C33-C5-C6	-3.67	120.48	124.48
14	A	4011	BCR	C11-C10-C9	-3.67	122.13	127.28
14	5	521	BCR	C24-C23-C22	-3.66	120.81	126.23
13	A	1133	CLA	C4A-NA-C1A	3.66	108.35	106.68
13	B	1216	CLA	C4A-NA-C1A	3.66	108.35	106.68
14	a	524	BCR	C7-C8-C9	-3.66	120.83	126.23
14	2	521	BCR	C20-C21-C22	-3.65	122.16	127.28
14	5	524	BCR	C16-C15-C14	-3.65	116.05	123.52
14	d	522	BCR	C16-C17-C18	-3.65	122.16	127.28
14	b	524	BCR	C7-C8-C9	-3.65	120.84	126.23
14	3	521	BCR	C24-C23-C22	-3.65	120.84	126.23
14	e	522	BCR	C38-C26-C25	-3.64	120.51	124.48
14	1	523	BCR	C24-C23-C22	-3.64	120.85	126.23
14	d	523	BCR	C20-C21-C22	-3.63	122.18	127.28
14	e	521	BCR	C28-C27-C26	-3.63	107.58	114.06
14	3	522	BCR	C20-C21-C22	-3.63	122.19	127.28
20	B	1843	LMU	C1B-O1B-C4'	-3.63	109.39	117.98
14	2	524	BCR	C7-C8-C9	-3.62	120.87	126.23
14	K	4001	BCR	C16-C17-C18	-3.62	122.20	127.28
14	1	524	BCR	C24-C23-C22	-3.62	120.88	126.23
15	B	1852	SQD	O47-C7-C8	3.62	119.31	111.48
14	M	4021	BCR	C33-C5-C6	-3.61	120.54	124.48
14	B	4005	BCR	C28-C27-C26	-3.61	107.62	114.06
14	g	521	BCR	C24-C23-C22	-3.61	120.89	126.23
14	g	524	BCR	C7-C8-C9	-3.61	120.89	126.23
14	c	524	BCR	C38-C26-C25	-3.61	120.55	124.48
15	2	822	SQD	O47-C7-C8	3.61	119.29	111.48
14	4	522	BCR	C7-C8-C9	-3.60	120.91	126.23
16	B	5002	LMG	O7-C10-C11	3.60	119.27	111.48
13	A	1102	CLA	O2D-CGD-O1D	-3.60	116.85	123.85
14	6	524	BCR	C3-C4-C5	-3.59	107.65	114.06
14	e	521	BCR	C24-C23-C22	-3.59	120.92	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	1	522	BCR	C38-C26-C25	-3.59	120.57	124.48
14	A	4008	BCR	C28-C27-C26	-3.59	107.65	114.06
14	4	523	BCR	C7-C8-C9	-3.58	120.93	126.23
14	F	4014	BCR	C33-C5-C6	-3.58	120.58	124.48
14	B	4005	BCR	C7-C8-C9	-3.57	120.95	126.23
14	1	521	BCR	C38-C26-C25	-3.57	120.59	124.48
14	3	522	BCR	C38-C26-C25	-3.57	120.59	124.48
14	4	524	BCR	C3-C4-C5	-3.56	107.71	114.06
14	2	523	BCR	C16-C17-C18	-3.56	122.29	127.28
14	d	523	BCR	C24-C23-C22	-3.55	120.98	126.23
14	3	523	BCR	C38-C26-C25	-3.55	120.61	124.48
14	4	523	BCR	C24-C23-C22	-3.55	120.98	126.23
14	B	4010	BCR	C8-C7-C6	-3.55	117.52	127.00
14	e	524	BCR	C38-C26-C25	-3.55	120.61	124.48
14	5	521	BCR	C3-C4-C5	-3.55	107.73	114.06
14	f	522	BCR	C38-C26-C25	-3.54	120.62	124.48
14	A	4003	BCR	C3-C4-C5	-3.54	107.75	114.06
13	b	506	CLA	O2D-CGD-O1D	-3.54	116.96	123.85
14	J	4013	BCR	C8-C7-C6	-3.54	117.55	127.00
14	a	524	BCR	C38-C26-C25	-3.53	120.63	124.48
14	B	4010	BCR	C33-C5-C6	-3.53	120.63	124.48
14	4	523	BCR	C33-C5-C6	-3.53	120.64	124.48
14	c	523	BCR	C20-C21-C22	-3.53	122.33	127.28
14	1	522	BCR	C16-C17-C18	-3.53	122.33	127.28
14	5	523	BCR	C33-C5-C6	-3.53	120.64	124.48
13	B	1224	CLA	O2D-CGD-O1D	-3.52	116.99	123.85
14	g	521	BCR	C28-C27-C26	-3.52	107.77	114.06
14	I	4020	BCR	C11-C10-C9	-3.52	122.34	127.28
14	2	522	BCR	C15-C16-C17	-3.52	116.31	123.52
14	6	521	BCR	C38-C26-C25	-3.52	120.64	124.48
14	A	4003	BCR	C38-C26-C25	-3.52	120.64	124.48
14	e	523	BCR	C28-C27-C26	-3.52	107.78	114.06
17	A	5003	LHG	O7-C7-C8	3.52	119.09	111.48
14	J	4013	BCR	C3-C4-C5	-3.51	107.79	114.06
14	b	522	BCR	C38-C26-C25	-3.51	120.65	124.48
15	a	822	SQD	O47-C7-C8	3.51	119.07	111.48
13	b	506	CLA	CHB-C1B-NB	3.51	129.31	124.05
14	c	521	BCR	C33-C5-C6	-3.50	120.66	124.48
14	f	521	BCR	C28-C27-C26	-3.50	107.81	114.06
14	3	521	BCR	C38-C26-C25	-3.50	120.66	124.48
14	c	522	BCR	C7-C8-C9	-3.49	121.07	126.23
14	2	522	BCR	C38-C26-C25	-3.48	120.69	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1236	CLA	O2D-CGD-O1D	-3.48	117.08	123.85
14	4	522	BCR	C20-C21-C22	-3.48	122.40	127.28
14	b	521	BCR	C3-C4-C5	-3.47	107.86	114.06
13	A	1140	CLA	O2D-CGD-O1D	-3.47	117.10	123.85
14	A	4003	BCR	C16-C17-C18	-3.47	122.41	127.28
14	M	4021	BCR	C3-C4-C5	-3.47	107.87	114.06
13	B	1222	CLA	O2D-CGD-O1D	-3.46	117.10	123.85
13	A	1013	CLA	O2D-CGD-O1D	-3.45	117.12	123.85
14	5	524	BCR	C33-C5-C6	-3.45	120.72	124.48
14	5	522	BCR	C23-C24-C25	-3.45	117.79	127.00
14	2	521	BCR	C3-C4-C5	-3.44	107.92	114.06
15	c	822	SQD	O47-C7-C8	3.44	118.92	111.48
14	F	4015	BCR	C2-C1-C6	3.44	115.43	110.44
14	d	521	BCR	C28-C27-C26	-3.43	107.94	114.06
14	6	522	BCR	C3-C4-C5	-3.43	107.94	114.06
14	B	4009	BCR	C8-C7-C6	-3.43	117.84	127.00
14	K	4001	BCR	C33-C5-C6	-3.43	120.75	124.48
14	b	521	BCR	C28-C27-C26	-3.43	107.95	114.06
14	2	522	BCR	C23-C24-C25	-3.42	117.86	127.00
14	d	524	BCR	C7-C8-C9	-3.42	121.18	126.23
14	1	522	BCR	C23-C24-C25	-3.42	117.87	127.00
13	a	501	CLA	O2D-CGD-O1D	-3.42	117.20	123.85
14	a	522	BCR	C23-C24-C25	-3.42	117.87	127.00
14	B	4017	BCR	C11-C10-C9	-3.41	122.49	127.28
14	3	522	BCR	C23-C24-C25	-3.41	117.88	127.00
14	5	522	BCR	C38-C26-C25	-3.41	120.76	124.48
14	a	524	BCR	C33-C5-C6	-3.41	120.76	124.48
14	6	521	BCR	C28-C27-C26	-3.41	107.97	114.06
14	2	524	BCR	C38-C26-C25	-3.41	120.76	124.48
14	a	523	BCR	C24-C23-C22	-3.41	121.19	126.23
14	A	4011	BCR	C24-C23-C22	-3.41	121.19	126.23
14	M	4021	BCR	C28-C27-C26	-3.41	107.98	114.06
15	5	822	SQD	O47-C7-C8	3.40	118.84	111.48
14	B	4017	BCR	C15-C14-C13	-3.40	122.51	127.28
14	5	524	BCR	C23-C22-C21	-3.40	113.66	119.01
14	B	4006	BCR	C20-C21-C22	-3.40	122.51	127.28
14	M	4021	BCR	C7-C8-C9	-3.40	121.20	126.23
14	J	4013	BCR	C11-C12-C13	-3.40	117.05	126.36
14	B	4005	BCR	C33-C5-C6	-3.40	120.78	124.48
14	4	523	BCR	C20-C21-C22	-3.38	122.53	127.28
14	F	4015	BCR	C3-C4-C5	-3.38	108.02	114.06
14	c	522	BCR	C8-C7-C6	-3.38	117.96	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	524	BCR	C3-C4-C5	-3.38	108.02	114.06
14	b	522	BCR	C7-C8-C9	-3.38	121.23	126.23
14	6	524	BCR	C33-C5-C6	-3.38	120.80	124.48
14	c	521	BCR	C7-C8-C9	-3.37	121.25	126.23
14	a	522	BCR	C38-C26-C25	-3.37	120.81	124.48
14	I	4019	BCR	C7-C8-C9	-3.37	121.25	126.23
14	b	524	BCR	C33-C5-C6	-3.36	120.82	124.48
14	1	523	BCR	C20-C21-C22	-3.36	122.56	127.28
14	1	524	BCR	C3-C4-C5	-3.36	108.06	114.06
13	B	1204	CLA	O2D-CGD-O1D	-3.36	117.31	123.85
14	3	524	BCR	C38-C26-C25	-3.36	120.82	124.48
14	3	523	BCR	C20-C21-C22	-3.36	122.57	127.28
14	a	522	BCR	C20-C21-C22	-3.35	122.58	127.28
14	M	4021	BCR	C38-C26-C25	-3.35	120.83	124.48
14	4	522	BCR	C33-C5-C6	-3.35	120.83	124.48
14	d	524	BCR	C38-C26-C25	-3.35	120.83	124.48
14	J	4012	BCR	C24-C23-C22	-3.35	121.28	126.23
14	e	522	BCR	C20-C21-C22	-3.34	122.59	127.28
13	B	1226	CLA	O2D-CGD-O1D	-3.34	117.35	123.85
15	b	822	SQD	O47-C7-C8	3.34	118.70	111.48
15	1	822	SQD	O47-C7-C8	3.34	118.70	111.48
14	4	522	BCR	C38-C26-C25	-3.34	120.84	124.48
13	J	1303	CLA	CMC-C2C-C1C	3.33	124.95	118.04
14	5	522	BCR	C28-C27-C26	-3.33	108.11	114.06
14	5	522	BCR	C20-C21-C22	-3.33	122.61	127.28
14	a	523	BCR	C8-C7-C6	-3.33	118.11	127.00
14	e	523	BCR	C11-C10-C9	-3.33	122.61	127.28
14	1	523	BCR	C7-C8-C9	-3.33	121.31	126.23
13	A	1137	CLA	O2D-CGD-O1D	-3.33	117.37	123.85
13	4	503	CLA	C1-C2-C3	-3.33	120.75	126.20
14	5	521	BCR	C28-C27-C26	-3.32	108.14	114.06
14	3	523	BCR	C16-C17-C18	-3.32	122.62	127.28
15	e	822	SQD	O47-C7-C8	3.30	118.62	111.48
14	2	522	BCR	C28-C27-C26	-3.30	108.17	114.06
13	X	1401	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
13	A	1125	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
14	B	4009	BCR	C11-C10-C9	-3.29	122.66	127.28
14	f	522	BCR	C23-C24-C25	-3.29	118.21	127.00
15	3	822	SQD	O47-C7-C8	3.29	118.59	111.48
13	B	1208	CLA	O2D-CGD-O1D	-3.28	117.45	123.85
14	3	523	BCR	C3-C4-C5	-3.28	108.20	114.06
14	6	524	BCR	C38-C26-C25	-3.28	120.90	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	c	521	BCR	C28-C27-C26	-3.28	108.20	114.06
14	b	522	BCR	C24-C23-C22	-3.28	121.38	126.23
13	B	1228	CLA	O2D-CGD-O1D	-3.28	117.46	123.85
13	A	1132	CLA	O2D-CGD-O1D	-3.28	117.47	123.85
14	b	522	BCR	C28-C27-C26	-3.28	108.21	114.06
14	f	522	BCR	C28-C27-C26	-3.27	108.23	114.06
14	d	523	BCR	C38-C26-C25	-3.27	120.92	124.48
14	c	522	BCR	C11-C12-C13	-3.26	117.41	126.36
13	A	1136	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
14	1	522	BCR	C3-C4-C5	-3.26	108.25	114.06
14	1	521	BCR	C3-C4-C5	-3.26	108.25	114.06
14	b	522	BCR	C16-C17-C18	-3.26	122.71	127.28
14	d	524	BCR	C33-C5-C6	-3.25	120.94	124.48
14	F	4016	BCR	C28-C27-C26	-3.25	108.26	114.06
14	e	521	BCR	C38-C26-C25	-3.25	120.94	124.48
14	I	4020	BCR	C33-C5-C6	-3.24	120.95	124.48
14	c	521	BCR	C3-C4-C5	-3.24	108.28	114.06
14	1	521	BCR	C28-C27-C26	-3.24	108.28	114.06
13	A	1103	CLA	O2D-CGD-O1D	-3.23	117.56	123.85
14	J	4013	BCR	C23-C24-C25	-3.23	118.37	127.00
14	B	4010	BCR	C3-C4-C5	-3.23	108.30	114.06
14	e	522	BCR	C23-C24-C25	-3.23	118.38	127.00
13	B	1218	CLA	O2D-CGD-O1D	-3.22	117.57	123.85
13	A	1101	CLA	O2D-CGD-O1D	-3.22	117.58	123.85
13	B	1202	CLA	O2D-CGD-O1D	-3.21	117.59	123.85
14	2	522	BCR	C3-C4-C5	-3.21	108.33	114.06
13	b	505	CLA	C1-C2-C3	-3.21	120.94	126.20
14	b	524	BCR	C20-C21-C22	-3.21	122.78	127.28
14	a	521	BCR	C3-C4-C5	-3.20	108.35	114.06
15	f	822	SQD	O47-C7-C8	3.20	118.40	111.48
14	4	523	BCR	C3-C4-C5	-3.20	108.36	114.06
13	B	1230	CLA	C1-C2-C3	-3.19	120.97	126.20
14	A	4002	BCR	C28-C27-C26	-3.19	108.36	114.06
13	A	1131	CLA	O2D-CGD-O1D	-3.19	117.64	123.85
14	6	522	BCR	C11-C12-C13	-3.19	117.62	126.36
14	4	522	BCR	C23-C24-C25	-3.19	118.48	127.00
13	A	1114	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
14	A	4008	BCR	C27-C26-C25	-3.18	118.41	122.70
14	B	4010	BCR	C15-C16-C17	-3.18	117.02	123.52
14	2	522	BCR	C20-C21-C22	-3.18	122.82	127.28
14	A	4011	BCR	C16-C15-C14	-3.18	117.02	123.52
13	A	1123	CLA	O2D-CGD-O1D	-3.17	117.67	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1234	CLA	O2D-CGD-O1D	-3.17	117.67	123.85
13	A	1130	CLA	O2D-CGD-O1D	-3.17	117.68	123.85
14	e	524	BCR	C20-C21-C22	-3.17	122.84	127.28
13	b	507	CLA	O2D-CGD-O1D	-3.17	117.69	123.85
13	A	1124	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
14	2	523	BCR	C3-C4-C5	-3.16	108.42	114.06
13	B	1223	CLA	O2D-CGD-O1D	-3.16	117.69	123.85
13	A	1128	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
13	A	1135	CLA	O2D-CGD-O1D	-3.16	117.70	123.85
14	3	522	BCR	C24-C23-C22	-3.16	121.56	126.23
13	A	1013	CLA	C4A-NA-C1A	3.16	108.12	106.68
14	3	523	BCR	C7-C8-C9	-3.16	121.57	126.23
14	g	521	BCR	C3-C4-C5	-3.15	108.43	114.06
14	5	523	BCR	C24-C23-C22	-3.15	121.57	126.23
14	M	4021	BCR	C16-C15-C14	-3.15	117.07	123.52
14	b	523	BCR	C15-C16-C17	-3.15	117.07	123.52
14	I	4020	BCR	C33-C5-C4	3.15	120.31	113.60
14	c	521	BCR	C38-C26-C25	-3.15	121.05	124.48
13	c	506	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
13	B	1201	CLA	O2D-CGD-O1D	-3.15	117.72	123.85
13	B	1230	CLA	O2D-CGD-O1D	-3.14	117.75	123.85
14	J	4013	BCR	C21-C20-C19	-3.13	114.12	123.20
14	B	4006	BCR	C38-C26-C25	-3.13	121.07	124.48
14	c	522	BCR	C3-C4-C5	-3.13	108.48	114.06
14	1	523	BCR	C27-C26-C25	-3.13	118.48	122.70
14	d	523	BCR	C15-C16-C17	-3.13	117.12	123.52
13	A	1134	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	f	522	BCR	C20-C21-C22	-3.12	122.90	127.28
13	B	1235	CLA	O2D-CGD-O1D	-3.12	117.77	123.85
14	A	4007	BCR	C23-C24-C25	-3.12	118.66	127.00
14	e	524	BCR	C16-C15-C14	-3.12	117.14	123.52
14	K	4001	BCR	C24-C23-C22	-3.12	121.62	126.23
14	3	524	BCR	C2-C1-C6	3.12	114.97	110.44
13	A	1105	CLA	O2D-CGD-O1D	-3.12	117.78	123.85
14	4	522	BCR	C28-C27-C26	-3.11	108.50	114.06
13	a	504	CLA	O2D-CGD-O1D	-3.11	117.79	123.85
14	g	522	BCR	C24-C23-C22	-3.11	121.64	126.23
14	I	4018	BCR	C30-C25-C26	-3.11	118.39	122.64
14	5	522	BCR	C3-C4-C5	-3.11	108.52	114.06
14	d	521	BCR	C38-C26-C25	-3.11	121.09	124.48
14	b	522	BCR	C23-C24-C25	-3.11	118.70	127.00
13	B	1231	CLA	O2D-CGD-O1D	-3.10	117.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	513	CLA	O2D-CGD-O1D	-3.10	117.81	123.85
14	b	522	BCR	C3-C4-C5	-3.10	108.53	114.06
14	a	523	BCR	C38-C26-C27	3.10	120.20	113.60
13	A	1109	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
13	B	1239	CLA	O2D-CGD-O1D	-3.10	117.82	123.85
13	a	508	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	A	1133	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
13	g	504	CLA	O2D-CGD-O1D	-3.09	117.83	123.85
14	6	524	BCR	C23-C24-C25	-3.09	118.75	127.00
14	I	4019	BCR	C11-C10-C9	-3.09	122.95	127.28
13	B	1023	CLA	CAC-C3C-C4C	3.09	128.81	124.79
13	3	510	CLA	C1-C2-C3	-3.09	121.14	126.20
13	B	1226	CLA	C1-C2-C3	-3.08	121.14	126.20
13	B	1219	CLA	C4D-ND-C1D	-3.08	104.01	106.39
13	A	1022	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
13	B	1214	CLA	O2D-CGD-O1D	-3.08	117.85	123.85
13	e	511	CLA	O2D-CGD-O1D	-3.08	117.86	123.85
14	5	523	BCR	C30-C25-C24	3.08	124.00	115.65
14	c	523	BCR	C33-C5-C6	-3.08	121.13	124.48
13	1	516	CLA	O2D-CGD-O1D	-3.07	117.87	123.85
14	d	522	BCR	C15-C16-C17	-3.07	117.23	123.52
14	e	522	BCR	C16-C17-C18	-3.07	122.97	127.28
14	4	521	BCR	C3-C4-C5	-3.07	108.58	114.06
14	B	4004	BCR	C38-C26-C25	-3.07	121.14	124.48
14	e	524	BCR	C11-C12-C13	-3.07	117.95	126.36
14	M	4021	BCR	C15-C14-C13	-3.06	122.98	127.28
14	3	521	BCR	C3-C4-C5	-3.06	108.59	114.06
13	B	1211	CLA	O2D-CGD-O1D	-3.06	117.88	123.85
13	A	1108	CLA	O2D-CGD-O1D	-3.06	117.89	123.85
17	A	5002	LHG	C5-O7-C7	-3.06	110.48	117.80
14	f	523	BCR	C16-C17-C18	-3.06	122.99	127.28
13	A	1106	CLA	O2D-CGD-O1D	-3.06	117.90	123.85
14	b	523	BCR	C38-C26-C25	-3.06	121.15	124.48
14	c	524	BCR	C24-C23-C22	-3.05	121.72	126.23
13	B	1205	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
13	3	501	CLA	O2D-CGD-O1D	-3.05	117.91	123.85
14	b	524	BCR	C8-C7-C6	-3.05	118.85	127.00
14	A	4002	BCR	C23-C24-C25	-3.05	118.86	127.00
14	J	4013	BCR	C11-C10-C9	-3.04	123.01	127.28
13	b	508	CLA	O2D-CGD-O1D	-3.04	117.92	123.85
14	B	4017	BCR	C7-C8-C9	-3.04	121.73	126.23
13	3	506	CLA	O2D-CGD-O1D	-3.04	117.93	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	A	4007	BCR	C28-C27-C26	-3.04	108.63	114.06
14	3	522	BCR	C8-C7-C6	-3.04	118.88	127.00
13	5	502	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
13	e	508	CLA	O2D-CGD-O1D	-3.04	117.94	123.85
14	B	4009	BCR	C3-C4-C5	-3.04	108.64	114.06
14	3	524	BCR	C20-C21-C22	-3.04	123.02	127.28
13	B	1227	CLA	O2D-CGD-O1D	-3.03	117.94	123.85
14	g	521	BCR	C38-C26-C25	-3.03	121.18	124.48
13	A	1117	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
13	a	506	CLA	O2D-CGD-O1D	-3.03	117.96	123.85
13	d	504	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
13	B	1213	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
14	1	523	BCR	C28-C27-C26	-3.02	108.66	114.06
13	K	1401	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	f	521	BCR	C15-C14-C13	-3.02	123.04	127.28
13	2	516	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
13	c	511	CLA	O2D-CGD-O1D	-3.02	117.97	123.85
14	e	521	BCR	C3-C4-C5	-3.02	108.68	114.06
13	5	519	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
13	A	1801	CLA	O2D-CGD-O1D	-3.01	117.98	123.85
14	5	521	BCR	C38-C26-C25	-3.01	121.20	124.48
14	B	4009	BCR	C33-C5-C4	3.01	120.01	113.60
13	d	519	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	3	517	CLA	O2D-CGD-O1D	-3.01	117.99	123.85
13	c	501	CLA	O2D-CGD-O1D	-3.01	118.00	123.85
13	2	507	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	A	1138	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	f	503	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
13	A	1237	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
13	f	512	CLA	O2D-CGD-O1D	-3.00	118.01	123.85
14	a	523	BCR	C23-C24-C25	-3.00	118.98	127.00
14	A	4011	BCR	C20-C19-C18	-3.00	118.14	126.36
14	a	521	BCR	C28-C27-C26	-3.00	108.71	114.06
13	4	506	CLA	O2D-CGD-O1D	-3.00	118.02	123.85
14	d	524	BCR	C24-C23-C22	-3.00	121.80	126.23
14	c	522	BCR	C23-C24-C25	-3.00	119.00	127.00
14	2	524	BCR	C20-C21-C22	-2.99	123.08	127.28
14	a	524	BCR	C28-C27-C26	-2.99	108.72	114.06
13	A	1103	CLA	C1-C2-C3	-2.99	121.29	126.20
13	f	501	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
13	e	506	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	A	1118	CLA	O2D-CGD-O1D	-2.99	118.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	c	502	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
14	1	524	BCR	C38-C26-C25	-2.99	121.22	124.48
14	A	4011	BCR	C15-C14-C13	-2.99	123.09	127.28
13	a	511	CLA	O2D-CGD-O1D	-2.99	118.03	123.85
13	4	519	CLA	O2D-CGD-O1D	-2.99	118.04	123.85
14	c	523	BCR	C7-C8-C9	-2.99	121.82	126.23
13	B	1209	CLA	O2D-CGD-CBD	2.98	116.45	111.23
13	4	511	CLA	C3B-C4B-NB	-2.98	107.87	110.53
13	5	501	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
14	4	522	BCR	C24-C23-C22	-2.98	121.83	126.23
15	B	1852	SQD	O48-C23-C24	2.98	120.92	111.83
13	g	512	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	4	516	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	B	1206	CLA	O2D-CGD-O1D	-2.98	118.05	123.85
13	B	1220	CLA	O2D-CGD-O1D	-2.98	118.06	123.85
14	I	4018	BCR	C27-C26-C25	-2.97	118.69	122.70
13	A	1110	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	c	512	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	B	1212	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	g	508	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
13	2	505	CLA	O2D-CGD-O1D	-2.97	118.06	123.85
14	B	4004	BCR	C11-C10-C9	-2.97	123.11	127.28
13	B	1205	CLA	O2A-CGA-O1A	-2.97	116.20	123.63
13	b	513	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
14	f	524	BCR	C29-C30-C25	2.97	114.75	110.44
13	f	511	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	6	508	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	B	1021	CLA	C1-C2-C3	-2.97	121.33	126.20
13	1	506	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
13	3	502	CLA	O2D-CGD-O1D	-2.97	118.08	123.85
14	B	4005	BCR	C3-C4-C5	-2.97	108.77	114.06
14	2	523	BCR	C11-C10-C9	-2.96	123.12	127.28
13	g	503	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	1	504	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
13	A	1119	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
14	b	524	BCR	C33-C5-C4	2.96	119.91	113.60
13	3	507	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	B	1229	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	d	501	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	A	1115	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
13	c	507	CLA	O2D-CGD-O1D	-2.96	118.09	123.85
14	5	523	BCR	C29-C30-C25	-2.96	106.14	110.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1229	CLA	C3B-C4B-NB	-2.96	107.89	110.53
14	f	524	BCR	C16-C15-C14	-2.95	117.47	123.52
13	6	506	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	A	1129	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	e	502	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
13	c	508	CLA	O2D-CGD-O1D	-2.95	118.10	123.85
14	I	4019	BCR	C33-C5-C6	-2.95	121.26	124.48
13	B	1215	CLA	C1-C2-C3	-2.95	121.36	126.20
14	g	522	BCR	C23-C24-C25	-2.95	119.12	127.00
13	d	511	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	b	504	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	4	508	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	1	501	CLA	O2D-CGD-O1D	-2.95	118.11	123.85
13	d	508	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	f	508	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	A	1107	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
15	e	822	SQD	O48-C23-C24	2.94	120.80	111.83
13	c	513	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
13	b	509	CLA	O2D-CGD-O1D	-2.94	118.12	123.85
14	g	524	BCR	C8-C7-C6	-2.94	119.14	127.00
13	a	512	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	I	4020	BCR	C4-C5-C6	-2.94	118.73	122.70
14	d	523	BCR	C16-C17-C18	-2.94	123.16	127.28
14	4	521	BCR	C38-C26-C25	-2.94	121.28	124.48
13	4	503	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
14	B	4010	BCR	C11-C12-C13	-2.94	118.31	126.36
14	f	523	BCR	C7-C8-C9	-2.94	121.89	126.23
13	5	504	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	1	513	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	f	502	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	c	519	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	A	1112	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	d	513	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
14	b	524	BCR	C16-C15-C14	-2.93	117.52	123.52
14	f	521	BCR	C38-C26-C25	-2.93	121.29	124.48
13	2	504	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
13	c	504	CLA	O2D-CGD-O1D	-2.93	118.15	123.85
13	A	1116	CLA	C1-C2-C3	-2.93	121.40	126.20
14	F	4014	BCR	C28-C27-C26	-2.93	108.84	114.06
13	2	513	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	f	506	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
17	A	5005	LHG	O8-C23-C24	2.92	120.75	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1215	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	4	509	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
13	2	519	CLA	O2D-CGD-O1D	-2.92	118.16	123.85
18	B	2002	PQN	C11-C3-C4	-2.92	115.50	118.58
14	I	4020	BCR	C1-C6-C7	2.92	123.57	115.65
14	1	522	BCR	C28-C27-C26	-2.92	108.85	114.06
13	5	508	CLA	O2D-CGD-O1D	-2.92	118.17	123.85
14	5	522	BCR	C11-C12-C13	-2.92	118.36	126.36
14	6	523	BCR	C38-C26-C25	-2.92	121.30	124.48
14	A	4011	BCR	C33-C5-C6	-2.92	121.30	124.48
13	f	518	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	3	508	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	a	522	BCR	C28-C27-C26	-2.91	108.86	114.06
14	5	523	BCR	C11-C10-C9	-2.91	123.20	127.28
13	2	502	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
13	A	1127	CLA	O2D-CGD-O1D	-2.91	118.18	123.85
14	b	524	BCR	C24-C23-C22	-2.91	121.93	126.23
14	e	523	BCR	C38-C26-C25	-2.91	121.31	124.48
13	5	506	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	1	507	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
13	6	504	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
14	2	523	BCR	C38-C26-C25	-2.90	121.31	124.48
13	b	501	CLA	O2D-CGD-O1D	-2.90	118.19	123.85
13	5	512	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	5	524	BCR	C24-C23-C22	-2.90	121.94	126.23
13	g	517	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	5	509	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	1	503	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
13	J	1302	CLA	O2D-CGD-O1D	-2.90	118.20	123.85
14	c	522	BCR	C24-C23-C22	-2.90	121.95	126.23
13	g	505	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	3	503	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	2	508	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
13	e	503	CLA	O2D-CGD-O1D	-2.90	118.21	123.85
14	2	521	BCR	C38-C26-C25	-2.90	121.33	124.48
13	6	512	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
15	d	822	SQD	O7-S-C6	2.89	111.08	106.76
13	1	508	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	2	517	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
14	g	522	BCR	C28-C27-C26	-2.89	108.90	114.06
13	d	506	CLA	O2D-CGD-O1D	-2.89	118.22	123.85
13	A	1138	CLA	C1-C2-C3	-2.89	121.46	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	512	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	6	517	CLA	O2D-CGD-O1D	-2.89	118.23	123.85
13	f	504	CLA	O2D-CGD-O1D	-2.88	118.23	123.85
14	6	524	BCR	C21-C20-C19	-2.88	114.84	123.20
13	a	519	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	F	1301	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
13	1	511	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
13	a	513	CLA	O2D-CGD-O1D	-2.87	118.25	123.85
14	J	4012	BCR	C38-C26-C25	-2.87	121.35	124.48
13	3	505	CLA	CHB-C4A-NA	2.87	128.55	124.40
13	1	505	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
13	B	1210	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
14	b	523	BCR	C28-C27-C26	-2.87	108.94	114.06
13	b	506	CLA	CMB-C2B-C3B	2.87	133.29	126.55
13	B	1216	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	5	503	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
13	A	1111	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	e	523	BCR	C8-C7-C6	-2.87	119.34	127.00
13	5	505	CLA	O2D-CGD-O1D	-2.87	118.27	123.85
14	c	523	BCR	C24-C23-C22	-2.86	122.00	126.23
13	3	505	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
13	g	519	CLA	O2D-CGD-O1D	-2.86	118.27	123.85
14	b	521	BCR	C38-C26-C25	-2.86	121.36	124.48
13	B	1012	CLA	O2D-CGD-CBD	2.86	116.24	111.23
15	c	822	SQD	O48-C23-C24	2.86	120.56	111.83
13	B	1221	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
14	F	4016	BCR	C38-C26-C25	-2.86	121.36	124.48
13	d	503	CLA	O2D-CGD-O1D	-2.86	118.28	123.85
13	6	519	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	e	504	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	5	511	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
14	2	523	BCR	C15-C16-C17	-2.86	117.67	123.52
13	2	506	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	3	510	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	4	501	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	6	511	CLA	O2D-CGD-O1D	-2.86	118.29	123.85
13	J	1303	CLA	C3B-C4B-NB	-2.86	107.98	110.53
13	3	518	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
13	d	517	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
13	4	512	CLA	O2D-CGD-O1D	-2.85	118.29	123.85
13	B	1225	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	e	518	CLA	O2D-CGD-O1D	-2.85	118.30	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	A	5001	LHG	C5-O7-C7	-2.85	110.97	117.80
13	g	506	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	b	511	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
14	6	523	BCR	C28-C27-C26	-2.85	108.97	114.06
13	2	501	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	e	507	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	e	510	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	1	519	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	e	519	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
13	5	518	CLA	C1-C2-C3	-2.85	121.53	126.20
13	6	503	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
13	f	507	CLA	O2D-CGD-O1D	-2.85	118.31	123.85
13	3	509	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
13	5	507	CLA	O2D-CGD-O1D	-2.84	118.31	123.85
13	c	505	CLA	C1-C2-C3	-2.84	121.54	126.20
13	a	517	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
13	a	507	CLA	O2D-CGD-O1D	-2.84	118.32	123.85
14	f	523	BCR	C15-C16-C17	-2.84	117.71	123.52
14	5	524	BCR	C11-C10-C9	-2.84	123.30	127.28
13	4	519	CLA	C1-C2-C3	-2.84	122.17	126.76
14	B	4017	BCR	C28-C27-C26	-2.84	109.00	114.06
13	1	518	CLA	O2D-CGD-O1D	-2.84	118.33	123.85
14	A	4008	BCR	C7-C8-C9	-2.84	122.04	126.23
14	I	4020	BCR	C15-C16-C17	-2.84	117.72	123.52
14	1	522	BCR	C11-C12-C13	-2.83	118.59	126.36
13	3	513	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
14	J	4012	BCR	C4-C5-C6	-2.83	118.87	122.70
13	6	513	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	B	1238	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	g	511	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
14	A	4002	BCR	C16-C15-C14	-2.83	117.72	123.52
13	1	517	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
14	e	524	BCR	C8-C7-C6	-2.83	119.43	127.00
14	1	522	BCR	C20-C21-C22	-2.83	123.31	127.28
14	g	523	BCR	C27-C26-C25	-2.83	118.88	122.70
13	b	513	CLA	C1-C2-C3	-2.83	122.18	126.76
13	A	1116	CLA	O2D-CGD-O1D	-2.83	118.33	123.85
13	4	502	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	f	505	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	6	518	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
13	3	504	CLA	O2D-CGD-O1D	-2.83	118.35	123.85
13	b	510	CLA	CMB-C2B-C1B	-2.83	121.12	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	d	521	BCR	C3-C4-C5	-2.83	109.02	114.06
14	B	4017	BCR	C39-C30-C25	-2.83	105.81	110.24
13	3	511	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
13	b	517	CLA	O2D-CGD-O1D	-2.82	118.35	123.85
14	g	524	BCR	C24-C23-C22	-2.82	122.06	126.23
14	d	524	BCR	C23-C24-C25	-2.82	119.46	127.00
13	g	513	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	B	1232	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	A	1120	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	B	1217	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	g	502	CLA	O2D-CGD-O1D	-2.82	118.36	123.85
13	5	513	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
13	b	518	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
13	b	519	CLA	O2D-CGD-O1D	-2.82	118.37	123.85
14	c	522	BCR	C33-C5-C4	2.82	119.60	113.60
14	b	523	BCR	C16-C17-C18	-2.82	123.33	127.28
14	a	522	BCR	C11-C12-C13	-2.82	118.64	126.36
14	3	522	BCR	C28-C27-C26	-2.81	109.04	114.06
13	f	517	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
13	4	510	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	F	4016	BCR	C23-C24-C25	-2.81	119.49	127.00
14	1	524	BCR	C33-C5-C4	2.81	119.59	113.60
13	e	505	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	b	502	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	1	524	BCR	C11-C12-C13	-2.81	118.66	126.36
13	B	1216	CLA	C3B-C4B-NB	-2.81	108.02	110.53
13	3	512	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	J	1303	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
13	g	501	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
14	f	524	BCR	C27-C26-C25	-2.81	118.91	122.70
14	6	522	BCR	C15-C16-C17	-2.80	117.78	123.52
16	2	5104	LMG	O8-C28-C29	2.80	120.39	111.83
13	A	1121	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
14	B	4017	BCR	C16-C15-C14	-2.80	117.78	123.52
14	f	522	BCR	C24-C23-C22	-2.80	122.09	126.23
13	B	1023	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
13	6	516	CLA	O2D-CGD-O1D	-2.80	118.40	123.85
14	F	4014	BCR	C11-C10-C9	-2.80	123.35	127.28
14	B	4005	BCR	C33-C5-C4	2.80	119.56	113.60
14	f	522	BCR	C38-C26-C27	2.79	119.56	113.60
14	b	522	BCR	C20-C21-C22	-2.79	123.36	127.28
13	5	516	CLA	O2D-CGD-O1D	-2.79	118.41	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	b	522	BCR	C11-C12-C13	-2.79	118.70	126.36
13	B	1021	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	2	518	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	e	517	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	2	510	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
13	1	502	CLA	O2D-CGD-O1D	-2.79	118.41	123.85
14	f	524	BCR	C3-C4-C5	-2.79	109.08	114.06
14	a	524	BCR	C3-C4-C5	-2.79	109.08	114.06
14	a	522	BCR	C38-C26-C27	2.79	119.55	113.60
14	a	523	BCR	C10-C11-C12	-2.79	115.12	123.20
14	4	524	BCR	C28-C27-C26	-2.79	109.08	114.06
14	c	522	BCR	C38-C26-C25	-2.79	121.44	124.48
14	1	522	BCR	C8-C7-C6	-2.79	119.55	127.00
13	3	509	CLA	CHB-C4A-NA	2.79	128.42	124.40
13	f	519	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
14	A	4008	BCR	C11-C10-C9	-2.79	123.37	127.28
13	A	1126	CLA	CMB-C2B-C3B	2.78	133.10	126.55
13	a	510	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
14	c	523	BCR	C3-C4-C5	-2.78	109.09	114.06
13	6	501	CLA	C1-C2-C3	-2.78	121.64	126.20
13	6	501	CLA	O2D-CGD-O1D	-2.78	118.43	123.85
14	F	4014	BCR	C10-C11-C12	-2.78	115.14	123.20
13	3	516	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
13	3	518	CLA	C1-C2-C3	-2.78	121.64	126.20
13	a	516	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
15	f	822	SQD	O48-C23-C24	2.78	120.30	111.83
14	1	523	BCR	C23-C24-C25	-2.78	119.58	127.00
14	A	4003	BCR	C28-C27-C26	-2.77	109.11	114.06
14	d	524	BCR	C8-C7-C6	-2.77	119.59	127.00
13	6	510	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
14	1	522	BCR	C7-C8-C9	-2.77	122.14	126.23
13	5	510	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
17	A	5001	LHG	O8-C23-C24	2.77	120.27	111.83
14	3	521	BCR	C28-C27-C26	-2.77	109.12	114.06
13	c	518	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
13	B	1233	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
13	5	518	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
14	3	522	BCR	C3-C4-C5	-2.76	109.13	114.06
13	6	502	CLA	O2D-CGD-O1D	-2.76	118.47	123.85
15	5	822	SQD	O48-C23-C24	2.76	120.25	111.83
14	e	522	BCR	C15-C16-C17	-2.76	117.87	123.52
13	1	509	CLA	O2D-CGD-O1D	-2.76	118.48	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	b	516	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
14	e	524	BCR	C3-C4-C5	-2.76	109.14	114.06
13	A	1117	CLA	C1-C2-C3	-2.76	121.68	126.20
14	d	523	BCR	C3-C4-C5	-2.75	109.14	114.06
13	4	504	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	I	4018	BCR	C28-C27-C26	-2.75	109.14	114.06
14	a	523	BCR	C3-C4-C5	-2.75	109.15	114.06
13	2	511	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
13	A	1113	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
14	J	4012	BCR	C20-C21-C22	-2.75	123.42	127.28
13	2	503	CLA	O2D-CGD-O1D	-2.75	118.49	123.85
13	5	517	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
14	K	4001	BCR	C16-C15-C14	-2.75	117.89	123.52
14	d	522	BCR	C11-C12-C13	-2.75	118.83	126.36
13	b	505	CLA	O2D-CGD-O1D	-2.75	118.50	123.85
13	c	517	CLA	O2D-CGD-O1D	-2.74	118.50	123.85
14	e	522	BCR	C11-C12-C13	-2.74	118.84	126.36
13	f	516	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	B	1207	CLA	C3B-C4B-NB	-2.74	108.08	110.53
14	c	524	BCR	C3-C4-C5	-2.74	109.17	114.06
13	6	507	CLA	O2D-CGD-O1D	-2.74	118.51	123.85
13	1	512	CLA	CHB-C4A-NA	2.74	128.35	124.40
13	6	509	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	A	1137	CLA	CHB-C4A-NA	2.74	128.35	124.40
14	e	524	BCR	C23-C24-C25	-2.74	119.69	127.00
14	4	523	BCR	C8-C7-C6	-2.74	119.69	127.00
13	d	505	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	4	517	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	e	501	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
13	g	510	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
15	3	822	SQD	O48-C23-C24	2.74	120.17	111.83
13	A	1131	CLA	C1-C2-C3	-2.73	121.72	126.20
14	f	522	BCR	C33-C5-C4	2.73	119.42	113.60
16	B	5002	LMG	O8-C28-C29	2.73	120.17	111.83
14	5	522	BCR	C38-C26-C27	2.73	119.42	113.60
13	d	512	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
13	a	513	CLA	C3B-C4B-NB	-2.73	108.09	110.53
16	6	5104	LMG	O8-C28-C29	2.73	120.15	111.83
13	B	1219	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	c	509	CLA	O2D-CGD-O1D	-2.73	118.54	123.85
13	2	512	CLA	C3B-C4B-NB	-2.73	108.10	110.53
14	A	4002	BCR	C38-C26-C27	2.72	119.41	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	518	CLA	O2D-CGD-O1D	-2.72	118.54	123.85
14	f	522	BCR	C11-C12-C13	-2.72	118.89	126.36
14	d	522	BCR	C33-C5-C4	2.72	119.40	113.60
14	a	521	BCR	C38-C26-C25	-2.72	121.51	124.48
14	e	522	BCR	C24-C23-C22	-2.72	122.21	126.23
15	6	822	SQD	O48-C23-C24	2.72	120.14	111.83
13	4	518	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	2	509	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	A	1139	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	6	505	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	a	505	CLA	O2D-CGD-O1D	-2.72	118.55	123.85
13	A	1126	CLA	CMB-C2B-C1B	-2.72	121.28	125.42
14	I	4020	BCR	C3-C4-C5	-2.72	109.21	114.06
13	a	502	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
13	d	502	CLA	O2D-CGD-O1D	-2.71	118.57	123.85
14	B	4004	BCR	C7-C8-C9	-2.71	122.23	126.23
14	c	523	BCR	C8-C7-C6	-2.71	119.76	127.00
14	J	4012	BCR	C33-C5-C4	2.71	119.37	113.60
13	b	510	CLA	CMB-C2B-C3B	2.70	132.91	126.55
13	d	510	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
14	a	524	BCR	C33-C5-C4	2.70	119.36	113.60
14	2	524	BCR	C23-C24-C25	-2.70	119.78	127.00
14	e	522	BCR	C28-C27-C26	-2.70	109.24	114.06
13	f	513	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
13	B	1214	CLA	C3B-C4B-NB	-2.70	108.12	110.53
14	2	522	BCR	C33-C5-C4	2.70	119.35	113.60
13	e	513	CLA	O2D-CGD-O1D	-2.70	118.60	123.85
13	c	513	CLA	C1-C2-C3	-2.70	122.40	126.76
14	A	4002	BCR	C24-C23-C22	-2.70	122.25	126.23
14	J	4013	BCR	C37-C22-C23	2.69	122.20	118.09
14	J	4012	BCR	C21-C20-C19	-2.69	115.39	123.20
14	1	522	BCR	C38-C26-C27	2.69	119.34	113.60
13	3	501	CLA	C1-C2-C3	-2.69	121.79	126.20
13	B	1207	CLA	CHB-C4A-NA	2.69	128.28	124.40
14	c	523	BCR	C11-C10-C9	-2.69	123.51	127.28
13	A	1116	CLA	C3B-C4B-NB	-2.69	108.13	110.53
16	g	5104	LMG	O8-C28-C29	2.68	120.02	111.83
13	b	503	CLA	O2D-CGD-O1D	-2.68	118.62	123.85
15	d	822	SQD	O48-C23-C24	2.68	120.02	111.83
13	A	1106	CLA	C1-C2-C3	-2.68	121.80	126.20
13	b	506	CLA	O2D-CGD-CBD	2.68	115.92	111.23
13	A	1129	CLA	C3B-C4B-NB	-2.68	108.14	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	521	BCR	C33-C5-C6	-2.68	121.56	124.48
13	3	519	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
13	g	516	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
13	A	1122	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
13	e	509	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
14	6	521	BCR	C3-C4-C5	-2.67	109.29	114.06
13	A	1104	CLA	O2D-CGD-O1D	-2.67	118.64	123.85
14	g	522	BCR	C38-C26-C27	2.67	119.30	113.60
14	6	522	BCR	C33-C5-C4	2.67	119.29	113.60
13	6	508	CLA	CHB-C4A-NA	2.67	128.25	124.40
14	4	523	BCR	C28-C27-C26	-2.67	109.30	114.06
14	F	4014	BCR	C20-C19-C18	-2.67	119.05	126.36
13	a	501	CLA	CHB-C4A-NA	2.66	128.25	124.40
16	6	5104	LMG	C8-O7-C10	-2.66	111.42	117.80
14	3	522	BCR	C38-C26-C27	2.66	119.28	113.60
13	A	1125	CLA	C1-C2-C3	-2.66	121.83	126.20
13	d	507	CLA	O2D-CGD-O1D	-2.66	118.67	123.85
14	B	4006	BCR	C11-C12-C13	-2.66	119.06	126.36
15	b	822	SQD	O48-C23-C24	2.66	119.95	111.83
13	J	1303	CLA	C4A-NA-C1A	2.66	109.10	106.28
13	c	509	CLA	CHB-C4A-NA	2.66	128.24	124.40
14	B	4009	BCR	C30-C25-C26	-2.66	119.00	122.64
14	F	4014	BCR	C8-C7-C6	-2.66	119.89	127.00
14	4	523	BCR	C38-C26-C25	-2.66	121.58	124.48
13	d	509	CLA	CHB-C4A-NA	2.66	128.24	124.40
13	4	505	CLA	O2D-CGD-O1D	-2.66	118.68	123.85
14	b	522	BCR	C15-C16-C17	-2.66	118.09	123.52
13	4	507	CLA	O2D-CGD-O1D	-2.65	118.68	123.85
13	A	1132	CLA	CHB-C4A-NA	2.65	128.23	124.40
14	f	524	BCR	C33-C5-C4	2.65	119.25	113.60
14	g	524	BCR	C3-C4-C5	-2.65	109.33	114.06
14	I	4018	BCR	C15-C16-C17	-2.65	118.10	123.52
13	B	1207	CLA	O2D-CGD-O1D	-2.65	118.69	123.85
14	2	522	BCR	C24-C23-C22	-2.65	122.32	126.23
13	B	1219	CLA	C4A-NA-C1A	2.65	107.89	106.68
13	f	507	CLA	C1-C2-C3	-2.65	121.86	126.20
13	f	513	CLA	C1-C2-C3	-2.65	122.48	126.76
13	e	512	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
13	c	505	CLA	O2D-CGD-O1D	-2.64	118.70	123.85
14	5	524	BCR	C37-C22-C23	2.64	122.12	118.09
13	e	518	CLA	C1-C2-C3	-2.64	121.87	126.20
14	c	523	BCR	C38-C26-C25	-2.64	121.60	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	1113	CLA	CHB-C4A-NA	2.64	128.21	124.40
14	1	521	BCR	C15-C16-C17	-2.64	118.12	123.52
14	A	4011	BCR	C39-C30-C25	-2.64	106.11	110.24
13	c	516	CLA	CHB-C4A-NA	2.64	128.21	124.40
13	4	518	CLA	C1-C2-C3	-2.64	121.88	126.20
14	A	4007	BCR	C38-C26-C27	2.64	119.22	113.60
13	B	1229	CLA	C1-C2-C3	-2.63	121.88	126.20
13	1	509	CLA	C1-C2-C3	-2.63	121.89	126.20
14	B	4004	BCR	C28-C27-C26	-2.63	109.37	114.06
13	g	507	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
13	e	505	CLA	C1-C2-C3	-2.63	121.89	126.20
15	2	822	SQD	C45-O47-C7	-2.63	111.51	117.80
13	1	510	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
13	c	510	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
13	3	513	CLA	C1-C2-C3	-2.62	122.52	126.76
14	d	524	BCR	C33-C5-C4	2.62	119.19	113.60
15	d	822	SQD	O9-S-C6	2.62	110.67	106.76
13	A	1104	CLA	C1-C2-C3	-2.62	121.91	126.20
14	3	524	BCR	C24-C23-C22	-2.62	122.36	126.23
13	A	1139	CLA	C3B-C4B-NB	-2.62	108.19	110.53
13	g	509	CLA	CHB-C4A-NA	2.62	128.18	124.40
15	2	822	SQD	O48-C23-C24	2.62	119.81	111.83
13	f	509	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
14	b	523	BCR	C3-C4-C5	-2.62	109.39	114.06
13	A	1101	CLA	CHB-C4A-NA	2.61	128.17	124.40
14	d	522	BCR	C38-C26-C25	-2.61	121.63	124.48
14	6	524	BCR	C33-C5-C4	2.61	119.17	113.60
13	a	509	CLA	O2D-CGD-O1D	-2.61	118.76	123.85
13	b	506	CLA	CMC-C2C-C1C	-2.61	120.95	125.03
14	5	522	BCR	C33-C5-C4	2.61	119.16	113.60
14	2	522	BCR	C11-C12-C13	-2.61	119.21	126.36
13	A	1118	CLA	CHB-C4A-NA	2.61	128.17	124.40
13	B	1203	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	c	503	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
13	2	509	CLA	CHB-C4A-NA	2.61	128.16	124.40
13	2	505	CLA	C1-C2-C3	-2.60	121.93	126.20
14	a	523	BCR	C15-C16-C17	-2.60	118.19	123.52
14	A	4007	BCR	C24-C23-C22	-2.60	122.38	126.23
13	A	1101	CLA	C3B-C4B-NB	-2.60	108.20	110.53
16	2	5104	LMG	C8-O7-C10	-2.60	111.56	117.80
14	f	523	BCR	C3-C4-C5	-2.60	109.41	114.06
14	f	521	BCR	C24-C23-C22	-2.60	122.39	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4005	BCR	C8-C7-C6	-2.60	120.05	127.00
14	5	522	BCR	C24-C23-C22	-2.60	122.39	126.23
14	B	4017	BCR	C8-C7-C6	-2.60	120.05	127.00
13	a	501	CLA	O2D-CGD-CBD	2.60	115.77	111.23
14	A	4003	BCR	C33-C5-C4	2.60	119.13	113.60
13	e	509	CLA	CHB-C4A-NA	2.60	128.15	124.40
14	F	4015	BCR	C33-C5-C6	-2.59	121.65	124.48
14	e	522	BCR	C38-C26-C27	2.59	119.12	113.60
14	1	523	BCR	C38-C26-C27	2.59	119.12	113.60
13	d	505	CLA	C1-C2-C3	-2.59	121.96	126.20
13	1	512	CLA	O2D-CGD-CBD	2.59	115.75	111.23
14	J	4012	BCR	C23-C24-C25	-2.59	120.09	127.00
13	c	518	CLA	CHB-C4A-NA	2.59	128.13	124.40
14	f	523	BCR	C38-C26-C25	-2.58	121.66	124.48
14	b	522	BCR	C33-C5-C4	2.58	119.10	113.60
13	5	509	CLA	CHB-C4A-NA	2.58	128.13	124.40
14	4	523	BCR	C21-C20-C19	-2.58	115.72	123.20
13	4	510	CLA	CMB-C2B-C1B	-2.58	121.49	125.42
14	e	523	BCR	C10-C11-C12	-2.58	115.72	123.20
13	5	506	CLA	C3B-C4B-NB	-2.58	108.23	110.53
15	a	822	SQD	O48-C23-C24	2.58	119.70	111.83
13	1	509	CLA	CHB-C4A-NA	2.58	128.12	124.40
14	b	524	BCR	C23-C24-C25	-2.58	120.11	127.00
14	g	524	BCR	C28-C27-C26	-2.58	109.46	114.06
13	A	1131	CLA	CHB-C4A-NA	2.58	128.12	124.40
13	e	517	CLA	C4A-NA-C1A	2.58	107.85	106.68
13	1	513	CLA	C3B-C4B-NB	-2.57	108.23	110.53
13	e	516	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
13	2	512	CLA	CHB-C4A-NA	2.57	128.11	124.40
13	A	1111	CLA	CHB-C4A-NA	2.57	128.11	124.40
14	A	4008	BCR	C38-C26-C27	2.57	119.08	113.60
13	f	510	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
14	3	522	BCR	C33-C5-C4	2.57	119.07	113.60
16	1	5104	LMG	O8-C28-C29	2.56	119.65	111.83
13	4	511	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
15	g	822	SQD	O48-C23-C24	2.56	119.65	111.83
14	4	524	BCR	C33-C5-C4	2.56	119.06	113.60
13	B	1223	CLA	CHB-C4A-NA	2.56	128.10	124.40
14	B	4006	BCR	C3-C4-C5	-2.56	109.49	114.06
14	M	4021	BCR	C10-C11-C12	-2.56	115.79	123.20
13	c	518	CLA	C1-C2-C3	-2.56	122.01	126.20
14	J	4013	BCR	C20-C21-C22	-2.55	123.70	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	d	522	BCR	C8-C7-C6	-2.55	120.18	127.00
13	A	1140	CLA	C3B-C4B-NB	-2.55	108.25	110.53
14	A	4008	BCR	C10-C11-C12	-2.55	115.81	123.20
14	c	522	BCR	C38-C26-C27	2.55	119.03	113.60
14	B	4004	BCR	C8-C7-C6	-2.55	120.19	127.00
13	a	502	CLA	C1-C2-C3	-2.55	122.03	126.20
14	4	522	BCR	C38-C26-C27	2.55	119.02	113.60
13	c	504	CLA	C1-C2-C3	-2.55	122.64	126.76
14	1	524	BCR	C28-C27-C26	-2.54	109.52	114.06
13	d	518	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
13	6	505	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	F	4016	BCR	C15-C16-C17	-2.54	118.32	123.52
13	f	502	CLA	CHB-C4A-NA	2.54	128.07	124.40
14	c	524	BCR	C23-C24-C25	-2.54	120.21	127.00
14	K	4001	BCR	C11-C12-C13	-2.54	119.39	126.36
15	1	822	SQD	O48-C23-C24	2.54	119.58	111.83
13	b	509	CLA	C1-C2-C3	-2.54	122.03	126.20
14	f	524	BCR	C8-C7-C6	-2.54	120.21	127.00
13	f	518	CLA	C1-C2-C3	-2.54	122.04	126.20
14	b	524	BCR	C4-C5-C6	-2.54	119.27	122.70
13	3	510	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	1	524	BCR	C15-C16-C17	-2.54	118.33	123.52
13	g	518	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
13	A	1135	CLA	CHB-C4A-NA	2.54	128.06	124.40
13	f	509	CLA	CHB-C4A-NA	2.54	128.06	124.40
14	e	523	BCR	C16-C15-C14	-2.54	118.33	123.52
14	a	524	BCR	C8-C7-C6	-2.54	120.22	127.00
13	c	510	CLA	CHB-C4A-NA	2.53	128.06	124.40
13	A	1107	CLA	C1-C2-C3	-2.53	122.05	126.20
13	6	510	CLA	CHB-C4A-NA	2.53	128.06	124.40
14	B	4004	BCR	C20-C19-C18	-2.53	119.42	126.36
14	2	523	BCR	C4-C5-C6	-2.53	119.28	122.70
14	4	522	BCR	C8-C7-C6	-2.53	120.23	127.00
13	4	508	CLA	CHB-C4A-NA	2.53	128.05	124.40
13	e	507	CLA	CHB-C4A-NA	2.53	128.05	124.40
14	a	523	BCR	C21-C20-C19	-2.53	115.87	123.20
14	4	522	BCR	C21-C20-C19	-2.53	115.88	123.20
13	A	1140	CLA	C1-C2-C3	-2.53	122.06	126.20
13	B	1220	CLA	C1-C2-C3	-2.53	122.67	126.76
14	4	524	BCR	C16-C15-C14	-2.53	118.35	123.52
13	A	1121	CLA	CHB-C4A-NA	2.52	128.04	124.40
14	M	4021	BCR	C11-C10-C9	-2.52	123.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	2	512	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
13	6	513	CLA	C1-C2-C3	-2.52	122.68	126.76
13	e	508	CLA	CHB-C4A-NA	2.52	128.04	124.40
13	A	1011	CLA	CBA-CAA-C2A	-2.52	106.30	113.79
13	A	1112	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	g	505	CLA	C3B-C4B-NB	-2.52	108.28	110.53
13	4	510	CLA	CMB-C2B-C3B	2.52	132.47	126.55
13	B	1012	CLA	O2A-CGA-O1A	-2.52	117.33	123.63
13	A	1137	CLA	C3B-C4B-NB	-2.51	108.28	110.53
13	5	510	CLA	CHB-C4A-NA	2.51	128.03	124.40
13	4	505	CLA	CHB-C4A-NA	2.51	128.03	124.40
13	a	518	CLA	CHB-C4A-NA	2.51	128.03	124.40
14	g	522	BCR	C11-C12-C13	-2.51	119.47	126.36
13	5	502	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	A	1013	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	6	524	BCR	C37-C22-C23	2.51	121.92	118.09
13	4	509	CLA	CHB-C4A-NA	2.51	128.02	124.40
14	g	522	BCR	C33-C5-C4	2.51	118.95	113.60
14	3	523	BCR	C15-C16-C17	-2.51	118.39	123.52
14	a	522	BCR	C24-C23-C22	-2.51	122.53	126.23
13	A	1102	CLA	CHB-C4A-NA	2.51	128.02	124.40
13	c	502	CLA	C1-C2-C3	-2.51	122.09	126.20
13	B	1221	CLA	CMB-C2B-C1B	-2.51	121.60	125.42
13	b	510	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	J	4013	BCR	C2-C1-C6	2.50	114.08	110.44
13	g	508	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	2	510	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	A	1103	CLA	CHB-C4A-NA	2.50	128.01	124.40
13	d	512	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	d	524	BCR	C16-C15-C14	-2.50	118.40	123.52
14	J	4012	BCR	C33-C5-C6	-2.50	121.76	124.48
13	4	503	CLA	CHB-C4A-NA	2.50	128.01	124.40
14	I	4018	BCR	C3-C4-C5	-2.50	109.60	114.06
13	B	1235	CLA	C3B-C4B-NB	-2.50	108.30	110.53
14	b	522	BCR	C21-C20-C19	-2.50	115.97	123.20
13	4	511	CLA	CHB-C1B-NB	2.49	127.79	124.05
13	d	516	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
13	B	1202	CLA	CHB-C4A-NA	2.49	128.00	124.40
13	2	505	CLA	C3B-C4B-NB	-2.49	108.31	110.53
13	A	1117	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
13	3	517	CLA	CHB-C4A-NA	2.49	127.99	124.40
13	B	1233	CLA	CHB-C4A-NA	2.49	127.99	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4014	BCR	C7-C8-C9	-2.49	122.55	126.23
14	c	523	BCR	C28-C27-C26	-2.49	109.62	114.06
14	3	522	BCR	C15-C16-C17	-2.49	118.43	123.52
13	A	1022	CLA	CMB-C2B-C1B	-2.49	121.63	125.42
13	f	507	CLA	CHB-C4A-NA	2.49	127.99	124.40
14	M	4021	BCR	C2-C1-C6	2.49	114.05	110.44
13	c	511	CLA	C1-C2-C3	-2.49	122.12	126.20
13	6	518	CLA	C1-C2-C3	-2.48	122.74	126.76
13	1	513	CLA	C1-C2-C3	-2.48	122.74	126.76
14	g	523	BCR	C38-C26-C27	2.48	118.89	113.60
13	d	518	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
14	a	522	BCR	C3-C4-C5	-2.48	109.63	114.06
13	f	513	CLA	O2A-CGA-O1A	-2.48	117.42	123.63
13	B	1201	CLA	CHB-C4A-NA	2.48	127.98	124.40
13	4	505	CLA	C1-C2-C3	-2.48	122.13	126.20
13	B	1221	CLA	CHB-C4A-NA	2.48	127.98	124.40
14	e	523	BCR	C7-C8-C9	-2.48	122.57	126.23
14	2	522	BCR	C8-C7-C6	-2.48	120.38	127.00
13	A	1124	CLA	CHB-C4A-NA	2.48	127.97	124.40
13	B	1222	CLA	CMB-C2B-C1B	-2.48	121.65	125.42
14	A	4008	BCR	C8-C7-C6	-2.47	120.39	127.00
15	B	1852	SQD	O7-S-C6	2.47	110.45	106.76
14	3	524	BCR	C23-C24-C25	-2.47	120.39	127.00
13	b	510	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
14	2	524	BCR	C24-C23-C22	-2.47	122.58	126.23
14	b	522	BCR	C8-C7-C6	-2.47	120.39	127.00
14	B	4009	BCR	C28-C27-C26	-2.47	109.65	114.06
14	2	522	BCR	C21-C20-C19	-2.47	116.05	123.20
13	a	502	CLA	CHB-C4A-NA	2.47	127.96	124.40
13	a	503	CLA	O2D-CGD-O1D	-2.47	119.05	123.85
13	c	510	CLA	C1-C2-C3	-2.47	122.16	126.20
13	B	1234	CLA	CHB-C4A-NA	2.47	127.96	124.40
13	A	1104	CLA	CHB-C4A-NA	2.47	127.96	124.40
13	A	1114	CLA	CHB-C4A-NA	2.46	127.96	124.40
13	3	507	CLA	CHB-C4A-NA	2.46	127.96	124.40
13	A	1123	CLA	CHB-C4A-NA	2.46	127.96	124.40
14	e	524	BCR	C20-C19-C18	-2.46	119.61	126.36
13	B	1023	CLA	C1-C2-C3	-2.46	122.16	126.20
13	2	503	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	A	4011	BCR	C23-C24-C25	-2.46	120.42	127.00
13	e	518	CLA	CHB-C4A-NA	2.46	127.95	124.40
14	3	523	BCR	C21-C20-C19	-2.46	116.07	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1023	CLA	CHB-C4A-NA	2.46	127.95	124.40
13	B	1209	CLA	CHB-C4A-NA	2.46	127.95	124.40
13	5	506	CLA	CHB-C4A-NA	2.46	127.95	124.40
13	c	508	CLA	CHB-C4A-NA	2.46	127.94	124.40
13	d	504	CLA	CHB-C4A-NA	2.46	127.94	124.40
13	e	502	CLA	CHB-C4A-NA	2.46	127.94	124.40
13	a	508	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	A	1109	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	B	1236	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	2	509	CLA	C1-C2-C3	-2.45	122.18	126.20
13	B	1212	CLA	CHB-C4A-NA	2.45	127.94	124.40
13	B	1021	CLA	C3B-C4B-NB	-2.45	108.34	110.53
13	a	503	CLA	CHB-C4A-NA	2.45	127.94	124.40
14	f	523	BCR	C11-C12-C13	-2.45	119.64	126.36
13	f	501	CLA	C1-C2-C3	-2.45	122.18	126.20
17	A	5002	LHG	O8-C23-C24	2.45	119.30	111.83
13	A	1104	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
13	B	1219	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	a	523	BCR	C27-C26-C25	-2.45	119.40	122.70
14	d	523	BCR	C33-C5-C6	-2.45	121.81	124.48
13	6	504	CLA	CHB-C4A-NA	2.45	127.93	124.40
14	2	524	BCR	C21-C20-C19	-2.45	116.11	123.20
13	B	1225	CLA	C3B-C4B-NB	-2.44	108.35	110.53
13	d	505	CLA	C3B-C4B-NB	-2.44	108.35	110.53
14	I	4018	BCR	C11-C12-C13	-2.44	119.67	126.36
13	A	1115	CLA	CHB-C4A-NA	2.44	127.92	124.40
13	c	505	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	A	4008	BCR	C30-C25-C26	-2.44	119.30	122.64
14	b	522	BCR	C38-C26-C27	2.44	118.80	113.60
13	b	508	CLA	CHB-C4A-NA	2.44	127.92	124.40
13	g	511	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	2	523	BCR	C33-C5-C4	2.44	118.79	113.60
13	4	512	CLA	C3B-C4B-NB	-2.44	108.35	110.53
13	e	510	CLA	CHB-C4A-NA	2.44	127.92	124.40
14	g	524	BCR	C38-C26-C25	-2.44	121.83	124.48
13	A	1127	CLA	CMB-C2B-C1B	-2.43	121.71	125.42
17	A	5003	LHG	O8-C23-C24	2.43	119.25	111.83
14	M	4021	BCR	C20-C19-C18	-2.43	119.69	126.36
13	d	516	CLA	CHB-C4A-NA	2.43	127.91	124.40
13	f	508	CLA	CHB-C4A-NA	2.43	127.91	124.40
13	X	1401	CLA	CHB-C4A-NA	2.43	127.91	124.40
13	d	506	CLA	CHB-C4A-NA	2.43	127.91	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	524	BCR	C8-C7-C6	-2.43	120.51	127.00
13	f	505	CLA	O2A-CGA-O1A	-2.43	117.55	123.63
13	A	1119	CLA	C1-C2-C3	-2.43	122.22	126.20
13	A	1126	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
14	3	522	BCR	C11-C12-C13	-2.43	119.70	126.36
13	A	1102	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	3	502	CLA	C1-C2-C3	-2.43	122.22	126.20
13	2	506	CLA	CHB-C4A-NA	2.43	127.90	124.40
13	J	1302	CLA	CHB-C4A-NA	2.43	127.90	124.40
14	g	521	BCR	C29-C30-C25	2.43	113.97	110.44
13	B	1236	CLA	C3B-C4B-NB	-2.43	108.36	110.53
13	B	1222	CLA	O2D-CGD-CBD	2.43	115.47	111.23
13	g	502	CLA	C1-C2-C3	-2.43	122.22	126.20
13	4	510	CLA	C1-C2-C3	-2.42	122.22	126.20
13	B	1211	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	A	4007	BCR	C33-C5-C4	2.42	118.76	113.60
13	f	506	CLA	CHB-C4A-NA	2.42	127.90	124.40
14	2	522	BCR	C16-C17-C18	-2.42	123.88	127.28
14	a	523	BCR	C37-C22-C23	2.42	121.79	118.09
14	1	523	BCR	C8-C7-C6	-2.42	120.53	127.00
13	e	506	CLA	CHB-C4A-NA	2.42	127.89	124.40
15	4	822	SQD	O48-C23-C24	2.42	119.22	111.83
13	4	505	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	A	1011	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	5	505	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	A	1133	CLA	C1-C2-C3	-2.42	122.23	126.20
14	J	4013	BCR	C34-C9-C8	2.42	121.78	118.09
14	g	522	BCR	C15-C16-C17	-2.42	118.57	123.52
13	e	504	CLA	CHB-C4A-NA	2.42	127.89	124.40
13	B	1012	CLA	CMB-C2B-C1B	-2.42	121.74	125.42
13	d	516	CLA	C3B-C4B-NB	-2.42	108.37	110.53
13	B	1206	CLA	C1-C2-C3	-2.42	122.24	126.20
14	4	523	BCR	C33-C5-C4	2.42	118.75	113.60
13	6	506	CLA	CHB-C4A-NA	2.41	127.88	124.40
13	2	506	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	A	1237	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	B	1205	CLA	C1-C2-C3	-2.41	122.24	126.20
13	B	1230	CLA	CHB-C4A-NA	2.41	127.88	124.40
13	c	502	CLA	O2A-CGA-O1A	-2.41	117.59	123.63
13	A	1011	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
14	d	522	BCR	C3-C4-C5	-2.41	109.76	114.06
14	J	4013	BCR	C33-C5-C4	2.41	118.73	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	522	BCR	C15-C16-C17	-2.41	118.59	123.52
13	2	501	CLA	C1-C2-C3	-2.41	122.25	126.20
13	a	510	CLA	CMB-C2B-C1B	-2.41	121.75	125.42
16	J	5104	LMG	O8-C28-C29	2.41	119.18	111.83
13	B	1232	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	f	507	CLA	C3B-C4B-NB	-2.41	108.38	110.53
13	B	1203	CLA	CHB-C4A-NA	2.41	127.87	124.40
13	d	508	CLA	CHB-C4A-NA	2.41	127.87	124.40
17	A	5004	LHG	O8-C23-C24	2.41	119.17	111.83
13	B	1217	CLA	CHB-C4A-NA	2.41	127.87	124.40
13	f	513	CLA	CHB-C4A-NA	2.41	127.87	124.40
13	2	512	CLA	C1-O2A-CGA	2.41	122.47	116.65
13	g	518	CLA	C1-C2-C3	-2.40	122.26	126.20
14	c	523	BCR	C10-C11-C12	-2.40	116.24	123.20
13	B	1226	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	a	509	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	c	524	BCR	C16-C15-C14	-2.40	118.61	123.52
14	B	4009	BCR	C38-C26-C25	-2.40	121.86	124.48
13	5	512	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	2	513	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	A	1138	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	2	523	BCR	C10-C11-C12	-2.40	116.25	123.20
14	4	522	BCR	C33-C5-C4	2.40	118.71	113.60
13	a	504	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	c	502	CLA	CHB-C4A-NA	2.40	127.86	124.40
13	3	503	CLA	CHB-C4A-NA	2.40	127.86	124.40
14	1	522	BCR	C33-C5-C4	2.40	118.70	113.60
13	J	1303	CLA	CHC-C4B-NB	2.39	126.33	120.96
14	f	523	BCR	C28-C27-C26	-2.39	109.79	114.06
14	g	524	BCR	C33-C5-C4	2.39	118.70	113.60
13	6	512	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	2	502	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	6	521	BCR	C20-C19-C18	-2.39	119.80	126.36
13	B	1220	CLA	O2A-CGA-O1A	-2.39	117.64	123.63
13	a	511	CLA	C3B-C4B-NB	-2.39	108.39	110.53
13	f	511	CLA	CMB-C2B-C1B	-2.39	121.78	125.42
13	B	1211	CLA	C1-C2-C3	-2.39	122.28	126.20
13	d	509	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
13	3	506	CLA	CHB-C4A-NA	2.39	127.85	124.40
14	A	4003	BCR	C15-C16-C17	-2.39	118.63	123.52
14	A	4003	BCR	C23-C24-C25	-2.39	120.62	127.00
13	d	501	CLA	CHB-C4A-NA	2.39	127.85	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1208	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	B	1227	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	g	519	CLA	CHB-C4A-NA	2.39	127.85	124.40
13	3	512	CLA	CHB-C4A-NA	2.39	127.84	124.40
13	e	516	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	c	524	BCR	C33-C5-C4	2.39	118.68	113.60
13	1	512	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
14	B	4010	BCR	C7-C8-C9	-2.39	122.71	126.23
13	5	503	CLA	CHB-C4A-NA	2.39	127.84	124.40
13	A	1119	CLA	CHB-C4A-NA	2.39	127.84	124.40
13	B	1213	CLA	CHB-C4A-NA	2.39	127.84	124.40
13	e	511	CLA	CHB-C4A-NA	2.39	127.84	124.40
13	f	505	CLA	CHB-C4A-NA	2.39	127.84	124.40
14	B	4006	BCR	C33-C5-C4	2.38	118.68	113.60
13	6	511	CLA	CHB-C4A-NA	2.38	127.84	124.40
13	B	1214	CLA	CHB-C4A-NA	2.38	127.84	124.40
14	B	4006	BCR	C8-C7-C6	-2.38	120.63	127.00
13	b	504	CLA	CHB-C4A-NA	2.38	127.84	124.40
14	B	4010	BCR	C21-C20-C19	-2.38	116.30	123.20
13	3	511	CLA	CHB-C4A-NA	2.38	127.84	124.40
14	a	524	BCR	C38-C26-C27	2.38	118.67	113.60
13	1	505	CLA	C3B-C4B-NB	-2.38	108.41	110.53
14	g	524	BCR	C23-C24-C25	-2.38	120.64	127.00
14	2	522	BCR	C38-C26-C27	2.38	118.67	113.60
13	B	1234	CLA	CMB-C2B-C1B	-2.38	121.80	125.42
13	g	513	CLA	C1-C2-C3	-2.38	122.92	126.76
14	A	4002	BCR	C36-C18-C17	-2.38	118.97	122.82
13	A	1110	CLA	CHB-C4A-NA	2.38	127.83	124.40
14	b	524	BCR	C36-C18-C19	2.38	121.72	118.09
13	3	513	CLA	CHB-C4A-NA	2.37	127.83	124.40
13	B	1222	CLA	CHB-C4A-NA	2.37	127.83	124.40
13	c	501	CLA	CHB-C4A-NA	2.37	127.83	124.40
14	b	521	BCR	C29-C30-C25	2.37	113.89	110.44
13	a	501	CLA	C3B-C4B-NB	-2.37	108.41	110.53
14	2	523	BCR	C33-C5-C6	-2.37	121.90	124.48
13	4	511	CLA	CHB-C4A-NA	2.37	127.82	124.40
13	B	1012	CLA	C1-C2-C3	-2.37	122.31	126.20
13	b	516	CLA	C3B-C4B-NB	-2.37	108.42	110.53
13	c	506	CLA	CHB-C4A-NA	2.37	127.82	124.40
14	g	521	BCR	C33-C5-C4	2.37	118.65	113.60
13	g	509	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
13	A	1130	CLA	C1-C2-C3	-2.37	122.32	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	c	522	BCR	C27-C26-C25	-2.37	119.51	122.70
14	d	524	BCR	C11-C12-C13	-2.37	119.88	126.36
15	4	822	SQD	O47-C7-C8	2.36	116.60	111.48
13	c	516	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
14	1	522	BCR	C24-C23-C22	-2.36	122.74	126.23
13	5	519	CLA	C1-C2-C3	-2.36	122.94	126.76
13	A	1120	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	A	4007	BCR	C8-C7-C6	-2.36	120.69	127.00
13	5	513	CLA	C3B-C4B-NB	-2.36	108.42	110.53
13	4	510	CLA	C3A-C2A-C1A	2.36	104.87	101.34
14	5	523	BCR	C3-C4-C5	-2.36	109.85	114.06
14	B	4009	BCR	C7-C8-C9	-2.36	122.74	126.23
13	B	1210	CLA	CHB-C4A-NA	2.36	127.81	124.40
13	b	506	CLA	C4B-C3B-C2B	-2.36	104.37	107.30
13	4	506	CLA	C3B-C4B-NB	-2.36	108.42	110.53
13	A	1133	CLA	C3B-C4B-NB	-2.36	108.42	110.53
14	e	524	BCR	C24-C23-C22	-2.36	122.75	126.23
13	A	1130	CLA	CMB-C2B-C1B	-2.36	121.83	125.42
14	F	4016	BCR	C24-C23-C22	-2.36	122.75	126.23
13	3	502	CLA	CHB-C4A-NA	2.36	127.80	124.40
13	6	513	CLA	CHB-C4A-NA	2.36	127.80	124.40
13	A	1122	CLA	CHB-C4A-NA	2.36	127.80	124.40
13	A	1134	CLA	CHB-C4A-NA	2.36	127.80	124.40
13	c	511	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	d	510	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	f	516	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	b	513	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	a	510	CLA	C1-C2-C3	-2.35	122.34	126.20
13	2	502	CLA	C1-C2-C3	-2.35	122.34	126.20
13	4	513	CLA	CHB-C4A-NA	2.35	127.80	124.40
13	d	518	CLA	CHB-C4A-NA	2.35	127.80	124.40
14	c	523	BCR	C23-C24-C25	-2.35	120.72	127.00
13	A	1116	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	A	1126	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	B	1224	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
13	B	1205	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	B	1231	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	g	503	CLA	CHB-C4A-NA	2.35	127.79	124.40
13	6	502	CLA	C1-C2-C3	-2.35	122.35	126.20
13	B	1203	CLA	C3B-C4B-NB	-2.35	108.43	110.53
13	5	508	CLA	CMB-C2B-C1B	-2.35	121.84	125.42
13	1	506	CLA	CHB-C4A-NA	2.35	127.79	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	5	523	BCR	C11-C12-C13	-2.35	119.92	126.36
13	b	502	CLA	CHB-C4A-NA	2.35	127.79	124.40
14	c	521	BCR	C15-C16-C17	-2.34	118.72	123.52
14	d	524	BCR	C20-C19-C18	-2.34	119.94	126.36
13	B	1229	CLA	CHB-C4A-NA	2.34	127.78	124.40
13	b	518	CLA	CHB-C4A-NA	2.34	127.78	124.40
13	1	504	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	F	4014	BCR	C3-C4-C5	-2.34	109.88	114.06
14	A	4007	BCR	C15-C16-C17	-2.34	118.73	123.52
13	1	510	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	g	523	BCR	C3-C4-C5	-2.34	109.88	114.06
13	B	1234	CLA	O2A-CGA-O1A	-2.34	117.77	123.63
13	A	1127	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	e	517	CLA	CHB-C4A-NA	2.34	127.78	124.40
14	g	524	BCR	C11-C12-C13	-2.34	119.94	126.36
13	3	512	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	B	1205	CLA	C3B-C4B-NB	-2.34	108.44	110.53
14	6	524	BCR	C20-C21-C22	-2.34	124.00	127.28
14	I	4018	BCR	C38-C26-C27	2.34	118.58	113.60
13	3	508	CLA	CHB-C4A-NA	2.34	127.78	124.40
13	3	506	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	A	1134	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	1	505	CLA	CHB-C4A-NA	2.34	127.78	124.40
13	b	510	CLA	CBC-CAC-C3C	2.34	118.76	112.42
13	4	517	CLA	CHB-C4A-NA	2.34	127.77	124.40
13	A	1135	CLA	C1-C2-C3	-2.34	122.37	126.20
13	B	1239	CLA	C3B-C4B-NB	-2.34	108.44	110.53
13	1	513	CLA	CHB-C4A-NA	2.34	127.77	124.40
14	3	521	BCR	C33-C5-C4	2.34	118.58	113.60
14	d	522	BCR	C23-C24-C25	-2.34	120.76	127.00
14	6	524	BCR	C15-C16-C17	-2.34	118.74	123.52
13	A	1105	CLA	CMB-C2B-C1B	-2.34	121.86	125.42
14	5	524	BCR	C10-C11-C12	-2.34	116.43	123.20
14	e	524	BCR	C33-C5-C4	2.33	118.57	113.60
13	2	517	CLA	CHB-C4A-NA	2.33	127.77	124.40
13	c	512	CLA	CHB-C4A-NA	2.33	127.77	124.40
13	f	506	CLA	C3B-C4B-NB	-2.33	108.45	110.53
14	A	4011	BCR	C38-C26-C27	2.33	118.57	113.60
14	b	521	BCR	C15-C16-C17	-2.33	118.74	123.52
13	c	504	CLA	CHB-C4A-NA	2.33	127.77	124.40
14	M	4021	BCR	C33-C5-C4	2.33	118.57	113.60
13	B	1228	CLA	CMB-C2B-C1B	-2.33	121.87	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	3	501	CLA	CHB-C4A-NA	2.33	127.77	124.40
13	f	511	CLA	CHB-C4A-NA	2.33	127.77	124.40
13	A	1113	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
13	a	511	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	4	506	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	B	1232	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	B	1234	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	J	1303	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	d	523	BCR	C28-C27-C26	-2.33	109.90	114.06
13	A	1140	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	b	516	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	2	503	CLA	C3B-C4B-NB	-2.33	108.45	110.53
13	4	519	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	A	1801	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	B	4010	BCR	C23-C24-C25	-2.33	120.78	127.00
13	6	509	CLA	CHB-C4A-NA	2.33	127.76	124.40
14	a	523	BCR	C33-C5-C4	2.33	118.56	113.60
13	5	517	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	A	1125	CLA	CHB-C4A-NA	2.33	127.76	124.40
13	A	1122	CLA	C1-C2-C3	-2.33	122.39	126.20
13	X	1401	CLA	C3B-C4B-NB	-2.32	108.45	110.53
13	d	506	CLA	C3B-C4B-NB	-2.32	108.45	110.53
14	d	522	BCR	C21-C20-C19	-2.32	116.47	123.20
13	A	1022	CLA	CMB-C2B-C3B	2.32	132.02	126.55
13	6	502	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	e	516	CLA	C3B-C4B-NB	-2.32	108.46	110.53
14	6	523	BCR	C3-C4-C5	-2.32	109.91	114.06
14	f	522	BCR	C3-C4-C5	-2.32	109.91	114.06
13	c	516	CLA	C3B-C4B-NB	-2.32	108.46	110.53
13	4	512	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	I	4020	BCR	C28-C27-C26	-2.32	109.92	114.06
13	5	503	CLA	O2A-CGA-O1A	-2.32	117.82	123.63
13	B	1219	CLA	C1-C2-C3	-2.32	122.39	126.20
13	e	501	CLA	C1-C2-C3	-2.32	122.39	126.20
13	1	501	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	b	505	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	1	517	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	B	4017	BCR	C10-C11-C12	-2.32	116.48	123.20
13	4	510	CLA	O2D-CGD-CBD	2.32	115.29	111.23
14	c	524	BCR	C8-C7-C6	-2.32	120.80	127.00
13	A	1237	CLA	CHB-C4A-NA	2.32	127.75	124.40
14	a	521	BCR	C11-C12-C13	-2.32	120.00	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	4	502	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	2	516	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	c	517	CLA	CHB-C4A-NA	2.32	127.75	124.40
13	B	1225	CLA	CMB-C2B-C1B	-2.32	121.89	125.42
14	B	4004	BCR	C16-C15-C14	-2.32	118.78	123.52
14	4	523	BCR	C15-C16-C17	-2.32	118.78	123.52
14	b	521	BCR	C33-C5-C4	2.32	118.53	113.60
14	A	4011	BCR	C29-C30-C25	2.32	113.80	110.44
14	A	4007	BCR	C20-C21-C22	-2.31	124.03	127.28
13	A	1128	CLA	CMB-C2B-C1B	-2.31	121.90	125.42
13	A	1126	CLA	C1-O2A-CGA	2.31	122.25	116.65
13	B	1223	CLA	C1-C2-C3	-2.31	122.41	126.20
13	1	508	CLA	CHB-C4A-NA	2.31	127.74	124.40
13	6	507	CLA	C1-C2-C3	-2.31	122.41	126.20
13	2	504	CLA	CHB-C4A-NA	2.31	127.74	124.40
13	d	503	CLA	CHB-C4A-NA	2.31	127.74	124.40
13	A	1108	CLA	CHB-C4A-NA	2.31	127.73	124.40
13	5	518	CLA	CHB-C4A-NA	2.31	127.73	124.40
13	B	1239	CLA	CHB-C4A-NA	2.31	127.73	124.40
13	6	503	CLA	O2A-CGA-O1A	-2.31	117.85	123.63
14	2	524	BCR	C8-C7-C6	-2.31	120.83	127.00
13	a	510	CLA	CHB-C4A-NA	2.31	127.73	124.40
13	A	1137	CLA	C1-C2-C3	-2.31	122.41	126.20
13	B	1224	CLA	O2D-CGD-CBD	2.31	115.27	111.23
13	2	511	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	A	4003	BCR	C38-C26-C27	2.31	118.52	113.60
14	e	522	BCR	C8-C7-C6	-2.31	120.83	127.00
16	J	5104	LMG	C8-O7-C10	-2.31	112.27	117.80
13	g	518	CLA	CHB-C4A-NA	2.31	127.73	124.40
14	F	4015	BCR	C33-C5-C4	2.31	118.51	113.60
13	e	512	CLA	CHB-C4A-NA	2.31	127.73	124.40
13	a	519	CLA	CHB-C4A-NA	2.30	127.73	124.40
13	4	519	CLA	C3B-C4B-NB	-2.30	108.47	110.53
14	4	523	BCR	C23-C24-C25	-2.30	120.85	127.00
13	5	519	CLA	CHB-C4A-NA	2.30	127.72	124.40
13	f	508	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
13	B	1216	CLA	CHB-C4A-NA	2.30	127.72	124.40
13	e	506	CLA	CMB-C2B-C1B	-2.30	121.91	125.42
14	A	4007	BCR	C21-C20-C19	-2.30	116.53	123.20
14	B	4006	BCR	C37-C22-C21	-2.30	119.09	122.82
13	6	519	CLA	CHB-C4A-NA	2.30	127.72	124.40
13	6	516	CLA	CHB-C4A-NA	2.30	127.72	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	518	CLA	CHB-C4A-NA	2.30	127.72	124.40
14	B	4004	BCR	C29-C30-C25	2.30	113.78	110.44
13	d	513	CLA	C1-C2-C3	-2.30	123.04	126.76
13	a	512	CLA	C3B-C4B-NB	-2.30	108.48	110.53
13	e	505	CLA	CHB-C4A-NA	2.30	127.72	124.40
13	3	516	CLA	CHB-C4A-NA	2.30	127.71	124.40
13	B	1207	CLA	O2A-CGA-O1A	-2.30	117.88	123.63
14	5	523	BCR	C33-C5-C4	2.30	118.49	113.60
13	B	1216	CLA	CHB-C1B-NB	2.30	127.49	124.05
13	A	1133	CLA	CHB-C4A-NA	2.30	127.71	124.40
13	K	1401	CLA	CHB-C4A-NA	2.30	127.71	124.40
14	e	523	BCR	C20-C19-C18	-2.30	120.07	126.36
13	4	513	CLA	C1-C2-C3	-2.29	123.05	126.76
13	g	510	CLA	CHB-C4A-NA	2.29	127.71	124.40
14	f	521	BCR	C16-C15-C14	-2.29	118.83	123.52
13	6	510	CLA	C1-C2-C3	-2.29	122.44	126.20
13	f	519	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	F	1301	CLA	CHB-C4A-NA	2.29	127.71	124.40
13	c	519	CLA	CHB-C4A-NA	2.29	127.71	124.40
13	d	508	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	A	1117	CLA	CHB-C1B-NB	2.29	127.49	124.05
14	3	522	BCR	C21-C20-C19	-2.29	116.56	123.20
14	B	4017	BCR	C33-C5-C4	2.29	118.48	113.60
13	4	504	CLA	CHB-C4A-NA	2.29	127.71	124.40
13	3	513	CLA	C3B-C4B-NB	-2.29	108.48	110.53
13	2	519	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	A	1013	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
13	4	501	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	2	501	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	B	1222	CLA	O2A-CGA-O1A	-2.29	117.90	123.63
13	a	506	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	d	521	BCR	C29-C30-C25	2.29	113.76	110.44
13	5	511	CLA	CHB-C4A-NA	2.29	127.70	124.40
13	2	505	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	b	521	BCR	C20-C19-C18	-2.29	120.09	126.36
13	4	507	CLA	CHB-C4A-NA	2.29	127.70	124.40
14	2	521	BCR	C33-C5-C4	2.29	118.47	113.60
14	a	524	BCR	C11-C12-C13	-2.29	120.09	126.36
13	b	510	CLA	C1-C2-C3	-2.29	122.45	126.20
13	6	504	CLA	CMB-C2B-C1B	-2.28	121.94	125.42
13	g	502	CLA	CHB-C4A-NA	2.28	127.70	124.40
14	5	523	BCR	C20-C21-C22	-2.28	124.07	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	a	522	BCR	C33-C5-C4	2.28	118.47	113.60
14	a	524	BCR	C23-C24-C25	-2.28	120.90	127.00
13	A	1138	CLA	C3B-C4B-NB	-2.28	108.49	110.53
13	3	519	CLA	CHB-C4A-NA	2.28	127.70	124.40
14	c	522	BCR	C16-C15-C14	-2.28	118.85	123.52
13	3	512	CLA	C1-C2-C3	-2.28	122.46	126.20
14	3	524	BCR	C4-C5-C6	-2.28	119.62	122.70
13	6	503	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	A	1119	CLA	C3B-C4B-NB	-2.28	108.49	110.53
13	B	1201	CLA	CMB-C2B-C1B	-2.28	121.95	125.42
13	A	1135	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
14	B	4009	BCR	C15-C16-C17	-2.28	118.86	123.52
13	6	517	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	f	517	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	e	501	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	g	506	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	b	519	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	a	516	CLA	CHB-C4A-NA	2.28	127.69	124.40
13	A	1107	CLA	O2A-CGA-O1A	-2.28	117.93	123.63
13	A	1130	CLA	C3B-C4B-NB	-2.28	108.50	110.53
13	5	504	CLA	CHB-C4A-NA	2.27	127.68	124.40
13	A	1105	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	c	523	BCR	C34-C9-C8	2.27	121.56	118.09
13	A	1140	CLA	O2D-CGD-CBD	2.27	115.20	111.23
13	d	517	CLA	C4A-NA-C1A	2.27	107.72	106.68
13	4	509	CLA	C1-C2-C3	-2.27	122.47	126.20
13	4	510	CLA	CHB-C4A-NA	2.27	127.68	124.40
13	b	512	CLA	CHB-C4A-NA	2.27	127.68	124.40
13	6	506	CLA	C3B-C4B-NB	-2.27	108.50	110.53
14	6	523	BCR	C8-C7-C6	-2.27	120.93	127.00
13	6	507	CLA	CHB-C4A-NA	2.27	127.68	124.40
13	A	1140	CLA	O2A-CGA-O1A	-2.27	117.95	123.63
14	d	523	BCR	C11-C12-C13	-2.27	120.14	126.36
13	d	513	CLA	CHB-C4A-NA	2.27	127.68	124.40
14	c	524	BCR	C28-C27-C26	-2.27	110.01	114.06
15	6	822	SQD	O6-C1-C2	2.27	111.72	108.27
13	d	517	CLA	CHB-C4A-NA	2.27	127.67	124.40
13	f	510	CLA	CHB-C4A-NA	2.27	127.67	124.40
13	3	503	CLA	C1-C2-C3	-2.27	122.48	126.20
17	A	5003	LHG	C5-O7-C7	-2.27	112.37	117.80
13	B	1230	CLA	O2D-CGD-CBD	2.27	115.19	111.23
13	5	501	CLA	CHB-C4A-NA	2.27	127.67	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	511	CLA	CHB-C4A-NA	2.27	127.67	124.40
13	B	1220	CLA	CHB-C4A-NA	2.27	127.67	124.40
14	2	521	BCR	C29-C30-C25	2.27	113.73	110.44
14	a	522	BCR	C27-C26-C25	-2.27	119.64	122.70
13	A	1106	CLA	CHB-C4A-NA	2.27	127.67	124.40
13	4	502	CLA	C1-C2-C3	-2.26	122.49	126.20
13	B	1210	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
14	c	523	BCR	C21-C20-C19	-2.26	116.64	123.20
13	B	1236	CLA	O2D-CGD-CBD	2.26	115.19	111.23
13	6	518	CLA	CHB-C4A-NA	2.26	127.67	124.40
13	b	501	CLA	CHB-C4A-NA	2.26	127.67	124.40
14	B	4005	BCR	C4-C5-C6	-2.26	119.65	122.70
13	a	503	CLA	O2A-CGA-O1A	-2.26	117.97	123.63
13	B	1012	CLA	CMB-C2B-C3B	2.26	131.87	126.55
14	6	522	BCR	C23-C24-C25	-2.26	120.96	127.00
13	3	504	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	3	524	BCR	C33-C5-C6	-2.26	122.02	124.48
15	B	1852	SQD	C45-O47-C7	-2.26	112.39	117.80
14	d	521	BCR	C33-C5-C4	2.26	118.42	113.60
13	A	1109	CLA	C3B-C4B-NB	-2.26	108.51	110.53
13	F	1301	CLA	C3B-C4B-NB	-2.26	108.51	110.53
13	B	1231	CLA	O1D-CGD-CBD	2.26	128.98	124.52
13	2	512	CLA	C3A-C2A-C1A	2.26	104.72	101.34
13	A	1013	CLA	O2D-CGD-CBD	2.26	115.18	111.23
13	d	502	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	B	1221	CLA	CMB-C2B-C3B	2.26	131.86	126.55
13	B	1215	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	e	510	CLA	C1-C2-C3	-2.26	122.50	126.20
13	c	513	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	b	503	CLA	CHB-C4A-NA	2.26	127.66	124.40
14	1	523	BCR	C3-C4-C5	-2.26	110.03	114.06
14	6	521	BCR	C11-C12-C13	-2.26	120.17	126.36
13	A	1130	CLA	CHB-C4A-NA	2.26	127.66	124.40
13	c	509	CLA	C1-C2-C3	-2.26	122.50	126.20
17	A	5004	LHG	C5-O7-C7	-2.26	112.40	117.80
13	B	1231	CLA	C3B-C4B-NB	-2.25	108.52	110.53
13	1	502	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	a	522	BCR	C8-C7-C6	-2.25	120.97	127.00
13	A	1112	CLA	CHB-C4A-NA	2.25	127.65	124.40
13	A	1125	CLA	C3B-C4B-NB	-2.25	108.52	110.53
14	F	4014	BCR	C35-C13-C12	2.25	121.53	118.09
13	g	505	CLA	CHB-C4A-NA	2.25	127.65	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	524	BCR	C20-C19-C18	-2.25	120.18	126.36
13	6	509	CLA	C1-C2-C3	-2.25	122.50	126.20
13	2	503	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
13	c	509	CLA	O2A-CGA-O1A	-2.25	117.99	123.63
13	B	1224	CLA	C3B-C4B-NB	-2.25	108.52	110.53
14	2	521	BCR	C38-C26-C27	2.25	118.40	113.60
13	B	1206	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
13	B	1235	CLA	C1-C2-C3	-2.25	122.51	126.20
13	B	1238	CLA	CHB-C4A-NA	2.25	127.65	124.40
14	A	4008	BCR	C15-C16-C17	-2.25	118.91	123.52
14	f	524	BCR	C20-C19-C18	-2.25	120.19	126.36
13	2	518	CLA	CHB-C4A-NA	2.25	127.65	124.40
13	A	1136	CLA	C3B-C4B-NB	-2.25	108.52	110.53
13	B	1023	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
13	g	512	CLA	C3B-C4B-NB	-2.25	108.52	110.53
13	3	503	CLA	O2A-CGA-O1A	-2.25	118.00	123.63
14	A	4008	BCR	C34-C9-C8	2.25	121.52	118.09
13	a	504	CLA	C1-C2-C3	-2.25	122.52	126.20
14	I	4020	BCR	C23-C24-C25	-2.25	121.00	127.00
14	K	4001	BCR	C21-C20-C19	-2.25	116.69	123.20
13	A	1126	CLA	C6-C7-C8	-2.25	108.50	115.97
14	1	521	BCR	C38-C26-C27	2.25	118.38	113.60
13	3	503	CLA	CAA-CBA-CGA	-2.25	106.83	113.21
14	F	4014	BCR	C34-C9-C8	2.25	121.52	118.09
14	g	523	BCR	C33-C5-C4	2.24	118.38	113.60
13	d	503	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
14	A	4003	BCR	C20-C19-C18	-2.24	120.22	126.36
13	2	508	CLA	CHB-C4A-NA	2.24	127.63	124.40
13	g	513	CLA	CHB-C4A-NA	2.24	127.63	124.40
13	B	1201	CLA	O2A-CGA-O1A	-2.24	118.02	123.63
13	A	1106	CLA	O2D-CGD-CBD	2.24	115.15	111.23
13	d	519	CLA	CHB-C4A-NA	2.24	127.63	124.40
14	6	524	BCR	C28-C27-C26	-2.24	110.06	114.06
14	K	4001	BCR	C3-C4-C5	-2.24	110.06	114.06
13	4	519	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
14	4	521	BCR	C16-C15-C14	-2.24	118.94	123.52
13	3	505	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
13	A	1125	CLA	CAA-CBA-CGA	-2.24	106.86	113.21
13	B	1235	CLA	O2A-CGA-O1A	-2.24	118.03	123.63
14	B	4017	BCR	C38-C26-C25	-2.24	122.04	124.48
13	e	506	CLA	C3B-C4B-NB	-2.24	108.53	110.53
13	A	1129	CLA	CHB-C4A-NA	2.24	127.63	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	524	BCR	C33-C5-C4	2.24	118.36	113.60
13	B	1202	CLA	C3B-C4B-NB	-2.23	108.53	110.53
13	b	506	CLA	CMC-C2C-C3C	2.23	132.19	126.15
13	b	506	CLA	CHA-C1A-NA	-2.23	121.33	126.39
13	3	518	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	5	513	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	A	1137	CLA	O2D-CGD-CBD	2.23	115.13	111.23
13	A	1133	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
14	d	522	BCR	C29-C30-C25	2.23	113.68	110.44
13	4	518	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	B	1236	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
14	b	521	BCR	C39-C30-C25	-2.23	106.75	110.24
13	B	1229	CLA	O2A-CGA-O1A	-2.23	118.05	123.63
13	4	511	CLA	CMB-C2B-C1B	-2.23	122.02	125.42
13	e	513	CLA	CHB-C4A-NA	2.23	127.62	124.40
13	3	511	CLA	C3B-C4B-NB	-2.23	108.54	110.53
14	1	522	BCR	C15-C16-C17	-2.23	118.96	123.52
13	d	512	CLA	CHB-C4A-NA	2.23	127.61	124.40
13	e	519	CLA	CHB-C4A-NA	2.23	127.61	124.40
13	B	1235	CLA	CHB-C4A-NA	2.23	127.61	124.40
13	3	505	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
14	a	523	BCR	C20-C21-C22	-2.23	124.16	127.28
13	c	513	CLA	O2A-CGA-O1A	-2.23	118.06	123.63
13	B	1209	CLA	C1-C2-C3	-2.22	122.55	126.20
13	5	516	CLA	C3B-C4B-NB	-2.22	108.54	110.53
13	B	1221	CLA	C3B-C4B-NB	-2.22	108.54	110.53
13	1	519	CLA	CHB-C4A-NA	2.22	127.61	124.40
13	f	518	CLA	CHB-C4A-NA	2.22	127.61	124.40
14	5	521	BCR	C16-C15-C14	-2.22	118.97	123.52
14	B	4006	BCR	C39-C30-C25	-2.22	106.76	110.24
14	2	521	BCR	C23-C24-C25	-2.22	121.07	127.00
13	5	511	CLA	CAA-CBA-CGA	-2.22	106.90	113.21
13	5	510	CLA	CMB-C2B-C1B	-2.22	122.04	125.42
13	5	508	CLA	CHB-C4A-NA	2.22	127.60	124.40
13	4	516	CLA	CHB-C4A-NA	2.22	127.60	124.40
13	1	507	CLA	CHB-C4A-NA	2.22	127.60	124.40
15	b	822	SQD	O9-S-C6	2.22	110.07	106.76
14	e	523	BCR	C23-C24-C25	-2.22	121.07	127.00
14	3	523	BCR	C28-C27-C26	-2.22	110.10	114.06
17	A	5004	LHG	O7-C7-O9	-2.22	118.52	123.70
13	g	501	CLA	CHB-C4A-NA	2.22	127.60	124.40
13	c	517	CLA	C4A-NA-C1A	2.22	107.69	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	1	516	CLA	CHB-C4A-NA	2.22	127.60	124.40
14	3	523	BCR	C33-C5-C6	-2.22	122.06	124.48
13	3	502	CLA	O2A-CGA-O1A	-2.22	118.08	123.63
14	c	524	BCR	C20-C19-C18	-2.22	120.28	126.36
14	B	4010	BCR	C36-C18-C19	2.22	121.47	118.09
14	4	524	BCR	C38-C26-C25	-2.22	122.06	124.48
13	f	502	CLA	C1-C2-C3	-2.22	122.56	126.20
13	2	510	CLA	C1-C2-C3	-2.22	122.57	126.20
13	2	517	CLA	C3B-C4B-NB	-2.22	108.55	110.53
13	A	1129	CLA	C1-C2-C3	-2.22	123.18	126.76
13	A	1124	CLA	C3B-C4B-NB	-2.21	108.55	110.53
13	d	502	CLA	C1-C2-C3	-2.21	122.57	126.20
13	6	504	CLA	CMB-C2B-C3B	2.21	131.76	126.55
13	e	508	CLA	C1-C2-C3	-2.21	122.57	126.20
13	B	1208	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
13	B	1224	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	6	505	CLA	C3B-C4B-NB	-2.21	108.56	110.53
13	f	511	CLA	C3B-C4B-NB	-2.21	108.56	110.53
13	A	1102	CLA	O2D-CGD-CBD	2.21	115.10	111.23
13	B	1226	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
13	e	501	CLA	O2A-CGA-O1A	-2.21	118.09	123.63
13	5	507	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	2	508	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
13	B	1213	CLA	CMB-C2B-C1B	-2.21	122.05	125.42
14	b	524	BCR	C1-C6-C5	-2.21	119.61	122.64
14	F	4014	BCR	C15-C14-C13	-2.21	124.18	127.28
13	B	1216	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
14	B	4010	BCR	C33-C5-C4	2.21	118.31	113.60
13	B	1218	CLA	C3B-C4B-NB	-2.21	108.56	110.53
13	a	510	CLA	CMB-C2B-C3B	2.21	131.75	126.55
13	A	1134	CLA	O2A-CGA-O1A	-2.21	118.10	123.63
13	B	1218	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
13	g	503	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
13	b	511	CLA	CHB-C4A-NA	2.21	127.59	124.40
13	a	502	CLA	O2A-CGA-O1A	-2.21	118.11	123.63
13	A	1127	CLA	CHB-C4A-NA	2.21	127.58	124.40
13	6	501	CLA	CHB-C4A-NA	2.21	127.58	124.40
13	A	1107	CLA	CAA-CBA-CGA	-2.20	106.95	113.21
13	3	510	CLA	CMB-C2B-C1B	-2.20	122.06	125.42
13	c	512	CLA	C3B-C4B-NB	-2.20	108.56	110.53
14	1	524	BCR	C8-C7-C6	-2.20	121.11	127.00
13	1	503	CLA	CHB-C4A-NA	2.20	127.58	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1220	CLA	C3B-C4B-NB	-2.20	108.56	110.53
13	c	519	CLA	C3B-C4B-NB	-2.20	108.56	110.53
13	1	510	CLA	C1-C2-C3	-2.20	122.59	126.20
14	6	521	BCR	C23-C24-C25	-2.20	121.11	127.00
13	f	504	CLA	CHB-C4A-NA	2.20	127.58	124.40
13	g	517	CLA	CHB-C4A-NA	2.20	127.58	124.40
14	B	4010	BCR	C34-C9-C8	2.20	121.45	118.09
14	B	4017	BCR	C20-C19-C18	-2.20	120.33	126.36
13	e	512	CLA	C1-C2-C3	-2.20	122.59	126.20
14	c	523	BCR	C15-C16-C17	-2.20	119.02	123.52
13	b	507	CLA	CHB-C4A-NA	2.20	127.57	124.40
14	1	522	BCR	C21-C20-C19	-2.20	116.83	123.20
13	6	511	CLA	C3B-C4B-NB	-2.20	108.57	110.53
13	f	519	CLA	CHB-C4A-NA	2.20	127.57	124.40
14	B	4004	BCR	C10-C11-C12	-2.20	116.83	123.20
16	g	5104	LMG	C8-O7-C10	-2.20	112.54	117.80
13	A	1127	CLA	CAA-CBA-CGA	-2.20	106.97	113.21
13	B	1218	CLA	CHB-C4A-NA	2.20	127.57	124.40
13	K	1401	CLA	O2A-CGA-O1A	-2.20	118.14	123.63
14	6	523	BCR	C33-C5-C4	2.19	118.28	113.60
13	d	510	CLA	C1-C2-C3	-2.19	122.60	126.20
13	g	506	CLA	C3B-C4B-NB	-2.19	108.57	110.53
14	F	4016	BCR	C11-C12-C13	-2.19	120.35	126.36
14	5	522	BCR	C15-C16-C17	-2.19	119.03	123.52
14	I	4018	BCR	C1-C6-C5	-2.19	119.64	122.64
13	d	505	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	b	517	CLA	CHB-C4A-NA	2.19	127.56	124.40
18	A	2001	PQN	C11-C3-C4	-2.19	116.27	118.58
13	B	1217	CLA	C1-C2-C3	-2.19	122.61	126.20
13	1	512	CLA	CAA-CBA-CGA	-2.19	106.99	113.21
14	M	4021	BCR	C38-C26-C27	2.19	118.26	113.60
13	e	504	CLA	C1-C2-C3	-2.19	122.61	126.20
13	2	512	CLA	O2D-CGD-CBD	2.19	115.06	111.23
13	3	507	CLA	O2A-CGA-O1A	-2.19	118.15	123.63
13	5	513	CLA	C1-C2-C3	-2.19	122.61	126.20
14	B	4009	BCR	C34-C9-C8	2.19	121.43	118.09
14	2	521	BCR	C16-C15-C14	-2.19	119.04	123.52
14	5	521	BCR	C33-C5-C4	2.19	118.26	113.60
13	f	518	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	B	1232	CLA	O2A-CGA-O1A	-2.19	117.71	123.33
13	A	1120	CLA	CHB-C4A-NA	2.19	127.56	124.40
13	c	502	CLA	C3B-C4B-NB	-2.19	108.58	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	3	524	BCR	C15-C16-C17	-2.19	119.05	123.52
14	2	524	BCR	C16-C15-C14	-2.19	119.05	123.52
13	B	1219	CLA	CMC-C2C-C3C	2.19	128.37	123.64
13	3	501	CLA	CMB-C2B-C1B	-2.19	122.09	125.42
13	g	511	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	b	505	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
13	g	518	CLA	O2A-CGA-O1A	-2.19	118.16	123.63
13	A	1106	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
13	b	503	CLA	O2A-CGA-O1A	-2.18	118.16	123.63
13	c	501	CLA	C3B-C4B-NB	-2.18	108.58	110.53
14	6	521	BCR	C38-C26-C27	2.18	118.25	113.60
13	g	504	CLA	O2D-CGD-CBD	2.18	115.05	111.23
13	4	513	CLA	C3B-C4B-NB	-2.18	108.58	110.53
13	B	1209	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	g	523	BCR	C15-C16-C17	-2.18	119.06	123.52
13	d	501	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	b	511	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	5	511	CLA	C3B-C4B-NB	-2.18	108.58	110.53
13	g	505	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	A	1111	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
14	B	4009	BCR	C20-C19-C18	-2.18	120.39	126.36
13	A	1116	CLA	O2A-CGA-O1A	-2.18	118.17	123.63
13	A	1119	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
14	5	524	BCR	C11-C12-C13	-2.18	120.39	126.36
13	e	505	CLA	C3B-C4B-NB	-2.18	108.58	110.53
13	B	1211	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	6	502	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	e	513	CLA	O2A-CGA-O1A	-2.18	118.18	123.63
13	B	1021	CLA	CHB-C4A-NA	2.18	127.54	124.40
13	e	512	CLA	C3B-C4B-NB	-2.18	108.59	110.53
14	6	524	BCR	C8-C7-C6	-2.17	121.19	127.00
13	A	1128	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	b	509	CLA	CHB-C4A-NA	2.17	127.54	124.40
13	d	511	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	d	504	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
13	K	1401	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	c	518	CLA	O2A-CGA-O1A	-2.17	118.19	123.63
14	F	4015	BCR	C21-C20-C19	-2.17	116.91	123.20
13	f	501	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	f	512	CLA	CHB-C4A-NA	2.17	127.53	124.40
13	d	501	CLA	C1-C2-C3	-2.17	122.64	126.20
14	a	524	BCR	C1-C6-C5	-2.17	119.67	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	509	CLA	C3B-C4B-NB	-2.17	108.59	110.53
15	2	822	SQD	O9-S-C6	2.17	110.00	106.76
13	f	519	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	5	505	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	A	1237	CLA	CMB-C2B-C1B	-2.17	122.11	125.42
13	f	505	CLA	C3B-C4B-NB	-2.17	108.59	110.53
13	f	511	CLA	C1-C2-C3	-2.17	122.64	126.20
13	e	511	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
13	e	518	CLA	O2A-CGA-O1A	-2.17	118.20	123.63
13	5	502	CLA	C1-C2-C3	-2.17	122.64	126.20
14	1	523	BCR	C21-C20-C19	-2.17	116.92	123.20
14	1	521	BCR	C20-C19-C18	-2.17	120.42	126.36
14	c	521	BCR	C20-C19-C18	-2.17	120.42	126.36
13	4	501	CLA	CMB-C2B-C1B	-2.17	122.12	125.42
14	3	523	BCR	C8-C7-C6	-2.17	121.21	127.00
14	1	521	BCR	C33-C5-C4	2.17	118.22	113.60
14	B	4009	BCR	C38-C26-C27	2.17	118.22	113.60
13	e	503	CLA	CHB-C4A-NA	2.17	127.53	124.40
14	F	4015	BCR	C32-C1-C6	-2.17	106.85	110.24
13	d	510	CLA	C3B-C4B-NB	-2.17	108.60	110.53
13	g	503	CLA	C3B-C4B-NB	-2.17	108.60	110.53
13	e	509	CLA	C1-C2-C3	-2.16	122.65	126.20
13	c	503	CLA	CHB-C4A-NA	2.16	127.52	124.40
13	5	505	CLA	C1-C2-C3	-2.16	122.65	126.20
14	4	521	BCR	C23-C24-C25	-2.16	121.22	127.00
13	A	1101	CLA	O2D-CGD-CBD	2.16	115.01	111.23
13	3	511	CLA	CAA-CBA-CGA	-2.16	107.07	113.21
13	A	1111	CLA	C1-C2-C3	-2.16	122.65	126.20
13	g	516	CLA	CHB-C4A-NA	2.16	127.52	124.40
13	5	502	CLA	C3B-C4B-NB	-2.16	108.60	110.53
14	e	521	BCR	C29-C30-C25	2.16	113.58	110.44
13	b	501	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	2	507	CLA	CMB-C2B-C1B	-2.16	122.13	125.42
13	B	1236	CLA	C1-C2-C3	-2.16	123.27	126.76
13	A	1113	CLA	CMB-C2B-C3B	2.16	131.62	126.55
13	3	509	CLA	C3B-C4B-NB	-2.16	108.60	110.53
13	A	1131	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	A	1011	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	B	1202	CLA	O2A-CGA-O1A	-2.16	118.23	123.63
13	d	507	CLA	CHB-C4A-NA	2.16	127.51	124.40
13	6	512	CLA	C3B-C4B-NB	-2.16	108.61	110.53
14	I	4019	BCR	C28-C27-C26	-2.16	110.21	114.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	g	524	BCR	C20-C19-C18	-2.16	120.45	126.36
13	e	504	CLA	O2A-CGA-O1A	-2.16	118.24	123.63
13	3	509	CLA	C1-C2-C3	-2.16	122.67	126.20
13	B	1227	CLA	C1-C2-C3	-2.16	122.67	126.20
13	A	1123	CLA	C1-C2-C3	-2.15	122.67	126.20
13	B	1234	CLA	O2D-CGD-CBD	2.15	115.00	111.23
14	e	521	BCR	C23-C24-C25	-2.15	121.25	127.00
13	5	516	CLA	CHB-C4A-NA	2.15	127.51	124.40
13	2	513	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	4	521	BCR	C29-C30-C25	2.15	113.56	110.44
13	c	513	CLA	C3B-C4B-NB	-2.15	108.61	110.53
14	4	522	BCR	C11-C12-C13	-2.15	120.46	126.36
14	e	522	BCR	C33-C5-C4	2.15	118.18	113.60
13	a	512	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	f	501	CLA	C3B-C4B-NB	-2.15	108.61	110.53
13	B	1231	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	5	507	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
13	a	513	CLA	CHB-C4A-NA	2.15	127.50	124.40
13	g	509	CLA	O2A-CGA-O1A	-2.15	118.25	123.63
14	a	523	BCR	C7-C8-C9	-2.15	123.06	126.23
13	1	518	CLA	O2A-CGA-O1A	-2.15	118.26	123.63
13	B	1228	CLA	O2D-CGD-CBD	2.15	114.98	111.23
13	3	508	CLA	CMB-C2B-C1B	-2.15	122.15	125.42
13	d	509	CLA	C1-C2-C3	-2.14	122.68	126.20
13	3	518	CLA	O2A-CGA-O1A	-2.14	118.26	123.63
14	1	524	BCR	C23-C24-C25	-2.14	121.27	127.00
13	6	510	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
14	e	521	BCR	C33-C5-C4	2.14	118.17	113.60
14	A	4008	BCR	C3-C4-C5	-2.14	110.23	114.06
14	b	523	BCR	C21-C20-C19	-2.14	116.99	123.20
13	4	510	CLA	C16-C15-C13	-2.14	108.84	115.97
13	B	1208	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
13	A	1112	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	2	512	CLA	CMD-C2D-C3D	2.14	132.60	127.69
13	4	503	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	2	502	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	f	510	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	g	519	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	5	507	CLA	C1-C2-C3	-2.14	122.69	126.20
14	6	523	BCR	C16-C15-C14	-2.14	119.14	123.52
14	B	4004	BCR	C39-C30-C25	-2.14	106.89	110.24
13	B	1238	CLA	O2A-CGA-O1A	-2.14	118.27	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	a	501	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	f	509	CLA	O2A-CGA-O1A	-2.14	118.27	123.63
13	A	1115	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	B	1023	CLA	C3B-C4B-NB	-2.14	108.62	110.53
14	5	521	BCR	C38-C26-C27	2.14	118.16	113.60
13	4	508	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	g	521	BCR	C16-C15-C14	-2.14	119.14	123.52
13	3	509	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	I	4019	BCR	C38-C26-C27	2.14	118.16	113.60
13	B	1210	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
14	5	522	BCR	C27-C26-C25	-2.14	119.81	122.70
14	1	521	BCR	C23-C24-C25	-2.14	121.28	127.00
13	1	511	CLA	CMB-C2B-C1B	-2.14	122.16	125.42
13	a	509	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	f	513	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	e	505	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
13	b	513	CLA	CMB-C2B-C1B	-2.14	122.17	125.42
14	a	521	BCR	C33-C5-C4	2.14	118.15	113.60
13	1	510	CLA	O2A-CGA-O1A	-2.14	118.28	123.63
14	d	524	BCR	C15-C16-C17	-2.14	119.15	123.52
15	1	822	SQD	O7-S-C6	2.14	109.95	106.76
13	5	504	CLA	C1-C2-C3	-2.14	122.70	126.20
17	A	5002	LHG	O7-C7-O9	-2.14	118.71	123.70
14	c	524	BCR	C36-C18-C19	2.14	121.35	118.09
14	f	522	BCR	C27-C26-C25	-2.14	119.82	122.70
13	A	1136	CLA	C1-C2-C3	-2.14	122.70	126.20
13	b	506	CLA	CHB-C1B-C2B	-2.14	121.23	127.43
13	A	1121	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	d	511	CLA	C3B-C4B-NB	-2.14	108.62	110.53
13	d	503	CLA	C1-C2-C3	-2.14	122.70	126.20
13	B	1023	CLA	O1D-CGD-CBD	2.13	128.73	124.52
14	c	523	BCR	C33-C5-C4	2.13	118.15	113.60
13	d	512	CLA	O2D-CGD-CBD	2.13	114.96	111.23
14	J	4012	BCR	C16-C15-C14	-2.13	119.15	123.52
14	B	4009	BCR	C10-C11-C12	-2.13	117.02	123.20
14	I	4020	BCR	C10-C11-C12	-2.13	117.02	123.20
14	d	522	BCR	C36-C18-C19	2.13	121.35	118.09
14	e	523	BCR	C3-C4-C5	-2.13	110.25	114.06
13	B	1213	CLA	C1-C2-C3	-2.13	122.70	126.20
13	B	1228	CLA	CHB-C4A-NA	2.13	127.48	124.40
14	g	521	BCR	C11-C12-C13	-2.13	120.52	126.36
13	B	1211	CLA	CMB-C2B-C1B	-2.13	122.17	125.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	d	511	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	J	1302	CLA	C3B-C4B-NB	-2.13	108.63	110.53
13	B	1201	CLA	CMB-C2B-C3B	2.13	131.56	126.55
13	e	503	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	6	521	BCR	C33-C5-C4	2.13	118.14	113.60
13	A	1011	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	g	501	CLA	C1-C2-C3	-2.13	122.71	126.20
13	g	501	CLA	C3B-C4B-NB	-2.13	108.63	110.53
17	A	5001	LHG	O7-C7-O9	-2.13	118.72	123.70
13	d	513	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	A	4008	BCR	C20-C19-C18	-2.13	120.52	126.36
13	B	1225	CLA	C1-C2-C3	-2.13	122.71	126.20
14	2	522	BCR	C36-C18-C19	2.13	121.34	118.09
14	g	523	BCR	C11-C12-C13	-2.13	120.52	126.36
13	c	506	CLA	C3B-C4B-NB	-2.13	108.63	110.53
13	1	503	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
13	f	511	CLA	CMB-C2B-C3B	2.13	131.56	126.55
13	b	507	CLA	O2A-CGA-O1A	-2.13	118.30	123.63
14	I	4018	BCR	C4-C5-C6	-2.13	119.83	122.70
14	3	524	BCR	C31-C1-C6	-2.13	106.91	110.24
13	g	516	CLA	O2A-CGA-O1A	-2.13	117.86	123.33
13	B	1225	CLA	CHB-C4A-NA	2.13	127.47	124.40
17	A	5004	LHG	O8-C23-O10	-2.13	118.31	123.63
14	c	521	BCR	C8-C7-C6	-2.13	121.32	127.00
13	d	503	CLA	C3B-C4B-NB	-2.13	108.63	110.53
13	B	1206	CLA	CHB-C4A-NA	2.13	127.47	124.40
13	2	519	CLA	C1-C2-C3	-2.13	123.32	126.76
17	A	5005	LHG	C5-O7-C7	-2.12	112.71	117.80
14	J	4012	BCR	C15-C16-C17	-2.12	119.17	123.52
13	A	1128	CLA	CHB-C4A-NA	2.12	127.47	124.40
13	A	1134	CLA	O2D-CGD-CBD	2.12	114.94	111.23
14	F	4015	BCR	C4-C5-C6	-2.12	119.83	122.70
15	5	822	SQD	O9-S-C6	2.12	109.93	106.76
13	f	501	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
14	4	521	BCR	C33-C5-C4	2.12	118.12	113.60
13	d	507	CLA	C1-C2-C3	-2.12	122.72	126.20
13	3	511	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
13	1	507	CLA	O2A-CGA-O1A	-2.12	118.32	123.63
13	B	1021	CLA	CBA-CAA-C2A	-2.12	107.48	113.79
14	B	4005	BCR	C15-C16-C17	-2.12	119.18	123.52
13	3	505	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	A	1104	CLA	C3B-C4B-NB	-2.12	108.64	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	e	513	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
13	A	1129	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
14	a	523	BCR	C16-C15-C14	-2.12	119.18	123.52
13	e	513	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	5	508	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	c	518	CLA	CMB-C2B-C1B	-2.12	122.19	125.42
15	4	822	SQD	C9-C8-C7	-2.12	105.94	113.69
14	J	4012	BCR	C2-C1-C6	2.12	113.51	110.44
13	B	1221	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	3	508	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	a	504	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	A	1107	CLA	CHB-C4A-NA	2.12	127.45	124.40
13	B	1212	CLA	C3B-C4B-NB	-2.12	108.64	110.53
13	2	507	CLA	O2A-CGA-O1A	-2.12	118.33	123.63
13	3	510	CLA	CMB-C2B-C3B	2.12	131.53	126.55
14	5	523	BCR	C37-C22-C21	-2.12	119.39	122.82
13	1	513	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
14	B	4017	BCR	C29-C30-C25	2.12	113.51	110.44
13	a	507	CLA	O2A-CGA-O1A	-2.12	118.34	123.63
13	b	517	CLA	C4A-NA-C1A	2.12	107.64	106.68
13	A	1105	CLA	CMB-C2B-C3B	2.12	131.53	126.55
13	2	509	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
13	1	501	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	A	4011	BCR	C10-C11-C12	-2.11	117.08	123.20
13	B	1224	CLA	C1-C2-C3	-2.11	122.73	126.20
13	g	512	CLA	CHB-C4A-NA	2.11	127.45	124.40
14	2	523	BCR	C21-C20-C19	-2.11	117.08	123.20
13	4	502	CLA	C3B-C4B-NB	-2.11	108.64	110.53
13	f	503	CLA	O2A-CGA-O1A	-2.11	118.34	123.63
14	5	524	BCR	C23-C24-C25	-2.11	121.36	127.00
13	f	513	CLA	CMB-C2B-C1B	-2.11	122.20	125.42
13	A	1118	CLA	C1-C2-C3	-2.11	122.74	126.20
14	F	4015	BCR	C34-C9-C10	-2.11	119.40	122.82
13	B	1239	CLA	O2A-CGA-O1A	-2.11	118.35	123.63
14	3	524	BCR	C21-C20-C19	-2.11	117.08	123.20
14	6	522	BCR	C38-C26-C27	2.11	118.10	113.60
13	5	512	CLA	C3B-C4B-NB	-2.11	108.65	110.53
13	B	1234	CLA	CMB-C2B-C3B	2.11	131.51	126.55
13	B	1012	CLA	CHB-C4A-NA	2.11	127.44	124.40
13	e	502	CLA	C1-C2-C3	-2.11	122.74	126.20
13	c	505	CLA	C3B-C4B-NB	-2.11	108.65	110.53
13	B	1227	CLA	O2A-CGA-O1A	-2.11	118.35	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1222	CLA	CMB-C2B-C3B	2.11	131.51	126.55
13	A	1013	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
13	5	511	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
13	6	513	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
13	g	504	CLA	CMB-C2B-C1B	-2.11	122.21	125.42
14	A	4002	BCR	C20-C19-C18	-2.11	120.59	126.36
13	g	504	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
13	4	501	CLA	C1-C2-C3	-2.11	122.75	126.20
13	1	511	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	B	4006	BCR	C28-C27-C26	-2.11	110.30	114.06
13	f	502	CLA	CAA-C2A-C3A	-2.11	107.31	113.00
13	B	1021	CLA	O2A-CGA-O1A	-2.11	118.36	123.63
14	a	521	BCR	C20-C19-C18	-2.10	120.59	126.36
14	2	523	BCR	C1-C6-C5	-2.10	119.76	122.64
14	d	524	BCR	C28-C27-C26	-2.10	110.31	114.06
14	2	521	BCR	C21-C20-C19	-2.10	117.11	123.20
13	X	1401	CLA	O2A-CGA-O1A	-2.10	117.92	123.33
14	1	523	BCR	C30-C25-C26	-2.10	119.76	122.64
13	6	518	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
13	d	508	CLA	O2A-CGA-O1A	-2.10	118.37	123.63
13	B	1208	CLA	O2D-CGD-CBD	2.10	114.90	111.23
13	A	1135	CLA	CMB-C2B-C1B	-2.10	122.22	125.42
14	2	522	BCR	C37-C22-C23	2.10	121.30	118.09
13	3	506	CLA	O1D-CGD-CBD	2.10	128.66	124.52
13	g	504	CLA	CHB-C4A-NA	2.10	127.43	124.40
13	A	1110	CLA	C3B-C4B-NB	-2.10	108.66	110.53
13	g	507	CLA	CHB-C4A-NA	2.10	127.43	124.40
14	c	524	BCR	C35-C13-C14	-2.10	119.42	122.82
13	c	503	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	2	507	CLA	CHB-C4A-NA	2.10	127.43	124.40
13	2	512	CLA	CMD-C2D-C1D	-2.10	121.03	124.73
14	4	524	BCR	C8-C7-C6	-2.10	121.39	127.00
13	a	505	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
13	4	509	CLA	O2A-CGA-O1A	-2.10	118.38	123.63
14	2	524	BCR	C15-C16-C17	-2.10	119.23	123.52
14	6	522	BCR	C8-C7-C6	-2.10	121.40	127.00
14	c	523	BCR	C16-C15-C14	-2.10	119.23	123.52
13	A	1013	CLA	C6-C7-C8	-2.10	109.00	115.97
14	B	4009	BCR	C27-C26-C25	-2.10	119.87	122.70
14	d	524	BCR	C4-C5-C6	-2.10	119.87	122.70
13	4	513	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
14	K	4001	BCR	C8-C7-C6	-2.09	121.40	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	4015	BCR	C28-C27-C26	-2.09	110.32	114.06
13	A	1130	CLA	CMB-C2B-C3B	2.09	131.48	126.55
14	a	524	BCR	C4-C5-C6	-2.09	119.87	122.70
14	a	524	BCR	C15-C16-C17	-2.09	119.23	123.52
13	B	1227	CLA	C3B-C4B-NB	-2.09	108.66	110.53
14	K	4001	BCR	C37-C22-C21	-2.09	119.43	122.82
13	B	1228	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
13	c	511	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
13	A	1138	CLA	O2A-CGA-O1A	-2.09	118.39	123.63
13	g	507	CLA	O1D-CGD-CBD	2.09	128.64	124.52
13	a	506	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
13	3	517	CLA	C3B-C4B-NB	-2.09	108.66	110.53
13	f	513	CLA	CMB-C2B-C3B	2.09	131.47	126.55
13	g	516	CLA	C3B-C4B-NB	-2.09	108.67	110.53
13	3	501	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	1	504	CLA	O2A-CGA-O1A	-2.09	118.40	123.63
13	F	1301	CLA	O2A-CGA-O1A	-2.09	117.96	123.33
14	5	523	BCR	C1-C6-C5	-2.09	119.78	122.64
13	c	511	CLA	CMB-C2B-C1B	-2.09	122.24	125.42
14	e	523	BCR	C37-C22-C23	2.09	121.28	118.09
13	B	1204	CLA	CHB-C4A-NA	2.09	127.41	124.40
13	3	504	CLA	O2A-CGA-O1A	-2.09	118.41	123.63
13	A	1123	CLA	C3B-C4B-NB	-2.09	108.67	110.53
13	K	1103	CLA	CHB-C4A-NA	2.08	127.41	124.40
13	c	508	CLA	C1-C2-C3	-2.08	122.78	126.20
13	g	509	CLA	C1-C2-C3	-2.08	122.78	126.20
13	1	501	CLA	C1-C2-C3	-2.08	122.78	126.20
13	A	1124	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	4	507	CLA	O2A-CGA-O1A	-2.08	118.42	123.63
13	B	1228	CLA	C3B-C4B-NB	-2.08	108.67	110.53
14	J	4012	BCR	C38-C26-C27	2.08	118.04	113.60
14	c	521	BCR	C33-C5-C4	2.08	118.03	113.60
13	g	506	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
13	B	1223	CLA	C3B-C4B-NB	-2.08	108.67	110.53
13	6	510	CLA	CMB-C2B-C3B	2.08	131.44	126.55
14	c	524	BCR	C11-C12-C13	-2.08	120.66	126.36
14	c	523	BCR	C37-C22-C23	2.08	121.27	118.09
13	f	506	CLA	CMB-C2B-C1B	-2.08	122.25	125.42
14	A	4007	BCR	C3-C4-C5	-2.08	110.35	114.06
13	f	505	CLA	C1-C2-C3	-2.08	122.79	126.20
13	A	1127	CLA	CMB-C2B-C3B	2.08	131.44	126.55
13	2	509	CLA	C3B-C4B-NB	-2.08	108.68	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	1213	CLA	C3B-C4B-NB	-2.08	108.68	110.53
13	A	1119	CLA	CMB-C2B-C1B	-2.08	122.26	125.42
13	2	501	CLA	O2A-CGA-O1A	-2.08	118.43	123.63
13	A	1117	CLA	CHB-C4A-NA	2.08	127.40	124.40
14	g	521	BCR	C23-C24-C25	-2.08	121.45	127.00
13	2	518	CLA	O2A-CGA-O1A	-2.08	118.44	123.63
13	5	509	CLA	C1-C2-C3	-2.08	122.80	126.20
13	5	517	CLA	C3B-C4B-NB	-2.08	108.68	110.53
13	e	501	CLA	C3B-C4B-NB	-2.08	108.68	110.53
14	b	524	BCR	C37-C22-C23	2.08	121.26	118.09
14	K	4001	BCR	C36-C18-C19	2.07	121.26	118.09
14	2	523	BCR	C28-C27-C26	-2.07	110.36	114.06
14	B	4004	BCR	C3-C4-C5	-2.07	110.36	114.06
13	b	519	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	e	509	CLA	O2A-CGA-O1A	-2.07	118.44	123.63
13	B	1209	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	b	511	CLA	C1-C2-C3	-2.07	122.80	126.20
13	a	517	CLA	CHB-C4A-NA	2.07	127.39	124.40
13	3	512	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	A	1101	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	1	502	CLA	C1-C2-C3	-2.07	122.80	126.20
13	B	1239	CLA	C1-C2-C3	-2.07	122.80	126.20
13	6	503	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	a	508	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	5	510	CLA	CMB-C2B-C3B	2.07	131.42	126.55
14	2	524	BCR	C37-C22-C23	2.07	121.25	118.09
14	M	4021	BCR	C8-C7-C6	-2.07	121.47	127.00
13	e	513	CLA	C1-C2-C3	-2.07	123.41	126.76
13	A	1111	CLA	CMB-C2B-C1B	-2.07	122.27	125.42
13	a	513	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	3	523	BCR	C36-C18-C19	2.07	121.25	118.09
14	4	522	BCR	C37-C22-C23	2.07	121.25	118.09
13	d	502	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	f	509	CLA	C3B-C4B-NB	-2.07	108.68	110.53
13	4	503	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	d	505	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
13	b	518	CLA	O2A-CGA-O1A	-2.07	118.45	123.63
14	f	521	BCR	C21-C20-C19	-2.07	117.21	123.20
13	2	518	CLA	C1-C2-C3	-2.07	122.81	126.20
13	a	503	CLA	C1-C2-C3	-2.07	122.81	126.20
13	A	1132	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
13	B	1229	CLA	O1D-CGD-CBD	2.07	128.60	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	5	510	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
13	g	513	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
13	A	1022	CLA	O2A-CGA-O1A	-2.07	118.46	123.63
14	3	523	BCR	C11-C12-C13	-2.07	120.70	126.36
15	f	822	SQD	O9-S-C6	2.07	109.84	106.76
14	B	4017	BCR	C3-C4-C5	-2.07	110.37	114.06
13	6	509	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
13	b	513	CLA	O2A-CGA-O1A	-2.06	118.46	123.63
13	3	506	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
14	4	524	BCR	C29-C30-C25	2.06	113.44	110.44
14	a	521	BCR	C16-C15-C14	-2.06	119.30	123.52
14	g	523	BCR	C38-C26-C25	-2.06	122.23	124.48
14	6	523	BCR	C11-C12-C13	-2.06	120.70	126.36
14	5	523	BCR	C40-C30-C29	2.06	116.87	108.95
14	e	523	BCR	C34-C9-C8	2.06	121.24	118.09
14	2	524	BCR	C33-C5-C4	2.06	117.99	113.60
13	A	1139	CLA	C1-C2-C3	-2.06	122.82	126.20
13	c	507	CLA	O2A-CGA-O1A	-2.06	118.47	123.63
14	e	523	BCR	C38-C26-C27	2.06	117.99	113.60
13	5	512	CLA	C1-C2-C3	-2.06	122.82	126.20
13	A	1122	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
13	3	505	CLA	CMB-C2B-C1B	-2.06	122.28	125.42
13	B	1201	CLA	O2D-CGD-CBD	2.06	114.83	111.23
13	4	507	CLA	C1-C2-C3	-2.06	122.83	126.20
14	d	521	BCR	C15-C16-C17	-2.06	119.31	123.52
14	B	4005	BCR	C21-C20-C19	-2.06	117.24	123.20
13	5	511	CLA	CMB-C2B-C1B	-2.06	122.29	125.42
13	a	506	CLA	C3B-C4B-NB	-2.06	108.69	110.53
14	g	523	BCR	C21-C20-C19	-2.06	117.24	123.20
13	c	504	CLA	O2A-CGA-O1A	-2.06	118.48	123.63
15	1	822	SQD	O9-S-C6	2.06	109.83	106.76
13	K	1401	CLA	O1D-CGD-CBD	2.06	128.57	124.52
13	c	507	CLA	C1-C2-C3	-2.06	122.83	126.20
13	4	518	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	a	512	CLA	O2A-CGA-O1A	-2.05	118.49	123.63
13	3	505	CLA	CMB-C2B-C3B	2.05	131.38	126.55
13	b	510	CLA	CHB-C4A-NA	2.05	127.36	124.40
13	B	1214	CLA	C1-C2-C3	-2.05	122.83	126.20
13	4	518	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	B	1222	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	c	507	CLA	CHB-C4A-NA	2.05	127.36	124.40
13	3	510	CLA	O2A-CGA-O1A	-2.05	118.49	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	e	522	BCR	C21-C20-C19	-2.05	117.25	123.20
13	a	505	CLA	CHB-C4A-NA	2.05	127.36	124.40
13	B	1210	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	1	505	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	b	509	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
14	d	521	BCR	C11-C12-C13	-2.05	120.74	126.36
13	A	1111	CLA	CMB-C2B-C3B	2.05	131.38	126.55
13	b	502	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	g	503	CLA	CAA-CBA-CGA	-2.05	107.38	113.21
13	A	1118	CLA	O2A-CGA-O1A	-2.05	118.50	123.63
13	A	1132	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	A	1136	CLA	O2D-CGD-CBD	2.05	114.81	111.23
13	b	505	CLA	C3A-C2A-C1A	2.05	104.41	101.34
13	3	502	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	d	509	CLA	C3B-C4B-NB	-2.05	108.70	110.53
14	5	521	BCR	C23-C24-C25	-2.05	121.53	127.00
14	6	522	BCR	C35-C13-C14	-2.05	119.50	122.82
16	J	5104	LMG	O7-C10-O9	-2.05	118.92	123.70
14	B	4010	BCR	C38-C26-C27	2.05	117.96	113.60
13	2	511	CLA	CMB-C2B-C1B	-2.05	122.30	125.42
13	2	518	CLA	C3B-C4B-NB	-2.05	108.70	110.53
13	b	519	CLA	O2A-CGA-O1A	-2.05	118.07	123.33
15	3	822	SQD	O9-S-C6	2.05	109.81	106.76
14	1	523	BCR	C15-C16-C17	-2.05	119.33	123.52
15	2	822	SQD	O7-S-C6	2.05	109.81	106.76
13	5	519	CLA	O2D-CGD-CBD	2.04	114.81	111.23
13	A	1107	CLA	O1D-CGD-CBD	2.04	128.55	124.52
14	f	521	BCR	C11-C12-C13	-2.04	120.76	126.36
13	3	503	CLA	CMB-C2B-C1B	-2.04	122.31	125.42
13	F	1301	CLA	O1A-CGA-CBA	2.04	129.57	123.09
13	A	1237	CLA	C1-C2-C3	-2.04	122.85	126.20
13	g	513	CLA	C3B-C4B-NB	-2.04	108.71	110.53
13	3	506	CLA	CMB-C2B-C3B	2.04	131.36	126.55
13	4	511	CLA	O2A-CGA-O1A	-2.04	118.08	123.33
13	1	512	CLA	CMD-C2D-C3D	2.04	132.37	127.69
13	A	1133	CLA	CMB-C2B-C3B	2.04	131.35	126.55
13	c	505	CLA	O2A-CGA-O1A	-2.04	118.52	123.63
13	A	1124	CLA	C1-C2-C3	-2.04	122.85	126.20
14	1	524	BCR	C38-C26-C27	2.04	117.95	113.60
13	2	516	CLA	C3B-C4B-NB	-2.04	108.71	110.53
13	1	508	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
14	5	523	BCR	C40-C30-C25	-2.04	107.05	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	B	4004	BCR	C34-C9-C8	2.04	121.20	118.09
14	2	524	BCR	C11-C12-C13	-2.04	120.78	126.36
14	d	522	BCR	C38-C26-C27	2.04	117.94	113.60
13	A	1117	CLA	C3B-C4B-NB	-2.04	108.71	110.53
13	A	1105	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	g	507	CLA	O2A-CGA-O1A	-2.04	118.53	123.63
13	2	508	CLA	O2A-CGA-O1A	-2.04	118.54	123.63
13	a	516	CLA	C3B-C4B-NB	-2.04	108.71	110.53
13	J	1302	CLA	O2A-CGA-O1A	-2.03	118.10	123.33
13	3	519	CLA	C3B-C4B-NB	-2.03	108.71	110.53
14	3	522	BCR	C36-C18-C19	2.03	121.19	118.09
13	f	510	CLA	O2A-CGA-O1A	-2.03	118.54	123.63
13	A	1137	CLA	CAA-CBA-CGA	-2.03	107.44	113.21
13	B	1202	CLA	CMB-C2B-C1B	-2.03	122.32	125.42
14	F	4015	BCR	C37-C22-C23	2.03	121.19	118.09
13	e	510	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
13	e	511	CLA	C3B-C4B-NB	-2.03	108.72	110.53
13	f	517	CLA	C3B-C4B-NB	-2.03	108.72	110.53
13	3	511	CLA	C1-C2-C3	-2.03	122.87	126.20
13	4	510	CLA	C3B-C4B-NB	-2.03	108.72	110.53
15	c	822	SQD	O9-S-C6	2.03	109.79	106.76
13	a	507	CLA	CHB-C4A-NA	2.03	127.33	124.40
14	a	522	BCR	C21-C20-C19	-2.03	117.32	123.20
13	2	511	CLA	O2A-CGA-O1A	-2.03	118.55	123.63
14	e	524	BCR	C37-C22-C23	2.03	121.19	118.09
13	c	501	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	g	502	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
14	b	521	BCR	C23-C24-C25	-2.03	121.58	127.00
13	e	508	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	6	507	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	c	508	CLA	O2A-CGA-O1A	-2.03	118.56	123.63
13	c	510	CLA	C3B-C4B-NB	-2.03	108.72	110.53
14	6	521	BCR	C16-C15-C14	-2.03	119.38	123.52
13	6	505	CLA	CAA-C2A-C3A	-2.02	107.53	113.00
13	A	1124	CLA	CHD-C1D-ND	-2.02	121.95	124.80
14	6	524	BCR	C10-C11-C12	-2.02	117.33	123.20
13	1	502	CLA	O2A-CGA-O1A	-2.02	118.56	123.63
14	I	4020	BCR	C34-C9-C8	2.02	121.18	118.09
14	2	521	BCR	C39-C30-C25	-2.02	107.07	110.24
13	B	1202	CLA	CMB-C2B-C3B	2.02	131.31	126.55
14	6	523	BCR	C20-C19-C18	-2.02	120.82	126.36
13	A	1109	CLA	O2A-CGA-O1A	-2.02	118.57	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	4	523	BCR	C10-C11-C12	-2.02	117.34	123.20
14	e	524	BCR	C36-C18-C19	2.02	121.18	118.09
13	1	509	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	2	511	CLA	C3B-C4B-NB	-2.02	108.72	110.53
13	c	517	CLA	O2A-CGA-O1A	-2.02	118.13	123.33
13	f	503	CLA	CHB-C4A-NA	2.02	127.32	124.40
14	b	524	BCR	C28-C27-C26	-2.02	110.45	114.06
14	c	522	BCR	C21-C20-C19	-2.02	117.34	123.20
13	5	512	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	A	1123	CLA	CAA-C2A-C3A	-2.02	107.54	113.00
14	F	4016	BCR	C3-C4-C5	-2.02	110.45	114.06
13	A	1130	CLA	O2A-CGA-O1A	-2.02	118.57	123.63
13	b	506	CLA	CHC-C1C-NC	2.02	127.35	124.31
13	B	1214	CLA	O2D-CGD-CBD	2.02	114.76	111.23
14	K	4001	BCR	C27-C26-C25	-2.02	119.97	122.70
13	f	502	CLA	C3B-C4B-NB	-2.02	108.73	110.53
13	4	519	CLA	CMB-C2B-C1B	-2.02	122.34	125.42
13	4	516	CLA	C3B-C4B-NB	-2.02	108.73	110.53
13	5	505	CLA	CMB-C2B-C3B	2.02	131.30	126.55
14	d	524	BCR	C34-C9-C8	2.02	121.17	118.09
13	c	517	CLA	C1D-ND-C4D	-2.02	104.90	106.31
13	d	510	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
13	g	501	CLA	O2A-CGA-O1A	-2.02	118.58	123.63
14	I	4020	BCR	C21-C20-C19	-2.02	117.36	123.20
13	6	517	CLA	O2A-CGA-O1A	-2.02	118.14	123.33
14	5	523	BCR	C23-C22-C21	2.02	122.18	119.01
13	A	1122	CLA	C3B-C4B-NB	-2.02	108.73	110.53
20	J	5105	LMU	C6'-C5'-C4'	-2.02	108.07	113.02
13	4	501	CLA	CMB-C2B-C3B	2.02	131.29	126.55
13	5	502	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
14	2	523	BCR	C35-C13-C12	2.01	121.17	118.09
13	A	1113	CLA	O2A-CGA-O1A	-2.01	118.59	123.63
13	A	1104	CLA	CMB-C2B-C1B	-2.01	122.35	125.42
13	5	503	CLA	CAA-CBA-CGA	-2.01	107.49	113.21
13	B	1211	CLA	CMB-C2B-C3B	2.01	131.28	126.55
13	A	1131	CLA	C3B-C4B-NB	-2.01	108.73	110.53
14	c	521	BCR	C29-C30-C25	2.01	113.36	110.44
13	A	1136	CLA	CHB-C4A-NA	2.01	127.30	124.40
13	b	510	CLA	C3A-C2A-C1A	2.01	104.35	101.34
13	1	506	CLA	C3B-C4B-NB	-2.01	108.73	110.53
13	g	511	CLA	C3B-C4B-NB	-2.01	108.73	110.53
13	d	504	CLA	C1-C2-C3	-2.01	122.90	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	f	523	BCR	C33-C5-C6	-2.01	122.29	124.48
13	J	1303	CLA	O2A-CGA-O1A	-2.01	118.16	123.33
14	e	523	BCR	C21-C20-C19	-2.01	117.37	123.20
13	2	507	CLA	CMB-C2B-C3B	2.01	131.28	126.55
13	6	517	CLA	C3B-C4B-NB	-2.01	108.73	110.53
13	A	1102	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	a	522	BCR	C34-C9-C10	-2.01	119.56	122.82
13	b	511	CLA	C3B-C4B-NB	-2.01	108.74	110.53
14	5	522	BCR	C21-C20-C19	-2.01	117.38	123.20
13	a	510	CLA	O2A-CGA-O1A	-2.01	118.60	123.63
14	B	4009	BCR	C36-C18-C19	2.01	121.16	118.09
14	d	521	BCR	C38-C26-C27	2.01	117.88	113.60
13	2	502	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
14	1	522	BCR	C37-C22-C23	2.01	121.16	118.09
13	6	501	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
13	c	518	CLA	C3B-C4B-NB	-2.01	108.74	110.53
13	B	1205	CLA	O2D-CGD-CBD	2.01	114.74	111.23
16	2	5104	LMG	O7-C10-O9	-2.01	119.02	123.70
13	d	509	CLA	O2A-CGA-O1A	-2.01	118.61	123.63
14	4	524	BCR	C36-C18-C17	-2.01	119.57	122.82
13	A	1133	CLA	O2A-CGA-O1A	-2.00	118.61	123.63
13	A	1140	CLA	CHB-C1B-NB	2.00	127.06	124.05
14	b	523	BCR	C23-C24-C25	-2.00	121.65	127.00
14	B	4005	BCR	C11-C12-C13	-2.00	120.87	126.36
13	c	511	CLA	C3B-C4B-NB	-2.00	108.74	110.53
13	A	1139	CLA	CHB-C4A-NA	2.00	127.29	124.40
13	A	1128	CLA	CMB-C2B-C3B	2.00	131.26	126.55
13	e	511	CLA	CMB-C2B-C3B	2.00	131.26	126.55
13	6	511	CLA	O2A-CGA-O1A	-2.00	118.19	123.33
13	A	1011	CLA	C1-C2-C3	-2.00	122.92	126.20
13	5	505	CLA	O2A-CGA-O1A	-2.00	118.62	123.63

All (303) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	3	501	CLA	ND
13	3	502	CLA	ND
13	3	503	CLA	ND
13	3	504	CLA	ND
13	3	505	CLA	ND
13	3	506	CLA	ND
13	3	507	CLA	ND

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Mol	Chain	Res	Type	Atom
13	3	508	CLA	ND
13	3	509	CLA	ND
13	3	510	CLA	ND
13	3	511	CLA	ND
13	3	512	CLA	ND
13	3	513	CLA	ND
13	3	516	CLA	ND
13	3	517	CLA	ND
13	3	518	CLA	ND
13	3	519	CLA	ND
13	4	501	CLA	ND
13	4	503	CLA	ND
13	4	504	CLA	ND
13	4	505	CLA	ND
13	4	506	CLA	ND
13	4	507	CLA	ND
13	4	508	CLA	ND
13	4	509	CLA	ND
13	4	510	CLA	ND
13	4	512	CLA	ND
13	4	513	CLA	ND
13	4	516	CLA	ND
13	4	517	CLA	ND
13	4	518	CLA	ND
13	4	519	CLA	ND
13	5	501	CLA	ND
13	5	502	CLA	ND
13	5	503	CLA	ND
13	5	504	CLA	ND
13	5	505	CLA	ND
13	5	506	CLA	ND
13	5	507	CLA	ND
13	5	508	CLA	ND
13	5	509	CLA	ND
13	5	510	CLA	ND
13	5	511	CLA	ND
13	5	512	CLA	ND
13	5	513	CLA	ND
13	5	516	CLA	ND
13	5	517	CLA	ND
13	5	518	CLA	ND
13	5	519	CLA	ND

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Mol	Chain	Res	Type	Atom
13	6	501	CLA	ND
13	6	502	CLA	ND
13	6	503	CLA	ND
13	6	504	CLA	ND
13	6	505	CLA	ND
13	6	506	CLA	ND
13	6	507	CLA	ND
13	6	508	CLA	ND
13	6	509	CLA	ND
13	6	510	CLA	ND
13	6	511	CLA	ND
13	6	512	CLA	ND
13	6	513	CLA	ND
13	6	516	CLA	ND
13	6	517	CLA	ND
13	6	518	CLA	ND
13	6	519	CLA	ND
13	2	501	CLA	ND
13	2	502	CLA	ND
13	2	503	CLA	ND
13	2	504	CLA	ND
13	2	505	CLA	ND
13	2	506	CLA	ND
13	2	507	CLA	ND
13	2	508	CLA	ND
13	2	509	CLA	ND
13	2	510	CLA	ND
13	2	511	CLA	ND
13	2	512	CLA	ND
13	2	513	CLA	ND
13	2	516	CLA	ND
13	2	517	CLA	ND
13	2	518	CLA	ND
13	2	519	CLA	ND
13	1	501	CLA	ND
13	1	502	CLA	ND
13	1	503	CLA	ND
13	1	504	CLA	ND
13	1	505	CLA	ND
13	1	506	CLA	ND
13	1	507	CLA	ND
13	1	508	CLA	ND

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Mol	Chain	Res	Type	Atom
13	1	509	CLA	ND
13	1	510	CLA	ND
13	1	511	CLA	ND
13	1	512	CLA	ND
13	1	513	CLA	ND
13	1	516	CLA	ND
13	1	517	CLA	ND
13	1	518	CLA	ND
13	1	519	CLA	ND
13	A	1022	CLA	ND
13	A	1013	CLA	ND
13	A	1101	CLA	ND
13	A	1102	CLA	ND
13	A	1103	CLA	ND
13	A	1104	CLA	ND
13	A	1105	CLA	ND
13	A	1106	CLA	ND
13	A	1107	CLA	ND
13	A	1108	CLA	ND
13	A	1109	CLA	ND
13	A	1110	CLA	ND
13	A	1111	CLA	ND
13	A	1112	CLA	ND
13	A	1113	CLA	ND
13	A	1114	CLA	ND
13	A	1115	CLA	ND
13	A	1116	CLA	ND
13	A	1117	CLA	ND
13	A	1118	CLA	ND
13	A	1119	CLA	ND
13	A	1120	CLA	ND
13	A	1121	CLA	ND
13	A	1122	CLA	ND
13	A	1123	CLA	ND
13	A	1125	CLA	ND
13	A	1126	CLA	ND
13	A	1127	CLA	ND
13	A	1128	CLA	ND
13	A	1129	CLA	ND
13	A	1130	CLA	ND
13	A	1131	CLA	ND
13	A	1132	CLA	ND

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Mol	Chain	Res	Type	Atom
13	A	1133	CLA	ND
13	A	1134	CLA	ND
13	A	1135	CLA	ND
13	A	1136	CLA	ND
13	A	1137	CLA	ND
13	A	1138	CLA	ND
13	A	1139	CLA	ND
13	A	1140	CLA	ND
13	A	1801	CLA	ND
13	A	1237	CLA	ND
13	A	1011	CLA	ND
13	B	1012	CLA	ND
13	B	1021	CLA	ND
13	B	1023	CLA	ND
13	B	1201	CLA	ND
13	B	1202	CLA	ND
13	B	1203	CLA	ND
13	B	1204	CLA	ND
13	B	1205	CLA	ND
13	B	1206	CLA	ND
13	B	1208	CLA	ND
13	B	1209	CLA	ND
13	B	1210	CLA	ND
13	B	1211	CLA	ND
13	B	1212	CLA	ND
13	B	1213	CLA	ND
13	B	1214	CLA	ND
13	B	1215	CLA	ND
13	B	1216	CLA	ND
13	B	1217	CLA	ND
13	B	1218	CLA	ND
13	B	1219	CLA	ND
13	B	1220	CLA	ND
13	B	1221	CLA	ND
13	B	1222	CLA	ND
13	B	1223	CLA	ND
13	B	1224	CLA	ND
13	B	1225	CLA	ND
13	B	1226	CLA	ND
13	B	1227	CLA	ND
13	B	1228	CLA	ND
13	B	1229	CLA	ND

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Mol	Chain	Res	Type	Atom
13	B	1230	CLA	ND
13	B	1231	CLA	ND
13	B	1232	CLA	ND
13	B	1233	CLA	ND
13	B	1234	CLA	ND
13	B	1236	CLA	ND
13	B	1238	CLA	ND
13	F	1301	CLA	ND
13	J	1302	CLA	ND
13	K	1103	CLA	ND
13	K	1401	CLA	ND
13	X	1401	CLA	ND
13	c	501	CLA	ND
13	c	502	CLA	ND
13	c	503	CLA	ND
13	c	504	CLA	ND
13	c	505	CLA	ND
13	c	506	CLA	ND
13	c	507	CLA	ND
13	c	508	CLA	ND
13	c	509	CLA	ND
13	c	510	CLA	ND
13	c	511	CLA	ND
13	c	512	CLA	ND
13	c	513	CLA	ND
13	c	516	CLA	ND
13	c	517	CLA	ND
13	c	518	CLA	ND
13	c	519	CLA	ND
13	d	501	CLA	ND
13	d	502	CLA	ND
13	d	503	CLA	ND
13	d	504	CLA	ND
13	d	505	CLA	ND
13	d	506	CLA	ND
13	d	507	CLA	ND
13	d	508	CLA	ND
13	d	509	CLA	ND
13	d	510	CLA	ND
13	d	511	CLA	ND
13	d	512	CLA	ND
13	d	513	CLA	ND

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Mol	Chain	Res	Type	Atom
13	d	516	CLA	ND
13	d	517	CLA	ND
13	d	518	CLA	ND
13	d	519	CLA	ND
13	e	501	CLA	ND
13	e	502	CLA	ND
13	e	503	CLA	ND
13	e	504	CLA	ND
13	e	505	CLA	ND
13	e	506	CLA	ND
13	e	507	CLA	ND
13	e	508	CLA	ND
13	e	509	CLA	ND
13	e	510	CLA	ND
13	e	511	CLA	ND
13	e	512	CLA	ND
13	e	513	CLA	ND
13	e	516	CLA	ND
13	e	517	CLA	ND
13	e	518	CLA	ND
13	e	519	CLA	ND
13	f	501	CLA	ND
13	f	502	CLA	ND
13	f	503	CLA	ND
13	f	504	CLA	ND
13	f	505	CLA	ND
13	f	507	CLA	ND
13	f	508	CLA	ND
13	f	509	CLA	ND
13	f	510	CLA	ND
13	f	511	CLA	ND
13	f	512	CLA	ND
13	f	513	CLA	ND
13	f	516	CLA	ND
13	f	517	CLA	ND
13	f	518	CLA	ND
13	f	519	CLA	ND
13	g	501	CLA	ND
13	g	502	CLA	ND
13	g	503	CLA	ND
13	g	504	CLA	ND
13	g	505	CLA	ND

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Mol	Chain	Res	Type	Atom
13	g	506	CLA	ND
13	g	507	CLA	ND
13	g	508	CLA	ND
13	g	509	CLA	ND
13	g	510	CLA	ND
13	g	511	CLA	ND
13	g	512	CLA	ND
13	g	513	CLA	ND
13	g	516	CLA	ND
13	g	517	CLA	ND
13	g	518	CLA	ND
13	g	519	CLA	ND
13	b	501	CLA	ND
13	b	502	CLA	ND
13	b	503	CLA	ND
13	b	504	CLA	ND
13	b	505	CLA	ND
13	b	507	CLA	ND
13	b	508	CLA	ND
13	b	509	CLA	ND
13	b	510	CLA	ND
13	b	511	CLA	ND
13	b	512	CLA	ND
13	b	513	CLA	ND
13	b	516	CLA	ND
13	b	517	CLA	ND
13	b	518	CLA	ND
13	b	519	CLA	ND
13	a	501	CLA	ND
13	a	502	CLA	ND
13	a	503	CLA	ND
13	a	504	CLA	ND
13	a	505	CLA	ND
13	a	506	CLA	ND
13	a	507	CLA	ND
13	a	508	CLA	ND
13	a	509	CLA	ND
13	a	510	CLA	ND
13	a	511	CLA	ND
13	a	512	CLA	ND
13	a	516	CLA	ND
13	a	517	CLA	ND

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Mol	Chain	Res	Type	Atom
13	a	518	CLA	ND
13	a	519	CLA	ND

All (3447) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	3	501	CLA	CAD-CBD-CGD-O1D
13	3	501	CLA	CAD-CBD-CGD-O2D
13	3	502	CLA	C4B-C3B-CAB-CBB
13	3	505	CLA	C6-C7-C8-C9
13	3	507	CLA	CAD-CBD-CGD-O1D
13	3	507	CLA	CAD-CBD-CGD-O2D
13	3	509	CLA	C3A-C2A-CAA-CBA
13	3	511	CLA	C1A-C2A-CAA-CBA
13	3	513	CLA	CBD-CGD-O2D-CED
13	3	516	CLA	C1A-C2A-CAA-CBA
13	4	501	CLA	CBD-CGD-O2D-CED
13	4	502	CLA	C2B-C3B-CAB-CBB
13	4	502	CLA	C4B-C3B-CAB-CBB
13	4	503	CLA	CBD-CGD-O2D-CED
13	4	504	CLA	CAD-CBD-CGD-O2D
13	4	505	CLA	C1A-C2A-CAA-CBA
13	4	505	CLA	C3A-C2A-CAA-CBA
13	4	505	CLA	CAD-CBD-CGD-O1D
13	4	505	CLA	CAD-CBD-CGD-O2D
13	4	506	CLA	CAD-CBD-CGD-O1D
13	4	506	CLA	CAD-CBD-CGD-O2D
13	4	506	CLA	CBD-CGD-O2D-CED
13	4	512	CLA	C3A-C2A-CAA-CBA
13	4	519	CLA	C1A-C2A-CAA-CBA
13	4	519	CLA	C3A-C2A-CAA-CBA
13	5	502	CLA	CHA-CBD-CGD-O1D
13	5	502	CLA	CHA-CBD-CGD-O2D
13	5	504	CLA	CAD-CBD-CGD-O1D
13	5	504	CLA	CAD-CBD-CGD-O2D
13	5	504	CLA	CBD-CGD-O2D-CED
13	5	506	CLA	CAD-CBD-CGD-O2D
13	5	507	CLA	CBD-CGD-O2D-CED
13	5	509	CLA	CAD-CBD-CGD-O1D
13	5	509	CLA	CAD-CBD-CGD-O2D
13	5	511	CLA	C1A-C2A-CAA-CBA
13	5	511	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	5	512	CLA	C1A-C2A-CAA-CBA
13	5	512	CLA	C3A-C2A-CAA-CBA
13	5	513	CLA	CBD-CGD-O2D-CED
13	5	516	CLA	C3A-C2A-CAA-CBA
13	5	516	CLA	CBD-CGD-O2D-CED
13	5	519	CLA	CHA-CBD-CGD-O1D
13	5	519	CLA	CHA-CBD-CGD-O2D
13	6	502	CLA	CHA-CBD-CGD-O1D
13	6	502	CLA	CHA-CBD-CGD-O2D
13	6	503	CLA	C11-C10-C8-C9
13	6	505	CLA	C1A-C2A-CAA-CBA
13	6	509	CLA	C1A-C2A-CAA-CBA
13	6	509	CLA	C3A-C2A-CAA-CBA
13	6	510	CLA	CHA-CBD-CGD-O1D
13	6	510	CLA	CHA-CBD-CGD-O2D
13	6	512	CLA	CHA-CBD-CGD-O1D
13	6	512	CLA	CHA-CBD-CGD-O2D
13	6	513	CLA	CBD-CGD-O2D-CED
13	6	516	CLA	C1A-C2A-CAA-CBA
13	6	516	CLA	C3A-C2A-CAA-CBA
13	2	501	CLA	CAD-CBD-CGD-O1D
13	2	501	CLA	CAD-CBD-CGD-O2D
13	2	502	CLA	CHA-CBD-CGD-O2D
13	2	505	CLA	CBD-CGD-O2D-CED
13	2	506	CLA	CHA-CBD-CGD-O2D
13	2	507	CLA	CAD-CBD-CGD-O1D
13	2	507	CLA	CAD-CBD-CGD-O2D
13	2	512	CLA	C3-C5-C6-C7
13	2	513	CLA	CBD-CGD-O2D-CED
13	2	516	CLA	C4B-C3B-CAB-CBB
13	2	516	CLA	CHA-CBD-CGD-O1D
13	2	516	CLA	CHA-CBD-CGD-O2D
13	2	517	CLA	CBD-CGD-O2D-CED
13	2	518	CLA	CBD-CGD-O2D-CED
13	1	501	CLA	CAD-CBD-CGD-O1D
13	1	501	CLA	CAD-CBD-CGD-O2D
13	1	502	CLA	CHA-CBD-CGD-O2D
13	1	502	CLA	CBD-CGD-O2D-CED
13	1	505	CLA	C1A-C2A-CAA-CBA
13	1	506	CLA	C1A-C2A-CAA-CBA
13	1	506	CLA	C3A-C2A-CAA-CBA
13	1	506	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	1	506	CLA	CAD-CBD-CGD-O2D
13	1	507	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	C1A-C2A-CAA-CBA
13	1	512	CLA	C3A-C2A-CAA-CBA
13	1	513	CLA	CBD-CGD-O2D-CED
13	1	516	CLA	CAD-CBD-CGD-O1D
13	1	516	CLA	CAD-CBD-CGD-O2D
13	1	518	CLA	C1A-C2A-CAA-CBA
13	1	518	CLA	CBD-CGD-O2D-CED
13	1	519	CLA	C3A-C2A-CAA-CBA
13	A	1022	CLA	CBD-CGD-O2D-CED
13	A	1101	CLA	CHA-CBD-CGD-O1D
13	A	1101	CLA	CHA-CBD-CGD-O2D
13	A	1102	CLA	C1A-C2A-CAA-CBA
13	A	1102	CLA	C3A-C2A-CAA-CBA
13	A	1103	CLA	CBA-CGA-O2A-C1
13	A	1103	CLA	O1A-CGA-O2A-C1
13	A	1104	CLA	C1A-C2A-CAA-CBA
13	A	1104	CLA	C6-C7-C8-C9
13	A	1106	CLA	C3A-C2A-CAA-CBA
13	A	1106	CLA	C6-C7-C8-C9
13	A	1109	CLA	CBD-CGD-O2D-CED
13	A	1112	CLA	C1A-C2A-CAA-CBA
13	A	1115	CLA	C2B-C3B-CAB-CBB
13	A	1115	CLA	C4B-C3B-CAB-CBB
13	A	1116	CLA	C1A-C2A-CAA-CBA
13	A	1116	CLA	C3A-C2A-CAA-CBA
13	A	1117	CLA	C1A-C2A-CAA-CBA
13	A	1117	CLA	C3A-C2A-CAA-CBA
13	A	1118	CLA	C3A-C2A-CAA-CBA
13	A	1119	CLA	CBD-CGD-O2D-CED
13	A	1121	CLA	CBD-CGD-O2D-CED
13	A	1126	CLA	C1A-C2A-CAA-CBA
13	A	1126	CLA	CBD-CGD-O2D-CED
13	A	1128	CLA	CHA-CBD-CGD-O1D
13	A	1128	CLA	CHA-CBD-CGD-O2D
13	A	1129	CLA	C3A-C2A-CAA-CBA
13	A	1132	CLA	C2B-C3B-CAB-CBB
13	A	1132	CLA	C4B-C3B-CAB-CBB
13	A	1132	CLA	CHA-CBD-CGD-O1D
13	A	1132	CLA	CHA-CBD-CGD-O2D
13	A	1134	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	1136	CLA	CAD-CBD-CGD-O1D
13	A	1136	CLA	CAD-CBD-CGD-O2D
13	A	1140	CLA	C4-C3-C5-C6
13	A	1801	CLA	CAD-CBD-CGD-O1D
13	A	1801	CLA	CAD-CBD-CGD-O2D
13	A	1801	CLA	CBD-CGD-O2D-CED
13	A	1011	CLA	CBD-CGD-O2D-CED
13	B	1012	CLA	CAD-CBD-CGD-O1D
13	B	1012	CLA	CAD-CBD-CGD-O2D
13	B	1021	CLA	C4B-C3B-CAB-CBB
13	B	1021	CLA	CBD-CGD-O2D-CED
13	B	1023	CLA	C2B-C3B-CAB-CBB
13	B	1023	CLA	C4B-C3B-CAB-CBB
13	B	1201	CLA	CHA-CBD-CGD-O1D
13	B	1201	CLA	CHA-CBD-CGD-O2D
13	B	1202	CLA	C3A-C2A-CAA-CBA
13	B	1203	CLA	C1A-C2A-CAA-CBA
13	B	1205	CLA	CHA-CBD-CGD-O1D
13	B	1205	CLA	CHA-CBD-CGD-O2D
13	B	1206	CLA	C1A-C2A-CAA-CBA
13	B	1206	CLA	C3A-C2A-CAA-CBA
13	B	1206	CLA	CBD-CGD-O2D-CED
13	B	1209	CLA	C1A-C2A-CAA-CBA
13	B	1209	CLA	C3A-C2A-CAA-CBA
13	B	1209	CLA	CBA-CGA-O2A-C1
13	B	1209	CLA	O1A-CGA-O2A-C1
13	B	1209	CLA	CHA-CBD-CGD-O1D
13	B	1209	CLA	CHA-CBD-CGD-O2D
13	B	1211	CLA	CHA-CBD-CGD-O1D
13	B	1211	CLA	CHA-CBD-CGD-O2D
13	B	1215	CLA	C3A-C2A-CAA-CBA
13	B	1216	CLA	C2B-C3B-CAB-CBB
13	B	1216	CLA	C4B-C3B-CAB-CBB
13	B	1217	CLA	C1A-C2A-CAA-CBA
13	B	1217	CLA	C3A-C2A-CAA-CBA
13	B	1218	CLA	C2B-C3B-CAB-CBB
13	B	1218	CLA	C4B-C3B-CAB-CBB
13	B	1222	CLA	CHA-CBD-CGD-O1D
13	B	1222	CLA	CHA-CBD-CGD-O2D
13	B	1224	CLA	C1A-C2A-CAA-CBA
13	B	1224	CLA	C3A-C2A-CAA-CBA
13	B	1225	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	B	1225	CLA	C3A-C2A-CAA-CBA
13	B	1227	CLA	C3A-C2A-CAA-CBA
13	B	1229	CLA	CAD-CBD-CGD-O1D
13	B	1229	CLA	CAD-CBD-CGD-O2D
13	B	1230	CLA	C4B-C3B-CAB-CBB
13	B	1231	CLA	C1A-C2A-CAA-CBA
13	B	1231	CLA	C3A-C2A-CAA-CBA
13	B	1232	CLA	C1A-C2A-CAA-CBA
13	B	1232	CLA	C3A-C2A-CAA-CBA
13	B	1232	CLA	C2B-C3B-CAB-CBB
13	B	1232	CLA	C4B-C3B-CAB-CBB
13	B	1238	CLA	CBD-CGD-O2D-CED
13	B	1239	CLA	CAD-CBD-CGD-O1D
13	B	1239	CLA	CAD-CBD-CGD-O2D
13	B	1207	CLA	CHA-CBD-CGD-O1D
13	B	1207	CLA	CHA-CBD-CGD-O2D
13	J	1302	CLA	CAD-CBD-CGD-O1D
13	J	1302	CLA	CAD-CBD-CGD-O2D
13	J	1302	CLA	CBD-CGD-O2D-CED
13	J	1303	CLA	C2C-C3C-C4C-CHD
13	J	1303	CLA	CAC-C3C-C4C-CHD
13	J	1303	CLA	CBD-CGD-O2D-CED
13	K	1103	CLA	C2B-C3B-CAB-CBB
13	K	1103	CLA	C4B-C3B-CAB-CBB
13	K	1401	CLA	C2B-C3B-CAB-CBB
13	K	1401	CLA	C4B-C3B-CAB-CBB
13	c	501	CLA	CAD-CBD-CGD-O2D
13	c	502	CLA	CHA-CBD-CGD-O1D
13	c	502	CLA	CHA-CBD-CGD-O2D
13	c	503	CLA	CBD-CGD-O2D-CED
13	c	506	CLA	CAD-CBD-CGD-O1D
13	c	506	CLA	CAD-CBD-CGD-O2D
13	c	507	CLA	C2B-C3B-CAB-CBB
13	c	507	CLA	C4B-C3B-CAB-CBB
13	c	507	CLA	CAD-CBD-CGD-O1D
13	c	507	CLA	CAD-CBD-CGD-O2D
13	c	512	CLA	C3A-C2A-CAA-CBA
13	c	513	CLA	C2B-C3B-CAB-CBB
13	c	513	CLA	C4B-C3B-CAB-CBB
13	c	513	CLA	CBD-CGD-O2D-CED
13	c	516	CLA	C2B-C3B-CAB-CBB
13	c	516	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	c	519	CLA	C1A-C2A-CAA-CBA
13	c	519	CLA	C3A-C2A-CAA-CBA
13	d	502	CLA	CBD-CGD-O2D-CED
13	d	503	CLA	CHA-CBD-CGD-O1D
13	d	503	CLA	CHA-CBD-CGD-O2D
13	d	503	CLA	CBD-CGD-O2D-CED
13	d	505	CLA	O1A-CGA-O2A-C1
13	d	506	CLA	C1A-C2A-CAA-CBA
13	d	506	CLA	C3A-C2A-CAA-CBA
13	d	506	CLA	C2B-C3B-CAB-CBB
13	d	506	CLA	C4B-C3B-CAB-CBB
13	d	511	CLA	CBD-CGD-O2D-CED
13	d	513	CLA	CBD-CGD-O2D-CED
13	d	516	CLA	C1A-C2A-CAA-CBA
13	d	519	CLA	CBD-CGD-O2D-CED
13	e	502	CLA	CAD-CBD-CGD-O1D
13	e	502	CLA	CAD-CBD-CGD-O2D
13	e	504	CLA	C1A-C2A-CAA-CBA
13	e	504	CLA	C2-C1-O2A-CGA
13	e	504	CLA	C4B-C3B-CAB-CBB
13	e	506	CLA	C1A-C2A-CAA-CBA
13	e	507	CLA	CAD-CBD-CGD-O2D
13	e	509	CLA	C1A-C2A-CAA-CBA
13	e	509	CLA	C3A-C2A-CAA-CBA
13	e	509	CLA	CBD-CGD-O2D-CED
13	e	513	CLA	CBD-CGD-O2D-CED
13	e	517	CLA	CBD-CGD-O2D-CED
13	e	518	CLA	CHA-CBD-CGD-O1D
13	e	518	CLA	CHA-CBD-CGD-O2D
13	e	519	CLA	C1A-C2A-CAA-CBA
13	e	519	CLA	C3A-C2A-CAA-CBA
13	e	519	CLA	CHA-CBD-CGD-O1D
13	e	519	CLA	CHA-CBD-CGD-O2D
13	f	502	CLA	CHA-CBD-CGD-O1D
13	f	502	CLA	CHA-CBD-CGD-O2D
13	f	502	CLA	CBD-CGD-O2D-CED
13	f	503	CLA	CBD-CGD-O2D-CED
13	f	504	CLA	C4B-C3B-CAB-CBB
13	f	505	CLA	CBA-CGA-O2A-C1
13	f	505	CLA	O1A-CGA-O2A-C1
13	f	512	CLA	C1A-C2A-CAA-CBA
13	f	513	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	f	516	CLA	CHA-CBD-CGD-O1D
13	f	516	CLA	CHA-CBD-CGD-O2D
13	f	517	CLA	CAD-CBD-CGD-O1D
13	f	517	CLA	CAD-CBD-CGD-O2D
13	f	519	CLA	C1A-C2A-CAA-CBA
13	g	502	CLA	CAD-CBD-CGD-O1D
13	g	502	CLA	CAD-CBD-CGD-O2D
13	g	502	CLA	CBD-CGD-O2D-CED
13	g	505	CLA	CBA-CGA-O2A-C1
13	g	505	CLA	O1A-CGA-O2A-C1
13	g	505	CLA	C4-C3-C5-C6
13	g	506	CLA	CAD-CBD-CGD-O1D
13	g	506	CLA	CAD-CBD-CGD-O2D
13	g	506	CLA	CBD-CGD-O2D-CED
13	g	507	CLA	CAD-CBD-CGD-O1D
13	g	507	CLA	CAD-CBD-CGD-O2D
13	g	510	CLA	CBD-CGD-O2D-CED
13	g	513	CLA	CBD-CGD-O2D-CED
13	g	513	CLA	O1D-CGD-O2D-CED
13	g	516	CLA	CAD-CBD-CGD-O1D
13	g	516	CLA	CAD-CBD-CGD-O2D
13	g	517	CLA	CHA-CBD-CGD-O2D
13	g	518	CLA	C2-C3-C5-C6
13	g	518	CLA	C4-C3-C5-C6
13	g	519	CLA	CBD-CGD-O2D-CED
13	b	503	CLA	C2-C3-C5-C6
13	b	503	CLA	C4-C3-C5-C6
13	b	504	CLA	C2B-C3B-CAB-CBB
13	b	504	CLA	C4B-C3B-CAB-CBB
13	b	505	CLA	CBD-CGD-O2D-CED
13	b	509	CLA	CBD-CGD-O2D-CED
13	b	512	CLA	C1A-C2A-CAA-CBA
13	b	512	CLA	C3A-C2A-CAA-CBA
13	b	513	CLA	CBD-CGD-O2D-CED
13	b	516	CLA	C1A-C2A-CAA-CBA
13	b	516	CLA	C3A-C2A-CAA-CBA
13	b	519	CLA	CBD-CGD-O2D-CED
13	a	502	CLA	CBD-CGD-O2D-CED
13	a	502	CLA	C6-C7-C8-C9
13	a	509	CLA	CBD-CGD-O2D-CED
13	a	510	CLA	CBD-CGD-O2D-CED
13	a	511	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	511	CLA	O1D-CGD-O2D-CED
13	a	512	CLA	C1A-C2A-CAA-CBA
13	a	512	CLA	C3A-C2A-CAA-CBA
13	a	512	CLA	C3-C5-C6-C7
13	a	513	CLA	C2B-C3B-CAB-CBB
13	a	513	CLA	C4B-C3B-CAB-CBB
13	a	513	CLA	CBD-CGD-O2D-CED
13	a	516	CLA	C1A-C2A-CAA-CBA
13	a	516	CLA	C3A-C2A-CAA-CBA
13	a	516	CLA	CAD-CBD-CGD-O1D
13	a	516	CLA	CAD-CBD-CGD-O2D
14	3	523	BCR	C21-C22-C23-C24
14	4	521	BCR	C7-C8-C9-C10
14	4	521	BCR	C7-C8-C9-C34
14	4	523	BCR	C7-C8-C9-C10
14	5	521	BCR	C7-C8-C9-C10
14	5	521	BCR	C7-C8-C9-C34
14	5	523	BCR	C7-C8-C9-C10
14	5	523	BCR	C7-C8-C9-C34
14	5	523	BCR	C11-C12-C13-C14
14	5	523	BCR	C17-C18-C19-C20
14	5	523	BCR	C36-C18-C19-C20
14	5	523	BCR	C21-C22-C23-C24
14	5	523	BCR	C37-C22-C23-C24
14	5	522	BCR	C7-C8-C9-C10
14	5	522	BCR	C7-C8-C9-C34
14	6	524	BCR	C15-C16-C17-C18
14	6	522	BCR	C5-C6-C7-C8
14	2	521	BCR	C7-C8-C9-C10
14	2	522	BCR	C7-C8-C9-C10
14	2	522	BCR	C7-C8-C9-C34
14	2	523	BCR	C7-C8-C9-C10
14	1	521	BCR	C7-C8-C9-C10
14	1	521	BCR	C7-C8-C9-C34
14	1	522	BCR	C5-C6-C7-C8
14	1	522	BCR	C7-C8-C9-C10
14	1	522	BCR	C7-C8-C9-C34
14	A	4002	BCR	C21-C22-C23-C24
14	A	4002	BCR	C37-C22-C23-C24
14	A	4003	BCR	C7-C8-C9-C34
14	A	4007	BCR	C21-C22-C23-C24
14	A	4008	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
14	A	4008	BCR	C37-C22-C23-C24
14	A	4011	BCR	C21-C22-C23-C24
14	A	4011	BCR	C37-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C10
14	B	4006	BCR	C7-C8-C9-C10
14	B	4009	BCR	C17-C18-C19-C20
14	B	4009	BCR	C21-C22-C23-C24
14	B	4017	BCR	C21-C22-C23-C24
14	B	4017	BCR	C37-C22-C23-C24
14	F	4014	BCR	C7-C8-C9-C10
14	F	4014	BCR	C17-C18-C19-C20
14	F	4014	BCR	C37-C22-C23-C24
14	I	4018	BCR	C7-C8-C9-C10
14	I	4018	BCR	C7-C8-C9-C34
14	I	4018	BCR	C21-C22-C23-C24
14	I	4018	BCR	C37-C22-C23-C24
14	I	4018	BCR	C23-C24-C25-C26
14	I	4018	BCR	C23-C24-C25-C30
14	I	4019	BCR	C21-C22-C23-C24
14	I	4019	BCR	C37-C22-C23-C24
14	c	524	BCR	C17-C18-C19-C20
14	c	524	BCR	C36-C18-C19-C20
14	d	522	BCR	C7-C8-C9-C10
14	d	522	BCR	C7-C8-C9-C34
14	d	523	BCR	C7-C8-C9-C10
14	d	523	BCR	C7-C8-C9-C34
14	d	524	BCR	C17-C18-C19-C20
14	d	524	BCR	C36-C18-C19-C20
14	e	522	BCR	C7-C8-C9-C10
14	e	522	BCR	C7-C8-C9-C34
14	e	524	BCR	C17-C18-C19-C20
14	e	524	BCR	C36-C18-C19-C20
14	f	522	BCR	C7-C8-C9-C10
14	f	522	BCR	C7-C8-C9-C34
14	f	523	BCR	C7-C8-C9-C10
14	f	523	BCR	C7-C8-C9-C34
14	g	522	BCR	C7-C8-C9-C10
14	b	523	BCR	C9-C10-C11-C12
14	b	521	BCR	C7-C8-C9-C10
14	b	522	BCR	C5-C6-C7-C8
14	b	522	BCR	C7-C8-C9-C10
14	b	522	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
14	b	524	BCR	C17-C18-C19-C20
14	b	524	BCR	C36-C18-C19-C20
14	b	524	BCR	C21-C22-C23-C24
14	a	523	BCR	C7-C8-C9-C10
14	a	524	BCR	C7-C8-C9-C10
14	a	524	BCR	C7-C8-C9-C34
15	5	822	SQD	O49-C7-O47-C45
15	5	822	SQD	C8-C7-O47-C45
15	B	1852	SQD	C5-C6-S-O7
15	B	1852	SQD	C5-C6-S-O8
15	B	1852	SQD	C5-C6-S-O9
15	d	822	SQD	C5-C6-S-O7
15	d	822	SQD	C5-C6-S-O8
15	d	822	SQD	C5-C6-S-O9
15	g	822	SQD	C8-C7-O47-C45
17	A	5005	LHG	C3-O3-P-O5
17	A	5004	LHG	C8-C7-O7-C5
17	A	5001	LHG	C1-C2-C3-O3
17	A	5002	LHG	C3-O3-P-O4
17	A	5002	LHG	C3-O3-P-O5
17	A	5002	LHG	C3-O3-P-O6
17	A	5002	LHG	C4-O6-P-O3
17	A	5002	LHG	C4-O6-P-O4
17	A	5003	LHG	C3-O3-P-O6
17	A	5003	LHG	C4-O6-P-O4
20	A	1848	LMU	O5'-C1'-O1'-C1
20	B	1843	LMU	C2'-C1'-O1'-C1
20	B	1843	LMU	O5'-C1'-O1'-C1
20	B	1843	LMU	C2-C1-O1'-C1'
13	3	513	CLA	O1D-CGD-O2D-CED
13	5	513	CLA	O1D-CGD-O2D-CED
13	6	502	CLA	O1D-CGD-O2D-CED
13	6	506	CLA	O1D-CGD-O2D-CED
13	6	513	CLA	O1D-CGD-O2D-CED
13	2	511	CLA	O1D-CGD-O2D-CED
13	2	513	CLA	O1D-CGD-O2D-CED
13	1	511	CLA	O1D-CGD-O2D-CED
13	1	513	CLA	O1D-CGD-O2D-CED
13	A	1011	CLA	O1D-CGD-O2D-CED
13	c	511	CLA	O1D-CGD-O2D-CED
13	c	513	CLA	O1D-CGD-O2D-CED
13	e	502	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	e	503	CLA	O1D-CGD-O2D-CED
13	e	506	CLA	O1D-CGD-O2D-CED
13	b	502	CLA	O1D-CGD-O2D-CED
13	b	505	CLA	O1D-CGD-O2D-CED
13	b	513	CLA	O1D-CGD-O2D-CED
13	3	503	CLA	O1D-CGD-O2D-CED
13	4	511	CLA	O1D-CGD-O2D-CED
13	5	504	CLA	O1D-CGD-O2D-CED
13	5	506	CLA	O1D-CGD-O2D-CED
13	2	506	CLA	O1D-CGD-O2D-CED
13	1	503	CLA	O1D-CGD-O2D-CED
13	1	506	CLA	O1D-CGD-O2D-CED
13	A	1121	CLA	O1D-CGD-O2D-CED
13	B	1211	CLA	O1D-CGD-O2D-CED
13	c	510	CLA	O1D-CGD-O2D-CED
13	d	502	CLA	O1D-CGD-O2D-CED
13	d	503	CLA	O1D-CGD-O2D-CED
13	d	513	CLA	O1D-CGD-O2D-CED
13	d	519	CLA	O1D-CGD-O2D-CED
13	e	513	CLA	O1D-CGD-O2D-CED
13	f	513	CLA	O1D-CGD-O2D-CED
13	g	506	CLA	O1D-CGD-O2D-CED
13	b	509	CLA	O1D-CGD-O2D-CED
13	b	517	CLA	O1D-CGD-O2D-CED
13	a	502	CLA	O1D-CGD-O2D-CED
13	a	513	CLA	O1D-CGD-O2D-CED
13	3	502	CLA	CBD-CGD-O2D-CED
13	3	503	CLA	CBD-CGD-O2D-CED
13	3	506	CLA	CBD-CGD-O2D-CED
13	3	508	CLA	CBD-CGD-O2D-CED
13	3	509	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	CBD-CGD-O2D-CED
13	4	507	CLA	CBD-CGD-O2D-CED
13	4	510	CLA	CBD-CGD-O2D-CED
13	4	511	CLA	CBD-CGD-O2D-CED
13	5	502	CLA	CBD-CGD-O2D-CED
13	5	503	CLA	CBD-CGD-O2D-CED
13	5	505	CLA	CBD-CGD-O2D-CED
13	5	506	CLA	CBD-CGD-O2D-CED
13	6	501	CLA	CBD-CGD-O2D-CED
13	6	502	CLA	CBD-CGD-O2D-CED
13	6	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	6	506	CLA	CBD-CGD-O2D-CED
13	6	509	CLA	CBD-CGD-O2D-CED
13	6	511	CLA	CBD-CGD-O2D-CED
13	6	518	CLA	CBD-CGD-O2D-CED
13	6	519	CLA	CBD-CGD-O2D-CED
13	2	503	CLA	CBD-CGD-O2D-CED
13	2	506	CLA	CBD-CGD-O2D-CED
13	2	507	CLA	CBD-CGD-O2D-CED
13	2	511	CLA	CBD-CGD-O2D-CED
13	2	512	CLA	CBD-CGD-O2D-CED
13	1	503	CLA	CBD-CGD-O2D-CED
13	1	505	CLA	CBD-CGD-O2D-CED
13	1	506	CLA	CBD-CGD-O2D-CED
13	1	510	CLA	CBD-CGD-O2D-CED
13	1	511	CLA	CBD-CGD-O2D-CED
13	A	1108	CLA	CBD-CGD-O2D-CED
13	A	1112	CLA	CBD-CGD-O2D-CED
13	A	1113	CLA	CBD-CGD-O2D-CED
13	A	1131	CLA	CBD-CGD-O2D-CED
13	A	1139	CLA	CBD-CGD-O2D-CED
13	B	1211	CLA	CBD-CGD-O2D-CED
13	B	1216	CLA	CBD-CGD-O2D-CED
13	B	1219	CLA	CBD-CGD-O2D-CED
13	B	1221	CLA	CBD-CGD-O2D-CED
13	B	1231	CLA	CBD-CGD-O2D-CED
13	B	1232	CLA	CBD-CGD-O2D-CED
13	c	502	CLA	CBD-CGD-O2D-CED
13	c	504	CLA	CBD-CGD-O2D-CED
13	c	506	CLA	CBD-CGD-O2D-CED
13	c	509	CLA	CBD-CGD-O2D-CED
13	c	510	CLA	CBD-CGD-O2D-CED
13	c	511	CLA	CBD-CGD-O2D-CED
13	c	517	CLA	CBD-CGD-O2D-CED
13	d	506	CLA	CBD-CGD-O2D-CED
13	d	517	CLA	CBD-CGD-O2D-CED
13	e	501	CLA	CBD-CGD-O2D-CED
13	e	502	CLA	CBD-CGD-O2D-CED
13	e	503	CLA	CBD-CGD-O2D-CED
13	e	506	CLA	CBD-CGD-O2D-CED
13	e	511	CLA	CBD-CGD-O2D-CED
13	f	501	CLA	CBD-CGD-O2D-CED
13	f	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	f	506	CLA	CBD-CGD-O2D-CED
13	f	507	CLA	CBD-CGD-O2D-CED
13	f	509	CLA	CBD-CGD-O2D-CED
13	f	510	CLA	CBD-CGD-O2D-CED
13	f	518	CLA	CBD-CGD-O2D-CED
13	f	519	CLA	CBD-CGD-O2D-CED
13	g	503	CLA	CBD-CGD-O2D-CED
13	g	504	CLA	CBD-CGD-O2D-CED
13	g	505	CLA	CBD-CGD-O2D-CED
13	g	511	CLA	CBD-CGD-O2D-CED
13	g	512	CLA	CBD-CGD-O2D-CED
13	b	501	CLA	CBD-CGD-O2D-CED
13	b	502	CLA	CBD-CGD-O2D-CED
13	b	503	CLA	CBD-CGD-O2D-CED
13	b	506	CLA	CBD-CGD-O2D-CED
13	b	508	CLA	CBD-CGD-O2D-CED
13	b	517	CLA	CBD-CGD-O2D-CED
13	b	518	CLA	CBD-CGD-O2D-CED
13	a	505	CLA	CBD-CGD-O2D-CED
13	a	506	CLA	CBD-CGD-O2D-CED
13	a	517	CLA	CBD-CGD-O2D-CED
13	a	519	CLA	CBD-CGD-O2D-CED
13	5	505	CLA	O1A-CGA-O2A-C1
13	2	509	CLA	O1A-CGA-O2A-C1
13	1	511	CLA	O1A-CGA-O2A-C1
13	A	1013	CLA	O1A-CGA-O2A-C1
13	c	505	CLA	O1A-CGA-O2A-C1
13	e	505	CLA	O1A-CGA-O2A-C1
13	A	1109	CLA	O1D-CGD-O2D-CED
13	B	1021	CLA	O1D-CGD-O2D-CED
13	B	1206	CLA	O1D-CGD-O2D-CED
13	4	510	CLA	O1D-CGD-O2D-CED
13	5	502	CLA	O1D-CGD-O2D-CED
13	6	503	CLA	O1D-CGD-O2D-CED
13	6	511	CLA	O1D-CGD-O2D-CED
13	A	1139	CLA	O1D-CGD-O2D-CED
13	c	506	CLA	O1D-CGD-O2D-CED
13	d	506	CLA	O1D-CGD-O2D-CED
13	d	517	CLA	O1D-CGD-O2D-CED
13	f	506	CLA	O1D-CGD-O2D-CED
13	f	518	CLA	O1D-CGD-O2D-CED
13	g	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	b	501	CLA	O1D-CGD-O2D-CED
13	b	503	CLA	O1D-CGD-O2D-CED
13	a	506	CLA	O1D-CGD-O2D-CED
13	3	510	CLA	CBA-CGA-O2A-C1
13	5	505	CLA	CBA-CGA-O2A-C1
13	c	505	CLA	CBA-CGA-O2A-C1
13	e	505	CLA	CBA-CGA-O2A-C1
13	2	510	CLA	CBD-CGD-O2D-CED
13	A	1111	CLA	CBD-CGD-O2D-CED
13	B	1209	CLA	CBD-CGD-O2D-CED
13	d	501	CLA	CBD-CGD-O2D-CED
13	d	505	CLA	CBD-CGD-O2D-CED
13	3	510	CLA	O1A-CGA-O2A-C1
13	4	505	CLA	O1A-CGA-O2A-C1
13	5	504	CLA	O1A-CGA-O2A-C1
13	5	510	CLA	O1A-CGA-O2A-C1
13	2	505	CLA	O1A-CGA-O2A-C1
13	1	505	CLA	O1A-CGA-O2A-C1
13	A	1113	CLA	O1A-CGA-O2A-C1
13	A	1118	CLA	O1A-CGA-O2A-C1
13	B	1217	CLA	O1A-CGA-O2A-C1
13	B	1219	CLA	O1A-CGA-O2A-C1
13	B	1231	CLA	O1A-CGA-O2A-C1
13	K	1401	CLA	O1A-CGA-O2A-C1
13	d	511	CLA	O1A-CGA-O2A-C1
13	f	507	CLA	O1A-CGA-O2A-C1
13	g	501	CLA	O1A-CGA-O2A-C1
13	g	511	CLA	O1A-CGA-O2A-C1
13	b	505	CLA	O1A-CGA-O2A-C1
20	A	1848	LMU	C4'-C5'-C6'-O6'
13	3	506	CLA	O1D-CGD-O2D-CED
13	4	501	CLA	O1D-CGD-O2D-CED
13	6	509	CLA	O1D-CGD-O2D-CED
13	A	1022	CLA	O1D-CGD-O2D-CED
13	A	1108	CLA	O1D-CGD-O2D-CED
13	J	1303	CLA	O1D-CGD-O2D-CED
13	e	509	CLA	O1D-CGD-O2D-CED
13	f	501	CLA	O1D-CGD-O2D-CED
13	f	502	CLA	O1D-CGD-O2D-CED
13	f	503	CLA	O1D-CGD-O2D-CED
13	b	518	CLA	O1D-CGD-O2D-CED
13	b	519	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	a	519	CLA	O1D-CGD-O2D-CED
13	4	503	CLA	O1D-CGD-O2D-CED
13	4	506	CLA	O1D-CGD-O2D-CED
13	5	507	CLA	O1D-CGD-O2D-CED
13	2	517	CLA	O1D-CGD-O2D-CED
13	2	518	CLA	O1D-CGD-O2D-CED
13	1	502	CLA	O1D-CGD-O2D-CED
13	1	507	CLA	O1D-CGD-O2D-CED
13	1	518	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	O1D-CGD-O2D-CED
13	B	1238	CLA	O1D-CGD-O2D-CED
13	J	1302	CLA	O1D-CGD-O2D-CED
13	c	503	CLA	O1D-CGD-O2D-CED
13	d	511	CLA	O1D-CGD-O2D-CED
13	e	517	CLA	O1D-CGD-O2D-CED
13	g	502	CLA	O1D-CGD-O2D-CED
13	g	510	CLA	O1D-CGD-O2D-CED
13	g	519	CLA	O1D-CGD-O2D-CED
13	a	509	CLA	O1D-CGD-O2D-CED
13	a	510	CLA	O1D-CGD-O2D-CED
13	2	509	CLA	CBD-CGD-O2D-CED
13	a	503	CLA	CBD-CGD-O2D-CED
15	g	822	SQD	O49-C7-O47-C45
13	3	507	CLA	C3-C5-C6-C7
13	3	510	CLA	C3-C5-C6-C7
13	4	501	CLA	C3-C5-C6-C7
13	4	510	CLA	C3-C5-C6-C7
13	5	511	CLA	C3-C5-C6-C7
13	2	505	CLA	C3-C5-C6-C7
13	1	501	CLA	C3-C5-C6-C7
13	1	504	CLA	C3-C5-C6-C7
13	A	1103	CLA	C3-C5-C6-C7
13	A	1138	CLA	C3-C5-C6-C7
13	A	1140	CLA	C3-C5-C6-C7
13	A	1011	CLA	C3-C5-C6-C7
13	B	1012	CLA	C3-C5-C6-C7
13	B	1202	CLA	C3-C5-C6-C7
13	B	1203	CLA	C3-C5-C6-C7
13	B	1221	CLA	C3-C5-C6-C7
13	B	1231	CLA	C3-C5-C6-C7
13	B	1235	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	B	1207	CLA	C3-C5-C6-C7
13	c	503	CLA	C3-C5-C6-C7
13	d	502	CLA	C3-C5-C6-C7
13	d	505	CLA	C3-C5-C6-C7
13	e	502	CLA	C3-C5-C6-C7
13	e	503	CLA	C3-C5-C6-C7
13	e	509	CLA	C3-C5-C6-C7
13	f	502	CLA	C3-C5-C6-C7
13	f	505	CLA	C3-C5-C6-C7
13	g	505	CLA	C3-C5-C6-C7
13	b	505	CLA	C3-C5-C6-C7
13	a	505	CLA	C3-C5-C6-C7
13	2	505	CLA	O1D-CGD-O2D-CED
13	4	505	CLA	CBA-CGA-O2A-C1
13	5	504	CLA	CBA-CGA-O2A-C1
13	5	510	CLA	CBA-CGA-O2A-C1
13	2	505	CLA	CBA-CGA-O2A-C1
13	2	509	CLA	CBA-CGA-O2A-C1
13	1	505	CLA	CBA-CGA-O2A-C1
13	1	511	CLA	CBA-CGA-O2A-C1
13	A	1013	CLA	CBA-CGA-O2A-C1
13	A	1113	CLA	CBA-CGA-O2A-C1
13	A	1121	CLA	CBA-CGA-O2A-C1
13	B	1213	CLA	CBA-CGA-O2A-C1
13	B	1219	CLA	CBA-CGA-O2A-C1
13	B	1231	CLA	CBA-CGA-O2A-C1
13	K	1401	CLA	CBA-CGA-O2A-C1
13	d	505	CLA	CBA-CGA-O2A-C1
13	f	507	CLA	CBA-CGA-O2A-C1
13	g	501	CLA	CBA-CGA-O2A-C1
13	g	511	CLA	CBA-CGA-O2A-C1
13	b	505	CLA	CBA-CGA-O2A-C1
13	b	513	CLA	CBA-CGA-O2A-C1
13	4	502	CLA	CBD-CGD-O2D-CED
13	4	519	CLA	CBD-CGD-O2D-CED
13	5	501	CLA	CBD-CGD-O2D-CED
13	5	508	CLA	CBD-CGD-O2D-CED
13	6	508	CLA	CBD-CGD-O2D-CED
13	6	517	CLA	CBD-CGD-O2D-CED
13	A	1115	CLA	CBD-CGD-O2D-CED
13	A	1118	CLA	CBD-CGD-O2D-CED
13	A	1120	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	A	1132	CLA	CBD-CGD-O2D-CED
13	A	1138	CLA	CBD-CGD-O2D-CED
13	B	1203	CLA	CBD-CGD-O2D-CED
13	B	1212	CLA	CBD-CGD-O2D-CED
13	B	1214	CLA	CBD-CGD-O2D-CED
13	B	1215	CLA	CBD-CGD-O2D-CED
13	B	1218	CLA	CBD-CGD-O2D-CED
13	B	1226	CLA	CBD-CGD-O2D-CED
13	B	1228	CLA	CBD-CGD-O2D-CED
13	B	1230	CLA	CBD-CGD-O2D-CED
13	B	1239	CLA	CBD-CGD-O2D-CED
13	c	501	CLA	CBD-CGD-O2D-CED
13	d	504	CLA	CBD-CGD-O2D-CED
13	e	519	CLA	CBD-CGD-O2D-CED
13	b	511	CLA	CBD-CGD-O2D-CED
13	b	512	CLA	CBD-CGD-O2D-CED
13	3	508	CLA	O1D-CGD-O2D-CED
13	5	503	CLA	O1D-CGD-O2D-CED
13	5	516	CLA	O1D-CGD-O2D-CED
13	c	504	CLA	O1D-CGD-O2D-CED
13	f	510	CLA	O1D-CGD-O2D-CED
13	a	517	CLA	O1D-CGD-O2D-CED
13	A	1801	CLA	O1D-CGD-O2D-CED
13	3	510	CLA	C4-C3-C5-C6
13	4	510	CLA	C4-C3-C5-C6
13	5	503	CLA	C4-C3-C5-C6
13	6	510	CLA	C4-C3-C5-C6
13	2	518	CLA	C4-C3-C5-C6
13	A	1115	CLA	C4-C3-C5-C6
13	B	1230	CLA	C4-C3-C5-C6
13	d	503	CLA	C4-C3-C5-C6
13	e	505	CLA	C4-C3-C5-C6
13	e	518	CLA	C4-C3-C5-C6
13	f	502	CLA	C4-C3-C5-C6
13	f	510	CLA	C4-C3-C5-C6
13	g	503	CLA	C4-C3-C5-C6
13	3	510	CLA	C2-C3-C5-C6
13	4	510	CLA	C2-C3-C5-C6
13	5	503	CLA	C2-C3-C5-C6
13	6	510	CLA	C2-C3-C5-C6
13	2	518	CLA	C2-C3-C5-C6
13	A	1140	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	f	510	CLA	C2-C3-C5-C6
13	g	503	CLA	C2-C3-C5-C6
13	g	505	CLA	C2-C3-C5-C6
13	6	516	CLA	CBD-CGD-O2D-CED
13	3	502	CLA	O1D-CGD-O2D-CED
13	1	505	CLA	O1D-CGD-O2D-CED
13	B	1232	CLA	O1D-CGD-O2D-CED
13	f	507	CLA	O1D-CGD-O2D-CED
13	g	512	CLA	O1D-CGD-O2D-CED
13	f	505	CLA	C2A-CAA-CBA-CGA
13	g	505	CLA	C2A-CAA-CBA-CGA
13	g	516	CLA	C2A-CAA-CBA-CGA
13	b	512	CLA	C3-C5-C6-C7
13	a	516	CLA	C2A-CAA-CBA-CGA
13	5	507	CLA	O1A-CGA-O2A-C1
13	3	518	CLA	C3-C5-C6-C7
13	4	518	CLA	C3-C5-C6-C7
13	5	503	CLA	C3-C5-C6-C7
13	6	501	CLA	C3-C5-C6-C7
13	A	1115	CLA	C3-C5-C6-C7
13	A	1133	CLA	C3-C5-C6-C7
13	B	1213	CLA	C3-C5-C6-C7
13	c	505	CLA	C3-C5-C6-C7
13	d	518	CLA	C3-C5-C6-C7
13	e	510	CLA	C3-C5-C6-C7
13	a	504	CLA	C3-C5-C6-C7
13	a	508	CLA	C3-C5-C6-C7
13	B	1023	CLA	C2C-C3C-CAC-CBC
13	1	504	CLA	CBA-CGA-O2A-C1
13	A	1117	CLA	CBA-CGA-O2A-C1
13	A	1118	CLA	CBA-CGA-O2A-C1
13	A	1127	CLA	CBA-CGA-O2A-C1
13	A	1130	CLA	CBA-CGA-O2A-C1
13	B	1021	CLA	CBA-CGA-O2A-C1
13	B	1214	CLA	CBA-CGA-O2A-C1
13	B	1217	CLA	CBA-CGA-O2A-C1
13	d	511	CLA	CBA-CGA-O2A-C1
13	e	504	CLA	CBA-CGA-O2A-C1
13	b	504	CLA	CBA-CGA-O2A-C1
13	a	502	CLA	CBA-CGA-O2A-C1
13	a	513	CLA	CBA-CGA-O2A-C1
14	4	524	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
14	2	524	BCR	C15-C16-C17-C18
13	3	501	CLA	O1A-CGA-O2A-C1
13	A	1119	CLA	O1A-CGA-O2A-C1
13	A	1121	CLA	O1A-CGA-O2A-C1
13	B	1021	CLA	O1A-CGA-O2A-C1
13	B	1213	CLA	O1A-CGA-O2A-C1
13	B	1214	CLA	O1A-CGA-O2A-C1
13	c	504	CLA	O1A-CGA-O2A-C1
13	e	504	CLA	O1A-CGA-O2A-C1
13	f	504	CLA	O1A-CGA-O2A-C1
13	b	513	CLA	O1A-CGA-O2A-C1
17	A	5004	LHG	O9-C7-O7-C5
13	A	1113	CLA	O1D-CGD-O2D-CED
13	B	1231	CLA	O1D-CGD-O2D-CED
13	f	504	CLA	O1D-CGD-O2D-CED
20	A	1848	LMU	O5'-C5'-C6'-O6'
13	3	518	CLA	O1D-CGD-O2D-CED
13	c	509	CLA	O1D-CGD-O2D-CED
13	4	505	CLA	C3-C5-C6-C7
13	5	510	CLA	C3-C5-C6-C7
13	2	518	CLA	C3-C5-C6-C7
13	e	518	CLA	C3-C5-C6-C7
13	f	503	CLA	C3-C5-C6-C7
13	b	503	CLA	C3-C5-C6-C7
13	5	509	CLA	CBD-CGD-O2D-CED
13	5	519	CLA	CBD-CGD-O2D-CED
13	1	512	CLA	CBD-CGD-O2D-CED
13	c	508	CLA	CBD-CGD-O2D-CED
13	g	509	CLA	CBD-CGD-O2D-CED
13	b	504	CLA	CBD-CGD-O2D-CED
13	a	504	CLA	CBD-CGD-O2D-CED
17	A	5005	LHG	O2-C2-C3-O3
17	A	5001	LHG	O2-C2-C3-O3
13	4	507	CLA	O1D-CGD-O2D-CED
13	5	505	CLA	O1D-CGD-O2D-CED
13	6	518	CLA	O1D-CGD-O2D-CED
13	6	519	CLA	O1D-CGD-O2D-CED
13	2	512	CLA	O1D-CGD-O2D-CED
13	c	502	CLA	O1D-CGD-O2D-CED
13	e	501	CLA	O1D-CGD-O2D-CED
13	g	511	CLA	O1D-CGD-O2D-CED
13	b	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	3	501	CLA	CBA-CGA-O2A-C1
13	2	502	CLA	CBA-CGA-O2A-C1
13	A	1136	CLA	CBA-CGA-O2A-C1
13	B	1215	CLA	CBA-CGA-O2A-C1
13	B	1228	CLA	CBA-CGA-O2A-C1
13	c	504	CLA	CBA-CGA-O2A-C1
13	g	502	CLA	CBA-CGA-O2A-C1
13	a	505	CLA	CBA-CGA-O2A-C1
20	B	1843	LMU	O5B-C5B-C6B-O6B
13	A	1130	CLA	O1A-CGA-O2A-C1
13	6	501	CLA	O1D-CGD-O2D-CED
13	g	504	CLA	O1D-CGD-O2D-CED
20	B	1843	LMU	C4'-C5'-C6'-O6'
13	3	504	CLA	CBD-CGD-O2D-CED
13	2	519	CLA	CBD-CGD-O2D-CED
13	e	504	CLA	CBD-CGD-O2D-CED
13	f	516	CLA	CBD-CGD-O2D-CED
15	6	822	SQD	C8-C7-O47-C45
17	A	5002	LHG	C8-C7-O7-C5
13	B	1216	CLA	O1D-CGD-O2D-CED
13	A	1117	CLA	O1A-CGA-O2A-C1
13	A	1136	CLA	O1A-CGA-O2A-C1
13	3	509	CLA	O1D-CGD-O2D-CED
13	2	503	CLA	O1D-CGD-O2D-CED
13	b	502	CLA	C3-C5-C6-C7
13	6	512	CLA	CBD-CGD-O2D-CED
13	1	501	CLA	CBD-CGD-O2D-CED
13	1	519	CLA	CBD-CGD-O2D-CED
13	A	1128	CLA	CBD-CGD-O2D-CED
13	c	516	CLA	CBD-CGD-O2D-CED
20	B	1843	LMU	C4B-C5B-C6B-O6B
13	1	510	CLA	O1D-CGD-O2D-CED
13	A	1131	CLA	O1D-CGD-O2D-CED
13	B	1219	CLA	O1D-CGD-O2D-CED
13	B	1221	CLA	O1D-CGD-O2D-CED
13	f	509	CLA	O1D-CGD-O2D-CED
13	b	508	CLA	O1D-CGD-O2D-CED
13	5	507	CLA	CBA-CGA-O2A-C1
13	A	1119	CLA	CBA-CGA-O2A-C1
13	f	504	CLA	CBA-CGA-O2A-C1
13	3	518	CLA	C4-C3-C5-C6
13	1	504	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	1	505	CLA	C4-C3-C5-C6
13	A	1118	CLA	C4-C3-C5-C6
13	A	1139	CLA	C4-C3-C5-C6
13	c	518	CLA	C4-C3-C5-C6
13	d	505	CLA	C4-C3-C5-C6
13	e	503	CLA	C4-C3-C5-C6
13	f	511	CLA	C4-C3-C5-C6
13	1	504	CLA	C2-C3-C5-C6
13	1	505	CLA	C2-C3-C5-C6
13	A	1115	CLA	C2-C3-C5-C6
13	A	1118	CLA	C2-C3-C5-C6
13	A	1122	CLA	C2-C3-C5-C6
13	A	1139	CLA	C2-C3-C5-C6
13	c	518	CLA	C2-C3-C5-C6
13	d	503	CLA	C2-C3-C5-C6
13	d	505	CLA	C2-C3-C5-C6
13	e	505	CLA	C2-C3-C5-C6
13	e	518	CLA	C2-C3-C5-C6
13	f	502	CLA	C2-C3-C5-C6
13	f	511	CLA	C2-C3-C5-C6
13	2	502	CLA	O1A-CGA-O2A-C1
13	1	504	CLA	O1A-CGA-O2A-C1
13	A	1127	CLA	O1A-CGA-O2A-C1
13	B	1215	CLA	O1A-CGA-O2A-C1
13	b	504	CLA	O1A-CGA-O2A-C1
13	a	502	CLA	O1A-CGA-O2A-C1
13	a	513	CLA	O1A-CGA-O2A-C1
15	6	822	SQD	O49-C7-O47-C45
16	J	5104	LMG	O6-C5-C6-O5
13	A	1112	CLA	O1D-CGD-O2D-CED
13	3	511	CLA	CBD-CGD-O2D-CED
13	1	505	CLA	C2A-CAA-CBA-CGA
13	B	1238	CLA	C2A-CAA-CBA-CGA
13	e	505	CLA	C2A-CAA-CBA-CGA
13	2	507	CLA	O1D-CGD-O2D-CED
13	2	510	CLA	O1D-CGD-O2D-CED
13	c	517	CLA	O1D-CGD-O2D-CED
13	d	501	CLA	O1D-CGD-O2D-CED
13	e	511	CLA	O1D-CGD-O2D-CED
13	a	505	CLA	O1A-CGA-O2A-C1
13	B	1218	CLA	C3-C5-C6-C7
20	A	1849	LMU	O5'-C1'-O1'-C1

