



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 12, 2020 – 02:26 PM EST

PDB ID : 6TCL
EMDB ID: : EMD-10461
Title : Photosystem I tetramer
Authors : Chen, M.; Perez-Boerema, A.; Li, S.; Amunts, A.
Deposited on : 2019-11-06
Resolution : 3.20 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB 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.

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

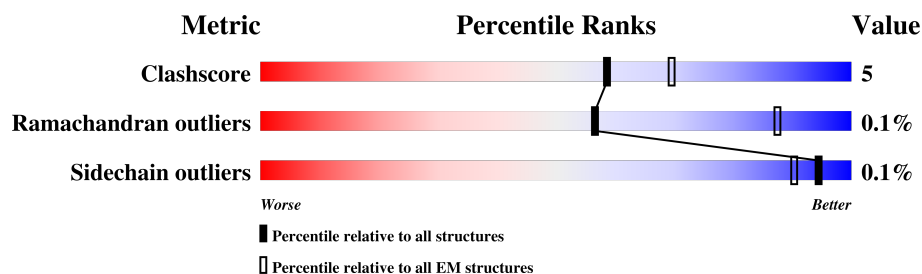
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 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.






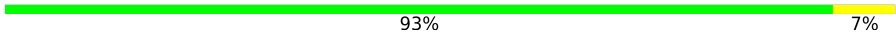
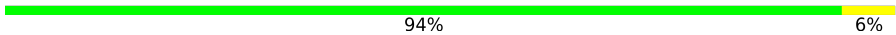

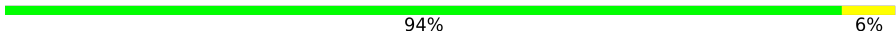






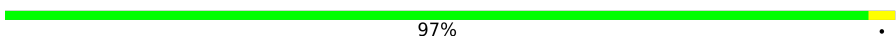
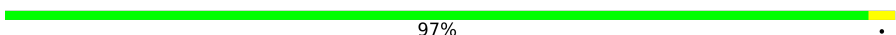





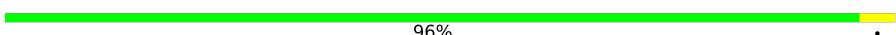



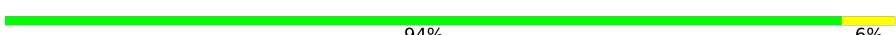
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	740	90% 10%
1	A1	740	89% 11%
1	A2	740	87% 13%
1	AA	740	91% 9%
2	B	739	87% 13%
2	B1	739	86% 14%
2	B2	739	86% 14%
2	BB	739	85% 15%
3	C	80	86% 14%

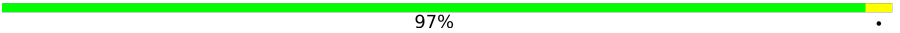
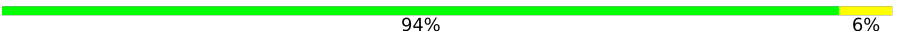



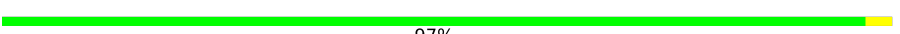








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Mol	Chain	Length	Quality of chain
3	C1	80	 84% 15%
3	C2	80	 88% 11%
3	CC	80	 84% 16%
4	D	134	 93% 7%
4	D1	134	 94% 6%
4	D2	134	 91% 9%
4	DD	134	 94% 6%
5	E1	60	 92% 8%
5	E2	60	 92% 8%
6	F	139	 92% 8%
6	F1	139	 90% 10%
6	FF	139	 88% 12%
7	I	31	 94% 6%
7	I1	31	 97%
7	II	31	 97%
8	J	48	 83% 6% 10%
8	J1	48	 81% 8% 10%
8	J2	48	 79% 10% 10%
8	JJ	48	 77% 13% 10%
9	K	74	 68% 14% 19%
9	K1	74	 96%
9	KK	74	 72% 9% 19%
10	L1	166	 89% 11%
11	M	31	 84% 16%
11	M1	31	 94% 6%

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Mol	Chain	Length	Quality of chain
11	M2	31	 97% .
11	MM	31	 94% 6%
12	X	39	 95% 5%
12	X1	39	 92% 8%
12	X2	39	 90% 10%
12	XX	39	 97% .
13	F2	137	 85% 13% ..
14	I2	33	 94% 6%
15	K2	73	 88% 12%
16	L2	167	 89% 10% .
17	E	63	 90% 10%
17	EE	63	 87% 13%
18	L	154	 95% 5%
18	LL	154	 94% 6%

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
19	CLA	A	801	X	-	-	-
19	CLA	A	804	X	-	-	-
19	CLA	A	805	X	-	-	-
19	CLA	A	806	X	-	-	-
19	CLA	A	807	X	-	-	-
19	CLA	A	808	X	-	-	-
19	CLA	A	809	X	-	-	-
19	CLA	A	810	X	-	-	-
19	CLA	A	811	X	-	-	-
19	CLA	A	812	X	-	-	-
19	CLA	A	813	X	-	-	-
19	CLA	A	814	X	-	-	-
19	CLA	A	815	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A	816	X	-	-	-
19	CLA	A	817	X	-	-	-
19	CLA	A	818	X	-	-	-
19	CLA	A	819	X	-	-	-
19	CLA	A	820	X	-	-	-
19	CLA	A	821	X	-	-	-
19	CLA	A	822	X	-	-	-
19	CLA	A	823	X	-	-	-
19	CLA	A	824	X	-	-	-
19	CLA	A	825	X	-	-	-
19	CLA	A	826	X	-	-	-
19	CLA	A	827	X	-	-	-
19	CLA	A	828	X	-	-	-
19	CLA	A	829	X	-	-	-
19	CLA	A	830	X	-	-	-
19	CLA	A	831	X	-	-	-
19	CLA	A	832	X	-	-	-
19	CLA	A	833	X	-	-	-
19	CLA	A	834	X	-	-	-
19	CLA	A	835	X	-	-	-
19	CLA	A	836	X	-	-	-
19	CLA	A	837	X	-	-	-
19	CLA	A	838	X	-	-	-
19	CLA	A	839	X	-	-	-
19	CLA	A	840	X	-	-	-
19	CLA	A	841	X	-	-	-
19	CLA	A	842	X	-	-	-
19	CLA	A	844	X	-	-	-
19	CLA	A	852	X	-	-	-
19	CLA	A1	801	X	-	-	-
19	CLA	A1	803	X	-	-	-
19	CLA	A1	804	X	-	-	-
19	CLA	A1	805	X	-	-	-
19	CLA	A1	806	X	-	-	-
19	CLA	A1	807	X	-	-	-
19	CLA	A1	808	X	-	-	-
19	CLA	A1	809	X	-	-	-
19	CLA	A1	810	X	-	-	-
19	CLA	A1	811	X	-	-	-
19	CLA	A1	812	X	-	-	-
19	CLA	A1	813	X	-	-	-
19	CLA	A1	814	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A1	815	X	-	-	-
19	CLA	A1	816	X	-	-	-
19	CLA	A1	817	X	-	-	-
19	CLA	A1	818	X	-	-	-
19	CLA	A1	819	X	-	-	-
19	CLA	A1	820	X	-	-	-
19	CLA	A1	821	X	-	-	-
19	CLA	A1	822	X	-	-	-
19	CLA	A1	823	X	-	-	-
19	CLA	A1	824	X	-	-	-
19	CLA	A1	825	X	-	-	-
19	CLA	A1	826	X	-	-	-
19	CLA	A1	827	X	-	-	-
19	CLA	A1	828	X	-	-	-
19	CLA	A1	829	X	-	-	-
19	CLA	A1	830	X	-	-	-
19	CLA	A1	831	X	-	-	-
19	CLA	A1	832	X	-	-	-
19	CLA	A1	833	X	-	-	-
19	CLA	A1	834	X	-	-	-
19	CLA	A1	835	X	-	-	-
19	CLA	A1	836	X	-	-	-
19	CLA	A1	837	X	-	-	-
19	CLA	A1	838	X	-	-	-
19	CLA	A1	839	X	-	-	-
19	CLA	A1	840	X	-	-	-
19	CLA	A1	841	X	-	-	-
19	CLA	A1	842	X	-	-	-
19	CLA	A1	844	X	-	-	-
19	CLA	A1	852	X	-	-	-
19	CLA	A2	801	X	-	-	-
19	CLA	A2	802	X	-	-	-
19	CLA	A2	804	X	-	-	-
19	CLA	A2	805	X	-	-	-
19	CLA	A2	806	X	-	-	-
19	CLA	A2	807	X	-	-	-
19	CLA	A2	808	X	-	-	-
19	CLA	A2	809	X	-	-	-
19	CLA	A2	810	X	-	-	-
19	CLA	A2	811	X	-	-	-
19	CLA	A2	812	X	-	-	-
19	CLA	A2	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	A2	814	X	-	-	-
19	CLA	A2	815	X	-	-	-
19	CLA	A2	816	X	-	-	-
19	CLA	A2	817	X	-	-	-
19	CLA	A2	818	X	-	-	-
19	CLA	A2	819	X	-	-	-
19	CLA	A2	820	X	-	-	-
19	CLA	A2	821	X	-	-	-
19	CLA	A2	822	X	-	-	-
19	CLA	A2	823	X	-	-	-
19	CLA	A2	824	X	-	-	-
19	CLA	A2	825	X	-	-	-
19	CLA	A2	826	X	-	-	-
19	CLA	A2	827	X	-	-	-
19	CLA	A2	828	X	-	-	-
19	CLA	A2	829	X	-	-	-
19	CLA	A2	830	X	-	-	-
19	CLA	A2	831	X	-	-	-
19	CLA	A2	832	X	-	-	-
19	CLA	A2	833	X	-	-	-
19	CLA	A2	834	X	-	-	-
19	CLA	A2	835	X	-	-	-
19	CLA	A2	836	X	-	-	-
19	CLA	A2	837	X	-	-	-
19	CLA	A2	838	X	-	-	-
19	CLA	A2	839	X	-	-	-
19	CLA	A2	840	X	-	-	-
19	CLA	A2	841	X	-	-	-
19	CLA	A2	842	X	-	-	-
19	CLA	A2	844	X	-	-	-
19	CLA	A2	852	X	-	-	-
19	CLA	AA	801	X	-	-	-
19	CLA	AA	804	X	-	-	-
19	CLA	AA	805	X	-	-	-
19	CLA	AA	806	X	-	-	-
19	CLA	AA	807	X	-	-	-
19	CLA	AA	808	X	-	-	-
19	CLA	AA	809	X	-	-	-
19	CLA	AA	810	X	-	-	-
19	CLA	AA	811	X	-	-	-
19	CLA	AA	812	X	-	-	-
19	CLA	AA	813	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	AA	814	X	-	-	-
19	CLA	AA	815	X	-	-	-
19	CLA	AA	816	X	-	-	-
19	CLA	AA	817	X	-	-	-
19	CLA	AA	818	X	-	-	-
19	CLA	AA	819	X	-	-	-
19	CLA	AA	820	X	-	-	-
19	CLA	AA	821	X	-	-	-
19	CLA	AA	822	X	-	-	-
19	CLA	AA	823	X	-	-	-
19	CLA	AA	824	X	-	-	-
19	CLA	AA	825	X	-	-	-
19	CLA	AA	826	X	-	-	-
19	CLA	AA	827	X	-	-	-
19	CLA	AA	828	X	-	-	-
19	CLA	AA	829	X	-	-	-
19	CLA	AA	830	X	-	-	-
19	CLA	AA	831	X	-	-	-
19	CLA	AA	832	X	-	-	-
19	CLA	AA	833	X	-	-	-
19	CLA	AA	834	X	-	-	-
19	CLA	AA	835	X	-	-	-
19	CLA	AA	836	X	-	-	-
19	CLA	AA	837	X	-	-	-
19	CLA	AA	838	X	-	-	-
19	CLA	AA	839	X	-	-	-
19	CLA	AA	840	X	-	-	-
19	CLA	AA	841	X	-	-	-
19	CLA	AA	842	X	-	-	-
19	CLA	AA	843	X	-	-	-
19	CLA	AA	845	X	-	-	-
19	CLA	AA	853	X	-	-	-
19	CLA	B	801	X	-	-	-
19	CLA	B	802	X	-	-	-
19	CLA	B	803	X	-	-	-
19	CLA	B	804	X	-	-	-
19	CLA	B	805	X	-	-	-
19	CLA	B	806	X	-	-	-
19	CLA	B	807	X	-	-	-
19	CLA	B	808	X	-	-	-
19	CLA	B	809	X	-	-	-
19	CLA	B	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B	811	X	-	-	-
19	CLA	B	812	X	-	-	-
19	CLA	B	813	X	-	-	-
19	CLA	B	814	X	-	-	-
19	CLA	B	815	X	-	-	-
19	CLA	B	816	X	-	-	-
19	CLA	B	817	X	-	-	-
19	CLA	B	818	X	-	-	-
19	CLA	B	819	X	-	-	-
19	CLA	B	820	X	-	-	-
19	CLA	B	821	X	-	-	-
19	CLA	B	822	X	-	-	-
19	CLA	B	823	X	-	-	-
19	CLA	B	824	X	-	-	-
19	CLA	B	825	X	-	-	-
19	CLA	B	826	X	-	-	-
19	CLA	B	827	X	-	-	-
19	CLA	B	828	X	-	-	-
19	CLA	B	829	X	-	-	-
19	CLA	B	830	X	-	-	-
19	CLA	B	831	X	-	-	-
19	CLA	B	832	X	-	-	-
19	CLA	B	833	X	-	-	-
19	CLA	B	834	X	-	-	-
19	CLA	B	835	X	-	-	-
19	CLA	B	836	X	-	-	-
19	CLA	B	837	X	-	-	-
19	CLA	B	846	X	-	-	-
19	CLA	B	854	X	-	-	-
19	CLA	B	858	X	-	-	-
19	CLA	B	859	X	-	-	-
19	CLA	B	860	X	-	-	-
19	CLA	B1	801	X	-	-	-
19	CLA	B1	802	X	-	-	-
19	CLA	B1	803	X	-	-	-
19	CLA	B1	804	X	-	-	-
19	CLA	B1	805	X	-	-	-
19	CLA	B1	806	X	-	-	-
19	CLA	B1	807	X	-	-	-
19	CLA	B1	808	X	-	-	-
19	CLA	B1	809	X	-	-	-
19	CLA	B1	810	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B1	811	X	-	-	-
19	CLA	B1	812	X	-	-	-
19	CLA	B1	813	X	-	-	-
19	CLA	B1	814	X	-	-	-
19	CLA	B1	815	X	-	-	-
19	CLA	B1	816	X	-	-	-
19	CLA	B1	817	X	-	-	-
19	CLA	B1	818	X	-	-	-
19	CLA	B1	819	X	-	-	-
19	CLA	B1	820	X	-	-	-
19	CLA	B1	821	X	-	-	-
19	CLA	B1	822	X	-	-	-
19	CLA	B1	823	X	-	-	-
19	CLA	B1	824	X	-	-	-
19	CLA	B1	825	X	-	-	-
19	CLA	B1	826	X	-	-	-
19	CLA	B1	827	X	-	-	-
19	CLA	B1	828	X	-	-	-
19	CLA	B1	829	X	-	-	-
19	CLA	B1	830	X	-	-	-
19	CLA	B1	831	X	-	-	-
19	CLA	B1	832	X	-	-	-
19	CLA	B1	833	X	-	-	-
19	CLA	B1	834	X	-	-	-
19	CLA	B1	835	X	-	-	-
19	CLA	B1	836	X	-	-	-
19	CLA	B1	845	X	-	-	-
19	CLA	B1	848	X	-	-	-
19	CLA	B1	849	X	-	-	-
19	CLA	B1	850	X	-	-	-
19	CLA	B2	801	X	-	-	-
19	CLA	B2	802	X	-	-	-
19	CLA	B2	803	X	-	-	-
19	CLA	B2	804	X	-	-	-
19	CLA	B2	805	X	-	-	-
19	CLA	B2	806	X	-	-	-
19	CLA	B2	807	X	-	-	-
19	CLA	B2	808	X	-	-	-
19	CLA	B2	809	X	-	-	-
19	CLA	B2	810	X	-	-	-
19	CLA	B2	811	X	-	-	-
19	CLA	B2	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	B2	813	X	-	-	-
19	CLA	B2	814	X	-	-	-
19	CLA	B2	815	X	-	-	-
19	CLA	B2	816	X	-	-	-
19	CLA	B2	817	X	-	-	-
19	CLA	B2	818	X	-	-	-
19	CLA	B2	819	X	-	-	-
19	CLA	B2	820	X	-	-	-
19	CLA	B2	821	X	-	-	-
19	CLA	B2	822	X	-	-	-
19	CLA	B2	823	X	-	-	-
19	CLA	B2	824	X	-	-	-
19	CLA	B2	825	X	-	-	-
19	CLA	B2	826	X	-	-	-
19	CLA	B2	827	X	-	-	-
19	CLA	B2	828	X	-	-	-
19	CLA	B2	829	X	-	-	-
19	CLA	B2	830	X	-	-	-
19	CLA	B2	831	X	-	-	-
19	CLA	B2	832	X	-	-	-
19	CLA	B2	833	X	-	-	-
19	CLA	B2	834	X	-	-	-
19	CLA	B2	835	X	-	-	-
19	CLA	B2	836	X	-	-	-
19	CLA	B2	837	X	-	-	-
19	CLA	B2	846	X	-	-	-
19	CLA	B2	849	X	-	-	-
19	CLA	B2	850	X	-	-	-
19	CLA	B2	851	X	-	-	-
19	CLA	B2	852	X	-	-	-
19	CLA	BB	801	X	-	-	-
19	CLA	BB	802	X	-	-	-
19	CLA	BB	803	X	-	-	-
19	CLA	BB	804	X	-	-	-
19	CLA	BB	805	X	-	-	-
19	CLA	BB	806	X	-	-	-
19	CLA	BB	807	X	-	-	-
19	CLA	BB	808	X	-	-	-
19	CLA	BB	809	X	-	-	-
19	CLA	BB	810	X	-	-	-
19	CLA	BB	811	X	-	-	-
19	CLA	BB	812	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	BB	813	X	-	-	-
19	CLA	BB	814	X	-	-	-
19	CLA	BB	815	X	-	-	-
19	CLA	BB	816	X	-	-	-
19	CLA	BB	817	X	-	-	-
19	CLA	BB	818	X	-	-	-
19	CLA	BB	819	X	-	-	-
19	CLA	BB	820	X	-	-	-
19	CLA	BB	821	X	-	-	-
19	CLA	BB	822	X	-	-	-
19	CLA	BB	823	X	-	-	-
19	CLA	BB	824	X	-	-	-
19	CLA	BB	825	X	-	-	-
19	CLA	BB	826	X	-	-	-
19	CLA	BB	827	X	-	-	-
19	CLA	BB	828	X	-	-	-
19	CLA	BB	829	X	-	-	-
19	CLA	BB	830	X	-	-	-
19	CLA	BB	831	X	-	-	-
19	CLA	BB	832	X	-	-	-
19	CLA	BB	833	X	-	-	-
19	CLA	BB	834	X	-	-	-
19	CLA	BB	835	X	-	-	-
19	CLA	BB	836	X	-	-	-
19	CLA	BB	845	X	-	-	-
19	CLA	BB	852	X	-	-	-
19	CLA	BB	855	X	-	-	-
19	CLA	BB	856	X	-	-	-
19	CLA	F	301	X	-	-	-
19	CLA	F	302	X	-	-	-
19	CLA	F1	301	X	-	-	-
19	CLA	F1	302	X	-	-	-
19	CLA	F1	305	X	-	-	-
19	CLA	F2	301	X	-	-	-
19	CLA	F2	302	X	-	-	-
19	CLA	FF	301	X	-	-	-
19	CLA	FF	302	X	-	-	-
19	CLA	FF	305	X	-	-	-
19	CLA	J	101	X	-	-	-
19	CLA	J	103	X	-	-	-
19	CLA	J1	101	X	-	-	-
19	CLA	J1	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
19	CLA	J2	101	X	-	-	-
19	CLA	J2	103	X	-	-	-
19	CLA	JJ	101	X	-	-	-
19	CLA	JJ	103	X	-	-	-
19	CLA	K	101	X	-	-	-
19	CLA	K	102	X	-	-	-
19	CLA	K1	102	X	-	-	-
19	CLA	K1	103	X	-	-	-
19	CLA	K1	105	X	-	-	-
19	CLA	K2	102	X	-	-	-
19	CLA	K2	104	X	-	-	-
19	CLA	KK	101	X	-	-	-
19	CLA	KK	102	X	-	-	-
19	CLA	L	202	X	-	-	-
19	CLA	L	203	X	-	-	-
19	CLA	L	204	X	-	-	-
19	CLA	L1	205	X	-	-	-
19	CLA	L1	206	X	-	-	-
19	CLA	L1	207	X	-	-	-
19	CLA	L2	204	X	-	-	-
19	CLA	L2	205	X	-	-	-
19	CLA	L2	206	X	-	-	-
19	CLA	LL	201	X	-	-	-
19	CLA	LL	202	X	-	-	-
19	CLA	LL	203	X	-	-	-
19	CLA	X	101	X	-	-	-
19	CLA	X1	101	X	-	-	-
19	CLA	X2	101	X	-	-	-
19	CLA	XX	101	X	-	-	-
20	CL0	A	803	X	-	-	-
20	CL0	A1	802	X	-	-	-
20	CL0	A2	803	X	-	-	-
20	CL0	AA	803	X	-	-	-
24	AJP	A	802	X	-	-	-
24	AJP	AA	802	X	-	-	-
24	AJP	B	849	X	-	-	-
24	AJP	B	850	X	-	-	-
24	AJP	BB	848	X	-	-	-
24	AJP	BB	849	X	-	-	-
24	AJP	I2	104	X	-	-	-
24	AJP	K	104	X	-	-	-
24	AJP	KK	104	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	AJP	L	208	X	-	-	-
24	AJP	L	209	X	-	-	-
24	AJP	L1	203	X	-	-	-
24	AJP	L1	204	X	-	-	-
24	AJP	L2	202	X	-	-	-
24	AJP	L2	203	X	-	-	-
24	AJP	M2	101	X	-	-	-

2 Entry composition

There are 28 unique types of molecules in this entry. The entry contains 199181 atoms, of which 99577 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A1	740	Total	C	H	N	O	S	0	0
			11478	3809	5672	1000	976	21		
1	A2	740	Total	C	H	N	O	S	0	0
			11486	3809	5680	1000	976	21		
1	A	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		
1	AA	740	Total	C	H	N	O	S	0	0
			11483	3809	5677	1000	976	21		

- Molecule 2 is a protein called Photosystem I P700 chlorophyll a apoprotein A2 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B1	739	Total	C	H	N	O	S	0	0
			11579	3905	5660	990	1006	18		
2	B2	739	Total	C	H	N	O	S	0	0
			11581	3905	5662	990	1006	18		
2	B	739	Total	C	H	N	O	S	0	0
			11586	3905	5667	990	1006	18		
2	BB	739	Total	C	H	N	O	S	0	0
			11595	3905	5676	990	1006	18		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
3	C1	80	Total	C	H	N	O	S	0	0
			1183	367	584	103	118	11		
3	C2	80	Total	C	H	N	O	S	0	0
			1179	367	580	103	118	11		
3	C	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		
3	CC	80	Total	C	H	N	O	S	0	0
			1181	367	582	103	118	11		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
4	D1	134	Total	C	H	N	O	S	0	0
			2073	664	1037	178	193	1		
4	D2	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	D	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		
4	DD	134	Total	C	H	N	O	S	0	0
			2078	664	1042	178	193	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E1	60	Total	C	H	N	O	0	0
			958	308	477	83	90		
5	E2	60	Total	C	H	N	O	0	0
			958	308	477	83	90		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
6	F1	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		
6	F	139	Total	C	H	N	O	S	0	0
			2111	678	1051	179	201	2		
6	FF	139	Total	C	H	N	O	S	0	0
			2112	678	1052	179	201	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I1	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	I	31	Total	C	H	N	O	0	0
			508	177	255	35	41		
7	II	31	Total	C	H	N	O	0	0
			508	177	255	35	41		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	J1	43	Total	C	H	N	O	0	0
			701	237	355	52	57		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	J2	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	J	43	Total	C	H	N	O	0	0
			701	237	355	52	57		
8	JJ	43	Total	C	H	N	O	0	0
			700	237	354	52	57		

- Molecule 9 is a protein called Photosystem I reaction center subunit PsaK 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
9	K1	74	Total	C	H	N	O	S	0	0
			1091	356	555	87	92	1		
9	K	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		
9	KK	60	Total	C	H	N	O	S	0	0
			900	289	461	72	77	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace	
10	L1	166	Total	C	H	N	O	S	0	0
			2483	810	1239	213	220	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	M1	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M2	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	M	31	Total	C	H	N	O	0	0
			496	160	256	37	43		
11	MM	31	Total	C	H	N	O	0	0
			496	160	256	37	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	X1	39	Total	C	H	N	O	0	0
			627	212	318	49	48		
12	X2	39	Total	C	H	N	O	0	0
			627	212	318	49	48		

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Mol	Chain	Residues	Atoms					AltConf	Trace
12	X	39	Total	C	H	N	O	0	0
			628	212	319	49	48		
12	XX	39	Total	C	H	N	O	0	0
			628	212	319	49	48		

- Molecule 13 is a protein called Photosystem I reaction center subunit III.

Mol	Chain	Residues	Atoms						AltConf	Trace
13	F2	137	Total	C	H	N	O	S	0	0
			2087	670	1040	177	198	2		

- Molecule 14 is a protein called Photosystem I reaction center subunit VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	I2	33	Total	C	H	N	O	0	0
			536	186	268	37	45		

- Molecule 15 is a protein called Photosystem I reaction center subunit Psak 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
15	K2	73	Total	C	H	N	O	S	0	0
			1081	353	550	86	91	1		

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

Mol	Chain	Residues	Atoms						AltConf	Trace
16	L2	167	Total	C	H	N	O	S	0	0
			2498	815	1245	215	222	1		

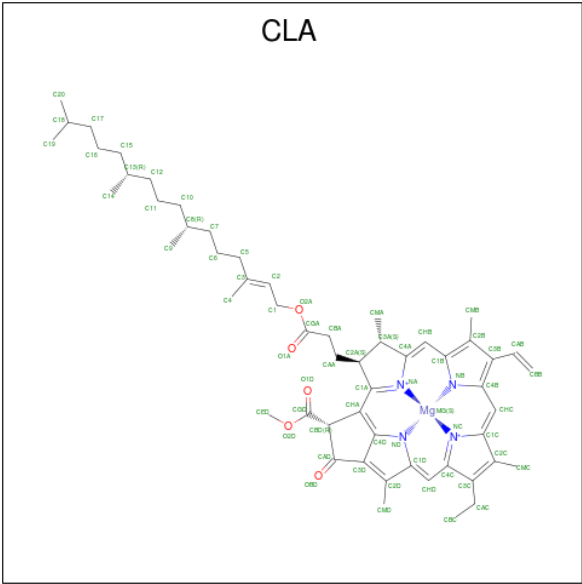
- Molecule 17 is a protein called Photosystem I reaction center subunit IV.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	E	63	Total	C	H	N	O	0	0
			994	321	492	86	95		
17	EE	63	Total	C	H	N	O	0	0
			994	321	492	86	95		

- Molecule 18 is a protein called Photosystem I reaction center subunit XI.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	L	154	Total	C	H	N	O	S	0	0
			2309	758	1153	196	201	1		
18	LL	154	Total	C	H	N	O	S	0	0
			2310	758	1154	196	201	1		

- Molecule 19 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	A1	1	Total	C	H	Mg	N	O	0
			4655	1974	2261	43	172	205	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	

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Mol	Chain	Residues	Atoms						AltConf
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	B1	1	Total	C	H	Mg	N	O	0
			4544	1905	2253	40	160	186	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	F1	1	Total	C	H	Mg	N	O	0
			269	119	122	3	12	13	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	J1	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	K1	1	Total	C	H	Mg	N	O	0
			223	103	92	3	12	13	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	
19	L1	1	Total	C	H	Mg	N	O	0
			393	161	202	3	12	15	

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Mol	Chain	Residues	Atoms						AltConf
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	
19	A2	1	Total	C	H	Mg	N	O	0
			4602	1955	2227	43	172	205	

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Mol	Chain	Residues	Atoms						AltConf
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	B2	1	Total	C	H	Mg	N	O	0
			4759	1995	2358	42	168	196	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	F2	1	Total	C	H	Mg	N	O	0
			191	84	89	2	8	8	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	J2	1	Total	C	H	Mg	N	O	0
			140	66	58	2	8	6	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	K2	1	Total	C	H	Mg	N	O	0
			147	68	61	2	8	8	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	L2	1	Total	C	H	Mg	N	O	0
			373	156	187	3	12	15	
19	X2	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	
19	A	1	Total	C	H	Mg	N	O	0
			4546	1927	2207	42	168	202	

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0

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Mol	Chain	Residues	Atoms						AltConf
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	A	1	Total 4546	C 1927	H 2207	Mg 42	N 168	O 202	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	
19	B	1	Total	C	H	Mg	N	O	0
			4758	1995	2357	42	168	196	

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Mol	Chain	Residues	Atoms						AltConf
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	B	1	Total 4758	C 1995	H 2357	Mg 42	N 168	O 196	0
19	F	1	Total 191	C 84	H 89	Mg 2	N 8	O 8	0
19	F	1	Total 191	C 84	H 89	Mg 2	N 8	O 8	0
19	J	1	Total 140	C 66	H 58	Mg 2	N 8	O 6	0
19	J	1	Total 140	C 66	H 58	Mg 2	N 8	O 6	0
19	K	1	Total 156	C 71	H 65	Mg 2	N 8	O 10	0
19	K	1	Total 156	C 71	H 65	Mg 2	N 8	O 10	0
19	L	1	Total 389	C 161	H 198	Mg 3	N 12	O 15	0
19	L	1	Total 389	C 161	H 198	Mg 3	N 12	O 15	0
19	L	1	Total 389	C 161	H 198	Mg 3	N 12	O 15	0

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0

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Mol	Chain	Residues	Atoms						AltConf
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	AA	1	Total 4683	C 1982	H 2279	Mg 43	N 172	O 207	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0
19	BB	1	Total 4490	C 1885	H 2219	Mg 40	N 160	O 186	0

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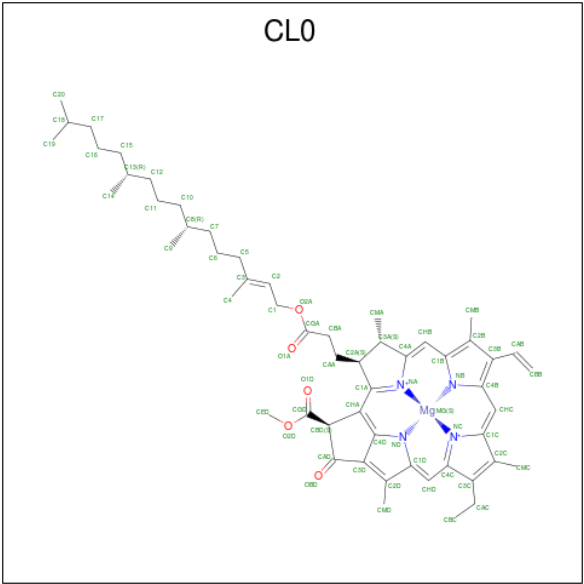
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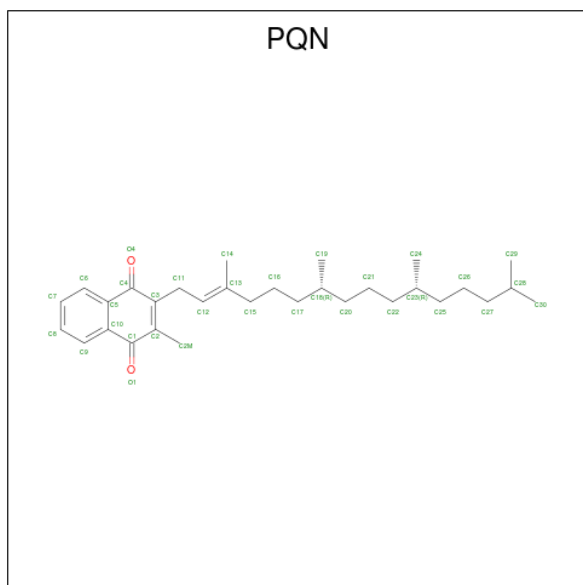
Mol	Chain	Residues	Atoms						AltConf
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	FF	1	Total	C	H	Mg	N	O	0
			328	139	161	3	12	13	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	JJ	1	Total	C	H	Mg	N	O	0
			139	66	57	2	8	6	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	KK	1	Total	C	H	Mg	N	O	0
			156	71	65	2	8	10	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	LL	1	Total	C	H	Mg	N	O	0
			323	140	155	3	12	13	
19	XX	1	Total	C	H	Mg	N	O	0
			77	35	32	1	4	5	

- Molecule 20 is CHLOROPHYLL A ISOMER (three-letter code: CL0) (formula: C₅₅H₇₂MgN₄O₅).



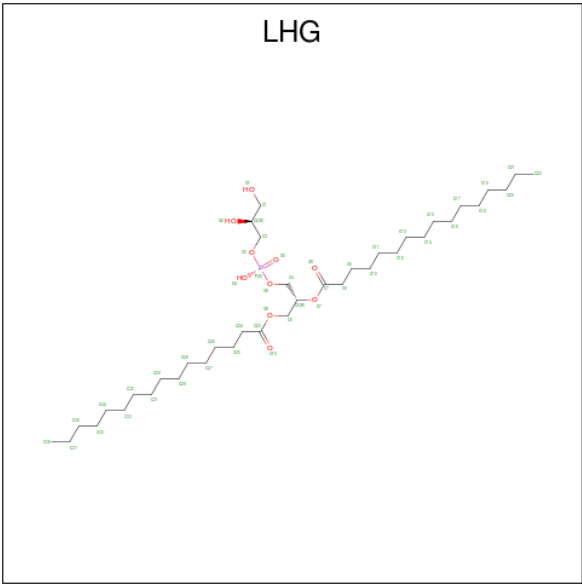
Mol	Chain	Residues	Atoms						AltConf
20	A1	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A2	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	A	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	
20	AA	1	Total	C	H	Mg	N	O	0
			137	55	72	1	4	5	

- Molecule 21 is PHYLLOQUINONE (three-letter code: PQN) (formula: $C_{31}H_{46}O_2$).



Mol	Chain	Residues	Atoms				AltConf
21	A1	1	Total	C	H	O	0
			79	31	46	2	
21	B1	1	Total	C	H	O	0
			79	31	46	2	
21	A2	1	Total	C	H	O	0
			79	31	46	2	
21	B2	1	Total	C	H	O	0
			79	31	46	2	
21	A	1	Total	C	H	O	0
			79	31	46	2	
21	B	1	Total	C	H	O	0
			79	31	46	2	
21	AA	1	Total	C	H	O	0
			79	31	46	2	
21	BB	1	Total	C	H	O	0
			79	31	46	2	

- Molecule 22 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P) (labeled as "Ligand of Interest" by author).



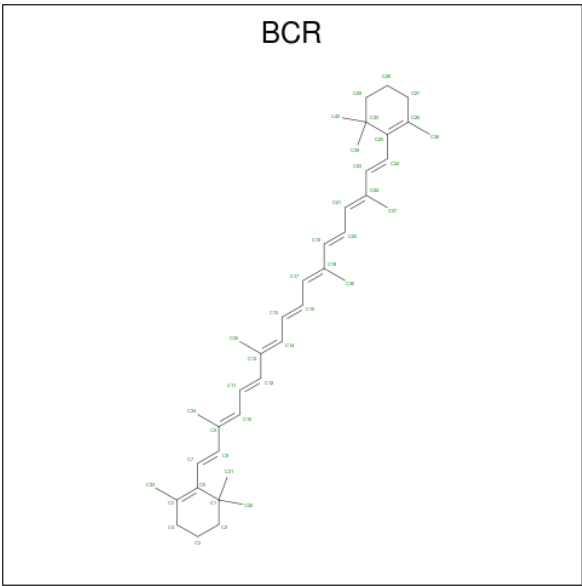
Mol	Chain	Residues	Atoms					AltConf
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A1	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B1	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L1	1	Total	C	H	O	P	0
			68	22	35	10	1	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X1	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A2	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B2	1	Total	C	H	O	P	0
			69	22	36	10	1	
22	L2	1	Total	C	H	O	P	0
			74	24	39	10	1	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	
22	X2	1	Total	C	H	O	P	0
			212	67	123	20	2	

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Mol	Chain	Residues	Atoms					AltConf
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	A	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	B	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	L	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	X	1	Total	C	H	O	P	0
			89	29	49	10	1	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	AA	1	Total	C	H	O	P	0
			209	65	122	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	BB	1	Total	C	H	O	P	0
			192	60	110	20	2	
22	LL	1	Total	C	H	O	P	0
			76	23	42	10	1	
22	XX	1	Total	C	H	O	P	0
			89	29	49	10	1	

- Molecule 23 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).



Mol	Chain	Residues	Atoms			AltConf
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	A1	1	Total	C	H	0
			572	239	333	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	B1	1	Total	C	H	0
			480	200	280	
23	F1	1	Total	C	H	0
			283	120	163	
23	F1	1	Total	C	H	0
			283	120	163	
23	F1	1	Total	C	H	0
			283	120	163	
23	I1	1	Total	C	H	0
			96	40	56	
23	J1	1	Total	C	H	0
			192	80	112	
23	J1	1	Total	C	H	0
			192	80	112	
23	K1	1	Total	C	H	0
			192	80	112	
23	K1	1	Total	C	H	0
			192	80	112	
23	L1	1	Total	C	H	0
			288	120	168	
23	L1	1	Total	C	H	0
			288	120	168	
23	L1	1	Total	C	H	0
			288	120	168	

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Mol	Chain	Residues	Atoms			AltConf
			Total	C	H	
23	M1	1	96	40	56	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	A2	1	572	239	333	0
23	B2	1	475	200	275	0
23	B2	1	475	200	275	0
23	B2	1	475	200	275	0
23	B2	1	475	200	275	0
23	B2	1	475	200	275	0
23	B2	1	475	200	275	0
23	F2	1	283	120	163	0
23	F2	1	283	120	163	0
23	F2	1	283	120	163	0
23	I2	1	288	120	168	0
23	I2	1	288	120	168	0
23	I2	1	288	120	168	0
23	J2	1	192	80	112	0
23	J2	1	192	80	112	0
23	K2	1	192	80	112	0

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Mol	Chain	Residues	Atoms			AltConf
23	K2	1	Total	C	H	0
			192	80	112	
23	L2	1	Total	C	H	0
			96	40	56	
23	M2	1	Total	C	H	0
			96	40	56	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	A	1	Total	C	H	0
			668	279	389	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	B	1	Total	C	H	0
			576	240	336	
23	F	1	Total	C	H	0
			283	120	163	
23	F	1	Total	C	H	0
			283	120	163	
23	F	1	Total	C	H	0
			283	120	163	
23	I	1	Total	C	H	0
			192	80	112	
23	I	1	Total	C	H	0
			192	80	112	

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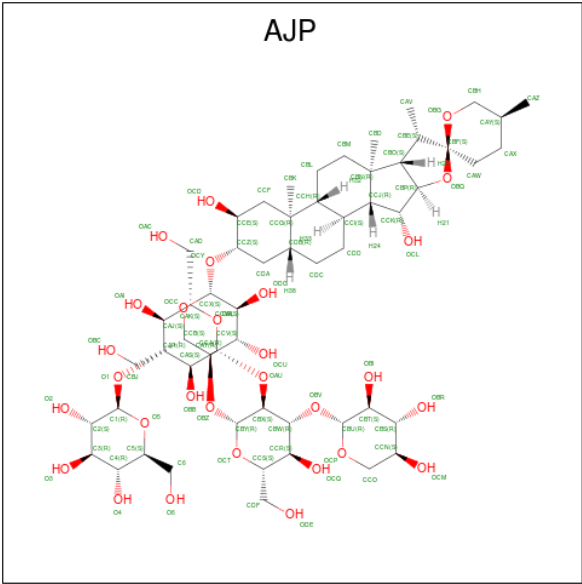
Mol	Chain	Residues	Atoms			AltConf
23	J	1	Total	C	H	0
			192	80	112	
23	J	1	Total	C	H	0
			192	80	112	
23	K	1	Total	C	H	0
			96	40	56	
23	L	1	Total	C	H	0
			192	80	112	
23	L	1	Total	C	H	0
			192	80	112	
23	M	1	Total	C	H	0
			91	40	51	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	AA	1	Total	C	H	0
			668	279	389	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	BB	1	Total	C	H	0
			576	240	336	
23	FF	1	Total	C	H	0
			283	120	163	
23	FF	1	Total	C	H	0
			283	120	163	

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Mol	Chain	Residues	Atoms			AltConf
23	FF	1	Total	C	H	0
			283	120	163	
23	II	1	Total	C	H	0
			288	120	168	
23	II	1	Total	C	H	0
			288	120	168	
23	II	1	Total	C	H	0
			288	120	168	
23	JJ	1	Total	C	H	0
			192	80	112	
23	JJ	1	Total	C	H	0
			192	80	112	
23	KK	1	Total	C	H	0
			96	40	56	
23	LL	1	Total	C	H	0
			96	40	56	
23	MM	1	Total	C	H	0
			93	40	53	

- Molecule 24 is Digitonin (three-letter code: AJP) (formula: C₅₆H₉₂O₂₉).



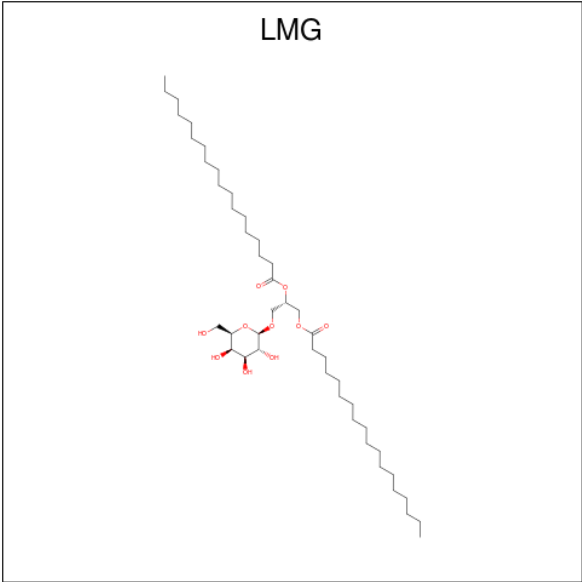
Mol	Chain	Residues	Atoms				AltConf
24	A1	1	Total	C	H	O	0
			171	60	96	15	
24	A1	1	Total	C	H	O	0
			171	60	96	15	

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Mol	Chain	Residues	Atoms				AltConf
24	L1	1	Total	C	H	O	0
			192	66	106	20	
24	L1	1	Total	C	H	O	0
			192	66	106	20	
24	A2	1	Total	C	H	O	0
			75	27	43	5	
24	I2	1	Total	C	H	O	0
			73	27	42	4	
24	L2	1	Total	C	H	O	0
			192	66	106	20	
24	L2	1	Total	C	H	O	0
			192	66	106	20	
24	M2	1	Total	C	H	O	0
			74	27	43	4	
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	A	1	Total	C	H	O	0
			153	56	88	9	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	B	1	Total	C	H	O	0
			288	99	159	30	
24	K	1	Total	C	H	O	0
			91	32	50	9	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	L	1	Total	C	H	O	0
			147	54	85	8	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	AA	1	Total	C	H	O	0
			153	56	88	9	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	BB	1	Total	C	H	O	0
			192	66	106	20	
24	KK	1	Total	C	H	O	0
			91	32	50	9	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀) (labeled as "Ligand of Interest" by author).



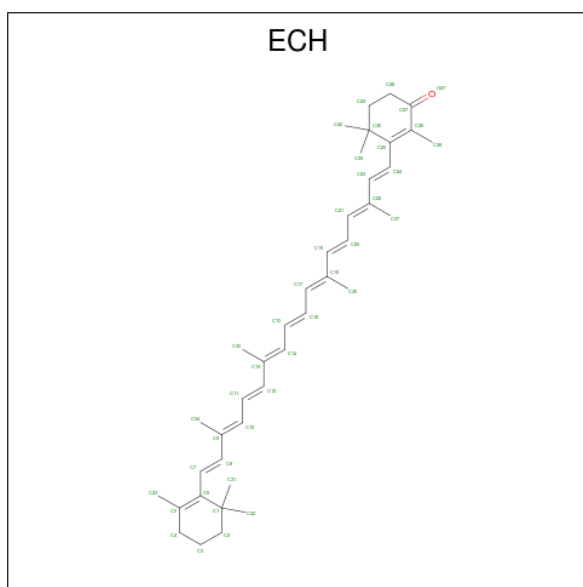
Mol	Chain	Residues	Atoms				AltConf
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	A1	1	Total	C	H	O	1
			152	48	84	20	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	B1	1	Total	C	H	O	0
			265	87	148	30	
25	I1	1	Total	C	H	O	0
			75	25	40	10	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	K1	1	Total	C	H	O	1
			120	38	62	20	
25	L1	1	Total	C	H	O	1
			223	71	132	20	
25	L1	1	Total	C	H	O	0
			223	71	132	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	A2	1	Total	C	H	O	1
			171	54	97	20	
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	B2	1	Total	C	H	O	0
			265	87	148	30	

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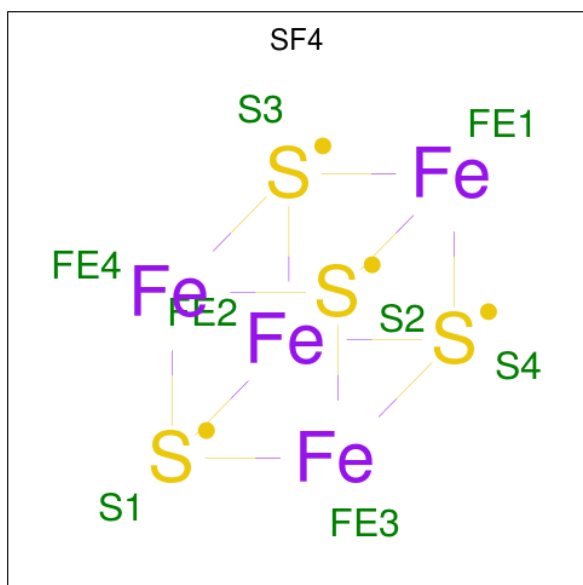
Mol	Chain	Residues	Atoms				AltConf
25	B2	1	Total	C	H	O	0
			265	87	148	30	
25	I2	1	Total	C	H	O	0
			75	25	40	10	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	K2	1	Total	C	H	O	1
			114	36	58	20	
25	L2	1	Total	C	H	O	1
			82	26	46	10	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	B	1	Total	C	H	O	0
			427	136	251	40	
25	B	1	Total	C	H	O	1
			427	136	251	40	
25	L	1	Total	C	H	O	1
			85	27	48	10	
25	M	1	Total	C	H	O	0
			105	36	59	10	
25	BB	1	Total	C	H	O	0
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	BB	1	Total	C	H	O	1
			289	92	167	30	
25	II	1	Total	C	H	O	1
			181	59	102	20	
25	II	1	Total	C	H	O	0
			181	59	102	20	

- Molecule 26 is beta,beta-caroten-4-one (three-letter code: ECH) (formula: $C_{40}H_{54}O$).



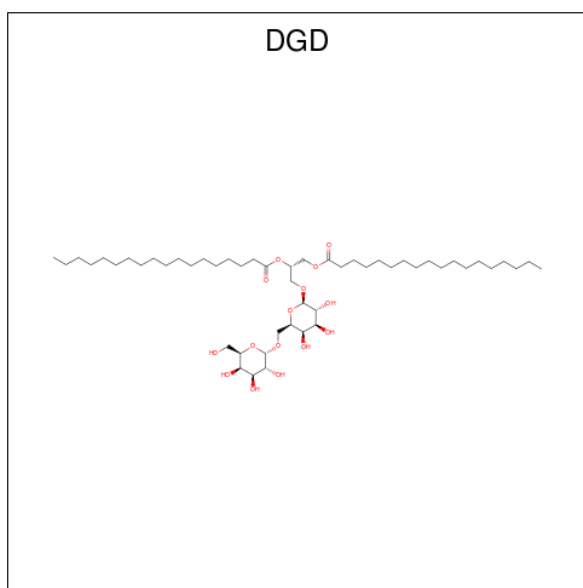
Mol	Chain	Residues	Atoms				AltConf
26	B1	1	Total	C	H	O	0
			95	40	54	1	
26	B2	1	Total	C	H	O	0
			95	40	54	1	
26	B	1	Total	C	H	O	0
			95	40	54	1	
26	BB	1	Total	C	H	O	0
			95	40	54	1	

- Molecule 27 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
27	B1	1	Total	Fe	S	0
			8	4	4	
27	C1	1	Total	Fe	S	0
			16	8	8	
27	C1	1	Total	Fe	S	0
			16	8	8	
27	B2	1	Total	Fe	S	0
			8	4	4	
27	C2	1	Total	Fe	S	0
			16	8	8	
27	C2	1	Total	Fe	S	0
			16	8	8	
27	B	1	Total	Fe	S	0
			8	4	4	
27	C	1	Total	Fe	S	0
			16	8	8	
27	C	1	Total	Fe	S	0
			16	8	8	
27	BB	1	Total	Fe	S	0
			8	4	4	
27	CC	1	Total	Fe	S	0
			16	8	8	
27	CC	1	Total	Fe	S	0
			16	8	8	

- Molecule 28 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$) (labeled as "Ligand of Interest" by author).

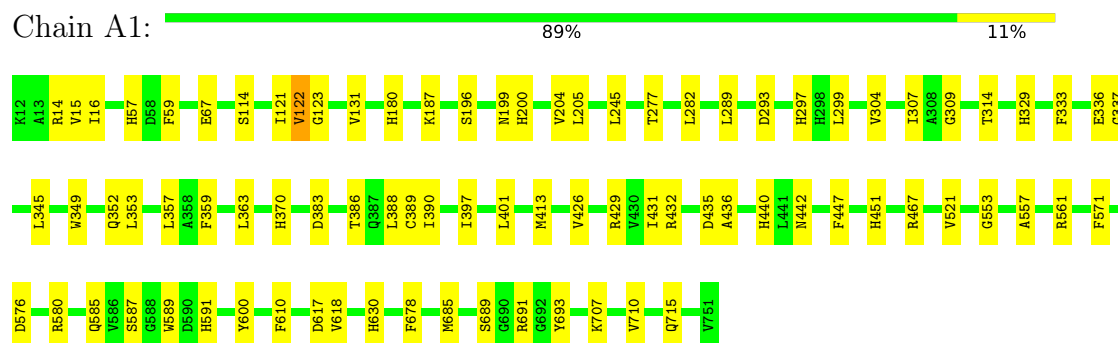


Mol	Chain	Residues	Atoms				AltConf
28	B	1	Total	C	H	O	0
			88	27	46	15	
28	BB	1	Total	C	H	O	0
			88	27	46	15	

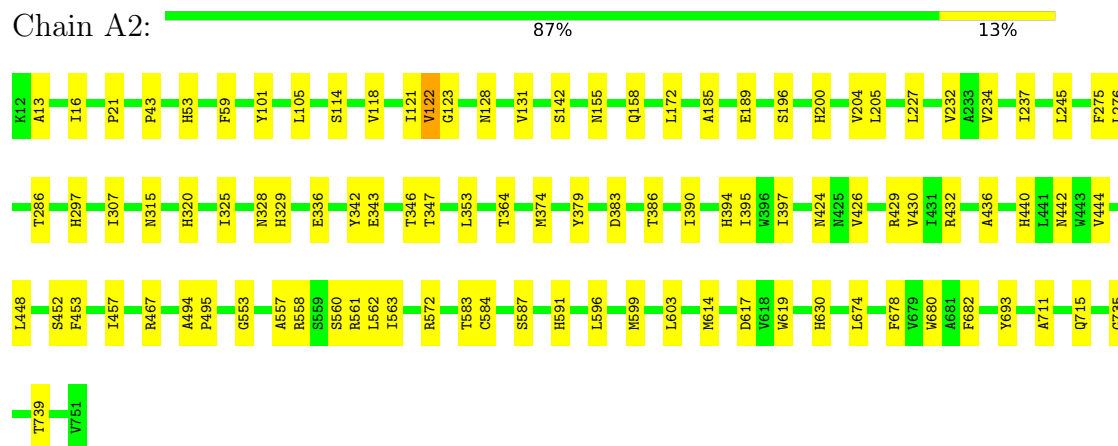
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

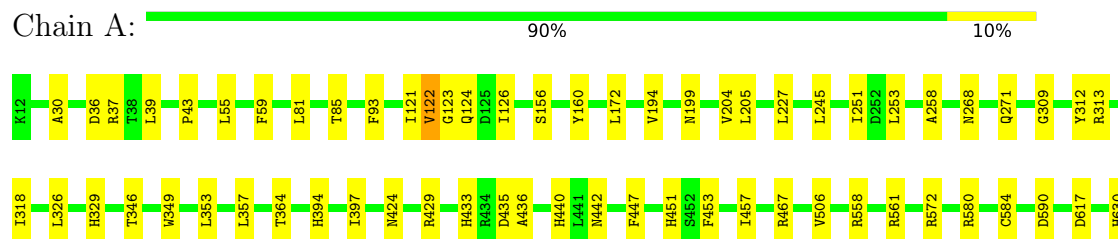
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

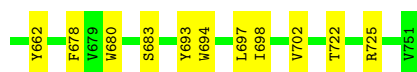


- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1



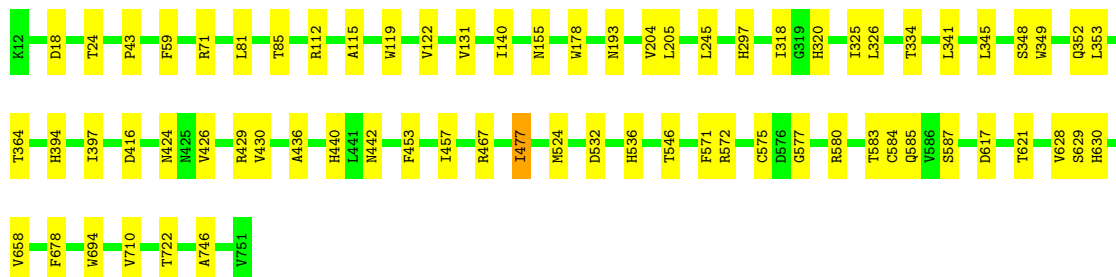
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1





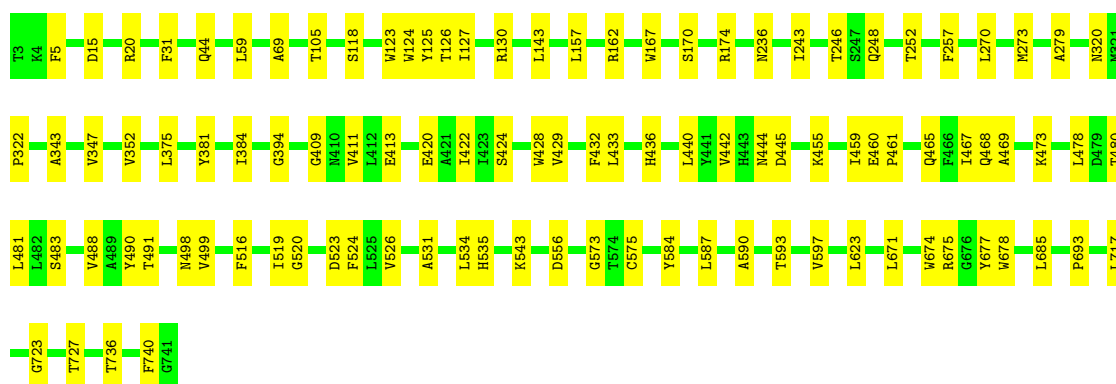
- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

Chain AA: 91% 9%



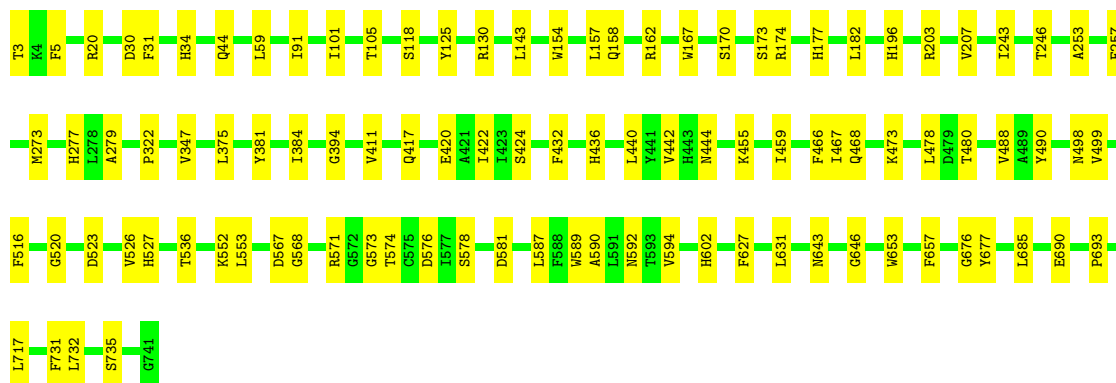
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B1: 86% 14%



- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B2: 86% 14%



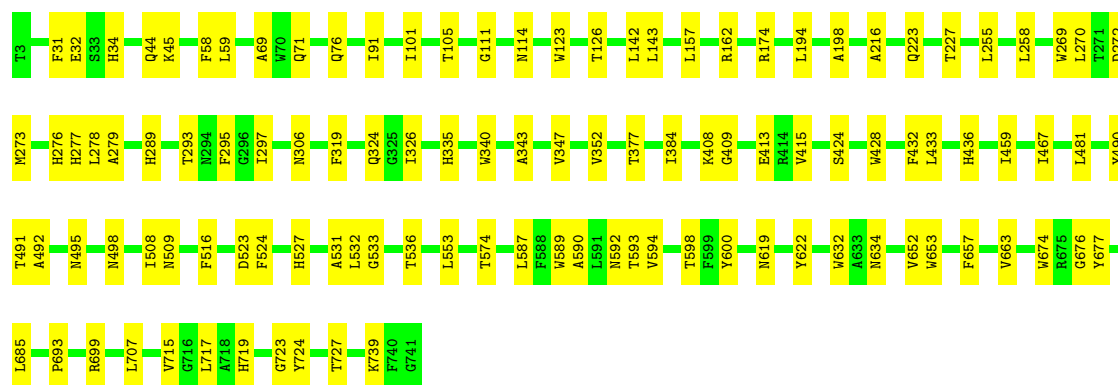
- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain B: 87% 13%



• Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2 1

Chain BB: 85% 15%



• Molecule 3: Photosystem I iron-sulfur center

Chain C1: 84% 15%



• Molecule 3: Photosystem I iron-sulfur center

Chain C2: 88% 11%



• Molecule 3: Photosystem I iron-sulfur center

Chain C: 86% 14%



• Molecule 3: Photosystem I iron-sulfur center

Chain CC: 84% 16%



- Molecule 4: Photosystem I reaction center subunit II

Chain D1: 94% 6%



- Molecule 4: Photosystem I reaction center subunit II

Chain D2: 91% 9%



- Molecule 4: Photosystem I reaction center subunit II

Chain D: 93% 7%



- Molecule 4: Photosystem I reaction center subunit II

Chain DD: 94% 6%



- Molecule 5: Photosystem I reaction center subunit IV

Chain E1: 92% 8%



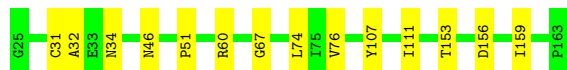
- Molecule 5: Photosystem I reaction center subunit IV

Chain E2: 92% 8%



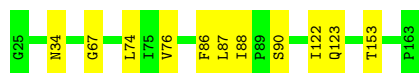
- Molecule 6: Photosystem I reaction center subunit III

Chain F1: 90% 10%




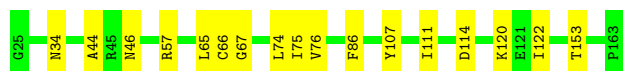
- Molecule 6: Photosystem I reaction center subunit III

Chain F:  92% 8%



- Molecule 6: Photosystem I reaction center subunit III

Chain FF:  88% 12%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I1:  97%



- Molecule 7: Photosystem I reaction center subunit VIII

Chain I:  94% 6%




- Molecule 7: Photosystem I reaction center subunit VIII

Chain II:  97%




- Molecule 8: Photosystem I reaction center subunit IX

Chain J1:  81% 8% 10%




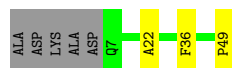
- Molecule 8: Photosystem I reaction center subunit IX

Chain J2:  79% 10% 10%

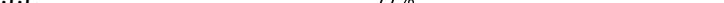


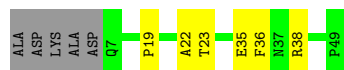
- Molecule 8: Photosystem I reaction center subunit IX

Chain J:  83% 6% 10%



- Molecule 8: Photosystem I reaction center subunit IX

Chain JJ:  77% 13% 10%



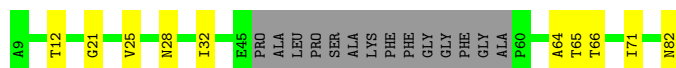
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K1:  96%



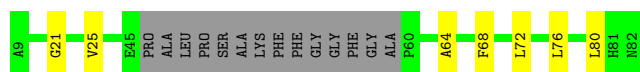
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain K: 68% 14% 19%

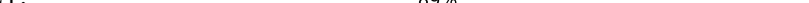


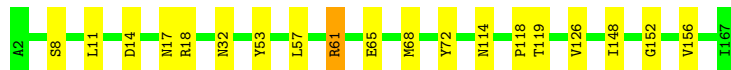
- Molecule 9: Photosystem I reaction center subunit PsaK 1

Chain KK:  72% 9% 19%



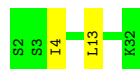
- Molecule 10: Photosystem I reaction center subunit XI

Chain L1:  89% 11%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M1: 94% 6%



- Molecule 11: Photosystem I reaction center subunit XII

Chain M2:  97%



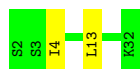
- Molecule 11: Photosystem I reaction center subunit XII

Chain M: 84% 16%



- Molecule 11: Photosystem I reaction center subunit XII

Chain MM: 94% 6%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X1: 92% 8%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X2: 90% 10%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain X: 95% 5%



- Molecule 12: Photosystem I 4.8 kDa protein

Chain XX: 97% 3%

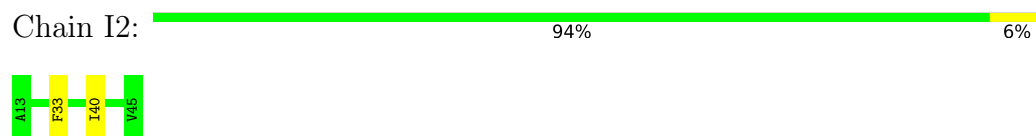


- Molecule 13: Photosystem I reaction center subunit III

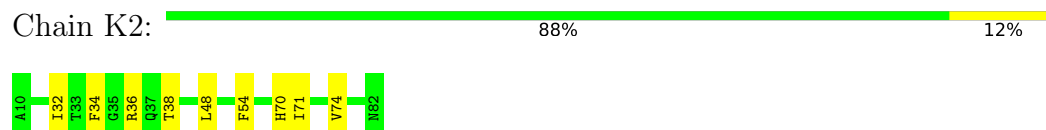
Chain F2: 85% 13% 2%



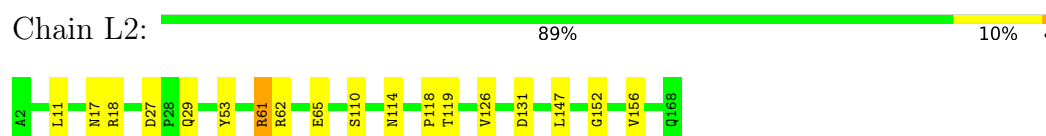
- Molecule 14: Photosystem I reaction center subunit VIII



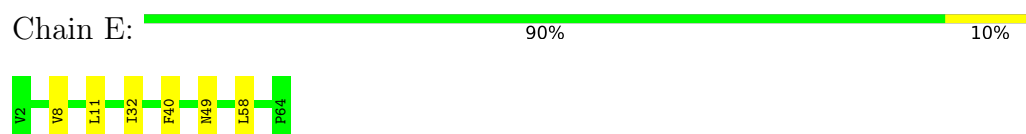
- Molecule 15: Photosystem I reaction center subunit PsaK 1



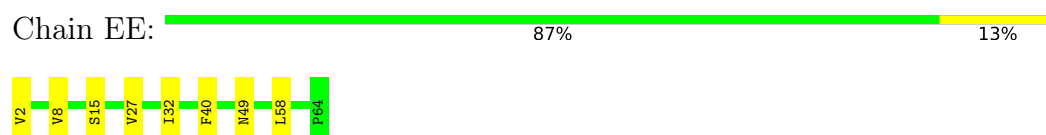
- Molecule 16: Photosystem I reaction center subunit XI



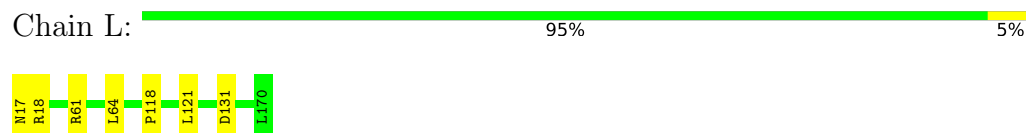
- Molecule 17: Photosystem I reaction center subunit IV



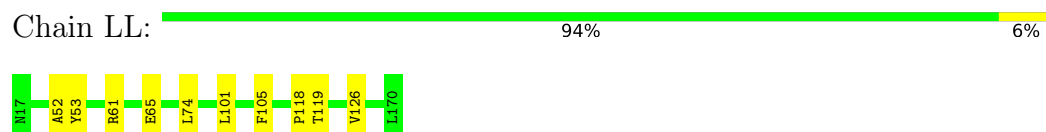
- Molecule 17: Photosystem I reaction center subunit IV



- Molecule 18: Photosystem I reaction center subunit XI



- Molecule 18: Photosystem I reaction center subunit XI



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	69247	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	42	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LHG, DGD, AJP, SF4, CLA, PQN, ECH, CL0, BCR, LMG

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 >2	RMSZ	# Z >2
1	A	0.29	0/6004	0.44	0/8193
1	A1	0.28	0/6004	0.45	0/8193
1	A2	0.29	0/6004	0.46	0/8193
1	AA	0.28	0/6004	0.44	0/8193
10	L1	0.30	0/1281	0.46	0/1756
11	M	0.26	0/244	0.37	0/334
11	M1	0.26	0/244	0.42	0/334
11	M2	0.25	0/244	0.41	0/334
11	MM	0.26	0/244	0.39	0/334
12	X	0.29	0/320	0.46	0/439
12	X1	0.27	0/320	0.43	0/439
12	X2	0.29	0/320	0.44	0/439
12	XX	0.29	0/320	0.44	0/439
13	F2	0.29	0/1070	0.52	0/1455
14	I2	0.30	0/277	0.42	0/379
15	K2	0.26	0/546	0.45	0/748
16	L2	0.31	0/1290	0.47	0/1768
17	E	0.29	0/512	0.49	0/696
17	EE	0.28	0/512	0.48	0/696
18	L	0.30	0/1191	0.47	0/1632
18	LL	0.30	0/1191	0.45	0/1632
2	B	0.32	0/6143	0.46	0/8396
2	B1	0.29	0/6143	0.44	0/8396
2	B2	0.30	0/6143	0.44	0/8396
2	BB	0.32	0/6143	0.45	0/8396
3	C	0.28	0/609	0.52	0/826
3	C1	0.28	0/609	0.52	0/826
3	C2	0.28	0/609	0.49	0/826
3	CC	0.28	0/609	0.51	0/826
4	D	0.28	0/1060	0.52	0/1431
4	D1	0.27	0/1060	0.50	0/1431
4	D2	0.27	0/1060	0.53	0/1431

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
4	DD	0.28	0/1060	0.52	0/1431
5	E1	0.27	0/490	0.49	0/665
5	E2	0.30	0/490	0.47	0/665
6	F	0.28	0/1084	0.47	0/1475
6	F1	0.26	0/1084	0.46	0/1475
6	FF	0.27	0/1084	0.47	0/1475
7	I	0.29	0/262	0.41	0/358
7	I1	0.30	0/262	0.40	0/358
7	II	0.30	0/262	0.41	0/358
8	J	0.28	0/358	0.46	0/491
8	J1	0.27	0/358	0.43	0/491
8	J2	0.27	0/358	0.41	0/491
8	JJ	0.27	0/358	0.42	0/491
9	K	0.25	0/448	0.41	0/613
9	K1	0.27	0/551	0.45	0/755
9	KK	0.25	0/448	0.44	0/613
All	All	0.29	0/73287	0.46	0/100012

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	F2	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	F2	158	GLU	Peptide
13	F2	159	ILE	Peptide

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	A	5806	5677	5682	58	0
1	A1	5806	5672	5682	73	0
1	A2	5806	5680	5682	73	0
1	AA	5806	5677	5682	56	0
2	B	5919	5667	5677	73	0
2	B1	5919	5660	5677	82	0
2	B2	5919	5662	5677	79	0
2	BB	5919	5676	5677	89	0
3	C	599	582	585	8	0
3	C1	599	584	585	10	0
3	C2	599	580	585	6	0
3	CC	599	582	585	10	0
4	D	1036	1042	1042	9	0
4	D1	1036	1037	1042	7	0
4	D2	1036	1042	1042	10	0
4	DD	1036	1042	1042	7	0
5	E1	481	477	478	4	0
5	E2	481	477	478	7	0
6	F	1060	1051	1054	8	0
6	F1	1060	1052	1054	11	0
6	FF	1060	1052	1054	11	0
7	I	253	255	255	2	0
7	I1	253	255	255	1	0
7	II	253	255	255	1	0
8	J	346	355	355	3	0
8	J1	346	355	355	4	0
8	J2	346	355	355	5	0
8	JJ	346	354	355	5	0
9	K	439	461	461	6	0
9	K1	536	555	555	2	0
9	KK	439	461	461	4	0
10	L1	1244	1239	1242	16	0
11	M	240	256	256	5	0
11	M1	240	256	256	3	0
11	M2	240	256	256	1	0
11	MM	240	256	256	4	0
12	X	309	319	319	2	0
12	X1	309	318	319	4	0
12	X2	309	318	319	5	0
12	XX	309	319	319	1	0
13	F2	1047	1040	1042	15	0
14	I2	268	268	268	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	K2	531	550	550	7	0
16	L2	1253	1245	1250	12	0
17	E	502	492	496	5	0
17	EE	502	492	496	6	0
18	L	1156	1153	1157	4	0
18	LL	1156	1154	1157	8	0
19	A	2339	2207	2215	48	0
19	A1	2394	2261	2275	59	0
19	A2	2375	2227	2236	47	0
19	AA	2404	2279	2287	43	0
19	B	2401	2357	2375	73	0
19	B1	2291	2253	2270	61	0
19	B2	2401	2358	2375	50	0
19	BB	2271	2219	2231	64	0
19	F	102	89	90	3	0
19	F1	147	122	123	5	0
19	F2	102	89	90	3	0
19	FF	167	161	162	6	0
19	J	82	58	58	4	0
19	J1	82	57	58	1	0
19	J2	82	58	58	2	0
19	JJ	82	57	58	1	0
19	K	91	65	66	0	0
19	K1	131	92	94	2	0
19	K2	86	61	62	1	0
19	KK	91	65	66	0	0
19	L	191	198	205	4	0
19	L1	191	202	205	5	0
19	L2	186	187	191	0	0
19	LL	168	155	164	7	0
19	X	45	32	33	0	0
19	X1	45	32	33	0	0
19	X2	45	32	33	1	0
19	XX	45	32	33	0	0
20	A	65	72	72	1	0
20	A1	65	72	71	3	0
20	A2	65	72	70	5	0
20	AA	65	72	71	1	0
21	A	33	46	46	3	0
21	A1	33	46	46	1	0
21	A2	33	46	46	1	0
21	AA	33	46	46	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	B	33	46	46	2	0
21	B1	33	46	46	0	0
21	B2	33	46	46	0	0
21	BB	33	46	46	2	0
22	A	87	122	123	3	0
22	A1	87	122	123	1	0
22	A2	87	122	123	2	0
22	AA	87	122	123	3	0
22	B	82	110	110	1	0
22	B1	33	36	36	1	0
22	B2	33	36	36	0	0
22	BB	82	110	110	0	0
22	L	34	42	38	0	0
22	L1	33	35	36	3	0
22	L2	35	39	40	2	0
22	LL	34	42	38	0	0
22	X	40	49	50	0	0
22	X1	89	123	124	0	0
22	X2	89	123	124	0	0
22	XX	40	49	50	0	0
23	A	279	389	389	7	0
23	A1	239	333	333	6	0
23	A2	239	333	333	7	0
23	AA	279	389	389	8	0
23	B	240	336	336	12	0
23	B1	200	280	280	7	0
23	B2	200	275	280	8	0
23	BB	240	336	336	10	0
23	F	120	163	168	8	0
23	F1	120	163	168	7	0
23	F2	120	163	168	7	0
23	FF	120	163	168	7	0
23	I	80	112	112	0	0
23	I1	40	56	56	1	0
23	I2	120	168	168	1	0
23	II	120	168	168	0	0
23	J	80	112	112	2	0
23	J1	80	112	112	2	0
23	J2	80	112	112	3	0
23	JJ	80	112	112	2	0
23	K	40	56	56	0	0
23	K1	80	112	112	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	K2	80	112	112	3	0
23	KK	40	56	56	0	0
23	L	80	112	112	1	0
23	L1	120	168	168	0	0
23	L2	40	56	56	0	0
23	LL	40	56	56	1	0
23	M	40	51	56	2	0
23	M1	40	56	56	0	0
23	M2	40	56	56	0	0
23	MM	40	53	56	1	0
24	A	65	88	0	0	0
24	A1	75	96	0	0	0
24	A2	32	43	0	0	0
24	AA	65	88	0	0	0
24	B	129	159	0	1	0
24	BB	86	106	0	1	0
24	I2	31	42	0	0	0
24	K	41	50	0	0	0
24	KK	41	50	0	0	0
24	L	62	85	0	0	0
24	L1	86	106	0	1	0
24	L2	86	106	0	1	0
24	M2	31	43	0	0	0
25	A1	68	84	0	0	0
25	A2	74	97	0	0	0
25	B	176	251	172	0	0
25	B1	117	148	150	0	0
25	B2	117	148	150	0	0
25	BB	122	167	86	0	0
25	I1	35	40	40	0	0
25	I2	35	40	40	1	0
25	II	79	102	54	0	0
25	K1	58	62	0	0	0
25	K2	56	58	0	0	0
25	L	37	48	0	0	0
25	L1	91	132	86	1	0
25	L2	36	46	0	0	0
25	M	46	59	62	1	0
26	B	41	54	54	1	0
26	B1	41	54	54	1	0
26	B2	41	54	54	1	0
26	BB	41	54	54	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	8	0	0	0	0
27	B1	8	0	0	0	0
27	B2	8	0	0	0	0
27	BB	8	0	0	0	0
27	C	16	0	0	1	0
27	C1	16	0	0	1	0
27	C2	16	0	0	0	0
27	CC	16	0	0	0	0
28	B	42	46	42	1	0
28	BB	42	46	42	1	0
All	All	99604	99577	98156	1039	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (1039) 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)
2:B2:587:LEU:HD23	2:B2:717:LEU:HD21	1.55	0.88
2:B:553:LEU:HD23	2:B:577:ILE:HD11	1.56	0.86
19:B2:822:CLA:H93	23:B2:843:BCR:H333	1.57	0.84
19:B1:822:CLA:H93	23:B1:842:BCR:H333	1.58	0.83
2:B1:534:LEU:HD12	19:B1:834:CLA:HED3	1.63	0.81
2:B:415:VAL:HG11	23:B:842:BCR:H401	1.62	0.81
19:B:834:CLA:H93	19:B:835:CLA:HBC1	1.63	0.79
19:BB:833:CLA:H93	19:BB:834:CLA:HBC1	1.64	0.79
1:A:199:ASN:ND2	1:A:309:GLY:O	2.16	0.79
19:B:822:CLA:H93	23:B:843:BCR:H333	1.66	0.78
19:B1:833:CLA:H93	19:B1:834:CLA:HBC1	1.66	0.77
1:A1:199:ASN:ND2	1:A1:309:GLY:O	2.18	0.77
1:A2:572:ARG:NH1	22:A2:845:LHG:O10	2.20	0.75
6:F1:31:CYS:SG	6:F1:32:ALA:N	2.59	0.75
19:BB:822:CLA:H93	23:BB:842:BCR:H333	1.68	0.75
2:B1:587:LEU:HD12	2:B1:717:LEU:HD21	1.69	0.75
2:B2:490:TYR:O	2:B2:498:ASN:ND2	2.21	0.74
1:A:693:TYR:O	2:B:543:LYS:NZ	2.20	0.74
2:B1:490:TYR:O	2:B1:498:ASN:ND2	2.21	0.74
4:D:105:LYS:O	4:D:110:ARG:NH2	2.22	0.73
2:B2:44:GLN:OE1	2:B2:162:ARG:NH2	2.22	0.73
2:B2:473:LYS:NZ	2:B2:516:PHE:O	2.20	0.72
2:BB:44:GLN:OE1	2:BB:162:ARG:NH2	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:473:LYS:NZ	2:B1:516:PHE:O	2.20	0.72
1:A1:693:TYR:O	2:B1:543:LYS:NZ	2.21	0.71
2:B:402:TYR:OH	2:B:413:GLU:OE2	2.08	0.71
19:B:834:CLA:HMC1	19:B:834:CLA:HBC3	1.72	0.71
19:BB:833:CLA:HMC1	19:BB:833:CLA:HBC3	1.72	0.71
6:F1:46:ASN:ND2	6:F1:51:PRO:O	2.23	0.70
13:F2:31:CYS:SG	13:F2:32:ALA:N	2.64	0.70
1:A1:576:ASP:OD2	1:A1:580:ARG:NH2	2.24	0.70
1:A2:715:GLN:NE2	5:E2:16:TYR:OH	2.25	0.69
2:B2:567:ASP:OD2	2:B2:571:ARG:NH2	2.25	0.69
2:BB:377:THR:HG23	2:BB:598:THR:HG21	1.73	0.69
4:D1:62:ARG:NH2	4:D1:64:GLU:OE1	2.26	0.69
18:LL:61:ARG:NH2	18:LL:65:GLU:OE1	2.26	0.69
1:A1:333:PHE:O	1:A1:429:ARG:NH1	2.25	0.68
1:A2:735:GLY:O	1:A2:739:THR:OG1	2.10	0.68
19:BB:829:CLA:HBC2	19:BB:829:CLA:HMC1	1.75	0.68
2:BB:306:ASN:ND2	2:BB:324:GLN:O	2.27	0.68
1:A1:435:ASP:OD2	1:A1:561:ARG:NH2	2.26	0.68
19:B1:833:CLA:HBC2	19:B1:834:CLA:HBC3	1.76	0.68
1:AA:722:THR:OG1	22:AA:846:LHG:O5	2.12	0.68
3:C1:61:ASP:OD1	5:E1:12:ARG:NH1	2.26	0.68
16:L2:114:ASN:ND2	22:L2:208:LHG:O9	2.28	0.67
1:AA:575:CYS:O	1:AA:583:THR:OG1	2.08	0.67
19:B1:821:CLA:HMA2	19:B1:821:CLA:O2A	1.94	0.67
23:A1:851:BCR:H362	19:A1:852:CLA:H43	1.77	0.67
1:A:722:THR:OG1	22:A:845:LHG:O5	2.13	0.67
23:A:851:BCR:H362	19:A:852:CLA:H43	1.76	0.67
4:D:62:ARG:NH2	4:D:64:GLU:OE1	2.27	0.67
19:B2:821:CLA:O2A	19:B2:821:CLA:HMA2	1.95	0.67
16:L2:11:LEU:O	16:L2:17:ASN:ND2	2.27	0.67
5:E2:19:GLN:NE2	13:F2:153:THR:O	2.28	0.67
19:A1:844:CLA:OBD	10:L1:18:ARG:NH2	2.28	0.67
1:A1:383:ASP:OD2	1:A1:386:THR:OG1	2.11	0.66
2:B1:409:GLY:N	2:B1:413:GLU:OE1	2.28	0.66
19:B:821:CLA:HMA2	19:B:821:CLA:O2A	1.95	0.66
2:B1:693:PRO:O	10:L1:53:TYR:OH	2.13	0.66
19:B1:832:CLA:CGD	19:B1:833:CLA:HMB1	2.26	0.66
19:B:834:CLA:HBB2	19:B:835:CLA:HED2	1.78	0.66
19:B2:834:CLA:HMC1	19:B2:834:CLA:HBC3	1.77	0.66
4:D2:62:ARG:NH2	4:D2:64:GLU:OE1	2.29	0.66
19:B:806:CLA:H18	25:M:102:LMG:H392	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BB:832:CLA:CGD	19:BB:833:CLA:HMB1	2.26	0.66
19:AA:804:CLA:O1A	2:BB:532:LEU:HD11	1.96	0.65
2:B2:384:ILE:CG2	2:B2:590:ALA:HB1	2.25	0.65
1:A1:571:PHE:O	1:A1:587:SER:OG	2.14	0.65
1:A2:329:HIS:O	22:A2:846:LHG:O2	2.10	0.65
2:B2:432:PHE:O	2:B2:436:HIS:ND1	2.29	0.65
19:BB:821:CLA:O2A	19:BB:821:CLA:HMA2	1.95	0.65
1:AA:580:ARG:NH1	4:DD:64:GLU:OE2	2.30	0.65
19:B:833:CLA:CGD	19:B:834:CLA:HMB1	2.27	0.65
19:BB:833:CLA:HBC2	19:BB:834:CLA:HBC3	1.78	0.65
3:C:64:SER:OG	27:C:102:SF4:S2	2.50	0.65
2:B1:236:ASN:ND2	2:B1:252:THR:OG1	2.22	0.65
3:C2:61:ASP:OD2	5:E2:15:SER:OG	2.09	0.65
1:A2:383:ASP:OD2	1:A2:386:THR:OG1	2.12	0.65
2:B1:432:PHE:O	2:B1:436:HIS:ND1	2.29	0.64
2:BB:490:TYR:O	2:BB:498:ASN:ND2	2.31	0.64
19:B1:833:CLA:HBC3	19:B1:833:CLA:HMC1	1.79	0.64
23:A2:851:BCR:H362	19:A2:852:CLA:H43	1.78	0.64
3:CC:9:ASP:OD1	3:CC:35:LYS:NZ	2.31	0.64
2:B:690:GLU:OE2	4:D:21:THR:OG1	2.16	0.64
1:AA:621:THR:OG1	1:AA:629:SER:OG	2.15	0.64
2:B2:693:PRO:O	16:L2:53:TYR:OH	2.14	0.64
3:C:25:VAL:HG23	3:C:44:ARG:O	1.99	0.63
3:C2:25:VAL:HG23	3:C2:44:ARG:O	1.99	0.63
2:B2:552:LYS:NZ	5:E2:15:SER:O	2.32	0.63
1:A2:205:LEU:HD11	19:A2:815:CLA:H42	1.80	0.63
19:AA:843:CLA:H202	19:BB:835:CLA:H192	1.81	0.63
1:A1:691:ARG:N	2:B1:575:CYS:SG	2.70	0.63
1:A1:467:ARG:NH2	19:A1:835:CLA:O1D	2.32	0.63
1:AA:397:ILE:HD13	19:AA:830:CLA:HBC3	1.79	0.63
13:F2:124:LEU:O	8:J2:16:SER:OG	2.16	0.63
1:A1:585:GLN:OE1	2:B1:674:TRP:N	2.32	0.62
1:AA:205:LEU:HD11	19:AA:815:CLA:H42	1.81	0.62
1:A1:277:THR:OG1	1:A1:293:ASP:OD1	2.17	0.62
1:A2:680:TRP:NE1	20:A2:803:CL0:O1A	2.32	0.62
2:BB:467:ILE:HD11	19:BB:832:CLA:H43	1.81	0.62
2:B2:440:LEU:O	2:B2:444:ASN:ND2	2.32	0.62
2:B:480:THR:O	2:B:484:ASN:N	2.33	0.62
1:A:122:VAL:HG11	19:B:830:CLA:HMD1	1.82	0.62
4:D2:101:VAL:HG11	4:D2:107:ASN:HB2	1.81	0.62
23:F2:305:BCR:HC8	23:F2:305:BCR:H311	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A1:852:CLA:HMB3	19:B1:848:CLA:H191	1.81	0.62
19:B:834:CLA:HBC2	19:B:835:CLA:HBC3	1.81	0.62
19:B:833:CLA:HED2	19:B:834:CLA:HBB1	1.81	0.62
2:BB:324:GLN:NE2	2:BB:408:LYS:O	2.33	0.62
1:A1:122:VAL:HG11	19:B1:829:CLA:HMD1	1.81	0.61
19:A2:830:CLA:HMC1	19:A2:830:CLA:HBC2	1.80	0.61
3:C1:25:VAL:HG23	3:C1:44:ARG:O	1.99	0.61
2:B1:384:ILE:HG23	2:B1:590:ALA:HB1	1.83	0.61
2:B:306:ASN:ND2	2:B:324:GLN:O	2.33	0.61
1:A:580:ARG:NH2	4:D:64:GLU:OE2	2.33	0.61
2:BB:273:MET:O	2:BB:277:HIS:ND1	2.26	0.61
4:D1:105:LYS:O	4:D1:110:ARG:NH1	2.33	0.61
9:K:12:THR:OG1	9:K:82:ASN:O	2.16	0.61
3:C2:21:CYS:SG	3:C2:24:ASP:N	2.73	0.61
2:B:692:THR:HG21	19:B:860:CLA:HMA2	1.82	0.61
2:B:326:ILE:HG21	19:B:820:CLA:HMD3	1.83	0.61
4:D:21:THR:HG21	18:L:121:LEU:HD11	1.83	0.61
1:AA:348:SER:OG	1:AA:416:ASP:OD2	2.15	0.61
1:A1:329:HIS:O	22:A1:846:LHG:O2	2.10	0.60
2:B:593:THR:O	2:B:597:VAL:HG23	2.00	0.60
1:A1:205:LEU:HD11	19:A1:814:CLA:H42	1.82	0.60
2:B1:723:GLY:O	2:B1:727:THR:HG22	2.01	0.60
1:A2:155:ASN:ND2	1:A2:158:GLN:OE1	2.34	0.60
19:B:801:CLA:H12	11:M:27:ALA:HB1	1.82	0.60
19:B1:832:CLA:O2D	19:B1:833:CLA:HMB1	2.00	0.60
2:BB:634:ASN:OD1	2:BB:739:LYS:NZ	2.35	0.60
1:A:436:ALA:O	1:A:440:HIS:ND1	2.34	0.60
1:A1:707:LYS:NZ	6:F1:156:ASP:OD1	2.30	0.60
19:B1:832:CLA:HED2	19:B1:833:CLA:CBB	2.32	0.60
2:B1:44:GLN:OE1	2:B1:162:ARG:NH2	2.35	0.60
2:B2:568:GLY:O	2:B2:574:THR:OG1	2.19	0.60
23:BB:841:BCR:H311	23:BB:841:BCR:H343	1.84	0.60
19:B:834:CLA:HAB	19:B:835:CLA:CGD	2.32	0.59
23:B:842:BCR:H343	23:B:842:BCR:H311	1.84	0.59
2:B2:203:ARG:NH2	2:B2:253:ALA:O	2.34	0.59
1:A:205:LEU:HD11	19:A:815:CLA:H42	1.83	0.59
1:AA:318:ILE:HG23	19:AA:822:CLA:HED1	1.84	0.59
6:FF:107:TYR:CZ	6:FF:111:ILE:HD11	2.37	0.59
19:B2:829:CLA:H142	23:F2:303:BCR:H333	1.83	0.59
2:B:279:ALA:HA	19:B:813:CLA:HMC3	1.85	0.59
13:F2:107:TYR:CZ	13:F2:111:ILE:HD11	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:674:LEU:HD11	2:B2:627:PHE:CZ	2.38	0.59
2:BB:432:PHE:O	2:BB:436:HIS:ND1	2.35	0.59
5:E2:19:GLN:NE2	13:F2:157:SER:OG	2.36	0.59
2:B1:440:LEU:O	2:B1:444:ASN:ND2	2.36	0.59
4:D2:105:LYS:O	4:D2:110:ARG:NH2	2.34	0.59
1:A1:363:LEU:HD21	19:A1:828:CLA:H43	1.85	0.59
2:BB:619:ASN:OD1	2:BB:622:TYR:OH	2.12	0.59
15:K2:34:PHE:O	15:K2:38:THR:OG1	2.15	0.59
23:F1:306:BCR:HC8	23:F1:306:BCR:H311	1.84	0.59
16:L2:110:SER:O	16:L2:114:ASN:ND2	2.35	0.59
1:A1:345:LEU:HD23	1:A1:352:GLN:OE1	2.03	0.58
1:A1:442:ASN:ND2	2:B1:685:LEU:HD21	2.18	0.58
2:B:31:PHE:CD2	19:B:802:CLA:HMC2	2.38	0.58
8:JJ:35:GLU:OE1	8:JJ:38:ARG:NE	2.35	0.58
19:A:852:CLA:HMB3	19:B:854:CLA:H191	1.84	0.58
1:AA:245:LEU:HD21	19:AA:818:CLA:HBC1	1.85	0.58
19:B:833:CLA:HED2	19:B:834:CLA:CBB	2.34	0.58
2:B:433:LEU:HD11	19:B:834:CLA:HMC3	1.85	0.58
6:F1:60:ARG:NH2	8:J1:42:ASP:O	2.36	0.58
2:B:459:ILE:HD11	2:B:524:PHE:CE1	2.38	0.58
19:B:810:CLA:H143	19:B:815:CLA:H42	1.85	0.58
1:AA:572:ARG:NH1	22:AA:846:LHG:O10	2.36	0.58
2:B:467:ILE:HD11	19:B:833:CLA:H43	1.85	0.58
19:BB:833:CLA:HAB	19:BB:834:CLA:CGD	2.33	0.58
19:BB:832:CLA:O2D	19:BB:833:CLA:HMB1	2.03	0.58
19:B1:828:CLA:H142	23:F1:303:BCR:H333	1.86	0.58
19:B1:833:CLA:O1D	6:F1:76:VAL:HG13	2.03	0.58
8:J2:35:GLU:OE2	8:J2:38:ARG:NH2	2.36	0.58
2:BB:459:ILE:HG22	6:FF:74:LEU:HB2	1.87	0.57
16:L2:53:TYR:CD2	16:L2:126:VAL:HG21	2.38	0.57
2:B1:243:ILE:O	2:B1:246:THR:OG1	2.17	0.57
2:BB:293:THR:HG21	19:BB:817:CLA:OBD	2.05	0.57
23:FF:306:BCR:H311	23:FF:306:BCR:HC8	1.85	0.57
2:B1:467:ILE:HD11	19:B1:832:CLA:H43	1.86	0.57
2:B:3:THR:OG1	2:B:20:ARG:NH2	2.38	0.57
13:F2:34:ASN:ND2	13:F2:67:GLY:O	2.36	0.57
19:LL:203:CLA:HMC1	19:LL:203:CLA:HBC3	1.86	0.57
1:A2:121:ILE:O	1:A2:123:GLY:N	2.37	0.57
1:AA:424:ASN:OD1	1:AA:429:ARG:NH2	2.37	0.57
1:AA:436:ALA:O	1:AA:440:HIS:ND1	2.37	0.57
2:B2:527:HIS:HB3	19:B2:833:CLA:HED1	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:DD:62:ARG:NH2	4:DD:64:GLU:OE1	2.37	0.57
17:EE:8:VAL:CG1	17:EE:58:LEU:HD22	2.34	0.57
23:F:305:BCR:HC8	23:F:305:BCR:H311	1.85	0.57
2:B:195:ILE:HA	2:B:199:ILE:HD12	1.87	0.57
2:B2:467:ILE:HD11	19:B2:833:CLA:H43	1.85	0.57
19:B2:836:CLA:H192	19:B2:852:CLA:H202	1.85	0.57
1:A:442:ASN:ND2	2:B:685:LEU:HD21	2.20	0.57
2:BB:433:LEU:HD11	19:BB:833:CLA:HMC3	1.87	0.57
19:BB:810:CLA:H143	19:BB:815:CLA:H42	1.84	0.57
19:B:833:CLA:O2D	19:B:834:CLA:HMB1	2.05	0.57
1:A:572:ARG:NH1	22:A:845:LHG:O10	2.37	0.56
2:B1:469:ALA:O	2:B1:483:SER:OG	2.21	0.56
20:A2:803:CL0:CBB	2:B2:631:LEU:HD13	2.35	0.56
2:BB:723:GLY:O	2:BB:727:THR:HG22	2.05	0.56
1:A2:424:ASN:OD1	1:A2:429:ARG:NH2	2.38	0.56
1:A2:599:MET:O	1:A2:603:LEU:HD23	2.05	0.56
2:B1:69:ALA:HB1	11:M1:4:ILE:HD11	1.86	0.56
19:B1:833:CLA:HBB2	19:B1:834:CLA:HED2	1.87	0.56
3:C:38:GLN:HB3	4:D:106:VAL:HG21	1.86	0.56
1:A1:14:ARG:NH2	1:A1:16:ILE:HD11	2.21	0.56
6:F1:107:TYR:CZ	6:F1:111:ILE:HD11	2.41	0.56
19:K1:105:CLA:HBC2	19:K1:105:CLA:HMC1	1.87	0.56
1:A1:401:LEU:HD21	19:A1:807:CLA:H142	1.88	0.56
1:AA:442:ASN:ND2	2:BB:685:LEU:HD21	2.21	0.56
2:B2:573:GLY:O	2:B2:574:THR:OG1	2.23	0.56
19:B:836:CLA:H192	19:B:860:CLA:H202	1.85	0.56
19:BB:832:CLA:HED2	19:BB:833:CLA:CBB	2.35	0.56
23:AA:852:BCR:H362	19:AA:853:CLA:H43	1.87	0.56
2:B1:727:THR:HG23	19:B1:848:CLA:O1D	2.06	0.56
2:BB:424:SER:OG	19:BB:856:CLA:HED3	2.06	0.56
1:A2:307:ILE:HG12	23:K2:105:BCR:H362	1.87	0.56
1:A1:617:ASP:O	1:A1:630:HIS:NE2	2.39	0.56
1:A2:142:SER:O	1:A2:390:ILE:HD11	2.05	0.56
2:B1:455:LYS:NZ	8:J1:42:ASP:OD1	2.29	0.56
10:L1:118:PRO:O	10:L1:119:THR:HG23	2.06	0.56
19:A2:820:CLA:CMD	19:A2:821:CLA:H202	2.36	0.56
2:B1:31:PHE:CD2	19:B1:802:CLA:HMC2	2.41	0.56
2:B:424:SER:OG	19:B:859:CLA:HED3	2.06	0.56
2:B2:455:LYS:NZ	8:J2:42:ASP:OD2	2.23	0.56
1:A2:328:ASN:OD1	19:A2:825:CLA:HED3	2.06	0.56
1:A:318:ILE:HG23	19:A:822:CLA:HED1	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:381:TYR:CE1	2:B2:594:VAL:HG11	2.41	0.56
2:BB:31:PHE:CD2	19:BB:802:CLA:HMC2	2.41	0.56
1:A:245:LEU:HD21	19:A:818:CLA:HBC1	1.89	0.55
1:A:617:ASP:O	1:A:630:HIS:NE2	2.39	0.55
2:B2:31:PHE:CD2	19:B2:802:CLA:HMC2	2.41	0.55
2:BB:459:ILE:HD11	2:BB:524:PHE:CE1	2.41	0.55
1:A:43:PRO:HG3	6:F:122:ILE:HD12	1.87	0.55
1:A2:227:LEU:O	1:A2:232:VAL:HG22	2.05	0.55
1:A2:343:GLU:O	1:A2:347:THR:OG1	2.12	0.55
19:B2:811:CLA:H43	26:B2:841:ECH:H36A	1.88	0.55
2:B:322:PRO:O	2:B:411:VAL:HG23	2.07	0.55
19:F1:301:CLA:H43	19:F1:302:CLA:CBC	2.36	0.55
2:B:123:TRP:CZ2	19:B:810:CLA:H191	2.41	0.55
19:B:811:CLA:H43	26:B:841:ECH:H36A	1.89	0.55
1:A:397:ILE:HD13	19:A:830:CLA:HBC3	1.88	0.55
1:A:467:ARG:NH2	19:A:836:CLA:O1D	2.40	0.55
8:JJ:19:PRO:O	8:JJ:23:THR:HG23	2.05	0.55
16:L2:61:ARG:NH2	16:L2:65:GLU:OE1	2.39	0.55
19:B1:804:CLA:HMD2	11:M1:13:LEU:HD21	1.89	0.55
2:B:320:ASN:ND2	22:B:852:LHG:O4	2.39	0.55
19:B1:833:CLA:HAB	19:B1:834:CLA:CGD	2.37	0.55
2:B1:5:PHE:CD1	7:I1:40:ILE:HG22	2.42	0.55
1:A1:363:LEU:CD2	19:A1:828:CLA:H43	2.35	0.55
19:AA:801:CLA:OBD	2:BB:677:TYR:OH	2.15	0.55
19:A1:842:CLA:H202	19:B1:835:CLA:H192	1.88	0.55
2:B1:320:ASN:ND2	22:B1:847:LHG:O4	2.39	0.55
19:BB:833:CLA:HBB2	19:BB:834:CLA:HED2	1.88	0.55
5:E2:10:ILE:HD11	5:E2:40:PHE:HZ	1.72	0.55
19:A:804:CLA:H193	19:A:852:CLA:H192	1.88	0.55
1:AA:617:ASP:O	1:AA:630:HIS:NE2	2.40	0.55
19:B1:833:CLA:H42	23:F1:303:BCR:H392	1.89	0.54
2:B2:417:GLN:OE1	12:X2:11:ASN:ND2	2.40	0.54
2:BB:508:ILE:HG23	2:BB:509:ASN:OD1	2.07	0.54
19:AA:853:CLA:HMB3	19:BB:852:CLA:H191	1.89	0.54
2:B1:520:GLY:N	2:B1:523:ASP:OD2	2.41	0.54
19:B2:826:CLA:H41	19:B2:826:CLA:C7	2.37	0.54
2:BB:663:VAL:HG22	19:BB:836:CLA:HMB3	1.89	0.54
1:A1:715:GLN:NE2	5:E1:16:TYR:OH	2.40	0.54
2:B2:173:SER:O	2:B2:177:HIS:ND1	2.40	0.54
9:K:32:ILE:HA	9:K:65:THR:HG21	1.88	0.54
11:MM:13:LEU:HB3	23:MM:101:BCR:H371	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:322:PRO:O	2:B1:411:VAL:HG13	2.08	0.54
2:B:291:TYR:HE1	2:B:301:ILE:HD11	1.72	0.54
2:BB:69:ALA:CB	11:MM:4:ILE:HD11	2.38	0.54
23:A2:851:BCR:H362	19:A2:852:CLA:C4	2.38	0.54
19:B1:826:CLA:H41	19:B1:826:CLA:C7	2.37	0.54
19:F2:301:CLA:H43	19:F2:302:CLA:CBC	2.37	0.54
19:F:301:CLA:H42	8:J:22:ALA:HA	1.90	0.54
23:A2:851:BCR:H403	23:A2:851:BCR:H23C	1.90	0.54
19:B1:811:CLA:H43	26:B1:840:ECH:H36A	1.87	0.54
25:L1:210:LMG:H161	2:BB:297:ILE:HD12	1.88	0.54
1:AA:345:LEU:HD22	1:AA:352:GLN:OE1	2.07	0.54
2:B1:478:LEU:O	12:X1:41:HIS:NE2	2.41	0.54
2:B2:322:PRO:O	2:B2:411:VAL:HG13	2.08	0.54
2:B2:553:LEU:HD21	2:B2:574:THR:HG22	1.89	0.54
1:A1:386:THR:HG22	1:A1:390:ILE:HD12	1.90	0.54
2:B2:417:GLN:NE2	12:X2:8:PRO:O	2.41	0.54
1:A2:122:VAL:HG11	19:B2:830:CLA:HMD1	1.89	0.54
23:B2:842:BCR:H382	23:B2:843:BCR:H21C	1.90	0.54
19:A:852:CLA:HMD3	19:B:854:CLA:O1A	2.08	0.54
19:BB:826:CLA:C7	19:BB:826:CLA:H41	2.38	0.54
22:L1:211:LHG:HC61	19:L:202:CLA:HBC1	1.90	0.54
19:B2:849:CLA:HMB3	19:B2:850:CLA:OBD	2.07	0.54
1:A1:691:ARG:NH1	2:B1:573:GLY:O	2.41	0.53
1:AA:397:ILE:CD1	19:AA:830:CLA:HBC3	2.38	0.53
2:B1:459:ILE:HD11	2:B1:524:PHE:CE1	2.43	0.53
6:FF:44:ALA:O	6:FF:57:ARG:NH2	2.41	0.53
1:A2:275:PHE:O	1:A2:276:LEU:HD12	2.09	0.53
19:A:805:CLA:C15	23:J:102:BCR:H353	2.38	0.53
3:CC:24:ASP:OD2	4:DD:96:HIS:ND1	2.41	0.53
15:K2:32:ILE:HG12	19:K2:104:CLA:HBA2	1.91	0.53
19:A2:804:CLA:HMC2	19:A2:852:CLA:CAC	2.38	0.53
1:AA:467:ARG:NH2	19:AA:836:CLA:O1D	2.41	0.53
17:EE:8:VAL:HG11	17:EE:58:LEU:HD22	1.90	0.53
19:B:837:CLA:HBC2	19:B:837:CLA:HHD	1.91	0.53
2:BB:289:HIS:CE1	23:BB:838:BCR:H363	2.43	0.53
19:LL:201:CLA:H92	19:LL:201:CLA:C4	2.38	0.53
1:A2:678:PHE:CD2	23:A2:851:BCR:H363	2.43	0.53
2:B2:578:SER:N	2:B2:581:ASP:OD2	2.41	0.53
2:B:581:ASP:OD1	2:B:713:ARG:NH1	2.41	0.53
2:B:731:PHE:O	2:B:735:SER:OG	2.10	0.53
1:A1:121:ILE:O	1:A1:123:GLY:N	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:678:PHE:CD2	23:A:851:BCR:H363	2.44	0.53
20:A:803:CL0:H13	19:A:852:CLA:OBD	2.08	0.53
2:B2:347:VAL:HB	19:B2:823:CLA:H43	1.89	0.53
2:B:688:ALA:O	2:B:692:THR:HG23	2.09	0.53
22:L2:208:LHG:HC92	19:LL:201:CLA:HMD2	1.91	0.53
19:AA:804:CLA:H193	19:AA:853:CLA:H192	1.91	0.53
19:BB:832:CLA:HED2	19:BB:833:CLA:HBB1	1.91	0.53
10:L1:8:SER:OG	10:L1:14:ASP:OD1	2.27	0.53
1:AA:353:LEU:HB2	19:AA:807:CLA:HMD3	1.91	0.53
5:E1:2:VAL:HG21	5:E1:24:VAL:HG21	1.91	0.53
1:AA:546:THR:HG21	19:AA:828:CLA:HBC3	1.91	0.53
2:B1:123:TRP:CZ2	19:B1:810:CLA:H191	2.44	0.53
25:I2:105:LMG:O5	25:I2:105:LMG:O4	2.14	0.53
1:A1:245:LEU:HD21	19:A1:817:CLA:HBC1	1.91	0.52
2:B2:424:SER:OG	19:B2:851:CLA:HED3	2.09	0.52
1:A2:442:ASN:HD22	2:B2:685:LEU:HD21	1.74	0.52
19:A:804:CLA:HMC2	19:A:852:CLA:CAC	2.40	0.52
2:B2:170:SER:OG	19:B2:810:CLA:HBC1	2.10	0.52
2:BB:553:LEU:HD21	2:BB:574:THR:HG22	1.91	0.52
17:E:8:VAL:CG2	17:E:58:LEU:HD22	2.38	0.52
6:FF:76:VAL:HG12	6:FF:86:PHE:HB2	1.90	0.52
9:K1:71:ILE:HD11	23:K1:106:BCR:C36	2.39	0.52
2:B1:248:GLN:N	2:B1:248:GLN:OE1	2.43	0.52
19:B:834:CLA:H42	23:F:303:BCR:H392	1.91	0.52
2:B:459:ILE:HG22	6:F:74:LEU:HB2	1.91	0.52
19:A:822:CLA:HMA2	9:K:64:ALA:HB2	1.92	0.52
19:LL:201:CLA:H92	19:LL:201:CLA:C3	2.40	0.52
1:A:172:LEU:HD11	19:A:812:CLA:HBC1	1.90	0.52
1:A1:14:ARG:HH21	1:A1:16:ILE:HD11	1.75	0.52
23:B1:841:BCR:H343	23:B1:841:BCR:H311	1.90	0.52
2:B:488:VAL:HG12	19:B:832:CLA:HMD3	1.92	0.52
1:A1:59:PHE:CD2	19:A1:806:CLA:HMC2	2.45	0.52
2:B:347:VAL:HB	19:B:823:CLA:H43	1.91	0.52
2:B2:384:ILE:HG21	2:B2:590:ALA:HB1	1.91	0.52
19:A2:805:CLA:C15	23:J2:102:BCR:H353	2.39	0.52
13:F2:157:SER:HB3	12:X2:9:VAL:HG11	1.90	0.52
1:A1:587:SER:O	1:A1:591:HIS:ND1	2.42	0.52
23:A1:851:BCR:H23C	23:A1:851:BCR:H403	1.91	0.52
2:BB:693:PRO:O	18:LL:53:TYR:OH	2.19	0.52
3:CC:38:GLN:HB3	4:DD:106:VAL:HG21	1.91	0.52
1:A1:67:GLU:N	1:A1:67:GLU:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AA:193:ASN:OD1	19:AA:815:CLA:HBC1	2.09	0.52
1:A:251:ILE:HD11	1:A:258:ALA:HB2	1.91	0.51
2:BB:279:ALA:HA	19:BB:813:CLA:HMC3	1.92	0.51
19:BB:828:CLA:O1A	6:FF:153:THR:HG21	2.10	0.51
19:A2:852:CLA:H42	2:B2:442:VAL:HG22	1.91	0.51
2:BB:340:TRP:CH2	23:BB:841:BCR:H372	2.46	0.51
19:F:301:CLA:H43	19:F:302:CLA:CBC	2.41	0.51
19:A2:816:CLA:CHC	23:A2:847:BCR:H352	2.40	0.51
19:AA:853:CLA:HMD3	19:BB:852:CLA:O1A	2.10	0.51
4:D2:5:LEU:CD1	4:D2:86:ILE:HD11	2.40	0.51
23:F1:306:BCR:H371	23:F1:306:BCR:H382	1.92	0.51
18:LL:74:LEU:HD13	18:LL:101:LEU:HD22	1.91	0.51
1:A1:357:LEU:HD11	1:A1:401:LEU:HD22	1.92	0.51
19:A1:801:CLA:OBD	2:B1:677:TYR:OH	2.27	0.51
1:A2:682:PHE:HZ	19:A2:842:CLA:HBC2	1.76	0.51
1:AA:678:PHE:CD2	23:AA:852:BCR:H363	2.45	0.51
1:A1:561:ARG:O	4:D1:62:ARG:NH1	2.43	0.51
2:B2:478:LEU:HB3	2:B2:480:THR:HG23	1.93	0.51
2:B2:520:GLY:N	2:B2:523:ASP:OD2	2.42	0.51
1:A:194:VAL:HG21	1:A:346:THR:HG22	1.92	0.51
19:BB:826:CLA:H72	19:BB:826:CLA:H41	1.93	0.51
1:A2:114:SER:HB3	1:A2:131:VAL:HG21	1.91	0.51
1:A2:286:THR:HG22	1:A2:379:TYR:CE2	2.45	0.51
19:A:852:CLA:H41	19:A:852:CLA:H71	1.93	0.51
19:AA:805:CLA:C15	23:JJ:102:BCR:H353	2.40	0.51
2:B2:488:VAL:HG12	19:B2:832:CLA:HMD3	1.93	0.51
19:B:828:CLA:HBC3	23:F:303:BCR:H362	1.91	0.51
2:BB:727:THR:HG23	19:BB:852:CLA:O1D	2.10	0.51
1:A2:374:MET:CE	19:A2:829:CLA:HMC2	2.41	0.51
19:B1:848:CLA:HMB3	19:B1:849:CLA:OBD	2.11	0.51
2:B2:466:PHE:HD1	2:B2:480:THR:HG21	1.76	0.51
2:B2:552:LYS:NZ	13:F2:158:GLU:OE1	2.42	0.51
2:B:467:ILE:CD1	19:B:831:CLA:HMC3	2.41	0.51
2:BB:653:TRP:O	2:BB:657:PHE:N	2.43	0.51
1:A2:467:ARG:NH2	19:A2:836:CLA:O1D	2.43	0.51
1:AA:453:PHE:CZ	1:AA:457:ILE:HD11	2.46	0.51
2:B1:236:ASN:HD21	2:B1:252:THR:HG1	1.54	0.51
2:BB:326:ILE:HG21	19:BB:820:CLA:HMD3	1.93	0.51
4:D:32:THR:HG22	4:D:57:LEU:HD13	1.92	0.51
17:EE:40:PHE:O	17:EE:49:ASN:ND2	2.41	0.51
19:A1:820:CLA:HBB1	19:A1:820:CLA:HMB1	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:587:SER:O	1:A2:591:HIS:ND1	2.44	0.51
2:B2:422:ILE:HG23	19:B2:835:CLA:CBB	2.41	0.51
2:B2:478:LEU:O	12:X2:41:HIS:NE2	2.44	0.51
2:B:44:GLN:OE1	2:B:162:ARG:NH2	2.44	0.51
19:A1:804:CLA:C15	23:J1:102:BCR:H353	2.40	0.50
1:AA:297:HIS:NE2	19:AA:821:CLA:HMB3	2.26	0.50
2:B1:352:VAL:HG22	19:B1:815:CLA:C2	2.41	0.50
19:B:830:CLA:H42	8:J:36:PHE:CE2	2.45	0.50
19:A1:805:CLA:HMA2	19:A1:812:CLA:HMD2	1.93	0.50
19:A:816:CLA:CHC	23:A:847:BCR:H352	2.41	0.50
2:B1:461:PRO:HG2	2:B1:519:ILE:HD12	1.93	0.50
2:BB:126:THR:CG2	2:BB:270:LEU:HD21	2.41	0.50
6:FF:34:ASN:ND2	6:FF:67:GLY:O	2.45	0.50
19:A1:803:CLA:HMC2	19:A1:852:CLA:CAC	2.41	0.50
1:A2:353:LEU:HB2	19:A2:807:CLA:HMD3	1.94	0.50
1:A:353:LEU:HB2	19:A:807:CLA:HMD3	1.93	0.50
23:A:854:BCR:H361	23:A:854:BCR:H21C	1.92	0.50
1:AA:571:PHE:O	1:AA:587:SER:OG	2.29	0.50
19:A1:852:CLA:HMD3	19:B1:848:CLA:O1A	2.11	0.50
1:A2:693:TYR:N	2:B2:576:ASP:O	2.45	0.50
1:A1:353:LEU:HB2	19:A1:806:CLA:HMD3	1.94	0.50
1:A2:245:LEU:HD21	19:A2:818:CLA:HBC1	1.93	0.50
1:A:680:TRP:O	1:A:683:SER:OG	2.25	0.50
1:AA:204:VAL:HG11	19:AA:815:CLA:CBB	2.42	0.50
2:B1:420:GLU:N	2:B1:420:GLU:OE1	2.45	0.50
15:K2:71:ILE:HD11	23:K2:105:BCR:C36	2.41	0.50
19:B2:820:CLA:HBC2	19:B2:820:CLA:HHD	1.93	0.50
3:CC:35:LYS:HA	17:EE:32:ILE:HG22	1.94	0.50
1:A1:204:VAL:HG11	19:A1:814:CLA:CBB	2.42	0.50
19:A2:833:CLA:HMA1	19:A2:834:CLA:O1D	2.12	0.50
18:L:17:ASN:OD1	18:L:18:ARG:N	2.44	0.50
19:B:854:CLA:HMB3	19:B:858:CLA:OBD	2.11	0.50
19:BB:828:CLA:HBC3	23:FF:303:BCR:H362	1.93	0.50
19:A:810:CLA:H43	19:A:830:CLA:HMD2	1.94	0.50
2:BB:592:ASN:OD1	19:BB:852:CLA:H42	2.11	0.50
19:A1:832:CLA:HMA1	19:A1:833:CLA:O1D	2.12	0.49
1:A2:297:HIS:HE1	19:A2:821:CLA:HMB3	1.76	0.49
1:A2:614:MET:O	1:A2:619:TRP:N	2.41	0.49
2:B2:157:LEU:O	2:B2:162:ARG:NE	2.43	0.49
23:F2:305:BCR:H382	23:F2:305:BCR:H371	1.94	0.49
2:B1:736:THR:O	2:B1:740:PHE:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:455:LYS:NZ	19:B2:830:CLA:OBD	2.39	0.49
19:B:828:CLA:O1A	6:F:153:THR:HG21	2.13	0.49
1:A2:320:HIS:CB	1:A2:325:ILE:HD11	2.43	0.49
23:AA:852:BCR:H23C	23:AA:852:BCR:H403	1.93	0.49
2:BB:523:ASP:O	2:BB:527:HIS:ND1	2.44	0.49
2:B1:556:ASP:OD1	3:C1:66:ARG:NH2	2.45	0.49
3:CC:61:ASP:OD2	17:EE:15:SER:OG	2.15	0.49
19:B2:829:CLA:HMC3	23:F2:305:BCR:C34	2.43	0.49
1:A1:436:ALA:O	1:A1:440:HIS:ND1	2.45	0.49
2:B1:445:ASP:OD1	2:B1:623:LEU:N	2.44	0.49
2:B2:154:TRP:O	2:B2:158:GLN:NE2	2.43	0.49
19:B2:804:CLA:HMD2	11:M2:13:LEU:HD21	1.94	0.49
19:A2:802:CLA:H3A	23:K2:103:BCR:H362	1.94	0.49
1:A:364:THR:HG22	1:A:394:HIS:HB3	1.93	0.49
19:AA:804:CLA:HMC2	19:AA:853:CLA:CAC	2.42	0.49
2:B2:257:PHE:HD2	2:B2:499:VAL:HG23	1.76	0.49
2:B2:422:ILE:HG23	19:B2:835:CLA:HBB2	1.94	0.49
3:CC:42:SER:O	4:DD:114:ARG:NH1	2.46	0.49
19:BB:833:CLA:H42	23:FF:303:BCR:H392	1.94	0.49
19:A2:821:CLA:HMB1	19:A2:821:CLA:HBB1	1.94	0.49
2:B:662:LEU:HD12	19:B:858:CLA:O1A	2.13	0.49
1:A2:711:ALA:O	13:F2:108:LEU:HD21	2.13	0.49
6:F:34:ASN:ND2	6:F:67:GLY:O	2.44	0.49
19:L:202:CLA:H92	19:L:202:CLA:C4	2.43	0.49
19:AA:816:CLA:CHC	23:AA:848:BCR:H352	2.42	0.49
2:B1:347:VAL:HB	19:B1:823:CLA:H43	1.95	0.49
2:B1:480:THR:OG1	2:B1:481:LEU:N	2.46	0.49
2:B2:690:GLU:OE1	4:D2:20:LEU:HD22	2.13	0.49
3:C1:29:VAL:HG12	4:D1:110:ARG:HB3	1.94	0.49
1:A:121:ILE:O	1:A:123:GLY:N	2.45	0.49
19:B:826:CLA:H41	19:B:826:CLA:C7	2.42	0.49
1:AA:364:THR:HG22	1:AA:394:HIS:HB3	1.95	0.49
2:B:334:LEU:HD22	19:B:802:CLA:H201	1.94	0.49
10:L1:68:MET:HE1	19:L1:205:CLA:HED2	1.95	0.49
1:A2:617:ASP:O	1:A2:630:HIS:NE2	2.46	0.49
1:A2:245:LEU:CD2	19:A2:818:CLA:HBC1	2.43	0.49
23:A:851:BCR:H403	23:A:851:BCR:H23C	1.93	0.49
19:B:820:CLA:HBC3	19:B:820:CLA:HHD	1.94	0.49
19:BB:828:CLA:CBB	19:FF:305:CLA:H202	2.43	0.49
1:A:30:ALA:O	6:F:123:GLN:NE2	2.45	0.49
1:A1:307:ILE:HG12	23:K1:106:BCR:H362	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:806:CLA:HMA2	19:A2:813:CLA:HMD2	1.95	0.48
19:BB:856:CLA:HMC3	19:FF:301:CLA:C4D	2.43	0.48
1:A1:297:HIS:HE1	19:A1:820:CLA:HMB3	1.78	0.48
19:B1:827:CLA:O1D	12:X1:11:ASN:ND2	2.46	0.48
19:B:859:CLA:HMC3	19:F:301:CLA:C4D	2.43	0.48
1:A1:710:VAL:HG12	1:A1:710:VAL:O	2.13	0.48
19:A1:815:CLA:CHC	23:A1:847:BCR:H352	2.43	0.48
1:A1:245:LEU:CD2	19:A1:817:CLA:HBC1	2.44	0.48
1:AA:18:ASP:OD2	1:AA:71:ARG:NH2	2.43	0.48
19:B:854:CLA:HMB3	19:B:858:CLA:CAD	2.43	0.48
2:BB:32:GLU:OE1	2:BB:335:HIS:NE2	2.43	0.48
2:BB:384:ILE:HG23	2:BB:590:ALA:HB1	1.94	0.48
13:F2:46:ASN:ND2	13:F2:51:PRO:O	2.46	0.48
9:K:28:ASN:HD21	9:K:66:THR:HG22	1.79	0.48
1:A2:204:VAL:HG11	19:A2:815:CLA:CBB	2.44	0.48
19:AA:820:CLA:CMD	19:AA:821:CLA:H202	2.43	0.48
19:B:828:CLA:CBB	19:B:829:CLA:H202	2.43	0.48
19:BB:833:CLA:C9	19:BB:834:CLA:HBC1	2.40	0.48
19:F1:301:CLA:H42	8:J1:22:ALA:HA	1.95	0.48
16:L2:152:GLY:O	16:L2:156:VAL:HG23	2.13	0.48
19:A:820:CLA:CMD	19:A:821:CLA:H202	2.43	0.48
1:AA:326:LEU:HD23	19:AA:826:CLA:O1D	2.14	0.48
19:B2:828:CLA:CBB	19:B2:829:CLA:H202	2.43	0.48
19:F2:301:CLA:H42	8:J2:22:ALA:HA	1.96	0.48
1:A1:337:GLY:C	1:A1:426:VAL:HG23	2.34	0.48
1:AA:24:THR:HG21	1:AA:178:TRP:HE1	1.77	0.48
1:AA:710:VAL:HG12	1:AA:710:VAL:O	2.13	0.48
23:B1:841:BCR:H343	23:B1:841:BCR:C31	2.43	0.48
3:CC:60:THR:OG1	3:CC:62:PHE:O	2.27	0.48
1:A1:299:LEU:HD13	19:A1:816:CLA:HMC1	1.95	0.48
2:B:272:ASP:O	2:B:276:HIS:N	2.47	0.48
3:C:60:THR:OG1	3:C:62:PHE:O	2.32	0.48
2:B:297:ILE:CG2	19:B:818:CLA:HMD1	2.43	0.48
2:BB:216:ALA:HA	19:BB:812:CLA:HED1	1.95	0.48
6:FF:66:CYS:SG	6:FF:67:GLY:N	2.86	0.48
20:A1:802:CL0:CAB	19:A1:852:CLA:HED1	2.43	0.48
1:A2:562:LEU:HD21	1:A2:583:THR:HG22	1.95	0.48
19:A2:806:CLA:HBC2	19:A2:832:CLA:H43	1.96	0.48
1:AA:122:VAL:HG21	19:BB:829:CLA:HMD1	1.96	0.48
1:AA:524:MET:CE	1:AA:628:VAL:HG11	2.44	0.48
19:AA:828:CLA:OBD	19:AA:828:CLA:HED2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:K1:103:CLA:H3A	23:K1:104:BCR:H362	1.95	0.48
18:LL:61:ARG:NH1	19:LL:201:CLA:O2D	2.47	0.48
1:A:122:VAL:CG1	19:B:830:CLA:HMD1	2.43	0.48
2:B1:460:GLU:OE2	2:B1:465:GLN:NE2	2.45	0.48
3:C1:2:SER:OG	3:C1:3:HIS:N	2.46	0.48
2:B1:459:ILE:HG22	6:F1:74:LEU:HB2	1.95	0.48
19:B2:834:CLA:H42	23:F2:303:BCR:H392	1.96	0.48
9:KK:21:GLY:O	9:KK:25:VAL:HG23	2.14	0.48
1:A1:447:PHE:O	1:A1:451:HIS:ND1	2.45	0.47
20:A1:802:CLO:H13	19:A1:852:CLA:OBD	2.14	0.47
1:A:326:LEU:HD23	19:A:826:CLA:O1D	2.14	0.47
2:B:594:VAL:O	2:B:598:THR:OG1	2.17	0.47
21:A:843:PQN:H211	19:B:859:CLA:HBC1	1.96	0.47
6:F:76:VAL:HG12	6:F:86:PHE:HB2	1.96	0.47
19:A1:839:CLA:H91	19:L1:206:CLA:H192	1.96	0.47
19:AA:830:CLA:HBB1	19:AA:830:CLA:HMB1	1.96	0.47
2:B1:124:TRP:HA	2:B1:127:ILE:HD12	1.95	0.47
2:B1:531:ALA:HB2	19:B1:833:CLA:HBB1	1.96	0.47
19:B:833:CLA:O1D	19:B:834:CLA:HMB1	2.13	0.47
28:BB:854:DGD:C1A	28:BB:854:DGD:HO2D	2.27	0.47
10:L1:68:MET:CE	19:L1:205:CLA:HED2	2.43	0.47
19:A:801:CLA:OBD	2:B:677:TYR:OH	2.22	0.47
1:AA:585:GLN:OE1	2:BB:674:TRP:N	2.41	0.47
2:B2:394:GLY:HA2	23:B2:843:BCR:H393	1.95	0.47
2:B:481:LEU:HD21	12:X:38:TYR:CD1	2.49	0.47
3:C1:14:CYS:N	27:C1:102:SF4:S1	2.87	0.47
1:A1:114:SER:HB3	1:A1:131:VAL:HG21	1.94	0.47
1:A2:561:ARG:O	4:D2:62:ARG:NH1	2.47	0.47
2:B1:123:TRP:NE1	2:B1:127:ILE:HD11	2.29	0.47
2:BB:123:TRP:CZ2	19:BB:810:CLA:H191	2.49	0.47
9:K:21:GLY:O	9:K:25:VAL:HG23	2.14	0.47
1:A:156:SER:O	1:A:160:TYR:N	2.47	0.47
1:A2:101:TYR:O	1:A2:105:LEU:HD23	2.13	0.47
1:A:435:ASP:OD2	1:A:561:ARG:NH2	2.47	0.47
2:B1:343:ALA:HB2	23:B1:842:BCR:H372	1.96	0.47
19:A1:852:CLA:H42	2:B1:442:VAL:HG22	1.96	0.47
4:DD:105:LYS:O	4:DD:110:ARG:NH2	2.47	0.47
19:A1:834:CLA:H93	19:B1:836:CLA:H142	1.96	0.47
2:B1:126:THR:CG2	2:B1:270:LEU:HD21	2.45	0.47
2:B2:3:THR:OG1	2:B2:20:ARG:NH2	2.47	0.47
2:B:326:ILE:CG2	19:B:820:CLA:HMD3	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:BB:804:CLA:HAA2	19:BB:806:CLA:HED1	1.96	0.47
19:BB:811:CLA:H43	26:BB:840:ECH:H36A	1.97	0.47
17:EE:2:VAL:O	17:EE:27:VAL:HG21	2.13	0.47
23:F1:306:BCR:H381	19:J1:103:CLA:HBC3	1.96	0.47
1:A1:114:SER:CB	1:A1:131:VAL:HG21	2.45	0.47
19:A1:841:CLA:H41	19:A1:841:CLA:H71	1.97	0.47
2:B1:157:LEU:O	2:B1:162:ARG:NE	2.43	0.47
2:B:297:ILE:HG22	19:B:818:CLA:HMD1	1.96	0.47
19:B1:828:CLA:H202	19:F1:305:CLA:CBB	2.44	0.47
19:A2:804:CLA:HMC2	19:A2:852:CLA:HAC1	1.96	0.47
19:A2:831:CLA:HMD2	19:A2:831:CLA:H92	1.97	0.47
2:B1:394:GLY:HA2	23:B1:842:BCR:H393	1.97	0.47
2:B2:273:MET:O	2:B2:277:HIS:ND1	2.46	0.47
2:BB:126:THR:HG23	2:BB:270:LEU:HD21	1.97	0.47
3:C2:17:CYS:SG	3:C2:18:VAL:N	2.87	0.47
1:A2:596:LEU:HD21	19:A2:832:CLA:HBC1	1.97	0.47
1:AA:349:TRP:HE3	19:AA:807:CLA:HMD2	1.80	0.47
2:B1:488:VAL:HG12	19:B1:831:CLA:HMD3	1.97	0.47
19:A2:852:CLA:HMB3	19:B2:849:CLA:H191	1.96	0.47
2:B2:91:ILE:HG22	19:B2:806:CLA:OBD	2.14	0.47
3:C:24:ASP:OD2	4:D:96:HIS:ND1	2.48	0.47
1:A2:59:PHE:CD2	19:A2:807:CLA:HMC2	2.50	0.47
19:A:828:CLA:OBD	19:A:828:CLA:HED2	2.15	0.47
19:AA:821:CLA:HBB1	19:AA:821:CLA:HMB1	1.97	0.47
2:B1:123:TRP:CE2	2:B1:127:ILE:HD11	2.50	0.47
2:B1:59:LEU:HD23	2:B1:143:LEU:HD23	1.95	0.47
2:BB:59:LEU:HD23	2:BB:143:LEU:HD23	1.97	0.47
2:BB:69:ALA:HB3	11:MM:4:ILE:HD11	1.97	0.47
10:L1:148:ILE:HD11	18:L:64:LEU:HD21	1.96	0.47
23:AA:855:BCR:H361	23:AA:855:BCR:H21C	1.97	0.47
2:B:71:GLN:NE2	19:B:804:CLA:O1D	2.47	0.47
3:CC:2:SER:OG	3:CC:71:ALA:O	2.22	0.47
6:F:87:LEU:O	6:F:90:SER:OG	2.13	0.47
1:A:121:ILE:HG22	1:A:124:GLN:HE21	1.80	0.46
19:A2:842:CLA:H71	19:A2:842:CLA:H41	1.97	0.46
1:A2:432:ARG:NH1	4:D2:14:GLY:O	2.46	0.46
1:A2:16:ILE:HD11	1:A2:189:GLU:HB2	1.97	0.46
19:BB:829:CLA:H42	8:JJ:36:PHE:CE2	2.50	0.46
3:C:35:LYS:HA	17:E:32:ILE:HG22	1.97	0.46
15:K2:70:HIS:O	15:K2:74:VAL:HG23	2.16	0.46
1:A1:337:GLY:O	1:A1:426:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B2:59:LEU:HD23	2:B2:143:LEU:HD23	1.97	0.46
2:BB:319:PHE:CD2	19:BB:820:CLA:HMA1	2.51	0.46
2:BB:523:ASP:OD1	2:BB:600:TYR:OH	2.20	0.46
1:AA:119:TRP:HE1	23:AA:854:BCR:H332	1.80	0.46
19:B1:804:CLA:HAA2	19:B1:806:CLA:HED1	1.97	0.46
19:B1:807:CLA:H162	19:B1:807:CLA:H141	1.72	0.46
19:B:826:CLA:H41	19:B:826:CLA:H72	1.96	0.46
8:J:49:PRO:HB3	19:J:103:CLA:HED1	1.96	0.46
15:K2:48:LEU:HD23	15:K2:54:PHE:CG	2.50	0.46
1:A:59:PHE:CD2	19:A:807:CLA:HMC2	2.51	0.46
2:B2:125:TYR:O	2:B2:130:ARG:NH1	2.48	0.46
2:B2:420:GLU:OE1	2:B2:420:GLU:N	2.49	0.46
2:B2:526:VAL:HG23	19:B2:849:CLA:H141	1.97	0.46
2:B:256:THR:HG1	2:B:271:THR:HG1	1.56	0.46
19:B:836:CLA:HAB	21:B:838:PQN:H192	1.98	0.46
19:BB:820:CLA:HBC3	19:BB:820:CLA:HHD	1.96	0.46
2:B1:170:SER:OG	19:B1:810:CLA:HBC1	2.14	0.46
2:B2:118:SER:O	2:B2:375:LEU:HD21	2.16	0.46
19:BB:820:CLA:O1A	23:BB:841:BCR:H352	2.15	0.46
1:AA:694:TRP:CZ2	21:AA:844:PQN:H2M3	2.50	0.46
2:B1:526:VAL:HG23	19:B1:848:CLA:H141	1.96	0.46
2:B2:174:ARG:HB2	19:B2:810:CLA:HBC2	1.96	0.46
1:A2:114:SER:CB	1:A2:131:VAL:HG21	2.46	0.46
1:A:453:PHE:CZ	1:A:457:ILE:HD11	2.51	0.46
1:A:349:TRP:HE3	19:A:807:CLA:HMD2	1.81	0.46
1:AA:155:ASN:OD1	1:AA:155:ASN:N	2.49	0.46
1:A1:15:VAL:HG11	19:A1:811:CLA:CBA	2.46	0.46
19:B1:833:CLA:C9	19:B1:834:CLA:HBC1	2.43	0.46
6:F1:153:THR:HG21	19:F1:305:CLA:O1A	2.16	0.46
19:A2:801:CLA:OBD	2:B2:677:TYR:OH	2.27	0.46
19:A:806:CLA:HBC2	19:A:832:CLA:H43	1.96	0.46
1:A1:122:VAL:CG1	19:B1:829:CLA:HMD1	2.46	0.46
2:B:524:PHE:O	2:B:528:HIS:ND1	2.48	0.46
2:BB:533:GLY:HA3	2:BB:593:THR:HG22	1.96	0.46
1:A1:678:PHE:CD2	23:A1:851:BCR:H363	2.51	0.45
1:A2:678:PHE:CG	23:A2:851:BCR:H363	2.51	0.45
19:A:852:CLA:HMB3	19:B:854:CLA:C19	2.45	0.45
1:AA:426:VAL:O	1:AA:430:VAL:HG23	2.16	0.45
19:B:837:CLA:HMB2	23:B:844:BCR:C12	2.46	0.45
2:BB:352:VAL:CG2	19:BB:815:CLA:H43	2.46	0.45
5:E2:10:ILE:HD11	5:E2:40:PHE:CZ	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:FF:65:LEU:HD12	6:FF:75:ILE:HD12	1.98	0.45
7:I:39:TYR:HH	11:M:31:TYR:HH	1.58	0.45
19:A1:803:CLA:H193	19:A1:852:CLA:H192	1.99	0.45
19:A:830:CLA:HMC1	19:A:830:CLA:HBC2	1.99	0.45
2:B1:174:ARG:HB2	19:B1:810:CLA:HBC2	1.98	0.45
19:B1:828:CLA:HMC3	23:F1:306:BCR:C34	2.46	0.45
1:A2:43:PRO:HG3	13:F2:122:ILE:HD12	1.98	0.45
8:J1:33:LEU:O	8:J1:37:ASN:ND2	2.48	0.45
19:B:827:CLA:O1D	12:X:11:ASN:ND2	2.49	0.45
19:A2:828:CLA:HAB	23:A2:850:BCR:H311	1.99	0.45
1:AA:59:PHE:CD2	19:AA:807:CLA:HMC2	2.51	0.45
19:AA:806:CLA:HBC2	19:AA:832:CLA:H43	1.98	0.45
2:B2:101:ILE:O	2:B2:105:THR:HG23	2.16	0.45
2:BB:343:ALA:HB2	23:BB:842:BCR:H372	1.97	0.45
16:L2:27:ASP:OD1	16:L2:29:GLN:NE2	2.49	0.45
1:A2:122:VAL:CG1	19:B2:830:CLA:HMD1	2.47	0.45
1:A:227:LEU:HD21	1:A:253:LEU:HD11	1.99	0.45
19:B:829:CLA:HMC3	23:F:305:BCR:C34	2.47	0.45
17:E:40:PHE:O	17:E:49:ASN:ND2	2.49	0.45
23:F2:305:BCR:H15C	23:F2:305:BCR:H351	1.79	0.45
1:A1:389:CYS:HB3	19:A1:829:CLA:HMA1	1.99	0.45
10:L1:126:VAL:HG13	10:L1:126:VAL:O	2.16	0.45
1:A2:584:CYS:O	2:B2:676:GLY:N	2.49	0.45
1:A2:172:LEU:HD11	19:A2:812:CLA:HBC1	1.98	0.45
2:B2:279:ALA:HA	19:B2:813:CLA:HMC3	1.99	0.45
19:BB:835:CLA:HAB	21:BB:837:PQN:H192	1.99	0.45
21:AA:844:PQN:H211	19:BB:856:CLA:HBC1	1.98	0.45
11:M:14:VAL:HG23	23:M:101:BCR:H391	1.98	0.45
19:A1:830:CLA:H92	19:A1:830:CLA:HMD2	1.99	0.45
23:B2:842:BCR:HC8	23:B2:842:BCR:H331	1.99	0.45
23:B:842:BCR:H343	23:B:842:BCR:C31	2.46	0.45
2:BB:58:PHE:HD1	2:BB:142:LEU:HD22	1.81	0.45
23:BB:841:BCR:C31	23:BB:841:BCR:H343	2.45	0.45
19:FF:305:CLA:HMC3	23:FF:306:BCR:C34	2.47	0.45
1:A2:560:SER:N	1:A2:563:ILE:O	2.49	0.45
1:A:268:ASN:ND2	1:A:271:GLN:OE1	2.50	0.45
19:A:806:CLA:HMA2	19:A:813:CLA:HMD2	1.97	0.45
19:A:852:CLA:H42	2:B:442:VAL:HG22	1.99	0.45
2:B1:381:TYR:HB3	19:B1:824:CLA:HMC3	1.99	0.45
18:LL:118:PRO:O	18:LL:119:THR:HG23	2.17	0.45
19:A2:852:CLA:H71	19:A2:852:CLA:H41	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:805:CLA:CGA	19:AA:842:CLA:H43	2.47	0.45
23:AA:852:BCR:H362	19:AA:853:CLA:C4	2.46	0.45
2:B1:279:ALA:HA	19:B1:813:CLA:HMC3	1.99	0.45
3:C1:25:VAL:HG21	3:C1:48:CYS:HB2	1.98	0.45
10:L1:114:ASN:ND2	22:L1:211:LHG:O9	2.50	0.45
16:L2:118:PRO:O	16:L2:119:THR:HG23	2.17	0.45
1:A:204:VAL:HG11	19:A:815:CLA:CBB	2.47	0.45
2:B2:468:GLN:OE1	19:B2:833:CLA:HMB1	2.17	0.45
2:BB:384:ILE:HD11	2:BB:594:VAL:HB	1.98	0.45
2:BB:69:ALA:HB1	11:MM:4:ILE:HD11	1.99	0.45
17:E:8:VAL:HG21	17:E:58:LEU:HD22	1.98	0.45
9:K1:21:GLY:O	9:K1:25:VAL:HG23	2.17	0.45
19:A2:844:CLA:OBD	16:L2:18:ARG:NH2	2.50	0.45
1:A1:336:GLU:OE1	1:A1:336:GLU:N	2.49	0.44
1:A1:553:GLY:O	1:A1:557:ALA:HB2	2.17	0.44
2:BB:101:ILE:O	2:BB:105:THR:HG23	2.17	0.44
2:BB:347:VAL:HB	19:BB:823:CLA:H43	1.99	0.44
2:BB:707:LEU:N	21:BB:837:PQN:O4	2.47	0.44
2:B2:5:PHE:CD1	14:I2:40:ILE:HG22	2.52	0.44
23:F:305:BCR:C28	19:J:103:CLA:HMD3	2.47	0.44
19:A:804:CLA:HMC2	19:A:852:CLA:HAC1	1.99	0.44
1:AA:658:VAL:HG22	1:AA:746:ALA:HB3	1.99	0.44
2:B2:59:LEU:CD2	2:B2:143:LEU:HD23	2.47	0.44
2:BB:76:GLN:N	2:BB:76:GLN:OE1	2.50	0.44
17:E:11:LEU:HD12	17:E:11:LEU:O	2.17	0.44
1:AA:43:PRO:HG3	6:FF:122:ILE:HD12	1.97	0.44
19:A1:803:CLA:HMC2	19:A1:852:CLA:HAC1	2.00	0.44
1:A:429:ARG:O	1:A:433:HIS:ND1	2.51	0.44
19:A:842:CLA:H41	19:A:842:CLA:H71	2.00	0.44
23:A:851:BCR:H362	19:A:852:CLA:C4	2.45	0.44
2:B:173:SER:HA	2:B:293:THR:HG22	1.99	0.44
2:B1:424:SER:OG	19:B1:850:CLA:HED3	2.17	0.44
23:B2:842:BCR:C8	23:B2:842:BCR:H331	2.46	0.44
19:B:804:CLA:HAA2	19:B:806:CLA:HED1	1.98	0.44
19:B:811:CLA:HMB1	19:B:811:CLA:HBB1	2.00	0.44
2:BB:492:ALA:HB3	2:BB:495:ASN:O	2.17	0.44
13:F2:107:TYR:CE2	13:F2:111:ILE:HD11	2.53	0.44
2:B2:243:ILE:O	2:B2:246:THR:OG1	2.33	0.44
2:BB:428:TRP:HZ3	19:BB:834:CLA:HBC2	1.82	0.44
2:BB:481:LEU:HD21	12:XX:38:TYR:CD1	2.52	0.44
1:A1:589:TRP:NE1	19:A1:831:CLA:HMD1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:453:PHE:CZ	1:A2:457:ILE:HD11	2.53	0.44
2:B:398:LEU:O	2:B:549:ARG:NH1	2.50	0.44
23:B:839:BCR:H311	23:B:839:BCR:HC8	1.98	0.44
23:F:305:BCR:H381	19:J:103:CLA:HBC3	1.98	0.44
6:F:88:ILE:HG12	19:J:103:CLA:HMB3	1.99	0.44
8:J2:38:ARG:HH11	23:J2:104:BCR:H311	1.82	0.44
19:A2:815:CLA:HBB1	19:A2:815:CLA:HMB1	1.99	0.44
19:A2:842:CLA:H93	21:A2:843:PQN:H293	2.00	0.44
1:AA:577:GLY:O	1:AA:583:THR:OG1	2.35	0.44
2:B2:587:LEU:HD23	2:B2:717:LEU:CD2	2.38	0.44
3:C2:14:CYS:O	3:C2:15:THR:OG1	2.23	0.44
4:D2:5:LEU:HD11	4:D2:86:ILE:HD11	1.99	0.44
19:A1:827:CLA:HAB	23:A1:850:BCR:H311	1.98	0.44
19:A1:852:CLA:H71	19:A1:852:CLA:H41	2.00	0.44
1:A2:397:ILE:HD13	19:A2:830:CLA:HBC3	1.99	0.44
19:B:806:CLA:H203	23:L:205:BCR:C31	2.47	0.44
19:B:822:CLA:H143	19:B:832:CLA:HBB2	2.00	0.44
2:BB:715:VAL:O	2:BB:719:HIS:ND1	2.50	0.44
23:BB:838:BCR:HC8	23:BB:838:BCR:H311	1.98	0.44
2:B:289:HIS:CE1	23:B:839:BCR:H363	2.53	0.44
15:K2:48:LEU:HD23	15:K2:54:PHE:CD2	2.53	0.44
1:A1:16:ILE:HG21	1:A1:187:LYS:HD3	2.00	0.44
1:A1:432:ARG:NH1	4:D1:13:ALA:HB3	2.33	0.44
1:A2:101:TYR:CZ	1:A2:105:LEU:HD21	2.53	0.44
2:B1:675:ARG:O	2:B1:678:TRP:N	2.46	0.44
2:B1:69:ALA:CB	11:M1:4:ILE:HD11	2.47	0.44
19:B1:814:CLA:HMD2	19:B1:815:CLA:H202	2.00	0.44
19:B1:850:CLA:C14	19:F1:301:CLA:HED2	2.48	0.44
2:BB:157:LEU:O	2:BB:162:ARG:NE	2.45	0.44
6:F1:76:VAL:O	6:F1:76:VAL:HG22	2.17	0.44
19:A1:804:CLA:CGA	19:A1:841:CLA:H43	2.48	0.43
1:A2:118:VAL:O	1:A2:128:ASN:ND2	2.50	0.43
1:A:506:VAL:HG23	19:A:837:CLA:HED3	2.00	0.43
1:A:590:ASP:OD1	1:A:725:ARG:NH1	2.51	0.43
19:B2:816:CLA:CMB	19:B2:821:CLA:HMA3	2.47	0.43
2:B:59:LEU:HD23	2:B:143:LEU:HD23	2.00	0.43
1:A1:349:TRP:HE3	19:A1:806:CLA:HMD2	1.83	0.43
2:B1:481:LEU:HD21	12:X1:38:TYR:CD1	2.53	0.43
1:A:584:CYS:O	2:B:676:GLY:N	2.51	0.43
23:F:305:BCR:H371	23:F:305:BCR:H382	2.00	0.43
1:A:447:PHE:O	1:A:451:HIS:ND1	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:AA:822:CLA:HMA2	9:KK:64:ALA:HB2	1.99	0.43
1:AA:341:LEU:HD13	19:AA:826:CLA:HMD3	1.99	0.43
2:B1:468:GLN:OE1	19:B1:832:CLA:HMB1	2.17	0.43
19:B:829:CLA:CAB	19:B:830:CLA:HMB2	2.48	0.43
2:BB:258:LEU:HD23	2:BB:269:TRP:CE2	2.53	0.43
2:BB:516:PHE:CE1	19:BB:823:CLA:HBC2	2.54	0.43
23:FF:303:BCR:H333	19:FF:305:CLA:H142	2.00	0.43
2:B1:531:ALA:HB2	19:B1:833:CLA:CBB	2.48	0.43
2:B:653:TRP:O	2:B:657:PHE:N	2.46	0.43
11:M:14:VAL:CG2	23:M:101:BCR:H391	2.48	0.43
1:A1:359:PHE:CG	19:A1:826:CLA:HMB2	2.54	0.43
1:A2:436:ALA:O	1:A2:440:HIS:ND1	2.52	0.43
1:A:694:TRP:CE2	21:A:843:PQN:H2M3	2.52	0.43
19:B1:820:CLA:HHD	19:B1:820:CLA:HBC2	2.01	0.43
23:J2:104:BCR:H392	23:J2:104:BCR:H23C	2.01	0.43
24:L2:203:AJP:OBC	24:L2:203:AJP:OBZ	2.36	0.43
1:A1:282:LEU:HD23	1:A1:289:LEU:HD23	2.00	0.43
19:A:830:CLA:HBB1	19:A:830:CLA:HMB1	2.01	0.43
19:AA:842:CLA:H71	19:AA:842:CLA:H41	2.01	0.43
2:B:531:ALA:HB2	19:B:834:CLA:CBB	2.49	0.43
28:B:856:DGD:HO2D	28:B:856:DGD:C1A	2.30	0.43
2:BB:531:ALA:HB2	19:BB:833:CLA:CBB	2.48	0.43
19:AA:806:CLA:HMA2	19:AA:813:CLA:HMD2	2.01	0.43
19:B2:821:CLA:HMB1	19:B2:821:CLA:HBB1	1.99	0.43
3:C:11:CYS:SG	3:C:12:ILE:N	2.92	0.43
24:L1:204:AJP:OBZ	24:L1:204:AJP:OBC	2.36	0.43
1:A:313:ARG:O	19:A:822:CLA:HED2	2.18	0.43
1:A:39:LEU:HD11	1:A:55:LEU:HD12	2.01	0.43
1:AA:477:ILE:O	1:AA:477:ILE:HG22	2.19	0.43
2:B2:257:PHE:CD2	2:B2:499:VAL:HG23	2.53	0.43
2:B2:30:ASP:O	2:B2:34:HIS:ND1	2.52	0.43
19:B2:831:CLA:HMD2	19:B2:832:CLA:CHC	2.49	0.43
2:B:43:TYR:CZ	2:B:334:LEU:HD21	2.54	0.43
2:BB:123:TRP:CH2	19:BB:810:CLA:H191	2.54	0.43
13:F2:88:ILE:HG12	19:J2:103:CLA:HMB3	2.01	0.43
19:B2:834:CLA:H43	19:X2:101:CLA:C4D	2.49	0.43
1:A1:196:SER:O	1:A1:200:HIS:ND1	2.45	0.43
19:A1:805:CLA:HBC2	19:A1:831:CLA:H43	2.00	0.43
19:A1:841:CLA:H93	21:A1:843:PQN:H293	2.00	0.43
19:A2:840:CLA:CBB	19:A2:841:CLA:HBC3	2.49	0.43
19:A2:805:CLA:CGA	19:A2:842:CLA:H43	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:TRP:CZ2	21:A:843:PQN:H2M3	2.54	0.43
2:B1:273:MET:SD	19:B1:815:CLA:HED1	2.59	0.43
23:B1:838:BCR:HC8	23:B1:838:BCR:H311	2.01	0.43
19:B2:809:CLA:CMC	23:B2:840:BCR:H343	2.49	0.43
4:D1:101:VAL:HG11	4:D1:107:ASN:HB2	2.00	0.43
3:C1:24:ASP:OD2	4:D1:96:HIS:ND1	2.51	0.43
1:A1:114:SER:OG	1:A1:131:VAL:HG21	2.19	0.43
19:A1:829:CLA:HBB1	19:A1:829:CLA:HMB1	2.00	0.43
19:A1:839:CLA:CBB	19:A1:840:CLA:HBC3	2.49	0.43
19:A1:815:CLA:HHB	23:A1:847:BCR:H331	2.00	0.43
1:AA:245:LEU:CD2	19:AA:818:CLA:HBC1	2.48	0.43
19:B:820:CLA:O1A	23:B:842:BCR:H352	2.19	0.43
2:BB:105:THR:HG22	2:BB:111:GLY:C	2.39	0.43
1:A2:13:ALA:HB3	1:A2:315:ASN:OD1	2.18	0.42
1:A2:342:TYR:O	1:A2:346:THR:OG1	2.23	0.42
1:A:424:ASN:OD1	1:A:429:ARG:NH1	2.52	0.42
19:A:833:CLA:HMA1	19:A:834:CLA:O1D	2.18	0.42
19:AA:826:CLA:HAB	19:AA:833:CLA:HMD2	2.00	0.42
2:B1:118:SER:O	2:B1:375:LEU:HD21	2.19	0.42
2:B1:428:TRP:HZ3	19:B1:834:CLA:HBC2	1.84	0.42
2:B1:433:LEU:HD11	19:B1:833:CLA:HMC3	2.01	0.42
2:B1:257:PHE:CD2	2:B1:499:VAL:HG23	2.53	0.42
19:B1:809:CLA:CMC	23:B1:839:BCR:H343	2.49	0.42
16:L2:147:LEU:HD21	19:LL:201:CLA:O1A	2.18	0.42
1:A1:521:VAL:HG11	1:A1:618:VAL:O	2.19	0.42
1:A1:57:HIS:O	19:A1:806:CLA:HMC3	2.19	0.42
1:A2:336:GLU:OE1	1:A2:336:GLU:N	2.52	0.42
2:B2:643:ASN:OD1	2:B2:646:GLY:N	2.48	0.42
2:B:478:LEU:HB3	2:B:480:THR:HG23	2.01	0.42
2:B:74:PHE:CZ	2:B:78:ILE:HD11	2.54	0.42
23:B:843:BCR:H371	23:B:843:BCR:H24C	1.92	0.42
2:BB:415:VAL:HG11	23:BB:841:BCR:H401	2.01	0.42
23:FF:306:BCR:H371	23:FF:306:BCR:H382	2.01	0.42
19:B1:827:CLA:HED3	12:X1:11:ASN:CB	2.49	0.42
19:A:820:CLA:H92	19:A:837:CLA:O1A	2.19	0.42
2:B2:466:PHE:CD1	2:B2:480:THR:HG21	2.54	0.42
22:L1:211:LHG:C9	19:L:202:CLA:HMD2	2.49	0.42
19:A2:815:CLA:HBA2	19:A2:815:CLA:H3A	1.89	0.42
1:AA:694:TRP:CE2	21:AA:844:PQN:H2M3	2.54	0.42
2:B1:125:TYR:O	2:B1:130:ARG:NH1	2.52	0.42
2:B1:167:TRP:CZ2	19:B1:808:CLA:HMA1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A2:835:CLA:H93	19:B2:837:CLA:H142	2.02	0.42
20:AA:803:CL0:H22	2:BB:632:TRP:HD1	1.84	0.42
18:LL:52:ALA:HB2	19:LL:202:CLA:HMD1	2.00	0.42
19:A1:824:CLA:HMC1	19:A1:828:CLA:H202	2.01	0.42
1:A2:553:GLY:O	1:A2:557:ALA:HB2	2.19	0.42
19:A2:805:CLA:H41	19:A2:805:CLA:H71	2.01	0.42
19:B1:830:CLA:HMD2	19:B1:831:CLA:CHC	2.50	0.42
19:B2:806:CLA:H41	19:B2:806:CLA:H72	2.01	0.42
23:B2:839:BCR:H311	23:B2:839:BCR:HC8	2.01	0.42
19:B:834:CLA:C9	19:B:835:CLA:HBC1	2.40	0.42
2:BB:223:GLN:NE2	2:BB:227:THR:OG1	2.53	0.42
9:KK:76:LEU:O	9:KK:80:LEU:HD23	2.20	0.42
1:A1:370:HIS:ND1	19:A1:819:CLA:OBD	2.53	0.42
1:A2:395:ILE:HG22	1:A2:603:LEU:HD12	2.01	0.42
1:AA:532:ASP:O	1:AA:536:HIS:ND1	2.46	0.42
1:AA:334:THR:HG21	22:AA:847:LHG:HC12	2.01	0.42
19:B1:831:CLA:CHD	19:B1:845:CLA:HMD2	2.50	0.42
2:B2:459:ILE:HG22	13:F2:74:LEU:HB2	2.00	0.42
2:B:46:ILE:O	2:B:49:THR:OG1	2.35	0.42
2:B:343:ALA:HB2	23:B:843:BCR:H372	2.01	0.42
2:BB:594:VAL:HG22	2:BB:598:THR:HG23	2.01	0.42
23:BB:841:BCR:H331	23:BB:841:BCR:C8	2.50	0.42
3:C1:7:ILE:HD13	3:C1:40:ALA:C	2.39	0.42
11:M:3:SER:OG	11:M:4:ILE:N	2.53	0.42
19:A1:814:CLA:HBB1	19:A1:814:CLA:HMB1	2.02	0.42
1:A2:21:PRO:HG3	1:A2:185:ALA:HB2	2.01	0.42
1:A2:343:GLU:N	1:A2:343:GLU:OE2	2.53	0.42
1:A:318:ILE:HG12	19:A:824:CLA:HMD1	2.01	0.42
2:B1:105:THR:O	2:B1:105:THR:HG23	2.19	0.42
20:A2:803:CL0:H48	19:B2:850:CLA:HMA3	2.01	0.42
2:BB:491:THR:O	2:BB:491:THR:HG23	2.20	0.42
19:BB:821:CLA:HBB1	19:BB:821:CLA:HMB1	2.02	0.42
1:A1:297:HIS:CE1	19:A1:820:CLA:HMB3	2.54	0.42
1:A2:196:SER:O	1:A2:200:HIS:ND1	2.43	0.42
1:A2:364:THR:HG22	1:A2:394:HIS:HB3	2.00	0.42
1:A2:448:LEU:O	1:A2:452:SER:N	2.53	0.42
1:A:357:LEU:HD21	19:A:832:CLA:CBB	2.50	0.42
23:B2:842:BCR:H371	23:B2:842:BCR:H24C	1.90	0.42
19:B2:832:CLA:CHD	19:B2:846:CLA:HMD2	2.50	0.42
23:J1:104:BCR:H392	23:J1:104:BCR:H23C	2.02	0.42
23:FF:306:BCR:H381	19:JJ:103:CLA:HBC3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A2:426:VAL:O	1:A2:430:VAL:HG23	2.20	0.42
2:B1:593:THR:O	2:B1:597:VAL:HG23	2.19	0.42
2:B2:182:LEU:HD21	19:B2:810:CLA:C2	2.50	0.42
2:B:514:SER:OG	2:B:514:SER:O	2.34	0.42
2:B:374:ALA:HB1	19:B:824:CLA:HMA1	2.01	0.42
2:B:707:LEU:N	21:B:838:PQN:O4	2.48	0.42
2:BB:174:ARG:HB2	19:BB:810:CLA:HBC2	2.01	0.42
8:JJ:23:THR:HG21	23:JJ:104:BCR:H403	2.02	0.42
9:KK:68:PHE:CE2	9:KK:72:LEU:HD11	2.55	0.42
19:L:202:CLA:H143	19:L:202:CLA:H91	2.01	0.42
18:LL:101:LEU:HD21	18:LL:105:PHE:CZ	2.55	0.42
1:A1:600:TYR:CE2	20:A1:802:CL0:H36	2.54	0.42
20:A2:803:CL0:H16	2:B2:631:LEU:HD22	2.02	0.42
19:A2:804:CLA:H193	19:A2:852:CLA:H192	2.00	0.42
1:A:698:ILE:O	1:A:702:VAL:HG23	2.20	0.42
19:B2:834:CLA:HBB2	19:B2:835:CLA:O2D	2.20	0.42
19:B2:849:CLA:HMB3	19:B2:850:CLA:CAD	2.50	0.42
2:B:534:LEU:HD12	19:B:835:CLA:CED	2.50	0.42
2:BB:71:GLN:NE2	19:BB:804:CLA:O1D	2.49	0.42
3:C:12:ILE:HD11	3:C:59:PRO:HG2	2.02	0.42
2:B1:440:LEU:HD11	23:F1:306:BCR:H311	2.01	0.42
6:F1:34:ASN:ND2	6:F1:67:GLY:O	2.50	0.42
18:LL:126:VAL:O	18:LL:126:VAL:HG13	2.20	0.42
19:A:805:CLA:H71	19:A:805:CLA:H41	2.02	0.41
19:AA:810:CLA:H43	19:AA:830:CLA:HMD2	2.01	0.41
23:F:305:BCR:H15C	23:F:305:BCR:H351	1.78	0.41
23:J:104:BCR:H23C	23:J:104:BCR:H392	2.02	0.41
23:LL:204:BCR:H15C	23:LL:204:BCR:H351	1.95	0.41
1:A1:707:LYS:HA	6:F1:159:ILE:HD11	2.01	0.41
20:A2:803:CL0:H4	19:A2:852:CLA:OBD	2.20	0.41
19:A:815:CLA:HBA2	19:A:815:CLA:H3A	1.90	0.41
19:A:805:CLA:CGA	19:A:842:CLA:H43	2.49	0.41
1:AA:112:ARG:HB2	1:AA:131:VAL:HG22	2.02	0.41
1:AA:81:LEU:O	1:AA:85:THR:HG23	2.19	0.41
2:B2:592:ASN:OD1	19:B2:849:CLA:H42	2.20	0.41
19:BB:832:CLA:O1D	19:BB:833:CLA:HMB1	2.20	0.41
2:BB:724:TYR:CD1	19:BB:852:CLA:HED1	2.56	0.41
1:A2:558:ARG:NH2	4:D2:42:GLU:OE2	2.52	0.41
10:L1:11:LEU:O	10:L1:17:ASN:ND2	2.53	0.41
1:AA:575:CYS:SG	1:AA:577:GLY:N	2.87	0.41
19:AA:830:CLA:HMC1	19:AA:830:CLA:HBC2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:B2:811:CLA:HMB1	19:B2:811:CLA:HBB1	2.01	0.41
2:B:536:THR:HG21	2:B:589:TRP:CZ2	2.55	0.41
2:B:630:TYR:O	2:B:634:ASN:ND2	2.53	0.41
19:B:833:CLA:C3D	19:B:833:CLA:HED3	2.51	0.41
2:BB:293:THR:O	2:BB:295:PHE:N	2.53	0.41
2:BB:45:LYS:NZ	19:BB:801:CLA:HED1	2.36	0.41
1:A:558:ARG:NH2	4:D:42:GLU:OE2	2.46	0.41
19:FF:301:CLA:H42	8:JJ:22:ALA:HA	2.02	0.41
1:A1:199:ASN:OD1	1:A1:314:THR:HG21	2.20	0.41
1:AA:341:LEU:CD1	19:AA:826:CLA:HMD3	2.50	0.41
2:B1:491:THR:HG23	2:B1:491:THR:O	2.21	0.41
19:B2:826:CLA:H72	19:B2:826:CLA:H41	2.02	0.41
14:I2:33:PHE:CE1	23:I2:103:BCR:H342	2.56	0.41
16:L2:62:ARG:NH1	16:L2:131:ASP:OD1	2.53	0.41
1:A:121:ILE:HG23	1:A:122:VAL:N	2.35	0.41
1:A:81:LEU:O	1:A:85:THR:HG23	2.21	0.41
1:AA:115:ALA:HB3	1:AA:140:ILE:CD1	2.51	0.41
2:B2:653:TRP:O	2:B2:657:PHE:N	2.50	0.41
2:B2:731:PHE:O	2:B2:735:SER:OG	2.29	0.41
2:B:422:ILE:HG23	19:B:835:CLA:HBB2	2.01	0.41
6:FF:46:ASN:N	6:FF:46:ASN:OD1	2.53	0.41
10:L1:152:GLY:O	10:L1:156:VAL:HG23	2.20	0.41
1:A1:413:MET:CE	1:A1:431:ILE:HD11	2.51	0.41
19:A:826:CLA:HAB	19:A:833:CLA:HMD2	2.03	0.41
1:AA:320:HIS:HB3	1:AA:325:ILE:HD11	2.02	0.41
2:B2:196:HIS:O	2:B2:207:VAL:HG11	2.21	0.41
19:B:818:CLA:HBB1	19:B:818:CLA:HHC	2.02	0.41
2:BB:536:THR:HG21	2:BB:589:TRP:CZ2	2.56	0.41
1:A2:494:ALA:HB3	1:A2:495:PRO:HD3	2.02	0.41
1:A:36:ASP:OD1	1:A:37:ARG:N	2.54	0.41
2:B2:167:TRP:CZ2	19:B2:808:CLA:HMA1	2.55	0.41
2:B:294:ASN:OD1	19:B:809:CLA:HMA2	2.20	0.41
2:BB:255:LEU:HD21	2:BB:278:LEU:HD23	2.03	0.41
2:BB:652:VAL:HG11	19:BB:805:CLA:CBC	2.51	0.41
19:A1:833:CLA:HED1	10:L1:32:ASN:OD1	2.21	0.41
10:L1:61:ARG:NH2	19:L1:205:CLA:HED1	2.35	0.41
1:A2:297:HIS:CE1	19:A2:821:CLA:HMB3	2.55	0.41
19:AA:825:CLA:HMA1	19:AA:845:CLA:HBC3	2.01	0.41
2:BB:724:TYR:CE1	19:BB:852:CLA:HED1	2.55	0.41
18:L:131:ASP:N	18:L:131:ASP:OD1	2.54	0.41
1:A1:685:MET:O	1:A1:689:SER:OG	2.32	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:A1:852:CLA:HMB3	19:B1:848:CLA:C19	2.50	0.41
19:A:831:CLA:H92	19:A:831:CLA:HMD2	2.03	0.41
1:A:93:PHE:HE1	19:A:809:CLA:HMD3	1.86	0.41
1:AA:584:CYS:O	2:BB:676:GLY:N	2.53	0.41
2:B1:429:VAL:HG11	2:B1:535:HIS:CD2	2.56	0.41
2:B2:536:THR:HG21	2:B2:589:TRP:CZ2	2.56	0.41
1:A:126:ILE:HG21	2:B:450:PHE:HA	2.03	0.41
1:A1:397:ILE:HD13	19:A1:829:CLA:HBC3	2.03	0.41
1:A:199:ASN:HD21	1:A:312:TYR:H	1.69	0.41
2:B1:15:ASP:O	2:B1:20:ARG:NH1	2.53	0.41
23:B:842:BCR:C8	23:B:842:BCR:H331	2.50	0.41
2:BB:272:ASP:O	2:BB:276:HIS:N	2.53	0.41
3:C2:42:SER:O	4:D2:114:ARG:NH1	2.54	0.41
23:F2:305:BCR:H381	19:J2:103:CLA:HBC3	2.03	0.41
1:A1:180:HIS:HE1	19:A1:811:CLA:HMA3	1.86	0.41
19:A2:826:CLA:HAB	19:A2:833:CLA:HMD2	2.02	0.41
23:A:854:BCR:H362	9:K:71:ILE:HD11	2.03	0.41
19:B1:811:CLA:HMB1	19:B1:811:CLA:HBB1	2.03	0.41
2:B2:602:HIS:CD2	2:B2:732:LEU:HD12	2.56	0.41
2:B:444:ASN:OD1	2:B:457:ILE:N	2.47	0.41
2:BB:587:LEU:HD12	2:BB:717:LEU:HD21	2.03	0.41
19:BB:806:CLA:H41	19:BB:806:CLA:H72	2.01	0.41
2:BB:91:ILE:HD11	2:BB:114:ASN:OD1	2.21	0.41
3:CC:13:GLY:O	3:CC:38:GLN:NE2	2.54	0.41
19:A1:834:CLA:HMA1	23:I1:101:BCR:H282	2.02	0.41
19:B2:827:CLA:HED3	12:X2:11:ASN:CB	2.51	0.41
19:A1:814:CLA:H3A	19:A1:814:CLA:HBA2	1.89	0.40
1:A2:234:VAL:HA	1:A2:237:ILE:HD12	2.03	0.40
19:AA:831:CLA:HMD2	19:AA:831:CLA:H92	2.02	0.40
2:B1:584:TYR:OH	2:B1:671:LEU:HD22	2.21	0.40
2:B:319:PHE:CD2	19:B:820:CLA:HMA1	2.56	0.40
2:BB:58:PHE:CD1	2:BB:142:LEU:HD22	2.54	0.40
2:BB:270:LEU:HD23	2:BB:273:MET:SD	2.61	0.40
2:BB:699:ARG:NH2	4:DD:25:GLU:OE2	2.54	0.40
10:L1:57:LEU:HD13	10:L1:61:ARG:HD3	2.03	0.40
1:A1:304:VAL:HG12	19:A1:822:CLA:HMC1	2.02	0.40
19:A1:819:CLA:H92	19:A1:836:CLA:O1A	2.21	0.40
1:A2:53:HIS:HD2	19:A2:806:CLA:HBC1	1.86	0.40
19:A:832:CLA:HMB1	19:A:832:CLA:HBB1	2.02	0.40
19:A:840:CLA:CBB	19:A:841:CLA:HBC3	2.51	0.40
2:B:534:LEU:HD12	19:B:835:CLA:HED3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BB:319:PHE:HD2	19:BB:820:CLA:HMA1	1.86	0.40
10:L1:72:TYR:OH	19:L1:207:CLA:OBD	2.29	0.40
1:A2:444:VAL:HG12	1:A2:448:LEU:HD12	2.04	0.40
1:A:329:HIS:O	22:A:846:LHG:O2	2.34	0.40
1:AA:122:VAL:CG2	19:BB:829:CLA:HMD1	2.50	0.40
2:B:638:LEU:HD21	2:B:657:PHE:CG	2.57	0.40
2:B:394:GLY:HA2	23:B:843:BCR:H393	2.03	0.40
19:B:854:CLA:H41	19:B:854:CLA:H62	1.96	0.40
2:BB:194:LEU:HA	2:BB:198:ALA:HB3	2.03	0.40
3:CC:17:CYS:SG	3:CC:18:VAL:N	2.95	0.40
19:FF:301:CLA:H43	19:FF:302:CLA:CBC	2.52	0.40
10:L1:61:ARG:NH2	10:L1:65:GLU:OE1	2.54	0.40
19:B2:852:CLA:HBC2	19:B2:852:CLA:HHD	2.02	0.40
1:A:662:TYR:OH	2:B:445:ASP:OD2	2.39	0.40
2:B:399:VAL:CG2	2:B:548:ALA:HB1	2.51	0.40
19:BB:822:CLA:H143	19:BB:831:CLA:HBB2	2.04	0.40
3:C1:35:LYS:HA	5:E1:32:ILE:HG22	2.02	0.40
13:F2:95:TYR:OH	13:F2:137:PHE:O	2.17	0.40
1:A1:388:LEU:HD23	1:A1:610:PHE:CD1	2.57	0.40
19:AA:828:CLA:HAB	23:AA:851:BCR:H311	2.03	0.40
2:B1:534:LEU:HD12	19:B1:834:CLA:CED	2.42	0.40
2:B1:422:ILE:HG23	19:B1:834:CLA:CBB	2.52	0.40
19:B2:851:CLA:HMC3	19:F2:301:CLA:C4D	2.52	0.40
1:A:697:LEU:HB2	2:B:543:LYS:HZ2	1.87	0.40
2:BB:409:GLY:N	2:BB:413:GLU:OE1	2.50	0.40
19:BB:832:CLA:HED3	19:BB:832:CLA:C3D	2.52	0.40
6:FF:114:ASP:OD1	6:FF:120:LYS:NZ	2.34	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	A	738/740 (100%)	713 (97%)	24 (3%)	1 (0%)	53	87
1	A1	738/740 (100%)	710 (96%)	27 (4%)	1 (0%)	53	87
1	A2	738/740 (100%)	714 (97%)	23 (3%)	1 (0%)	53	87
1	AA	738/740 (100%)	709 (96%)	28 (4%)	1 (0%)	53	87
2	B	737/739 (100%)	712 (97%)	25 (3%)	0	100	100
2	B1	737/739 (100%)	715 (97%)	22 (3%)	0	100	100
2	B2	737/739 (100%)	713 (97%)	24 (3%)	0	100	100
2	BB	737/739 (100%)	710 (96%)	27 (4%)	0	100	100
3	C	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	C1	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
3	C2	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
3	CC	78/80 (98%)	75 (96%)	3 (4%)	0	100	100
4	D	132/134 (98%)	122 (92%)	10 (8%)	0	100	100
4	D1	132/134 (98%)	121 (92%)	11 (8%)	0	100	100
4	D2	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
4	DD	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
5	E1	58/60 (97%)	56 (97%)	2 (3%)	0	100	100
5	E2	58/60 (97%)	54 (93%)	4 (7%)	0	100	100
6	F	137/139 (99%)	132 (96%)	5 (4%)	0	100	100
6	F1	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
6	FF	137/139 (99%)	131 (96%)	6 (4%)	0	100	100
7	I	29/31 (94%)	29 (100%)	0	0	100	100
7	I1	29/31 (94%)	29 (100%)	0	0	100	100
7	II	29/31 (94%)	29 (100%)	0	0	100	100
8	J	41/48 (85%)	40 (98%)	1 (2%)	0	100	100
8	J1	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
8	J2	41/48 (85%)	39 (95%)	2 (5%)	0	100	100
8	JJ	41/48 (85%)	38 (93%)	3 (7%)	0	100	100
9	K	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
9	K1	72/74 (97%)	71 (99%)	1 (1%)	0	100	100
9	KK	56/74 (76%)	55 (98%)	1 (2%)	0	100	100
10	L1	164/166 (99%)	160 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	M	29/31 (94%)	29 (100%)	0	0	100	100
11	M1	29/31 (94%)	29 (100%)	0	0	100	100
11	M2	29/31 (94%)	29 (100%)	0	0	100	100
11	MM	29/31 (94%)	29 (100%)	0	0	100	100
12	X	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X1	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	X2	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
12	XX	37/39 (95%)	35 (95%)	2 (5%)	0	100	100
13	F2	135/137 (98%)	125 (93%)	7 (5%)	3 (2%)	7	39
14	I2	31/33 (94%)	31 (100%)	0	0	100	100
15	K2	71/73 (97%)	70 (99%)	1 (1%)	0	100	100
16	L2	165/167 (99%)	160 (97%)	5 (3%)	0	100	100
17	E	61/63 (97%)	61 (100%)	0	0	100	100
17	EE	61/63 (97%)	60 (98%)	1 (2%)	0	100	100
18	L	152/154 (99%)	146 (96%)	5 (3%)	1 (1%)	24	66
18	LL	152/154 (99%)	148 (97%)	4 (3%)	0	100	100
All	All	8958/9106 (98%)	8634 (96%)	316 (4%)	8 (0%)	56	87

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A2	122	VAL
13	F2	159	ILE
1	A1	122	VAL
1	A	122	VAL
1	AA	477	ILE
13	F2	158	GLU
13	F2	160	THR
18	L	118	PRO

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	594/594 (100%)	594 (100%)	0	100	100
1	A1	594/594 (100%)	594 (100%)	0	100	100
1	A2	594/594 (100%)	594 (100%)	0	100	100
1	AA	594/594 (100%)	594 (100%)	0	100	100
2	B	601/601 (100%)	601 (100%)	0	100	100
2	B1	601/601 (100%)	601 (100%)	0	100	100
2	B2	601/601 (100%)	601 (100%)	0	100	100
2	BB	601/601 (100%)	600 (100%)	1 (0%)	94	98
3	C	68/68 (100%)	68 (100%)	0	100	100
3	C1	68/68 (100%)	67 (98%)	1 (2%)	67	88
3	C2	68/68 (100%)	67 (98%)	1 (2%)	67	88
3	CC	68/68 (100%)	68 (100%)	0	100	100
4	D	107/107 (100%)	107 (100%)	0	100	100
4	D1	107/107 (100%)	107 (100%)	0	100	100
4	D2	107/107 (100%)	107 (100%)	0	100	100
4	DD	107/107 (100%)	107 (100%)	0	100	100
5	E1	53/53 (100%)	53 (100%)	0	100	100
5	E2	53/53 (100%)	53 (100%)	0	100	100
6	F	108/108 (100%)	108 (100%)	0	100	100
6	F1	108/108 (100%)	108 (100%)	0	100	100
6	FF	108/108 (100%)	108 (100%)	0	100	100
7	I	28/28 (100%)	28 (100%)	0	100	100
7	I1	28/28 (100%)	28 (100%)	0	100	100
7	II	28/28 (100%)	28 (100%)	0	100	100
8	J	38/41 (93%)	38 (100%)	0	100	100
8	J1	38/41 (93%)	38 (100%)	0	100	100
8	J2	38/41 (93%)	38 (100%)	0	100	100
8	JJ	38/41 (93%)	38 (100%)	0	100	100
9	K	46/54 (85%)	46 (100%)	0	100	100
9	K1	54/54 (100%)	54 (100%)	0	100	100
9	KK	46/54 (85%)	46 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	L1	127/127 (100%)	126 (99%)	1 (1%)	83	94
11	M	26/26 (100%)	26 (100%)	0	100	100
11	M1	26/26 (100%)	26 (100%)	0	100	100
11	M2	26/26 (100%)	26 (100%)	0	100	100
11	MM	26/26 (100%)	26 (100%)	0	100	100
12	X	31/31 (100%)	31 (100%)	0	100	100
12	X1	31/31 (100%)	31 (100%)	0	100	100
12	X2	31/31 (100%)	31 (100%)	0	100	100
12	XX	31/31 (100%)	31 (100%)	0	100	100
13	F2	106/106 (100%)	106 (100%)	0	100	100
14	I2	30/30 (100%)	30 (100%)	0	100	100
15	K2	54/54 (100%)	54 (100%)	0	100	100
16	L2	128/128 (100%)	127 (99%)	1 (1%)	83	94
17	E	55/55 (100%)	55 (100%)	0	100	100
17	EE	55/55 (100%)	55 (100%)	0	100	100
18	L	117/117 (100%)	116 (99%)	1 (1%)	81	93
18	LL	117/117 (100%)	117 (100%)	0	100	100
All	All	7309/7337 (100%)	7303 (100%)	6 (0%)	94	98

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C1	44	ARG
10	L1	61	ARG
3	C2	44	ARG
16	L2	61	ARG
18	L	61	ARG
2	BB	34	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A1	158	GLN
1	A1	180	HIS
1	A1	199	ASN

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Mol	Chain	Res	Type
1	A1	715	GLN
2	B1	29	ASN
2	B1	468	GLN
2	B1	610	GLN
5	E1	19	GLN
5	E1	51	ASN
10	L1	114	ASN
1	A2	53	HIS
1	A2	715	GLN
2	B2	114	ASN
2	B2	341	HIS
2	B2	468	GLN
2	B2	610	GLN
5	E2	19	GLN
16	L2	114	ASN
1	A	216	HIS
2	B	41	ASN
2	B	289	HIS
2	B	306	ASN
2	B	380	GLN
4	D	125	ASN
4	D	128	GLN
17	E	51	ASN
1	AA	158	GLN
2	BB	223	GLN
2	BB	498	ASN
17	EE	51	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

594 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$
19	CLA	A	801	-	57,73,73	1.04	5 (8%)	66,113,113	1.48	9 (13%)
24	AJP	A	802	-	35,35,95	4.43	22 (62%)	52,58,149	4.37	28 (53%)
20	CL0	A	803	-	57,73,73	1.85	11 (19%)	66,113,113	2.32	21 (31%)
19	CLA	A	804	-	57,73,73	1.06	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	A	805	-	52,68,73	1.08	4 (7%)	60,107,113	1.56	9 (15%)
19	CLA	A	806	-	48,64,73	1.14	6 (12%)	55,102,113	1.69	12 (21%)
19	CLA	A	807	-	57,73,73	1.06	5 (8%)	66,113,113	1.34	8 (12%)
19	CLA	A	808	-	57,73,73	1.04	4 (7%)	66,113,113	1.47	10 (15%)
19	CLA	A	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.65	10 (20%)
19	CLA	A	810	1	57,73,73	1.02	5 (8%)	66,113,113	1.57	12 (18%)
19	CLA	A	811	1	43,59,73	1.24	7 (16%)	49,96,113	1.67	9 (18%)
19	CLA	A	812	-	38,54,73	1.23	4 (10%)	43,90,113	1.72	8 (18%)
19	CLA	A	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	9 (13%)
19	CLA	A	814	-	34,50,73	1.28	4 (11%)	38,85,113	1.66	7 (18%)
19	CLA	A	815	-	47,63,73	1.13	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	A	816	-	42,58,73	1.20	4 (9%)	48,95,113	1.60	9 (18%)
19	CLA	A	817	-	36,52,73	1.24	4 (11%)	39,87,113	1.72	8 (20%)
19	CLA	A	818	-	34,53,73	1.28	4 (11%)	37,89,113	1.70	6 (16%)
19	CLA	A	819	-	52,68,73	1.08	5 (9%)	60,107,113	1.51	9 (15%)
19	CLA	A	820	-	50,66,73	1.16	7 (14%)	57,104,113	1.58	11 (19%)
19	CLA	A	821	-	57,73,73	1.00	5 (8%)	66,113,113	1.54	11 (16%)
19	CLA	A	822	-	43,59,73	1.19	4 (9%)	49,96,113	1.58	7 (14%)
19	CLA	A	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.62	10 (16%)
19	CLA	A	824	-	34,53,73	1.26	4 (11%)	37,89,113	1.82	8 (21%)
19	CLA	A	825	-	44,60,73	1.16	4 (9%)	50,97,113	1.59	8 (16%)
19	CLA	A	826	-	34,53,73	1.28	5 (14%)	37,89,113	1.72	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A	827	-	57,73,73	1.05	6 (10%)	66,113,113	1.34	4 (6%)
19	CLA	A	828	-	48,64,73	1.11	4 (8%)	55,102,113	1.56	8 (14%)
19	CLA	A	829	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	A	830	-	54,70,73	1.01	5 (9%)	62,109,113	1.50	9 (14%)
19	CLA	A	831	-	57,73,73	1.05	4 (7%)	66,113,113	1.41	8 (12%)
19	CLA	A	832	-	57,73,73	1.01	5 (8%)	66,113,113	1.51	11 (16%)
19	CLA	A	833	-	42,58,73	1.20	6 (14%)	48,95,113	1.52	6 (12%)
19	CLA	A	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.74	8 (21%)
19	CLA	A	835	-	57,73,73	1.06	4 (7%)	66,113,113	1.41	9 (13%)
19	CLA	A	836	-	57,73,73	1.03	6 (10%)	66,113,113	1.44	7 (10%)
19	CLA	A	837	-	34,53,73	1.31	4 (11%)	37,89,113	1.74	8 (21%)
19	CLA	A	838	-	36,52,73	1.25	4 (11%)	39,87,113	1.81	8 (20%)
19	CLA	A	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.62	9 (18%)
19	CLA	A	840	-	48,64,73	1.12	5 (10%)	55,102,113	1.54	8 (14%)
19	CLA	A	841	-	38,54,73	1.21	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	A	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	12 (18%)
21	PQN	A	843	-	34,34,34	0.59	0	42,45,45	1.07	3 (7%)
19	CLA	A	844	-	33,49,73	1.30	4 (12%)	37,84,113	1.81	7 (18%)
22	LHG	A	845	-	48,48,48	0.79	2 (4%)	51,54,54	0.97	3 (5%)
22	LHG	A	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
23	BCR	A	847	-	40,40,41	1.09	2 (5%)	53,54,56	1.26	9 (16%)
23	BCR	A	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	8 (14%)
23	BCR	A	849	-	41,41,41	1.07	2 (4%)	56,56,56	1.26	10 (17%)
23	BCR	A	850	-	41,41,41	1.13	2 (4%)	56,56,56	1.23	4 (7%)
23	BCR	A	851	-	41,41,41	1.06	1 (2%)	56,56,56	1.46	8 (14%)
19	CLA	A	852	-	57,73,73	1.07	7 (12%)	66,113,113	1.45	10 (15%)
23	BCR	A	853	-	41,41,41	1.13	2 (4%)	56,56,56	1.35	10 (17%)
23	BCR	A	854	-	41,41,41	1.12	2 (4%)	56,56,56	1.29	8 (14%)
24	AJP	A	855	-	40,40,95	4.24	24 (60%)	57,65,149	3.45	19 (33%)
19	CLA	A1	801	-	57,73,73	1.04	5 (8%)	66,113,113	1.51	10 (15%)
20	CL0	A1	802	-	57,73,73	1.87	12 (21%)	66,113,113	2.27	23 (34%)
19	CLA	A1	803	-	57,73,73	1.03	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	A1	804	-	52,68,73	1.07	4 (7%)	60,107,113	1.43	9 (15%)
19	CLA	A1	805	-	48,64,73	1.15	7 (14%)	55,102,113	1.52	8 (14%)
19	CLA	A1	806	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	8 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A1	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.48	8 (12%)
19	CLA	A1	808	-	42,58,73	1.19	4 (9%)	48,95,113	1.70	9 (18%)
19	CLA	A1	809	-	57,73,73	1.02	5 (8%)	66,113,113	1.49	12 (18%)
19	CLA	A1	810	-	43,59,73	1.22	7 (16%)	49,96,113	1.68	9 (18%)
19	CLA	A1	811	-	38,54,73	1.24	4 (10%)	43,90,113	1.69	9 (20%)
19	CLA	A1	812	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	9 (13%)
19	CLA	A1	813	-	34,50,73	1.26	4 (11%)	38,85,113	1.70	8 (21%)
19	CLA	A1	814	-	47,63,73	1.12	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	A1	815	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	9 (18%)
19	CLA	A1	816	-	36,52,73	1.26	5 (13%)	39,87,113	1.71	8 (20%)
19	CLA	A1	817	-	34,53,73	1.29	4 (11%)	37,89,113	1.73	8 (21%)
19	CLA	A1	818	-	52,68,73	1.09	4 (7%)	60,107,113	1.50	8 (13%)
19	CLA	A1	819	-	50,66,73	1.17	7 (14%)	57,104,113	1.55	10 (17%)
19	CLA	A1	820	-	57,73,73	0.99	5 (8%)	66,113,113	1.55	12 (18%)
19	CLA	A1	821	-	43,59,73	1.19	4 (9%)	49,96,113	1.61	9 (18%)
19	CLA	A1	822	-	52,68,73	1.09	6 (11%)	60,107,113	1.57	10 (16%)
19	CLA	A1	823	-	34,53,73	1.28	4 (11%)	37,89,113	1.84	8 (21%)
19	CLA	A1	824	-	34,50,73	1.32	5 (14%)	38,85,113	1.69	8 (21%)
19	CLA	A1	825	-	34,53,73	1.28	4 (11%)	37,89,113	1.77	7 (18%)
19	CLA	A1	826	-	57,73,73	1.06	6 (10%)	66,113,113	1.42	5 (7%)
19	CLA	A1	827	-	48,64,73	1.13	4 (8%)	55,102,113	1.57	9 (16%)
19	CLA	A1	828	-	57,73,73	1.02	4 (7%)	66,113,113	1.49	10 (15%)
19	CLA	A1	829	-	54,70,73	1.03	4 (7%)	62,109,113	1.46	9 (14%)
19	CLA	A1	830	-	57,73,73	1.05	4 (7%)	66,113,113	1.40	10 (15%)
19	CLA	A1	831	-	57,73,73	1.01	5 (8%)	66,113,113	1.49	8 (12%)
19	CLA	A1	832	-	42,58,73	1.21	6 (14%)	48,95,113	1.55	7 (14%)
19	CLA	A1	833	-	33,49,73	1.31	5 (15%)	37,84,113	1.76	8 (21%)
19	CLA	A1	834	-	57,73,73	1.06	6 (10%)	66,113,113	1.41	10 (15%)
19	CLA	A1	835	-	57,73,73	1.04	6 (10%)	66,113,113	1.43	7 (10%)
19	CLA	A1	836	-	34,53,73	1.32	5 (14%)	37,89,113	1.75	8 (21%)
19	CLA	A1	837	1	36,52,73	1.24	4 (11%)	39,87,113	1.86	9 (23%)
19	CLA	A1	838	-	44,60,73	1.17	4 (9%)	50,97,113	1.64	7 (14%)
19	CLA	A1	839	-	48,64,73	1.12	4 (8%)	55,102,113	1.49	7 (12%)
19	CLA	A1	840	-	38,54,73	1.23	4 (10%)	43,90,113	1.70	7 (16%)
19	CLA	A1	841	-	57,73,73	1.03	6 (10%)	66,113,113	1.52	9 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A1	842	-	57,73,73	1.08	6 (10%)	66,113,113	1.70	12 (18%)
21	PQN	A1	843	-	34,34,34	0.62	0	42,45,45	1.07	3 (7%)
19	CLA	A1	844	-	33,49,73	1.30	4 (12%)	37,84,113	1.78	7 (18%)
22	LHG	A1	845	-	48,48,48	0.77	2 (4%)	51,54,54	0.95	3 (5%)
22	LHG	A1	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.00	3 (7%)
23	BCR	A1	847	-	40,40,41	1.10	2 (5%)	53,54,56	1.24	7 (13%)
23	BCR	A1	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	A1	849	-	41,41,41	1.08	2 (4%)	56,56,56	1.25	7 (12%)
23	BCR	A1	850	-	41,41,41	1.17	2 (4%)	56,56,56	1.26	6 (10%)
23	BCR	A1	851	-	41,41,41	1.07	1 (2%)	56,56,56	1.47	8 (14%)
19	CLA	A1	852	-	57,73,73	1.05	6 (10%)	66,113,113	1.41	7 (10%)
23	BCR	A1	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	9 (16%)
24	AJP	A1	854	-	49,49,95	3.88	25 (51%)	71,80,149	3.22	19 (26%)
24	AJP	A1	855	-	37,37,95	4.35	24 (64%)	56,62,149	3.41	21 (37%)
19	CLA	A2	801	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	8 (12%)
19	CLA	A2	802	-	38,54,73	1.22	4 (10%)	43,90,113	1.69	7 (16%)
20	CL0	A2	803	-	57,73,73	1.79	12 (21%)	66,113,113	2.39	20 (30%)
19	CLA	A2	804	-	57,73,73	1.03	5 (8%)	66,113,113	1.44	9 (13%)
19	CLA	A2	805	-	52,68,73	1.07	4 (7%)	60,107,113	1.54	10 (16%)
19	CLA	A2	806	-	48,64,73	1.14	7 (14%)	55,102,113	1.68	10 (18%)
19	CLA	A2	807	-	57,73,73	1.06	5 (8%)	66,113,113	1.39	8 (12%)
19	CLA	A2	808	-	57,73,73	1.02	5 (8%)	66,113,113	1.42	8 (12%)
19	CLA	A2	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.68	8 (16%)
19	CLA	A2	810	1	57,73,73	1.03	5 (8%)	66,113,113	1.54	12 (18%)
19	CLA	A2	811	-	43,59,73	1.22	7 (16%)	49,96,113	1.69	9 (18%)
19	CLA	A2	812	-	38,54,73	1.23	5 (13%)	43,90,113	1.68	10 (23%)
19	CLA	A2	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.47	9 (13%)
19	CLA	A2	814	-	34,50,73	1.27	4 (11%)	38,85,113	1.69	7 (18%)
19	CLA	A2	815	-	47,63,73	1.12	4 (8%)	54,101,113	1.50	8 (14%)
19	CLA	A2	816	-	42,58,73	1.19	4 (9%)	48,95,113	1.62	9 (18%)
19	CLA	A2	817	-	36,52,73	1.26	4 (11%)	39,87,113	1.72	8 (20%)
19	CLA	A2	818	-	34,53,73	1.30	4 (11%)	37,89,113	1.72	8 (21%)
19	CLA	A2	819	-	52,68,73	1.09	5 (9%)	60,107,113	1.49	8 (13%)
19	CLA	A2	820	-	50,66,73	1.17	7 (14%)	57,104,113	1.58	10 (17%)
19	CLA	A2	821	-	57,73,73	0.99	5 (8%)	66,113,113	1.49	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	A2	822	-	43,59,73	1.19	4 (9%)	49,96,113	1.62	8 (16%)
19	CLA	A2	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.67	11 (18%)
19	CLA	A2	824	-	34,53,73	1.28	4 (11%)	37,89,113	1.81	8 (21%)
19	CLA	A2	825	-	34,50,73	1.32	6 (17%)	38,85,113	1.76	8 (21%)
19	CLA	A2	826	-	34,53,73	1.29	6 (17%)	37,89,113	1.77	7 (18%)
19	CLA	A2	827	-	57,73,73	1.06	6 (10%)	66,113,113	1.49	8 (12%)
19	CLA	A2	828	-	48,64,73	1.12	4 (8%)	55,102,113	1.58	8 (14%)
19	CLA	A2	829	-	57,73,73	1.06	7 (12%)	66,113,113	1.42	11 (16%)
19	CLA	A2	830	-	54,70,73	1.04	4 (7%)	62,109,113	1.48	10 (16%)
19	CLA	A2	831	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	8 (12%)
19	CLA	A2	832	-	57,73,73	1.02	5 (8%)	66,113,113	1.51	9 (13%)
19	CLA	A2	833	-	42,58,73	1.21	6 (14%)	48,95,113	1.49	8 (16%)
19	CLA	A2	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.77	10 (27%)
19	CLA	A2	835	-	57,73,73	1.07	6 (10%)	66,113,113	1.44	10 (15%)
19	CLA	A2	836	-	57,73,73	1.06	6 (10%)	66,113,113	1.54	9 (13%)
19	CLA	A2	837	-	34,53,73	1.33	5 (14%)	37,89,113	1.77	8 (21%)
19	CLA	A2	838	-	36,52,73	1.24	4 (11%)	39,87,113	1.85	9 (23%)
19	CLA	A2	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.62	8 (16%)
19	CLA	A2	840	-	48,64,73	1.11	4 (8%)	55,102,113	1.52	7 (12%)
19	CLA	A2	841	-	38,54,73	1.22	4 (10%)	43,90,113	1.71	7 (16%)
19	CLA	A2	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.57	10 (15%)
21	PQN	A2	843	-	34,34,34	0.62	0	42,45,45	1.07	3 (7%)
19	CLA	A2	844	-	33,49,73	1.30	5 (15%)	37,84,113	1.77	7 (18%)
22	LHG	A2	845	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
22	LHG	A2	846	-	37,37,48	0.81	1 (2%)	40,43,54	1.01	3 (7%)
23	BCR	A2	847	-	40,40,41	1.09	2 (5%)	53,54,56	1.24	7 (13%)
23	BCR	A2	848	-	41,41,41	1.14	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	A2	849	-	41,41,41	1.04	2 (4%)	56,56,56	1.25	8 (14%)
23	BCR	A2	850	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	A2	851	-	41,41,41	1.06	1 (2%)	56,56,56	1.48	10 (17%)
19	CLA	A2	852	-	57,73,73	1.08	6 (10%)	66,113,113	1.49	8 (12%)
23	BCR	A2	853	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	8 (14%)
24	AJP	A2	854	-	37,37,95	4.35	24 (64%)	56,62,149	3.42	20 (35%)
19	CLA	AA	801	-	57,73,73	1.04	7 (12%)	66,113,113	1.45	7 (10%)
24	AJP	AA	802	-	35,35,95	4.43	22 (62%)	52,58,149	4.37	28 (53%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CL0	AA	803	-	57,73,73	1.84	12 (21%)	66,113,113	2.42	20 (30%)
19	CLA	AA	804	-	57,73,73	1.05	4 (7%)	66,113,113	1.46	9 (13%)
19	CLA	AA	805	-	52,68,73	1.07	4 (7%)	60,107,113	1.57	10 (16%)
19	CLA	AA	806	-	48,64,73	1.15	6 (12%)	55,102,113	1.68	11 (20%)
19	CLA	AA	807	-	57,73,73	1.05	5 (8%)	66,113,113	1.33	6 (9%)
19	CLA	AA	808	-	57,73,73	1.02	4 (7%)	66,113,113	1.40	8 (12%)
19	CLA	AA	809	-	42,58,73	1.19	4 (9%)	48,95,113	1.66	9 (18%)
19	CLA	AA	810	-	57,73,73	1.03	5 (8%)	66,113,113	1.56	13 (19%)
19	CLA	AA	811	1	43,59,73	1.23	6 (13%)	49,96,113	1.69	8 (16%)
19	CLA	AA	812	-	38,54,73	1.24	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	AA	813	-	57,73,73	1.02	4 (7%)	66,113,113	1.45	9 (13%)
19	CLA	AA	814	-	34,50,73	1.28	4 (11%)	38,85,113	1.70	8 (21%)
19	CLA	AA	815	-	47,63,73	1.13	4 (8%)	54,101,113	1.53	7 (12%)
19	CLA	AA	816	-	42,58,73	1.21	5 (11%)	48,95,113	1.61	10 (20%)
19	CLA	AA	817	-	36,52,73	1.25	4 (11%)	39,87,113	1.71	8 (20%)
19	CLA	AA	818	-	34,53,73	1.28	4 (11%)	37,89,113	1.72	7 (18%)
19	CLA	AA	819	-	52,68,73	1.09	4 (7%)	60,107,113	1.48	9 (15%)
19	CLA	AA	820	-	50,66,73	1.15	7 (14%)	57,104,113	1.58	10 (17%)
19	CLA	AA	821	-	57,73,73	1.00	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	AA	822	-	43,59,73	1.18	4 (9%)	49,96,113	1.59	8 (16%)
19	CLA	AA	823	-	52,68,73	1.09	5 (9%)	60,107,113	1.61	10 (16%)
19	CLA	AA	824	-	34,53,73	1.27	4 (11%)	37,89,113	1.81	8 (21%)
19	CLA	AA	825	-	44,60,73	1.16	4 (9%)	50,97,113	1.56	7 (14%)
19	CLA	AA	826	-	34,53,73	1.28	5 (14%)	37,89,113	1.71	7 (18%)
19	CLA	AA	827	-	57,73,73	1.05	5 (8%)	66,113,113	1.33	4 (6%)
19	CLA	AA	828	-	48,64,73	1.11	4 (8%)	55,102,113	1.59	8 (14%)
19	CLA	AA	829	-	57,73,73	1.02	4 (7%)	66,113,113	1.49	9 (13%)
19	CLA	AA	830	-	54,70,73	1.01	5 (9%)	62,109,113	1.48	9 (14%)
19	CLA	AA	831	-	57,73,73	1.05	4 (7%)	66,113,113	1.40	9 (13%)
19	CLA	AA	832	-	57,73,73	1.02	5 (8%)	66,113,113	1.47	10 (15%)
19	CLA	AA	833	-	42,58,73	1.20	6 (14%)	48,95,113	1.46	5 (10%)
19	CLA	AA	834	-	33,49,73	1.31	5 (15%)	37,84,113	1.73	8 (21%)
19	CLA	AA	835	-	57,73,73	1.07	4 (7%)	66,113,113	1.41	9 (13%)
19	CLA	AA	836	-	57,73,73	1.03	6 (10%)	66,113,113	1.42	7 (10%)
19	CLA	AA	837	-	34,53,73	1.31	5 (14%)	37,89,113	1.75	8 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	AA	838	-	36,52,73	1.25	4 (11%)	39,87,113	1.83	8 (20%)
19	CLA	AA	839	-	44,60,73	1.16	4 (9%)	50,97,113	1.61	8 (16%)
19	CLA	AA	840	-	48,64,73	1.11	5 (10%)	55,102,113	1.47	6 (10%)
19	CLA	AA	841	-	38,54,73	1.21	4 (10%)	43,90,113	1.71	8 (18%)
19	CLA	AA	842	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	11 (16%)
19	CLA	AA	843	-	57,73,73	1.07	5 (8%)	66,113,113	1.65	11 (16%)
21	PQN	AA	844	-	34,34,34	0.64	0	42,45,45	1.03	3 (7%)
19	CLA	AA	845	-	33,49,73	1.30	4 (12%)	37,84,113	1.82	7 (18%)
22	LHG	AA	846	-	48,48,48	0.79	2 (4%)	51,54,54	0.96	3 (5%)
22	LHG	AA	847	-	37,37,48	0.81	1 (2%)	40,43,54	1.00	3 (7%)
23	BCR	AA	848	-	40,40,41	1.09	2 (5%)	53,54,56	1.25	9 (16%)
23	BCR	AA	849	-	41,41,41	1.14	2 (4%)	56,56,56	1.20	7 (12%)
23	BCR	AA	850	-	41,41,41	1.05	2 (4%)	56,56,56	1.26	8 (14%)
23	BCR	AA	851	-	41,41,41	1.13	2 (4%)	56,56,56	1.24	5 (8%)
23	BCR	AA	852	-	41,41,41	1.09	1 (2%)	56,56,56	1.44	7 (12%)
19	CLA	AA	853	-	57,73,73	1.07	7 (12%)	66,113,113	1.38	10 (15%)
23	BCR	AA	854	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	12 (21%)
23	BCR	AA	855	-	41,41,41	1.14	2 (4%)	56,56,56	1.29	8 (14%)
24	AJP	AA	856	-	40,40,95	4.24	24 (60%)	57,65,149	3.45	19 (33%)
19	CLA	B	801	-	57,73,73	1.00	4 (7%)	66,113,113	1.77	14 (21%)
19	CLA	B	802	-	57,73,73	1.06	6 (10%)	66,113,113	1.42	8 (12%)
19	CLA	B	803	-	57,73,73	1.04	5 (8%)	66,113,113	1.53	9 (13%)
19	CLA	B	804	-	54,70,73	1.07	5 (9%)	62,109,113	1.48	11 (17%)
19	CLA	B	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.57	11 (17%)
19	CLA	B	806	-	57,73,73	1.03	5 (8%)	66,113,113	1.55	11 (16%)
19	CLA	B	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.52	8 (12%)
19	CLA	B	808	-	52,68,73	1.09	4 (7%)	60,107,113	1.37	7 (11%)
19	CLA	B	809	-	34,53,73	1.29	5 (14%)	37,89,113	1.81	9 (24%)
19	CLA	B	810	-	57,73,73	1.03	5 (8%)	66,113,113	1.49	9 (13%)
19	CLA	B	811	-	53,69,73	1.05	5 (9%)	61,108,113	1.39	6 (9%)
19	CLA	B	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.91	10 (27%)
19	CLA	B	813	-	34,50,73	1.30	5 (14%)	38,85,113	1.69	9 (23%)
19	CLA	B	814	-	51,67,73	1.12	5 (9%)	58,105,113	1.60	11 (18%)
19	CLA	B	815	-	57,73,73	1.01	4 (7%)	66,113,113	1.58	11 (16%)
19	CLA	B	816	-	49,65,73	1.16	6 (12%)	56,103,113	1.54	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.84	9 (23%)
19	CLA	B	818	-	33,49,73	1.20	3 (9%)	37,84,113	1.67	6 (16%)
19	CLA	B	819	-	33,49,73	1.29	4 (12%)	37,84,113	1.78	8 (21%)
19	CLA	B	820	-	34,53,73	1.34	5 (14%)	37,89,113	2.09	11 (29%)
19	CLA	B	821	2	57,73,73	1.00	4 (7%)	66,113,113	1.50	8 (12%)
19	CLA	B	822	-	57,73,73	1.04	5 (8%)	66,113,113	1.45	7 (10%)
19	CLA	B	823	-	57,73,73	1.04	5 (8%)	66,113,113	1.44	6 (9%)
19	CLA	B	824	-	47,63,73	1.13	4 (8%)	54,101,113	1.49	8 (14%)
19	CLA	B	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.47	8 (12%)
19	CLA	B	826	-	57,73,73	1.08	6 (10%)	66,113,113	1.57	12 (18%)
19	CLA	B	827	-	34,53,73	1.32	5 (14%)	37,89,113	1.67	6 (16%)
19	CLA	B	828	-	34,53,73	1.27	5 (14%)	37,89,113	1.71	7 (18%)
19	CLA	B	829	-	57,73,73	1.04	4 (7%)	66,113,113	1.41	8 (12%)
19	CLA	B	830	-	48,64,73	1.10	5 (10%)	55,102,113	1.60	11 (20%)
19	CLA	B	831	-	48,64,73	1.11	4 (8%)	55,102,113	1.51	9 (16%)
19	CLA	B	832	-	34,53,73	1.35	6 (17%)	37,89,113	1.60	5 (13%)
19	CLA	B	833	-	57,73,73	1.06	5 (8%)	66,113,113	1.60	13 (19%)
19	CLA	B	834	-	57,73,73	1.09	6 (10%)	66,113,113	1.76	16 (24%)
19	CLA	B	835	-	34,53,73	1.29	4 (11%)	37,89,113	1.76	8 (21%)
19	CLA	B	836	-	57,73,73	1.05	5 (8%)	66,113,113	1.43	9 (13%)
19	CLA	B	837	-	52,68,73	1.09	5 (9%)	60,107,113	1.46	7 (11%)
21	PQN	B	838	-	34,34,34	0.63	0	42,45,45	0.85	1 (2%)
23	BCR	B	839	-	41,41,41	1.14	2 (4%)	56,56,56	1.27	8 (14%)
23	BCR	B	840	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
26	ECH	B	841	-	42,42,42	0.89	1 (2%)	55,58,58	2.49	22 (40%)
23	BCR	B	842	-	41,41,41	1.09	2 (4%)	56,56,56	1.34	6 (10%)
23	BCR	B	843	-	41,41,41	1.19	2 (4%)	56,56,56	1.18	6 (10%)
23	BCR	B	844	-	41,41,41	1.24	4 (9%)	56,56,56	1.22	7 (12%)
25	LMG	B	845	-	55,55,55	0.69	0	63,63,63	1.25	4 (6%)
19	CLA	B	846	-	31,47,73	1.29	4 (12%)	33,80,113	1.92	9 (27%)
23	BCR	B	848	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
24	AJP	B	849	-	49,49,95	3.88	23 (46%)	71,80,149	4.32	42 (59%)
24	AJP	B	850	-	49,49,95	3.89	25 (51%)	71,80,149	4.24	43 (60%)
25	LMG	B	851	-	55,55,55	0.67	0	63,63,63	1.27	7 (11%)
22	LHG	B	852	-	32,32,48	0.89	1 (3%)	35,38,54	1.01	3 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	B	853	-	48,48,48	0.75	1 (2%)	51,54,54	0.97	4 (7%)
19	CLA	B	854	-	57,73,73	1.03	6 (10%)	66,113,113	1.47	5 (7%)
28	DGD	B	856	-	43,43,67	1.06	0	57,57,81	1.39	6 (10%)
24	AJP	B	857	-	49,49,95	3.87	25 (51%)	71,80,149	3.20	20 (28%)
19	CLA	B	858	-	57,73,73	1.06	5 (8%)	66,113,113	1.41	10 (15%)
19	CLA	B	859	-	52,68,73	1.10	6 (11%)	60,107,113	1.84	17 (28%)
19	CLA	B	860	-	57,73,73	1.07	5 (8%)	66,113,113	1.68	12 (18%)
27	SF4	B	861	-	0,12,12	0.00	-	-	-	-
19	CLA	B1	801	-	57,73,73	1.01	4 (7%)	66,113,113	1.63	11 (16%)
19	CLA	B1	802	-	57,73,73	1.04	5 (8%)	66,113,113	1.40	10 (15%)
19	CLA	B1	803	-	57,73,73	1.05	7 (12%)	66,113,113	1.49	9 (13%)
19	CLA	B1	804	-	54,70,73	1.07	5 (9%)	62,109,113	1.50	10 (16%)
19	CLA	B1	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.57	11 (17%)
19	CLA	B1	806	-	57,73,73	1.02	5 (8%)	66,113,113	1.56	12 (18%)
19	CLA	B1	807	-	57,73,73	1.06	4 (7%)	66,113,113	1.61	11 (16%)
19	CLA	B1	808	-	52,68,73	1.08	4 (7%)	60,107,113	1.42	7 (11%)
19	CLA	B1	809	-	34,53,73	1.28	4 (11%)	37,89,113	1.78	9 (24%)
19	CLA	B1	810	-	57,73,73	1.03	4 (7%)	66,113,113	1.45	11 (16%)
19	CLA	B1	811	-	53,69,73	1.07	4 (7%)	61,108,113	1.36	6 (9%)
19	CLA	B1	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.83	7 (18%)
19	CLA	B1	813	-	34,50,73	1.29	4 (11%)	38,85,113	1.69	9 (23%)
19	CLA	B1	814	-	51,67,73	1.11	4 (7%)	58,105,113	1.47	8 (13%)
19	CLA	B1	815	-	57,73,73	1.01	4 (7%)	66,113,113	1.63	11 (16%)
19	CLA	B1	816	-	49,65,73	1.14	5 (10%)	56,103,113	1.47	8 (14%)
19	CLA	B1	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.76	7 (18%)
19	CLA	B1	818	-	33,49,73	1.28	4 (12%)	37,84,113	1.73	7 (18%)
19	CLA	B1	819	-	33,49,73	1.28	4 (12%)	37,84,113	1.78	9 (24%)
19	CLA	B1	820	-	34,53,73	1.30	4 (11%)	37,89,113	1.71	9 (24%)
19	CLA	B1	821	2	57,73,73	1.01	5 (8%)	66,113,113	1.47	10 (15%)
19	CLA	B1	822	-	57,73,73	1.03	5 (8%)	66,113,113	1.41	9 (13%)
19	CLA	B1	823	-	57,73,73	1.03	4 (7%)	66,113,113	1.45	7 (10%)
19	CLA	B1	824	-	47,63,73	1.18	6 (12%)	54,101,113	1.48	9 (16%)
19	CLA	B1	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.49	8 (12%)
19	CLA	B1	826	-	57,73,73	1.08	6 (10%)	66,113,113	1.58	12 (18%)
19	CLA	B1	827	-	34,53,73	1.31	5 (14%)	37,89,113	1.65	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B1	828	-	57,73,73	1.04	4 (7%)	66,113,113	1.36	8 (12%)
19	CLA	B1	829	-	48,64,73	1.14	7 (14%)	55,102,113	1.59	10 (18%)
19	CLA	B1	830	-	48,64,73	1.11	4 (8%)	55,102,113	1.52	8 (14%)
19	CLA	B1	831	-	34,53,73	1.33	6 (17%)	37,89,113	1.61	5 (13%)
19	CLA	B1	832	-	57,73,73	1.02	4 (7%)	66,113,113	1.53	11 (16%)
19	CLA	B1	833	-	57,73,73	1.09	7 (12%)	66,113,113	1.79	16 (24%)
19	CLA	B1	834	-	34,53,73	1.27	4 (11%)	37,89,113	1.73	7 (18%)
19	CLA	B1	835	-	57,73,73	1.04	6 (10%)	66,113,113	1.36	7 (10%)
19	CLA	B1	836	-	52,68,73	1.09	4 (7%)	60,107,113	1.56	9 (15%)
21	PQN	B1	837	-	34,34,34	0.70	0	42,45,45	0.86	0
23	BCR	B1	838	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	10 (17%)
23	BCR	B1	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.16	3 (5%)
26	ECH	B1	840	-	42,42,42	0.81	1 (2%)	55,58,58	2.43	19 (34%)
23	BCR	B1	841	-	41,41,41	1.06	2 (4%)	56,56,56	1.35	6 (10%)
23	BCR	B1	842	-	41,41,41	1.18	2 (4%)	56,56,56	1.22	6 (10%)
23	BCR	B1	843	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
25	LMG	B1	844	-	55,55,55	0.68	0	63,63,63	1.27	3 (4%)
19	CLA	B1	845	-	31,47,73	1.29	4 (12%)	33,80,113	1.87	9 (27%)
25	LMG	B1	846	-	32,32,55	0.93	0	40,40,63	1.20	4 (10%)
22	LHG	B1	847	-	32,32,48	0.87	1 (3%)	35,38,54	1.03	3 (8%)
19	CLA	B1	848	-	57,73,73	1.06	6 (10%)	66,113,113	1.48	6 (9%)
19	CLA	B1	849	-	57,73,73	1.05	6 (10%)	66,113,113	1.35	7 (10%)
19	CLA	B1	850	-	52,68,73	1.10	5 (9%)	60,107,113	1.80	17 (28%)
27	SF4	B1	851	-	0,12,12	0.00	-	-	-	-
25	LMG	B1	852	-	30,30,55	0.99	0	38,38,63	1.22	4 (10%)
19	CLA	B2	801	-	57,73,73	1.01	4 (7%)	66,113,113	1.65	11 (16%)
19	CLA	B2	802	-	57,73,73	1.05	4 (7%)	66,113,113	1.42	9 (13%)
19	CLA	B2	803	-	57,73,73	1.04	6 (10%)	66,113,113	1.53	9 (13%)
19	CLA	B2	804	-	54,70,73	1.07	6 (11%)	62,109,113	1.52	10 (16%)
19	CLA	B2	805	-	56,72,73	1.04	5 (8%)	64,111,113	1.57	11 (17%)
19	CLA	B2	806	2	57,73,73	1.02	5 (8%)	66,113,113	1.53	11 (16%)
19	CLA	B2	807	-	57,73,73	1.06	4 (7%)	66,113,113	1.63	11 (16%)
19	CLA	B2	808	-	52,68,73	1.08	4 (7%)	60,107,113	1.44	7 (11%)
19	CLA	B2	809	-	34,53,73	1.28	4 (11%)	37,89,113	1.78	9 (24%)
19	CLA	B2	810	-	57,73,73	1.02	4 (7%)	66,113,113	1.45	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B2	811	-	53,69,73	1.06	4 (7%)	61,108,113	1.37	6 (9%)
19	CLA	B2	812	-	33,49,73	1.28	4 (12%)	37,84,113	1.84	8 (21%)
19	CLA	B2	813	-	34,50,73	1.28	4 (11%)	38,85,113	1.67	9 (23%)
19	CLA	B2	814	-	51,67,73	1.12	5 (9%)	58,105,113	1.47	7 (12%)
19	CLA	B2	815	-	57,73,73	1.03	4 (7%)	66,113,113	1.56	11 (16%)
19	CLA	B2	816	-	49,65,73	1.13	5 (10%)	56,103,113	1.50	7 (12%)
19	CLA	B2	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.77	8 (21%)
19	CLA	B2	818	-	33,49,73	1.28	4 (12%)	37,84,113	1.73	8 (21%)
19	CLA	B2	819	-	33,49,73	1.29	5 (15%)	37,84,113	1.83	8 (21%)
19	CLA	B2	820	-	34,53,73	1.34	5 (14%)	37,89,113	1.99	12 (32%)
19	CLA	B2	821	-	57,73,73	1.00	4 (7%)	66,113,113	1.51	11 (16%)
19	CLA	B2	822	-	57,73,73	1.06	5 (8%)	66,113,113	1.45	8 (12%)
19	CLA	B2	823	-	57,73,73	1.03	4 (7%)	66,113,113	1.46	7 (10%)
19	CLA	B2	824	-	47,63,73	1.14	4 (8%)	54,101,113	1.54	8 (14%)
19	CLA	B2	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.49	9 (13%)
19	CLA	B2	826	-	57,73,73	1.07	5 (8%)	66,113,113	1.58	11 (16%)
19	CLA	B2	827	-	34,53,73	1.33	6 (17%)	37,89,113	1.65	6 (16%)
19	CLA	B2	828	-	34,53,73	1.26	4 (11%)	37,89,113	1.71	7 (18%)
19	CLA	B2	829	-	57,73,73	1.05	4 (7%)	66,113,113	1.33	7 (10%)
19	CLA	B2	830	-	48,64,73	1.14	7 (14%)	55,102,113	1.60	10 (18%)
19	CLA	B2	831	-	48,64,73	1.10	4 (8%)	55,102,113	1.54	8 (14%)
19	CLA	B2	832	-	34,53,73	1.31	5 (14%)	37,89,113	1.59	5 (13%)
19	CLA	B2	833	-	57,73,73	1.02	4 (7%)	66,113,113	1.64	13 (19%)
19	CLA	B2	834	-	57,73,73	1.11	6 (10%)	66,113,113	1.74	15 (22%)
19	CLA	B2	835	-	34,53,73	1.29	4 (11%)	37,89,113	1.68	6 (16%)
19	CLA	B2	836	-	57,73,73	1.05	6 (10%)	66,113,113	1.36	6 (9%)
19	CLA	B2	837	-	52,68,73	1.09	4 (7%)	60,107,113	1.54	9 (15%)
21	PQN	B2	838	-	34,34,34	0.61	0	42,45,45	0.84	0
23	BCR	B2	839	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	10 (17%)
23	BCR	B2	840	-	41,41,41	1.09	2 (4%)	56,56,56	1.20	5 (8%)
26	ECH	B2	841	-	42,42,42	0.79	1 (2%)	55,58,58	2.41	18 (32%)
23	BCR	B2	842	-	41,41,41	1.01	2 (4%)	56,56,56	1.35	7 (12%)
23	BCR	B2	843	-	41,41,41	1.16	2 (4%)	56,56,56	1.17	6 (10%)
23	BCR	B2	844	-	41,41,41	1.21	3 (7%)	56,56,56	1.19	6 (10%)
25	LMG	B2	845	-	55,55,55	0.68	0	63,63,63	1.26	4 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	B2	846	-	31,47,73	1.29	4 (12%)	33,80,113	1.87	9 (27%)
25	LMG	B2	847	-	32,32,55	0.93	0	40,40,63	1.21	2 (5%)
22	LHG	B2	848	-	32,32,48	0.89	2 (6%)	35,38,54	0.98	2 (5%)
19	CLA	B2	849	-	57,73,73	1.05	5 (8%)	66,113,113	1.46	5 (7%)
19	CLA	B2	850	-	57,73,73	1.07	7 (12%)	66,113,113	1.40	7 (10%)
19	CLA	B2	851	-	52,68,73	1.09	5 (9%)	60,107,113	1.81	16 (26%)
19	CLA	B2	852	-	57,73,73	1.07	5 (8%)	66,113,113	1.66	12 (18%)
27	SF4	B2	853	-	0,12,12	0.00	-	-		
25	LMG	B2	854	-	30,30,55	0.99	0	38,38,63	1.22	4 (10%)
19	CLA	BB	801	-	57,73,73	1.00	4 (7%)	66,113,113	1.75	11 (16%)
19	CLA	BB	802	-	57,73,73	1.07	6 (10%)	66,113,113	1.40	9 (13%)
19	CLA	BB	803	-	57,73,73	1.04	5 (8%)	66,113,113	1.50	9 (13%)
19	CLA	BB	804	-	54,70,73	1.07	6 (11%)	62,109,113	1.49	11 (17%)
19	CLA	BB	805	-	56,72,73	1.04	6 (10%)	64,111,113	1.56	11 (17%)
19	CLA	BB	806	-	57,73,73	1.04	5 (8%)	66,113,113	1.52	12 (18%)
19	CLA	BB	807	-	57,73,73	1.04	4 (7%)	66,113,113	1.53	8 (12%)
19	CLA	BB	808	-	52,68,73	1.11	5 (9%)	60,107,113	1.45	8 (13%)
19	CLA	BB	809	-	34,53,73	1.29	5 (14%)	37,89,113	1.82	9 (24%)
19	CLA	BB	810	-	57,73,73	1.02	4 (7%)	66,113,113	1.44	10 (15%)
19	CLA	BB	811	-	53,69,73	1.06	5 (9%)	61,108,113	1.41	7 (11%)
19	CLA	BB	812	-	33,49,73	1.30	4 (12%)	37,84,113	1.82	8 (21%)
19	CLA	BB	813	-	34,50,73	1.28	4 (11%)	38,85,113	1.75	9 (23%)
19	CLA	BB	814	-	51,67,73	1.12	7 (13%)	58,105,113	1.57	9 (15%)
19	CLA	BB	815	-	57,73,73	1.02	4 (7%)	66,113,113	1.56	9 (13%)
19	CLA	BB	816	-	49,65,73	1.15	6 (12%)	56,103,113	1.54	9 (16%)
19	CLA	BB	817	-	34,50,73	1.28	4 (11%)	38,85,113	1.79	8 (21%)
19	CLA	BB	818	-	33,49,73	1.34	4 (12%)	37,84,113	1.64	6 (16%)
19	CLA	BB	819	-	33,49,73	1.28	4 (12%)	37,84,113	1.80	10 (27%)
19	CLA	BB	820	-	34,53,73	1.36	5 (14%)	37,89,113	2.14	13 (35%)
19	CLA	BB	821	-	57,73,73	1.01	4 (7%)	66,113,113	1.39	8 (12%)
19	CLA	BB	822	-	57,73,73	1.01	6 (10%)	66,113,113	1.46	6 (9%)
19	CLA	BB	823	-	57,73,73	1.04	5 (8%)	66,113,113	1.44	7 (10%)
19	CLA	BB	824	-	47,63,73	1.15	5 (10%)	54,101,113	1.51	8 (14%)
19	CLA	BB	825	-	57,73,73	1.03	4 (7%)	66,113,113	1.47	8 (12%)
19	CLA	BB	826	-	57,73,73	1.12	6 (10%)	66,113,113	1.59	12 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	BB	827	-	34,53,73	1.32	6 (17%)	37,89,113	1.66	6 (16%)
19	CLA	BB	828	-	34,53,73	1.27	5 (14%)	37,89,113	1.76	7 (18%)
19	CLA	BB	829	-	48,64,73	1.17	6 (12%)	55,102,113	1.54	10 (18%)
19	CLA	BB	830	-	48,64,73	1.11	4 (8%)	55,102,113	1.50	9 (16%)
19	CLA	BB	831	-	34,53,73	1.35	6 (17%)	37,89,113	1.66	6 (16%)
19	CLA	BB	832	-	57,73,73	1.08	6 (10%)	66,113,113	1.58	11 (16%)
19	CLA	BB	833	-	57,73,73	1.08	6 (10%)	66,113,113	1.76	16 (24%)
19	CLA	BB	834	-	34,53,73	1.28	5 (14%)	37,89,113	1.76	6 (16%)
19	CLA	BB	835	-	57,73,73	1.06	6 (10%)	66,113,113	1.39	9 (13%)
19	CLA	BB	836	-	52,68,73	1.12	5 (9%)	60,107,113	1.87	13 (21%)
21	PQN	BB	837	-	34,34,34	0.65	0	42,45,45	0.83	0
23	BCR	BB	838	-	41,41,41	1.16	2 (4%)	56,56,56	1.26	7 (12%)
23	BCR	BB	839	-	41,41,41	1.10	2 (4%)	56,56,56	1.20	6 (10%)
26	ECH	BB	840	-	42,42,42	0.88	0	55,58,58	2.44	18 (32%)
23	BCR	BB	841	-	41,41,41	1.09	2 (4%)	56,56,56	1.35	6 (10%)
23	BCR	BB	842	-	41,41,41	1.19	2 (4%)	56,56,56	1.19	5 (8%)
23	BCR	BB	843	-	41,41,41	1.21	4 (9%)	56,56,56	1.19	6 (10%)
25	LMG	BB	844	-	55,55,55	0.69	1 (1%)	63,63,63	1.26	4 (6%)
19	CLA	BB	845	-	31,47,73	1.29	4 (12%)	33,80,113	1.93	9 (27%)
23	BCR	BB	847	-	41,41,41	1.17	2 (4%)	56,56,56	1.34	8 (14%)
24	AJP	BB	848	-	49,49,95	3.87	24 (48%)	71,80,149	4.25	40 (56%)
24	AJP	BB	849	-	49,49,95	3.92	25 (51%)	71,80,149	4.23	44 (61%)
22	LHG	BB	850	-	32,32,48	0.89	1 (3%)	35,38,54	1.02	3 (8%)
22	LHG	BB	851	-	48,48,48	0.76	2 (4%)	51,54,54	0.97	4 (7%)
19	CLA	BB	852	-	57,73,73	1.04	5 (8%)	66,113,113	1.53	7 (10%)
28	DGD	BB	854	-	43,43,67	1.05	0	57,57,81	1.40	7 (12%)
19	CLA	BB	855	-	57,73,73	1.05	7 (12%)	66,113,113	1.45	7 (10%)
19	CLA	BB	856	-	52,68,73	1.10	6 (11%)	60,107,113	1.83	17 (28%)
27	SF4	BB	857	-	0,12,12	0.00	-	-	-	-
27	SF4	C	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C	102	3	0,12,12	0.00	-	-	-	-
27	SF4	C1	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C1	102	-	0,12,12	0.00	-	-	-	-
27	SF4	C2	101	-	0,12,12	0.00	-	-	-	-
27	SF4	C2	102	-	0,12,12	0.00	-	-	-	-
27	SF4	CC	101	-	0,12,12	0.00	-	-	-	-
27	SF4	CC	102	-	0,12,12	0.00	-	-	-	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	F	301	-	52,68,73	1.06	5 (9%)	60,107,113	1.66	11 (18%)
19	CLA	F	302	-	34,50,73	1.28	4 (11%)	38,85,113	1.82	9 (23%)
23	BCR	F	303	-	41,41,41	1.13	2 (4%)	56,56,56	1.31	9 (16%)
23	BCR	F	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.29	9 (16%)
23	BCR	F	305	-	41,41,41	1.15	3 (7%)	56,56,56	1.49	10 (17%)
19	CLA	F1	301	-	52,68,73	1.07	5 (9%)	60,107,113	1.65	11 (18%)
19	CLA	F1	302	-	34,50,73	1.28	5 (14%)	38,85,113	1.85	10 (26%)
23	BCR	F1	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.27	7 (12%)
23	BCR	F1	304	-	41,41,41	1.21	2 (4%)	56,56,56	1.28	9 (16%)
19	CLA	F1	305	-	34,53,73	1.26	4 (11%)	37,89,113	1.71	7 (18%)
23	BCR	F1	306	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	8 (14%)
19	CLA	F2	301	-	52,68,73	1.06	5 (9%)	60,107,113	1.60	11 (18%)
19	CLA	F2	302	-	34,50,73	1.28	5 (14%)	38,85,113	1.85	9 (23%)
23	BCR	F2	303	-	41,41,41	1.09	2 (4%)	56,56,56	1.29	8 (14%)
23	BCR	F2	304	-	41,41,41	1.20	2 (4%)	56,56,56	1.25	9 (16%)
23	BCR	F2	305	-	41,41,41	1.12	2 (4%)	56,56,56	1.48	9 (16%)
19	CLA	FF	301	-	52,68,73	1.08	4 (7%)	60,107,113	1.51	12 (20%)
19	CLA	FF	302	-	34,50,73	1.28	4 (11%)	38,85,113	1.83	9 (23%)
23	BCR	FF	303	-	41,41,41	1.12	2 (4%)	56,56,56	1.33	9 (16%)
23	BCR	FF	304	-	41,41,41	1.22	2 (4%)	56,56,56	1.29	9 (16%)
19	CLA	FF	305	-	57,73,73	1.04	4 (7%)	66,113,113	1.39	8 (12%)
23	BCR	FF	306	-	41,41,41	1.15	3 (7%)	56,56,56	1.48	10 (17%)
23	BCR	I	101	-	41,41,41	1.18	2 (4%)	56,56,56	1.21	6 (10%)
23	BCR	I	102	-	41,41,41	1.15	2 (4%)	56,56,56	1.19	7 (12%)
23	BCR	I1	101	-	41,41,41	1.23	2 (4%)	56,56,56	1.27	8 (14%)
25	LMG	I1	102	-	35,35,55	1.04	1 (2%)	43,43,63	1.26	3 (6%)
23	BCR	I2	101	-	41,41,41	1.22	2 (4%)	56,56,56	1.27	9 (16%)
23	BCR	I2	102	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
23	BCR	I2	103	-	41,41,41	1.13	2 (4%)	56,56,56	1.36	9 (16%)
24	AJP	I2	104	-	36,36,95	4.36	22 (61%)	54,60,149	4.41	31 (57%)
25	LMG	I2	105	-	35,35,55	0.92	1 (2%)	43,43,63	1.21	4 (9%)
23	BCR	II	101	-	41,41,41	1.19	2 (4%)	56,56,56	1.22	8 (14%)
23	BCR	II	102	-	41,41,41	1.15	3 (7%)	56,56,56	1.19	5 (8%)
23	BCR	II	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.32	8 (14%)
25	LMG	II	105	-	42,42,55	0.82	1 (2%)	50,50,63	1.23	5 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	J	101	8	33,49,73	1.30	4 (12%)	37,84,113	1.76	8 (21%)
23	BCR	J	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.38	9 (16%)
19	CLA	J	103	-	33,49,73	1.31	5 (15%)	37,84,113	1.70	7 (18%)
23	BCR	J	104	-	41,41,41	1.12	2 (4%)	56,56,56	1.36	7 (12%)
19	CLA	J1	101	-	33,49,73	1.30	4 (12%)	37,84,113	1.73	8 (21%)
23	BCR	J1	102	-	41,41,41	1.20	2 (4%)	56,56,56	1.36	9 (16%)
19	CLA	J1	103	-	33,49,73	1.30	4 (12%)	37,84,113	1.73	7 (18%)
23	BCR	J1	104	-	41,41,41	1.13	2 (4%)	56,56,56	1.33	6 (10%)
19	CLA	J2	101	8	33,49,73	1.31	4 (12%)	37,84,113	1.71	8 (21%)
23	BCR	J2	102	-	41,41,41	1.19	2 (4%)	56,56,56	1.35	8 (14%)
19	CLA	J2	103	-	33,49,73	1.30	4 (12%)	37,84,113	1.70	7 (18%)
23	BCR	J2	104	-	41,41,41	1.15	2 (4%)	56,56,56	1.31	9 (16%)
19	CLA	JJ	101	8	33,49,73	1.30	4 (12%)	37,84,113	1.76	8 (21%)
23	BCR	JJ	102	-	41,41,41	1.24	2 (4%)	56,56,56	1.37	10 (17%)
19	CLA	JJ	103	-	33,49,73	1.31	4 (12%)	37,84,113	1.73	7 (18%)
23	BCR	JJ	104	-	41,41,41	1.17	3 (7%)	56,56,56	1.24	7 (12%)
19	CLA	K	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	K	102	-	38,54,73	1.21	4 (10%)	43,90,113	1.67	8 (18%)
23	BCR	K	103	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	7 (12%)
24	AJP	K	104	-	47,47,95	3.94	24 (51%)	68,77,149	4.30	38 (55%)
19	CLA	K1	102	-	34,53,73	1.28	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	K1	103	-	38,54,73	1.23	4 (10%)	43,90,113	1.68	7 (16%)
23	BCR	K1	104	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	K1	105	9	31,48,73	1.35	4 (12%)	35,82,113	1.92	11 (31%)
23	BCR	K1	106	-	41,41,41	1.14	2 (4%)	56,56,56	1.35	10 (17%)
19	CLA	K2	102	-	34,53,73	1.28	4 (11%)	37,89,113	1.80	9 (24%)
23	BCR	K2	103	-	41,41,41	1.15	3 (7%)	56,56,56	1.18	6 (10%)
19	CLA	K2	104	-	30,49,73	1.31	4 (13%)	31,83,113	1.93	9 (29%)
23	BCR	K2	105	-	41,41,41	1.13	2 (4%)	56,56,56	1.32	9 (16%)
19	CLA	KK	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.89	9 (24%)
19	CLA	KK	102	-	38,54,73	1.22	4 (10%)	43,90,113	1.68	8 (18%)
23	BCR	KK	103	-	41,41,41	1.12	2 (4%)	56,56,56	1.34	9 (16%)
24	AJP	KK	104	-	47,47,95	3.93	24 (51%)	68,77,149	4.33	38 (55%)
19	CLA	L	202	18	53,69,73	1.07	5 (9%)	61,108,113	1.71	10 (16%)
19	CLA	L	203	-	57,73,73	1.07	6 (10%)	66,113,113	1.49	10 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CLA	L	204	-	57,73,73	1.01	4 (7%)	66,113,113	1.62	11 (16%)
23	BCR	L	205	-	41,41,41	1.14	2 (4%)	56,56,56	1.32	9 (16%)
23	BCR	L	206	-	41,41,41	1.17	2 (4%)	56,56,56	1.25	9 (16%)
22	LHG	L	207	-	33,33,48	0.94	3 (9%)	36,39,54	1.05	4 (11%)
24	AJP	L	208	-	36,36,95	4.44	24 (66%)	54,60,149	4.64	33 (61%)
24	AJP	L	209	-	36,36,95	4.47	24 (66%)	54,60,149	4.56	31 (57%)
23	BCR	L1	201	-	41,41,41	1.16	2 (4%)	56,56,56	1.23	6 (10%)
24	AJP	L1	203	-	49,49,95	3.87	24 (48%)	71,80,149	3.74	35 (49%)
24	AJP	L1	204	-	49,49,95	3.84	23 (46%)	71,80,149	4.02	45 (63%)
19	CLA	L1	205	10	53,69,73	1.06	4 (7%)	61,108,113	1.57	12 (19%)
19	CLA	L1	206	-	57,73,73	1.05	6 (10%)	66,113,113	1.52	10 (15%)
19	CLA	L1	207	-	57,73,73	0.98	4 (7%)	66,113,113	1.47	7 (10%)
23	BCR	L1	208	-	41,41,41	1.12	2 (4%)	56,56,56	1.35	10 (17%)
23	BCR	L1	209	-	41,41,41	1.14	2 (4%)	56,56,56	1.26	9 (16%)
25	LMG	L1	210	-	55,55,55	0.68	0	63,63,63	1.27	6 (9%)
22	LHG	L1	211	-	32,32,48	0.95	3 (9%)	35,38,54	1.02	3 (8%)
24	AJP	L2	202	-	49,49,95	3.88	23 (46%)	71,80,149	4.36	44 (61%)
24	AJP	L2	203	-	49,49,95	3.84	22 (44%)	71,80,149	4.02	44 (61%)
19	CLA	L2	204	16	53,69,73	1.06	4 (7%)	61,108,113	1.54	11 (18%)
19	CLA	L2	205	-	51,67,73	1.09	6 (11%)	58,105,113	1.67	9 (15%)
19	CLA	L2	206	-	57,73,73	0.98	4 (7%)	66,113,113	1.47	8 (12%)
23	BCR	L2	207	-	41,41,41	1.15	2 (4%)	56,56,56	1.27	8 (14%)
22	LHG	L2	208	-	34,34,48	0.86	1 (2%)	37,40,54	1.05	3 (8%)
19	CLA	LL	201	18	53,69,73	1.07	4 (7%)	61,108,113	1.75	10 (16%)
19	CLA	LL	202	-	57,73,73	1.07	7 (12%)	66,113,113	1.53	10 (15%)
19	CLA	LL	203	-	34,50,73	1.32	4 (11%)	38,85,113	1.98	8 (21%)
23	BCR	LL	204	-	41,41,41	1.14	2 (4%)	56,56,56	1.19	6 (10%)
22	LHG	LL	205	-	33,33,48	0.94	3 (9%)	36,39,54	1.04	4 (11%)
23	BCR	M	101	-	41,41,41	1.21	3 (7%)	56,56,56	1.33	10 (17%)
25	LMG	M	102	-	46,46,55	0.82	0	54,54,63	1.27	7 (12%)
23	BCR	M1	101	-	41,41,41	1.13	3 (7%)	56,56,56	1.24	7 (12%)
24	AJP	M2	101	-	36,36,95	4.46	23 (63%)	54,60,149	4.47	30 (55%)
23	BCR	M2	102	-	41,41,41	1.12	3 (7%)	56,56,56	1.24	9 (16%)
23	BCR	MM	101	-	41,41,41	1.20	3 (7%)	56,56,56	1.36	10 (17%)
19	CLA	X	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.77	7 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
22	LHG	X	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.94	2 (4%)
19	CLA	X1	101	-	34,53,73	1.26	4 (11%)	37,89,113	1.77	7 (18%)
22	LHG	X1	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
22	LHG	X1	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	3 (5%)
19	CLA	X2	101	-	34,53,73	1.26	4 (11%)	37,89,113	1.74	7 (18%)
22	LHG	X2	102	-	39,39,48	0.81	2 (5%)	42,45,54	0.93	2 (4%)
22	LHG	X2	103	-	48,48,48	0.76	1 (2%)	51,54,54	0.95	4 (7%)
19	CLA	XX	101	-	34,53,73	1.27	4 (11%)	37,89,113	1.77	7 (18%)
22	LHG	XX	102	-	39,39,48	0.80	2 (5%)	42,45,54	0.93	2 (4%)