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Mol	Chain	Res	Type	Atoms
20	J	5105	LMU	O5'-C5'-C6'-O6'
13	f	519	CLA	O1D-CGD-O2D-CED
13	g	505	CLA	O1D-CGD-O2D-CED
13	a	505	CLA	O1D-CGD-O2D-CED
13	6	502	CLA	CBA-CGA-O2A-C1
13	A	1109	CLA	CBA-CGA-O2A-C1
13	d	518	CLA	CBA-CGA-O2A-C1
13	4	509	CLA	CBD-CGD-O2D-CED
13	4	517	CLA	CBD-CGD-O2D-CED
13	2	502	CLA	CBD-CGD-O2D-CED
13	1	504	CLA	CBD-CGD-O2D-CED
13	1	509	CLA	CBD-CGD-O2D-CED
13	A	1116	CLA	CBD-CGD-O2D-CED
13	B	1210	CLA	CBD-CGD-O2D-CED
13	X	1401	CLA	CBD-CGD-O2D-CED
13	d	510	CLA	CBD-CGD-O2D-CED
13	d	512	CLA	CBD-CGD-O2D-CED
13	e	518	CLA	CBD-CGD-O2D-CED
13	f	511	CLA	CBD-CGD-O2D-CED
13	g	517	CLA	CBD-CGD-O2D-CED
13	b	510	CLA	CBD-CGD-O2D-CED
20	B	1843	LMU	O5'-C5'-C6'-O6'
13	a	503	CLA	O1D-CGD-O2D-CED
13	B	1228	CLA	O1A-CGA-O2A-C1
13	g	502	CLA	O1A-CGA-O2A-C1
13	2	509	CLA	O1D-CGD-O2D-CED
13	A	1111	CLA	O1D-CGD-O2D-CED
13	B	1209	CLA	O1D-CGD-O2D-CED
13	d	505	CLA	O1D-CGD-O2D-CED
13	B	1227	CLA	CBD-CGD-O2D-CED
13	a	501	CLA	CBD-CGD-O2D-CED
13	2	503	CLA	C3-C5-C6-C7
14	5	523	BCR	C13-C14-C15-C16
14	f	521	BCR	C9-C10-C11-C12
14	f	524	BCR	C15-C16-C17-C18
13	A	1109	CLA	O1A-CGA-O2A-C1
17	A	5002	LHG	O9-C7-O7-C5
13	3	502	CLA	CBA-CGA-O2A-C1
13	3	504	CLA	CBA-CGA-O2A-C1
13	3	509	CLA	CBA-CGA-O2A-C1
13	3	511	CLA	CBA-CGA-O2A-C1
13	5	502	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	5	511	CLA	CBA-CGA-O2A-C1
13	6	501	CLA	CBA-CGA-O2A-C1
13	6	510	CLA	CBA-CGA-O2A-C1
13	1	502	CLA	CBA-CGA-O2A-C1
13	A	1106	CLA	CBA-CGA-O2A-C1
13	A	1110	CLA	CBA-CGA-O2A-C1
13	A	1111	CLA	CBA-CGA-O2A-C1
13	A	1120	CLA	CBA-CGA-O2A-C1
13	A	1126	CLA	CBA-CGA-O2A-C1
13	A	1135	CLA	CBA-CGA-O2A-C1
13	B	1012	CLA	CBA-CGA-O2A-C1
13	B	1202	CLA	CBA-CGA-O2A-C1
13	B	1203	CLA	CBA-CGA-O2A-C1
13	B	1206	CLA	CBA-CGA-O2A-C1
13	B	1238	CLA	CBA-CGA-O2A-C1
13	d	502	CLA	CBA-CGA-O2A-C1
13	d	512	CLA	CBA-CGA-O2A-C1
13	e	502	CLA	CBA-CGA-O2A-C1
13	f	502	CLA	CBA-CGA-O2A-C1
13	a	510	CLA	CBA-CGA-O2A-C1
17	A	5004	LHG	C24-C23-O8-C6
13	A	1120	CLA	O1D-CGD-O2D-CED
13	B	1218	CLA	O1D-CGD-O2D-CED
13	B	1226	CLA	O1D-CGD-O2D-CED
13	3	503	CLA	C4-C3-C5-C6
13	6	503	CLA	C4-C3-C5-C6
13	2	503	CLA	C4-C3-C5-C6
13	A	1122	CLA	C4-C3-C5-C6
13	B	1221	CLA	C4-C3-C5-C6
13	6	503	CLA	C2-C3-C5-C6
13	2	503	CLA	C2-C3-C5-C6
13	B	1221	CLA	C2-C3-C5-C6
13	B	1230	CLA	C2-C3-C5-C6
13	e	503	CLA	C2-C3-C5-C6
13	5	508	CLA	C3-C5-C6-C7
13	f	508	CLA	C3-C5-C6-C7
13	f	518	CLA	C3-C5-C6-C7
13	g	510	CLA	C3-C5-C6-C7
13	g	511	CLA	C3-C5-C6-C7
13	c	518	CLA	CBD-CGD-O2D-CED
13	3	507	CLA	C6-C7-C8-C9
13	4	505	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	5	509	CLA	C6-C7-C8-C9
13	6	502	CLA	C6-C7-C8-C9
13	6	509	CLA	C6-C7-C8-C9
13	2	502	CLA	C11-C10-C8-C9
13	2	509	CLA	C6-C7-C8-C9
13	2	510	CLA	C11-C12-C13-C14
13	1	503	CLA	C11-C10-C8-C9
13	1	503	CLA	C11-C12-C13-C14
13	1	507	CLA	C6-C7-C8-C9
13	1	509	CLA	C14-C13-C15-C16
13	A	1022	CLA	C14-C13-C15-C16
13	A	1102	CLA	C6-C7-C8-C9
13	A	1103	CLA	C6-C7-C8-C9
13	A	1107	CLA	C6-C7-C8-C9
13	A	1116	CLA	C6-C7-C8-C9
13	A	1125	CLA	C6-C7-C8-C9
13	A	1138	CLA	C6-C7-C8-C9
13	A	1139	CLA	C6-C7-C8-C9
13	B	1202	CLA	C6-C7-C8-C9
13	B	1222	CLA	C11-C10-C8-C9
13	B	1226	CLA	C11-C12-C13-C14
13	d	502	CLA	C6-C7-C8-C9
13	d	509	CLA	C6-C7-C8-C9
13	d	510	CLA	C14-C13-C15-C16
13	e	502	CLA	C11-C10-C8-C9
13	e	505	CLA	C11-C10-C8-C9
13	f	501	CLA	C14-C13-C15-C16
13	g	502	CLA	C11-C10-C8-C9
13	b	507	CLA	C11-C10-C8-C9
13	a	505	CLA	C6-C7-C8-C9
13	a	509	CLA	C6-C7-C8-C9
18	A	2001	PQN	C21-C22-C23-C24
13	5	501	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	O1D-CGD-O2D-CED
13	B	1215	CLA	O1D-CGD-O2D-CED
13	d	504	CLA	O1D-CGD-O2D-CED
20	A	1849	LMU	C2'-C1'-O1'-C1
13	A	1115	CLA	O1D-CGD-O2D-CED
13	1	502	CLA	O1A-CGA-O2A-C1
13	B	1202	CLA	CBD-CGD-O2D-CED
13	5	508	CLA	O1D-CGD-O2D-CED
13	B	1212	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
14	3	521	BCR	C7-C8-C9-C34
14	3	523	BCR	C37-C22-C23-C24
14	4	523	BCR	C7-C8-C9-C34
14	4	524	BCR	C37-C22-C23-C24
14	5	523	BCR	C11-C12-C13-C35
14	6	521	BCR	C7-C8-C9-C34
14	6	522	BCR	C7-C8-C9-C34
14	2	521	BCR	C7-C8-C9-C34
14	2	523	BCR	C7-C8-C9-C34
14	A	4007	BCR	C37-C22-C23-C24
14	B	4004	BCR	C7-C8-C9-C34
14	B	4005	BCR	C37-C22-C23-C24
14	B	4006	BCR	C7-C8-C9-C34
14	B	4009	BCR	C36-C18-C19-C20
14	B	4009	BCR	C37-C22-C23-C24
14	B	4010	BCR	C37-C22-C23-C24
14	F	4014	BCR	C7-C8-C9-C34
14	F	4014	BCR	C36-C18-C19-C20
14	M	4021	BCR	C37-C22-C23-C24
14	c	522	BCR	C7-C8-C9-C34
14	d	521	BCR	C7-C8-C9-C34
14	f	521	BCR	C7-C8-C9-C34
14	g	521	BCR	C7-C8-C9-C34
14	g	522	BCR	C7-C8-C9-C34
14	b	523	BCR	C7-C8-C9-C34
14	b	521	BCR	C7-C8-C9-C34
14	b	524	BCR	C37-C22-C23-C24
14	a	523	BCR	C7-C8-C9-C34
14	a	523	BCR	C37-C22-C23-C24
14	3	521	BCR	C7-C8-C9-C10
14	4	524	BCR	C21-C22-C23-C24
14	A	4003	BCR	C7-C8-C9-C10
14	B	4005	BCR	C21-C22-C23-C24
14	F	4014	BCR	C21-C22-C23-C24
14	M	4021	BCR	C21-C22-C23-C24
14	c	522	BCR	C7-C8-C9-C10
14	d	521	BCR	C7-C8-C9-C10
14	f	521	BCR	C7-C8-C9-C10
14	g	521	BCR	C7-C8-C9-C10
14	b	523	BCR	C7-C8-C9-C10
14	a	523	BCR	C21-C22-C23-C24
13	3	512	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	A	1140	CLA	C2A-CAA-CBA-CGA
13	c	505	CLA	C2A-CAA-CBA-CGA
13	f	512	CLA	C2A-CAA-CBA-CGA
13	b	504	CLA	C2A-CAA-CBA-CGA
16	2	5104	LMG	C28-C29-C30-C31
17	A	5002	LHG	C23-C24-C25-C26
13	A	1132	CLA	O1D-CGD-O2D-CED
13	3	511	CLA	O1A-CGA-O2A-C1
13	A	1110	CLA	O1A-CGA-O2A-C1
13	A	1126	CLA	O1A-CGA-O2A-C1
13	A	1135	CLA	O1A-CGA-O2A-C1
13	B	1012	CLA	O1A-CGA-O2A-C1
13	f	502	CLA	O1A-CGA-O2A-C1
17	A	5004	LHG	O10-C23-O8-C6
13	5	502	CLA	C3-C5-C6-C7
13	A	1013	CLA	C3-C5-C6-C7
13	A	1123	CLA	C3-C5-C6-C7
13	c	509	CLA	C3-C5-C6-C7
16	1	5104	LMG	O7-C8-C9-O8
13	4	519	CLA	O1D-CGD-O2D-CED
13	4	502	CLA	CBA-CGA-O2A-C1
13	A	1134	CLA	CBA-CGA-O2A-C1
13	c	510	CLA	CBA-CGA-O2A-C1
13	g	504	CLA	CBA-CGA-O2A-C1
13	2	510	CLA	C10-C11-C12-C13
13	A	1101	CLA	C8-C10-C11-C12
13	A	1106	CLA	C5-C6-C7-C8
13	B	1210	CLA	C5-C6-C7-C8
13	e	518	CLA	C5-C6-C7-C8
13	3	504	CLA	C2-C1-O2A-CGA
13	3	502	CLA	O1A-CGA-O2A-C1
13	6	508	CLA	O1D-CGD-O2D-CED
13	6	517	CLA	O1D-CGD-O2D-CED
13	A	1138	CLA	O1D-CGD-O2D-CED
13	B	1228	CLA	O1D-CGD-O2D-CED
13	c	501	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	CBD-CGD-O2D-CED
13	e	505	CLA	C13-C15-C16-C17
13	B	1217	CLA	C3-C5-C6-C7
13	A	1118	CLA	O1D-CGD-O2D-CED
13	3	504	CLA	O1A-CGA-O2A-C1
13	B	1238	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	B	1224	CLA	C8-C10-C11-C12
13	3	510	CLA	C12-C13-C15-C16
13	5	501	CLA	C12-C13-C15-C16
13	A	1107	CLA	C11-C10-C8-C7
13	B	1214	CLA	C12-C13-C15-C16
13	d	503	CLA	C12-C13-C15-C16
13	b	511	CLA	O1D-CGD-O2D-CED
13	B	1203	CLA	C13-C15-C16-C17
13	e	519	CLA	O1D-CGD-O2D-CED
14	5	523	BCR	C19-C20-C21-C22
14	5	524	BCR	C9-C10-C11-C12
14	5	524	BCR	C15-C16-C17-C18
13	3	509	CLA	O1A-CGA-O2A-C1
13	B	1238	CLA	C3-C5-C6-C7
13	f	501	CLA	C3-C5-C6-C7
13	6	510	CLA	C10-C11-C12-C13
13	A	1122	CLA	C5-C6-C7-C8
13	e	502	CLA	C5-C6-C7-C8
13	f	501	CLA	C15-C16-C17-C18
13	a	510	CLA	C5-C6-C7-C8
13	b	512	CLA	O1D-CGD-O2D-CED
13	4	502	CLA	O1A-CGA-O2A-C1
13	5	511	CLA	O1A-CGA-O2A-C1
13	6	501	CLA	O1A-CGA-O2A-C1
13	A	1106	CLA	O1A-CGA-O2A-C1
13	B	1206	CLA	O1A-CGA-O2A-C1
13	d	502	CLA	O1A-CGA-O2A-C1
13	e	502	CLA	O1A-CGA-O2A-C1
13	a	510	CLA	O1A-CGA-O2A-C1
13	B	1223	CLA	CBD-CGD-O2D-CED
13	4	502	CLA	O1D-CGD-O2D-CED
13	3	503	CLA	C8-C10-C11-C12
13	A	1104	CLA	C10-C11-C12-C13
13	A	1139	CLA	C5-C6-C7-C8
13	A	1237	CLA	C5-C6-C7-C8
13	B	1021	CLA	C15-C16-C17-C18
13	c	502	CLA	C10-C11-C12-C13
13	d	501	CLA	C10-C11-C12-C13
13	3	504	CLA	C2A-CAA-CBA-CGA
13	3	510	CLA	C2A-CAA-CBA-CGA
13	6	501	CLA	C2A-CAA-CBA-CGA
13	6	511	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	6	513	CLA	C2A-CAA-CBA-CGA
13	1	511	CLA	C2A-CAA-CBA-CGA
13	1	512	CLA	C2A-CAA-CBA-CGA
13	A	1237	CLA	C2A-CAA-CBA-CGA
13	B	1213	CLA	C2A-CAA-CBA-CGA
13	B	1218	CLA	C2A-CAA-CBA-CGA
13	B	1224	CLA	C2A-CAA-CBA-CGA
13	B	1227	CLA	C2A-CAA-CBA-CGA
13	c	504	CLA	C2A-CAA-CBA-CGA
13	d	505	CLA	C2A-CAA-CBA-CGA
13	e	511	CLA	C2A-CAA-CBA-CGA
13	f	507	CLA	C2A-CAA-CBA-CGA
13	b	505	CLA	C2A-CAA-CBA-CGA
13	b	513	CLA	C2A-CAA-CBA-CGA
13	6	503	CLA	C8-C10-C11-C12
13	2	502	CLA	C5-C6-C7-C8
13	2	505	CLA	C8-C10-C11-C12
13	2	509	CLA	C15-C16-C17-C18
13	1	501	CLA	C13-C15-C16-C17
13	1	505	CLA	C8-C10-C11-C12
13	A	1103	CLA	C15-C16-C17-C18
13	A	1136	CLA	C13-C15-C16-C17
13	A	1140	CLA	C15-C16-C17-C18
13	B	1203	CLA	C10-C11-C12-C13
13	B	1210	CLA	C10-C11-C12-C13
13	B	1210	CLA	C15-C16-C17-C18
13	B	1211	CLA	C15-C16-C17-C18
13	B	1235	CLA	C13-C15-C16-C17
13	e	505	CLA	C10-C11-C12-C13
13	e	509	CLA	C5-C6-C7-C8
13	f	508	CLA	C5-C6-C7-C8
13	g	510	CLA	C10-C11-C12-C13
13	a	505	CLA	C5-C6-C7-C8
13	a	509	CLA	C5-C6-C7-C8
13	6	510	CLA	O1A-CGA-O2A-C1
13	A	1111	CLA	O1A-CGA-O2A-C1
13	A	1120	CLA	O1A-CGA-O2A-C1
13	B	1203	CLA	O1A-CGA-O2A-C1
13	d	512	CLA	O1A-CGA-O2A-C1
13	2	502	CLA	C3-C5-C6-C7
20	J	5105	LMU	O5'-C1'-O1'-C1
13	B	1230	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	4	501	CLA	C13-C15-C16-C17
13	4	509	CLA	C8-C10-C11-C12
13	5	503	CLA	C8-C10-C11-C12
13	6	502	CLA	C8-C10-C11-C12
13	6	505	CLA	C5-C6-C7-C8
13	A	1022	CLA	C5-C6-C7-C8
13	A	1103	CLA	C8-C10-C11-C12
13	A	1106	CLA	C8-C10-C11-C12
13	A	1106	CLA	C10-C11-C12-C13
13	A	1126	CLA	C10-C11-C12-C13
13	A	1133	CLA	C8-C10-C11-C12
13	A	1138	CLA	C5-C6-C7-C8
13	B	1023	CLA	C10-C11-C12-C13
13	B	1202	CLA	C10-C11-C12-C13
13	B	1204	CLA	C5-C6-C7-C8
13	B	1214	CLA	C8-C10-C11-C12
13	c	508	CLA	C5-C6-C7-C8
13	e	510	CLA	C15-C16-C17-C18
13	b	504	CLA	C5-C6-C7-C8
13	b	510	CLA	C13-C15-C16-C17
13	a	510	CLA	C15-C16-C17-C18
13	3	512	CLA	CBA-CGA-O2A-C1
13	2	503	CLA	CBA-CGA-O2A-C1
13	1	513	CLA	CBA-CGA-O2A-C1
13	B	1210	CLA	CBA-CGA-O2A-C1
13	5	502	CLA	O1A-CGA-O2A-C1
13	6	502	CLA	O1A-CGA-O2A-C1
13	B	1202	CLA	O1A-CGA-O2A-C1
13	B	1221	CLA	C8-C10-C11-C12
13	B	1229	CLA	C15-C16-C17-C18
13	1	508	CLA	C3-C5-C6-C7
13	A	1125	CLA	C3-C5-C6-C7
13	d	503	CLA	C3-C5-C6-C7
13	6	516	CLA	O1D-CGD-O2D-CED
13	B	1214	CLA	O1D-CGD-O2D-CED
13	B	1239	CLA	O1D-CGD-O2D-CED
13	g	509	CLA	O1D-CGD-O2D-CED
13	b	504	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C8-C10-C11-C12
13	e	505	CLA	C15-C16-C17-C18
13	g	509	CLA	C8-C10-C11-C12
13	b	505	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
13	A	1013	CLA	CBD-CGD-O2D-CED
13	3	518	CLA	C2-C3-C5-C6
13	5	519	CLA	O1D-CGD-O2D-CED
13	1	512	CLA	O1D-CGD-O2D-CED
13	3	507	CLA	C5-C6-C7-C8
13	4	510	CLA	C10-C11-C12-C13
13	A	1125	CLA	C13-C15-C16-C17
13	b	510	CLA	C15-C16-C17-C18
18	A	2001	PQN	C25-C26-C27-C28
13	3	505	CLA	CBA-CGA-O2A-C1
13	1	509	CLA	CBA-CGA-O2A-C1
13	d	510	CLA	CBA-CGA-O2A-C1
15	4	822	SQD	C8-C7-O47-C45
13	c	510	CLA	O1A-CGA-O2A-C1
13	d	518	CLA	O1A-CGA-O2A-C1
13	g	504	CLA	O1A-CGA-O2A-C1
13	B	1205	CLA	C8-C10-C11-C12
13	1	503	CLA	C3-C5-C6-C7
13	B	1205	CLA	C3-C5-C6-C7
13	g	504	CLA	C3-C5-C6-C7
13	g	518	CLA	C3-C5-C6-C7
20	A	1849	LMU	C4'-C5'-C6'-O6'
13	B	1214	CLA	C5-C6-C7-C8
15	4	822	SQD	O49-C7-O47-C45
13	4	501	CLA	C2A-CAA-CBA-CGA
13	1	518	CLA	C2A-CAA-CBA-CGA
13	A	1113	CLA	C2A-CAA-CBA-CGA
13	A	1120	CLA	C2A-CAA-CBA-CGA
13	B	1217	CLA	C2A-CAA-CBA-CGA
13	g	513	CLA	C2A-CAA-CBA-CGA
13	b	506	CLA	C2A-CAA-CBA-CGA
13	a	501	CLA	C2A-CAA-CBA-CGA
13	a	505	CLA	C2A-CAA-CBA-CGA
13	a	511	CLA	C2A-CAA-CBA-CGA
13	2	510	CLA	CBA-CGA-O2A-C1
13	g	503	CLA	CBA-CGA-O2A-C1
13	3	502	CLA	C5-C6-C7-C8
13	2	501	CLA	C8-C10-C11-C12
13	1	501	CLA	C8-C10-C11-C12
13	1	503	CLA	C5-C6-C7-C8
13	A	1109	CLA	C15-C16-C17-C18
13	A	1118	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	B	1214	CLA	C13-C15-C16-C17
13	B	1218	CLA	C5-C6-C7-C8
13	c	501	CLA	C8-C10-C11-C12
13	b	508	CLA	C5-C6-C7-C8
13	a	510	CLA	C10-C11-C12-C13
13	5	509	CLA	O1D-CGD-O2D-CED
13	a	504	CLA	O1D-CGD-O2D-CED
13	B	1229	CLA	CBD-CGD-O2D-CED
13	c	508	CLA	O1D-CGD-O2D-CED
13	f	516	CLA	O1D-CGD-O2D-CED
13	2	505	CLA	C13-C15-C16-C17
13	A	1109	CLA	C8-C10-C11-C12
13	B	1012	CLA	C5-C6-C7-C8
13	3	504	CLA	O1D-CGD-O2D-CED
13	4	502	CLA	C5-C6-C7-C8
13	5	508	CLA	C5-C6-C7-C8
13	1	505	CLA	C5-C6-C7-C8
13	A	1103	CLA	C13-C15-C16-C17
13	A	1107	CLA	C5-C6-C7-C8
13	A	1115	CLA	C5-C6-C7-C8
13	B	1203	CLA	C5-C6-C7-C8
13	B	1235	CLA	C15-C16-C17-C18
13	d	505	CLA	C13-C15-C16-C17
13	f	505	CLA	C15-C16-C17-C18
13	g	501	CLA	C15-C16-C17-C18
13	g	503	CLA	C5-C6-C7-C8
13	e	504	CLA	O1D-CGD-O2D-CED
13	A	1126	CLA	C15-C16-C17-C18
13	B	1221	CLA	C5-C6-C7-C8
13	c	505	CLA	C13-C15-C16-C17
13	f	510	CLA	C5-C6-C7-C8
13	f	510	CLA	C3-C5-C6-C7
13	5	505	CLA	C6-C7-C8-C9
13	c	516	CLA	O1D-CGD-O2D-CED
20	J	5105	LMU	C2'-C1'-O1'-C1
13	5	501	CLA	C13-C15-C16-C17
13	1	502	CLA	C5-C6-C7-C8
13	d	511	CLA	C5-C6-C7-C8
13	4	519	CLA	CBA-CGA-O2A-C1
13	d	504	CLA	CBA-CGA-O2A-C1
13	6	507	CLA	C11-C12-C13-C15
13	B	1231	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	d	511	CLA	C6-C7-C8-C10
13	2	501	CLA	C13-C15-C16-C17
13	B	1210	CLA	C3-C5-C6-C7
13	2	519	CLA	O1D-CGD-O2D-CED
13	1	503	CLA	C10-C11-C12-C13
14	3	523	BCR	C7-C8-C9-C34
14	5	524	BCR	C7-C8-C9-C34
14	J	4012	BCR	C11-C12-C13-C35
14	c	524	BCR	C37-C22-C23-C24
14	e	521	BCR	C7-C8-C9-C34
14	e	523	BCR	C37-C22-C23-C24
14	f	524	BCR	C37-C22-C23-C24
14	b	521	BCR	C36-C18-C19-C20
14	a	522	BCR	C7-C8-C9-C34
14	a	521	BCR	C7-C8-C9-C34
14	3	523	BCR	C7-C8-C9-C10
14	5	524	BCR	C7-C8-C9-C10
14	6	522	BCR	C7-C8-C9-C10
14	e	523	BCR	C21-C22-C23-C24
14	f	524	BCR	C21-C22-C23-C24
14	a	522	BCR	C7-C8-C9-C10
14	a	521	BCR	C7-C8-C9-C10
13	3	505	CLA	O1A-CGA-O2A-C1
13	4	516	CLA	C2A-CAA-CBA-CGA
13	6	504	CLA	C2A-CAA-CBA-CGA
13	6	505	CLA	C2A-CAA-CBA-CGA
13	1	504	CLA	C2A-CAA-CBA-CGA
13	A	1022	CLA	C2A-CAA-CBA-CGA
13	A	1111	CLA	C2A-CAA-CBA-CGA
13	A	1126	CLA	C2A-CAA-CBA-CGA
13	B	1225	CLA	C2A-CAA-CBA-CGA
13	d	511	CLA	C2A-CAA-CBA-CGA
13	f	518	CLA	C2A-CAA-CBA-CGA
13	g	501	CLA	C2A-CAA-CBA-CGA
13	a	510	CLA	C2A-CAA-CBA-CGA
13	2	510	CLA	C8-C10-C11-C12
13	b	505	CLA	C13-C15-C16-C17
13	b	510	CLA	C10-C11-C12-C13
13	6	505	CLA	C16-C17-C18-C20
13	2	518	CLA	C6-C7-C8-C10
13	1	501	CLA	C16-C17-C18-C19
13	A	1111	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	c	505	CLA	C16-C17-C18-C20
13	d	511	CLA	C6-C7-C8-C9
13	b	502	CLA	C11-C12-C13-C15
13	1	519	CLA	O1D-CGD-O2D-CED
13	A	1128	CLA	O1D-CGD-O2D-CED
13	3	512	CLA	O1A-CGA-O2A-C1
13	1	509	CLA	O1A-CGA-O2A-C1
13	1	513	CLA	O1A-CGA-O2A-C1
13	A	1134	CLA	O1A-CGA-O2A-C1
13	g	503	CLA	O1A-CGA-O2A-C1
13	A	1130	CLA	C3-C5-C6-C7
13	B	1219	CLA	C3-C5-C6-C7
13	e	504	CLA	C3-C5-C6-C7
13	b	504	CLA	C3-C5-C6-C7
13	3	510	CLA	C13-C15-C16-C17
13	2	502	CLA	C10-C11-C12-C13
13	e	505	CLA	C8-C10-C11-C12
13	f	501	CLA	C8-C10-C11-C12
13	3	503	CLA	C2-C3-C5-C6
13	6	512	CLA	O1D-CGD-O2D-CED
13	1	501	CLA	O1D-CGD-O2D-CED
13	1	507	CLA	CBA-CGA-O2A-C1
13	b	502	CLA	CBA-CGA-O2A-C1
13	b	510	CLA	CBA-CGA-O2A-C1
13	1	502	CLA	C10-C11-C12-C13
13	6	510	CLA	C2-C1-O2A-CGA
13	2	509	CLA	C2-C1-O2A-CGA
13	4	507	CLA	C11-C12-C13-C14
13	6	507	CLA	C11-C12-C13-C14
13	2	505	CLA	C16-C17-C18-C20
13	1	501	CLA	C16-C17-C18-C20
13	B	1225	CLA	C16-C17-C18-C19
13	e	504	CLA	C6-C7-C8-C10
13	g	504	CLA	C6-C7-C8-C10
13	2	510	CLA	O1A-CGA-O2A-C1
13	1	507	CLA	C5-C6-C7-C8
13	d	503	CLA	C5-C6-C7-C8
13	g	501	CLA	C13-C15-C16-C17
13	b	509	CLA	C5-C6-C7-C8
13	3	511	CLA	O1D-CGD-O2D-CED
13	2	503	CLA	O1A-CGA-O2A-C1
13	d	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
13	5	519	CLA	CBA-CGA-O2A-C1
13	g	513	CLA	CBA-CGA-O2A-C1
20	A	1849	LMU	C2-C1-O1'-C1'
13	g	517	CLA	O1D-CGD-O2D-CED
13	3	518	CLA	C4B-C3B-CAB-CBB
13	4	518	CLA	C4B-C3B-CAB-CBB
13	6	508	CLA	C4B-C3B-CAB-CBB
13	6	518	CLA	C4B-C3B-CAB-CBB
13	1	513	CLA	C4B-C3B-CAB-CBB
13	A	1013	CLA	C4B-C3B-CAB-CBB
13	A	1121	CLA	C4B-C3B-CAB-CBB
13	A	1136	CLA	C4B-C3B-CAB-CBB
13	A	1011	CLA	C4B-C3B-CAB-CBB
13	B	1209	CLA	C4B-C3B-CAB-CBB
13	B	1227	CLA	C4B-C3B-CAB-CBB
13	B	1239	CLA	C4B-C3B-CAB-CBB
13	F	1301	CLA	C4B-C3B-CAB-CBB
13	d	518	CLA	C4B-C3B-CAB-CBB
13	f	512	CLA	C4B-C3B-CAB-CBB
13	g	511	CLA	C4B-C3B-CAB-CBB
13	g	517	CLA	C4B-C3B-CAB-CBB
13	b	501	CLA	C4B-C3B-CAB-CBB
13	b	512	CLA	C4B-C3B-CAB-CBB
13	b	518	CLA	C4B-C3B-CAB-CBB
13	a	504	CLA	C4B-C3B-CAB-CBB
13	a	517	CLA	C4B-C3B-CAB-CBB
13	4	507	CLA	C11-C12-C13-C15
13	2	505	CLA	C16-C17-C18-C19
13	1	504	CLA	C6-C7-C8-C9
13	1	504	CLA	C6-C7-C8-C10
13	A	1111	CLA	C11-C12-C13-C15
13	A	1126	CLA	C16-C17-C18-C20
13	B	1202	CLA	C16-C17-C18-C20
13	B	1203	CLA	C16-C17-C18-C19
13	B	1203	CLA	C16-C17-C18-C20
13	e	504	CLA	C6-C7-C8-C9
13	b	502	CLA	C11-C12-C13-C14
18	B	2002	PQN	C26-C27-C28-C29
13	4	517	CLA	O1D-CGD-O2D-CED
13	b	510	CLA	O1D-CGD-O2D-CED
13	1	506	CLA	C2A-CAA-CBA-CGA
13	A	1013	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	c	501	CLA	C2A-CAA-CBA-CGA
13	d	518	CLA	C2A-CAA-CBA-CGA
13	g	511	CLA	C2A-CAA-CBA-CGA
13	b	501	CLA	C2A-CAA-CBA-CGA
13	4	509	CLA	C15-C16-C17-C18
13	5	511	CLA	C5-C6-C7-C8
13	d	505	CLA	C8-C10-C11-C12
13	g	501	CLA	C5-C6-C7-C8
15	d	822	SQD	C8-C7-O47-C45
16	6	5104	LMG	C11-C10-O7-C8
20	A	1849	LMU	O5'-C5'-C6'-O6'
13	4	505	CLA	C11-C12-C13-C15
13	5	503	CLA	C6-C7-C8-C10
13	5	510	CLA	C12-C13-C15-C16
13	6	502	CLA	C11-C10-C8-C7
13	B	1021	CLA	C12-C13-C15-C16
13	B	1203	CLA	C11-C10-C8-C7
13	B	1223	CLA	C6-C7-C8-C10
13	e	503	CLA	C12-C13-C15-C16
13	g	503	CLA	C6-C7-C8-C10
13	b	510	CLA	C11-C12-C13-C15
15	5	822	SQD	C7-C8-C9-C10
13	c	508	CLA	CBA-CGA-O2A-C1
13	f	503	CLA	C8-C10-C11-C12
13	B	1210	CLA	O1A-CGA-O2A-C1
16	J	5104	LMG	C4-C5-C6-O5
13	1	502	CLA	C3-C5-C6-C7
13	f	509	CLA	C3-C5-C6-C7
13	3	516	CLA	C3A-C2A-CAA-CBA
13	1	505	CLA	C3A-C2A-CAA-CBA
13	1	518	CLA	C3A-C2A-CAA-CBA
13	A	1101	CLA	C3A-C2A-CAA-CBA
13	A	1104	CLA	C3A-C2A-CAA-CBA
13	A	1134	CLA	C3A-C2A-CAA-CBA
13	A	1135	CLA	C3A-C2A-CAA-CBA
13	A	1801	CLA	C3A-C2A-CAA-CBA
13	B	1203	CLA	C3A-C2A-CAA-CBA
13	B	1230	CLA	C3A-C2A-CAA-CBA
13	B	1238	CLA	C4-C3-C5-C6
13	d	516	CLA	C3A-C2A-CAA-CBA
13	e	504	CLA	C3A-C2A-CAA-CBA
13	e	506	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	e	516	CLA	C3A-C2A-CAA-CBA
13	f	519	CLA	C3A-C2A-CAA-CBA
13	3	505	CLA	C15-C16-C17-C18
13	4	510	CLA	C13-C15-C16-C17
13	2	510	CLA	C13-C15-C16-C17
13	A	1126	CLA	C13-C15-C16-C17
13	1	504	CLA	O1D-CGD-O2D-CED
13	d	510	CLA	O1D-CGD-O2D-CED
14	6	522	BCR	C9-C10-C11-C12
14	2	522	BCR	C9-C10-C11-C12
14	J	4013	BCR	C13-C14-C15-C16
13	c	505	CLA	C16-C17-C18-C19
18	B	2002	PQN	C26-C27-C28-C30
20	A	1849	LMU	C5-C6-C7-C8
13	d	512	CLA	O1D-CGD-O2D-CED
13	4	508	CLA	CBA-CGA-O2A-C1
13	A	1137	CLA	CBA-CGA-O2A-C1
13	c	503	CLA	CBA-CGA-O2A-C1
13	4	509	CLA	C5-C6-C7-C8
13	f	511	CLA	O1D-CGD-O2D-CED
17	A	5001	LHG	C28-C29-C30-C31
13	1	507	CLA	O1A-CGA-O2A-C1
20	B	1843	LMU	C6-C7-C8-C9
13	4	509	CLA	O1D-CGD-O2D-CED
13	A	1116	CLA	O1D-CGD-O2D-CED
13	X	1401	CLA	O1D-CGD-O2D-CED
13	B	1210	CLA	O1D-CGD-O2D-CED
13	e	518	CLA	O1D-CGD-O2D-CED
17	A	5004	LHG	C26-C27-C28-C29
13	B	1225	CLA	C16-C17-C18-C20
13	4	519	CLA	O1A-CGA-O2A-C1
13	d	504	CLA	O1A-CGA-O2A-C1
13	3	502	CLA	C2B-C3B-CAB-CBB
13	4	518	CLA	C2B-C3B-CAB-CBB
13	5	516	CLA	C2B-C3B-CAB-CBB
13	6	503	CLA	C2B-C3B-CAB-CBB
13	2	516	CLA	C2B-C3B-CAB-CBB
13	1	513	CLA	C2B-C3B-CAB-CBB
13	A	1121	CLA	C2B-C3B-CAB-CBB
13	A	1136	CLA	C2B-C3B-CAB-CBB
13	B	1021	CLA	C2B-C3B-CAB-CBB
13	B	1209	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	B	1230	CLA	C2B-C3B-CAB-CBB
13	d	518	CLA	C2B-C3B-CAB-CBB
13	e	504	CLA	C2B-C3B-CAB-CBB
13	e	516	CLA	C2B-C3B-CAB-CBB
13	e	517	CLA	C2B-C3B-CAB-CBB
13	f	504	CLA	C2B-C3B-CAB-CBB
13	f	512	CLA	C2B-C3B-CAB-CBB
13	f	517	CLA	C2B-C3B-CAB-CBB
13	b	501	CLA	C2B-C3B-CAB-CBB
13	b	512	CLA	C2B-C3B-CAB-CBB
13	b	516	CLA	C2B-C3B-CAB-CBB
13	a	504	CLA	C2B-C3B-CAB-CBB
13	a	517	CLA	C2B-C3B-CAB-CBB
14	4	522	BCR	C1-C6-C7-C8
14	5	521	BCR	C1-C6-C7-C8
14	5	522	BCR	C1-C6-C7-C8
14	5	522	BCR	C5-C6-C7-C8
14	6	524	BCR	C1-C6-C7-C8
14	6	524	BCR	C5-C6-C7-C8
14	6	522	BCR	C1-C6-C7-C8
14	2	521	BCR	C1-C6-C7-C8
14	2	521	BCR	C5-C6-C7-C8
14	2	522	BCR	C1-C6-C7-C8
14	2	522	BCR	C5-C6-C7-C8
14	1	521	BCR	C1-C6-C7-C8
14	1	521	BCR	C23-C24-C25-C30
14	1	522	BCR	C1-C6-C7-C8
14	A	4003	BCR	C1-C6-C7-C8
14	A	4003	BCR	C5-C6-C7-C8
14	B	4004	BCR	C1-C6-C7-C8
14	B	4004	BCR	C5-C6-C7-C8
14	B	4009	BCR	C23-C24-C25-C26
14	I	4019	BCR	C23-C24-C25-C26
14	I	4019	BCR	C23-C24-C25-C30
14	J	4012	BCR	C1-C6-C7-C8
14	J	4012	BCR	C5-C6-C7-C8
14	J	4013	BCR	C1-C6-C7-C8
14	J	4013	BCR	C23-C24-C25-C26
14	J	4013	BCR	C23-C24-C25-C30
14	M	4021	BCR	C1-C6-C7-C8
14	c	521	BCR	C1-C6-C7-C8
14	d	524	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
14	d	524	BCR	C5-C6-C7-C8
14	f	521	BCR	C23-C24-C25-C26
14	f	521	BCR	C23-C24-C25-C30
14	g	522	BCR	C1-C6-C7-C8
14	g	522	BCR	C5-C6-C7-C8
14	g	523	BCR	C1-C6-C7-C8
14	g	523	BCR	C5-C6-C7-C8
14	b	522	BCR	C1-C6-C7-C8
17	A	5002	LHG	C27-C28-C29-C30
13	B	1217	CLA	CBD-CGD-O2D-CED
15	3	822	SQD	C8-C7-O47-C45
15	2	822	SQD	C8-C7-O47-C45
15	1	822	SQD	C8-C7-O47-C45
15	c	822	SQD	C8-C7-O47-C45
13	2	519	CLA	CBA-CGA-O2A-C1
13	5	505	CLA	C8-C10-C11-C12
13	2	503	CLA	C13-C15-C16-C17
13	d	501	CLA	C15-C16-C17-C18
13	B	1229	CLA	C3-C5-C6-C7
17	A	5003	LHG	C9-C10-C11-C12
20	B	1843	LMU	C4-C5-C6-C7
13	3	501	CLA	C2A-CAA-CBA-CGA
13	5	501	CLA	C2A-CAA-CBA-CGA
13	2	518	CLA	C2A-CAA-CBA-CGA
13	1	501	CLA	C2A-CAA-CBA-CGA
13	A	1106	CLA	C2A-CAA-CBA-CGA
13	A	1116	CLA	C2A-CAA-CBA-CGA
13	A	1134	CLA	C2A-CAA-CBA-CGA
13	A	1135	CLA	C2A-CAA-CBA-CGA
13	B	1012	CLA	C2A-CAA-CBA-CGA
17	A	5005	LHG	C7-C8-C9-C10
13	e	502	CLA	C10-C11-C12-C13
18	B	2002	PQN	C18-C20-C21-C22
13	5	519	CLA	O1A-CGA-O2A-C1
13	A	1137	CLA	O1A-CGA-O2A-C1
13	c	508	CLA	O1A-CGA-O2A-C1
13	b	502	CLA	O1A-CGA-O2A-C1
13	b	510	CLA	O1A-CGA-O2A-C1
15	d	822	SQD	O49-C7-O47-C45
16	6	5104	LMG	O9-C10-O7-C8
13	1	518	CLA	C4-C3-C5-C6
13	c	503	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	d	501	CLA	C4-C3-C5-C6
13	b	512	CLA	C4-C3-C5-C6
13	a	501	CLA	O1D-CGD-O2D-CED
13	A	1139	CLA	C8-C10-C11-C12
13	2	518	CLA	C6-C7-C8-C9
13	B	1231	CLA	C6-C7-C8-C9
13	6	503	CLA	CBA-CGA-O2A-C1
13	1	503	CLA	CBA-CGA-O2A-C1
13	1	510	CLA	CBA-CGA-O2A-C1
13	c	502	CLA	CBA-CGA-O2A-C1
13	f	503	CLA	CBA-CGA-O2A-C1
13	f	518	CLA	CBA-CGA-O2A-C1
13	4	508	CLA	O1A-CGA-O2A-C1
13	g	513	CLA	O1A-CGA-O2A-C1
13	5	502	CLA	C6-C7-C8-C9
13	c	510	CLA	C14-C13-C15-C16
13	a	503	CLA	C11-C12-C13-C14
13	B	1226	CLA	C13-C15-C16-C17
13	c	509	CLA	C8-C10-C11-C12
20	A	1849	LMU	C4-C5-C6-C7
20	A	1848	LMU	C7-C8-C9-C10
13	f	505	CLA	C8-C10-C11-C12
13	2	502	CLA	O1D-CGD-O2D-CED
13	1	509	CLA	O1D-CGD-O2D-CED
13	A	1117	CLA	C3-C5-C6-C7
13	5	511	CLA	C6-C7-C8-C10
13	6	505	CLA	C16-C17-C18-C19
13	g	504	CLA	C6-C7-C8-C9
15	a	822	SQD	C8-C7-O47-C45
17	A	5005	LHG	C8-C7-O7-C5
16	B	5002	LMG	C31-C32-C33-C34
13	A	1115	CLA	C10-C11-C12-C13
14	3	522	BCR	C7-C8-C9-C34
14	M	4021	BCR	C7-C8-C9-C34
14	d	524	BCR	C37-C22-C23-C24
14	b	524	BCR	C7-C8-C9-C34
13	A	1118	CLA	C3-C5-C6-C7
13	B	1021	CLA	C3-C5-C6-C7
14	6	521	BCR	C7-C8-C9-C10
14	B	4010	BCR	C21-C22-C23-C24
13	B	1211	CLA	C2A-CAA-CBA-CGA
13	a	512	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	3	508	CLA	C6-C7-C8-C9
13	A	1118	CLA	C11-C12-C13-C14
13	A	1118	CLA	C11-C12-C13-C15
13	A	1127	CLA	C16-C17-C18-C20
13	4	503	CLA	C4-C3-C5-C6
13	e	510	CLA	C4-C3-C5-C6
13	B	1238	CLA	C2-C3-C5-C6
13	d	502	CLA	C5-C6-C7-C8
13	c	503	CLA	O1A-CGA-O2A-C1
20	A	1849	LMU	C6-C7-C8-C9
17	A	5005	LHG	O9-C7-O7-C5
13	c	503	CLA	C15-C16-C17-C18
18	A	2001	PQN	C18-C20-C21-C22
16	B	5002	LMG	C30-C31-C32-C33
13	2	519	CLA	O1A-CGA-O2A-C1
16	1	5104	LMG	O6-C5-C6-O5
20	J	5105	LMU	C1-C2-C3-C4
13	3	505	CLA	C5-C6-C7-C8
13	5	502	CLA	C5-C6-C7-C8
13	A	1127	CLA	C5-C6-C7-C8
13	B	1231	CLA	C5-C6-C7-C8
13	c	518	CLA	C5-C6-C7-C8
13	a	501	CLA	C13-C15-C16-C17
18	B	2002	PQN	C25-C26-C27-C28
13	2	508	CLA	C3-C5-C6-C7
13	e	505	CLA	C3-C5-C6-C7
15	4	822	SQD	O47-C45-C46-O48
13	B	1227	CLA	O1D-CGD-O2D-CED
13	A	1136	CLA	C8-C10-C11-C12
13	B	1213	CLA	C5-C6-C7-C8
13	1	518	CLA	C5-C6-C7-C8
13	B	1225	CLA	C10-C11-C12-C13
13	d	501	CLA	C13-C15-C16-C17
16	B	5002	LMG	O6-C5-C6-O5
13	2	510	CLA	C4-C3-C5-C6
13	c	510	CLA	C4-C3-C5-C6
13	B	1201	CLA	C3-C5-C6-C7
13	4	503	CLA	C2-C3-C5-C6
13	d	501	CLA	C2-C3-C5-C6
13	b	512	CLA	C2-C3-C5-C6
15	3	822	SQD	O49-C7-O47-C45
15	a	822	SQD	O49-C7-O47-C45

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Mol	Chain	Res	Type	Atoms
13	B	1234	CLA	C8-C10-C11-C12
13	5	516	CLA	C2A-CAA-CBA-CGA
13	A	1121	CLA	C2A-CAA-CBA-CGA
13	d	504	CLA	C2A-CAA-CBA-CGA
13	e	501	CLA	C2A-CAA-CBA-CGA
13	f	513	CLA	C2A-CAA-CBA-CGA
13	f	517	CLA	C2A-CAA-CBA-CGA
13	g	504	CLA	C2A-CAA-CBA-CGA
13	g	518	CLA	C2A-CAA-CBA-CGA
13	g	518	CLA	CBA-CGA-O2A-C1
13	c	518	CLA	O1D-CGD-O2D-CED
13	A	1106	CLA	C15-C16-C17-C18
16	6	5104	LMG	C28-C29-C30-C31
16	B	5002	LMG	C29-C30-C31-C32
17	A	5004	LHG	C28-C29-C30-C31
20	B	1843	LMU	C7-C8-C9-C10
13	5	511	CLA	C6-C7-C8-C9
13	A	1117	CLA	C16-C17-C18-C20
13	6	503	CLA	O1A-CGA-O2A-C1
13	1	510	CLA	O1A-CGA-O2A-C1
13	c	502	CLA	O1A-CGA-O2A-C1
13	f	503	CLA	O1A-CGA-O2A-C1
13	4	508	CLA	C3-C5-C6-C7
13	b	508	CLA	C3-C5-C6-C7
13	3	503	CLA	C1A-C2A-CAA-CBA
13	3	509	CLA	C1A-C2A-CAA-CBA
13	4	501	CLA	C1A-C2A-CAA-CBA
13	4	503	CLA	C1A-C2A-CAA-CBA
13	4	511	CLA	C1A-C2A-CAA-CBA
13	4	512	CLA	C1A-C2A-CAA-CBA
13	5	503	CLA	C1A-C2A-CAA-CBA
13	5	516	CLA	C1A-C2A-CAA-CBA
13	6	501	CLA	C1A-C2A-CAA-CBA
13	6	503	CLA	C1A-C2A-CAA-CBA
13	6	511	CLA	C1A-C2A-CAA-CBA
13	2	503	CLA	C1A-C2A-CAA-CBA
13	2	511	CLA	C1A-C2A-CAA-CBA
13	1	501	CLA	C1A-C2A-CAA-CBA
13	1	513	CLA	C1A-C2A-CAA-CBA
13	1	519	CLA	C1A-C2A-CAA-CBA
13	A	1101	CLA	C1A-C2A-CAA-CBA
13	A	1106	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
13	A	1107	CLA	C1A-C2A-CAA-CBA
13	A	1118	CLA	C1A-C2A-CAA-CBA
13	A	1129	CLA	C1A-C2A-CAA-CBA
13	A	1130	CLA	C1A-C2A-CAA-CBA
13	A	1135	CLA	C1A-C2A-CAA-CBA
13	A	1137	CLA	C1A-C2A-CAA-CBA
13	A	1801	CLA	C1A-C2A-CAA-CBA
13	B	1202	CLA	C1A-C2A-CAA-CBA
13	B	1213	CLA	C1A-C2A-CAA-CBA
13	B	1215	CLA	C1A-C2A-CAA-CBA
13	B	1221	CLA	C1A-C2A-CAA-CBA
13	B	1227	CLA	C1A-C2A-CAA-CBA
13	B	1230	CLA	C1A-C2A-CAA-CBA
13	B	1236	CLA	C1A-C2A-CAA-CBA
13	B	1239	CLA	C1A-C2A-CAA-CBA
13	J	1303	CLA	C1A-C2A-CAA-CBA
13	c	508	CLA	C1A-C2A-CAA-CBA
13	c	511	CLA	C1A-C2A-CAA-CBA
13	c	512	CLA	C1A-C2A-CAA-CBA
13	c	518	CLA	C1A-C2A-CAA-CBA
13	d	503	CLA	C1A-C2A-CAA-CBA
13	d	505	CLA	C1A-C2A-CAA-CBA
13	e	501	CLA	C1A-C2A-CAA-CBA
13	e	518	CLA	C1A-C2A-CAA-CBA
13	f	511	CLA	C1A-C2A-CAA-CBA
13	f	516	CLA	C1A-C2A-CAA-CBA
13	g	502	CLA	C1A-C2A-CAA-CBA
13	g	511	CLA	C1A-C2A-CAA-CBA
13	b	501	CLA	C1A-C2A-CAA-CBA
13	b	508	CLA	C1A-C2A-CAA-CBA
13	b	511	CLA	C1A-C2A-CAA-CBA
13	b	513	CLA	C1A-C2A-CAA-CBA
13	b	519	CLA	C1A-C2A-CAA-CBA
13	a	501	CLA	C1A-C2A-CAA-CBA
13	a	506	CLA	C1A-C2A-CAA-CBA
13	a	513	CLA	C1A-C2A-CAA-CBA
13	A	1127	CLA	C8-C10-C11-C12
15	1	822	SQD	O49-C7-O47-C45
15	c	822	SQD	O49-C7-O47-C45
13	6	503	CLA	C15-C16-C17-C18
13	4	502	CLA	C3-C5-C6-C7
13	3	505	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	5	503	CLA	C12-C13-C15-C16
13	1	502	CLA	C11-C10-C8-C7
13	1	510	CLA	C11-C10-C8-C7
13	A	1104	CLA	C6-C7-C8-C10
13	A	1109	CLA	C11-C10-C8-C7
13	A	1115	CLA	C6-C7-C8-C10
13	A	1117	CLA	C11-C12-C13-C15
13	A	1132	CLA	C12-C13-C15-C16
13	A	1133	CLA	C11-C12-C13-C15
13	A	1138	CLA	C11-C10-C8-C7
13	A	1139	CLA	C6-C7-C8-C10
13	B	1210	CLA	C6-C7-C8-C10
13	B	1211	CLA	C6-C7-C8-C10
13	B	1213	CLA	C12-C13-C15-C16
13	B	1222	CLA	C11-C10-C8-C7
13	B	1224	CLA	C6-C7-C8-C10
13	B	1225	CLA	C12-C13-C15-C16
13	B	1207	CLA	C11-C12-C13-C15
13	c	501	CLA	C11-C12-C13-C15
13	d	501	CLA	C11-C10-C8-C7
13	e	505	CLA	C11-C10-C8-C7
13	f	505	CLA	C12-C13-C15-C16
13	b	503	CLA	C12-C13-C15-C16
13	a	505	CLA	C11-C12-C13-C15
13	a	505	CLA	C12-C13-C15-C16
13	a	510	CLA	C6-C7-C8-C10
18	A	2001	PQN	C17-C18-C20-C21
18	B	2002	PQN	C17-C18-C20-C21
13	A	1116	CLA	C11-C12-C13-C15
13	e	510	CLA	C5-C6-C7-C8
13	1	503	CLA	O1A-CGA-O2A-C1
13	1	505	CLA	C10-C11-C12-C13
15	1	822	SQD	C7-C8-C9-C10
20	J	5105	LMU	C4'-C5'-C6'-O6'
13	4	518	CLA	C2A-CAA-CBA-CGA
13	5	510	CLA	C2A-CAA-CBA-CGA
13	5	512	CLA	C2A-CAA-CBA-CGA
13	2	510	CLA	C2A-CAA-CBA-CGA
13	2	519	CLA	C2A-CAA-CBA-CGA
13	A	1115	CLA	C2A-CAA-CBA-CGA
13	B	1202	CLA	C2A-CAA-CBA-CGA
13	B	1203	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	B	1214	CLA	C2A-CAA-CBA-CGA
13	B	1219	CLA	C2A-CAA-CBA-CGA
13	B	1231	CLA	C2A-CAA-CBA-CGA
13	c	510	CLA	C2A-CAA-CBA-CGA
13	d	510	CLA	C2A-CAA-CBA-CGA
13	3	510	CLA	C14-C13-C15-C16
13	4	505	CLA	C14-C13-C15-C16
13	2	505	CLA	C11-C12-C13-C14
13	A	1104	CLA	C14-C13-C15-C16
13	A	1117	CLA	C11-C12-C13-C14
13	B	1021	CLA	C11-C12-C13-C14
13	B	1203	CLA	C6-C7-C8-C9
13	B	1203	CLA	C14-C13-C15-C16
13	B	1210	CLA	C6-C7-C8-C9
13	B	1210	CLA	C14-C13-C15-C16
13	B	1213	CLA	C14-C13-C15-C16
13	B	1223	CLA	C6-C7-C8-C9
13	B	1225	CLA	C14-C13-C15-C16
13	B	1229	CLA	C14-C13-C15-C16
13	c	505	CLA	C14-C13-C15-C16
13	d	502	CLA	C11-C10-C8-C9
13	f	501	CLA	C11-C12-C13-C14
13	f	503	CLA	C6-C7-C8-C9
13	a	510	CLA	C6-C7-C8-C9
13	4	510	CLA	CBA-CGA-O2A-C1
13	A	1125	CLA	CBA-CGA-O2A-C1
13	A	1022	CLA	C10-C11-C12-C13
13	A	1140	CLA	C8-C10-C11-C12
13	g	516	CLA	CBD-CGD-O2D-CED
13	3	510	CLA	C5-C6-C7-C8
15	4	822	SQD	C44-C45-C46-O48
15	g	822	SQD	C44-C45-C46-O48
17	A	5004	LHG	C4-C5-C6-O8
13	B	1202	CLA	O1D-CGD-O2D-CED
13	A	1137	CLA	C5-C6-C7-C8
13	A	1107	CLA	CBA-CGA-O2A-C1
13	A	1112	CLA	CBA-CGA-O2A-C1
13	5	504	CLA	C6-C7-C8-C10
13	B	1217	CLA	C6-C7-C8-C9
13	e	501	CLA	C16-C17-C18-C20
13	f	518	CLA	O1A-CGA-O2A-C1
20	J	5105	LMU	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
13	3	509	CLA	C5-C6-C7-C8
13	5	509	CLA	C10-C11-C12-C13
17	A	5005	LHG	C25-C26-C27-C28
13	A	1138	CLA	C2-C3-C5-C6
13	c	503	CLA	C2-C3-C5-C6
13	2	510	CLA	C15-C16-C17-C18
13	B	1229	CLA	C13-C15-C16-C17
13	d	509	CLA	C15-C16-C17-C18
13	2	502	CLA	C11-C12-C13-C14
13	A	1117	CLA	C16-C17-C18-C19
14	e	521	BCR	C7-C8-C9-C10
13	B	1023	CLA	C4C-C3C-CAC-CBC
13	A	1133	CLA	C10-C11-C12-C13
13	B	1202	CLA	C15-C16-C17-C18
13	A	1110	CLA	C2A-CAA-CBA-CGA
13	A	1125	CLA	O1A-CGA-O2A-C1
13	a	507	CLA	CBA-CGA-O2A-C1
13	A	1126	CLA	O2A-C1-C2-C3
15	4	822	SQD	C44-C45-O47-C7
20	A	1849	LMU	C1-C2-C3-C4
13	4	507	CLA	C5-C6-C7-C8
13	A	1116	CLA	C5-C6-C7-C8
13	B	1203	CLA	C15-C16-C17-C18
13	b	502	CLA	C10-C11-C12-C13
17	A	5005	LHG	C23-C24-C25-C26
13	g	518	CLA	O1A-CGA-O2A-C1
13	d	508	CLA	CBD-CGD-O2D-CED
13	1	508	CLA	C5-C6-C7-C8
13	B	1224	CLA	O1D-CGD-O2D-CED
13	B	1230	CLA	CBA-CGA-O2A-C1
13	a	509	CLA	CBA-CGA-O2A-C1
13	B	1012	CLA	CBD-CGD-O2D-CED
13	A	1126	CLA	C4-C3-C5-C6
13	f	518	CLA	C4-C3-C5-C6
13	a	512	CLA	C4-C3-C5-C6
13	1	509	CLA	C2-C3-C5-C6
13	A	1136	CLA	C2-C3-C5-C6
13	5	504	CLA	C6-C7-C8-C9
13	5	507	CLA	C11-C12-C13-C15
13	A	1116	CLA	C11-C12-C13-C14
13	b	505	CLA	C16-C17-C18-C20
13	A	1110	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
20	B	1843	LMU	C5-C6-C7-C8
20	A	1848	LMU	C1-C2-C3-C4
13	f	503	CLA	C15-C16-C17-C18
13	4	518	CLA	CAA-CBA-CGA-O2A
13	6	505	CLA	CAA-CBA-CGA-O2A
13	g	518	CLA	CAA-CBA-CGA-O2A
13	b	512	CLA	C2A-CAA-CBA-CGA
13	2	501	CLA	C3-C5-C6-C7
15	2	822	SQD	O49-C7-O47-C45
13	2	512	CLA	C2-C1-O2A-CGA
13	e	501	CLA	C16-C17-C18-C19
20	B	1843	LMU	C11-C10-C9-C8
13	2	501	CLA	CBA-CGA-O2A-C1
13	1	518	CLA	CBA-CGA-O2A-C1
13	B	1226	CLA	CBA-CGA-O2A-C1
13	c	518	CLA	CBA-CGA-O2A-C1
13	B	1230	CLA	C10-C11-C12-C13
15	b	822	SQD	C8-C7-O47-C45
20	A	1848	LMU	C9-C10-C11-C12
13	4	501	CLA	C8-C10-C11-C12
13	A	1011	CLA	C8-C10-C11-C12
13	A	1117	CLA	C15-C16-C17-C18
13	A	1013	CLA	O1D-CGD-O2D-CED
17	A	5002	LHG	C11-C12-C13-C14
13	A	1138	CLA	C4-C3-C5-C6
13	B	1224	CLA	C4-C3-C5-C6
13	5	503	CLA	CBA-CGA-O2A-C1
13	a	512	CLA	CBA-CGA-O2A-C1
15	f	822	SQD	C24-C23-O48-C46
13	e	508	CLA	C5-C6-C7-C8
16	B	5002	LMG	C40-C41-C42-C43
13	d	511	CLA	C3-C5-C6-C7
13	3	505	CLA	C14-C13-C15-C16
13	5	510	CLA	C11-C10-C8-C9
13	5	510	CLA	C14-C13-C15-C16
13	6	502	CLA	C11-C10-C8-C9
13	2	503	CLA	C11-C10-C8-C9
13	2	510	CLA	C6-C7-C8-C9
13	1	502	CLA	C11-C10-C8-C9
13	A	1109	CLA	C11-C10-C8-C9
13	A	1123	CLA	C6-C7-C8-C9
13	A	1126	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	A	1132	CLA	C14-C13-C15-C16
13	A	1133	CLA	C11-C12-C13-C14
13	A	1138	CLA	C11-C10-C8-C9
13	B	1012	CLA	C11-C10-C8-C9
13	B	1202	CLA	C14-C13-C15-C16
13	B	1204	CLA	C6-C7-C8-C9
13	B	1211	CLA	C11-C12-C13-C14
13	B	1214	CLA	C11-C12-C13-C14
13	B	1214	CLA	C14-C13-C15-C16
13	B	1224	CLA	C6-C7-C8-C9
13	B	1207	CLA	C11-C12-C13-C14
13	c	501	CLA	C11-C12-C13-C14
13	f	501	CLA	C6-C7-C8-C9
13	f	505	CLA	C14-C13-C15-C16
13	b	503	CLA	C14-C13-C15-C16
13	a	505	CLA	C11-C12-C13-C14
13	a	505	CLA	C14-C13-C15-C16
18	A	2001	PQN	C19-C18-C20-C21
13	B	1223	CLA	O1D-CGD-O2D-CED
13	4	510	CLA	C5-C6-C7-C8
13	c	501	CLA	C5-C6-C7-C8
13	g	510	CLA	C13-C15-C16-C17
13	4	503	CLA	C4B-C3B-CAB-CBB
13	5	507	CLA	C4B-C3B-CAB-CBB
13	5	516	CLA	C4B-C3B-CAB-CBB
13	6	503	CLA	C4B-C3B-CAB-CBB
13	6	506	CLA	C4B-C3B-CAB-CBB
13	1	517	CLA	C4B-C3B-CAB-CBB
13	1	518	CLA	C4B-C3B-CAB-CBB
13	1	519	CLA	C4B-C3B-CAB-CBB
13	B	1203	CLA	C4B-C3B-CAB-CBB
13	B	1238	CLA	C4B-C3B-CAB-CBB
13	d	503	CLA	C4B-C3B-CAB-CBB
13	d	516	CLA	C4B-C3B-CAB-CBB
13	d	517	CLA	C4B-C3B-CAB-CBB
13	e	502	CLA	C4B-C3B-CAB-CBB
13	e	516	CLA	C4B-C3B-CAB-CBB
13	e	517	CLA	C4B-C3B-CAB-CBB
13	f	517	CLA	C4B-C3B-CAB-CBB
13	g	507	CLA	C4B-C3B-CAB-CBB
13	b	516	CLA	C4B-C3B-CAB-CBB
13	a	511	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	6	509	CLA	C8-C10-C11-C12
13	1	503	CLA	C8-C10-C11-C12
13	A	1125	CLA	C10-C11-C12-C13
13	b	501	CLA	C5-C6-C7-C8
13	e	518	CLA	C6-C7-C8-C9
13	b	505	CLA	C16-C17-C18-C19
13	6	518	CLA	C2A-CAA-CBA-CGA
13	K	1103	CLA	C2A-CAA-CBA-CGA
17	A	5004	LHG	O6-C4-C5-C6
13	3	505	CLA	C12-C13-C15-C16
13	4	505	CLA	C12-C13-C15-C16
13	5	509	CLA	C11-C12-C13-C15
13	5	510	CLA	C11-C10-C8-C7
13	6	503	CLA	C11-C10-C8-C7
13	6	505	CLA	C6-C7-C8-C10
13	6	509	CLA	C6-C7-C8-C10
13	2	503	CLA	C11-C10-C8-C7
13	2	505	CLA	C12-C13-C15-C16
13	2	507	CLA	C6-C7-C8-C10
13	2	510	CLA	C6-C7-C8-C10
13	1	509	CLA	C12-C13-C15-C16
13	A	1103	CLA	C11-C10-C8-C7
13	A	1104	CLA	C12-C13-C15-C16
13	A	1126	CLA	C12-C13-C15-C16
13	B	1012	CLA	C11-C10-C8-C7
13	B	1021	CLA	C11-C12-C13-C15
13	B	1201	CLA	C11-C10-C8-C7
13	B	1202	CLA	C6-C7-C8-C10
13	B	1203	CLA	C6-C7-C8-C10
13	B	1204	CLA	C6-C7-C8-C10
13	B	1210	CLA	C11-C12-C13-C15
13	B	1210	CLA	C12-C13-C15-C16
13	B	1214	CLA	C11-C12-C13-C15
13	B	1229	CLA	C12-C13-C15-C16
13	B	1235	CLA	C12-C13-C15-C16
13	c	505	CLA	C12-C13-C15-C16
13	c	507	CLA	C6-C7-C8-C10
13	d	502	CLA	C11-C10-C8-C7
13	f	501	CLA	C11-C12-C13-C15
13	f	501	CLA	C12-C13-C15-C16
13	f	503	CLA	C6-C7-C8-C10
13	g	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	b	510	CLA	C6-C7-C8-C10
13	4	503	CLA	C8-C10-C11-C12
13	A	1111	CLA	C10-C11-C12-C13
13	A	1112	CLA	O1A-CGA-O2A-C1
13	A	1107	CLA	O1A-CGA-O2A-C1
16	2	5104	LMG	C31-C32-C33-C34
13	2	512	CLA	C3A-C2A-CAA-CBA
13	2	517	CLA	C3A-C2A-CAA-CBA
13	1	509	CLA	C4-C3-C5-C6
13	A	1112	CLA	C3A-C2A-CAA-CBA
13	A	1117	CLA	C4-C3-C5-C6
13	A	1125	CLA	C4-C3-C5-C6
13	A	1126	CLA	C3A-C2A-CAA-CBA
13	A	1130	CLA	C3A-C2A-CAA-CBA
13	A	1136	CLA	C4-C3-C5-C6
13	B	1213	CLA	C3A-C2A-CAA-CBA
13	B	1221	CLA	C3A-C2A-CAA-CBA
13	f	512	CLA	C3A-C2A-CAA-CBA
13	2	509	CLA	C5-C6-C7-C8
13	B	1225	CLA	C13-C15-C16-C17
13	a	508	CLA	C5-C6-C7-C8
13	1	518	CLA	C2-C3-C5-C6
13	4	510	CLA	O1A-CGA-O2A-C1
13	a	507	CLA	O1A-CGA-O2A-C1
13	b	512	CLA	CBA-CGA-O2A-C1
14	3	523	BCR	C9-C10-C11-C12
14	5	524	BCR	C13-C14-C15-C16
14	d	523	BCR	C9-C10-C11-C12
13	B	1216	CLA	C3-C5-C6-C7
13	g	502	CLA	C3-C5-C6-C7
13	A	1140	CLA	C13-C15-C16-C17
14	e	521	BCR	C11-C12-C13-C35
14	J	4012	BCR	C11-C12-C13-C14
13	A	1119	CLA	C2A-CAA-CBA-CGA
13	J	1302	CLA	C2A-CAA-CBA-CGA
13	g	519	CLA	C2A-CAA-CBA-CGA
13	B	1229	CLA	O1D-CGD-O2D-CED
13	3	509	CLA	C15-C16-C17-C18
16	1	5104	LMG	C7-C8-C9-O8
13	c	508	CLA	C3-C5-C6-C7
16	B	5002	LMG	C32-C33-C34-C35
13	A	1134	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
13	g	502	CLA	C11-C12-C13-C14
13	A	1116	CLA	C4-C3-C5-C6
13	f	507	CLA	C4-C3-C5-C6
13	d	504	CLA	C5-C6-C7-C8
13	5	507	CLA	C11-C12-C13-C14
13	a	501	CLA	C16-C17-C18-C19
13	5	507	CLA	C2B-C3B-CAB-CBB
13	B	1239	CLA	C2B-C3B-CAB-CBB
13	B	1207	CLA	C2B-C3B-CAB-CBB
13	c	501	CLA	C2B-C3B-CAB-CBB
13	d	516	CLA	C2B-C3B-CAB-CBB
13	g	517	CLA	C2B-C3B-CAB-CBB
13	b	517	CLA	C2B-C3B-CAB-CBB
14	3	524	BCR	C1-C6-C7-C8
14	5	521	BCR	C5-C6-C7-C8
14	5	521	BCR	C23-C24-C25-C30
14	5	524	BCR	C1-C6-C7-C8
14	2	521	BCR	C23-C24-C25-C30
14	1	521	BCR	C5-C6-C7-C8
14	1	521	BCR	C23-C24-C25-C26
14	A	4002	BCR	C1-C6-C7-C8
14	A	4011	BCR	C23-C24-C25-C30
14	e	522	BCR	C1-C6-C7-C8
14	a	522	BCR	C1-C6-C7-C8
13	3	518	CLA	CAA-CBA-CGA-O2A
13	b	518	CLA	CAA-CBA-CGA-O2A
13	6	510	CLA	C5-C6-C7-C8
13	e	505	CLA	C5-C6-C7-C8
16	B	5002	LMG	C33-C34-C35-C36
20	A	1848	LMU	C4-C5-C6-C7
13	B	1202	CLA	C16-C17-C18-C19
13	B	1217	CLA	C6-C7-C8-C10
13	3	519	CLA	C2A-CAA-CBA-CGA
13	B	1228	CLA	C5-C6-C7-C8
13	g	510	CLA	C5-C6-C7-C8
15	2	822	SQD	O6-C44-C45-O47
15	e	822	SQD	O47-C45-C46-O48
15	g	822	SQD	O47-C45-C46-O48
13	5	505	CLA	C13-C15-C16-C17
13	1	501	CLA	C15-C16-C17-C18
13	A	1124	CLA	C5-C6-C7-C8
13	B	1224	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
13	f	507	CLA	C2-C3-C5-C6
13	A	1126	CLA	C16-C17-C18-C19
13	e	518	CLA	C6-C7-C8-C10
13	g	502	CLA	C11-C12-C13-C15
17	A	5004	LHG	C10-C11-C12-C13
16	1	5104	LMG	C28-C29-C30-C31
13	f	504	CLA	C3-C5-C6-C7
13	1	517	CLA	CBD-CGD-O2D-CED
13	6	503	CLA	C11-C12-C13-C14
13	2	507	CLA	C6-C7-C8-C9
13	A	1103	CLA	C11-C10-C8-C9
13	A	1118	CLA	C6-C7-C8-C9
13	B	1202	CLA	C11-C10-C8-C9
13	B	1211	CLA	C11-C10-C8-C9
13	B	1225	CLA	C11-C12-C13-C14
13	c	507	CLA	C6-C7-C8-C9
13	d	501	CLA	C11-C10-C8-C9
13	a	509	CLA	O1A-CGA-O2A-C1
13	A	1113	CLA	O2A-C1-C2-C3
13	5	510	CLA	CBD-CGD-O2D-CED
13	B	1217	CLA	O1D-CGD-O2D-CED
13	e	513	CLA	C2A-CAA-CBA-CGA
13	a	506	CLA	C2A-CAA-CBA-CGA
13	e	512	CLA	CBA-CGA-O2A-C1
13	A	1137	CLA	C4-C3-C5-C6
14	e	521	BCR	C9-C10-C11-C12
13	A	1117	CLA	C2-C3-C5-C6
13	A	1125	CLA	C2-C3-C5-C6
13	A	1134	CLA	C6-C7-C8-C9
13	e	502	CLA	C11-C12-C13-C14
13	a	501	CLA	C16-C17-C18-C20
17	A	5005	LHG	C1-C2-C3-O3
13	b	503	CLA	CBA-CGA-O2A-C1
13	A	1123	CLA	C13-C15-C16-C17
13	3	508	CLA	C6-C7-C8-C10
13	1	507	CLA	C11-C12-C13-C15
13	A	1127	CLA	C16-C17-C18-C19
13	B	1234	CLA	C11-C12-C13-C15
13	c	502	CLA	C11-C12-C13-C15
13	5	504	CLA	C5-C6-C7-C8
13	6	509	CLA	C10-C11-C12-C13
20	J	5105	LMU	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
13	3	507	CLA	C6-C7-C8-C10
13	5	509	CLA	C6-C7-C8-C10
13	5	509	CLA	C11-C10-C8-C7
13	6	502	CLA	C6-C7-C8-C10
13	6	505	CLA	C12-C13-C15-C16
13	6	510	CLA	C6-C7-C8-C10
13	1	507	CLA	C6-C7-C8-C10
13	A	1022	CLA	C12-C13-C15-C16
13	A	1107	CLA	C6-C7-C8-C10
13	A	1107	CLA	C11-C12-C13-C15
13	A	1118	CLA	C6-C7-C8-C10
13	A	1125	CLA	C6-C7-C8-C10
13	B	1202	CLA	C11-C10-C8-C7
13	B	1211	CLA	C11-C10-C8-C7
13	B	1216	CLA	C11-C10-C8-C7
13	B	1226	CLA	C11-C10-C8-C7
13	d	507	CLA	C6-C7-C8-C10
13	d	509	CLA	C6-C7-C8-C10
13	d	510	CLA	C12-C13-C15-C16
13	e	501	CLA	C12-C13-C15-C16
13	g	503	CLA	C11-C10-C8-C7
13	g	509	CLA	C11-C12-C13-C15
13	g	510	CLA	C6-C7-C8-C10
13	b	507	CLA	C6-C7-C8-C10
13	b	509	CLA	C12-C13-C15-C16
13	b	510	CLA	C12-C13-C15-C16
13	a	510	CLA	C11-C12-C13-C15
18	A	2001	PQN	C21-C22-C23-C25
16	B	5002	LMG	C28-C29-C30-C31
13	d	502	CLA	C10-C11-C12-C13
14	c	524	BCR	C21-C22-C23-C24
14	b	521	BCR	C17-C18-C19-C20
13	B	1234	CLA	CBA-CGA-O2A-C1
13	a	508	CLA	CBA-CGA-O2A-C1
13	5	503	CLA	O1A-CGA-O2A-C1
13	2	501	CLA	O1A-CGA-O2A-C1
13	g	502	CLA	C5-C6-C7-C8
13	4	503	CLA	C2A-CAA-CBA-CGA
13	2	501	CLA	C2A-CAA-CBA-CGA
13	2	512	CLA	C2A-CAA-CBA-CGA
13	c	513	CLA	C2A-CAA-CBA-CGA
13	d	501	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
13	a	518	CLA	C2A-CAA-CBA-CGA
13	2	502	CLA	C11-C12-C13-C15
13	1	518	CLA	O1A-CGA-O2A-C1
13	B	1226	CLA	O1A-CGA-O2A-C1
13	c	518	CLA	O1A-CGA-O2A-C1
13	a	512	CLA	O1A-CGA-O2A-C1
15	f	822	SQD	O10-C23-O48-C46
17	A	5004	LHG	O1-C1-C2-C3
13	3	509	CLA	C3-C5-C6-C7
13	A	1101	CLA	C10-C11-C12-C13
15	3	822	SQD	C46-C45-O47-C7
15	c	822	SQD	C46-C45-O47-C7
15	d	822	SQD	C46-C45-O47-C7
15	g	822	SQD	C46-C45-O47-C7
13	B	1230	CLA	O1A-CGA-O2A-C1
13	b	512	CLA	O1A-CGA-O2A-C1
13	4	505	CLA	C16-C17-C18-C20
13	A	1237	CLA	C10-C11-C12-C13
13	1	505	CLA	C13-C15-C16-C17
15	b	822	SQD	O49-C7-O47-C45
17	A	5002	LHG	O6-C4-C5-O7
15	g	822	SQD	O6-C44-C45-C46
13	4	505	CLA	C15-C16-C17-C18
13	3	518	CLA	C2A-CAA-CBA-CGA
13	f	504	CLA	C2A-CAA-CBA-CGA
13	e	510	CLA	C2-C3-C5-C6
13	2	505	CLA	C15-C16-C17-C18
13	A	1128	CLA	C5-C6-C7-C8
18	A	2001	PQN	C23-C25-C26-C27
13	e	508	CLA	C3-C5-C6-C7
15	6	822	SQD	O6-C44-C45-O47
15	f	822	SQD	O47-C45-C46-O48
17	A	5004	LHG	O7-C5-C6-O8
13	6	501	CLA	C13-C15-C16-C17
13	3	503	CLA	C11-C10-C8-C9
13	6	505	CLA	C6-C7-C8-C9
13	6	510	CLA	C6-C7-C8-C9
13	B	1211	CLA	C6-C7-C8-C9
13	B	1216	CLA	C11-C10-C8-C9
13	B	1221	CLA	C11-C10-C8-C9
13	B	1226	CLA	C11-C10-C8-C9
13	d	503	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	d	507	CLA	C6-C7-C8-C9
13	e	501	CLA	C14-C13-C15-C16
13	g	509	CLA	C11-C12-C13-C14
13	a	509	CLA	C14-C13-C15-C16
13	e	502	CLA	C11-C12-C13-C15
20	J	5105	LMU	C5-C6-C7-C8
13	e	512	CLA	O1A-CGA-O2A-C1
13	a	508	CLA	O1A-CGA-O2A-C1
17	A	5003	LHG	C24-C23-O8-C6
13	a	501	CLA	C5-C6-C7-C8
17	A	5004	LHG	C25-C26-C27-C28
13	g	516	CLA	O1D-CGD-O2D-CED
13	A	1119	CLA	C4-C3-C5-C6
13	1	518	CLA	C3-C5-C6-C7
13	c	502	CLA	C3-C5-C6-C7
13	b	509	CLA	C3-C5-C6-C7
13	6	505	CLA	C10-C11-C12-C13
13	A	1106	CLA	C16-C17-C18-C20
13	A	1115	CLA	C11-C12-C13-C15
13	A	1132	CLA	C16-C17-C18-C20
13	f	518	CLA	C6-C7-C8-C9
13	A	1116	CLA	C3-C5-C6-C7
13	a	510	CLA	C3-C5-C6-C7
13	b	503	CLA	O1A-CGA-O2A-C1
13	c	511	CLA	CBA-CGA-O2A-C1
17	A	5004	LHG	O1-C1-C2-O2
13	6	508	CLA	C3-C5-C6-C7
13	A	1126	CLA	C3-C5-C6-C7
13	A	1237	CLA	C3-C5-C6-C7
13	B	1224	CLA	C10-C11-C12-C13
14	B	4006	BCR	C11-C12-C13-C35
13	3	516	CLA	C4B-C3B-CAB-CBB
13	5	501	CLA	C1A-C2A-CAA-CBA
13	5	506	CLA	C4B-C3B-CAB-CBB
13	5	508	CLA	C1A-C2A-CAA-CBA
13	5	513	CLA	C1A-C2A-CAA-CBA
13	5	517	CLA	C4B-C3B-CAB-CBB
13	6	512	CLA	C4B-C3B-CAB-CBB
13	6	517	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	C1A-C2A-CAA-CBA
13	2	503	CLA	C4B-C3B-CAB-CBB
13	2	506	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	2	508	CLA	C1A-C2A-CAA-CBA
13	2	512	CLA	C1A-C2A-CAA-CBA
13	2	517	CLA	C1A-C2A-CAA-CBA
13	2	517	CLA	C4B-C3B-CAB-CBB
13	1	508	CLA	C1A-C2A-CAA-CBA
13	1	512	CLA	C4B-C3B-CAB-CBB
13	1	516	CLA	C4B-C3B-CAB-CBB
13	1	517	CLA	C1A-C2A-CAA-CBA
13	A	1109	CLA	C4B-C3B-CAB-CBB
13	A	1110	CLA	C4B-C3B-CAB-CBB
13	A	1114	CLA	C4B-C3B-CAB-CBB
13	A	1116	CLA	C4B-C3B-CAB-CBB
13	A	1122	CLA	C1A-C2A-CAA-CBA
13	A	1128	CLA	C1A-C2A-CAA-CBA
13	A	1129	CLA	C4B-C3B-CAB-CBB
13	A	1134	CLA	C4B-C3B-CAB-CBB
13	A	1137	CLA	C4B-C3B-CAB-CBB
13	A	1139	CLA	C4B-C3B-CAB-CBB
13	A	1237	CLA	C4B-C3B-CAB-CBB
13	B	1214	CLA	C4B-C3B-CAB-CBB
13	B	1207	CLA	C4B-C3B-CAB-CBB
13	c	501	CLA	C4B-C3B-CAB-CBB
13	c	517	CLA	C4B-C3B-CAB-CBB
13	d	501	CLA	C4B-C3B-CAB-CBB
13	d	508	CLA	C1A-C2A-CAA-CBA
13	d	512	CLA	C4B-C3B-CAB-CBB
13	e	501	CLA	C4B-C3B-CAB-CBB
13	e	516	CLA	C1A-C2A-CAA-CBA
13	f	501	CLA	C4B-C3B-CAB-CBB
13	f	503	CLA	C4B-C3B-CAB-CBB
13	f	508	CLA	C1A-C2A-CAA-CBA
13	f	518	CLA	C4B-C3B-CAB-CBB
13	g	508	CLA	C1A-C2A-CAA-CBA
13	g	516	CLA	C4B-C3B-CAB-CBB
13	b	517	CLA	C4B-C3B-CAB-CBB
13	a	501	CLA	C4B-C3B-CAB-CBB
13	a	511	CLA	C1A-C2A-CAA-CBA
13	d	508	CLA	O1D-CGD-O2D-CED
13	A	1133	CLA	CBA-CGA-O2A-C1
13	1	503	CLA	C4-C3-C5-C6
13	B	1218	CLA	C4-C3-C5-C6
13	B	1021	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
13	6	518	CLA	CAA-CBA-CGA-O2A
13	A	1011	CLA	CAA-CBA-CGA-O2A
14	M	4021	BCR	C7-C8-C9-C10
14	d	524	BCR	C21-C22-C23-C24
13	A	1122	CLA	C11-C12-C13-C15
13	b	510	CLA	C2A-CAA-CBA-CGA
13	A	1105	CLA	CBD-CGD-O2D-CED
13	4	505	CLA	C5-C6-C7-C8
13	e	501	CLA	C3-C5-C6-C7
13	3	501	CLA	C11-C12-C13-C15
13	4	501	CLA	C11-C10-C8-C7
13	4	501	CLA	C11-C12-C13-C15
13	5	503	CLA	C11-C10-C8-C7
13	6	507	CLA	C11-C10-C8-C7
13	6	510	CLA	C12-C13-C15-C16
13	2	509	CLA	C6-C7-C8-C10
13	2	509	CLA	C11-C10-C8-C7
13	2	510	CLA	C11-C12-C13-C15
13	1	505	CLA	C12-C13-C15-C16
13	A	1103	CLA	C11-C12-C13-C15
13	A	1116	CLA	C6-C7-C8-C10
13	A	1123	CLA	C11-C10-C8-C7
13	A	1131	CLA	C12-C13-C15-C16
13	A	1237	CLA	C6-C7-C8-C10
13	A	1011	CLA	C11-C10-C8-C7
13	B	1012	CLA	C11-C12-C13-C15
13	B	1213	CLA	C6-C7-C8-C10
13	B	1218	CLA	C6-C7-C8-C10
13	B	1235	CLA	C11-C12-C13-C15
13	c	509	CLA	C11-C10-C8-C7
13	d	505	CLA	C11-C10-C8-C7
13	d	509	CLA	C11-C10-C8-C7
13	f	502	CLA	C11-C10-C8-C7
13	g	501	CLA	C6-C7-C8-C10
13	g	501	CLA	C11-C10-C8-C7
13	g	502	CLA	C6-C7-C8-C10
13	b	505	CLA	C11-C12-C13-C15
13	a	509	CLA	C6-C7-C8-C10
18	A	2001	PQN	C22-C23-C25-C26
18	B	2002	PQN	C16-C17-C18-C20
13	4	505	CLA	C16-C17-C18-C19
13	B	1215	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
13	e	505	CLA	C16-C17-C18-C19
13	f	518	CLA	C6-C7-C8-C10
13	b	508	CLA	C6-C7-C8-C9
13	B	1234	CLA	O1A-CGA-O2A-C1
13	B	1210	CLA	C3A-C2A-CAA-CBA
13	3	502	CLA	C11-C12-C13-C15
13	B	1234	CLA	C11-C12-C13-C14
13	5	509	CLA	C8-C10-C11-C12
17	A	5001	LHG	C24-C23-O8-C6
17	A	5004	LHG	O6-C4-C5-O7
13	b	518	CLA	C2A-CAA-CBA-CGA
13	5	501	CLA	C14-C13-C15-C16
13	6	505	CLA	C14-C13-C15-C16
13	2	501	CLA	C6-C7-C8-C9
13	2	505	CLA	C14-C13-C15-C16
13	A	1107	CLA	C11-C12-C13-C14
13	g	503	CLA	C11-C10-C8-C9
13	g	510	CLA	C6-C7-C8-C9
13	b	507	CLA	C6-C7-C8-C9
13	b	509	CLA	C14-C13-C15-C16
13	b	510	CLA	C6-C7-C8-C9
13	b	510	CLA	C14-C13-C15-C16
13	c	511	CLA	O1A-CGA-O2A-C1
13	4	501	CLA	C10-C11-C12-C13
13	B	1218	CLA	C8-C10-C11-C12
14	2	522	BCR	C13-C14-C15-C16
14	b	521	BCR	C9-C10-C11-C12
18	B	2002	PQN	C13-C15-C16-C17
13	5	509	CLA	C15-C16-C17-C18
15	f	822	SQD	O6-C44-C45-O47
15	g	822	SQD	O6-C44-C45-O47
15	b	822	SQD	O6-C44-C45-O47
13	a	503	CLA	C13-C15-C16-C17
13	1	507	CLA	C11-C12-C13-C14
15	2	822	SQD	O6-C44-C45-C46
15	f	822	SQD	O6-C44-C45-C46
15	b	822	SQD	O6-C44-C45-C46
13	3	505	CLA	C4-C3-C5-C6
13	6	508	CLA	C4-C3-C5-C6
13	4	505	CLA	C8-C10-C11-C12
13	3	502	CLA	CAD-CBD-CGD-O2D
13	3	506	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
13	4	501	CLA	CAD-CBD-CGD-O2D
13	4	507	CLA	CAD-CBD-CGD-O2D
13	4	517	CLA	CAD-CBD-CGD-O2D
13	5	516	CLA	CAD-CBD-CGD-O2D
13	5	517	CLA	CAD-CBD-CGD-O2D
13	6	501	CLA	CAD-CBD-CGD-O2D
13	6	505	CLA	CAD-CBD-CGD-O2D
13	6	517	CLA	CAD-CBD-CGD-O2D
13	2	517	CLA	CAD-CBD-CGD-O2D
13	1	504	CLA	CAD-CBD-CGD-O2D
13	A	1111	CLA	CAD-CBD-CGD-O2D
13	B	1202	CLA	CAD-CBD-CGD-O2D
13	K	1401	CLA	CAD-CBD-CGD-O2D
13	d	507	CLA	CAD-CBD-CGD-O2D
13	e	506	CLA	CAD-CBD-CGD-O2D
13	f	507	CLA	CAD-CBD-CGD-O2D
13	f	510	CLA	CAD-CBD-CGD-O2D
13	g	519	CLA	CAD-CBD-CGD-O2D
13	b	509	CLA	CAD-CBD-CGD-O2D
13	a	507	CLA	CAD-CBD-CGD-O2D
13	4	510	CLA	C16-C17-C18-C20
13	a	503	CLA	C3-C5-C6-C7
13	B	1207	CLA	C2A-CAA-CBA-CGA
13	c	512	CLA	C2A-CAA-CBA-CGA
20	B	1843	LMU	C1-C2-C3-C4
13	B	1223	CLA	C5-C6-C7-C8
17	A	5003	LHG	O10-C23-O8-C6
13	A	1133	CLA	O1A-CGA-O2A-C1
13	3	502	CLA	CAD-CBD-CGD-O1D
13	3	506	CLA	CAD-CBD-CGD-O1D
13	3	516	CLA	CHA-CBD-CGD-O1D
13	3	516	CLA	CHA-CBD-CGD-O2D
13	4	501	CLA	CAD-CBD-CGD-O1D
13	4	504	CLA	CAD-CBD-CGD-O1D
13	4	507	CLA	CAD-CBD-CGD-O1D
13	4	517	CLA	CAD-CBD-CGD-O1D
13	4	518	CLA	CHA-CBD-CGD-O1D
13	4	518	CLA	CHA-CBD-CGD-O2D
13	5	506	CLA	CAD-CBD-CGD-O1D
13	5	510	CLA	CHA-CBD-CGD-O1D
13	5	510	CLA	CHA-CBD-CGD-O2D
13	5	516	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	5	517	CLA	CAD-CBD-CGD-O1D
13	5	518	CLA	CHA-CBD-CGD-O1D
13	5	518	CLA	CHA-CBD-CGD-O2D
13	6	501	CLA	CAD-CBD-CGD-O1D
13	6	504	CLA	CAD-CBD-CGD-O1D
13	6	505	CLA	CAD-CBD-CGD-O1D
13	6	516	CLA	CHA-CBD-CGD-O1D
13	6	516	CLA	CHA-CBD-CGD-O2D
13	6	517	CLA	CAD-CBD-CGD-O1D
13	6	519	CLA	CHA-CBD-CGD-O2D
13	2	502	CLA	CHA-CBD-CGD-O1D
13	2	504	CLA	CAD-CBD-CGD-O1D
13	2	506	CLA	CHA-CBD-CGD-O1D
13	2	517	CLA	CAD-CBD-CGD-O1D
13	1	502	CLA	CHA-CBD-CGD-O1D
13	1	504	CLA	CAD-CBD-CGD-O1D
13	A	1103	CLA	CAD-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O1D
13	A	1106	CLA	CHA-CBD-CGD-O2D
13	A	1111	CLA	CAD-CBD-CGD-O1D
13	A	1131	CLA	CAD-CBD-CGD-O1D
13	B	1202	CLA	CAD-CBD-CGD-O1D
13	B	1232	CLA	CHA-CBD-CGD-O1D
13	K	1401	CLA	CAD-CBD-CGD-O1D
13	c	501	CLA	CAD-CBD-CGD-O1D
13	d	502	CLA	CHA-CBD-CGD-O1D
13	d	502	CLA	CHA-CBD-CGD-O2D
13	d	507	CLA	CAD-CBD-CGD-O1D
13	d	509	CLA	CHA-CBD-CGD-O2D
13	d	510	CLA	CHA-CBD-CGD-O1D
13	d	510	CLA	CHA-CBD-CGD-O2D
13	d	518	CLA	CHA-CBD-CGD-O1D
13	d	518	CLA	CHA-CBD-CGD-O2D
13	e	506	CLA	CAD-CBD-CGD-O1D
13	e	507	CLA	CAD-CBD-CGD-O1D
13	f	507	CLA	CAD-CBD-CGD-O1D
13	f	510	CLA	CAD-CBD-CGD-O1D
13	f	518	CLA	CHA-CBD-CGD-O1D
13	f	518	CLA	CHA-CBD-CGD-O2D
13	f	519	CLA	CHA-CBD-CGD-O1D
13	f	519	CLA	CHA-CBD-CGD-O2D
13	g	517	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
13	g	518	CLA	CHA-CBD-CGD-O1D
13	g	518	CLA	CHA-CBD-CGD-O2D
13	g	519	CLA	CAD-CBD-CGD-O1D
13	b	502	CLA	CHA-CBD-CGD-O1D
13	b	502	CLA	CHA-CBD-CGD-O2D
13	b	504	CLA	CAD-CBD-CGD-O1D
13	b	509	CLA	CAD-CBD-CGD-O1D
13	b	518	CLA	CHA-CBD-CGD-O1D
13	b	518	CLA	CHA-CBD-CGD-O2D
13	a	502	CLA	CHA-CBD-CGD-O1D
13	a	502	CLA	CHA-CBD-CGD-O2D
13	a	503	CLA	CHA-CBD-CGD-O1D
13	a	503	CLA	CHA-CBD-CGD-O2D
13	a	507	CLA	CAD-CBD-CGD-O1D
13	a	511	CLA	CHA-CBD-CGD-O1D
13	a	517	CLA	CHA-CBD-CGD-O1D
13	a	517	CLA	CHA-CBD-CGD-O2D
14	4	524	BCR	C19-C20-C21-C22
14	F	4015	BCR	C9-C10-C11-C12
14	f	522	BCR	C13-C14-C15-C16
14	a	523	BCR	C19-C20-C21-C22
17	A	5005	LHG	C4-O6-P-O5
17	A	5001	LHG	C3-O3-P-O5
17	A	5002	LHG	C4-O6-P-O5
17	A	5003	LHG	C3-O3-P-O5
13	d	511	CLA	C4-C3-C5-C6
13	f	504	CLA	C4-C3-C5-C6
13	f	505	CLA	C4-C3-C5-C6
13	3	518	CLA	C2B-C3B-CAB-CBB
13	5	506	CLA	C2B-C3B-CAB-CBB
13	5	517	CLA	C2B-C3B-CAB-CBB
13	6	508	CLA	C2B-C3B-CAB-CBB
13	6	512	CLA	C2B-C3B-CAB-CBB
13	6	517	CLA	C2B-C3B-CAB-CBB
13	6	518	CLA	C2B-C3B-CAB-CBB
13	2	506	CLA	C2B-C3B-CAB-CBB
13	1	512	CLA	C2B-C3B-CAB-CBB
13	1	516	CLA	C2B-C3B-CAB-CBB
13	1	517	CLA	C2B-C3B-CAB-CBB
13	A	1013	CLA	C2B-C3B-CAB-CBB
13	A	1114	CLA	C2B-C3B-CAB-CBB
13	A	1116	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	A	1134	CLA	C2B-C3B-CAB-CBB
13	A	1011	CLA	C2B-C3B-CAB-CBB
13	B	1203	CLA	C2B-C3B-CAB-CBB
13	B	1227	CLA	C2B-C3B-CAB-CBB
13	F	1301	CLA	C2B-C3B-CAB-CBB
13	c	517	CLA	C2B-C3B-CAB-CBB
13	f	501	CLA	C2B-C3B-CAB-CBB
13	f	503	CLA	C2B-C3B-CAB-CBB
13	f	518	CLA	C2B-C3B-CAB-CBB
13	g	507	CLA	C2B-C3B-CAB-CBB
13	g	511	CLA	C2B-C3B-CAB-CBB
13	b	518	CLA	C2B-C3B-CAB-CBB
13	a	501	CLA	C2B-C3B-CAB-CBB
14	4	522	BCR	C5-C6-C7-C8
14	B	4009	BCR	C23-C24-C25-C30
14	c	521	BCR	C5-C6-C7-C8
17	A	5003	LHG	C17-C18-C19-C20
13	5	518	CLA	CAA-CBA-CGA-O2A
13	2	510	CLA	C2-C3-C5-C6
13	c	510	CLA	C2-C3-C5-C6
13	1	502	CLA	C8-C10-C11-C12
13	e	507	CLA	C8-C10-C11-C12
14	B	4004	BCR	C37-C22-C23-C24
14	b	522	BCR	C37-C22-C23-C24
13	a	509	CLA	C3-C5-C6-C7
13	f	503	CLA	C5-C6-C7-C8
13	B	1219	CLA	C6-C7-C8-C9
13	e	508	CLA	C6-C7-C8-C9
13	f	518	CLA	CAA-CBA-CGA-O2A
14	3	522	BCR	C7-C8-C9-C10
13	B	1213	CLA	C13-C15-C16-C17
13	F	1301	CLA	CBD-CGD-O2D-CED
13	B	1229	CLA	C2C-C3C-CAC-CBC
13	4	509	CLA	C3-C5-C6-C7
13	g	509	CLA	C3-C5-C6-C7
13	6	503	CLA	C10-C11-C12-C13
13	1	517	CLA	O1D-CGD-O2D-CED
13	B	1229	CLA	CAA-CBA-CGA-O2A
13	1	510	CLA	C5-C6-C7-C8
13	4	508	CLA	C5-C6-C7-C8
13	B	1205	CLA	C13-C15-C16-C17
15	6	822	SQD	C44-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
15	1	822	SQD	C44-C45-O47-C7
15	b	822	SQD	C46-C45-O47-C7
15	a	822	SQD	C46-C45-O47-C7
13	6	509	CLA	C5-C6-C7-C8
13	A	1119	CLA	C2-C3-C5-C6
13	A	1106	CLA	C16-C17-C18-C19
13	A	1115	CLA	C11-C12-C13-C14
13	a	509	CLA	C15-C16-C17-C18
13	5	509	CLA	C11-C10-C8-C9
13	5	509	CLA	C11-C12-C13-C14
13	6	503	CLA	C14-C13-C15-C16
13	1	503	CLA	C14-C13-C15-C16
13	A	1022	CLA	C11-C10-C8-C9
13	A	1107	CLA	C11-C10-C8-C9
13	A	1119	CLA	C11-C10-C8-C9
13	A	1125	CLA	C11-C10-C8-C9
13	A	1139	CLA	C11-C10-C8-C9
13	A	1237	CLA	C6-C7-C8-C9
13	B	1201	CLA	C11-C10-C8-C9
13	B	1214	CLA	C11-C10-C8-C9
13	B	1235	CLA	C14-C13-C15-C16
13	B	1239	CLA	C14-C13-C15-C16
13	f	502	CLA	C11-C10-C8-C9
13	g	501	CLA	C11-C10-C8-C9
13	g	507	CLA	C11-C10-C8-C9
13	a	507	CLA	C6-C7-C8-C9
13	6	503	CLA	C12-C13-C15-C16
13	1	501	CLA	C12-C13-C15-C16
13	A	1022	CLA	C11-C10-C8-C7
13	A	1104	CLA	C11-C10-C8-C7
13	A	1119	CLA	C11-C10-C8-C7
13	A	1138	CLA	C6-C7-C8-C10
13	B	1238	CLA	C11-C12-C13-C15
13	B	1239	CLA	C12-C13-C15-C16
13	a	505	CLA	C6-C7-C8-C10
13	a	505	CLA	C11-C10-C8-C7
13	c	503	CLA	C5-C6-C7-C8
13	A	1132	CLA	C16-C17-C18-C19
13	B	1221	CLA	C11-C12-C13-C15
13	2	518	CLA	CAA-CBA-CGA-O2A
13	B	1202	CLA	CAA-CBA-CGA-O2A
13	6	509	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
13	B	1012	CLA	O1D-CGD-O2D-CED
13	2	512	CLA	C4-C3-C5-C6
13	f	518	CLA	C2-C3-C5-C6
13	a	512	CLA	C2-C3-C5-C6
13	5	510	CLA	O1D-CGD-O2D-CED
13	b	508	CLA	C6-C7-C8-C10
13	e	504	CLA	CAA-CBA-CGA-O2A
17	A	5005	LHG	C24-C23-O8-C6
13	B	1206	CLA	C16-C17-C18-C20
15	6	822	SQD	O47-C7-C8-C9
13	A	1138	CLA	C2A-CAA-CBA-CGA
13	d	503	CLA	C2A-CAA-CBA-CGA
13	B	1201	CLA	CBD-CGD-O2D-CED
13	5	511	CLA	C2-C1-O2A-CGA
13	B	1206	CLA	CAA-CBA-CGA-O2A
15	6	822	SQD	O6-C44-C45-C46
13	2	501	CLA	C5-C6-C7-C8
13	A	1102	CLA	CAA-CBA-CGA-O2A
13	e	518	CLA	CAA-CBA-CGA-O2A
13	B	1238	CLA	C16-C17-C18-C20
13	f	509	CLA	C16-C17-C18-C19
13	5	501	CLA	C3-C5-C6-C7
13	d	501	CLA	C3-C5-C6-C7
14	b	524	BCR	C7-C8-C9-C10
13	B	1206	CLA	C5-C6-C7-C8
13	1	519	CLA	C2C-C3C-CAC-CBC
13	6	512	CLA	C2A-CAA-CBA-CGA
13	1	513	CLA	C2A-CAA-CBA-CGA
13	A	1136	CLA	C2A-CAA-CBA-CGA
13	e	516	CLA	C2A-CAA-CBA-CGA
14	M	4021	BCR	C19-C20-C21-C22
13	b	518	CLA	C4-C3-C5-C6
13	a	503	CLA	C5-C6-C7-C8
13	d	503	CLA	C15-C16-C17-C18
20	A	1849	LMU	C2-C3-C4-C5
17	A	5001	LHG	O10-C23-O8-C6
13	6	505	CLA	CAA-CBA-CGA-O1A
13	c	502	CLA	C11-C12-C13-C14
13	5	503	CLA	C11-C10-C8-C9
13	6	507	CLA	C11-C10-C8-C9
13	2	510	CLA	C14-C13-C15-C16
13	A	1011	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	B	1012	CLA	C11-C12-C13-C14
13	B	1239	CLA	C11-C12-C13-C14
13	c	509	CLA	C11-C10-C8-C9
13	d	503	CLA	C14-C13-C15-C16
13	g	501	CLA	C6-C7-C8-C9
13	g	502	CLA	C6-C7-C8-C9
13	b	505	CLA	C11-C12-C13-C14
18	A	2001	PQN	C24-C23-C25-C26
13	3	503	CLA	CBA-CGA-O2A-C1
13	4	518	CLA	CBA-CGA-O2A-C1
13	A	1022	CLA	CBA-CGA-O2A-C1
13	g	509	CLA	CBA-CGA-O2A-C1
13	5	502	CLA	C4B-C3B-CAB-CBB
13	2	501	CLA	C4B-C3B-CAB-CBB
13	1	504	CLA	C4B-C3B-CAB-CBB
13	1	505	CLA	C4B-C3B-CAB-CBB
13	A	1112	CLA	C4B-C3B-CAB-CBB
13	A	1125	CLA	C4B-C3B-CAB-CBB
13	A	1131	CLA	C4B-C3B-CAB-CBB
13	J	1303	CLA	C4B-C3B-CAB-CBB
13	e	518	CLA	C4B-C3B-CAB-CBB
13	A	1125	CLA	CBD-CGD-O2D-CED
13	K	1401	CLA	C6-C7-C8-C10
13	B	1227	CLA	CBA-CGA-O2A-C1
13	c	507	CLA	CBA-CGA-O2A-C1
13	c	513	CLA	CBA-CGA-O2A-C1
13	f	501	CLA	CBA-CGA-O2A-C1
13	5	516	CLA	CAA-CBA-CGA-O2A
13	1	509	CLA	C15-C16-C17-C18
13	c	502	CLA	C5-C6-C7-C8
13	d	518	CLA	C5-C6-C7-C8
13	b	509	CLA	C8-C10-C11-C12
17	A	5002	LHG	C28-C29-C30-C31
13	g	509	CLA	O1A-CGA-O2A-C1
14	f	524	BCR	C19-C20-C21-C22
13	A	1139	CLA	C10-C11-C12-C13
13	b	502	CLA	C5-C6-C7-C8
13	4	510	CLA	C16-C17-C18-C19
13	A	1122	CLA	C11-C12-C13-C14
13	B	1206	CLA	C16-C17-C18-C19
13	B	1219	CLA	C6-C7-C8-C10
13	B	1221	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	e	508	CLA	C6-C7-C8-C10
13	A	1105	CLA	O1D-CGD-O2D-CED
13	e	509	CLA	CAA-CBA-CGA-O2A
13	6	510	CLA	C11-C10-C8-C7
13	2	510	CLA	C12-C13-C15-C16
13	1	510	CLA	C6-C7-C8-C10
13	B	1223	CLA	C11-C10-C8-C7
13	e	503	CLA	C6-C7-C8-C10
13	g	505	CLA	C11-C12-C13-C15
13	3	503	CLA	O1A-CGA-O2A-C1
13	4	518	CLA	O1A-CGA-O2A-C1
13	A	1022	CLA	O1A-CGA-O2A-C1
13	c	507	CLA	O1A-CGA-O2A-C1
13	c	513	CLA	O1A-CGA-O2A-C1
13	f	501	CLA	O1A-CGA-O2A-C1
13	f	512	CLA	CBD-CGD-O2D-CED
13	f	510	CLA	CBA-CGA-O2A-C1
15	6	822	SQD	C7-C8-C9-C10
13	B	1201	CLA	O1D-CGD-O2D-CED
13	5	505	CLA	C15-C16-C17-C18
13	c	502	CLA	C8-C10-C11-C12
13	B	1227	CLA	O1A-CGA-O2A-C1
16	B	5002	LMG	O7-C8-C9-O8
13	3	511	CLA	C3A-C2A-CAA-CBA
13	2	513	CLA	C3A-C2A-CAA-CBA
13	A	1107	CLA	C3A-C2A-CAA-CBA
13	A	1115	CLA	C3A-C2A-CAA-CBA
13	B	1214	CLA	C3A-C2A-CAA-CBA
13	g	506	CLA	C3A-C2A-CAA-CBA
13	2	512	CLA	C2-C3-C5-C6
14	A	4011	BCR	C11-C10-C9-C34
14	A	4011	BCR	C16-C17-C18-C36
14	B	4006	BCR	C11-C10-C9-C34
14	B	4006	BCR	C20-C21-C22-C37
14	F	4016	BCR	C35-C13-C14-C15
14	I	4020	BCR	C20-C21-C22-C37
13	g	518	CLA	CAA-CBA-CGA-O1A
13	A	1107	CLA	C10-C11-C12-C13
13	d	517	CLA	CAA-CBA-CGA-O2A
13	5	510	CLA	C15-C16-C17-C18
13	b	509	CLA	C2-C1-O2A-CGA
14	1	521	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
14	I	4020	BCR	C15-C16-C17-C18
14	I	4020	BCR	C19-C20-C21-C22
14	b	522	BCR	C9-C10-C11-C12
13	5	516	CLA	CAA-CBA-CGA-O1A
13	6	519	CLA	CAA-CBA-CGA-O1A
13	2	504	CLA	CAA-CBA-CGA-O2A
13	a	518	CLA	CAA-CBA-CGA-O1A
13	e	516	CLA	CBD-CGD-O2D-CED
13	6	505	CLA	C15-C16-C17-C18
13	b	501	CLA	CBA-CGA-O2A-C1
13	B	1205	CLA	C4-C3-C5-C6
13	6	509	CLA	CAA-CBA-CGA-O2A
13	6	508	CLA	C2-C3-C5-C6
13	B	1218	CLA	C2-C3-C5-C6
13	3	510	CLA	C10-C11-C12-C13
13	5	518	CLA	C2A-CAA-CBA-CGA
13	X	1401	CLA	C2A-CAA-CBA-CGA
13	6	512	CLA	CAA-CBA-CGA-O1A
17	A	5005	LHG	C32-C33-C34-C35
13	d	516	CLA	CAA-CBA-CGA-O1A
13	e	511	CLA	CAA-CBA-CGA-O1A
13	e	511	CLA	CAA-CBA-CGA-O2A
13	g	517	CLA	CAA-CBA-CGA-O2A
13	3	501	CLA	C11-C12-C13-C14
13	3	505	CLA	C11-C12-C13-C14
13	6	505	CLA	C11-C10-C8-C9
13	6	509	CLA	C14-C13-C15-C16
13	2	510	CLA	C11-C10-C8-C9
13	1	510	CLA	C6-C7-C8-C9
13	A	1103	CLA	C11-C12-C13-C14
13	A	1118	CLA	C11-C10-C8-C9
13	A	1131	CLA	C6-C7-C8-C9
13	A	1140	CLA	C11-C10-C8-C9
13	B	1012	CLA	C6-C7-C8-C9
13	B	1021	CLA	C14-C13-C15-C16
13	B	1218	CLA	C11-C10-C8-C9
13	d	505	CLA	C14-C13-C15-C16
13	e	501	CLA	C6-C7-C8-C9
13	e	510	CLA	C6-C7-C8-C9
13	f	507	CLA	C6-C7-C8-C9
13	f	507	CLA	C11-C10-C8-C9
13	g	505	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
13	4	518	CLA	CAA-CBA-CGA-O1A
13	4	519	CLA	CAA-CBA-CGA-O2A
13	A	1116	CLA	CAA-CBA-CGA-O2A
15	5	822	SQD	C46-C45-O47-C7
15	e	822	SQD	C46-C45-O47-C7
15	f	822	SQD	C46-C45-O47-C7
14	a	522	BCR	C13-C14-C15-C16
13	a	517	CLA	CAA-CBA-CGA-O2A
13	6	501	CLA	C4-C3-C5-C6
17	A	5002	LHG	C33-C34-C35-C36
13	e	512	CLA	CBD-CGD-O2D-CED
17	A	5005	LHG	O10-C23-O8-C6
13	A	1122	CLA	C3-C5-C6-C7
13	4	517	CLA	CAA-CBA-CGA-O1A
13	d	517	CLA	CAA-CBA-CGA-O1A
13	g	516	CLA	CAA-CBA-CGA-O2A
13	g	517	CLA	CAA-CBA-CGA-O1A
13	3	509	CLA	C2A-CAA-CBA-CGA
13	B	1204	CLA	C2A-CAA-CBA-CGA
13	c	518	CLA	C2A-CAA-CBA-CGA
13	e	507	CLA	C2A-CAA-CBA-CGA
13	A	1124	CLA	C8-C10-C11-C12
13	2	502	CLA	C1A-C2A-CAA-CBA
13	2	505	CLA	C1A-C2A-CAA-CBA
13	2	513	CLA	C1A-C2A-CAA-CBA
13	A	1132	CLA	C1A-C2A-CAA-CBA
13	B	1210	CLA	C1A-C2A-CAA-CBA
13	B	1214	CLA	C1A-C2A-CAA-CBA
13	B	1229	CLA	C1A-C2A-CAA-CBA
13	d	502	CLA	C1A-C2A-CAA-CBA
13	e	505	CLA	C1A-C2A-CAA-CBA
13	f	501	CLA	C1A-C2A-CAA-CBA
13	g	506	CLA	C1A-C2A-CAA-CBA
13	g	516	CLA	C1A-C2A-CAA-CBA
13	b	502	CLA	C1A-C2A-CAA-CBA
13	b	505	CLA	C1A-C2A-CAA-CBA
13	a	518	CLA	C1A-C2A-CAA-CBA
14	A	4011	BCR	C11-C10-C9-C8
14	A	4011	BCR	C16-C17-C18-C19
14	B	4006	BCR	C11-C10-C9-C8
14	B	4006	BCR	C20-C21-C22-C23
14	F	4016	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
14	I	4020	BCR	C20-C21-C22-C23
13	B	1232	CLA	CAA-CBA-CGA-O1A
13	K	1103	CLA	CAA-CBA-CGA-O2A
13	b	516	CLA	CAA-CBA-CGA-O2A
13	a	518	CLA	CAA-CBA-CGA-O2A
13	4	509	CLA	C10-C11-C12-C13
13	3	516	CLA	C2B-C3B-CAB-CBB
13	4	503	CLA	C2B-C3B-CAB-CBB
13	5	518	CLA	C2B-C3B-CAB-CBB
13	2	501	CLA	C2B-C3B-CAB-CBB
13	2	503	CLA	C2B-C3B-CAB-CBB
13	2	517	CLA	C2B-C3B-CAB-CBB
13	1	504	CLA	C2B-C3B-CAB-CBB
13	1	505	CLA	C2B-C3B-CAB-CBB
13	1	519	CLA	C2B-C3B-CAB-CBB
13	A	1101	CLA	C2B-C3B-CAB-CBB
13	A	1109	CLA	C2B-C3B-CAB-CBB
13	A	1110	CLA	C2B-C3B-CAB-CBB
13	A	1112	CLA	C2B-C3B-CAB-CBB
13	A	1125	CLA	C2B-C3B-CAB-CBB
13	A	1129	CLA	C2B-C3B-CAB-CBB
13	A	1131	CLA	C2B-C3B-CAB-CBB
13	A	1137	CLA	C2B-C3B-CAB-CBB
13	A	1139	CLA	C2B-C3B-CAB-CBB
13	A	1237	CLA	C2B-C3B-CAB-CBB
13	B	1214	CLA	C2B-C3B-CAB-CBB
13	B	1238	CLA	C2B-C3B-CAB-CBB
13	c	502	CLA	C2B-C3B-CAB-CBB
13	d	501	CLA	C2B-C3B-CAB-CBB
13	d	503	CLA	C2B-C3B-CAB-CBB
13	d	512	CLA	C2B-C3B-CAB-CBB
13	e	501	CLA	C2B-C3B-CAB-CBB
13	e	518	CLA	C2B-C3B-CAB-CBB
13	g	509	CLA	C2B-C3B-CAB-CBB
13	g	516	CLA	C2B-C3B-CAB-CBB
13	a	511	CLA	C2B-C3B-CAB-CBB
14	3	521	BCR	C1-C6-C7-C8
14	3	523	BCR	C1-C6-C7-C8
14	3	523	BCR	C23-C24-C25-C30
14	3	524	BCR	C5-C6-C7-C8
14	4	521	BCR	C23-C24-C25-C30
14	5	521	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
14	5	523	BCR	C23-C24-C25-C30
14	5	524	BCR	C5-C6-C7-C8
14	6	523	BCR	C23-C24-C25-C30
14	2	521	BCR	C23-C24-C25-C26
14	A	4002	BCR	C5-C6-C7-C8
14	A	4011	BCR	C23-C24-C25-C26
14	J	4013	BCR	C5-C6-C7-C8
14	M	4021	BCR	C5-C6-C7-C8
14	c	523	BCR	C23-C24-C25-C30
14	d	521	BCR	C23-C24-C25-C30
14	d	522	BCR	C23-C24-C25-C30
14	e	522	BCR	C5-C6-C7-C8
14	g	523	BCR	C23-C24-C25-C30
14	a	522	BCR	C5-C6-C7-C8
14	a	521	BCR	C1-C6-C7-C8
14	a	521	BCR	C5-C6-C7-C8
14	a	521	BCR	C23-C24-C25-C30
13	3	517	CLA	CAA-CBA-CGA-O2A
13	B	1232	CLA	CAA-CBA-CGA-O2A
13	b	506	CLA	CAA-CBA-CGA-O2A
17	A	5005	LHG	C9-C10-C11-C12
13	b	501	CLA	O1A-CGA-O2A-C1
13	f	512	CLA	O1D-CGD-O2D-CED
13	3	502	CLA	C3-C5-C6-C7
13	3	505	CLA	CBD-CGD-O2D-CED
13	6	510	CLA	C13-C15-C16-C17
13	6	512	CLA	CAA-CBA-CGA-O2A
13	c	516	CLA	CAA-CBA-CGA-O1A
13	e	517	CLA	CAA-CBA-CGA-O1A
13	e	517	CLA	CAA-CBA-CGA-O2A
13	b	504	CLA	C4-C3-C5-C6
17	A	5002	LHG	O6-C4-C5-C6
13	A	1137	CLA	C2-C3-C5-C6
15	B	1852	SQD	C10-C11-C12-C13
13	A	1125	CLA	O1D-CGD-O2D-CED
17	A	5005	LHG	C11-C12-C13-C14
13	K	1103	CLA	CAA-CBA-CGA-O1A
13	g	516	CLA	CAA-CBA-CGA-O1A
13	4	510	CLA	C6-C7-C8-C10
13	5	507	CLA	C6-C7-C8-C10
13	6	509	CLA	C11-C10-C8-C7
13	2	502	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	2	510	CLA	C11-C10-C8-C7
13	1	503	CLA	C11-C12-C13-C15
13	1	503	CLA	C12-C13-C15-C16
13	A	1106	CLA	C6-C7-C8-C10
13	A	1118	CLA	C11-C10-C8-C7
13	A	1125	CLA	C11-C10-C8-C7
13	B	1012	CLA	C12-C13-C15-C16
13	B	1023	CLA	C12-C13-C15-C16
13	B	1225	CLA	C11-C10-C8-C7
13	B	1226	CLA	C11-C12-C13-C15
13	B	1239	CLA	C11-C12-C13-C15
13	f	503	CLA	C11-C10-C8-C7
13	f	509	CLA	C12-C13-C15-C16
13	g	509	CLA	C11-C10-C8-C7
13	f	501	CLA	C2A-CAA-CBA-CGA
13	f	510	CLA	C2A-CAA-CBA-CGA
13	g	503	CLA	C8-C10-C11-C12
13	6	519	CLA	CAA-CBA-CGA-O2A
13	a	517	CLA	CAA-CBA-CGA-O1A
13	d	508	CLA	C5-C6-C7-C8
13	3	517	CLA	CAA-CBA-CGA-O1A
13	4	517	CLA	CAA-CBA-CGA-O2A
20	A	1848	LMU	C5-C6-C7-C8
13	B	1021	CLA	C8-C10-C11-C12
13	3	518	CLA	C6-C7-C8-C9
13	B	1021	CLA	C16-C17-C18-C20
13	g	509	CLA	C13-C15-C16-C17
14	a	524	BCR	C37-C22-C23-C24
13	5	517	CLA	CAA-CBA-CGA-O2A
13	1	517	CLA	CAA-CBA-CGA-O1A
13	g	519	CLA	CAA-CBA-CGA-O2A
13	6	505	CLA	C4-C3-C5-C6
13	A	1106	CLA	C4-C3-C5-C6
13	B	1021	CLA	C4-C3-C5-C6
13	a	510	CLA	C4-C3-C5-C6
13	A	1116	CLA	C2-C3-C5-C6
13	A	1126	CLA	C2-C3-C5-C6
13	g	503	CLA	C15-C16-C17-C18
13	f	517	CLA	CAA-CBA-CGA-O2A
14	e	521	BCR	C11-C12-C13-C14
13	A	1132	CLA	C2C-C3C-CAC-CBC
13	B	1226	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
13	f	510	CLA	O1A-CGA-O2A-C1
13	4	512	CLA	C2A-CAA-CBA-CGA
13	J	1303	CLA	C2A-CAA-CBA-CGA
13	a	504	CLA	C2A-CAA-CBA-CGA
13	b	506	CLA	CAA-CBA-CGA-O1A
13	3	501	CLA	C11-C10-C8-C9
13	3	510	CLA	C6-C7-C8-C9
14	5	522	BCR	C9-C10-C11-C12
14	e	524	BCR	C13-C14-C15-C16
13	c	507	CLA	C5-C6-C7-C8
13	1	517	CLA	CAA-CBA-CGA-O2A
13	c	516	CLA	CAA-CBA-CGA-O2A
13	b	516	CLA	CAA-CBA-CGA-O1A
16	B	5002	LMG	C17-C18-C19-C20
13	5	507	CLA	C4-C3-C5-C6
13	B	1202	CLA	C4-C3-C5-C6
13	B	1234	CLA	C4-C3-C5-C6
13	b	507	CLA	C4-C3-C5-C6
13	3	516	CLA	CAA-CBA-CGA-O2A
16	6	5104	LMG	C11-C12-C13-C14
13	3	505	CLA	C2-C3-C5-C6
13	4	518	CLA	C5-C6-C7-C8
13	f	503	CLA	C13-C15-C16-C17
13	A	1013	CLA	C8-C10-C11-C12
13	a	501	CLA	C15-C16-C17-C18
13	d	506	CLA	CAA-CBA-CGA-O2A
13	a	511	CLA	CAA-CBA-CGA-O2A
17	A	5004	LHG	C11-C10-C9-C8
13	6	516	CLA	C2A-CAA-CBA-CGA
13	e	518	CLA	C2A-CAA-CBA-CGA
13	A	1013	CLA	C15-C16-C17-C18
13	d	516	CLA	CAA-CBA-CGA-O2A
13	g	519	CLA	CAA-CBA-CGA-O1A
13	5	511	CLA	C4-C3-C5-C6
13	e	504	CLA	C4-C3-C5-C6
13	g	511	CLA	C4-C3-C5-C6
14	c	521	BCR	C9-C10-C11-C12
13	2	504	CLA	CAA-CBA-CGA-O1A
13	A	1114	CLA	CAA-CBA-CGA-O2A
13	A	1107	CLA	CAA-CBA-CGA-O2A
13	1	503	CLA	C2-C3-C5-C6
13	a	508	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	5	501	CLA	C4B-C3B-CAB-CBB
13	5	518	CLA	C4B-C3B-CAB-CBB
13	A	1101	CLA	C4B-C3B-CAB-CBB
13	A	1122	CLA	C4B-C3B-CAB-CBB
13	B	1231	CLA	C4B-C3B-CAB-CBB
13	c	503	CLA	C4B-C3B-CAB-CBB
13	e	509	CLA	C4B-C3B-CAB-CBB
13	c	519	CLA	CAA-CBA-CGA-O2A
13	e	506	CLA	CAA-CBA-CGA-O2A
13	e	516	CLA	O1D-CGD-O2D-CED
13	B	1224	CLA	CAA-CBA-CGA-O2A
15	c	822	SQD	O47-C7-C8-C9
13	A	1136	CLA	C10-C11-C12-C13
13	B	1223	CLA	C16-C17-C18-C20
13	c	508	CLA	C6-C7-C8-C9
13	d	504	CLA	C6-C7-C8-C9
13	3	505	CLA	O1D-CGD-O2D-CED
13	5	517	CLA	CAA-CBA-CGA-O1A
13	6	517	CLA	CAA-CBA-CGA-O2A
13	c	517	CLA	CAA-CBA-CGA-O2A
13	b	519	CLA	CAA-CBA-CGA-O1A
13	F	1301	CLA	O1D-CGD-O2D-CED
13	5	505	CLA	C16-C17-C18-C20
13	B	1216	CLA	C11-C12-C13-C15
13	f	512	CLA	CAA-CBA-CGA-O2A
15	3	822	SQD	O47-C7-C8-C9
13	e	501	CLA	C13-C15-C16-C17
13	3	501	CLA	C11-C10-C8-C7
13	d	505	CLA	C12-C13-C15-C16
13	e	510	CLA	C6-C7-C8-C10
13	b	503	CLA	C15-C16-C17-C18
13	c	512	CLA	CAA-CBA-CGA-O2A
13	e	516	CLA	CAA-CBA-CGA-O2A
13	B	1216	CLA	C10-C11-C12-C13
14	F	4015	BCR	C15-C16-C17-C18
14	d	524	BCR	C19-C20-C21-C22
13	A	1801	CLA	CAA-CBA-CGA-O2A
13	c	512	CLA	CAA-CBA-CGA-O1A
13	b	519	CLA	CAA-CBA-CGA-O2A
14	B	4004	BCR	C21-C22-C23-C24
13	4	501	CLA	C11-C12-C13-C14
13	5	501	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	5	503	CLA	C6-C7-C8-C9
13	1	505	CLA	C14-C13-C15-C16
13	A	1101	CLA	C11-C10-C8-C9
13	A	1106	CLA	C11-C12-C13-C14
13	A	1123	CLA	C11-C10-C8-C9
13	B	1206	CLA	C11-C12-C13-C14
13	A	1126	CLA	CAA-CBA-CGA-O2A
13	1	516	CLA	O1D-CGD-O2D-CED
13	3	518	CLA	CAA-CBA-CGA-O1A
13	b	518	CLA	CAA-CBA-CGA-O1A
13	3	519	CLA	CAA-CBA-CGA-O2A
13	2	504	CLA	C2A-CAA-CBA-CGA
13	A	1103	CLA	C2A-CAA-CBA-CGA
13	e	506	CLA	C2A-CAA-CBA-CGA
13	5	504	CLA	C2-C1-O2A-CGA
13	A	1124	CLA	C2-C1-O2A-CGA
13	B	1207	CLA	C2-C1-O2A-CGA
13	K	1401	CLA	C2-C1-O2A-CGA
13	c	503	CLA	C2-C1-O2A-CGA
13	e	503	CLA	C2-C1-O2A-CGA
13	e	512	CLA	C2-C1-O2A-CGA
13	b	503	CLA	C2-C1-O2A-CGA
13	6	513	CLA	C3A-C2A-CAA-CBA
13	2	503	CLA	C3A-C2A-CAA-CBA
13	1	517	CLA	C3A-C2A-CAA-CBA
13	A	1137	CLA	C3A-C2A-CAA-CBA
13	B	1216	CLA	C3A-C2A-CAA-CBA
13	B	1236	CLA	C3A-C2A-CAA-CBA
13	g	516	CLA	C3A-C2A-CAA-CBA
13	2	513	CLA	CAA-CBA-CGA-O2A
13	d	506	CLA	CAA-CBA-CGA-O1A
15	b	822	SQD	O47-C7-C8-C9
13	d	511	CLA	C2-C3-C5-C6
13	f	505	CLA	C2-C3-C5-C6
13	e	512	CLA	O1D-CGD-O2D-CED
13	6	503	CLA	C3-C5-C6-C7
13	d	508	CLA	C3-C5-C6-C7
13	5	503	CLA	C10-C11-C12-C13
13	6	505	CLA	C13-C15-C16-C17
13	2	516	CLA	CAA-CBA-CGA-O2A
13	c	517	CLA	CAA-CBA-CGA-O1A
13	f	517	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
13	A	1134	CLA	O1D-CGD-O2D-CED
13	2	516	CLA	CAA-CBA-CGA-O1A
13	2	517	CLA	CAA-CBA-CGA-O2A
13	f	519	CLA	CAA-CBA-CGA-O2A
13	A	1140	CLA	C5-C6-C7-C8
13	B	1214	CLA	C15-C16-C17-C18
14	5	523	BCR	C9-C10-C11-C12
13	e	503	CLA	O1A-CGA-O2A-C1
13	3	516	CLA	CAA-CBA-CGA-O1A
13	d	519	CLA	CAA-CBA-CGA-O2A
13	b	517	CLA	CAA-CBA-CGA-O2A
13	a	511	CLA	CAA-CBA-CGA-O1A
13	A	1108	CLA	CAA-CBA-CGA-O2A
13	A	1114	CLA	CAA-CBA-CGA-O1A
13	c	519	CLA	CAA-CBA-CGA-O1A
13	B	1205	CLA	C2-C3-C5-C6
13	f	504	CLA	C2-C3-C5-C6
13	e	503	CLA	CBA-CGA-O2A-C1
13	B	1206	CLA	C13-C15-C16-C17
13	e	510	CLA	C16-C17-C18-C19
13	6	517	CLA	CAA-CBA-CGA-O1A
13	2	513	CLA	CAA-CBA-CGA-O1A
13	f	512	CLA	CAA-CBA-CGA-O1A
13	6	504	CLA	CAA-CBA-CGA-O2A
13	A	1801	CLA	CAA-CBA-CGA-O1A
13	e	506	CLA	CAA-CBA-CGA-O1A
13	1	516	CLA	CBD-CGD-O2D-CED
13	B	1207	CLA	CBD-CGD-O2D-CED
13	d	509	CLA	C5-C6-C7-C8
13	d	519	CLA	C2A-CAA-CBA-CGA
13	B	1230	CLA	CAA-CBA-CGA-O2A
17	A	5002	LHG	O7-C7-C8-C9
13	2	517	CLA	CAA-CBA-CGA-O1A
13	B	1213	CLA	C16-C17-C18-C20
13	A	1102	CLA	C13-C15-C16-C17
13	g	511	CLA	C5-C6-C7-C8
13	b	517	CLA	CAA-CBA-CGA-O1A
13	3	505	CLA	CAA-CBA-CGA-O2A
13	A	1237	CLA	CAA-CBA-CGA-O2A
13	B	1217	CLA	CAA-CBA-CGA-O2A
13	a	508	CLA	O1D-CGD-O2D-CED
16	B	5002	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
20	A	1848	LMU	C2-C3-C4-C5
13	3	519	CLA	CAA-CBA-CGA-O1A
13	d	519	CLA	CAA-CBA-CGA-O1A
13	f	519	CLA	CAA-CBA-CGA-O1A
13	4	501	CLA	C11-C10-C8-C9
13	4	505	CLA	C11-C10-C8-C9
13	4	510	CLA	C6-C7-C8-C9
13	6	510	CLA	C14-C13-C15-C16
13	1	505	CLA	C11-C12-C13-C14
13	A	1103	CLA	C14-C13-C15-C16
13	A	1107	CLA	C14-C13-C15-C16
13	B	1213	CLA	C6-C7-C8-C9
13	B	1218	CLA	C6-C7-C8-C9
13	B	1226	CLA	C6-C7-C8-C9
13	B	1235	CLA	C11-C12-C13-C14
13	c	502	CLA	C11-C10-C8-C9
13	e	503	CLA	C14-C13-C15-C16
13	b	510	CLA	C11-C12-C13-C14
18	B	2002	PQN	C16-C17-C18-C19
16	2	5104	LMG	C32-C33-C34-C35
20	A	1848	LMU	O1'-C1-C2-C3
13	c	518	CLA	CAA-CBA-CGA-O2A
13	B	1216	CLA	O1A-CGA-O2A-C1
13	A	1108	CLA	CAA-CBA-CGA-O1A
13	e	516	CLA	CAA-CBA-CGA-O1A
13	5	504	CLA	C3-C5-C6-C7
13	2	507	CLA	CAA-CBA-CGA-O2A
13	e	512	CLA	CAA-CBA-CGA-O2A
13	B	1012	CLA	C16-C17-C18-C20
13	4	516	CLA	CAA-CBA-CGA-O2A
13	B	1216	CLA	CBA-CGA-O2A-C1
13	3	510	CLA	C6-C7-C8-C10
13	5	501	CLA	C11-C10-C8-C7
13	6	501	CLA	C6-C7-C8-C10
13	6	509	CLA	C11-C12-C13-C15
13	A	1101	CLA	C11-C10-C8-C7
13	A	1106	CLA	C11-C12-C13-C15
13	A	1138	CLA	C11-C12-C13-C15
13	A	1011	CLA	C12-C13-C15-C16
13	B	1224	CLA	C11-C10-C8-C7
13	c	503	CLA	C12-C13-C15-C16
13	e	502	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	f	507	CLA	C6-C7-C8-C10
13	g	501	CLA	C12-C13-C15-C16
13	g	502	CLA	C11-C10-C8-C7
13	a	502	CLA	C6-C7-C8-C10
13	3	519	CLA	C2B-C3B-CAB-CBB
13	5	502	CLA	C2B-C3B-CAB-CBB
13	6	506	CLA	C2B-C3B-CAB-CBB
13	1	518	CLA	C2B-C3B-CAB-CBB
13	c	503	CLA	C2B-C3B-CAB-CBB
13	c	511	CLA	C2B-C3B-CAB-CBB
13	d	517	CLA	C2B-C3B-CAB-CBB
13	e	502	CLA	C2B-C3B-CAB-CBB
13	e	509	CLA	C2B-C3B-CAB-CBB
13	e	519	CLA	C2B-C3B-CAB-CBB
13	g	518	CLA	C2B-C3B-CAB-CBB
14	3	521	BCR	C5-C6-C7-C8
14	3	523	BCR	C5-C6-C7-C8
14	3	523	BCR	C23-C24-C25-C26
14	4	521	BCR	C1-C6-C7-C8
14	4	521	BCR	C5-C6-C7-C8
14	4	521	BCR	C23-C24-C25-C26
14	4	523	BCR	C23-C24-C25-C26
14	4	523	BCR	C23-C24-C25-C30
14	6	521	BCR	C1-C6-C7-C8
14	6	521	BCR	C5-C6-C7-C8
14	6	523	BCR	C23-C24-C25-C26
14	2	524	BCR	C1-C6-C7-C8
14	2	524	BCR	C5-C6-C7-C8
14	B	4004	BCR	C23-C24-C25-C26
14	c	523	BCR	C23-C24-C25-C26
14	d	521	BCR	C1-C6-C7-C8
14	d	521	BCR	C5-C6-C7-C8
14	d	521	BCR	C23-C24-C25-C26
14	d	522	BCR	C23-C24-C25-C26
14	d	523	BCR	C1-C6-C7-C8
14	f	522	BCR	C5-C6-C7-C8
14	f	523	BCR	C1-C6-C7-C8
14	g	521	BCR	C1-C6-C7-C8
14	g	521	BCR	C5-C6-C7-C8
14	g	523	BCR	C23-C24-C25-C26
14	b	521	BCR	C23-C24-C25-C26
14	b	521	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
14	a	521	BCR	C23-C24-C25-C26
13	A	1135	CLA	CAA-CBA-CGA-O2A
13	6	518	CLA	C2-C1-O2A-CGA
13	a	507	CLA	C2-C1-O2A-CGA
13	g	507	CLA	C5-C6-C7-C8
13	A	1013	CLA	CAA-CBA-CGA-O2A
13	A	1134	CLA	CBD-CGD-O2D-CED
13	e	507	CLA	C3-C5-C6-C7
13	1	518	CLA	CAA-CBA-CGA-O2A
13	B	1235	CLA	C2-C3-C5-C6
18	B	2002	PQN	C23-C25-C26-C27
13	A	1011	CLA	O1A-CGA-O2A-C1
13	B	1201	CLA	O1A-CGA-O2A-C1
13	3	505	CLA	C2A-CAA-CBA-CGA
13	B	1210	CLA	C2A-CAA-CBA-CGA
13	A	1110	CLA	C5-C6-C7-C8
13	A	1127	CLA	C15-C16-C17-C18
13	A	1119	CLA	CAA-CBA-CGA-O2A
13	d	509	CLA	C10-C11-C12-C13
13	B	1222	CLA	O1D-CGD-O2D-CED
15	f	822	SQD	O47-C7-C8-C9
17	A	5001	LHG	C13-C14-C15-C16
13	5	505	CLA	C4-C3-C5-C6
13	B	1235	CLA	C4-C3-C5-C6
13	d	504	CLA	C4-C3-C5-C6
20	A	1849	LMU	C11-C10-C9-C8
13	b	518	CLA	C2-C3-C5-C6
13	1	501	CLA	C10-C11-C12-C13
13	f	505	CLA	C13-C15-C16-C17
13	1	510	CLA	C2A-CAA-CBA-CGA
13	4	506	CLA	CAA-CBA-CGA-O2A
13	6	516	CLA	CAA-CBA-CGA-O2A
13	A	1127	CLA	C2C-C3C-CAC-CBC
20	A	1848	LMU	C6-C7-C8-C9
13	a	503	CLA	CBA-CGA-O2A-C1
13	a	503	CLA	O1A-CGA-O2A-C1
13	f	501	CLA	C5-C6-C7-C8
13	4	516	CLA	CAA-CBA-CGA-O1A
13	3	509	CLA	C6-C7-C8-C9
13	3	510	CLA	C11-C12-C13-C14
13	A	1123	CLA	C11-C12-C13-C14
13	A	1131	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
13	B	1207	CLA	C6-C7-C8-C9
13	c	507	CLA	C11-C10-C8-C9
13	d	505	CLA	C11-C10-C8-C9
13	g	509	CLA	C11-C10-C8-C9
13	b	509	CLA	C6-C7-C8-C9
13	b	509	CLA	C11-C12-C13-C14
18	B	2002	PQN	C19-C18-C20-C21
14	f	521	BCR	C36-C18-C19-C20
13	A	1115	CLA	CAA-CBA-CGA-O2A
13	B	1239	CLA	CAA-CBA-CGA-O2A
13	f	510	CLA	CAA-CBA-CGA-O2A
13	3	508	CLA	C1A-C2A-CAA-CBA
13	3	512	CLA	C4B-C3B-CAB-CBB
13	3	517	CLA	C4B-C3B-CAB-CBB
13	4	506	CLA	C4B-C3B-CAB-CBB
13	5	503	CLA	C4B-C3B-CAB-CBB
13	6	508	CLA	C1A-C2A-CAA-CBA
13	6	511	CLA	C4B-C3B-CAB-CBB
13	6	513	CLA	C1A-C2A-CAA-CBA
13	2	518	CLA	C1A-C2A-CAA-CBA
13	1	503	CLA	C4B-C3B-CAB-CBB
13	A	1109	CLA	C1A-C2A-CAA-CBA
13	A	1115	CLA	C1A-C2A-CAA-CBA
13	A	1138	CLA	C4B-C3B-CAB-CBB
13	B	1021	CLA	C1A-C2A-CAA-CBA
13	B	1205	CLA	C4B-C3B-CAB-CBB
13	B	1211	CLA	C1A-C2A-CAA-CBA
13	B	1212	CLA	C4B-C3B-CAB-CBB
13	B	1222	CLA	C1A-C2A-CAA-CBA
13	B	1226	CLA	C1A-C2A-CAA-CBA
13	B	1236	CLA	C4B-C3B-CAB-CBB
13	J	1302	CLA	C4B-C3B-CAB-CBB
13	K	1103	CLA	C1A-C2A-CAA-CBA
13	c	502	CLA	C4B-C3B-CAB-CBB
13	c	509	CLA	C1A-C2A-CAA-CBA
13	d	504	CLA	C4B-C3B-CAB-CBB
13	e	508	CLA	C1A-C2A-CAA-CBA
13	f	509	CLA	C1A-C2A-CAA-CBA
13	f	516	CLA	C4B-C3B-CAB-CBB
13	g	501	CLA	C4B-C3B-CAB-CBB
13	g	503	CLA	C1A-C2A-CAA-CBA
13	g	503	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
13	g	509	CLA	C4B-C3B-CAB-CBB
13	g	518	CLA	C4B-C3B-CAB-CBB
13	a	512	CLA	C4B-C3B-CAB-CBB
13	6	504	CLA	CAA-CBA-CGA-O1A
13	3	511	CLA	C4-C3-C5-C6
16	J	5104	LMG	C12-C13-C14-C15
13	A	1127	CLA	CAA-CBA-CGA-O2A
13	A	1137	CLA	CAA-CBA-CGA-O2A
13	b	504	CLA	C2-C3-C5-C6
14	B	4006	BCR	C11-C12-C13-C14
14	b	522	BCR	C21-C22-C23-C24
13	c	509	CLA	O1A-CGA-O2A-C1
13	c	518	CLA	C6-C7-C8-C9
13	A	1011	CLA	CBA-CGA-O2A-C1
13	c	509	CLA	CBA-CGA-O2A-C1
13	a	519	CLA	CAA-CBA-CGA-O1A
13	6	513	CLA	CAA-CBA-CGA-O2A
13	e	507	CLA	CAA-CBA-CGA-O2A
13	b	504	CLA	CAA-CBA-CGA-O2A
16	g	5104	LMG	O7-C10-C11-C12
13	e	517	CLA	C2A-CAA-CBA-CGA
13	f	509	CLA	C13-C15-C16-C17
13	A	1120	CLA	CAA-CBA-CGA-O2A
13	A	1133	CLA	CAA-CBA-CGA-O2A
13	g	501	CLA	CAA-CBA-CGA-O2A
13	2	505	CLA	C5-C6-C7-C8
13	J	1303	CLA	CAA-CBA-CGA-O1A
13	4	513	CLA	C2-C1-O2A-CGA
13	A	1127	CLA	C2-C1-O2A-CGA
13	A	1237	CLA	C2-C1-O2A-CGA
13	c	504	CLA	C2-C1-O2A-CGA
13	c	518	CLA	C2-C1-O2A-CGA
13	d	511	CLA	C2-C1-O2A-CGA
13	a	502	CLA	C2-C1-O2A-CGA
13	a	509	CLA	C2-C1-O2A-CGA
13	3	507	CLA	C11-C10-C8-C7
13	4	510	CLA	C11-C10-C8-C7
13	A	1102	CLA	C6-C7-C8-C10
13	A	1237	CLA	C11-C10-C8-C7
13	B	1206	CLA	C11-C12-C13-C15
13	g	509	CLA	C12-C13-C15-C16
13	b	507	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
13	6	501	CLA	C2-C3-C5-C6
13	A	1106	CLA	C2-C3-C5-C6
13	a	519	CLA	CAA-CBA-CGA-O2A
13	5	505	CLA	C16-C17-C18-C19
13	A	1103	CLA	C16-C17-C18-C20
13	3	505	CLA	O2A-C1-C2-C3
13	1	511	CLA	O2A-C1-C2-C3
13	A	1013	CLA	O2A-C1-C2-C3
15	5	822	SQD	C44-C45-O47-C7
15	e	822	SQD	C44-C45-O47-C7
13	A	1115	CLA	C8-C10-C11-C12
17	A	5003	LHG	C10-C11-C12-C13
13	3	503	CLA	C5-C6-C7-C8
13	3	517	CLA	C2A-CAA-CBA-CGA
18	A	2001	PQN	C20-C21-C22-C23
13	g	506	CLA	CAA-CBA-CGA-O2A
13	2	512	CLA	CAA-CBA-CGA-O2A
13	5	503	CLA	C3A-C2A-CAA-CBA
13	2	511	CLA	C3A-C2A-CAA-CBA
13	B	1223	CLA	C4-C3-C5-C6
13	J	1303	CLA	C3A-C2A-CAA-CBA
13	d	503	CLA	C3A-C2A-CAA-CBA
13	f	503	CLA	C10-C11-C12-C13
13	4	503	CLA	C15-C16-C17-C18
13	1	518	CLA	CAA-CBA-CGA-O1A
13	e	512	CLA	CAA-CBA-CGA-O1A
13	2	510	CLA	CAA-CBA-CGA-O2A
13	e	510	CLA	CAA-CBA-CGA-O2A
13	3	505	CLA	CAA-CBA-CGA-O1A
13	2	507	CLA	CAA-CBA-CGA-O1A
13	A	1013	CLA	CAA-CBA-CGA-O1A
13	A	1135	CLA	CAA-CBA-CGA-O1A
13	B	1023	CLA	C15-C16-C17-C18
13	g	509	CLA	C10-C11-C12-C13
13	B	1201	CLA	CBA-CGA-O2A-C1
13	5	507	CLA	C6-C7-C8-C9
13	6	509	CLA	C11-C10-C8-C9
13	2	509	CLA	C11-C10-C8-C9
13	1	510	CLA	C11-C10-C8-C9
13	B	1023	CLA	C14-C13-C15-C16
13	B	1224	CLA	C11-C10-C8-C9
13	B	1225	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
13	d	509	CLA	C11-C10-C8-C9
13	f	509	CLA	C14-C13-C15-C16
13	a	505	CLA	C11-C10-C8-C9
16	g	5104	LMG	C31-C32-C33-C34
13	B	1239	CLA	CAA-CBA-CGA-O1A
13	c	509	CLA	C15-C16-C17-C18
14	1	522	BCR	C9-C10-C11-C12
14	I	4020	BCR	C9-C10-C11-C12
13	6	516	CLA	CAA-CBA-CGA-O1A
13	2	505	CLA	C4-C3-C5-C6
13	c	505	CLA	C4-C3-C5-C6
13	6	513	CLA	CAA-CBA-CGA-O1A
13	A	1133	CLA	CAA-CBA-CGA-O1A
13	f	510	CLA	CAA-CBA-CGA-O1A
17	A	5002	LHG	O9-C7-C8-C9
15	6	822	SQD	O5-C5-C6-S
13	4	506	CLA	CAA-CBA-CGA-O1A
13	4	505	CLA	C13-C15-C16-C17
17	A	5003	LHG	C14-C15-C16-C17
13	e	510	CLA	C16-C17-C18-C20
13	g	510	CLA	C16-C17-C18-C19
13	A	1237	CLA	CAA-CBA-CGA-O1A
13	B	1230	CLA	CAA-CBA-CGA-O1A
13	e	507	CLA	CAA-CBA-CGA-O1A
13	A	1102	CLA	C15-C16-C17-C18
16	J	5104	LMG	C8-C7-O1-C1
15	f	822	SQD	O49-C7-O47-C45
17	A	5001	LHG	O9-C7-O7-C5
17	A	5003	LHG	C1-C2-C3-O3
13	J	1303	CLA	CAA-CBA-CGA-O2A
13	f	516	CLA	CAA-CBA-CGA-O2A
13	g	501	CLA	CAA-CBA-CGA-O1A
13	1	504	CLA	C5-C6-C7-C8
13	F	1301	CLA	CAA-CBA-CGA-O2A
13	B	1217	CLA	CAA-CBA-CGA-O1A
17	A	5005	LHG	C27-C28-C29-C30
13	B	1234	CLA	C5-C6-C7-C8
13	b	503	CLA	C5-C6-C7-C8
13	b	507	CLA	C5-C6-C7-C8
13	3	501	CLA	CAA-CBA-CGA-O2A
13	3	510	CLA	CAA-CBA-CGA-O2A
13	B	1218	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
15	e	822	SQD	O47-C7-C8-C9
15	a	822	SQD	O47-C7-C8-C9
16	2	5104	LMG	O7-C10-C11-C12
13	3	505	CLA	C3-C5-C6-C7
16	g	5104	LMG	O9-C10-C11-C12
13	B	1213	CLA	C16-C17-C18-C19
13	3	517	CLA	CAD-CBD-CGD-O2D
13	4	513	CLA	CAD-CBD-CGD-O2D
13	6	506	CLA	CAD-CBD-CGD-O2D
13	2	504	CLA	CAD-CBD-CGD-O2D
13	A	1103	CLA	CAD-CBD-CGD-O2D
13	A	1131	CLA	CAD-CBD-CGD-O2D
13	B	1227	CLA	CAD-CBD-CGD-O2D
13	d	506	CLA	CAD-CBD-CGD-O2D
13	f	504	CLA	CAD-CBD-CGD-O2D
13	b	504	CLA	CAD-CBD-CGD-O2D
13	b	506	CLA	CAD-CBD-CGD-O2D
13	b	516	CLA	CAD-CBD-CGD-O2D
13	a	506	CLA	CAD-CBD-CGD-O2D
13	a	510	CLA	CAD-CBD-CGD-O2D
13	4	510	CLA	CAA-CBA-CGA-O2A
13	B	1223	CLA	C3-C5-C6-C7
13	A	1115	CLA	CAA-CBA-CGA-O1A
13	A	1127	CLA	CAA-CBA-CGA-O1A
13	3	510	CLA	C15-C16-C17-C18
13	f	512	CLA	C4C-C3C-CAC-CBC
16	J	5104	LMG	C11-C12-C13-C14
13	6	502	CLA	C2-C1-O2A-CGA
13	F	1301	CLA	CAA-CBA-CGA-O1A
13	A	1137	CLA	CAA-CBA-CGA-O1A
15	1	822	SQD	O47-C7-C8-C9
15	d	822	SQD	O47-C7-C8-C9
13	B	1229	CLA	O1A-CGA-O2A-C1
13	f	511	CLA	C6-C7-C8-C9
13	1	509	CLA	C13-C15-C16-C17
13	A	1140	CLA	C10-C11-C12-C13
13	A	1119	CLA	CAA-CBA-CGA-O1A
13	A	1106	CLA	CAA-CBA-CGA-O2A
15	f	822	SQD	C8-C7-O47-C45
13	A	1120	CLA	CAA-CBA-CGA-O1A
13	A	1119	CLA	C10-C11-C12-C13
13	B	1207	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
13	3	507	CLA	CAA-CBA-CGA-O2A
13	3	513	CLA	CAA-CBA-CGA-O2A
13	B	1213	CLA	CAA-CBA-CGA-O2A
13	B	1228	CLA	CAA-CBA-CGA-O2A
13	f	507	CLA	CAA-CBA-CGA-O2A
13	g	512	CLA	CAA-CBA-CGA-O2A
15	2	822	SQD	O47-C7-C8-C9
13	5	503	CLA	C15-C16-C17-C18
13	b	504	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

382 monomers are involved in 1314 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	1	504	CLA	3	0
14	f	523	BCR	8	0
13	5	511	CLA	1	0
13	a	509	CLA	11	0
13	6	502	CLA	4	0
13	5	501	CLA	8	0
18	B	2002	PQN	4	0
13	3	505	CLA	8	0
13	B	1239	CLA	4	0
13	A	1105	CLA	6	0
13	4	508	CLA	3	0
13	c	506	CLA	4	0
13	2	501	CLA	5	0
14	I	4020	BCR	4	0
13	B	1201	CLA	4	0
13	g	503	CLA	8	0
13	B	1204	CLA	6	0
13	a	503	CLA	8	0
17	A	5005	LHG	14	0
13	K	1401	CLA	4	0
14	a	524	BCR	7	0
13	d	511	CLA	2	0
13	A	1129	CLA	4	0
13	A	1113	CLA	3	0
13	6	504	CLA	3	0
13	e	508	CLA	2	0
13	f	502	CLA	8	0
14	e	524	BCR	8	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	d	517	CLA	3	0
13	d	504	CLA	2	0
13	f	504	CLA	1	0
13	f	518	CLA	2	0
13	c	503	CLA	5	0
13	e	518	CLA	2	0
14	c	524	BCR	10	0
14	g	523	BCR	6	0
17	A	5002	LHG	2	0
13	c	508	CLA	5	0
13	1	507	CLA	4	0
14	d	521	BCR	5	0
13	1	519	CLA	6	0
13	1	503	CLA	5	0
13	2	512	CLA	2	0
13	1	508	CLA	5	0
13	4	507	CLA	4	0
13	A	1136	CLA	4	0
13	c	517	CLA	3	0
13	a	516	CLA	1	0
13	a	512	CLA	2	0
13	5	512	CLA	1	0
13	A	1115	CLA	4	0
13	A	1123	CLA	6	0
13	B	1228	CLA	5	0
13	1	513	CLA	2	0
13	A	1125	CLA	7	0
13	a	510	CLA	9	0
13	B	1231	CLA	4	0
13	B	1220	CLA	2	0
13	g	502	CLA	9	0
13	g	506	CLA	1	0
14	A	4007	BCR	6	0
13	g	504	CLA	1	0
13	d	509	CLA	4	0
13	c	507	CLA	5	0
13	A	1118	CLA	3	0
13	2	505	CLA	6	0
13	f	507	CLA	9	0
13	2	511	CLA	2	0
13	b	502	CLA	3	0
14	1	521	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	f	510	CLA	2	0
13	A	1128	CLA	7	0
13	4	510	CLA	3	0
13	e	503	CLA	6	0
13	A	1133	CLA	2	0
13	b	518	CLA	3	0
13	4	506	CLA	2	0
13	A	1112	CLA	3	0
13	1	505	CLA	2	0
14	4	521	BCR	4	0
13	B	1202	CLA	4	0
13	B	1219	CLA	1	0
13	e	512	CLA	3	0
13	d	512	CLA	3	0
13	B	1225	CLA	9	0
14	5	524	BCR	4	0
15	B	1852	SQD	2	0
13	1	501	CLA	7	0
13	g	509	CLA	3	0
13	A	1022	CLA	8	0
13	e	511	CLA	4	0
13	A	1127	CLA	6	0
13	d	501	CLA	6	0
14	f	521	BCR	2	0
13	A	1102	CLA	6	0
13	A	1011	CLA	6	0
13	f	513	CLA	7	0
16	2	5104	LMG	1	0
13	6	519	CLA	3	0
13	f	508	CLA	2	0
13	B	1235	CLA	2	0
13	A	1013	CLA	9	0
13	B	1021	CLA	6	0
13	d	510	CLA	3	0
13	b	512	CLA	4	0
14	B	4005	BCR	2	0
13	a	511	CLA	2	0
13	A	1106	CLA	9	0
13	g	517	CLA	2	0
13	e	509	CLA	8	0
13	5	506	CLA	4	0
13	a	504	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	1229	CLA	7	0
13	B	1215	CLA	4	0
13	B	1232	CLA	2	0
13	J	1302	CLA	1	0
14	5	523	BCR	6	0
13	a	502	CLA	11	0
14	g	521	BCR	7	0
14	3	522	BCR	10	0
13	a	518	CLA	1	0
13	3	501	CLA	5	0
13	A	1107	CLA	8	0
13	6	503	CLA	6	0
13	F	1301	CLA	1	0
13	6	517	CLA	1	0
14	2	523	BCR	2	0
14	f	524	BCR	7	0
13	b	501	CLA	5	0
13	1	516	CLA	1	0
13	c	509	CLA	9	0
13	4	511	CLA	3	0
13	A	1801	CLA	1	0
13	B	1221	CLA	5	0
13	c	502	CLA	8	0
13	g	519	CLA	1	0
13	A	1139	CLA	9	0
14	b	524	BCR	5	0
13	b	511	CLA	5	0
14	2	524	BCR	5	0
14	B	4017	BCR	5	0
13	4	505	CLA	5	0
13	3	511	CLA	3	0
13	5	504	CLA	1	0
14	I	4018	BCR	9	0
13	B	1207	CLA	2	0
13	f	503	CLA	3	0
13	a	507	CLA	7	0
13	B	1234	CLA	4	0
13	B	1012	CLA	10	0
13	A	1134	CLA	4	0
13	f	511	CLA	3	0
19	C	3002	SF4	1	0
13	2	510	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	2	516	CLA	2	0
13	e	517	CLA	2	0
17	A	5003	LHG	3	0
14	B	4010	BCR	10	0
14	5	522	BCR	4	0
13	g	511	CLA	3	0
13	c	510	CLA	5	0
13	g	501	CLA	6	0
13	4	512	CLA	2	0
13	6	512	CLA	4	0
13	2	518	CLA	5	0
14	3	524	BCR	4	0
13	6	510	CLA	12	0
14	2	522	BCR	2	0
13	A	1116	CLA	5	0
13	5	502	CLA	4	0
14	c	523	BCR	3	0
13	A	1140	CLA	7	0
13	d	518	CLA	2	0
17	A	5004	LHG	2	0
14	d	522	BCR	4	0
14	e	521	BCR	2	0
13	3	513	CLA	2	0
15	2	822	SQD	3	0
13	B	1213	CLA	3	0
13	d	508	CLA	2	0
13	4	509	CLA	9	0
13	6	509	CLA	11	0
13	B	1205	CLA	6	0
14	b	523	BCR	7	0
13	f	509	CLA	11	0
20	J	5105	LMU	10	0
13	B	1227	CLA	2	0
13	e	519	CLA	2	0
13	6	501	CLA	4	0
14	1	522	BCR	5	0
13	c	518	CLA	4	0
13	B	1208	CLA	1	0
13	A	1138	CLA	9	0
13	g	505	CLA	6	0
13	a	506	CLA	3	0
13	d	507	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	a	523	BCR	7	0
13	1	510	CLA	4	0
15	g	822	SQD	1	0
13	B	1209	CLA	2	0
14	e	523	BCR	4	0
13	B	1224	CLA	7	0
13	6	505	CLA	5	0
13	6	506	CLA	4	0
13	B	1223	CLA	7	0
13	b	508	CLA	3	0
13	A	1111	CLA	2	0
17	A	5001	LHG	1	0
14	F	4014	BCR	6	0
13	f	517	CLA	3	0
13	A	1110	CLA	1	0
19	C	3003	SF4	1	0
15	4	822	SQD	7	0
15	6	822	SQD	2	0
13	e	501	CLA	7	0
13	e	513	CLA	5	0
14	3	523	BCR	3	0
13	a	513	CLA	4	0
13	A	1237	CLA	6	0
13	A	1119	CLA	10	0
13	f	506	CLA	2	0
13	B	1226	CLA	2	0
13	2	513	CLA	1	0
14	a	521	BCR	5	0
13	5	518	CLA	2	0
13	d	503	CLA	6	0
13	A	1126	CLA	4	0
13	d	519	CLA	1	0
13	B	1210	CLA	5	0
13	5	505	CLA	4	0
13	b	507	CLA	4	0
13	3	510	CLA	5	0
13	a	508	CLA	6	0
13	e	505	CLA	11	0
13	a	505	CLA	4	0
14	M	4021	BCR	3	0
16	g	5104	LMG	1	0
13	4	501	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	4	523	BCR	2	0
13	X	1401	CLA	2	0
13	6	508	CLA	9	0
13	A	1124	CLA	4	0
13	c	519	CLA	2	0
14	1	524	BCR	8	0
18	A	2001	PQN	2	0
13	3	504	CLA	1	0
13	1	506	CLA	3	0
14	J	4013	BCR	6	0
13	b	510	CLA	4	0
13	A	1131	CLA	2	0
13	c	504	CLA	1	0
13	B	1023	CLA	14	0
14	b	521	BCR	5	0
13	g	516	CLA	1	0
13	4	502	CLA	4	0
13	B	1206	CLA	6	0
13	B	1212	CLA	2	0
19	A	3001	SF4	1	0
13	A	1104	CLA	6	0
13	4	518	CLA	1	0
13	B	1236	CLA	3	0
13	6	516	CLA	1	0
13	3	506	CLA	3	0
13	A	1108	CLA	2	0
13	b	517	CLA	2	0
13	f	501	CLA	10	0
14	d	523	BCR	3	0
13	3	502	CLA	4	0
13	4	516	CLA	1	0
13	2	508	CLA	2	0
13	3	507	CLA	4	0
13	2	503	CLA	5	0
13	3	512	CLA	2	0
13	g	510	CLA	3	0
14	f	522	BCR	5	0
13	5	509	CLA	3	0
14	4	522	BCR	4	0
13	a	519	CLA	1	0
13	f	505	CLA	8	0
13	A	1132	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	3	509	CLA	6	0
13	B	1222	CLA	4	0
20	A	1848	LMU	2	0
13	B	1203	CLA	5	0
13	1	512	CLA	1	0
13	6	507	CLA	3	0
13	2	502	CLA	5	0
14	1	523	BCR	4	0
13	A	1135	CLA	1	0
14	J	4012	BCR	2	0
13	A	1122	CLA	7	0
20	B	1843	LMU	1	0
13	B	1238	CLA	7	0
14	B	4004	BCR	1	0
14	3	521	BCR	3	0
13	c	513	CLA	5	0
13	d	505	CLA	8	0
20	A	1849	LMU	1	0
13	B	1214	CLA	7	0
13	A	1117	CLA	4	0
14	g	522	BCR	4	0
13	1	502	CLA	8	0
13	1	518	CLA	2	0
13	A	1137	CLA	7	0
13	A	1120	CLA	2	0
13	2	506	CLA	1	0
13	3	503	CLA	6	0
13	f	512	CLA	5	0
14	6	521	BCR	5	0
14	I	4019	BCR	4	0
14	c	521	BCR	4	0
14	b	522	BCR	5	0
14	B	4009	BCR	5	0
13	5	510	CLA	9	0
13	c	505	CLA	10	0
13	4	519	CLA	2	0
13	b	513	CLA	2	0
13	d	502	CLA	3	0
13	f	519	CLA	2	0
14	A	4002	BCR	7	0
13	2	507	CLA	6	0
14	F	4016	BCR	2	0