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
19	CLA	A	801	-	3/3/25/25	11/37/135/135	-
24	AJP	A	802	-	3/3/14/38	-	0/6/6/11
20	CL0	A	803	-	4/4/25/25	18/37/135/135	-
19	CLA	A	804	-	3/3/25/25	17/37/135/135	-
19	CLA	A	805	-	3/3/24/25	8/31/129/135	-
19	CLA	A	806	-	3/3/23/25	8/27/125/135	-
19	CLA	A	807	-	3/3/25/25	17/37/135/135	-
19	CLA	A	808	-	3/3/25/25	13/37/135/135	-
19	CLA	A	809	-	3/3/22/25	2/19/117/135	-
19	CLA	A	810	1	3/3/25/25	11/37/135/135	-
19	CLA	A	811	1	3/3/22/25	6/21/119/135	-
19	CLA	A	812	-	3/3/20/25	7/15/113/135	-
19	CLA	A	813	-	3/3/25/25	9/37/135/135	-
19	CLA	A	814	-	3/3/19/25	3/10/108/135	-
19	CLA	A	815	-	3/3/23/25	9/25/123/135	-
19	CLA	A	816	-	3/3/22/25	7/19/117/135	-
19	CLA	A	817	-	3/3/19/25	3/11/110/135	-
19	CLA	A	818	-	3/3/20/25	1/11/111/135	-
19	CLA	A	819	-	3/3/24/25	11/31/129/135	-
19	CLA	A	820	-	2/2/23/25	11/29/127/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A	821	-	3/3/25/25	13/37/135/135	-
19	CLA	A	822	-	3/3/22/25	7/21/119/135	-
19	CLA	A	823	-	3/3/24/25	14/31/129/135	-
19	CLA	A	824	-	3/3/20/25	9/11/111/135	-
19	CLA	A	825	-	3/3/22/25	3/22/120/135	-
19	CLA	A	826	-	3/3/20/25	7/11/111/135	-
19	CLA	A	827	-	3/3/25/25	16/37/135/135	-
19	CLA	A	828	-	3/3/23/25	11/27/125/135	-
19	CLA	A	829	-	3/3/25/25	14/37/135/135	-
19	CLA	A	830	-	3/3/24/25	15/34/132/135	-
19	CLA	A	831	-	3/3/25/25	12/37/135/135	-
19	CLA	A	832	-	3/3/25/25	9/37/135/135	-
19	CLA	A	833	-	3/3/22/25	5/19/117/135	-
19	CLA	A	834	-	3/3/19/25	4/8/106/135	-
19	CLA	A	835	-	3/3/25/25	8/37/135/135	-
19	CLA	A	836	-	3/3/25/25	13/37/135/135	-
19	CLA	A	837	-	3/3/20/25	2/11/111/135	-
19	CLA	A	838	-	3/3/19/25	5/11/110/135	-
19	CLA	A	839	-	3/3/22/25	8/22/120/135	-
19	CLA	A	840	-	3/3/23/25	5/27/125/135	-
19	CLA	A	841	-	3/3/20/25	4/15/113/135	-
19	CLA	A	842	-	3/3/25/25	11/37/135/135	-
21	PQN	A	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A	844	-	3/3/19/25	4/8/106/135	-
22	LHG	A	845	-	-	19/53/53/53	-
22	LHG	A	846	-	-	12/42/42/53	-
23	BCR	A	847	-	-	14/27/61/63	0/2/2/2
23	BCR	A	848	-	-	19/29/63/63	0/2/2/2
23	BCR	A	849	-	-	18/29/63/63	0/2/2/2
23	BCR	A	850	-	-	15/29/63/63	0/2/2/2
23	BCR	A	851	-	-	19/29/63/63	0/2/2/2
19	CLA	A	852	-	3/3/25/25	16/37/135/135	-
23	BCR	A	853	-	-	18/29/63/63	0/2/2/2
23	BCR	A	854	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	AJP	A	855	-	-	2/4/99/220	1/6/6/11
19	CLA	A1	801	-	3/3/25/25	13/37/135/135	-
20	CL0	A1	802	-	4/4/25/25	13/37/135/135	-
19	CLA	A1	803	-	3/3/25/25	17/37/135/135	-
19	CLA	A1	804	-	3/3/24/25	9/31/129/135	-
19	CLA	A1	805	-	2/2/23/25	6/27/125/135	-
19	CLA	A1	806	-	3/3/25/25	16/37/135/135	-
19	CLA	A1	807	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	808	-	3/3/22/25	1/19/117/135	-
19	CLA	A1	809	-	3/3/25/25	11/37/135/135	-
19	CLA	A1	810	-	3/3/22/25	7/21/119/135	-
19	CLA	A1	811	-	3/3/20/25	5/15/113/135	-
19	CLA	A1	812	-	3/3/25/25	9/37/135/135	-
19	CLA	A1	813	-	3/3/19/25	4/10/108/135	-
19	CLA	A1	814	-	3/3/23/25	9/25/123/135	-
19	CLA	A1	815	-	3/3/22/25	9/19/117/135	-
19	CLA	A1	816	-	3/3/19/25	2/11/110/135	-
19	CLA	A1	817	-	3/3/20/25	1/11/111/135	-
19	CLA	A1	818	-	3/3/24/25	13/31/129/135	-
19	CLA	A1	819	-	2/2/23/25	9/29/127/135	-
19	CLA	A1	820	-	3/3/25/25	18/37/135/135	-
19	CLA	A1	821	-	3/3/22/25	4/21/119/135	-
19	CLA	A1	822	-	3/3/24/25	15/31/129/135	-
19	CLA	A1	823	-	3/3/20/25	6/11/111/135	-
19	CLA	A1	824	-	3/3/19/25	2/10/108/135	-
19	CLA	A1	825	-	3/3/20/25	7/11/111/135	-
19	CLA	A1	826	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	827	-	3/3/23/25	11/27/125/135	-
19	CLA	A1	828	-	3/3/25/25	20/37/135/135	-
19	CLA	A1	829	-	3/3/24/25	16/34/132/135	-
19	CLA	A1	830	-	3/3/25/25	14/37/135/135	-
19	CLA	A1	831	-	3/3/25/25	8/37/135/135	-
19	CLA	A1	832	-	3/3/22/25	9/19/117/135	-
19	CLA	A1	833	-	3/3/19/25	4/8/106/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A1	834	-	3/3/25/25	7/37/135/135	-
19	CLA	A1	835	-	3/3/25/25	11/37/135/135	-
19	CLA	A1	836	-	3/3/20/25	4/11/111/135	-
19	CLA	A1	837	1	3/3/19/25	4/11/110/135	-
19	CLA	A1	838	-	3/3/22/25	8/22/120/135	-
19	CLA	A1	839	-	3/3/23/25	7/27/125/135	-
19	CLA	A1	840	-	3/3/20/25	6/15/113/135	-
19	CLA	A1	841	-	3/3/25/25	9/37/135/135	-
19	CLA	A1	842	-	3/3/25/25	15/37/135/135	-
21	PQN	A1	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A1	844	-	3/3/19/25	3/8/106/135	-
22	LHG	A1	845	-	-	20/53/53/53	-
22	LHG	A1	846	-	-	12/42/42/53	-
23	BCR	A1	847	-	-	12/27/61/63	0/2/2/2
23	BCR	A1	848	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	849	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	850	-	-	14/29/63/63	0/2/2/2
23	BCR	A1	851	-	-	19/29/63/63	0/2/2/2
19	CLA	A1	852	-	3/3/25/25	18/37/135/135	-
23	BCR	A1	853	-	-	16/29/63/63	0/2/2/2
24	AJP	A1	854	-	-	2/6/121/220	0/7/7/11
24	AJP	A1	855	-	-	-	0/6/6/11
19	CLA	A2	801	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	802	-	3/3/20/25	9/15/113/135	-
20	CL0	A2	803	-	4/4/25/25	16/37/135/135	-
19	CLA	A2	804	-	3/3/25/25	19/37/135/135	-
19	CLA	A2	805	-	3/3/24/25	8/31/129/135	-
19	CLA	A2	806	-	3/3/23/25	9/27/125/135	-
19	CLA	A2	807	-	3/3/25/25	16/37/135/135	-
19	CLA	A2	808	-	3/3/25/25	15/37/135/135	-
19	CLA	A2	809	-	3/3/22/25	2/19/117/135	-
19	CLA	A2	810	1	3/3/25/25	9/37/135/135	-
19	CLA	A2	811	-	3/3/22/25	6/21/119/135	-
19	CLA	A2	812	-	3/3/20/25	5/15/113/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	A2	813	-	3/3/25/25	11/37/135/135	-
19	CLA	A2	814	-	3/3/19/25	4/10/108/135	-
19	CLA	A2	815	-	3/3/23/25	9/25/123/135	-
19	CLA	A2	816	-	3/3/22/25	6/19/117/135	-
19	CLA	A2	817	-	3/3/19/25	1/11/110/135	-
19	CLA	A2	818	-	3/3/20/25	1/11/111/135	-
19	CLA	A2	819	-	3/3/24/25	9/31/129/135	-
19	CLA	A2	820	-	3/3/23/25	11/29/127/135	-
19	CLA	A2	821	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	822	-	3/3/22/25	5/21/119/135	-
19	CLA	A2	823	-	3/3/24/25	12/31/129/135	-
19	CLA	A2	824	-	3/3/20/25	4/11/111/135	-
19	CLA	A2	825	-	3/3/19/25	3/10/108/135	-
19	CLA	A2	826	-	3/3/20/25	7/11/111/135	-
19	CLA	A2	827	-	3/3/25/25	14/37/135/135	-
19	CLA	A2	828	-	3/3/23/25	11/27/125/135	-
19	CLA	A2	829	-	3/3/25/25	17/37/135/135	-
19	CLA	A2	830	-	3/3/24/25	18/34/132/135	-
19	CLA	A2	831	-	3/3/25/25	13/37/135/135	-
19	CLA	A2	832	-	3/3/25/25	6/37/135/135	-
19	CLA	A2	833	-	3/3/22/25	5/19/117/135	-
19	CLA	A2	834	-	3/3/19/25	4/8/106/135	-
19	CLA	A2	835	-	3/3/25/25	7/37/135/135	-
19	CLA	A2	836	-	2/2/25/25	14/37/135/135	-
19	CLA	A2	837	-	3/3/20/25	4/11/111/135	-
19	CLA	A2	838	-	3/3/19/25	4/11/110/135	-
19	CLA	A2	839	-	3/3/22/25	8/22/120/135	-
19	CLA	A2	840	-	3/3/23/25	4/27/125/135	-
19	CLA	A2	841	-	3/3/20/25	6/15/113/135	-
19	CLA	A2	842	-	3/3/25/25	10/37/135/135	-
21	PQN	A2	843	-	-	8/23/43/43	0/2/2/2
19	CLA	A2	844	-	3/3/19/25	3/8/106/135	-
22	LHG	A2	845	-	-	16/53/53/53	-
22	LHG	A2	846	-	-	12/42/42/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	A2	847	-	-	12/27/61/63	0/2/2/2
23	BCR	A2	848	-	-	15/29/63/63	0/2/2/2
23	BCR	A2	849	-	-	13/29/63/63	0/2/2/2
23	BCR	A2	850	-	-	13/29/63/63	0/2/2/2
23	BCR	A2	851	-	-	17/29/63/63	0/2/2/2
19	CLA	A2	852	-	3/3/25/25	13/37/135/135	-
23	BCR	A2	853	-	-	17/29/63/63	0/2/2/2
24	AJP	A2	854	-	-	-	0/6/6/11
19	CLA	AA	801	-	3/3/25/25	13/37/135/135	-
24	AJP	AA	802	-	3/3/14/38	-	0/6/6/11
20	CL0	AA	803	-	4/4/25/25	15/37/135/135	-
19	CLA	AA	804	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	805	-	3/3/24/25	8/31/129/135	-
19	CLA	AA	806	-	3/3/23/25	8/27/125/135	-
19	CLA	AA	807	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	808	-	3/3/25/25	14/37/135/135	-
19	CLA	AA	809	-	3/3/22/25	2/19/117/135	-
19	CLA	AA	810	-	3/3/25/25	10/37/135/135	-
19	CLA	AA	811	1	3/3/22/25	6/21/119/135	-
19	CLA	AA	812	-	3/3/20/25	7/15/113/135	-
19	CLA	AA	813	-	3/3/25/25	9/37/135/135	-
19	CLA	AA	814	-	3/3/19/25	3/10/108/135	-
19	CLA	AA	815	-	3/3/23/25	9/25/123/135	-
19	CLA	AA	816	-	3/3/22/25	9/19/117/135	-
19	CLA	AA	817	-	3/3/19/25	2/11/110/135	-
19	CLA	AA	818	-	3/3/20/25	1/11/111/135	-
19	CLA	AA	819	-	3/3/24/25	13/31/129/135	-
19	CLA	AA	820	-	3/3/23/25	11/29/127/135	-
19	CLA	AA	821	-	3/3/25/25	15/37/135/135	-
19	CLA	AA	822	-	2/2/22/25	8/21/119/135	-
19	CLA	AA	823	-	3/3/24/25	13/31/129/135	-
19	CLA	AA	824	-	3/3/20/25	9/11/111/135	-
19	CLA	AA	825	-	3/3/22/25	2/22/120/135	-
19	CLA	AA	826	-	3/3/20/25	7/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	AA	827	-	3/3/25/25	16/37/135/135	-
19	CLA	AA	828	-	3/3/23/25	11/27/125/135	-
19	CLA	AA	829	-	3/3/25/25	14/37/135/135	-
19	CLA	AA	830	-	3/3/24/25	14/34/132/135	-
19	CLA	AA	831	-	3/3/25/25	13/37/135/135	-
19	CLA	AA	832	-	3/3/25/25	6/37/135/135	-
19	CLA	AA	833	-	3/3/22/25	4/19/117/135	-
19	CLA	AA	834	-	3/3/19/25	4/8/106/135	-
19	CLA	AA	835	-	3/3/25/25	8/37/135/135	-
19	CLA	AA	836	-	3/3/25/25	15/37/135/135	-
19	CLA	AA	837	-	3/3/20/25	0/11/111/135	-
19	CLA	AA	838	-	3/3/19/25	4/11/110/135	-
19	CLA	AA	839	-	3/3/22/25	8/22/120/135	-
19	CLA	AA	840	-	3/3/23/25	7/27/125/135	-
19	CLA	AA	841	-	3/3/20/25	4/15/113/135	-
19	CLA	AA	842	-	3/3/25/25	10/37/135/135	-
19	CLA	AA	843	-	3/3/25/25	15/37/135/135	-
21	PQN	AA	844	-	-	4/23/43/43	0/2/2/2
19	CLA	AA	845	-	3/3/19/25	3/8/106/135	-
22	LHG	AA	846	-	-	20/53/53/53	-
22	LHG	AA	847	-	-	12/42/42/53	-
23	BCR	AA	848	-	-	13/27/61/63	0/2/2/2
23	BCR	AA	849	-	-	19/29/63/63	0/2/2/2
23	BCR	AA	850	-	-	16/29/63/63	0/2/2/2
23	BCR	AA	851	-	-	15/29/63/63	0/2/2/2
23	BCR	AA	852	-	-	19/29/63/63	0/2/2/2
19	CLA	AA	853	-	3/3/25/25	18/37/135/135	-
23	BCR	AA	854	-	-	18/29/63/63	0/2/2/2
23	BCR	AA	855	-	-	18/29/63/63	0/2/2/2
24	AJP	AA	856	-	-	2/4/99/220	0/6/6/11
19	CLA	B	801	-	3/3/25/25	17/37/135/135	-
19	CLA	B	802	-	3/3/25/25	11/37/135/135	-
19	CLA	B	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B	804	-	3/3/24/25	8/34/132/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B	806	-	3/3/25/25	15/37/135/135	-
19	CLA	B	807	-	3/3/25/25	11/37/135/135	-
19	CLA	B	808	-	3/3/24/25	10/31/129/135	-
19	CLA	B	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B	810	-	3/3/25/25	15/37/135/135	-
19	CLA	B	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B	812	-	3/3/19/25	4/8/106/135	-
19	CLA	B	813	-	3/3/19/25	6/10/108/135	-
19	CLA	B	814	-	3/3/23/25	10/30/128/135	-
19	CLA	B	815	-	3/3/25/25	18/37/135/135	-
19	CLA	B	816	-	3/3/23/25	9/28/126/135	-
19	CLA	B	817	-	3/3/19/25	3/10/108/135	-
19	CLA	B	818	-	3/3/19/25	4/8/106/135	-
19	CLA	B	819	-	3/3/19/25	2/8/106/135	-
19	CLA	B	820	-	3/3/20/25	7/11/111/135	-
19	CLA	B	821	2	3/3/25/25	14/37/135/135	-
19	CLA	B	822	-	3/3/25/25	4/37/135/135	-
19	CLA	B	823	-	3/3/25/25	14/37/135/135	-
19	CLA	B	824	-	3/3/23/25	12/25/123/135	-
19	CLA	B	825	-	3/3/25/25	20/37/135/135	-
19	CLA	B	826	-	3/3/25/25	14/37/135/135	-
19	CLA	B	827	-	3/3/20/25	6/11/111/135	-
19	CLA	B	828	-	3/3/20/25	2/11/111/135	-
19	CLA	B	829	-	3/3/25/25	13/37/135/135	-
19	CLA	B	830	-	3/3/23/25	4/27/125/135	-
19	CLA	B	831	-	3/3/23/25	5/27/125/135	-
19	CLA	B	832	-	3/3/20/25	4/11/111/135	-
19	CLA	B	833	-	2/2/25/25	12/37/135/135	-
19	CLA	B	834	-	3/3/24/25	18/37/135/135	-
19	CLA	B	835	-	3/3/20/25	1/11/111/135	-
19	CLA	B	836	-	3/3/25/25	9/37/135/135	-
19	CLA	B	837	-	3/3/24/25	10/31/129/135	-
21	PQN	B	838	-	-	7/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	B	839	-	-	16/29/63/63	0/2/2/2
23	BCR	B	840	-	-	9/29/63/63	0/2/2/2
26	ECH	B	841	-	-	16/29/66/66	0/2/2/2
23	BCR	B	842	-	-	19/29/63/63	0/2/2/2
23	BCR	B	843	-	-	16/29/63/63	0/2/2/2
23	BCR	B	844	-	-	15/29/63/63	0/2/2/2
25	LMG	B	845	-	-	19/50/70/70	0/1/1/1
19	CLA	B	846	-	3/3/17/25	1/5/99/135	-
23	BCR	B	848	-	-	17/29/63/63	0/2/2/2
24	AJP	B	849	-	8/8/19/38	3/6/121/220	0/7/7/11
24	AJP	B	850	-	7/7/19/38	2/6/121/220	0/7/7/11
25	LMG	B	851	-	-	17/50/70/70	0/1/1/1
22	LHG	B	852	-	-	13/37/37/53	-
22	LHG	B	853	-	-	23/53/53/53	-
19	CLA	B	854	-	3/3/25/25	13/37/135/135	-
28	DGD	B	856	-	-	21/31/71/95	0/2/2/2
24	AJP	B	857	-	-	0/6/121/220	0/7/7/11
19	CLA	B	858	-	3/3/25/25	5/37/135/135	-
19	CLA	B	859	-	3/3/24/25	13/31/129/135	-
19	CLA	B	860	-	3/3/25/25	15/37/135/135	-
27	SF4	B	861	-	-	-	0/6/5/5
19	CLA	B1	801	-	3/3/25/25	20/37/135/135	-
19	CLA	B1	802	-	3/3/25/25	14/37/135/135	-
19	CLA	B1	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B1	804	-	3/3/24/25	10/34/132/135	-
19	CLA	B1	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B1	806	-	3/3/25/25	15/37/135/135	-
19	CLA	B1	807	-	3/3/25/25	11/37/135/135	-
19	CLA	B1	808	-	3/3/24/25	11/31/129/135	-
19	CLA	B1	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B1	810	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B1	812	-	3/3/19/25	6/8/106/135	-
19	CLA	B1	813	-	3/3/19/25	6/10/108/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	814	-	3/3/23/25	12/30/128/135	-
19	CLA	B1	815	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	816	-	3/3/23/25	9/28/126/135	-
19	CLA	B1	817	-	3/3/19/25	2/10/108/135	-
19	CLA	B1	818	-	3/3/19/25	2/8/106/135	-
19	CLA	B1	819	-	3/3/19/25	3/8/106/135	-
19	CLA	B1	820	-	3/3/20/25	7/11/111/135	-
19	CLA	B1	821	2	3/3/25/25	14/37/135/135	-
19	CLA	B1	822	-	3/3/25/25	2/37/135/135	-
19	CLA	B1	823	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	824	-	3/3/23/25	13/25/123/135	-
19	CLA	B1	825	-	3/3/25/25	18/37/135/135	-
19	CLA	B1	826	-	3/3/25/25	15/37/135/135	-
19	CLA	B1	827	-	3/3/20/25	6/11/111/135	-
19	CLA	B1	828	-	3/3/25/25	11/37/135/135	-
19	CLA	B1	829	-	3/3/23/25	5/27/125/135	-
19	CLA	B1	830	-	3/3/23/25	8/27/125/135	-
19	CLA	B1	831	-	3/3/20/25	4/11/111/135	-
19	CLA	B1	832	-	3/3/25/25	12/37/135/135	-
19	CLA	B1	833	-	3/3/24/25	18/37/135/135	-
19	CLA	B1	834	-	3/3/20/25	1/11/111/135	-
19	CLA	B1	835	-	3/3/25/25	10/37/135/135	-
19	CLA	B1	836	-	3/3/24/25	10/31/129/135	-
21	PQN	B1	837	-	-	7/23/43/43	0/2/2/2
23	BCR	B1	838	-	-	19/29/63/63	0/2/2/2
23	BCR	B1	839	-	-	9/29/63/63	0/2/2/2
26	ECH	B1	840	-	-	16/29/66/66	0/2/2/2
23	BCR	B1	841	-	-	19/29/63/63	0/2/2/2
23	BCR	B1	842	-	-	16/29/63/63	0/2/2/2
23	BCR	B1	843	-	-	13/29/63/63	0/2/2/2
25	LMG	B1	844	-	-	20/50/70/70	0/1/1/1
19	CLA	B1	845	-	3/3/17/25	0/5/99/135	-
25	LMG	B1	846	-	-	10/27/47/70	0/1/1/1
22	LHG	B1	847	-	-	14/37/37/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B1	848	-	3/3/25/25	16/37/135/135	-
19	CLA	B1	849	-	3/3/25/25	4/37/135/135	-
19	CLA	B1	850	-	3/3/24/25	10/31/129/135	-
27	SF4	B1	851	-	-	-	0/6/5/5
25	LMG	B1	852	-	-	5/25/45/70	0/1/1/1
19	CLA	B2	801	-	3/3/25/25	18/37/135/135	-
19	CLA	B2	802	-	3/3/25/25	9/37/135/135	-
19	CLA	B2	803	-	3/3/25/25	13/37/135/135	-
19	CLA	B2	804	-	3/3/24/25	9/34/132/135	-
19	CLA	B2	805	-	3/3/24/25	9/36/134/135	-
19	CLA	B2	806	2	3/3/25/25	15/37/135/135	-
19	CLA	B2	807	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	808	-	3/3/24/25	11/31/129/135	-
19	CLA	B2	809	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	810	-	3/3/25/25	16/37/135/135	-
19	CLA	B2	811	-	3/3/24/25	15/33/131/135	-
19	CLA	B2	812	-	3/3/19/25	4/8/106/135	-
19	CLA	B2	813	-	3/3/19/25	6/10/108/135	-
19	CLA	B2	814	-	3/3/23/25	12/30/128/135	-
19	CLA	B2	815	-	3/3/25/25	15/37/135/135	-
19	CLA	B2	816	-	3/3/23/25	8/28/126/135	-
19	CLA	B2	817	-	3/3/19/25	2/10/108/135	-
19	CLA	B2	818	-	3/3/19/25	2/8/106/135	-
19	CLA	B2	819	-	3/3/19/25	3/8/106/135	-
19	CLA	B2	820	-	3/3/20/25	8/11/111/135	-
19	CLA	B2	821	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	822	-	3/3/25/25	7/37/135/135	-
19	CLA	B2	823	-	3/3/25/25	17/37/135/135	-
19	CLA	B2	824	-	3/3/23/25	13/25/123/135	-
19	CLA	B2	825	-	3/3/25/25	20/37/135/135	-
19	CLA	B2	826	-	3/3/25/25	16/37/135/135	-
19	CLA	B2	827	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	828	-	3/3/20/25	1/11/111/135	-
19	CLA	B2	829	-	3/3/25/25	13/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	B2	830	-	3/3/23/25	4/27/125/135	-
19	CLA	B2	831	-	3/3/23/25	9/27/125/135	-
19	CLA	B2	832	-	3/3/20/25	4/11/111/135	-
19	CLA	B2	833	-	2/2/25/25	11/37/135/135	-
19	CLA	B2	834	-	3/3/24/25	20/37/135/135	-
19	CLA	B2	835	-	3/3/20/25	2/11/111/135	-
19	CLA	B2	836	-	3/3/25/25	11/37/135/135	-
19	CLA	B2	837	-	3/3/24/25	10/31/129/135	-
21	PQN	B2	838	-	-	7/23/43/43	0/2/2/2
23	BCR	B2	839	-	-	19/29/63/63	0/2/2/2
23	BCR	B2	840	-	-	8/29/63/63	0/2/2/2
26	ECH	B2	841	-	-	16/29/66/66	0/2/2/2
23	BCR	B2	842	-	-	21/29/63/63	0/2/2/2
23	BCR	B2	843	-	-	18/29/63/63	0/2/2/2
23	BCR	B2	844	-	-	13/29/63/63	0/2/2/2
25	LMG	B2	845	-	-	21/50/70/70	0/1/1/1
19	CLA	B2	846	-	3/3/17/25	0/5/99/135	-
25	LMG	B2	847	-	-	9/27/47/70	0/1/1/1
22	LHG	B2	848	-	-	9/37/37/53	-
19	CLA	B2	849	-	3/3/25/25	14/37/135/135	-
19	CLA	B2	850	-	3/3/25/25	4/37/135/135	-
19	CLA	B2	851	-	3/3/24/25	11/31/129/135	-
19	CLA	B2	852	-	3/3/25/25	15/37/135/135	-
27	SF4	B2	853	-	-	-	0/6/5/5
25	LMG	B2	854	-	-	5/25/45/70	0/1/1/1
19	CLA	BB	801	-	3/3/25/25	20/37/135/135	-
19	CLA	BB	802	-	3/3/25/25	16/37/135/135	-
19	CLA	BB	803	-	3/3/25/25	14/37/135/135	-
19	CLA	BB	804	-	3/3/24/25	9/34/132/135	-
19	CLA	BB	805	-	3/3/24/25	9/36/134/135	-
19	CLA	BB	806	-	3/3/25/25	15/37/135/135	-
19	CLA	BB	807	-	3/3/25/25	11/37/135/135	-
19	CLA	BB	808	-	3/3/24/25	13/31/129/135	-
19	CLA	BB	809	-	3/3/20/25	4/11/111/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	BB	810	-	3/3/25/25	16/37/135/135	-
19	CLA	BB	811	-	3/3/24/25	17/33/131/135	-
19	CLA	BB	812	-	3/3/19/25	6/8/106/135	-
19	CLA	BB	813	-	3/3/19/25	6/10/108/135	-
19	CLA	BB	814	-	3/3/23/25	11/30/128/135	-
19	CLA	BB	815	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	816	-	3/3/23/25	8/28/126/135	-
19	CLA	BB	817	-	3/3/19/25	1/10/108/135	-
19	CLA	BB	818	-	3/3/19/25	2/8/106/135	-
19	CLA	BB	819	-	3/3/19/25	2/8/106/135	-
19	CLA	BB	820	-	3/3/20/25	8/11/111/135	-
19	CLA	BB	821	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	822	-	3/3/25/25	8/37/135/135	-
19	CLA	BB	823	-	3/3/25/25	14/37/135/135	-
19	CLA	BB	824	-	3/3/23/25	12/25/123/135	-
19	CLA	BB	825	-	3/3/25/25	20/37/135/135	-
19	CLA	BB	826	-	3/3/25/25	17/37/135/135	-
19	CLA	BB	827	-	3/3/20/25	2/11/111/135	-
19	CLA	BB	828	-	3/3/20/25	1/11/111/135	-
19	CLA	BB	829	-	3/3/23/25	6/27/125/135	-
19	CLA	BB	830	-	3/3/23/25	8/27/125/135	-
19	CLA	BB	831	-	3/3/20/25	4/11/111/135	-
19	CLA	BB	832	-	2/2/25/25	12/37/135/135	-
19	CLA	BB	833	-	3/3/24/25	16/37/135/135	-
19	CLA	BB	834	-	3/3/20/25	1/11/111/135	-
19	CLA	BB	835	-	3/3/25/25	9/37/135/135	-
19	CLA	BB	836	-	3/3/24/25	10/31/129/135	-
21	PQN	BB	837	-	-	7/23/43/43	0/2/2/2
23	BCR	BB	838	-	-	15/29/63/63	0/2/2/2
23	BCR	BB	839	-	-	9/29/63/63	0/2/2/2
26	ECH	BB	840	-	-	15/29/66/66	0/2/2/2
23	BCR	BB	841	-	-	20/29/63/63	0/2/2/2
23	BCR	BB	842	-	-	16/29/63/63	0/2/2/2
23	BCR	BB	843	-	-	13/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	BB	844	-	-	18/50/70/70	0/1/1/1
19	CLA	BB	845	-	3/3/17/25	1/5/99/135	-
23	BCR	BB	847	-	-	17/29/63/63	0/2/2/2
24	AJP	BB	848	-	7/7/19/38	3/6/121/220	0/7/7/11
24	AJP	BB	849	-	7/7/19/38	3/6/121/220	0/7/7/11
22	LHG	BB	850	-	-	14/37/37/53	-
22	LHG	BB	851	-	-	20/53/53/53	-
19	CLA	BB	852	-	3/3/25/25	13/37/135/135	-
28	DGD	BB	854	-	-	21/31/71/95	0/2/2/2
19	CLA	BB	855	-	3/3/25/25	6/37/135/135	-
19	CLA	BB	856	-	3/3/24/25	13/31/129/135	-
27	SF4	BB	857	-	-	-	0/6/5/5
27	SF4	C	101	-	-	-	0/6/5/5
27	SF4	C	102	3	-	-	0/6/5/5
27	SF4	C1	101	-	-	-	0/6/5/5
27	SF4	C1	102	-	-	-	0/6/5/5
27	SF4	C2	101	-	-	-	0/6/5/5
27	SF4	C2	102	-	-	-	0/6/5/5
27	SF4	CC	101	-	-	-	0/6/5/5
27	SF4	CC	102	-	-	-	0/6/5/5
19	CLA	F	301	-	3/3/24/25	12/31/129/135	-
19	CLA	F	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F	303	-	-	18/29/63/63	0/2/2/2
23	BCR	F	304	-	-	15/29/63/63	0/2/2/2
23	BCR	F	305	-	-	23/29/63/63	0/2/2/2
19	CLA	F1	301	-	3/3/24/25	11/31/129/135	-
19	CLA	F1	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F1	303	-	-	17/29/63/63	0/2/2/2
23	BCR	F1	304	-	-	15/29/63/63	0/2/2/2
19	CLA	F1	305	-	3/3/20/25	2/11/111/135	-
23	BCR	F1	306	-	-	25/29/63/63	0/2/2/2
19	CLA	F2	301	-	3/3/24/25	11/31/129/135	-
19	CLA	F2	302	-	3/3/19/25	4/10/108/135	-
23	BCR	F2	303	-	-	20/29/63/63	0/2/2/2
23	BCR	F2	304	-	-	15/29/63/63	0/2/2/2
23	BCR	F2	305	-	-	26/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CLA	FF	301	-	3/3/24/25	13/31/129/135	-
19	CLA	FF	302	-	3/3/19/25	4/10/108/135	-
23	BCR	FF	303	-	-	19/29/63/63	0/2/2/2
23	BCR	FF	304	-	-	14/29/63/63	0/2/2/2
19	CLA	FF	305	-	3/3/25/25	11/37/135/135	-
23	BCR	FF	306	-	-	22/29/63/63	0/2/2/2
23	BCR	I	101	-	-	20/29/63/63	0/2/2/2
23	BCR	I	102	-	-	10/29/63/63	0/2/2/2
23	BCR	I1	101	-	-	18/29/63/63	0/2/2/2
25	LMG	I1	102	-	-	18/30/50/70	0/1/1/1
23	BCR	I2	101	-	-	17/29/63/63	0/2/2/2
23	BCR	I2	102	-	-	11/29/63/63	0/2/2/2
23	BCR	I2	103	-	-	18/29/63/63	0/2/2/2
24	AJP	I2	104	-	3/3/14/38	-	0/6/6/11
25	LMG	I2	105	-	-	10/29/49/70	0/1/1/1
23	BCR	II	101	-	-	17/29/63/63	0/2/2/2
23	BCR	II	102	-	-	9/29/63/63	0/2/2/2
23	BCR	II	104	-	-	18/29/63/63	0/2/2/2
25	LMG	II	105	-	-	20/37/57/70	0/1/1/1
19	CLA	J	101	8	3/3/19/25	3/8/106/135	-
23	BCR	J	102	-	-	19/29/63/63	0/2/2/2
19	CLA	J	103	-	2/2/19/25	6/8/106/135	-
23	BCR	J	104	-	-	16/29/63/63	0/2/2/2
19	CLA	J1	101	-	3/3/18/25	3/8/106/135	-
23	BCR	J1	102	-	-	19/29/63/63	0/2/2/2
19	CLA	J1	103	-	3/3/19/25	0/8/106/135	-
23	BCR	J1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	J2	101	8	3/3/19/25	3/8/106/135	-
23	BCR	J2	102	-	-	18/29/63/63	0/2/2/2
19	CLA	J2	103	-	3/3/19/25	0/8/106/135	-
23	BCR	J2	104	-	-	16/29/63/63	0/2/2/2
19	CLA	JJ	101	8	3/3/19/25	3/8/106/135	-
23	BCR	JJ	102	-	-	20/29/63/63	0/2/2/2
19	CLA	JJ	103	-	3/3/19/25	0/8/106/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	JJ	104	-	-	16/29/63/63	0/2/2/2
19	CLA	K	101	-	3/3/20/25	1/11/111/135	-
19	CLA	K	102	-	3/3/20/25	11/15/113/135	-
23	BCR	K	103	-	-	19/29/63/63	0/2/2/2
24	AJP	K	104	-	6/6/19/38	2/4/116/220	0/7/7/11
19	CLA	K1	102	-	3/3/20/25	2/11/111/135	-
19	CLA	K1	103	-	3/3/20/25	8/15/113/135	-
23	BCR	K1	104	-	-	18/29/63/63	0/2/2/2
19	CLA	K1	105	9	3/3/18/25	6/8/102/135	-
23	BCR	K1	106	-	-	17/29/63/63	0/2/2/2
19	CLA	K2	102	-	3/3/20/25	1/11/111/135	-
23	BCR	K2	103	-	-	12/29/63/63	0/2/2/2
19	CLA	K2	104	-	3/3/18/25	2/5/101/135	-
23	BCR	K2	105	-	-	16/29/63/63	0/2/2/2
19	CLA	KK	101	-	3/3/20/25	1/11/111/135	-
19	CLA	KK	102	-	3/3/20/25	10/15/113/135	-
23	BCR	KK	103	-	-	19/29/63/63	0/2/2/2
24	AJP	KK	104	-	6/6/19/38	2/4/116/220	0/7/7/11
19	CLA	L	202	18	3/3/24/25	14/33/131/135	-
19	CLA	L	203	-	3/3/25/25	7/37/135/135	-
19	CLA	L	204	-	3/3/25/25	16/37/135/135	-
23	BCR	L	205	-	-	17/29/63/63	0/2/2/2
23	BCR	L	206	-	-	18/29/63/63	0/2/2/2
22	LHG	L	207	-	-	13/38/38/53	-
24	AJP	L	208	-	4/4/14/38	-	0/6/6/11
24	AJP	L	209	-	4/4/14/38	-	0/6/6/11
23	BCR	L1	201	-	-	12/29/63/63	0/2/2/2
24	AJP	L1	203	-	5/5/19/38	4/6/121/220	0/7/7/11
24	AJP	L1	204	-	5/5/19/38	3/6/121/220	0/7/7/11
19	CLA	L1	205	10	3/3/24/25	11/33/131/135	-
19	CLA	L1	206	-	3/3/25/25	3/37/135/135	-
19	CLA	L1	207	-	3/3/25/25	12/37/135/135	-
23	BCR	L1	208	-	-	17/29/63/63	0/2/2/2
23	BCR	L1	209	-	-	18/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	LMG	L1	210	-	-	16/50/70/70	0/1/1/1
22	LHG	L1	211	-	-	13/37/37/53	-
24	AJP	L2	202	-	7/7/19/38	3/6/121/220	0/7/7/11
24	AJP	L2	203	-	6/6/19/38	4/6/121/220	0/7/7/11
19	CLA	L2	204	16	3/3/24/25	15/33/131/135	-
19	CLA	L2	205	-	3/3/23/25	6/30/128/135	-
19	CLA	L2	206	-	3/3/25/25	14/37/135/135	-
23	BCR	L2	207	-	-	19/29/63/63	0/2/2/2
22	LHG	L2	208	-	-	17/39/39/53	-
19	CLA	LL	201	18	3/3/24/25	13/33/131/135	-
19	CLA	LL	202	-	3/3/25/25	6/37/135/135	-
19	CLA	LL	203	-	3/3/19/25	8/10/108/135	-
23	BCR	LL	204	-	-	18/29/63/63	0/2/2/2
22	LHG	LL	205	-	-	13/38/38/53	-
23	BCR	M	101	-	-	22/29/63/63	0/2/2/2
25	LMG	M	102	-	-	15/41/61/70	0/1/1/1
23	BCR	M1	101	-	-	17/29/63/63	0/2/2/2
24	AJP	M2	101	-	3/3/14/38	-	0/6/6/11
23	BCR	M2	102	-	-	18/29/63/63	0/2/2/2
23	BCR	MM	101	-	-	23/29/63/63	0/2/2/2
19	CLA	X	101	-	3/3/20/25	1/11/111/135	-
22	LHG	X	102	-	-	18/44/44/53	-
19	CLA	X1	101	-	3/3/20/25	2/11/111/135	-
22	LHG	X1	102	-	-	17/44/44/53	-
22	LHG	X1	103	-	-	19/53/53/53	-
19	CLA	X2	101	-	3/3/20/25	3/11/111/135	-
22	LHG	X2	102	-	-	15/44/44/53	-
22	LHG	X2	103	-	-	22/53/53/53	-
19	CLA	XX	101	-	3/3/20/25	5/11/111/135	-
22	LHG	XX	102	-	-	18/44/44/53	-

All (2620) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	802	AJP	CBL-CCH	-10.99	1.35	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	802	AJP	CBL-CCH	-10.93	1.35	1.53
24	L	208	AJP	CBL-CCH	-10.78	1.35	1.53
24	BB	849	AJP	CBL-CCH	-10.74	1.35	1.53
24	AA	856	AJP	CCI-CCJ	-10.73	1.39	1.54
24	L2	202	AJP	CCI-CCJ	-10.72	1.39	1.54
24	A	855	AJP	CCI-CCJ	-10.71	1.39	1.54
24	L1	203	AJP	CCI-CCJ	-10.69	1.39	1.54
24	BB	848	AJP	CCI-CCJ	-10.64	1.39	1.54
24	AA	802	AJP	CCI-CCJ	-10.59	1.39	1.54
24	L1	204	AJP	CCI-CCJ	-10.58	1.39	1.54
24	A	802	AJP	CCI-CCJ	-10.57	1.39	1.54
24	B	849	AJP	CCI-CCJ	-10.53	1.40	1.54
24	A1	854	AJP	CCI-CCJ	-10.50	1.40	1.54
24	L2	202	AJP	CBL-CCH	-10.49	1.36	1.53
24	B	850	AJP	CCI-CCJ	-10.44	1.40	1.54
24	K	104	AJP	CCI-CCJ	-10.42	1.40	1.54
24	B	850	AJP	CBL-CCH	-10.39	1.36	1.53
24	M2	101	AJP	CBL-CCH	-10.34	1.36	1.53
24	L1	203	AJP	CBL-CCH	-10.34	1.36	1.53
24	M2	101	AJP	CCI-CCJ	-10.34	1.40	1.54
24	B	857	AJP	CCI-CCJ	-10.33	1.40	1.54
24	L2	203	AJP	CBL-CCH	-10.33	1.36	1.53
24	L	209	AJP	CCI-CCJ	-10.33	1.40	1.54
24	L	209	AJP	CBL-CCH	-10.31	1.36	1.53
24	I2	104	AJP	CCI-CCJ	-10.29	1.40	1.54
24	L2	203	AJP	CCI-CCJ	-10.29	1.40	1.54
24	L1	204	AJP	CBL-CCH	-10.28	1.36	1.53
24	B	849	AJP	CBL-CCH	-10.22	1.36	1.53
24	KK	104	AJP	CBL-CCH	-10.21	1.36	1.53
24	BB	849	AJP	CCI-CCJ	-10.19	1.40	1.54
24	K	104	AJP	CBL-CCH	-10.15	1.36	1.53
24	BB	848	AJP	CBL-CCH	-10.14	1.36	1.53
24	B	857	AJP	CBL-CCH	-10.09	1.36	1.53
24	KK	104	AJP	CCI-CCJ	-10.08	1.40	1.54
24	A1	855	AJP	CCI-CCJ	-10.08	1.40	1.54
24	A2	854	AJP	CCI-CCJ	-10.06	1.40	1.54
24	A1	854	AJP	CBL-CCH	-10.00	1.36	1.53
24	A1	855	AJP	CBL-CCH	-9.99	1.36	1.53
24	A2	854	AJP	CBL-CCH	-9.98	1.36	1.53
24	I2	104	AJP	CBL-CCH	-9.96	1.36	1.53
24	A	855	AJP	CBL-CCH	-9.65	1.37	1.53
24	AA	856	AJP	CBL-CCH	-9.65	1.37	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L	208	AJP	CCI-CCJ	-9.46	1.41	1.54
24	BB	848	AJP	CDC-CDD	-9.20	1.29	1.52
24	B	849	AJP	CDC-CDD	-9.12	1.29	1.52
24	L1	203	AJP	CDC-CDD	-9.10	1.29	1.52
24	L2	202	AJP	CDC-CDD	-9.10	1.29	1.52
24	BB	849	AJP	CBM-CBN	-8.97	1.37	1.54
24	AA	856	AJP	CBM-CBN	-8.95	1.37	1.54
24	B	857	AJP	CBM-CBN	-8.95	1.37	1.54
24	A1	854	AJP	CBM-CBN	-8.95	1.37	1.54
24	A	855	AJP	CBM-CBN	-8.94	1.37	1.54
24	L	209	AJP	CBM-CBN	-8.90	1.37	1.54
24	L	208	AJP	CBM-CBN	-8.88	1.38	1.54
24	I2	104	AJP	CDC-CDD	-8.88	1.30	1.52
24	L1	204	AJP	CDC-CDD	-8.87	1.30	1.52
24	A1	855	AJP	CDC-CDD	-8.87	1.30	1.52
24	A2	854	AJP	CDC-CDD	-8.86	1.30	1.52
24	AA	802	AJP	CDC-CDD	-8.85	1.30	1.52
24	L	208	AJP	CDC-CDD	-8.85	1.30	1.52
24	KK	104	AJP	CDC-CDD	-8.85	1.30	1.52
24	A	802	AJP	CDC-CDD	-8.84	1.30	1.52
24	K	104	AJP	CDC-CDD	-8.83	1.30	1.52
24	BB	849	AJP	CDC-CDD	-8.79	1.30	1.52
24	M2	101	AJP	CBM-CBN	-8.79	1.38	1.54
24	B	850	AJP	CDC-CDD	-8.77	1.30	1.52
24	A1	855	AJP	CBM-CBN	-8.74	1.38	1.54
24	L2	202	AJP	CBM-CBN	-8.73	1.38	1.54
24	L1	203	AJP	CBM-CBN	-8.72	1.38	1.54
24	B	850	AJP	CBM-CBN	-8.71	1.38	1.54
24	L2	203	AJP	CDC-CDD	-8.71	1.30	1.52
24	A1	854	AJP	CDC-CDD	-8.70	1.30	1.52
24	K	104	AJP	CBM-CBN	-8.70	1.38	1.54
24	A	855	AJP	CDC-CDD	-8.69	1.30	1.52
24	AA	856	AJP	CDC-CDD	-8.69	1.30	1.52
24	L2	203	AJP	CBM-CBN	-8.68	1.38	1.54
24	B	857	AJP	CDC-CDD	-8.67	1.31	1.52
24	A2	854	AJP	CBM-CBN	-8.65	1.38	1.54
24	M2	101	AJP	CDC-CDD	-8.65	1.31	1.52
24	L	209	AJP	CDC-CDD	-8.65	1.31	1.52
24	L1	204	AJP	CBM-CBN	-8.58	1.38	1.54
24	KK	104	AJP	CBM-CBN	-8.57	1.38	1.54
24	B	849	AJP	CBM-CBN	-8.57	1.38	1.54
24	A	802	AJP	CBM-CBN	-8.48	1.38	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	AA	802	AJP	CBM-CBN	-8.48	1.38	1.54
24	I2	104	AJP	CBM-CBN	-8.31	1.39	1.54
24	BB	848	AJP	CBM-CBN	-8.23	1.39	1.54
24	L2	203	AJP	OBQ-CBF	7.80	1.59	1.42
24	BB	849	AJP	OBQ-CBF	7.80	1.59	1.42
24	A1	855	AJP	OBQ-CBF	7.79	1.59	1.42
24	A	802	AJP	OBQ-CBF	7.77	1.59	1.42
24	KK	104	AJP	OBQ-CBF	7.77	1.59	1.42
24	A2	854	AJP	OBQ-CBF	7.76	1.59	1.42
24	AA	802	AJP	OBQ-CBF	7.76	1.59	1.42
24	L	208	AJP	OBQ-CBF	7.71	1.59	1.42
24	B	850	AJP	OBQ-CBF	7.68	1.59	1.42
24	B	849	AJP	OBQ-CBF	7.68	1.59	1.42
24	K	104	AJP	OBQ-CBF	7.67	1.59	1.42
24	A	855	AJP	OBQ-CBF	7.67	1.59	1.42
24	AA	856	AJP	OBQ-CBF	7.67	1.59	1.42
24	L	209	AJP	OBQ-CBF	7.66	1.59	1.42
24	M2	101	AJP	OBQ-CBF	7.66	1.59	1.42
24	A1	854	AJP	OBQ-CBF	7.65	1.59	1.42
24	B	857	AJP	OBQ-CBF	7.65	1.59	1.42
24	L2	202	AJP	OBQ-CBF	7.62	1.59	1.42
24	I2	104	AJP	OBQ-CBF	7.59	1.59	1.42
24	L1	204	AJP	OBQ-CBF	7.56	1.59	1.42
24	BB	848	AJP	OBQ-CBF	7.55	1.59	1.42
24	L1	203	AJP	OBQ-CBF	7.39	1.59	1.42
24	L	209	AJP	CBM-CBL	-6.94	1.38	1.53
24	L	208	AJP	CBM-CBL	-6.94	1.38	1.53
24	B	857	AJP	CBM-CBL	-6.78	1.38	1.53
24	A	802	AJP	CBM-CBL	-6.74	1.38	1.53
24	AA	802	AJP	CBM-CBL	-6.71	1.38	1.53
24	AA	856	AJP	CBM-CBL	-6.71	1.39	1.53
24	A	855	AJP	CBM-CBL	-6.70	1.39	1.53
24	M2	101	AJP	CBM-CBL	-6.70	1.39	1.53
24	A1	854	AJP	CBM-CBL	-6.68	1.39	1.53
24	A2	854	AJP	CBM-CBL	-6.60	1.39	1.53
24	KK	104	AJP	CBM-CBL	-6.54	1.39	1.53
24	A1	855	AJP	CBM-CBL	-6.52	1.39	1.53
24	L2	202	AJP	CBM-CBL	-6.43	1.39	1.53
24	BB	849	AJP	CBM-CBL	-6.43	1.39	1.53
24	B	849	AJP	CBM-CBL	-6.43	1.39	1.53
24	L1	203	AJP	CBM-CBL	-6.41	1.39	1.53
24	K	104	AJP	CBM-CBL	-6.39	1.39	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	BB	848	AJP	CBM-CBL	-6.38	1.39	1.53
24	B	850	AJP	CBM-CBL	-6.29	1.39	1.53
24	L2	203	AJP	CBM-CBL	-6.14	1.40	1.53
24	L1	204	AJP	CBM-CBL	-5.96	1.40	1.53
24	I2	104	AJP	CBM-CBL	-5.87	1.40	1.53
24	I2	104	AJP	CBK-CCG	5.80	1.64	1.54
24	I2	104	AJP	CCF-CCE	5.77	1.60	1.52
24	I2	104	AJP	CBN-CBO	5.71	1.68	1.56
24	L	208	AJP	CCF-CCE	5.70	1.60	1.52
24	L1	203	AJP	CCF-CCE	5.69	1.61	1.53
24	B	850	AJP	CBK-CCG	5.65	1.64	1.54
24	M2	101	AJP	CCF-CCE	5.64	1.60	1.52
24	A1	854	AJP	CCF-CCE	5.61	1.61	1.53
24	BB	848	AJP	CCF-CCE	5.61	1.61	1.53
24	L1	204	AJP	CBK-CCG	5.57	1.64	1.54
24	B	850	AJP	CBN-CBO	5.57	1.67	1.56
24	L	209	AJP	CCF-CCE	5.52	1.60	1.52
24	L2	203	AJP	CBK-CCG	5.51	1.64	1.54
24	L2	202	AJP	CCF-CCE	5.51	1.61	1.53
24	B	849	AJP	CCF-CCE	5.49	1.61	1.53
24	B	857	AJP	CCF-CCE	5.48	1.61	1.53
24	B	849	AJP	CBN-CBO	5.48	1.67	1.56
24	BB	849	AJP	CBK-CCG	5.43	1.64	1.54
24	K	104	AJP	CBN-CBO	5.42	1.67	1.56
24	M2	101	AJP	CBN-CBO	5.42	1.67	1.56
24	BB	848	AJP	CBN-CBO	5.42	1.67	1.56
24	K	104	AJP	CBK-CCG	5.40	1.64	1.54
24	KK	104	AJP	CBK-CCG	5.39	1.63	1.54
24	L2	202	AJP	CBN-CBO	5.35	1.67	1.56
24	KK	104	AJP	CBN-CBO	5.34	1.67	1.56
24	L	209	AJP	CBN-CBO	5.32	1.67	1.56
24	L	208	AJP	CBN-CBO	5.25	1.67	1.56
24	AA	856	AJP	CCF-CCE	5.24	1.61	1.53
24	A	855	AJP	CCF-CCE	5.23	1.61	1.53
24	BB	848	AJP	CBK-CCG	5.23	1.63	1.54
24	AA	802	AJP	CBN-CBO	5.22	1.67	1.56
24	B	849	AJP	CBK-CCG	5.20	1.63	1.54
24	A	802	AJP	CBN-CBO	5.20	1.66	1.56
24	M2	101	AJP	CBK-CCG	5.19	1.63	1.54
24	L1	204	AJP	CCF-CCE	5.18	1.61	1.53
24	BB	849	AJP	CCF-CCE	5.11	1.61	1.53
24	BB	849	AJP	CBN-CBO	5.08	1.66	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	L1	204	AJP	CBN-CBO	5.06	1.66	1.56
24	L	209	AJP	CBK-CCG	5.04	1.63	1.54
24	L2	202	AJP	CBK-CCG	5.04	1.63	1.54
24	L1	203	AJP	CBK-CCG	5.03	1.63	1.54
24	L2	203	AJP	CCF-CCE	5.02	1.60	1.53
20	A	803	CL0	O2D-CGD	4.96	1.45	1.33
24	B	850	AJP	CCF-CCE	4.96	1.60	1.53
24	L1	203	AJP	CBN-CBO	4.93	1.66	1.56
24	L	208	AJP	CBK-CCG	4.93	1.63	1.54
24	A	855	AJP	CBN-CBO	4.86	1.66	1.56
24	AA	856	AJP	CBN-CBO	4.86	1.66	1.56
24	A2	854	AJP	CBN-CBO	4.85	1.66	1.56
24	A1	855	AJP	CBN-CBO	4.82	1.66	1.56
24	B	857	AJP	CBN-CBO	4.82	1.66	1.56
24	A1	854	AJP	CBN-CBO	4.82	1.66	1.56
24	A1	855	AJP	CCF-CCE	4.79	1.60	1.53
24	L2	203	AJP	CBN-CBO	4.78	1.66	1.56
20	A1	802	CL0	C3B-C2B	4.77	1.47	1.40
20	AA	803	CL0	C3B-C2B	4.77	1.47	1.40
24	AA	802	AJP	CBK-CCG	4.71	1.62	1.54
24	A	802	AJP	CBK-CCG	4.70	1.62	1.54
24	A2	854	AJP	CCF-CCE	4.69	1.60	1.53
20	A1	802	CL0	O2D-CGD	4.69	1.44	1.33
20	A1	802	CL0	CHC-C1C	4.67	1.47	1.35
20	AA	803	CL0	O2D-CGD	4.67	1.44	1.33
24	L1	203	AJP	OCL-CCK	-4.62	1.32	1.43
20	AA	803	CL0	CHC-C1C	4.61	1.47	1.35
20	A	803	CL0	CHC-C1C	4.60	1.47	1.35
20	A1	802	CL0	C3C-C2C	4.60	1.46	1.36
20	A	803	CL0	OBD-CAD	4.55	1.28	1.22
24	AA	856	AJP	CCI-CCH	4.55	1.62	1.53
24	A	855	AJP	CCI-CCH	4.55	1.62	1.53
20	A	803	CL0	C3B-C2B	4.54	1.46	1.40
20	AA	803	CL0	OBD-CAD	4.53	1.28	1.22
24	M2	101	AJP	CCG-CCH	-4.51	1.47	1.56
24	A2	854	AJP	CBK-CCG	4.50	1.62	1.54
24	A1	855	AJP	CCI-CCH	4.50	1.62	1.53
24	A2	854	AJP	CCI-CCH	4.50	1.62	1.53
20	A2	803	CL0	OBD-CAD	4.49	1.28	1.22
24	A1	855	AJP	CBK-CCG	4.49	1.62	1.54
24	A1	854	AJP	CBK-CCG	4.49	1.62	1.54
20	A1	802	CL0	OBD-CAD	4.49	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A2	803	CL0	O2D-CGD	4.49	1.44	1.33
20	A2	803	CL0	CHC-C1C	4.48	1.47	1.35
24	AA	856	AJP	CBK-CCG	4.47	1.62	1.54
24	KK	104	AJP	CCF-CCE	4.47	1.60	1.53
24	A1	854	AJP	CCI-CCH	4.47	1.62	1.53
24	A	855	AJP	CBK-CCG	4.47	1.62	1.54
24	B	857	AJP	CBK-CCG	4.46	1.62	1.54
24	K	104	AJP	CCF-CCE	4.45	1.60	1.53
24	A1	854	AJP	CBN-CCJ	-4.42	1.46	1.56
20	AA	803	CL0	C3C-C2C	4.41	1.46	1.36
24	B	857	AJP	CBN-CCJ	-4.40	1.47	1.56
24	B	857	AJP	CCI-CCH	4.40	1.62	1.53
24	L	209	AJP	CCG-CCH	-4.38	1.47	1.56
24	B	857	AJP	OCL-CCK	-4.36	1.32	1.43
20	A	803	CL0	C3C-C2C	4.36	1.45	1.36
24	A1	855	AJP	OCL-CCK	-4.35	1.32	1.43
24	A2	854	AJP	CBN-CCJ	-4.35	1.47	1.56
24	A1	855	AJP	CBN-CCJ	-4.35	1.47	1.56
24	A2	854	AJP	OCL-CCK	-4.35	1.32	1.43
24	A1	854	AJP	OCL-CCK	-4.34	1.32	1.43
24	A	855	AJP	CBN-CCJ	-4.34	1.47	1.56
24	AA	856	AJP	CBN-CCJ	-4.33	1.47	1.56
24	A	855	AJP	OCL-CCK	-4.31	1.32	1.43
24	AA	856	AJP	OCL-CCK	-4.31	1.32	1.43
24	L1	203	AJP	CBN-CCJ	-4.31	1.47	1.56
24	BB	849	AJP	CCJ-CCK	4.30	1.61	1.53
24	BB	849	AJP	CCG-CCH	-4.29	1.48	1.56
24	L2	203	AJP	CCG-CCH	-4.28	1.48	1.56
20	A2	803	CL0	C3B-C2B	4.28	1.46	1.40
24	L	208	AJP	CCJ-CCK	4.28	1.61	1.53
20	A2	803	CL0	C3C-C2C	4.22	1.45	1.36
24	B	850	AJP	CCG-CCH	-4.17	1.48	1.56
23	AA	855	BCR	C1-C6	-4.14	1.48	1.53
23	A	854	BCR	C1-C6	-4.12	1.48	1.53
24	L	209	AJP	CCJ-CCK	4.12	1.61	1.53
24	BB	848	AJP	OCL-CCK	-4.10	1.33	1.43
23	BB	839	BCR	C1-C6	-4.10	1.48	1.53
23	K2	105	BCR	C1-C6	-4.09	1.48	1.53
24	A	802	AJP	CCJ-CCK	4.09	1.61	1.53
24	L2	203	AJP	CBN-CCJ	-4.08	1.47	1.56
24	AA	802	AJP	CCJ-CCK	4.08	1.61	1.53
24	L1	204	AJP	CBN-CCJ	-4.08	1.47	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	K1	106	BCR	C1-C6	-4.07	1.48	1.53
20	A1	802	CL0	O2A-CGA	4.06	1.45	1.33
23	B	844	BCR	C30-C25	-4.04	1.48	1.53
23	B1	839	BCR	C1-C6	-4.04	1.48	1.53
24	KK	104	AJP	CCJ-CCK	4.03	1.61	1.53
23	B	840	BCR	C1-C6	-4.03	1.48	1.53
24	L1	204	AJP	CCG-CCH	-4.03	1.48	1.56
23	JJ	104	BCR	C1-C6	-4.02	1.48	1.53
24	A2	854	AJP	CCJ-CCK	4.02	1.61	1.53
23	B2	840	BCR	C1-C6	-4.01	1.48	1.53
24	A1	854	AJP	CCJ-CCK	3.99	1.61	1.53
24	B	857	AJP	CCJ-CCK	3.98	1.61	1.53
20	A1	802	CL0	C3D-C2D	3.98	1.47	1.39
24	A1	855	AJP	CCJ-CCK	3.97	1.61	1.53
24	L2	202	AJP	OCL-CCK	-3.96	1.33	1.43
23	B2	844	BCR	C30-C25	-3.95	1.48	1.53
24	L	208	AJP	CCG-CCH	-3.95	1.48	1.56
24	I2	104	AJP	CCJ-CCK	3.94	1.61	1.53
23	M	101	BCR	C1-C6	-3.94	1.48	1.53
24	M2	101	AJP	CCJ-CCK	3.93	1.61	1.53
20	AA	803	CL0	C3D-C2D	3.93	1.47	1.39
20	A2	803	CL0	C3D-C2D	3.93	1.47	1.39
24	L	209	AJP	OCL-CCK	-3.93	1.33	1.43
23	B1	843	BCR	C30-C25	-3.93	1.48	1.53
24	AA	856	AJP	CCG-CCH	-3.92	1.48	1.56
23	J	102	BCR	C1-C6	-3.92	1.48	1.53
24	A	855	AJP	CCG-CCH	-3.92	1.48	1.56
24	L	208	AJP	OCL-CCK	-3.92	1.33	1.43
24	KK	104	AJP	OCL-CCK	-3.92	1.33	1.43
24	L	209	AJP	CCI-CCH	3.91	1.61	1.53
23	MM	101	BCR	C1-C6	-3.91	1.48	1.53
24	K	104	AJP	OCL-CCK	-3.91	1.33	1.43
24	AA	856	AJP	CCJ-CCK	3.90	1.61	1.53
24	I2	104	AJP	OCL-CCK	-3.90	1.33	1.43
24	A	855	AJP	CCJ-CCK	3.90	1.61	1.53
24	L1	204	AJP	OCL-CCK	-3.89	1.33	1.43
24	B	850	AJP	OCL-CCK	-3.89	1.33	1.43
24	K	104	AJP	CCJ-CCK	3.88	1.61	1.53
20	A	803	CL0	C3D-C2D	3.88	1.47	1.39
23	BB	847	BCR	C1-C6	-3.87	1.48	1.53
23	J2	104	BCR	C1-C6	-3.87	1.48	1.53
23	F1	304	BCR	C30-C25	-3.86	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	850	AJP	CCJ-CCK	3.85	1.61	1.53
23	B	848	BCR	C1-C6	-3.85	1.48	1.53
24	L2	203	AJP	CCJ-CCK	3.85	1.61	1.53
23	BB	842	BCR	C1-C6	-3.85	1.48	1.53
24	B	849	AJP	OCL-CCK	-3.84	1.33	1.43
24	KK	104	AJP	CCI-CCH	3.84	1.61	1.53
23	J2	102	BCR	C1-C6	-3.84	1.48	1.53
23	JJ	102	BCR	C1-C6	-3.84	1.48	1.53
24	M2	101	AJP	OCL-CCK	-3.83	1.33	1.43
24	L2	202	AJP	CBN-CCJ	-3.82	1.48	1.56
23	JJ	102	BCR	C30-C25	-3.82	1.48	1.53
23	B	843	BCR	C1-C6	-3.82	1.48	1.53
24	B	850	AJP	CBN-CCJ	-3.80	1.48	1.56
20	AA	803	CL0	O2A-CGA	3.79	1.44	1.33
23	BB	843	BCR	C30-C25	-3.79	1.48	1.53
24	BB	849	AJP	OCL-CCK	-3.79	1.34	1.43
24	M2	101	AJP	CCI-CCH	3.79	1.60	1.53
24	AA	802	AJP	OCL-CCK	-3.79	1.34	1.43
24	A	802	AJP	OCL-CCK	-3.78	1.34	1.43
24	K	104	AJP	CBN-CCJ	-3.78	1.48	1.56
24	BB	848	AJP	CBN-CCJ	-3.78	1.48	1.56
23	I1	101	BCR	C30-C25	-3.78	1.48	1.53
23	FF	304	BCR	C30-C25	-3.77	1.48	1.53
23	B1	842	BCR	C1-C6	-3.77	1.48	1.53
23	BB	838	BCR	C1-C6	-3.77	1.48	1.53
23	J1	102	BCR	C1-C6	-3.77	1.48	1.53
23	B2	843	BCR	C1-C6	-3.77	1.48	1.53
24	I2	104	AJP	CBN-CCJ	-3.76	1.48	1.56
24	BB	849	AJP	CBN-CCJ	-3.76	1.48	1.56
24	AA	856	AJP	CDA-CDB	3.76	1.60	1.53
24	A	855	AJP	CDA-CDB	3.76	1.60	1.53
24	K	104	AJP	CCI-CCH	3.76	1.60	1.53
23	B	839	BCR	C1-C6	-3.75	1.48	1.53
23	F2	304	BCR	C30-C25	-3.75	1.48	1.53
23	J1	102	BCR	C30-C25	-3.75	1.48	1.53
23	F	304	BCR	C1-C6	-3.75	1.48	1.53
24	L2	202	AJP	CCJ-CCK	3.74	1.60	1.53
24	A2	854	AJP	CCG-CCH	-3.74	1.49	1.56
24	B	849	AJP	CCI-CCH	3.74	1.60	1.53
24	L2	203	AJP	CCI-CCH	3.73	1.60	1.53
23	J	102	BCR	C30-C25	-3.73	1.48	1.53
20	A	803	CL0	O2A-CGA	3.73	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	F	305	BCR	C1-C6	-3.72	1.48	1.53
23	FF	306	BCR	C1-C6	-3.71	1.48	1.53
23	I2	101	BCR	C30-C25	-3.71	1.48	1.53
23	AA	852	BCR	C1-C6	-3.71	1.48	1.53
24	BB	848	AJP	CCI-CCH	3.71	1.60	1.53
24	K	104	AJP	CCG-CCH	-3.71	1.49	1.56
23	F2	304	BCR	C1-C6	-3.71	1.48	1.53
24	L2	203	AJP	OCL-CCK	-3.70	1.34	1.43
23	KK	103	BCR	C1-C6	-3.70	1.48	1.53
23	BB	843	BCR	C1-C6	-3.70	1.48	1.53
23	B	844	BCR	C1-C6	-3.70	1.48	1.53
23	F1	304	BCR	C1-C6	-3.70	1.48	1.53
23	FF	304	BCR	C1-C6	-3.69	1.48	1.53
24	KK	104	AJP	CCG-CCH	-3.69	1.49	1.56
23	K2	103	BCR	C1-C6	-3.69	1.48	1.53
24	I2	104	AJP	CCI-CCH	3.68	1.60	1.53
23	K1	104	BCR	C1-C6	-3.68	1.48	1.53
23	M1	101	BCR	C1-C6	-3.68	1.48	1.53
24	K	104	AJP	CDA-CDB	3.68	1.59	1.53
24	L1	204	AJP	CCJ-CCK	3.68	1.60	1.53
20	A2	803	CL0	O2A-CGA	3.68	1.44	1.33
24	B	849	AJP	CBN-CCJ	-3.68	1.48	1.56
24	BB	848	AJP	CCJ-CCK	3.67	1.60	1.53
24	M2	101	AJP	CBN-CCJ	-3.67	1.48	1.56
24	L	208	AJP	CCI-CCH	3.67	1.60	1.53
23	K	103	BCR	C1-C6	-3.67	1.48	1.53
23	L	206	BCR	C1-C6	-3.66	1.48	1.53
24	A1	855	AJP	CCG-CCH	-3.66	1.49	1.56
23	B1	838	BCR	C1-C6	-3.66	1.48	1.53
24	B	857	AJP	CCG-CCH	-3.65	1.49	1.56
23	B2	839	BCR	C1-C6	-3.65	1.48	1.53
24	L	209	AJP	CBN-CCJ	-3.65	1.48	1.56
24	BB	849	AJP	CCI-CCH	3.65	1.60	1.53
24	B	849	AJP	CCJ-CCK	3.64	1.60	1.53
23	I2	101	BCR	C1-C6	-3.64	1.48	1.53
23	I1	101	BCR	C1-C6	-3.63	1.48	1.53
23	J2	102	BCR	C30-C25	-3.63	1.48	1.53
23	A1	850	BCR	C1-C6	-3.62	1.48	1.53
23	F	304	BCR	C30-C25	-3.62	1.48	1.53
24	B	850	AJP	CCI-CCH	3.62	1.60	1.53
23	A2	848	BCR	C1-C6	-3.62	1.48	1.53
24	A1	855	AJP	CDA-CDB	3.61	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A2	854	AJP	CDA-CDB	3.61	1.59	1.53
23	A1	848	BCR	C1-C6	-3.61	1.48	1.53
23	AA	854	BCR	C30-C25	-3.61	1.48	1.53
23	A2	850	BCR	C1-C6	-3.61	1.48	1.53
23	II	101	BCR	C1-C6	-3.61	1.48	1.53
23	A1	847	BCR	C1-C6	-3.60	1.48	1.53
23	A	853	BCR	C30-C25	-3.60	1.48	1.53
24	A	802	AJP	CCG-CCH	-3.59	1.49	1.56
23	B1	843	BCR	C1-C6	-3.59	1.48	1.53
23	M2	102	BCR	C1-C6	-3.59	1.48	1.53
24	KK	104	AJP	CDA-CDB	3.58	1.59	1.53
23	II	104	BCR	C1-C6	-3.58	1.48	1.53
23	A2	847	BCR	C1-C6	-3.58	1.48	1.53
23	I	101	BCR	C1-C6	-3.58	1.48	1.53
23	B2	844	BCR	C1-C6	-3.57	1.49	1.53
24	L1	204	AJP	CCI-CCH	3.57	1.60	1.53
23	L1	209	BCR	C1-C6	-3.57	1.49	1.53
23	II	102	BCR	C1-C6	-3.57	1.49	1.53
23	A1	853	BCR	C30-C25	-3.56	1.49	1.53
23	L2	207	BCR	C1-C6	-3.56	1.49	1.53
24	L1	203	AJP	CCI-CCH	3.56	1.60	1.53
23	A2	853	BCR	C30-C25	-3.56	1.49	1.53
19	BB	826	CLA	CMB-C2B	-3.56	1.44	1.51
23	AA	849	BCR	C1-C6	-3.56	1.49	1.53
23	I2	103	BCR	C1-C6	-3.55	1.49	1.53
23	A	847	BCR	C1-C6	-3.55	1.49	1.53
24	B	850	AJP	CDA-CDB	3.55	1.59	1.53
23	A	848	BCR	C1-C6	-3.55	1.49	1.53
23	L	205	BCR	C1-C6	-3.55	1.49	1.53
24	AA	802	AJP	CCG-CCH	-3.54	1.49	1.56
23	L	206	BCR	C30-C25	-3.54	1.49	1.53
23	J1	104	BCR	C1-C6	-3.54	1.49	1.53
20	A	803	CL0	C1D-C2D	3.54	1.50	1.42
23	AA	848	BCR	C1-C6	-3.54	1.49	1.53
23	L1	201	BCR	C1-C6	-3.54	1.49	1.53
24	L2	202	AJP	CCG-CCH	-3.54	1.49	1.56
24	KK	104	AJP	CBN-CCJ	-3.52	1.48	1.56
24	BB	848	AJP	CCG-CCH	-3.52	1.49	1.56
23	F1	306	BCR	C1-C6	-3.52	1.49	1.53
24	L2	202	AJP	CCI-CCH	3.52	1.60	1.53
24	A1	854	AJP	CCG-CCH	-3.51	1.49	1.56
24	B	849	AJP	CCG-CCH	-3.51	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	848	BCR	C30-C25	-3.50	1.49	1.53
23	F2	305	BCR	C1-C6	-3.50	1.49	1.53
24	L1	203	AJP	CCJ-CCK	3.49	1.60	1.53
23	I2	102	BCR	C1-C6	-3.49	1.49	1.53
23	BB	847	BCR	C30-C25	-3.49	1.49	1.53
24	AA	802	AJP	CCI-CCH	3.49	1.60	1.53
23	II	101	BCR	C30-C25	-3.48	1.49	1.53
23	F1	303	BCR	C1-C6	-3.48	1.49	1.53
23	AA	854	BCR	C1-C6	-3.47	1.49	1.53
24	L2	203	AJP	CBO-CBE	-3.47	1.42	1.54
23	I	101	BCR	C30-C25	-3.47	1.49	1.53
23	LL	204	BCR	C30-C25	-3.47	1.49	1.53
24	A	802	AJP	CCI-CCH	3.47	1.60	1.53
23	I	102	BCR	C1-C6	-3.46	1.49	1.53
24	AA	802	AJP	CBN-CCJ	-3.46	1.48	1.56
23	A	853	BCR	C1-C6	-3.46	1.49	1.53
24	BB	849	AJP	CDA-CDB	3.46	1.59	1.53
24	BB	849	AJP	CBO-CBE	-3.46	1.42	1.54
20	A2	803	CL0	C1D-C2D	3.45	1.50	1.42
24	L2	203	AJP	CDA-CDB	3.45	1.59	1.53
24	A	802	AJP	CBN-CCJ	-3.44	1.49	1.56
23	AA	851	BCR	C1-C6	-3.44	1.49	1.53
24	L1	204	AJP	CDA-CDB	3.44	1.59	1.53
23	A	851	BCR	C1-C6	-3.44	1.49	1.53
24	A	802	AJP	CBO-CBE	-3.44	1.42	1.54
23	B1	842	BCR	C30-C25	-3.43	1.49	1.53
23	LL	204	BCR	C1-C6	-3.43	1.49	1.53
23	A	850	BCR	C1-C6	-3.43	1.49	1.53
24	AA	802	AJP	CBO-CBE	-3.43	1.42	1.54
23	M	101	BCR	C30-C25	-3.43	1.49	1.53
23	L1	208	BCR	C1-C6	-3.43	1.49	1.53
23	B2	843	BCR	C30-C25	-3.42	1.49	1.53
23	L2	207	BCR	C30-C25	-3.42	1.49	1.53
20	A1	802	CL0	C1D-C2D	3.42	1.50	1.42
23	K2	103	BCR	C30-C25	-3.42	1.49	1.53
23	A2	851	BCR	C1-C6	-3.42	1.49	1.53
23	B	842	BCR	C1-C6	-3.42	1.49	1.53
23	BB	841	BCR	C1-C6	-3.41	1.49	1.53
23	K1	104	BCR	C30-C25	-3.41	1.49	1.53
23	A1	853	BCR	C1-C6	-3.41	1.49	1.53
23	FF	303	BCR	C1-C6	-3.40	1.49	1.53
23	A1	851	BCR	C1-C6	-3.40	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	857	AJP	CDA-CDB	3.39	1.59	1.53
23	B1	841	BCR	C1-C6	-3.39	1.49	1.53
23	F	303	BCR	C1-C6	-3.39	1.49	1.53
23	L1	209	BCR	C30-C25	-3.38	1.49	1.53
23	A2	853	BCR	C1-C6	-3.38	1.49	1.53
24	AA	856	AJP	CBO-CBE	-3.37	1.43	1.54
24	A	855	AJP	CBO-CBE	-3.37	1.43	1.54
23	J	104	BCR	C30-C25	-3.36	1.49	1.53
23	B	843	BCR	C30-C25	-3.35	1.49	1.53
24	BB	848	AJP	CDA-CDB	3.33	1.59	1.53
23	F2	303	BCR	C1-C6	-3.33	1.49	1.53
24	A1	854	AJP	CDA-CDB	3.33	1.59	1.53
24	L	209	AJP	CBO-CBE	-3.33	1.43	1.54
23	J	104	BCR	C1-C6	-3.33	1.49	1.53
24	L2	202	AJP	CBO-CBE	-3.32	1.43	1.54
23	BB	842	BCR	C30-C25	-3.32	1.49	1.53
24	A1	855	AJP	CBO-CBE	-3.32	1.43	1.54
23	I	102	BCR	C30-C25	-3.31	1.49	1.53
24	AA	802	AJP	CCF-CCE	3.31	1.61	1.52
24	KK	104	AJP	CBO-CBE	-3.30	1.43	1.54
24	A	802	AJP	CCF-CCE	3.30	1.61	1.52
20	AA	803	CL0	C1D-C2D	3.30	1.50	1.42
23	B1	838	BCR	C30-C25	-3.30	1.49	1.53
24	A2	854	AJP	CBO-CBE	-3.30	1.43	1.54
23	B2	839	BCR	C30-C25	-3.29	1.49	1.53
24	L1	204	AJP	CBO-CBE	-3.29	1.43	1.54
23	J2	104	BCR	C30-C25	-3.29	1.49	1.53
24	L	208	AJP	CBO-CBE	-3.28	1.43	1.54
24	I2	104	AJP	CCG-CCH	-3.28	1.50	1.56
23	AA	849	BCR	C30-C25	-3.28	1.49	1.53
19	B	826	CLA	CMB-C2B	-3.28	1.44	1.51
23	B2	842	BCR	C1-C6	-3.28	1.49	1.53
23	A1	850	BCR	C30-C25	-3.28	1.49	1.53
23	J1	104	BCR	C30-C25	-3.27	1.49	1.53
23	A	848	BCR	C30-C25	-3.27	1.49	1.53
24	L	208	AJP	CBN-CCJ	-3.26	1.49	1.56
23	A2	850	BCR	C30-C25	-3.25	1.49	1.53
23	II	102	BCR	C30-C25	-3.24	1.49	1.53
23	I2	102	BCR	C30-C25	-3.24	1.49	1.53
24	B	849	AJP	CBO-CBE	-3.24	1.43	1.54
23	L1	201	BCR	C30-C25	-3.23	1.49	1.53
23	BB	838	BCR	C30-C25	-3.23	1.49	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	M2	101	AJP	CBO-CBE	-3.23	1.43	1.54
24	L1	203	AJP	CCG-CCH	-3.23	1.50	1.56
23	B	839	BCR	C30-C25	-3.21	1.49	1.53
25	I1	102	LMG	C4-C5	3.21	1.59	1.53
23	MM	101	BCR	C30-C25	-3.20	1.49	1.53
24	K	104	AJP	CBO-CBE	-3.20	1.43	1.54
24	A1	854	AJP	CBO-CBE	-3.19	1.43	1.54
19	B1	824	CLA	CHC-C1C	3.19	1.43	1.35
24	BB	848	AJP	OCD-CCE	-3.19	1.36	1.43
19	B1	826	CLA	CMB-C2B	-3.18	1.45	1.51
24	B	850	AJP	CBO-CBE	-3.18	1.43	1.54
23	AA	851	BCR	C30-C25	-3.18	1.49	1.53
24	B	857	AJP	CBO-CBE	-3.18	1.43	1.54
19	B2	820	CLA	CHC-C1C	3.17	1.43	1.35
19	B2	834	CLA	CHC-C1C	3.17	1.43	1.35
23	A	850	BCR	C30-C25	-3.16	1.49	1.53
24	B	849	AJP	CDA-CDB	3.16	1.59	1.53
23	JJ	104	BCR	C30-C25	-3.16	1.49	1.53
24	L1	204	AJP	OCD-CCE	-3.16	1.36	1.43
19	B2	849	CLA	CMB-C2B	-3.15	1.45	1.51
24	L2	203	AJP	OCD-CCE	-3.15	1.36	1.43
24	L1	203	AJP	CBO-CBE	-3.15	1.43	1.54
23	M1	101	BCR	C30-C25	-3.14	1.49	1.53
23	A1	848	BCR	C30-C25	-3.14	1.49	1.53
23	A2	848	BCR	C30-C25	-3.13	1.49	1.53
24	B	850	AJP	OCD-CCE	-3.13	1.36	1.43
24	BB	848	AJP	CBO-CBE	-3.13	1.43	1.54
23	F	303	BCR	C30-C25	-3.12	1.49	1.53
24	BB	849	AJP	OCD-CCE	-3.12	1.36	1.43
19	B1	848	CLA	CMB-C2B	-3.12	1.45	1.51
19	A2	815	CLA	CHC-C1C	3.12	1.43	1.35
19	B2	826	CLA	CMB-C2B	-3.11	1.45	1.51
19	A2	806	CLA	CHC-C1C	3.11	1.43	1.35
19	A	804	CLA	CHC-C1C	3.10	1.43	1.35
19	A	810	CLA	CHC-C1C	3.10	1.43	1.35
23	M2	102	BCR	C30-C25	-3.10	1.49	1.53
24	L2	202	AJP	OCD-CCE	-3.10	1.36	1.43
19	B2	829	CLA	CHC-C1C	3.09	1.43	1.35
23	A1	849	BCR	C30-C25	-3.09	1.49	1.53
24	B	849	AJP	OCD-CCE	-3.09	1.36	1.43
24	A2	854	AJP	OCD-CCE	-3.09	1.36	1.43
19	A1	814	CLA	CHC-C1C	3.09	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	852	CLA	CMB-C2B	-3.08	1.45	1.51
19	B1	850	CLA	CHC-C1C	3.08	1.43	1.35
19	BB	821	CLA	CHC-C1C	3.08	1.43	1.35
24	BB	848	AJP	CAV-CBE	3.08	1.60	1.53
23	KK	103	BCR	C30-C25	-3.08	1.49	1.53
24	A1	854	AJP	OCD-CCE	-3.08	1.36	1.43
19	A2	804	CLA	CHC-C1C	3.08	1.43	1.35
23	K	103	BCR	C30-C25	-3.08	1.49	1.53
19	FF	305	CLA	CHC-C1C	3.08	1.43	1.35
24	B	857	AJP	OCD-CCE	-3.08	1.36	1.43
24	A1	855	AJP	OCD-CCE	-3.07	1.36	1.43
19	AA	806	CLA	CHC-C1C	3.07	1.43	1.35
19	AA	804	CLA	CHC-C1C	3.07	1.43	1.35
19	B1	820	CLA	CHC-C1C	3.06	1.43	1.35
23	A1	849	BCR	C1-C6	-3.06	1.49	1.53
23	II	104	BCR	C30-C25	-3.06	1.49	1.53
23	F2	305	BCR	C30-C25	-3.06	1.49	1.53
19	B1	828	CLA	CHC-C1C	3.06	1.43	1.35
23	A2	849	BCR	C30-C25	-3.06	1.49	1.53
23	A	849	BCR	C30-C25	-3.06	1.49	1.53
24	L	208	AJP	CDC-CDB	-3.06	1.45	1.53
19	B2	827	CLA	CHC-C1C	3.06	1.43	1.35
23	AA	850	BCR	C30-C25	-3.06	1.49	1.53
23	F1	306	BCR	C30-C25	-3.06	1.49	1.53
19	AA	816	CLA	CHC-C1C	3.06	1.43	1.35
23	FF	303	BCR	C30-C25	-3.05	1.49	1.53
19	A	806	CLA	CHC-C1C	3.05	1.43	1.35
19	A1	806	CLA	CHC-C1C	3.05	1.43	1.35
24	L1	203	AJP	OCD-CCE	-3.05	1.36	1.43
19	B2	851	CLA	CHC-C1C	3.05	1.43	1.35
19	AA	823	CLA	CHC-C1C	3.05	1.43	1.35
19	BB	818	CLA	CHC-C1C	3.05	1.43	1.35
19	AA	810	CLA	CHC-C1C	3.05	1.43	1.35
19	A	823	CLA	CHC-C1C	3.04	1.43	1.35
24	KK	104	AJP	OCD-CCE	-3.04	1.36	1.43
19	B2	816	CLA	CHC-C1C	3.04	1.43	1.35
19	B	822	CLA	CHC-C1C	3.04	1.43	1.35
19	A2	807	CLA	CHC-C1C	3.03	1.43	1.35
19	B	813	CLA	CHC-C1C	3.03	1.43	1.35
19	B2	802	CLA	CHC-C1C	3.03	1.43	1.35
23	A	849	BCR	C1-C6	-3.03	1.49	1.53
24	K	104	AJP	OCD-CCE	-3.03	1.36	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	856	CLA	CHC-C1C	3.03	1.43	1.35
24	AA	856	AJP	OCD-CCE	-3.02	1.36	1.43
19	A2	810	CLA	CHC-C1C	3.02	1.43	1.35
19	B1	813	CLA	CHC-C1C	3.02	1.43	1.35
24	L2	202	AJP	CDA-CDB	3.02	1.58	1.53
19	A2	823	CLA	CHC-C1C	3.02	1.43	1.35
24	A	855	AJP	OCD-CCE	-3.02	1.36	1.43
19	B2	811	CLA	CHC-C1C	3.02	1.43	1.35
19	B1	827	CLA	CHC-C1C	3.02	1.43	1.35
19	B	859	CLA	CHC-C1C	3.01	1.43	1.35
23	AA	848	BCR	C30-C25	-3.01	1.49	1.53
19	A1	815	CLA	CHC-C1C	3.01	1.43	1.35
19	A1	805	CLA	CHC-C1C	3.01	1.43	1.35
19	BB	822	CLA	CHC-C1C	3.01	1.43	1.35
19	B1	811	CLA	CHC-C1C	3.01	1.43	1.35
19	B	829	CLA	CHC-C1C	3.01	1.43	1.35
19	B1	802	CLA	CHC-C1C	3.01	1.43	1.35
23	L	205	BCR	C30-C25	-3.01	1.49	1.53
19	B2	813	CLA	CHC-C1C	3.01	1.43	1.35
19	B2	809	CLA	CHC-C1C	3.01	1.43	1.35
23	A	847	BCR	C30-C25	-3.00	1.49	1.53
19	B	816	CLA	CHC-C1C	3.00	1.43	1.35
19	A2	835	CLA	CHC-C1C	3.00	1.43	1.35
19	B1	809	CLA	CHC-C1C	3.00	1.43	1.35
19	A2	829	CLA	CHC-C1C	3.00	1.43	1.35
19	B	811	CLA	CHC-C1C	3.00	1.43	1.35
19	B1	816	CLA	CHC-C1C	3.00	1.43	1.35
23	F2	303	BCR	C30-C25	-2.99	1.49	1.53
19	A2	816	CLA	CHC-C1C	2.99	1.43	1.35
19	AA	815	CLA	CHC-C1C	2.99	1.43	1.35
19	A	815	CLA	CHC-C1C	2.99	1.43	1.35
19	BB	827	CLA	CHC-C1C	2.99	1.43	1.35
19	BB	813	CLA	CHC-C1C	2.99	1.43	1.35
19	A	816	CLA	CHC-C1C	2.99	1.43	1.35
19	BB	820	CLA	CHC-C1C	2.99	1.43	1.35
19	J1	101	CLA	CHC-C1C	2.99	1.43	1.35
19	A1	822	CLA	CHC-C1C	2.99	1.43	1.35
19	AA	842	CLA	CHC-C1C	2.99	1.43	1.35
19	A	814	CLA	CHC-C1C	2.99	1.43	1.35
19	J2	101	CLA	CHC-C1C	2.99	1.43	1.35
23	B	842	BCR	C30-C25	-2.99	1.49	1.53
19	A	842	CLA	CHC-C1C	2.99	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	802	CLA	CHC-C1C	2.99	1.43	1.35
19	A	807	CLA	CHC-C1C	2.98	1.43	1.35
19	K	101	CLA	CHC-C1C	2.98	1.43	1.35
19	A	835	CLA	CHC-C1C	2.98	1.43	1.35
19	AA	835	CLA	CHC-C1C	2.98	1.43	1.35
19	AA	814	CLA	CHC-C1C	2.98	1.43	1.35
19	BB	811	CLA	CHC-C1C	2.98	1.43	1.35
19	B1	819	CLA	CHC-C1C	2.98	1.43	1.35
19	B2	834	CLA	CMB-C2B	-2.98	1.45	1.51
19	B2	807	CLA	CHC-C1C	2.97	1.43	1.35
19	BB	823	CLA	CHC-C1C	2.97	1.43	1.35
19	K2	102	CLA	CHC-C1C	2.97	1.43	1.35
19	B	804	CLA	CHC-C1C	2.97	1.43	1.35
19	B1	833	CLA	CHC-C1C	2.97	1.43	1.35
19	A1	834	CLA	CHC-C1C	2.97	1.43	1.35
19	KK	101	CLA	CHC-C1C	2.97	1.43	1.35
19	B	802	CLA	CHC-C1C	2.97	1.43	1.35
19	B2	846	CLA	CHC-C1C	2.97	1.43	1.35
24	L1	203	AJP	CDA-CDB	2.97	1.58	1.53
19	B	820	CLA	CHC-C1C	2.97	1.43	1.35
19	A2	817	CLA	CHC-C1C	2.97	1.43	1.35
19	B1	845	CLA	CHC-C1C	2.97	1.43	1.35
23	BB	841	BCR	C30-C25	-2.97	1.49	1.53
19	A1	837	CLA	CHC-C1C	2.97	1.43	1.35
19	A1	809	CLA	CHC-C1C	2.96	1.43	1.35
19	B	809	CLA	CHC-C1C	2.96	1.43	1.35
19	B1	807	CLA	CHC-C1C	2.96	1.43	1.35
19	AA	807	CLA	CHC-C1C	2.96	1.43	1.35
19	AA	820	CLA	CHC-C1C	2.96	1.43	1.35
19	BB	829	CLA	CHC-C1C	2.96	1.43	1.35
19	B1	823	CLA	CHC-C1C	2.95	1.43	1.35
19	FF	301	CLA	CHC-C1C	2.95	1.43	1.35
19	B	805	CLA	CHC-C1C	2.95	1.43	1.35
19	A2	809	CLA	CHC-C1C	2.95	1.43	1.35
19	A1	816	CLA	CHC-C1C	2.95	1.43	1.35
19	A1	841	CLA	CHC-C1C	2.95	1.43	1.35
19	BB	816	CLA	CHC-C1C	2.95	1.43	1.35
19	F1	301	CLA	CHC-C1C	2.95	1.43	1.35
19	A	852	CLA	CHC-C1C	2.95	1.43	1.35
19	B	831	CLA	CHC-C1C	2.95	1.43	1.35
19	BB	809	CLA	CHC-C1C	2.95	1.43	1.35
19	AA	809	CLA	CHC-C1C	2.95	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	846	CLA	CHC-C1C	2.95	1.43	1.35
19	B1	818	CLA	CHC-C1C	2.95	1.43	1.35
19	A1	803	CLA	CHC-C1C	2.95	1.43	1.35
19	BB	826	CLA	CMD-C2D	-2.95	1.44	1.51
19	A1	817	CLA	CHC-C1C	2.94	1.43	1.35
19	B2	818	CLA	CHC-C1C	2.94	1.43	1.35
24	M2	101	AJP	CAV-CBE	2.94	1.59	1.53
19	B1	829	CLA	CHC-C1C	2.94	1.43	1.35
19	BB	804	CLA	CHC-C1C	2.94	1.43	1.35
24	BB	849	AJP	CBO-CBP	-2.94	1.48	1.53
24	I2	104	AJP	CBO-CBE	-2.94	1.44	1.54
19	BB	845	CLA	CHC-C1C	2.94	1.43	1.35
23	A1	847	BCR	C30-C25	-2.94	1.49	1.53
19	B1	814	CLA	CHC-C1C	2.94	1.43	1.35
19	B	823	CLA	CHC-C1C	2.94	1.43	1.35
19	A1	826	CLA	CHC-C1C	2.94	1.43	1.35
19	BB	831	CLA	CHC-C1C	2.93	1.43	1.35
19	B2	822	CLA	CHC-C1C	2.93	1.43	1.35
23	I2	103	BCR	C30-C25	-2.93	1.49	1.53
19	AA	819	CLA	CHC-C1C	2.93	1.43	1.35
19	BB	808	CLA	CHC-C1C	2.93	1.43	1.35
19	F1	305	CLA	CHC-C1C	2.93	1.43	1.35
19	BB	807	CLA	CHC-C1C	2.93	1.43	1.35
19	B	828	CLA	CHC-C1C	2.93	1.42	1.35
19	AA	801	CLA	CHC-C1C	2.93	1.42	1.35
19	B	827	CLA	CHC-C1C	2.93	1.42	1.35
19	K1	102	CLA	CHC-C1C	2.93	1.42	1.35
19	BB	805	CLA	CHC-C1C	2.93	1.42	1.35
19	BB	824	CLA	CHC-C1C	2.93	1.42	1.35
19	JJ	101	CLA	CHC-C1C	2.93	1.42	1.35
19	A2	818	CLA	CHC-C1C	2.93	1.42	1.35
19	A	844	CLA	CHC-C1C	2.92	1.42	1.35
19	B	832	CLA	CHC-C1C	2.92	1.42	1.35
19	A1	808	CLA	CHC-C1C	2.92	1.42	1.35
19	A2	838	CLA	CHC-C1C	2.92	1.42	1.35
19	A2	814	CLA	CHC-C1C	2.92	1.42	1.35
19	B	807	CLA	CHC-C1C	2.92	1.42	1.35
19	B	808	CLA	CHC-C1C	2.92	1.42	1.35
19	A1	813	CLA	CHC-C1C	2.92	1.42	1.35
23	A2	847	BCR	C30-C25	-2.92	1.49	1.53
19	F2	301	CLA	CHC-C1C	2.92	1.42	1.35
19	B1	810	CLA	CHC-C1C	2.92	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	853	CLA	CHC-C1C	2.92	1.42	1.35
19	J	101	CLA	CHC-C1C	2.92	1.42	1.35
19	B2	823	CLA	CHC-C1C	2.92	1.42	1.35
19	B	819	CLA	CHC-C1C	2.92	1.42	1.35
19	B	817	CLA	CHC-C1C	2.92	1.42	1.35
19	BB	828	CLA	CHC-C1C	2.92	1.42	1.35
19	B1	822	CLA	CHC-C1C	2.92	1.42	1.35
19	A1	810	CLA	CHC-C1C	2.91	1.42	1.35
19	A	817	CLA	CHC-C1C	2.91	1.42	1.35
19	A1	812	CLA	CHC-C1C	2.91	1.42	1.35
19	AA	817	CLA	CHC-C1C	2.91	1.42	1.35
19	BB	817	CLA	CHC-C1C	2.91	1.42	1.35
19	B2	828	CLA	CHC-C1C	2.91	1.42	1.35
19	B1	817	CLA	CHC-C1C	2.91	1.42	1.35
19	K1	103	CLA	CHC-C1C	2.91	1.42	1.35
19	A	811	CLA	CHC-C1C	2.91	1.42	1.35
23	B1	841	BCR	C30-C25	-2.91	1.49	1.53
19	KK	102	CLA	CHC-C1C	2.91	1.42	1.35
19	B1	804	CLA	CHC-C1C	2.91	1.42	1.35
19	L	203	CLA	CMB-C2B	-2.91	1.45	1.51
19	B2	804	CLA	CHC-C1C	2.91	1.42	1.35
19	K2	104	CLA	CHC-C1C	2.91	1.42	1.35
19	A2	852	CLA	CHC-C1C	2.91	1.42	1.35
19	B2	817	CLA	CHC-C1C	2.91	1.42	1.35
19	A1	852	CLA	CHC-C1C	2.91	1.42	1.35
19	A2	802	CLA	CHC-C1C	2.91	1.42	1.35
19	A2	840	CLA	CHC-C1C	2.90	1.42	1.35
19	A	801	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	801	CLA	CHC-C1C	2.90	1.42	1.35
19	B2	819	CLA	CHC-C1C	2.90	1.42	1.35
23	FF	306	BCR	C30-C25	-2.90	1.49	1.53
24	B	849	AJP	CAV-CBE	2.90	1.59	1.53
19	A2	813	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	839	CLA	CHC-C1C	2.90	1.42	1.35
19	AA	838	CLA	CHC-C1C	2.90	1.42	1.35
19	B1	830	CLA	CHC-C1C	2.90	1.42	1.35
19	A	809	CLA	CHC-C1C	2.90	1.42	1.35
19	B2	810	CLA	CHC-C1C	2.90	1.42	1.35
19	A	818	CLA	CHC-C1C	2.90	1.42	1.35
19	AA	818	CLA	CHC-C1C	2.90	1.42	1.35
19	A	827	CLA	CHC-C1C	2.90	1.42	1.35
19	A1	818	CLA	CHC-C1C	2.90	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	836	CLA	CHC-C1C	2.89	1.42	1.35
19	LL	202	CLA	CHC-C1C	2.89	1.42	1.35
19	A2	842	CLA	CHC-C1C	2.89	1.42	1.35
19	A	838	CLA	CHC-C1C	2.89	1.42	1.35
19	BB	833	CLA	CMB-C2B	-2.89	1.45	1.51
19	BB	835	CLA	CHC-C1C	2.89	1.42	1.35
19	A	837	CLA	CHC-C1C	2.89	1.42	1.35
19	B2	824	CLA	CHC-C1C	2.89	1.42	1.35
24	BB	848	AJP	CDC-CDB	-2.89	1.45	1.53
19	A2	801	CLA	CHC-C1C	2.89	1.42	1.35
19	A1	811	CLA	CHC-C1C	2.89	1.42	1.35
19	J1	103	CLA	CHC-C1C	2.89	1.42	1.35
19	A1	827	CLA	CHC-C1C	2.89	1.42	1.35
19	AA	845	CLA	CHC-C1C	2.89	1.42	1.35
23	L1	208	BCR	C30-C25	-2.89	1.49	1.53
19	A2	837	CLA	CMB-C2B	-2.89	1.45	1.51
19	J2	103	CLA	CHC-C1C	2.89	1.42	1.35
19	B1	808	CLA	CHC-C1C	2.88	1.42	1.35
19	BB	810	CLA	CHC-C1C	2.88	1.42	1.35
19	A2	811	CLA	CHC-C1C	2.88	1.42	1.35
19	AA	837	CLA	CHC-C1C	2.88	1.42	1.35
19	K	102	CLA	CHC-C1C	2.88	1.42	1.35
19	B	810	CLA	CHC-C1C	2.88	1.42	1.35
19	A2	805	CLA	CHC-C1C	2.88	1.42	1.35
19	AA	828	CLA	CHC-C1C	2.88	1.42	1.35
19	A2	827	CLA	CHC-C1C	2.88	1.42	1.35
19	B2	831	CLA	CHC-C1C	2.88	1.42	1.35
24	L	209	AJP	CAV-CBE	2.88	1.59	1.53
19	A2	819	CLA	CHC-C1C	2.88	1.42	1.35
19	L	203	CLA	CHC-C1C	2.88	1.42	1.35
19	B1	812	CLA	CHC-C1C	2.88	1.42	1.35
23	F	305	BCR	C30-C25	-2.87	1.49	1.53
19	B	834	CLA	CMB-C2B	-2.87	1.45	1.51
19	B2	830	CLA	CHC-C1C	2.87	1.42	1.35
19	JJ	103	CLA	CHC-C1C	2.87	1.42	1.35
24	L2	202	AJP	CDC-CDB	-2.87	1.45	1.53
19	B1	815	CLA	CHC-C1C	2.87	1.42	1.35
19	AA	811	CLA	CHC-C1C	2.87	1.42	1.35
19	B	837	CLA	CHC-C1C	2.87	1.42	1.35
19	A2	822	CLA	CHC-C1C	2.87	1.42	1.35
19	A	826	CLA	CHC-C1C	2.87	1.42	1.35
19	L1	206	CLA	CHC-C1C	2.87	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	827	CLA	CHC-C1C	2.87	1.42	1.35
19	A1	824	CLA	CHC-C1C	2.87	1.42	1.35
19	B2	812	CLA	CHC-C1C	2.86	1.42	1.35
19	B2	837	CLA	CHC-C1C	2.86	1.42	1.35
19	A2	812	CLA	CHC-C1C	2.86	1.42	1.35
24	L1	203	AJP	CBF-CBE	2.86	1.59	1.53
19	L2	205	CLA	CHC-C1C	2.86	1.42	1.35
19	K1	105	CLA	CHC-C1C	2.86	1.42	1.35
19	B2	815	CLA	CHC-C1C	2.86	1.42	1.35
19	A	828	CLA	CHC-C1C	2.86	1.42	1.35
19	F2	302	CLA	CHC-C1C	2.86	1.42	1.35
19	A	812	CLA	CHC-C1C	2.86	1.42	1.35
19	B2	808	CLA	CHC-C1C	2.86	1.42	1.35
19	A1	821	CLA	CHC-C1C	2.86	1.42	1.35
19	A1	804	CLA	CHC-C1C	2.86	1.42	1.35
19	B1	836	CLA	CHC-C1C	2.86	1.42	1.35
19	X1	101	CLA	CHC-C1C	2.85	1.42	1.35
19	AA	812	CLA	CHC-C1C	2.85	1.42	1.35
24	B	849	AJP	CDC-CDB	-2.85	1.45	1.53
23	F1	303	BCR	C30-C25	-2.85	1.49	1.53
19	B	824	CLA	CHC-C1C	2.85	1.42	1.35
19	A	840	CLA	CHC-C1C	2.85	1.42	1.35
19	AA	813	CLA	CHC-C1C	2.85	1.42	1.35
19	F	301	CLA	CHC-C1C	2.85	1.42	1.35
19	BB	816	CLA	CMB-C2B	-2.85	1.45	1.51
19	X2	101	CLA	CHC-C1C	2.85	1.42	1.35
19	A	822	CLA	CHC-C1C	2.85	1.42	1.35
19	B1	801	CLA	CHC-C1C	2.85	1.42	1.35
19	A1	838	CLA	CHC-C1C	2.85	1.42	1.35
19	A1	836	CLA	CHC-C1C	2.85	1.42	1.35
19	A2	828	CLA	CHC-C1C	2.85	1.42	1.35
19	A	808	CLA	CHC-C1C	2.85	1.42	1.35
19	B	814	CLA	CHC-C1C	2.85	1.42	1.35
19	B2	814	CLA	CHC-C1C	2.84	1.42	1.35
19	X	101	CLA	CHC-C1C	2.84	1.42	1.35
19	B1	833	CLA	CMB-C2B	-2.84	1.45	1.51
19	A	805	CLA	CHC-C1C	2.84	1.42	1.35
19	B2	801	CLA	CHC-C1C	2.84	1.42	1.35
19	FF	302	CLA	CHC-C1C	2.84	1.42	1.35
19	A2	836	CLA	CMB-C2B	-2.84	1.45	1.51
24	AA	802	AJP	CDC-CDB	-2.84	1.45	1.53
19	B	834	CLA	CHC-C1C	2.84	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	836	CLA	CHC-C1C	2.84	1.42	1.35
24	L1	203	AJP	CDC-CDB	-2.84	1.45	1.53
20	A1	802	CL0	C4B-CHC	2.84	1.47	1.40
19	XX	101	CLA	CHC-C1C	2.84	1.42	1.35
19	B2	805	CLA	CHC-C1C	2.84	1.42	1.35
19	A	833	CLA	CHC-C1C	2.84	1.42	1.35
19	AA	825	CLA	CHC-C1C	2.84	1.42	1.35
19	B	818	CLA	CHC-C1C	2.84	1.42	1.35
19	J	103	CLA	CHC-C1C	2.84	1.42	1.35
19	A2	837	CLA	CHC-C1C	2.83	1.42	1.35
19	B2	832	CLA	CHC-C1C	2.83	1.42	1.35
19	AA	805	CLA	CHC-C1C	2.83	1.42	1.35
19	A2	833	CLA	CHC-C1C	2.83	1.42	1.35
19	A	825	CLA	CHC-C1C	2.83	1.42	1.35
19	B1	805	CLA	CHC-C1C	2.83	1.42	1.35
24	L1	204	AJP	CAV-CBE	2.83	1.59	1.53
19	B1	821	CLA	CHC-C1C	2.83	1.42	1.35
19	AA	840	CLA	CHC-C1C	2.83	1.42	1.35
24	A	802	AJP	CDC-CDB	-2.83	1.45	1.53
23	AA	850	BCR	C1-C6	-2.83	1.50	1.53
19	AA	833	CLA	CHC-C1C	2.83	1.42	1.35
19	A2	820	CLA	CHC-C1C	2.83	1.42	1.35
19	BB	836	CLA	CHC-C1C	2.83	1.42	1.35
19	A	821	CLA	CHC-C1C	2.83	1.42	1.35
19	A2	825	CLA	CHC-C1C	2.83	1.42	1.35
19	F1	302	CLA	CHC-C1C	2.82	1.42	1.35
19	A	819	CLA	CHC-C1C	2.82	1.42	1.35
19	A2	834	CLA	CHC-C1C	2.82	1.42	1.35
24	L	209	AJP	CDC-CDB	-2.82	1.45	1.53
19	AA	808	CLA	CHC-C1C	2.82	1.42	1.35
19	F	302	CLA	CHC-C1C	2.82	1.42	1.35
19	A2	839	CLA	CHC-C1C	2.82	1.42	1.35
19	A	813	CLA	CHC-C1C	2.82	1.42	1.35
19	A1	829	CLA	CHC-C1C	2.82	1.42	1.35
19	AA	826	CLA	CHC-C1C	2.82	1.42	1.35
19	A	820	CLA	CHC-C1C	2.82	1.42	1.35
19	A1	833	CLA	CHC-C1C	2.82	1.42	1.35
19	A1	828	CLA	CHC-C1C	2.82	1.42	1.35
19	A2	844	CLA	CHC-C1C	2.82	1.42	1.35
19	B1	835	CLA	CHC-C1C	2.82	1.42	1.35
24	L2	203	AJP	CAV-CBE	2.82	1.59	1.53
19	AA	822	CLA	CHC-C1C	2.81	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	812	CLA	CHC-C1C	2.81	1.42	1.35
19	A2	821	CLA	CHC-C1C	2.81	1.42	1.35
19	BB	825	CLA	CHC-C1C	2.81	1.42	1.35
19	B1	834	CLA	CHC-C1C	2.81	1.42	1.35
19	A1	844	CLA	CHC-C1C	2.81	1.42	1.35
19	BB	819	CLA	CHC-C1C	2.81	1.42	1.35
19	BB	814	CLA	CHC-C1C	2.81	1.42	1.35
19	AA	821	CLA	CHC-C1C	2.81	1.42	1.35
19	AA	839	CLA	CHC-C1C	2.81	1.42	1.35
19	AA	824	CLA	CHC-C1C	2.81	1.42	1.35
19	A1	825	CLA	CHC-C1C	2.81	1.42	1.35
19	B	801	CLA	CHC-C1C	2.81	1.42	1.35
19	BB	803	CLA	CHC-C1C	2.81	1.42	1.35
24	K	104	AJP	CAV-CBE	2.81	1.59	1.53
19	B	803	CLA	CHC-C1C	2.80	1.42	1.35
19	B	825	CLA	CHC-C1C	2.80	1.42	1.35
19	A1	819	CLA	CHC-C1C	2.80	1.42	1.35
19	A	834	CLA	CHC-C1C	2.80	1.42	1.35
19	BB	830	CLA	CHC-C1C	2.80	1.42	1.35
19	AA	830	CLA	CHC-C1C	2.80	1.42	1.35
19	B	816	CLA	CMB-C2B	-2.80	1.45	1.51
19	A2	824	CLA	CHC-C1C	2.80	1.42	1.35
20	A	803	CL0	C4B-CHC	2.80	1.47	1.40
19	A	824	CLA	CHC-C1C	2.80	1.42	1.35
19	A	839	CLA	CHC-C1C	2.80	1.42	1.35
19	A1	832	CLA	CHC-C1C	2.80	1.42	1.35
19	L1	205	CLA	CHC-C1C	2.80	1.42	1.35
19	A1	820	CLA	CHC-C1C	2.80	1.42	1.35
19	AA	834	CLA	CHC-C1C	2.80	1.42	1.35
24	L	208	AJP	CAV-CBE	2.80	1.59	1.53
19	L2	204	CLA	CHC-C1C	2.79	1.42	1.35
20	AA	803	CL0	C4B-CHC	2.79	1.47	1.40
19	A1	823	CLA	CHC-C1C	2.79	1.42	1.35
19	AA	836	CLA	CHC-C1C	2.79	1.42	1.35
19	A2	808	CLA	CHC-C1C	2.79	1.42	1.35
19	A1	836	CLA	CMB-C2B	-2.79	1.45	1.51
19	B1	825	CLA	CHC-C1C	2.79	1.42	1.35
19	L2	206	CLA	CHC-C1C	2.79	1.42	1.35
19	BB	812	CLA	CHC-C1C	2.79	1.42	1.35
19	L	204	CLA	CHC-C1C	2.79	1.42	1.35
19	A1	807	CLA	CHC-C1C	2.79	1.42	1.35
19	B1	806	CLA	CHC-C1C	2.78	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	849	CLA	CHC-C1C	2.78	1.42	1.35
19	B	806	CLA	CHC-C1C	2.78	1.42	1.35
19	B	815	CLA	CHC-C1C	2.78	1.42	1.35
19	B2	835	CLA	CHC-C1C	2.78	1.42	1.35
19	A2	830	CLA	CHC-C1C	2.78	1.42	1.35
19	BB	808	CLA	CMB-C2B	-2.78	1.45	1.51
19	B2	803	CLA	CHC-C1C	2.78	1.42	1.35
19	B	821	CLA	CHC-C1C	2.78	1.42	1.35
19	BB	815	CLA	CHC-C1C	2.78	1.42	1.35
19	B1	831	CLA	CHC-C1C	2.78	1.42	1.35
19	L1	207	CLA	CHC-C1C	2.78	1.42	1.35
19	BB	834	CLA	CHC-C1C	2.77	1.42	1.35
19	B2	850	CLA	CHC-C1C	2.77	1.42	1.35
23	B1	839	BCR	C30-C25	-2.77	1.50	1.53
19	BB	806	CLA	CHC-C1C	2.77	1.42	1.35
19	B2	821	CLA	CHC-C1C	2.77	1.42	1.35
19	B1	803	CLA	CHC-C1C	2.77	1.42	1.35
19	B	854	CLA	CMB-C2B	-2.76	1.45	1.51
19	A	836	CLA	CHC-C1C	2.76	1.42	1.35
24	M2	101	AJP	CDC-CDB	-2.76	1.46	1.53
19	B	830	CLA	CHC-C1C	2.76	1.42	1.35
19	A2	826	CLA	CHC-C1C	2.76	1.42	1.35
19	B2	850	CLA	CMB-C2B	-2.76	1.45	1.51
19	AA	837	CLA	CMB-C2B	-2.76	1.45	1.51
19	B2	834	CLA	C3B-C2B	-2.75	1.36	1.40
19	AA	831	CLA	CHC-C1C	2.75	1.42	1.35
19	B	835	CLA	CHC-C1C	2.75	1.42	1.35
19	L	202	CLA	CHC-C1C	2.75	1.42	1.35
19	BB	833	CLA	CHC-C1C	2.75	1.42	1.35
19	A	831	CLA	CMB-C2B	-2.75	1.45	1.51
19	A	829	CLA	CHC-C1C	2.75	1.42	1.35
19	B2	825	CLA	CHC-C1C	2.75	1.42	1.35
19	AA	820	CLA	CMB-C2B	-2.74	1.45	1.51
23	A2	849	BCR	C1-C6	-2.74	1.50	1.53
19	A2	831	CLA	CHC-C1C	2.74	1.42	1.35
24	KK	104	AJP	CAV-CBE	2.74	1.59	1.53
19	BB	802	CLA	CMB-C2B	-2.74	1.46	1.51
19	A	837	CLA	CMB-C2B	-2.74	1.46	1.51
19	AA	832	CLA	CMB-C2B	-2.73	1.46	1.51
19	AA	811	CLA	C1D-C2D	2.73	1.48	1.42
19	BB	801	CLA	CHC-C1C	2.73	1.42	1.35
19	A	831	CLA	CHC-C1C	2.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	LL	201	CLA	CHC-C1C	2.73	1.42	1.35
19	L2	205	CLA	CMB-C2B	-2.73	1.46	1.51
19	L1	206	CLA	CMB-C2B	-2.73	1.46	1.51
23	K1	106	BCR	C30-C25	-2.73	1.50	1.53
19	A	830	CLA	CHC-C1C	2.73	1.42	1.35
19	B	858	CLA	CHC-C1C	2.73	1.42	1.35
24	I2	104	AJP	CAV-CBE	2.73	1.59	1.53
24	L1	204	AJP	CDC-CDB	-2.73	1.46	1.53
19	A1	830	CLA	CHC-C1C	2.72	1.42	1.35
19	B	860	CLA	CMB-C2B	-2.72	1.46	1.51
19	B2	852	CLA	CMB-C2B	-2.72	1.46	1.51
24	B	857	AJP	CAV-CBE	2.72	1.59	1.53
19	A1	842	CLA	CHC-C1C	2.72	1.42	1.35
23	BB	839	BCR	C30-C25	-2.72	1.50	1.53
19	A2	827	CLA	CMB-C2B	-2.72	1.46	1.51
19	A1	835	CLA	CHC-C1C	2.72	1.42	1.35
19	B2	814	CLA	CMB-C2B	-2.72	1.46	1.51
19	B	802	CLA	CMB-C2B	-2.72	1.46	1.51
24	A1	854	AJP	CAV-CBE	2.72	1.59	1.53
24	L	209	AJP	CDD-CCI	2.72	1.58	1.53
24	AA	802	AJP	CAV-CBE	2.72	1.59	1.53
24	L2	202	AJP	CBO-CBP	-2.72	1.49	1.53
19	AA	829	CLA	CHC-C1C	2.71	1.42	1.35
19	BB	820	CLA	C1D-C2D	2.71	1.48	1.42
19	AA	807	CLA	C1D-C2D	2.71	1.48	1.42
19	B2	852	CLA	CHC-C1C	2.71	1.42	1.35
19	B	818	CLA	C1D-C2D	2.71	1.48	1.42
19	B2	806	CLA	CHC-C1C	2.71	1.42	1.35
23	B	840	BCR	C30-C25	-2.71	1.50	1.53
24	L1	203	AJP	CBO-CBP	-2.71	1.49	1.53
19	A	822	CLA	C1D-C2D	2.71	1.48	1.42
19	A	807	CLA	C1D-C2D	2.71	1.48	1.42
24	BB	849	AJP	CDC-CDB	-2.71	1.46	1.53
19	BB	826	CLA	CHC-C1C	2.71	1.42	1.35
24	L2	202	AJP	CAV-CBE	2.71	1.59	1.53
24	A2	854	AJP	CAV-CBE	2.71	1.59	1.53
19	A2	832	CLA	CHC-C1C	2.71	1.42	1.35
19	B2	826	CLA	CHC-C1C	2.70	1.42	1.35
19	A1	824	CLA	CMB-C2B	-2.70	1.46	1.51
19	A	820	CLA	CMB-C2B	-2.70	1.46	1.51
19	A2	831	CLA	CMB-C2B	-2.70	1.46	1.51
24	A	802	AJP	CAV-CBE	2.70	1.59	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	845	CLA	C1D-C2D	2.70	1.48	1.42
19	B2	846	CLA	C1D-C2D	2.70	1.48	1.42
24	B	850	AJP	CBO-CBP	-2.70	1.49	1.53
19	BB	831	CLA	C3B-C2B	-2.70	1.36	1.40
19	AA	831	CLA	CMB-C2B	-2.70	1.46	1.51
24	L	208	AJP	CBO-CBP	-2.70	1.49	1.53
19	J2	103	CLA	C1D-C2D	2.69	1.48	1.42
19	B2	832	CLA	C1D-C2D	2.69	1.48	1.42
24	B	850	AJP	CDC-CDB	-2.69	1.46	1.53
24	L2	203	AJP	CDC-CDB	-2.69	1.46	1.53
19	A1	818	CLA	C1D-C2D	2.69	1.48	1.42
19	A2	825	CLA	CMB-C2B	-2.69	1.46	1.51
19	AA	832	CLA	CHC-C1C	2.69	1.42	1.35
19	B1	816	CLA	CMB-C2B	-2.69	1.46	1.51
19	LL	202	CLA	CMB-C2B	-2.69	1.46	1.51
24	KK	104	AJP	CBD-CBN	2.69	1.59	1.54
19	A1	830	CLA	CMB-C2B	-2.69	1.46	1.51
19	AA	843	CLA	CHC-C1C	2.68	1.42	1.35
19	AA	826	CLA	C1D-C2D	2.68	1.48	1.42
19	A1	840	CLA	CHC-C1C	2.68	1.42	1.35
19	B1	831	CLA	C1D-C2D	2.68	1.48	1.42
19	A	811	CLA	C1D-C2D	2.68	1.48	1.42
19	LL	203	CLA	CHC-C1C	2.68	1.42	1.35
24	M2	101	AJP	CBO-CBP	-2.68	1.49	1.53
19	A2	836	CLA	CHC-C1C	2.67	1.42	1.35
19	A1	831	CLA	CMB-C2B	-2.67	1.46	1.51
19	A	841	CLA	CHC-C1C	2.67	1.42	1.35
24	L	209	AJP	CBO-CBP	-2.67	1.49	1.53
19	A2	820	CLA	CMB-C2B	-2.67	1.46	1.51
19	A2	832	CLA	CMB-C2B	-2.67	1.46	1.51
19	AA	841	CLA	CHC-C1C	2.67	1.42	1.35
19	A	809	CLA	C1D-C2D	2.67	1.48	1.42
24	I2	104	AJP	CDA-CDB	2.67	1.59	1.53
19	LL	203	CLA	C1D-C2D	2.67	1.48	1.42
19	A2	807	CLA	C1D-C2D	2.66	1.48	1.42
19	A2	841	CLA	CHC-C1C	2.66	1.42	1.35
19	A2	823	CLA	CMB-C2B	-2.66	1.46	1.51
19	B	860	CLA	CHC-C1C	2.66	1.42	1.35
19	F2	302	CLA	CMB-C2B	-2.66	1.46	1.51
19	A1	806	CLA	C1D-C2D	2.66	1.48	1.42
19	J1	103	CLA	C1D-C2D	2.66	1.48	1.42
19	BB	855	CLA	CHC-C1C	2.66	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	819	CLA	C1D-C2D	2.66	1.48	1.42
19	B1	803	CLA	CMB-C2B	-2.66	1.46	1.51
19	B1	825	CLA	C1D-C2D	2.66	1.48	1.42
19	J2	101	CLA	C1D-C2D	2.66	1.48	1.42
19	A1	819	CLA	CMB-C2B	-2.65	1.46	1.51
19	J	103	CLA	C1D-C2D	2.65	1.48	1.42
19	B1	826	CLA	CHC-C1C	2.65	1.42	1.35
24	K	104	AJP	CDC-CDB	-2.65	1.46	1.53
19	B	814	CLA	CMB-C2B	-2.65	1.46	1.51
19	FF	301	CLA	CMB-C2B	-2.65	1.46	1.51
19	A2	824	CLA	CMB-C2B	-2.65	1.46	1.51
19	A2	818	CLA	C1D-C2D	2.65	1.48	1.42
19	B1	807	CLA	CMD-C2D	-2.65	1.45	1.51
19	BB	845	CLA	C1D-C2D	2.65	1.48	1.42
19	B2	811	CLA	C1D-C2D	2.65	1.48	1.42
19	BB	855	CLA	CMB-C2B	-2.65	1.46	1.51
23	AA	855	BCR	C30-C25	-2.64	1.50	1.53
19	AA	809	CLA	C1D-C2D	2.64	1.48	1.42
19	A1	817	CLA	C1D-C2D	2.64	1.48	1.42
19	BB	814	CLA	CMB-C2B	-2.64	1.46	1.51
19	A1	812	CLA	C1D-C2D	2.64	1.48	1.42
19	J1	101	CLA	C1D-C2D	2.64	1.48	1.42
19	A2	811	CLA	CMB-C2B	-2.64	1.46	1.51
19	B	826	CLA	CHC-C1C	2.64	1.42	1.35
24	BB	849	AJP	CAV-CBE	2.64	1.59	1.53
23	B2	840	BCR	C30-C25	-2.64	1.50	1.53
19	LL	201	CLA	CMB-C2B	-2.64	1.46	1.51
19	B	825	CLA	C1D-C2D	2.64	1.48	1.42
23	B2	842	BCR	C30-C25	-2.64	1.50	1.53
19	A	822	CLA	CMB-C2B	-2.64	1.46	1.51
19	B	833	CLA	CHC-C1C	2.64	1.42	1.35
19	B	803	CLA	CMB-C2B	-2.64	1.46	1.51
19	JJ	103	CLA	C1D-C2D	2.63	1.48	1.42
19	B	846	CLA	C1D-C2D	2.63	1.48	1.42
19	BB	825	CLA	C1D-C2D	2.63	1.48	1.42
19	A1	831	CLA	CHC-C1C	2.63	1.42	1.35
19	K1	103	CLA	C1D-C2D	2.63	1.48	1.42
19	AA	812	CLA	CMB-C2B	-2.63	1.46	1.51
19	B2	803	CLA	CMB-C2B	-2.63	1.46	1.51
19	A1	823	CLA	CMB-C2B	-2.63	1.46	1.51
19	F1	302	CLA	CMB-C2B	-2.63	1.46	1.51
19	LL	201	CLA	C1D-C2D	2.63	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	802	CLA	C1D-C2D	2.63	1.48	1.42
19	B	829	CLA	CMB-C2B	-2.63	1.46	1.51
23	K2	105	BCR	C30-C25	-2.63	1.50	1.53
24	B	849	AJP	CBO-CBP	-2.63	1.49	1.53
19	A	818	CLA	C1D-C2D	2.63	1.48	1.42
19	A	836	CLA	CMB-C2B	-2.63	1.46	1.51
24	A1	855	AJP	CAV-CBE	2.63	1.59	1.53
19	F	302	CLA	CMB-C2B	-2.63	1.46	1.51
19	AA	835	CLA	CMB-C2B	-2.63	1.46	1.51
19	BB	835	CLA	C1D-C2D	2.63	1.48	1.42
19	AA	818	CLA	C1D-C2D	2.63	1.48	1.42
24	AA	856	AJP	CBO-CBP	-2.62	1.49	1.53
19	A2	820	CLA	C3B-CAB	-2.62	1.42	1.47
19	B1	811	CLA	C1D-C2D	2.62	1.48	1.42
19	A	833	CLA	C1D-C2D	2.62	1.48	1.42
24	KK	104	AJP	CDC-CDB	-2.62	1.46	1.53
19	A2	825	CLA	C1D-C2D	2.62	1.48	1.42
19	A	832	CLA	CMB-C2B	-2.62	1.46	1.51
19	B2	805	CLA	CMB-C2B	-2.62	1.46	1.51
19	BB	803	CLA	CMB-C2B	-2.62	1.46	1.51
19	B	858	CLA	CMB-C2B	-2.62	1.46	1.51
19	AA	834	CLA	CMB-C2B	-2.62	1.46	1.51
19	AA	836	CLA	CMB-C2B	-2.62	1.46	1.51
19	BB	852	CLA	CHC-C1C	2.62	1.42	1.35
19	A1	836	CLA	C1D-C2D	2.62	1.48	1.42
19	B2	816	CLA	CMB-C2B	-2.62	1.46	1.51
24	A	855	AJP	CBO-CBP	-2.62	1.49	1.53
19	BB	805	CLA	CMB-C2B	-2.62	1.46	1.51
19	A1	842	CLA	C1D-C2D	2.62	1.48	1.42
19	AA	853	CLA	C1D-C2D	2.62	1.48	1.42
19	B	836	CLA	CMB-C2B	-2.62	1.46	1.51
19	B2	833	CLA	CHC-C1C	2.62	1.42	1.35
19	LL	203	CLA	CMD-C2D	-2.62	1.45	1.51
19	A1	811	CLA	CMB-C2B	-2.62	1.46	1.51
19	BB	832	CLA	CHC-C1C	2.62	1.42	1.35
24	B	849	AJP	CBF-CBE	2.62	1.58	1.53
19	A	832	CLA	CHC-C1C	2.62	1.42	1.35
19	A2	802	CLA	C1D-C2D	2.61	1.48	1.42
19	B2	802	CLA	C1D-C2D	2.61	1.48	1.42
24	A	802	AJP	CDA-CDB	2.61	1.59	1.53
19	B	820	CLA	C1D-C2D	2.61	1.48	1.42
19	B	832	CLA	C3B-C2B	-2.61	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	824	CLA	CMB-C2B	-2.61	1.46	1.51
19	A2	815	CLA	C1D-C2D	2.61	1.48	1.42
19	B1	805	CLA	CMB-C2B	-2.61	1.46	1.51
19	B	832	CLA	CMB-C2B	-2.61	1.46	1.51
19	A	824	CLA	CMB-C2B	-2.61	1.46	1.51
24	BB	848	AJP	OCY-CCX	2.61	1.49	1.41
19	B	825	CLA	CMB-C2B	-2.61	1.46	1.51
19	A	812	CLA	CMB-C2B	-2.61	1.46	1.51
24	AA	802	AJP	CDA-CDB	2.61	1.59	1.53
19	A	823	CLA	CMB-C2B	-2.61	1.46	1.51
24	A1	855	AJP	CBF-CBE	2.61	1.58	1.53
24	I2	104	AJP	CDC-CDB	-2.61	1.46	1.53
19	A2	809	CLA	C1D-C2D	2.61	1.48	1.42
19	A2	852	CLA	CMB-C2B	-2.61	1.46	1.51
19	AA	829	CLA	CMB-C2B	-2.61	1.46	1.51
19	AA	837	CLA	C1D-C2D	2.61	1.48	1.42
19	A1	808	CLA	C1D-C2D	2.61	1.48	1.42
19	B	805	CLA	CMB-C2B	-2.61	1.46	1.51
19	B2	807	CLA	CMD-C2D	-2.61	1.45	1.51
19	A	834	CLA	CMB-C2B	-2.60	1.46	1.51
19	B2	825	CLA	C1D-C2D	2.60	1.48	1.42
19	BB	825	CLA	CMB-C2B	-2.60	1.46	1.51
19	AA	823	CLA	CMB-C2B	-2.60	1.46	1.51
19	A1	810	CLA	CMB-C2B	-2.60	1.46	1.51
24	L1	204	AJP	OCY-CCX	2.60	1.49	1.41
19	A1	832	CLA	CMB-C2B	-2.60	1.46	1.51
19	A	805	CLA	CMB-C2B	-2.60	1.46	1.51
19	A	840	CLA	CMB-C2B	-2.60	1.46	1.51
19	B2	814	CLA	C1D-C2D	2.60	1.48	1.42
19	BB	808	CLA	C1D-C2D	2.60	1.48	1.42
19	A2	837	CLA	C1D-C2D	2.60	1.48	1.42
24	AA	856	AJP	CBD-CBN	2.60	1.59	1.54
19	A	812	CLA	C1D-C2D	2.60	1.48	1.42
24	A1	855	AJP	CDC-CDB	-2.60	1.46	1.53
19	AA	805	CLA	CMB-C2B	-2.60	1.46	1.51
19	B2	829	CLA	CMB-C2B	-2.60	1.46	1.51
24	K	104	AJP	CBO-CBP	-2.60	1.49	1.53
19	AA	812	CLA	C1D-C2D	2.60	1.48	1.42
19	B2	825	CLA	CMB-C2B	-2.60	1.46	1.51
19	A2	833	CLA	CMB-C2B	-2.60	1.46	1.51
19	A2	812	CLA	C1D-C2D	2.60	1.48	1.42
19	A	829	CLA	CMB-C2B	-2.60	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	822	CLA	CMB-C2B	-2.60	1.46	1.51
19	A2	835	CLA	CMB-C2B	-2.59	1.46	1.51
24	L2	203	AJP	OCY-CCX	2.59	1.49	1.41
19	A	837	CLA	C1D-C2D	2.59	1.48	1.42
19	A1	824	CLA	C1D-C2D	2.59	1.48	1.42
19	A	835	CLA	CMB-C2B	-2.59	1.46	1.51
19	B2	807	CLA	CMB-C2B	-2.59	1.46	1.51
24	A	855	AJP	CBD-CBN	2.59	1.59	1.54
19	A	839	CLA	C1D-C2D	2.59	1.48	1.42
19	A1	819	CLA	C3B-CAB	-2.59	1.42	1.47
19	B2	822	CLA	C1D-C2D	2.59	1.48	1.42
19	BB	811	CLA	C1D-C2D	2.59	1.48	1.42
19	B	813	CLA	CMB-C2B	-2.59	1.46	1.51
19	A2	834	CLA	CMB-C2B	-2.59	1.46	1.51
19	A	819	CLA	C1D-C2D	2.59	1.48	1.42
19	FF	302	CLA	CMB-C2B	-2.59	1.46	1.51
19	JJ	101	CLA	C1D-C2D	2.59	1.48	1.42
19	L	202	CLA	CMB-C2B	-2.59	1.46	1.51
24	B	857	AJP	CBF-CBE	2.59	1.58	1.53
19	B1	828	CLA	CMB-C2B	-2.59	1.46	1.51
24	I2	104	AJP	CBO-CBP	-2.59	1.49	1.53
19	BB	836	CLA	CMB-C2B	-2.58	1.46	1.51
19	A1	833	CLA	CMB-C2B	-2.58	1.46	1.51
19	B2	828	CLA	C1D-C2D	2.58	1.48	1.42
19	A2	826	CLA	C1D-C2D	2.58	1.48	1.42
19	F	301	CLA	CMB-C2B	-2.58	1.46	1.51
24	A2	854	AJP	CBF-CBE	2.58	1.58	1.53
22	L1	211	LHG	P-O3	2.58	1.69	1.59
19	AA	815	CLA	C1D-C2D	2.58	1.48	1.42
19	A1	811	CLA	C1D-C2D	2.58	1.48	1.42
19	B	854	CLA	CHC-C1C	2.58	1.42	1.35
19	J	101	CLA	C1D-C2D	2.58	1.48	1.42
19	BB	809	CLA	CMB-C2B	-2.58	1.46	1.51
19	B	859	CLA	CMB-C2B	-2.58	1.46	1.51
19	A2	822	CLA	CMB-C2B	-2.58	1.46	1.51
19	BB	804	CLA	C1D-C2D	2.58	1.48	1.42
19	B2	836	CLA	C1D-C2D	2.58	1.48	1.42
19	A1	834	CLA	C1D-C2D	2.58	1.48	1.42
19	A2	820	CLA	C3B-C2B	-2.58	1.36	1.40
19	L2	204	CLA	CMB-C2B	-2.58	1.46	1.51
19	BB	831	CLA	CMB-C2B	-2.58	1.46	1.51
19	AA	825	CLA	C1D-C2D	2.58	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	804	CLA	CMB-C2B	-2.58	1.46	1.51
19	AA	843	CLA	C1D-C2D	2.58	1.48	1.42
19	B1	807	CLA	CMB-C2B	-2.57	1.46	1.51
19	A	825	CLA	C1D-C2D	2.57	1.48	1.42
19	B1	812	CLA	C1D-C2D	2.57	1.48	1.42
19	BB	813	CLA	CMB-C2B	-2.57	1.46	1.51
24	A2	854	AJP	CDC-CDB	-2.57	1.46	1.53
19	A	826	CLA	C1D-C2D	2.57	1.48	1.42
19	A	824	CLA	C1D-C2D	2.57	1.48	1.42
19	A2	813	CLA	C1D-C2D	2.57	1.48	1.42
19	A1	821	CLA	CMB-C2B	-2.57	1.46	1.51
19	A1	834	CLA	CMB-C2B	-2.57	1.46	1.51
19	A2	818	CLA	CMB-C2B	-2.57	1.46	1.51
19	F1	305	CLA	C1D-C2D	2.57	1.48	1.42
19	B2	829	CLA	C1D-C2D	2.57	1.48	1.42
19	B1	814	CLA	CMB-C2B	-2.57	1.46	1.51
19	A1	805	CLA	C1D-C2D	2.57	1.48	1.42
19	B2	804	CLA	CMB-C2B	-2.57	1.46	1.51
19	AA	811	CLA	CMB-C2B	-2.57	1.46	1.51
19	B	860	CLA	C1D-C2D	2.57	1.48	1.42
19	B1	834	CLA	C1D-C2D	2.57	1.48	1.42
19	B1	830	CLA	C1D-C2D	2.57	1.48	1.42
19	B2	851	CLA	CMB-C2B	-2.57	1.46	1.51
24	M2	101	AJP	CDD-CCI	2.57	1.58	1.53
19	B1	804	CLA	C1D-C2D	2.57	1.48	1.42
19	B2	852	CLA	C1D-C2D	2.57	1.48	1.42
19	A2	810	CLA	C1D-C2D	2.57	1.48	1.42
19	A	811	CLA	CMB-C2B	-2.57	1.46	1.51
19	B	809	CLA	CMB-C2B	-2.57	1.46	1.51
19	BB	835	CLA	CMB-C2B	-2.57	1.46	1.51
19	A1	842	CLA	CMB-C2B	-2.57	1.46	1.51
20	A2	803	CL0	C4B-CHC	2.57	1.47	1.40
19	BB	812	CLA	CMB-C2B	-2.56	1.46	1.51
19	A	852	CLA	C1D-C2D	2.56	1.48	1.42
19	AA	835	CLA	C1D-C2D	2.56	1.48	1.42
19	B1	831	CLA	CMB-C2B	-2.56	1.46	1.51
19	L1	205	CLA	CMB-C2B	-2.56	1.46	1.51
19	B2	804	CLA	C1D-C2D	2.56	1.48	1.42
24	A1	854	AJP	CBF-CBE	2.56	1.58	1.53
19	AA	838	CLA	C1D-C2D	2.56	1.48	1.42
19	B1	824	CLA	CMB-C2B	-2.56	1.46	1.51
19	A	807	CLA	CMB-C2B	-2.56	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	804	CLA	C1D-C2D	2.56	1.48	1.42
19	LL	203	CLA	CMB-C2B	-2.56	1.46	1.51
19	AA	816	CLA	C1D-C2D	2.56	1.48	1.42
19	B	837	CLA	C1D-C2D	2.56	1.48	1.42
19	FF	305	CLA	CMB-C2B	-2.56	1.46	1.51
19	B1	850	CLA	C1D-C2D	2.56	1.48	1.42
19	A	815	CLA	C1D-C2D	2.56	1.48	1.42
19	B1	814	CLA	C1D-C2D	2.56	1.48	1.42
19	A	838	CLA	C1D-C2D	2.56	1.48	1.42
19	AA	843	CLA	CMB-C2B	-2.56	1.46	1.51
19	B2	812	CLA	C1D-C2D	2.56	1.48	1.42
19	A	835	CLA	C1D-C2D	2.56	1.48	1.42
24	L	208	AJP	CDD-CCI	2.56	1.58	1.53
19	B1	849	CLA	CMB-C2B	-2.55	1.46	1.51
19	KK	102	CLA	C1D-C2D	2.55	1.48	1.42
19	L1	205	CLA	C1D-C2D	2.55	1.48	1.42
19	X2	101	CLA	C1D-C2D	2.55	1.48	1.42
19	A	806	CLA	C1D-C2D	2.55	1.48	1.42
19	B	811	CLA	C1D-C2D	2.55	1.48	1.42
19	BB	818	CLA	CMD-C2D	-2.55	1.45	1.51
19	B1	828	CLA	C1D-C2D	2.55	1.48	1.42
19	A2	805	CLA	CMB-C2B	-2.55	1.46	1.51
19	AA	806	CLA	C1D-C2D	2.55	1.48	1.42
19	A1	809	CLA	C1D-C2D	2.55	1.48	1.42
19	BB	824	CLA	CMB-C2B	-2.55	1.46	1.51
19	A1	814	CLA	C1D-C2D	2.55	1.48	1.42
19	B1	816	CLA	C1D-C2D	2.55	1.48	1.42
19	B1	825	CLA	CMB-C2B	-2.55	1.46	1.51
19	B2	827	CLA	C1D-C2D	2.55	1.48	1.42
19	BB	834	CLA	C1D-C2D	2.55	1.48	1.42
19	K	102	CLA	C1D-C2D	2.55	1.48	1.42
19	B2	816	CLA	C1D-C2D	2.55	1.48	1.42
19	A2	842	CLA	CMB-C2B	-2.55	1.46	1.51
19	BB	856	CLA	CMB-C2B	-2.55	1.46	1.51
19	B2	802	CLA	CMB-C2B	-2.54	1.46	1.51
19	B	836	CLA	C1D-C2D	2.54	1.48	1.42
23	A	854	BCR	C30-C25	-2.54	1.50	1.53
19	AA	810	CLA	C1D-C2D	2.54	1.48	1.42
19	AA	822	CLA	CMB-C2B	-2.54	1.46	1.51
19	BB	829	CLA	CMB-C2B	-2.54	1.46	1.51
19	B2	808	CLA	C1D-C2D	2.54	1.48	1.42
19	A2	832	CLA	C1D-C2D	2.54	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	842	CLA	CMB-C2B	-2.54	1.46	1.51
19	B	835	CLA	C1D-C2D	2.54	1.48	1.42
19	AA	807	CLA	CMB-C2B	-2.54	1.46	1.51
19	A	813	CLA	C1D-C2D	2.54	1.48	1.42
19	B2	851	CLA	C1D-C2D	2.54	1.48	1.42
19	BB	820	CLA	CMB-C2B	-2.54	1.46	1.51
19	B1	832	CLA	CHC-C1C	2.54	1.41	1.35
19	B1	815	CLA	C1D-C2D	2.54	1.48	1.42
19	B	826	CLA	C1D-C2D	2.54	1.48	1.42
24	BB	848	AJP	CBO-CBP	-2.54	1.49	1.53
19	B2	815	CLA	CMB-C2B	-2.54	1.46	1.51
19	A1	825	CLA	CMB-C2B	-2.54	1.46	1.51
19	B	808	CLA	C1D-C2D	2.54	1.48	1.42
19	L	202	CLA	C1D-C2D	2.54	1.48	1.42
19	A1	833	CLA	C1D-C2D	2.54	1.48	1.42
19	K2	104	CLA	C1D-C2D	2.54	1.48	1.42
19	AA	842	CLA	CMB-C2B	-2.54	1.46	1.51
19	A2	814	CLA	C1D-C2D	2.54	1.48	1.42
19	A2	840	CLA	C1D-C2D	2.54	1.48	1.42
19	A	814	CLA	CMB-C2B	-2.54	1.46	1.51
19	A2	826	CLA	CMB-C2B	-2.54	1.46	1.51
19	A1	839	CLA	C1D-C2D	2.54	1.48	1.42
19	B2	818	CLA	C1D-C2D	2.54	1.48	1.42
19	B	816	CLA	C1D-C2D	2.54	1.48	1.42
19	B2	813	CLA	C1D-C2D	2.54	1.48	1.42
19	AA	819	CLA	C1D-C2D	2.54	1.48	1.42
19	AA	838	CLA	CMB-C2B	-2.54	1.46	1.51
19	A	810	CLA	C1D-C2D	2.54	1.48	1.42
19	BB	816	CLA	C1D-C2D	2.54	1.48	1.42
19	B2	819	CLA	C1D-C2D	2.53	1.48	1.42
19	BB	832	CLA	CMB-C2B	-2.53	1.46	1.51
19	B	833	CLA	CMB-C2B	-2.53	1.46	1.51
19	B	820	CLA	CMB-C2B	-2.53	1.46	1.51
19	AA	833	CLA	C1D-C2D	2.53	1.48	1.42
19	A2	829	CLA	CMB-C2B	-2.53	1.46	1.51
19	AA	839	CLA	C1D-C2D	2.53	1.48	1.42
19	A	834	CLA	C1D-C2D	2.53	1.48	1.42
19	B1	801	CLA	CMB-C2B	-2.53	1.46	1.51
19	A	820	CLA	C3B-CAB	-2.53	1.42	1.47
19	B2	822	CLA	CMB-C2B	-2.53	1.46	1.51
24	KK	104	AJP	CBO-CBP	-2.53	1.49	1.53
24	B	849	AJP	OCY-CCX	2.53	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	832	CLA	C1D-C2D	2.53	1.48	1.42
19	B2	808	CLA	CMB-C2B	-2.53	1.46	1.51
19	B2	826	CLA	CMD-C2D	-2.53	1.45	1.51
19	B	858	CLA	C1D-C2D	2.53	1.48	1.42
19	A1	844	CLA	C1D-C2D	2.53	1.48	1.42
19	A	816	CLA	C1D-C2D	2.53	1.48	1.42
19	B1	826	CLA	CMD-C2D	-2.53	1.45	1.51
19	B1	835	CLA	C1D-C2D	2.53	1.48	1.42
19	A1	813	CLA	C1D-C2D	2.53	1.48	1.42
19	A2	835	CLA	C1D-C2D	2.53	1.48	1.42
19	B	829	CLA	C1D-C2D	2.53	1.48	1.42
19	A1	810	CLA	C1D-C2D	2.53	1.48	1.42
19	B1	819	CLA	C1D-C2D	2.53	1.48	1.42
19	B	834	CLA	CMD-C2D	-2.53	1.45	1.51
19	BB	802	CLA	C1D-C2D	2.52	1.48	1.42
19	A	838	CLA	CMB-C2B	-2.52	1.46	1.51
19	BB	836	CLA	C1D-C2D	2.52	1.48	1.42
19	L2	204	CLA	C1D-C2D	2.52	1.48	1.42
19	B1	808	CLA	C1D-C2D	2.52	1.48	1.42
19	AA	827	CLA	C1D-C2D	2.52	1.48	1.42
19	B2	824	CLA	CMB-C2B	-2.52	1.46	1.51
19	A1	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	A	825	CLA	CMB-C2B	-2.52	1.46	1.51
19	A1	819	CLA	C3B-C2B	-2.52	1.36	1.40
19	BB	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	850	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	817	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	827	CLA	CMB-C2B	-2.52	1.46	1.51
19	F1	301	CLA	CMB-C2B	-2.52	1.46	1.51
19	FF	305	CLA	C1D-C2D	2.52	1.48	1.42
19	B1	808	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	802	CLA	CMB-C2B	-2.52	1.46	1.51
19	B1	813	CLA	C1D-C2D	2.52	1.48	1.42
24	L1	203	AJP	CAW-CBF	2.52	1.56	1.52
19	AA	825	CLA	CMB-C2B	-2.52	1.46	1.51
19	A	842	CLA	C1D-C2D	2.52	1.48	1.42
19	AA	813	CLA	C1D-C2D	2.52	1.48	1.42
19	BB	829	CLA	C1D-C2D	2.52	1.48	1.42
19	B	808	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	807	CLA	CMB-C2B	-2.52	1.46	1.51
19	B	826	CLA	C3B-C2B	-2.52	1.36	1.40
19	A2	819	CLA	CMB-C2B	-2.52	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	828	CLA	C1D-C2D	2.52	1.48	1.42
19	A1	816	CLA	CMB-C2B	-2.52	1.46	1.51
19	A2	828	CLA	CMB-C2B	-2.52	1.46	1.51
19	BB	827	CLA	CMB-C2B	-2.52	1.46	1.51
19	B2	830	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	806	CLA	CMB-C2B	-2.51	1.46	1.51
24	A2	854	AJP	CAW-CBF	2.51	1.56	1.52
19	BB	807	CLA	CMD-C2D	-2.51	1.45	1.51
19	AA	814	CLA	C1D-C2D	2.51	1.48	1.42
19	B1	829	CLA	CMB-C2B	-2.51	1.46	1.51
19	A	814	CLA	C1D-C2D	2.51	1.48	1.42
19	B2	849	CLA	CHC-C1C	2.51	1.41	1.35
19	A1	818	CLA	CMB-C2B	-2.51	1.46	1.51
19	BB	830	CLA	C1D-C2D	2.51	1.48	1.42
19	A1	835	CLA	CMB-C2B	-2.51	1.46	1.51
19	F2	301	CLA	CMB-C2B	-2.51	1.46	1.51
24	A	855	AJP	CAV-CBE	2.51	1.58	1.53
19	A2	844	CLA	C1D-C2D	2.51	1.48	1.42
19	A	844	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	803	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	807	CLA	CMD-C2D	-2.51	1.45	1.51
19	B2	809	CLA	C1D-C2D	2.51	1.48	1.42
19	B1	820	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	816	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	817	CLA	C1D-C2D	2.51	1.48	1.42
24	AA	856	AJP	CAV-CBE	2.51	1.58	1.53
19	B2	831	CLA	C1D-C2D	2.51	1.48	1.42
19	B1	818	CLA	C1D-C2D	2.51	1.48	1.42
19	A1	808	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	845	CLA	CMB-C2B	-2.51	1.46	1.51
19	B	831	CLA	C1D-C2D	2.51	1.48	1.42
19	B2	837	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	831	CLA	C1D-C2D	2.51	1.48	1.42
19	B1	836	CLA	CMB-C2B	-2.51	1.46	1.51
19	A2	842	CLA	C1D-C2D	2.51	1.48	1.42
19	A2	834	CLA	C1D-C2D	2.51	1.48	1.42
19	A1	840	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	844	CLA	CMB-C2B	-2.51	1.46	1.51
19	AA	853	CLA	CMB-C2B	-2.51	1.46	1.51
19	A1	828	CLA	CMB-C2B	-2.51	1.46	1.51
19	L	204	CLA	CMB-C2B	-2.51	1.46	1.51
19	BB	831	CLA	C1D-C2D	2.51	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	820	CLA	C1D-C2D	2.50	1.48	1.42
19	B2	836	CLA	CMB-C2B	-2.50	1.46	1.51
19	B1	827	CLA	C1D-C2D	2.50	1.48	1.42
19	BB	834	CLA	CMB-C2B	-2.50	1.46	1.51
19	K1	102	CLA	CMB-C2B	-2.50	1.46	1.51
19	LL	202	CLA	C1D-C2D	2.50	1.48	1.42
19	B	807	CLA	CMB-C2B	-2.50	1.46	1.51
19	BB	815	CLA	C1D-C2D	2.50	1.48	1.42
19	A1	827	CLA	CMB-C2B	-2.50	1.46	1.51
19	BB	845	CLA	CMB-C2B	-2.50	1.46	1.51
19	B2	801	CLA	CMB-C2B	-2.50	1.46	1.51
19	B1	809	CLA	C1D-C2D	2.50	1.48	1.42
24	M2	101	AJP	CDA-CDB	2.50	1.59	1.53
19	AA	845	CLA	C1D-C2D	2.50	1.48	1.42
19	A	840	CLA	C1D-C2D	2.50	1.48	1.42
19	AA	808	CLA	CMB-C2B	-2.50	1.46	1.51
19	A2	808	CLA	CMB-C2B	-2.50	1.46	1.51
19	A	804	CLA	CMB-C2B	-2.50	1.46	1.51
19	A1	823	CLA	C1D-C2D	2.50	1.48	1.42
19	B2	817	CLA	C1D-C2D	2.50	1.48	1.42
19	A1	815	CLA	C1D-C2D	2.50	1.48	1.42
19	B1	822	CLA	C1D-C2D	2.50	1.48	1.42
19	AA	814	CLA	CMB-C2B	-2.50	1.46	1.51
19	A1	841	CLA	C1D-C2D	2.50	1.48	1.42
19	B	804	CLA	CMB-C2B	-2.50	1.46	1.51
19	A2	816	CLA	C1D-C2D	2.50	1.48	1.42
19	A	841	CLA	CMB-C2B	-2.50	1.46	1.51
19	A1	838	CLA	CMB-C2B	-2.50	1.46	1.51
19	AA	840	CLA	C1D-C2D	2.50	1.48	1.42
19	AA	822	CLA	C1D-C2D	2.49	1.48	1.42
19	B	817	CLA	CMB-C2B	-2.49	1.46	1.51
19	A1	839	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	804	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	846	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	835	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	821	CLA	CMD-C2D	-2.49	1.45	1.51
19	A	821	CLA	C1D-C2D	2.49	1.48	1.42
19	A	808	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	841	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	826	CLA	CMB-C2B	-2.49	1.46	1.51
19	BB	806	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	813	CLA	CMB-C2B	-2.49	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	AA	826	CLA	CMB-C2B	-2.49	1.46	1.51
19	B1	803	CLA	C1D-C2D	2.49	1.48	1.42
19	AA	833	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	833	CLA	CMB-C2B	-2.49	1.46	1.51
19	B	859	CLA	C1D-C2D	2.49	1.48	1.42
19	AA	810	CLA	CMB-C2B	-2.49	1.46	1.51
19	A	816	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	813	CLA	CMB-C2B	-2.49	1.46	1.51
19	B2	823	CLA	CMB-C2B	-2.49	1.46	1.51
19	B2	832	CLA	CMB-C2B	-2.49	1.46	1.51
24	L1	203	AJP	OCY-CCX	2.49	1.48	1.41
19	BB	819	CLA	C1D-C2D	2.49	1.48	1.42
19	A	819	CLA	CMB-C2B	-2.49	1.46	1.51
19	A2	844	CLA	CMB-C2B	-2.49	1.46	1.51
19	AA	841	CLA	C1D-C2D	2.49	1.48	1.42
19	A2	806	CLA	C1D-C2D	2.49	1.48	1.42
19	A1	817	CLA	CMB-C2B	-2.49	1.46	1.51
19	K1	105	CLA	C1D-C2D	2.49	1.48	1.42
19	A	832	CLA	C1D-C2D	2.49	1.48	1.42
19	BB	817	CLA	CMB-C2B	-2.49	1.46	1.51
19	B2	815	CLA	C1D-C2D	2.48	1.48	1.42
19	A1	819	CLA	CMD-C2D	-2.48	1.45	1.51
19	BB	815	CLA	CMB-C2B	-2.48	1.46	1.51
19	B1	823	CLA	CMB-C2B	-2.48	1.46	1.51
19	B1	817	CLA	C1D-C2D	2.48	1.48	1.42
19	AA	818	CLA	CMB-C2B	-2.48	1.46	1.51
19	A2	841	CLA	CMB-C2B	-2.48	1.46	1.51
19	AA	819	CLA	CMB-C2B	-2.48	1.46	1.51
19	A1	852	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	815	CLA	C1D-C2D	2.48	1.48	1.42
19	B	801	CLA	CMB-C2B	-2.48	1.46	1.51
19	B2	837	CLA	C1D-C2D	2.48	1.48	1.42
24	L1	203	AJP	CAV-CBE	2.48	1.58	1.53
19	K2	102	CLA	CMB-C2B	-2.48	1.46	1.51
19	B2	813	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	814	CLA	C1D-C2D	2.48	1.48	1.42
19	A2	833	CLA	C1D-C2D	2.48	1.48	1.42
19	A1	829	CLA	CMD-C2D	-2.48	1.45	1.51
19	A	820	CLA	CMD-C2D	-2.48	1.45	1.51
19	A	820	CLA	C3B-C2B	-2.48	1.36	1.40
19	A	828	CLA	CMB-C2B	-2.48	1.46	1.51
19	B2	827	CLA	CMB-C2B	-2.48	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	812	CLA	CMB-C2B	-2.48	1.46	1.51
19	B1	813	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	824	CLA	CMD-C2D	-2.48	1.45	1.51
19	B	823	CLA	CMB-C2B	-2.48	1.46	1.51
19	AA	821	CLA	C1D-C2D	2.48	1.48	1.42
19	B2	803	CLA	C1D-C2D	2.48	1.48	1.42
19	AA	828	CLA	CMB-C2B	-2.48	1.46	1.51
19	B	813	CLA	C1D-C2D	2.48	1.48	1.42
19	BB	809	CLA	C1D-C2D	2.48	1.48	1.42
19	X	101	CLA	C1D-C2D	2.48	1.48	1.42
19	BB	803	CLA	C1D-C2D	2.48	1.48	1.42
19	A2	822	CLA	C1D-C2D	2.48	1.48	1.42
19	A2	814	CLA	CMB-C2B	-2.48	1.46	1.51
19	BB	856	CLA	C1D-C2D	2.48	1.48	1.42
19	A1	804	CLA	C1D-C2D	2.47	1.48	1.42
19	AA	806	CLA	CMB-C2B	-2.47	1.46	1.51
19	A1	812	CLA	CMB-C2B	-2.47	1.46	1.51
19	A2	841	CLA	C1D-C2D	2.47	1.48	1.42
19	A2	820	CLA	CMD-C2D	-2.47	1.45	1.51
19	BB	823	CLA	CMB-C2B	-2.47	1.46	1.51
19	A	817	CLA	C1D-C2D	2.47	1.48	1.42
19	A2	804	CLA	CMD-C2D	-2.47	1.45	1.51
19	A	810	CLA	CMB-C2B	-2.47	1.46	1.51
19	A	806	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	809	CLA	C1D-C2D	2.47	1.48	1.42
19	AA	804	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	803	CLA	C1D-C2D	2.47	1.48	1.42
19	A	852	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	827	CLA	CMD-C2D	-2.47	1.45	1.51
19	BB	818	CLA	CMB-C2B	-2.47	1.46	1.51
24	B	849	AJP	CAW-CBF	2.47	1.56	1.52
19	B1	836	CLA	C1D-C2D	2.47	1.48	1.42
19	A	804	CLA	CMD-C2D	-2.47	1.45	1.51
19	A1	841	CLA	CMB-C2B	-2.47	1.46	1.51
19	A1	832	CLA	CMD-C2D	-2.47	1.45	1.51
19	AA	834	CLA	C1D-C2D	2.47	1.48	1.42
19	B2	820	CLA	CMB-C2B	-2.47	1.46	1.51
19	A1	822	CLA	C1D-C2D	2.47	1.48	1.42
19	XX	101	CLA	C1D-C2D	2.47	1.48	1.42
19	A	841	CLA	C1D-C2D	2.47	1.48	1.42
19	B2	810	CLA	C1D-C2D	2.47	1.48	1.42
19	BB	801	CLA	CMB-C2B	-2.47	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A1	826	CLA	CMB-C2B	-2.47	1.46	1.51
19	B	812	CLA	CMB-C2B	-2.47	1.46	1.51
19	A2	830	CLA	C1D-C2D	2.47	1.48	1.42
19	BB	828	CLA	C1D-C2D	2.47	1.48	1.42
19	A2	813	CLA	CMB-C2B	-2.47	1.46	1.51
19	AA	840	CLA	CMB-C2B	-2.46	1.46	1.51
19	B1	810	CLA	C1D-C2D	2.46	1.48	1.42
24	B	850	AJP	CBF-CBE	2.46	1.58	1.53
19	BB	824	CLA	CMD-C2D	-2.46	1.45	1.51
19	A1	821	CLA	C1D-C2D	2.46	1.48	1.42
19	A2	852	CLA	C1D-C2D	2.46	1.48	1.42
19	B1	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	A2	839	CLA	C1D-C2D	2.46	1.48	1.42
19	A	823	CLA	C1D-C2D	2.46	1.48	1.42
19	JJ	101	CLA	CMB-C2B	-2.46	1.46	1.51
19	L1	207	CLA	CMB-C2B	-2.46	1.46	1.51
24	B	850	AJP	CAV-CBE	2.46	1.58	1.53
19	A2	839	CLA	CMB-C2B	-2.46	1.46	1.51
19	F	302	CLA	C1D-C2D	2.46	1.48	1.42
24	M2	101	AJP	CBF-CBE	2.46	1.58	1.53
19	BB	833	CLA	CMD-C2D	-2.46	1.45	1.51
19	L	203	CLA	C1D-C2D	2.46	1.48	1.42
19	A	839	CLA	CMB-C2B	-2.46	1.46	1.51
19	J	101	CLA	CMB-C2B	-2.46	1.46	1.51
19	A2	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	A1	805	CLA	CMB-C2B	-2.46	1.46	1.51
19	A	805	CLA	CMD-C2D	-2.46	1.45	1.51
19	B1	833	CLA	CMD-C2D	-2.46	1.45	1.51
19	B2	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	B1	848	CLA	CHC-C1C	2.46	1.41	1.35
19	A	818	CLA	CMB-C2B	-2.46	1.46	1.51
24	A1	854	AJP	CBO-CBP	-2.46	1.49	1.53
19	A1	809	CLA	CMB-C2B	-2.46	1.46	1.51
19	F2	302	CLA	C1D-C2D	2.46	1.48	1.42
19	BB	814	CLA	C1D-C2D	2.46	1.48	1.42
19	B	832	CLA	C1D-C2D	2.46	1.48	1.42
19	B	801	CLA	CMD-C2D	-2.46	1.45	1.51
19	BB	812	CLA	C1D-C2D	2.45	1.48	1.42
19	A1	837	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	809	CLA	CMB-C2B	-2.45	1.46	1.51
19	B	819	CLA	C1D-C2D	2.45	1.48	1.42
19	AA	823	CLA	C1D-C2D	2.45	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	838	CLA	CMB-C2B	-2.45	1.46	1.51
19	A	828	CLA	C1D-C2D	2.45	1.48	1.42
19	B	824	CLA	CMB-C2B	-2.45	1.46	1.51
19	B1	827	CLA	CMB-C2B	-2.45	1.46	1.51
19	A2	811	CLA	C1D-C2D	2.45	1.48	1.42
19	A1	840	CLA	C1D-C2D	2.45	1.48	1.42
19	B	806	CLA	CMB-C2B	-2.45	1.46	1.51
19	A1	816	CLA	C1D-C2D	2.45	1.48	1.42
19	BB	826	CLA	C3B-C2B	-2.45	1.37	1.40
19	K	101	CLA	CMB-C2B	-2.45	1.46	1.51
19	AA	824	CLA	C1D-C2D	2.45	1.48	1.42
19	AA	820	CLA	C3B-CAB	-2.45	1.42	1.47
19	B1	806	CLA	C1D-C2D	2.45	1.48	1.42
19	A	827	CLA	C1D-C2D	2.45	1.48	1.42
19	A1	820	CLA	C1D-C2D	2.45	1.48	1.42
19	BB	817	CLA	C1D-C2D	2.45	1.48	1.42
19	B	830	CLA	C1D-C2D	2.45	1.48	1.42
19	A2	821	CLA	C1D-C2D	2.45	1.48	1.42
19	AA	842	CLA	C1D-C2D	2.45	1.48	1.42
19	BB	827	CLA	CMD-C2D	-2.44	1.45	1.51
19	B1	817	CLA	CMB-C2B	-2.44	1.46	1.51
19	AA	820	CLA	CMD-C2D	-2.44	1.45	1.51
19	F1	302	CLA	C1D-C2D	2.44	1.48	1.42
19	B1	848	CLA	CMD-C2D	-2.44	1.45	1.51
19	AA	839	CLA	CMB-C2B	-2.44	1.46	1.51
19	A2	840	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	822	CLA	CMB-C2B	-2.44	1.46	1.51
19	B2	817	CLA	CMB-C2B	-2.44	1.46	1.51
19	B1	812	CLA	CMB-C2B	-2.44	1.46	1.51
19	B	802	CLA	C1D-C2D	2.44	1.48	1.42
19	A1	813	CLA	CMB-C2B	-2.44	1.46	1.51
24	B	857	AJP	CBO-CBP	-2.44	1.49	1.53
24	L	208	AJP	CBF-CBE	2.44	1.58	1.53
19	A2	824	CLA	C1D-C2D	2.44	1.48	1.42
19	B	812	CLA	C1D-C2D	2.44	1.48	1.42
19	B2	835	CLA	CMB-C2B	-2.44	1.46	1.51
19	L2	206	CLA	CMD-C2D	-2.44	1.45	1.51
19	A2	810	CLA	CMB-C2B	-2.44	1.46	1.51
24	L	209	AJP	CDA-CDB	2.44	1.59	1.53
19	B	827	CLA	C1D-C2D	2.44	1.48	1.42
24	AA	802	AJP	CBO-CBP	-2.44	1.49	1.53
19	B	821	CLA	CMD-C2D	-2.43	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	801	CLA	CMC-C2C	-2.43	1.45	1.50
19	B1	835	CLA	CMB-C2B	-2.43	1.46	1.51
22	X1	102	LHG	P-O3	2.43	1.69	1.59
19	A2	831	CLA	C1D-C2D	2.43	1.48	1.42
19	KK	101	CLA	CMB-C2B	-2.43	1.46	1.51
19	AA	830	CLA	C1D-C2D	2.43	1.48	1.42
24	A	802	AJP	CBO-CBP	-2.43	1.49	1.53
19	B1	826	CLA	C1D-C2D	2.43	1.48	1.42
19	A	827	CLA	CMB-C2B	-2.43	1.46	1.51
19	B1	830	CLA	CMB-C2B	-2.43	1.46	1.51
19	B	817	CLA	C1D-C2D	2.43	1.48	1.42
19	B1	824	CLA	C1D-C2D	2.43	1.48	1.42
19	A1	807	CLA	CMD-C2D	-2.43	1.45	1.51
19	B	810	CLA	CMB-C2B	-2.43	1.46	1.51
19	BB	802	CLA	C3B-C2B	-2.43	1.37	1.40
19	AA	804	CLA	CMD-C2D	-2.43	1.45	1.51
19	A	844	CLA	C1D-C2D	2.43	1.48	1.42
19	A1	827	CLA	C1D-C2D	2.43	1.48	1.42
19	AA	801	CLA	CMB-C2B	-2.43	1.46	1.51
19	X1	101	CLA	C1D-C2D	2.43	1.48	1.42
19	B2	824	CLA	CMD-C2D	-2.43	1.45	1.51
19	L	202	CLA	CMD-C2D	-2.43	1.45	1.51
19	B1	829	CLA	C1D-C2D	2.43	1.48	1.42
24	B	850	AJP	CAW-CBF	2.43	1.55	1.52
19	A1	826	CLA	C3B-C2B	-2.42	1.37	1.40
19	A2	806	CLA	CMB-C2B	-2.42	1.46	1.51
19	FF	302	CLA	C1D-C2D	2.42	1.48	1.42
19	J2	101	CLA	CMB-C2B	-2.42	1.46	1.51
19	K	101	CLA	C1D-C2D	2.42	1.48	1.42
19	A1	801	CLA	CMC-C2C	-2.42	1.45	1.50
19	B2	850	CLA	C3B-C2B	-2.42	1.37	1.40
19	A	815	CLA	CMB-C2B	-2.42	1.46	1.51
19	B1	826	CLA	C3B-C2B	-2.42	1.37	1.40
24	A1	854	AJP	CDC-CDB	-2.42	1.46	1.53
19	BB	832	CLA	C3B-C2B	-2.42	1.37	1.40
19	BB	813	CLA	C1D-C2D	2.42	1.48	1.42
19	AA	820	CLA	C3B-C2B	-2.42	1.37	1.40
19	AA	809	CLA	CMB-C2B	-2.42	1.46	1.51
19	A1	815	CLA	CMB-C2B	-2.42	1.46	1.51
19	B1	831	CLA	C3B-C2B	-2.42	1.37	1.40
19	J1	101	CLA	CMB-C2B	-2.42	1.46	1.51
19	KK	101	CLA	C1D-C2D	2.42	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	834	CLA	CMB-C2B	-2.42	1.46	1.51
19	A1	801	CLA	CMB-C2B	-2.42	1.46	1.51
19	B2	850	CLA	C1D-C2D	2.42	1.48	1.42
24	A1	855	AJP	CBO-CBP	-2.42	1.49	1.53
24	K	104	AJP	OCY-CCX	2.42	1.48	1.41
22	X2	102	LHG	P-O3	2.42	1.69	1.59
19	A1	838	CLA	C1D-C2D	2.42	1.48	1.42
19	B1	820	CLA	C1D-C2D	2.41	1.48	1.42
19	B1	822	CLA	CMB-C2B	-2.41	1.46	1.51
19	A	808	CLA	C1D-C2D	2.41	1.48	1.42
19	A2	817	CLA	C1D-C2D	2.41	1.48	1.42
19	B2	812	CLA	CMB-C2B	-2.41	1.46	1.51
19	BB	818	CLA	C1D-C2D	2.41	1.48	1.42
19	BB	855	CLA	C1D-C2D	2.41	1.48	1.42
19	XX	101	CLA	CMB-C2B	-2.41	1.46	1.51
19	BB	852	CLA	CMD-C2D	-2.41	1.45	1.51
19	A1	832	CLA	C1D-C2D	2.41	1.48	1.42
22	B2	848	LHG	P-O3	2.41	1.69	1.59
19	A1	819	CLA	C1D-C2D	2.41	1.48	1.42
19	AA	805	CLA	CMD-C2D	-2.41	1.45	1.51
19	B1	824	CLA	CMD-C2D	-2.41	1.45	1.51
19	A1	828	CLA	CMD-C2D	-2.41	1.45	1.51
19	B	815	CLA	CMB-C2B	-2.41	1.46	1.51
19	AA	820	CLA	C1D-C2D	2.41	1.48	1.42
19	B2	822	CLA	CMD-C2D	-2.41	1.45	1.51
19	A1	830	CLA	C1D-C2D	2.41	1.48	1.42
19	A	827	CLA	CMD-C2D	-2.41	1.45	1.51
19	BB	830	CLA	CMB-C2B	-2.41	1.46	1.51
19	A	811	CLA	C3B-CAB	-2.41	1.43	1.47
19	A	831	CLA	C1D-C2D	2.40	1.48	1.42
19	A	801	CLA	CMB-C2B	-2.40	1.46	1.51
19	LL	202	CLA	C3B-C2B	-2.40	1.37	1.40
19	AA	828	CLA	C1D-C2D	2.40	1.48	1.42
19	B1	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	A2	816	CLA	CMB-C2B	-2.40	1.46	1.51
19	A	820	CLA	C1D-C2D	2.40	1.48	1.42
24	BB	848	AJP	CBD-CBN	2.40	1.58	1.54
24	B	857	AJP	CDC-CDB	-2.40	1.46	1.53
19	A1	830	CLA	CMD-C2D	-2.40	1.45	1.51
19	B	831	CLA	CMB-C2B	-2.40	1.46	1.51
19	AA	815	CLA	CMB-C2B	-2.40	1.46	1.51
19	A2	828	CLA	C1D-C2D	2.40	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	810	CLA	CMB-C2B	-2.40	1.46	1.51
19	A2	831	CLA	CMD-C2D	-2.40	1.45	1.51
19	L1	207	CLA	CMD-C2D	-2.40	1.45	1.51
19	B1	845	CLA	CMB-C2B	-2.40	1.46	1.51
19	B1	848	CLA	C3B-C2B	-2.40	1.37	1.40
19	X	101	CLA	CMB-C2B	-2.40	1.46	1.51
19	X1	101	CLA	CMB-C2B	-2.40	1.46	1.51
19	B1	810	CLA	CMB-C2B	-2.40	1.46	1.51
19	AA	817	CLA	CMB-C2B	-2.40	1.46	1.51
19	BB	832	CLA	C1D-C2D	2.40	1.48	1.42
19	A1	837	CLA	C1D-C2D	2.39	1.48	1.42
19	JJ	103	CLA	CMB-C2B	-2.39	1.46	1.51
19	A2	827	CLA	C1D-C2D	2.39	1.48	1.42
19	BB	828	CLA	CMB-C2B	-2.39	1.46	1.51
19	X2	101	CLA	CMB-C2B	-2.39	1.46	1.51
24	KK	104	AJP	OCY-CCX	2.39	1.48	1.41
19	B2	806	CLA	CMB-C2B	-2.39	1.46	1.51
19	A	817	CLA	CMB-C2B	-2.39	1.46	1.51
19	AA	831	CLA	C1D-C2D	2.39	1.48	1.42
19	B2	801	CLA	CMD-C2D	-2.39	1.45	1.51
19	B1	832	CLA	C1D-C2D	2.39	1.48	1.42
24	A	802	AJP	CAW-CBF	2.39	1.55	1.52
19	AA	827	CLA	CMB-C2B	-2.39	1.46	1.51
19	B2	819	CLA	CMB-C2B	-2.39	1.46	1.51
19	B1	833	CLA	C3B-C2B	-2.39	1.37	1.40
22	A1	845	LHG	O7-C5	-2.39	1.40	1.46
19	BB	827	CLA	C1D-C2D	2.39	1.48	1.42
19	B	828	CLA	CMB-C2B	-2.39	1.46	1.51
19	A2	811	CLA	C3B-CAB	-2.39	1.43	1.47
19	BB	806	CLA	C1D-C2D	2.39	1.48	1.42
19	A	830	CLA	C1D-C2D	2.39	1.48	1.42
24	AA	856	AJP	CDA-CCZ	2.38	1.56	1.52
19	K1	103	CLA	CMB-C2B	-2.38	1.46	1.51
22	XX	102	LHG	P-O3	2.38	1.68	1.59
19	A1	807	CLA	C1D-C2D	2.38	1.48	1.42
19	B2	831	CLA	CMB-C2B	-2.38	1.46	1.51
19	K1	105	CLA	CMB-C2B	-2.38	1.46	1.51
19	B	830	CLA	CMB-C2B	-2.38	1.46	1.51
19	LL	201	CLA	CMD-C2D	-2.38	1.45	1.51
19	B2	846	CLA	CMB-C2B	-2.38	1.46	1.51
19	B2	830	CLA	C1D-C2D	2.38	1.48	1.42
19	J1	103	CLA	CMB-C2B	-2.38	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	810	CLA	CMB-C2B	-2.38	1.46	1.51
19	B1	849	CLA	C1D-C2D	2.38	1.48	1.42
19	AA	805	CLA	C1D-C2D	2.38	1.48	1.42
19	AA	843	CLA	C3B-C2B	-2.38	1.37	1.40
24	AA	802	AJP	CAW-CBF	2.38	1.55	1.52
19	AA	827	CLA	CMD-C2D	-2.38	1.45	1.51
19	A1	825	CLA	C1D-C2D	2.38	1.48	1.42
19	A2	838	CLA	C1D-C2D	2.38	1.48	1.42
19	BB	833	CLA	C3B-CAB	-2.38	1.43	1.47
19	A1	803	CLA	CMD-C2D	-2.38	1.45	1.51
19	A1	840	CLA	CMD-C2D	-2.38	1.45	1.51
19	L	204	CLA	CMD-C2D	-2.38	1.45	1.51
19	B1	818	CLA	CMB-C2B	-2.38	1.46	1.51
19	BB	811	CLA	CMB-C2B	-2.38	1.46	1.51
19	B	833	CLA	C1D-C2D	2.38	1.47	1.42
19	B2	818	CLA	CMB-C2B	-2.37	1.46	1.51
19	B2	826	CLA	C1D-C2D	2.37	1.47	1.42
19	A	801	CLA	CMC-C2C	-2.37	1.45	1.50
19	B2	835	CLA	C1D-C2D	2.37	1.47	1.42
19	B	824	CLA	C1D-C2D	2.37	1.47	1.42
19	B	834	CLA	C3B-CAB	-2.37	1.43	1.47
19	A2	801	CLA	CMB-C2B	-2.37	1.46	1.51
24	A1	855	AJP	CAW-CBF	2.37	1.55	1.52
19	B	819	CLA	CMB-C2B	-2.37	1.46	1.51
19	K2	102	CLA	C1D-C2D	2.37	1.47	1.42
19	KK	102	CLA	CMB-C2B	-2.37	1.46	1.51
24	A	855	AJP	CDA-CCZ	2.37	1.56	1.52
19	A1	852	CLA	C1D-C2D	2.37	1.47	1.42
19	BB	819	CLA	CMB-C2B	-2.37	1.46	1.51
19	B2	806	CLA	C1D-C2D	2.37	1.47	1.42
19	A2	805	CLA	C1D-C2D	2.37	1.47	1.42
19	A2	802	CLA	CMB-C2B	-2.37	1.46	1.51
19	B1	801	CLA	C1D-C2D	2.36	1.47	1.42
19	B2	834	CLA	C3B-CAB	-2.36	1.43	1.47
19	K2	104	CLA	CMB-C2B	-2.36	1.46	1.51
19	AA	836	CLA	C1D-C2D	2.36	1.47	1.42
19	A1	826	CLA	C1D-C2D	2.36	1.47	1.42
19	A	808	CLA	CMD-C2D	-2.36	1.45	1.51
24	A2	854	AJP	CBO-CBP	-2.36	1.49	1.53
19	J	103	CLA	CMB-C2B	-2.36	1.46	1.51
19	A1	835	CLA	C1D-C2D	2.36	1.47	1.42
19	BB	824	CLA	C1D-C2D	2.36	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	L	207	LHG	C6-C5	2.36	1.58	1.50
19	A	836	CLA	C1D-C2D	2.36	1.47	1.42
19	B2	821	CLA	CMD-C2D	-2.36	1.45	1.51
19	A	831	CLA	CMD-C2D	-2.36	1.45	1.51
19	A1	825	CLA	CMD-C2D	-2.36	1.45	1.51
24	L2	202	AJP	OCY-CCX	2.36	1.48	1.41
19	B	822	CLA	C1D-C2D	2.35	1.47	1.42
19	F1	305	CLA	CMB-C2B	-2.35	1.46	1.51
19	BB	801	CLA	CMD-C2D	-2.35	1.45	1.51
19	BB	822	CLA	CMB-C2B	-2.35	1.46	1.51
19	A2	823	CLA	C1D-C2D	2.35	1.47	1.42
19	A2	827	CLA	C3B-C2B	-2.35	1.37	1.40
19	AA	831	CLA	CMD-C2D	-2.35	1.45	1.51
19	A2	833	CLA	CMD-C2D	-2.35	1.45	1.51
19	B	835	CLA	CMD-C2D	-2.35	1.45	1.51
22	LL	205	LHG	C6-C5	2.35	1.58	1.50
24	AA	802	AJP	CBF-CBE	2.35	1.58	1.53
20	A1	802	CL0	C1C-C2C	2.35	1.49	1.44
19	B2	834	CLA	CMD-C2D	-2.35	1.45	1.51
19	A	821	CLA	CMB-C2B	-2.35	1.46	1.51
19	B	810	CLA	C1D-C2D	2.35	1.47	1.42
24	L	208	AJP	CAW-CBF	2.35	1.55	1.52
22	X	102	LHG	P-O3	2.35	1.68	1.59
19	A1	829	CLA	CMB-C2B	-2.35	1.46	1.51
19	B2	824	CLA	C1D-C2D	2.35	1.47	1.42
19	B2	828	CLA	CMB-C2B	-2.35	1.46	1.51
19	L1	206	CLA	C1D-C2D	2.35	1.47	1.42
19	K	102	CLA	CMB-C2B	-2.35	1.46	1.51
19	A2	805	CLA	CMD-C2D	-2.35	1.45	1.51
19	J2	103	CLA	CMB-C2B	-2.35	1.46	1.51
19	AA	808	CLA	C1D-C2D	2.35	1.47	1.42
19	B	805	CLA	CMD-C2D	-2.35	1.45	1.51
24	I2	104	AJP	CAW-CBF	2.35	1.55	1.52
19	A	805	CLA	C1D-C2D	2.34	1.47	1.42
19	A1	836	CLA	CMD-C2D	-2.34	1.45	1.51
19	K1	102	CLA	C1D-C2D	2.34	1.47	1.42
24	M2	101	AJP	CAW-CBF	2.34	1.55	1.52
19	A	827	CLA	C3B-C2B	-2.34	1.37	1.40
22	A	845	LHG	O7-C5	-2.34	1.40	1.46
19	B1	806	CLA	CMB-C2B	-2.34	1.46	1.51
24	B	857	AJP	CAW-CBF	2.34	1.55	1.52
19	B	816	CLA	CMD-C2D	-2.34	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	829	CLA	CMD-C2D	-2.34	1.45	1.51
19	B2	833	CLA	C1D-C2D	2.34	1.47	1.42
19	B1	833	CLA	C3B-CAB	-2.34	1.43	1.47
24	L2	202	AJP	CBF-CBE	2.34	1.58	1.53
19	A1	804	CLA	CMB-C2B	-2.34	1.46	1.51
19	BB	855	CLA	C3B-C2B	-2.34	1.37	1.40
19	A2	830	CLA	CMB-C2B	-2.34	1.46	1.51
20	AA	803	CL0	C4C-C3C	2.34	1.49	1.45
19	B1	821	CLA	CMD-C2D	-2.34	1.45	1.51
19	B1	811	CLA	CMB-C2B	-2.33	1.46	1.51
19	B2	849	CLA	CMD-C2D	-2.33	1.46	1.51
19	B1	836	CLA	CMD-C2D	-2.33	1.46	1.51
19	B1	801	CLA	CMD-C2D	-2.33	1.46	1.51
19	A2	837	CLA	CMD-C2D	-2.33	1.46	1.51
19	A2	804	CLA	CMB-C2B	-2.33	1.46	1.51
19	BB	814	CLA	CMD-C2D	-2.33	1.46	1.51
19	B1	816	CLA	CMD-C2D	-2.33	1.46	1.51
19	B	834	CLA	C3B-C2B	-2.33	1.37	1.40
19	BB	810	CLA	C1D-C2D	2.33	1.47	1.42
19	B1	819	CLA	CMB-C2B	-2.33	1.46	1.51
19	A2	801	CLA	CMD-C2D	-2.33	1.46	1.51
24	BB	849	AJP	CBD-CBN	2.33	1.58	1.54
19	AA	833	CLA	CMD-C2D	-2.33	1.46	1.51
24	A	802	AJP	CBF-CBE	2.33	1.58	1.53
19	L	204	CLA	C1D-C2D	2.33	1.47	1.42
19	B1	824	CLA	C3B-C2B	-2.33	1.37	1.40
19	B	822	CLA	CMD-C2D	-2.33	1.46	1.51
19	A2	827	CLA	CMD-C2D	-2.33	1.46	1.51
19	BB	836	CLA	CMD-C2D	-2.33	1.46	1.51
20	A2	803	CL0	C1C-C2C	2.33	1.49	1.44
19	A	842	CLA	CMD-C2D	-2.33	1.46	1.51
19	B	811	CLA	CMB-C2B	-2.33	1.46	1.51
19	AA	808	CLA	CMD-C2D	-2.32	1.46	1.51
19	A2	833	CLA	C3B-C2B	-2.32	1.37	1.40
19	FF	301	CLA	C1D-C2D	2.32	1.47	1.42
24	L	208	AJP	CDA-CDB	2.32	1.59	1.53
19	A2	828	CLA	CMD-C2D	-2.32	1.46	1.51
19	B	814	CLA	CMD-C2D	-2.32	1.46	1.51
19	A1	842	CLA	CMD-C2D	-2.32	1.46	1.51
22	AA	846	LHG	O7-C5	-2.32	1.40	1.46
19	AA	801	CLA	CMD-C2D	-2.32	1.46	1.51
19	A2	820	CLA	C1D-C2D	2.32	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	826	CLA	C1D-C2D	2.32	1.47	1.42
19	A	829	CLA	CMD-C2D	-2.32	1.46	1.51
19	BB	823	CLA	CMD-C2D	-2.32	1.46	1.51
19	BB	833	CLA	C3B-C2B	-2.32	1.37	1.40
19	A2	836	CLA	C1D-C2D	2.32	1.47	1.42
24	A1	854	AJP	CAW-CBF	2.32	1.55	1.52
19	A1	829	CLA	C1D-C2D	2.32	1.47	1.42
19	B2	837	CLA	CMD-C2D	-2.32	1.46	1.51
19	A	801	CLA	CMD-C2D	-2.32	1.46	1.51
19	B2	811	CLA	CMB-C2B	-2.32	1.46	1.51
19	A1	838	CLA	CMD-C2D	-2.31	1.46	1.51
19	B	854	CLA	CMD-C2D	-2.31	1.46	1.51
19	A2	852	CLA	C3B-C2B	-2.31	1.37	1.40
19	B1	827	CLA	CMD-C2D	-2.31	1.46	1.51
24	L	209	AJP	CBF-CBE	2.31	1.58	1.53
19	A1	814	CLA	CMB-C2B	-2.31	1.46	1.51
19	A	830	CLA	CMB-C2B	-2.31	1.46	1.51
19	B2	823	CLA	C1D-C2D	2.31	1.47	1.42
19	B	836	CLA	CMD-C2D	-2.31	1.46	1.51
19	AA	843	CLA	CMD-C2D	-2.31	1.46	1.51
19	A2	808	CLA	CMD-C2D	-2.31	1.46	1.51
19	FF	301	CLA	CMD-C2D	-2.31	1.46	1.51
19	BB	807	CLA	C1D-C2D	2.31	1.47	1.42
19	B1	823	CLA	C1D-C2D	2.31	1.47	1.42
19	B	823	CLA	C1D-C2D	2.30	1.47	1.42
19	B2	827	CLA	CMD-C2D	-2.30	1.46	1.51
22	L	207	LHG	P-O3	2.30	1.68	1.59
22	LL	205	LHG	P-O3	2.30	1.68	1.59
22	BB	850	LHG	P-O3	2.30	1.68	1.59
19	B2	827	CLA	C3B-C2B	-2.30	1.37	1.40
19	B2	807	CLA	C1D-C2D	2.30	1.47	1.42
19	A	835	CLA	CMD-C2D	-2.30	1.46	1.51
19	B	806	CLA	CMD-C2D	-2.30	1.46	1.51
19	A2	836	CLA	CMD-C2D	-2.30	1.46	1.51
19	A1	810	CLA	C3B-CAB	-2.30	1.43	1.47
19	BB	834	CLA	CMD-C2D	-2.30	1.46	1.51
19	B	807	CLA	C1D-C2D	2.30	1.47	1.42
19	A1	804	CLA	CMD-C2D	-2.30	1.46	1.51
19	B	837	CLA	CMD-C2D	-2.30	1.46	1.51
19	A1	841	CLA	CMD-C2D	-2.30	1.46	1.51
19	B	823	CLA	CMD-C2D	-2.30	1.46	1.51
19	AA	811	CLA	C3B-CAB	-2.30	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	808	CLA	C1D-C2D	2.30	1.47	1.42
19	B	832	CLA	CMD-C2D	-2.30	1.46	1.51
19	A2	841	CLA	CMD-C2D	-2.29	1.46	1.51
19	B	811	CLA	CMD-C2D	-2.29	1.46	1.51
19	A2	842	CLA	CMD-C2D	-2.29	1.46	1.51
19	B2	852	CLA	CMD-C2D	-2.29	1.46	1.51
19	AA	829	CLA	CMD-C2D	-2.29	1.46	1.51
19	B2	816	CLA	CMD-C2D	-2.29	1.46	1.51
19	AA	853	CLA	C3B-C2B	-2.29	1.37	1.40
19	F2	301	CLA	C1D-C2D	2.29	1.47	1.42
19	AA	835	CLA	CMD-C2D	-2.29	1.46	1.51
19	B1	832	CLA	CMB-C2B	-2.29	1.46	1.51
19	K1	105	CLA	CMD-C2D	-2.29	1.46	1.51
19	B2	832	CLA	C3B-C2B	-2.29	1.37	1.40
19	A2	839	CLA	CMD-C2D	-2.29	1.46	1.51
19	A	811	CLA	CMD-C2D	-2.29	1.46	1.51
19	B1	805	CLA	CMD-C2D	-2.29	1.46	1.51
19	AA	824	CLA	CMD-C2D	-2.29	1.46	1.51
19	B2	849	CLA	C3B-C2B	-2.29	1.37	1.40
19	AA	842	CLA	CMD-C2D	-2.29	1.46	1.51
19	B1	835	CLA	CMD-C2D	-2.29	1.46	1.51
19	B2	833	CLA	CMB-C2B	-2.29	1.46	1.51
19	AA	801	CLA	CMC-C2C	-2.29	1.45	1.50
19	BB	827	CLA	C3B-C2B	-2.29	1.37	1.40
19	K2	102	CLA	CMD-C2D	-2.29	1.46	1.51
19	L2	206	CLA	C1D-C2D	2.29	1.47	1.42
19	A1	827	CLA	CMD-C2D	-2.29	1.46	1.51
19	A1	824	CLA	CMD-C2D	-2.29	1.46	1.51
24	A	855	AJP	CBF-CBE	2.28	1.58	1.53
19	B	860	CLA	CMD-C2D	-2.28	1.46	1.51
19	B	837	CLA	CMB-C2B	-2.28	1.46	1.51
19	BB	816	CLA	C3B-C2B	-2.28	1.37	1.40
19	B1	849	CLA	CMD-C2D	-2.28	1.46	1.51
19	A2	842	CLA	CMC-C2C	-2.28	1.45	1.50
19	B1	807	CLA	C1D-C2D	2.28	1.47	1.42
19	A1	801	CLA	CMD-C2D	-2.28	1.46	1.51
19	B	826	CLA	CMD-C2D	-2.28	1.46	1.51
19	B2	852	CLA	C3B-C2B	-2.28	1.37	1.40
19	B1	834	CLA	CMD-C2D	-2.28	1.46	1.51
19	A1	852	CLA	CMD-C2D	-2.28	1.46	1.51
19	B2	826	CLA	C3B-C2B	-2.28	1.37	1.40
20	A2	803	CL0	CHD-C4C	2.28	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A	836	CLA	CMD-C2D	-2.28	1.46	1.51
19	A1	835	CLA	CMD-C2D	-2.28	1.46	1.51
19	B	815	CLA	CMD-C2D	-2.28	1.46	1.51
24	BB	849	AJP	CAW-CBF	2.28	1.55	1.52
19	A1	826	CLA	CMD-C2D	-2.28	1.46	1.51
19	AA	836	CLA	CMD-C2D	-2.28	1.46	1.51
19	B2	850	CLA	CMD-C2D	-2.28	1.46	1.51
24	AA	856	AJP	CBF-CBE	2.28	1.58	1.53
19	B2	805	CLA	CMD-C2D	-2.28	1.46	1.51
19	B2	801	CLA	C1D-C2D	2.28	1.47	1.42
19	AA	821	CLA	CMB-C2B	-2.28	1.46	1.51
22	X2	103	LHG	P-O3	2.27	1.68	1.59
19	BB	832	CLA	CMD-C2D	-2.27	1.46	1.51
19	B	860	CLA	C3B-C2B	-2.27	1.37	1.40
19	B	816	CLA	C3B-C2B	-2.27	1.37	1.40
19	A	852	CLA	C3B-C2B	-2.27	1.37	1.40
19	B1	814	CLA	CMD-C2D	-2.27	1.46	1.51
19	B	819	CLA	CMD-C2D	-2.27	1.46	1.51
19	A2	810	CLA	C3B-C2B	-2.27	1.37	1.40
19	AA	827	CLA	C3B-C2B	-2.27	1.37	1.40
19	A2	830	CLA	CMD-C2D	-2.27	1.46	1.51
19	L1	206	CLA	CMD-C2D	-2.27	1.46	1.51
19	AA	810	CLA	C3B-C2B	-2.27	1.37	1.40
19	AA	819	CLA	CMD-C2D	-2.27	1.46	1.51
19	AA	834	CLA	CMD-C2D	-2.27	1.46	1.51
19	B2	815	CLA	CMD-C2D	-2.27	1.46	1.51
19	K1	102	CLA	CMD-C2D	-2.27	1.46	1.51
24	BB	848	AJP	CBF-CBE	2.27	1.58	1.53
19	L2	205	CLA	CMD-C2D	-2.27	1.46	1.51
19	L2	206	CLA	CMB-C2B	-2.27	1.46	1.51
24	L1	204	AJP	CBF-CBE	2.27	1.58	1.53
24	A	855	AJP	CDC-CDB	-2.27	1.47	1.53
19	B1	818	CLA	CMD-C2D	-2.26	1.46	1.51
22	B	852	LHG	P-O3	2.26	1.68	1.59
19	A2	823	CLA	CMD-C2D	-2.26	1.46	1.51
19	A	828	CLA	CMD-C2D	-2.26	1.46	1.51
24	L	208	AJP	OCD-CCE	-2.26	1.36	1.43
19	A1	822	CLA	CMD-C2D	-2.26	1.46	1.51
19	BB	829	CLA	CMD-C2D	-2.26	1.46	1.51
19	L2	205	CLA	C1D-C2D	2.26	1.47	1.42
19	A1	821	CLA	CMD-C2D	-2.26	1.46	1.51
19	B2	836	CLA	CMD-C2D	-2.26	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	840	CLA	CMD-C2D	-2.26	1.46	1.51
19	B1	822	CLA	CMD-C2D	-2.26	1.46	1.51
19	B	858	CLA	C3B-C2B	-2.26	1.37	1.40
19	A	841	CLA	CMD-C2D	-2.26	1.46	1.51
19	BB	835	CLA	CMD-C2D	-2.26	1.46	1.51
19	BB	823	CLA	C1D-C2D	2.26	1.47	1.42
19	B	827	CLA	C3B-C2B	-2.26	1.37	1.40
19	A1	810	CLA	CMD-C2D	-2.26	1.46	1.51
19	BB	810	CLA	CMD-C2D	-2.26	1.46	1.51
19	B2	834	CLA	C1D-C2D	2.26	1.47	1.42
19	BB	815	CLA	CMD-C2D	-2.26	1.46	1.51
19	B	822	CLA	C3B-C2B	-2.26	1.37	1.40
19	B	826	CLA	CMC-C2C	-2.26	1.46	1.50
19	B1	832	CLA	CMD-C2D	-2.26	1.46	1.51
19	A2	811	CLA	CMD-C2D	-2.26	1.46	1.51
19	AA	811	CLA	CMD-C2D	-2.26	1.46	1.51
19	A	833	CLA	C3B-C2B	-2.26	1.37	1.40
19	B2	829	CLA	CMD-C2D	-2.26	1.46	1.51
19	B	817	CLA	CMD-C2D	-2.25	1.46	1.51
19	BB	822	CLA	CMD-C2D	-2.25	1.46	1.51
19	A	834	CLA	CMD-C2D	-2.25	1.46	1.51
19	BB	822	CLA	C3B-C2B	-2.25	1.37	1.40
24	M2	101	AJP	OCD-CCE	-2.25	1.36	1.43
24	AA	856	AJP	CDC-CDB	-2.25	1.47	1.53
20	AA	803	CL0	CHD-C4C	2.25	1.47	1.41
19	B	833	CLA	CMD-C2D	-2.25	1.46	1.51
19	AA	830	CLA	CMD-C2D	-2.25	1.46	1.51
19	B1	811	CLA	CMD-C2D	-2.25	1.46	1.51
19	AA	839	CLA	CMD-C2D	-2.25	1.46	1.51
22	X1	103	LHG	P-O3	2.25	1.68	1.59
19	A1	801	CLA	C1D-C2D	2.25	1.47	1.42
19	B	802	CLA	CMD-C2D	-2.25	1.46	1.51
19	B2	818	CLA	CMD-C2D	-2.25	1.46	1.51
19	B	804	CLA	CMD-C2D	-2.25	1.46	1.51
19	BB	804	CLA	CMD-C2D	-2.25	1.46	1.51
19	A1	834	CLA	CMD-C2D	-2.25	1.46	1.51
19	F	301	CLA	CMD-C2D	-2.25	1.46	1.51
19	A2	815	CLA	CMB-C2B	-2.25	1.47	1.51
19	B2	814	CLA	CMD-C2D	-2.25	1.46	1.51
19	LL	202	CLA	CMD-C2D	-2.25	1.46	1.51
19	A	833	CLA	CMD-C2D	-2.25	1.46	1.51
22	BB	851	LHG	P-O3	2.25	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	806	CLA	C3B-C2B	-2.25	1.37	1.40
19	B2	805	CLA	C1D-C2D	2.25	1.47	1.42
19	A2	835	CLA	CMD-C2D	-2.25	1.46	1.51
19	FF	302	CLA	CMD-C2D	-2.25	1.46	1.51
19	A1	835	CLA	C3B-C2B	-2.25	1.37	1.40
19	L	203	CLA	C3B-C2B	-2.25	1.37	1.40
24	BB	849	AJP	CBF-CBE	2.25	1.57	1.53
19	A2	822	CLA	CMD-C2D	-2.24	1.46	1.51
19	B	802	CLA	C3B-C2B	-2.24	1.37	1.40
19	AA	841	CLA	CMD-C2D	-2.24	1.46	1.51
19	A2	826	CLA	CMD-C2D	-2.24	1.46	1.51
19	B1	804	CLA	CMD-C2D	-2.24	1.46	1.51
19	A2	824	CLA	CMD-C2D	-2.24	1.46	1.51
19	B1	821	CLA	C1D-C2D	2.24	1.47	1.42
24	L1	204	AJP	CDD-CCI	2.24	1.57	1.53
19	BB	806	CLA	CMD-C2D	-2.24	1.46	1.51
19	A	830	CLA	CMD-C2D	-2.24	1.46	1.51
19	AA	853	CLA	C3B-CAB	-2.24	1.43	1.47
19	B	806	CLA	C1D-C2D	2.24	1.47	1.42
19	F1	301	CLA	C1D-C2D	2.24	1.47	1.42
19	BB	811	CLA	CMD-C2D	-2.24	1.46	1.51
24	KK	104	AJP	CDD-CCI	2.24	1.57	1.53
19	BB	816	CLA	CMD-C2D	-2.24	1.46	1.51
19	B	837	CLA	C3B-C2B	-2.24	1.37	1.40
19	A2	825	CLA	CMD-C2D	-2.24	1.46	1.51
19	BB	829	CLA	C3B-CAB	-2.24	1.43	1.47
19	BB	812	CLA	CMD-C2D	-2.24	1.46	1.51
19	B2	823	CLA	CMD-C2D	-2.24	1.46	1.51
24	L	209	AJP	OCD-CCE	-2.24	1.36	1.43
19	A2	821	CLA	CMB-C2B	-2.24	1.47	1.51
19	B1	803	CLA	CMD-C2D	-2.24	1.46	1.51
19	A1	832	CLA	C3B-C2B	-2.24	1.37	1.40
19	B	810	CLA	CMD-C2D	-2.24	1.46	1.51
19	AA	828	CLA	CMD-C2D	-2.24	1.46	1.51
19	B2	804	CLA	CMD-C2D	-2.24	1.46	1.51
19	B1	827	CLA	C3B-C2B	-2.24	1.37	1.40
19	B	828	CLA	CMD-C2D	-2.24	1.46	1.51
19	A	806	CLA	CMD-C2D	-2.24	1.46	1.51
19	BB	805	CLA	C1D-C2D	2.24	1.47	1.42
19	AA	833	CLA	C3B-C2B	-2.24	1.37	1.40
19	A1	839	CLA	CMD-C2D	-2.24	1.46	1.51
19	AA	842	CLA	CMC-C2C	-2.23	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	805	CLA	CMD-C2D	-2.23	1.46	1.51
19	BB	828	CLA	CMD-C2D	-2.23	1.46	1.51
19	AA	806	CLA	CMD-C2D	-2.23	1.46	1.51
19	A2	810	CLA	CMD-C2D	-2.23	1.46	1.51
19	A2	811	CLA	C3B-C2B	-2.23	1.37	1.40
20	A2	803	CL0	C4C-C3C	2.23	1.48	1.45
19	BB	801	CLA	C1D-C2D	2.23	1.47	1.42
24	L2	203	AJP	CDD-CCI	2.23	1.57	1.53
19	B	803	CLA	CMD-C2D	-2.23	1.46	1.51
19	B	812	CLA	CMD-C2D	-2.23	1.46	1.51
19	B1	849	CLA	C3B-C2B	-2.23	1.37	1.40
19	A2	844	CLA	CMD-C2D	-2.23	1.46	1.51
19	FF	305	CLA	CMD-C2D	-2.23	1.46	1.51
19	A1	842	CLA	C3B-C2B	-2.23	1.37	1.40
19	B1	815	CLA	CMD-C2D	-2.23	1.46	1.51
19	F2	302	CLA	CMD-C2D	-2.23	1.46	1.51
19	AA	810	CLA	CMD-C2D	-2.23	1.46	1.51
19	F	302	CLA	CMD-C2D	-2.22	1.46	1.51
19	A1	809	CLA	CMD-C2D	-2.22	1.46	1.51
19	A1	805	CLA	CMD-C2D	-2.22	1.46	1.51
19	A	839	CLA	CMD-C2D	-2.22	1.46	1.51
19	B	829	CLA	CMD-C2D	-2.22	1.46	1.51
19	AA	809	CLA	CMD-C2D	-2.22	1.46	1.51
19	B2	835	CLA	CMD-C2D	-2.22	1.46	1.51
19	BB	802	CLA	CMD-C2D	-2.22	1.46	1.51
19	AA	837	CLA	CMD-C2D	-2.22	1.46	1.51
19	B2	803	CLA	CMD-C2D	-2.22	1.46	1.51
19	A	810	CLA	CMD-C2D	-2.22	1.46	1.51
19	AA	830	CLA	CMB-C2B	-2.22	1.47	1.51
19	A	837	CLA	CMD-C2D	-2.22	1.46	1.51
19	A	811	CLA	C3B-C2B	-2.22	1.37	1.40
19	A1	805	CLA	C3B-C2B	-2.22	1.37	1.40
19	B	809	CLA	CMD-C2D	-2.22	1.46	1.51
22	L2	208	LHG	P-O3	2.22	1.68	1.59
19	BB	856	CLA	CMD-C2D	-2.22	1.46	1.51
19	KK	101	CLA	CMD-C2D	-2.22	1.46	1.51
19	L1	207	CLA	C1D-C2D	2.22	1.47	1.42
19	A1	814	CLA	CMD-C2D	-2.22	1.46	1.51
19	BB	803	CLA	CMD-C2D	-2.22	1.46	1.51
19	K	101	CLA	CMD-C2D	-2.22	1.46	1.51
22	X2	102	LHG	P-O6	2.22	1.68	1.59
19	A2	837	CLA	C3B-C2B	-2.22	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	811	CLA	CMD-C2D	-2.22	1.46	1.51
19	B	821	CLA	C1D-C2D	2.22	1.47	1.42
19	BB	831	CLA	C3B-CAB	-2.22	1.43	1.47
19	B1	828	CLA	CMD-C2D	-2.21	1.46	1.51
19	A	815	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	809	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	855	CLA	CMD-C2D	-2.21	1.46	1.51
19	B	858	CLA	CMD-C2D	-2.21	1.46	1.51
19	B2	821	CLA	C1D-C2D	2.21	1.47	1.42
19	AA	821	CLA	CMD-C2D	-2.21	1.46	1.51
19	B2	821	CLA	CMB-C2B	-2.21	1.47	1.51
19	A	821	CLA	CMD-C2D	-2.21	1.46	1.51
19	A2	852	CLA	CMD-C2D	-2.21	1.46	1.51
19	AA	822	CLA	CMD-C2D	-2.21	1.46	1.51
19	A	814	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	817	CLA	CMD-C2D	-2.21	1.46	1.51
19	A2	806	CLA	CMD-C2D	-2.21	1.46	1.51
19	B1	824	CLA	C3B-CAB	-2.21	1.43	1.47
19	B	825	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	825	CLA	CMD-C2D	-2.21	1.46	1.51
22	AA	846	LHG	P-O3	2.21	1.68	1.59
19	B	859	CLA	CMD-C2D	-2.21	1.46	1.51
19	AA	815	CLA	CMD-C2D	-2.21	1.46	1.51
19	A	819	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	813	CLA	CMD-C2D	-2.21	1.46	1.51
19	B2	810	CLA	CMD-C2D	-2.21	1.46	1.51
19	A2	815	CLA	CMD-C2D	-2.21	1.46	1.51
19	AA	823	CLA	CMD-C2D	-2.21	1.46	1.51
19	A	823	CLA	CMD-C2D	-2.21	1.46	1.51
19	B1	850	CLA	CMD-C2D	-2.21	1.46	1.51
19	B2	851	CLA	CMD-C2D	-2.21	1.46	1.51
19	B1	821	CLA	CMB-C2B	-2.21	1.47	1.51
19	A1	841	CLA	CMC-C2C	-2.21	1.46	1.50
19	A2	814	CLA	CMD-C2D	-2.21	1.46	1.51
19	BB	830	CLA	CMD-C2D	-2.21	1.46	1.51
19	B1	810	CLA	CMD-C2D	-2.21	1.46	1.51
19	A	801	CLA	C1D-C2D	2.21	1.47	1.42
19	A1	820	CLA	CMD-C2D	-2.21	1.46	1.51
19	B2	806	CLA	CMD-C2D	-2.20	1.46	1.51
19	BB	821	CLA	C1D-C2D	2.20	1.47	1.42
19	F1	302	CLA	CMD-C2D	-2.20	1.46	1.51
19	BB	819	CLA	CMD-C2D	-2.20	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B2	830	CLA	CMD-C2D	-2.20	1.46	1.51
19	B	854	CLA	C1D-C2D	2.20	1.47	1.42
19	AA	814	CLA	CMD-C2D	-2.20	1.46	1.51
19	BB	856	CLA	C3B-C2B	-2.20	1.37	1.40
19	BB	822	CLA	C1D-C2D	2.20	1.47	1.42
19	A2	821	CLA	CMD-C2D	-2.20	1.46	1.51
19	B2	833	CLA	CMD-C2D	-2.20	1.46	1.51
19	B1	823	CLA	CMD-C2D	-2.20	1.46	1.51
19	B1	817	CLA	CMD-C2D	-2.20	1.46	1.51
24	I2	104	AJP	OCD-CCE	-2.20	1.36	1.43
19	A1	823	CLA	CMD-C2D	-2.20	1.46	1.51
19	B2	850	CLA	C3B-CAB	-2.20	1.43	1.47
19	A2	836	CLA	CMC-C2C	-2.20	1.46	1.50
20	AA	803	CL0	C1C-C2C	2.20	1.48	1.44
19	AA	840	CLA	CMD-C2D	-2.20	1.46	1.51
19	B2	814	CLA	C3B-C2B	-2.20	1.37	1.40
19	BB	829	CLA	C3B-C2B	-2.20	1.37	1.40
23	B1	843	BCR	C38-C26	-2.20	1.47	1.50
19	AA	813	CLA	CMD-C2D	-2.20	1.46	1.51
19	A1	820	CLA	CMB-C2B	-2.20	1.47	1.51
19	A1	837	CLA	CMD-C2D	-2.20	1.46	1.51
19	A	852	CLA	C3B-CAB	-2.20	1.43	1.47
19	A	825	CLA	CMD-C2D	-2.20	1.46	1.51
19	A2	817	CLA	CMD-C2D	-2.20	1.46	1.51
22	X1	102	LHG	P-O6	2.20	1.68	1.59
19	A1	816	CLA	CMD-C2D	-2.19	1.46	1.51
19	B	808	CLA	CMD-C2D	-2.19	1.46	1.51
19	B1	819	CLA	CMD-C2D	-2.19	1.46	1.51
19	AA	825	CLA	CMD-C2D	-2.19	1.46	1.51
19	XX	101	CLA	CMD-C2D	-2.19	1.46	1.51
19	B	830	CLA	CMD-C2D	-2.19	1.46	1.51
19	A1	809	CLA	C3B-C2B	-2.19	1.37	1.40
19	A1	818	CLA	CMD-C2D	-2.19	1.46	1.51
19	A	809	CLA	CMD-C2D	-2.19	1.46	1.51
19	A2	836	CLA	C3B-C2B	-2.19	1.37	1.40
24	K	104	AJP	CDD-CCI	2.19	1.57	1.53
24	BB	849	AJP	OCY-CCX	2.19	1.48	1.41
19	A	813	CLA	CMD-C2D	-2.19	1.46	1.51
19	A	840	CLA	CMD-C2D	-2.19	1.46	1.51
19	A2	801	CLA	C1D-C2D	2.19	1.47	1.42
19	A2	834	CLA	CMD-C2D	-2.19	1.46	1.51
22	B	853	LHG	P-O3	2.19	1.68	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B2	844	BCR	C38-C26	-2.19	1.47	1.50
19	B	831	CLA	CMD-C2D	-2.19	1.46	1.51
19	B	801	CLA	C1D-C2D	2.19	1.47	1.42
19	A1	812	CLA	CMD-C2D	-2.19	1.46	1.51
19	B1	808	CLA	CMD-C2D	-2.19	1.46	1.51
19	X	101	CLA	CMD-C2D	-2.19	1.46	1.51
19	A2	838	CLA	CMD-C2D	-2.19	1.46	1.51
24	I2	104	AJP	CBF-CBE	2.19	1.57	1.53
19	B1	805	CLA	C1D-C2D	2.19	1.47	1.42
19	B2	819	CLA	CMD-C2D	-2.19	1.46	1.51
19	A1	833	CLA	CMD-C2D	-2.19	1.46	1.51
19	B	813	CLA	CMD-C2D	-2.19	1.46	1.51
19	A	844	CLA	CMD-C2D	-2.19	1.46	1.51
19	AA	806	CLA	C3B-C2B	-2.19	1.37	1.40
19	A1	835	CLA	CMC-C2C	-2.18	1.46	1.50
19	L	203	CLA	CMD-C2D	-2.18	1.46	1.51
19	B	859	CLA	C3B-C2B	-2.18	1.37	1.40
24	A	855	AJP	CAW-CBF	2.18	1.55	1.52
19	A2	806	CLA	CMC-C2C	-2.18	1.46	1.50
19	A	812	CLA	CMD-C2D	-2.18	1.46	1.51
19	B1	809	CLA	CMD-C2D	-2.18	1.46	1.51
24	AA	856	AJP	CAW-CBF	2.18	1.55	1.52
19	A2	813	CLA	CMD-C2D	-2.18	1.46	1.51
19	A1	810	CLA	C3B-C2B	-2.18	1.37	1.40
19	K1	103	CLA	CMD-C2D	-2.18	1.46	1.51
19	AA	812	CLA	CMD-C2D	-2.18	1.46	1.51
19	A1	811	CLA	CMD-C2D	-2.18	1.46	1.51
19	AA	836	CLA	CMC-C2C	-2.18	1.46	1.50
19	B2	809	CLA	CMD-C2D	-2.18	1.46	1.51
22	A1	845	LHG	P-O3	2.18	1.68	1.59
24	L	209	AJP	CAW-CBF	2.18	1.55	1.52
19	B2	820	CLA	CMD-C2D	-2.18	1.46	1.51
19	F1	301	CLA	C3B-C2B	-2.18	1.37	1.40
19	B2	817	CLA	CMD-C2D	-2.18	1.46	1.51
19	B1	829	CLA	CMD-C2D	-2.18	1.46	1.51
19	AA	811	CLA	C3B-C2B	-2.18	1.37	1.40
19	B1	806	CLA	CMD-C2D	-2.17	1.46	1.51
24	L1	203	AJP	CBD-CBN	2.17	1.58	1.54
19	B	846	CLA	CMD-C2D	-2.17	1.46	1.51
24	BB	848	AJP	CAW-CBF	2.17	1.55	1.52
22	B1	847	LHG	P-O3	2.17	1.68	1.59
19	B2	825	CLA	CMD-C2D	-2.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	BB	808	CLA	CMD-C2D	-2.17	1.46	1.51
19	A	818	CLA	CMD-C2D	-2.17	1.46	1.51
19	F1	301	CLA	CMD-C2D	-2.17	1.46	1.51
26	B	841	ECH	C1-C6	-2.17	1.50	1.53
19	A2	802	CLA	CMD-C2D	-2.17	1.46	1.51
19	A	826	CLA	CMD-C2D	-2.17	1.46	1.51
19	BB	833	CLA	C1D-C2D	2.17	1.47	1.42
19	A2	819	CLA	CMD-C2D	-2.17	1.46	1.51
19	B2	808	CLA	CMD-C2D	-2.17	1.46	1.51
19	A2	812	CLA	CMD-C2D	-2.17	1.46	1.51
19	BB	802	CLA	C3B-CAB	-2.17	1.43	1.47
19	B2	827	CLA	C3B-CAB	-2.17	1.43	1.47
19	A2	821	CLA	CMC-C2C	-2.17	1.46	1.50
19	B2	828	CLA	CMD-C2D	-2.17	1.46	1.51
19	X1	101	CLA	CMD-C2D	-2.17	1.46	1.51
19	AA	818	CLA	CMD-C2D	-2.17	1.46	1.51
19	B1	820	CLA	CMD-C2D	-2.17	1.46	1.51
19	AA	804	CLA	C1D-C2D	2.17	1.47	1.42
19	A1	826	CLA	C3B-CAB	-2.17	1.43	1.47
19	KK	102	CLA	CMD-C2D	-2.17	1.46	1.51
19	A	842	CLA	C3B-C2B	-2.17	1.37	1.40
19	B	821	CLA	CMB-C2B	-2.16	1.47	1.51
19	B1	825	CLA	CMD-C2D	-2.16	1.46	1.51
19	A2	852	CLA	C3B-CAB	-2.16	1.43	1.47
19	A	836	CLA	CMC-C2C	-2.16	1.46	1.50
19	BB	836	CLA	C3B-C2B	-2.16	1.37	1.40
19	F1	305	CLA	CMD-C2D	-2.16	1.46	1.51
22	A	845	LHG	P-O3	2.16	1.68	1.59
20	A	803	CL0	CHD-C4C	2.16	1.47	1.41
19	F	301	CLA	C1D-C2D	2.16	1.47	1.42
19	A1	803	CLA	C1D-C2D	2.16	1.47	1.42
19	A2	829	CLA	C3B-CAB	-2.16	1.43	1.47
19	JJ	103	CLA	CMD-C2D	-2.16	1.46	1.51
19	BB	845	CLA	CMD-C2D	-2.16	1.46	1.51
20	A1	802	CL0	CHD-C4C	2.16	1.47	1.41
19	B1	813	CLA	CMD-C2D	-2.15	1.46	1.51
19	AA	817	CLA	CMD-C2D	-2.15	1.46	1.51
19	X2	101	CLA	CMD-C2D	-2.15	1.46	1.51
19	A2	827	CLA	C3B-CAB	-2.15	1.43	1.47
24	B	850	AJP	OCY-CCX	2.15	1.47	1.41
19	B2	813	CLA	CMD-C2D	-2.15	1.46	1.51
19	B	823	CLA	CMC-C2C	-2.15	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	K	104	AJP	CBF-CBE	2.15	1.57	1.53
19	A2	825	CLA	C3B-C2B	-2.15	1.37	1.40
19	A1	844	CLA	CMD-C2D	-2.15	1.46	1.51
19	B2	802	CLA	CMD-C2D	-2.15	1.46	1.51
19	J	101	CLA	CMD-C2D	-2.15	1.46	1.51
19	B1	802	CLA	CMD-C2D	-2.15	1.46	1.51
19	JJ	101	CLA	CMD-C2D	-2.15	1.46	1.51
19	A	817	CLA	CMD-C2D	-2.15	1.46	1.51
19	A2	818	CLA	CMD-C2D	-2.15	1.46	1.51
19	A1	810	CLA	CMC-C2C	-2.15	1.46	1.50
19	A	852	CLA	CMD-C2D	-2.15	1.46	1.51
19	B1	829	CLA	C3B-CAB	-2.15	1.43	1.47
19	K	102	CLA	CMD-C2D	-2.15	1.46	1.51
24	L2	202	AJP	CAW-CBF	2.15	1.55	1.52
19	AA	845	CLA	CMD-C2D	-2.15	1.46	1.51
22	A2	846	LHG	P-O3	2.15	1.68	1.59
19	A2	816	CLA	CMD-C2D	-2.15	1.46	1.51
19	A1	815	CLA	CMD-C2D	-2.15	1.46	1.51
19	B	805	CLA	C1D-C2D	2.14	1.47	1.42
19	A1	817	CLA	CMD-C2D	-2.14	1.46	1.51
19	B2	822	CLA	C3B-C2B	-2.14	1.37	1.40
19	A	810	CLA	C3B-C2B	-2.14	1.37	1.40
19	J	103	CLA	CMD-C2D	-2.14	1.46	1.51
19	A	806	CLA	C3B-C2B	-2.14	1.37	1.40
23	B	844	BCR	C38-C26	-2.14	1.47	1.50
19	AA	838	CLA	CMD-C2D	-2.14	1.46	1.51
19	F2	301	CLA	CMD-C2D	-2.14	1.46	1.51
19	B1	812	CLA	CMD-C2D	-2.14	1.46	1.51
19	A	816	CLA	CMD-C2D	-2.14	1.46	1.51
24	A2	854	AJP	CBD-CBN	2.14	1.58	1.54
19	BB	852	CLA	C3B-C2B	-2.14	1.37	1.40
19	B2	812	CLA	CMD-C2D	-2.14	1.46	1.51
19	L1	205	CLA	CMD-C2D	-2.14	1.46	1.51
19	B	832	CLA	C3B-CAB	-2.14	1.43	1.47
19	A1	820	CLA	CMC-C2C	-2.14	1.46	1.50
19	A1	813	CLA	CMD-C2D	-2.14	1.46	1.51
19	BB	820	CLA	CMD-C2D	-2.14	1.46	1.51
19	A	838	CLA	CMD-C2D	-2.14	1.46	1.51
19	AA	829	CLA	C1D-C2D	2.14	1.47	1.42
19	L2	204	CLA	CMD-C2D	-2.14	1.46	1.51
19	A1	808	CLA	CMD-C2D	-2.14	1.46	1.51
20	A	803	CL0	C1C-C2C	2.13	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A2	845	LHG	P-O3	2.13	1.67	1.59
19	A2	809	CLA	CMD-C2D	-2.13	1.46	1.51
19	B	806	CLA	CMC-C2C	-2.13	1.46	1.50
19	BB	803	CLA	CMC-C2C	-2.13	1.46	1.50
19	AA	801	CLA	C1D-C2D	2.13	1.47	1.42
19	AA	816	CLA	CMD-C2D	-2.13	1.46	1.51
19	A1	806	CLA	CMD-C2D	-2.13	1.46	1.51
24	L	209	AJP	CBD-CBN	2.13	1.58	1.54
19	A	807	CLA	CMD-C2D	-2.13	1.46	1.51
19	J1	103	CLA	CMD-C2D	-2.13	1.46	1.51
19	A2	823	CLA	C3B-C2B	-2.13	1.37	1.40
22	A1	846	LHG	P-O3	2.13	1.67	1.59
19	B1	816	CLA	C3B-C2B	-2.13	1.37	1.40
19	A	807	CLA	C3B-C2B	-2.13	1.37	1.40
24	B	857	AJP	OCY-CCX	2.13	1.47	1.41
19	B	804	CLA	C3B-C2B	-2.13	1.37	1.40
19	B	803	CLA	CMC-C2C	-2.13	1.46	1.50
19	A1	828	CLA	C1D-C2D	2.12	1.47	1.42
19	J2	103	CLA	CMD-C2D	-2.12	1.46	1.51
24	KK	104	AJP	CBF-CBE	2.12	1.57	1.53
19	A	824	CLA	CMD-C2D	-2.12	1.46	1.51
19	J1	101	CLA	CMD-C2D	-2.12	1.46	1.51
19	A	842	CLA	CMC-C2C	-2.12	1.46	1.50
22	AA	847	LHG	P-O3	2.12	1.67	1.59
24	A1	854	AJP	OCY-CCX	2.12	1.47	1.41
19	A1	852	CLA	C3B-CAB	-2.12	1.43	1.47
19	AA	807	CLA	CMD-C2D	-2.12	1.46	1.51
19	K2	104	CLA	CMD-C2D	-2.12	1.46	1.51
19	J2	101	CLA	CMD-C2D	-2.12	1.46	1.51
19	AA	836	CLA	C3B-C2B	-2.12	1.37	1.40
19	BB	831	CLA	CMD-C2D	-2.12	1.46	1.51
19	A2	832	CLA	CMD-C2D	-2.12	1.46	1.51
19	B1	822	CLA	C3B-C2B	-2.12	1.37	1.40
19	A2	829	CLA	C1D-C2D	2.12	1.47	1.42
19	B1	805	CLA	CMC-C2C	-2.12	1.46	1.50
19	BB	832	CLA	C3B-CAB	-2.12	1.43	1.47
19	A2	820	CLA	CMC-C2C	-2.12	1.46	1.50
19	AA	853	CLA	CMD-C2D	-2.12	1.46	1.51
19	A2	807	CLA	CMD-C2D	-2.11	1.46	1.51
19	AA	832	CLA	CMD-C2D	-2.11	1.46	1.51
24	L2	203	AJP	CBO-CBP	-2.11	1.50	1.53
19	A	821	CLA	CMC-C2C	-2.11	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B1	831	CLA	CMD-C2D	-2.11	1.46	1.51
19	BB	804	CLA	C3B-C2B	-2.11	1.37	1.40
24	A1	855	AJP	CCK-CBP	2.11	1.57	1.52
19	AA	842	CLA	C3B-C2B	-2.11	1.37	1.40
19	AA	807	CLA	C3B-C2B	-2.11	1.37	1.40
19	F	301	CLA	C3B-C2B	-2.11	1.37	1.40
24	A2	854	AJP	CCK-CBP	2.11	1.57	1.52
19	AA	830	CLA	CMC-C2C	-2.11	1.46	1.50
19	A	804	CLA	C1D-C2D	2.11	1.47	1.42
19	A2	804	CLA	CMC-C2C	-2.11	1.46	1.50
19	B2	819	CLA	CMC-C2C	-2.11	1.46	1.50
19	B	820	CLA	CMD-C2D	-2.11	1.46	1.51
19	BB	820	CLA	C3B-C2B	-2.11	1.37	1.40
26	B1	840	ECH	C1-C6	-2.11	1.50	1.53
23	FF	306	BCR	C33-C5	-2.11	1.47	1.50
19	B2	830	CLA	C3B-CAB	-2.11	1.43	1.47
19	AA	826	CLA	CMD-C2D	-2.11	1.46	1.51
19	A2	804	CLA	C1D-C2D	2.10	1.47	1.42
19	B2	832	CLA	CMD-C2D	-2.10	1.46	1.51
19	BB	826	CLA	CMC-C2C	-2.10	1.46	1.50
19	B1	850	CLA	C3B-C2B	-2.10	1.37	1.40
19	B	830	CLA	CMC-C2C	-2.10	1.46	1.50
19	A2	833	CLA	CMC-C2C	-2.10	1.46	1.50
22	XX	102	LHG	P-O6	2.10	1.67	1.59
19	AA	833	CLA	CMC-C2C	-2.10	1.46	1.50
23	F	305	BCR	C33-C5	-2.10	1.47	1.50
19	B2	836	CLA	C3B-C2B	-2.10	1.37	1.40
19	B1	829	CLA	C3B-C2B	-2.10	1.37	1.40
19	A	832	CLA	CMD-C2D	-2.10	1.46	1.51
19	A1	824	CLA	C3B-C2B	-2.10	1.37	1.40
19	B1	805	CLA	C3B-C2B	-2.10	1.37	1.40
19	B1	829	CLA	CMC-C2C	-2.10	1.46	1.50
19	A	832	CLA	CMC-C2C	-2.10	1.46	1.50
23	BB	843	BCR	C38-C26	-2.10	1.47	1.50
19	B1	826	CLA	CMC-C2C	-2.10	1.46	1.50
19	B	813	CLA	C3B-C2B	-2.10	1.37	1.40
19	A	836	CLA	C3B-C2B	-2.10	1.37	1.40
24	BB	849	AJP	CDD-CCI	2.10	1.57	1.53
24	A	802	AJP	CBD-CBN	2.09	1.58	1.54
19	B	818	CLA	CMD-C2D	-2.09	1.46	1.51
19	F2	301	CLA	C3B-C2B	-2.09	1.37	1.40
19	BB	806	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	A	846	LHG	P-O3	2.09	1.67	1.59
26	B2	841	ECH	C1-C6	-2.09	1.51	1.53
19	A1	836	CLA	C3B-C2B	-2.09	1.37	1.40
19	B1	833	CLA	C1D-C2D	2.09	1.47	1.42
19	A1	831	CLA	CMC-C2C	-2.09	1.46	1.50
19	B2	805	CLA	C3B-C2B	-2.09	1.37	1.40
19	B2	850	CLA	CMC-C2C	-2.09	1.46	1.50
19	BB	856	CLA	C3B-CAB	-2.09	1.43	1.47
19	A1	831	CLA	CMD-C2D	-2.09	1.46	1.51
19	B2	846	CLA	CMD-C2D	-2.09	1.46	1.51
19	B1	848	CLA	C1D-C2D	2.09	1.47	1.42
19	B2	831	CLA	CMD-C2D	-2.09	1.46	1.51
19	BB	805	CLA	C3B-C2B	-2.09	1.37	1.40
19	B	833	CLA	C3B-C2B	-2.09	1.37	1.40
19	A2	811	CLA	CMC-C2C	-2.08	1.46	1.50
24	AA	802	AJP	CBD-CBN	2.08	1.58	1.54
19	BB	808	CLA	C3B-C2B	-2.08	1.37	1.40
19	BB	852	CLA	C1D-C2D	2.08	1.47	1.42
19	A	811	CLA	CMC-C2C	-2.08	1.46	1.50
19	A1	852	CLA	C3B-C2B	-2.08	1.37	1.40
19	A	829	CLA	C1D-C2D	2.08	1.47	1.42
19	A	822	CLA	CMD-C2D	-2.08	1.46	1.51
24	L1	204	AJP	CBO-CBP	-2.08	1.50	1.53
19	B	854	CLA	CMC-C2C	-2.08	1.46	1.50
19	L1	206	CLA	C3B-C2B	-2.08	1.37	1.40
19	B1	845	CLA	CMD-C2D	-2.08	1.46	1.51
19	LL	202	CLA	C3B-CAB	-2.08	1.43	1.47
19	B2	849	CLA	C1D-C2D	2.08	1.47	1.42
19	A	833	CLA	CMC-C2C	-2.08	1.46	1.50
19	A2	829	CLA	CMC-C2C	-2.07	1.46	1.50
19	B1	803	CLA	C3B-C2B	-2.07	1.37	1.40
19	B2	804	CLA	C3B-C2B	-2.07	1.37	1.40
19	A1	806	CLA	C3B-C2B	-2.07	1.37	1.40
22	B2	848	LHG	P-O6	2.07	1.67	1.59
19	B	805	CLA	C3B-C2B	-2.07	1.37	1.40
19	AA	821	CLA	CMC-C2C	-2.07	1.46	1.50
22	BB	851	LHG	P-O6	2.07	1.67	1.59
19	B	859	CLA	C3B-CAB	-2.07	1.43	1.47
19	A2	807	CLA	C3B-C2B	-2.07	1.37	1.40
19	B1	806	CLA	CMC-C2C	-2.07	1.46	1.50
19	A	819	CLA	CMC-C2C	-2.07	1.46	1.50
19	B2	830	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	A2	832	CLA	CMC-C2C	-2.07	1.46	1.50
19	B2	836	CLA	CMC-C2C	-2.07	1.46	1.50
19	A2	835	CLA	C3B-C2B	-2.07	1.37	1.40
19	A	829	CLA	C3B-CAB	-2.07	1.43	1.47
22	X	102	LHG	P-O6	2.07	1.67	1.59
19	A1	819	CLA	CMC-C2C	-2.07	1.46	1.50
19	B2	820	CLA	C3B-C2B	-2.06	1.37	1.40
19	A2	831	CLA	C3B-CAB	-2.06	1.43	1.47
19	B1	835	CLA	C3B-C2B	-2.06	1.37	1.40
22	L1	211	LHG	O7-C5	-2.06	1.41	1.46
19	B	816	CLA	C3B-CAB	-2.06	1.43	1.47
19	J	103	CLA	C3B-C2B	-2.06	1.37	1.40
19	B1	849	CLA	CMC-C2C	-2.06	1.46	1.50
19	A2	825	CLA	CMC-C2C	-2.06	1.46	1.50
19	A2	826	CLA	CMC-C2C	-2.06	1.46	1.50
19	BB	814	CLA	C3B-C2B	-2.06	1.37	1.40
19	B	809	CLA	C3B-C2B	-2.06	1.37	1.40
19	A1	832	CLA	CMC-C2C	-2.06	1.46	1.50
19	B1	830	CLA	CMD-C2D	-2.06	1.46	1.51
24	K	104	AJP	CBD-CBN	2.06	1.58	1.54
19	B2	851	CLA	C3B-C2B	-2.06	1.37	1.40
19	A2	835	CLA	CMC-C2C	-2.06	1.46	1.50
19	A1	834	CLA	CMC-C2C	-2.06	1.46	1.50
24	B	857	AJP	CCK-CBP	2.06	1.57	1.52
23	MM	101	BCR	C33-C5	-2.06	1.47	1.50
19	A2	819	CLA	CMC-C2C	-2.06	1.46	1.50
19	AA	820	CLA	CMC-C2C	-2.06	1.46	1.50
22	L	207	LHG	P-O6	2.06	1.67	1.59
22	LL	205	LHG	P-O6	2.06	1.67	1.59
19	BB	824	CLA	C3B-C2B	-2.06	1.37	1.40
19	B1	821	CLA	C3B-CAB	-2.05	1.43	1.47
19	AA	806	CLA	C3B-CAB	-2.05	1.43	1.47
19	B1	804	CLA	C3B-C2B	-2.05	1.37	1.40
19	BB	814	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	834	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	823	CLA	CMC-C2C	-2.05	1.46	1.50
25	I2	105	LMG	C4-C5	2.05	1.57	1.53
19	BB	816	CLA	C3B-CAB	-2.05	1.43	1.47
19	A	826	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	811	CLA	CMC-C2C	-2.05	1.46	1.50
24	A1	854	AJP	CBD-CBN	2.05	1.58	1.54
19	A1	834	CLA	C3B-C2B	-2.05	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	B	805	CLA	CMC-C2C	-2.05	1.46	1.50
19	BB	835	CLA	C3B-C2B	-2.04	1.37	1.40
19	B	834	CLA	C1D-C2D	2.04	1.47	1.42
19	B	811	CLA	CMC-C2C	-2.04	1.46	1.50
19	B1	803	CLA	C3B-CAB	-2.04	1.43	1.47
23	M	101	BCR	C33-C5	-2.04	1.47	1.50
23	K2	103	BCR	C33-C5	-2.04	1.47	1.50
24	B	850	AJP	CDD-CCI	2.04	1.57	1.53
19	BB	814	CLA	C3B-CAB	-2.04	1.43	1.47
19	B1	802	CLA	C3B-C2B	-2.04	1.37	1.40
19	BB	804	CLA	CMC-C2C	-2.04	1.46	1.50
19	BB	827	CLA	CMC-C2C	-2.04	1.46	1.50
19	BB	805	CLA	CMC-C2C	-2.04	1.46	1.50
19	BB	828	CLA	CMC-C2C	-2.03	1.46	1.50
24	A1	855	AJP	CBD-CBN	2.03	1.58	1.54
19	A	830	CLA	CMC-C2C	-2.03	1.46	1.50
19	AA	840	CLA	CMC-C2C	-2.03	1.46	1.50
19	B2	803	CLA	CMC-C2C	-2.03	1.46	1.50
19	AA	853	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	854	CLA	C3B-C2B	-2.03	1.37	1.40
20	A1	802	CL0	C4C-C3C	2.03	1.48	1.45
19	B	814	CLA	CMC-C2C	-2.03	1.46	1.50
24	L	208	AJP	CCF-CCG	2.03	1.57	1.54
19	A	827	CLA	CMC-C2C	-2.03	1.46	1.50
19	A	852	CLA	CMC-C2C	-2.03	1.46	1.50
19	A2	806	CLA	C3B-CAB	-2.03	1.43	1.47
19	B2	816	CLA	C3B-C2B	-2.03	1.37	1.40
19	A2	834	CLA	CMC-C2C	-2.03	1.46	1.50
19	AA	834	CLA	CMC-C2C	-2.03	1.46	1.50
19	B	802	CLA	C3B-CAB	-2.03	1.43	1.47
19	BB	822	CLA	CMC-C2C	-2.03	1.46	1.50
19	A1	841	CLA	C3B-C2B	-2.03	1.37	1.40
19	A1	833	CLA	CMC-C2C	-2.03	1.46	1.50
19	B1	848	CLA	CMC-C2C	-2.03	1.46	1.50
22	L1	211	LHG	P-O6	2.03	1.67	1.59
19	B1	803	CLA	CMC-C2C	-2.03	1.46	1.50
19	BB	855	CLA	CMC-C2C	-2.03	1.46	1.50
23	M1	101	BCR	C33-C5	-2.03	1.47	1.50
19	A2	842	CLA	C3B-C2B	-2.02	1.37	1.40
19	B2	830	CLA	C3B-C2B	-2.02	1.37	1.40
19	B	828	CLA	CMC-C2C	-2.02	1.46	1.50
19	L2	205	CLA	CMC-C2C	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	B	857	AJP	CBD-CBN	2.02	1.57	1.54
19	B1	835	CLA	CMC-C2C	-2.02	1.46	1.50
23	K1	104	BCR	C33-C5	-2.02	1.47	1.50
24	A1	854	AJP	CCK-CBP	2.02	1.57	1.52
19	AA	837	CLA	C3B-C2B	-2.02	1.37	1.40
23	II	102	BCR	C33-C5	-2.02	1.47	1.50
19	BB	809	CLA	C3B-C2B	-2.02	1.37	1.40
23	K	103	BCR	C33-C5	-2.02	1.47	1.50
19	AA	801	CLA	C3B-CAB	-2.02	1.43	1.47
19	AA	801	CLA	C3B-C2B	-2.02	1.37	1.40
23	BB	843	BCR	C33-C5	-2.02	1.47	1.50
19	A1	805	CLA	CMC-C2C	-2.02	1.46	1.50
19	B	836	CLA	CMC-C2C	-2.02	1.46	1.50
25	BB	844	LMG	C7-C8	2.02	1.56	1.50
19	A1	822	CLA	C3B-C2B	-2.02	1.37	1.40
19	A1	822	CLA	CMC-C2C	-2.02	1.46	1.50
19	AA	826	CLA	CMC-C2C	-2.02	1.46	1.50
19	L2	205	CLA	C3B-C2B	-2.02	1.37	1.40
19	A2	829	CLA	C3B-C2B	-2.02	1.37	1.40
19	AA	816	CLA	C3B-C2B	-2.02	1.37	1.40
19	A1	842	CLA	C4C-C3C	2.02	1.48	1.45
23	JJ	104	BCR	C33-C5	-2.02	1.47	1.50
19	L	202	CLA	CMC-C2C	-2.02	1.46	1.50
19	A	840	CLA	CMC-C2C	-2.02	1.46	1.50
19	BB	821	CLA	CMB-C2B	-2.02	1.47	1.51
19	B1	831	CLA	C3B-CAB	-2.02	1.43	1.47
19	A1	816	CLA	C3B-C2B	-2.01	1.37	1.40
19	F1	302	CLA	C3B-C2B	-2.01	1.37	1.40
19	A1	806	CLA	C3B-CAB	-2.01	1.43	1.47
19	AA	832	CLA	CMC-C2C	-2.01	1.46	1.50
19	L	203	CLA	CMC-C2C	-2.01	1.46	1.50
19	B	810	CLA	CMC-C2C	-2.01	1.46	1.50
19	B2	804	CLA	CMC-C2C	-2.01	1.46	1.50
23	M2	102	BCR	C33-C5	-2.01	1.47	1.50
19	A2	826	CLA	C3B-C2B	-2.01	1.37	1.40
19	F2	302	CLA	C3B-C2B	-2.01	1.37	1.40
24	B	850	AJP	CBD-CBN	2.01	1.57	1.54
19	B1	833	CLA	C3C-C2C	2.01	1.41	1.36
19	A	806	CLA	C3B-CAB	-2.01	1.43	1.47
19	A	820	CLA	CMC-C2C	-2.01	1.46	1.50
19	A2	844	CLA	CMC-C2C	-2.01	1.46	1.50
19	A2	808	CLA	CMC-C2C	-2.01	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	B	844	BCR	C33-C5	-2.01	1.47	1.50
19	A	834	CLA	CMC-C2C	-2.01	1.46	1.50
19	A2	812	CLA	C3B-C2B	-2.01	1.37	1.40
19	L1	206	CLA	CMC-C2C	-2.01	1.46	1.50
19	B2	803	CLA	C3B-CAB	-2.01	1.43	1.47
25	II	105	LMG	C7-C8	2.01	1.56	1.50
19	B2	806	CLA	CMC-C2C	-2.00	1.46	1.50
19	A2	831	CLA	C3B-C2B	-2.00	1.37	1.40
19	A	823	CLA	C3B-C2B	-2.00	1.37	1.40
19	BB	835	CLA	C3B-CAB	-2.00	1.43	1.47
19	AA	823	CLA	C3B-C2B	-2.00	1.37	1.40
19	LL	202	CLA	CMC-C2C	-2.00	1.46	1.50
19	A1	805	CLA	C3B-CAB	-2.00	1.43	1.47
19	B	820	CLA	C3B-C2B	-2.00	1.37	1.40
19	BB	855	CLA	C3B-CAB	-2.00	1.43	1.47

All (5097) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A1	854	AJP	CBK-CCG-CCF	-13.21	88.84	108.95
24	B	857	AJP	CBK-CCG-CCF	-13.13	88.97	108.95
24	L1	203	AJP	CBK-CCG-CCF	-13.04	89.10	108.95
24	L2	202	AJP	CBK-CCG-CCF	-12.69	89.64	108.95
24	L	208	AJP	CBK-CCG-CCF	-12.63	89.73	108.95
24	B	849	AJP	CBK-CCG-CCF	-12.57	89.81	108.95
24	BB	849	AJP	OBQ-CBP-CCK	12.02	135.15	110.23
24	AA	856	AJP	CBK-CCG-CCF	-12.02	90.66	108.95
24	A	855	AJP	CBK-CCG-CCF	-12.00	90.68	108.95
24	BB	848	AJP	CBK-CCG-CCF	-11.97	90.72	108.95
24	I2	104	AJP	CBK-CCG-CCF	-11.86	90.89	108.95
24	L	209	AJP	CBK-CCG-CCF	-11.86	90.90	108.95
24	KK	104	AJP	CBK-CCG-CCF	-11.73	91.09	108.95
24	L1	204	AJP	CBK-CCG-CCF	-11.70	91.15	108.95
24	K	104	AJP	CBK-CCG-CCF	-11.61	91.27	108.95
24	M2	101	AJP	CBK-CCG-CCF	-11.59	91.31	108.95
24	B	857	AJP	CCF-CCG-CDB	11.58	120.63	107.10
24	L2	203	AJP	CBK-CCG-CCF	-11.55	91.37	108.95
24	M2	101	AJP	CCF-CCG-CDB	11.44	120.47	107.10
24	A1	855	AJP	CBK-CCG-CCF	-11.40	91.59	108.95
24	L	209	AJP	OBQ-CBP-CCK	11.40	133.86	110.23
24	A2	854	AJP	CBK-CCG-CCF	-11.39	91.62	108.95
24	A1	854	AJP	CCF-CCG-CDB	11.34	120.35	107.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	KK	104	AJP	OBQ-CBP-CCK	11.28	133.62	110.23
24	L	209	AJP	CCF-CCG-CDB	11.26	120.26	107.10
24	BB	849	AJP	CBK-CCG-CCF	-11.21	91.88	108.95
24	B	850	AJP	CBK-CCG-CCF	-11.20	91.90	108.95
24	A	802	AJP	OBQ-CBP-CCK	11.10	133.26	110.23
24	B	850	AJP	OBQ-CBP-CCK	11.08	133.20	110.23
24	M2	101	AJP	OBQ-CBP-CCK	11.07	133.19	110.23
24	L	208	AJP	CCF-CCG-CCH	11.07	127.09	110.13
24	AA	802	AJP	OBQ-CBP-CCK	11.07	133.19	110.23
24	I2	104	AJP	OBQ-CBP-CCK	11.03	133.10	110.23
24	L	208	AJP	OBQ-CBP-CCK	10.91	132.87	110.23
24	K	104	AJP	OBQ-CBP-CCK	10.89	132.81	110.23
24	AA	802	AJP	CBK-CCG-CCF	-10.88	90.58	108.25
24	A	802	AJP	CBK-CCG-CCF	-10.84	90.65	108.25
24	B	849	AJP	OBQ-CBP-CCK	10.82	132.68	110.23
24	AA	856	AJP	CCF-CCG-CDB	10.80	119.72	107.10
24	A	855	AJP	CCF-CCG-CDB	10.78	119.70	107.10
24	L2	202	AJP	OBQ-CBP-CCK	10.75	132.53	110.23
24	BB	848	AJP	OBQ-CBP-CCK	10.71	132.44	110.23
24	L2	203	AJP	CCF-CCG-CDB	10.70	119.60	107.10
24	BB	848	AJP	CCF-CCG-CCH	10.52	126.24	110.13
24	B	850	AJP	CCF-CCG-CDB	10.39	119.24	107.10
24	L1	203	AJP	CCF-CCG-CCH	10.24	125.81	110.13
24	B	849	AJP	CCF-CCG-CCH	10.19	125.74	110.13
24	KK	104	AJP	CCF-CCG-CCH	10.13	125.64	110.13
24	BB	849	AJP	CCF-CCG-CDB	10.12	118.92	107.10
24	L	209	AJP	CCF-CCG-CCH	10.10	125.59	110.13
24	L1	204	AJP	CCF-CCG-CDB	10.08	118.89	107.10
24	L	208	AJP	CCF-CCG-CDB	10.05	118.85	107.10
24	I2	104	AJP	CCF-CCG-CCH	9.96	125.38	110.13
24	K	104	AJP	CCF-CCG-CCH	9.94	125.35	110.13
24	A2	854	AJP	CCF-CCG-CDB	9.93	118.71	107.10
24	L2	202	AJP	CCF-CCG-CCH	9.90	125.28	110.13
26	B	841	ECH	C16-C17-C18	-9.89	113.19	127.31
26	B1	840	ECH	C16-C17-C18	-9.84	113.27	127.31
26	B2	841	ECH	C16-C17-C18	-9.81	113.30	127.31
24	K	104	AJP	CCF-CCG-CDB	9.72	118.46	107.10
24	A1	855	AJP	CCF-CCG-CDB	9.71	118.45	107.10
24	KK	104	AJP	CCF-CCG-CDB	9.65	118.38	107.10
24	L1	204	AJP	CCF-CCG-CCH	9.57	124.79	110.13
26	BB	840	ECH	C16-C17-C18	-9.54	113.70	127.31
24	BB	848	AJP	CCF-CCG-CDB	9.35	118.03	107.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	M2	101	AJP	CCF-CCG-CCH	9.30	124.38	110.13
24	B	849	AJP	CCF-CCG-CDB	9.29	117.96	107.10
24	L2	203	AJP	CCF-CCG-CCH	9.15	124.14	110.13
24	B	850	AJP	CAX-CAY-CBH	9.08	121.50	108.51
24	A1	854	AJP	CCF-CCG-CCH	9.04	123.97	110.13
24	I2	104	AJP	CCF-CCG-CDB	9.00	117.61	107.10
24	L2	202	AJP	CAX-CAY-CBH	8.97	121.34	108.51
24	L2	202	AJP	CCF-CCG-CDB	8.95	117.56	107.10
24	BB	849	AJP	CCF-CCG-CCH	8.81	123.62	110.13
24	B	857	AJP	CCF-CCG-CCH	8.64	123.36	110.13
24	KK	104	AJP	CAX-CAY-CBH	8.55	120.74	108.51
24	A	802	AJP	CBL-CCH-CCG	8.54	123.99	113.92
24	AA	802	AJP	CBL-CCH-CCG	8.53	123.97	113.92
24	B	850	AJP	CCF-CCG-CCH	8.51	123.16	110.13
24	K	104	AJP	CAX-CAY-CBH	8.46	120.61	108.51
24	AA	802	AJP	CCF-CCG-CCH	8.42	124.70	111.36
24	A	802	AJP	CCF-CCG-CCH	8.37	124.63	111.36
19	BB	801	CLA	C4A-NA-C1A	8.33	110.45	106.71
20	AA	803	CL0	O2D-CGD-CBD	8.32	125.81	111.25
24	A1	855	AJP	CCF-CCG-CCH	8.30	122.85	110.13
24	I2	104	AJP	CBL-CCH-CCG	8.29	123.69	113.92
24	L2	202	AJP	OCC-CCB-CCA	8.24	124.72	109.68
24	L1	203	AJP	CCF-CCG-CDB	8.23	116.72	107.10
24	A2	854	AJP	CCF-CCG-CCH	8.17	122.65	110.13
24	B	849	AJP	CAX-CAY-CBH	8.10	120.10	108.51
19	B	801	CLA	C4A-NA-C1A	8.09	110.34	106.71
19	B1	848	CLA	C4A-NA-C1A	8.02	110.31	106.71
24	AA	802	AJP	CBK-CCG-CCH	-7.94	100.11	111.17
24	A	802	AJP	CBK-CCG-CCH	-7.94	100.12	111.17
24	BB	848	AJP	CBK-CCG-CCH	-7.87	100.22	111.17
19	L2	205	CLA	C4A-NA-C1A	7.85	110.23	106.71
19	B2	801	CLA	C4A-NA-C1A	7.84	110.23	106.71
19	B1	801	CLA	C4A-NA-C1A	7.77	110.20	106.71
24	AA	856	AJP	CCF-CCG-CCH	7.75	122.01	110.13
24	A	855	AJP	CCF-CCG-CCH	7.75	122.01	110.13
19	B	805	CLA	C4A-NA-C1A	7.75	110.19	106.71
24	A1	854	AJP	CBK-CCG-CCH	-7.72	100.42	111.17
20	A	803	CL0	O2D-CGD-CBD	7.70	124.73	111.25
19	A2	836	CLA	C4A-NA-C1A	7.68	110.16	106.71
19	BB	852	CLA	C4A-NA-C1A	7.62	110.13	106.71
24	L	208	AJP	CBL-CCH-CCG	7.56	122.83	113.92
19	B	854	CLA	C4A-NA-C1A	7.56	110.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	805	CLA	C4A-NA-C1A	7.56	110.11	106.71
24	B	849	AJP	CBK-CCG-CCH	-7.56	100.65	111.17
24	B	857	AJP	CBK-CCG-CCH	-7.53	100.69	111.17
19	L1	206	CLA	C4A-NA-C1A	7.47	110.07	106.71
24	KK	104	AJP	OBQ-CBF-CAW	7.46	126.55	108.58
19	B2	805	CLA	C4A-NA-C1A	7.46	110.06	106.71
24	M2	101	AJP	CBL-CCH-CCI	7.44	122.56	111.74
24	L1	203	AJP	CBK-CCG-CCH	-7.42	100.84	111.17
19	LL	202	CLA	C4A-NA-C1A	7.41	110.04	106.71
24	L2	202	AJP	CBK-CCG-CCH	-7.39	100.89	111.17
19	L	204	CLA	C4A-NA-C1A	7.37	110.02	106.71
19	A2	801	CLA	C4A-NA-C1A	7.36	110.02	106.71
19	A	836	CLA	C4A-NA-C1A	7.36	110.01	106.71
19	B1	805	CLA	C4A-NA-C1A	7.35	110.01	106.71
19	A1	835	CLA	C4A-NA-C1A	7.35	110.01	106.71
19	B	859	CLA	C4A-NA-C1A	7.34	110.01	106.71
24	BB	849	AJP	CBK-CCG-CCH	-7.33	100.97	111.17
19	A	832	CLA	C4A-NA-C1A	7.31	109.99	106.71
19	BB	856	CLA	C4A-NA-C1A	7.30	109.99	106.71
19	A2	842	CLA	C4A-NA-C1A	7.27	109.97	106.71
20	A2	803	CL0	C2C-C1C-NC	7.27	116.78	109.97
24	A	855	AJP	CBK-CCG-CCH	-7.25	101.08	111.17
24	AA	856	AJP	CBK-CCG-CCH	-7.25	101.08	111.17
19	A2	813	CLA	C4A-NA-C1A	7.25	109.96	106.71
19	AA	813	CLA	C4A-NA-C1A	7.24	109.96	106.71
19	B2	849	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	K	104	AJP	CBK-CCG-CCH	-7.22	101.12	111.17
19	A1	829	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	B	817	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	A1	801	CLA	C4A-NA-C1A	7.20	109.94	106.71
19	AA	836	CLA	C4A-NA-C1A	7.19	109.94	106.71
24	L	209	AJP	CBK-CCG-CCH	-7.19	101.16	111.17
19	B2	851	CLA	C4A-NA-C1A	7.19	109.94	106.71
24	M2	101	AJP	CBK-CCG-CCH	-7.18	101.17	111.17
19	A	825	CLA	C4A-NA-C1A	7.18	109.93	106.71
24	L1	204	AJP	CBK-CCG-CCH	-7.17	101.19	111.17
19	B1	826	CLA	C4A-NA-C1A	7.16	109.92	106.71
24	KK	104	AJP	CBK-CCG-CCH	-7.15	101.22	111.17
24	BB	848	AJP	CBL-CCH-CCG	7.15	122.34	113.92
19	B2	826	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	A	801	CLA	C4A-NA-C1A	7.14	109.92	106.71
19	B1	836	CLA	C4A-NA-C1A	7.14	109.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	849	AJP	CBL-CCH-CCI	7.14	122.13	111.74
24	L2	203	AJP	OBQ-CBP-CCK	7.13	125.02	110.23
19	A1	841	CLA	C4A-NA-C1A	7.13	109.91	106.71
19	A	813	CLA	C4A-NA-C1A	7.13	109.91	106.71
24	A1	855	AJP	CBK-CCG-CCH	-7.12	101.25	111.17
19	AA	801	CLA	C4A-NA-C1A	7.12	109.91	106.71
24	L1	203	AJP	OCC-CCB-CCA	7.12	122.67	109.68
19	A2	838	CLA	C4A-NA-C1A	7.11	109.90	106.71
24	L2	203	AJP	CBK-CCG-CCH	-7.11	101.28	111.17
19	BB	822	CLA	C4A-NA-C1A	7.11	109.90	106.71
19	B	833	CLA	C4A-NA-C1A	7.11	109.90	106.71
24	B	849	AJP	CBL-CCH-CCI	7.09	122.06	111.74
19	A1	831	CLA	C4A-NA-C1A	7.07	109.88	106.71
19	B2	837	CLA	C4A-NA-C1A	7.05	109.88	106.71
24	B	850	AJP	CBK-CCG-CCH	-7.04	101.37	111.17
19	B1	850	CLA	C4A-NA-C1A	7.04	109.87	106.71
24	A2	854	AJP	CBK-CCG-CCH	-7.03	101.39	111.17
19	B	822	CLA	C4A-NA-C1A	7.03	109.86	106.71
24	L1	204	AJP	CBL-CCH-CCG	7.00	122.17	113.92
19	B1	832	CLA	C4A-NA-C1A	6.97	109.84	106.71
19	A	830	CLA	C4A-NA-C1A	6.97	109.84	106.71
24	L	209	AJP	CBL-CCH-CCI	6.97	121.88	111.74
19	BB	817	CLA	C4A-NA-C1A	6.96	109.84	106.71
19	A2	832	CLA	C4A-NA-C1A	6.96	109.83	106.71
24	A1	855	AJP	CBL-CCH-CCG	6.96	122.11	113.92
19	A2	823	CLA	C4A-NA-C1A	6.95	109.83	106.71
19	AA	845	CLA	C4A-NA-C1A	6.95	109.83	106.71
19	A1	807	CLA	C4A-NA-C1A	6.95	109.83	106.71
24	K	104	AJP	OBQ-CBF-CAW	6.94	125.30	108.58
24	L2	202	AJP	CBL-CCH-CCI	6.94	121.84	111.74
19	AA	825	CLA	C4A-NA-C1A	6.94	109.83	106.71
19	A2	825	CLA	C4A-NA-C1A	6.94	109.82	106.71
20	A1	802	CL0	C2C-C1C-NC	6.92	116.46	109.97
19	K2	104	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	A	808	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	B	821	CLA	C4A-NA-C1A	6.92	109.82	106.71
19	B	826	CLA	C4A-NA-C1A	6.91	109.81	106.71
19	A	819	CLA	C4A-NA-C1A	6.91	109.81	106.71
24	A	802	AJP	CCJ-CCI-CCH	-6.90	97.14	109.25
19	B2	821	CLA	C4A-NA-C1A	6.90	109.81	106.71
19	A1	803	CLA	C4A-NA-C1A	6.89	109.80	106.71
19	B1	803	CLA	C4A-NA-C1A	6.88	109.80	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	823	CLA	C4A-NA-C1A	6.88	109.80	106.71
24	L	208	AJP	CBK-CCG-CCH	-6.88	101.60	111.17
20	AA	803	CL0	C2C-C1C-NC	6.87	116.41	109.97
19	AA	832	CLA	C4A-NA-C1A	6.87	109.80	106.71
24	L	208	AJP	CCJ-CCI-CCH	-6.87	97.20	109.25
19	A1	825	CLA	C4A-NA-C1A	6.87	109.79	106.71
24	L2	203	AJP	CBL-CCH-CCI	6.87	121.74	111.74
19	AA	842	CLA	C4A-NA-C1A	6.87	109.79	106.71
24	AA	802	AJP	CCJ-CCI-CCH	-6.86	97.21	109.25
19	B1	823	CLA	C4A-NA-C1A	6.86	109.79	106.71
24	BB	848	AJP	CBL-CCH-CCI	6.85	121.72	111.74
19	A1	812	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	A	828	CLA	C4A-NA-C1A	6.85	109.79	106.71
19	A1	822	CLA	C4A-NA-C1A	6.85	109.78	106.71
19	A1	837	CLA	C4A-NA-C1A	6.85	109.78	106.71
19	B2	833	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	B2	836	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	AA	828	CLA	C4A-NA-C1A	6.83	109.78	106.71
19	B1	821	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	A2	822	CLA	C4A-NA-C1A	6.82	109.77	106.71
19	A2	826	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	AA	822	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	B	823	CLA	C4A-NA-C1A	6.81	109.77	106.71
19	AA	821	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	A2	808	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	B	812	CLA	C4A-NA-C1A	6.80	109.76	106.71
19	AA	823	CLA	C4A-NA-C1A	6.79	109.76	106.71
24	B	850	AJP	CBL-CCH-CCG	6.79	121.92	113.92
19	K	102	CLA	C4A-NA-C1A	6.78	109.75	106.71
24	B	850	AJP	CBF-CBE-CBO	6.78	114.76	103.39
19	AA	818	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A1	821	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A2	827	CLA	C4A-NA-C1A	6.78	109.75	106.71
19	A1	823	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	A	817	CLA	C4A-NA-C1A	6.77	109.75	106.71
19	B1	806	CLA	C4A-NA-C1A	6.77	109.75	106.71
20	A2	803	CL0	O2D-CGD-CBD	6.77	123.09	111.25
19	B	803	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	B2	817	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	A1	826	CLA	C4A-NA-C1A	6.76	109.75	106.71
19	X1	101	CLA	C4A-NA-C1A	6.76	109.74	106.71
19	F	301	CLA	C4A-NA-C1A	6.76	109.74	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	828	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	A	844	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	B	802	CLA	C4A-NA-C1A	6.75	109.74	106.71
19	B1	817	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	L2	203	AJP	OBQ-CBF-CAW	6.74	124.81	108.58
19	B1	804	CLA	C4A-NA-C1A	6.74	109.73	106.71
19	B2	825	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	B1	835	CLA	C4A-NA-C1A	6.73	109.73	106.71
19	A	818	CLA	C4A-NA-C1A	6.73	109.73	106.71
24	L2	202	AJP	CBF-CBE-CBO	6.72	114.66	103.39
19	A	815	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	F1	302	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A	821	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	B2	830	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	BB	832	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A1	838	CLA	C4A-NA-C1A	6.72	109.73	106.71
19	A	824	CLA	C4A-NA-C1A	6.72	109.72	106.71
19	B2	804	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	A	823	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	B	830	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	A2	802	CLA	C4A-NA-C1A	6.71	109.72	106.71
19	AA	830	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	BB	823	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	AA	804	CLA	C4A-NA-C1A	6.70	109.72	106.71
19	A2	841	CLA	C4A-NA-C1A	6.70	109.72	106.71
24	AA	856	AJP	OBQ-CBF-CAW	6.69	124.70	108.58
19	B	809	CLA	C4A-NA-C1A	6.69	109.72	106.71
24	K	104	AJP	CBL-CCH-CCG	6.69	121.80	113.92
19	L	202	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	A	855	AJP	OBQ-CBF-CAW	6.68	124.68	108.58
24	A2	854	AJP	CBL-CCH-CCG	6.68	121.79	113.92
19	B2	824	CLA	C4A-NA-C1A	6.68	109.71	106.71
19	AA	839	CLA	C4A-NA-C1A	6.67	109.71	106.71
19	A1	840	CLA	C4A-NA-C1A	6.67	109.71	106.71
19	BB	809	CLA	C4A-NA-C1A	6.67	109.70	106.71
19	B1	815	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	AA	856	AJP	CBK-CCG-CDB	-6.66	98.96	110.34
20	A	803	CL0	C2C-C1C-NC	6.66	116.21	109.97
19	B2	803	CLA	C4A-NA-C1A	6.66	109.70	106.71
24	BB	849	AJP	OCC-CCB-CCA	6.66	121.82	109.68
24	A	855	AJP	CBK-CCG-CDB	-6.65	98.97	110.34
19	BB	831	CLA	C4A-NA-C1A	6.65	109.70	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	844	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	A1	808	CLA	C4A-NA-C1A	6.65	109.70	106.71
19	L1	205	CLA	C4A-NA-C1A	6.65	109.69	106.71
24	KK	104	AJP	CBL-CCH-CCG	6.64	121.74	113.92
19	A1	818	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	A2	809	CLA	C4A-NA-C1A	6.64	109.69	106.71
19	XX	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	BB	828	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	B1	807	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	A2	830	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	AA	817	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	KK	102	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	A1	827	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	X	101	CLA	C4A-NA-C1A	6.63	109.69	106.71
19	A2	819	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	B1	812	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A2	824	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	L2	204	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	B	807	CLA	C4A-NA-C1A	6.62	109.68	106.71
19	A	838	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	A2	821	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	B2	831	CLA	C4A-NA-C1A	6.61	109.68	106.71
19	B	836	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	AA	815	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	B2	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A2	852	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	BB	812	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A1	817	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	A	839	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	BB	836	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	BB	803	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	AA	805	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	AA	838	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	K1	103	CLA	C4A-NA-C1A	6.59	109.67	106.71
19	A	805	CLA	C4A-NA-C1A	6.58	109.67	106.71
19	BB	807	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	BB	830	CLA	C4A-NA-C1A	6.58	109.66	106.71
19	B2	807	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	A2	818	CLA	C4A-NA-C1A	6.57	109.66	106.71
24	I2	104	AJP	CBK-CCG-CCH	-6.57	102.03	111.17
19	AA	841	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	A2	844	CLA	C4A-NA-C1A	6.56	109.66	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	839	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	BB	813	CLA	C4A-NA-C1A	6.56	109.66	106.71
19	A2	816	CLA	C4A-NA-C1A	6.56	109.66	106.71
24	B	850	AJP	CBL-CCH-CCI	6.56	121.28	111.74
19	A	841	CLA	C4A-NA-C1A	6.56	109.65	106.71
19	AA	808	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	A	842	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	BB	804	CLA	C4A-NA-C1A	6.55	109.65	106.71
19	B1	822	CLA	C4A-NA-C1A	6.54	109.65	106.71
19	A	812	CLA	C4A-NA-C1A	6.54	109.64	106.71
19	F2	302	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	B	806	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	B2	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
24	KK	104	AJP	CBL-CCH-CCI	6.52	121.23	111.74
19	A1	824	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	B1	825	CLA	C4A-NA-C1A	6.52	109.64	106.71
19	JJ	101	CLA	C4A-NA-C1A	6.52	109.64	106.71
24	K	104	AJP	CBL-CCH-CCI	6.52	121.23	111.74
19	J	101	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	AA	824	CLA	C4A-NA-C1A	6.51	109.64	106.71
19	A2	805	CLA	C4A-NA-C1A	6.50	109.63	106.71
24	B	849	AJP	CBF-CBE-CBO	6.50	114.28	103.39
19	X2	101	CLA	C4A-NA-C1A	6.50	109.63	106.71
19	B1	808	CLA	C4A-NA-C1A	6.49	109.63	106.71
19	A	804	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	B	810	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	A2	817	CLA	C4A-NA-C1A	6.49	109.62	106.71
19	A1	820	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	A1	832	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	A	829	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B	829	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B1	830	CLA	C4A-NA-C1A	6.48	109.62	106.71
19	B1	802	CLA	C4A-NA-C1A	6.47	109.62	106.71
19	B	804	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	A	816	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	A1	828	CLA	C4A-NA-C1A	6.46	109.61	106.71
19	BB	835	CLA	C4A-NA-C1A	6.45	109.61	106.71
19	FF	302	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	B1	809	CLA	C4A-NA-C1A	6.44	109.60	106.71
19	B2	809	CLA	C4A-NA-C1A	6.44	109.60	106.71
24	A	802	AJP	OBQ-CBF-CAW	6.44	124.09	108.58
24	L1	203	AJP	CBL-CCH-CCI	6.44	121.11	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	831	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	AA	829	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	B	860	CLA	CAC-C3C-C4C	6.43	133.23	124.82
19	A2	806	CLA	C4A-NA-C1A	6.43	109.60	106.71
19	BB	821	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	AA	812	CLA	C4A-NA-C1A	6.42	109.59	106.71
24	L1	204	AJP	CBL-CCH-CCI	6.42	121.09	111.74
19	BB	806	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B2	819	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	LL	201	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	FF	301	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B	827	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	B1	829	CLA	C4A-NA-C1A	6.42	109.59	106.71
19	F1	301	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	A1	815	CLA	C4A-NA-C1A	6.41	109.59	106.71
19	B2	802	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	BB	845	CLA	C4A-NA-C1A	6.40	109.58	106.71
19	F	302	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	AA	819	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	A	833	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	B2	806	CLA	C4A-NA-C1A	6.39	109.58	106.71
19	A	831	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	B2	828	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	A1	804	CLA	C4A-NA-C1A	6.38	109.57	106.71
19	BB	826	CLA	C4A-NA-C1A	6.38	109.57	106.71
24	AA	802	AJP	OBQ-CBF-CAW	6.38	123.94	108.58
19	BB	824	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	A	822	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	AA	843	CLA	CAC-C3C-C4C	6.37	133.15	124.82
19	B2	832	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	L1	204	AJP	OBQ-CBP-CCK	6.36	123.42	110.23
19	A1	842	CLA	CAC-C3C-C4C	6.36	133.13	124.82
24	L	208	AJP	CBF-CBE-CBO	6.35	114.04	103.39
19	A1	814	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	A2	804	CLA	C4A-NA-C1A	6.35	109.56	106.71
19	A2	807	CLA	C4A-NA-C1A	6.35	109.56	106.71
24	BB	849	AJP	OBQ-CBF-CAW	6.35	123.87	108.58
24	A2	854	AJP	OBQ-CBF-CAW	6.35	123.86	108.58
19	A1	816	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	B	828	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	AA	809	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	B	846	CLA	C4A-NA-C1A	6.34	109.56	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	822	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	AA	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	B	831	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	B2	815	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	L	203	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	BB	827	CLA	C4A-NA-C1A	6.33	109.55	106.71
19	A	809	CLA	C4A-NA-C1A	6.32	109.55	106.71
24	BB	848	AJP	CAZ-CAY-CBH	6.31	122.52	111.22
19	AA	827	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	A2	812	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	K1	105	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	F2	301	CLA	C4A-NA-C1A	6.30	109.54	106.71
19	B1	834	CLA	C4A-NA-C1A	6.29	109.53	106.71
24	KK	104	AJP	OBQ-CBP-CBO	6.28	118.46	103.90
19	AA	826	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	B1	813	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	K	104	AJP	CBF-CBE-CBO	6.28	113.92	103.39
19	BB	825	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	B	816	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	K1	102	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	AA	840	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	B	813	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	B	824	CLA	C4A-NA-C1A	6.27	109.53	106.71
19	A	826	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	B	825	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	B	819	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	A2	835	CLA	C4A-NA-C1A	6.26	109.52	106.71
19	B	832	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	A1	806	CLA	C4A-NA-C1A	6.25	109.52	106.71
19	J1	103	CLA	C4A-NA-C1A	6.25	109.51	106.71
19	B	837	CLA	C4A-NA-C1A	6.25	109.51	106.71
19	A2	814	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	A2	854	AJP	CBK-CCG-CDB	-6.24	99.67	110.34
19	A	840	CLA	C4A-NA-C1A	6.24	109.51	106.71
19	A2	811	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	A	806	CLA	C4A-NA-C1A	6.23	109.51	106.71
19	FF	305	CLA	C4A-NA-C1A	6.23	109.51	106.71
24	L2	202	AJP	OBQ-CBP-CBO	6.23	118.35	103.90
19	B2	814	CLA	C4A-NA-C1A	6.23	109.50	106.71
24	A1	855	AJP	CBK-CCG-CDB	-6.22	99.71	110.34
19	A	827	CLA	C4A-NA-C1A	6.22	109.50	106.71
19	A1	833	CLA	C4A-NA-C1A	6.22	109.50	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	849	AJP	OCY-CCX-CCW	6.21	124.46	108.10
24	M2	101	AJP	CBF-CBE-CBO	6.21	113.80	103.39
24	AA	802	AJP	CBF-CBE-CBO	6.21	113.80	103.39
19	B2	813	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	BB	808	CLA	C4A-NA-C1A	6.21	109.50	106.71
19	F1	305	CLA	C4A-NA-C1A	6.21	109.50	106.71
24	L1	203	AJP	OCY-CCX-CCW	6.20	124.43	108.10
19	B2	846	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	B2	810	CLA	C4A-NA-C1A	6.20	109.49	106.71
19	B2	835	CLA	C4A-NA-C1A	6.20	109.49	106.71
24	I2	104	AJP	CBK-CCG-CDB	-6.20	99.75	110.34
19	A1	813	CLA	C4A-NA-C1A	6.20	109.49	106.71
24	I2	104	AJP	CBF-CBE-CBO	6.20	113.77	103.39
19	B1	845	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	L1	204	AJP	OCC-CCB-CCA	6.19	120.97	109.68
24	L2	203	AJP	CAX-CAY-CBH	6.19	117.36	108.51
19	AA	833	CLA	C4A-NA-C1A	6.19	109.49	106.71
24	A	802	AJP	CBF-CBE-CBO	6.18	113.75	103.39
24	L1	203	AJP	CBL-CCH-CCG	6.18	121.19	113.92
19	B2	852	CLA	CAC-C3C-C4C	6.17	132.89	124.82
19	J1	101	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	J2	103	CLA	C4A-NA-C1A	6.17	109.48	106.71
19	B	814	CLA	C4A-NA-C1A	6.17	109.48	106.71
24	L2	203	AJP	CBL-CCH-CCG	6.16	121.18	113.92
19	AA	814	CLA	C4A-NA-C1A	6.16	109.48	106.71
24	B	849	AJP	OCC-CCB-CCA	6.16	120.91	109.68
19	LL	203	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	B1	819	CLA	C4A-NA-C1A	6.15	109.47	106.71
24	K	104	AJP	CBK-CCG-CDB	-6.15	99.83	110.34
24	B	849	AJP	OBQ-CBP-CBO	6.15	118.16	103.90
24	B	850	AJP	OCC-CCB-CCA	6.15	120.90	109.68
19	B	835	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	BB	834	CLA	C4A-NA-C1A	6.15	109.47	106.71
19	BB	810	CLA	C4A-NA-C1A	6.15	109.47	106.71
24	B	857	AJP	CBK-CCG-CDB	-6.14	99.84	110.34
19	A1	830	CLA	C4A-NA-C1A	6.14	109.47	106.71
19	BB	814	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A1	810	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	B	808	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A1	836	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	A2	834	CLA	C4A-NA-C1A	6.13	109.46	106.71
19	JJ	103	CLA	C4A-NA-C1A	6.13	109.46	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	834	CLA	C4A-NA-C1A	6.13	109.46	106.71
24	BB	848	AJP	OCY-CCX-CCW	6.13	124.23	108.10
24	K	104	AJP	OBQ-CBP-CBO	6.12	118.10	103.90
19	AA	837	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	B1	828	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	A	837	CLA	C4A-NA-C1A	6.12	109.46	106.71
24	BB	849	AJP	OBQ-CBP-CBO	6.12	118.09	103.90
19	AA	806	CLA	C4A-NA-C1A	6.12	109.46	106.71
24	KK	104	AJP	CBK-CCG-CDB	-6.12	99.88	110.34
19	J	103	CLA	C4A-NA-C1A	6.12	109.46	106.71
19	A1	839	CLA	C4A-NA-C1A	6.12	109.46	106.71
24	KK	104	AJP	CBF-CBE-CBO	6.11	113.64	103.39
19	B1	827	CLA	C4A-NA-C1A	6.11	109.45	106.71
24	BB	848	AJP	OCC-CCB-CCA	6.11	120.83	109.68
19	AA	816	CLA	C4A-NA-C1A	6.11	109.45	106.71
19	A	814	CLA	C4A-NA-C1A	6.11	109.45	106.71
24	A1	854	AJP	CBK-CCG-CDB	-6.10	99.91	110.34
19	A1	834	CLA	C4A-NA-C1A	6.10	109.45	106.71
19	A2	820	CLA	C4A-NA-C1A	6.08	109.44	106.71
19	BB	819	CLA	C4A-NA-C1A	6.08	109.44	106.71
19	J2	101	CLA	C4A-NA-C1A	6.07	109.44	106.71
19	AA	807	CLA	C4A-NA-C1A	6.07	109.43	106.71
19	K2	102	CLA	C4A-NA-C1A	6.06	109.43	106.71
19	BB	802	CLA	C4A-NA-C1A	6.06	109.43	106.71
19	B1	810	CLA	C4A-NA-C1A	6.05	109.43	106.71
19	AA	834	CLA	C4A-NA-C1A	6.05	109.42	106.71
19	A2	837	CLA	C4A-NA-C1A	6.04	109.42	106.71
19	A	807	CLA	C4A-NA-C1A	6.02	109.41	106.71
24	A	802	AJP	OBQ-CBP-CBO	6.02	117.86	103.90
24	AA	802	AJP	OBQ-CBP-CBO	6.02	117.86	103.90
19	B1	818	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	BB	816	CLA	C4A-NA-C1A	6.01	109.41	106.71
24	L	209	AJP	CBF-CBE-CBO	6.01	113.46	103.39
19	L2	206	CLA	C4A-NA-C1A	6.01	109.41	106.71
19	A2	840	CLA	C4A-NA-C1A	6.00	109.41	106.71
19	B2	816	CLA	C4A-NA-C1A	6.00	109.41	106.71
24	M2	101	AJP	OBQ-CBP-CBO	6.00	117.81	103.90
24	I2	104	AJP	OBQ-CBF-CAW	6.00	123.02	108.58
19	BB	855	CLA	C4A-NA-C1A	5.99	109.40	106.71
24	BB	849	AJP	OCL-CCK-CBP	5.98	128.11	111.15
24	B	850	AJP	OBQ-CBP-CBO	5.98	117.77	103.90
24	A	802	AJP	CCG-CCH-CCI	5.98	118.78	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	I2	104	AJP	OBQ-CBP-CBO	5.98	117.76	103.90
19	A2	815	CLA	C4A-NA-C1A	5.98	109.39	106.71
19	K	101	CLA	C4A-NA-C1A	5.98	109.39	106.71
24	AA	802	AJP	CCG-CCH-CCI	5.97	118.77	112.42
19	B1	814	CLA	C4A-NA-C1A	5.97	109.39	106.71
24	KK	104	AJP	OCL-CCK-CBP	5.96	128.06	111.15
24	M2	101	AJP	OBQ-CBF-CAW	5.96	122.94	108.58
19	B2	818	CLA	C4A-NA-C1A	5.96	109.39	106.71
19	KK	101	CLA	C4A-NA-C1A	5.95	109.38	106.71
24	B	849	AJP	OBG-CBF-OBQ	-5.95	92.49	109.74
19	BB	815	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	B2	850	CLA	C4A-NA-C1A	5.95	109.38	106.71
19	A2	831	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	A	835	CLA	C4A-NA-C1A	5.94	109.38	106.71
19	B	818	CLA	C4A-NA-C1A	5.94	109.38	106.71
24	L	209	AJP	OBQ-CBP-CBO	5.94	117.67	103.90
24	L	209	AJP	OBQ-CBF-CAW	5.93	122.86	108.58
24	A1	855	AJP	OBQ-CBP-CCK	5.92	122.52	110.23
19	B1	849	CLA	C4A-NA-C1A	5.92	109.37	106.71
19	B	811	CLA	C4A-NA-C1A	5.92	109.37	106.71
24	L	209	AJP	OCL-CCK-CBP	5.91	127.92	111.15
24	BB	848	AJP	OBQ-CBF-CAW	5.90	122.79	108.58
19	BB	836	CLA	CAC-C3C-C4C	5.90	132.53	124.82
19	B	815	CLA	C4A-NA-C1A	5.90	109.36	106.71
19	A	852	CLA	C4A-NA-C1A	5.88	109.35	106.71
19	A2	833	CLA	C4A-NA-C1A	5.87	109.35	106.71
19	BB	811	CLA	C4A-NA-C1A	5.87	109.35	106.71
19	A2	829	CLA	C4A-NA-C1A	5.87	109.34	106.71
19	A1	809	CLA	C4A-NA-C1A	5.87	109.34	106.71
24	A	802	AJP	OCL-CCK-CBP	5.86	127.76	111.15
24	AA	802	AJP	OCL-CCK-CBP	5.85	127.72	111.15
19	B2	829	CLA	C4A-NA-C1A	5.85	109.33	106.71
19	A1	811	CLA	C4A-NA-C1A	5.84	109.33	106.71
19	B	860	CLA	C4A-NA-C1A	5.83	109.33	106.71
19	A1	852	CLA	C4A-NA-C1A	5.82	109.32	106.71
24	L2	203	AJP	OCC-CCB-CCA	5.82	120.30	109.68
24	B	849	AJP	OCL-CCK-CBP	5.82	127.66	111.15
19	L1	207	CLA	C4A-NA-C1A	5.82	109.32	106.71
19	BB	829	CLA	C4A-NA-C1A	5.81	109.32	106.71
24	L	209	AJP	CBK-CCG-CDB	-5.79	100.44	110.34
19	B2	827	CLA	C4A-NA-C1A	5.79	109.31	106.71
24	B	849	AJP	CBL-CCH-CCG	5.79	120.74	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	811	CLA	C4A-NA-C1A	5.79	109.31	106.71
24	A1	854	AJP	OBQ-CBF-CAW	5.78	122.51	108.58
24	M2	101	AJP	CBK-CCG-CDB	-5.78	100.46	110.34
24	L2	202	AJP	OBQ-CBF-CAW	5.78	122.50	108.58
24	B	850	AJP	CBK-CCG-CDB	-5.76	100.50	110.34
24	L2	202	AJP	OBG-CBF-OBQ	-5.76	93.06	109.74
19	B1	816	CLA	C4A-NA-C1A	5.75	109.29	106.71
24	K	104	AJP	OCL-CCK-CBP	5.74	127.43	111.15
19	AA	820	CLA	C4A-NA-C1A	5.74	109.28	106.71
24	B	857	AJP	OBQ-CBF-CAW	5.74	122.40	108.58
19	AA	843	CLA	C4A-NA-C1A	5.73	109.28	106.71
24	BB	849	AJP	CAX-CAY-CBH	5.73	116.70	108.51
20	AA	803	CL0	CHB-C4A-NA	5.72	132.42	124.51
19	A	811	CLA	C4A-NA-C1A	5.72	109.28	106.71
19	BB	818	CLA	C4A-NA-C1A	5.72	109.28	106.71
24	BB	849	AJP	CBF-CBE-CBO	5.71	112.96	103.39
19	B2	852	CLA	C4A-NA-C1A	5.71	109.27	106.71
24	A2	854	AJP	OBQ-CBP-CCK	5.70	122.06	110.23
24	KK	104	AJP	OCC-CCX-CCW	5.69	118.58	110.10
24	I2	104	AJP	CAZ-CAY-CBH	5.69	121.40	111.22
24	B	850	AJP	OCL-CCK-CBP	5.69	127.28	111.15
24	L1	204	AJP	CAZ-CAY-CBH	5.69	121.39	111.22
19	AA	811	CLA	C4A-NA-C1A	5.69	109.26	106.71
24	M2	101	AJP	OCL-CCK-CBP	5.68	127.25	111.15
24	L2	203	AJP	CBK-CCG-CDB	-5.67	100.65	110.34
24	L1	204	AJP	CBK-CCG-CDB	-5.67	100.66	110.34
24	A1	854	AJP	OBG-CBF-OBQ	-5.67	93.32	109.74
19	LL	201	CLA	C4-C3-C5	5.66	125.04	115.29
24	L	208	AJP	CCG-CCH-CCI	5.66	118.43	112.42
24	L2	202	AJP	OCL-CCK-CBP	5.65	127.18	111.15
19	AA	810	CLA	C4A-NA-C1A	5.65	109.25	106.71
20	A1	802	CL0	CHB-C4A-NA	5.64	132.32	124.51
24	L	208	AJP	OBQ-CBP-CBO	5.64	116.98	103.90
24	KK	104	AJP	OCU-CCV-CCA	5.64	120.50	110.02
19	B1	820	CLA	C4A-NA-C1A	5.64	109.24	106.71
20	A1	802	CL0	O2D-CGD-CBD	5.64	121.11	111.25
24	BB	848	AJP	OBQ-CBP-CBO	5.63	116.96	103.90
24	I2	104	AJP	OCL-CCK-CBP	5.63	127.11	111.15
24	L	209	AJP	CDC-CDD-CCI	5.63	121.52	112.13
26	B	841	ECH	C19-C18-C17	5.63	127.58	118.94
20	A	803	CL0	CHB-C4A-NA	5.62	132.29	124.51
24	K	104	AJP	OCU-CCV-CCA	5.62	120.46	110.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	820	CLA	C4A-NA-C1A	5.61	109.23	106.71
24	L1	204	AJP	CAX-CAY-CBH	5.60	116.52	108.51
24	AA	802	AJP	CAZ-CAY-CBH	5.59	121.22	111.22
24	B	857	AJP	OBQ-CBP-CCK	5.59	121.82	110.23
19	A1	805	CLA	C4A-NA-C1A	5.59	109.22	106.71
24	L2	202	AJP	CBL-CCH-CCG	5.58	120.49	113.92
24	A	802	AJP	CAZ-CAY-CBH	5.58	121.19	111.22
24	B	849	AJP	OBQ-CBF-CAW	5.58	122.01	108.58
24	L2	203	AJP	OCL-CCK-CBP	5.57	126.95	111.15
24	A	802	AJP	OBG-CBF-OBQ	-5.57	93.59	109.74
24	L	208	AJP	OBQ-CBF-CAW	5.57	122.00	108.58
24	BB	849	AJP	CBL-CCH-CCG	5.57	120.48	113.92
24	L	208	AJP	CDC-CDD-CCI	5.56	121.39	112.13
19	AA	853	CLA	C4A-NA-C1A	5.56	109.20	106.71
24	B	857	AJP	OBG-CBF-OBQ	-5.55	93.65	109.74
24	B	850	AJP	OBQ-CBF-CAW	5.55	121.94	108.58
24	BB	848	AJP	OBG-CBF-OBQ	-5.55	93.67	109.74
19	AA	835	CLA	C4A-NA-C1A	5.54	109.20	106.71
24	AA	802	AJP	OBG-CBF-OBQ	-5.53	93.71	109.74
24	BB	849	AJP	CBK-CCG-CDB	-5.53	100.89	110.34
24	M2	101	AJP	CAX-CAY-CBH	5.53	116.41	108.51
19	B	834	CLA	C4A-NA-C1A	5.52	109.19	106.71
19	A	810	CLA	C4A-NA-C1A	5.52	109.19	106.71
19	A	820	CLA	C4A-NA-C1A	5.51	109.18	106.71
24	K	104	AJP	OCY-CCX-CCW	5.51	122.61	108.10
24	A1	855	AJP	OBQ-CBF-CAW	5.50	121.83	108.58
19	A1	842	CLA	C4A-NA-C1A	5.50	109.18	106.71
19	B1	811	CLA	C4A-NA-C1A	5.49	109.17	106.71
24	K	104	AJP	OCC-CCX-CCW	5.47	118.25	110.10
24	L	209	AJP	CAX-CAY-CBH	5.46	116.32	108.51
19	B	858	CLA	C4A-NA-C1A	5.46	109.16	106.71
24	BB	848	AJP	CBK-CCG-CDB	-5.45	101.03	110.34
24	L1	204	AJP	OBQ-CBF-CAW	5.44	121.69	108.58
24	A1	854	AJP	OBQ-CBP-CCK	5.41	121.46	110.23
24	L1	204	AJP	OCL-CCK-CBP	5.39	126.43	111.15
26	B2	841	ECH	C19-C18-C17	5.38	127.20	118.94
24	L2	203	AJP	CAZ-CAY-CBH	5.38	120.84	111.22
24	L	209	AJP	CBL-CCH-CCG	5.37	120.25	113.92
24	A	855	AJP	OBQ-CBP-CCK	5.37	121.36	110.23
24	L1	204	AJP	OCC-CCX-CCW	5.36	121.77	110.35
24	L	208	AJP	CAZ-CAY-CBH	5.36	120.80	111.22
19	BB	820	CLA	C4A-NA-C1A	5.35	109.11	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	856	AJP	OBQ-CBP-CCK	5.35	121.32	110.23
19	A1	819	CLA	C4A-NA-C1A	5.33	109.10	106.71
24	L	208	AJP	CAX-CAY-CBH	5.33	116.13	108.51
24	I2	104	AJP	CAX-CAY-CBH	5.33	116.13	108.51
20	AA	803	CL0	CAA-C2A-C1A	5.32	129.41	111.97
26	BB	840	ECH	C19-C18-C17	5.31	127.09	118.94
26	B1	840	ECH	C19-C18-C17	5.31	127.09	118.94
24	A	802	AJP	CAX-CAY-CBH	5.31	116.10	108.51
20	A1	802	CL0	CAA-C2A-C1A	5.31	129.36	111.97
24	AA	802	AJP	CAX-CAY-CBH	5.31	116.10	108.51
19	BB	833	CLA	C4A-NA-C1A	5.30	109.09	106.71
24	B	849	AJP	CBK-CCG-CDB	-5.28	101.31	110.34
19	B1	833	CLA	C4A-NA-C1A	5.28	109.08	106.71
24	I2	104	AJP	CBL-CCH-CCI	5.28	119.42	111.74
24	L	208	AJP	CBK-CCG-CDB	-5.28	101.32	110.34
24	A2	854	AJP	OBG-CBF-OBQ	-5.27	94.45	109.74
24	L	208	AJP	OCL-CCK-CBP	5.27	126.10	111.15
24	L	209	AJP	CAZ-CAY-CBH	5.27	120.65	111.22
19	B1	824	CLA	C4A-NA-C1A	5.27	109.08	106.71
19	A2	810	CLA	C4A-NA-C1A	5.27	109.08	106.71
24	L2	202	AJP	CBK-CCG-CDB	-5.26	101.34	110.34
24	L1	203	AJP	OBG-CBF-OBQ	-5.25	94.51	109.74
24	BB	848	AJP	OCC-CCB-CBJ	5.25	119.52	106.43
24	M2	101	AJP	CAZ-CAY-CBH	5.24	120.59	111.22
24	A1	855	AJP	OBG-CBF-OBQ	-5.24	94.56	109.74
24	AA	802	AJP	CBK-CCG-CDB	-5.24	101.39	110.34
24	BB	848	AJP	CBF-CBE-CBO	5.23	112.16	103.39
24	KK	104	AJP	OCY-CCX-CCW	5.22	121.85	108.10
24	A	802	AJP	CBK-CCG-CDB	-5.22	101.42	110.34
19	L	202	CLA	C4-C3-C5	5.21	124.27	115.29
24	L2	203	AJP	OCC-CCB-CBJ	5.21	119.42	106.43
24	L2	202	AJP	OCY-CCX-CCW	5.20	121.79	108.10
24	L1	203	AJP	OBQ-CBP-CCK	5.20	121.01	110.23
24	L1	203	AJP	ODG-CCW-CCX	5.19	122.70	110.06
24	A1	854	AJP	CBL-CCH-CCG	5.17	120.00	113.92
24	BB	849	AJP	CAZ-CAY-CBH	5.15	120.44	111.22
20	A2	803	CL0	CHB-C4A-NA	5.15	131.63	124.51
19	B2	820	CLA	CAC-C3C-C4C	5.15	131.55	124.82
24	L1	203	AJP	CBK-CCG-CDB	-5.14	101.55	110.34
20	A2	803	CL0	CMC-C2C-C1C	5.14	132.85	125.03
19	BB	820	CLA	CAC-C3C-C4C	5.14	131.53	124.82
24	L1	204	AJP	OCC-CCB-CBJ	5.13	119.23	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	820	CLA	CAC-C3C-C4C	5.11	131.50	124.82
24	M2	101	AJP	OBG-CBF-OBQ	-5.10	94.97	109.74
24	BB	848	AJP	ODG-CCW-CCX	5.09	122.48	110.06
24	B	849	AJP	ODG-CCW-CCX	5.09	122.48	110.06
24	BB	849	AJP	CAV-CBE-CBF	5.09	124.45	114.90
24	B	850	AJP	OBG-CBF-OBQ	-5.08	95.03	109.74
24	BB	848	AJP	OCL-CCK-CBP	5.07	125.51	111.15
24	A	855	AJP	CBL-CCH-CCG	5.05	119.87	113.92
24	L	208	AJP	OBG-CBF-OBQ	-5.05	95.11	109.74
26	B1	840	ECH	C24-C23-C22	-5.03	118.66	126.21
24	B	850	AJP	OCC-CCB-CBJ	5.02	118.94	106.43
24	AA	856	AJP	CBL-CCH-CCG	5.02	119.83	113.92
24	AA	856	AJP	CDD-CCI-CCH	-5.01	104.21	110.50
24	BB	849	AJP	OBG-CBF-OBQ	-5.00	95.24	109.74
24	B	857	AJP	CDD-CCI-CCH	-4.99	104.23	110.50
24	A	855	AJP	CDD-CCI-CCH	-4.99	104.24	110.50
26	B	841	ECH	C24-C23-C22	-4.99	118.71	126.21
24	L	209	AJP	CCG-CCH-CCI	4.98	117.72	112.42
24	M2	101	AJP	CBL-CCH-CCG	4.98	119.79	113.92
24	L1	204	AJP	CAV-CBE-CBF	4.96	124.22	114.90
24	M2	101	AJP	CDC-CDD-CCI	4.95	120.39	112.13
19	LL	203	CLA	CMB-C2B-C1B	-4.95	120.86	128.46
24	A1	854	AJP	CDD-CCI-CCH	-4.95	104.30	110.50
24	BB	848	AJP	CCA-CCV-CCW	4.94	119.50	110.82
28	BB	854	DGD	O3G-C3G-C2G	-4.93	99.00	110.90
24	B	857	AJP	CBL-CCH-CCG	4.93	119.73	113.92
24	L2	202	AJP	CCG-CCH-CCI	4.92	117.65	112.42
24	L1	203	AJP	CCG-CCH-CCI	4.92	117.65	112.42
24	AA	802	AJP	CCH-CCG-CDB	4.90	115.56	108.59
24	A	802	AJP	CCH-CCG-CDB	4.89	115.54	108.59
24	BB	849	AJP	OCC-CCB-CBJ	4.89	118.61	106.43
24	L2	203	AJP	OCC-CCX-CCW	4.88	120.76	110.35
24	L	209	AJP	CAV-CBE-CBF	4.88	124.06	114.90
24	K	104	AJP	ODG-CCW-CCX	4.88	121.95	110.06
20	A2	803	CL0	O1D-CGD-CBD	-4.87	114.39	124.48
19	B	815	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
24	L	209	AJP	OBG-CBF-OBQ	-4.86	95.65	109.74
24	M2	101	AJP	CCG-CCH-CCI	4.86	117.58	112.42
24	AA	856	AJP	OBG-CBF-OBQ	-4.85	95.68	109.74
24	A	855	AJP	OBG-CBF-OBQ	-4.84	95.71	109.74
24	A	802	AJP	CCF-CCG-CDB	4.84	115.04	107.77
24	B	849	AJP	CCA-CCV-CCW	4.84	119.32	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	834	CLA	C4A-NA-C1A	4.84	108.88	106.71
26	BB	840	ECH	C24-C23-C22	-4.84	118.95	126.21
24	B	849	AJP	OCC-CCB-CBJ	4.83	118.47	106.43
19	BB	826	CLA	CMB-C2B-C1B	-4.83	121.05	128.46
24	M2	101	AJP	CAV-CBE-CBF	4.81	123.93	114.90
24	AA	802	AJP	CCF-CCG-CDB	4.81	114.99	107.77
19	B2	820	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	L2	203	AJP	CAV-CBE-CBF	4.78	123.88	114.90
24	KK	104	AJP	ODG-CCW-CCX	4.77	121.70	110.06
28	B	856	DGD	O3G-C3G-C2G	-4.77	99.39	110.90
19	B1	833	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
19	BB	833	CLA	CMB-C2B-C1B	-4.77	121.14	128.46
24	B	850	AJP	OCC-CCX-CCW	4.74	120.45	110.35
26	B2	841	ECH	C24-C23-C22	-4.73	119.11	126.21
19	BB	815	CLA	CMB-C2B-C1B	-4.72	121.21	128.46
24	L	209	AJP	CCJ-CCI-CCH	-4.72	100.98	109.25
26	B	841	ECH	C36-C18-C19	-4.71	110.63	118.09
19	B	834	CLA	CMB-C2B-C1B	-4.68	121.27	128.46
24	KK	104	AJP	OBG-CBF-OBQ	-4.68	96.18	109.74
24	L1	203	AJP	OCC-CCB-CBJ	4.68	118.09	106.43
20	A2	803	CL0	C1C-C2C-C3C	-4.66	102.01	106.95
24	BB	849	AJP	CCG-CCH-CCI	4.63	117.34	112.42
20	A2	803	CL0	CAA-C2A-C1A	4.63	127.14	111.97
24	I2	104	AJP	CAV-CBE-CBF	4.62	123.57	114.90
24	A1	855	AJP	CCJ-CBN-CBO	-4.62	92.16	100.22
24	A2	854	AJP	CCJ-CBN-CBO	-4.61	92.17	100.22
19	A2	810	CLA	CAA-C2A-C1A	-4.60	96.91	111.97
24	L	208	AJP	CBL-CCH-CCI	4.58	118.41	111.74
24	L1	203	AJP	OBQ-CBF-CAW	4.57	119.59	108.58
19	AA	810	CLA	CAA-C2A-C1A	-4.56	97.02	111.97
24	L2	202	AJP	OCC-CCX-CCW	4.56	120.07	110.35
24	I2	104	AJP	CDD-CCI-CCH	-4.54	104.80	110.50
24	BB	848	AJP	CAX-CAY-CBH	4.52	114.97	108.51
24	L2	202	AJP	ODG-CCW-CCX	4.50	121.02	110.06
24	B	849	AJP	CCG-CCH-CCI	4.50	117.20	112.42
19	B2	834	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
24	L2	203	AJP	ODG-CCW-CCV	4.46	120.71	110.34
24	AA	802	AJP	CAV-CBE-CBF	4.46	123.27	114.90
20	A2	803	CL0	O2D-CGD-O1D	-4.44	115.07	123.83
24	A	802	AJP	CAV-CBE-CBF	4.43	123.22	114.90
24	L1	204	AJP	ODG-CCW-CCV	4.43	120.62	110.34
24	L2	202	AJP	CCX-OCC-CCB	4.42	122.41	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	849	AJP	CAZ-CAY-CBH	4.41	119.10	111.22
24	BB	849	AJP	OCC-CCX-CCW	4.40	119.74	110.35
26	BB	840	ECH	C36-C18-C19	-4.40	111.11	118.09
24	BB	849	AJP	CCA-CCV-CCW	4.40	118.55	110.82
24	KK	104	AJP	OCY-CCX-OCC	4.39	118.60	109.20
26	B2	841	ECH	C36-C18-C19	-4.39	111.14	118.09
24	B	850	AJP	CCA-CCV-CCW	4.38	118.51	110.82
24	I2	104	AJP	CBM-CBL-CCH	4.38	120.74	113.12
24	K	104	AJP	OBG-CBF-OBQ	-4.37	97.08	109.74
24	L2	203	AJP	CCG-CCH-CCI	4.37	117.06	112.42
24	BB	848	AJP	OCL-CCK-CCJ	4.36	129.07	113.73
24	L1	204	AJP	OBG-CBF-OBQ	-4.35	97.14	109.74
19	B	860	CLA	CAC-C3C-C2C	-4.34	120.11	127.53
24	K	104	AJP	OCU-CCV-CCW	4.34	120.42	110.34
26	B1	840	ECH	C36-C18-C19	-4.34	111.21	118.09
24	KK	104	AJP	CCG-CCH-CCI	4.33	117.03	112.42
19	B1	815	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
20	A1	802	CL0	C3C-C4C-NC	4.33	115.43	110.57
24	KK	104	AJP	OCU-CCV-CCW	4.33	120.39	110.34
20	A	803	CL0	C1C-C2C-C3C	-4.32	102.37	106.95
20	A1	802	CL0	C1C-C2C-C3C	-4.32	102.37	106.95
24	K	104	AJP	CAZ-CAY-CBH	4.31	118.94	111.22
24	KK	104	AJP	ODG-CCW-CCV	4.31	120.36	110.34
24	AA	856	AJP	CCJ-CBN-CBO	-4.31	92.70	100.22
24	M2	101	AJP	CCJ-CCI-CCH	-4.31	101.69	109.25
24	L2	203	AJP	CCA-CCV-CCW	4.31	118.38	110.82
24	A	855	AJP	CCJ-CBN-CBO	-4.30	92.71	100.22
24	BB	848	AJP	OCU-CCV-CCA	4.30	120.32	110.34
24	B	849	AJP	CCJ-CCI-CCH	-4.29	101.72	109.25
24	K	104	AJP	CCG-CCH-CCI	4.29	116.97	112.42
19	AA	843	CLA	CAC-C3C-C2C	-4.29	120.21	127.53
24	L	208	AJP	OCL-CCK-CCJ	4.28	128.80	113.73
24	BB	848	AJP	CAV-CBE-CBF	4.28	122.93	114.90
24	A1	854	AJP	CCJ-CBN-CBO	-4.28	92.76	100.22
24	L1	204	AJP	OCU-CCV-CCW	4.27	120.26	110.34
19	A1	842	CLA	CAC-C3C-C2C	-4.26	120.25	127.53
21	A1	843	PQN	C14-C13-C15	4.26	122.62	115.29
20	AA	803	CL0	O2D-CGD-O1D	-4.25	115.43	123.83
24	L2	202	AJP	OCU-CCV-CCA	4.25	120.20	110.34
24	I2	104	AJP	OBG-CBF-OBQ	-4.25	97.43	109.74
19	B2	852	CLA	CAC-C3C-C2C	-4.25	120.28	127.53
24	B	850	AJP	ODG-CCW-CCV	4.24	120.19	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L1	203	AJP	OCU-CCV-CCA	4.24	120.19	110.34
24	BB	849	AJP	OCY-CCX-CCW	4.23	119.23	108.10
24	L2	202	AJP	OCU-CCV-CCW	4.23	120.16	110.34
19	B2	826	CLA	CMB-C2B-C1B	-4.23	121.97	128.46
24	B	850	AJP	CAV-CBE-CBF	4.23	122.83	114.90
19	A	810	CLA	CAA-C2A-C1A	-4.23	98.13	111.97
24	BB	849	AJP	OCL-CCK-CCJ	4.22	128.58	113.73
20	AA	803	CL0	O1D-CGD-CBD	-4.22	115.74	124.48
24	K	104	AJP	ODG-CCW-CCV	4.21	120.12	110.34
19	BB	803	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
24	L1	203	AJP	CCA-CCV-CCW	4.21	118.22	110.82
24	L1	203	AJP	OCU-CCV-CCW	4.21	120.11	110.34
19	B2	807	CLA	O2D-CGD-CBD	4.21	118.61	111.25
24	AA	802	AJP	CCF-CCE-CCZ	4.20	117.92	111.38
19	L1	207	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
26	BB	840	ECH	C16-C15-C14	-4.20	114.69	123.51
24	BB	849	AJP	ODG-CCW-CCX	4.20	120.29	110.06
24	AA	802	AJP	OCL-CCK-CCJ	4.19	128.49	113.73
24	L	208	AJP	CDC-CDB-CCG	4.19	120.04	112.31
24	A	802	AJP	OCL-CCK-CCJ	4.19	128.48	113.73
24	L1	204	AJP	OCU-CCV-CCA	4.19	120.07	110.34
21	A2	843	PQN	C14-C13-C15	4.19	122.50	115.29
19	BB	833	CLA	CMB-C2B-C3B	4.18	132.65	124.80
24	KK	104	AJP	CAV-CBE-CBF	4.18	122.75	114.90
24	K	104	AJP	OCY-CCX-OCC	4.18	118.14	109.20
24	B	850	AJP	OCU-CCV-CCW	4.17	120.04	110.34
24	KK	104	AJP	CAZ-CAY-CBH	4.17	118.69	111.22
24	L1	204	AJP	CBM-CBL-CCH	4.16	120.37	113.12
24	B	857	AJP	CCJ-CBN-CBO	-4.16	92.96	100.22
24	L2	202	AJP	OCC-CCB-CBJ	4.16	116.80	106.43
24	A	802	AJP	CCF-CCE-CCZ	4.16	117.85	111.38
20	A2	803	CL0	CAC-C3C-C4C	4.15	130.25	124.82
19	AA	805	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
19	B	803	CLA	CMB-C2B-C1B	-4.15	122.08	128.46
24	BB	849	AJP	OCU-CCV-CCW	4.15	119.98	110.34
24	B	850	AJP	OCY-CCX-CCW	4.14	119.00	108.10
24	L2	203	AJP	OCU-CCV-CCW	4.14	119.95	110.34
20	A	803	CL0	O2A-CGA-CBA	4.14	125.21	111.93
24	BB	849	AJP	ODG-CCW-CCV	4.13	119.94	110.34
19	B1	826	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
24	B	849	AJP	CAV-CBE-CBF	4.13	122.65	114.90
24	L2	203	AJP	OCU-CCV-CCA	4.13	119.92	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	850	AJP	ODG-CCW-CCX	4.12	120.10	110.06
24	I2	104	AJP	CCG-CCH-CCI	4.12	116.80	112.42
24	B	850	AJP	CCG-CCH-CCI	4.12	116.80	112.42
21	A	843	PQN	C14-C13-C15	4.11	122.37	115.29
19	B	815	CLA	CMB-C2B-C3B	4.11	132.51	124.80
24	L2	202	AJP	CCA-CCV-CCW	4.11	118.04	110.82
19	B2	803	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
19	A	852	CLA	C7-C6-C5	4.10	124.27	113.25
24	L1	204	AJP	CAV-CBE-CBO	4.10	123.79	114.54
19	L2	206	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
20	AA	803	CL0	CAC-C3C-C4C	4.09	130.17	124.82
24	L2	203	AJP	OCY-CCX-CCW	4.09	118.88	108.10
19	A	805	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
24	K	104	AJP	CAV-CBE-CBF	4.09	122.58	114.90
24	L2	203	AJP	ODG-CCW-CCX	4.08	120.01	110.06
19	B	834	CLA	CMB-C2B-C3B	4.08	132.45	124.80
24	BB	849	AJP	OCU-CCV-CCA	4.08	119.82	110.34
24	B	850	AJP	CAZ-CAY-CBH	4.07	118.51	111.22
19	B	846	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
19	B1	833	CLA	CMB-C2B-C3B	4.06	132.42	124.80
24	L1	204	AJP	CCA-CCV-CCW	4.06	117.95	110.82
23	F1	306	BCR	C15-C16-C17	-4.06	114.99	123.51
24	B	850	AJP	OCU-CCV-CCA	4.05	119.74	110.34
19	BB	845	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
23	F2	305	BCR	C15-C16-C17	-4.05	115.00	123.51
24	L2	203	AJP	OBQ-CBF-CBE	-4.04	98.28	104.44
19	B1	807	CLA	O2D-CGD-CBD	4.04	118.32	111.25
24	L2	202	AJP	ODG-CCW-CCV	4.04	119.72	110.34
19	L	204	CLA	CMB-C2B-C1B	-4.04	122.26	128.46
19	BB	807	CLA	O2D-CGD-CBD	4.04	118.31	111.25
24	L1	204	AJP	CCG-CCH-CCI	4.03	116.70	112.42
24	L1	203	AJP	CCX-OCC-CCB	4.02	121.62	113.70
24	L2	203	AJP	CAV-CBE-CBO	4.02	123.61	114.54
24	L1	204	AJP	CCX-CCW-CCV	4.02	118.38	109.98
24	B	850	AJP	CCX-CCW-CCV	4.02	118.37	109.98
24	L2	203	AJP	CBM-CBL-CCH	4.01	120.11	113.12
24	BB	849	AJP	CCX-CCW-CCV	4.01	118.36	109.98
20	AA	803	CL0	C1C-C2C-C3C	-4.01	102.70	106.95
24	L2	202	AJP	OCL-CCK-CCJ	4.01	127.83	113.73
24	B	849	AJP	CCX-CCW-CCV	4.01	118.35	109.98
19	B	814	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
19	B2	815	CLA	CMB-C2B-C1B	-3.98	122.35	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	B	850	AJP	CBM-CBL-CCH	3.98	120.05	113.12
24	M2	101	AJP	OCL-CCK-CCJ	3.98	127.72	113.73
24	L1	204	AJP	ODG-CCW-CCX	3.98	119.75	110.06
24	B	849	AJP	OCU-CCV-CCA	3.97	119.55	110.34
19	B1	828	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
24	B	849	AJP	OCU-CCV-CCW	3.96	119.53	110.34
19	B	829	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
24	L1	204	AJP	OBQ-CBF-CBE	-3.94	98.43	104.44
19	A2	852	CLA	C7-C6-C5	3.94	123.85	113.25
24	L	209	AJP	CDC-CDB-CCG	3.94	119.58	112.31
24	L2	202	AJP	CCJ-CCI-CCH	-3.94	102.34	109.25
24	K	104	AJP	CBM-CBL-CCH	3.93	119.96	113.12
24	B	850	AJP	OCL-CCK-CCJ	3.93	127.55	113.73
24	KK	104	AJP	OCL-CCK-CCJ	3.92	127.53	113.73
24	BB	848	AJP	CCX-CCW-CCV	3.92	118.17	109.98
19	BB	815	CLA	CMB-C2B-C3B	3.91	132.14	124.80
20	AA	803	CL0	C3C-C4C-NC	3.91	114.96	110.57
24	K	104	AJP	OCL-CCK-CCJ	3.91	127.50	113.73
19	A2	805	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
24	L1	203	AJP	CCJ-CBN-CBO	-3.91	93.41	100.22
19	B	807	CLA	O2D-CGD-CBD	3.90	118.08	111.25
24	A	855	AJP	CCH-CCG-CDB	3.90	114.14	108.59
24	AA	856	AJP	CCH-CCG-CDB	3.89	114.12	108.59
19	LL	201	CLA	C6-C5-C3	3.89	122.35	113.01
19	A2	837	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
24	L	209	AJP	OCL-CCK-CCJ	3.89	127.41	113.73
24	L2	202	AJP	CAZ-CAY-CBH	3.88	118.16	111.22
24	B	849	AJP	OCC-CCX-CCW	3.88	118.61	110.35
24	I2	104	AJP	OCL-CCK-CCJ	3.87	127.36	113.73
24	L	208	AJP	CAV-CBE-CBF	3.87	122.16	114.90
24	L1	203	AJP	OCC-CCX-CCW	3.86	118.58	110.35
24	L2	203	AJP	CCX-CCW-CCV	3.85	118.03	109.98
19	KK	101	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
24	L1	203	AJP	CCJ-CCI-CCH	-3.85	102.50	109.25
26	B	841	ECH	C33-C5-C6	-3.85	120.23	124.51
19	B2	807	CLA	O2D-CGD-O1D	-3.84	116.24	123.83
19	L	203	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
19	BB	834	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
24	L2	203	AJP	CBF-CBE-CBO	3.84	109.82	103.39
24	BB	849	AJP	CBM-CBL-CCH	3.83	119.80	113.12
19	FF	305	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
24	BB	848	AJP	OCC-CCX-CCW	3.83	118.52	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	K	104	AJP	CCA-CCV-CCW	3.83	117.54	110.89
19	B2	846	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
24	L	208	AJP	CAZ-CAY-CAX	3.83	120.58	112.08
19	B	826	CLA	CMB-C2B-C1B	-3.82	122.59	128.46
24	L2	202	AJP	CCX-CCW-CCV	3.81	117.95	109.98
24	KK	104	AJP	CCA-CCV-CCW	3.81	117.50	110.89
19	AA	824	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
19	A2	823	CLA	O2D-CGD-O1D	-3.81	116.31	123.83
19	AA	838	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
24	B	849	AJP	OCL-CKK-CCJ	3.81	127.12	113.73
19	B1	845	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
19	B2	833	CLA	CGD-CBD-CAD	-3.79	98.44	110.73
19	A	837	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
20	A2	803	CL0	C3B-C4B-NB	3.79	114.11	109.21
19	B1	807	CLA	O2D-CGD-O1D	-3.78	116.37	123.83
19	B2	829	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	A	823	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	A1	837	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	K	101	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
19	BB	807	CLA	O2D-CGD-O1D	-3.76	116.41	123.83
19	AA	829	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
20	A	803	CL0	C3C-C4C-NC	3.75	114.77	110.57
23	J	104	BCR	C2-C1-C6	3.75	116.28	110.48
24	BB	848	AJP	CAV-CBE-CBO	3.74	122.98	114.54
19	AA	837	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	AA	823	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	A	824	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
19	LL	203	CLA	CMB-C2B-C3B	3.73	131.80	124.80
24	L	209	AJP	CAZ-CAY-CAX	3.73	120.36	112.08
19	AA	835	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
19	AA	820	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
24	L1	203	AJP	CCX-CCW-CCV	3.72	117.75	109.98
19	A2	832	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	M2	101	AJP	CAZ-CAY-CAX	3.71	120.32	112.08
19	B	807	CLA	O2D-CGD-O1D	-3.71	116.50	123.83
19	A	831	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	L2	202	AJP	CAV-CBE-CBF	3.71	121.86	114.90
19	A1	836	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
19	B1	833	CLA	O2D-CGD-CBD	3.70	117.73	111.25
24	BB	849	AJP	CAZ-CAY-CAX	3.70	120.29	112.08
23	BB	841	BCR	C15-C14-C13	-3.70	122.03	127.31
19	B1	825	CLA	O2D-CGD-O1D	-3.70	116.53	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	842	BCR	C15-C14-C13	-3.69	122.04	127.31
19	B	821	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
19	BB	814	CLA	CMB-C2B-C1B	-3.69	122.80	128.46
26	B2	841	ECH	C33-C5-C6	-3.69	120.40	124.51
26	BB	840	ECH	C33-C5-C6	-3.69	120.41	124.51
20	AA	803	CL0	C3B-C4B-NB	3.69	113.98	109.21
26	B1	840	ECH	C33-C5-C6	-3.69	120.41	124.51
26	BB	840	ECH	C12-C13-C14	-3.68	113.29	118.94
20	A2	803	CL0	C3C-C4C-NC	3.68	114.70	110.57
23	BB	847	BCR	C15-C16-C17	-3.67	115.80	123.51
26	B1	840	ECH	C16-C15-C14	-3.67	115.80	123.51
24	AA	802	AJP	CBL-CCH-CCI	3.67	117.08	111.74
19	A2	823	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
19	A	839	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
19	A2	831	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
24	L1	203	AJP	CAW-CBF-CBE	3.65	123.43	115.72
23	F1	306	BCR	C15-C14-C13	-3.65	122.10	127.31
19	B2	825	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
23	F2	305	BCR	C15-C14-C13	-3.65	122.10	127.31
19	B	825	CLA	O2D-CGD-O1D	-3.65	116.63	123.83
19	A	838	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
19	A1	823	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
19	B	801	CLA	O2D-CGD-O1D	-3.64	116.64	123.83
24	A1	855	AJP	CCH-CCG-CDB	3.64	113.76	108.59
21	AA	844	PQN	C14-C13-C15	3.64	121.55	115.29
24	A	802	AJP	CBL-CCH-CCI	3.64	117.03	111.74
19	B	825	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
19	BB	803	CLA	CMB-C2B-C3B	3.63	131.61	124.80
20	A1	802	CL0	O1D-CGD-CBD	-3.63	116.97	124.48
19	B2	834	CLA	O2D-CGD-O1D	-3.63	116.67	123.83
19	BB	825	CLA	O2D-CGD-O1D	-3.62	116.68	123.83
24	L1	204	AJP	CBF-CBE-CBO	3.62	109.46	103.39
19	AA	839	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
19	B2	834	CLA	CMB-C2B-C3B	3.62	131.59	124.80
23	B	848	BCR	C15-C16-C17	-3.62	115.91	123.51
19	B1	803	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
19	B2	834	CLA	O2D-CGD-CBD	3.61	117.58	111.25
19	A1	830	CLA	CMB-C2B-C1B	-3.60	122.92	128.46
19	BB	836	CLA	CAC-C3C-C2C	-3.60	121.38	127.53
19	BB	825	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
19	B	801	CLA	C4-C3-C2	-3.60	114.33	123.68
19	B1	815	CLA	CMB-C2B-C3B	3.59	131.54	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	802	AJP	CAZ-CAY-CAX	3.59	120.06	112.08
26	B1	840	ECH	C7-C8-C9	-3.59	120.82	126.21
20	A	803	CL0	C3B-C4B-NB	3.59	113.85	109.21
23	F	305	BCR	C15-C16-C17	-3.59	115.96	123.51
19	B	812	CLA	O2D-CGD-O1D	-3.59	116.74	123.83
19	A1	828	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
24	M2	101	AJP	CDC-CDB-CCG	3.59	118.92	112.31
19	BB	816	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
24	BB	848	AJP	CDC-CDB-CCG	3.58	118.92	112.31
23	B2	842	BCR	C1-C6-C5	-3.58	117.59	122.59
24	AA	802	AJP	CAZ-CAY-CAX	3.58	120.03	112.08
24	L1	204	AJP	OCY-CCX-CCW	3.57	117.51	108.10
24	L1	203	AJP	CDA-CDB-CCG	3.57	116.48	112.65
24	L	208	AJP	CDA-CDB-CDC	-3.57	107.17	112.56
19	L	202	CLA	C6-C5-C3	3.57	121.58	113.01
26	B2	841	ECH	C7-C8-C9	-3.57	120.86	126.21
24	A2	854	AJP	CCH-CCG-CDB	3.56	113.66	108.59
19	B2	801	CLA	O2D-CGD-O1D	-3.56	116.79	123.83
26	B2	841	ECH	C16-C15-C14	-3.56	116.03	123.51
19	A2	824	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
19	B2	803	CLA	CMB-C2B-C3B	3.55	131.47	124.80
19	A	829	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
20	A1	802	CL0	C3B-C4B-NB	3.55	113.80	109.21
19	A1	838	CLA	CMB-C2B-C1B	-3.55	123.01	128.46
19	A2	839	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
19	B	803	CLA	CMB-C2B-C3B	3.54	131.44	124.80
19	L2	205	CLA	CMB-C2B-C1B	-3.54	123.03	128.46
19	B2	825	CLA	O2D-CGD-O1D	-3.54	116.85	123.83
24	BB	848	AJP	OCU-CCV-CCW	3.53	118.55	110.34
24	BB	848	AJP	CCJ-CCI-CCH	-3.53	103.05	109.25
19	A2	823	CLA	O2D-CGD-CBD	3.53	117.43	111.25
19	B1	801	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
23	F1	304	BCR	C24-C23-C22	-3.53	120.91	126.21
23	FF	306	BCR	C15-C14-C13	-3.53	122.28	127.31
19	A	810	CLA	CMB-C2B-C1B	-3.52	123.05	128.46
19	BB	801	CLA	O2D-CGD-CBD	3.52	117.41	111.25
19	B	835	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
28	BB	854	DGD	O6D-C1D-O3G	-3.51	101.64	109.94
19	A1	819	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
23	J1	102	BCR	C15-C16-C17	-3.51	116.13	123.51
19	AA	831	CLA	CMB-C2B-C1B	-3.51	123.07	128.46
26	B	841	ECH	C7-C8-C9	-3.50	120.95	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	FF	306	BCR	C15-C16-C17	-3.50	116.15	123.51
19	B1	825	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
19	B2	850	CLA	CMB-C2B-C1B	-3.50	123.08	128.46
24	I2	104	AJP	CAZ-CAY-CAX	3.50	119.86	112.08
19	BB	808	CLA	CMB-C2B-C1B	-3.49	123.09	128.46
19	BB	801	CLA	O2D-CGD-O1D	-3.49	116.93	123.83
19	A	820	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
19	B	836	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
19	F	301	CLA	O2D-CGD-CBD	3.48	117.35	111.25
23	J	102	BCR	C15-C16-C17	-3.48	116.20	123.51
26	B	841	ECH	C16-C15-C14	-3.47	116.22	123.51
20	A	803	CL0	O1D-CGD-CBD	-3.46	117.31	124.48
19	B2	801	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
23	A1	850	BCR	C15-C16-C17	-3.46	116.24	123.51
19	AA	832	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
19	F	302	CLA	O2D-CGD-O1D	-3.46	117.00	123.83
23	F	305	BCR	C15-C14-C13	-3.46	122.38	127.31
19	B1	830	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
19	B2	816	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	B2	842	BCR	C15-C16-C17	-3.45	116.26	123.51
19	F2	302	CLA	O2D-CGD-O1D	-3.45	117.02	123.83
19	B2	831	CLA	CMB-C2B-C1B	-3.44	123.18	128.46
19	B	816	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	AA	854	BCR	C15-C16-C17	-3.43	116.30	123.51
23	A2	850	BCR	C15-C16-C17	-3.43	116.30	123.51
19	L2	206	CLA	CMB-C2B-C3B	3.43	131.23	124.80
23	J2	102	BCR	C15-C16-C17	-3.43	116.31	123.51
19	A2	832	CLA	O2D-CGD-O1D	-3.43	117.06	123.83
19	K1	103	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	A	840	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
19	A1	808	CLA	CMB-C2B-C1B	-3.42	123.20	128.46
24	KK	104	AJP	CDA-CDB-CCG	3.42	116.32	112.65
19	BB	855	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	A	822	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	K1	102	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
19	B2	812	CLA	O2D-CGD-O1D	-3.42	117.08	123.83
24	L1	204	AJP	CAZ-CAY-CAX	3.42	119.67	112.08
19	BB	807	CLA	CMB-C2B-C1B	-3.42	123.22	128.46
23	A	853	BCR	C15-C16-C17	-3.41	116.33	123.51
19	A	814	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
19	B	801	CLA	O2D-CGD-CBD	3.41	117.23	111.25
19	B2	835	CLA	CMB-C2B-C1B	-3.41	123.22	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	849	AJP	OCY-CCX-OCC	3.41	120.26	110.67
19	KK	101	CLA	O2D-CGD-O1D	-3.41	117.10	123.83
24	L1	204	AJP	OCY-CCX-OCC	3.40	120.25	110.67
19	A1	831	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
19	AA	838	CLA	O2D-CGD-O1D	-3.40	117.11	123.83
23	JJ	102	BCR	C15-C16-C17	-3.40	116.36	123.51
20	AA	803	CL0	CMC-C2C-C1C	3.40	130.21	125.03
23	B1	841	BCR	C15-C14-C13	-3.40	122.46	127.31
28	B	856	DGD	O6D-C1D-O3G	-3.40	101.91	109.94
19	B2	807	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
24	L	208	AJP	CDD-CDC-CDB	3.40	118.77	111.87
24	BB	848	AJP	CAZ-CAY-CAX	3.40	119.63	112.08
19	B1	834	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
19	B2	849	CLA	CMD-C2D-C3D	3.39	131.16	124.80
19	L1	207	CLA	CMB-C2B-C3B	3.39	131.16	124.80
19	K	101	CLA	O2D-CGD-O1D	-3.39	117.14	123.83
23	FF	303	BCR	C35-C13-C14	-3.39	118.17	122.92
19	BB	856	CLA	CHB-C4A-NA	3.39	129.20	124.51
19	F1	301	CLA	O2D-CGD-O1D	-3.39	117.14	123.83
23	L	205	BCR	C15-C16-C17	-3.39	116.39	123.51
19	A2	806	CLA	CAA-C2A-C1A	-3.39	100.88	111.97
19	A	838	CLA	O2D-CGD-O1D	-3.38	117.15	123.83
19	AA	805	CLA	CMB-C2B-C3B	3.38	131.14	124.80
19	A1	852	CLA	C7-C6-C5	3.38	122.35	113.25
19	K1	102	CLA	O2D-CGD-O1D	-3.38	117.15	123.83
19	B	858	CLA	O2D-CGD-O1D	-3.38	117.15	123.83
19	F1	301	CLA	CAA-C2A-C3A	-3.38	103.53	112.78
19	B1	824	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
19	A1	822	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
19	BB	809	CLA	O2D-CGD-O1D	-3.37	117.17	123.83
19	BB	833	CLA	O2D-CGD-O1D	-3.37	117.17	123.83
19	F	301	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	B	806	CLA	C5-C3-C2	3.37	128.04	121.11
19	FF	302	CLA	O2D-CGD-O1D	-3.37	117.18	123.83
19	L1	206	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
19	A2	838	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	A	832	CLA	O2D-CGD-O1D	-3.36	117.19	123.83
19	A1	812	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	B1	807	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
19	A	812	CLA	CMB-C2B-C1B	-3.36	123.31	128.46
24	L	208	AJP	CAV-CBE-CBO	3.35	122.11	114.54
23	A	851	BCR	C2-C1-C6	3.35	115.67	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	820	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
19	BB	805	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
19	B	859	CLA	CHB-C4A-NA	3.35	129.15	124.51
19	FF	301	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
19	A	835	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
23	F	304	BCR	C24-C23-C22	-3.34	121.19	126.21
19	A2	802	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
20	A1	802	CL0	O2D-CGD-O1D	-3.34	117.23	123.83
24	L2	203	AJP	CCJ-CCI-CCH	-3.34	103.39	109.25
24	L2	203	AJP	CAZ-CAY-CAX	3.34	119.49	112.08
23	FF	304	BCR	C24-C23-C22	-3.34	121.20	126.21
19	A	823	CLA	O2D-CGD-O1D	-3.33	117.24	123.83
24	KK	104	AJP	CBM-CBL-CCH	3.33	118.92	113.12
19	A	805	CLA	CMB-C2B-C3B	3.33	131.04	124.80
19	A1	814	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
19	BB	810	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
19	A1	819	CLA	CMB-C2B-C3B	3.33	131.04	124.80
19	B	810	CLA	CMB-C2B-C1B	-3.32	123.35	128.46
19	B1	801	CLA	O2D-CGD-O1D	-3.32	117.27	123.83
24	A2	854	AJP	CDA-CCZ-CCE	3.32	114.39	110.27
19	B1	816	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	A2	815	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	BB	806	CLA	C5-C3-C2	3.32	127.92	121.11
19	B	820	CLA	C1D-CHD-C4C	3.32	127.02	122.48
24	L2	202	AJP	CBM-CBL-CCH	3.31	118.89	113.12
24	BB	848	AJP	CCG-CCH-CCI	3.31	115.94	112.42
19	B2	805	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	A2	829	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	B2	851	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
19	B	820	CLA	O2D-CGD-O1D	-3.31	117.29	123.83
19	A1	831	CLA	O2D-CGD-O1D	-3.31	117.29	123.83
19	BB	836	CLA	O2D-CGD-O1D	-3.31	117.30	123.83
19	F1	302	CLA	O2D-CGD-O1D	-3.31	117.30	123.83
24	L2	203	AJP	OCY-CCX-OCC	3.31	119.98	110.67
19	A1	827	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
19	F1	305	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
19	B1	812	CLA	O2D-CGD-O1D	-3.30	117.31	123.83
19	A1	805	CLA	O2D-CGD-O1D	-3.30	117.31	123.83
19	B	833	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
19	B	821	CLA	CMB-C2B-C3B	3.30	130.99	124.80
23	F	303	BCR	C35-C13-C14	-3.30	118.31	122.92
19	A2	813	CLA	CMB-C2B-C1B	-3.30	123.40	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	812	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
19	B1	836	CLA	O2D-CGD-O1D	-3.29	117.33	123.83
19	B2	837	CLA	O2D-CGD-O1D	-3.29	117.33	123.83
19	B	805	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	K2	102	CLA	O2D-CGD-O1D	-3.29	117.33	123.83
19	A1	813	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	KK	102	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	BB	812	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
19	B1	814	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
19	BB	801	CLA	CHB-C4A-NA	3.28	129.05	124.51
19	L	203	CLA	O2D-CGD-O1D	-3.28	117.35	123.83
19	BB	836	CLA	CHB-C4A-NA	3.28	129.05	124.51
24	B	849	AJP	CDC-CDB-CCG	3.28	118.36	112.31
24	L2	202	AJP	CDA-CDB-CCG	3.28	116.17	112.65
19	AA	828	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	K1	105	CLA	CBD-CHA-C1A	3.28	132.49	128.57
19	A2	814	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
19	B	807	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
26	BB	840	ECH	C7-C8-C9	-3.28	121.29	126.21
19	B1	850	CLA	CHB-C4A-NA	3.27	129.04	124.51
24	B	849	AJP	OBG-CBF-CAW	3.27	113.91	110.81
19	A2	809	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
19	B	824	CLA	CMB-C2B-C1B	-3.27	123.43	128.46
19	B	846	CLA	CMB-C2B-C3B	3.27	130.94	124.80
20	A	803	CL0	O2A-CGA-O1A	-3.27	115.20	123.56
19	B2	801	CLA	O2D-CGD-CBD	3.27	116.97	111.25
19	AA	823	CLA	O2D-CGD-O1D	-3.27	117.38	123.83
24	B	849	AJP	CBM-CBL-CCH	3.27	118.81	113.12
24	K	104	AJP	CDA-CDB-CCG	3.27	116.16	112.65
19	F2	301	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
19	B1	805	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
19	A2	828	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
19	AA	811	CLA	CMB-C2B-C1B	-3.26	123.45	128.46
23	F2	304	BCR	C24-C23-C22	-3.26	121.31	126.21
19	B2	851	CLA	CHB-C4A-NA	3.26	129.02	124.51
19	A1	809	CLA	O2D-CGD-O1D	-3.26	117.39	123.83
19	B1	806	CLA	C5-C3-C2	3.26	127.80	121.11
24	L1	203	AJP	ODG-CCW-CCV	3.26	117.91	110.34
19	BB	845	CLA	CMB-C2B-C3B	3.26	130.91	124.80
19	A	820	CLA	CMB-C2B-C3B	3.25	130.90	124.80
19	B	811	CLA	CMB-C2B-C1B	-3.25	123.46	128.46
19	AA	806	CLA	CBA-CAA-C2A	3.25	123.53	113.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	I2	103	BCR	C15-C16-C17	-3.25	116.67	123.51
24	A1	855	AJP	CDA-CCZ-CCE	3.25	114.30	110.27
19	BB	820	CLA	O2D-CGD-O1D	-3.25	117.41	123.83
19	AA	820	CLA	CMB-C2B-C3B	3.25	130.89	124.80
19	B	809	CLA	O2D-CGD-O1D	-3.24	117.42	123.83
24	A1	854	AJP	CDC-CDB-CCG	3.24	118.30	112.31
19	LL	202	CLA	O2D-CGD-O1D	-3.24	117.43	123.83
26	B	841	ECH	C28-C27-C26	-3.24	115.62	118.68
19	A2	852	CLA	C6-C5-C3	3.24	120.79	113.01
19	BB	824	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
19	B2	815	CLA	CMB-C2B-C3B	3.24	130.87	124.80
19	A2	805	CLA	CMB-C2B-C3B	3.24	130.87	124.80
19	A	806	CLA	CBA-CAA-C2A	3.23	123.47	113.85
19	L	202	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	AA	814	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	B	837	CLA	O2D-CGD-O1D	-3.23	117.45	123.83
19	AA	838	CLA	CMB-C2B-C3B	3.23	130.86	124.80
19	BB	820	CLA	C1D-CHD-C4C	3.23	126.90	122.48
19	A2	840	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	B	812	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
19	A2	820	CLA	CMB-C2B-C3B	3.22	130.85	124.80
19	F2	301	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
19	A1	818	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
23	B2	842	BCR	C15-C14-C13	-3.22	122.71	127.31
23	A1	851	BCR	C2-C1-C6	3.22	115.47	110.48
19	F	301	CLA	O2D-CGD-O1D	-3.22	117.47	123.83
24	B	850	AJP	CBE-CBO-CBP	-3.22	98.27	104.35
19	AA	832	CLA	O2D-CGD-O1D	-3.22	117.47	123.83
24	B	850	AJP	OCY-CCX-OCC	3.22	119.73	110.67
24	I2	104	AJP	CBE-CBO-CBP	-3.22	98.28	104.35
19	B1	833	CLA	O2D-CGD-O1D	-3.21	117.48	123.83
24	BB	848	AJP	ODG-CCW-CCV	3.21	117.80	110.34
24	M2	101	AJP	CBM-CBL-CCH	3.21	118.71	113.12
19	B1	811	CLA	CMB-C2B-C1B	-3.21	123.53	128.46
19	BB	855	CLA	O2D-CGD-O1D	-3.21	117.50	123.83
19	A2	827	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
23	K1	106	BCR	C24-C23-C22	-3.20	121.40	126.21
19	B1	832	CLA	CHB-C4A-NA	3.20	128.94	124.51
19	KK	101	CLA	CMB-C2B-C3B	3.20	130.80	124.80
19	B	801	CLA	CHB-C4A-NA	3.20	128.94	124.51
26	B1	840	ECH	C12-C13-C14	-3.20	114.03	118.94
19	B2	820	CLA	O2D-CGD-O1D	-3.20	117.52	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	805	CLA	CMD-C2D-C3D	3.20	130.80	124.80
19	B1	820	CLA	O2D-CGD-O1D	-3.20	117.52	123.83
24	B	849	AJP	ODG-CCW-CCV	3.20	117.77	110.34
19	B1	850	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
19	F1	301	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
19	B	814	CLA	CMB-C2B-C3B	3.19	130.79	124.80
19	B1	804	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	A2	808	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	BB	805	CLA	O2D-CGD-O1D	-3.19	117.53	123.83
19	A2	810	CLA	O2D-CGD-O1D	-3.19	117.53	123.83
19	B2	811	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
19	A	841	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
23	L1	208	BCR	C15-C16-C17	-3.19	116.81	123.51
19	B	834	CLA	O2D-CGD-O1D	-3.19	117.53	123.83
19	B2	806	CLA	C5-C3-C2	3.19	127.66	121.11
19	B2	805	CLA	O2D-CGD-O1D	-3.19	117.54	123.83
19	L1	205	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
19	B	859	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
19	A1	842	CLA	C1D-CHD-C4C	3.18	126.84	122.48
26	B2	841	ECH	C12-C13-C14	-3.18	114.06	118.94
23	J2	104	BCR	C24-C23-C22	-3.18	121.43	126.21
19	AA	830	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	B2	819	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	B1	820	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	AA	841	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	LL	201	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
19	A2	830	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
24	L1	204	AJP	CBE-CBO-CBP	-3.17	98.36	104.35
20	A2	803	CL0	C9-C8-C10	3.17	122.86	111.30
23	A2	851	BCR	C2-C1-C6	3.17	115.39	110.48
19	B2	834	CLA	C1D-CHD-C4C	3.17	126.82	122.48
23	B2	842	BCR	C30-C25-C26	-3.17	118.16	122.59
19	B1	836	CLA	CHB-C4A-NA	3.17	128.90	124.51
24	L2	203	AJP	OBG-CBF-OBQ	-3.17	100.56	109.74
19	A	830	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
19	BB	811	CLA	CMB-C2B-C1B	-3.17	123.60	128.46
19	B	859	CLA	O2D-CGD-O1D	-3.16	117.58	123.83
19	BB	832	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
25	I1	102	LMG	O6-C1-O1	-3.16	102.47	109.94
19	F2	301	CLA	O2D-CGD-O1D	-3.16	117.59	123.83
19	B2	810	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
24	L1	203	AJP	CCH-CCG-CDB	3.16	113.08	108.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K	101	CLA	CAA-C2A-C3A	-3.16	104.13	112.78
19	L1	206	CLA	O2D-CGD-O1D	-3.16	117.59	123.83
26	B	841	ECH	C12-C13-C14	-3.16	114.10	118.94
24	I2	104	AJP	CCG-CCF-CCE	-3.16	110.32	113.91
19	B2	809	CLA	O2D-CGD-O1D	-3.16	117.60	123.83
19	A1	822	CLA	O2D-CGD-O1D	-3.16	117.60	123.83
19	AA	835	CLA	CMB-C2B-C3B	3.15	130.71	124.80
19	B2	846	CLA	CMB-C2B-C3B	3.15	130.71	124.80
19	B2	828	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
19	K	101	CLA	CMB-C2B-C3B	3.15	130.71	124.80
19	F	301	CLA	CHB-C4A-NA	3.15	128.87	124.51
23	J1	104	BCR	C2-C1-C6	3.15	115.35	110.48
19	B2	837	CLA	CHB-C4A-NA	3.15	128.87	124.51
24	B	857	AJP	CDC-CDB-CCG	3.15	118.12	112.31
23	A1	849	BCR	C2-C1-C6	3.15	115.35	110.48
19	A1	837	CLA	CMB-C2B-C3B	3.15	130.70	124.80
19	A2	810	CLA	O2D-CGD-CBD	3.15	116.76	111.25
19	BB	829	CLA	O2D-CGD-O1D	-3.15	117.62	123.83
19	L2	205	CLA	CMD-C2D-C3D	3.15	130.70	124.80
19	B1	809	CLA	O2D-CGD-O1D	-3.14	117.62	123.83
19	A1	811	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
19	FF	302	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
19	B2	818	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B1	812	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	AA	801	CLA	CMD-C2D-C3D	3.14	130.69	124.80
19	BB	856	CLA	O2D-CGD-O1D	-3.14	117.63	123.83
19	B1	803	CLA	CMB-C2B-C3B	3.14	130.69	124.80
19	A	828	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B2	826	CLA	O2D-CGD-O1D	-3.14	117.63	123.83
24	L2	202	AJP	CAV-CBE-CBO	3.14	121.62	114.54
19	A1	810	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	L	204	CLA	CMB-C2B-C3B	3.14	130.69	124.80
19	L2	205	CLA	O2D-CGD-O1D	-3.14	117.64	123.83
19	B1	819	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	B2	804	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
19	BB	826	CLA	O2D-CGD-O1D	-3.13	117.64	123.83
19	B	823	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	A	819	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	B1	826	CLA	O2D-CGD-O1D	-3.13	117.64	123.83
19	B1	815	CLA	O2D-CGD-O1D	-3.13	117.64	123.83
19	A	806	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	A2	819	CLA	CMB-C2B-C1B	-3.13	123.65	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	807	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	B1	845	CLA	CMB-C2B-C3B	3.13	130.67	124.80
23	A1	853	BCR	C15-C16-C17	-3.13	116.93	123.51
23	AA	850	BCR	C2-C1-C6	3.13	115.33	110.48
19	BB	813	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	BB	823	CLA	CMB-C2B-C1B	-3.13	123.65	128.46
19	B1	809	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	A2	835	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	LL	201	CLA	O2D-CGD-O1D	-3.13	117.66	123.83
19	BB	809	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	LL	202	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
19	BB	833	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
23	A2	853	BCR	C15-C16-C17	-3.12	116.94	123.51
19	F2	302	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
24	B	850	AJP	CCJ-CCI-CCH	-3.12	103.77	109.25
23	AA	852	BCR	C2-C1-C6	3.12	115.31	110.48
19	B1	805	CLA	O2D-CGD-O1D	-3.12	117.66	123.83
23	A2	849	BCR	C2-C1-C6	3.12	115.31	110.48
19	A2	841	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	AA	806	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	KK	101	CLA	CAA-C2A-C3A	-3.12	104.24	112.78
19	K2	102	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
24	KK	104	AJP	CCX-CCW-CCV	3.12	116.50	109.98
19	B1	818	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	B2	833	CLA	O2D-CGD-O1D	-3.12	117.67	123.83
19	BB	801	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
19	B	809	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
19	B2	809	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
24	L1	203	AJP	CBM-CBL-CCH	3.11	118.54	113.12
24	K	104	AJP	CCX-CCW-CCV	3.11	116.48	109.98
19	A1	837	CLA	O2D-CGD-O1D	-3.11	117.69	123.83
24	K	104	AJP	CCJ-CCI-CCH	-3.11	103.79	109.25
23	A	854	BCR	C24-C23-C22	-3.11	121.54	126.21
19	A	804	CLA	CMD-C2D-C3D	3.11	130.63	124.80
23	A	850	BCR	C15-C16-C17	-3.11	116.98	123.51
19	F1	301	CLA	CHB-C4A-NA	3.11	128.81	124.51
23	M	101	BCR	C15-C16-C17	-3.10	116.99	123.51
19	A1	832	CLA	O2D-CGD-O1D	-3.10	117.70	123.83
19	AA	811	CLA	O2D-CGD-O1D	-3.10	117.70	123.83
19	B	826	CLA	O2D-CGD-O1D	-3.10	117.70	123.83
19	A2	806	CLA	CBA-CAA-C2A	3.10	123.08	113.85
19	B	834	CLA	O2A-CGA-O1A	-3.10	115.63	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	X2	101	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	B1	849	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	B	805	CLA	O2D-CGD-O1D	-3.10	117.71	123.83
19	B2	824	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
19	BB	813	CLA	O2D-CGD-O1D	-3.10	117.72	123.83
19	A2	838	CLA	O2D-CGD-O1D	-3.09	117.72	123.83
19	A	810	CLA	CBA-CAA-C2A	3.09	123.06	113.85
23	J1	104	BCR	C24-C23-C22	-3.09	121.56	126.21
23	K	103	BCR	C15-C16-C17	-3.09	117.01	123.51
23	F	305	BCR	C11-C10-C9	-3.09	122.90	127.31
19	AA	813	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	A	838	CLA	CMB-C2B-C3B	3.09	130.60	124.80
19	X	101	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	BB	835	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
19	A	809	CLA	O2D-CGD-O1D	-3.09	117.73	123.83
19	BB	852	CLA	CMD-C2D-C3D	3.09	130.59	124.80
20	A	803	CL0	CMC-C2C-C1C	3.09	129.73	125.03
19	B2	812	CLA	CMB-C2B-C1B	-3.09	123.72	128.46
20	A	803	CL0	O2A-C1-C2	3.09	116.75	108.64
19	L1	205	CLA	O2D-CGD-O1D	-3.08	117.74	123.83
19	A1	819	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
19	BB	834	CLA	CMB-C2B-C3B	3.08	130.58	124.80
19	J1	101	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	F1	301	CLA	CMD-C2D-C3D	3.08	130.58	124.80
19	XX	101	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
19	B	834	CLA	CAA-C2A-C3A	-3.08	104.35	112.78
19	AA	841	CLA	O2D-CGD-O1D	-3.08	117.75	123.83
19	AA	819	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
19	X1	101	CLA	CMB-C2B-C1B	-3.07	123.74	128.46
19	B2	820	CLA	C1D-CHD-C4C	3.07	126.68	122.48
19	L	202	CLA	O2D-CGD-O1D	-3.07	117.77	123.83
19	B1	833	CLA	C1D-CHD-C4C	3.07	126.68	122.48
19	B1	810	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
19	A	810	CLA	O2D-CGD-O1D	-3.07	117.77	123.83
19	A	832	CLA	O2D-CGD-CBD	3.07	116.62	111.25
19	A	815	CLA	CHB-C4A-NA	3.06	128.75	124.51
19	BB	852	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	A2	805	CLA	O2D-CGD-O1D	-3.06	117.78	123.83
19	B2	822	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
19	B1	850	CLA	O2D-CGD-O1D	-3.06	117.78	123.83
19	BB	833	CLA	O2A-CGA-O1A	-3.06	115.73	123.56
19	A1	814	CLA	CHB-C4A-NA	3.06	128.75	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	821	CLA	CHB-C4A-NA	3.06	128.75	124.51
19	AA	805	CLA	O2D-CGD-O1D	-3.06	117.78	123.83
23	II	104	BCR	C15-C16-C17	-3.06	117.07	123.51
19	BB	814	CLA	CMB-C2B-C3B	3.06	130.54	124.80
24	L1	204	AJP	OBG-CBF-CAW	3.06	113.71	110.81
24	L	208	AJP	CBE-CBO-CBP	-3.06	98.58	104.35
24	A1	855	AJP	CDA-CDB-CCG	3.06	115.93	112.65
23	AA	851	BCR	C15-C16-C17	-3.06	117.08	123.51
19	AA	808	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	A1	825	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	A1	839	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
19	B2	801	CLA	CHB-C4A-NA	3.06	128.74	124.51
19	B2	814	CLA	O2D-CGD-O1D	-3.06	117.80	123.83
19	B2	820	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
19	B	818	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
19	A2	815	CLA	CHB-C4A-NA	3.05	128.74	124.51
19	AA	829	CLA	CMB-C2B-C3B	3.05	130.53	124.80
19	A	841	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
23	F2	305	BCR	C11-C10-C9	-3.05	122.96	127.31
19	B	817	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
19	B2	834	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
19	A1	840	CLA	CMB-C2B-C1B	-3.05	123.78	128.46
19	A1	804	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
19	A2	822	CLA	O2D-CGD-O1D	-3.05	117.81	123.83
19	BB	836	CLA	C1D-CHD-C4C	3.04	126.65	122.48
19	B1	833	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
19	B1	814	CLA	O2D-CGD-O1D	-3.04	117.82	123.83
19	A	839	CLA	O2D-CGD-O1D	-3.04	117.82	123.83
19	AA	845	CLA	O2D-CGD-O1D	-3.04	117.82	123.83
23	A	849	BCR	C2-C1-C6	3.04	115.19	110.48
19	B	828	CLA	CMB-C2B-C1B	-3.04	123.79	128.46
19	BB	814	CLA	O2D-CGD-O1D	-3.04	117.83	123.83
19	AA	804	CLA	O2D-CGD-O1D	-3.04	117.83	123.83
19	B2	851	CLA	CBA-CAA-C2A	3.04	122.89	113.85
24	B	849	AJP	CAV-CBE-CBO	3.04	121.39	114.54
24	KK	104	AJP	CAV-CBE-CBO	3.04	121.39	114.54
19	AA	810	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	A1	816	CLA	CMB-C2B-C1B	-3.04	123.80	128.46
19	A	823	CLA	CMB-C2B-C3B	3.04	130.49	124.80
23	F1	306	BCR	C11-C10-C9	-3.03	122.98	127.31
19	B	830	CLA	O2D-CGD-O1D	-3.03	117.84	123.83
19	B	859	CLA	CAA-C2A-C3A	-3.03	104.47	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	805	CLA	CMD-C2D-C3D	3.03	130.49	124.80
19	A1	803	CLA	CMD-C2D-C3D	3.03	130.49	124.80
19	F1	302	CLA	CMB-C2B-C1B	-3.03	123.80	128.46
19	B2	833	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	A1	842	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
19	A	808	CLA	O2A-CGA-O1A	-3.03	115.82	123.56
19	AA	853	CLA	O2D-CGD-O1D	-3.03	117.85	123.83
19	AA	815	CLA	CHB-C4A-NA	3.03	128.70	124.51
19	B	804	CLA	O2D-CGD-O1D	-3.03	117.85	123.83
19	B1	801	CLA	O2D-CGD-CBD	3.03	116.55	111.25
19	AA	843	CLA	C1D-CHD-C4C	3.03	126.62	122.48
19	AA	801	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	A2	801	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	F2	301	CLA	CMD-C2D-C3D	3.02	130.47	124.80
19	L2	204	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
19	B	834	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
19	F2	301	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	B	837	CLA	CHB-C4A-NA	3.02	128.69	124.51
19	BB	829	CLA	C1D-CHD-C4C	3.02	126.61	122.48
19	A	839	CLA	CMB-C2B-C3B	3.02	130.46	124.80
24	L1	204	AJP	OCL-CCK-CCJ	3.02	124.35	113.73
19	BB	804	CLA	O2D-CGD-O1D	-3.02	117.87	123.83
19	A	811	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
19	A	801	CLA	CHB-C4A-NA	3.02	128.68	124.51
19	B	806	CLA	CMD-C2D-C3D	3.02	130.46	124.80
24	L	208	AJP	CBM-CBN-CBO	-3.02	110.50	115.48
19	B	825	CLA	CMB-C2B-C3B	3.02	130.46	124.80
23	B1	843	BCR	C33-C5-C6	-3.02	121.15	124.51
19	BB	819	CLA	CMB-C2B-C1B	-3.02	123.83	128.46
19	A1	828	CLA	CMB-C2B-C3B	3.02	130.46	124.80
23	J	104	BCR	C24-C23-C22	-3.02	121.68	126.21
19	A1	809	CLA	O2D-CGD-CBD	3.01	116.53	111.25
19	B1	850	CLA	C6-C5-C3	3.01	120.25	113.01
19	A	844	CLA	O2D-CGD-O1D	-3.01	117.88	123.83
19	B	814	CLA	O2D-CGD-O1D	-3.01	117.88	123.83
19	BB	856	CLA	CMB-C2B-C1B	-3.01	123.83	128.46
19	L	204	CLA	CMD-C2D-C3D	3.01	130.45	124.80
19	A1	844	CLA	O2D-CGD-O1D	-3.01	117.88	123.83
19	A2	804	CLA	CMD-C2D-C3D	3.01	130.44	124.80
19	B2	806	CLA	CMD-C2D-C3D	3.01	130.44	124.80
19	B	858	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	AA	842	CLA	C6-C5-C3	3.01	120.23	113.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	828	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
24	B	849	AJP	CBE-CBO-CBP	-3.01	98.67	104.35
19	B2	852	CLA	C1D-CHD-C4C	3.01	126.60	122.48
19	A	829	CLA	CMB-C2B-C3B	3.01	130.44	124.80
19	AA	823	CLA	CMB-C2B-C3B	3.01	130.44	124.80
19	B2	850	CLA	CMB-C2B-C3B	3.01	130.44	124.80
19	A1	834	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
19	A2	831	CLA	CMB-C2B-C3B	3.00	130.44	124.80
23	J1	104	BCR	C1-C6-C5	-3.00	118.39	122.59
19	B2	851	CLA	C6-C5-C3	3.00	120.22	113.01
19	B2	807	CLA	CHB-C4A-NA	3.00	128.66	124.51
19	B2	820	CLA	CAC-C3C-C2C	-3.00	122.40	127.53
19	JJ	101	CLA	CMB-C2B-C1B	-3.00	123.85	128.46
23	I2	103	BCR	C24-C23-C22	-3.00	121.70	126.21
19	B2	821	CLA	CMD-C2D-C3D	3.00	130.43	124.80
19	A2	832	CLA	O2D-CGD-CBD	3.00	116.50	111.25
19	A1	808	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
19	B2	817	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
19	AA	809	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
19	A	805	CLA	O2D-CGD-O1D	-3.00	117.91	123.83
24	B	849	AJP	CAX-CAW-CBF	3.00	117.26	111.95
19	B	817	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
19	AA	824	CLA	CMB-C2B-C3B	3.00	130.42	124.80
23	B2	844	BCR	C33-C5-C6	-2.99	121.17	124.51
19	A	842	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	A2	844	CLA	O2D-CGD-O1D	-2.99	117.92	123.83
24	K	104	AJP	CDC-CDB-CCG	2.99	117.83	112.31
19	A2	817	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	B2	813	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	BB	820	CLA	CAC-C3C-C2C	-2.99	122.42	127.53
19	A	821	CLA	CHB-C4A-NA	2.99	128.65	124.51
19	B2	806	CLA	CMB-C2B-C1B	-2.99	123.86	128.46
19	BB	833	CLA	C1D-CHD-C4C	2.99	126.57	122.48
19	A1	840	CLA	O2D-CGD-O1D	-2.99	117.93	123.83
20	A	803	CL0	O2D-CGD-O1D	-2.99	117.93	123.83
23	B	848	BCR	C1-C6-C5	-2.99	118.42	122.59
19	B	802	CLA	O2D-CGD-O1D	-2.99	117.93	123.83
19	A2	811	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
19	F	302	CLA	CMB-C2B-C1B	-2.99	123.88	128.46
23	BB	843	BCR	C33-C5-C6	-2.98	121.19	124.51
19	A2	809	CLA	O2D-CGD-O1D	-2.98	117.94	123.83
19	B1	823	CLA	CMB-C2B-C1B	-2.98	123.88	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	833	CLA	O2D-CGD-O1D	-2.98	117.94	123.83
19	B	833	CLA	CHB-C4A-NA	2.98	128.64	124.51
19	AA	839	CLA	CMB-C2B-C3B	2.98	130.39	124.80
19	B	860	CLA	C1D-CHD-C4C	2.98	126.56	122.48
19	A	826	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
23	B	844	BCR	C33-C5-C6	-2.98	121.19	124.51
19	J2	101	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	B2	823	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	A	808	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
19	A1	801	CLA	CHB-C4A-NA	2.98	128.63	124.51
19	A1	809	CLA	CAA-C2A-C1A	-2.98	102.22	111.97
19	AA	809	CLA	CMB-C2B-C1B	-2.98	123.89	128.46
23	J	102	BCR	C15-C14-C13	-2.98	123.06	127.31
19	A1	807	CLA	O2A-CGA-O1A	-2.98	115.96	123.56
24	L2	203	AJP	CDC-CDB-CCG	2.98	117.80	112.31
19	A	821	CLA	O2D-CGD-O1D	-2.98	117.95	123.83
23	M2	102	BCR	C35-C13-C14	-2.98	118.75	122.92
19	B	834	CLA	C1D-CHD-C4C	2.98	126.55	122.48
19	BB	852	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
19	B1	804	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
19	AA	814	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
23	K2	105	BCR	C24-C23-C22	-2.97	121.74	126.21
19	B2	825	CLA	CMB-C2B-C3B	2.97	130.38	124.80
19	BB	814	CLA	CHB-C4A-NA	2.97	128.62	124.51
19	B	813	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
19	B1	833	CLA	O2A-CGA-O1A	-2.97	115.96	123.56
19	AA	842	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
19	A2	815	CLA	CMB-C2B-C3B	2.97	130.38	124.80
19	B1	829	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
19	B1	813	CLA	O2D-CGD-O1D	-2.97	117.96	123.83
19	A	852	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
19	A2	821	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
19	J	101	CLA	CMB-C2B-C1B	-2.97	123.90	128.46
19	A2	824	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
23	F2	304	BCR	C2-C1-C6	2.97	115.07	110.48
19	BB	856	CLA	CAA-C2A-C3A	-2.97	104.65	112.78
19	B	801	CLA	CMB-C2B-C1B	-2.97	123.91	128.46
19	AA	821	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
19	B1	801	CLA	CHB-C4A-NA	2.97	128.61	124.51
19	AA	810	CLA	O2D-CGD-O1D	-2.97	117.97	123.83
19	K2	104	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	L2	204	CLA	O2D-CGD-O1D	-2.96	117.97	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	AA	856	AJP	CBL-CCH-CCI	2.96	116.06	111.74
19	A1	821	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
19	B2	852	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
24	L2	203	AJP	OCL-CCK-CCJ	2.96	124.16	113.73
24	L2	202	AJP	CBE-CBO-CBP	-2.96	98.76	104.35
19	A1	806	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
19	B2	804	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
19	A2	823	CLA	CHB-C4A-NA	2.96	128.61	124.51
19	A2	810	CLA	CMB-C2B-C1B	-2.96	123.91	128.46
23	B2	839	BCR	C15-C14-C13	-2.96	123.08	127.31
23	FF	306	BCR	C11-C10-C9	-2.96	123.08	127.31
19	BB	828	CLA	O2D-CGD-O1D	-2.96	117.98	123.83
19	A2	833	CLA	O2D-CGD-O1D	-2.96	117.99	123.83
19	B1	817	CLA	O2D-CGD-O1D	-2.96	117.99	123.83
19	K1	102	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
19	A	813	CLA	CMB-C2B-C1B	-2.96	123.92	128.46
19	AA	839	CLA	O2D-CGD-O1D	-2.96	117.99	123.83
19	B	818	CLA	O2D-CGD-O1D	-2.96	117.99	123.83
24	BB	849	AJP	CDA-CDB-CCG	2.96	115.82	112.65
19	B	827	CLA	CHB-C4A-NA	2.95	128.60	124.51
19	BB	825	CLA	CMB-C2B-C3B	2.95	130.34	124.80
19	B1	848	CLA	CMD-C2D-C3D	2.95	130.34	124.80
19	A2	840	CLA	O2D-CGD-O1D	-2.95	118.00	123.83
20	A2	803	CL0	O2A-CGA-CBA	2.95	121.41	111.93
19	A1	824	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	A	801	CLA	CMD-C2D-C3D	2.95	130.33	124.80
23	FF	304	BCR	C2-C1-C6	2.95	115.05	110.48
19	BB	817	CLA	CMB-C2B-C1B	-2.95	123.93	128.46
19	B2	834	CLA	O2A-CGA-O1A	-2.95	116.03	123.56
19	A2	807	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
19	A2	822	CLA	CMB-C2B-C1B	-2.94	123.94	128.46
24	L	208	AJP	CDD-CCI-CCH	2.94	114.19	110.50
19	B1	824	CLA	CMB-C2B-C3B	2.94	130.32	124.80
19	A2	830	CLA	O2D-CGD-O1D	-2.94	118.02	123.83
19	K2	102	CLA	CAA-C2A-C3A	-2.94	104.73	112.78
19	B1	850	CLA	CBA-CAA-C2A	2.94	122.60	113.85
19	B1	817	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
19	K1	105	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
24	L	208	AJP	CDD-CCI-CCJ	2.94	116.59	112.32
19	A2	842	CLA	CMB-C2B-C1B	-2.93	123.95	128.46
24	B	850	AJP	CDA-CDB-CCG	2.93	115.80	112.65
19	BB	830	CLA	CMB-C2B-C1B	-2.93	123.95	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	A	855	AJP	CBL-CCH-CCI	2.93	116.01	111.74
23	KK	103	BCR	C15-C16-C17	-2.93	117.34	123.51
23	B1	838	BCR	C15-C14-C13	-2.93	123.12	127.31
19	B1	807	CLA	CHB-C4A-NA	2.93	128.57	124.51
19	B1	806	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	A	831	CLA	CMB-C2B-C3B	2.93	130.29	124.80
19	A1	821	CLA	CMB-C2B-C1B	-2.93	123.96	128.46
19	BB	855	CLA	CMB-C2B-C3B	2.93	130.29	124.80
19	AA	804	CLA	CMD-C2D-C3D	2.93	130.29	124.80
19	B2	802	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
23	F1	304	BCR	C2-C1-C6	2.93	115.01	110.48
19	B1	816	CLA	O2D-CGD-O1D	-2.93	118.05	123.83
19	A	820	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
19	A	832	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
23	FF	306	BCR	C33-C5-C6	-2.92	121.25	124.51
23	AA	852	BCR	C28-C27-C26	-2.92	108.90	113.99
23	M1	101	BCR	C35-C13-C14	-2.92	118.83	122.92
23	F1	306	BCR	C24-C23-C22	-2.92	121.82	126.21
19	B	859	CLA	CBA-CAA-C2A	2.92	122.55	113.85
23	A	851	BCR	C28-C27-C26	-2.92	108.91	113.99
19	BB	802	CLA	CMB-C2B-C1B	-2.92	123.97	128.46
19	B1	806	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
19	B	828	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
19	A2	841	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
19	B1	802	CLA	O2D-CGD-O1D	-2.92	118.06	123.83
19	B2	831	CLA	CMB-C2B-C3B	2.92	130.28	124.80
23	J2	104	BCR	C1-C6-C5	-2.92	118.51	122.59
24	BB	848	AJP	CBE-CBO-CBP	-2.92	98.84	104.35
19	AA	806	CLA	CAA-C2A-C1A	-2.92	102.41	111.97
19	A2	806	CLA	CHB-C4A-NA	2.92	128.55	124.51
19	B2	821	CLA	O2D-CGD-O1D	-2.92	118.07	123.83
19	A2	836	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
20	A	803	CL0	CMD-C2D-C3D	-2.92	119.33	124.80
19	BB	827	CLA	CHB-C4A-NA	2.92	128.55	124.51
24	A	802	AJP	CAV-CBE-CBO	2.92	121.12	114.54
19	BB	832	CLA	CMB-C2B-C3B	2.92	130.27	124.80
19	A1	814	CLA	CMB-C2B-C3B	2.92	130.27	124.80
19	A	824	CLA	CMB-C2B-C3B	2.92	130.27	124.80
23	A1	850	BCR	C33-C5-C6	-2.92	121.26	124.51
20	AA	803	CL0	CMB-C2B-C3B	2.92	130.27	124.80
19	A2	823	CLA	CMB-C2B-C3B	2.91	130.26	124.80
19	B	816	CLA	O2D-CGD-O1D	-2.91	118.08	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	855	BCR	C24-C23-C22	-2.91	121.84	126.21
19	A	806	CLA	CAA-C2A-C1A	-2.91	102.43	111.97
19	B2	851	CLA	O2D-CGD-O1D	-2.91	118.08	123.83
19	B	831	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
19	B	803	CLA	O2D-CGD-O1D	-2.91	118.08	123.83
24	A	855	AJP	CCJ-CCI-CCH	-2.91	104.14	109.25
19	F2	302	CLA	O2D-CGD-CBD	2.91	116.34	111.25
19	A	842	CLA	O2D-CGD-O1D	-2.91	118.09	123.83
19	BB	807	CLA	CHB-C4A-NA	2.91	128.53	124.51
19	B	806	CLA	CMB-C2B-C1B	-2.91	123.99	128.46
24	KK	104	AJP	CDC-CDB-CCG	2.91	117.67	112.31
25	B2	847	LMG	O6-C1-O1	-2.91	103.08	109.94
19	A2	801	CLA	CMD-C2D-C3D	2.91	130.25	124.80
24	AA	856	AJP	CCJ-CCI-CCH	-2.91	104.15	109.25
19	B1	825	CLA	CMB-C2B-C3B	2.91	130.25	124.80
19	B	854	CLA	CMD-C2D-C3D	2.91	130.25	124.80
19	B2	806	CLA	O2D-CGD-O1D	-2.90	118.09	123.83
19	B	833	CLA	CMB-C2B-C3B	2.90	130.25	124.80
19	A1	838	CLA	CMB-C2B-C3B	2.90	130.25	124.80
19	A	829	CLA	CMD-C2D-C3D	2.90	130.24	124.80
19	AA	842	CLA	O2D-CGD-O1D	-2.90	118.10	123.83
19	B	814	CLA	CHB-C4A-NA	2.90	128.52	124.51
19	BB	820	CLA	O2D-CGD-CBD	2.90	116.33	111.25
23	F2	303	BCR	C35-C13-C14	-2.90	118.86	122.92
19	A1	831	CLA	O2D-CGD-CBD	2.90	116.33	111.25
25	I1	102	LMG	O6-C5-C4	2.90	114.97	109.68
24	L	209	AJP	CDD-CCI-CCH	2.90	114.13	110.50
19	A1	829	CLA	O2D-CGD-O1D	-2.90	118.11	123.83
19	B	801	CLA	C4-C3-C5	2.90	120.28	115.29
19	A2	825	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
19	A1	820	CLA	O2D-CGD-O1D	-2.90	118.11	123.83
19	A1	830	CLA	CMB-C2B-C3B	2.90	130.23	124.80
19	BB	856	CLA	CBA-CAA-C2A	2.89	122.47	113.85
19	AA	820	CLA	O2A-CGA-O1A	-2.89	116.17	123.56
19	B1	806	CLA	CHB-C4A-NA	2.89	128.51	124.51
19	B	835	CLA	CMB-C2B-C3B	2.89	130.22	124.80
19	AA	826	CLA	CMB-C2B-C1B	-2.89	124.02	128.46
19	BB	833	CLA	O2D-CGD-CBD	2.89	116.31	111.25
23	KK	103	BCR	C35-C13-C14	-2.89	118.87	122.92
19	B1	815	CLA	CHB-C4A-NA	2.89	128.51	124.51
24	L	209	AJP	CDD-CDC-CDB	2.89	117.73	111.87
19	B	834	CLA	O2D-CGD-CBD	2.89	116.31	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	839	CLA	CMB-C2B-C3B	2.89	130.22	124.80
20	AA	803	CL0	CHC-C1C-C2C	-2.89	118.75	126.71
19	A2	830	CLA	CMB-C2B-C3B	2.89	130.22	124.80
19	BB	831	CLA	O2D-CGD-O1D	-2.89	118.13	123.83
19	A1	820	CLA	CHB-C4A-NA	2.89	128.50	124.51
19	BB	818	CLA	O2D-CGD-O1D	-2.88	118.13	123.83
23	L1	208	BCR	C24-C23-C22	-2.88	121.88	126.21
19	B2	802	CLA	CMB-C2B-C1B	-2.88	124.03	128.46
19	AA	811	CLA	CMB-C2B-C3B	2.88	130.20	124.80
19	A	823	CLA	O2D-CGD-CBD	2.88	116.29	111.25
19	AA	817	CLA	CHB-C4A-NA	2.88	128.49	124.51
23	A	851	BCR	C3-C4-C5	-2.88	108.98	113.99
19	B2	830	CLA	O2D-CGD-O1D	-2.88	118.14	123.83
19	B2	821	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
24	A2	854	AJP	CDA-CDB-CCG	2.88	115.74	112.65
19	B2	835	CLA	CMB-C2B-C3B	2.88	130.20	124.80
24	K	104	AJP	CCG-CCF-CCE	-2.88	109.25	114.00
19	A	804	CLA	O2D-CGD-O1D	-2.88	118.15	123.83
26	BB	840	ECH	C8-C7-C6	-2.88	119.22	127.28
19	A	842	CLA	C6-C5-C3	2.88	119.92	113.01
19	AA	819	CLA	O2D-CGD-O1D	-2.88	118.15	123.83
19	B1	802	CLA	CHB-C4A-NA	2.88	128.49	124.51
19	B2	817	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
19	B1	830	CLA	CMB-C2B-C3B	2.88	130.19	124.80
19	B1	827	CLA	CHB-C4A-NA	2.88	128.49	124.51
19	B2	813	CLA	O2D-CGD-O1D	-2.88	118.15	123.83
19	B	829	CLA	CMB-C2B-C3B	2.87	130.19	124.80
19	B2	850	CLA	C1B-CHB-C4A	-2.87	124.42	130.12
19	BB	856	CLA	C6-C5-C3	2.87	119.91	113.01
19	A1	826	CLA	O2D-CGD-O1D	-2.87	118.16	123.83
19	BB	832	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
19	B2	814	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	A	817	CLA	CHB-C4A-NA	2.87	128.48	124.51
19	B1	801	CLA	CMB-C2B-C3B	2.87	130.18	124.80
24	K	104	AJP	CAV-CBE-CBO	2.87	121.02	114.54
19	B	831	CLA	O2D-CGD-O1D	-2.87	118.17	123.83
24	L	209	AJP	CAV-CBE-CBO	2.87	121.01	114.54
19	L	203	CLA	O2D-CGD-CBD	2.86	116.27	111.25
24	AA	802	AJP	CAV-CBE-CBO	2.86	121.01	114.54
19	JJ	103	CLA	O2D-CGD-O1D	-2.86	118.17	123.83
19	BB	832	CLA	CHB-C4A-NA	2.86	128.47	124.51
19	A1	823	CLA	CMB-C2B-C3B	2.86	130.17	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	814	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
19	A	825	CLA	O2D-CGD-O1D	-2.86	118.17	123.83
26	B2	841	ECH	C37-C22-C21	2.86	126.93	122.92
19	BB	822	CLA	CMD-C2D-C3D	2.86	130.17	124.80
19	F1	301	CLA	O2D-CGD-CBD	2.86	116.26	111.25
19	A	835	CLA	CMB-C2B-C3B	2.86	130.17	124.80
19	AA	816	CLA	O2D-CGD-O1D	-2.86	118.18	123.83
19	A2	834	CLA	CMD-C2D-C3D	2.86	130.17	124.80
26	B	841	ECH	C8-C7-C6	-2.86	119.27	127.28
19	A	844	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
19	BB	805	CLA	CMD-C2D-C3D	2.86	130.17	124.80
19	A	827	CLA	O2D-CGD-O1D	-2.86	118.18	123.83
19	A1	835	CLA	CHB-C4A-NA	2.86	128.47	124.51
23	AA	855	BCR	C33-C5-C6	-2.86	121.33	124.51
19	B	807	CLA	CHB-C4A-NA	2.86	128.46	124.51
19	A2	805	CLA	CMD-C2D-C3D	2.86	130.16	124.80
23	I2	101	BCR	C33-C5-C6	-2.86	121.33	124.51
19	A1	810	CLA	O2D-CGD-O1D	-2.86	118.19	123.83
20	A1	802	CL0	CMC-C2C-C1C	2.86	129.38	125.03
20	A1	802	CL0	C9-C8-C7	2.86	121.71	111.30
24	A1	855	AJP	CCJ-CCI-CCH	-2.86	104.24	109.25
19	B1	829	CLA	CMB-C2B-C1B	-2.86	124.08	128.46
23	F1	306	BCR	C33-C5-C6	-2.86	121.33	124.51
19	BB	856	CLA	CAA-CBA-CGA	2.86	121.67	113.26
19	B	819	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	A1	808	CLA	CMB-C2B-C3B	2.85	130.15	124.80
23	B2	839	BCR	C35-C13-C14	-2.85	118.92	122.92
19	B	820	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
24	L1	204	AJP	CCJ-CCI-CCH	-2.85	104.24	109.25
23	AA	851	BCR	C33-C5-C6	-2.85	121.33	124.51
19	A2	828	CLA	CHB-C4A-NA	2.85	128.46	124.51
19	A1	828	CLA	CMD-C2D-C3D	2.85	130.15	124.80
19	A1	815	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
19	B1	823	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
19	KK	102	CLA	O2D-CGD-O1D	-2.85	118.20	123.83
19	A2	826	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	A2	834	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
19	A2	820	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
19	K1	103	CLA	CMB-C2B-C3B	2.85	130.14	124.80
19	A2	829	CLA	CMB-C2B-C3B	2.85	130.14	124.80
19	FF	305	CLA	CMB-C2B-C3B	2.85	130.14	124.80
19	B1	828	CLA	CMB-C2B-C3B	2.85	130.14	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	MM	101	BCR	C33-C5-C6	-2.85	121.34	124.51
19	A1	827	CLA	CHB-C4A-NA	2.85	128.45	124.51
23	K2	103	BCR	C33-C5-C6	-2.85	121.34	124.51
23	F	305	BCR	C33-C5-C6	-2.85	121.34	124.51
19	B2	834	CLA	CHB-C4A-NA	2.84	128.45	124.51
19	A1	841	CLA	C6-C5-C3	2.84	119.84	113.01
19	A2	816	CLA	CHB-C4A-NA	2.84	128.44	124.51
19	B	859	CLA	C6-C5-C3	2.84	119.84	113.01
19	A1	803	CLA	O2D-CGD-O1D	-2.84	118.21	123.83
19	BB	816	CLA	O2D-CGD-O1D	-2.84	118.22	123.83
19	A1	838	CLA	O2D-CGD-O1D	-2.84	118.22	123.83
19	BB	810	CLA	CMB-C2B-C3B	2.84	130.13	124.80
23	A	850	BCR	C33-C5-C6	-2.84	121.34	124.51
23	I1	101	BCR	C33-C5-C6	-2.84	121.34	124.51
19	B2	833	CLA	C5-C3-C2	2.84	126.95	121.11
19	BB	820	CLA	CMB-C2B-C1B	-2.84	124.09	128.46
19	A1	823	CLA	CHB-C4A-NA	2.84	128.44	124.51
23	K	103	BCR	C33-C5-C6	-2.84	121.34	124.51
19	B1	813	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	B	810	CLA	CMB-C2B-C3B	2.84	130.13	124.80
19	B	802	CLA	CMB-C2B-C1B	-2.84	124.10	128.46
19	K	102	CLA	O2D-CGD-O1D	-2.84	118.22	123.83
23	B1	839	BCR	C1-C6-C5	-2.84	118.62	122.59
19	B2	816	CLA	O2D-CGD-O1D	-2.84	118.22	123.83
19	B1	810	CLA	O2D-CGD-O1D	-2.84	118.22	123.83
19	AA	825	CLA	O2D-CGD-O1D	-2.84	118.23	123.83
24	L2	202	AJP	CCH-CCG-CDB	2.84	112.62	108.59
26	B	841	ECH	C37-C22-C21	2.84	126.90	122.92
19	LL	203	CLA	C1B-CHB-C4A	-2.84	124.50	130.12
23	B1	838	BCR	C33-C5-C6	-2.84	121.35	124.51
23	A2	850	BCR	C33-C5-C6	-2.84	121.35	124.51
23	B2	840	BCR	C1-C6-C5	-2.84	118.63	122.59
19	A	815	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
23	K1	104	BCR	C33-C5-C6	-2.83	121.35	124.51
19	B1	821	CLA	O2D-CGD-O1D	-2.83	118.23	123.83
19	B1	821	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
23	JJ	104	BCR	C24-C23-C22	-2.83	121.96	126.21
19	A	821	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
19	A2	812	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
19	A2	832	CLA	CMB-C2B-C3B	2.83	130.11	124.80
19	K2	104	CLA	CHB-C4A-NA	2.83	128.43	124.51
23	II	101	BCR	C33-C5-C6	-2.83	121.36	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	854	BCR	C33-C5-C6	-2.83	121.36	124.51
19	K	102	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
19	F	301	CLA	CMD-C2D-C3D	2.83	130.11	124.80
19	B1	811	CLA	CMB-C2B-C3B	2.83	130.11	124.80
19	BB	808	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
23	F	304	BCR	C2-C1-C6	2.83	114.86	110.48
19	A2	825	CLA	O2D-CGD-O1D	-2.83	118.24	123.83
24	KK	104	AJP	CCG-CCF-CCE	-2.83	109.33	114.00
19	B	813	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
19	L	203	CLA	CMB-C2B-C3B	2.83	130.10	124.80
19	A1	801	CLA	CMB-C2B-C1B	-2.83	124.12	128.46
19	B	817	CLA	CHB-C4A-NA	2.83	128.42	124.51
19	B1	821	CLA	CMD-C2D-C3D	2.83	130.10	124.80
23	I	101	BCR	C33-C5-C6	-2.83	121.36	124.51
19	A2	842	CLA	C6-C5-C3	2.83	119.79	113.01
24	BB	848	AJP	CBM-CBL-CCH	2.83	118.04	113.12
19	B1	848	CLA	O2D-CGD-O1D	-2.82	118.25	123.83
24	L	209	AJP	CBM-CBN-CBO	-2.82	110.82	115.48
19	B2	801	CLA	CMB-C2B-C3B	2.82	130.09	124.80
19	A	837	CLA	CMB-C2B-C3B	2.82	130.09	124.80
19	B1	824	CLA	O2D-CGD-O1D	-2.82	118.26	123.83
23	B	842	BCR	C28-C27-C26	-2.82	109.08	113.99
19	B2	834	CLA	C3A-C2A-C1A	2.82	105.56	101.34
19	K1	102	CLA	CMB-C2B-C3B	2.82	130.09	124.80
19	A2	842	CLA	O2D-CGD-O1D	-2.82	118.26	123.83
24	A2	854	AJP	CDC-CDB-CCG	2.82	117.51	112.31
23	M	101	BCR	C33-C5-C6	-2.82	121.37	124.51
23	FF	306	BCR	C35-C13-C14	-2.82	118.97	122.92
23	A2	851	BCR	C28-C27-C26	-2.82	109.08	113.99
19	A2	836	CLA	CHB-C4A-NA	2.82	128.41	124.51
19	A1	811	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
19	AA	827	CLA	O2D-CGD-O1D	-2.82	118.27	123.83
19	A1	834	CLA	C1-C2-C3	-2.82	121.17	126.04
19	A1	827	CLA	CMB-C2B-C3B	2.82	130.08	124.80
24	K	104	AJP	CDC-CDD-CCI	2.82	116.82	112.13
19	A1	852	CLA	C6-C5-C3	2.82	119.77	113.01
26	BB	840	ECH	C29-C30-C25	-2.82	106.13	110.48
23	B2	839	BCR	C33-C5-C6	-2.82	121.37	124.51
23	B	840	BCR	C1-C6-C5	-2.82	118.65	122.59
19	BB	804	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
19	A	842	CLA	C4-C3-C5	2.82	120.14	115.29
19	BB	817	CLA	CHB-C4A-NA	2.82	128.41	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	821	CLA	C5-C3-C2	2.82	126.89	121.11
19	B	805	CLA	CMD-C2D-C3D	2.81	130.08	124.80
19	B2	819	CLA	O2D-CGD-O1D	-2.81	118.27	123.83
19	B1	834	CLA	CMB-C2B-C3B	2.81	130.08	124.80
23	B1	842	BCR	C15-C16-C17	-2.81	117.60	123.51
19	A2	820	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	B2	850	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	A	836	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	B1	833	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	B1	850	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
19	A	819	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	B2	823	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	A1	839	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	B1	833	CLA	C3A-C2A-C1A	2.81	105.55	101.34
19	A	806	CLA	CHB-C4A-NA	2.81	128.40	124.51
19	B	804	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	A1	809	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	BB	802	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
19	A2	827	CLA	O2D-CGD-O1D	-2.81	118.28	123.83
23	J1	102	BCR	C15-C14-C13	-2.81	123.31	127.31
19	AA	815	CLA	CMB-C2B-C1B	-2.81	124.15	128.46
19	A	823	CLA	CHB-C4A-NA	2.81	128.39	124.51
19	A2	818	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
19	BB	855	CLA	C1B-CHB-C4A	-2.80	124.56	130.12
23	M2	102	BCR	C33-C5-C6	-2.80	121.39	124.51
23	BB	847	BCR	C1-C6-C5	-2.80	118.67	122.59
19	A2	835	CLA	C1-C2-C3	-2.80	121.19	126.04
19	AA	831	CLA	CMB-C2B-C3B	2.80	130.06	124.80
19	B	859	CLA	CMB-C2B-C3B	2.80	130.06	124.80
19	A2	821	CLA	CHB-C4A-NA	2.80	128.39	124.51
19	B	832	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
19	B2	827	CLA	CHB-C4A-NA	2.80	128.38	124.51
19	AA	828	CLA	CHB-C4A-NA	2.80	128.38	124.51
19	A2	839	CLA	O2D-CGD-O1D	-2.80	118.30	123.83
24	A2	854	AJP	CCJ-CCI-CCH	-2.80	104.34	109.25
19	B2	807	CLA	O2A-CGA-O1A	-2.80	116.42	123.56
19	A1	827	CLA	O2D-CGD-O1D	-2.80	118.31	123.83
19	B	824	CLA	CMB-C2B-C3B	2.80	130.04	124.80
19	AA	829	CLA	CMD-C2D-C3D	2.80	130.04	124.80
19	A2	838	CLA	CMB-C2B-C3B	2.79	130.04	124.80
26	B1	840	ECH	C8-C7-C6	-2.79	119.45	127.28
25	L1	210	LMG	O6-C1-O1	-2.79	103.34	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	842	CLA	C5-C3-C2	-2.79	115.37	121.11
19	A2	802	CLA	CMB-C2B-C3B	2.79	130.04	124.80
19	A2	829	CLA	CMD-C2D-C3D	2.79	130.04	124.80
19	B1	818	CLA	O2D-CGD-O1D	-2.79	118.31	123.83
26	B2	841	ECH	C8-C7-C6	-2.79	119.46	127.28
19	BB	826	CLA	CMB-C2B-C3B	2.79	130.04	124.80
24	A1	855	AJP	CDC-CDB-CCG	2.79	117.46	112.31
19	A	810	CLA	CMB-C2B-C3B	2.79	130.03	124.80
19	AA	836	CLA	CHB-C4A-NA	2.79	128.37	124.51
20	A2	803	CL0	CHC-C1C-C2C	-2.79	119.02	126.71
19	BB	802	CLA	CHB-C4A-NA	2.79	128.37	124.51
19	A2	828	CLA	O2D-CGD-O1D	-2.79	118.32	123.83
19	LL	201	CLA	C4-C3-C2	-2.79	116.43	123.68
19	BB	824	CLA	CMB-C2B-C3B	2.79	130.03	124.80
19	B2	833	CLA	C2A-C1A-CHA	2.79	128.74	123.86
23	B1	838	BCR	C35-C13-C14	-2.79	119.02	122.92
23	II	104	BCR	C24-C23-C22	-2.79	122.02	126.21
19	B2	818	CLA	O2D-CGD-O1D	-2.79	118.33	123.83
19	A	824	CLA	O2D-CGD-O1D	-2.79	118.33	123.83
19	A2	828	CLA	CMB-C2B-C3B	2.79	130.03	124.80
19	A	834	CLA	CMB-C2B-C1B	-2.79	124.18	128.46
19	B1	832	CLA	C5-C3-C2	2.79	126.83	121.11
19	B2	851	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
24	L2	202	AJP	CDC-CDB-CCG	2.79	117.45	112.31
20	A	803	CL0	CHC-C1C-C2C	-2.79	119.03	126.71
25	B	851	LMG	O6-C1-O1	-2.79	103.36	109.94
19	BB	806	CLA	O2D-CGD-O1D	-2.78	118.33	123.83
19	A2	816	CLA	O2D-CGD-O1D	-2.78	118.33	123.83
24	A2	854	AJP	CDD-CCI-CCH	-2.78	107.00	110.50
19	B	806	CLA	O2D-CGD-O1D	-2.78	118.33	123.83
23	B1	841	BCR	C30-C25-C26	-2.78	118.70	122.59
23	A1	847	BCR	C23-C22-C21	-2.78	118.61	124.84
19	A	836	CLA	CHB-C4A-NA	2.78	128.36	124.51
23	F2	303	BCR	C33-C5-C6	-2.78	121.41	124.51
19	AA	806	CLA	CHB-C4A-NA	2.78	128.36	124.51
19	A2	824	CLA	CMB-C2B-C3B	2.78	130.02	124.80
19	B2	824	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
19	AA	805	CLA	CMD-C2D-C3D	2.78	130.01	124.80
19	A1	841	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
23	A1	853	BCR	C27-C26-C25	2.78	126.79	122.74
19	B1	822	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
19	AA	809	CLA	CHB-C4A-NA	2.78	128.35	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	827	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
19	A	835	CLA	O2D-CGD-O1D	-2.78	118.34	123.83
23	A2	853	BCR	C27-C26-C25	2.78	126.79	122.74
19	AA	823	CLA	CHB-C4A-NA	2.78	128.35	124.51
19	B	836	CLA	CMB-C2B-C3B	2.78	130.01	124.80
23	L	206	BCR	C33-C5-C6	-2.78	121.42	124.51
23	A2	847	BCR	C23-C22-C21	-2.78	118.62	124.84
19	A2	837	CLA	CMB-C2B-C3B	2.78	130.01	124.80
23	JJ	104	BCR	C33-C5-C6	-2.78	121.42	124.51
20	A1	802	CL0	CHD-C4C-C3C	-2.78	120.82	124.87
19	B	859	CLA	CAA-CBA-CGA	2.78	121.43	113.26
23	F2	305	BCR	C33-C5-C6	-2.78	121.42	124.51
19	A	820	CLA	O2A-CGA-O1A	-2.78	116.47	123.56
19	BB	823	CLA	O2D-CGD-O1D	-2.78	118.35	123.83
19	F1	302	CLA	CHB-C4A-NA	2.77	128.35	124.51
19	L1	205	CLA	C4-C3-C2	-2.77	116.47	123.68
24	L	209	AJP	CDA-CDB-CDC	-2.77	108.37	112.56
19	A2	809	CLA	CMB-C2B-C3B	2.77	130.00	124.80
23	A	848	BCR	C33-C5-C6	-2.77	121.42	124.51
19	A2	811	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	B	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
23	BB	847	BCR	C33-C5-C6	-2.77	121.42	124.51
23	KK	103	BCR	C33-C5-C6	-2.77	121.42	124.51
19	A	844	CLA	CMD-C2D-C3D	2.77	130.00	124.80
19	B2	803	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
23	A1	851	BCR	C28-C27-C26	-2.77	109.17	113.99
23	AA	849	BCR	C33-C5-C6	-2.77	121.42	124.51
19	A	811	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	A2	804	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	A1	842	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	A1	817	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
19	A	808	CLA	C1-O2A-CGA	2.77	124.11	116.54
19	AA	824	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	BB	803	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	B2	805	CLA	CHB-C4A-NA	2.77	128.34	124.51
19	A1	833	CLA	CMB-C2B-C1B	-2.77	124.21	128.46
23	A	853	BCR	C27-C26-C25	2.77	126.78	122.74
23	AA	854	BCR	C27-C26-C25	2.77	126.78	122.74
19	A1	819	CLA	O2D-CGD-O1D	-2.77	118.36	123.83
19	B1	829	CLA	C1D-CHD-C4C	2.77	126.27	122.48
19	B	822	CLA	O2D-CGD-O1D	-2.77	118.37	123.83
19	B	829	CLA	O2D-CGD-O1D	-2.77	118.37	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L1	204	AJP	CDC-CDB-CCG	2.77	117.41	112.31
19	AA	840	CLA	O2D-CGD-O1D	-2.77	118.37	123.83
19	B1	819	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
19	A	812	CLA	O2D-CGD-O1D	-2.76	118.37	123.83
24	AA	856	AJP	CDC-CDB-CCG	2.76	117.41	112.31
19	A	809	CLA	CHB-C4A-NA	2.76	128.34	124.51
24	A	855	AJP	CDC-CDB-CCG	2.76	117.41	112.31
23	BB	841	BCR	C15-C16-C17	-2.76	117.70	123.51
19	A1	822	CLA	CMB-C2B-C3B	2.76	129.98	124.80
19	AA	833	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	B1	814	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	F	302	CLA	O2D-CGD-CBD	2.76	116.09	111.25
23	J2	102	BCR	C15-C14-C13	-2.76	123.37	127.31
19	J2	103	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	A	828	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	BB	856	CLA	C1B-CHB-C4A	-2.76	124.65	130.12
19	AA	830	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	AA	837	CLA	CMB-C2B-C3B	2.76	129.97	124.80
19	A2	807	CLA	CHB-C4A-NA	2.76	128.33	124.51
19	A2	824	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	FF	303	BCR	C33-C5-C6	-2.76	121.44	124.51
19	B	820	CLA	CAC-C3C-C2C	-2.76	122.82	127.53
19	A	817	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	A	840	CLA	O2D-CGD-O1D	-2.76	118.38	123.83
19	B	858	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
19	BB	819	CLA	O2D-CGD-O1D	-2.76	118.39	123.83
19	B1	825	CLA	O2D-CGD-CBD	2.76	116.08	111.25
19	FF	301	CLA	O2D-CGD-CBD	2.76	116.08	111.25
19	B2	851	CLA	CMB-C2B-C3B	2.76	129.97	124.80
19	AA	845	CLA	CMB-C2B-C1B	-2.76	124.23	128.46
19	A1	805	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
20	A1	802	CL0	CHC-C1C-C2C	-2.76	119.11	126.71
19	A	811	CLA	CMB-C2B-C3B	2.76	129.97	124.80
19	A2	811	CLA	CMD-C2D-C3D	2.75	129.97	124.80
19	F2	302	CLA	CHB-C4A-NA	2.75	128.32	124.51
19	A2	819	CLA	O2D-CGD-O1D	-2.75	118.39	123.83
19	JJ	101	CLA	O2D-CGD-O1D	-2.75	118.39	123.83
19	XX	101	CLA	O2D-CGD-O1D	-2.75	118.39	123.83
19	B	860	CLA	O2D-CGD-O1D	-2.75	118.40	123.83
19	B	815	CLA	O2D-CGD-O1D	-2.75	118.40	123.83
19	A	816	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A2	810	CLA	C1B-CHB-C4A	-2.75	124.67	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	801	CLA	C4-C3-C2	-2.75	116.53	123.68
19	A1	810	CLA	CMB-C2B-C3B	2.75	129.96	124.80
23	AA	848	BCR	C23-C22-C21	-2.75	118.69	124.84
19	AA	830	CLA	CMB-C2B-C3B	2.75	129.95	124.80
23	F	303	BCR	C33-C5-C6	-2.75	121.45	124.51
19	A	828	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A	811	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	A1	805	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
19	A2	842	CLA	CHB-C4A-NA	2.75	128.31	124.51
19	BB	821	CLA	C5-C3-C2	2.74	126.75	121.11
19	LL	202	CLA	O2D-CGD-CBD	2.74	116.05	111.25
24	BB	849	AJP	CAV-CBE-CBO	2.74	120.73	114.54
23	F1	303	BCR	C33-C5-C6	-2.74	121.45	124.51
19	A1	815	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
19	A	842	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	AA	817	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
19	J2	101	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
23	I1	101	BCR	C8-C7-C6	-2.74	119.60	127.28
19	A1	822	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	AA	828	CLA	CMB-C2B-C3B	2.74	129.94	124.80
19	B1	849	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
19	AA	812	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
19	B	806	CLA	CHB-C4A-NA	2.74	128.30	124.51
19	AA	843	CLA	O2D-CGD-O1D	-2.74	118.42	123.83
19	L2	204	CLA	C4-C3-C2	-2.74	116.56	123.68
19	B1	827	CLA	O2D-CGD-O1D	-2.74	118.43	123.83
19	B1	850	CLA	CMB-C2B-C3B	2.74	129.93	124.80
24	K	104	AJP	CBE-CBO-CBP	-2.74	99.19	104.35
19	A	818	CLA	O2D-CGD-O1D	-2.74	118.43	123.83
19	B2	811	CLA	CMB-C2B-C3B	2.73	129.93	124.80
23	BB	841	BCR	C28-C27-C26	-2.73	109.23	113.99
19	B1	821	CLA	CMB-C2B-C3B	2.73	129.93	124.80
19	B1	805	CLA	CHB-C4A-NA	2.73	128.29	124.51
19	A2	842	CLA	C5-C3-C2	-2.73	115.50	121.11
23	F1	304	BCR	C38-C26-C25	-2.73	121.47	124.51
19	J1	103	CLA	O2D-CGD-O1D	-2.73	118.43	123.83
19	B2	810	CLA	O2D-CGD-O1D	-2.73	118.43	123.83
19	B1	814	CLA	CMB-C2B-C3B	2.73	129.92	124.80
23	MM	101	BCR	C15-C16-C17	-2.73	117.77	123.51
19	B	811	CLA	CMB-C2B-C3B	2.73	129.92	124.80
19	A	816	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
19	A	809	CLA	CMB-C2B-C1B	-2.73	124.27	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	841	CLA	CHB-C4A-NA	2.73	128.29	124.51
19	J1	101	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
19	B2	830	CLA	C1D-CHD-C4C	2.73	126.21	122.48
19	BB	808	CLA	CMB-C2B-C3B	2.73	129.92	124.80
23	A1	851	BCR	C3-C4-C5	-2.73	109.24	113.99
19	A	830	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
19	BB	821	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
19	L2	205	CLA	CMB-C2B-C3B	2.73	129.91	124.80
19	B1	849	CLA	CMB-C2B-C3B	2.73	129.91	124.80
23	BB	839	BCR	C1-C6-C5	-2.73	118.78	122.59
19	B	819	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
19	A1	818	CLA	O2D-CGD-O1D	-2.73	118.44	123.83
23	B	842	BCR	C15-C16-C17	-2.73	117.78	123.51
19	AA	834	CLA	CMD-C2D-C3D	2.73	129.91	124.80
19	A	830	CLA	CMB-C2B-C3B	2.73	129.91	124.80
19	B	812	CLA	CMB-C2B-C3B	2.73	129.91	124.80
19	AA	823	CLA	O2D-CGD-CBD	2.73	116.02	111.25
19	AA	806	CLA	O2D-CGD-O1D	-2.73	118.45	123.83
19	B	830	CLA	C1D-CHD-C4C	2.73	126.21	122.48
23	II	101	BCR	C8-C7-C6	-2.72	119.65	127.28
24	L2	203	AJP	CDC-CDD-CCI	2.72	116.67	112.13
20	A1	802	CL0	CMB-C2B-C3B	2.72	129.91	124.80
19	A	840	CLA	CMB-C2B-C3B	2.72	129.91	124.80
19	AA	818	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
23	M1	101	BCR	C33-C5-C6	-2.72	121.48	124.51
19	AA	829	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
19	L	202	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	B1	850	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
19	B1	808	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
19	B	823	CLA	O2D-CGD-O1D	-2.72	118.46	123.83
23	B1	841	BCR	C15-C16-C17	-2.72	117.80	123.51
19	X	101	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	B	834	CLA	CHB-C4A-NA	2.72	128.27	124.51
19	AA	822	CLA	CMB-C2B-C1B	-2.72	124.29	128.46
19	B2	810	CLA	CMB-C2B-C3B	2.72	129.89	124.80
19	BB	831	CLA	CHB-C4A-NA	2.72	128.27	124.51
23	B	848	BCR	C33-C5-C6	-2.72	121.49	124.51
19	A1	836	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
19	A2	817	CLA	CHB-C4A-NA	2.71	128.27	124.51
19	B2	806	CLA	CHB-C4A-NA	2.71	128.27	124.51
19	A2	816	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
19	A1	828	CLA	O2D-CGD-O1D	-2.71	118.47	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	BB	849	AJP	OBG-CBF-CAW	2.71	113.38	110.81
23	A	847	BCR	C23-C22-C21	-2.71	118.76	124.84
19	B2	833	CLA	C3D-CAD-CBD	-2.71	103.96	107.61
19	J	101	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
19	AA	828	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
26	BB	840	ECH	C37-C22-C21	2.71	126.72	122.92
19	AA	811	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B	859	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
19	B	837	CLA	C1D-CHD-C4C	2.71	126.19	122.48
19	BB	833	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	A2	801	CLA	O2D-CGD-O1D	-2.71	118.47	123.83
19	B2	829	CLA	CMB-C2B-C3B	2.71	129.88	124.80
24	AA	802	AJP	CDA-CDB-CCG	2.71	117.31	112.31
19	B	832	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	BB	805	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	KK	101	CLA	O2D-CGD-CBD	2.71	116.00	111.25
24	L2	203	AJP	OBG-CBF-CAW	2.71	113.38	110.81
26	B1	840	ECH	C40-C30-C25	2.71	114.69	110.30
19	B1	807	CLA	O2A-CGA-O1A	-2.71	116.64	123.56
19	BB	816	CLA	CMB-C2B-C3B	2.71	129.88	124.80
19	K1	102	CLA	O2D-CGD-CBD	2.71	115.99	111.25
19	B2	817	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	B1	848	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	BB	836	CLA	CBC-CAC-C3C	2.71	119.94	112.43
19	B	836	CLA	O2D-CGD-O1D	-2.71	118.48	123.83
19	A1	806	CLA	CHB-C4A-NA	2.71	128.26	124.51
19	AA	816	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
23	K1	106	BCR	C38-C26-C25	-2.71	121.50	124.51
23	F	305	BCR	C24-C23-C22	-2.71	122.14	126.21
19	F	301	CLA	C2A-C1A-CHA	2.71	128.59	123.86
19	B1	817	CLA	CHB-C4A-NA	2.71	128.25	124.51
24	BB	848	AJP	CDA-CDB-CCG	2.71	115.55	112.65
19	A1	841	CLA	C5-C3-C2	-2.71	115.55	121.11
19	BB	806	CLA	CMD-C2D-C3D	2.70	129.87	124.80
19	AA	810	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
19	AA	836	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
19	B	824	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
19	K1	105	CLA	O2D-CGD-O1D	-2.70	118.49	123.83
19	AA	816	CLA	CHB-C4A-NA	2.70	128.25	124.51
20	A	803	CL0	CAA-C2A-C1A	2.70	120.83	111.97
19	A2	820	CLA	O2A-CGA-O1A	-2.70	116.65	123.56
19	A	820	CLA	CHB-C4A-NA	2.70	128.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L1	205	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	A1	815	CLA	CHB-C4A-NA	2.70	128.25	124.51
19	BB	856	CLA	CMB-C2B-C3B	2.70	129.87	124.80
19	BB	827	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
19	BB	835	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
19	A2	829	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
23	I2	101	BCR	C8-C7-C6	-2.70	119.72	127.28
21	A	843	PQN	C15-C13-C12	-2.70	115.57	121.11
19	AA	826	CLA	O2D-CGD-O1D	-2.70	118.50	123.83
24	B	857	AJP	CCH-CCG-CDB	2.70	112.42	108.59
19	B	815	CLA	C5-C3-C2	2.70	126.65	121.11
23	F	305	BCR	C35-C13-C14	-2.70	119.14	122.92
19	B1	822	CLA	CMB-C2B-C1B	-2.70	124.32	128.46
19	L1	206	CLA	CMD-C2D-C3D	2.70	129.85	124.80
19	B2	802	CLA	CHB-C4A-NA	2.70	128.24	124.51
19	B	826	CLA	C6-C5-C3	2.69	119.48	113.01
24	B	850	AJP	OBQ-CBF-CBE	-2.69	100.33	104.44
19	K	101	CLA	CHB-C4A-NA	2.69	128.24	124.51
19	BB	807	CLA	CMB-C2B-C3B	2.69	129.85	124.80
23	F1	306	BCR	C35-C13-C14	-2.69	119.15	122.92
23	F2	305	BCR	C35-C13-C14	-2.69	119.15	122.92
19	KK	102	CLA	CMB-C2B-C3B	2.69	129.85	124.80
19	A	829	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	B	823	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	A2	818	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
24	L1	204	AJP	CDA-CDB-CCG	2.69	115.54	112.65
19	BB	824	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
19	F	302	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	F1	305	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
26	B	841	ECH	C21-C20-C19	-2.69	115.22	123.31
19	A2	806	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
23	BB	841	BCR	C30-C25-C26	-2.69	118.83	122.59
19	B	833	CLA	C5-C3-C2	2.69	126.63	121.11
19	BB	832	CLA	CED-O2D-CGD	2.69	122.09	115.95
19	B	854	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
19	XX	101	CLA	CHB-C4A-NA	2.69	128.23	124.51
19	A2	840	CLA	CMB-C2B-C3B	2.69	129.84	124.80
19	A2	844	CLA	CMB-C2B-C1B	-2.69	124.33	128.46
19	X	101	CLA	O2D-CGD-O1D	-2.69	118.52	123.83
19	A1	819	CLA	O2A-CGA-O1A	-2.69	116.69	123.56
19	B2	804	CLA	C1-C2-C3	-2.69	121.40	126.04
19	F1	305	CLA	CMB-C2B-C3B	2.69	129.84	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	824	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
19	B	810	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	BB	825	CLA	O2D-CGD-CBD	2.68	115.95	111.25
19	A2	806	CLA	O2D-CGD-O1D	-2.68	118.53	123.83
24	B	849	AJP	CAZ-CAY-CAX	2.68	118.04	112.08
19	B2	806	CLA	CMB-C2B-C3B	2.68	129.83	124.80
23	L1	209	BCR	C33-C5-C6	-2.68	121.52	124.51
19	L2	204	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	X1	101	CLA	CHB-C4A-NA	2.68	128.22	124.51
24	A	802	AJP	CDA-CDB-CCG	2.68	117.26	112.31
19	A2	841	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	B2	824	CLA	CMB-C2B-C3B	2.68	129.83	124.80
23	L2	207	BCR	C33-C5-C6	-2.68	121.53	124.51
23	A2	851	BCR	C3-C4-C5	-2.68	109.33	113.99
20	A	803	CL0	CAC-C3C-C4C	2.68	128.32	124.82
19	B2	851	CLA	C1B-CHB-C4A	-2.68	124.81	130.12
26	BB	840	ECH	C21-C20-C19	-2.68	115.25	123.31
23	F2	303	BCR	C2-C1-C6	2.68	114.63	110.48
19	B1	850	CLA	CAA-CBA-CGA	2.68	121.15	113.26
19	BB	821	CLA	CHB-C4A-NA	2.68	128.22	124.51
19	BB	811	CLA	CMB-C2B-C3B	2.68	129.82	124.80
19	FF	305	CLA	O2D-CGD-O1D	-2.68	118.54	123.83
24	I2	104	AJP	OBQ-CBF-CBE	-2.68	100.36	104.44
19	B2	830	CLA	C5-C3-C2	2.68	126.61	121.11
19	BB	805	CLA	CMB-C2B-C3B	2.68	129.82	124.80
19	AA	842	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	AA	804	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	A	812	CLA	CMB-C2B-C3B	2.68	129.82	124.80
24	M2	101	AJP	CBE-CBO-CBP	-2.68	99.30	104.35
19	A1	816	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	B1	803	CLA	O2D-CGD-O1D	-2.68	118.55	123.83
19	B2	809	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	B2	804	CLA	CHB-C4A-NA	2.68	128.21	124.51
19	A	834	CLA	O2D-CGD-O1D	-2.68	118.55	123.83
23	I	102	BCR	C2-C1-C6	2.67	114.62	110.48
19	A2	842	CLA	C4-C3-C5	2.67	119.89	115.29
19	B2	849	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
19	A2	835	CLA	O2D-CGD-O1D	-2.67	118.55	123.83
19	BB	823	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	A	825	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	A	806	CLA	CMB-C2B-C3B	2.67	129.81	124.80
19	A2	809	CLA	CHB-C4A-NA	2.67	128.21	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F1	303	BCR	C35-C13-C14	-2.67	119.18	122.92
19	B	810	CLA	CMD-C2D-C3D	2.67	129.81	124.80
19	A2	837	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	BB	804	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	AA	845	CLA	CHB-C4A-NA	2.67	128.21	124.51
19	AA	811	CLA	C1B-CHB-C4A	-2.67	124.83	130.12
24	KK	104	AJP	CAZ-CAY-CAX	2.67	118.01	112.08
23	J	104	BCR	C1-C6-C5	-2.67	118.86	122.59
19	A	829	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	A	807	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	B2	815	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	A2	803	CL0	O2A-CGA-O1A	-2.67	116.74	123.56
19	A1	817	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	AA	806	CLA	CMB-C2B-C3B	2.67	129.81	124.80
19	B2	816	CLA	CMB-C2B-C3B	2.67	129.81	124.80
19	A1	816	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	A	804	CLA	CMB-C2B-C1B	-2.67	124.36	128.46
19	K1	103	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	F1	302	CLA	O2D-CGD-CBD	2.67	115.92	111.25
19	L1	206	CLA	O2D-CGD-CBD	2.67	115.92	111.25
19	A1	812	CLA	CMB-C2B-C3B	2.67	129.80	124.80
19	BB	833	CLA	C3A-C2A-C1A	2.67	105.33	101.34
19	X2	101	CLA	O2D-CGD-O1D	-2.67	118.56	123.83
19	AA	810	CLA	CBA-CAA-C2A	2.67	121.79	113.85
19	A1	841	CLA	C4-C3-C5	2.67	119.88	115.29
23	I1	101	BCR	C38-C26-C25	-2.67	121.54	124.51
19	B	804	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	B1	813	CLA	CHB-C4A-NA	2.67	128.20	124.51
19	A2	835	CLA	CMB-C2B-C3B	2.67	129.80	124.80
19	A	810	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
19	BB	806	CLA	CHB-C4A-NA	2.66	128.20	124.51
23	B1	843	BCR	C27-C26-C25	2.66	126.63	122.74
19	BB	806	CLA	CMB-C2B-C1B	-2.66	124.37	128.46
19	A1	840	CLA	CHB-C4A-NA	2.66	128.20	124.51
20	AA	803	CL0	C9-C8-C7	2.66	121.01	111.30
23	L2	207	BCR	C15-C16-C17	-2.66	117.92	123.51
19	B2	826	CLA	CMB-C2B-C3B	2.66	129.79	124.80
19	A2	802	CLA	O2D-CGD-O1D	-2.66	118.58	123.83
19	FF	302	CLA	CHB-C4A-NA	2.66	128.19	124.51
23	II	104	BCR	C33-C5-C6	-2.66	121.55	124.51
19	F1	301	CLA	C2A-C1A-CHA	2.66	128.51	123.86
19	A	816	CLA	CMB-C2B-C1B	-2.66	124.38	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	BB	841	BCR	C35-C13-C14	-2.66	119.20	122.92
19	BB	833	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
19	B	805	CLA	CMB-C2B-C3B	2.66	129.78	124.80
19	B2	822	CLA	O2D-CGD-O1D	-2.66	118.59	123.83
19	BB	801	CLA	C5-C3-C2	2.65	126.56	121.11
19	A1	833	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
23	MM	101	BCR	C27-C26-C25	2.65	126.61	122.74
19	B1	808	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
19	A1	838	CLA	CHB-C4A-NA	2.65	128.18	124.51
23	K1	106	BCR	C33-C5-C6	-2.65	121.56	124.51
19	A2	811	CLA	CMB-C2B-C3B	2.65	129.78	124.80
19	A1	830	CLA	O2D-CGD-O1D	-2.65	118.59	123.83
20	A	803	CL0	CHD-C4C-C3C	-2.65	121.00	124.87
19	BB	826	CLA	C6-C5-C3	2.65	119.38	113.01
19	BB	812	CLA	CMB-C2B-C3B	2.65	129.77	124.80
24	M2	101	AJP	CAV-CBE-CBO	2.65	120.52	114.54
23	B1	841	BCR	C28-C27-C26	-2.65	109.38	113.99
19	B1	806	CLA	CMD-C2D-C3D	2.65	129.77	124.80
19	B1	830	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
24	A1	855	AJP	CDD-CCI-CCH	-2.65	107.17	110.50
19	A2	808	CLA	CHB-C4A-NA	2.65	128.18	124.51
19	B1	836	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
24	L	208	AJP	CCG-CCF-CCE	2.65	116.92	113.91
26	B	841	ECH	C40-C30-C25	2.65	114.59	110.30
19	B1	809	CLA	CHB-C4A-NA	2.65	128.17	124.51
19	B1	802	CLA	CMB-C2B-C1B	-2.65	124.39	128.46
19	A1	835	CLA	O2D-CGD-O1D	-2.65	118.60	123.83
19	A1	808	CLA	CHB-C4A-NA	2.65	128.17	124.51
26	BB	840	ECH	C40-C30-C25	2.65	114.58	110.30
19	B	812	CLA	CMD-C2D-C3D	2.64	129.76	124.80
19	A2	815	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
23	A1	848	BCR	C33-C5-C6	-2.64	121.57	124.51
19	K1	102	CLA	CHB-C4A-NA	2.64	128.17	124.51
19	A2	806	CLA	C1B-CHB-C4A	-2.64	124.88	130.12
19	A1	801	CLA	O2D-CGD-O1D	-2.64	118.61	123.83
24	I2	104	AJP	CDA-CDB-CCG	2.64	117.18	112.31
19	B2	805	CLA	CMB-C2B-C3B	2.64	129.75	124.80
19	AA	843	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	AA	825	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
19	A	811	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
19	A1	844	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
23	A2	848	BCR	C33-C5-C6	-2.64	121.57	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	817	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
19	A2	825	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A2	811	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A	805	CLA	CMD-C2D-C3D	2.64	129.75	124.80
19	AA	843	CLA	CHD-C4C-C3C	2.64	128.71	124.87
19	BB	836	CLA	CMB-C2B-C1B	-2.64	124.41	128.46
19	A2	834	CLA	O2D-CGD-O1D	-2.64	118.62	123.83
19	AA	806	CLA	C1B-CHB-C4A	-2.64	124.89	130.12
23	I	101	BCR	C8-C7-C6	-2.64	119.89	127.28
19	AA	808	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	A2	839	CLA	CHB-C4A-NA	2.64	128.16	124.51
19	B1	818	CLA	CMD-C2D-C3D	2.64	129.74	124.80
19	AA	835	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
19	BB	829	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
19	A1	809	CLA	C1B-CHB-C4A	-2.63	124.90	130.12
23	K2	105	BCR	C33-C5-C6	-2.63	121.58	124.51
19	L1	207	CLA	CMD-C2D-C3D	2.63	129.74	124.80
19	A1	833	CLA	CMD-C2D-C3D	2.63	129.74	124.80
19	A1	805	CLA	O2D-CGD-CBD	2.63	115.86	111.25
19	BB	811	CLA	O2D-CGD-O1D	-2.63	118.63	123.83
19	B	821	CLA	CMD-C2D-C3D	2.63	129.74	124.80
19	B	803	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	A	810	CLA	O2A-CGA-O1A	-2.63	116.84	123.56
23	A1	853	BCR	C15-C14-C13	-2.63	123.56	127.31
20	A1	802	CL0	O2A-C1-C2	2.63	115.55	108.64
19	B1	805	CLA	CMB-C2B-C3B	2.63	129.73	124.80
19	B1	835	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	B	816	CLA	CMB-C2B-C3B	2.63	129.73	124.80
19	A1	820	CLA	CMD-C2D-C3D	2.63	129.73	124.80
19	X2	101	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	B2	808	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
19	BB	815	CLA	O2D-CGD-O1D	-2.63	118.64	123.83
19	B	854	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	A2	853	BCR	C33-C5-C6	-2.63	121.58	124.51
19	B2	818	CLA	CMD-C2D-C3D	2.63	129.73	124.80
24	BB	849	AJP	CCJ-CCI-CCH	-2.63	104.64	109.25
19	B2	820	CLA	CBC-CAC-C3C	2.63	119.71	112.43
19	A1	801	CLA	CMD-C2D-C3D	2.63	129.72	124.80
19	BB	852	CLA	CHB-C4A-NA	2.63	128.14	124.51
19	AA	838	CLA	C1B-CHB-C4A	-2.62	124.92	130.12
25	II	105	LMG	O6-C1-O1	-2.62	103.74	109.94
19	B	830	CLA	CMB-C2B-C1B	-2.62	124.43	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	851	CLA	CAA-CBA-CGA	2.62	120.99	113.26
19	B2	832	CLA	CHB-C4A-NA	2.62	128.14	124.51
23	L1	209	BCR	C15-C16-C17	-2.62	118.00	123.51
19	B1	806	CLA	CMB-C2B-C3B	2.62	129.72	124.80
19	B2	807	CLA	CMB-C2B-C3B	2.62	129.72	124.80
19	B2	819	CLA	CMB-C2B-C3B	2.62	129.72	124.80
19	X1	101	CLA	O2D-CGD-O1D	-2.62	118.65	123.83
19	KK	101	CLA	CHB-C4A-NA	2.62	128.14	124.51
19	A1	803	CLA	CMB-C2B-C1B	-2.62	124.44	128.46
23	AA	854	BCR	C33-C5-C6	-2.62	121.59	124.51
19	LL	201	CLA	CHB-C4A-NA	2.62	128.13	124.51
19	A2	832	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	K	104	AJP	CAZ-CAY-CAX	2.62	117.90	112.08
19	B1	833	CLA	C2A-C1A-CHA	2.62	128.44	123.86
19	A1	836	CLA	CMB-C2B-C3B	2.62	129.71	124.80
19	A	813	CLA	O2D-CGD-O1D	-2.62	118.66	123.83
19	AA	812	CLA	CMB-C2B-C3B	2.62	129.71	124.80
19	AA	853	CLA	C1B-CHB-C4A	-2.62	124.93	130.12
19	A	806	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
19	B1	824	CLA	C1B-CHB-C4A	-2.62	124.94	130.12
19	A1	823	CLA	O2D-CGD-O1D	-2.61	118.67	123.83
19	B1	820	CLA	O2D-CGD-CBD	2.61	115.83	111.25
19	A1	842	CLA	CHD-C4C-C3C	2.61	128.68	124.87
19	A	828	CLA	CMB-C2B-C3B	2.61	129.70	124.80
19	A2	813	CLA	CMB-C2B-C3B	2.61	129.70	124.80
19	AA	842	CLA	C4-C3-C5	2.61	119.79	115.29
19	B1	819	CLA	CMB-C2B-C3B	2.61	129.70	124.80
19	BB	809	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	B2	841	ECH	C21-C20-C19	-2.61	115.45	123.31
19	AA	810	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	BB	845	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	F	301	CLA	CMB-C2B-C3B	2.61	129.70	124.80
19	LL	202	CLA	CMB-C2B-C3B	2.61	129.70	124.80
23	A	853	BCR	C33-C5-C6	-2.61	121.60	124.51
19	B	820	CLA	CBC-CAC-C3C	2.61	119.67	112.43
23	B2	843	BCR	C15-C16-C17	-2.61	118.03	123.51
19	B2	810	CLA	CMD-C2D-C3D	2.61	129.69	124.80
19	B1	845	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	B	831	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	BB	810	CLA	CHB-C4A-NA	2.61	128.12	124.51
19	LL	203	CLA	CAC-C3C-C4C	2.61	128.23	124.82
19	BB	815	CLA	C5-C3-C2	2.61	126.47	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	FF	306	BCR	C24-C23-C22	-2.61	122.29	126.21
19	B2	821	CLA	CMB-C2B-C3B	2.61	129.69	124.80
19	B2	830	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
23	A2	848	BCR	C15-C16-C17	-2.61	118.03	123.51
19	B	810	CLA	O2D-CGD-O1D	-2.61	118.69	123.83
19	A1	807	CLA	C1-O2A-CGA	2.61	123.66	116.54
19	B1	810	CLA	CMB-C2B-C3B	2.61	129.69	124.80
19	B	834	CLA	C3A-C2A-C1A	2.61	105.24	101.34
19	B2	837	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
19	AA	832	CLA	CMB-C2B-C3B	2.60	129.68	124.80
22	A2	846	LHG	O4-P-O5	2.60	125.26	112.21
19	LL	202	CLA	CHB-C4A-NA	2.60	128.11	124.51
22	A1	846	LHG	O4-P-O5	2.60	125.26	112.21
19	A2	835	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
19	A	814	CLA	CMB-C2B-C3B	2.60	129.68	124.80
19	A	810	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	L1	209	BCR	C11-C10-C9	-2.60	123.60	127.31
19	AA	813	CLA	O2D-CGD-O1D	-2.60	118.69	123.83
19	B2	846	CLA	CHB-C4A-NA	2.60	128.11	124.51
19	B2	834	CLA	CAA-C2A-C3A	-2.60	105.66	112.78
23	F	303	BCR	C2-C1-C6	2.60	114.50	110.48
19	FF	302	CLA	O2D-CGD-CBD	2.60	115.80	111.25
23	LL	204	BCR	C33-C5-C6	-2.60	121.61	124.51
22	A	846	LHG	O4-P-O5	2.60	125.24	112.21
23	J2	102	BCR	C1-C6-C5	-2.60	118.96	122.59
19	AA	804	CLA	C1-C2-C3	-2.60	121.55	126.04
26	B1	840	ECH	C21-C20-C19	-2.60	115.49	123.31
23	K	103	BCR	C24-C23-C22	-2.60	122.31	126.21
19	A	844	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	A2	807	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
19	B1	835	CLA	O2D-CGD-O1D	-2.60	118.70	123.83
19	AA	829	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	AA	835	CLA	C1-C2-C3	-2.60	121.55	126.04
19	BB	836	CLA	O2D-CGD-CBD	2.60	115.80	111.25
19	B	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	A1	810	CLA	CHB-C4A-NA	2.60	128.10	124.51
19	BB	815	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	I2	104	AJP	CAV-CBE-CBO	2.60	120.40	114.54
19	B1	823	CLA	CHB-C4A-NA	2.59	128.10	124.51
19	A	841	CLA	CMB-C2B-C3B	2.59	129.67	124.80
19	B	808	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
19	B2	828	CLA	CMB-C2B-C3B	2.59	129.66	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	820	CLA	CMB-C2B-C3B	2.59	129.66	124.80
23	M	101	BCR	C27-C26-C25	2.59	126.52	122.74
19	F	301	CLA	CAA-C2A-C3A	-2.59	105.68	112.78
20	AA	803	CL0	CMA-C3A-C4A	-2.59	104.81	111.77
19	BB	826	CLA	C1B-CHB-C4A	-2.59	124.98	130.12
25	B1	846	LMG	O6-C1-O1	-2.59	103.82	109.94
23	FF	303	BCR	C8-C7-C6	-2.59	120.02	127.28
19	AA	834	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	J	103	CLA	O2D-CGD-O1D	-2.59	118.71	123.83
19	A1	829	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
19	BB	832	CLA	C5-C3-C2	2.59	126.43	121.11
19	A1	825	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
19	A	817	CLA	CMB-C2B-C1B	-2.59	124.48	128.46
24	B	850	AJP	CCX-OCY-CCZ	-2.59	111.33	115.33
19	A2	817	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
19	A2	813	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
19	A2	808	CLA	CMB-C2B-C3B	2.59	129.66	124.80
19	A	822	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
22	X1	103	LHG	O4-P-O5	2.59	125.19	112.21
19	AA	820	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
23	I	102	BCR	C33-C5-C6	-2.59	121.63	124.51
19	B	822	CLA	CMB-C2B-C1B	-2.59	124.49	128.46
19	B1	836	CLA	O2D-CGD-CBD	2.59	115.78	111.25
19	K2	102	CLA	CMB-C2B-C3B	2.59	129.65	124.80
19	A	801	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
19	A2	822	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	BB	810	CLA	CMD-C2D-C3D	2.59	129.65	124.80
19	B	858	CLA	CMB-C2B-C3B	2.59	129.65	124.80
23	J1	102	BCR	C1-C6-C5	-2.59	118.97	122.59
19	BB	825	CLA	C1D-CHD-C4C	2.59	126.02	122.48
19	BB	830	CLA	CHB-C4A-NA	2.59	128.09	124.51
23	L	205	BCR	C33-C5-C6	-2.59	121.63	124.51
19	BB	810	CLA	O2D-CGD-O1D	-2.59	118.72	123.83
19	B1	829	CLA	CMD-C2D-C3D	2.59	129.65	124.80
19	L1	206	CLA	CMB-C2B-C3B	2.59	129.65	124.80
19	BB	821	CLA	CMD-C2D-C3D	2.58	129.65	124.80
19	A1	820	CLA	CMB-C2B-C1B	-2.58	124.49	128.46
19	B	821	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
19	BB	812	CLA	CMD-C2D-C3D	2.58	129.65	124.80
19	LL	203	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
19	A1	812	CLA	O2D-CGD-O1D	-2.58	118.73	123.83
23	B2	842	BCR	C28-C27-C26	-2.58	109.50	113.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	815	CLA	O2D-CGD-CBD	2.58	115.77	111.25
19	F2	301	CLA	C2A-C1A-CHA	2.58	128.37	123.86
19	B2	830	CLA	CMD-C2D-C3D	2.58	129.64	124.80
19	B2	837	CLA	O2D-CGD-CBD	2.58	115.77	111.25
19	AA	841	CLA	CMB-C2B-C3B	2.58	129.64	124.80
19	B	807	CLA	O2A-CGA-O1A	-2.58	116.97	123.56
19	A1	828	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	K	103	BCR	C38-C26-C25	-2.58	121.64	124.51
19	B1	826	CLA	CMB-C2B-C3B	2.58	129.63	124.80
19	B1	812	CLA	CMB-C2B-C3B	2.58	129.63	124.80
19	K2	102	CLA	O2D-CGD-CBD	2.58	115.76	111.25
19	B2	825	CLA	C1D-CHD-C4C	2.58	126.01	122.48
19	B2	820	CLA	CMB-C2B-C3B	2.58	129.63	124.80
24	BB	848	AJP	CDC-CDD-CCI	2.58	116.42	112.13
19	B	825	CLA	O2D-CGD-CBD	2.58	115.76	111.25
19	A	806	CLA	O2D-CGD-O1D	-2.58	118.74	123.83
19	AA	807	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	A1	803	CLA	CHB-C4A-NA	2.58	128.07	124.51
19	B2	812	CLA	CMB-C2B-C3B	2.57	129.63	124.80
19	B2	811	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
19	B2	852	CLA	CHD-C4C-C3C	2.57	128.62	124.87
28	B	856	DGD	O5D-C6D-C5D	-2.57	104.22	109.14
19	B	811	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
19	A	820	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
19	A	835	CLA	C1-C2-C3	-2.57	121.59	126.04
23	I1	101	BCR	C24-C23-C22	-2.57	122.35	126.21
23	I2	103	BCR	C33-C5-C6	-2.57	121.64	124.51
23	KK	103	BCR	C24-C23-C22	-2.57	122.35	126.21
19	B2	803	CLA	CHB-C4A-NA	2.57	128.07	124.51
19	A	838	CLA	C1B-CHB-C4A	-2.57	125.02	130.12
19	A1	834	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
19	B1	811	CLA	O2D-CGD-O1D	-2.57	118.75	123.83
23	KK	103	BCR	C38-C26-C25	-2.57	121.65	124.51
19	L	202	CLA	CMB-C2B-C3B	2.57	129.62	124.80
19	A	822	CLA	CMB-C2B-C3B	2.57	129.62	124.80
23	B	842	BCR	C30-C25-C26	-2.57	119.00	122.59
19	AA	810	CLA	O2D-CGD-CBD	2.57	115.75	111.25
19	B	802	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	AA	817	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
19	A	826	CLA	O2D-CGD-O1D	-2.57	118.76	123.83
19	B	807	CLA	CMB-C2B-C3B	2.57	129.62	124.80
22	L2	208	LHG	O4-P-O5	2.57	125.09	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	853	LHG	O4-P-O5	2.57	125.09	112.21
23	FF	303	BCR	C2-C1-C6	2.57	114.46	110.48
23	B	844	BCR	C27-C26-C25	2.57	126.49	122.74
19	B	846	CLA	CHB-C4A-NA	2.57	128.06	124.51
19	A2	810	CLA	CBA-CAA-C2A	2.57	121.49	113.85
19	B1	804	CLA	CHB-C4A-NA	2.57	128.06	124.51
23	K1	106	BCR	C28-C27-C26	-2.57	109.53	113.99
23	AA	854	BCR	C15-C14-C13	-2.57	123.65	127.31
24	L2	202	AJP	CAZ-CAY-CAX	2.57	117.78	112.08
22	X2	103	LHG	O4-P-O5	2.57	125.07	112.21
23	B	840	BCR	C28-C27-C26	-2.57	109.53	113.99
19	A1	804	CLA	CMD-C2D-C3D	2.57	129.61	124.80
24	BB	849	AJP	OBQ-CBF-CBE	-2.56	100.53	104.44
22	AA	847	LHG	O4-P-O5	2.56	125.07	112.21
23	I2	103	BCR	C7-C8-C9	-2.56	122.36	126.21
23	II	102	BCR	C2-C1-C6	2.56	114.45	110.48
19	B	820	CLA	CHB-C4A-NA	2.56	128.06	124.51
19	B1	807	CLA	CMB-C2B-C3B	2.56	129.61	124.80
23	A	853	BCR	C15-C14-C13	-2.56	123.65	127.31
19	A1	810	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
19	B2	834	CLA	C2A-C1A-CHA	2.56	128.34	123.86
19	A2	841	CLA	CMB-C2B-C3B	2.56	129.60	124.80
19	BB	809	CLA	O2D-CGD-CBD	2.56	115.74	111.25
23	BB	838	BCR	C33-C5-C6	-2.56	121.66	124.51
23	A2	851	BCR	C24-C23-C22	-2.56	122.36	126.21
24	L	209	AJP	CBE-CBO-CBP	-2.56	99.52	104.35
24	A1	854	AJP	CCH-CCG-CDB	2.56	112.23	108.59
23	II	102	BCR	C7-C8-C9	-2.56	122.37	126.21
19	AA	834	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
19	AA	807	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
19	AA	809	CLA	CMB-C2B-C3B	2.56	129.60	124.80
19	AA	835	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
19	AA	822	CLA	O2D-CGD-O1D	-2.56	118.78	123.83
19	L1	205	CLA	CMB-C2B-C3B	2.56	129.60	124.80
23	A2	853	BCR	C15-C14-C13	-2.56	123.66	127.31
23	L1	208	BCR	C33-C5-C6	-2.56	121.66	124.51
20	AA	803	CL0	C9-C8-C10	2.56	120.62	111.30
19	B	820	CLA	O2D-CGD-CBD	2.56	115.73	111.25
19	B1	849	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
19	AA	832	CLA	O2D-CGD-CBD	2.56	115.72	111.25
19	BB	832	CLA	O2A-CGA-O1A	-2.55	117.03	123.56
22	AA	846	LHG	O4-P-O5	2.55	125.02	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	L1	204	AJP	CBD-CBN-CCJ	2.55	117.95	111.69
19	B1	825	CLA	C1D-CHD-C4C	2.55	125.97	122.48
23	L1	208	BCR	C2-C1-C6	2.55	114.43	110.48
24	AA	802	AJP	CBE-CBO-CBP	-2.55	99.53	104.35
19	B	809	CLA	O2D-CGD-CBD	2.55	115.72	111.25
19	B1	815	CLA	C5-C3-C2	2.55	126.35	121.11
19	B	806	CLA	CMB-C2B-C3B	2.55	129.59	124.80
23	F	305	BCR	C7-C8-C9	-2.55	122.38	126.21
22	B1	847	LHG	O4-P-O5	2.55	125.00	112.21
19	B1	810	CLA	CMD-C2D-C3D	2.55	129.58	124.80
19	BB	813	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	A1	821	CLA	CHB-C4A-NA	2.55	128.04	124.51
19	A	832	CLA	CHB-C4A-NA	2.55	128.04	124.51
22	A	845	LHG	O4-P-O5	2.55	124.98	112.21
23	M	101	BCR	C15-C14-C13	-2.55	123.67	127.31
19	B1	810	CLA	C6-C5-C3	2.55	119.13	113.01
23	B	842	BCR	C35-C13-C14	-2.55	119.36	122.92
23	FF	304	BCR	C15-C16-C17	-2.55	118.16	123.51
22	A1	845	LHG	O4-P-O5	2.55	124.98	112.21
22	LL	205	LHG	O4-P-O5	2.55	124.98	112.21
23	II	102	BCR	C33-C5-C6	-2.55	121.67	124.51
19	A2	826	CLA	CHB-C4A-NA	2.55	128.03	124.51
19	K2	102	CLA	CHB-C4A-NA	2.55	128.03	124.51
22	L	207	LHG	O4-P-O5	2.55	124.97	112.21
23	BB	839	BCR	C8-C7-C6	-2.55	120.15	127.28
19	AA	831	CLA	O2D-CGD-O1D	-2.55	118.80	123.83
19	B	823	CLA	CMB-C2B-C3B	2.55	129.57	124.80
23	I2	101	BCR	C38-C26-C25	-2.55	121.67	124.51
19	B	825	CLA	C1D-CHD-C4C	2.55	125.96	122.48
19	X1	101	CLA	CMD-C2D-C3D	2.54	129.57	124.80
24	A2	854	AJP	CCG-CCF-CCE	-2.54	109.80	114.00
24	A1	854	AJP	CBM-CBL-CCH	2.54	117.55	113.12
23	B	839	BCR	C33-C5-C6	-2.54	121.68	124.51
19	A2	830	CLA	C1B-CHB-C4A	-2.54	125.08	130.12
19	A1	811	CLA	CMB-C2B-C3B	2.54	129.57	124.80
19	FF	301	CLA	CMB-C2B-C3B	2.54	129.57	124.80
19	K2	104	CLA	CMB-C2B-C3B	2.54	129.57	124.80
19	B1	833	CLA	CAA-C2A-C3A	-2.54	105.81	112.78
19	A1	809	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	L	202	CLA	C4-C3-C2	-2.54	117.07	123.68
19	AA	842	CLA	C5-C3-C2	-2.54	115.89	121.11
19	A1	825	CLA	CMB-C2B-C3B	2.54	129.57	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	840	ECH	C35-C13-C14	2.54	126.48	122.92
19	B2	836	CLA	CHB-C4A-NA	2.54	128.03	124.51
19	A2	844	CLA	CHB-C4A-NA	2.54	128.03	124.51
23	L	205	BCR	C24-C23-C22	-2.54	122.39	126.21
19	A2	827	CLA	CMB-C2B-C3B	2.54	129.57	124.80
19	AA	804	CLA	CMB-C2B-C1B	-2.54	124.56	128.46
22	XX	102	LHG	O4-P-O5	2.54	124.95	112.21
19	AA	838	CLA	O2D-CGD-CBD	2.54	115.70	111.25
19	BB	822	CLA	O2D-CGD-O1D	-2.54	118.81	123.83
19	B2	828	CLA	O2D-CGD-O1D	-2.54	118.82	123.83
19	B	833	CLA	CED-O2D-CGD	2.54	121.75	115.95
19	AA	814	CLA	CMD-C2D-C3D	2.54	129.56	124.80
19	BB	835	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	A1	826	CLA	CMD-C2D-C3D	2.54	129.56	124.80
19	B1	831	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	A1	844	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	B	848	BCR	C27-C26-C25	2.54	126.44	122.74
23	A	850	BCR	C8-C7-C6	-2.54	120.17	127.28
19	BB	819	CLA	CMB-C2B-C3B	2.54	129.56	124.80
19	A2	817	CLA	CMD-C2D-C3D	2.54	129.56	124.80
19	A1	852	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
19	BB	823	CLA	CMB-C2B-C3B	2.54	129.56	124.80
19	BB	804	CLA	C1-C2-C3	-2.54	121.66	126.04
19	B1	829	CLA	CMB-C2B-C3B	2.54	129.56	124.80
19	K	101	CLA	O2D-CGD-CBD	2.54	115.69	111.25
19	B2	815	CLA	O2D-CGD-O1D	-2.54	118.82	123.83
19	B	836	CLA	CHB-C4A-NA	2.54	128.02	124.51
19	A	852	CLA	C1B-CHB-C4A	-2.54	125.09	130.12
23	L1	201	BCR	C33-C5-C6	-2.54	121.69	124.51
19	B1	821	CLA	CHB-C4A-NA	2.54	128.02	124.51
23	B2	844	BCR	C27-C26-C25	2.54	126.44	122.74
22	A2	845	LHG	O4-P-O5	2.53	124.92	112.21
23	B	843	BCR	C15-C16-C17	-2.53	118.18	123.51
22	X	102	LHG	O4-P-O5	2.53	124.92	112.21
19	A1	806	CLA	CMB-C2B-C3B	2.53	129.55	124.80
19	L1	205	CLA	C6-C5-C3	2.53	119.09	113.01
19	A2	811	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
19	A	824	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	B1	804	CLA	C1-C2-C3	-2.53	121.66	126.04
23	F	303	BCR	C8-C7-C6	-2.53	120.19	127.28
19	BB	807	CLA	O2A-CGA-O1A	-2.53	117.09	123.56
19	B2	820	CLA	C1B-CHB-C4A	-2.53	125.10	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	821	CLA	CMD-C2D-C3D	2.53	129.55	124.80
23	BB	839	BCR	C28-C27-C26	-2.53	109.58	113.99
19	B	801	CLA	C6-C5-C3	2.53	119.09	113.01
19	AA	814	CLA	CMB-C2B-C3B	2.53	129.55	124.80
23	I	102	BCR	C7-C8-C9	-2.53	122.41	126.21
19	A1	806	CLA	O2D-CGD-O1D	-2.53	118.83	123.83
23	I2	102	BCR	C2-C1-C6	2.53	114.40	110.48
19	A1	813	CLA	CMD-C2D-C3D	2.53	129.54	124.80
19	AA	822	CLA	CHB-C4A-NA	2.53	128.01	124.51
19	A1	840	CLA	CMB-C2B-C3B	2.53	129.54	124.80
26	B2	841	ECH	C40-C30-C25	2.53	114.39	110.30
19	BB	820	CLA	OBD-CAD-CBD	-2.53	122.20	125.91
19	BB	828	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	B	850	AJP	CDC-CDD-CCI	2.53	116.34	112.13
22	B1	847	LHG	P-O3-C3	-2.53	106.86	121.68
19	A2	807	CLA	CMB-C2B-C3B	2.53	129.54	124.80
19	B2	810	CLA	C4-C3-C5	2.53	119.64	115.29
19	B2	835	CLA	O2D-CGD-O1D	-2.53	118.84	123.83
19	B	828	CLA	CMB-C2B-C3B	2.53	129.54	124.80
19	B2	819	CLA	CMD-C2D-C3D	2.53	129.54	124.80
19	BB	801	CLA	CMB-C2B-C3B	2.52	129.53	124.80
19	A1	813	CLA	CMB-C2B-C3B	2.52	129.53	124.80
19	B2	823	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	A2	804	CLA	CMB-C2B-C1B	-2.52	124.58	128.46
24	B	849	AJP	CBJ-CCB-CCA	2.52	118.93	113.00
19	BB	827	CLA	CMD-C2D-C3D	2.52	129.53	124.80
24	M2	101	AJP	CDD-CDC-CDB	2.52	116.99	111.87
22	BB	851	LHG	O4-P-O5	2.52	124.86	112.21
19	AA	801	CLA	O2D-CGD-O1D	-2.52	118.85	123.83
23	FF	304	BCR	C38-C26-C25	-2.52	121.70	124.51
23	AA	851	BCR	C8-C7-C6	-2.52	120.21	127.28
23	L	206	BCR	C27-C26-C25	2.52	126.42	122.74
23	B2	840	BCR	C28-C27-C26	-2.52	109.60	113.99
24	B	850	AJP	CCH-CCG-CDB	2.52	112.18	108.59
19	A2	813	CLA	CHB-C4A-NA	2.52	128.00	124.51
23	BB	847	BCR	C27-C26-C25	2.52	126.42	122.74
19	A1	814	CLA	O2D-CGD-O1D	-2.52	118.85	123.83
23	AA	855	BCR	C28-C27-C26	-2.52	109.60	113.99
24	A	802	AJP	CBE-CBO-CBP	-2.52	99.59	104.35
23	A	847	BCR	C33-C5-C6	-2.52	121.70	124.51
19	AA	853	CLA	OBD-CAD-CBD	-2.52	122.21	125.91
19	A1	829	CLA	CHB-C4A-NA	2.52	128.00	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	831	CLA	O2D-CGD-O1D	-2.52	118.85	123.83
19	B	860	CLA	CHD-C4C-C3C	2.52	128.54	124.87
24	L	209	AJP	OBG-CBF-CAW	2.52	113.19	110.81
19	B	833	CLA	O2A-CGA-O1A	-2.52	117.12	123.56
19	A	801	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
19	B1	819	CLA	CMD-C2D-C3D	2.52	129.52	124.80
19	K1	105	CLA	CMB-C2B-C3B	2.52	129.52	124.80
22	X1	102	LHG	O4-P-O5	2.52	124.83	112.21
19	BB	820	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	BB	822	CLA	CMB-C2B-C1B	-2.52	124.59	128.46
23	A2	847	BCR	C33-C5-C6	-2.52	121.71	124.51
24	L2	202	AJP	OCY-CCZ-CDA	-2.52	104.81	109.66
19	B2	812	CLA	CHB-C4A-NA	2.52	127.99	124.51
26	B2	841	ECH	C29-C30-C25	-2.52	106.59	110.48
23	L	206	BCR	C11-C10-C9	-2.52	123.72	127.31
19	AA	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	A	841	CLA	CHB-C4A-NA	2.52	127.99	124.51
22	X2	102	LHG	O4-P-O5	2.51	124.82	112.21
19	BB	832	CLA	C2A-C1A-CHA	2.51	128.26	123.86
26	B1	840	ECH	C37-C22-C21	2.51	126.44	122.92
19	B2	815	CLA	C5-C3-C2	2.51	126.28	121.11
23	F1	303	BCR	C2-C1-C6	2.51	114.37	110.48
19	AA	838	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	B2	831	CLA	CHB-C4A-NA	2.51	127.99	124.51
19	B	833	CLA	C2A-C1A-CHA	2.51	128.25	123.86
19	A	815	CLA	CMB-C2B-C3B	2.51	129.51	124.80
19	A1	842	CLA	CMB-C2B-C3B	2.51	129.51	124.80
19	F1	301	CLA	CMB-C2B-C3B	2.51	129.51	124.80
19	A2	814	CLA	O2D-CGD-O1D	-2.51	118.87	123.83
19	BB	828	CLA	CMB-C2B-C3B	2.51	129.51	124.80
23	AA	852	BCR	C1-C6-C5	-2.51	119.08	122.59
19	K	102	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	A	831	CLA	O2D-CGD-O1D	-2.51	118.87	123.83
19	B2	836	CLA	O2D-CGD-O1D	-2.51	118.87	123.83
26	B1	840	ECH	C29-C30-C25	-2.51	106.61	110.48
19	A1	834	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
19	B2	820	CLA	O2D-CGD-CBD	2.51	115.64	111.25
19	B	819	CLA	CMD-C2D-C3D	2.51	129.50	124.80
19	BB	855	CLA	CMD-C2D-C3D	2.51	129.50	124.80
23	L1	201	BCR	C2-C1-C6	2.51	114.36	110.48
19	A	807	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	F2	304	BCR	C33-C5-C6	-2.51	121.72	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	819	CLA	CMB-C2B-C3B	2.51	129.50	124.80
19	AA	824	CLA	CHB-C4A-NA	2.51	127.98	124.51
19	B	809	CLA	CMB-C2B-C3B	2.51	129.50	124.80
23	LL	204	BCR	C27-C26-C25	2.51	126.39	122.74
19	B1	816	CLA	CMB-C2B-C3B	2.50	129.50	124.80
19	A1	820	CLA	C6-C5-C3	2.50	119.02	113.01
19	AA	845	CLA	CMD-C2D-C3D	2.50	129.50	124.80
19	A1	837	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A1	831	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A	826	CLA	CMB-C2B-C3B	2.50	129.49	124.80
19	BB	809	CLA	CMD-C2D-C3D	2.50	129.49	124.80
23	B1	839	BCR	C33-C5-C6	-2.50	121.72	124.51
19	B1	804	CLA	CMB-C2B-C3B	2.50	129.49	124.80
19	BB	835	CLA	CMB-C2B-C3B	2.50	129.49	124.80
24	L1	204	AJP	CAW-CAX-CAY	-2.50	106.36	111.82
19	BB	830	CLA	CMB-C2B-C3B	2.50	129.49	124.80
19	A2	804	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	B2	808	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
19	A1	816	CLA	CMD-C2D-C3D	2.50	129.49	124.80
24	L2	203	AJP	CBE-CBO-CBP	-2.50	99.63	104.35
19	A	838	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	A1	807	CLA	CMB-C2B-C3B	2.50	129.49	124.80
19	FF	301	CLA	CMD-C2D-C3D	2.50	129.49	124.80
25	I2	105	LMG	O6-C1-O1	-2.50	104.04	109.94
26	BB	840	ECH	C8-C9-C10	2.50	122.78	118.94
19	B1	830	CLA	CHB-C4A-NA	2.50	127.97	124.51
23	MM	101	BCR	C35-C13-C14	-2.50	119.42	122.92
19	AA	820	CLA	C1B-CHB-C4A	-2.50	125.17	130.12
19	L2	204	CLA	C6-C5-C3	2.50	119.01	113.01
19	BB	819	CLA	CMD-C2D-C3D	2.50	129.48	124.80
19	B	825	CLA	CHB-C4A-NA	2.50	127.97	124.51
22	BB	850	LHG	O4-P-O5	2.50	124.73	112.21
19	B2	849	CLA	CHB-C4A-NA	2.50	127.96	124.51
19	AA	813	CLA	CHB-C4A-NA	2.50	127.96	124.51
23	J	104	BCR	C15-C16-C17	-2.50	118.26	123.51
19	B	821	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B2	833	CLA	O2A-CGA-O1A	-2.49	117.19	123.56
23	K2	105	BCR	C28-C27-C26	-2.49	109.65	113.99
19	L	203	CLA	CMD-C2D-C3D	2.49	129.48	124.80
19	A1	839	CLA	CMB-C2B-C3B	2.49	129.48	124.80
19	B1	820	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	B1	826	CLA	CHB-C4A-NA	2.49	127.96	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	805	CLA	CMD-C2D-C3D	2.49	129.48	124.80
23	J	102	BCR	C1-C6-C5	-2.49	119.11	122.59
19	B1	812	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B1	807	CLA	C11-C12-C13	-2.49	107.99	115.77
19	B	831	CLA	CMB-C2B-C3B	2.49	129.47	124.80
19	A1	844	CLA	CMD-C2D-C3D	2.49	129.47	124.80
19	B1	826	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
19	AA	815	CLA	CMB-C2B-C3B	2.49	129.47	124.80
19	A1	818	CLA	CMB-C2B-C3B	2.49	129.47	124.80
19	B1	824	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	B2	852	CLA	CHB-C4A-NA	2.49	127.96	124.51
19	A	835	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
22	B	852	LHG	O4-P-O5	2.49	124.69	112.21
19	B1	823	CLA	CMD-C2D-C3D	2.49	129.47	124.80
19	BB	834	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	B	816	CLA	C1B-CHB-C4A	-2.49	125.19	130.12
23	J1	104	BCR	C15-C16-C17	-2.49	118.28	123.51
19	A2	814	CLA	CMB-C2B-C3B	2.49	129.46	124.80
19	AA	840	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	AA	826	CLA	CMB-C2B-C3B	2.49	129.46	124.80
19	B	822	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	B	835	CLA	CED-O2D-CGD	2.49	121.63	115.95
19	A1	834	CLA	CMB-C2B-C3B	2.49	129.46	124.80
20	A1	802	CL0	CMD-C2D-C3D	-2.49	120.14	124.80
21	A2	843	PQN	C15-C13-C12	-2.48	116.00	121.11
24	A1	855	AJP	CCG-CCF-CCE	-2.48	109.90	114.00
24	L2	203	AJP	CBJ-CCB-CCA	2.48	118.84	113.00
19	A	804	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	A2	823	CLA	C5-C3-C2	2.48	126.21	121.11
19	B2	822	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
21	A1	843	PQN	C15-C13-C12	-2.48	116.01	121.11
23	AA	854	BCR	C2-C1-C6	2.48	114.32	110.48
19	A2	813	CLA	C1B-CHB-C4A	-2.48	125.20	130.12
19	A	807	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
19	B	834	CLA	C2A-C1A-CHA	2.48	128.20	123.86
19	B1	832	CLA	O2A-CGA-O1A	-2.48	117.22	123.56
19	K2	104	CLA	CMD-C2D-C3D	2.48	129.45	124.80
19	A	836	CLA	CMB-C2B-C1B	-2.48	124.65	128.46
19	FF	302	CLA	CMD-C2D-C3D	2.48	129.45	124.80
19	A2	802	CLA	CHB-C4A-NA	2.48	127.94	124.51
23	FF	304	BCR	C27-C26-C25	2.48	126.36	122.74
23	F2	304	BCR	C27-C26-C25	2.48	126.36	122.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	815	CLA	O2D-CGD-O1D	-2.48	118.94	123.83
19	B	859	CLA	O2A-CGA-O1A	-2.48	117.23	123.56
23	L	205	BCR	C2-C1-C6	2.48	114.32	110.48
23	J	104	BCR	C27-C26-C25	2.48	126.35	122.74
19	B	819	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B2	804	CLA	CMB-C2B-C3B	2.48	129.45	124.80
23	A	853	BCR	C2-C1-C6	2.48	114.32	110.48
23	F1	304	BCR	C27-C26-C25	2.48	126.35	122.74
19	A1	841	CLA	CMB-C2B-C1B	-2.48	124.66	128.46
19	B1	803	CLA	CHB-C4A-NA	2.48	127.94	124.51
19	B	837	CLA	O2D-CGD-CBD	2.48	115.59	111.25
19	F2	301	CLA	CMB-C2B-C3B	2.48	129.44	124.80
23	K2	103	BCR	C27-C26-C25	2.48	126.35	122.74
24	I2	104	AJP	CDA-CDB-CDC	-2.48	108.82	112.56
23	I2	103	BCR	C2-C1-C6	2.48	114.31	110.48
19	B2	825	CLA	O2D-CGD-CBD	2.47	115.58	111.25
19	BB	809	CLA	CMB-C2B-C3B	2.47	129.44	124.80
19	A2	821	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
23	I	101	BCR	C24-C23-C22	-2.47	122.50	126.21
23	F	304	BCR	C38-C26-C25	-2.47	121.75	124.51
23	F	303	BCR	C27-C26-C25	2.47	126.35	122.74
19	A2	836	CLA	O2D-CGD-O1D	-2.47	118.95	123.83
19	BB	826	CLA	O2D-CGD-CBD	2.47	115.58	111.25
19	BB	805	CLA	O2D-CGD-CBD	2.47	115.58	111.25
19	B	833	CLA	C1B-CHB-C4A	-2.47	125.22	130.12
19	B	809	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	B	812	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	MM	101	BCR	C15-C14-C13	-2.47	123.78	127.31
23	F1	303	BCR	C11-C10-C9	-2.47	123.78	127.31
23	K1	104	BCR	C27-C26-C25	2.47	126.34	122.74
23	J2	104	BCR	C27-C26-C25	2.47	126.34	122.74
22	L1	211	LHG	O4-P-O5	2.47	124.58	112.21
19	A2	852	CLA	C1B-CHB-C4A	-2.47	125.23	130.12
19	A	819	CLA	CMB-C2B-C3B	2.47	129.43	124.80
19	A1	811	CLA	CBA-CAA-C2A	2.47	121.19	113.85
19	A	830	CLA	CMD-C2D-C3D	2.47	129.43	124.80
23	A1	848	BCR	C15-C16-C17	-2.47	118.33	123.51
19	J1	101	CLA	CMB-C2B-C3B	2.47	129.43	124.80
19	B1	832	CLA	CED-O2D-CGD	2.47	121.58	115.95
19	B	809	CLA	CMD-C2D-C3D	2.47	129.42	124.80
19	B	813	CLA	CHB-C4A-NA	2.47	127.92	124.51
19	B2	812	CLA	CMD-C2D-C3D	2.46	129.42	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	K1	105	CLA	C1B-CHB-C4A	-2.46	125.23	130.12
19	AA	820	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	A1	809	CLA	O2A-CGA-O1A	-2.46	117.26	123.56
22	A	846	LHG	P-O3-C3	-2.46	107.23	121.68
19	A	810	CLA	O2D-CGD-CBD	2.46	115.56	111.25
19	AA	810	CLA	O2A-CGA-O1A	-2.46	117.27	123.56
19	A	813	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	B	843	BCR	C33-C5-C6	-2.46	121.77	124.51
19	A2	810	CLA	CHB-C4A-NA	2.46	127.92	124.51
24	L1	204	AJP	CDC-CDD-CCI	2.46	116.23	112.13
19	K1	105	CLA	CMD-C2D-C3D	2.46	129.42	124.80
19	A1	837	CLA	CMD-C2D-C3D	2.46	129.42	124.80
19	B1	805	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
19	B2	809	CLA	CMB-C2B-C3B	2.46	129.42	124.80
19	A	829	CLA	C5-C3-C2	2.46	126.17	121.11
19	B2	819	CLA	CHB-C4A-NA	2.46	127.92	124.51
19	BB	814	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
19	FF	301	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	XX	101	CLA	CMB-C2B-C3B	2.46	129.41	124.80
19	K	102	CLA	CMD-C2D-C3D	2.46	129.41	124.80
23	F	303	BCR	C11-C10-C9	-2.46	123.80	127.31
19	A	838	CLA	O2D-CGD-CBD	2.46	115.56	111.25
23	A2	853	BCR	C2-C1-C6	2.46	114.29	110.48
23	JJ	104	BCR	C15-C16-C17	-2.46	118.34	123.51
19	B2	807	CLA	C11-C12-C13	-2.46	108.10	115.77
19	B2	822	CLA	C5-C3-C2	2.46	126.16	121.11
25	M	102	LMG	O1-C7-C8	-2.46	104.97	110.90
19	A2	826	CLA	O2D-CGD-O1D	-2.46	118.97	123.83
22	AA	847	LHG	P-O3-C3	-2.46	107.27	121.68
19	A2	830	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	A1	812	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
23	F1	304	BCR	C15-C16-C17	-2.46	118.34	123.51
19	B1	809	CLA	CMB-C2B-C3B	2.46	129.41	124.80
23	F1	304	BCR	C33-C5-C6	-2.46	121.77	124.51
19	JJ	101	CLA	CHB-C4A-NA	2.46	127.91	124.51
23	I2	101	BCR	C24-C23-C22	-2.46	122.52	126.21
19	B2	813	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	B2	822	CLA	CMB-C2B-C3B	2.46	129.41	124.80
19	J	101	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	KK	101	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
19	B1	808	CLA	CMD-C2D-C3D	2.46	129.41	124.80
23	M	101	BCR	C24-C23-C22	-2.46	122.52	126.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	830	CLA	CMD-C2D-C3D	2.45	129.40	124.80
23	BB	838	BCR	C15-C16-C17	-2.45	118.35	123.51
23	A1	847	BCR	C33-C5-C6	-2.45	121.78	124.51
22	A1	845	LHG	P-O6-C4	-2.45	107.29	121.68
23	A1	853	BCR	C33-C5-C6	-2.45	121.78	124.51
19	A2	835	CLA	CMD-C2D-C3D	2.45	129.40	124.80
23	A2	847	BCR	C2-C1-C6	2.45	114.28	110.48
19	BB	813	CLA	O2D-CGD-CBD	2.45	115.55	111.25
19	B1	828	CLA	O2D-CGD-O1D	-2.45	118.99	123.83
23	BB	843	BCR	C27-C26-C25	2.45	126.32	122.74
19	A2	820	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	LL	204	BCR	C38-C26-C25	-2.45	121.78	124.51
19	A	821	CLA	CMB-C2B-C3B	2.45	129.40	124.80
19	BB	820	CLA	CMB-C2B-C3B	2.45	129.40	124.80
23	II	104	BCR	C2-C1-C6	2.45	114.28	110.48
19	B	836	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	B	835	CLA	CHB-C4A-NA	2.45	127.90	124.51
19	BB	852	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	BB	816	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
19	A1	819	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	A1	849	BCR	C33-C5-C6	-2.45	121.78	124.51
23	BB	839	BCR	C33-C5-C6	-2.45	121.78	124.51
19	A2	820	CLA	CBA-CAA-C2A	2.45	121.14	113.85
19	B2	826	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	B	857	AJP	CCJ-CCI-CCH	-2.45	104.95	109.25
23	A1	847	BCR	C2-C1-C6	2.45	114.27	110.48
24	L1	204	AJP	CCX-OCY-CCZ	2.45	119.12	115.33
24	L1	203	AJP	CCG-CCF-CCE	2.45	118.05	114.00
19	BB	824	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
23	J2	102	BCR	C38-C26-C25	-2.45	121.78	124.51
23	J1	104	BCR	C38-C26-C25	-2.45	121.78	124.51
19	AA	821	CLA	O2A-CGA-O1A	-2.45	117.31	123.56
25	B	851	LMG	O1-C7-C8	-2.45	104.99	110.90
19	LL	201	CLA	CMB-C2B-C3B	2.45	129.39	124.80
19	B2	808	CLA	CMD-C2D-C3D	2.45	129.39	124.80
19	K1	102	CLA	CMD-C2D-C3D	2.45	129.39	124.80
23	L1	201	BCR	C7-C8-C9	-2.45	122.53	126.21
19	B2	821	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	B2	840	BCR	C8-C7-C6	-2.45	120.42	127.28
19	A2	838	CLA	CHB-C4A-NA	2.45	127.89	124.51
19	B1	850	CLA	C4-C3-C5	2.45	119.50	115.29
19	B2	831	CLA	CMD-C2D-C3D	2.45	129.39	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	821	CLA	CMD-C2D-C3D	2.45	129.39	124.80
19	BB	820	CLA	CBC-CAC-C3C	2.45	119.21	112.43
19	AA	830	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	A2	838	CLA	CMD-C2D-C3D	2.44	129.38	124.80
19	BB	856	CLA	O2A-CGA-O1A	-2.44	117.31	123.56
19	X	101	CLA	CMB-C2B-C3B	2.44	129.38	124.80
19	A1	809	CLA	CMD-C2D-C3D	2.44	129.38	124.80
19	L	204	CLA	O2D-CGD-O1D	-2.44	119.00	123.83
24	L1	203	AJP	CDC-CDB-CCG	2.44	116.82	112.31
23	J2	104	BCR	C33-C5-C6	-2.44	121.79	124.51
19	A1	822	CLA	C5-C3-C2	2.44	126.13	121.11
19	A	817	CLA	CMD-C2D-C3D	2.44	129.38	124.80
19	FF	301	CLA	O2D-CGD-O1D	-2.44	119.01	123.83
19	KK	101	CLA	CMD-C2D-C3D	2.44	129.38	124.80
19	A2	806	CLA	CMD-C2D-C3D	2.44	129.38	124.80
23	J2	104	BCR	C38-C26-C25	-2.44	121.79	124.51
23	FF	303	BCR	C27-C26-C25	2.44	126.30	122.74
19	A	839	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	A	810	CLA	CMD-C2D-C3D	2.44	129.37	124.80
19	AA	808	CLA	CMB-C2B-C3B	2.44	129.37	124.80
23	II	104	BCR	C27-C26-C25	2.44	126.30	122.74
24	B	857	AJP	CAW-CBF-CBE	2.44	120.86	115.72
19	A	834	CLA	CMD-C2D-C3D	2.44	129.37	124.80
19	B1	829	CLA	C5-C3-C2	2.44	126.12	121.11
23	F1	306	BCR	C7-C8-C9	-2.44	122.55	126.21
19	L2	205	CLA	CHB-C4A-NA	2.44	127.88	124.51
24	I2	104	AJP	CCH-CCG-CDB	2.44	112.06	108.59
23	F	304	BCR	C33-C5-C6	-2.44	121.80	124.51
19	B	814	CLA	C1B-CHB-C4A	-2.44	125.29	130.12
23	K2	105	BCR	C20-C21-C22	-2.44	123.83	127.31
23	B1	839	BCR	C8-C7-C6	-2.44	120.45	127.28
23	JJ	102	BCR	C15-C14-C13	-2.44	123.83	127.31
24	AA	856	AJP	CDD-CDC-CDB	2.44	116.81	111.87
22	L	207	LHG	P-O3-C3	-2.44	107.40	121.68
23	B	840	BCR	C8-C7-C6	-2.44	120.46	127.28
19	B1	812	CLA	CMD-C2D-C3D	2.44	129.37	124.80
23	B1	841	BCR	C35-C13-C14	-2.44	119.51	122.92
23	I2	102	BCR	C15-C16-C17	-2.43	118.39	123.51
23	M2	102	BCR	C24-C23-C22	-2.43	122.55	126.21
19	A	823	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	B	805	CLA	O2D-CGD-CBD	2.43	115.51	111.25
19	A1	822	CLA	O2D-CGD-CBD	2.43	115.51	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F1	303	BCR	C27-C26-C25	2.43	126.29	122.74
19	L	204	CLA	CAC-C3C-C4C	2.43	128.00	124.82
19	BB	820	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
22	A2	846	LHG	P-O3-C3	-2.43	107.41	121.68
19	B2	824	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	B	826	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	A1	801	CLA	CMB-C2B-C3B	2.43	129.36	124.80
19	B2	825	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	A	830	CLA	CHB-C4A-NA	2.43	127.88	124.51
21	A	843	PQN	C21-C22-C23	-2.43	108.18	115.77
22	LL	205	LHG	P-O3-C3	-2.43	107.42	121.68
19	B	822	CLA	CMD-C2D-C3D	2.43	129.36	124.80
23	I	101	BCR	C15-C16-C17	-2.43	118.40	123.51
23	A2	851	BCR	C1-C6-C5	-2.43	119.19	122.59
19	AA	831	CLA	CHB-C4A-NA	2.43	127.88	124.51
19	B2	823	CLA	CMD-C2D-C3D	2.43	129.36	124.80
19	BB	818	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
24	BB	849	AJP	CCH-CCG-CDB	2.43	112.05	108.59
23	M1	101	BCR	C24-C23-C22	-2.43	122.56	126.21
19	A	808	CLA	CHB-C4A-NA	2.43	127.87	124.51
19	AA	823	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
19	AA	832	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	M	102	LMG	C7-O1-C1	2.43	118.63	113.75
19	B	804	CLA	C1-C2-C3	-2.43	121.84	126.04
19	B	801	CLA	CMB-C2B-C3B	2.43	129.35	124.80
23	AA	848	BCR	C33-C5-C6	-2.43	121.81	124.51
19	A	842	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	A1	810	CLA	CMD-C2D-C3D	2.43	129.35	124.80
23	F2	305	BCR	C7-C8-C9	-2.43	122.56	126.21
23	F2	303	BCR	C27-C26-C25	2.43	126.28	122.74
23	K2	105	BCR	C1-C6-C5	-2.43	119.20	122.59
19	J2	101	CLA	CMB-C2B-C3B	2.43	129.35	124.80
19	AA	813	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	J1	104	BCR	C27-C26-C25	2.43	126.28	122.74
23	J	102	BCR	C38-C26-C25	-2.43	121.81	124.51
23	J	104	BCR	C38-C26-C25	-2.43	121.81	124.51
22	A2	845	LHG	P-O6-C4	-2.43	107.45	121.68
19	B	813	CLA	CMD-C2D-C3D	2.43	129.35	124.80
19	A2	822	CLA	CMD-C2D-C3D	2.43	129.35	124.80
19	B2	805	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
19	B2	829	CLA	O2D-CGD-O1D	-2.42	119.04	123.83
19	A1	829	CLA	CAC-C3C-C4C	2.42	127.99	124.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	814	CLA	CMD-C2D-C3D	2.42	129.35	124.80
19	B2	818	CLA	CMB-C2B-C3B	2.42	129.35	124.80
19	A1	832	CLA	CMB-C2B-C1B	-2.42	124.74	128.46
19	L2	205	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	L1	209	BCR	C38-C26-C25	-2.42	121.81	124.51
19	AA	828	CLA	CMD-C2D-C3D	2.42	129.34	124.80
19	B2	813	CLA	CMD-C2D-C3D	2.42	129.34	124.80
19	A1	803	CLA	C1-C2-C3	-2.42	121.85	126.04
19	A1	825	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	A	833	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	A1	837	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
23	L1	201	BCR	C15-C16-C17	-2.42	118.42	123.51
23	L	205	BCR	C27-C26-C25	2.42	126.27	122.74
19	B1	820	CLA	CMD-C2D-C3D	2.42	129.34	124.80
19	BB	829	CLA	CMB-C2B-C3B	2.42	129.34	124.80
24	L2	203	AJP	CBD-CBN-CCJ	2.42	117.63	111.69
23	L	205	BCR	C7-C8-C9	-2.42	122.57	126.21
19	B1	849	CLA	CMD-C2D-C3D	2.42	129.34	124.80
23	JJ	102	BCR	C1-C6-C5	-2.42	119.21	122.59
19	B1	825	CLA	CHB-C4A-NA	2.42	127.86	124.51
19	B2	850	CLA	CMD-C2D-C3D	2.42	129.34	124.80
23	A	854	BCR	C1-C6-C5	-2.42	119.21	122.59
19	A1	817	CLA	CHB-C4A-NA	2.42	127.86	124.51
23	B2	840	BCR	C33-C5-C6	-2.42	121.82	124.51
19	B1	813	CLA	CMD-C2D-C3D	2.42	129.34	124.80
23	AA	848	BCR	C15-C16-C17	-2.42	118.43	123.51
19	F	301	CLA	C1B-CHB-C4A	-2.42	125.33	130.12
19	A1	831	CLA	CMB-C2B-C3B	2.42	129.33	124.80
19	AA	833	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	A2	812	CLA	CHB-C4A-NA	2.42	127.85	124.51
19	A2	819	CLA	CMB-C2B-C3B	2.42	129.33	124.80
19	A1	815	CLA	CMD-C2D-C3D	2.42	129.33	124.80
19	K1	103	CLA	CHB-C4A-NA	2.42	127.85	124.51
22	B2	848	LHG	O4-P-O5	2.42	124.32	112.21
23	K1	104	BCR	C38-C26-C25	-2.41	121.82	124.51
19	X1	101	CLA	CMB-C2B-C3B	2.41	129.33	124.80
19	A1	838	CLA	CMD-C2D-C3D	2.41	129.33	124.80
26	B	841	ECH	C33-C5-C4	2.41	118.09	113.57
19	BB	835	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	BB	842	BCR	C33-C5-C6	-2.41	121.82	124.51
19	KK	102	CLA	CHB-C4A-NA	2.41	127.85	124.51
19	K	101	CLA	C1B-CHB-C4A	-2.41	125.34	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L2	204	CLA	CMB-C2B-C3B	2.41	129.32	124.80
19	X2	101	CLA	CMB-C2B-C3B	2.41	129.32	124.80
23	J1	102	BCR	C38-C26-C25	-2.41	121.82	124.51
19	AA	822	CLA	CMD-C2D-C3D	2.41	129.32	124.80
19	BB	819	CLA	OBD-CAD-CBD	-2.41	122.37	125.91
19	BB	808	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	F	304	BCR	C15-C16-C17	-2.41	118.44	123.51
28	BB	854	DGD	C1D-C2D-C3D	-2.41	104.95	109.98
19	L1	206	CLA	C1-O2A-CGA	2.41	123.13	116.54
19	AA	810	CLA	CMB-C2B-C3B	2.41	129.32	124.80
19	B1	814	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
19	A1	812	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	AA	818	CLA	CHB-C4A-NA	2.41	127.84	124.51
19	BB	802	CLA	CMB-C2B-C3B	2.41	129.32	124.80
23	I2	101	BCR	C15-C16-C17	-2.41	118.44	123.51
24	L	209	AJP	CBM-CBL-CCH	2.41	117.32	113.12
19	B1	829	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	A1	850	BCR	C8-C7-C6	-2.41	120.53	127.28
24	A	855	AJP	CDD-CDC-CDB	2.41	116.76	111.87
23	F2	304	BCR	C38-C26-C25	-2.41	121.83	124.51
24	AA	856	AJP	CBM-CBL-CCH	2.41	117.31	113.12
23	FF	306	BCR	C7-C8-C9	-2.41	122.59	126.21
23	A1	853	BCR	C2-C1-C6	2.41	114.21	110.48
19	A	842	CLA	CMB-C2B-C3B	2.41	129.32	124.80
19	BB	813	CLA	CMD-C2D-C3D	2.41	129.32	124.80
23	F2	303	BCR	C11-C10-C9	-2.41	123.87	127.31
23	AA	848	BCR	C2-C1-C6	2.41	114.21	110.48
23	II	101	BCR	C38-C26-C25	-2.41	121.83	124.51
19	A2	807	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
19	BB	825	CLA	CHB-C4A-NA	2.41	127.84	124.51
23	MM	101	BCR	C11-C10-C9	-2.41	123.88	127.31
19	A	808	CLA	CMB-C2B-C3B	2.40	129.31	124.80
19	B1	831	CLA	O2D-CGD-O1D	-2.40	119.08	123.83
23	A	847	BCR	C15-C16-C17	-2.40	118.46	123.51
23	A1	847	BCR	C15-C16-C17	-2.40	118.46	123.51
19	A2	826	CLA	CMB-C2B-C3B	2.40	129.31	124.80
19	B2	803	CLA	CMD-C2D-C3D	2.40	129.31	124.80
19	BB	830	CLA	O2D-CGD-O1D	-2.40	119.08	123.83
19	BB	805	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	B2	833	CLA	O2D-CGD-CBD	2.40	115.46	111.25
24	A	802	AJP	CBD-CBN-CCJ	2.40	117.59	111.69
19	A2	812	CLA	CMB-C2B-C1B	-2.40	124.77	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	B	853	LHG	P-O3-C3	-2.40	107.59	121.68
24	B	849	AJP	CDA-CDB-CCG	2.40	115.23	112.65
19	A2	829	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
23	II	101	BCR	C2-C1-C6	2.40	114.20	110.48
23	L2	207	BCR	C38-C26-C25	-2.40	121.83	124.51
23	I1	101	BCR	C15-C16-C17	-2.40	118.46	123.51
19	B	828	CLA	CMD-C2D-C3D	2.40	129.31	124.80
19	K	101	CLA	CMD-C2D-C3D	2.40	129.31	124.80
24	L2	202	AJP	CCG-CCF-CCE	2.40	117.97	114.00
20	A1	802	CL0	C4C-C3C-C2C	-2.40	103.41	106.89
19	K2	102	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	K1	102	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
19	LL	202	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
25	M	102	LMG	C38-C37-C36	-2.40	102.04	114.44
19	B1	820	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	B2	814	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
23	F1	303	BCR	C8-C7-C6	-2.40	120.56	127.28
23	I	101	BCR	C2-C1-C6	2.40	114.19	110.48
19	A1	816	CLA	CMB-C2B-C3B	2.40	129.29	124.80
19	A2	814	CLA	CMD-C2D-C3D	2.40	129.29	124.80
19	A	809	CLA	C1D-CHD-C4C	2.40	125.76	122.48
19	BB	812	CLA	CHB-C4A-NA	2.40	127.83	124.51
19	BB	816	CLA	CMD-C2D-C3D	2.40	129.29	124.80
19	AA	818	CLA	CMB-C2B-C1B	-2.39	124.78	128.46
19	A2	812	CLA	CBA-CAA-C2A	2.39	120.98	113.85
19	A	812	CLA	CHB-C4A-NA	2.39	127.82	124.51
23	BB	847	BCR	C15-C14-C13	-2.39	123.89	127.31
19	B	803	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	B	817	CLA	CMB-C2B-C3B	2.39	129.29	124.80
19	BB	834	CLA	CMD-C2D-C3D	2.39	129.29	124.80
24	A	855	AJP	CBM-CBL-CCH	2.39	117.29	113.12
19	A1	822	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	A1	802	CL0	CGD-CBD-CAD	-2.39	102.98	110.73
23	B1	842	BCR	C2-C1-C6	2.39	114.19	110.48
23	A	847	BCR	C8-C7-C6	-2.39	120.58	127.28
23	I2	102	BCR	C7-C8-C9	-2.39	122.62	126.21
19	A	844	CLA	CMB-C2B-C3B	2.39	129.29	124.80
19	A2	823	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
19	A1	826	CLA	CHB-C4A-NA	2.39	127.82	124.51
19	J	101	CLA	CMD-C2D-C3D	2.39	129.28	124.80
19	BB	828	CLA	CMD-C2D-C3D	2.39	129.28	124.80
19	A	813	CLA	C1B-CHB-C4A	-2.39	125.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F2	303	BCR	C8-C7-C6	-2.39	120.59	127.28
19	F1	305	CLA	CMD-C2D-C3D	2.39	129.28	124.80
23	A	849	BCR	C33-C5-C6	-2.39	121.85	124.51
19	B1	832	CLA	C2A-C1A-CHA	2.39	128.04	123.86
20	A	803	CL0	C9-C8-C7	2.39	120.01	111.30
23	F1	306	BCR	C27-C26-C25	2.39	126.22	122.74
23	KK	103	BCR	C8-C7-C6	-2.39	120.59	127.28
19	A	830	CLA	CAC-C3C-C4C	2.39	127.94	124.82
24	L2	202	AJP	OBG-CBF-CAW	2.39	113.07	110.81
19	AA	813	CLA	CMB-C2B-C3B	2.39	129.28	124.80
19	B1	823	CLA	CMB-C2B-C3B	2.39	129.28	124.80
19	B1	810	CLA	CHB-C4A-NA	2.39	127.81	124.51
24	M2	101	AJP	OBG-CBF-CAW	2.39	113.07	110.81
19	AA	826	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
23	K	103	BCR	C2-C1-C6	2.38	114.17	110.48
19	A2	826	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
19	A	813	CLA	CMD-C2D-C3D	2.38	129.27	124.80
19	A1	852	CLA	OBD-CAD-CBD	-2.38	122.41	125.91
23	A	847	BCR	C2-C1-C6	2.38	114.17	110.48
19	B	819	CLA	CMB-C2B-C3B	2.38	129.27	124.80
19	A	821	CLA	CMD-C2D-C3D	2.38	129.27	124.80
19	K1	105	CLA	C1D-CHD-C4C	2.38	125.74	122.48
20	AA	803	CL0	CMD-C2D-C3D	-2.38	120.33	124.80
19	AA	837	CLA	CHB-C4A-NA	2.38	127.81	124.51
19	F1	302	CLA	CMD-C2D-C3D	2.38	129.27	124.80
19	B	834	CLA	C4-C3-C5	2.38	119.39	115.29
23	F2	304	BCR	C15-C16-C17	-2.38	118.50	123.51
19	A	820	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	A2	816	CLA	C1-C2-C3	-2.38	122.90	126.75
19	B2	824	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	BB	829	CLA	C5-C3-C2	2.38	126.00	121.11
19	B2	802	CLA	CMB-C2B-C3B	2.38	129.26	124.80
19	AA	836	CLA	CMD-C2D-C3D	2.38	129.26	124.80
23	I2	103	BCR	C27-C26-C25	2.38	126.21	122.74
19	BB	803	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	A2	810	CLA	CMB-C2B-C3B	2.38	129.26	124.80
19	A1	807	CLA	CHB-C4A-NA	2.38	127.80	124.51
24	AA	802	AJP	CBD-CBN-CCJ	2.38	117.52	111.69
19	KK	102	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	A1	820	CLA	O2A-CGA-O1A	-2.38	117.49	123.56
19	BB	826	CLA	CHB-C4A-NA	2.38	127.80	124.51
19	B1	818	CLA	CMB-C2B-C3B	2.38	129.26	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	805	CLA	CMB-C2B-C3B	2.38	129.26	124.80
24	L1	203	AJP	OCY-CCZ-CDA	-2.38	105.08	109.66
19	B	805	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	FF	303	BCR	C11-C10-C9	-2.38	123.92	127.31
19	B2	828	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	A2	816	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	AA	812	CLA	CMD-C2D-C3D	2.38	129.26	124.80
19	B2	821	CLA	C4-C3-C2	-2.38	117.50	123.68
19	A2	817	CLA	CMB-C2B-C3B	2.38	129.25	124.80
23	A2	853	BCR	C30-C25-C26	-2.38	119.27	122.59
23	JJ	102	BCR	C38-C26-C25	-2.37	121.86	124.51
19	A1	820	CLA	CMB-C2B-C3B	2.37	129.25	124.80
23	A2	850	BCR	C8-C7-C6	-2.37	120.63	127.28
19	BB	824	CLA	CHB-C4A-NA	2.37	127.79	124.51
22	A1	846	LHG	P-O3-C3	-2.37	107.76	121.68
19	K2	102	CLA	CMD-C2D-C3D	2.37	129.25	124.80
23	L	206	BCR	C38-C26-C25	-2.37	121.87	124.51
23	B1	842	BCR	C33-C5-C6	-2.37	121.87	124.51
19	B	829	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	B	860	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	A1	801	CLA	O2A-CGA-O1A	-2.37	117.50	123.56
19	B	820	CLA	CMB-C2B-C3B	2.37	129.25	124.80
19	B1	809	CLA	CMD-C2D-C3D	2.37	129.25	124.80
19	B	830	CLA	C5-C3-C2	2.37	125.98	121.11
19	AA	829	CLA	C5-C3-C2	2.37	125.98	121.11
24	B	850	AJP	CBJ-CCB-CCA	2.37	118.57	113.00
23	K2	105	BCR	C15-C14-C13	-2.37	123.92	127.31
19	B2	809	CLA	CMD-C2D-C3D	2.37	129.25	124.80
19	AA	813	CLA	CMD-C2D-C3D	2.37	129.25	124.80
23	K1	106	BCR	C1-C6-C5	-2.37	119.28	122.59
24	BB	849	AJP	CDC-CDB-CCG	2.37	116.69	112.31
19	BB	822	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	F2	305	BCR	C27-C26-C25	2.37	126.20	122.74
19	A1	835	CLA	O2D-CGD-CBD	2.37	115.40	111.25
19	BB	856	CLA	C2A-C1A-CHA	2.37	128.00	123.86
19	A1	819	CLA	CBA-CAA-C2A	2.37	120.91	113.85
19	JJ	101	CLA	CMB-C2B-C3B	2.37	129.25	124.80
19	F	302	CLA	CMD-C2D-C3D	2.37	129.25	124.80
19	A2	840	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	B2	810	CLA	CHB-C4A-NA	2.37	127.79	124.51
23	K1	106	BCR	C15-C14-C13	-2.37	123.93	127.31
19	B2	816	CLA	C1B-CHB-C4A	-2.37	125.42	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	808	CLA	O2D-CGD-O1D	-2.37	119.15	123.83
19	A1	801	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	A2	801	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
19	F1	301	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	X1	103	LHG	P-O3-C3	-2.37	107.79	121.68
19	A1	835	CLA	CMD-C2D-C3D	2.37	129.24	124.80
19	L	203	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
22	L2	208	LHG	P-O3-C3	-2.37	107.80	121.68
24	M2	101	AJP	CBM-CBN-CBO	-2.37	111.57	115.48
19	AA	841	CLA	CMD-C2D-C3D	2.37	129.24	124.80
19	A1	806	CLA	C1B-CHB-C4A	-2.37	125.43	130.12
24	I2	104	AJP	OBG-CBF-CAW	2.37	113.05	110.81
24	B	850	AJP	CDC-CDB-CCG	2.37	116.67	112.31
23	JJ	102	BCR	C2-C1-C6	2.37	114.14	110.48
23	J	102	BCR	C27-C26-C25	2.36	126.19	122.74
19	K1	103	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
19	B2	826	CLA	C1B-CHB-C4A	-2.36	125.43	130.12
19	B2	851	CLA	O2A-CGA-O1A	-2.36	117.52	123.56
24	I2	104	AJP	CDC-CDB-CCG	2.36	116.67	112.31
19	B	859	CLA	O2D-CGD-CBD	2.36	115.39	111.25
19	A	841	CLA	CMD-C2D-C3D	2.36	129.23	124.80
23	A2	853	BCR	C35-C13-C14	-2.36	119.61	122.92
22	BB	851	LHG	P-O3-C3	-2.36	107.83	121.68
19	B2	813	CLA	CMB-C2B-C3B	2.36	129.23	124.80
19	A2	836	CLA	CMD-C2D-C3D	2.36	129.23	124.80
19	JJ	101	CLA	CMD-C2D-C3D	2.36	129.23	124.80
19	F2	301	CLA	O2D-CGD-CBD	2.36	115.39	111.25
19	J	101	CLA	CMB-C2B-C3B	2.36	129.23	124.80
23	A2	847	BCR	C8-C7-C6	-2.36	120.67	127.28
19	B2	805	CLA	O2D-CGD-CBD	2.36	115.38	111.25
19	B2	837	CLA	C1D-CHD-C4C	2.36	125.71	122.48
25	I2	105	LMG	O3-C3-C2	-2.36	104.87	110.34
19	A1	820	CLA	CBA-CAA-C2A	2.36	120.88	113.85
19	A2	801	CLA	CMB-C2B-C1B	-2.36	124.84	128.46
25	L1	210	LMG	O1-C7-C8	-2.36	105.20	110.90
19	B	835	CLA	CMD-C2D-C3D	2.36	129.22	124.80
23	B	848	BCR	C15-C14-C13	-2.36	123.94	127.31
19	B	802	CLA	CMD-C2D-C3D	2.36	129.22	124.80
19	B	825	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
19	BB	829	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
20	AA	803	CL0	C4C-C3C-C2C	-2.36	103.47	106.89
24	L1	203	AJP	CBN-CBO-CBE	2.36	128.95	120.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	806	CLA	O2A-CGA-O1A	-2.36	117.54	123.56
23	A1	851	BCR	C1-C6-C5	-2.36	119.30	122.59
19	AA	804	CLA	C1D-CHD-C4C	2.36	125.71	122.48
23	K2	103	BCR	C38-C26-C25	-2.36	121.89	124.51
24	L1	203	AJP	OBQ-CBF-CBE	-2.36	100.85	104.44
19	F2	301	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	A1	854	AJP	CCJ-CCI-CCH	-2.36	105.11	109.25
19	B2	809	CLA	O2D-CGD-CBD	2.36	115.38	111.25
19	B1	809	CLA	O2D-CGD-CBD	2.36	115.38	111.25
19	B1	805	CLA	O2A-CGA-O1A	-2.36	117.54	123.56
19	L2	204	CLA	CMD-C2D-C3D	2.35	129.22	124.80
19	AA	821	CLA	CMD-C2D-C3D	2.35	129.22	124.80
23	F1	303	BCR	C15-C16-C17	-2.35	118.56	123.51
19	B1	806	CLA	O2A-CGA-O1A	-2.35	117.55	123.56
23	F2	305	BCR	C24-C23-C22	-2.35	122.68	126.21
19	A1	832	CLA	CHB-C4A-NA	2.35	127.77	124.51
19	B1	817	CLA	CMB-C2B-C3B	2.35	129.21	124.80
19	B2	821	CLA	C5-C3-C2	2.35	125.94	121.11
19	A2	806	CLA	CMB-C2B-C3B	2.35	129.21	124.80
19	L1	207	CLA	O2D-CGD-O1D	-2.35	119.19	123.83
19	AA	810	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	A	812	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	AA	817	CLA	CMD-C2D-C3D	2.35	129.21	124.80
23	A1	851	BCR	C24-C23-C22	-2.35	122.68	126.21
23	BB	838	BCR	C7-C8-C9	-2.35	122.68	126.21
23	A1	853	BCR	C30-C25-C26	-2.35	119.30	122.59
19	AA	837	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	A2	829	CLA	C5-C3-C2	2.35	125.94	121.11
19	A	822	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	A1	836	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	AA	823	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	BB	813	CLA	CMB-C2B-C3B	2.35	129.21	124.80
19	A1	808	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
19	B1	850	CLA	O2A-CGA-O1A	-2.35	117.56	123.56
23	L1	208	BCR	C7-C8-C9	-2.35	122.68	126.21
19	A	840	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	A	836	CLA	O2D-CGD-CBD	2.35	115.36	111.25
19	B1	803	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	L1	205	CLA	CMD-C2D-C3D	2.35	129.21	124.80
19	B2	805	CLA	O2A-CGA-O1A	-2.35	117.56	123.56
19	A2	832	CLA	C1D-CHD-C4C	2.35	125.69	122.48
19	B1	819	CLA	CHB-C4A-NA	2.35	127.76	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	851	CLA	C4-C3-C5	2.35	119.33	115.29
23	KK	103	BCR	C2-C1-C6	2.35	114.11	110.48
19	A	825	CLA	C1D-CHD-C4C	2.35	125.69	122.48
19	A2	833	CLA	CMB-C2B-C1B	-2.35	124.86	128.46
19	A2	838	CLA	O2D-CGD-CBD	2.35	115.36	111.25
19	A	836	CLA	CMD-C2D-C3D	2.35	129.20	124.80
26	BB	840	ECH	C33-C5-C4	2.35	117.97	113.57
19	AA	842	CLA	C1B-CHB-C4A	-2.35	125.47	130.12
19	J2	101	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	BB	803	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	BB	856	CLA	O2D-CGD-CBD	2.35	115.36	111.25
19	B	828	CLA	CHB-C4A-NA	2.35	127.76	124.51
19	B2	817	CLA	CMD-C2D-C3D	2.35	129.20	124.80
19	A2	814	CLA	CHB-C4A-NA	2.35	127.75	124.51
23	B2	843	BCR	C2-C1-C6	2.35	114.11	110.48
19	AA	816	CLA	O2D-CGD-CBD	2.34	115.36	111.25
19	B	816	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	819	CLA	CHB-C4A-NA	2.34	127.75	124.51
23	B	848	BCR	C38-C26-C25	-2.34	121.90	124.51
19	BB	806	CLA	O2A-CGA-O1A	-2.34	117.57	123.56
19	AA	807	CLA	CMB-C2B-C1B	-2.34	124.86	128.46
19	B1	833	CLA	C4-C3-C5	2.34	119.32	115.29
19	B	860	CLA	CBC-CAC-C3C	2.34	118.93	112.43
20	A2	803	CL0	CMD-C2D-C3D	-2.34	120.41	124.80
19	B2	806	CLA	O2A-CGA-O1A	-2.34	117.58	123.56
19	B	804	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A1	811	CLA	CMD-C2D-C3D	2.34	129.19	124.80
24	L1	204	AJP	OCY-CCZ-CDA	-2.34	105.15	109.66
19	A2	825	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A1	830	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A	818	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A2	852	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	A	837	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	B	820	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
23	B2	843	BCR	C33-C5-C6	-2.34	121.90	124.51
24	L2	202	AJP	CAX-CAW-CBF	2.34	116.10	111.95
19	B1	834	CLA	CHB-C4A-NA	2.34	127.75	124.51
19	JJ	103	CLA	CHB-C4A-NA	2.34	127.75	124.51
24	KK	104	AJP	OBG-CBF-CAW	-2.34	108.59	110.81
19	B2	802	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
19	A2	831	CLA	C1B-CHB-C4A	-2.34	125.48	130.12
21	AA	844	PQN	C15-C13-C12	-2.34	116.31	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	825	CLA	C1D-CHD-C4C	2.34	125.68	122.48
19	BB	825	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
24	B	850	AJP	CAV-CBE-CBO	2.34	119.82	114.54
19	A1	809	CLA	CBA-CAA-C2A	2.34	120.81	113.85
19	A2	829	CLA	CHB-C4A-NA	2.34	127.75	124.51
22	A	845	LHG	P-O6-C4	-2.34	107.97	121.68
19	AA	801	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	A2	842	CLA	CMB-C2B-C3B	2.34	129.18	124.80
19	AA	840	CLA	CMD-C2D-C3D	2.34	129.18	124.80
19	A	811	CLA	CAC-C3C-C4C	2.34	127.87	124.82
23	JJ	104	BCR	C38-C26-C25	-2.34	121.91	124.51
19	A1	842	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A	840	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	A1	839	CLA	CHB-C4A-NA	2.34	127.74	124.51
19	B2	831	CLA	O2D-CGD-O1D	-2.34	119.22	123.83
20	A1	802	CL0	C4-C3-C5	2.34	119.31	115.29
19	A1	837	CLA	O2D-CGD-CBD	2.34	115.34	111.25
19	A1	815	CLA	C1-C2-C3	-2.34	122.97	126.75
19	A2	809	CLA	C1D-CHD-C4C	2.34	125.68	122.48
19	J	103	CLA	C1D-CHD-C4C	2.34	125.68	122.48
19	A1	836	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
19	L2	206	CLA	CMD-C2D-C3D	2.33	129.18	124.80
19	A2	842	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
23	A1	853	BCR	C35-C13-C14	-2.33	119.65	122.92
19	B1	822	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	B1	830	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
19	A2	836	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	L2	205	CLA	O2D-CGD-CBD	2.33	115.34	111.25
19	AA	836	CLA	O2D-CGD-CBD	2.33	115.33	111.25
19	A2	818	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	FF	305	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	BB	817	CLA	CMB-C2B-C3B	2.33	129.17	124.80
19	K	102	CLA	CMB-C2B-C3B	2.33	129.17	124.80
19	A	821	CLA	O2A-CGA-O1A	-2.33	117.60	123.56
19	A2	802	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	AA	839	CLA	CHB-C4A-NA	2.33	127.74	124.51
19	A2	827	CLA	CMD-C2D-C3D	2.33	129.17	124.80
25	II	105	LMG	O1-C1-C2	-2.33	104.55	108.26
19	BB	836	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	B1	843	BCR	C24-C23-C22	-2.33	122.71	126.21
19	A1	813	CLA	O2D-CGD-O1D	-2.33	119.23	123.83
22	B	852	LHG	P-O6-C4	-2.33	108.02	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	M2	102	BCR	C7-C8-C9	-2.33	122.71	126.21
19	J	103	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	A1	833	CLA	CHB-C4A-NA	2.33	127.73	124.51
23	A2	849	BCR	C33-C5-C6	-2.33	121.92	124.51
19	B1	822	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	A	837	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	BB	804	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
23	II	104	BCR	C7-C8-C9	-2.33	122.71	126.21
24	BB	849	AJP	CDC-CDD-CCI	2.33	116.01	112.13
19	BB	814	CLA	C1D-CHD-C4C	2.33	125.67	122.48
19	AA	812	CLA	CHB-C4A-NA	2.33	127.73	124.51
19	A1	811	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
19	A2	810	CLA	CMD-C2D-C3D	2.33	129.17	124.80
23	B	844	BCR	C8-C7-C6	-2.33	120.76	127.28
19	B2	820	CLA	CHB-C4A-NA	2.33	127.73	124.51
21	AA	844	PQN	C21-C22-C23	-2.33	108.51	115.77
19	A	809	CLA	CMB-C2B-C3B	2.33	129.16	124.80
19	AA	842	CLA	CMB-C2B-C3B	2.33	129.16	124.80
23	BB	847	BCR	C35-C13-C14	-2.33	119.66	122.92
19	A	807	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
19	AA	819	CLA	CMD-C2D-C3D	2.33	129.16	124.80
19	BB	845	CLA	CAC-C3C-C4C	2.33	127.86	124.82
19	J1	103	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
19	B1	806	CLA	C4-C3-C2	-2.33	117.63	123.68
19	A1	828	CLA	C4-C3-C5	2.33	119.29	115.29
19	B	829	CLA	CMD-C2D-C3D	2.33	129.16	124.80
19	B1	845	CLA	C1D-CHD-C4C	2.33	125.66	122.48
23	AA	852	BCR	C24-C23-C22	-2.33	122.72	126.21
19	AA	836	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
19	A	801	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	B1	802	CLA	C1B-CHB-C4A	-2.32	125.51	130.12
19	BB	816	CLA	CHB-C4A-NA	2.32	127.73	124.51
19	B1	833	CLA	CMD-C2D-C3D	2.32	129.16	124.80
21	A1	843	PQN	C21-C22-C23	-2.32	108.52	115.77
19	A1	815	CLA	CMB-C2B-C3B	2.32	129.16	124.80
23	L1	208	BCR	C27-C26-C25	2.32	126.13	122.74
19	BB	802	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	BB	801	CLA	C6-C5-C3	2.32	118.59	113.01
19	A1	825	CLA	CMD-C2D-C3D	2.32	129.16	124.80
19	B	805	CLA	O2A-CGA-O1A	-2.32	117.63	123.56
19	A	812	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
24	L	208	AJP	CBD-CBN-CCJ	2.32	117.39	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	I2	103	BCR	C11-C10-C9	-2.32	124.00	127.31
19	B	824	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B1	828	CLA	CMD-C2D-C3D	2.32	129.15	124.80
23	A	848	BCR	C38-C26-C25	-2.32	121.92	124.51
19	B2	828	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	B2	816	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	FF	301	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	BB	806	CLA	CMB-C2B-C3B	2.32	129.15	124.80
19	AA	830	CLA	CAC-C3C-C4C	2.32	127.85	124.82
19	AA	853	CLA	C7-C6-C5	2.32	119.49	113.25
19	JJ	103	CLA	CMB-C2B-C1B	-2.32	124.90	128.46
19	AA	826	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	A1	820	CLA	CAC-C3C-C4C	2.32	127.85	124.82
19	A2	809	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
19	B1	827	CLA	CMD-C2D-C3D	2.32	129.15	124.80
19	A2	834	CLA	CHB-C4A-NA	2.32	127.72	124.51
19	AA	824	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	A1	831	CLA	C1D-CHD-C4C	2.32	125.65	122.48
19	A	813	CLA	CMB-C2B-C3B	2.32	129.15	124.80
19	A	823	CLA	CMD-C2D-C3D	2.32	129.15	124.80
23	J	102	BCR	C33-C5-C6	-2.32	121.93	124.51
22	X2	103	LHG	P-O3-C3	-2.32	108.09	121.68
20	A1	802	CL0	CMA-C3A-C4A	-2.32	105.55	111.77
23	B1	843	BCR	C8-C7-C6	-2.32	120.79	127.28
19	FF	305	CLA	CMD-C2D-C3D	2.32	129.15	124.80
23	F1	304	BCR	C37-C22-C21	-2.32	119.68	122.92
19	A	837	CLA	O2D-CGD-O1D	-2.32	119.26	123.83
19	AA	812	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	L1	206	CLA	CHB-C4A-NA	2.32	127.72	124.51
22	A	845	LHG	P-O3-C3	-2.32	108.10	121.68
19	A1	825	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
19	B	846	CLA	CAC-C3C-C4C	2.32	127.85	124.82
19	B1	850	CLA	O2D-CGD-CBD	2.32	115.31	111.25
19	B	837	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
19	LL	201	CLA	C1D-CHD-C4C	2.31	125.65	122.48
19	BB	812	CLA	O2D-CGD-O1D	-2.31	119.26	123.83
23	B2	844	BCR	C8-C7-C6	-2.31	120.80	127.28
19	B2	801	CLA	CBA-CAA-C2A	2.31	120.74	113.85
19	B1	803	CLA	C11-C12-C13	-2.31	108.55	115.77
19	A2	813	CLA	CMD-C2D-C3D	2.31	129.14	124.80
19	BB	845	CLA	C1B-CHB-C4A	-2.31	125.53	130.12
24	BB	849	AJP	CDD-CCI-CCH	-2.31	107.60	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	852	CLA	CMD-C2D-C3D	2.31	129.14	124.80
20	A1	802	CL0	C9-C8-C10	2.31	119.73	111.30
23	B1	842	BCR	C27-C26-C25	2.31	126.11	122.74
19	AA	819	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	K1	105	CLA	CHB-C4A-NA	2.31	127.71	124.51
19	B2	806	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	B2	835	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	A1	852	CLA	CMD-C2D-C3D	2.31	129.13	124.80
23	AA	848	BCR	C8-C7-C6	-2.31	120.81	127.28
21	A2	843	PQN	C21-C22-C23	-2.31	108.56	115.77
19	B2	846	CLA	C1D-CHD-C4C	2.31	125.64	122.48
19	AA	809	CLA	C1D-CHD-C4C	2.31	125.64	122.48
19	B2	817	CLA	CMB-C2B-C3B	2.31	129.13	124.80
23	F2	303	BCR	C38-C26-C25	-2.31	121.94	124.51
19	B2	809	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
19	B2	815	CLA	C4-C3-C2	-2.31	117.67	123.68
23	JJ	102	BCR	C27-C26-C25	2.31	126.11	122.74
19	A2	801	CLA	O2A-CGA-O1A	-2.31	117.66	123.56
23	A1	849	BCR	C7-C8-C9	-2.31	122.74	126.21
19	A	805	CLA	C5-C3-C2	2.31	125.85	121.11
23	L1	209	BCR	C16-C15-C14	-2.31	118.66	123.51
19	B1	801	CLA	C5-C3-C2	2.31	125.85	121.11
19	B2	826	CLA	O2D-CGD-CBD	2.31	115.29	111.25
19	FF	302	CLA	CMB-C2B-C3B	2.31	129.13	124.80
19	J1	103	CLA	CHB-C4A-NA	2.31	127.70	124.51
23	II	101	BCR	C24-C23-C22	-2.31	122.75	126.21
23	AA	849	BCR	C38-C26-C25	-2.31	121.94	124.51
19	A2	838	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	JJ	102	BCR	C8-C7-C6	-2.31	120.82	127.28
19	B1	831	CLA	C1B-CHB-C4A	-2.31	125.55	130.12
23	BB	843	BCR	C16-C15-C14	-2.31	118.66	123.51
22	BB	850	LHG	P-O6-C4	-2.31	108.16	121.68
23	K1	106	BCR	C15-C16-C17	-2.31	118.66	123.51
19	A	831	CLA	CHB-C4A-NA	2.31	127.70	124.51
19	F1	305	CLA	CHB-C4A-NA	2.31	127.70	124.51
19	B1	830	CLA	CMD-C2D-C3D	2.31	129.12	124.80
22	AA	846	LHG	P-O6-C4	-2.31	108.16	121.68
19	A2	821	CLA	O2A-CGA-O1A	-2.30	117.67	123.56
22	A2	845	LHG	P-O3-C3	-2.30	108.17	121.68
23	B	848	BCR	C35-C13-C14	-2.30	119.69	122.92
19	A2	821	CLA	CBA-CAA-C2A	2.30	120.71	113.85
19	B	846	CLA	C1B-CHB-C4A	-2.30	125.55	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	816	CLA	CMD-C2D-C3D	2.30	129.12	124.80
19	B	802	CLA	CMB-C2B-C3B	2.30	129.12	124.80
23	L2	207	BCR	C24-C23-C22	-2.30	122.75	126.21
19	AA	820	CLA	CMD-C2D-C3D	2.30	129.12	124.80
23	F	304	BCR	C37-C22-C21	-2.30	119.70	122.92
19	AA	845	CLA	CMB-C2B-C3B	2.30	129.12	124.80
19	AA	816	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	B2	826	CLA	C6-C5-C3	2.30	118.54	113.01
19	B2	832	CLA	O2D-CGD-O1D	-2.30	119.28	123.83
23	A2	851	BCR	C37-C22-C21	-2.30	119.70	122.92
23	BB	842	BCR	C15-C16-C17	-2.30	118.67	123.51
19	A	828	CLA	CMD-C2D-C3D	2.30	129.12	124.80
19	A	826	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	AA	831	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
23	BB	843	BCR	C8-C7-C6	-2.30	120.83	127.28
23	F1	304	BCR	C20-C21-C22	-2.30	124.03	127.31
23	F2	305	BCR	C20-C21-C22	-2.30	124.03	127.31
19	A	829	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	B	824	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	AA	830	CLA	CMD-C2D-C3D	2.30	129.11	124.80
23	II	102	BCR	C15-C16-C17	-2.30	118.68	123.51
23	BB	838	BCR	C24-C23-C22	-2.30	122.76	126.21
23	JJ	104	BCR	C27-C26-C25	2.30	126.09	122.74
19	B	827	CLA	CMD-C2D-C3D	2.30	129.11	124.80
19	BB	817	CLA	CMD-C2D-C3D	2.30	129.11	124.80
19	B1	805	CLA	O2D-CGD-CBD	2.30	115.28	111.25
19	B	858	CLA	O2D-CGD-CBD	2.30	115.28	111.25
23	A2	851	BCR	C8-C7-C6	-2.30	120.84	127.28
19	BB	815	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	A	825	CLA	CHB-C4A-NA	2.30	127.69	124.51
23	B	844	BCR	C16-C15-C14	-2.30	118.68	123.51
19	B2	833	CLA	CMD-C2D-C3D	2.30	129.11	124.80
19	AA	807	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
23	A2	849	BCR	C7-C8-C9	-2.30	122.76	126.21
19	B	803	CLA	CMD-C2D-C3D	2.30	129.11	124.80
19	B	806	CLA	C4-C3-C2	-2.30	117.71	123.68
28	BB	854	DGD	O5D-C6D-C5D	-2.30	104.75	109.14
19	A2	828	CLA	CMD-C2D-C3D	2.30	129.11	124.80
24	KK	104	AJP	CDC-CDD-CCI	2.30	115.96	112.13
19	B2	831	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	B2	852	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	A2	810	CLA	O2A-CGA-O1A	-2.30	117.69	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A	816	CLA	CMD-C2D-C3D	2.30	129.10	124.80
19	J2	103	CLA	CHB-C4A-NA	2.30	127.69	124.51
19	B1	824	CLA	O2A-CGA-O1A	-2.30	117.70	123.56
19	B2	832	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
19	F2	302	CLA	CMD-C2D-C3D	2.29	129.10	124.80
23	B	843	BCR	C2-C1-C6	2.29	114.03	110.48
23	BB	842	BCR	C2-C1-C6	2.29	114.03	110.48
19	AA	819	CLA	CHB-C4A-NA	2.29	127.69	124.51
19	B2	823	CLA	CMB-C2B-C3B	2.29	129.10	124.80
19	A	823	CLA	C5-C3-C2	2.29	125.82	121.11
19	A	822	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
20	AA	803	CL0	C5-C3-C2	-2.29	116.40	121.11
23	A	849	BCR	C7-C8-C9	-2.29	122.77	126.21
19	BB	833	CLA	CMD-C2D-C3D	2.29	129.10	124.80
23	K	103	BCR	C8-C7-C6	-2.29	120.86	127.28
19	A	828	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A	826	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	B1	809	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A	821	CLA	CBA-CAA-C2A	2.29	120.67	113.85
19	B2	815	CLA	O2D-CGD-CBD	2.29	115.27	111.25
19	B2	804	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	LL	202	CLA	C1D-CHD-C4C	2.29	125.62	122.48
19	A2	819	CLA	O2A-CGA-O1A	-2.29	117.70	123.56
19	A1	818	CLA	O2A-CGA-O1A	-2.29	117.70	123.56
24	A1	854	AJP	CBN-CBO-CBE	2.29	128.72	120.59
23	FF	304	BCR	C33-C5-C6	-2.29	121.96	124.51
19	B1	801	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A2	812	CLA	CMD-C2D-C3D	2.29	129.10	124.80
19	BB	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	AA	853	CLA	O2D-CGD-CBD	2.29	115.26	111.25
19	L1	206	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
19	A1	819	CLA	CMD-C2D-C3D	2.29	129.09	124.80
19	A2	808	CLA	CMD-C2D-C3D	2.29	129.09	124.80
19	B	818	CLA	CHB-C4A-NA	2.29	127.68	124.51
19	A	831	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	JJ	104	BCR	C8-C7-C6	-2.29	120.87	127.28
23	F	304	BCR	C20-C21-C22	-2.29	124.05	127.31
23	B1	843	BCR	C16-C15-C14	-2.29	118.70	123.51
19	A1	823	CLA	C1D-CHD-C4C	2.29	125.61	122.48
24	B	857	AJP	CBN-CBO-CBE	2.29	128.70	120.59
19	AA	809	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	B2	827	CLA	C1B-CHB-C4A	-2.29	125.59	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	829	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	B	859	CLA	C2A-C1A-CHA	2.29	127.86	123.86
19	AA	806	CLA	CMD-C2D-C3D	2.29	129.09	124.80
19	A2	831	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	J	103	CLA	CHB-C4A-NA	2.29	127.67	124.51
19	A	819	CLA	C1D-CHD-C4C	2.29	125.61	122.48
19	B1	845	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
19	A1	827	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	A	851	BCR	C1-C6-C5	-2.29	119.39	122.59
19	A1	832	CLA	O2D-CGD-CBD	2.29	115.25	111.25
23	M	101	BCR	C8-C7-C6	-2.29	120.88	127.28
23	J	104	BCR	C3-C4-C5	-2.29	110.01	113.99
24	A1	855	AJP	CAW-CBF-CBE	2.29	120.54	115.72
19	A1	808	CLA	C1D-CHD-C4C	2.28	125.61	122.48
19	B2	830	CLA	CMB-C2B-C3B	2.28	129.08	124.80
19	L1	205	CLA	C4-C3-C5	2.28	119.22	115.29
19	B1	801	CLA	CBA-CAA-C2A	2.28	120.65	113.85
19	B1	817	CLA	CMD-C2D-C3D	2.28	129.08	124.80
19	JJ	103	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
19	AA	821	CLA	CBA-CAA-C2A	2.28	120.65	113.85
19	A1	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	B1	842	BCR	C38-C26-C25	-2.28	121.97	124.51
23	L1	208	BCR	C11-C10-C9	-2.28	124.05	127.31
19	B	801	CLA	CMD-C2D-C3D	2.28	129.08	124.80
19	B1	813	CLA	CMB-C2B-C3B	2.28	129.08	124.80
24	BB	849	AJP	CCX-OCY-CCZ	-2.28	111.81	115.33
24	B	850	AJP	CAZ-CAY-CAX	2.28	117.15	112.08
19	A	852	CLA	O2D-CGD-CBD	2.28	115.24	111.25
19	AA	834	CLA	CHB-C4A-NA	2.28	127.67	124.51
19	B2	833	CLA	CHA-C1A-NA	-2.28	121.18	126.40
19	BB	833	CLA	C2A-C1A-CHA	2.28	127.84	123.86
19	B1	803	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
25	I1	102	LMG	O3-C3-C2	-2.28	105.05	110.34
24	B	849	AJP	CCH-CCG-CDB	2.28	111.83	108.59
20	AA	803	CL0	C1-O2A-CGA	-2.28	110.32	116.54
19	B1	836	CLA	C1D-CHD-C4C	2.28	125.60	122.48
19	A1	830	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	B	829	CLA	C1B-CHB-C4A	-2.28	125.60	130.12
23	F1	304	BCR	C8-C7-C6	-2.28	120.90	127.28
24	L2	202	AJP	OCY-CCX-OCC	2.28	117.08	110.67
19	A2	844	CLA	CMD-C2D-C3D	2.28	129.07	124.80
24	A1	854	AJP	CAW-CBF-CBE	2.28	120.52	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	J2	101	CLA	CMD-C2D-C3D	2.28	129.07	124.80
19	A1	805	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	A1	842	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	B	826	CLA	CHB-C4A-NA	2.28	127.66	124.51
19	A	836	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
19	AA	805	CLA	O2D-CGD-CBD	2.28	115.24	111.25
19	AA	804	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	X1	103	LHG	P-O6-C4	-2.28	108.33	121.68
23	B	844	BCR	C15-C16-C17	-2.28	118.73	123.51
19	A	806	CLA	CMD-C2D-C3D	2.28	129.07	124.80
19	A2	834	CLA	CMB-C2B-C3B	2.28	129.07	124.80
19	BB	836	CLA	CHD-C4C-C3C	2.28	128.19	124.87
19	AA	836	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
22	BB	850	LHG	P-O3-C3	-2.28	108.34	121.68
24	L2	202	AJP	CBH-OBG-CBF	2.28	118.13	113.74
19	A	815	CLA	O2D-CGD-O1D	-2.27	119.34	123.83
23	B2	839	BCR	C24-C23-C22	-2.27	122.79	126.21
19	JJ	103	CLA	C1D-CHD-C4C	2.27	125.59	122.48
23	BB	847	BCR	C38-C26-C25	-2.27	121.98	124.51
19	B2	846	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
19	B1	826	CLA	O2D-CGD-CBD	2.27	115.23	111.25
22	X2	103	LHG	P-O6-C4	-2.27	108.35	121.68
19	B	830	CLA	CMB-C2B-C3B	2.27	129.06	124.80
19	B2	849	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
26	B1	840	ECH	C28-C27-C26	-2.27	116.53	118.68
23	F2	304	BCR	C8-C7-C6	-2.27	120.92	127.28
19	AA	805	CLA	C5-C3-C2	2.27	125.78	121.11
19	B1	834	CLA	CMD-C2D-C3D	2.27	129.06	124.80
23	B2	839	BCR	C15-C16-C17	-2.27	118.74	123.51
23	B2	839	BCR	C7-C8-C9	-2.27	122.80	126.21
19	AA	842	CLA	CMD-C2D-C3D	2.27	129.06	124.80
19	AA	816	CLA	CMB-C2B-C3B	2.27	129.06	124.80
19	AA	826	CLA	C1D-CHD-C4C	2.27	125.59	122.48
23	L1	209	BCR	C27-C26-C25	2.27	126.05	122.74
23	II	101	BCR	C15-C16-C17	-2.27	118.74	123.51
19	BB	806	CLA	C4-C3-C2	-2.27	117.78	123.68
19	B2	806	CLA	C4-C3-C2	-2.27	117.78	123.68
19	BB	856	CLA	CMD-C2D-C3D	2.27	129.06	124.80
23	B2	843	BCR	C38-C26-C25	-2.27	121.98	124.51
23	MM	101	BCR	C24-C23-C22	-2.27	122.80	126.21
19	BB	820	CLA	CHD-C4C-C3C	2.27	128.18	124.87
23	JJ	102	BCR	C33-C5-C6	-2.27	121.98	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	BB	840	ECH	C23-C24-C25	-2.27	120.92	127.28
19	B	860	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	B1	838	BCR	C7-C8-C9	-2.27	122.80	126.21
19	B2	827	CLA	O2D-CGD-O1D	-2.27	119.35	123.83
19	A2	828	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	A	824	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
19	B	846	CLA	C1D-CHD-C4C	2.27	125.58	122.48
20	A1	802	CL0	C1-C2-C3	2.27	129.97	126.04
19	J1	101	CLA	CMD-C2D-C3D	2.27	129.05	124.80
23	AA	855	BCR	C1-C6-C5	-2.27	119.42	122.59
23	K2	105	BCR	C15-C16-C17	-2.27	118.75	123.51
19	A1	841	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
19	B2	822	CLA	CHB-C4A-NA	2.27	127.65	124.51
23	K1	104	BCR	C15-C16-C17	-2.27	118.75	123.51
23	B2	844	BCR	C16-C15-C14	-2.27	118.75	123.51
23	J	102	BCR	C8-C7-C6	-2.27	120.93	127.28
19	A1	827	CLA	CMD-C2D-C3D	2.27	129.05	124.80
19	B	804	CLA	CMB-C2B-C3B	2.27	129.05	124.80
19	A2	816	CLA	CMB-C2B-C3B	2.26	129.05	124.80
23	AA	852	BCR	C15-C16-C17	-2.26	118.75	123.51
23	A	854	BCR	C15-C16-C17	-2.26	118.75	123.51
19	A1	816	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
23	L1	209	BCR	C8-C7-C6	-2.26	120.94	127.28
19	B2	826	CLA	O2A-CGA-O1A	-2.26	117.78	123.56
19	B	826	CLA	CMB-C2B-C3B	2.26	129.05	124.80
19	A1	812	CLA	O2A-CGA-O1A	-2.26	117.78	123.56
19	A2	841	CLA	CMD-C2D-C3D	2.26	129.04	124.80
19	X	101	CLA	CMD-C2D-C3D	2.26	129.04	124.80
23	BB	842	BCR	C27-C26-C25	2.26	126.04	122.74
23	F	304	BCR	C27-C26-C25	2.26	126.04	122.74
23	B1	838	BCR	C24-C23-C22	-2.26	122.81	126.21
19	L	204	CLA	C6-C5-C3	2.26	118.44	113.01
19	JJ	103	CLA	CMD-C2D-C3D	2.26	129.04	124.80
19	A2	831	CLA	C1D-CHD-C4C	2.26	125.58	122.48
19	B	834	CLA	C4-C3-C2	-2.26	117.80	123.68
19	A2	827	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	B2	824	CLA	O2A-CGA-O1A	-2.26	117.79	123.56
23	A1	851	BCR	C15-C16-C17	-2.26	118.76	123.51
23	F2	303	BCR	C15-C16-C17	-2.26	118.76	123.51
19	AA	832	CLA	C1D-CHD-C4C	2.26	125.57	122.48
23	MM	101	BCR	C8-C7-C6	-2.26	120.95	127.28
19	B	815	CLA	C1B-CHB-C4A	-2.26	125.64	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	L1	207	CLA	O2A-CGA-O1A	-2.26	117.79	123.56
19	A1	824	CLA	CHB-C4A-NA	2.26	127.64	124.51
19	A	852	CLA	C6-C5-C3	2.26	118.43	113.01
19	A2	852	CLA	O2D-CGD-O1D	-2.26	119.37	123.83
19	A2	829	CLA	C4-C3-C2	-2.26	117.81	123.68
23	J	102	BCR	C35-C13-C14	-2.26	119.76	122.92
19	B2	821	CLA	O2A-CGA-O1A	-2.26	117.80	123.56
19	B1	828	CLA	C1D-CHD-C4C	2.26	125.57	122.48
19	B2	829	CLA	CMD-C2D-C3D	2.26	129.03	124.80
19	AA	828	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
19	J2	101	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
19	A2	830	CLA	CMD-C2D-C3D	2.26	129.03	124.80
23	B	840	BCR	C33-C5-C6	-2.26	122.00	124.51
22	AA	846	LHG	P-O3-C3	-2.26	108.46	121.68
19	B1	848	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	B2	815	CLA	CMD-C2D-C3D	2.25	129.03	124.80
19	A	809	CLA	C1B-CHB-C4A	-2.25	125.65	130.12
19	B1	801	CLA	O2A-CGA-O1A	-2.25	117.80	123.56
25	B	851	LMG	O1-C1-C2	-2.25	104.67	108.26
19	A1	818	CLA	CHB-C4A-NA	2.25	127.63	124.51
23	II	101	BCR	C16-C15-C14	-2.25	118.78	123.51
19	B1	804	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	I2	102	BCR	C8-C7-C6	-2.25	120.97	127.28
19	A1	828	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	J2	103	CLA	C1D-CHD-C4C	2.25	125.56	122.48
19	J1	101	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
23	AA	855	BCR	C20-C21-C22	-2.25	124.10	127.31
19	A	831	CLA	C1D-CHD-C4C	2.25	125.56	122.48
19	AA	843	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	BB	845	CLA	C1D-CHD-C4C	2.25	125.56	122.48
19	B	834	CLA	CMD-C2D-C3D	2.25	129.02	124.80
19	FF	305	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	A2	834	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	B1	802	CLA	CMB-C2B-C3B	2.25	129.02	124.80
19	A1	804	CLA	C5-C3-C2	2.25	125.73	121.11
19	A	852	CLA	OBD-CAD-CBD	-2.25	122.61	125.91
22	X	102	LHG	P-O3-C3	-2.25	108.50	121.68
19	AA	825	CLA	C1D-CHD-C4C	2.25	125.56	122.48
19	BB	801	CLA	CMD-C2D-C3D	2.25	129.01	124.80
19	A2	822	CLA	CMB-C2B-C3B	2.25	129.01	124.80
19	B	813	CLA	O2D-CGD-CBD	2.25	115.19	111.25
19	A2	833	CLA	C1B-CHB-C4A	-2.25	125.67	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	830	CLA	C1D-CHD-C4C	2.25	125.56	122.48
19	B2	815	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
19	A	834	CLA	CHB-C4A-NA	2.25	127.62	124.51
19	A	816	CLA	C1-C2-C3	-2.24	123.12	126.75
23	J1	102	BCR	C27-C26-C25	2.24	126.01	122.74
19	A	819	CLA	O2A-CGA-O1A	-2.24	117.83	123.56
19	BB	831	CLA	CMD-C2D-C3D	2.24	129.01	124.80
22	X2	102	LHG	P-O3-C3	-2.24	108.52	121.68
23	AA	850	BCR	C7-C8-C9	-2.24	122.84	126.21
19	A	804	CLA	C1-C2-C3	-2.24	122.16	126.04
19	A1	811	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	BB	805	CLA	O2A-CGA-O1A	-2.24	117.83	123.56
23	B	839	BCR	C7-C8-C9	-2.24	122.84	126.21
23	L2	207	BCR	C8-C7-C6	-2.24	121.00	127.28
19	A	804	CLA	C1B-CHB-C4A	-2.24	125.67	130.12
19	B2	801	CLA	CMD-C2D-C3D	2.24	129.01	124.80
25	B1	846	LMG	O3-C3-C2	-2.24	105.14	110.34
19	AA	829	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	I1	101	BCR	C27-C26-C25	2.24	126.01	122.74
19	BB	832	CLA	CHA-C1A-NA	-2.24	121.26	126.40
26	B1	840	ECH	C33-C5-C4	2.24	117.77	113.57
19	B2	818	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	B	821	CLA	C4-C3-C2	-2.24	117.85	123.68
19	A2	823	CLA	O2A-CGA-O1A	-2.24	117.83	123.56
23	F	305	BCR	C27-C26-C25	2.24	126.01	122.74
19	LL	203	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	B2	801	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	B1	815	CLA	C4-C3-C2	-2.24	117.85	123.68
19	A1	821	CLA	CMB-C2B-C3B	2.24	129.00	124.80
19	A1	804	CLA	CHB-C4A-NA	2.24	127.61	124.51
19	J1	101	CLA	CHB-C4A-NA	2.24	127.61	124.51
23	B1	838	BCR	C15-C16-C17	-2.24	118.80	123.51
23	A2	848	BCR	C38-C26-C25	-2.24	122.02	124.51
23	AA	850	BCR	C33-C5-C6	-2.24	122.02	124.51
19	B	824	CLA	O2A-CGA-O1A	-2.24	117.84	123.56
19	B2	830	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	L2	206	CLA	O2D-CGD-O1D	-2.24	119.41	123.83
19	A1	840	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	A1	822	CLA	O2A-CGA-O1A	-2.24	117.84	123.56
19	AA	808	CLA	CMD-C2D-C3D	2.24	129.00	124.80
23	I	102	BCR	C15-C16-C17	-2.24	118.80	123.51
19	A2	837	CLA	C1B-CHB-C4A	-2.24	125.68	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	817	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
24	L1	204	AJP	CBJ-CCB-CCA	2.24	118.26	113.00
19	B	814	CLA	C1D-CHD-C4C	2.24	125.54	122.48
19	L	204	CLA	C1D-CHD-C4C	2.24	125.54	122.48
19	AA	818	CLA	CMD-C2D-C3D	2.24	129.00	124.80
19	X2	101	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
26	B2	841	ECH	C33-C5-C4	2.24	117.76	113.57
19	B	826	CLA	O2D-CGD-CBD	2.24	115.17	111.25
23	B	843	BCR	C27-C26-C25	2.24	126.00	122.74
25	B2	847	LMG	O3-C3-C2	-2.24	105.15	110.34
19	A	818	CLA	CMB-C2B-C1B	-2.24	125.03	128.46
19	F2	302	CLA	CMB-C2B-C3B	2.24	128.99	124.80
19	A1	834	CLA	CMD-C2D-C3D	2.24	128.99	124.80
23	FF	304	BCR	C37-C22-C21	-2.24	119.79	122.92
23	F	303	BCR	C15-C16-C17	-2.24	118.81	123.51
23	J2	102	BCR	C33-C5-C6	-2.24	122.02	124.51
19	A1	822	CLA	CMD-C2D-C3D	2.24	128.99	124.80
23	BB	843	BCR	C15-C16-C17	-2.23	118.81	123.51
19	BB	808	CLA	CMD-C2D-C3D	2.23	128.99	124.80
19	A	804	CLA	CMB-C2B-C3B	2.23	128.99	124.80
19	A2	836	CLA	CMB-C2B-C3B	2.23	128.99	124.80
19	A2	835	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	A	830	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	A2	812	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
23	I2	101	BCR	C2-C1-C6	2.23	113.94	110.48
23	K2	103	BCR	C15-C16-C17	-2.23	118.81	123.51
23	I2	101	BCR	C27-C26-C25	2.23	126.00	122.74
19	J1	103	CLA	C1D-CHD-C4C	2.23	125.54	122.48
24	L2	203	AJP	CCJ-CBN-CBO	-2.23	96.32	100.22
23	A1	847	BCR	C8-C7-C6	-2.23	121.02	127.28
19	A	825	CLA	CMD-C2D-C3D	2.23	128.99	124.80
19	BB	804	CLA	CMB-C2B-C3B	2.23	128.99	124.80
24	L2	203	AJP	CCX-OCY-CCZ	2.23	118.79	115.33
19	L	202	CLA	C1D-CHD-C4C	2.23	125.54	122.48
19	B1	806	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	J1	103	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
19	XX	101	CLA	CMD-C2D-C3D	2.23	128.99	124.80
19	B2	814	CLA	CMB-C2B-C3B	2.23	128.99	124.80
19	B	814	CLA	C4-C3-C5	-2.23	111.44	115.29
19	A	818	CLA	CMD-C2D-C3D	2.23	128.99	124.80
19	B1	818	CLA	CHB-C4A-NA	2.23	127.60	124.51
19	A1	818	CLA	C1B-CHB-C4A	-2.23	125.70	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	808	CLA	CHB-C4A-NA	2.23	127.60	124.51
23	A2	847	BCR	C15-C16-C17	-2.23	118.82	123.51
19	AA	820	CLA	CBA-CAA-C2A	2.23	120.49	113.85
19	B	810	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	B1	825	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	L2	207	BCR	C27-C26-C25	2.23	125.99	122.74
19	B1	816	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
19	A2	824	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
23	KK	103	BCR	C16-C15-C14	-2.23	118.82	123.51
23	I1	101	BCR	C16-C15-C14	-2.23	118.82	123.51
19	A	820	CLA	C1-C2-C3	-2.23	122.19	126.04
19	B2	808	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	B1	835	CLA	O2A-CGA-O1A	-2.23	117.86	123.56
22	B	852	LHG	P-O3-C3	-2.23	108.61	121.68
23	J2	102	BCR	C8-C7-C6	-2.23	121.03	127.28
23	FF	303	BCR	C38-C26-C25	-2.23	122.03	124.51
23	A1	848	BCR	C2-C1-C6	2.23	113.93	110.48
23	A2	848	BCR	C2-C1-C6	2.23	113.93	110.48
19	AA	829	CLA	C4-C3-C2	-2.23	117.89	123.68
19	AA	823	CLA	C5-C3-C2	2.23	125.69	121.11
19	A	826	CLA	C1D-CHD-C4C	2.23	125.53	122.48
19	A2	821	CLA	CAC-C3C-C4C	2.23	127.73	124.82
19	J	101	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
25	B1	852	LMG	O3-C3-C2	-2.23	105.17	110.34
19	B	813	CLA	CMB-C2B-C3B	2.23	128.98	124.80
19	A1	813	CLA	CHB-C4A-NA	2.23	127.59	124.51
19	AA	806	CLA	O2A-CGA-O1A	-2.23	117.87	123.56
19	AA	801	CLA	CMB-C2B-C1B	-2.23	125.04	128.46
19	A2	837	CLA	C1D-CHD-C4C	2.23	125.53	122.48
25	B2	854	LMG	O3-C3-C2	-2.23	105.18	110.34
23	B2	840	BCR	C29-C30-C25	2.23	113.93	110.48
19	A	806	CLA	O2A-CGA-O1A	-2.23	117.87	123.56
19	AA	843	CLA	CBC-CAC-C3C	2.23	118.61	112.43
19	A2	806	CLA	O2A-CGA-O1A	-2.23	117.87	123.56
19	B2	805	CLA	C1D-CHD-C4C	2.23	125.53	122.48
19	A	844	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	A2	841	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	F1	302	CLA	CMB-C2B-C3B	2.23	128.97	124.80
19	A	819	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	BB	830	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	A	840	CLA	C1B-CHB-C4A	-2.23	125.71	130.12
19	AA	837	CLA	CMD-C2D-C3D	2.22	128.97	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	844	CLA	CMB-C2B-C3B	2.22	128.97	124.80
19	BB	815	CLA	CMD-C2D-C3D	2.22	128.97	124.80
26	B	841	ECH	C7-C6-C5	-2.22	116.08	121.48
19	L2	204	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
19	AA	801	CLA	O2A-CGA-O1A	-2.22	117.88	123.56
24	BB	849	AJP	CBM-CBN-CBO	-2.22	111.81	115.48
19	A	819	CLA	CMD-C2D-C3D	2.22	128.97	124.80
19	B2	803	CLA	C11-C12-C13	-2.22	108.84	115.77
19	B2	836	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
19	A1	804	CLA	CMB-C2B-C1B	-2.22	125.05	128.46
19	B2	846	CLA	OBD-CAD-C3D	2.22	129.43	127.11
19	A	838	CLA	CMD-C2D-C3D	2.22	128.97	124.80
19	B	859	CLA	CMD-C2D-C3D	2.22	128.97	124.80
23	A1	848	BCR	C38-C26-C25	-2.22	122.04	124.51
23	JJ	102	BCR	C11-C10-C9	-2.22	124.14	127.31
19	A	814	CLA	O2D-CGD-O1D	-2.22	119.45	123.83
25	B	845	LMG	O3-C3-C2	-2.22	105.19	110.34
19	B1	807	CLA	C16-C15-C13	-2.22	108.84	115.77
19	A2	836	CLA	O2D-CGD-CBD	2.22	115.14	111.25
19	A1	834	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A	837	CLA	CMD-C2D-C3D	2.22	128.96	124.80
19	BB	809	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
19	BB	826	CLA	C1D-CHD-C4C	2.22	125.52	122.48
23	J1	102	BCR	C35-C13-C14	-2.22	119.81	122.92
24	KK	104	AJP	CBE-CBO-CBP	-2.22	100.16	104.35
19	B2	802	CLA	O2A-CGA-O1A	-2.22	117.89	123.56
19	A	805	CLA	O2D-CGD-CBD	2.22	115.14	111.25
19	A	814	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A1	823	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
25	M	102	LMG	C1-C2-C3	-2.22	105.36	109.98
23	A	854	BCR	C20-C21-C22	-2.22	124.14	127.31
26	B2	841	ECH	C23-C24-C25	-2.22	121.07	127.28
23	J1	102	BCR	C33-C5-C6	-2.22	122.04	124.51
22	X1	102	LHG	P-O3-C3	-2.22	108.68	121.68
19	B1	821	CLA	O2D-CGD-CBD	2.22	115.13	111.25
19	B2	819	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	A2	813	CLA	O2A-CGA-O1A	-2.22	117.90	123.56
24	I2	104	AJP	CAW-CAX-CAY	-2.22	106.98	111.82
19	A	816	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	BB	833	CLA	C4-C3-C5	2.22	119.10	115.29
19	AA	831	CLA	C1D-CHD-C4C	2.22	125.51	122.48
19	L1	205	CLA	C1B-CHB-C4A	-2.22	125.73	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	821	CLA	C1B-CHB-C4A	-2.22	125.73	130.12
19	AA	827	CLA	CHB-C4A-NA	2.22	127.58	124.51
23	A1	849	BCR	C38-C26-C25	-2.22	122.04	124.51
19	A1	842	CLA	CBC-CAC-C3C	2.22	118.58	112.43
23	FF	303	BCR	C15-C16-C17	-2.22	118.85	123.51
19	B1	828	CLA	CHB-C4A-NA	2.22	127.58	124.51
19	A1	817	CLA	CMD-C2D-C3D	2.21	128.95	124.80
23	K1	104	BCR	C2-C1-C6	2.21	113.91	110.48
23	B	840	BCR	C29-C30-C25	2.21	113.91	110.48
24	L2	203	AJP	CAW-CAX-CAY	-2.21	106.99	111.82
19	B1	810	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B	826	CLA	C4-C3-C5	2.21	119.10	115.29
19	A2	836	CLA	C1D-CHD-C4C	2.21	125.51	122.48
23	BB	839	BCR	C15-C16-C17	-2.21	118.86	123.51
19	AA	832	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	A1	809	CLA	CMB-C2B-C3B	2.21	128.95	124.80
23	L	206	BCR	C8-C7-C6	-2.21	121.08	127.28
19	AA	823	CLA	O2A-CGA-O1A	-2.21	117.91	123.56
22	XX	102	LHG	P-O3-C3	-2.21	108.70	121.68
19	B1	818	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	BB	810	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	JJ	101	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B	835	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B1	813	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
19	B1	850	CLA	C2A-C1A-CHA	2.21	127.73	123.86
19	BB	824	CLA	O2A-CGA-O1A	-2.21	117.91	123.56
23	J1	102	BCR	C8-C7-C6	-2.21	121.08	127.28
19	B1	845	CLA	OBD-CAD-C3D	2.21	129.42	127.11
19	AA	832	CLA	CMD-C2D-C3D	2.21	128.95	124.80
19	A2	820	CLA	CMD-C2D-C3D	2.21	128.95	124.80
26	BB	840	ECH	C7-C6-C5	-2.21	116.11	121.48
19	A2	804	CLA	CMB-C2B-C3B	2.21	128.95	124.80
19	AA	807	CLA	C1D-CHD-C4C	2.21	125.51	122.48
19	BB	826	CLA	C16-C15-C13	-2.21	108.87	115.77
19	B	817	CLA	CMD-C2D-C3D	2.21	128.95	124.80
19	AA	825	CLA	CMD-C2D-C3D	2.21	128.95	124.80
19	B2	807	CLA	C1-O2A-CGA	2.21	122.58	116.54
19	B	860	CLA	CMD-C2D-C3D	2.21	128.95	124.80
19	AA	831	CLA	CMD-C2D-C3D	2.21	128.95	124.80
24	B	857	AJP	CBM-CBL-CCH	2.21	116.97	113.12
23	LL	204	BCR	C15-C16-C17	-2.21	118.86	123.51
23	B	839	BCR	C15-C16-C17	-2.21	118.86	123.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A2	820	CLA	O2D-CGD-CBD	2.21	115.12	111.25
19	A2	804	CLA	C1-C2-C3	-2.21	122.22	126.04
19	BB	833	CLA	C4-C3-C2	-2.21	117.93	123.68
23	A	848	BCR	C8-C7-C6	-2.21	121.09	127.28
19	B	808	CLA	CMD-C2D-C3D	2.21	128.94	124.80
24	A1	854	AJP	OCY-CCZ-CDA	-2.21	105.41	109.66
19	BB	802	CLA	CMD-C2D-C3D	2.21	128.94	124.80
19	A1	817	CLA	CMB-C2B-C3B	2.21	128.94	124.80
23	BB	839	BCR	C29-C30-C25	2.21	113.90	110.48
19	A1	801	CLA	O1D-CGD-CBD	2.21	129.06	124.48
19	B2	825	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	A	815	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	B2	814	CLA	C1D-CHD-C4C	2.21	125.50	122.48
19	A	804	CLA	C1D-CHD-C4C	2.21	125.50	122.48
19	J2	103	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
19	A1	844	CLA	C1B-CHB-C4A	-2.21	125.74	130.12
23	M2	102	BCR	C2-C1-C6	2.21	113.90	110.48
19	AA	845	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
23	FF	304	BCR	C20-C21-C22	-2.21	124.16	127.31
23	I2	103	BCR	C15-C14-C13	-2.21	124.16	127.31
23	B	843	BCR	C8-C7-C6	-2.21	121.10	127.28
23	AA	849	BCR	C8-C7-C6	-2.21	121.10	127.28
23	J2	102	BCR	C27-C26-C25	2.21	125.96	122.74
19	L	202	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
19	B	831	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
22	B2	848	LHG	P-O3-C3	-2.21	108.74	121.68
19	B2	810	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
19	A2	811	CLA	CAA-C2A-C1A	-2.21	104.75	111.97
26	B2	841	ECH	C8-C9-C10	2.21	122.33	118.94
19	B1	806	CLA	C1-C2-C3	2.21	129.86	126.04
19	A	824	CLA	C1D-CHD-C4C	2.21	125.50	122.48
19	A	827	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	A	835	CLA	CHB-C4A-NA	2.21	127.56	124.51
19	A	801	CLA	CMB-C2B-C3B	2.21	128.94	124.80
19	AA	838	CLA	CMD-C2D-C3D	2.21	128.94	124.80
23	B	844	BCR	C24-C23-C22	-2.21	122.90	126.21
23	A	851	BCR	C24-C23-C22	-2.21	122.90	126.21
19	B2	831	CLA	C1D-CHD-C4C	2.20	125.50	122.48
19	A1	833	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
19	B2	824	CLA	CMD-C2D-C3D	2.20	128.94	124.80
23	JJ	102	BCR	C35-C13-C14	-2.20	119.83	122.92
22	B	853	LHG	P-O6-C4	-2.20	108.76	121.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	803	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
19	A	831	CLA	CMD-C2D-C3D	2.20	128.93	124.80
19	A2	819	CLA	C1D-CHD-C4C	2.20	125.50	122.48
19	B1	828	CLA	C1B-CHB-C4A	-2.20	125.75	130.12
23	AA	849	BCR	C2-C1-C6	2.20	113.89	110.48
22	A1	845	LHG	P-O3-C3	-2.20	108.76	121.68
19	AA	814	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	A2	818	CLA	CMD-C2D-C3D	2.20	128.93	124.80
23	A2	851	BCR	C15-C16-C17	-2.20	118.88	123.51
23	MM	101	BCR	C7-C8-C9	-2.20	122.90	126.21
23	I1	101	BCR	C2-C1-C6	2.20	113.89	110.48
23	B2	843	BCR	C27-C26-C25	2.20	125.95	122.74
19	A	807	CLA	C1D-CHD-C4C	2.20	125.50	122.48
19	L	203	CLA	C1D-CHD-C4C	2.20	125.50	122.48
19	A2	824	CLA	C1D-CHD-C4C	2.20	125.50	122.48
19	A	805	CLA	CHB-C4A-NA	2.20	127.56	124.51
19	B2	850	CLA	CHB-C4A-NA	2.20	127.56	124.51
25	M	102	LMG	O3-C3-C2	-2.20	105.23	110.34
19	A2	840	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
22	L2	208	LHG	O7-C7-C8	2.20	116.32	111.51
19	B2	852	CLA	C3C-C4C-NC	-2.20	108.10	110.57
19	B	809	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	B	802	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	L2	204	CLA	C4-C3-C5	2.20	119.08	115.29
23	II	104	BCR	C15-C14-C13	-2.20	124.17	127.31
23	L	206	BCR	C15-C16-C17	-2.20	118.89	123.51
19	B1	821	CLA	C5-C3-C2	2.20	125.63	121.11
19	A1	832	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	A2	825	CLA	CMB-C2B-C3B	2.20	128.93	124.80
19	A1	833	CLA	CMB-C2B-C3B	2.20	128.93	124.80
19	B	826	CLA	C16-C15-C13	-2.20	108.91	115.77
23	F2	304	BCR	C20-C21-C22	-2.20	124.17	127.31
24	A1	855	AJP	CBN-CBO-CBE	2.20	128.39	120.59
19	B2	812	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	BB	834	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	A	801	CLA	O2A-CGA-O1A	-2.20	117.94	123.56
19	B2	830	CLA	O2A-CGA-O1A	-2.20	117.94	123.56
19	A2	822	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
19	BB	811	CLA	CMD-C2D-C3D	2.20	128.92	124.80
19	A2	821	CLA	CMB-C2B-C3B	2.20	128.92	124.80
19	LL	202	CLA	CMD-C2D-C3D	2.20	128.92	124.80
19	B1	810	CLA	C1D-CHD-C4C	2.20	125.49	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	834	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
19	B	830	CLA	CHB-C4A-NA	2.20	127.55	124.51
19	B1	812	CLA	C1B-CHB-C4A	-2.20	125.77	130.12
23	JJ	104	BCR	C2-C1-C6	2.20	113.88	110.48
25	BB	844	LMG	O3-C3-C2	-2.19	105.25	110.34
25	B2	845	LMG	O3-C3-C2	-2.19	105.25	110.34
19	BB	831	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
23	B2	842	BCR	C35-C13-C14	-2.19	119.85	122.92
23	A1	853	BCR	C7-C8-C9	-2.19	122.92	126.21
19	B2	818	CLA	CHB-C4A-NA	2.19	127.55	124.51
25	B1	844	LMG	O3-C3-C2	-2.19	105.25	110.34
25	B1	846	LMG	O1-C7-C8	-2.19	105.61	110.90
19	B2	801	CLA	C5-C3-C2	2.19	125.61	121.11
19	A2	805	CLA	O2D-CGD-CBD	2.19	115.09	111.25
24	B	849	AJP	CBH-OBG-CBF	2.19	117.97	113.74
19	BB	806	CLA	C1B-CHB-C4A	-2.19	125.77	130.12
19	AA	837	CLA	O2D-CGD-O1D	-2.19	119.50	123.83
23	A	848	BCR	C2-C1-C6	2.19	113.88	110.48
19	AA	819	CLA	O2A-CGA-O1A	-2.19	117.96	123.56
19	BB	812	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	B1	805	CLA	C1D-CHD-C4C	2.19	125.48	122.48
19	A1	806	CLA	C1D-CHD-C4C	2.19	125.48	122.48
23	A	854	BCR	C28-C27-C26	-2.19	110.18	113.99
24	L1	204	AJP	CCJ-CBN-CBO	-2.19	96.40	100.22
19	L	204	CLA	C1-C2-C3	-2.19	122.25	126.04
23	A2	848	BCR	C8-C7-C6	-2.19	121.14	127.28
23	FF	306	BCR	C35-C13-C12	2.19	121.56	118.09
19	B	836	CLA	O2A-CGA-O1A	-2.19	117.96	123.56
23	K1	106	BCR	C35-C13-C14	-2.19	119.86	122.92
23	A	851	BCR	C15-C16-C17	-2.19	118.91	123.51
25	L1	210	LMG	O3-C3-C2	-2.19	105.26	110.34
19	B2	829	CLA	CHB-C4A-NA	2.19	127.54	124.51
23	M2	102	BCR	C15-C16-C17	-2.19	118.91	123.51
23	A	853	BCR	C38-C26-C25	-2.19	122.07	124.51
24	BB	848	AJP	CBJ-CCB-CCA	2.19	118.14	113.00
19	A2	819	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	FF	301	CLA	CGD-CBD-CAD	-2.19	103.64	110.73
23	L	205	BCR	C8-C7-C6	-2.19	121.15	127.28
19	B	858	CLA	CMD-C2D-C3D	2.19	128.90	124.80
19	A	841	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
23	L1	208	BCR	C8-C7-C6	-2.19	121.15	127.28
19	BB	801	CLA	C2A-C1A-CHA	2.19	127.68	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	815	CLA	CBA-CAA-C2A	2.19	120.36	113.85
19	A	809	CLA	C1-C2-C3	-2.19	123.21	126.75
19	B	833	CLA	CHA-C1A-NA	-2.19	121.39	126.40
19	B1	822	CLA	CMB-C2B-C3B	2.19	128.90	124.80
19	B2	817	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
19	A2	827	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	BB	803	CLA	C11-C12-C13	-2.19	108.95	115.77
19	X1	101	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	A	827	CLA	O2A-CGA-O1A	-2.19	117.97	123.56
19	A2	839	CLA	CMD-C2D-C3D	2.19	128.90	124.80
19	X2	101	CLA	CMD-C2D-C3D	2.19	128.90	124.80
19	A1	824	CLA	CMB-C2B-C3B	2.19	128.90	124.80
23	A	848	BCR	C15-C16-C17	-2.19	118.92	123.51
19	XX	101	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	B	806	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	A	823	CLA	O2A-CGA-O1A	-2.19	117.98	123.56
19	J1	101	CLA	C1D-CHD-C4C	2.19	125.47	122.48
19	A2	844	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	A2	804	CLA	C1B-CHB-C4A	-2.19	125.79	130.12
19	AA	843	CLA	CMD-C2D-C3D	2.18	128.90	124.80
19	A1	844	CLA	CMB-C2B-C3B	2.18	128.90	124.80
23	F	305	BCR	C20-C21-C22	-2.18	124.19	127.31
23	A	847	BCR	C15-C14-C13	-2.18	124.19	127.31
19	AA	841	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
19	A2	807	CLA	C1D-CHD-C4C	2.18	125.47	122.48
19	AA	834	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
19	BB	823	CLA	CMD-C2D-C3D	2.18	128.90	124.80
19	B	831	CLA	C1D-CHD-C4C	2.18	125.47	122.48
19	B1	820	CLA	C1D-CHD-C4C	2.18	125.47	122.48
23	L	205	BCR	C15-C14-C13	-2.18	124.19	127.31
19	A2	805	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	B	823	CLA	C1B-CHB-C4A	-2.18	125.79	130.12
19	B	810	CLA	C1D-CHD-C4C	2.18	125.47	122.48
19	B2	810	CLA	C1D-CHD-C4C	2.18	125.47	122.48
19	L2	206	CLA	C6-C5-C3	2.18	118.25	113.01
19	BB	810	CLA	C6-C5-C3	2.18	118.25	113.01
23	L2	207	BCR	C11-C10-C9	-2.18	124.19	127.31
19	B2	834	CLA	C4-C3-C5	2.18	119.05	115.29
25	II	105	LMG	O2-C2-C1	-2.18	104.74	110.06
23	A1	848	BCR	C8-C7-C6	-2.18	121.17	127.28
23	M1	101	BCR	C15-C16-C17	-2.18	118.92	123.51
26	B	841	ECH	C29-C30-C25	-2.18	107.11	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	BB	851	LHG	O7-C7-C8	2.18	116.27	111.51
19	A2	819	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	BB	819	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	A1	817	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
26	B	841	ECH	C23-C24-C25	-2.18	121.17	127.28
19	B	812	CLA	CMA-C3A-C2A	-2.18	110.91	116.06
19	BB	808	CLA	CHB-C4A-NA	2.18	127.53	124.51
19	B2	807	CLA	C16-C15-C13	-2.18	108.97	115.77
19	A	829	CLA	C4-C3-C2	-2.18	118.01	123.68
23	F	303	BCR	C38-C26-C25	-2.18	122.08	124.51
23	K2	103	BCR	C8-C7-C6	-2.18	121.17	127.28
19	B2	835	CLA	CHB-C4A-NA	2.18	127.53	124.51
25	B	851	LMG	O3-C3-C2	-2.18	105.29	110.34
19	A	813	CLA	O2A-CGA-O1A	-2.18	117.99	123.56
19	A1	815	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	A1	838	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
19	B	817	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
20	A1	802	CL0	C5-C3-C2	-2.18	116.64	121.11
24	A	802	AJP	CBH-OBG-CBF	2.18	117.94	113.74
25	B1	852	LMG	C1-C2-C3	-2.18	105.44	109.98
23	J2	102	BCR	C35-C13-C14	-2.18	119.87	122.92
19	BB	835	CLA	C1D-CHD-C4C	2.18	125.46	122.48
23	II	104	BCR	C8-C7-C6	-2.18	121.18	127.28
19	B	832	CLA	CMD-C2D-C3D	2.18	128.88	124.80
19	B2	820	CLA	CMD-C2D-C3D	2.18	128.88	124.80
19	B	805	CLA	C3A-C2A-C1A	2.18	104.60	101.34
19	BB	816	CLA	C1D-CHD-C4C	2.18	125.46	122.48
19	A1	839	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
19	B1	817	CLA	C1B-CHB-C4A	-2.18	125.81	130.12
19	A2	830	CLA	CAC-C3C-C4C	2.18	127.66	124.82
19	BB	835	CLA	O2A-CGA-O1A	-2.18	118.00	123.56
19	AA	808	CLA	O2D-CGD-O1D	-2.18	119.53	123.83
19	L1	207	CLA	C6-C5-C3	2.18	118.23	113.01
19	BB	810	CLA	C1D-CHD-C4C	2.17	125.46	122.48
23	FF	303	BCR	C15-C14-C13	-2.17	124.21	127.31
25	B1	844	LMG	C40-C39-C38	-2.17	103.20	114.44
19	BB	829	CLA	CMD-C2D-C3D	2.17	128.88	124.80
26	B1	840	ECH	C8-C9-C10	2.17	122.28	118.94
26	B2	841	ECH	C7-C6-C5	-2.17	116.20	121.48
19	A	821	CLA	CAC-C3C-C4C	2.17	127.66	124.82
19	X	101	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
23	BB	838	BCR	C8-C7-C6	-2.17	121.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	805	CLA	C1D-CHD-C4C	2.17	125.46	122.48
19	AA	827	CLA	O2A-CGA-O1A	-2.17	118.01	123.56
23	A2	849	BCR	C15-C16-C17	-2.17	118.94	123.51
23	I2	101	BCR	C16-C15-C14	-2.17	118.94	123.51
23	J2	104	BCR	C15-C16-C17	-2.17	118.94	123.51
19	B	832	CLA	C1B-CHB-C4A	-2.17	125.81	130.12
19	B1	813	CLA	O2D-CGD-CBD	2.17	115.05	111.25
24	A1	855	AJP	CCF-CCE-CCZ	2.17	113.89	111.36
19	BB	826	CLA	C3A-C2A-C1A	2.17	104.59	101.34
19	B	860	CLA	CMB-C2B-C1B	-2.17	125.13	128.46
19	AA	804	CLA	CMB-C2B-C3B	2.17	128.87	124.80
19	L	203	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	AA	854	BCR	C38-C26-C25	-2.17	122.09	124.51
24	KK	104	AJP	CBD-CBN-CCJ	2.17	117.01	111.69
19	A1	814	CLA	CMD-C2D-C3D	2.17	128.87	124.80
19	AA	835	CLA	CMD-C2D-C3D	2.17	128.87	124.80
28	B	856	DGD	C1D-C2D-C3D	-2.17	105.46	109.98
19	AA	835	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	A1	851	BCR	C8-C7-C6	-2.17	121.20	127.28
19	B	816	CLA	O2A-CGA-O1A	-2.17	118.02	123.56
19	BB	831	CLA	O2D-CGD-CBD	2.17	115.05	111.25
19	B1	816	CLA	CHB-C4A-NA	2.17	127.51	124.51
25	B2	854	LMG	C7-O1-C1	2.17	118.11	113.75
19	A	834	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
19	B1	845	CLA	CAC-C3C-C4C	2.17	127.65	124.82
20	A2	803	CL0	CGD-CBD-CAD	-2.17	103.71	110.73
19	AA	825	CLA	CHB-C4A-NA	2.17	127.51	124.51
23	FF	304	BCR	C8-C7-C6	-2.17	121.21	127.28
25	B	845	LMG	C40-C39-C38	-2.17	103.24	114.44
19	A2	814	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
19	AA	817	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
24	B	850	AJP	CBD-CBN-CCJ	2.17	117.01	111.69
19	B1	832	CLA	CHA-C1A-NA	-2.17	121.44	126.40
19	A	832	CLA	C1D-CHD-C4C	2.17	125.45	122.48
19	KK	102	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	AA	816	CLA	C1-C2-C3	-2.17	123.25	126.75
26	B1	840	ECH	C7-C6-C5	-2.17	116.22	121.48
19	BB	815	CLA	CBA-CAA-C2A	2.17	120.30	113.85
24	L	208	AJP	CBH-OBG-CBF	2.17	117.92	113.74
19	A	810	CLA	C1D-CHD-C4C	2.17	125.45	122.48
25	B2	854	LMG	C1-C2-C3	-2.17	105.46	109.98
24	A2	854	AJP	CCF-CCE-CCZ	2.17	113.89	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	841	ECH	C8-C9-C10	2.17	122.26	118.94
19	A	833	CLA	C1D-CHD-C4C	2.17	125.44	122.48
23	I2	102	BCR	C33-C5-C6	-2.17	122.10	124.51
19	A1	824	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	B1	836	CLA	C1B-CHB-C4A	-2.17	125.83	130.12
19	A2	823	CLA	CMD-C2D-C3D	2.17	128.86	124.80
24	BB	849	AJP	CBE-CBO-CBP	-2.16	100.26	104.35
25	B	851	LMG	O2-C2-C1	-2.16	104.78	110.06
19	BB	845	CLA	CMD-C2D-C3D	2.16	128.86	124.80
19	BB	823	CLA	C1B-CHB-C4A	-2.16	125.83	130.12
22	L1	211	LHG	P-O6-C4	-2.16	108.99	121.68
19	A2	816	CLA	C1D-CHD-C4C	2.16	125.44	122.48
19	AA	813	CLA	O2A-CGA-O1A	-2.16	118.04	123.56
24	AA	802	AJP	OBG-CBF-CAW	2.16	112.86	110.81
19	B	831	CLA	CMD-C2D-C3D	2.16	128.85	124.80
22	A2	846	LHG	P-O6-C4	-2.16	109.00	121.68
25	II	105	LMG	O3-C3-C2	-2.16	105.33	110.34
19	B	829	CLA	C1D-CHD-C4C	2.16	125.44	122.48
19	B1	845	CLA	CMD-C2D-C3D	2.16	128.85	124.80
19	A	834	CLA	CMB-C2B-C3B	2.16	128.85	124.80
23	AA	848	BCR	C38-C26-C25	-2.16	122.10	124.51
19	B1	810	CLA	C5-C3-C2	2.16	125.55	121.11
19	BB	805	CLA	C3A-C2A-C1A	2.16	104.57	101.34
19	A2	805	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
23	M1	101	BCR	C27-C26-C25	2.16	125.89	122.74
23	B	842	BCR	C1-C6-C5	-2.16	119.57	122.59
19	A	821	CLA	C1D-CHD-C4C	2.16	125.44	122.48
19	B1	826	CLA	O2A-CGA-O1A	-2.16	118.05	123.56
24	L	208	AJP	OBG-CBF-CAW	2.16	112.85	110.81
19	AA	809	CLA	CAC-C3C-C4C	2.16	127.64	124.82
24	A2	854	AJP	CBN-CBO-CBE	2.16	128.24	120.59
23	K1	104	BCR	C8-C7-C6	-2.16	121.24	127.28
19	AA	835	CLA	C1D-CHD-C4C	2.16	125.43	122.48
19	A2	816	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	BB	821	CLA	CMB-C2B-C3B	2.16	128.85	124.80
19	B1	822	CLA	CMD-C2D-C3D	2.16	128.85	124.80
24	M2	101	AJP	CDA-CDB-CDC	-2.16	109.30	112.56
23	BB	842	BCR	C8-C7-C6	-2.16	121.24	127.28
19	A	814	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	AA	815	CLA	C1B-CHB-C4A	-2.16	125.84	130.12
19	B2	852	CLA	CBC-CAC-C3C	2.16	118.41	112.43
19	B1	808	CLA	CHB-C4A-NA	2.16	127.49	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	805	CLA	CHB-C4A-NA	2.16	127.49	124.51
23	B1	838	BCR	C27-C26-C25	2.16	125.88	122.74
19	B	809	CLA	C1D-CHD-C4C	2.16	125.43	122.48
19	A2	818	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	B1	808	CLA	CMB-C2B-C3B	2.16	128.84	124.80
19	B2	851	CLA	CMD-C2D-C3D	2.16	128.84	124.80
19	A	805	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	B	854	CLA	C1B-CHB-C4A	-2.16	125.85	130.12
19	A2	833	CLA	CHB-C4A-NA	2.16	127.49	124.51
19	A	842	CLA	O2A-C1-C2	-2.15	102.97	108.64
19	B	846	CLA	OBD-CAD-C3D	2.15	129.36	127.11
26	B	841	ECH	C10-C11-C12	-2.15	116.83	123.31
19	B2	810	CLA	CAC-C3C-C4C	2.15	127.64	124.82
19	B	804	CLA	C1D-CHD-C4C	2.15	125.43	122.48
19	B1	826	CLA	C3A-C2A-C1A	2.15	104.57	101.34
23	B	840	BCR	C15-C16-C17	-2.15	118.98	123.51
19	B2	826	CLA	C1D-CHD-C4C	2.15	125.43	122.48
19	A1	835	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	B1	827	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	A1	810	CLA	CAA-C2A-C1A	-2.15	104.92	111.97
19	B2	837	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	BB	824	CLA	CMD-C2D-C3D	2.15	128.84	124.80
19	K2	104	CLA	C1D-CHD-C4C	2.15	125.43	122.48
19	BB	830	CLA	C1D-CHD-C4C	2.15	125.43	122.48
19	B	813	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
19	FF	302	CLA	C1B-CHB-C4A	-2.15	125.85	130.12
22	LL	205	LHG	P-O6-C4	-2.15	109.06	121.68
22	L	207	LHG	P-O6-C4	-2.15	109.06	121.68
23	AA	849	BCR	C15-C16-C17	-2.15	118.99	123.51
23	A	847	BCR	C38-C26-C25	-2.15	122.11	124.51
23	L1	201	BCR	C24-C23-C22	-2.15	122.98	126.21
19	B2	827	CLA	CMD-C2D-C3D	2.15	128.84	124.80
23	A1	853	BCR	C8-C7-C6	-2.15	121.25	127.28
24	K	104	AJP	CBD-CBN-CCJ	2.15	116.97	111.69
19	B1	814	CLA	C1D-CHD-C4C	2.15	125.42	122.48
23	I	101	BCR	C16-C15-C14	-2.15	118.99	123.51
25	L1	210	LMG	O2-C2-C1	-2.15	104.82	110.06
26	B2	841	ECH	C10-C11-C12	-2.15	116.84	123.31
19	J1	103	CLA	CMD-C2D-C3D	2.15	128.83	124.80
19	A	826	CLA	CMD-C2D-C3D	2.15	128.83	124.80
25	B1	852	LMG	C7-O1-C1	2.15	118.07	113.75
19	A1	829	CLA	CMB-C2B-C3B	2.15	128.83	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B2	839	BCR	C27-C26-C25	2.15	125.87	122.74
19	B	830	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
19	AA	809	CLA	O2A-CGA-O1A	-2.15	118.07	123.56
23	LL	204	BCR	C11-C10-C9	-2.15	124.24	127.31
25	L1	210	LMG	C38-C37-C36	-2.15	103.34	114.44
19	B1	823	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	AA	824	CLA	CMD-C2D-C3D	2.15	128.83	124.80
19	B1	832	CLA	C1D-CHD-C4C	2.15	125.42	122.48
23	AA	850	BCR	C15-C16-C17	-2.15	119.00	123.51
21	B	838	PQN	C26-C25-C23	-2.15	109.07	115.77
25	B1	844	LMG	O2-C2-C1	-2.15	104.83	110.06
19	A2	815	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	B1	835	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
19	B2	815	CLA	CBA-CAA-C2A	2.15	120.24	113.85
19	AA	840	CLA	CMB-C2B-C1B	-2.15	125.17	128.46
19	B1	815	CLA	C1B-CHB-C4A	-2.15	125.87	130.12
19	B2	851	CLA	C2A-C1A-CHA	2.15	127.61	123.86
23	M1	101	BCR	C7-C8-C9	-2.15	122.99	126.21
19	B2	846	CLA	CMD-C2D-C3D	2.14	128.82	124.80
19	A2	809	CLA	CMD-C2D-C3D	2.14	128.82	124.80
19	A1	818	CLA	C1D-CHD-C4C	2.14	125.42	122.48
19	A	839	CLA	O2D-CGD-CBD	2.14	115.01	111.25
28	B	856	DGD	O6E-C1E-O5D	-2.14	104.88	109.94
19	AA	833	CLA	C1B-CHB-C4A	-2.14	125.87	130.12
19	F	302	CLA	CMB-C2B-C3B	2.14	128.82	124.80
19	A2	802	CLA	CMD-C2D-C3D	2.14	128.82	124.80
19	A2	818	CLA	CMB-C2B-C3B	2.14	128.82	124.80
23	A1	850	BCR	C2-C1-C6	2.14	113.80	110.48
23	A2	853	BCR	C8-C7-C6	-2.14	121.28	127.28
22	A1	846	LHG	P-O6-C4	-2.14	109.11	121.68
19	A	809	CLA	CAC-C3C-C4C	2.14	127.62	124.82
19	A	822	CLA	C1D-CHD-C4C	2.14	125.41	122.48
19	A	808	CLA	CED-O2D-CGD	2.14	120.84	115.95
19	A1	804	CLA	O2D-CGD-CBD	2.14	115.00	111.25
19	L	203	CLA	C1-O2A-CGA	2.14	122.39	116.54
19	AA	837	CLA	C1D-CHD-C4C	2.14	125.41	122.48
19	AA	810	CLA	C1D-CHD-C4C	2.14	125.41	122.48
26	B1	840	ECH	C10-C11-C12	-2.14	116.87	123.31
19	A	817	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	AA	843	CLA	C3C-C4C-NC	-2.14	108.17	110.57
19	A1	814	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	F1	302	CLA	C1B-CHB-C4A	-2.14	125.88	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	828	CLA	C4-C3-C2	-2.14	118.11	123.68
19	A	816	CLA	CMB-C2B-C3B	2.14	128.81	124.80
23	L	205	BCR	C11-C10-C9	-2.14	124.26	127.31
23	I	102	BCR	C24-C23-C22	-2.14	123.00	126.21
19	BB	817	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	B1	804	CLA	CBA-CAA-C2A	2.14	120.22	113.85
23	A	848	BCR	C16-C15-C14	-2.14	119.01	123.51
19	B	805	CLA	C1D-CHD-C4C	2.14	125.41	122.48
19	B2	825	CLA	CMD-C2D-C3D	2.14	128.81	124.80
19	A	830	CLA	O2A-CGA-O1A	-2.14	118.09	123.56
19	BB	828	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
23	A2	849	BCR	C38-C26-C25	-2.14	122.13	124.51
23	AA	850	BCR	C3-C4-C5	-2.14	110.27	113.99
24	B	857	AJP	CDD-CDC-CDB	2.14	116.21	111.87
19	B	804	CLA	CBA-CAA-C2A	2.14	120.21	113.85
23	AA	854	BCR	C11-C10-C9	-2.14	124.26	127.31
19	F2	302	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
19	A	832	CLA	OBD-CAD-CBD	-2.14	122.77	125.91
19	B2	836	CLA	O2A-CGA-O1A	-2.14	118.10	123.56
25	BB	844	LMG	O2-C2-C1	-2.14	104.85	110.06
19	B2	804	CLA	CBA-CAA-C2A	2.14	120.21	113.85
22	AA	847	LHG	P-O6-C4	-2.14	109.16	121.68
19	B	817	CLA	O2D-CGD-CBD	2.14	114.99	111.25
19	A1	836	CLA	C1D-CHD-C4C	2.14	125.40	122.48
23	B	839	BCR	C8-C7-C6	-2.14	121.30	127.28
23	A	849	BCR	C38-C26-C25	-2.13	122.13	124.51
19	B2	813	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
23	K2	103	BCR	C2-C1-C6	2.13	113.78	110.48
26	B	841	ECH	C23-C22-C21	-2.13	115.67	118.94
19	BB	816	CLA	O2A-CGA-O1A	-2.13	118.11	123.56
19	BB	809	CLA	C1D-CHD-C4C	2.13	125.40	122.48
23	A2	850	BCR	C2-C1-C6	2.13	113.78	110.48
19	B2	808	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
19	BB	822	CLA	O2D-CGD-CBD	2.13	114.99	111.25
19	L1	206	CLA	C1D-CHD-C4C	2.13	125.40	122.48
19	B2	801	CLA	O2A-CGA-O1A	-2.13	118.11	123.56
24	BB	848	AJP	OCD-CCE-CCZ	-2.13	105.60	109.98
19	B	835	CLA	O2D-CGD-CBD	2.13	114.98	111.25
19	A	833	CLA	C1B-CHB-C4A	-2.13	125.89	130.12
19	BB	855	CLA	CHB-C4A-NA	2.13	127.46	124.51
23	A	851	BCR	C8-C7-C6	-2.13	121.31	127.28
23	BB	841	BCR	C1-C6-C5	-2.13	119.61	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	I2	102	BCR	C37-C22-C21	-2.13	119.94	122.92
25	B2	845	LMG	O2-C2-C1	-2.13	104.86	110.06
19	BB	829	CLA	CHB-C4A-NA	2.13	127.46	124.51
19	BB	804	CLA	C1D-CHD-C4C	2.13	125.40	122.48
23	AA	850	BCR	C38-C26-C25	-2.13	122.14	124.51
23	B	839	BCR	C35-C13-C14	-2.13	119.94	122.92
28	BB	854	DGD	O3E-C3E-C2E	-2.13	105.40	110.34
19	B	813	CLA	C1D-CHD-C4C	2.13	125.40	122.48
19	B1	826	CLA	C1D-CHD-C4C	2.13	125.39	122.48
19	B2	811	CLA	C1D-CHD-C4C	2.13	125.39	122.48
19	B1	819	CLA	C1D-CHD-C4C	2.13	125.39	122.48
19	B	816	CLA	C1D-CHD-C4C	2.13	125.39	122.48
19	B	810	CLA	C6-C5-C3	2.13	118.12	113.01
22	A	846	LHG	P-O6-C4	-2.13	109.20	121.68
19	B2	830	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	B	818	CLA	C1D-CHD-C4C	2.13	125.39	122.48
24	B	857	AJP	OCY-CCZ-CDA	-2.13	105.56	109.66
19	L	204	CLA	CHB-C4A-NA	2.13	127.45	124.51
19	BB	836	CLA	CMB-C2B-C3B	2.13	128.79	124.80
19	B	815	CLA	CMD-C2D-C3D	2.13	128.79	124.80
19	B1	835	CLA	CMD-C2D-C3D	2.13	128.79	124.80
19	BB	804	CLA	CBA-CAA-C2A	2.13	120.18	113.85
25	B	851	LMG	C38-C37-C36	-2.13	103.45	114.44
19	A1	819	CLA	C1-C2-C3	-2.13	122.37	126.04
19	B1	816	CLA	C1D-CHD-C4C	2.13	125.39	122.48
23	A2	847	BCR	C21-C20-C19	-2.13	119.31	124.68
26	B1	840	ECH	C23-C24-C25	-2.13	121.33	127.28
19	F1	305	CLA	C1B-CHB-C4A	-2.13	125.91	130.12
19	A	821	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	B	844	BCR	C38-C26-C25	-2.12	122.14	124.51
19	AA	805	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
19	AA	830	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
23	K1	106	BCR	C20-C21-C22	-2.12	124.28	127.31
24	L2	202	AJP	CBD-CBN-CCJ	2.12	116.90	111.69
19	J	103	CLA	CMD-C2D-C3D	2.12	128.78	124.80
19	B	801	CLA	CBA-CAA-C2A	2.12	120.17	113.85
19	B	834	CLA	C6-C7-C8	-2.12	109.14	115.77
23	A1	847	BCR	C16-C15-C14	-2.12	119.05	123.51
19	A1	813	CLA	C1B-CHB-C4A	-2.12	125.91	130.12
19	J	103	CLA	CAC-C3C-C4C	2.12	127.59	124.82
23	B2	839	BCR	C38-C26-C25	-2.12	122.14	124.51
19	B	822	CLA	CMB-C2B-C3B	2.12	128.78	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	805	CLA	C3A-C2A-C1A	2.12	104.52	101.34
19	B	826	CLA	C1D-CHD-C4C	2.12	125.39	122.48
25	I2	105	LMG	C1-C2-C3	-2.12	105.55	109.98
23	AA	848	BCR	C15-C14-C13	-2.12	124.28	127.31
19	BB	830	CLA	O2A-CGA-O1A	-2.12	118.14	123.56
23	A	853	BCR	C8-C7-C6	-2.12	121.33	127.28
23	AA	855	BCR	C15-C16-C17	-2.12	119.05	123.51
23	M2	102	BCR	C27-C26-C25	2.12	125.83	122.74
23	K2	105	BCR	C35-C13-C14	-2.12	119.95	122.92
19	A2	815	CLA	C1D-CHD-C4C	2.12	125.39	122.48
19	FF	305	CLA	C1D-CHD-C4C	2.12	125.39	122.48
19	K1	103	CLA	CMD-C2D-C3D	2.12	128.78	124.80
19	A1	803	CLA	CMB-C2B-C3B	2.12	128.78	124.80
19	A1	824	CLA	C1D-CHD-C4C	2.12	125.38	122.48
19	A	817	CLA	CMB-C2B-C3B	2.12	128.78	124.80
19	B2	807	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	AA	818	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	AA	811	CLA	CAA-C2A-C1A	-2.12	105.03	111.97
19	A	816	CLA	C1D-CHD-C4C	2.12	125.38	122.48
19	B2	852	CLA	CMD-C2D-C3D	2.12	128.78	124.80
23	BB	838	BCR	C11-C10-C9	-2.12	124.28	127.31
19	B	836	CLA	C1D-CHD-C4C	2.12	125.38	122.48
23	L	206	BCR	C16-C15-C14	-2.12	119.06	123.51
19	B	828	CLA	C1B-CHB-C4A	-2.12	125.92	130.12
19	BB	811	CLA	C1D-CHD-C4C	2.12	125.38	122.48
19	B1	821	CLA	C4-C3-C2	-2.12	118.17	123.68
19	A2	824	CLA	CMD-C2D-C3D	2.12	128.77	124.80
19	B	815	CLA	C4-C3-C2	-2.12	118.17	123.68
19	BB	856	CLA	C4-C3-C5	2.12	118.93	115.29
19	B	859	CLA	C1D-CHD-C4C	2.12	125.38	122.48
19	B1	805	CLA	C3A-C2A-C1A	2.12	104.51	101.34
23	I2	101	BCR	C16-C17-C18	-2.12	124.29	127.31
19	B1	849	CLA	CHB-C4A-NA	2.12	127.44	124.51
23	AA	848	BCR	C21-C20-C19	-2.12	119.33	124.68
19	B2	852	CLA	CMB-C2B-C1B	-2.12	125.21	128.46
19	B1	802	CLA	C1D-CHD-C4C	2.12	125.38	122.48
19	AA	822	CLA	C1B-CHB-C4A	-2.12	125.93	130.12
25	B	845	LMG	O2-C2-C1	-2.12	104.90	110.06
19	A1	803	CLA	C1D-CHD-C4C	2.11	125.38	122.48
19	B1	815	CLA	CBA-CAA-C2A	2.11	120.14	113.85
23	L1	208	BCR	C37-C22-C21	-2.11	119.96	122.92
19	A2	837	CLA	CHB-C4A-NA	2.11	127.44	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	839	CLA	CMD-C2D-C3D	2.11	128.76	124.80
19	AA	808	CLA	C1B-CHB-C4A	-2.11	125.93	130.12
24	A	802	AJP	OBG-CBF-CAW	2.11	112.81	110.81
19	A	801	CLA	O1D-CGD-CBD	2.11	128.86	124.48
19	BB	830	CLA	CMD-C2D-C3D	2.11	128.76	124.80
19	B2	822	CLA	C1D-CHD-C4C	2.11	125.37	122.48
23	AA	854	BCR	C7-C8-C9	-2.11	123.04	126.21
19	AA	853	CLA	CMD-C2D-C3D	2.11	128.76	124.80
19	F	302	CLA	C1B-CHB-C4A	-2.11	125.94	130.12
25	B2	854	LMG	O2-C2-C1	-2.11	104.91	110.06
19	B2	802	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	A2	830	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	B2	837	CLA	O2A-CGA-O1A	-2.11	118.17	123.56
19	BB	845	CLA	OBD-CAD-C3D	2.11	129.31	127.11
19	B1	833	CLA	C4-C3-C2	-2.11	118.19	123.68
19	A1	808	CLA	CMD-C2D-C3D	2.11	128.76	124.80
19	B	811	CLA	CMD-C2D-C3D	2.11	128.76	124.80
28	B	856	DGD	O3E-C3E-C2E	-2.11	105.45	110.34
19	BB	806	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	AA	841	CLA	O2D-CGD-CBD	2.11	114.94	111.25
19	AA	853	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	FF	301	CLA	OBD-CAD-CBD	-2.11	122.81	125.91
19	A1	834	CLA	C11-C10-C8	-2.11	109.19	115.77
19	B1	801	CLA	CMD-C2D-C3D	2.11	128.75	124.80
19	A1	814	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	B	819	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	AA	821	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	B1	811	CLA	C1D-CHD-C4C	2.11	125.37	122.48
23	B1	838	BCR	C38-C26-C25	-2.11	122.16	124.51
19	B2	803	CLA	C1D-CHD-C4C	2.11	125.37	122.48
19	A	808	CLA	CMD-C2D-C3D	2.11	128.75	124.80
23	L1	208	BCR	C15-C14-C13	-2.11	124.30	127.31
19	A	834	CLA	C1D-CHD-C4C	2.11	125.36	122.48
19	BB	817	CLA	C1D-CHD-C4C	2.11	125.36	122.48
23	F	303	BCR	C15-C14-C13	-2.11	124.30	127.31
19	AA	824	CLA	C1D-CHD-C4C	2.11	125.36	122.48
19	B	801	CLA	C1D-CHD-C4C	2.11	125.36	122.48
19	B1	808	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
19	B1	850	CLA	C1D-CHD-C4C	2.11	125.36	122.48
19	B	819	CLA	C1B-CHB-C4A	-2.11	125.95	130.12
23	B2	844	BCR	C38-C26-C25	-2.11	122.17	124.51
19	B	858	CLA	CHB-C4A-NA	2.11	127.42	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	850	BCR	C27-C26-C25	2.10	125.81	122.74
19	K	102	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
23	L1	201	BCR	C8-C7-C6	-2.10	121.38	127.28
19	B2	846	CLA	CAC-C3C-C4C	2.10	127.57	124.82
19	B	812	CLA	O1D-CGD-CBD	2.10	128.84	124.48
23	I2	103	BCR	C8-C7-C6	-2.10	121.39	127.28
23	B2	844	BCR	C15-C16-C17	-2.10	119.09	123.51
23	AA	854	BCR	C8-C7-C6	-2.10	121.39	127.28
19	B1	830	CLA	C1D-CHD-C4C	2.10	125.36	122.48
20	A2	803	CL0	O2A-C1-C2	2.10	114.16	108.64
19	B	812	CLA	C1B-CHB-C4A	-2.10	125.95	130.12
19	A1	821	CLA	O2D-CGD-CBD	2.10	114.93	111.25
23	L1	209	BCR	C24-C23-C22	-2.10	123.05	126.21
19	A2	826	CLA	C1D-CHD-C4C	2.10	125.36	122.48
23	B1	843	BCR	C15-C16-C17	-2.10	119.09	123.51
23	AA	852	BCR	C33-C5-C6	-2.10	122.17	124.51
23	F	304	BCR	C8-C7-C6	-2.10	121.39	127.28
25	L1	210	LMG	O1-C1-C2	-2.10	104.92	108.26
19	A2	815	CLA	CMD-C2D-C3D	2.10	128.74	124.80
24	B	849	AJP	CBD-CBN-CCJ	2.10	116.84	111.69
20	A2	803	CL0	C9-C8-C7	2.10	118.96	111.30
19	B2	809	CLA	C1D-CHD-C4C	2.10	125.36	122.48
19	AA	814	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B1	824	CLA	CMD-C2D-C3D	2.10	128.74	124.80
19	BB	813	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	A	837	CLA	C1D-CHD-C4C	2.10	125.36	122.48
19	A	807	CLA	C1-C2-C3	-2.10	122.41	126.04
23	A2	849	BCR	C11-C10-C9	-2.10	124.31	127.31
19	B1	819	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B	817	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	A1	832	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	F	301	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	AA	811	CLA	C1D-CHD-C4C	2.10	125.35	122.48
23	F2	304	BCR	C37-C22-C21	-2.10	119.98	122.92
19	B1	832	CLA	CMD-C2D-C3D	2.10	128.74	124.80
24	A	855	AJP	CDA-CDB-CCG	2.10	114.90	112.65
19	A1	839	CLA	C1D-CHD-C4C	2.10	125.35	122.48
25	B1	852	LMG	O2-C2-C1	-2.10	104.94	110.06
19	B2	802	CLA	CMD-C2D-C3D	2.10	128.74	124.80
23	B	839	BCR	C15-C14-C13	-2.10	124.32	127.31
19	A2	839	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	B2	828	CLA	C1B-CHB-C4A	-2.10	125.96	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	LL	201	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
23	A	848	BCR	C27-C26-C25	2.10	125.80	122.74
19	A	808	CLA	C1B-CHB-C4A	-2.10	125.96	130.12
19	FF	301	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
19	B2	833	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	B1	829	CLA	CHB-C4A-NA	2.10	127.41	124.51
19	A	818	CLA	C1B-CHB-C4A	-2.10	125.97	130.12
23	A1	847	BCR	C21-C20-C19	-2.10	119.38	124.68
23	J1	102	BCR	C2-C1-C6	2.10	113.73	110.48
19	B	837	CLA	O2A-CGA-O1A	-2.10	118.20	123.56
19	B2	851	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	BB	802	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	B2	816	CLA	C1D-CHD-C4C	2.10	125.35	122.48
19	A	835	CLA	CMD-C2D-C3D	2.09	128.73	124.80
19	AA	817	CLA	CMB-C2B-C3B	2.09	128.73	124.80
19	A	825	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
23	A1	848	BCR	C27-C26-C25	2.09	125.79	122.74
19	A	811	CLA	C1D-CHD-C4C	2.09	125.35	122.48
24	BB	848	AJP	CAW-CAX-CAY	-2.09	107.25	111.82
19	A2	852	CLA	CMB-C2B-C1B	-2.09	125.25	128.46
19	K2	104	CLA	OBD-CAD-C3D	2.09	129.30	127.11
19	BB	829	CLA	O2A-CGA-O1A	-2.09	118.21	123.56
19	AA	819	CLA	C1D-CHD-C4C	2.09	125.35	122.48
19	B1	836	CLA	O2A-CGA-O1A	-2.09	118.21	123.56
19	A2	811	CLA	C1-O2A-CGA	2.09	122.26	116.54
19	B2	804	CLA	CMD-C2D-C3D	2.09	128.73	124.80
19	BB	856	CLA	O2A-CGA-CBA	2.09	118.65	111.93
19	A1	833	CLA	C1D-CHD-C4C	2.09	125.35	122.48
19	AA	833	CLA	C1D-CHD-C4C	2.09	125.34	122.48
19	B2	833	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
19	B1	829	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
19	A2	808	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
22	B1	847	LHG	P-O6-C4	-2.09	109.42	121.68
19	BB	836	CLA	O2A-CGA-O1A	-2.09	118.22	123.56
19	BB	833	CLA	C6-C7-C8	-2.09	109.25	115.77
19	B	808	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	BB	803	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	B	822	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	AA	825	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	B	860	CLA	C3C-C4C-NC	-2.09	108.23	110.57
28	BB	854	DGD	O6E-C5E-C4E	2.09	113.49	109.68
19	A2	822	CLA	O2D-CGD-CBD	2.09	114.91	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	AA	849	BCR	C27-C26-C25	2.09	125.79	122.74
19	AA	820	CLA	C1-C2-C3	-2.09	122.43	126.04
28	BB	854	DGD	C3G-C2G-C1G	-2.09	106.81	111.79
19	A1	830	CLA	CMD-C2D-C3D	2.09	128.72	124.80
22	B	853	LHG	O7-C7-C8	2.09	116.07	111.51
23	A	849	BCR	C16-C15-C14	-2.09	119.12	123.51
23	A	849	BCR	C24-C23-C22	-2.09	123.07	126.21
25	M	102	LMG	O2-C2-C1	-2.09	104.97	110.06
19	B	827	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
19	BB	818	CLA	C1B-CHB-C4A	-2.09	125.98	130.12
23	A1	849	BCR	C15-C16-C17	-2.09	119.12	123.51
19	BB	819	CLA	CMA-C3A-C2A	-2.09	111.13	116.06
23	A2	851	BCR	C16-C15-C14	-2.09	119.12	123.51
19	B	846	CLA	CMD-C2D-C3D	2.09	128.71	124.80
23	A2	847	BCR	C16-C15-C14	-2.09	119.12	123.51
22	BB	851	LHG	P-O6-C4	-2.09	109.45	121.68
19	B	815	CLA	O2D-CGD-CBD	2.09	114.90	111.25
19	A2	833	CLA	O2D-CGD-CBD	2.09	114.90	111.25
25	BB	844	LMG	C40-C39-C38	-2.09	103.67	114.44
19	A2	837	CLA	CMD-C2D-C3D	2.09	128.71	124.80
23	A	847	BCR	C21-C20-C19	-2.09	119.41	124.68
23	A	853	BCR	C7-C8-C9	-2.08	123.08	126.21
19	A1	816	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	J	101	CLA	C1D-CHD-C4C	2.08	125.33	122.48
23	M	101	BCR	C11-C10-C9	-2.08	124.34	127.31
19	FF	301	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	AA	806	CLA	C1D-CHD-C4C	2.08	125.33	122.48
24	AA	856	AJP	CDA-CDB-CCG	2.08	114.89	112.65
19	BB	827	CLA	C1B-CHB-C4A	-2.08	125.99	130.12
19	A1	842	CLA	C3C-C4C-NC	-2.08	108.24	110.57
24	M2	101	AJP	CBD-CBN-CCJ	2.08	116.80	111.69
19	F2	302	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	L2	205	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	A2	821	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	AA	816	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	AA	812	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	BB	819	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
19	B1	850	CLA	CMD-C2D-C3D	2.08	128.70	124.80
19	A	813	CLA	C1D-CHD-C4C	2.08	125.33	122.48
23	L	206	BCR	C24-C23-C22	-2.08	123.09	126.21
19	L2	206	CLA	C1D-CHD-C4C	2.08	125.33	122.48
23	B	839	BCR	C11-C10-C9	-2.08	124.34	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B2	813	CLA	O2D-CGD-CBD	2.08	114.89	111.25
19	A	839	CLA	C1B-CHB-C4A	-2.08	126.00	130.12
26	B	841	ECH	C35-C13-C14	2.08	125.83	122.92
19	B	808	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
19	B1	815	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	B1	802	CLA	CMD-C2D-C3D	2.08	128.70	124.80
19	AA	815	CLA	C1D-CHD-C4C	2.08	125.33	122.48
19	B1	810	CLA	CAC-C3C-C4C	2.08	127.53	124.82
19	B	804	CLA	CMD-C2D-C3D	2.08	128.70	124.80
23	A	854	BCR	C8-C7-C6	-2.08	121.46	127.28
19	A	811	CLA	CAA-C2A-C1A	-2.08	105.17	111.97
19	AA	822	CLA	C1D-CHD-C4C	2.08	125.32	122.48
19	K1	105	CLA	C2A-C1A-CHA	2.08	125.93	122.71
19	A2	835	CLA	C11-C10-C8	-2.08	109.29	115.77
19	A1	823	CLA	CMD-C2D-C3D	2.08	128.69	124.80
19	BB	807	CLA	C1D-CHD-C4C	2.08	125.32	122.48
23	AA	851	BCR	C27-C26-C25	2.08	125.77	122.74
19	J2	103	CLA	CMD-C2D-C3D	2.08	128.69	124.80
19	AA	813	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	A	832	CLA	CMB-C2B-C3B	2.07	128.69	124.80
19	B2	851	CLA	O2D-CGD-CBD	2.07	114.88	111.25
24	A	855	AJP	CBN-CBO-CBE	2.07	127.95	120.59
23	A	853	BCR	C11-C10-C9	-2.07	124.35	127.31
19	BB	827	CLA	C1D-CHD-C4C	2.07	125.32	122.48
23	L	206	BCR	C10-C11-C12	-2.07	117.07	123.31
19	BB	826	CLA	O2A-CGA-O1A	-2.07	118.26	123.56
24	AA	856	AJP	CBN-CBO-CBE	2.07	127.94	120.59
24	AA	802	AJP	CBH-OBG-CBF	2.07	117.74	113.74
19	AA	834	CLA	C1D-CHD-C4C	2.07	125.32	122.48
23	A2	849	BCR	C8-C7-C6	-2.07	121.47	127.28
19	A2	805	CLA	C5-C3-C2	2.07	125.37	121.11
19	B	803	CLA	C11-C12-C13	-2.07	109.30	115.77
20	A	803	CL0	C9-C8-C10	2.07	118.86	111.30
19	A2	823	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	FF	302	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	F	302	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	B2	827	CLA	C1D-CHD-C4C	2.07	125.32	122.48
25	BB	844	LMG	O1-C1-C2	-2.07	104.96	108.26
19	B1	807	CLA	C1B-CHB-C4A	-2.07	126.01	130.12
19	LL	203	CLA	CHC-C1C-NC	2.07	127.35	124.20
19	A2	812	CLA	CAA-C2A-C1A	-2.07	105.19	111.97
19	A1	812	CLA	CMD-C2D-C3D	2.07	128.69	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	817	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	A	806	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	BB	803	CLA	C1D-CHD-C4C	2.07	125.32	122.48
19	A2	834	CLA	C1D-CHD-C4C	2.07	125.32	122.48
23	J2	104	BCR	C8-C7-C6	-2.07	121.48	127.28
24	B	850	AJP	CBH-OBG-CBF	2.07	117.73	113.74
25	B	845	LMG	O1-C7-C8	-2.07	105.90	110.90
19	B2	823	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
19	BB	812	CLA	C1D-CHD-C4C	2.07	125.31	122.48
19	B	814	CLA	O2D-CGD-CBD	2.07	114.88	111.25
19	B	804	CLA	O2D-CGD-CBD	2.07	114.88	111.25
19	A1	829	CLA	O2A-CGA-O1A	-2.07	118.27	123.56
19	F2	301	CLA	C1D-CHD-C4C	2.07	125.31	122.48
20	A	803	CL0	C4C-C3C-C2C	-2.07	103.89	106.89
23	AA	849	BCR	C16-C15-C14	-2.07	119.16	123.51
23	II	101	BCR	C27-C26-C25	2.07	125.76	122.74
19	A2	808	CLA	O1D-CGD-CBD	2.07	128.77	124.48
24	L1	204	AJP	CBN-CBO-CBE	2.07	127.93	120.59
19	B2	836	CLA	C1D-CHD-C4C	2.07	125.31	122.48
19	BB	810	CLA	CAC-C3C-C4C	2.07	127.52	124.82
19	A1	836	CLA	CMD-C2D-C3D	2.07	128.68	124.80
19	B1	833	CLA	C6-C7-C8	-2.07	109.32	115.77
19	BB	821	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
19	A	832	CLA	CMD-C2D-C3D	2.07	128.68	124.80
19	BB	856	CLA	C1D-CHD-C4C	2.07	125.31	122.48
23	A1	849	BCR	C11-C10-C9	-2.07	124.36	127.31
19	B1	835	CLA	C1D-CHD-C4C	2.07	125.31	122.48
19	A	820	CLA	CBA-CAA-C2A	2.07	120.00	113.85
23	FF	306	BCR	C20-C21-C22	-2.07	124.36	127.31
23	K1	106	BCR	C8-C7-C6	-2.07	121.49	127.28
19	BB	832	CLA	CMD-C2D-C3D	2.07	128.68	124.80
19	A	852	CLA	CHB-C4A-NA	2.07	127.37	124.51
19	B	803	CLA	C1D-CHD-C4C	2.07	125.31	122.48
20	A	803	CL0	CGD-CBD-CAD	-2.07	104.05	110.73
19	BB	811	CLA	OBd-CAD-CBD	-2.06	122.88	125.91
23	A	851	BCR	C38-C26-C25	-2.06	122.21	124.51
23	AA	850	BCR	C24-C23-C22	-2.06	123.11	126.21
22	L1	211	LHG	O7-C7-C8	2.06	116.02	111.51
19	A1	820	CLA	C1D-CHD-C4C	2.06	125.31	122.48
19	B	831	CLA	O2A-CGA-O1A	-2.06	118.29	123.56
19	LL	202	CLA	C1-O2A-CGA	2.06	122.18	116.54
19	B1	811	CLA	CMD-C2D-C3D	2.06	128.67	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
19	A1	811	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	B2	813	CLA	C1D-CHD-C4C	2.06	125.30	122.48
23	B1	842	BCR	C8-C7-C6	-2.06	121.50	127.28
23	L2	207	BCR	C15-C14-C13	-2.06	124.37	127.31
19	B2	826	CLA	C3A-C2A-C1A	2.06	104.43	101.34
19	BB	808	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	B1	826	CLA	C6-C5-C3	2.06	117.96	113.01
19	A2	801	CLA	CMB-C2B-C3B	2.06	128.67	124.80
20	A2	803	CL0	CHD-C4C-C3C	-2.06	121.86	124.87
19	B2	818	CLA	C1D-CHD-C4C	2.06	125.30	122.48
24	BB	849	AJP	CBJ-CCB-CCA	2.06	117.84	113.00
19	B	801	CLA	C5-C3-C2	2.06	125.34	121.11
19	B1	822	CLA	O2D-CGD-CBD	2.06	114.86	111.25
19	A	832	CLA	C1-C2-C3	-2.06	122.48	126.04
19	A	852	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	AA	832	CLA	C1-C2-C3	-2.06	122.48	126.04
19	A2	839	CLA	O2A-CGA-O1A	-2.06	118.30	123.56
19	BB	802	CLA	C4-C3-C5	2.06	118.83	115.29
19	A	839	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	B1	809	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	B	801	CLA	C2A-C1A-CHA	2.06	127.46	123.86
23	A2	848	BCR	C27-C26-C25	2.06	125.74	122.74
19	K	102	CLA	C1D-CHD-C4C	2.06	125.30	122.48
19	A2	842	CLA	CMD-C2D-C3D	2.06	128.66	124.80
23	FF	306	BCR	C27-C26-C25	2.06	125.74	122.74
19	BB	821	CLA	C4-C3-C2	-2.06	118.33	123.68
23	K2	105	BCR	C8-C7-C6	-2.06	121.52	127.28
19	B	858	CLA	C1D-CHD-C4C	2.05	125.29	122.48
23	M	101	BCR	C16-C15-C14	-2.05	119.19	123.51
19	L2	206	CLA	CHB-C4A-NA	2.05	127.35	124.51
19	B1	807	CLA	C1-O2A-CGA	2.05	122.16	116.54
19	JJ	101	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	B	833	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	A2	840	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	B2	804	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	B1	836	CLA	CMB-C2B-C3B	2.05	128.65	124.80
23	M2	102	BCR	C38-C26-C25	-2.05	122.22	124.51
19	B	858	CLA	C6-C5-C3	2.05	117.94	113.01
23	J2	104	BCR	C2-C3-C4	2.05	115.99	111.37
19	B1	802	CLA	O2A-CGA-O1A	-2.05	118.32	123.56
19	BB	814	CLA	O2D-CGD-CBD	2.05	114.84	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	B1	813	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	B	814	CLA	CMD-C2D-C3D	2.05	128.65	124.80
23	M	101	BCR	C7-C8-C9	-2.05	123.13	126.21
19	B1	831	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	A1	804	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	A1	834	CLA	C1D-CHD-C4C	2.05	125.29	122.48
19	BB	804	CLA	O2D-CGD-CBD	2.05	114.84	111.25
23	B1	838	BCR	C8-C7-C6	-2.05	121.54	127.28
25	B1	846	LMG	C1-C2-C3	-2.05	105.70	109.98
19	A	820	CLA	C1D-CHD-C4C	2.05	125.29	122.48
24	A1	854	AJP	CDD-CDC-CDB	2.05	116.03	111.87
19	A1	837	CLA	C1D-CHD-C4C	2.05	125.29	122.48
23	A1	851	BCR	C37-C22-C21	-2.05	120.05	122.92
19	B2	811	CLA	CMD-C2D-C3D	2.05	128.64	124.80
19	A2	829	CLA	C1D-CHD-C4C	2.05	125.28	122.48
19	A2	812	CLA	C1D-CHD-C4C	2.05	125.28	122.48
23	B2	843	BCR	C8-C7-C6	-2.05	121.54	127.28
23	AA	855	BCR	C8-C7-C6	-2.05	121.54	127.28
19	B1	850	CLA	O2A-CGA-CBA	2.05	118.51	111.93
19	AA	821	CLA	CMB-C2B-C1B	-2.05	125.32	128.46
19	B2	812	CLA	O1D-CGD-CBD	2.05	128.72	124.48
19	K2	104	CLA	C1B-CHB-C4A	-2.05	126.06	130.12
19	B	859	CLA	C4-C3-C5	2.05	118.81	115.29
23	AA	848	BCR	C16-C15-C14	-2.05	119.21	123.51
23	L1	209	BCR	C34-C9-C10	-2.05	120.06	122.92
19	B2	819	CLA	C1D-CHD-C4C	2.05	125.28	122.48
19	AA	814	CLA	C1D-CHD-C4C	2.05	125.28	122.48
19	A2	818	CLA	C1D-CHD-C4C	2.05	125.28	122.48
23	B2	839	BCR	C8-C7-C6	-2.05	121.55	127.28
23	II	102	BCR	C24-C23-C22	-2.05	123.14	126.21
23	M	101	BCR	C38-C26-C25	-2.04	122.23	124.51
19	A1	817	CLA	C1D-CHD-C4C	2.04	125.28	122.48
23	K	103	BCR	C27-C26-C25	2.04	125.72	122.74
19	A2	834	CLA	CAA-C2A-C3A	-2.04	111.23	116.06
19	A1	841	CLA	CMD-C2D-C3D	2.04	128.63	124.80
19	A2	833	CLA	C1D-CHD-C4C	2.04	125.28	122.48
23	AA	852	BCR	C8-C7-C6	-2.04	121.55	127.28
19	B2	821	CLA	CBA-CAA-C2A	2.04	119.94	113.85
19	A	812	CLA	C1D-CHD-C4C	2.04	125.28	122.48
19	A1	809	CLA	C1D-CHD-C4C	2.04	125.28	122.48
23	A	849	BCR	C3-C4-C5	-2.04	110.43	113.99
19	AA	840	CLA	C1B-CHB-C4A	-2.04	126.07	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	853	CLA	CMB-C2B-C1B	-2.04	125.32	128.46
19	B1	819	CLA	CMA-C3A-C2A	-2.04	111.24	116.06
19	F1	302	CLA	CAA-C2A-C3A	-2.04	109.11	114.24
23	B	839	BCR	C24-C23-C22	-2.04	123.14	126.21
19	B	833	CLA	CMD-C2D-C3D	2.04	128.63	124.80
19	J2	101	CLA	C1D-CHD-C4C	2.04	125.28	122.48
19	F1	301	CLA	C1D-CHD-C4C	2.04	125.28	122.48
19	B	802	CLA	C1D-CHD-C4C	2.04	125.28	122.48
23	A1	849	BCR	C8-C7-C6	-2.04	121.56	127.28
19	AA	831	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
23	B1	841	BCR	C36-C18-C19	2.04	121.33	118.09
23	KK	103	BCR	C27-C26-C25	2.04	125.72	122.74
23	AA	854	BCR	C35-C13-C14	-2.04	120.06	122.92
19	K1	105	CLA	CAC-C3C-C4C	2.04	127.49	124.82
19	AA	839	CLA	O2A-CGA-O1A	-2.04	118.34	123.56
23	A1	850	BCR	C24-C23-C22	-2.04	123.14	126.21
19	B1	803	CLA	C1D-CHD-C4C	2.04	125.28	122.48
19	B2	832	CLA	C1D-CHD-C4C	2.04	125.28	122.48
19	F1	302	CLA	C1D-CHD-C4C	2.04	125.28	122.48
26	B	841	ECH	C39-C30-C25	-2.04	107.00	110.30
19	A1	827	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
23	B	848	BCR	C7-C8-C9	-2.04	123.15	126.21
19	B1	824	CLA	C1D-CHD-C4C	2.04	125.27	122.48
19	A	841	CLA	O2D-CGD-CBD	2.04	114.82	111.25
23	A	849	BCR	C15-C16-C17	-2.04	119.23	123.51
19	A	839	CLA	O2A-CGA-O1A	-2.04	118.35	123.56
23	M1	101	BCR	C38-C26-C25	-2.04	122.24	124.51
23	A1	850	BCR	C27-C26-C25	2.04	125.71	122.74
19	B	836	CLA	CMD-C2D-C3D	2.04	128.62	124.80
19	B	833	CLA	O2D-CGD-O1D	-2.04	119.81	123.83
19	A2	832	CLA	C1B-CHB-C4A	-2.04	126.08	130.12
24	L2	203	AJP	CDA-CDB-CCG	2.04	114.84	112.65
19	A2	810	CLA	C1D-CHD-C4C	2.04	125.27	122.48
19	A2	805	CLA	C1D-CHD-C4C	2.04	125.27	122.48
19	K2	104	CLA	CHA-C1A-NA	-2.04	121.73	126.40
22	X2	103	LHG	O7-C7-C8	2.04	115.95	111.51
19	A2	812	CLA	CMB-C2B-C3B	2.03	128.62	124.80
19	A1	826	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
19	AA	808	CLA	O2A-CGA-O1A	-2.03	118.36	123.56
24	L1	203	AJP	CBJ-CCB-CCA	2.03	117.78	113.00
19	B	827	CLA	C1D-CHD-C4C	2.03	125.27	122.48
19	A	815	CLA	C1D-CHD-C4C	2.03	125.27	122.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	102	BCR	C11-C10-C9	-2.03	124.41	127.31
19	A	808	CLA	O2D-CGD-O1D	-2.03	119.82	123.83
19	AA	810	CLA	CAA-CBA-CGA	-2.03	107.27	113.26
19	B2	821	CLA	O2D-CGD-CBD	2.03	114.81	111.25
19	B	814	CLA	C6-C5-C3	2.03	117.89	113.01
19	A1	829	CLA	C1B-CHB-C4A	-2.03	126.09	130.12
25	B2	845	LMG	C1-C2-C3	-2.03	105.74	109.98
19	BB	806	CLA	C1-C2-C3	2.03	129.56	126.04
25	B2	845	LMG	C40-C39-C38	-2.03	103.94	114.44
23	AA	850	BCR	C16-C15-C14	-2.03	119.24	123.51
19	B1	814	CLA	O2D-CGD-CBD	2.03	114.81	111.25
19	B1	848	CLA	O2D-CGD-CBD	2.03	114.81	111.25
19	A2	825	CLA	CMD-C2D-C3D	2.03	128.61	124.80
24	A2	854	AJP	OBG-CBF-CBE	-2.03	99.96	107.37
19	B	816	CLA	CMD-C2D-C3D	2.03	128.61	124.80
19	A2	817	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	B	859	CLA	O2A-CGA-CBA	2.03	118.45	111.93
19	A2	832	CLA	OBD-CAD-CBD	-2.03	122.93	125.91
23	A2	850	BCR	C24-C23-C22	-2.03	123.16	126.21
23	AA	854	BCR	C36-C18-C17	-2.03	120.08	122.92
19	A2	813	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	A1	830	CLA	CAC-C3C-C4C	2.03	127.47	124.82
19	B	818	CLA	CMB-C2B-C3B	2.03	128.60	124.80
19	B	811	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	B2	806	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	AA	821	CLA	C1B-CHB-C4A	-2.03	126.10	130.12
19	B	824	CLA	CMD-C2D-C3D	2.03	128.60	124.80
19	B1	832	CLA	CAA-C2A-C1A	2.03	118.62	111.97
24	B	849	AJP	CDC-CDD-CCI	2.03	115.51	112.13
23	B2	842	BCR	C24-C23-C22	-2.03	123.17	126.21
19	A1	830	CLA	O2A-CGA-O1A	-2.03	118.38	123.56
19	B2	817	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	A1	827	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	A	835	CLA	C1D-CHD-C4C	2.03	125.26	122.48
19	AA	822	CLA	CMB-C2B-C3B	2.03	128.60	124.80
24	L	209	AJP	CBD-CBN-CCJ	2.03	116.66	111.69
19	A	833	CLA	O2D-CGD-CBD	2.03	114.80	111.25
23	MM	101	BCR	C16-C15-C14	-2.03	119.25	123.51
19	B2	834	CLA	CBA-CAA-C2A	2.03	119.88	113.85
23	J2	104	BCR	C35-C13-C14	-2.03	120.08	122.92
19	AA	834	CLA	CMB-C2B-C3B	2.03	128.60	124.80
23	LL	204	BCR	C8-C7-C6	-2.03	121.60	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	BB	852	CLA	CMB-C2B-C3B	2.03	128.60	124.80
19	A	809	CLA	O2A-CGA-O1A	-2.03	118.39	123.56
24	BB	848	AJP	OCY-CCX-OCC	2.03	116.37	110.67
19	A	825	CLA	CMB-C2B-C3B	2.03	128.60	124.80
23	A	849	BCR	C35-C13-C12	2.03	121.30	118.09
19	A1	810	CLA	C1-O2A-CGA	2.03	122.08	116.54
23	A2	850	BCR	C27-C26-C25	2.03	125.69	122.74
24	KK	104	AJP	CDD-CCI-CCH	-2.03	107.96	110.50
19	B1	804	CLA	CMD-C2D-C3D	2.02	128.60	124.80
19	B1	832	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
19	A1	852	CLA	CMB-C2B-C1B	-2.02	125.35	128.46
23	BB	843	BCR	C24-C23-C22	-2.02	123.17	126.21
19	A	842	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	B1	822	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	A2	828	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
19	B1	802	CLA	C4-C3-C5	2.02	118.77	115.29
19	AA	839	CLA	C1B-CHB-C4A	-2.02	126.11	130.12
19	AA	853	CLA	CHB-C4A-NA	2.02	127.31	124.51
19	AA	828	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
24	L1	203	AJP	CBH-OBG-CBF	2.02	117.64	113.74
24	K	104	AJP	CCH-CCG-CDB	2.02	111.47	108.59
19	A2	807	CLA	C1-C2-C3	-2.02	122.54	126.04
19	A1	835	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	BB	813	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	B1	821	CLA	O2A-CGA-O1A	-2.02	118.39	123.56
19	KK	102	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	B	806	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	B	812	CLA	C1D-CHD-C4C	2.02	125.25	122.48
25	B	851	LMG	C40-C39-C38	-2.02	104.00	114.44
23	A2	849	BCR	C16-C15-C14	-2.02	119.26	123.51
19	A1	840	CLA	CMD-C2D-C3D	2.02	128.59	124.80
19	A1	804	CLA	CMB-C2B-C3B	2.02	128.59	124.80
24	L2	203	AJP	CBH-OBG-CBF	2.02	117.64	113.74
19	A1	801	CLA	CMC-C2C-C1C	-2.02	121.96	125.03
23	AA	855	BCR	C29-C30-C25	2.02	113.61	110.48
23	A	853	BCR	C36-C18-C17	-2.02	120.09	122.92
19	B2	837	CLA	CMB-C2B-C3B	2.02	128.59	124.80
19	AA	830	CLA	C1D-CHD-C4C	2.02	125.25	122.48
19	AA	818	CLA	C1D-CHD-C4C	2.02	125.25	122.48
23	A	849	BCR	C8-C7-C6	-2.02	121.62	127.28
19	A	842	CLA	CMD-C2D-C3D	2.02	128.59	124.80
24	B	857	AJP	CCG-CCF-CCE	2.02	117.34	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	A1	831	CLA	OBD-CAD-CBD	-2.02	122.95	125.91
19	A	807	CLA	CMB-C2B-C3B	2.02	128.59	124.80
19	A	824	CLA	CMD-C2D-C3D	2.02	128.59	124.80
25	M	102	LMG	O6-C1-O1	-2.02	105.18	109.94
23	M2	102	BCR	C35-C13-C12	2.02	121.29	118.09
19	B1	804	CLA	C1D-CHD-C4C	2.02	125.24	122.48
19	BB	818	CLA	C1D-CHD-C4C	2.02	125.24	122.48
23	B1	838	BCR	C11-C10-C9	-2.02	124.43	127.31
23	BB	838	BCR	C20-C21-C22	-2.02	124.43	127.31
23	A	854	BCR	C15-C14-C13	-2.02	124.43	127.31
19	A2	835	CLA	C1D-CHD-C4C	2.02	125.24	122.48
23	A	847	BCR	C35-C13-C14	-2.02	120.10	122.92
19	L	204	CLA	C1B-CHB-C4A	-2.02	126.12	130.12
19	B	807	CLA	C1D-CHD-C4C	2.02	125.24	122.48
19	B1	834	CLA	O2D-CGD-CBD	2.01	114.78	111.25
23	I	102	BCR	C8-C7-C6	-2.01	121.64	127.28
23	A2	851	BCR	C33-C5-C6	-2.01	122.27	124.51
19	J2	103	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
19	B1	826	CLA	C16-C15-C13	-2.01	109.49	115.77
19	A	828	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
19	B	808	CLA	C1D-CHD-C4C	2.01	125.24	122.48
19	A2	831	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
19	A2	827	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
19	B1	816	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
19	BB	835	CLA	O2D-CGD-CBD	2.01	114.77	111.25
19	A	852	CLA	CMD-C2D-C3D	2.01	128.57	124.80
19	A1	813	CLA	C1D-CHD-C4C	2.01	125.23	122.48
19	A1	815	CLA	C1D-CHD-C4C	2.01	125.23	122.48
19	A1	808	CLA	O2A-CGA-O1A	-2.01	118.42	123.56
25	I2	105	LMG	O2-C2-C1	-2.01	105.16	110.06
19	A1	820	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	B2	839	BCR	C11-C10-C9	-2.01	124.44	127.31
23	AA	854	BCR	C30-C25-C26	-2.01	119.78	122.59
19	AA	805	CLA	C4-C3-C2	-2.01	118.45	123.68
19	L1	205	CLA	O2A-CGA-O1A	-2.01	118.43	123.56
19	A2	830	CLA	O2A-CGA-O1A	-2.01	118.43	123.56
19	A1	812	CLA	C1D-CHD-C4C	2.01	125.23	122.48
19	L2	204	CLA	O2A-CGA-O1A	-2.01	118.43	123.56
19	A1	807	CLA	C1B-CHB-C4A	-2.01	126.14	130.12
23	I	102	BCR	C38-C26-C25	-2.01	122.27	124.51
23	BB	847	BCR	C8-C7-C6	-2.01	121.66	127.28
19	A1	821	CLA	O2A-CGA-O1A	-2.01	118.43	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	AA	842	CLA	O2A-C1-C2	-2.01	103.36	108.64
19	B2	808	CLA	C1D-CHD-C4C	2.01	125.23	122.48
24	A1	855	AJP	CBH-OBG-CBF	2.01	117.61	113.74
19	A	806	CLA	CAA-C2A-C3A	2.01	118.27	112.78
19	B	830	CLA	O2D-CGD-CBD	2.01	114.77	111.25
22	L	207	LHG	O7-C7-C8	2.01	115.89	111.51
19	L1	205	CLA	C1D-CHD-C4C	2.01	125.23	122.48
19	BB	804	CLA	CMD-C2D-C3D	2.01	128.56	124.80
23	B	843	BCR	C38-C26-C25	-2.01	122.28	124.51
19	A1	824	CLA	CMD-C2D-C3D	2.01	128.56	124.80
19	A1	829	CLA	CMD-C2D-C3D	2.01	128.56	124.80
19	A1	806	CLA	C1-C2-C3	-2.00	122.58	126.04
19	A1	828	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	A	832	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	II	105	LMG	C38-C37-C36	-2.00	104.09	114.44
19	BB	814	CLA	C4-C3-C5	-2.00	111.83	115.29
19	A2	834	CLA	CMA-C3A-C2A	-2.00	111.33	116.06
23	F	305	BCR	C35-C13-C12	2.00	121.27	118.09
19	A2	829	CLA	CAC-C3C-C4C	2.00	127.44	124.82
19	B1	806	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	A	817	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	B	830	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
19	BB	819	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	A2	804	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	A1	807	CLA	CMD-C2D-C3D	2.00	128.55	124.80
19	A	815	CLA	CMD-C2D-C3D	2.00	128.55	124.80
19	B2	834	CLA	C3B-C4B-NB	-2.00	106.62	109.21
19	A2	833	CLA	O2A-CGA-O1A	-2.00	118.45	123.56
19	B1	827	CLA	C1D-CHD-C4C	2.00	125.22	122.48
23	A	848	BCR	C24-C23-C22	-2.00	123.21	126.21
22	LL	205	LHG	O7-C7-C8	2.00	115.88	111.51
23	AA	851	BCR	C2-C1-C6	2.00	113.58	110.48
19	A2	838	CLA	C1D-CHD-C4C	2.00	125.22	122.48
19	A	840	CLA	C1D-CHD-C4C	2.00	125.22	122.48