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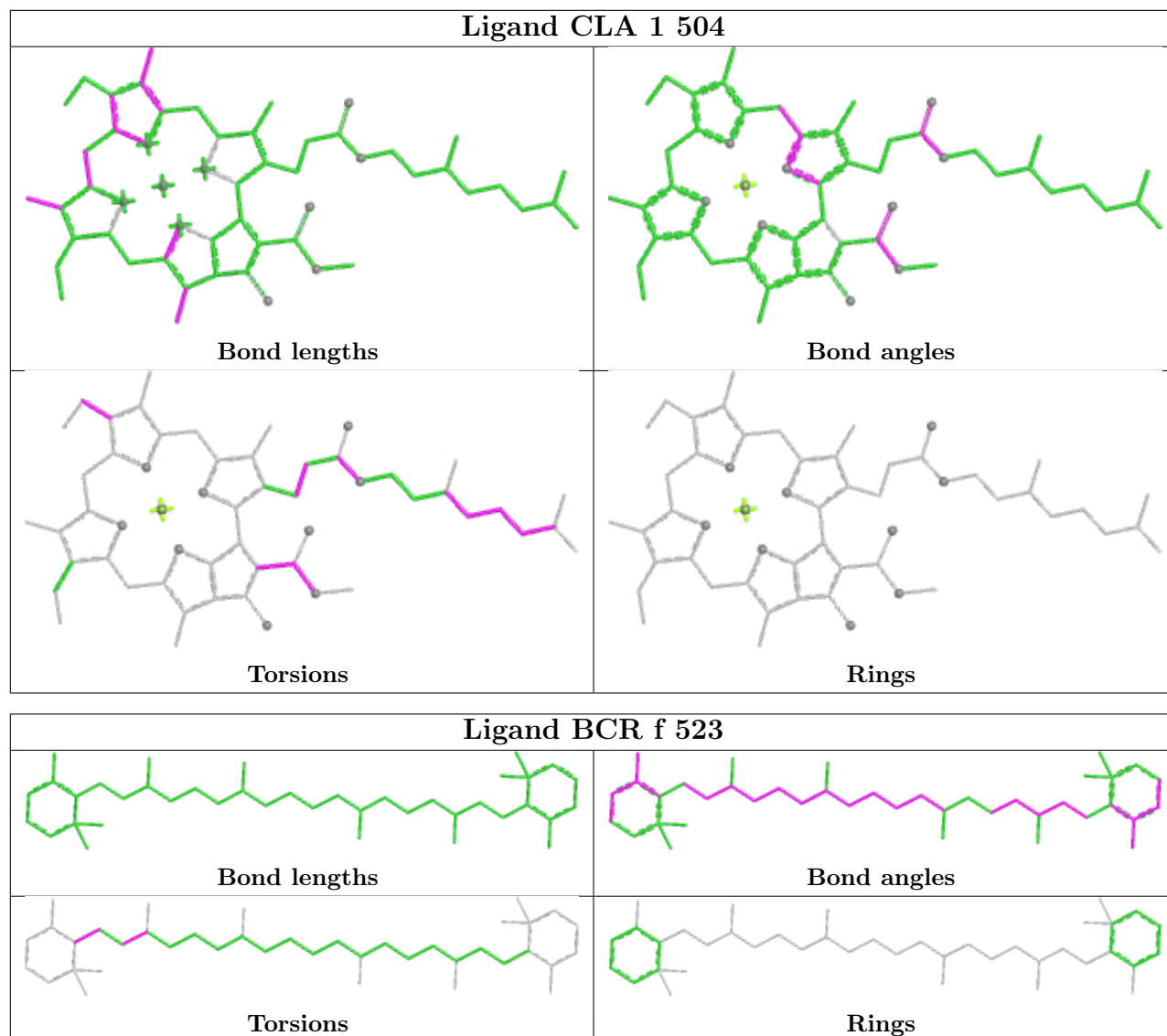
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	c	501	CLA	7	0
13	3	508	CLA	6	0
13	5	507	CLA	7	0
13	1	509	CLA	4	0
13	a	517	CLA	3	0
13	B	1217	CLA	2	0
13	A	1101	CLA	7	0
13	a	501	CLA	8	0
13	2	509	CLA	4	0
14	6	523	BCR	5	0
14	A	4008	BCR	9	0
13	b	505	CLA	11	0
14	A	4011	BCR	3	0
13	5	513	CLA	4	0
14	B	4006	BCR	3	0
13	A	1130	CLA	1	0
14	4	524	BCR	4	0
14	6	524	BCR	6	0
13	c	511	CLA	5	0
13	3	518	CLA	3	0
13	g	507	CLA	6	0
14	2	521	BCR	8	0
13	g	512	CLA	3	0
13	d	506	CLA	6	0
14	d	524	BCR	6	0
13	B	1216	CLA	5	0
13	g	508	CLA	2	0
14	g	524	BCR	8	0
13	5	519	CLA	2	0
13	5	503	CLA	6	0
14	a	522	BCR	8	0
13	e	510	CLA	3	0
14	5	521	BCR	8	0
13	e	502	CLA	5	0
13	5	508	CLA	4	0
14	A	4003	BCR	7	0
14	e	522	BCR	6	0
13	2	519	CLA	2	0
13	g	513	CLA	5	0
13	2	517	CLA	1	0
13	B	1230	CLA	2	0
13	B	1233	CLA	2	0

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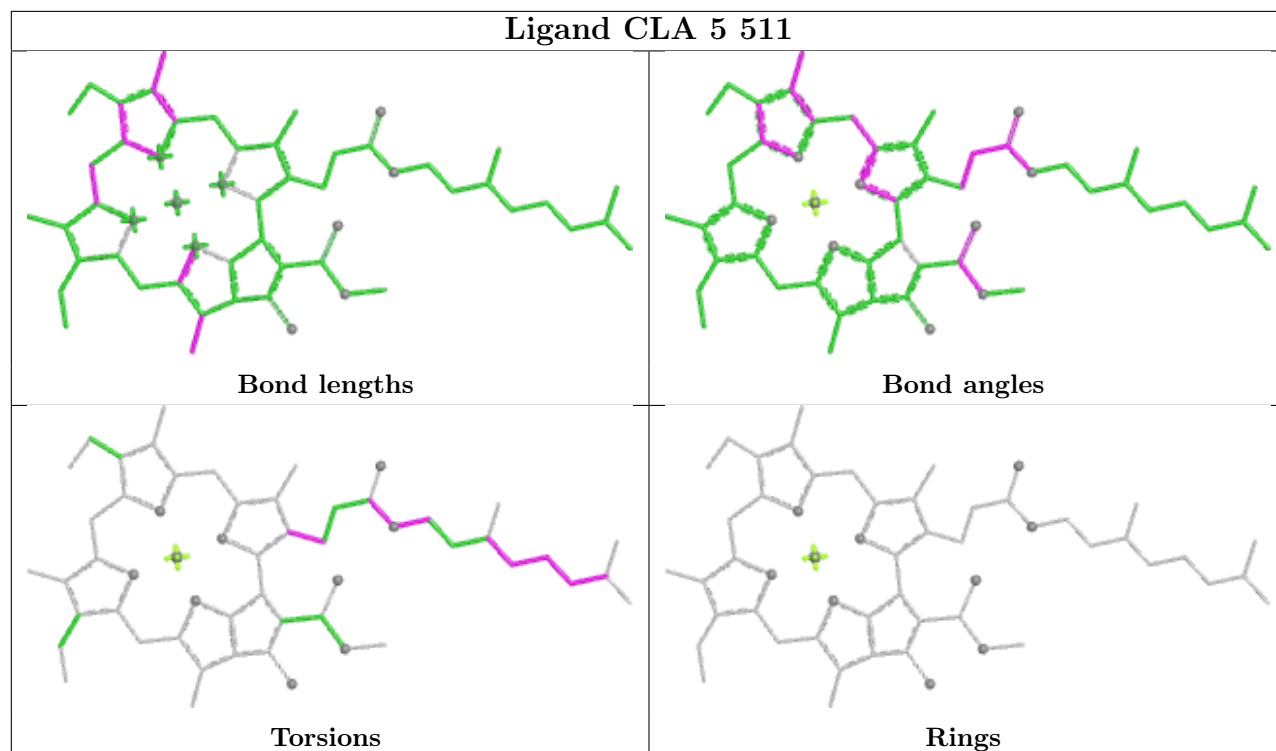
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	4	503	CLA	5	0
15	5	822	SQD	2	0
14	F	4015	BCR	7	0
13	g	518	CLA	2	0
13	b	503	CLA	6	0
13	b	509	CLA	7	0
13	A	1109	CLA	3	0
13	6	511	CLA	5	0
13	e	507	CLA	1	0
14	c	522	BCR	9	0
14	K	4001	BCR	6	0
13	A	1103	CLA	8	0
14	6	522	BCR	2	0
13	B	1211	CLA	4	0
13	b	506	CLA	1	0
16	6	5104	LMG	2	0
16	B	5002	LMG	5	0
13	c	512	CLA	2	0

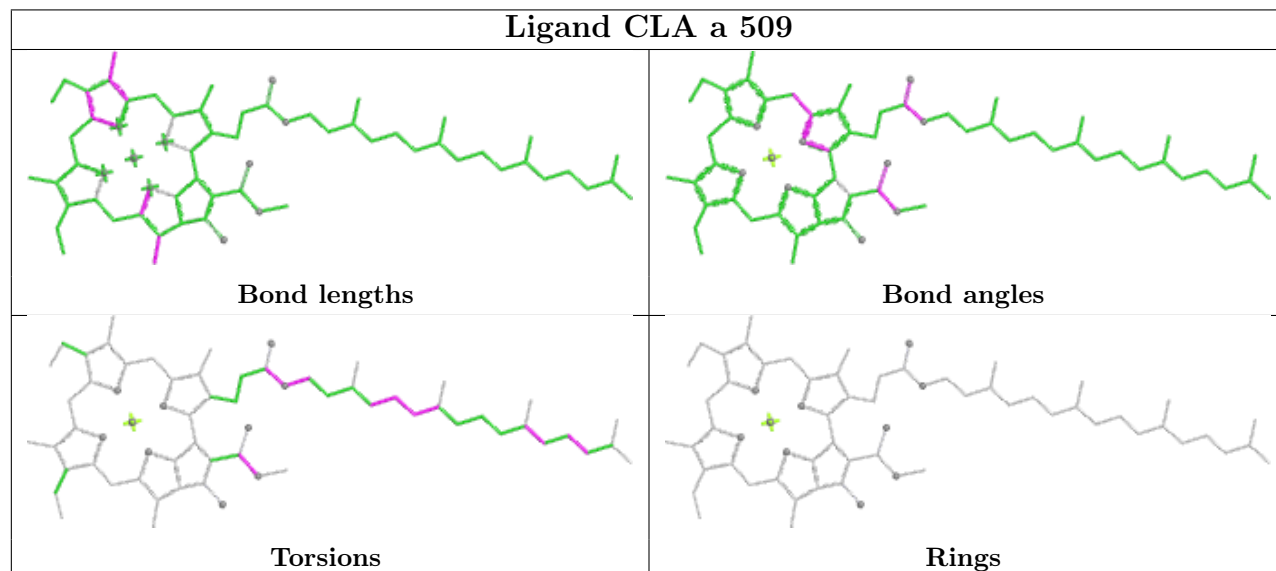
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

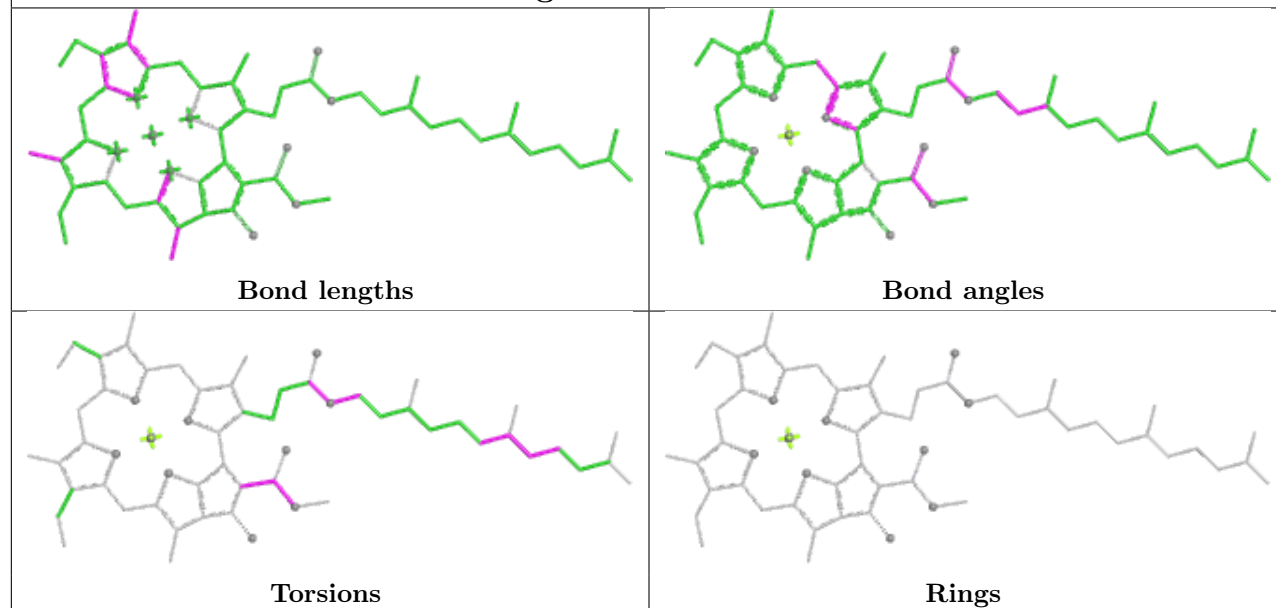
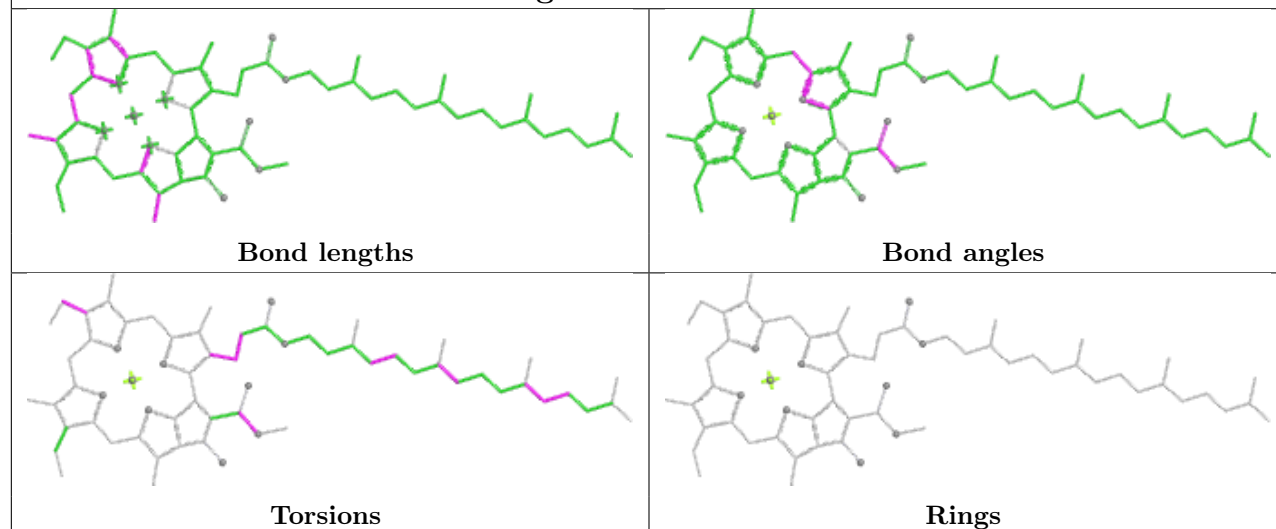
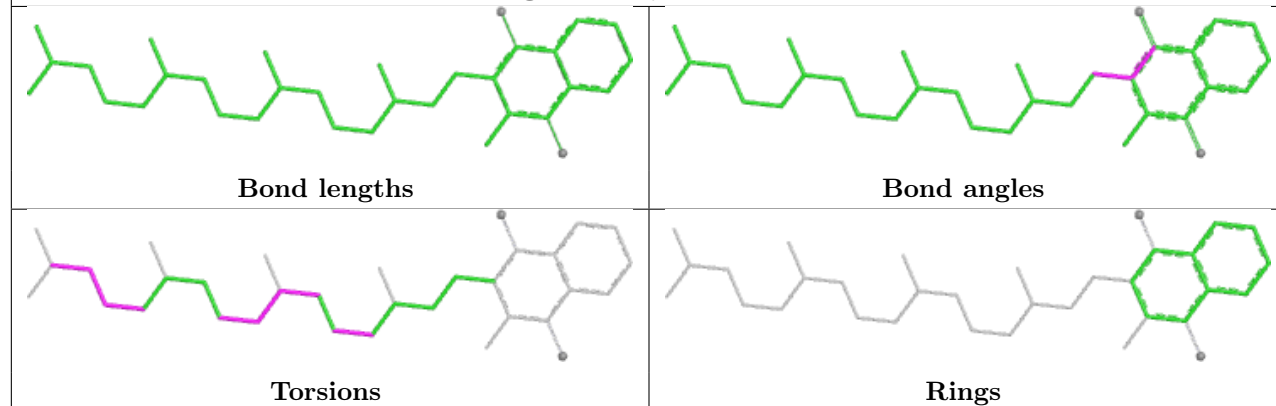


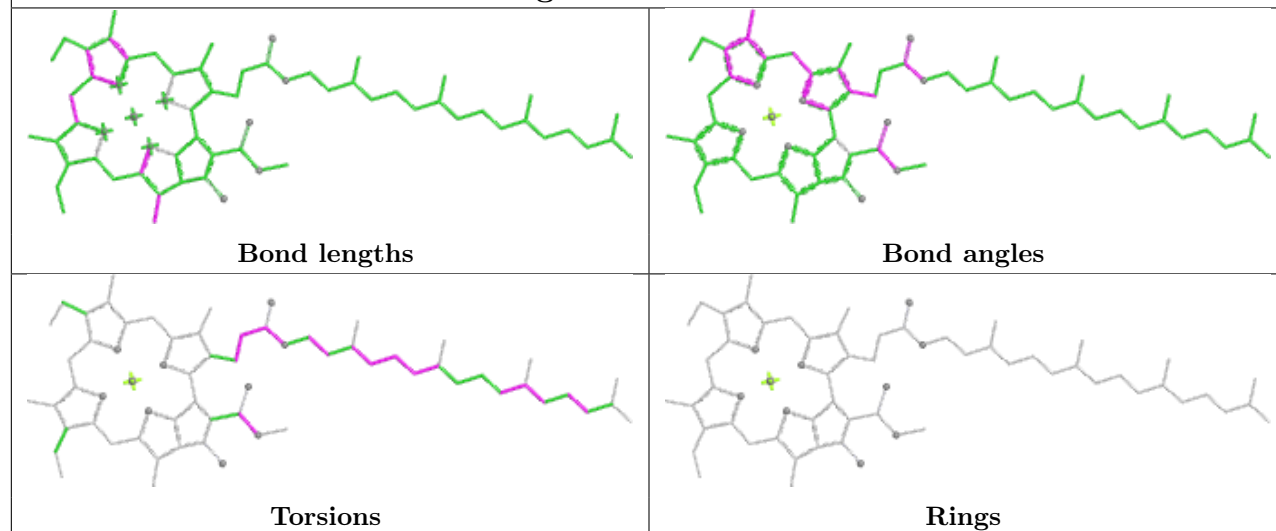
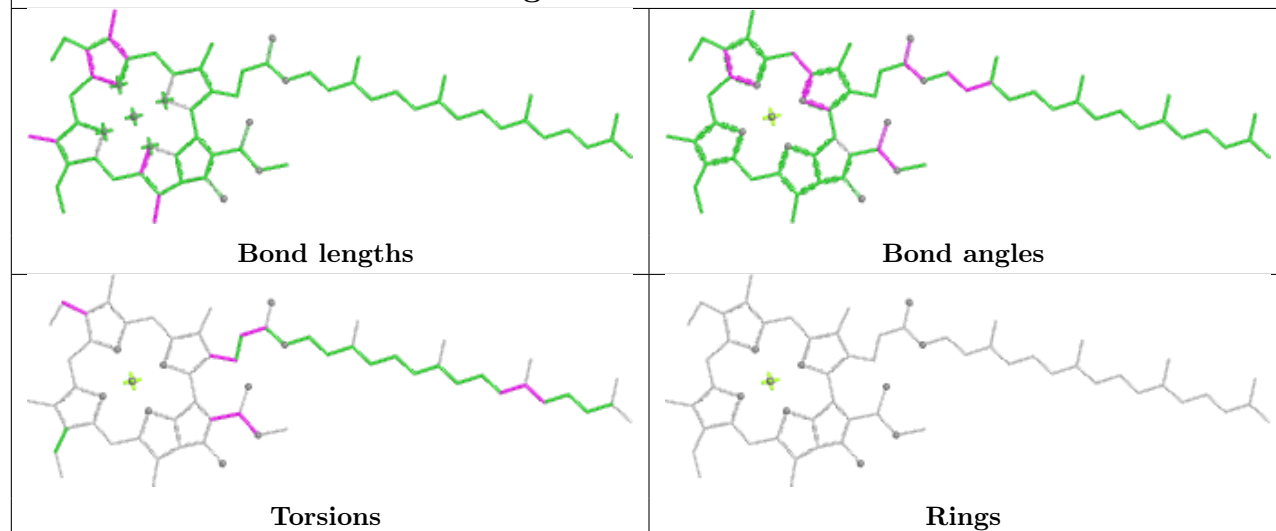
Ligand CLA 5 511



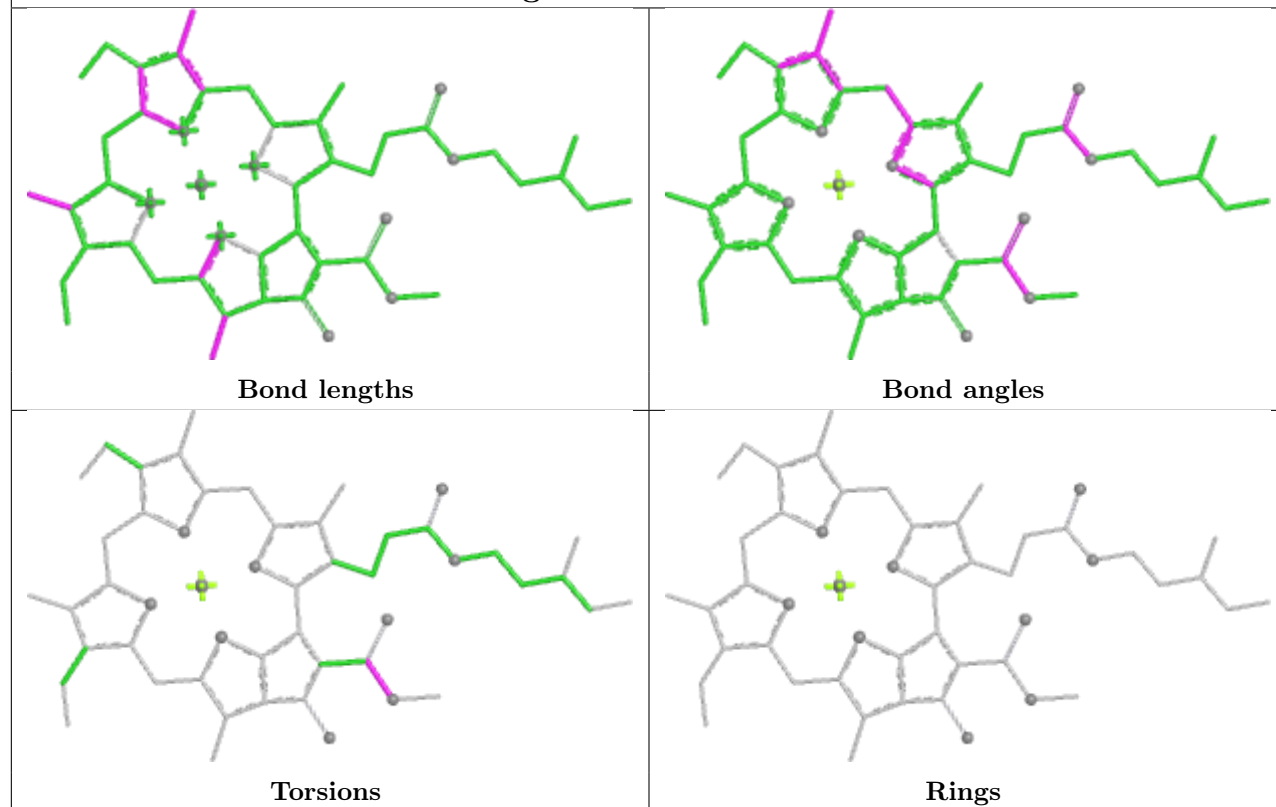
Ligand CLA a 509



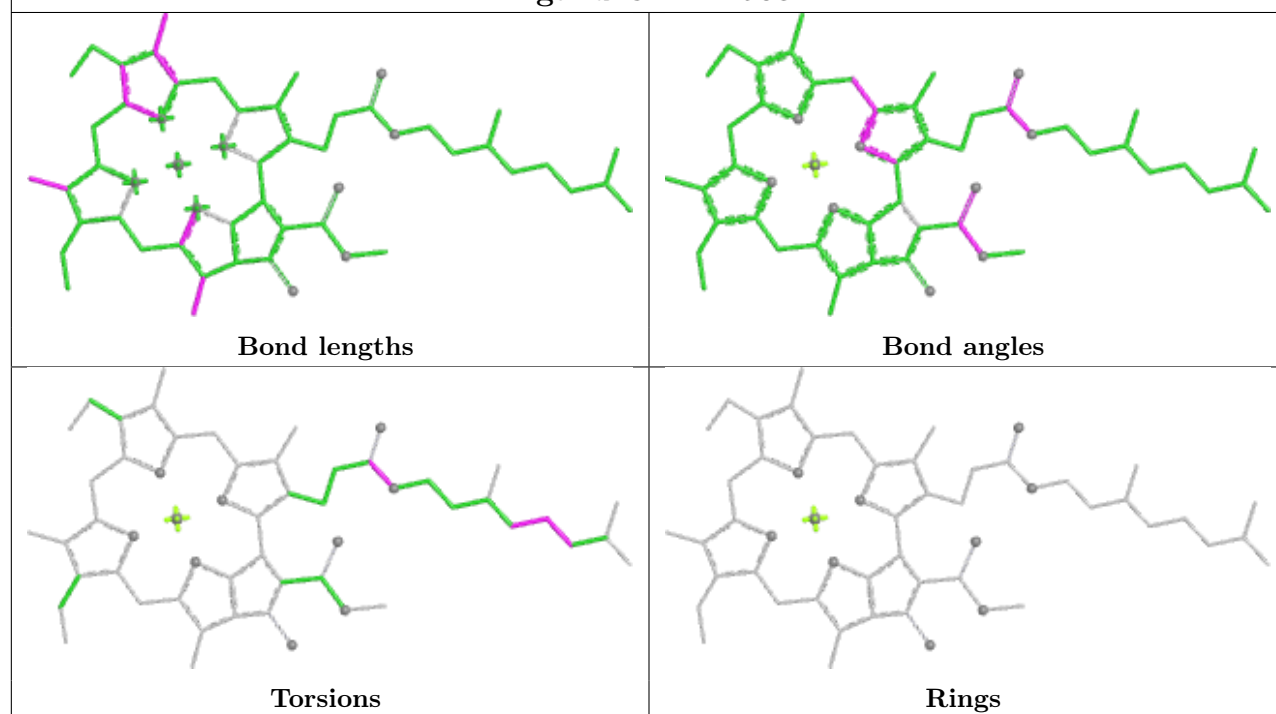
Ligand CLA 6 502**Ligand CLA 5 501****Ligand PQN B 2002**

Ligand CLA 3 505**Ligand CLA B 1239**

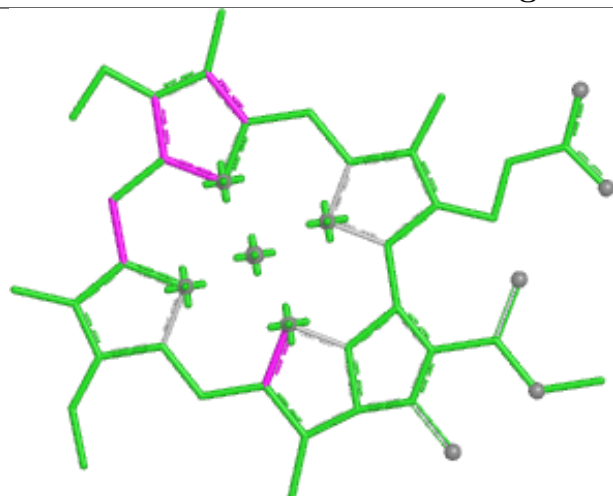
Ligand CLA A 1105



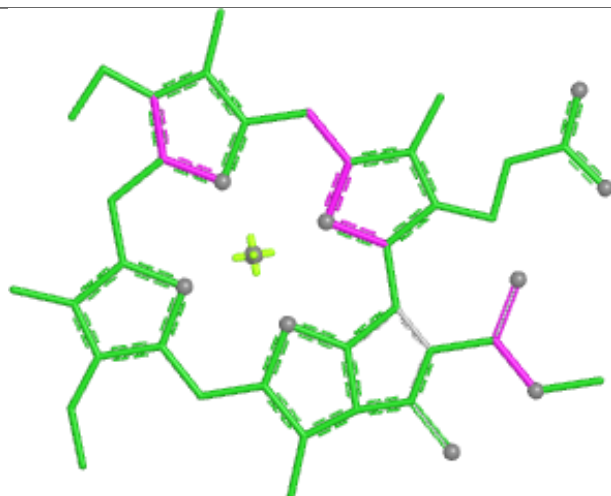
Ligand CLA 4 508



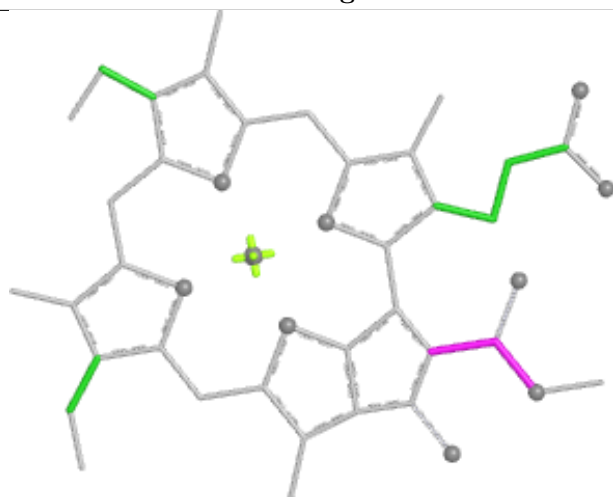
Ligand CLA c 506



Bond lengths



Bond angles

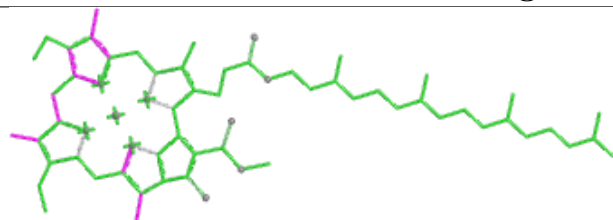


Torsions

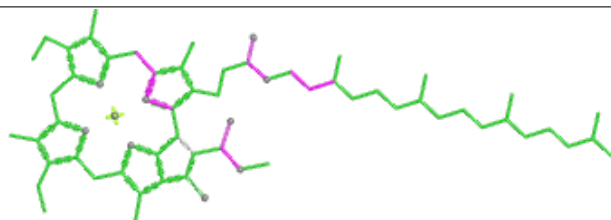


Rings

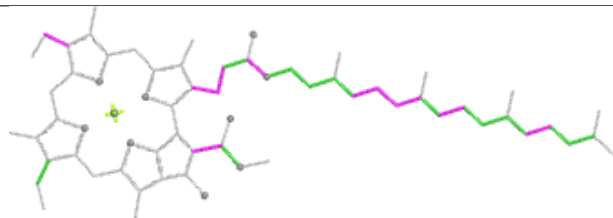
Ligand CLA 2 501



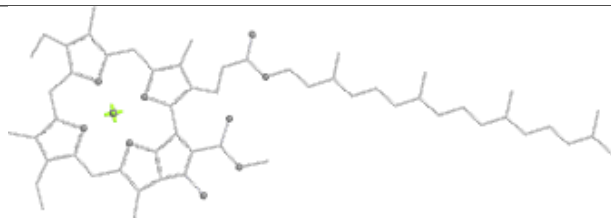
Bond lengths



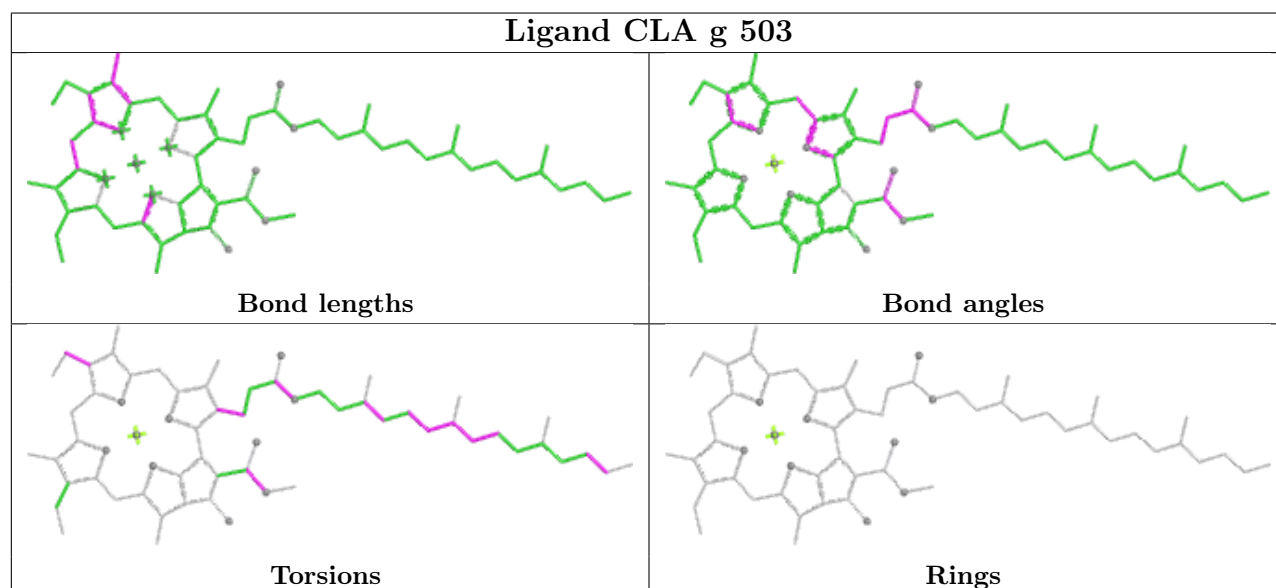
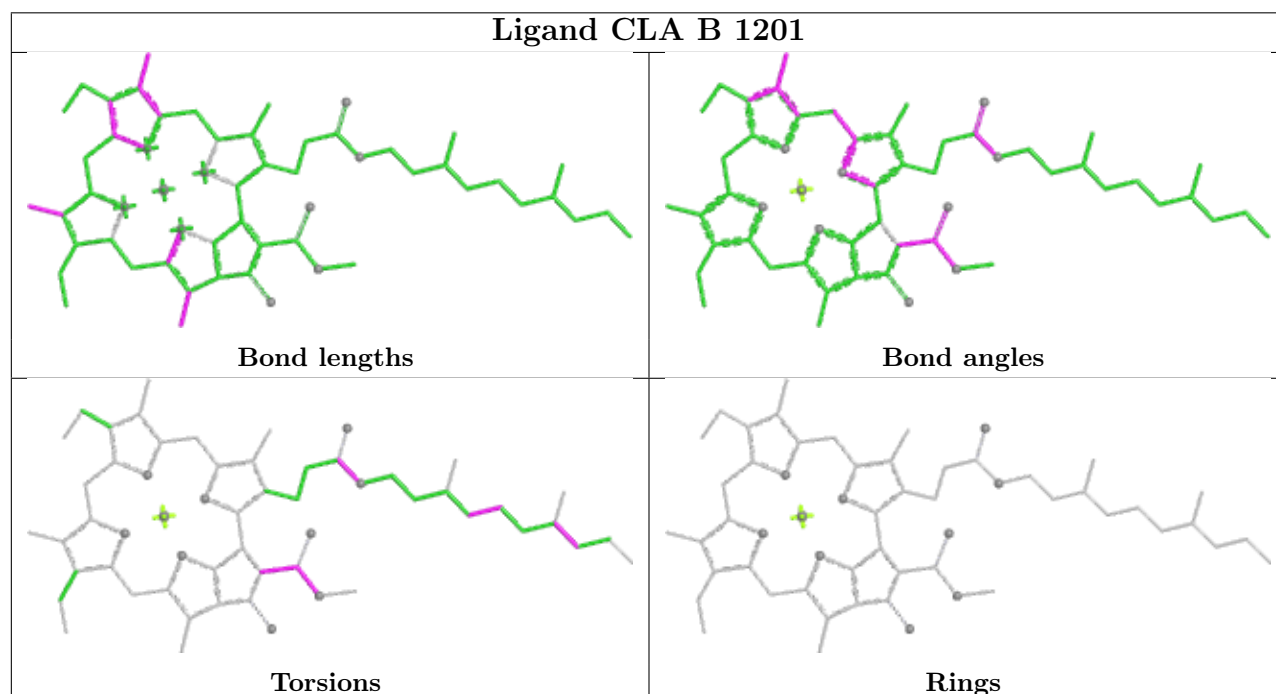
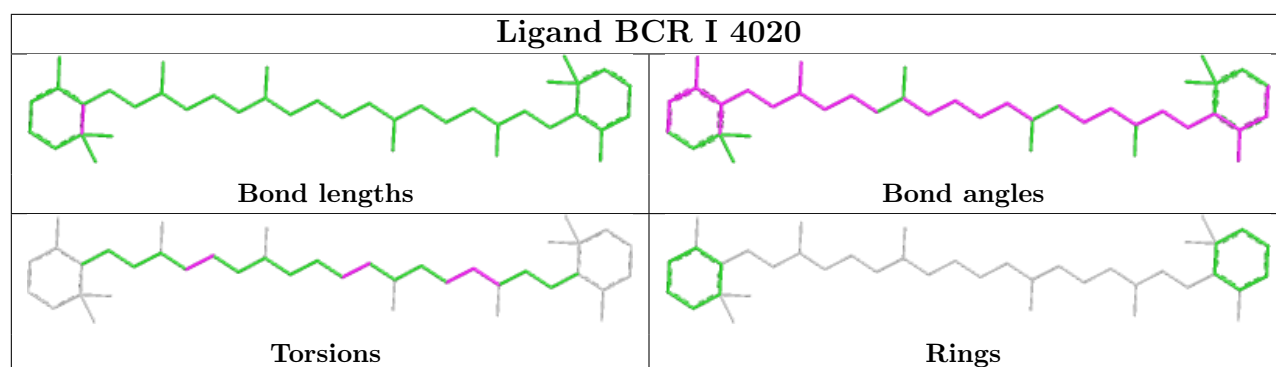
Bond angles

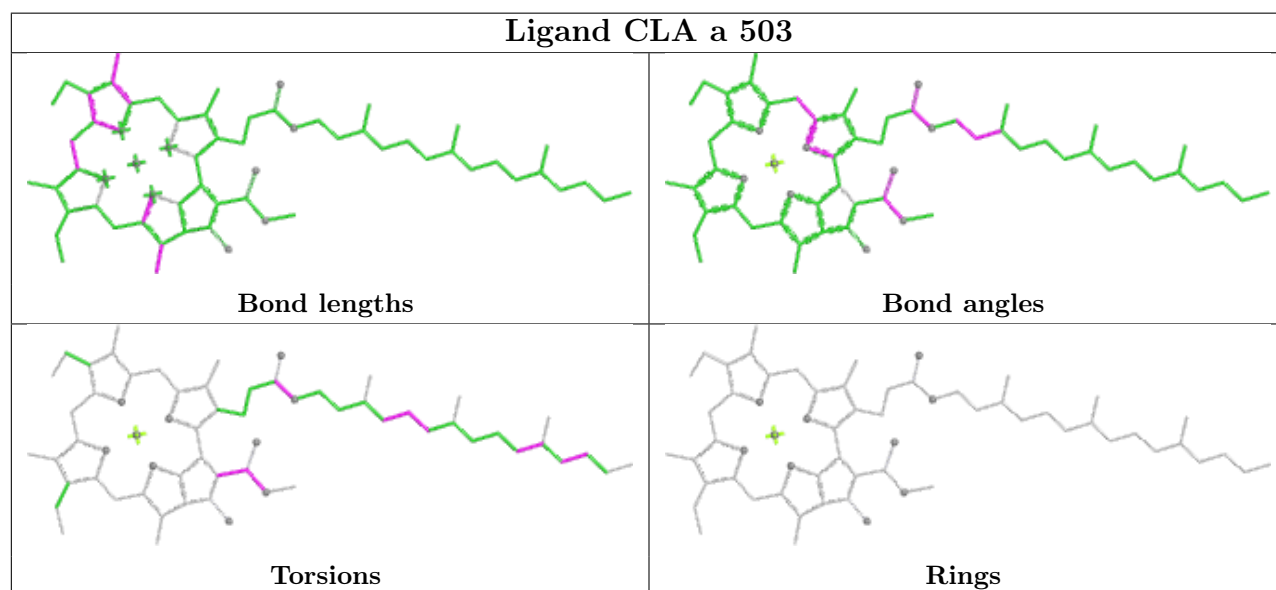
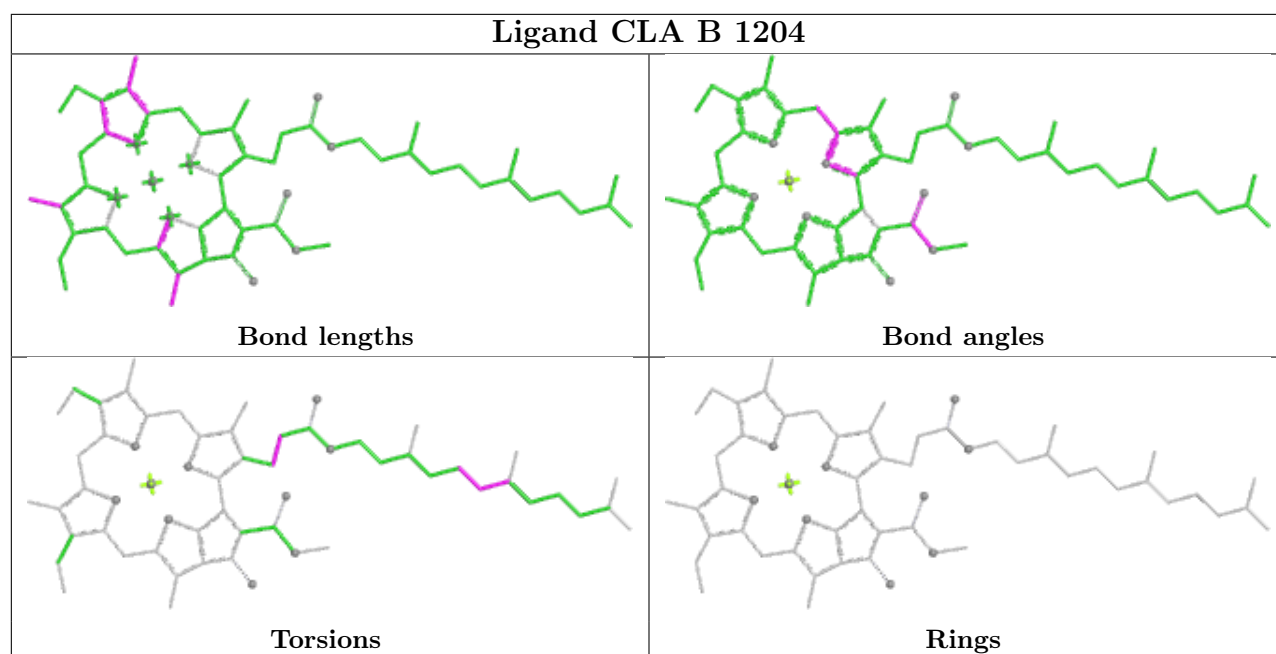


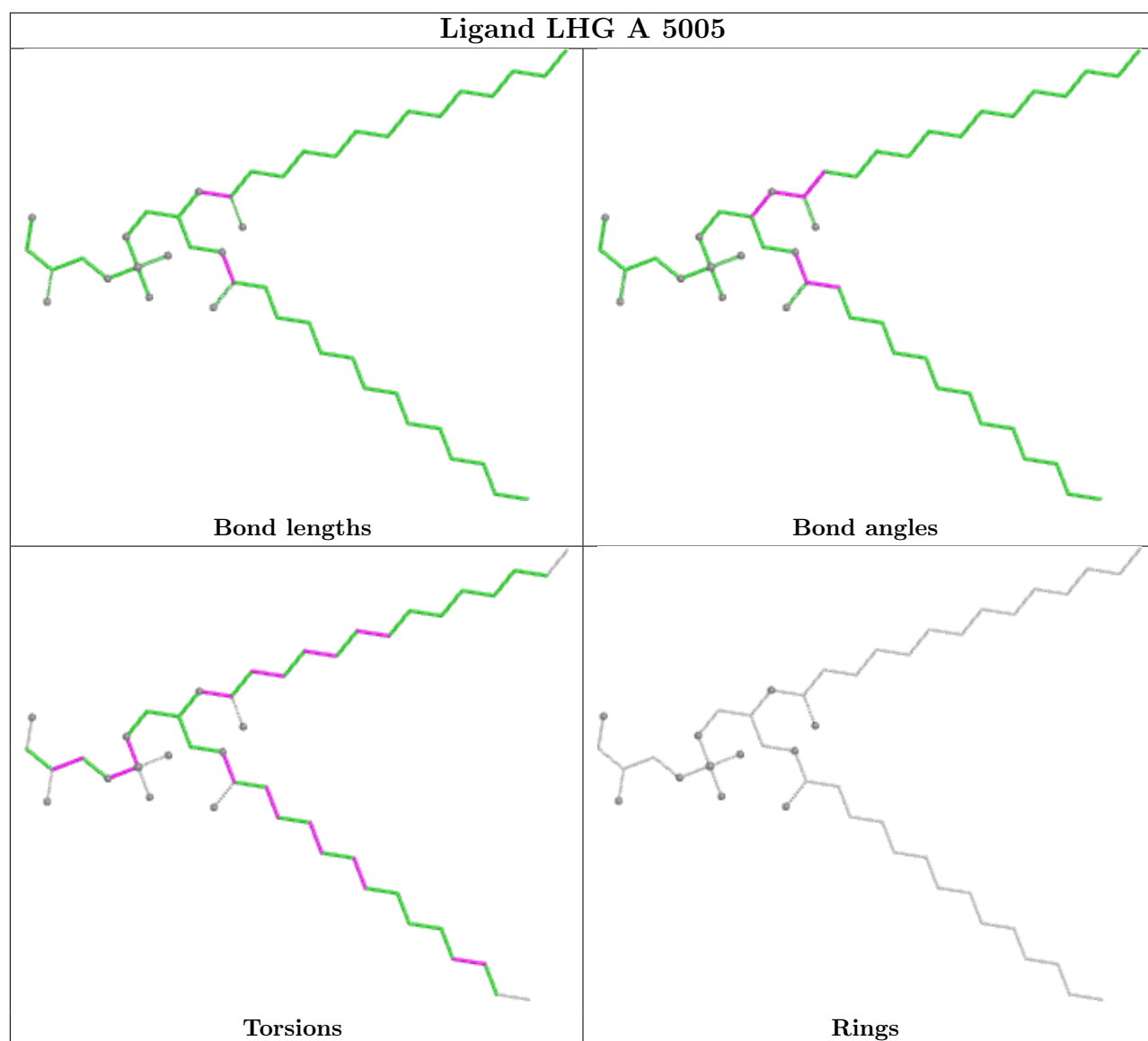
Torsions

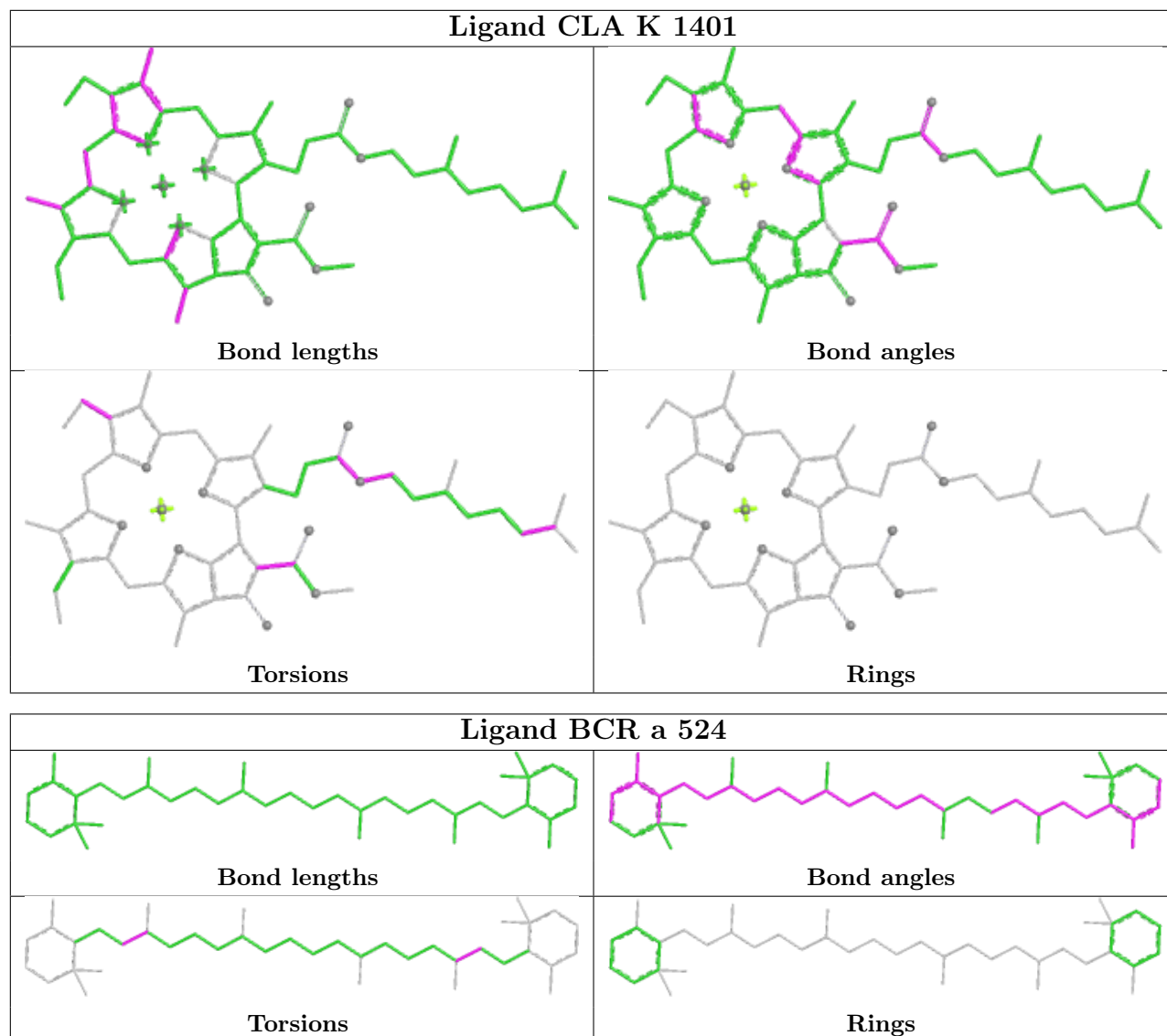


Rings

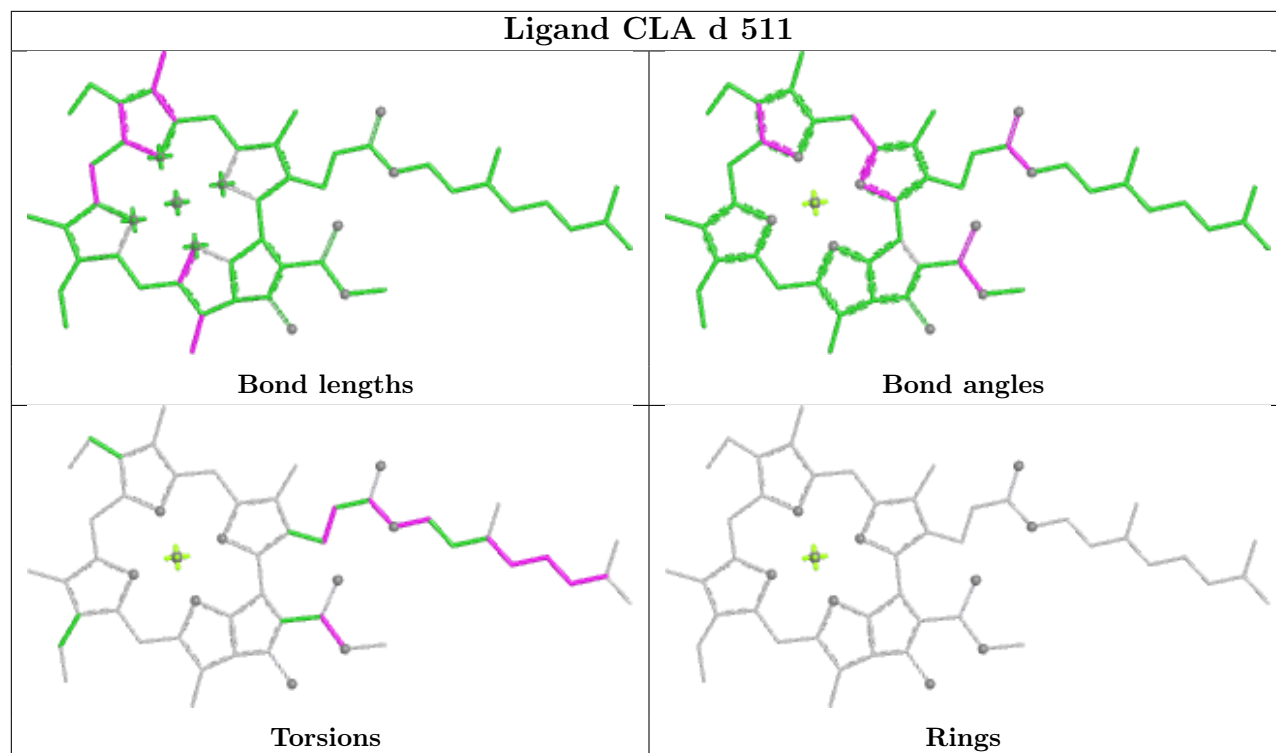




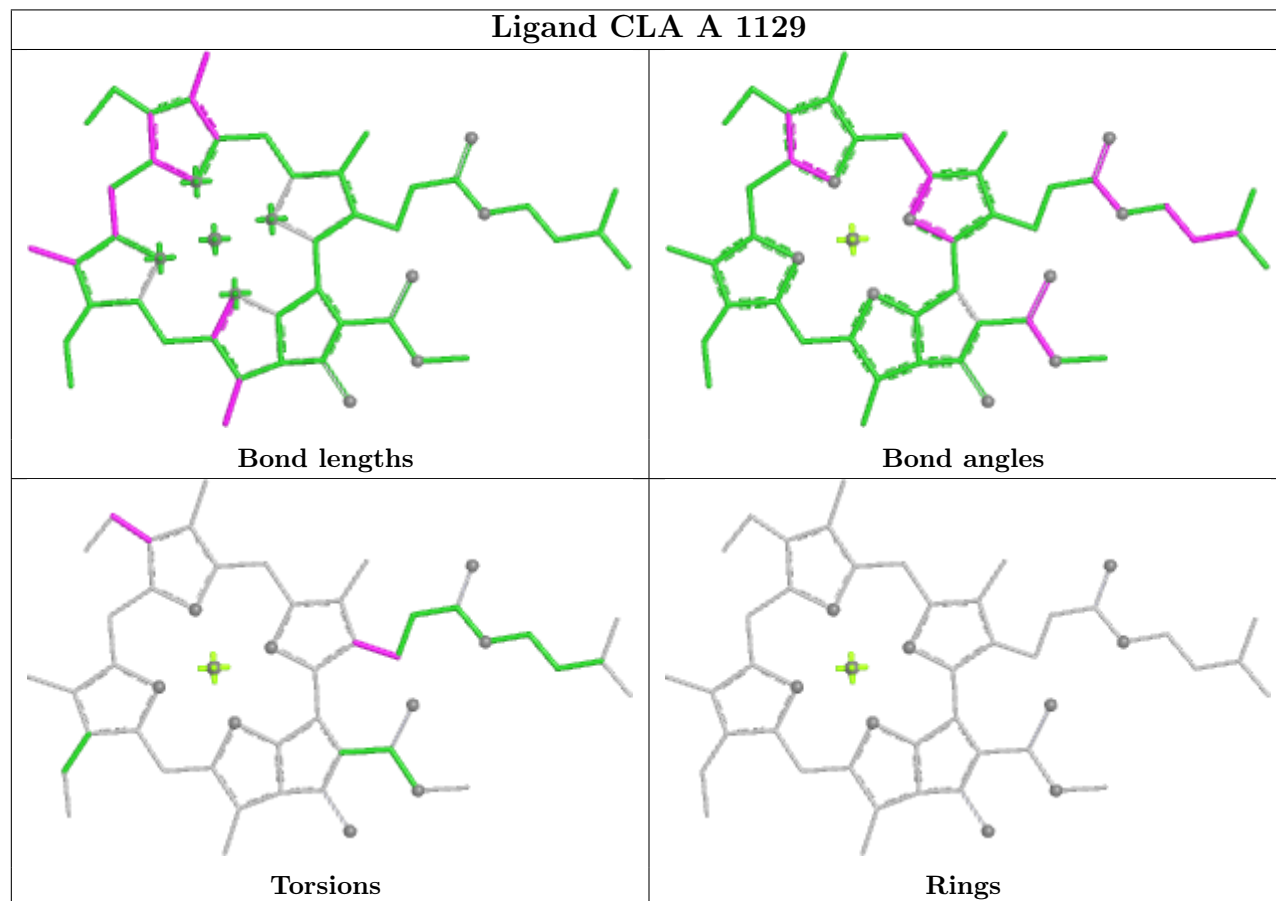


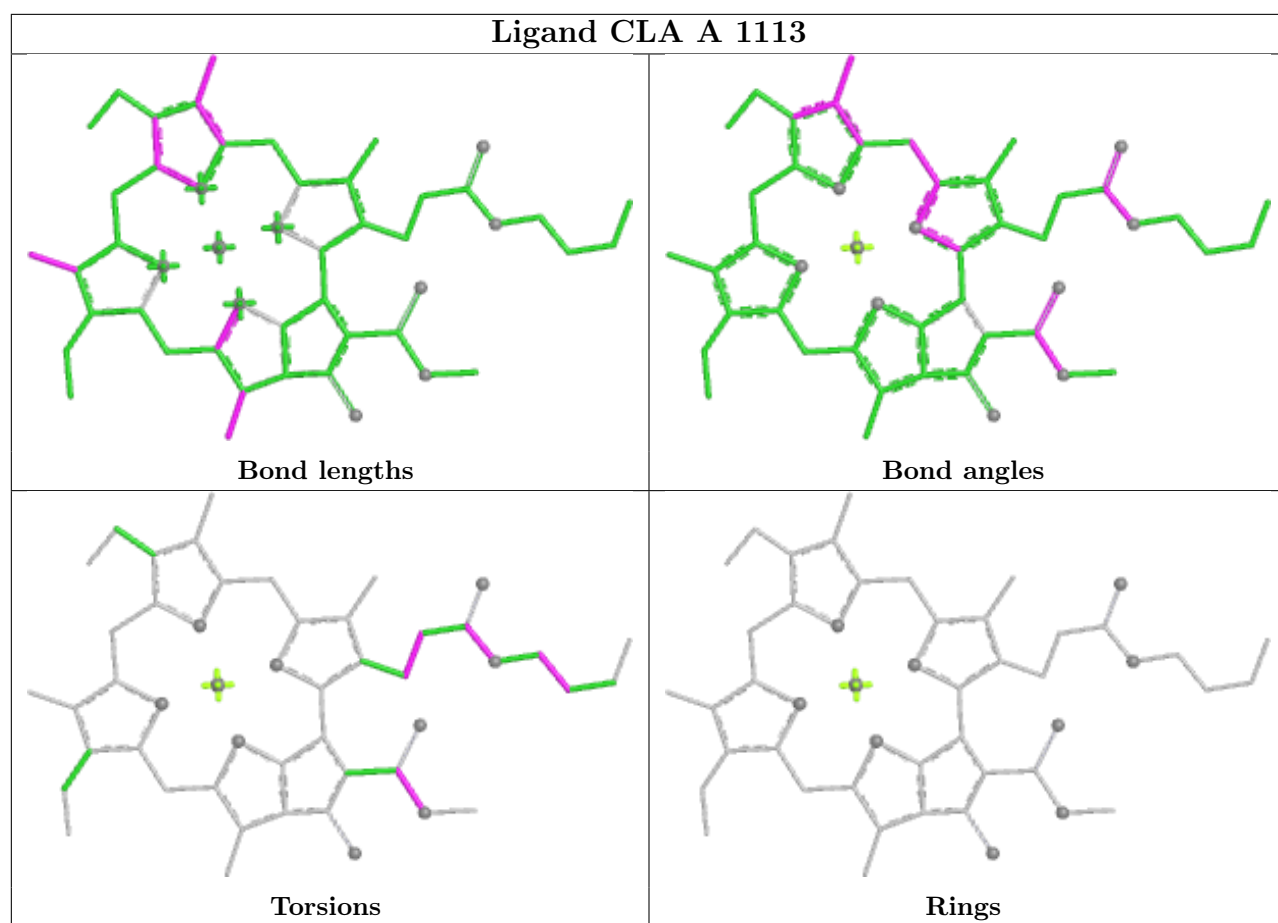


Ligand CLA d 511

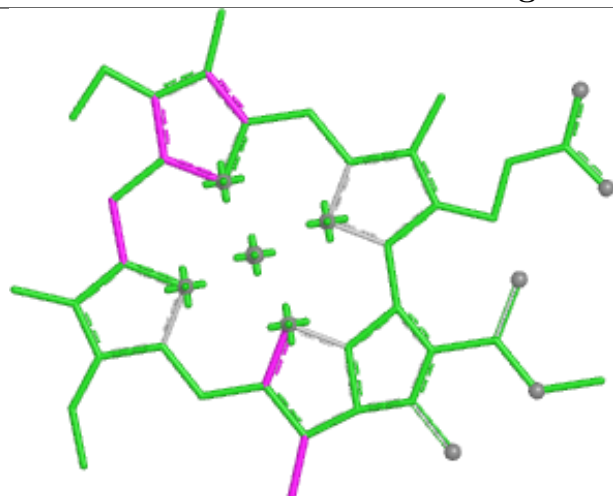


Ligand CLA A 1129

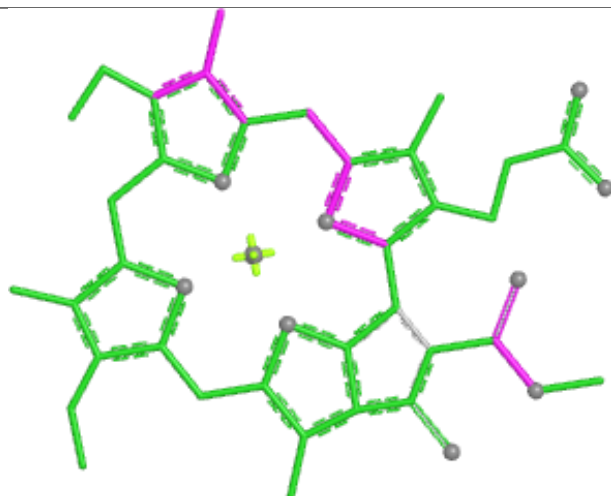




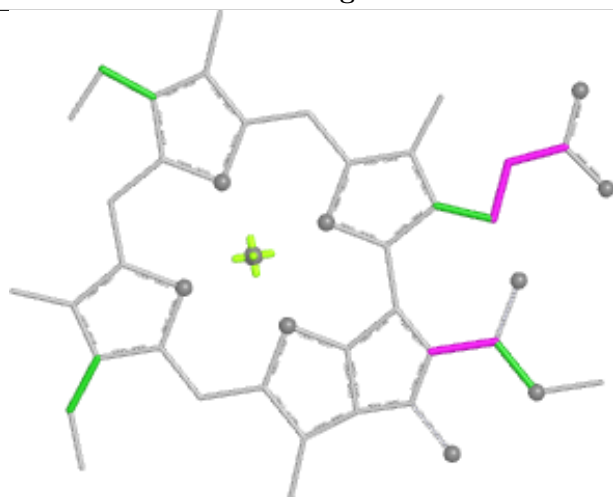
Ligand CLA 6 504



Bond lengths



Bond angles

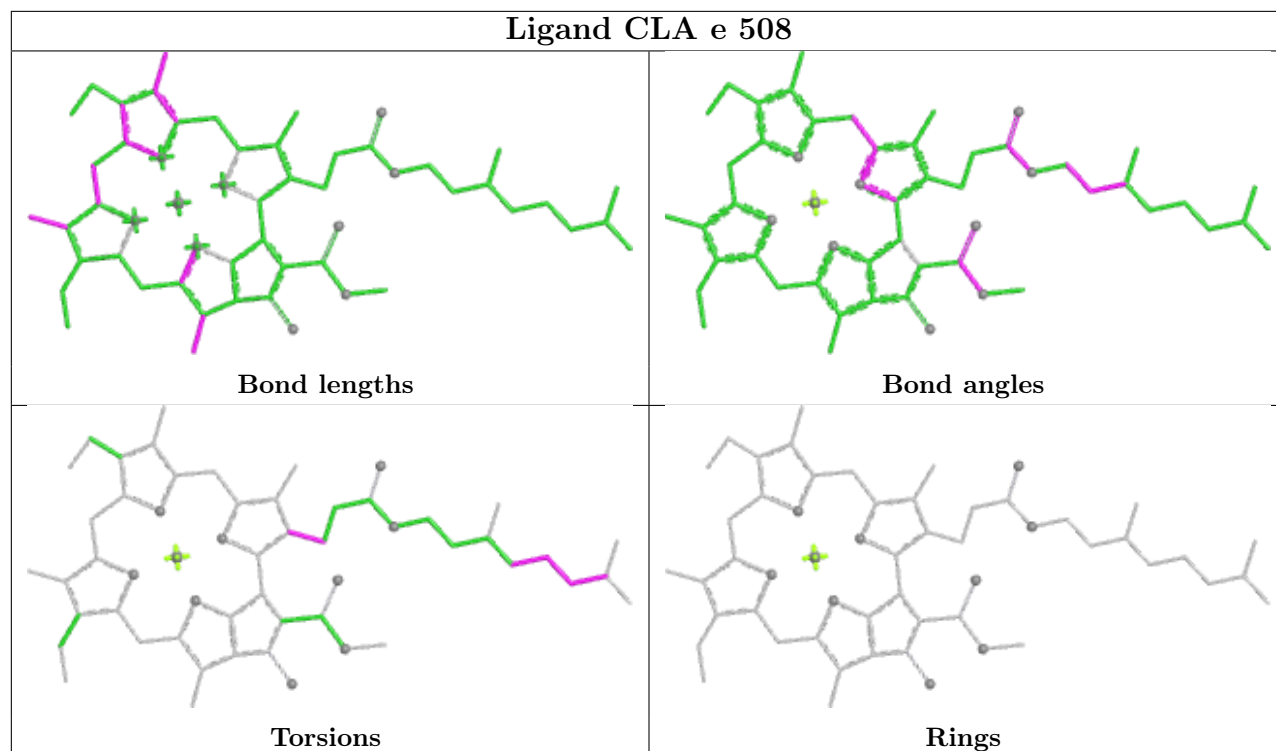


Torsions

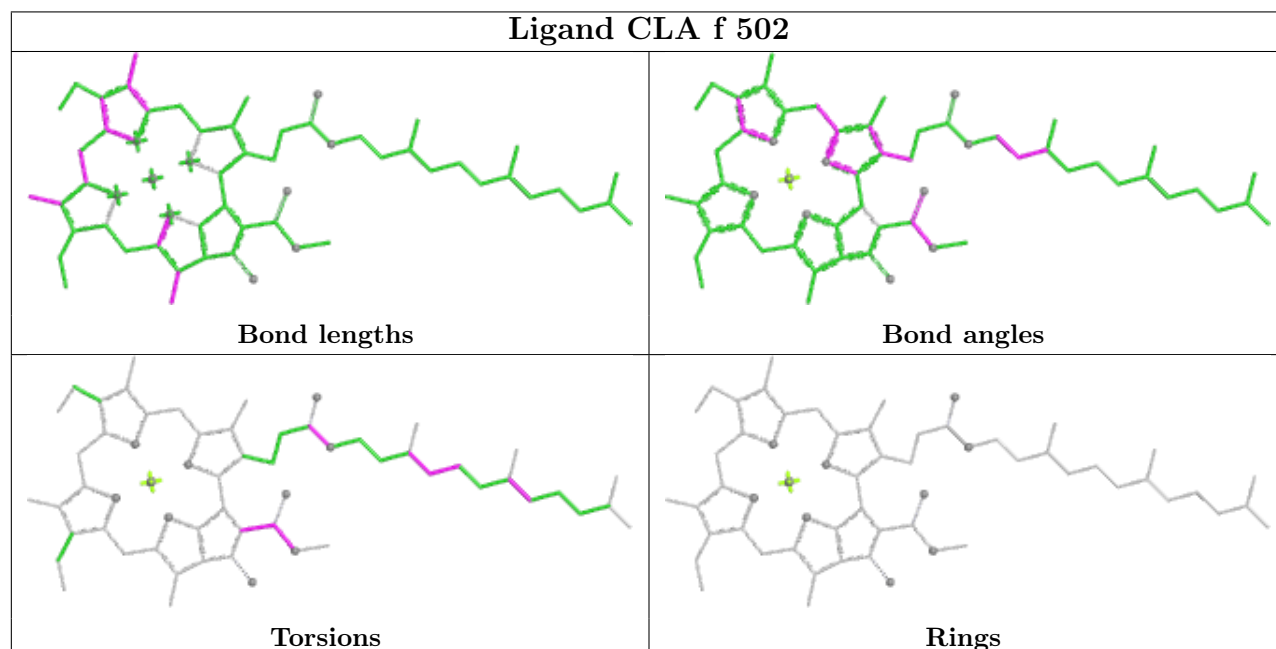


Rings

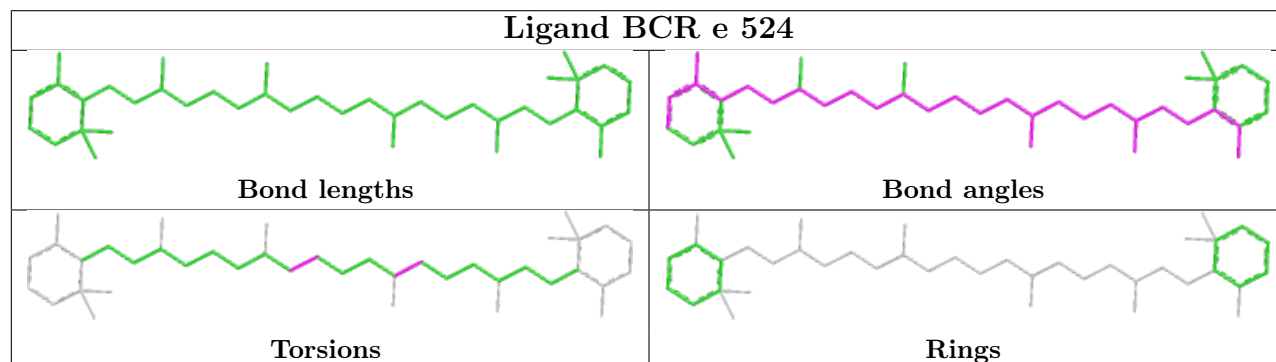
Ligand CLA e 508



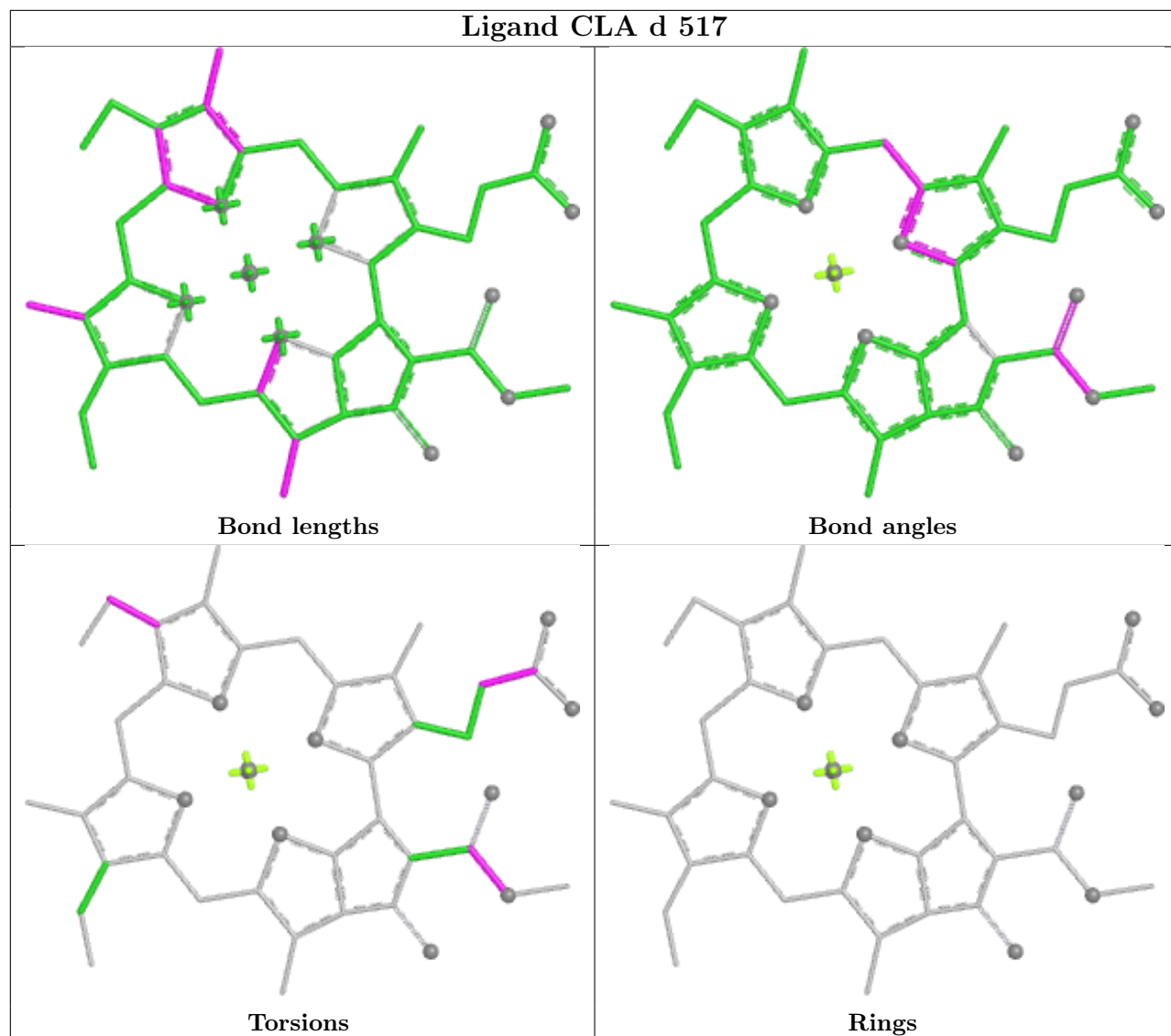
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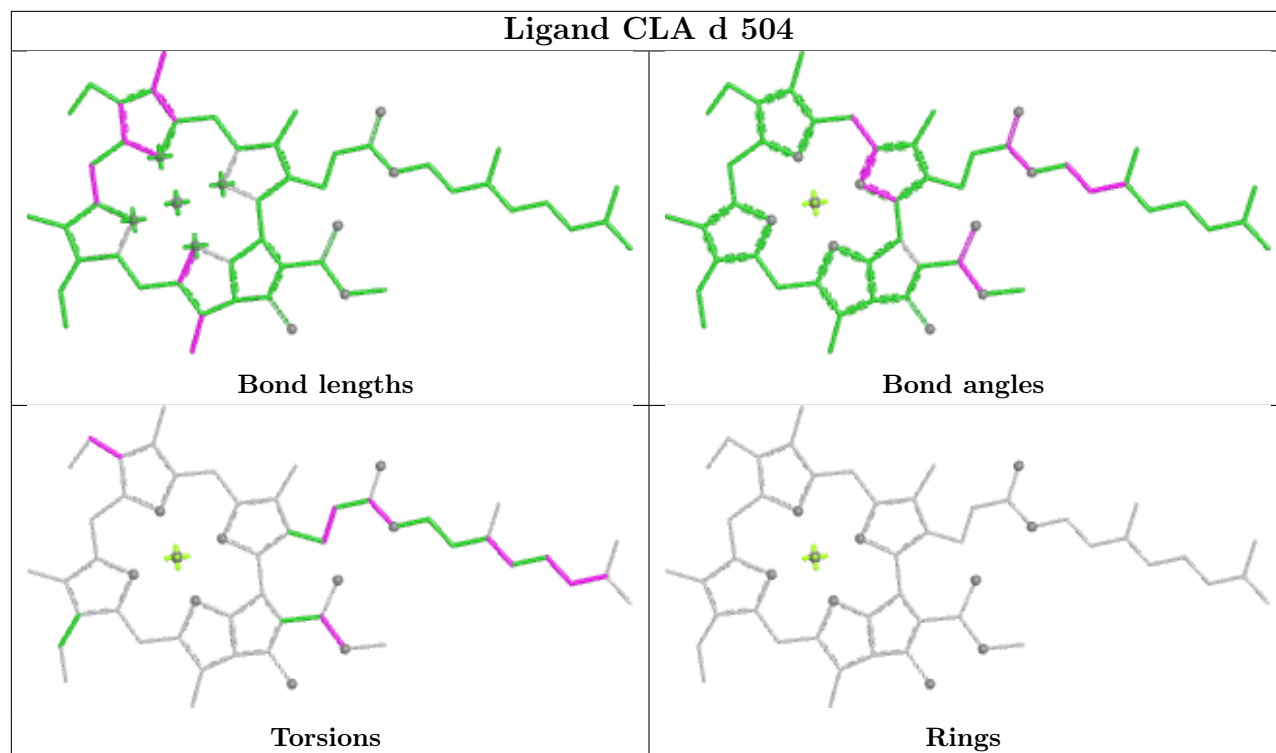
Ligand BCR e 524



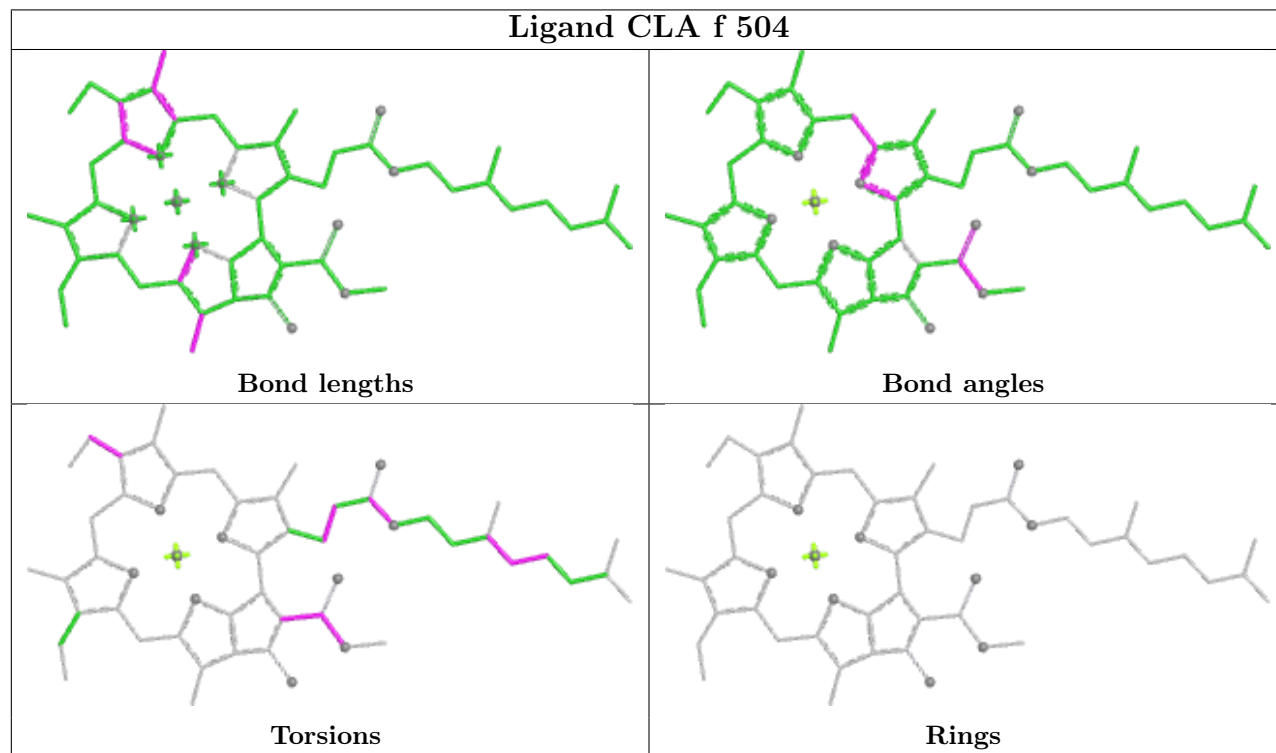
Ligand CLA d 517



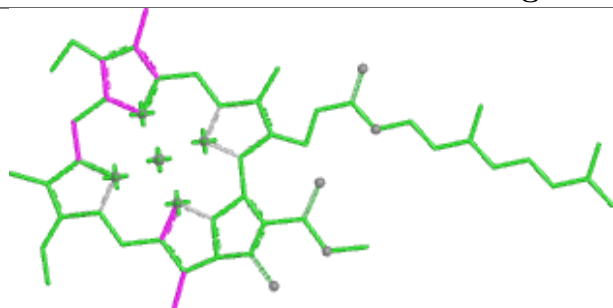
Ligand CLA d 504



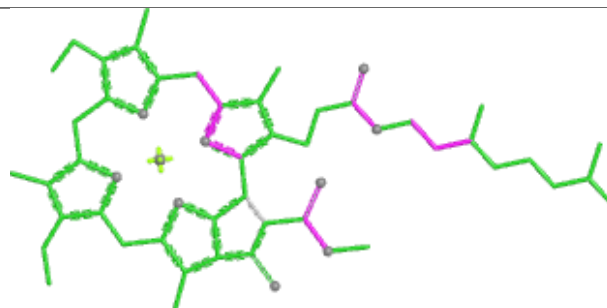
Ligand CLA f 504



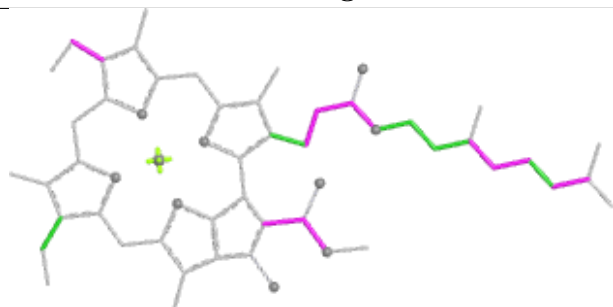
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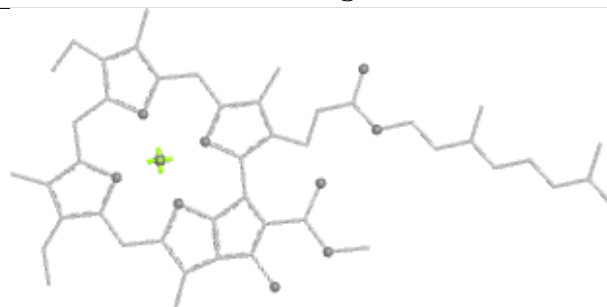
Bond lengths



Bond angles

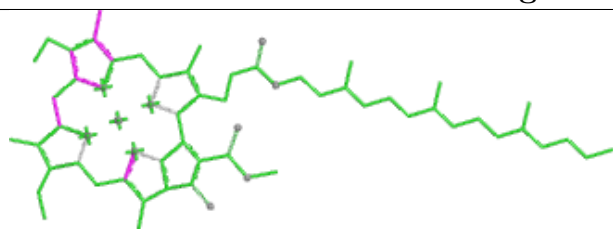


Torsions

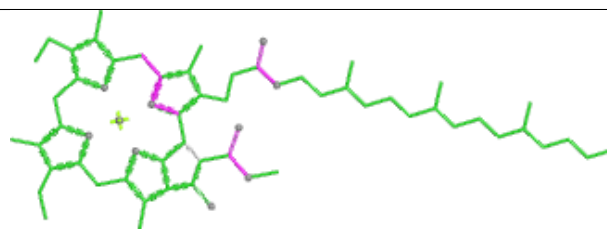


Rings

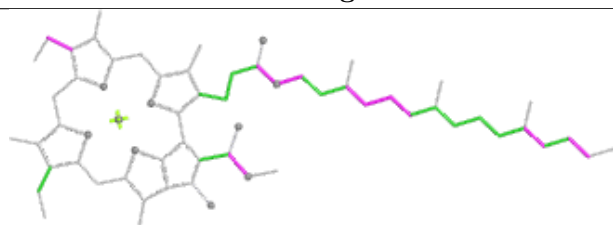
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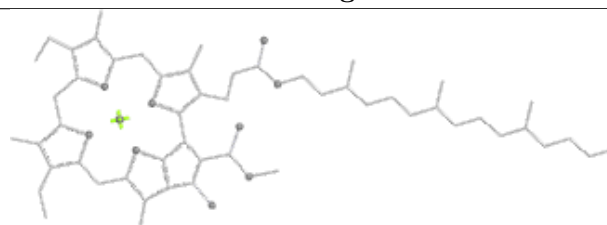
Bond lengths



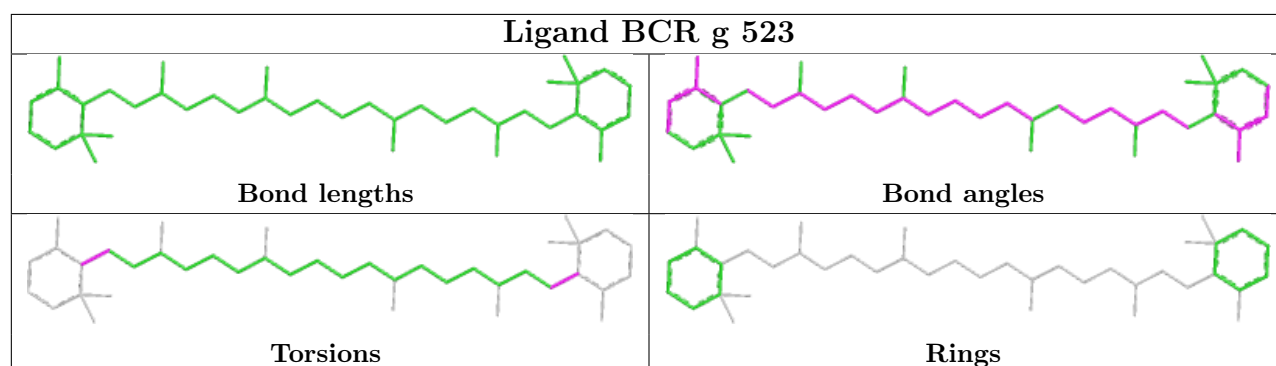
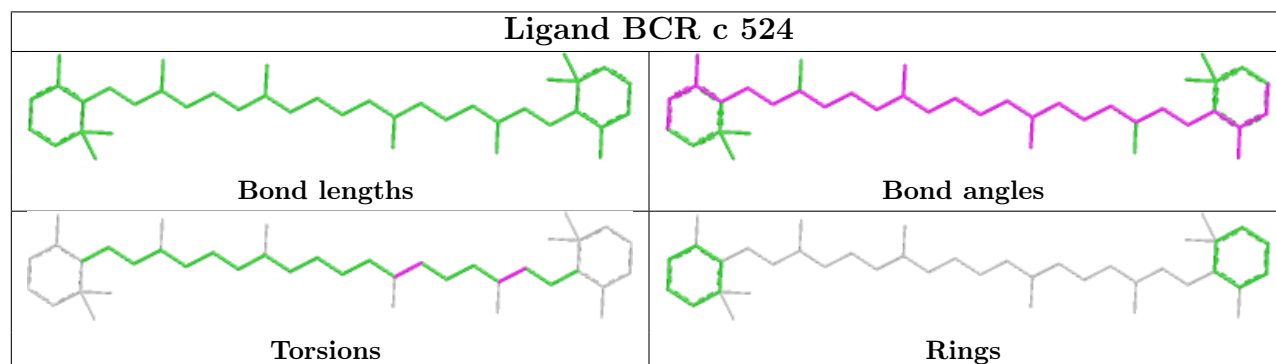
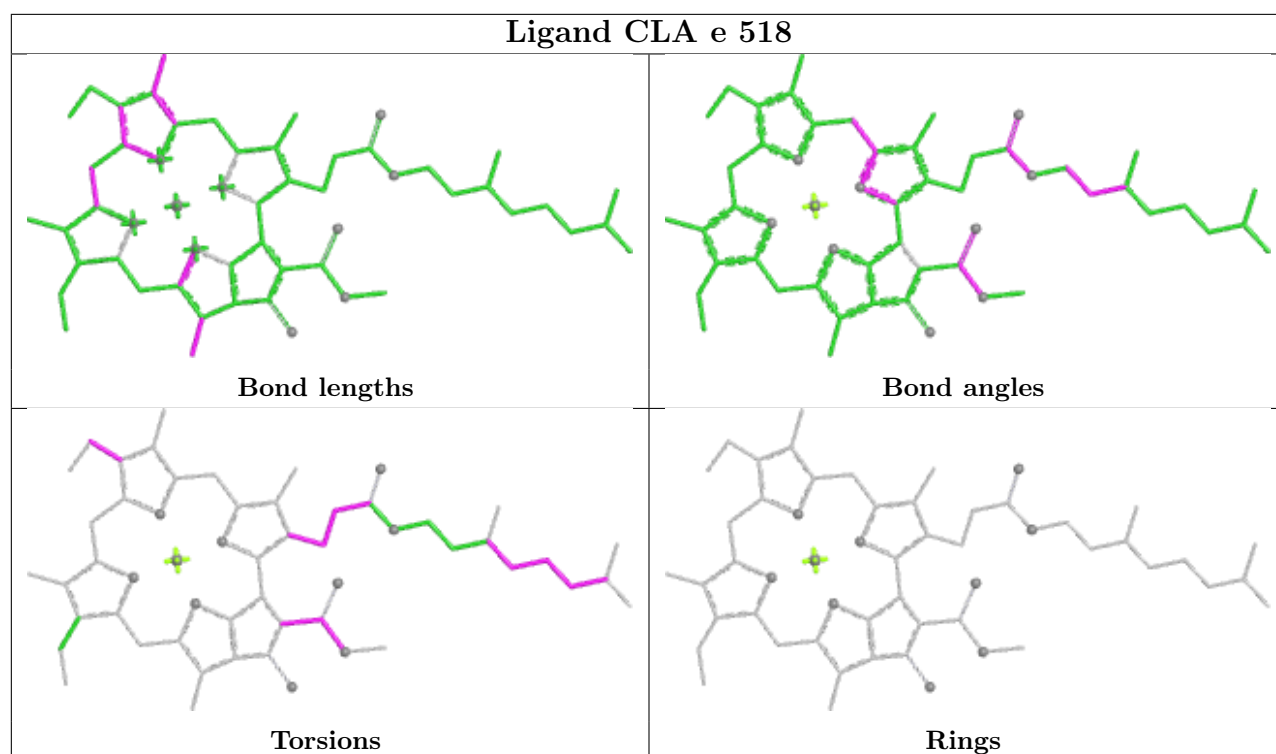
Bond angles

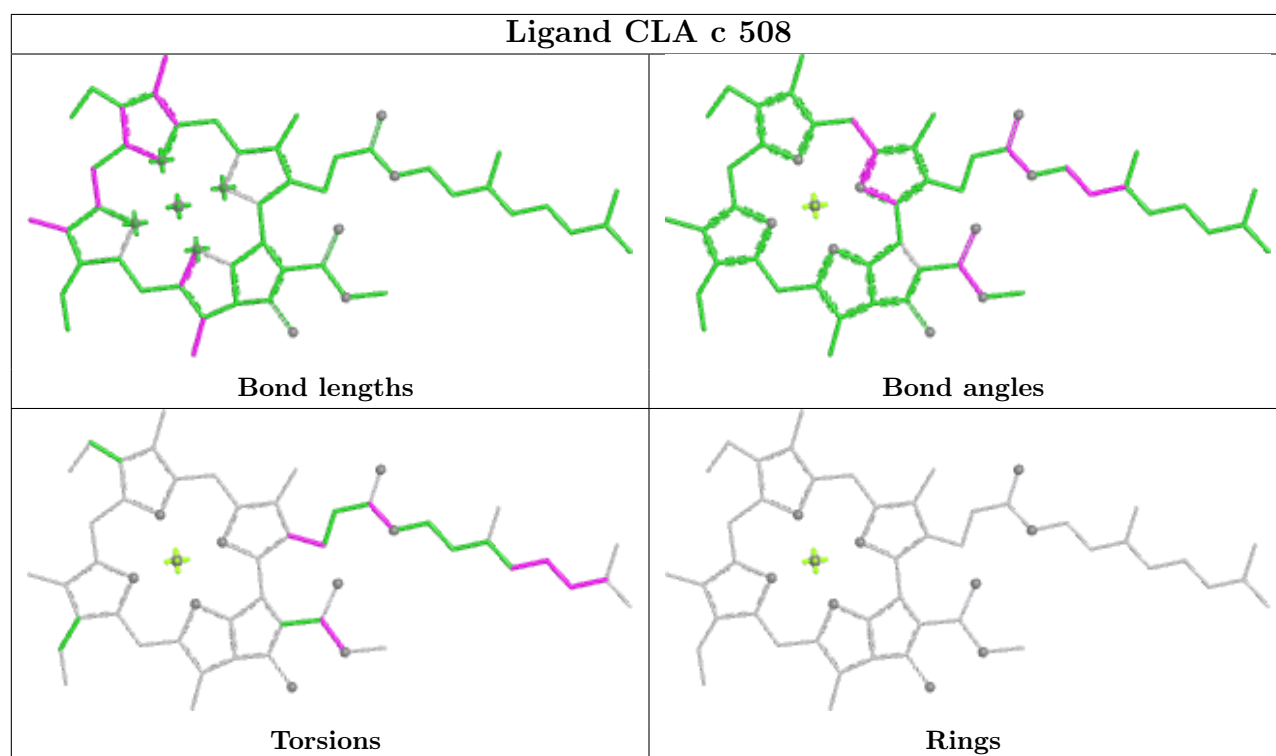
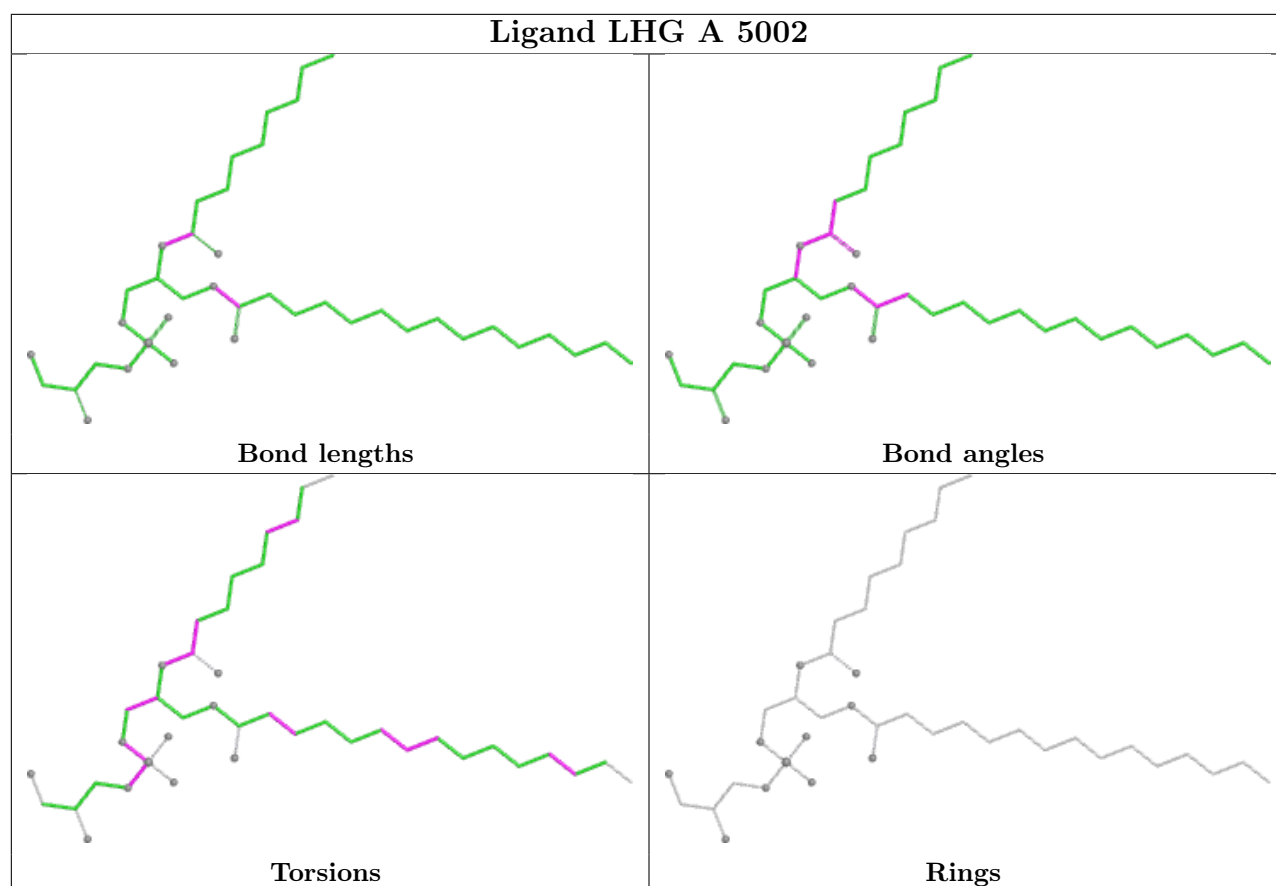


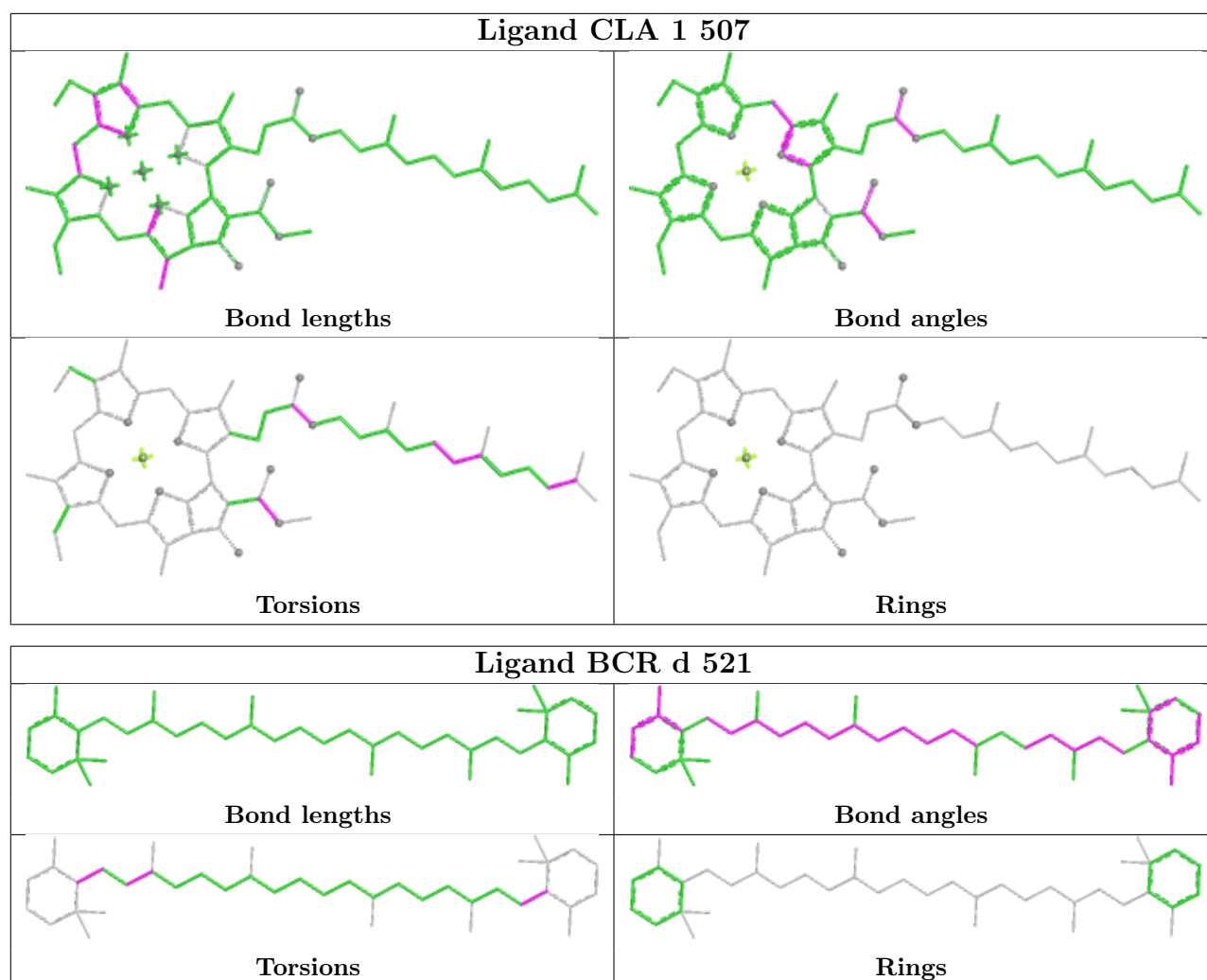
Torsions



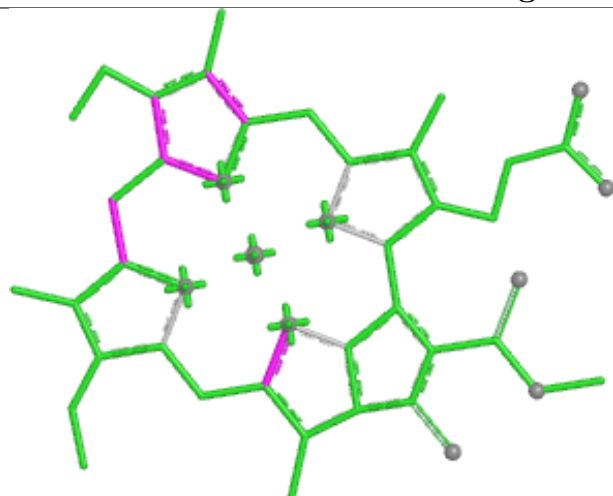
Rings



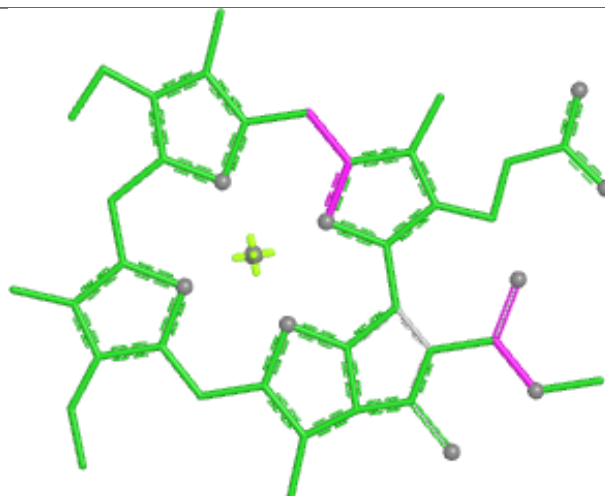




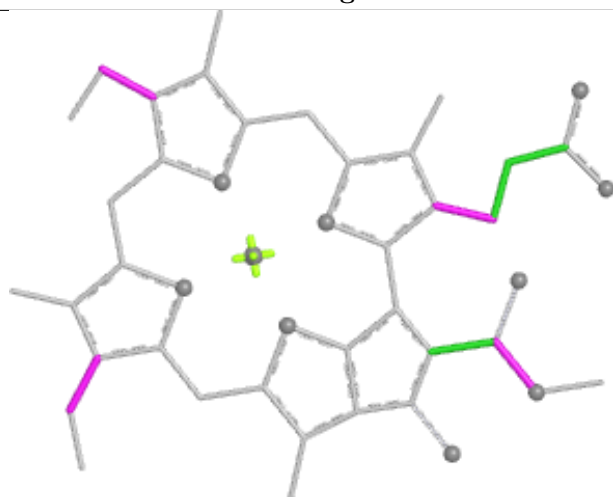
Ligand CLA 1 519



Bond lengths



Bond angles

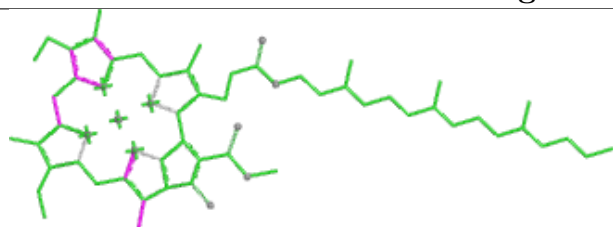


Torsions

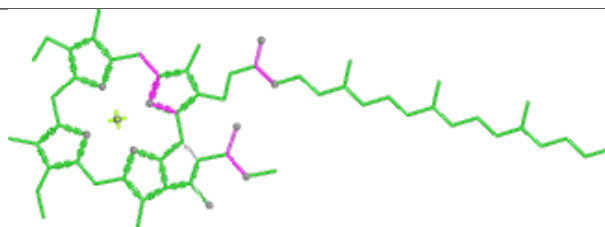


Rings

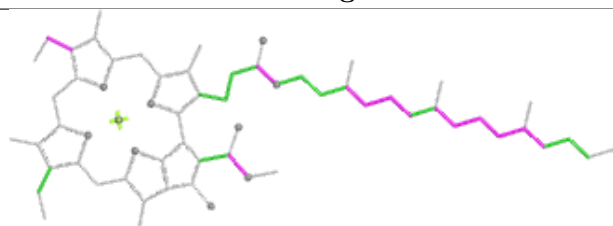
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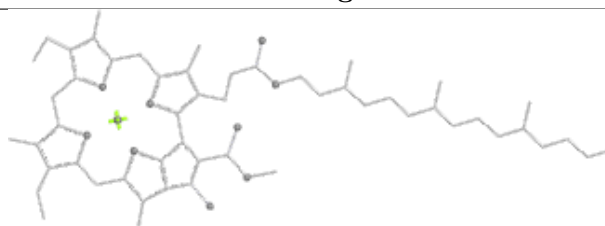
Bond lengths



Bond angles

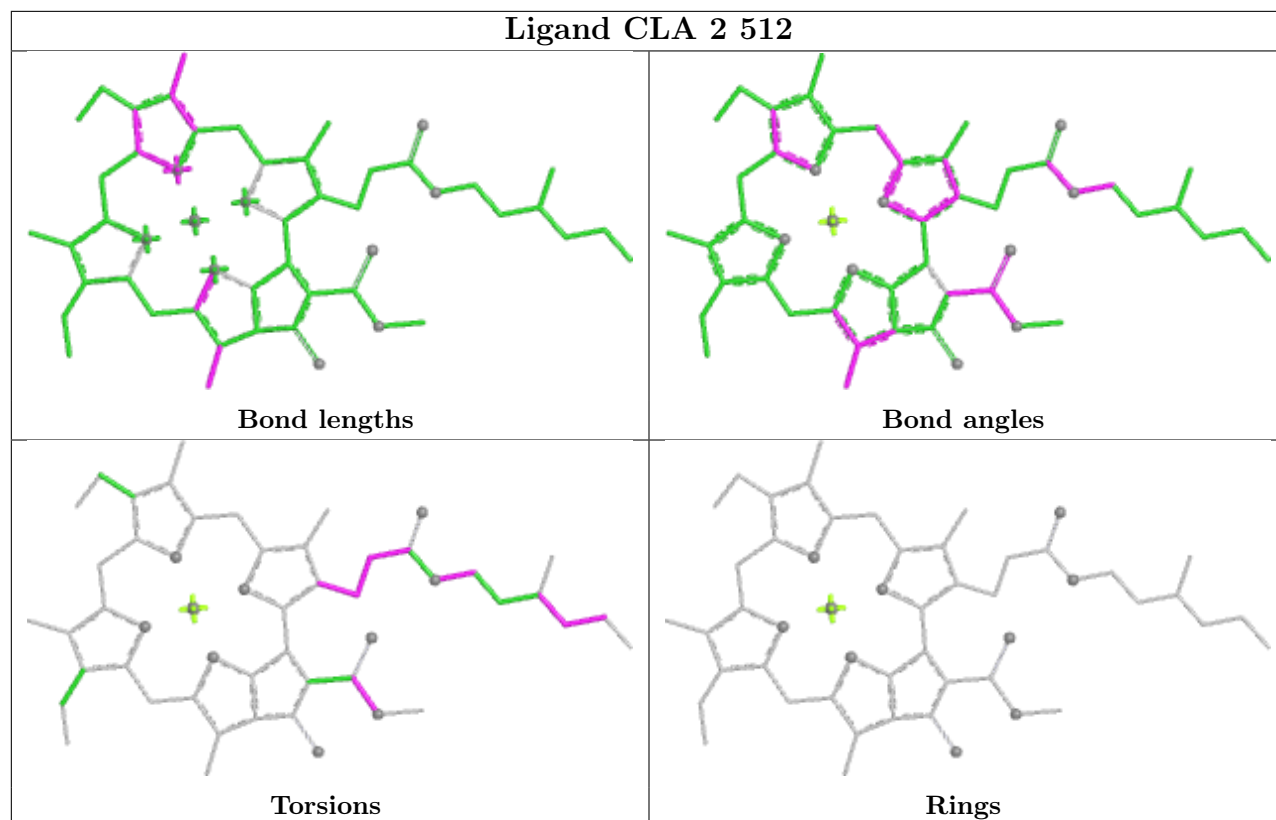


Torsions

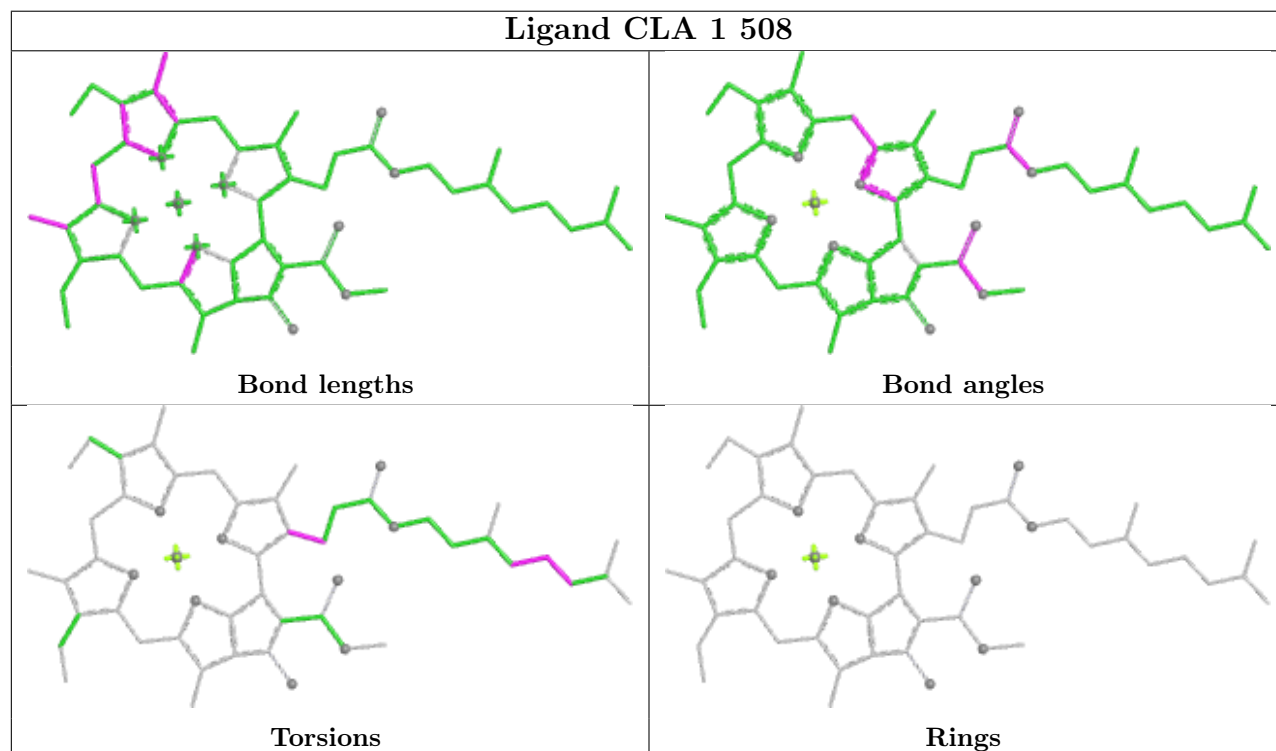


Rings

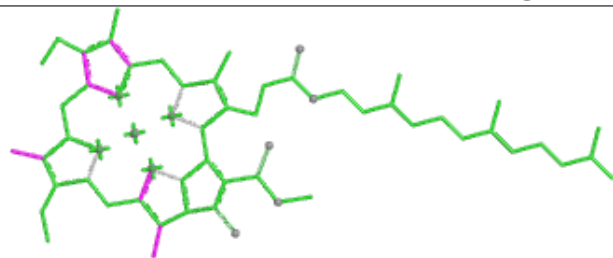
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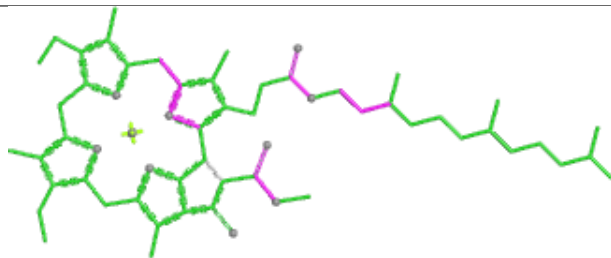
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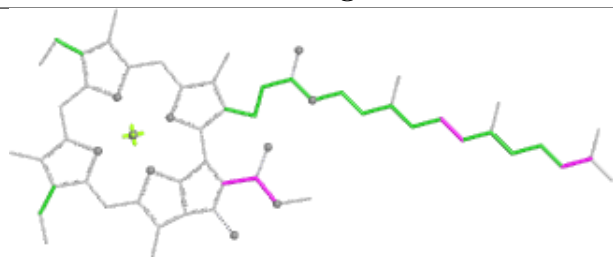
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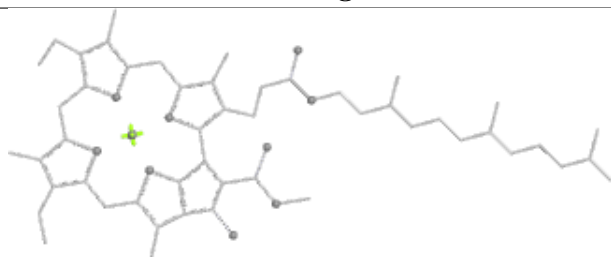
Bond lengths



Bond angles

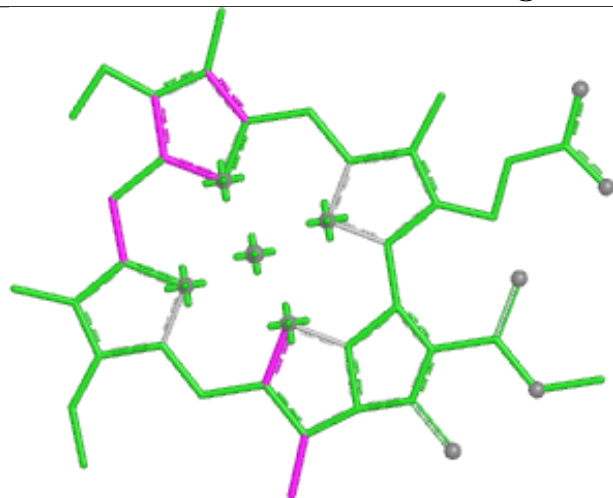


Torsions

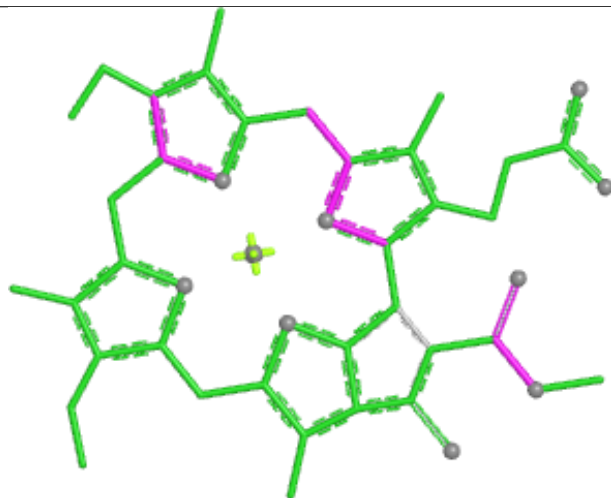


Rings

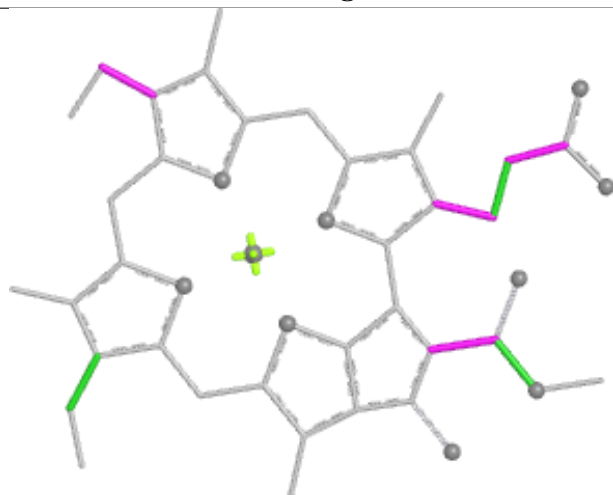
Ligand CLA b 516



Bond lengths



Bond angles

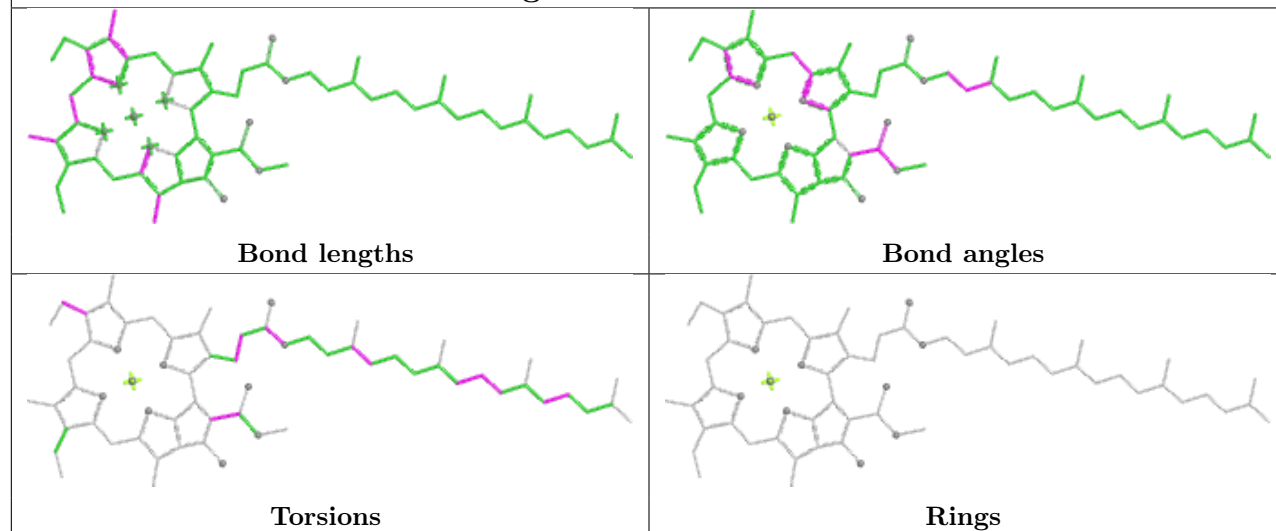


Torsions

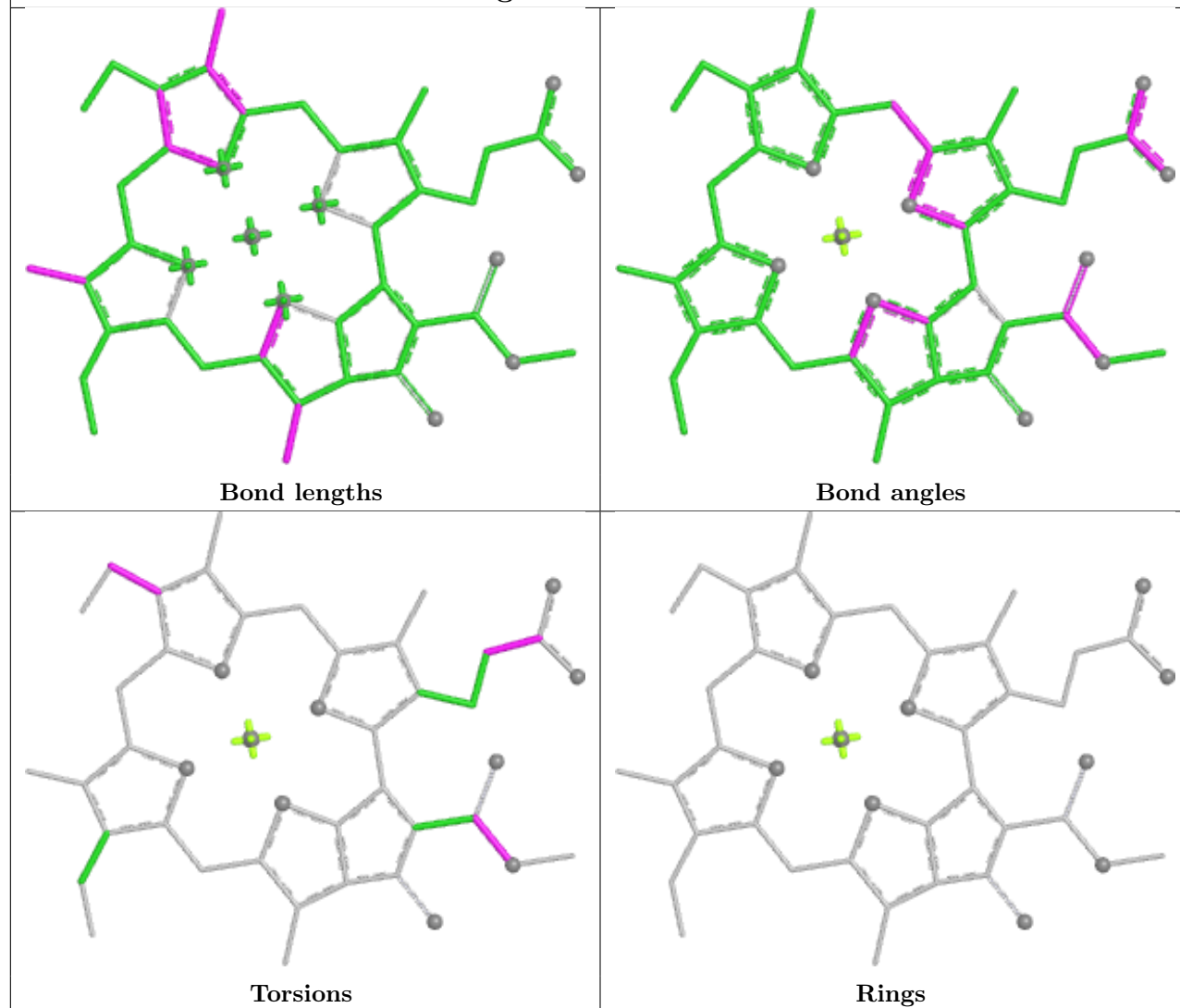


Rings

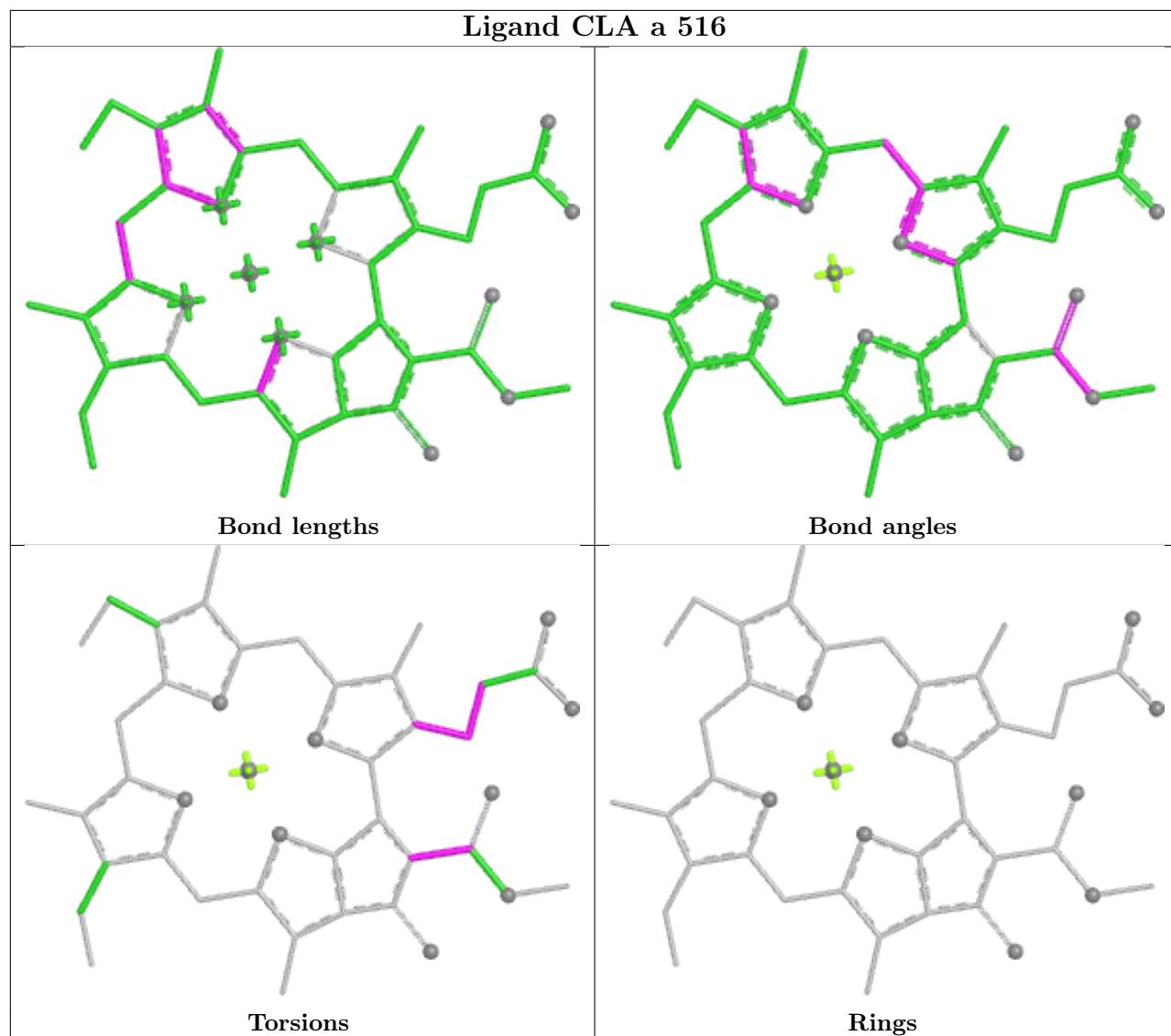
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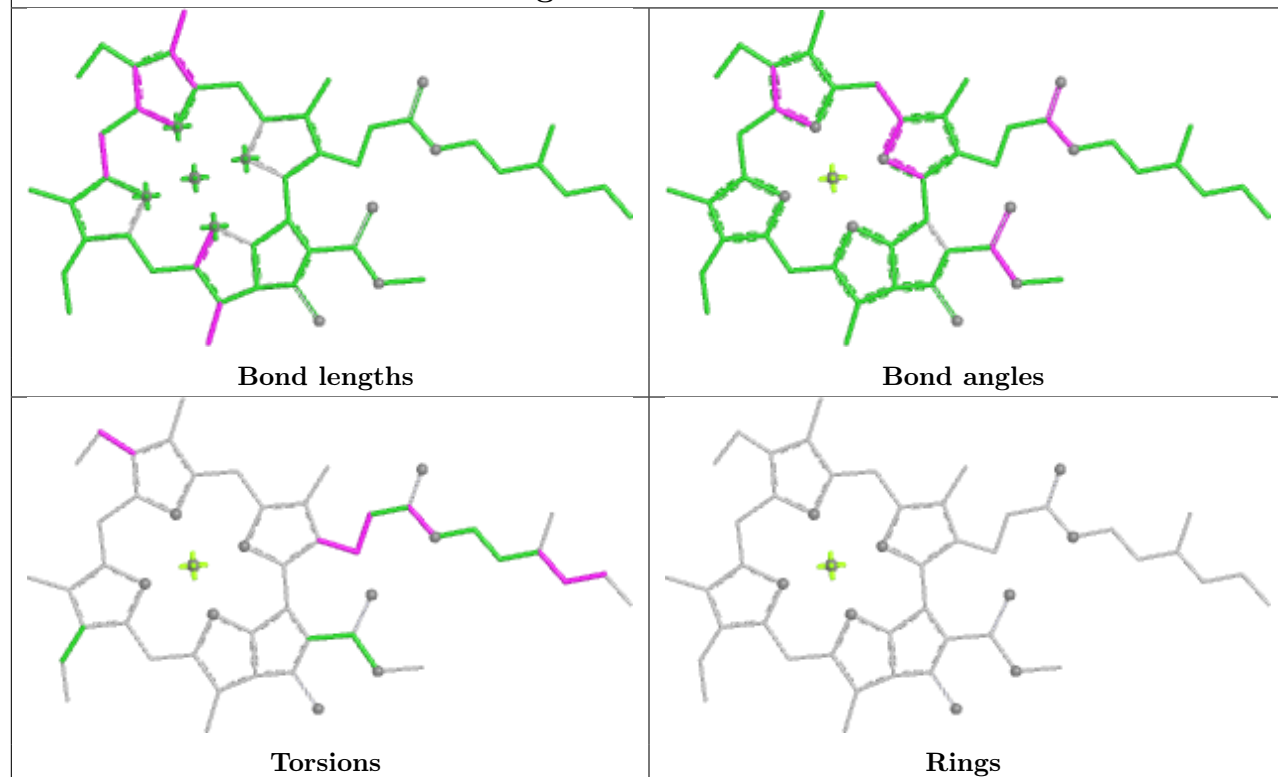
Ligand CLA c 517



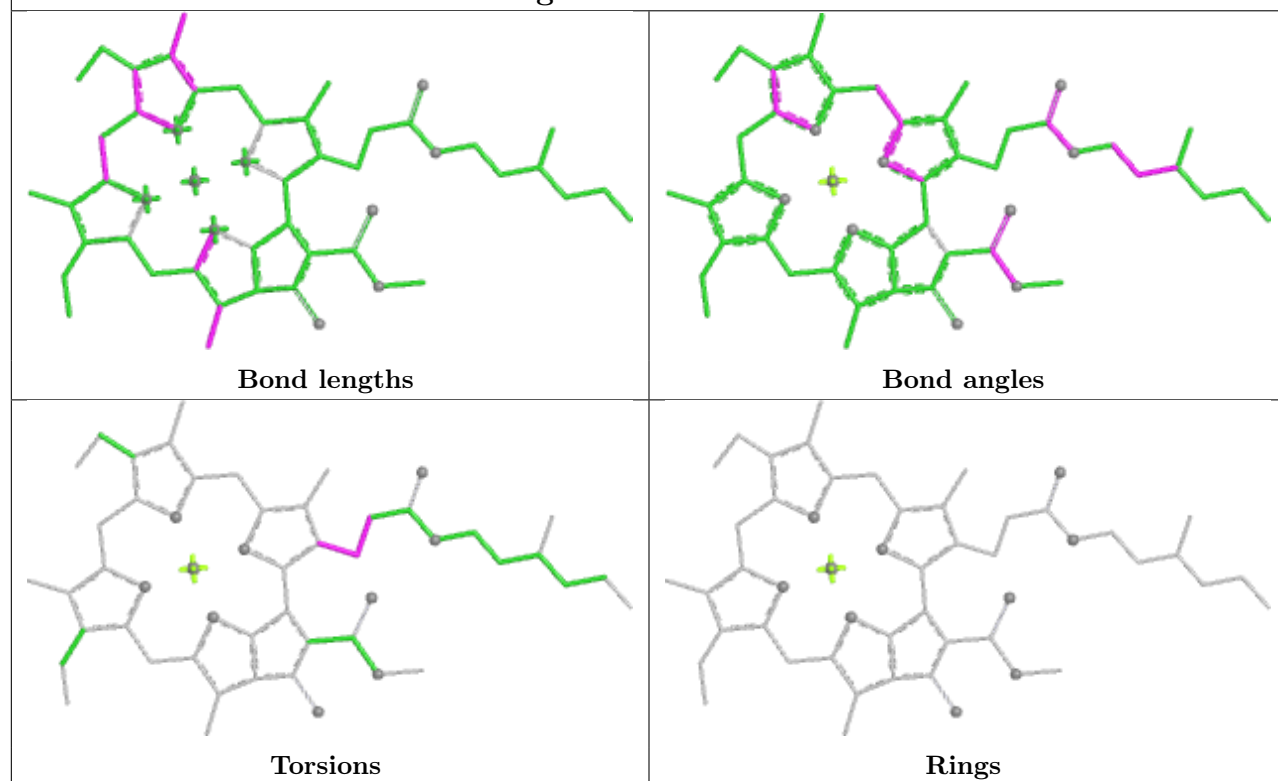
Ligand CLA a 516

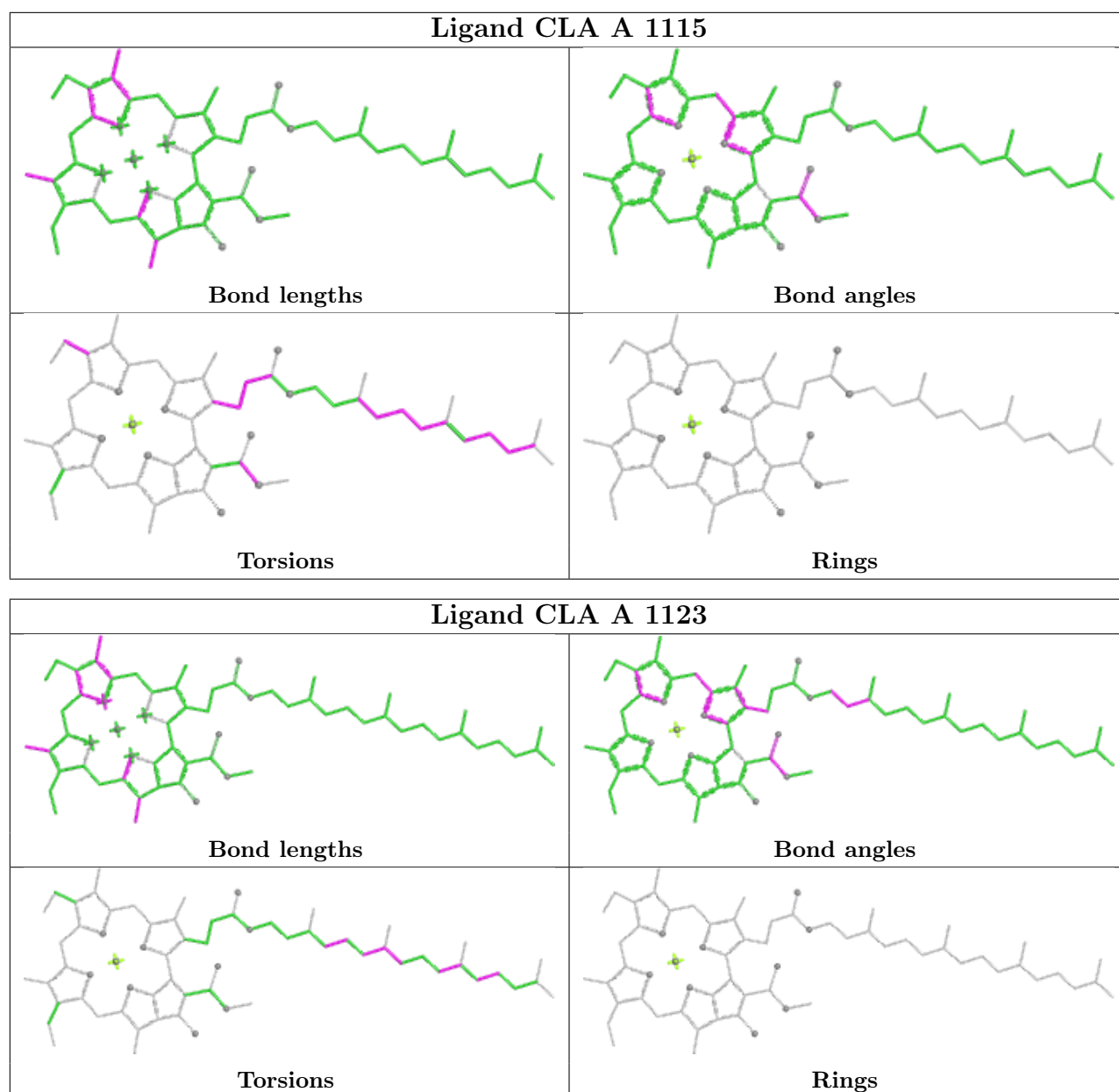


Ligand CLA a 512

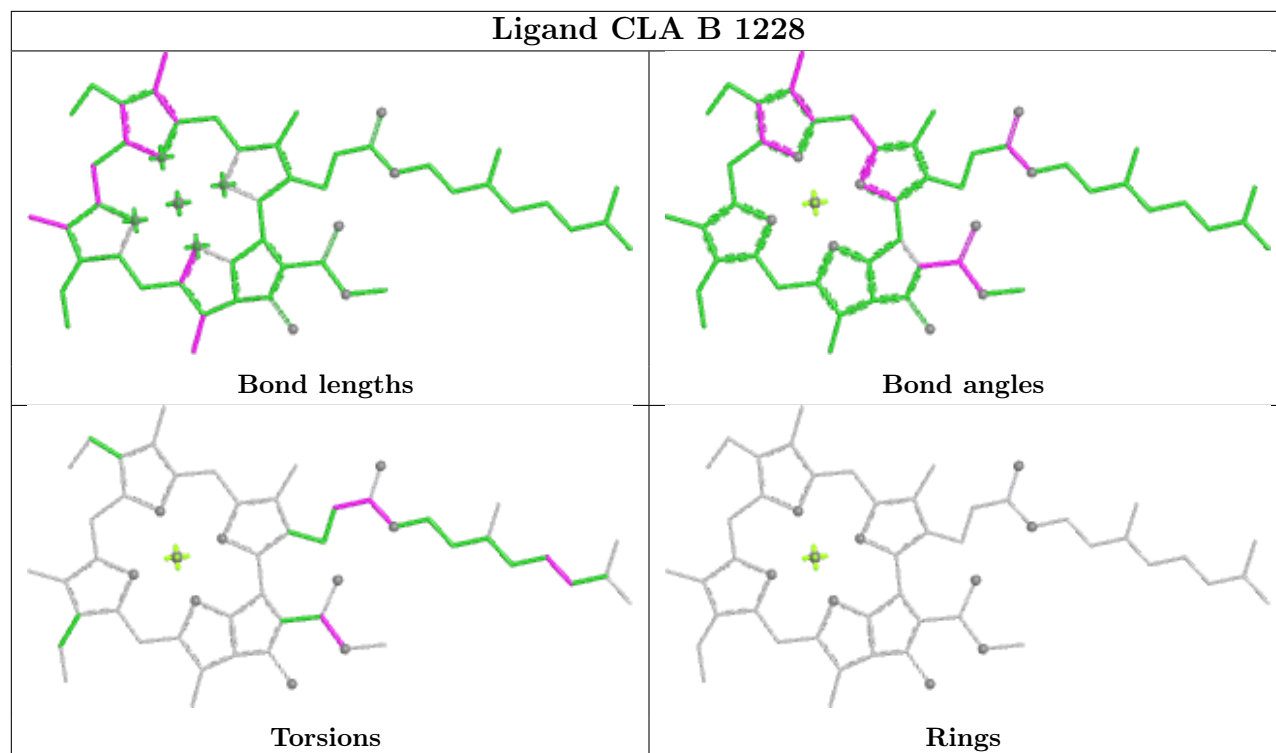


Ligand CLA 5 512

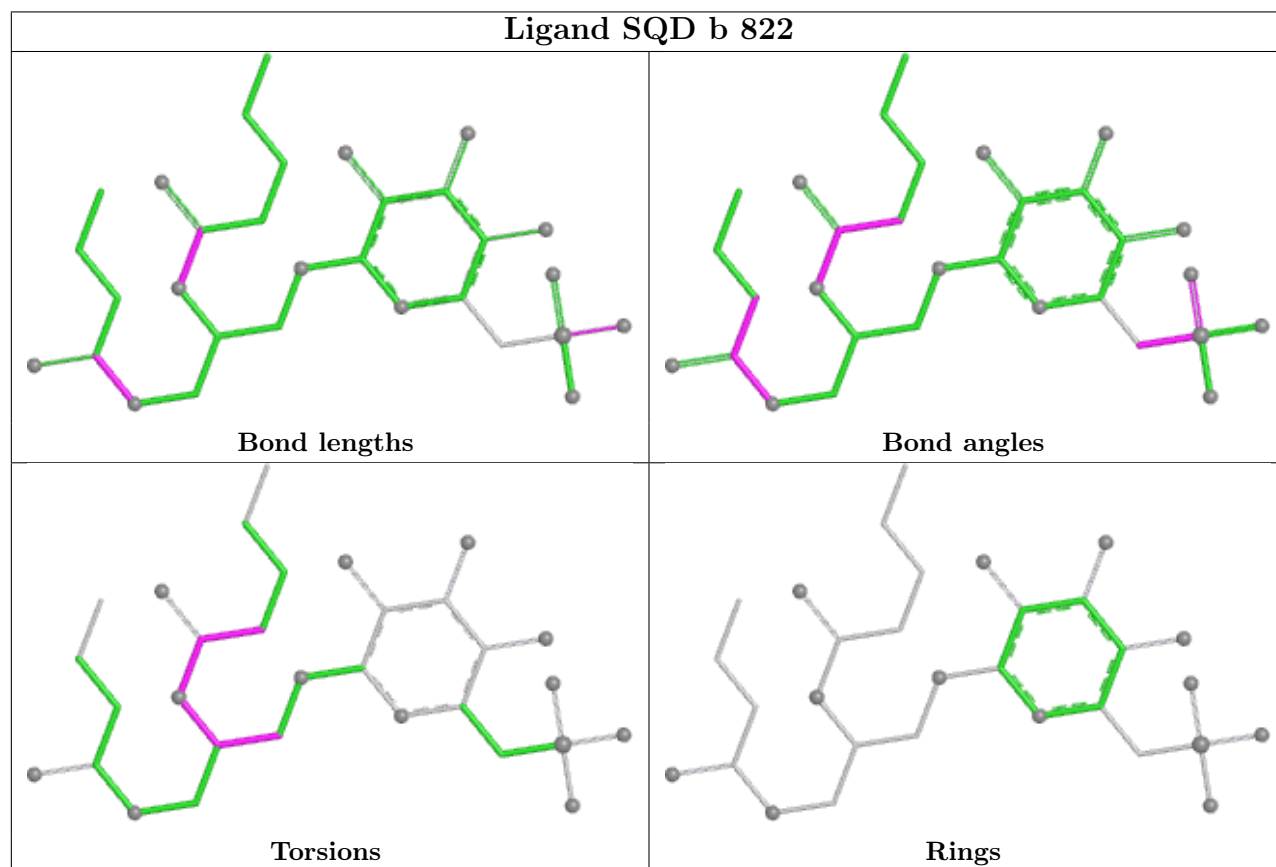




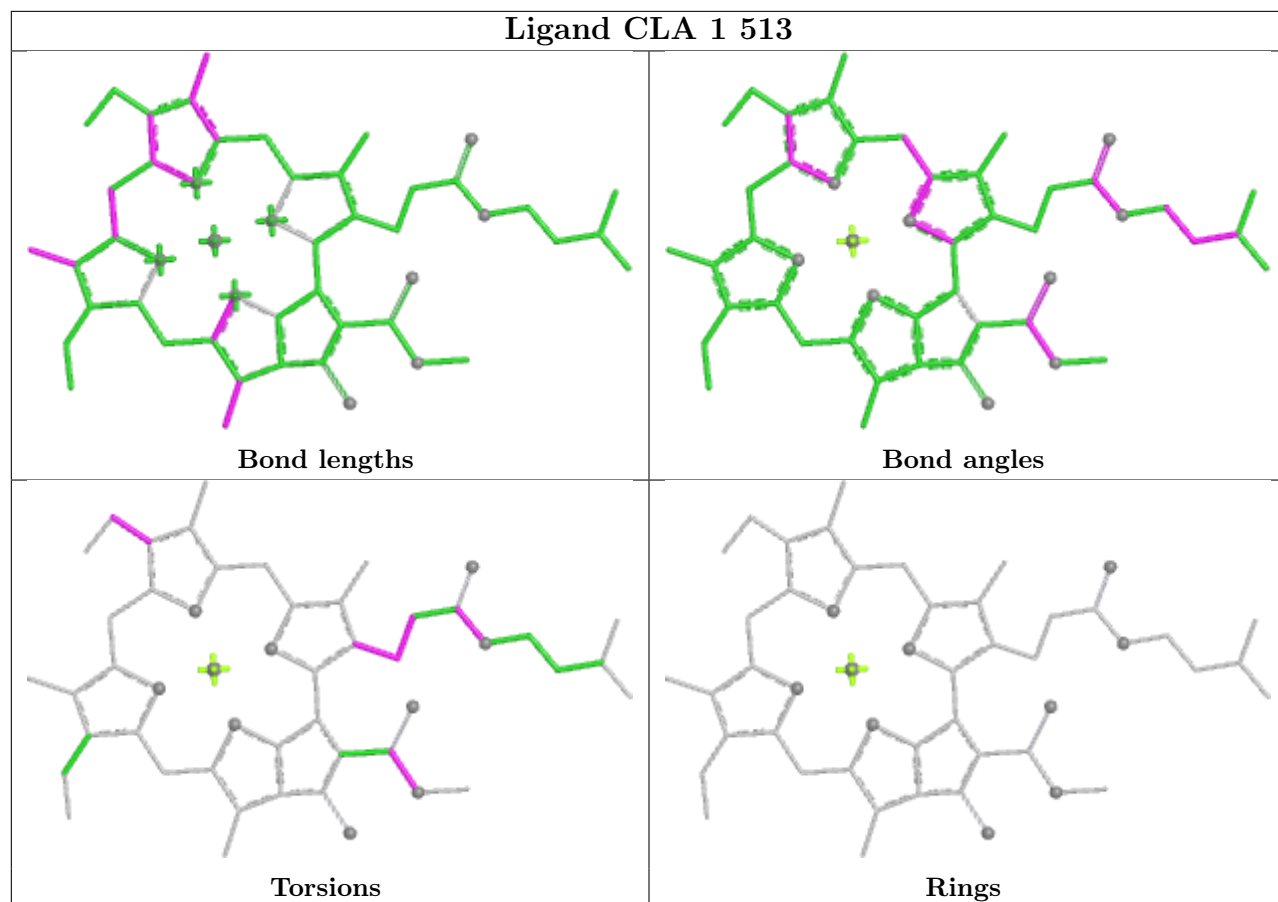
Ligand CLA B 1228



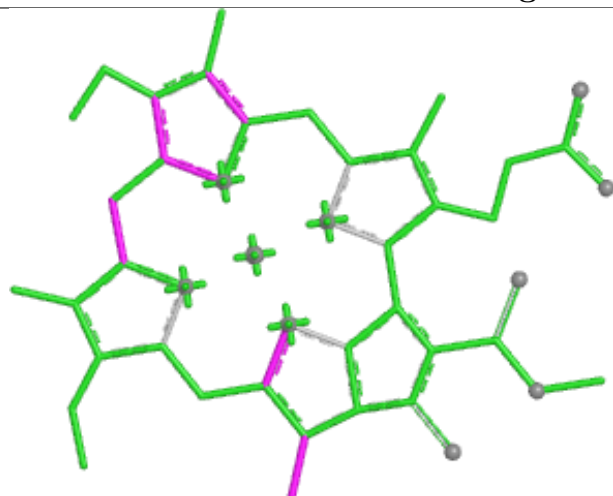
Ligand SQD b 822



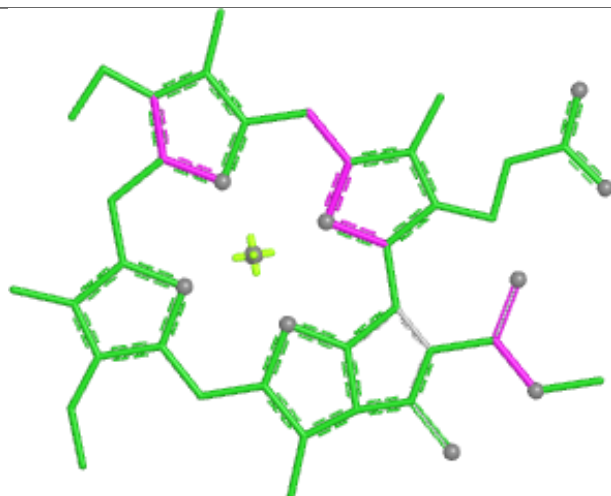
Ligand CLA 1 513



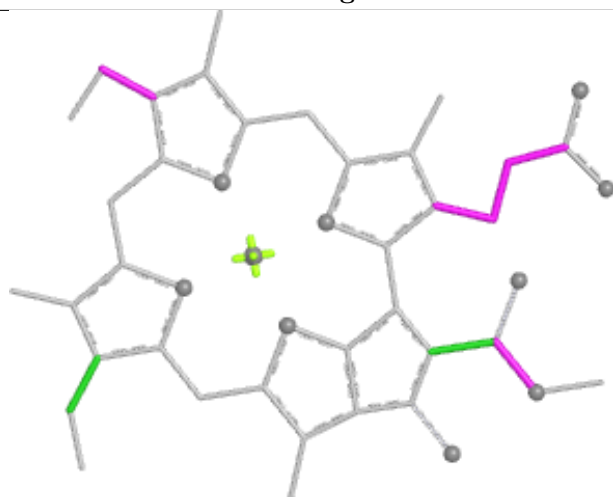
Ligand CLA e 516



Bond lengths



Bond angles

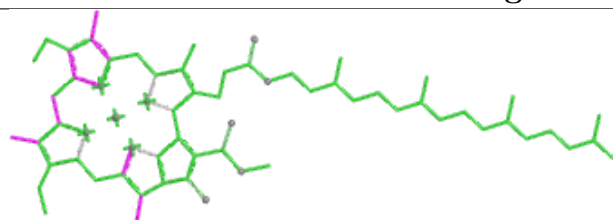


Torsions

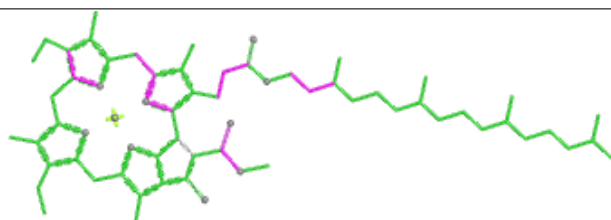


Rings

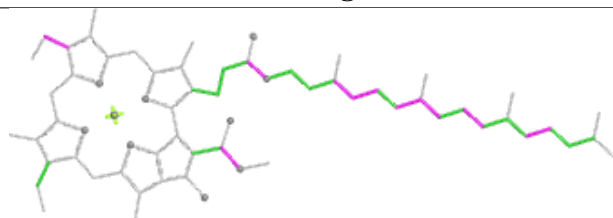
Ligand CLA A 1125



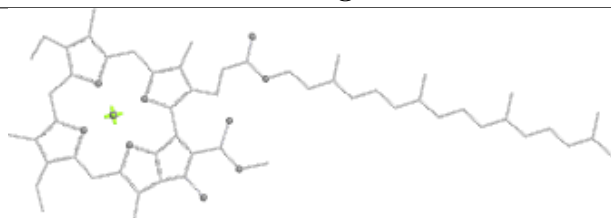
Bond lengths



Bond angles

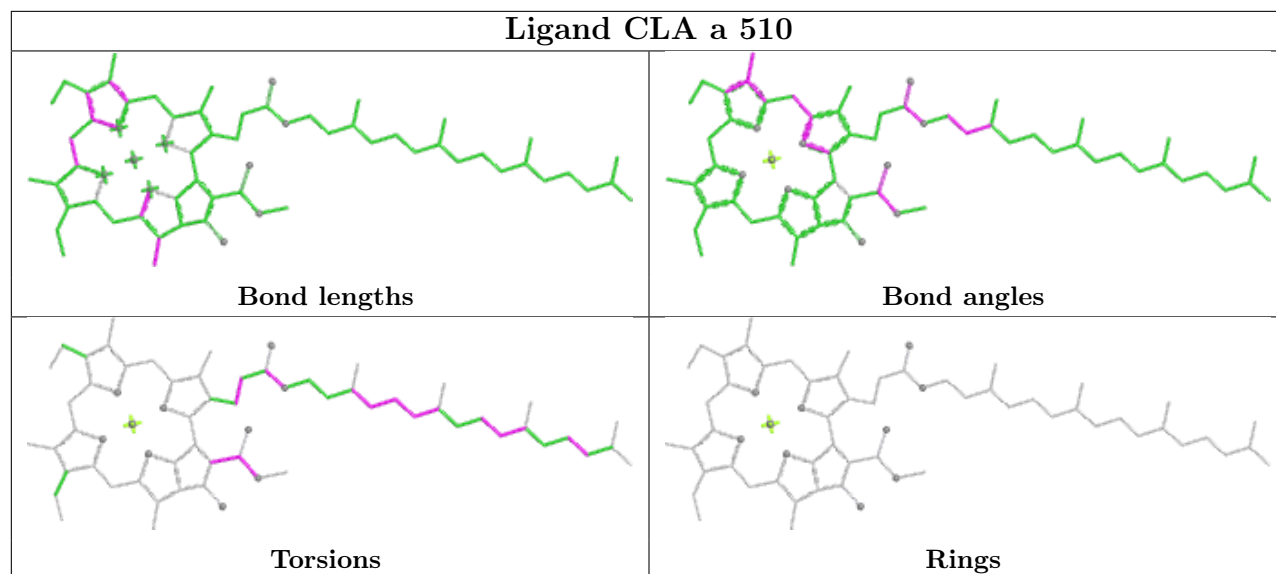


Torsions

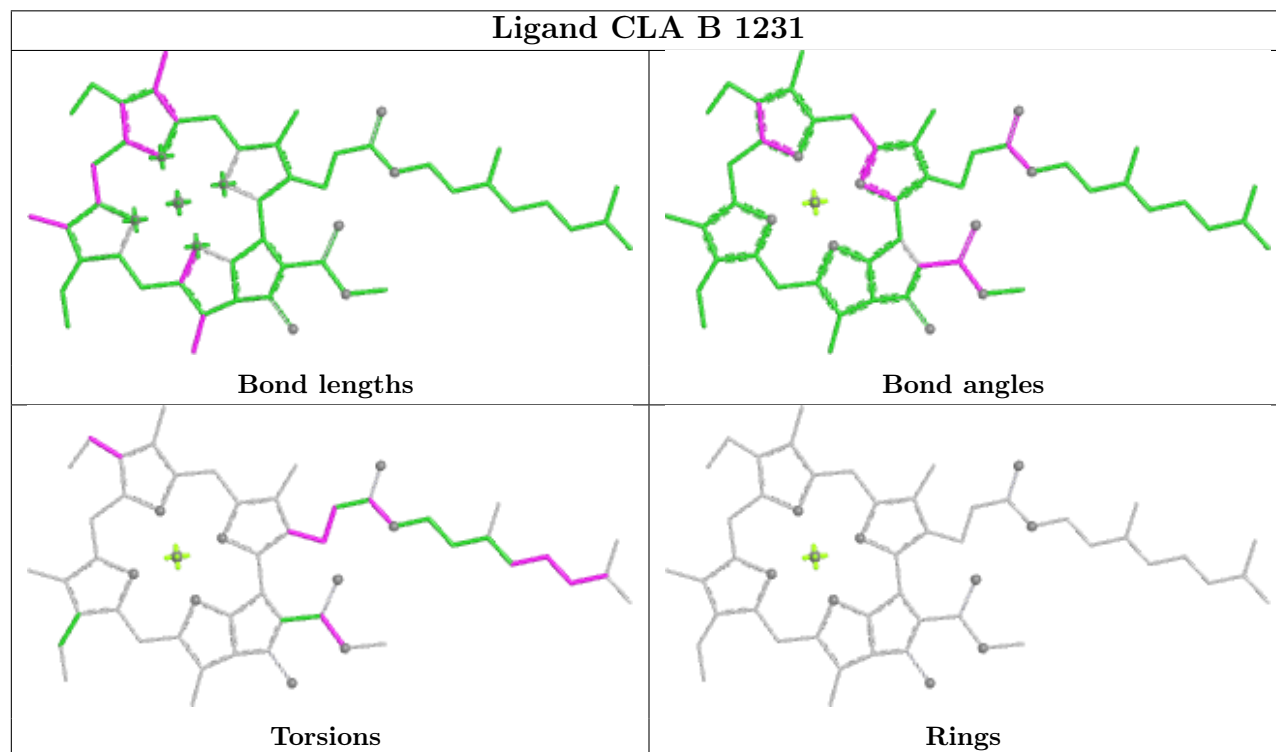


Rings

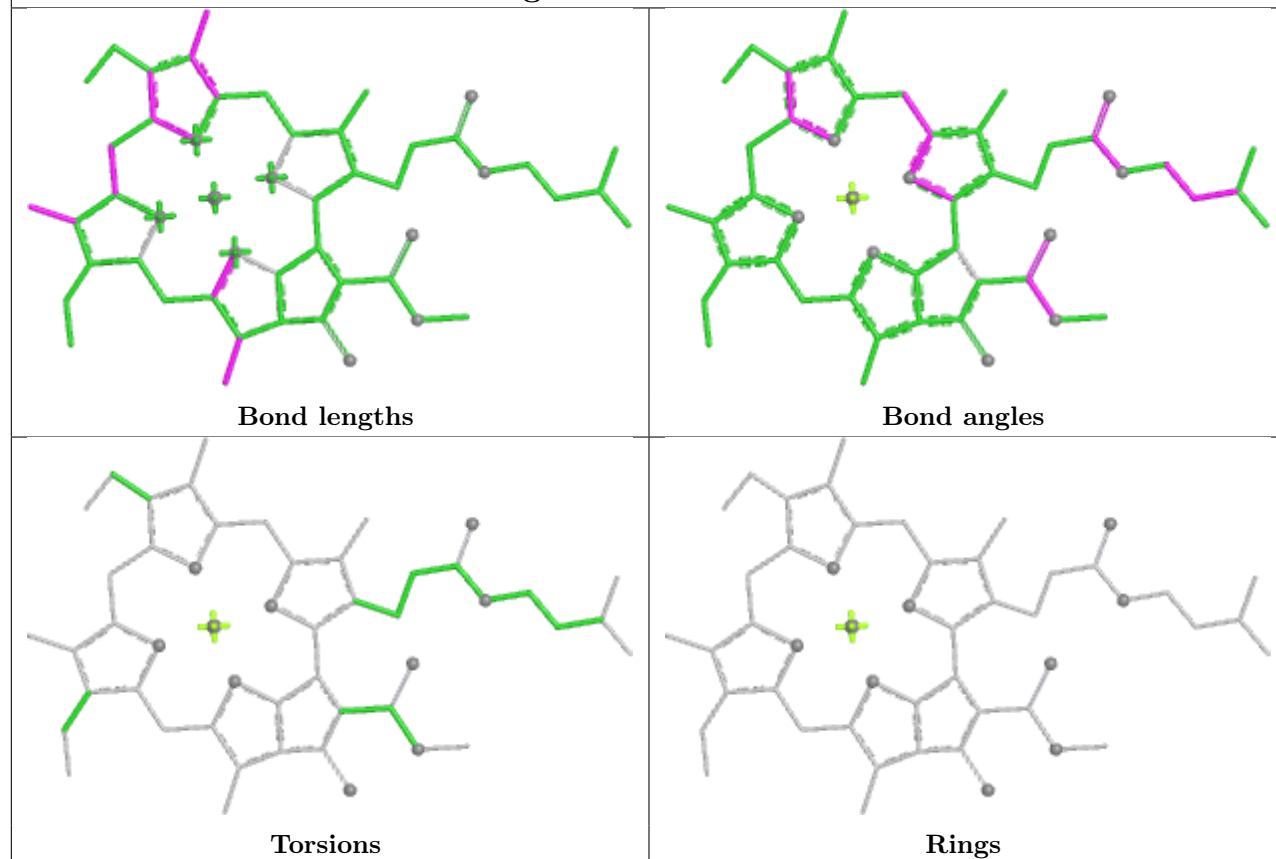
Ligand CLA a 510



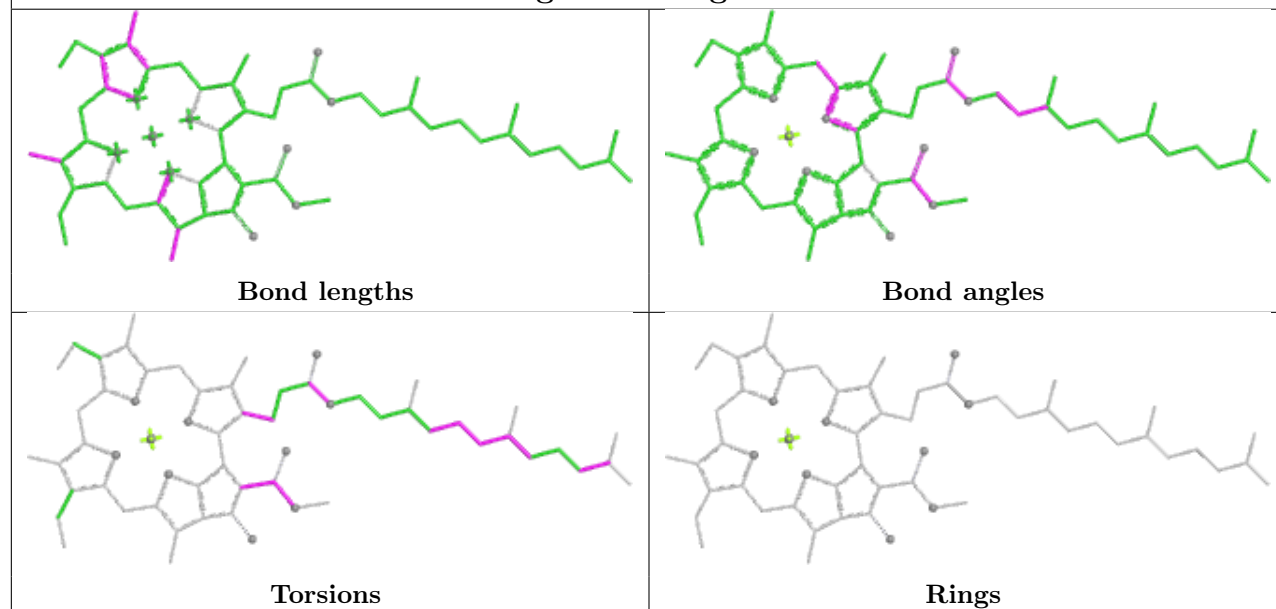
Ligand CLA B 1231



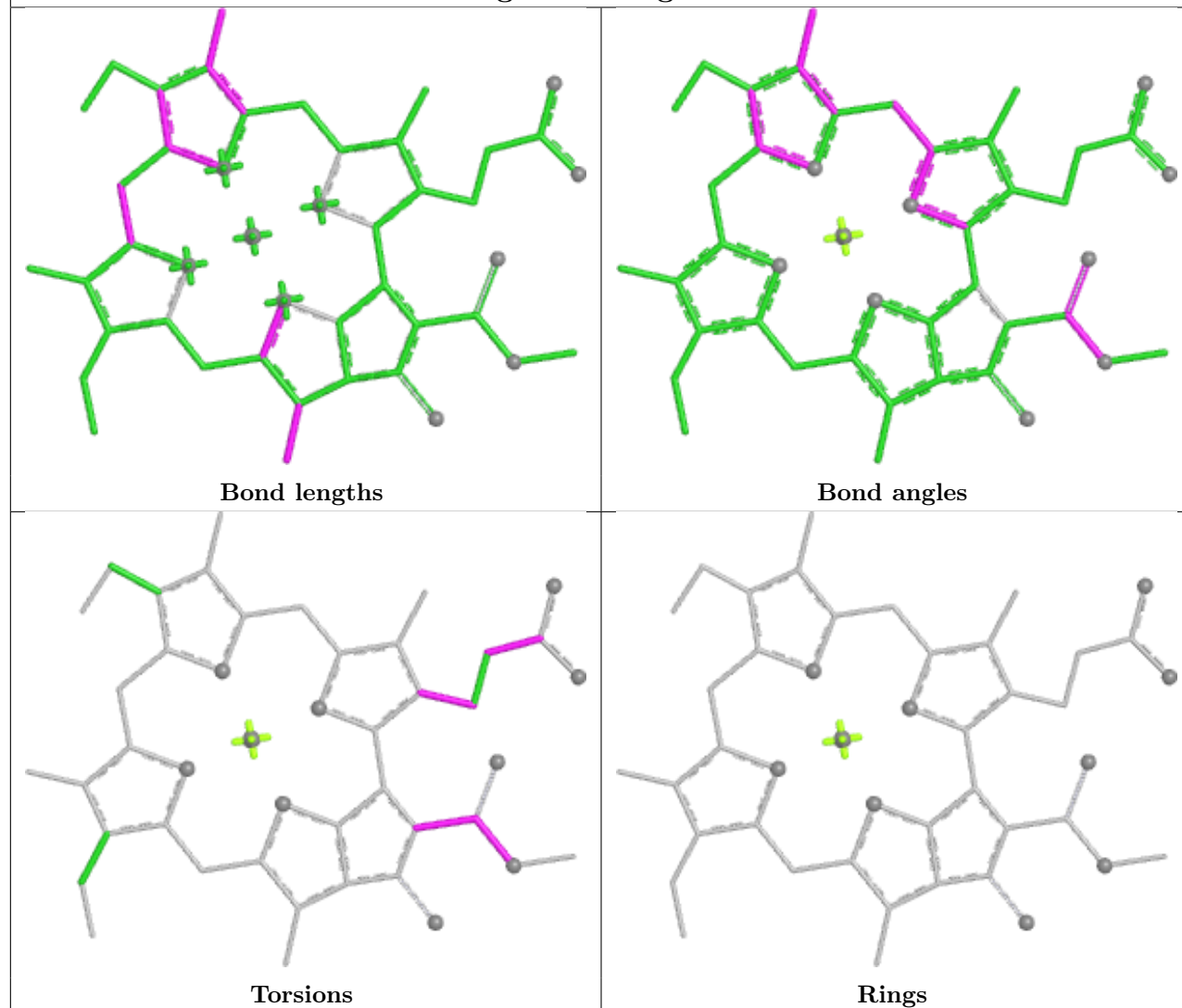
Ligand CLA B 1220



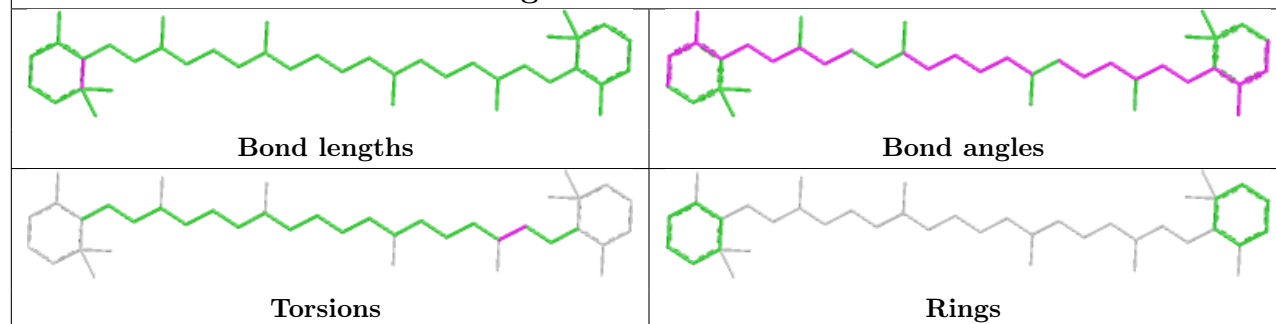
Ligand CLA g 502



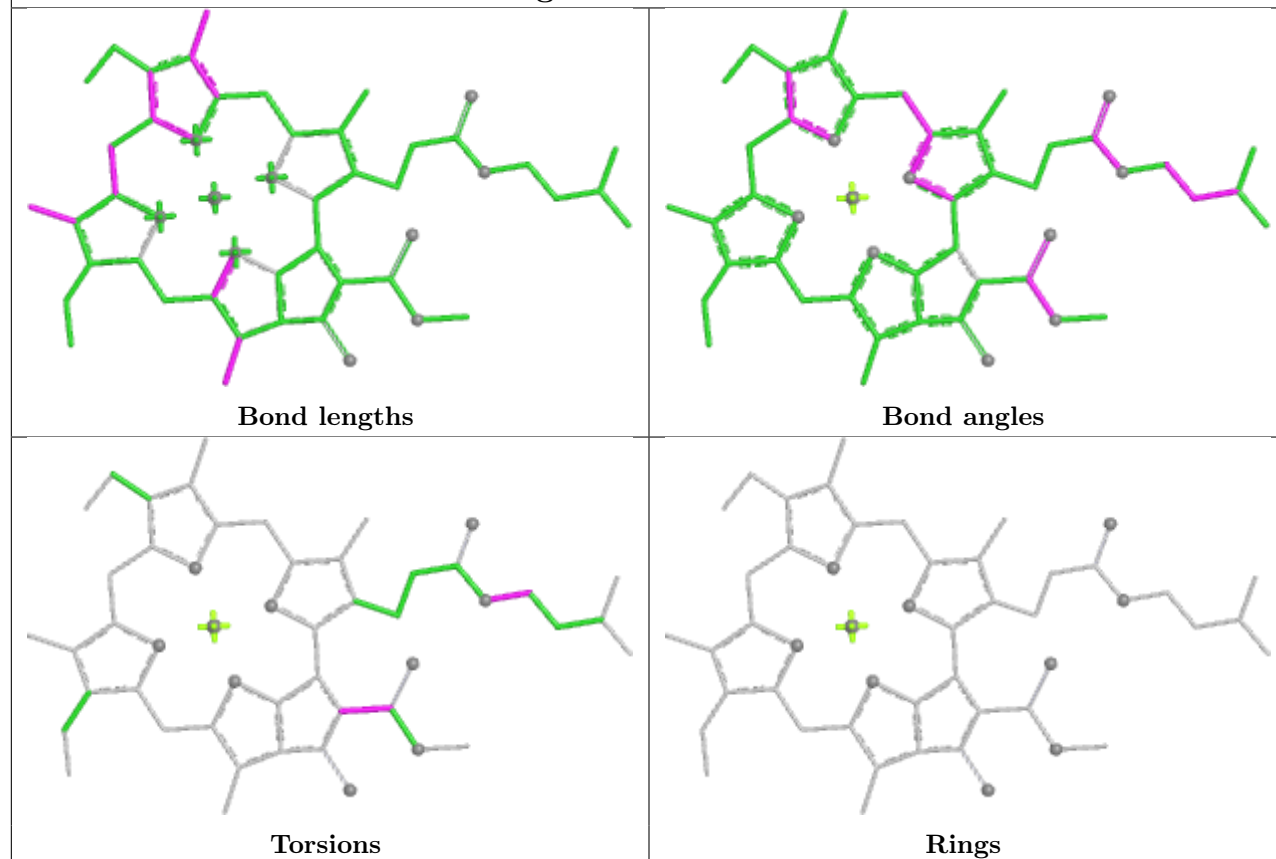
Ligand CLA g 506



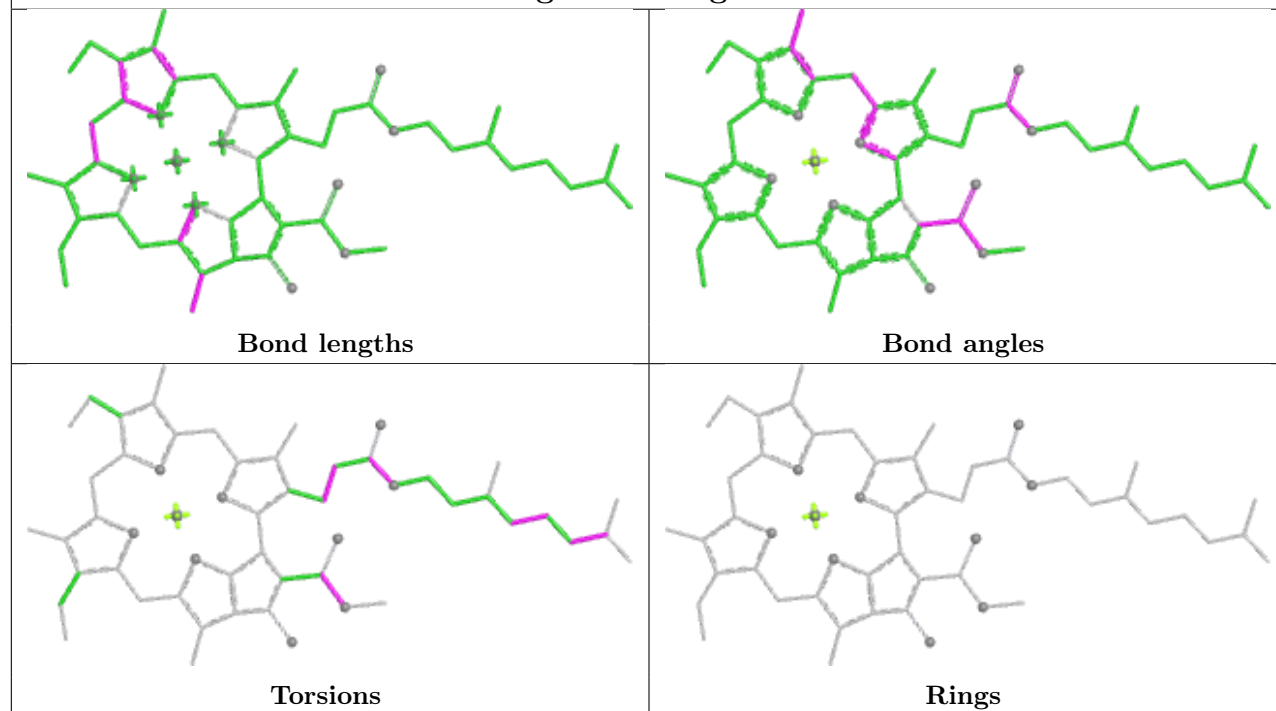
Ligand BCR A 4007



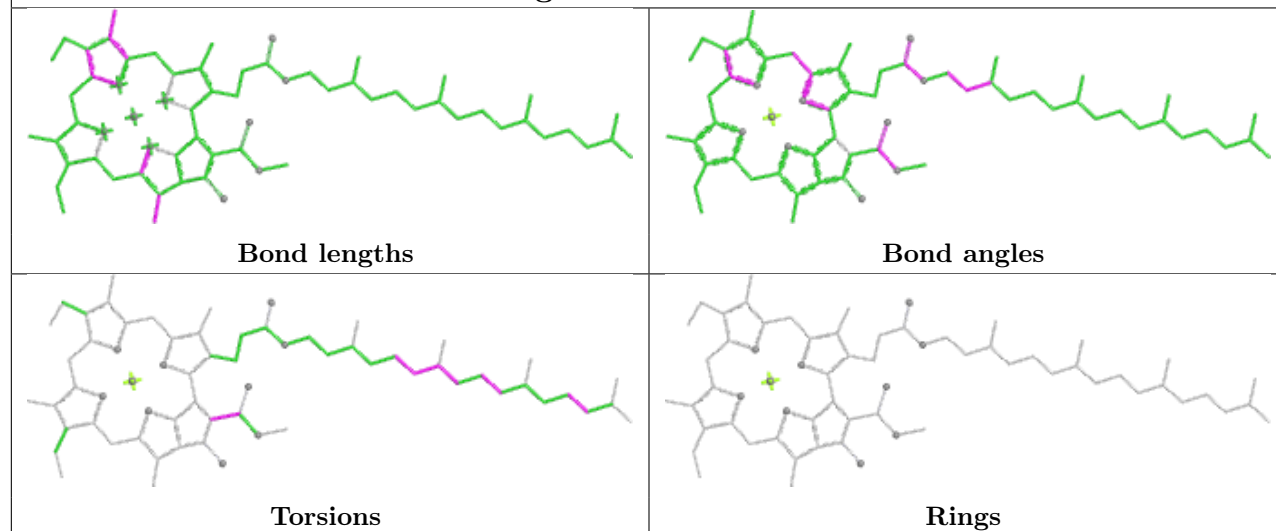
Ligand CLA 4 513



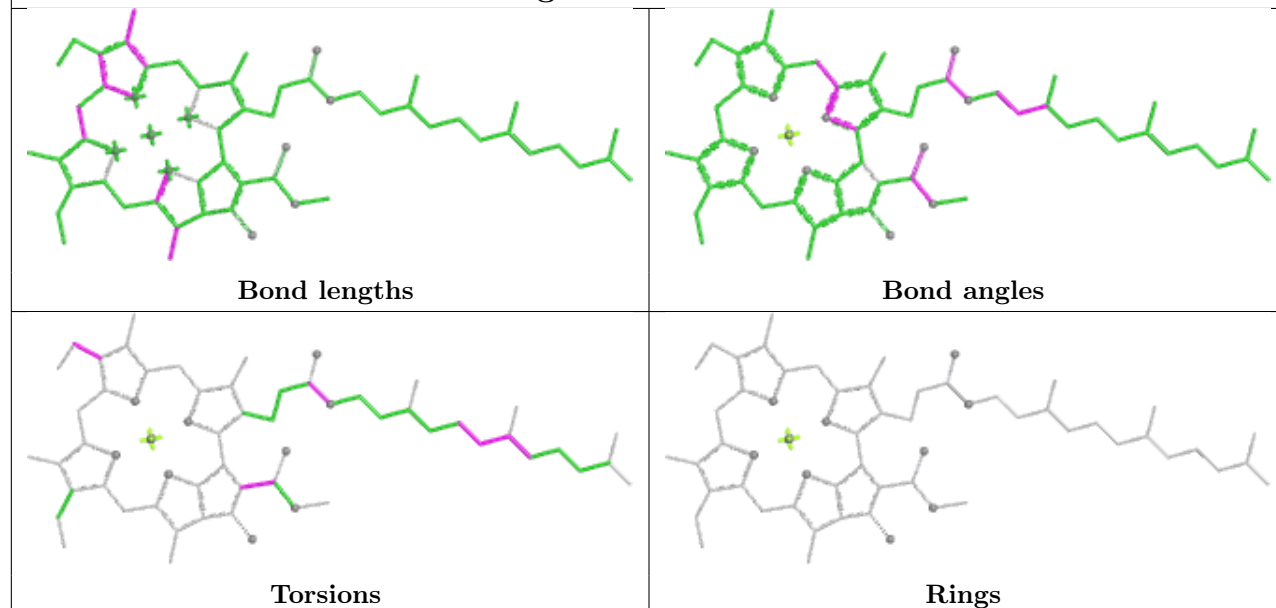
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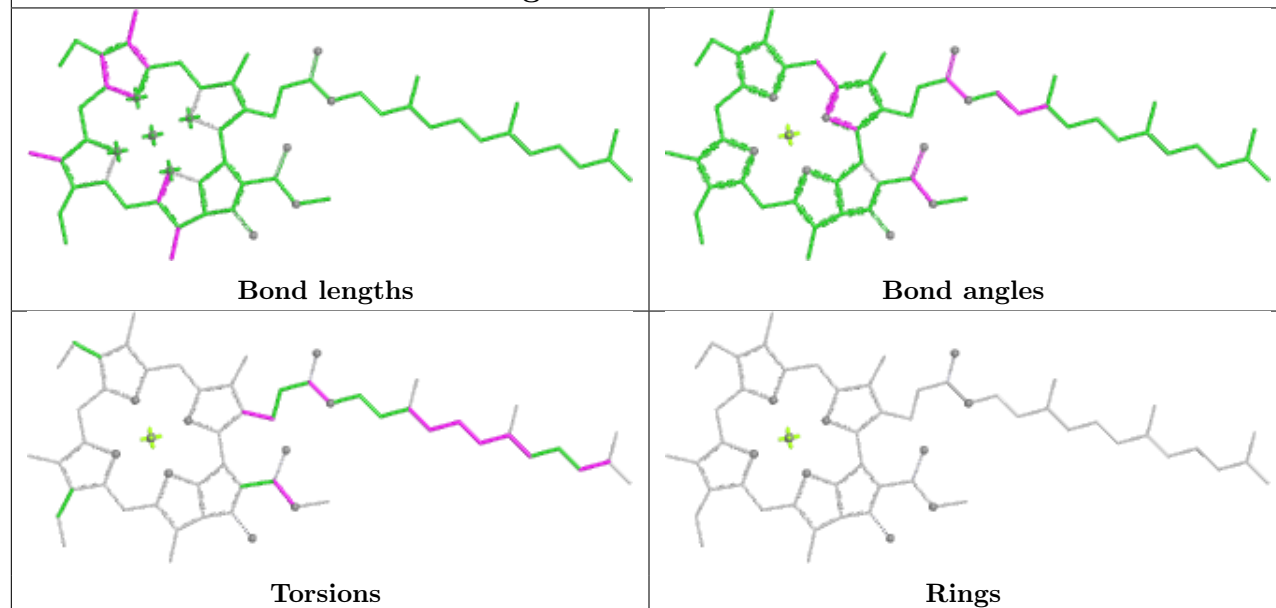
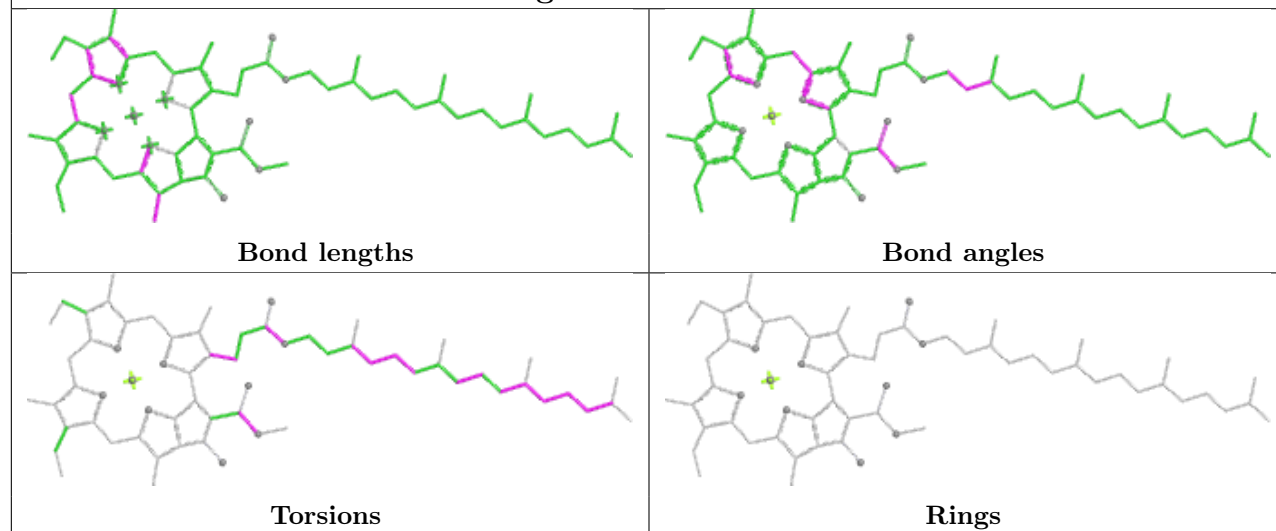