All (1225) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	B2	817	CLA	NC
19	B2	817	CLA	ND
19	B2	817	CLA	NA
19	B1	806	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B1	806	CLA	ND
19	B1	806	CLA	NA
19	BB	856	CLA	NC
19	BB	856	CLA	ND
19	BB	856	CLA	NA
24	L2	202	AJP	CBP
24	L2	202	AJP	CCB
24	L2	202	AJP	CCH
24	L2	202	AJP	CCV
24	L2	202	AJP	CCW
24	L2	202	AJP	CCK
24	L2	202	AJP	CCX
19	BB	801	CLA	NC
19	BB	801	CLA	ND
19	BB	801	CLA	NA
19	B	834	CLA	NC
19	B	834	CLA	NA
19	B	834	CLA	ND
19	KK	102	CLA	NC
19	KK	102	CLA	ND
19	KK	102	CLA	NA
19	AA	843	CLA	NC
19	AA	843	CLA	ND
19	AA	843	CLA	NA
19	B1	828	CLA	NC
19	B1	828	CLA	ND
19	B1	828	CLA	NA
19	A1	816	CLA	NC
19	A1	816	CLA	ND
19	A1	816	CLA	NA
19	B1	834	CLA	NC
19	B1	834	CLA	ND
19	B1	834	CLA	NA
19	B2	825	CLA	NC
19	B2	825	CLA	NA
19	B2	825	CLA	ND
19	A1	811	CLA	NC
19	A1	811	CLA	ND
19	A1	811	CLA	NA
19	A2	814	CLA	NC
19	A2	814	CLA	ND
19	A2	814	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B	813	CLA	NC
19	B	813	CLA	ND
19	B	813	CLA	NA
19	AA	834	CLA	NC
19	AA	834	CLA	ND
19	AA	834	CLA	NA
19	A	831	CLA	NC
19	A	831	CLA	ND
19	A	831	CLA	NA
19	A2	823	CLA	NC
19	A2	823	CLA	ND
19	A2	823	CLA	NA
24	I2	104	AJP	CCH
24	I2	104	AJP	CCK
24	I2	104	AJP	CBP
19	A2	839	CLA	NC
19	A2	839	CLA	ND
19	A2	839	CLA	NA
19	A	827	CLA	NC
19	A	827	CLA	ND
19	A	827	CLA	NA
19	BB	836	CLA	NC
19	BB	836	CLA	ND
19	BB	836	CLA	NA
19	B2	824	CLA	NC
19	B2	824	CLA	ND
19	B2	824	CLA	NA
19	F2	302	CLA	NC
19	F2	302	CLA	ND
19	F2	302	CLA	NA
19	B	810	CLA	NC
19	B	810	CLA	ND
19	B	810	CLA	NA
19	A2	840	CLA	NC
19	A2	840	CLA	ND
19	A2	840	CLA	NA
19	B	803	CLA	NC
19	B	803	CLA	ND
19	B	803	CLA	NA
19	A	839	CLA	NC
19	A	839	CLA	ND
19	A	839	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B2	822	CLA	NC
19	B2	822	CLA	ND
19	B2	822	CLA	NA
19	AA	832	CLA	NC
19	AA	832	CLA	ND
19	AA	832	CLA	NA
19	L2	204	CLA	NC
19	L2	204	CLA	ND
19	L2	204	CLA	NA
19	B1	845	CLA	NC
19	B1	845	CLA	ND
19	B1	845	CLA	NA
19	B	828	CLA	NC
19	B	828	CLA	ND
19	B	828	CLA	NA
19	B2	818	CLA	NC
19	B2	818	CLA	ND
19	B2	818	CLA	NA
19	B2	835	CLA	NC
19	B2	835	CLA	ND
19	B2	835	CLA	NA
19	JJ	103	CLA	NC
19	JJ	103	CLA	ND
19	JJ	103	CLA	NA
19	K1	105	CLA	NC
19	K1	105	CLA	NA
19	K1	105	CLA	ND
19	B	817	CLA	NC
19	B	817	CLA	ND
19	B	817	CLA	NA
20	AA	803	CL0	C8
20	AA	803	CL0	NC
20	AA	803	CL0	ND
20	AA	803	CL0	NA
19	K1	103	CLA	NC
19	K1	103	CLA	ND
19	K1	103	CLA	NA
24	B	849	AJP	CBE
24	B	849	AJP	CBP
24	B	849	AJP	CCB
24	B	849	AJP	CCH
24	B	849	AJP	CCV

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Mol	Chain	Res	Type	Atom
24	B	849	AJP	CCW
24	B	849	AJP	CCK
24	B	849	AJP	CCX
19	AA	822	CLA	NC
19	AA	822	CLA	NA
19	B	807	CLA	NC
19	B	807	CLA	ND
19	B	807	CLA	NA
19	B	860	CLA	NC
19	B	860	CLA	ND
19	B	860	CLA	NA
19	A	801	CLA	NC
19	A	801	CLA	ND
19	A	801	CLA	NA
19	AA	828	CLA	NC
19	AA	828	CLA	ND
19	AA	828	CLA	NA
19	BB	832	CLA	NC
19	BB	832	CLA	NA
19	B2	802	CLA	NC
19	B2	802	CLA	ND
19	B2	802	CLA	NA
19	BB	808	CLA	NC
19	BB	808	CLA	ND
19	BB	808	CLA	NA
19	BB	831	CLA	NC
19	BB	831	CLA	ND
19	BB	831	CLA	NA
19	LL	203	CLA	NC
19	LL	203	CLA	ND
19	LL	203	CLA	NA
19	A	805	CLA	NC
19	A	805	CLA	ND
19	A	805	CLA	NA
19	B	808	CLA	NC
19	B	808	CLA	ND
19	B	808	CLA	NA
19	A	808	CLA	NC
19	A	808	CLA	ND
19	A	808	CLA	NA
19	B1	831	CLA	NC
19	B1	831	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B1	831	CLA	NA
19	B2	812	CLA	NC
19	B2	812	CLA	ND
19	B2	812	CLA	NA
19	B1	818	CLA	NC
19	B1	818	CLA	ND
19	B1	818	CLA	NA
19	L2	205	CLA	NC
19	L2	205	CLA	ND
19	L2	205	CLA	NA
19	BB	806	CLA	NC
19	BB	806	CLA	ND
19	BB	806	CLA	NA
19	BB	811	CLA	NC
19	BB	811	CLA	ND
19	BB	811	CLA	NA
19	BB	814	CLA	NC
19	BB	814	CLA	ND
19	BB	814	CLA	NA
19	A	810	CLA	NC
19	A	810	CLA	ND
19	A	810	CLA	NA
19	B	825	CLA	NC
19	B	825	CLA	NA
19	B	825	CLA	ND
19	A	807	CLA	NC
19	A	807	CLA	ND
19	A	807	CLA	NA
19	A2	825	CLA	NC
19	A2	825	CLA	ND
19	A2	825	CLA	NA
19	A1	807	CLA	NC
19	A1	807	CLA	ND
19	A1	807	CLA	NA
19	B2	846	CLA	NC
19	B2	846	CLA	ND
19	B2	846	CLA	NA
19	AA	838	CLA	NC
19	AA	838	CLA	ND
19	AA	838	CLA	NA
19	AA	837	CLA	NC
19	AA	837	CLA	ND

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Mol	Chain	Res	Type	Atom
19	AA	837	CLA	NA
19	L2	206	CLA	NC
19	L2	206	CLA	ND
19	L2	206	CLA	NA
19	XX	101	CLA	NC
19	XX	101	CLA	ND
19	XX	101	CLA	NA
19	FF	302	CLA	NC
19	FF	302	CLA	ND
19	FF	302	CLA	NA
19	B1	826	CLA	NC
19	B1	826	CLA	NA
19	B1	826	CLA	ND
19	A	825	CLA	NC
19	A	825	CLA	ND
19	A	825	CLA	NA
19	B1	825	CLA	NC
19	B1	825	CLA	ND
19	B1	825	CLA	NA
19	A	844	CLA	NC
19	A	844	CLA	ND
19	A	844	CLA	NA
19	A2	837	CLA	NC
19	A2	837	CLA	ND
19	A2	837	CLA	NA
19	BB	827	CLA	NC
19	BB	827	CLA	ND
19	BB	827	CLA	NA
19	B1	832	CLA	NC
19	B1	832	CLA	ND
19	B1	832	CLA	NA
19	AA	833	CLA	NC
19	AA	833	CLA	ND
19	AA	833	CLA	NA
19	BB	825	CLA	NC
19	BB	825	CLA	NA
19	BB	825	CLA	ND
19	B1	808	CLA	NC
19	B1	808	CLA	ND
19	B1	808	CLA	NA
19	B	830	CLA	NC
19	B	830	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	830	CLA	NA
19	B2	815	CLA	NC
19	B2	815	CLA	ND
19	B2	815	CLA	NA
20	A1	802	CL0	C8
20	A1	802	CL0	NC
20	A1	802	CL0	ND
20	A1	802	CL0	NA
24	M2	101	AJP	CCH
24	M2	101	AJP	CCK
24	M2	101	AJP	CBP
19	A2	811	CLA	NC
19	A2	811	CLA	ND
19	A2	811	CLA	NA
19	A1	832	CLA	NC
19	A1	832	CLA	ND
19	A1	832	CLA	NA
19	B2	814	CLA	NC
19	B2	814	CLA	ND
19	B2	814	CLA	NA
19	KK	101	CLA	NC
19	KK	101	CLA	ND
19	KK	101	CLA	NA
19	A	836	CLA	NC
19	A	836	CLA	ND
19	A	836	CLA	NA
19	A1	823	CLA	NC
19	A1	823	CLA	ND
19	A1	823	CLA	NA
19	A	829	CLA	NC
19	A	829	CLA	ND
19	A	829	CLA	NA
19	A2	821	CLA	NC
19	A2	821	CLA	ND
19	A2	821	CLA	NA
19	J	101	CLA	NC
19	J	101	CLA	ND
19	J	101	CLA	NA
19	X2	101	CLA	NC
19	X2	101	CLA	ND
19	X2	101	CLA	NA
19	B	827	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B	827	CLA	ND
19	B	827	CLA	NA
19	B1	803	CLA	NC
19	B1	803	CLA	ND
19	B1	803	CLA	NA
19	A1	814	CLA	NC
19	A1	814	CLA	ND
19	A1	814	CLA	NA
24	KK	104	AJP	CBP
24	KK	104	AJP	CCH
24	KK	104	AJP	CCV
24	KK	104	AJP	CCW
24	KK	104	AJP	CCK
24	KK	104	AJP	CCX
19	A1	835	CLA	NC
19	A1	835	CLA	ND
19	A1	835	CLA	NA
19	B1	849	CLA	NC
19	B1	849	CLA	ND
19	B1	849	CLA	NA
24	B	850	AJP	CBP
24	B	850	AJP	CCB
24	B	850	AJP	CCH
24	B	850	AJP	CCV
24	B	850	AJP	CCW
24	B	850	AJP	CCK
24	B	850	AJP	CCX
19	B1	805	CLA	NC
19	B1	805	CLA	NA
19	B1	805	CLA	ND
19	A	806	CLA	NC
19	A	806	CLA	ND
19	A	806	CLA	NA
19	B	819	CLA	NC
19	B	819	CLA	ND
19	B	819	CLA	NA
19	AA	831	CLA	NC
19	AA	831	CLA	ND
19	AA	831	CLA	NA
19	A	809	CLA	NC
19	A	809	CLA	ND
19	A	809	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B2	832	CLA	NC
19	B2	832	CLA	ND
19	B2	832	CLA	NA
19	BB	824	CLA	NC
19	BB	824	CLA	ND
19	BB	824	CLA	NA
19	L1	205	CLA	NC
19	L1	205	CLA	ND
19	L1	205	CLA	NA
19	B	806	CLA	NC
19	B	806	CLA	ND
19	B	806	CLA	NA
19	BB	809	CLA	NC
19	BB	809	CLA	NA
19	BB	809	CLA	ND
19	A2	831	CLA	NC
19	A2	831	CLA	ND
19	A2	831	CLA	NA
19	A	830	CLA	NC
19	A	830	CLA	ND
19	A	830	CLA	NA
19	A	815	CLA	NC
19	A	815	CLA	ND
19	A	815	CLA	NA
19	AA	839	CLA	NC
19	AA	839	CLA	ND
19	AA	839	CLA	NA
19	AA	841	CLA	NC
19	AA	841	CLA	ND
19	AA	841	CLA	NA
19	B2	809	CLA	NC
19	B2	809	CLA	NA
19	B2	809	CLA	ND
19	B	805	CLA	NC
19	B	805	CLA	ND
19	B	805	CLA	NA
19	AA	823	CLA	NC
19	AA	823	CLA	ND
19	AA	823	CLA	NA
19	A2	819	CLA	NC
19	A2	819	CLA	ND
19	A2	819	CLA	NA

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Mol	Chain	Res	Type	Atom
19	AA	842	CLA	NC
19	AA	842	CLA	ND
19	AA	842	CLA	NA
19	F1	302	CLA	NC
19	F1	302	CLA	ND
19	F1	302	CLA	NA
19	B	832	CLA	NC
19	B	832	CLA	ND
19	B	832	CLA	NA
19	A1	808	CLA	NC
19	A1	808	CLA	ND
19	A1	808	CLA	NA
19	A1	818	CLA	NC
19	A1	818	CLA	ND
19	A1	818	CLA	NA
19	B2	811	CLA	NC
19	B2	811	CLA	ND
19	B2	811	CLA	NA
19	B2	828	CLA	NC
19	B2	828	CLA	ND
19	B2	828	CLA	NA
19	B	809	CLA	NC
19	B	809	CLA	NA
19	B	809	CLA	ND
19	AA	821	CLA	NC
19	AA	821	CLA	ND
19	AA	821	CLA	NA
19	BB	819	CLA	NC
19	BB	819	CLA	ND
19	BB	819	CLA	NA
19	L	202	CLA	NC
19	L	202	CLA	ND
19	L	202	CLA	NA
19	A	822	CLA	NC
19	A	822	CLA	ND
19	A	822	CLA	NA
19	A1	840	CLA	NC
19	A1	840	CLA	ND
19	A1	840	CLA	NA
19	A2	838	CLA	NC
19	A2	838	CLA	ND
19	A2	838	CLA	NA

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Mol	Chain	Res	Type	Atom
19	AA	801	CLA	NC
19	AA	801	CLA	ND
19	AA	801	CLA	NA
19	A	828	CLA	NC
19	A	828	CLA	ND
19	A	828	CLA	NA
19	BB	828	CLA	NC
19	BB	828	CLA	ND
19	BB	828	CLA	NA
19	BB	834	CLA	NC
19	BB	834	CLA	ND
19	BB	834	CLA	NA
19	B	831	CLA	NC
19	B	831	CLA	ND
19	B	831	CLA	NA
19	AA	805	CLA	NC
19	AA	805	CLA	ND
19	AA	805	CLA	NA
19	A2	817	CLA	NC
19	A2	817	CLA	ND
19	A2	817	CLA	NA
19	AA	808	CLA	NC
19	AA	808	CLA	ND
19	AA	808	CLA	NA
19	A1	813	CLA	NC
19	A1	813	CLA	ND
19	A1	813	CLA	NA
19	A1	804	CLA	NC
19	A1	804	CLA	ND
19	A1	804	CLA	NA
19	B	815	CLA	NC
19	B	815	CLA	ND
19	B	815	CLA	NA
19	A1	801	CLA	NC
19	A1	801	CLA	ND
19	A1	801	CLA	NA
19	AA	810	CLA	NC
19	AA	810	CLA	ND
19	AA	810	CLA	NA
19	B2	804	CLA	NC
19	B2	804	CLA	ND
19	B2	804	CLA	NA

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Mol	Chain	Res	Type	Atom
19	AA	807	CLA	NC
19	AA	807	CLA	ND
19	AA	807	CLA	NA
19	A2	820	CLA	NC
19	A2	820	CLA	ND
19	A2	820	CLA	NA
19	B2	849	CLA	NC
19	B2	849	CLA	ND
19	B2	849	CLA	NA
19	A	816	CLA	NC
19	A	816	CLA	ND
19	A	816	CLA	NA
19	J1	103	CLA	NC
19	J1	103	CLA	ND
19	J1	103	CLA	NA
19	A1	820	CLA	NC
19	A1	820	CLA	ND
19	A1	820	CLA	NA
19	A	804	CLA	NC
19	A	804	CLA	NA
19	A	804	CLA	ND
19	BB	810	CLA	NC
19	BB	810	CLA	ND
19	BB	810	CLA	NA
19	B	821	CLA	NC
19	B	821	CLA	ND
19	B	821	CLA	NA
19	B2	837	CLA	NC
19	B2	837	CLA	ND
19	B2	837	CLA	NA
19	A2	809	CLA	NC
19	A2	809	CLA	ND
19	A2	809	CLA	NA
19	BB	821	CLA	NC
19	BB	821	CLA	ND
19	BB	821	CLA	NA
19	A	814	CLA	NC
19	A	814	CLA	ND
19	A	814	CLA	NA
19	A2	841	CLA	NC
19	A2	841	CLA	ND
19	A2	841	CLA	NA

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Mol	Chain	Res	Type	Atom
19	A2	826	CLA	NC
19	A2	826	CLA	ND
19	A2	826	CLA	NA
19	A	813	CLA	NC
19	A	813	CLA	ND
19	A	813	CLA	NA
19	B	811	CLA	NC
19	B	811	CLA	ND
19	B	811	CLA	NA
19	A1	827	CLA	NC
19	A1	827	CLA	ND
19	A1	827	CLA	NA
19	L1	207	CLA	NC
19	L1	207	CLA	ND
19	L1	207	CLA	NA
19	J2	103	CLA	NC
19	J2	103	CLA	ND
19	J2	103	CLA	NA
19	AA	820	CLA	NC
19	AA	820	CLA	ND
19	AA	820	CLA	NA
19	AA	826	CLA	NC
19	AA	826	CLA	ND
19	AA	826	CLA	NA
19	AA	836	CLA	NC
19	AA	836	CLA	ND
19	AA	836	CLA	NA
19	A	811	CLA	NC
19	A	811	CLA	ND
19	A	811	CLA	NA
19	K2	102	CLA	NC
19	K2	102	CLA	ND
19	K2	102	CLA	NA
19	A1	824	CLA	NC
19	A1	824	CLA	ND
19	A1	824	CLA	NA
19	BB	807	CLA	NC
19	BB	807	CLA	ND
19	BB	807	CLA	NA
19	A2	828	CLA	NC
19	A2	828	CLA	ND
19	A2	828	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B2	807	CLA	NC
19	B2	807	CLA	ND
19	B2	807	CLA	NA
19	BB	826	CLA	NC
19	BB	826	CLA	ND
19	BB	826	CLA	NA
19	A2	801	CLA	NC
19	A2	801	CLA	ND
19	A2	801	CLA	NA
24	L1	203	AJP	CCB
24	L1	203	AJP	CCH
24	L1	203	AJP	CCV
24	L1	203	AJP	CCX
24	L1	203	AJP	CCW
19	AA	824	CLA	NC
19	AA	824	CLA	ND
19	AA	824	CLA	NA
19	B1	819	CLA	NC
19	B1	819	CLA	ND
19	B1	819	CLA	NA
19	B2	819	CLA	NC
19	B2	819	CLA	ND
19	B2	819	CLA	NA
19	JJ	101	CLA	NC
19	JJ	101	CLA	ND
19	JJ	101	CLA	NA
19	B2	803	CLA	NC
19	B2	803	CLA	ND
19	B2	803	CLA	NA
24	A	802	AJP	CCH
24	A	802	AJP	CCK
24	A	802	AJP	CBP
19	F	302	CLA	NC
19	F	302	CLA	ND
19	F	302	CLA	NA
19	AA	806	CLA	NC
19	AA	806	CLA	ND
19	AA	806	CLA	NA
19	B	816	CLA	NC
19	B	816	CLA	ND
19	B	816	CLA	NA
19	A2	842	CLA	NC

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Mol	Chain	Res	Type	Atom
19	A2	842	CLA	ND
19	A2	842	CLA	NA
19	AA	809	CLA	NC
19	AA	809	CLA	ND
19	AA	809	CLA	NA
19	B1	801	CLA	NC
19	B1	801	CLA	ND
19	B1	801	CLA	NA
19	B	859	CLA	NC
19	B	859	CLA	ND
19	B	859	CLA	NA
19	J2	101	CLA	NC
19	J2	101	CLA	ND
19	J2	101	CLA	NA
19	AA	853	CLA	NC
19	AA	853	CLA	NA
19	AA	853	CLA	ND
19	B	824	CLA	NC
19	B	824	CLA	ND
19	B	824	CLA	NA
19	A1	841	CLA	NC
19	A1	841	CLA	ND
19	A1	841	CLA	NA
24	L2	203	AJP	CCB
24	L2	203	AJP	CCH
24	L2	203	AJP	CCV
24	L2	203	AJP	CCW
24	L2	203	AJP	CCK
24	L2	203	AJP	CCX
19	AA	830	CLA	NC
19	AA	830	CLA	ND
19	AA	830	CLA	NA
19	AA	815	CLA	NC
19	AA	815	CLA	ND
19	AA	815	CLA	NA
19	BB	852	CLA	NC
19	BB	852	CLA	ND
19	BB	852	CLA	NA
19	A	841	CLA	NC
19	A	841	CLA	ND
19	A	841	CLA	NA
19	B1	821	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B1	821	CLA	ND
19	B1	821	CLA	NA
19	A1	842	CLA	NC
19	A1	842	CLA	ND
19	A1	842	CLA	NA
19	A	823	CLA	NC
19	A	823	CLA	ND
19	A	823	CLA	NA
19	X	101	CLA	NC
19	X	101	CLA	ND
19	X	101	CLA	NA
19	A1	815	CLA	NC
19	A1	815	CLA	ND
19	A1	815	CLA	NA
19	A2	827	CLA	NC
19	A2	827	CLA	ND
19	A2	827	CLA	NA
19	A	842	CLA	NC
19	A	842	CLA	ND
19	A	842	CLA	NA
19	B	814	CLA	NC
19	B	814	CLA	ND
19	B	814	CLA	NA
19	A	819	CLA	NC
19	A	819	CLA	ND
19	A	819	CLA	NA
19	B1	850	CLA	NC
19	B1	850	CLA	ND
19	B1	850	CLA	NA
19	B2	834	CLA	NC
19	B2	834	CLA	NA
19	B2	834	CLA	ND
19	A1	828	CLA	NC
19	A1	828	CLA	ND
19	A1	828	CLA	NA
19	A1	844	CLA	NC
19	A1	844	CLA	ND
19	A1	844	CLA	NA
19	A	821	CLA	NC
19	A	821	CLA	ND
19	A	821	CLA	NA
19	A2	806	CLA	NC

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Mol	Chain	Res	Type	Atom
19	A2	806	CLA	ND
19	A2	806	CLA	NA
19	A1	833	CLA	NC
19	A1	833	CLA	ND
19	A1	833	CLA	NA
19	BB	845	CLA	NC
19	BB	845	CLA	ND
19	BB	845	CLA	NA
19	BB	816	CLA	NC
19	BB	816	CLA	ND
19	BB	816	CLA	NA
19	BB	813	CLA	NC
19	BB	813	CLA	ND
19	BB	813	CLA	NA
19	F2	301	CLA	NC
19	F2	301	CLA	ND
19	F2	301	CLA	NA
24	L1	204	AJP	CCB
24	L1	204	AJP	CCH
24	L1	204	AJP	CCV
24	L1	204	AJP	CCX
24	L1	204	AJP	CCW
19	B2	827	CLA	NC
19	B2	827	CLA	ND
19	B2	827	CLA	NA
19	BB	802	CLA	NC
19	BB	802	CLA	ND
19	BB	802	CLA	NA
19	J	103	CLA	NC
19	J	103	CLA	NA
19	B2	851	CLA	NC
19	B2	851	CLA	ND
19	B2	851	CLA	NA
19	A	835	CLA	NC
19	A	835	CLA	ND
19	A	835	CLA	NA
19	B	820	CLA	NC
19	B	820	CLA	ND
19	B	820	CLA	NA
19	B2	831	CLA	NC
19	B2	831	CLA	NA
19	B2	831	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A2	802	CLA	NC
19	A2	802	CLA	ND
19	A2	802	CLA	NA
19	B1	824	CLA	NC
19	B1	824	CLA	ND
19	B1	824	CLA	NA
19	B	823	CLA	NC
19	B	823	CLA	ND
19	B	823	CLA	NA
19	X1	101	CLA	NC
19	X1	101	CLA	ND
19	X1	101	CLA	NA
19	A	818	CLA	NC
19	A	818	CLA	ND
19	A	818	CLA	NA
19	A	812	CLA	NC
19	A	812	CLA	ND
19	A	812	CLA	NA
19	B1	836	CLA	NC
19	B1	836	CLA	ND
19	B1	836	CLA	NA
19	AA	840	CLA	NC
19	AA	840	CLA	ND
19	AA	840	CLA	NA
19	A1	830	CLA	NC
19	A1	830	CLA	ND
19	A1	830	CLA	NA
19	A1	829	CLA	NC
19	A1	829	CLA	ND
19	A1	829	CLA	NA
19	B	846	CLA	NC
19	B	846	CLA	ND
19	B	846	CLA	NA
19	A1	825	CLA	NC
19	A1	825	CLA	ND
19	A1	825	CLA	NA
19	AA	816	CLA	NC
19	AA	816	CLA	ND
19	AA	816	CLA	NA
19	AA	804	CLA	NC
19	AA	804	CLA	NA
19	AA	804	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B2	816	CLA	NC
19	B2	816	CLA	ND
19	B2	816	CLA	NA
19	A1	805	CLA	NC
19	A1	805	CLA	NA
19	B2	801	CLA	NC
19	B2	801	CLA	ND
19	B2	801	CLA	NA
19	F1	301	CLA	NC
19	F1	301	CLA	ND
19	F1	301	CLA	NA
24	L	208	AJP	CBE
24	L	208	AJP	CCH
24	L	208	AJP	CCK
24	L	208	AJP	CBP
19	A2	833	CLA	NC
19	A2	833	CLA	ND
19	A2	833	CLA	NA
19	A2	808	CLA	NC
19	A2	808	CLA	ND
19	A2	808	CLA	NA
19	B2	810	CLA	NC
19	B2	810	CLA	ND
19	B2	810	CLA	NA
19	B1	804	CLA	NC
19	B1	804	CLA	ND
19	B1	804	CLA	NA
19	B2	820	CLA	NC
19	B2	820	CLA	ND
19	B2	820	CLA	NA
19	LL	201	CLA	NC
19	LL	201	CLA	ND
19	LL	201	CLA	NA
19	AA	814	CLA	NC
19	AA	814	CLA	ND
19	AA	814	CLA	NA
19	B1	820	CLA	NC
19	B1	820	CLA	ND
19	B1	820	CLA	NA
19	A2	815	CLA	NC
19	A2	815	CLA	ND
19	A2	815	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B	801	CLA	NC
19	B	801	CLA	ND
19	B	801	CLA	NA
19	B2	821	CLA	NC
19	B2	821	CLA	ND
19	B2	821	CLA	NA
19	BB	805	CLA	NC
19	BB	805	CLA	NA
19	BB	805	CLA	ND
19	B	835	CLA	NC
19	B	835	CLA	ND
19	B	835	CLA	NA
19	B2	833	CLA	NC
19	B2	833	CLA	NA
19	AA	813	CLA	NC
19	AA	813	CLA	ND
19	AA	813	CLA	NA
19	A	817	CLA	NC
19	A	817	CLA	ND
19	A	817	CLA	NA
19	A2	816	CLA	NC
19	A2	816	CLA	ND
19	A2	816	CLA	NA
19	B2	805	CLA	NC
19	B2	805	CLA	NA
19	B2	805	CLA	ND
19	B	837	CLA	NC
19	B	837	CLA	ND
19	B	837	CLA	NA
19	BB	829	CLA	NC
19	BB	829	CLA	ND
19	BB	829	CLA	NA
19	F	301	CLA	NC
19	F	301	CLA	ND
19	F	301	CLA	NA
19	BB	822	CLA	NC
19	BB	822	CLA	ND
19	BB	822	CLA	NA
24	AA	802	AJP	CCH
24	AA	802	AJP	CCK
24	AA	802	AJP	CBP
19	B1	823	CLA	NC