Ligand CLA d 509

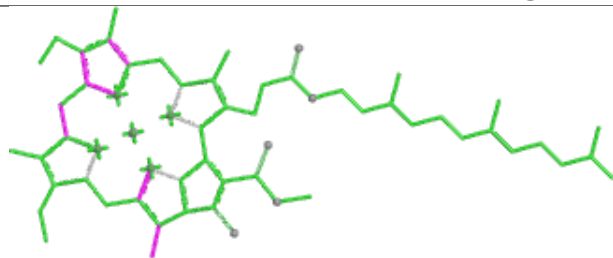


Ligand CLA c 507

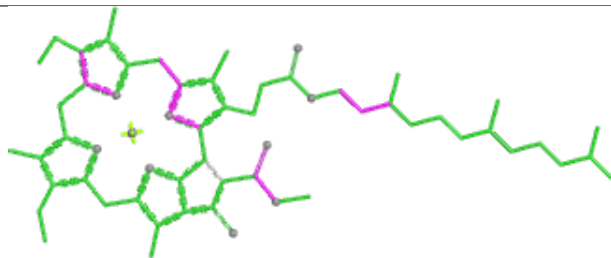


Ligand CLA A 1118**Ligand CLA 2 505**

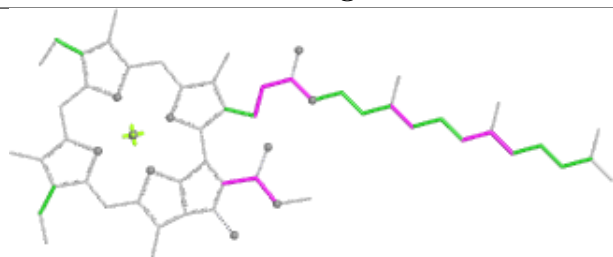
Ligand CLA f 507



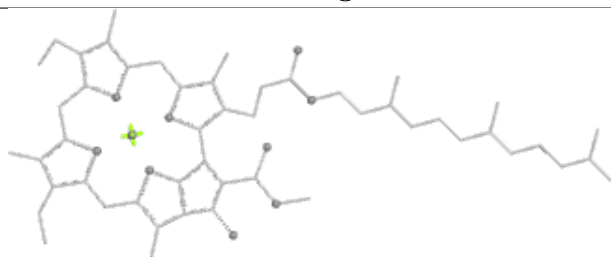
Bond lengths



Bond angles

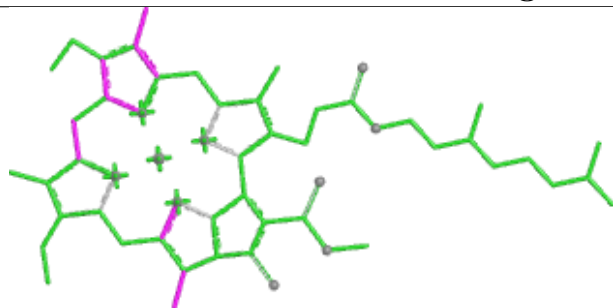


Torsions

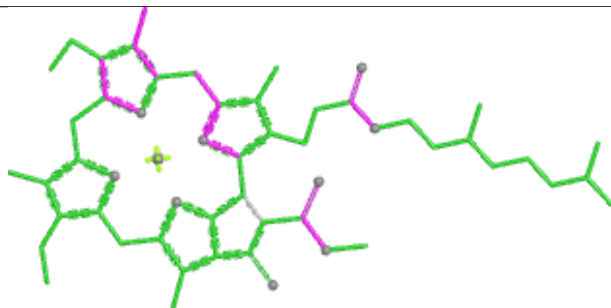


Rings

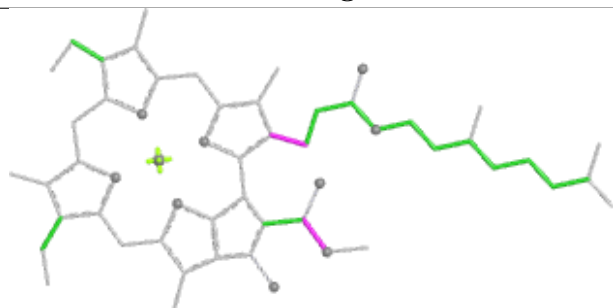
Ligand CLA 2 511



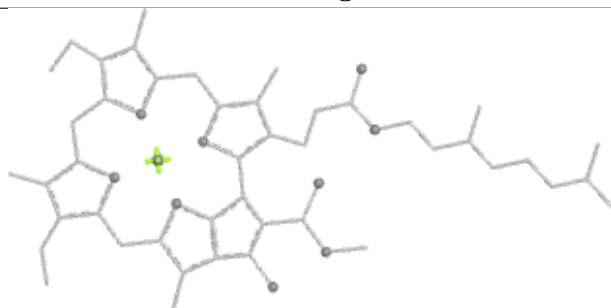
Bond lengths



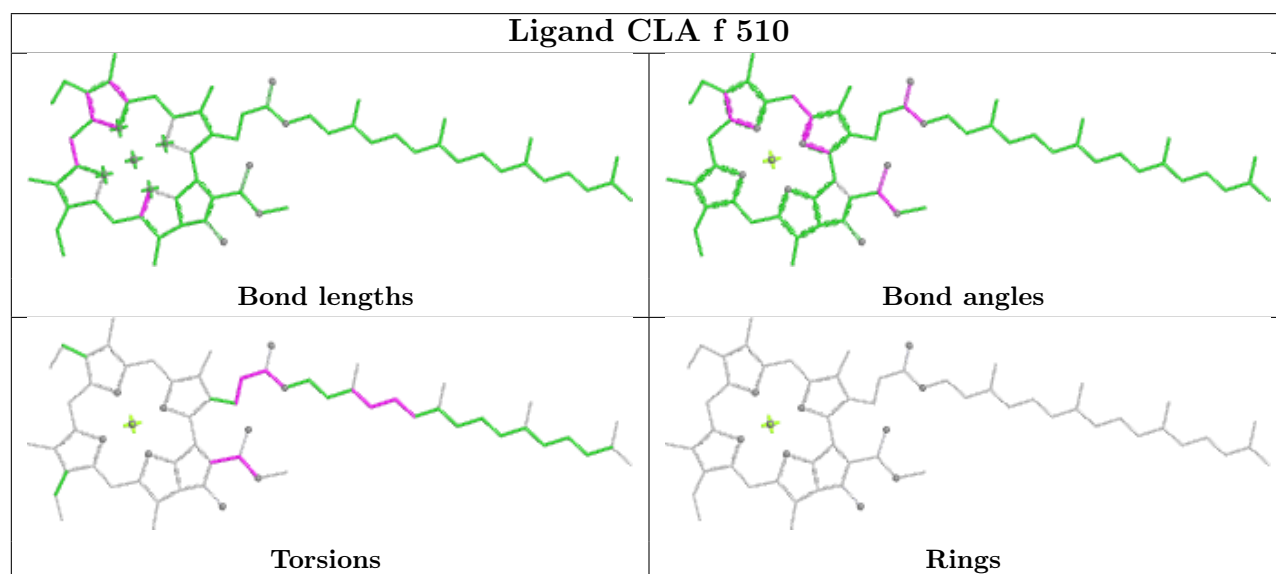
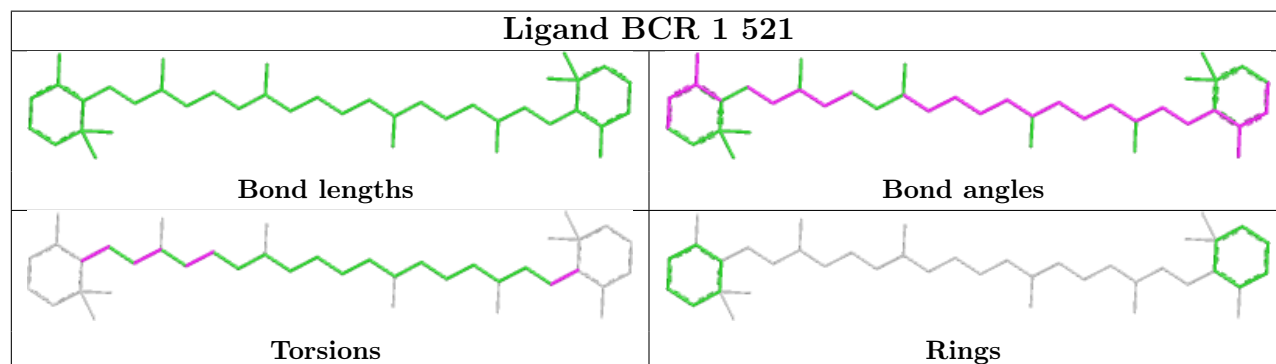
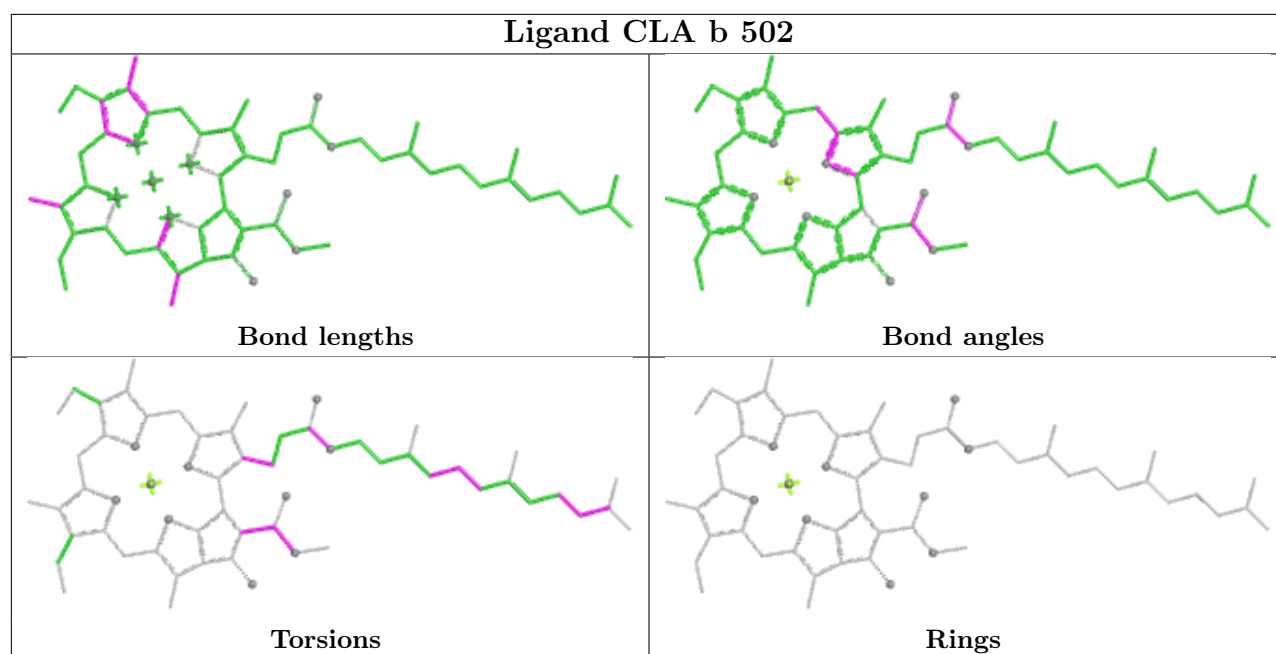
Bond angles

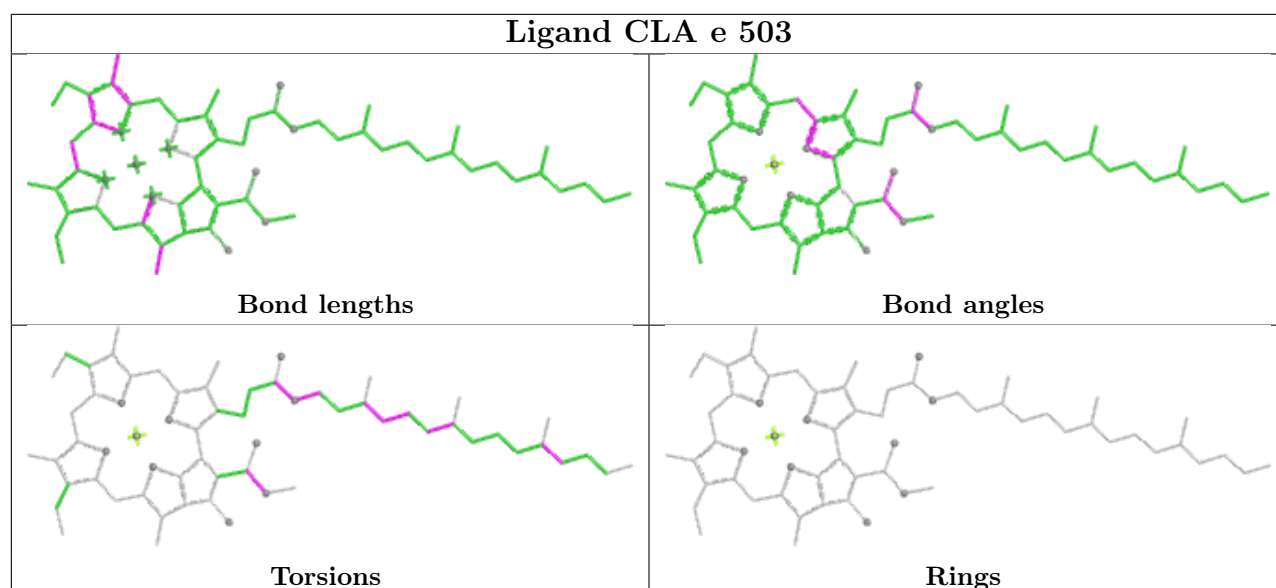
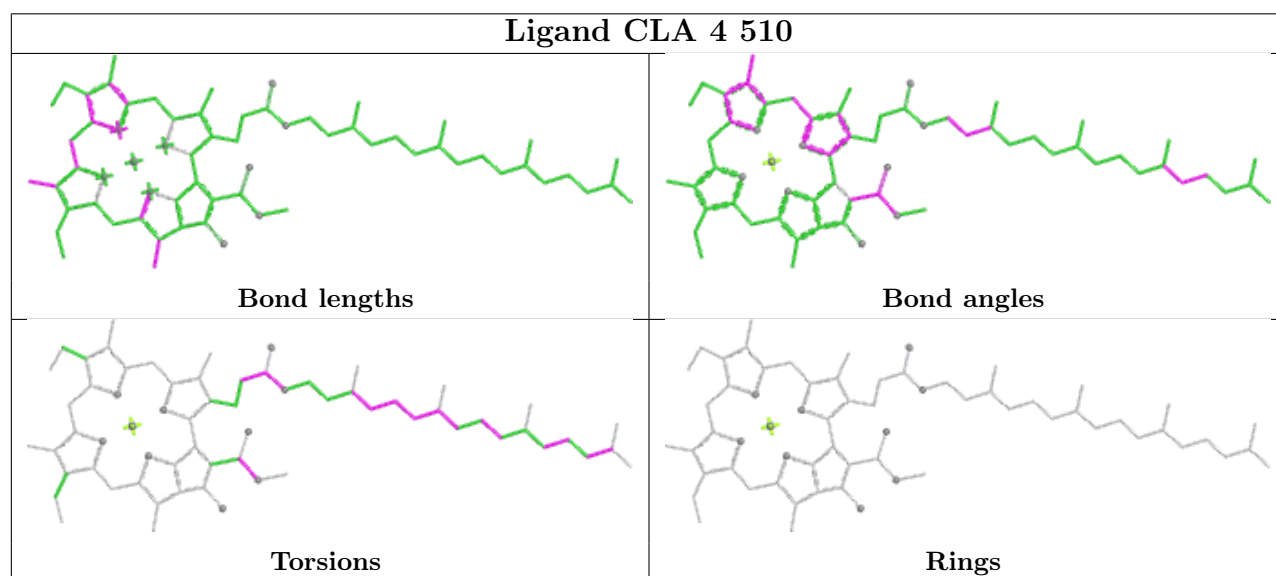
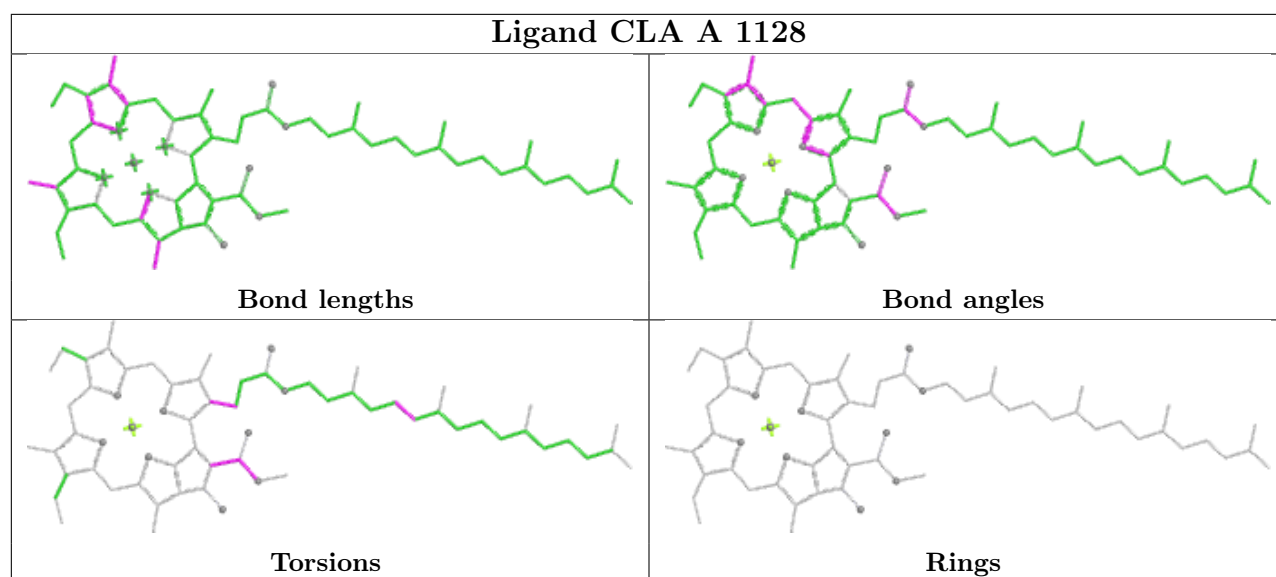


Torsions

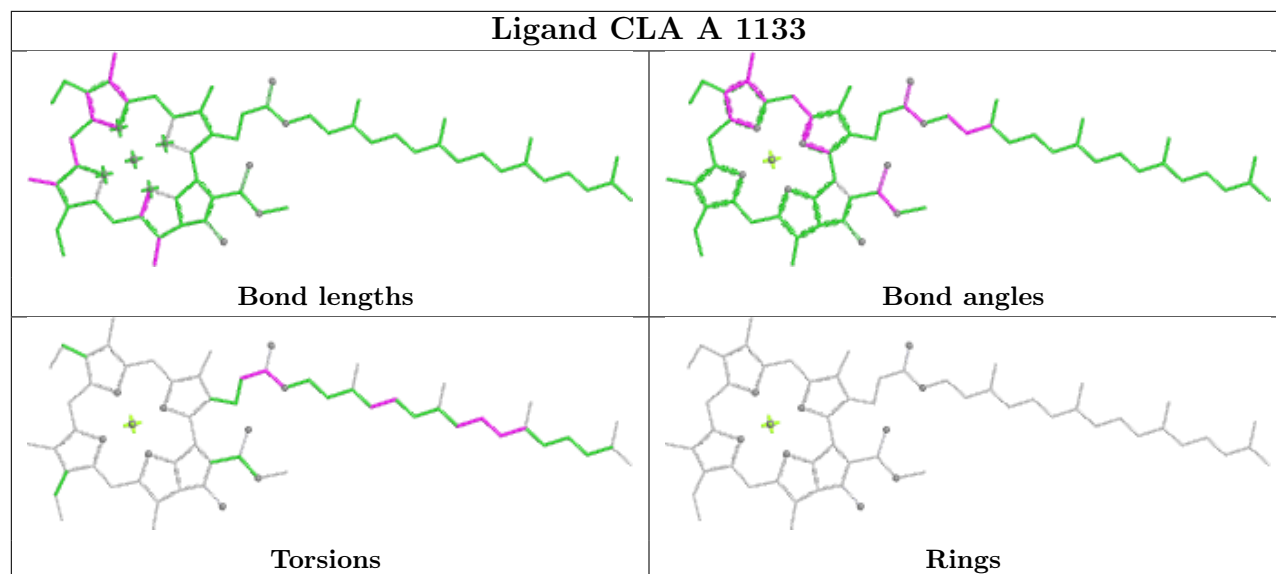


Rings

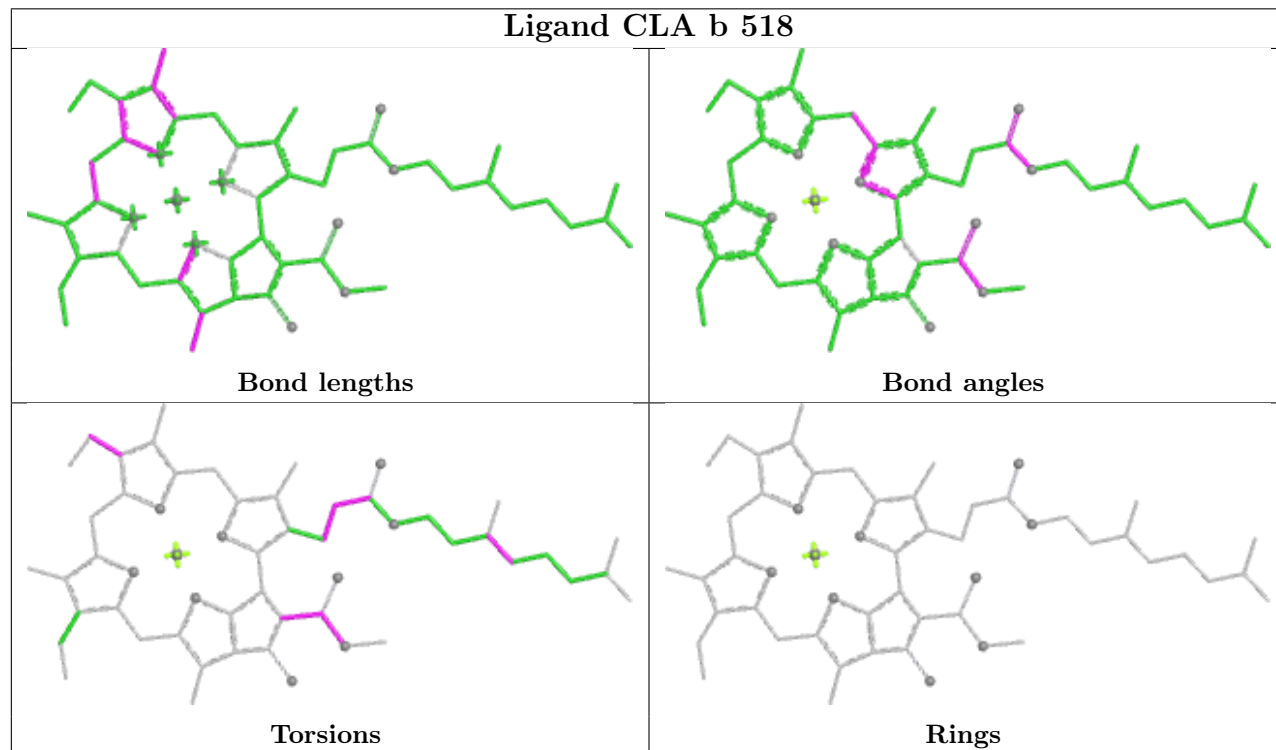




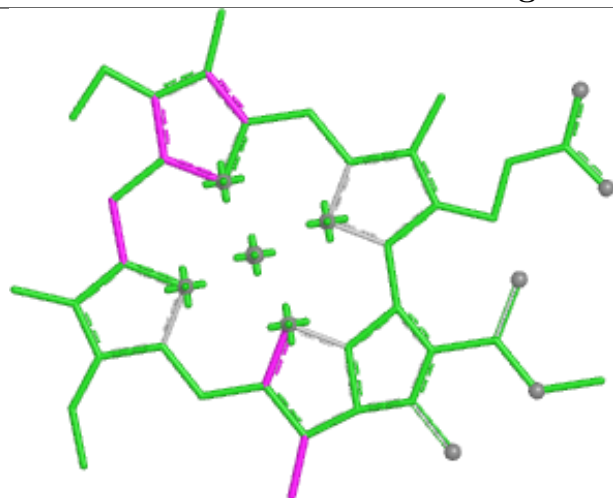
Ligand CLA A 1133



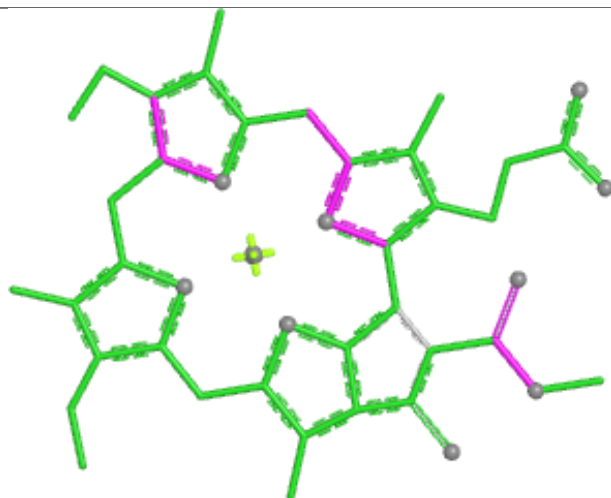
Ligand CLA b 518



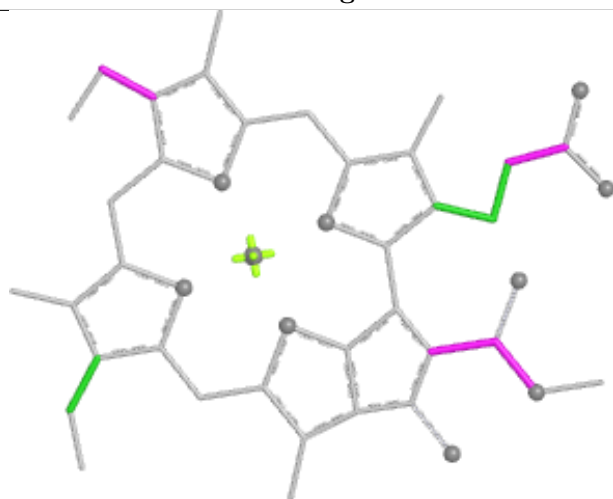
Ligand CLA 4 506



Bond lengths



Bond angles

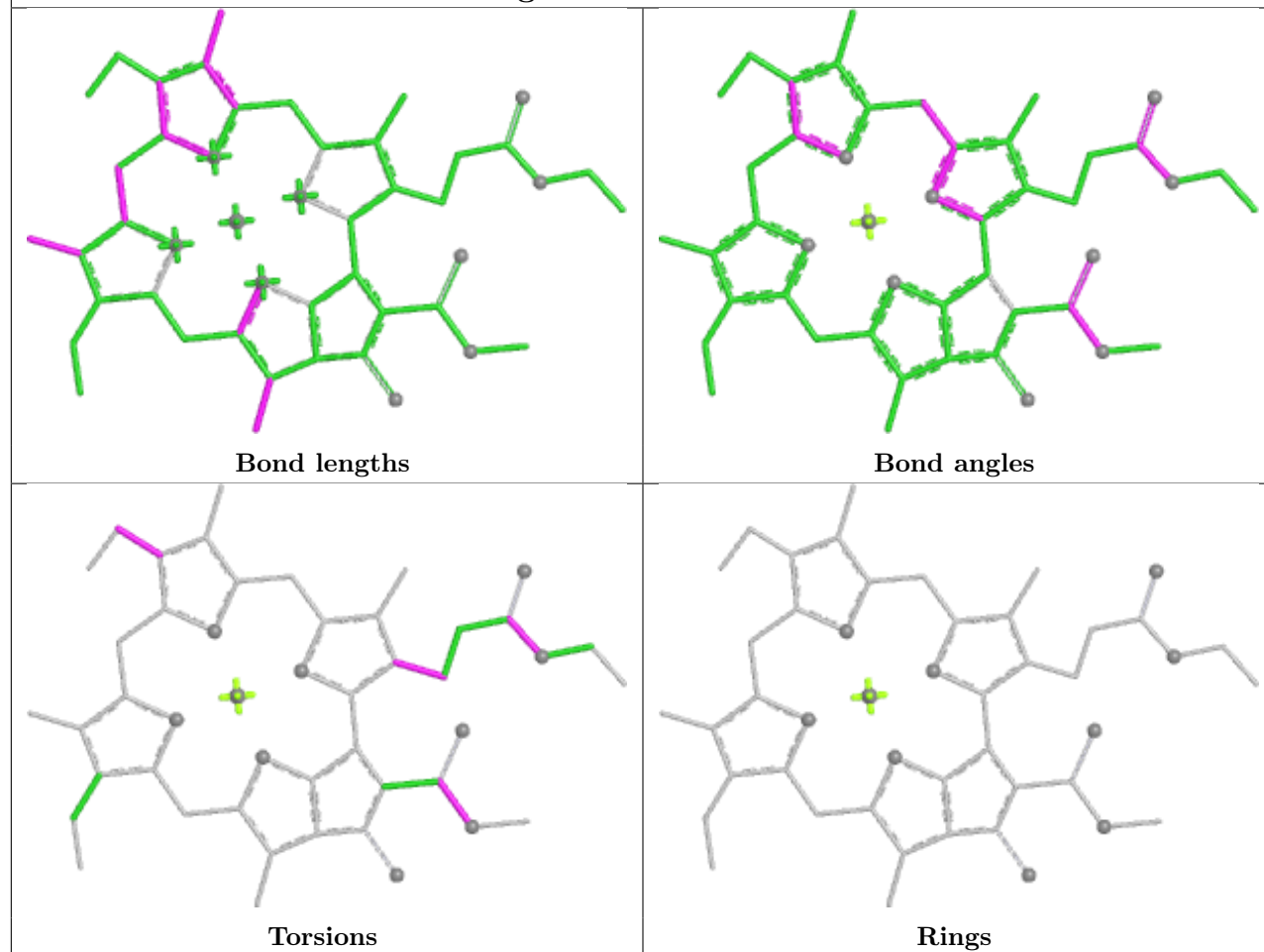


Torsions

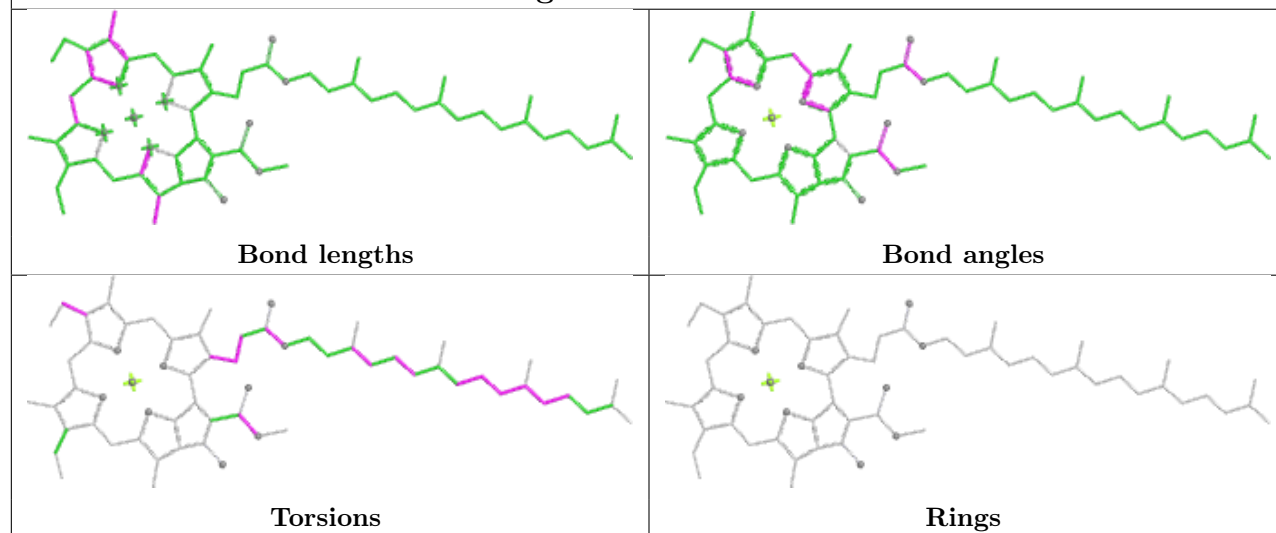


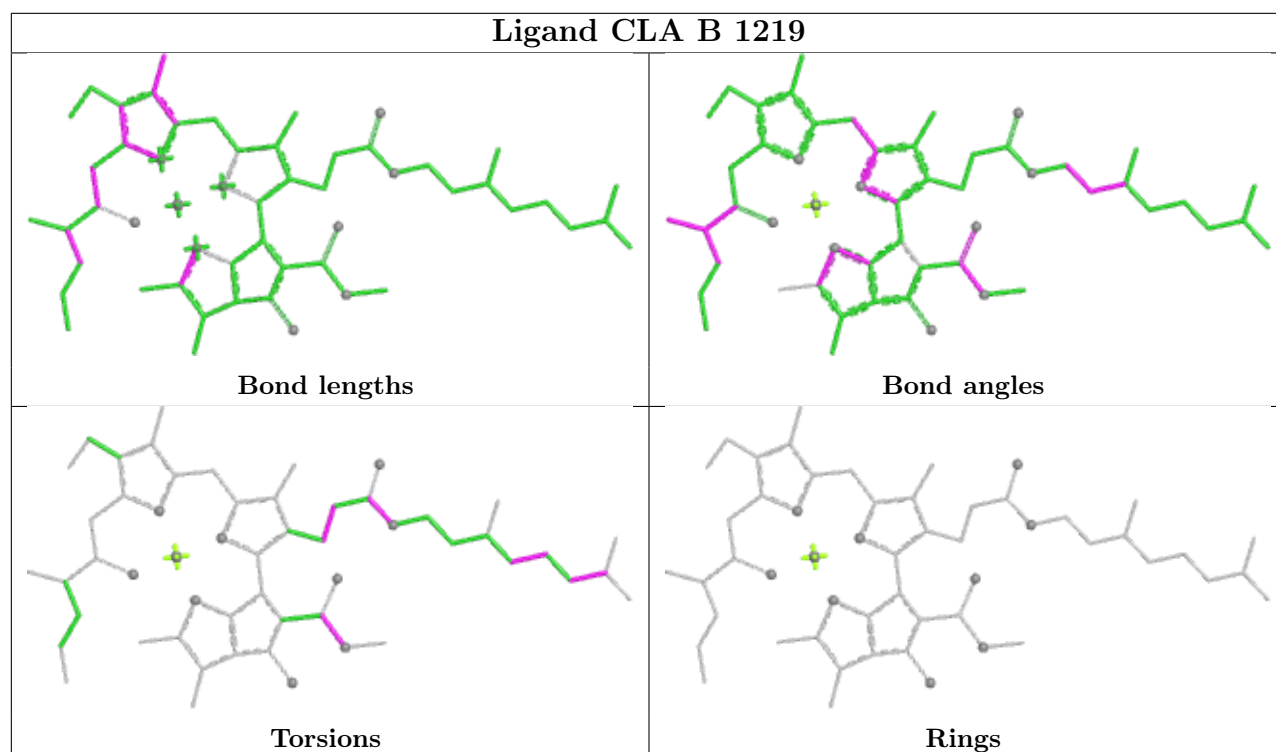
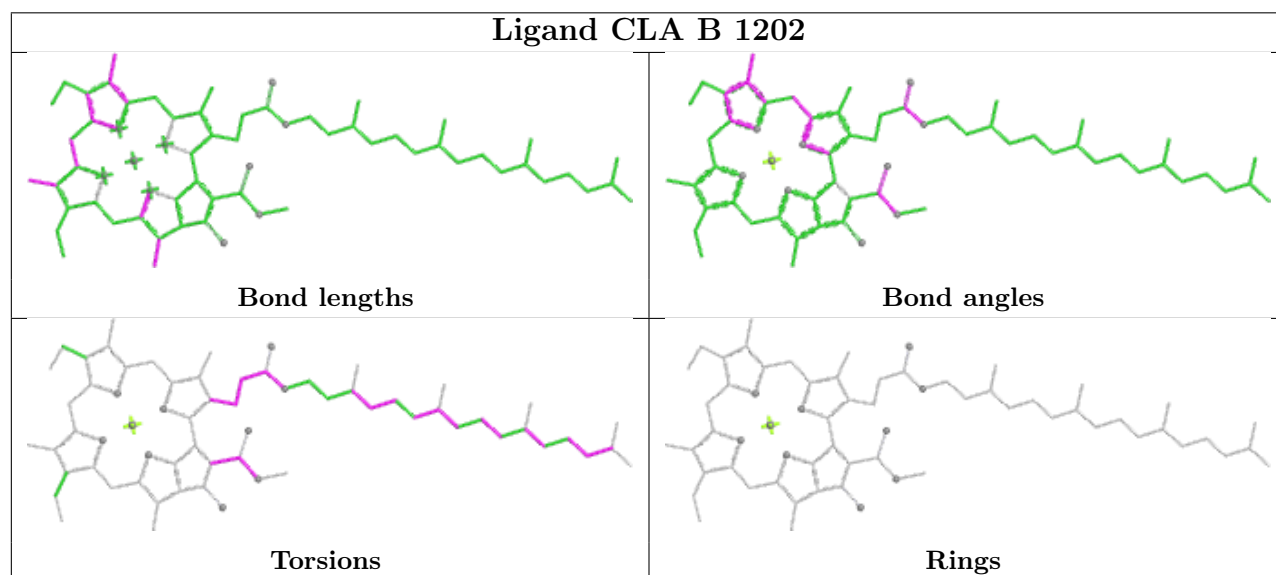
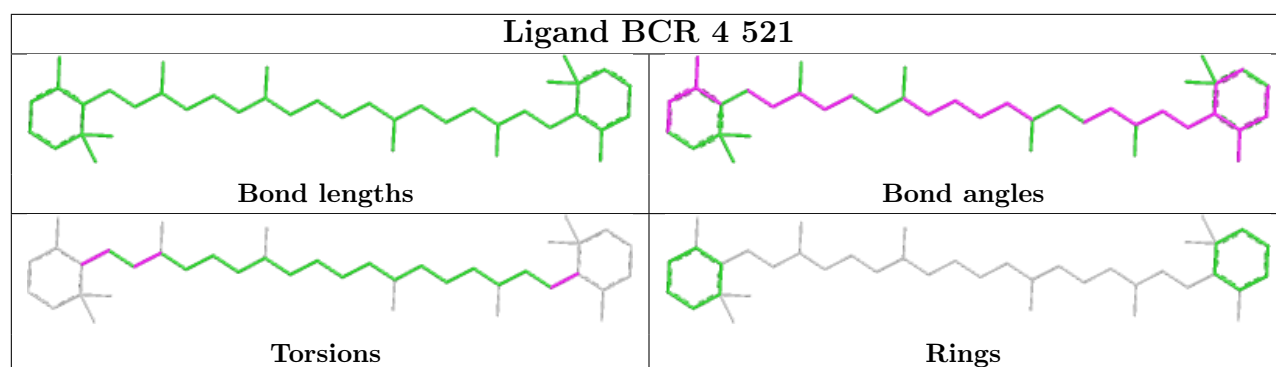
Rings

Ligand CLA A 1112

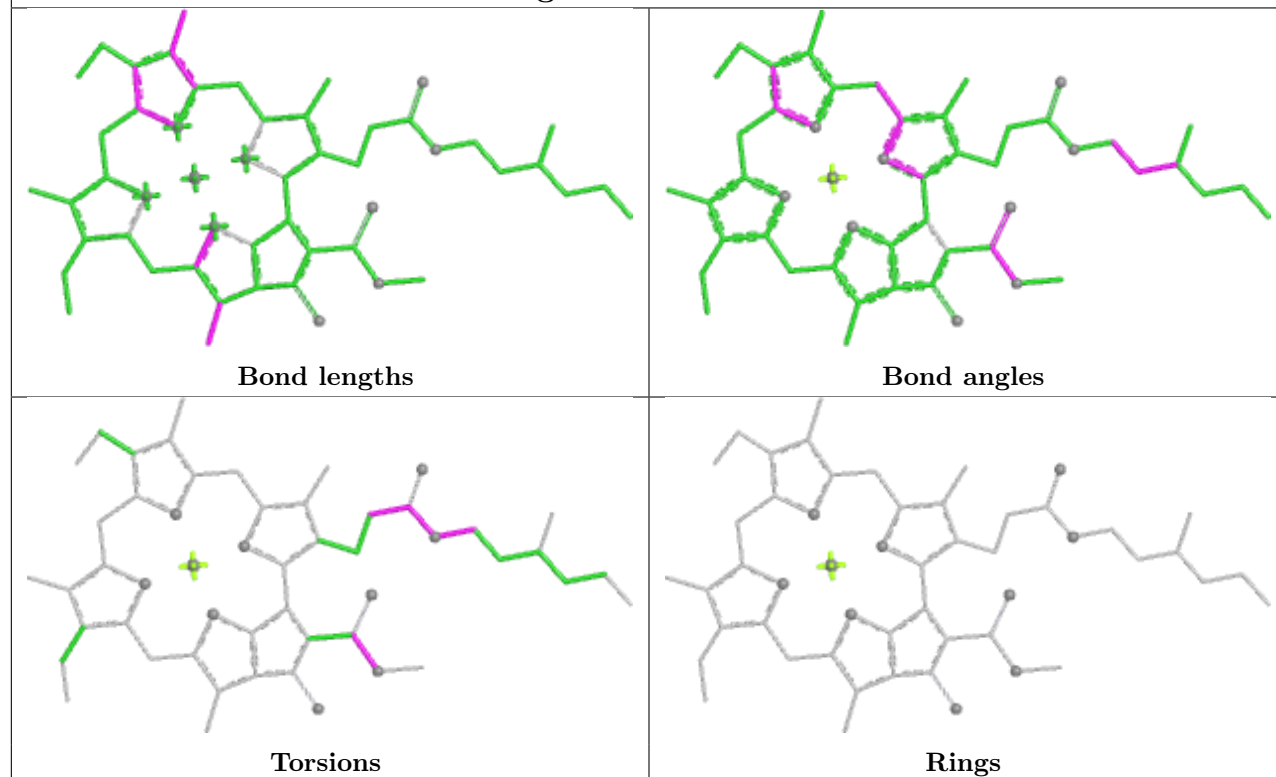


Ligand CLA 1 505

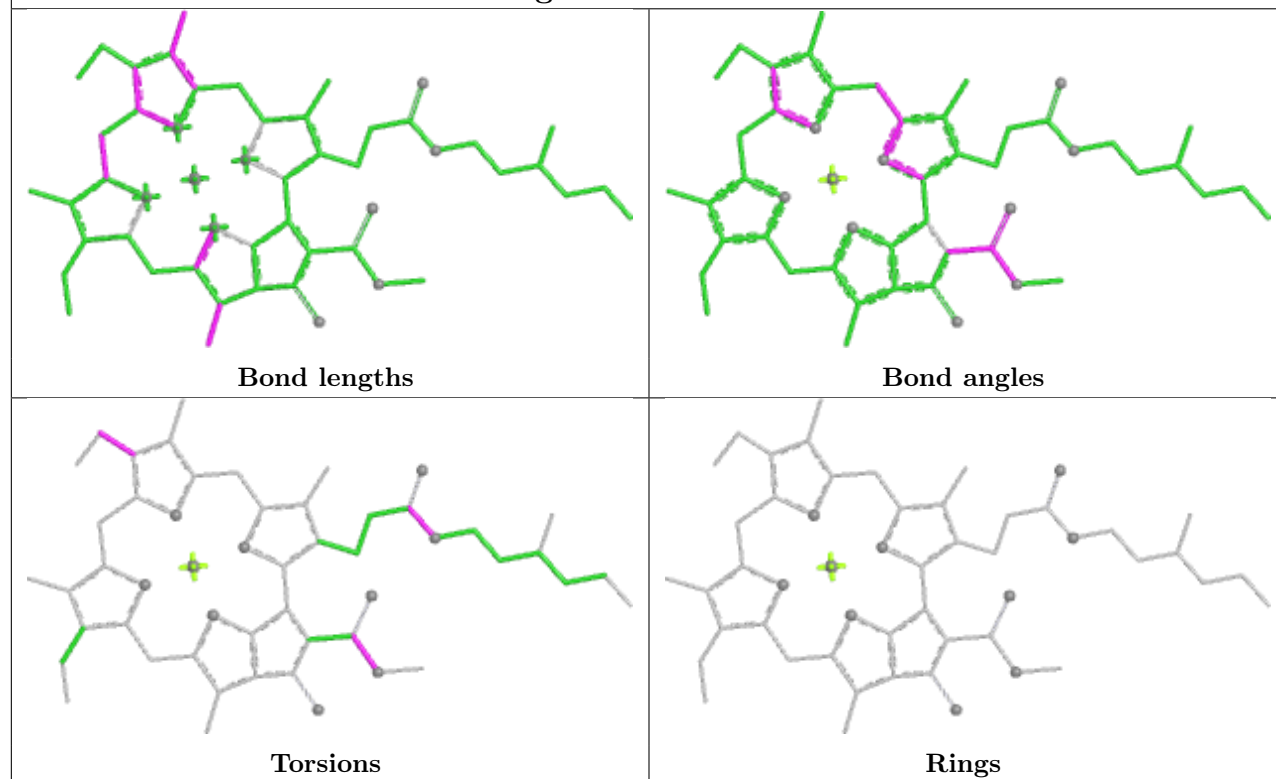




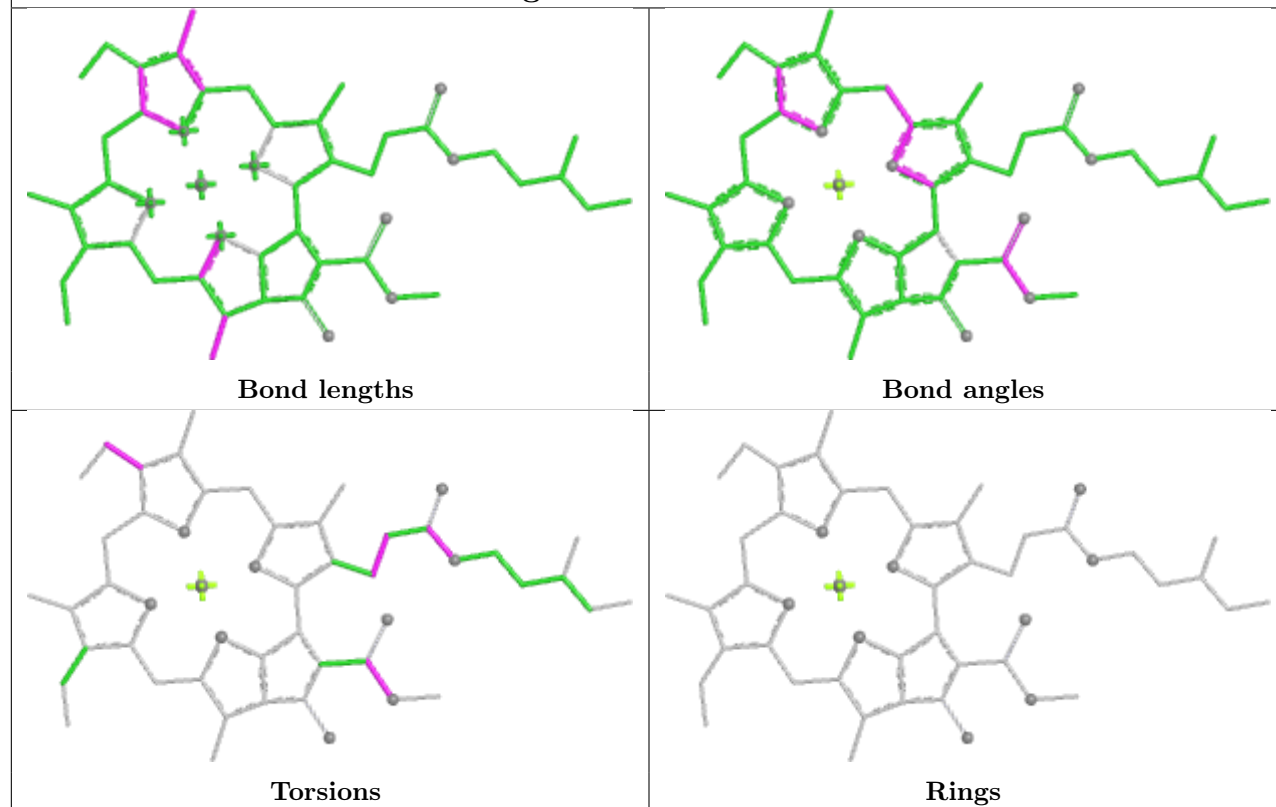
Ligand CLA e 512



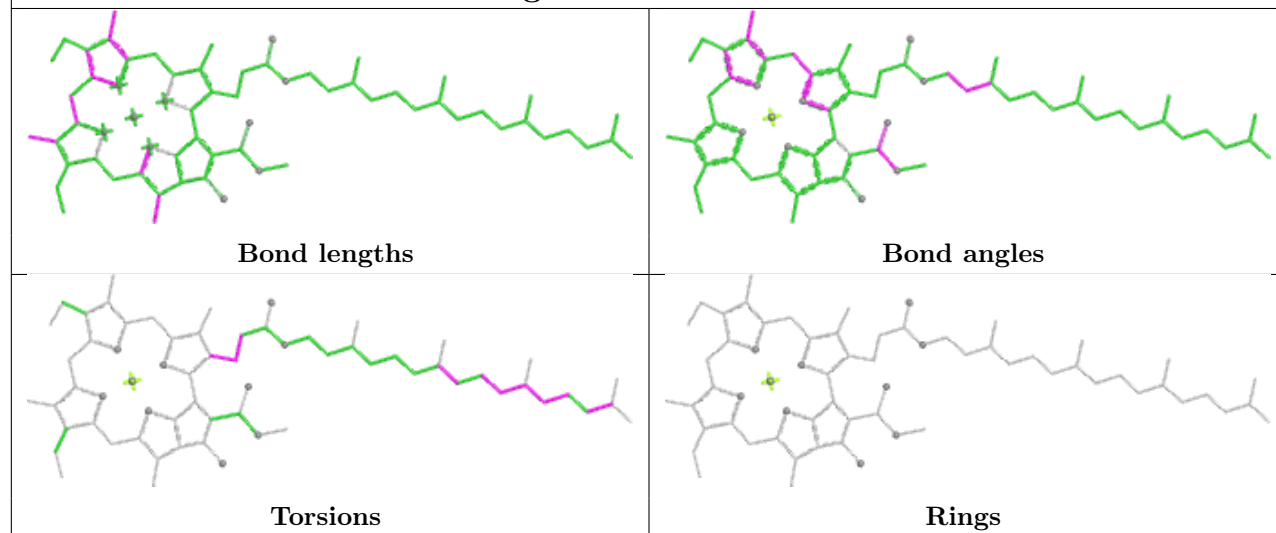
Ligand CLA d 512

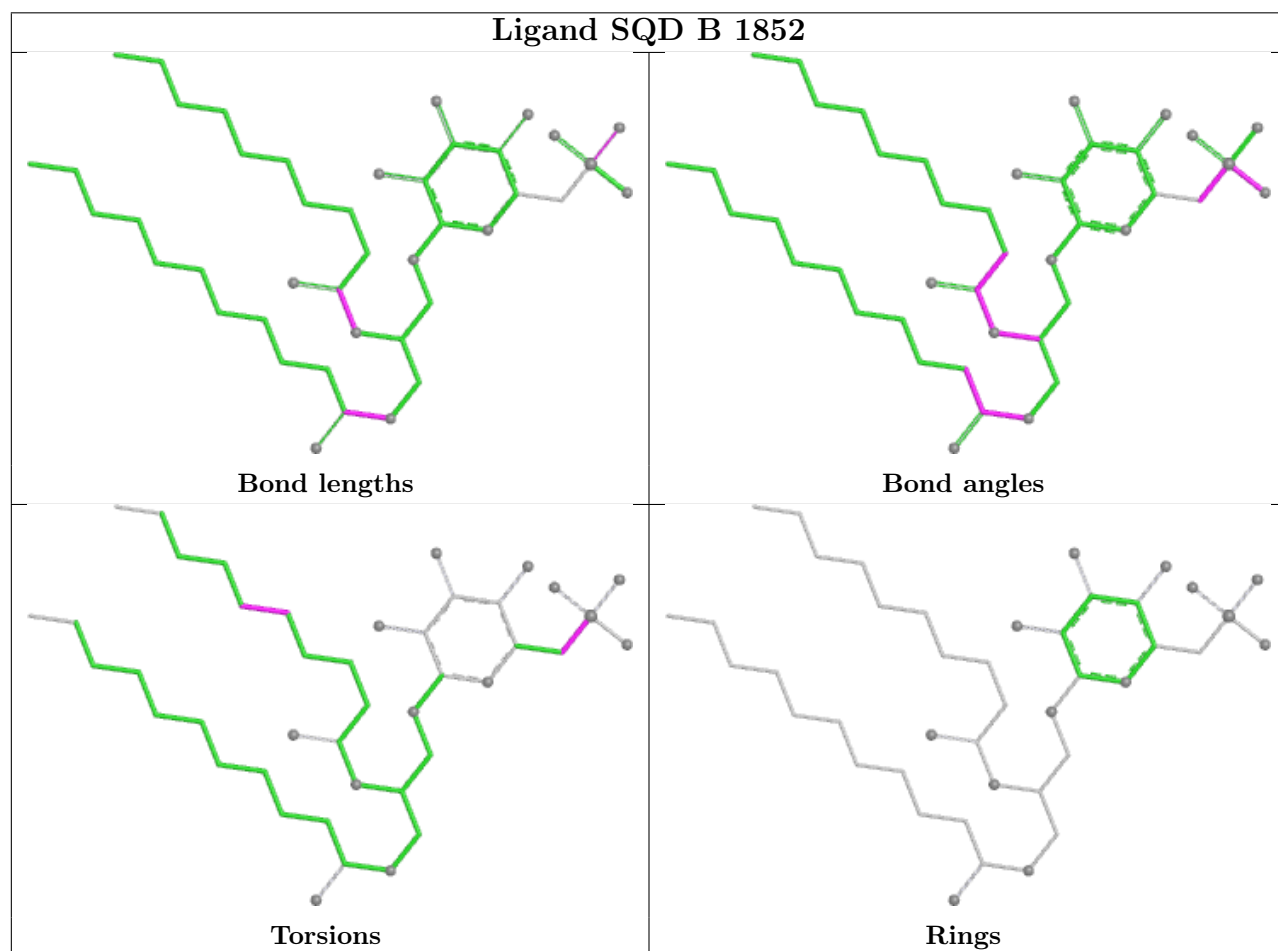
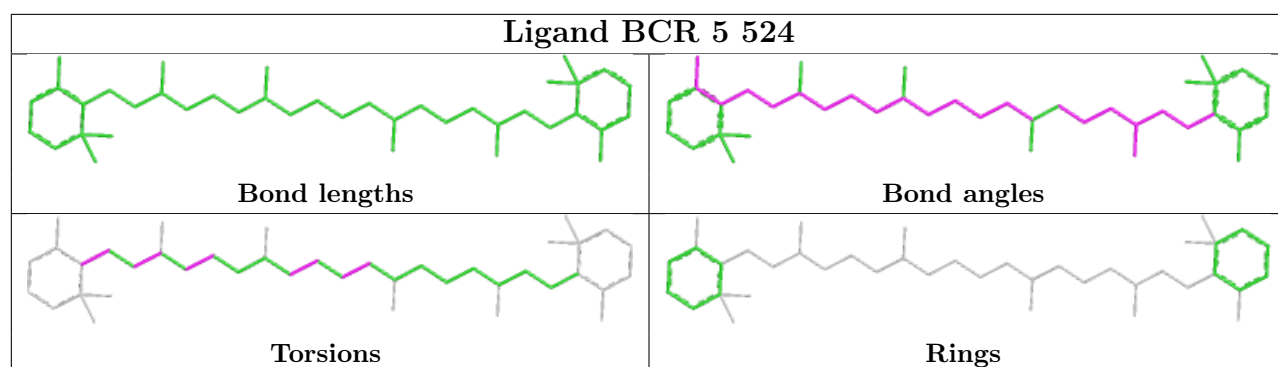


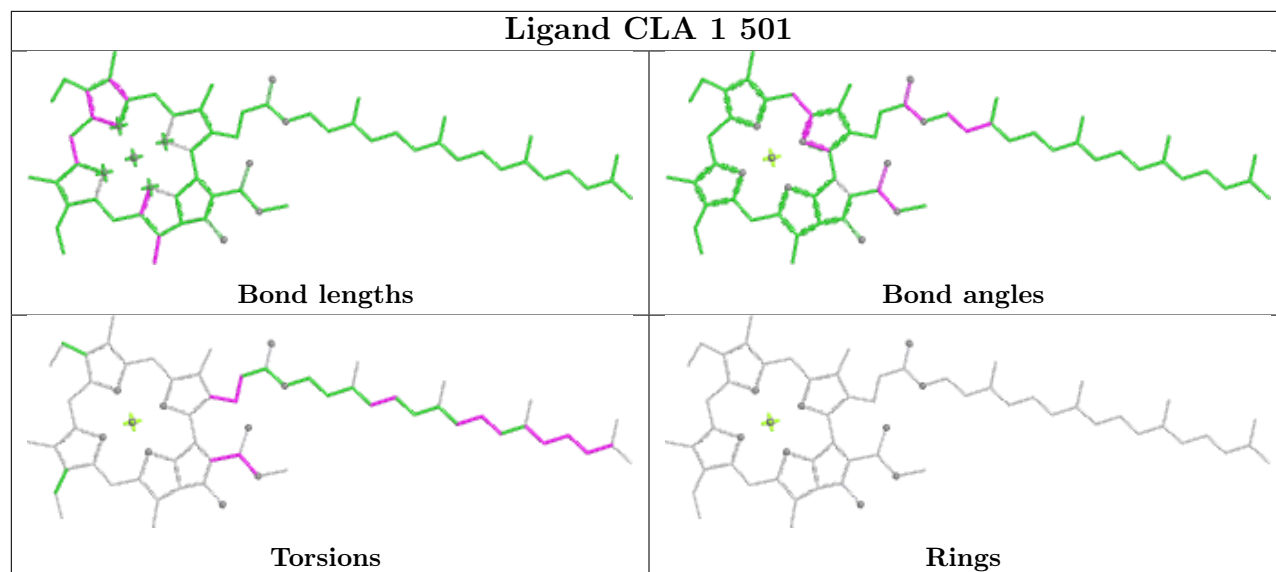
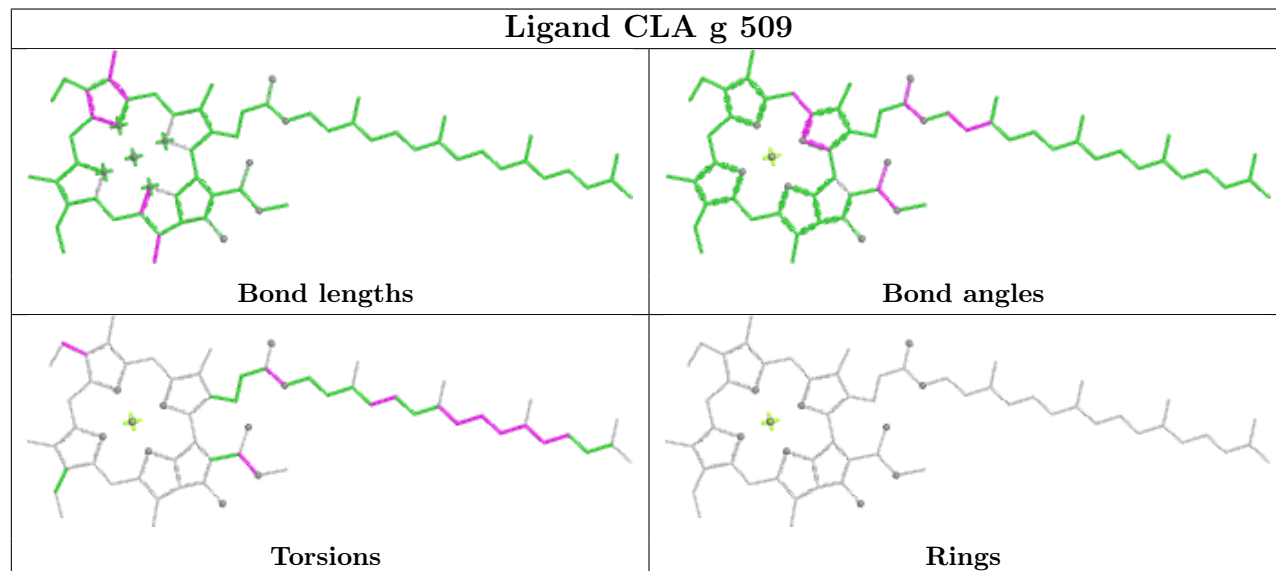
Ligand CLA A 1121



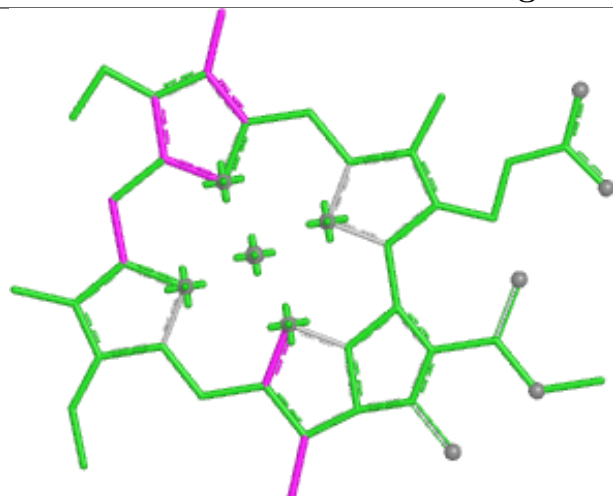
Ligand CLA B 1225



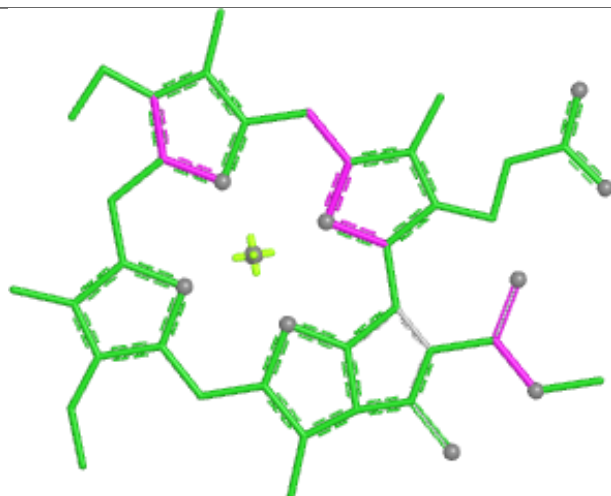


Ligand CLA 1 501**Ligand CLA g 509**

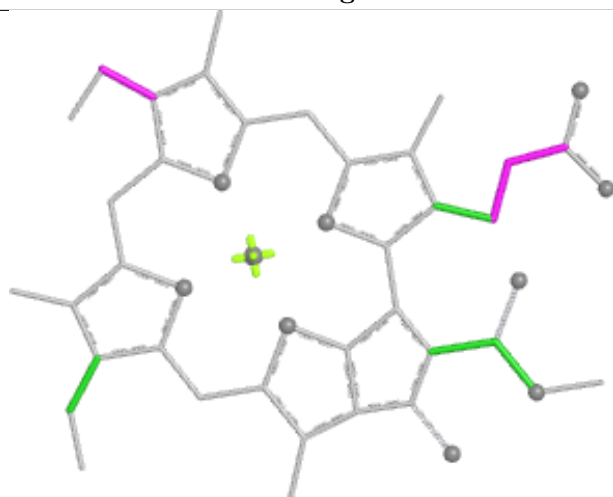
Ligand CLA 3 519



Bond lengths



Bond angles

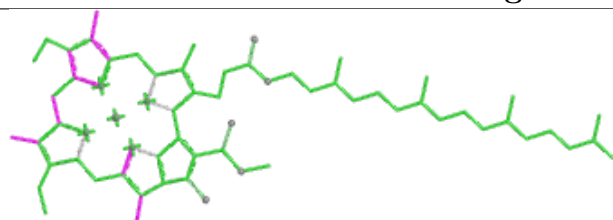


Torsions

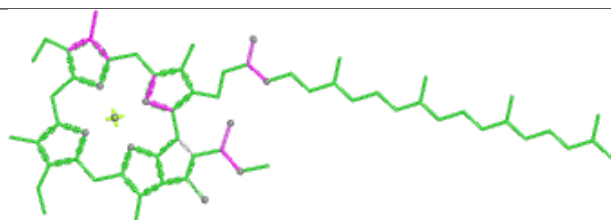


Rings

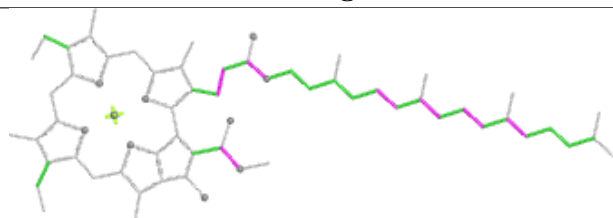
Ligand CLA A 1022



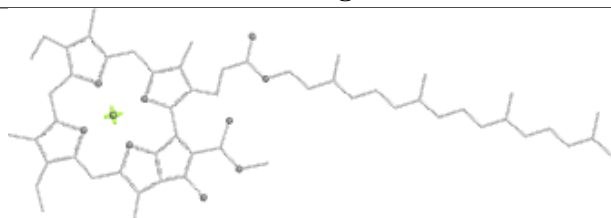
Bond lengths



Bond angles

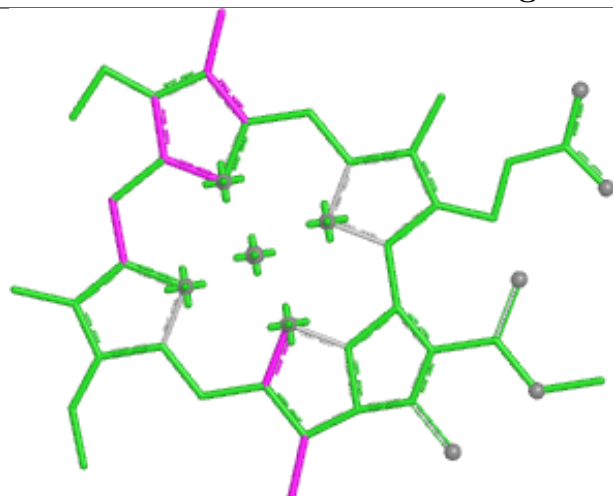


Torsions

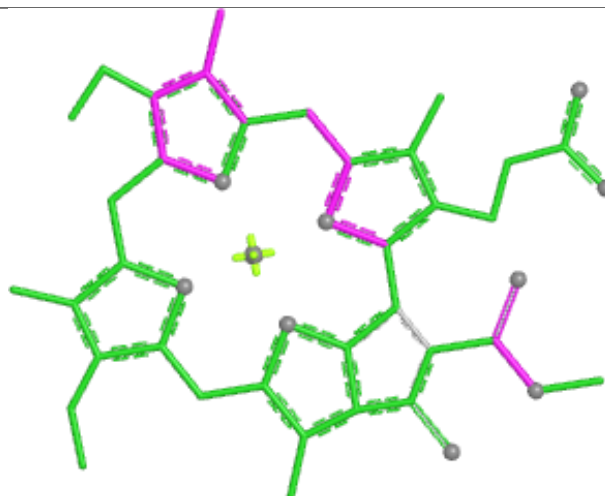


Rings

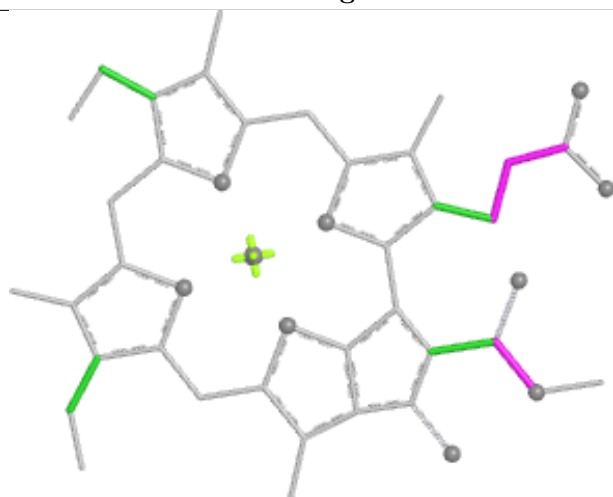
Ligand CLA e 511



Bond lengths



Bond angles

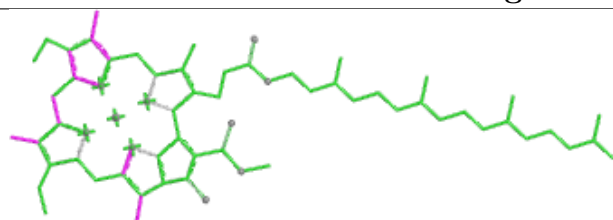


Torsions

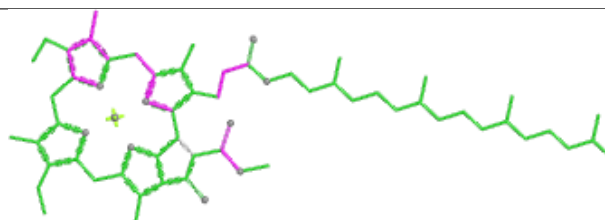


Rings

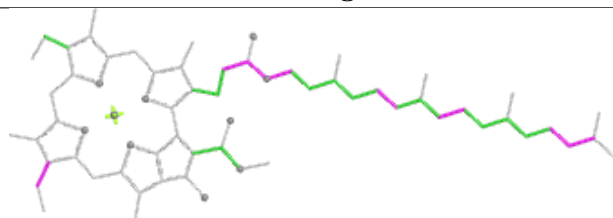
Ligand CLA A 1127



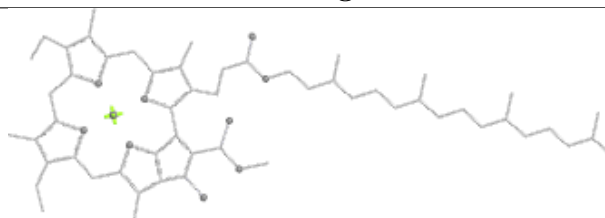
Bond lengths



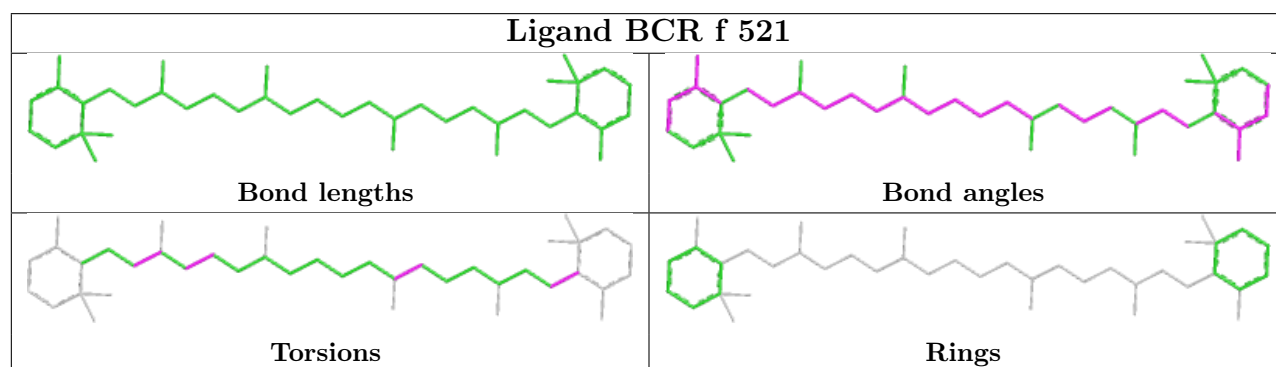
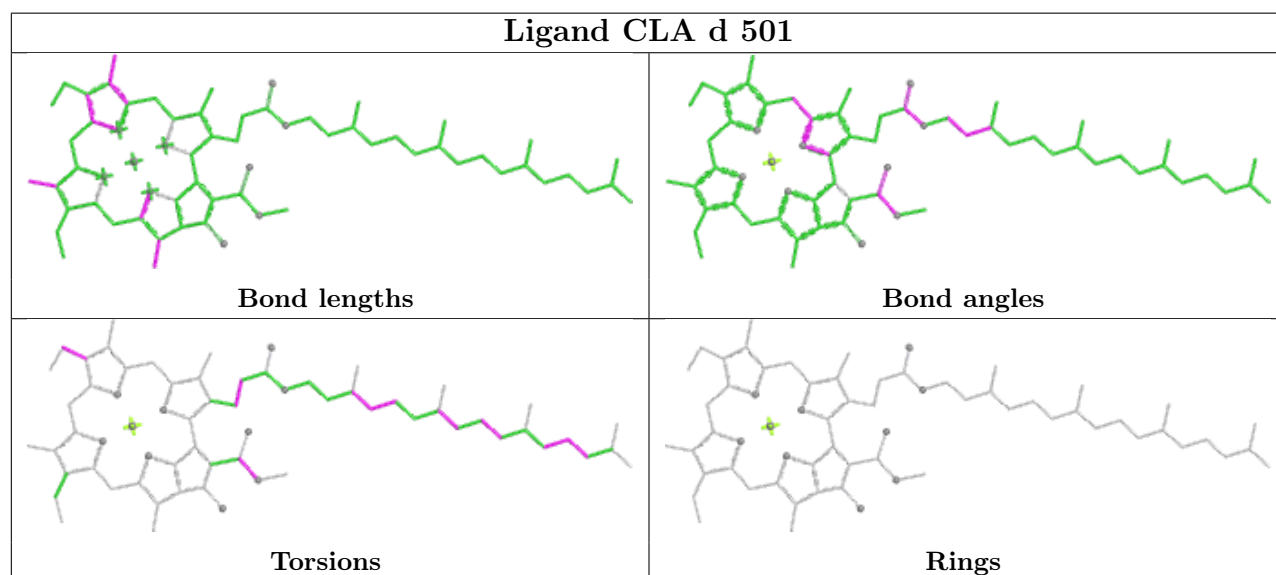
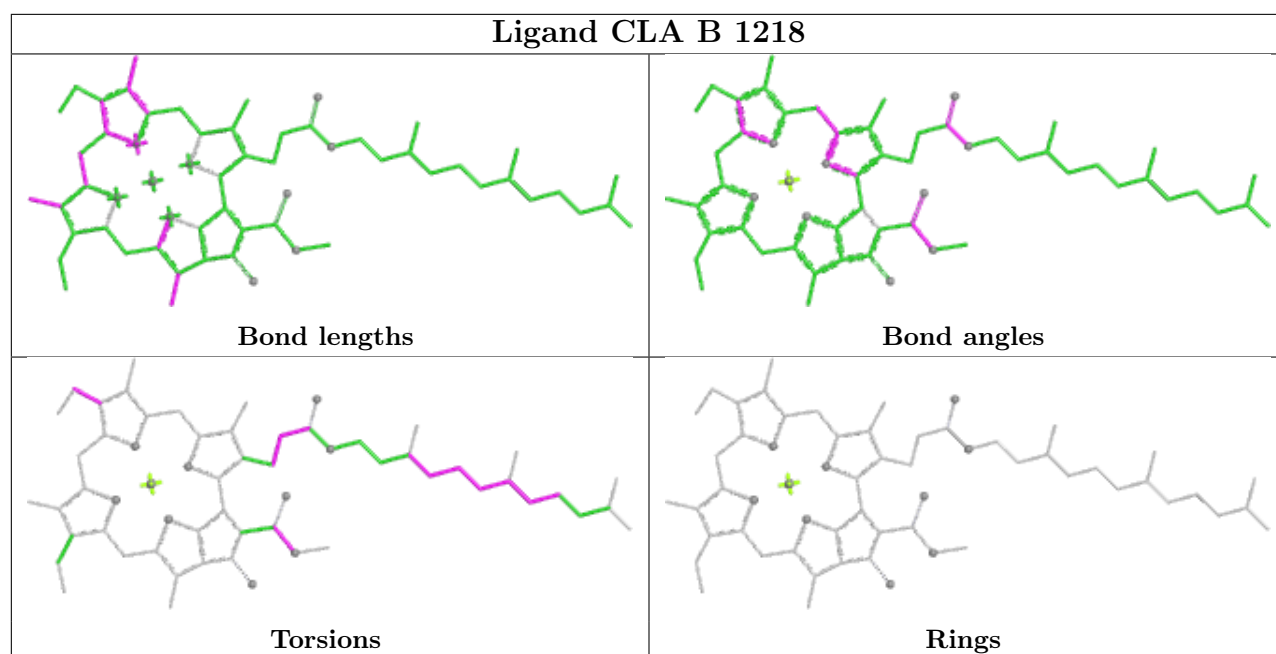
Bond angles

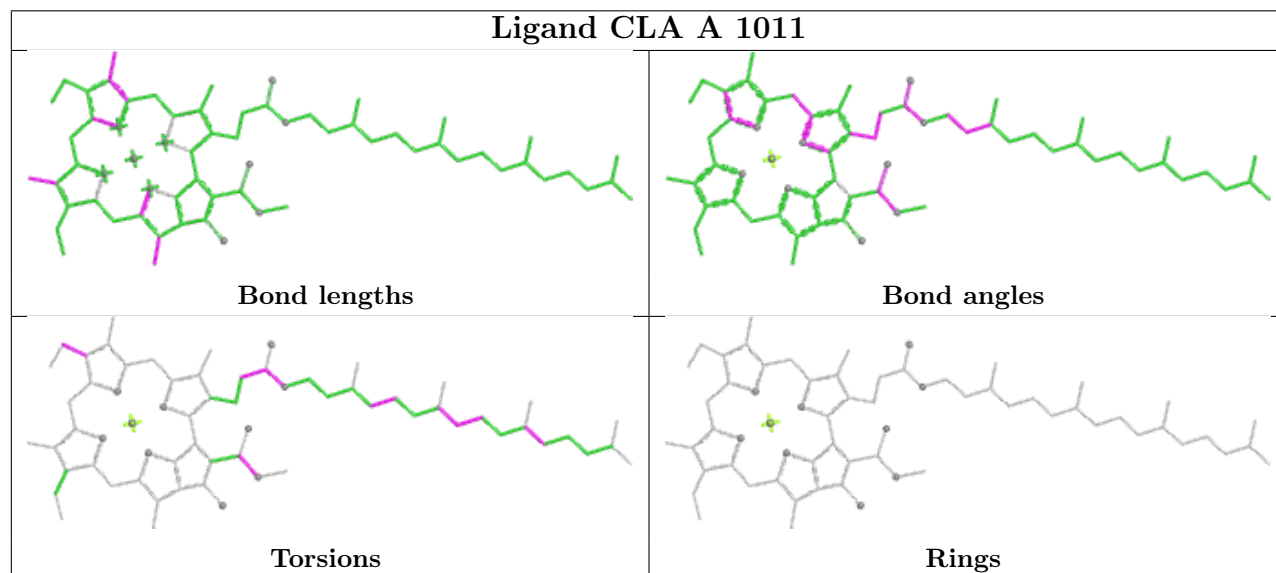
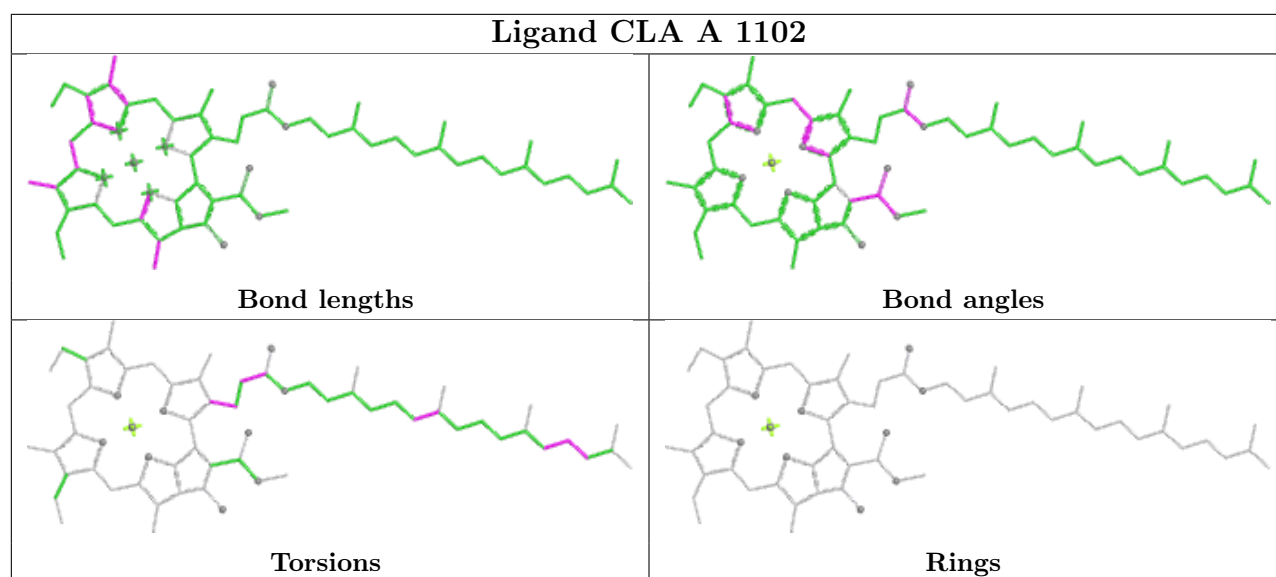


Torsions

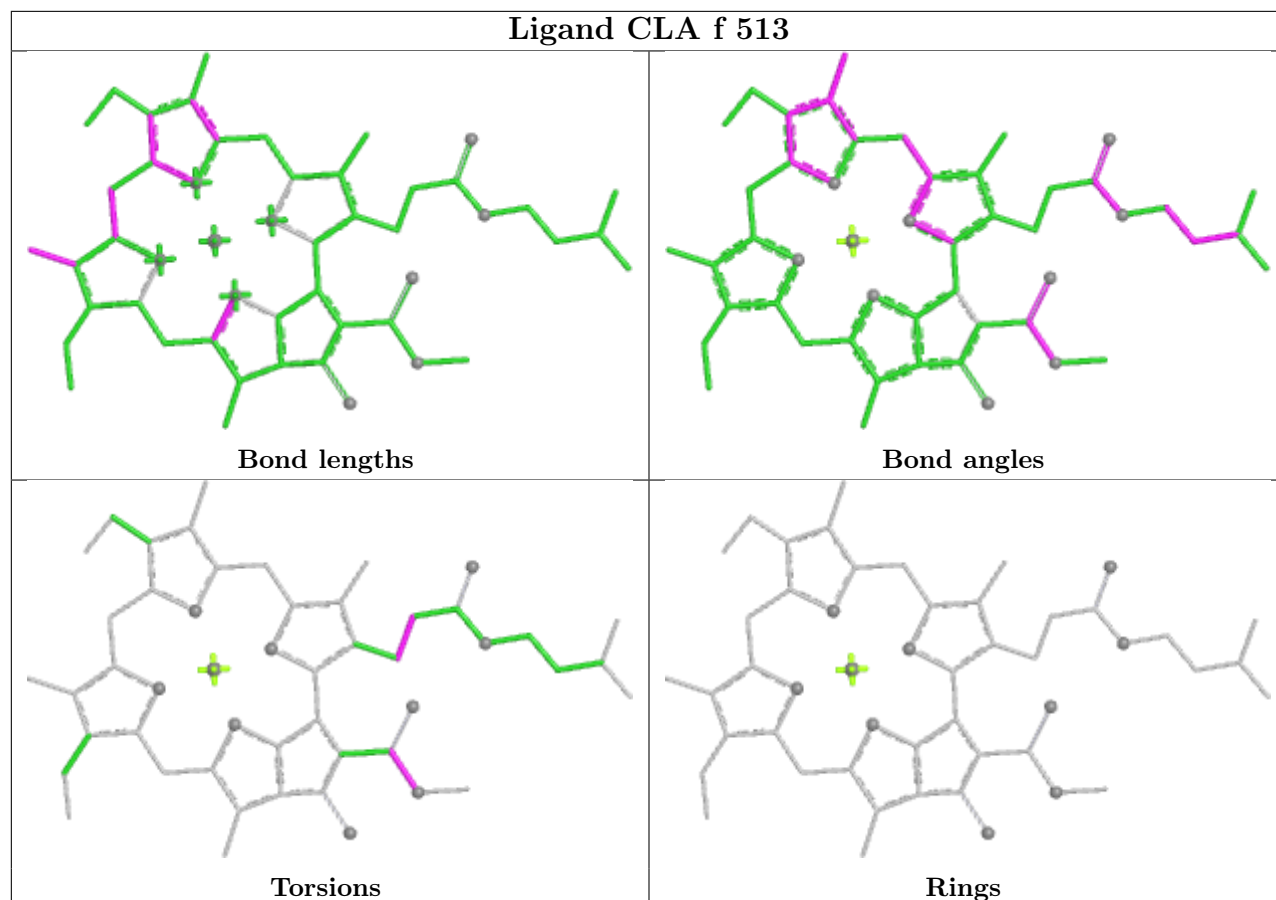


Rings

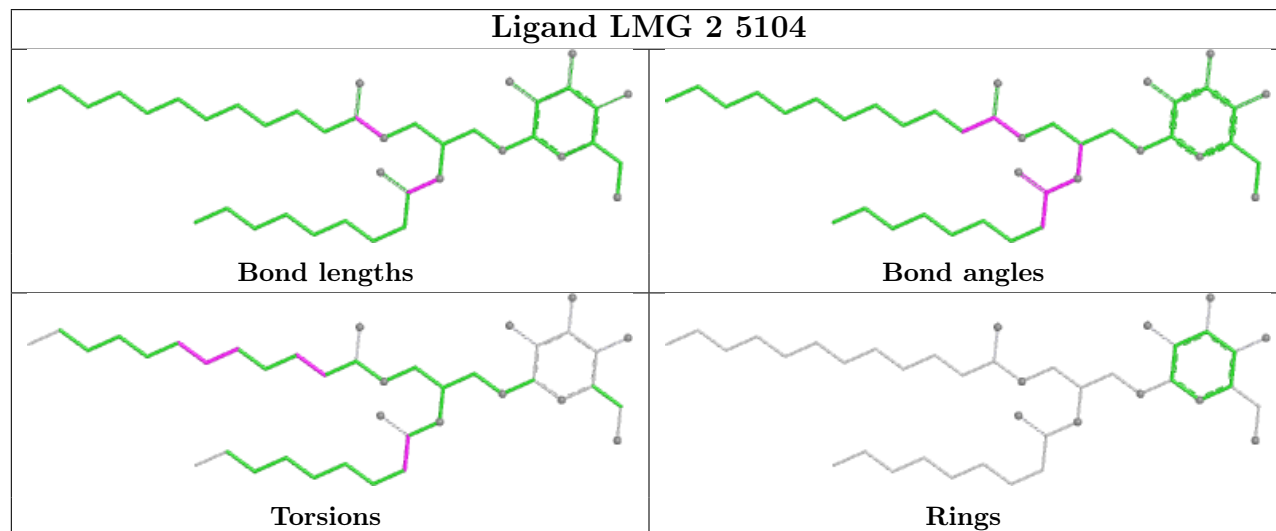


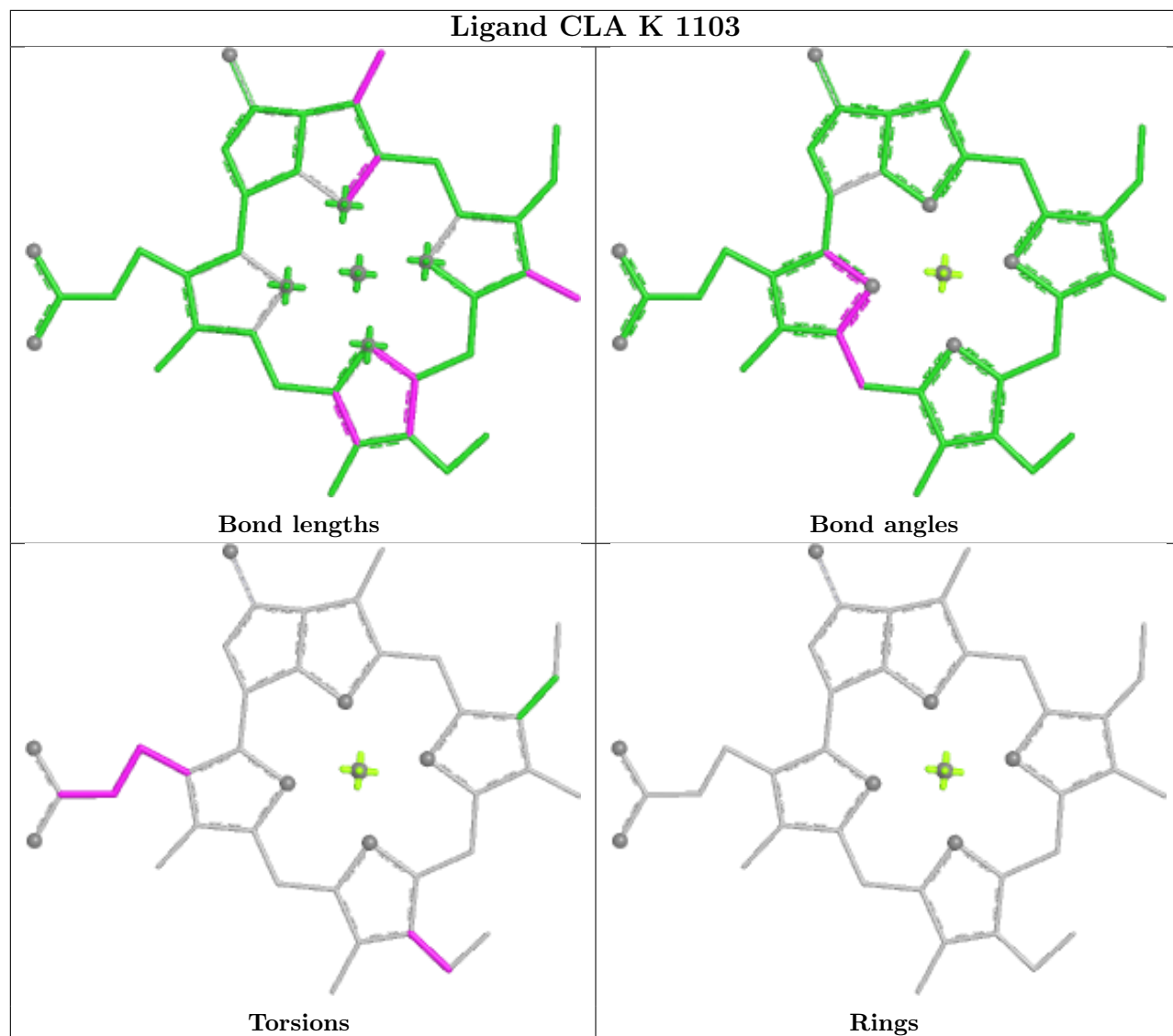


Ligand CLA f 513

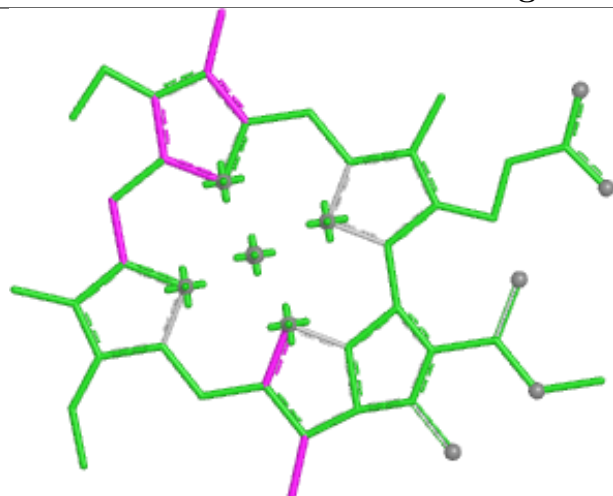


Ligand LMG 2 5104

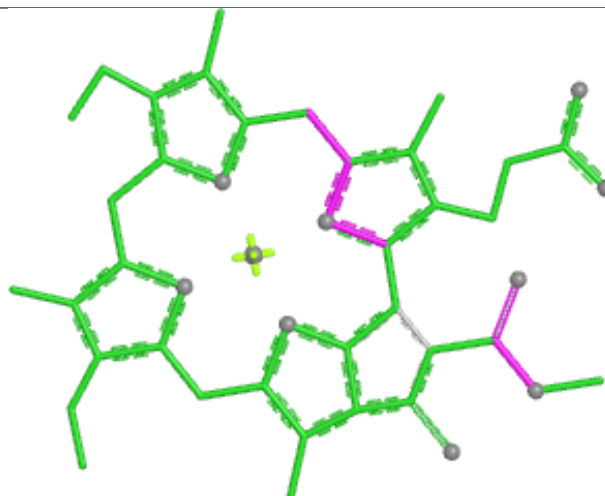




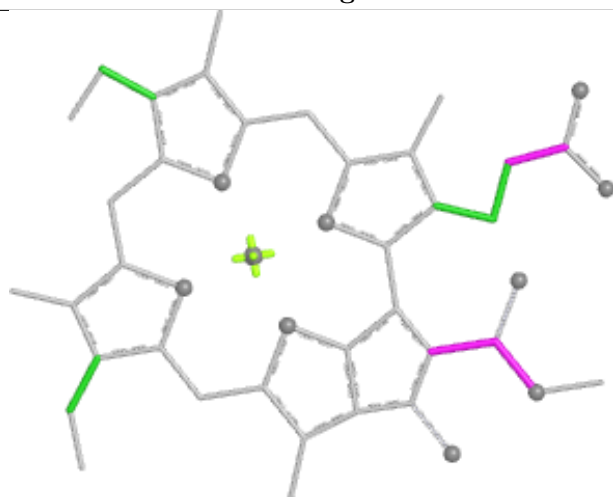
Ligand CLA 6 519



Bond lengths



Bond angles

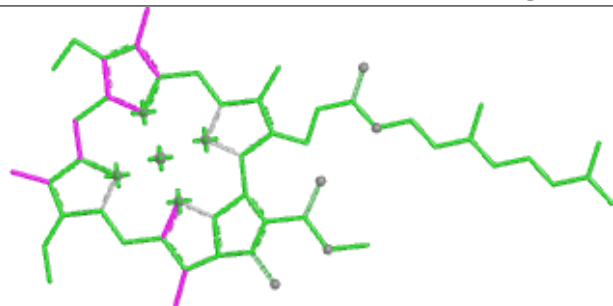


Torsions

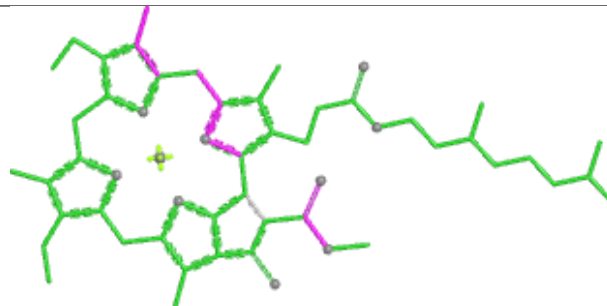


Rings

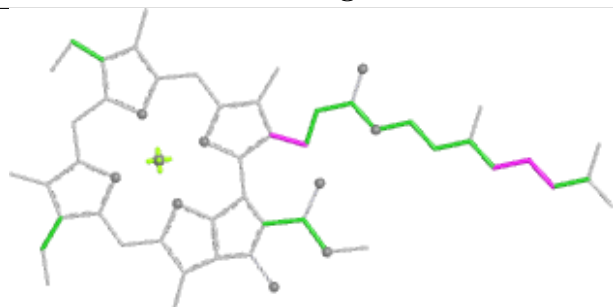
Ligand CLA f 508



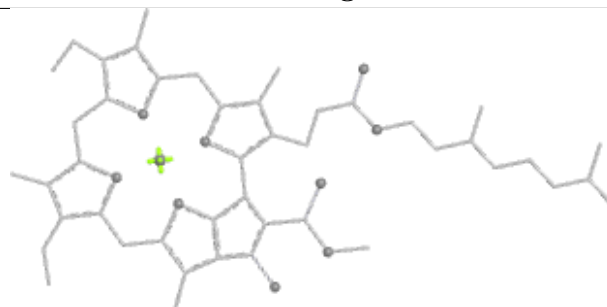
Bond lengths



Bond angles

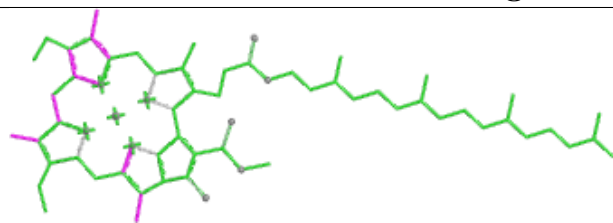


Torsions

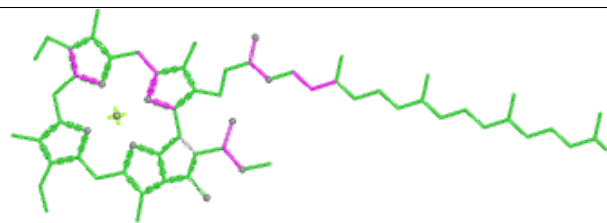


Rings

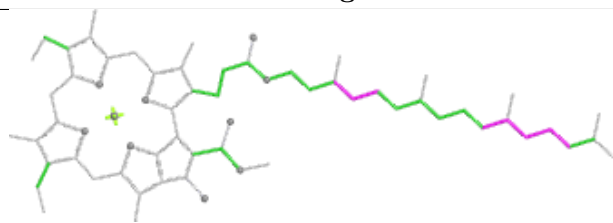
Ligand CLA B 1235



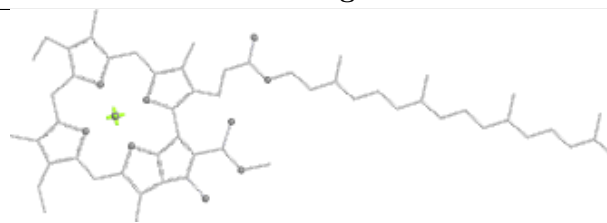
Bond lengths



Bond angles

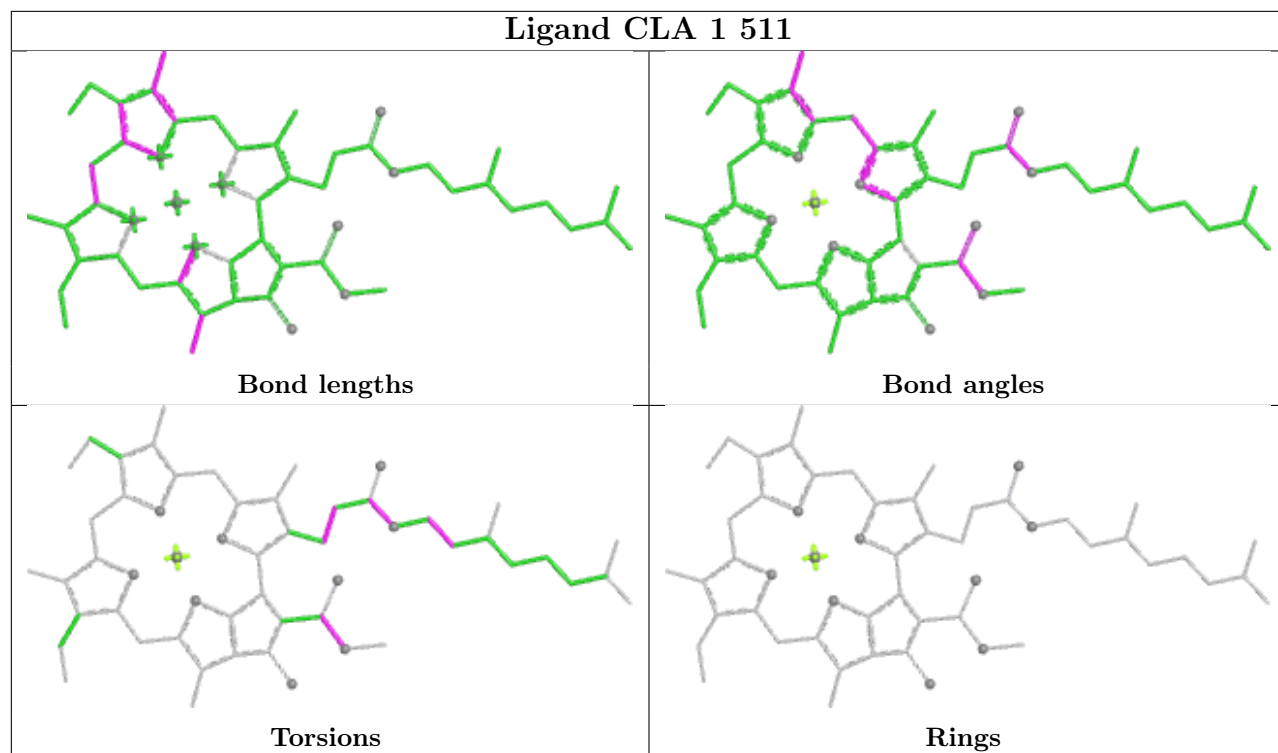


Torsions

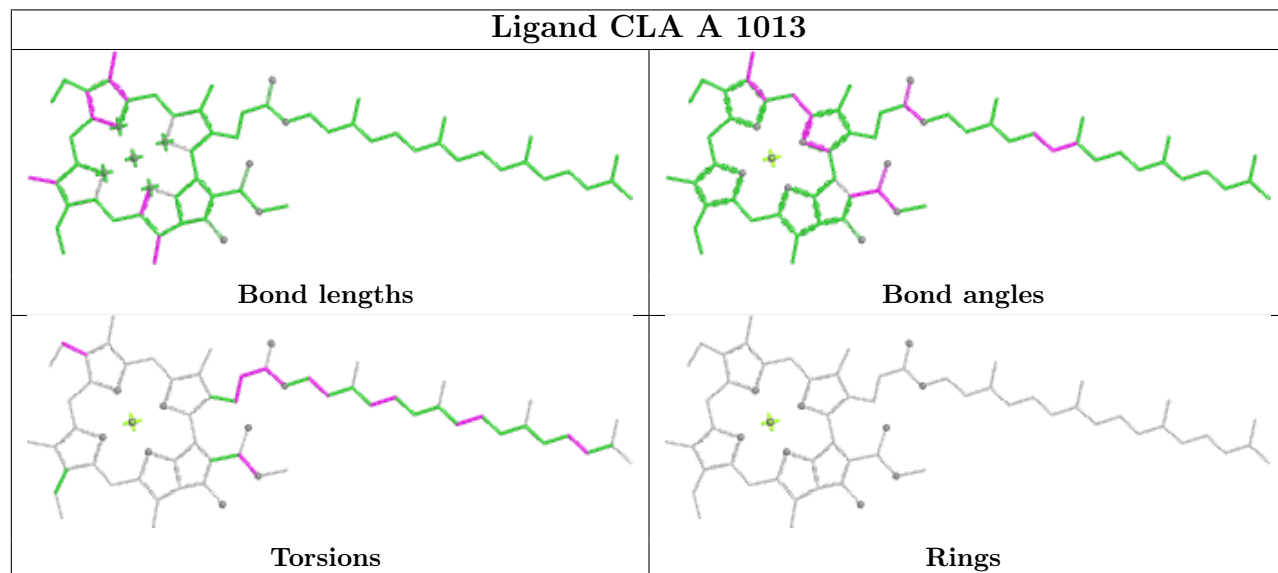


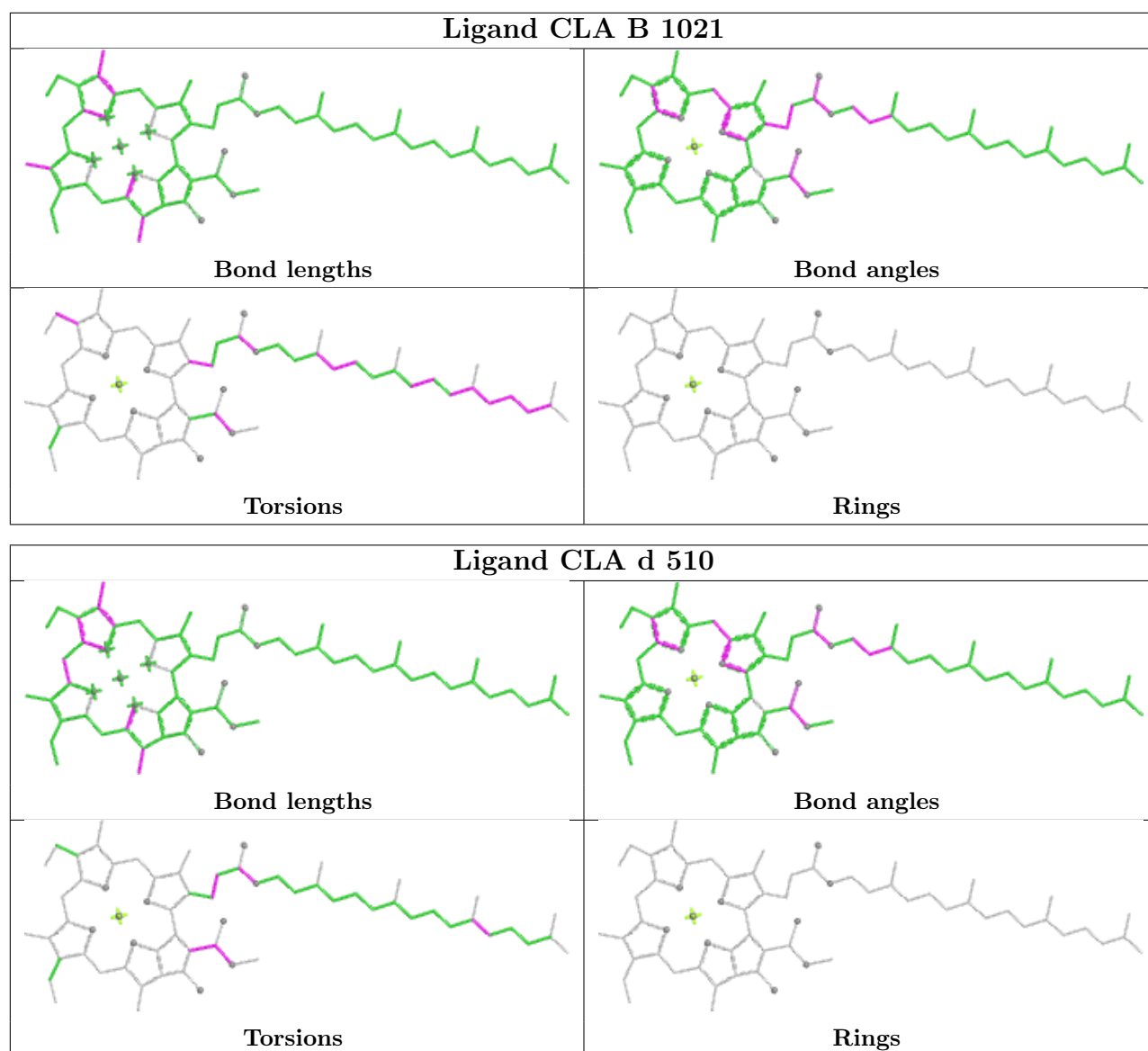
Rings

Ligand CLA 1 511

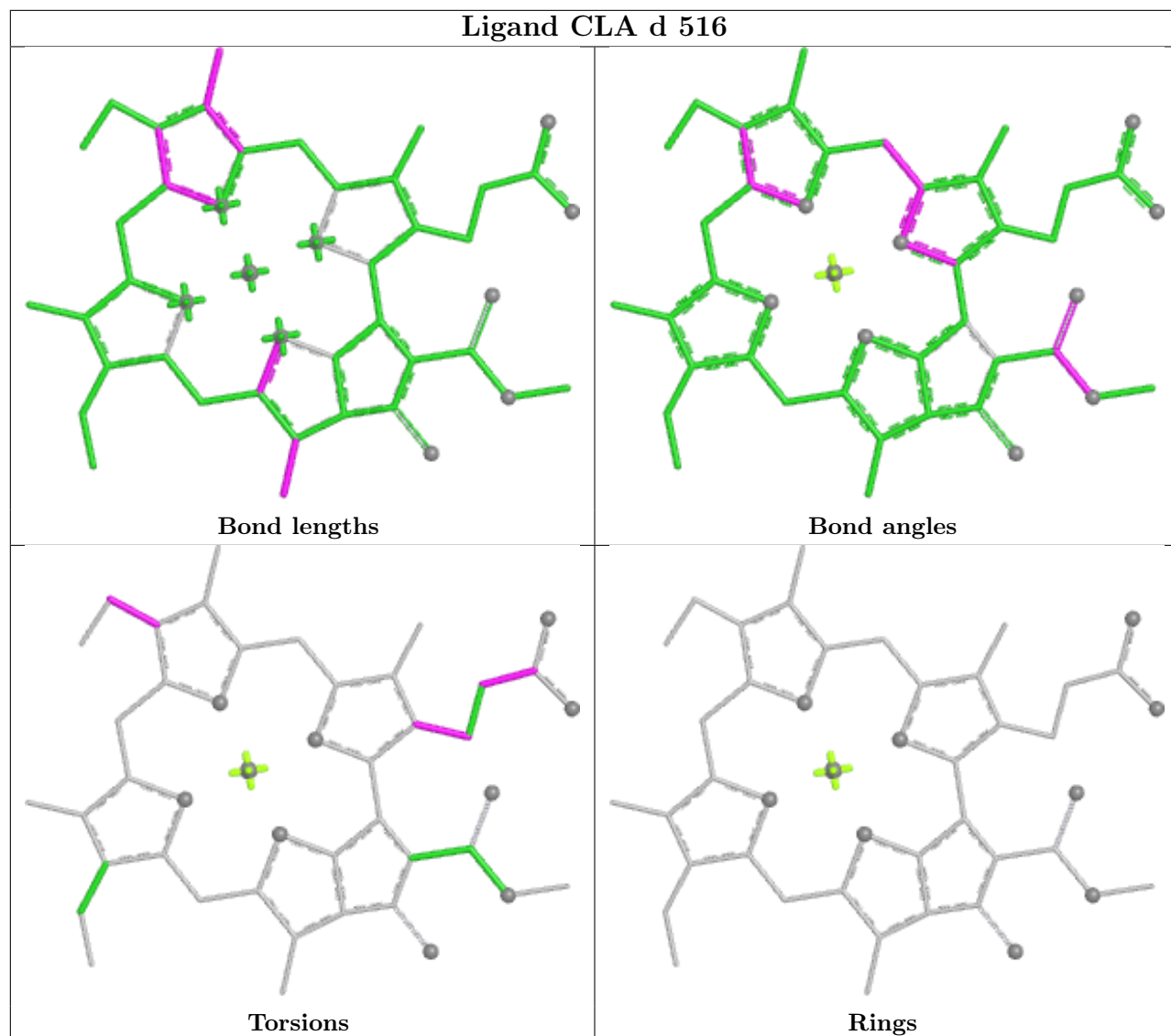


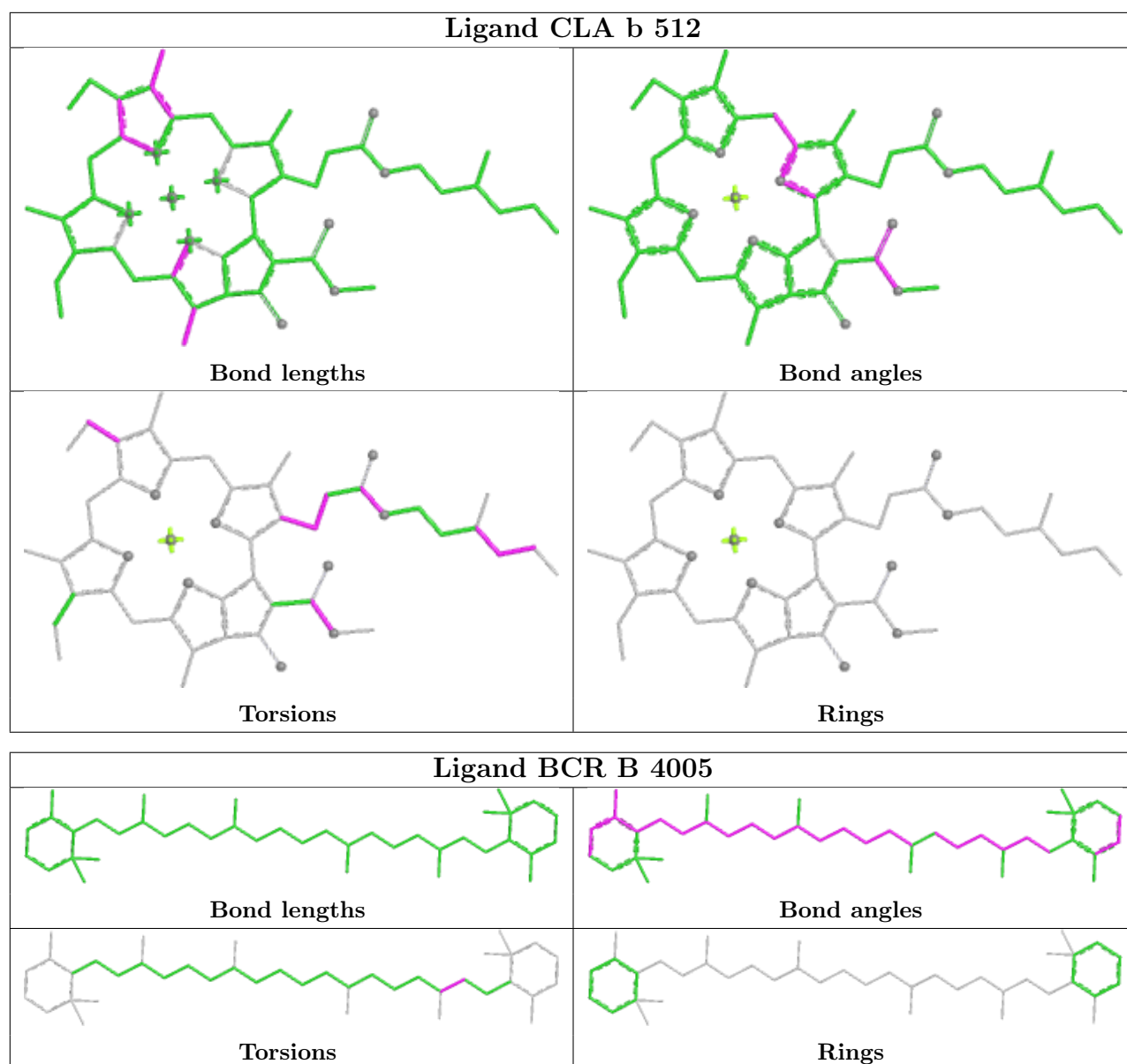
Ligand CLA A 1013



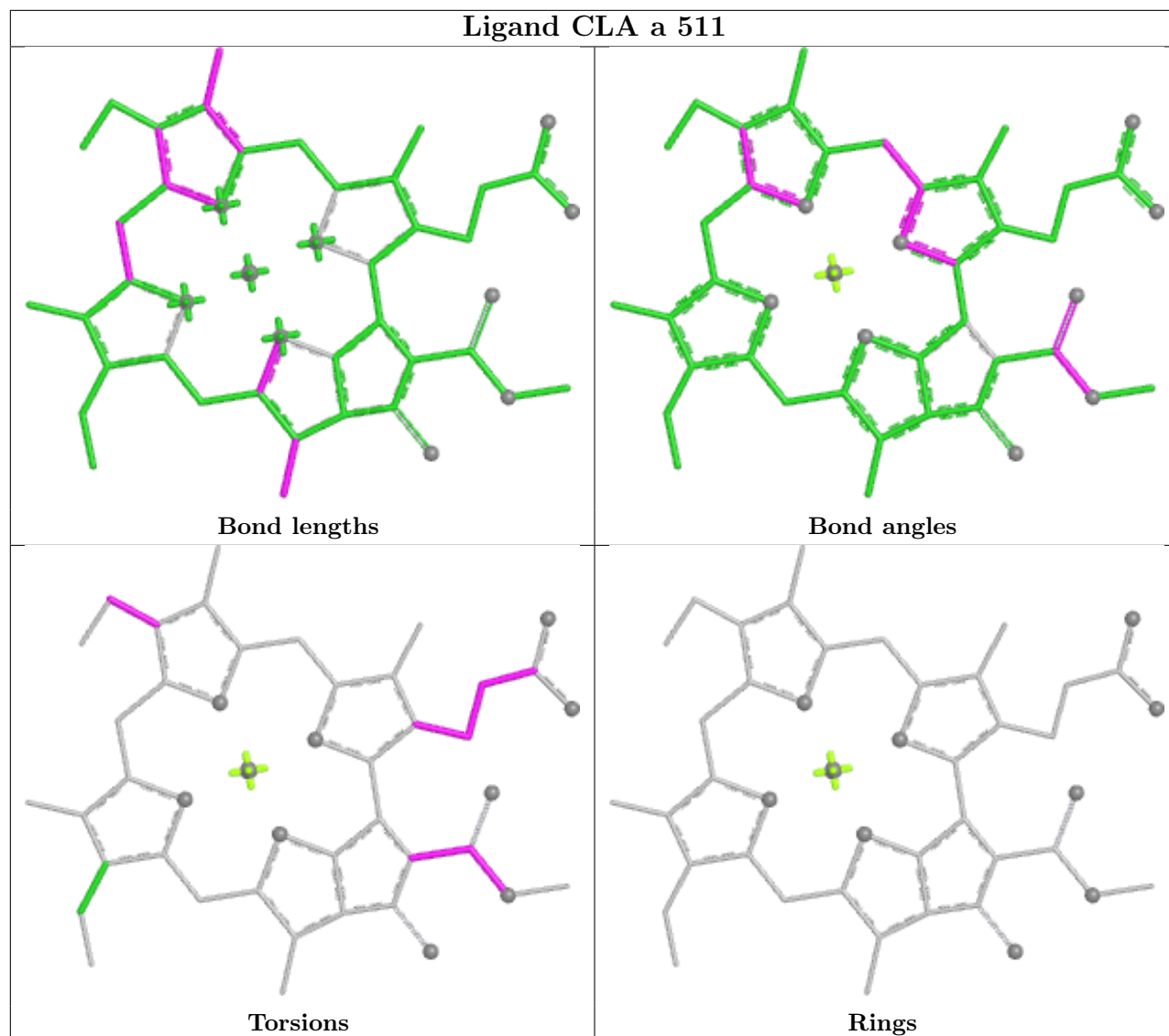


Ligand CLA d 516

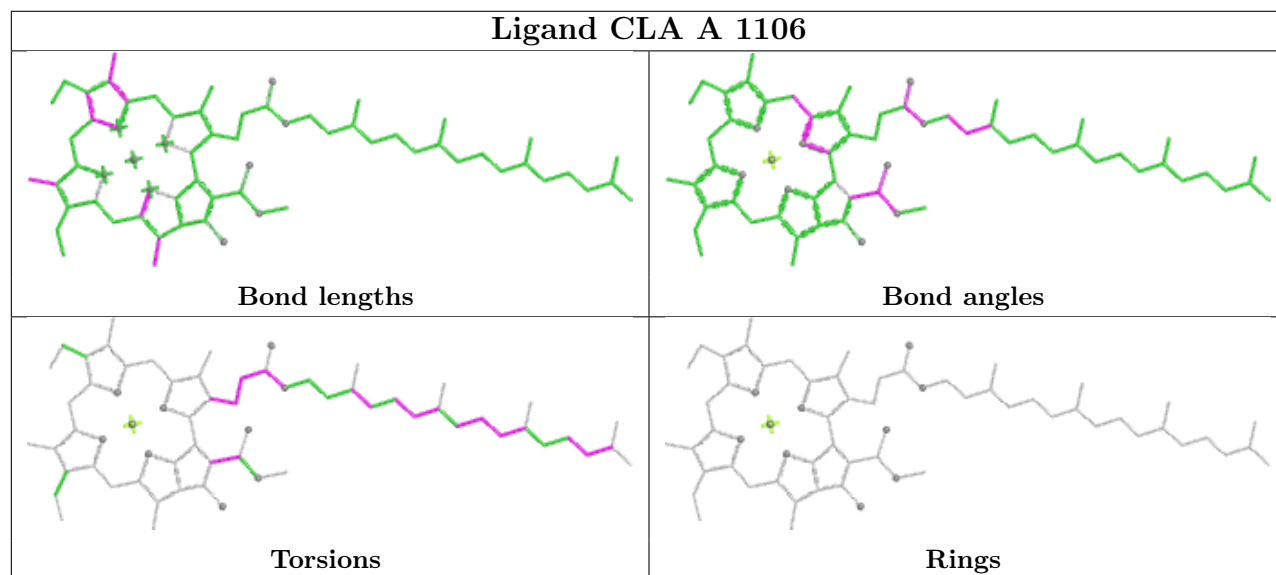




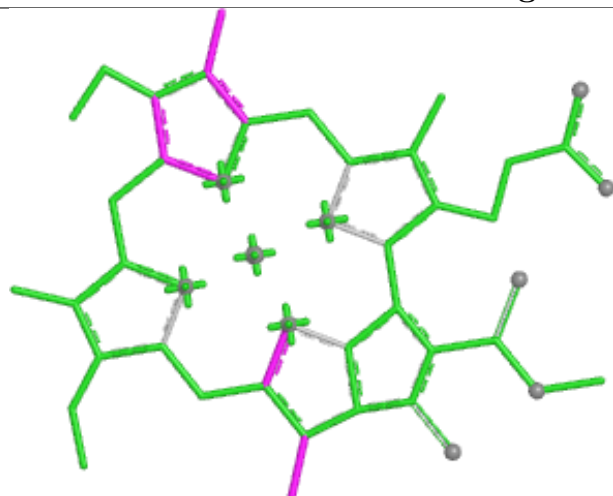
Ligand CLA a 511



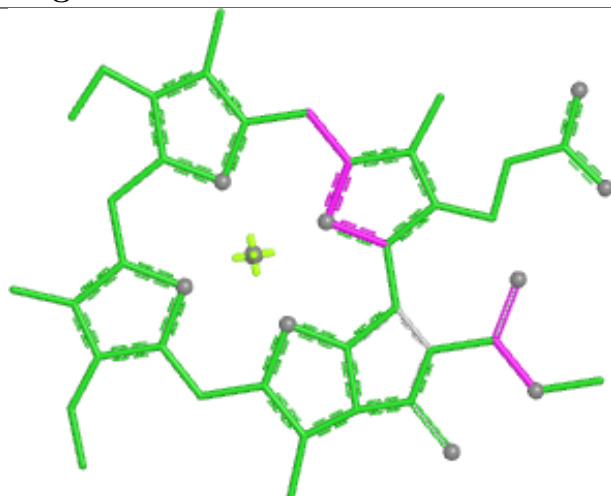
Ligand CLA A 1106



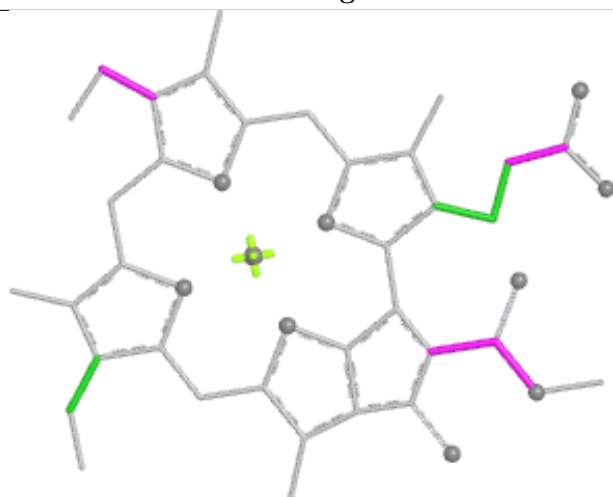
Ligand CLA g 517



Bond lengths



Bond angles

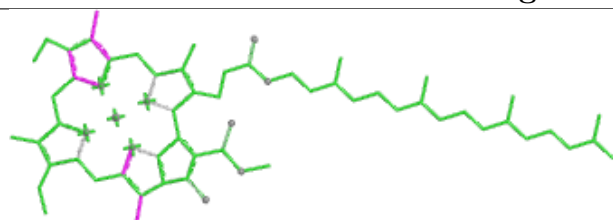


Torsions

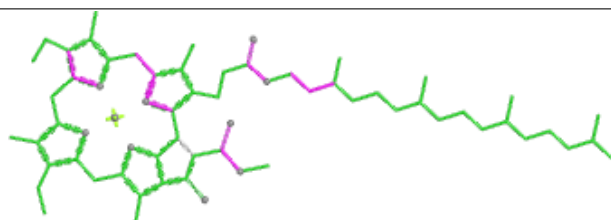


Rings

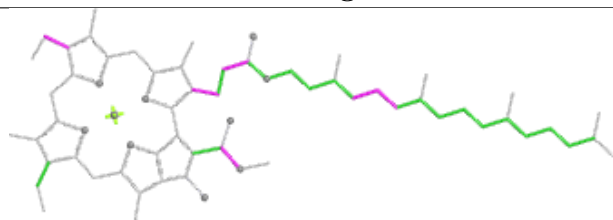
Ligand CLA e 509



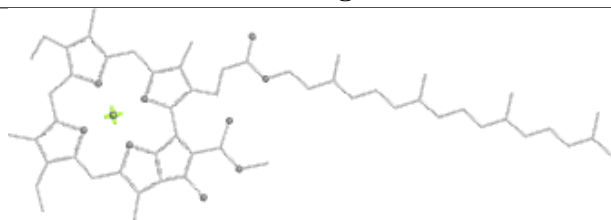
Bond lengths



Bond angles

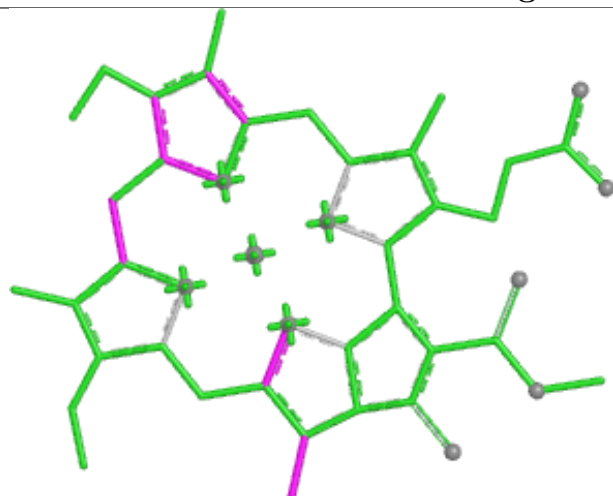


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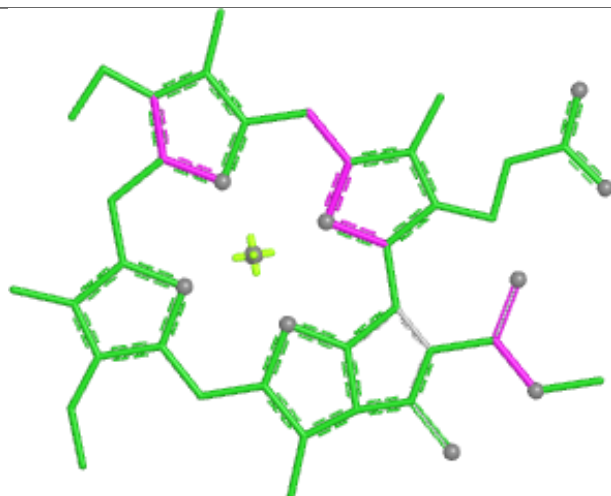


Rings

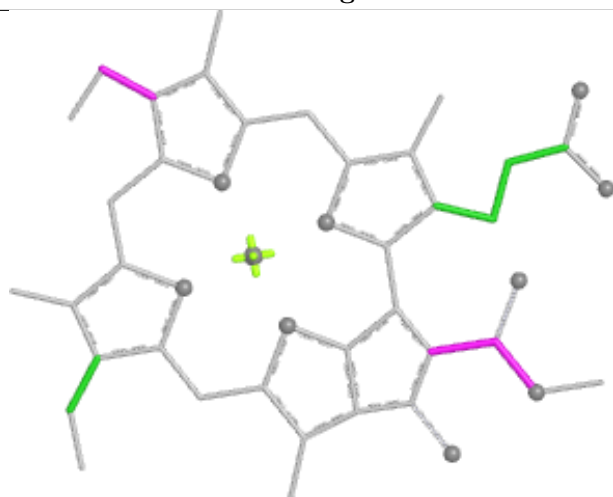
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Bond lengths



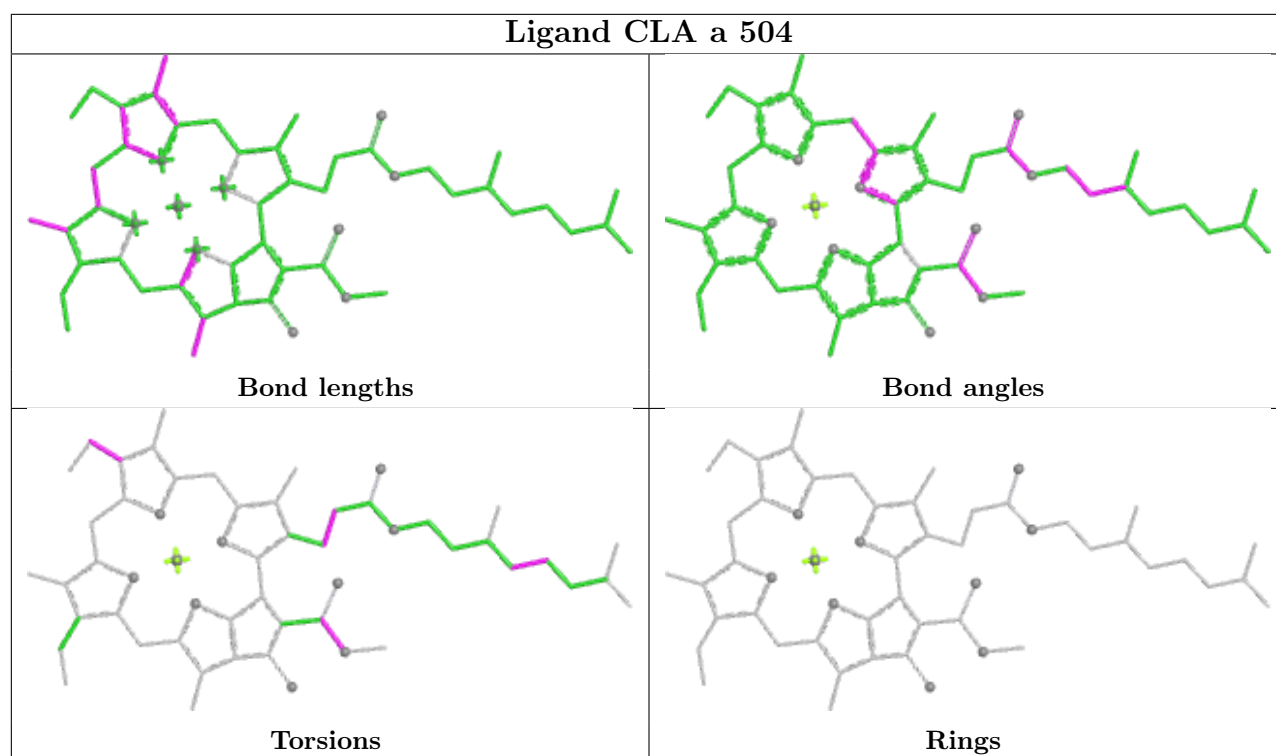
Bond angles



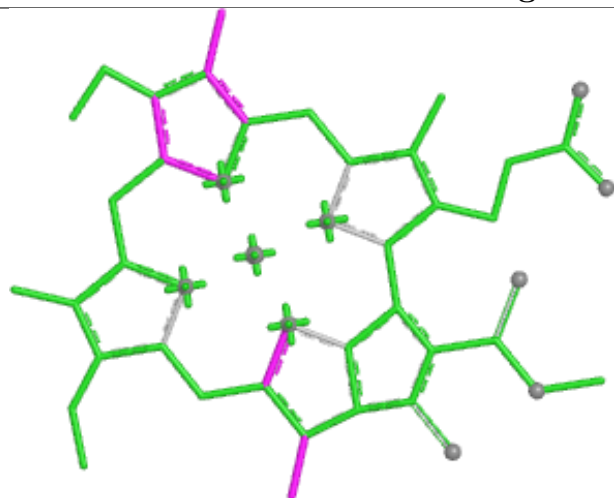
Torsions



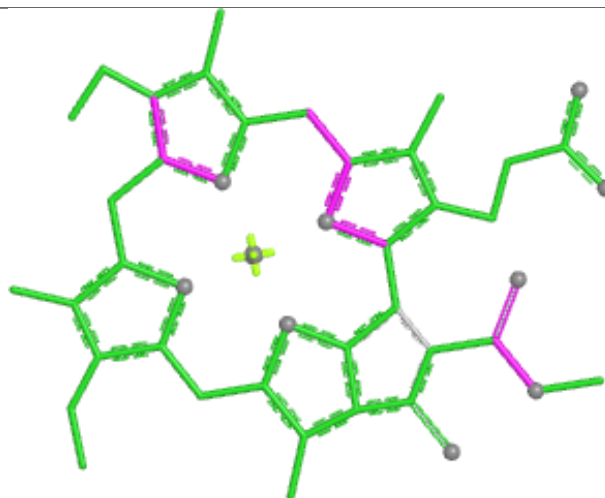
Rings



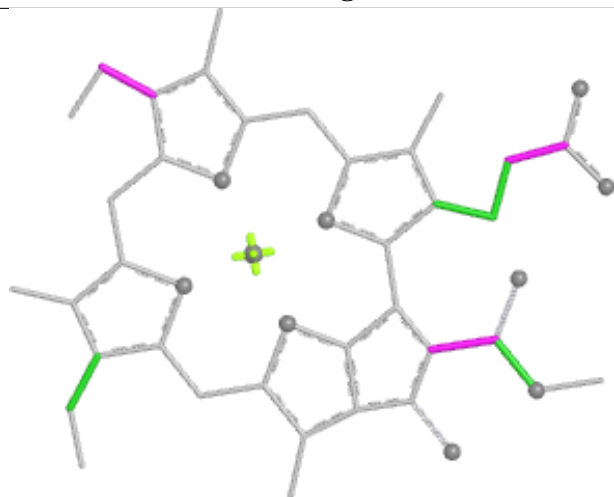
Ligand CLA 5 517



Bond lengths



Bond angles

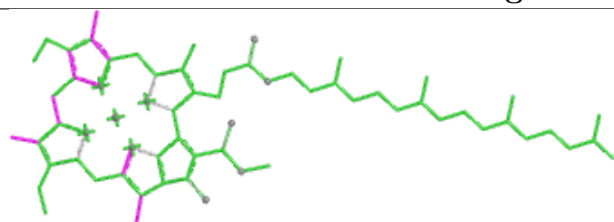


Torsions

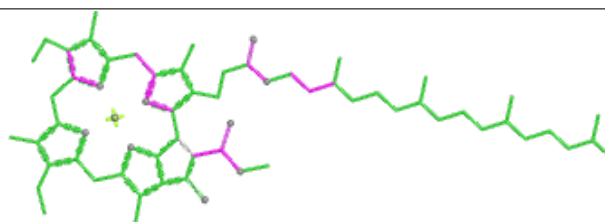


Rings

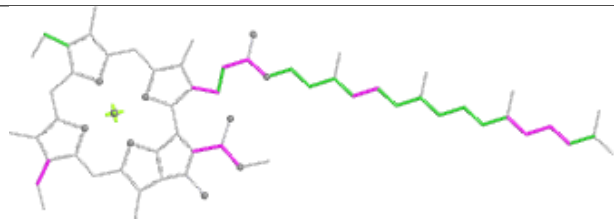
Ligand CLA B 1229



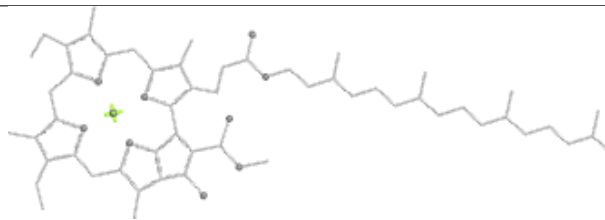
Bond lengths



Bond angles

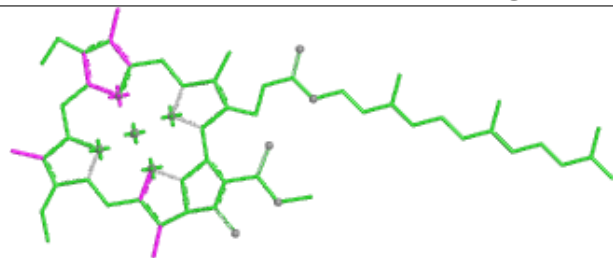


Torsions

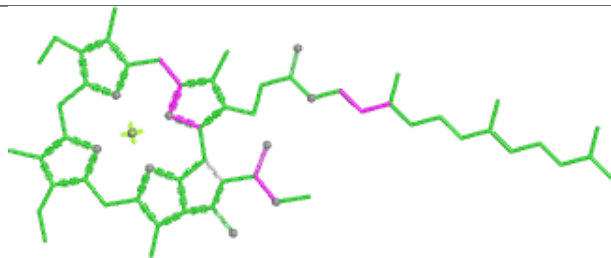


Rings

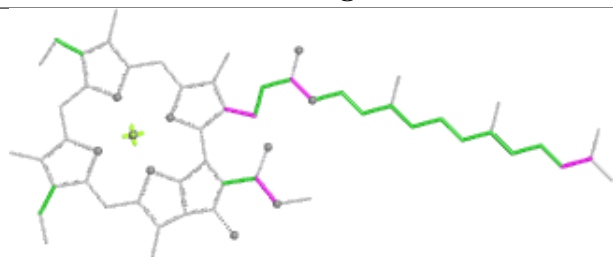
Ligand CLA B 1215



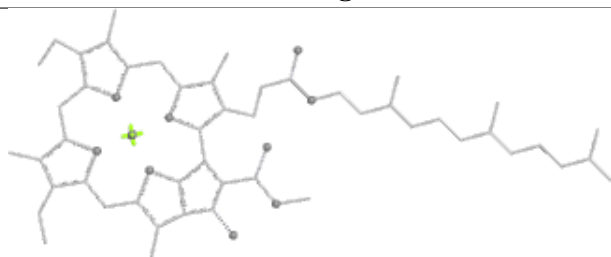
Bond lengths



Bond angles

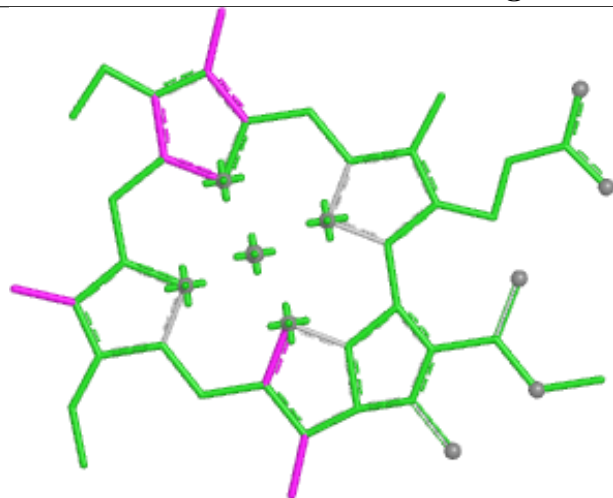


Torsions

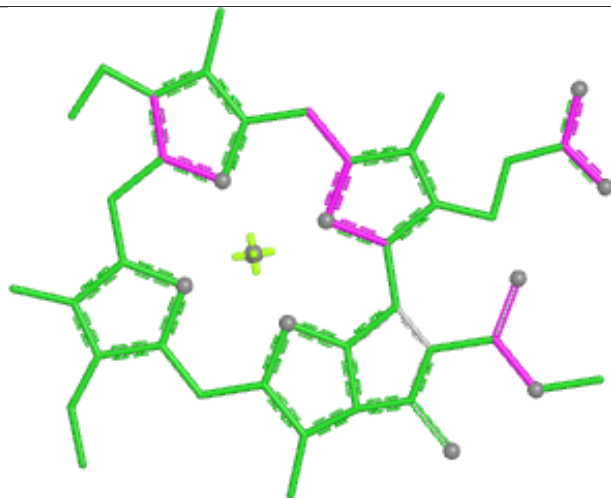


Rings

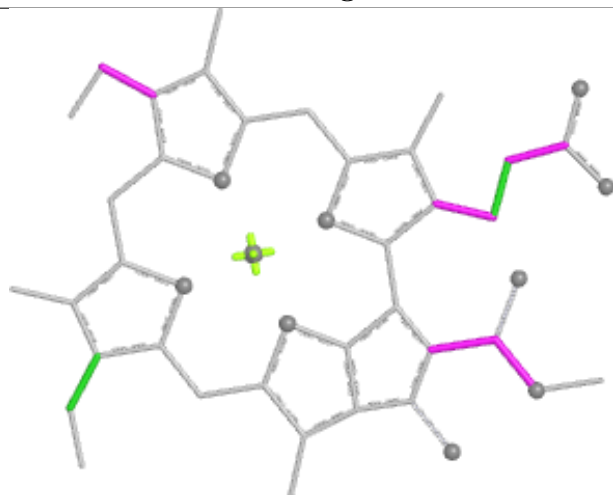
Ligand CLA B 1232



Bond lengths



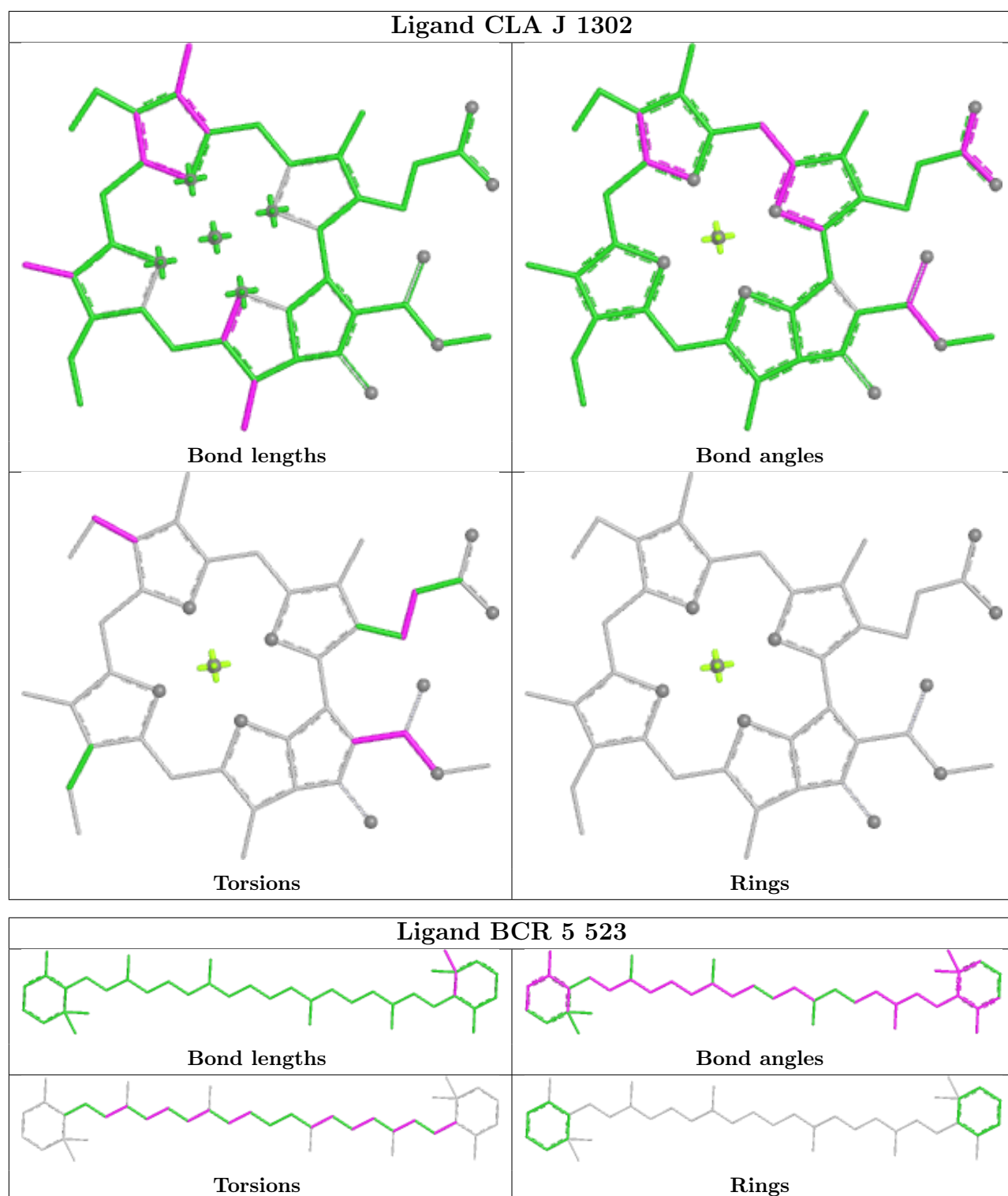
Bond angles

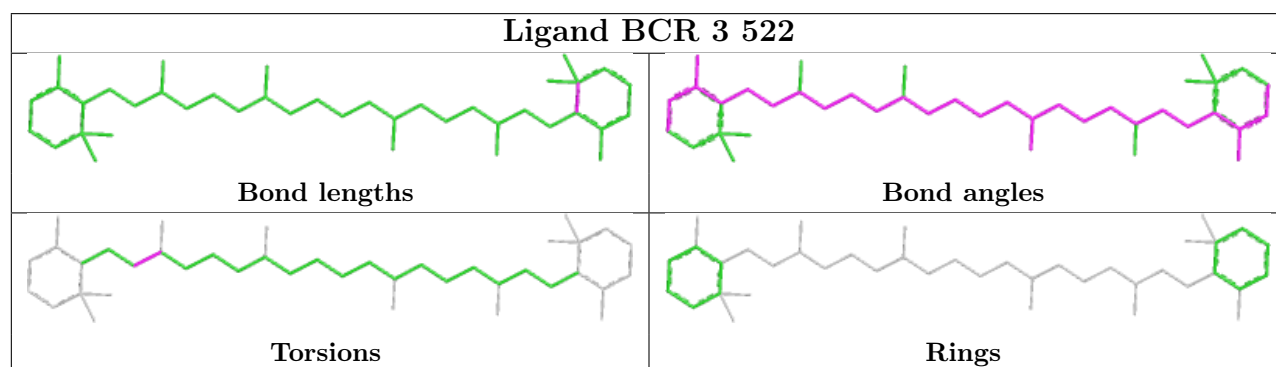
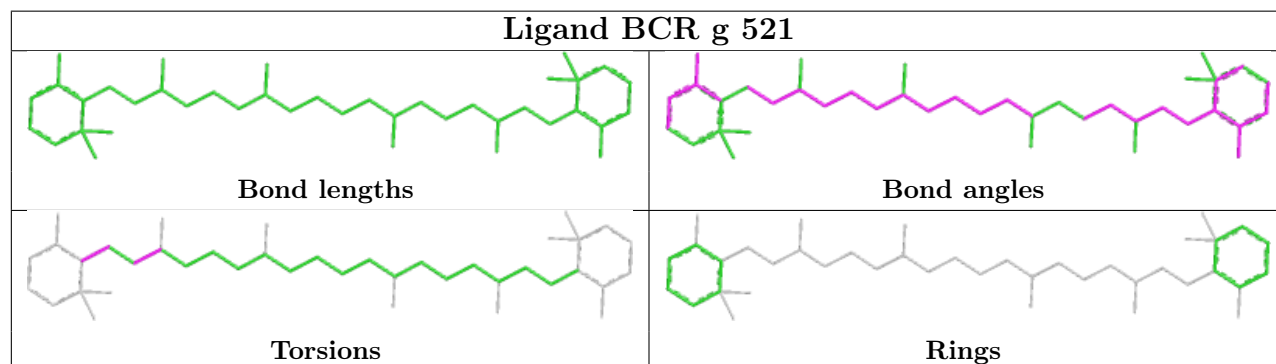
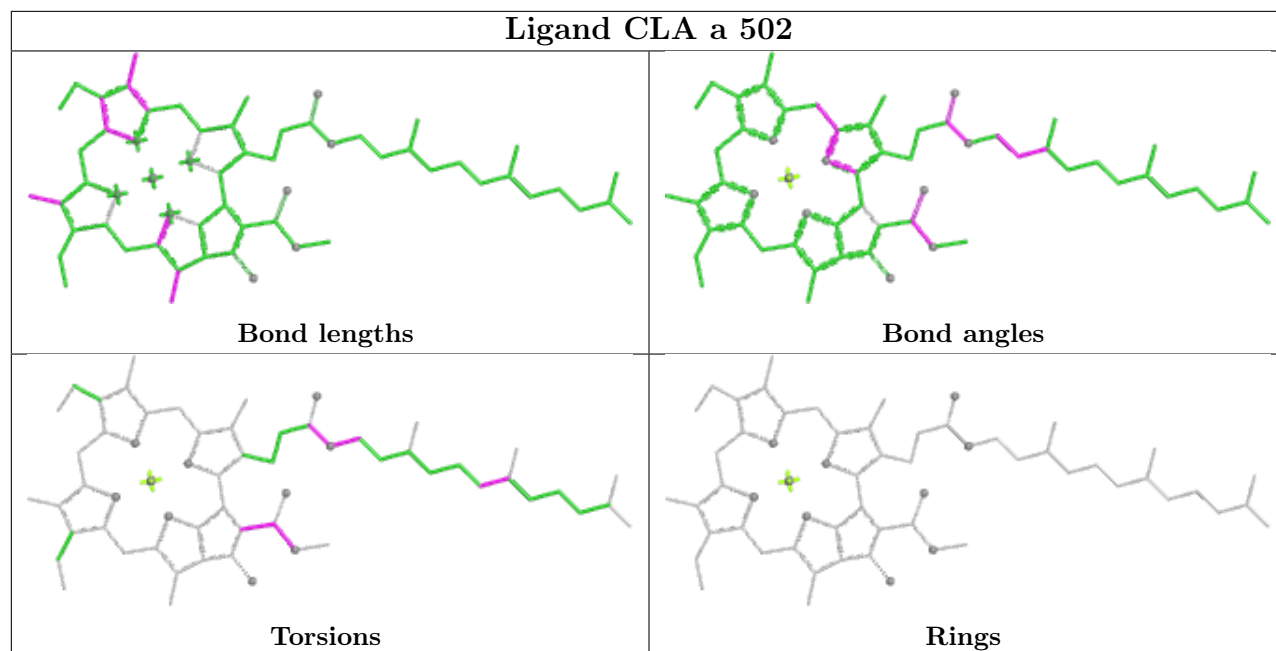


Torsions

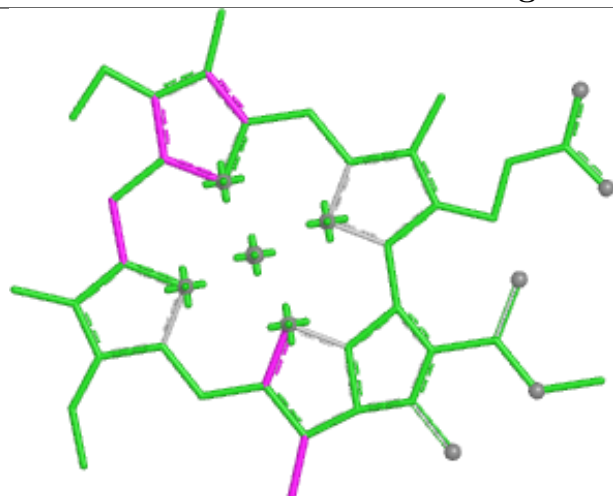


Rings

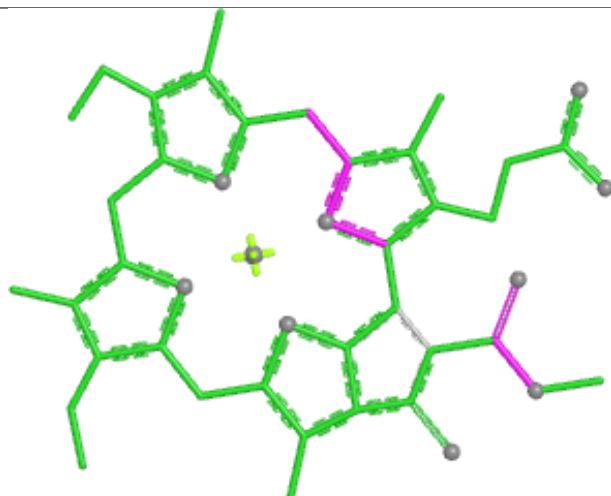




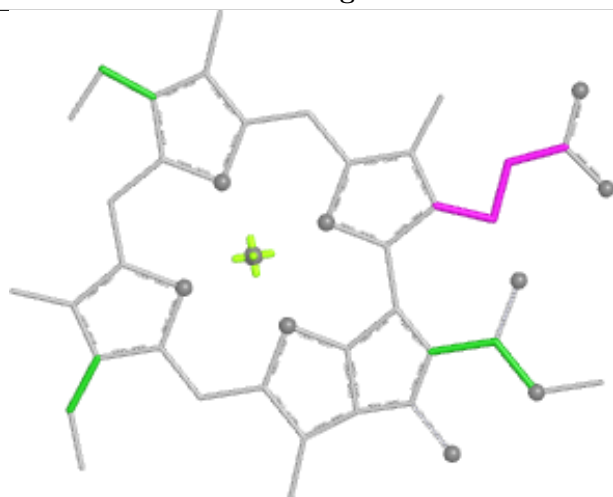
Ligand CLA a 518



Bond lengths



Bond angles

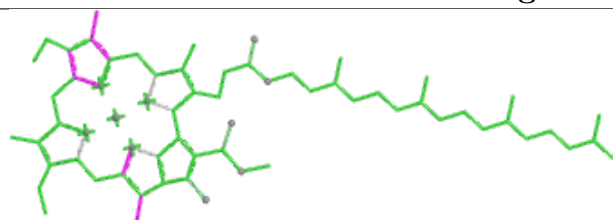


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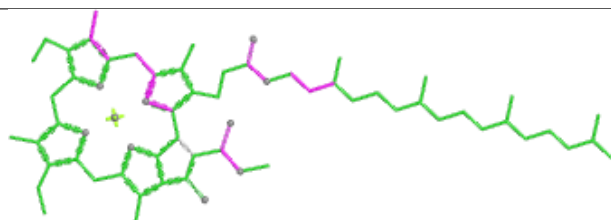


Rings

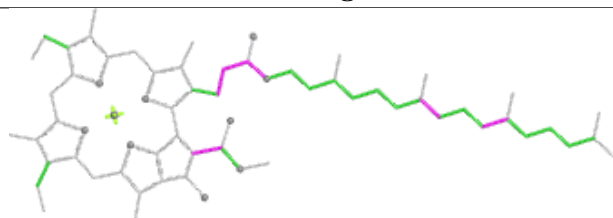
Ligand CLA 3 501



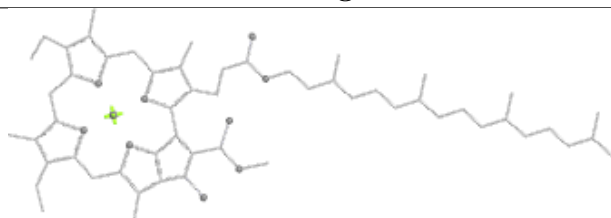
Bond lengths



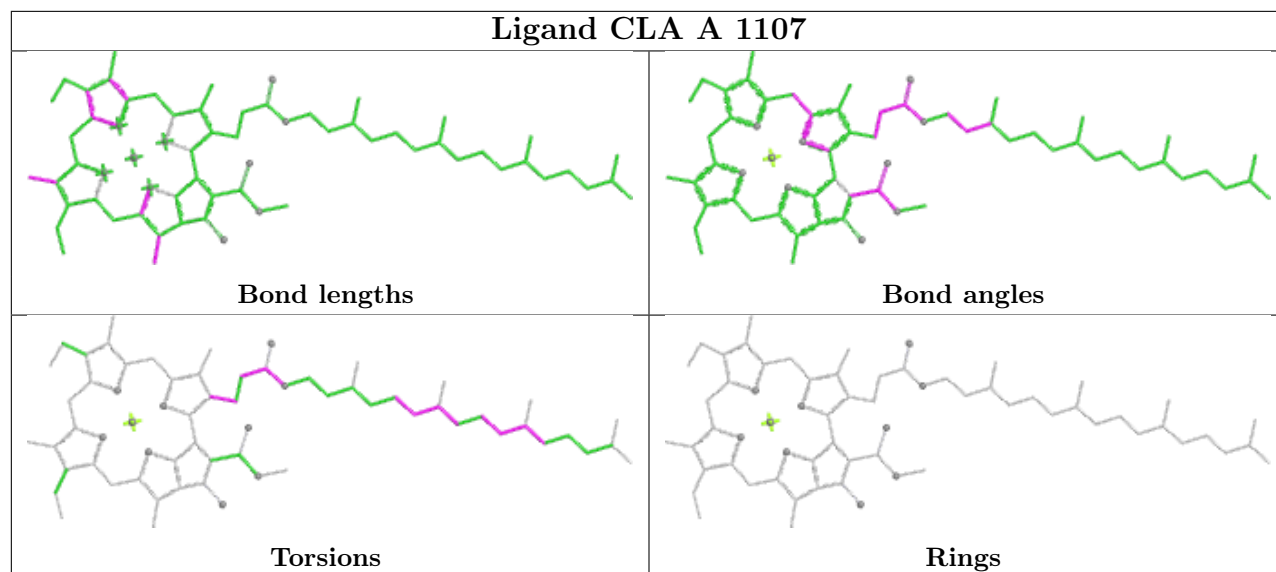
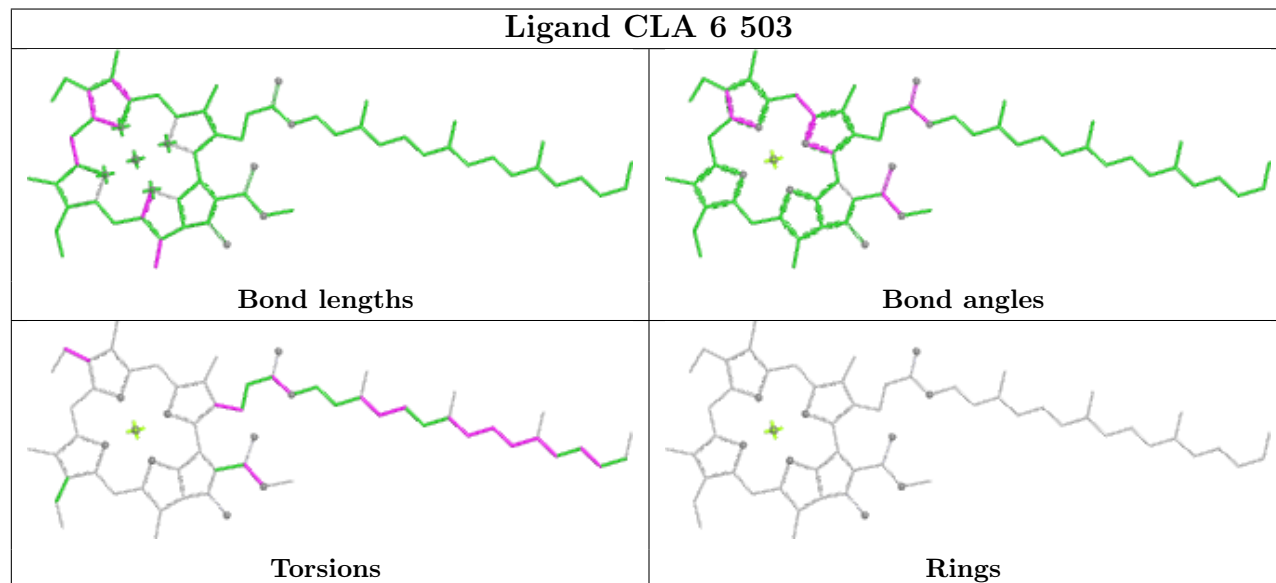
Bond angles

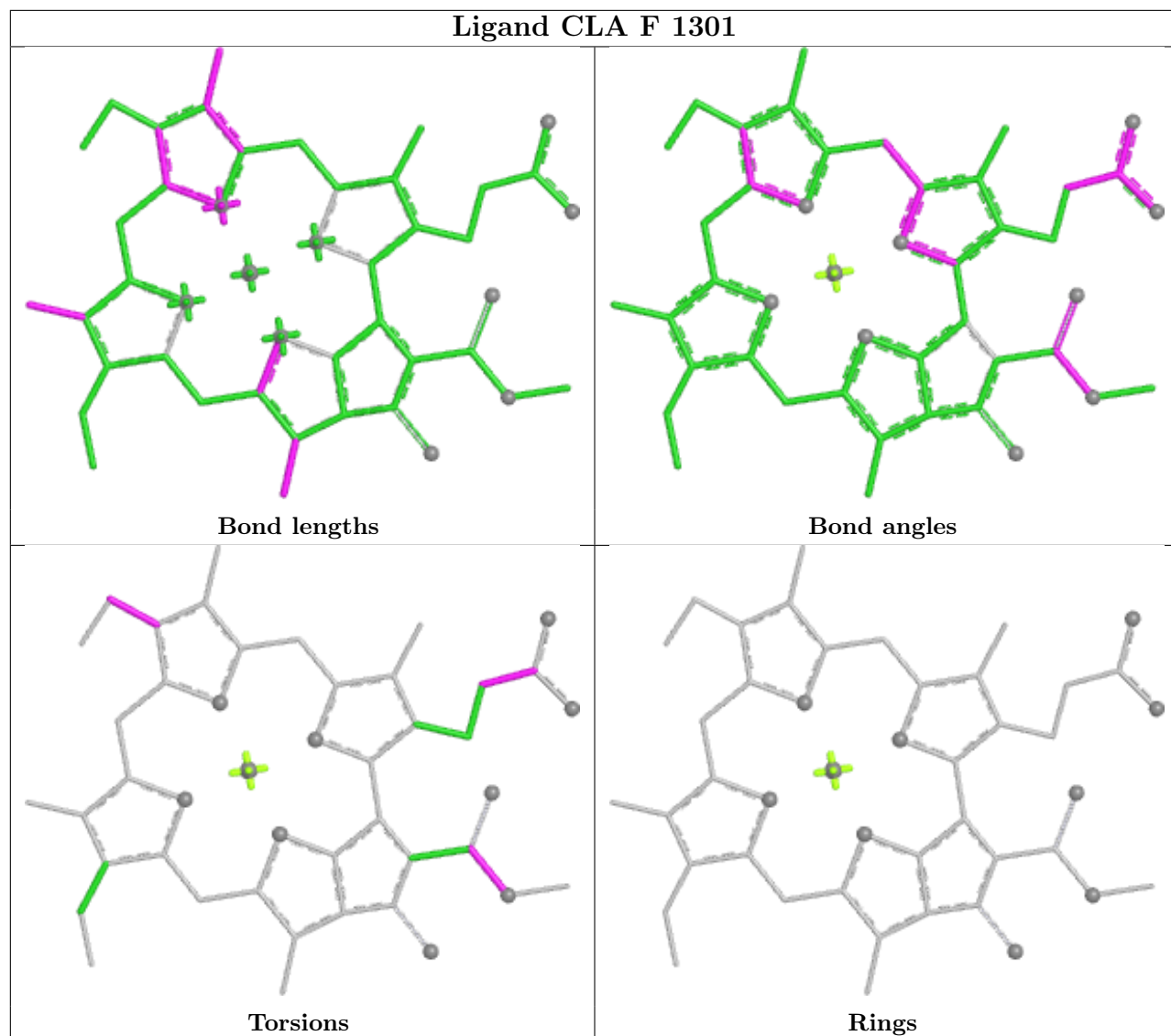


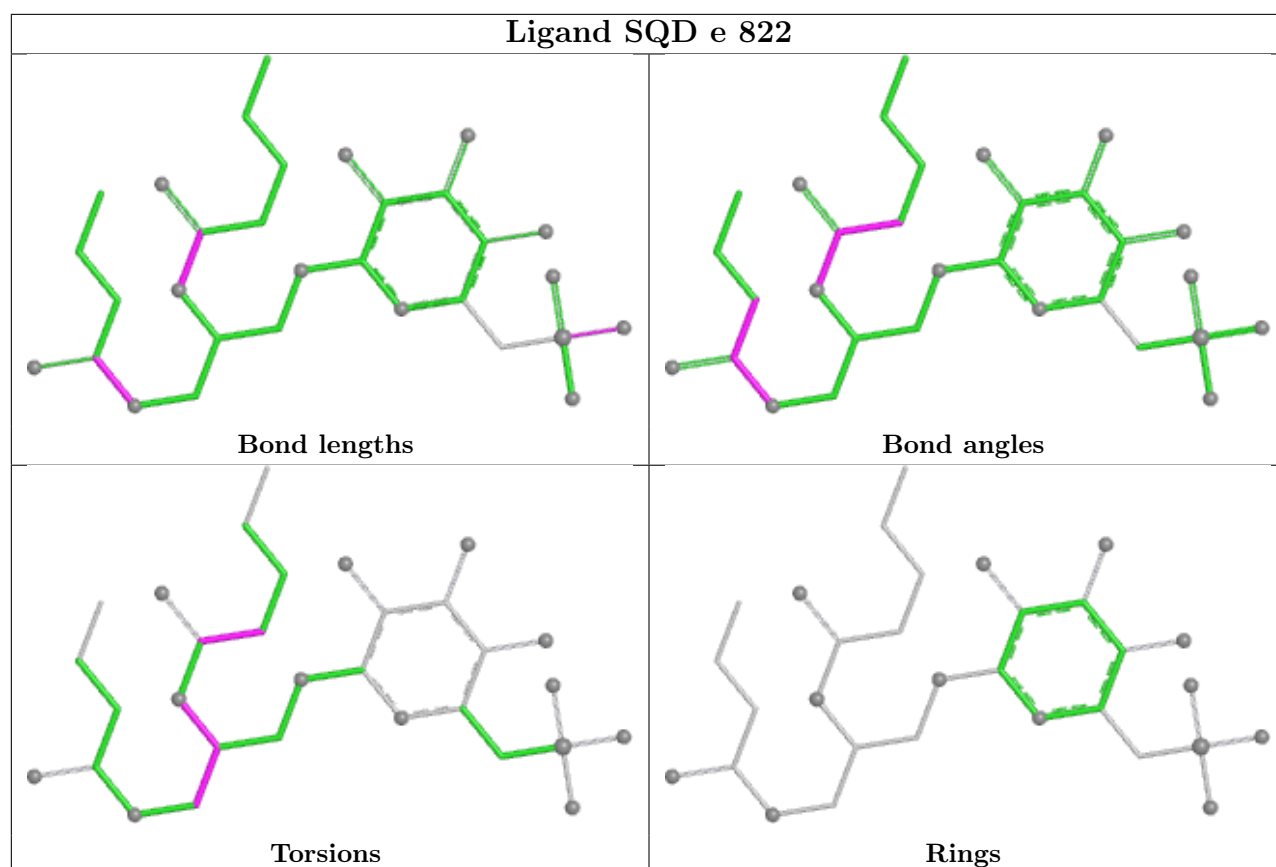
Torsions



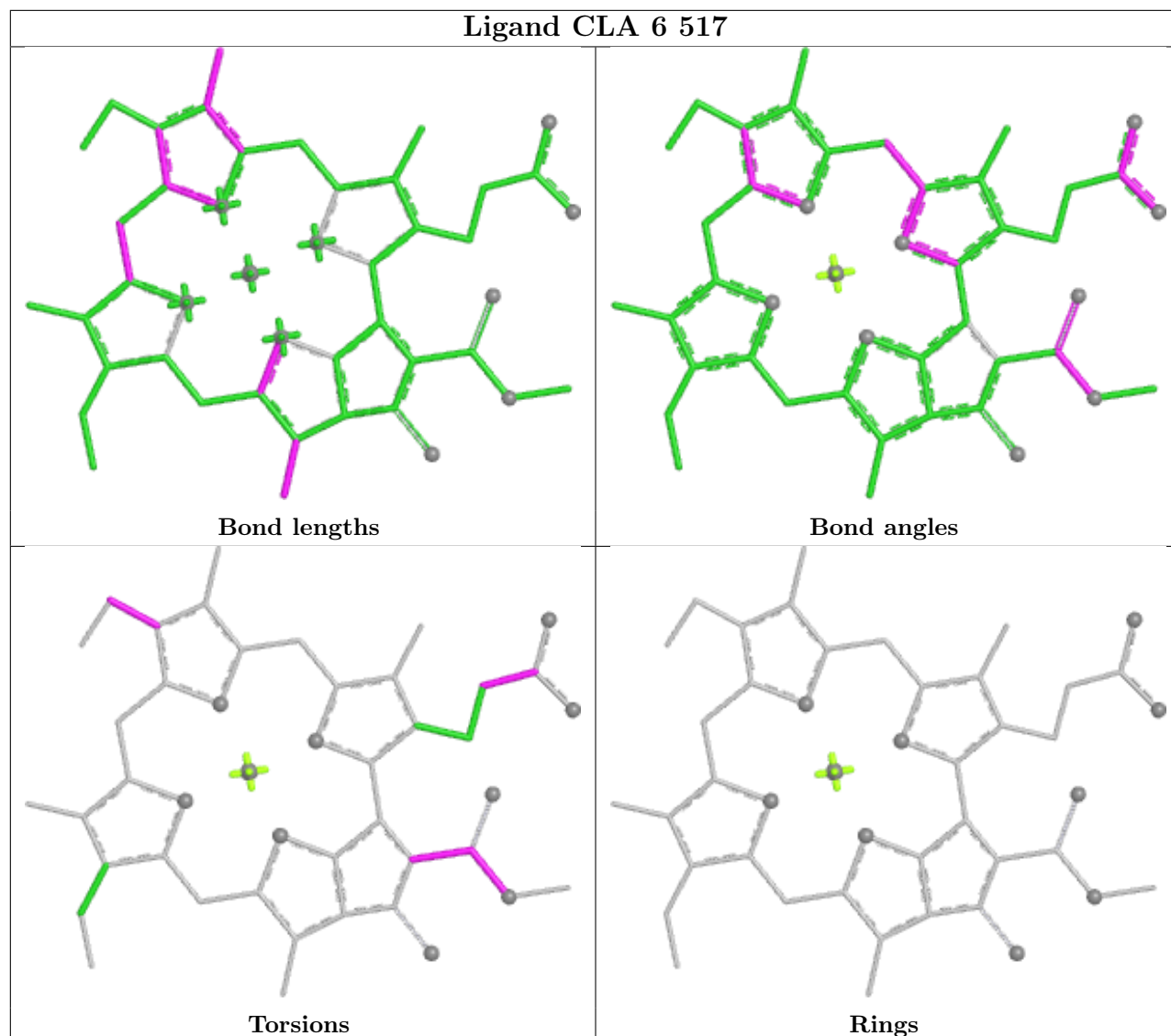
Rings

Ligand CLA A 1107**Ligand CLA 6 503**

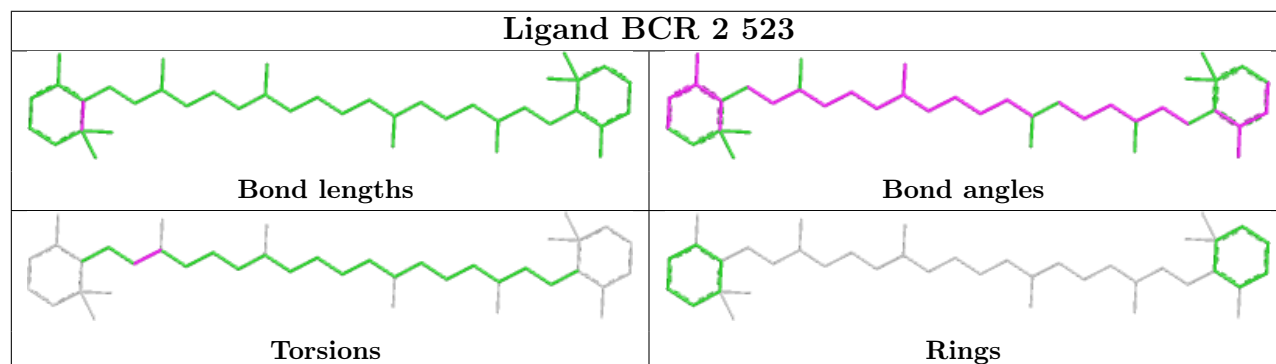


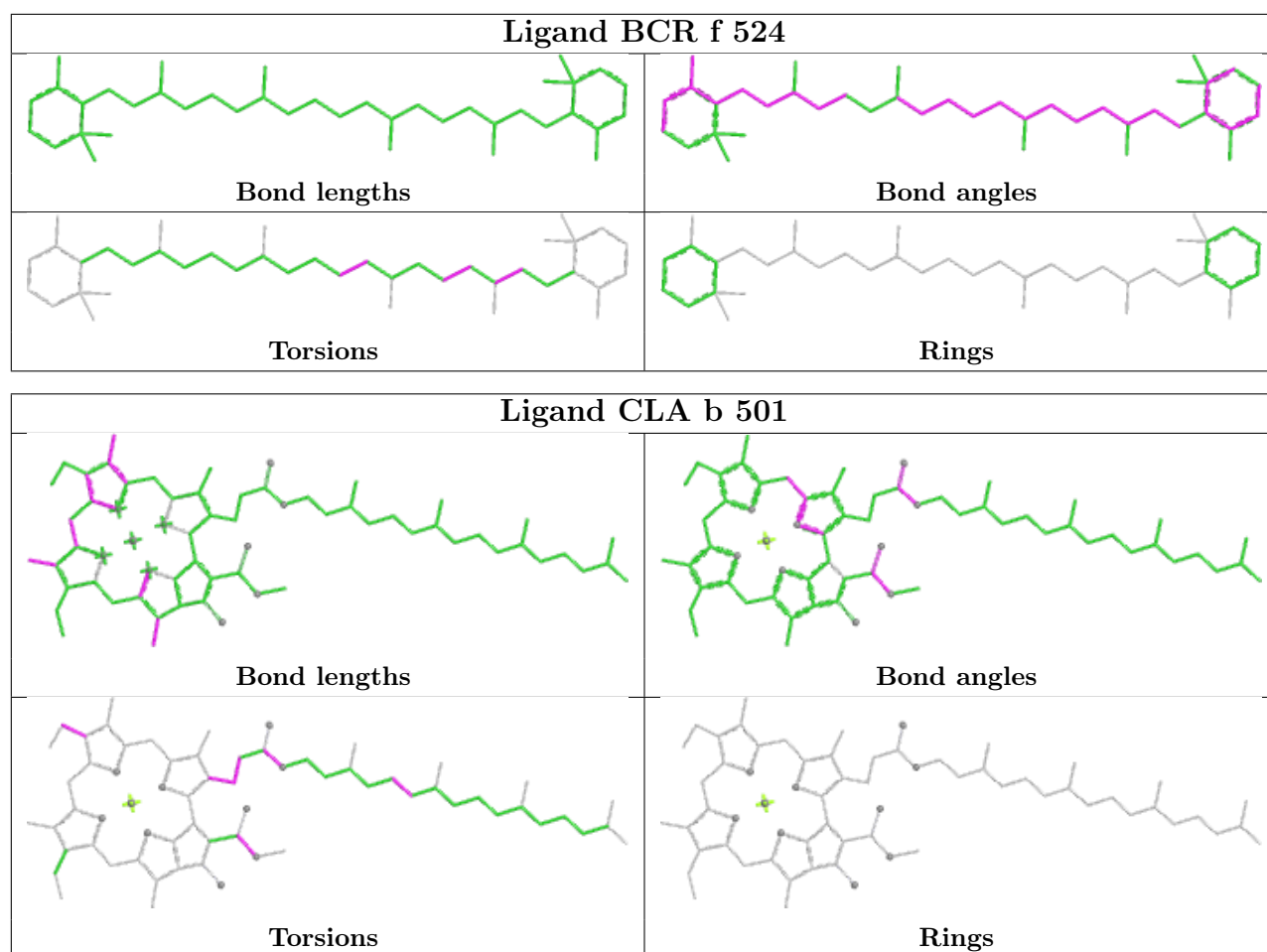


Ligand CLA 6 517

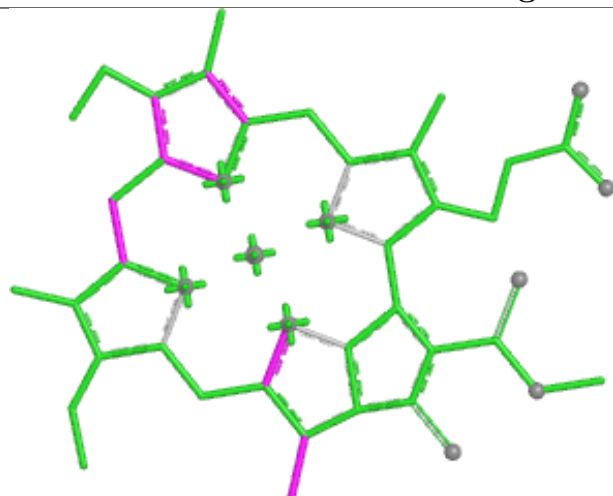


Ligand BCR 2 523

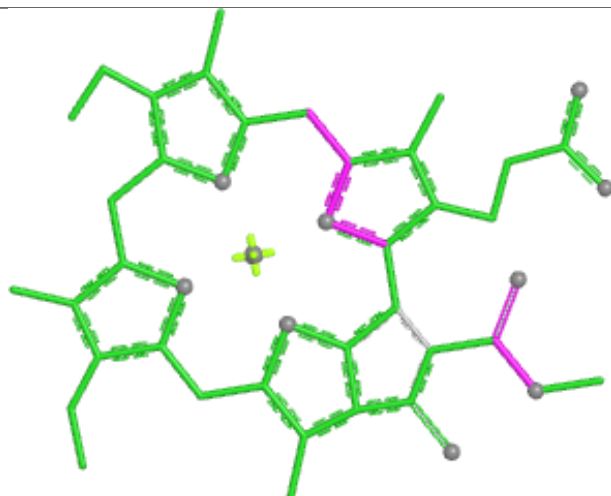




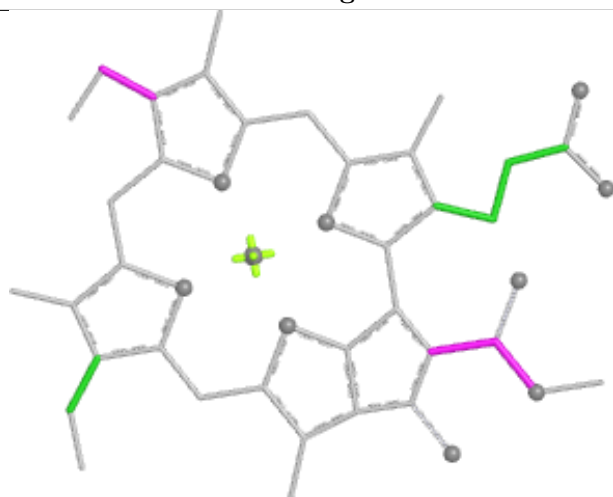
Ligand CLA 1 516



Bond lengths



Bond angles

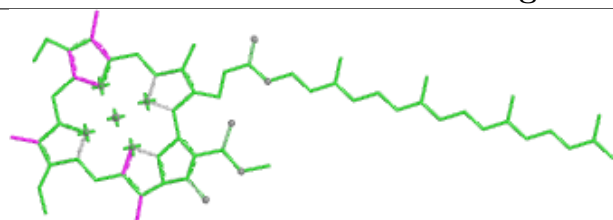


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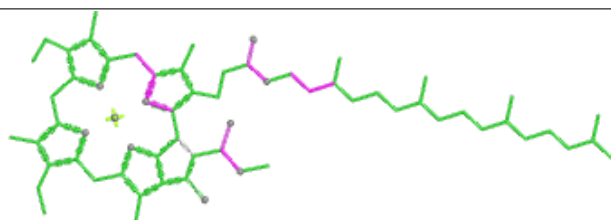