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Mol	Chain	Res	Type	Atom
19	B1	823	CLA	ND
19	B1	823	CLA	NA
19	B1	829	CLA	NC
19	B1	829	CLA	ND
19	B1	829	CLA	NA
19	A2	835	CLA	NC
19	A2	835	CLA	ND
19	A2	835	CLA	NA
19	A	820	CLA	NC
19	A	820	CLA	NA
19	B1	814	CLA	NC
19	B1	814	CLA	ND
19	B1	814	CLA	NA
19	A1	837	CLA	NC
19	A1	837	CLA	ND
19	A1	837	CLA	NA
19	K	102	CLA	NC
19	K	102	CLA	ND
19	K	102	CLA	NA
19	A	826	CLA	NC
19	A	826	CLA	ND
19	A	826	CLA	NA
19	AA	811	CLA	NC
19	AA	811	CLA	ND
19	AA	811	CLA	NA
19	B1	848	CLA	NC
19	B1	848	CLA	ND
19	B1	848	CLA	NA
19	A1	826	CLA	NC
19	A1	826	CLA	ND
19	A1	826	CLA	NA
19	K	101	CLA	NC
19	K	101	CLA	ND
19	K	101	CLA	NA
19	B	829	CLA	NC
19	B	829	CLA	ND
19	B	829	CLA	NA
19	B1	809	CLA	NC
19	B1	809	CLA	ND
19	B1	809	CLA	NA
19	A1	812	CLA	NC
19	A1	812	CLA	ND

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Mol	Chain	Res	Type	Atom
19	A1	812	CLA	NA
19	A1	831	CLA	NC
19	A1	831	CLA	ND
19	A1	831	CLA	NA
19	BB	835	CLA	NC
19	BB	835	CLA	ND
19	BB	835	CLA	NA
19	B	804	CLA	NC
19	B	804	CLA	ND
19	B	804	CLA	NA
19	L1	206	CLA	NC
19	L1	206	CLA	ND
19	L1	206	CLA	NA
19	BB	803	CLA	NC
19	BB	803	CLA	ND
19	BB	803	CLA	NA
19	A	824	CLA	NC
19	A	824	CLA	ND
19	A	824	CLA	NA
19	B2	836	CLA	NC
19	B2	836	CLA	ND
19	B2	836	CLA	NA
19	B2	813	CLA	NC
19	B2	813	CLA	ND
19	B2	813	CLA	NA
24	K	104	AJP	CBP
24	K	104	AJP	CCH
24	K	104	AJP	CCV
24	K	104	AJP	CCW
24	K	104	AJP	CCK
24	K	104	AJP	CCX
19	BB	804	CLA	NC
19	BB	804	CLA	ND
19	BB	804	CLA	NA
19	B1	817	CLA	NC
19	B1	817	CLA	ND
19	B1	817	CLA	NA
19	B2	852	CLA	NC
19	B2	852	CLA	ND
19	B2	852	CLA	NA
19	B	818	CLA	NC
19	B	818	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	818	CLA	NA
19	A2	844	CLA	NC
19	A2	844	CLA	ND
19	A2	844	CLA	NA
19	K2	104	CLA	NC
19	K2	104	CLA	ND
19	K2	104	CLA	NA
19	A	834	CLA	NC
19	A	834	CLA	ND
19	A	834	CLA	NA
19	A1	836	CLA	NC
19	A1	836	CLA	ND
19	A1	836	CLA	NA
19	B2	808	CLA	NC
19	B2	808	CLA	ND
19	B2	808	CLA	NA
19	A2	804	CLA	NC
19	A2	804	CLA	NA
19	A2	804	CLA	ND
19	A1	809	CLA	NC
19	A1	809	CLA	ND
19	A1	809	CLA	NA
19	B	836	CLA	NC
19	B	836	CLA	ND
19	B	836	CLA	NA
19	AA	827	CLA	NC
19	AA	827	CLA	ND
19	AA	827	CLA	NA
19	B2	830	CLA	NC
19	B2	830	CLA	ND
19	B2	830	CLA	NA
19	BB	830	CLA	NC
19	BB	830	CLA	NA
19	BB	830	CLA	ND
19	FF	301	CLA	NC
19	FF	301	CLA	ND
19	FF	301	CLA	NA
19	A2	810	CLA	NC
19	A2	810	CLA	ND
19	A2	810	CLA	NA
24	BB	848	AJP	CBP
24	BB	848	AJP	CCB

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Mol	Chain	Res	Type	Atom
24	BB	848	AJP	CCH
24	BB	848	AJP	CCV
24	BB	848	AJP	CCW
24	BB	848	AJP	CCK
24	BB	848	AJP	CCX
19	A	832	CLA	NC
19	A	832	CLA	ND
19	A	832	CLA	NA
19	BB	820	CLA	NC
19	BB	820	CLA	ND
19	BB	820	CLA	NA
19	AA	819	CLA	NC
19	AA	819	CLA	ND
19	AA	819	CLA	NA
19	A1	834	CLA	NC
19	A1	834	CLA	ND
19	A1	834	CLA	NA
19	A1	819	CLA	NC
19	A1	819	CLA	NA
19	B2	823	CLA	NC
19	B2	823	CLA	ND
19	B2	823	CLA	NA
19	L	203	CLA	NC
19	L	203	CLA	ND
19	L	203	CLA	NA
19	AA	845	CLA	NC
19	AA	845	CLA	ND
19	AA	845	CLA	NA
19	A2	834	CLA	NC
19	A2	834	CLA	ND
19	A2	834	CLA	NA
19	B1	815	CLA	NC
19	B1	815	CLA	ND
19	B1	815	CLA	NA
19	A2	829	CLA	NC
19	A2	829	CLA	ND
19	A2	829	CLA	NA
19	B1	810	CLA	NC
19	B1	810	CLA	ND
19	B1	810	CLA	NA
19	A1	803	CLA	NC
19	A1	803	CLA	NA

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Mol	Chain	Res	Type	Atom
19	A1	803	CLA	ND
19	A1	806	CLA	NC
19	A1	806	CLA	ND
19	A1	806	CLA	NA
19	A2	813	CLA	NC
19	A2	813	CLA	ND
19	A2	813	CLA	NA
19	A2	832	CLA	NC
19	A2	832	CLA	ND
19	A2	832	CLA	NA
19	A2	822	CLA	NC
19	A2	822	CLA	ND
19	A2	822	CLA	NA
19	A1	817	CLA	NC
19	A1	817	CLA	ND
19	A1	817	CLA	NA
19	AA	835	CLA	NC
19	AA	835	CLA	ND
19	AA	835	CLA	NA
19	B1	822	CLA	NC
19	B1	822	CLA	ND
19	B1	822	CLA	NA
19	B1	835	CLA	NC
19	B1	835	CLA	ND
19	B1	835	CLA	NA
19	B1	816	CLA	NC
19	B1	816	CLA	ND
19	B1	816	CLA	NA
24	L	209	AJP	CBE
24	L	209	AJP	CCH
24	L	209	AJP	CCK
24	L	209	AJP	CBP
19	B	826	CLA	NC
19	B	826	CLA	NA
19	B	826	CLA	ND
19	B1	807	CLA	NC
19	B1	807	CLA	ND
19	B1	807	CLA	NA
24	BB	849	AJP	CBP
24	BB	849	AJP	CCB
24	BB	849	AJP	CCH
24	BB	849	AJP	CCV

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Mol	Chain	Res	Type	Atom
24	BB	849	AJP	CCW
24	BB	849	AJP	CCK
24	BB	849	AJP	CCX
19	BB	823	CLA	NC
19	BB	823	CLA	ND
19	BB	823	CLA	NA
19	B1	833	CLA	NC
19	B1	833	CLA	NA
19	B1	833	CLA	ND
20	A2	803	CL0	C8
20	A2	803	CL0	NC
20	A2	803	CL0	ND
20	A2	803	CL0	NA
19	A2	830	CLA	NC
19	A2	830	CLA	ND
19	A2	830	CLA	NA
19	B1	812	CLA	NC
19	B1	812	CLA	ND
19	B1	812	CLA	NA
19	AA	818	CLA	NC
19	AA	818	CLA	ND
19	AA	818	CLA	NA
19	B	854	CLA	NC
19	B	854	CLA	ND
19	B	854	CLA	NA
19	AA	812	CLA	NC
19	AA	812	CLA	ND
19	AA	812	CLA	NA
19	BB	855	CLA	NC
19	BB	855	CLA	ND
19	BB	855	CLA	NA
19	A	840	CLA	NC
19	A	840	CLA	ND
19	A	840	CLA	NA
19	A1	852	CLA	NC
19	A1	852	CLA	NA
19	A1	852	CLA	ND
19	A2	852	CLA	NC
19	A2	852	CLA	ND
19	A2	852	CLA	NA
19	B	822	CLA	NC
19	B	822	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B	822	CLA	NA
19	B	812	CLA	NC
19	B	812	CLA	ND
19	B	812	CLA	NA
19	B1	811	CLA	NC
19	B1	811	CLA	ND
19	B1	811	CLA	NA
19	BB	812	CLA	NC
19	BB	812	CLA	ND
19	BB	812	CLA	NA
19	A	838	CLA	NC
19	A	838	CLA	ND
19	A	838	CLA	NA
19	A	837	CLA	NC
19	A	837	CLA	ND
19	A	837	CLA	NA
19	J1	101	CLA	NC
19	J1	101	CLA	ND
19	J1	101	CLA	NA
19	BB	833	CLA	NC
19	BB	833	CLA	NA
19	BB	833	CLA	ND
19	BB	815	CLA	NC
19	BB	815	CLA	ND
19	BB	815	CLA	NA
19	K1	102	CLA	NC
19	K1	102	CLA	ND
19	K1	102	CLA	NA
19	BB	817	CLA	NC
19	BB	817	CLA	ND
19	BB	817	CLA	NA
19	A2	807	CLA	NC
19	A2	807	CLA	ND
19	A2	807	CLA	NA
20	A	803	CL0	C8
20	A	803	CL0	NC
20	A	803	CL0	ND
20	A	803	CL0	NA
19	B	833	CLA	NC
19	B	833	CLA	NA
19	AA	825	CLA	NC
19	AA	825	CLA	ND

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Mol	Chain	Res	Type	Atom
19	AA	825	CLA	NA
19	A2	824	CLA	NC
19	A2	824	CLA	ND
19	A2	824	CLA	NA
19	F1	305	CLA	NC
19	F1	305	CLA	ND
19	F1	305	CLA	NA
19	B1	802	CLA	NC
19	B1	802	CLA	ND
19	B1	802	CLA	NA
19	A1	810	CLA	NC
19	A1	810	CLA	ND
19	A1	810	CLA	NA
19	B	858	CLA	NC
19	B	858	CLA	ND
19	B	858	CLA	NA
19	A	833	CLA	NC
19	A	833	CLA	ND
19	A	833	CLA	NA
19	AA	817	CLA	NC
19	AA	817	CLA	ND
19	AA	817	CLA	NA
19	B2	850	CLA	NC
19	B2	850	CLA	ND
19	B2	850	CLA	NA
19	BB	818	CLA	NC
19	BB	818	CLA	ND
19	BB	818	CLA	NA
19	A1	822	CLA	NC
19	A1	822	CLA	ND
19	A1	822	CLA	NA
19	LL	202	CLA	NC
19	LL	202	CLA	ND
19	LL	202	CLA	NA
19	A1	839	CLA	NC
19	A1	839	CLA	ND
19	A1	839	CLA	NA
19	B1	813	CLA	NC
19	B1	813	CLA	ND
19	B1	813	CLA	NA
19	B2	829	CLA	NC
19	B2	829	CLA	ND

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Mol	Chain	Res	Type	Atom
19	B2	829	CLA	NA
19	A2	818	CLA	NC
19	A2	818	CLA	ND
19	A2	818	CLA	NA
19	A	852	CLA	NC
19	A	852	CLA	NA
19	A	852	CLA	ND
19	A1	838	CLA	NC
19	A1	838	CLA	ND
19	A1	838	CLA	NA
19	A1	821	CLA	NC
19	A1	821	CLA	ND
19	A1	821	CLA	NA
19	A2	812	CLA	NC
19	A2	812	CLA	ND
19	A2	812	CLA	NA
19	A2	836	CLA	NC
19	A2	836	CLA	NA
19	A2	805	CLA	NC
19	A2	805	CLA	ND
19	A2	805	CLA	NA
19	B1	827	CLA	NC
19	B1	827	CLA	ND
19	B1	827	CLA	NA
19	B2	826	CLA	NC
19	B2	826	CLA	NA
19	B2	826	CLA	ND
19	L	204	CLA	NC
19	L	204	CLA	ND
19	L	204	CLA	NA
19	AA	829	CLA	NC
19	AA	829	CLA	ND
19	AA	829	CLA	NA
19	B1	830	CLA	NC
19	B1	830	CLA	ND
19	B1	830	CLA	NA
19	B	802	CLA	NC
19	B	802	CLA	ND
19	B	802	CLA	NA
19	FF	305	CLA	NC
19	FF	305	CLA	ND
19	FF	305	CLA	NA

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Mol	Chain	Res	Type	Atom
19	B2	806	CLA	NC
19	B2	806	CLA	ND
19	B2	806	CLA	NA

All (5794) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	B1	806	CLA	CHA-CBD-CGD-O1D
19	B1	806	CLA	CHA-CBD-CGD-O2D
19	BB	801	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C1A-C2A-CAA-CBA
19	B	834	CLA	C4-C3-C5-C6
19	KK	102	CLA	C1A-C2A-CAA-CBA
19	KK	102	CLA	C3A-C2A-CAA-CBA
19	KK	102	CLA	CBA-CGA-O2A-C1
19	KK	102	CLA	O1A-CGA-O2A-C1
19	KK	102	CLA	CHA-CBD-CGD-O1D
19	KK	102	CLA	CHA-CBD-CGD-O2D
19	AA	843	CLA	C2C-C3C-CAC-CBC
19	AA	843	CLA	C4C-C3C-CAC-CBC
26	BB	840	ECH	C5-C6-C7-C8
26	BB	840	ECH	C7-C8-C9-C10
26	BB	840	ECH	C7-C8-C9-C34
26	BB	840	ECH	C11-C12-C13-C14
26	BB	840	ECH	C11-C12-C13-C35
26	BB	840	ECH	C13-C14-C15-C16
19	B2	825	CLA	CHA-CBD-CGD-O1D
19	B2	825	CLA	CHA-CBD-CGD-O2D
19	B2	825	CLA	CAD-CBD-CGD-O1D
19	A1	811	CLA	C1A-C2A-CAA-CBA
19	A1	811	CLA	C3A-C2A-CAA-CBA
19	A1	811	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	C1A-C2A-CAA-CBA
19	B	813	CLA	CHA-CBD-CGD-O2D
19	AA	834	CLA	CHA-CBD-CGD-O1D
19	AA	834	CLA	CHA-CBD-CGD-O2D
19	A	831	CLA	CHA-CBD-CGD-O1D
19	A	831	CLA	CHA-CBD-CGD-O2D
23	B	848	BCR	C7-C8-C9-C10
23	B	848	BCR	C7-C8-C9-C34
23	B	848	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	B	848	BCR	C16-C17-C18-C36
23	B	848	BCR	C36-C18-C19-C20
23	B	848	BCR	C19-C20-C21-C22
19	A2	823	CLA	CBD-CGD-O2D-CED
23	L	206	BCR	C1-C6-C7-C8
23	L	206	BCR	C5-C6-C7-C8
23	L	206	BCR	C11-C10-C9-C8
23	L	206	BCR	C11-C10-C9-C34
23	L	206	BCR	C9-C10-C11-C12
23	L	206	BCR	C10-C11-C12-C13
23	L	206	BCR	C11-C12-C13-C14
23	L	206	BCR	C11-C12-C13-C35
23	L	206	BCR	C16-C17-C18-C36
23	L	206	BCR	C17-C18-C19-C20
23	L	206	BCR	C20-C21-C22-C37
23	L	206	BCR	C21-C22-C23-C24
23	K1	104	BCR	C7-C8-C9-C34
23	K1	104	BCR	C11-C12-C13-C35
23	K1	104	BCR	C36-C18-C19-C20
23	K1	104	BCR	C20-C21-C22-C23
23	K1	104	BCR	C20-C21-C22-C37
23	K1	104	BCR	C21-C22-C23-C24
23	A2	849	BCR	C7-C8-C9-C34
23	A2	849	BCR	C11-C10-C9-C34
23	A2	849	BCR	C11-C12-C13-C35
23	A2	849	BCR	C18-C19-C20-C21
23	A2	849	BCR	C21-C22-C23-C24
23	A2	849	BCR	C37-C22-C23-C24
23	A2	849	BCR	C23-C24-C25-C30
23	L1	201	BCR	C11-C12-C13-C35
23	L1	201	BCR	C17-C18-C19-C20
23	L1	201	BCR	C36-C18-C19-C20
23	L1	201	BCR	C37-C22-C23-C24
19	BB	836	CLA	C2C-C3C-CAC-CBC
19	BB	836	CLA	C4C-C3C-CAC-CBC
22	BB	851	LHG	C3-O3-P-O5
22	BB	851	LHG	C3-O3-P-O6
22	BB	851	LHG	O9-C7-O7-C5
22	BB	851	LHG	C8-C7-O7-C5
19	B2	824	CLA	C1A-C2A-CAA-CBA
19	B2	824	CLA	C3A-C2A-CAA-CBA
19	B2	824	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B2	824	CLA	CHA-CBD-CGD-O2D
19	F2	302	CLA	C1A-C2A-CAA-CBA
19	F2	302	CLA	C3A-C2A-CAA-CBA
19	F2	302	CLA	CBD-CGD-O2D-CED
19	B	810	CLA	CHA-CBD-CGD-O1D
19	B	810	CLA	CHA-CBD-CGD-O2D
19	B	810	CLA	CBD-CGD-O2D-CED
19	B	803	CLA	CHA-CBD-CGD-O1D
19	B	803	CLA	CBD-CGD-O2D-CED
19	A	839	CLA	CHA-CBD-CGD-O1D
19	A	839	CLA	CHA-CBD-CGD-O2D
22	L2	208	LHG	C1-C2-C3-O3
22	L2	208	LHG	O9-C7-O7-C5
23	B2	842	BCR	C6-C7-C8-C9
23	B2	842	BCR	C7-C8-C9-C34
23	B2	842	BCR	C11-C10-C9-C34
23	B2	842	BCR	C10-C11-C12-C13
23	B2	842	BCR	C11-C12-C13-C35
23	B2	842	BCR	C35-C13-C14-C15
23	B2	842	BCR	C14-C15-C16-C17
23	B2	842	BCR	C18-C19-C20-C21
23	B2	842	BCR	C20-C21-C22-C37
23	B2	842	BCR	C22-C23-C24-C25
22	A	846	LHG	O1-C1-C2-C3
19	B2	818	CLA	CHA-CBD-CGD-O1D
19	B2	818	CLA	CHA-CBD-CGD-O2D
23	B	843	BCR	C6-C7-C8-C9
23	B	843	BCR	C7-C8-C9-C10
23	B	843	BCR	C7-C8-C9-C34
23	B	843	BCR	C11-C10-C9-C8
23	B	843	BCR	C11-C10-C9-C34
23	B	843	BCR	C10-C11-C12-C13
23	B	843	BCR	C11-C12-C13-C14
23	B	843	BCR	C11-C12-C13-C35
23	B	843	BCR	C36-C18-C19-C20
23	B	843	BCR	C20-C21-C22-C23
23	B	843	BCR	C20-C21-C22-C37
23	B	843	BCR	C23-C24-C25-C30
19	K1	105	CLA	CHA-CBD-CGD-O1D
19	K1	105	CLA	CHA-CBD-CGD-O2D
19	K1	105	CLA	CBD-CGD-O2D-CED
23	A	848	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	A	848	BCR	C11-C10-C9-C34
23	A	848	BCR	C11-C12-C13-C35
23	A	848	BCR	C16-C17-C18-C36
23	A	848	BCR	C36-C18-C19-C20
23	A	848	BCR	C21-C22-C23-C24
20	AA	803	CL0	C2A-CAA-CBA-CGA
20	AA	803	CL0	C2-C1-O2A-CGA
19	K1	103	CLA	C1A-C2A-CAA-CBA
19	K1	103	CLA	C3A-C2A-CAA-CBA
19	K1	103	CLA	CBA-CGA-O2A-C1
19	K1	103	CLA	O1A-CGA-O2A-C1
24	B	849	AJP	CCW-CCX-OCY-CCZ
19	B	807	CLA	O1A-CGA-O2A-C1
19	B	860	CLA	C2C-C3C-CAC-CBC
19	B	860	CLA	C4C-C3C-CAC-CBC
19	AA	828	CLA	C1A-C2A-CAA-CBA
19	AA	828	CLA	CBD-CGD-O2D-CED
19	BB	832	CLA	CBD-CGD-O2D-CED
23	F2	303	BCR	C7-C8-C9-C34
23	F2	303	BCR	C11-C10-C9-C8
23	F2	303	BCR	C11-C10-C9-C34
23	F2	303	BCR	C10-C11-C12-C13
23	F2	303	BCR	C11-C12-C13-C35
23	F2	303	BCR	C16-C17-C18-C36
23	F2	303	BCR	C21-C22-C23-C24
23	F2	303	BCR	C23-C24-C25-C30
19	B2	802	CLA	CHA-CBD-CGD-O1D
19	B2	802	CLA	CHA-CBD-CGD-O2D
19	B2	802	CLA	CAD-CBD-CGD-O1D
23	L	205	BCR	C7-C8-C9-C10
23	L	205	BCR	C7-C8-C9-C34
23	L	205	BCR	C11-C10-C9-C34
23	L	205	BCR	C11-C12-C13-C35
23	L	205	BCR	C37-C22-C23-C24
23	L	205	BCR	C23-C24-C25-C26
23	L	205	BCR	C23-C24-C25-C30
19	LL	203	CLA	C1A-C2A-CAA-CBA
19	LL	203	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	CHA-CBD-CGD-O2D
22	AA	847	LHG	O1-C1-C2-C3
19	A	808	CLA	O1A-CGA-O2A-C1
19	B1	831	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B1	831	CLA	C3A-C2A-CAA-CBA
19	B2	812	CLA	CAD-CBD-CGD-O1D
19	B2	812	CLA	CAD-CBD-CGD-O2D
19	B1	818	CLA	CHA-CBD-CGD-O1D
19	B1	818	CLA	CHA-CBD-CGD-O2D
19	BB	806	CLA	CHA-CBD-CGD-O1D
19	BB	806	CLA	CHA-CBD-CGD-O2D
19	BB	806	CLA	CBD-CGD-O2D-CED
19	BB	811	CLA	CHA-CBD-CGD-O1D
19	BB	811	CLA	CHA-CBD-CGD-O2D
19	BB	811	CLA	CAD-CBD-CGD-O1D
23	J2	104	BCR	C6-C7-C8-C9
23	J2	104	BCR	C11-C10-C9-C34
23	J2	104	BCR	C11-C12-C13-C35
23	J2	104	BCR	C16-C17-C18-C19
23	J2	104	BCR	C16-C17-C18-C36
23	J2	104	BCR	C36-C18-C19-C20
23	J2	104	BCR	C21-C22-C23-C24
23	J2	104	BCR	C23-C24-C25-C26
23	A1	851	BCR	C7-C8-C9-C34
23	A1	851	BCR	C11-C10-C9-C8
23	A1	851	BCR	C11-C10-C9-C34
23	A1	851	BCR	C10-C11-C12-C13
23	A1	851	BCR	C16-C17-C18-C19
23	A1	851	BCR	C16-C17-C18-C36
23	A1	851	BCR	C36-C18-C19-C20
23	A1	851	BCR	C18-C19-C20-C21
23	A1	851	BCR	C20-C21-C22-C37
23	A1	851	BCR	C37-C22-C23-C24
23	A1	851	BCR	C22-C23-C24-C25
25	B	845	LMG	C2-C1-O1-C7
25	B	845	LMG	O6-C1-O1-C7
19	B	825	CLA	CHA-CBD-CGD-O1D
19	B	825	CLA	CHA-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	C1A-C2A-CAA-CBA
19	A	807	CLA	C3A-C2A-CAA-CBA
19	A	807	CLA	CHA-CBD-CGD-O1D
19	A	807	CLA	CHA-CBD-CGD-O2D
23	B1	838	BCR	C1-C6-C7-C8
23	B1	838	BCR	C5-C6-C7-C8
23	B1	838	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	B1	838	BCR	C11-C12-C13-C35
23	B1	838	BCR	C16-C17-C18-C36
23	B1	838	BCR	C17-C18-C19-C20
23	B1	838	BCR	C20-C21-C22-C37
23	BB	838	BCR	C1-C6-C7-C8
23	BB	838	BCR	C5-C6-C7-C8
23	BB	838	BCR	C7-C8-C9-C10
23	BB	838	BCR	C16-C17-C18-C36
23	BB	838	BCR	C18-C19-C20-C21
23	BB	838	BCR	C20-C21-C22-C23
23	BB	838	BCR	C20-C21-C22-C37
19	A2	825	CLA	CBD-CGD-O2D-CED
19	A1	807	CLA	O1A-CGA-O2A-C1
19	L2	206	CLA	CHA-CBD-CGD-O1D
19	L2	206	CLA	CHA-CBD-CGD-O2D
19	L2	206	CLA	CBD-CGD-O2D-CED
23	BB	847	BCR	C1-C6-C7-C8
23	BB	847	BCR	C7-C8-C9-C10
23	BB	847	BCR	C7-C8-C9-C34
23	BB	847	BCR	C12-C13-C14-C15
23	BB	847	BCR	C36-C18-C19-C20
23	BB	847	BCR	C19-C20-C21-C22
23	M	101	BCR	C7-C8-C9-C10
23	M	101	BCR	C7-C8-C9-C34
23	M	101	BCR	C11-C10-C9-C8
23	M	101	BCR	C11-C10-C9-C34
23	M	101	BCR	C10-C11-C12-C13
23	M	101	BCR	C11-C12-C13-C14
23	M	101	BCR	C11-C12-C13-C35
23	M	101	BCR	C12-C13-C14-C15
23	M	101	BCR	C35-C13-C14-C15
23	M	101	BCR	C14-C15-C16-C17
23	M	101	BCR	C15-C16-C17-C18
23	M	101	BCR	C16-C17-C18-C19
23	M	101	BCR	C16-C17-C18-C36
23	M	101	BCR	C36-C18-C19-C20
23	M	101	BCR	C18-C19-C20-C21
23	M	101	BCR	C21-C22-C23-C24
23	M	101	BCR	C37-C22-C23-C24
23	M	101	BCR	C23-C24-C25-C26
23	A1	848	BCR	C7-C8-C9-C10
23	A1	848	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A1	848	BCR	C11-C12-C13-C35
23	A1	848	BCR	C16-C17-C18-C36
23	A1	848	BCR	C36-C18-C19-C20
23	A1	848	BCR	C37-C22-C23-C24
23	B	844	BCR	C7-C8-C9-C34
23	B	844	BCR	C11-C12-C13-C35
23	B	844	BCR	C16-C17-C18-C36
23	B	844	BCR	C36-C18-C19-C20
23	B	844	BCR	C20-C21-C22-C23
23	B	844	BCR	C20-C21-C22-C37
23	B	844	BCR	C22-C23-C24-C25
19	FF	302	CLA	C1A-C2A-CAA-CBA
19	FF	302	CLA	C3A-C2A-CAA-CBA
19	FF	302	CLA	CBD-CGD-O2D-CED
23	A	850	BCR	C7-C8-C9-C34
23	A	850	BCR	C11-C10-C9-C8
23	A	850	BCR	C11-C10-C9-C34
23	A	850	BCR	C11-C12-C13-C14
23	A	850	BCR	C11-C12-C13-C35
23	A	850	BCR	C16-C17-C18-C19
23	A	850	BCR	C16-C17-C18-C36
23	A	850	BCR	C20-C21-C22-C37
23	A	850	BCR	C37-C22-C23-C24
19	B1	825	CLA	CHA-CBD-CGD-O1D
19	B1	825	CLA	CHA-CBD-CGD-O2D
19	B1	825	CLA	CAD-CBD-CGD-O1D
19	A	844	CLA	CAD-CBD-CGD-O1D
19	BB	827	CLA	C3A-C2A-CAA-CBA
19	B1	832	CLA	CBD-CGD-O2D-CED
19	BB	825	CLA	CHA-CBD-CGD-O1D
19	BB	825	CLA	CHA-CBD-CGD-O2D
19	BB	825	CLA	CAD-CBD-CGD-O1D
23	A	853	BCR	C11-C12-C13-C35
23	A	853	BCR	C13-C14-C15-C16
23	A	853	BCR	C16-C17-C18-C36
23	A	853	BCR	C36-C18-C19-C20
23	A	853	BCR	C18-C19-C20-C21
19	B2	815	CLA	C3A-C2A-CAA-CBA
19	B2	815	CLA	C14-C13-C15-C16
20	A1	802	CL0	C2-C1-O2A-CGA
20	A1	802	CL0	C2-C3-C5-C6
20	A1	802	CL0	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A2	811	CLA	C3A-C2A-CAA-CBA
19	A2	811	CLA	C2-C3-C5-C6
19	A2	811	CLA	C4-C3-C5-C6
21	A2	843	PQN	C14-C13-C15-C16
19	B2	814	CLA	CHA-CBD-CGD-O1D
19	B2	814	CLA	CHA-CBD-CGD-O2D
23	A2	850	BCR	C7-C8-C9-C34
23	A2	850	BCR	C11-C10-C9-C8
23	A2	850	BCR	C11-C10-C9-C34
23	A2	850	BCR	C10-C11-C12-C13
23	A2	850	BCR	C11-C12-C13-C14
23	A2	850	BCR	C16-C17-C18-C19
23	A2	850	BCR	C16-C17-C18-C36
23	A2	850	BCR	C37-C22-C23-C24
21	A	843	PQN	C14-C13-C15-C16
19	A1	823	CLA	CHA-CBD-CGD-O1D
19	A1	823	CLA	CHA-CBD-CGD-O2D
19	A	829	CLA	CHA-CBD-CGD-O1D
19	A	829	CLA	CHA-CBD-CGD-O2D
25	BB	844	LMG	C2-C1-O1-C7
25	BB	844	LMG	O6-C1-O1-C7
19	A2	821	CLA	C1A-C2A-CAA-CBA
19	A2	821	CLA	C3A-C2A-CAA-CBA
23	K2	105	BCR	C7-C8-C9-C10
23	K2	105	BCR	C35-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C36
23	K2	105	BCR	C17-C18-C19-C20
23	K2	105	BCR	C36-C18-C19-C20
23	K2	105	BCR	C18-C19-C20-C21
23	K2	105	BCR	C20-C21-C22-C23
23	K2	105	BCR	C20-C21-C22-C37
19	B	827	CLA	C3A-C2A-CAA-CBA
19	B	827	CLA	CHA-CBD-CGD-O1D
19	B	827	CLA	CHA-CBD-CGD-O2D
19	B1	803	CLA	CHA-CBD-CGD-O1D
19	B1	803	CLA	CHA-CBD-CGD-O2D
22	LL	205	LHG	O9-C7-O7-C5
19	A1	814	CLA	CHA-CBD-CGD-O1D
19	A1	814	CLA	CHA-CBD-CGD-O2D
23	K2	103	BCR	C11-C12-C13-C35
23	K2	103	BCR	C36-C18-C19-C20
23	K2	103	BCR	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
23	K2	103	BCR	C20-C21-C22-C23
23	K2	103	BCR	C20-C21-C22-C37
23	J	102	BCR	C7-C8-C9-C34
23	J	102	BCR	C11-C10-C9-C34
23	J	102	BCR	C9-C10-C11-C12
23	J	102	BCR	C11-C12-C13-C14
23	J	102	BCR	C12-C13-C14-C15
23	J	102	BCR	C35-C13-C14-C15
23	J	102	BCR	C16-C17-C18-C36
23	J	102	BCR	C17-C18-C19-C20
23	J	102	BCR	C21-C22-C23-C24
23	J	102	BCR	C37-C22-C23-C24
23	J	102	BCR	C23-C24-C25-C30
25	I1	102	LMG	C2-C1-O1-C7
25	I1	102	LMG	O6-C1-O1-C7
19	A	806	CLA	C1A-C2A-CAA-CBA
19	A	806	CLA	C3A-C2A-CAA-CBA
19	A	806	CLA	CHA-CBD-CGD-O1D
19	A	806	CLA	CHA-CBD-CGD-O2D
19	A	806	CLA	CAD-CBD-CGD-O1D
19	AA	831	CLA	CHA-CBD-CGD-O1D
19	AA	831	CLA	CHA-CBD-CGD-O2D
22	B1	847	LHG	C3-O3-P-O5
19	B2	832	CLA	C1A-C2A-CAA-CBA
19	B2	832	CLA	C3A-C2A-CAA-CBA
19	BB	824	CLA	CHA-CBD-CGD-O1D
19	BB	824	CLA	CHA-CBD-CGD-O2D
19	B	806	CLA	CHA-CBD-CGD-O1D
19	B	806	CLA	CHA-CBD-CGD-O2D
19	BB	809	CLA	CHA-CBD-CGD-O1D
19	BB	809	CLA	CHA-CBD-CGD-O2D
19	BB	809	CLA	CAD-CBD-CGD-O1D
19	BB	809	CLA	CAD-CBD-CGD-O2D
19	A2	831	CLA	CHA-CBD-CGD-O1D
19	A2	831	CLA	CHA-CBD-CGD-O2D
22	A2	846	LHG	O1-C1-C2-C3
19	A	830	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CHA-CBD-CGD-O1D
19	A	815	CLA	CHA-CBD-CGD-O2D
19	AA	839	CLA	CHA-CBD-CGD-O2D
19	AA	841	CLA	CHA-CBD-CGD-O1D
19	AA	841	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B2	809	CLA	CHA-CBD-CGD-O1D
19	B2	809	CLA	CHA-CBD-CGD-O2D
19	B2	809	CLA	CAD-CBD-CGD-O1D
23	II	104	BCR	C7-C8-C9-C10
23	II	104	BCR	C7-C8-C9-C34
23	II	104	BCR	C11-C10-C9-C34
23	II	104	BCR	C11-C12-C13-C35
23	II	104	BCR	C16-C17-C18-C36
23	II	104	BCR	C37-C22-C23-C24
23	II	104	BCR	C23-C24-C25-C26
23	II	104	BCR	C23-C24-C25-C30
19	B	805	CLA	CHA-CBD-CGD-O1D
19	B	805	CLA	CHA-CBD-CGD-O2D
28	B	856	DGD	C2D-C1D-O3G-C3G
28	B	856	DGD	O6D-C1D-O3G-C3G
28	B	856	DGD	C2E-C1E-O5D-C6D
28	B	856	DGD	O6E-C1E-O5D-C6D
19	F1	302	CLA	C1A-C2A-CAA-CBA
19	F1	302	CLA	C3A-C2A-CAA-CBA
19	F1	302	CLA	CBD-CGD-O2D-CED
22	A1	846	LHG	O1-C1-C2-C3
19	B	832	CLA	C1A-C2A-CAA-CBA
23	I	101	BCR	C11-C10-C9-C34
23	I	101	BCR	C11-C12-C13-C35
23	I	101	BCR	C35-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C36
23	I	101	BCR	C36-C18-C19-C20
23	I	101	BCR	C20-C21-C22-C37
23	I	101	BCR	C21-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
22	AA	846	LHG	C1-C2-C3-O3
22	AA	846	LHG	O2-C2-C3-O3
19	B2	811	CLA	CHA-CBD-CGD-O1D
19	B2	811	CLA	CHA-CBD-CGD-O2D
19	B2	811	CLA	CAD-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O1D
19	B	809	CLA	CHA-CBD-CGD-O2D
19	B	809	CLA	CAD-CBD-CGD-O1D
19	AA	821	CLA	C1A-C2A-CAA-CBA
19	AA	821	CLA	C3A-C2A-CAA-CBA
23	FF	304	BCR	C7-C8-C9-C10
23	FF	304	BCR	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
23	FF	304	BCR	C11-C10-C9-C8
23	FF	304	BCR	C11-C10-C9-C34
23	FF	304	BCR	C11-C12-C13-C35
23	FF	304	BCR	C35-C13-C14-C15
23	FF	304	BCR	C36-C18-C19-C20
23	FF	304	BCR	C18-C19-C20-C21
23	FF	304	BCR	C20-C21-C22-C23
23	FF	304	BCR	C21-C22-C23-C24
22	X	102	LHG	O1-C1-C2-O2
22	X	102	LHG	O1-C1-C2-C3
22	X	102	LHG	C3-O3-P-O5
23	F	305	BCR	C1-C6-C7-C8
23	F	305	BCR	C5-C6-C7-C8
23	F	305	BCR	C6-C7-C8-C9
23	F	305	BCR	C7-C8-C9-C10
23	F	305	BCR	C10-C11-C12-C13
23	F	305	BCR	C11-C12-C13-C14
23	F	305	BCR	C11-C12-C13-C35
23	F	305	BCR	C15-C16-C17-C18
23	F	305	BCR	C16-C17-C18-C19
23	F	305	BCR	C16-C17-C18-C36
23	F	305	BCR	C17-C18-C19-C20
23	F	305	BCR	C18-C19-C20-C21
23	F	305	BCR	C21-C22-C23-C24
23	F	305	BCR	C37-C22-C23-C24
23	F	305	BCR	C22-C23-C24-C25
19	L	202	CLA	CHA-CBD-CGD-O1D
19	L	202	CLA	CHA-CBD-CGD-O2D
19	L	202	CLA	CAD-CBD-CGD-O1D
19	L	202	CLA	CAD-CBD-CGD-O2D
19	A	822	CLA	CHA-CBD-CGD-O1D
19	A	822	CLA	CHA-CBD-CGD-O2D
23	JJ	102	BCR	C7-C8-C9-C34
23	JJ	102	BCR	C11-C10-C9-C34
23	JJ	102	BCR	C9-C10-C11-C12
23	JJ	102	BCR	C11-C12-C13-C14
23	JJ	102	BCR	C35-C13-C14-C15
23	JJ	102	BCR	C16-C17-C18-C36
23	JJ	102	BCR	C36-C18-C19-C20
23	JJ	102	BCR	C21-C22-C23-C24
23	JJ	102	BCR	C37-C22-C23-C24
23	JJ	102	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
19	A1	840	CLA	CHA-CBD-CGD-O1D
19	A1	840	CLA	CHA-CBD-CGD-O2D
19	A	828	CLA	CBD-CGD-O2D-CED
22	L	207	LHG	O9-C7-O7-C5
23	B1	842	BCR	C6-C7-C8-C9
23	B1	842	BCR	C7-C8-C9-C10
23	B1	842	BCR	C7-C8-C9-C34
23	B1	842	BCR	C11-C10-C9-C8
23	B1	842	BCR	C11-C12-C13-C14
23	B1	842	BCR	C11-C12-C13-C35
23	B1	842	BCR	C17-C18-C19-C20
23	B1	842	BCR	C36-C18-C19-C20
23	B1	842	BCR	C20-C21-C22-C23
23	B1	842	BCR	C20-C21-C22-C37
23	I2	103	BCR	C7-C8-C9-C10
23	I2	103	BCR	C7-C8-C9-C34
23	I2	103	BCR	C11-C10-C9-C34
23	I2	103	BCR	C10-C11-C12-C13
23	I2	103	BCR	C11-C12-C13-C35
23	I2	103	BCR	C16-C17-C18-C36
23	I2	103	BCR	C37-C22-C23-C24
23	I2	103	BCR	C23-C24-C25-C26
23	I2	103	BCR	C23-C24-C25-C30
22	XX	102	LHG	O1-C1-C2-O2
22	XX	102	LHG	O1-C1-C2-C3
22	XX	102	LHG	C4-O6-P-O3
22	XX	102	LHG	C4-O6-P-O4
22	XX	102	LHG	C4-O6-P-O5
26	B	841	ECH	C1-C6-C7-C8
26	B	841	ECH	C5-C6-C7-C8
26	B	841	ECH	C7-C8-C9-C10
26	B	841	ECH	C7-C8-C9-C34
23	I2	102	BCR	C11-C12-C13-C35
23	I2	102	BCR	C36-C18-C19-C20
23	I2	102	BCR	C37-C22-C23-C24
19	B	831	CLA	CHA-CBD-CGD-O1D
19	B	831	CLA	CHA-CBD-CGD-O2D
19	AA	805	CLA	C3A-C2A-CAA-CBA
19	AA	805	CLA	CHA-CBD-CGD-O1D
19	AA	805	CLA	CHA-CBD-CGD-O2D
23	AA	852	BCR	C7-C8-C9-C34
23	AA	852	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	AA	852	BCR	C10-C11-C12-C13
23	AA	852	BCR	C12-C13-C14-C15
23	AA	852	BCR	C16-C17-C18-C19
23	AA	852	BCR	C16-C17-C18-C36
23	AA	852	BCR	C36-C18-C19-C20
23	AA	852	BCR	C18-C19-C20-C21
23	AA	852	BCR	C20-C21-C22-C37
23	AA	852	BCR	C37-C22-C23-C24
23	AA	852	BCR	C22-C23-C24-C25
19	AA	808	CLA	C1A-C2A-CAA-CBA
23	L1	208	BCR	C7-C8-C9-C10
23	L1	208	BCR	C7-C8-C9-C34
23	L1	208	BCR	C11-C10-C9-C34
23	L1	208	BCR	C11-C12-C13-C35
23	L1	208	BCR	C16-C17-C18-C36
23	L1	208	BCR	C37-C22-C23-C24
23	L1	208	BCR	C23-C24-C25-C26
23	L1	208	BCR	C23-C24-C25-C30
19	A1	813	CLA	C1A-C2A-CAA-CBA
19	A1	804	CLA	C1A-C2A-CAA-CBA
19	A1	804	CLA	C3A-C2A-CAA-CBA
19	A1	804	CLA	CHA-CBD-CGD-O1D
19	A1	804	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	C1A-C2A-CAA-CBA
19	B	815	CLA	C3A-C2A-CAA-CBA
19	B	815	CLA	CHA-CBD-CGD-O1D
19	B	815	CLA	CHA-CBD-CGD-O2D
19	B	815	CLA	C14-C13-C15-C16
22	L1	211	LHG	O9-C7-O7-C5
19	B2	804	CLA	CHA-CBD-CGD-O1D
19	B2	804	CLA	CHA-CBD-CGD-O2D
19	AA	807	CLA	C1A-C2A-CAA-CBA
19	AA	807	CLA	C3A-C2A-CAA-CBA
19	AA	807	CLA	CHA-CBD-CGD-O1D
19	AA	807	CLA	CHA-CBD-CGD-O2D
19	AA	807	CLA	CAD-CBD-CGD-O1D
19	A2	820	CLA	C3A-C2A-CAA-CBA
19	B2	849	CLA	CHA-CBD-CGD-O1D
19	B2	849	CLA	CHA-CBD-CGD-O2D
19	B2	849	CLA	CBD-CGD-O2D-CED
19	B2	849	CLA	C2-C3-C5-C6
19	B2	849	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
23	B2	843	BCR	C6-C7-C8-C9
23	B2	843	BCR	C7-C8-C9-C10
23	B2	843	BCR	C7-C8-C9-C34
23	B2	843	BCR	C11-C10-C9-C8
23	B2	843	BCR	C10-C11-C12-C13
23	B2	843	BCR	C11-C12-C13-C14
23	B2	843	BCR	C17-C18-C19-C20
23	B2	843	BCR	C36-C18-C19-C20
23	B2	843	BCR	C20-C21-C22-C37
19	A	816	CLA	C1A-C2A-CAA-CBA
19	A	816	CLA	C3A-C2A-CAA-CBA
19	A	816	CLA	CBD-CGD-O2D-CED
19	A1	820	CLA	C1A-C2A-CAA-CBA
19	A1	820	CLA	C3A-C2A-CAA-CBA
23	I	102	BCR	C11-C12-C13-C35
23	I	102	BCR	C36-C18-C19-C20
19	BB	810	CLA	CHA-CBD-CGD-O1D
19	BB	810	CLA	CHA-CBD-CGD-O2D
19	BB	810	CLA	CBD-CGD-O2D-CED
23	A	847	BCR	C11-C10-C9-C34
23	A	847	BCR	C11-C12-C13-C35
19	BB	821	CLA	CHA-CBD-CGD-O2D
23	LL	204	BCR	C1-C6-C7-C8
23	LL	204	BCR	C5-C6-C7-C8
23	LL	204	BCR	C6-C7-C8-C9
23	LL	204	BCR	C11-C10-C9-C8
23	LL	204	BCR	C11-C10-C9-C34
23	LL	204	BCR	C11-C12-C13-C14
23	LL	204	BCR	C11-C12-C13-C35
23	LL	204	BCR	C16-C17-C18-C36
23	LL	204	BCR	C17-C18-C19-C20
23	LL	204	BCR	C20-C21-C22-C37
23	LL	204	BCR	C21-C22-C23-C24
19	A	814	CLA	C1A-C2A-CAA-CBA
23	J2	102	BCR	C7-C8-C9-C34
23	J2	102	BCR	C11-C10-C9-C34
23	J2	102	BCR	C11-C12-C13-C14
23	J2	102	BCR	C35-C13-C14-C15
23	J2	102	BCR	C36-C18-C19-C20
23	J2	102	BCR	C21-C22-C23-C24
23	J2	102	BCR	C37-C22-C23-C24
23	J2	102	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
19	A2	841	CLA	CHA-CBD-CGD-O1D
19	A2	841	CLA	CHA-CBD-CGD-O2D
22	X2	102	LHG	O1-C1-C2-O2
22	X2	102	LHG	O1-C1-C2-C3
22	X2	102	LHG	C3-O3-P-O5
22	X2	102	LHG	C4-O6-P-O3
22	X2	102	LHG	C4-O6-P-O4
19	A2	826	CLA	C1A-C2A-CAA-CBA
19	A2	826	CLA	CHA-CBD-CGD-O1D
19	A2	826	CLA	CHA-CBD-CGD-O2D
23	K1	106	BCR	C7-C8-C9-C10
23	K1	106	BCR	C35-C13-C14-C15
23	K1	106	BCR	C36-C18-C19-C20
23	K1	106	BCR	C18-C19-C20-C21
23	K1	106	BCR	C20-C21-C22-C37
23	K1	106	BCR	C22-C23-C24-C25
23	B	839	BCR	C1-C6-C7-C8
23	B	839	BCR	C5-C6-C7-C8
23	B	839	BCR	C7-C8-C9-C10
23	B	839	BCR	C11-C12-C13-C35
23	B	839	BCR	C16-C17-C18-C36
23	B	839	BCR	C17-C18-C19-C20
23	B	839	BCR	C18-C19-C20-C21
23	B	839	BCR	C20-C21-C22-C37
28	BB	854	DGD	C2D-C1D-O3G-C3G
28	BB	854	DGD	O6D-C1D-O3G-C3G
28	BB	854	DGD	C2E-C1E-O5D-C6D
28	BB	854	DGD	O6E-C1E-O5D-C6D
19	B	811	CLA	CHA-CBD-CGD-O1D
19	B	811	CLA	CHA-CBD-CGD-O2D
19	B	811	CLA	CAD-CBD-CGD-O1D
23	L1	209	BCR	C1-C6-C7-C8
23	L1	209	BCR	C5-C6-C7-C8
23	L1	209	BCR	C11-C10-C9-C8
23	L1	209	BCR	C11-C10-C9-C34
23	L1	209	BCR	C9-C10-C11-C12
23	L1	209	BCR	C10-C11-C12-C13
23	L1	209	BCR	C11-C12-C13-C14
23	L1	209	BCR	C11-C12-C13-C35
23	L1	209	BCR	C16-C17-C18-C36
23	L1	209	BCR	C20-C21-C22-C37
23	L1	209	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	A1	827	CLA	C1A-C2A-CAA-CBA
19	L1	207	CLA	CHA-CBD-CGD-O1D
19	L1	207	CLA	CHA-CBD-CGD-O2D
19	AA	820	CLA	C3A-C2A-CAA-CBA
23	B	842	BCR	C6-C7-C8-C9
23	B	842	BCR	C11-C12-C13-C35
23	B	842	BCR	C35-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C36
23	B	842	BCR	C21-C22-C23-C24
23	B	842	BCR	C37-C22-C23-C24
23	B	842	BCR	C23-C24-C25-C26
23	B	842	BCR	C23-C24-C25-C30
25	B1	846	LMG	C2-C1-O1-C7
25	B1	846	LMG	O6-C1-O1-C7
22	X1	103	LHG	C3-O3-P-O5
22	X1	103	LHG	O9-C7-O7-C5
22	X1	103	LHG	C8-C7-O7-C5
19	AA	826	CLA	C1A-C2A-CAA-CBA
19	AA	826	CLA	C3A-C2A-CAA-CBA
19	AA	826	CLA	CHA-CBD-CGD-O1D
19	AA	826	CLA	CHA-CBD-CGD-O2D
19	A	811	CLA	CBD-CGD-O2D-CED
19	A	811	CLA	C2-C3-C5-C6
19	A	811	CLA	C4-C3-C5-C6
22	X2	103	LHG	C3-O3-P-O5
22	X2	103	LHG	C3-O3-P-O6
22	X2	103	LHG	O9-C7-O7-C5
22	X2	103	LHG	C8-C7-O7-C5
19	A1	824	CLA	C1A-C2A-CAA-CBA
23	BB	842	BCR	C6-C7-C8-C9
23	BB	842	BCR	C7-C8-C9-C10
23	BB	842	BCR	C7-C8-C9-C34
23	BB	842	BCR	C11-C10-C9-C8
23	BB	842	BCR	C11-C10-C9-C34
23	BB	842	BCR	C11-C12-C13-C14
23	BB	842	BCR	C11-C12-C13-C35
23	BB	842	BCR	C16-C17-C18-C36
23	BB	842	BCR	C36-C18-C19-C20
23	BB	842	BCR	C20-C21-C22-C23
23	BB	842	BCR	C20-C21-C22-C37
19	A2	828	CLA	C1A-C2A-CAA-CBA
19	A2	828	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
21	A1	843	PQN	C12-C13-C15-C16
21	A1	843	PQN	C14-C13-C15-C16
23	AA	849	BCR	C7-C8-C9-C10
23	AA	849	BCR	C11-C10-C9-C34
23	AA	849	BCR	C11-C12-C13-C35
23	AA	849	BCR	C16-C17-C18-C36
23	AA	849	BCR	C36-C18-C19-C20
23	AA	849	BCR	C21-C22-C23-C24
19	BB	826	CLA	CHA-CBD-CGD-O2D
19	BB	826	CLA	C2-C3-C5-C6
19	BB	826	CLA	C4-C3-C5-C6
23	F1	306	BCR	C1-C6-C7-C8
23	F1	306	BCR	C5-C6-C7-C8
23	F1	306	BCR	C6-C7-C8-C9
23	F1	306	BCR	C7-C8-C9-C10
23	F1	306	BCR	C11-C10-C9-C8
23	F1	306	BCR	C10-C11-C12-C13
23	F1	306	BCR	C11-C12-C13-C14
23	F1	306	BCR	C11-C12-C13-C35
23	F1	306	BCR	C16-C17-C18-C19
23	F1	306	BCR	C16-C17-C18-C36
23	F1	306	BCR	C36-C18-C19-C20
23	F1	306	BCR	C18-C19-C20-C21
23	F1	306	BCR	C21-C22-C23-C24
23	F1	306	BCR	C37-C22-C23-C24
23	F1	306	BCR	C22-C23-C24-C25
24	L1	203	AJP	CCW-CCX-OCY-CCZ
23	L2	207	BCR	C1-C6-C7-C8
23	L2	207	BCR	C5-C6-C7-C8
23	L2	207	BCR	C7-C8-C9-C34
23	L2	207	BCR	C11-C10-C9-C8
23	L2	207	BCR	C11-C10-C9-C34
23	L2	207	BCR	C10-C11-C12-C13
23	L2	207	BCR	C11-C12-C13-C14
23	L2	207	BCR	C11-C12-C13-C35
23	L2	207	BCR	C16-C17-C18-C36
23	L2	207	BCR	C20-C21-C22-C37
23	L2	207	BCR	C21-C22-C23-C24
23	M1	101	BCR	C6-C7-C8-C9
23	M1	101	BCR	C7-C8-C9-C10
23	M1	101	BCR	C7-C8-C9-C34
23	M1	101	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	M1	101	BCR	C11-C10-C9-C34
23	M1	101	BCR	C10-C11-C12-C13
23	M1	101	BCR	C12-C13-C14-C15
23	M1	101	BCR	C35-C13-C14-C15
23	M1	101	BCR	C14-C15-C16-C17
23	M1	101	BCR	C17-C18-C19-C20
23	M1	101	BCR	C36-C18-C19-C20
23	M1	101	BCR	C18-C19-C20-C21
23	M1	101	BCR	C21-C22-C23-C24
23	M1	101	BCR	C37-C22-C23-C24
19	AA	824	CLA	C1A-C2A-CAA-CBA
19	AA	824	CLA	C3A-C2A-CAA-CBA
19	AA	824	CLA	CHA-CBD-CGD-O1D
19	AA	824	CLA	CHA-CBD-CGD-O2D
19	AA	824	CLA	CAD-CBD-CGD-O1D
19	B2	803	CLA	CHA-CBD-CGD-O1D
23	J1	102	BCR	C7-C8-C9-C34
23	J1	102	BCR	C11-C10-C9-C34
23	J1	102	BCR	C11-C12-C13-C14
23	J1	102	BCR	C35-C13-C14-C15
23	J1	102	BCR	C16-C17-C18-C36
23	J1	102	BCR	C36-C18-C19-C20
23	J1	102	BCR	C21-C22-C23-C24
23	J1	102	BCR	C37-C22-C23-C24
23	J1	102	BCR	C23-C24-C25-C30
23	II	101	BCR	C11-C10-C9-C34
23	II	101	BCR	C11-C12-C13-C35
23	II	101	BCR	C16-C17-C18-C36
23	II	101	BCR	C36-C18-C19-C20
23	II	101	BCR	C21-C22-C23-C24
23	II	101	BCR	C37-C22-C23-C24
19	F	302	CLA	C1A-C2A-CAA-CBA
19	F	302	CLA	C3A-C2A-CAA-CBA
19	F	302	CLA	CBD-CGD-O2D-CED
19	AA	806	CLA	C1A-C2A-CAA-CBA
19	AA	806	CLA	C3A-C2A-CAA-CBA
19	AA	806	CLA	CHA-CBD-CGD-O1D
19	AA	806	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	C4-C3-C5-C6
19	A2	842	CLA	C4-C3-C5-C6
23	JJ	104	BCR	C11-C10-C9-C34
23	JJ	104	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
23	JJ	104	BCR	C16-C17-C18-C36
23	JJ	104	BCR	C17-C18-C19-C20
23	JJ	104	BCR	C36-C18-C19-C20
23	JJ	104	BCR	C23-C24-C25-C26
23	B2	839	BCR	C1-C6-C7-C8
23	B2	839	BCR	C5-C6-C7-C8
23	B2	839	BCR	C7-C8-C9-C10
23	B2	839	BCR	C11-C12-C13-C35
23	B2	839	BCR	C16-C17-C18-C36
23	B2	839	BCR	C17-C18-C19-C20
23	B2	839	BCR	C20-C21-C22-C37
19	AA	853	CLA	C1A-C2A-CAA-CBA
19	AA	853	CLA	C2A-CAA-CBA-CGA
19	B	824	CLA	CHA-CBD-CGD-O1D
19	B	824	CLA	CHA-CBD-CGD-O2D
19	A1	841	CLA	C4-C3-C5-C6
19	AA	830	CLA	CHA-CBD-CGD-O1D
19	AA	830	CLA	CHA-CBD-CGD-O2D
19	AA	830	CLA	CBD-CGD-O2D-CED
19	AA	815	CLA	CHA-CBD-CGD-O1D
19	AA	815	CLA	CHA-CBD-CGD-O2D
19	BB	852	CLA	CBD-CGD-O2D-CED
19	BB	852	CLA	C4-C3-C5-C6
19	A	841	CLA	CHA-CBD-CGD-O1D
19	A	841	CLA	CHA-CBD-CGD-O2D
19	B1	821	CLA	CHA-CBD-CGD-O1D
19	B1	821	CLA	CHA-CBD-CGD-O2D
22	A2	845	LHG	C1-C2-C3-O3
22	A2	845	LHG	O2-C2-C3-O3
19	A1	842	CLA	C2C-C3C-CAC-CBC
19	A1	842	CLA	C4C-C3C-CAC-CBC
23	A2	847	BCR	C11-C10-C9-C34
23	A2	847	BCR	C11-C12-C13-C35
23	A2	847	BCR	C36-C18-C19-C20
19	A	823	CLA	CAD-CBD-CGD-O2D
19	A1	815	CLA	C1A-C2A-CAA-CBA
19	A1	815	CLA	C3A-C2A-CAA-CBA
19	A1	815	CLA	CBD-CGD-O2D-CED
26	B1	840	ECH	C1-C6-C7-C8
26	B1	840	ECH	C5-C6-C7-C8
26	B1	840	ECH	C7-C8-C9-C10
26	B1	840	ECH	C7-C8-C9-C34

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Mol	Chain	Res	Type	Atoms
26	B1	840	ECH	C11-C12-C13-C14
26	B1	840	ECH	C11-C12-C13-C35
19	B2	834	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C1A-C2A-CAA-CBA
19	A1	828	CLA	C3A-C2A-CAA-CBA
19	A1	828	CLA	CHA-CBD-CGD-O1D
19	A1	828	CLA	CHA-CBD-CGD-O2D
19	A1	828	CLA	C11-C10-C8-C9
19	A1	844	CLA	CBD-CGD-O2D-CED
25	II	105	LMG	C11-C10-O7-C8
19	A	821	CLA	C1A-C2A-CAA-CBA
19	A	821	CLA	C3A-C2A-CAA-CBA
19	A2	806	CLA	C1A-C2A-CAA-CBA
19	A2	806	CLA	CHA-CBD-CGD-O1D
19	A2	806	CLA	CHA-CBD-CGD-O2D
19	A2	806	CLA	CAD-CBD-CGD-O1D
19	A1	833	CLA	CHA-CBD-CGD-O1D
19	A1	833	CLA	CHA-CBD-CGD-O2D
19	A1	833	CLA	CBD-CGD-O2D-CED
23	AA	848	BCR	C11-C10-C9-C34
23	AA	848	BCR	C10-C11-C12-C13
23	AA	848	BCR	C11-C12-C13-C35
23	BB	843	BCR	C7-C8-C9-C34
23	BB	843	BCR	C11-C12-C13-C35
23	BB	843	BCR	C35-C13-C14-C15
23	BB	843	BCR	C16-C17-C18-C36
23	BB	843	BCR	C36-C18-C19-C20
23	BB	843	BCR	C20-C21-C22-C23
23	BB	843	BCR	C20-C21-C22-C37
23	BB	843	BCR	C22-C23-C24-C25
23	AA	855	BCR	C7-C8-C9-C10
23	AA	855	BCR	C35-C13-C14-C15
23	AA	855	BCR	C36-C18-C19-C20
23	AA	855	BCR	C18-C19-C20-C21
23	AA	855	BCR	C19-C20-C21-C22
23	AA	855	BCR	C20-C21-C22-C23
23	AA	855	BCR	C20-C21-C22-C37
23	AA	855	BCR	C37-C22-C23-C24
23	AA	855	BCR	C23-C24-C25-C30
19	BB	813	CLA	C1A-C2A-CAA-CBA
19	BB	813	CLA	CHA-CBD-CGD-O1D
19	BB	813	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	F2	301	CLA	C1A-C2A-CAA-CBA
19	F2	301	CLA	CHA-CBD-CGD-O1D
19	F2	301	CLA	CHA-CBD-CGD-O2D
19	B2	827	CLA	C3A-C2A-CAA-CBA
19	BB	802	CLA	CHA-CBD-CGD-O1D
19	BB	802	CLA	CHA-CBD-CGD-O2D
19	BB	802	CLA	CAD-CBD-CGD-O1D
19	J	103	CLA	CHA-CBD-CGD-O1D
19	J	103	CLA	CHA-CBD-CGD-O2D
19	B2	851	CLA	CBD-CGD-O2D-CED
19	A	835	CLA	CBD-CGD-O2D-CED
23	AA	851	BCR	C7-C8-C9-C34
23	AA	851	BCR	C11-C10-C9-C8
23	AA	851	BCR	C11-C10-C9-C34
23	AA	851	BCR	C10-C11-C12-C13
23	AA	851	BCR	C11-C12-C13-C14
23	AA	851	BCR	C11-C12-C13-C35
23	AA	851	BCR	C16-C17-C18-C19
23	AA	851	BCR	C16-C17-C18-C36
23	AA	851	BCR	C20-C21-C22-C37
23	AA	851	BCR	C37-C22-C23-C24
23	KK	103	BCR	C7-C8-C9-C34
23	KK	103	BCR	C11-C10-C9-C34
23	KK	103	BCR	C11-C12-C13-C35
23	KK	103	BCR	C16-C17-C18-C36
23	KK	103	BCR	C17-C18-C19-C20
23	KK	103	BCR	C20-C21-C22-C37
23	KK	103	BCR	C21-C22-C23-C24
23	KK	103	BCR	C37-C22-C23-C24
23	KK	103	BCR	C23-C24-C25-C30
19	B	820	CLA	C2C-C3C-CAC-CBC
19	B	820	CLA	C4C-C3C-CAC-CBC
19	B	820	CLA	CHA-CBD-CGD-O1D
19	B	820	CLA	CHA-CBD-CGD-O2D
19	B2	831	CLA	CHA-CBD-CGD-O1D
19	B2	831	CLA	CHA-CBD-CGD-O2D
19	B2	831	CLA	CAD-CBD-CGD-O1D
19	B2	831	CLA	CAD-CBD-CGD-O2D
19	A2	802	CLA	C1A-C2A-CAA-CBA
19	A2	802	CLA	C3A-C2A-CAA-CBA
19	A2	802	CLA	CBA-CGA-O2A-C1
19	A2	802	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A2	802	CLA	CHA-CBD-CGD-O1D
19	A2	802	CLA	CHA-CBD-CGD-O2D
19	A2	802	CLA	CAD-CBD-CGD-O1D
19	B1	824	CLA	C1A-C2A-CAA-CBA
19	B1	824	CLA	C3A-C2A-CAA-CBA
19	B1	824	CLA	CHA-CBD-CGD-O1D
19	B1	824	CLA	CHA-CBD-CGD-O2D
19	B1	824	CLA	CBD-CGD-O2D-CED
19	B	823	CLA	CHA-CBD-CGD-O1D
19	B	823	CLA	CHA-CBD-CGD-O2D
19	B	823	CLA	C6-C7-C8-C9
19	A	812	CLA	C1A-C2A-CAA-CBA
19	A	812	CLA	C3A-C2A-CAA-CBA
19	A	812	CLA	CBD-CGD-O2D-CED
19	A	812	CLA	O1D-CGD-O2D-CED
23	FF	306	BCR	C1-C6-C7-C8
23	FF	306	BCR	C5-C6-C7-C8
23	FF	306	BCR	C6-C7-C8-C9
23	FF	306	BCR	C7-C8-C9-C10
23	FF	306	BCR	C11-C10-C9-C8
23	FF	306	BCR	C10-C11-C12-C13
23	FF	306	BCR	C11-C12-C13-C14
23	FF	306	BCR	C11-C12-C13-C35
23	FF	306	BCR	C15-C16-C17-C18
23	FF	306	BCR	C16-C17-C18-C19
23	FF	306	BCR	C16-C17-C18-C36
23	FF	306	BCR	C17-C18-C19-C20
23	FF	306	BCR	C18-C19-C20-C21
23	FF	306	BCR	C21-C22-C23-C24
23	FF	306	BCR	C37-C22-C23-C24
23	FF	306	BCR	C22-C23-C24-C25
23	A2	848	BCR	C7-C8-C9-C10
23	A2	848	BCR	C11-C12-C13-C35
23	A2	848	BCR	C36-C18-C19-C20
23	A2	848	BCR	C37-C22-C23-C24
23	M2	102	BCR	C6-C7-C8-C9
23	M2	102	BCR	C7-C8-C9-C10
23	M2	102	BCR	C7-C8-C9-C34
23	M2	102	BCR	C11-C10-C9-C8
23	M2	102	BCR	C11-C10-C9-C34
23	M2	102	BCR	C10-C11-C12-C13
23	M2	102	BCR	C12-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
23	M2	102	BCR	C35-C13-C14-C15
23	M2	102	BCR	C14-C15-C16-C17
23	M2	102	BCR	C17-C18-C19-C20
23	M2	102	BCR	C36-C18-C19-C20
23	M2	102	BCR	C18-C19-C20-C21
23	M2	102	BCR	C37-C22-C23-C24
19	A1	825	CLA	C1A-C2A-CAA-CBA
19	A1	825	CLA	C3A-C2A-CAA-CBA
19	A1	825	CLA	CHA-CBD-CGD-O1D
19	A1	825	CLA	CHA-CBD-CGD-O2D
19	AA	816	CLA	C1A-C2A-CAA-CBA
19	AA	816	CLA	C3A-C2A-CAA-CBA
19	AA	816	CLA	CBD-CGD-O2D-CED
23	B2	844	BCR	C1-C6-C7-C8
23	B2	844	BCR	C11-C12-C13-C35
23	B2	844	BCR	C16-C17-C18-C36
23	B2	844	BCR	C36-C18-C19-C20
23	B2	844	BCR	C20-C21-C22-C23
23	B2	844	BCR	C20-C21-C22-C37
23	B2	844	BCR	C22-C23-C24-C25
19	AA	804	CLA	CBD-CGD-O2D-CED
19	B2	816	CLA	CBD-CGD-O2D-CED
19	A1	805	CLA	C1A-C2A-CAA-CBA
19	A1	805	CLA	C3A-C2A-CAA-CBA
23	I2	101	BCR	C1-C6-C7-C8
23	I2	101	BCR	C11-C10-C9-C34
23	I2	101	BCR	C11-C12-C13-C35
23	I2	101	BCR	C16-C17-C18-C36
23	I2	101	BCR	C36-C18-C19-C20
23	I2	101	BCR	C20-C21-C22-C37
23	I2	101	BCR	C21-C22-C23-C24
19	F1	301	CLA	C1A-C2A-CAA-CBA
23	B1	843	BCR	C1-C6-C7-C8
23	B1	843	BCR	C11-C12-C13-C35
23	B1	843	BCR	C14-C15-C16-C17
23	B1	843	BCR	C16-C17-C18-C36
23	B1	843	BCR	C36-C18-C19-C20
23	B1	843	BCR	C20-C21-C22-C37
23	B1	843	BCR	C22-C23-C24-C25
19	B2	810	CLA	CHA-CBD-CGD-O1D
19	B2	810	CLA	CHA-CBD-CGD-O2D
19	B2	810	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B1	804	CLA	CHA-CBD-CGD-O1D
19	B1	804	CLA	CHA-CBD-CGD-O2D
19	B2	820	CLA	C2C-C3C-CAC-CBC
19	B2	820	CLA	C4C-C3C-CAC-CBC
19	AA	814	CLA	C1A-C2A-CAA-CBA
19	A2	815	CLA	CHA-CBD-CGD-O1D
19	A2	815	CLA	CHA-CBD-CGD-O2D
19	B	801	CLA	CBD-CGD-O2D-CED
19	B2	821	CLA	C1A-C2A-CAA-CBA
19	B2	821	CLA	C3A-C2A-CAA-CBA
19	BB	805	CLA	CHA-CBD-CGD-O2D
19	B2	833	CLA	CHA-CBD-CGD-O2D
19	A2	816	CLA	C1A-C2A-CAA-CBA
19	A2	816	CLA	C3A-C2A-CAA-CBA
23	B	840	BCR	C37-C22-C23-C24
19	F	301	CLA	C1A-C2A-CAA-CBA
23	F2	304	BCR	C7-C8-C9-C10
23	F2	304	BCR	C7-C8-C9-C34
23	F2	304	BCR	C11-C10-C9-C8
23	F2	304	BCR	C11-C10-C9-C34
23	F2	304	BCR	C11-C12-C13-C35
23	F2	304	BCR	C18-C19-C20-C21
23	F2	304	BCR	C20-C21-C22-C23
23	F2	304	BCR	C21-C22-C23-C24
22	B	853	LHG	C3-O3-P-O5
22	B	853	LHG	C3-O3-P-O6
22	B	853	LHG	O9-C7-O7-C5
22	B	853	LHG	C8-C7-O7-C5
19	B1	823	CLA	CHA-CBD-CGD-O1D
19	B1	823	CLA	CHA-CBD-CGD-O2D
19	A2	835	CLA	CBD-CGD-O2D-CED
26	B2	841	ECH	C1-C6-C7-C8
26	B2	841	ECH	C5-C6-C7-C8
26	B2	841	ECH	C7-C8-C9-C10
26	B2	841	ECH	C7-C8-C9-C34
26	B2	841	ECH	C11-C12-C13-C14
26	B2	841	ECH	C11-C12-C13-C35
19	A	820	CLA	C3A-C2A-CAA-CBA
19	B1	814	CLA	CHA-CBD-CGD-O1D
19	B1	814	CLA	CHA-CBD-CGD-O2D
19	K	102	CLA	C1A-C2A-CAA-CBA
19	K	102	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	K	102	CLA	CBA-CGA-O2A-C1
19	K	102	CLA	O1A-CGA-O2A-C1
19	K	102	CLA	CHA-CBD-CGD-O1D
19	K	102	CLA	CHA-CBD-CGD-O2D
19	K	102	CLA	CAD-CBD-CGD-O1D
19	A	826	CLA	C1A-C2A-CAA-CBA
19	A	826	CLA	C3A-C2A-CAA-CBA
23	MM	101	BCR	C7-C8-C9-C10
23	MM	101	BCR	C11-C10-C9-C8
23	MM	101	BCR	C11-C10-C9-C34
23	MM	101	BCR	C10-C11-C12-C13
23	MM	101	BCR	C11-C12-C13-C14
23	MM	101	BCR	C12-C13-C14-C15
23	MM	101	BCR	C35-C13-C14-C15
23	MM	101	BCR	C14-C15-C16-C17
23	MM	101	BCR	C16-C17-C18-C19
23	MM	101	BCR	C16-C17-C18-C36
23	MM	101	BCR	C36-C18-C19-C20
23	MM	101	BCR	C18-C19-C20-C21
23	MM	101	BCR	C20-C21-C22-C23
23	MM	101	BCR	C20-C21-C22-C37
23	MM	101	BCR	C21-C22-C23-C24
23	MM	101	BCR	C37-C22-C23-C24
23	A1	853	BCR	C11-C12-C13-C35
23	A1	853	BCR	C16-C17-C18-C36
23	A1	853	BCR	C36-C18-C19-C20
23	A1	853	BCR	C18-C19-C20-C21
23	A1	853	BCR	C20-C21-C22-C37
19	AA	811	CLA	CBD-CGD-O2D-CED
19	AA	811	CLA	C2-C3-C5-C6
19	AA	811	CLA	C4-C3-C5-C6
19	B1	848	CLA	CHA-CBD-CGD-O1D
19	B1	848	CLA	CBD-CGD-O2D-CED
23	A	854	BCR	C7-C8-C9-C10
23	A	854	BCR	C35-C13-C14-C15
23	A	854	BCR	C14-C15-C16-C17
23	A	854	BCR	C17-C18-C19-C20
23	A	854	BCR	C36-C18-C19-C20
23	A	854	BCR	C18-C19-C20-C21
23	A	854	BCR	C19-C20-C21-C22
23	A	854	BCR	C20-C21-C22-C23
23	A	854	BCR	C20-C21-C22-C37

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Mol	Chain	Res	Type	Atoms
23	A	854	BCR	C37-C22-C23-C24
23	A	854	BCR	C23-C24-C25-C30
19	B1	809	CLA	CHA-CBD-CGD-O1D
19	B1	809	CLA	CHA-CBD-CGD-O2D
19	B1	809	CLA	CAD-CBD-CGD-O1D
22	A	845	LHG	C1-C2-C3-O3
22	A	845	LHG	O2-C2-C3-O3
19	B	804	CLA	CHA-CBD-CGD-O1D
19	B	804	CLA	CHA-CBD-CGD-O2D
23	K	103	BCR	C11-C10-C9-C34
23	K	103	BCR	C10-C11-C12-C13
23	K	103	BCR	C16-C17-C18-C36
23	K	103	BCR	C17-C18-C19-C20
23	K	103	BCR	C20-C21-C22-C37
23	K	103	BCR	C21-C22-C23-C24
23	K	103	BCR	C37-C22-C23-C24
23	K	103	BCR	C23-C24-C25-C30
23	A2	851	BCR	C7-C8-C9-C34
23	A2	851	BCR	C11-C10-C9-C8
23	A2	851	BCR	C11-C10-C9-C34
23	A2	851	BCR	C10-C11-C12-C13
23	A2	851	BCR	C35-C13-C14-C15
23	A2	851	BCR	C18-C19-C20-C21
23	A2	851	BCR	C20-C21-C22-C37
23	A2	851	BCR	C37-C22-C23-C24
23	A2	851	BCR	C22-C23-C24-C25
23	B1	841	BCR	C6-C7-C8-C9
23	B1	841	BCR	C11-C12-C13-C35
23	B1	841	BCR	C35-C13-C14-C15
23	B1	841	BCR	C16-C17-C18-C19
23	B1	841	BCR	C36-C18-C19-C20
23	B1	841	BCR	C18-C19-C20-C21
23	B1	841	BCR	C21-C22-C23-C24
23	B1	841	BCR	C37-C22-C23-C24
23	B1	841	BCR	C23-C24-C25-C26
23	B1	841	BCR	C23-C24-C25-C30
19	BB	803	CLA	CHA-CBD-CGD-O1D
19	BB	803	CLA	CHA-CBD-CGD-O2D
19	BB	803	CLA	CBD-CGD-O2D-CED
19	A	824	CLA	CHA-CBD-CGD-O1D
19	A	824	CLA	CHA-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B2	813	CLA	C1A-C2A-CAA-CBA
23	A2	853	BCR	C11-C12-C13-C35
23	A2	853	BCR	C16-C17-C18-C36
23	A2	853	BCR	C36-C18-C19-C20
23	A2	853	BCR	C18-C19-C20-C21
23	A2	853	BCR	C20-C21-C22-C37
25	B2	847	LMG	C2-C1-O1-C7
25	B2	847	LMG	O6-C1-O1-C7
24	K	104	AJP	CCW-CCX-OCY-CCZ
19	BB	804	CLA	CHA-CBD-CGD-O1D
19	BB	804	CLA	CHA-CBD-CGD-O2D
19	B2	852	CLA	C2C-C3C-CAC-CBC
19	B2	852	CLA	C4C-C3C-CAC-CBC
19	B	818	CLA	CHA-CBD-CGD-O1D
19	B	818	CLA	CHA-CBD-CGD-O2D
19	A2	844	CLA	CBD-CGD-O2D-CED
19	K2	104	CLA	C3A-C2A-CAA-CBA
23	F	304	BCR	C7-C8-C9-C10
23	F	304	BCR	C11-C10-C9-C8
23	F	304	BCR	C11-C12-C13-C35
23	F	304	BCR	C35-C13-C14-C15
23	F	304	BCR	C17-C18-C19-C20
23	F	304	BCR	C36-C18-C19-C20
23	F	304	BCR	C18-C19-C20-C21
23	F	304	BCR	C20-C21-C22-C23
23	F	304	BCR	C21-C22-C23-C24
19	A	834	CLA	CHA-CBD-CGD-O1D
19	A	834	CLA	CHA-CBD-CGD-O2D
19	A1	836	CLA	CHA-CBD-CGD-O1D
19	A1	836	CLA	CHA-CBD-CGD-O2D
19	A2	804	CLA	CBD-CGD-O2D-CED
19	A1	809	CLA	C3A-C2A-CAA-CBA
19	A1	809	CLA	C2-C3-C5-C6
19	A1	809	CLA	C4-C3-C5-C6
25	B1	844	LMG	C2-C1-O1-C7
25	B1	844	LMG	O6-C1-O1-C7
19	BB	830	CLA	CHA-CBD-CGD-O1D
19	BB	830	CLA	CHA-CBD-CGD-O2D
19	FF	301	CLA	CHA-CBD-CGD-O1D
19	FF	301	CLA	CHA-CBD-CGD-O2D
19	A2	810	CLA	C2-C3-C5-C6
19	A2	810	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	BB	848	AJP	CCW-CCX-OCY-CCZ
19	BB	820	CLA	C2C-C3C-CAC-CBC
19	BB	820	CLA	C4C-C3C-CAC-CBC
19	BB	820	CLA	CAD-CBD-CGD-O2D
22	X1	102	LHG	O1-C1-C2-O2
22	X1	102	LHG	O1-C1-C2-C3
22	X1	102	LHG	C3-O3-P-O5
22	X1	102	LHG	C4-O6-P-O3
22	X1	102	LHG	C4-O6-P-O4
22	X1	102	LHG	C4-O6-P-O5
23	A	849	BCR	C7-C8-C9-C34
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C35-C13-C14-C15
23	A	849	BCR	C17-C18-C19-C20
23	A	849	BCR	C20-C21-C22-C37
23	A	849	BCR	C37-C22-C23-C24
23	A	849	BCR	C23-C24-C25-C30
23	B1	839	BCR	C35-C13-C14-C15
23	B1	839	BCR	C20-C21-C22-C37
23	B1	839	BCR	C37-C22-C23-C24
19	A1	819	CLA	C3A-C2A-CAA-CBA
23	A1	849	BCR	C7-C8-C9-C34
23	A1	849	BCR	C11-C10-C9-C34
23	A1	849	BCR	C11-C12-C13-C14
23	A1	849	BCR	C11-C12-C13-C35
23	A1	849	BCR	C17-C18-C19-C20
23	A1	849	BCR	C20-C21-C22-C37
23	A1	849	BCR	C37-C22-C23-C24
23	A1	849	BCR	C23-C24-C25-C30
19	B2	823	CLA	CHA-CBD-CGD-O1D
19	B2	823	CLA	CHA-CBD-CGD-O2D
19	B2	823	CLA	C6-C7-C8-C9
19	L	203	CLA	C1A-C2A-CAA-CBA
19	L	203	CLA	C3A-C2A-CAA-CBA
19	AA	845	CLA	CBD-CGD-O2D-CED
19	A2	834	CLA	CHA-CBD-CGD-O1D
19	A2	834	CLA	CHA-CBD-CGD-O2D
19	A2	834	CLA	CBD-CGD-O2D-CED
19	B1	815	CLA	C3A-C2A-CAA-CBA
19	B1	815	CLA	C14-C13-C15-C16
19	A2	829	CLA	C1A-C2A-CAA-CBA
19	A2	829	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A2	829	CLA	C2A-CAA-CBA-CGA
19	A2	829	CLA	CHA-CBD-CGD-O1D
19	A2	829	CLA	CHA-CBD-CGD-O2D
19	B1	810	CLA	CHA-CBD-CGD-O1D
19	B1	810	CLA	CHA-CBD-CGD-O2D
19	A1	803	CLA	CBD-CGD-O2D-CED
21	AA	844	PQN	C12-C13-C15-C16
21	AA	844	PQN	C14-C13-C15-C16
19	A1	806	CLA	C1A-C2A-CAA-CBA
19	A1	806	CLA	C3A-C2A-CAA-CBA
19	A1	806	CLA	CHA-CBD-CGD-O1D
19	A1	806	CLA	CHA-CBD-CGD-O2D
19	A1	806	CLA	CAD-CBD-CGD-O1D
23	F1	304	BCR	C7-C8-C9-C10
23	F1	304	BCR	C7-C8-C9-C34
23	F1	304	BCR	C11-C10-C9-C34
23	F1	304	BCR	C11-C12-C13-C35
23	F1	304	BCR	C36-C18-C19-C20
23	F1	304	BCR	C18-C19-C20-C21
23	F1	304	BCR	C20-C21-C22-C23
23	F1	304	BCR	C21-C22-C23-C24
19	AA	835	CLA	CBD-CGD-O2D-CED
23	A	851	BCR	C7-C8-C9-C34
23	A	851	BCR	C11-C10-C9-C8
23	A	851	BCR	C10-C11-C12-C13
23	A	851	BCR	C12-C13-C14-C15
23	A	851	BCR	C16-C17-C18-C19
23	A	851	BCR	C16-C17-C18-C36
23	A	851	BCR	C18-C19-C20-C21
23	A	851	BCR	C20-C21-C22-C37
23	A	851	BCR	C37-C22-C23-C24
23	A	851	BCR	C22-C23-C24-C25
19	B1	835	CLA	C6-C7-C8-C9
23	AA	854	BCR	C11-C12-C13-C35
23	AA	854	BCR	C13-C14-C15-C16
23	AA	854	BCR	C16-C17-C18-C36
23	AA	854	BCR	C36-C18-C19-C20
23	AA	854	BCR	C18-C19-C20-C21
23	AA	854	BCR	C20-C21-C22-C37
23	AA	854	BCR	C21-C22-C23-C24
19	B	826	CLA	C4-C3-C5-C6
19	B1	807	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	BB	823	CLA	CHA-CBD-CGD-O1D
19	BB	823	CLA	CHA-CBD-CGD-O2D
19	B1	833	CLA	C1A-C2A-CAA-CBA
20	A2	803	CL0	C6-C7-C8-C9
19	B1	812	CLA	CAD-CBD-CGD-O1D
19	B1	812	CLA	CAD-CBD-CGD-O2D
23	I1	101	BCR	C1-C6-C7-C8
23	I1	101	BCR	C11-C10-C9-C34
23	I1	101	BCR	C11-C12-C13-C35
23	I1	101	BCR	C16-C17-C18-C36
23	I1	101	BCR	C36-C18-C19-C20
23	I1	101	BCR	C20-C21-C22-C37
23	I1	101	BCR	C21-C22-C23-C24
19	B	854	CLA	CHA-CBD-CGD-O1D
19	B	854	CLA	CHA-CBD-CGD-O2D
19	B	854	CLA	C2-C3-C5-C6
19	B	854	CLA	C4-C3-C5-C6
19	AA	812	CLA	C1A-C2A-CAA-CBA
19	AA	812	CLA	C3A-C2A-CAA-CBA
19	AA	812	CLA	CBD-CGD-O2D-CED
19	BB	855	CLA	CHA-CBD-CGD-O1D
19	BB	855	CLA	CHA-CBD-CGD-O2D
23	II	102	BCR	C11-C12-C13-C35
23	II	102	BCR	C35-C13-C14-C15
23	II	102	BCR	C17-C18-C19-C20
23	II	102	BCR	C36-C18-C19-C20
19	A1	852	CLA	C2A-CAA-CBA-CGA
19	A1	852	CLA	CHA-CBD-CGD-O1D
19	A1	852	CLA	CHA-CBD-CGD-O2D
19	A1	852	CLA	CAD-CBD-CGD-O1D
23	J	104	BCR	C6-C7-C8-C9
23	J	104	BCR	C11-C10-C9-C34
23	J	104	BCR	C11-C12-C13-C35
23	J	104	BCR	C16-C17-C18-C36
23	J	104	BCR	C17-C18-C19-C20
23	J	104	BCR	C36-C18-C19-C20
23	J	104	BCR	C21-C22-C23-C24
23	J	104	BCR	C23-C24-C25-C26
19	B	812	CLA	CAD-CBD-CGD-O1D
19	B	812	CLA	CAD-CBD-CGD-O2D
19	B1	811	CLA	CHA-CBD-CGD-O1D
19	B1	811	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
23	A1	847	BCR	C11-C10-C9-C34
23	A1	847	BCR	C11-C12-C13-C35
23	A1	847	BCR	C36-C18-C19-C20
23	F2	305	BCR	C1-C6-C7-C8
23	F2	305	BCR	C5-C6-C7-C8
23	F2	305	BCR	C7-C8-C9-C10
23	F2	305	BCR	C7-C8-C9-C34
23	F2	305	BCR	C11-C10-C9-C8
23	F2	305	BCR	C10-C11-C12-C13
23	F2	305	BCR	C11-C12-C13-C14
23	F2	305	BCR	C11-C12-C13-C35
23	F2	305	BCR	C15-C16-C17-C18
23	F2	305	BCR	C16-C17-C18-C19
23	F2	305	BCR	C16-C17-C18-C36
23	F2	305	BCR	C17-C18-C19-C20
23	F2	305	BCR	C18-C19-C20-C21
23	F2	305	BCR	C20-C21-C22-C23
23	F2	305	BCR	C20-C21-C22-C37
23	F2	305	BCR	C22-C23-C24-C25
19	BB	812	CLA	CHA-CBD-CGD-O1D
19	BB	812	CLA	CHA-CBD-CGD-O2D
19	BB	812	CLA	CAD-CBD-CGD-O1D
23	BB	841	BCR	C6-C7-C8-C9
23	BB	841	BCR	C11-C12-C13-C35
23	BB	841	BCR	C35-C13-C14-C15
23	BB	841	BCR	C16-C17-C18-C36
23	BB	841	BCR	C17-C18-C19-C20
23	BB	841	BCR	C21-C22-C23-C24
23	BB	841	BCR	C37-C22-C23-C24
23	BB	841	BCR	C23-C24-C25-C26
23	BB	841	BCR	C23-C24-C25-C30
23	BB	839	BCR	C37-C22-C23-C24
23	F	303	BCR	C7-C8-C9-C34
23	F	303	BCR	C11-C10-C9-C8
23	F	303	BCR	C11-C10-C9-C34
23	F	303	BCR	C10-C11-C12-C13
23	F	303	BCR	C12-C13-C14-C15
23	F	303	BCR	C16-C17-C18-C36
23	F	303	BCR	C23-C24-C25-C30
19	BB	833	CLA	C1A-C2A-CAA-CBA
19	BB	815	CLA	C1A-C2A-CAA-CBA
19	BB	815	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	BB	815	CLA	CHA-CBD-CGD-O1D
19	BB	815	CLA	CHA-CBD-CGD-O2D
19	A2	807	CLA	C1A-C2A-CAA-CBA
19	A2	807	CLA	C3A-C2A-CAA-CBA
19	A2	807	CLA	CHA-CBD-CGD-O1D
19	A2	807	CLA	CHA-CBD-CGD-O2D
19	A2	807	CLA	CAD-CBD-CGD-O1D
20	A	803	CL0	C1A-C2A-CAA-CBA
20	A	803	CL0	C2-C1-O2A-CGA
19	B	833	CLA	CBD-CGD-O2D-CED
23	AA	850	BCR	C7-C8-C9-C34
23	AA	850	BCR	C11-C10-C9-C34
23	AA	850	BCR	C35-C13-C14-C15
23	AA	850	BCR	C17-C18-C19-C20
23	AA	850	BCR	C36-C18-C19-C20
23	AA	850	BCR	C20-C21-C22-C37
23	AA	850	BCR	C37-C22-C23-C24
23	AA	850	BCR	C23-C24-C25-C30
19	A2	824	CLA	CHA-CBD-CGD-O1D
19	A2	824	CLA	CHA-CBD-CGD-O2D
19	B1	802	CLA	CHA-CBD-CGD-O1D
19	B1	802	CLA	CHA-CBD-CGD-O2D
19	A1	810	CLA	CBD-CGD-O2D-CED
19	A1	810	CLA	C2-C3-C5-C6
19	A1	810	CLA	C4-C3-C5-C6
25	B2	845	LMG	C2-C1-O1-C7
25	B2	845	LMG	O6-C1-O1-C7
19	BB	818	CLA	CHA-CBD-CGD-O1D
19	BB	818	CLA	CHA-CBD-CGD-O2D
19	A1	822	CLA	CBD-CGD-O2D-CED
23	B2	840	BCR	C35-C13-C14-C15
23	B2	840	BCR	C16-C17-C18-C36
23	B2	840	BCR	C21-C22-C23-C24
23	B2	840	BCR	C37-C22-C23-C24
23	J1	104	BCR	C11-C10-C9-C34
23	J1	104	BCR	C11-C12-C13-C35
23	J1	104	BCR	C16-C17-C18-C36
23	J1	104	BCR	C36-C18-C19-C20
23	J1	104	BCR	C21-C22-C23-C24
23	J1	104	BCR	C23-C24-C25-C26
19	B1	813	CLA	C1A-C2A-CAA-CBA
19	B1	813	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B1	813	CLA	CHA-CBD-CGD-O2D
19	A	852	CLA	C2A-CAA-CBA-CGA
23	A1	850	BCR	C7-C8-C9-C34
23	A1	850	BCR	C11-C10-C9-C8
23	A1	850	BCR	C11-C10-C9-C34
23	A1	850	BCR	C10-C11-C12-C13
23	A1	850	BCR	C11-C12-C13-C14
23	A1	850	BCR	C16-C17-C18-C19
23	A1	850	BCR	C16-C17-C18-C36
23	A1	850	BCR	C37-C22-C23-C24
19	A2	812	CLA	C1A-C2A-CAA-CBA
19	A2	812	CLA	C3A-C2A-CAA-CBA
19	A2	812	CLA	CBD-CGD-O2D-CED
19	A2	805	CLA	C1A-C2A-CAA-CBA
19	A2	805	CLA	C3A-C2A-CAA-CBA
19	A2	805	CLA	CHA-CBD-CGD-O1D
19	A2	805	CLA	CHA-CBD-CGD-O2D
23	F1	303	BCR	C7-C8-C9-C34
23	F1	303	BCR	C11-C10-C9-C8
23	F1	303	BCR	C11-C10-C9-C34
23	F1	303	BCR	C10-C11-C12-C13
23	F1	303	BCR	C11-C12-C13-C35
23	F1	303	BCR	C12-C13-C14-C15
23	F1	303	BCR	C16-C17-C18-C36
23	F1	303	BCR	C23-C24-C25-C30
19	B1	827	CLA	C3A-C2A-CAA-CBA
19	B1	827	CLA	CBD-CGD-O2D-CED
19	B2	826	CLA	C2-C3-C5-C6
19	B2	826	CLA	C4-C3-C5-C6
19	L	204	CLA	CHA-CBD-CGD-O1D
19	L	204	CLA	CHA-CBD-CGD-O2D
19	L	204	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	C1A-C2A-CAA-CBA
19	AA	829	CLA	C3A-C2A-CAA-CBA
19	AA	829	CLA	CHA-CBD-CGD-O1D
19	AA	829	CLA	CHA-CBD-CGD-O2D
19	B1	830	CLA	CHA-CBD-CGD-O1D
19	B1	830	CLA	CHA-CBD-CGD-O2D
23	FF	303	BCR	C6-C7-C8-C9
23	FF	303	BCR	C7-C8-C9-C34
23	FF	303	BCR	C11-C10-C9-C8
23	FF	303	BCR	C11-C10-C9-C34

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Mol	Chain	Res	Type	Atoms
23	FF	303	BCR	C10-C11-C12-C13
23	FF	303	BCR	C12-C13-C14-C15
23	FF	303	BCR	C16-C17-C18-C36
23	FF	303	BCR	C21-C22-C23-C24
23	FF	303	BCR	C23-C24-C25-C30
19	B	802	CLA	C1A-C2A-CAA-CBA
19	B2	806	CLA	CHA-CBD-CGD-O1D
19	B2	806	CLA	CHA-CBD-CGD-O2D
19	B2	806	CLA	CBD-CGD-O2D-CED
19	BB	829	CLA	C4C-C3C-CAC-CBC
19	B1	833	CLA	C4C-C3C-CAC-CBC
19	BB	832	CLA	O1D-CGD-O2D-CED
19	BB	806	CLA	O1D-CGD-O2D-CED
19	B1	832	CLA	O1D-CGD-O2D-CED
19	B1	803	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	O1D-CGD-O2D-CED
19	AA	823	CLA	O1D-CGD-O2D-CED
19	A1	827	CLA	O1D-CGD-O2D-CED
19	A2	801	CLA	O1D-CGD-O2D-CED
19	A	823	CLA	O1D-CGD-O2D-CED
19	BB	816	CLA	O1D-CGD-O2D-CED
19	B	854	CLA	O1D-CGD-O2D-CED
19	AA	812	CLA	O1D-CGD-O2D-CED
19	A2	812	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	C2C-C3C-CAC-CBC
19	BB	833	CLA	C2C-C3C-CAC-CBC
19	BB	833	CLA	C4C-C3C-CAC-CBC
19	B1	806	CLA	O1D-CGD-O2D-CED
19	BB	856	CLA	O1D-CGD-O2D-CED
19	A1	811	CLA	O1D-CGD-O2D-CED
19	AA	828	CLA	O1D-CGD-O2D-CED
19	BB	808	CLA	O1D-CGD-O2D-CED
19	A	828	CLA	O1D-CGD-O2D-CED
19	A2	828	CLA	O1D-CGD-O2D-CED
19	B2	803	CLA	O1D-CGD-O2D-CED
19	B	816	CLA	O1D-CGD-O2D-CED
19	B	859	CLA	O1D-CGD-O2D-CED
19	BB	852	CLA	O1D-CGD-O2D-CED
19	F1	301	CLA	O1D-CGD-O2D-CED
19	B1	848	CLA	O1D-CGD-O2D-CED
19	BB	803	CLA	O1D-CGD-O2D-CED
19	B1	816	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	833	CLA	O1D-CGD-O2D-CED
19	A1	822	CLA	O1D-CGD-O2D-CED
19	B2	806	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	CBD-CGD-O2D-CED
19	BB	856	CLA	CBD-CGD-O2D-CED
19	BB	801	CLA	CBD-CGD-O2D-CED
19	A	831	CLA	CBD-CGD-O2D-CED
19	B2	824	CLA	CBD-CGD-O2D-CED
19	AA	822	CLA	CBD-CGD-O2D-CED
19	A	801	CLA	CBD-CGD-O2D-CED
19	BB	808	CLA	CBD-CGD-O2D-CED
19	BB	831	CLA	CBD-CGD-O2D-CED
19	LL	203	CLA	CBD-CGD-O2D-CED
19	B2	812	CLA	CBD-CGD-O2D-CED
19	A2	837	CLA	CBD-CGD-O2D-CED
19	A2	811	CLA	CBD-CGD-O2D-CED
19	B	827	CLA	CBD-CGD-O2D-CED
19	B1	803	CLA	CBD-CGD-O2D-CED
19	BB	824	CLA	CBD-CGD-O2D-CED
19	B	806	CLA	CBD-CGD-O2D-CED
19	A2	831	CLA	CBD-CGD-O2D-CED
19	AA	823	CLA	CBD-CGD-O2D-CED
19	B	832	CLA	CBD-CGD-O2D-CED
19	AA	801	CLA	CBD-CGD-O2D-CED
19	A1	801	CLA	CBD-CGD-O2D-CED
19	A	804	CLA	CBD-CGD-O2D-CED
19	A1	827	CLA	CBD-CGD-O2D-CED
19	L1	207	CLA	CBD-CGD-O2D-CED
19	A2	801	CLA	CBD-CGD-O2D-CED
19	B2	803	CLA	CBD-CGD-O2D-CED
19	B	816	CLA	CBD-CGD-O2D-CED
19	B1	801	CLA	CBD-CGD-O2D-CED
19	B	859	CLA	CBD-CGD-O2D-CED
19	J2	101	CLA	CBD-CGD-O2D-CED
19	B	824	CLA	CBD-CGD-O2D-CED
19	A	823	CLA	CBD-CGD-O2D-CED
19	B1	850	CLA	CBD-CGD-O2D-CED
19	BB	816	CLA	CBD-CGD-O2D-CED
19	F2	301	CLA	CBD-CGD-O2D-CED
19	B2	827	CLA	CBD-CGD-O2D-CED
19	J	103	CLA	CBD-CGD-O2D-CED
19	A1	830	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A1	829	CLA	CBD-CGD-O2D-CED
19	B2	801	CLA	CBD-CGD-O2D-CED
19	F1	301	CLA	CBD-CGD-O2D-CED
19	A2	816	CLA	CBD-CGD-O2D-CED
19	F	301	CLA	CBD-CGD-O2D-CED
19	A	820	CLA	CBD-CGD-O2D-CED
19	A	824	CLA	CBD-CGD-O2D-CED
19	B2	852	CLA	CBD-CGD-O2D-CED
19	A1	836	CLA	CBD-CGD-O2D-CED
19	BB	830	CLA	CBD-CGD-O2D-CED
19	FF	301	CLA	CBD-CGD-O2D-CED
19	BB	820	CLA	CBD-CGD-O2D-CED
19	A1	834	CLA	CBD-CGD-O2D-CED
19	B1	815	CLA	CBD-CGD-O2D-CED
19	B1	810	CLA	CBD-CGD-O2D-CED
19	A2	832	CLA	CBD-CGD-O2D-CED
19	B1	816	CLA	CBD-CGD-O2D-CED
19	A2	830	CLA	CBD-CGD-O2D-CED
19	B	854	CLA	CBD-CGD-O2D-CED
19	B	812	CLA	CBD-CGD-O2D-CED
19	J1	101	CLA	CBD-CGD-O2D-CED
19	A2	836	CLA	CBD-CGD-O2D-CED
19	AA	829	CLA	CBD-CGD-O2D-CED
19	B1	806	CLA	O1A-CGA-O2A-C1
19	BB	806	CLA	O1A-CGA-O2A-C1
20	A1	802	CL0	O1A-CGA-O2A-C1
19	B	806	CLA	O1A-CGA-O2A-C1
22	L1	211	LHG	O10-C23-O8-C6
19	B2	807	CLA	O1A-CGA-O2A-C1
19	B1	807	CLA	O1A-CGA-O2A-C1
19	B2	806	CLA	O1A-CGA-O2A-C1
24	L2	202	AJP	CCW-CCX-OCY-CCZ
24	KK	104	AJP	CCW-CCX-OCY-CCZ
25	I2	105	LMG	C4-C5-C6-O5
19	B	803	CLA	O1D-CGD-O2D-CED
19	LL	203	CLA	O1D-CGD-O2D-CED
19	B	827	CLA	O1D-CGD-O2D-CED
19	BB	824	CLA	O1D-CGD-O2D-CED
19	B2	849	CLA	O1D-CGD-O2D-CED
19	A1	815	CLA	O1D-CGD-O2D-CED
19	B1	850	CLA	O1D-CGD-O2D-CED
19	F	301	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	FF	301	CLA	O1D-CGD-O2D-CED
19	B1	810	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	C4C-C3C-CAC-CBC
19	A2	823	CLA	O1D-CGD-O2D-CED
19	B2	824	CLA	O1D-CGD-O2D-CED
19	F2	302	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	O1D-CGD-O2D-CED
19	K1	105	CLA	O1D-CGD-O2D-CED
19	A2	825	CLA	O1D-CGD-O2D-CED
19	L2	206	CLA	O1D-CGD-O2D-CED
19	A	816	CLA	O1D-CGD-O2D-CED
19	BB	810	CLA	O1D-CGD-O2D-CED
19	L1	207	CLA	O1D-CGD-O2D-CED
19	A	811	CLA	O1D-CGD-O2D-CED
19	F	302	CLA	O1D-CGD-O2D-CED
19	B	824	CLA	O1D-CGD-O2D-CED
19	A1	844	CLA	O1D-CGD-O2D-CED
19	F2	301	CLA	O1D-CGD-O2D-CED
19	AA	816	CLA	O1D-CGD-O2D-CED
19	B2	810	CLA	O1D-CGD-O2D-CED
19	A2	816	CLA	O1D-CGD-O2D-CED
19	AA	811	CLA	O1D-CGD-O2D-CED
19	A2	844	CLA	O1D-CGD-O2D-CED
19	AA	845	CLA	O1D-CGD-O2D-CED
19	A1	810	CLA	O1D-CGD-O2D-CED
19	L	204	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	CBA-CGA-O2A-C1
19	BB	806	CLA	CBA-CGA-O2A-C1
25	B	845	LMG	C29-C28-O8-C9
25	B1	852	LMG	C29-C28-O8-C9
19	B	806	CLA	CBA-CGA-O2A-C1
25	B2	854	LMG	C29-C28-O8-C9
19	B2	807	CLA	CBA-CGA-O2A-C1
25	B1	844	LMG	C29-C28-O8-C9
19	B1	807	CLA	CBA-CGA-O2A-C1
25	B2	845	LMG	C29-C28-O8-C9
19	B2	806	CLA	CBA-CGA-O2A-C1
19	BB	829	CLA	C2C-C3C-CAC-CBC
19	KK	102	CLA	CBD-CGD-O2D-CED
19	A2	814	CLA	CBD-CGD-O2D-CED
19	AA	834	CLA	CBD-CGD-O2D-CED
19	B1	831	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	A	844	CLA	CBD-CGD-O2D-CED
19	A	836	CLA	CBD-CGD-O2D-CED
19	A1	823	CLA	CBD-CGD-O2D-CED
19	A	829	CLA	CBD-CGD-O2D-CED
19	J	101	CLA	CBD-CGD-O2D-CED
19	A1	835	CLA	CBD-CGD-O2D-CED
19	AA	831	CLA	CBD-CGD-O2D-CED
19	B2	832	CLA	CBD-CGD-O2D-CED
19	A2	838	CLA	CBD-CGD-O2D-CED
19	B	815	CLA	CBD-CGD-O2D-CED
19	B2	837	CLA	CBD-CGD-O2D-CED
19	A2	826	CLA	CBD-CGD-O2D-CED
19	A	813	CLA	CBD-CGD-O2D-CED
19	AA	820	CLA	CBD-CGD-O2D-CED
19	AA	836	CLA	CBD-CGD-O2D-CED
19	JJ	101	CLA	CBD-CGD-O2D-CED
19	A1	828	CLA	CBD-CGD-O2D-CED
19	B1	836	CLA	CBD-CGD-O2D-CED
19	A1	825	CLA	CBD-CGD-O2D-CED
19	A2	808	CLA	CBD-CGD-O2D-CED
19	B1	820	CLA	CBD-CGD-O2D-CED
19	B	837	CLA	CBD-CGD-O2D-CED
19	A1	837	CLA	CBD-CGD-O2D-CED
19	K	102	CLA	CBD-CGD-O2D-CED
19	A1	831	CLA	CBD-CGD-O2D-CED
19	A	834	CLA	CBD-CGD-O2D-CED
19	A1	819	CLA	CBD-CGD-O2D-CED
19	A2	829	CLA	CBD-CGD-O2D-CED
19	A1	852	CLA	CBD-CGD-O2D-CED
19	BB	815	CLA	CBD-CGD-O2D-CED
19	AA	817	CLA	CBD-CGD-O2D-CED
19	B2	829	CLA	CBD-CGD-O2D-CED
19	B	834	CLA	O1A-CGA-O2A-C1
19	A2	839	CLA	O1A-CGA-O2A-C1
19	A	839	CLA	O1A-CGA-O2A-C1
22	L2	208	LHG	O10-C23-O8-C6
20	AA	803	CL0	O1A-CGA-O2A-C1
19	B2	802	CLA	O1A-CGA-O2A-C1
25	B1	852	LMG	O10-C28-O8-C9
19	A1	814	CLA	O1A-CGA-O2A-C1
25	I1	102	LMG	O10-C28-O8-C9
19	A	815	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	AA	839	CLA	O1A-CGA-O2A-C1
28	B	856	DGD	O1A-C1A-O1G-C1G
28	BB	854	DGD	O1A-C1A-O1G-C1G
25	B1	846	LMG	O10-C28-O8-C9
25	B2	854	LMG	O10-C28-O8-C9
19	BB	807	CLA	O1A-CGA-O2A-C1
19	AA	815	CLA	O1A-CGA-O2A-C1
19	B2	834	CLA	O1A-CGA-O2A-C1
19	BB	802	CLA	O1A-CGA-O2A-C1
19	A2	815	CLA	O1A-CGA-O2A-C1
25	B2	847	LMG	O10-C28-O8-C9
19	FF	301	CLA	O1A-CGA-O2A-C1
19	B	826	CLA	O1A-CGA-O2A-C1
19	B1	833	CLA	O1A-CGA-O2A-C1
19	BB	833	CLA	O1A-CGA-O2A-C1
19	FF	302	CLA	O1D-CGD-O2D-CED
19	A	830	CLA	O1D-CGD-O2D-CED
19	F1	302	CLA	O1D-CGD-O2D-CED
19	B1	824	CLA	O1D-CGD-O2D-CED
19	A2	804	CLA	O1D-CGD-O2D-CED
19	A1	803	CLA	O1D-CGD-O2D-CED
19	B	834	CLA	C2C-C3C-CAC-CBC
19	B2	834	CLA	C4C-C3C-CAC-CBC
19	AA	830	CLA	O1D-CGD-O2D-CED
19	A1	833	CLA	O1D-CGD-O2D-CED
19	B2	851	CLA	O1D-CGD-O2D-CED
19	A	835	CLA	O1D-CGD-O2D-CED
19	B2	816	CLA	O1D-CGD-O2D-CED
19	A2	834	CLA	O1D-CGD-O2D-CED
19	B1	827	CLA	O1D-CGD-O2D-CED
19	B	819	CLA	CBD-CGD-O2D-CED
19	AA	813	CLA	CBD-CGD-O2D-CED
19	A	817	CLA	CBD-CGD-O2D-CED
19	B1	833	CLA	CBD-CGD-O2D-CED
25	I1	102	LMG	O9-C10-O7-C8
28	B	856	DGD	O1B-C1B-O2G-C2G
28	BB	854	DGD	O1B-C1B-O2G-C2G
25	II	105	LMG	O9-C10-O7-C8
24	L2	203	AJP	OBC-CBJ-CCB-CCA
19	A1	830	CLA	O1D-CGD-O2D-CED
19	AA	804	CLA	O1D-CGD-O2D-CED
19	B2	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	801	CLA	O1D-CGD-O2D-CED
19	A2	835	CLA	O1D-CGD-O2D-CED
19	A1	836	CLA	O1D-CGD-O2D-CED
19	A1	834	CLA	O1D-CGD-O2D-CED
19	AA	835	CLA	O1D-CGD-O2D-CED
25	B	845	LMG	O10-C28-O8-C9
19	BB	826	CLA	O1A-CGA-O2A-C1
19	A2	823	CLA	C3-C5-C6-C7
19	L2	205	CLA	C3-C5-C6-C7
19	AA	823	CLA	C3-C5-C6-C7
19	AA	808	CLA	C3-C5-C6-C7
19	B2	804	CLA	C3-C5-C6-C7
19	A	823	CLA	C3-C5-C6-C7
19	A	835	CLA	C3-C5-C6-C7
19	B	804	CLA	C3-C5-C6-C7
19	BB	804	CLA	C3-C5-C6-C7
19	FF	301	CLA	C3-C5-C6-C7
19	AA	835	CLA	C3-C5-C6-C7
19	A1	822	CLA	C3-C5-C6-C7
24	B	849	AJP	OBC-CBJ-CCB-OCC
25	I2	105	LMG	O6-C5-C6-O5
19	B	834	CLA	CBA-CGA-O2A-C1
22	L2	208	LHG	C24-C23-O8-C6
20	AA	803	CL0	CBA-CGA-O2A-C1
19	B	807	CLA	CBA-CGA-O2A-C1
19	A	801	CLA	CBA-CGA-O2A-C1
20	A1	802	CL0	CBA-CGA-O2A-C1
25	BB	844	LMG	C29-C28-O8-C9
19	A1	814	CLA	CBA-CGA-O2A-C1
19	A	815	CLA	CBA-CGA-O2A-C1
19	A1	801	CLA	CBA-CGA-O2A-C1
22	L1	211	LHG	C24-C23-O8-C6
19	A	813	CLA	CBA-CGA-O2A-C1
25	B1	846	LMG	C29-C28-O8-C9
19	A2	801	CLA	CBA-CGA-O2A-C1
19	AA	815	CLA	CBA-CGA-O2A-C1
19	B2	834	CLA	CBA-CGA-O2A-C1
19	BB	816	CLA	CBA-CGA-O2A-C1
19	A2	815	CLA	CBA-CGA-O2A-C1
19	AA	813	CLA	CBA-CGA-O2A-C1
25	B2	847	LMG	C29-C28-O8-C9
19	B1	833	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	BB	833	CLA	CBA-CGA-O2A-C1
19	A1	821	CLA	CBA-CGA-O2A-C1
22	L2	208	LHG	C8-C7-O7-C5
22	LL	205	LHG	C8-C7-O7-C5
22	L	207	LHG	C8-C7-O7-C5
22	L1	211	LHG	C8-C7-O7-C5
19	B2	834	CLA	C2C-C3C-CAC-CBC
19	BB	801	CLA	O1D-CGD-O2D-CED
19	A2	811	CLA	O1D-CGD-O2D-CED
19	A	804	CLA	O1D-CGD-O2D-CED
19	A	824	CLA	O1D-CGD-O2D-CED
19	AA	838	CLA	CBD-CGD-O2D-CED
19	B1	808	CLA	CBD-CGD-O2D-CED
19	AA	808	CLA	CBD-CGD-O2D-CED
19	A2	820	CLA	CBD-CGD-O2D-CED
19	B2	834	CLA	CBD-CGD-O2D-CED
19	B2	831	CLA	CBD-CGD-O2D-CED
19	A1	812	CLA	CBD-CGD-O2D-CED
19	A2	813	CLA	CBD-CGD-O2D-CED
19	B1	812	CLA	CBD-CGD-O2D-CED
19	BB	812	CLA	CBD-CGD-O2D-CED
19	A1	820	CLA	O1A-CGA-O2A-C1
19	A1	812	CLA	O1A-CGA-O2A-C1
24	L1	204	AJP	OBC-CBJ-CCB-CCA
19	A	825	CLA	C3-C5-C6-C7
19	AA	825	CLA	C3-C5-C6-C7
24	BB	848	AJP	OBC-CBJ-CCB-OCC
19	A1	811	CLA	C2A-CAA-CBA-CGA
19	A	830	CLA	C2A-CAA-CBA-CGA
19	AA	830	CLA	C2A-CAA-CBA-CGA
19	A1	828	CLA	C2A-CAA-CBA-CGA
19	A1	829	CLA	C2A-CAA-CBA-CGA
19	BB	835	CLA	C2A-CAA-CBA-CGA
19	B2	836	CLA	C2A-CAA-CBA-CGA
19	FF	301	CLA	C2A-CAA-CBA-CGA
19	B1	835	CLA	C2A-CAA-CBA-CGA
19	A2	830	CLA	C2A-CAA-CBA-CGA
19	A2	852	CLA	C2A-CAA-CBA-CGA
19	B	860	CLA	CBD-CGD-O2D-CED
19	XX	101	CLA	CBD-CGD-O2D-CED
19	BB	819	CLA	CBD-CGD-O2D-CED
19	AA	853	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B2	820	CLA	CBD-CGD-O2D-CED
19	B1	826	CLA	C4-C3-C5-C6
19	BB	833	CLA	C4-C3-C5-C6
19	B	834	CLA	C2-C3-C5-C6
19	B1	826	CLA	C2-C3-C5-C6
21	A2	843	PQN	C12-C13-C15-C16
21	A	843	PQN	C12-C13-C15-C16
19	B	816	CLA	C2-C3-C5-C6
19	BB	852	CLA	C2-C3-C5-C6
19	B	826	CLA	C2-C3-C5-C6
19	AA	808	CLA	O1A-CGA-O2A-C1
19	B2	801	CLA	O1A-CGA-O2A-C1
19	A2	808	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	O10-C28-O8-C9
25	B2	845	LMG	O10-C28-O8-C9
19	A1	838	CLA	O1A-CGA-O2A-C1
19	A1	829	CLA	O1D-CGD-O2D-CED
19	A	820	CLA	O1D-CGD-O2D-CED
19	B	807	CLA	C3-C5-C6-C7
19	BB	807	CLA	C3-C5-C6-C7
19	A2	808	CLA	C3-C5-C6-C7
19	B1	804	CLA	C3-C5-C6-C7
20	A	803	CL0	C3-C5-C6-C7
25	B1	846	LMG	C4-C5-C6-O5
19	BB	801	CLA	CBA-CGA-O2A-C1
19	AA	843	CLA	CBA-CGA-O2A-C1
19	A2	839	CLA	CBA-CGA-O2A-C1
19	A	839	CLA	CBA-CGA-O2A-C1
19	BB	832	CLA	CBA-CGA-O2A-C1
19	B2	802	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	CBA-CGA-O2A-C1
19	A1	807	CLA	CBA-CGA-O2A-C1
19	AA	839	CLA	CBA-CGA-O2A-C1
28	B	856	DGD	C2A-C1A-O1G-C1G
19	AA	801	CLA	CBA-CGA-O2A-C1
28	BB	854	DGD	C2A-C1A-O1G-C1G
19	BB	807	CLA	CBA-CGA-O2A-C1
19	BB	826	CLA	CBA-CGA-O2A-C1
19	B	816	CLA	CBA-CGA-O2A-C1
19	A	819	CLA	CBA-CGA-O2A-C1
25	II	105	LMG	C29-C28-O8-C9
19	BB	802	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	B	823	CLA	CBA-CGA-O2A-C1
19	B2	801	CLA	CBA-CGA-O2A-C1
19	F	301	CLA	CBA-CGA-O2A-C1
19	A1	812	CLA	CBA-CGA-O2A-C1
19	FF	301	CLA	CBA-CGA-O2A-C1
19	AA	819	CLA	CBA-CGA-O2A-C1
19	A2	813	CLA	CBA-CGA-O2A-C1
19	B	826	CLA	CBA-CGA-O2A-C1
20	A	803	CL0	CBA-CGA-O2A-C1
19	A2	837	CLA	O1D-CGD-O2D-CED
19	B	832	CLA	O1D-CGD-O2D-CED
19	BB	836	CLA	CBD-CGD-O2D-CED
20	AA	803	CL0	CBD-CGD-O2D-CED
19	A	808	CLA	CBD-CGD-O2D-CED
19	A1	807	CLA	CBD-CGD-O2D-CED
19	A1	814	CLA	CBD-CGD-O2D-CED
19	A	815	CLA	CBD-CGD-O2D-CED
19	A	822	CLA	CBD-CGD-O2D-CED
19	B1	819	CLA	CBD-CGD-O2D-CED
19	AA	815	CLA	CBD-CGD-O2D-CED
19	A1	842	CLA	CBD-CGD-O2D-CED
19	BB	813	CLA	CBD-CGD-O2D-CED
19	A2	815	CLA	CBD-CGD-O2D-CED
19	A	832	CLA	CBD-CGD-O2D-CED
20	A2	803	CL0	CBD-CGD-O2D-CED
19	A	838	CLA	CBD-CGD-O2D-CED
19	A	852	CLA	CBD-CGD-O2D-CED
19	B1	830	CLA	CBD-CGD-O2D-CED
24	B	849	AJP	OCC-CCX-OCY-CCZ
19	A	831	CLA	O1D-CGD-O2D-CED
19	AA	822	CLA	O1D-CGD-O2D-CED
19	A1	801	CLA	O1D-CGD-O2D-CED
19	B1	801	CLA	O1D-CGD-O2D-CED
19	B2	827	CLA	O1D-CGD-O2D-CED
19	J	103	CLA	O1D-CGD-O2D-CED
19	BB	820	CLA	O1D-CGD-O2D-CED
19	J1	101	CLA	O1D-CGD-O2D-CED
19	A1	840	CLA	CBA-CGA-O2A-C1
19	A2	841	CLA	CBA-CGA-O2A-C1
19	AA	843	CLA	O1A-CGA-O2A-C1
19	B	860	CLA	O1A-CGA-O2A-C1
19	B1	826	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	BB	844	LMG	O10-C28-O8-C9
19	A2	821	CLA	O1A-CGA-O2A-C1
19	A2	819	CLA	O1A-CGA-O2A-C1
19	A1	818	CLA	O1A-CGA-O2A-C1
25	M	102	LMG	O10-C28-O8-C9
19	AA	821	CLA	O1A-CGA-O2A-C1
19	B1	801	CLA	O1A-CGA-O2A-C1
19	A	819	CLA	O1A-CGA-O2A-C1
19	A	821	CLA	O1A-CGA-O2A-C1
19	B	801	CLA	O1A-CGA-O2A-C1
19	B2	852	CLA	O1A-CGA-O2A-C1
19	AA	819	CLA	O1A-CGA-O2A-C1
19	A2	813	CLA	O1A-CGA-O2A-C1
19	A2	822	CLA	O1A-CGA-O2A-C1
19	B1	802	CLA	O1A-CGA-O2A-C1
19	A1	821	CLA	O1A-CGA-O2A-C1
19	B2	826	CLA	O1A-CGA-O2A-C1
19	B	802	CLA	O1A-CGA-O2A-C1
19	BB	831	CLA	O1D-CGD-O2D-CED
23	A	853	BCR	C15-C16-C17-C18
23	LL	204	BCR	C9-C10-C11-C12
23	F1	306	BCR	C15-C16-C17-C18
23	L2	207	BCR	C9-C10-C11-C12
23	I2	101	BCR	C9-C10-C11-C12
23	MM	101	BCR	C19-C20-C21-C22
23	A1	853	BCR	C13-C14-C15-C16
23	A2	853	BCR	C13-C14-C15-C16
23	A2	853	BCR	C15-C16-C17-C18
23	AA	854	BCR	C15-C16-C17-C18
19	AA	826	CLA	CBD-CGD-O2D-CED
19	B	823	CLA	CBD-CGD-O2D-CED
19	A	826	CLA	CBD-CGD-O2D-CED
19	B2	823	CLA	CBD-CGD-O2D-CED
19	BB	823	CLA	CBD-CGD-O2D-CED
19	A	801	CLA	O1D-CGD-O2D-CED
19	BB	830	CLA	O1D-CGD-O2D-CED
19	A2	830	CLA	O1D-CGD-O2D-CED
24	B	850	AJP	OBC-CBJ-CCB-OCC
25	M	102	LMG	O6-C5-C6-O5
19	A	801	CLA	O1A-CGA-O2A-C1
19	AA	801	CLA	O1A-CGA-O2A-C1
19	A1	801	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A	813	CLA	O1A-CGA-O2A-C1
19	A2	801	CLA	O1A-CGA-O2A-C1
19	A1	842	CLA	O1A-CGA-O2A-C1
25	II	105	LMG	O10-C28-O8-C9
19	BB	816	CLA	O1A-CGA-O2A-C1
19	AA	813	CLA	O1A-CGA-O2A-C1
19	F	301	CLA	O1A-CGA-O2A-C1
19	A2	823	CLA	CBA-CGA-O2A-C1
19	B	860	CLA	CBA-CGA-O2A-C1
19	B1	832	CLA	CBA-CGA-O2A-C1
19	A1	835	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	C29-C28-O8-C9
19	A2	819	CLA	CBA-CGA-O2A-C1
25	M	102	LMG	C29-C28-O8-C9
19	AA	821	CLA	CBA-CGA-O2A-C1
19	B	831	CLA	CBA-CGA-O2A-C1
19	AA	808	CLA	CBA-CGA-O2A-C1
19	A2	820	CLA	CBA-CGA-O2A-C1
19	AA	820	CLA	CBA-CGA-O2A-C1
19	A	821	CLA	CBA-CGA-O2A-C1
19	F2	301	CLA	CBA-CGA-O2A-C1
19	B2	831	CLA	CBA-CGA-O2A-C1
19	A2	808	CLA	CBA-CGA-O2A-C1
19	B2	833	CLA	CBA-CGA-O2A-C1
19	A	820	CLA	CBA-CGA-O2A-C1
19	B2	852	CLA	CBA-CGA-O2A-C1
19	A1	809	CLA	CBA-CGA-O2A-C1
19	BB	830	CLA	CBA-CGA-O2A-C1
19	B2	823	CLA	CBA-CGA-O2A-C1
19	BB	823	CLA	CBA-CGA-O2A-C1
19	B	833	CLA	CBA-CGA-O2A-C1
19	A1	822	CLA	CBA-CGA-O2A-C1
19	A1	838	CLA	CBA-CGA-O2A-C1
19	B2	826	CLA	CBA-CGA-O2A-C1
19	B1	830	CLA	CBA-CGA-O2A-C1
22	BB	851	LHG	O2-C2-C3-O3
22	L2	208	LHG	O2-C2-C3-O3
22	B1	847	LHG	O2-C2-C3-O3
22	B2	848	LHG	O2-C2-C3-O3
22	B	853	LHG	O2-C2-C3-O3
22	A1	845	LHG	O2-C2-C3-O3
19	A2	831	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	B	812	CLA	O1D-CGD-O2D-CED
19	AA	829	CLA	O1D-CGD-O2D-CED
19	AA	812	CLA	CBA-CGA-O2A-C1
25	M	102	LMG	C4-C5-C6-O5
19	AA	843	CLA	CBD-CGD-O2D-CED
19	A1	826	CLA	CBD-CGD-O2D-CED
19	B1	815	CLA	O1D-CGD-O2D-CED
19	A2	832	CLA	O1D-CGD-O2D-CED
19	A2	836	CLA	O1D-CGD-O2D-CED
24	L2	202	AJP	OBC-CBJ-CCB-OCC
25	B1	846	LMG	O6-C5-C6-O5
24	A1	854	AJP	OBC-CBJ-CCB-CCA
23	A	848	BCR	C14-C15-C16-C17
23	AA	849	BCR	C14-C15-C16-C17
23	B2	844	BCR	C14-C15-C16-C17
19	J2	101	CLA	O1D-CGD-O2D-CED
19	B2	815	CLA	C3-C5-C6-C7
19	B1	815	CLA	C3-C5-C6-C7
19	A2	805	CLA	C3-C5-C6-C7
19	AA	834	CLA	O1D-CGD-O2D-CED
19	A1	835	CLA	O1D-CGD-O2D-CED
19	AA	831	CLA	O1D-CGD-O2D-CED
19	B2	852	CLA	O1D-CGD-O2D-CED
19	B1	826	CLA	CBA-CGA-O2A-C1
19	A2	821	CLA	CBA-CGA-O2A-C1
19	AA	823	CLA	CBA-CGA-O2A-C1
19	A1	818	CLA	CBA-CGA-O2A-C1
19	A1	820	CLA	CBA-CGA-O2A-C1
19	B1	801	CLA	CBA-CGA-O2A-C1
19	A1	842	CLA	CBA-CGA-O2A-C1
19	A	823	CLA	CBA-CGA-O2A-C1
19	B	801	CLA	CBA-CGA-O2A-C1
19	A2	822	CLA	CBA-CGA-O2A-C1
19	B1	802	CLA	CBA-CGA-O2A-C1
19	B	802	CLA	CBA-CGA-O2A-C1
19	BB	801	CLA	O1A-CGA-O2A-C1
19	B1	832	CLA	O1A-CGA-O2A-C1
19	B	831	CLA	O1A-CGA-O2A-C1
19	AA	820	CLA	O1A-CGA-O2A-C1
19	B	816	CLA	O1A-CGA-O2A-C1
19	B	823	CLA	O1A-CGA-O2A-C1
19	B2	833	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	L1	210	LMG	O10-C28-O8-C9
19	A1	809	CLA	O1A-CGA-O2A-C1
19	B2	823	CLA	O1A-CGA-O2A-C1
19	BB	823	CLA	O1A-CGA-O2A-C1
19	B	833	CLA	O1A-CGA-O2A-C1
24	A1	854	AJP	OBC-CBJ-CCB-OCC
19	B	836	CLA	C2A-CAA-CBA-CGA
19	A2	812	CLA	C2A-CAA-CBA-CGA
19	AA	829	CLA	C2A-CAA-CBA-CGA
19	BB	856	CLA	C4-C3-C5-C6
20	AA	803	CL0	C4-C3-C5-C6
19	BB	811	CLA	C4-C3-C5-C6
19	A	810	CLA	C4-C3-C5-C6
19	A2	819	CLA	C4-C3-C5-C6
19	AA	842	CLA	C4-C3-C5-C6
19	A1	818	CLA	C4-C3-C5-C6
19	B2	811	CLA	C4-C3-C5-C6
19	L	202	CLA	C4-C3-C5-C6
19	AA	810	CLA	C4-C3-C5-C6
19	B	811	CLA	C4-C3-C5-C6
19	B	859	CLA	C4-C3-C5-C6
19	A	842	CLA	C4-C3-C5-C6
19	A	819	CLA	C4-C3-C5-C6
19	B1	850	CLA	C4-C3-C5-C6
19	B2	834	CLA	C4-C3-C5-C6
19	A1	828	CLA	C4-C3-C5-C6
19	BB	816	CLA	C4-C3-C5-C6
19	B2	851	CLA	C4-C3-C5-C6
19	B	823	CLA	C4-C3-C5-C6
19	B2	816	CLA	C4-C3-C5-C6
19	LL	201	CLA	C4-C3-C5-C6
19	B1	823	CLA	C4-C3-C5-C6
19	AA	819	CLA	C4-C3-C5-C6
19	B2	823	CLA	C4-C3-C5-C6
19	B1	816	CLA	C4-C3-C5-C6
19	BB	823	CLA	C4-C3-C5-C6
19	B1	833	CLA	C4-C3-C5-C6
19	B1	811	CLA	C4-C3-C5-C6
19	BB	856	CLA	C2-C3-C5-C6
20	AA	803	CL0	C2-C3-C5-C6
19	BB	811	CLA	C2-C3-C5-C6
19	A	810	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	A2	819	CLA	C2-C3-C5-C6
19	AA	842	CLA	C2-C3-C5-C6
19	A1	818	CLA	C2-C3-C5-C6
19	B2	811	CLA	C2-C3-C5-C6
19	L	202	CLA	C2-C3-C5-C6
19	AA	810	CLA	C2-C3-C5-C6
19	B	811	CLA	C2-C3-C5-C6
19	A2	842	CLA	C2-C3-C5-C6
19	B	859	CLA	C2-C3-C5-C6
19	A1	841	CLA	C2-C3-C5-C6
19	A	842	CLA	C2-C3-C5-C6
19	A	819	CLA	C2-C3-C5-C6
19	B1	850	CLA	C2-C3-C5-C6
19	B2	834	CLA	C2-C3-C5-C6
19	A1	828	CLA	C2-C3-C5-C6
19	BB	816	CLA	C2-C3-C5-C6
19	B2	851	CLA	C2-C3-C5-C6
19	B	823	CLA	C2-C3-C5-C6
19	B2	816	CLA	C2-C3-C5-C6
19	LL	201	CLA	C2-C3-C5-C6
19	B1	823	CLA	C2-C3-C5-C6
19	AA	819	CLA	C2-C3-C5-C6
19	B2	823	CLA	C2-C3-C5-C6
19	B1	816	CLA	C2-C3-C5-C6
19	BB	823	CLA	C2-C3-C5-C6
19	B1	833	CLA	C2-C3-C5-C6
19	B1	811	CLA	C2-C3-C5-C6
19	BB	833	CLA	C2-C3-C5-C6
24	BB	849	AJP	OBC-CBJ-CCB-CCA
19	A2	830	CLA	C2C-C3C-CAC-CBC
19	A2	823	CLA	O1A-CGA-O2A-C1
19	BB	832	CLA	O1A-CGA-O2A-C1
19	A1	835	CLA	O1A-CGA-O2A-C1
19	F2	301	CLA	O1A-CGA-O2A-C1
19	B2	831	CLA	O1A-CGA-O2A-C1
19	A	820	CLA	O1A-CGA-O2A-C1
19	BB	830	CLA	O1A-CGA-O2A-C1
20	A	803	CL0	O1A-CGA-O2A-C1
19	A1	822	CLA	O1A-CGA-O2A-C1
19	B1	830	CLA	O1A-CGA-O2A-C1
19	B2	812	CLA	O1D-CGD-O2D-CED
19	A1	823	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	AA	801	CLA	O1D-CGD-O2D-CED
19	B	837	CLA	O1D-CGD-O2D-CED
19	A	821	CLA	C8-C10-C11-C12
19	B1	831	CLA	O1D-CGD-O2D-CED
19	A	836	CLA	O1D-CGD-O2D-CED
19	AA	820	CLA	O1D-CGD-O2D-CED
19	A1	825	CLA	O1D-CGD-O2D-CED
19	A2	808	CLA	O1D-CGD-O2D-CED
19	A1	837	CLA	O1D-CGD-O2D-CED
19	A1	831	CLA	O1D-CGD-O2D-CED
19	A1	852	CLA	O1D-CGD-O2D-CED
19	A1	813	CLA	CBD-CGD-O2D-CED
22	A2	846	LHG	C24-C23-O8-C6
19	B2	811	CLA	CBA-CGA-O2A-C1
19	L	202	CLA	CBA-CGA-O2A-C1
22	B2	848	LHG	C24-C23-O8-C6
19	B	811	CLA	CBA-CGA-O2A-C1
19	F1	301	CLA	CBA-CGA-O2A-C1
19	A1	819	CLA	CBA-CGA-O2A-C1
20	A2	803	CL0	CBA-CGA-O2A-C1
19	A1	801	CLA	C8-C10-C11-C12
24	L1	203	AJP	OBC-CBJ-CCB-CCA
19	AA	823	CLA	O1A-CGA-O2A-C1
19	A2	820	CLA	O1A-CGA-O2A-C1
19	A	823	CLA	O1A-CGA-O2A-C1
19	A2	838	CLA	O1D-CGD-O2D-CED
19	B1	820	CLA	O1D-CGD-O2D-CED
22	B1	847	LHG	C1-C2-C3-O3
19	B	836	CLA	CBD-CGD-O2D-CED
19	B1	835	CLA	CBD-CGD-O2D-CED
25	II	105	LMG	O6-C5-C6-O5
24	L1	204	AJP	OBC-CBJ-CCB-OCC
24	BB	848	AJP	OCC-CCX-OCY-CCZ
19	K	102	CLA	O1D-CGD-O2D-CED
19	K1	105	CLA	C2C-C3C-CAC-CBC
19	A	808	CLA	C10-C11-C12-C13
19	A2	821	CLA	C8-C10-C11-C12
19	AA	808	CLA	C10-C11-C12-C13
19	B	815	CLA	C10-C11-C12-C13
19	B2	807	CLA	C15-C16-C17-C18
19	BB	803	CLA	C8-C10-C11-C12
19	A2	829	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
19	B1	807	CLA	C15-C16-C17-C18
19	B	815	CLA	C3-C5-C6-C7
19	F1	301	CLA	C3-C5-C6-C7
19	A2	815	CLA	C3-C5-C6-C7
19	F1	301	CLA	O1A-CGA-O2A-C1
19	A1	819	CLA	O1A-CGA-O2A-C1
20	A2	803	CL0	O1A-CGA-O2A-C1
19	A	827	CLA	CBA-CGA-O2A-C1
22	BB	851	LHG	C24-C23-O8-C6
19	A	805	CLA	CBA-CGA-O2A-C1
19	A	810	CLA	CBA-CGA-O2A-C1
22	A1	846	LHG	C24-C23-O8-C6
19	AA	805	CLA	CBA-CGA-O2A-C1
19	A1	804	CLA	CBA-CGA-O2A-C1
19	AA	810	CLA	CBA-CGA-O2A-C1
22	X2	103	LHG	C24-C23-O8-C6
19	B1	821	CLA	CBA-CGA-O2A-C1
19	LL	201	CLA	CBA-CGA-O2A-C1
19	B2	821	CLA	CBA-CGA-O2A-C1
22	B	853	LHG	C24-C23-O8-C6
19	B1	823	CLA	CBA-CGA-O2A-C1
19	BB	803	CLA	CBA-CGA-O2A-C1
25	L1	210	LMG	C29-C28-O8-C9
19	AA	827	CLA	CBA-CGA-O2A-C1
19	A2	810	CLA	CBA-CGA-O2A-C1
19	A2	836	CLA	CBA-CGA-O2A-C1
19	A2	805	CLA	CBA-CGA-O2A-C1
19	AA	821	CLA	C8-C10-C11-C12
19	B1	801	CLA	C5-C6-C7-C8
19	B	822	CLA	C13-C15-C16-C17
26	BB	840	ECH	C15-C16-C17-C18
23	B	842	BCR	C13-C14-C15-C16
23	A1	853	BCR	C15-C16-C17-C18
23	B1	841	BCR	C13-C14-C15-C16
23	I1	101	BCR	C9-C10-C11-C12
19	B2	803	CLA	C8-C10-C11-C12
28	B	856	DGD	O6E-C5E-C6E-O5E
24	BB	849	AJP	OBC-CBJ-CCB-OCC
19	B2	819	CLA	CBD-CGD-O2D-CED
19	A	837	CLA	CBD-CGD-O2D-CED
19	A	844	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
19	J	101	CLA	O1D-CGD-O2D-CED
19	A2	826	CLA	O1D-CGD-O2D-CED
19	AA	836	CLA	O1D-CGD-O2D-CED
19	JJ	101	CLA	O1D-CGD-O2D-CED
19	A1	828	CLA	O1D-CGD-O2D-CED
19	LL	203	CLA	C2C-C3C-CAC-CBC
19	B	837	CLA	C2C-C3C-CAC-CBC
19	BB	815	CLA	C3-C5-C6-C7
19	B	834	CLA	C14-C13-C15-C16
19	B2	825	CLA	C14-C13-C15-C16
19	A	827	CLA	C14-C13-C15-C16
20	AA	803	CL0	C6-C7-C8-C9
19	B	807	CLA	C6-C7-C8-C9
19	B	807	CLA	C14-C13-C15-C16
19	L2	205	CLA	C6-C7-C8-C9
19	B	825	CLA	C14-C13-C15-C16
19	B1	825	CLA	C14-C13-C15-C16
19	BB	825	CLA	C14-C13-C15-C16
19	A	829	CLA	C11-C10-C8-C9
19	A	804	CLA	C6-C7-C8-C9
19	BB	807	CLA	C6-C7-C8-C9
19	BB	807	CLA	C14-C13-C15-C16
19	B2	807	CLA	C6-C7-C8-C9
19	AA	853	CLA	C11-C10-C8-C9
19	AA	804	CLA	C6-C7-C8-C9
19	B2	816	CLA	C6-C7-C8-C9
19	B1	823	CLA	C6-C7-C8-C9
19	BB	835	CLA	C6-C7-C8-C9
19	B2	836	CLA	C6-C7-C8-C9
19	A2	804	CLA	C6-C7-C8-C9
19	B	836	CLA	C6-C7-C8-C9
19	A2	829	CLA	C11-C10-C8-C9
19	A1	803	CLA	C6-C7-C8-C9
19	A2	813	CLA	C6-C7-C8-C9
19	B1	816	CLA	C6-C7-C8-C9
19	BB	823	CLA	C6-C7-C8-C9
19	B1	833	CLA	C14-C13-C15-C16
20	A2	803	CL0	C11-C10-C8-C9
19	A1	852	CLA	C11-C10-C8-C9
19	A2	852	CLA	C11-C10-C8-C9
19	BB	815	CLA	C14-C13-C15-C16
19	A	852	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	AA	829	CLA	C11-C10-C8-C9
19	B1	803	CLA	C13-C15-C16-C17
19	A1	835	CLA	C5-C6-C7-C8
19	A2	801	CLA	C10-C11-C12-C13
19	AA	804	CLA	C10-C11-C12-C13
19	B2	801	CLA	C10-C11-C12-C13
19	BB	822	CLA	C13-C15-C16-C17
19	AA	819	CLA	C8-C10-C11-C12
19	B2	823	CLA	C13-C15-C16-C17
19	A1	803	CLA	C13-C15-C16-C17
21	B1	837	PQN	C25-C26-C27-C28
19	A2	807	CLA	C5-C6-C7-C8
23	B	848	BCR	C11-C12-C13-C35
23	B	848	BCR	C37-C22-C23-C24
23	K1	104	BCR	C37-C22-C23-C24
23	L1	201	BCR	C7-C8-C9-C34
23	A	848	BCR	C37-C22-C23-C24
23	J2	104	BCR	C37-C22-C23-C24
23	B1	838	BCR	C7-C8-C9-C34
23	B1	838	BCR	C37-C22-C23-C24
23	BB	838	BCR	C7-C8-C9-C34
23	BB	838	BCR	C37-C22-C23-C24
23	BB	847	BCR	C11-C12-C13-C35
23	BB	847	BCR	C37-C22-C23-C24
23	A1	848	BCR	C7-C8-C9-C34
23	A2	850	BCR	C11-C12-C13-C35
23	K2	105	BCR	C7-C8-C9-C34
23	J	102	BCR	C11-C12-C13-C35
23	J	102	BCR	C36-C18-C19-C20
23	F	305	BCR	C7-C8-C9-C34
23	JJ	102	BCR	C11-C12-C13-C35
26	B	841	ECH	C11-C12-C13-C35
23	AA	852	BCR	C11-C12-C13-C35
23	B2	843	BCR	C11-C12-C13-C35
23	I	102	BCR	C7-C8-C9-C34
23	A	847	BCR	C7-C8-C9-C34
23	J2	102	BCR	C11-C12-C13-C35
23	K1	106	BCR	C7-C8-C9-C34
23	B	839	BCR	C7-C8-C9-C34
23	B	839	BCR	C37-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C34
23	AA	849	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	F1	306	BCR	C7-C8-C9-C34
23	J1	102	BCR	C11-C12-C13-C35
23	JJ	104	BCR	C37-C22-C23-C24
23	B2	839	BCR	C7-C8-C9-C34
23	B2	839	BCR	C37-C22-C23-C24
23	AA	855	BCR	C7-C8-C9-C34
23	KK	103	BCR	C36-C18-C19-C20
23	FF	306	BCR	C7-C8-C9-C34
23	A2	848	BCR	C7-C8-C9-C34
23	MM	101	BCR	C7-C8-C9-C34
23	A1	853	BCR	C7-C8-C9-C34
23	A1	853	BCR	C37-C22-C23-C24
23	A	854	BCR	C7-C8-C9-C34
23	K	103	BCR	C36-C18-C19-C20
23	B1	841	BCR	C7-C8-C9-C34
23	A2	853	BCR	C7-C8-C9-C34
23	A2	853	BCR	C37-C22-C23-C24
23	F	304	BCR	C7-C8-C9-C34
23	A	851	BCR	C11-C12-C13-C35
23	II	102	BCR	C7-C8-C9-C34
23	II	102	BCR	C37-C22-C23-C24
23	F2	305	BCR	C36-C18-C19-C20
23	F2	305	BCR	C37-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C34
23	A1	850	BCR	C11-C12-C13-C35
23	FF	303	BCR	C11-C12-C13-C35
19	AA	843	CLA	C2A-CAA-CBA-CGA
19	A	829	CLA	C2A-CAA-CBA-CGA
19	B1	836	CLA	C2A-CAA-CBA-CGA
19	F1	301	CLA	C2A-CAA-CBA-CGA
20	A	803	CL0	C2A-CAA-CBA-CGA
19	A	810	CLA	O1A-CGA-O2A-C1
25	B	851	LMG	O10-C28-O8-C9
19	B1	823	CLA	O1A-CGA-O2A-C1
19	A2	810	CLA	O1A-CGA-O2A-C1
23	B	848	BCR	C17-C18-C19-C20
23	B	848	BCR	C21-C22-C23-C24
23	L1	201	BCR	C7-C8-C9-C10
23	B1	838	BCR	C21-C22-C23-C24
23	BB	838	BCR	C21-C22-C23-C24
23	BB	847	BCR	C17-C18-C19-C20
23	BB	847	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	A	853	BCR	C7-C8-C9-C10
23	A	853	BCR	C21-C22-C23-C24
23	I2	102	BCR	C7-C8-C9-C10
23	I	102	BCR	C7-C8-C9-C10
23	K1	106	BCR	C17-C18-C19-C20
23	B	839	BCR	C21-C22-C23-C24
23	B	842	BCR	C7-C8-C9-C10
23	F1	306	BCR	C17-C18-C19-C20
23	JJ	104	BCR	C21-C22-C23-C24
23	B2	839	BCR	C21-C22-C23-C24
23	AA	855	BCR	C17-C18-C19-C20
23	M2	102	BCR	C21-C22-C23-C24
23	A1	853	BCR	C7-C8-C9-C10
23	A1	853	BCR	C21-C22-C23-C24
23	B1	841	BCR	C7-C8-C9-C10
23	A2	853	BCR	C7-C8-C9-C10
23	A2	853	BCR	C21-C22-C23-C24
23	AA	854	BCR	C7-C8-C9-C10
23	II	102	BCR	C7-C8-C9-C10
23	F2	305	BCR	C21-C22-C23-C24
23	BB	841	BCR	C7-C8-C9-C10
19	A2	814	CLA	O1D-CGD-O2D-CED
19	B	815	CLA	O1D-CGD-O2D-CED
19	A1	819	CLA	O1D-CGD-O2D-CED
19	B2	808	CLA	CBD-CGD-O2D-CED
19	B1	821	CLA	C4-C3-C5-C6
25	I1	102	LMG	C11-C10-O7-C8
28	B	856	DGD	C2B-C1B-O2G-C2G
28	BB	854	DGD	C2B-C1B-O2G-C2G
19	KK	102	CLA	O1D-CGD-O2D-CED
19	B1	806	CLA	C8-C10-C11-C12
19	B2	825	CLA	C10-C11-C12-C13
19	A2	840	CLA	C5-C6-C7-C8
19	B	803	CLA	C8-C10-C11-C12
19	B2	822	CLA	C13-C15-C16-C17
20	AA	803	CL0	C13-C15-C16-C17
19	A	801	CLA	C10-C11-C12-C13
19	A	807	CLA	C5-C6-C7-C8
19	A1	807	CLA	C10-C11-C12-C13
19	B1	826	CLA	C10-C11-C12-C13
19	B1	832	CLA	C15-C16-C17-C18
21	A	843	PQN	C23-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
19	A	829	CLA	C10-C11-C12-C13
19	B1	803	CLA	C8-C10-C11-C12
19	B	806	CLA	C8-C10-C11-C12
19	A1	801	CLA	C10-C11-C12-C13
19	AA	807	CLA	C5-C6-C7-C8
19	A	804	CLA	C10-C11-C12-C13
21	B2	838	PQN	C25-C26-C27-C28
19	B2	803	CLA	C13-C15-C16-C17
19	B1	801	CLA	C10-C11-C12-C13
19	A1	842	CLA	C13-C15-C16-C17
19	AA	804	CLA	C13-C15-C16-C17
19	B2	801	CLA	C5-C6-C7-C8
19	BB	803	CLA	C13-C15-C16-C17
19	B1	822	CLA	C13-C15-C16-C17
19	BB	815	CLA	C10-C11-C12-C13
19	AA	829	CLA	C10-C11-C12-C13
19	B2	806	CLA	C8-C10-C11-C12
19	AA	841	CLA	CBA-CGA-O2A-C1
19	A	805	CLA	O1A-CGA-O2A-C1
19	A1	804	CLA	O1A-CGA-O2A-C1
19	AA	810	CLA	O1A-CGA-O2A-C1
19	B1	821	CLA	O1A-CGA-O2A-C1
19	B2	821	CLA	O1A-CGA-O2A-C1
19	A2	805	CLA	O1A-CGA-O2A-C1
19	BB	815	CLA	O1D-CGD-O2D-CED
19	B	813	CLA	CBD-CGD-O2D-CED
19	B	825	CLA	CBD-CGD-O2D-CED
19	B1	823	CLA	CBD-CGD-O2D-CED
19	B1	813	CLA	CBD-CGD-O2D-CED
19	BB	801	CLA	C5-C6-C7-C8
19	B	860	CLA	C13-C15-C16-C17
19	A	801	CLA	C8-C10-C11-C12
19	BB	806	CLA	C8-C10-C11-C12
19	AA	801	CLA	C8-C10-C11-C12
19	A	804	CLA	C8-C10-C11-C12
19	A2	801	CLA	C8-C10-C11-C12
19	AA	853	CLA	C13-C15-C16-C17
19	B	814	CLA	C5-C6-C7-C8
19	B2	833	CLA	C15-C16-C17-C18
19	B1	823	CLA	C8-C10-C11-C12
19	A1	803	CLA	C10-C11-C12-C13
19	A1	806	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	C10-C11-C12-C13
22	A2	846	LHG	C7-C8-C9-C10
22	X	102	LHG	C7-C8-C9-C10
22	A	846	LHG	C24-C23-O8-C6
19	BB	811	CLA	CBA-CGA-O2A-C1
25	B	851	LMG	C29-C28-O8-C9
19	B1	803	CLA	CBA-CGA-O2A-C1
19	A2	827	CLA	CBA-CGA-O2A-C1
19	A1	831	CLA	CBA-CGA-O2A-C1
19	B2	832	CLA	O1D-CGD-O2D-CED
19	A	813	CLA	O1D-CGD-O2D-CED
19	B1	836	CLA	O1D-CGD-O2D-CED
19	A	834	CLA	O1D-CGD-O2D-CED
19	A2	829	CLA	O1D-CGD-O2D-CED
19	B1	825	CLA	C10-C11-C12-C13
19	AA	801	CLA	C10-C11-C12-C13
19	L1	207	CLA	C13-C15-C16-C17
19	AA	804	CLA	C8-C10-C11-C12
19	A2	808	CLA	C10-C11-C12-C13
19	B	829	CLA	C13-C15-C16-C17
19	A2	804	CLA	C10-C11-C12-C13
28	BB	854	DGD	O6E-C5E-C6E-O5E
24	L2	203	AJP	OBC-CBJ-CCB-OCC
19	BB	822	CLA	CBD-CGD-O2D-CED
19	B2	829	CLA	O1D-CGD-O2D-CED
23	AA	855	BCR	C14-C15-C16-C17
22	AA	847	LHG	C7-C8-C9-C10
25	B	851	LMG	C28-C29-C30-C31
25	I1	102	LMG	C10-C11-C12-C13
22	A1	846	LHG	C7-C8-C9-C10
22	XX	102	LHG	C7-C8-C9-C10
22	X1	102	LHG	C7-C8-C9-C10
19	BB	832	CLA	C15-C16-C17-C18
20	A1	802	CL0	C13-C15-C16-C17
19	AA	831	CLA	C5-C6-C7-C8
21	B	838	PQN	C25-C26-C27-C28
19	B2	834	CLA	C13-C15-C16-C17
19	A1	828	CLA	C10-C11-C12-C13
19	B	801	CLA	C5-C6-C7-C8
19	B	836	CLA	C13-C15-C16-C17
20	A	803	CL0	C8-C10-C11-C12
22	A1	846	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
19	A2	835	CLA	C3-C5-C6-C7
19	A1	834	CLA	C3-C5-C6-C7
19	B	825	CLA	C10-C11-C12-C13
19	A	819	CLA	C8-C10-C11-C12
19	B1	815	CLA	C10-C11-C12-C13
19	A1	852	CLA	C13-C15-C16-C17
19	A2	807	CLA	C13-C15-C16-C17
19	B	833	CLA	C15-C16-C17-C18
19	A	836	CLA	CBA-CGA-O2A-C1
22	X1	103	LHG	C24-C23-O8-C6
19	A1	826	CLA	CBA-CGA-O2A-C1
19	B1	811	CLA	CBA-CGA-O2A-C1
19	A	808	CLA	C2-C1-O2A-CGA
19	A1	807	CLA	C2-C1-O2A-CGA
19	B2	807	CLA	C2-C1-O2A-CGA
19	A2	827	CLA	C2-C1-O2A-CGA
19	A1	826	CLA	C2-C1-O2A-CGA
19	B1	807	CLA	C2-C1-O2A-CGA
22	X2	102	LHG	C7-C8-C9-C10
19	B	819	CLA	O1D-CGD-O2D-CED
24	AA	856	AJP	ODG-CCW-CCX-OCY
19	A	841	CLA	CBA-CGA-O2A-C1
19	BB	811	CLA	C6-C7-C8-C10
19	BB	811	CLA	C11-C12-C13-C15
19	A	807	CLA	C11-C10-C8-C7
21	A2	843	PQN	C16-C17-C18-C20
21	A2	843	PQN	C21-C22-C23-C25
19	A1	823	CLA	C2A-CAA-CBA-CGA
19	A1	820	CLA	C11-C10-C8-C7
19	B	811	CLA	C6-C7-C8-C10
21	A1	843	PQN	C16-C17-C18-C20
21	A1	843	PQN	C21-C22-C23-C25
19	A2	801	CLA	C11-C10-C8-C7
19	A1	826	CLA	C11-C10-C8-C7
19	A	824	CLA	C2A-CAA-CBA-CGA
19	A2	824	CLA	C2A-CAA-CBA-CGA
19	B2	829	CLA	C12-C13-C15-C16
19	B1	826	CLA	C5-C6-C7-C8
19	BB	825	CLA	C10-C11-C12-C13
19	A	804	CLA	C13-C15-C16-C17
19	A2	829	CLA	C5-C6-C7-C8
19	B1	835	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	A1	839	CLA	C5-C6-C7-C8
19	B2	826	CLA	C5-C6-C7-C8
19	FF	305	CLA	C13-C15-C16-C17
19	B2	837	CLA	O1D-CGD-O2D-CED
19	B2	831	CLA	O1D-CGD-O2D-CED
19	AA	813	CLA	O1D-CGD-O2D-CED
19	A	817	CLA	O1D-CGD-O2D-CED
19	BB	812	CLA	O1D-CGD-O2D-CED
19	AA	817	CLA	O1D-CGD-O2D-CED
19	BB	836	CLA	C2A-CAA-CBA-CGA
19	B2	822	CLA	C2A-CAA-CBA-CGA
19	B	860	CLA	C2A-CAA-CBA-CGA
19	BB	814	CLA	C2A-CAA-CBA-CGA
20	A1	802	CL0	C2A-CAA-CBA-CGA
19	B2	837	CLA	C2A-CAA-CBA-CGA
19	F	301	CLA	C2A-CAA-CBA-CGA
19	BB	822	CLA	C2A-CAA-CBA-CGA
19	B	822	CLA	C2A-CAA-CBA-CGA
19	B	858	CLA	C2A-CAA-CBA-CGA
23	A	853	BCR	C19-C20-C21-C22
23	K2	105	BCR	C13-C14-C15-C16
23	F	305	BCR	C9-C10-C11-C12
26	B	841	ECH	C13-C14-C15-C16
23	J2	102	BCR	C9-C10-C11-C12
23	K1	106	BCR	C13-C14-C15-C16
23	F1	306	BCR	C9-C10-C11-C12
23	F1	306	BCR	C19-C20-C21-C22
23	J1	102	BCR	C9-C10-C11-C12
23	II	101	BCR	C9-C10-C11-C12
23	FF	306	BCR	C9-C10-C11-C12
23	MM	101	BCR	C15-C16-C17-C18
23	AA	854	BCR	C19-C20-C21-C22
19	A	808	CLA	C15-C16-C17-C18
19	AA	823	CLA	C5-C6-C7-C8
19	A	823	CLA	C5-C6-C7-C8
19	A2	804	CLA	C13-C15-C16-C17
19	A1	822	CLA	C8-C10-C11-C12
22	BB	851	LHG	O10-C23-O8-C6
19	B2	811	CLA	O1A-CGA-O2A-C1
19	AA	805	CLA	O1A-CGA-O2A-C1
22	X2	103	LHG	O10-C23-O8-C6
19	LL	201	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	BB	803	CLA	O1A-CGA-O2A-C1
19	A2	836	CLA	O1A-CGA-O2A-C1
19	B2	836	CLA	CBD-CGD-O2D-CED
19	A	827	CLA	C4-C3-C5-C6
19	L2	206	CLA	C4-C3-C5-C6
19	B2	814	CLA	C4-C3-C5-C6
19	B1	849	CLA	C4-C3-C5-C6
19	L1	207	CLA	C4-C3-C5-C6
19	AA	827	CLA	C4-C3-C5-C6
19	A	827	CLA	C2-C3-C5-C6
19	B	810	CLA	C2-C3-C5-C6
19	L2	206	CLA	C2-C3-C5-C6
19	B1	849	CLA	C2-C3-C5-C6
19	L1	207	CLA	C2-C3-C5-C6
19	A1	840	CLA	O1A-CGA-O2A-C1
19	A2	841	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	C10-C11-C12-C13
19	B1	828	CLA	C13-C15-C16-C17
19	A	831	CLA	C5-C6-C7-C8
19	L2	204	CLA	C5-C6-C7-C8
19	BB	814	CLA	C5-C6-C7-C8
19	BB	814	CLA	C8-C10-C11-C12
19	A	807	CLA	C10-C11-C12-C13
19	B1	832	CLA	C5-C6-C7-C8
19	B2	814	CLA	C8-C10-C11-C12
19	AA	807	CLA	C13-C15-C16-C17
19	A1	820	CLA	C8-C10-C11-C12
19	A	804	CLA	C5-C6-C7-C8
21	B	838	PQN	C15-C16-C17-C18
21	A1	843	PQN	C23-C25-C26-C27
19	BB	826	CLA	C10-C11-C12-C13
19	A	823	CLA	C8-C10-C11-C12
19	B	823	CLA	C15-C16-C17-C18
19	A1	830	CLA	C5-C6-C7-C8
19	AA	804	CLA	C5-C6-C7-C8
19	B	801	CLA	C10-C11-C12-C13
19	B2	833	CLA	C5-C6-C7-C8
19	B1	814	CLA	C5-C6-C7-C8
19	B1	814	CLA	C8-C10-C11-C12
19	A1	831	CLA	C8-C10-C11-C12
19	B	836	CLA	C8-C10-C11-C12
19	AA	827	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	A2	832	CLA	C8-C10-C11-C12
19	A	852	CLA	C13-C15-C16-C17
19	B2	826	CLA	C10-C11-C12-C13
19	A	827	CLA	O1A-CGA-O2A-C1
19	L	202	CLA	O1A-CGA-O2A-C1
19	AA	827	CLA	O1A-CGA-O2A-C1
19	B	818	CLA	CBD-CGD-O2D-CED
23	K1	104	BCR	C18-C19-C20-C21
23	A	848	BCR	C10-C11-C12-C13
23	L	205	BCR	C10-C11-C12-C13
23	B1	838	BCR	C18-C19-C20-C21
23	B	844	BCR	C18-C19-C20-C21
23	A	850	BCR	C10-C11-C12-C13
23	II	104	BCR	C10-C11-C12-C13
23	I	101	BCR	C18-C19-C20-C21
23	B1	842	BCR	C10-C11-C12-C13
23	I2	102	BCR	C18-C19-C20-C21
23	L1	208	BCR	C10-C11-C12-C13
23	A	847	BCR	C10-C11-C12-C13
23	A	847	BCR	C18-C19-C20-C21
23	LL	204	BCR	C10-C11-C12-C13
23	B	842	BCR	C18-C19-C20-C21
23	BB	842	BCR	C10-C11-C12-C13
23	AA	849	BCR	C10-C11-C12-C13
23	II	101	BCR	C18-C19-C20-C21
23	B2	839	BCR	C18-C19-C20-C21
23	A2	847	BCR	C10-C11-C12-C13
23	A2	847	BCR	C18-C19-C20-C21
23	AA	848	BCR	C18-C19-C20-C21
23	KK	103	BCR	C10-C11-C12-C13
23	K	103	BCR	C18-C19-C20-C21
23	A	849	BCR	C10-C11-C12-C13
23	A	849	BCR	C18-C19-C20-C21
23	A1	849	BCR	C18-C19-C20-C21
23	I1	101	BCR	C18-C19-C20-C21
23	A1	847	BCR	C10-C11-C12-C13
23	A1	847	BCR	C18-C19-C20-C21
23	BB	841	BCR	C18-C19-C20-C21
23	AA	850	BCR	C10-C11-C12-C13
23	AA	850	BCR	C18-C19-C20-C21
19	B1	806	CLA	C15-C16-C17-C18
19	A2	823	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
21	BB	837	PQN	C25-C26-C27-C28
19	A1	807	CLA	C15-C16-C17-C18
21	A2	843	PQN	C25-C26-C27-C28
19	AA	823	CLA	C8-C10-C11-C12
19	B2	810	CLA	C8-C10-C11-C12
19	B1	810	CLA	C8-C10-C11-C12
19	A1	806	CLA	C13-C15-C16-C17
19	BB	823	CLA	C15-C16-C17-C18
19	B	833	CLA	C5-C6-C7-C8
19	B2	806	CLA	C15-C16-C17-C18
19	B1	805	CLA	C3-C5-C6-C7
19	B	805	CLA	C3-C5-C6-C7
23	M1	101	BCR	C22-C23-C24-C25
23	M2	102	BCR	C22-C23-C24-C25
23	F2	305	BCR	C6-C7-C8-C9
23	J1	104	BCR	C6-C7-C8-C9
19	AA	838	CLA	O1D-CGD-O2D-CED
19	A1	812	CLA	O1D-CGD-O2D-CED
19	B1	833	CLA	O1D-CGD-O2D-CED
19	A1	820	CLA	CBD-CGD-O2D-CED
22	L2	208	LHG	C4-O6-P-O3
22	X	102	LHG	C4-O6-P-O3
22	L1	211	LHG	C3-O3-P-O6
19	BB	811	CLA	O1A-CGA-O2A-C1
19	B1	803	CLA	O1A-CGA-O2A-C1
22	A2	846	LHG	O10-C23-O8-C6
22	B2	848	LHG	O10-C23-O8-C6
19	B	811	CLA	O1A-CGA-O2A-C1
22	B	853	LHG	O10-C23-O8-C6
19	BB	821	CLA	CBA-CGA-O2A-C1
19	BB	801	CLA	C10-C11-C12-C13
19	AA	843	CLA	C13-C15-C16-C17
19	A2	823	CLA	C8-C10-C11-C12
19	B	803	CLA	C13-C15-C16-C17
19	AA	832	CLA	C8-C10-C11-C12
19	BB	832	CLA	C5-C6-C7-C8
19	A	807	CLA	C13-C15-C16-C17
19	L2	206	CLA	C13-C15-C16-C17
21	A2	843	PQN	C23-C25-C26-C27
19	A2	819	CLA	C8-C10-C11-C12
19	A1	818	CLA	C8-C10-C11-C12
19	AA	808	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	A1	820	CLA	C15-C16-C17-C18
21	A1	843	PQN	C25-C26-C27-C28
19	B2	834	CLA	C10-C11-C12-C13
19	A2	808	CLA	C15-C16-C17-C18
19	B1	823	CLA	C13-C15-C16-C17
19	B2	852	CLA	C13-C15-C16-C17
19	A	832	CLA	C8-C10-C11-C12
19	A2	852	CLA	C13-C15-C16-C17
25	I2	105	LMG	C11-C10-O7-C8
21	A	843	PQN	C25-C26-C27-C28
19	A1	804	CLA	C8-C10-C11-C12
19	B	823	CLA	C8-C10-C11-C12
19	BB	835	CLA	C13-C15-C16-C17
19	A1	803	CLA	C5-C6-C7-C8
19	B1	833	CLA	C10-C11-C12-C13
19	BB	833	CLA	C10-C11-C12-C13
22	A	846	LHG	C7-C8-C9-C10
22	A1	845	LHG	C7-C8-C9-C10
24	L1	203	AJP	OCC-CCX-OCY-CCZ
22	X1	103	LHG	O10-C23-O8-C6
19	A2	827	CLA	O1A-CGA-O2A-C1
19	B1	811	CLA	O1A-CGA-O2A-C1
19	B1	808	CLA	O1D-CGD-O2D-CED
19	BB	805	CLA	C3-C5-C6-C7
19	B2	805	CLA	C3-C5-C6-C7
25	I1	102	LMG	O6-C5-C6-O5
25	B2	845	LMG	C4-C5-C6-O5
19	A2	813	CLA	O1D-CGD-O2D-CED
19	L2	204	CLA	CBA-CGA-O2A-C1
22	AA	847	LHG	C24-C23-O8-C6
22	B1	847	LHG	C24-C23-O8-C6
19	L1	205	CLA	CBA-CGA-O2A-C1
19	B	821	CLA	CBA-CGA-O2A-C1
19	A1	827	CLA	CBA-CGA-O2A-C1
19	B2	808	CLA	CBA-CGA-O2A-C1
19	A2	832	CLA	CBA-CGA-O2A-C1
19	B1	816	CLA	CBA-CGA-O2A-C1
25	L1	210	LMG	O9-C10-O7-C8
25	I2	105	LMG	O9-C10-O7-C8
19	A1	826	CLA	O1A-CGA-O2A-C1
19	A1	831	CLA	O1A-CGA-O2A-C1
19	B2	814	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	A	804	CLA	C2A-CAA-CBA-CGA
19	A2	801	CLA	C2A-CAA-CBA-CGA
19	A1	842	CLA	C2A-CAA-CBA-CGA
19	B	814	CLA	C2A-CAA-CBA-CGA
19	F2	301	CLA	C2A-CAA-CBA-CGA
19	AA	804	CLA	C2A-CAA-CBA-CGA
19	B1	814	CLA	C2A-CAA-CBA-CGA
19	B2	852	CLA	C2A-CAA-CBA-CGA
19	A2	804	CLA	C2A-CAA-CBA-CGA
19	BB	855	CLA	C2A-CAA-CBA-CGA
19	A2	820	CLA	O1D-CGD-O2D-CED
19	A	829	CLA	C5-C6-C7-C8
19	AA	812	CLA	O1A-CGA-O2A-C1
19	AA	840	CLA	CBD-CGD-O2D-CED
19	B2	814	CLA	C3-C5-C6-C7
19	F2	301	CLA	C3-C5-C6-C7
24	A	855	AJP	ODG-CCW-CCX-OCY
19	B	810	CLA	C4-C3-C5-C6
19	BB	810	CLA	C4-C3-C5-C6
19	B	829	CLA	C4-C3-C5-C6
19	B2	829	CLA	C4-C3-C5-C6
19	FF	305	CLA	C4-C3-C5-C6
19	A2	826	CLA	C2A-CAA-CBA-CGA
19	AA	826	CLA	C2A-CAA-CBA-CGA
19	A1	825	CLA	C2A-CAA-CBA-CGA
19	A	826	CLA	C2A-CAA-CBA-CGA
19	B1	828	CLA	C2-C3-C5-C6
19	B2	814	CLA	C2-C3-C5-C6
19	BB	810	CLA	C2-C3-C5-C6
19	A1	826	CLA	C2-C3-C5-C6
19	B	829	CLA	C2-C3-C5-C6
19	AA	827	CLA	C2-C3-C5-C6
19	B2	829	CLA	C2-C3-C5-C6
19	FF	305	CLA	C2-C3-C5-C6
21	BB	837	PQN	C15-C16-C17-C18
19	B2	815	CLA	C10-C11-C12-C13
19	B1	835	CLA	C13-C15-C16-C17
20	A2	803	CL0	C15-C16-C17-C18
24	B	850	AJP	OBC-CBJ-CCB-CCA
23	B	848	BCR	C35-C13-C14-C15
23	K1	104	BCR	C35-C13-C14-C15
23	K1	104	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	A2	849	BCR	C20-C21-C22-C37
23	L1	201	BCR	C35-C13-C14-C15
23	B	843	BCR	C16-C17-C18-C36
23	A	848	BCR	C35-C13-C14-C15
23	F2	303	BCR	C20-C21-C22-C37
23	L	205	BCR	C16-C17-C18-C36
23	L	205	BCR	C20-C21-C22-C37
23	J2	104	BCR	C20-C21-C22-C37
23	A1	851	BCR	C35-C13-C14-C15
23	BB	847	BCR	C35-C13-C14-C15
23	BB	847	BCR	C16-C17-C18-C36
23	A1	848	BCR	C11-C10-C9-C34
23	A1	848	BCR	C20-C21-C22-C37
23	B	844	BCR	C35-C13-C14-C15
23	A	853	BCR	C35-C13-C14-C15
23	A	853	BCR	C20-C21-C22-C37
23	A2	850	BCR	C20-C21-C22-C37
23	K2	103	BCR	C11-C10-C9-C34
23	K2	103	BCR	C16-C17-C18-C36
23	F	305	BCR	C20-C21-C22-C37
23	B1	842	BCR	C11-C10-C9-C34
23	I2	103	BCR	C35-C13-C14-C15
23	I2	103	BCR	C20-C21-C22-C37
23	I2	102	BCR	C11-C10-C9-C34
23	I2	102	BCR	C35-C13-C14-C15
23	AA	852	BCR	C11-C10-C9-C34
23	AA	852	BCR	C35-C13-C14-C15
23	L1	208	BCR	C35-C13-C14-C15
23	L1	208	BCR	C20-C21-C22-C37
23	B2	843	BCR	C11-C10-C9-C34
23	B2	843	BCR	C16-C17-C18-C36
23	I	102	BCR	C35-C13-C14-C15
23	A	847	BCR	C35-C13-C14-C15
23	A	847	BCR	C16-C17-C18-C36
23	J2	102	BCR	C16-C17-C18-C36
23	K1	106	BCR	C16-C17-C18-C36
23	B	839	BCR	C11-C10-C9-C34
23	AA	849	BCR	C35-C13-C14-C15
23	F1	306	BCR	C20-C21-C22-C37
23	J1	102	BCR	C20-C21-C22-C37
23	II	101	BCR	C20-C21-C22-C37
23	A2	847	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	AA	848	BCR	C35-C13-C14-C15
23	AA	848	BCR	C16-C17-C18-C36
23	A2	848	BCR	C11-C10-C9-C34
23	A2	848	BCR	C16-C17-C18-C36
23	A2	848	BCR	C20-C21-C22-C37
23	B2	844	BCR	C35-C13-C14-C15
23	I2	101	BCR	C35-C13-C14-C15
23	B1	843	BCR	C35-C13-C14-C15
23	B	840	BCR	C11-C10-C9-C34
23	B	840	BCR	C35-C13-C14-C15
23	B	840	BCR	C16-C17-C18-C36
23	F2	304	BCR	C35-C13-C14-C15
23	F2	304	BCR	C16-C17-C18-C36
23	A1	853	BCR	C35-C13-C14-C15
23	K	103	BCR	C35-C13-C14-C15
23	B1	841	BCR	C16-C17-C18-C36
23	A2	853	BCR	C35-C13-C14-C15
23	A	849	BCR	C16-C17-C18-C36
23	B1	839	BCR	C11-C10-C9-C34
23	B1	839	BCR	C16-C17-C18-C36
23	F1	304	BCR	C35-C13-C14-C15
23	F1	304	BCR	C16-C17-C18-C36
23	A	851	BCR	C11-C10-C9-C34
23	A	851	BCR	C35-C13-C14-C15
23	AA	854	BCR	C35-C13-C14-C15
23	I1	101	BCR	C35-C13-C14-C15
23	J	104	BCR	C20-C21-C22-C37
23	A1	847	BCR	C16-C17-C18-C36
23	F2	305	BCR	C11-C10-C9-C34
23	BB	841	BCR	C20-C21-C22-C37
23	BB	839	BCR	C11-C10-C9-C34
23	BB	839	BCR	C35-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C36
23	F	303	BCR	C35-C13-C14-C15
23	F	303	BCR	C20-C21-C22-C37
23	B2	840	BCR	C11-C10-C9-C34
23	J1	104	BCR	C20-C21-C22-C37
23	A1	850	BCR	C20-C21-C22-C37
23	F1	303	BCR	C20-C21-C22-C37
23	FF	303	BCR	C35-C13-C14-C15
23	FF	303	BCR	C20-C21-C22-C37
22	A	845	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
19	AA	832	CLA	CBA-CGA-O2A-C1
19	B1	808	CLA	CBA-CGA-O2A-C1
19	A2	831	CLA	CBA-CGA-O2A-C1
19	AA	836	CLA	CBA-CGA-O2A-C1
19	A2	828	CLA	CBA-CGA-O2A-C1
19	B	859	CLA	CBA-CGA-O2A-C1
19	B1	829	CLA	CBA-CGA-O2A-C1
19	A	832	CLA	CBA-CGA-O2A-C1
19	B2	834	CLA	O1D-CGD-O2D-CED
19	B1	812	CLA	O1D-CGD-O2D-CED
22	AA	846	LHG	C26-C27-C28-C29
25	M	102	LMG	C32-C33-C34-C35
22	A	845	LHG	C26-C27-C28-C29
25	B1	844	LMG	C22-C23-C24-C25
25	B1	844	LMG	C30-C31-C32-C33
19	BB	819	CLA	O1D-CGD-O2D-CED
19	AA	808	CLA	O1D-CGD-O2D-CED
19	B2	820	CLA	O1D-CGD-O2D-CED
22	LL	205	LHG	C23-C24-C25-C26
23	B	848	BCR	C15-C16-C17-C18
23	BB	847	BCR	C15-C16-C17-C18
26	B	841	ECH	C15-C16-C17-C18
26	B1	840	ECH	C15-C16-C17-C18
23	AA	855	BCR	C13-C14-C15-C16
26	B2	841	ECH	C15-C16-C17-C18
23	A1	853	BCR	C19-C20-C21-C22
23	A	854	BCR	C13-C14-C15-C16
23	A2	853	BCR	C19-C20-C21-C22
23	F2	305	BCR	C9-C10-C11-C12
23	BB	841	BCR	C13-C14-C15-C16
22	AA	846	LHG	C27-C28-C29-C30
22	X2	103	LHG	C14-C15-C16-C17
22	B	853	LHG	C30-C31-C32-C33
25	I2	105	LMG	C16-C17-C18-C19
22	A1	845	LHG	C8-C7-O7-C5
22	BB	851	LHG	C30-C31-C32-C33
19	K1	105	CLA	C4C-C3C-CAC-CBC
25	B	851	LMG	C19-C20-C21-C22
22	X1	103	LHG	C30-C31-C32-C33
19	A1	814	CLA	C3-C5-C6-C7
19	A1	842	CLA	C3-C5-C6-C7
25	B	851	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
22	A1	845	LHG	O9-C7-O7-C5
25	B2	847	LMG	O9-C10-O7-C8
19	XX	101	CLA	O1D-CGD-O2D-CED
19	B1	819	CLA	O1D-CGD-O2D-CED
19	A2	823	CLA	C11-C12-C13-C15
19	BB	825	CLA	C16-C17-C18-C19
19	AA	823	CLA	C11-C12-C13-C15
21	B2	838	PQN	C26-C27-C28-C30
19	A	823	CLA	C11-C12-C13-C15
19	AA	813	CLA	C16-C17-C18-C20
19	A1	812	CLA	C16-C17-C18-C20
19	A1	822	CLA	C11-C12-C13-C15
25	B	851	LMG	C30-C31-C32-C33
22	B	853	LHG	C11-C10-C9-C8
19	A	836	CLA	O1A-CGA-O2A-C1
23	L	206	BCR	C16-C17-C18-C19
23	L	206	BCR	C20-C21-C22-C23
23	A2	849	BCR	C11-C10-C9-C8
23	B2	842	BCR	C11-C10-C9-C8
23	B2	842	BCR	C12-C13-C14-C15
23	F2	303	BCR	C12-C13-C14-C15
23	F2	303	BCR	C16-C17-C18-C19
23	L	205	BCR	C11-C10-C9-C8
23	J2	104	BCR	C11-C10-C9-C8
23	A1	851	BCR	C12-C13-C14-C15
23	B1	838	BCR	C16-C17-C18-C19
23	B1	838	BCR	C20-C21-C22-C23
23	BB	838	BCR	C16-C17-C18-C19
23	A	853	BCR	C16-C17-C18-C19
23	K2	105	BCR	C12-C13-C14-C15
23	K2	105	BCR	C16-C17-C18-C19
23	II	104	BCR	C11-C10-C9-C8
23	I	101	BCR	C11-C10-C9-C8
23	I	101	BCR	C12-C13-C14-C15
23	I	101	BCR	C16-C17-C18-C19
23	I	101	BCR	C20-C21-C22-C23
23	F	305	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C11-C10-C9-C8
23	JJ	102	BCR	C12-C13-C14-C15
23	JJ	102	BCR	C20-C21-C22-C23
23	I2	103	BCR	C11-C10-C9-C8
23	I2	102	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	L1	208	BCR	C11-C10-C9-C8
23	A	847	BCR	C11-C10-C9-C8
23	LL	204	BCR	C16-C17-C18-C19
23	LL	204	BCR	C20-C21-C22-C23
23	J2	102	BCR	C12-C13-C14-C15
23	K1	106	BCR	C12-C13-C14-C15
23	K1	106	BCR	C16-C17-C18-C19
23	K1	106	BCR	C20-C21-C22-C23
23	B	839	BCR	C20-C21-C22-C23
23	L1	209	BCR	C20-C21-C22-C23
23	B	842	BCR	C12-C13-C14-C15
23	B	842	BCR	C16-C17-C18-C19
23	F1	306	BCR	C20-C21-C22-C23
23	L2	207	BCR	C16-C17-C18-C19
23	L2	207	BCR	C20-C21-C22-C23
23	J1	102	BCR	C12-C13-C14-C15
23	J1	102	BCR	C20-C21-C22-C23
23	II	101	BCR	C11-C10-C9-C8
23	II	101	BCR	C16-C17-C18-C19
23	II	101	BCR	C20-C21-C22-C23
23	JJ	104	BCR	C11-C10-C9-C8
23	JJ	104	BCR	C16-C17-C18-C19
23	B2	839	BCR	C20-C21-C22-C23
23	A2	847	BCR	C11-C10-C9-C8
23	AA	848	BCR	C11-C10-C9-C8
23	AA	855	BCR	C12-C13-C14-C15
23	KK	103	BCR	C16-C17-C18-C19
23	I2	101	BCR	C16-C17-C18-C19
23	B1	843	BCR	C20-C21-C22-C23
23	F2	304	BCR	C16-C17-C18-C19
23	A1	853	BCR	C16-C17-C18-C19
23	A	854	BCR	C12-C13-C14-C15
23	K	103	BCR	C16-C17-C18-C19
23	A2	851	BCR	C12-C13-C14-C15
23	A2	851	BCR	C20-C21-C22-C23
23	A2	853	BCR	C16-C17-C18-C19
23	F	304	BCR	C12-C13-C14-C15
23	A	849	BCR	C12-C13-C14-C15
23	A	849	BCR	C20-C21-C22-C23
23	B1	839	BCR	C16-C17-C18-C19
23	A1	849	BCR	C11-C10-C9-C8
23	F1	304	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	F1	304	BCR	C16-C17-C18-C19
23	AA	854	BCR	C16-C17-C18-C19
23	I1	101	BCR	C16-C17-C18-C19
23	J	104	BCR	C11-C10-C9-C8
23	J	104	BCR	C16-C17-C18-C19
23	A1	847	BCR	C11-C10-C9-C8
23	BB	841	BCR	C16-C17-C18-C19
23	F	303	BCR	C16-C17-C18-C19
23	AA	850	BCR	C12-C13-C14-C15
23	AA	850	BCR	C20-C21-C22-C23
23	B2	840	BCR	C16-C17-C18-C19
23	J1	104	BCR	C11-C10-C9-C8
23	J1	104	BCR	C12-C13-C14-C15
23	J1	104	BCR	C16-C17-C18-C19
23	F1	303	BCR	C16-C17-C18-C19
23	FF	303	BCR	C16-C17-C18-C19
19	A	822	CLA	O1D-CGD-O2D-CED
19	AA	853	CLA	O1D-CGD-O2D-CED
25	B	851	LMG	C18-C19-C20-C21
22	LL	205	LHG	C11-C12-C13-C14
22	L	207	LHG	C11-C12-C13-C14
22	A1	845	LHG	C27-C28-C29-C30
19	AA	828	CLA	CBA-CGA-O2A-C1
19	B2	815	CLA	CBA-CGA-O2A-C1
19	A1	830	CLA	CBA-CGA-O2A-C1
19	B2	830	CLA	CBA-CGA-O2A-C1
25	M	102	LMG	C34-C35-C36-C37
22	X1	103	LHG	C14-C15-C16-C17
19	B	860	CLA	O1D-CGD-O2D-CED
25	B	845	LMG	C22-C23-C24-C25
19	L1	205	CLA	C5-C6-C7-C8
19	B	814	CLA	C8-C10-C11-C12
21	AA	844	PQN	C25-C26-C27-C28
19	BB	823	CLA	C8-C10-C11-C12
25	B2	845	LMG	C41-C42-C43-C44
19	A	832	CLA	O1D-CGD-O2D-CED
19	A	838	CLA	O1D-CGD-O2D-CED
28	B	856	DGD	C1B-C2B-C3B-C4B
22	L	207	LHG	C23-C24-C25-C26
28	BB	854	DGD	C1B-C2B-C3B-C4B
19	BB	801	CLA	C3-C5-C6-C7
19	F	301	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	BB	851	LHG	C14-C15-C16-C17
25	BB	844	LMG	C22-C23-C24-C25
25	I1	102	LMG	C12-C13-C14-C15
22	X2	103	LHG	C11-C10-C9-C8
22	A2	845	LHG	C27-C28-C29-C30
22	B	853	LHG	C14-C15-C16-C17
25	L1	210	LMG	C19-C20-C21-C22
25	B2	845	LMG	C22-C23-C24-C25
25	B2	845	LMG	C30-C31-C32-C33
19	A1	814	CLA	O1D-CGD-O2D-CED
19	A	815	CLA	O1D-CGD-O2D-CED
19	BB	813	CLA	O1D-CGD-O2D-CED
19	B1	830	CLA	O1D-CGD-O2D-CED
19	B1	828	CLA	C14-C13-C15-C16
19	B1	825	CLA	C11-C10-C8-C9
20	A1	802	CL0	C6-C7-C8-C9
21	A2	843	PQN	C21-C22-C23-C24
19	B1	803	CLA	C11-C12-C13-C14
19	B2	811	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C12-C13-C14
19	B	815	CLA	C11-C10-C8-C9
19	B2	849	CLA	C6-C7-C8-C9
19	A1	820	CLA	C11-C12-C13-C14
19	A1	820	CLA	C14-C13-C15-C16
19	BB	810	CLA	C6-C7-C8-C9
19	A2	801	CLA	C11-C10-C8-C9
19	B2	803	CLA	C11-C12-C13-C14
19	A1	841	CLA	C6-C7-C8-C9
19	A	842	CLA	C6-C7-C8-C9
19	BB	803	CLA	C11-C12-C13-C14
19	AA	827	CLA	C11-C10-C8-C9
19	B1	811	CLA	C6-C7-C8-C9
19	B1	811	CLA	C11-C12-C13-C14
19	BB	833	CLA	C14-C13-C15-C16
19	B2	829	CLA	C14-C13-C15-C16
19	A	827	CLA	C15-C16-C17-C18
22	B	853	LHG	C17-C18-C19-C20
19	A1	822	CLA	C5-C6-C7-C8
23	A	848	BCR	C7-C8-C9-C34
23	A	853	BCR	C7-C8-C9-C34
23	A	853	BCR	C37-C22-C23-C24
23	FF	304	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
23	I2	102	BCR	C7-C8-C9-C34
23	AA	849	BCR	C7-C8-C9-C34
23	F2	304	BCR	C37-C22-C23-C24
23	F	304	BCR	C37-C22-C23-C24
23	F1	304	BCR	C37-C22-C23-C24
23	AA	854	BCR	C7-C8-C9-C34
23	AA	854	BCR	C37-C22-C23-C24
23	J	104	BCR	C37-C22-C23-C24
23	J1	104	BCR	C37-C22-C23-C24
21	BB	837	PQN	C26-C27-C28-C29
19	AA	823	CLA	C11-C12-C13-C14
19	A	804	CLA	C16-C17-C18-C19
21	B	838	PQN	C26-C27-C28-C29
19	A2	813	CLA	C16-C17-C18-C20
19	A	801	CLA	C2A-CAA-CBA-CGA
19	AA	801	CLA	C2A-CAA-CBA-CGA
19	A1	801	CLA	C2A-CAA-CBA-CGA
19	B	837	CLA	C2A-CAA-CBA-CGA
22	A	846	LHG	O10-C23-O8-C6
19	A2	828	CLA	O1A-CGA-O2A-C1
19	B2	808	CLA	O1A-CGA-O2A-C1
19	A	832	CLA	O1A-CGA-O2A-C1
19	B1	816	CLA	O1A-CGA-O2A-C1
23	A2	849	BCR	C11-C12-C13-C14
23	L	205	BCR	C21-C22-C23-C24
23	II	104	BCR	C21-C22-C23-C24
23	I2	103	BCR	C21-C22-C23-C24
23	I2	102	BCR	C17-C18-C19-C20
23	L1	208	BCR	C21-C22-C23-C24
23	I	102	BCR	C17-C18-C19-C20
23	L1	209	BCR	C17-C18-C19-C20
23	F	303	BCR	C21-C22-C23-C24
22	BB	851	LHG	C17-C18-C19-C20
22	X	102	LHG	C23-C24-C25-C26
22	XX	102	LHG	C23-C24-C25-C26
25	L1	210	LMG	C28-C29-C30-C31
22	X1	103	LHG	O2-C2-C3-O3
19	A	812	CLA	CBA-CGA-O2A-C1
22	BB	851	LHG	C11-C10-C9-C8
19	A2	831	CLA	C5-C6-C7-C8
22	L1	211	LHG	C9-C10-C11-C12
19	BB	810	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
22	X1	103	LHG	C17-C18-C19-C20
22	A2	845	LHG	C13-C14-C15-C16
25	L1	210	LMG	C30-C31-C32-C33
22	B	852	LHG	C11-C12-C13-C14
19	B1	828	CLA	C4-C3-C5-C6
19	BB	808	CLA	C4-C3-C5-C6
19	A2	821	CLA	C4-C3-C5-C6
19	A1	835	CLA	C4-C3-C5-C6
19	A1	820	CLA	C4-C3-C5-C6
19	A2	827	CLA	C4-C3-C5-C6
19	B1	814	CLA	C4-C3-C5-C6
19	A1	826	CLA	C4-C3-C5-C6
19	B2	808	CLA	C4-C3-C5-C6
19	BB	808	CLA	C2-C3-C5-C6
19	B	808	CLA	C2-C3-C5-C6
19	A2	821	CLA	C2-C3-C5-C6
19	A1	835	CLA	C2-C3-C5-C6
19	A2	827	CLA	C2-C3-C5-C6
19	B1	814	CLA	C2-C3-C5-C6
19	BB	855	CLA	C2-C3-C5-C6
19	B	858	CLA	C2-C3-C5-C6
22	BB	851	LHG	C15-C16-C17-C18
25	B	845	LMG	C29-C30-C31-C32
22	BB	850	LHG	C11-C12-C13-C14
25	II	105	LMG	C34-C35-C36-C37
19	B2	830	CLA	C4C-C3C-CAC-CBC
25	B2	847	LMG	C11-C10-O7-C8
19	L2	204	CLA	O1A-CGA-O2A-C1
19	L1	205	CLA	O1A-CGA-O2A-C1
19	B	821	CLA	O1A-CGA-O2A-C1
19	BB	821	CLA	O1A-CGA-O2A-C1
19	A2	832	CLA	O1A-CGA-O2A-C1
19	A1	807	CLA	C3-C5-C6-C7
19	L	202	CLA	C3-C5-C6-C7
19	B2	837	CLA	C3-C5-C6-C7
19	B2	852	CLA	C3-C5-C6-C7
19	B	810	CLA	C10-C11-C12-C13
22	X2	103	LHG	C15-C16-C17-C18
25	B1	844	LMG	C18-C19-C20-C21
22	AA	846	LHG	C13-C14-C15-C16
22	B2	848	LHG	C11-C10-C9-C8
25	L1	210	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	BB	836	CLA	O1D-CGD-O2D-CED
19	BB	856	CLA	CBA-CGA-O2A-C1
19	B2	803	CLA	CBA-CGA-O2A-C1
19	B	824	CLA	CBA-CGA-O2A-C1
19	A2	823	CLA	C11-C12-C13-C14
19	A	813	CLA	C16-C17-C18-C20
21	B2	838	PQN	C26-C27-C28-C29
19	A	823	CLA	C11-C12-C13-C14
21	B1	837	PQN	C26-C27-C28-C30
25	B	845	LMG	C41-C42-C43-C44
19	XX	101	CLA	C2A-CAA-CBA-CGA
19	AA	824	CLA	C2A-CAA-CBA-CGA
19	X	101	CLA	C2A-CAA-CBA-CGA
19	X1	101	CLA	C2A-CAA-CBA-CGA
19	A1	807	CLA	O1D-CGD-O2D-CED
19	A	852	CLA	O1D-CGD-O2D-CED
19	BB	856	CLA	C3A-C2A-CAA-CBA
19	A2	839	CLA	C3A-C2A-CAA-CBA
19	A	827	CLA	C3A-C2A-CAA-CBA
19	A	839	CLA	C3A-C2A-CAA-CBA
19	B2	802	CLA	C3A-C2A-CAA-CBA
19	A	805	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	C3A-C2A-CAA-CBA
19	A1	807	CLA	C3A-C2A-CAA-CBA
19	A	829	CLA	C3A-C2A-CAA-CBA
19	BB	824	CLA	C3A-C2A-CAA-CBA
19	AA	839	CLA	C3A-C2A-CAA-CBA
19	AA	808	CLA	C3A-C2A-CAA-CBA
19	A2	826	CLA	C3A-C2A-CAA-CBA
19	A	811	CLA	C3A-C2A-CAA-CBA
19	AA	853	CLA	C3A-C2A-CAA-CBA
19	A2	827	CLA	C3A-C2A-CAA-CBA
19	B1	850	CLA	C3A-C2A-CAA-CBA
19	B2	834	CLA	C3A-C2A-CAA-CBA
19	B2	851	CLA	C3A-C2A-CAA-CBA
19	B	820	CLA	C3A-C2A-CAA-CBA
19	A2	808	CLA	C3A-C2A-CAA-CBA
19	B2	820	CLA	C3A-C2A-CAA-CBA
19	B1	820	CLA	C3A-C2A-CAA-CBA
19	AA	811	CLA	C3A-C2A-CAA-CBA
19	A1	826	CLA	C3A-C2A-CAA-CBA
19	AA	827	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	FF	301	CLA	C3A-C2A-CAA-CBA
19	BB	820	CLA	C3A-C2A-CAA-CBA
20	A	803	CL0	C3A-C2A-CAA-CBA
19	B1	802	CLA	C3A-C2A-CAA-CBA
19	A1	810	CLA	C3A-C2A-CAA-CBA
19	A	852	CLA	C3A-C2A-CAA-CBA
19	A1	838	CLA	C3A-C2A-CAA-CBA
19	B	802	CLA	C3A-C2A-CAA-CBA
19	A	808	CLA	O1D-CGD-O2D-CED
19	A1	842	CLA	O1D-CGD-O2D-CED
19	B	810	CLA	C8-C10-C11-C12
19	BB	806	CLA	C15-C16-C17-C18
19	B2	814	CLA	C5-C6-C7-C8
22	X1	103	LHG	C11-C10-C9-C8
22	B	853	LHG	C15-C16-C17-C18
19	AA	843	CLA	C3-C5-C6-C7
24	BB	849	AJP	OCC-CCX-OCY-CCZ
19	AA	815	CLA	O1D-CGD-O2D-CED
19	A	826	CLA	O1D-CGD-O2D-CED
28	BB	854	DGD	C1G-C2G-C3G-O3G
22	AA	847	LHG	O10-C23-O8-C6
19	A1	827	CLA	O1A-CGA-O2A-C1
19	B	859	CLA	O1A-CGA-O2A-C1
25	BB	844	LMG	C29-C30-C31-C32
19	A2	815	CLA	O1D-CGD-O2D-CED
23	I	101	BCR	C9-C10-C11-C12
22	X2	103	LHG	C30-C31-C32-C33
19	A1	828	CLA	C5-C6-C7-C8
22	A1	846	LHG	O9-C7-O7-C5
22	AA	846	LHG	O9-C7-O7-C5
19	B2	851	CLA	CBA-CGA-O2A-C1
19	AA	826	CLA	O1D-CGD-O2D-CED
22	X2	103	LHG	C17-C18-C19-C20
21	B	838	PQN	C26-C27-C28-C30
21	B1	837	PQN	C26-C27-C28-C29
19	A1	822	CLA	C11-C12-C13-C14
19	AA	832	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	C13-C14-C15-C16
20	A	803	CL0	CBD-CGD-O2D-CED
19	A	805	CLA	C3-C5-C6-C7
19	AA	805	CLA	C3-C5-C6-C7
19	B1	836	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
22	A	846	LHG	C8-C7-O7-C5
22	AA	847	LHG	C8-C7-O7-C5
22	A2	846	LHG	C8-C7-O7-C5
22	A1	846	LHG	C8-C7-O7-C5
22	AA	846	LHG	C8-C7-O7-C5
22	A	845	LHG	C8-C7-O7-C5
25	L1	210	LMG	C11-C10-O7-C8
22	B1	847	LHG	C11-C12-C13-C14
25	L1	210	LMG	C15-C16-C17-C18
22	A	846	LHG	O1-C1-C2-O2
22	AA	847	LHG	O1-C1-C2-O2
23	B	844	BCR	C14-C15-C16-C17
22	A1	846	LHG	O1-C1-C2-O2
23	F	305	BCR	C14-C15-C16-C17
23	BB	843	BCR	C14-C15-C16-C17
23	KK	103	BCR	C14-C15-C16-C17
25	BB	844	LMG	C41-C42-C43-C44
25	B	845	LMG	C13-C14-C15-C16
28	B	856	DGD	C2B-C3B-C4B-C5B
19	B	808	CLA	CBA-CGA-O2A-C1
19	BB	829	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	C4-C3-C5-C6
19	BB	855	CLA	C4-C3-C5-C6
22	B1	847	LHG	C11-C10-C9-C8
19	A	821	CLA	C15-C16-C17-C18
22	A	845	LHG	C12-C13-C14-C15
19	A1	820	CLA	C2-C3-C5-C6
19	B2	808	CLA	C2-C3-C5-C6
19	A2	836	CLA	C2-C3-C5-C6
21	BB	837	PQN	C26-C27-C28-C30
19	B1	829	CLA	C4C-C3C-CAC-CBC
25	B1	844	LMG	C29-C30-C31-C32
22	BB	851	LHG	C1-C2-C3-O3
19	A2	831	CLA	C13-C15-C16-C17
19	BB	810	CLA	C8-C10-C11-C12
22	X1	103	LHG	C15-C16-C17-C18
19	AA	830	CLA	C2C-C3C-CAC-CBC
25	L1	210	LMG	C11-C12-C13-C14
19	B2	836	CLA	C13-C15-C16-C17
19	B1	810	CLA	C10-C11-C12-C13
25	B2	845	LMG	C18-C19-C20-C21
25	B2	845	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
19	A	852	CLA	C8-C10-C11-C12
19	AA	824	CLA	CBD-CGD-O2D-CED
19	BB	833	CLA	CBD-CGD-O2D-CED
26	BB	840	ECH	C1-C6-C7-C8
26	BB	840	ECH	C23-C24-C25-C26
23	A2	849	BCR	C23-C24-C25-C26
23	B2	842	BCR	C23-C24-C25-C26
23	B2	842	BCR	C23-C24-C25-C30
23	B	843	BCR	C23-C24-C25-C26
23	F2	303	BCR	C23-C24-C25-C26
23	J2	104	BCR	C23-C24-C25-C30
23	A1	851	BCR	C23-C24-C25-C26
23	A1	851	BCR	C23-C24-C25-C30
23	BB	847	BCR	C5-C6-C7-C8
23	M	101	BCR	C23-C24-C25-C30
23	B	844	BCR	C1-C6-C7-C8
23	B	844	BCR	C5-C6-C7-C8
23	I	101	BCR	C1-C6-C7-C8
26	B	841	ECH	C23-C24-C25-C26
23	J2	102	BCR	C23-C24-C25-C26
23	K1	106	BCR	C23-C24-C25-C26
23	K1	106	BCR	C23-C24-C25-C30
23	BB	842	BCR	C23-C24-C25-C30
23	J1	102	BCR	C23-C24-C25-C26
23	JJ	104	BCR	C23-C24-C25-C30
26	B1	840	ECH	C23-C24-C25-C26
23	BB	843	BCR	C1-C6-C7-C8
23	BB	843	BCR	C5-C6-C7-C8
23	AA	855	BCR	C23-C24-C25-C26
23	KK	103	BCR	C23-C24-C25-C26
23	B2	844	BCR	C5-C6-C7-C8
23	I2	101	BCR	C5-C6-C7-C8
23	B1	843	BCR	C5-C6-C7-C8
26	B2	841	ECH	C23-C24-C25-C26
23	A	854	BCR	C23-C24-C25-C26
23	K	103	BCR	C23-C24-C25-C26
23	A2	851	BCR	C23-C24-C25-C26
23	A2	851	BCR	C23-C24-C25-C30
23	A	849	BCR	C23-C24-C25-C26
23	A1	849	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C26
23	A	851	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
23	I1	101	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C30
23	F2	305	BCR	C23-C24-C25-C26
23	F2	305	BCR	C23-C24-C25-C30
23	F	303	BCR	C23-C24-C25-C26
23	AA	850	BCR	C23-C24-C25-C26
23	J1	104	BCR	C23-C24-C25-C30
23	FF	303	BCR	C23-C24-C25-C26
22	A	845	LHG	O9-C7-O7-C5
19	BB	856	CLA	O1A-CGA-O2A-C1
19	AA	828	CLA	O1A-CGA-O2A-C1
19	B1	808	CLA	O1A-CGA-O2A-C1
19	B2	815	CLA	O1A-CGA-O2A-C1
19	A2	831	CLA	O1A-CGA-O2A-C1
19	AA	836	CLA	O1A-CGA-O2A-C1
19	B2	851	CLA	O1A-CGA-O2A-C1
19	AA	831	CLA	CBA-CGA-O2A-C1
19	BB	824	CLA	CBA-CGA-O2A-C1
19	B1	850	CLA	CBA-CGA-O2A-C1
19	B2	816	CLA	CBA-CGA-O2A-C1
19	B1	815	CLA	CBA-CGA-O2A-C1
19	A	833	CLA	CBA-CGA-O2A-C1
19	A1	832	CLA	CBD-CGD-O2D-CED
19	B2	813	CLA	CBD-CGD-O2D-CED
22	A1	845	LHG	C12-C13-C14-C15
19	A2	830	CLA	C4C-C3C-CAC-CBC
19	B1	806	CLA	C2-C1-O2A-CGA
19	B1	828	CLA	C2-C1-O2A-CGA
19	A	827	CLA	C2-C1-O2A-CGA
19	B	807	CLA	C2-C1-O2A-CGA
19	BB	806	CLA	C2-C1-O2A-CGA
19	B	806	CLA	C2-C1-O2A-CGA
19	BB	807	CLA	C2-C1-O2A-CGA
19	B	829	CLA	C2-C1-O2A-CGA
19	AA	827	CLA	C2-C1-O2A-CGA
20	A2	803	CL0	C2-C1-O2A-CGA
19	B2	829	CLA	C2-C1-O2A-CGA
19	FF	305	CLA	C2-C1-O2A-CGA
19	B2	806	CLA	C2-C1-O2A-CGA
22	X2	102	LHG	C23-C24-C25-C26
22	X1	102	LHG	C23-C24-C25-C26
19	AA	829	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
19	AA	813	CLA	C16-C17-C18-C19
19	B	834	CLA	C6-C7-C8-C10
19	B1	828	CLA	C12-C13-C15-C16
19	A	827	CLA	C11-C10-C8-C7
19	B	810	CLA	C6-C7-C8-C10
19	A	801	CLA	C11-C10-C8-C7
21	A	843	PQN	C16-C17-C18-C20
19	B1	805	CLA	C6-C7-C8-C10
19	B	805	CLA	C6-C7-C8-C10
19	AA	842	CLA	C6-C7-C8-C10
19	B2	811	CLA	C6-C7-C8-C10
19	B2	811	CLA	C11-C12-C13-C15
19	A1	801	CLA	C11-C10-C8-C7
19	A	804	CLA	C6-C7-C8-C10
19	BB	810	CLA	C6-C7-C8-C10
19	B	811	CLA	C11-C12-C13-C15
19	A2	827	CLA	C11-C10-C8-C7
19	A	842	CLA	C6-C7-C8-C10
19	B2	834	CLA	C6-C7-C8-C10
19	AA	804	CLA	C6-C7-C8-C10
19	BB	805	CLA	C6-C7-C8-C10
19	B2	805	CLA	C6-C7-C8-C10
19	B	829	CLA	C12-C13-C15-C16
19	L1	206	CLA	C11-C12-C13-C15
19	A2	804	CLA	C12-C13-C15-C16
19	L	203	CLA	C11-C12-C13-C15
19	A1	803	CLA	C6-C7-C8-C10
19	B1	833	CLA	C6-C7-C8-C10
19	B1	811	CLA	C6-C7-C8-C10
19	B1	811	CLA	C11-C12-C13-C15
19	BB	833	CLA	C6-C7-C8-C10
19	LL	202	CLA	C11-C12-C13-C15
19	FF	305	CLA	C12-C13-C15-C16
22	B1	847	LHG	O10-C23-O8-C6
19	BB	824	CLA	O1A-CGA-O2A-C1
19	B2	803	CLA	O1A-CGA-O2A-C1
19	B	824	CLA	O1A-CGA-O2A-C1
19	B1	850	CLA	O1A-CGA-O2A-C1
19	A1	830	CLA	O1A-CGA-O2A-C1
19	B1	829	CLA	O1A-CGA-O2A-C1
19	B2	830	CLA	O1A-CGA-O2A-C1
22	L2	208	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	C2C-C3C-CAC-CBC
22	A1	845	LHG	C13-C14-C15-C16
19	B	826	CLA	C5-C6-C7-C8
19	A1	813	CLA	O1D-CGD-O2D-CED
19	B2	823	CLA	O1D-CGD-O2D-CED
19	BB	823	CLA	O1D-CGD-O2D-CED
19	B1	828	CLA	CBA-CGA-O2A-C1
19	AA	833	CLA	CBA-CGA-O2A-C1
19	B	830	CLA	CBA-CGA-O2A-C1
19	A	828	CLA	CBA-CGA-O2A-C1
19	B1	824	CLA	CBA-CGA-O2A-C1
19	B	829	CLA	CBA-CGA-O2A-C1
19	A	840	CLA	CBA-CGA-O2A-C1
19	B2	829	CLA	CBA-CGA-O2A-C1
19	FF	305	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	O1A-CGA-O2A-C1
19	A	805	CLA	C8-C10-C11-C12
19	B2	849	CLA	C13-C15-C16-C17
19	BB	826	CLA	C5-C6-C7-C8
19	B1	848	CLA	C13-C15-C16-C17
19	B2	836	CLA	C8-C10-C11-C12
19	A1	803	CLA	C8-C10-C11-C12
19	A2	852	CLA	C8-C10-C11-C12
19	B1	849	CLA	C2A-CAA-CBA-CGA
19	A	812	CLA	C2A-CAA-CBA-CGA
19	A2	808	CLA	C2A-CAA-CBA-CGA
19	A1	803	CLA	C2A-CAA-CBA-CGA
19	B2	850	CLA	C2A-CAA-CBA-CGA
22	A	846	LHG	O9-C7-O7-C5
22	AA	847	LHG	O9-C7-O7-C5
22	A2	846	LHG	O9-C7-O7-C5
25	B1	844	LMG	C4-C5-C6-O5
19	B	823	CLA	O1D-CGD-O2D-CED
19	A2	828	CLA	C3-C5-C6-C7
19	B2	829	CLA	C3-C5-C6-C7
23	A	853	BCR	C9-C10-C11-C12
23	B	842	BCR	C9-C10-C11-C12
23	KK	103	BCR	C9-C10-C11-C12
23	AA	854	BCR	C9-C10-C11-C12
23	BB	841	BCR	C9-C10-C11-C12
19	A	836	CLA	C13-C15-C16-C17
25	BB	844	LMG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
19	BB	835	CLA	C8-C10-C11-C12
19	B2	806	CLA	C5-C6-C7-C8
19	B1	808	CLA	C4-C3-C5-C6
19	AA	821	CLA	C4-C3-C5-C6
19	B	858	CLA	C4-C3-C5-C6
22	AA	846	LHG	C12-C13-C14-C15
28	BB	854	DGD	C2B-C3B-C4B-C5B
22	AA	846	LHG	C24-C23-O8-C6
19	B	814	CLA	CBA-CGA-O2A-C1
19	AA	804	CLA	CBA-CGA-O2A-C1
19	A	827	CLA	C5-C6-C7-C8
19	B	829	CLA	C5-C6-C7-C8
19	B2	829	CLA	C13-C15-C16-C17
22	A	846	LHG	O6-C4-C5-O7
22	AA	847	LHG	O6-C4-C5-O7
22	A2	846	LHG	O6-C4-C5-O7
22	BB	850	LHG	O6-C4-C5-O7
25	B	845	LMG	C18-C19-C20-C21
25	B1	844	LMG	C41-C42-C43-C44
19	B1	828	CLA	C3-C5-C6-C7
19	B	860	CLA	C3-C5-C6-C7
19	A	815	CLA	C3-C5-C6-C7
19	LL	201	CLA	C3-C5-C6-C7
19	B1	828	CLA	C5-C6-C7-C8
19	A2	821	CLA	C15-C16-C17-C18
19	BB	852	CLA	C13-C15-C16-C17
19	B	823	CLA	C13-C15-C16-C17
19	A1	809	CLA	C10-C11-C12-C13
21	B1	837	PQN	C15-C16-C17-C18
19	FF	305	CLA	C5-C6-C7-C8
25	B1	852	LMG	O6-C5-C6-O5
22	BB	850	LHG	C8-C7-O7-C5
19	B	825	CLA	C16-C17-C18-C19
19	B1	825	CLA	C16-C17-C18-C19
19	B2	816	CLA	O1A-CGA-O2A-C1
19	BB	829	CLA	O1A-CGA-O2A-C1
19	B1	815	CLA	O1A-CGA-O2A-C1
19	B1	806	CLA	C5-C6-C7-C8
25	BB	844	LMG	C18-C19-C20-C21
25	B2	854	LMG	O6-C5-C6-O5
25	B2	847	LMG	O6-C5-C6-O5
19	B	803	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	L2	205	CLA	CBA-CGA-O2A-C1
19	B	815	CLA	CBA-CGA-O2A-C1
25	I1	102	LMG	C11-C12-C13-C14
22	A1	845	LHG	C26-C27-C28-C29
23	L2	207	BCR	C18-C19-C20-C21
23	KK	103	BCR	C18-C19-C20-C21
19	BB	806	CLA	C5-C6-C7-C8
19	A2	827	CLA	C15-C16-C17-C18
19	B2	829	CLA	C5-C6-C7-C8
23	K1	104	BCR	C14-C15-C16-C17
23	A1	847	BCR	C14-C15-C16-C17
23	L	206	BCR	C6-C7-C8-C9
23	K1	104	BCR	C22-C23-C24-C25
23	K2	105	BCR	C22-C23-C24-C25
23	B	839	BCR	C6-C7-C8-C9
23	L2	207	BCR	C6-C7-C8-C9
23	JJ	104	BCR	C6-C7-C8-C9
23	AA	855	BCR	C22-C23-C24-C25
23	A	854	BCR	C22-C23-C24-C25
19	B1	806	CLA	C6-C7-C8-C9
19	B	834	CLA	C6-C7-C8-C9
19	A	831	CLA	C6-C7-C8-C9
19	A	827	CLA	C11-C10-C8-C9
19	B	810	CLA	C6-C7-C8-C9
19	L2	204	CLA	C6-C7-C8-C9
19	A	801	CLA	C11-C10-C8-C9
19	BB	806	CLA	C6-C7-C8-C9
19	BB	811	CLA	C6-C7-C8-C9
19	BB	811	CLA	C11-C12-C13-C14
19	AA	831	CLA	C6-C7-C8-C9
19	L1	205	CLA	C6-C7-C8-C9
19	B	806	CLA	C6-C7-C8-C9
19	A2	831	CLA	C6-C7-C8-C9
19	AA	842	CLA	C6-C7-C8-C9
19	AA	801	CLA	C11-C10-C8-C9
19	A1	801	CLA	C11-C10-C8-C9
19	AA	807	CLA	C11-C12-C13-C14
19	A1	820	CLA	C11-C10-C8-C9
19	BB	821	CLA	C6-C7-C8-C9
19	B	811	CLA	C6-C7-C8-C9
19	B	811	CLA	C11-C12-C13-C14
21	A1	843	PQN	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	A2	827	CLA	C11-C10-C8-C9
19	B2	834	CLA	C6-C7-C8-C9
19	A1	826	CLA	C11-C10-C8-C9
19	B	829	CLA	C14-C13-C15-C16
19	L1	206	CLA	C11-C12-C13-C14
19	A2	804	CLA	C14-C13-C15-C16
19	L	203	CLA	C11-C12-C13-C14
19	A1	803	CLA	C14-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C14
19	B1	833	CLA	C6-C7-C8-C9
19	BB	833	CLA	C6-C7-C8-C9
19	LL	202	CLA	C11-C12-C13-C14
19	L	204	CLA	C6-C7-C8-C9
19	FF	305	CLA	C14-C13-C15-C16
19	B2	806	CLA	C6-C7-C8-C9
19	BB	856	CLA	C1A-C2A-CAA-CBA
19	B1	828	CLA	C1A-C2A-CAA-CBA
19	B1	834	CLA	C1A-C2A-CAA-CBA
19	B2	825	CLA	C1A-C2A-CAA-CBA
19	A2	823	CLA	C1A-C2A-CAA-CBA
19	A2	839	CLA	C1A-C2A-CAA-CBA
19	A	827	CLA	C1A-C2A-CAA-CBA
19	A	839	CLA	C1A-C2A-CAA-CBA
19	B2	835	CLA	C1A-C2A-CAA-CBA
19	AA	822	CLA	C1A-C2A-CAA-CBA
19	B2	802	CLA	C1A-C2A-CAA-CBA
19	BB	808	CLA	C1A-C2A-CAA-CBA
19	A	805	CLA	C1A-C2A-CAA-CBA
19	A	808	CLA	C1A-C2A-CAA-CBA
19	A	810	CLA	C1A-C2A-CAA-CBA
19	B	825	CLA	C1A-C2A-CAA-CBA
19	A1	807	CLA	C1A-C2A-CAA-CBA
19	A	825	CLA	C1A-C2A-CAA-CBA
19	B1	825	CLA	C1A-C2A-CAA-CBA
19	BB	827	CLA	C1A-C2A-CAA-CBA
19	BB	825	CLA	C1A-C2A-CAA-CBA
19	B2	815	CLA	C1A-C2A-CAA-CBA
19	A2	811	CLA	C1A-C2A-CAA-CBA
19	A	829	CLA	C1A-C2A-CAA-CBA
19	B	827	CLA	C1A-C2A-CAA-CBA
19	BB	824	CLA	C1A-C2A-CAA-CBA
19	AA	839	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	A	822	CLA	C1A-C2A-CAA-CBA
19	A	828	CLA	C1A-C2A-CAA-CBA
19	AA	805	CLA	C1A-C2A-CAA-CBA
19	B2	804	CLA	C1A-C2A-CAA-CBA
19	A2	820	CLA	C1A-C2A-CAA-CBA
19	AA	820	CLA	C1A-C2A-CAA-CBA
19	A	811	CLA	C1A-C2A-CAA-CBA
19	B	859	CLA	C1A-C2A-CAA-CBA
19	A2	827	CLA	C1A-C2A-CAA-CBA
19	B1	850	CLA	C1A-C2A-CAA-CBA
19	B2	827	CLA	C1A-C2A-CAA-CBA
19	B2	851	CLA	C1A-C2A-CAA-CBA
19	B	820	CLA	C1A-C2A-CAA-CBA
19	A	818	CLA	C1A-C2A-CAA-CBA
19	A2	808	CLA	C1A-C2A-CAA-CBA
19	B1	804	CLA	C1A-C2A-CAA-CBA
19	B2	820	CLA	C1A-C2A-CAA-CBA
19	B1	820	CLA	C1A-C2A-CAA-CBA
19	A	820	CLA	C1A-C2A-CAA-CBA
19	AA	811	CLA	C1A-C2A-CAA-CBA
19	A1	826	CLA	C1A-C2A-CAA-CBA
19	B	829	CLA	C1A-C2A-CAA-CBA
19	B	804	CLA	C1A-C2A-CAA-CBA
19	BB	804	CLA	C1A-C2A-CAA-CBA
19	K2	104	CLA	C1A-C2A-CAA-CBA
19	A1	809	CLA	C1A-C2A-CAA-CBA
19	AA	827	CLA	C1A-C2A-CAA-CBA
19	FF	301	CLA	C1A-C2A-CAA-CBA
19	A1	819	CLA	C1A-C2A-CAA-CBA
19	B1	815	CLA	C1A-C2A-CAA-CBA
19	A1	817	CLA	C1A-C2A-CAA-CBA
19	AA	818	CLA	C1A-C2A-CAA-CBA
19	AA	825	CLA	C1A-C2A-CAA-CBA
19	A1	810	CLA	C1A-C2A-CAA-CBA
19	A1	822	CLA	C1A-C2A-CAA-CBA
19	A2	818	CLA	C1A-C2A-CAA-CBA
19	A	852	CLA	C1A-C2A-CAA-CBA
19	A1	838	CLA	C1A-C2A-CAA-CBA
19	B1	827	CLA	C1A-C2A-CAA-CBA
19	A2	804	CLA	C5-C6-C7-C8
19	BB	855	CLA	C15-C16-C17-C18
19	A	837	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	II	105	LMG	C28-C29-C30-C31
25	B1	852	LMG	C2-C1-O1-C7
23	A	847	BCR	C36-C18-C19-C20
23	L1	209	BCR	C7-C8-C9-C34
25	B2	854	LMG	C2-C1-O1-C7
23	K	103	BCR	C7-C8-C9-C34
23	A	849	BCR	C36-C18-C19-C20
23	F1	303	BCR	C36-C18-C19-C20
19	A1	812	CLA	C16-C17-C18-C19
19	B1	822	CLA	C2A-CAA-CBA-CGA
19	AA	812	CLA	C2A-CAA-CBA-CGA
19	X2	101	CLA	C2A-CAA-CBA-CGA
22	X1	103	LHG	C3-O3-P-O6
19	LL	203	CLA	C4C-C3C-CAC-CBC
25	B	845	LMG	C33-C34-C35-C36
19	AA	831	CLA	O1A-CGA-O2A-C1
19	B1	824	CLA	O1A-CGA-O2A-C1
19	A	833	CLA	O1A-CGA-O2A-C1
23	FF	304	BCR	C17-C18-C19-C20
23	B	842	BCR	C17-C18-C19-C20
23	II	101	BCR	C17-C18-C19-C20
23	A2	848	BCR	C11-C12-C13-C14
23	I2	101	BCR	C17-C18-C19-C20
23	A	854	BCR	C21-C22-C23-C24
23	A1	849	BCR	C21-C22-C23-C24
23	F1	304	BCR	C17-C18-C19-C20
19	A1	826	CLA	O1D-CGD-O2D-CED
19	BB	815	CLA	CBA-CGA-O2A-C1
19	AA	815	CLA	C3-C5-C6-C7
22	B	853	LHG	C23-C24-C25-C26
19	AA	843	CLA	O1D-CGD-O2D-CED
21	B2	838	PQN	C15-C16-C17-C18
19	B1	850	CLA	C5-C6-C7-C8
19	B2	851	CLA	C5-C6-C7-C8
19	AA	828	CLA	C4-C3-C5-C6
19	A	821	CLA	C4-C3-C5-C6
19	B2	821	CLA	C4-C3-C5-C6
19	B2	850	CLA	C4-C3-C5-C6
19	A2	836	CLA	C4-C3-C5-C6
19	AA	828	CLA	C2-C3-C5-C6
19	B1	808	CLA	C2-C3-C5-C6
19	AA	821	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
19	B1	821	CLA	C2-C3-C5-C6
22	A	846	LHG	O6-C4-C5-C6
25	B	851	LMG	C11-C10-O7-C8
22	X	102	LHG	C8-C7-O7-C5
22	L1	211	LHG	O6-C4-C5-C6
22	A2	845	LHG	C8-C7-O7-C5
24	K	104	AJP	OCC-CCX-OCY-CCZ
25	B2	845	LMG	O6-C5-C6-O5
19	BB	856	CLA	C5-C6-C7-C8
19	AA	820	CLA	C8-C10-C11-C12
19	A	813	CLA	C16-C17-C18-C19
19	B	808	CLA	CBD-CGD-O2D-CED
19	B2	824	CLA	CBA-CGA-O2A-C1
23	B2	842	BCR	C19-C20-C21-C22
23	KK	103	BCR	C15-C16-C17-C18
23	B1	841	BCR	C9-C10-C11-C12
19	B2	822	CLA	C3-C5-C6-C7
19	A1	827	CLA	C3-C5-C6-C7
19	B	829	CLA	C3-C5-C6-C7
19	FF	305	CLA	C3-C5-C6-C7
19	A	827	CLA	C10-C11-C12-C13
19	AA	805	CLA	C8-C10-C11-C12
19	BB	823	CLA	C13-C15-C16-C17
19	B1	835	CLA	O1D-CGD-O2D-CED
19	B	806	CLA	C5-C6-C7-C8
19	A2	801	CLA	C5-C6-C7-C8
19	B2	823	CLA	C8-C10-C11-C12
19	B1	802	CLA	C15-C16-C17-C18
22	A1	845	LHG	C1-C2-C3-O3
19	B	803	CLA	O1A-CGA-O2A-C1
19	AA	833	CLA	O1A-CGA-O2A-C1
19	B	830	CLA	O1A-CGA-O2A-C1
19	A	828	CLA	O1A-CGA-O2A-C1
19	B	829	CLA	O1A-CGA-O2A-C1
19	A	840	CLA	O1A-CGA-O2A-C1
19	FF	305	CLA	O1A-CGA-O2A-C1
19	B2	819	CLA	O1D-CGD-O2D-CED
22	L2	208	LHG	C4-C5-C6-O8
22	B1	847	LHG	C4-C5-C6-O8
28	B	856	DGD	C1G-C2G-C3G-O3G
25	M	102	LMG	O1-C7-C8-C9
22	L1	211	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
22	B2	848	LHG	C4-C5-C6-O8
25	B2	847	LMG	O1-C7-C8-C9
19	K1	103	CLA	C2A-CAA-CBA-CGA
25	B	845	LMG	C30-C31-C32-C33
19	A	820	CLA	C8-C10-C11-C12
19	A2	810	CLA	C10-C11-C12-C13
25	II	105	LMG	C4-C5-C6-O5
19	A2	814	CLA	C3A-C2A-CAA-CBA
19	B	813	CLA	C3A-C2A-CAA-CBA
19	A1	813	CLA	C3A-C2A-CAA-CBA
19	A	814	CLA	C3A-C2A-CAA-CBA
19	BB	813	CLA	C3A-C2A-CAA-CBA
19	AA	814	CLA	C3A-C2A-CAA-CBA
19	B2	813	CLA	C3A-C2A-CAA-CBA
19	B1	813	CLA	C3A-C2A-CAA-CBA
19	B2	824	CLA	O1A-CGA-O2A-C1
19	L2	205	CLA	O1A-CGA-O2A-C1
19	B	814	CLA	O1A-CGA-O2A-C1
19	B2	829	CLA	O1A-CGA-O2A-C1
19	B	834	CLA	C13-C15-C16-C17
25	B	851	LMG	C37-C38-C39-C40
19	AA	810	CLA	C10-C11-C12-C13
19	B2	850	CLA	C15-C16-C17-C18
24	L1	203	AJP	OBC-CBJ-CCB-OCC
25	B2	854	LMG	C14-C15-C16-C17
19	A	828	CLA	C4-C3-C5-C6
19	B2	808	CLA	O1D-CGD-O2D-CED
19	B	836	CLA	O1D-CGD-O2D-CED
19	B1	828	CLA	O1A-CGA-O2A-C1
19	AA	821	CLA	C15-C16-C17-C18
19	L1	207	CLA	C10-C11-C12-C13
19	B1	801	CLA	C13-C15-C16-C17
25	B2	845	LMG	C33-C34-C35-C36
23	L	205	BCR	C35-C13-C14-C15
23	BB	838	BCR	C35-C13-C14-C15
23	K2	103	BCR	C35-C13-C14-C15
23	II	104	BCR	C20-C21-C22-C37
23	AA	849	BCR	C20-C21-C22-C37
23	F1	306	BCR	C11-C10-C9-C34
23	B1	841	BCR	C20-C21-C22-C37
25	M	102	LMG	C15-C16-C17-C18
25	II	105	LMG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
19	A1	830	CLA	C13-C15-C16-C17
22	BB	850	LHG	C23-C24-C25-C26
23	F2	303	BCR	C14-C15-C16-C17
23	L	205	BCR	C14-C15-C16-C17
22	A2	846	LHG	O1-C1-C2-O2
23	FF	306	BCR	C14-C15-C16-C17
23	A2	848	BCR	C14-C15-C16-C17
19	A1	804	CLA	C3-C5-C6-C7
19	B	830	CLA	C4C-C3C-CAC-CBC
19	B1	849	CLA	C15-C16-C17-C18
19	BB	826	CLA	C15-C16-C17-C18
19	B2	801	CLA	C13-C15-C16-C17
19	B1	823	CLA	C15-C16-C17-C18
19	B	826	CLA	C15-C16-C17-C18
25	B	851	LMG	C9-C8-O7-C10
28	B	856	DGD	C1G-C2G-O2G-C1B
28	BB	854	DGD	C1G-C2G-O2G-C1B
25	L1	210	LMG	C9-C8-O7-C10
19	B	815	CLA	O1A-CGA-O2A-C1
19	A	841	CLA	O1A-CGA-O2A-C1
19	A	801	CLA	C5-C6-C7-C8
19	B2	803	CLA	C5-C6-C7-C8
19	B1	833	CLA	C13-C15-C16-C17
19	BB	822	CLA	O1D-CGD-O2D-CED
22	L2	208	LHG	C24-C25-C26-C27
19	B1	813	CLA	O1D-CGD-O2D-CED
22	LL	205	LHG	C24-C23-O8-C6
19	B1	803	CLA	C5-C6-C7-C8
19	B2	810	CLA	C10-C11-C12-C13
19	B2	830	CLA	C2C-C3C-CAC-CBC
19	A2	807	CLA	C10-C11-C12-C13
25	B2	845	LMG	C35-C36-C37-C38
19	A2	802	CLA	C2A-CAA-CBA-CGA
19	B	813	CLA	O1D-CGD-O2D-CED
22	A1	846	LHG	O6-C4-C5-O7
19	B	822	CLA	C16-C17-C18-C19
19	A2	807	CLA	C16-C17-C18-C19
20	AA	803	CL0	C2C-C3C-CAC-CBC
25	B1	852	LMG	C14-C15-C16-C17
22	X2	102	LHG	C25-C26-C27-C28
19	AA	804	CLA	O1A-CGA-O2A-C1
23	B2	842	BCR	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
23	A1	851	BCR	C20-C21-C22-C23
23	J	102	BCR	C11-C10-C9-C8
25	I1	102	LMG	C8-C7-O1-C1
23	FF	304	BCR	C12-C13-C14-C15
23	B	839	BCR	C16-C17-C18-C19
23	L1	209	BCR	C16-C17-C18-C19
23	AA	849	BCR	C16-C17-C18-C19
23	B2	839	BCR	C16-C17-C18-C19
23	M2	102	BCR	C16-C17-C18-C19
23	B	840	BCR	C16-C17-C18-C19
23	B1	841	BCR	C11-C10-C9-C8
23	B1	841	BCR	C12-C13-C14-C15
19	B1	823	CLA	O1D-CGD-O2D-CED
19	A	810	CLA	C8-C10-C11-C12
19	BB	808	CLA	CBA-CGA-O2A-C1
19	A1	832	CLA	CBA-CGA-O2A-C1
22	L	207	LHG	C24-C23-O8-C6
19	AA	853	CLA	CBA-CGA-O2A-C1
19	AA	840	CLA	CBA-CGA-O2A-C1
19	A2	804	CLA	CBA-CGA-O2A-C1
19	A1	839	CLA	CBA-CGA-O2A-C1
19	BB	814	CLA	C4-C3-C5-C6
19	A1	827	CLA	C4-C3-C5-C6
19	B2	850	CLA	C2-C3-C5-C6
25	M	102	LMG	C12-C13-C14-C15
25	M	102	LMG	C17-C18-C19-C20
22	X1	102	LHG	C25-C26-C27-C28
19	A1	820	CLA	O1D-CGD-O2D-CED
22	AA	846	LHG	O10-C23-O8-C6
19	BB	815	CLA	O1A-CGA-O2A-C1
25	I2	105	LMG	O1-C7-C8-O7
19	A1	807	CLA	C5-C6-C7-C8
19	BB	802	CLA	C15-C16-C17-C18
25	L1	210	LMG	C37-C38-C39-C40
22	A2	845	LHG	C12-C13-C14-C15
19	B2	825	CLA	C16-C17-C18-C19
19	B	822	CLA	C16-C17-C18-C20
19	B1	806	CLA	C6-C7-C8-C10
19	A	831	CLA	C6-C7-C8-C10
19	A2	823	CLA	C6-C7-C8-C10
19	L2	204	CLA	C6-C7-C8-C10
19	BB	832	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	BB	806	CLA	C6-C7-C8-C10
19	A	807	CLA	C11-C12-C13-C15
19	A	807	CLA	C12-C13-C15-C16
19	B1	832	CLA	C6-C7-C8-C10
21	A	843	PQN	C21-C22-C23-C25
19	AA	831	CLA	C6-C7-C8-C10
19	L1	205	CLA	C6-C7-C8-C10
19	B	806	CLA	C6-C7-C8-C10
19	A2	831	CLA	C6-C7-C8-C10
19	A	830	CLA	C11-C10-C8-C7
19	AA	823	CLA	C6-C7-C8-C10
19	B2	811	CLA	C11-C10-C8-C7
19	AA	821	CLA	C11-C12-C13-C15
19	AA	801	CLA	C11-C10-C8-C7
19	B	815	CLA	C12-C13-C15-C16
19	AA	807	CLA	C11-C12-C13-C15
19	B2	849	CLA	C6-C7-C8-C10
19	A1	820	CLA	C12-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C10
19	BB	821	CLA	C6-C7-C8-C10
19	A	813	CLA	C11-C12-C13-C15
21	B2	838	PQN	C21-C22-C23-C25
21	B	838	PQN	C21-C22-C23-C25
19	BB	826	CLA	C6-C7-C8-C10
19	B1	801	CLA	C12-C13-C15-C16
19	AA	830	CLA	C11-C10-C8-C7
19	B1	821	CLA	C6-C7-C8-C10
19	A	823	CLA	C6-C7-C8-C10
19	A	821	CLA	C11-C12-C13-C15
19	A	835	CLA	C12-C13-C15-C16
19	A1	830	CLA	C6-C7-C8-C10
19	A1	829	CLA	C11-C10-C8-C7
19	AA	804	CLA	C12-C13-C15-C16
19	B2	810	CLA	C6-C7-C8-C10
19	B2	821	CLA	C6-C7-C8-C10
19	B2	833	CLA	C6-C7-C8-C10
19	AA	813	CLA	C11-C12-C13-C15
19	BB	835	CLA	C6-C7-C8-C10
19	B2	836	CLA	C6-C7-C8-C10
19	A2	804	CLA	C6-C7-C8-C10
19	B	836	CLA	C6-C7-C8-C10
19	B1	815	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	B1	815	CLA	C12-C13-C15-C16
19	A1	803	CLA	C12-C13-C15-C16
19	A1	806	CLA	C11-C12-C13-C15
19	A2	813	CLA	C11-C12-C13-C15
19	B	826	CLA	C6-C7-C8-C10
19	A2	830	CLA	C11-C10-C8-C7
19	B1	811	CLA	C11-C10-C8-C7
19	A2	807	CLA	C11-C12-C13-C15
19	A2	807	CLA	C12-C13-C15-C16
20	A	803	CL0	C12-C13-C15-C16
19	A1	822	CLA	C6-C7-C8-C10
19	B2	826	CLA	C6-C7-C8-C10
19	AA	829	CLA	C11-C10-C8-C7
19	B2	806	CLA	C6-C7-C8-C10
19	B	858	CLA	C15-C16-C17-C18
25	B2	845	LMG	C13-C14-C15-C16
22	L2	208	LHG	C13-C14-C15-C16
25	II	105	LMG	C35-C36-C37-C38
25	L1	210	LMG	C21-C22-C23-C24
25	B2	845	LMG	C38-C39-C40-C41
19	A	830	CLA	C3-C5-C6-C7
19	A	828	CLA	C3-C5-C6-C7
19	BB	801	CLA	C14-C13-C15-C16
19	A2	823	CLA	C6-C7-C8-C9
19	B	803	CLA	C11-C12-C13-C14
19	BB	832	CLA	C6-C7-C8-C9
19	A	807	CLA	C11-C10-C8-C9
19	A	807	CLA	C11-C12-C13-C14
19	A	807	CLA	C14-C13-C15-C16
19	B1	832	CLA	C6-C7-C8-C9
19	B2	815	CLA	C11-C10-C8-C9
21	A2	843	PQN	C16-C17-C18-C19
21	A	843	PQN	C21-C22-C23-C24
19	A	836	CLA	C14-C13-C15-C16
19	A2	821	CLA	C11-C12-C13-C14
19	AA	823	CLA	C6-C7-C8-C9
19	AA	821	CLA	C11-C12-C13-C14
19	B2	849	CLA	C11-C10-C8-C9
19	A	804	CLA	C14-C13-C15-C16
19	B	821	CLA	C6-C7-C8-C9
19	A	813	CLA	C11-C12-C13-C14
19	AA	836	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
19	BB	826	CLA	C6-C7-C8-C9
19	B1	801	CLA	C14-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C14
19	BB	852	CLA	C11-C10-C8-C9
19	B1	821	CLA	C6-C7-C8-C9
19	A	823	CLA	C6-C7-C8-C9
19	A	821	CLA	C11-C12-C13-C14
19	A1	830	CLA	C6-C7-C8-C9
19	AA	804	CLA	C14-C13-C15-C16
19	B2	810	CLA	C6-C7-C8-C9
19	B	801	CLA	C14-C13-C15-C16
19	B2	821	CLA	C6-C7-C8-C9
19	B2	833	CLA	C6-C7-C8-C9
19	AA	813	CLA	C11-C12-C13-C14
19	B1	848	CLA	C11-C10-C8-C9
19	B2	823	CLA	C11-C12-C13-C14
19	B1	815	CLA	C11-C10-C8-C9
19	B1	810	CLA	C11-C10-C8-C9
19	B	826	CLA	C6-C7-C8-C9
19	A2	830	CLA	C11-C12-C13-C14
19	B	854	CLA	C11-C10-C8-C9
19	BB	815	CLA	C11-C10-C8-C9
19	A2	807	CLA	C11-C12-C13-C14
19	A2	807	CLA	C14-C13-C15-C16
20	A	803	CL0	C6-C7-C8-C9
19	B	833	CLA	C6-C7-C8-C9
19	A1	822	CLA	C6-C7-C8-C9
19	B2	826	CLA	C6-C7-C8-C9
19	AA	841	CLA	O1A-CGA-O2A-C1
19	A	810	CLA	C10-C11-C12-C13
19	AA	810	CLA	C8-C10-C11-C12
19	B	859	CLA	C5-C6-C7-C8
19	A1	852	CLA	C8-C10-C11-C12
26	BB	840	ECH	C37-C22-C23-C24
23	L	206	BCR	C7-C8-C9-C34
23	L	206	BCR	C37-C22-C23-C24
25	M	102	LMG	C2-C1-O1-C7
26	B	841	ECH	C37-C22-C23-C24
26	B1	840	ECH	C37-C22-C23-C24
23	I2	101	BCR	C37-C22-C23-C24
26	B2	841	ECH	C37-C22-C23-C24
23	I1	101	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
19	A1	803	CLA	C16-C17-C18-C19
19	A2	813	CLA	C16-C17-C18-C19
25	B1	844	LMG	C16-C17-C18-C19
19	K	102	CLA	C2A-CAA-CBA-CGA
20	A2	803	CL0	C2A-CAA-CBA-CGA
19	B2	836	CLA	O1D-CGD-O2D-CED
26	BB	840	ECH	C21-C22-C23-C24
23	A2	849	BCR	C17-C18-C19-C20
23	B2	842	BCR	C11-C12-C13-C14
23	A1	848	BCR	C21-C22-C23-C24
23	A	853	BCR	C17-C18-C19-C20
23	A2	850	BCR	C21-C22-C23-C24
23	JJ	102	BCR	C17-C18-C19-C20
26	B	841	ECH	C21-C22-C23-C24
23	L2	207	BCR	C17-C18-C19-C20
26	B1	840	ECH	C21-C22-C23-C24
23	F2	304	BCR	C17-C18-C19-C20
26	B2	841	ECH	C17-C18-C19-C20
26	B2	841	ECH	C21-C22-C23-C24
23	AA	854	BCR	C17-C18-C19-C20
22	A	845	LHG	C24-C23-O8-C6
19	A1	803	CLA	CBA-CGA-O2A-C1
19	B	803	CLA	C5-C6-C7-C8
19	L2	206	CLA	C10-C11-C12-C13
19	AA	830	CLA	C5-C6-C7-C8
19	BB	803	CLA	C5-C6-C7-C8
19	AA	827	CLA	C15-C16-C17-C18
19	BB	823	CLA	C10-C11-C12-C13
21	B1	837	PQN	C18-C20-C21-C22
19	L	204	CLA	C8-C10-C11-C12
19	B	818	CLA	O1D-CGD-O2D-CED
22	B	852	LHG	C23-C24-C25-C26
19	AA	830	CLA	C3-C5-C6-C7
28	B	856	DGD	C4B-C5B-C6B-C7B
19	AA	843	CLA	C15-C16-C17-C18
19	AA	831	CLA	C13-C15-C16-C17
19	A	830	CLA	C5-C6-C7-C8
19	B1	810	CLA	C5-C6-C7-C8
19	A2	830	CLA	C5-C6-C7-C8
22	B2	848	LHG	C1-C2-C3-O3
19	A	821	CLA	C2-C3-C5-C6
19	BB	801	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	F1	301	CLA	C10-C11-C12-C13
19	A1	826	CLA	C15-C16-C17-C18
22	AA	847	LHG	O6-C4-C5-C6
22	A2	846	LHG	O6-C4-C5-C6
22	A1	846	LHG	O6-C4-C5-C6
19	A	831	CLA	CBA-CGA-O2A-C1
19	A	804	CLA	CBA-CGA-O2A-C1
19	A2	833	CLA	CBA-CGA-O2A-C1
19	B	825	CLA	O1D-CGD-O2D-CED
25	BB	844	LMG	C13-C14-C15-C16
19	A1	829	CLA	C5-C6-C7-C8
19	B2	852	CLA	C15-C16-C17-C18
25	B	851	LMG	C21-C22-C23-C24
19	A1	801	CLA	C5-C6-C7-C8
28	B	856	DGD	C1A-C2A-C3A-C4A
19	A1	815	CLA	CBA-CGA-O2A-C1
19	B	804	CLA	CBA-CGA-O2A-C1
19	BB	804	CLA	CBA-CGA-O2A-C1
19	B1	825	CLA	C3-C5-C6-C7
19	B1	814	CLA	C3-C5-C6-C7
19	A1	803	CLA	C3-C5-C6-C7
19	AA	804	CLA	C16-C17-C18-C19
19	A2	807	CLA	C16-C17-C18-C20
20	A	803	CL0	C16-C17-C18-C19
25	B	851	LMG	C11-C12-C13-C14
19	A1	809	CLA	C8-C10-C11-C12
25	L1	210	LMG	C34-C35-C36-C37
22	BB	850	LHG	O9-C7-O7-C5
19	AA	828	CLA	C3A-C2A-CAA-CBA
19	A1	814	CLA	C3A-C2A-CAA-CBA
19	A	815	CLA	C3A-C2A-CAA-CBA
19	B	832	CLA	C3A-C2A-CAA-CBA
19	A	828	CLA	C3A-C2A-CAA-CBA
19	B	821	CLA	C3A-C2A-CAA-CBA
19	BB	821	CLA	C3A-C2A-CAA-CBA
19	A1	827	CLA	C3A-C2A-CAA-CBA
19	A2	828	CLA	C3A-C2A-CAA-CBA
19	B	859	CLA	C3A-C2A-CAA-CBA
19	B	824	CLA	C3A-C2A-CAA-CBA
19	AA	815	CLA	C3A-C2A-CAA-CBA
19	B1	821	CLA	C3A-C2A-CAA-CBA
19	A2	806	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	B1	804	CLA	C3A-C2A-CAA-CBA
19	LL	201	CLA	C3A-C2A-CAA-CBA
19	A2	815	CLA	C3A-C2A-CAA-CBA
19	B	804	CLA	C3A-C2A-CAA-CBA
19	A	824	CLA	C3A-C2A-CAA-CBA
19	BB	804	CLA	C3A-C2A-CAA-CBA
19	AA	840	CLA	O1D-CGD-O2D-CED
19	L	202	CLA	C2A-CAA-CBA-CGA
19	BB	801	CLA	C8-C10-C11-C12
19	AA	801	CLA	C5-C6-C7-C8
22	A2	845	LHG	C29-C30-C31-C32
19	A1	829	CLA	C2C-C3C-CAC-CBC
25	BB	844	LMG	C16-C17-C18-C19
25	BB	844	LMG	C38-C39-C40-C41
19	B	837	CLA	C4C-C3C-CAC-CBC
23	B	848	BCR	C18-C19-C20-C21
22	B	852	LHG	C8-C7-O7-C5
22	A	846	LHG	C14-C15-C16-C17
25	II	105	LMG	C11-C12-C13-C14
22	B	853	LHG	C34-C35-C36-C37
25	B1	844	LMG	C38-C39-C40-C41
19	B2	804	CLA	CBA-CGA-O2A-C1
19	A1	805	CLA	CBA-CGA-O2A-C1
23	BB	838	BCR	C6-C7-C8-C9
23	L1	209	BCR	C6-C7-C8-C9
23	MM	101	BCR	C22-C23-C24-C25
23	BB	841	BCR	C22-C23-C24-C25
23	F	303	BCR	C6-C7-C8-C9
25	I1	102	LMG	O1-C7-C8-C9
25	B1	846	LMG	O1-C7-C8-C9
22	X1	102	LHG	C4-C5-C6-O8
19	BB	821	CLA	C4-C3-C5-C6
28	BB	854	DGD	C4B-C5B-C6B-C7B
19	A	828	CLA	C2-C3-C5-C6
19	A1	827	CLA	C2-C3-C5-C6
23	L	205	BCR	C15-C16-C17-C18
23	B	844	BCR	C9-C10-C11-C12
23	K2	105	BCR	C19-C20-C21-C22
23	J	102	BCR	C15-C16-C17-C18
26	B1	840	ECH	C13-C14-C15-C16
26	B2	841	ECH	C13-C14-C15-C16
23	K	103	BCR	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
19	B	805	CLA	C5-C6-C7-C8
19	B	811	CLA	C8-C10-C11-C12
19	BB	805	CLA	C5-C6-C7-C8
19	BB	833	CLA	C13-C15-C16-C17
22	AA	847	LHG	C14-C15-C16-C17
19	AA	828	CLA	C3-C5-C6-C7
19	A2	804	CLA	C3-C5-C6-C7
22	X	102	LHG	O9-C7-O7-C5
22	A2	845	LHG	O9-C7-O7-C5
19	BB	814	CLA	CBA-CGA-O2A-C1
19	BB	852	CLA	CBA-CGA-O2A-C1
19	B1	804	CLA	CBA-CGA-O2A-C1
19	AA	804	CLA	C16-C17-C18-C20
19	BB	825	CLA	CBD-CGD-O2D-CED
19	B1	820	CLA	C2C-C3C-CAC-CBC
19	AA	853	CLA	O1A-CGA-O2A-C1
19	A	808	CLA	C5-C6-C7-C8
19	AA	836	CLA	C13-C15-C16-C17
19	F2	301	CLA	C10-C11-C12-C13
19	A2	810	CLA	C8-C10-C11-C12
22	B	852	LHG	O6-C4-C5-O7
22	A	845	LHG	C7-C8-C9-C10
19	AA	832	CLA	C3-C5-C6-C7
19	A	831	CLA	C13-C15-C16-C17
19	B	860	CLA	C15-C16-C17-C18
19	L	202	CLA	C5-C6-C7-C8
19	B1	801	CLA	C15-C16-C17-C18
19	A1	852	CLA	C5-C6-C7-C8
19	BB	815	CLA	C13-C15-C16-C17
23	B	848	BCR	C14-C15-C16-C17
23	BB	847	BCR	C14-C15-C16-C17
23	A1	848	BCR	C14-C15-C16-C17
23	A	847	BCR	C20-C21-C22-C23
23	AA	848	BCR	C20-C21-C22-C23
22	B	853	LHG	O1-C1-C2-O2
23	A	849	BCR	C14-C15-C16-C17
25	B1	844	LMG	O6-C5-C6-O5
22	BB	851	LHG	C34-C35-C36-C37
19	B	801	CLA	C16-C17-C18-C20
20	A	803	CL0	C16-C17-C18-C20
19	BB	808	CLA	O1A-CGA-O2A-C1
19	A1	832	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
22	LL	205	LHG	O10-C23-O8-C6
19	AA	840	CLA	O1A-CGA-O2A-C1
19	A2	804	CLA	O1A-CGA-O2A-C1
19	A1	839	CLA	O1A-CGA-O2A-C1
25	B	845	LMG	C35-C36-C37-C38
25	B2	845	LMG	C16-C17-C18-C19
25	I1	102	LMG	O1-C7-C8-O7
28	B	856	DGD	O2G-C2G-C3G-O3G
25	M	102	LMG	O1-C7-C8-O7
25	M	102	LMG	O7-C8-C9-O8
19	B1	805	CLA	C5-C6-C7-C8
19	B2	805	CLA	C5-C6-C7-C8
19	BB	836	CLA	C3-C5-C6-C7
19	B2	849	CLA	CBA-CGA-O2A-C1
19	AA	816	CLA	CBA-CGA-O2A-C1
19	BB	826	CLA	CBD-CGD-O2D-CED
19	AA	824	CLA	O1D-CGD-O2D-CED
22	L	207	LHG	O10-C23-O8-C6
19	A2	828	CLA	C4-C3-C5-C6
25	B	845	LMG	C38-C39-C40-C41
28	B	856	DGD	C4E-C5E-C6E-O5E
19	B2	825	CLA	C16-C17-C18-C20
19	A2	804	CLA	C16-C17-C18-C20
19	L2	204	CLA	C10-C11-C12-C13
22	X2	103	LHG	C2-C3-O3-P
22	B	853	LHG	C2-C3-O3-P
19	AA	804	CLA	C3-C5-C6-C7
22	B	853	LHG	C1-C2-C3-O3
19	A2	816	CLA	CBA-CGA-O2A-C1
23	K1	104	BCR	C23-C24-C25-C26
23	K1	104	BCR	C23-C24-C25-C30
23	F2	303	BCR	C1-C6-C7-C8
23	F2	303	BCR	C5-C6-C7-C8
23	L	205	BCR	C5-C6-C7-C8
23	A1	851	BCR	C5-C6-C7-C8
19	A2	825	CLA	C1A-C2A-CAA-CBA
23	M	101	BCR	C1-C6-C7-C8
19	B1	826	CLA	C6-C7-C8-C9
23	A	850	BCR	C5-C6-C7-C8
23	A2	850	BCR	C5-C6-C7-C8
23	K2	105	BCR	C23-C24-C25-C30
23	J	102	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	J	102	BCR	C5-C6-C7-C8
23	J	102	BCR	C23-C24-C25-C26
19	B1	805	CLA	C11-C12-C13-C14
23	II	104	BCR	C5-C6-C7-C8
19	B	805	CLA	C11-C12-C13-C14
23	I	101	BCR	C5-C6-C7-C8
23	F	305	BCR	C23-C24-C25-C26
23	F	305	BCR	C23-C24-C25-C30
23	JJ	102	BCR	C1-C6-C7-C8
23	JJ	102	BCR	C5-C6-C7-C8
23	JJ	102	BCR	C23-C24-C25-C26
23	B1	842	BCR	C23-C24-C25-C30
23	AA	852	BCR	C5-C6-C7-C8
23	AA	852	BCR	C23-C24-C25-C26
23	B2	843	BCR	C23-C24-C25-C26
23	B2	843	BCR	C23-C24-C25-C30
23	L1	209	BCR	C23-C24-C25-C26
23	L1	209	BCR	C23-C24-C25-C30
23	BB	842	BCR	C23-C24-C25-C26
23	L2	207	BCR	C23-C24-C25-C26
23	L2	207	BCR	C23-C24-C25-C30
23	II	101	BCR	C1-C6-C7-C8
23	II	101	BCR	C5-C6-C7-C8
19	A2	842	CLA	C6-C7-C8-C9
19	A2	827	CLA	C14-C13-C15-C16
19	BB	816	CLA	C6-C7-C8-C9
19	A	835	CLA	C14-C13-C15-C16
23	AA	851	BCR	C5-C6-C7-C8
19	B2	801	CLA	C14-C13-C15-C16
19	BB	805	CLA	C11-C12-C13-C14
19	AA	813	CLA	C6-C7-C8-C9
19	B2	805	CLA	C11-C12-C13-C14
23	MM	101	BCR	C1-C6-C7-C8
23	MM	101	BCR	C5-C6-C7-C8
19	A1	812	CLA	C11-C12-C13-C14
23	A2	851	BCR	C5-C6-C7-C8
19	BB	803	CLA	C6-C7-C8-C9
19	B2	836	CLA	C14-C13-C15-C16
19	A1	806	CLA	C14-C13-C15-C16
19	A2	813	CLA	C11-C12-C13-C14
23	A	851	BCR	C5-C6-C7-C8
23	F	303	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	F	303	BCR	C5-C6-C7-C8
23	A1	850	BCR	C5-C6-C7-C8
23	F1	303	BCR	C1-C6-C7-C8
23	F1	303	BCR	C23-C24-C25-C26
23	FF	303	BCR	C1-C6-C7-C8
23	FF	303	BCR	C5-C6-C7-C8
22	B	852	LHG	O9-C7-O7-C5
25	B1	844	LMG	C13-C14-C15-C16
25	B	851	LMG	C32-C33-C34-C35
22	X1	103	LHG	C10-C11-C12-C13
23	K2	103	BCR	C7-C8-C9-C34
23	AA	848	BCR	C36-C18-C19-C20
26	B2	841	ECH	C36-C18-C19-C20
19	B1	825	CLA	C16-C17-C18-C20
19	A1	803	CLA	C16-C17-C18-C20
19	AA	808	CLA	C2A-CAA-CBA-CGA
19	A	804	CLA	O1A-CGA-O2A-C1
25	BB	844	LMG	C33-C34-C35-C36
23	L1	201	BCR	C11-C12-C13-C14
23	L1	201	BCR	C21-C22-C23-C24
23	B	843	BCR	C17-C18-C19-C20
23	AA	852	BCR	C7-C8-C9-C10
23	J2	102	BCR	C17-C18-C19-C20
23	M1	101	BCR	C11-C12-C13-C14
23	J1	102	BCR	C17-C18-C19-C20
23	AA	851	BCR	C21-C22-C23-C24
23	A2	848	BCR	C21-C22-C23-C24
23	M2	102	BCR	C11-C12-C13-C14
23	J1	104	BCR	C11-C12-C13-C14
23	A1	850	BCR	C21-C22-C23-C24
23	FF	303	BCR	C7-C8-C9-C10
19	B1	829	CLA	C2C-C3C-CAC-CBC
19	L1	205	CLA	C10-C11-C12-C13
25	B1	844	LMG	C35-C36-C37-C38
19	BB	801	CLA	C2-C1-O2A-CGA
19	L2	204	CLA	C2-C1-O2A-CGA
19	L1	205	CLA	C2-C1-O2A-CGA
19	A	804	CLA	C2-C1-O2A-CGA
19	B	824	CLA	C2-C1-O2A-CGA
19	LL	201	CLA	C2-C1-O2A-CGA
22	A	845	LHG	O10-C23-O8-C6
19	A1	803	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	B	851	LMG	C15-C16-C17-C18
22	B1	847	LHG	C12-C13-C14-C15
25	II	105	LMG	C30-C31-C32-C33
19	B	823	CLA	C10-C11-C12-C13
19	F	301	CLA	C10-C11-C12-C13
19	B	825	CLA	C16-C17-C18-C20
19	B1	806	CLA	C12-C13-C15-C16
19	BB	801	CLA	C12-C13-C15-C16
19	B	803	CLA	C6-C7-C8-C10
20	AA	803	CL0	C11-C10-C8-C7
19	A	808	CLA	C6-C7-C8-C10
19	L2	205	CLA	C6-C7-C8-C10
19	BB	806	CLA	C12-C13-C15-C16
19	B	825	CLA	C12-C13-C15-C16
21	BB	837	PQN	C21-C22-C23-C25
19	A1	807	CLA	C6-C7-C8-C10
19	B1	826	CLA	C6-C7-C8-C10
19	B1	826	CLA	C12-C13-C15-C16
19	B1	825	CLA	C11-C10-C8-C7
19	B2	815	CLA	C11-C10-C8-C7
19	B2	815	CLA	C12-C13-C15-C16
19	A2	821	CLA	C11-C12-C13-C15
19	B1	803	CLA	C6-C7-C8-C10
19	A1	835	CLA	C12-C13-C15-C16
19	AA	808	CLA	C6-C7-C8-C10
19	B	815	CLA	C11-C10-C8-C7
19	B2	849	CLA	C11-C10-C8-C7
19	A1	820	CLA	C11-C12-C13-C15
19	A	804	CLA	C12-C13-C15-C16
19	BB	810	CLA	C11-C10-C8-C7
19	AA	836	CLA	C12-C13-C15-C16
19	BB	826	CLA	C12-C13-C15-C16
19	AA	853	CLA	C11-C12-C13-C15
19	BB	852	CLA	C11-C10-C8-C7
19	A1	828	CLA	C11-C10-C8-C7
19	B	823	CLA	C6-C7-C8-C10
19	B2	801	CLA	C12-C13-C15-C16
19	A2	808	CLA	C6-C7-C8-C10
19	B	801	CLA	C12-C13-C15-C16
19	B1	823	CLA	C6-C7-C8-C10
19	A2	835	CLA	C12-C13-C15-C16
19	B1	848	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
19	BB	835	CLA	C12-C13-C15-C16
19	BB	803	CLA	C6-C7-C8-C10
19	B2	836	CLA	C12-C13-C15-C16
19	A1	834	CLA	C12-C13-C15-C16
19	B2	823	CLA	C6-C7-C8-C10
19	B1	810	CLA	C11-C10-C8-C7
19	A1	806	CLA	C12-C13-C15-C16
19	A2	813	CLA	C6-C7-C8-C10
19	AA	835	CLA	C12-C13-C15-C16
19	B1	835	CLA	C6-C7-C8-C10
19	B1	807	CLA	C6-C7-C8-C10
19	BB	823	CLA	C6-C7-C8-C10
19	B	854	CLA	C11-C10-C8-C7
19	A1	852	CLA	C11-C10-C8-C7
19	BB	815	CLA	C12-C13-C15-C16
20	A	803	CL0	C11-C10-C8-C7
19	B	833	CLA	C6-C7-C8-C10
19	B2	826	CLA	C12-C13-C15-C16
19	B2	806	CLA	C12-C13-C15-C16
19	A2	828	CLA	C2-C3-C5-C6
21	B2	838	PQN	C18-C20-C21-C22
19	A2	804	CLA	C8-C10-C11-C12
19	AA	830	CLA	C13-C15-C16-C17
23	B	848	BCR	C20-C21-C22-C37
23	K1	104	BCR	C11-C10-C9-C34
23	L1	201	BCR	C11-C10-C9-C34
23	A	848	BCR	C20-C21-C22-C37
23	B1	838	BCR	C11-C10-C9-C34
23	B1	838	BCR	C35-C13-C14-C15
23	BB	838	BCR	C11-C10-C9-C34
23	II	104	BCR	C35-C13-C14-C15
23	B1	842	BCR	C16-C17-C18-C36
23	B2	843	BCR	C35-C13-C14-C15
23	B	842	BCR	C20-C21-C22-C37
23	II	101	BCR	C35-C13-C14-C15
23	JJ	104	BCR	C20-C21-C22-C37
23	FF	306	BCR	C20-C21-C22-C37
23	A2	848	BCR	C35-C13-C14-C15
23	B	840	BCR	C20-C21-C22-C37
23	F	304	BCR	C11-C10-C9-C34
23	A1	847	BCR	C35-C13-C14-C15
19	B2	825	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
23	A	847	BCR	C14-C15-C16-C17
23	AA	848	BCR	C14-C15-C16-C17
23	F2	305	BCR	C14-C15-C16-C17
19	BB	825	CLA	C16-C17-C18-C20
19	A	804	CLA	C16-C17-C18-C20
25	BB	844	LMG	C35-C36-C37-C38
19	BB	811	CLA	C8-C10-C11-C12
19	B	815	CLA	C13-C15-C16-C17
19	KK	102	CLA	C2A-CAA-CBA-CGA
22	LL	205	LHG	C6-C5-O7-C7
22	L	207	LHG	C6-C5-O7-C7
19	B2	813	CLA	O1D-CGD-O2D-CED
19	A	831	CLA	O1A-CGA-O2A-C1
19	B2	804	CLA	O1A-CGA-O2A-C1
19	B1	804	CLA	O1A-CGA-O2A-C1
19	A2	830	CLA	C3-C5-C6-C7
20	A	803	CL0	C5-C6-C7-C8
23	A	848	BCR	C9-C10-C11-C12
23	F	305	BCR	C19-C20-C21-C22
23	K1	106	BCR	C19-C20-C21-C22
23	JJ	104	BCR	C9-C10-C11-C12
26	B1	840	ECH	C9-C10-C11-C12
23	KK	103	BCR	C19-C20-C21-C22
23	FF	306	BCR	C19-C20-C21-C22
23	B1	843	BCR	C9-C10-C11-C12
26	B2	841	ECH	C9-C10-C11-C12
23	MM	101	BCR	C13-C14-C15-C16
23	K	103	BCR	C19-C20-C21-C22
23	J	104	BCR	C9-C10-C11-C12
19	BB	835	CLA	CBD-CGD-O2D-CED
19	A	835	CLA	CBA-CGA-O2A-C1
19	B	808	CLA	O1D-CGD-O2D-CED
19	BB	833	CLA	O1D-CGD-O2D-CED
25	B	845	LMG	C16-C17-C18-C19
19	L1	206	CLA	C8-C10-C11-C12
19	A2	852	CLA	C5-C6-C7-C8
19	A1	816	CLA	CAD-CBD-CGD-O2D
19	B2	825	CLA	CAD-CBD-CGD-O2D
19	A	827	CLA	CAD-CBD-CGD-O2D
19	B	828	CLA	CAD-CBD-CGD-O2D
19	BB	832	CLA	CAD-CBD-CGD-O2D
19	B1	825	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B2	809	CLA	CAD-CBD-CGD-O2D
19	AA	823	CLA	CAD-CBD-CGD-O2D
19	A2	819	CLA	CAD-CBD-CGD-O2D
19	A1	818	CLA	CAD-CBD-CGD-O2D
19	B2	828	CLA	CAD-CBD-CGD-O2D
19	B	809	CLA	CAD-CBD-CGD-O2D
19	BB	828	CLA	CAD-CBD-CGD-O2D
19	A	816	CLA	CAD-CBD-CGD-O2D
19	A	814	CLA	CAD-CBD-CGD-O2D
19	A1	824	CLA	CAD-CBD-CGD-O2D
19	AA	824	CLA	CAD-CBD-CGD-O2D
19	B2	819	CLA	CAD-CBD-CGD-O2D
19	A	819	CLA	CAD-CBD-CGD-O2D
19	A2	802	CLA	CAD-CBD-CGD-O2D
19	AA	814	CLA	CAD-CBD-CGD-O2D
19	B1	809	CLA	CAD-CBD-CGD-O2D
19	A	824	CLA	CAD-CBD-CGD-O2D
19	AA	819	CLA	CAD-CBD-CGD-O2D
19	A1	806	CLA	CAD-CBD-CGD-O2D
19	A1	852	CLA	CAD-CBD-CGD-O2D
19	BB	812	CLA	CAD-CBD-CGD-O2D
19	K1	102	CLA	CAD-CBD-CGD-O2D
19	BB	817	CLA	CAD-CBD-CGD-O2D
19	A2	807	CLA	CAD-CBD-CGD-O2D
19	B	833	CLA	CAD-CBD-CGD-O2D
19	AA	830	CLA	C4C-C3C-CAC-CBC
22	X1	103	LHG	C2-C3-O3-P
19	B1	801	CLA	C8-C10-C11-C12
19	A	808	CLA	C3-C5-C6-C7
19	A1	829	CLA	C3-C5-C6-C7
19	B	804	CLA	O1A-CGA-O2A-C1
19	BB	804	CLA	O1A-CGA-O2A-C1
19	A	830	CLA	C4C-C3C-CAC-CBC
19	B1	825	CLA	CBA-CGA-O2A-C1
25	B	845	LMG	O1-C7-C8-C9
22	LL	205	LHG	C4-C5-C6-O8
22	X	102	LHG	C4-C5-C6-O8
22	L	207	LHG	C4-C5-C6-O8
22	XX	102	LHG	C4-C5-C6-O8
22	X2	102	LHG	C4-C5-C6-O8
25	II	105	LMG	O1-C7-C8-C9
25	B2	845	LMG	O1-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	A1	826	CLA	C5-C6-C7-C8
22	L1	211	LHG	O6-C4-C5-O7
19	L	204	CLA	C2C-C3C-CAC-CBC
22	X2	102	LHG	C27-C28-C29-C30
19	B2	834	CLA	C15-C16-C17-C18
22	A1	845	LHG	C15-C16-C17-C18
23	A	848	BCR	C16-C17-C18-C19
23	F2	303	BCR	C20-C21-C22-C23
23	I2	103	BCR	C16-C17-C18-C19
23	L1	208	BCR	C16-C17-C18-C19
23	M1	101	BCR	C16-C17-C18-C19
23	I2	101	BCR	C20-C21-C22-C23
23	B1	839	BCR	C20-C21-C22-C23
23	I1	101	BCR	C20-C21-C22-C23
23	BB	841	BCR	C12-C13-C14-C15
23	BB	839	BCR	C12-C13-C14-C15
23	BB	839	BCR	C16-C17-C18-C19
19	B1	835	CLA	C3-C5-C6-C7
19	BB	810	CLA	C5-C6-C7-C8
19	A2	827	CLA	C5-C6-C7-C8
19	A1	818	CLA	C2A-CAA-CBA-CGA
19	AA	806	CLA	C2A-CAA-CBA-CGA
19	A2	842	CLA	C2A-CAA-CBA-CGA
19	A	842	CLA	C2A-CAA-CBA-CGA
19	B2	823	CLA	C15-C16-C17-C18
25	B	845	LMG	O1-C7-C8-O7
22	B1	847	LHG	O7-C5-C6-O8
22	X	102	LHG	O7-C5-C6-O8
22	XX	102	LHG	O7-C5-C6-O8
22	X2	102	LHG	O7-C5-C6-O8
22	B2	848	LHG	O7-C5-C6-O8
22	A1	845	LHG	O7-C5-C6-O8
22	X1	102	LHG	O7-C5-C6-O8
25	B2	845	LMG	O1-C7-C8-O7
19	BB	801	CLA	C16-C17-C18-C20
19	AA	843	CLA	C16-C17-C18-C19
19	B	801	CLA	C16-C17-C18-C19
19	A2	816	CLA	O1A-CGA-O2A-C1
22	X2	103	LHG	C10-C11-C12-C13
19	BB	814	CLA	O1A-CGA-O2A-C1
19	B2	849	CLA	O1A-CGA-O2A-C1
19	A1	805	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	A2	833	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	C32-C33-C34-C35
19	B2	817	CLA	CHA-CBD-CGD-O1D
19	B2	817	CLA	CHA-CBD-CGD-O2D
19	B	813	CLA	CHA-CBD-CGD-O1D
19	A2	839	CLA	CHA-CBD-CGD-O1D
19	A2	839	CLA	CHA-CBD-CGD-O2D
19	BB	836	CLA	CHA-CBD-CGD-O1D
19	BB	836	CLA	CHA-CBD-CGD-O2D
19	B	803	CLA	CHA-CBD-CGD-O2D
19	AA	832	CLA	CHA-CBD-CGD-O1D
19	AA	832	CLA	CHA-CBD-CGD-O2D
19	L2	204	CLA	CHA-CBD-CGD-O1D
19	L2	204	CLA	CHA-CBD-CGD-O2D
19	B	817	CLA	CHA-CBD-CGD-O1D
19	B	817	CLA	CHA-CBD-CGD-O2D
19	K1	103	CLA	CHA-CBD-CGD-O1D
19	K1	103	CLA	CHA-CBD-CGD-O2D
19	AA	822	CLA	CHA-CBD-CGD-O1D
19	LL	203	CLA	CHA-CBD-CGD-O1D
19	A	805	CLA	CHA-CBD-CGD-O1D
19	AA	838	CLA	CHA-CBD-CGD-O1D
19	AA	838	CLA	CHA-CBD-CGD-O2D
19	B1	826	CLA	CHA-CBD-CGD-O1D
19	B1	826	CLA	CHA-CBD-CGD-O2D
19	B2	815	CLA	CHA-CBD-CGD-O1D
19	B2	815	CLA	CHA-CBD-CGD-O2D
20	A1	802	CL0	CHA-CBD-CGD-O2D
19	A1	832	CLA	CHA-CBD-CGD-O1D
19	A1	832	CLA	CHA-CBD-CGD-O2D
19	A	836	CLA	CHA-CBD-CGD-O1D
19	A	836	CLA	CHA-CBD-CGD-O2D
19	A1	835	CLA	CHA-CBD-CGD-O1D
19	A1	835	CLA	CHA-CBD-CGD-O2D
19	B1	805	CLA	CHA-CBD-CGD-O1D
19	B1	805	CLA	CHA-CBD-CGD-O2D
19	AA	839	CLA	CHA-CBD-CGD-O1D
19	A2	838	CLA	CHA-CBD-CGD-O1D
19	A2	838	CLA	CHA-CBD-CGD-O2D
19	B	821	CLA	CHA-CBD-CGD-O1D
19	B	821	CLA	CHA-CBD-CGD-O2D
19	B2	837	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	B2	837	CLA	CHA-CBD-CGD-O2D
19	BB	821	CLA	CHA-CBD-CGD-O1D
19	AA	836	CLA	CHA-CBD-CGD-O1D
19	AA	836	CLA	CHA-CBD-CGD-O2D
19	BB	826	CLA	CHA-CBD-CGD-O1D
19	B2	803	CLA	CHA-CBD-CGD-O2D
19	BB	852	CLA	CHA-CBD-CGD-O1D
19	BB	852	CLA	CHA-CBD-CGD-O2D
19	A1	815	CLA	CHA-CBD-CGD-O1D
19	A1	815	CLA	CHA-CBD-CGD-O2D
19	B2	834	CLA	CHA-CBD-CGD-O1D
19	B2	834	CLA	CHA-CBD-CGD-O2D
19	B2	851	CLA	CHA-CBD-CGD-O1D
19	B1	836	CLA	CHA-CBD-CGD-O1D
19	B1	836	CLA	CHA-CBD-CGD-O2D
19	A1	830	CLA	CHA-CBD-CGD-O1D
19	A1	830	CLA	CHA-CBD-CGD-O2D
19	AA	816	CLA	CHA-CBD-CGD-O1D
19	F1	301	CLA	CHA-CBD-CGD-O1D
19	F1	301	CLA	CHA-CBD-CGD-O2D
19	B2	820	CLA	CHA-CBD-CGD-O1D
19	B2	820	CLA	CHA-CBD-CGD-O2D
19	LL	201	CLA	CHA-CBD-CGD-O1D
19	LL	201	CLA	CHA-CBD-CGD-O2D
19	B1	820	CLA	CHA-CBD-CGD-O1D
19	B1	820	CLA	CHA-CBD-CGD-O2D
19	B2	821	CLA	CHA-CBD-CGD-O1D
19	B2	821	CLA	CHA-CBD-CGD-O2D
19	BB	805	CLA	CHA-CBD-CGD-O1D
19	B2	833	CLA	CHA-CBD-CGD-O1D
19	B2	805	CLA	CHA-CBD-CGD-O1D
19	B2	805	CLA	CHA-CBD-CGD-O2D
19	F	301	CLA	CHA-CBD-CGD-O1D
19	A1	837	CLA	CHA-CBD-CGD-O1D
19	A1	837	CLA	CHA-CBD-CGD-O2D
19	A	826	CLA	CHA-CBD-CGD-O1D
19	A	826	CLA	CHA-CBD-CGD-O2D
19	B1	848	CLA	CHA-CBD-CGD-O2D
19	B2	813	CLA	CHA-CBD-CGD-O1D
19	B2	813	CLA	CHA-CBD-CGD-O2D
19	B1	817	CLA	CHA-CBD-CGD-O1D
19	B1	817	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	B	826	CLA	CHA-CBD-CGD-O1D
19	B	826	CLA	CHA-CBD-CGD-O2D
19	B1	833	CLA	CHA-CBD-CGD-O1D
19	B1	833	CLA	CHA-CBD-CGD-O2D
20	A2	803	CL0	CHA-CBD-CGD-O2D
19	A2	852	CLA	CHA-CBD-CGD-O1D
19	A2	852	CLA	CHA-CBD-CGD-O2D
19	A	838	CLA	CHA-CBD-CGD-O1D
19	A	838	CLA	CHA-CBD-CGD-O2D
19	A1	822	CLA	CHA-CBD-CGD-O1D
19	A	852	CLA	CHA-CBD-CGD-O1D
19	A1	838	CLA	CHA-CBD-CGD-O1D
19	A1	838	CLA	CHA-CBD-CGD-O2D
19	B2	826	CLA	CHA-CBD-CGD-O1D
19	B2	826	CLA	CHA-CBD-CGD-O2D
19	B	802	CLA	CHA-CBD-CGD-O1D
19	B	802	CLA	CHA-CBD-CGD-O2D
25	II	105	LMG	C13-C14-C15-C16
22	X1	102	LHG	C27-C28-C29-C30
19	L1	205	CLA	C4-C3-C5-C6
19	B	824	CLA	C4-C3-C5-C6
19	B1	848	CLA	C4-C3-C5-C6
19	B1	826	CLA	C15-C16-C17-C18
19	B	859	CLA	C8-C10-C11-C12
19	B	801	CLA	C15-C16-C17-C18
19	B1	815	CLA	C13-C15-C16-C17
19	B1	825	CLA	O1A-CGA-O2A-C1
19	A1	815	CLA	O1A-CGA-O2A-C1
19	AA	816	CLA	O1A-CGA-O2A-C1
23	B1	838	BCR	C6-C7-C8-C9
23	BB	847	BCR	C22-C23-C24-C25
23	B2	839	BCR	C6-C7-C8-C9
23	A2	848	BCR	C22-C23-C24-C25
22	A	845	LHG	C15-C16-C17-C18
19	BB	801	CLA	C13-C15-C16-C17
19	B2	815	CLA	C13-C15-C16-C17
19	B1	806	CLA	C14-C13-C15-C16
19	B2	825	CLA	C11-C10-C8-C9
19	B	803	CLA	C6-C7-C8-C9
19	A	808	CLA	C6-C7-C8-C9
21	BB	837	PQN	C21-C22-C23-C24
19	B1	803	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
19	AA	807	CLA	C14-C13-C15-C16
19	A	813	CLA	C6-C7-C8-C9
19	B2	803	CLA	C6-C7-C8-C9
19	B	816	CLA	C6-C7-C8-C9
19	A2	835	CLA	C14-C13-C15-C16
19	BB	835	CLA	C14-C13-C15-C16
19	AA	827	CLA	C14-C13-C15-C16
19	AA	835	CLA	C14-C13-C15-C16
20	A2	803	CL0	C11-C12-C13-C14
19	B2	826	CLA	C14-C13-C15-C16
19	B2	806	CLA	C14-C13-C15-C16
19	B	828	CLA	C1A-C2A-CAA-CBA
19	L2	205	CLA	C1A-C2A-CAA-CBA
19	AA	823	CLA	C1A-C2A-CAA-CBA
19	BB	834	CLA	C1A-C2A-CAA-CBA
19	B	821	CLA	C1A-C2A-CAA-CBA
19	BB	821	CLA	C1A-C2A-CAA-CBA
19	B	824	CLA	C1A-C2A-CAA-CBA
19	A	823	CLA	C1A-C2A-CAA-CBA
19	B2	801	CLA	C1A-C2A-CAA-CBA
19	B	835	CLA	C1A-C2A-CAA-CBA
19	B2	833	CLA	C1A-C2A-CAA-CBA
19	F1	305	CLA	C1A-C2A-CAA-CBA
19	B1	802	CLA	C1A-C2A-CAA-CBA
19	B2	829	CLA	C1A-C2A-CAA-CBA
19	FF	305	CLA	C1A-C2A-CAA-CBA
19	BB	852	CLA	O1A-CGA-O2A-C1
19	L	202	CLA	C10-C11-C12-C13
19	A2	842	CLA	C5-C6-C7-C8
26	BB	840	ECH	C36-C18-C19-C20
23	F2	303	BCR	C37-C22-C23-C24
26	B	841	ECH	C36-C18-C19-C20
23	I	102	BCR	C37-C22-C23-C24
26	B1	840	ECH	C36-C18-C19-C20
23	B2	844	BCR	C7-C8-C9-C34
23	B1	843	BCR	C7-C8-C9-C34
23	F2	304	BCR	C36-C18-C19-C20
23	F	303	BCR	C11-C12-C13-C35
19	BB	825	CLA	C3-C5-C6-C7
20	A2	803	CL0	C3-C5-C6-C7
26	BB	840	ECH	C17-C18-C19-C20
23	B1	838	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
23	A	850	BCR	C21-C22-C23-C24
26	B	841	ECH	C17-C18-C19-C20
23	II	101	BCR	C11-C12-C13-C14
23	JJ	104	BCR	C11-C12-C13-C14
23	B2	839	BCR	C11-C12-C13-C14
26	B1	840	ECH	C17-C18-C19-C20
23	B1	841	BCR	C17-C18-C19-C20
23	I1	101	BCR	C17-C18-C19-C20
23	AA	850	BCR	C21-C22-C23-C24
25	B2	845	LMG	C39-C40-C41-C42
22	X	102	LHG	C29-C30-C31-C32
19	A	812	CLA	O1A-CGA-O2A-C1
22	BB	851	LHG	C2-C3-O3-P
22	L2	208	LHG	C2-C3-O3-P
22	L2	208	LHG	C4-O6-P-O5
22	X	102	LHG	C4-O6-P-O4
22	X	102	LHG	C4-O6-P-O5
22	L1	211	LHG	C3-O3-P-O5
22	X2	102	LHG	C4-O6-P-O5
25	L1	210	LMG	C42-C43-C44-C45
19	A1	832	CLA	O1D-CGD-O2D-CED
19	BB	808	CLA	C11-C12-C13-C15
19	A1	842	CLA	C16-C17-C18-C19
19	L	204	CLA	C16-C17-C18-C20
22	AA	846	LHG	C32-C33-C34-C35
19	B	814	CLA	C10-C11-C12-C13
19	BB	814	CLA	C2-C3-C5-C6
25	B	851	LMG	C42-C43-C44-C45
22	B	853	LHG	C10-C11-C12-C13
22	B	852	LHG	O6-C4-C5-C6
19	BB	826	CLA	O1D-CGD-O2D-CED
21	B	838	PQN	C18-C20-C21-C22
19	KK	102	CLA	CAD-CBD-CGD-O1D
19	B	810	CLA	CAD-CBD-CGD-O1D
19	L2	204	CLA	CAD-CBD-CGD-O1D
19	K1	103	CLA	CAD-CBD-CGD-O1D
19	A	807	CLA	CAD-CBD-CGD-O1D
19	A1	823	CLA	CAD-CBD-CGD-O1D
19	B	831	CLA	CAD-CBD-CGD-O1D
19	BB	810	CLA	CAD-CBD-CGD-O1D
19	AA	806	CLA	CAD-CBD-CGD-O1D
19	A1	815	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A1	844	CLA	CAD-CBD-CGD-O1D
19	AA	816	CLA	CAD-CBD-CGD-O1D
19	B2	810	CLA	CAD-CBD-CGD-O1D
19	LL	201	CLA	CAD-CBD-CGD-O1D
19	A2	844	CLA	CAD-CBD-CGD-O1D
19	BB	830	CLA	CAD-CBD-CGD-O1D
19	AA	845	CLA	CAD-CBD-CGD-O1D
19	B1	810	CLA	CAD-CBD-CGD-O1D
19	A2	852	CLA	CAD-CBD-CGD-O1D
19	B1	811	CLA	CAD-CBD-CGD-O1D
19	A2	824	CLA	CAD-CBD-CGD-O1D
19	B1	802	CLA	CAD-CBD-CGD-O1D
19	B1	830	CLA	CAD-CBD-CGD-O1D
19	B	802	CLA	CAD-CBD-CGD-O1D
25	B	851	LMG	C34-C35-C36-C37
19	B	808	CLA	C11-C12-C13-C15
19	B1	808	CLA	C11-C12-C13-C15
19	B2	808	CLA	C11-C12-C13-C15
19	A1	806	CLA	C16-C17-C18-C19
19	L2	206	CLA	CBA-CGA-O2A-C1
23	JJ	102	BCR	C15-C16-C17-C18
23	I2	103	BCR	C15-C16-C17-C18
26	B	841	ECH	C9-C10-C11-C12
23	J2	102	BCR	C15-C16-C17-C18
23	BB	843	BCR	C9-C10-C11-C12
23	K	103	BCR	C9-C10-C11-C12
22	AA	846	LHG	C16-C17-C18-C19
22	XX	102	LHG	C29-C30-C31-C32
19	B	858	CLA	C5-C6-C7-C8
19	A	806	CLA	C2A-CAA-CBA-CGA
19	A2	819	CLA	C2A-CAA-CBA-CGA
19	A1	841	CLA	C2A-CAA-CBA-CGA
19	A	819	CLA	C2A-CAA-CBA-CGA
19	B	834	CLA	C15-C16-C17-C18
19	A1	839	CLA	CBD-CGD-O2D-CED
19	B2	825	CLA	C6-C7-C8-C10
19	B2	825	CLA	C12-C13-C15-C16
19	BB	836	CLA	C6-C7-C8-C10
19	B	810	CLA	C11-C10-C8-C7
19	BB	832	CLA	C11-C12-C13-C15
19	BB	811	CLA	C11-C10-C8-C7
19	B	825	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	B1	825	CLA	C6-C7-C8-C10
19	B1	832	CLA	C11-C12-C13-C15
19	BB	825	CLA	C6-C7-C8-C10
19	A	836	CLA	C12-C13-C15-C16
19	A	829	CLA	C11-C10-C8-C7
19	B	806	CLA	C12-C13-C15-C16
19	A2	819	CLA	C11-C10-C8-C7
19	B	815	CLA	C6-C7-C8-C10
19	AA	807	CLA	C12-C13-C15-C16
19	B2	837	CLA	C6-C7-C8-C10
19	B	811	CLA	C11-C10-C8-C7
19	B2	807	CLA	C6-C7-C8-C10
19	B2	803	CLA	C6-C7-C8-C10
19	AA	806	CLA	C6-C7-C8-C10
19	AA	853	CLA	C11-C10-C8-C7
19	B2	834	CLA	C11-C10-C8-C7
19	A2	806	CLA	C6-C7-C8-C10
19	B1	836	CLA	C6-C7-C8-C10
19	A1	805	CLA	C6-C7-C8-C10
19	B2	833	CLA	C11-C12-C13-C15
19	A1	812	CLA	C11-C12-C13-C15
19	B	836	CLA	C12-C13-C15-C16
19	A2	829	CLA	C11-C10-C8-C7
19	B1	835	CLA	C12-C13-C15-C16
19	B	826	CLA	C12-C13-C15-C16
20	A2	803	CL0	C11-C12-C13-C15
21	B1	837	PQN	C21-C22-C23-C25
19	A1	852	CLA	C11-C12-C13-C15
19	A2	852	CLA	C11-C10-C8-C7
19	BB	815	CLA	C6-C7-C8-C10
19	B	833	CLA	C11-C12-C13-C15
19	A	852	CLA	C11-C10-C8-C7
19	A2	836	CLA	C12-C13-C15-C16
19	A	835	CLA	O1A-CGA-O2A-C1
22	A	845	LHG	C16-C17-C18-C19
19	BB	829	CLA	C3-C5-C6-C7
19	B2	804	CLA	C3A-C2A-CAA-CBA
22	BB	851	LHG	C10-C11-C12-C13
19	A2	820	CLA	C8-C10-C11-C12
19	A1	841	CLA	C5-C6-C7-C8
22	X2	103	LHG	C23-C24-C25-C26
19	A1	829	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
19	L2	204	CLA	C4-C3-C5-C6
19	BB	824	CLA	C4-C3-C5-C6
19	B	821	CLA	C4-C3-C5-C6
19	B	810	CLA	C5-C6-C7-C8
19	B	824	CLA	C2-C3-C5-C6
19	A2	836	CLA	C5-C6-C7-C8
20	A1	802	CL0	C16-C17-C18-C19
19	B2	823	CLA	C16-C17-C18-C20
22	XX	102	LHG	O9-C7-O7-C5
19	L2	206	CLA	O1A-CGA-O2A-C1
19	AA	807	CLA	C10-C11-C12-C13
19	A1	842	CLA	C15-C16-C17-C18
19	A	832	CLA	C3-C5-C6-C7
25	II	105	LMG	C37-C38-C39-C40
22	L1	211	LHG	C24-C25-C26-C27
19	B1	823	CLA	C10-C11-C12-C13
25	BB	844	LMG	O1-C7-C8-C9
25	B1	844	LMG	O1-C7-C8-C9
22	L2	208	LHG	O7-C5-C6-O8
25	BB	844	LMG	O1-C7-C8-O7
22	L1	211	LHG	O7-C5-C6-O8
28	BB	854	DGD	O2G-C2G-C3G-O3G
25	B1	846	LMG	O1-C7-C8-O7
25	B2	847	LMG	O1-C7-C8-O7
19	B	830	CLA	C2C-C3C-CAC-CBC
22	L1	211	LHG	C2-C3-O3-P
19	AA	843	CLA	C16-C17-C18-C20
22	AA	846	LHG	C7-C8-C9-C10
19	LL	202	CLA	C3-C5-C6-C7
23	A2	853	BCR	C9-C10-C11-C12
20	AA	803	CL0	C8-C10-C11-C12
19	A	835	CLA	C15-C16-C17-C18
19	B2	801	CLA	C15-C16-C17-C18
19	AA	819	CLA	CBD-CGD-O2D-CED
19	B1	814	CLA	C10-C11-C12-C13
22	BB	851	LHG	C25-C26-C27-C28
19	B	825	CLA	C3-C5-C6-C7
19	AA	840	CLA	C5-C6-C7-C8
19	B	860	CLA	C16-C17-C18-C19
22	A2	845	LHG	C7-C8-C9-C10
19	B1	814	CLA	O1A-CGA-O2A-C1
25	B1	844	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	BB	844	LMG	C19-C20-C21-C22
25	B1	844	LMG	C19-C20-C21-C22
19	BB	806	CLA	C14-C13-C15-C16
19	B	825	CLA	C11-C10-C8-C9
19	A1	807	CLA	C6-C7-C8-C9
19	B1	826	CLA	C14-C13-C15-C16
19	BB	825	CLA	C11-C10-C8-C9
19	AA	808	CLA	C6-C7-C8-C9
19	BB	810	CLA	C11-C10-C8-C9
21	B2	838	PQN	C21-C22-C23-C24
21	B	838	PQN	C21-C22-C23-C24
21	A1	843	PQN	C16-C17-C18-C19
19	BB	826	CLA	C14-C13-C15-C16
19	A1	828	CLA	C11-C12-C13-C14
19	A2	808	CLA	C6-C7-C8-C9
19	A2	810	CLA	C14-C13-C15-C16
19	A1	834	CLA	C14-C13-C15-C16
21	B1	837	PQN	C21-C22-C23-C24
19	L1	207	CLA	CBA-CGA-O2A-C1
19	B1	814	CLA	CBA-CGA-O2A-C1
19	AA	853	CLA	C5-C6-C7-C8
23	JJ	102	BCR	C20-C21-C22-C37
23	A2	847	BCR	C35-C13-C14-C15
23	A	851	BCR	C36-C18-C19-C20
23	F	303	BCR	C36-C18-C19-C20
23	B2	840	BCR	C11-C12-C13-C35
23	FF	303	BCR	C36-C18-C19-C20
19	AA	842	CLA	C2A-CAA-CBA-CGA
19	L	204	CLA	C2A-CAA-CBA-CGA
19	BB	825	CLA	O1A-CGA-O2A-C1
19	L1	207	CLA	O1A-CGA-O2A-C1
19	B1	825	CLA	CBD-CGD-O2D-CED
23	A2	847	BCR	C14-C15-C16-C17
26	B	841	ECH	C11-C12-C13-C14
23	BB	842	BCR	C17-C18-C19-C20
23	AA	855	BCR	C21-C22-C23-C24
23	BB	839	BCR	C21-C22-C23-C24
23	J1	104	BCR	C17-C18-C19-C20
24	KK	104	AJP	OCC-CCX-OCY-CCZ
19	A2	830	CLA	C13-C15-C16-C17
19	B2	825	CLA	O1A-CGA-O2A-C1
22	AA	846	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	L2	202	AJP	OCC-CCX-OCY-CCZ
25	M	102	LMG	C30-C31-C32-C33
19	A2	827	CLA	C10-C11-C12-C13
23	M	101	BCR	C13-C14-C15-C16
19	B2	814	CLA	C11-C12-C13-C14
22	X1	103	LHG	C25-C26-C27-C28
22	X1	102	LHG	O9-C7-O7-C5
19	B2	824	CLA	C4-C3-C5-C6
19	AA	836	CLA	C4-C3-C5-C6
19	B1	824	CLA	C4-C3-C5-C6
19	BB	856	CLA	C8-C10-C11-C12
22	A2	845	LHG	C26-C27-C28-C29
19	L1	205	CLA	C2-C3-C5-C6
22	XX	102	LHG	C8-C7-O7-C5
22	BB	850	LHG	O6-C4-C5-C6
22	X1	102	LHG	C8-C7-O7-C5
19	BB	801	CLA	C16-C17-C18-C19
19	A2	835	CLA	CBA-CGA-O2A-C1
19	A1	834	CLA	CBA-CGA-O2A-C1
19	AA	835	CLA	CBA-CGA-O2A-C1
22	LL	205	LHG	C5-C4-O6-P
22	L	207	LHG	C5-C4-O6-P
19	BB	821	CLA	O1D-CGD-O2D-CED
25	B	845	LMG	C19-C20-C21-C22
19	A	831	CLA	C2A-CAA-CBA-CGA
23	A2	849	BCR	C6-C7-C8-C9
23	A	850	BCR	C22-C23-C24-C25
22	A1	845	LHG	C9-C10-C11-C12
19	AA	853	CLA	C8-C10-C11-C12
19	B1	814	CLA	C11-C12-C13-C14
22	A1	845	LHG	C29-C30-C31-C32
23	A	848	BCR	C1-C6-C7-C8
23	L	205	BCR	C1-C6-C7-C8
23	A1	851	BCR	C1-C6-C7-C8
23	M	101	BCR	C5-C6-C7-C8
23	A	850	BCR	C1-C6-C7-C8
23	A2	850	BCR	C1-C6-C7-C8
23	K2	105	BCR	C23-C24-C25-C26
23	II	104	BCR	C1-C6-C7-C8
23	B1	842	BCR	C23-C24-C25-C26
23	I2	103	BCR	C5-C6-C7-C8
23	AA	852	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	L1	208	BCR	C5-C6-C7-C8
23	J2	102	BCR	C1-C6-C7-C8
23	J2	102	BCR	C5-C6-C7-C8
23	AA	849	BCR	C1-C6-C7-C8
23	F1	306	BCR	C23-C24-C25-C30
23	J1	102	BCR	C1-C6-C7-C8
23	AA	851	BCR	C1-C6-C7-C8
23	A2	851	BCR	C1-C6-C7-C8
23	A	851	BCR	C1-C6-C7-C8
23	F1	303	BCR	C5-C6-C7-C8
19	B1	801	CLA	C16-C17-C18-C20
19	A1	842	CLA	C16-C17-C18-C20
19	A1	806	CLA	C16-C17-C18-C20
25	B2	845	LMG	C19-C20-C21-C22
23	B	844	BCR	C16-C17-C18-C19
23	B2	843	BCR	C20-C21-C22-C23
23	I	102	BCR	C20-C21-C22-C23
23	J2	102	BCR	C11-C10-C9-C8
23	B	842	BCR	C11-C10-C9-C8
23	B	840	BCR	C12-C13-C14-C15
23	K	103	BCR	C11-C10-C9-C8
23	BB	841	BCR	C11-C10-C9-C8
23	FF	303	BCR	C20-C21-C22-C23
19	BB	835	CLA	O1D-CGD-O2D-CED
19	AA	819	CLA	O1D-CGD-O2D-CED
22	A	846	LHG	C3-O3-P-O6
22	AA	847	LHG	C3-O3-P-O6
22	LL	205	LHG	C3-O3-P-O6
22	B1	847	LHG	C3-O3-P-O6
22	A2	846	LHG	C3-O3-P-O6
22	A1	846	LHG	C3-O3-P-O6
22	AA	846	LHG	C4-O6-P-O3
22	X	102	LHG	C3-O3-P-O6
22	L	207	LHG	C3-O3-P-O6
22	XX	102	LHG	C3-O3-P-O6
22	X2	102	LHG	C3-O3-P-O6
22	A2	845	LHG	C4-O6-P-O3
22	BB	850	LHG	C4-O6-P-O3
22	A	845	LHG	C4-O6-P-O3
22	A1	845	LHG	C4-O6-P-O3
22	B	852	LHG	C4-O6-P-O3
22	X1	102	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
19	B	825	CLA	O1A-CGA-O2A-C1
19	A	809	CLA	O1A-CGA-O2A-C1
19	A2	835	CLA	O1A-CGA-O2A-C1
20	AA	803	CL0	C4C-C3C-CAC-CBC
19	L2	204	CLA	C2-C3-C5-C6
19	A1	834	CLA	O1A-CGA-O2A-C1
25	II	105	LMG	O1-C7-C8-O7
25	B1	844	LMG	O1-C7-C8-O7
19	B	805	CLA	C16-C17-C18-C19
22	B2	848	LHG	C12-C13-C14-C15
19	BB	824	CLA	C2-C1-O2A-CGA
19	LL	201	CLA	C10-C11-C12-C13
23	J1	102	BCR	C15-C16-C17-C18
19	B2	801	CLA	C16-C17-C18-C20
19	B	805	CLA	C11-C12-C13-C15
19	BB	805	CLA	C11-C12-C13-C15
19	B2	805	CLA	C11-C12-C13-C15
19	AA	827	CLA	C11-C10-C8-C7
19	AA	819	CLA	C6-C7-C8-C10
19	B1	810	CLA	C6-C7-C8-C10
19	L	204	CLA	C6-C7-C8-C10
19	B	801	CLA	C13-C15-C16-C17
22	AA	846	LHG	C18-C19-C20-C21
22	X1	103	LHG	C34-C35-C36-C37
19	B2	826	CLA	C15-C16-C17-C18
19	AA	835	CLA	O1A-CGA-O2A-C1
19	L	204	CLA	C10-C11-C12-C13
19	A1	820	CLA	C16-C17-C18-C20
19	B1	823	CLA	C16-C17-C18-C20
22	B	853	LHG	C18-C19-C20-C21
19	BB	801	CLA	C6-C7-C8-C9
19	B	810	CLA	C11-C10-C8-C9
20	AA	803	CL0	C11-C10-C8-C9
19	BB	811	CLA	C11-C10-C8-C9
19	B1	826	CLA	C11-C12-C13-C14
19	A1	835	CLA	C14-C13-C15-C16
19	B1	805	CLA	C6-C7-C8-C9
19	A	830	CLA	C11-C10-C8-C9
19	A	830	CLA	C11-C12-C13-C14
19	B	805	CLA	C6-C7-C8-C9
19	B2	811	CLA	C11-C10-C8-C9
19	B	811	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
19	AA	830	CLA	C11-C10-C8-C9
19	B2	834	CLA	C14-C13-C15-C16
19	A2	806	CLA	C6-C7-C8-C9
19	A1	829	CLA	C11-C10-C8-C9
19	A1	805	CLA	C6-C7-C8-C9
19	BB	805	CLA	C6-C7-C8-C9
19	B2	805	CLA	C6-C7-C8-C9
19	A1	812	CLA	C6-C7-C8-C9
19	B1	835	CLA	C14-C13-C15-C16
19	B	826	CLA	C14-C13-C15-C16
19	A2	830	CLA	C11-C10-C8-C9
19	B1	811	CLA	C11-C10-C8-C9
20	A	803	CL0	C14-C13-C15-C16
19	A2	836	CLA	C11-C10-C8-C9
19	B2	826	CLA	C11-C12-C13-C14
25	M	102	LMG	C37-C38-C39-C40
19	LL	202	CLA	C8-C10-C11-C12
19	B2	821	CLA	C2-C3-C5-C6
19	BB	821	CLA	CBD-CGD-O2D-CED
19	B2	825	CLA	CBA-CGA-O2A-C1
19	BB	825	CLA	CBA-CGA-O2A-C1
25	II	105	LMG	C32-C33-C34-C35
19	A1	829	CLA	C4C-C3C-CAC-CBC
19	A	840	CLA	C5-C6-C7-C8
23	F2	303	BCR	C36-C18-C19-C20
23	A	849	BCR	C21-C22-C23-C24
23	A	851	BCR	C7-C8-C9-C10
23	J	104	BCR	C11-C12-C13-C14
23	AA	850	BCR	C7-C8-C9-C10
19	A	809	CLA	CBA-CGA-O2A-C1
19	LL	201	CLA	C5-C6-C7-C8
24	L1	204	AJP	CCW-CCX-OCY-CCZ
23	B2	842	BCR	C15-C16-C17-C18
23	B1	838	BCR	C9-C10-C11-C12
23	B1	838	BCR	C13-C14-C15-C16
23	A1	848	BCR	C9-C10-C11-C12
23	AA	849	BCR	C9-C10-C11-C12
23	B2	839	BCR	C9-C10-C11-C12
23	B2	839	BCR	C13-C14-C15-C16
23	B2	844	BCR	C9-C10-C11-C12
23	A1	853	BCR	C9-C10-C11-C12
23	F2	305	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	J1	104	BCR	C15-C16-C17-C18
19	BB	808	CLA	C11-C12-C13-C14
19	B	808	CLA	C11-C12-C13-C14
20	A1	802	CL0	C16-C17-C18-C20
19	A1	801	CLA	C16-C17-C18-C19
19	A2	801	CLA	C16-C17-C18-C19
19	A2	804	CLA	C16-C17-C18-C19
19	B2	823	CLA	C16-C17-C18-C19
22	A1	845	LHG	O10-C23-O8-C6
19	B	825	CLA	CBA-CGA-O2A-C1
22	A1	845	LHG	C24-C23-O8-C6
22	BB	851	LHG	C18-C19-C20-C21
23	J	102	BCR	C14-C15-C16-C17
19	A	836	CLA	C4-C3-C5-C6
19	B	860	CLA	C16-C17-C18-C20
22	XX	102	LHG	C25-C26-C27-C28
19	B	829	CLA	C2C-C3C-CAC-CBC
19	B	824	CLA	C2A-CAA-CBA-CGA
19	AA	819	CLA	C2A-CAA-CBA-CGA
19	A1	819	CLA	C2A-CAA-CBA-CGA
22	L2	208	LHG	C10-C11-C12-C13
22	X	102	LHG	C25-C26-C27-C28
19	B2	801	CLA	C8-C10-C11-C12
25	II	105	LMG	C31-C32-C33-C34
28	BB	854	DGD	O6D-C5D-C6D-O5D
19	BB	805	CLA	C16-C17-C18-C19
19	A	807	CLA	C16-C17-C18-C19
22	A2	846	LHG	C11-C12-C13-C14
20	A	803	CL0	O1D-CGD-O2D-CED
19	A	842	CLA	C5-C6-C7-C8
22	A1	846	LHG	C11-C12-C13-C14
19	B2	805	CLA	C16-C17-C18-C19
19	B	859	CLA	C10-C11-C12-C13
19	A1	818	CLA	CBD-CGD-O2D-CED
23	J2	104	BCR	C15-C16-C17-C18
23	BB	838	BCR	C9-C10-C11-C12
23	I	101	BCR	C13-C14-C15-C16
23	L1	208	BCR	C15-C16-C17-C18
23	B2	843	BCR	C19-C20-C21-C22
23	B	839	BCR	C9-C10-C11-C12
23	BB	842	BCR	C9-C10-C11-C12
23	A2	848	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
23	F	304	BCR	C19-C20-C21-C22
23	F1	304	BCR	C19-C20-C21-C22
23	J	104	BCR	C15-C16-C17-C18
22	X2	103	LHG	C25-C26-C27-C28
19	J	103	CLA	C2C-C3C-CAC-CBC
19	AA	842	CLA	C16-C17-C18-C20
19	B	814	CLA	C4-C3-C5-C6
19	B2	810	CLA	C4-C3-C5-C6
19	B	814	CLA	C2-C3-C5-C6
25	I1	102	LMG	C19-C20-C21-C22
22	X2	102	LHG	C31-C32-C33-C34
22	X2	103	LHG	C28-C29-C30-C31
28	BB	854	DGD	C4D-C5D-C6D-O5D
19	B2	815	CLA	C5-C6-C7-C8
19	B	802	CLA	C15-C16-C17-C18
19	BB	801	CLA	C3A-C2A-CAA-CBA
19	L2	204	CLA	C3A-C2A-CAA-CBA
19	A	810	CLA	C3A-C2A-CAA-CBA
19	AA	836	CLA	C3A-C2A-CAA-CBA
19	B2	807	CLA	C3A-C2A-CAA-CBA
19	BB	802	CLA	C3A-C2A-CAA-CBA
19	B2	801	CLA	C3A-C2A-CAA-CBA
19	F	301	CLA	C3A-C2A-CAA-CBA
19	B1	810	CLA	C3A-C2A-CAA-CBA
24	A	855	AJP	CCW-CCX-OCY-CCZ
24	AA	856	AJP	CCW-CCX-OCY-CCZ
19	A1	839	CLA	O1D-CGD-O2D-CED
19	B1	808	CLA	C11-C12-C13-C14
19	A	842	CLA	C16-C17-C18-C20
19	B2	808	CLA	C11-C12-C13-C14
19	L	204	CLA	C16-C17-C18-C19
22	A	845	LHG	C18-C19-C20-C21
26	BB	840	ECH	C11-C10-C9-C34
23	L1	201	BCR	C20-C21-C22-C37
23	B2	842	BCR	C16-C17-C18-C36
23	F2	303	BCR	C35-C13-C14-C15
26	B	841	ECH	C11-C10-C9-C34
23	I	102	BCR	C20-C21-C22-C37
23	B2	839	BCR	C11-C10-C9-C34
26	B1	840	ECH	C11-C10-C9-C34
26	B2	841	ECH	C11-C10-C9-C34
23	A2	851	BCR	C16-C17-C18-C36