Rings

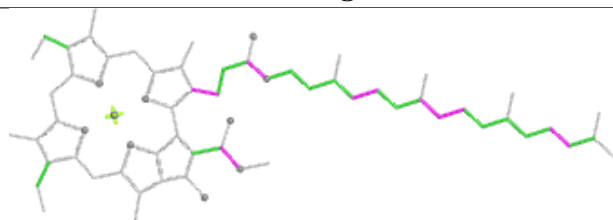
Ligand CLA c 509



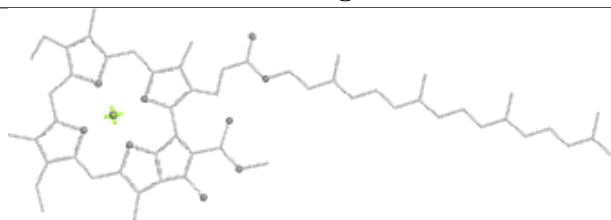
Bond lengths



Bond angles

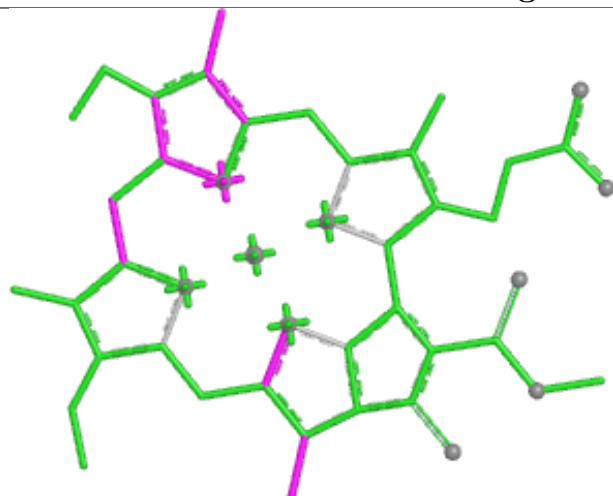


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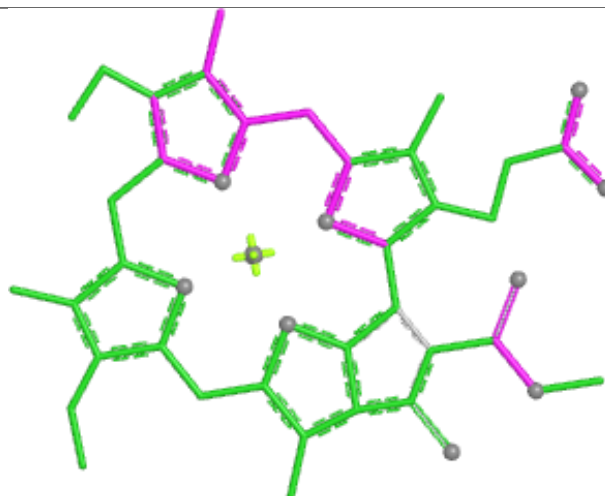


Rings

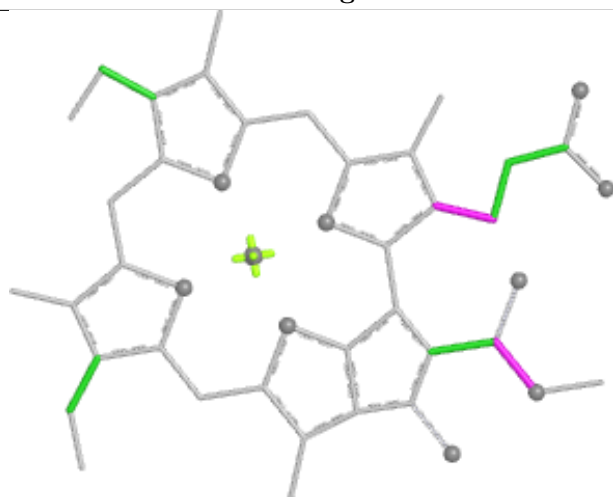
Ligand CLA 4 511



Bond lengths



Bond angles

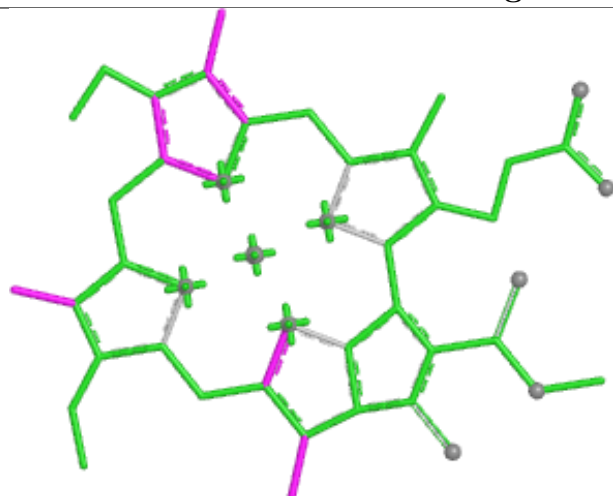


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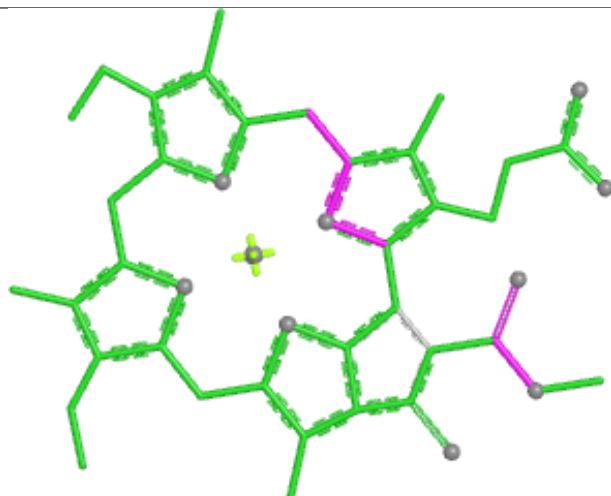


Rings

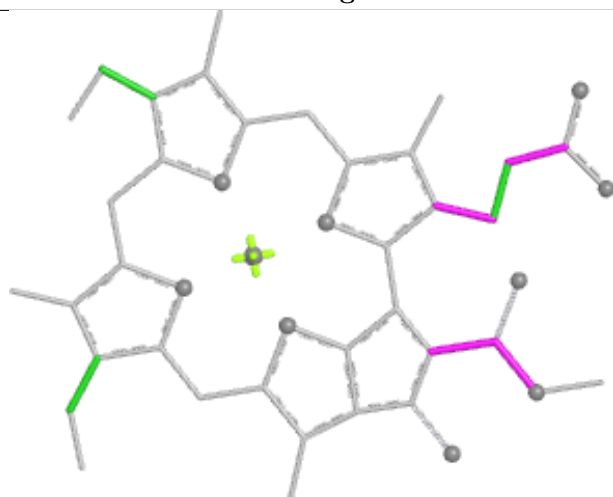
Ligand CLA A 1801



Bond lengths



Bond angles

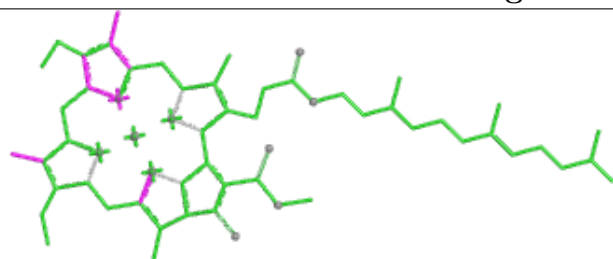


Torsions

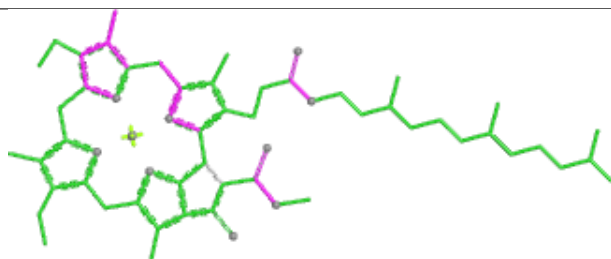


Rings

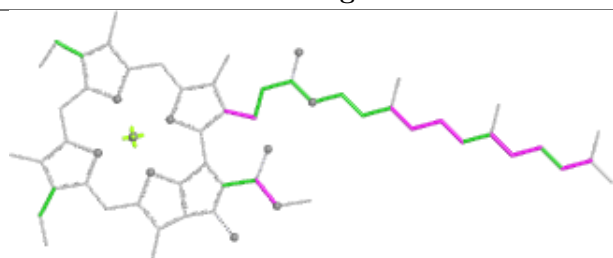
Ligand CLA B 1221



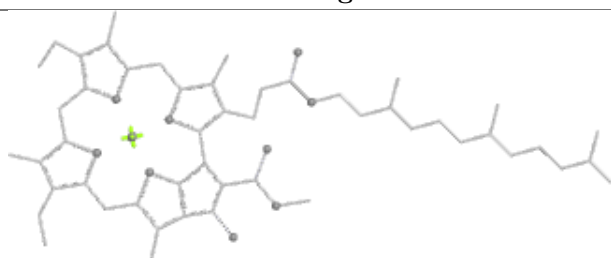
Bond lengths



Bond angles

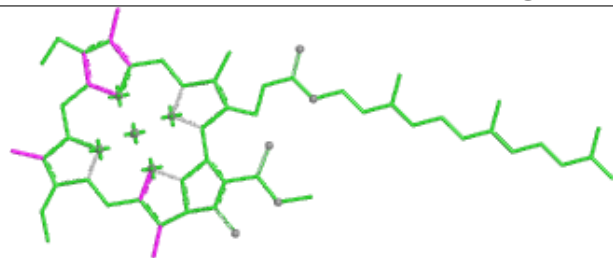


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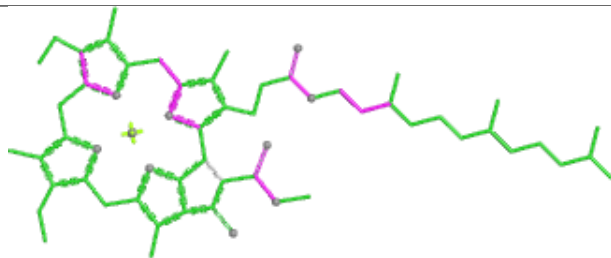


Rings

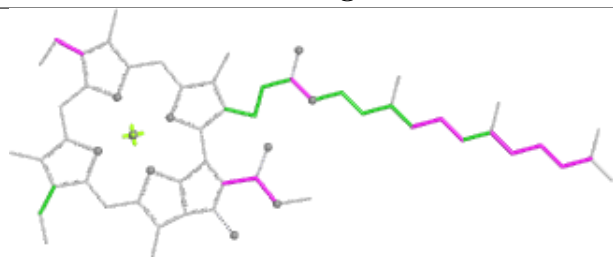
Ligand CLA c 502



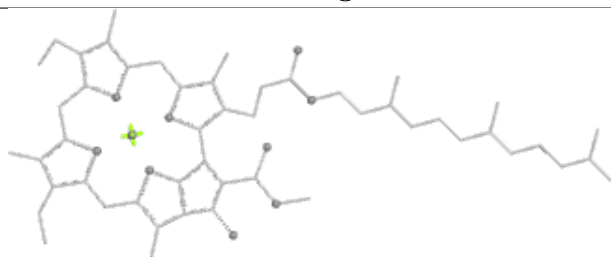
Bond lengths



Bond angles

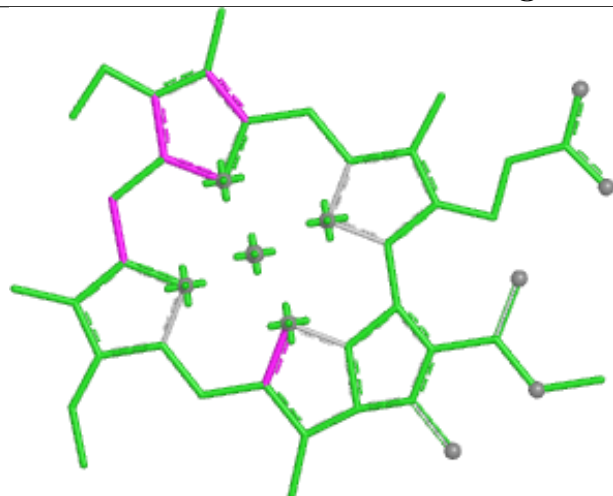


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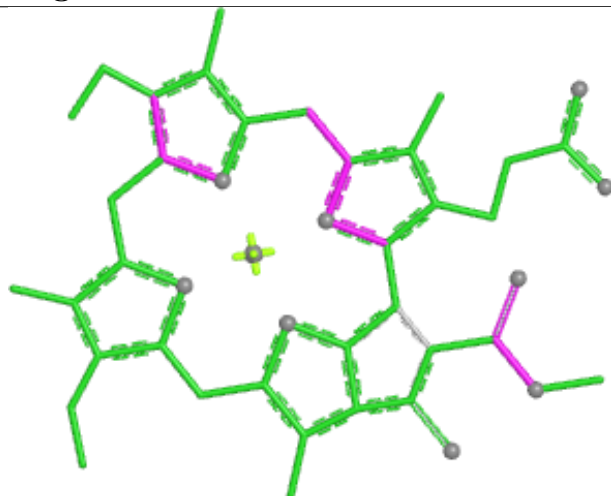


Rings

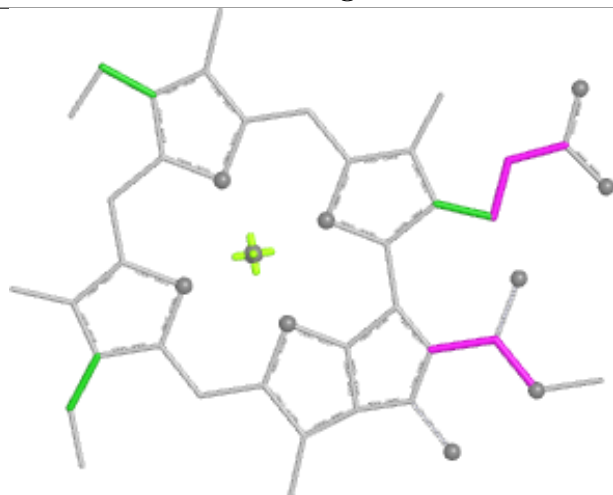
Ligand CLA g 519



Bond lengths



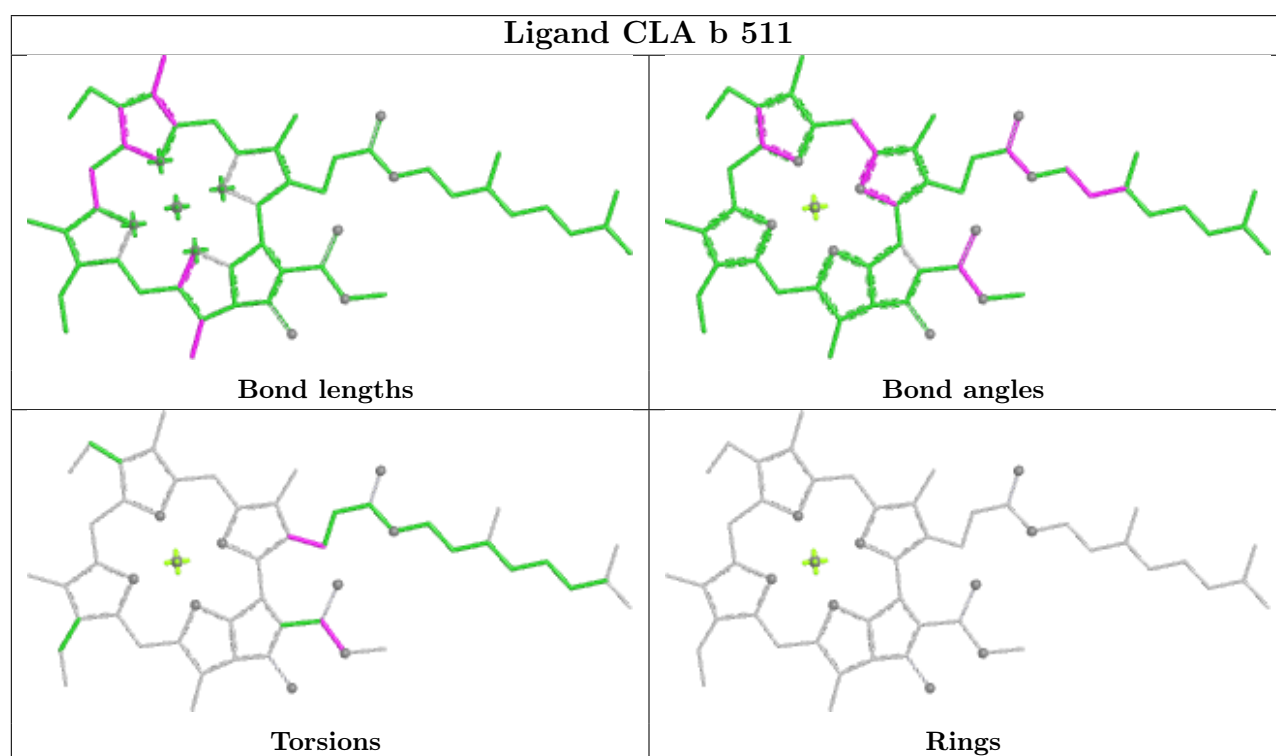
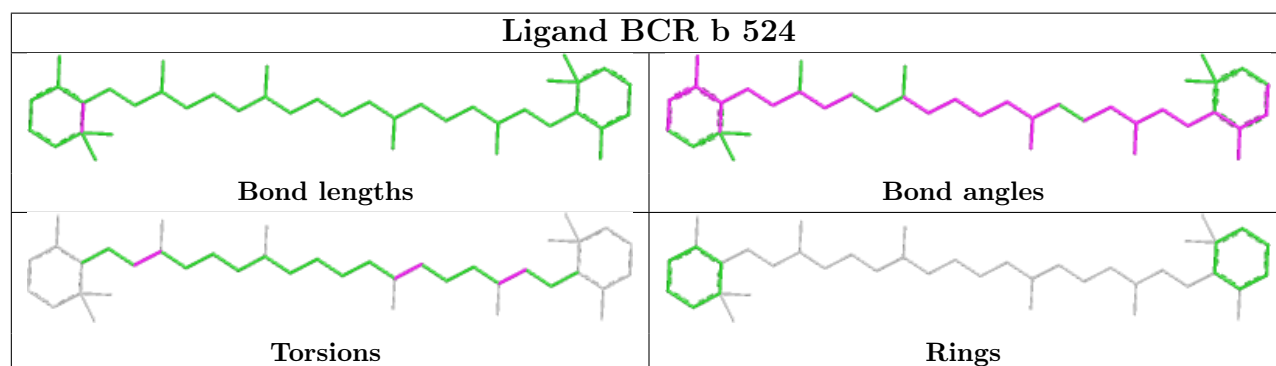
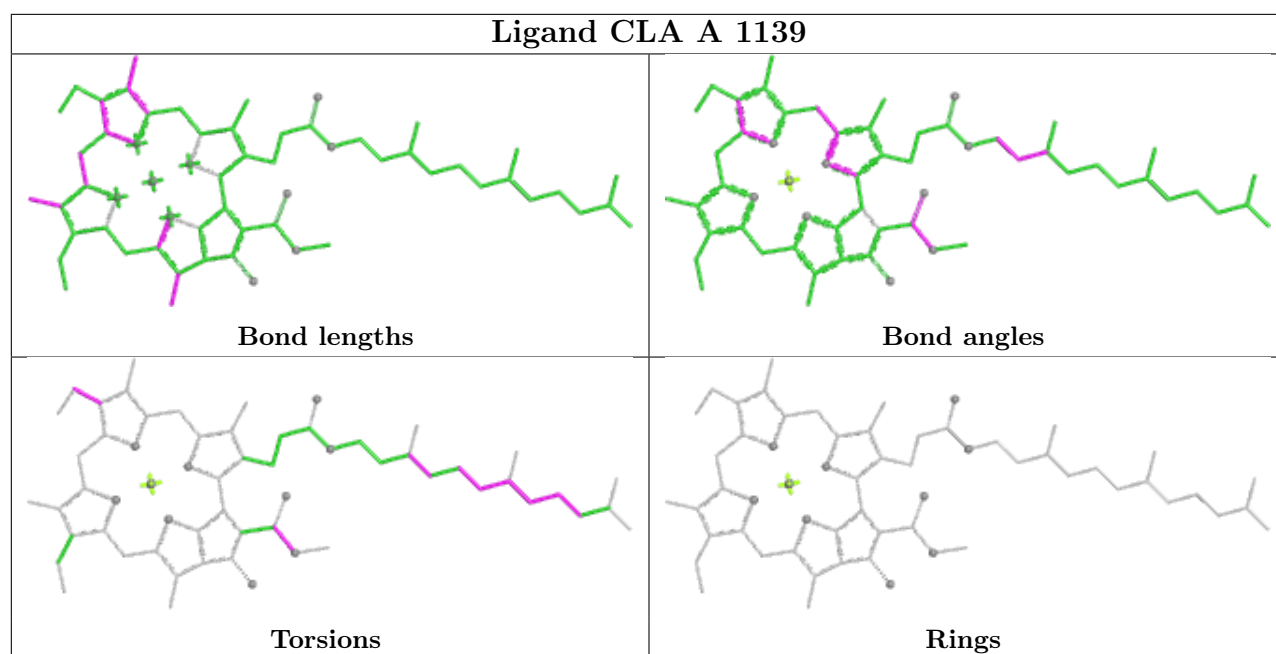
Bond angles

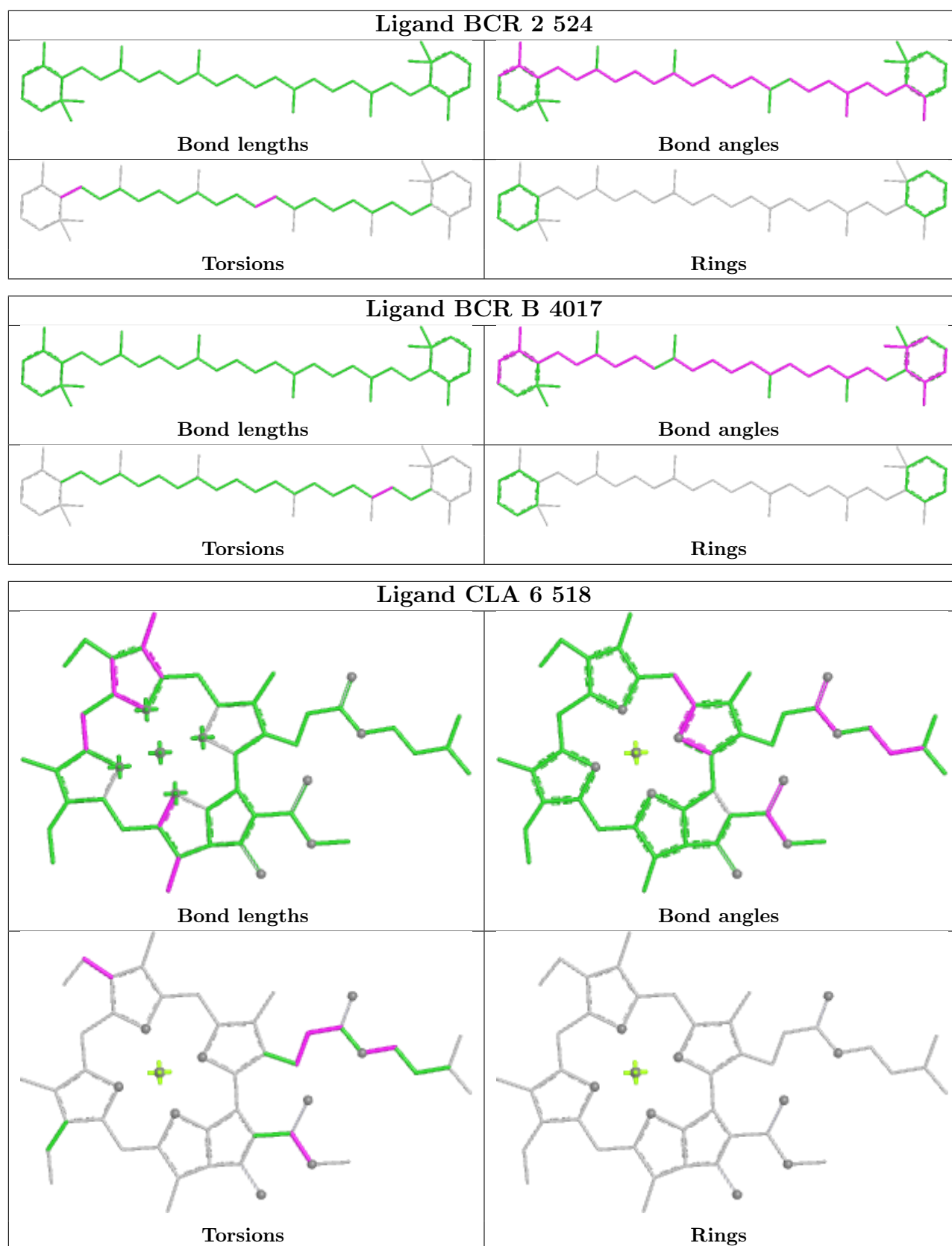


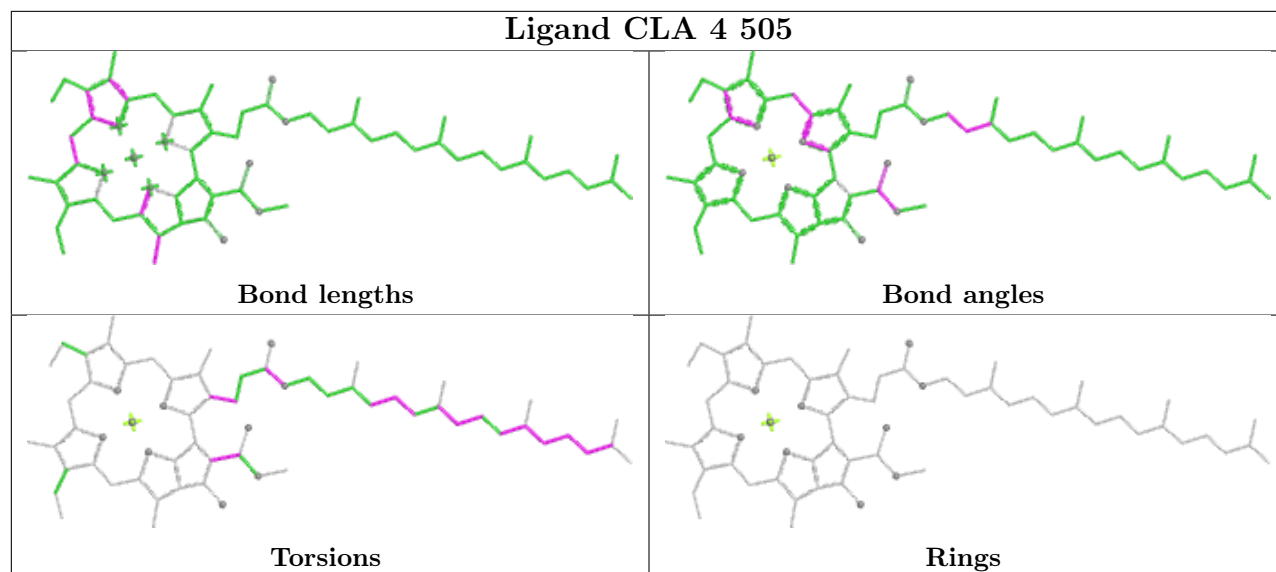
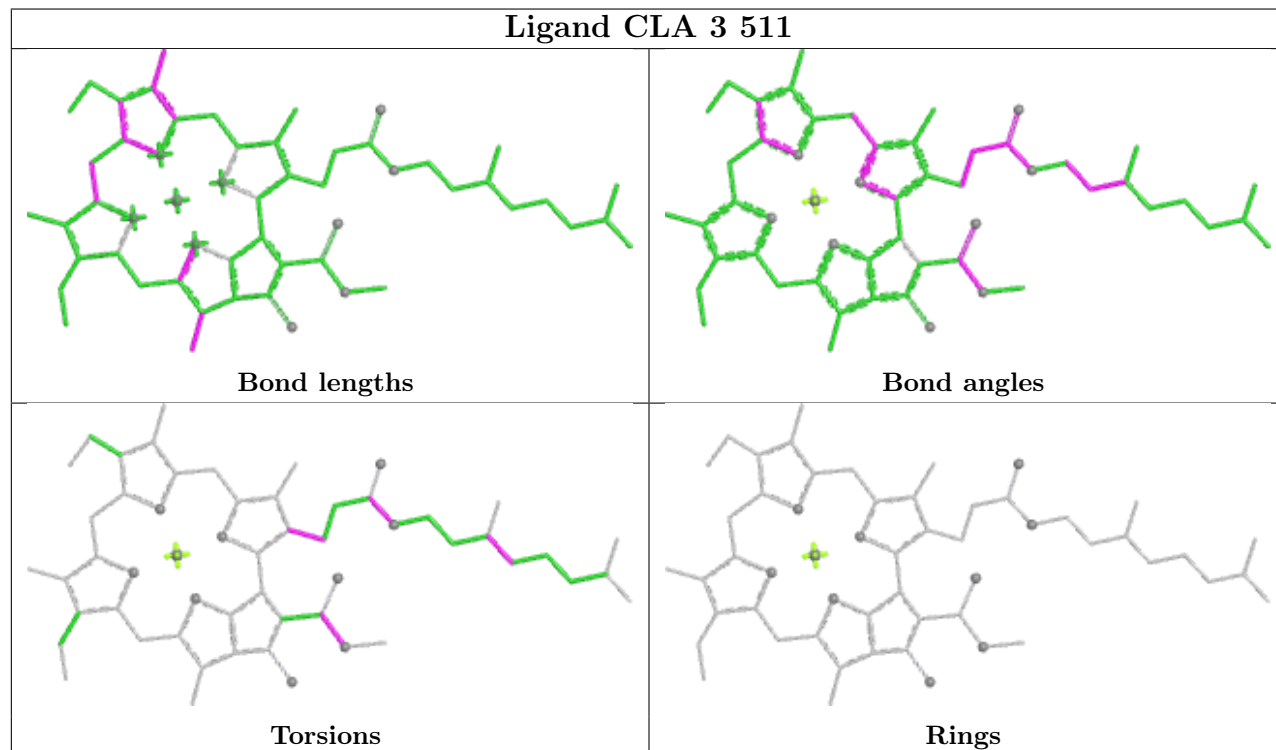
Torsions



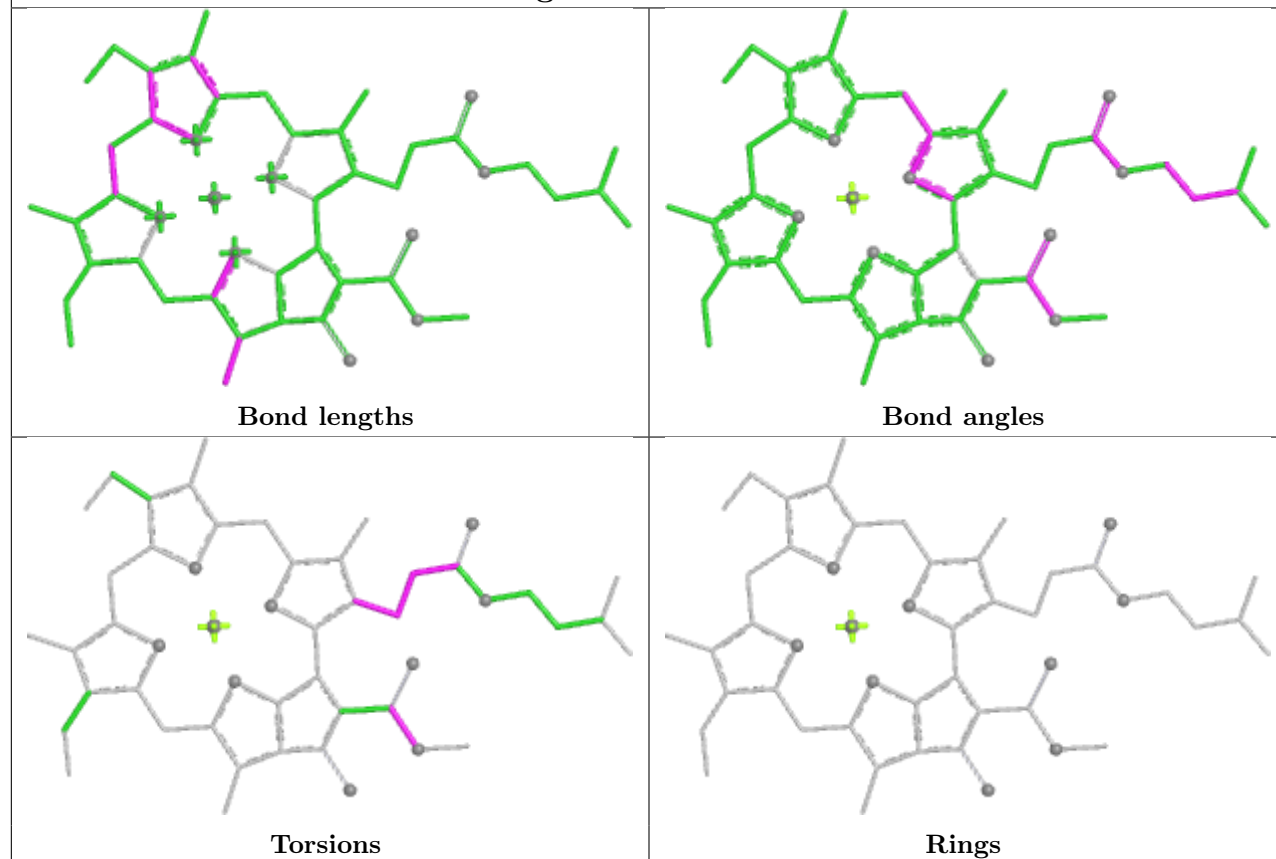
Rings



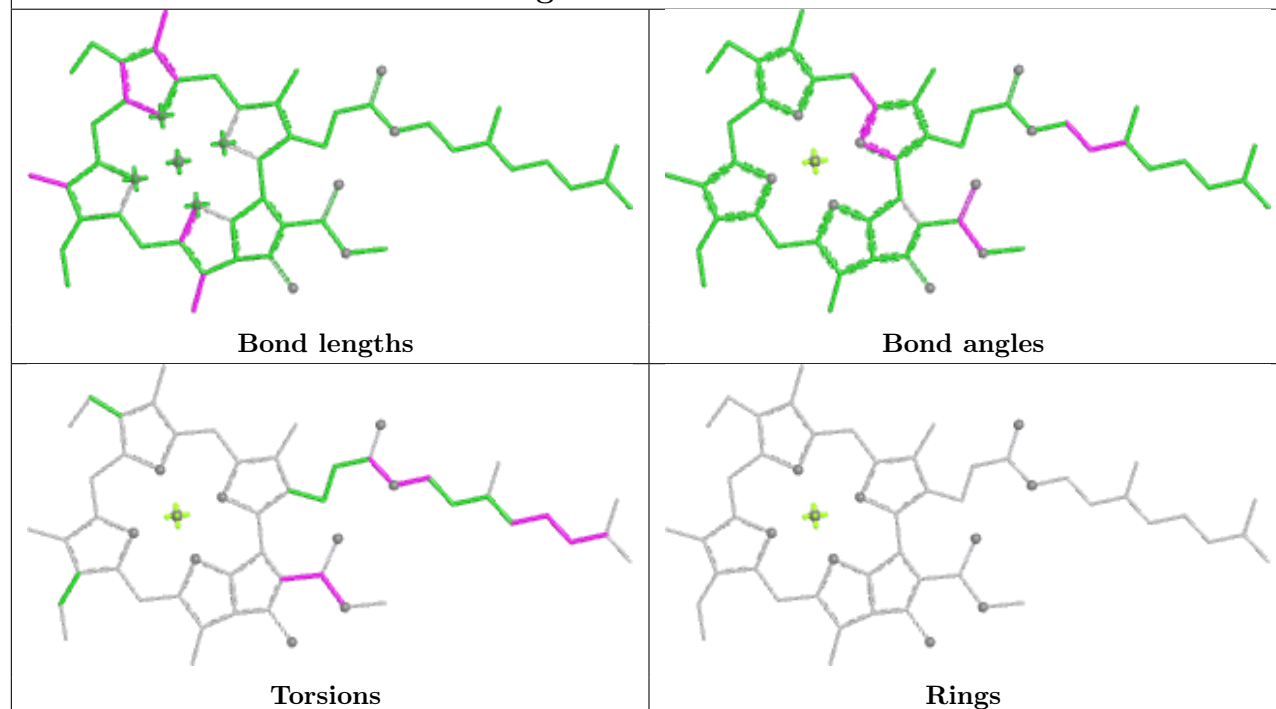


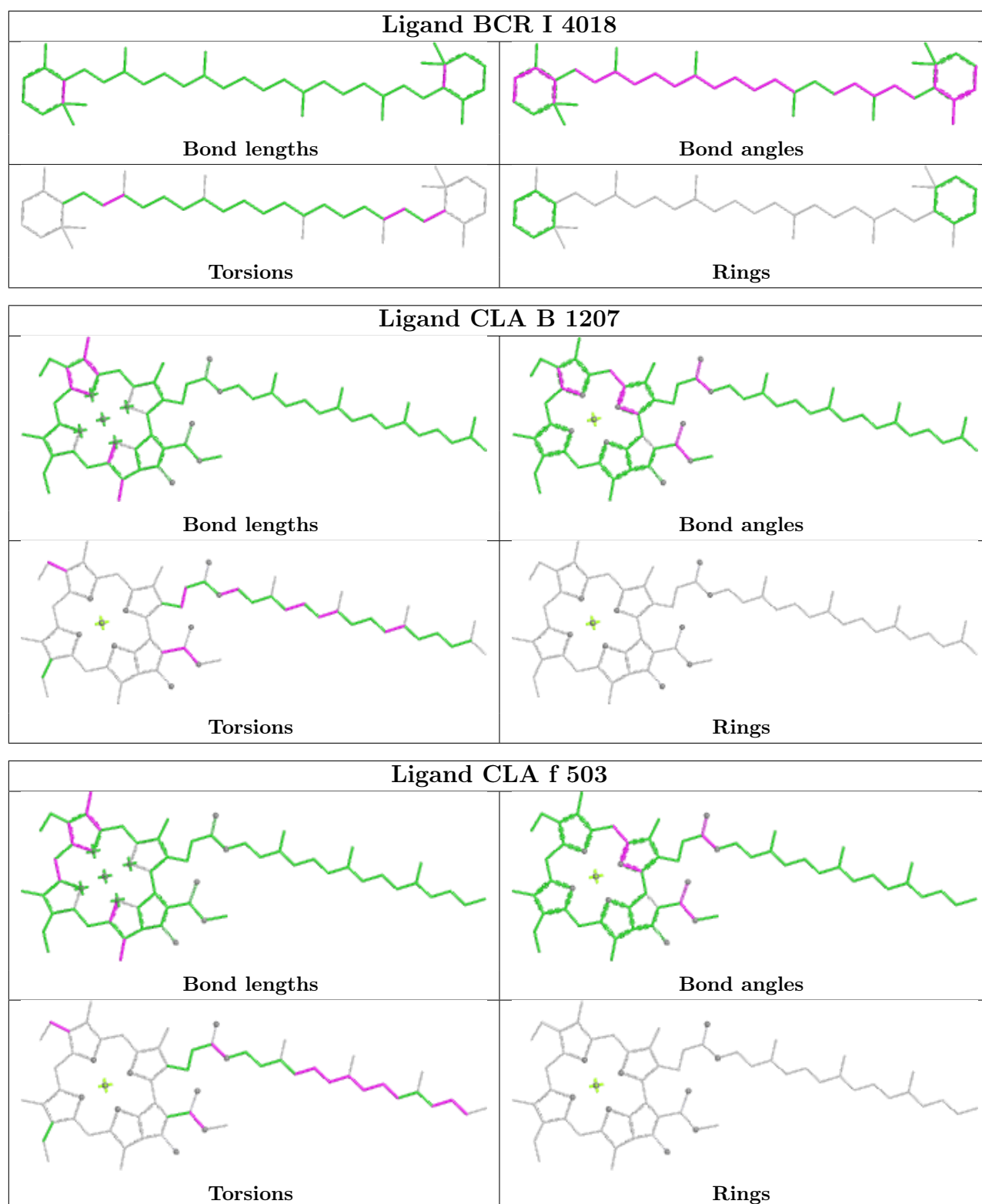
Ligand CLA 4 505**Ligand CLA 3 511**

Ligand CLA 6 513

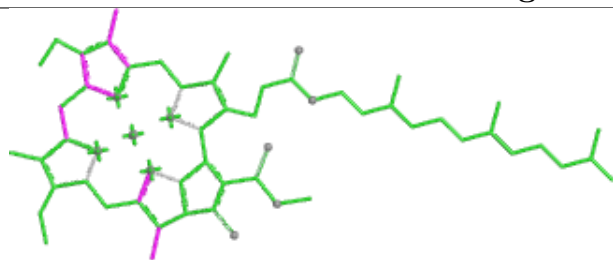


Ligand CLA 5 504

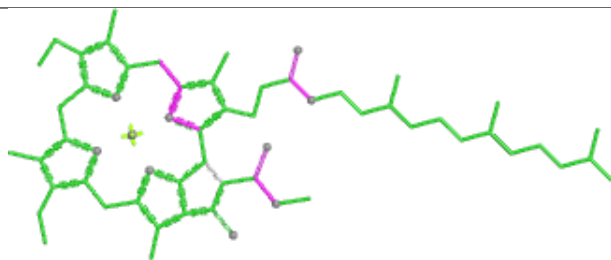




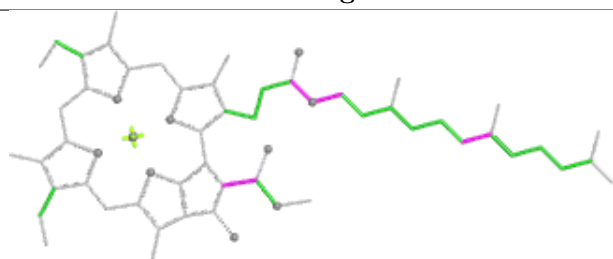
Ligand CLA a 507



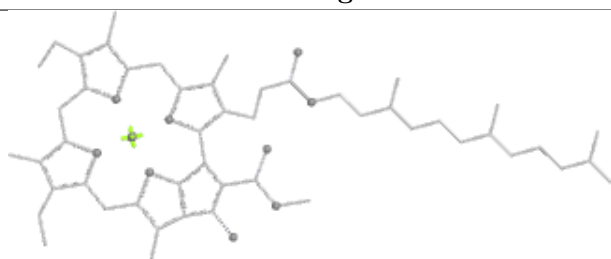
Bond lengths



Bond angles

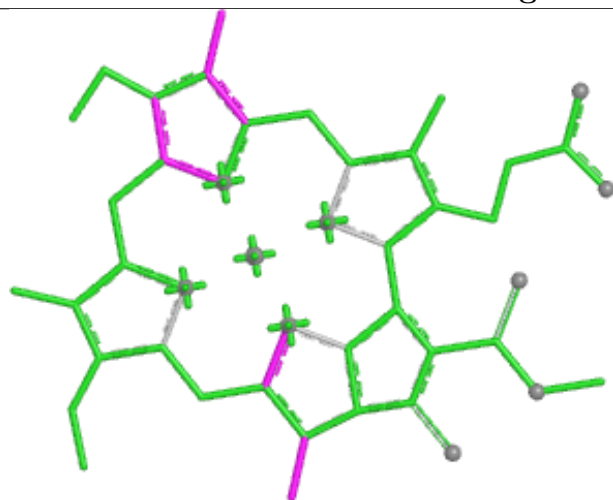


Torsions

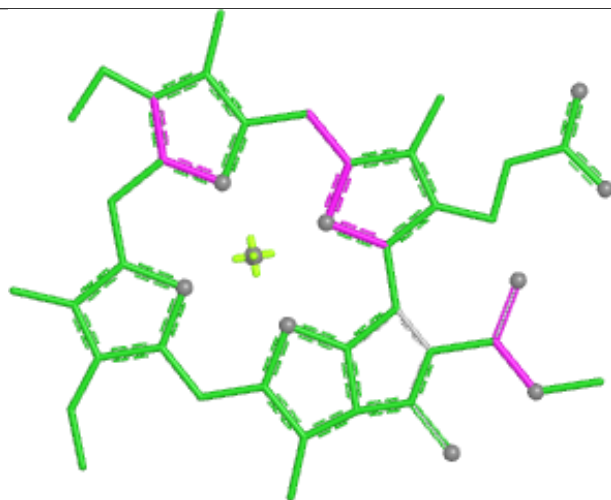


Rings

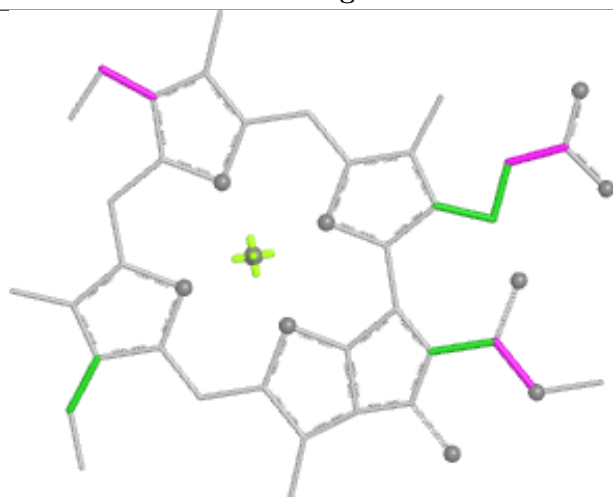
Ligand CLA c 516



Bond lengths



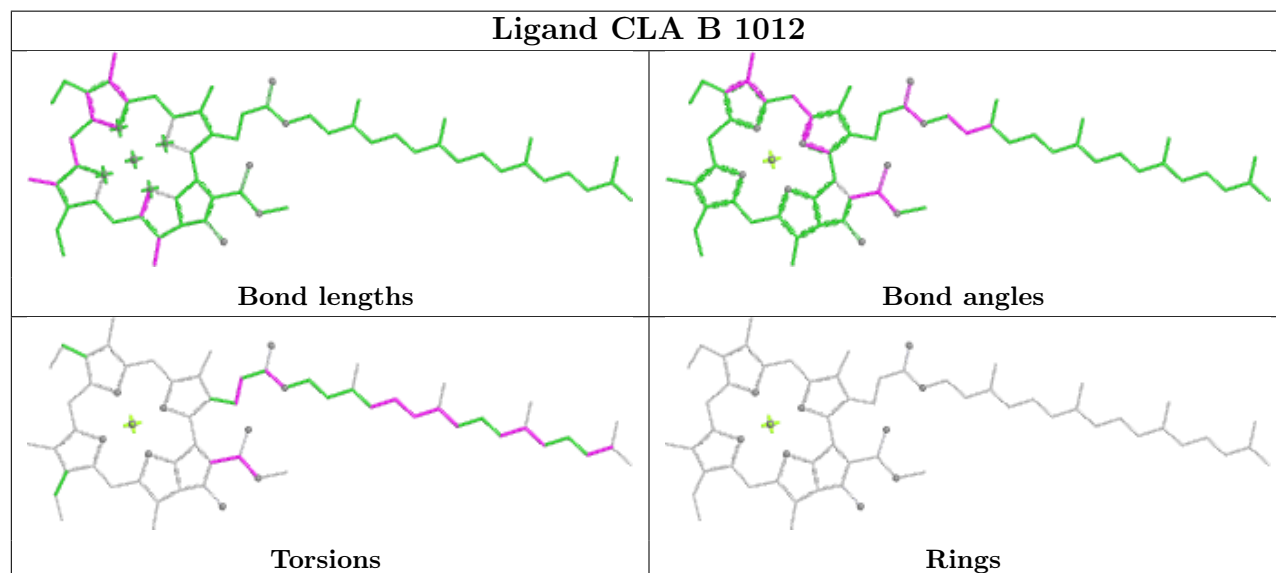
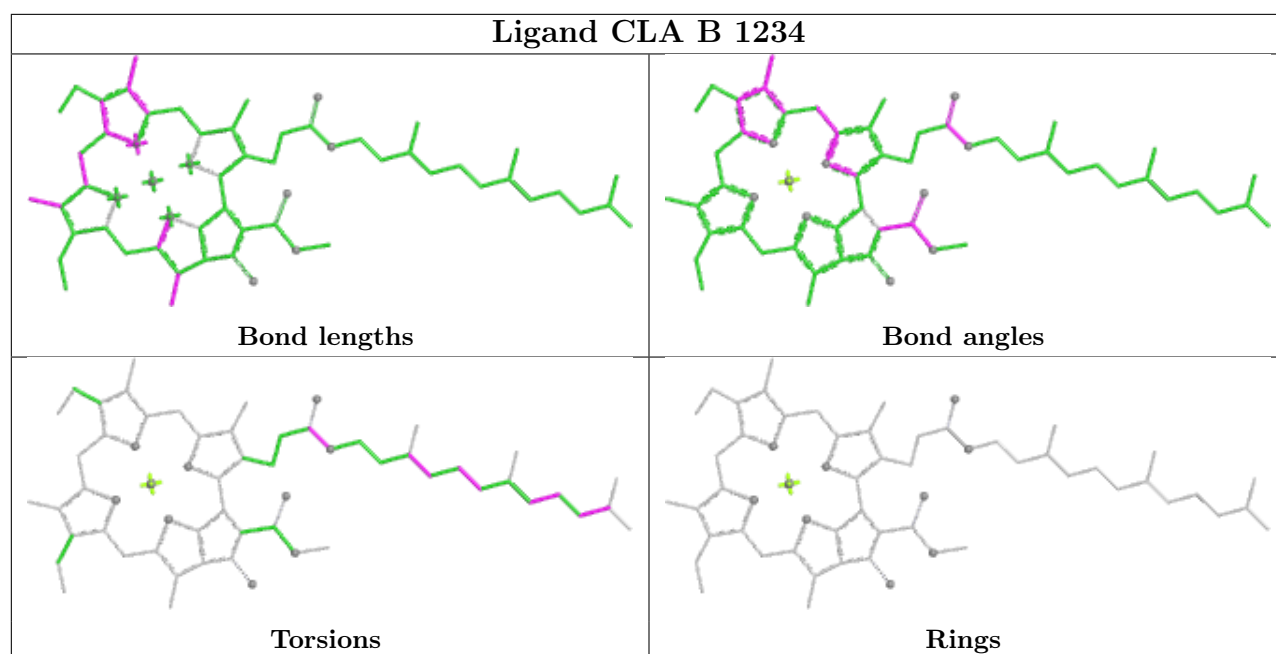
Bond angles



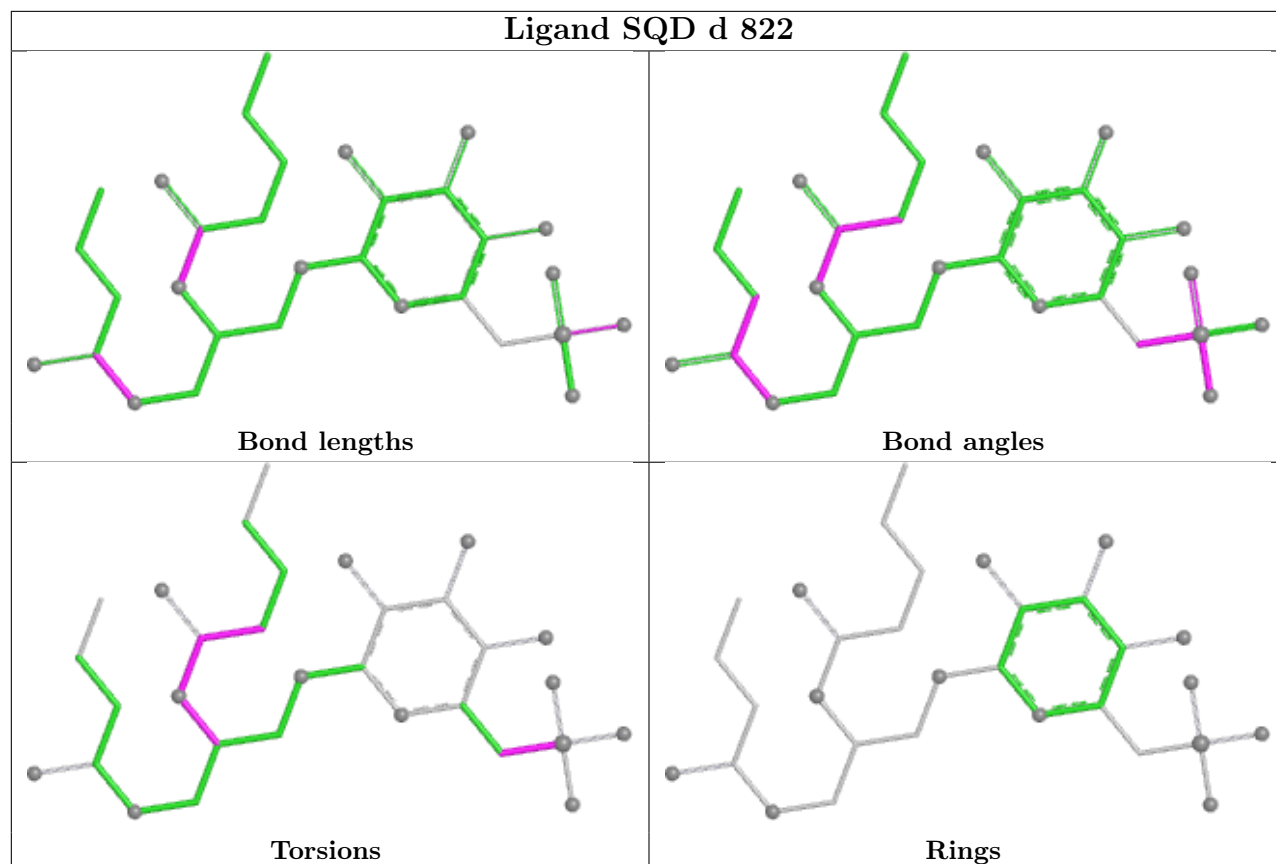
Torsions



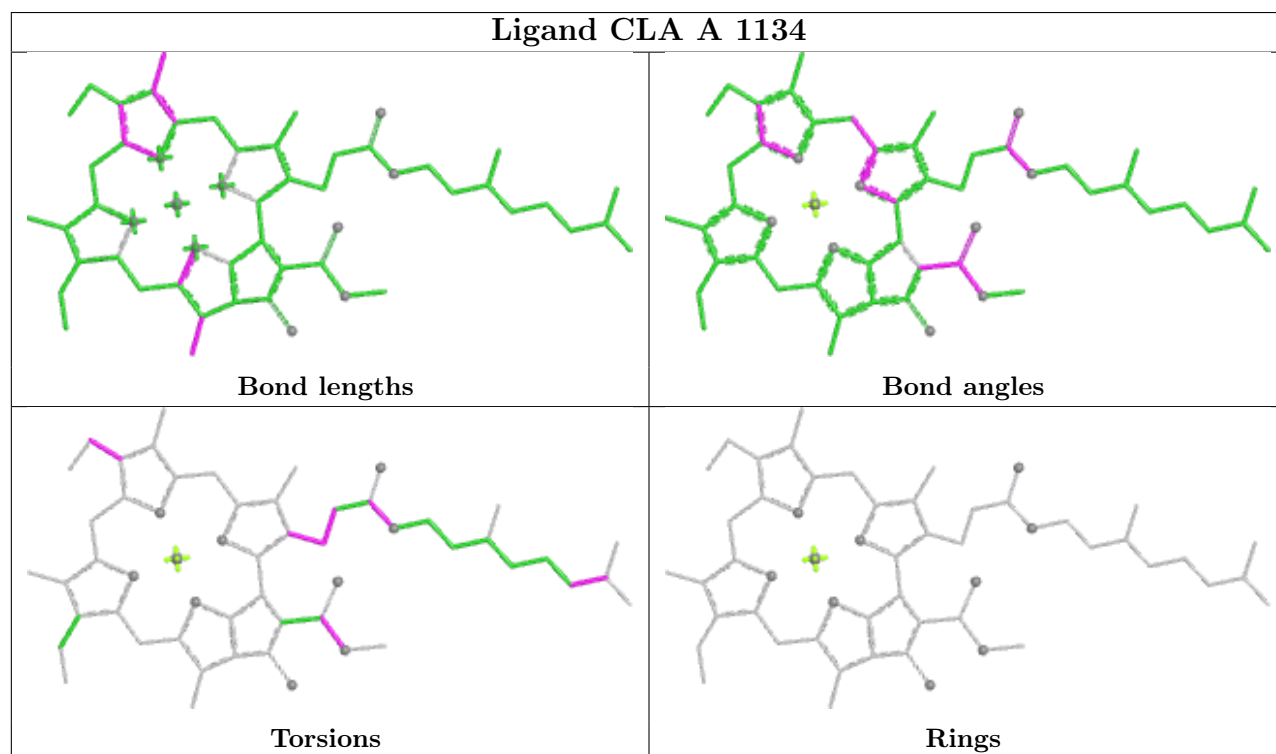
Rings



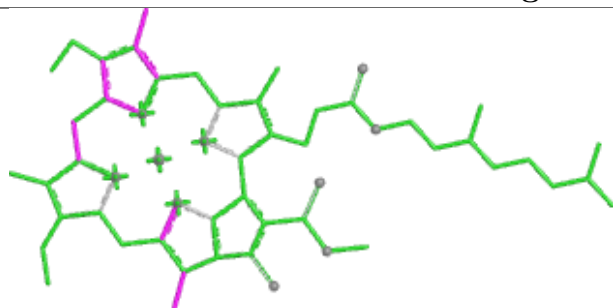
Ligand SQD d 822



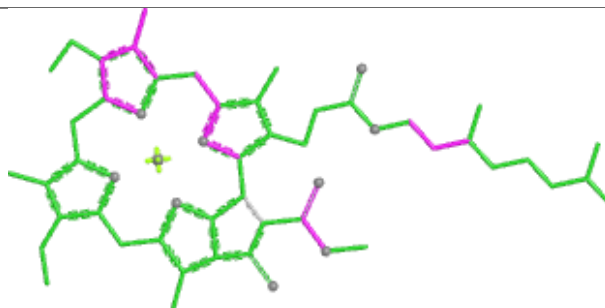
Ligand CLA A 1134



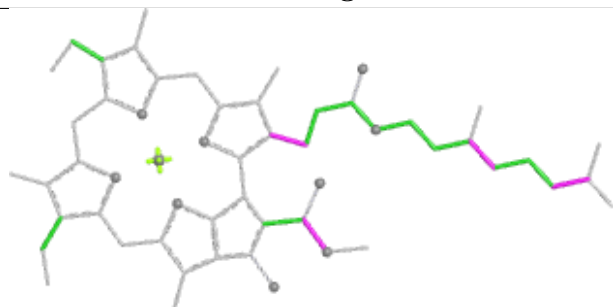
Ligand CLA f 511



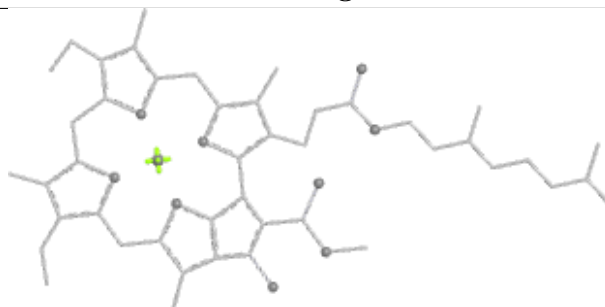
Bond lengths



Bond angles

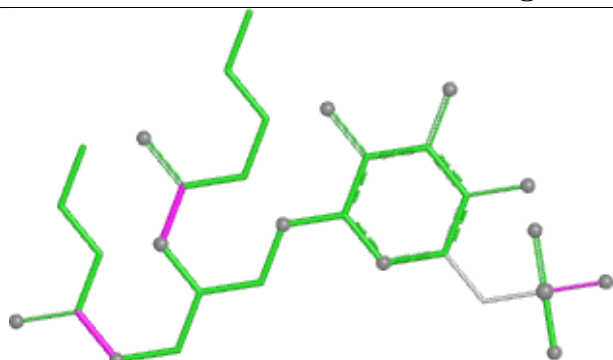


Torsions

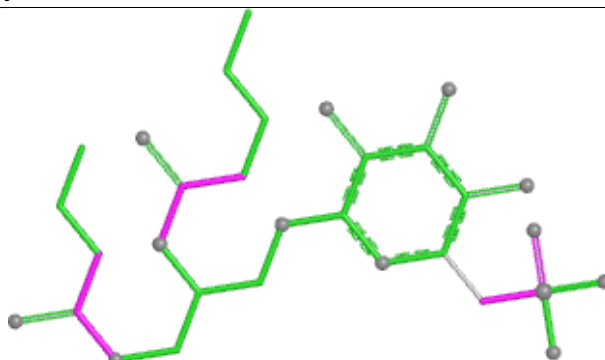


Rings

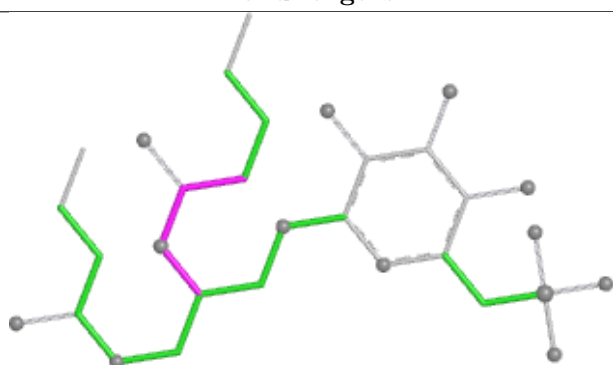
Ligand SQD 3 822



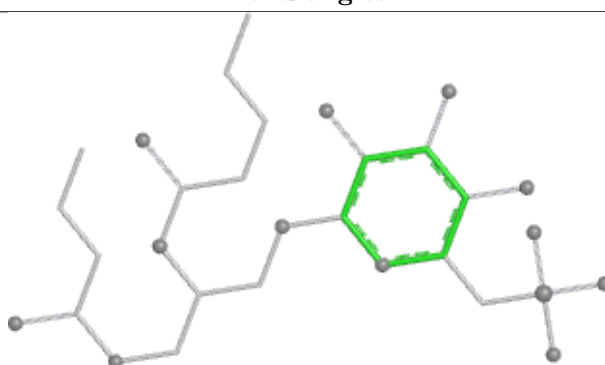
Bond lengths



Bond angles

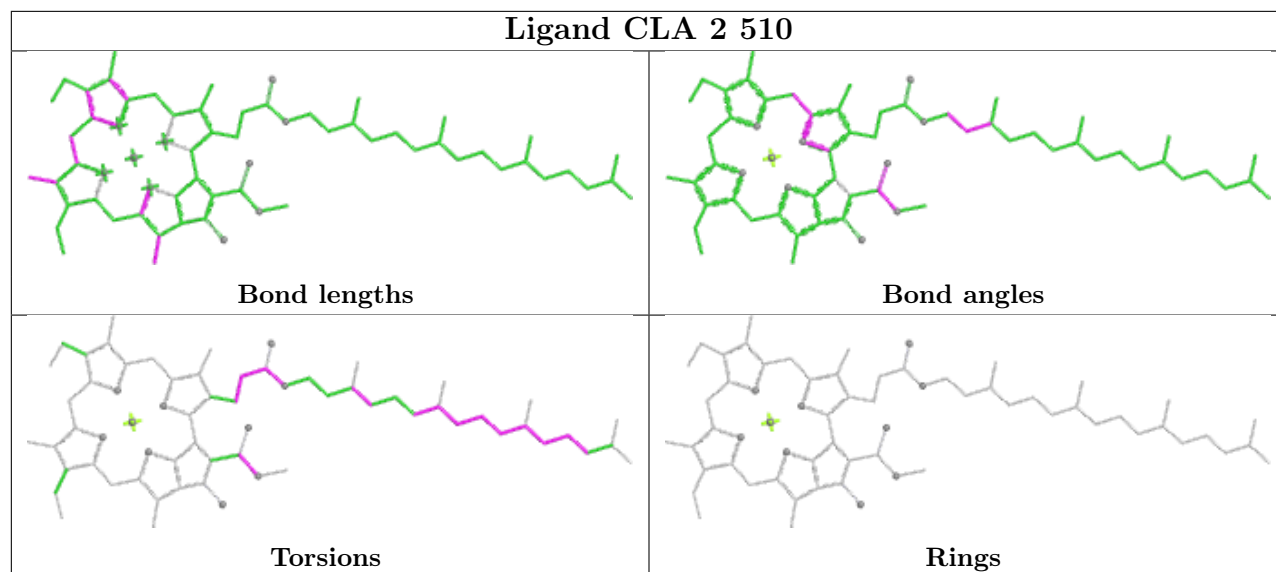


Torsions

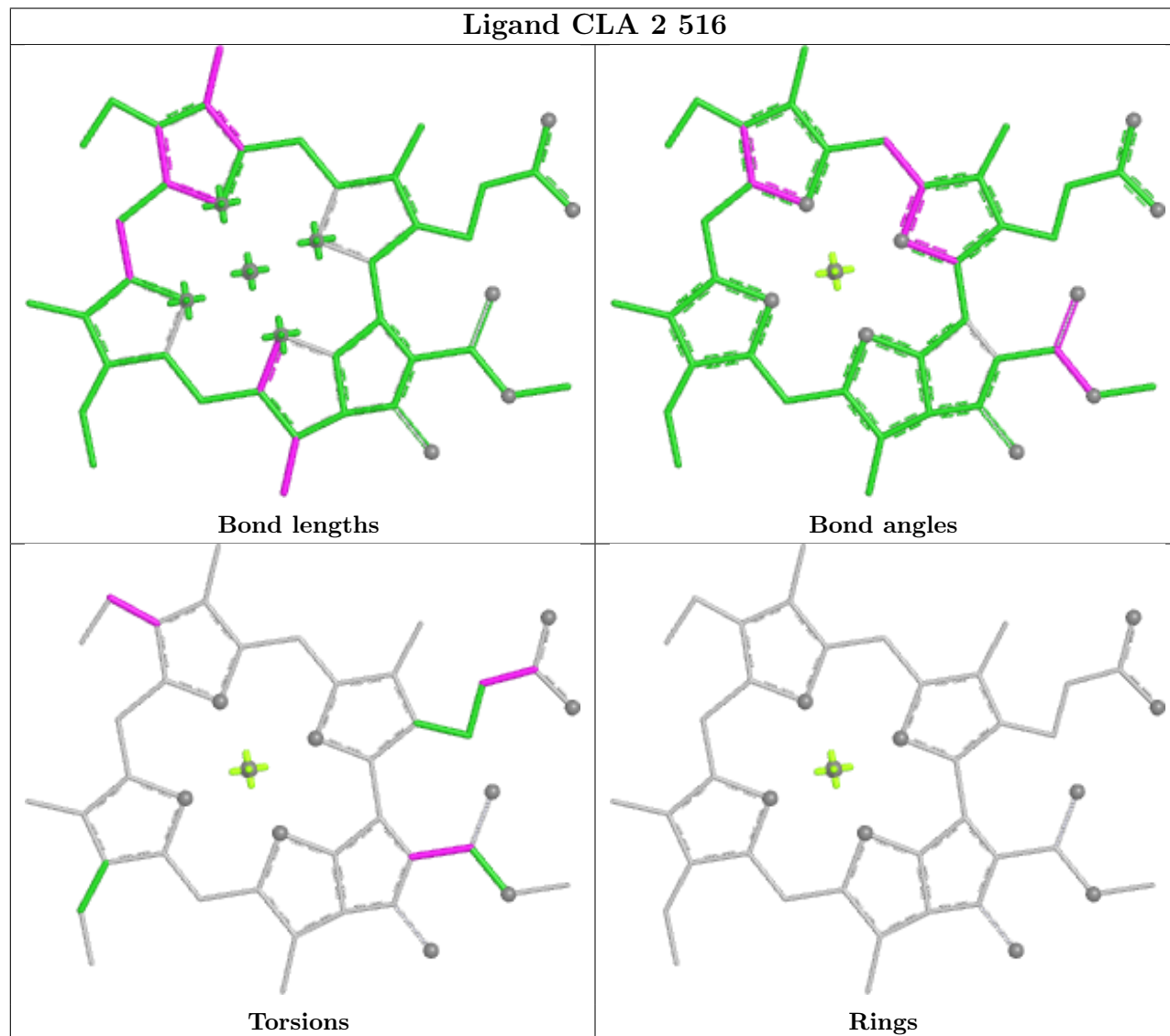


Rings

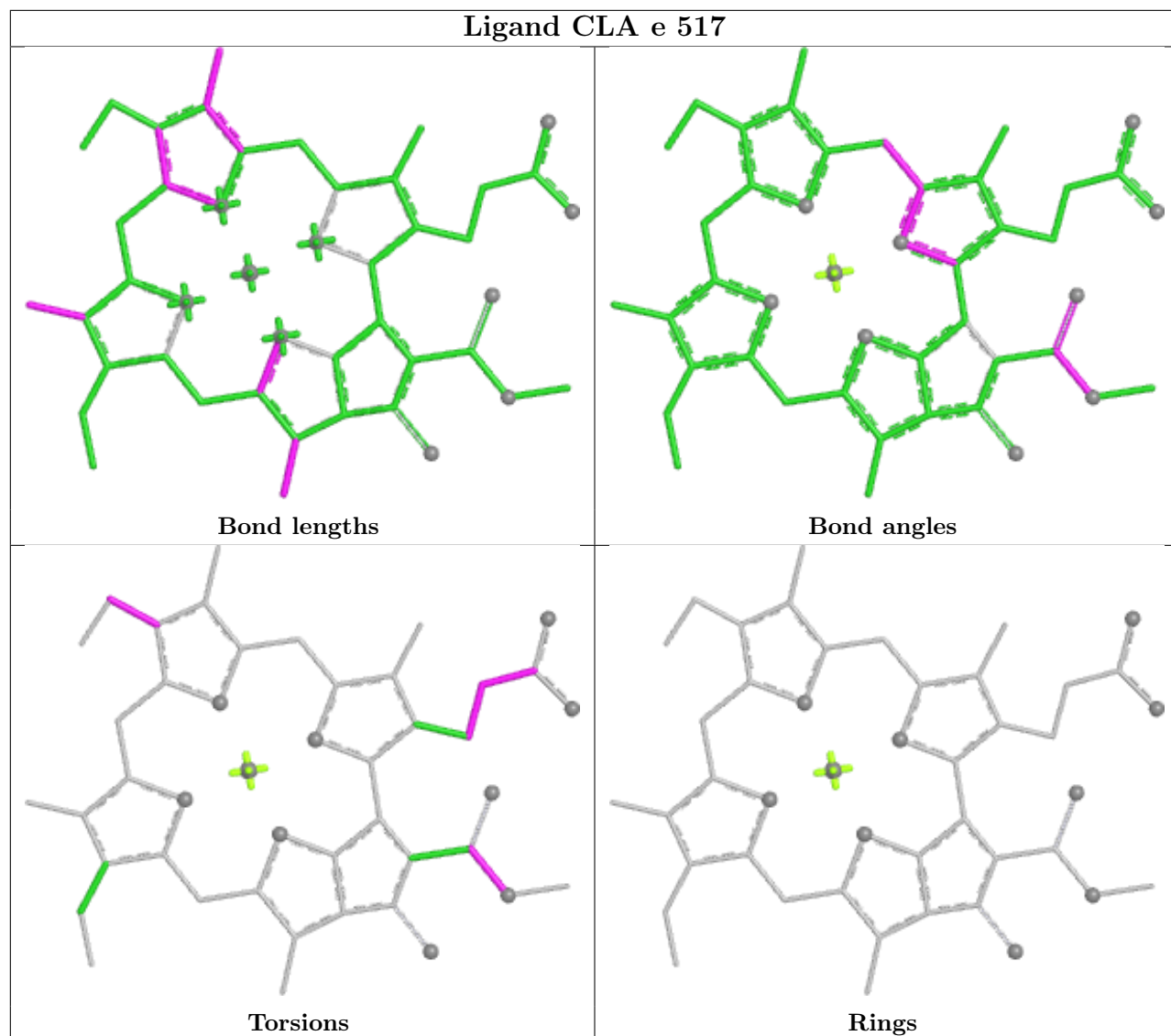
Ligand CLA 2 510

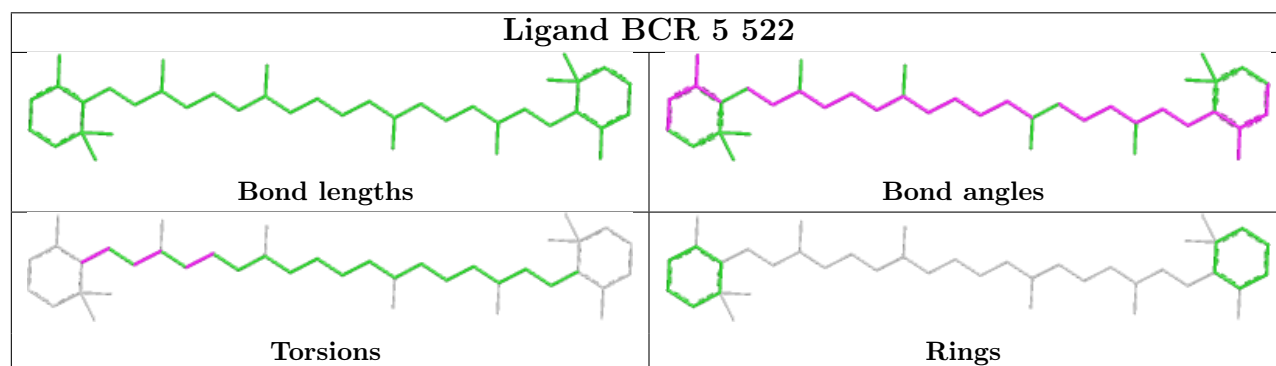
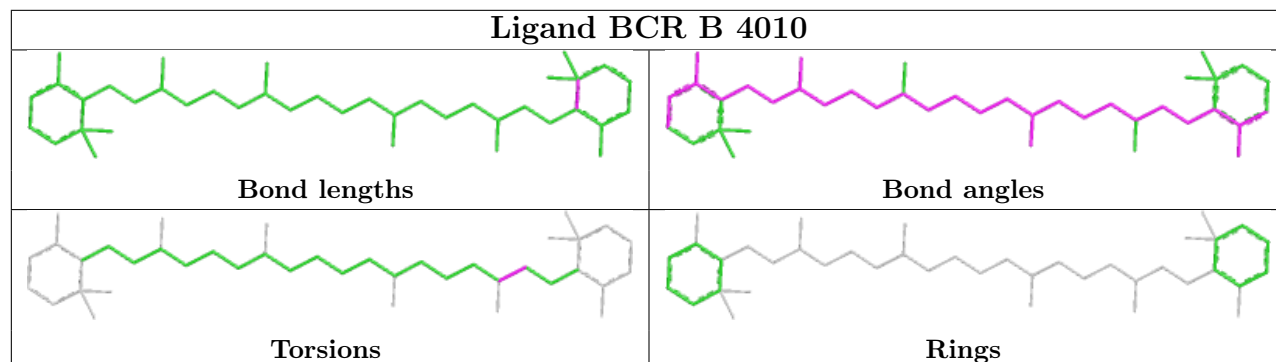
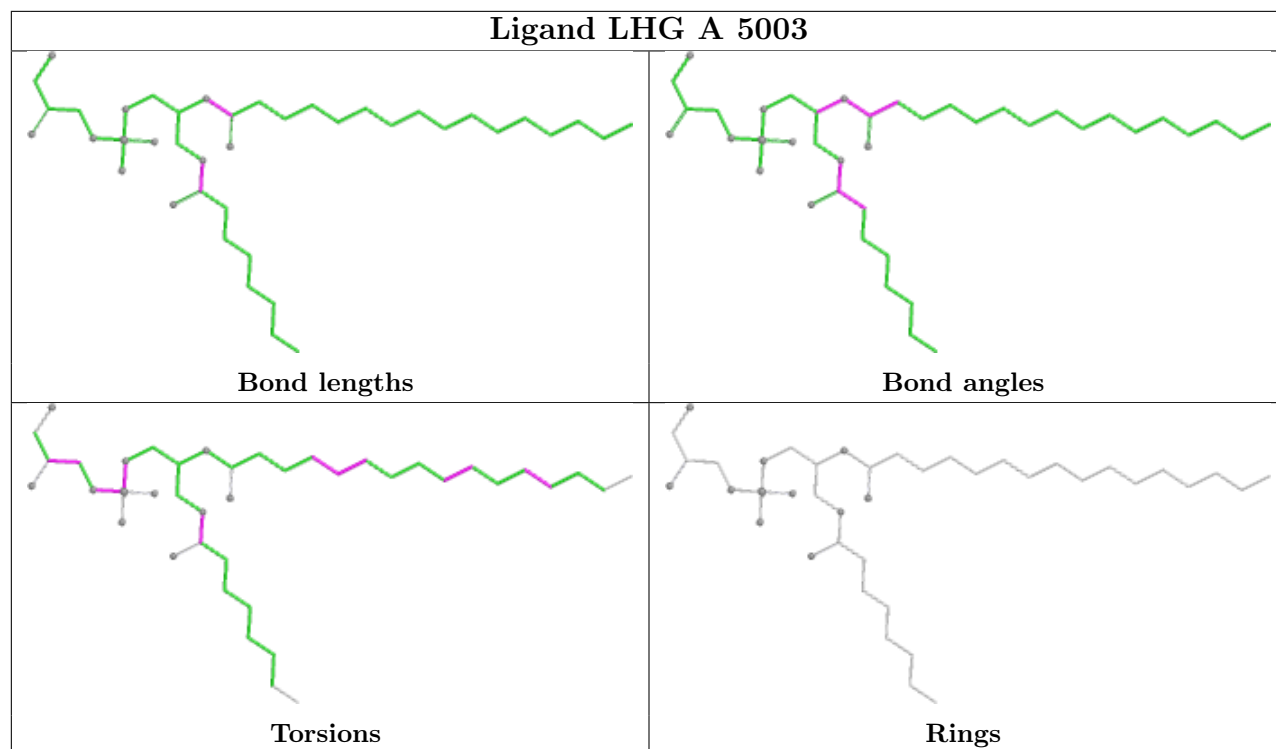


Ligand CLA 2 516

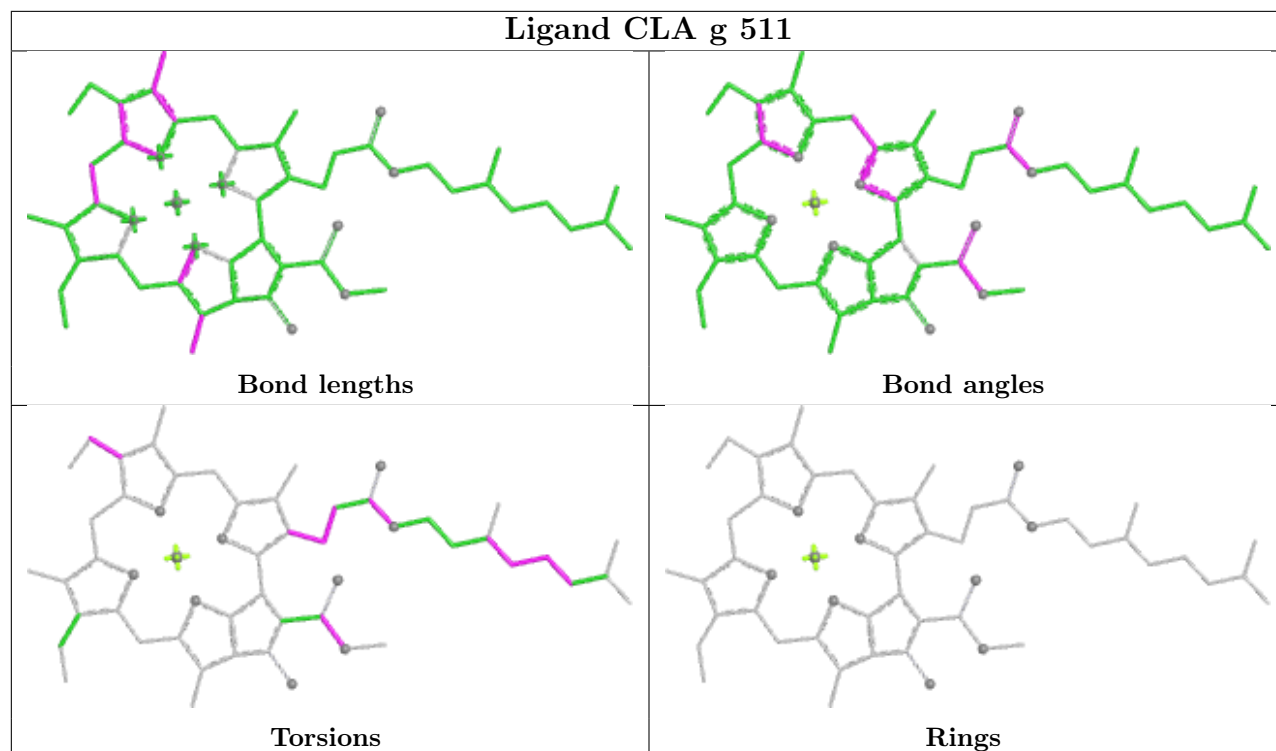


Ligand CLA e 517

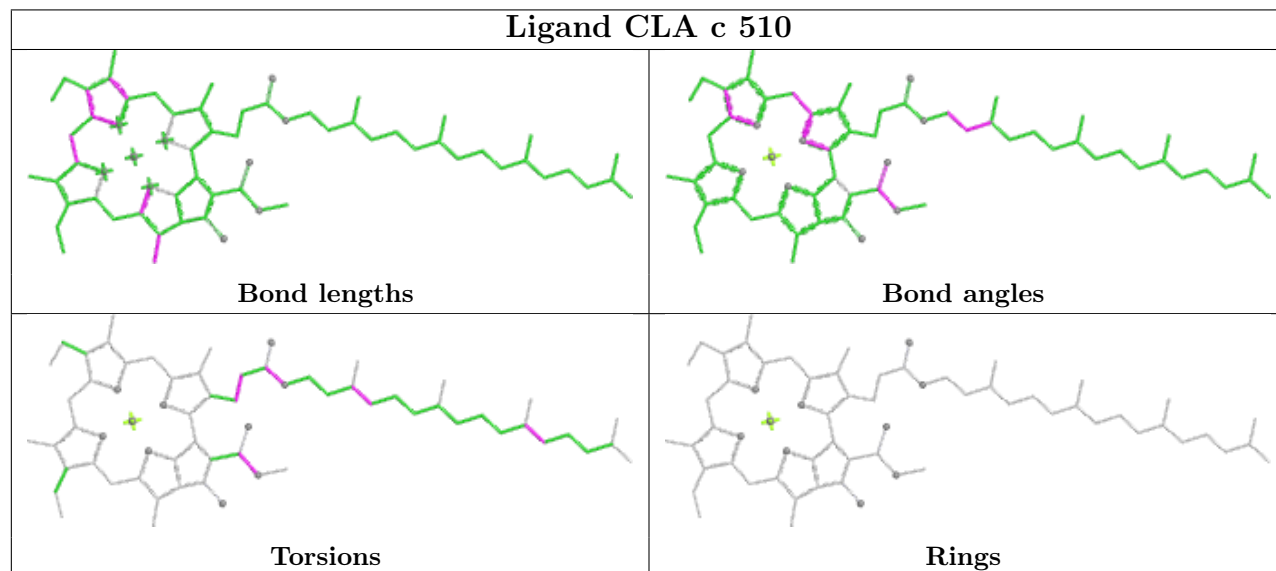


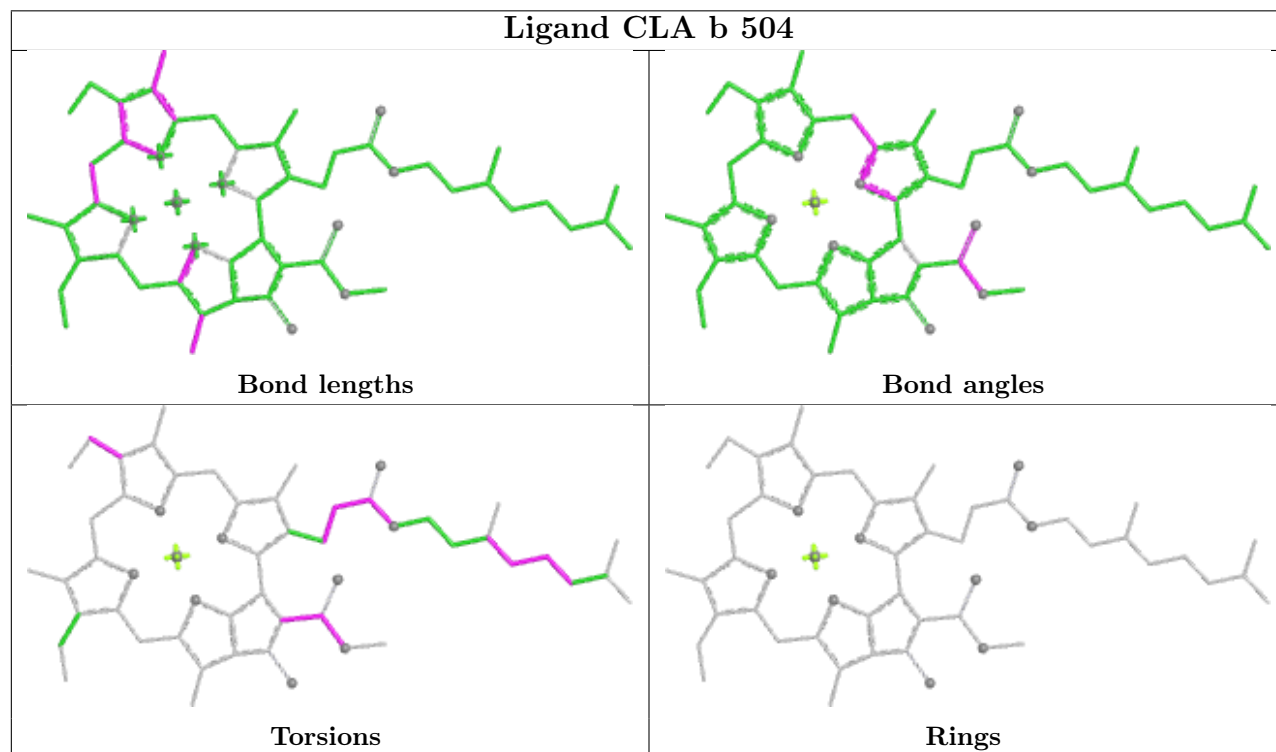
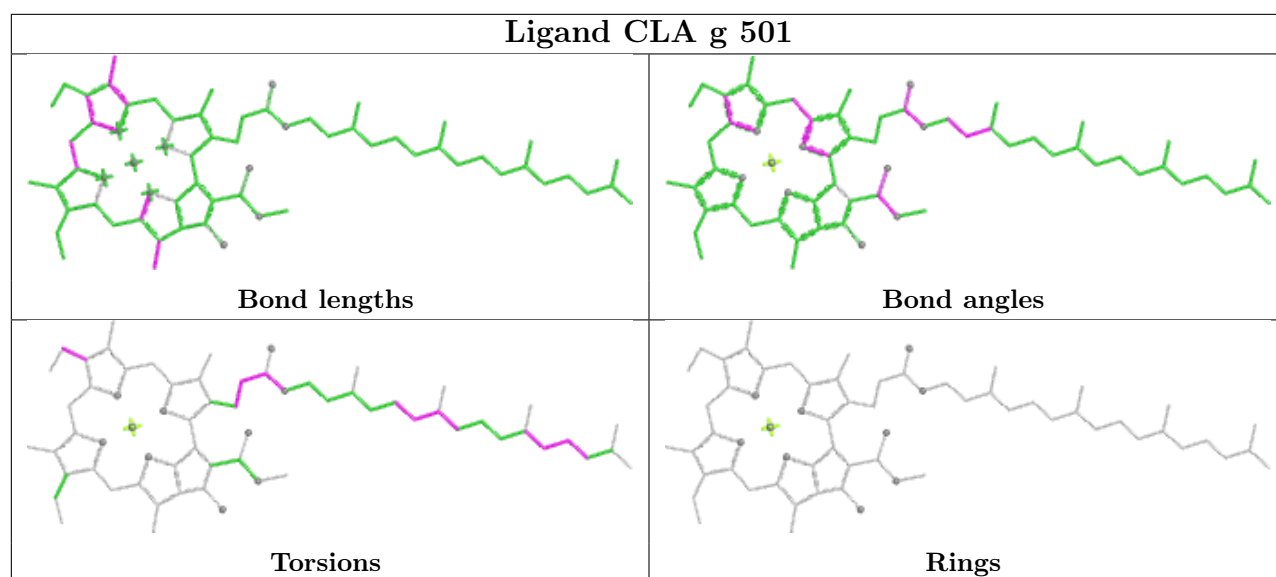


Ligand CLA g 511

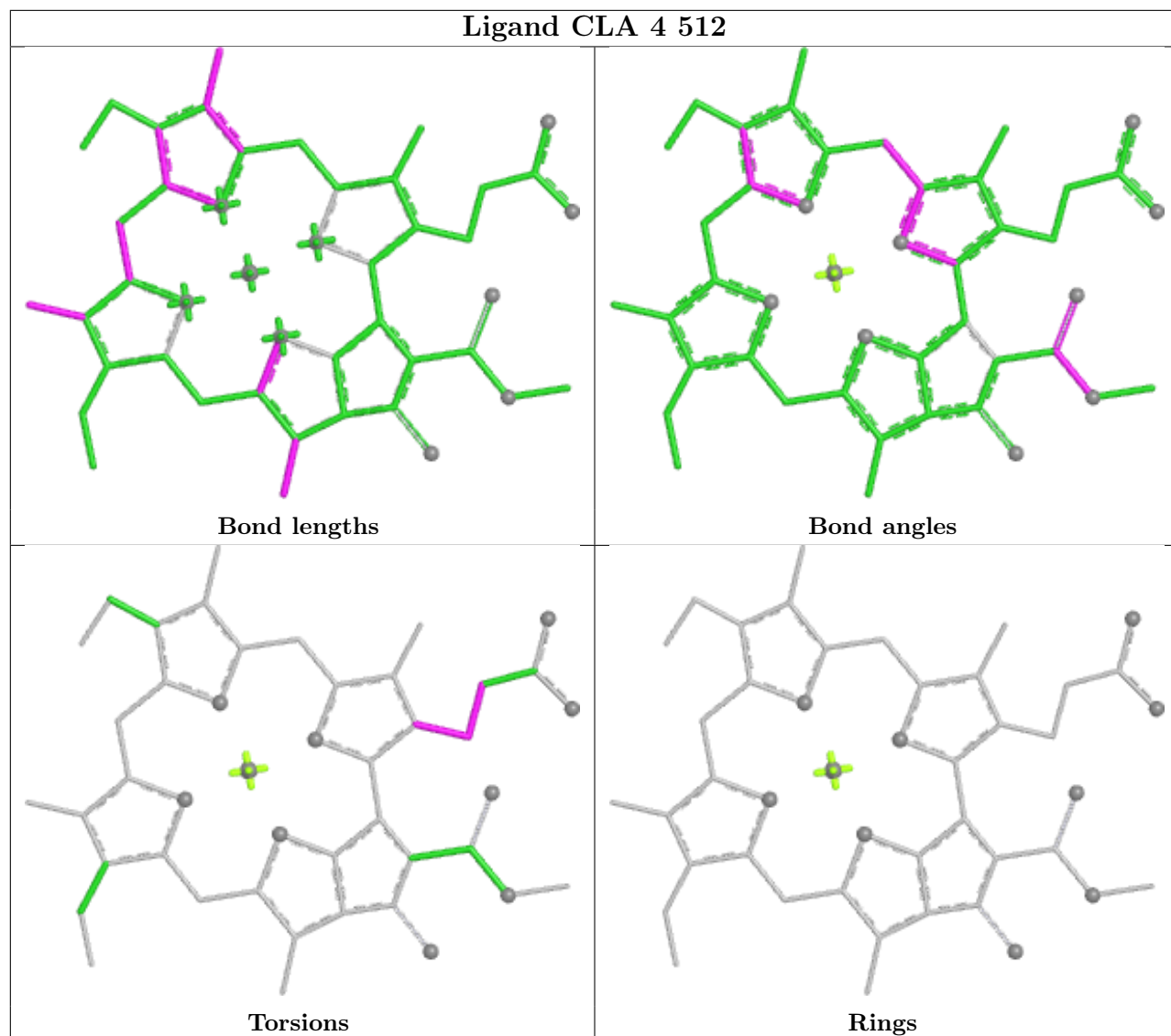


Ligand CLA c 510

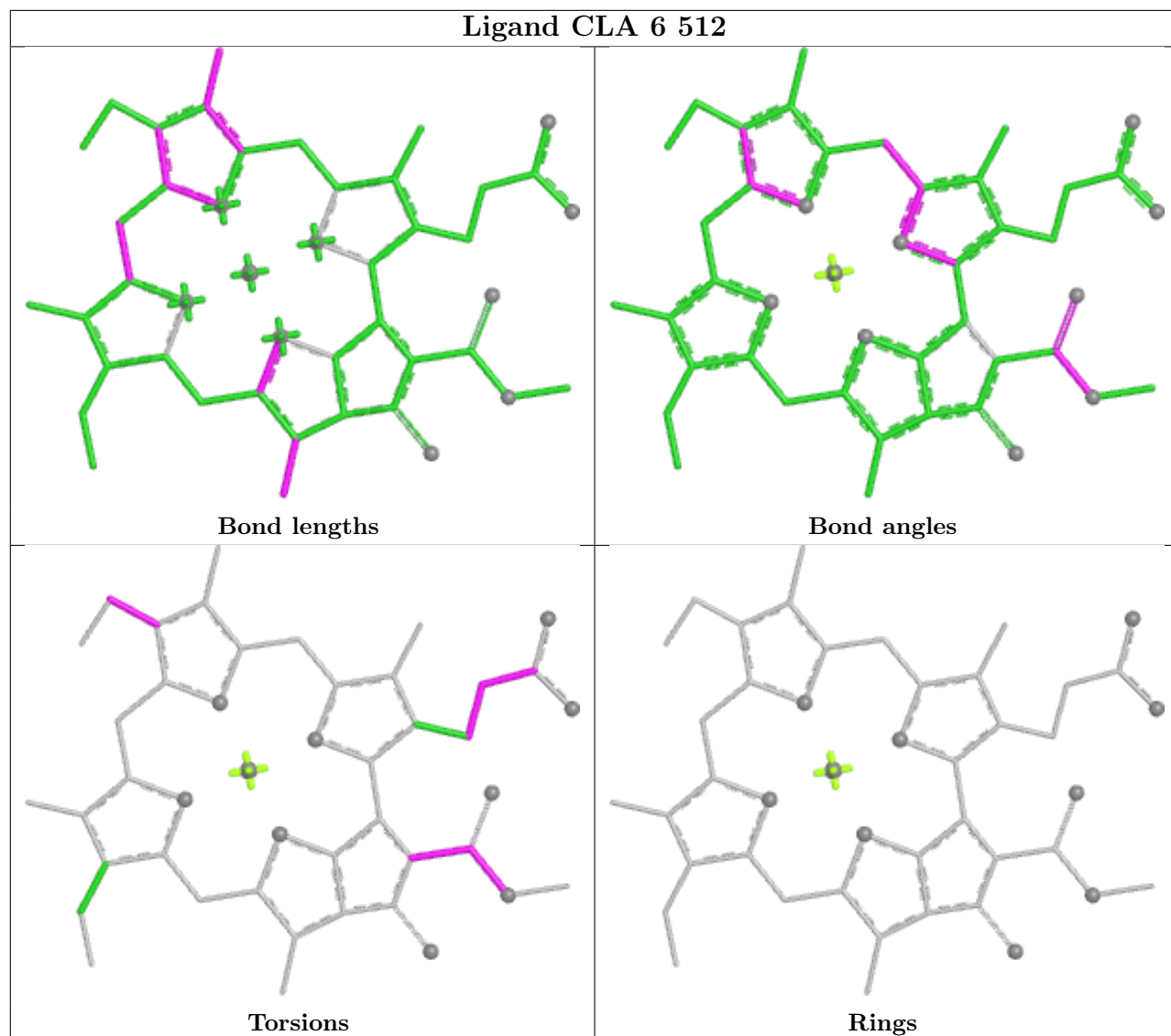


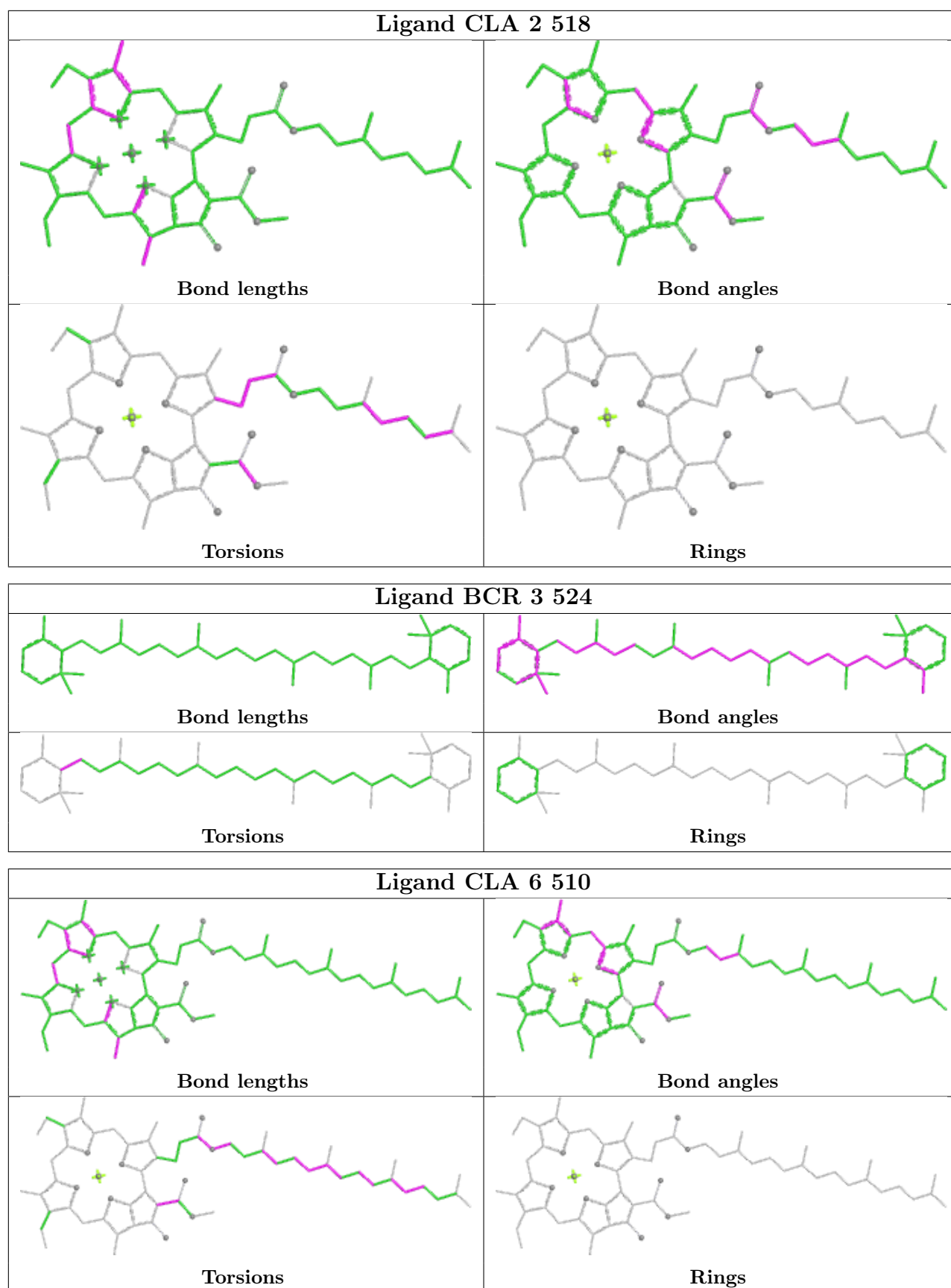


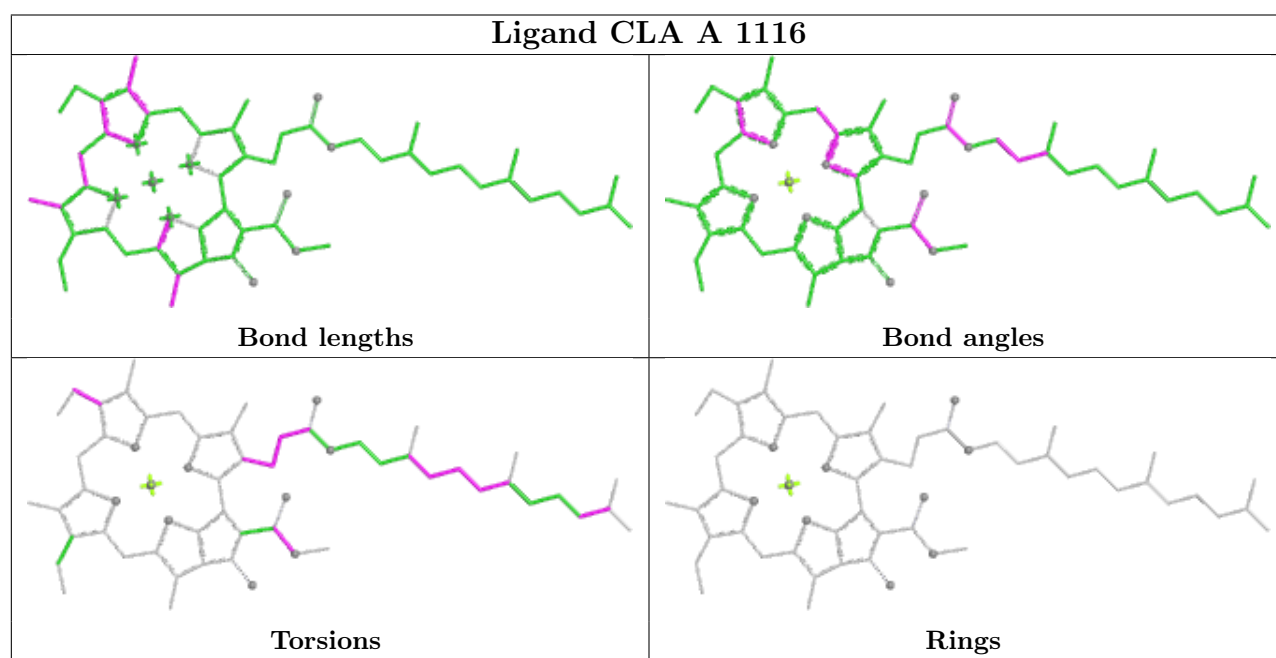
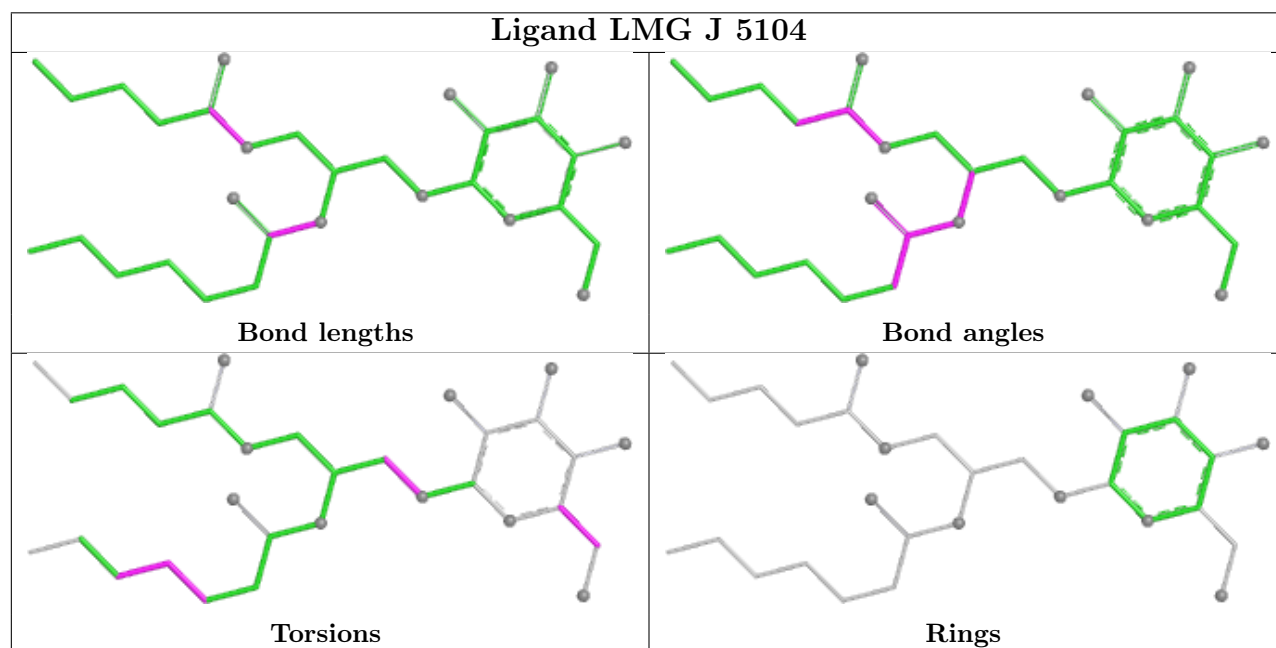
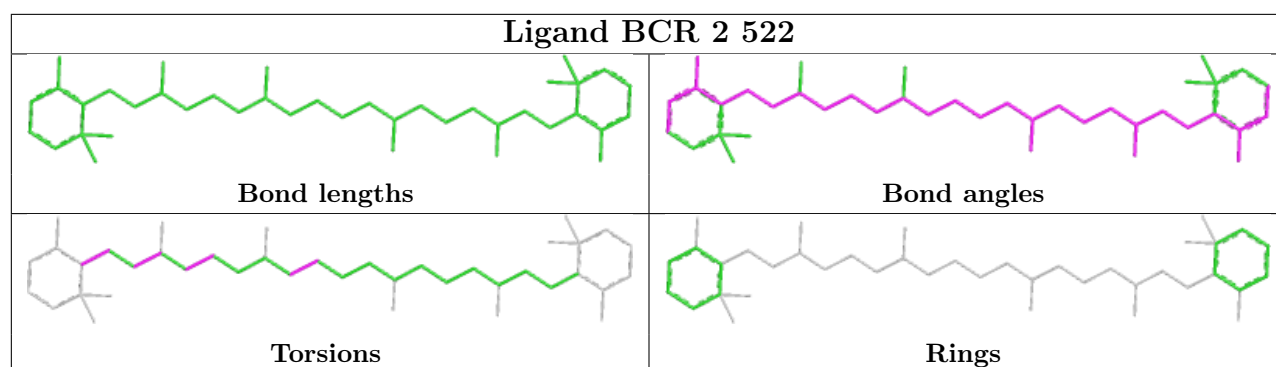
Ligand CLA 4 512

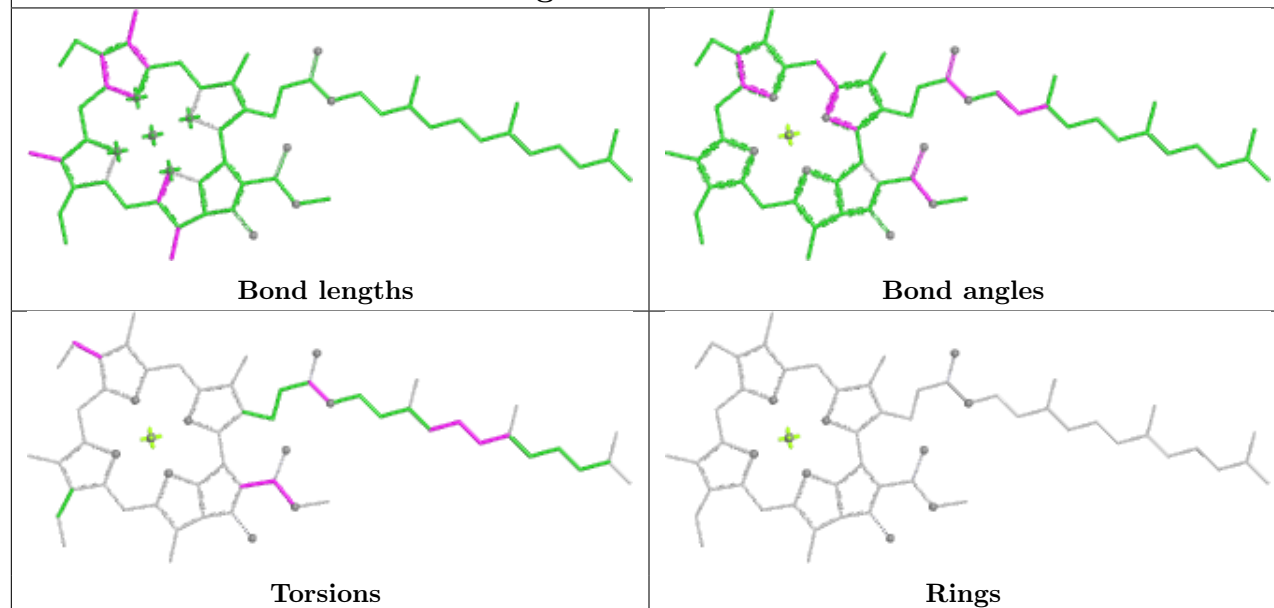
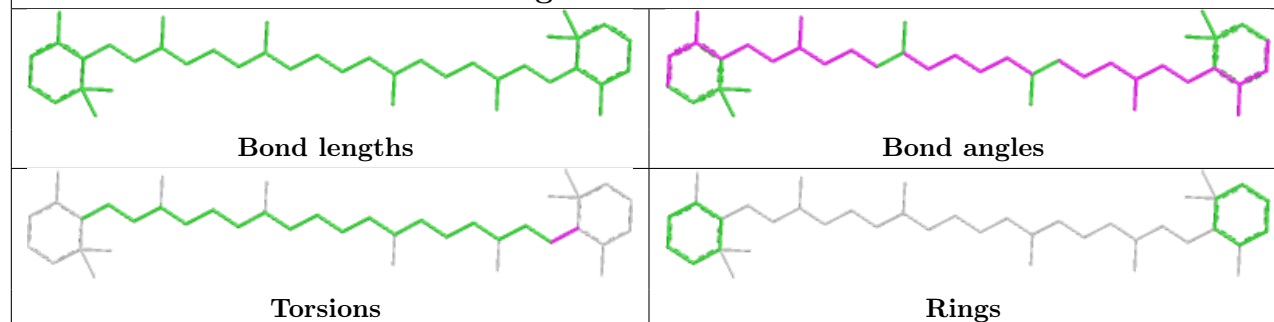
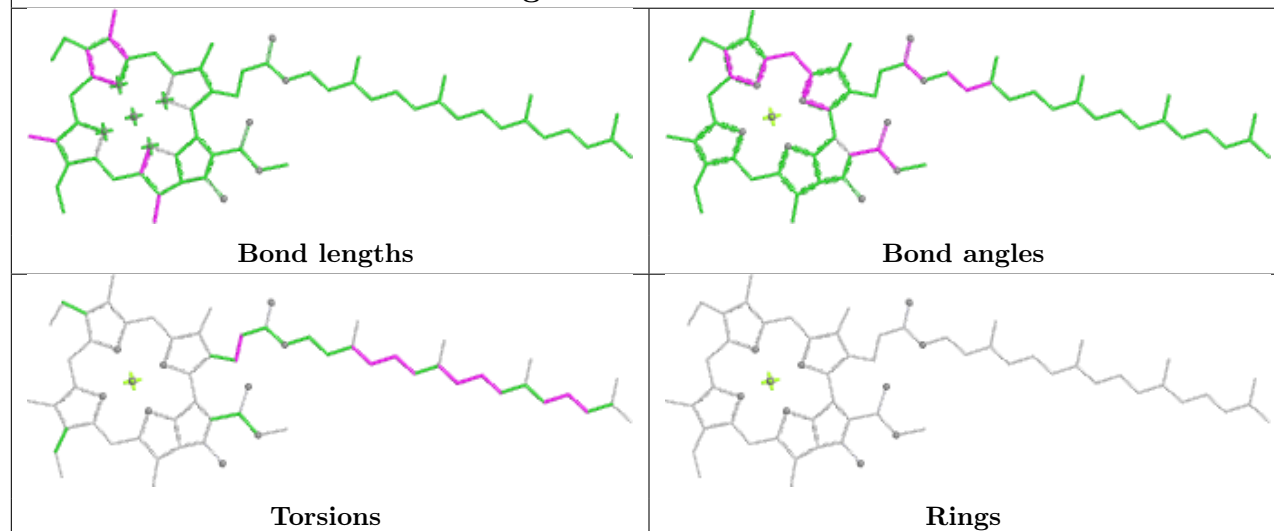


Ligand CLA 6 512

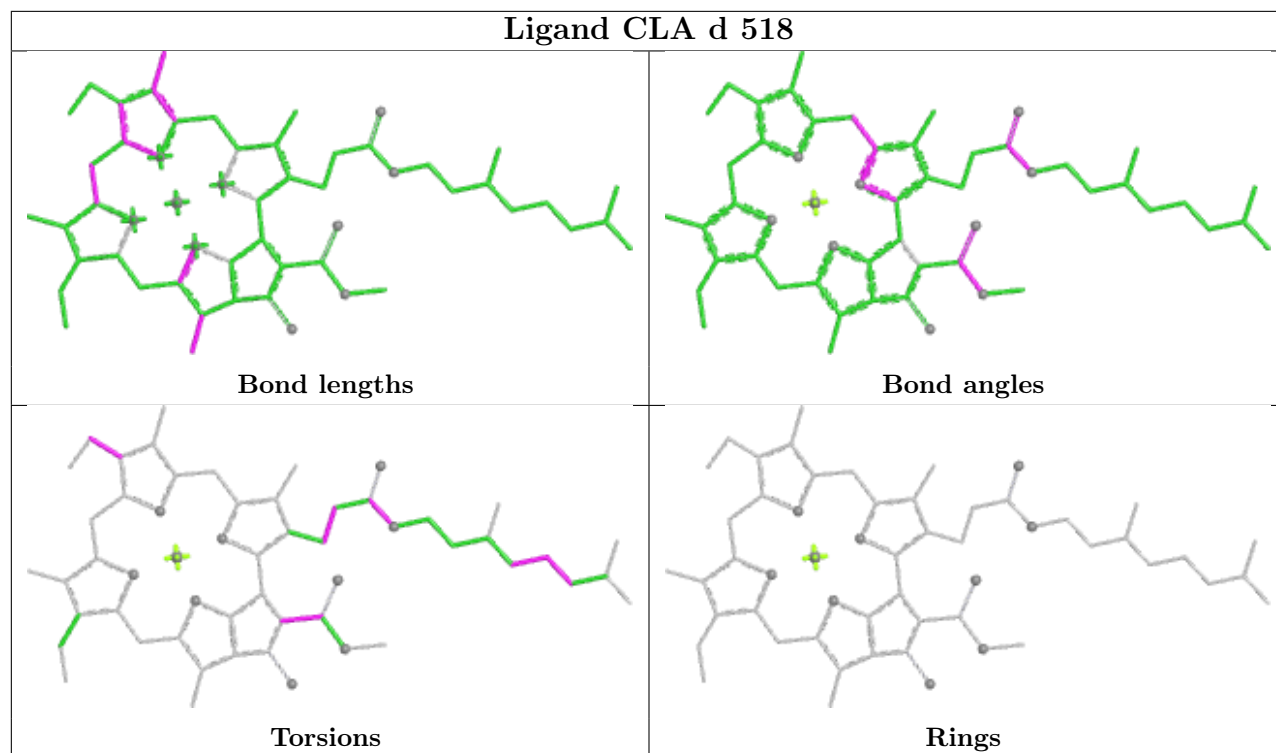




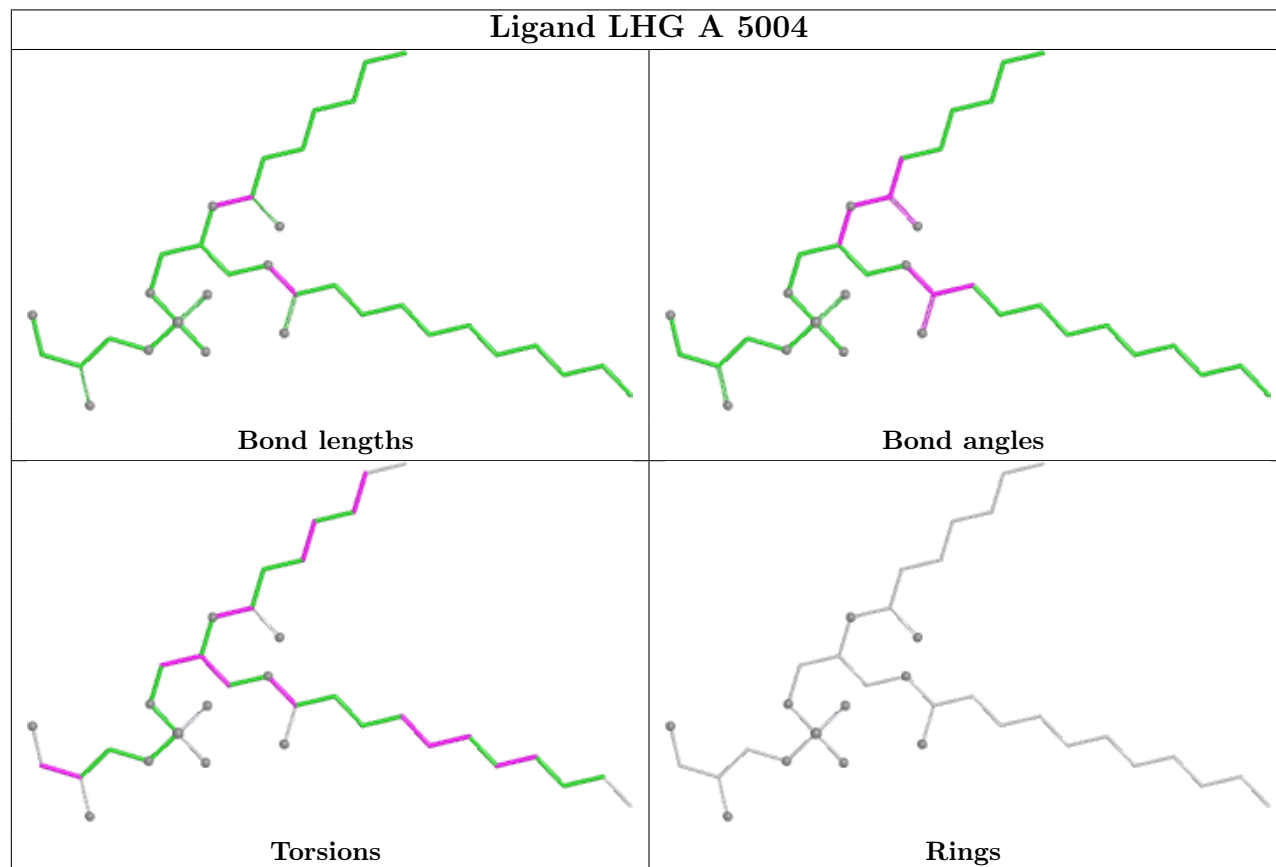


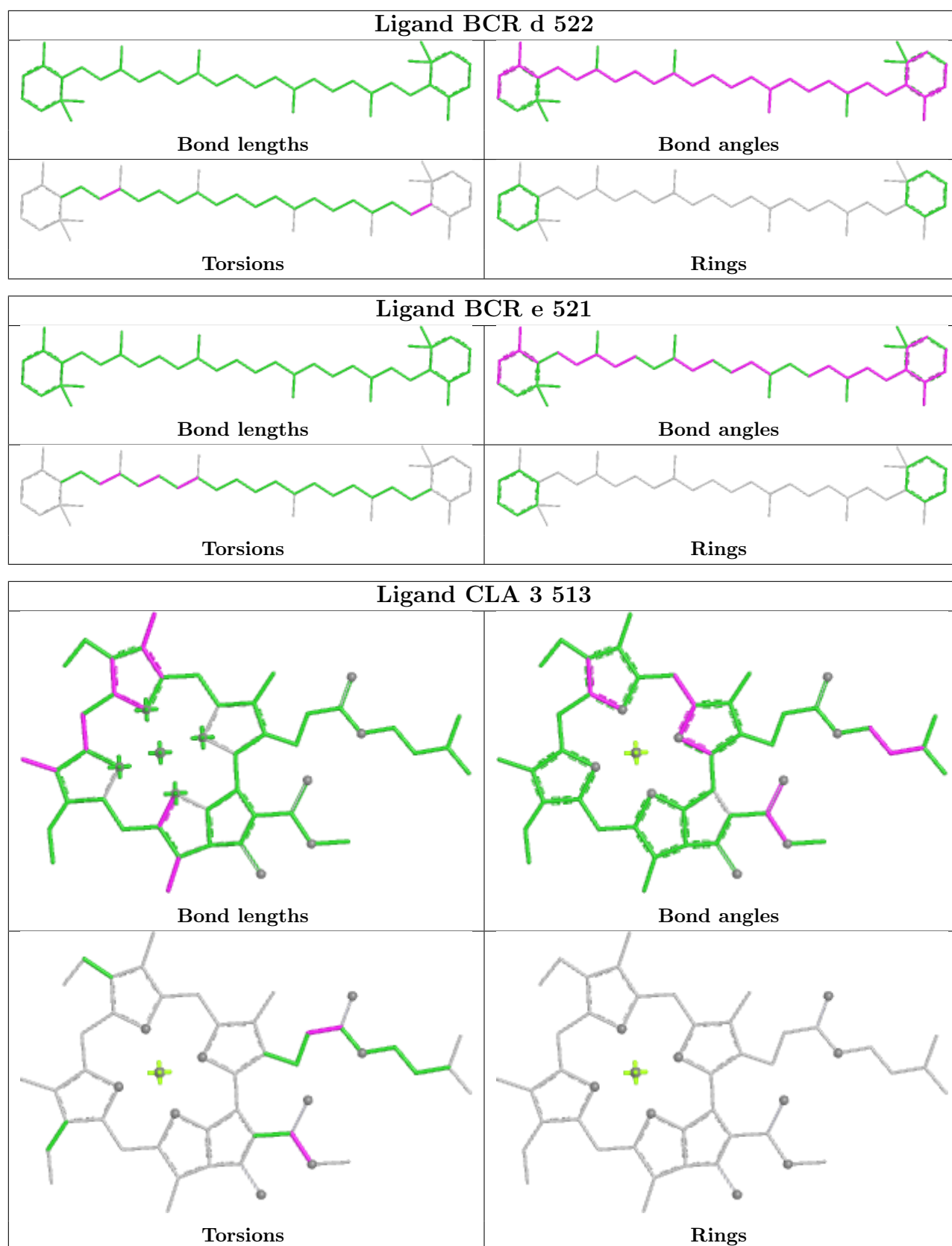
Ligand CLA 5 502**Ligand BCR c 523****Ligand CLA A 1140**

Ligand CLA d 518

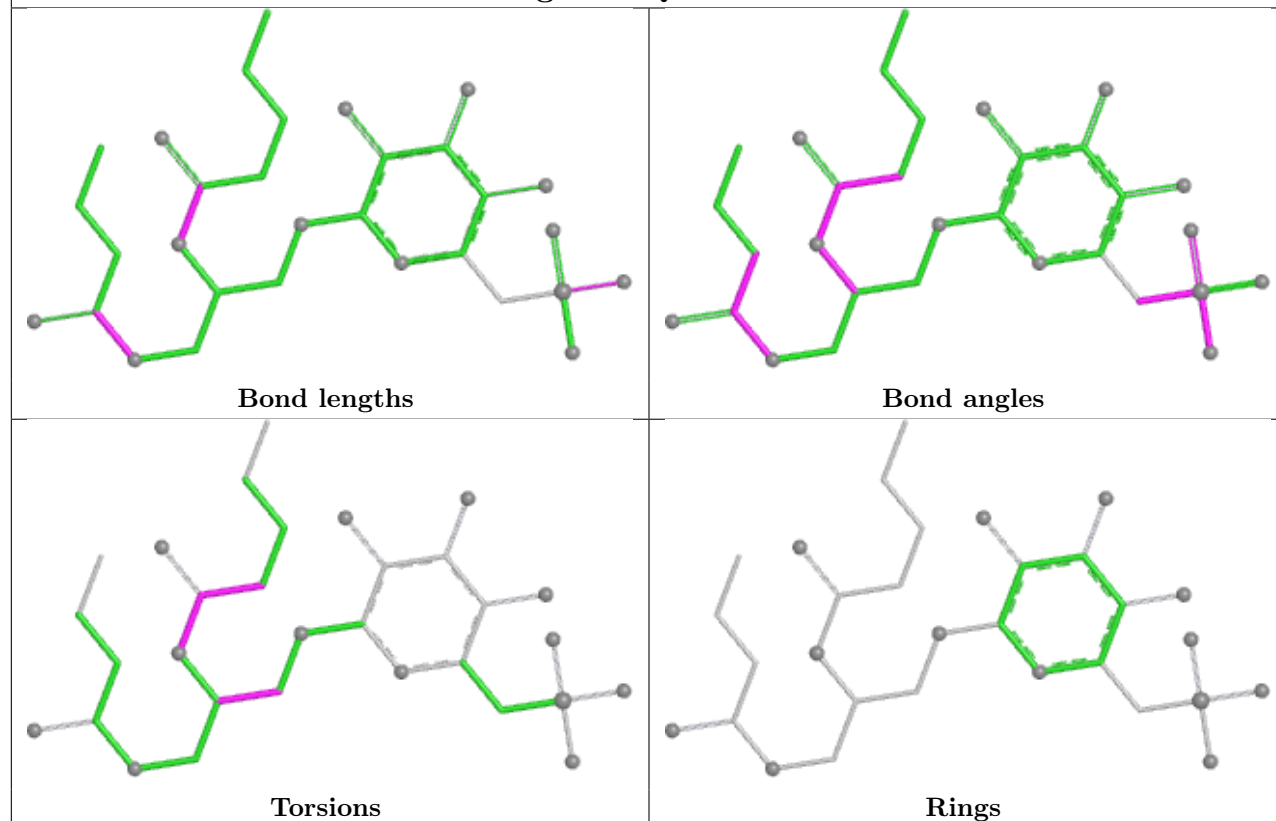


Ligand LHG A 5004

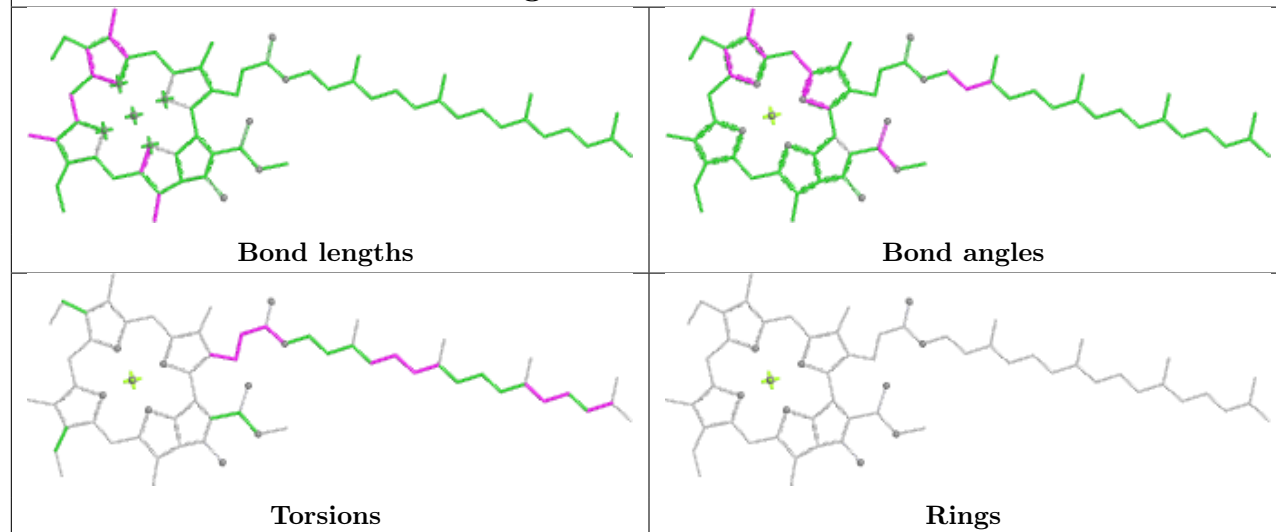




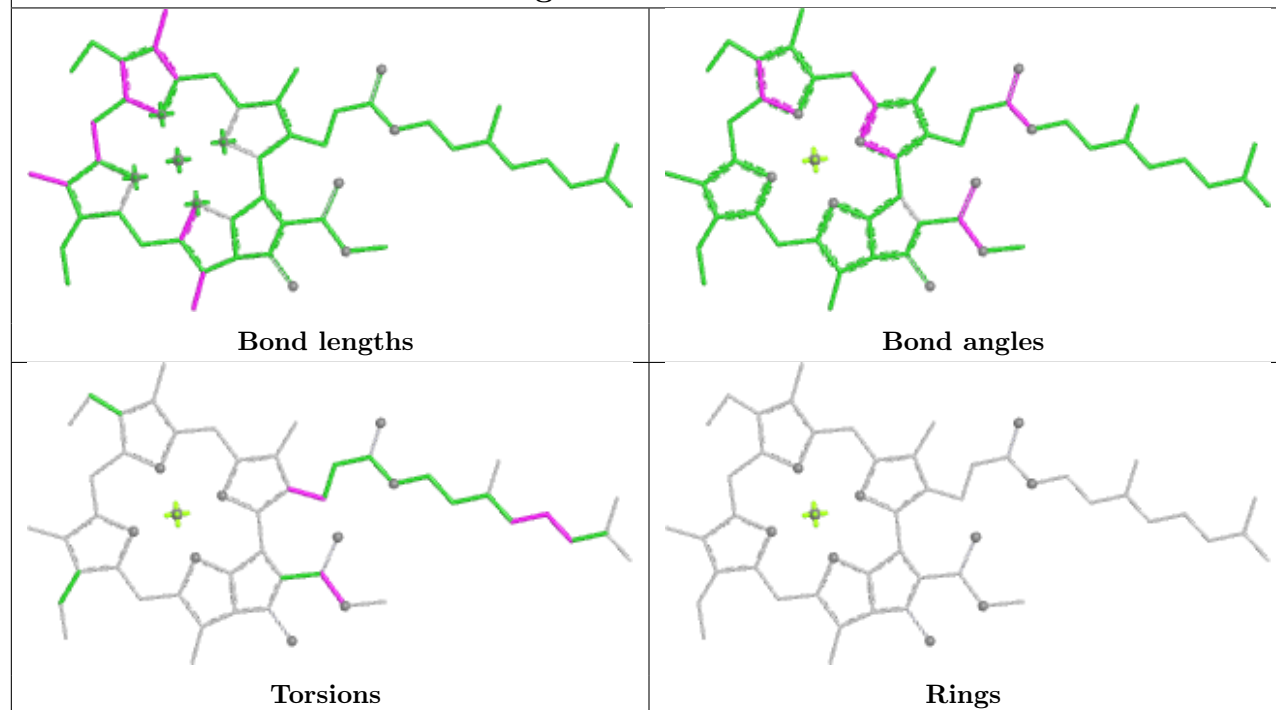
Ligand SQD 2 822



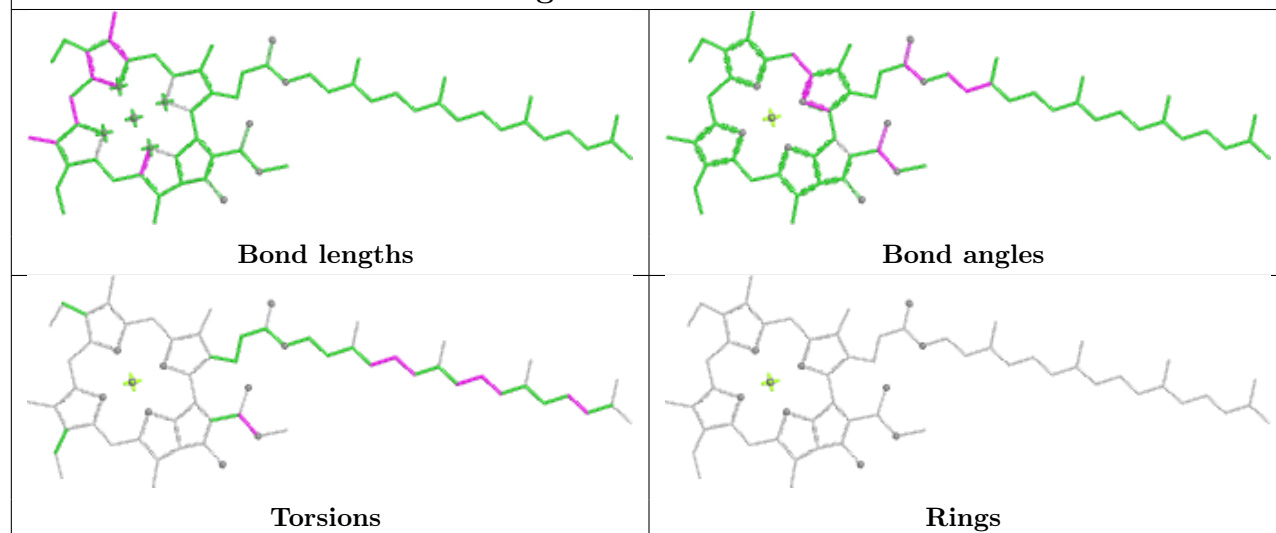
Ligand CLA B 1213



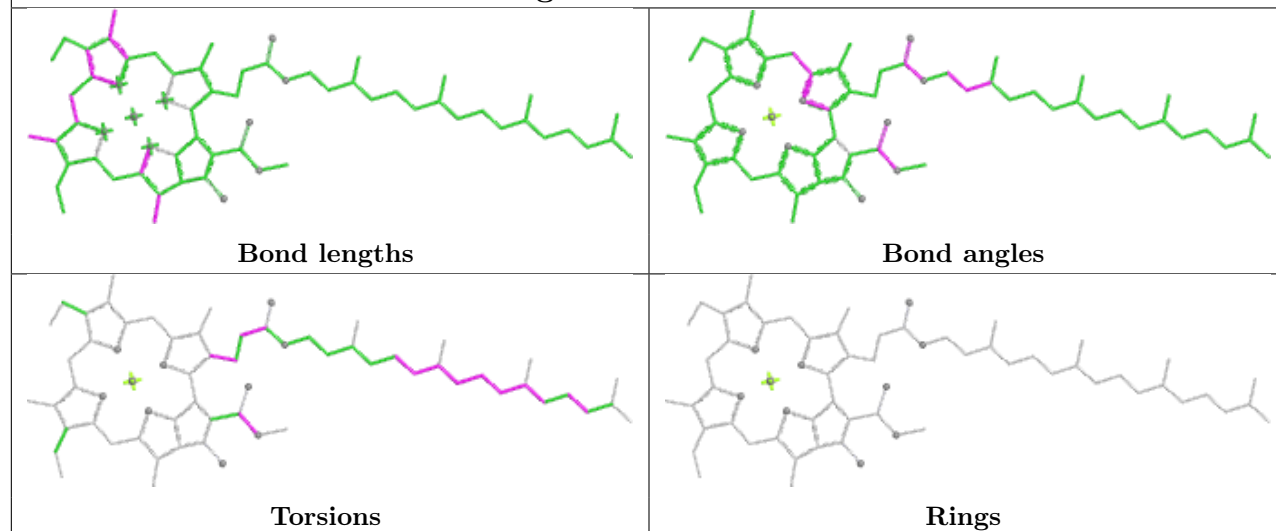
Ligand CLA d 508



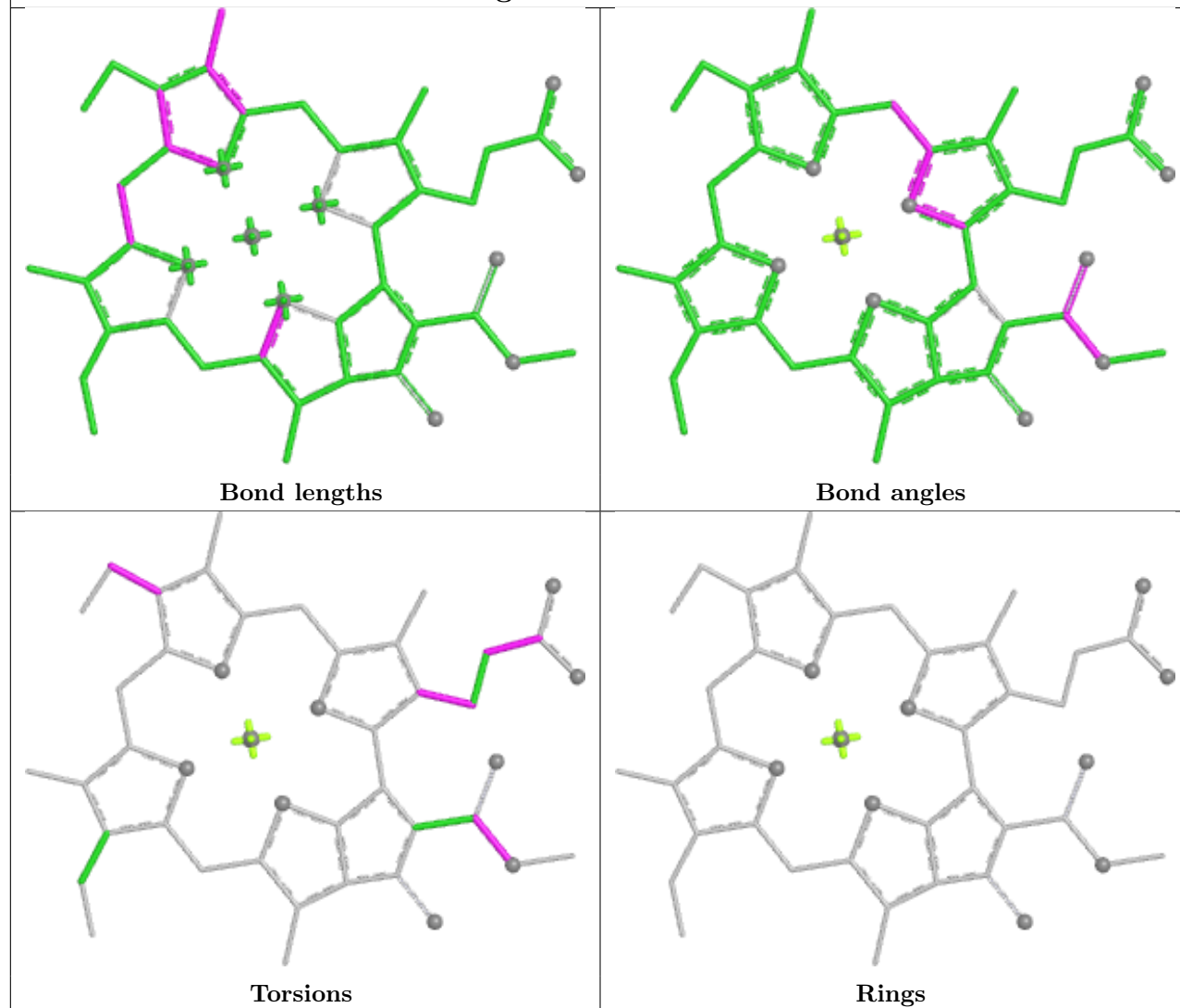
Ligand CLA 4 509

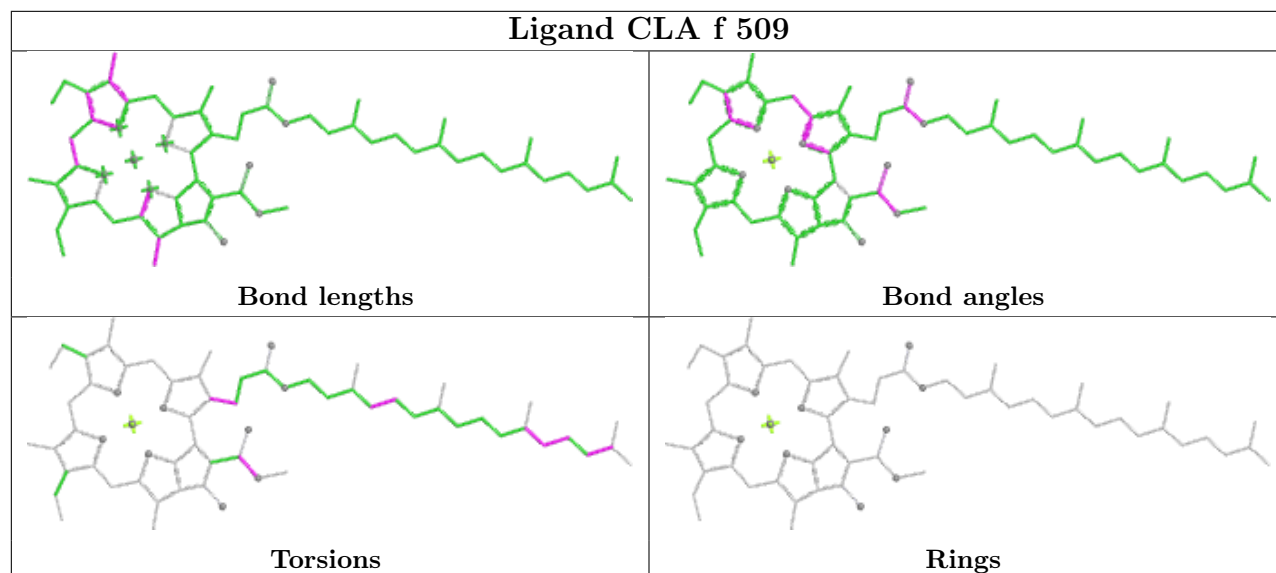
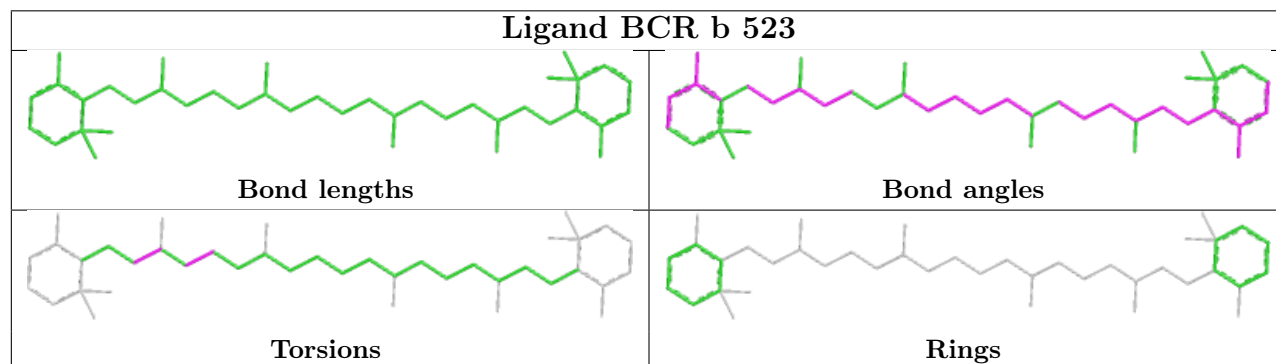
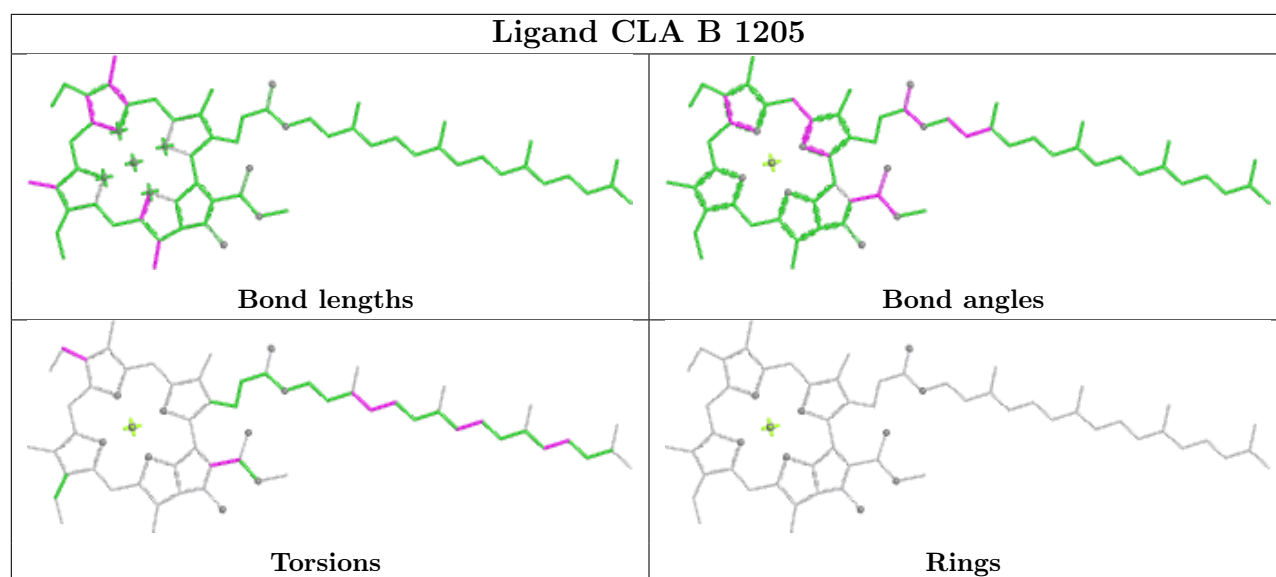


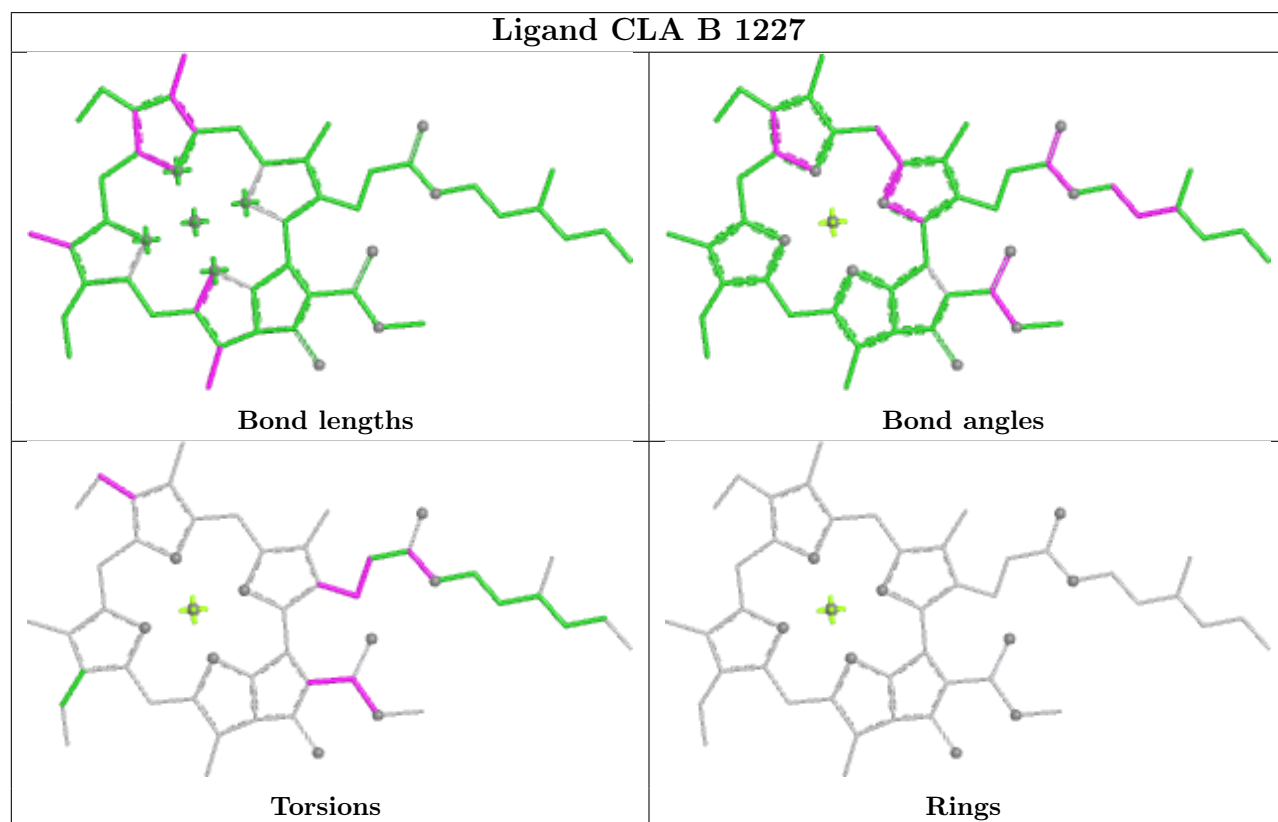
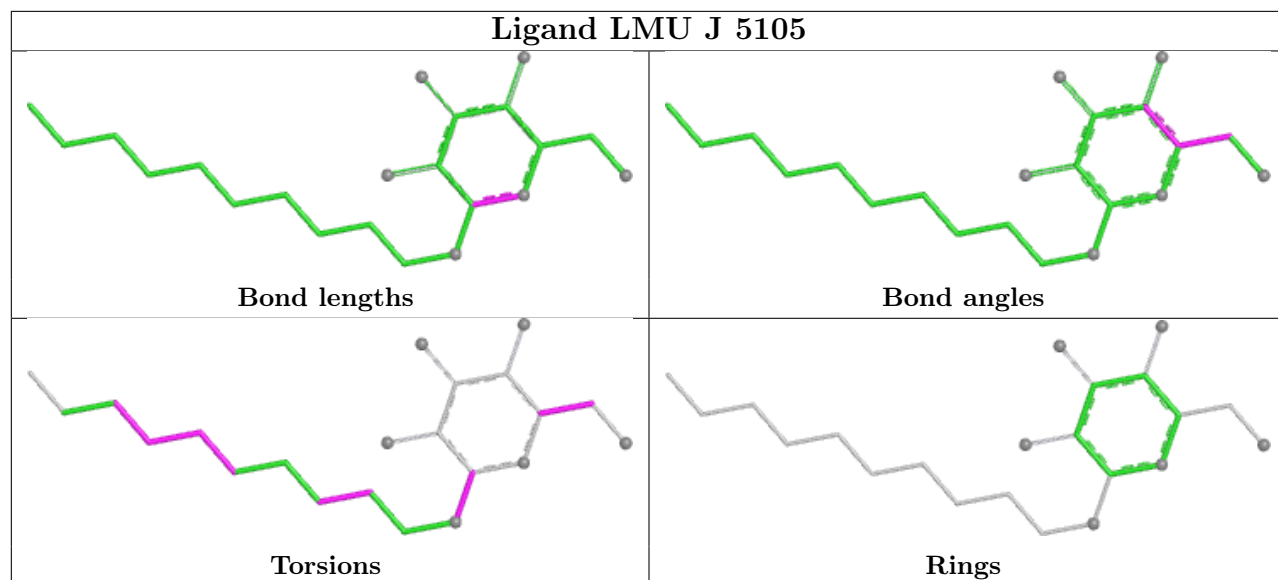
Ligand CLA 6 509



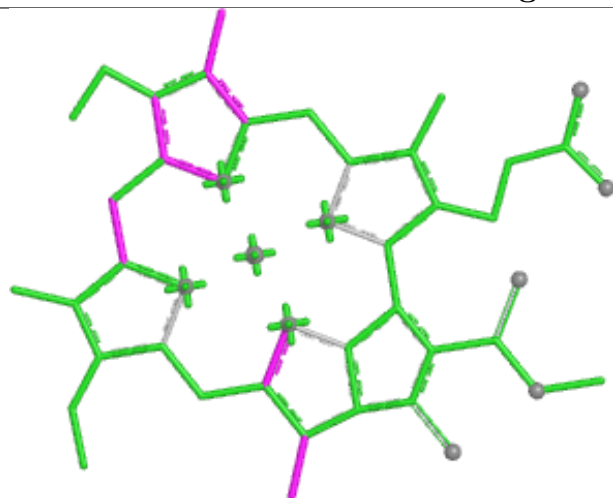
Ligand CLA 1 517



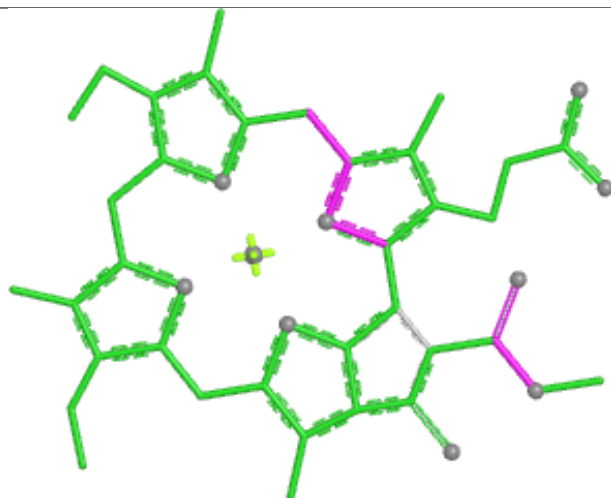




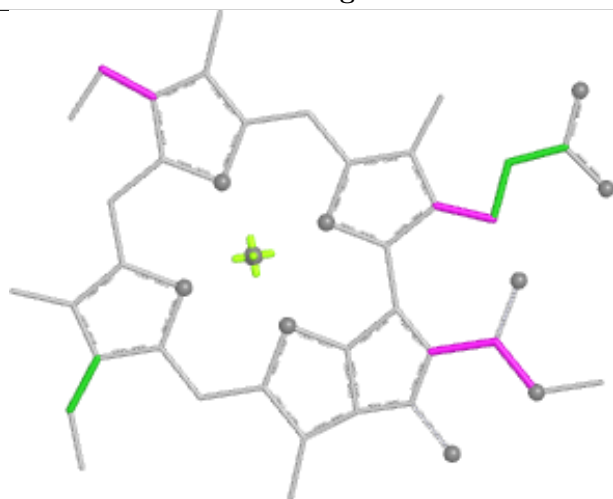
Ligand CLA e 519



Bond lengths



Bond angles

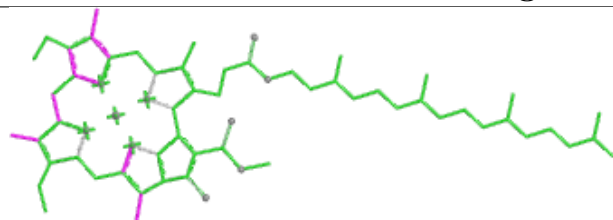


Torsions

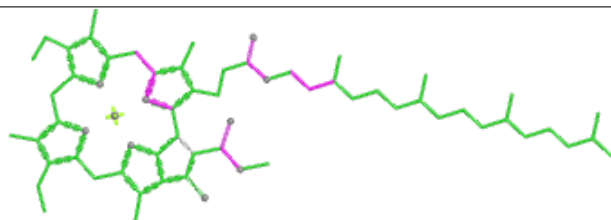


Rings

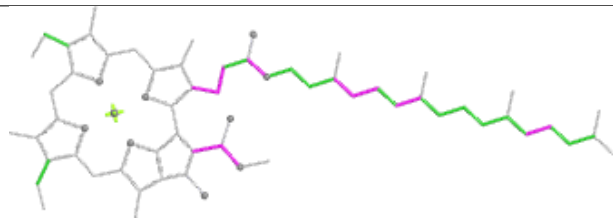
Ligand CLA 6 501



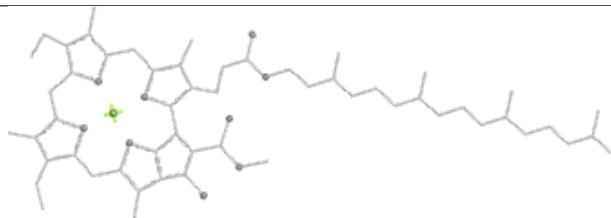
Bond lengths



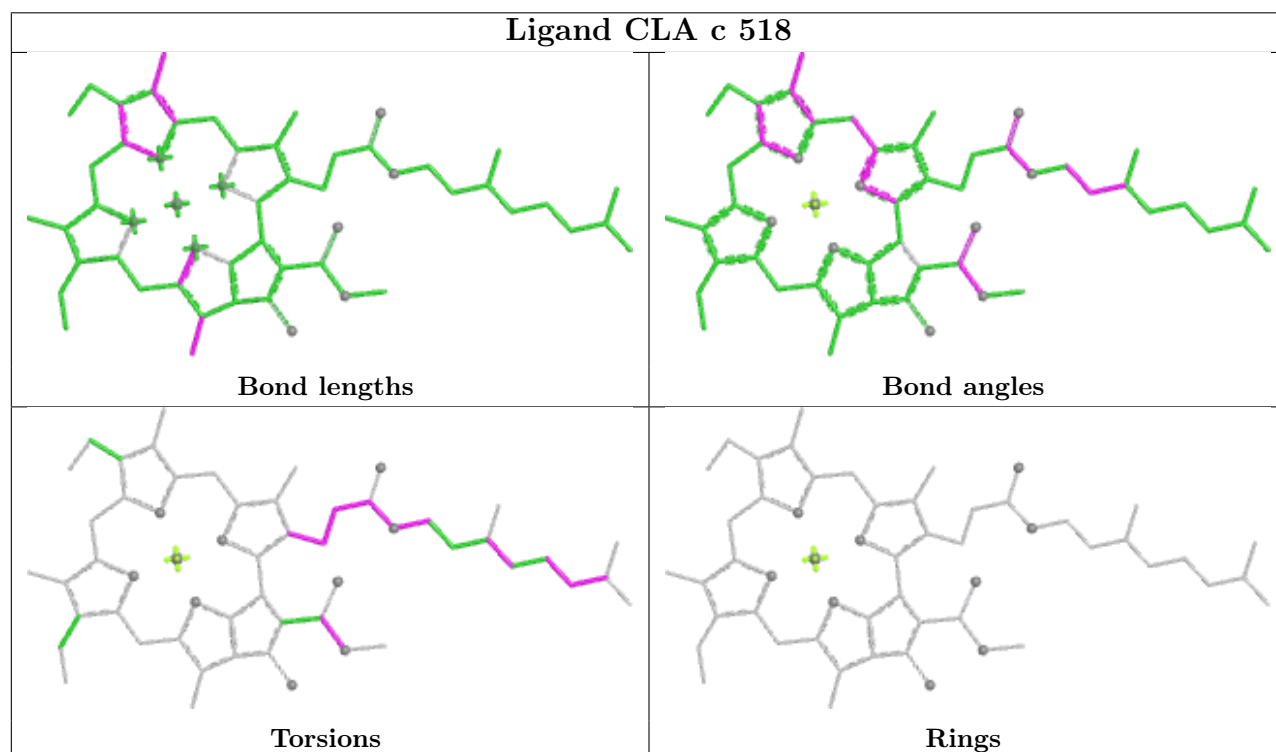
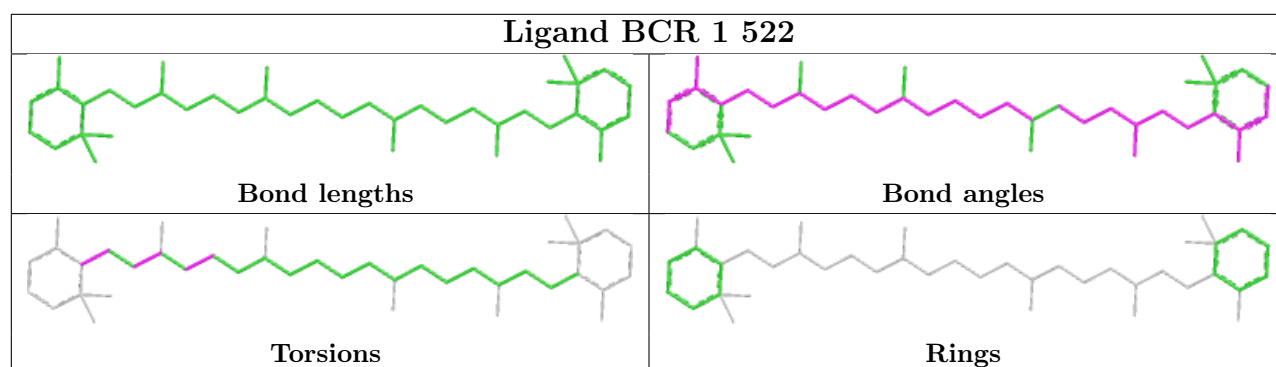
Bond angles



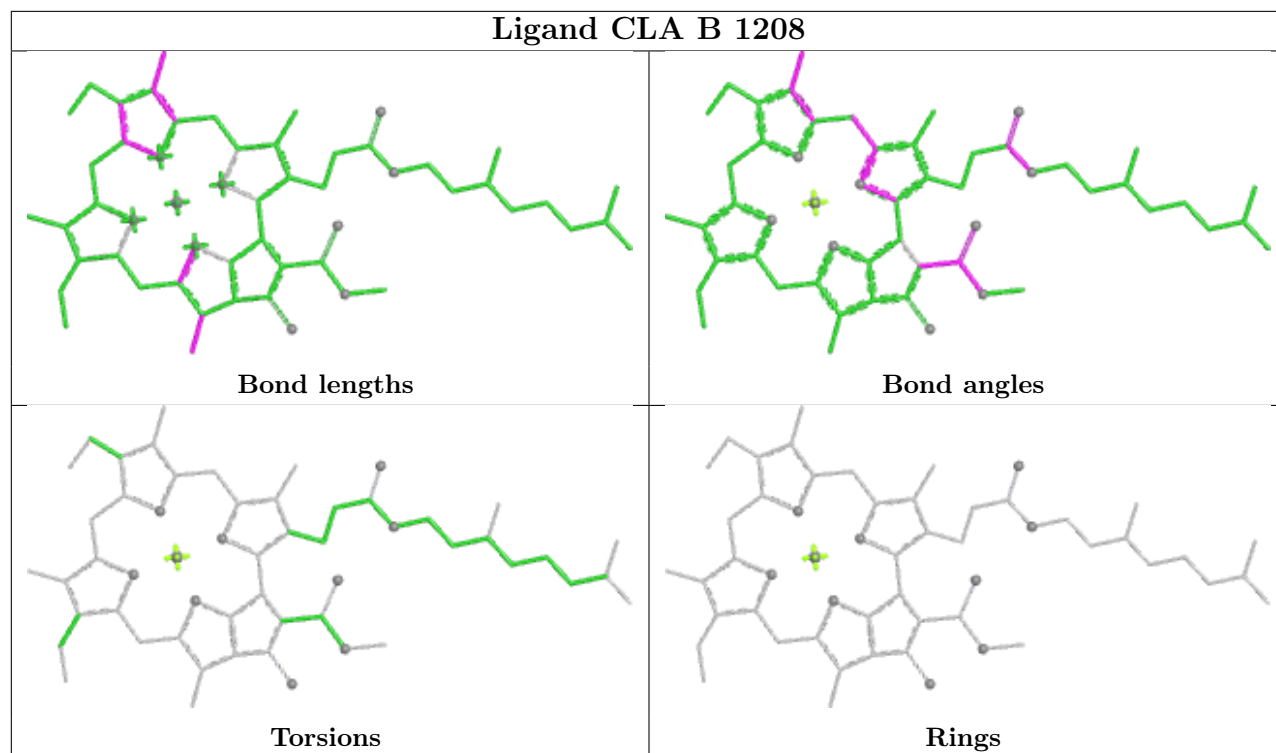
Torsions



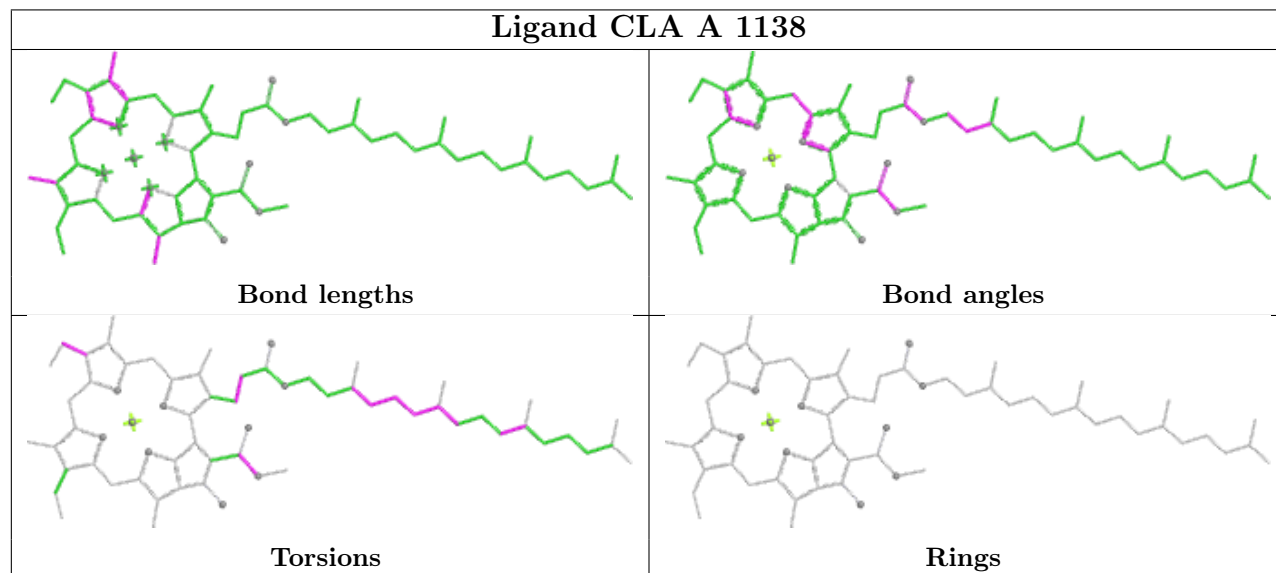
Rings

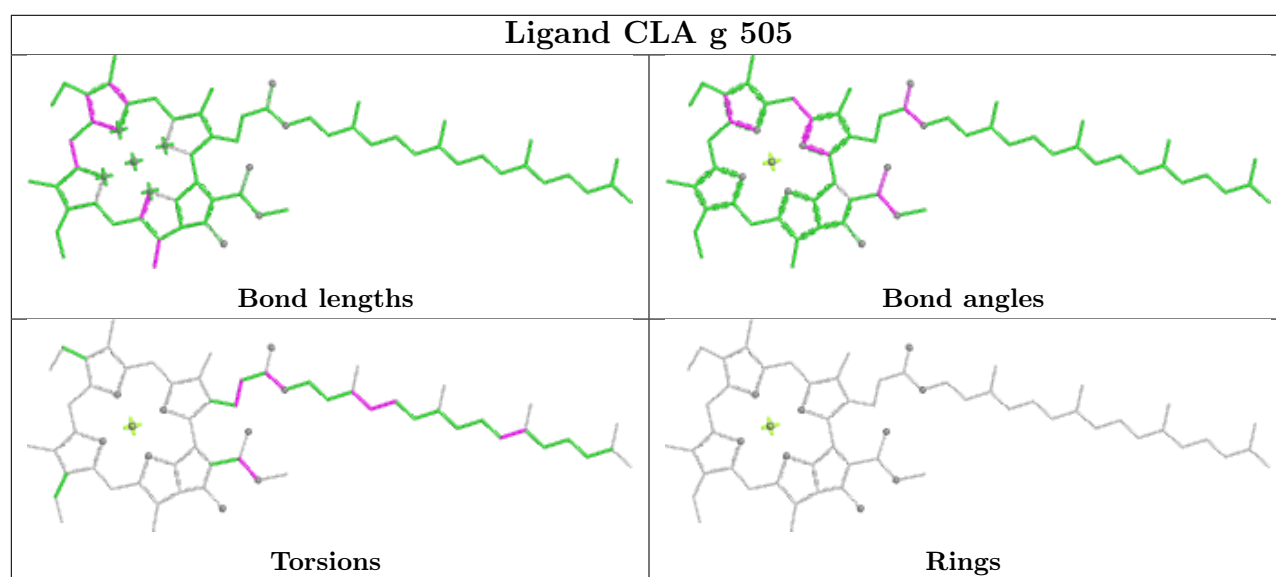
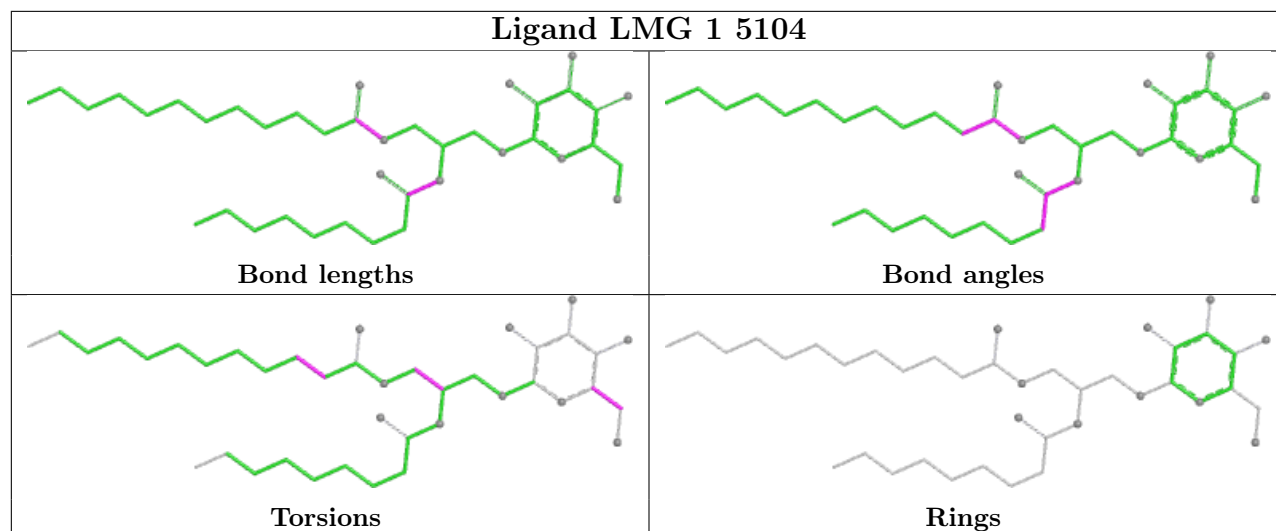


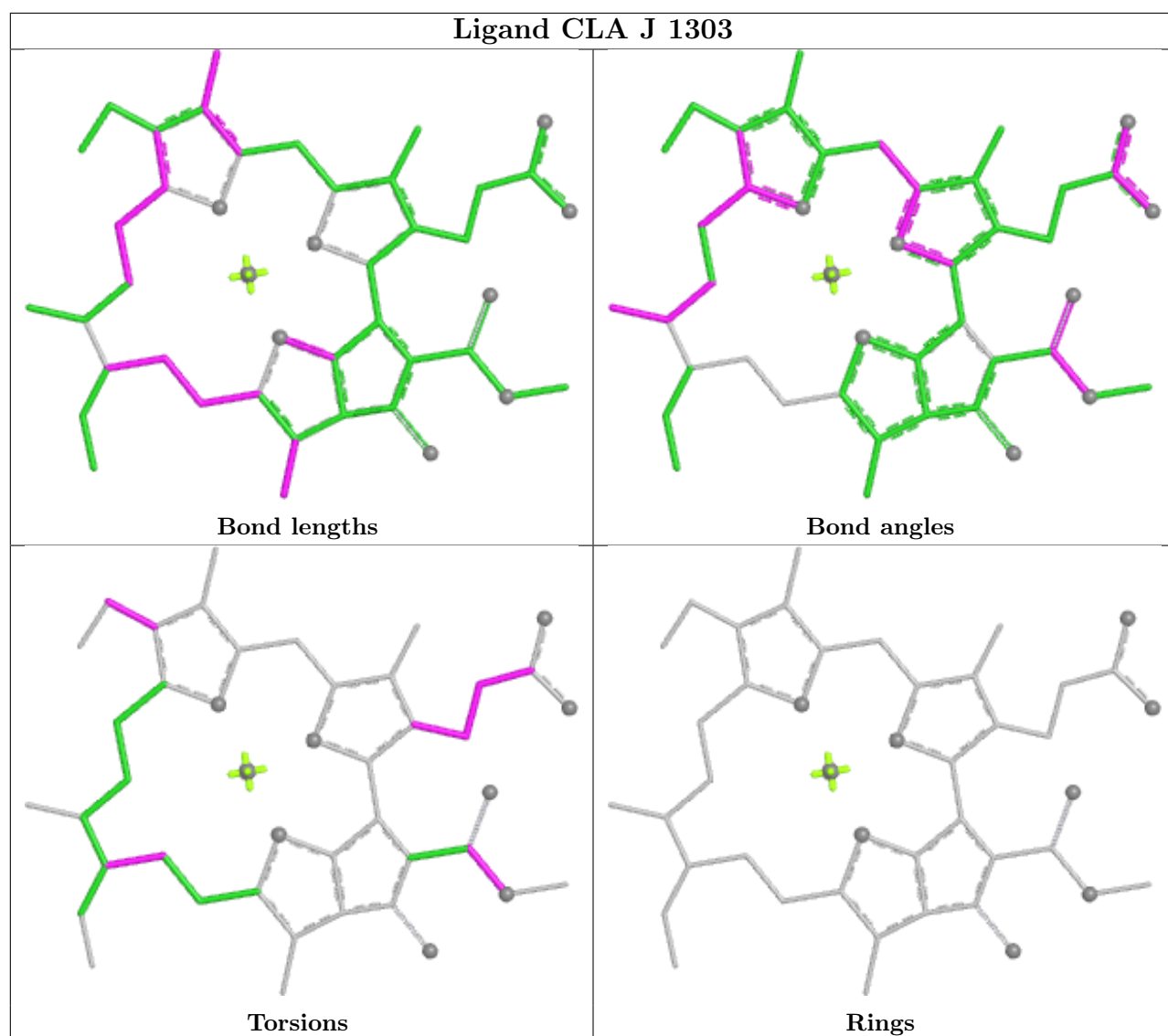
Ligand CLA B 1208



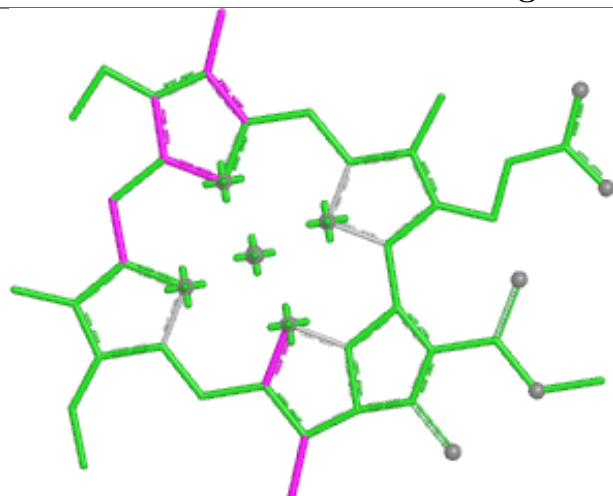
Ligand CLA A 1138



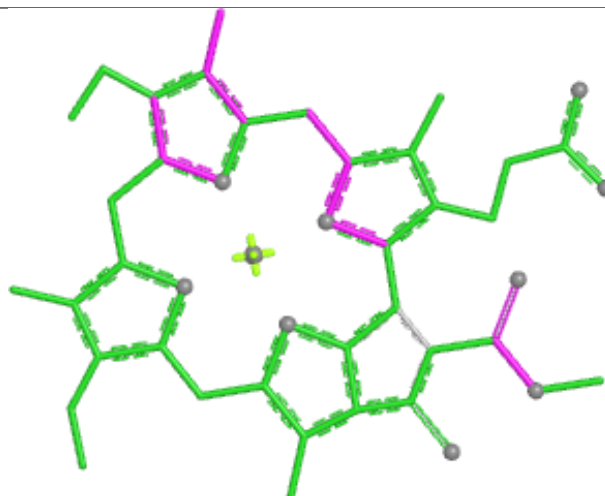




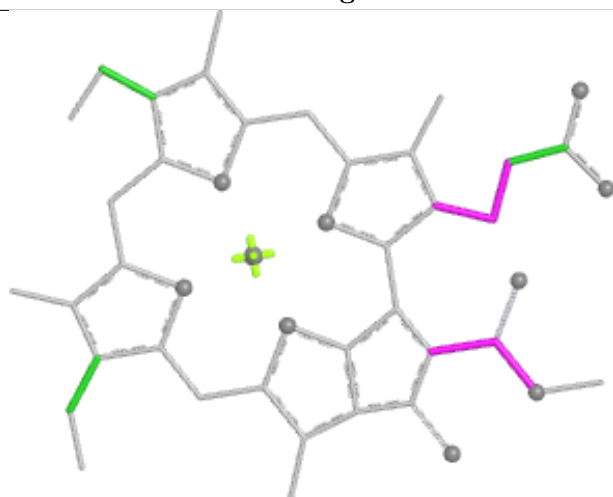
Ligand CLA a 506



Bond lengths



Bond angles

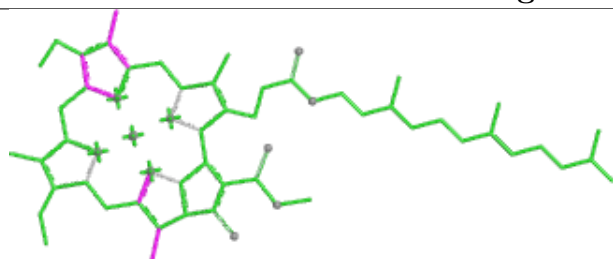


Torsions

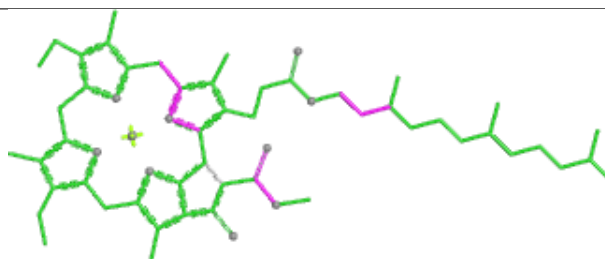


Rings

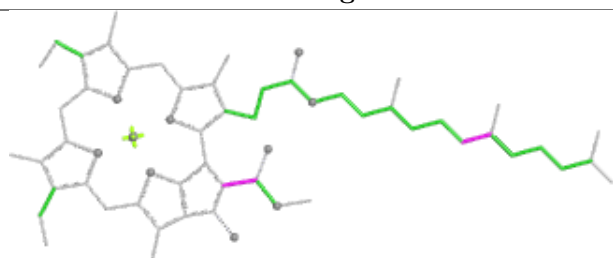
Ligand CLA d 507



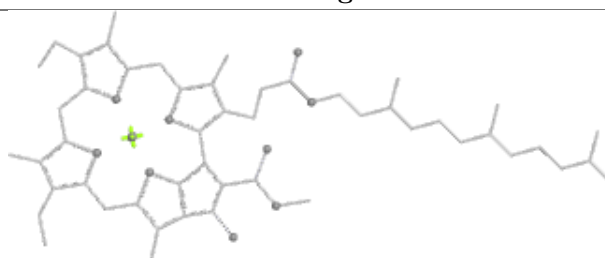
Bond lengths



Bond angles

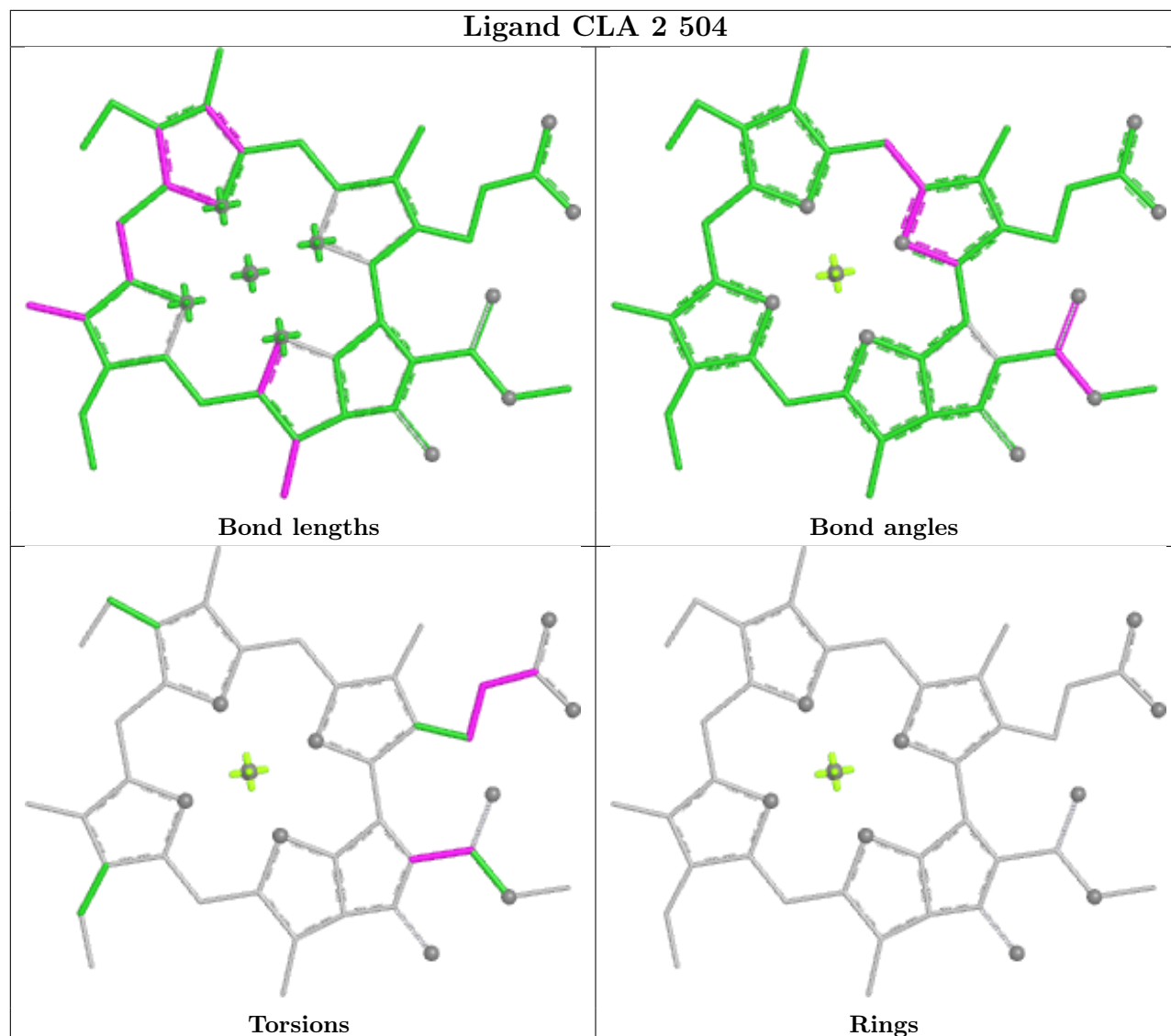


Torsions

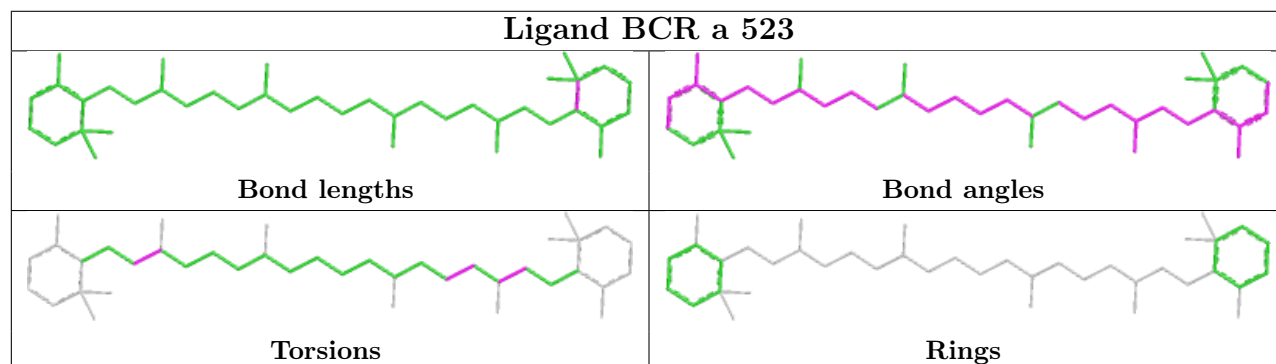


Rings

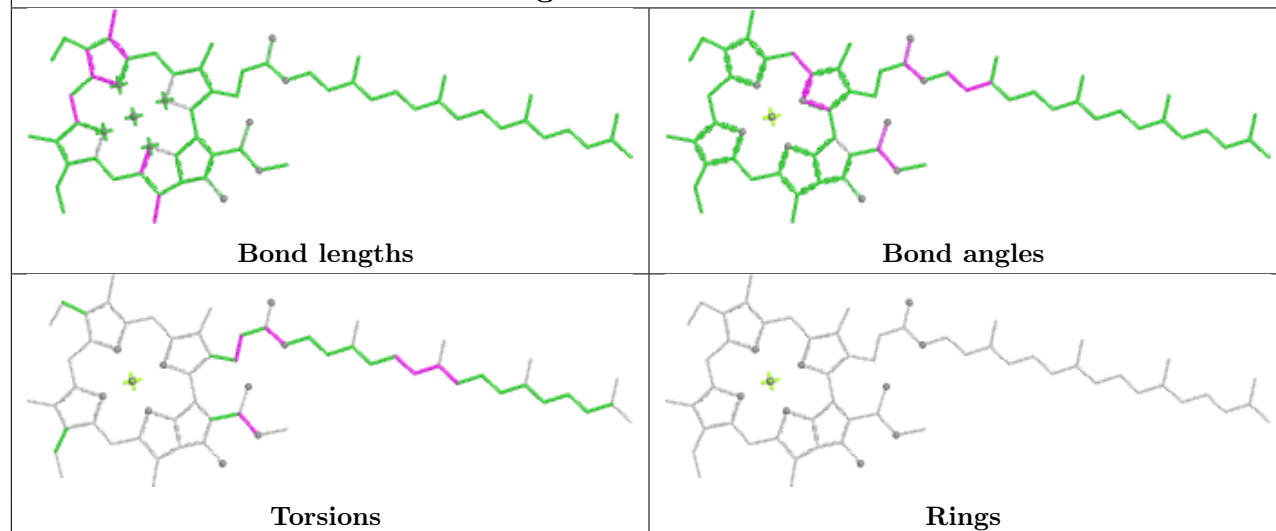
Ligand CLA 2 504



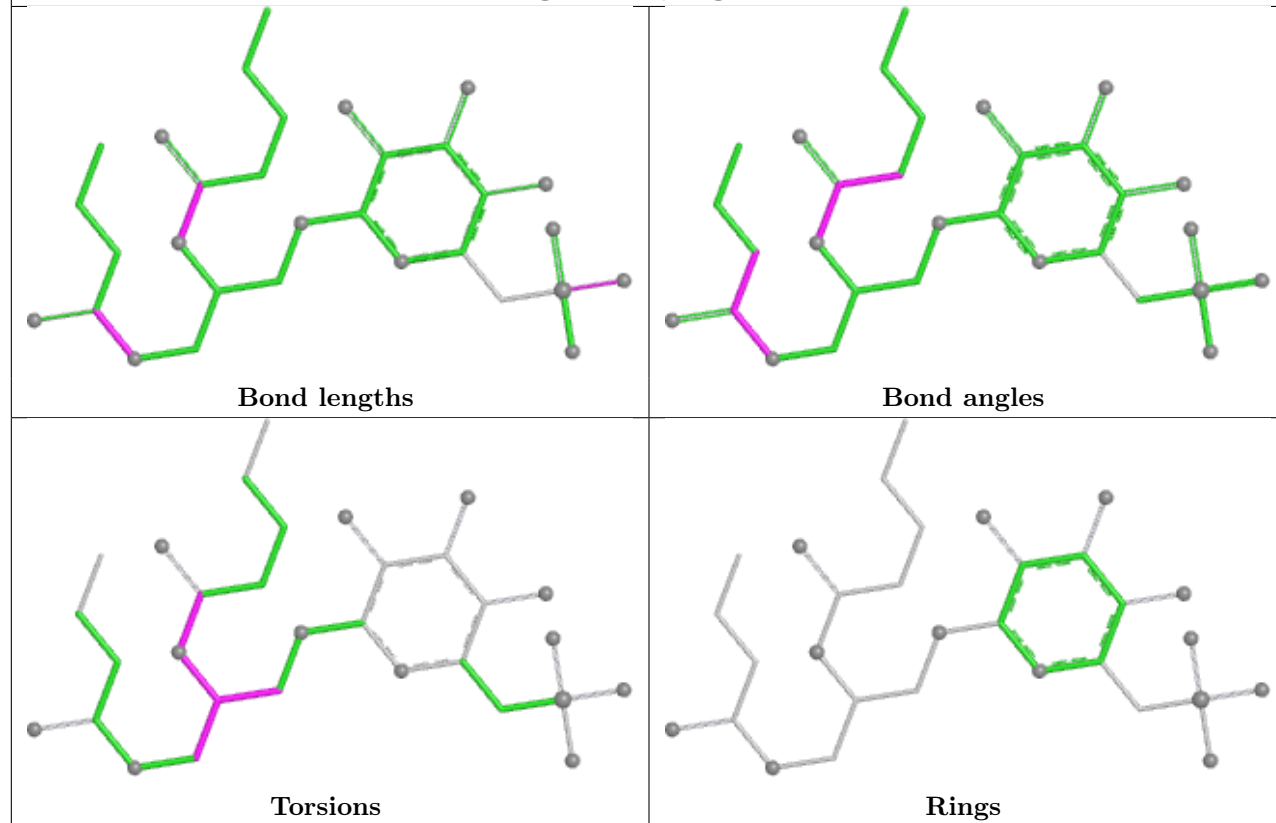
Ligand BCR a 523

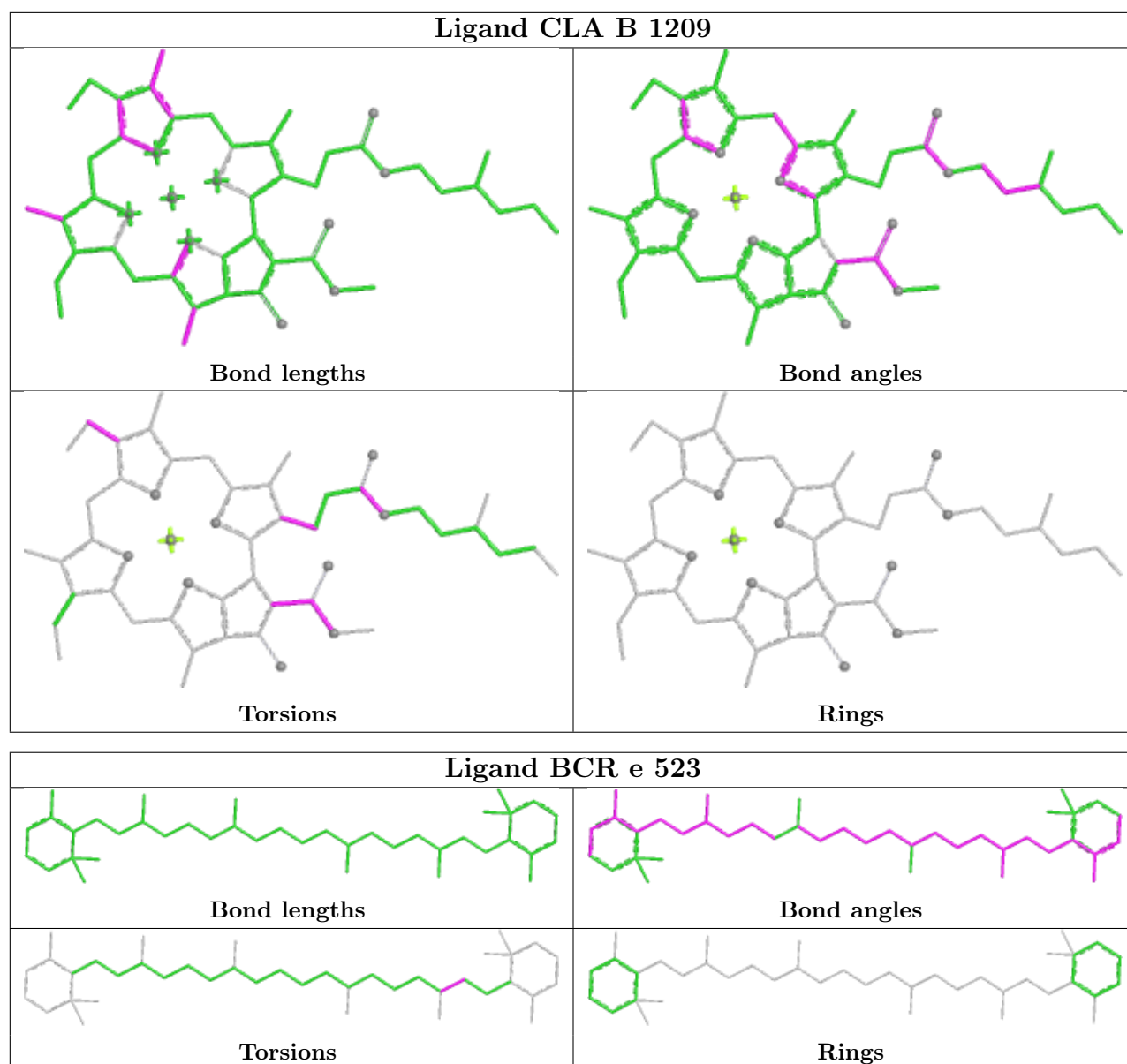


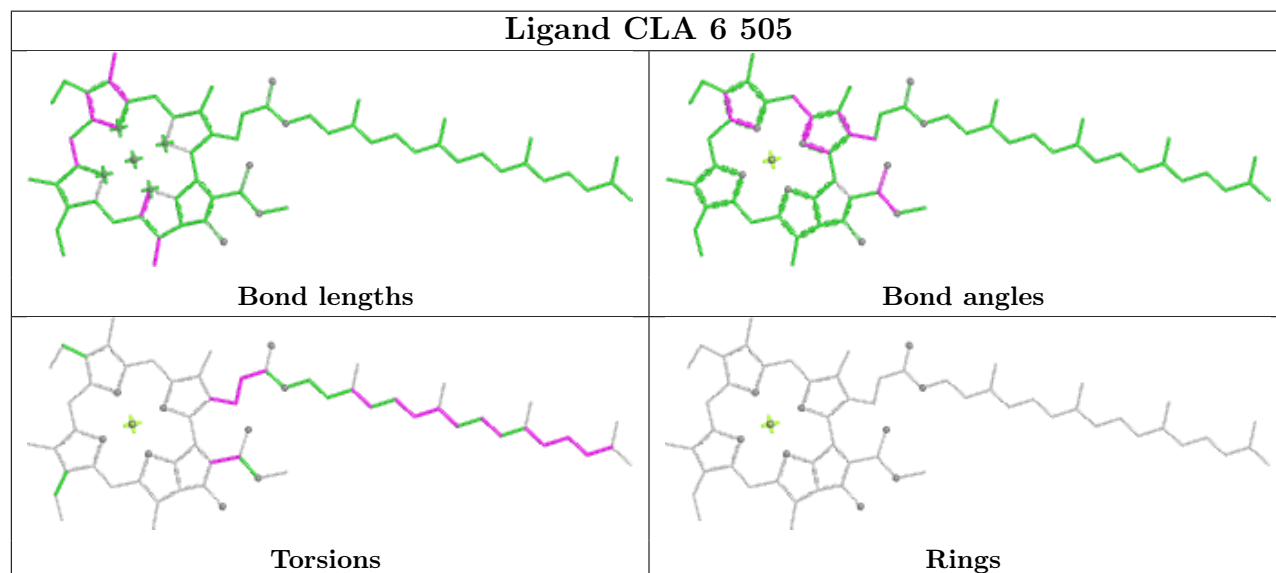
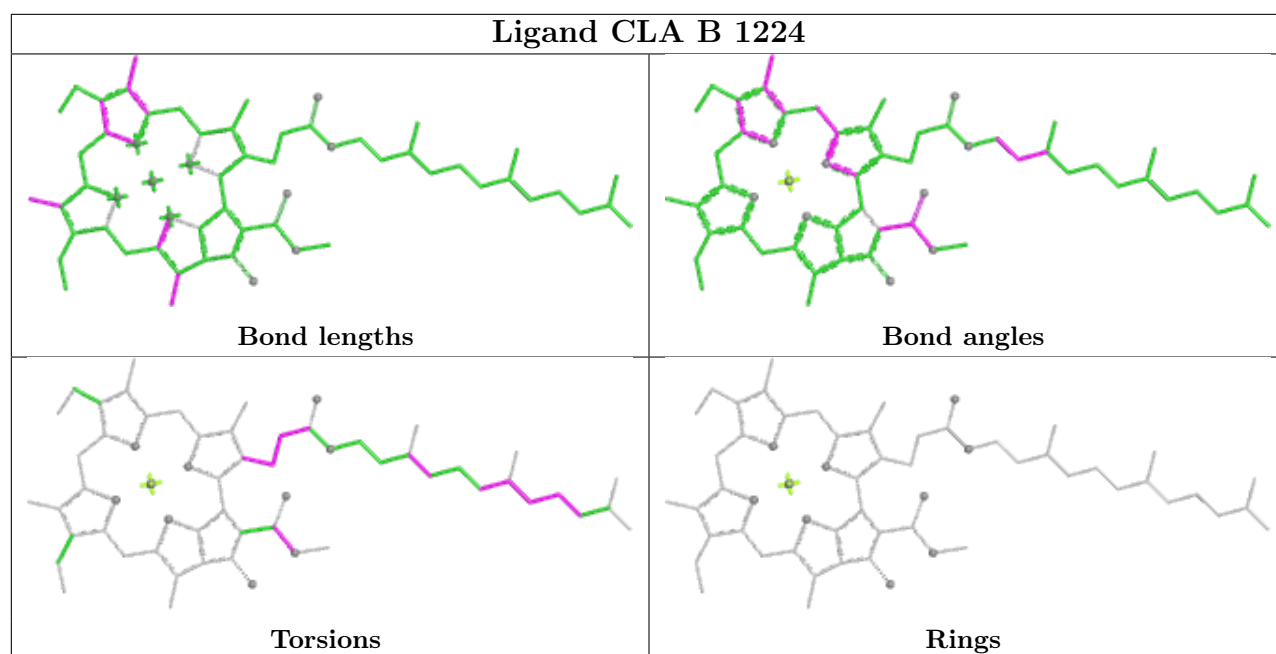
Ligand CLA 1 510



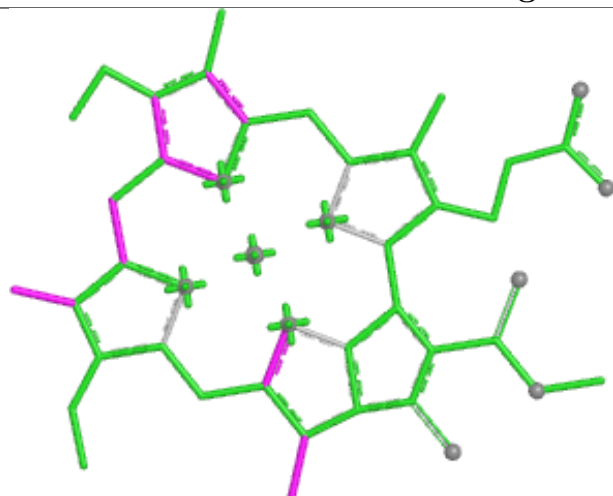
Ligand SQD g 822



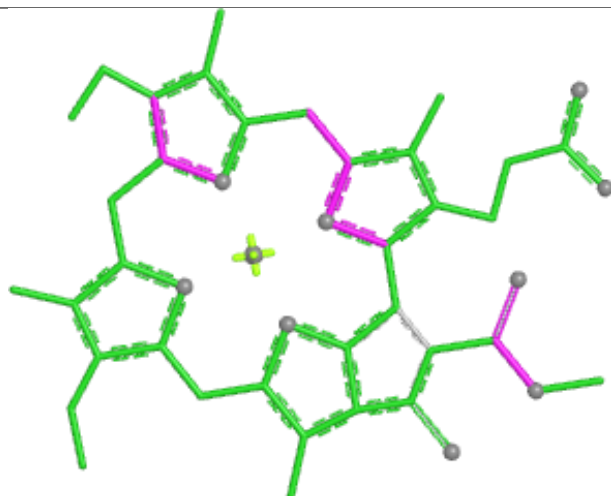




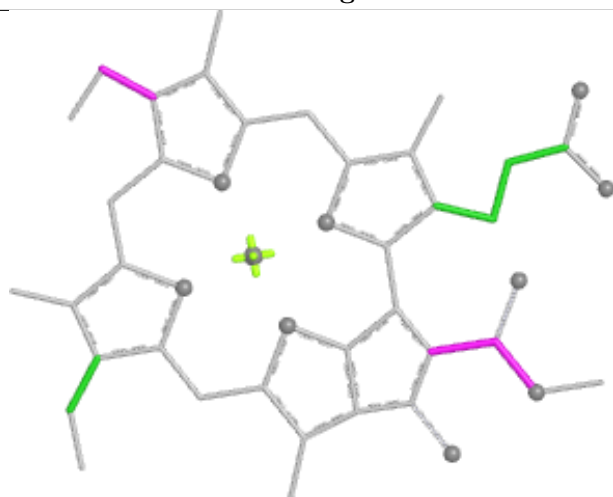
Ligand CLA 6 506



Bond lengths



Bond angles

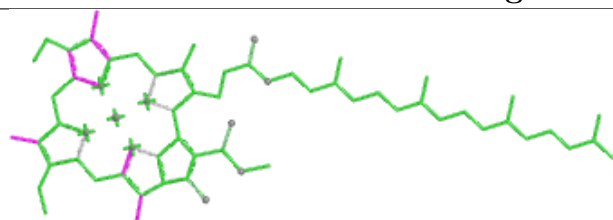


Torsions

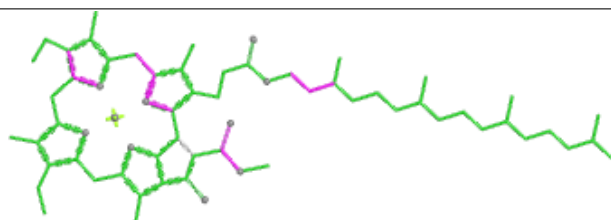


Rings

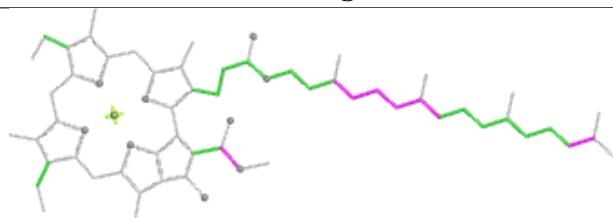
Ligand CLA B 1223



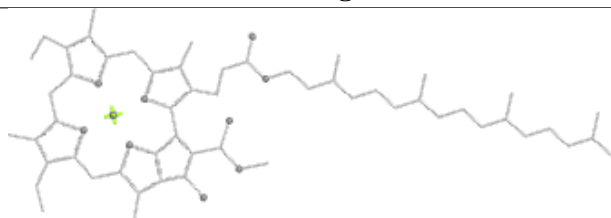
Bond lengths



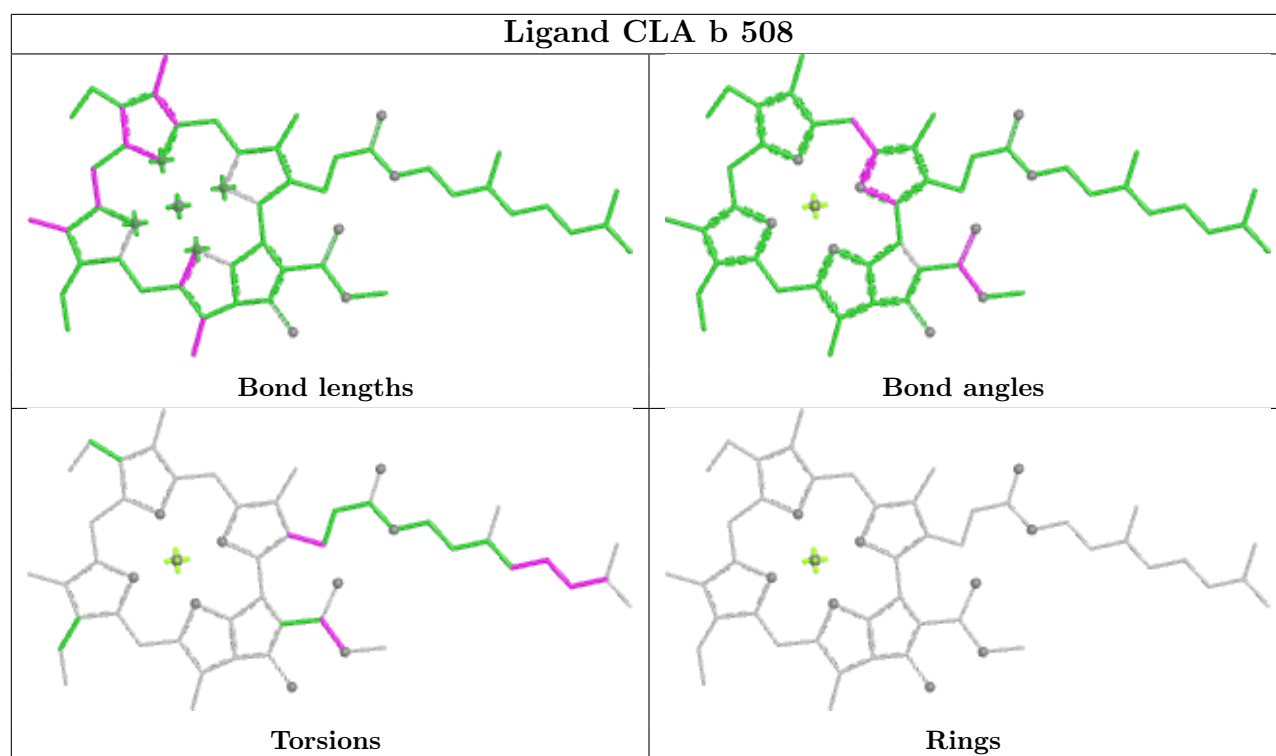
Bond angles



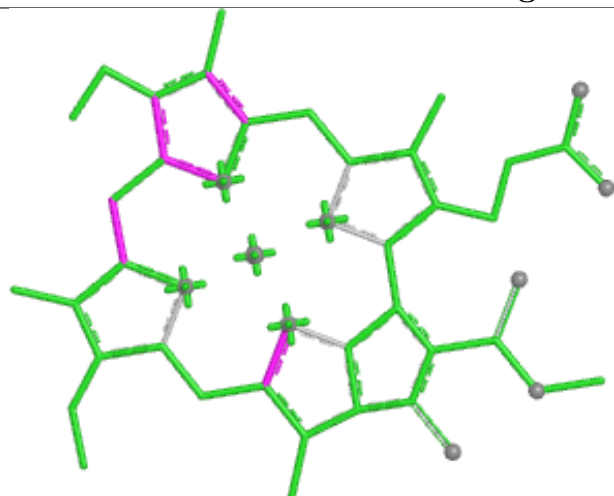
Torsions



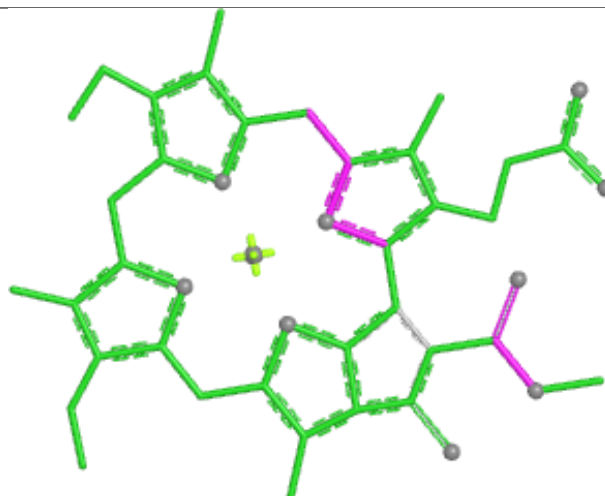
Rings



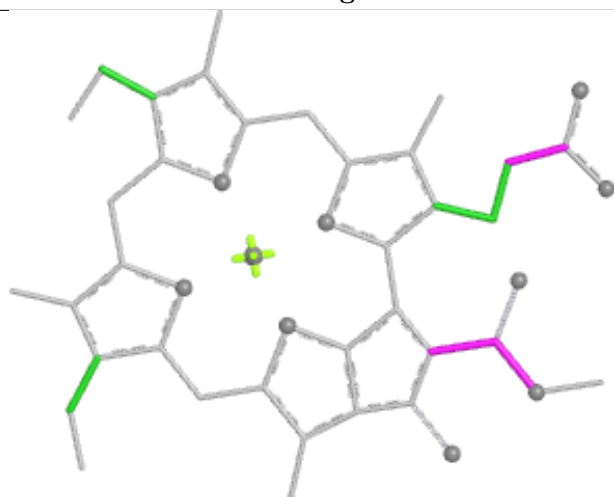
Ligand CLA 4 517



Bond lengths



Bond angles

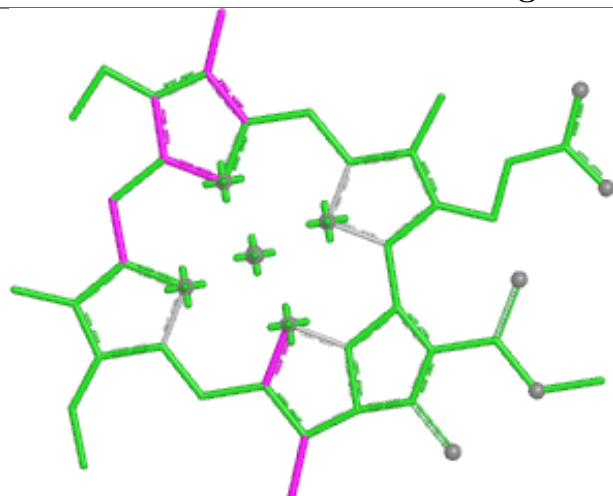


Torsions

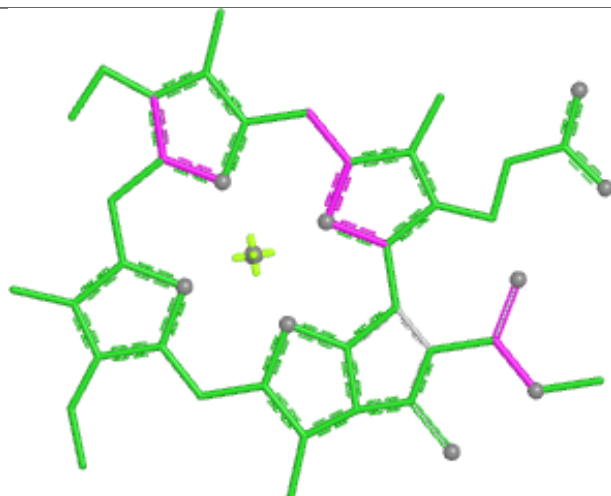


Rings

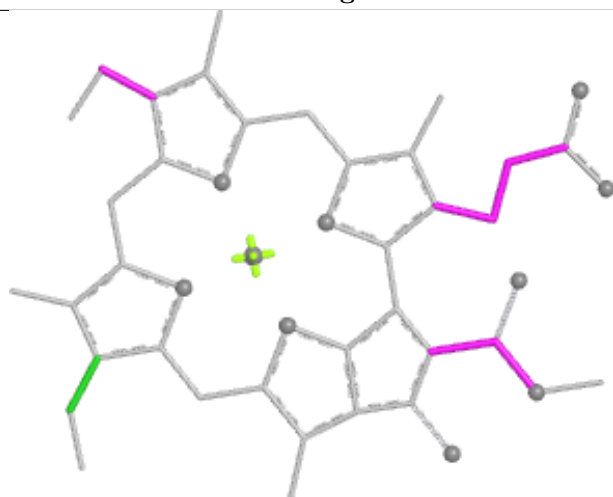
Ligand CLA 5 516



Bond lengths



Bond angles

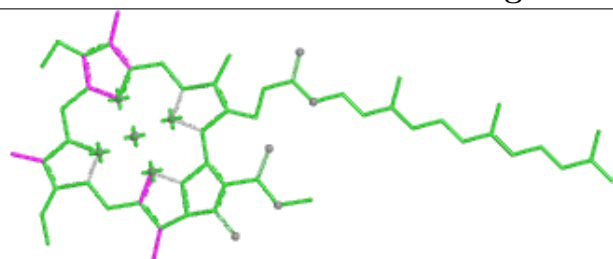


Torsions

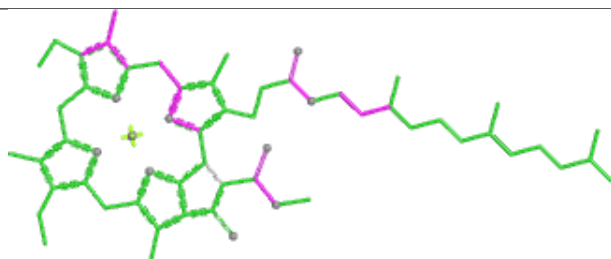


Rings

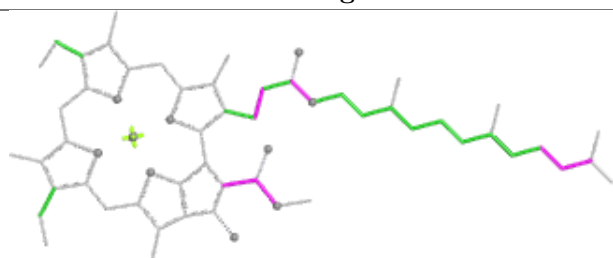
Ligand CLA A 1111



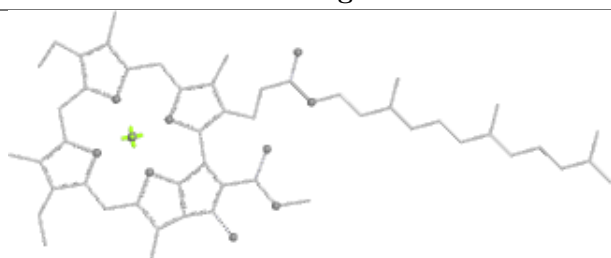
Bond lengths



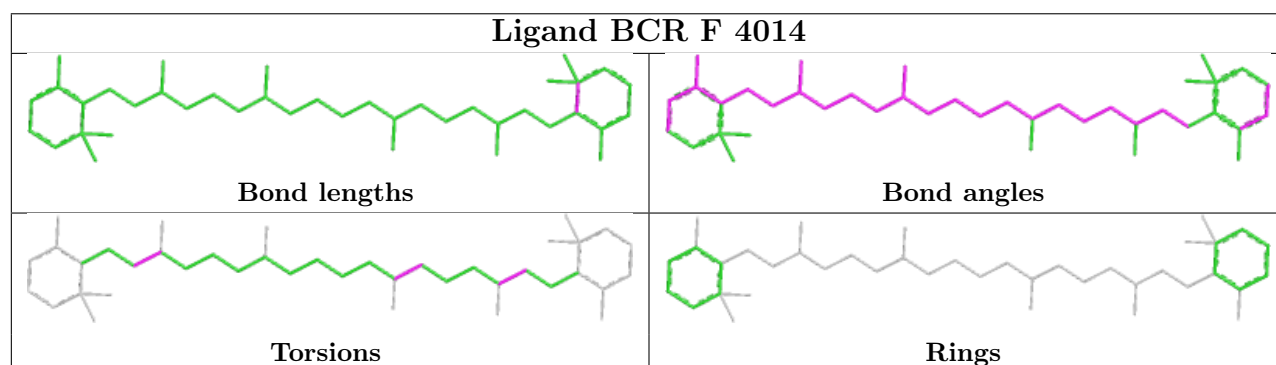
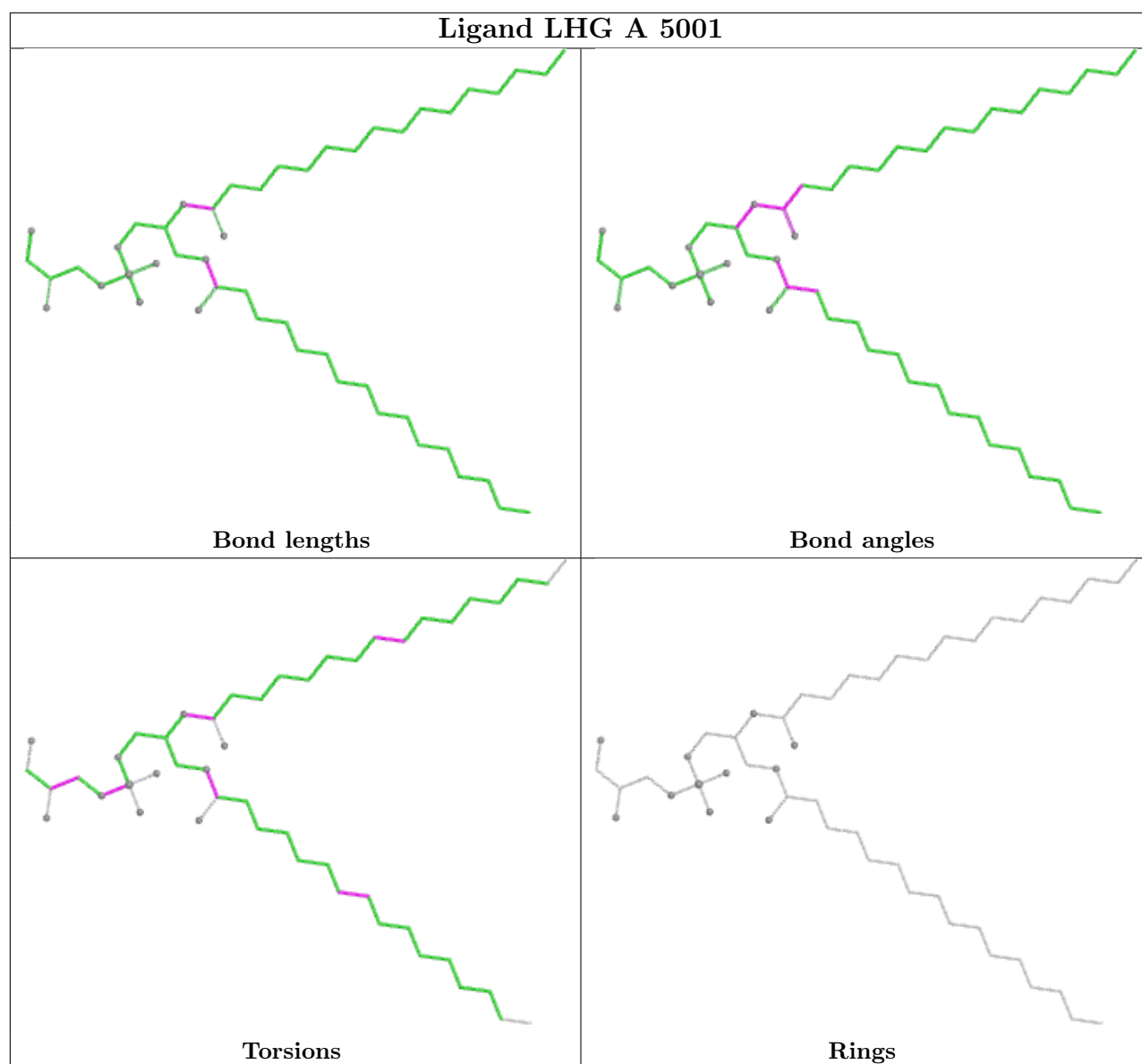
Bond angles



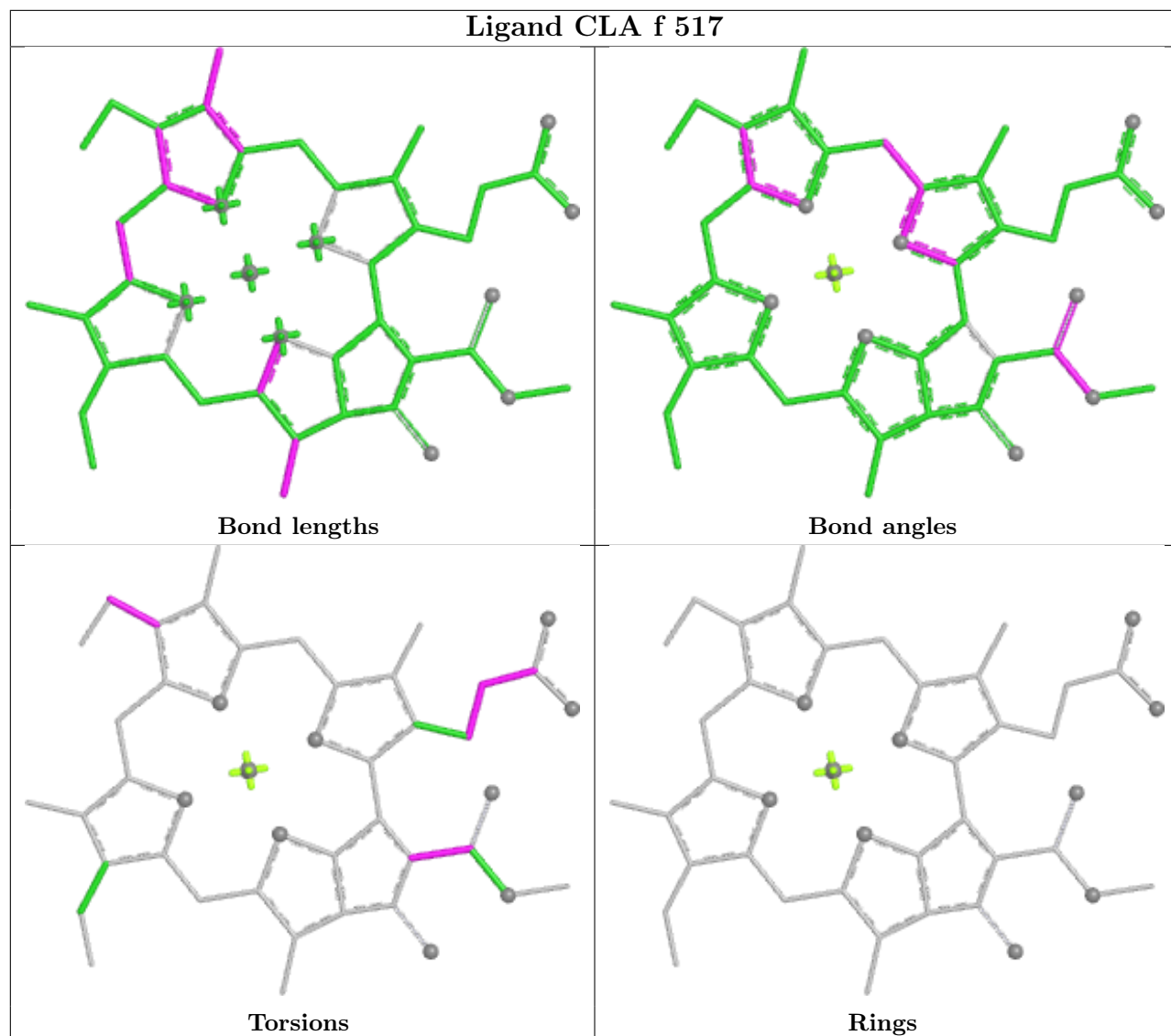
Torsions

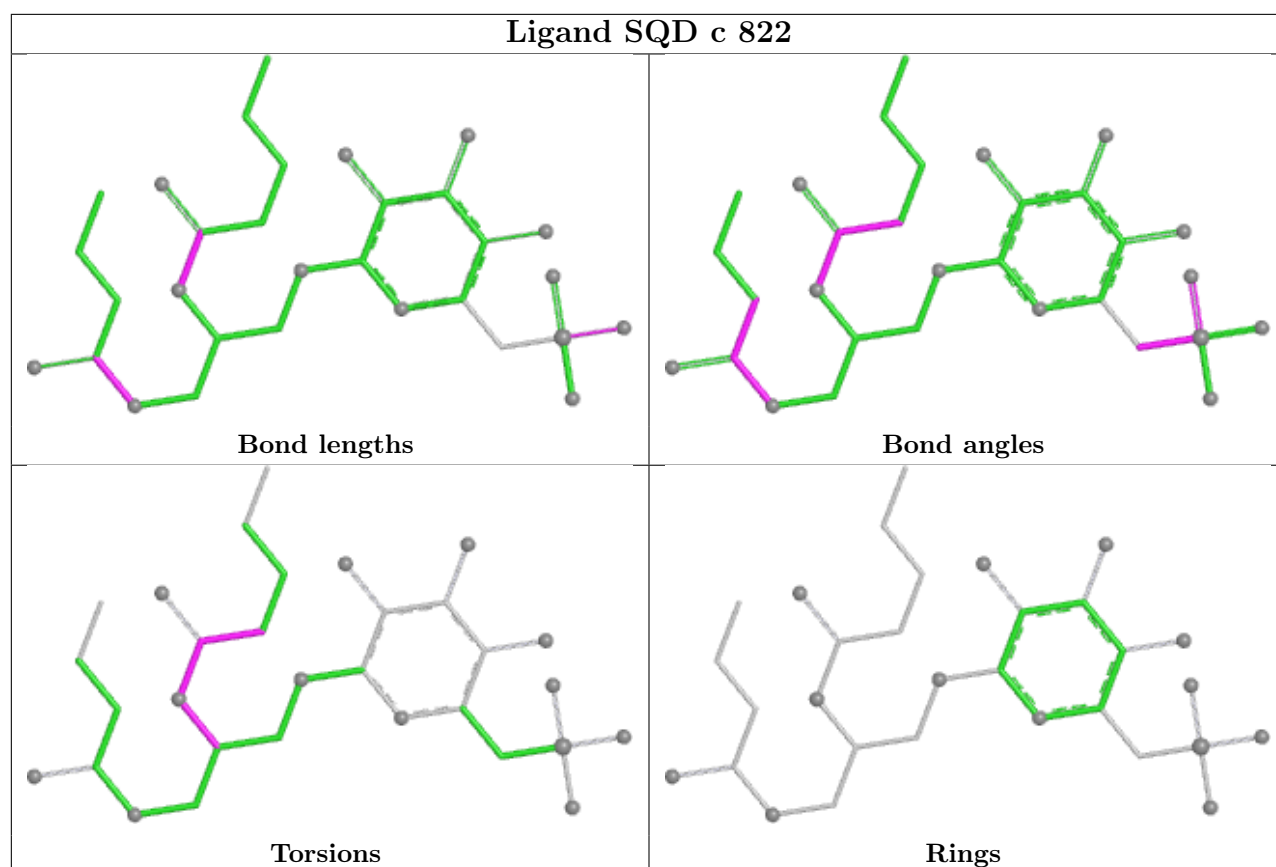


Rings

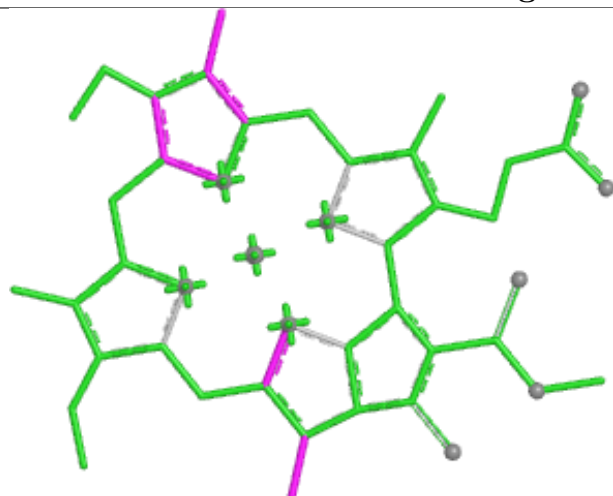


Ligand CLA f 517

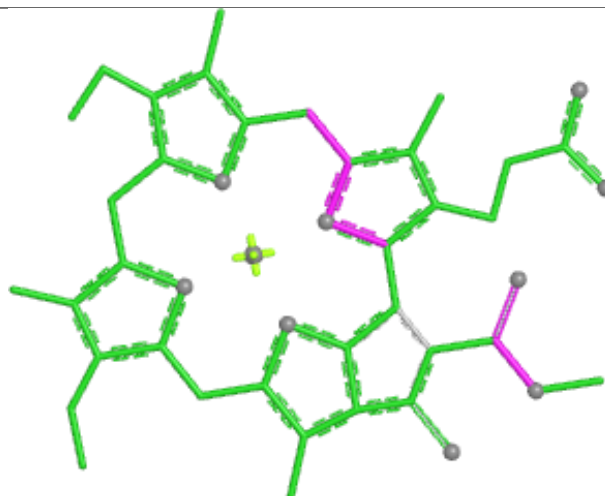




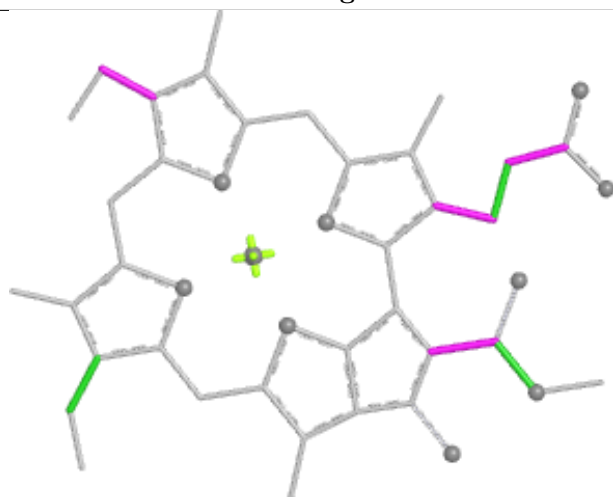
Ligand CLA 3 516



Bond lengths



Bond angles

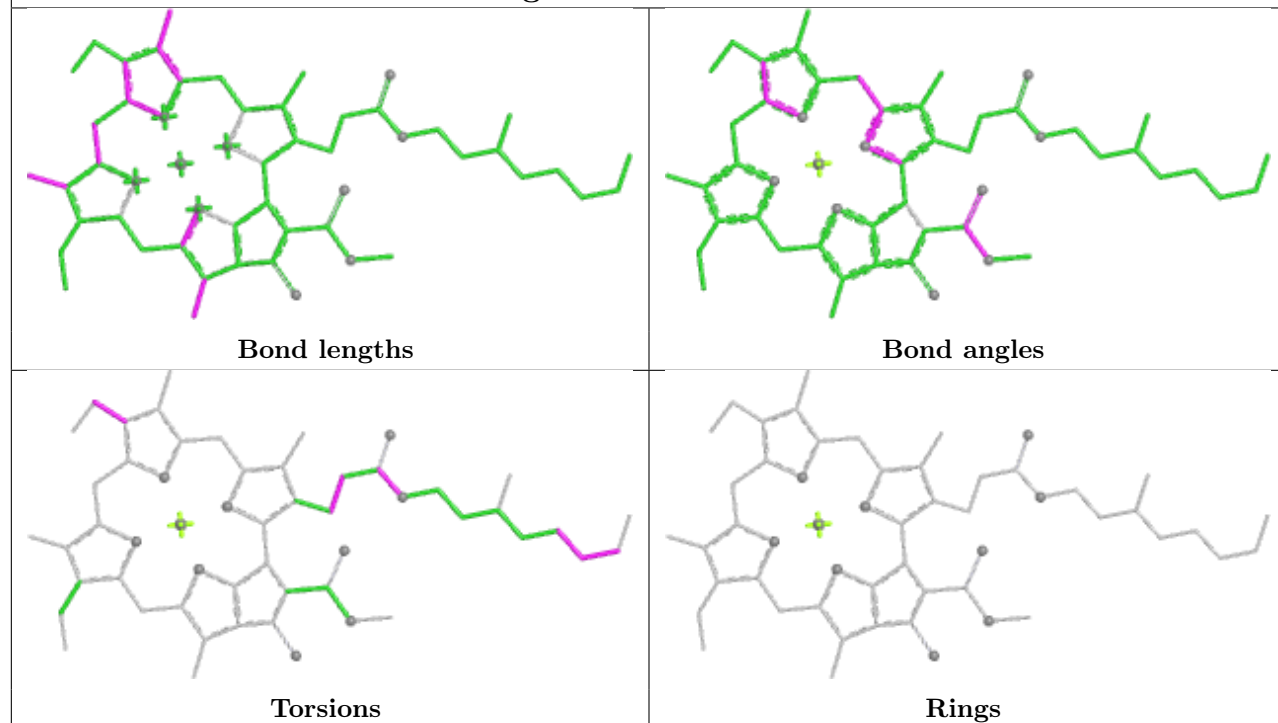


Torsions

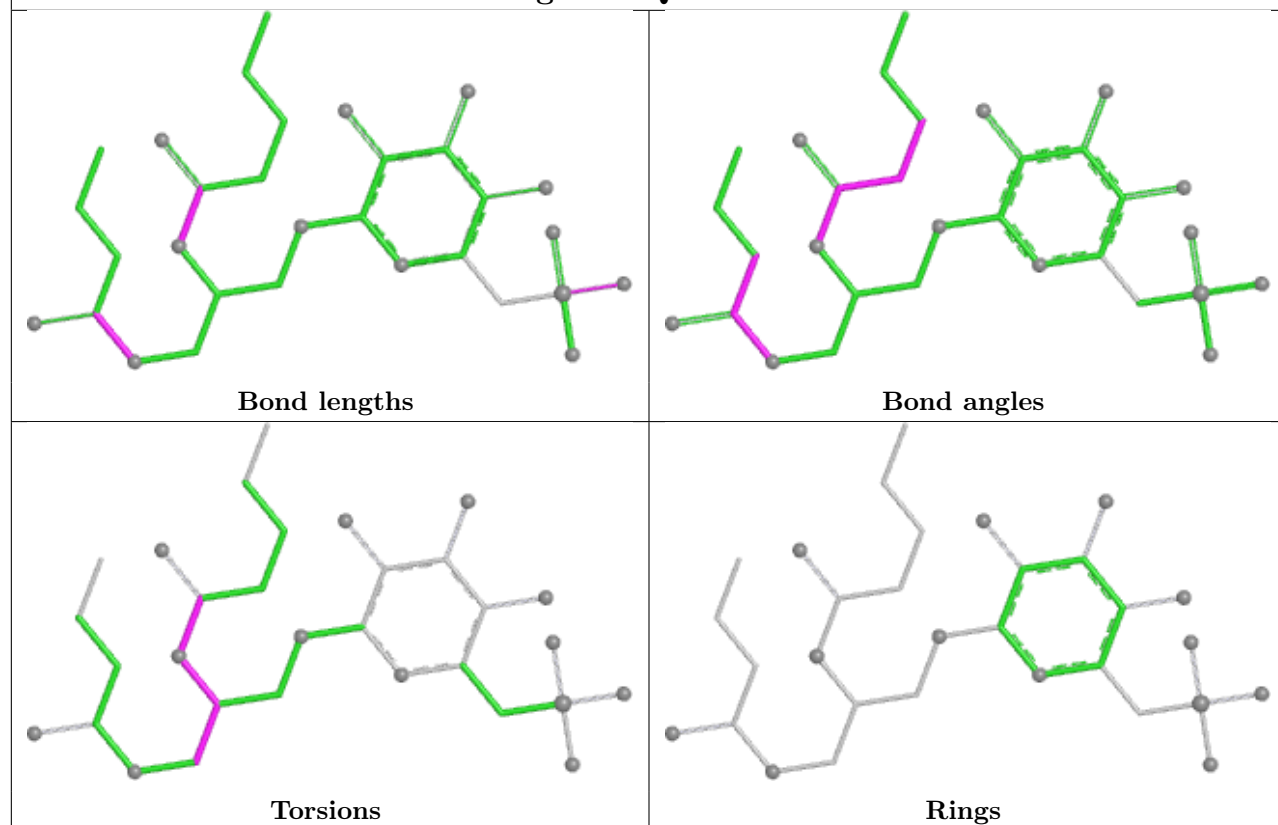


Rings

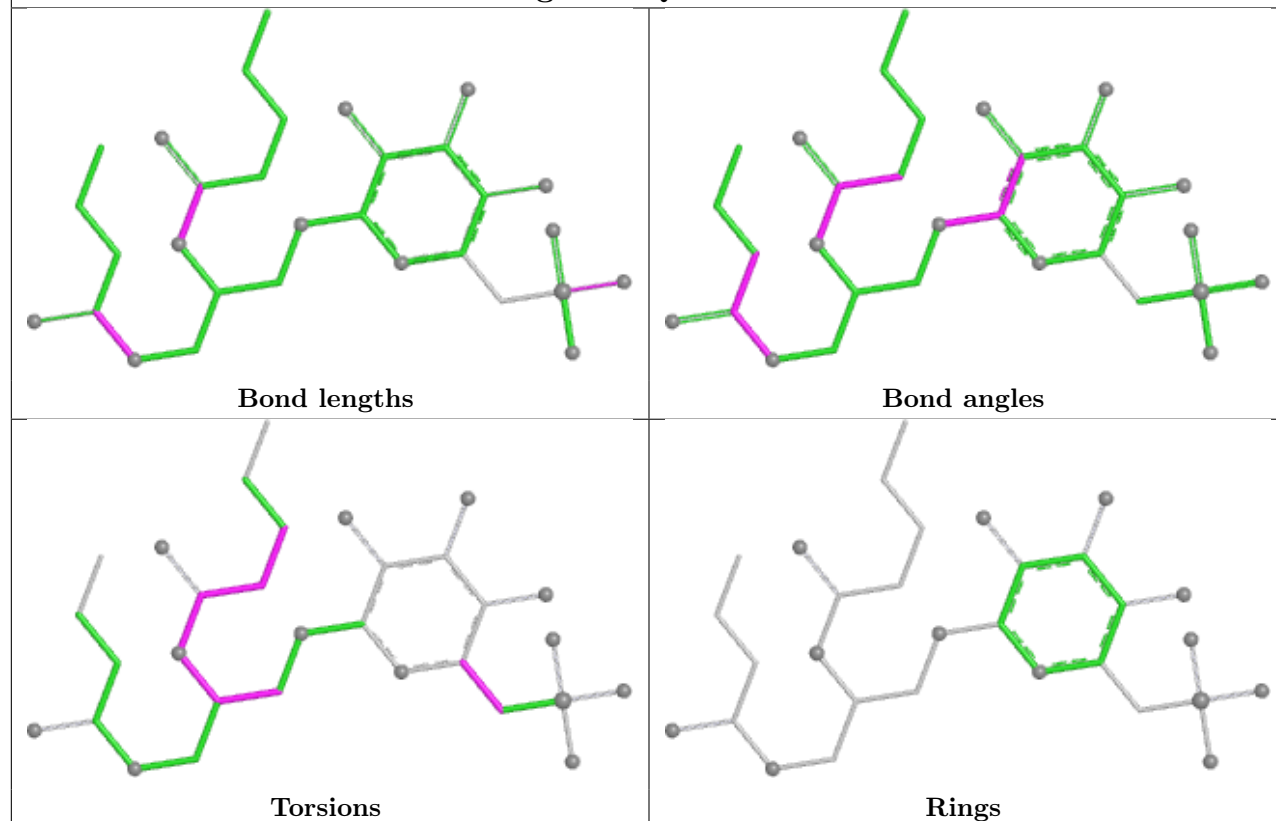
Ligand CLA A 1110



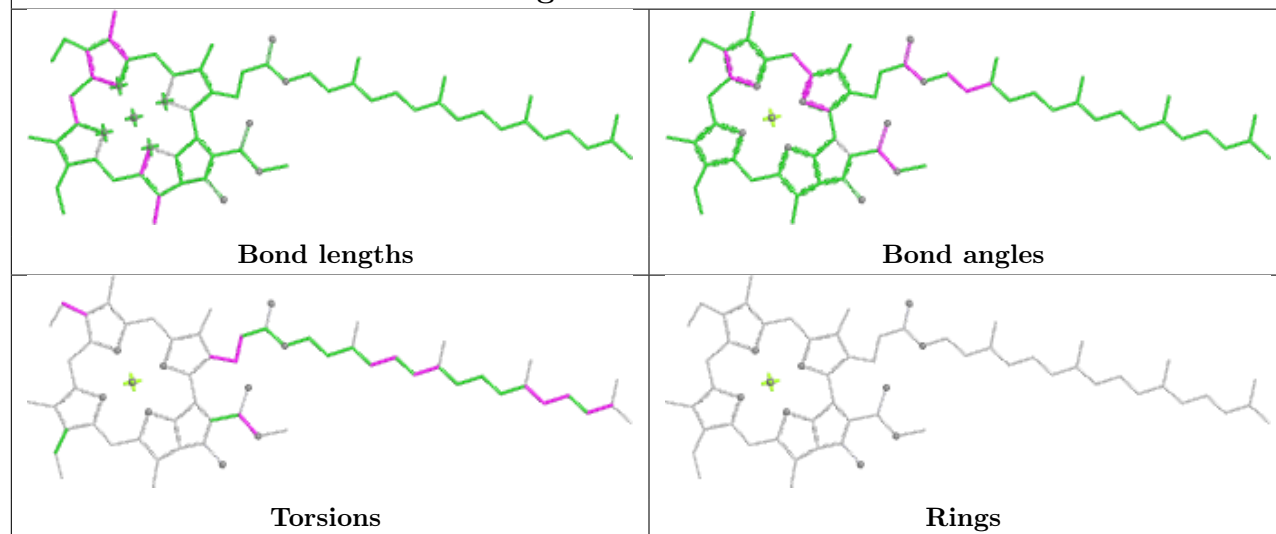
Ligand SQD 4 822



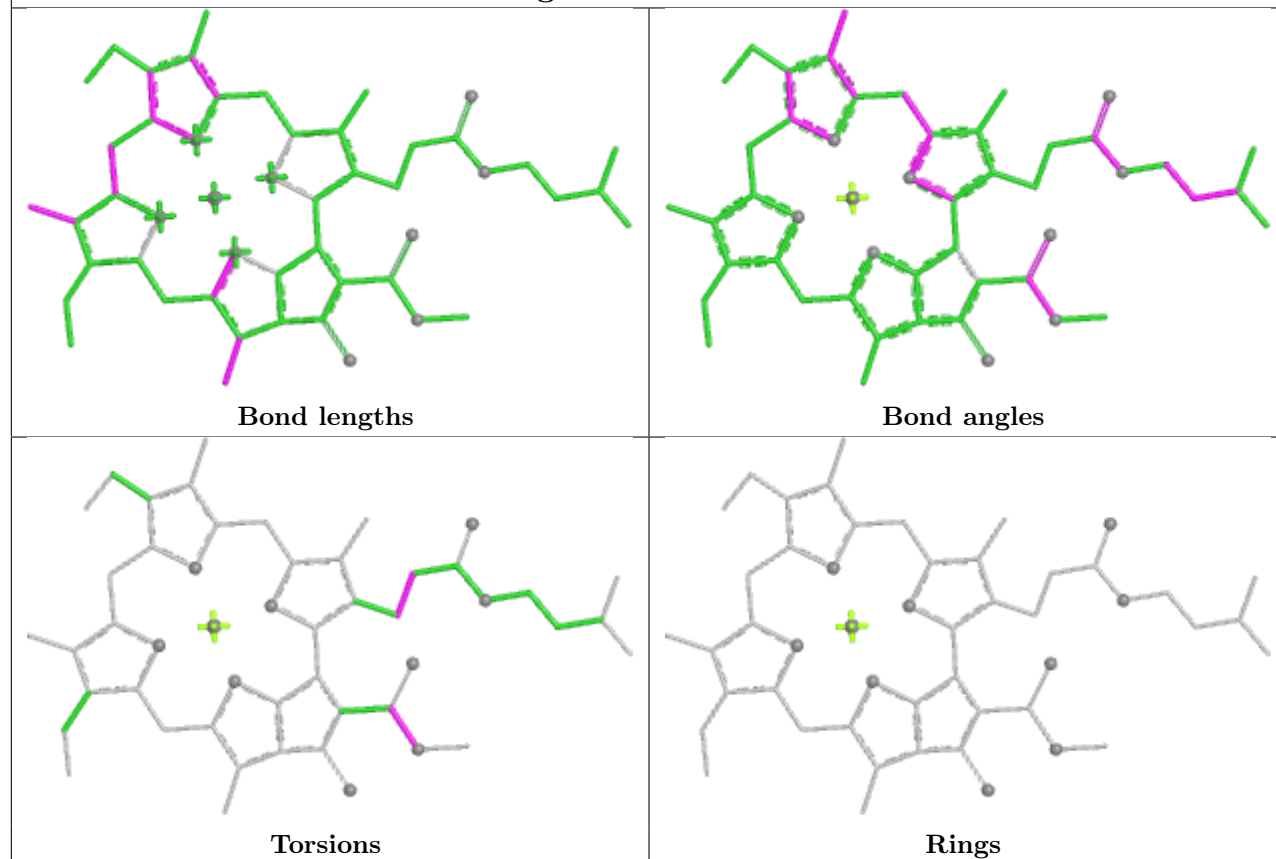
Ligand SQD 6 822



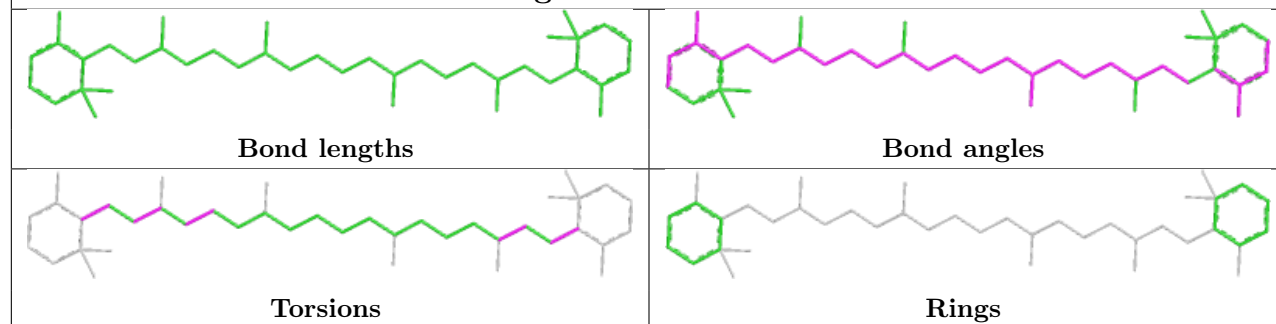
Ligand CLA e 501



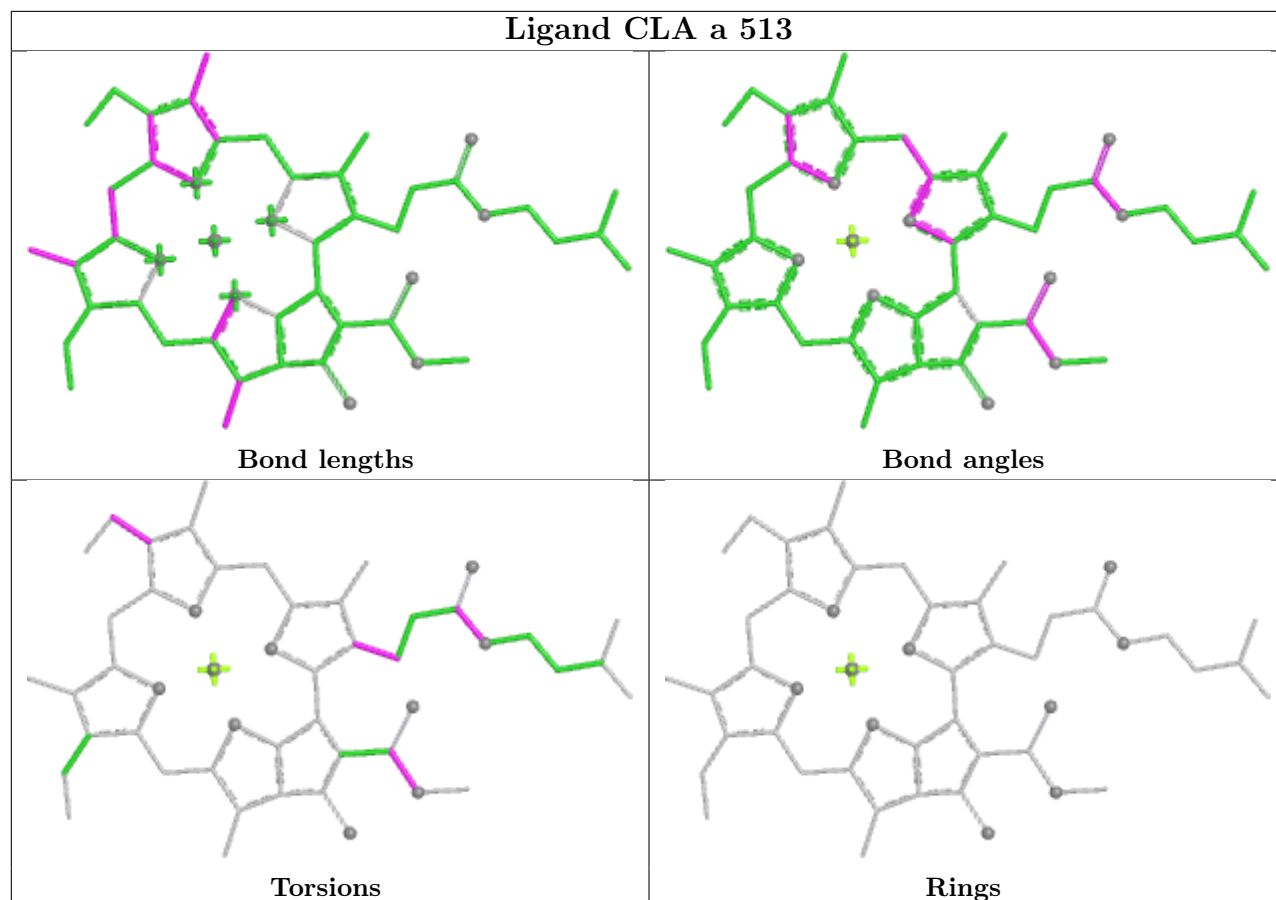
Ligand CLA e 513



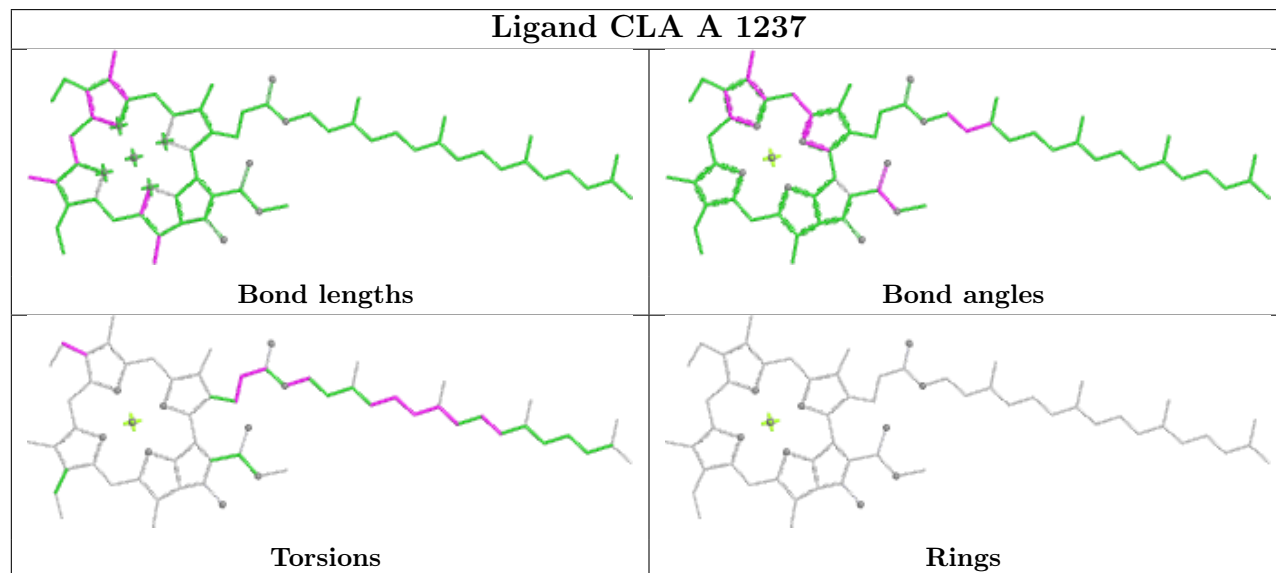
Ligand BCR 3 523



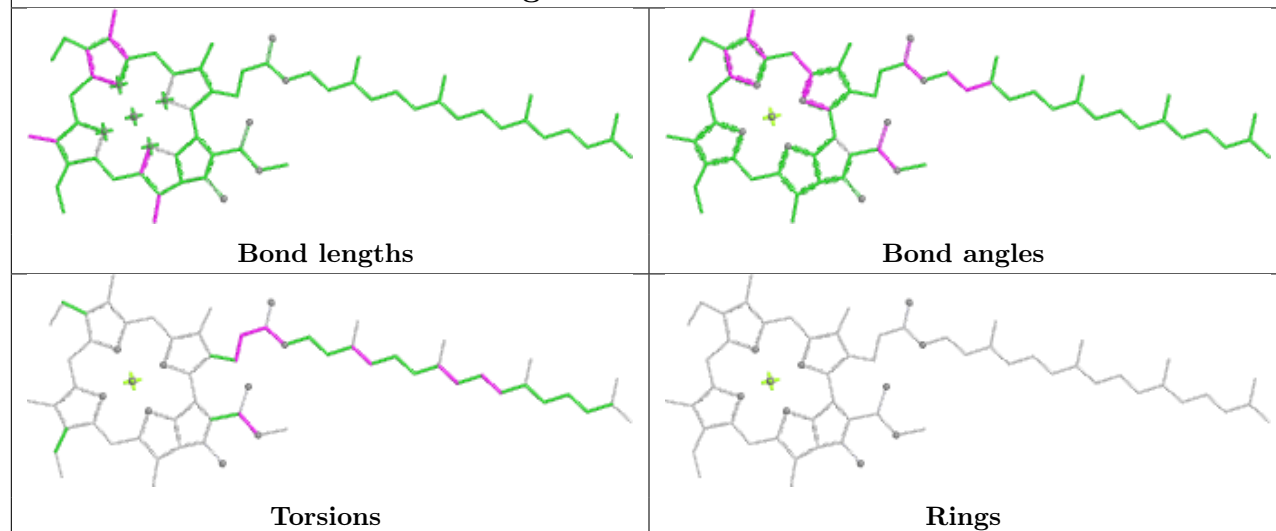
Ligand CLA a 513



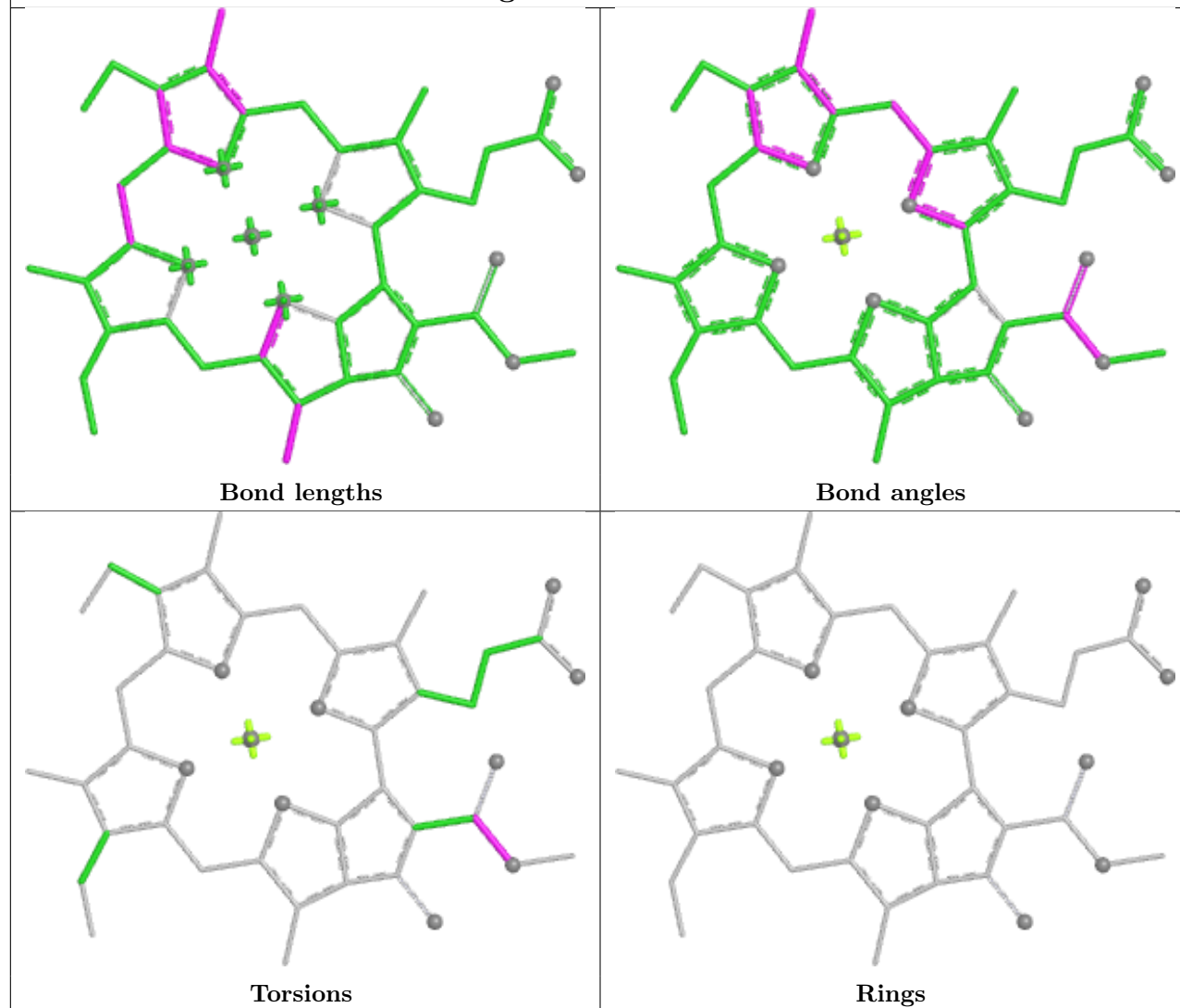
Ligand CLA A 1237



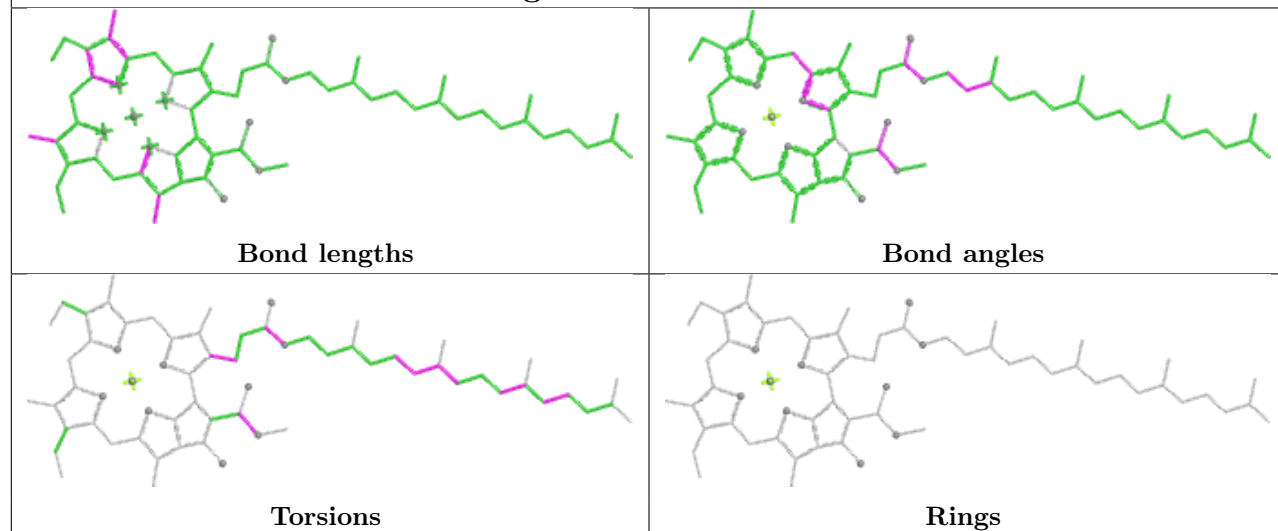
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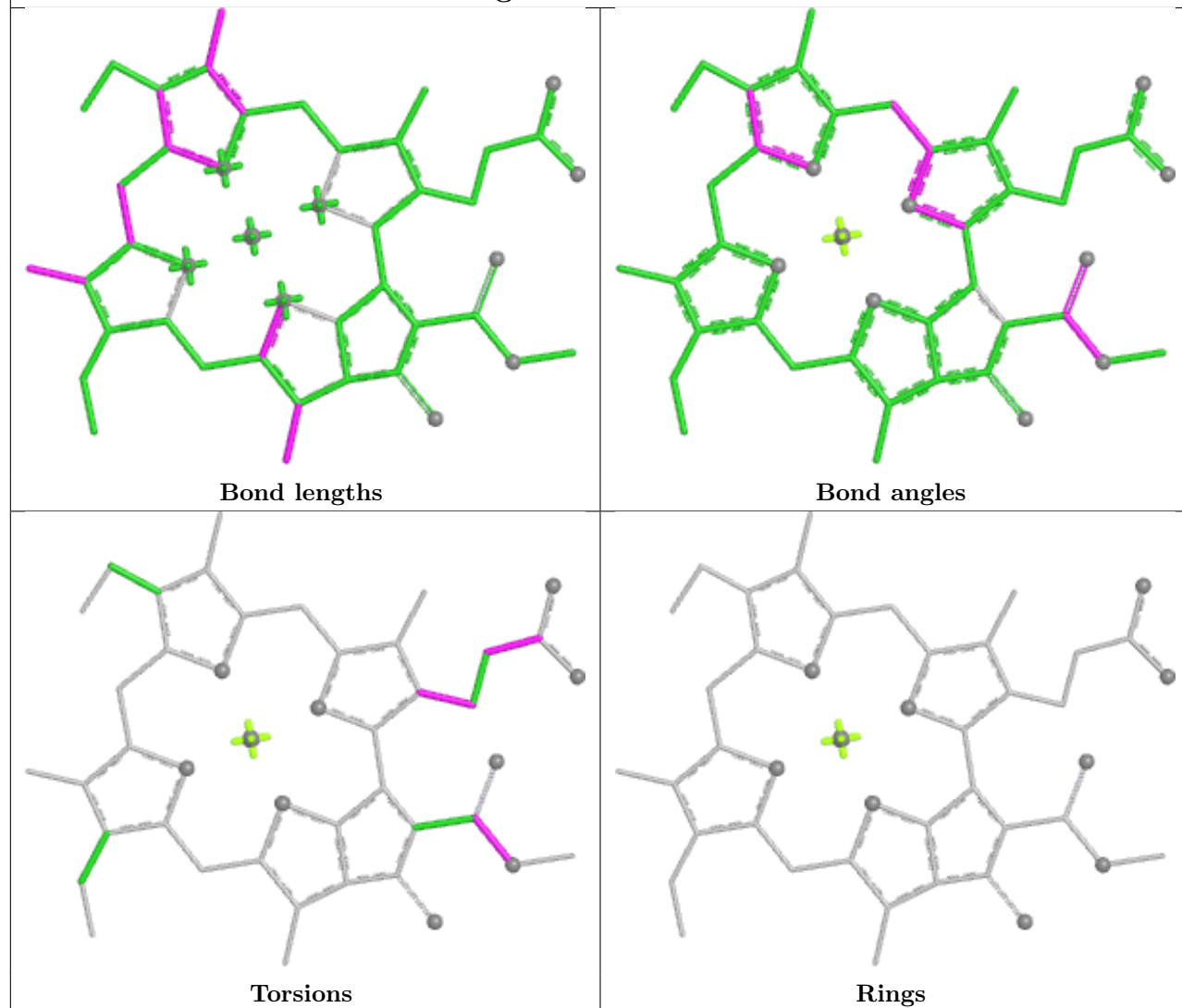
Ligand CLA f 506

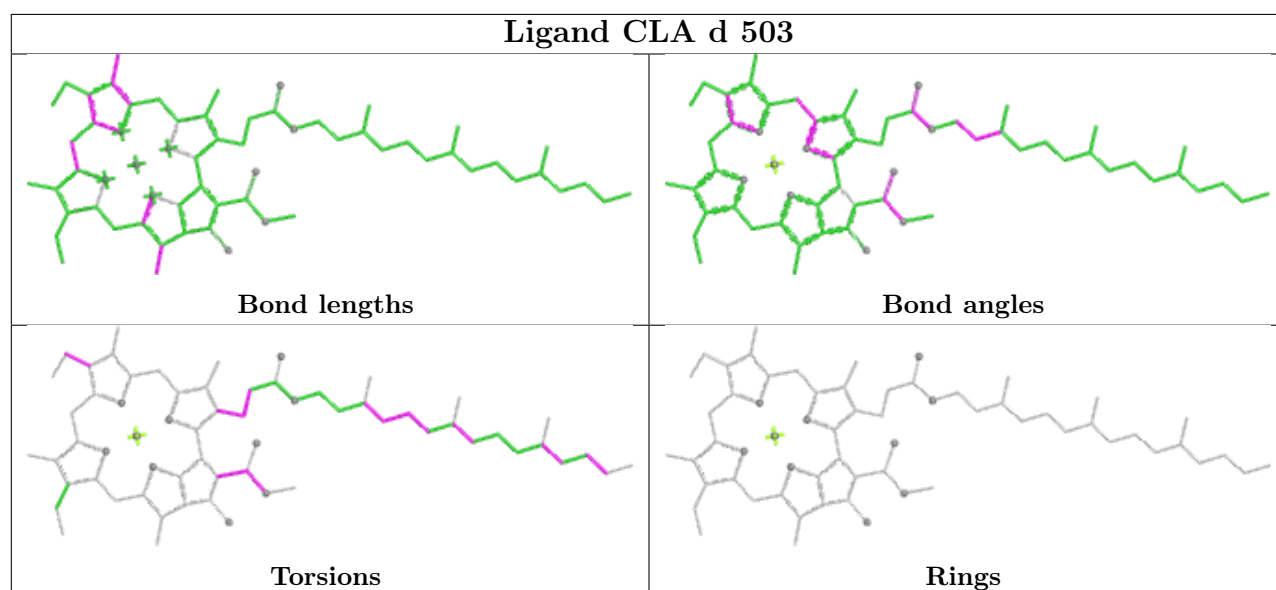
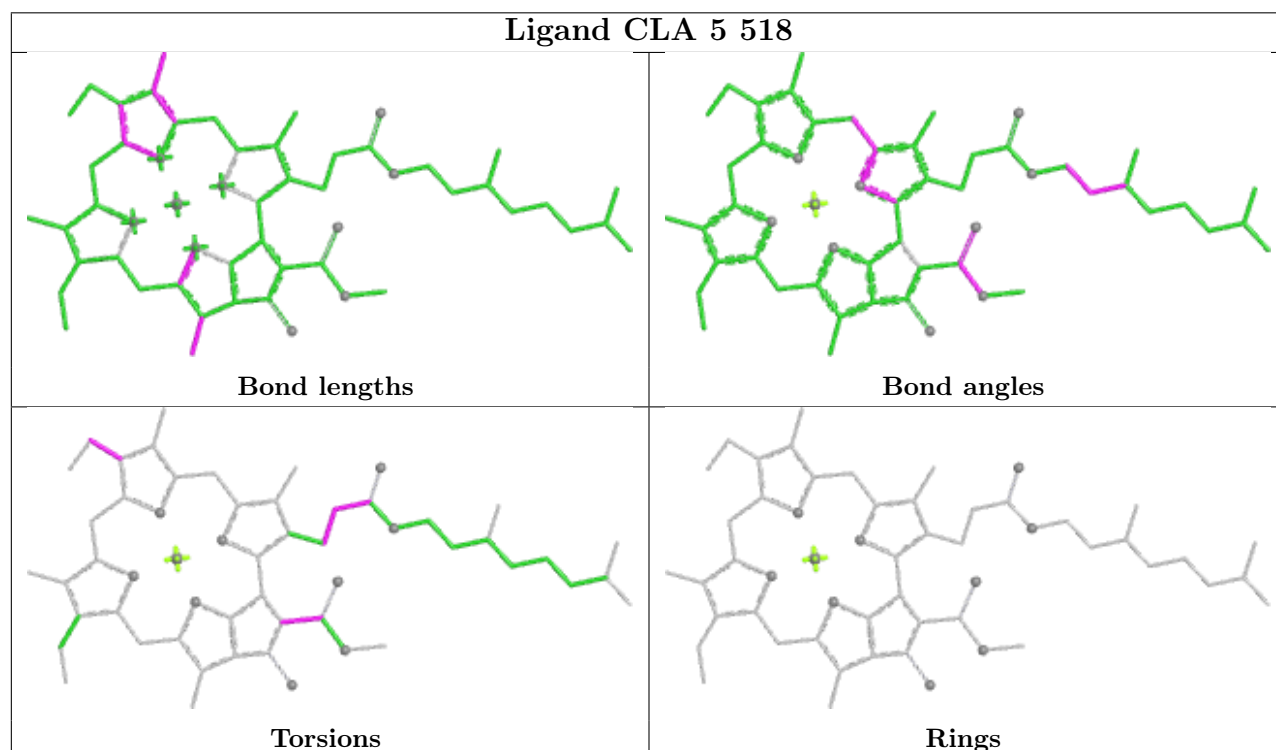
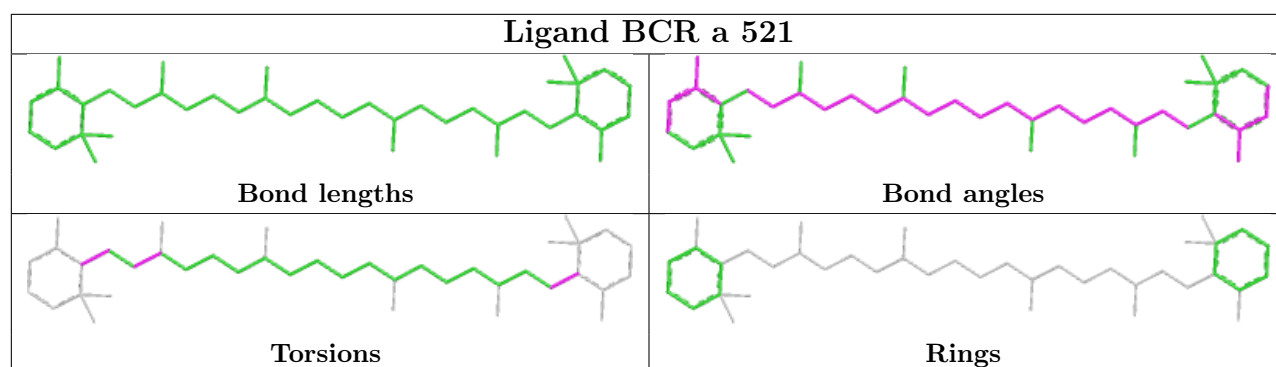


Ligand CLA B 1226

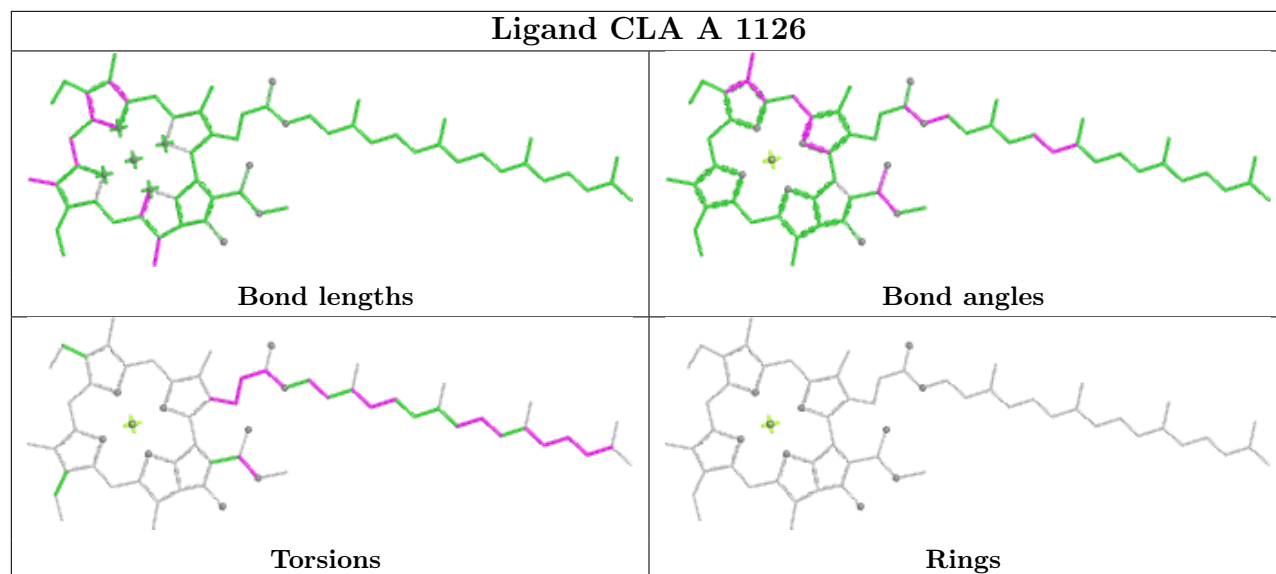


Ligand CLA 2 513

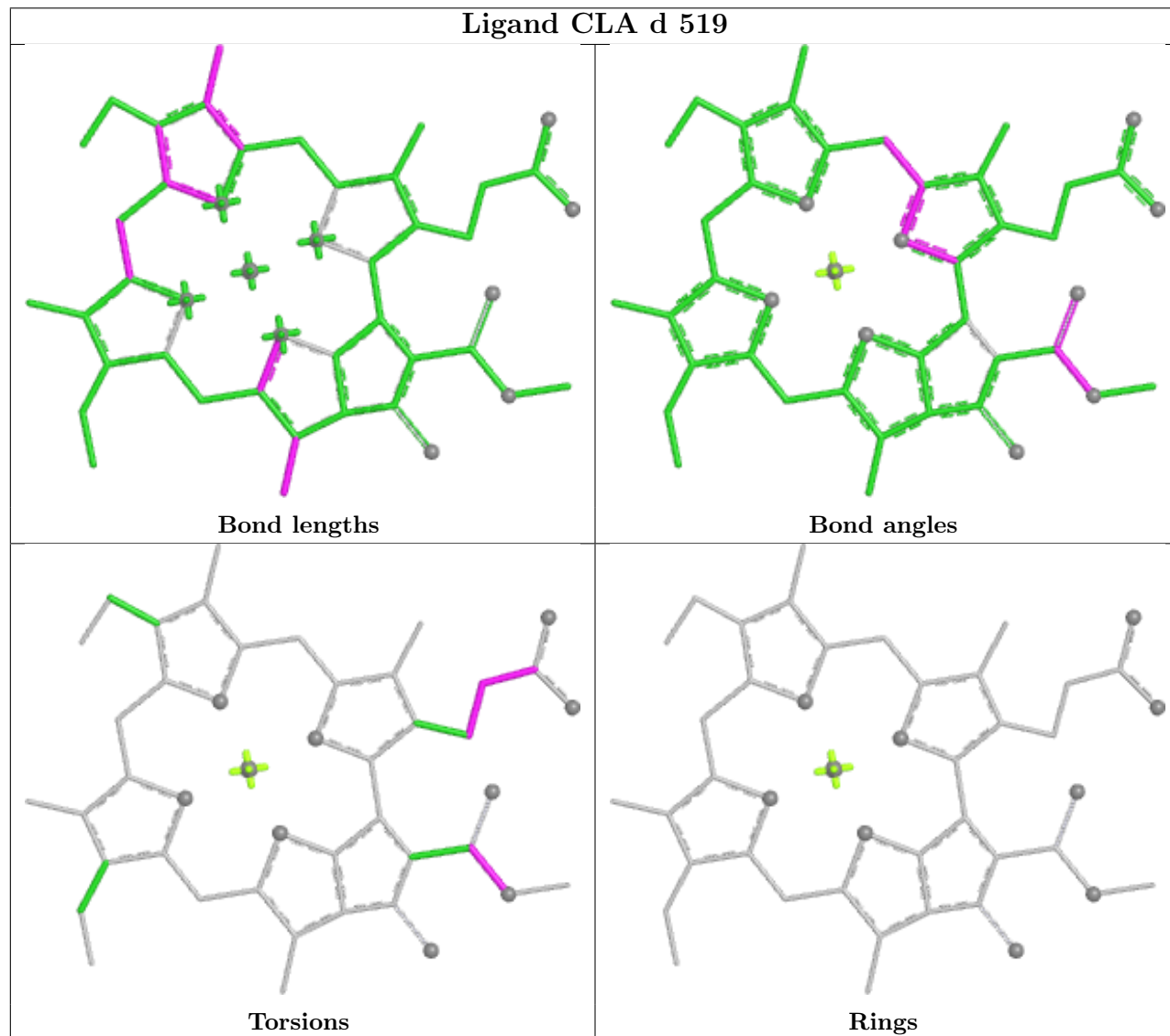


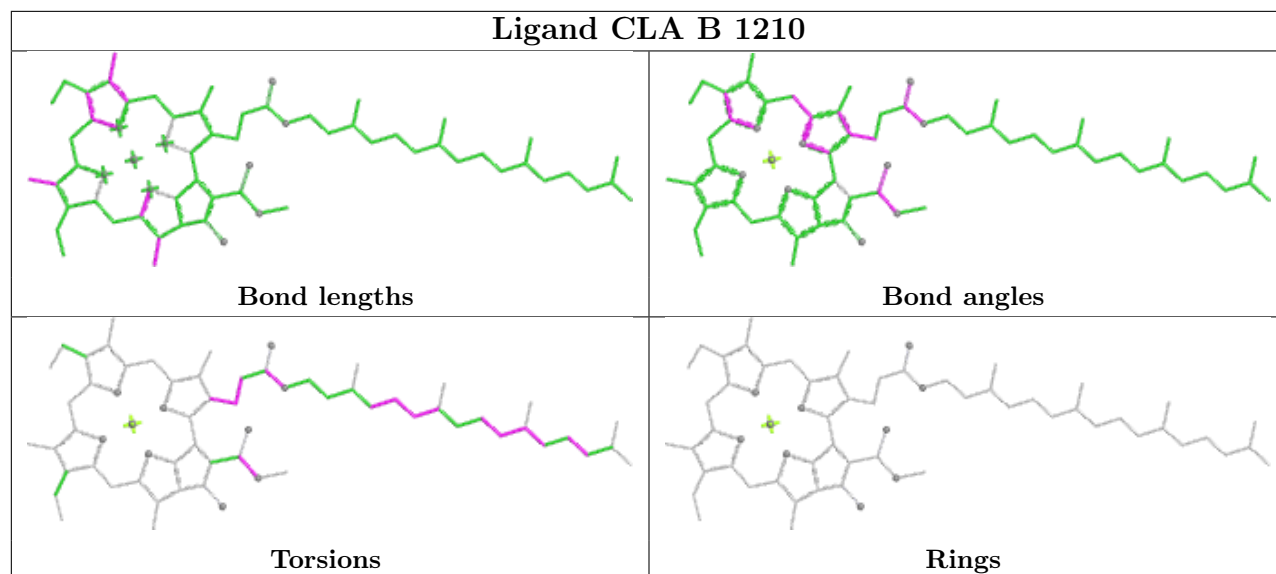
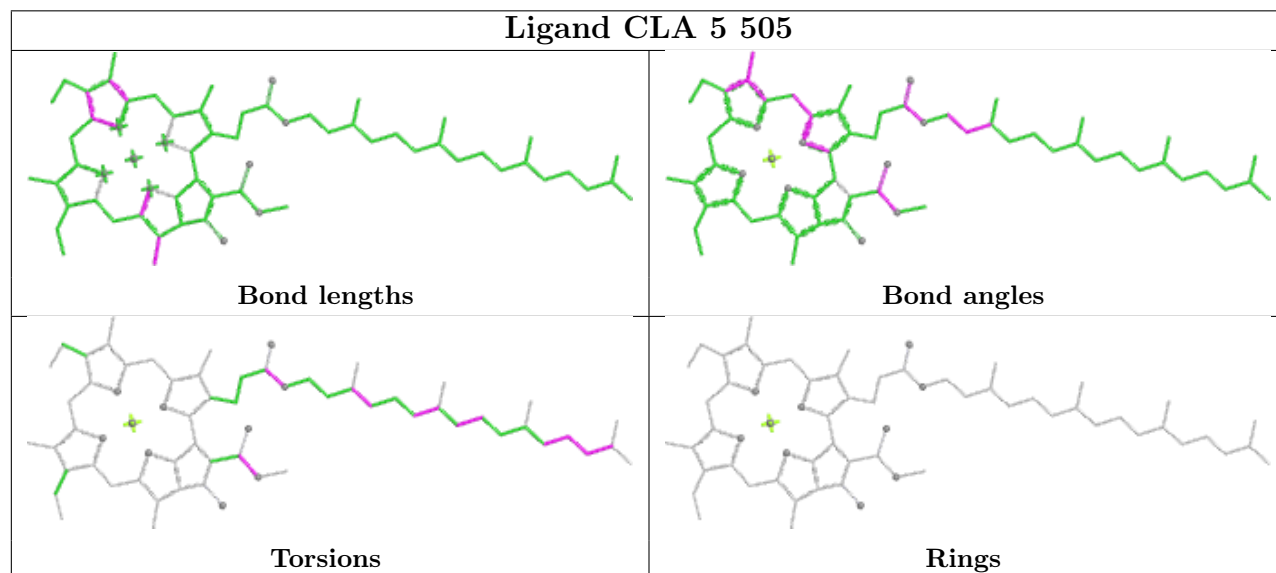


Ligand CLA A 1126

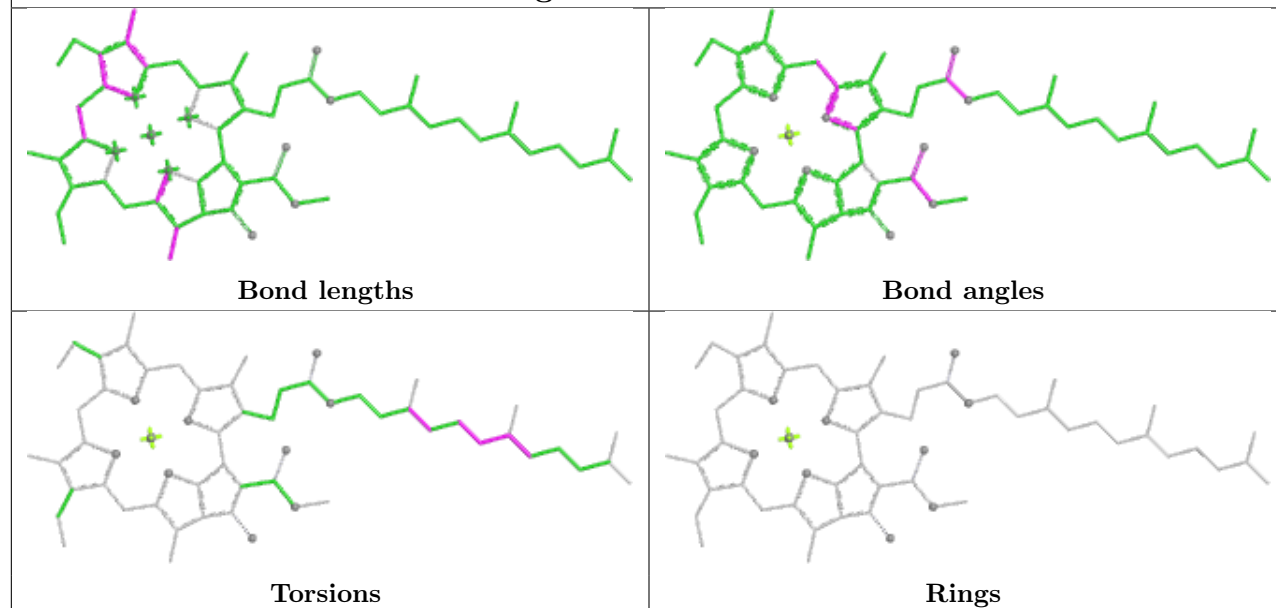


Ligand CLA d 519

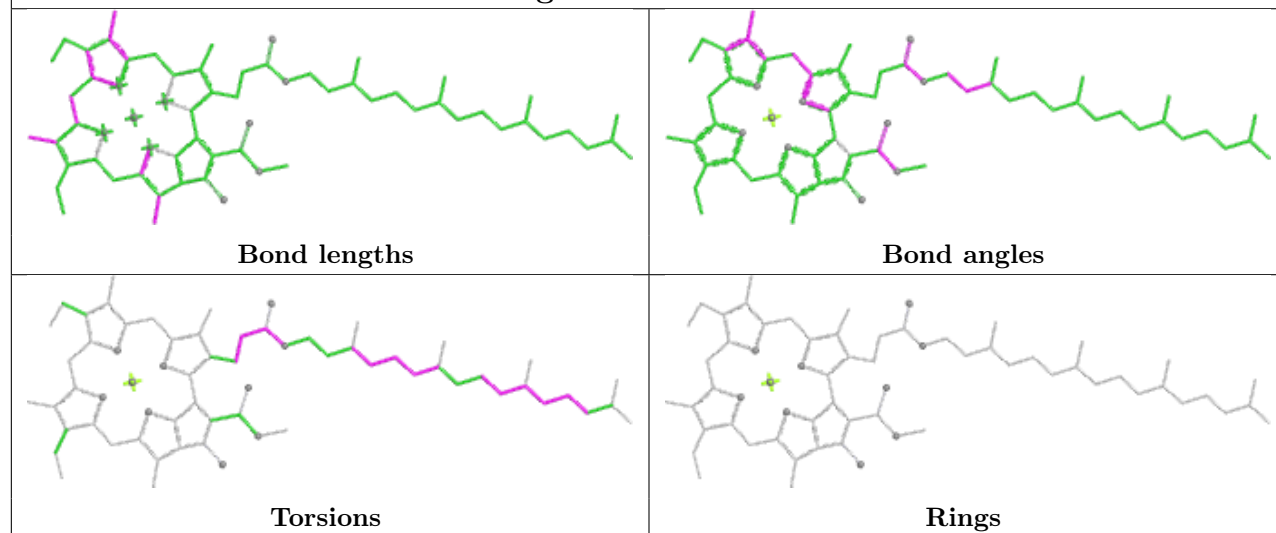


Ligand CLA B 1210**Ligand CLA 5 505**

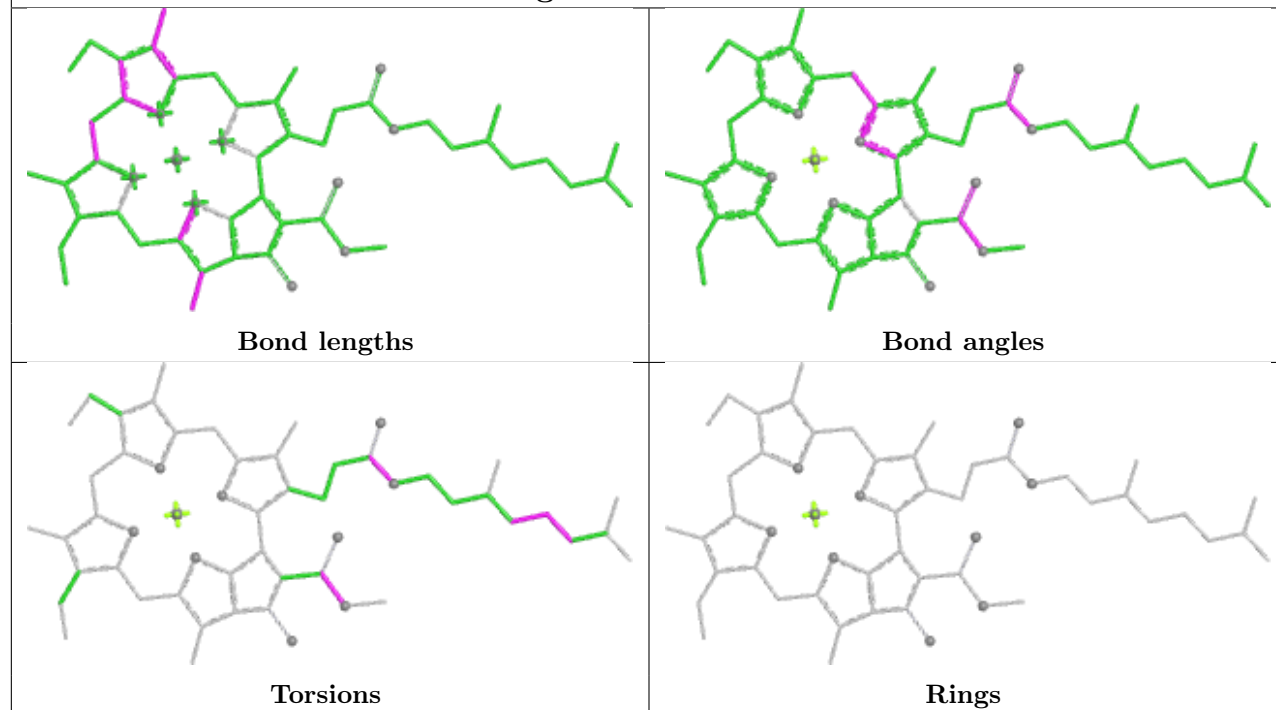
Ligand CLA b 507



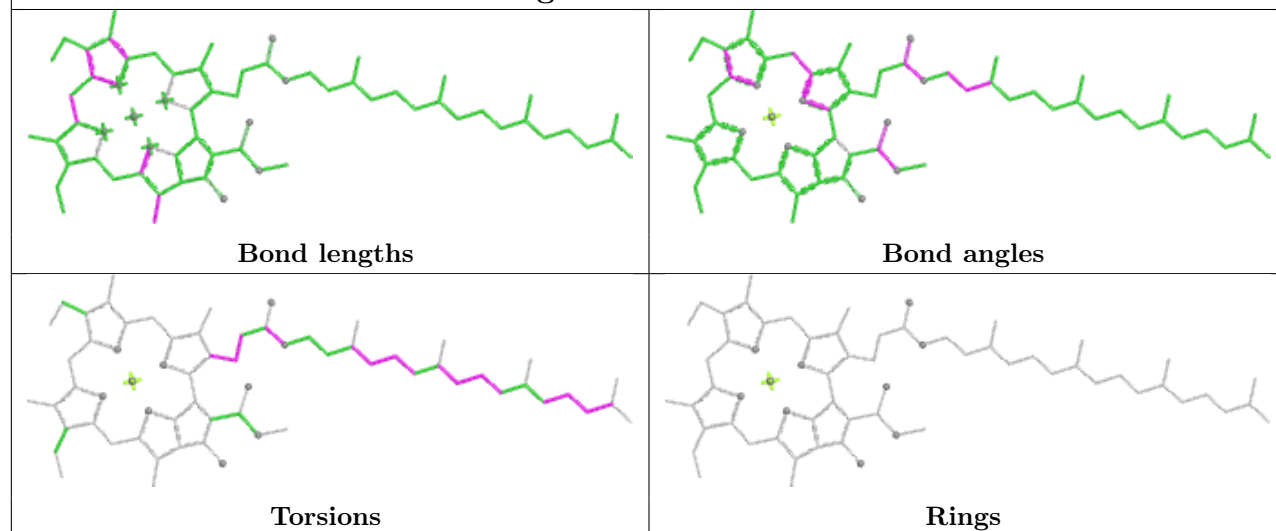
Ligand CLA 3 510

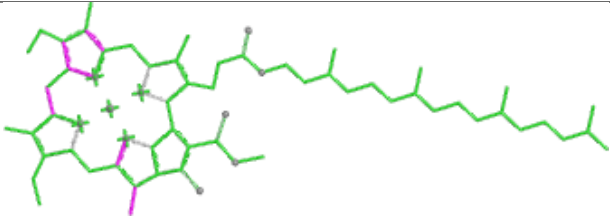
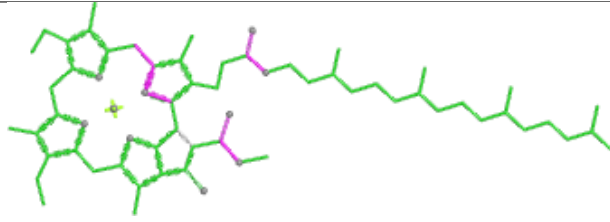
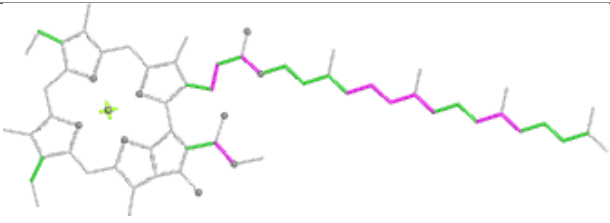
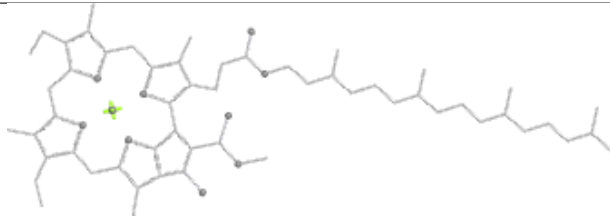
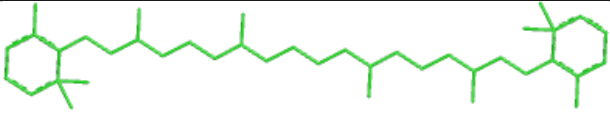
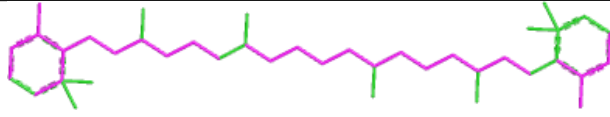
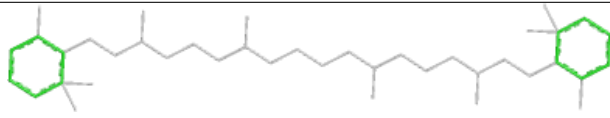
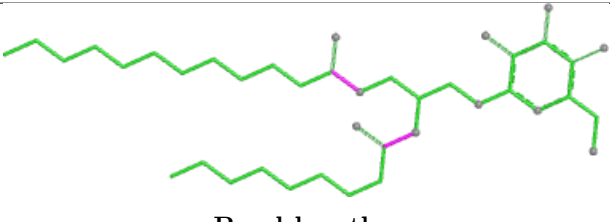
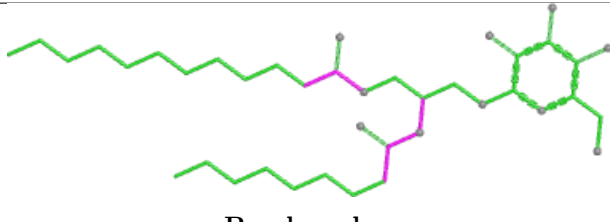
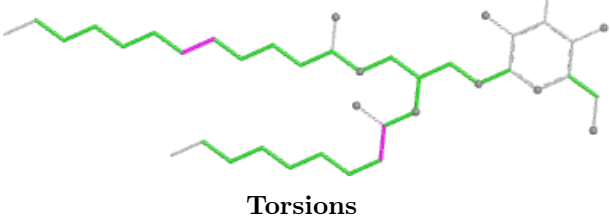
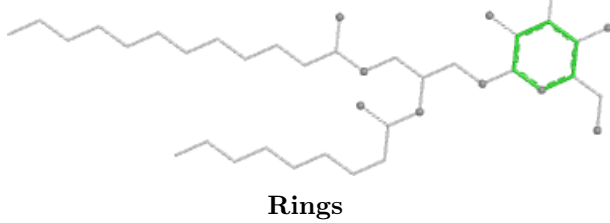


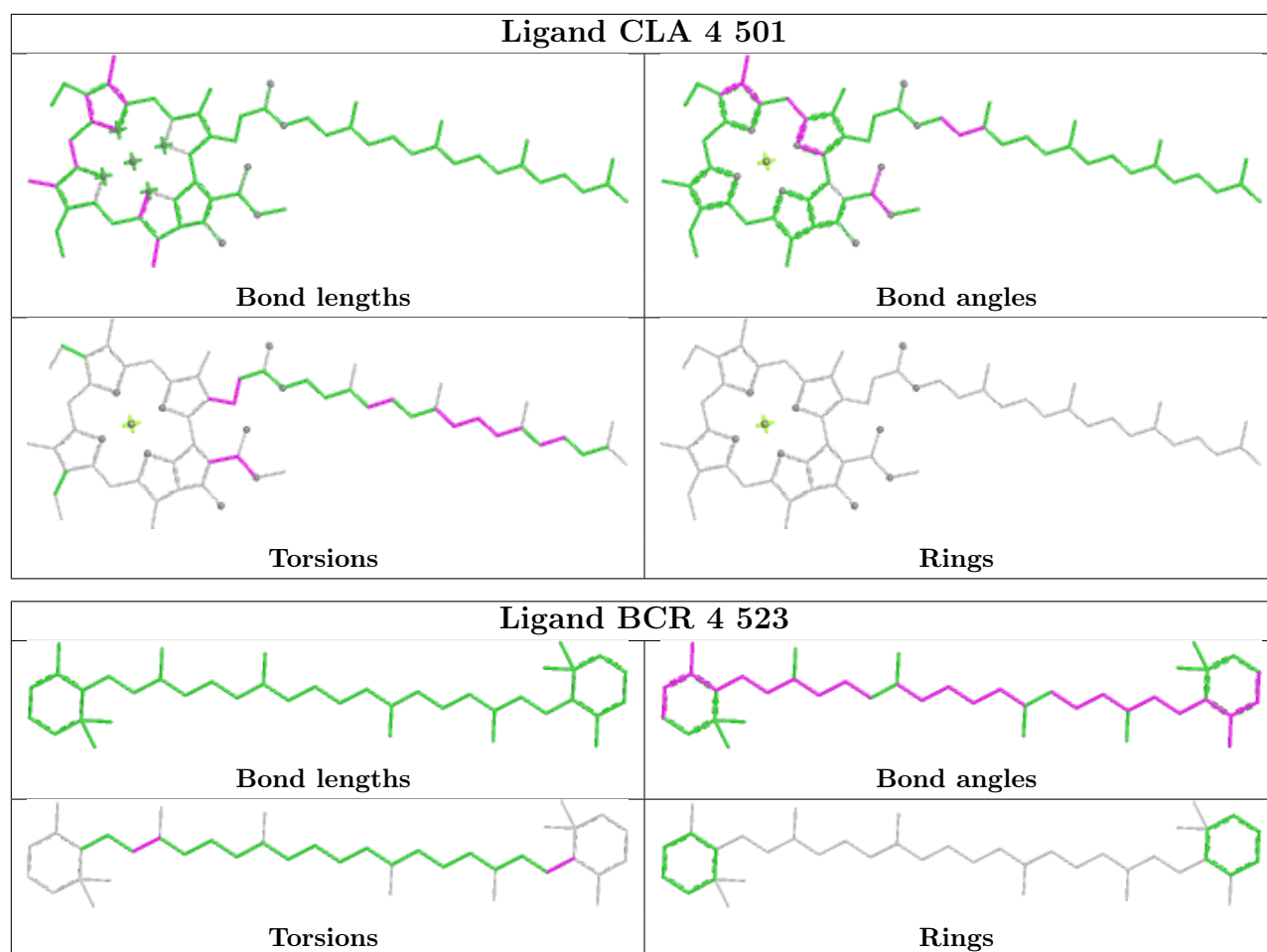
Ligand CLA a 508

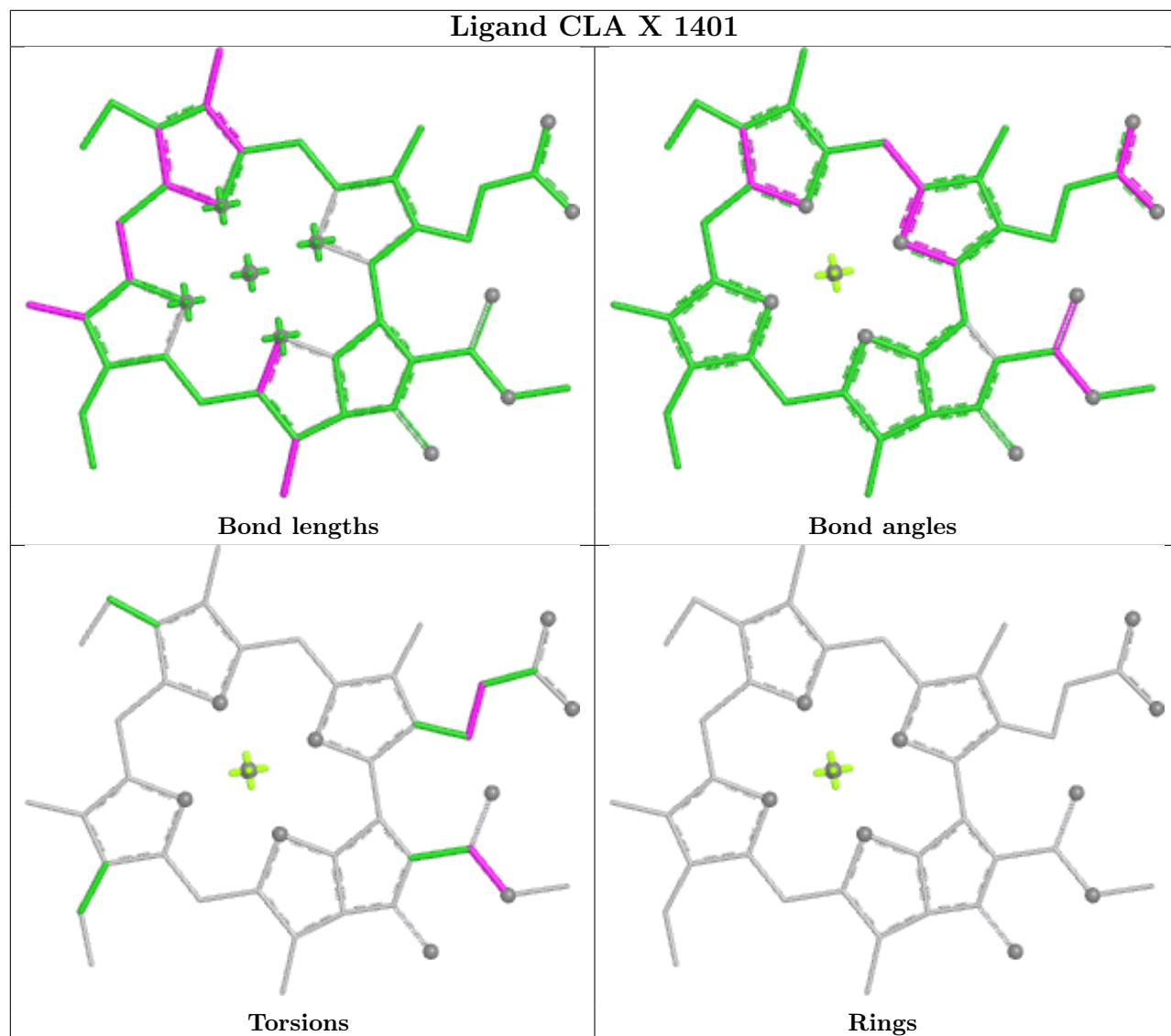


Ligand CLA e 505

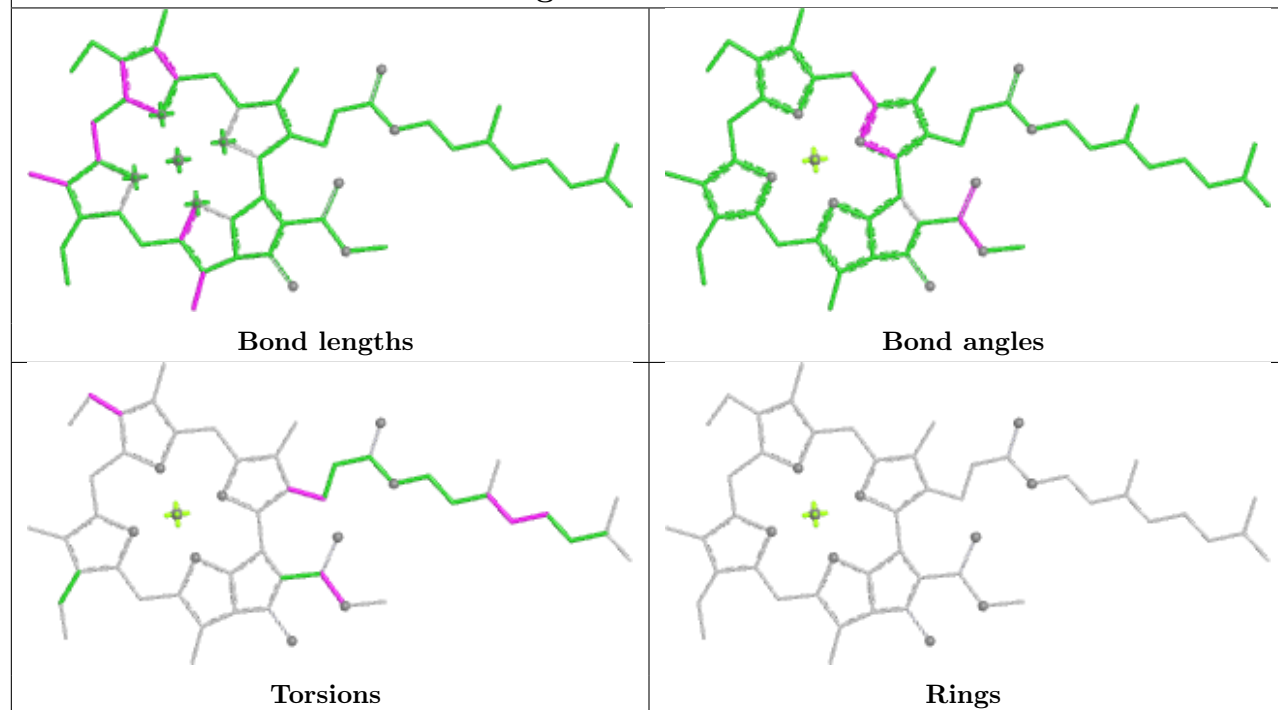


Ligand CLA a 505	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR M 4021	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand LMG g 5104	
 Bond lengths	 Bond angles
 Torsions	 Rings

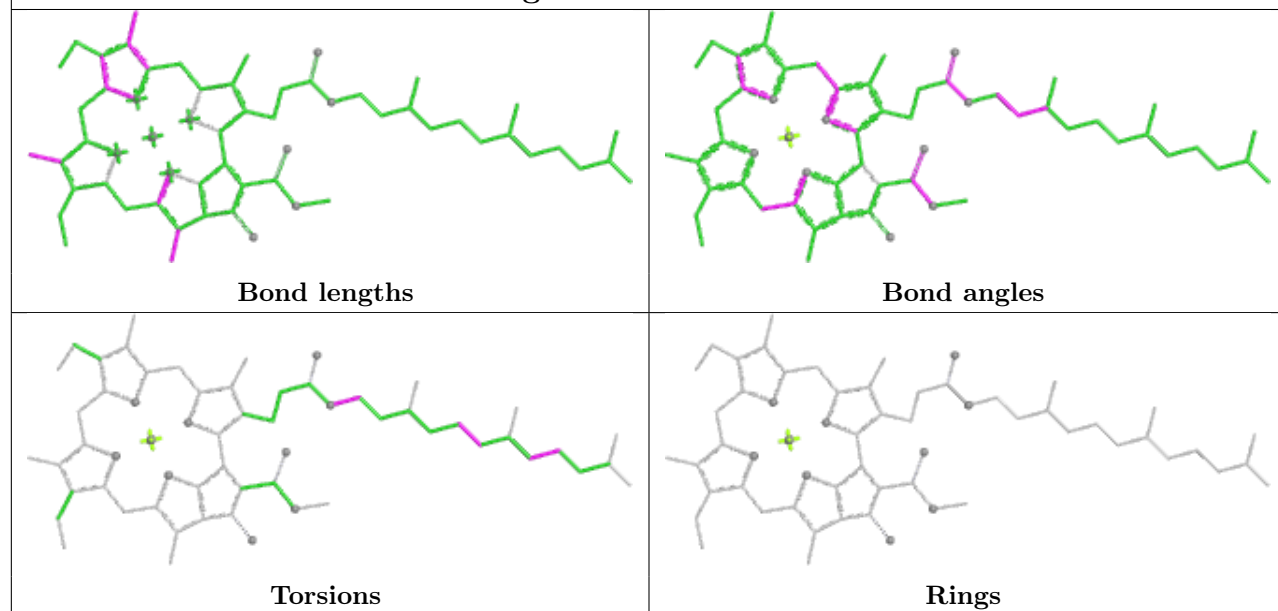


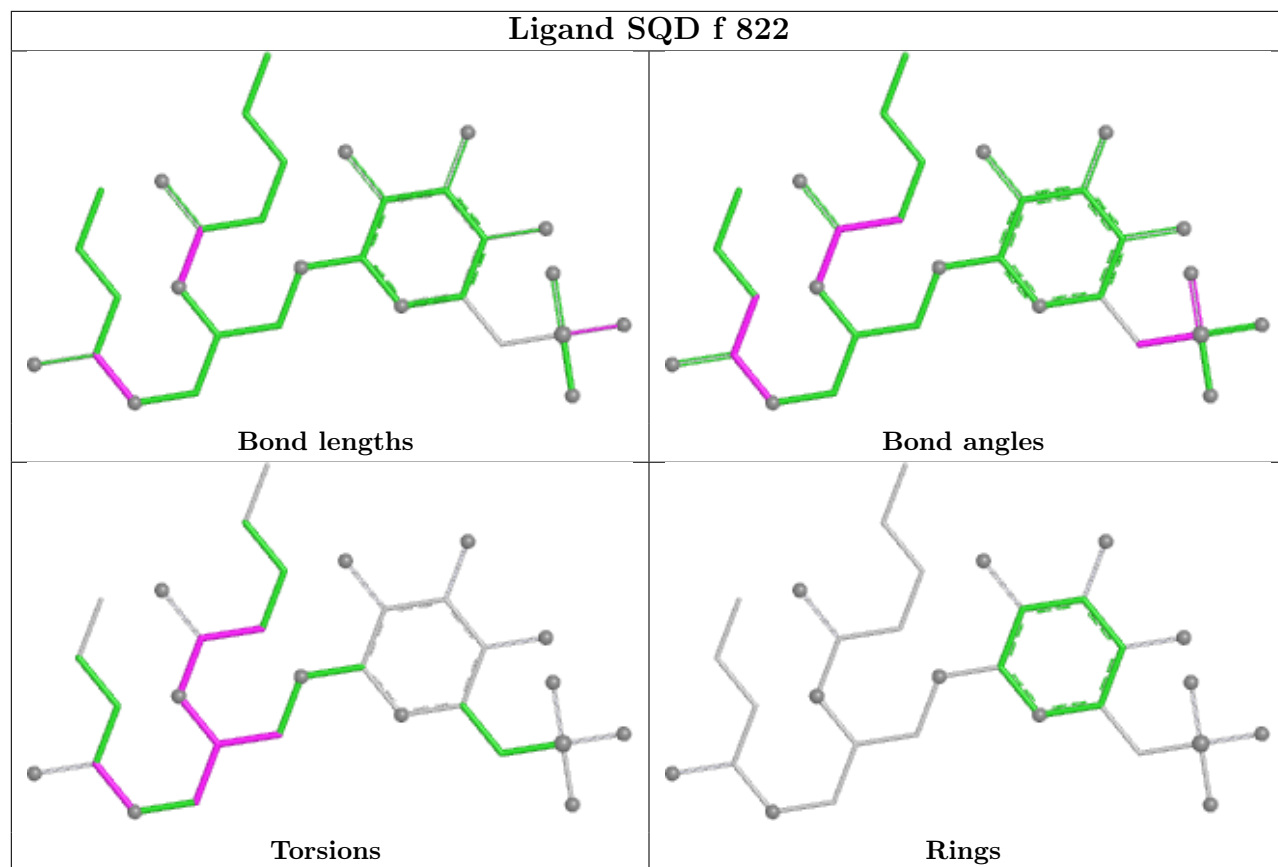


Ligand CLA 6 508

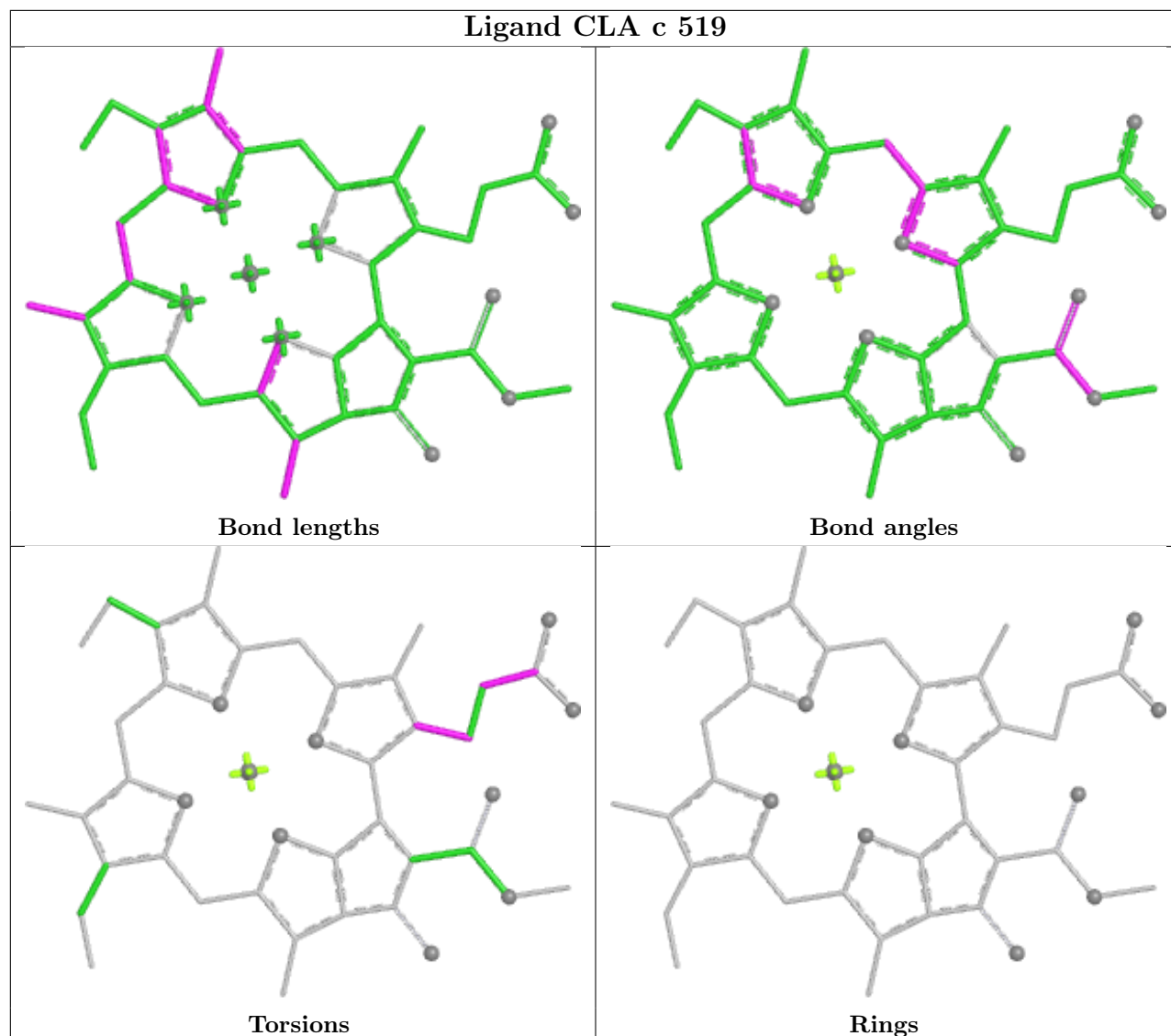


Ligand CLA A 1124

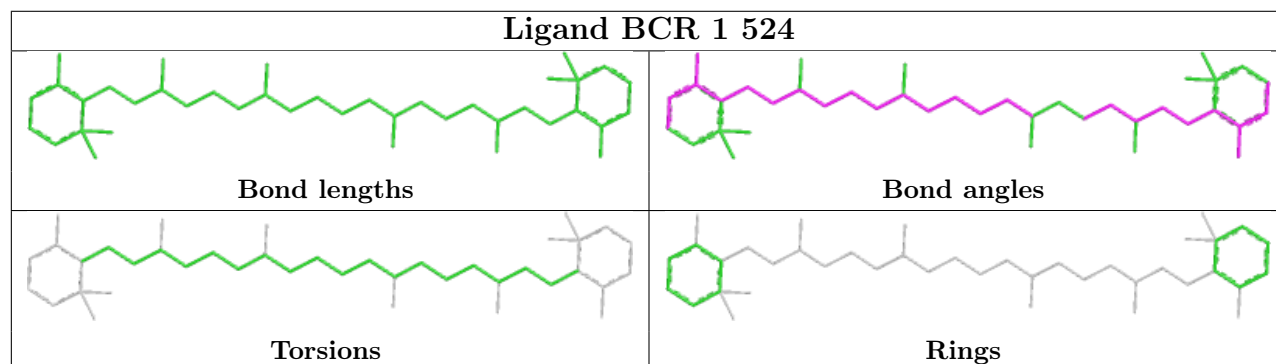


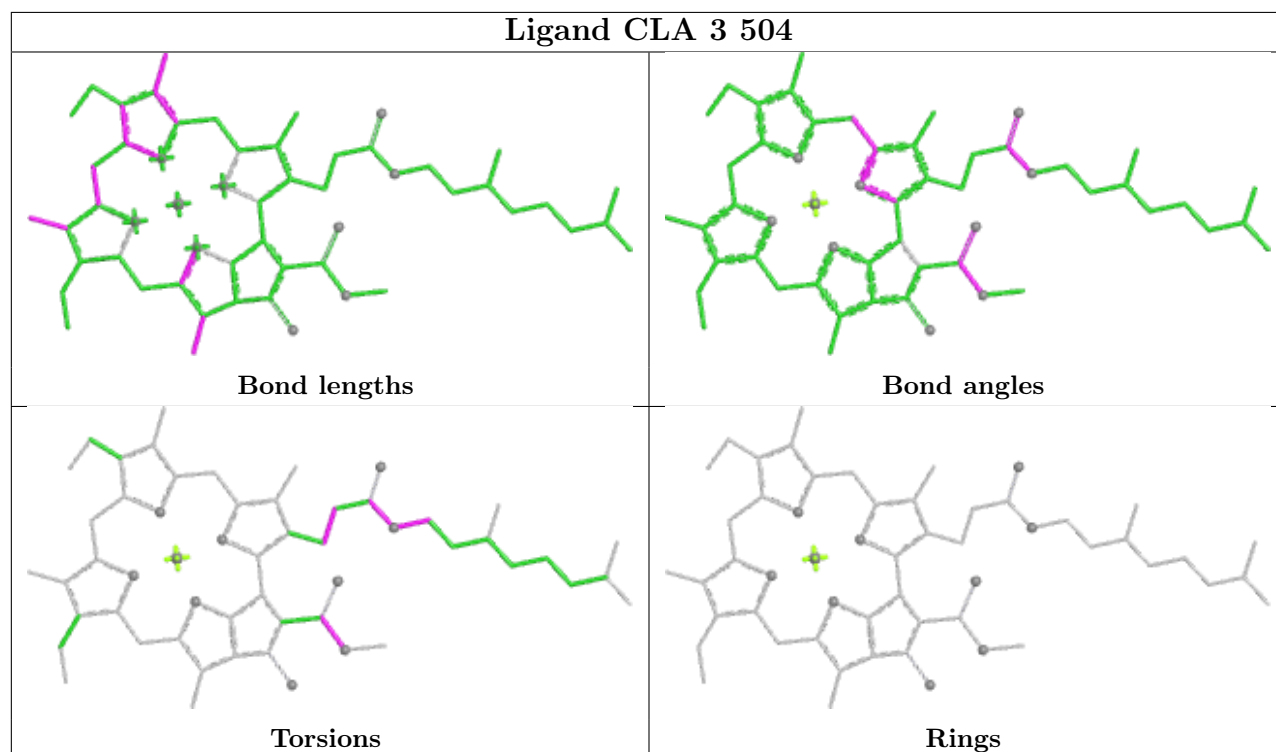
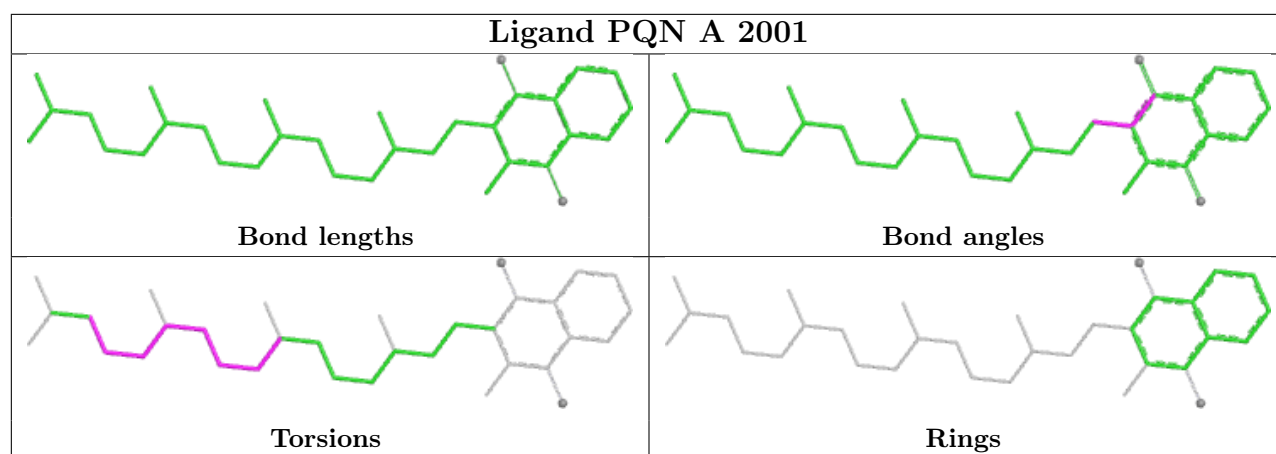


Ligand CLA c 519

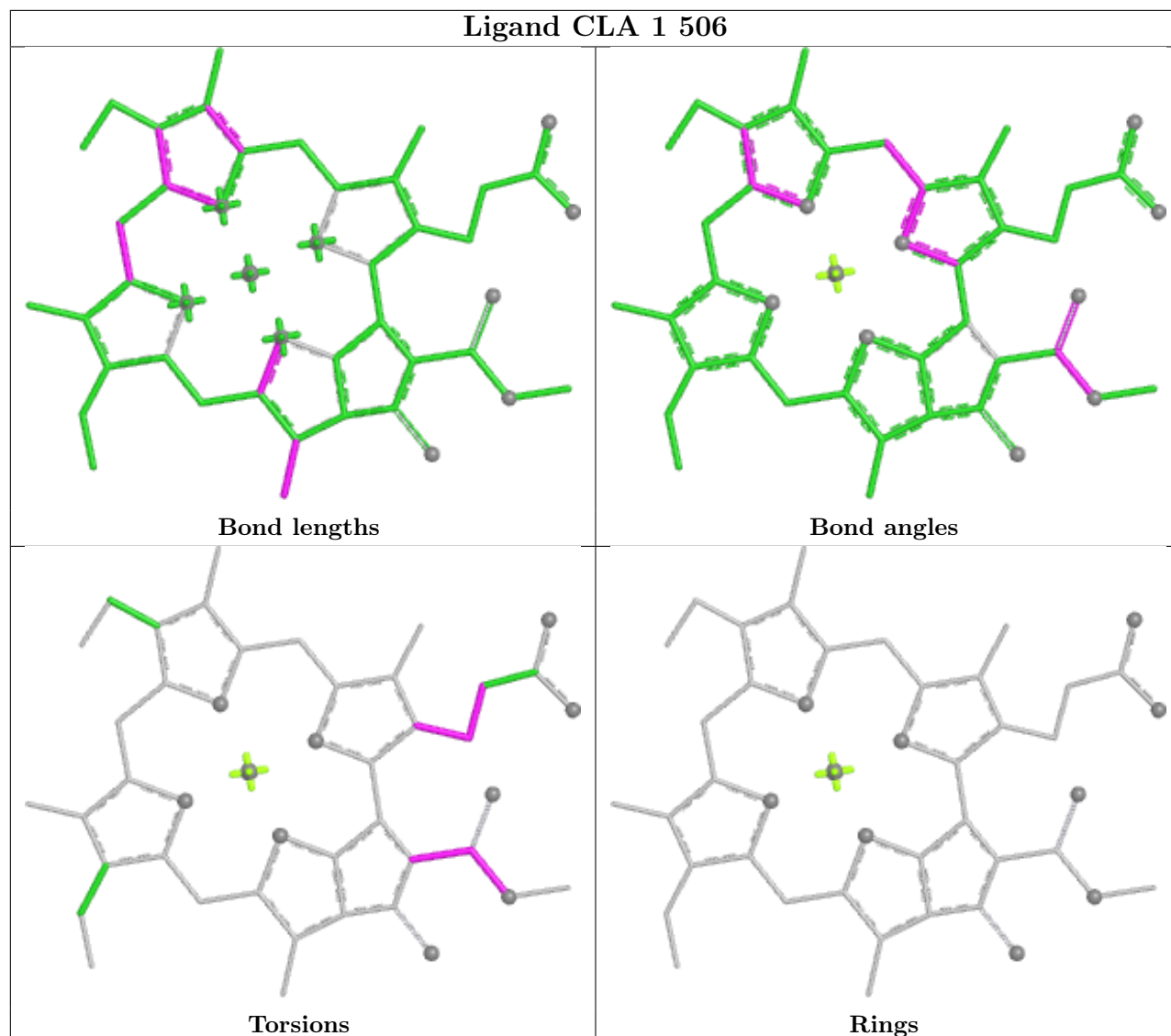


Ligand BCR 1 524

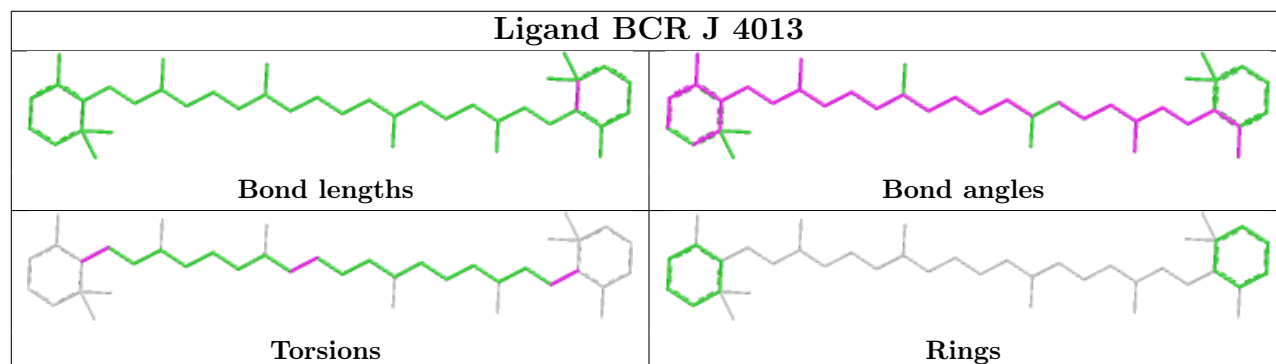


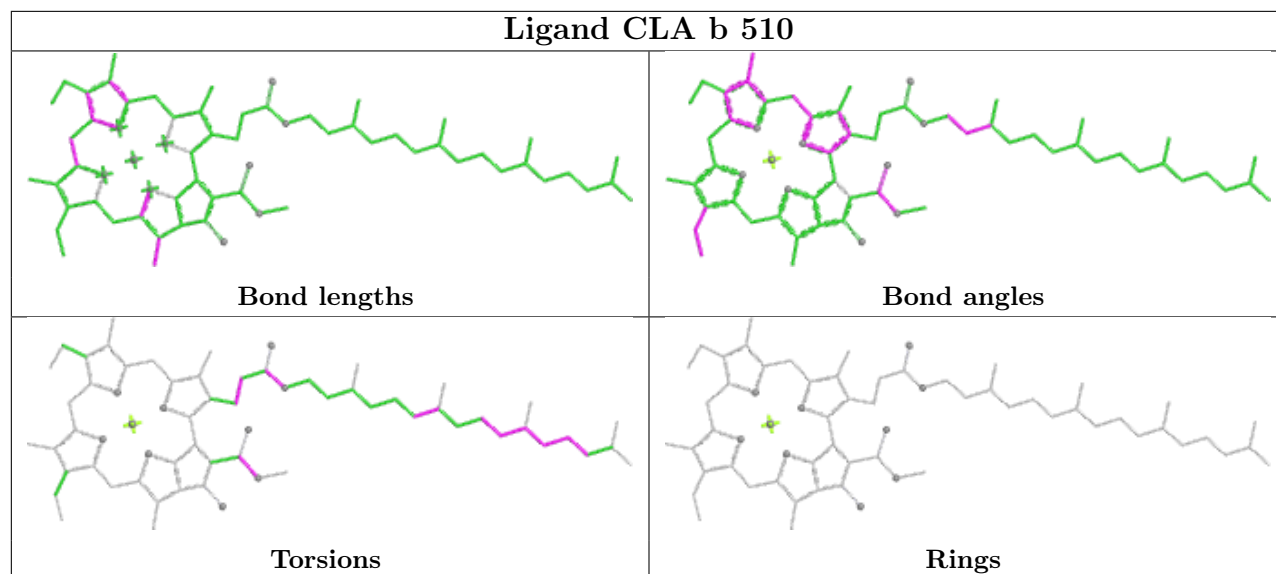
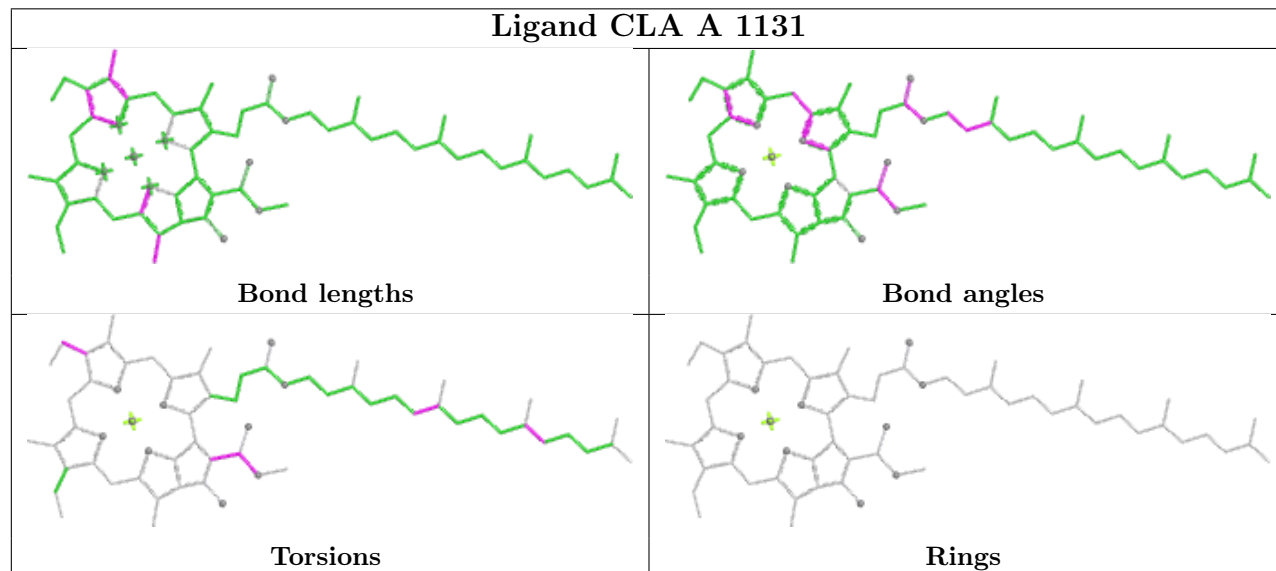


Ligand CLA 1 506

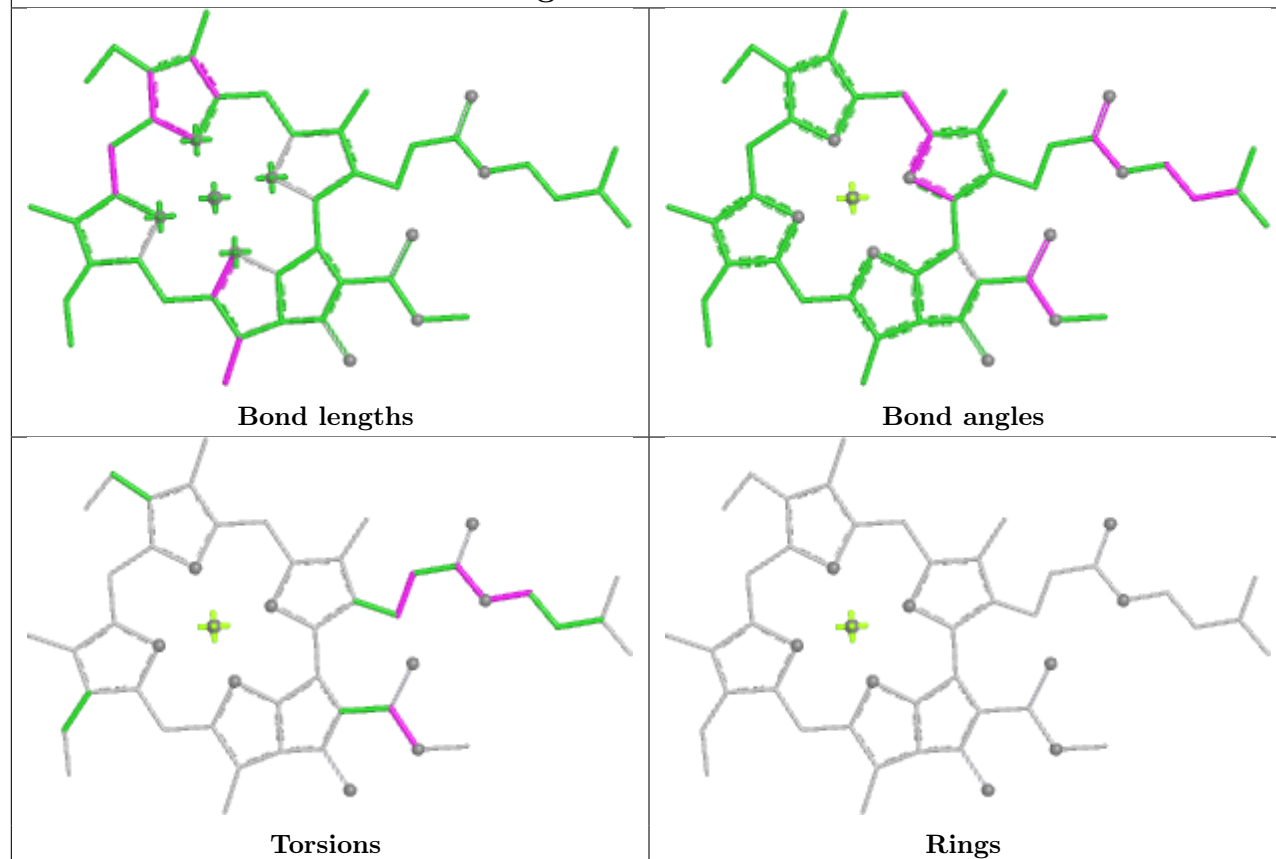


Ligand BCR J 4013

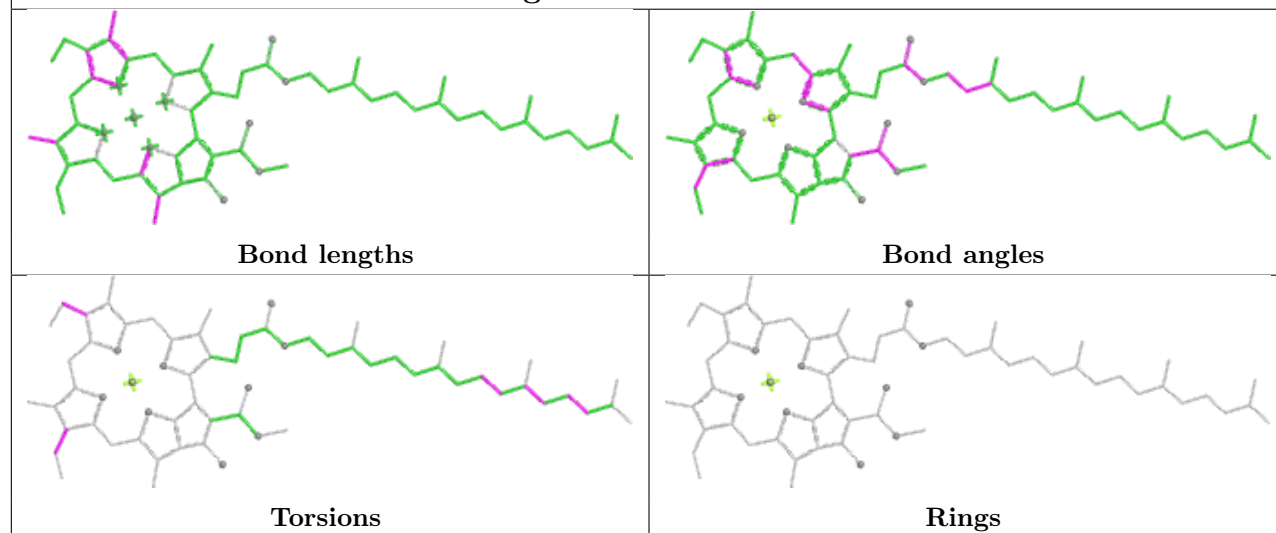


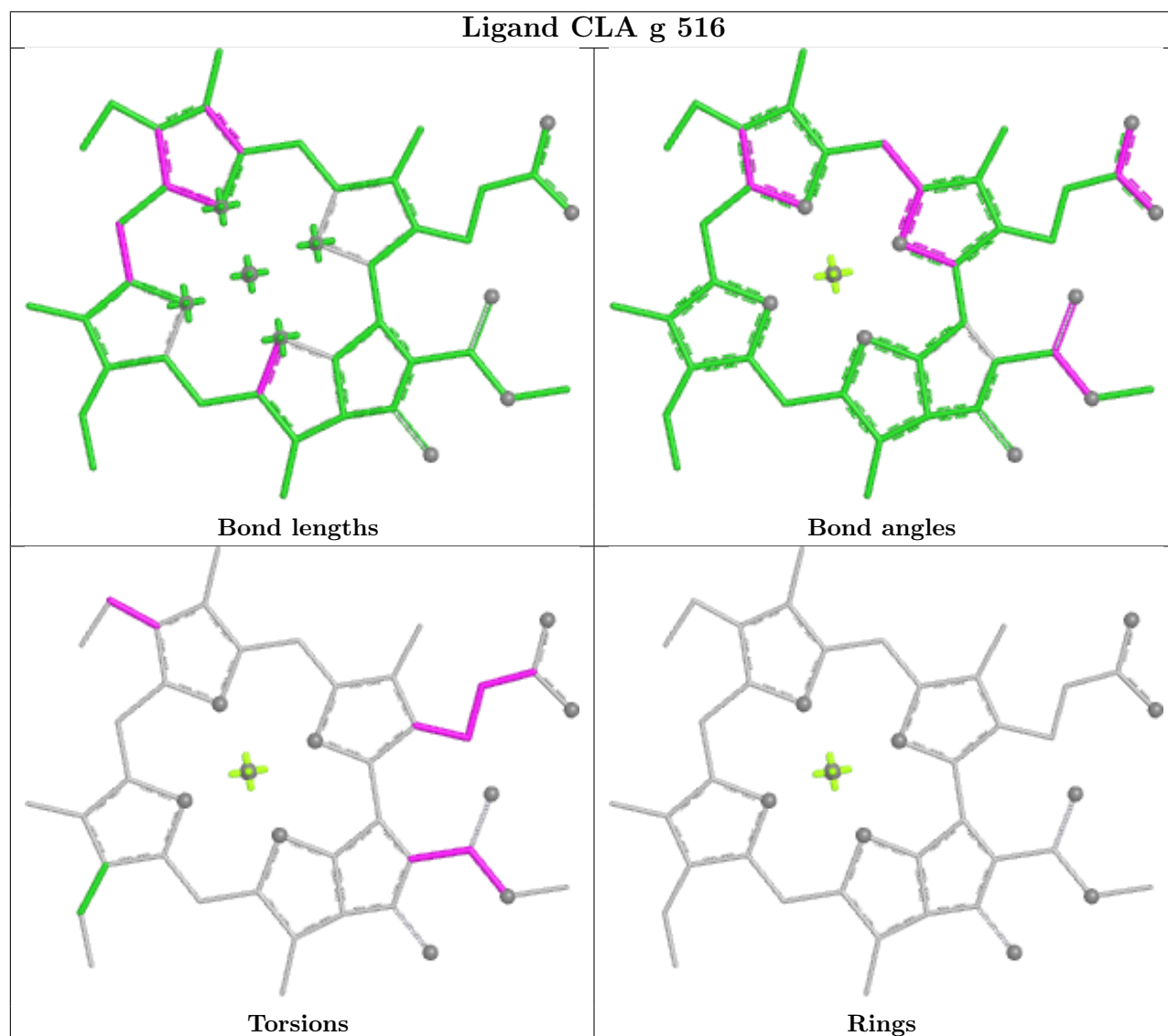
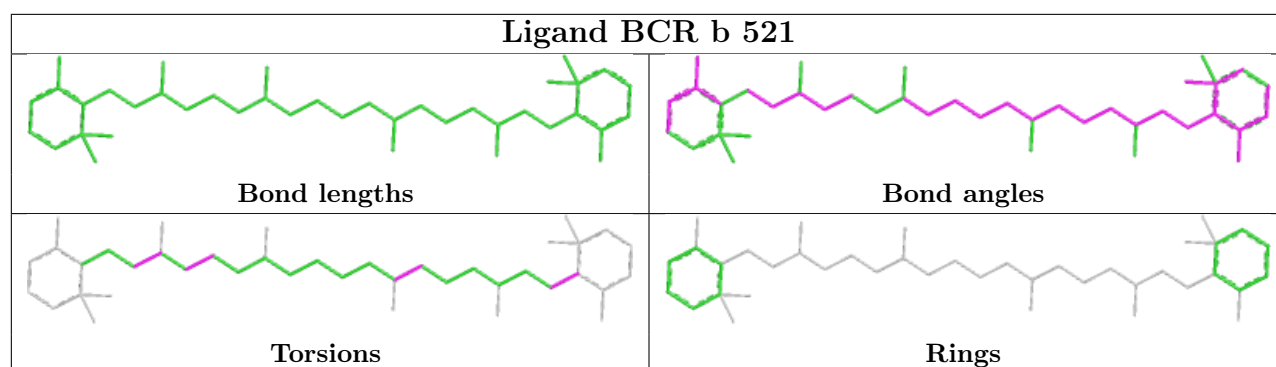
Ligand CLA b 510**Ligand CLA A 1131**

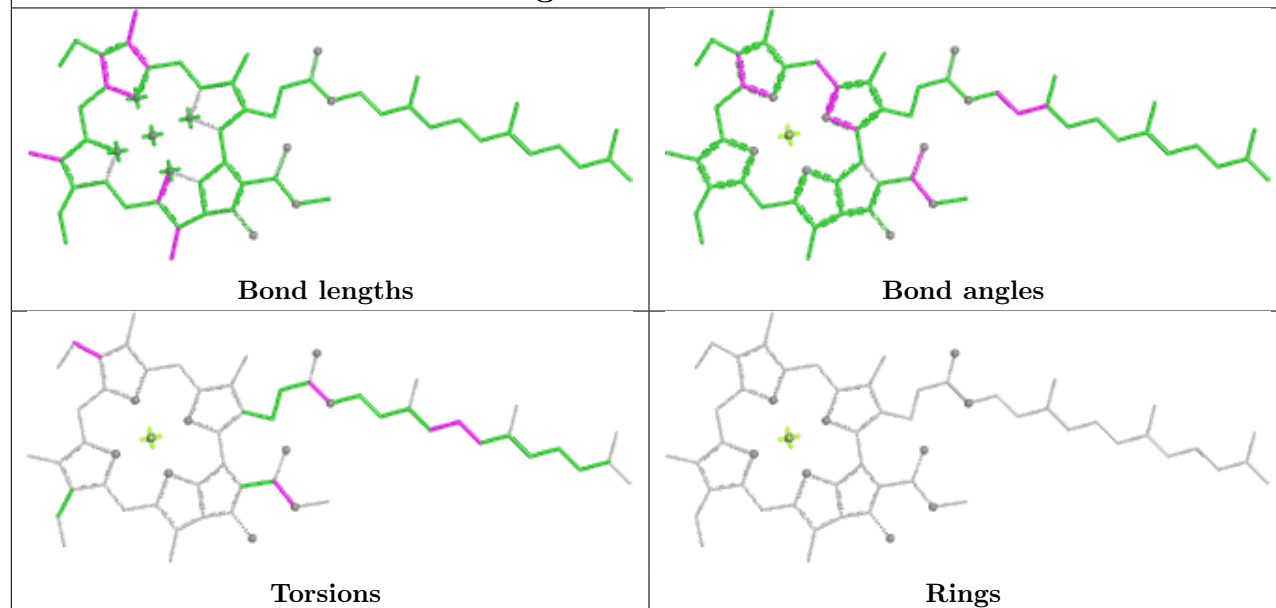
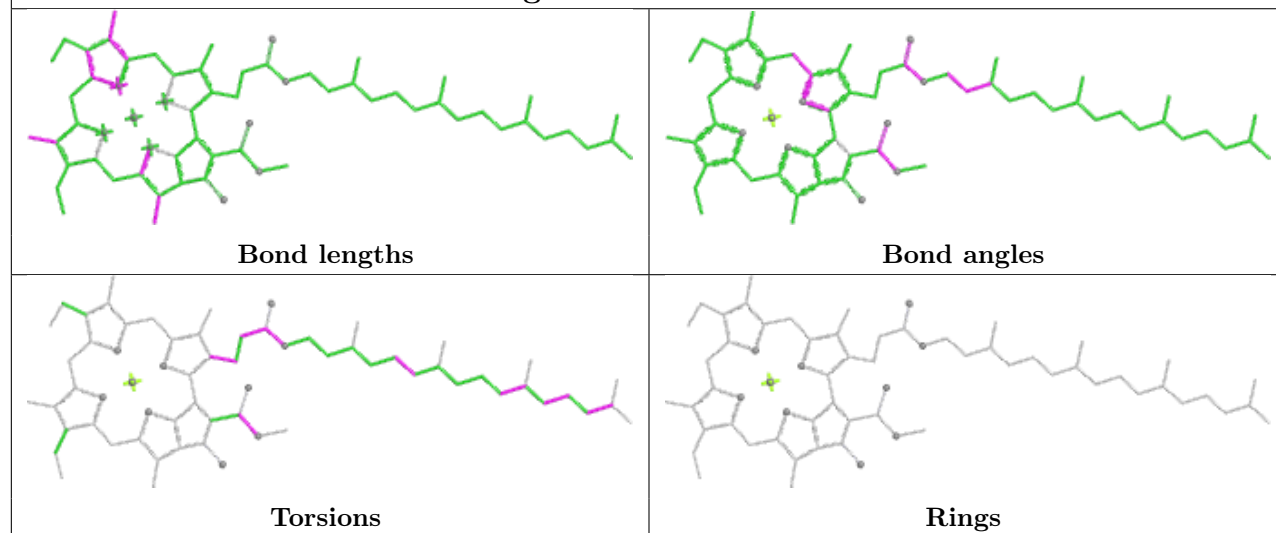
Ligand CLA c 504