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Mol	Chain	Res	Type	Atoms
23	II	102	BCR	C20-C21-C22-C37
23	F1	303	BCR	C35-C13-C14-C15
19	AA	827	CLA	C10-C11-C12-C13
19	BB	807	CLA	C2C-C3C-CAC-CBC
23	I	101	BCR	C10-C11-C12-C13
23	I	102	BCR	C18-C19-C20-C21
23	I2	101	BCR	C18-C19-C20-C21
23	F1	303	BCR	C18-C19-C20-C21
19	BB	825	CLA	O1D-CGD-O2D-CED
19	A1	819	CLA	C8-C10-C11-C12
19	A	827	CLA	O2A-C1-C2-C3
19	BB	821	CLA	O2A-C1-C2-C3
19	AA	827	CLA	O2A-C1-C2-C3
19	B	834	CLA	CBD-CGD-O2D-CED
23	A1	848	BCR	C22-C23-C24-C25
23	AA	851	BCR	C22-C23-C24-C25
19	BB	814	CLA	C10-C11-C12-C13
19	B	806	CLA	C10-C11-C12-C13
22	X1	103	LHG	C18-C19-C20-C21
19	B2	823	CLA	C10-C11-C12-C13
19	A2	842	CLA	C16-C17-C18-C20
19	B1	823	CLA	C16-C17-C18-C19
22	A1	845	LHG	C4-C5-C6-O8
19	B	825	CLA	C6-C7-C8-C9
19	B1	825	CLA	C6-C7-C8-C9
21	A	843	PQN	C16-C17-C18-C19
19	AA	821	CLA	C11-C10-C8-C9
19	B2	837	CLA	C6-C7-C8-C9
19	A1	809	CLA	C14-C13-C15-C16
19	B1	810	CLA	C6-C7-C8-C9
19	B1	801	CLA	C2-C1-O2A-CGA
19	B1	824	CLA	C2-C1-O2A-CGA
19	B2	808	CLA	C2-C1-O2A-CGA
19	B1	806	CLA	C10-C11-C12-C13
25	I1	102	LMG	C7-C8-O7-C10
20	AA	803	CL0	C1A-C2A-CAA-CBA
19	BB	831	CLA	C1A-C2A-CAA-CBA
19	B1	832	CLA	C1A-C2A-CAA-CBA
19	A1	814	CLA	C1A-C2A-CAA-CBA
19	A	815	CLA	C1A-C2A-CAA-CBA
19	AA	810	CLA	C1A-C2A-CAA-CBA
19	B1	801	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
19	AA	815	CLA	C1A-C2A-CAA-CBA
19	B1	821	CLA	C1A-C2A-CAA-CBA
19	BB	802	CLA	C1A-C2A-CAA-CBA
19	B2	810	CLA	C1A-C2A-CAA-CBA
19	LL	201	CLA	C1A-C2A-CAA-CBA
19	A2	815	CLA	C1A-C2A-CAA-CBA
19	B	801	CLA	C1A-C2A-CAA-CBA
19	A	824	CLA	C1A-C2A-CAA-CBA
19	A2	810	CLA	C1A-C2A-CAA-CBA
19	BB	820	CLA	C1A-C2A-CAA-CBA
19	B1	810	CLA	C1A-C2A-CAA-CBA
19	A1	852	CLA	C1A-C2A-CAA-CBA
19	B1	811	CLA	C1A-C2A-CAA-CBA
19	B	833	CLA	C1A-C2A-CAA-CBA
19	BB	802	CLA	C4-C3-C5-C6
19	A2	808	CLA	C4-C3-C5-C6
19	B1	802	CLA	C4-C3-C5-C6
19	B1	848	CLA	CBA-CGA-O2A-C1
19	B	854	CLA	CBA-CGA-O2A-C1
19	AA	842	CLA	C5-C6-C7-C8
19	B2	806	CLA	C10-C11-C12-C13
19	BB	824	CLA	C2-C3-C5-C6
23	A2	847	BCR	C7-C8-C9-C34
23	B2	842	BCR	C13-C14-C15-C16
23	B	843	BCR	C9-C10-C11-C12
23	A	847	BCR	C13-C14-C15-C16
19	A1	801	CLA	C16-C17-C18-C20
19	A2	801	CLA	C16-C17-C18-C20
19	L2	206	CLA	C2A-CAA-CBA-CGA
19	BB	824	CLA	C2A-CAA-CBA-CGA
19	B2	825	CLA	C11-C10-C8-C7
19	BB	808	CLA	C6-C7-C8-C10
19	BB	825	CLA	C11-C10-C8-C7
19	B2	815	CLA	C6-C7-C8-C10
19	B1	803	CLA	C11-C12-C13-C15
19	B1	805	CLA	C11-C12-C13-C15
19	A	806	CLA	C6-C7-C8-C10
19	A1	818	CLA	C11-C10-C8-C7
19	B2	804	CLA	C11-C10-C8-C7
19	B2	807	CLA	C11-C12-C13-C15
19	B2	803	CLA	C11-C12-C13-C15
19	A1	841	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	A	819	CLA	C11-C10-C8-C7
19	B1	804	CLA	C11-C10-C8-C7
19	BB	803	CLA	C11-C12-C13-C15
19	B1	815	CLA	C6-C7-C8-C10
19	B1	807	CLA	C11-C12-C13-C15
19	BB	815	CLA	C11-C10-C8-C7
25	I1	102	LMG	C17-C18-C19-C20
19	BB	802	CLA	O1D-CGD-O2D-CED
19	BB	806	CLA	C10-C11-C12-C13
19	A1	828	CLA	C13-C15-C16-C17
19	B1	805	CLA	C16-C17-C18-C19
22	B	853	LHG	C12-C13-C14-C15
19	B1	801	CLA	C16-C17-C18-C19
22	X2	103	LHG	O2-C2-C3-O3
19	A1	818	CLA	O1D-CGD-O2D-CED
19	B2	837	CLA	C2C-C3C-CAC-CBC
19	BB	825	CLA	C5-C6-C7-C8
25	II	105	LMG	C29-C30-C31-C32
19	BB	802	CLA	CBD-CGD-O2D-CED
22	B1	847	LHG	O6-C4-C5-O7
25	B1	846	LMG	O7-C10-C11-C12
19	B1	825	CLA	C5-C6-C7-C8
19	BB	822	CLA	C16-C17-C18-C19
19	AA	836	CLA	C2-C3-C5-C6
21	BB	837	PQN	C18-C20-C21-C22
26	BB	840	ECH	C11-C10-C9-C8
23	L1	201	BCR	C20-C21-C22-C23
23	B2	842	BCR	C16-C17-C18-C19
23	A	850	BCR	C20-C21-C22-C23
26	B	841	ECH	C11-C10-C9-C8
26	B1	840	ECH	C11-C10-C9-C8
26	B2	841	ECH	C11-C10-C9-C8
19	A	829	CLA	C13-C15-C16-C17
22	X2	103	LHG	O1-C1-C2-O2
22	X1	102	LHG	C31-C32-C33-C34
28	B	856	DGD	C4D-C5D-C6D-O5D
19	B2	807	CLA	C13-C15-C16-C17
19	BB	804	CLA	C10-C11-C12-C13
20	A2	803	CL0	C10-C11-C12-C13
19	B2	807	CLA	C3-C5-C6-C7
19	B1	829	CLA	C3-C5-C6-C7
19	B2	801	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
23	AA	848	BCR	C13-C14-C15-C16
23	F	304	BCR	C15-C16-C17-C18
19	B2	825	CLA	C5-C6-C7-C8
19	B	854	CLA	C13-C15-C16-C17
19	A2	805	CLA	C8-C10-C11-C12
19	AA	829	CLA	C13-C15-C16-C17
22	AA	846	LHG	C33-C34-C35-C36
28	B	856	DGD	O6D-C5D-C6D-O5D
19	A	807	CLA	C16-C17-C18-C20
19	AA	801	CLA	C16-C17-C18-C19
22	X	102	LHG	C31-C32-C33-C34
19	AA	808	CLA	C4-C3-C5-C6
19	B2	849	CLA	C8-C10-C11-C12
19	A1	806	CLA	C10-C11-C12-C13
19	B2	824	CLA	C2-C3-C5-C6
19	B1	824	CLA	C2-C3-C5-C6
19	B	834	CLA	O1D-CGD-O2D-CED
19	AA	831	CLA	C2A-CAA-CBA-CGA
19	L1	207	CLA	C2A-CAA-CBA-CGA
19	A2	806	CLA	C2A-CAA-CBA-CGA
19	A1	810	CLA	C2A-CAA-CBA-CGA
19	B	802	CLA	C2A-CAA-CBA-CGA
22	B	853	LHG	C28-C29-C30-C31
19	B2	814	CLA	C10-C11-C12-C13
19	B1	833	CLA	C15-C16-C17-C18
19	B	837	CLA	C3-C5-C6-C7
22	B	852	LHG	C1-C2-C3-O3
19	B1	848	CLA	O1A-CGA-O2A-C1
19	A2	830	CLA	O1A-CGA-O2A-C1
19	A1	820	CLA	C16-C17-C18-C19
22	A2	845	LHG	C15-C16-C17-C18
19	BB	845	CLA	C2A-CAA-CBA-CGA
23	B	848	BCR	C23-C24-C25-C30
23	L	206	BCR	C23-C24-C25-C30
23	K1	104	BCR	C1-C6-C7-C8
23	A	848	BCR	C23-C24-C25-C30
19	L2	206	CLA	C11-C12-C13-C14
23	BB	847	BCR	C23-C24-C25-C30
23	A1	848	BCR	C1-C6-C7-C8
23	A	853	BCR	C23-C24-C25-C30
19	A2	821	CLA	C11-C10-C8-C9
23	K2	103	BCR	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
23	K2	103	BCR	C23-C24-C25-C30
23	I2	103	BCR	C1-C6-C7-C8
23	AA	852	BCR	C23-C24-C25-C30
23	L1	208	BCR	C1-C6-C7-C8
23	A	847	BCR	C1-C6-C7-C8
23	A	847	BCR	C23-C24-C25-C30
23	LL	204	BCR	C23-C24-C25-C30
23	AA	849	BCR	C23-C24-C25-C30
19	BB	826	CLA	C11-C12-C13-C14
23	F1	306	BCR	C23-C24-C25-C26
23	A2	847	BCR	C1-C6-C7-C8
19	A	819	CLA	C6-C7-C8-C9
23	AA	848	BCR	C1-C6-C7-C8
23	AA	848	BCR	C23-C24-C25-C30
23	AA	855	BCR	C1-C6-C7-C8
19	BB	802	CLA	C6-C7-C8-C9
23	KK	103	BCR	C1-C6-C7-C8
23	FF	306	BCR	C23-C24-C25-C30
19	A1	829	CLA	C11-C12-C13-C14
23	A2	848	BCR	C1-C6-C7-C8
23	M2	102	BCR	C1-C6-C7-C8
19	B1	848	CLA	C6-C7-C8-C9
23	A	854	BCR	C1-C6-C7-C8
23	K	103	BCR	C1-C6-C7-C8
23	A2	853	BCR	C1-C6-C7-C8
19	AA	819	CLA	C6-C7-C8-C9
23	A	849	BCR	C1-C6-C7-C8
23	B1	839	BCR	C1-C6-C7-C8
23	A1	849	BCR	C1-C6-C7-C8
19	A2	829	CLA	C11-C12-C13-C14
23	AA	854	BCR	C23-C24-C25-C30
19	B	826	CLA	C11-C12-C13-C14
23	A1	847	BCR	C1-C6-C7-C8
23	BB	839	BCR	C1-C6-C7-C8
23	AA	850	BCR	C1-C6-C7-C8
19	B1	802	CLA	C6-C7-C8-C9
23	B2	840	BCR	C1-C6-C7-C8
23	A1	850	BCR	C1-C6-C7-C8
22	LL	205	LHG	C10-C11-C12-C13
23	J2	104	BCR	C9-C10-C11-C12
23	II	104	BCR	C15-C16-C17-C18
23	FF	304	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
23	B1	842	BCR	C9-C10-C11-C12
23	F2	304	BCR	C19-C20-C21-C22
22	X2	103	LHG	C18-C19-C20-C21
22	X2	103	LHG	C31-C32-C33-C34
19	B1	848	CLA	C8-C10-C11-C12
19	B2	825	CLA	O1D-CGD-O2D-CED
19	A2	840	CLA	C4-C3-C5-C6
19	B	807	CLA	C4-C3-C5-C6
19	A2	809	CLA	O1A-CGA-O2A-C1
19	AA	809	CLA	O1A-CGA-O2A-C1
19	B	854	CLA	O1A-CGA-O2A-C1
23	F1	303	BCR	C14-C15-C16-C17
19	A	836	CLA	C2-C3-C5-C6
22	B	853	LHG	O1-C1-C2-C3
19	A2	831	CLA	C2A-CAA-CBA-CGA
19	B	807	CLA	C2C-C3C-CAC-CBC
19	B2	825	CLA	C3-C5-C6-C7
19	B2	811	CLA	C8-C10-C11-C12
19	BB	821	CLA	C5-C6-C7-C8
22	B	852	LHG	C11-C10-C9-C8
19	B1	811	CLA	C8-C10-C11-C12
23	I	101	BCR	C17-C18-C19-C20
23	BB	843	BCR	C7-C8-C9-C10
23	A	849	BCR	C7-C8-C9-C10
23	I1	101	BCR	C11-C12-C13-C14
19	BB	856	CLA	C10-C11-C12-C13
19	B	825	CLA	C5-C6-C7-C8
19	A2	829	CLA	C13-C15-C16-C17
19	BB	833	CLA	C15-C16-C17-C18
22	X	102	LHG	C30-C31-C32-C33
21	AA	844	PQN	C23-C25-C26-C27
22	BB	851	LHG	C12-C13-C14-C15
19	A	830	CLA	C13-C15-C16-C17
19	A1	841	CLA	C16-C17-C18-C20
19	B2	852	CLA	C16-C17-C18-C19
23	A	848	BCR	C22-C23-C24-C25
23	AA	849	BCR	C22-C23-C24-C25
19	B2	802	CLA	C4-C3-C5-C6
19	BB	807	CLA	C4-C3-C5-C6
19	B	825	CLA	C11-C10-C8-C7
19	B1	826	CLA	C11-C12-C13-C15
19	A	819	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
19	A1	828	CLA	C11-C12-C13-C15
19	A1	809	CLA	C12-C13-C15-C16
19	A2	810	CLA	C12-C13-C15-C16
19	B1	802	CLA	C6-C7-C8-C10
19	AA	809	CLA	CBA-CGA-O2A-C1
19	AA	808	CLA	C2-C3-C5-C6
19	B2	810	CLA	C2-C3-C5-C6
22	XX	102	LHG	C31-C32-C33-C34
22	X2	103	LHG	C12-C13-C14-C15
23	LL	204	BCR	C13-C14-C15-C16
23	A1	847	BCR	C13-C14-C15-C16
23	J1	104	BCR	C9-C10-C11-C12
23	J1	104	BCR	C19-C20-C21-C22
19	A1	830	CLA	C2A-CAA-CBA-CGA
19	AA	822	CLA	CAA-CBA-CGA-O2A
19	B1	848	CLA	CAA-CBA-CGA-O2A
19	A2	830	CLA	CAA-CBA-CGA-O2A
22	BB	850	LHG	C11-C10-C9-C8
19	A	839	CLA	CAA-CBA-CGA-O2A
19	L	202	CLA	CAA-CBA-CGA-O2A
19	B	854	CLA	CAA-CBA-CGA-O2A
19	A1	838	CLA	CAA-CBA-CGA-O2A
19	A	816	CLA	O1A-CGA-O2A-C1
19	AA	822	CLA	C2-C3-C5-C6
23	I2	102	BCR	C20-C21-C22-C37
23	B2	839	BCR	C35-C13-C14-C15
23	AA	851	BCR	C35-C13-C14-C15
23	B2	844	BCR	C11-C10-C9-C34
23	B1	843	BCR	C11-C10-C9-C34
19	A1	801	CLA	C3-C5-C6-C7
19	A2	801	CLA	C3-C5-C6-C7
22	L2	208	LHG	C3-O3-P-O6
22	XX	102	LHG	C30-C31-C32-C33
19	AA	831	CLA	CAA-CBA-CGA-O2A
19	A2	842	CLA	CAA-CBA-CGA-O2A
19	B1	801	CLA	CAA-CBA-CGA-O2A
19	BB	852	CLA	CAA-CBA-CGA-O2A
19	A	842	CLA	CAA-CBA-CGA-O2A
19	A1	830	CLA	CAA-CBA-CGA-O2A
20	A2	803	CL0	CAA-CBA-CGA-O2A
19	BB	822	CLA	C16-C17-C18-C20
19	A2	804	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	B	845	LMG	C39-C40-C41-C42
19	AA	843	CLA	CAA-CBA-CGA-O2A
19	A2	839	CLA	CAA-CBA-CGA-O2A
25	B	851	LMG	O7-C10-C11-C12
19	A1	841	CLA	CAA-CBA-CGA-O2A
19	A1	828	CLA	CAA-CBA-CGA-O2A
19	A1	829	CLA	CAA-CBA-CGA-O2A
19	B1	810	CLA	CAA-CBA-CGA-O2A
19	A1	821	CLA	CAA-CBA-CGA-O2A
19	BB	821	CLA	C2-C3-C5-C6
19	BB	802	CLA	C2-C3-C5-C6
19	A2	808	CLA	C2-C3-C5-C6
19	B1	802	CLA	C2-C3-C5-C6
19	B1	815	CLA	C5-C6-C7-C8
25	I1	102	LMG	C9-C8-O7-C10
19	A	816	CLA	CBA-CGA-O2A-C1
19	A2	809	CLA	CBA-CGA-O2A-C1
22	L	207	LHG	C10-C11-C12-C13
19	A1	828	CLA	C16-C17-C18-C20
19	AA	839	CLA	CAA-CBA-CGA-O2A
19	A	822	CLA	CAA-CBA-CGA-O2A
19	A2	852	CLA	CAA-CBA-CGA-O2A
19	A	852	CLA	CAA-CBA-CGA-O2A
19	B1	801	CLA	C3-C5-C6-C7
23	B	840	BCR	C13-C14-C15-C16
19	B	834	CLA	C3A-C2A-CAA-CBA
19	BB	831	CLA	C3A-C2A-CAA-CBA
19	AA	833	CLA	C3A-C2A-CAA-CBA
19	A1	832	CLA	C3A-C2A-CAA-CBA
19	A	836	CLA	C3A-C2A-CAA-CBA
19	B1	801	CLA	C3A-C2A-CAA-CBA
19	A2	833	CLA	C3A-C2A-CAA-CBA
19	B2	810	CLA	C3A-C2A-CAA-CBA
19	B1	807	CLA	C3A-C2A-CAA-CBA
19	B1	833	CLA	C3A-C2A-CAA-CBA
19	A1	852	CLA	C3A-C2A-CAA-CBA
19	A2	836	CLA	C3A-C2A-CAA-CBA
19	AA	842	CLA	CAA-CBA-CGA-O2A
20	A	803	CL0	CAA-CBA-CGA-O2A
19	B2	825	CLA	C6-C7-C8-C9
19	BB	836	CLA	C6-C7-C8-C9
19	BB	832	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
19	B1	832	CLA	C11-C12-C13-C14
19	BB	825	CLA	C6-C7-C8-C9
19	A2	819	CLA	C11-C10-C8-C9
19	A1	818	CLA	C6-C7-C8-C9
19	B	815	CLA	C6-C7-C8-C9
19	AA	806	CLA	C6-C7-C8-C9
19	B1	836	CLA	C6-C7-C8-C9
19	B1	804	CLA	C11-C10-C8-C9
19	B2	833	CLA	C11-C12-C13-C14
19	B	836	CLA	C14-C13-C15-C16
19	A1	852	CLA	C11-C12-C13-C14
19	BB	815	CLA	C6-C7-C8-C9
19	B	833	CLA	C11-C12-C13-C14
19	A2	836	CLA	C14-C13-C15-C16
19	B	802	CLA	C6-C7-C8-C9
19	BB	803	CLA	C3-C5-C6-C7
19	A2	813	CLA	C3-C5-C6-C7
19	BB	856	CLA	CAD-CBD-CGD-O2D
19	AA	822	CLA	CAD-CBD-CGD-O2D
19	B2	802	CLA	CAD-CBD-CGD-O2D
19	BB	811	CLA	CAD-CBD-CGD-O2D
19	B	825	CLA	CAD-CBD-CGD-O2D
19	XX	101	CLA	CAD-CBD-CGD-O2D
19	A	844	CLA	CAD-CBD-CGD-O2D
19	B1	832	CLA	CAD-CBD-CGD-O2D
19	BB	825	CLA	CAD-CBD-CGD-O2D
19	KK	101	CLA	CAD-CBD-CGD-O2D
19	J	101	CLA	CAD-CBD-CGD-O2D
19	X2	101	CLA	CAD-CBD-CGD-O2D
19	A1	808	CLA	CAD-CBD-CGD-O2D
19	A2	817	CLA	CAD-CBD-CGD-O2D
19	B	811	CLA	CAD-CBD-CGD-O2D
19	K2	102	CLA	CAD-CBD-CGD-O2D
19	B1	819	CLA	CAD-CBD-CGD-O2D
19	B	859	CLA	CAD-CBD-CGD-O2D
19	J2	101	CLA	CAD-CBD-CGD-O2D
19	B1	850	CLA	CAD-CBD-CGD-O2D
19	A2	806	CLA	CAD-CBD-CGD-O2D
19	BB	816	CLA	CAD-CBD-CGD-O2D
19	A	817	CLA	CAD-CBD-CGD-O2D
19	BB	829	CLA	CAD-CBD-CGD-O2D
19	BB	822	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
19	K	102	CLA	CAD-CBD-CGD-O2D
19	K	101	CLA	CAD-CBD-CGD-O2D
19	B	829	CLA	CAD-CBD-CGD-O2D
19	A2	804	CLA	CAD-CBD-CGD-O2D
19	AA	827	CLA	CAD-CBD-CGD-O2D
19	F1	305	CLA	CAD-CBD-CGD-O2D
19	A1	822	CLA	CAD-CBD-CGD-O2D
22	A2	845	LHG	C11-C12-C13-C14
19	A1	827	CLA	CAA-CBA-CGA-O2A
22	BB	850	LHG	O8-C23-C24-C25
19	B2	852	CLA	CAA-CBA-CGA-O2A
19	A1	852	CLA	CAA-CBA-CGA-O2A
19	B	846	CLA	C2A-CAA-CBA-CGA
19	A	804	CLA	C4-C3-C5-C6
20	A2	803	CL0	C4-C3-C5-C6
19	AA	807	CLA	C15-C16-C17-C18
19	A1	806	CLA	C15-C16-C17-C18
19	L	204	CLA	C13-C15-C16-C17
19	A1	832	CLA	O2A-C1-C2-C3
19	B	821	CLA	O2A-C1-C2-C3
19	B1	821	CLA	O2A-C1-C2-C3
19	A2	827	CLA	O2A-C1-C2-C3
19	A2	833	CLA	O2A-C1-C2-C3
19	A1	826	CLA	O2A-C1-C2-C3
19	A	833	CLA	O2A-C1-C2-C3
19	AA	801	CLA	C16-C17-C18-C20
19	A1	804	CLA	C11-C12-C13-C15
19	B	817	CLA	CBD-CGD-O2D-CED
19	A2	804	CLA	C2-C3-C5-C6
19	B	860	CLA	CAA-CBA-CGA-O2A
19	A1	842	CLA	CAA-CBA-CGA-O2A
19	B2	801	CLA	CAA-CBA-CGA-O2A
22	B	852	LHG	O8-C23-C24-C25
19	A	840	CLA	CAA-CBA-CGA-O2A
19	FF	301	CLA	C2C-C3C-CAC-CBC
19	A2	829	CLA	C2C-C3C-CAC-CBC
23	K1	104	BCR	C11-C12-C13-C14
23	K1	104	BCR	C17-C18-C19-C20
23	F2	303	BCR	C7-C8-C9-C10
23	J2	104	BCR	C11-C12-C13-C14
23	J2	104	BCR	C17-C18-C19-C20
23	A1	851	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
23	A2	847	BCR	C11-C12-C13-C14
23	B	840	BCR	C21-C22-C23-C24
23	A2	853	BCR	C17-C18-C19-C20
23	A1	847	BCR	C11-C12-C13-C14
23	F	303	BCR	C7-C8-C9-C10
28	BB	854	DGD	O1G-C1G-C2G-C3G
25	I2	105	LMG	O1-C7-C8-C9
25	I2	105	LMG	C7-C8-C9-O8
19	A	801	CLA	C3-C5-C6-C7
19	AA	801	CLA	C3-C5-C6-C7
19	AA	821	CLA	C16-C17-C18-C19
22	A2	845	LHG	C33-C34-C35-C36
25	I2	105	LMG	C13-C14-C15-C16
23	II	104	BCR	C14-C15-C16-C17
23	I2	103	BCR	C14-C15-C16-C17
19	A	829	CLA	CAA-CBA-CGA-O2A
19	B1	821	CLA	CAA-CBA-CGA-O2A
19	AA	840	CLA	CAA-CBA-CGA-O2A
19	A2	822	CLA	CAA-CBA-CGA-O2A
22	X1	103	LHG	C28-C29-C30-C31
19	L	204	CLA	C4C-C3C-CAC-CBC
23	A2	851	BCR	C16-C17-C18-C19
23	I1	101	BCR	C11-C10-C9-C8
23	II	102	BCR	C20-C21-C22-C23
23	BB	841	BCR	C20-C21-C22-C23
23	A1	850	BCR	C20-C21-C22-C23
22	B1	847	LHG	C24-C25-C26-C27
19	AA	830	CLA	CAA-CBA-CGA-O2A
22	XX	102	LHG	C27-C28-C29-C30
25	I2	105	LMG	C20-C21-C22-C23
19	AA	842	CLA	C16-C17-C18-C19
19	B2	836	CLA	C16-C17-C18-C19
22	A1	846	LHG	C14-C15-C16-C17
19	A	827	CLA	C2A-CAA-CBA-CGA
19	A1	807	CLA	C2A-CAA-CBA-CGA
19	B1	848	CLA	C2-C3-C5-C6
20	A2	803	CL0	C2-C3-C5-C6
24	L2	203	AJP	CCW-CCX-OCY-CCZ
22	A	845	LHG	O7-C5-C6-O8
19	AA	821	CLA	C16-C17-C18-C20
19	B2	837	CLA	C11-C12-C13-C15
19	B2	852	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
19	B2	824	CLA	C2-C1-O2A-CGA
22	BB	850	LHG	C1-C2-C3-O3
19	A2	830	CLA	CBA-CGA-O2A-C1
19	B1	821	CLA	C5-C6-C7-C8
19	L2	204	CLA	C8-C10-C11-C12
19	L1	205	CLA	C8-C10-C11-C12
19	A	831	CLA	CAA-CBA-CGA-O2A
22	B1	847	LHG	C25-C26-C27-C28
19	A	820	CLA	C5-C6-C7-C8
19	A	852	CLA	C5-C6-C7-C8
19	B2	822	CLA	C16-C17-C18-C19
19	A	842	CLA	C16-C17-C18-C19
19	B	808	CLA	C6-C7-C8-C10
19	BB	825	CLA	C12-C13-C15-C16
19	AA	810	CLA	C11-C12-C13-C15
19	A2	842	CLA	C6-C7-C8-C10
19	BB	802	CLA	C6-C7-C8-C10
19	B	837	CLA	C6-C7-C8-C10
19	AA	819	CLA	C11-C10-C8-C7
19	A2	852	CLA	C11-C12-C13-C15
19	A	852	CLA	C11-C12-C13-C15
19	B	802	CLA	C6-C7-C8-C10
22	X	102	LHG	C27-C28-C29-C30
19	B2	836	CLA	C3-C5-C6-C7
19	BB	856	CLA	CHA-CBD-CGD-O1D
19	BB	801	CLA	CHA-CBD-CGD-O1D
19	BB	801	CLA	CHA-CBD-CGD-O2D
19	B	834	CLA	CHA-CBD-CGD-O1D
19	B	834	CLA	CHA-CBD-CGD-O2D
19	A1	816	CLA	CHA-CBD-CGD-O2D
19	B2	822	CLA	CHA-CBD-CGD-O2D
19	B2	835	CLA	CHA-CBD-CGD-O2D
19	B	807	CLA	CHA-CBD-CGD-O1D
19	B	807	CLA	CHA-CBD-CGD-O2D
19	BB	808	CLA	CHA-CBD-CGD-O1D
19	BB	808	CLA	CHA-CBD-CGD-O2D
19	LL	203	CLA	CHA-CBD-CGD-O2D
19	BB	814	CLA	CHA-CBD-CGD-O1D
19	BB	814	CLA	CHA-CBD-CGD-O2D
19	A2	837	CLA	CHA-CBD-CGD-O1D
19	A2	837	CLA	CHA-CBD-CGD-O2D
19	A	830	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A	830	CLA	CHA-CBD-CGD-O2D
19	A2	820	CLA	CHA-CBD-CGD-O1D
19	A2	820	CLA	CHA-CBD-CGD-O2D
19	AA	820	CLA	CHA-CBD-CGD-O1D
19	AA	820	CLA	CHA-CBD-CGD-O2D
19	BB	807	CLA	CHA-CBD-CGD-O1D
19	BB	807	CLA	CHA-CBD-CGD-O2D
19	B2	807	CLA	CHA-CBD-CGD-O1D
19	B2	807	CLA	CHA-CBD-CGD-O2D
19	B	816	CLA	CHA-CBD-CGD-O1D
19	B1	801	CLA	CHA-CBD-CGD-O1D
19	B	859	CLA	CHA-CBD-CGD-O1D
19	AA	853	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O1D
19	B	814	CLA	CHA-CBD-CGD-O2D
19	B2	851	CLA	CHA-CBD-CGD-O2D
19	A1	829	CLA	CHA-CBD-CGD-O1D
19	A1	829	CLA	CHA-CBD-CGD-O2D
19	AA	816	CLA	CHA-CBD-CGD-O2D
19	B2	801	CLA	CHA-CBD-CGD-O1D
19	B	801	CLA	CHA-CBD-CGD-O1D
19	B	837	CLA	CHA-CBD-CGD-O1D
19	B	837	CLA	CHA-CBD-CGD-O2D
19	F	301	CLA	CHA-CBD-CGD-O2D
19	A	820	CLA	CHA-CBD-CGD-O1D
19	A	820	CLA	CHA-CBD-CGD-O2D
19	A1	831	CLA	CHA-CBD-CGD-O1D
19	A1	831	CLA	CHA-CBD-CGD-O2D
19	A	832	CLA	CHA-CBD-CGD-O1D
19	A	832	CLA	CHA-CBD-CGD-O2D
19	B1	815	CLA	CHA-CBD-CGD-O2D
19	B1	816	CLA	CHA-CBD-CGD-O1D
19	B1	807	CLA	CHA-CBD-CGD-O2D
19	A2	830	CLA	CHA-CBD-CGD-O1D
19	A2	830	CLA	CHA-CBD-CGD-O2D
19	B1	812	CLA	CHA-CBD-CGD-O1D
19	B1	812	CLA	CHA-CBD-CGD-O2D
19	A	833	CLA	CHA-CBD-CGD-O1D
19	A	833	CLA	CHA-CBD-CGD-O2D
19	A1	822	CLA	CHA-CBD-CGD-O2D
19	A	852	CLA	CHA-CBD-CGD-O2D
19	A2	836	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
19	A2	836	CLA	CHA-CBD-CGD-O2D
19	B1	827	CLA	CHA-CBD-CGD-O1D
19	B1	827	CLA	CHA-CBD-CGD-O2D
19	A2	831	CLA	CAA-CBA-CGA-O2A
19	B2	810	CLA	CAA-CBA-CGA-O2A
28	BB	854	DGD	C4E-C5E-C6E-O5E
19	B1	824	CLA	C2A-CAA-CBA-CGA
19	B2	810	CLA	C2A-CAA-CBA-CGA
19	AA	827	CLA	C2A-CAA-CBA-CGA
23	B2	843	BCR	C9-C10-C11-C12
23	BB	839	BCR	C13-C14-C15-C16
23	LL	204	BCR	C18-C19-C20-C21
22	B	853	LHG	C25-C26-C27-C28
19	A2	829	CLA	C4C-C3C-CAC-CBC
19	A1	828	CLA	C16-C17-C18-C19
22	BB	850	LHG	O1-C1-C2-O2
22	B	852	LHG	O1-C1-C2-O2
22	X2	102	LHG	O9-C7-O7-C5
22	X2	103	LHG	C34-C35-C36-C37
23	B	848	BCR	C22-C23-C24-C25
23	B	842	BCR	C22-C23-C24-C25
23	A1	849	BCR	C6-C7-C8-C9
23	I1	101	BCR	C22-C23-C24-C25
19	A2	828	CLA	CAA-CBA-CGA-O2A
19	BB	808	CLA	C6-C7-C8-C9
19	A	810	CLA	C14-C13-C15-C16
19	B1	808	CLA	C6-C7-C8-C9
20	A1	802	CL0	C11-C10-C8-C9
19	A	806	CLA	C6-C7-C8-C9
19	B	806	CLA	C14-C13-C15-C16
19	A1	818	CLA	C11-C10-C8-C9
19	B2	804	CLA	C11-C10-C8-C9
19	BB	821	CLA	C11-C10-C8-C9
19	A	842	CLA	C11-C10-C8-C9
19	A	819	CLA	C11-C10-C8-C9
19	B2	834	CLA	C11-C10-C8-C9
19	A	821	CLA	C11-C10-C8-C9
19	B2	831	CLA	C6-C7-C8-C9
19	B	837	CLA	C6-C7-C8-C9
19	B1	830	CLA	C6-C7-C8-C9
19	A	821	CLA	C16-C17-C18-C19
19	B1	836	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	L	204	CLA	CAA-CBA-CGA-O2A
22	A2	846	LHG	C14-C15-C16-C17
22	X1	103	LHG	C31-C32-C33-C34
19	A2	842	CLA	CAA-CBA-CGA-O1A
19	B1	848	CLA	CAA-CBA-CGA-O1A
19	B	854	CLA	CAA-CBA-CGA-O1A
19	B	810	CLA	C1A-C2A-CAA-CBA
19	L2	204	CLA	C1A-C2A-CAA-CBA
19	BB	832	CLA	C1A-C2A-CAA-CBA
19	BB	811	CLA	C1A-C2A-CAA-CBA
19	L2	206	CLA	C1A-C2A-CAA-CBA
19	XX	101	CLA	C1A-C2A-CAA-CBA
19	AA	833	CLA	C1A-C2A-CAA-CBA
20	A1	802	CL0	C1A-C2A-CAA-CBA
19	A1	832	CLA	C1A-C2A-CAA-CBA
19	A	836	CLA	C1A-C2A-CAA-CBA
19	X2	101	CLA	C1A-C2A-CAA-CBA
19	B2	811	CLA	C1A-C2A-CAA-CBA
19	BB	810	CLA	C1A-C2A-CAA-CBA
19	L1	207	CLA	C1A-C2A-CAA-CBA
19	AA	836	CLA	C1A-C2A-CAA-CBA
19	B2	807	CLA	C1A-C2A-CAA-CBA
19	X1	101	CLA	C1A-C2A-CAA-CBA
19	A2	833	CLA	C1A-C2A-CAA-CBA
19	A1	831	CLA	C1A-C2A-CAA-CBA
19	BB	830	CLA	C1A-C2A-CAA-CBA
19	A	832	CLA	C1A-C2A-CAA-CBA
19	A2	832	CLA	C1A-C2A-CAA-CBA
19	B1	807	CLA	C1A-C2A-CAA-CBA
19	A2	852	CLA	C1A-C2A-CAA-CBA
19	A2	836	CLA	C1A-C2A-CAA-CBA
19	A1	830	CLA	CAA-CBA-CGA-O1A
19	B1	810	CLA	CAA-CBA-CGA-O1A
19	AA	828	CLA	CAA-CBA-CGA-O2A
19	A	830	CLA	CAA-CBA-CGA-O2A
19	A	828	CLA	CAA-CBA-CGA-O2A
19	BB	821	CLA	CAA-CBA-CGA-O2A
19	B2	821	CLA	CAA-CBA-CGA-O2A
25	L1	210	LMG	O7-C10-C11-C12
19	L	203	CLA	CAA-CBA-CGA-O2A
19	A	807	CLA	C15-C16-C17-C18
23	B1	839	BCR	C11-C12-C13-C35

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Mol	Chain	Res	Type	Atoms
19	F	301	CLA	C11-C12-C13-C15
22	L	207	LHG	C13-C14-C15-C16
19	B2	824	CLA	C2A-CAA-CBA-CGA
19	B	860	CLA	CAA-CBA-CGA-O1A
19	AA	842	CLA	CAA-CBA-CGA-O1A
19	AA	830	CLA	CAA-CBA-CGA-O1A
19	A1	828	CLA	CAA-CBA-CGA-O1A
19	A2	822	CLA	CAA-CBA-CGA-O1A
19	B	860	CLA	C5-C6-C7-C8
19	A1	829	CLA	O1A-CGA-O2A-C1
19	B1	836	CLA	C2C-C3C-CAC-CBC
19	A1	839	CLA	CAA-CBA-CGA-O2A
23	B	844	BCR	C7-C8-C9-C10
23	II	104	BCR	C11-C12-C13-C14
23	I2	101	BCR	C11-C12-C13-C14
23	A1	853	BCR	C17-C18-C19-C20
19	A1	830	CLA	C8-C10-C11-C12
19	L	203	CLA	C8-C10-C11-C12
19	A	839	CLA	CAA-CBA-CGA-O1A
19	AA	822	CLA	CAA-CBA-CGA-O1A
25	B	845	LMG	O10-C28-C29-C30
25	BB	844	LMG	O10-C28-C29-C30
19	L	202	CLA	CAA-CBA-CGA-O1A
19	B1	801	CLA	CAA-CBA-CGA-O1A
19	BB	852	CLA	CAA-CBA-CGA-O1A
19	B2	801	CLA	CAA-CBA-CGA-O1A
22	B	852	LHG	O10-C23-C24-C25
22	A2	845	LHG	C18-C19-C20-C21
23	JJ	104	BCR	C15-C16-C17-C18
23	I2	101	BCR	C15-C16-C17-C18
22	L2	208	LHG	C3-O3-P-O5
22	AA	846	LHG	C4-O6-P-O5
22	XX	102	LHG	C3-O3-P-O5
22	A2	845	LHG	C4-O6-P-O5
22	BB	850	LHG	C3-O3-P-O5
22	A	845	LHG	C4-O6-P-O5
22	A1	845	LHG	C4-O6-P-O5
22	B	852	LHG	C4-O6-P-O5
19	B1	821	CLA	CAA-CBA-CGA-O1A
22	BB	850	LHG	O10-C23-C24-C25
19	B2	852	CLA	CAA-CBA-CGA-O1A
19	A	852	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
22	BB	851	LHG	C28-C29-C30-C31
28	B	856	DGD	O1G-C1G-C2G-C3G
19	BB	811	CLA	O1D-CGD-O2D-CED
22	A	845	LHG	C33-C34-C35-C36
19	B1	804	CLA	C10-C11-C12-C13
19	AA	843	CLA	CAA-CBA-CGA-O1A
19	A2	839	CLA	CAA-CBA-CGA-O1A
19	A	830	CLA	CAA-CBA-CGA-O1A
19	A1	841	CLA	CAA-CBA-CGA-O1A
19	A1	842	CLA	CAA-CBA-CGA-O1A
19	A1	821	CLA	CAA-CBA-CGA-O1A
19	A	825	CLA	O1D-CGD-O2D-CED
19	AA	807	CLA	C16-C17-C18-C20
23	I	101	BCR	C14-C15-C16-C17
19	A	829	CLA	CAA-CBA-CGA-O1A
19	AA	831	CLA	CAA-CBA-CGA-O1A
28	B	856	DGD	O1B-C1B-C2B-C3B
19	A1	829	CLA	CAA-CBA-CGA-O1A
19	B2	821	CLA	CAA-CBA-CGA-O1A
19	A2	830	CLA	CAA-CBA-CGA-O1A
19	A2	852	CLA	CAA-CBA-CGA-O1A
19	B2	814	CLA	CBA-CGA-O2A-C1
23	A	848	BCR	C5-C6-C7-C8
23	A	848	BCR	C23-C24-C25-C26
23	A	853	BCR	C1-C6-C7-C8
23	K2	103	BCR	C5-C6-C7-C8
23	K1	106	BCR	C1-C6-C7-C8
23	AA	849	BCR	C5-C6-C7-C8
23	AA	849	BCR	C23-C24-C25-C26
23	J1	102	BCR	C5-C6-C7-C8
23	AA	854	BCR	C1-C6-C7-C8
19	A	820	CLA	C2A-CAA-CBA-CGA
19	B	821	CLA	C5-C6-C7-C8
19	A1	803	CLA	C4-C3-C5-C6
19	B	821	CLA	C2-C3-C5-C6
19	A1	819	CLA	C5-C6-C7-C8
19	AA	828	CLA	CAA-CBA-CGA-O1A
19	AA	839	CLA	CAA-CBA-CGA-O1A
19	A1	852	CLA	CAA-CBA-CGA-O1A
19	A1	838	CLA	CAA-CBA-CGA-O1A
19	AA	836	CLA	C16-C17-C18-C20
19	A2	842	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
22	AA	846	LHG	C25-C26-C27-C28
19	A2	807	CLA	C15-C16-C17-C18
19	BB	814	CLA	CAD-CBD-CGD-O1D
19	AA	821	CLA	CAD-CBD-CGD-O1D
19	A2	820	CLA	CAD-CBD-CGD-O1D
19	AA	820	CLA	CAD-CBD-CGD-O1D
19	AA	836	CLA	CAD-CBD-CGD-O1D
19	JJ	101	CLA	CAD-CBD-CGD-O1D
19	B	816	CLA	CAD-CBD-CGD-O1D
19	AA	853	CLA	CAD-CBD-CGD-O1D
19	A	823	CLA	CAD-CBD-CGD-O1D
19	A	821	CLA	CAD-CBD-CGD-O1D
19	B	820	CLA	CAD-CBD-CGD-O1D
19	BB	820	CLA	CAD-CBD-CGD-O1D
19	A2	822	CLA	CAD-CBD-CGD-O1D
19	B1	816	CLA	CAD-CBD-CGD-O1D
19	A2	830	CLA	CAD-CBD-CGD-O1D
19	A	838	CLA	CAD-CBD-CGD-O1D
19	J1	101	CLA	CAD-CBD-CGD-O1D
19	A	852	CLA	CAD-CBD-CGD-O1D
19	AA	820	CLA	CAA-CBA-CGA-O2A
19	BB	821	CLA	CAA-CBA-CGA-O1A
28	BB	854	DGD	O1B-C1B-C2B-C3B
19	A2	828	CLA	CAA-CBA-CGA-O1A
19	A2	821	CLA	O1D-CGD-O2D-CED
19	J	103	CLA	C4C-C3C-CAC-CBC
19	A2	829	CLA	C15-C16-C17-C18
24	L2	203	AJP	OCC-CCX-OCY-CCZ
19	A	828	CLA	CAA-CBA-CGA-O1A
22	LL	205	LHG	C12-C13-C14-C15
19	B2	852	CLA	C5-C6-C7-C8
19	A2	841	CLA	CAA-CBA-CGA-O2A
25	II	105	LMG	O8-C28-C29-C30
19	B1	824	CLA	CAA-CBA-CGA-O2A
19	FF	301	CLA	CAA-CBA-CGA-O2A
19	B2	822	CLA	C16-C17-C18-C20
19	AA	835	CLA	C16-C17-C18-C20
22	A	846	LHG	C11-C12-C13-C14
19	A	822	CLA	CAA-CBA-CGA-O1A
19	A	842	CLA	CAA-CBA-CGA-O1A
19	AA	840	CLA	CAA-CBA-CGA-O1A
19	A	840	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	B2	845	LMG	O10-C28-C29-C30
19	A1	839	CLA	CAA-CBA-CGA-O1A
22	LL	205	LHG	C13-C14-C15-C16
22	X1	102	LHG	C29-C30-C31-C32
19	B	815	CLA	C5-C6-C7-C8
19	A1	842	CLA	C5-C6-C7-C8
28	BB	854	DGD	O2G-C1B-C2B-C3B
22	BB	850	LHG	O7-C7-C8-C9
19	BB	802	CLA	CAA-CBA-CGA-O2A
19	A2	820	CLA	C2A-CAA-CBA-CGA
22	AA	847	LHG	C11-C12-C13-C14
19	B1	808	CLA	C2-C1-O2A-CGA
19	A1	827	CLA	CAA-CBA-CGA-O1A
19	FF	301	CLA	CAA-CBA-CGA-O1A
19	AA	807	CLA	C16-C17-C18-C19
19	B	806	CLA	C13-C15-C16-C17
19	B	804	CLA	C10-C11-C12-C13
22	L	207	LHG	C12-C13-C14-C15
19	B2	824	CLA	CAA-CBA-CGA-O2A
19	B	821	CLA	CAA-CBA-CGA-O2A
19	B1	802	CLA	CAA-CBA-CGA-O2A
19	LL	202	CLA	CAA-CBA-CGA-O2A
25	B1	846	LMG	C14-C15-C16-C17
22	B2	848	LHG	C2-C3-O3-P
19	A2	841	CLA	CAA-CBA-CGA-O1A
22	A1	845	LHG	C16-C17-C18-C19
19	L2	206	CLA	C8-C10-C11-C12
19	B	808	CLA	C6-C7-C8-C9
19	AA	810	CLA	C11-C12-C13-C14
19	AA	810	CLA	C14-C13-C15-C16
19	B2	807	CLA	C11-C12-C13-C14
19	B	801	CLA	C11-C10-C8-C9
19	B2	808	CLA	C6-C7-C8-C9
19	AA	819	CLA	C11-C10-C8-C9
19	B1	807	CLA	C11-C12-C13-C14
19	L	203	CLA	C3-C5-C6-C7
19	A1	840	CLA	CAA-CBA-CGA-O1A
19	B	821	CLA	CAA-CBA-CGA-O1A
19	B	801	CLA	CAA-CBA-CGA-O1A
25	B1	844	LMG	O10-C28-C29-C30
19	B	801	CLA	CAA-CBA-CGA-O2A
19	B	803	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
19	B2	822	CLA	C11-C10-C8-C7
19	B	807	CLA	C6-C7-C8-C10
19	A	810	CLA	C11-C12-C13-C15
19	A	810	CLA	C12-C13-C15-C16
19	B1	808	CLA	C6-C7-C8-C10
19	A2	821	CLA	C11-C10-C8-C7
19	A1	818	CLA	C6-C7-C8-C10
19	AA	821	CLA	C11-C10-C8-C7
19	AA	807	CLA	C11-C10-C8-C7
19	BB	807	CLA	C6-C7-C8-C10
19	BB	826	CLA	C11-C12-C13-C15
19	B2	816	CLA	C6-C7-C8-C10
19	BB	822	CLA	C11-C10-C8-C7
19	B1	848	CLA	C6-C7-C8-C10
19	BB	804	CLA	C11-C10-C8-C7
19	B2	808	CLA	C6-C7-C8-C10
19	A2	829	CLA	C11-C12-C13-C15
19	B2	826	CLA	C11-C12-C13-C15
19	L	204	CLA	C12-C13-C15-C16
19	AA	843	CLA	C5-C6-C7-C8
19	A2	808	CLA	C5-C6-C7-C8
19	A2	840	CLA	CAA-CBA-CGA-O1A
19	A2	831	CLA	CAA-CBA-CGA-O1A
19	AA	853	CLA	CAA-CBA-CGA-O1A
19	BB	802	CLA	CAA-CBA-CGA-O1A
19	LL	202	CLA	CAA-CBA-CGA-O1A
19	AA	829	CLA	CAA-CBA-CGA-O1A
19	A2	840	CLA	CAA-CBA-CGA-O2A
25	I1	102	LMG	O7-C10-C11-C12
19	L1	205	CLA	CAA-CBA-CGA-O2A
19	AA	853	CLA	CAA-CBA-CGA-O2A
19	AA	829	CLA	CAA-CBA-CGA-O2A
19	B2	814	CLA	O1A-CGA-O2A-C1
19	BB	810	CLA	C3A-C2A-CAA-CBA
19	F2	301	CLA	C3A-C2A-CAA-CBA
19	F1	301	CLA	C3A-C2A-CAA-CBA
19	BB	833	CLA	C3A-C2A-CAA-CBA
19	K1	102	CLA	C3A-C2A-CAA-CBA
19	B2	821	CLA	C5-C6-C7-C8
19	B2	821	CLA	C13-C15-C16-C17
19	A1	809	CLA	C5-C6-C7-C8
22	A1	845	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
19	B2	810	CLA	CAA-CBA-CGA-O1A
19	B2	826	CLA	C2A-CAA-CBA-CGA
22	AA	846	LHG	C11-C12-C13-C14
19	A1	840	CLA	CAA-CBA-CGA-O2A
19	B1	802	CLA	CAA-CBA-CGA-O1A

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	855	AJP	CCE-CCF-CCG-CCZ-CDA-CDB

350 monomers are involved in 569 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	801	CLA	1	0
20	A	803	CL0	1	0
19	A	804	CLA	3	0
19	A	805	CLA	3	0
19	A	806	CLA	2	0
19	A	807	CLA	3	0
19	A	809	CLA	1	0
19	A	810	CLA	1	0
19	A	812	CLA	1	0
19	A	813	CLA	1	0
19	A	815	CLA	3	0
19	A	816	CLA	1	0
19	A	818	CLA	1	0
19	A	820	CLA	2	0
19	A	821	CLA	1	0
19	A	822	CLA	3	0
19	A	824	CLA	1	0
19	A	826	CLA	2	0
19	A	828	CLA	1	0
19	A	830	CLA	4	0
19	A	831	CLA	1	0
19	A	832	CLA	3	0
19	A	833	CLA	2	0
19	A	834	CLA	1	0
19	A	836	CLA	1	0
19	A	837	CLA	2	0
19	A	840	CLA	1	0
19	A	841	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	A	842	CLA	2	0
21	A	843	PQN	3	0
22	A	845	LHG	2	0
22	A	846	LHG	1	0
23	A	847	BCR	1	0
23	A	851	BCR	4	0
19	A	852	CLA	11	0
23	A	854	BCR	2	0
19	A1	801	CLA	1	0
20	A1	802	CL0	3	0
19	A1	803	CLA	3	0
19	A1	804	CLA	2	0
19	A1	805	CLA	2	0
19	A1	806	CLA	4	0
19	A1	807	CLA	1	0
19	A1	811	CLA	2	0
19	A1	812	CLA	1	0
19	A1	814	CLA	4	0
19	A1	815	CLA	2	0
19	A1	816	CLA	1	0
19	A1	817	CLA	2	0
19	A1	819	CLA	2	0
19	A1	820	CLA	3	0
19	A1	822	CLA	1	0
19	A1	824	CLA	1	0
19	A1	826	CLA	1	0
19	A1	827	CLA	1	0
19	A1	828	CLA	3	0
19	A1	829	CLA	3	0
19	A1	830	CLA	1	0
19	A1	831	CLA	2	0
19	A1	832	CLA	1	0
19	A1	833	CLA	2	0
19	A1	834	CLA	2	0
19	A1	835	CLA	1	0
19	A1	836	CLA	1	0
19	A1	839	CLA	2	0
19	A1	840	CLA	1	0
19	A1	841	CLA	3	0
19	A1	842	CLA	1	0
21	A1	843	PQN	1	0
19	A1	844	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
22	A1	846	LHG	1	0
23	A1	847	BCR	2	0
23	A1	850	BCR	1	0
23	A1	851	BCR	3	0
19	A1	852	CLA	11	0
19	A2	801	CLA	1	0
19	A2	802	CLA	1	0
20	A2	803	CL0	5	0
19	A2	804	CLA	3	0
19	A2	805	CLA	3	0
19	A2	806	CLA	3	0
19	A2	807	CLA	2	0
19	A2	812	CLA	1	0
19	A2	813	CLA	1	0
19	A2	815	CLA	4	0
19	A2	816	CLA	1	0
19	A2	818	CLA	2	0
19	A2	820	CLA	1	0
19	A2	821	CLA	4	0
19	A2	825	CLA	1	0
19	A2	826	CLA	1	0
19	A2	828	CLA	1	0
19	A2	829	CLA	1	0
19	A2	830	CLA	2	0
19	A2	831	CLA	1	0
19	A2	832	CLA	2	0
19	A2	833	CLA	2	0
19	A2	834	CLA	1	0
19	A2	835	CLA	1	0
19	A2	836	CLA	1	0
19	A2	840	CLA	1	0
19	A2	841	CLA	1	0
19	A2	842	CLA	4	0
21	A2	843	PQN	1	0
19	A2	844	CLA	1	0
22	A2	845	LHG	1	0
22	A2	846	LHG	1	0
23	A2	847	BCR	1	0
23	A2	850	BCR	1	0
23	A2	851	BCR	5	0
19	A2	852	CLA	9	0
19	AA	801	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	AA	803	CL0	1	0
19	AA	804	CLA	3	0
19	AA	805	CLA	2	0
19	AA	806	CLA	2	0
19	AA	807	CLA	3	0
19	AA	810	CLA	1	0
19	AA	813	CLA	1	0
19	AA	815	CLA	3	0
19	AA	816	CLA	1	0
19	AA	818	CLA	2	0
19	AA	820	CLA	1	0
19	AA	821	CLA	3	0
19	AA	822	CLA	2	0
19	AA	825	CLA	1	0
19	AA	826	CLA	4	0
19	AA	828	CLA	3	0
19	AA	830	CLA	5	0
19	AA	831	CLA	1	0
19	AA	832	CLA	1	0
19	AA	833	CLA	1	0
19	AA	836	CLA	1	0
19	AA	842	CLA	2	0
19	AA	843	CLA	1	0
21	AA	844	PQN	3	0
19	AA	845	CLA	1	0
22	AA	846	LHG	2	0
22	AA	847	LHG	1	0
23	AA	848	BCR	1	0
23	AA	851	BCR	1	0
23	AA	852	BCR	4	0
19	AA	853	CLA	6	0
23	AA	854	BCR	1	0
23	AA	855	BCR	1	0
19	B	801	CLA	1	0
19	B	802	CLA	2	0
19	B	804	CLA	2	0
19	B	806	CLA	3	0
19	B	809	CLA	1	0
19	B	810	CLA	2	0
19	B	811	CLA	2	0
19	B	813	CLA	1	0
19	B	815	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B	818	CLA	3	0
19	B	820	CLA	5	0
19	B	821	CLA	1	0
19	B	822	CLA	2	0
19	B	823	CLA	1	0
19	B	824	CLA	1	0
19	B	826	CLA	2	0
19	B	827	CLA	1	0
19	B	828	CLA	3	0
19	B	829	CLA	3	0
19	B	830	CLA	4	0
19	B	831	CLA	1	0
19	B	832	CLA	2	0
19	B	833	CLA	7	0
19	B	834	CLA	14	0
19	B	835	CLA	8	0
19	B	836	CLA	2	0
19	B	837	CLA	2	0
21	B	838	PQN	2	0
23	B	839	BCR	2	0
26	B	841	ECH	1	0
23	B	842	BCR	5	0
23	B	843	BCR	4	0
23	B	844	BCR	1	0
24	B	849	AJP	1	0
22	B	852	LHG	1	0
19	B	854	CLA	6	0
28	B	856	DGD	1	0
19	B	858	CLA	3	0
19	B	859	CLA	3	0
19	B	860	CLA	2	0
19	B1	802	CLA	1	0
19	B1	804	CLA	2	0
19	B1	806	CLA	1	0
19	B1	807	CLA	1	0
19	B1	808	CLA	1	0
19	B1	809	CLA	1	0
19	B1	810	CLA	3	0
19	B1	811	CLA	2	0
19	B1	813	CLA	1	0
19	B1	814	CLA	1	0
19	B1	815	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B1	820	CLA	1	0
19	B1	821	CLA	1	0
19	B1	822	CLA	1	0
19	B1	823	CLA	1	0
19	B1	824	CLA	1	0
19	B1	826	CLA	1	0
19	B1	827	CLA	2	0
19	B1	828	CLA	3	0
19	B1	829	CLA	2	0
19	B1	830	CLA	1	0
19	B1	831	CLA	3	0
19	B1	832	CLA	5	0
19	B1	833	CLA	14	0
19	B1	834	CLA	9	0
19	B1	835	CLA	1	0
19	B1	836	CLA	1	0
23	B1	838	BCR	1	0
23	B1	839	BCR	1	0
26	B1	840	ECH	1	0
23	B1	841	BCR	2	0
23	B1	842	BCR	3	0
19	B1	845	CLA	1	0
22	B1	847	LHG	1	0
19	B1	848	CLA	6	0
19	B1	849	CLA	1	0
19	B1	850	CLA	2	0
19	B2	802	CLA	1	0
19	B2	804	CLA	1	0
19	B2	806	CLA	2	0
19	B2	808	CLA	1	0
19	B2	809	CLA	1	0
19	B2	810	CLA	3	0
19	B2	811	CLA	2	0
19	B2	813	CLA	1	0
19	B2	816	CLA	1	0
19	B2	820	CLA	1	0
19	B2	821	CLA	3	0
19	B2	822	CLA	1	0
19	B2	823	CLA	1	0
19	B2	826	CLA	2	0
19	B2	827	CLA	1	0
19	B2	828	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	B2	829	CLA	3	0
19	B2	830	CLA	3	0
19	B2	831	CLA	1	0
19	B2	832	CLA	3	0
19	B2	833	CLA	3	0
19	B2	834	CLA	4	0
19	B2	835	CLA	3	0
19	B2	836	CLA	1	0
19	B2	837	CLA	1	0
23	B2	839	BCR	1	0
23	B2	840	BCR	1	0
26	B2	841	ECH	1	0
23	B2	842	BCR	4	0
23	B2	843	BCR	3	0
19	B2	846	CLA	1	0
19	B2	849	CLA	5	0
19	B2	850	CLA	3	0
19	B2	851	CLA	2	0
19	B2	852	CLA	2	0
19	BB	801	CLA	1	0
19	BB	802	CLA	1	0
19	BB	804	CLA	2	0
19	BB	805	CLA	1	0
19	BB	806	CLA	2	0
19	BB	810	CLA	4	0
19	BB	811	CLA	1	0
19	BB	812	CLA	1	0
19	BB	813	CLA	1	0
19	BB	815	CLA	2	0
19	BB	817	CLA	1	0
19	BB	820	CLA	5	0
19	BB	821	CLA	2	0
19	BB	822	CLA	2	0
19	BB	823	CLA	2	0
19	BB	826	CLA	2	0
19	BB	828	CLA	3	0
19	BB	829	CLA	4	0
19	BB	831	CLA	1	0
19	BB	832	CLA	7	0
19	BB	833	CLA	14	0
19	BB	834	CLA	6	0
19	BB	835	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
19	BB	836	CLA	1	0
21	BB	837	PQN	2	0
23	BB	838	BCR	2	0
26	BB	840	ECH	1	0
23	BB	841	BCR	6	0
23	BB	842	BCR	2	0
24	BB	848	AJP	1	0
19	BB	852	CLA	6	0
28	BB	854	DGD	1	0
19	BB	856	CLA	3	0
27	C	102	SF4	1	0
27	C1	102	SF4	1	0
19	F	301	CLA	3	0
19	F	302	CLA	1	0
23	F	303	BCR	2	0
23	F	305	BCR	6	0
19	F1	301	CLA	3	0
19	F1	302	CLA	1	0
23	F1	303	BCR	2	0
19	F1	305	CLA	2	0
23	F1	306	BCR	5	0
19	F2	301	CLA	3	0
19	F2	302	CLA	1	0
23	F2	303	BCR	2	0
23	F2	305	BCR	5	0
19	FF	301	CLA	3	0
19	FF	302	CLA	1	0
23	FF	303	BCR	3	0
19	FF	305	CLA	3	0
23	FF	306	BCR	4	0
23	I1	101	BCR	1	0
23	I2	103	BCR	1	0
25	I2	105	LMG	1	0
23	J	102	BCR	1	0
19	J	103	CLA	4	0
23	J	104	BCR	1	0
23	J1	102	BCR	1	0
19	J1	103	CLA	1	0
23	J1	104	BCR	1	0
23	J2	102	BCR	1	0
19	J2	103	CLA	2	0
23	J2	104	BCR	2	0

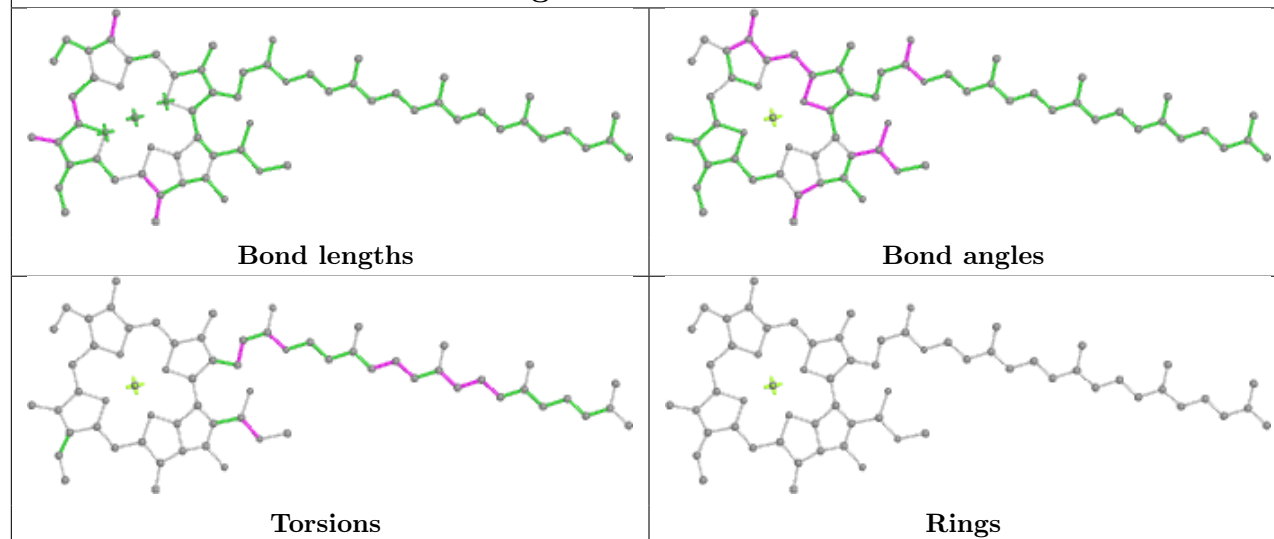
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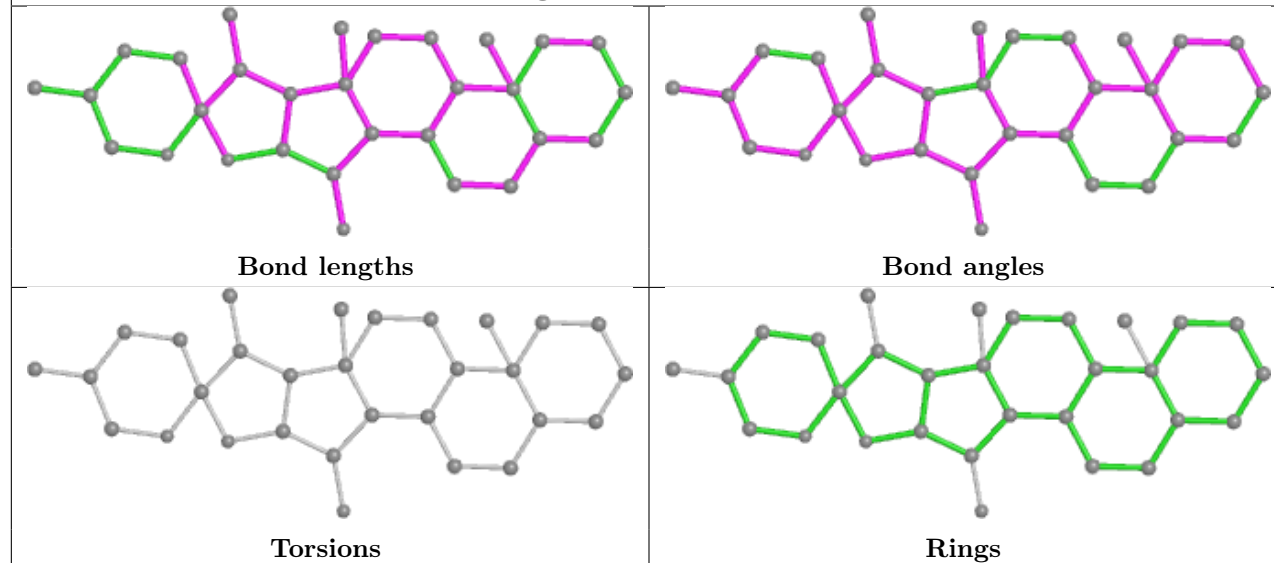
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	JJ	102	BCR	1	0
19	JJ	103	CLA	1	0
23	JJ	104	BCR	1	0
19	K1	103	CLA	1	0
23	K1	104	BCR	1	0
19	K1	105	CLA	1	0
23	K1	106	BCR	2	0
23	K2	103	BCR	1	0
19	K2	104	CLA	1	0
23	K2	105	BCR	2	0
19	L	202	CLA	4	0
23	L	205	BCR	1	0
24	L1	204	AJP	1	0
19	L1	205	CLA	3	0
19	L1	206	CLA	1	0
19	L1	207	CLA	1	0
25	L1	210	LMG	1	0
22	L1	211	LHG	3	0
24	L2	203	AJP	1	0
22	L2	208	LHG	2	0
19	LL	201	CLA	5	0
19	LL	202	CLA	1	0
19	LL	203	CLA	1	0
23	LL	204	BCR	1	0
23	M	101	BCR	2	0
25	M	102	LMG	1	0
23	MM	101	BCR	1	0
19	X2	101	CLA	1	0

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

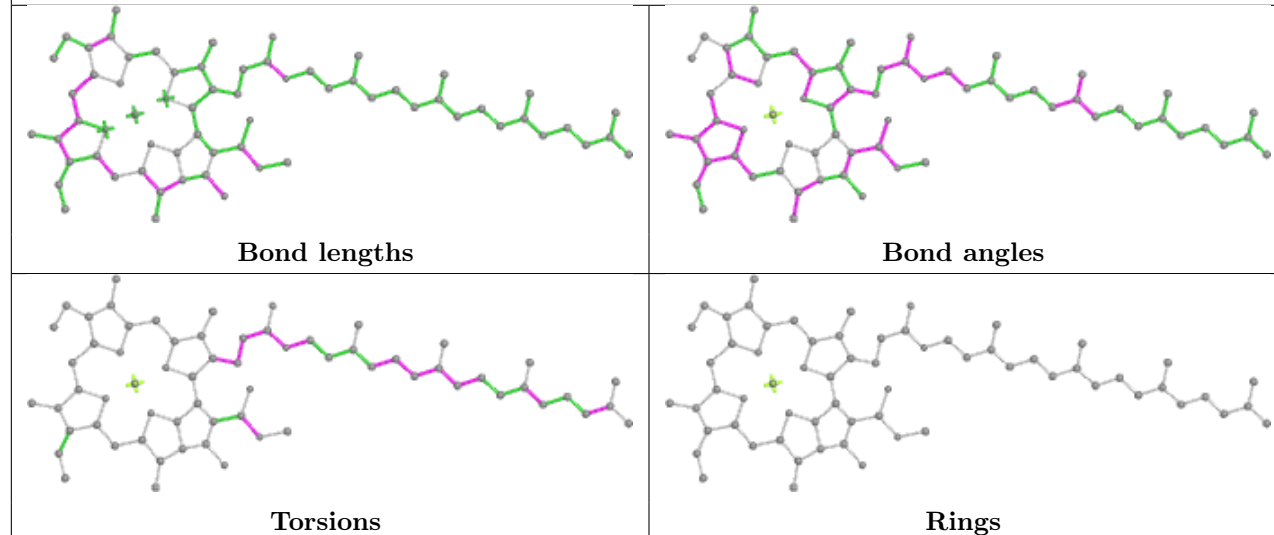
Ligand CLA A 801



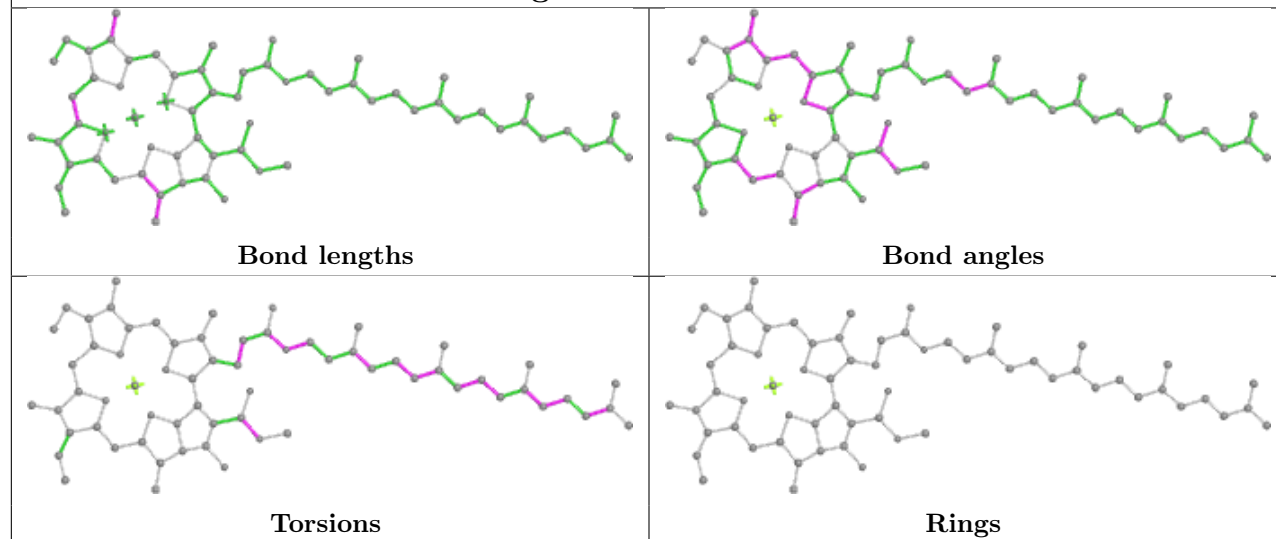
Ligand AJP A 802



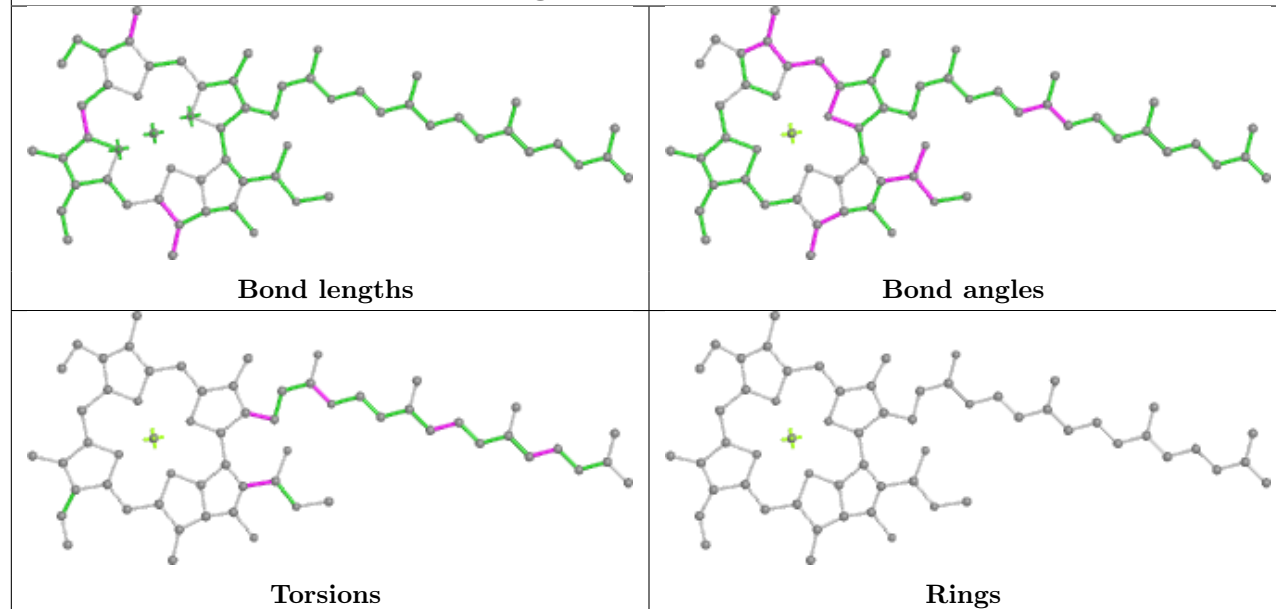
Ligand CL0 A 803



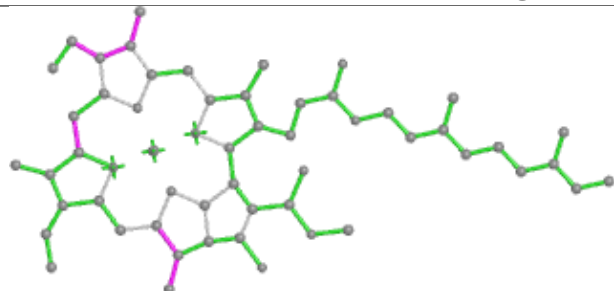
Ligand CLA A 804



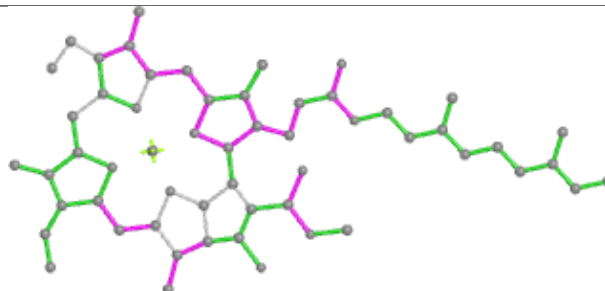
Ligand CLA A 805



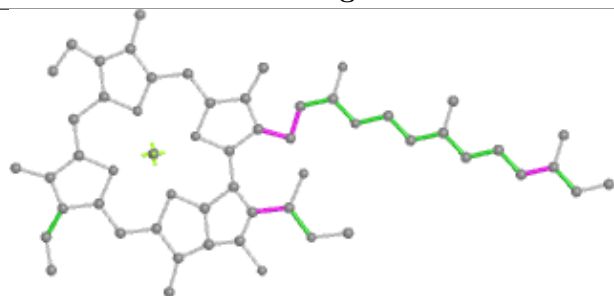
Ligand CLA A 806



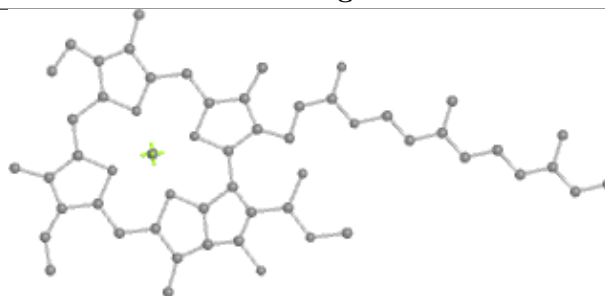
Bond lengths



Bond angles

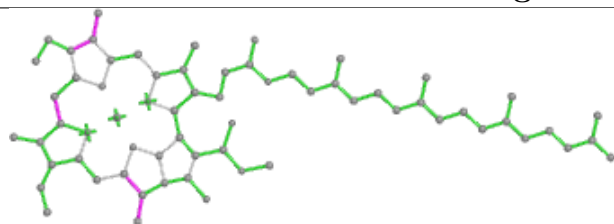


Torsions

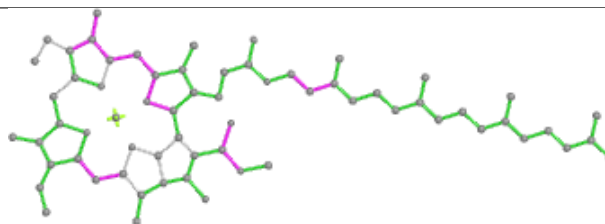


Rings

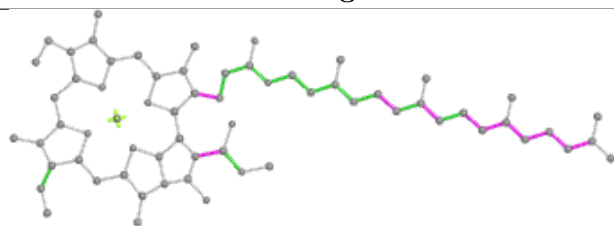
Ligand CLA A 807



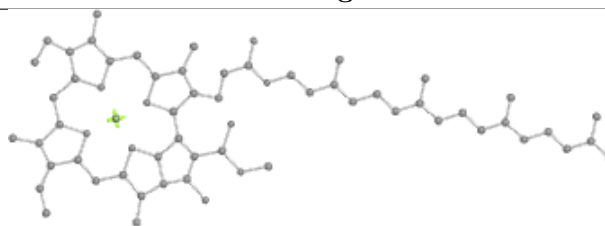
Bond lengths



Bond angles

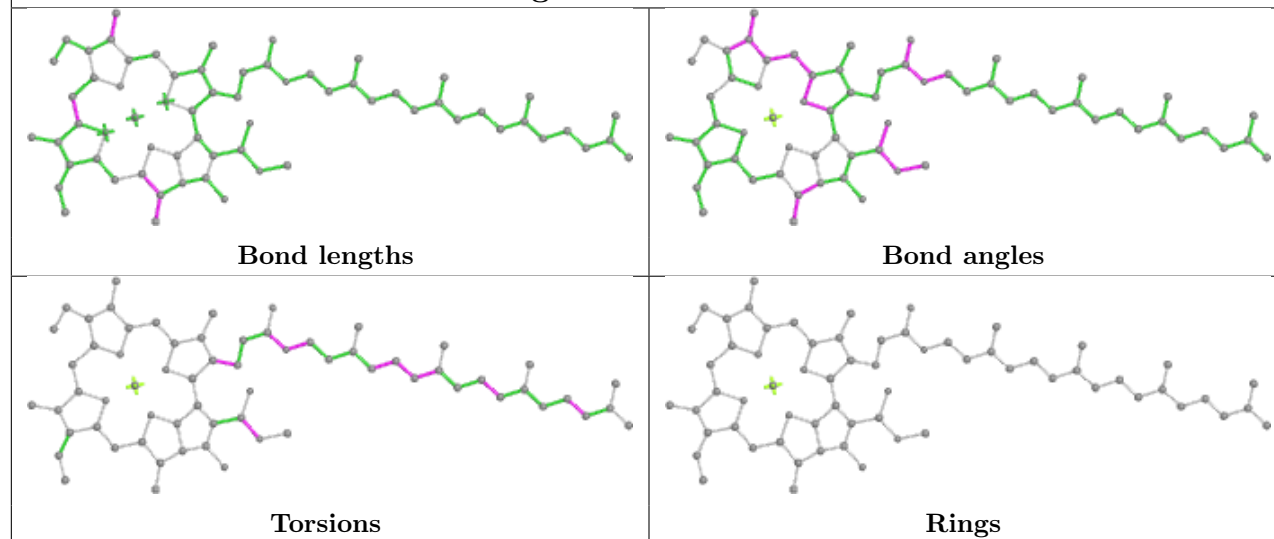


Torsions

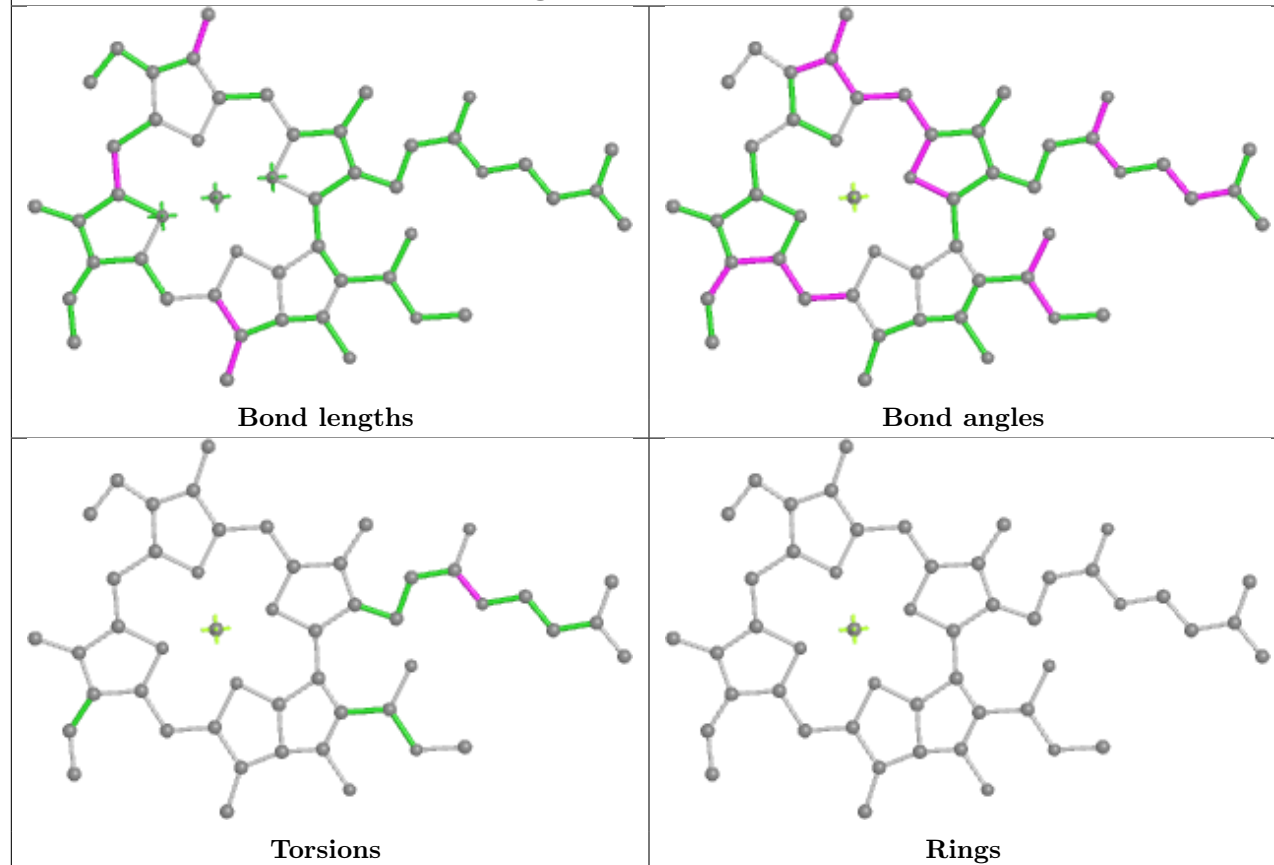


Rings

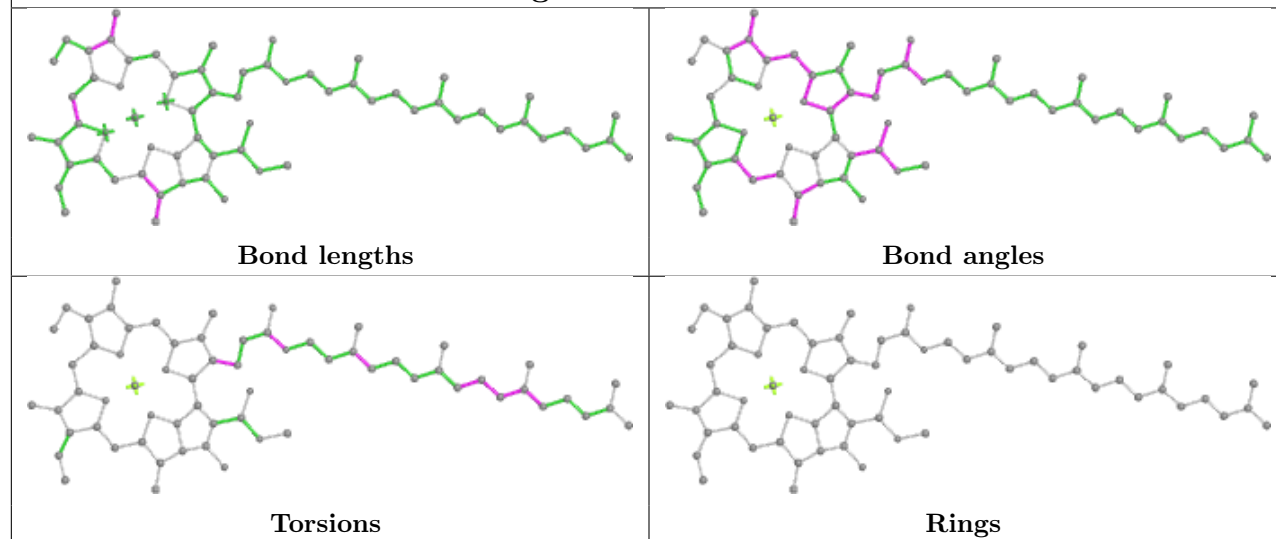
Ligand CLA A 808



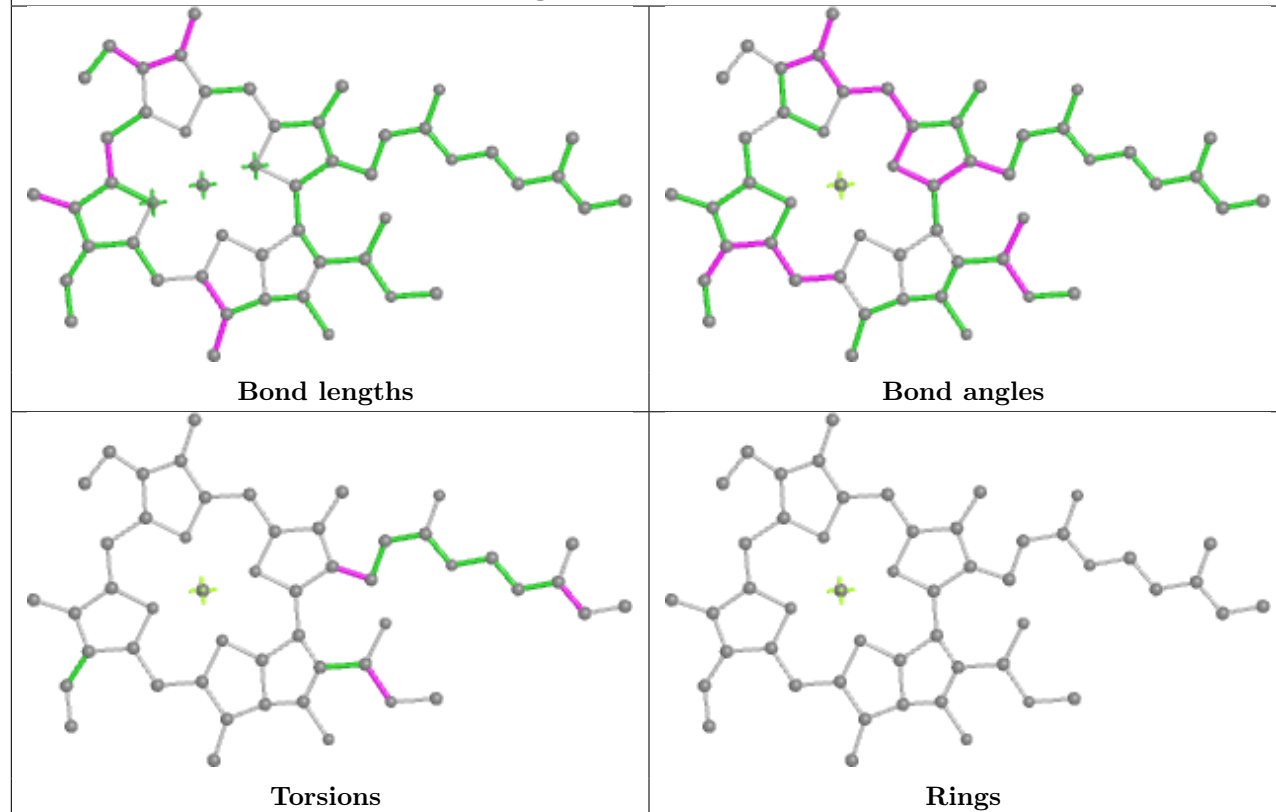
Ligand CLA A 809



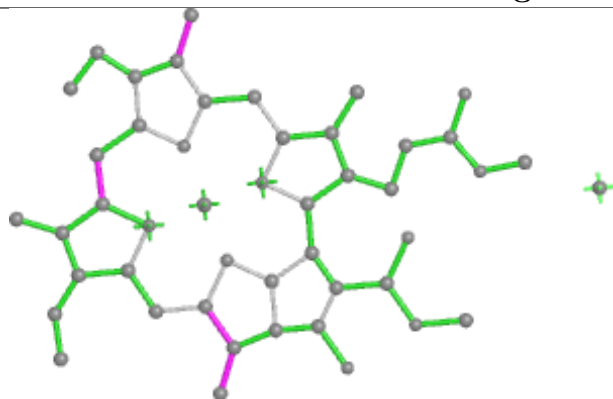
Ligand CLA A 810



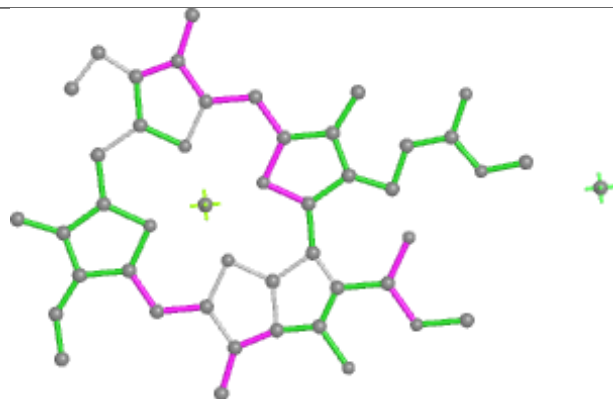
Ligand CLA A 811



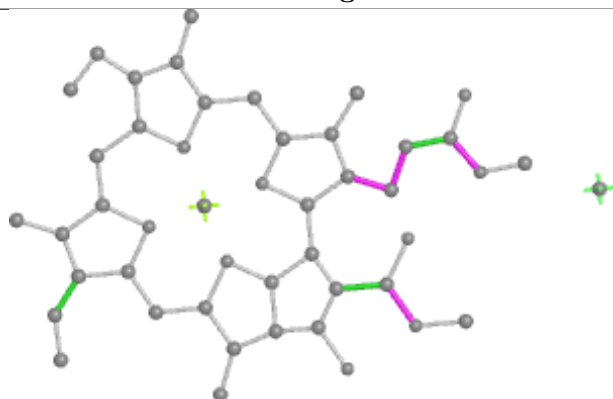
Ligand CLA A 812



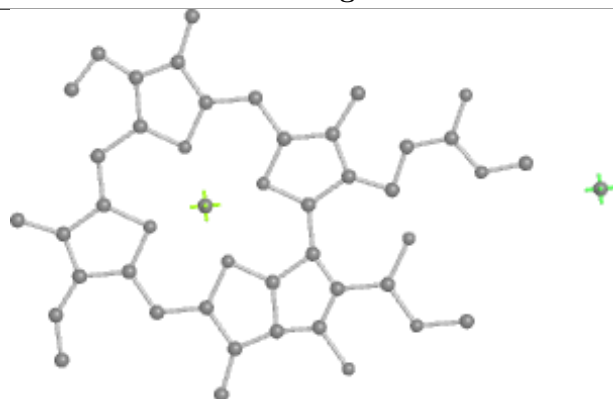
Bond lengths



Bond angles

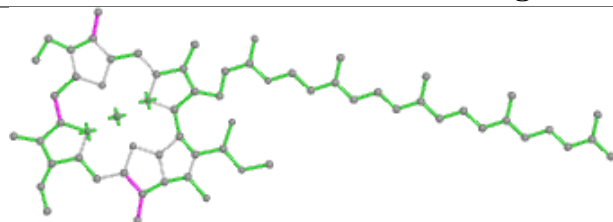


Torsions

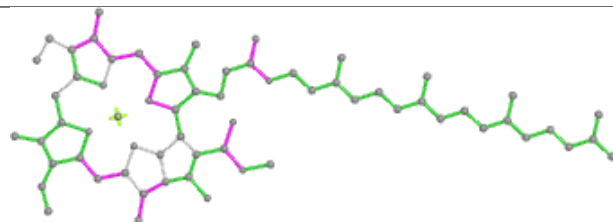


Rings

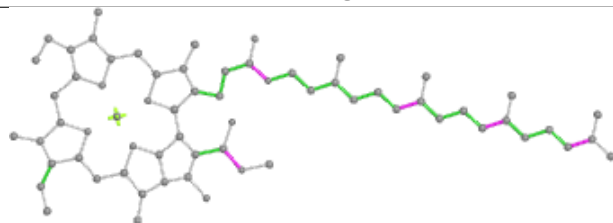
Ligand CLA A 813



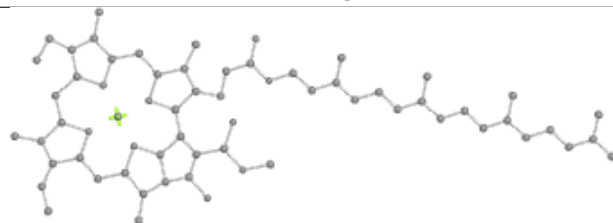
Bond lengths



Bond angles

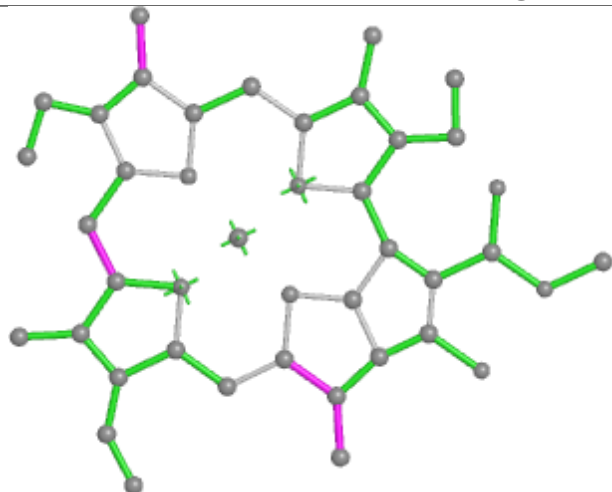


Torsions

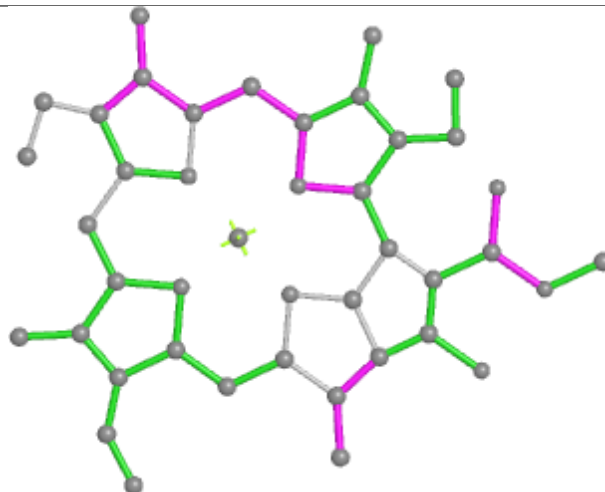


Rings

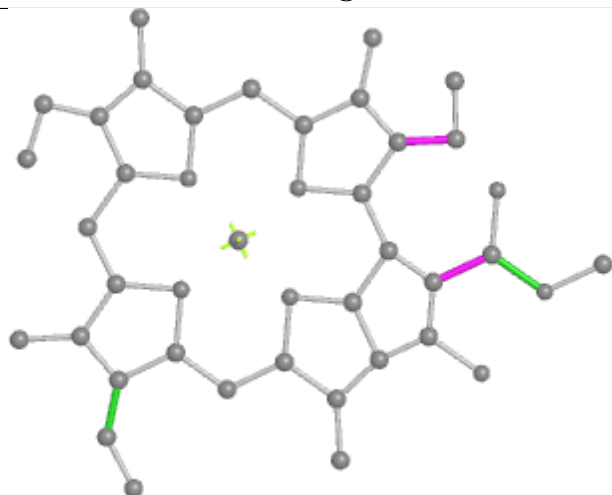
Ligand CLA A 814



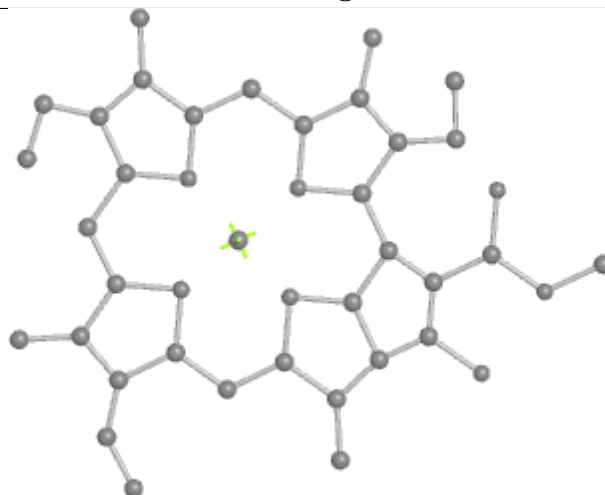
Bond lengths



Bond angles

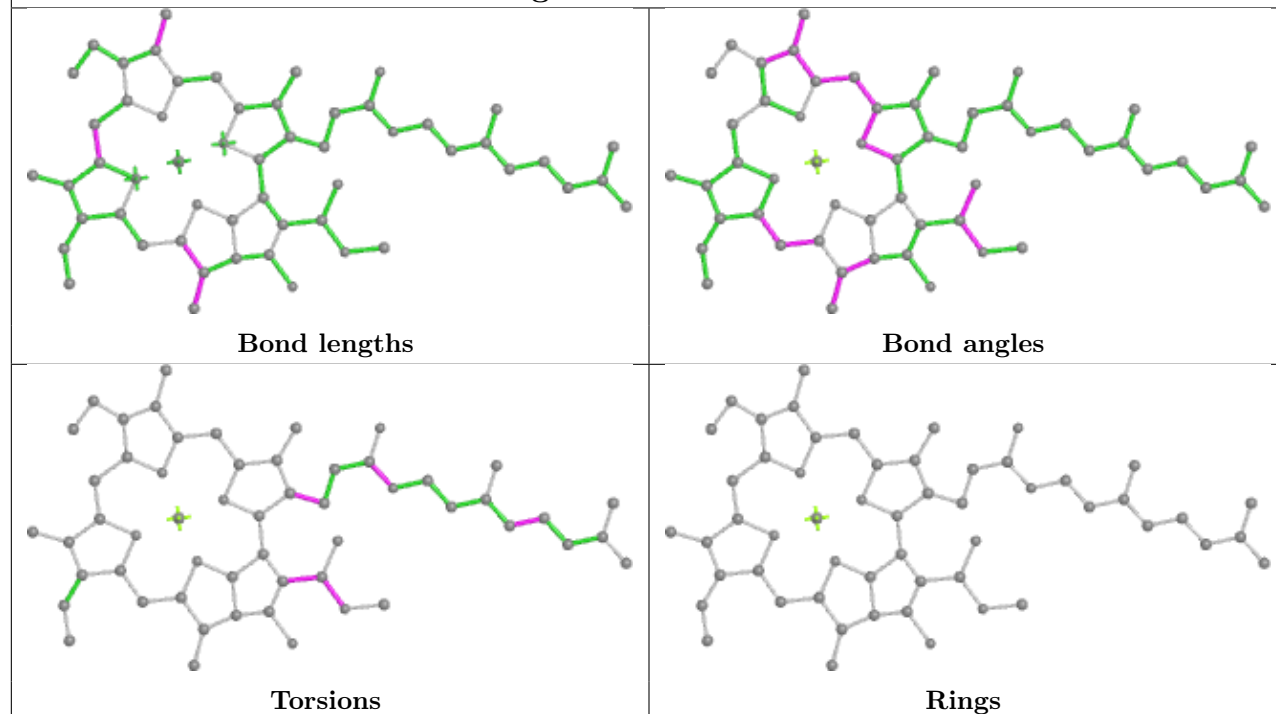


Torsions

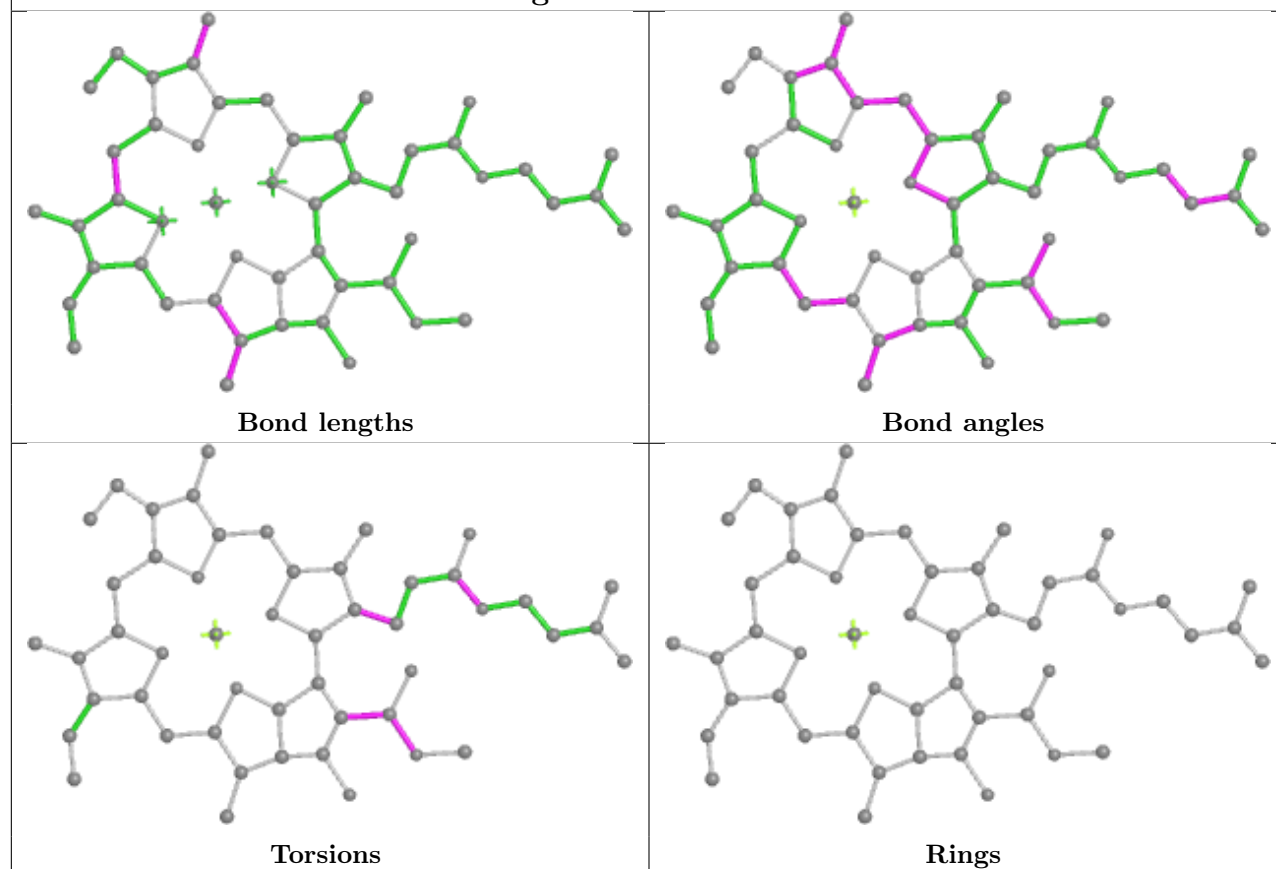


Rings

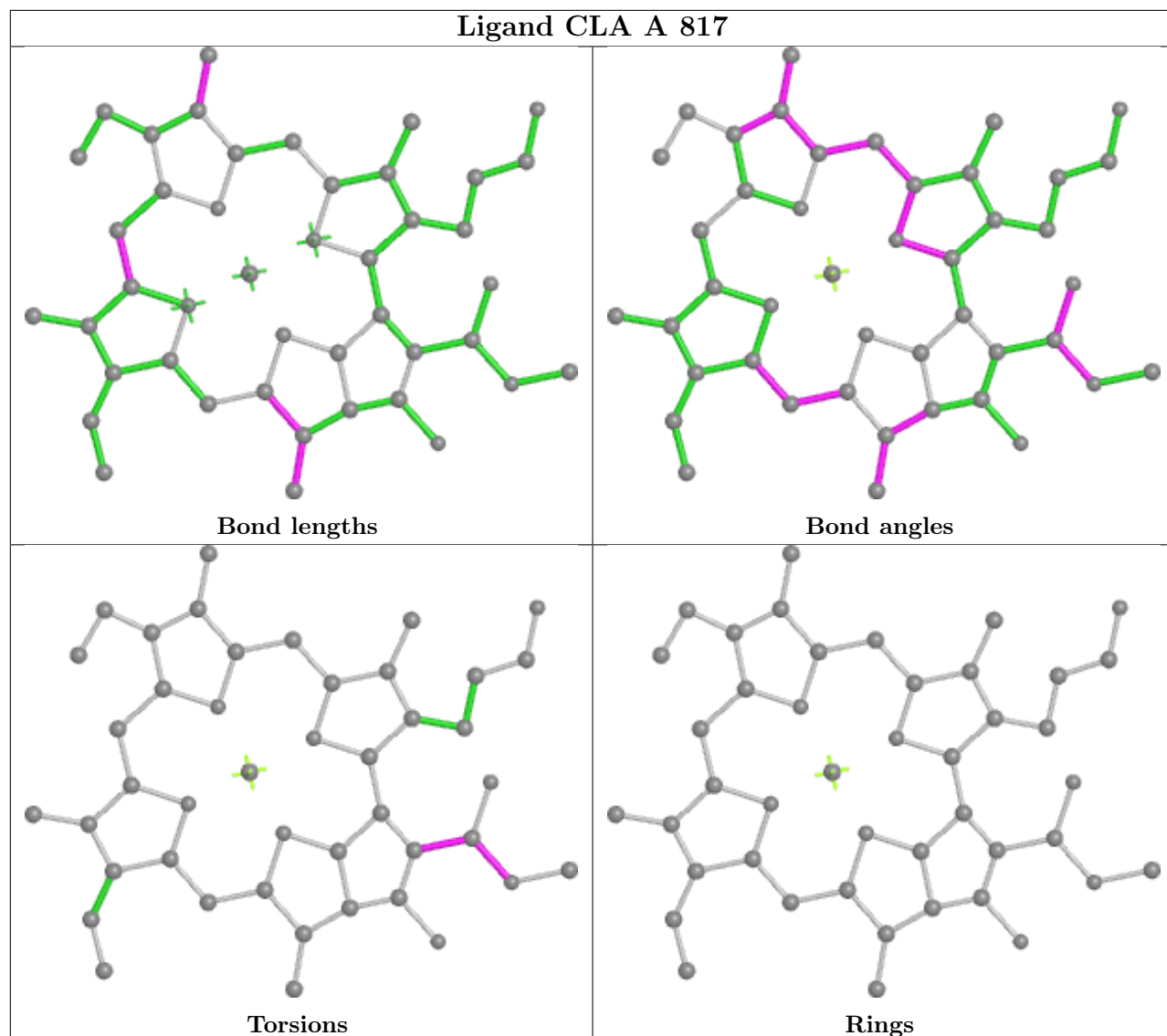
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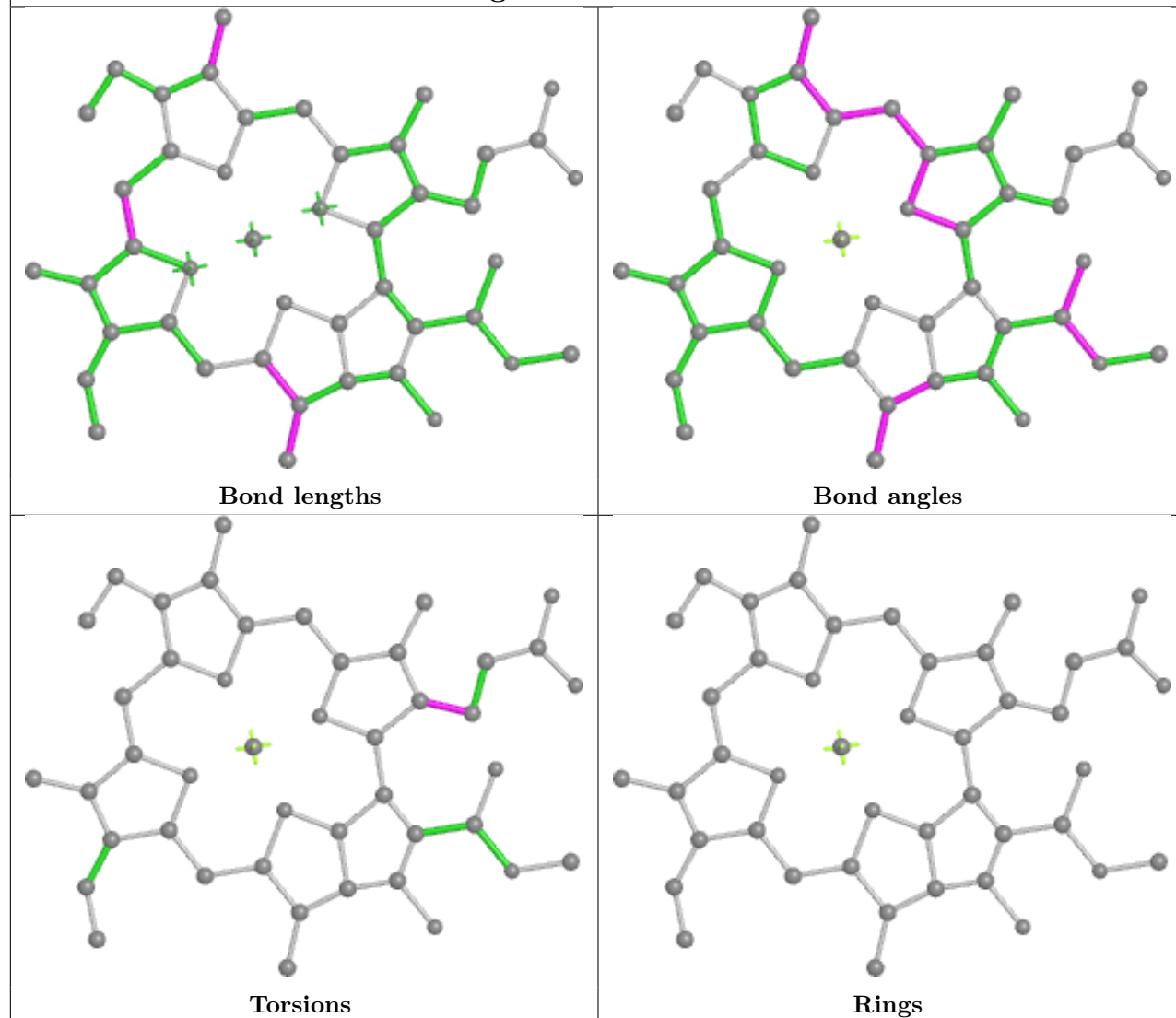
Ligand CLA A 816



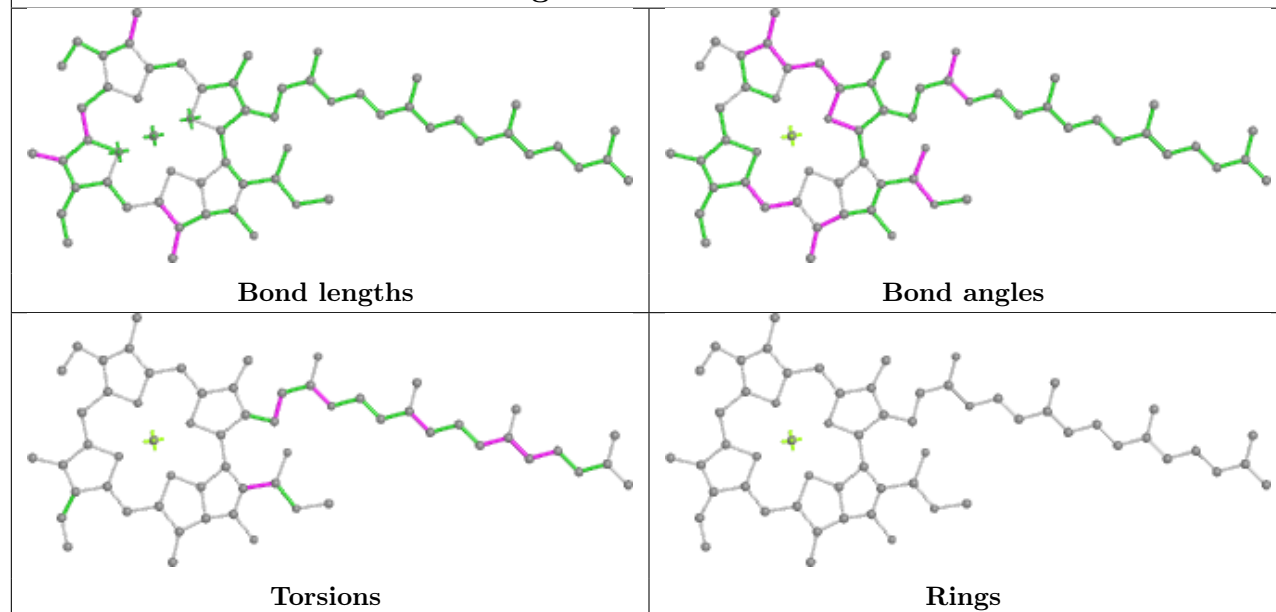
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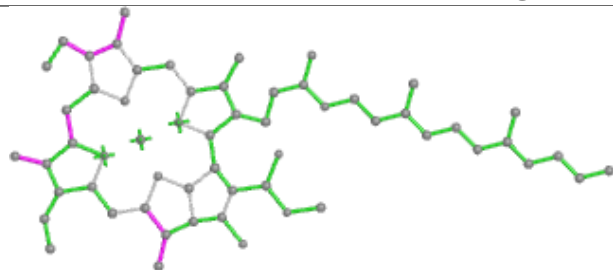
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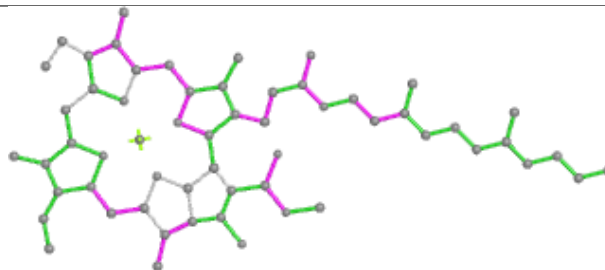
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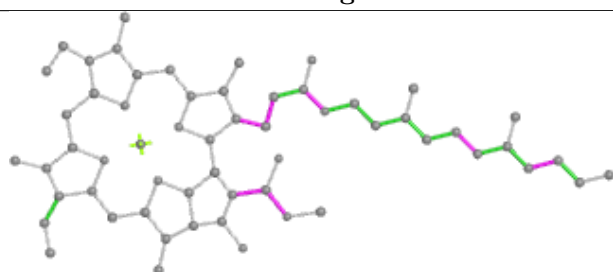
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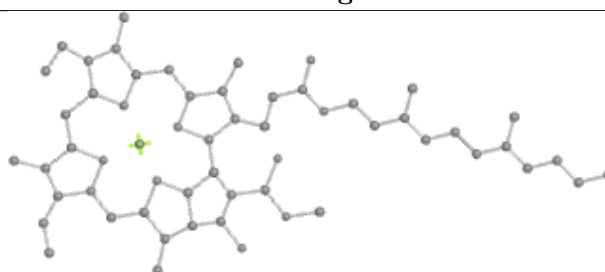
Bond lengths



Bond angles

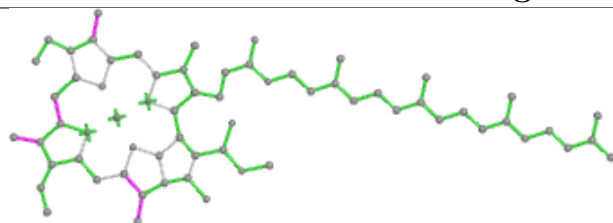


Torsions

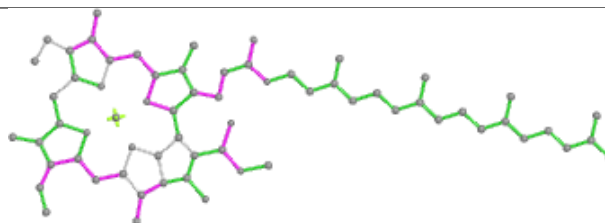


Rings

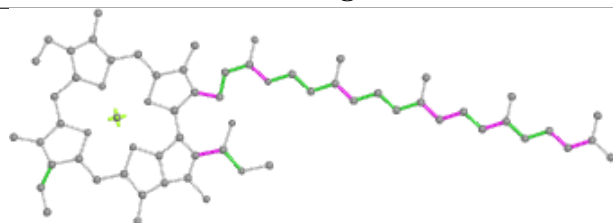
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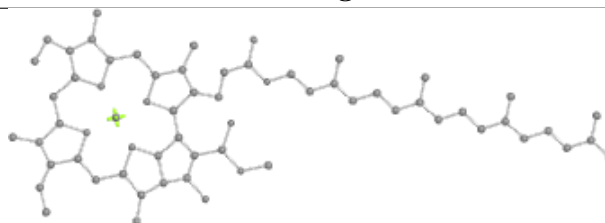
Bond lengths