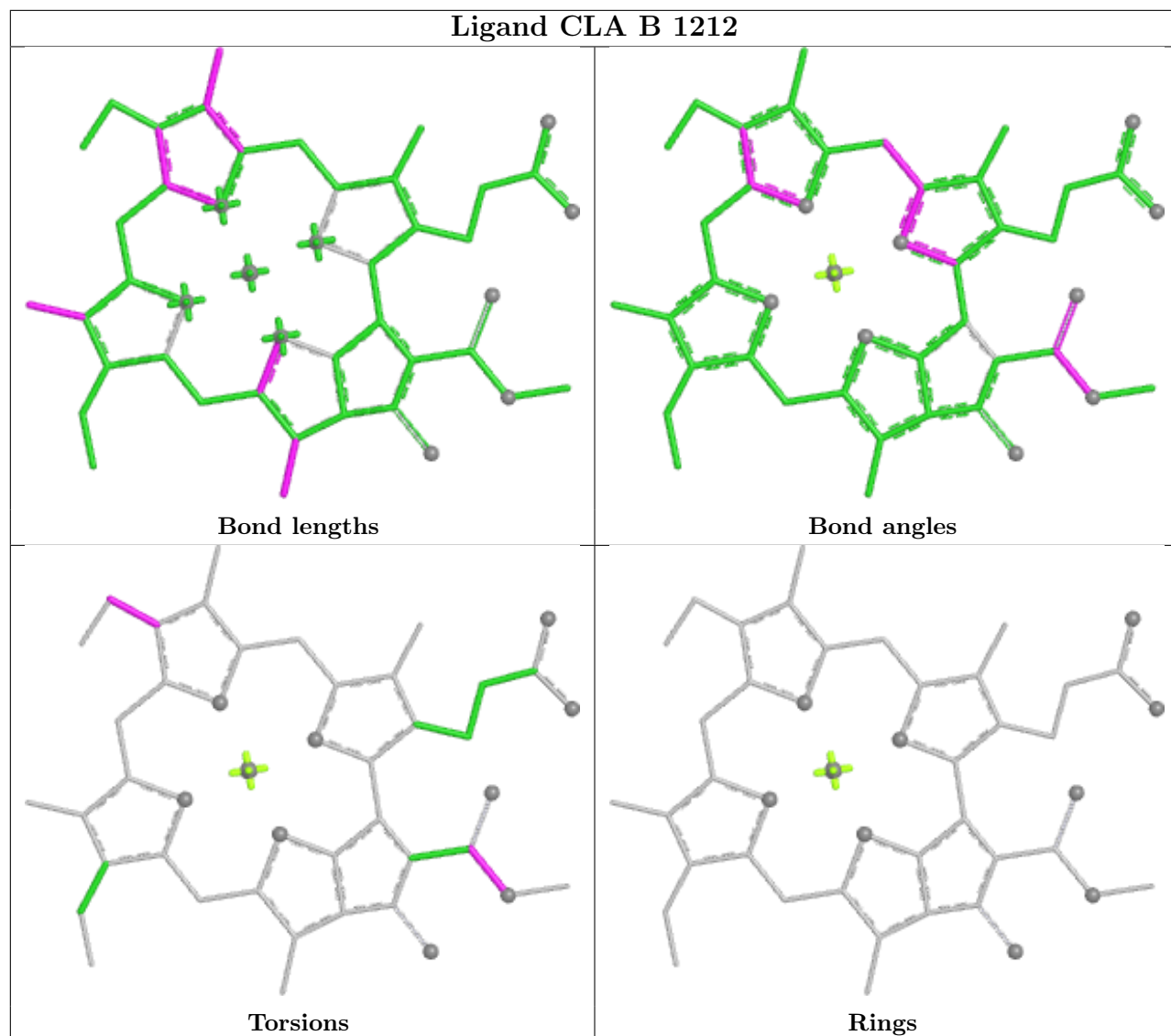


Ligand CLA B 1023

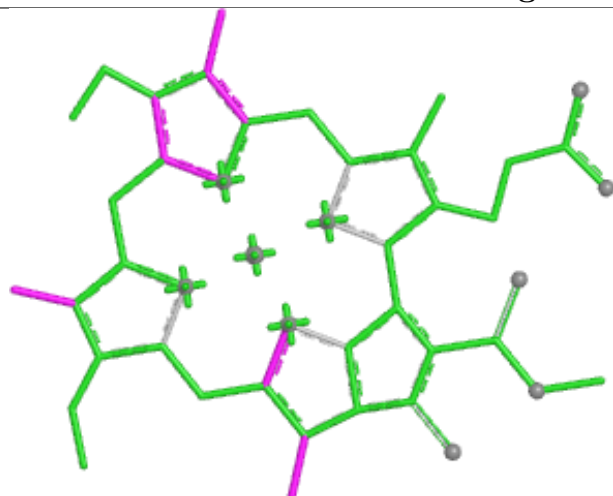




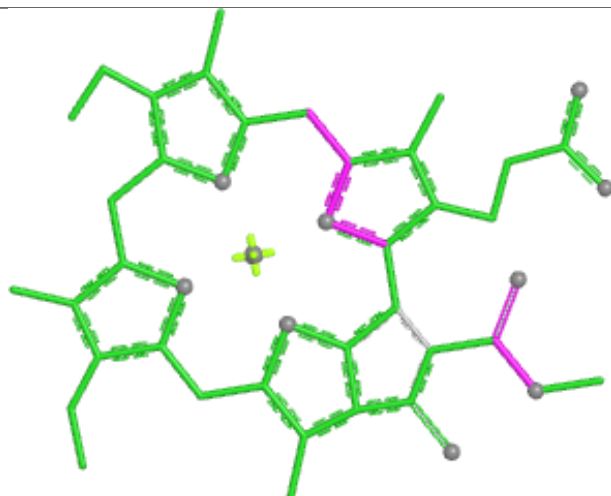
Ligand CLA 4 502**Ligand CLA B 1206**



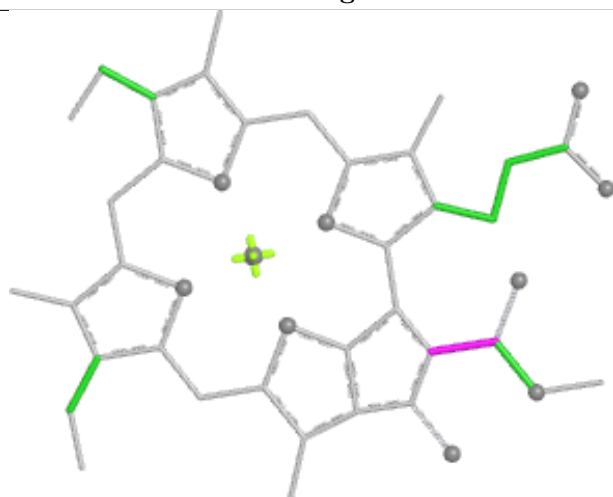
Ligand CLA 4 504



Bond lengths



Bond angles

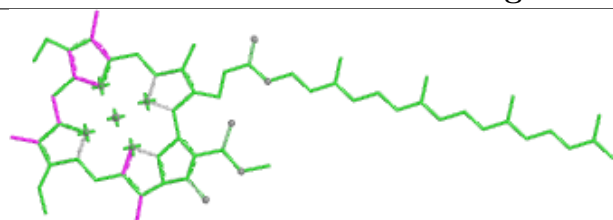


Torsions

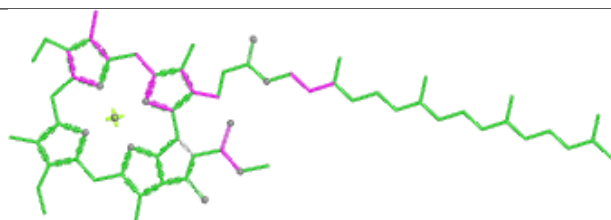


Rings

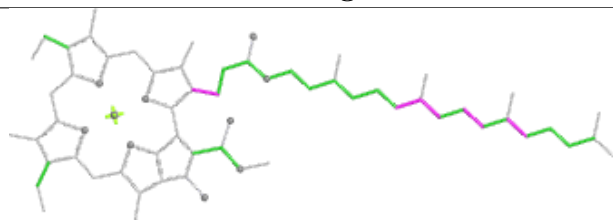
Ligand CLA A 1104



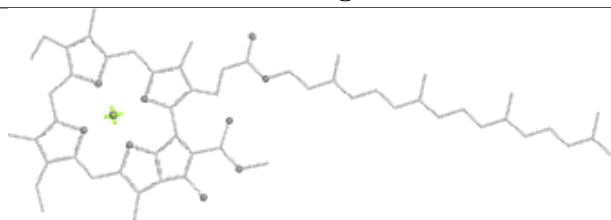
Bond lengths



Bond angles

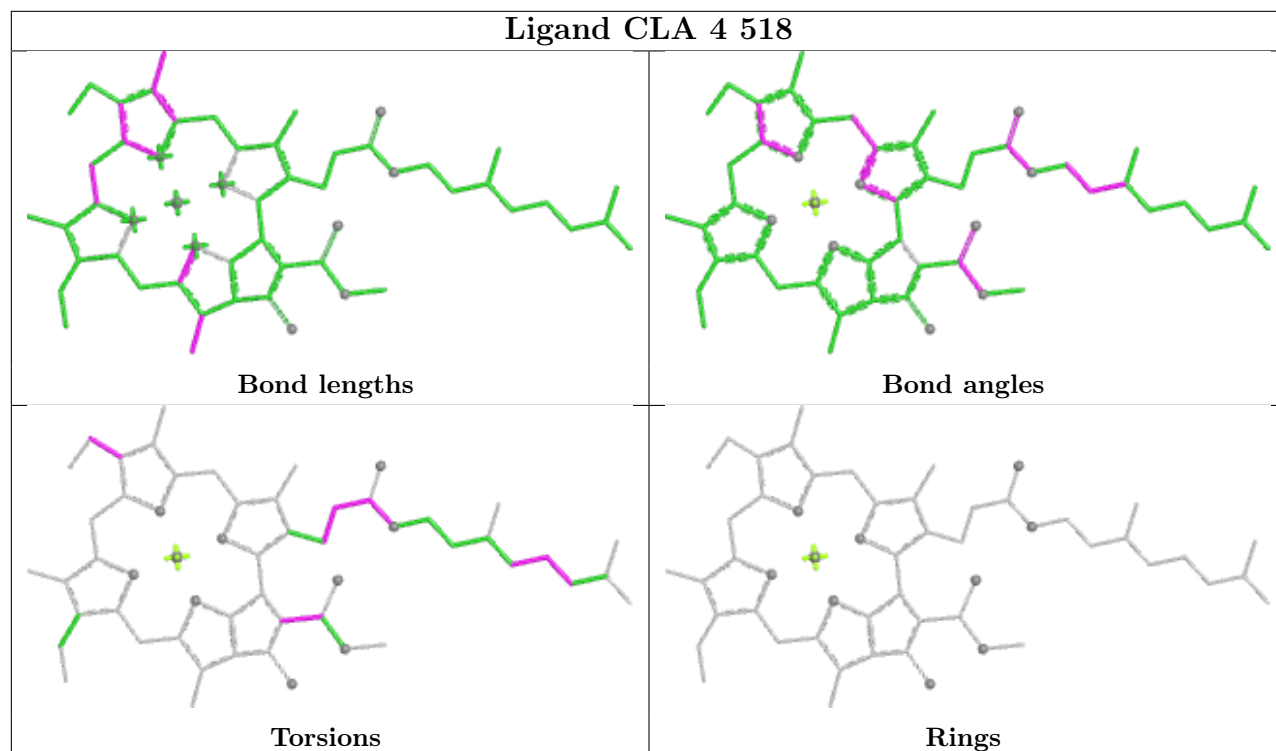


Torsions

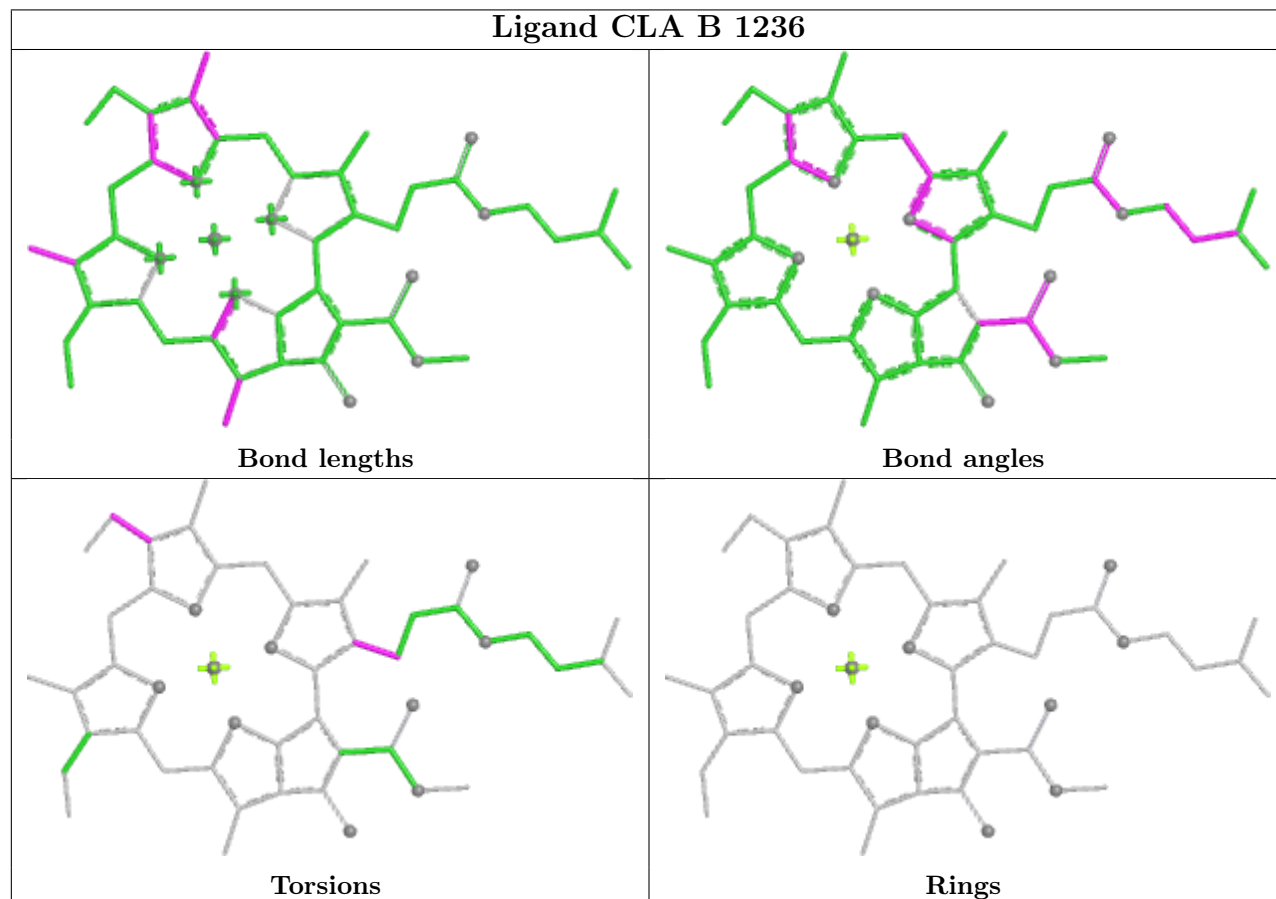


Rings

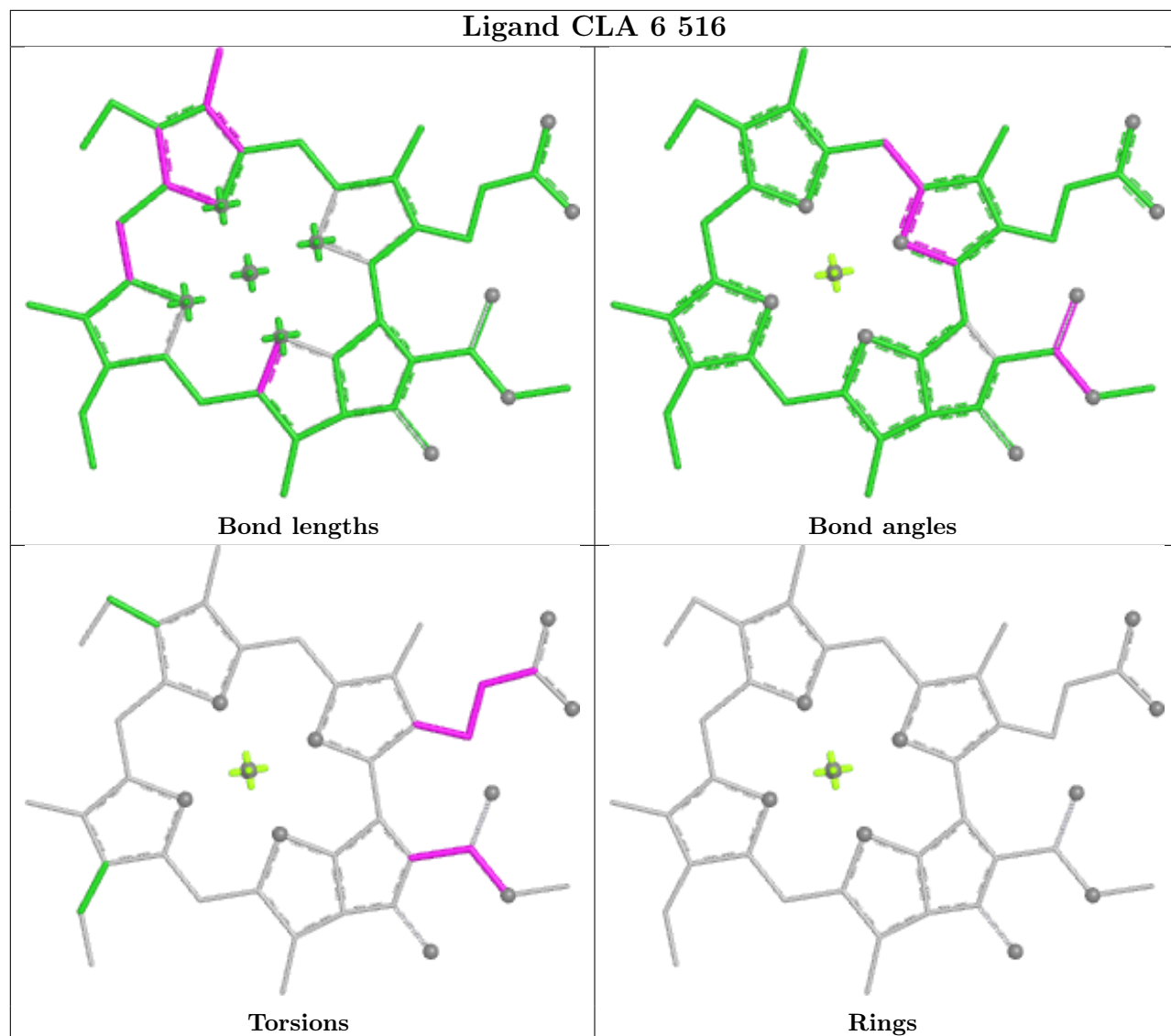
Ligand CLA 4 518



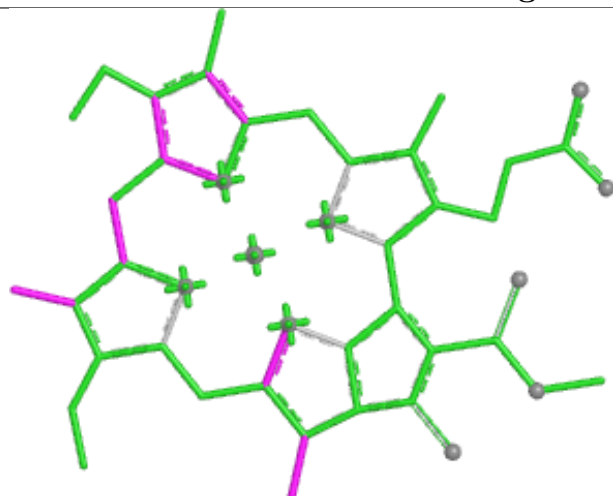
Ligand CLA B 1236



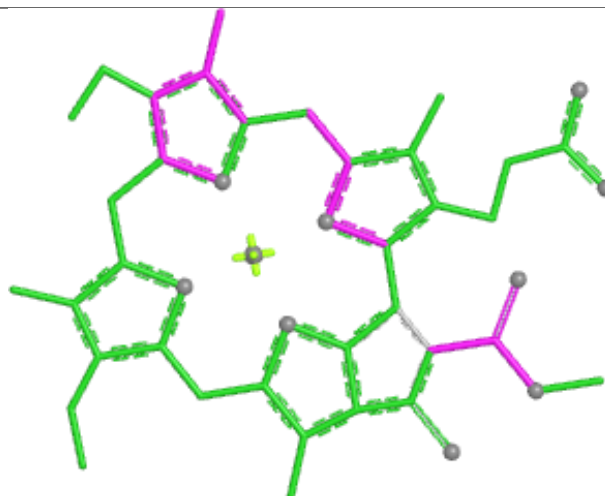
Ligand CLA 6 516



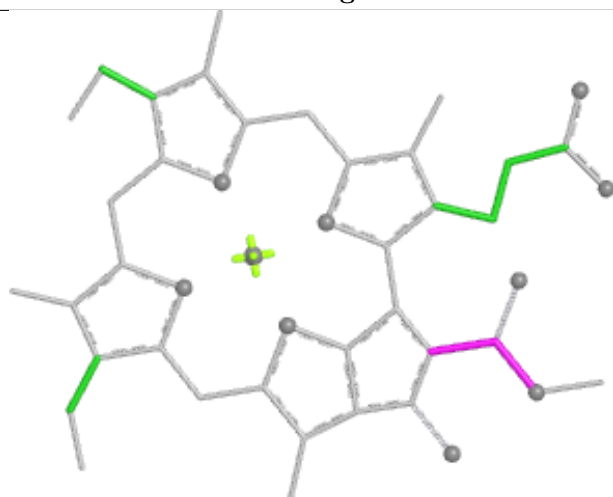
Ligand CLA 3 506



Bond lengths



Bond angles

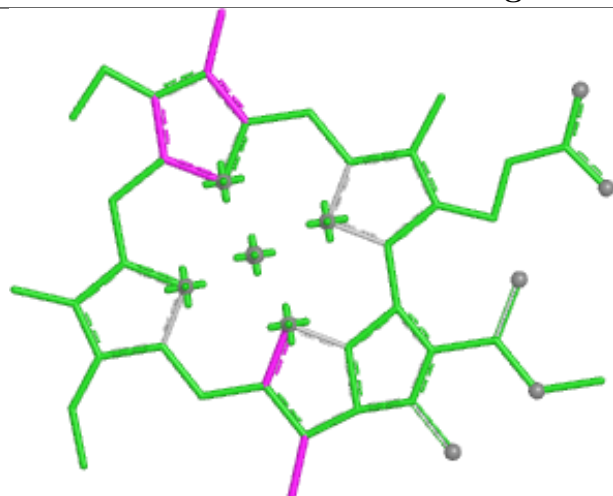


Torsions

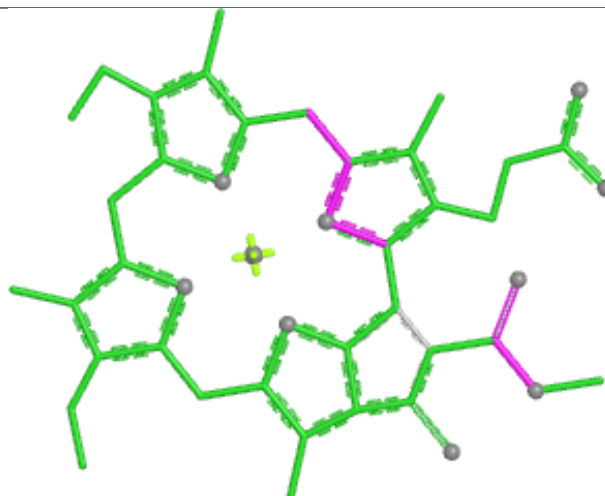


Rings

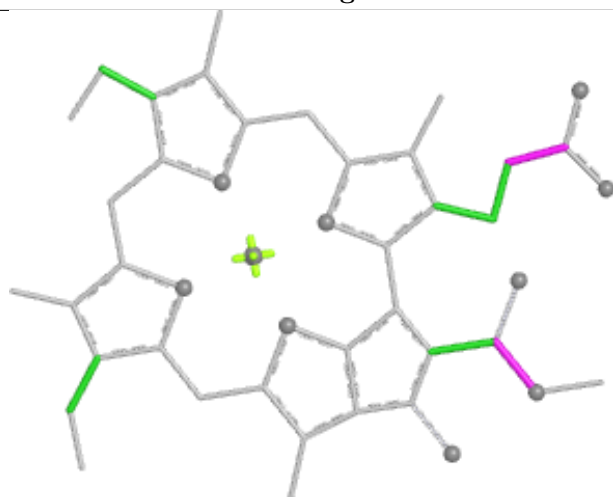
Ligand CLA A 1108



Bond lengths



Bond angles

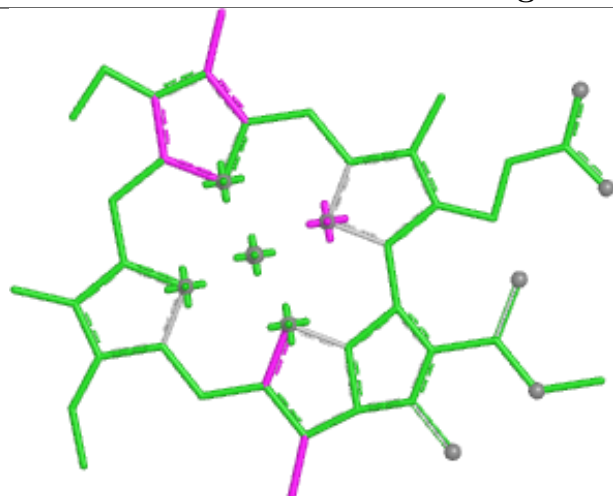


Torsions

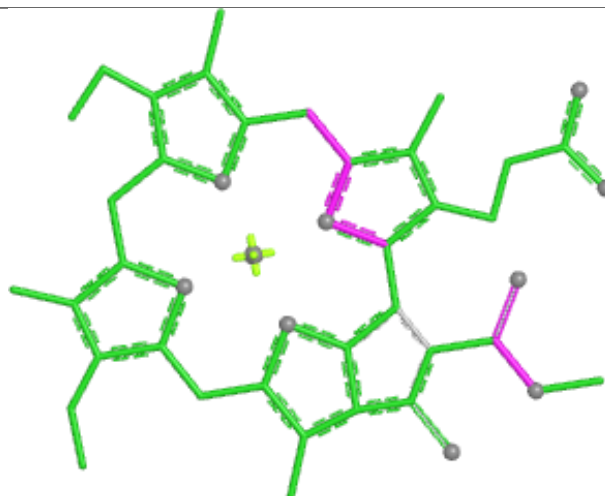


Rings

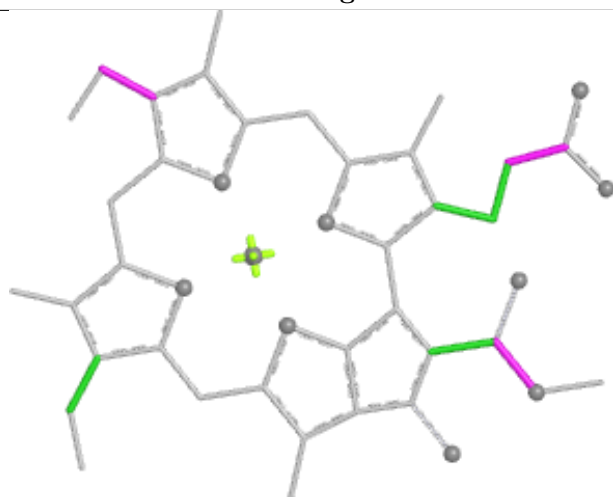
Ligand CLA b 517



Bond lengths



Bond angles

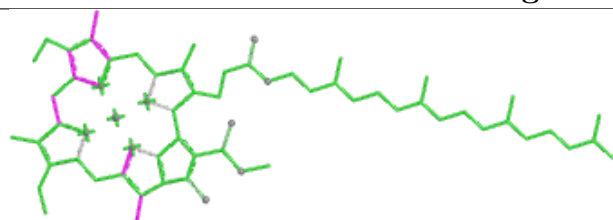


Torsions

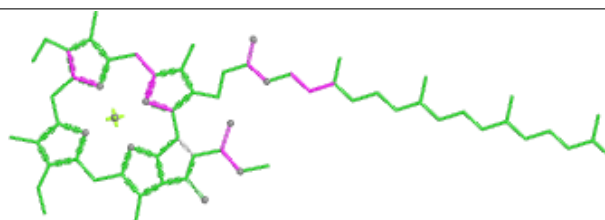


Rings

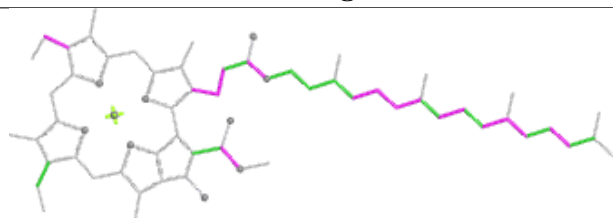
Ligand CLA f 501



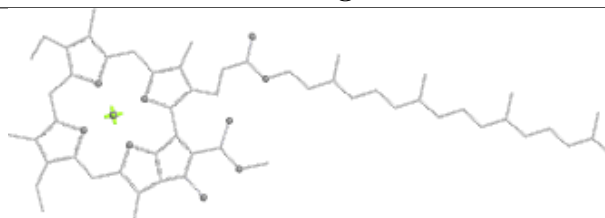
Bond lengths



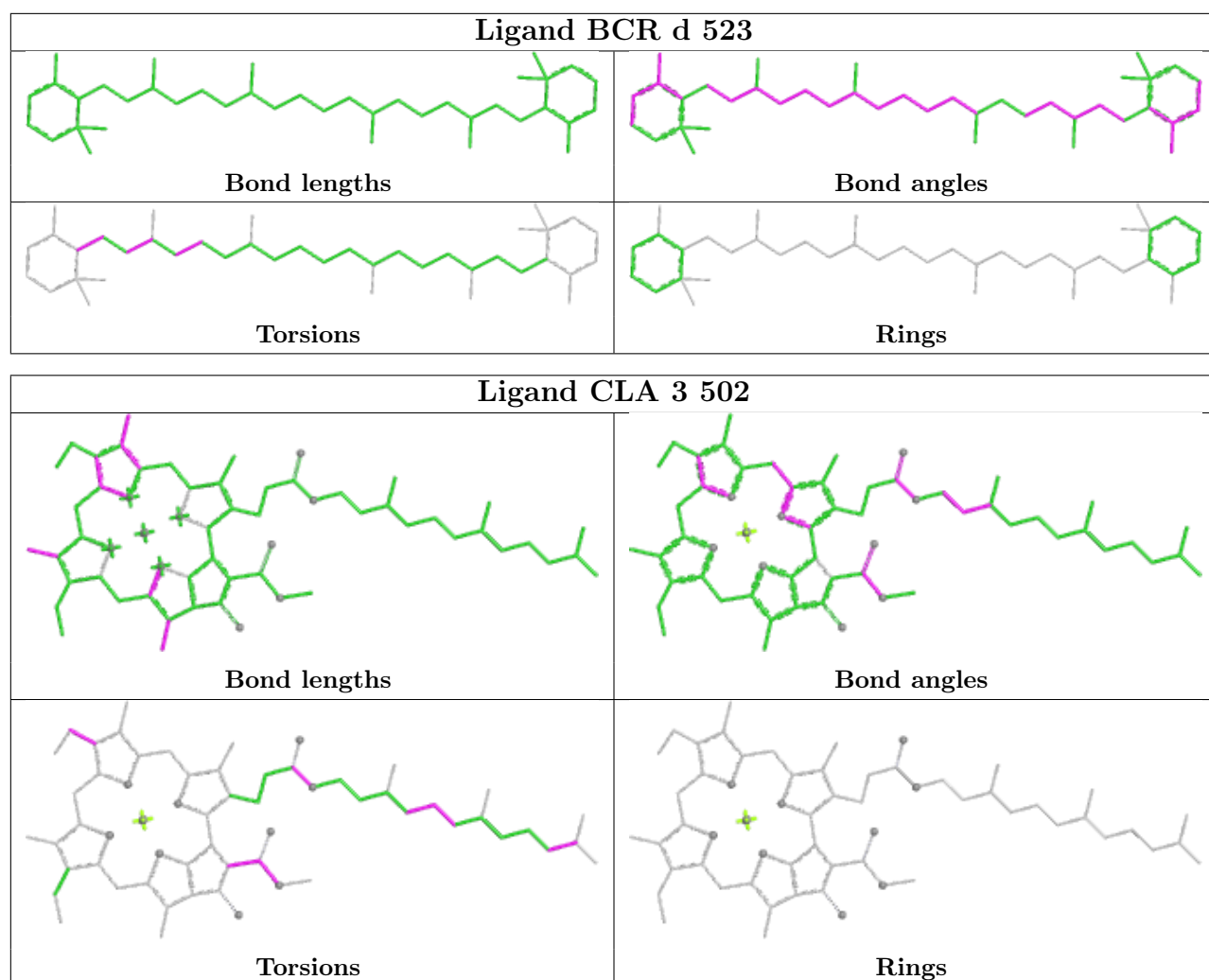
Bond angles



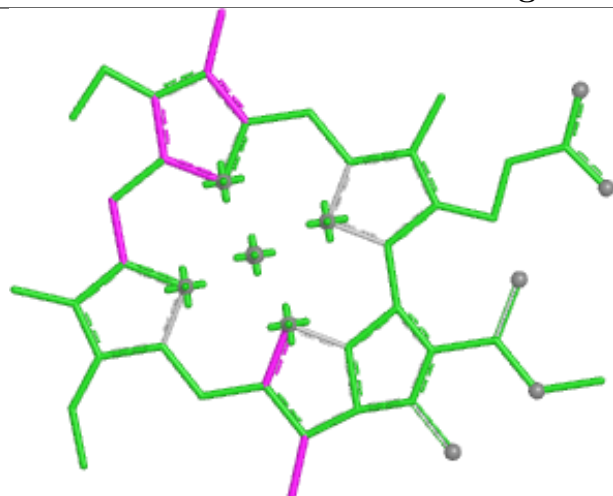
Torsions



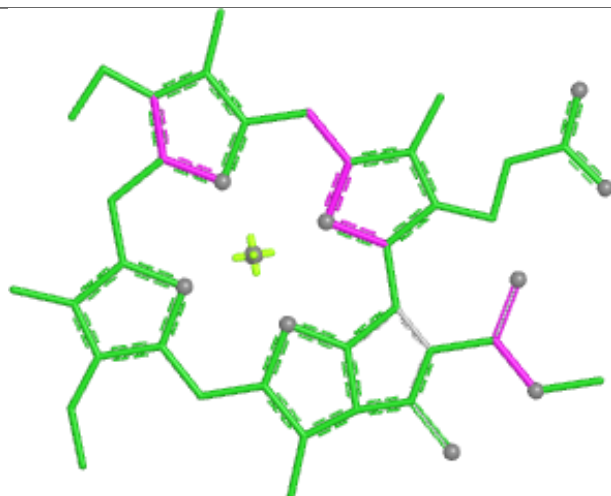
Rings



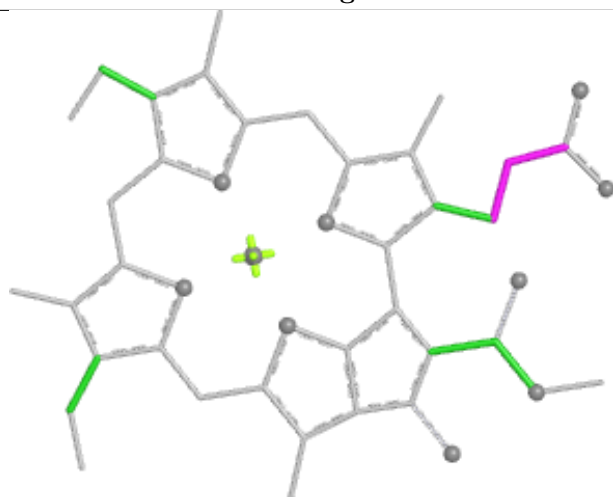
Ligand CLA 4 516



Bond lengths



Bond angles

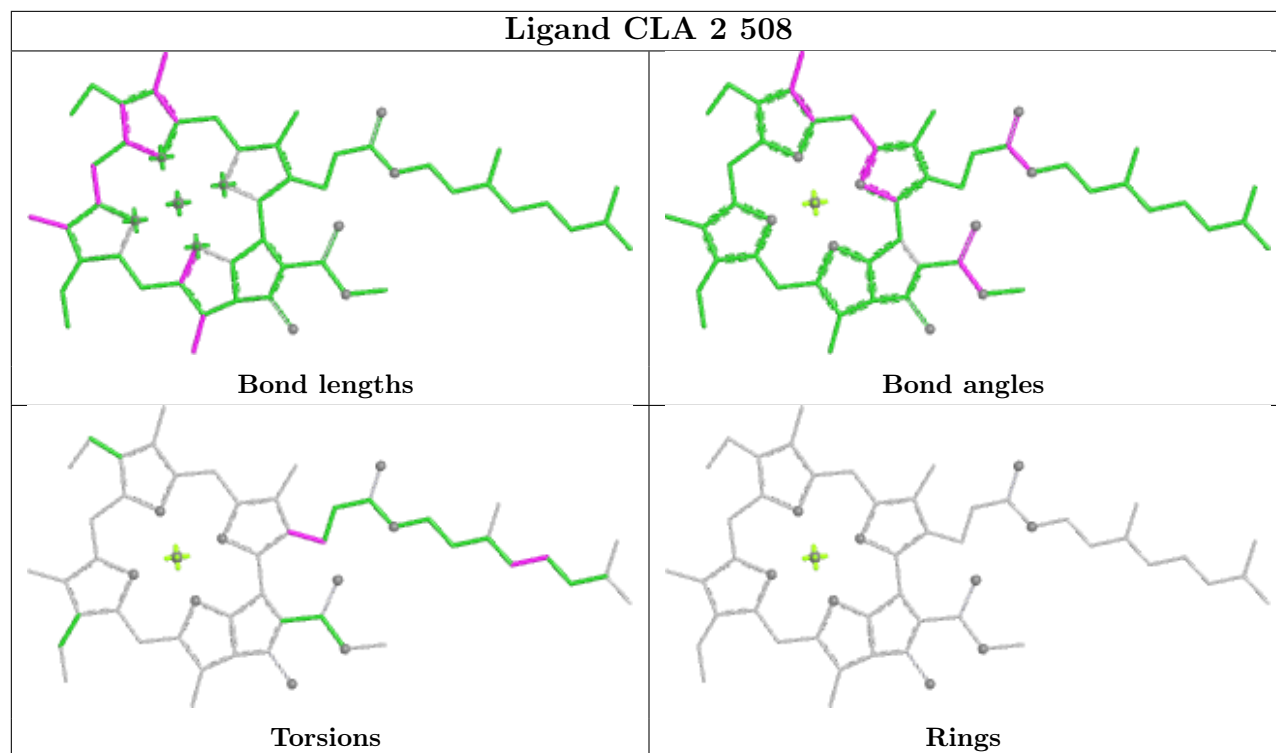


Torsions

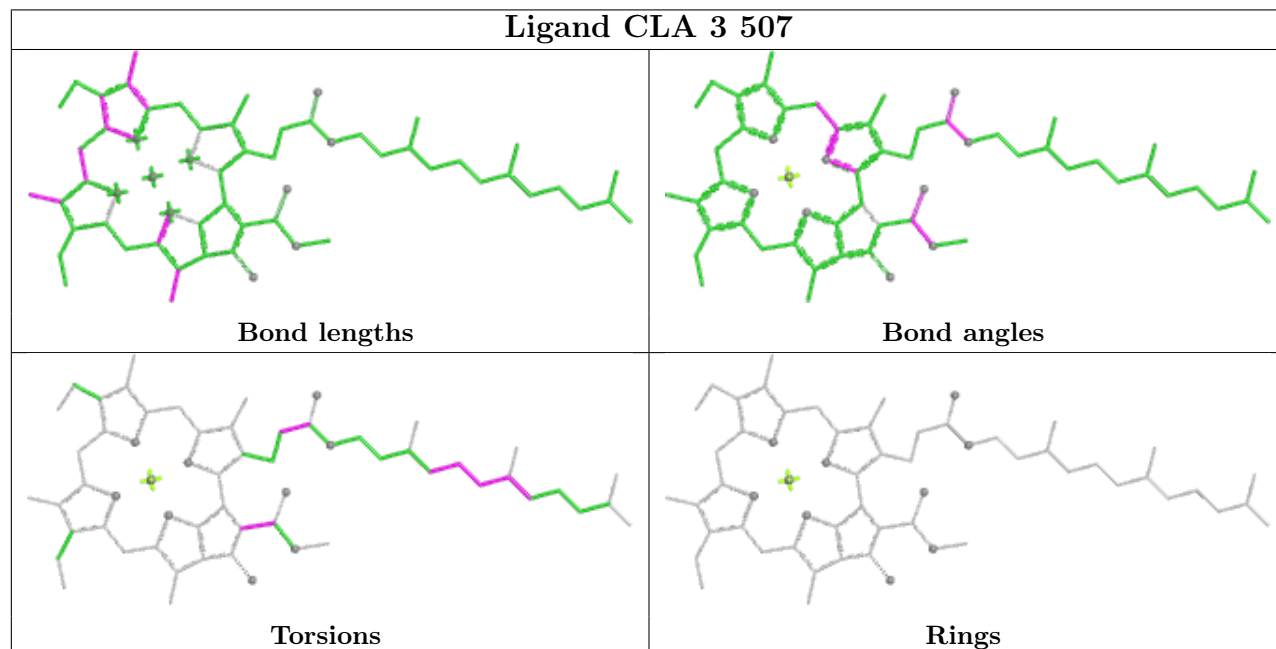


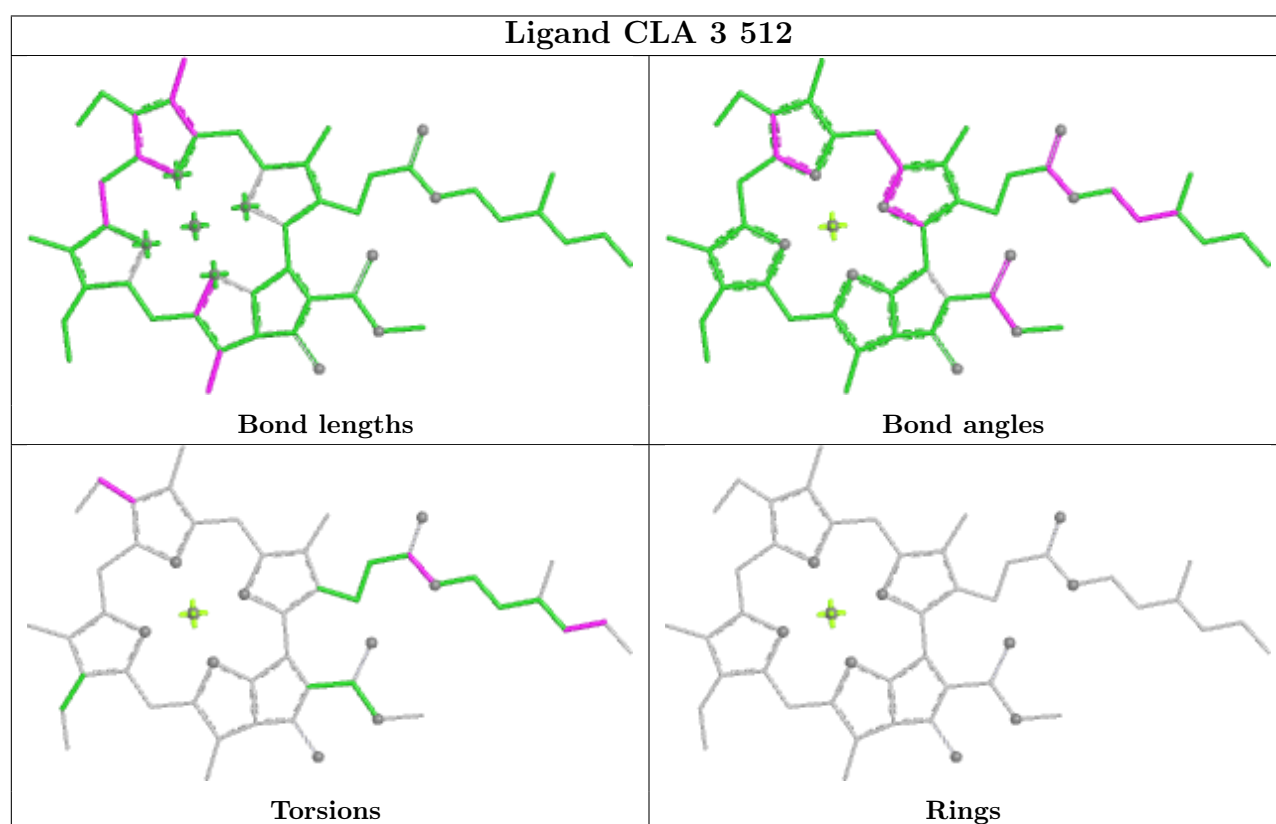
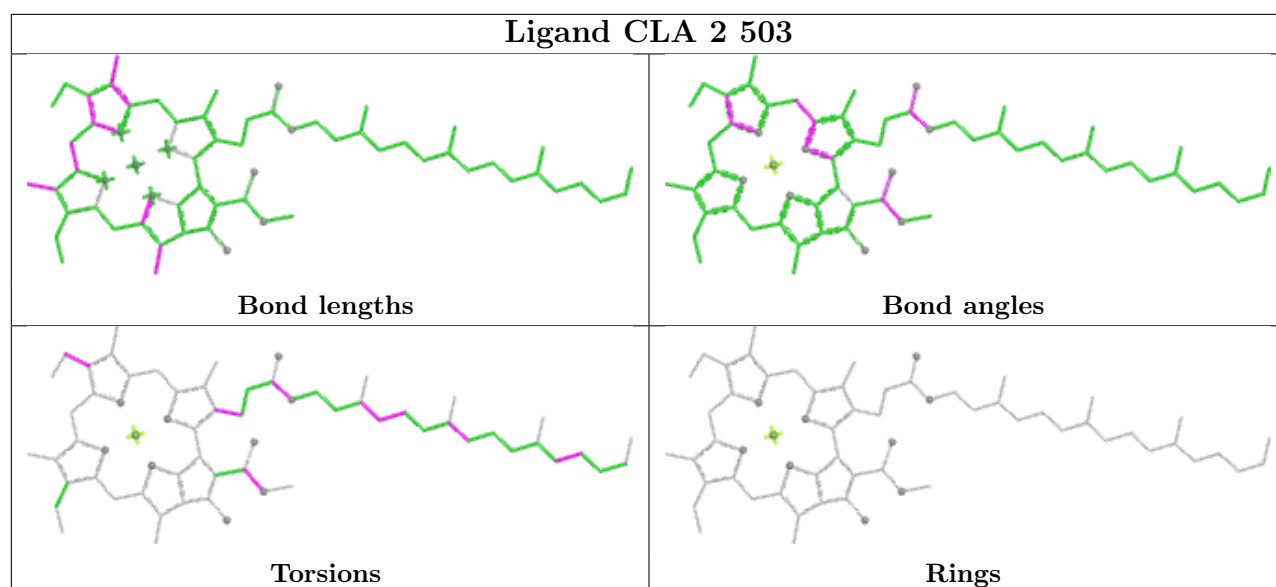
Rings

Ligand CLA 2 508

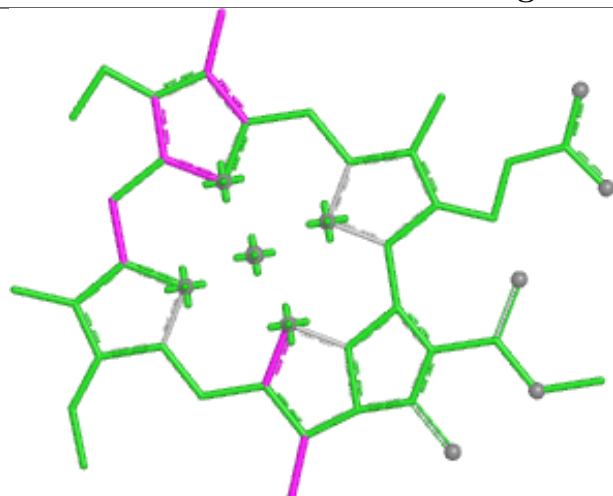


Ligand CLA 3 507

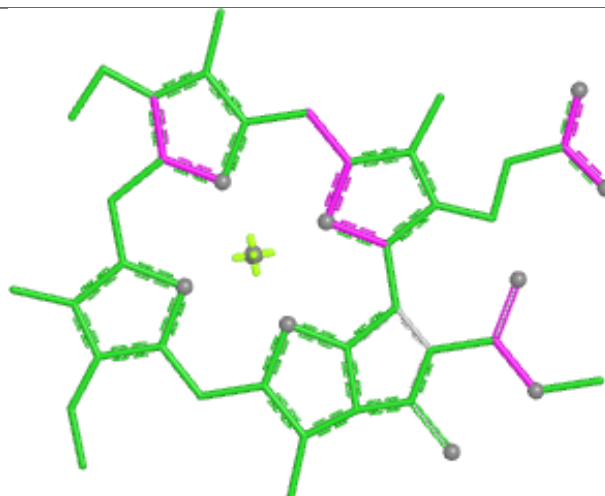




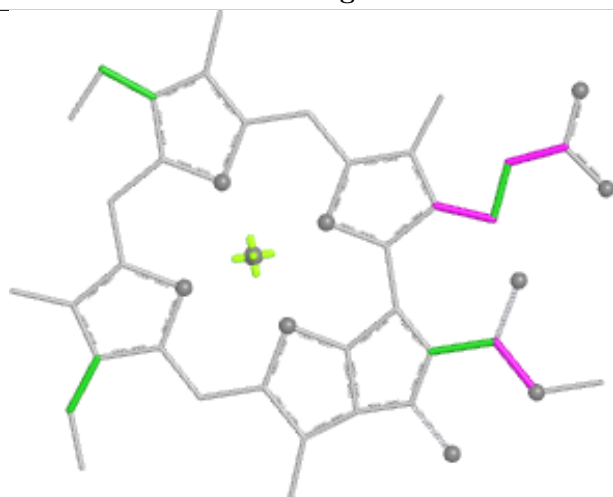
Ligand CLA b 519



Bond lengths



Bond angles

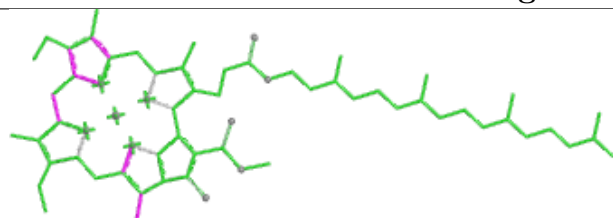


Torsions

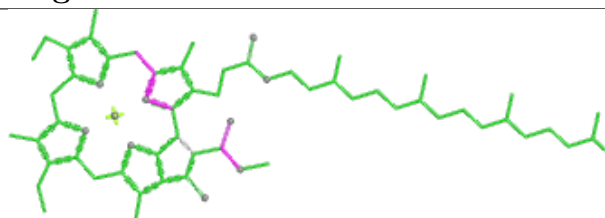


Rings

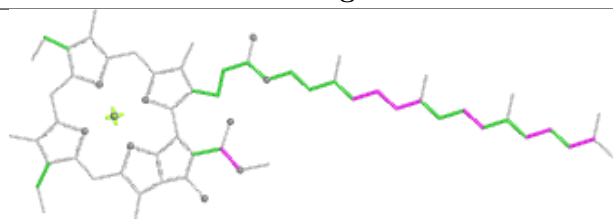
Ligand CLA g 510



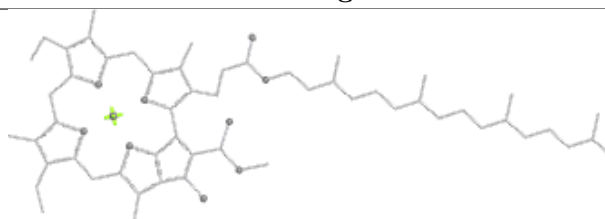
Bond lengths



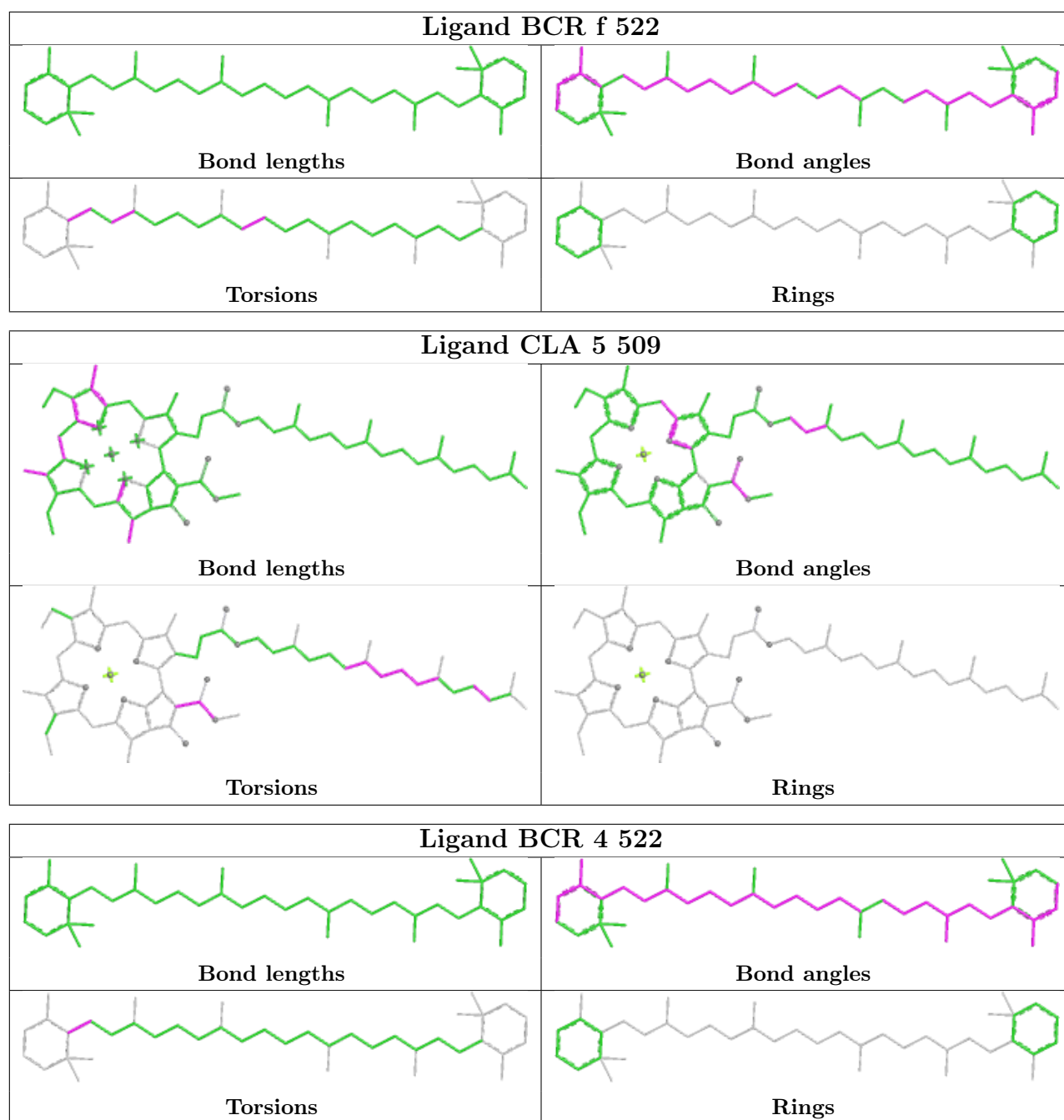
Bond angles



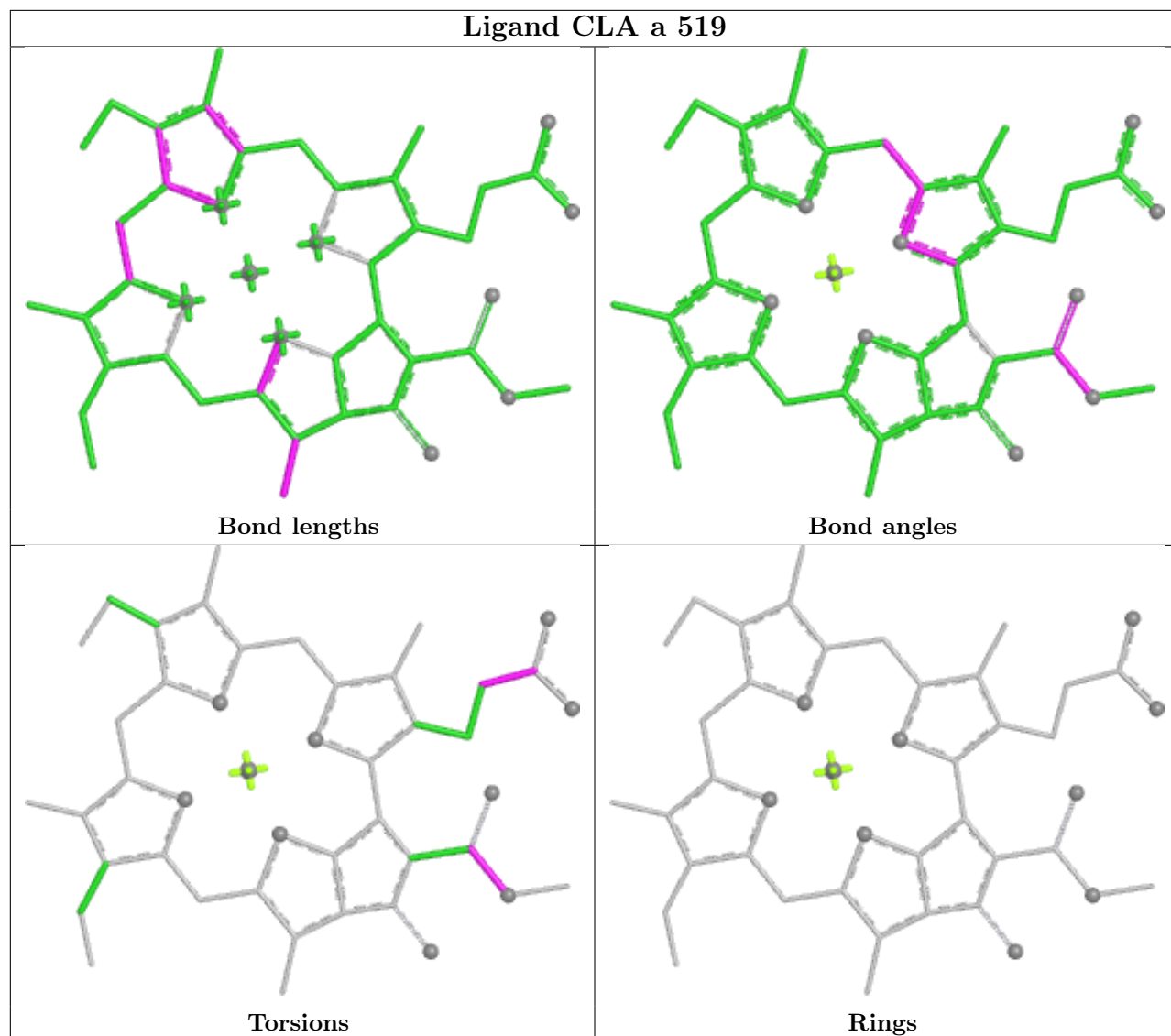
Torsions



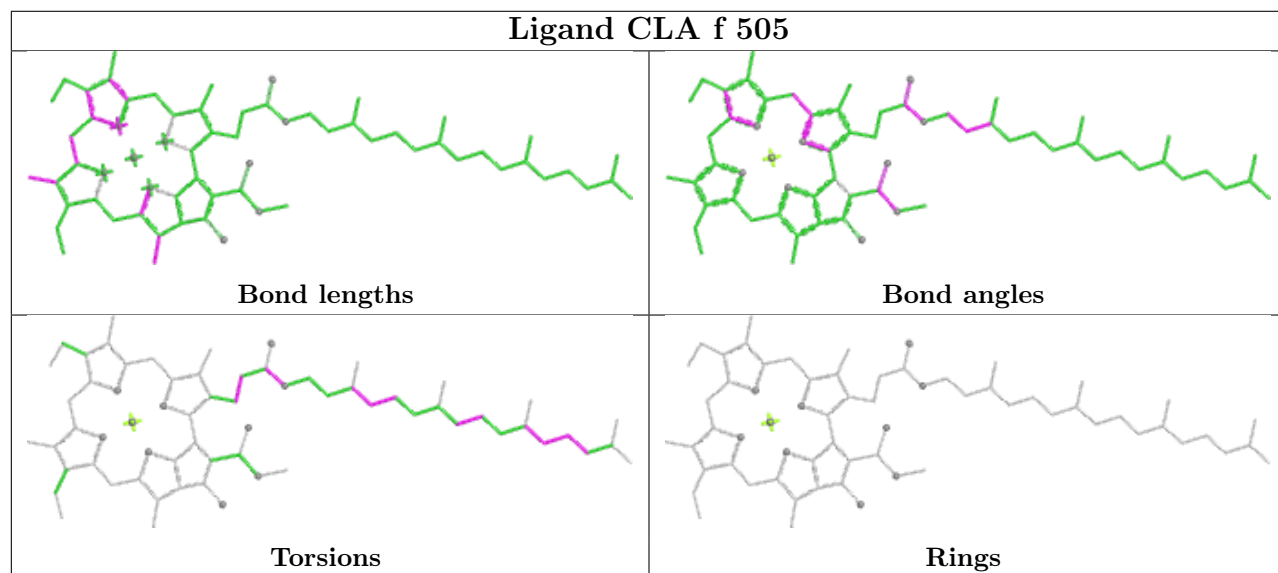
Rings

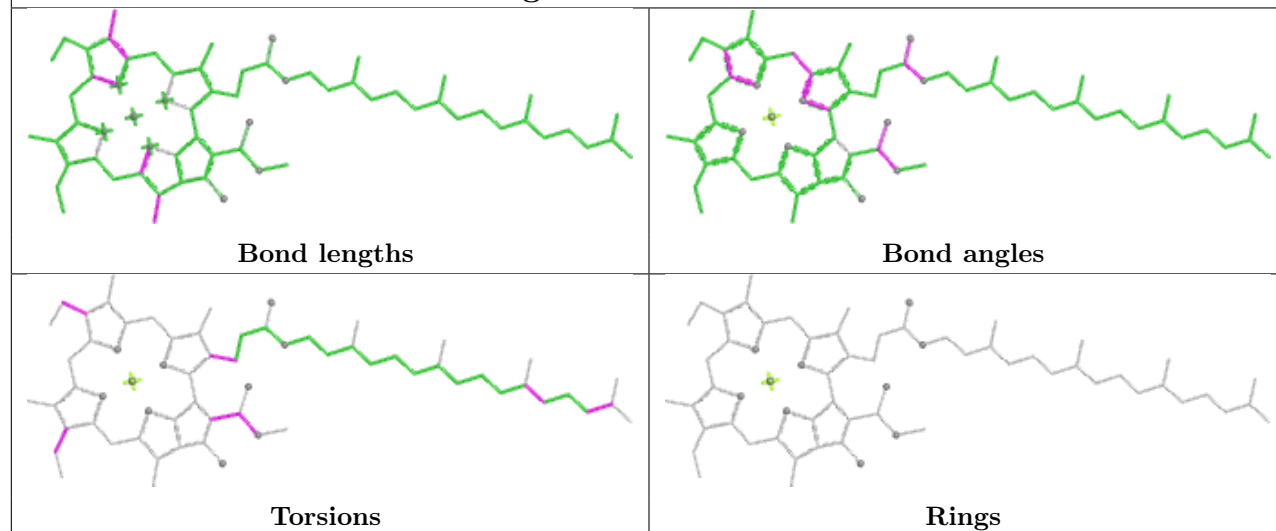
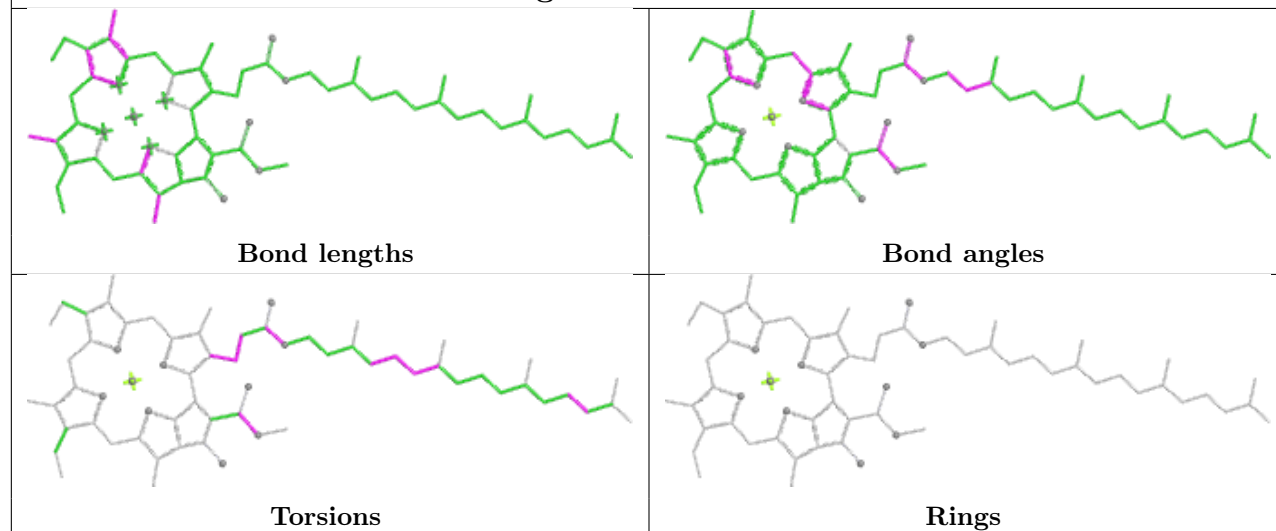


Ligand CLA a 519

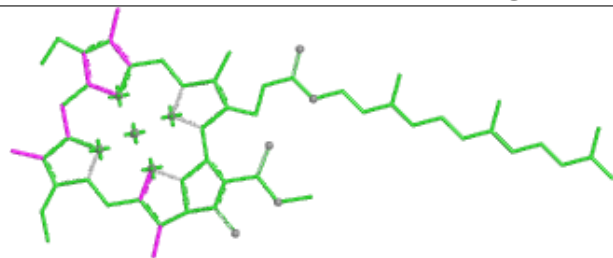


Ligand CLA f 505

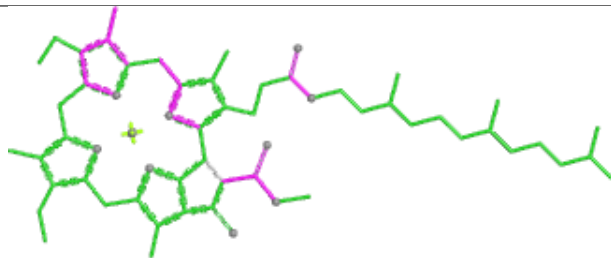


Ligand CLA A 1132**Ligand CLA 3 509**

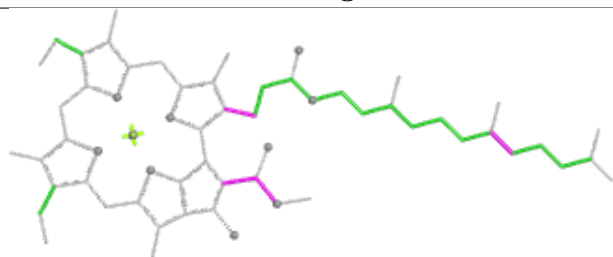
Ligand CLA B 1222



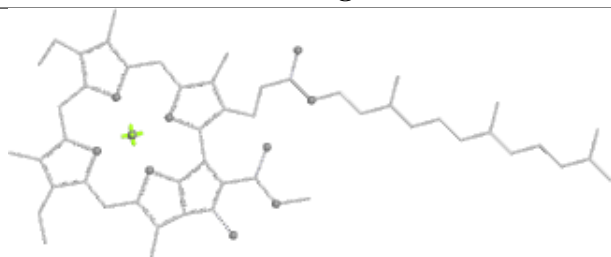
Bond lengths



Bond angles

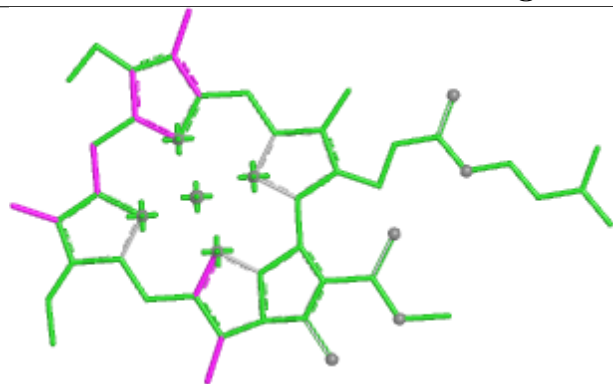


Torsions

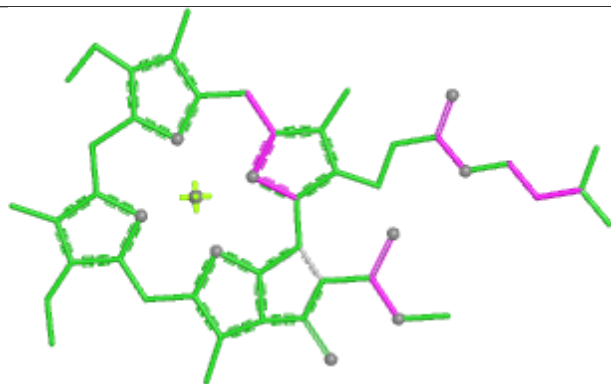


Rings

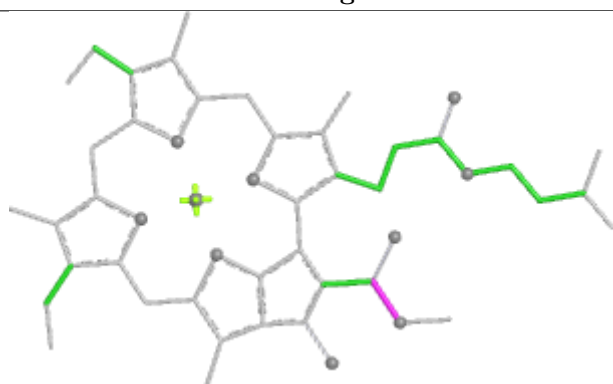
Ligand CLA d 513



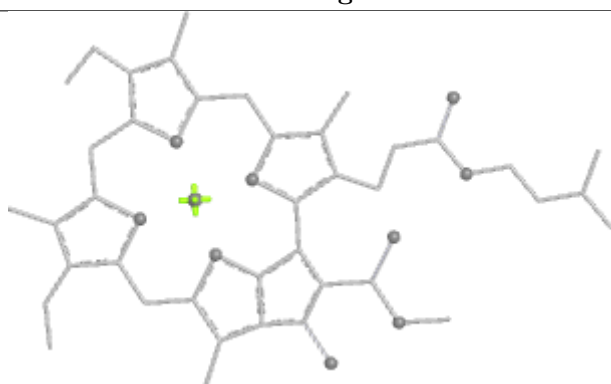
Bond lengths



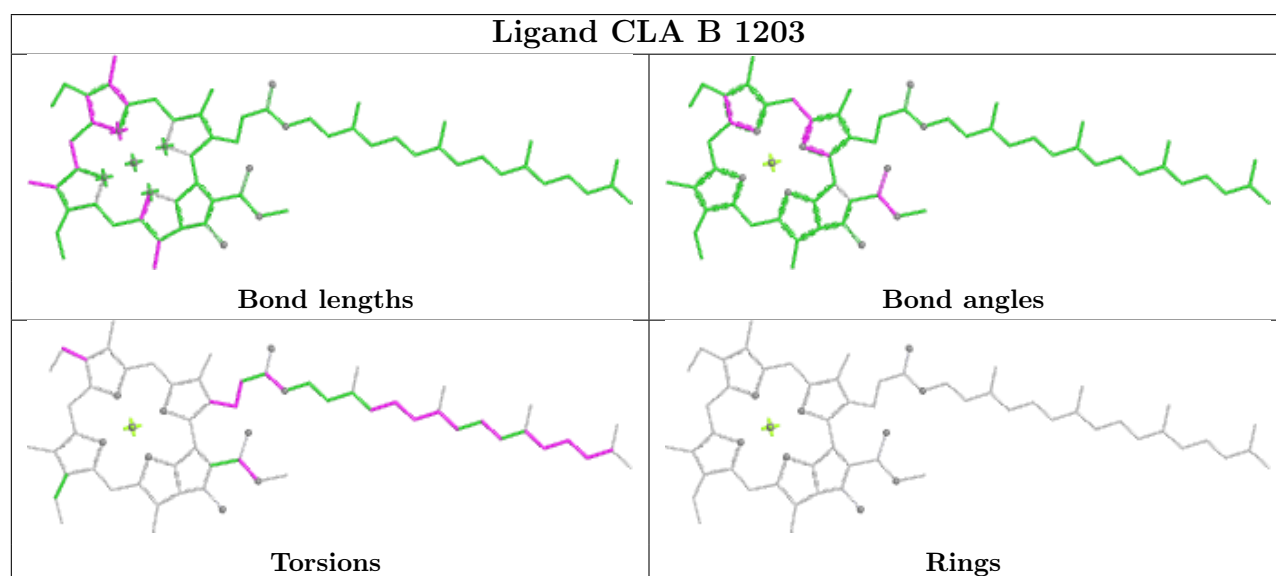
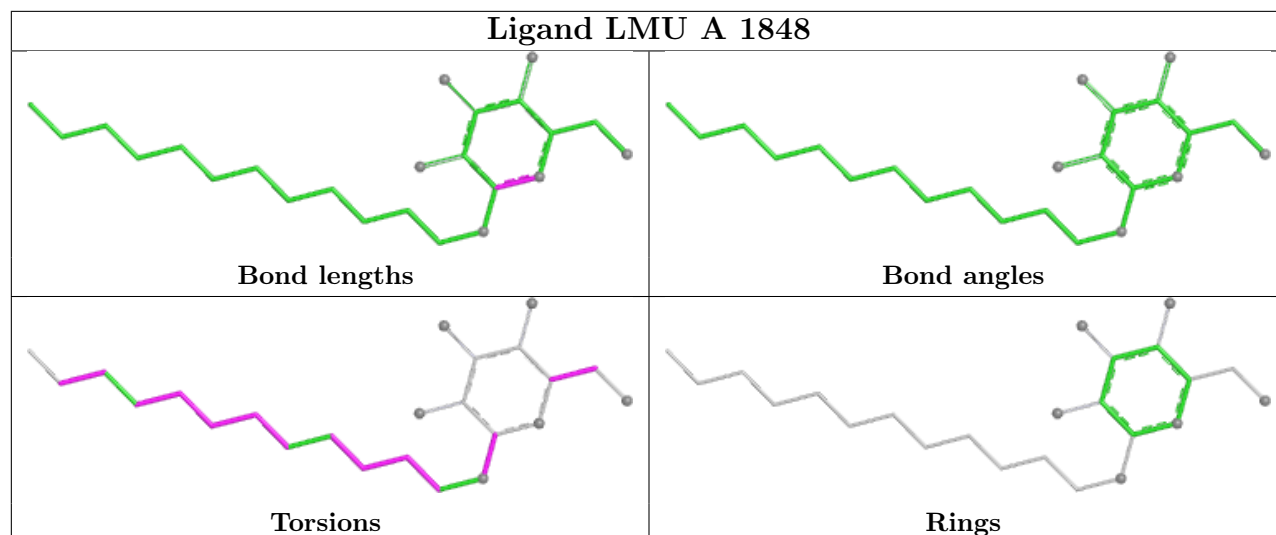
Bond angles



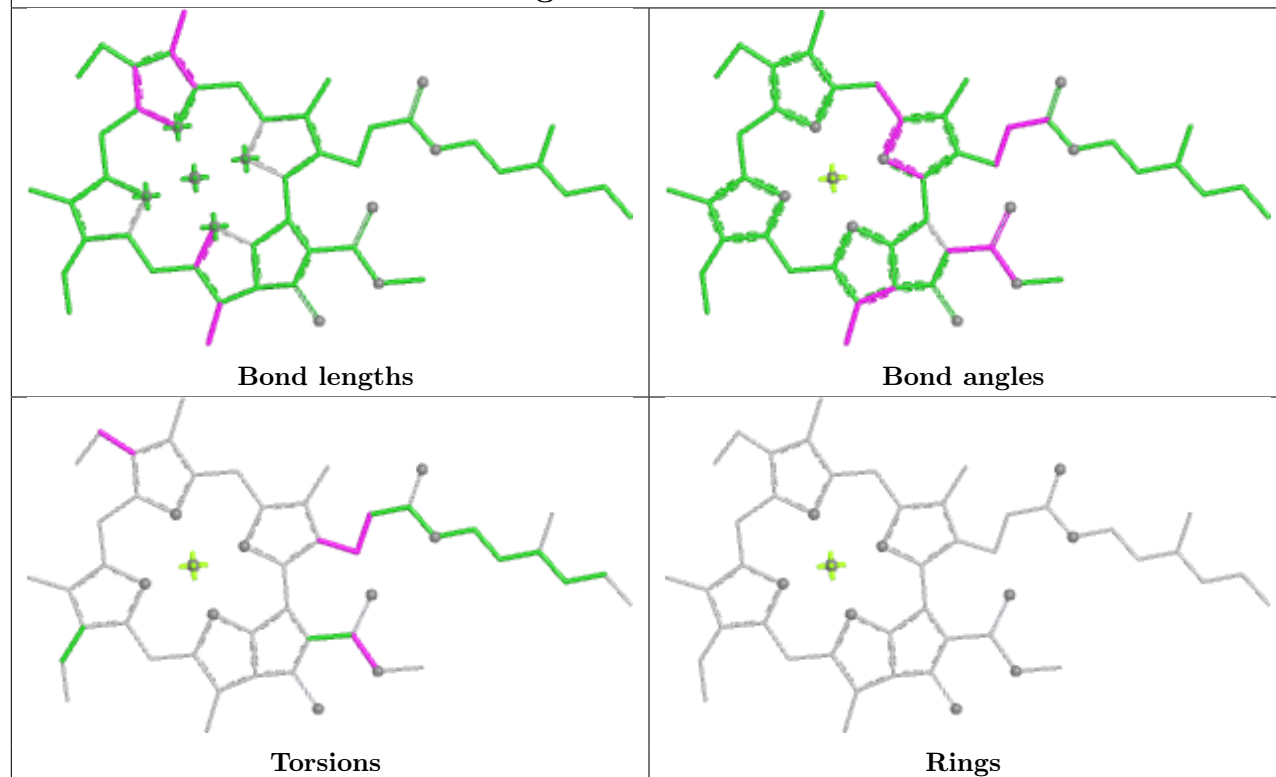
Torsions



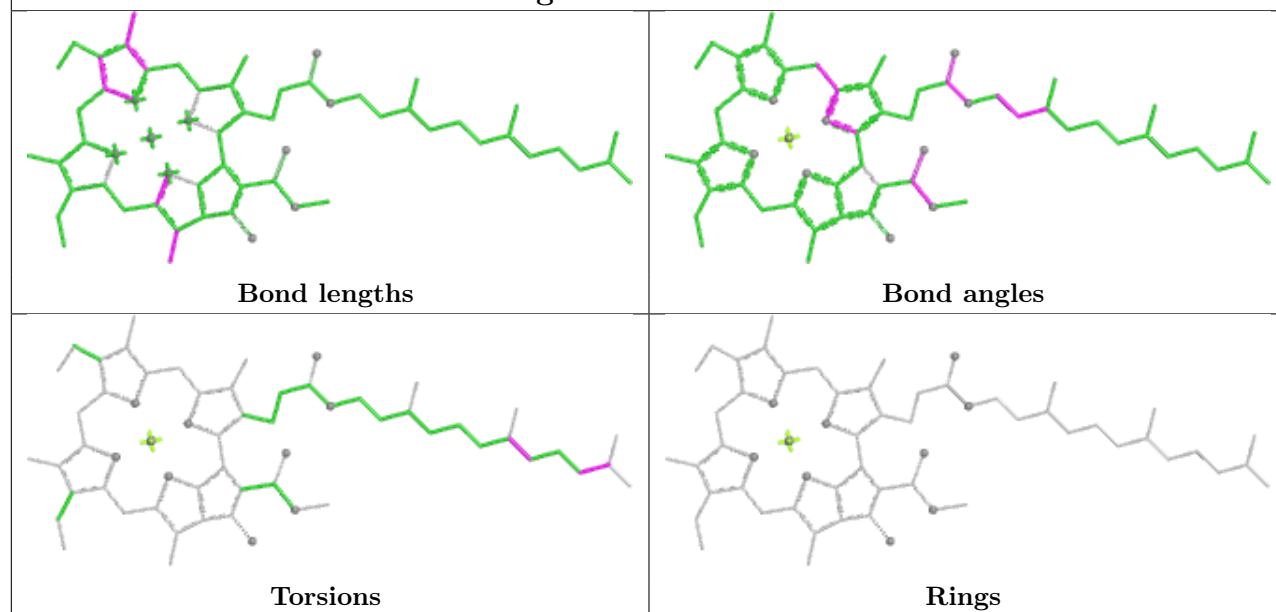
Rings

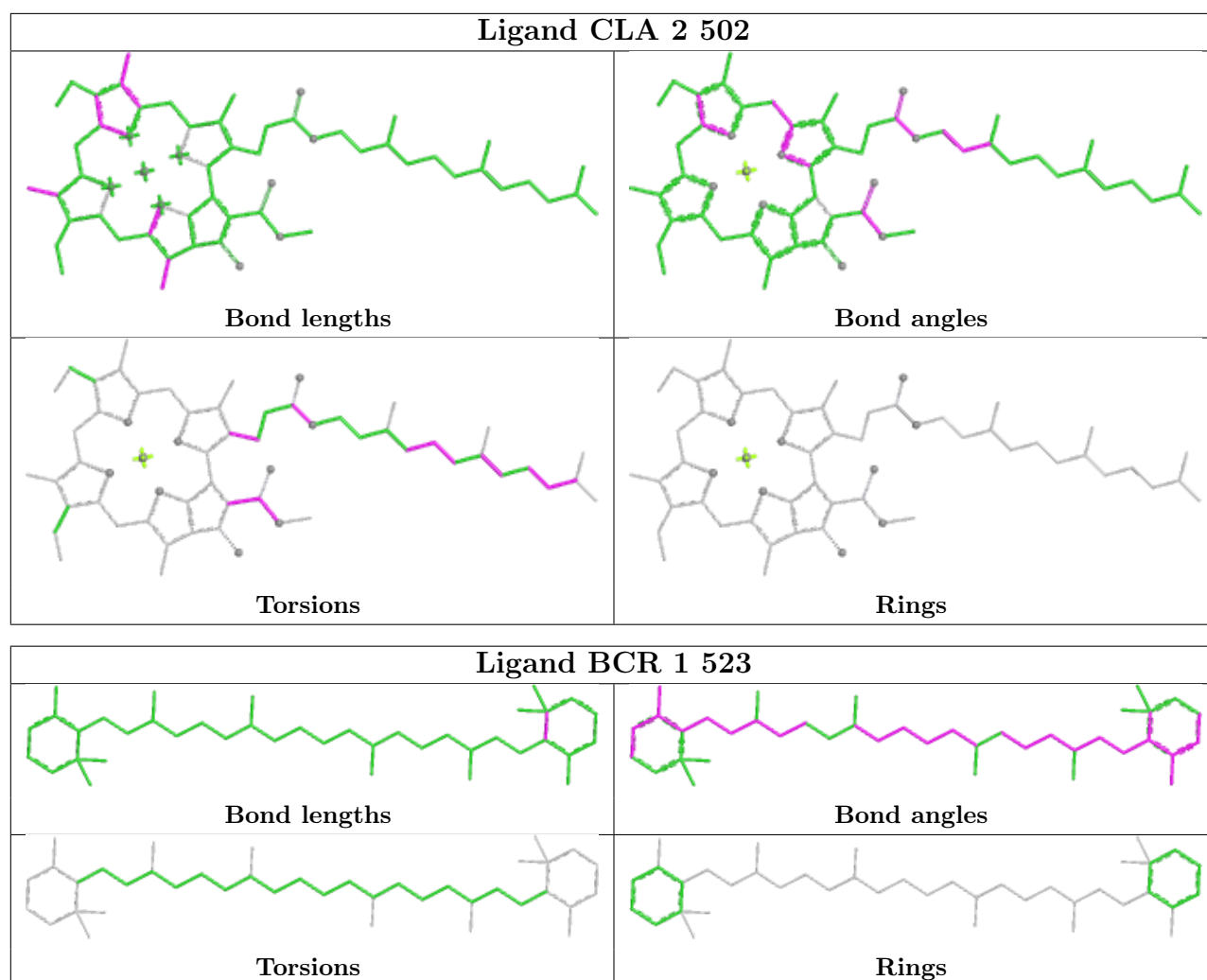


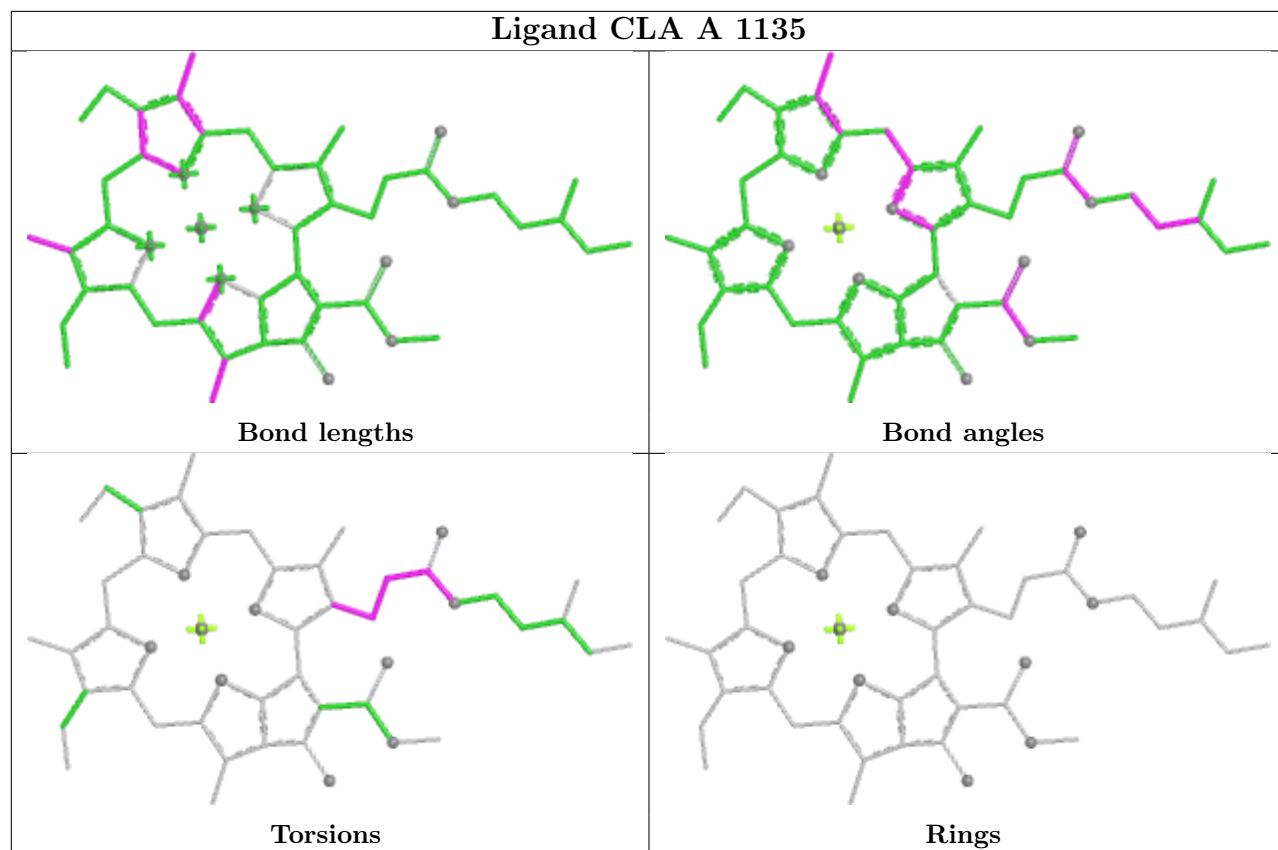
Ligand CLA 1 512



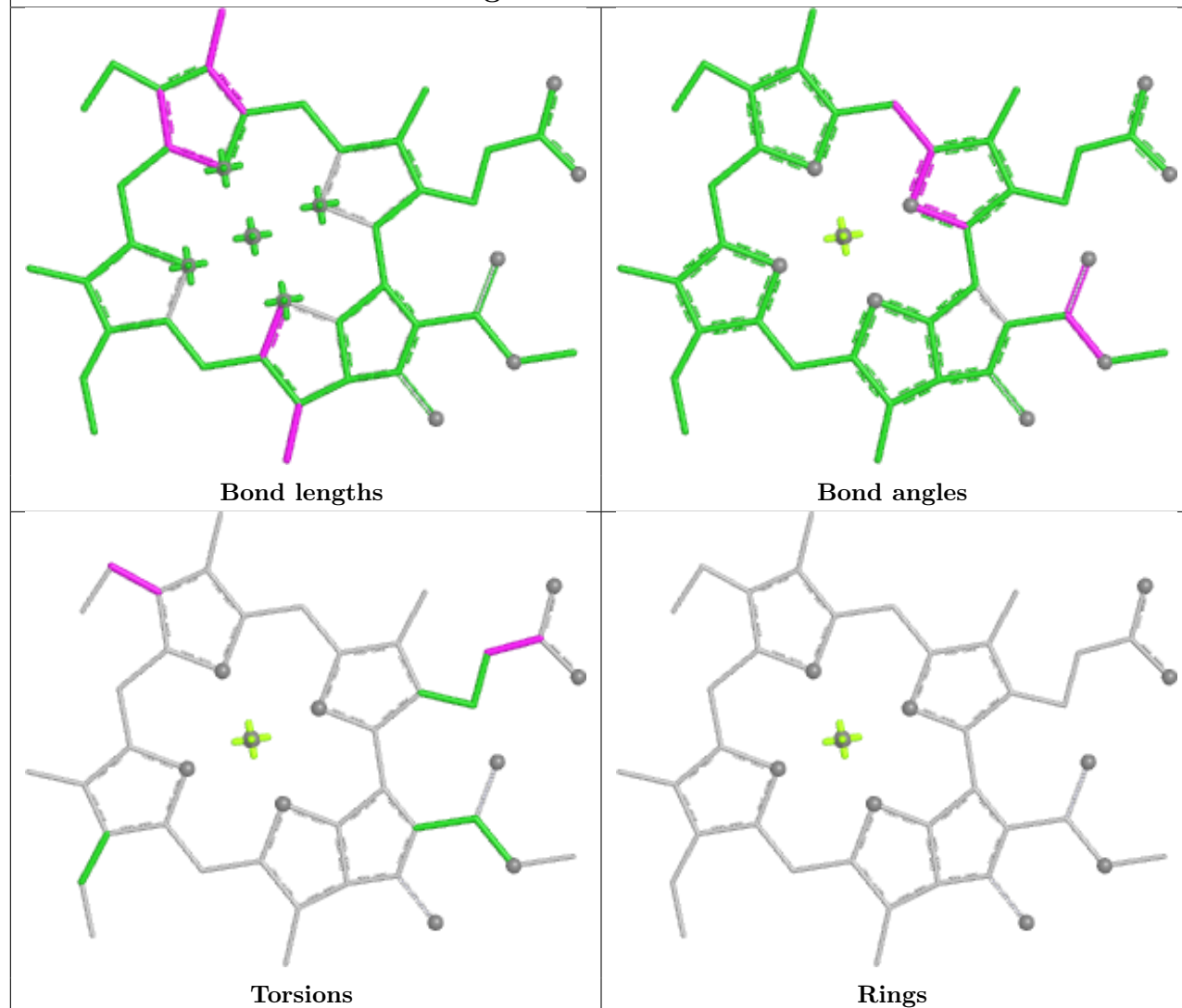
Ligand CLA 6 507



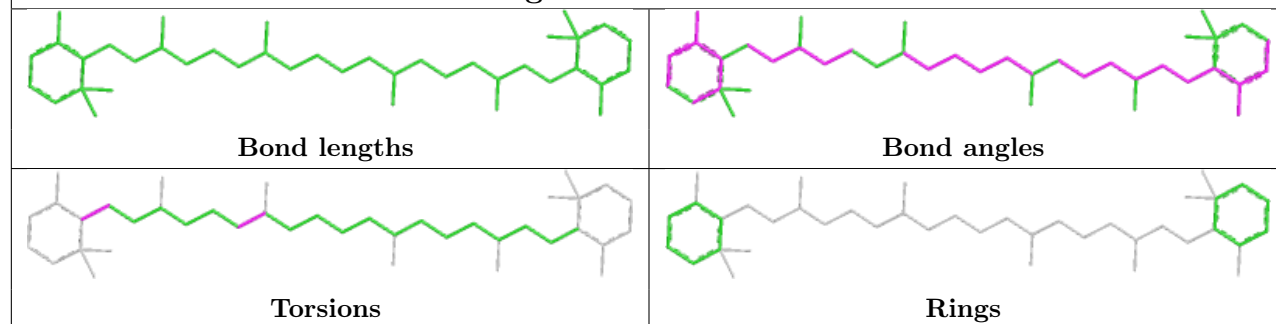


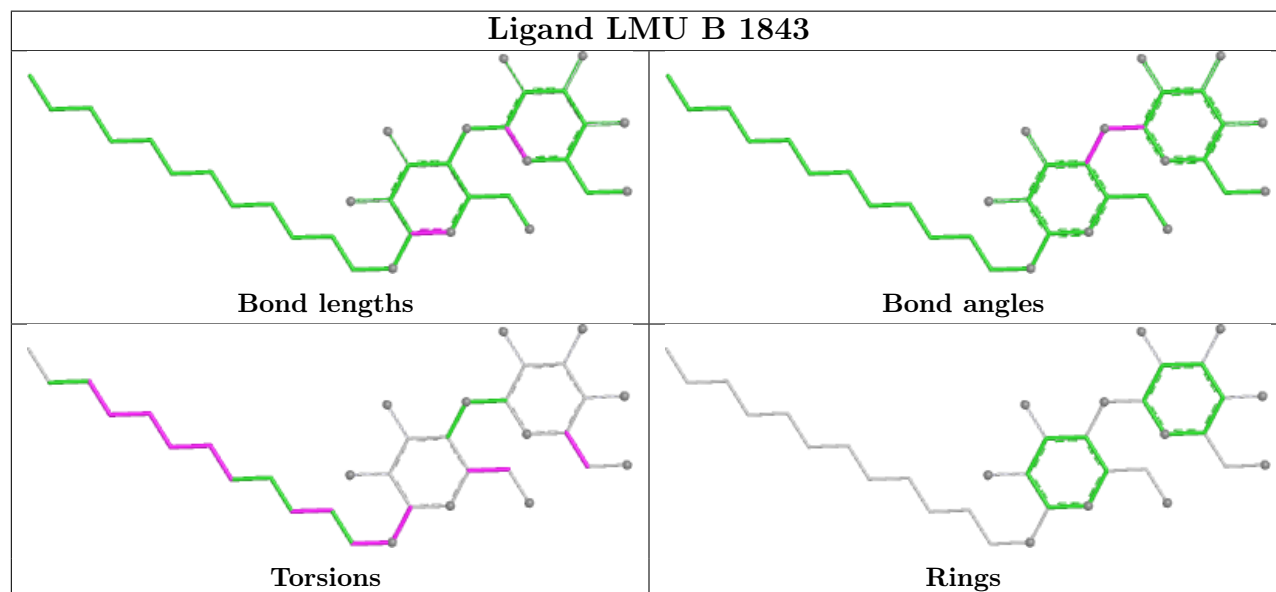
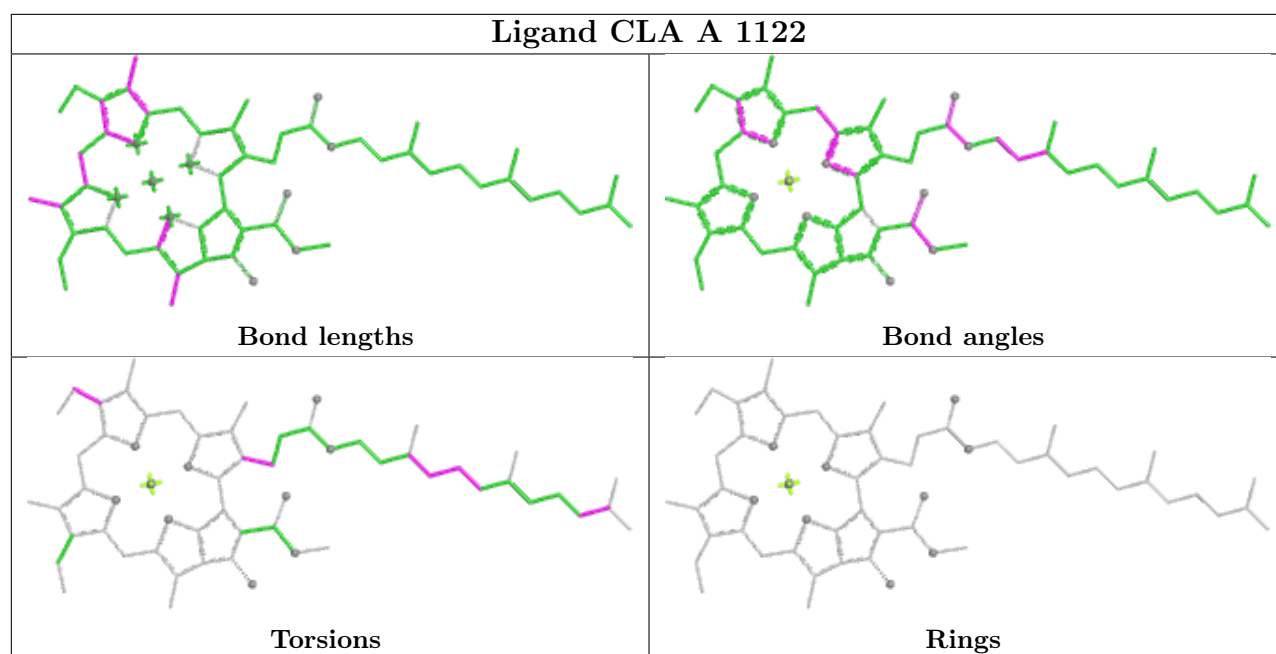


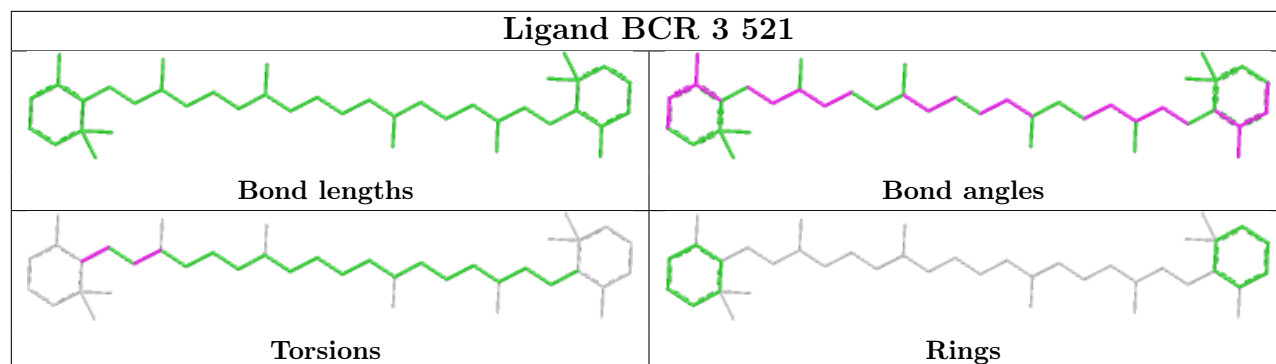
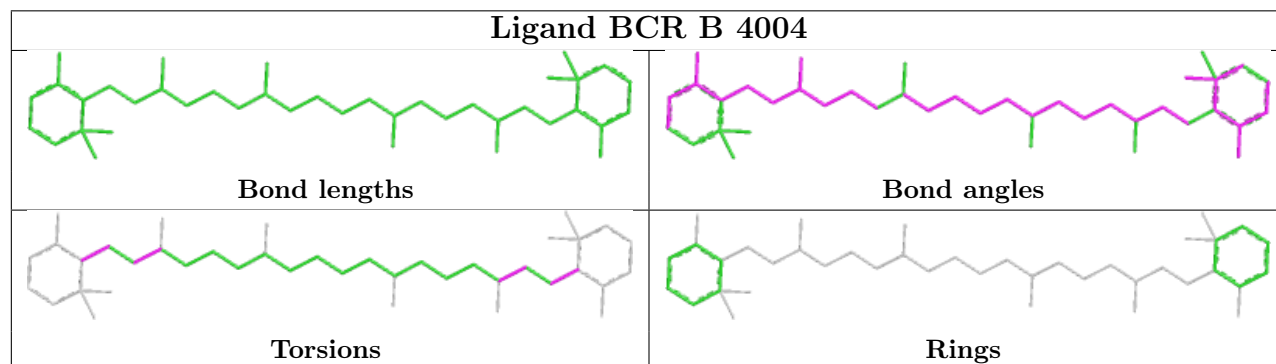
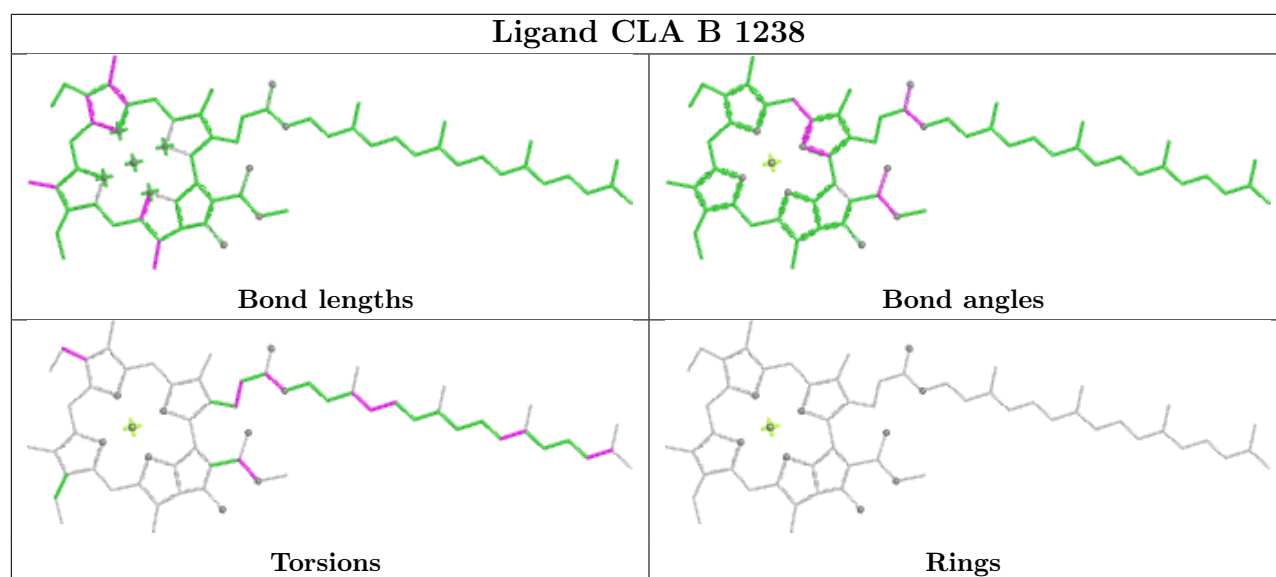
Ligand CLA A 1114



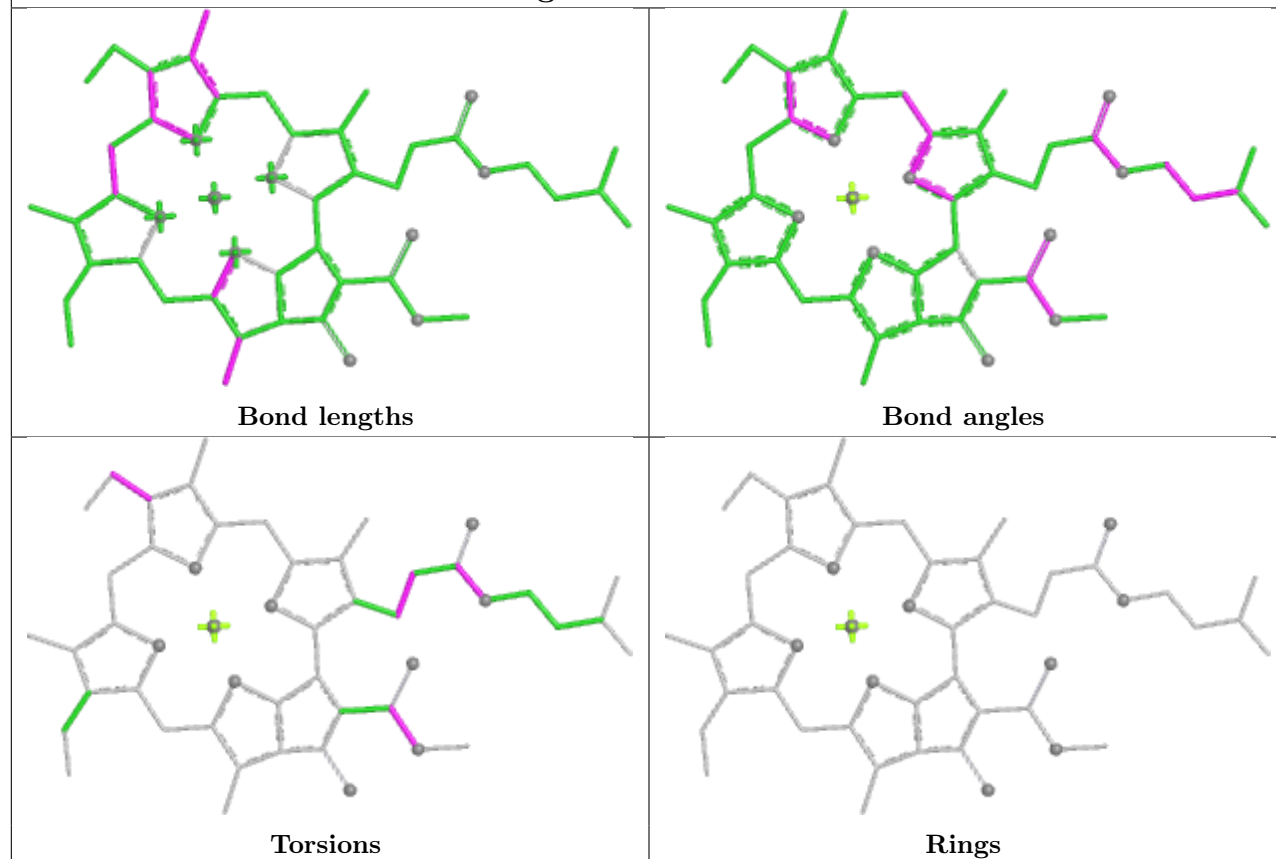
Ligand BCR J 4012



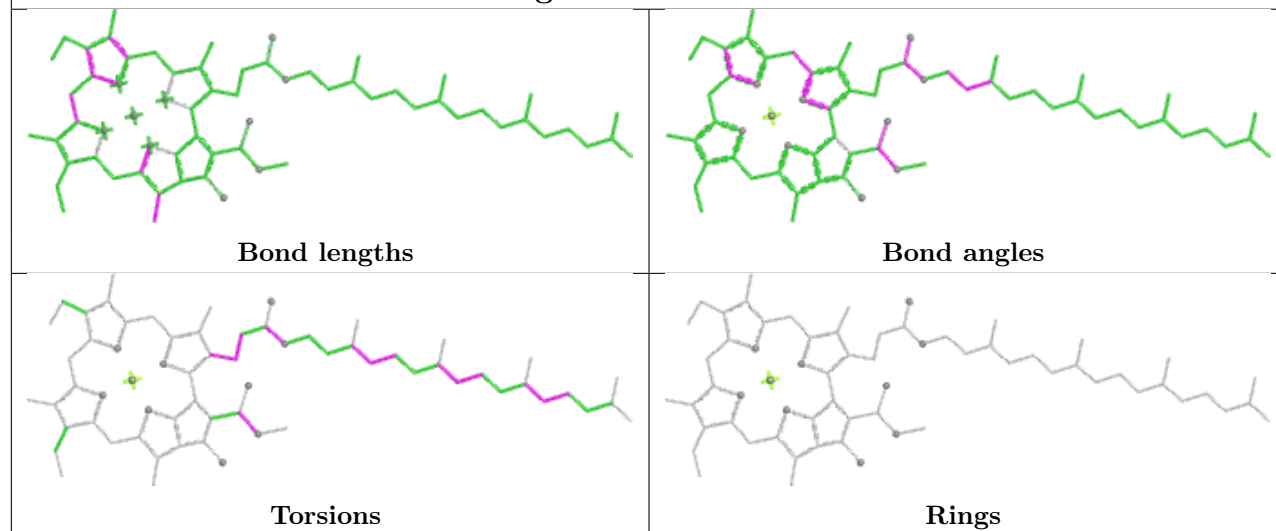


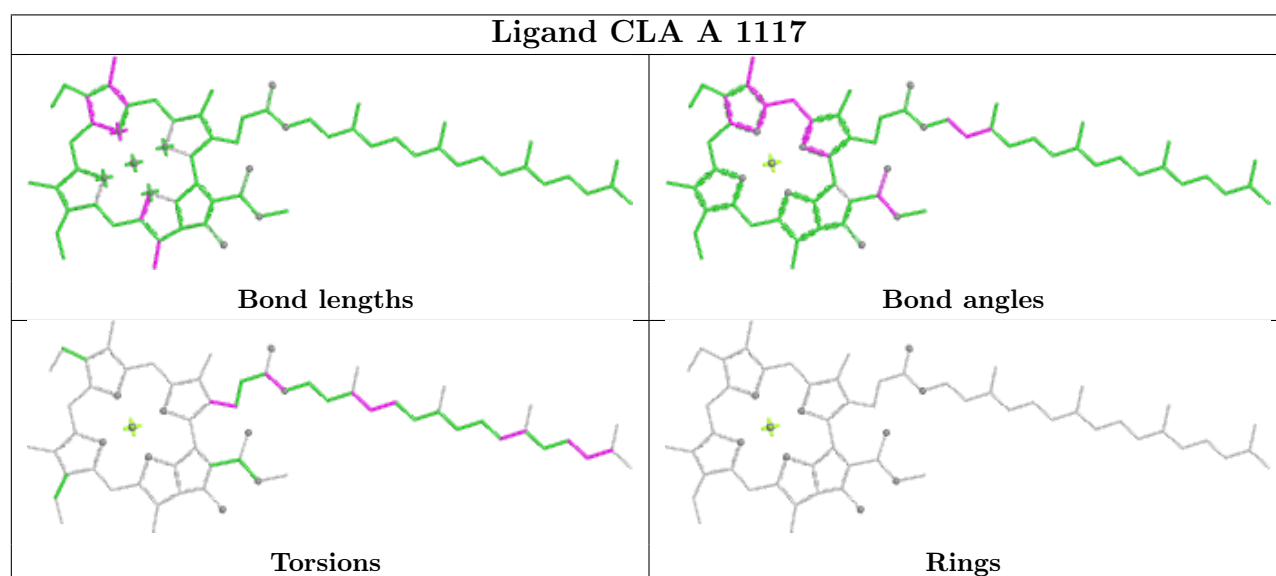
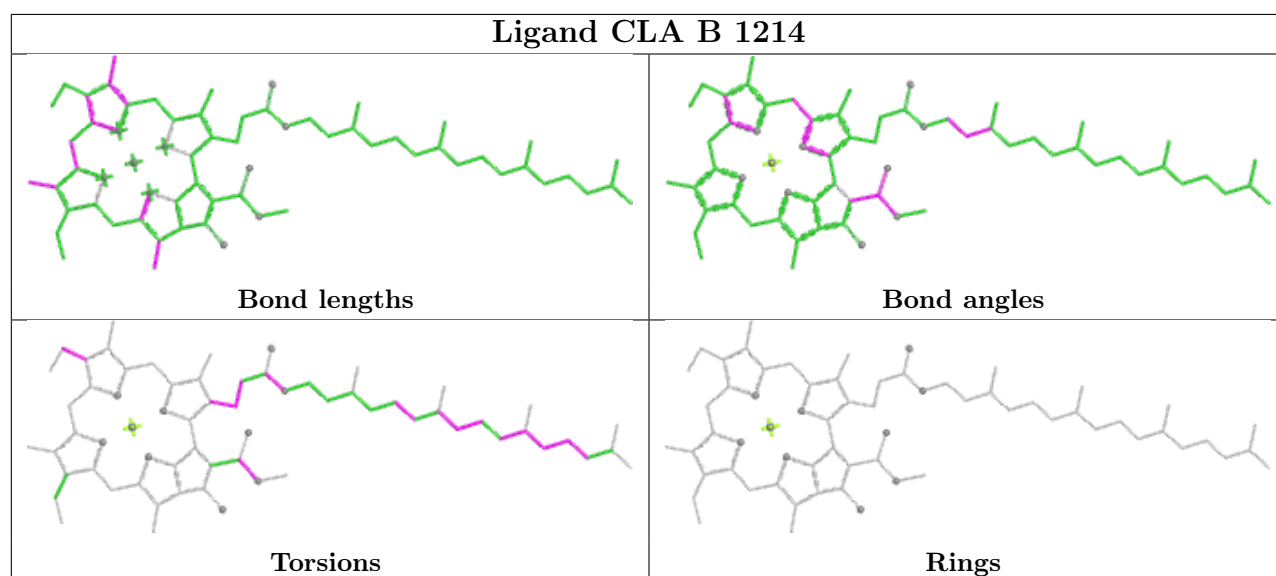
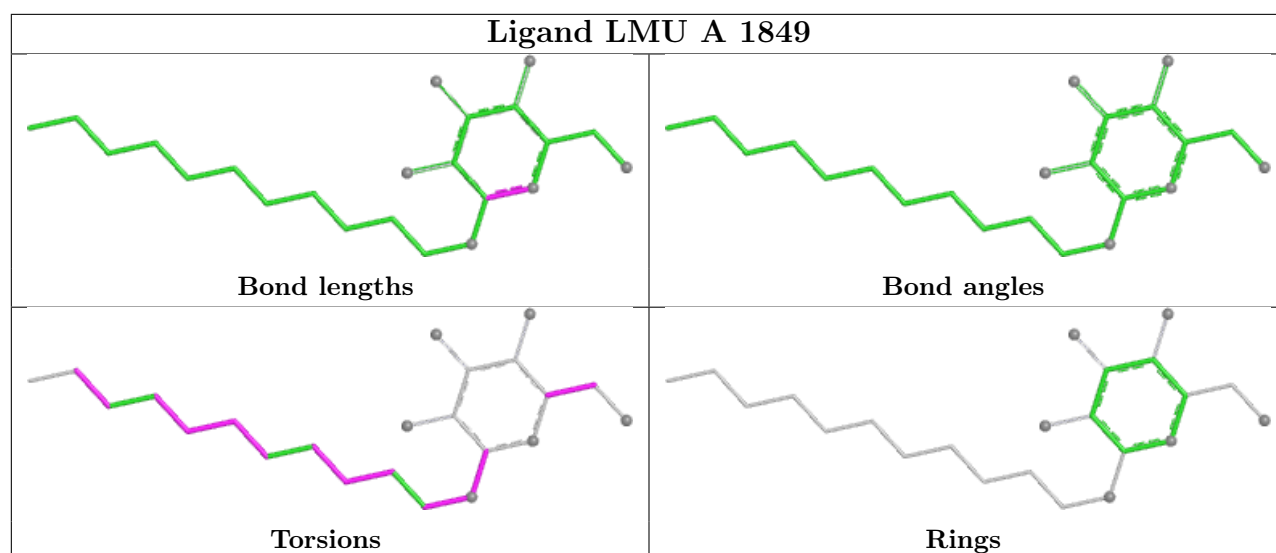


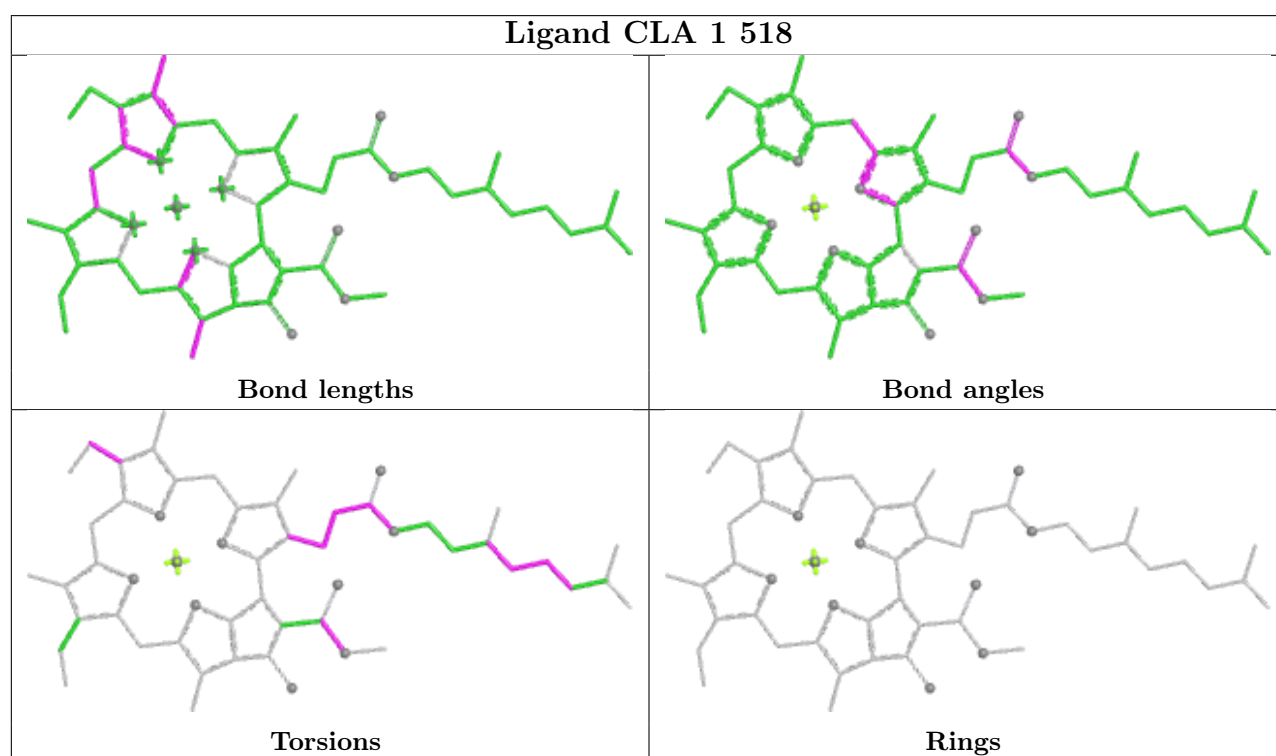
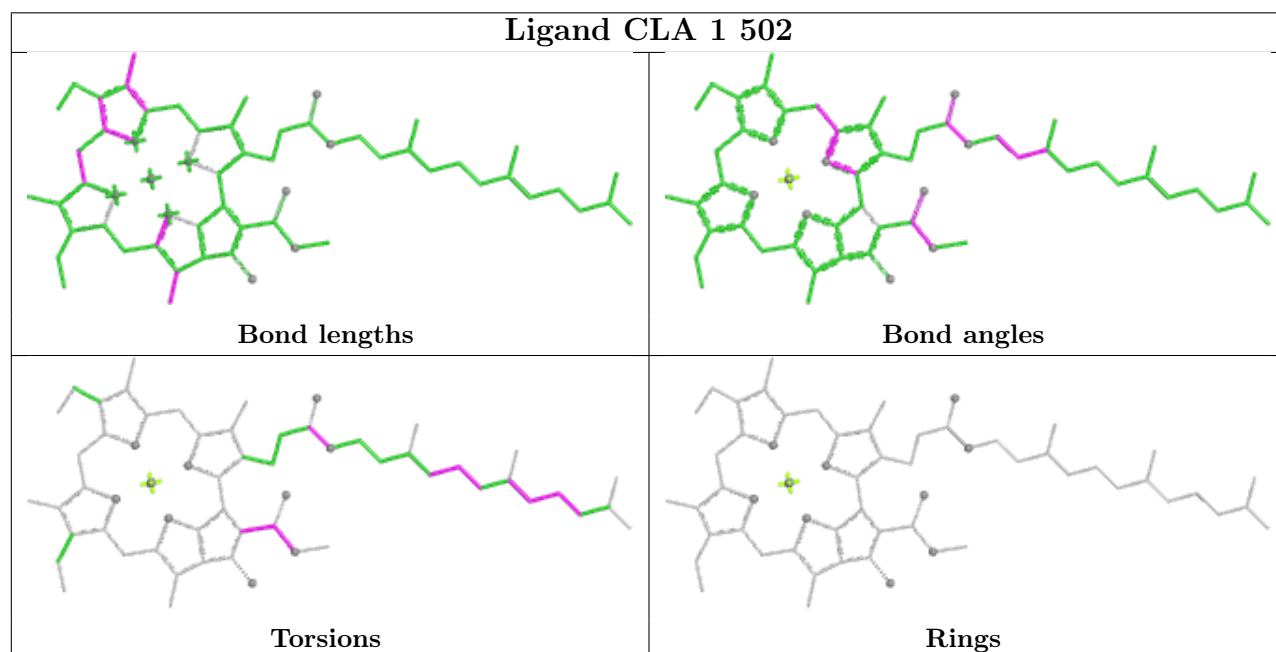
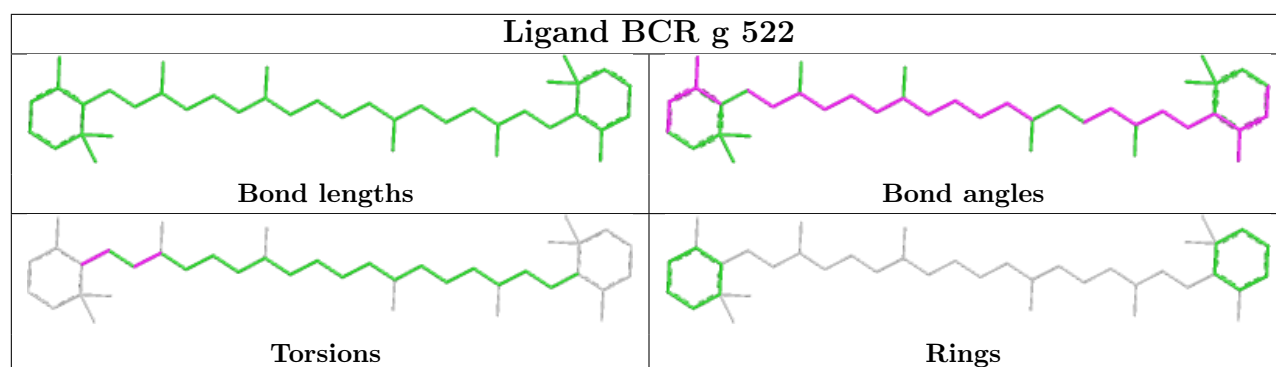
Ligand CLA c 513



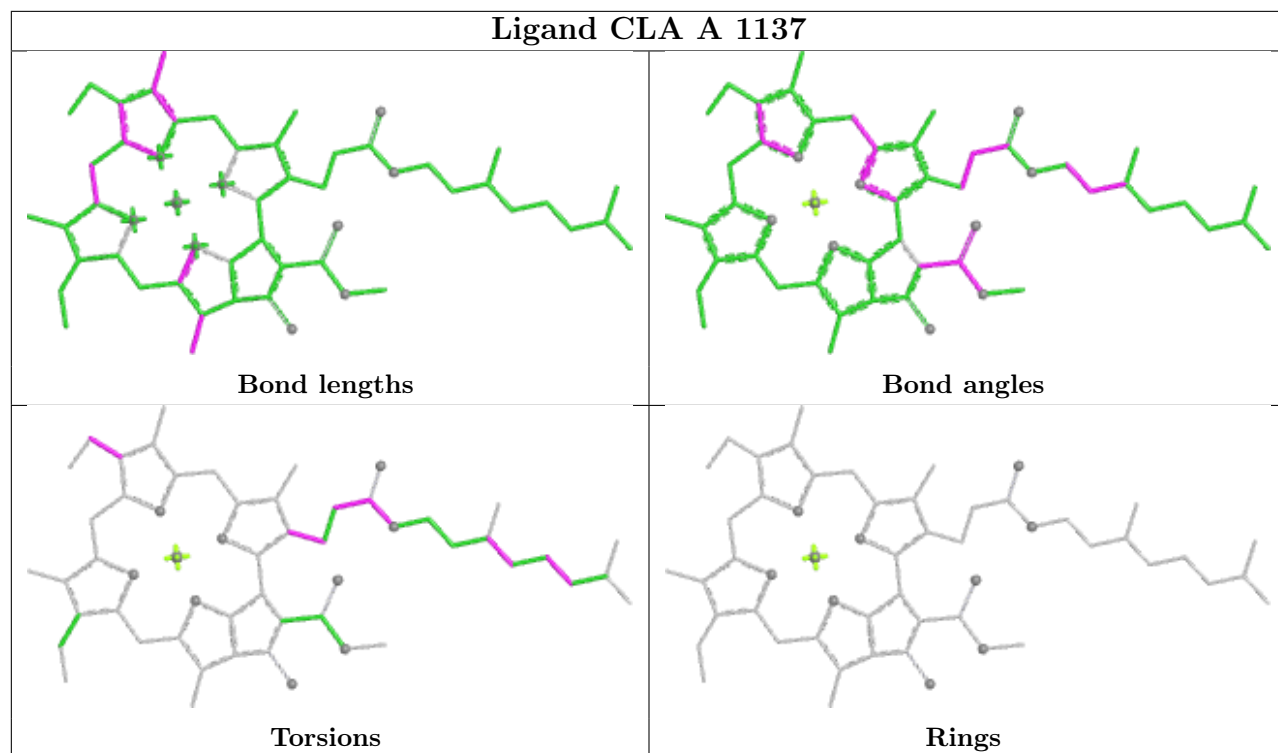
Ligand CLA d 505



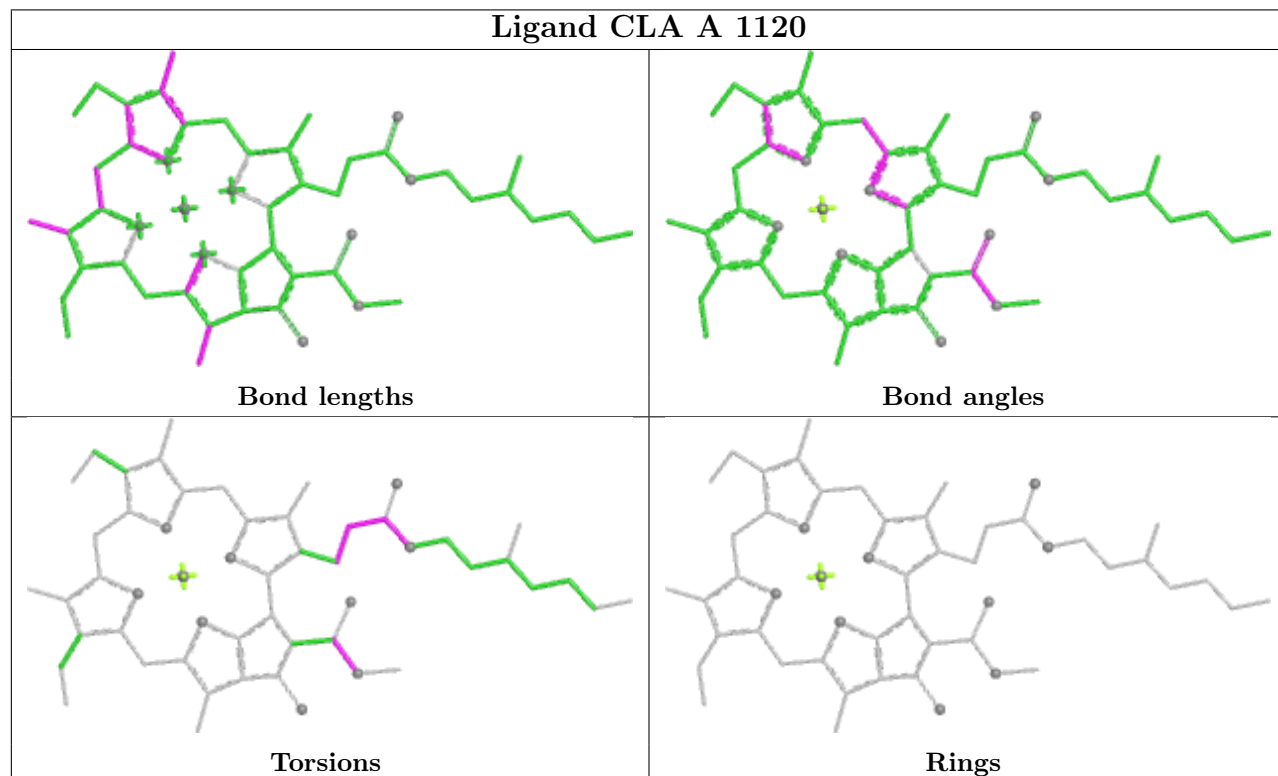




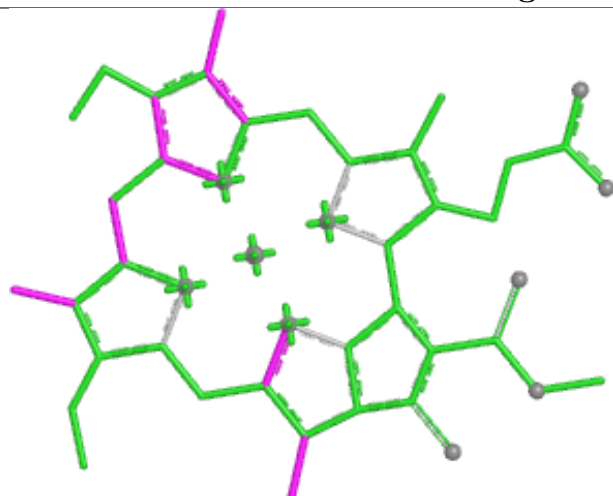
Ligand CLA A 1137



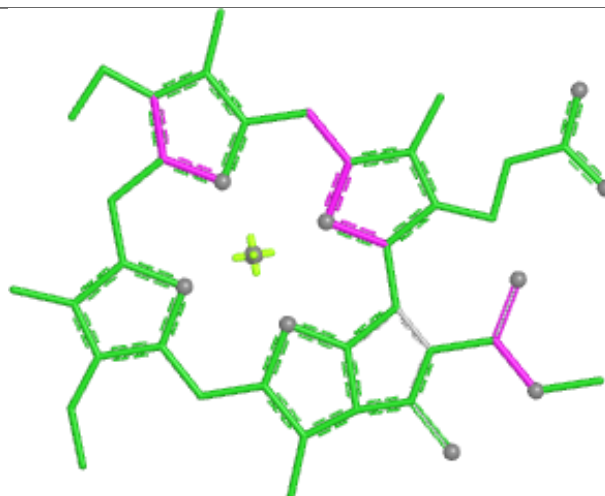
Ligand CLA A 1120



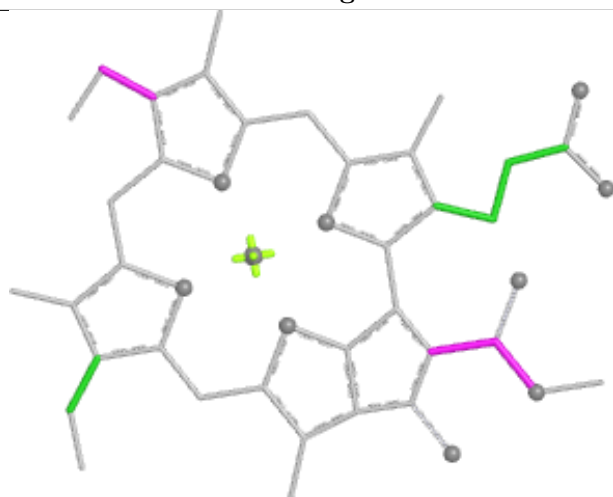
Ligand CLA 2 506



Bond lengths



Bond angles

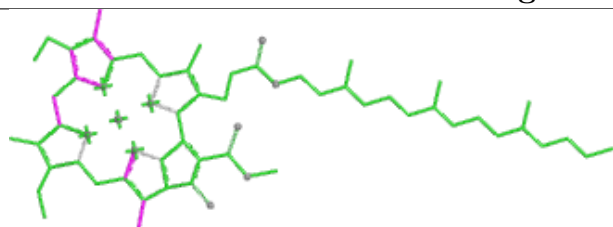


Torsions

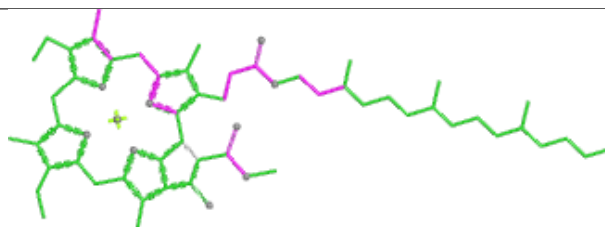


Rings

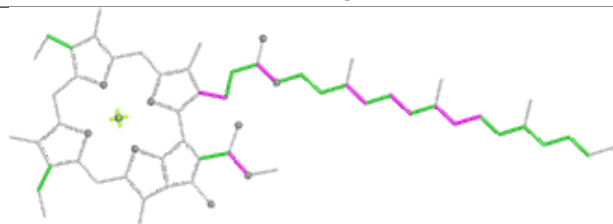
Ligand CLA 3 503



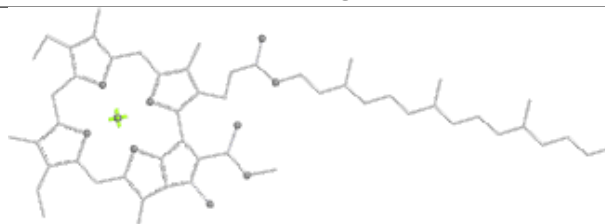
Bond lengths



Bond angles

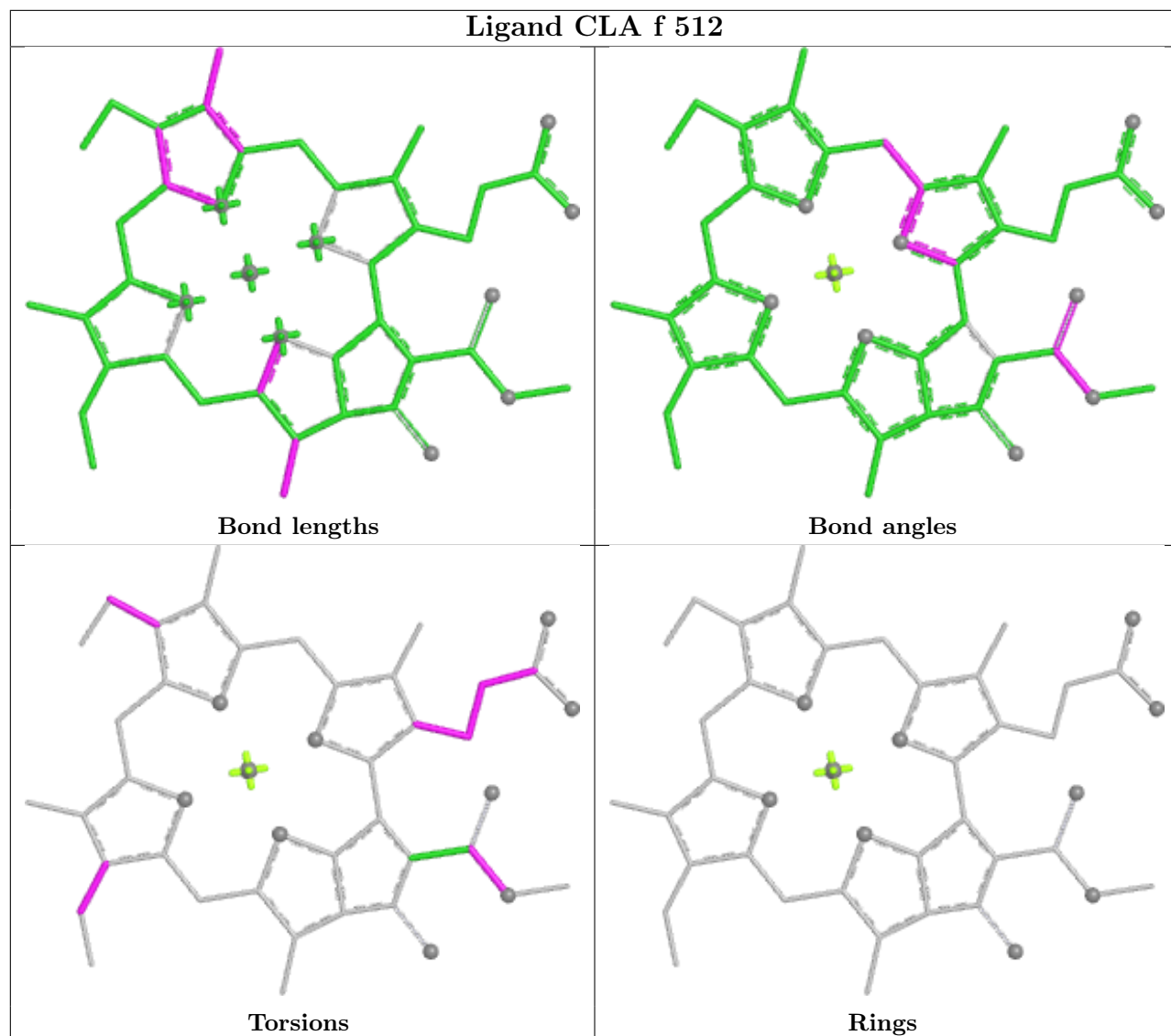


Torsions

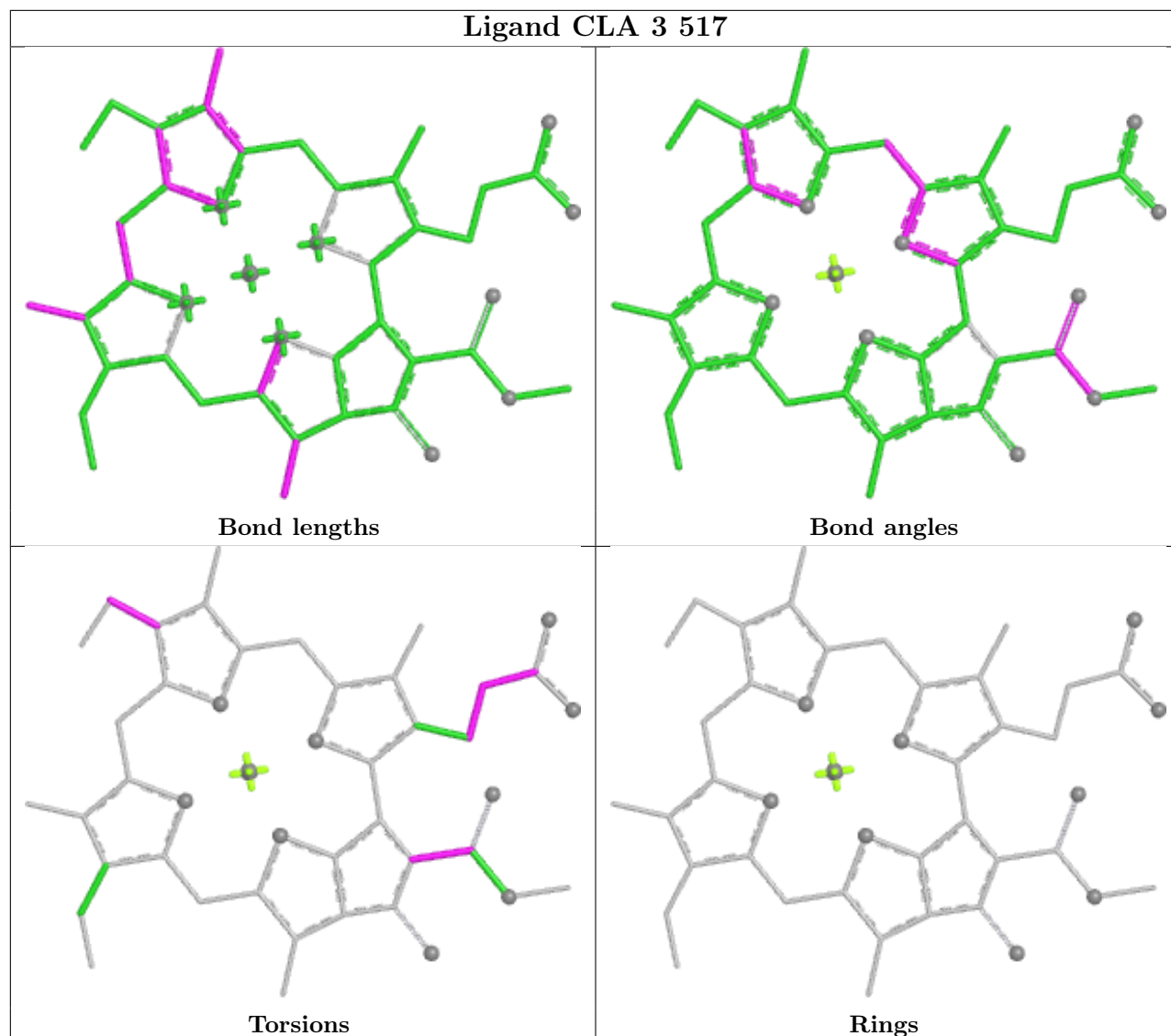


Rings

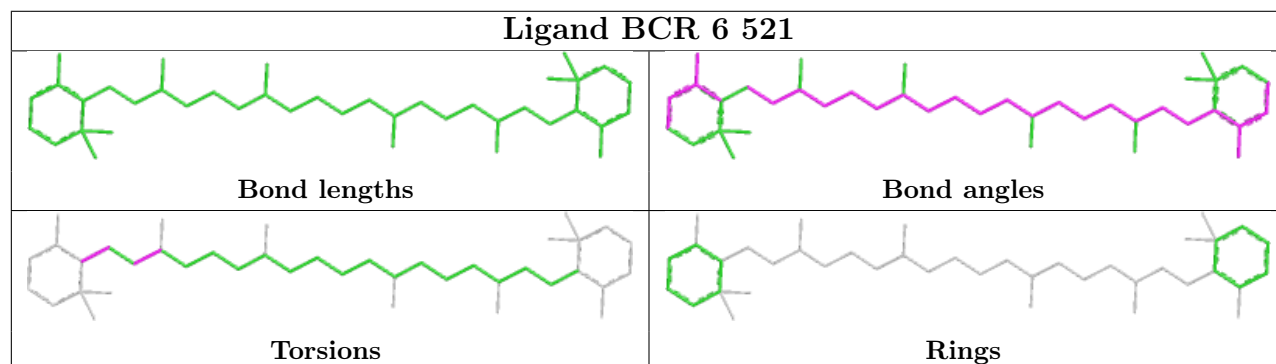
Ligand CLA f 512

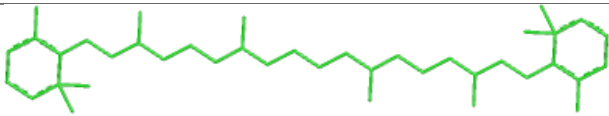
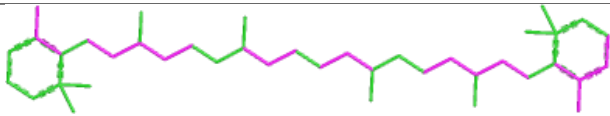
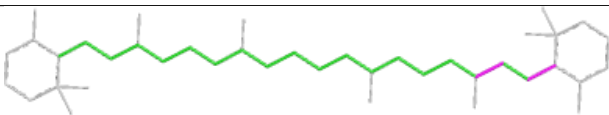
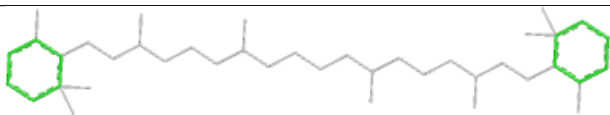


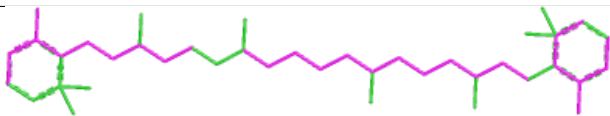
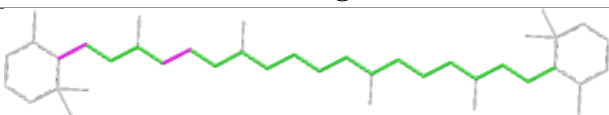
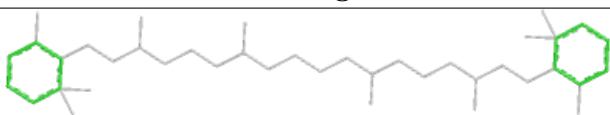
Ligand CLA 3 517

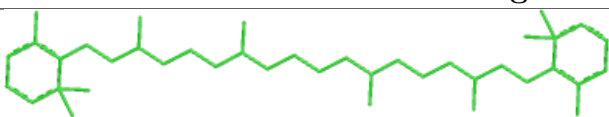
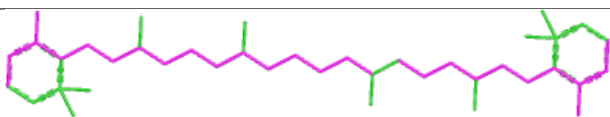
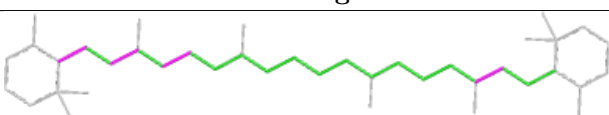
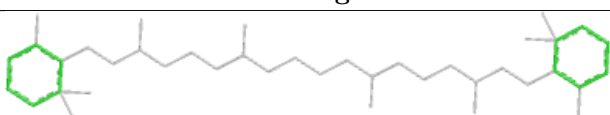


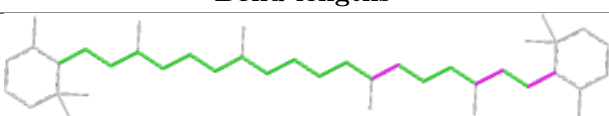
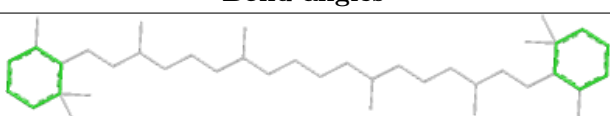
Ligand BCR 6 521

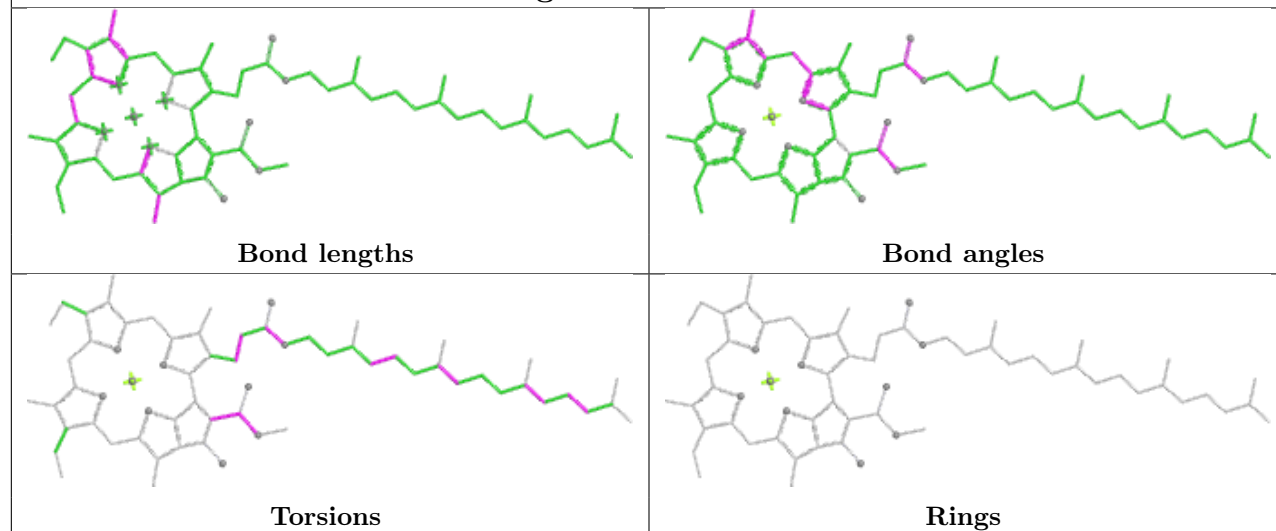
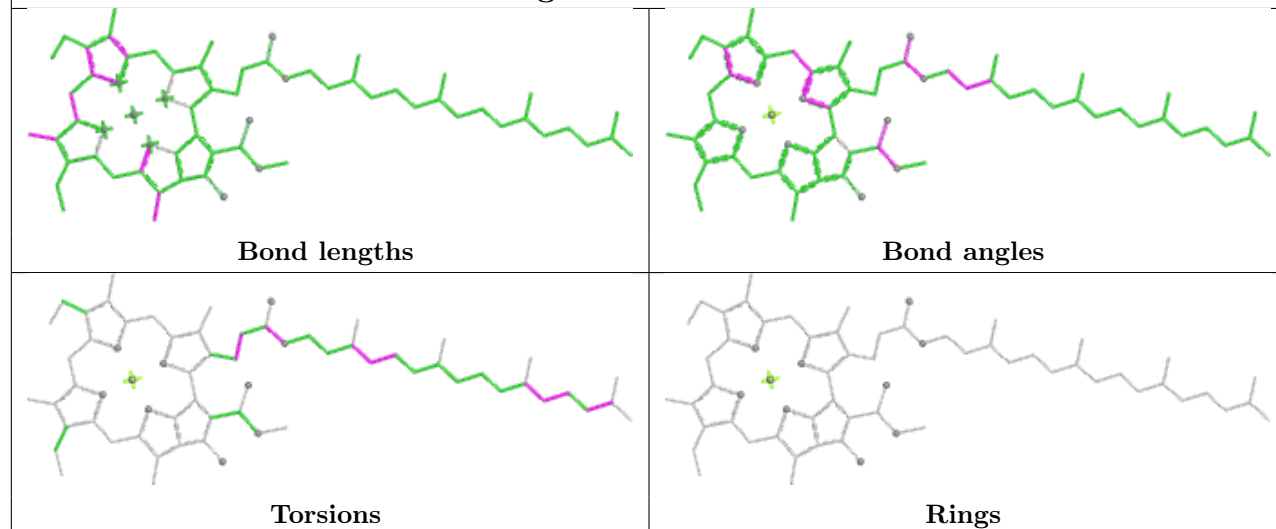


Ligand BCR I 4019	
	
Bond lengths	Bond angles
	
Torsions	Rings

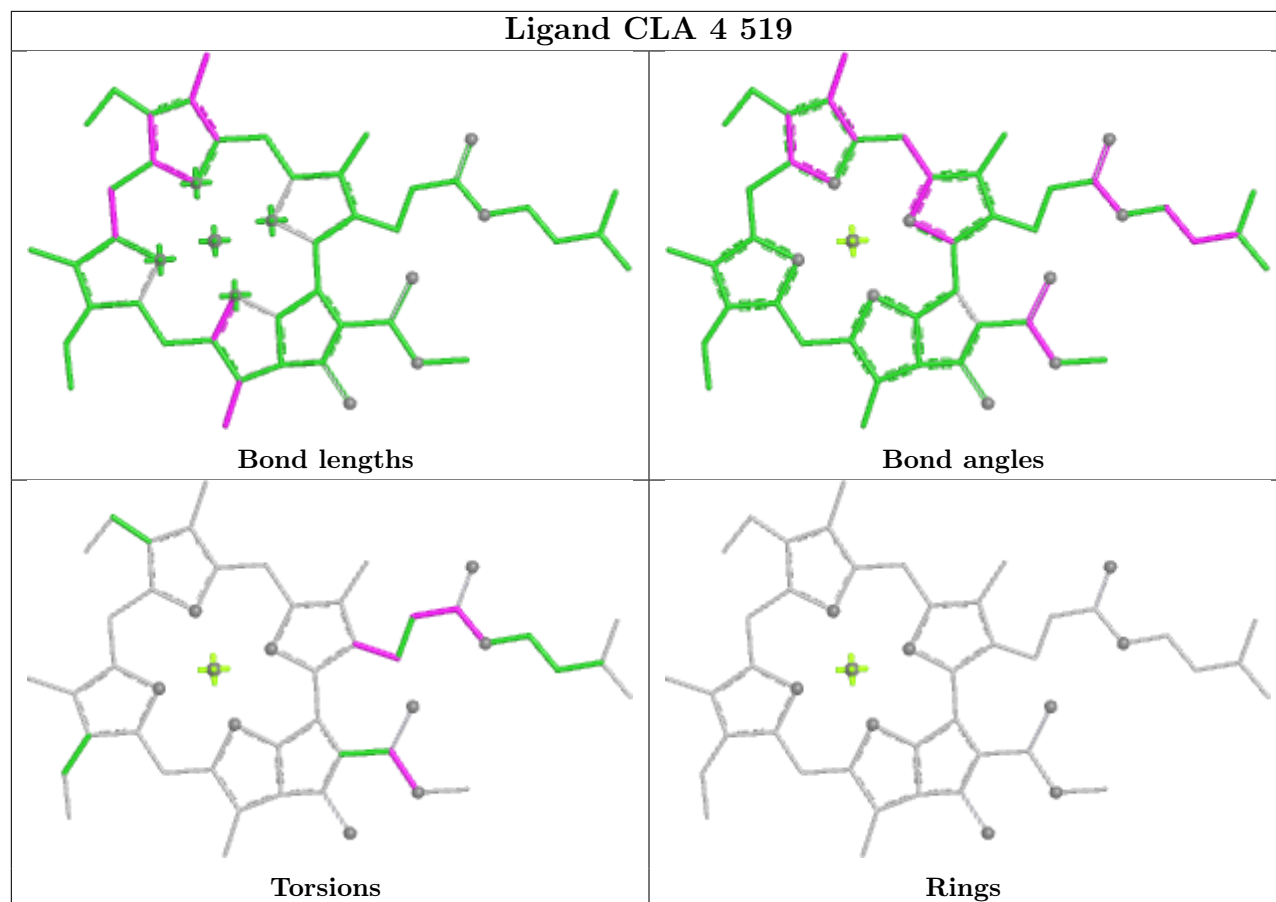
Ligand BCR c 521	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR b 522	
	
Bond lengths	Bond angles
	
Torsions	Rings

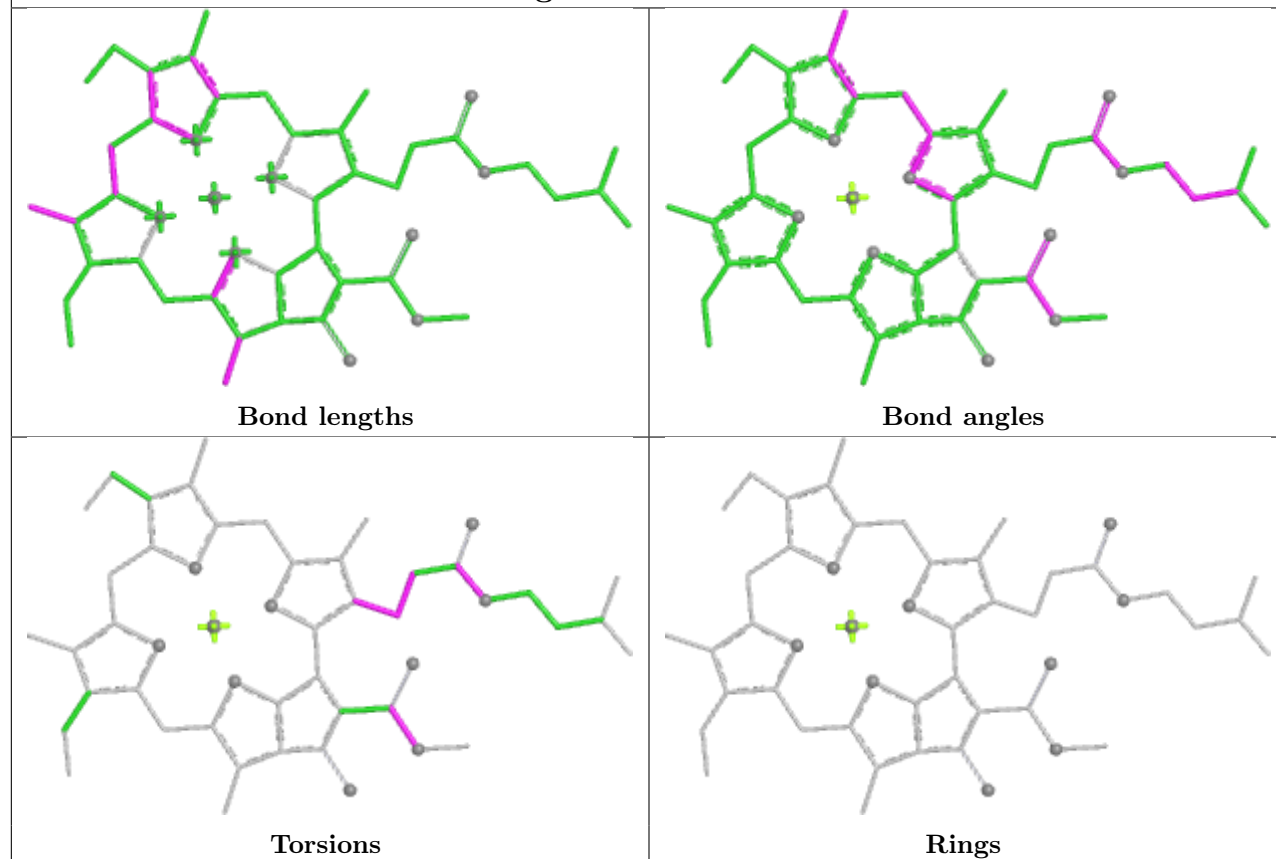
Ligand BCR B 4009	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 510**Ligand CLA c 505**

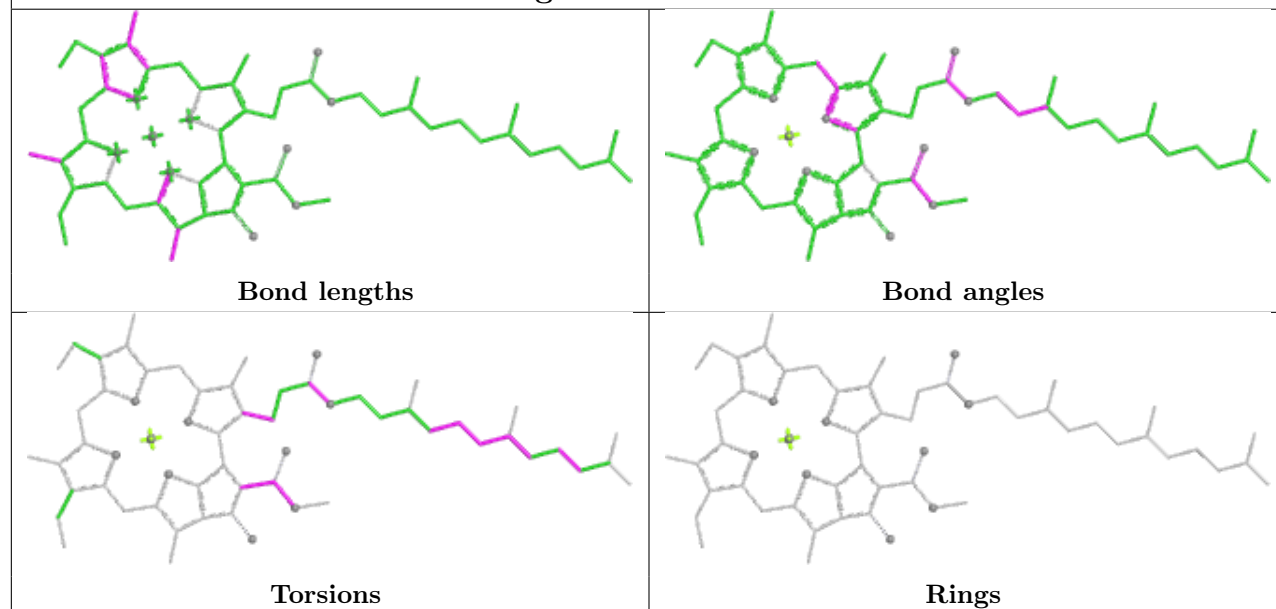
Ligand CLA 4 519



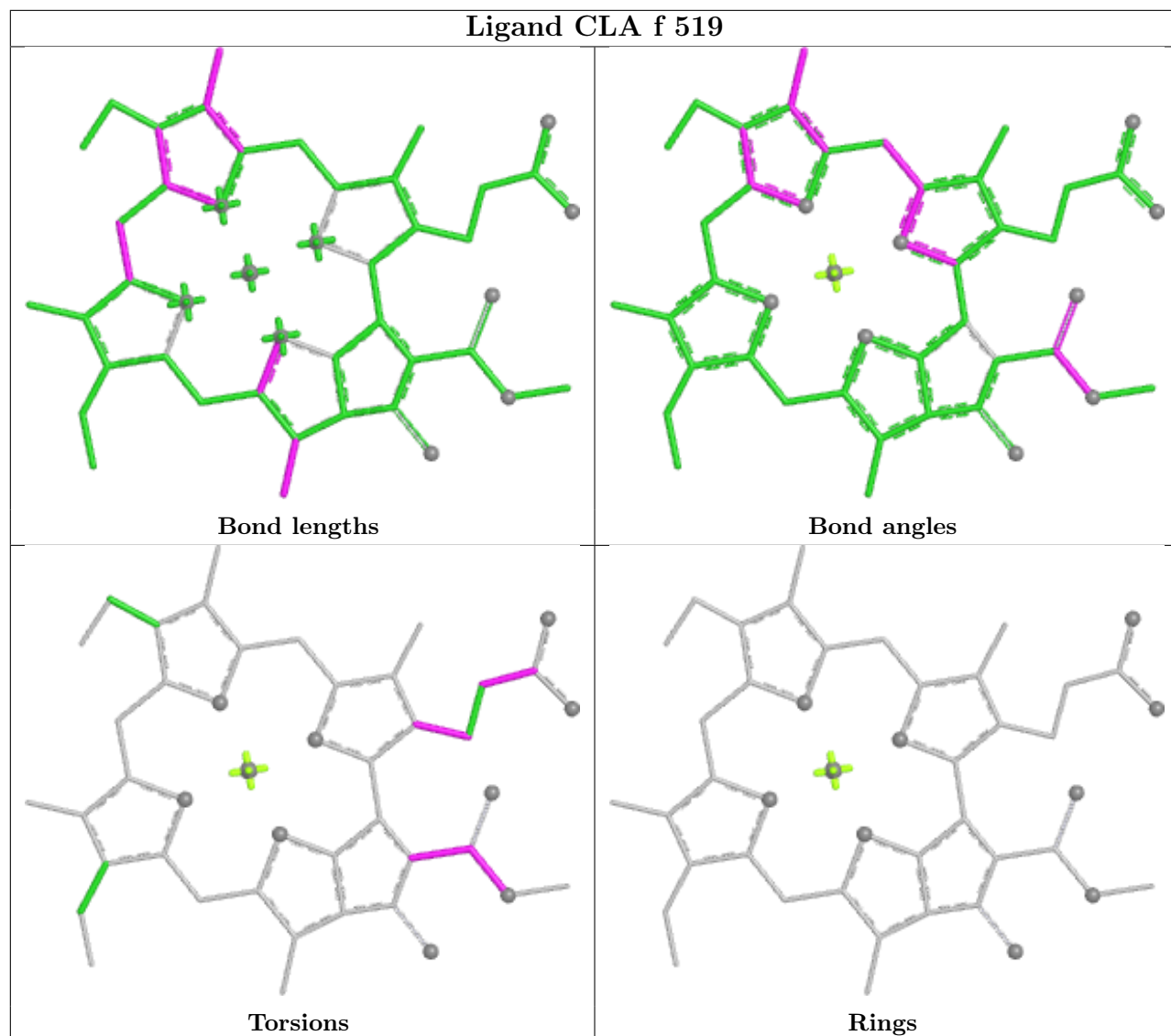
Ligand CLA b 513



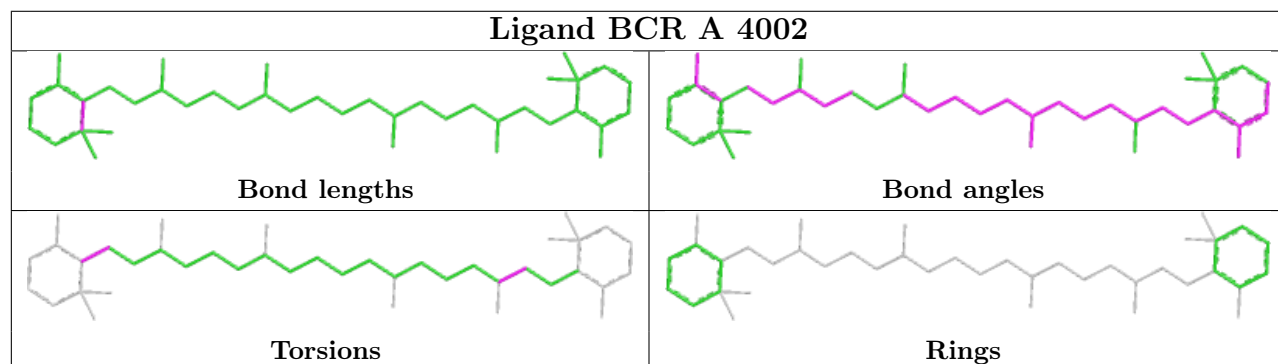
Ligand CLA d 502



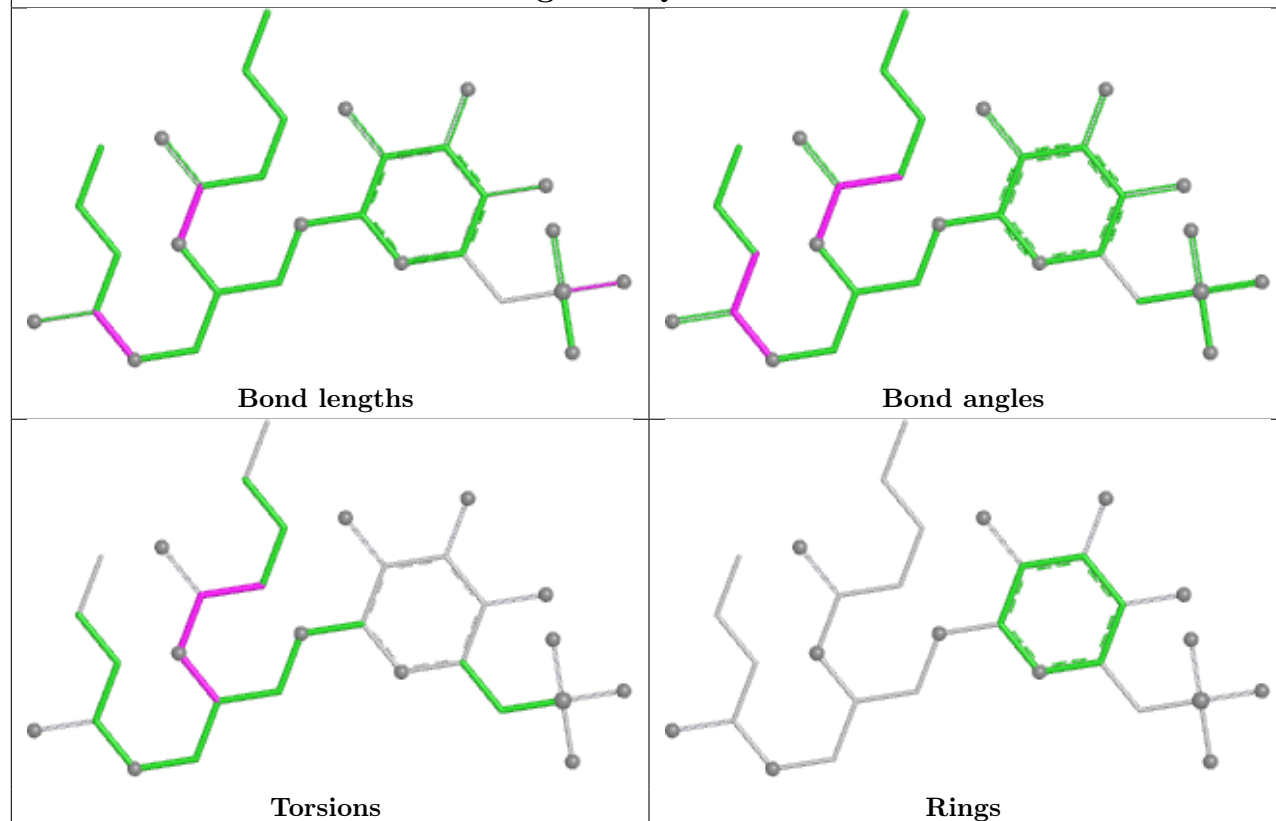
Ligand CLA f 519



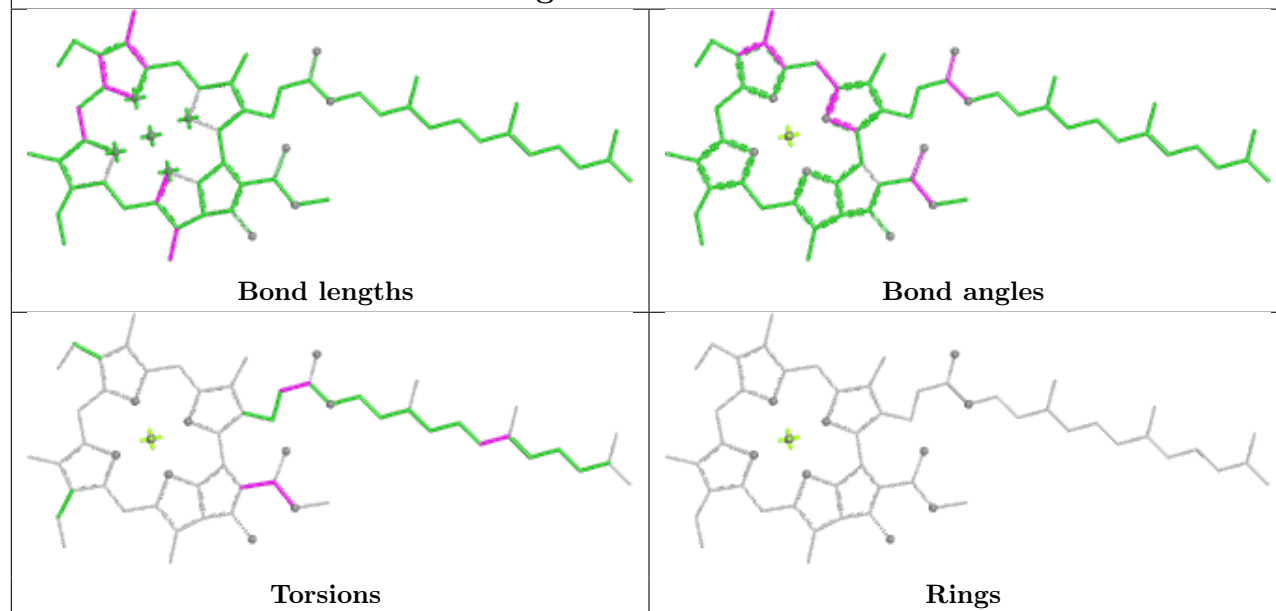
Ligand BCR A 4002

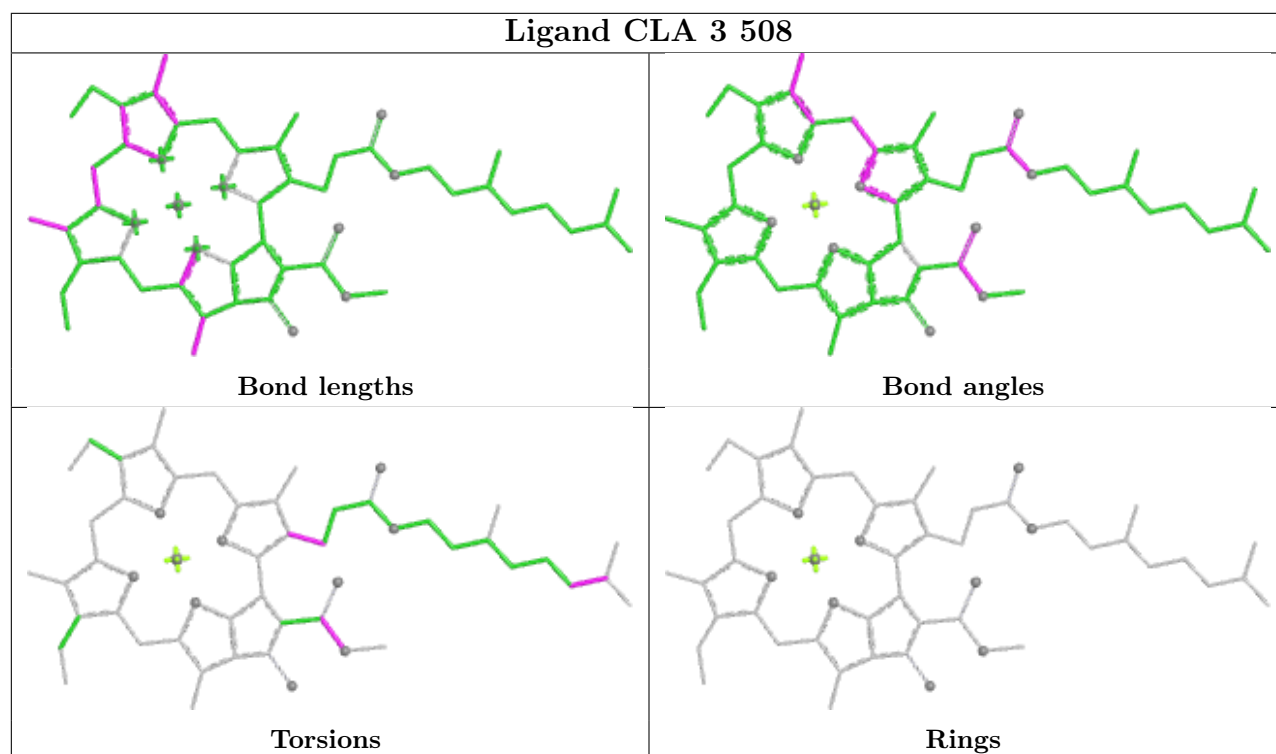
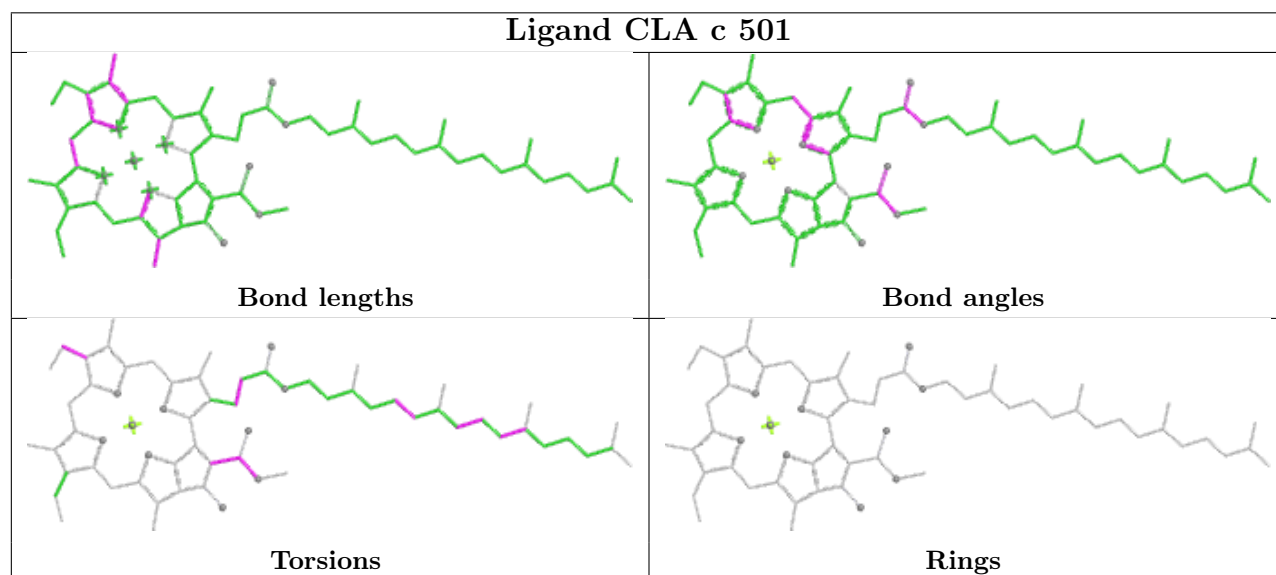
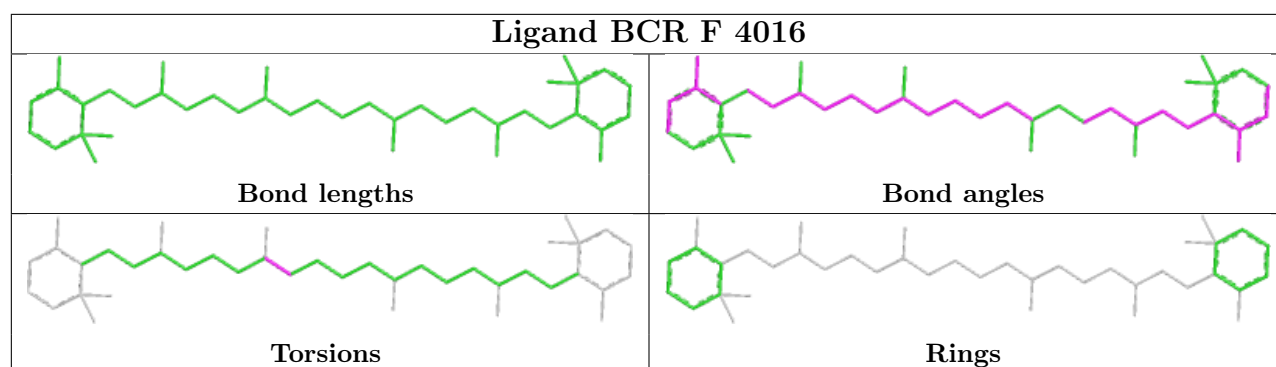


Ligand SQD a 822

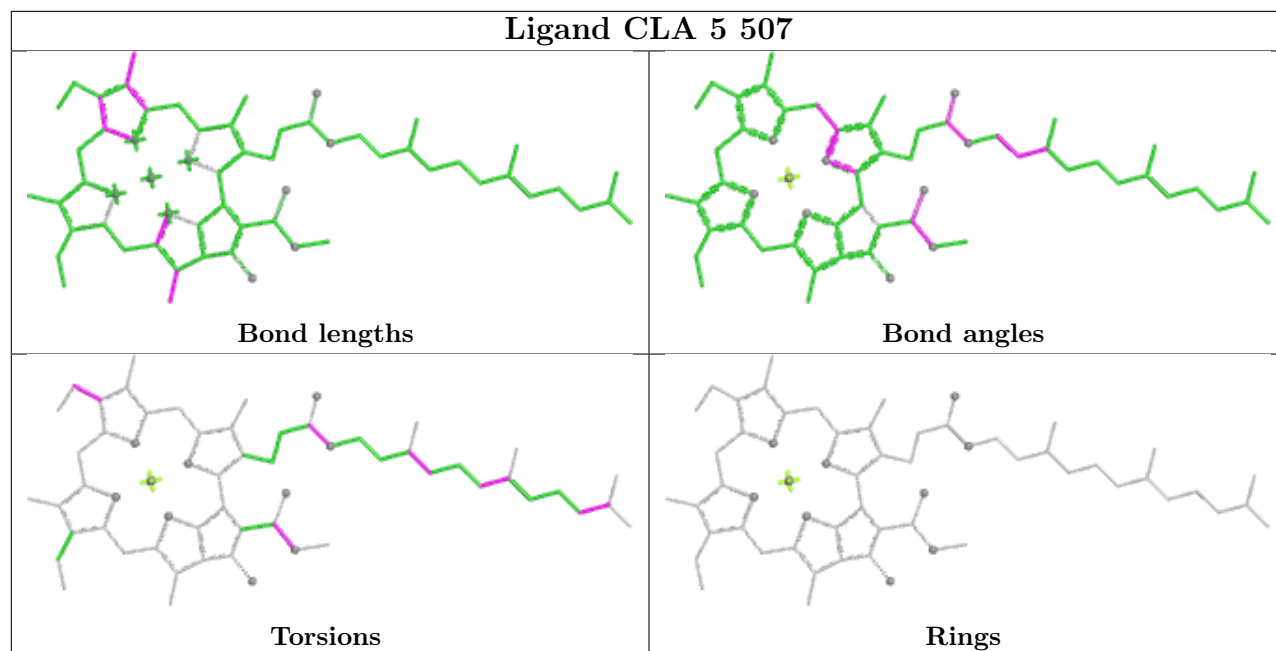


Ligand CLA 2 507

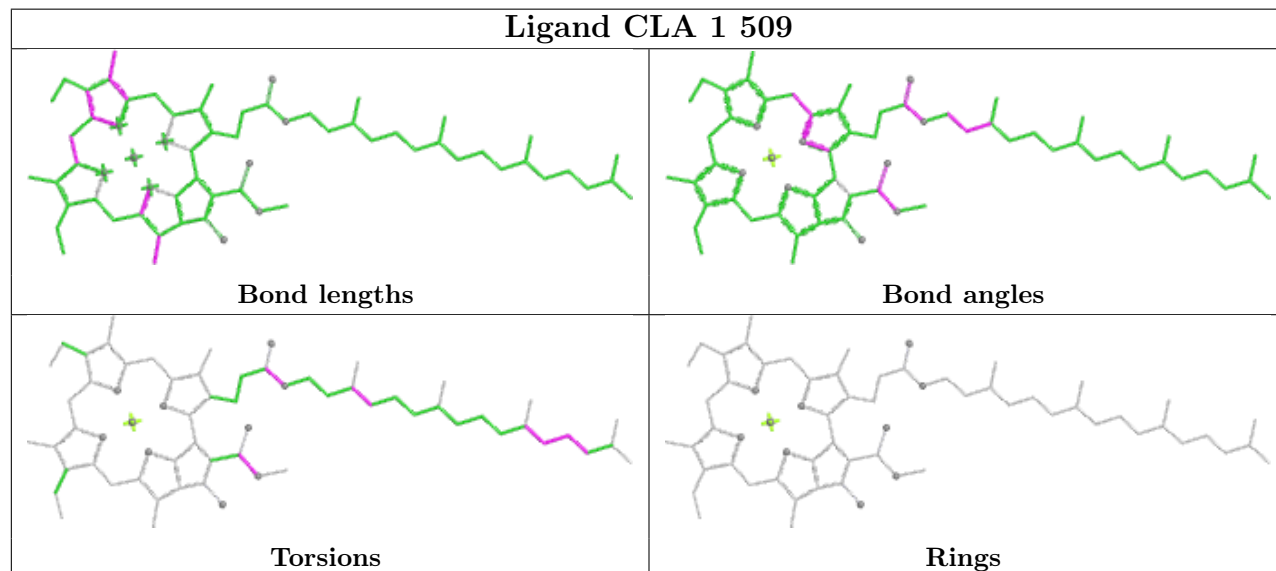




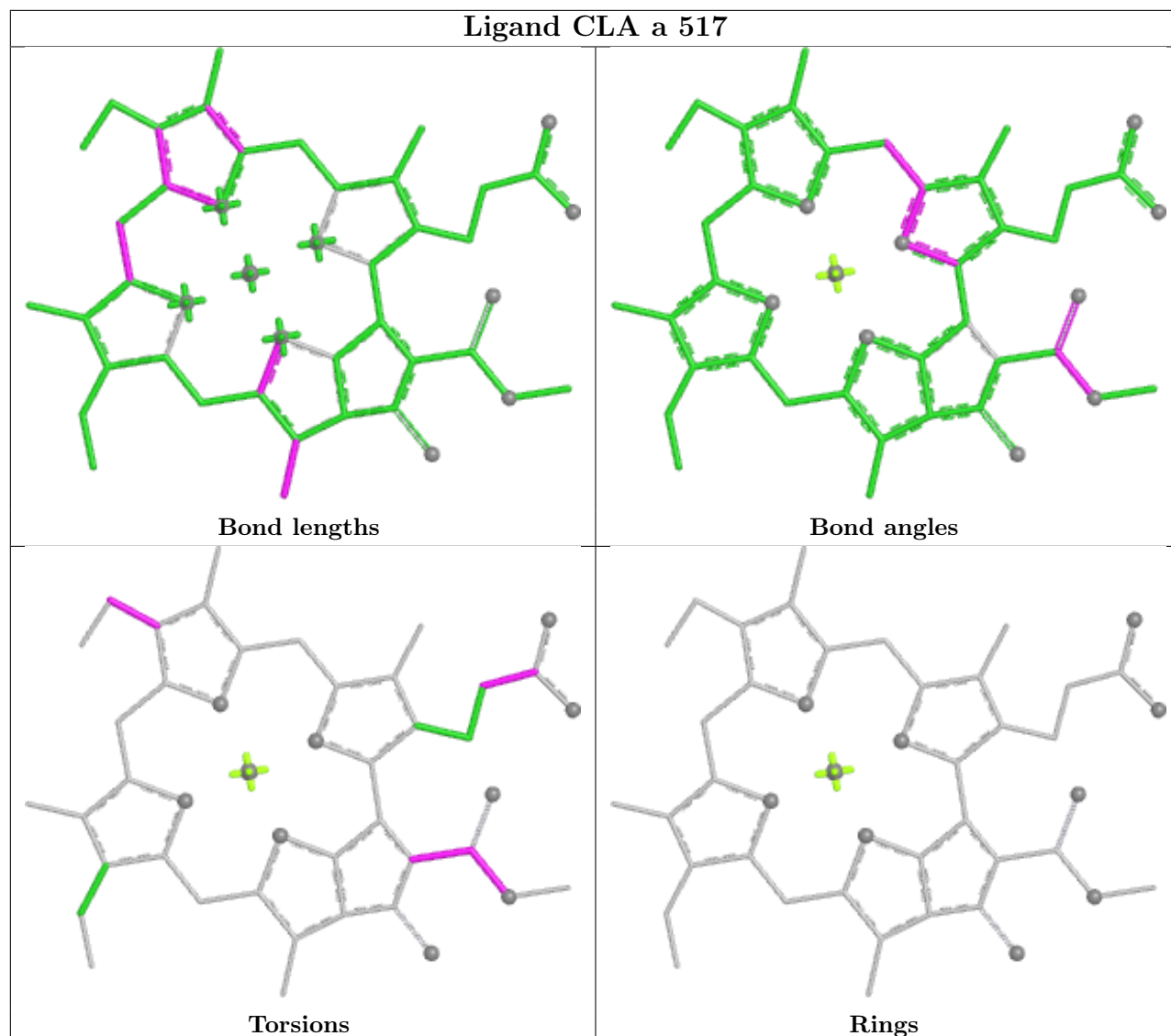
Ligand CLA 5 507



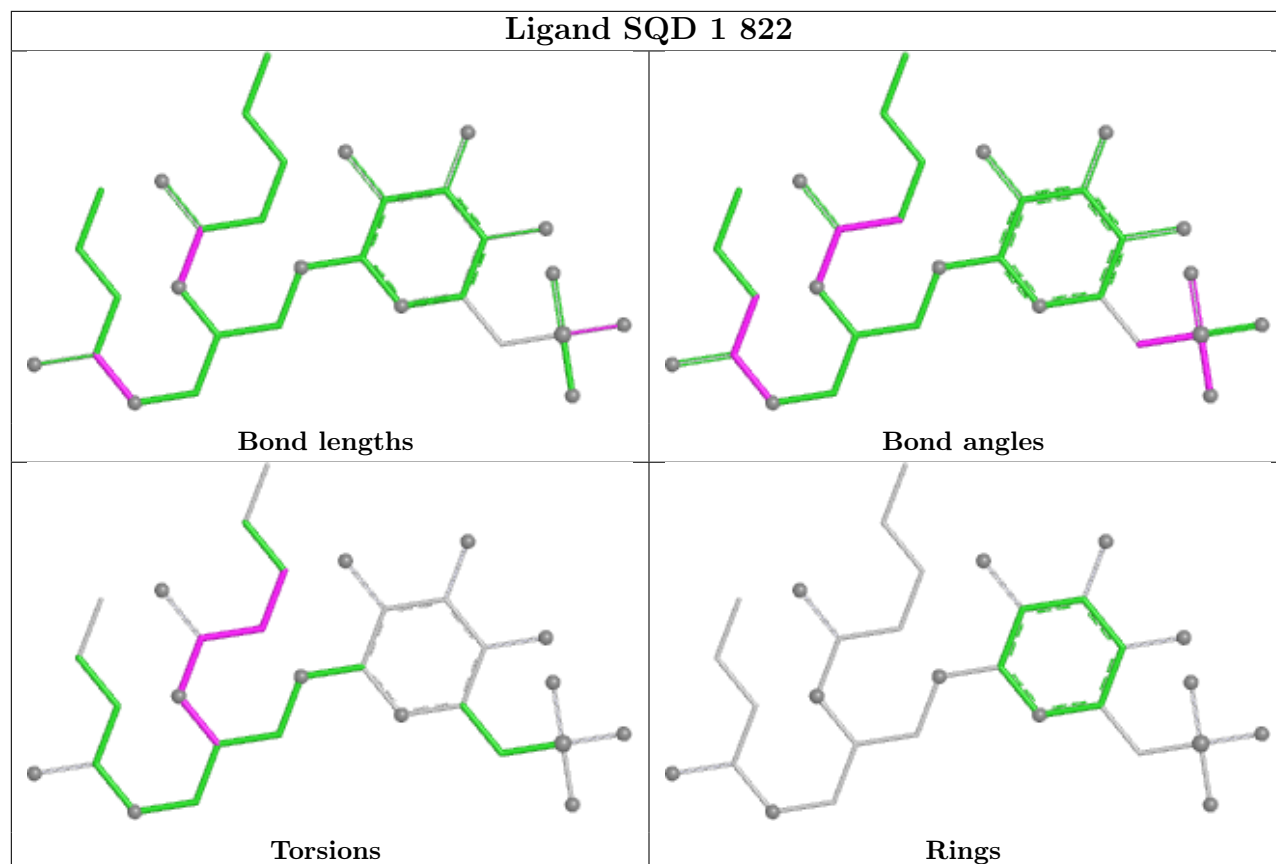
Ligand CLA 1 509



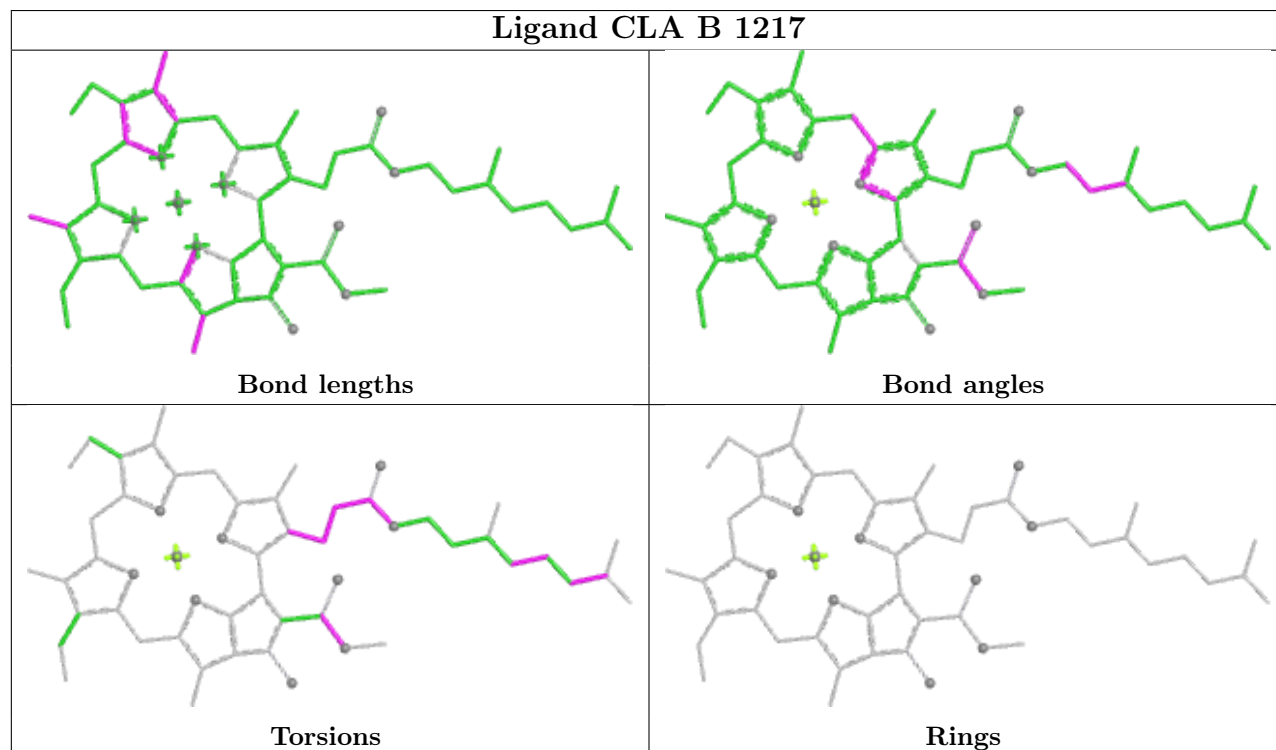
Ligand CLA a 517

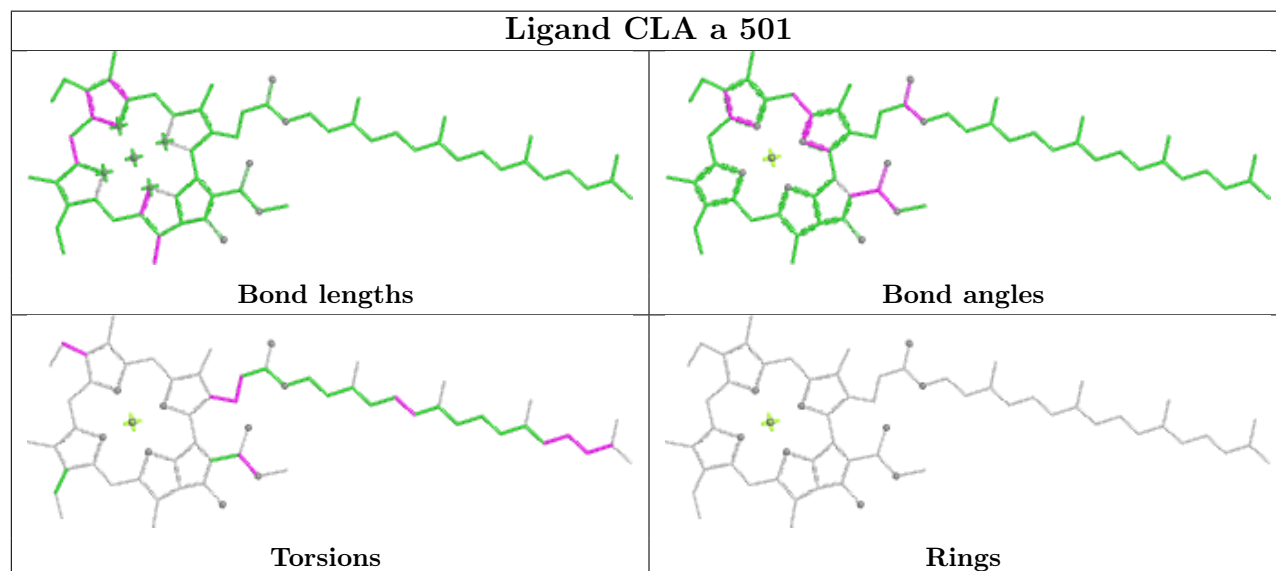
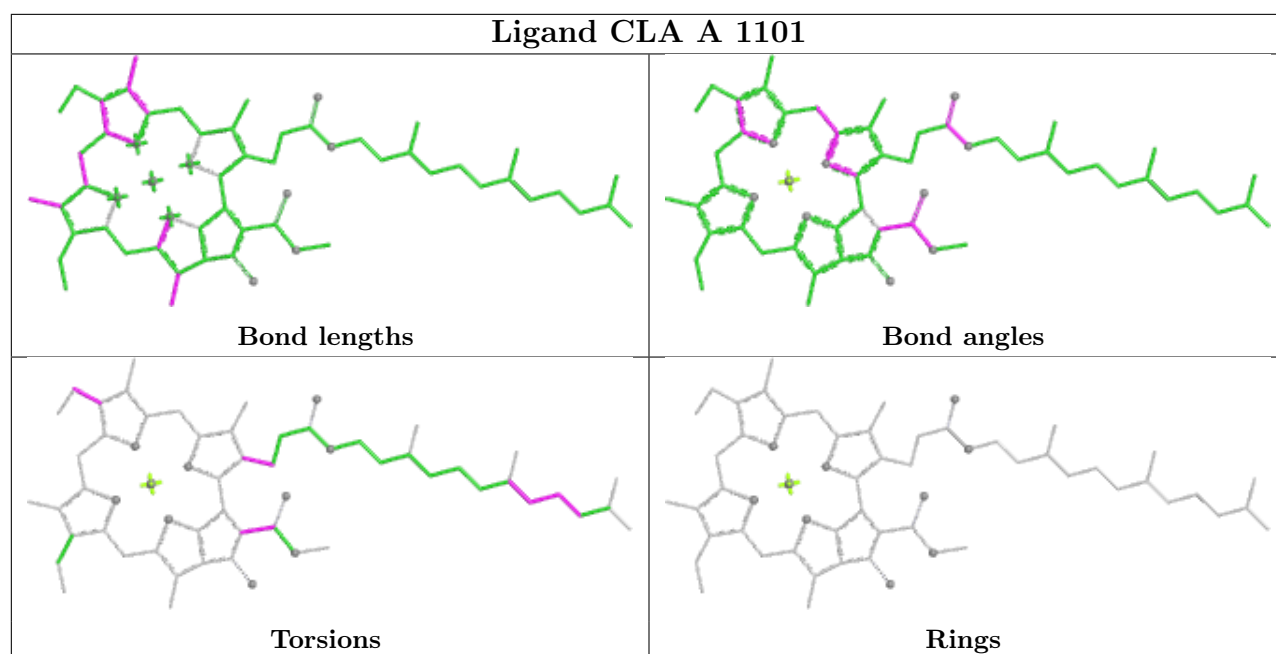


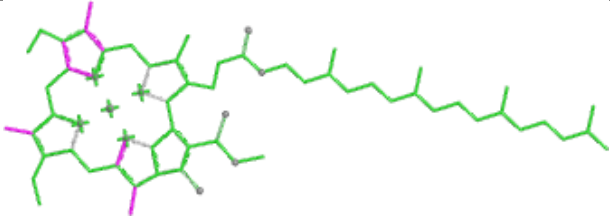
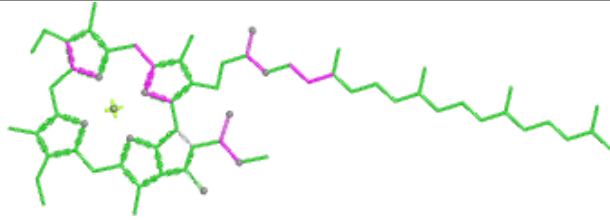
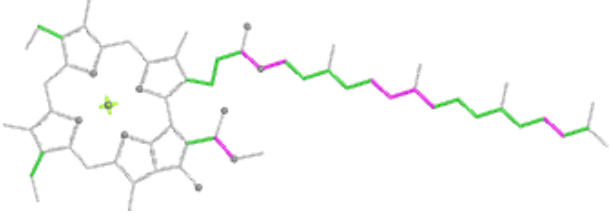
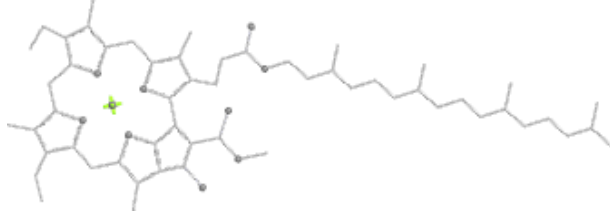
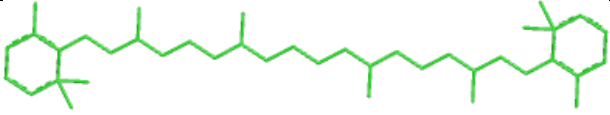
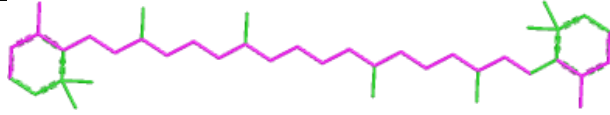
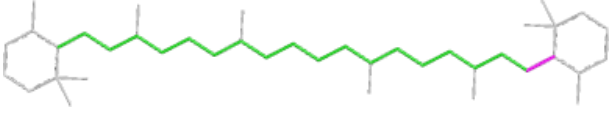
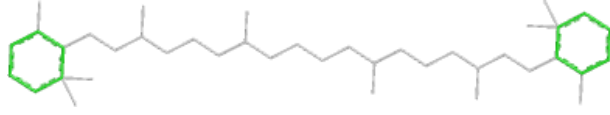
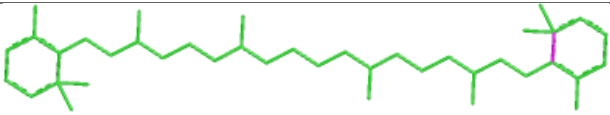
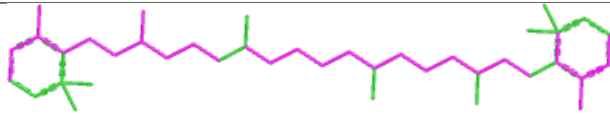
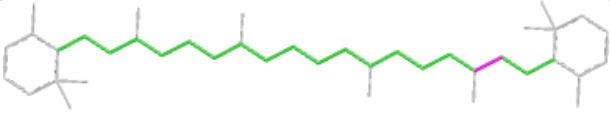
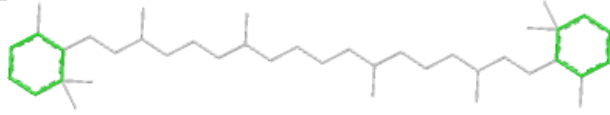
Ligand SQD 1 822



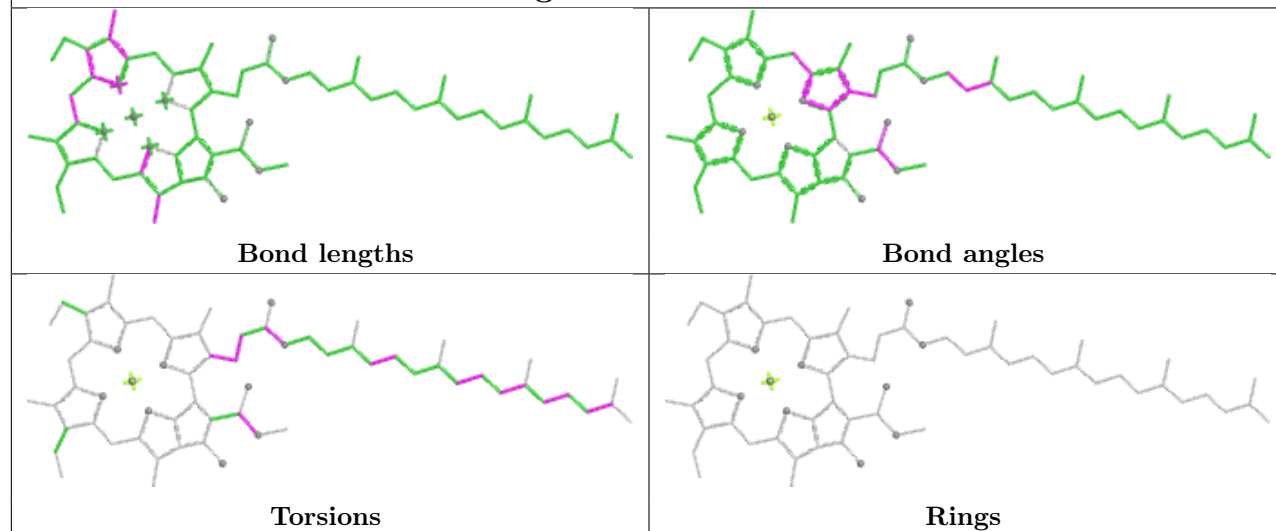
Ligand CLA B 1217



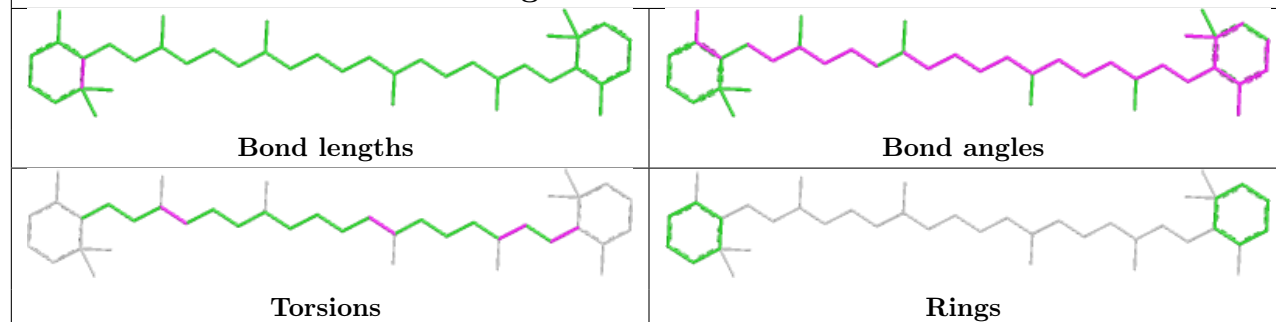


Ligand CLA 2 509	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR 6 523	
 Bond lengths	 Bond angles
 Torsions	 Rings
Ligand BCR A 4008	
 Bond lengths	 Bond angles
 Torsions	 Rings

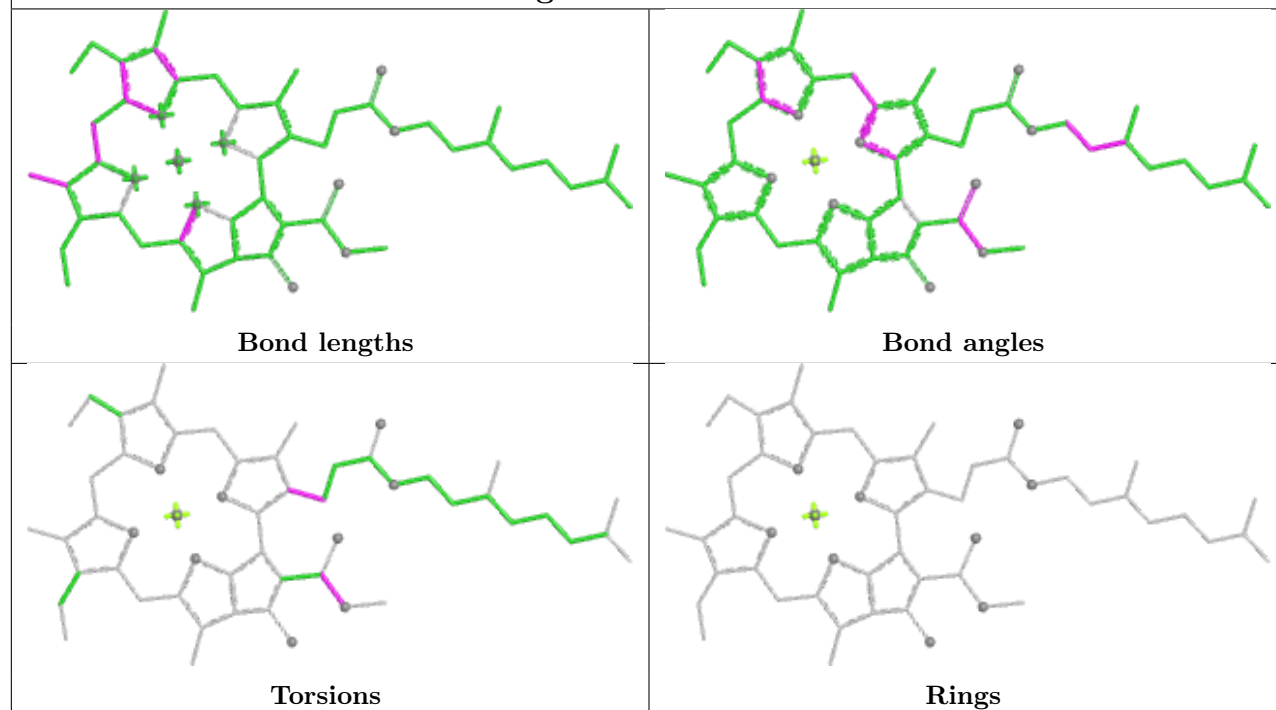
Ligand CLA b 505



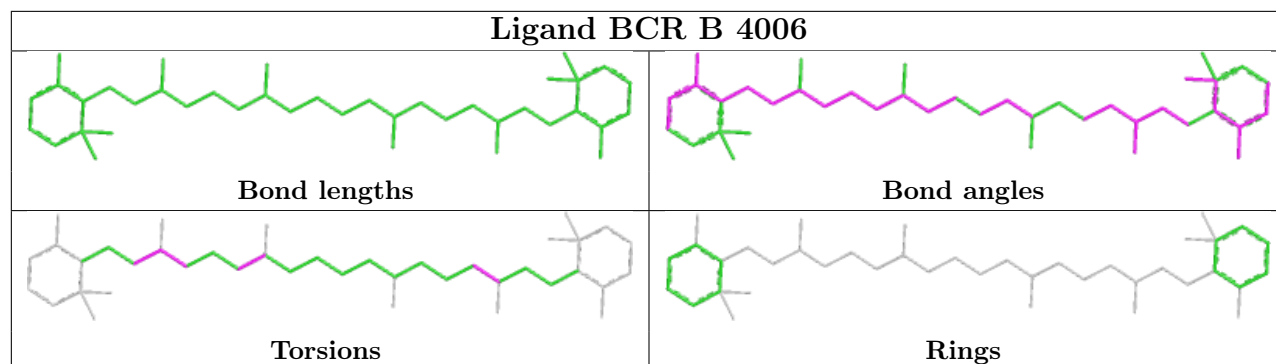
Ligand BCR A 4011



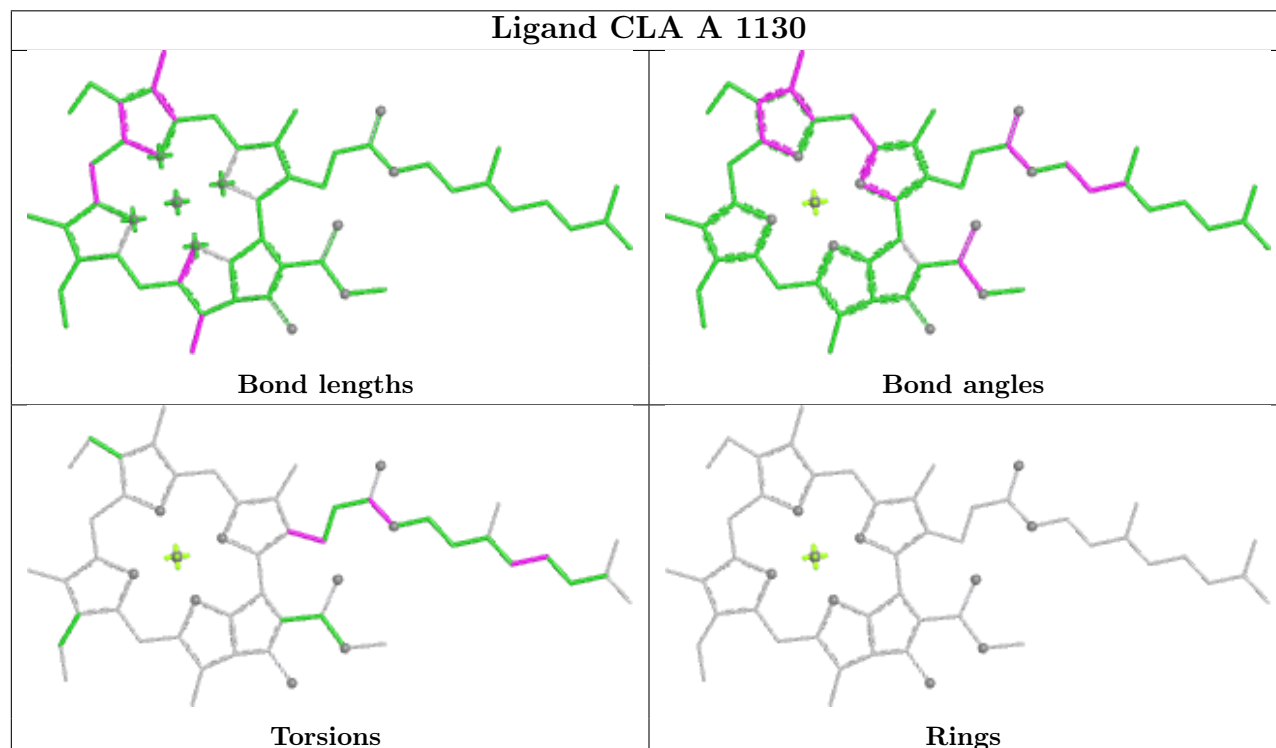
Ligand CLA 5 513



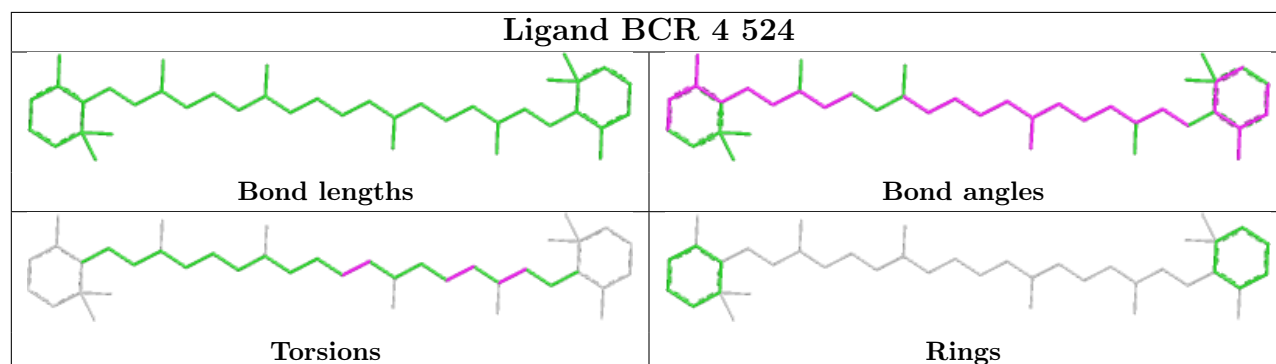
Ligand BCR B 4006

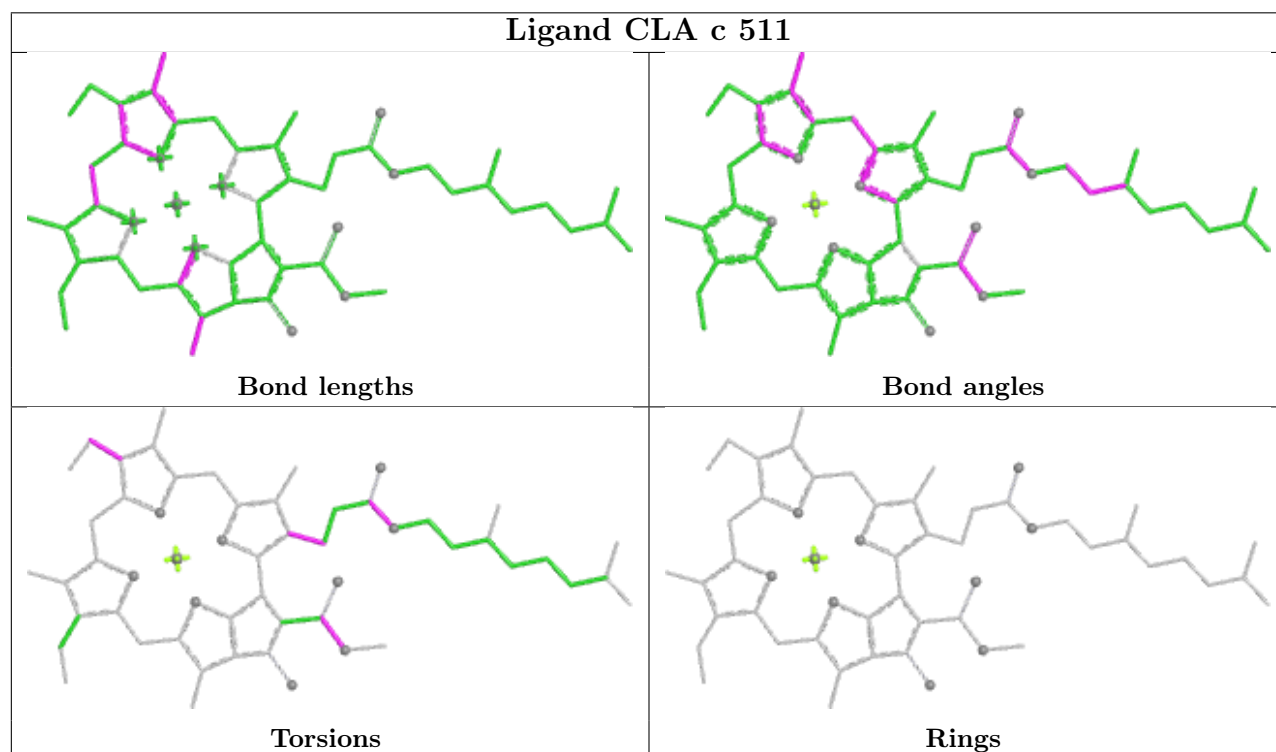
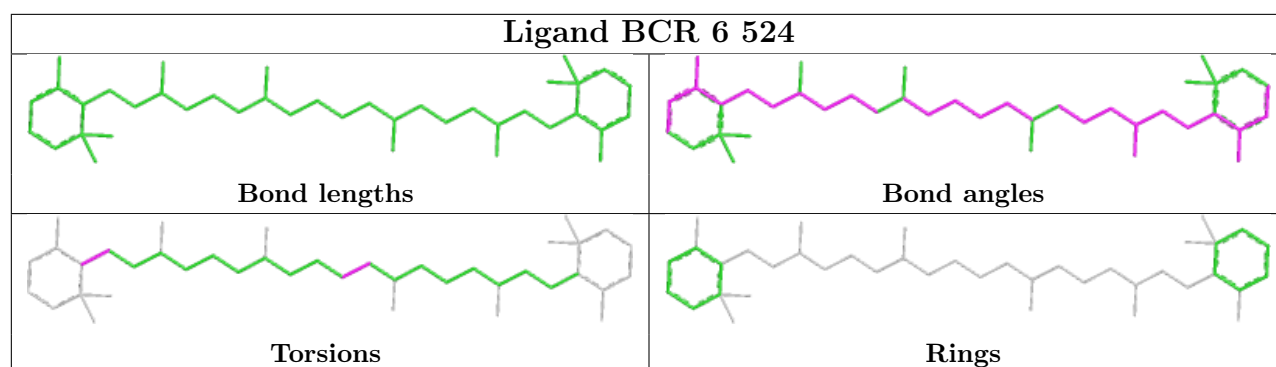


Ligand CLA A 1130

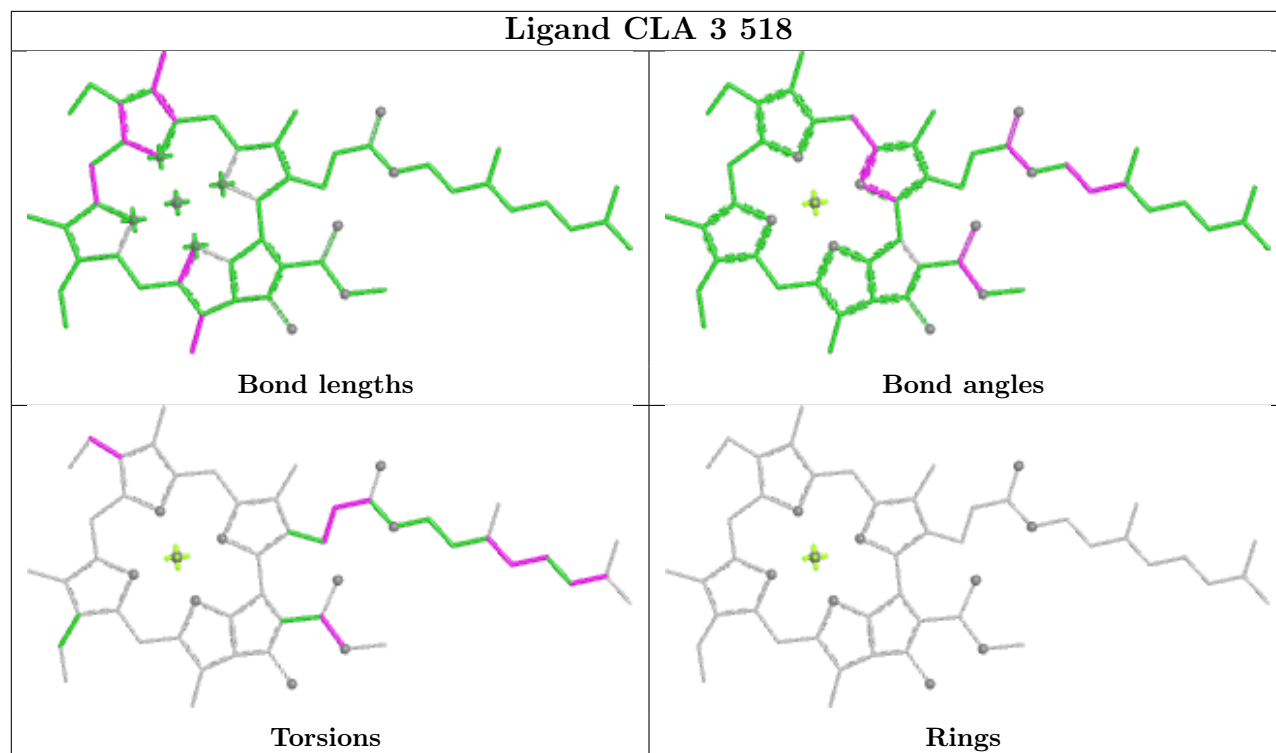


Ligand BCR 4 524

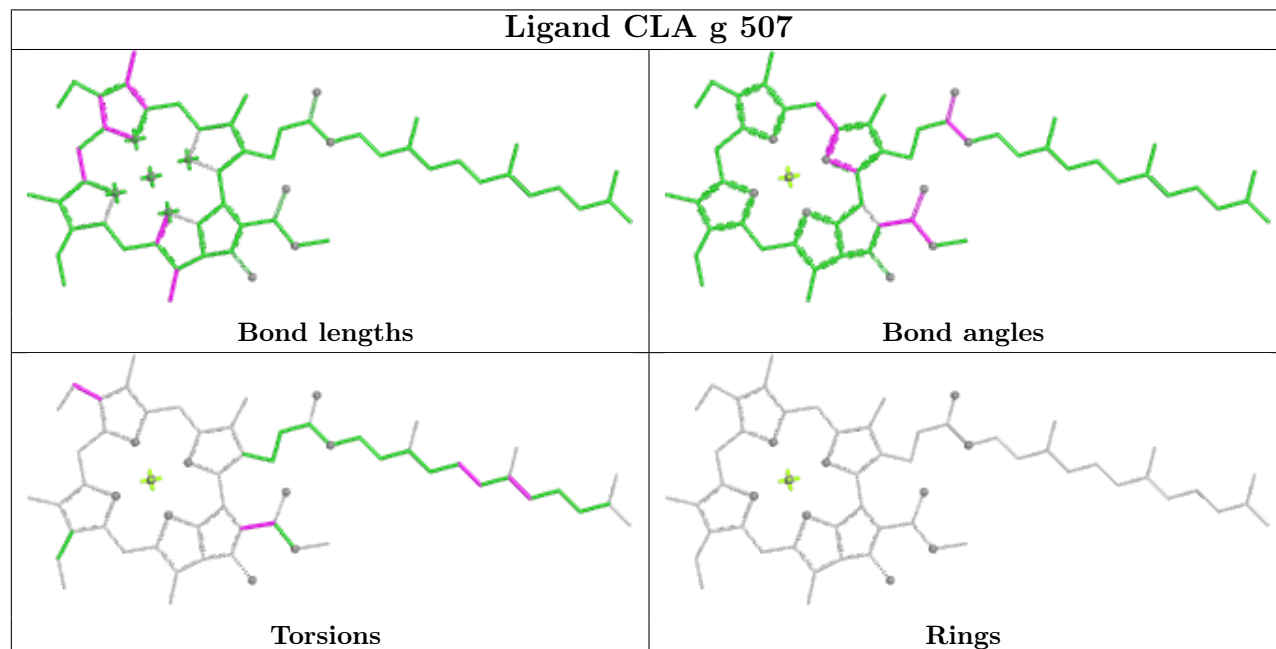




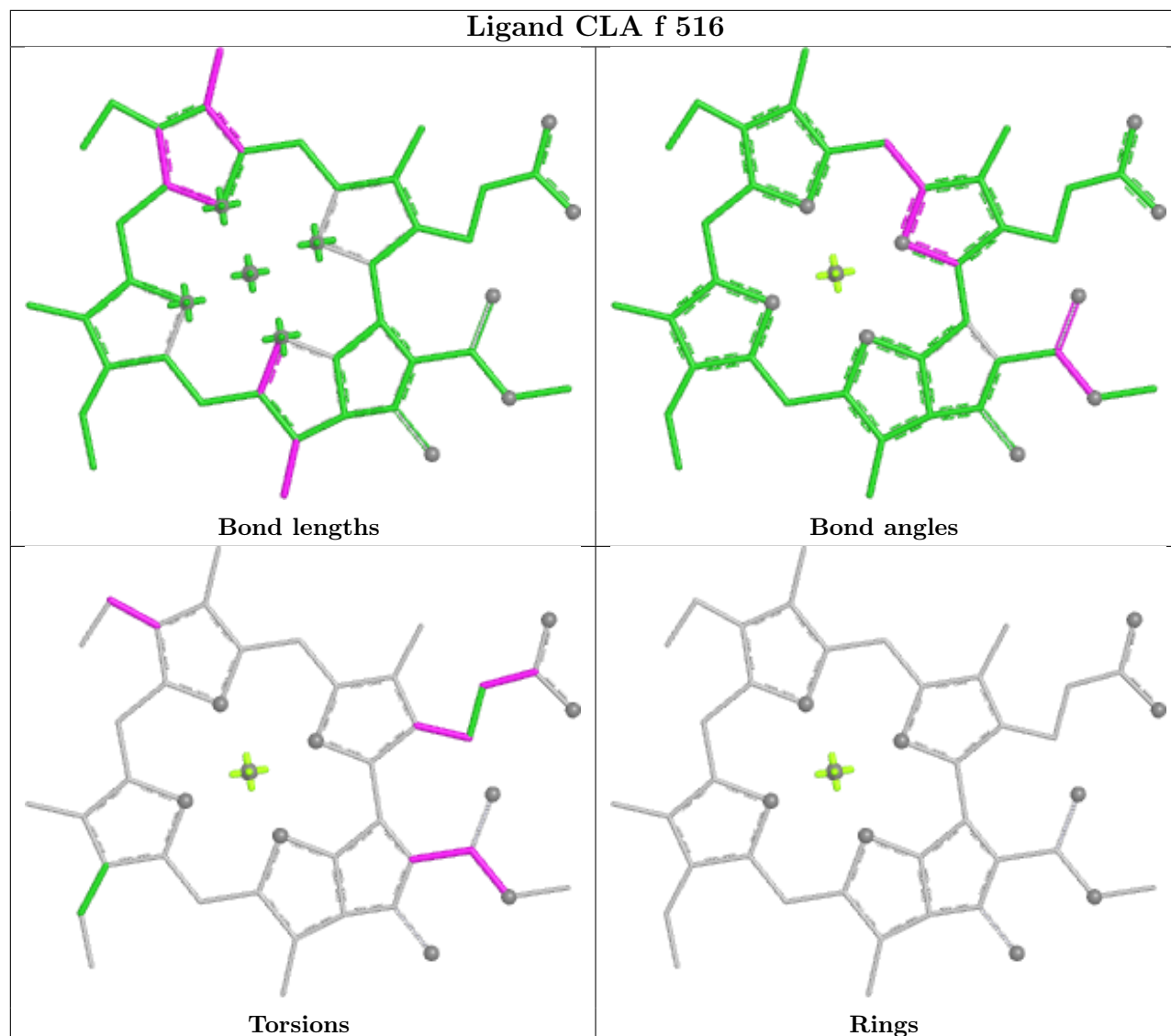
Ligand CLA 3 518



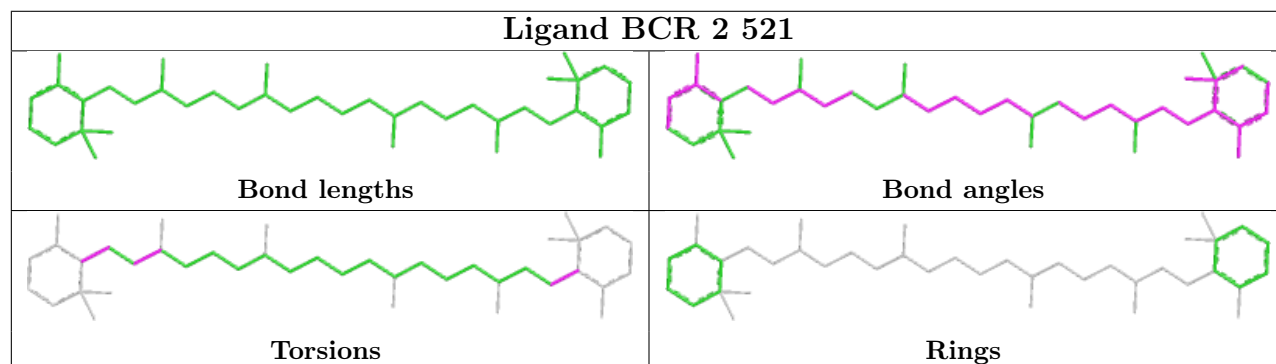
Ligand CLA g 507

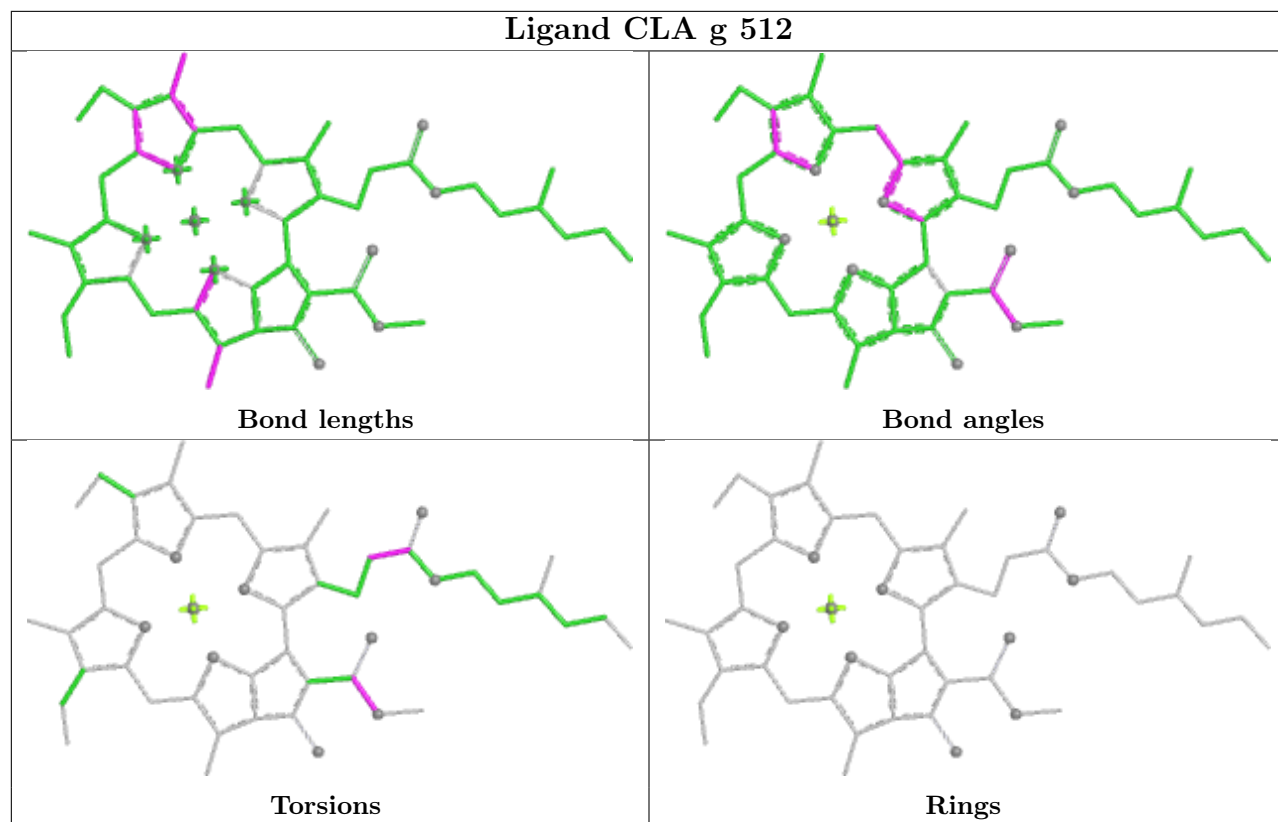


Ligand CLA f 516

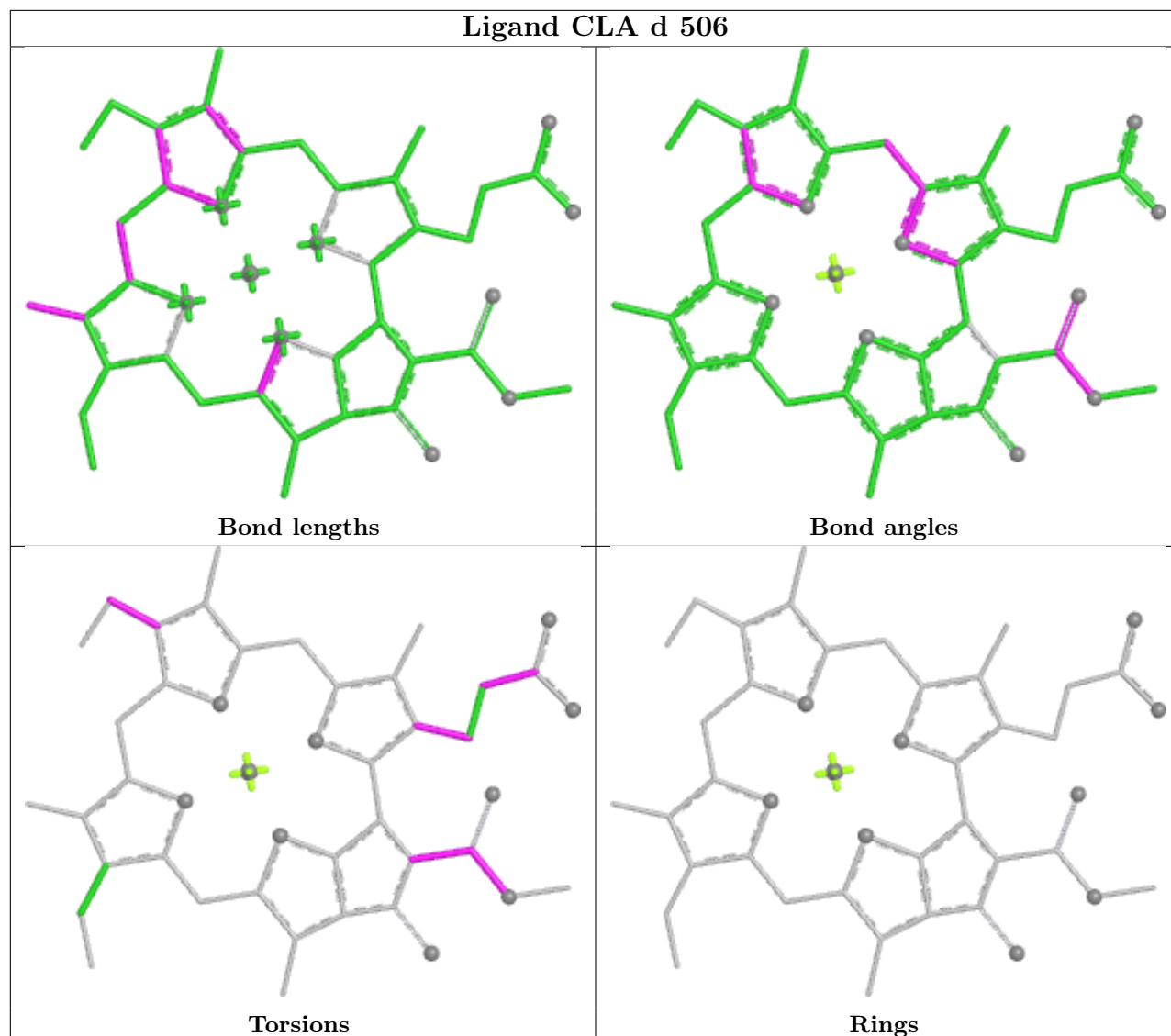


Ligand BCR 2 521

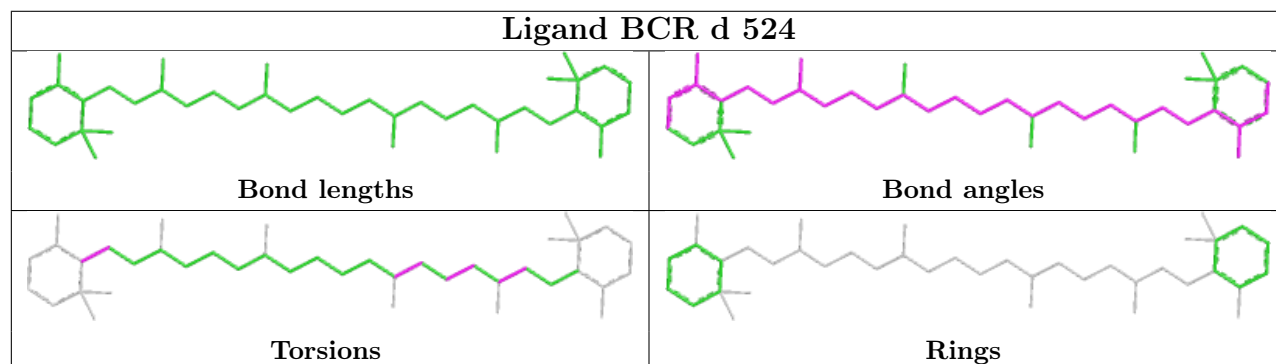




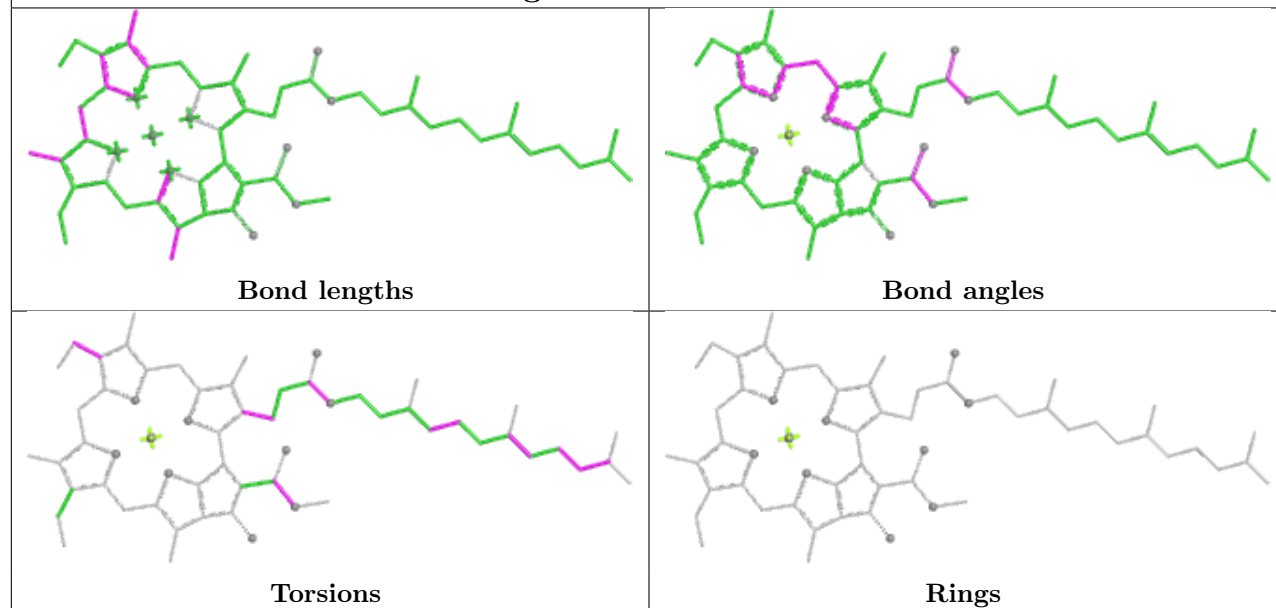
Ligand CLA d 506



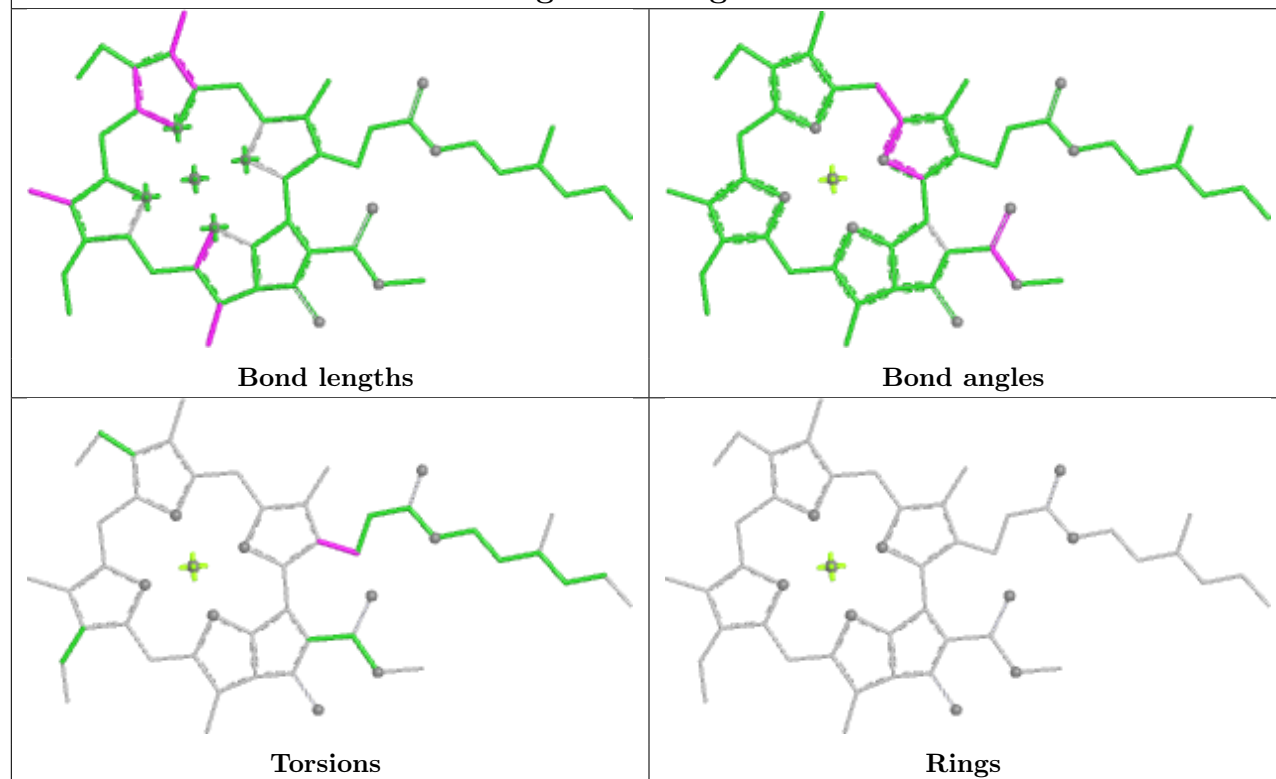
Ligand BCR d 524

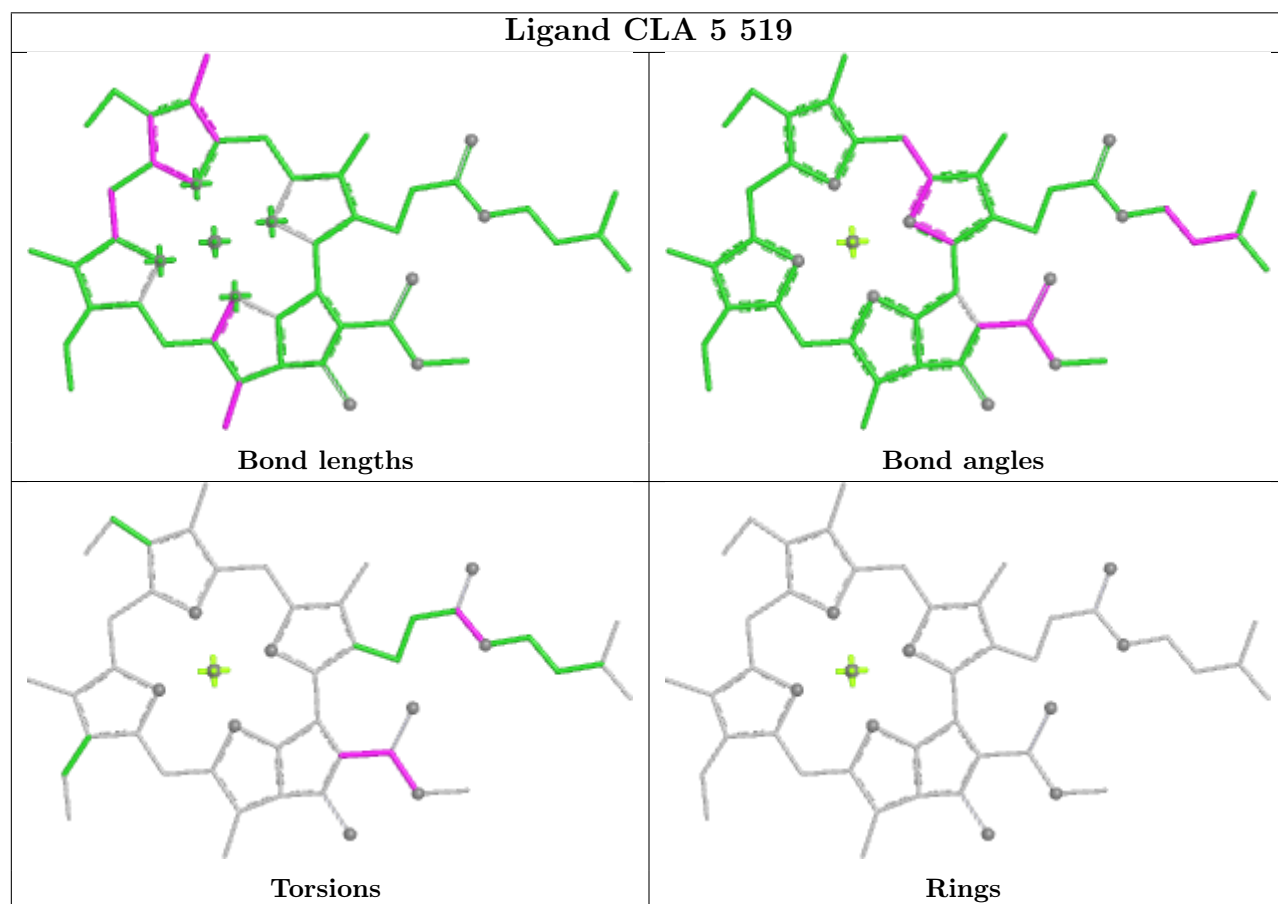
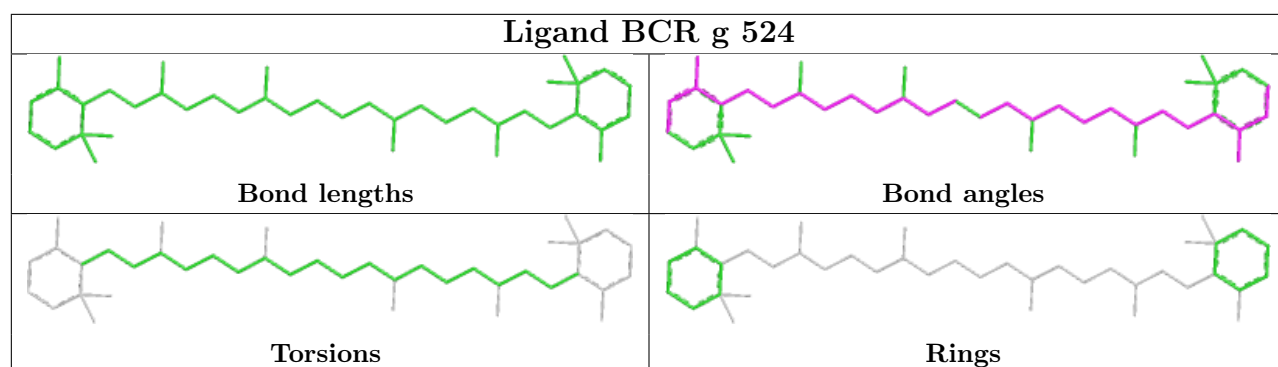


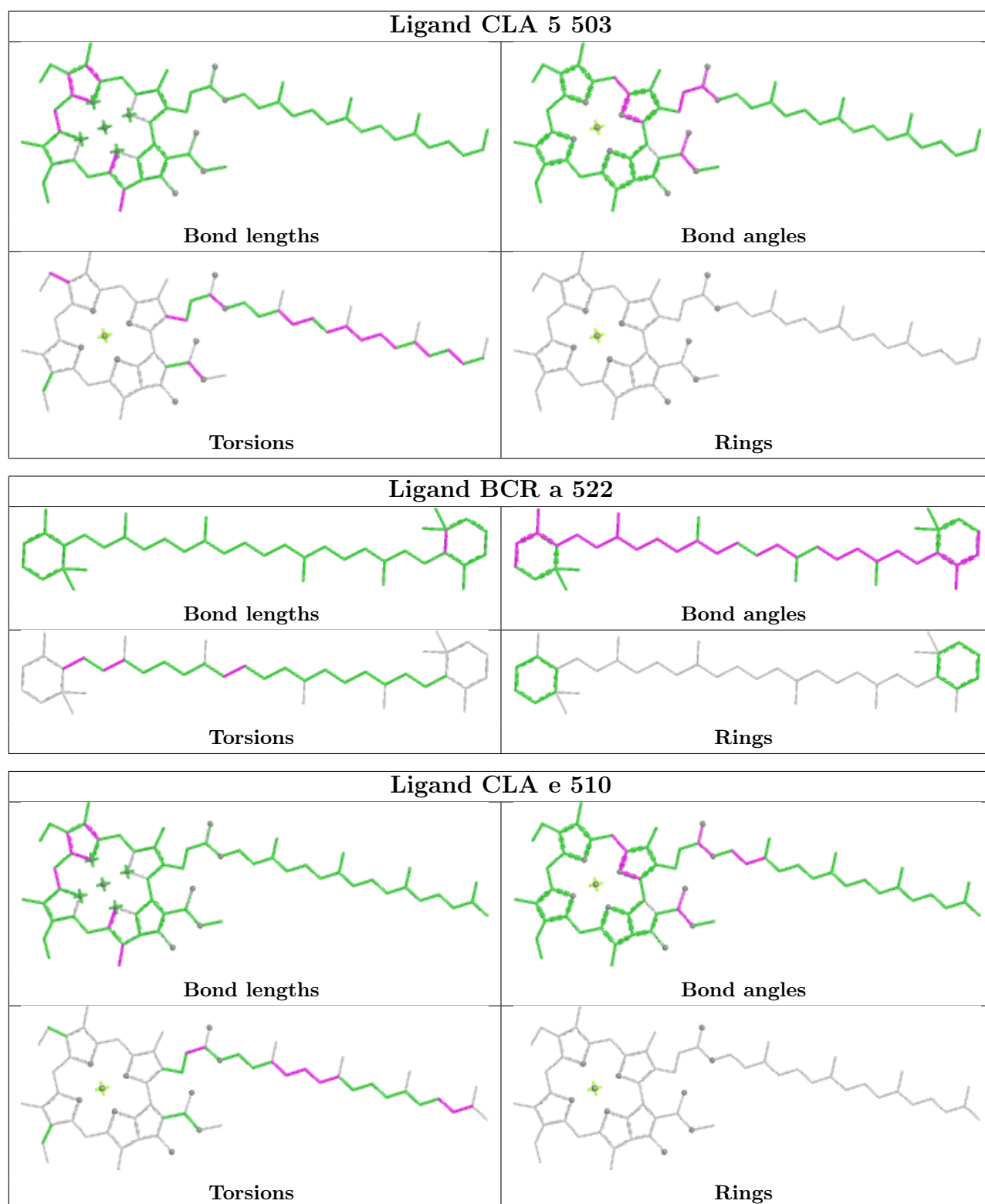
Ligand CLA B 1216



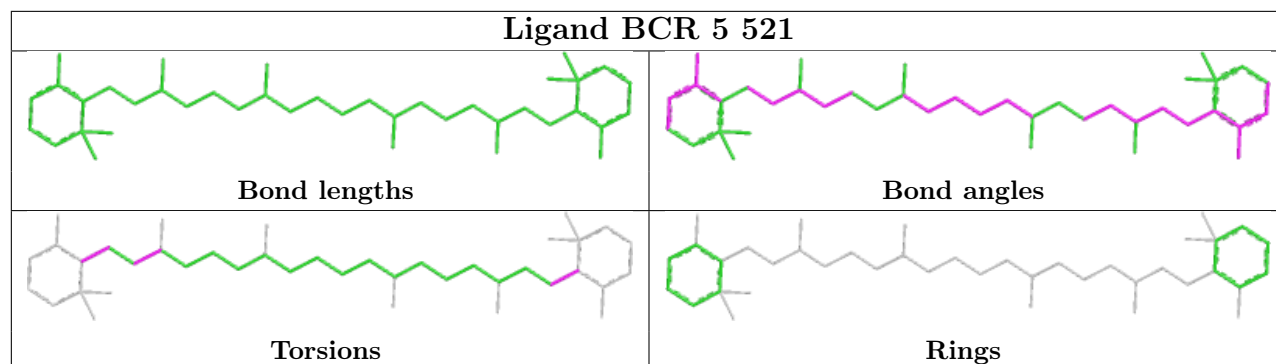
Ligand CLA g 508



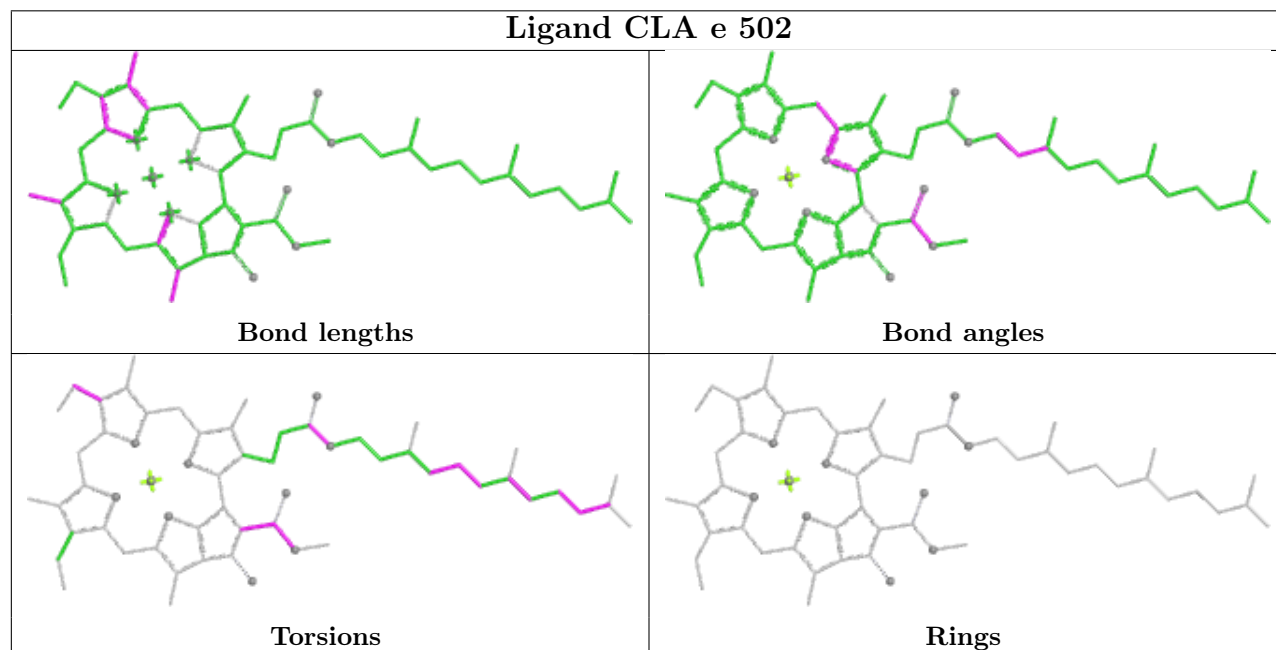




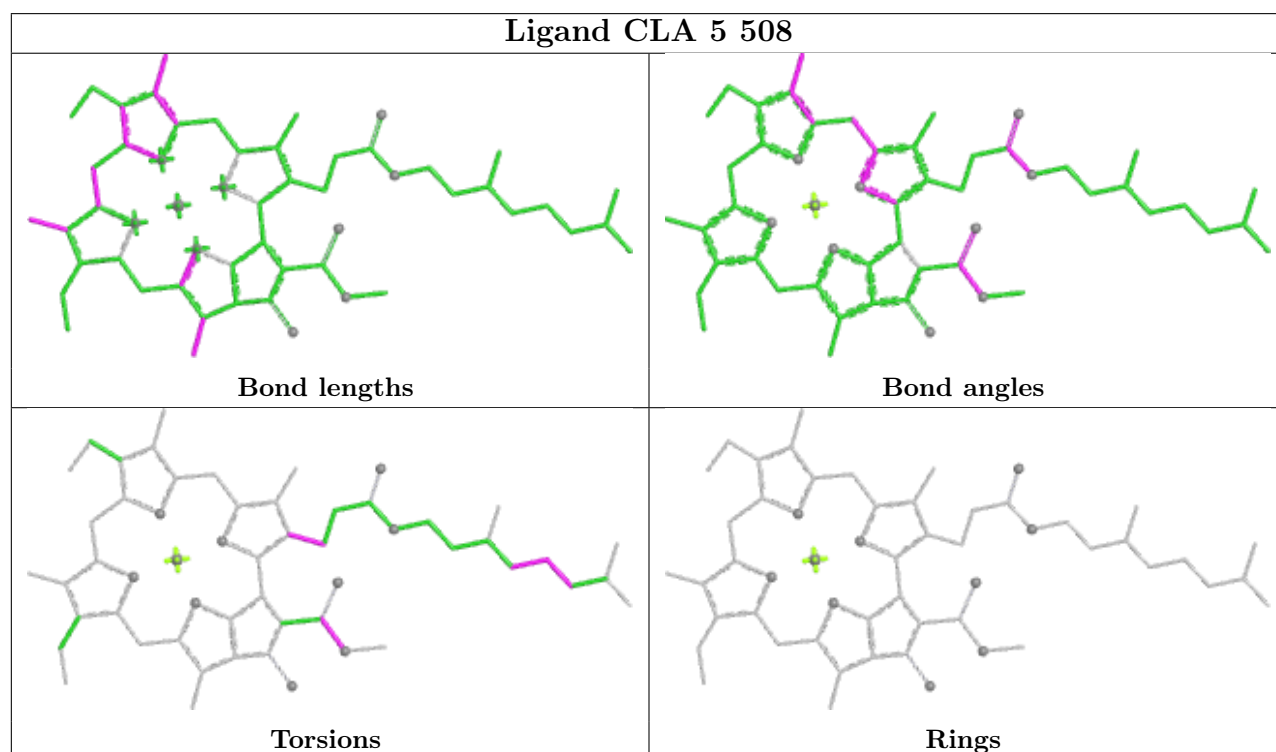
Ligand BCR 5 521



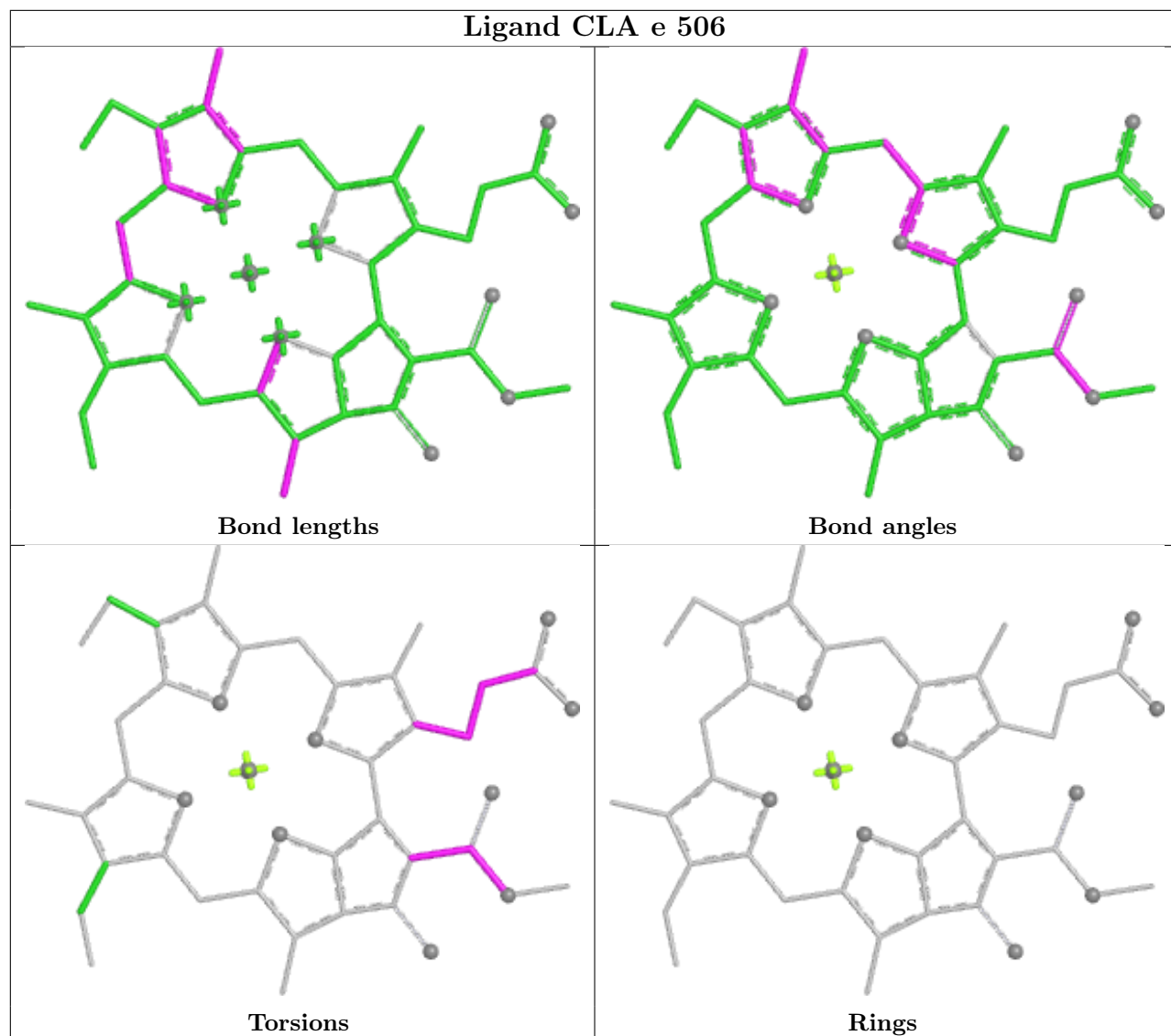
Ligand CLA e 502

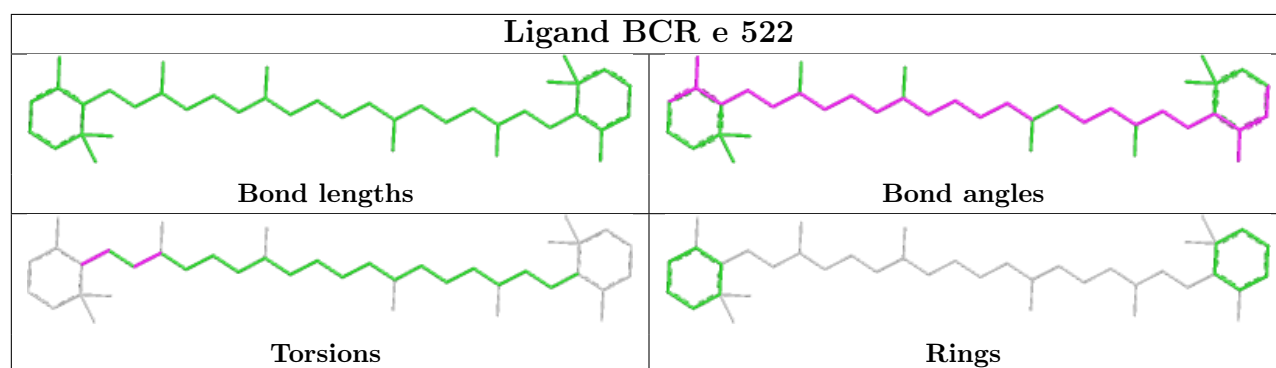
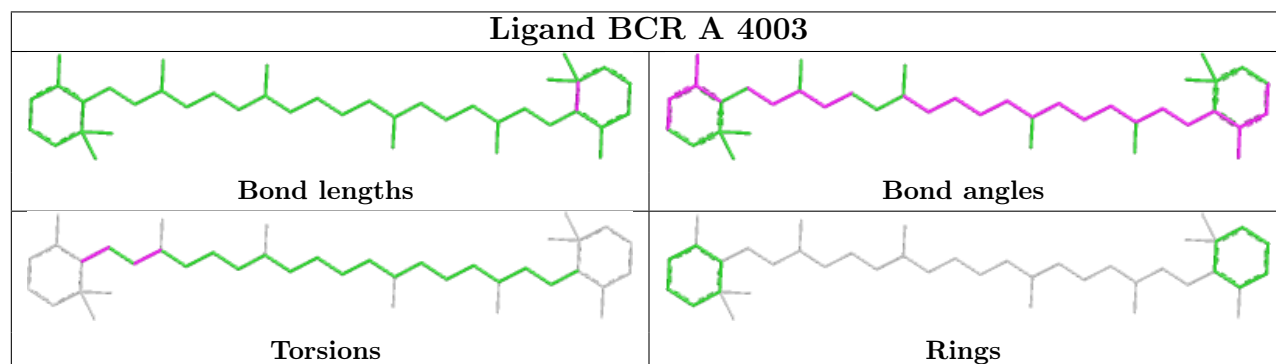
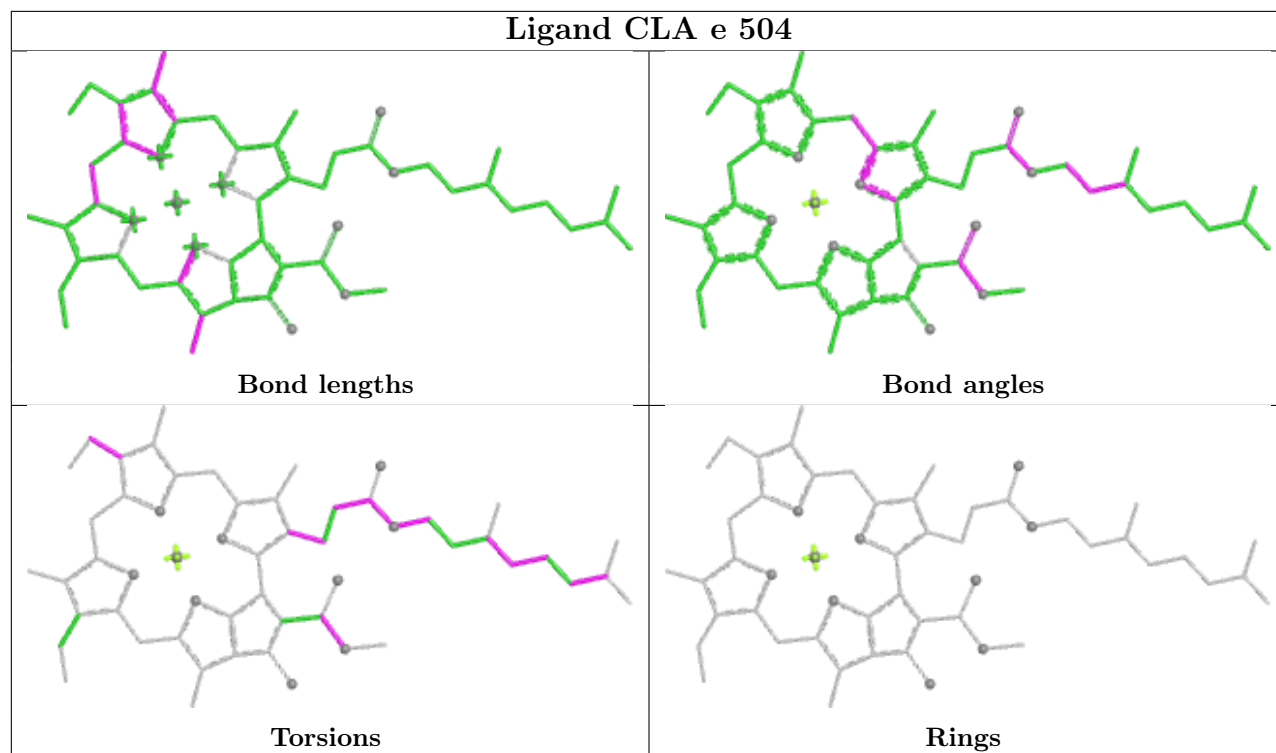


Ligand CLA 5 508

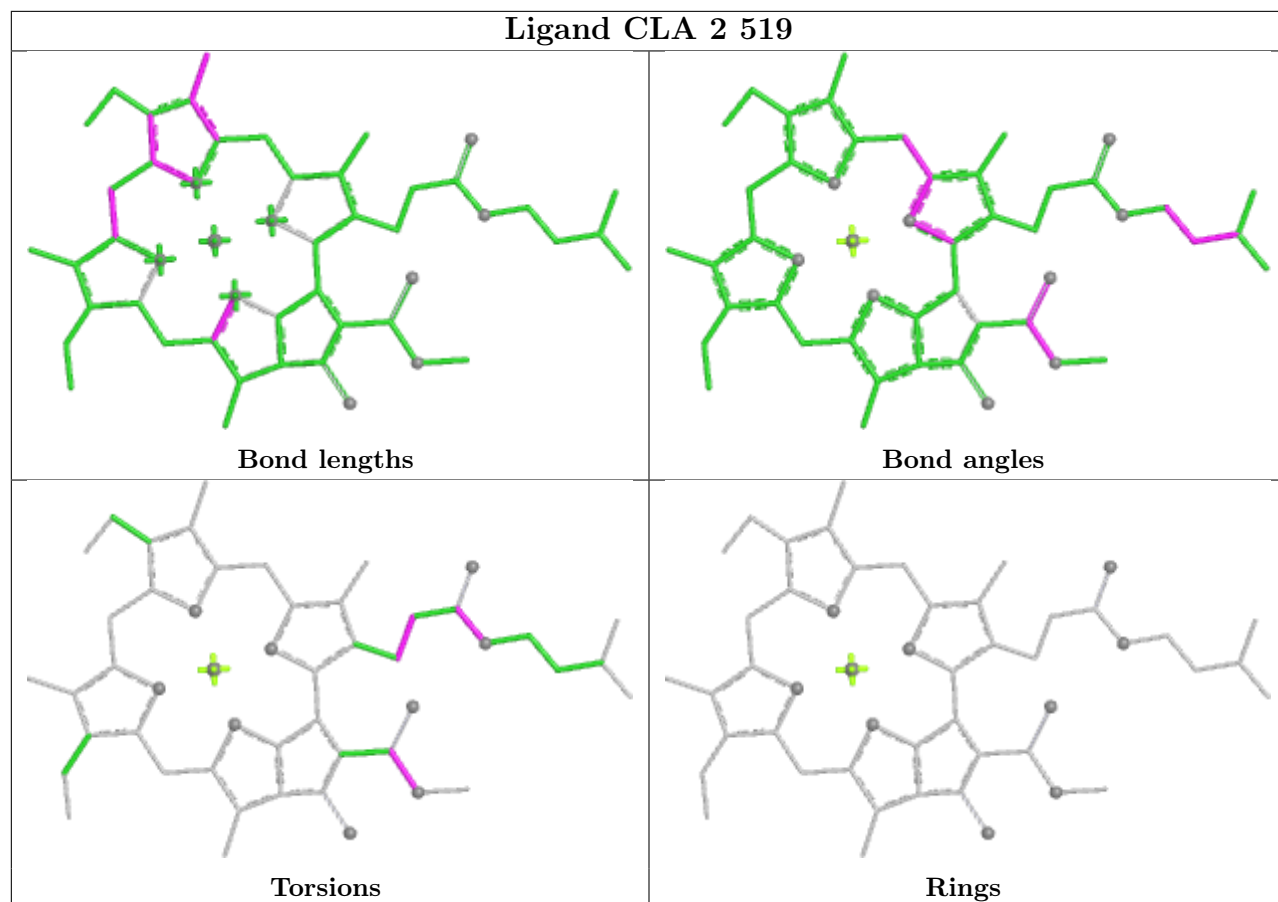


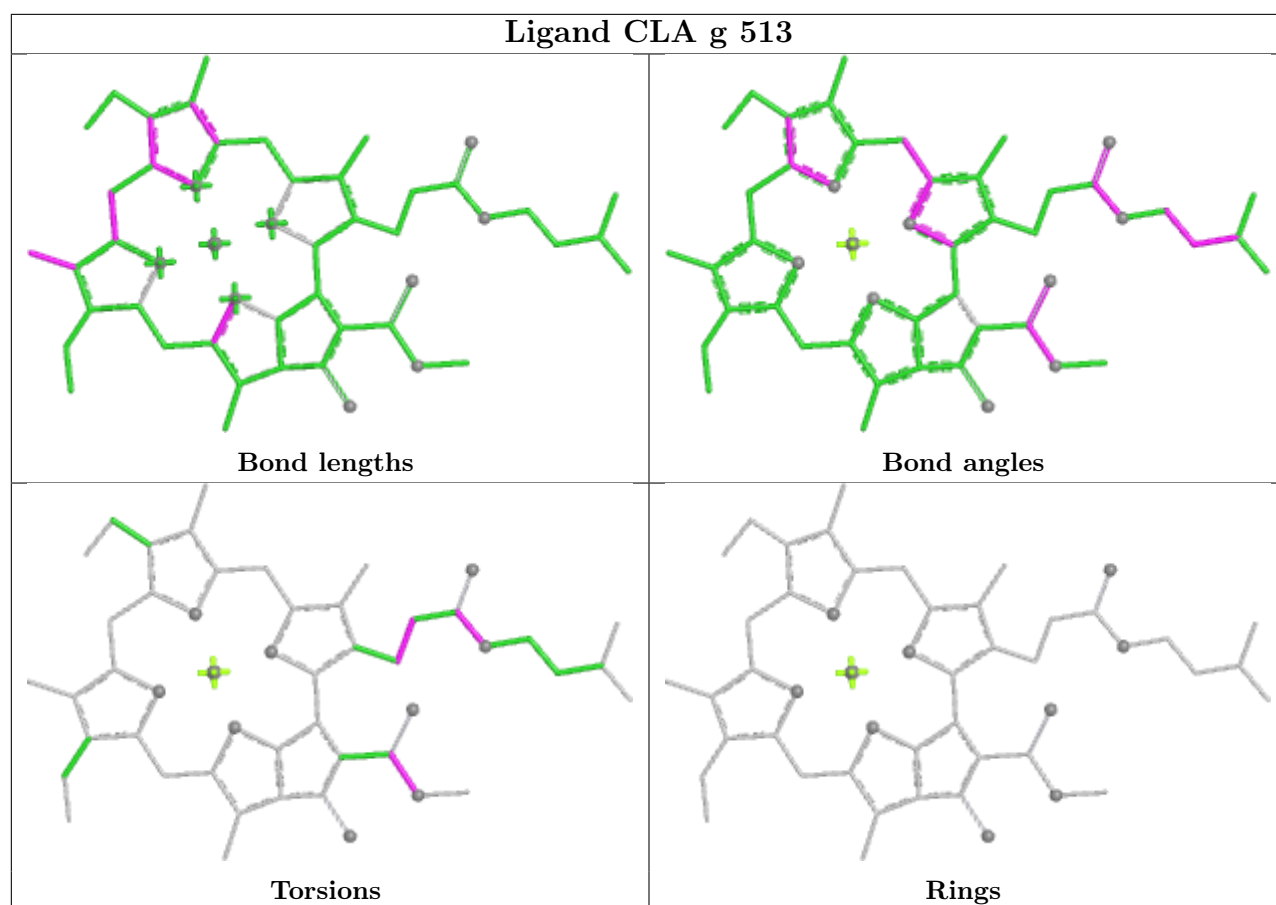
Ligand CLA e 506



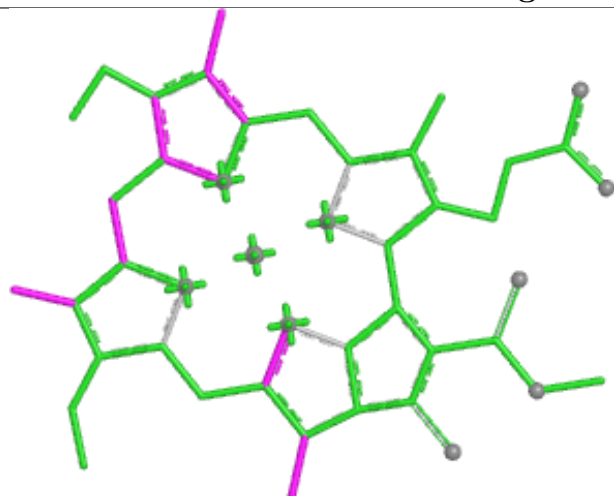


Ligand CLA 2 519

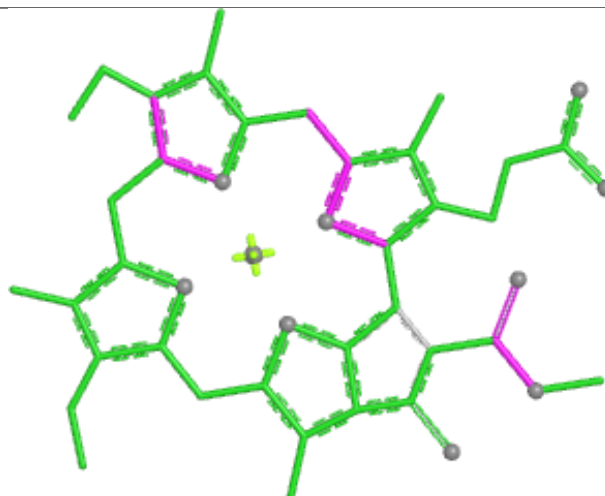




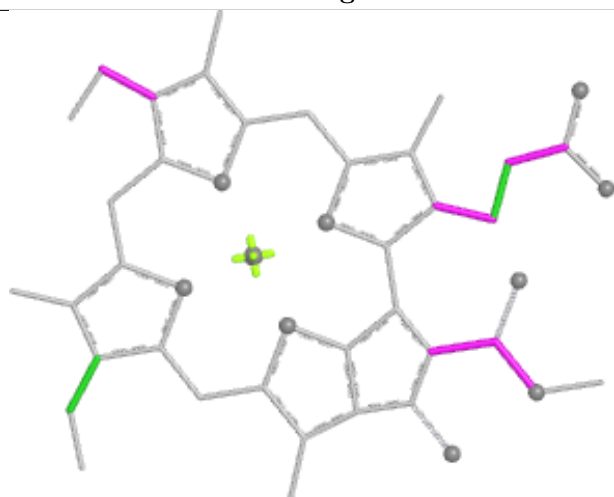
Ligand CLA 2 517



Bond lengths



Bond angles

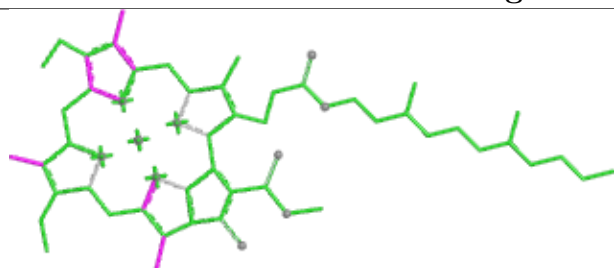


Torsions

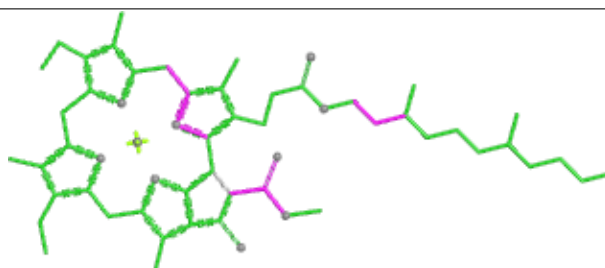


Rings

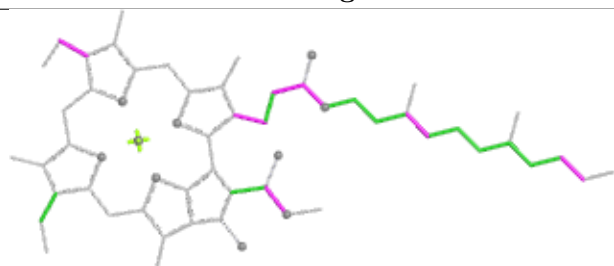
Ligand CLA B 1230



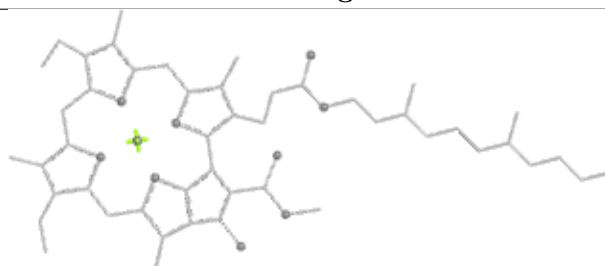
Bond lengths



Bond angles

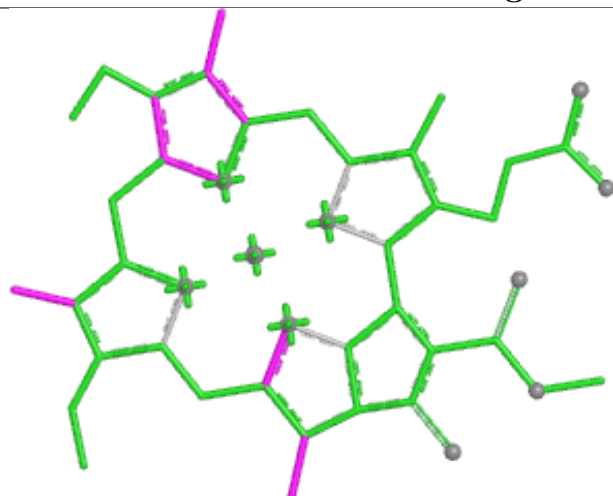


Torsions

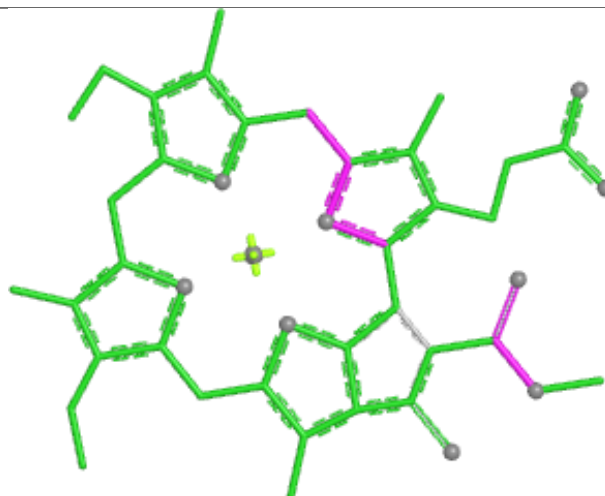


Rings

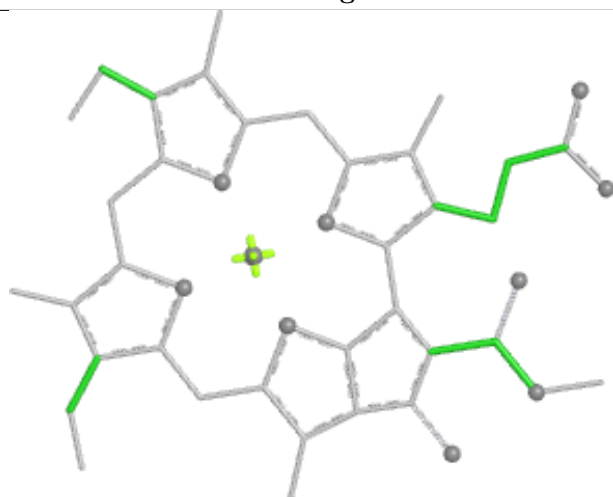
Ligand CLA B 1233



Bond lengths



Bond angles

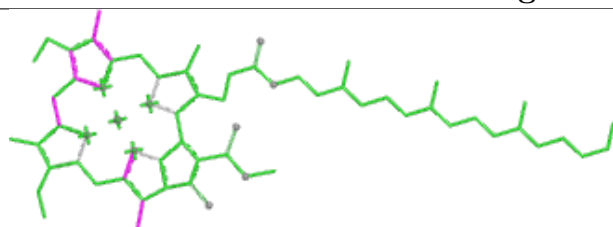


Torsions

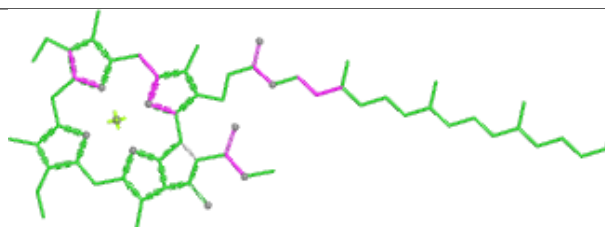


Rings

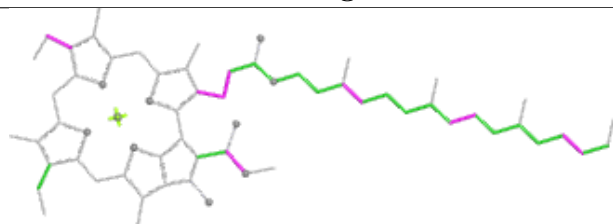
Ligand CLA 4 503



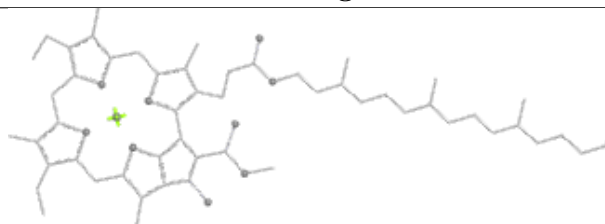
Bond lengths



Bond angles

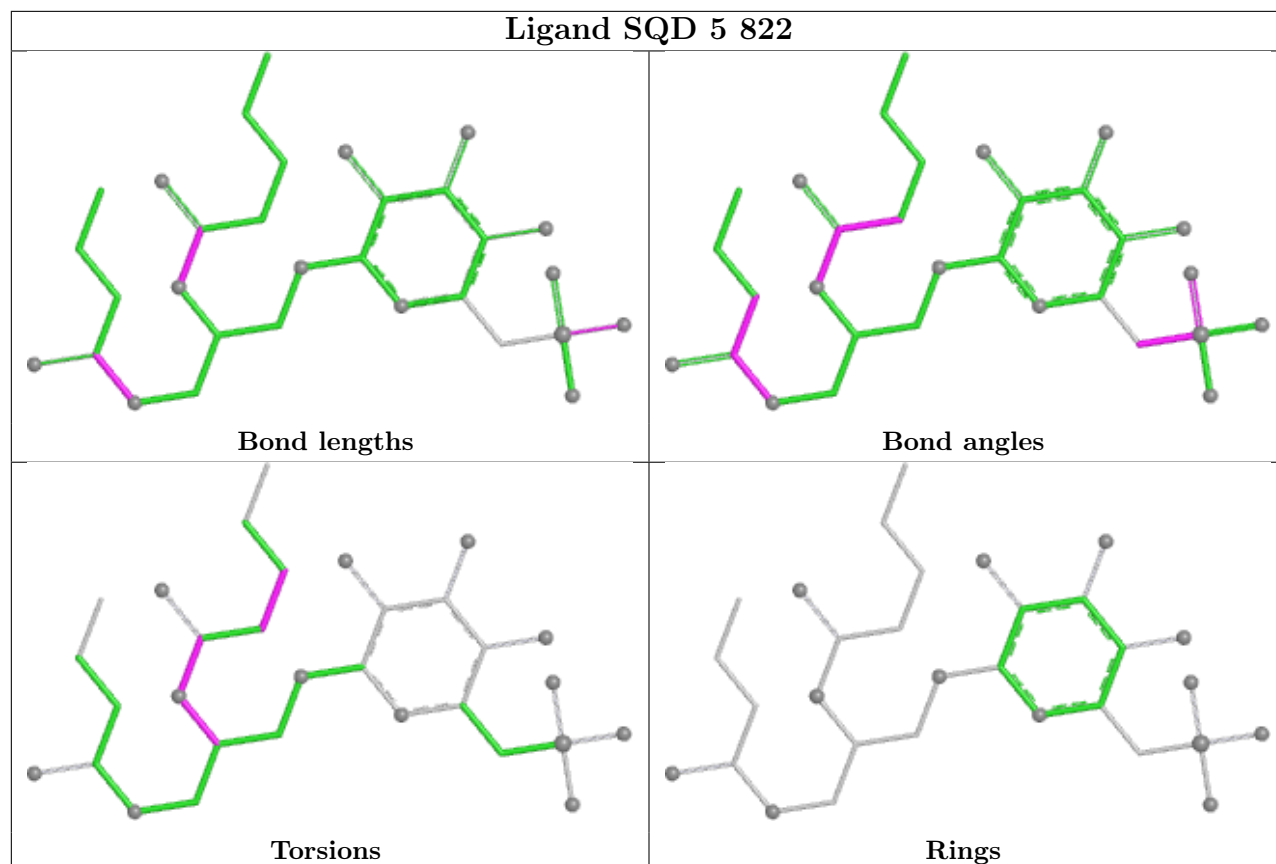


Torsions

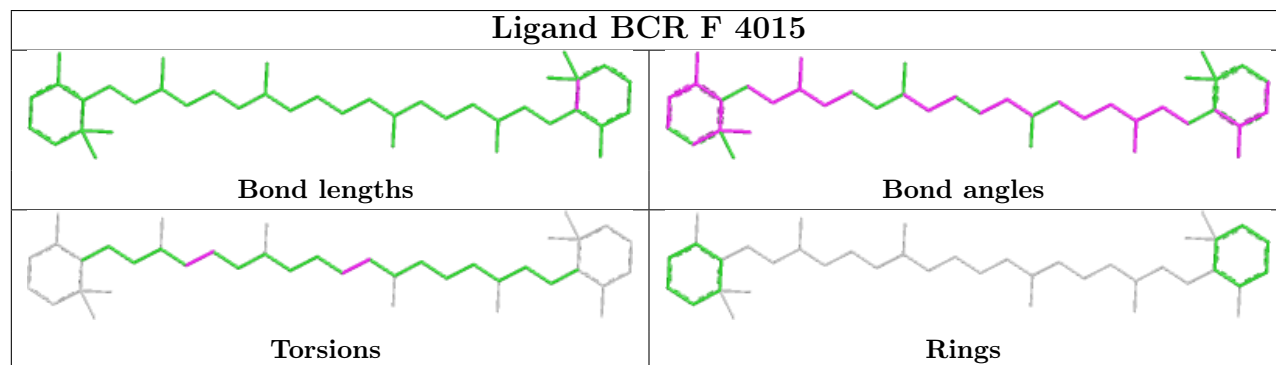


Rings

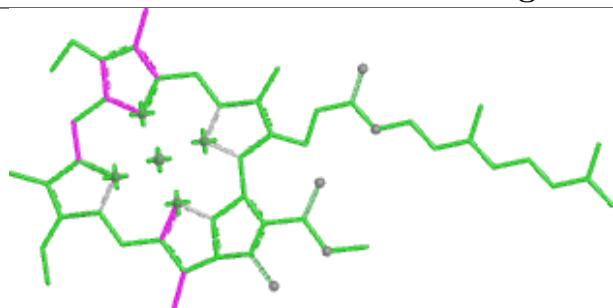
Ligand SQD 5 822



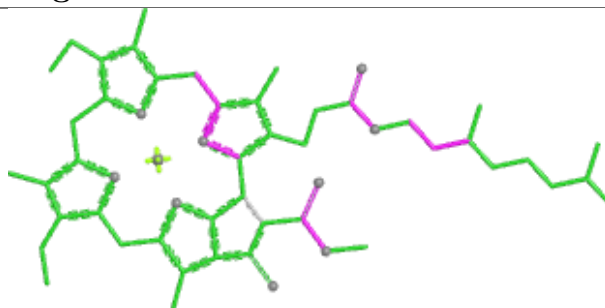
Ligand BCR F 4015



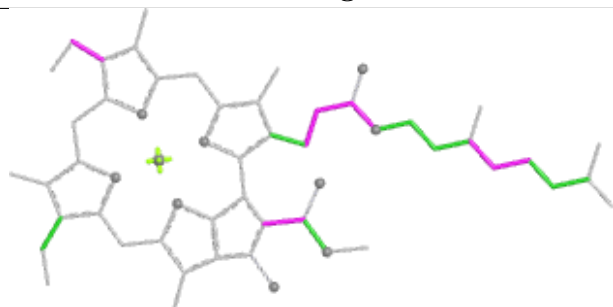
Ligand CLA g 518



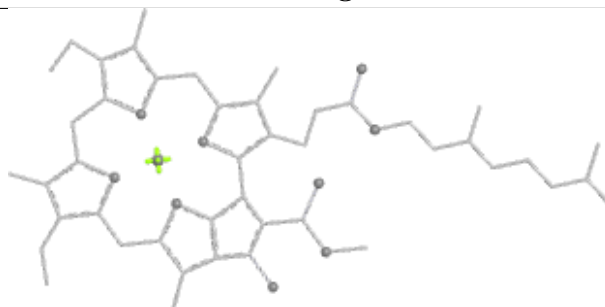
Bond lengths



Bond angles

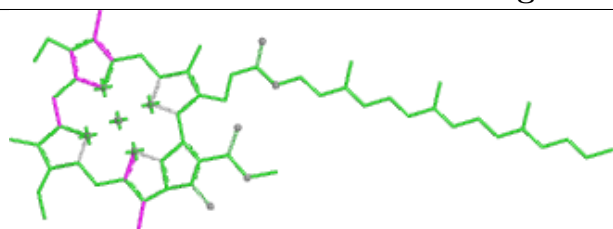


Torsions

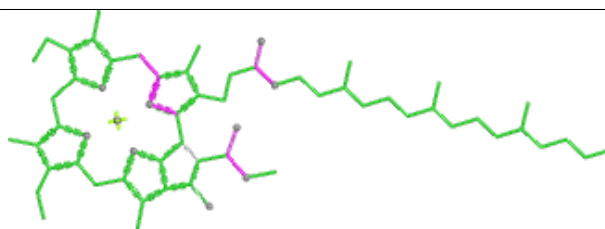


Rings

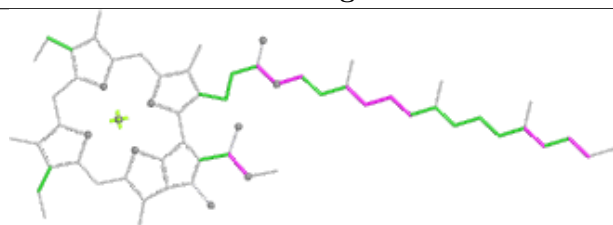
Ligand CLA b 503



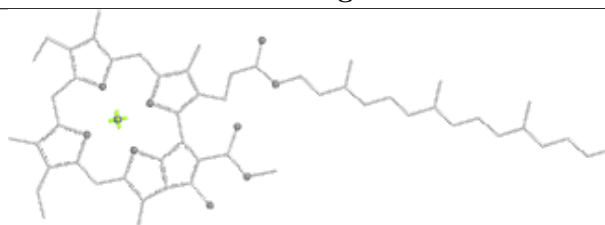
Bond lengths



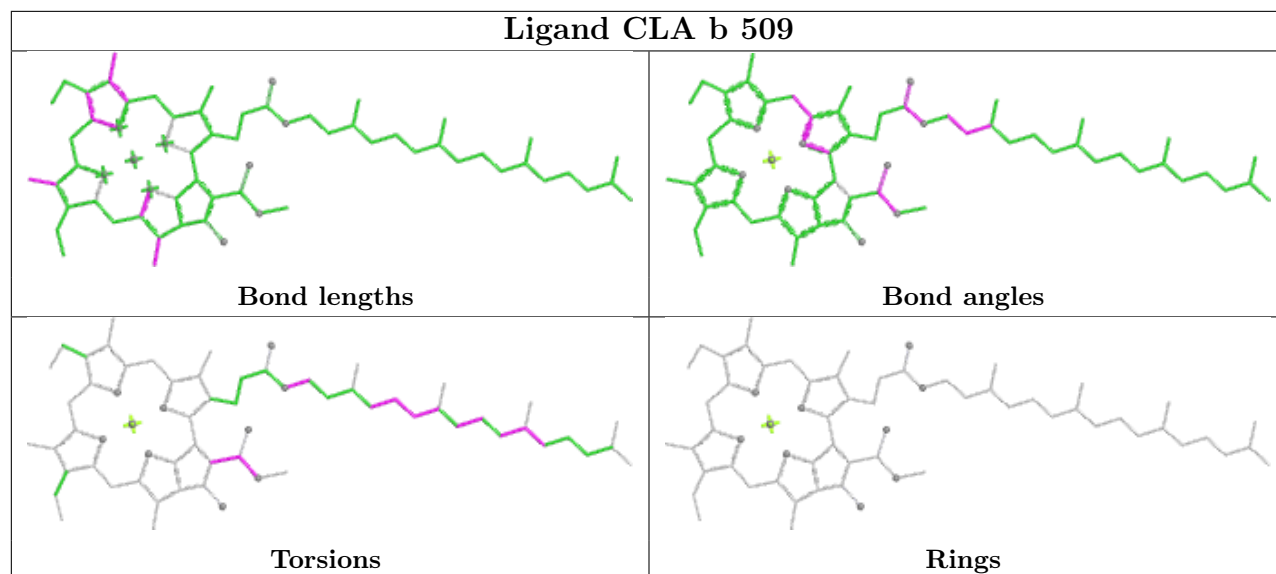
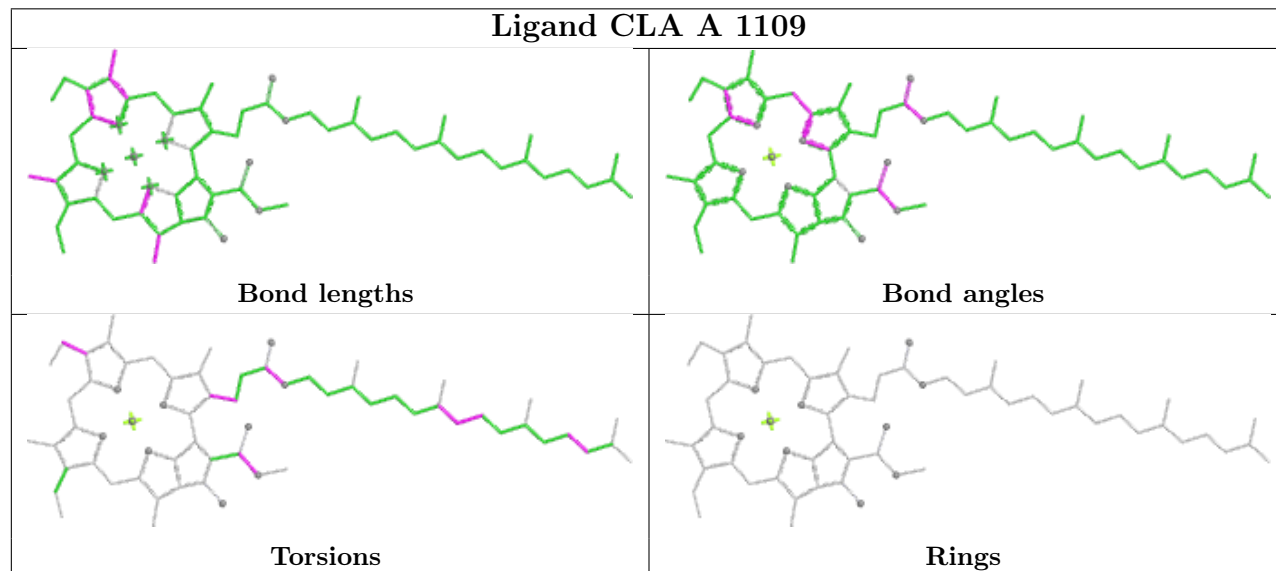
Bond angles



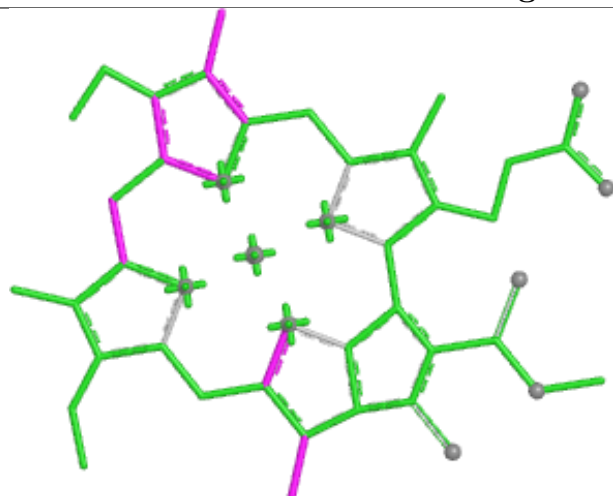
Torsions



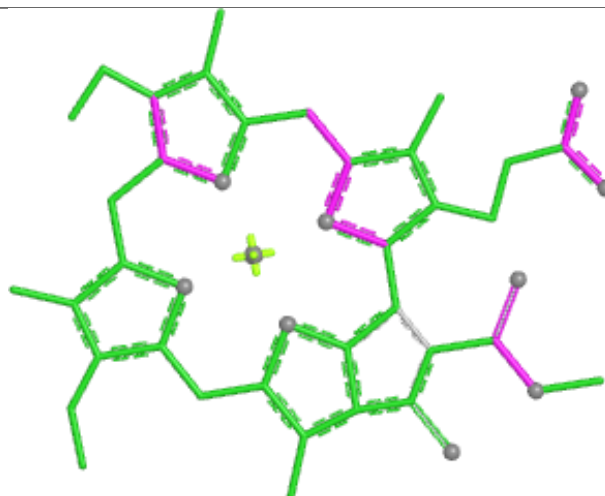
Rings

Ligand CLA b 509**Ligand CLA A 1109**

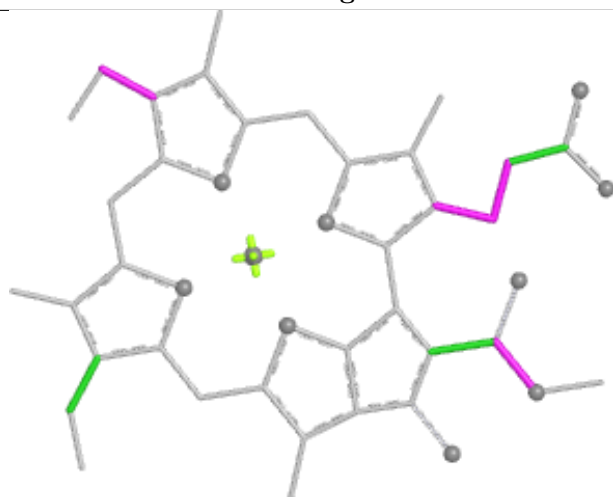
Ligand CLA 6 511



Bond lengths



Bond angles

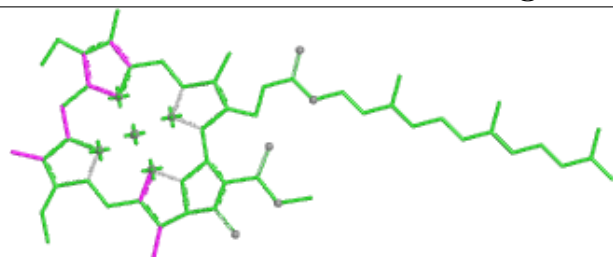


Torsions

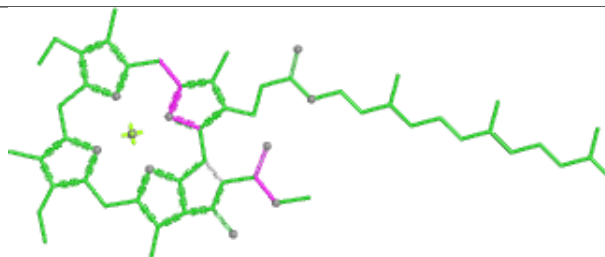


Rings

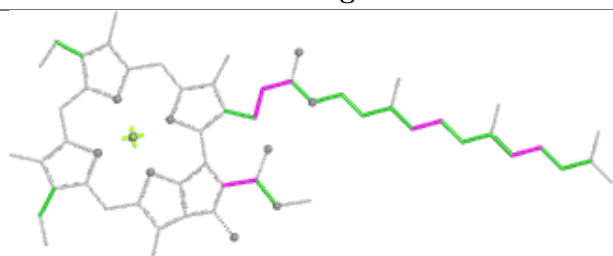
Ligand CLA e 507



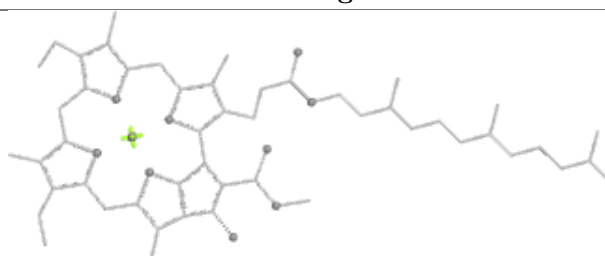
Bond lengths



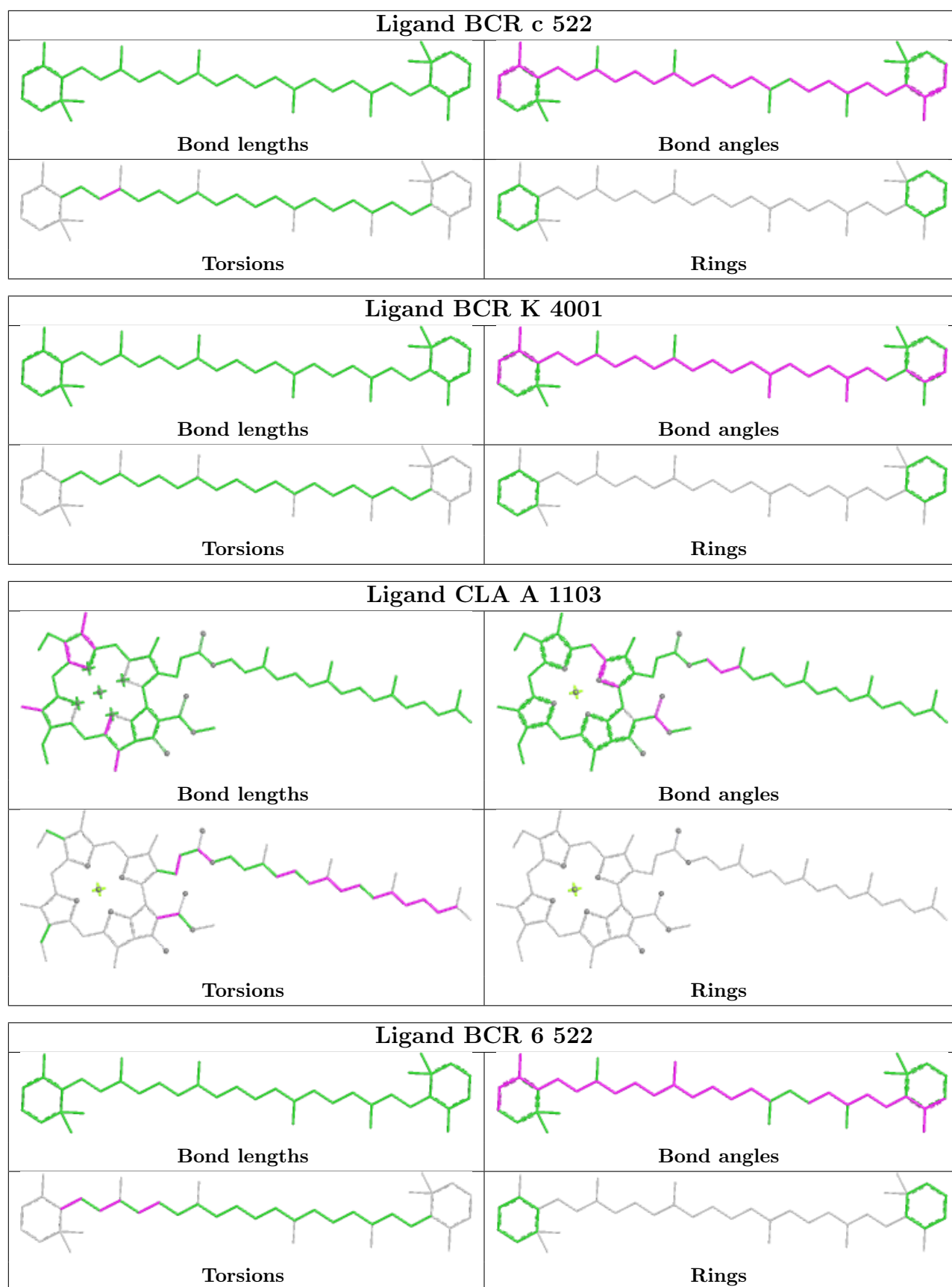
Bond angles



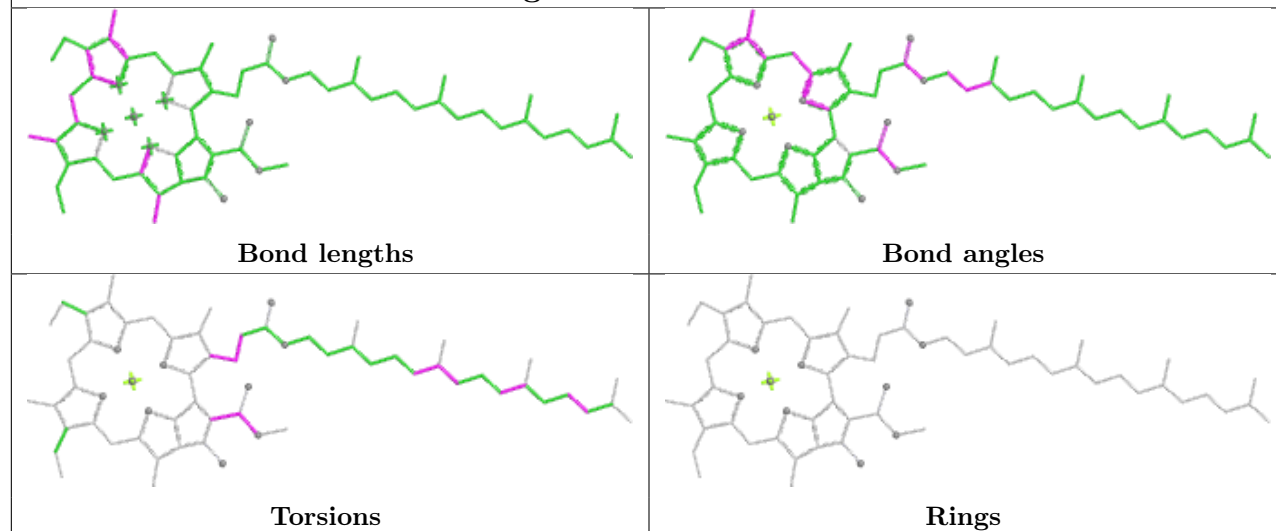
Torsions



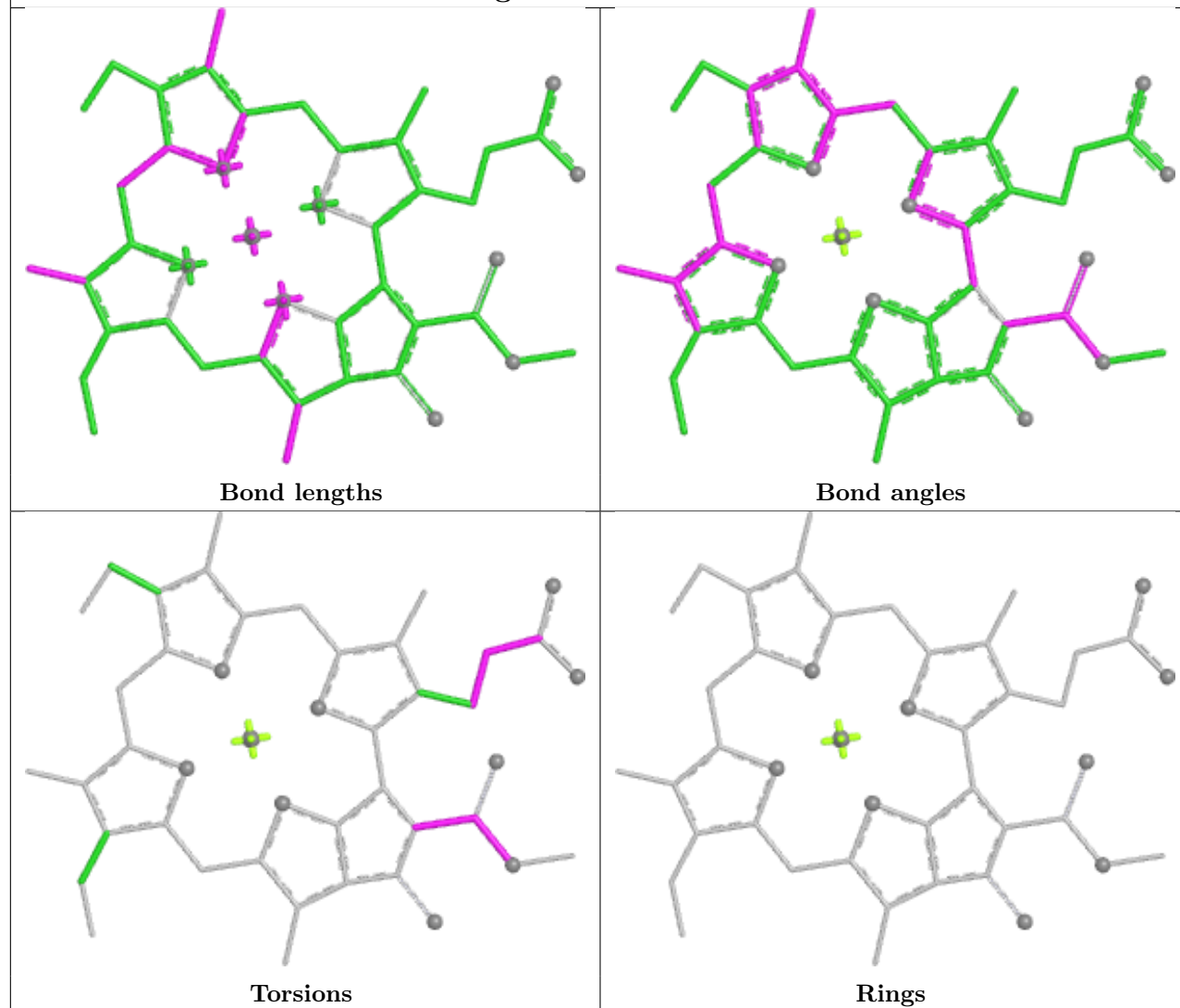
Rings

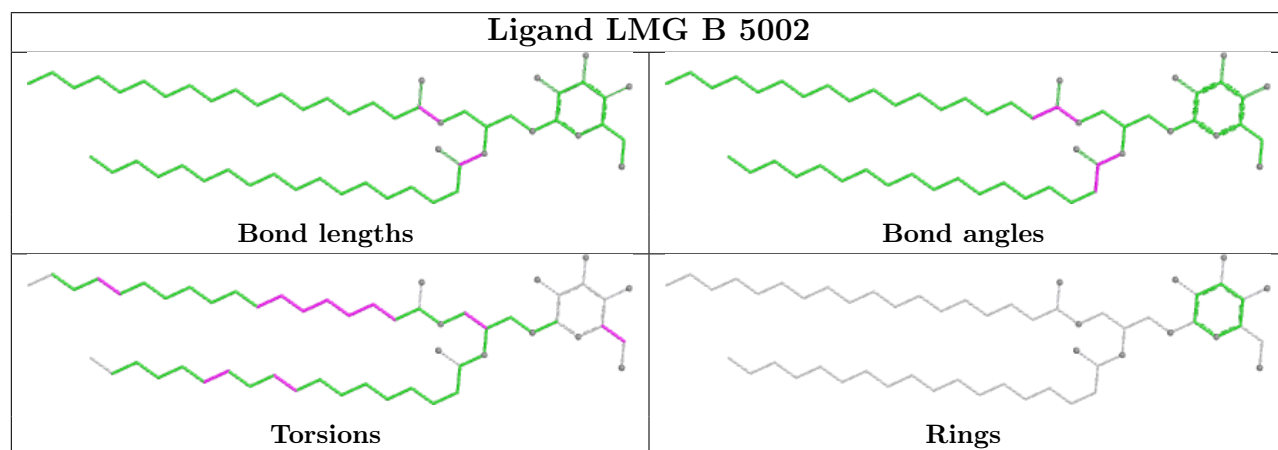
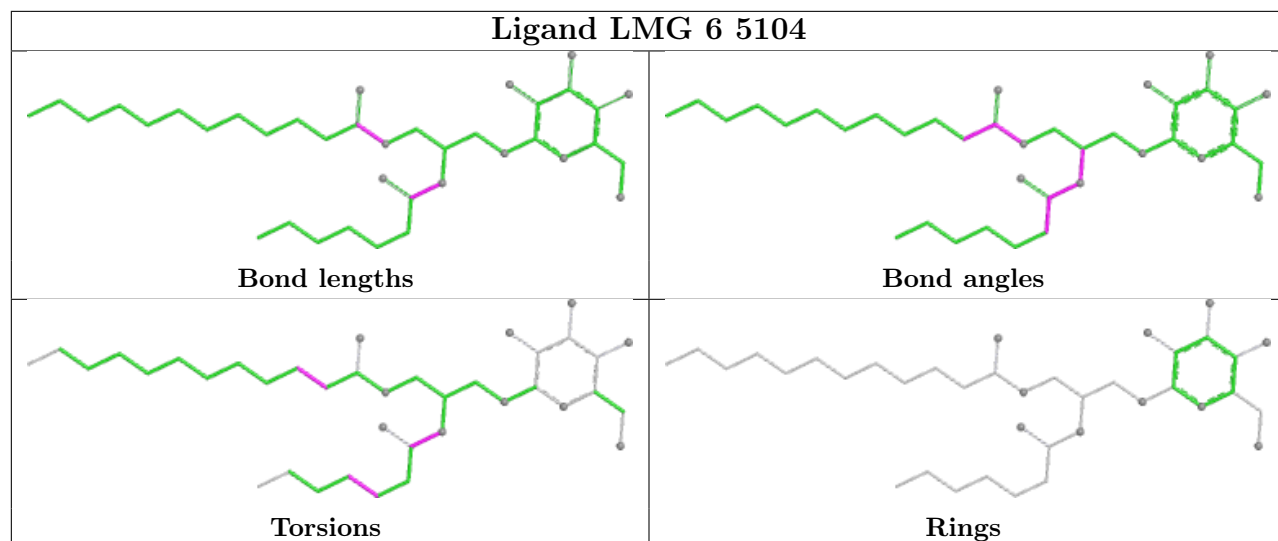


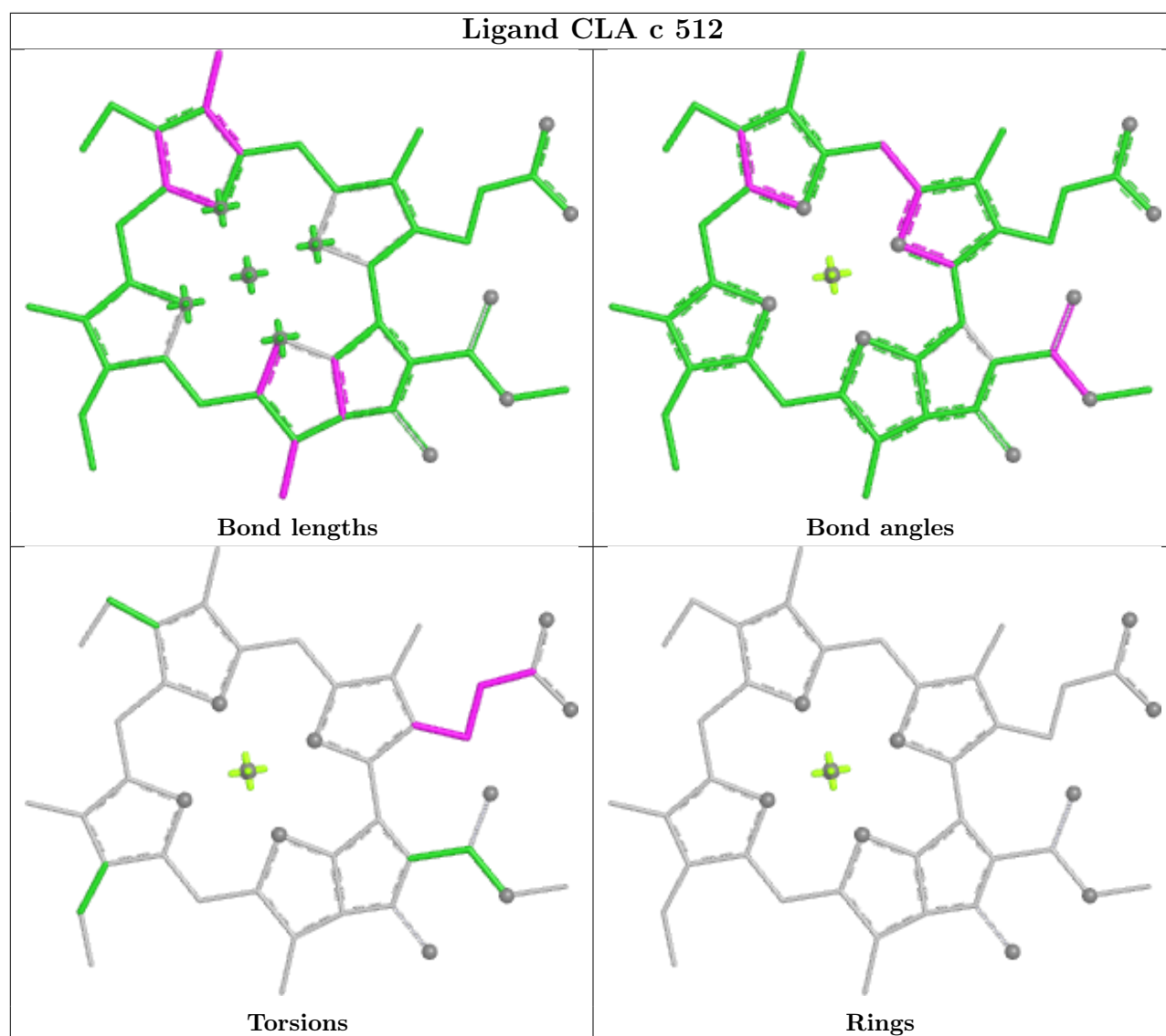
Ligand CLA B 1211



Ligand CLA b 506







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-63528. These allow visual inspection of the internal detail of the map and identification of artifacts.

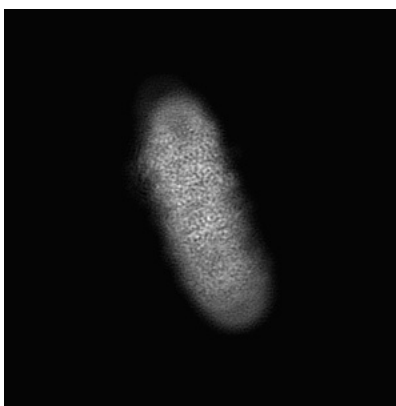
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

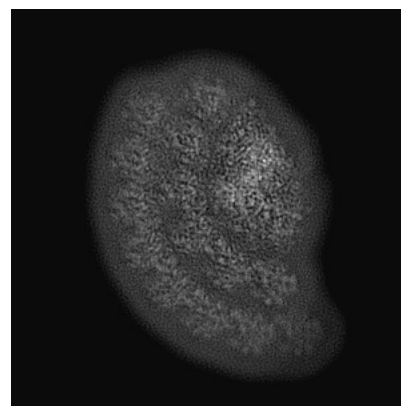
6.1.1 Primary map



X

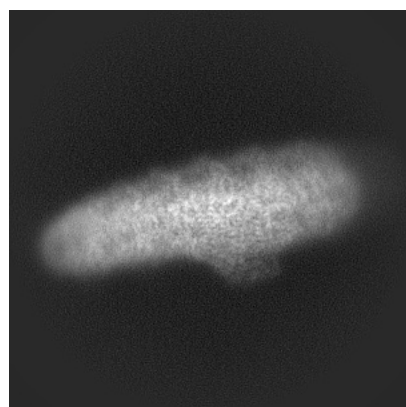


Y

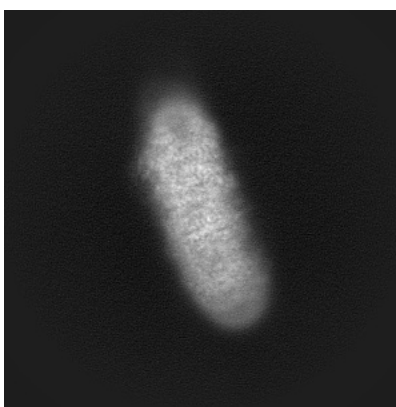


Z

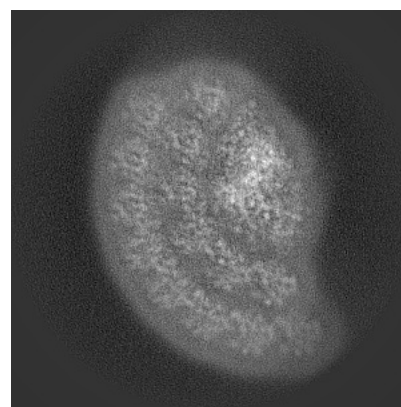
6.1.2 Raw map



X



Y

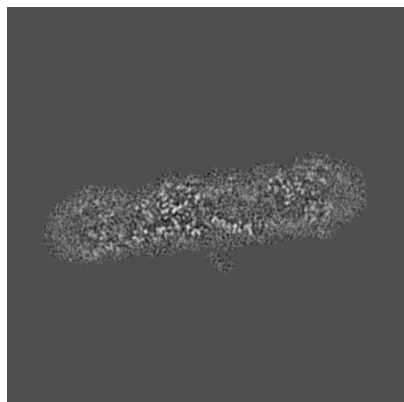


Z

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

6.2 Central slices [i](#)

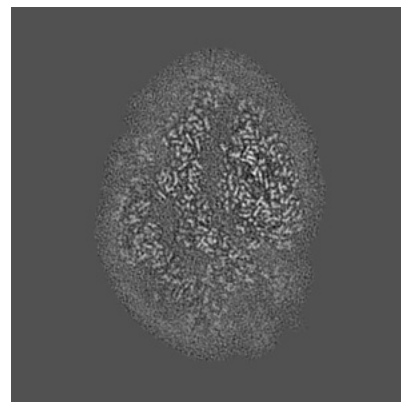
6.2.1 Primary map



X Index: 175

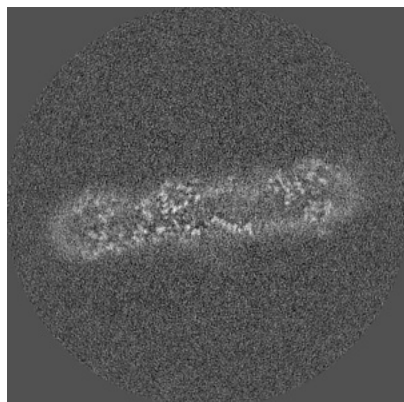


Y Index: 175

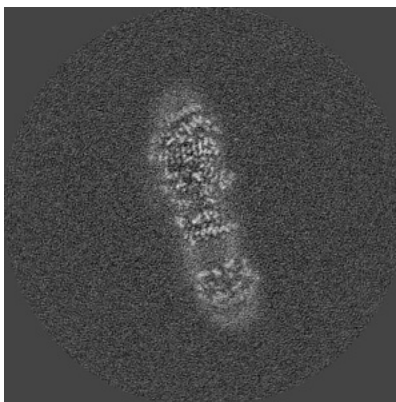


Z Index: 175

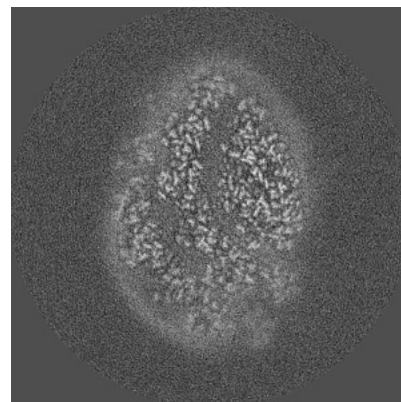
6.2.2 Raw map



X Index: 175



Y Index: 175

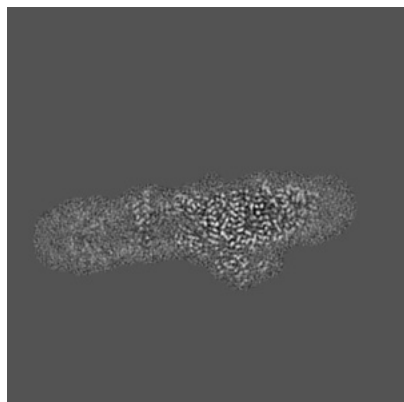


Z Index: 175

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

6.3 Largest variance slices [i](#)

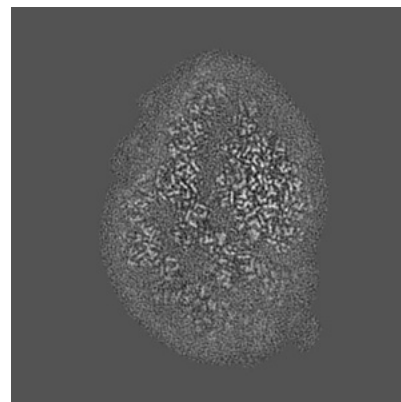
6.3.1 Primary map



X Index: 209

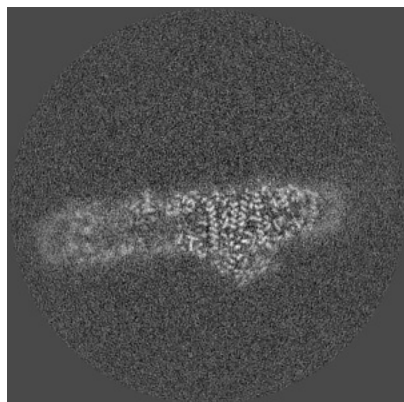


Y Index: 186

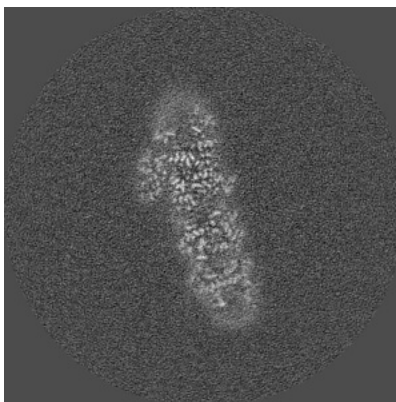


Z Index: 171

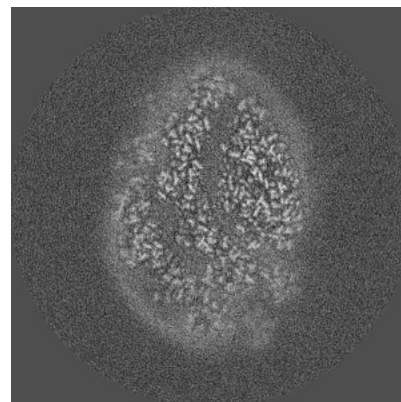
6.3.2 Raw map



X Index: 210



Y Index: 186

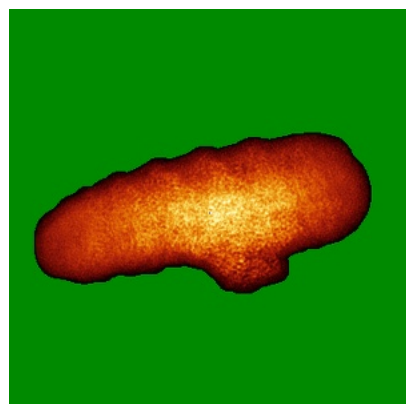


Z Index: 175

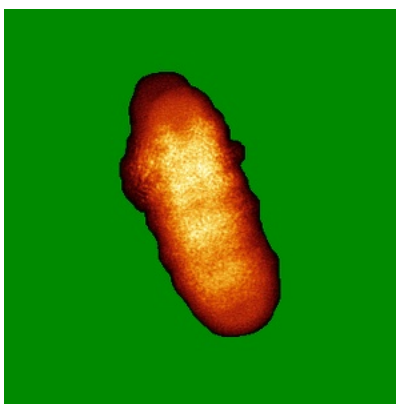
The images above show the largest variance slices of the map in three orthogonal directions.

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

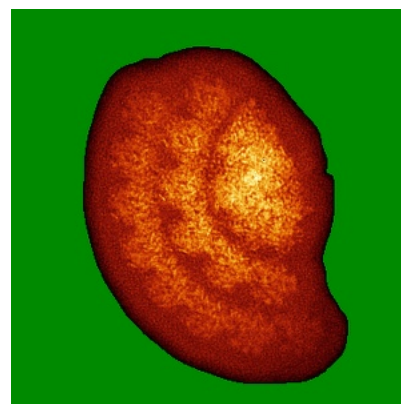
6.4.1 Primary map



X

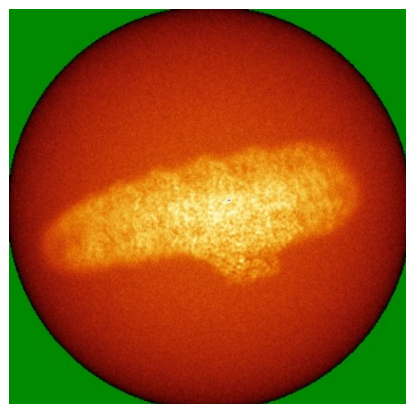


Y

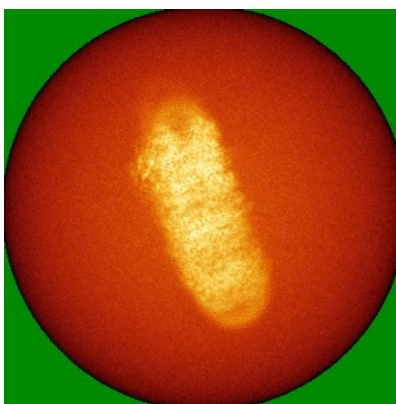


Z

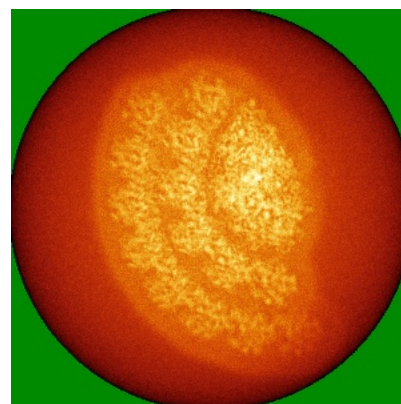
6.4.2 Raw map



X



Y

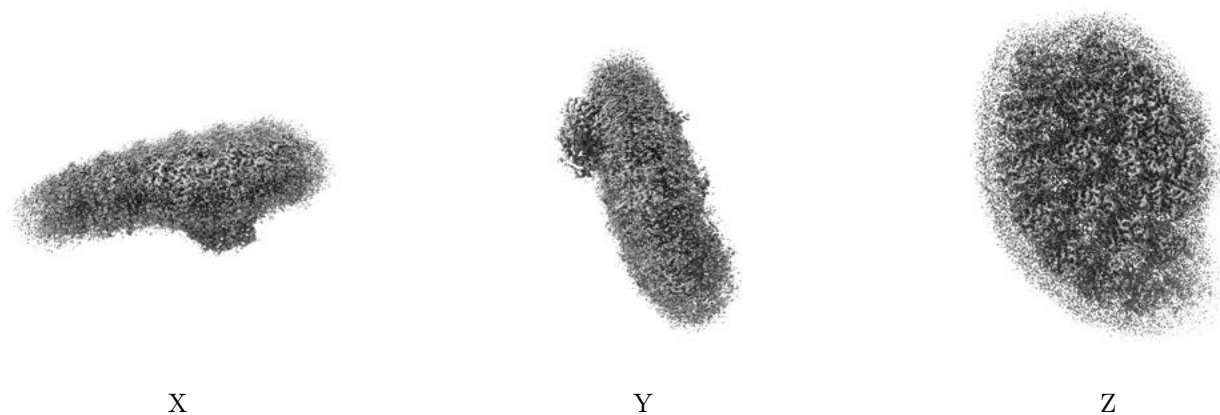


Z

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

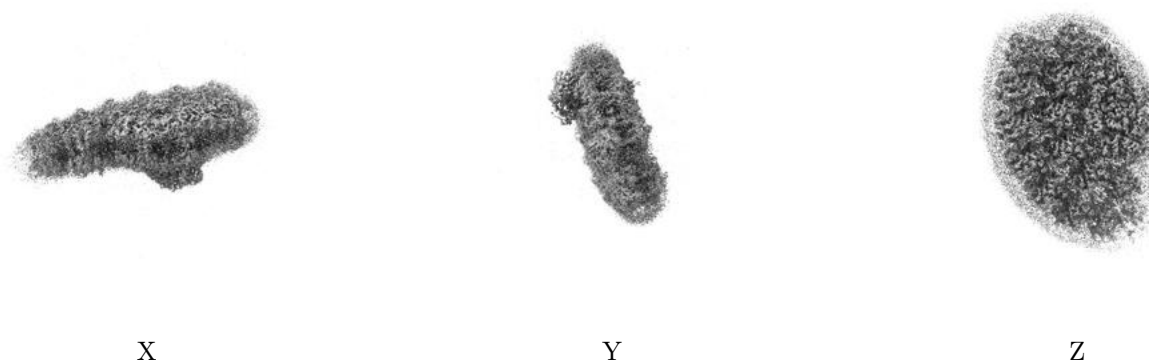
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.023. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

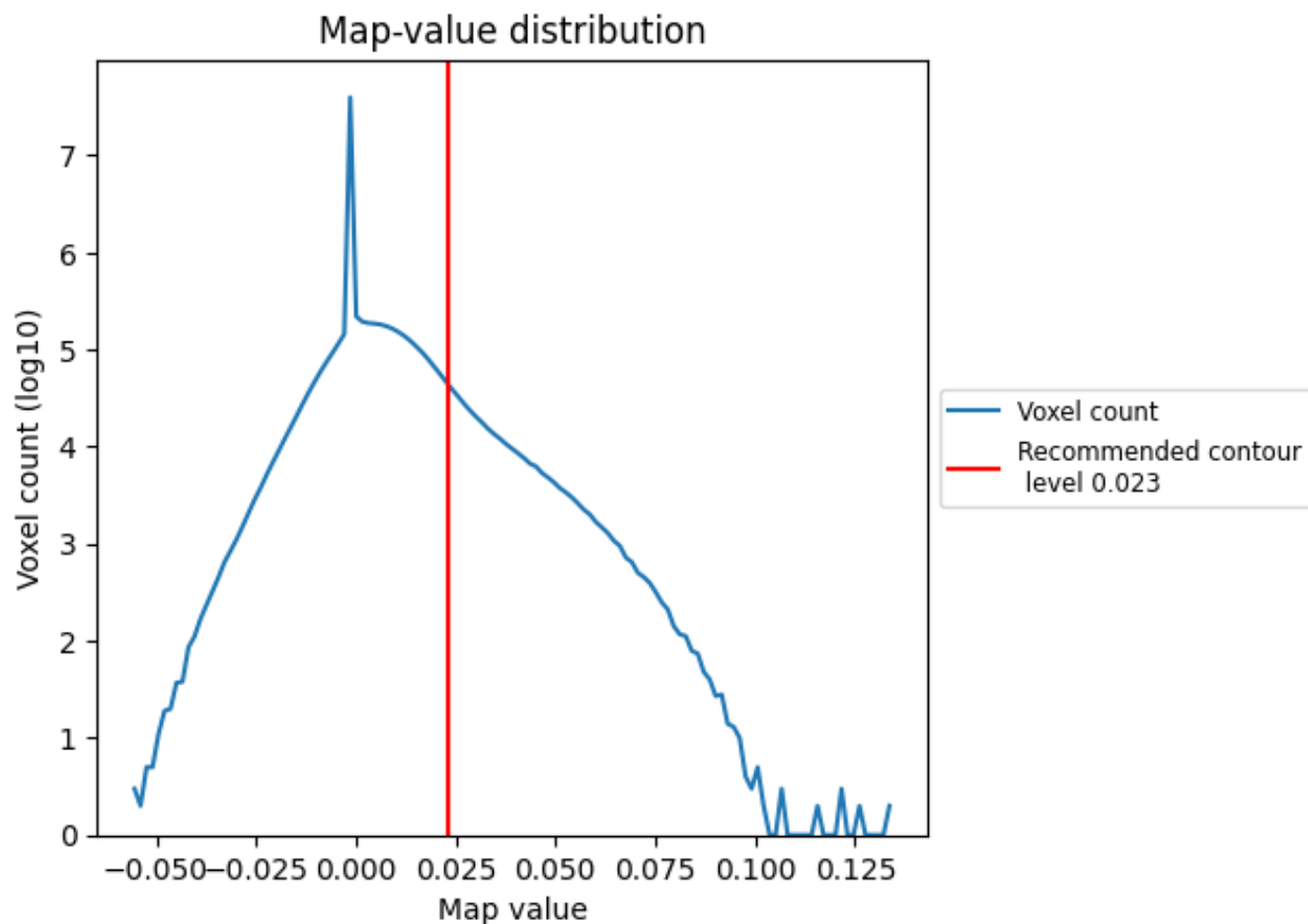
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

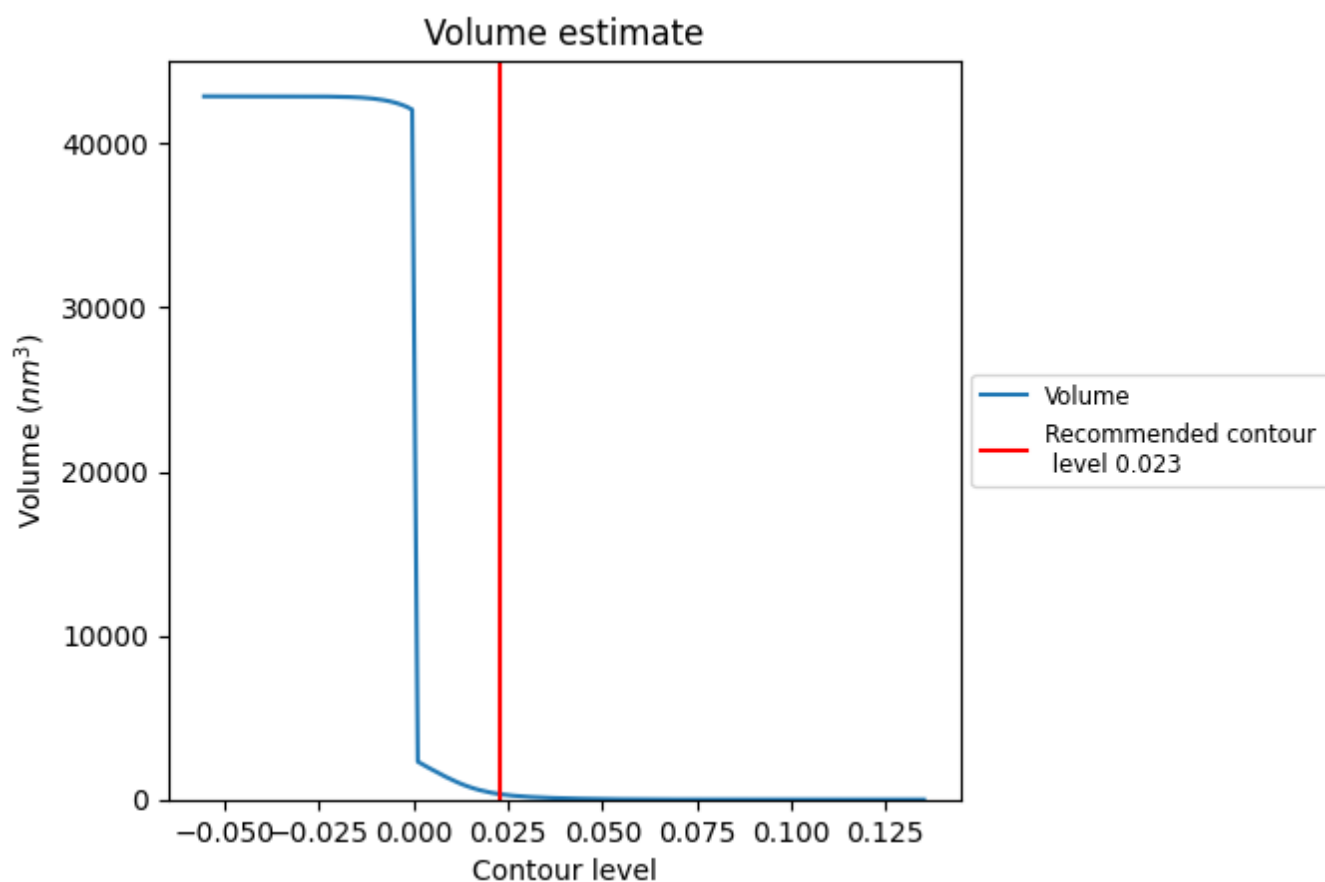
This section contains the results of statistical analysis of the map.

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.

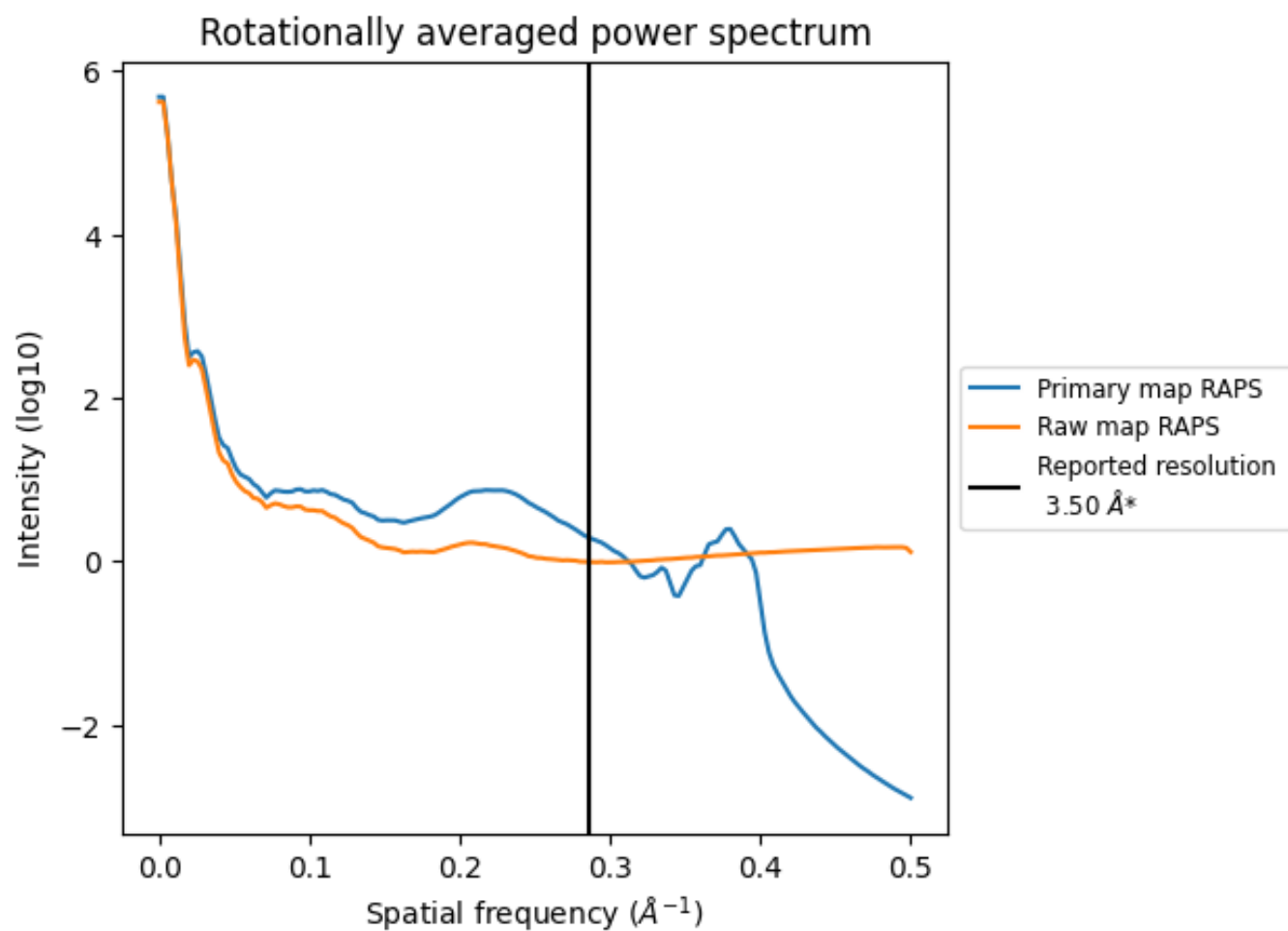
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 329 nm³; this corresponds to an approximate mass of 297 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 ⓘ

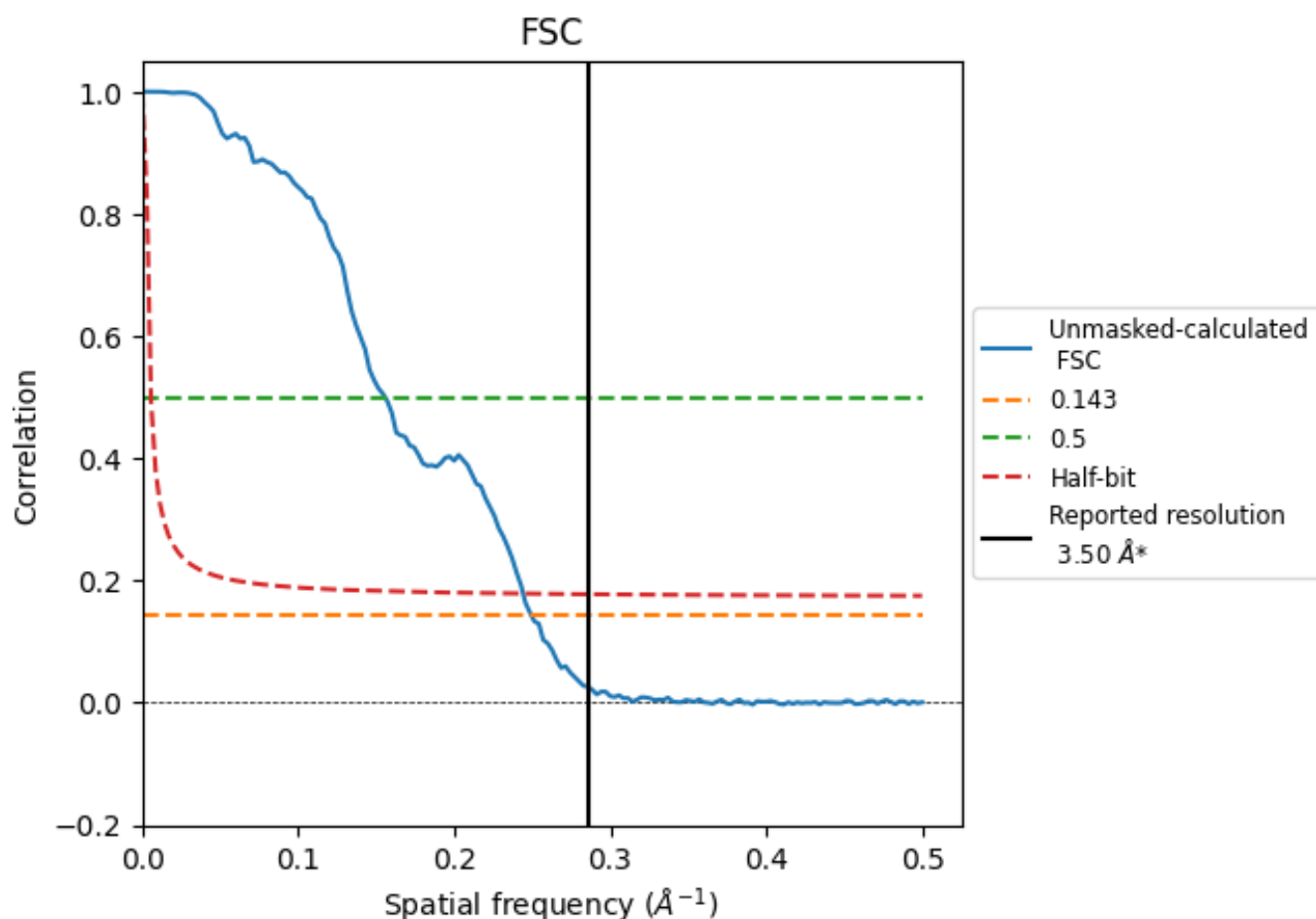


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	6.43	4.10

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.01 differs from the reported value 3.5 by more than 10 %

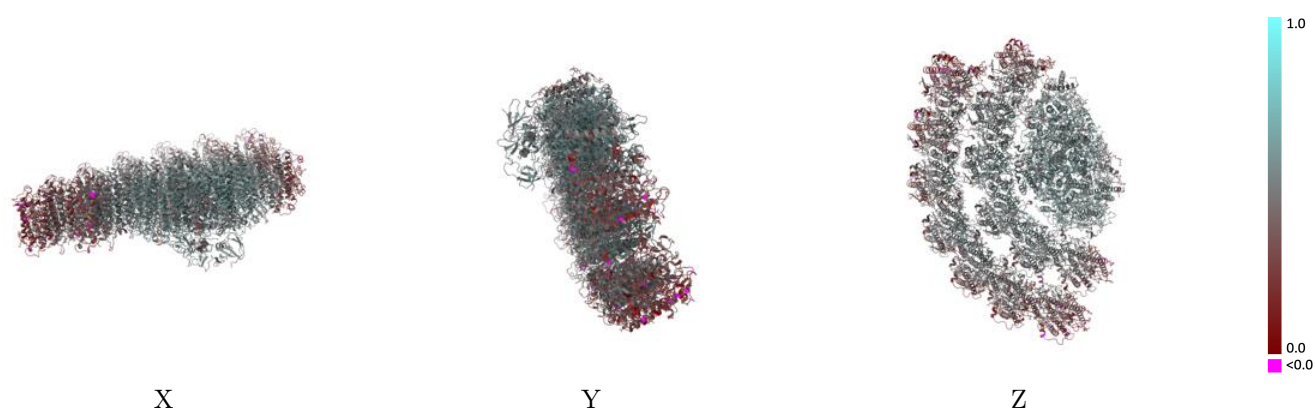
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-63528 and PDB model 9LZK. Per-residue inclusion information can be found in section 3 on page 39.

9.1 Map-model overlay [i](#)

This section was not generated.

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

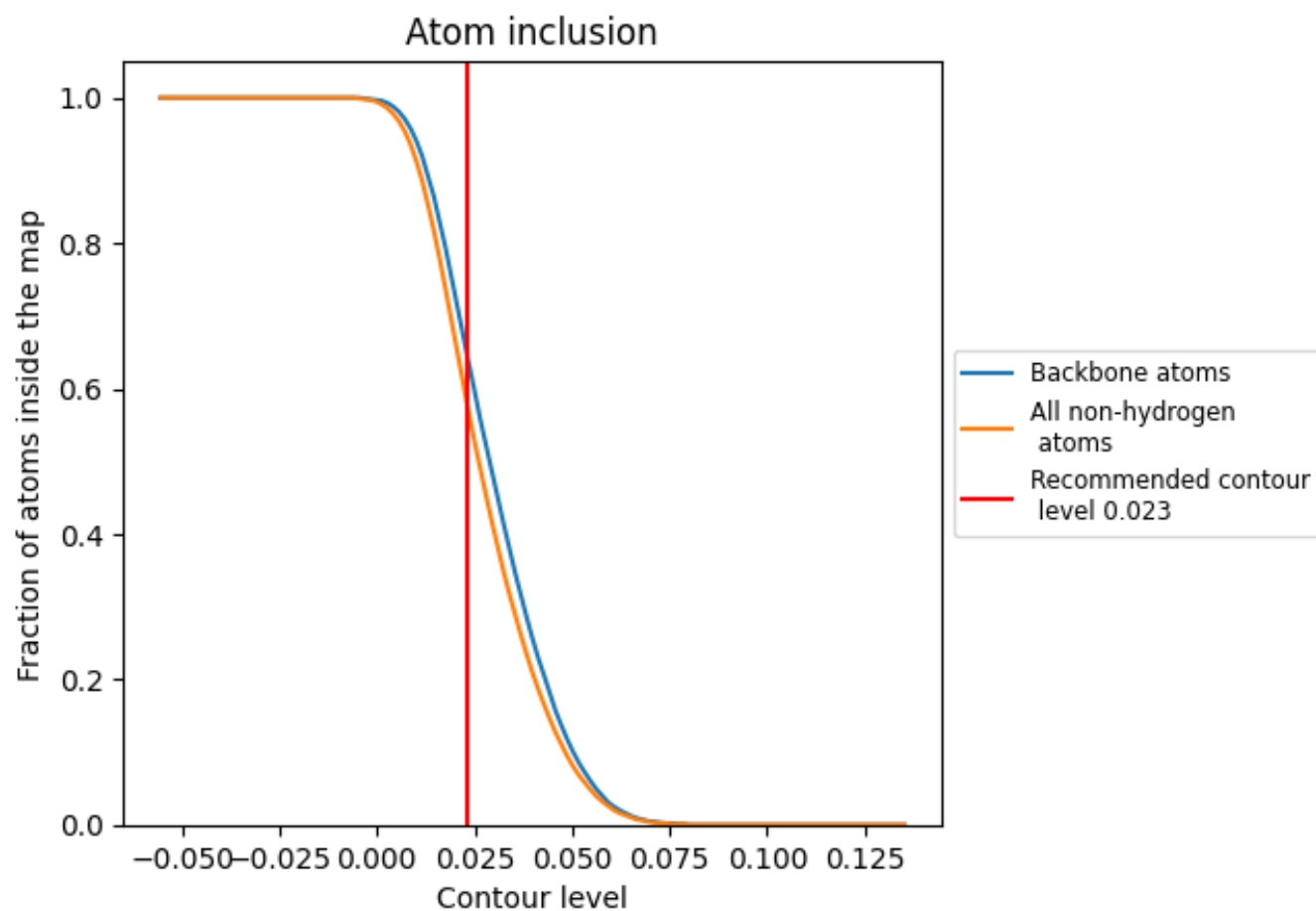


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 58% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5820	 0.4600
1	 0.4000	 0.3510
2	 0.6700	 0.4970
3	 0.7250	 0.5240
4	 0.7170	 0.5220
5	 0.6520	 0.4890
6	 0.4060	 0.3670
A	 0.7710	 0.5600
B	 0.7590	 0.5540
C	 0.7430	 0.5320
D	 0.5880	 0.4880
E	 0.6340	 0.5280
F	 0.7310	 0.5500
I	 0.2230	 0.3910
J	 0.7510	 0.5470
K	 0.5520	 0.4540
M	 0.4910	 0.4560
X	 0.8170	 0.5670
a	 0.3340	 0.3240
b	 0.4870	 0.4040
c	 0.5550	 0.4370
d	 0.5760	 0.4630
e	 0.5000	 0.4230
f	 0.3910	 0.3690
g	 0.2330	 0.2860