Bond angles

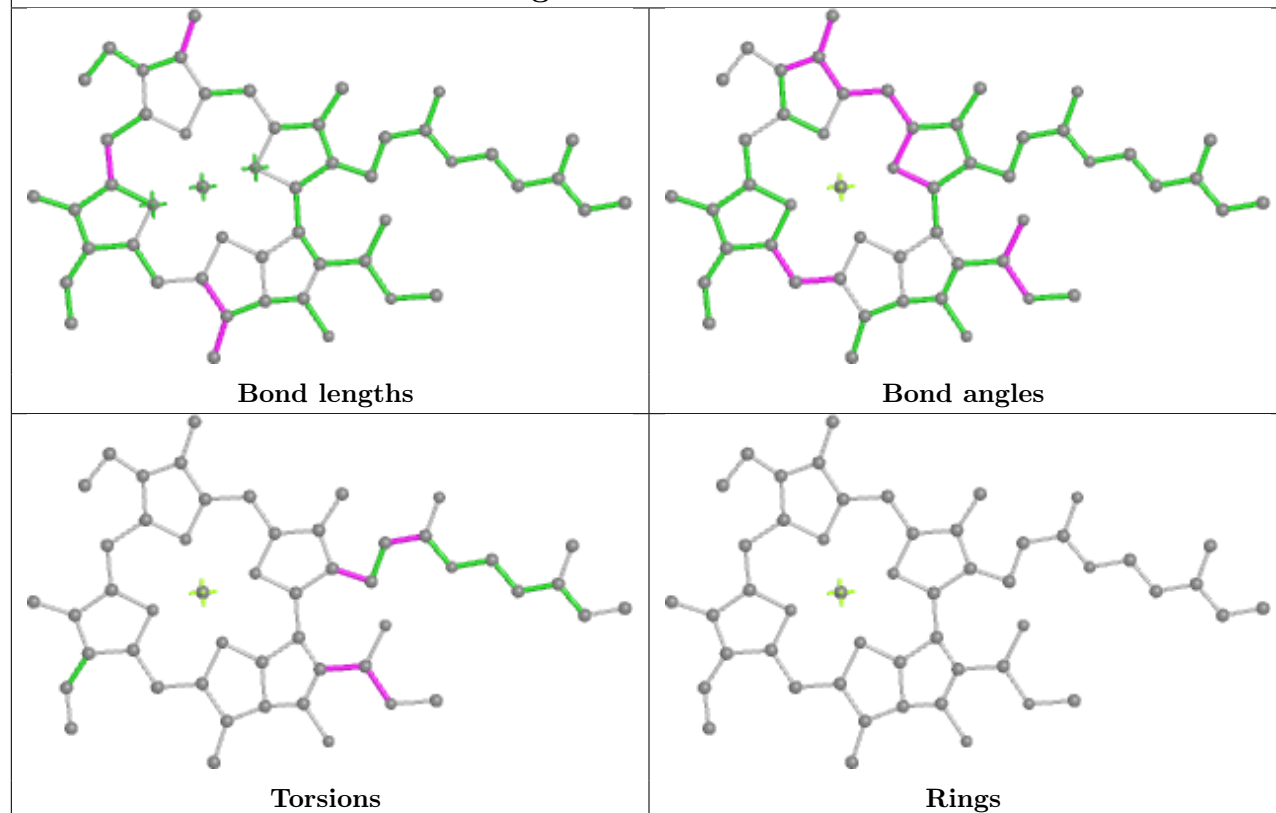


Torsions

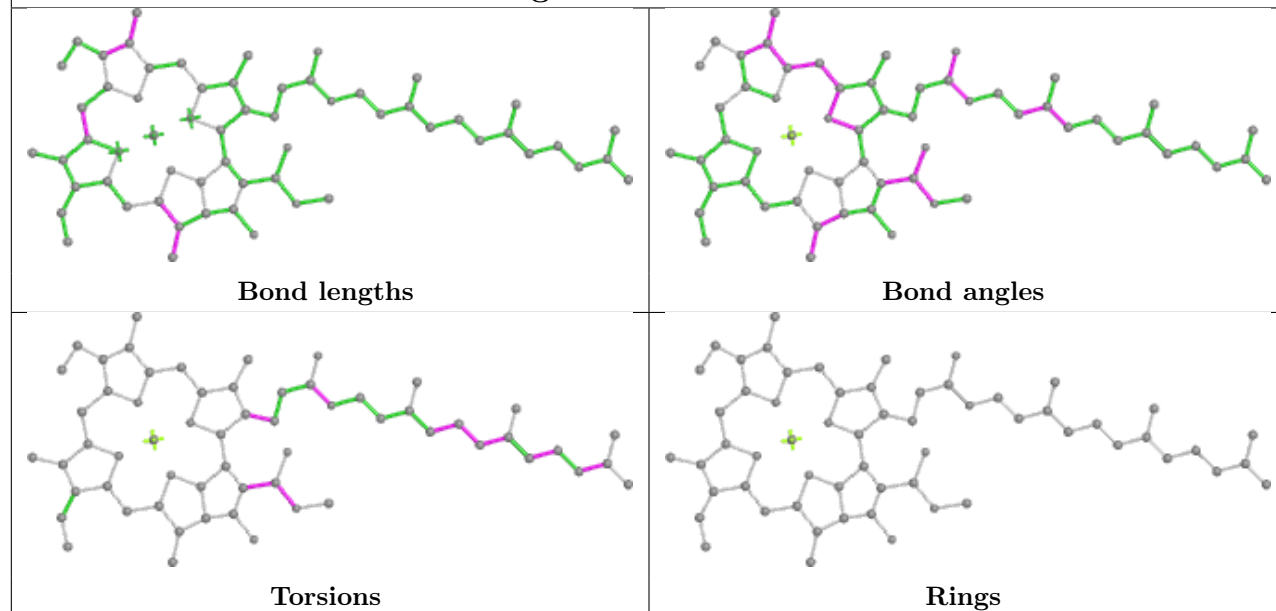


Rings

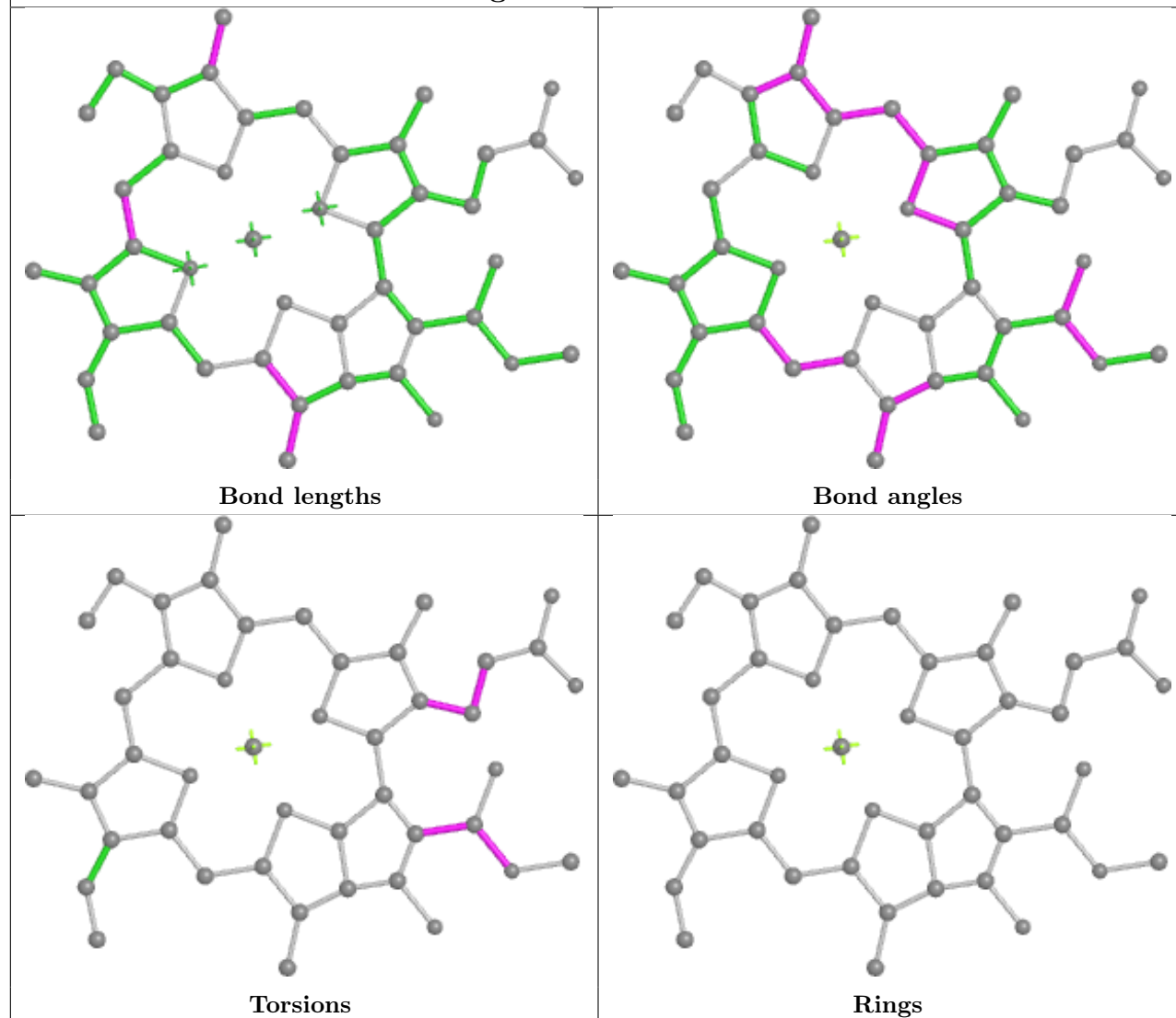
Ligand CLA A 822

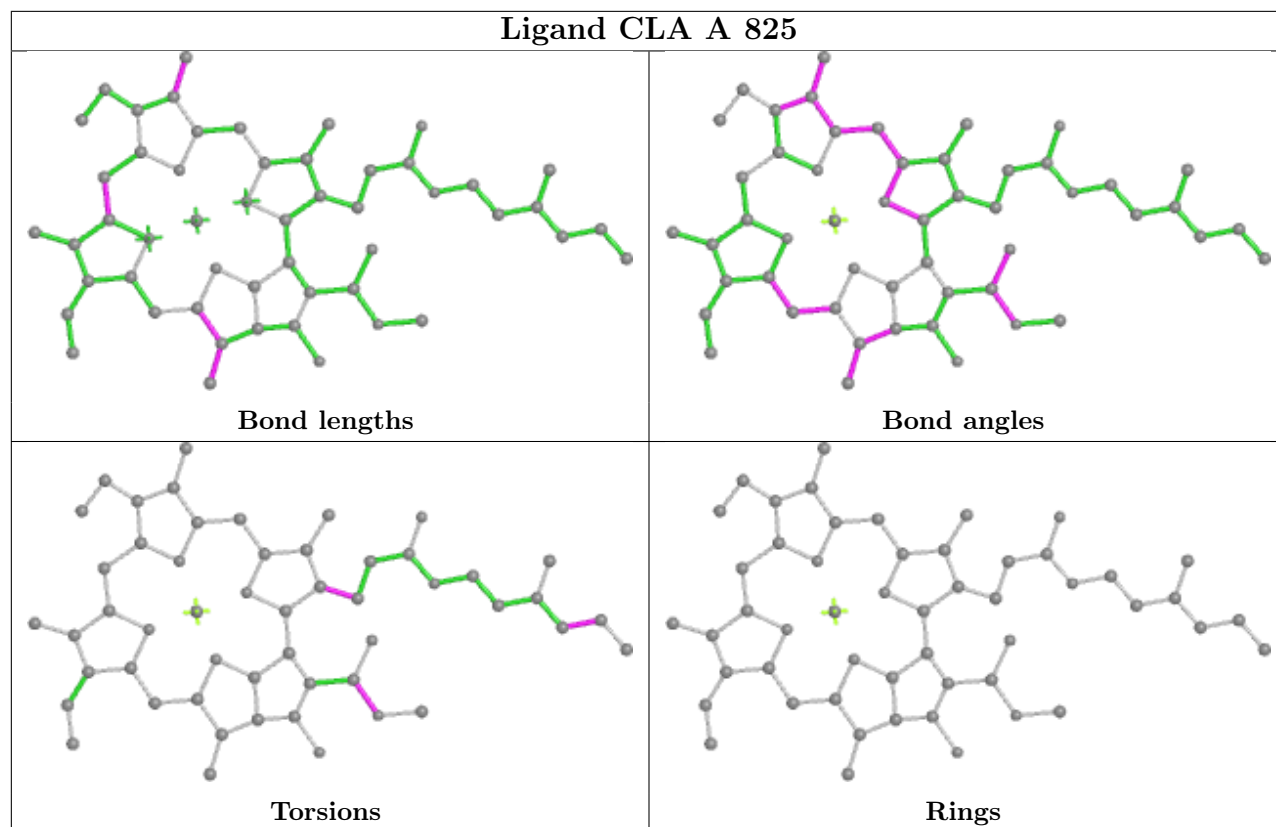


Ligand CLA A 823

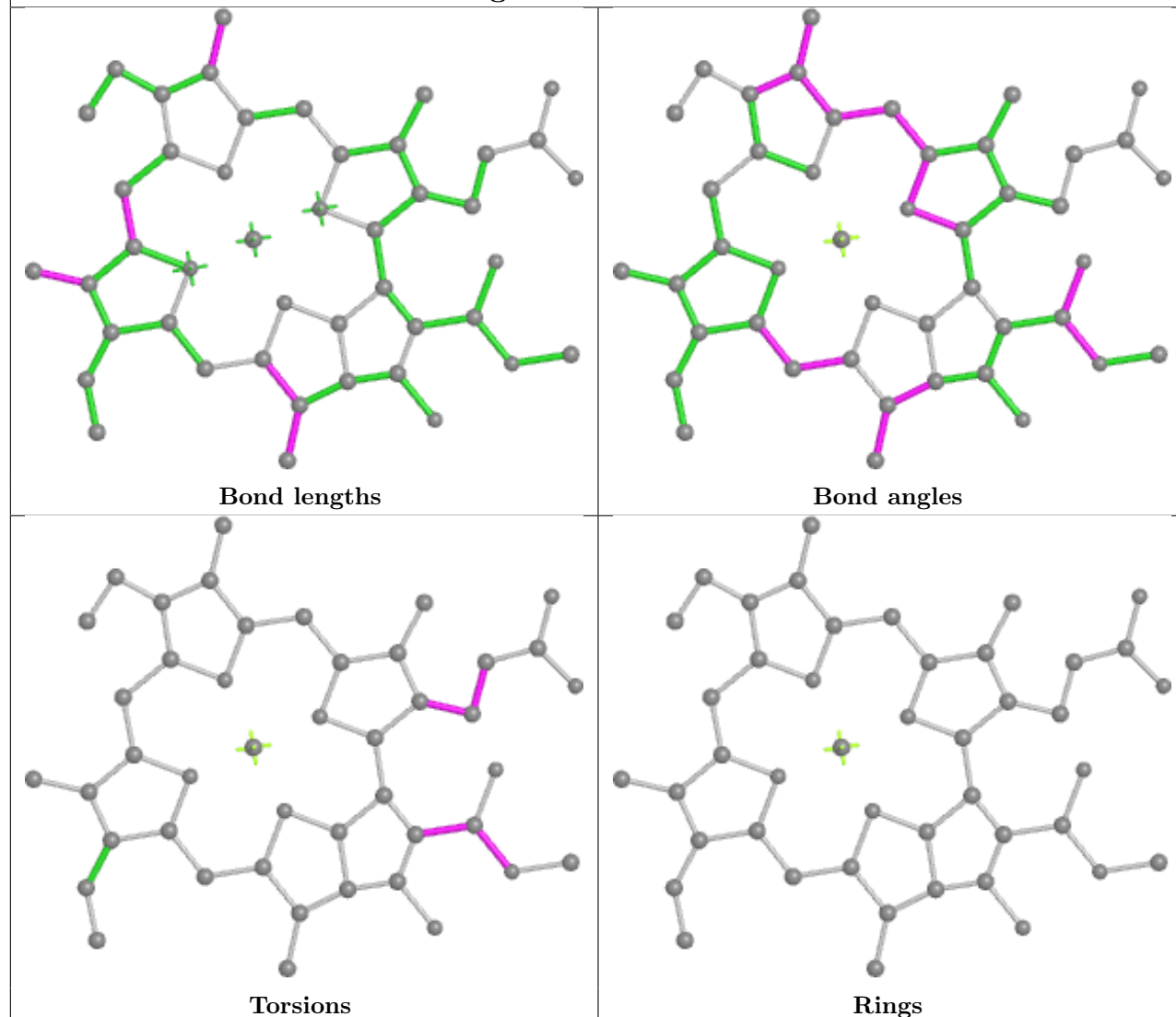


Ligand CLA A 824

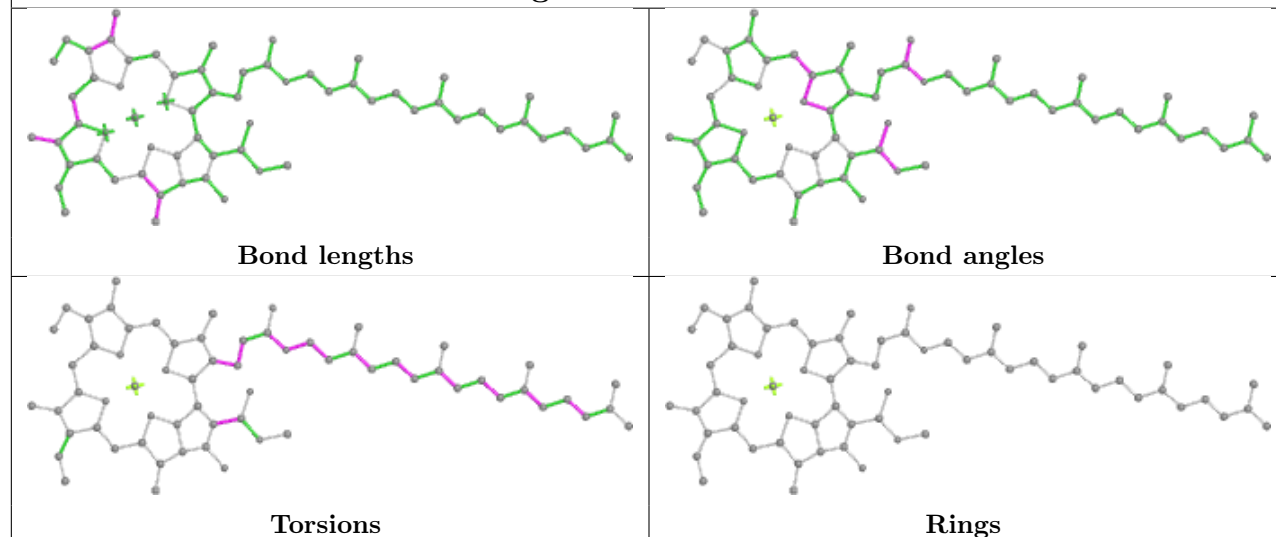




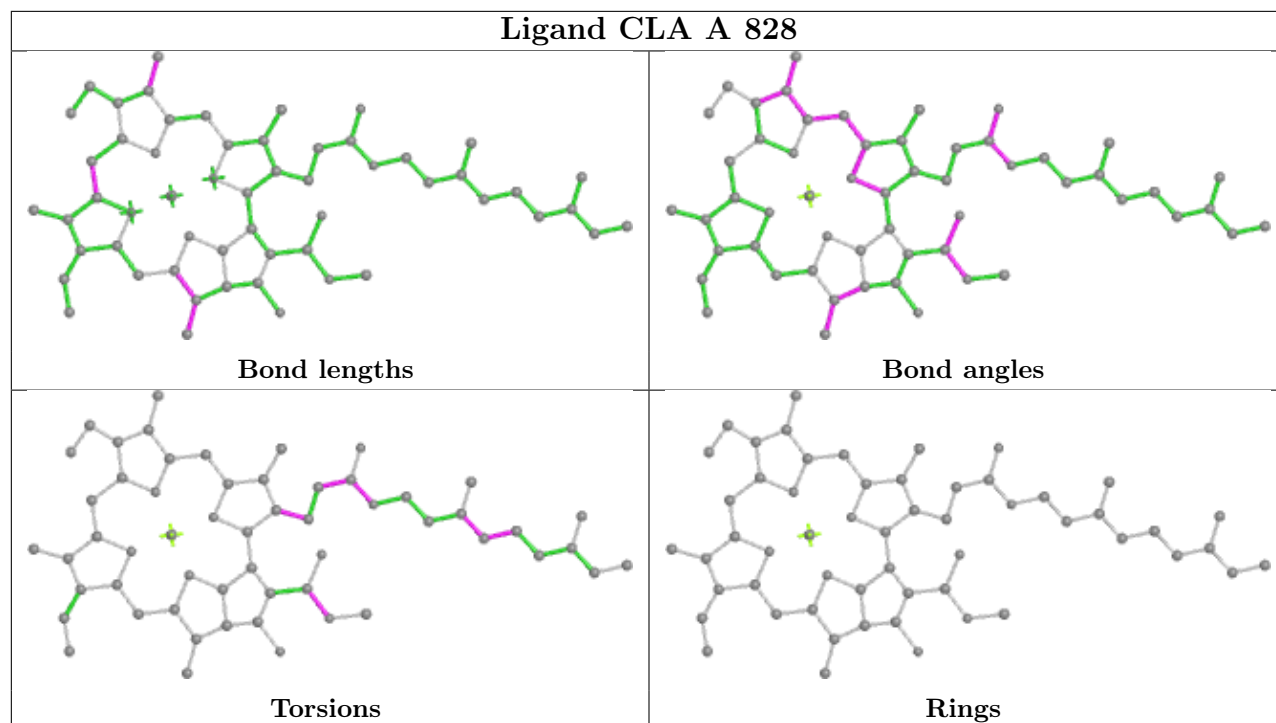
Ligand CLA A 826



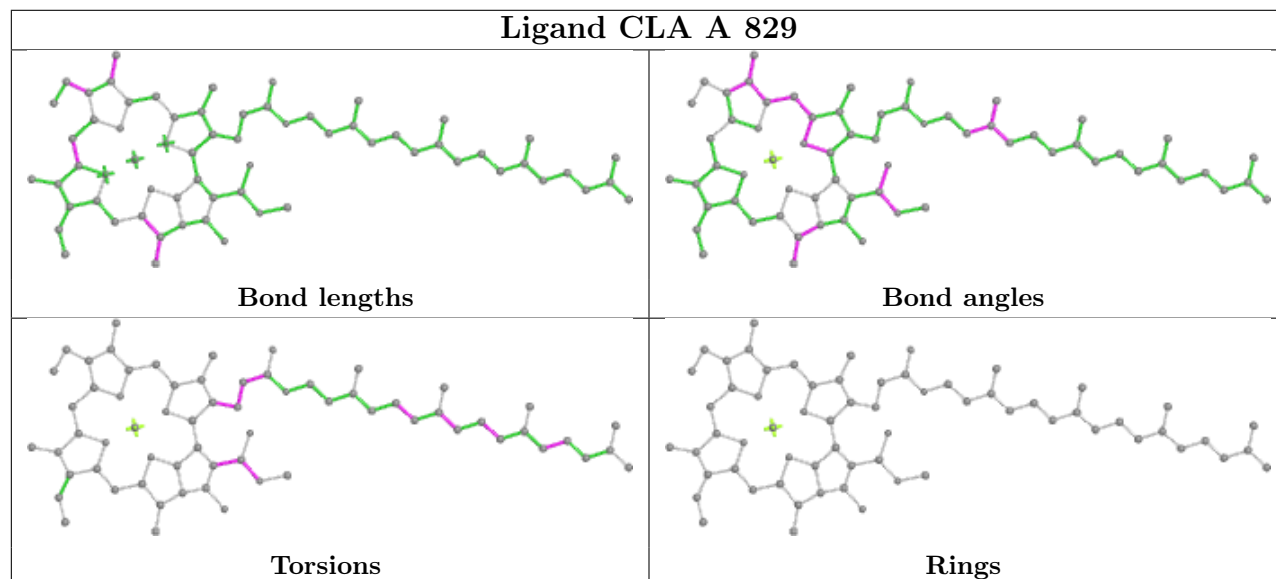
Ligand CLA A 827

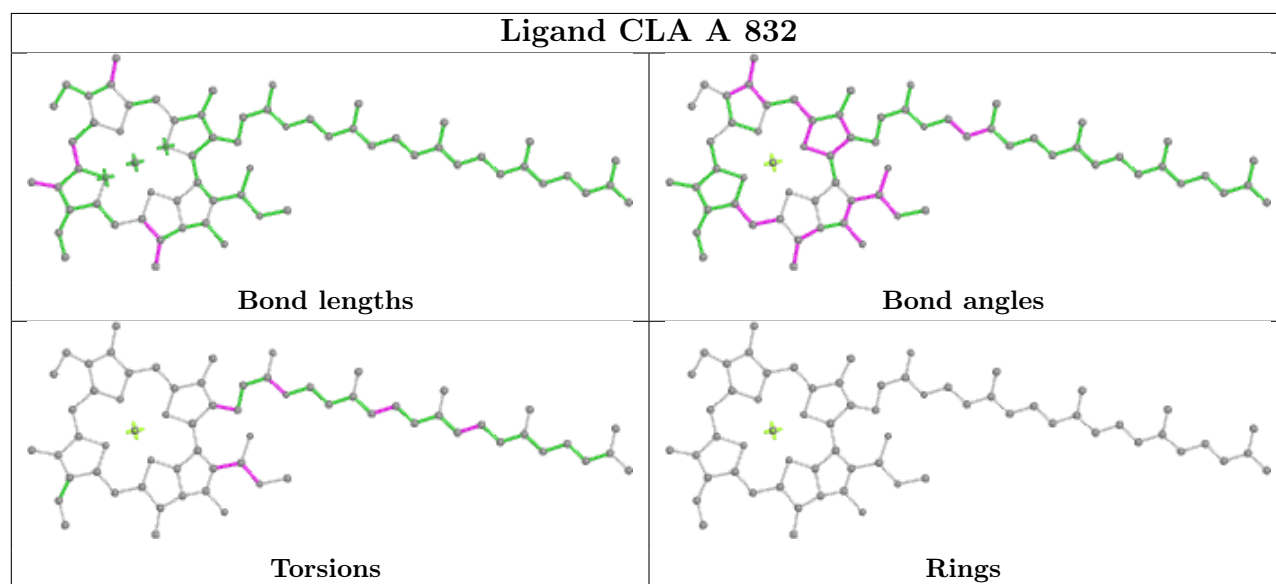
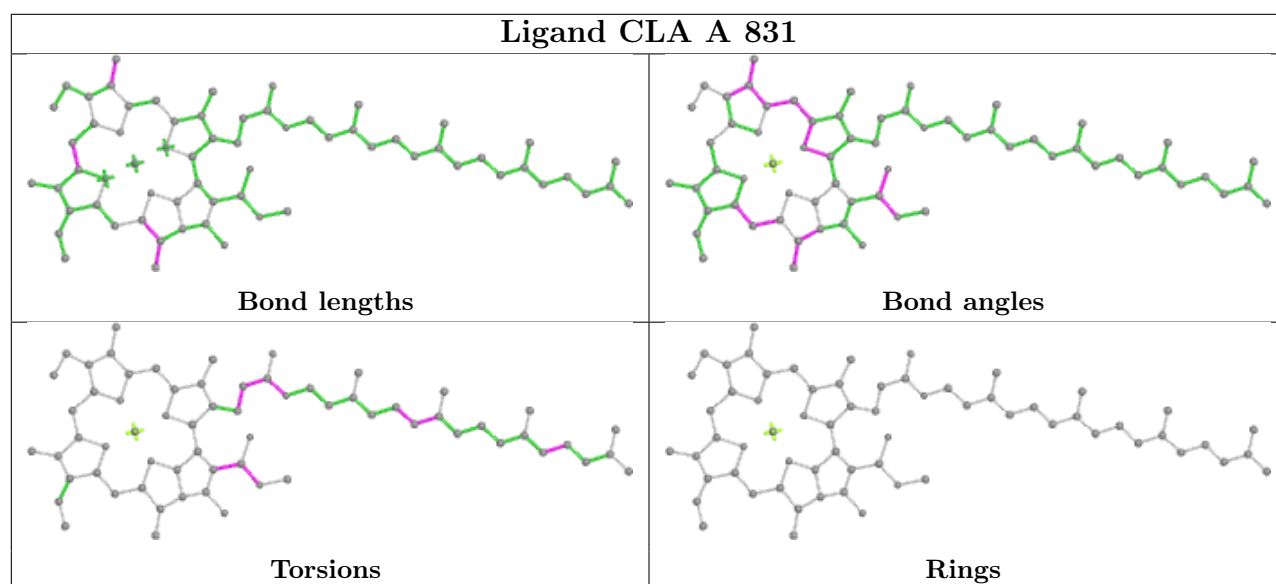
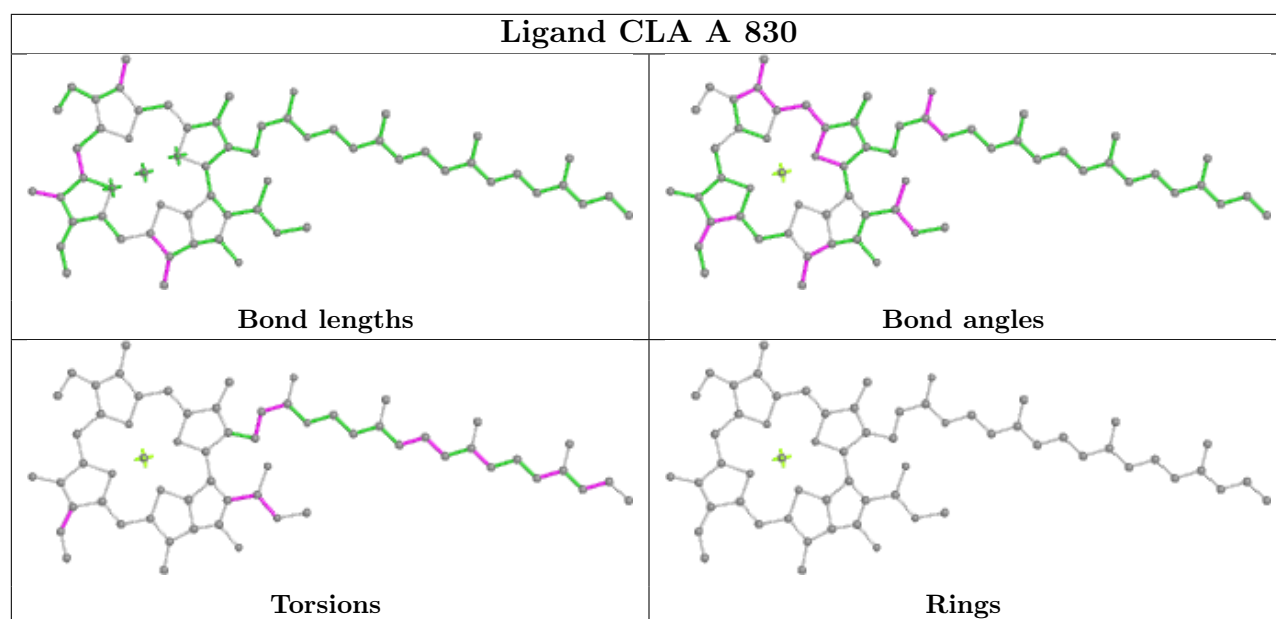


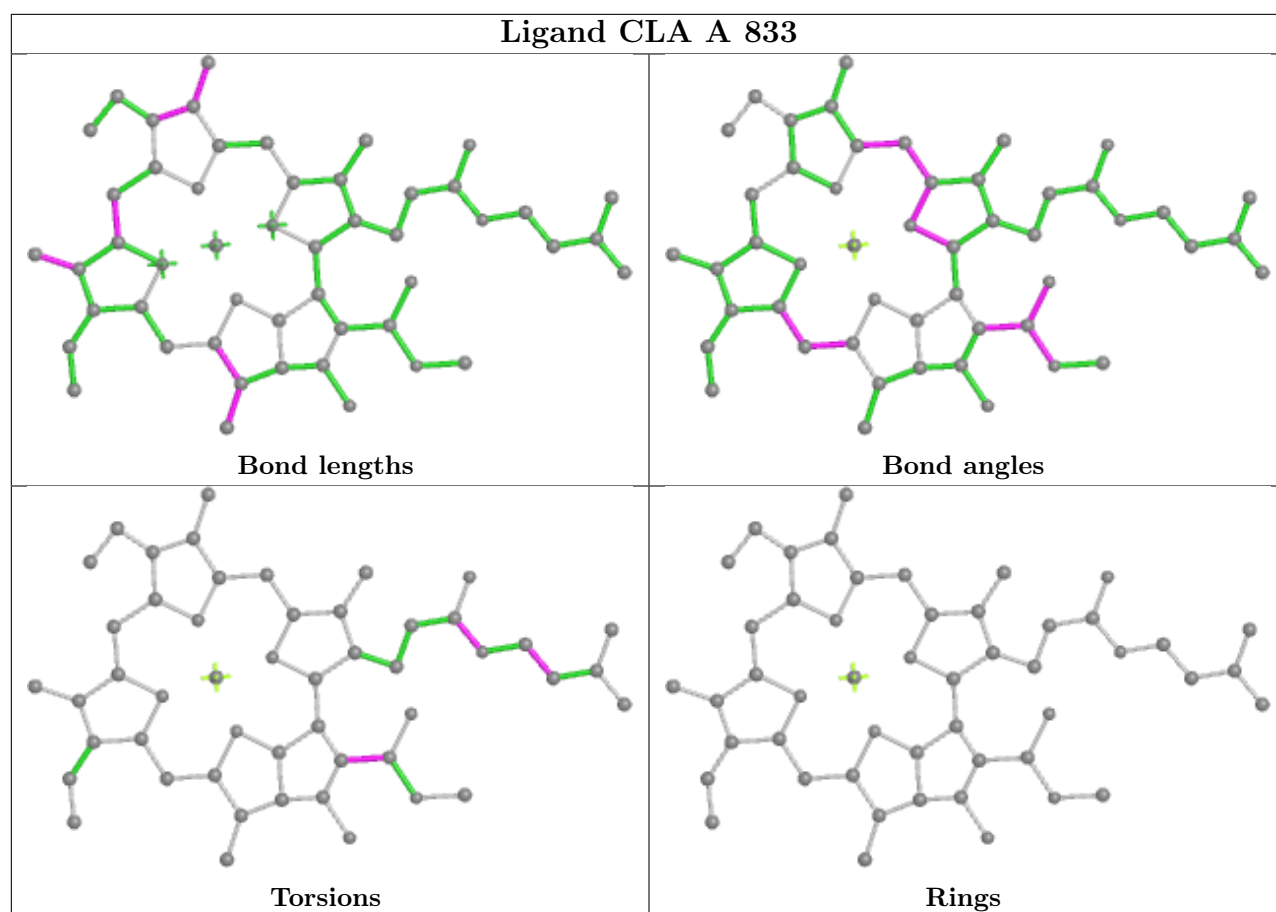
Ligand CLA A 828



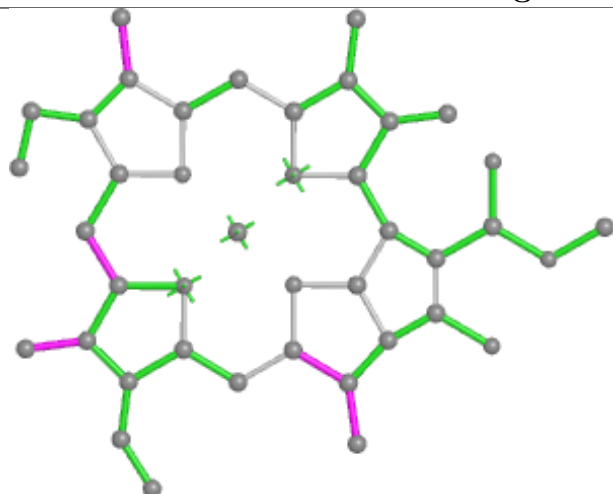
Ligand CLA A 829



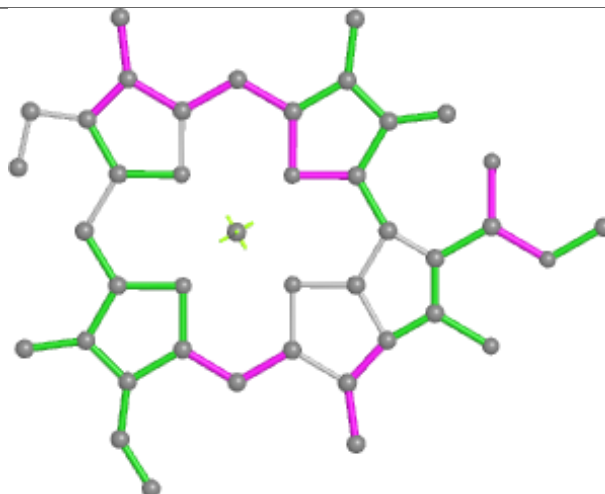




Ligand CLA A 834



Bond lengths



Bond angles

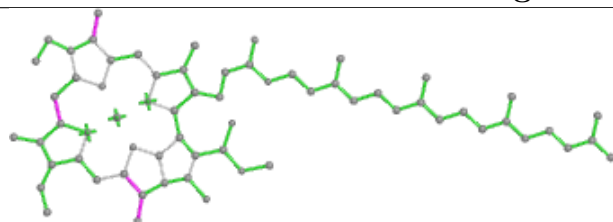


Torsions

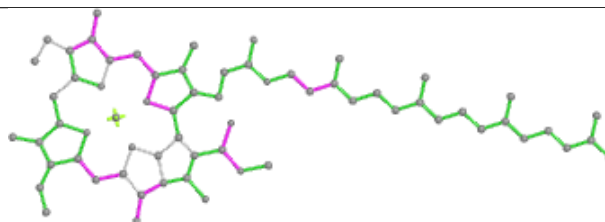


Rings

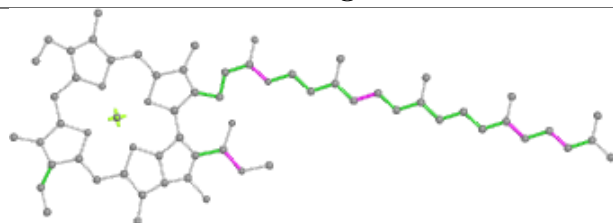
Ligand CLA A 835



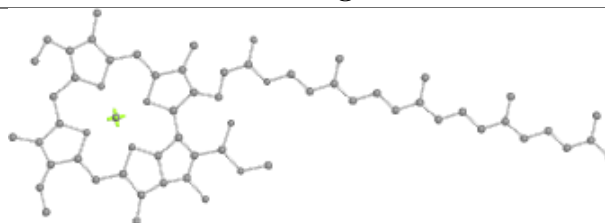
Bond lengths



Bond angles

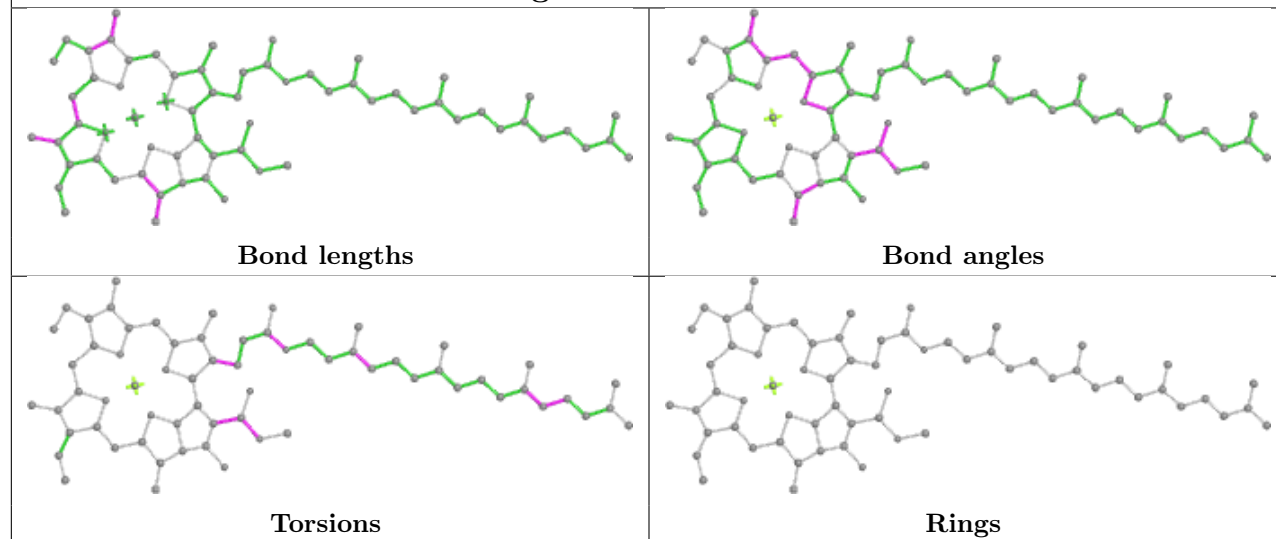


Torsions

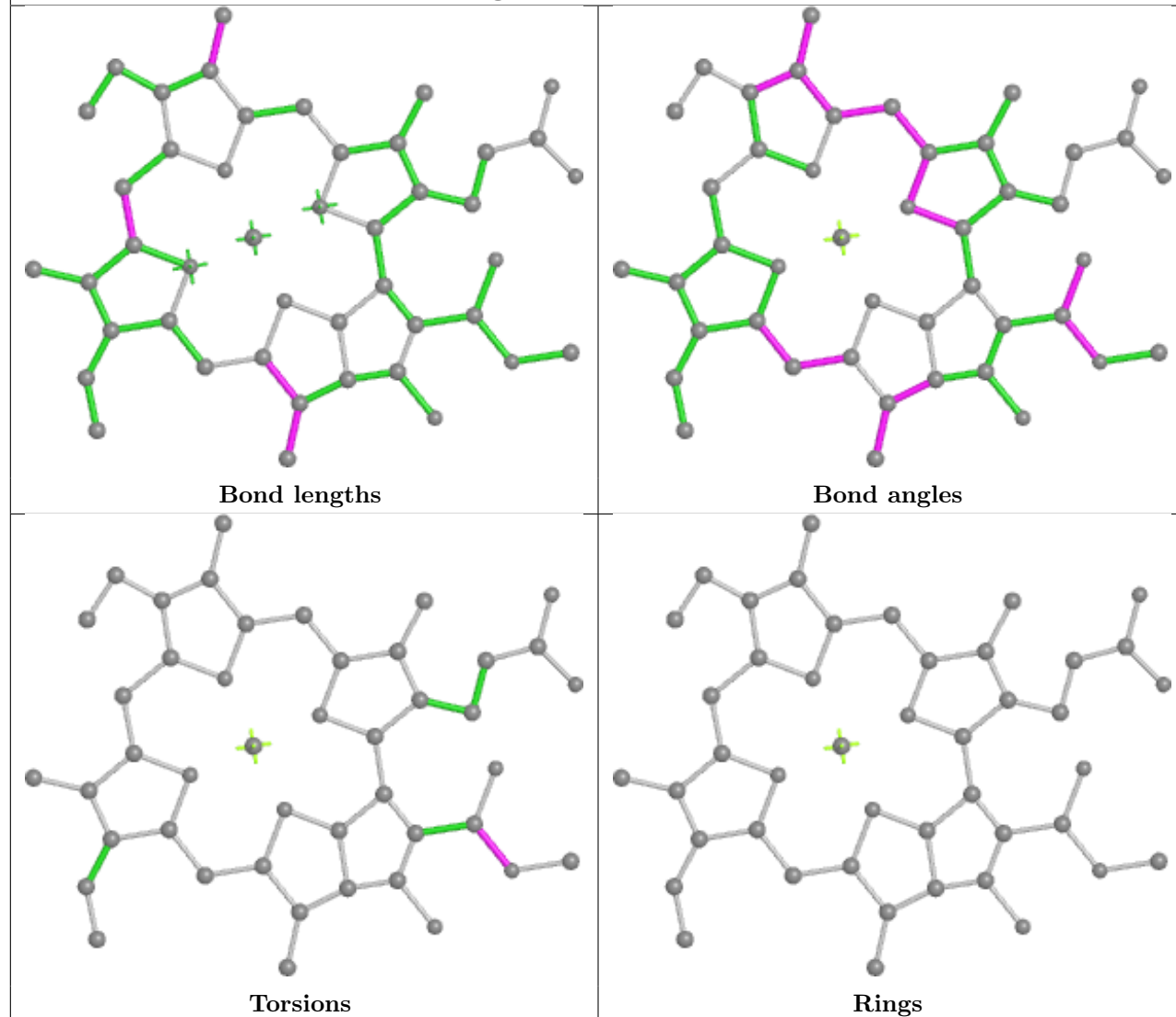


Rings

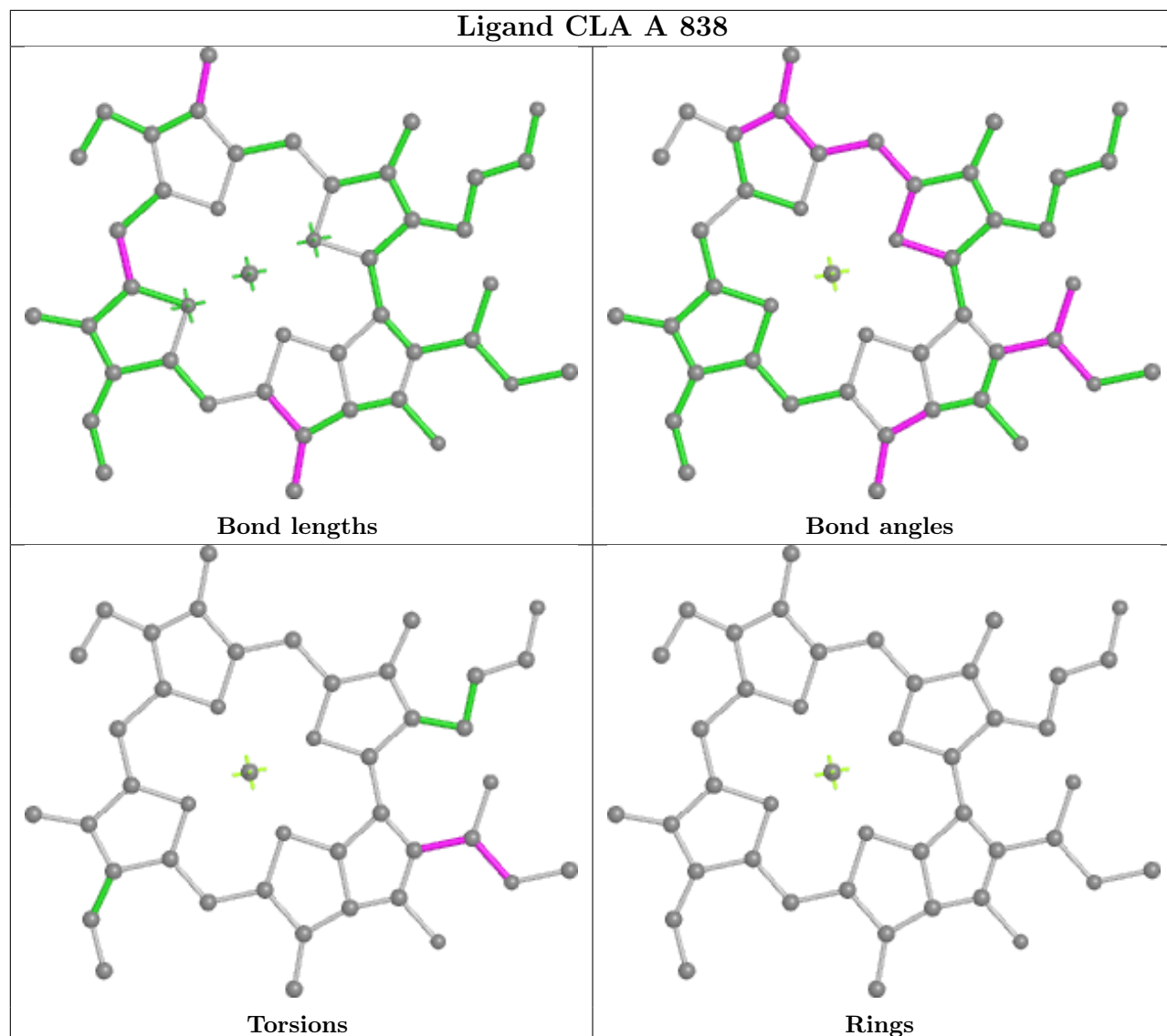
Ligand CLA A 836



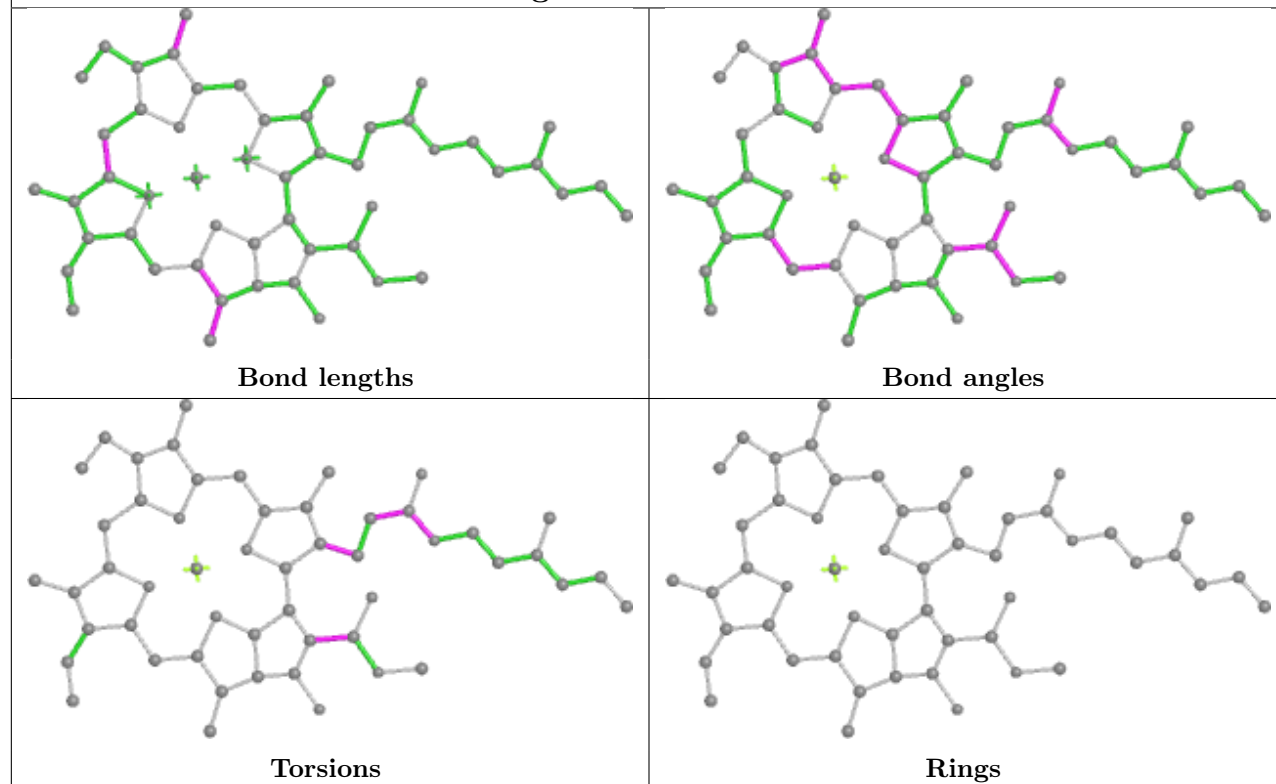
Ligand CLA A 837



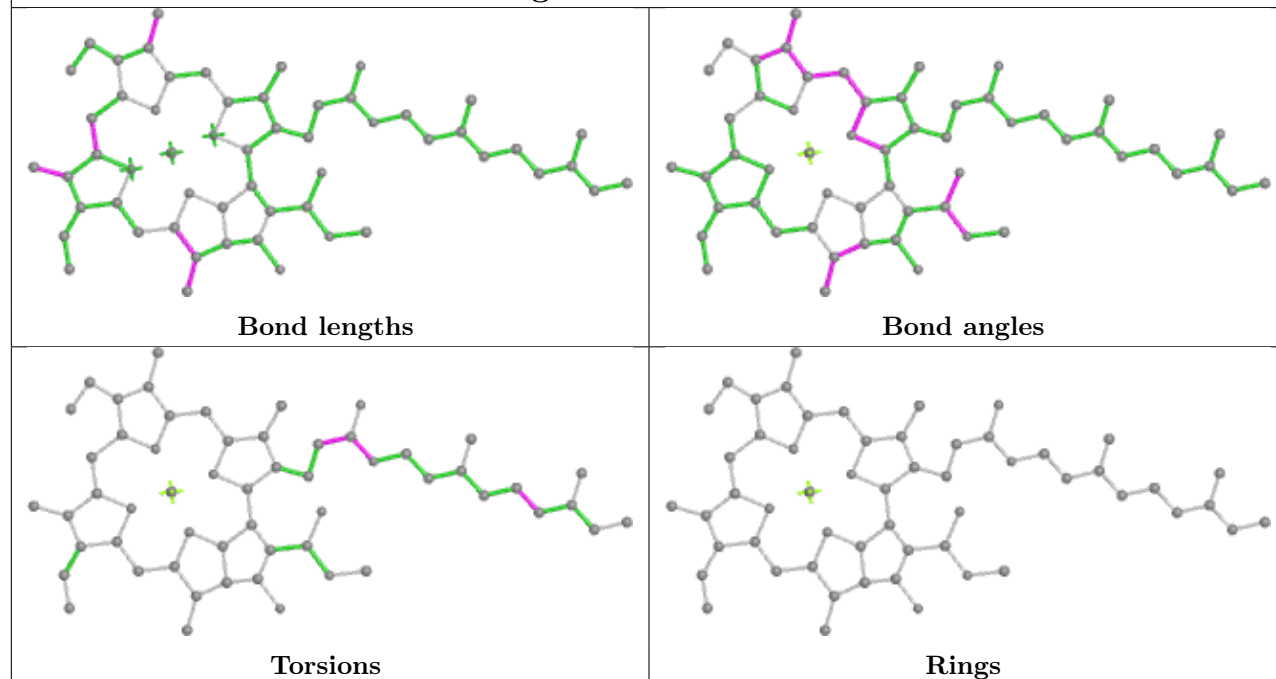
Ligand CLA A 838



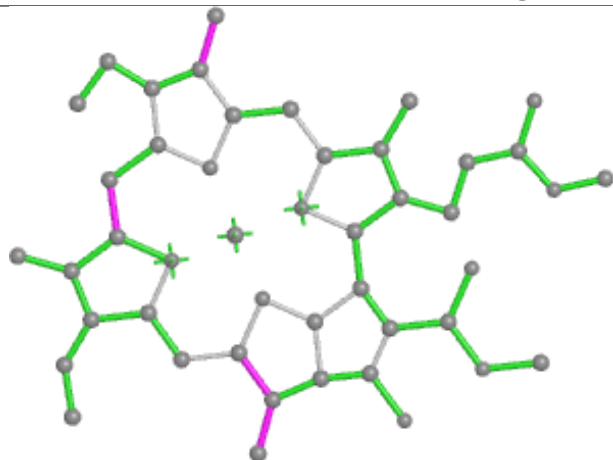
Ligand CLA A 839



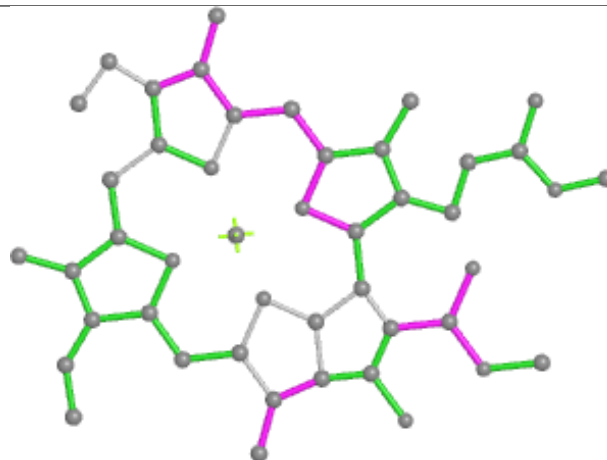
Ligand CLA A 840



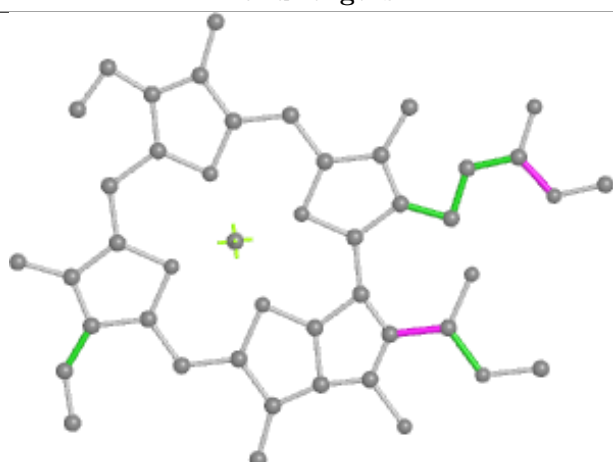
Ligand CLA A 841



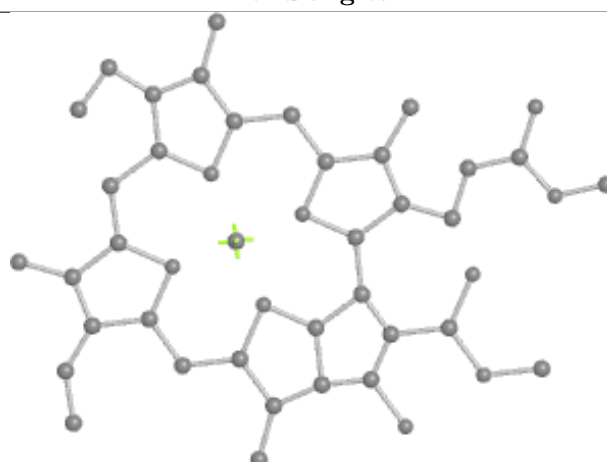
Bond lengths



Bond angles

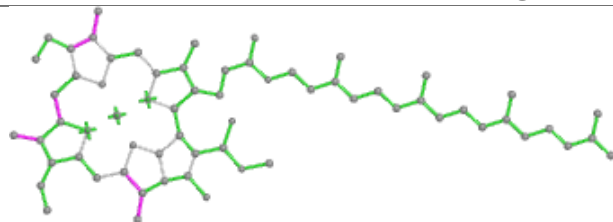


Torsions

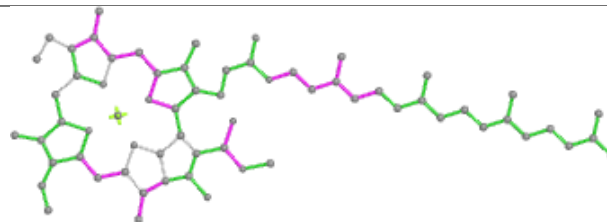


Rings

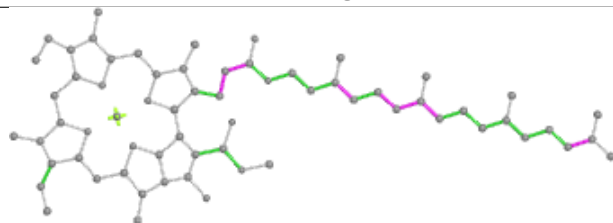
Ligand CLA A 842



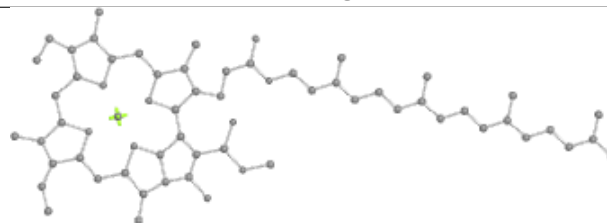
Bond lengths



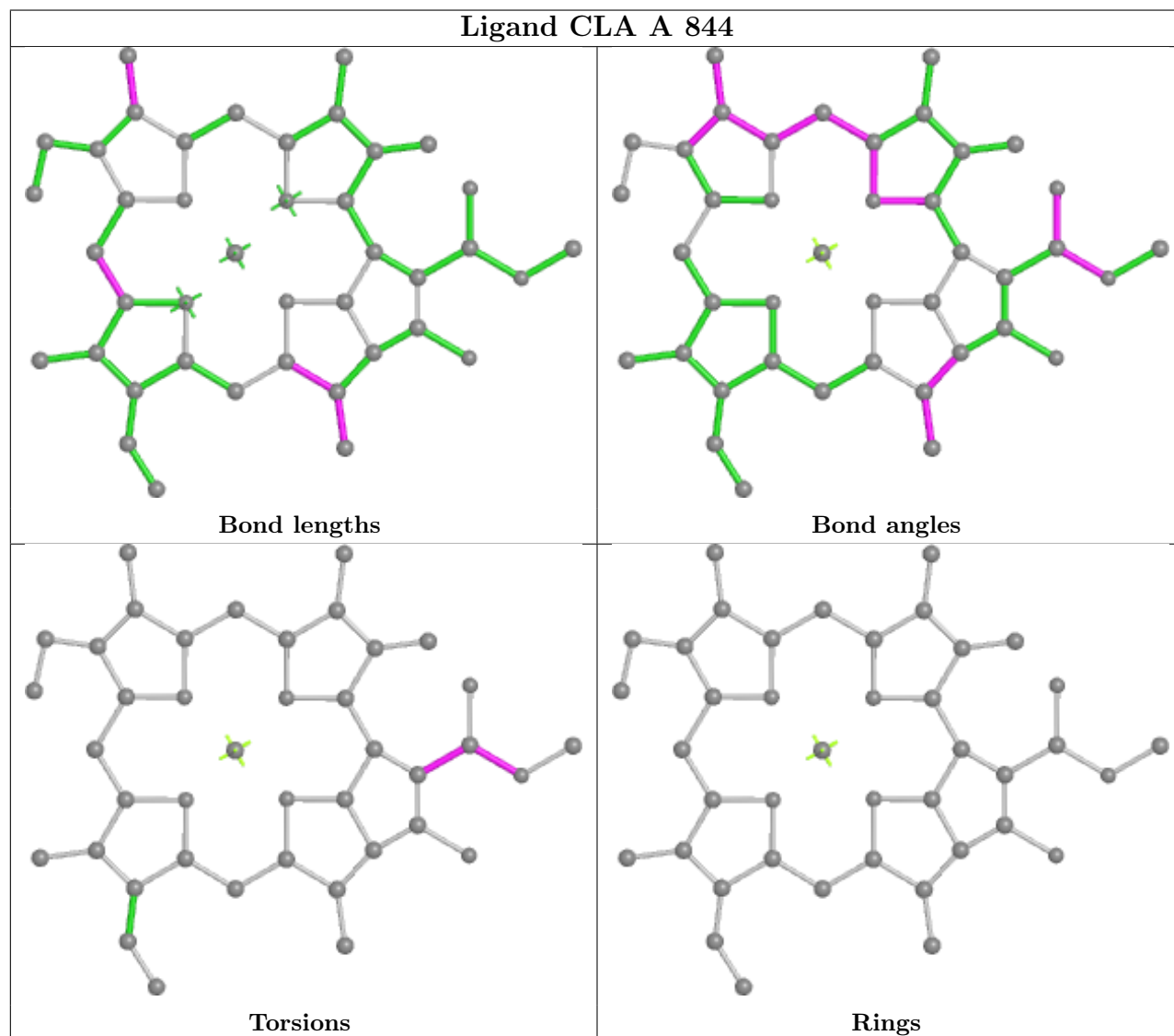
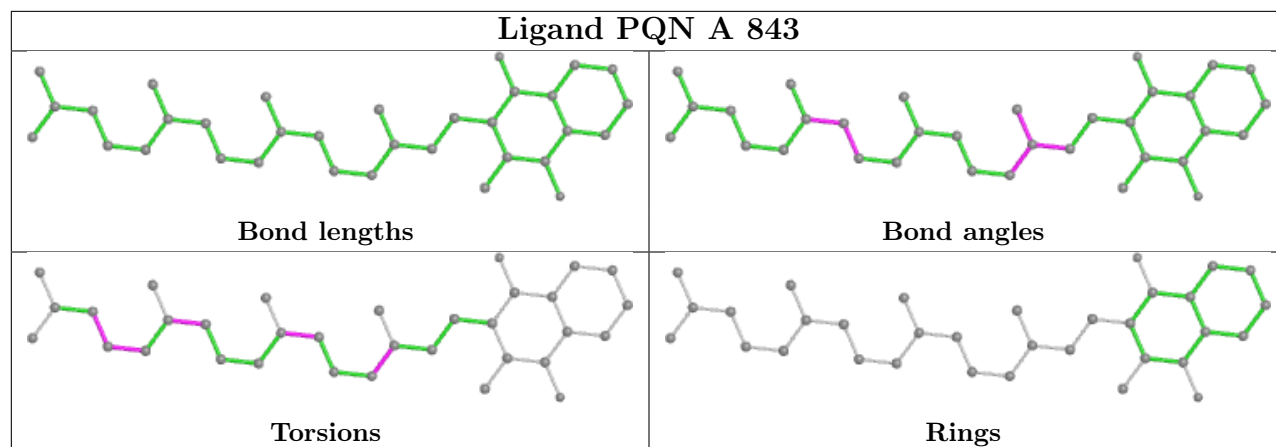
Bond angles

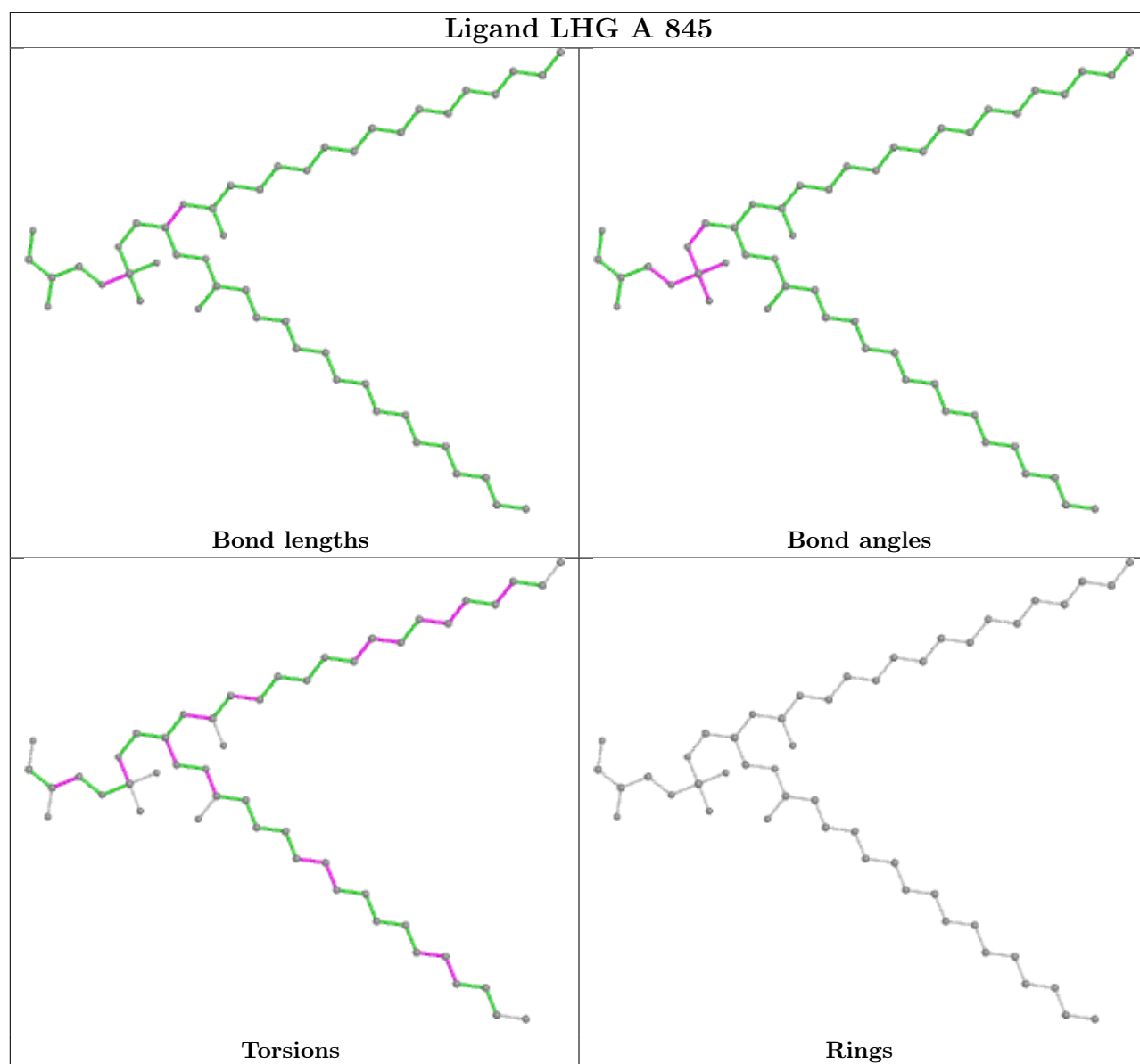


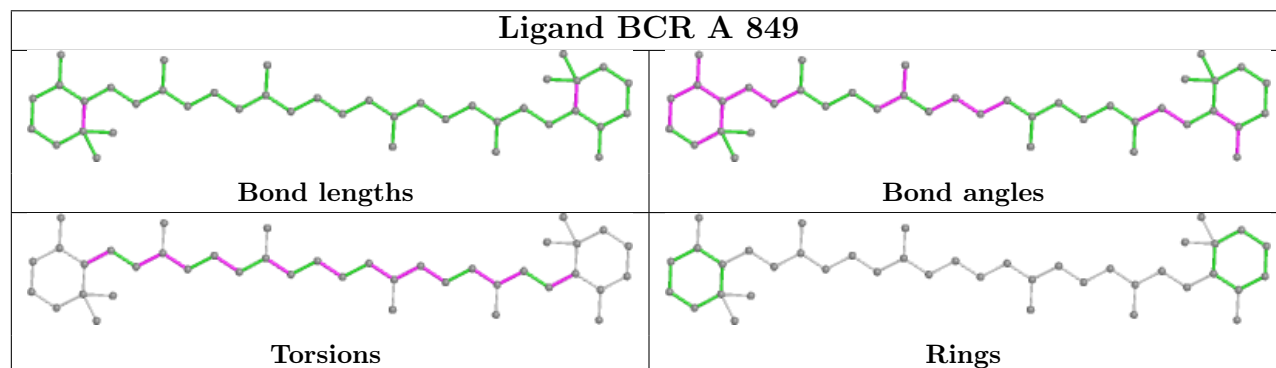
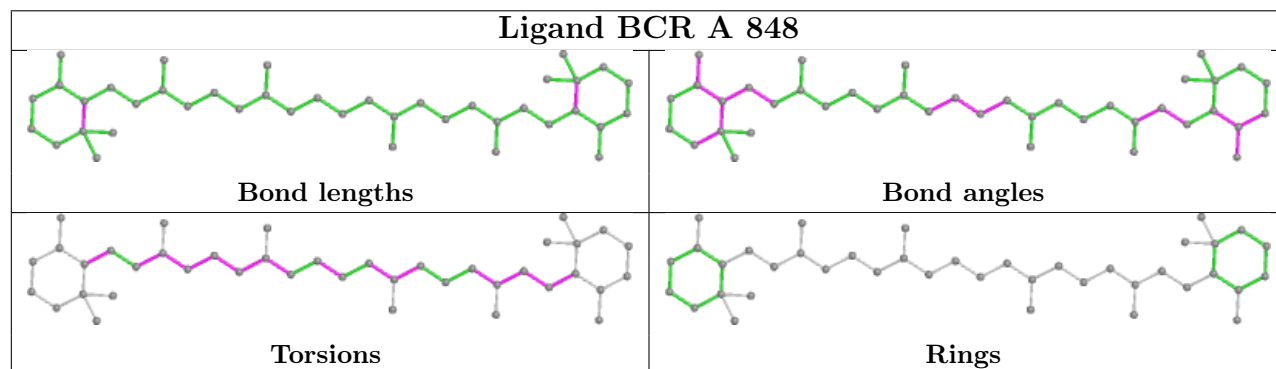
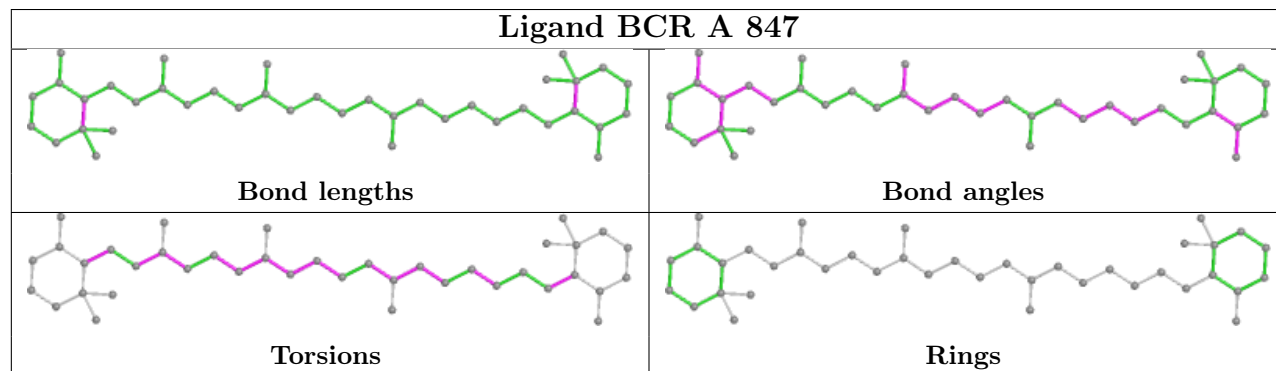
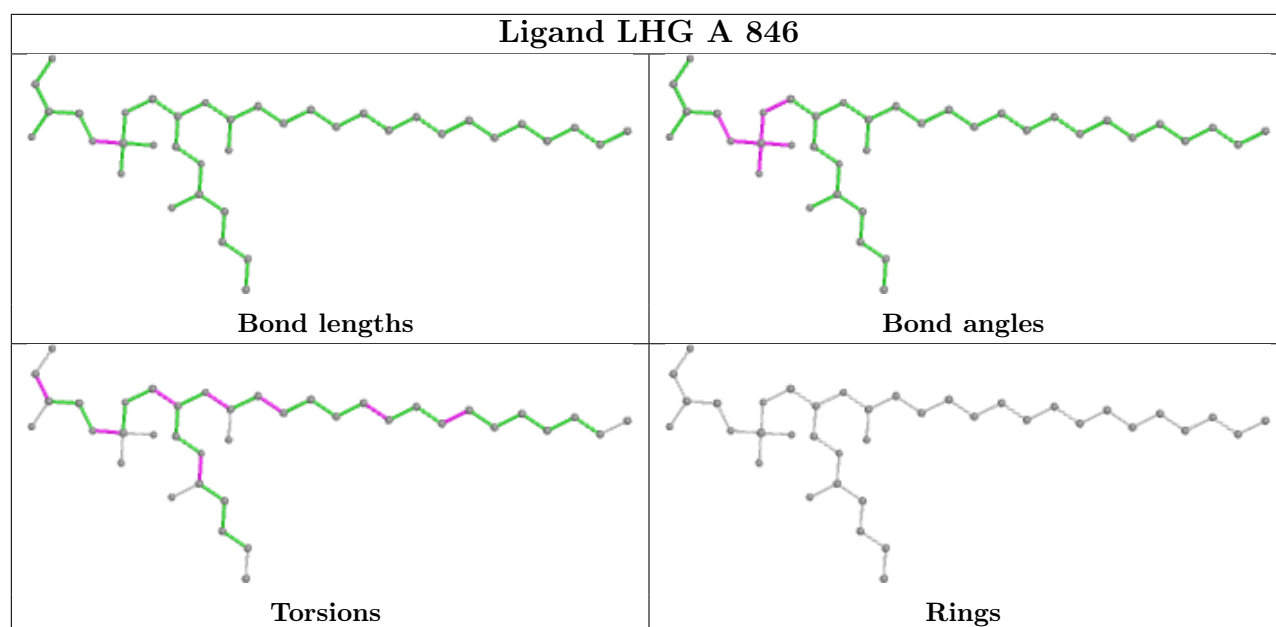
Torsions

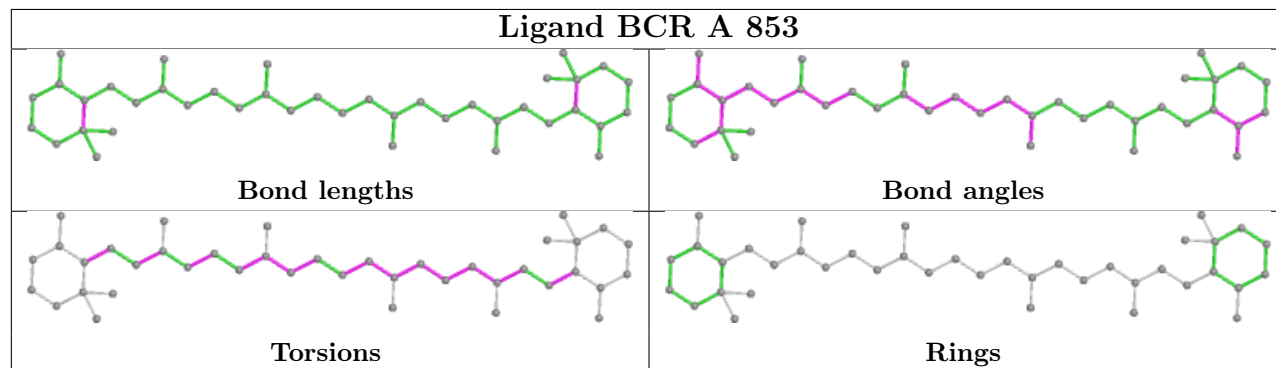
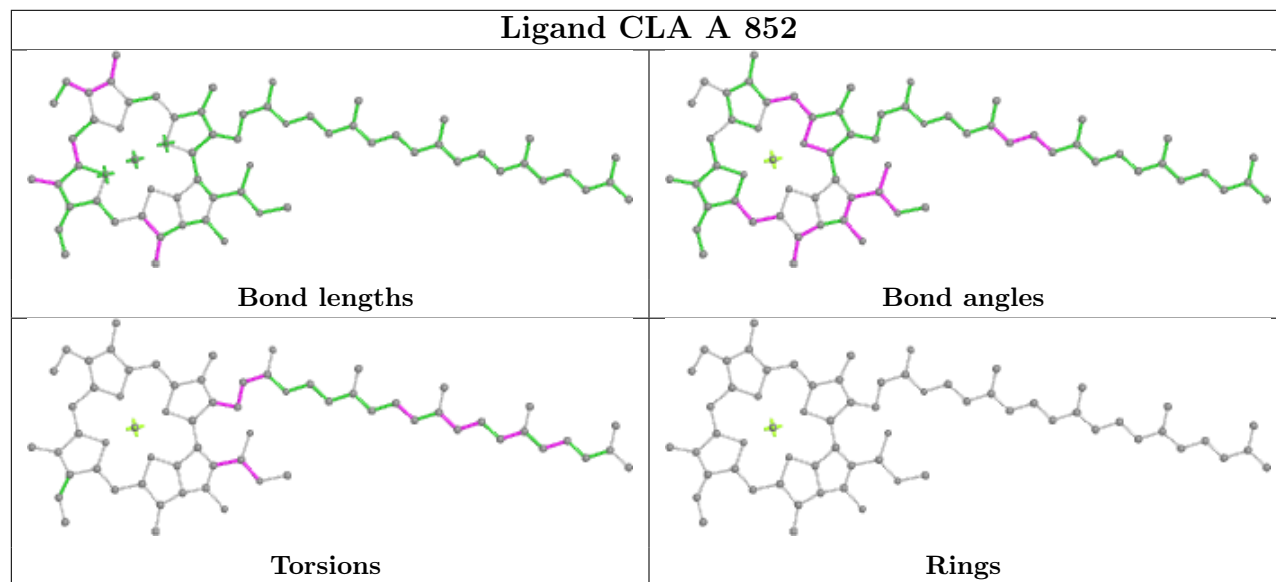
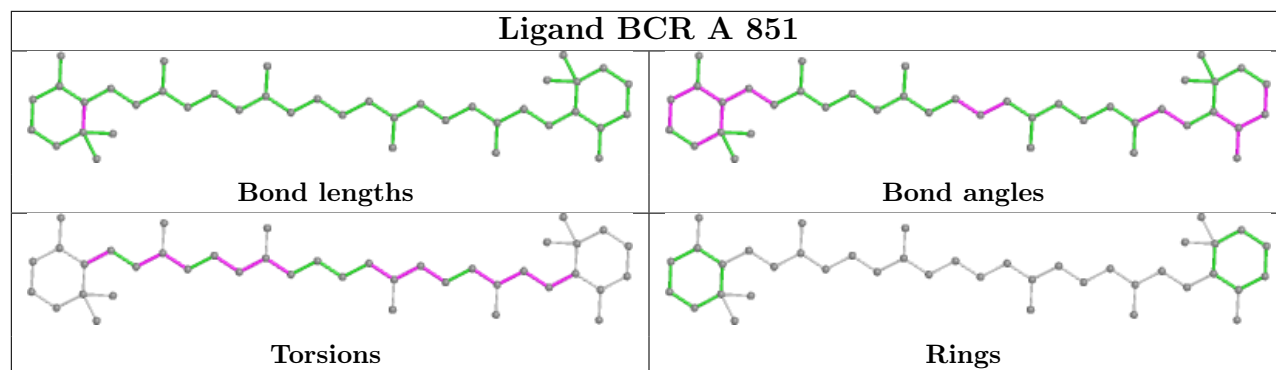
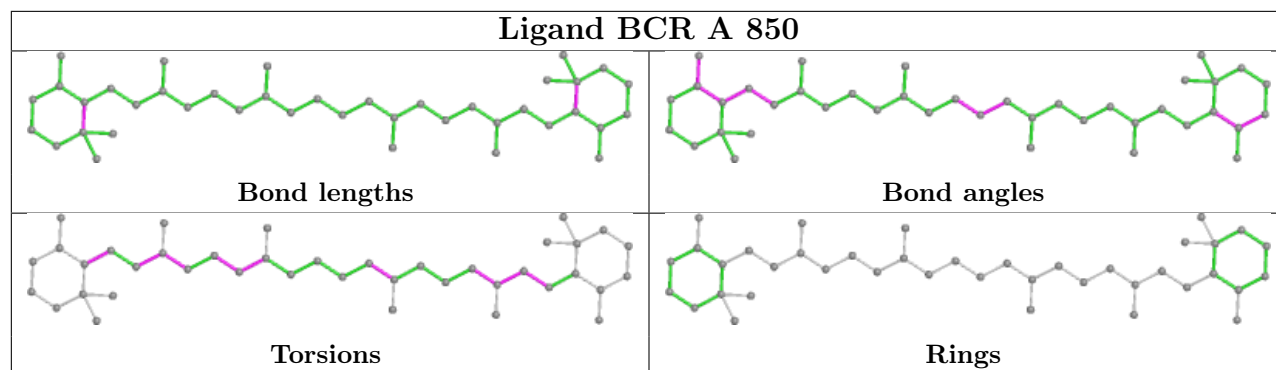


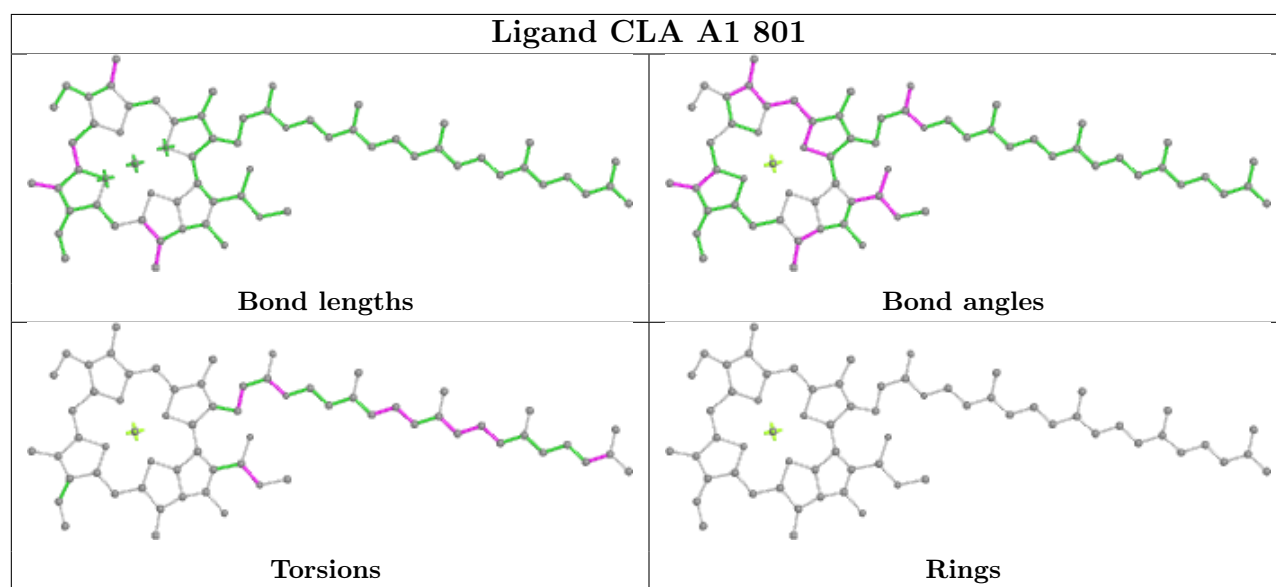
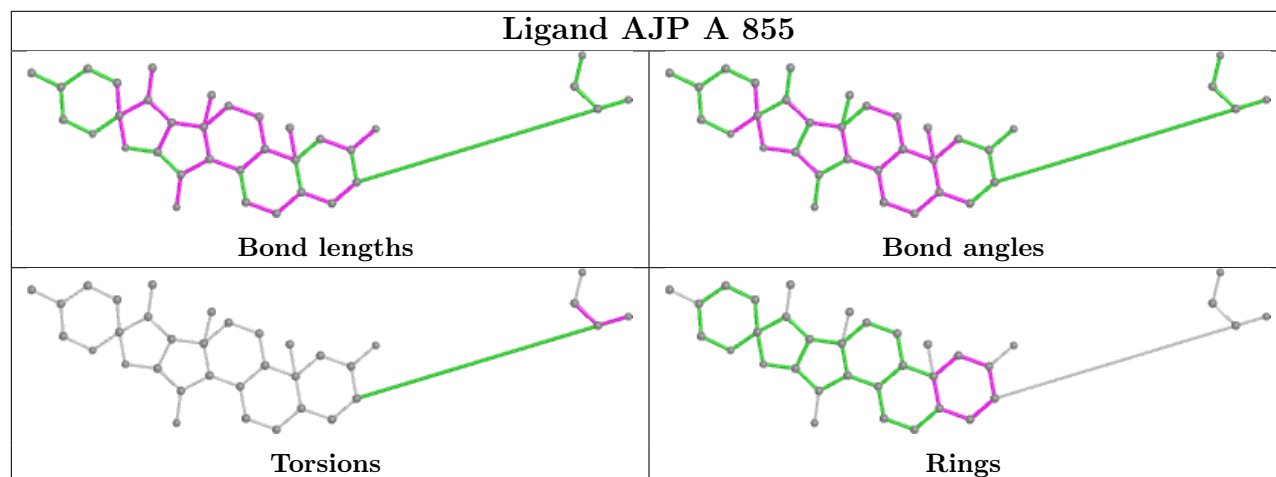
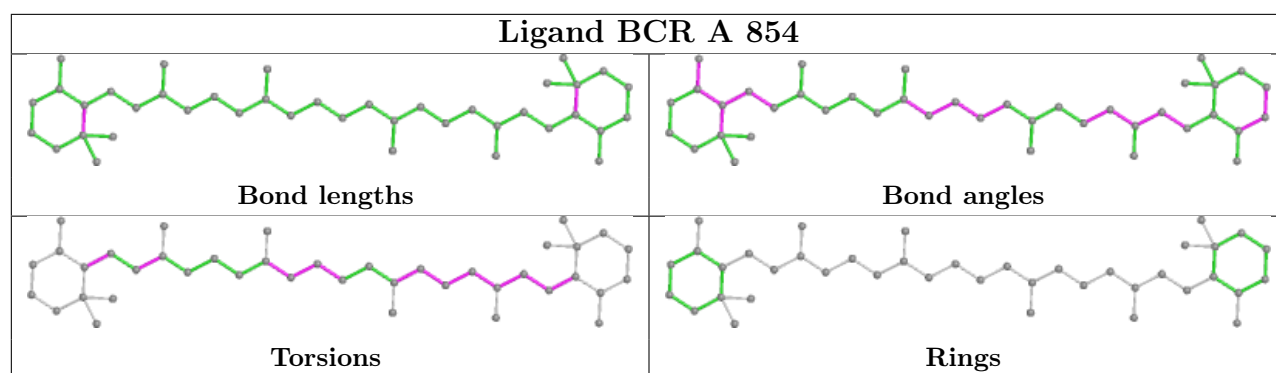
Rings

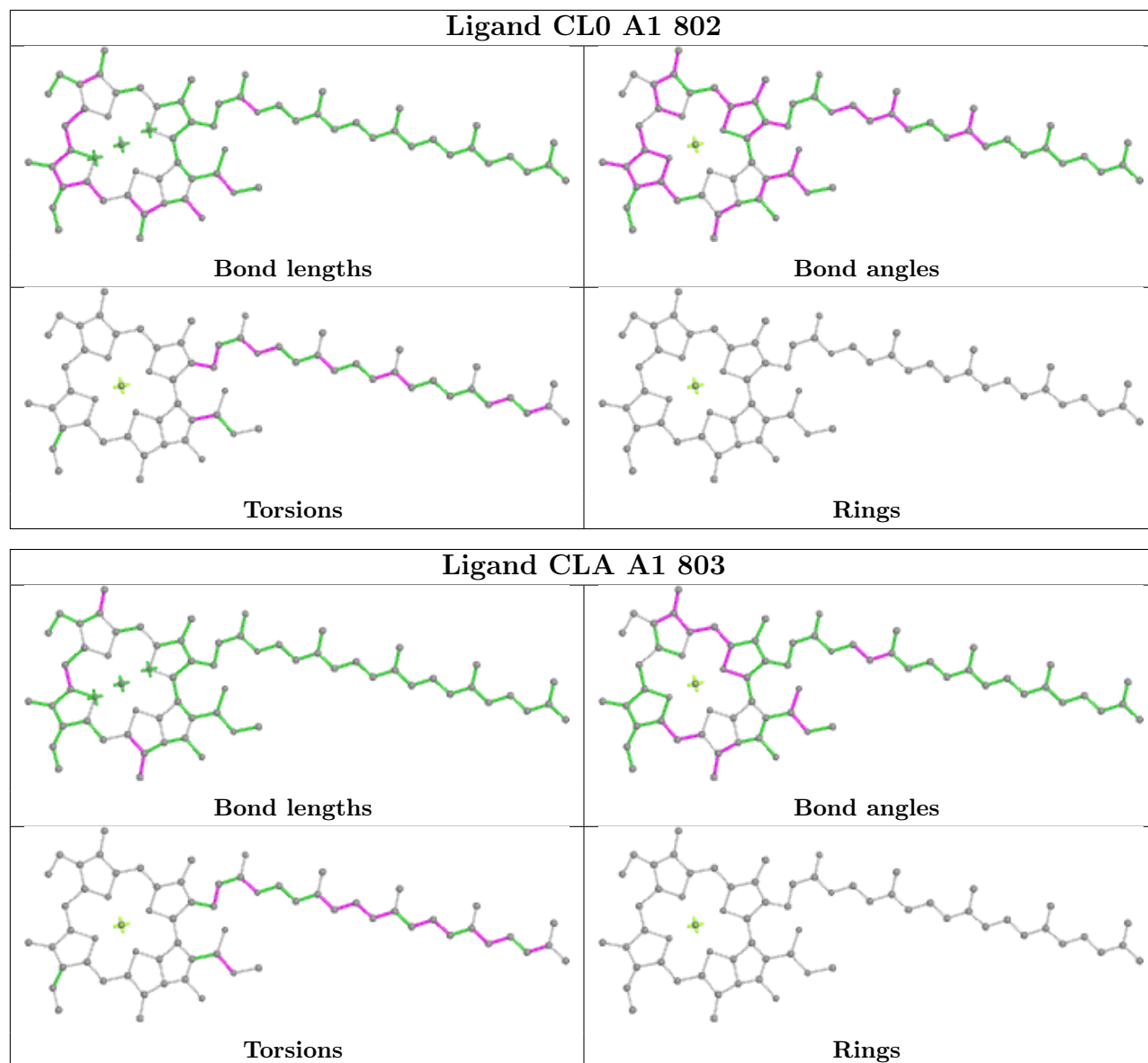




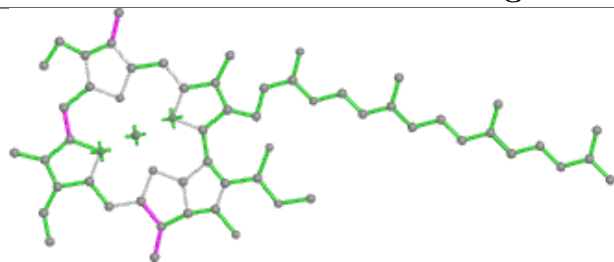




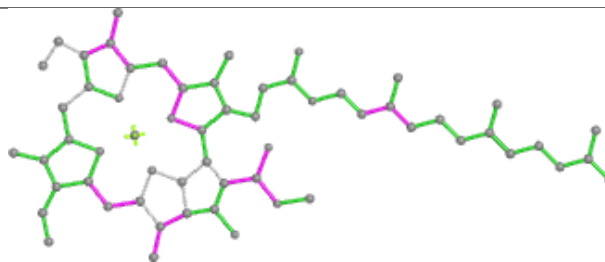




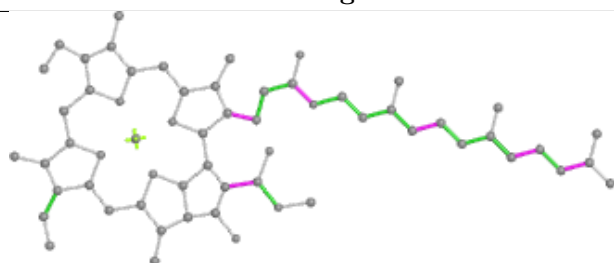
Ligand CLA A1 804



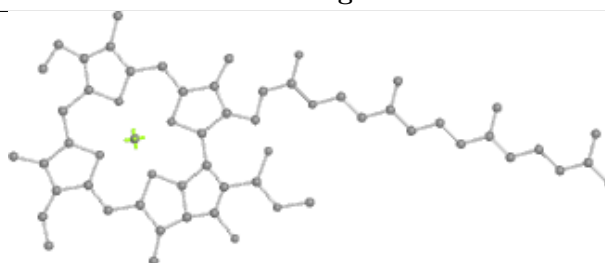
Bond lengths



Bond angles

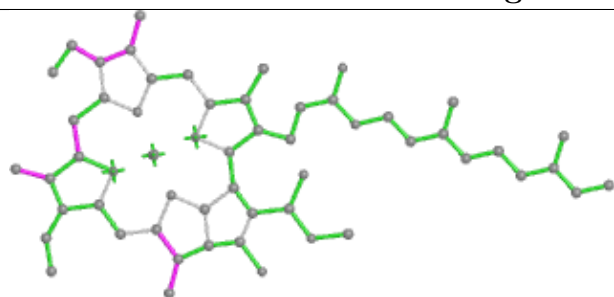


Torsions

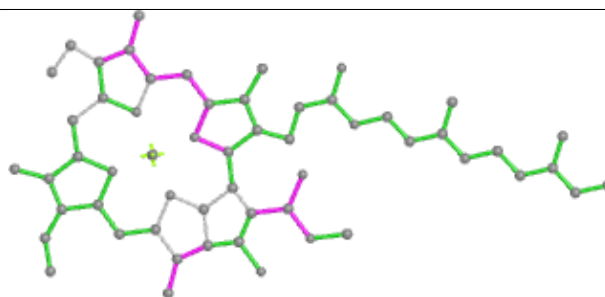


Rings

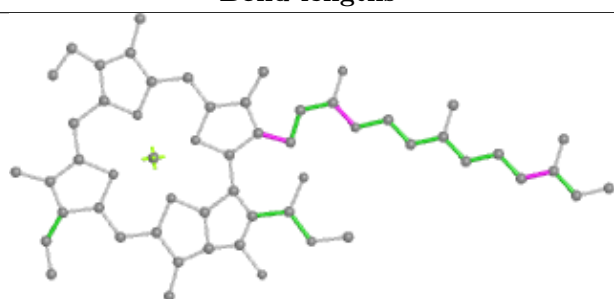
Ligand CLA A1 805



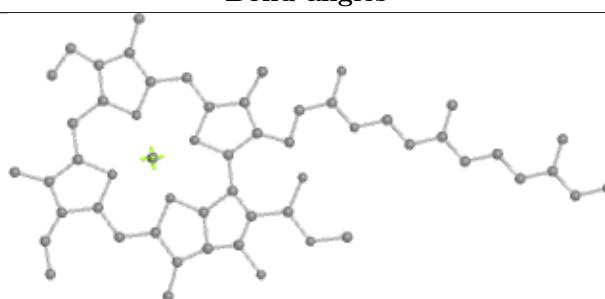
Bond lengths



Bond angles

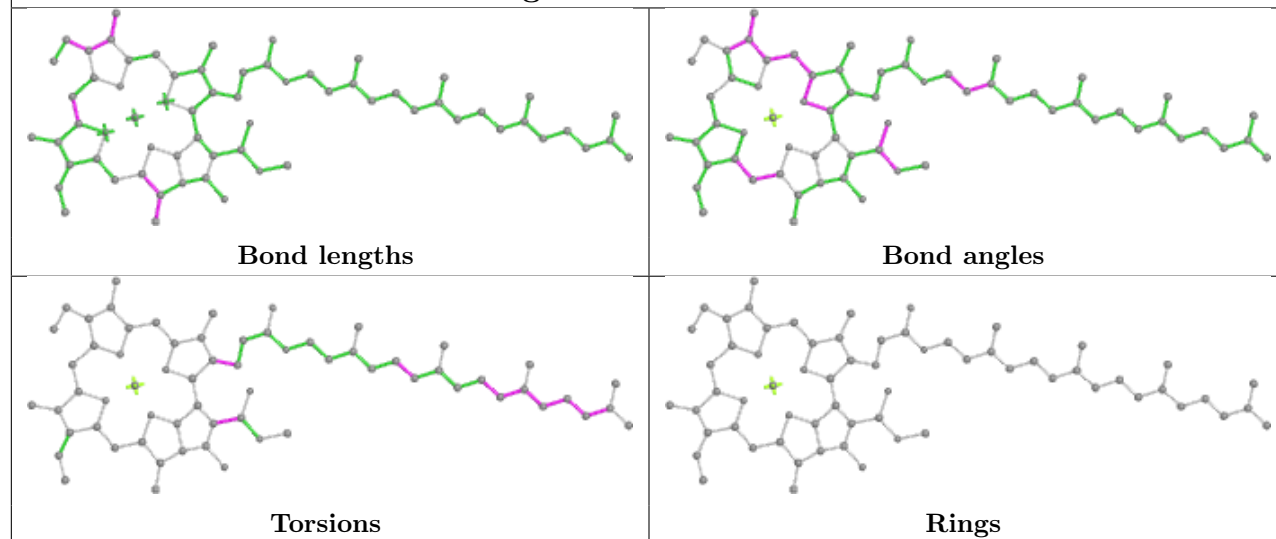


Torsions

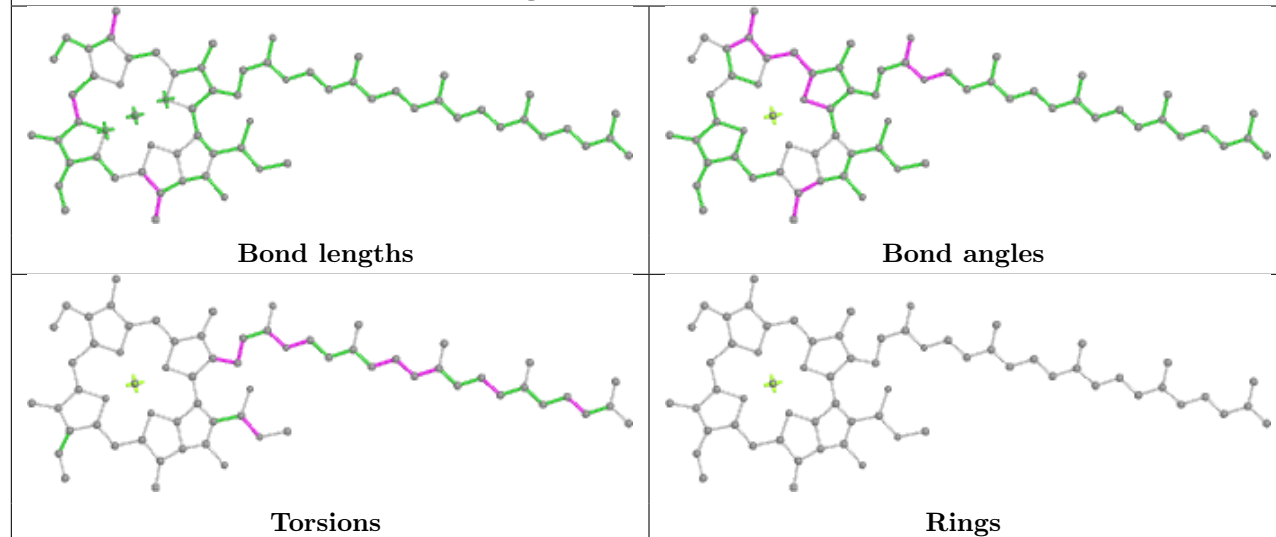


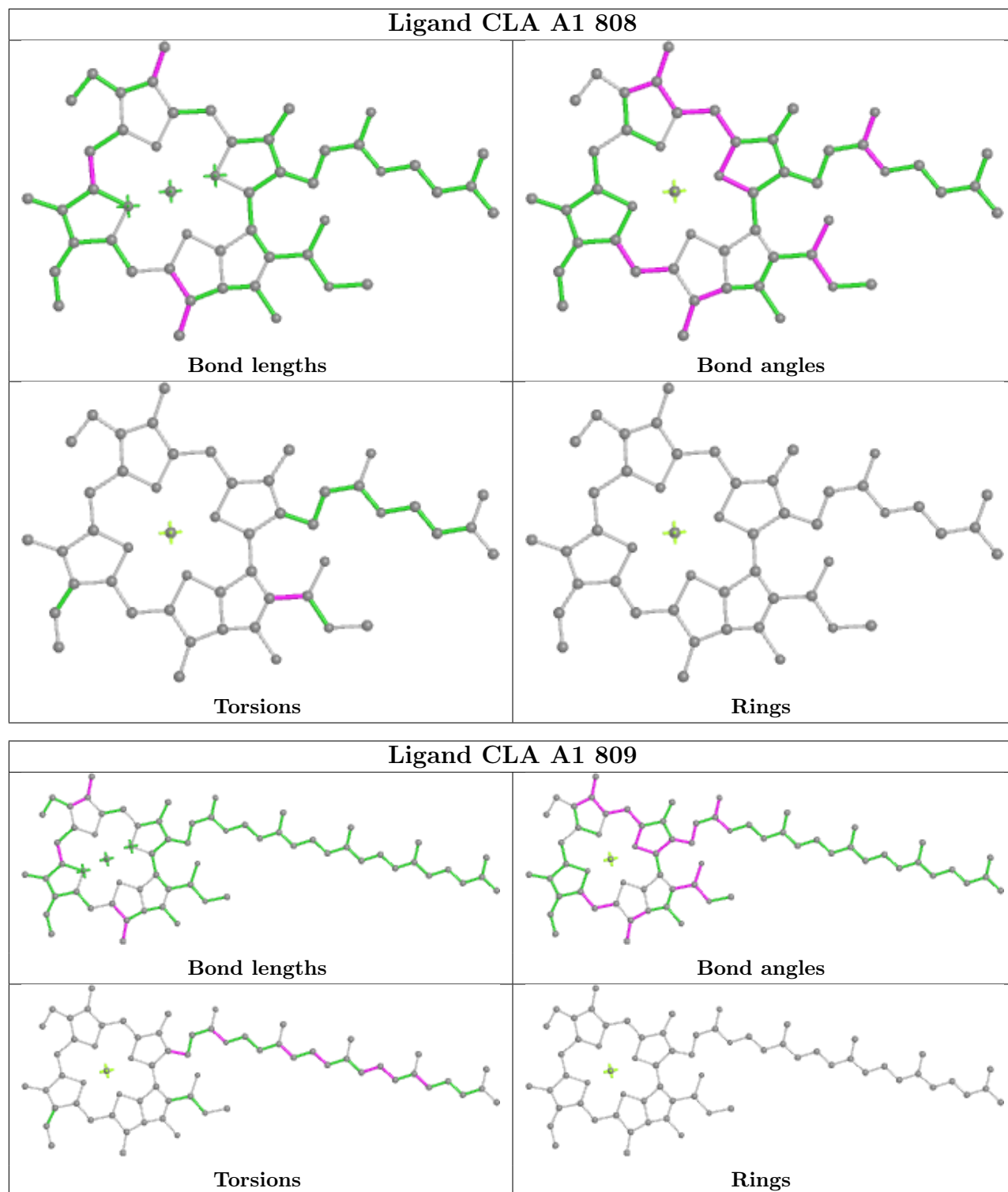
Rings

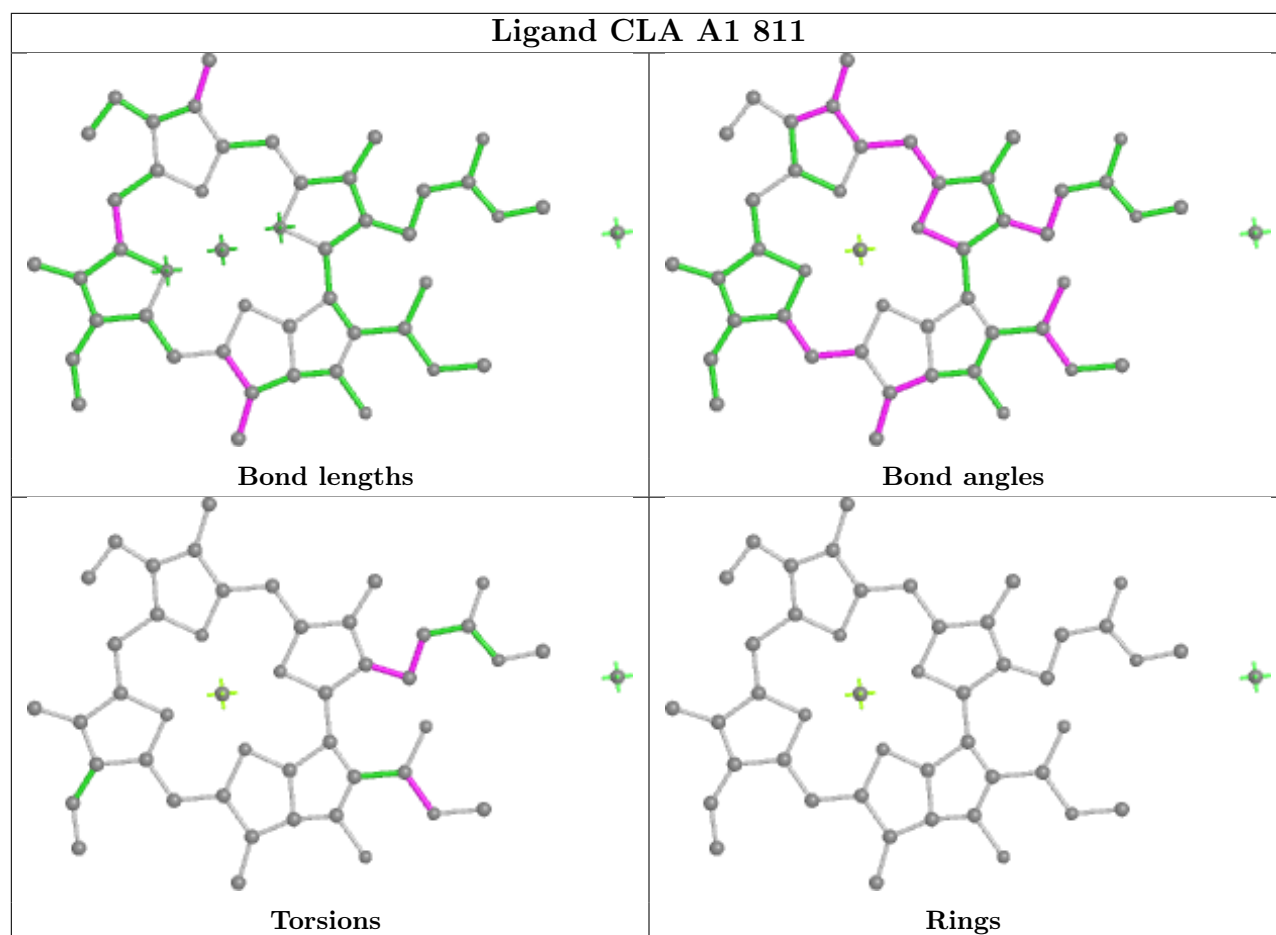
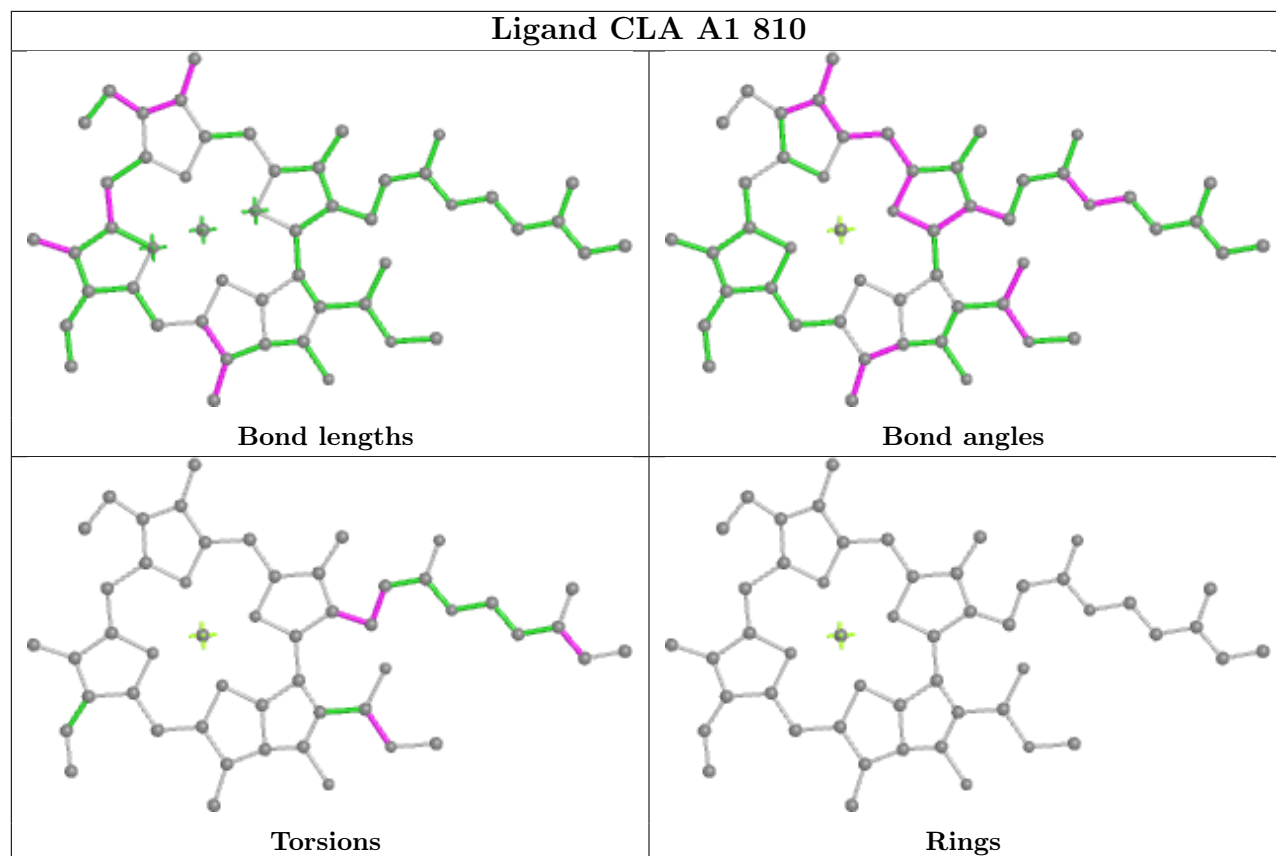
Ligand CLA A1 806



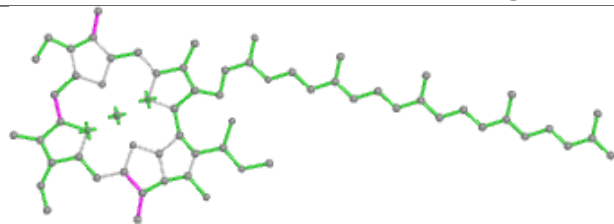
Ligand CLA A1 807



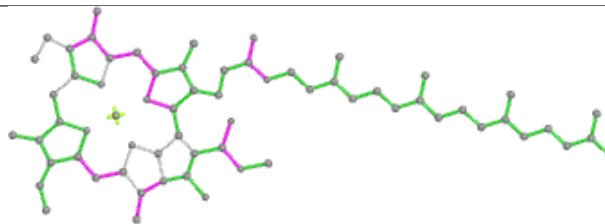




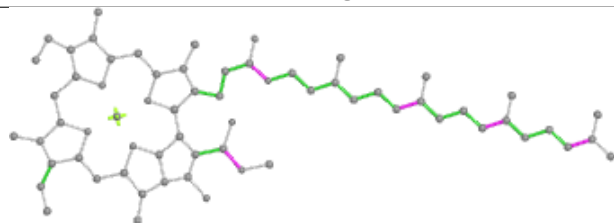
Ligand CLA A1 812



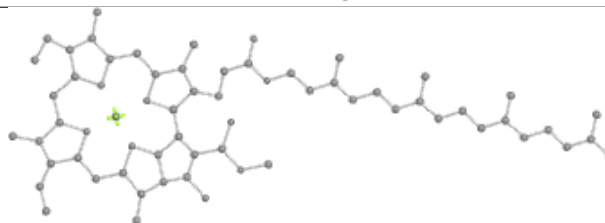
Bond lengths



Bond angles

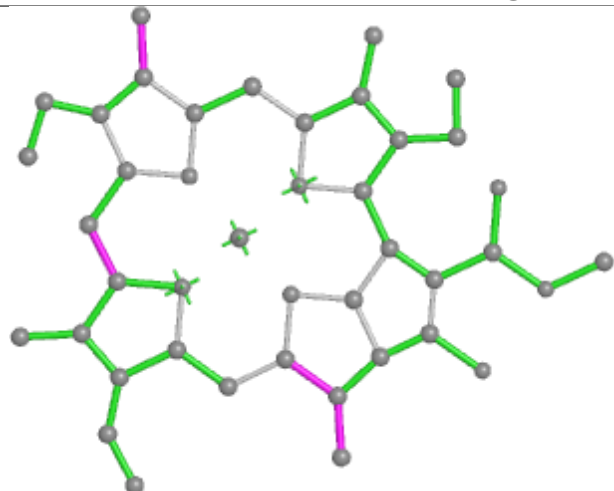


Torsions

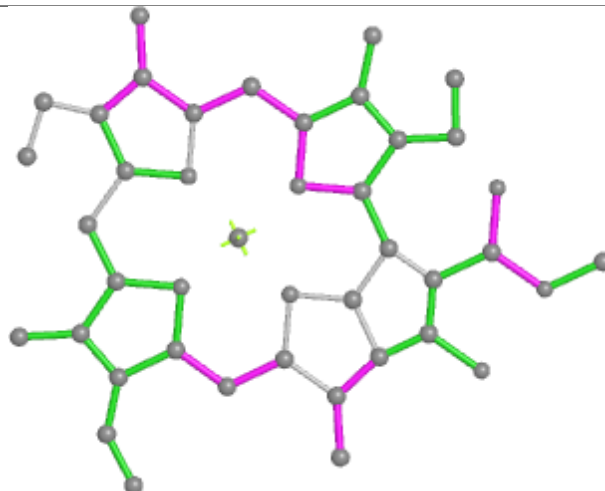


Rings

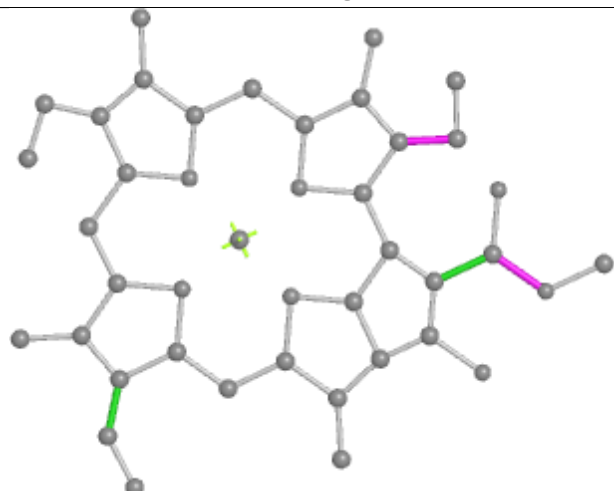
Ligand CLA A1 813



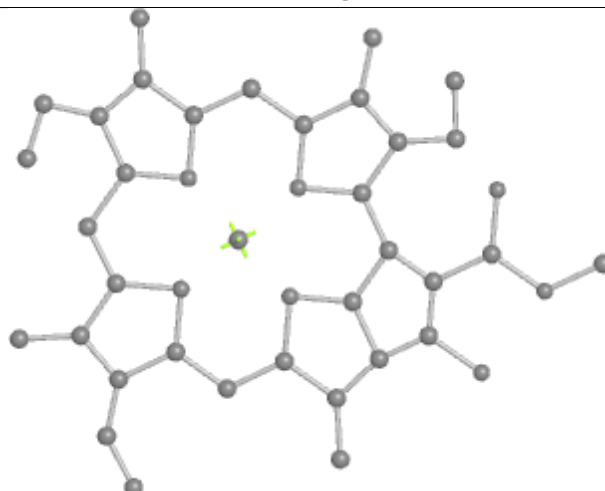
Bond lengths



Bond angles

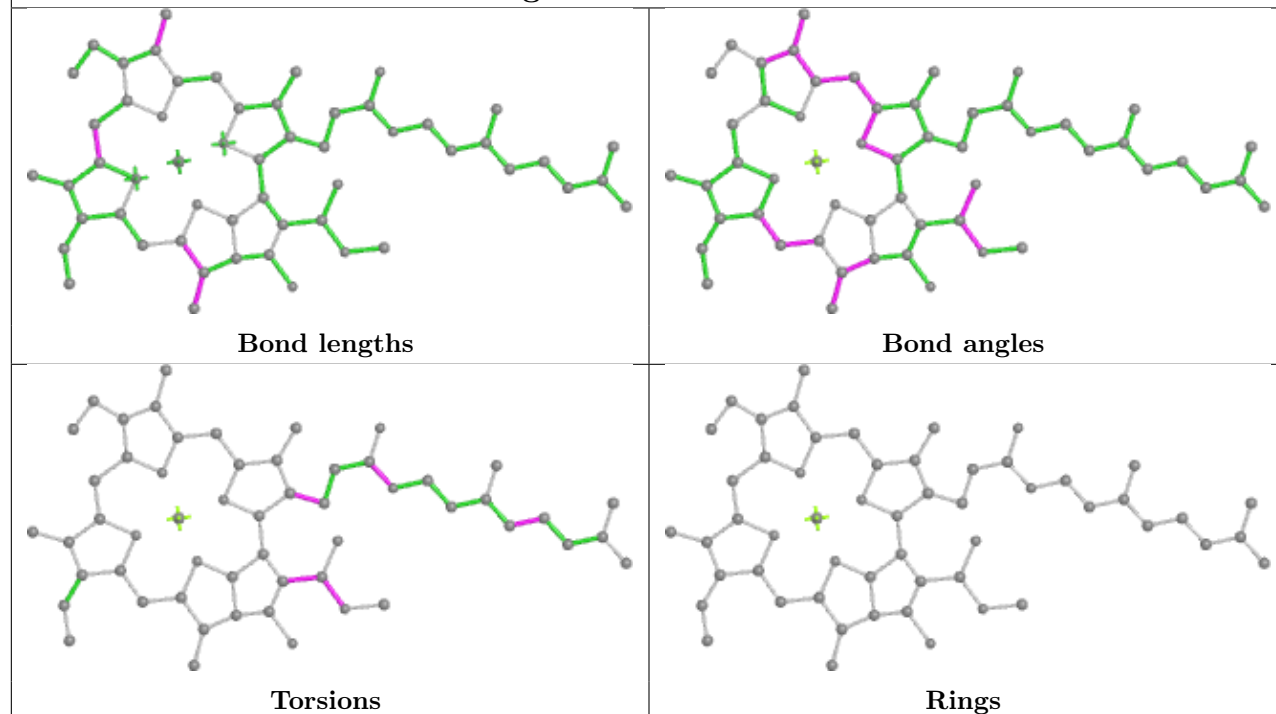


Torsions

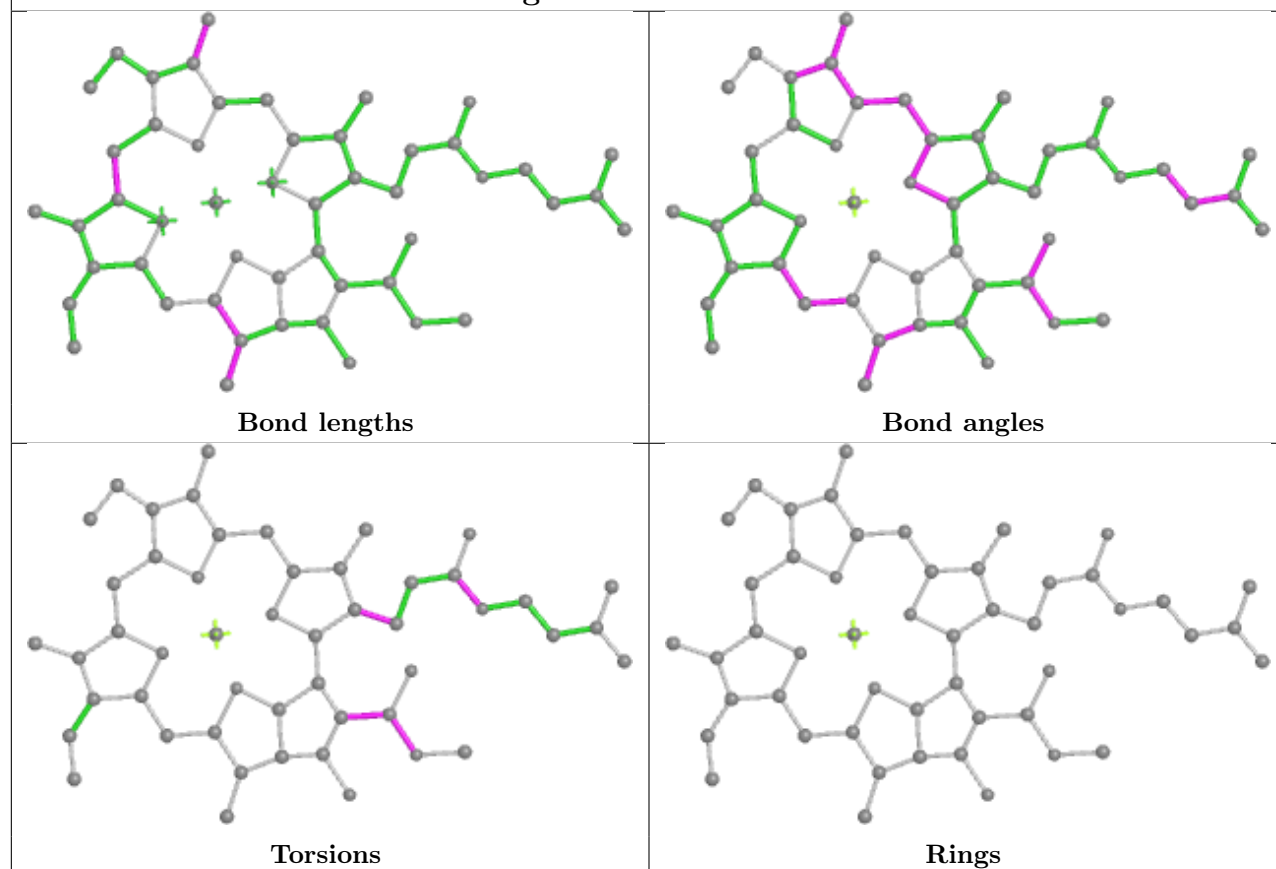


Rings

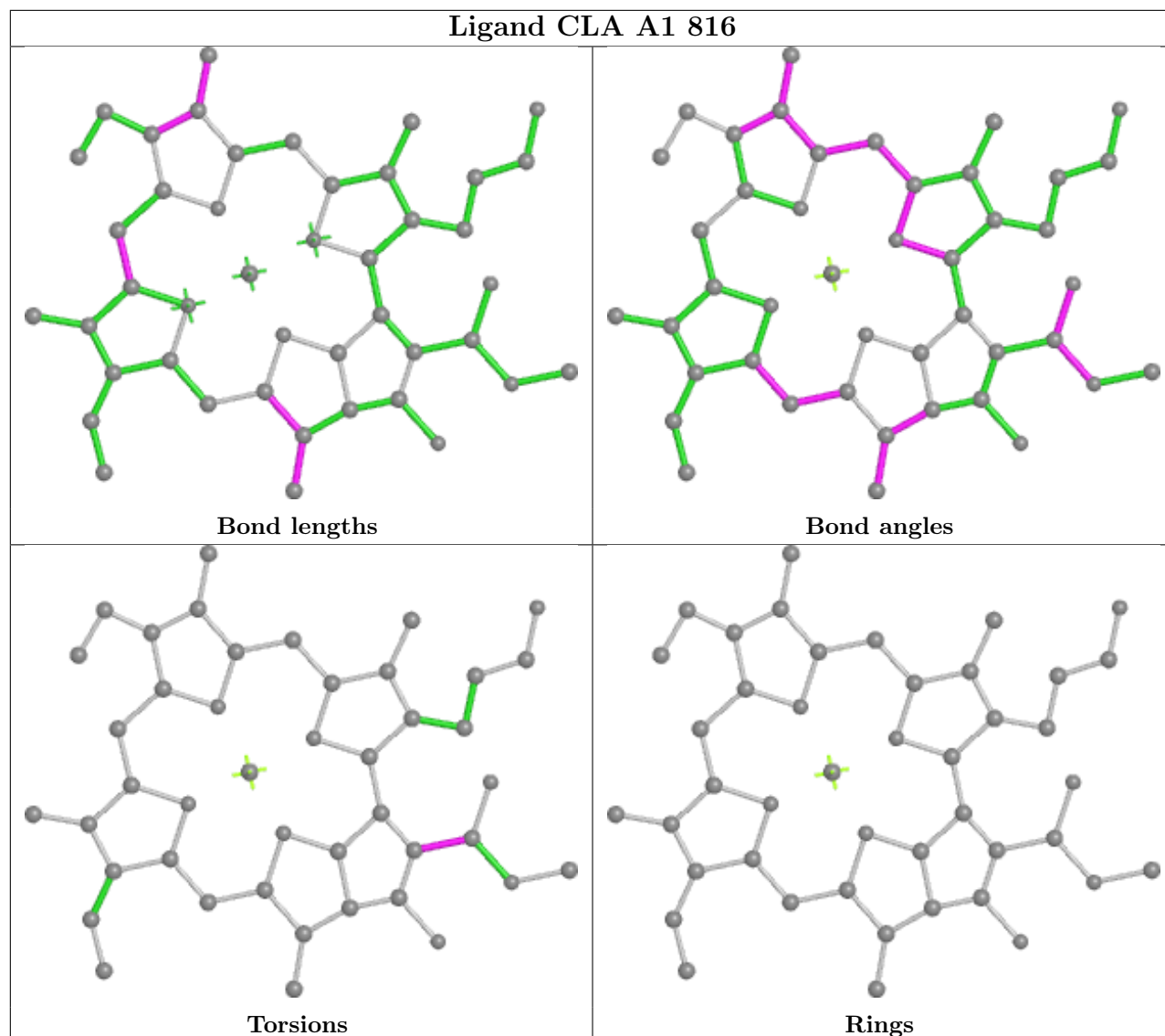
Ligand CLA A1 814



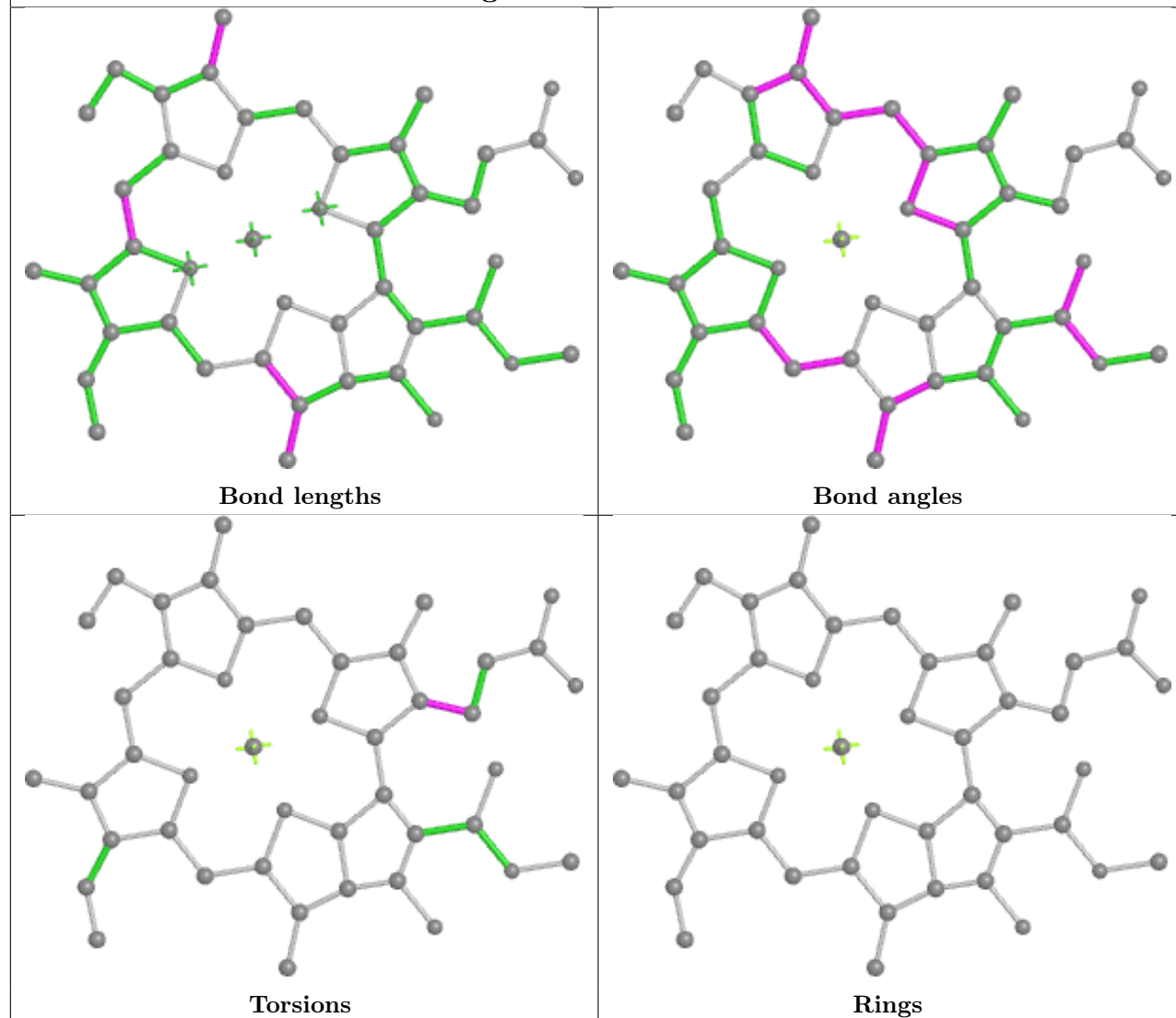
Ligand CLA A1 815



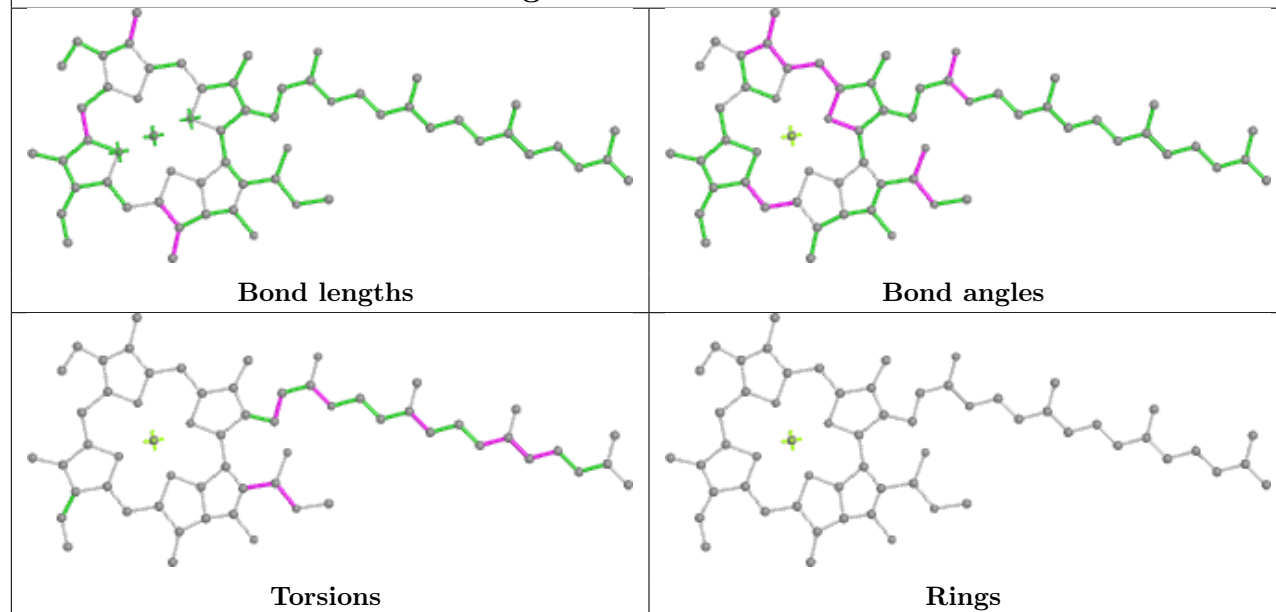
Ligand CLA A1 816



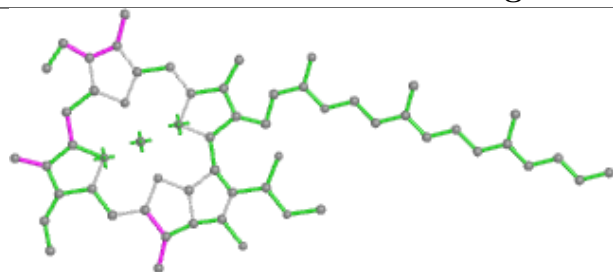
Ligand CLA A1 817



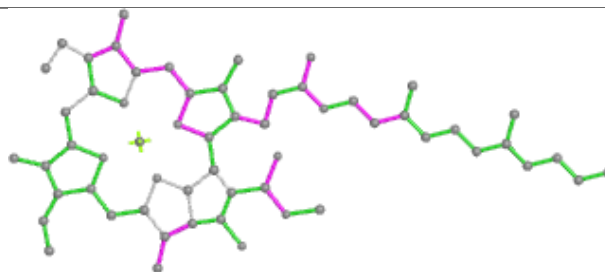
Ligand CLA A1 818



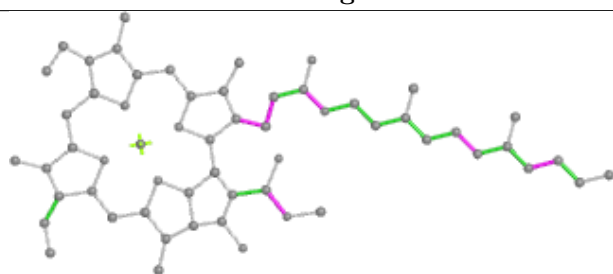
Ligand CLA A1 819



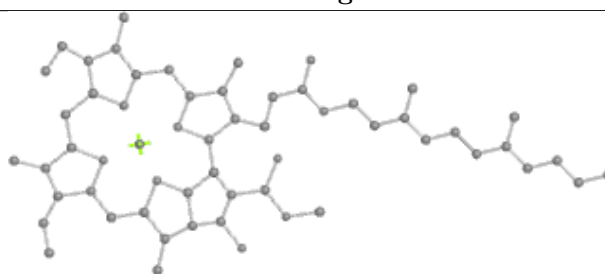
Bond lengths



Bond angles

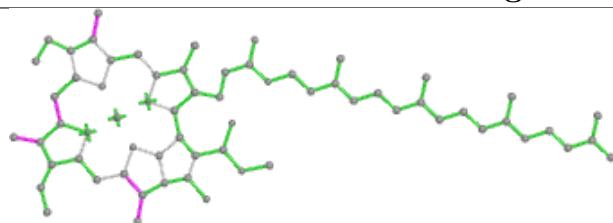


Torsions

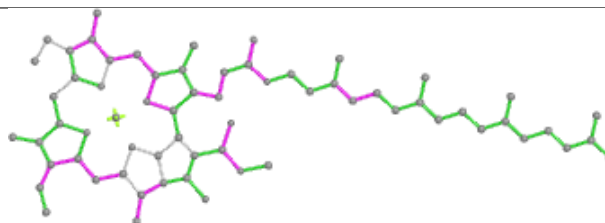


Rings

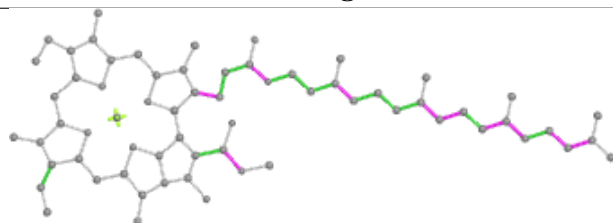
Ligand CLA A1 820



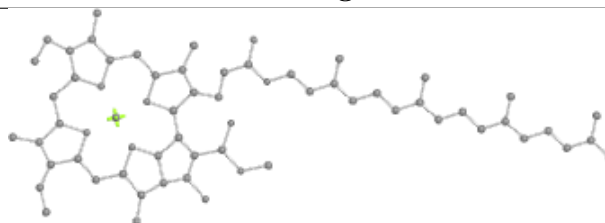
Bond lengths



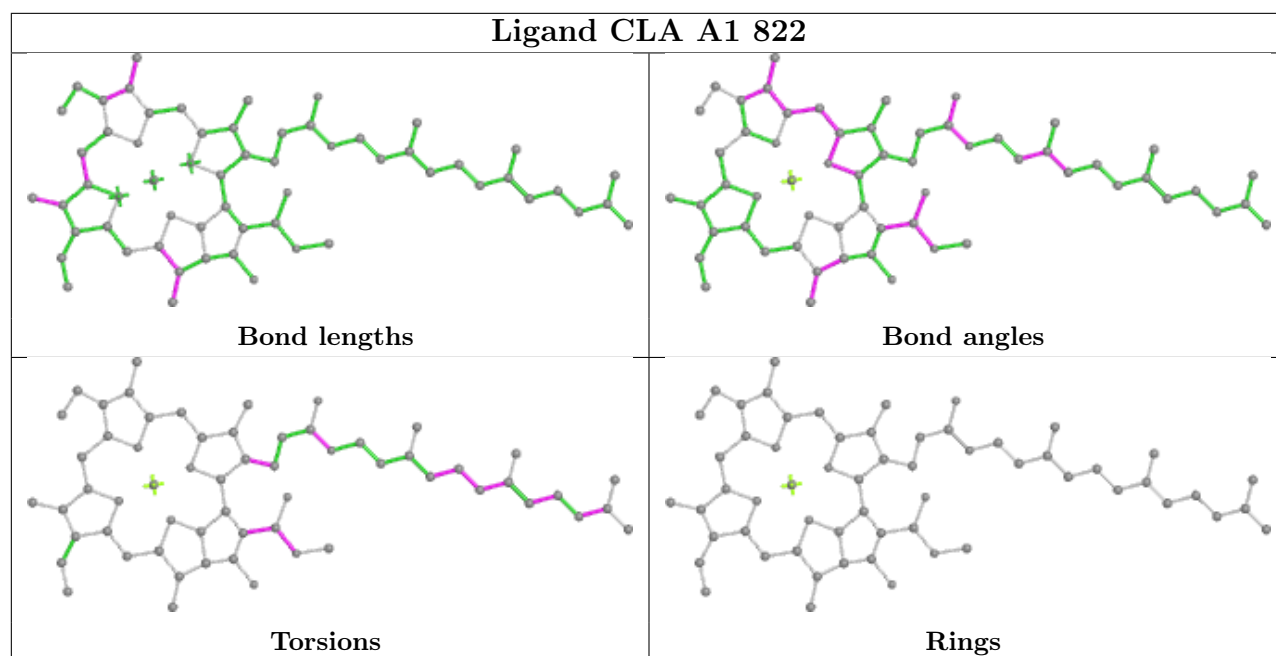
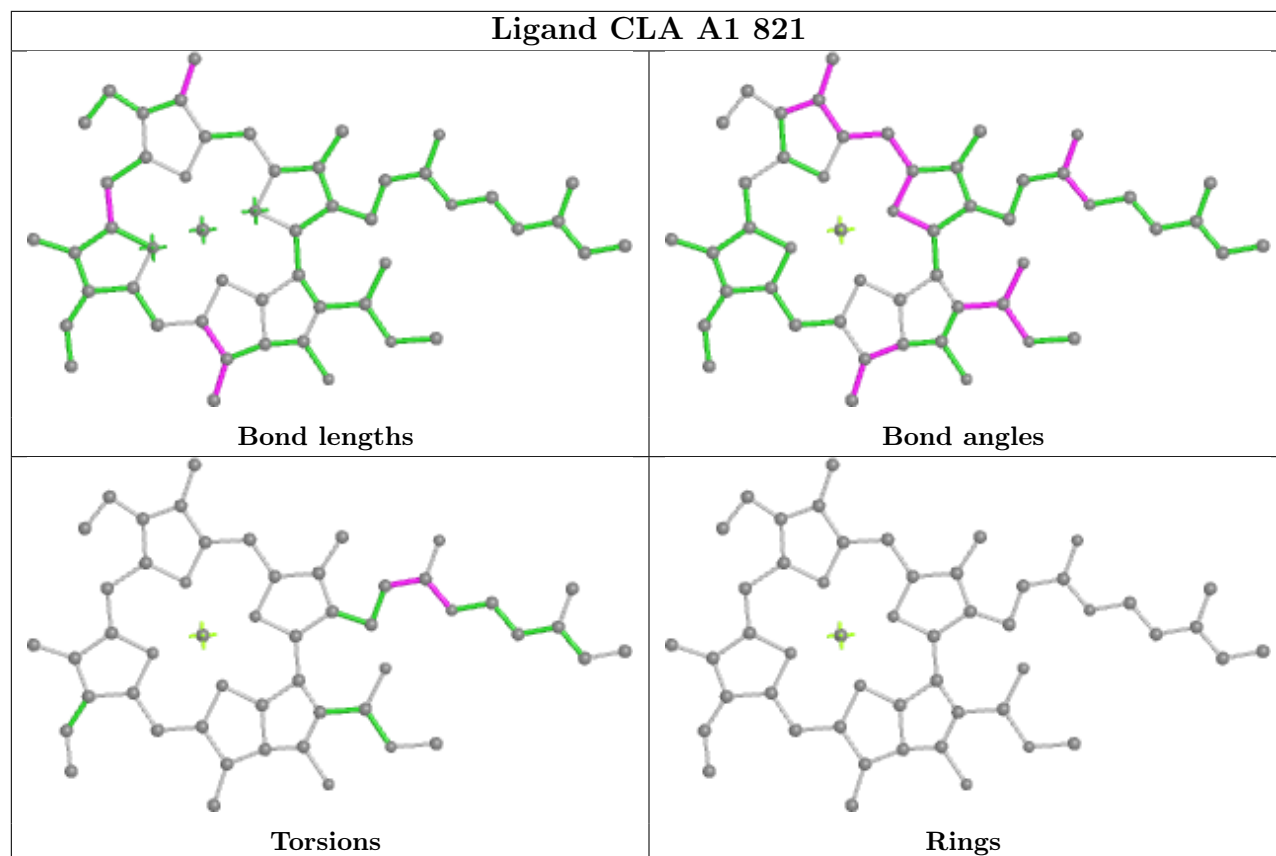
Bond angles



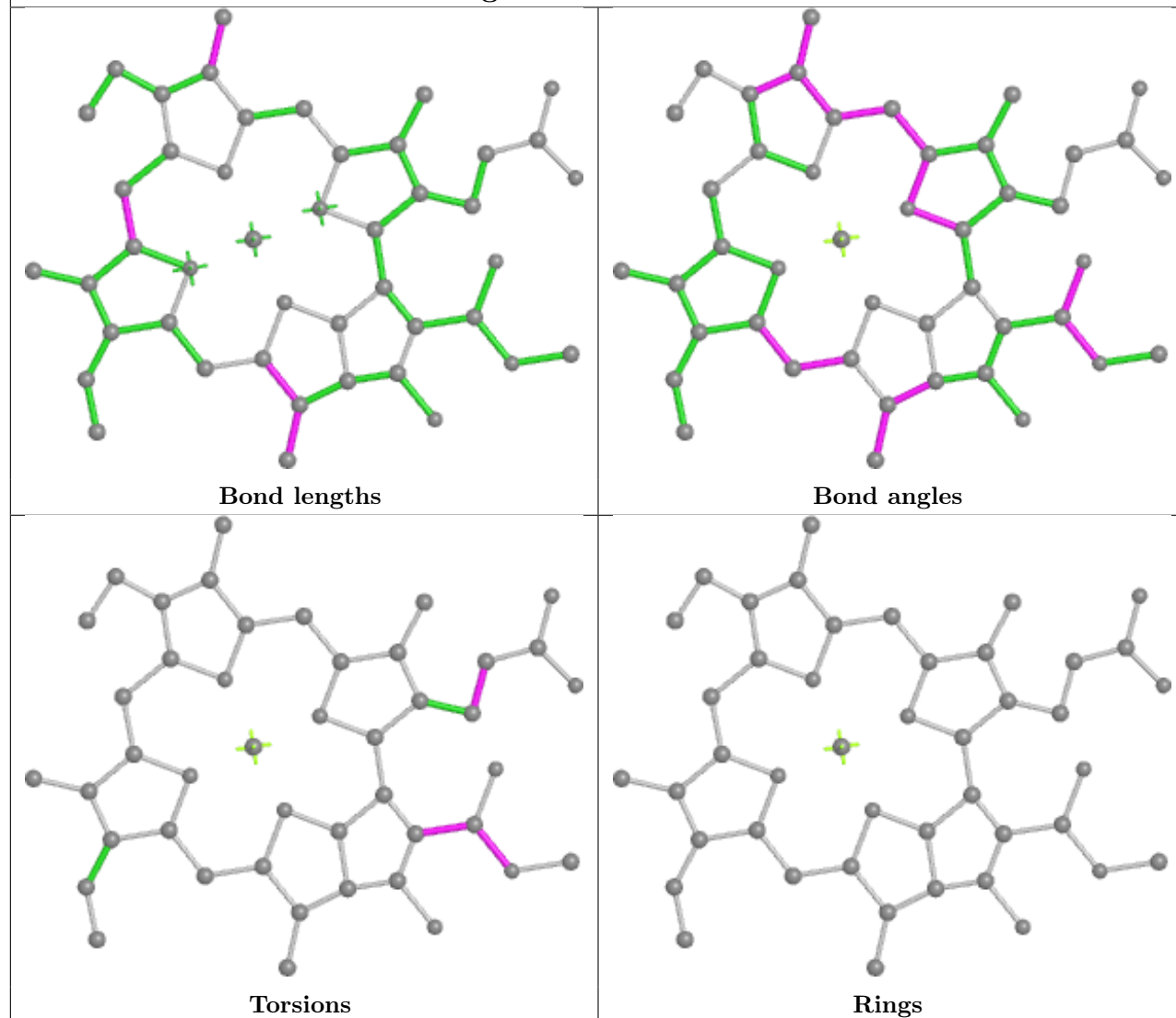
Torsions



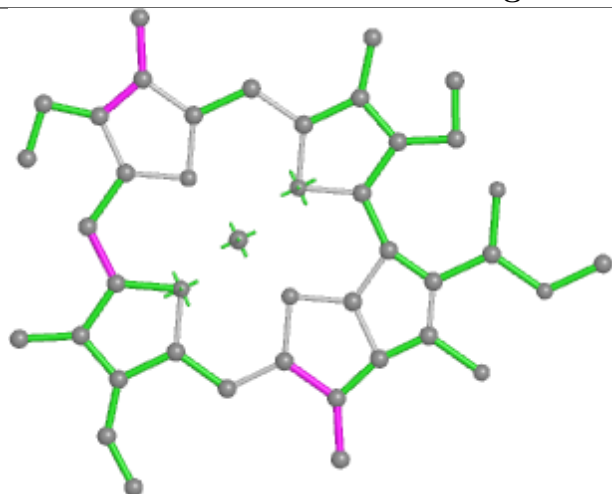
Rings



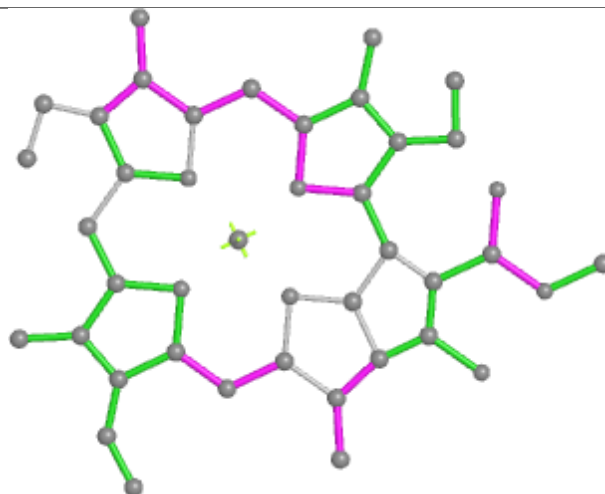
Ligand CLA A1 823



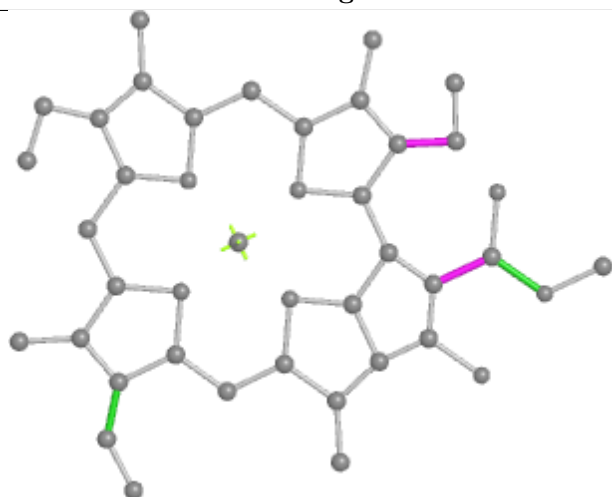
Ligand CLA A1 824



Bond lengths



Bond angles

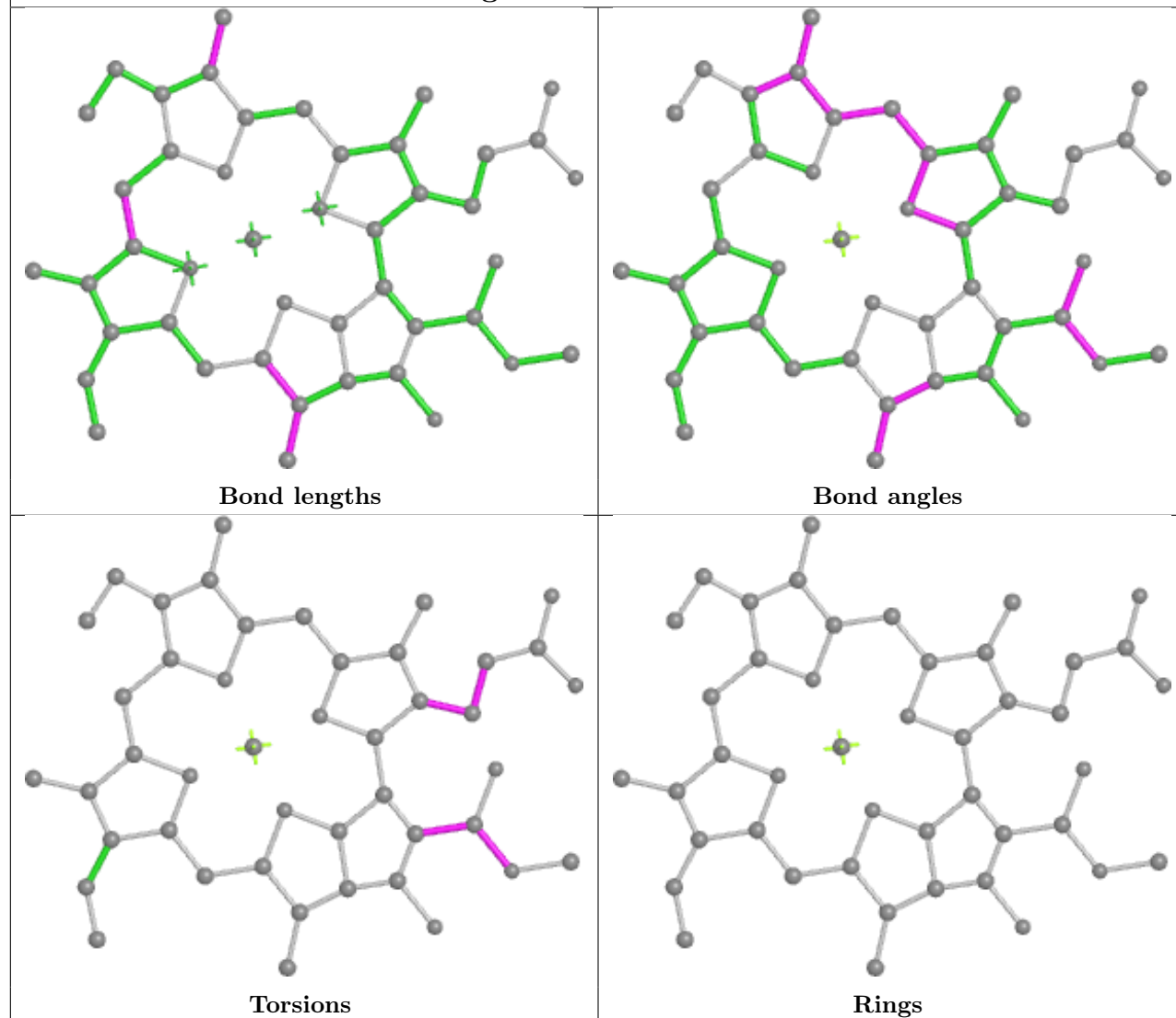


Torsions

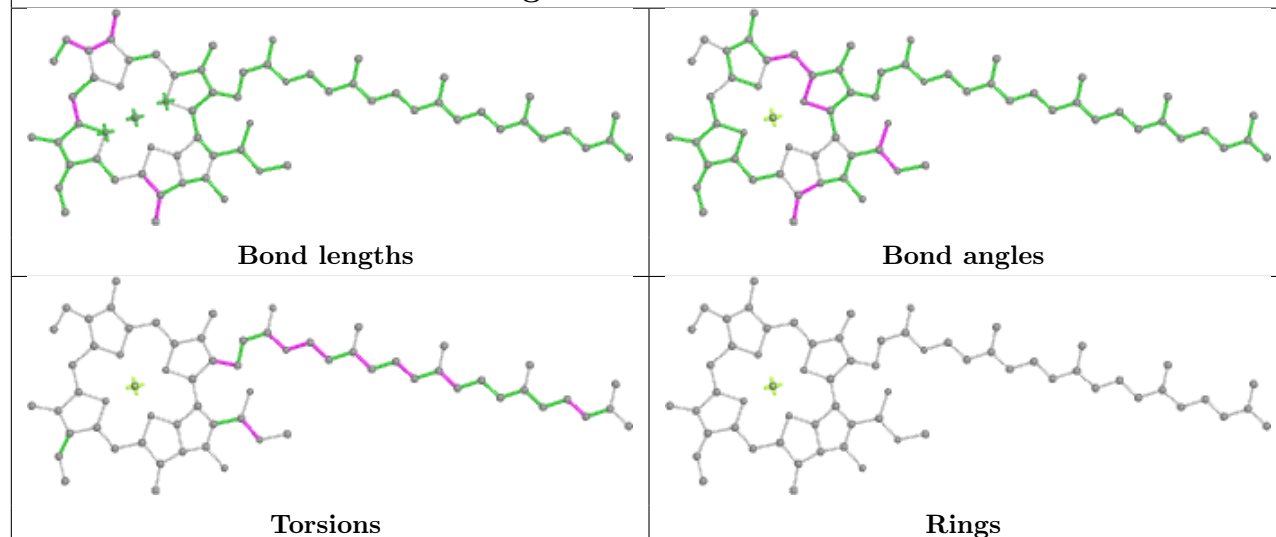


Rings

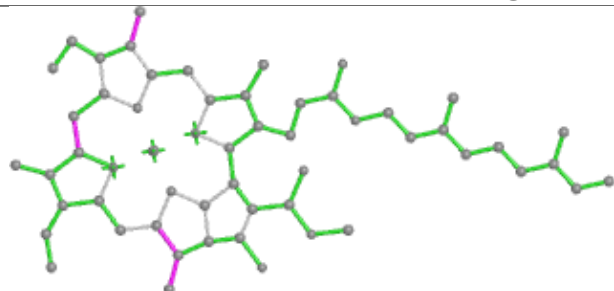
Ligand CLA A1 825



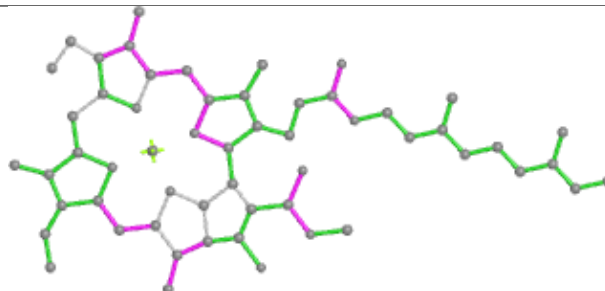
Ligand CLA A1 826



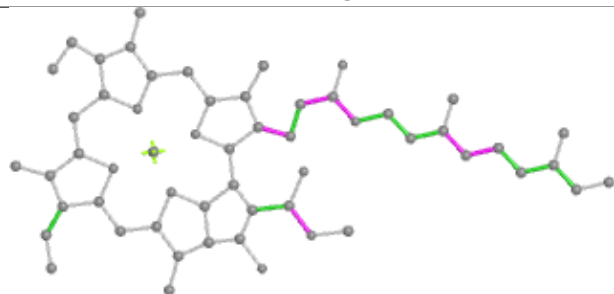
Ligand CLA A1 827



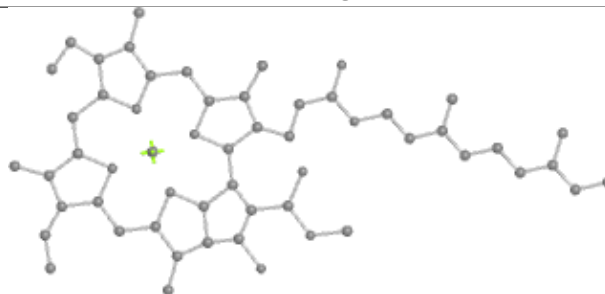
Bond lengths



Bond angles

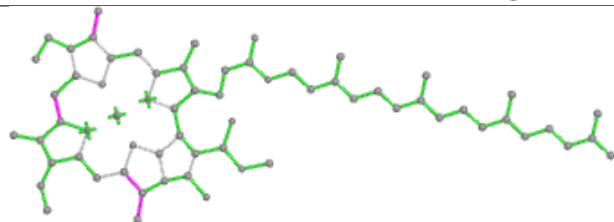


Torsions

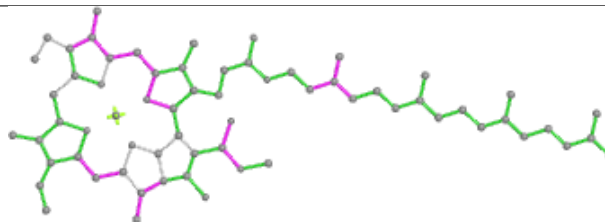


Rings

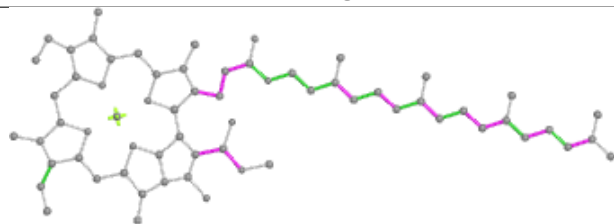
Ligand CLA A1 828



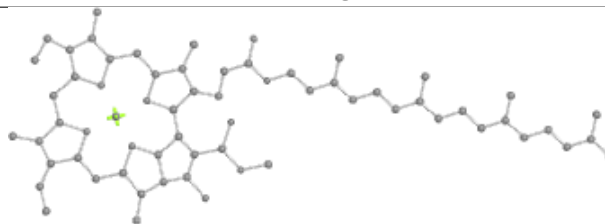
Bond lengths



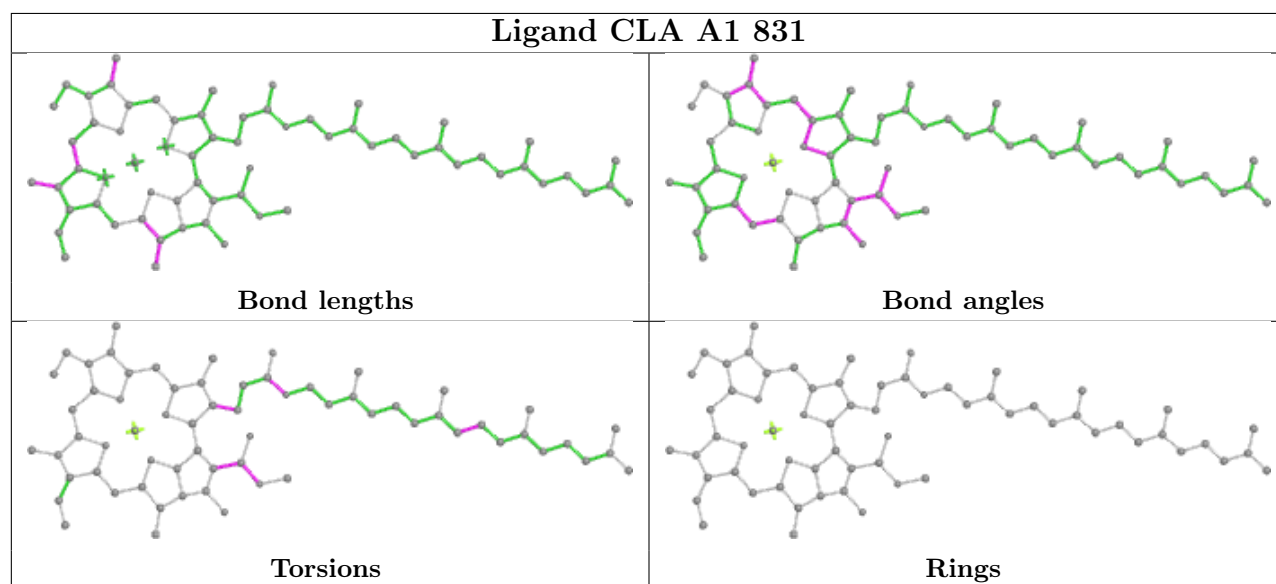
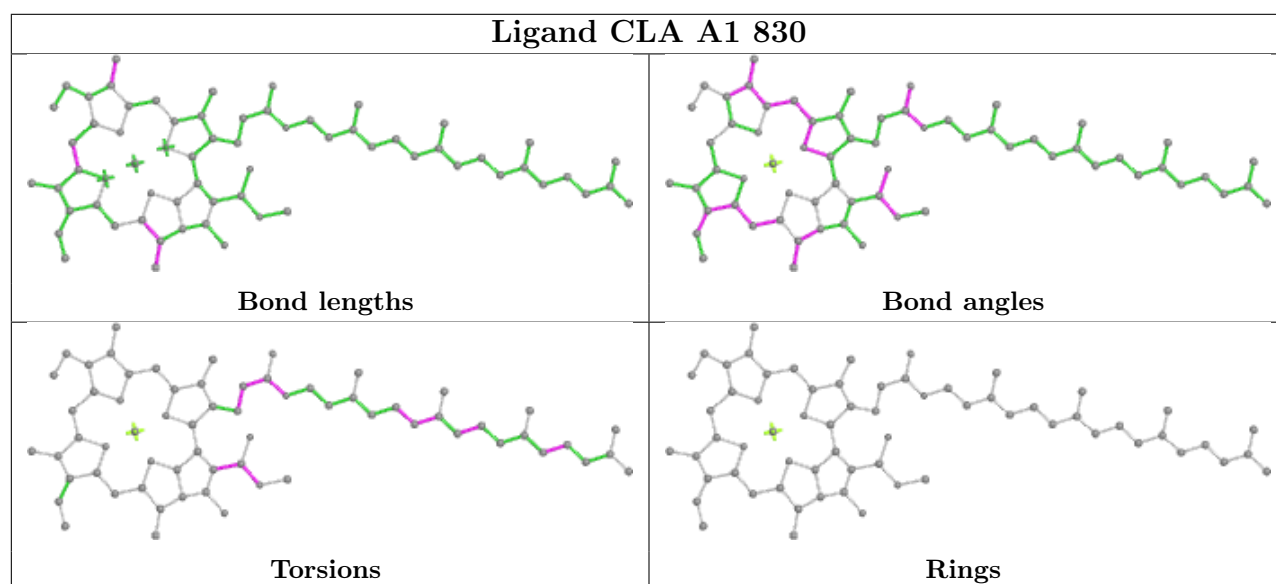
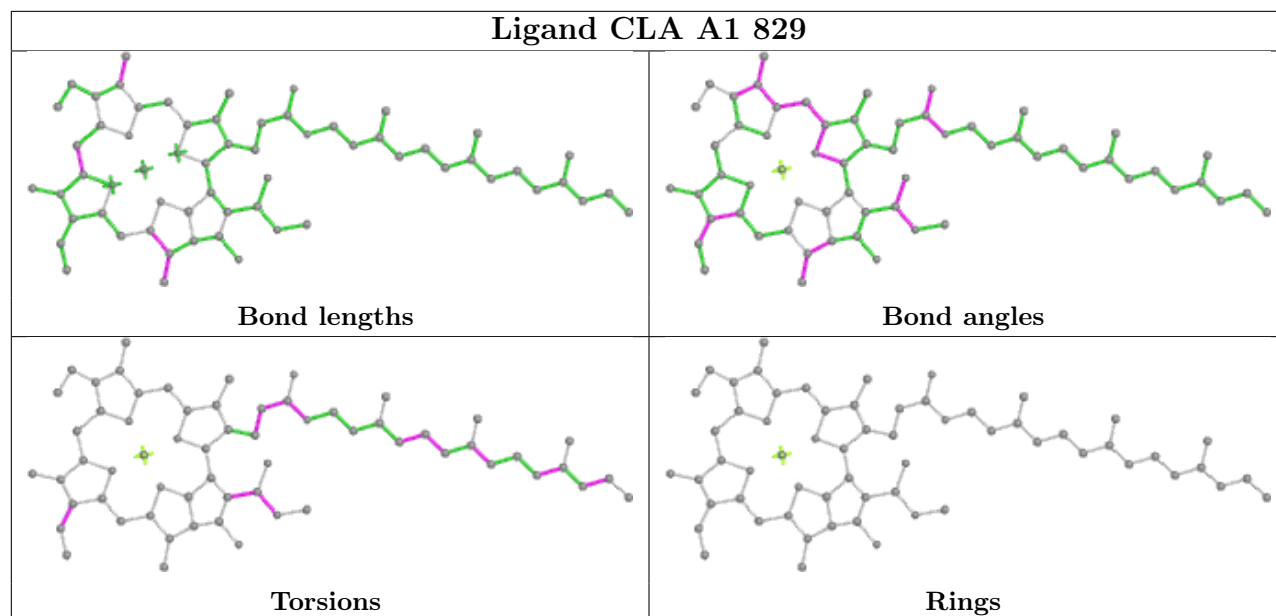
Bond angles



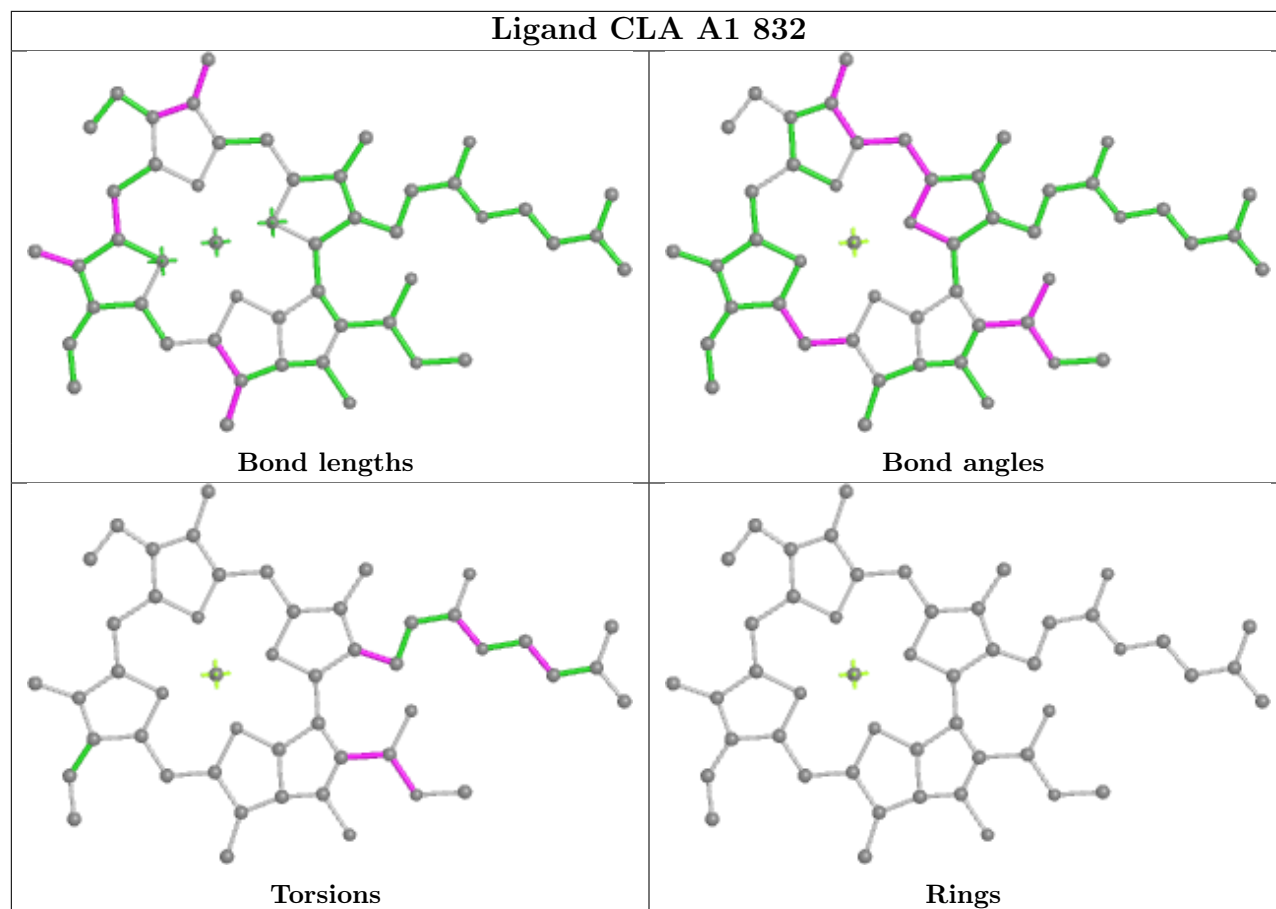
Torsions



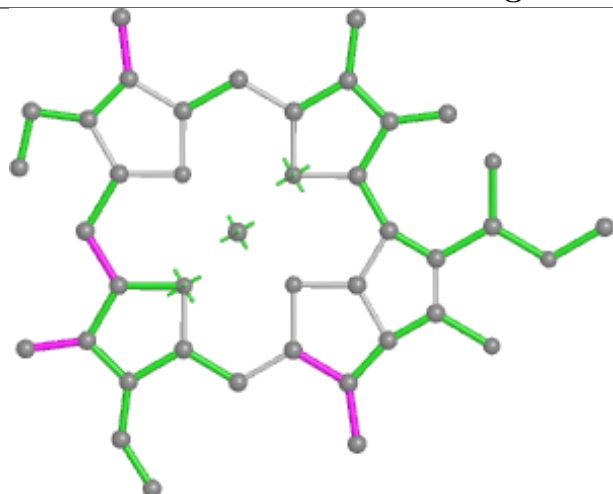
Rings



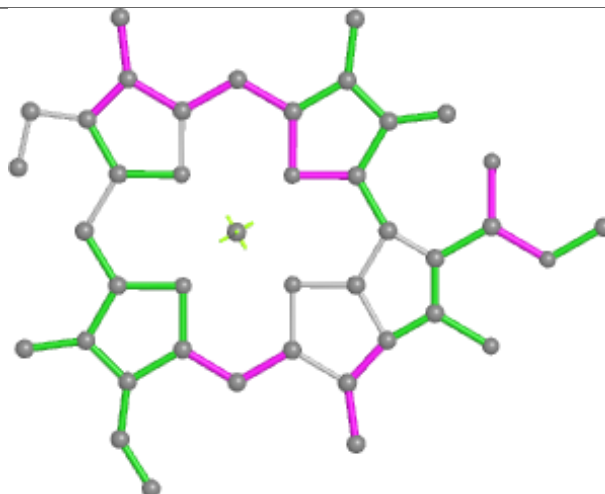
Ligand CLA A1 832



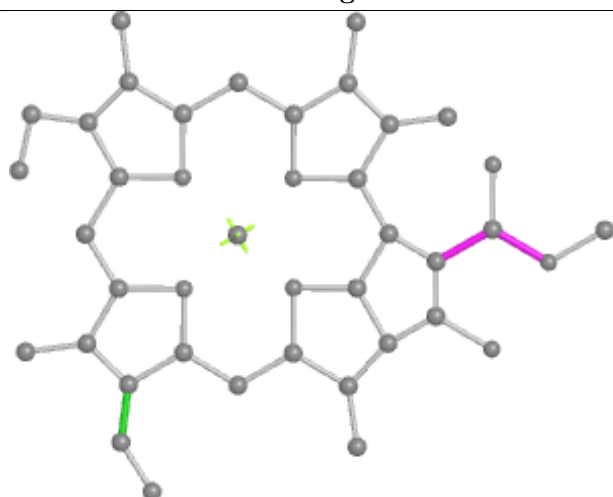
Ligand CLA A1 833



Bond lengths



Bond angles

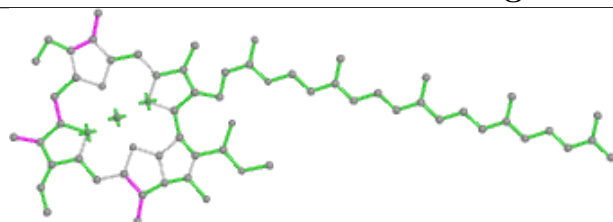


Torsions

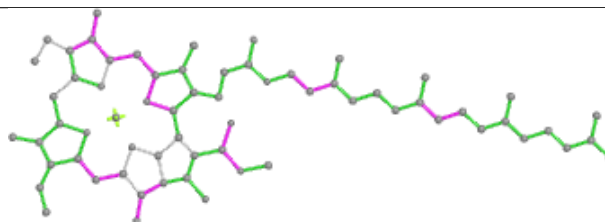


Rings

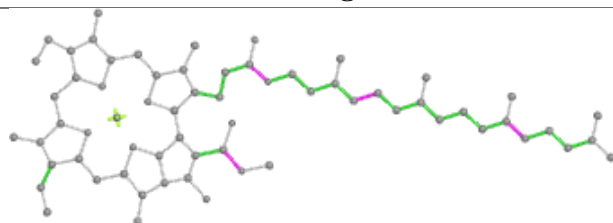
Ligand CLA A1 834



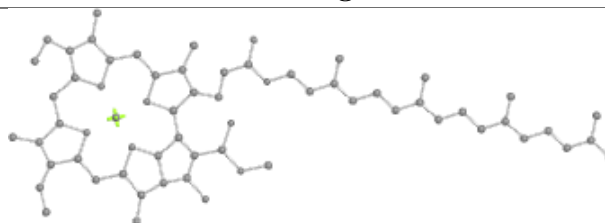
Bond lengths



Bond angles

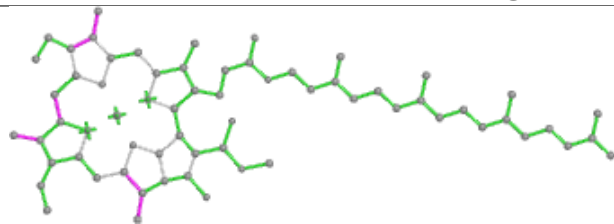


Torsions

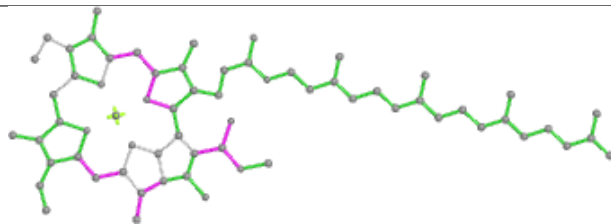


Rings

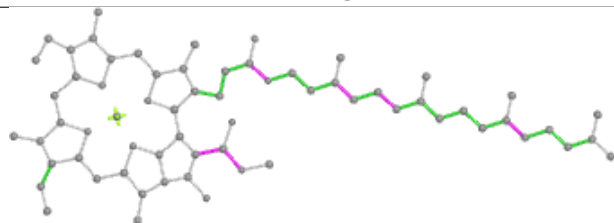
Ligand CLA A1 835



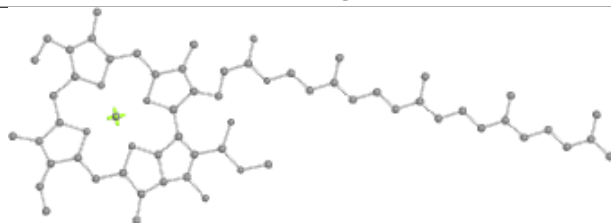
Bond lengths



Bond angles

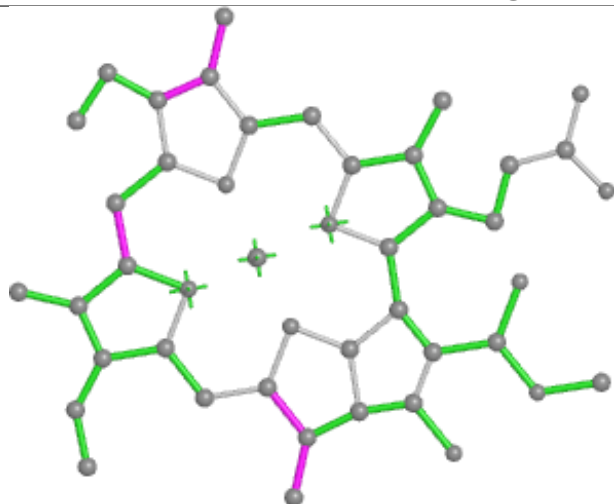


Torsions

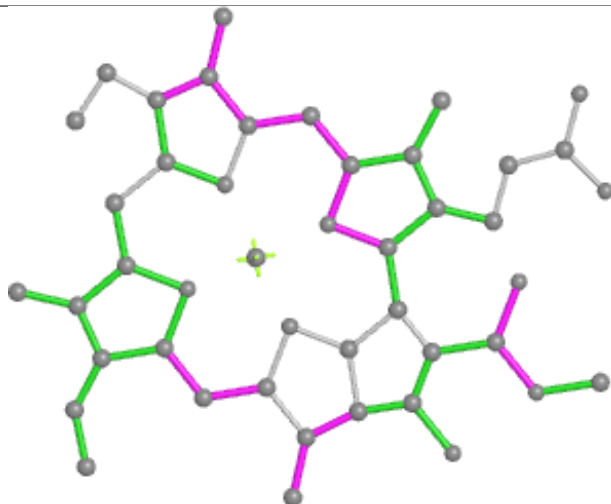


Rings

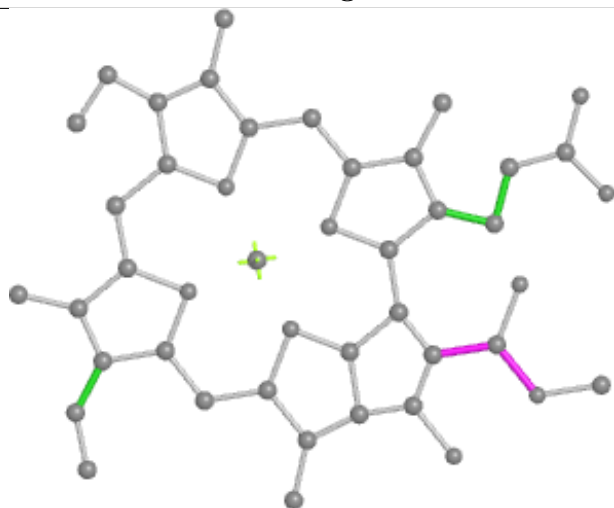
Ligand CLA A1 836



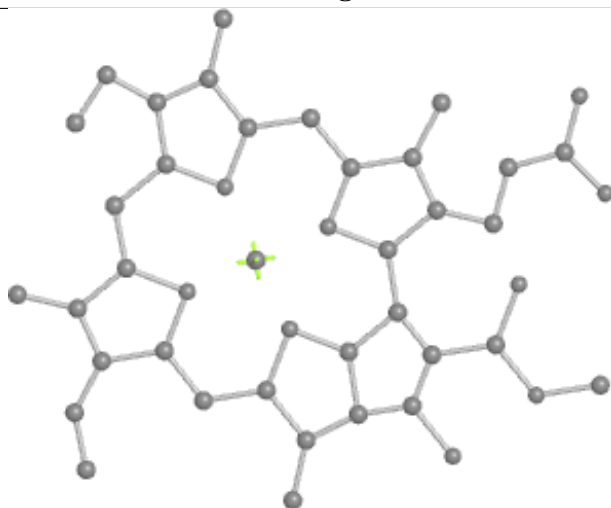
Bond lengths



Bond angles

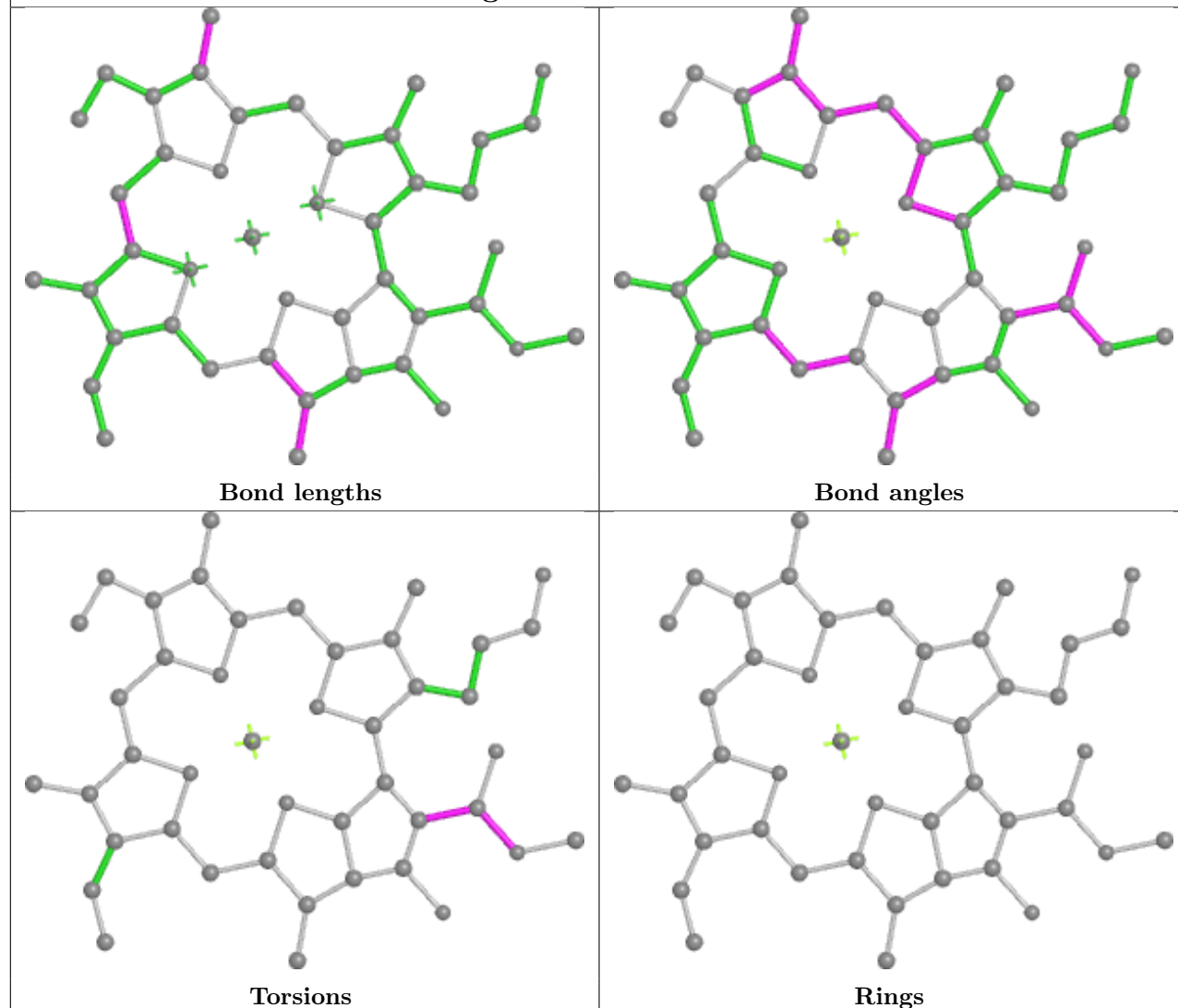


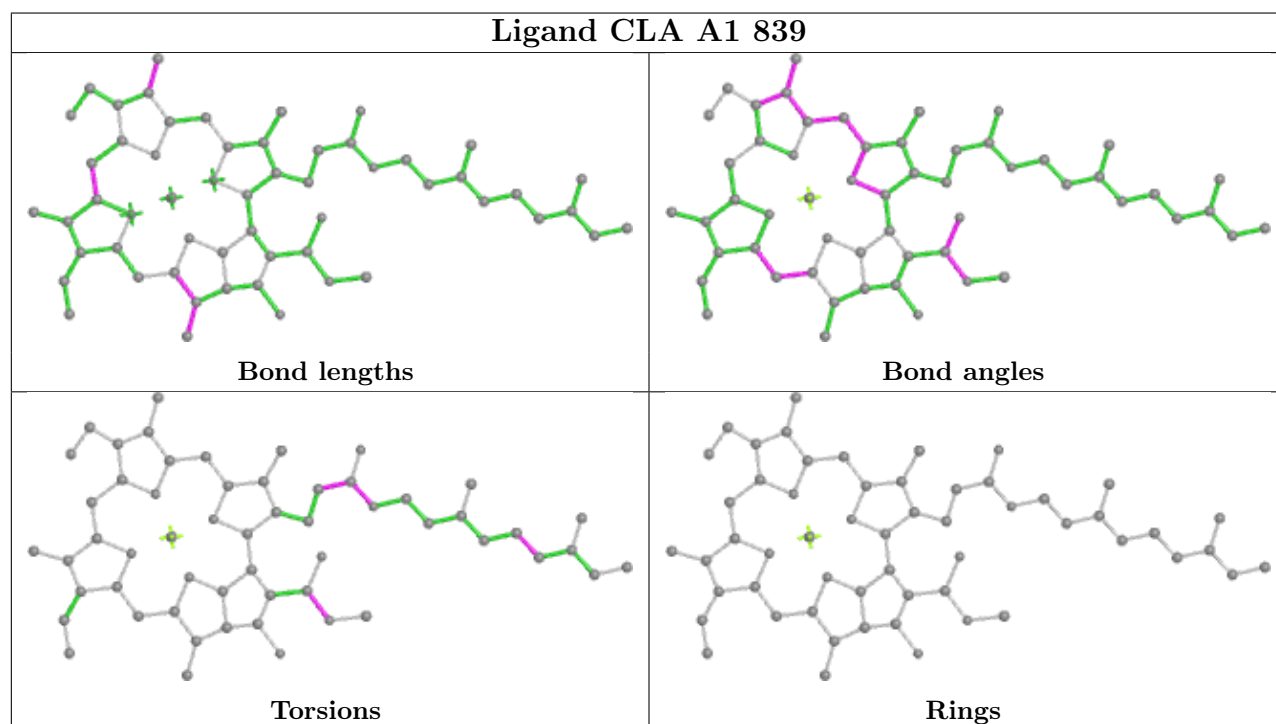
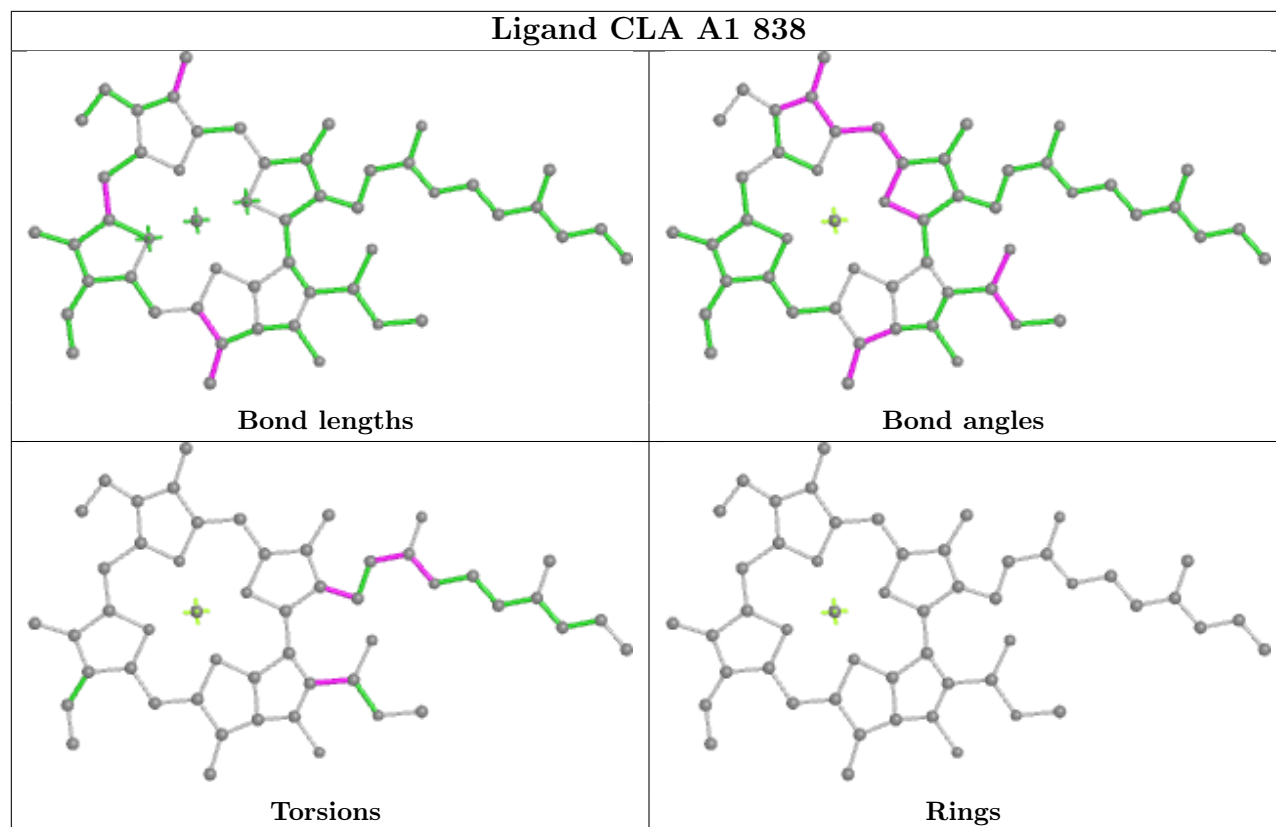
Torsions



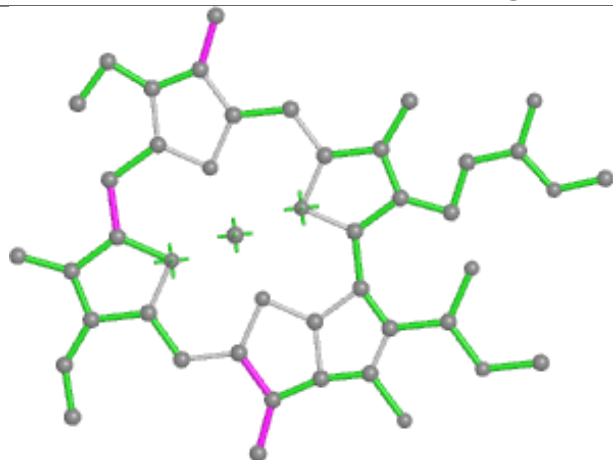
Rings

Ligand CLA A1 837

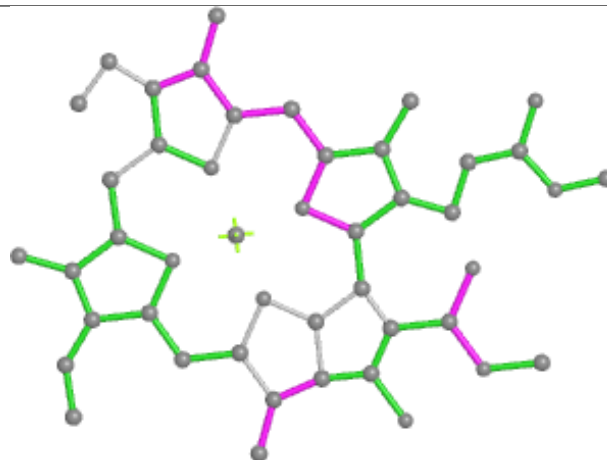




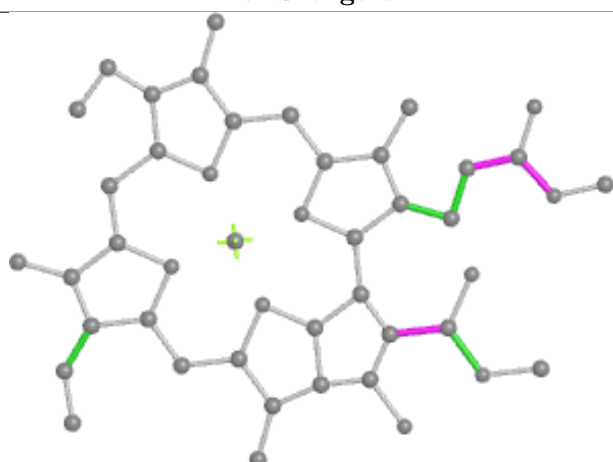
Ligand CLA A1 840



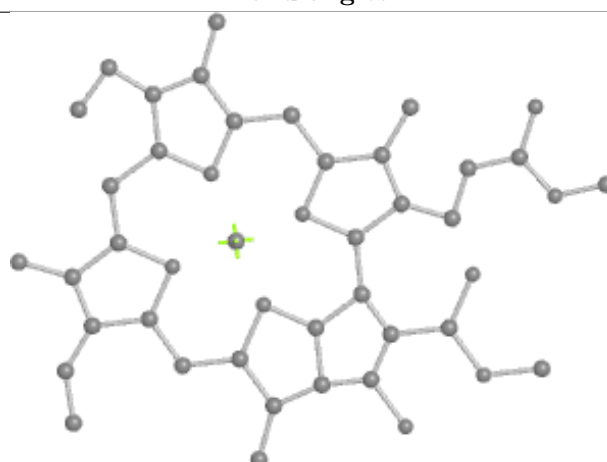
Bond lengths



Bond angles

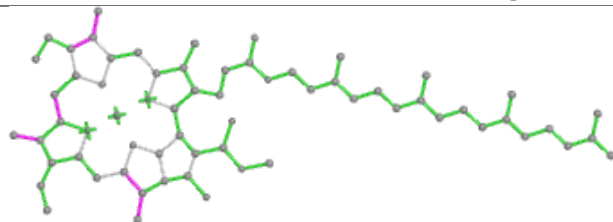


Torsions

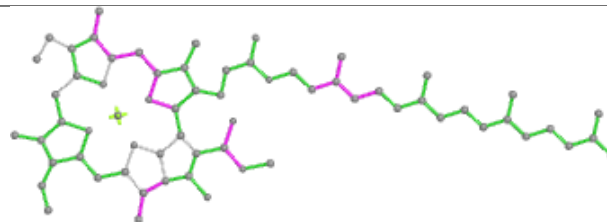


Rings

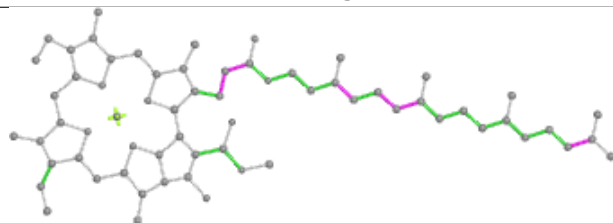
Ligand CLA A1 841



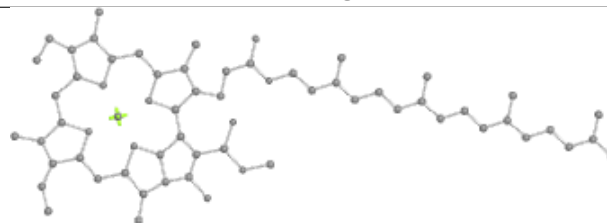
Bond lengths



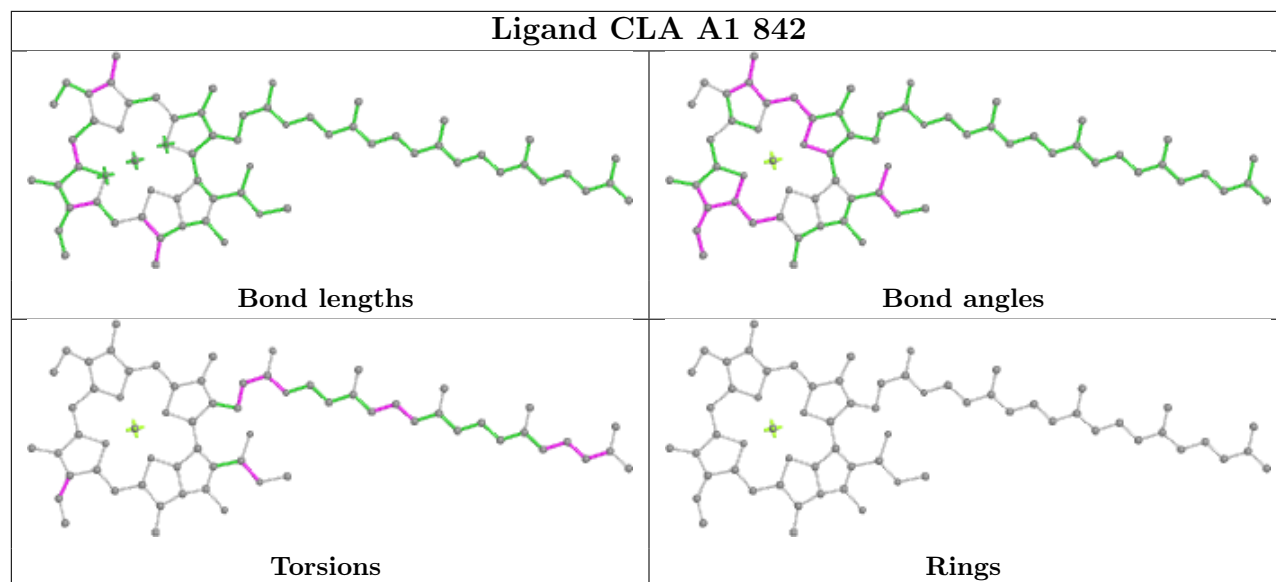
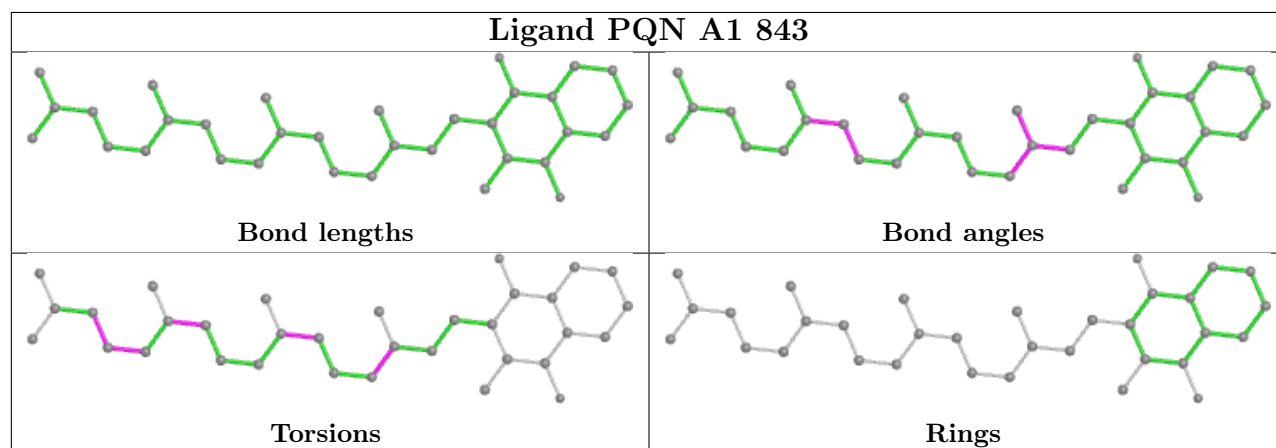
Bond angles



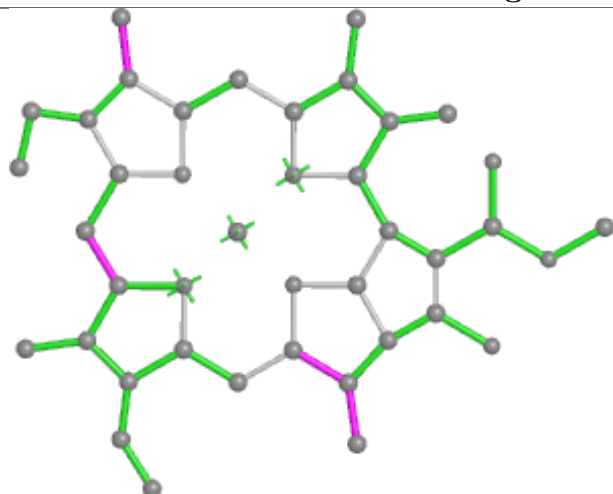
Torsions



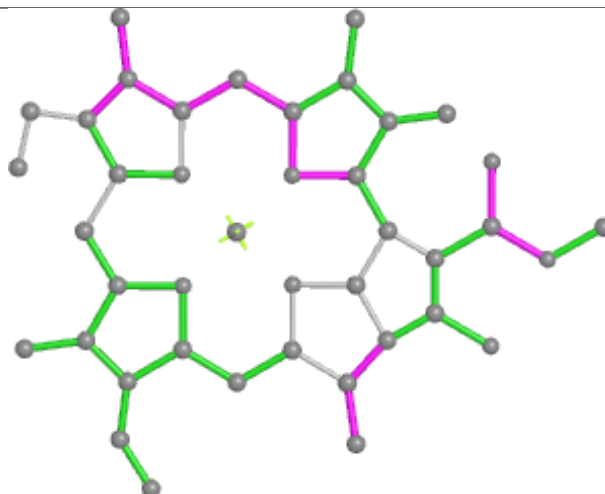
Rings

Ligand CLA A1 842**Ligand PQN A1 843**

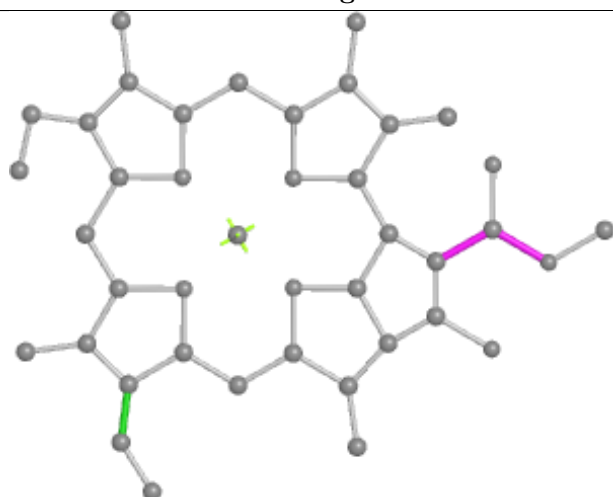
Ligand CLA A1 844



Bond lengths



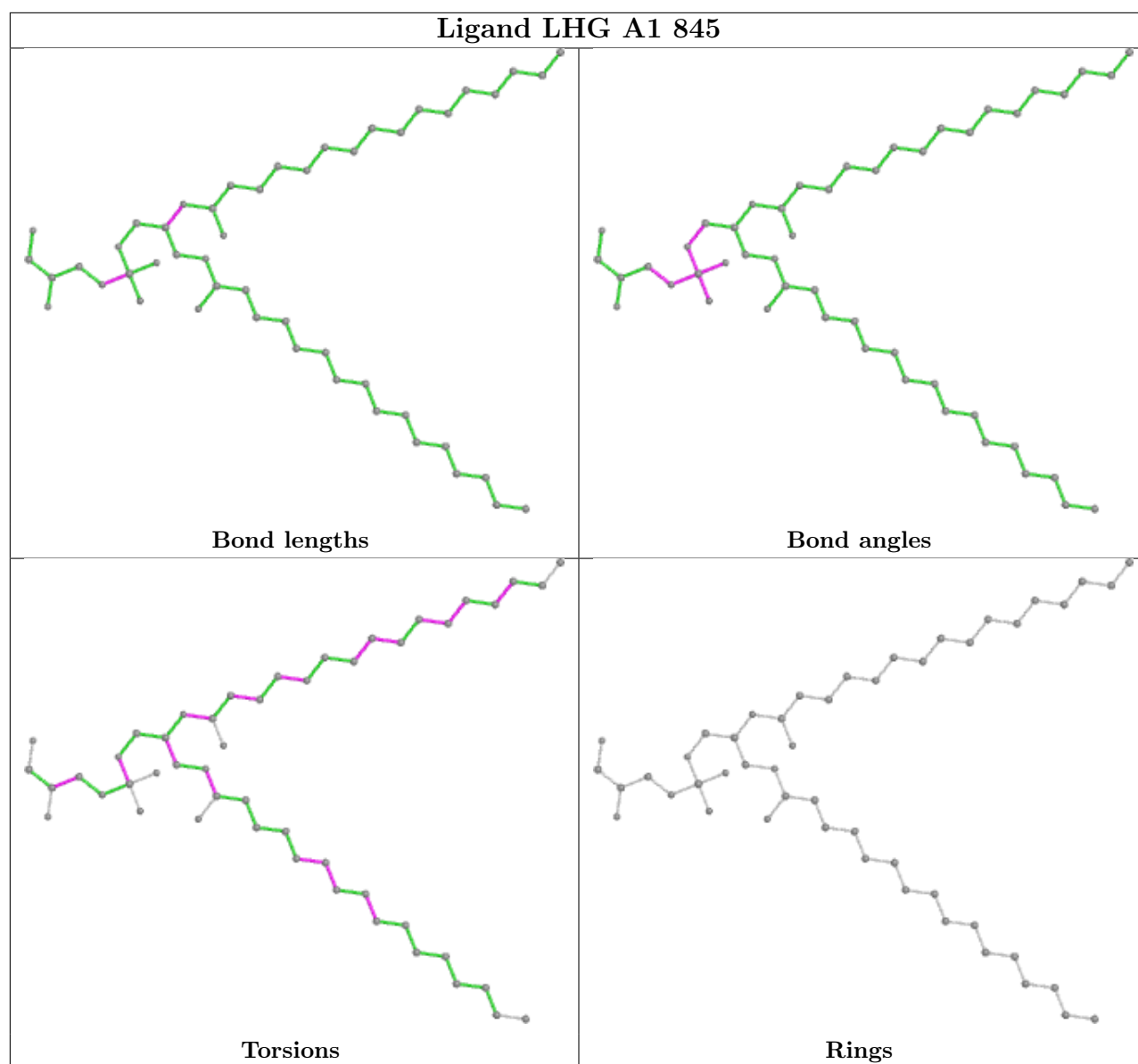
Bond angles

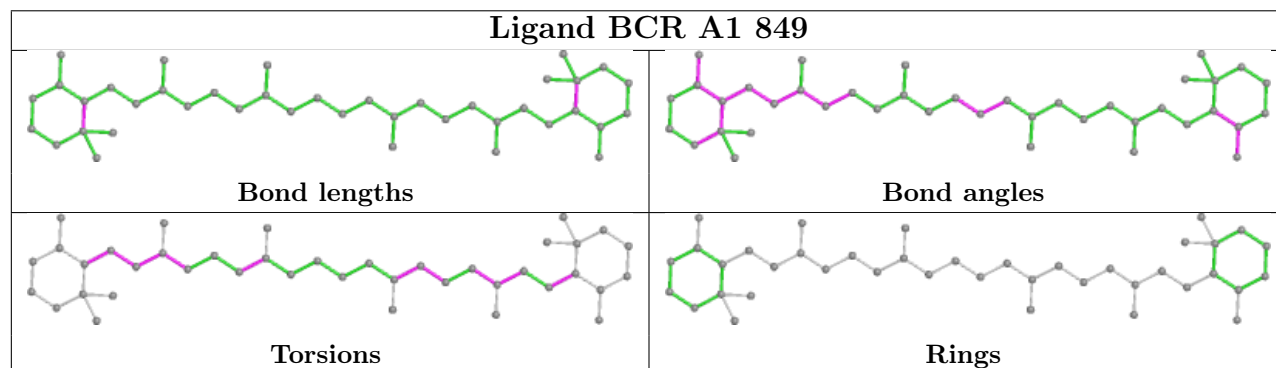
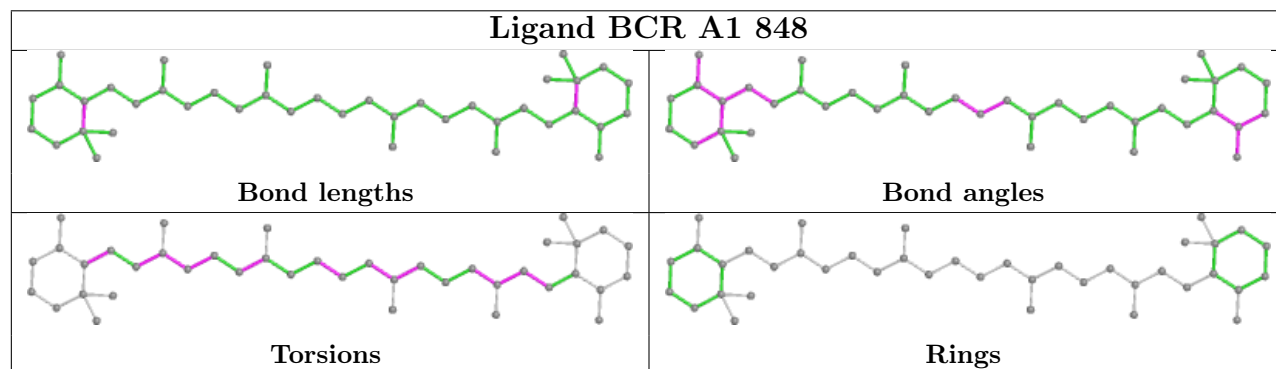
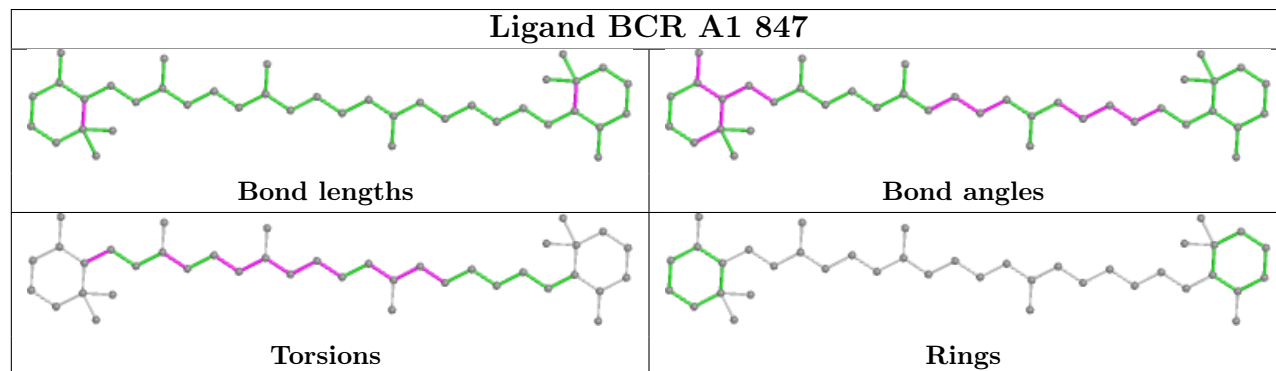
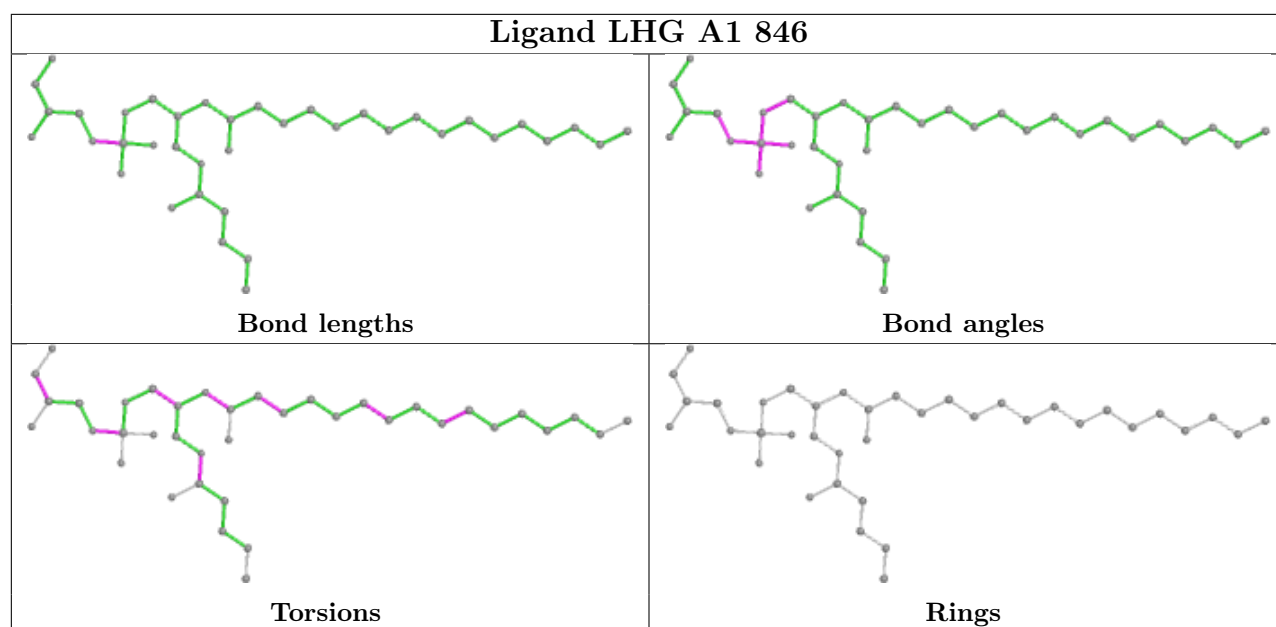


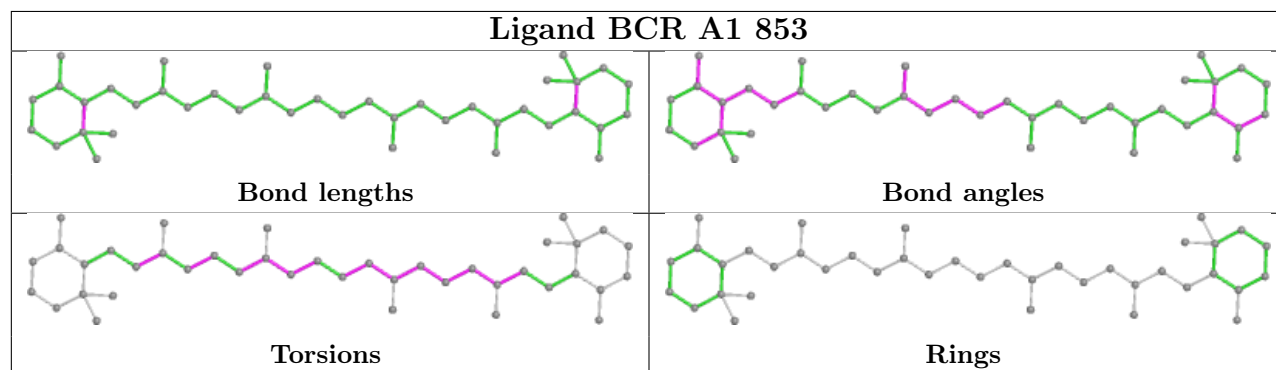
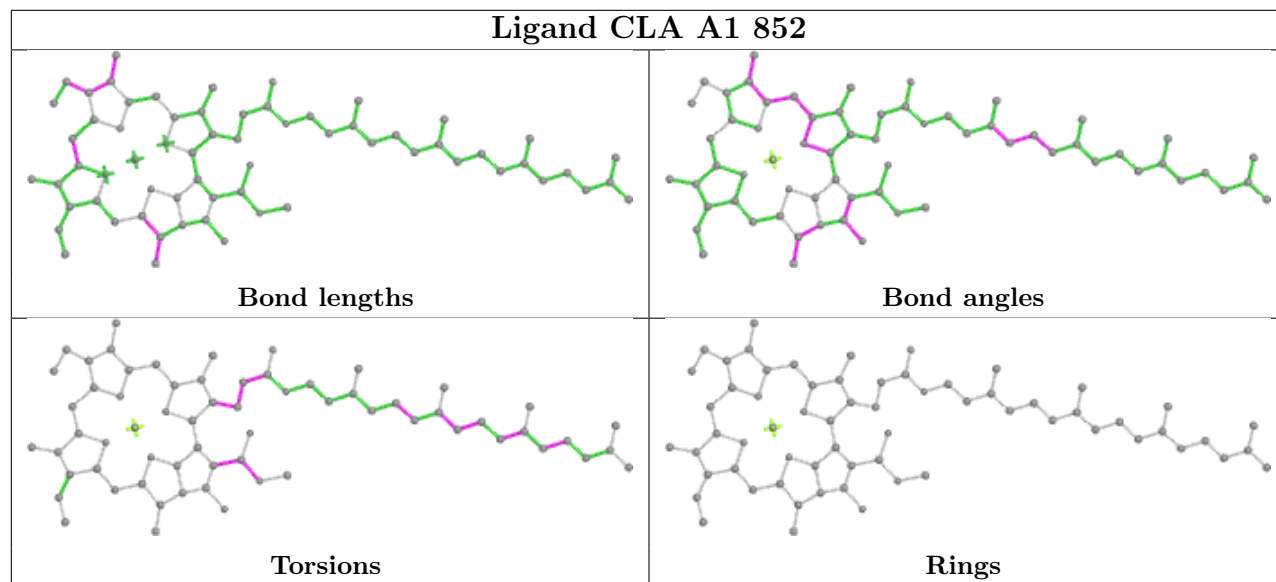
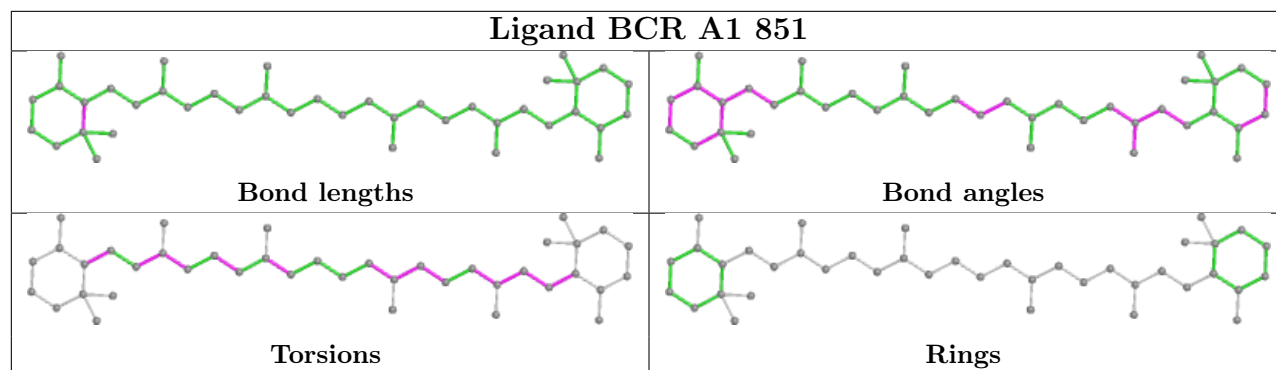
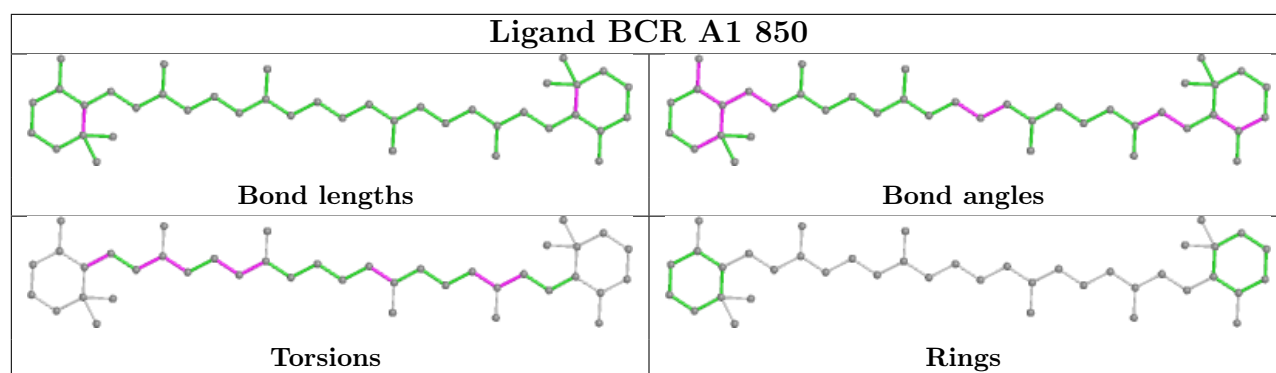
Torsions

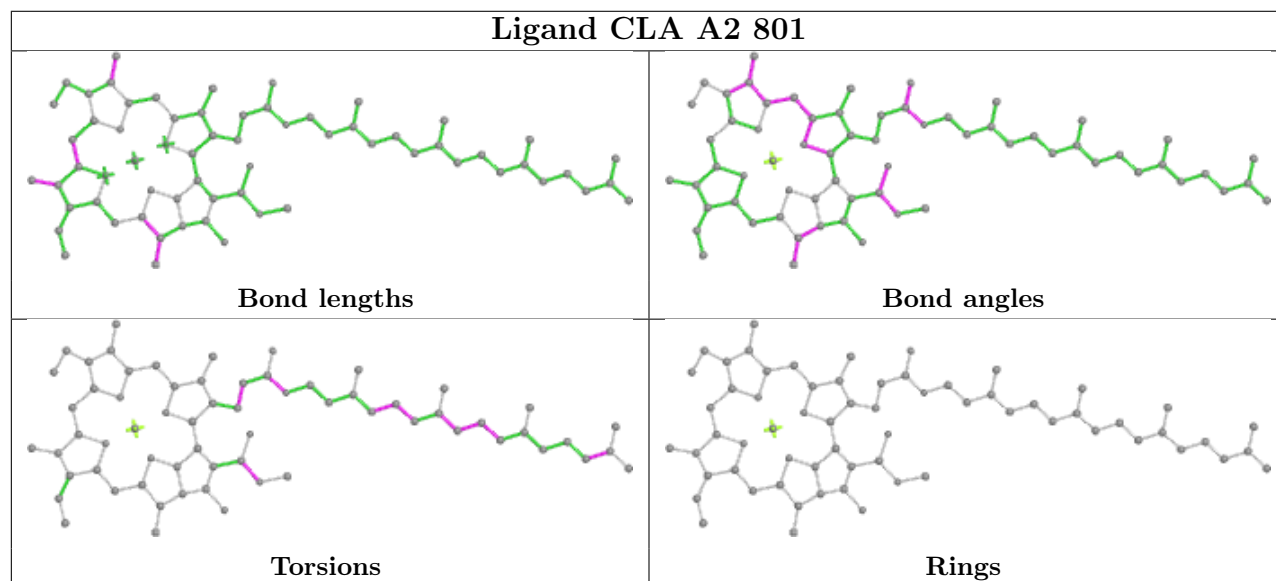
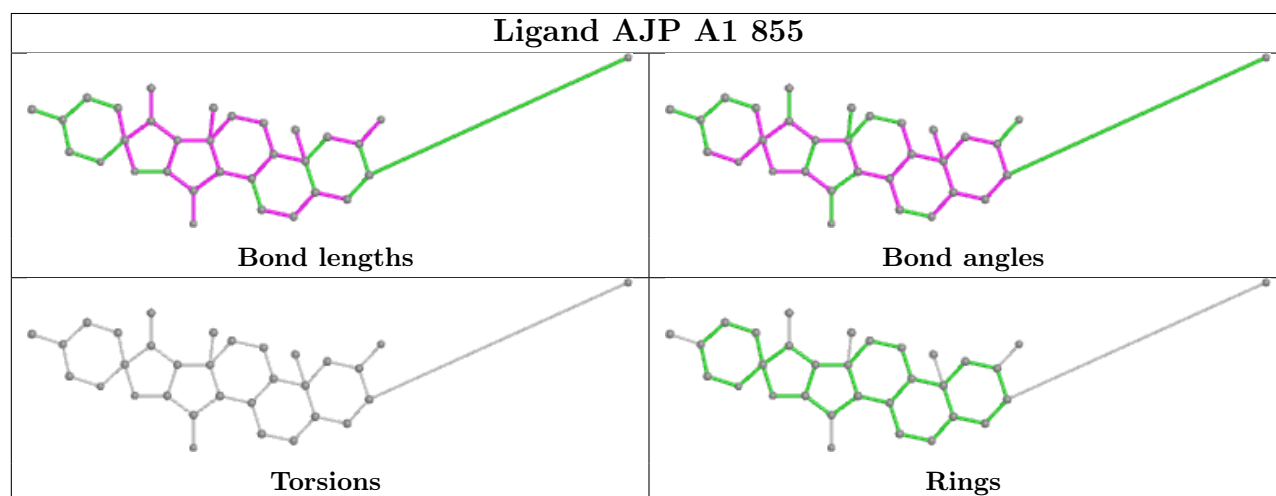
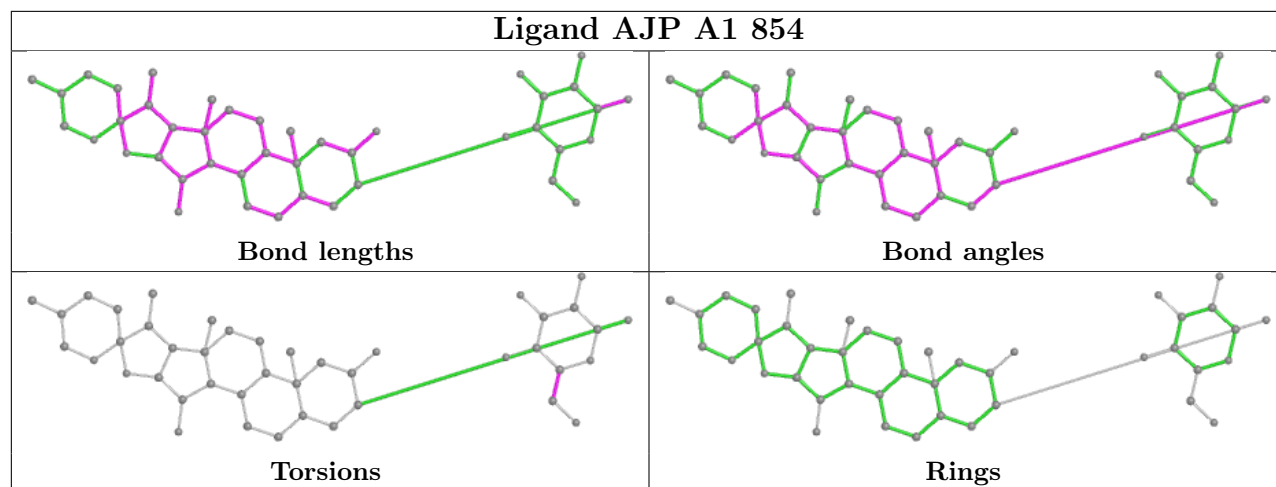


Rings

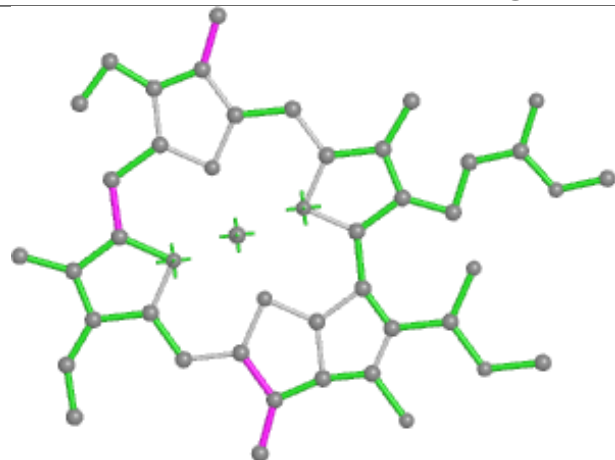




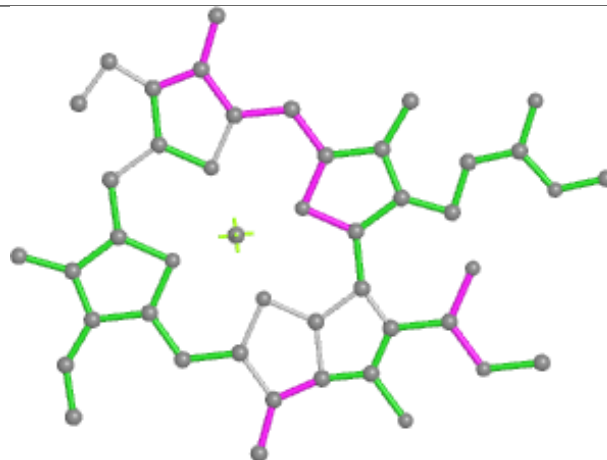




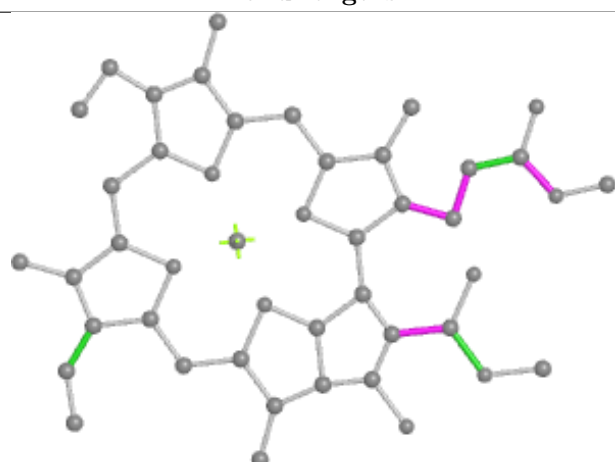
Ligand CLA A2 802



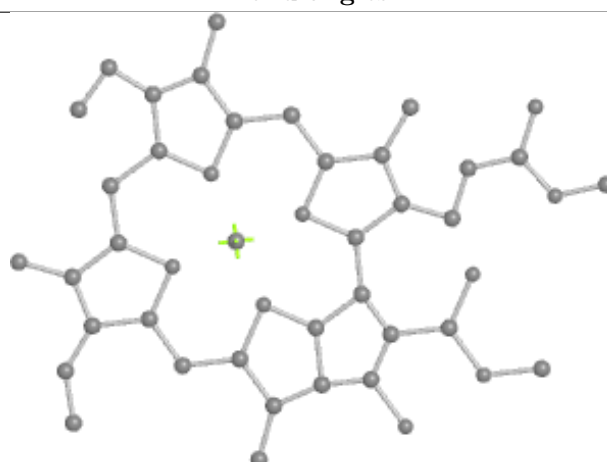
Bond lengths



Bond angles

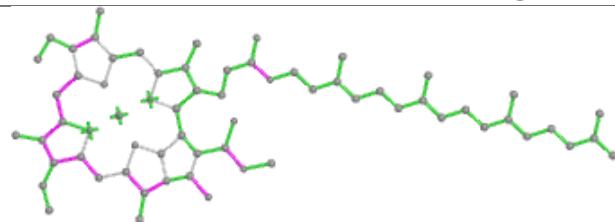


Torsions

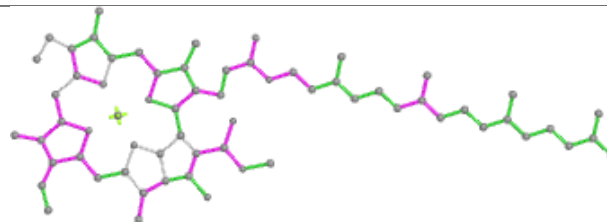


Rings

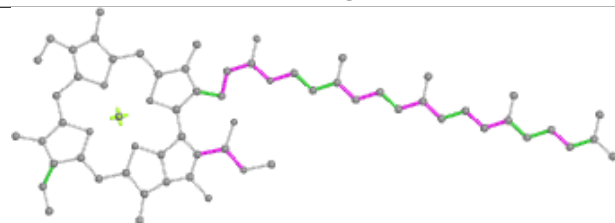
Ligand CL0 A2 803



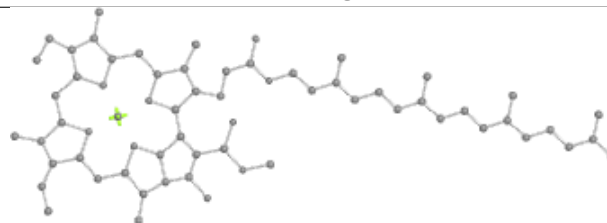
Bond lengths



Bond angles

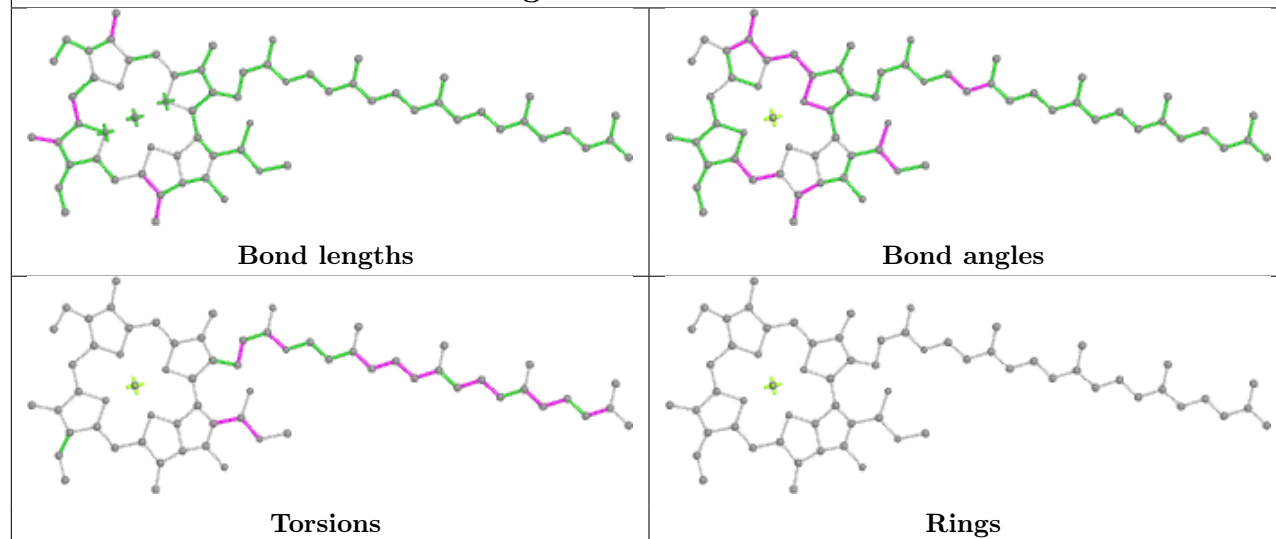


Torsions

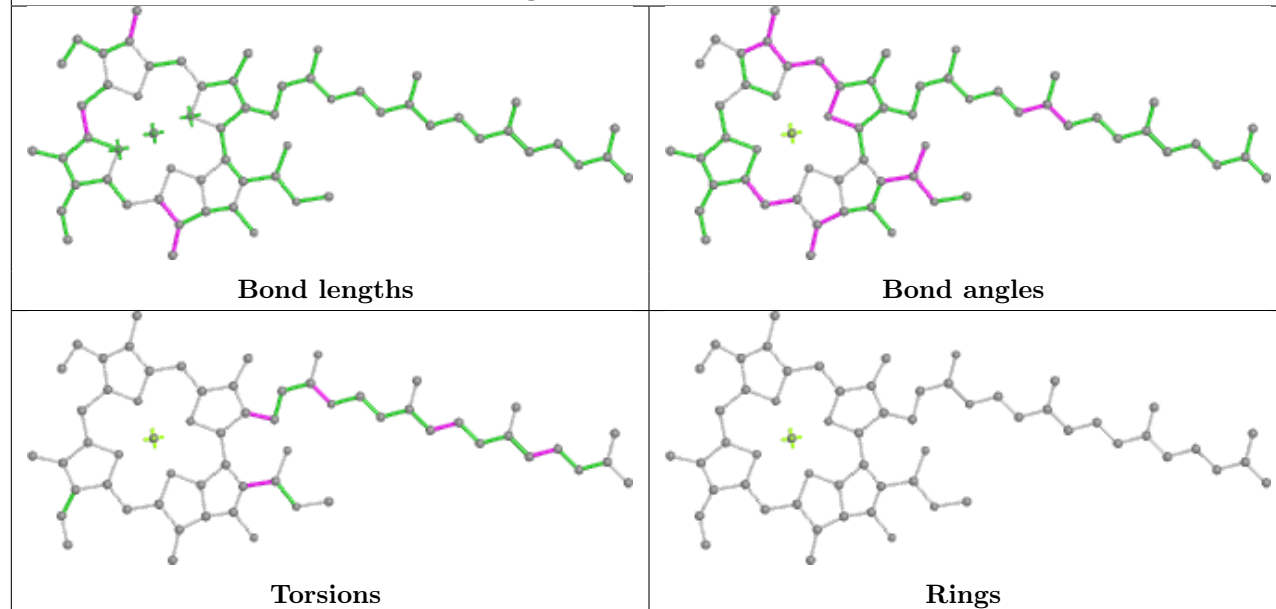


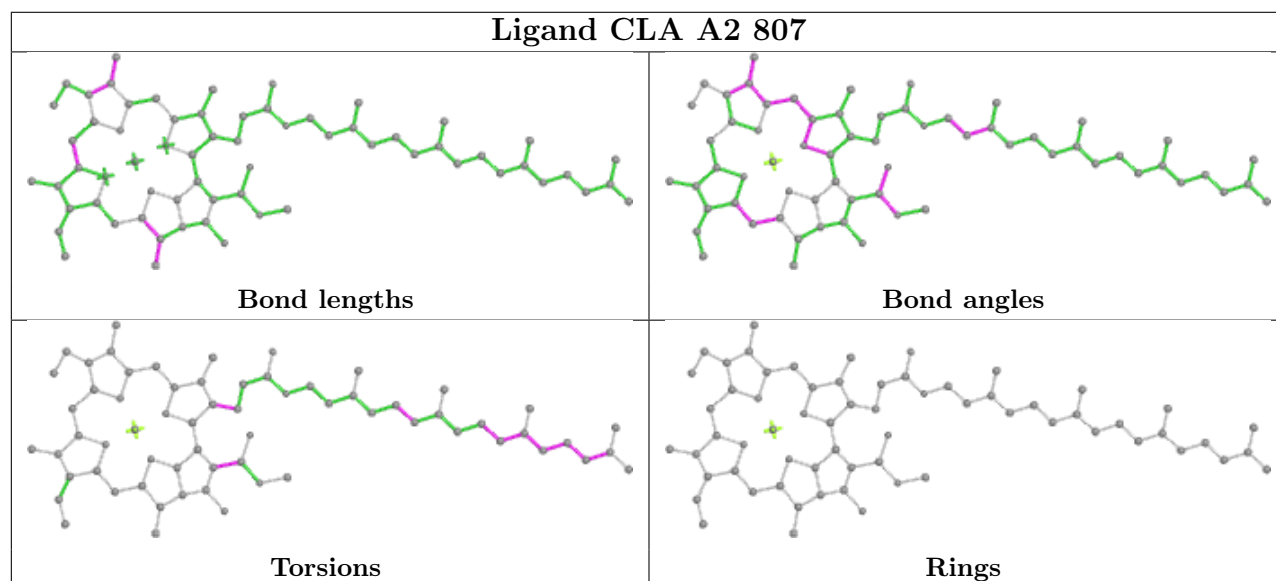
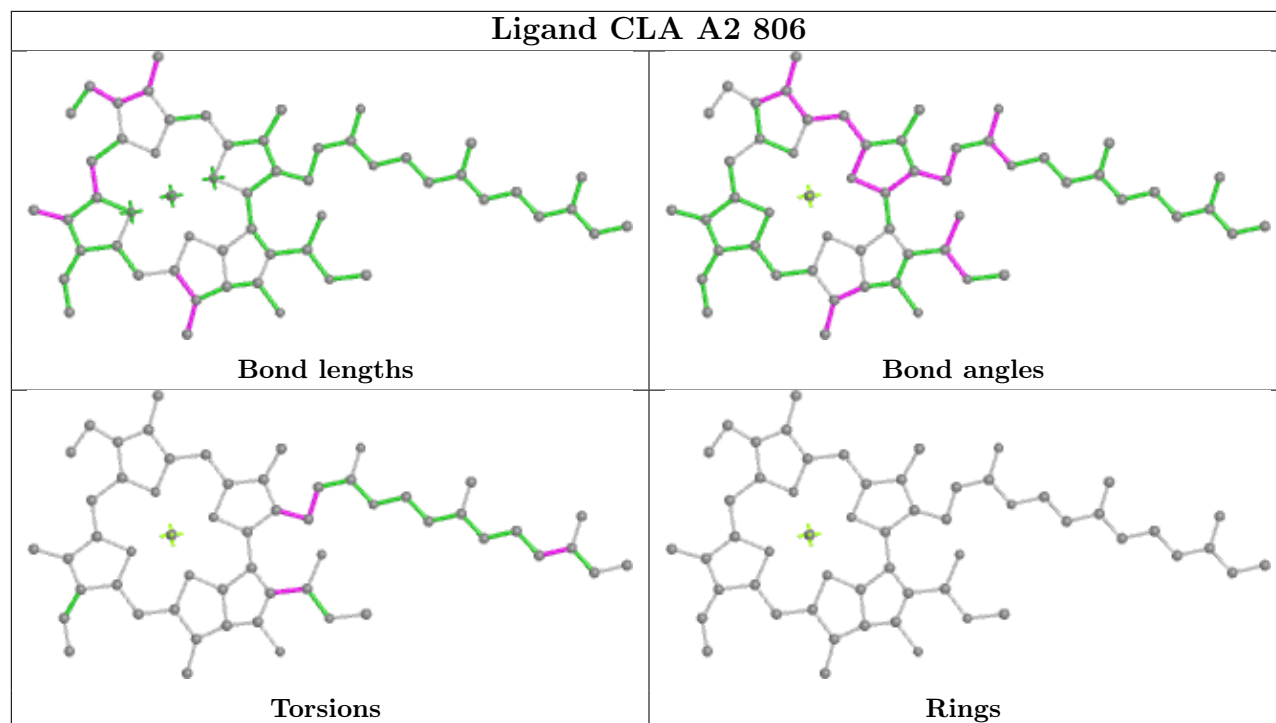
Rings

Ligand CLA A2 804

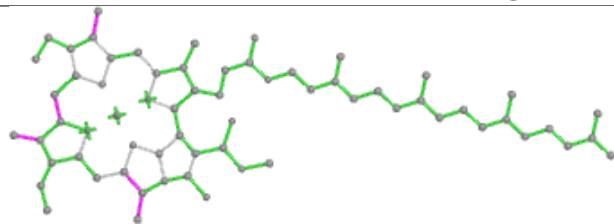


Ligand CLA A2 805

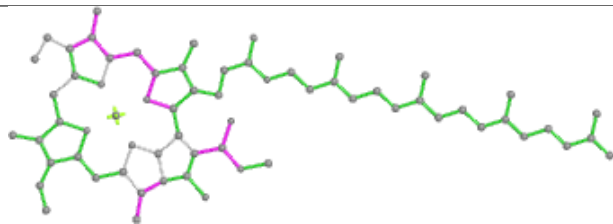




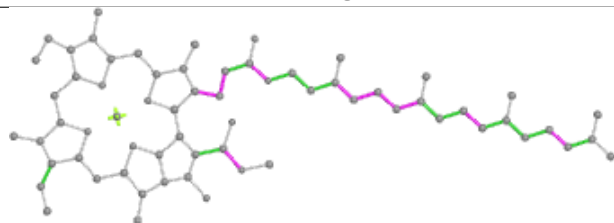
Ligand CLA A2 808



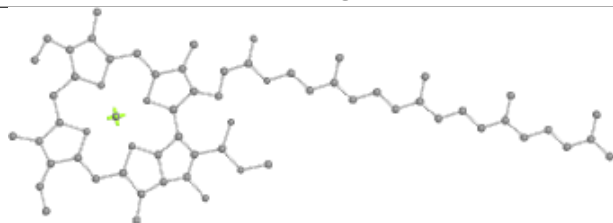
Bond lengths



Bond angles

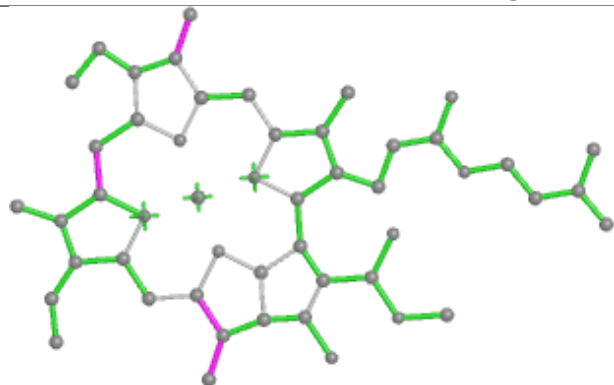


Torsions

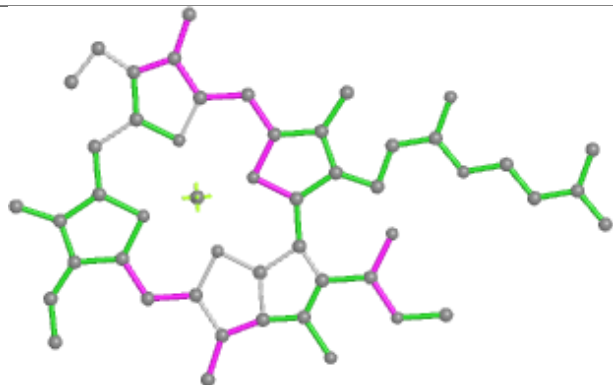


Rings

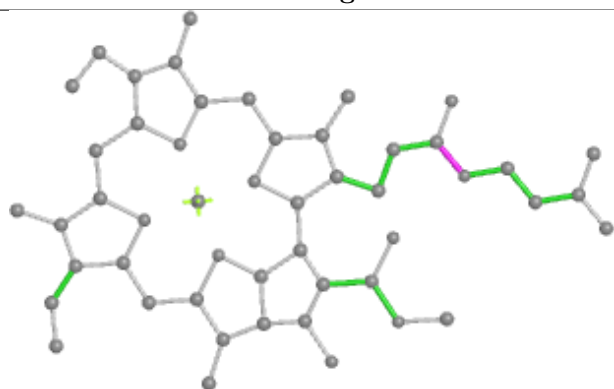
Ligand CLA A2 809



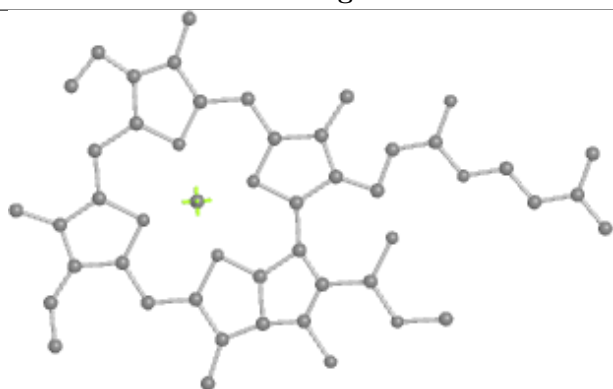
Bond lengths



Bond angles

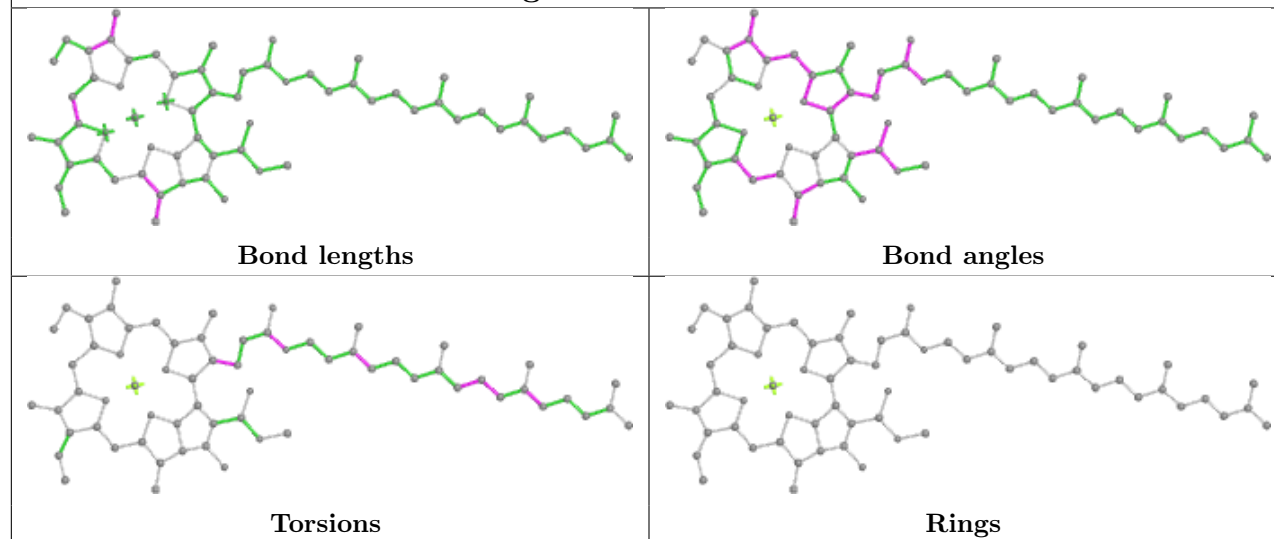


Torsions

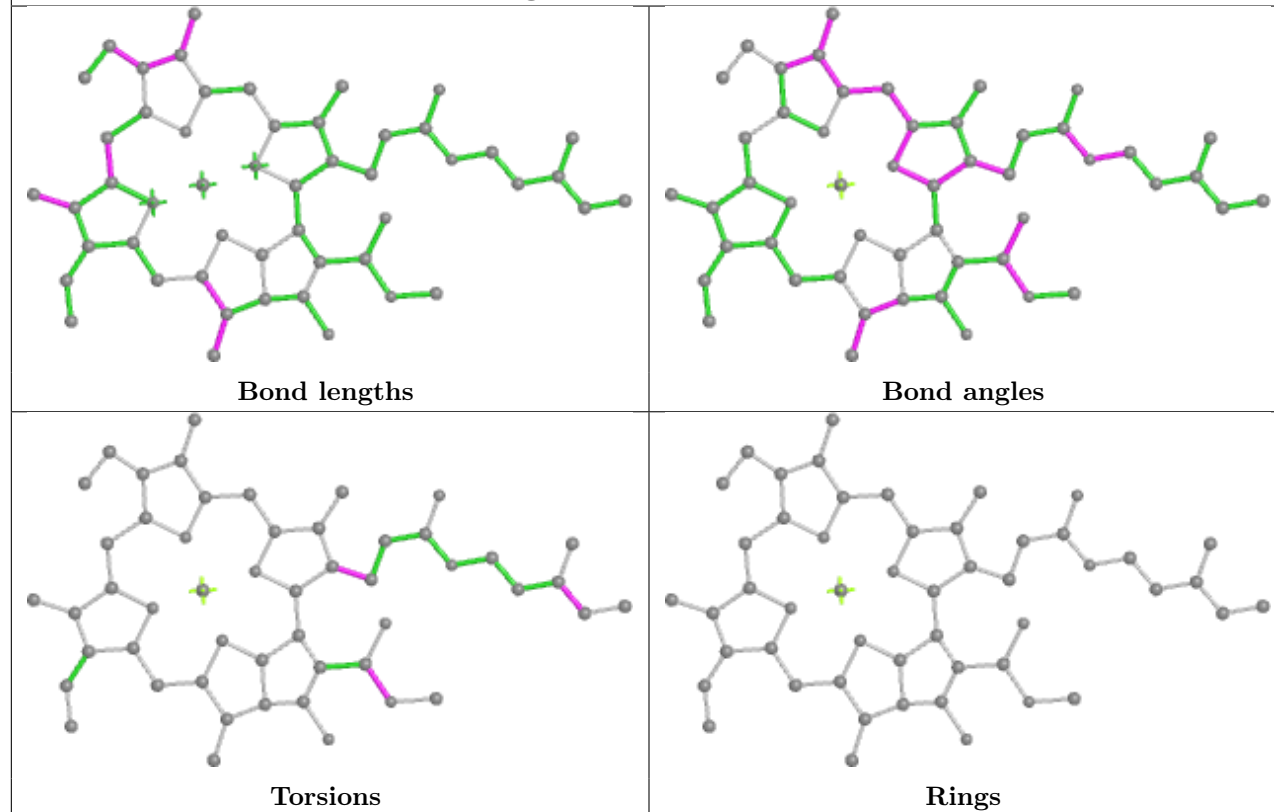


Rings

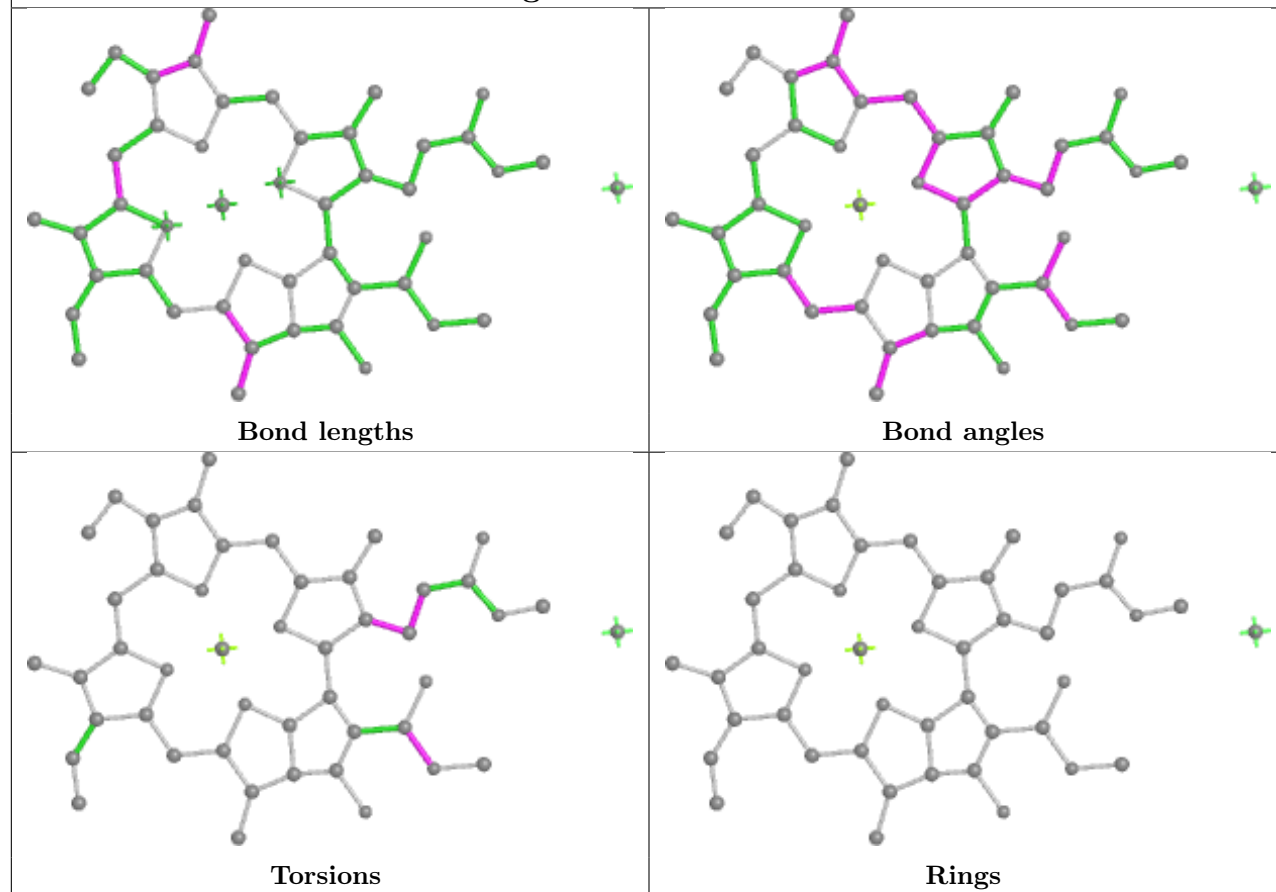
Ligand CLA A2 810



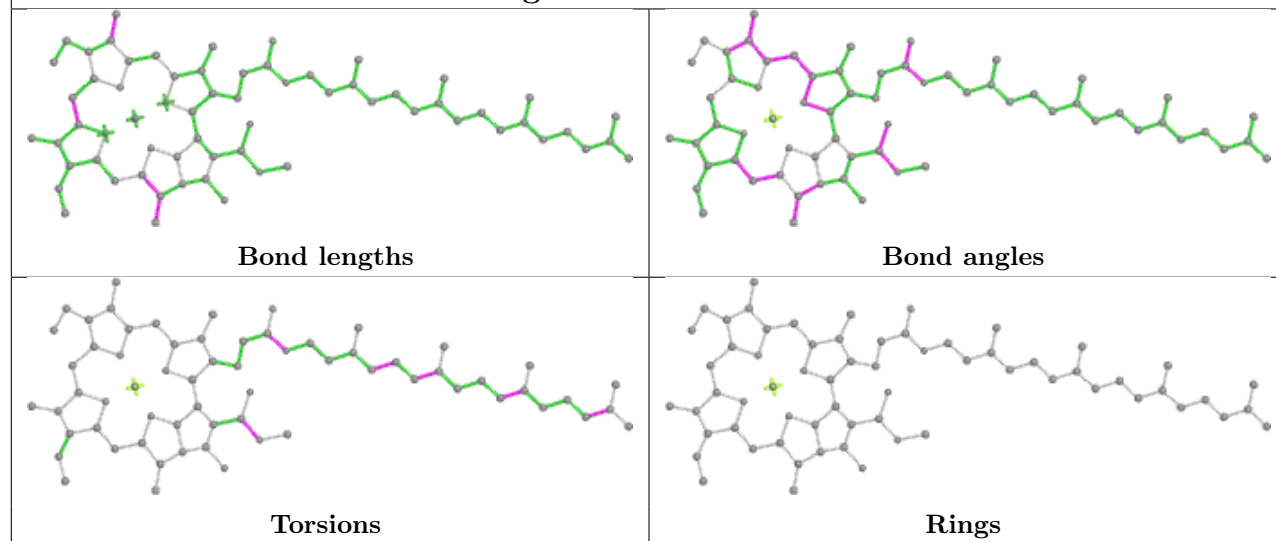
Ligand CLA A2 811



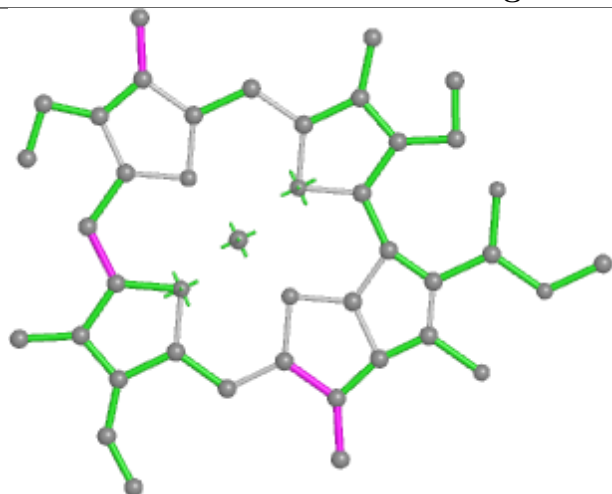
Ligand CLA A2 812



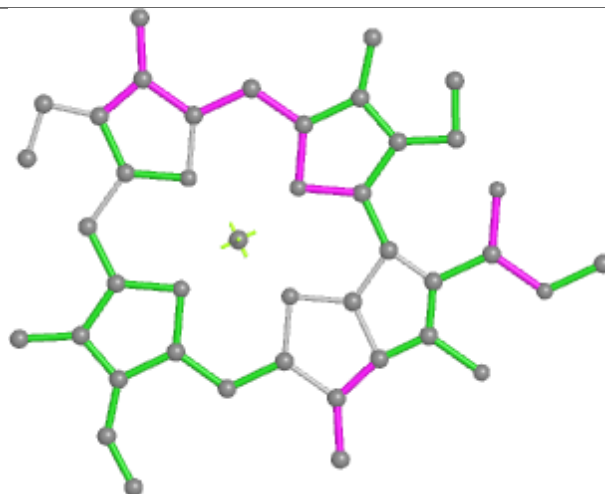
Ligand CLA A2 813



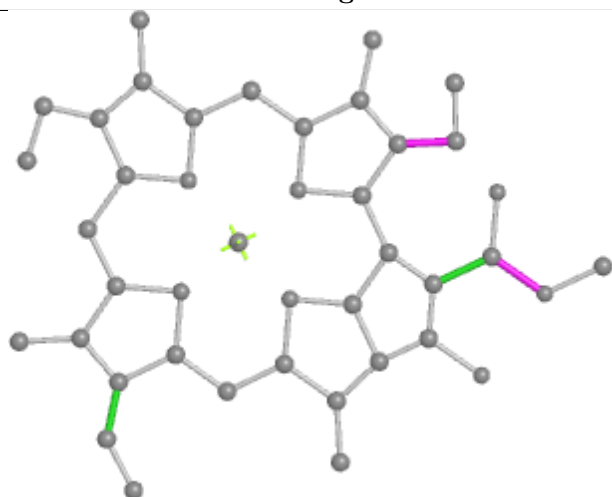
Ligand CLA A2 814



Bond lengths



Bond angles

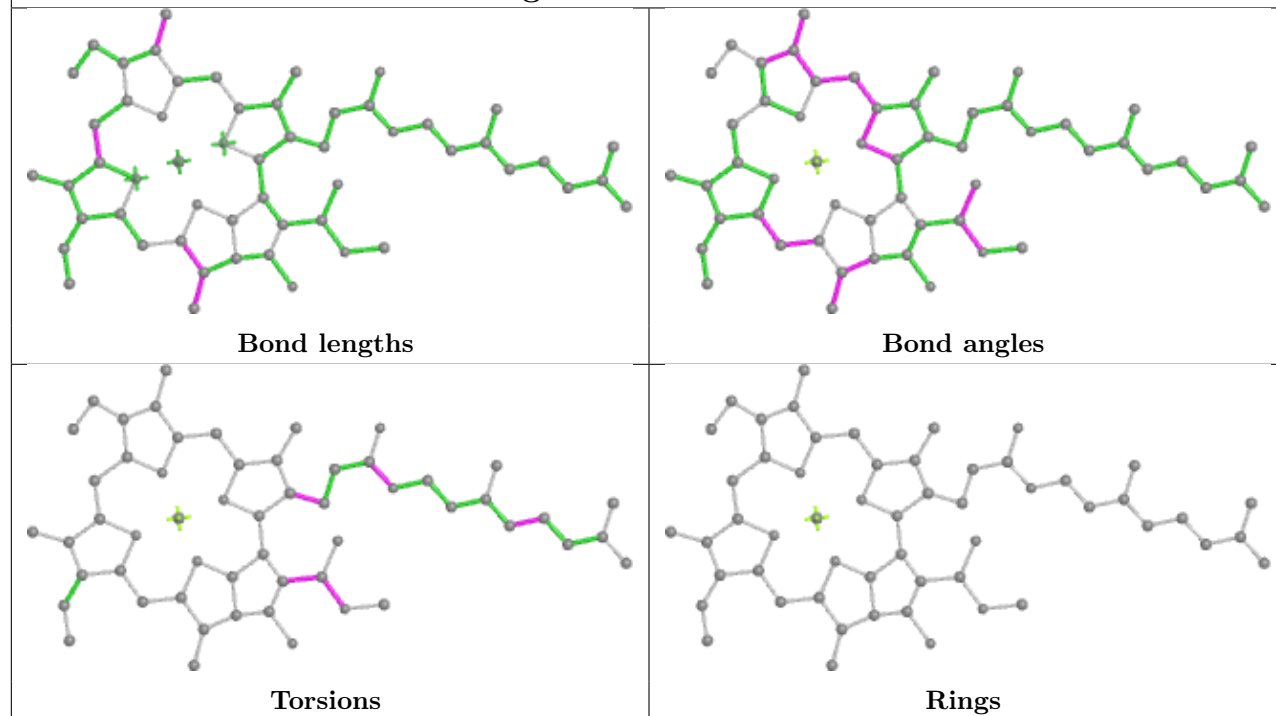


Torsions

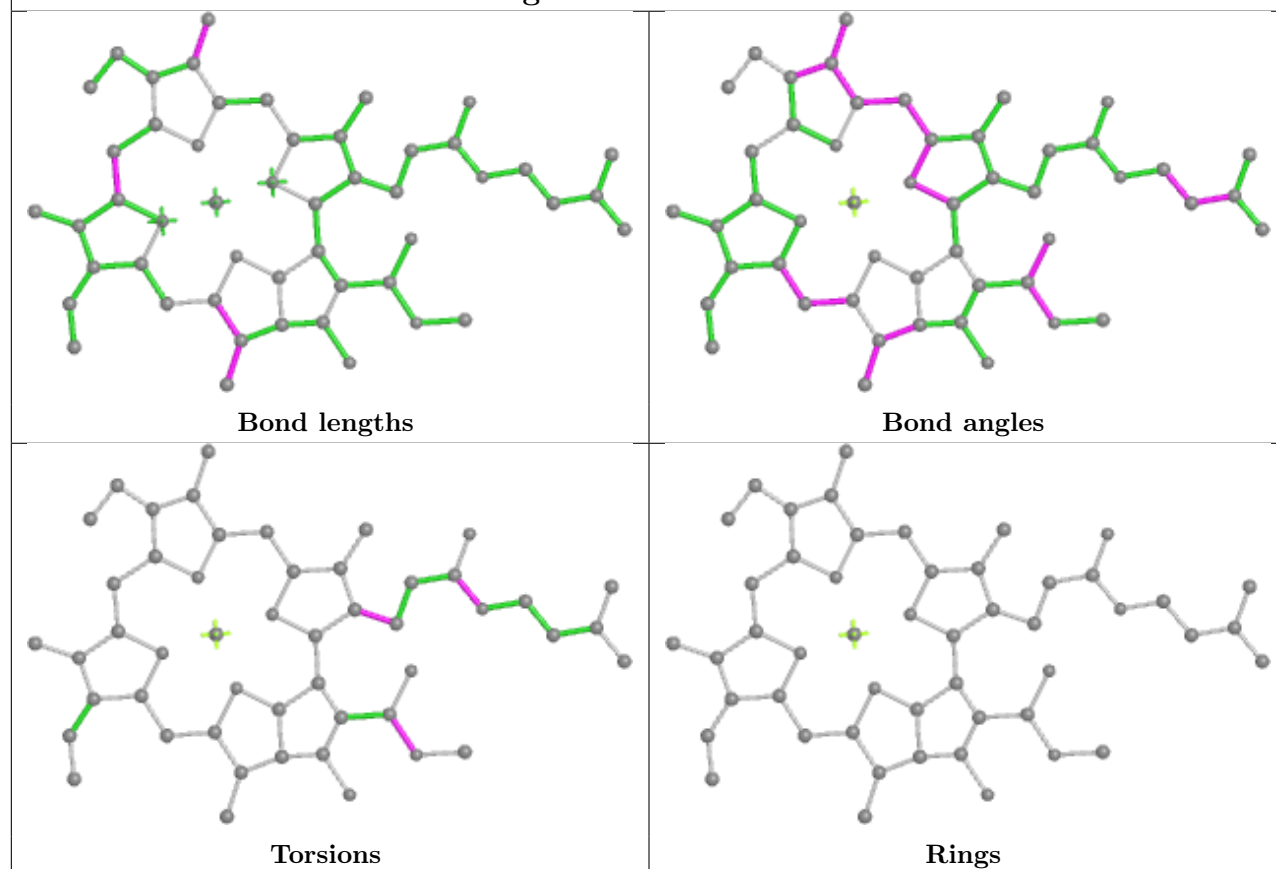


Rings

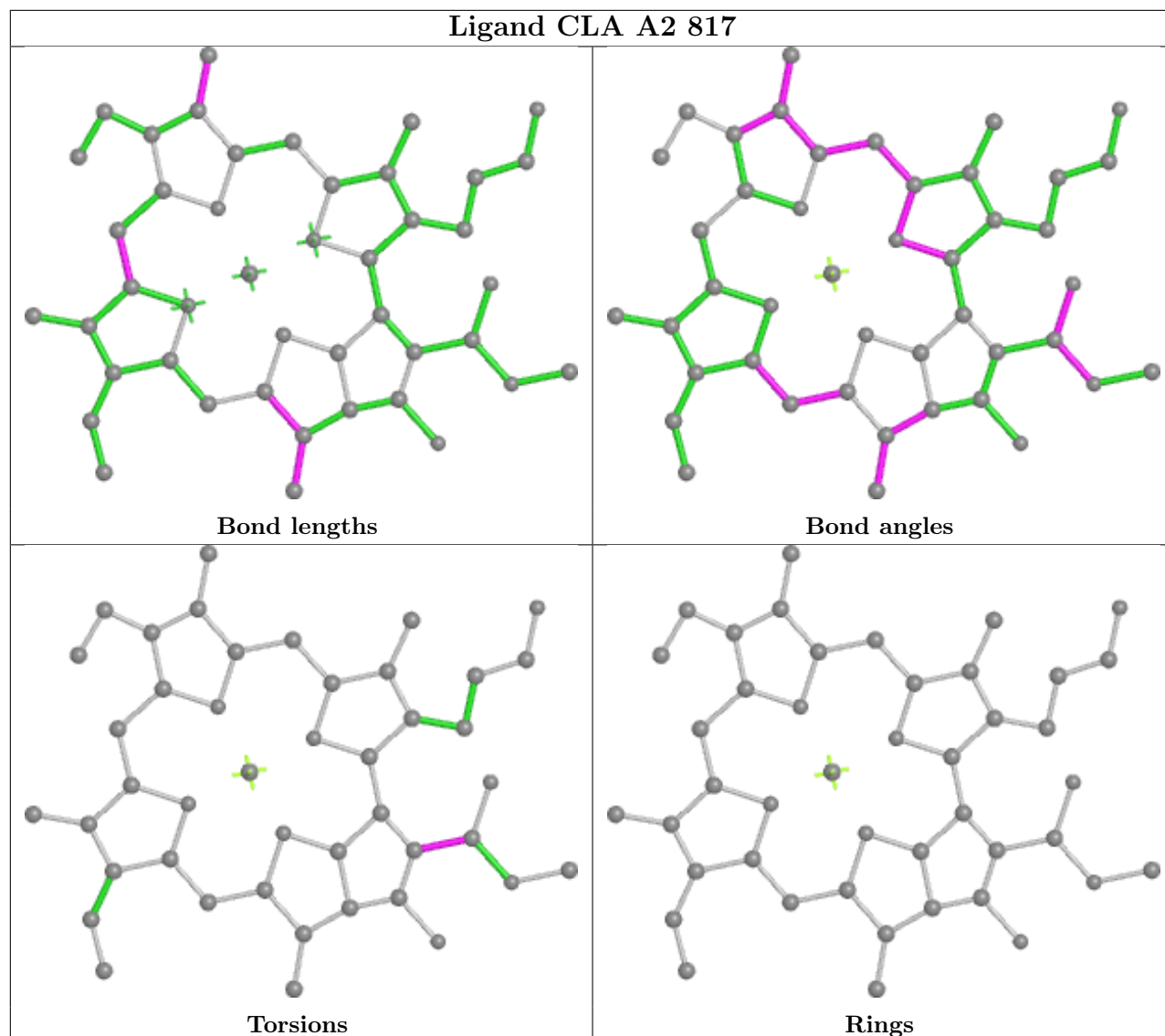
Ligand CLA A2 815



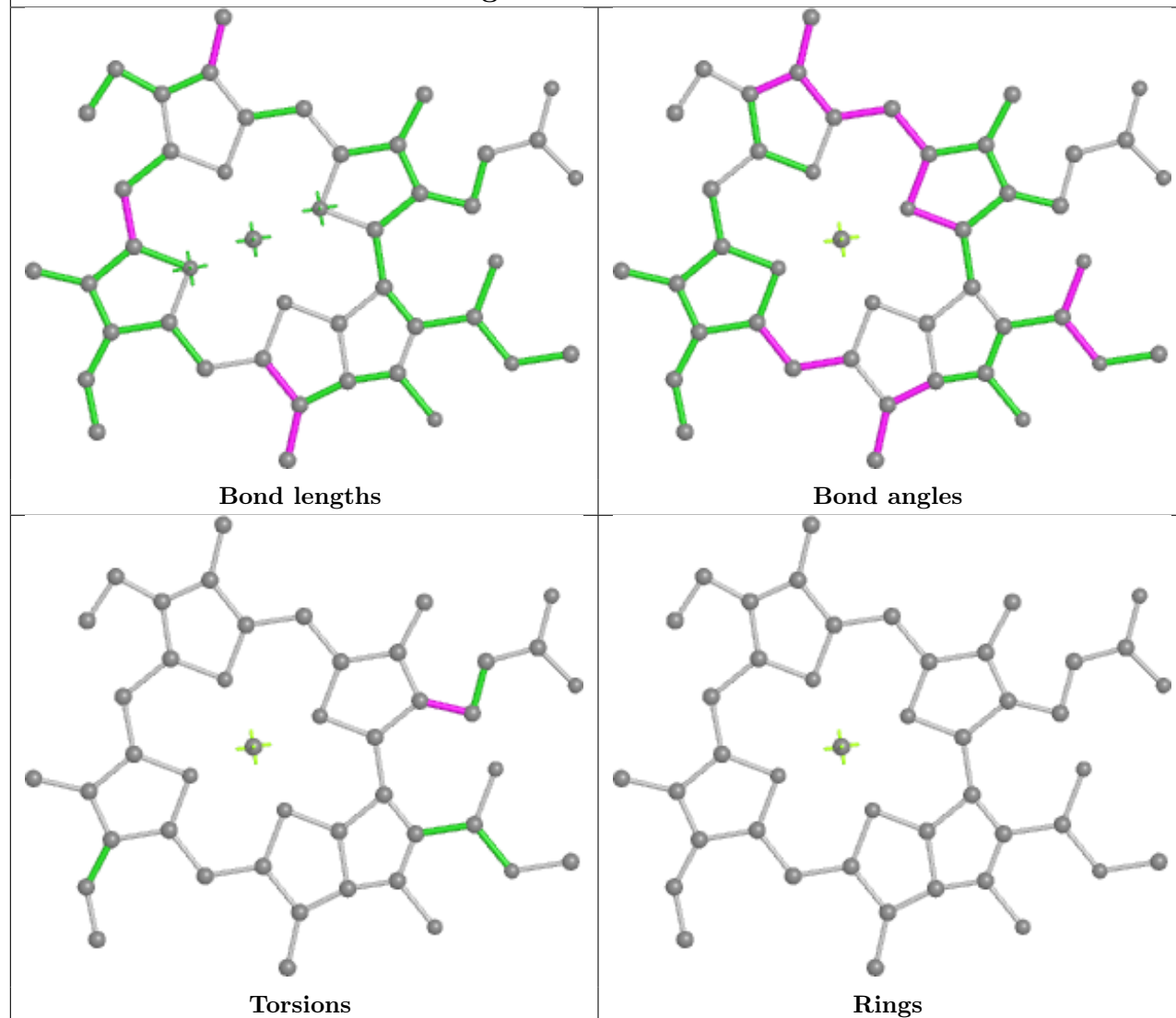
Ligand CLA A2 816



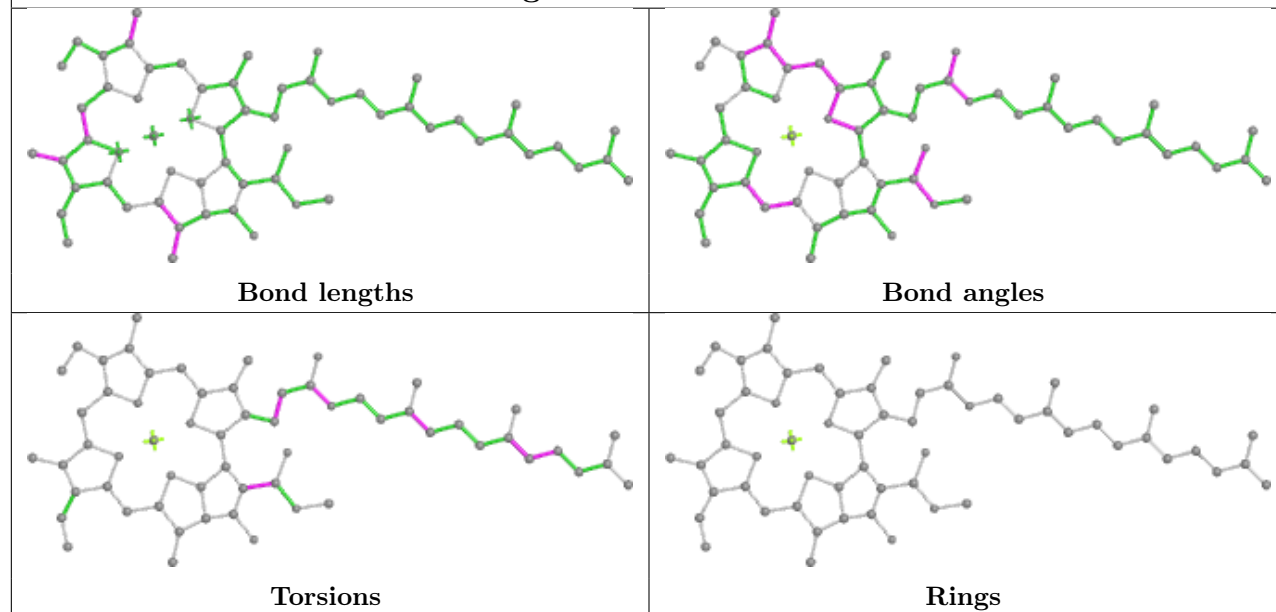
Ligand CLA A2 817



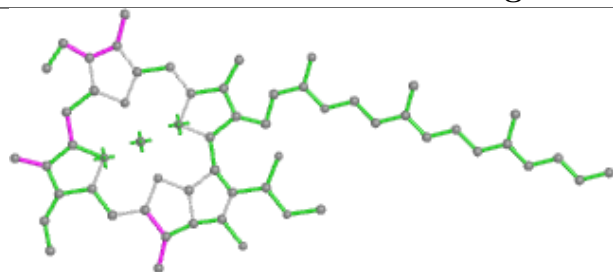
Ligand CLA A2 818



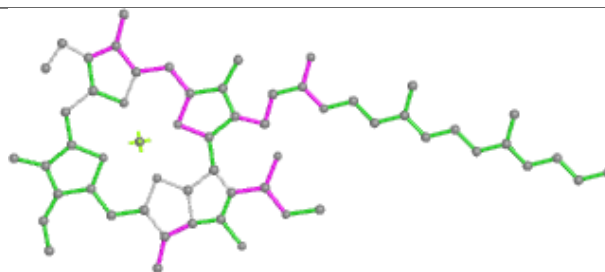
Ligand CLA A2 819



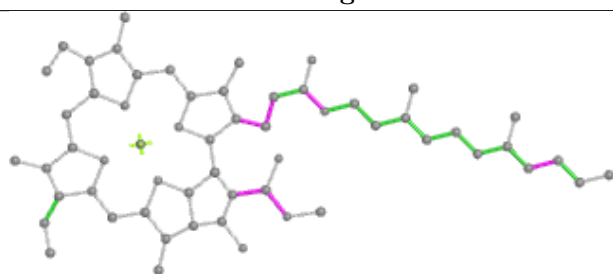
Ligand CLA A2 820



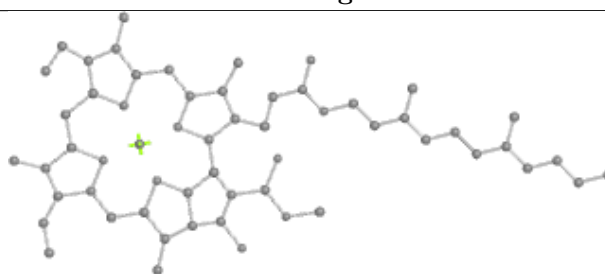
Bond lengths



Bond angles

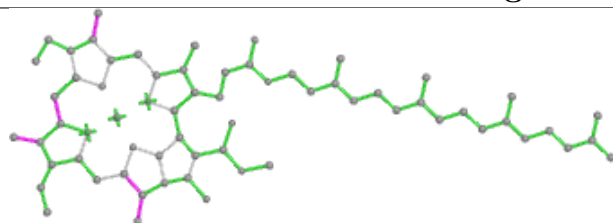


Torsions

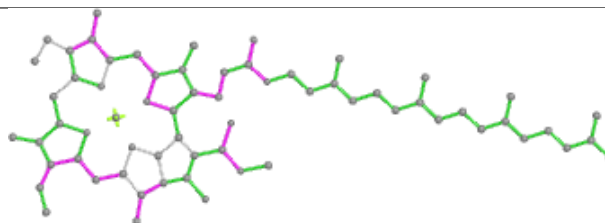


Rings

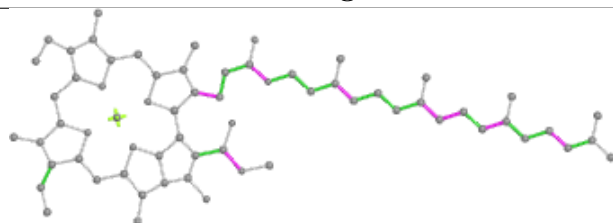
Ligand CLA A2 821



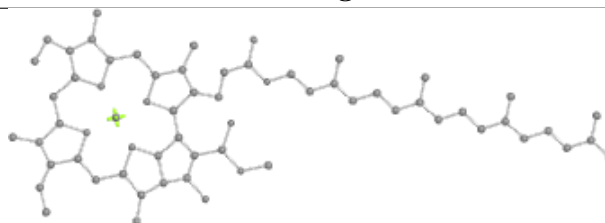
Bond lengths



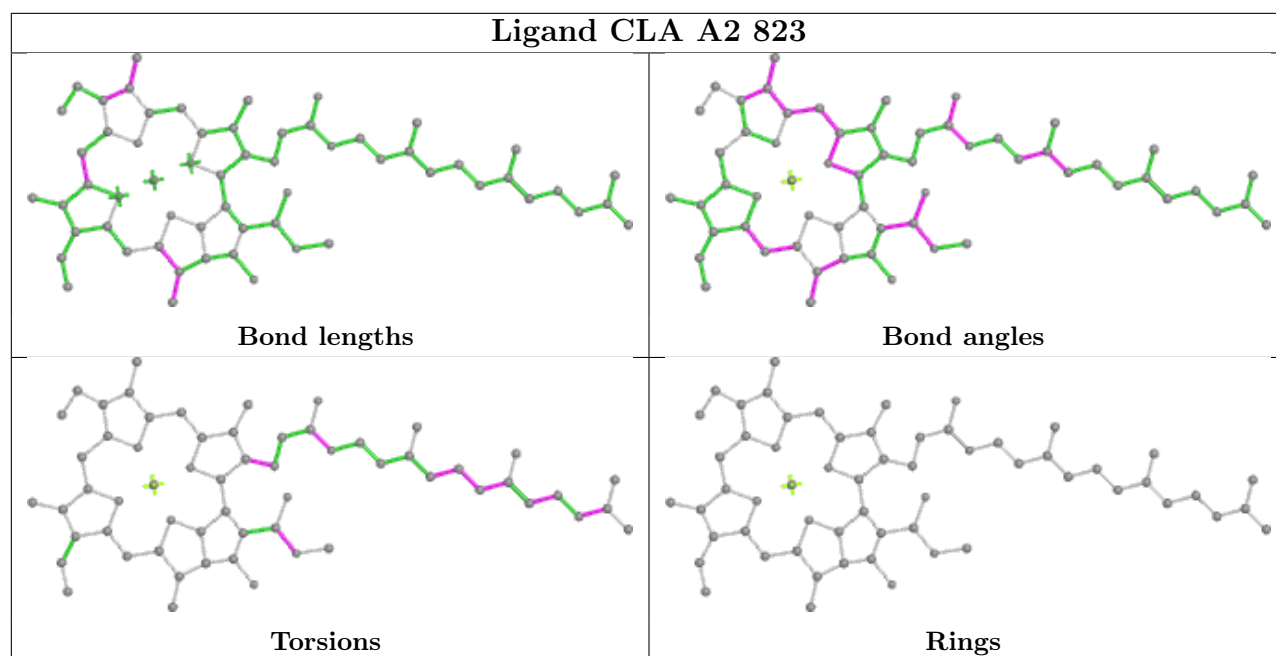
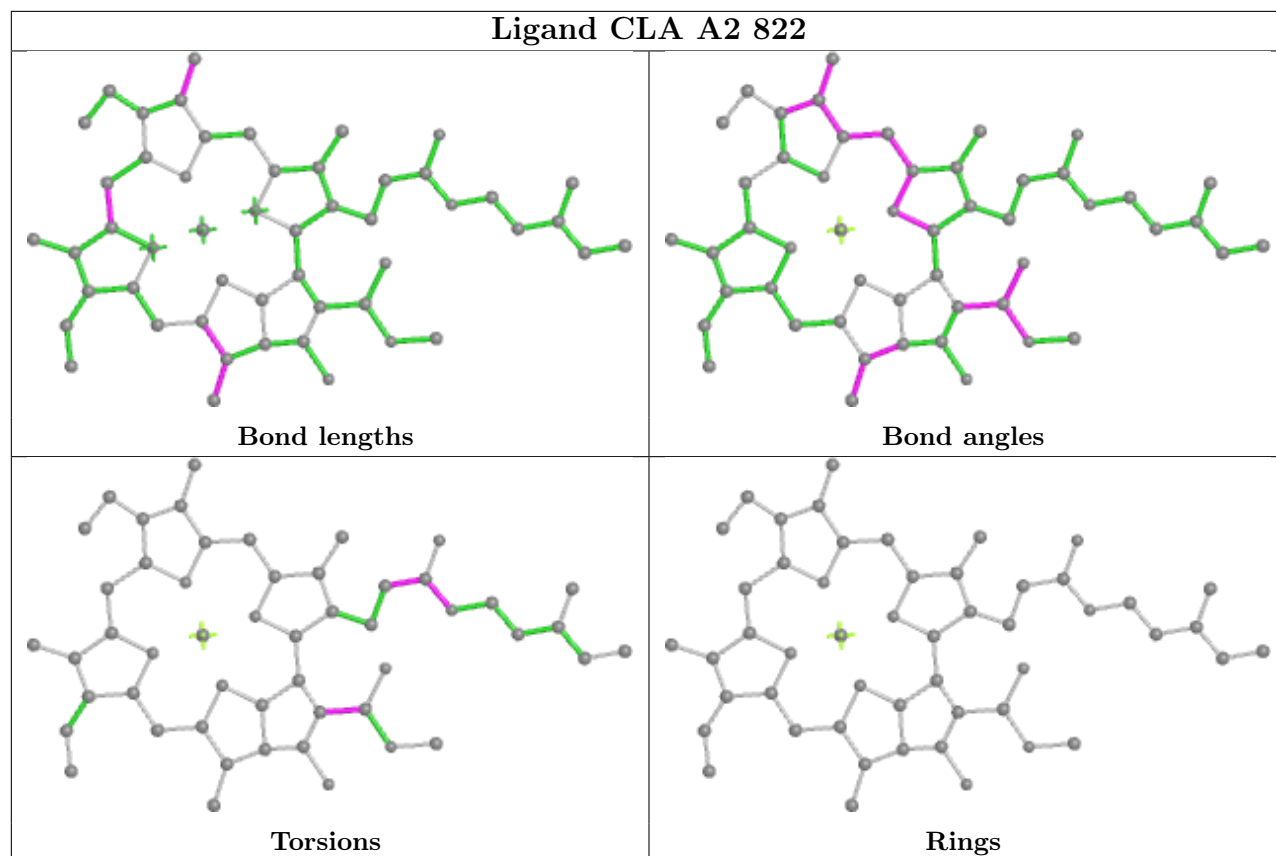
Bond angles



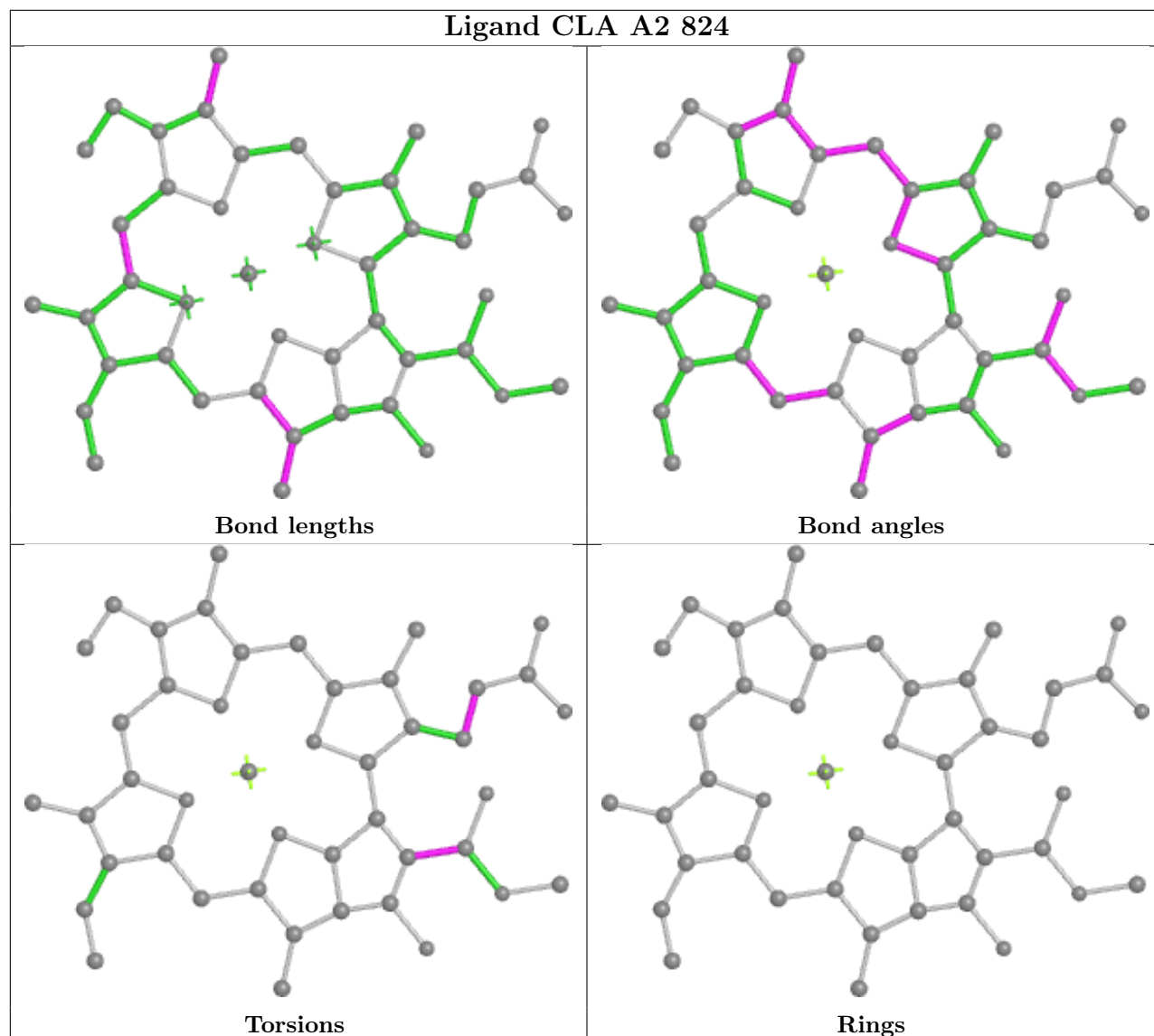
Torsions



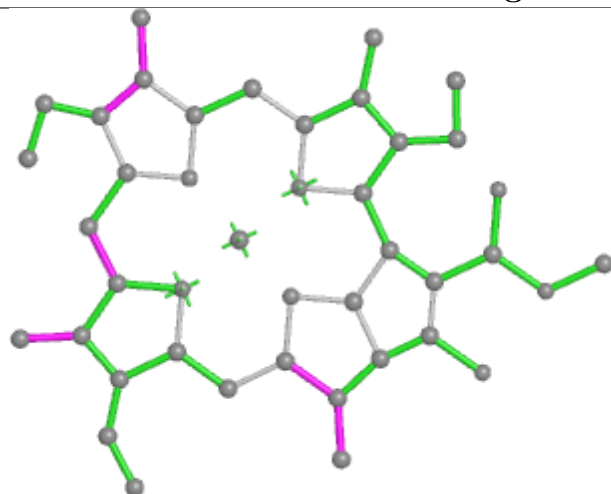
Rings



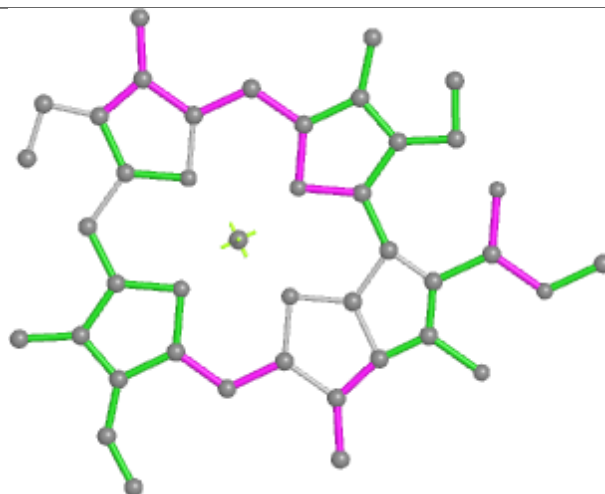
Ligand CLA A2 824



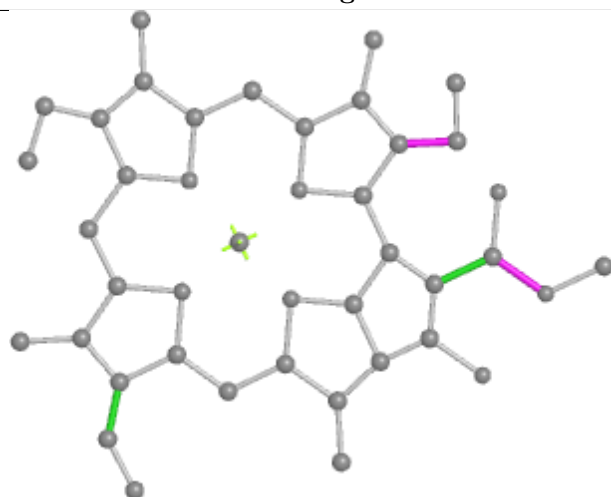
Ligand CLA A2 825



Bond lengths



Bond angles

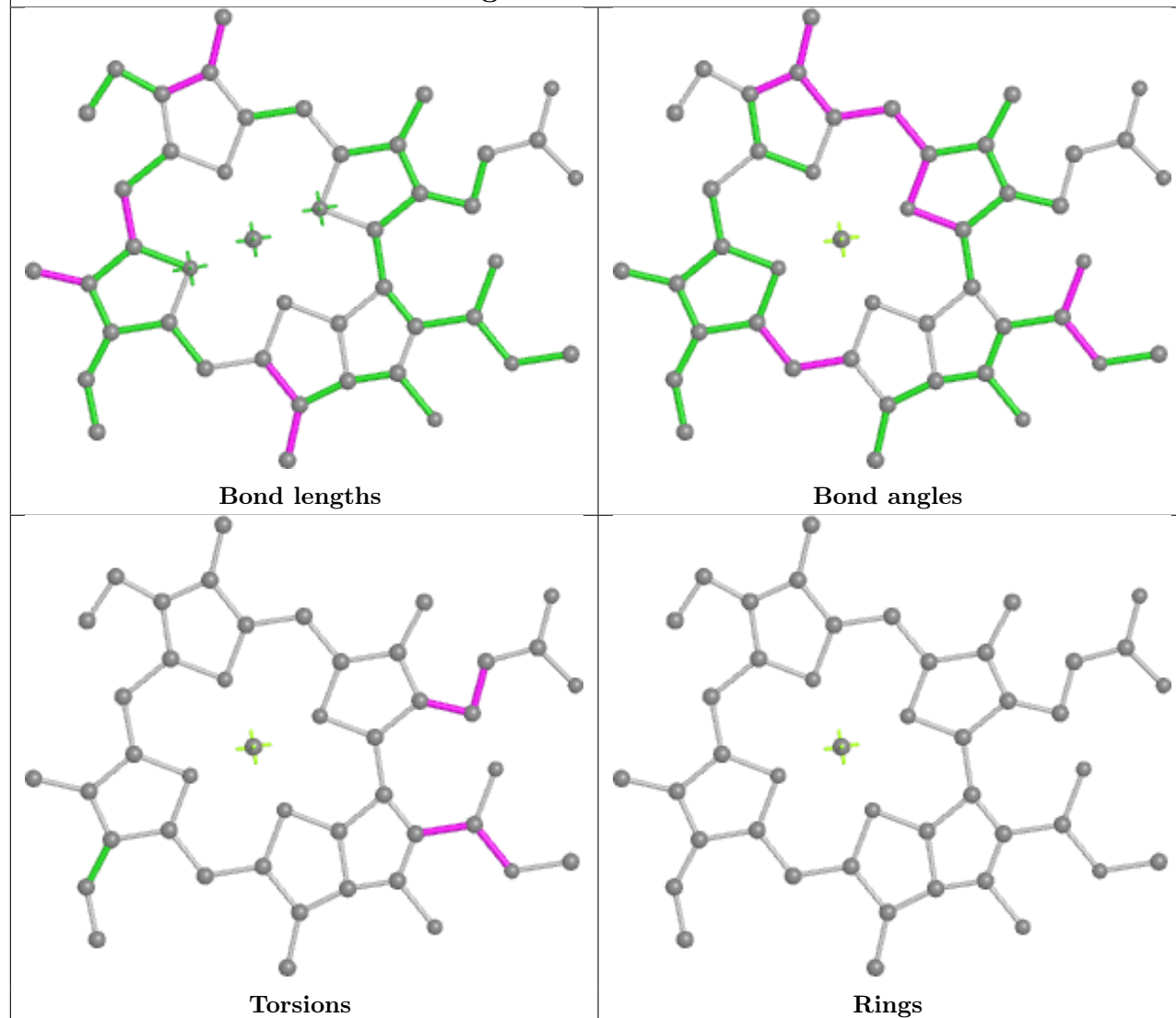


Torsions

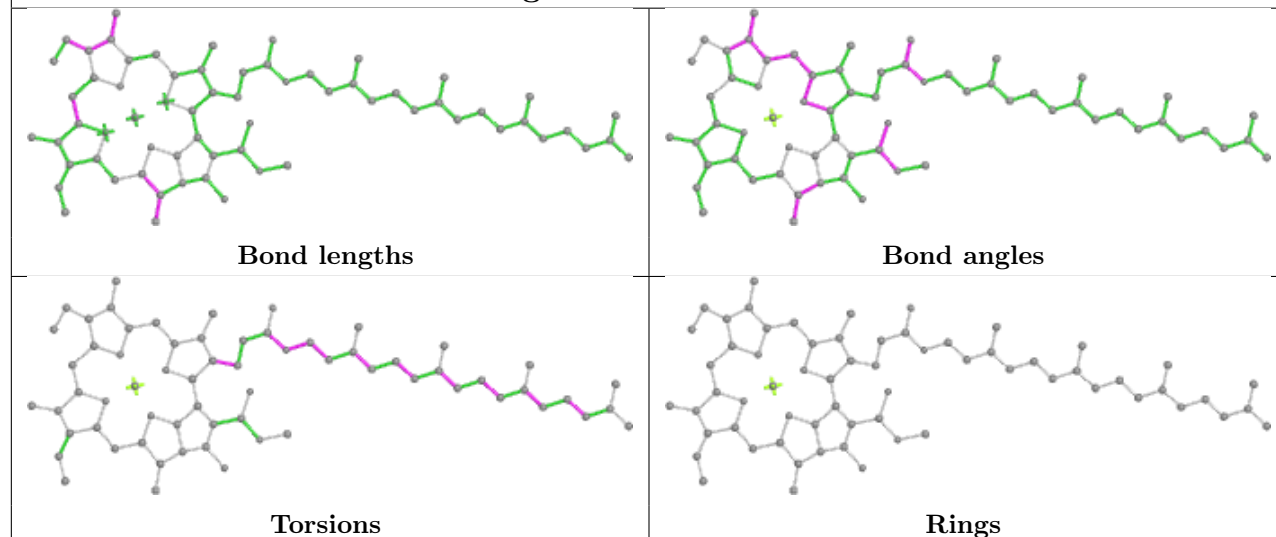


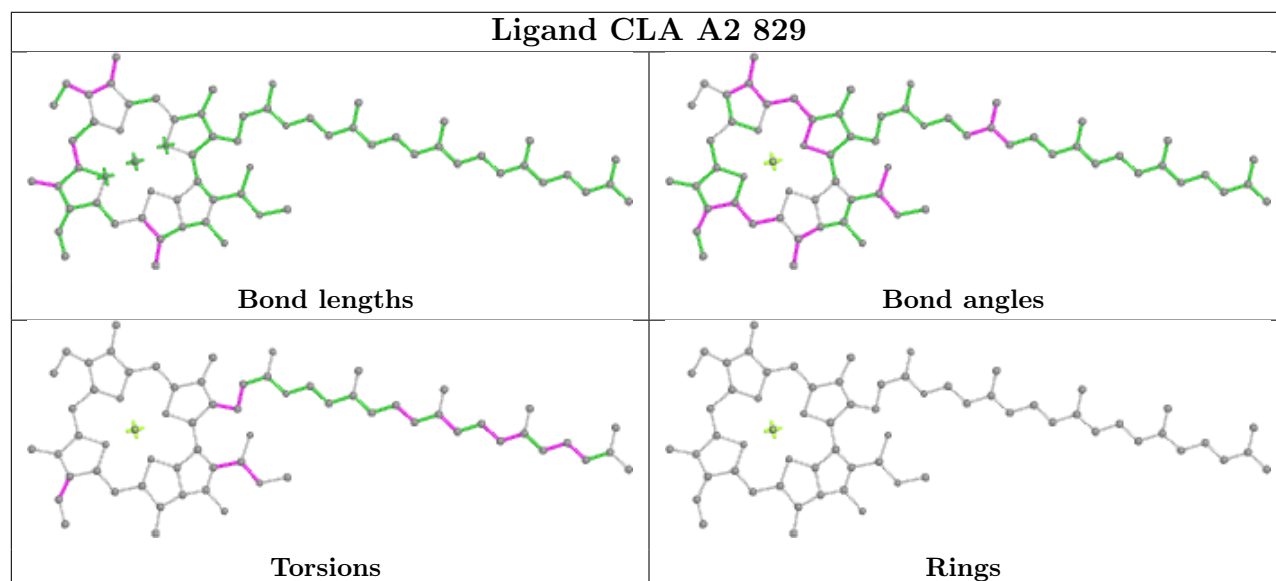
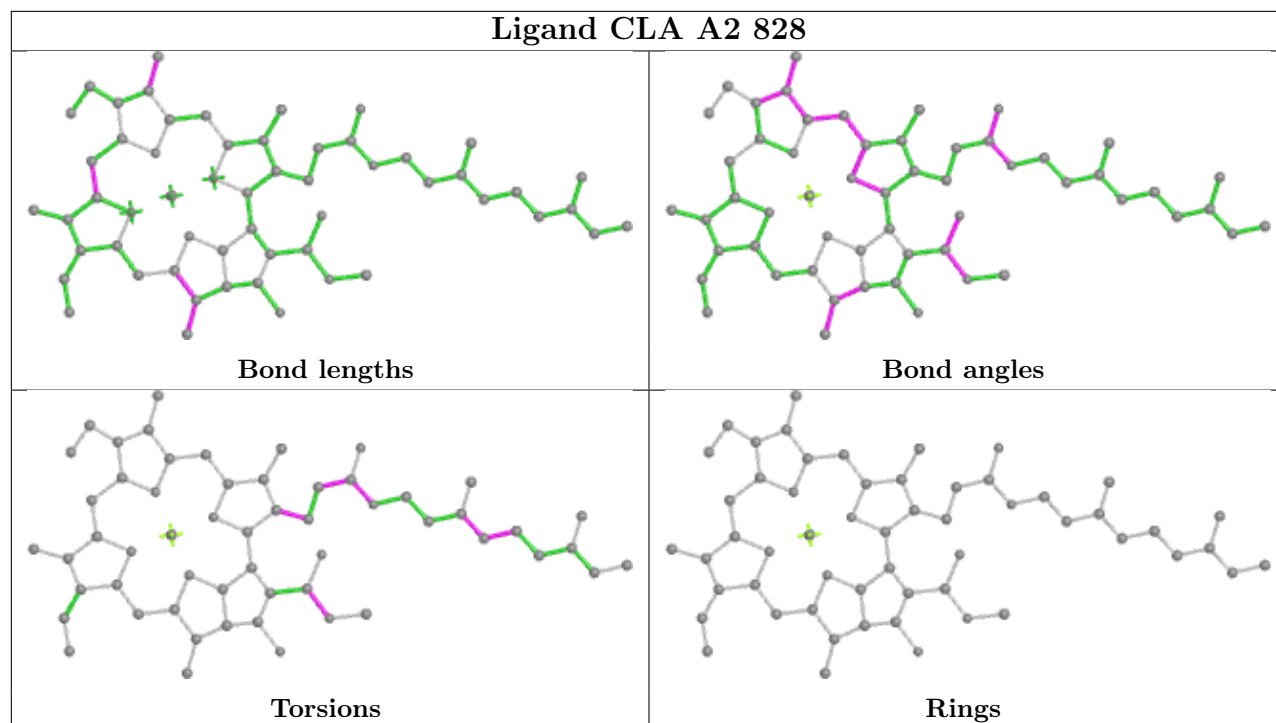
Rings

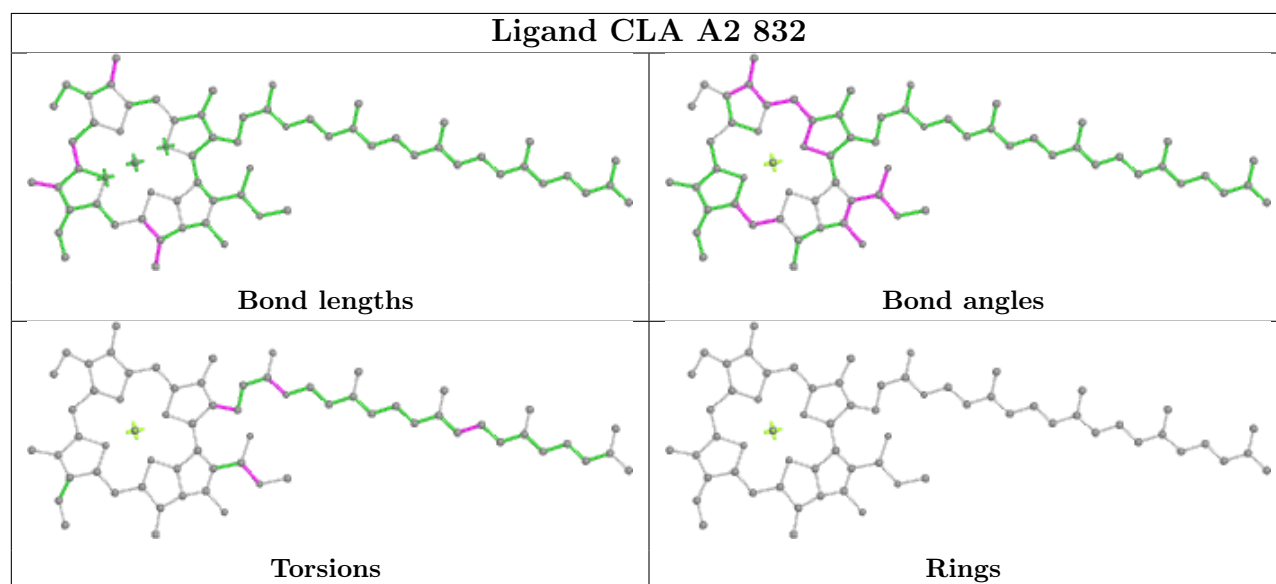
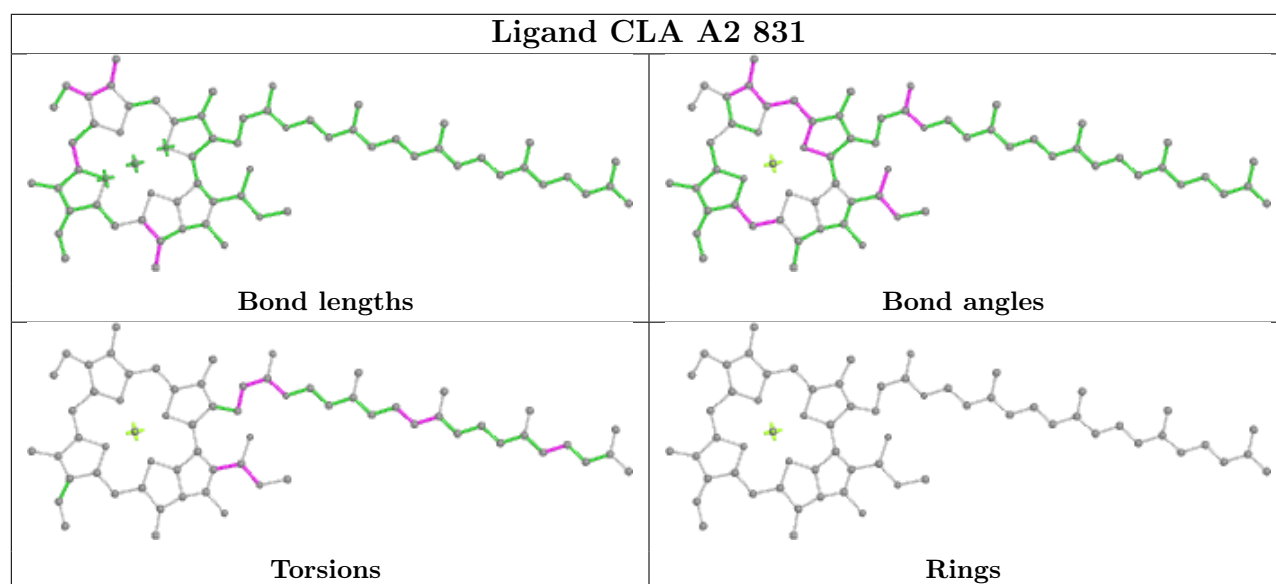
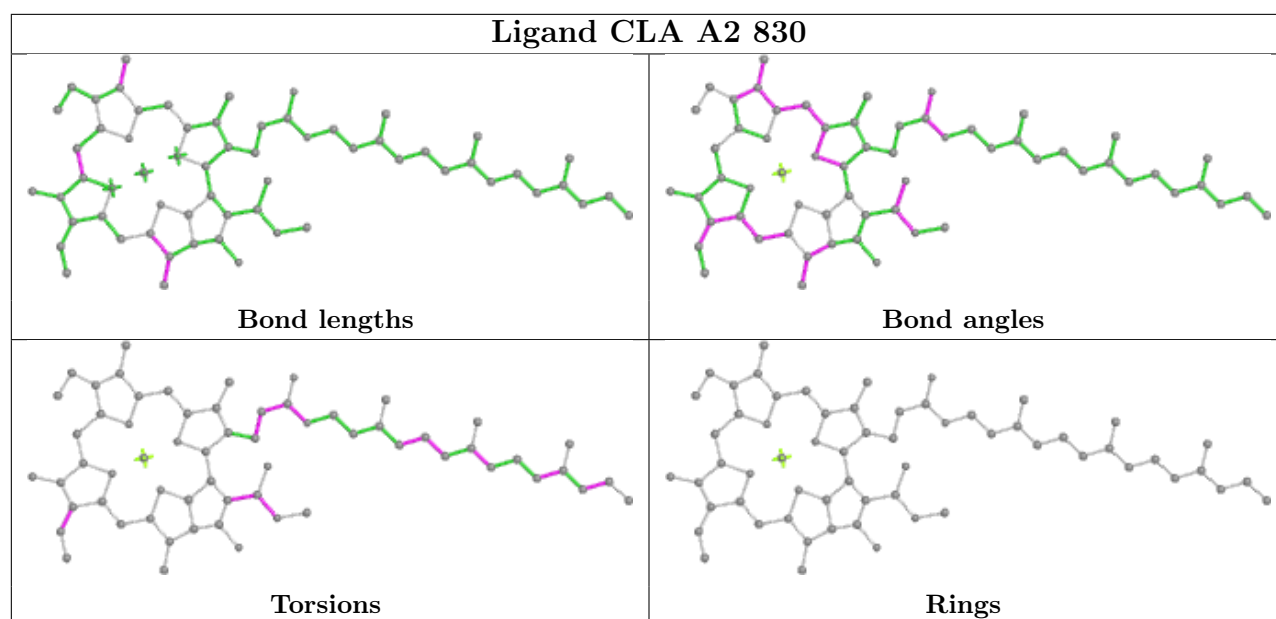
Ligand CLA A2 826



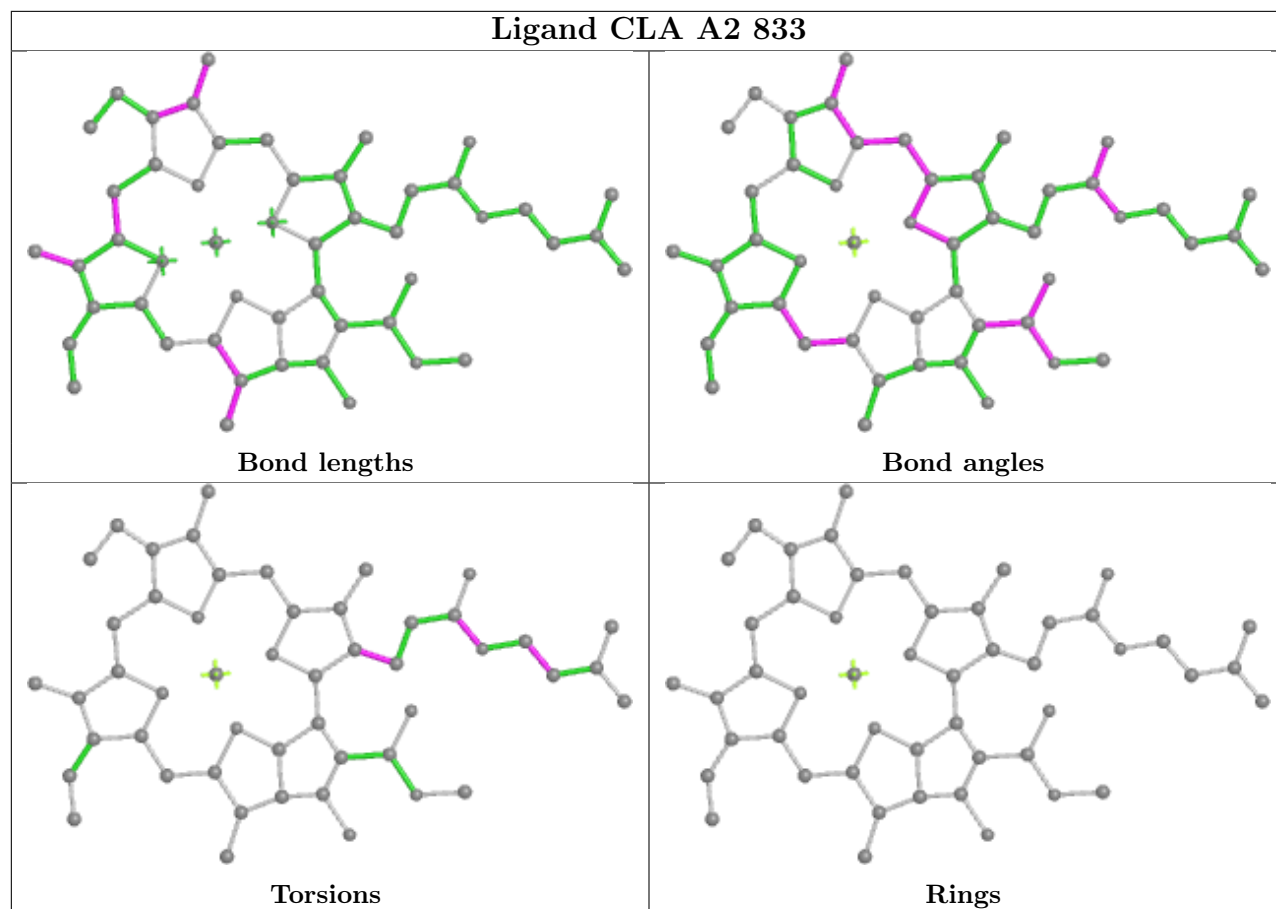
Ligand CLA A2 827



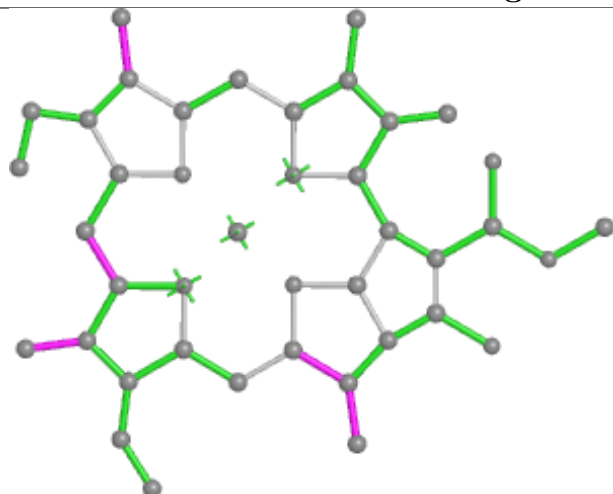




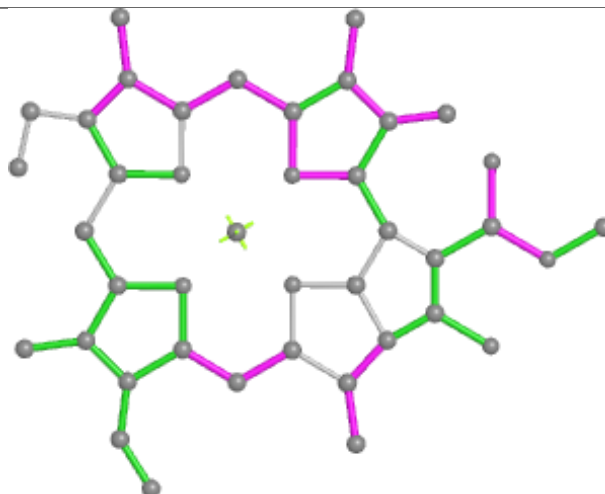
Ligand CLA A2 833



Ligand CLA A2 834



Bond lengths



Bond angles

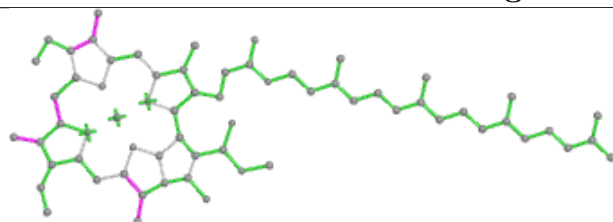


Torsions

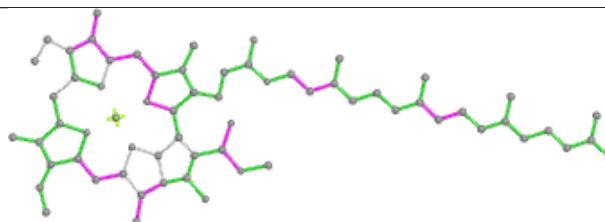


Rings

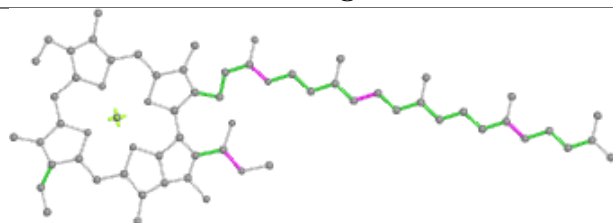
Ligand CLA A2 835



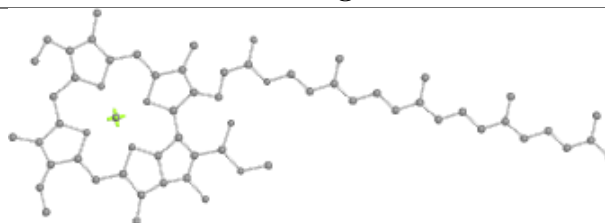
Bond lengths



Bond angles

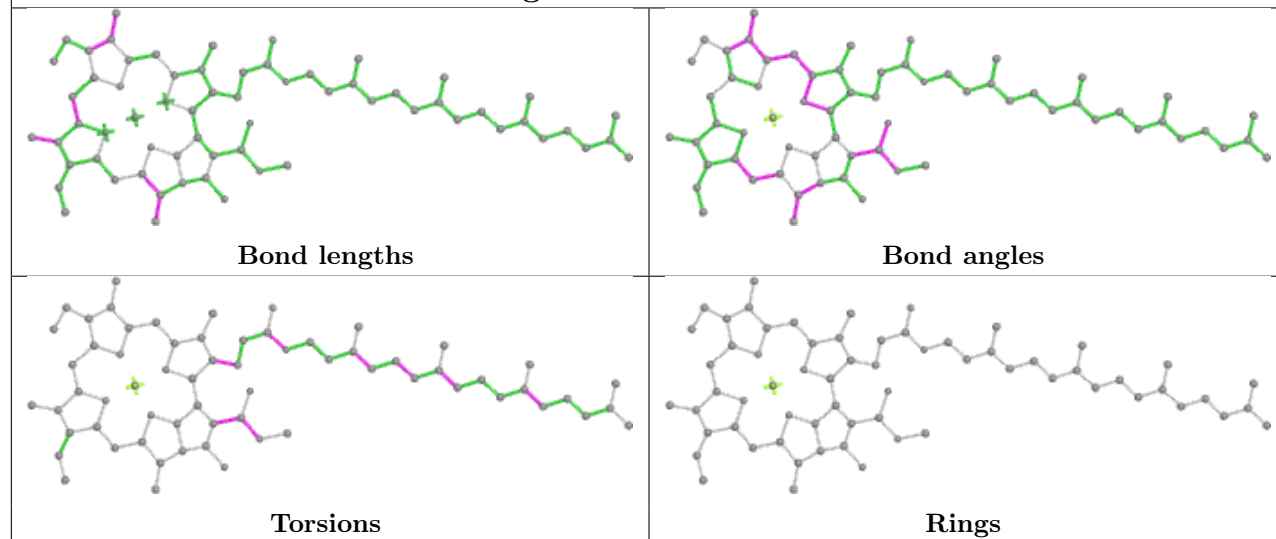


Torsions

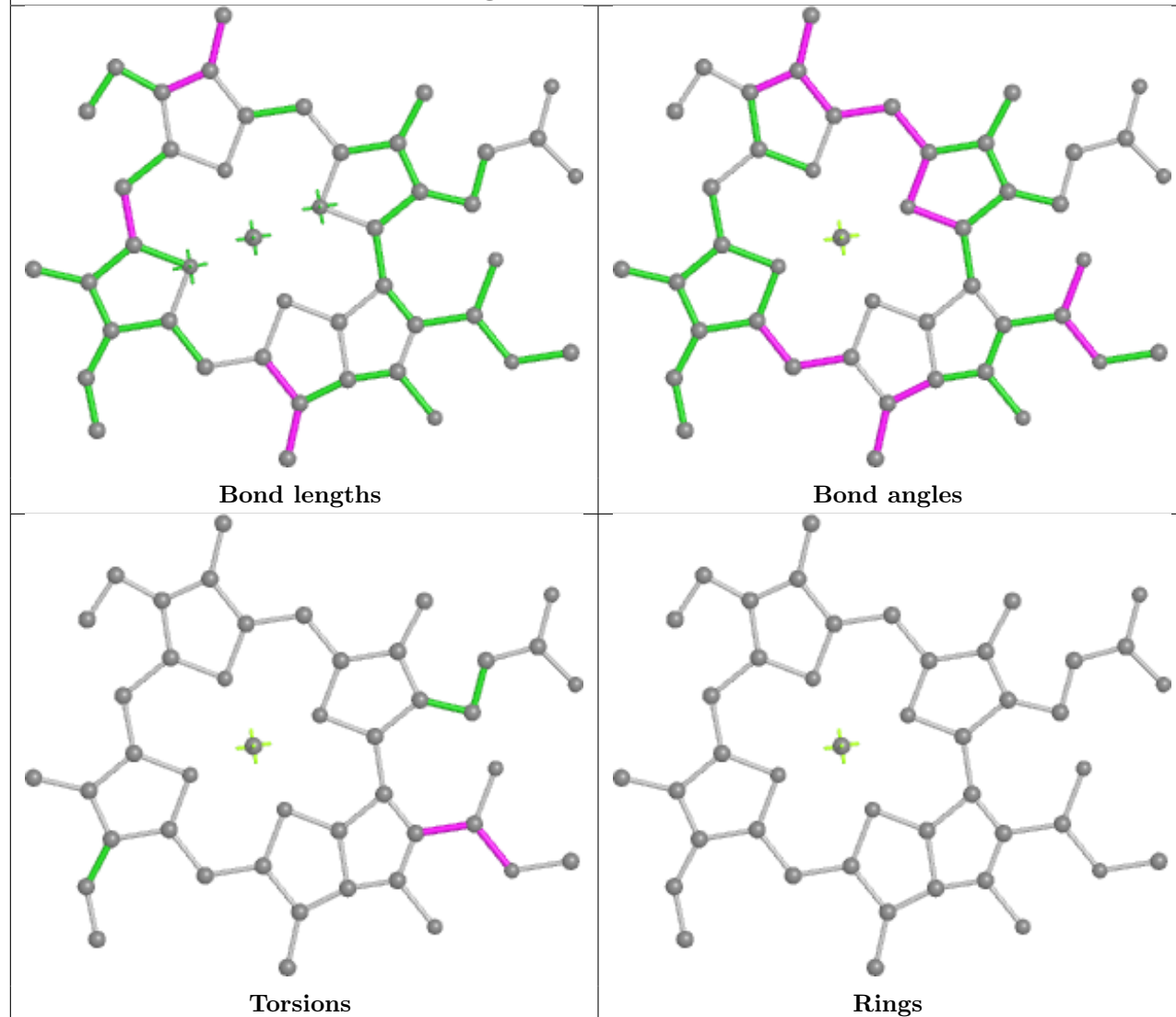


Rings

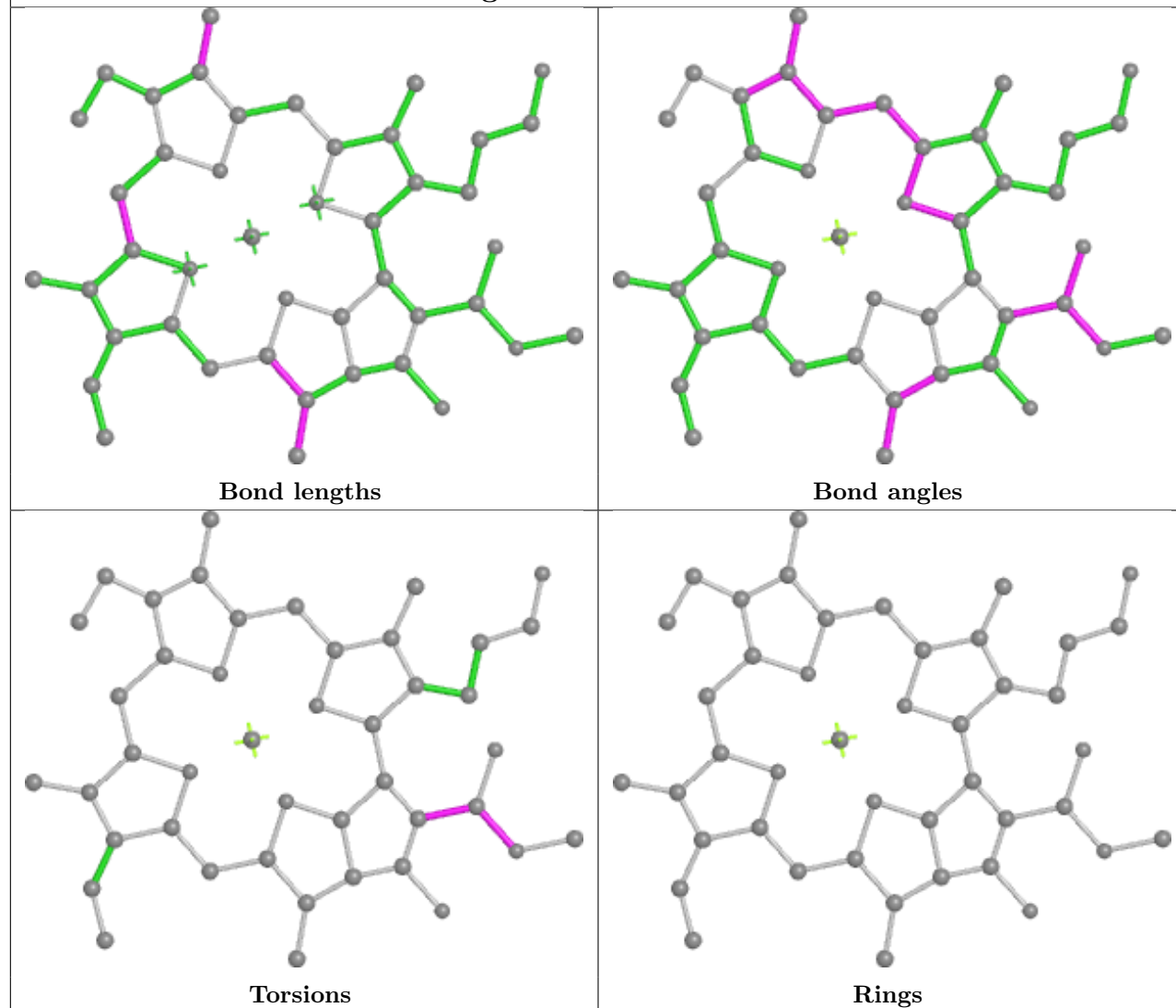
Ligand CLA A2 836



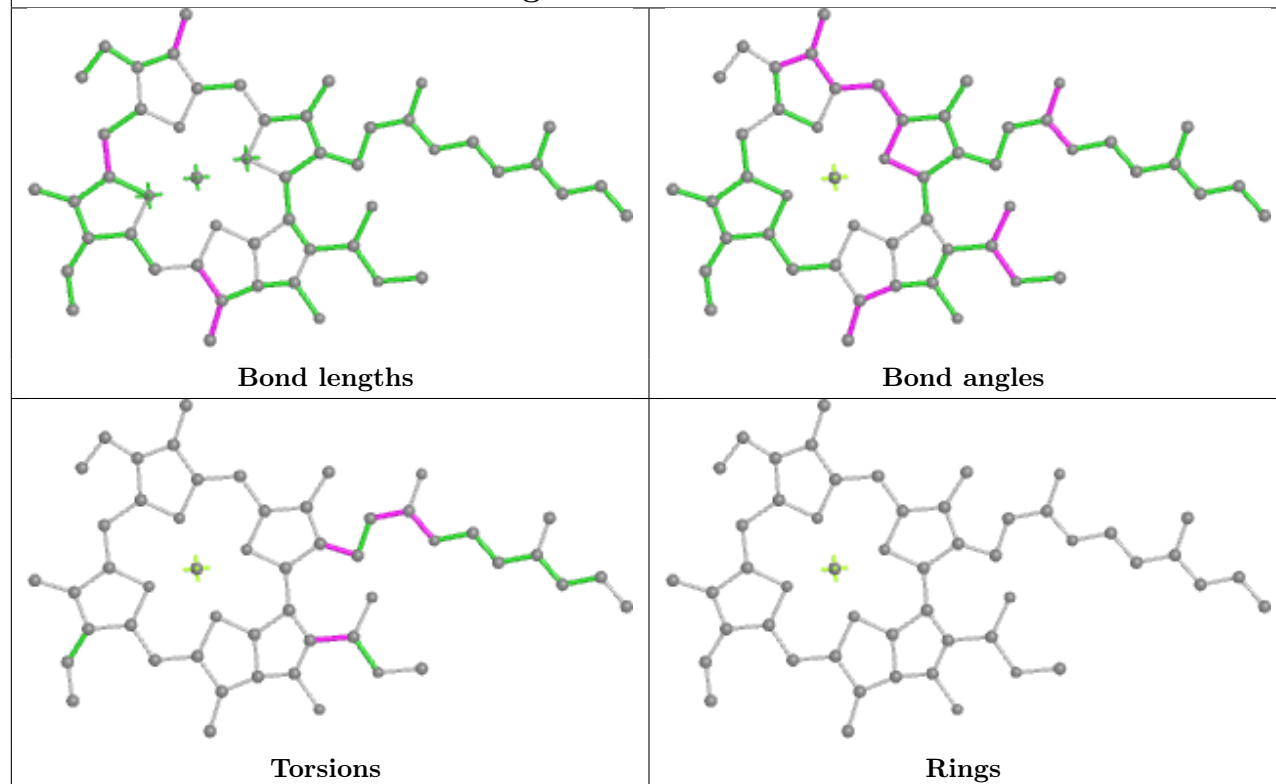
Ligand CLA A2 837



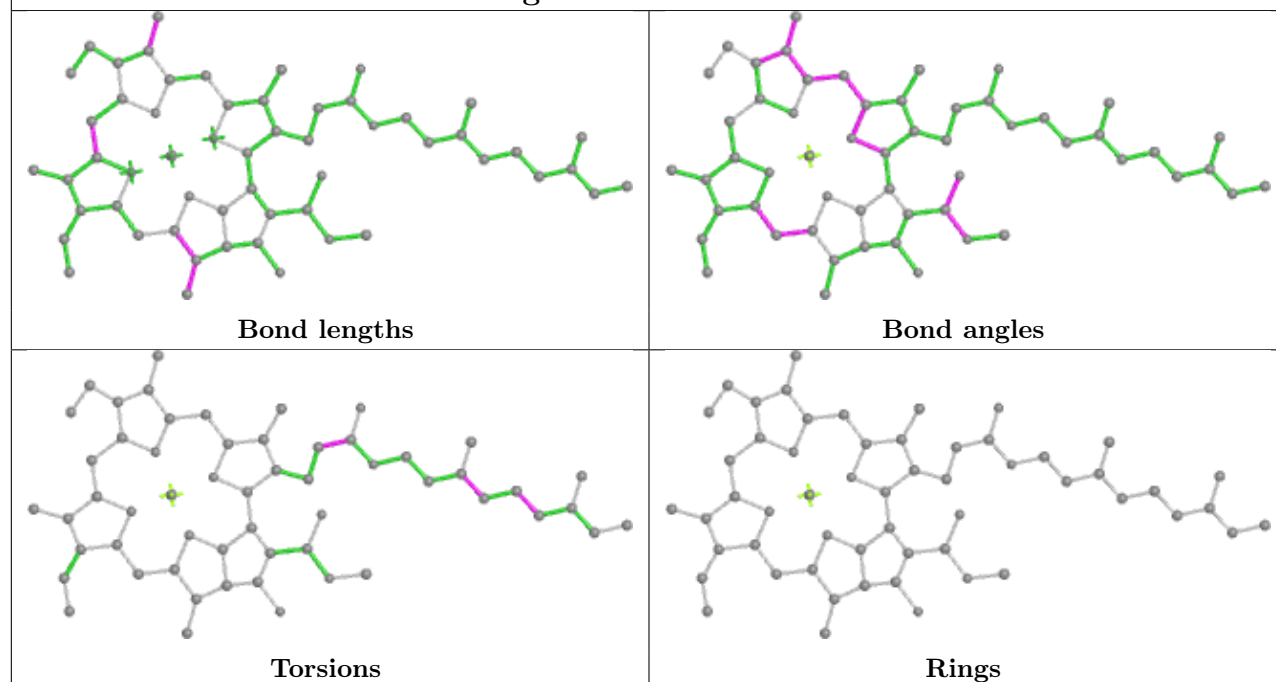
Ligand CLA A2 838



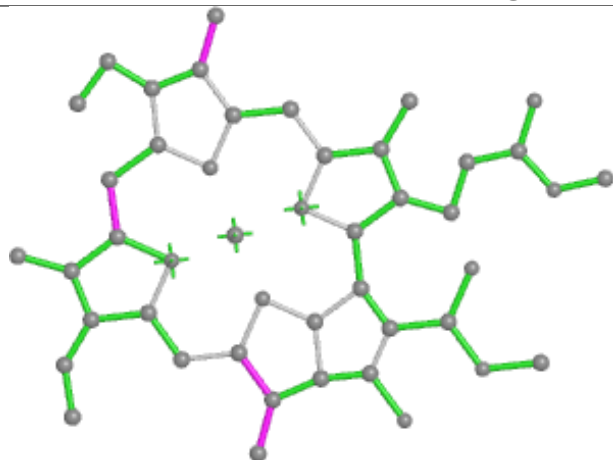
Ligand CLA A2 839



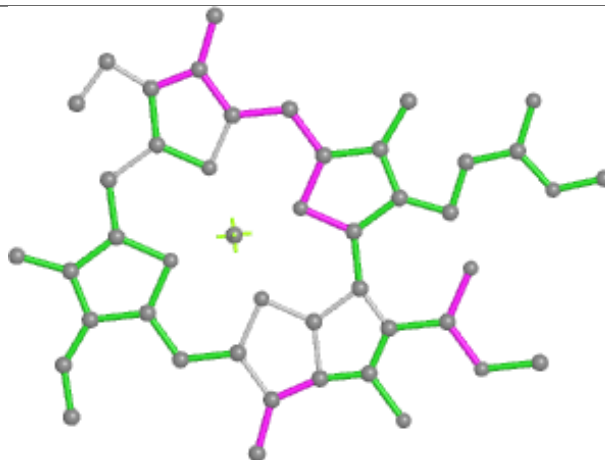
Ligand CLA A2 840



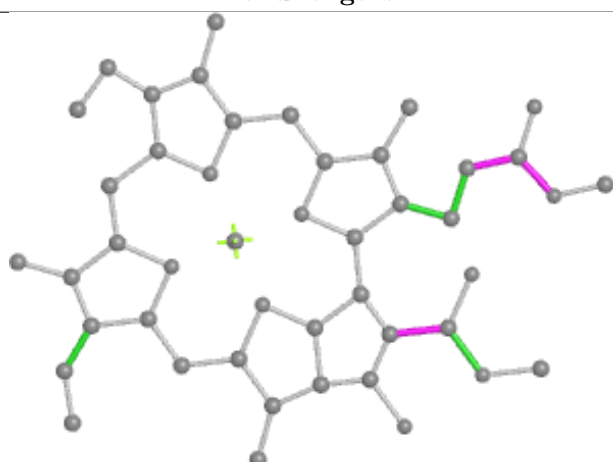
Ligand CLA A2 841



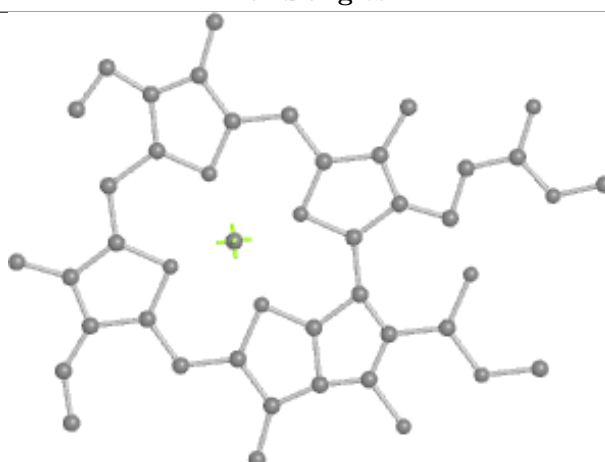
Bond lengths



Bond angles

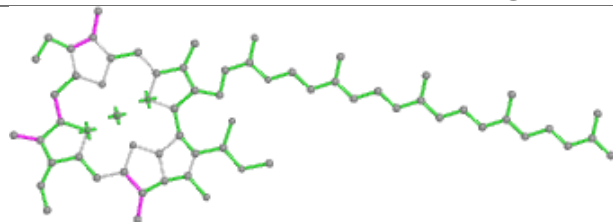


Torsions

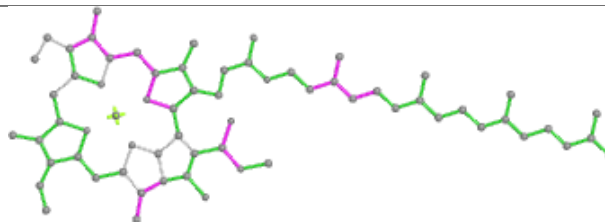


Rings

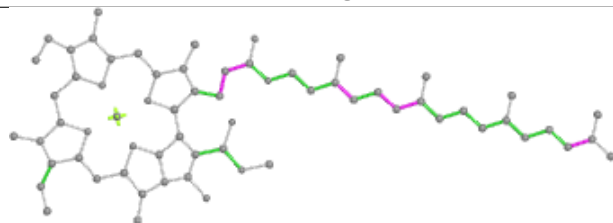
Ligand CLA A2 842



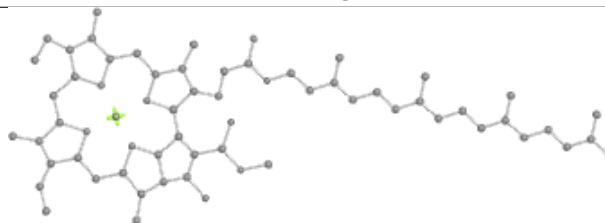
Bond lengths



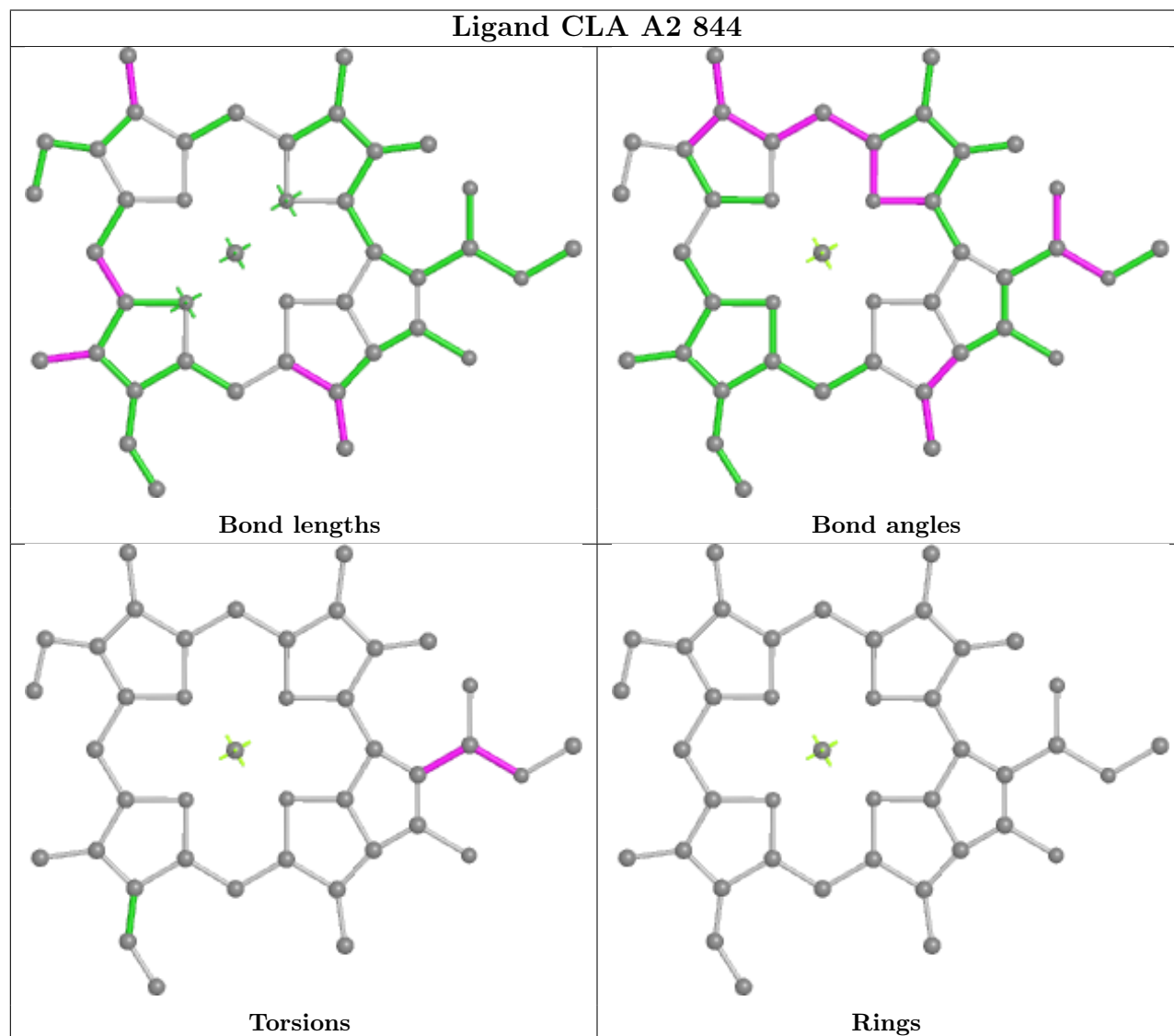
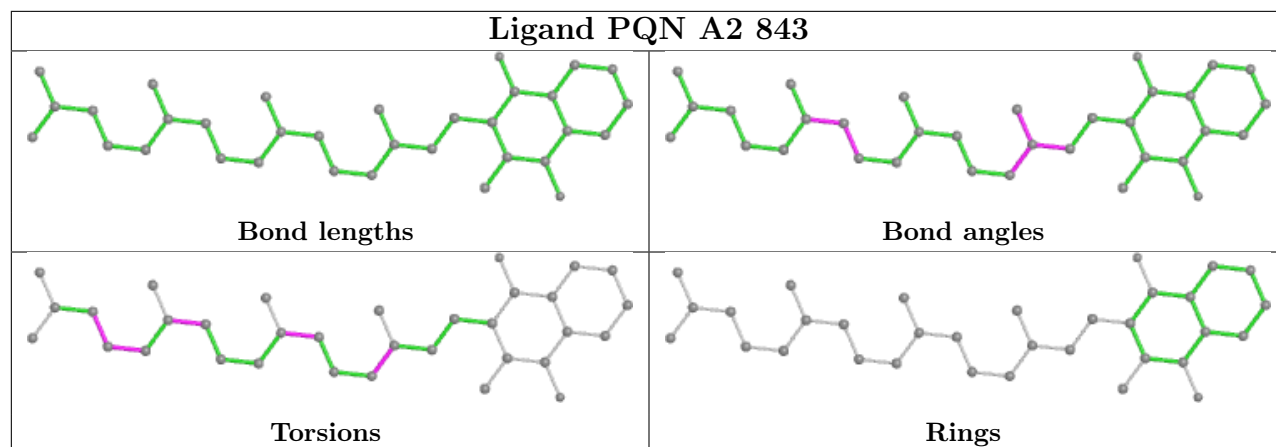
Bond angles

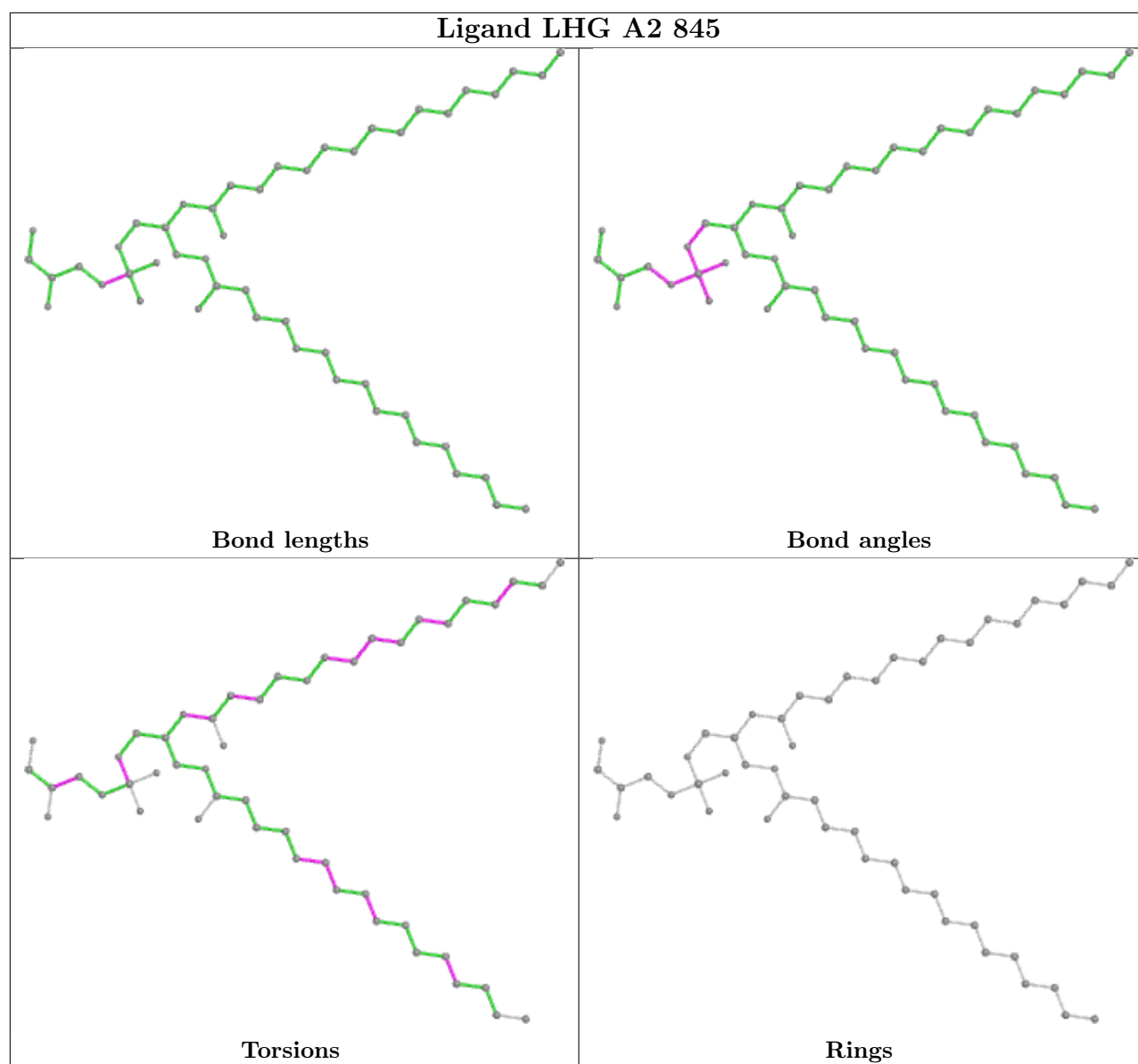


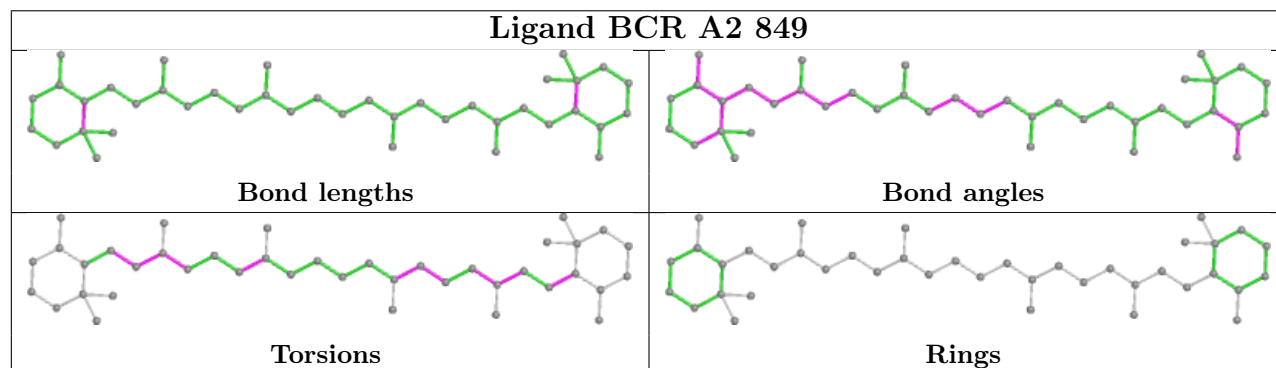
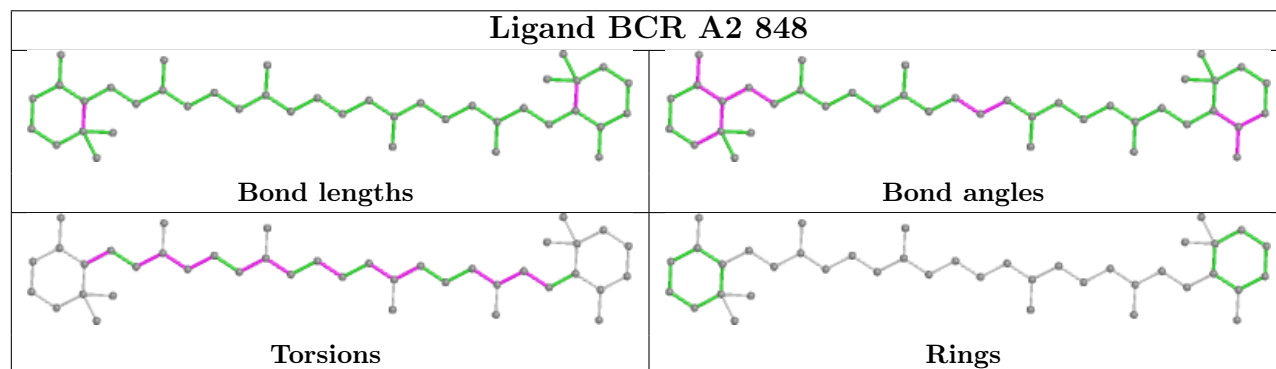
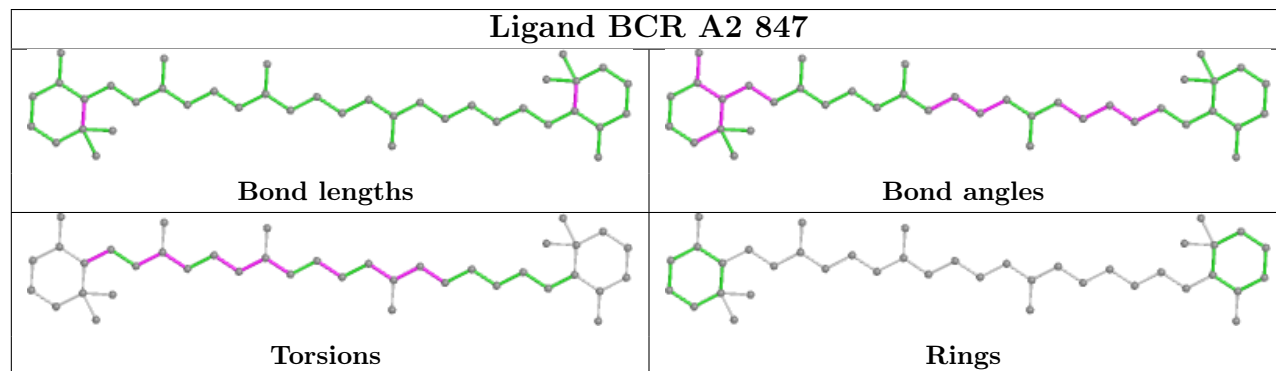
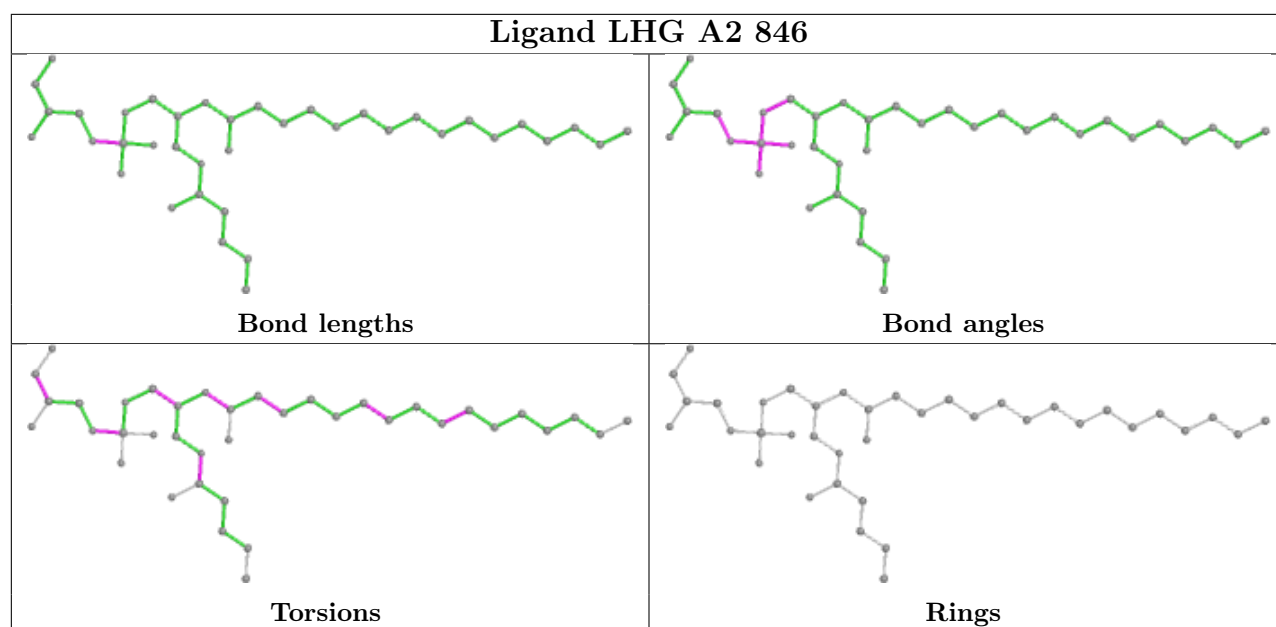
Torsions

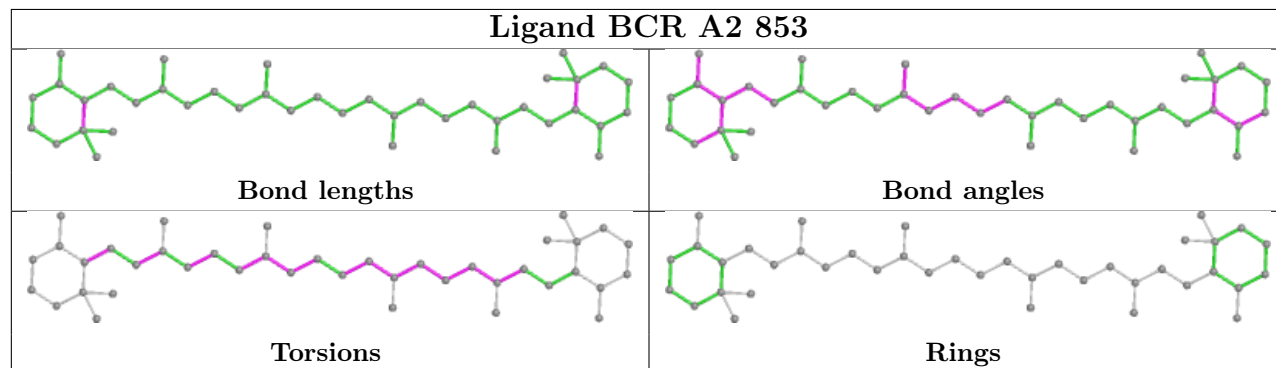
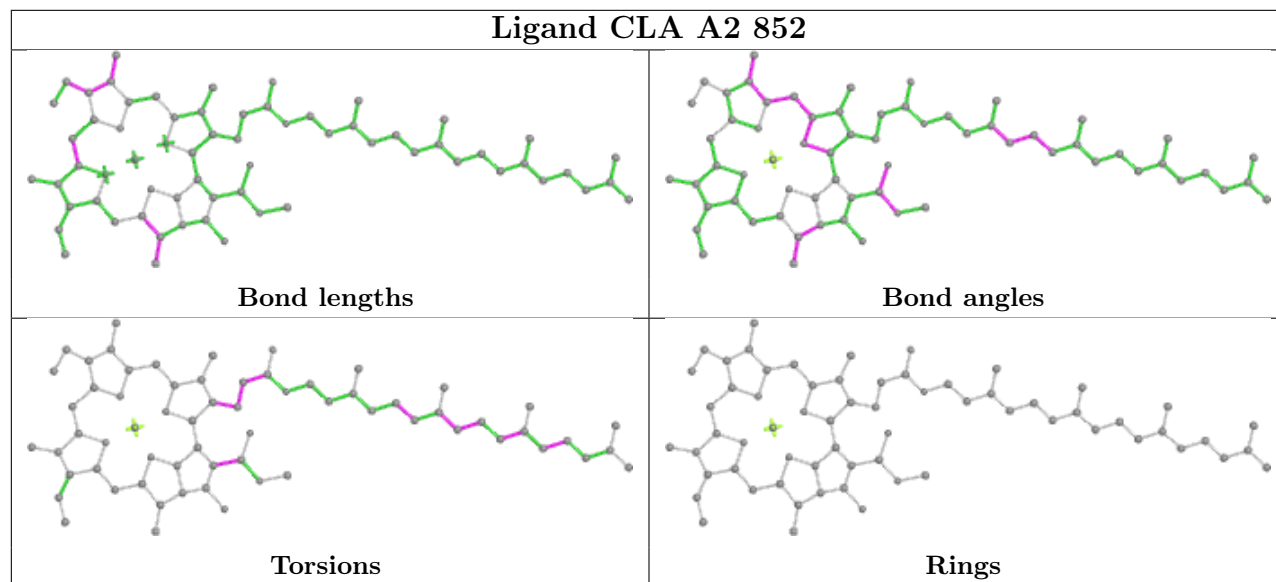
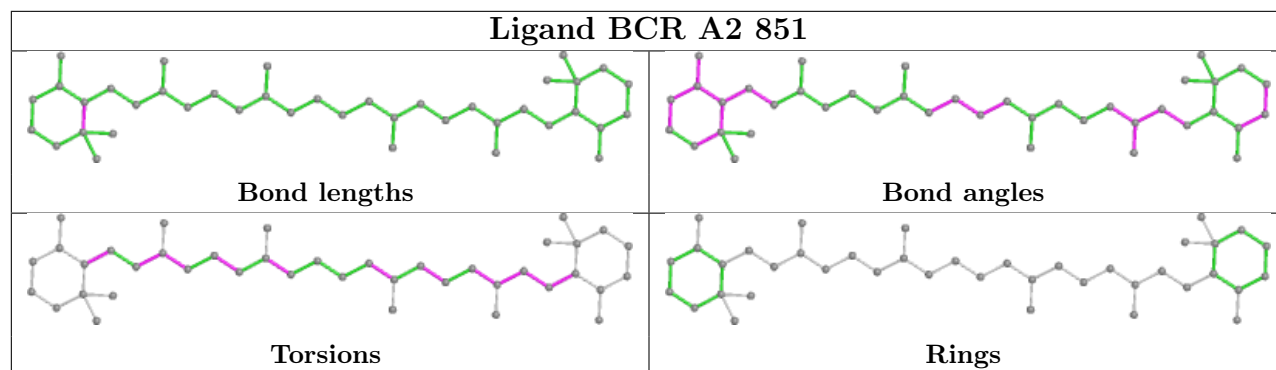
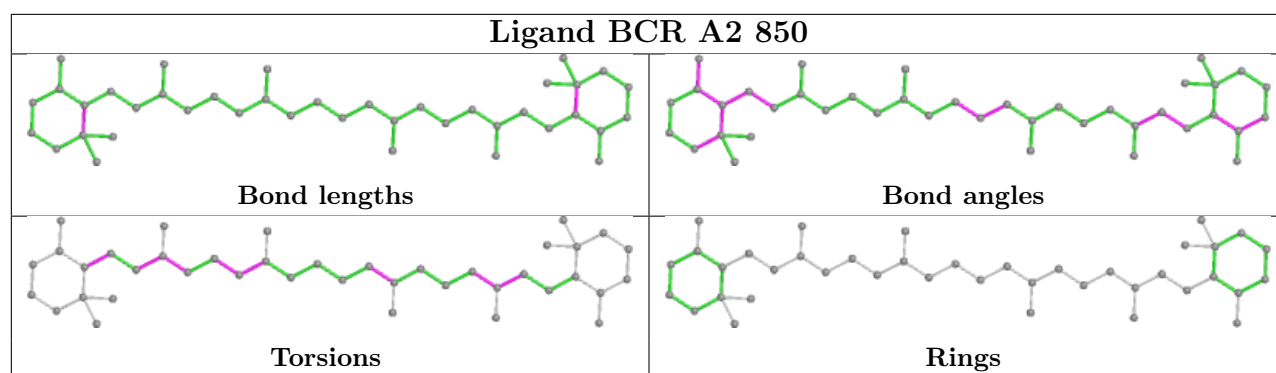


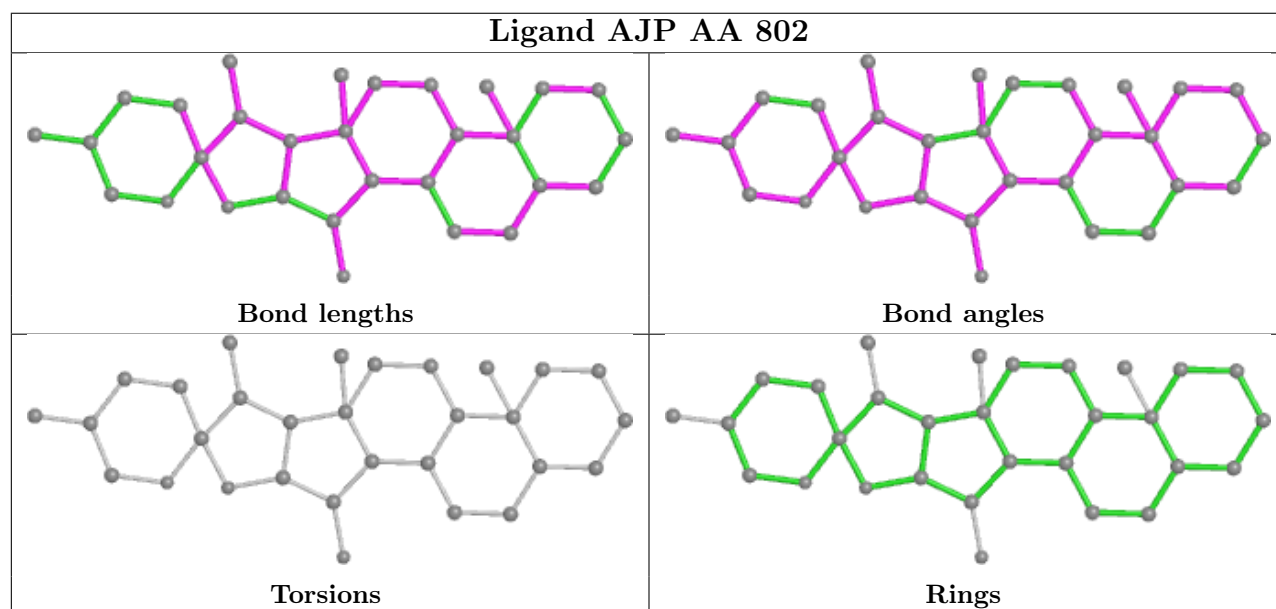
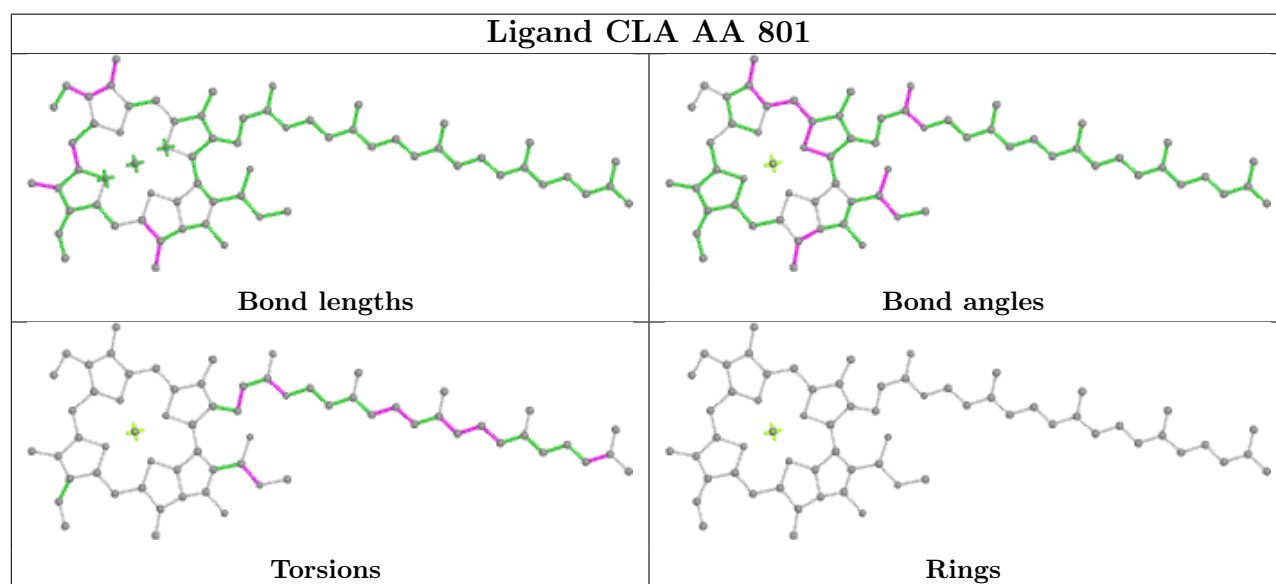
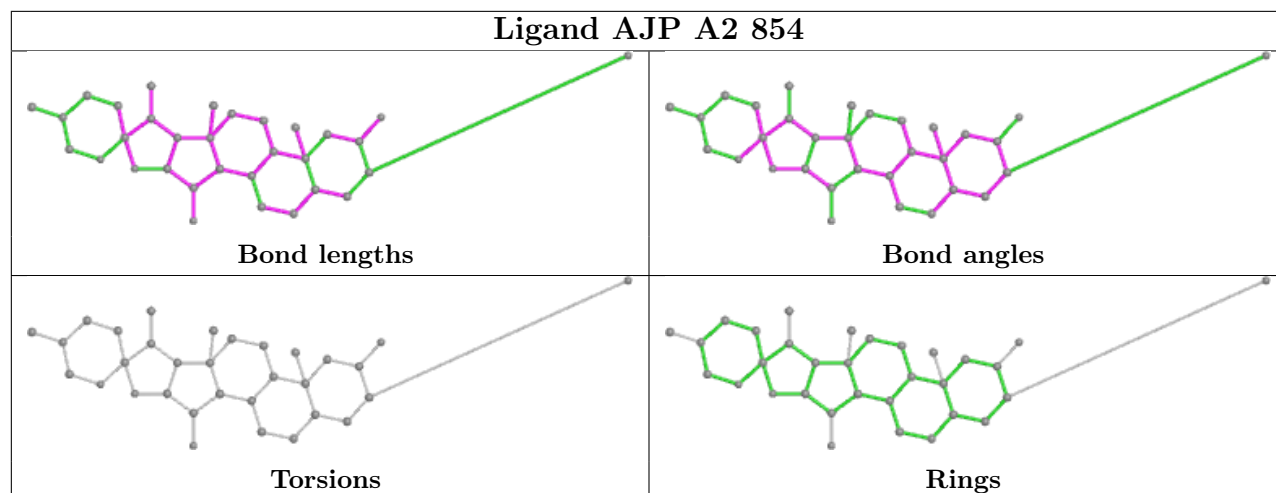
Rings

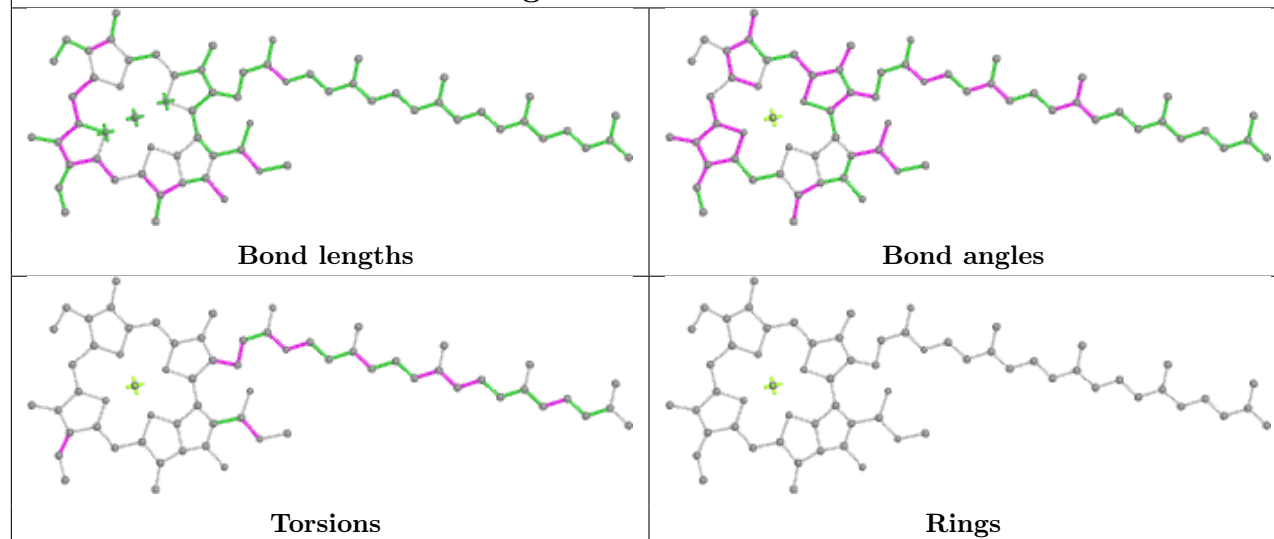
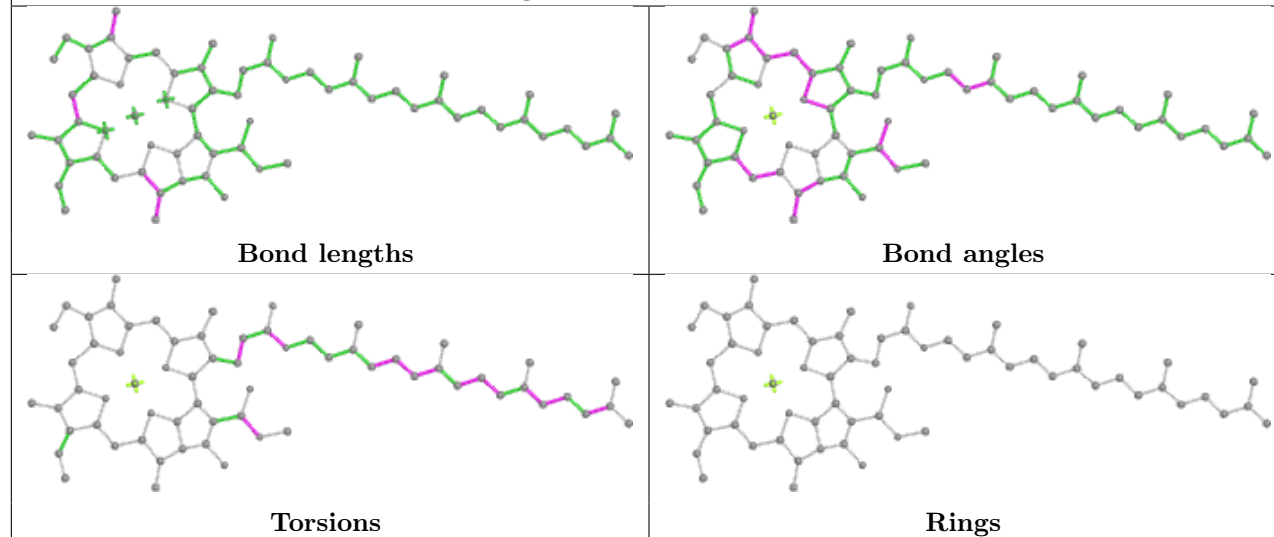




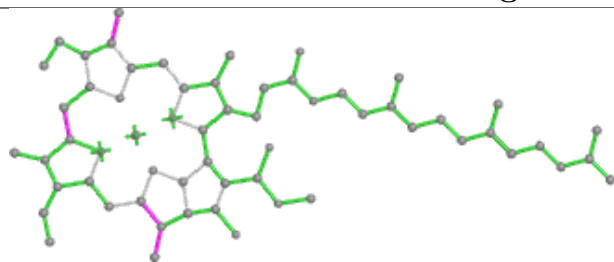




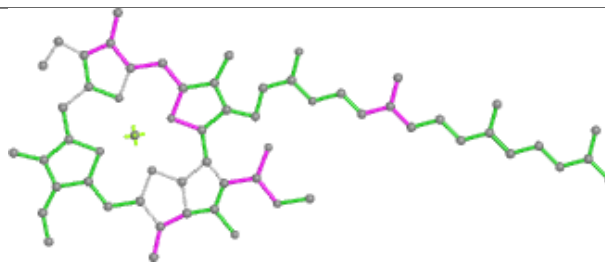


Ligand CL0 AA 803**Ligand CLA AA 804**

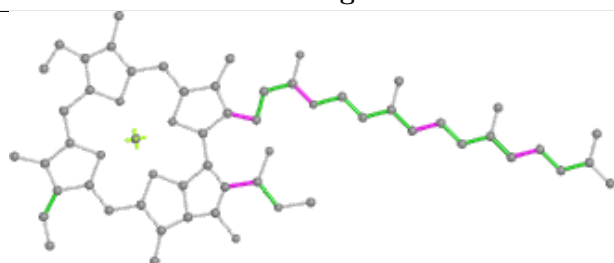
Ligand CLA AA 805



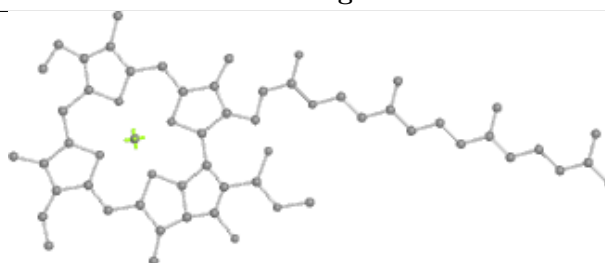
Bond lengths



Bond angles

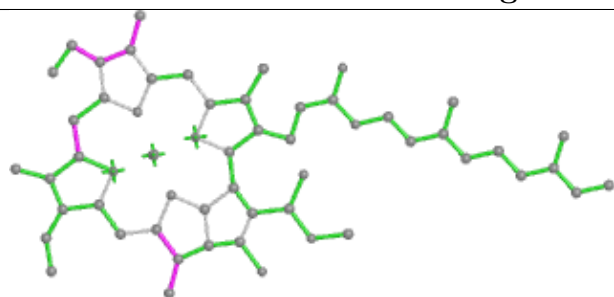


Torsions

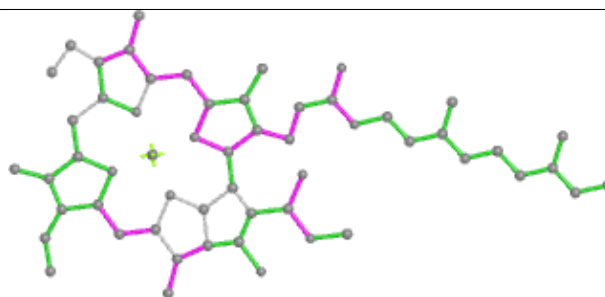


Rings

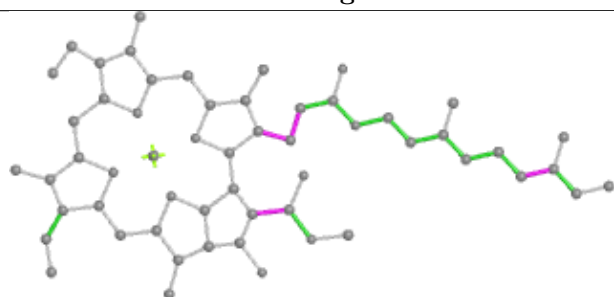
Ligand CLA AA 806



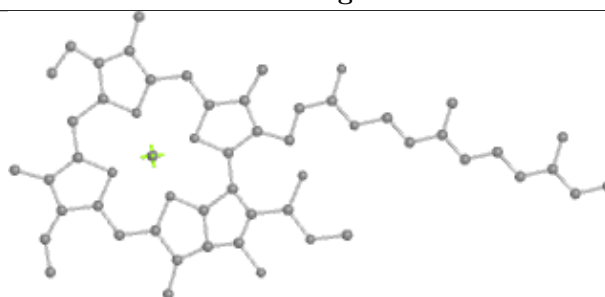
Bond lengths



Bond angles

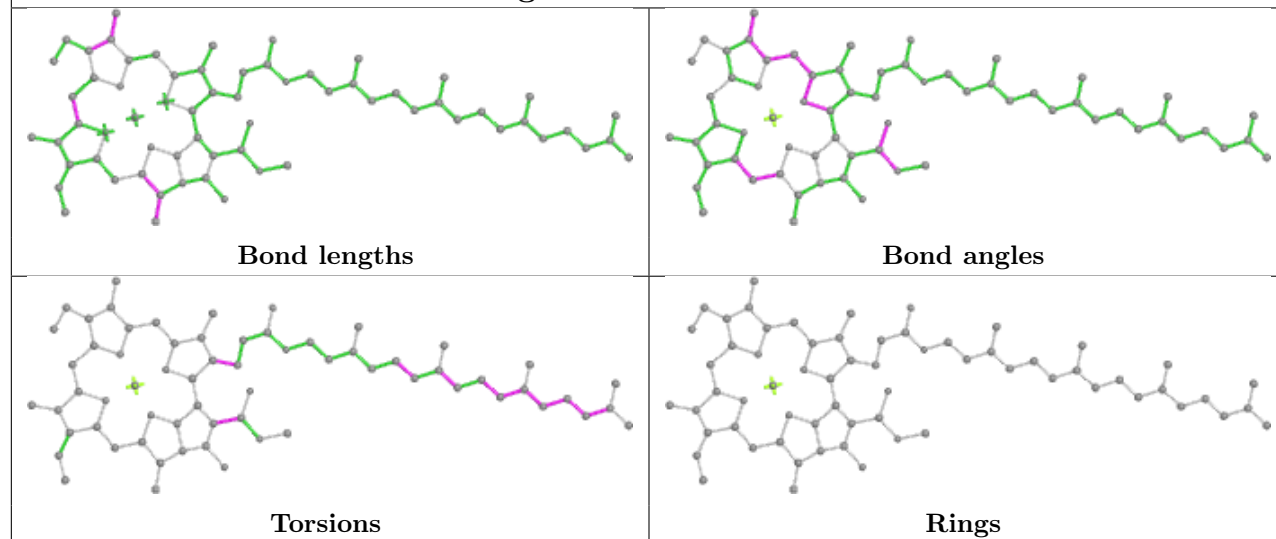


Torsions

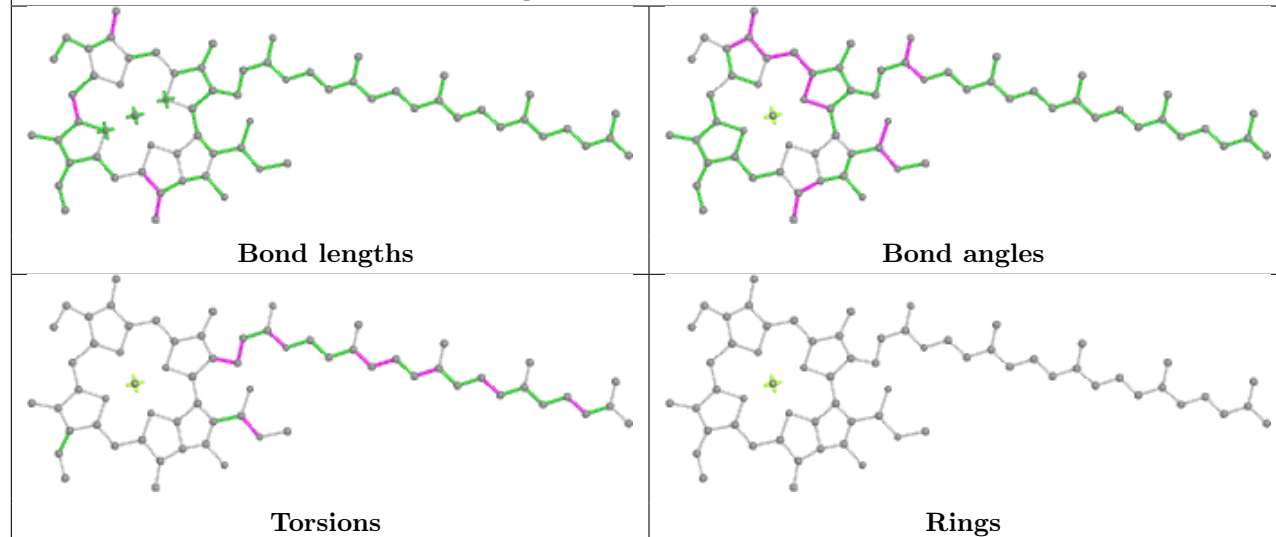


Rings

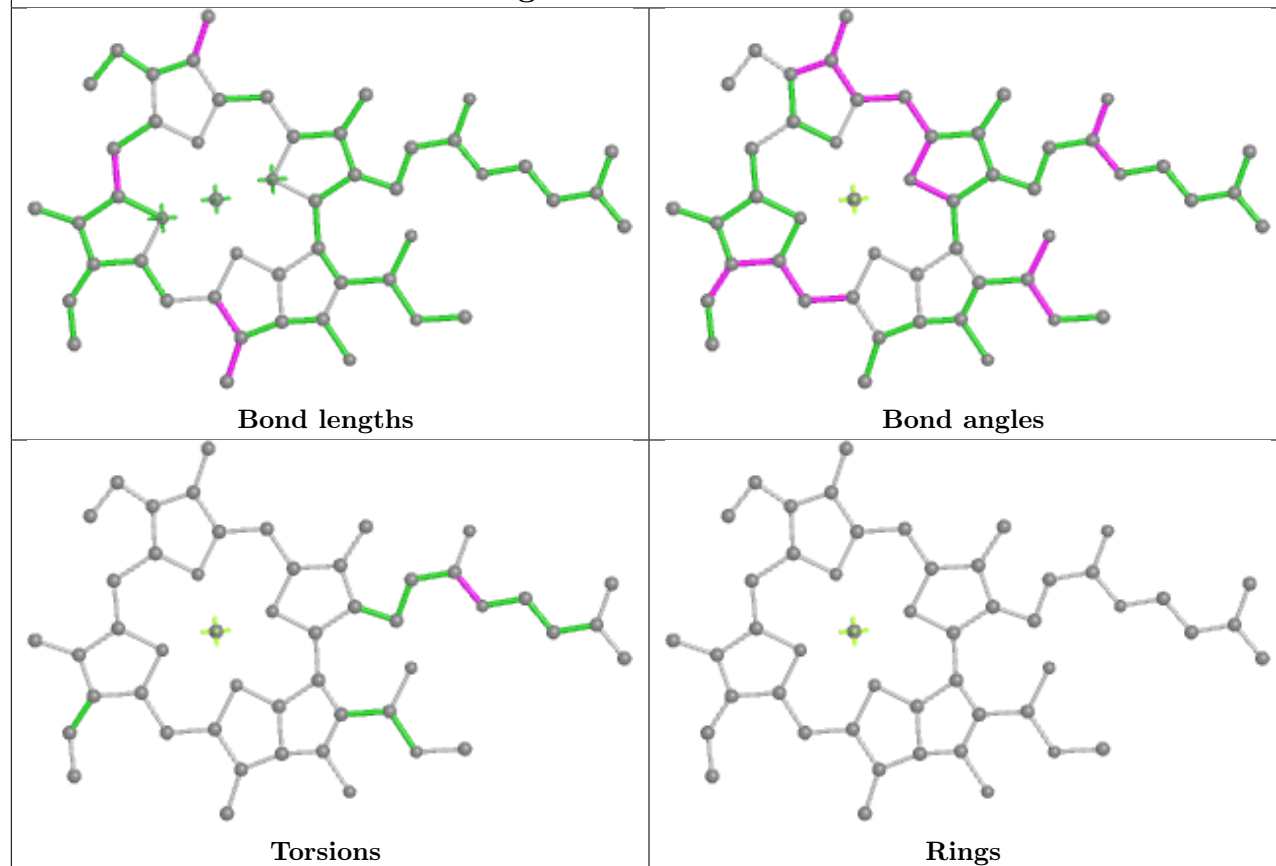
Ligand CLA AA 807



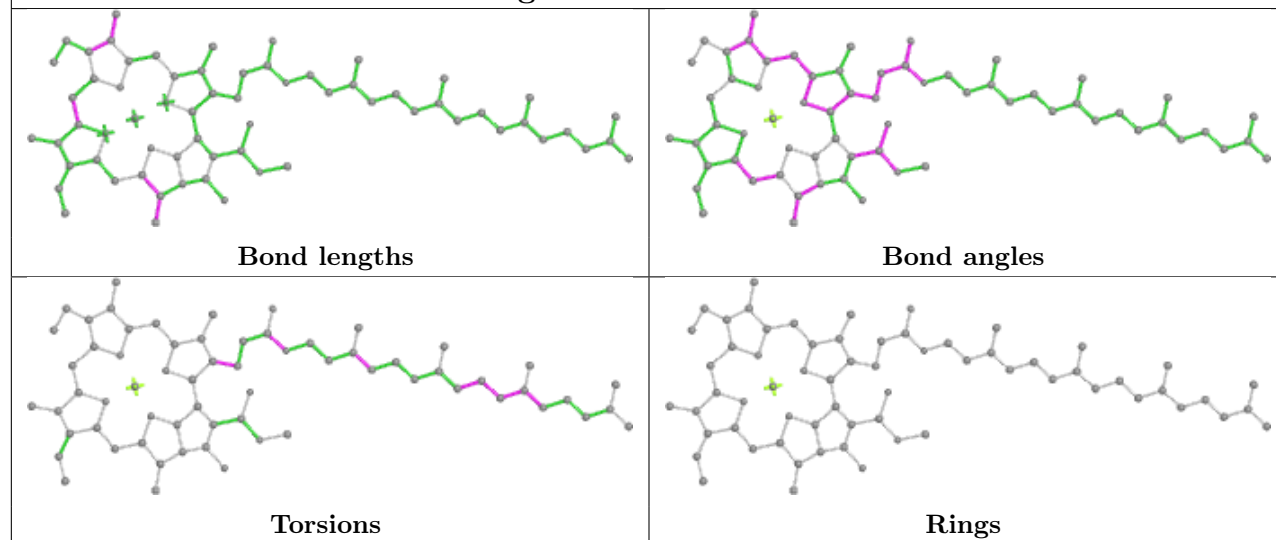
Ligand CLA AA 808



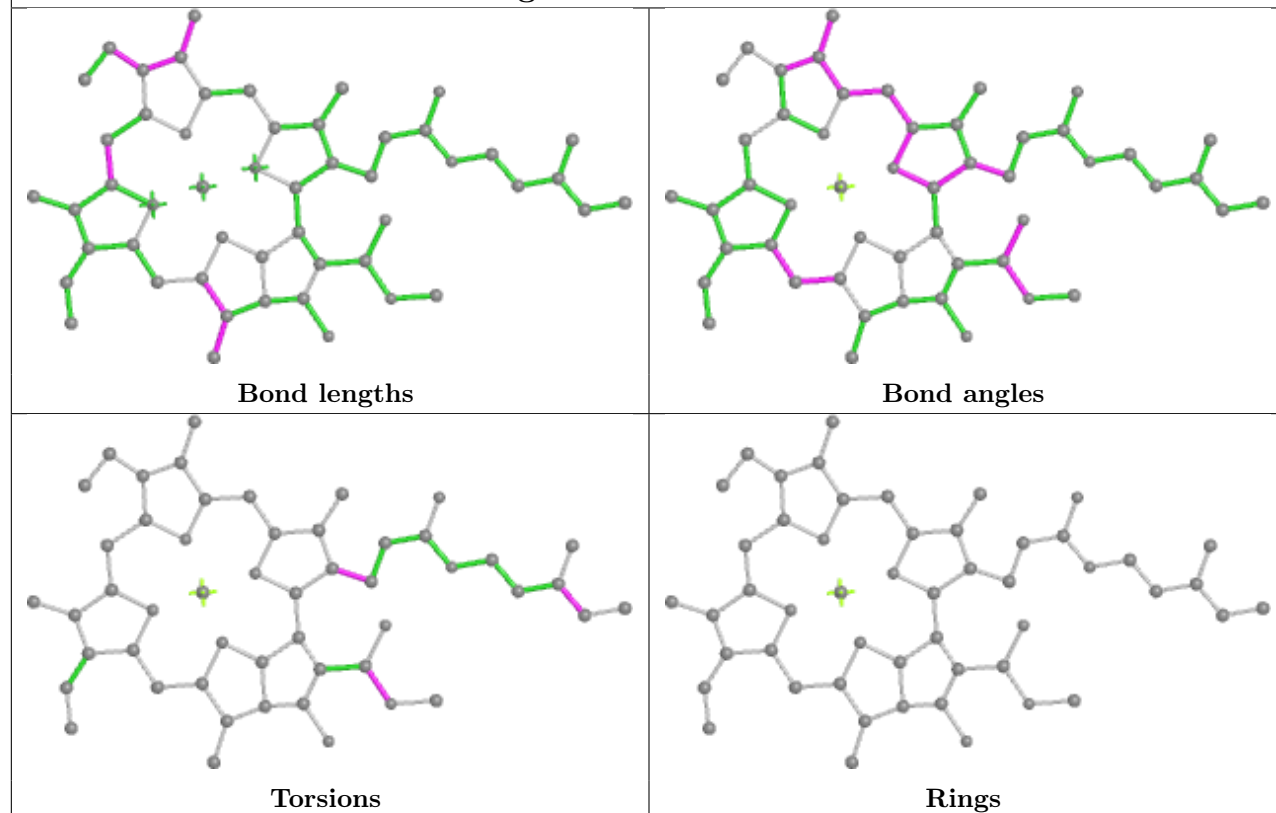
Ligand CLA AA 809



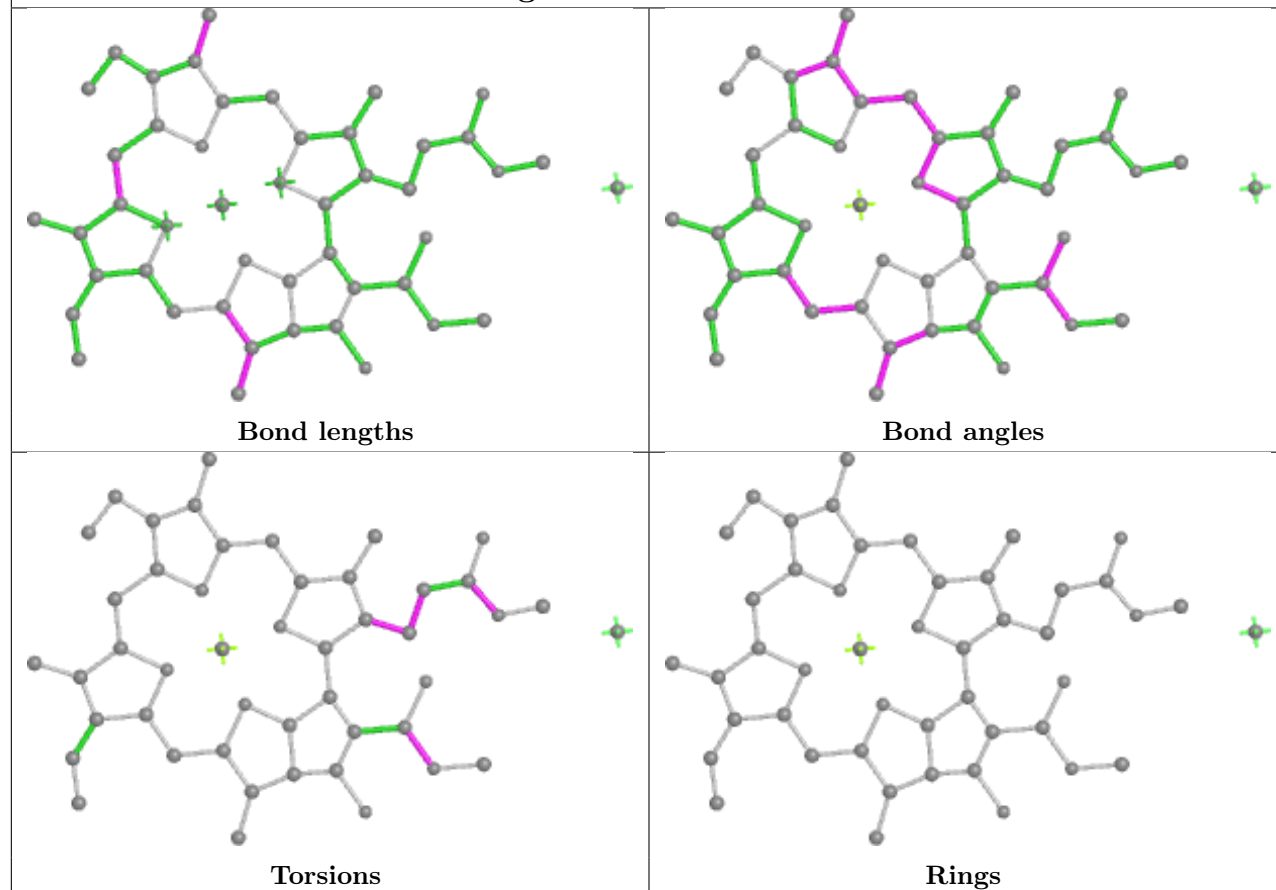
Ligand CLA AA 810



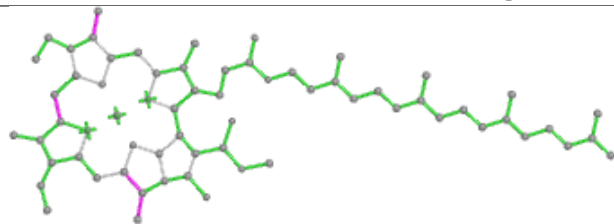
Ligand CLA AA 811



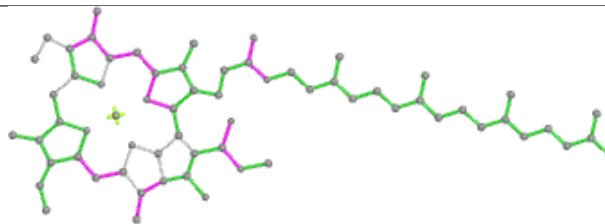
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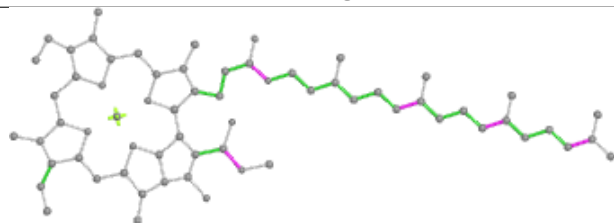
Ligand CLA AA 813



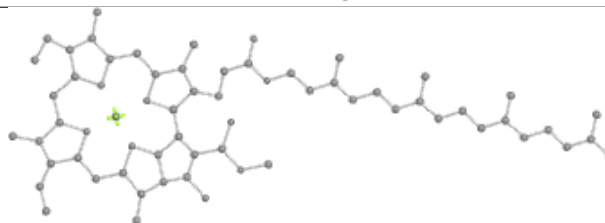
Bond lengths



Bond angles

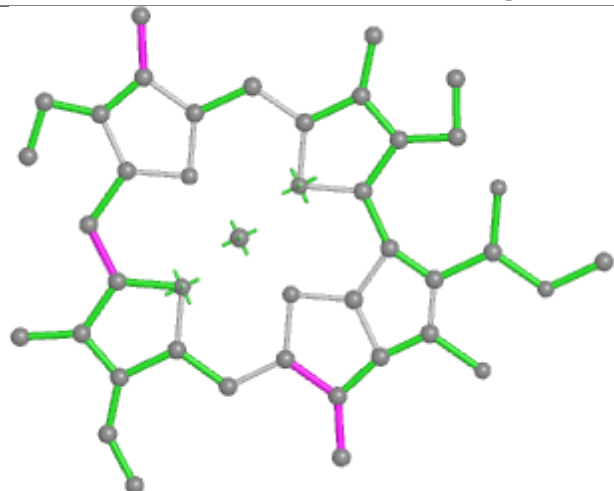


Torsions

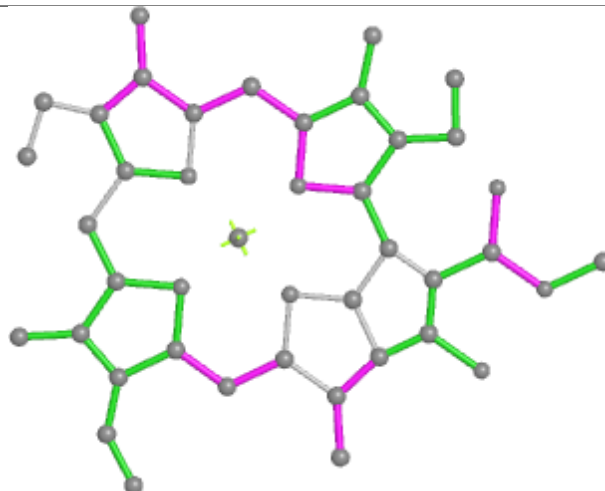


Rings

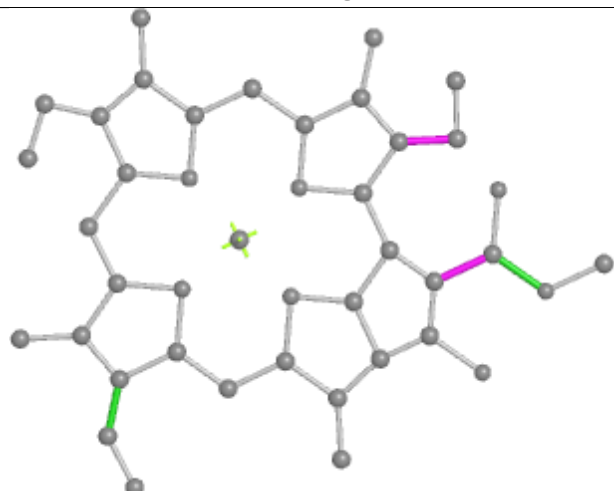
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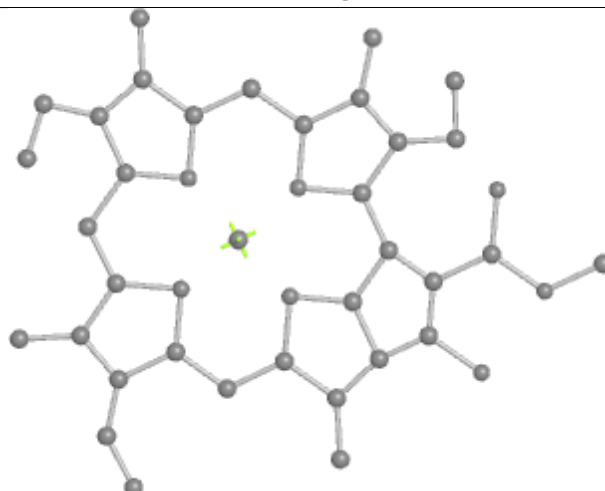
Bond lengths



Bond angles

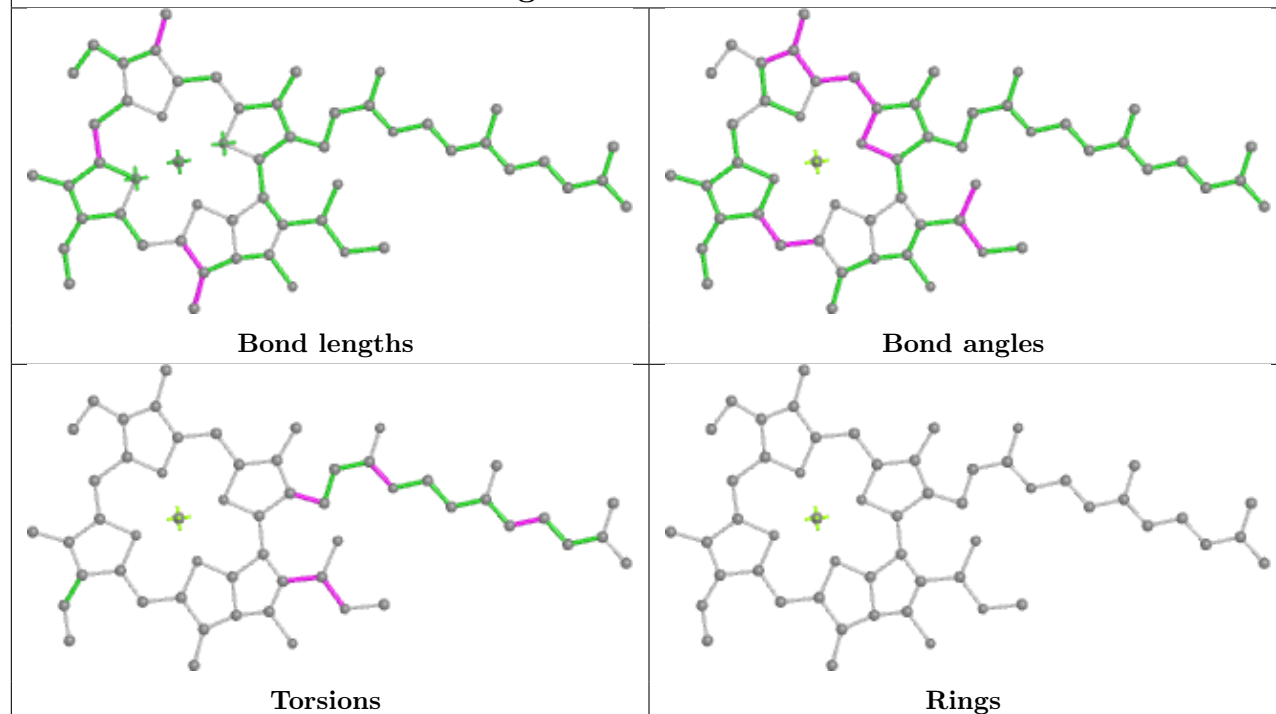


Torsions

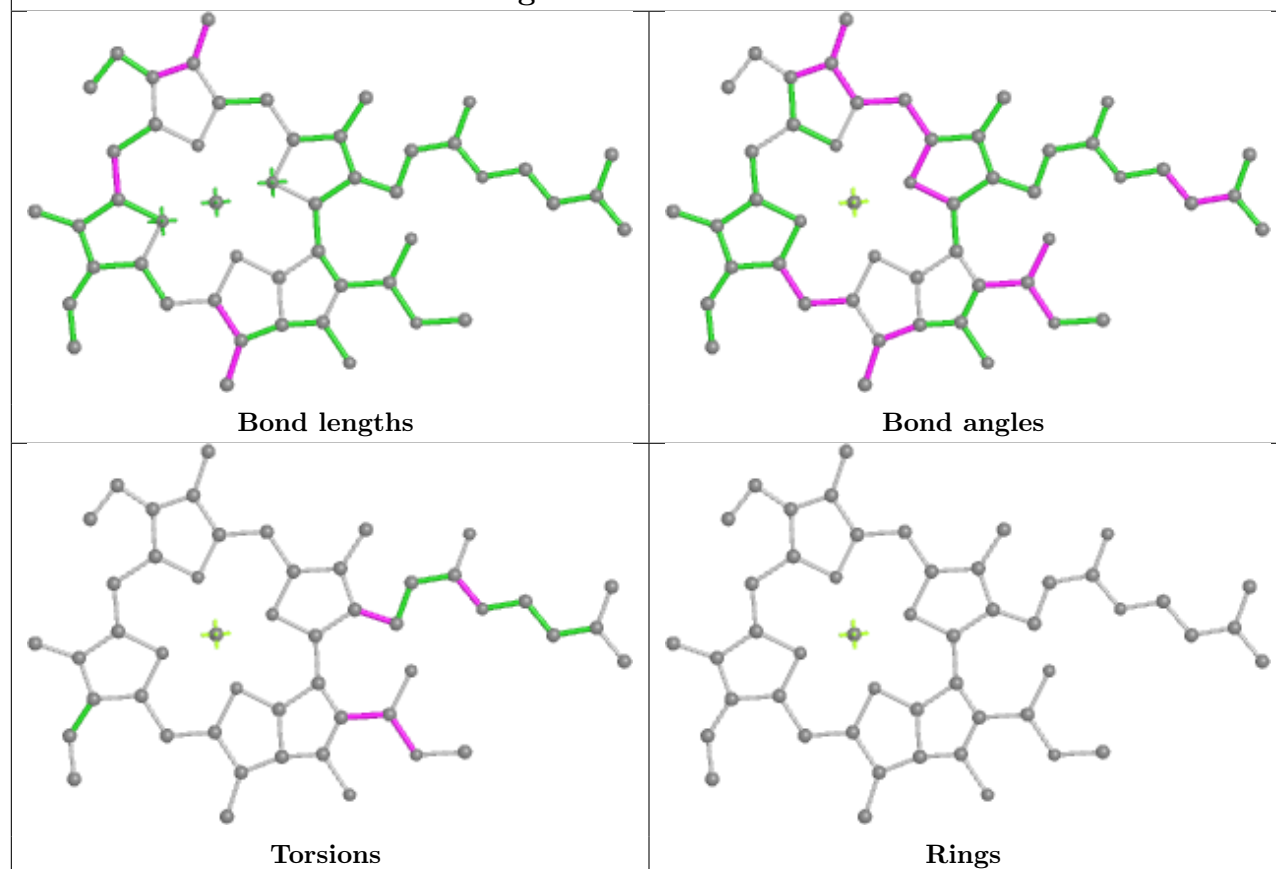


Rings

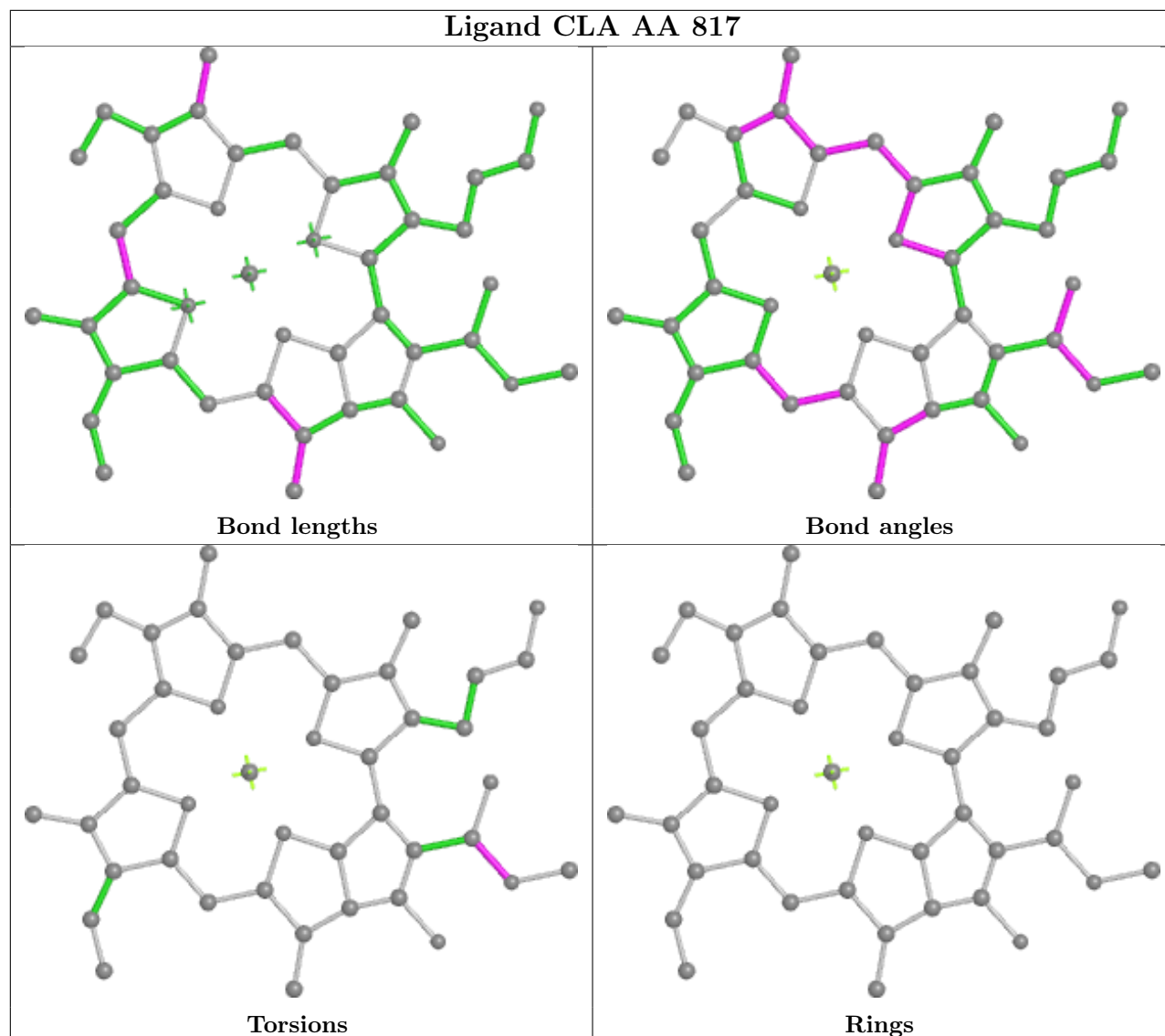
Ligand CLA AA 815



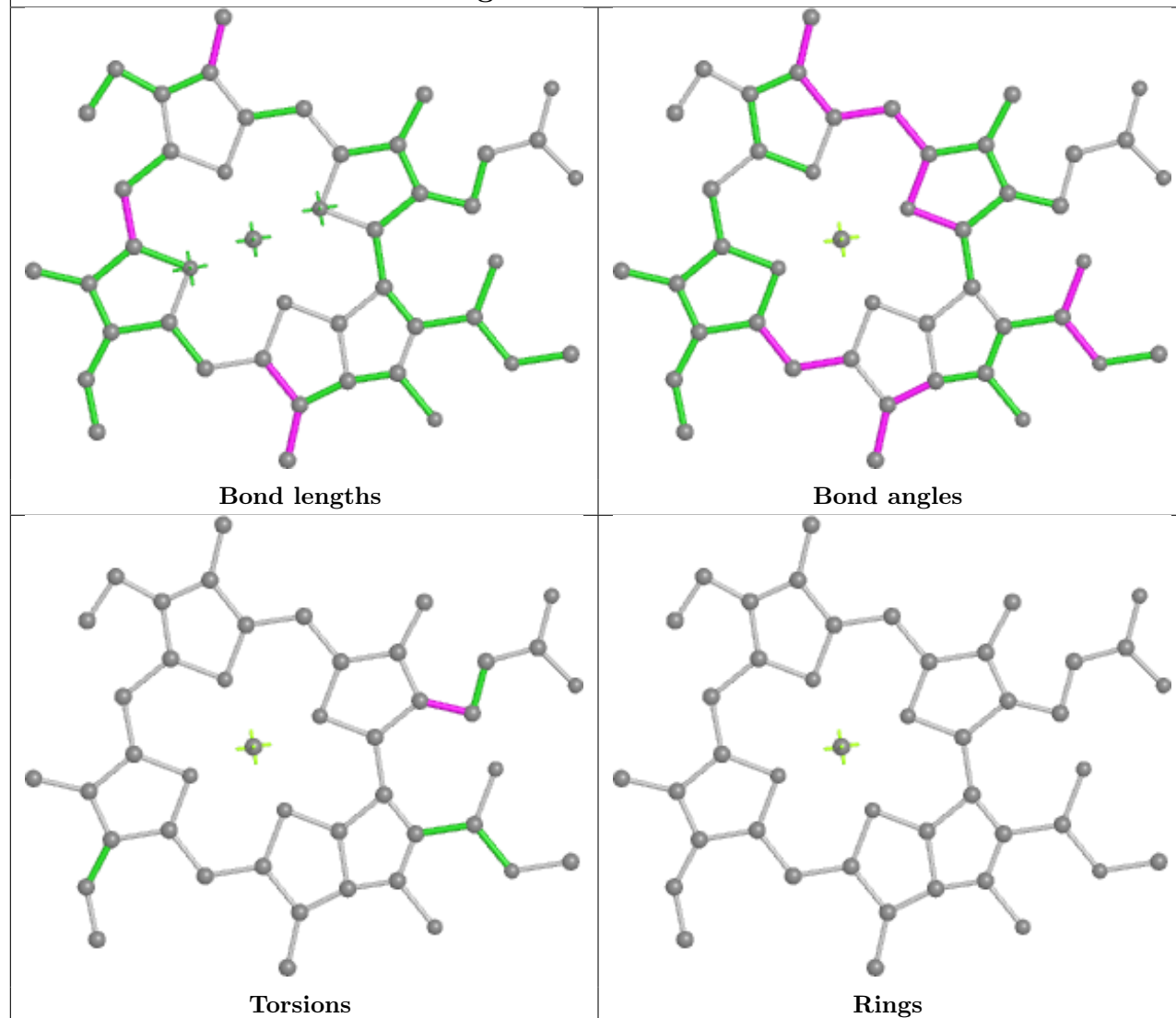
Ligand CLA AA 816



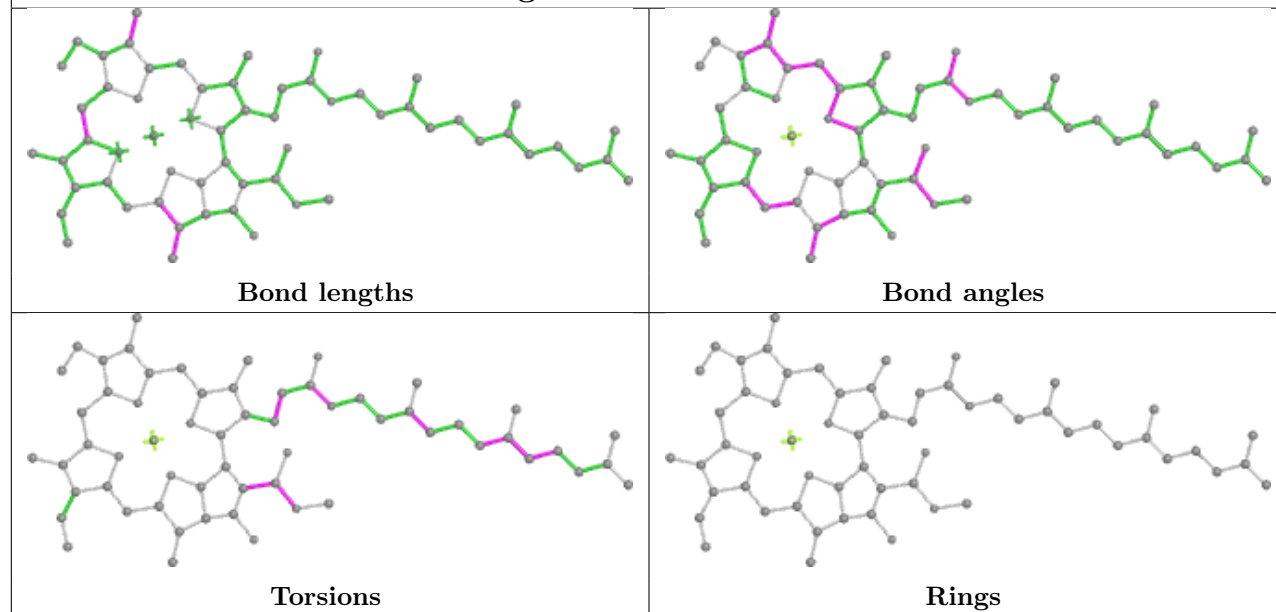
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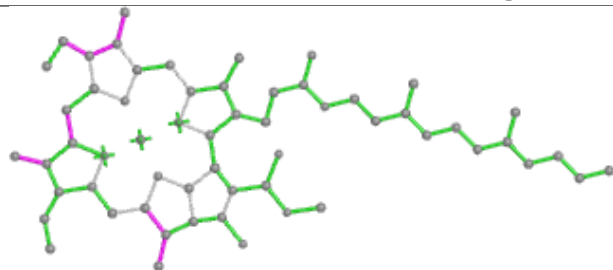
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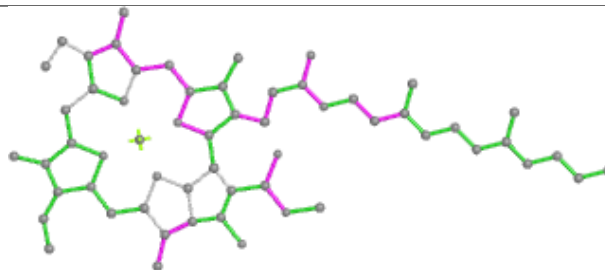
Ligand CLA AA 819



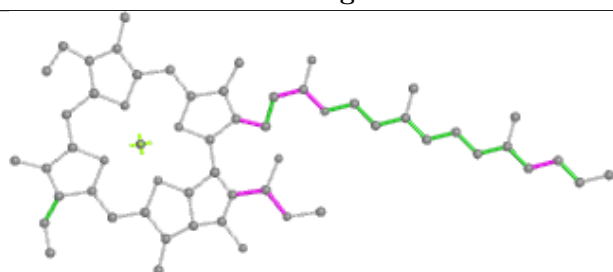
Ligand CLA AA 820



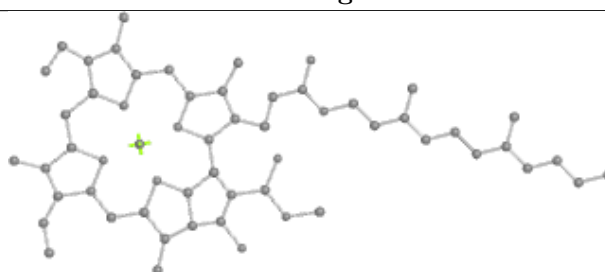
Bond lengths



Bond angles

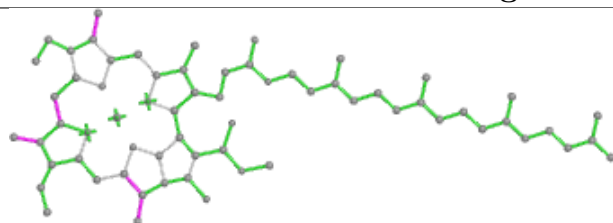


Torsions

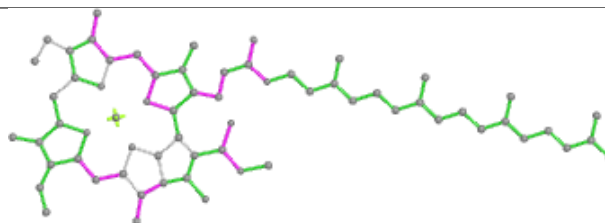


Rings

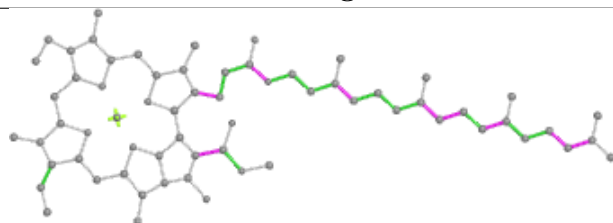
Ligand CLA AA 821



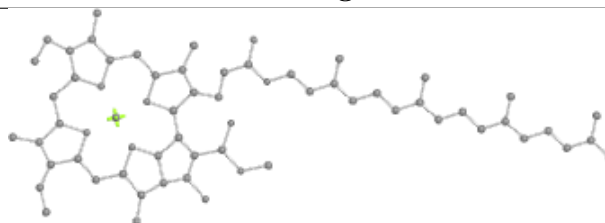
Bond lengths



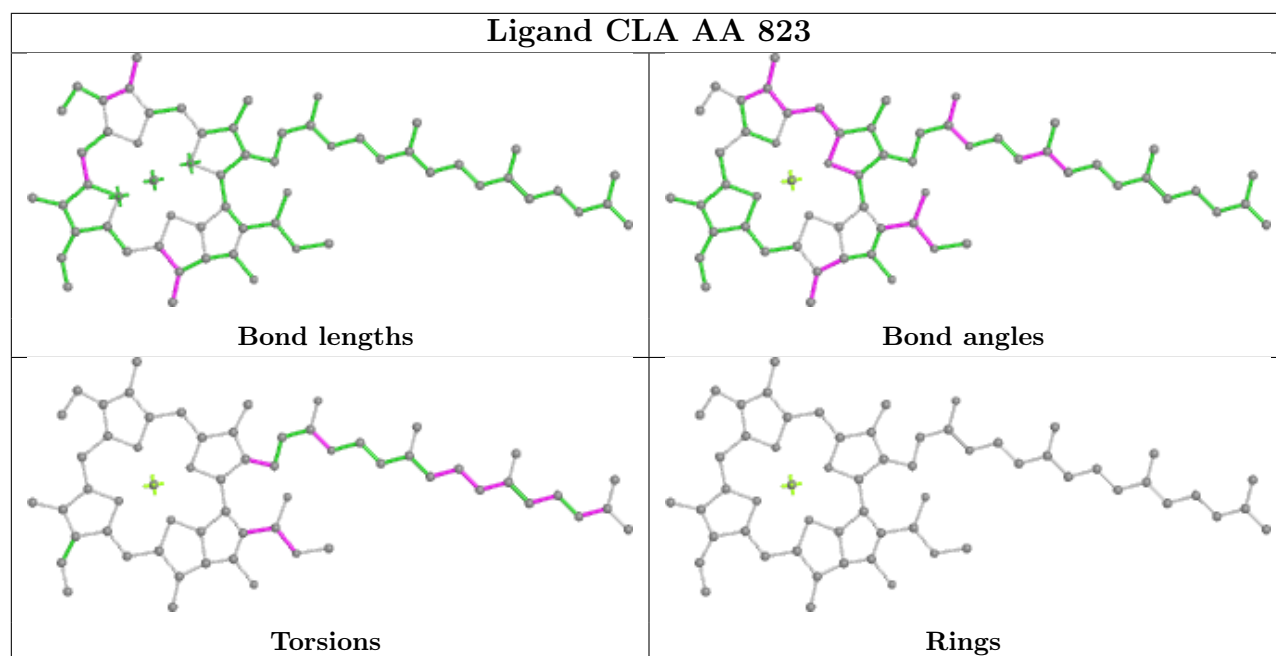
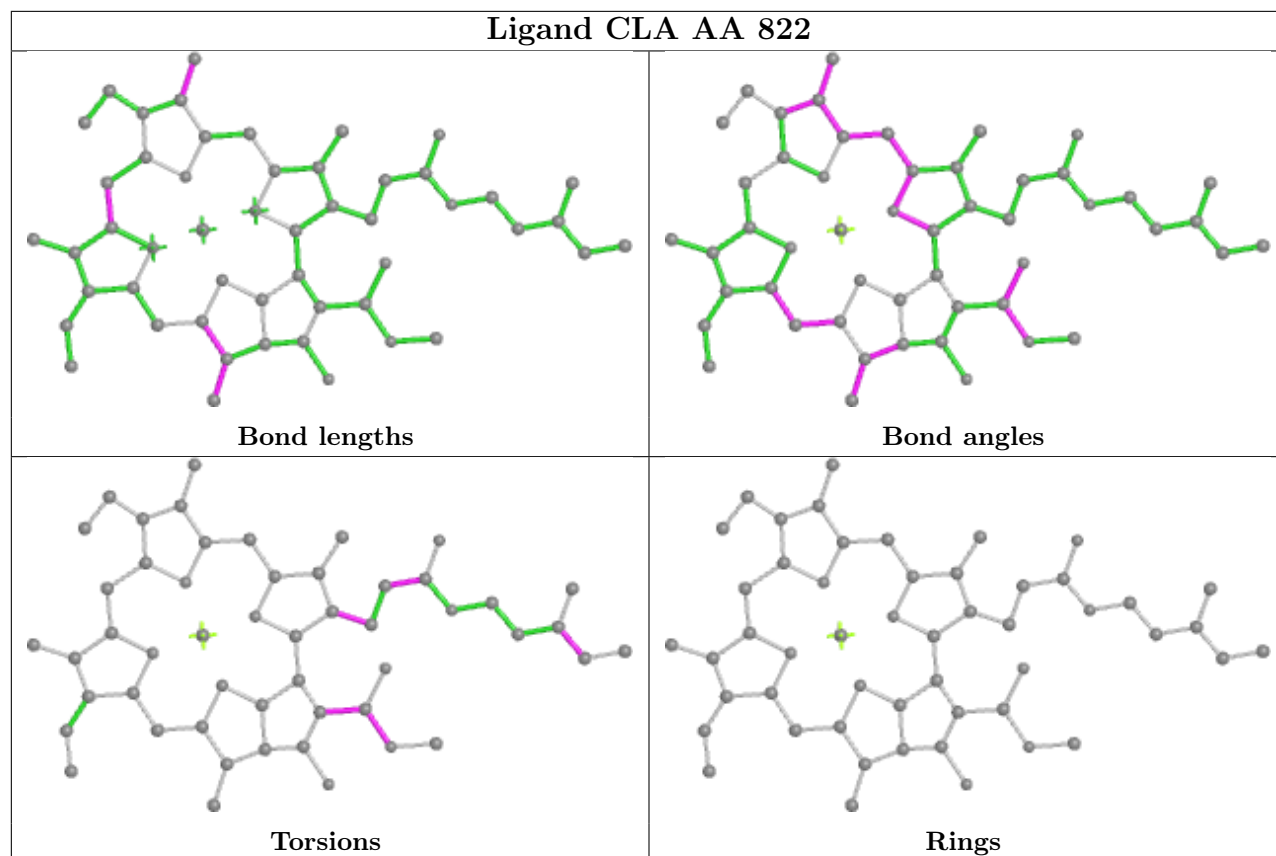
Bond angles



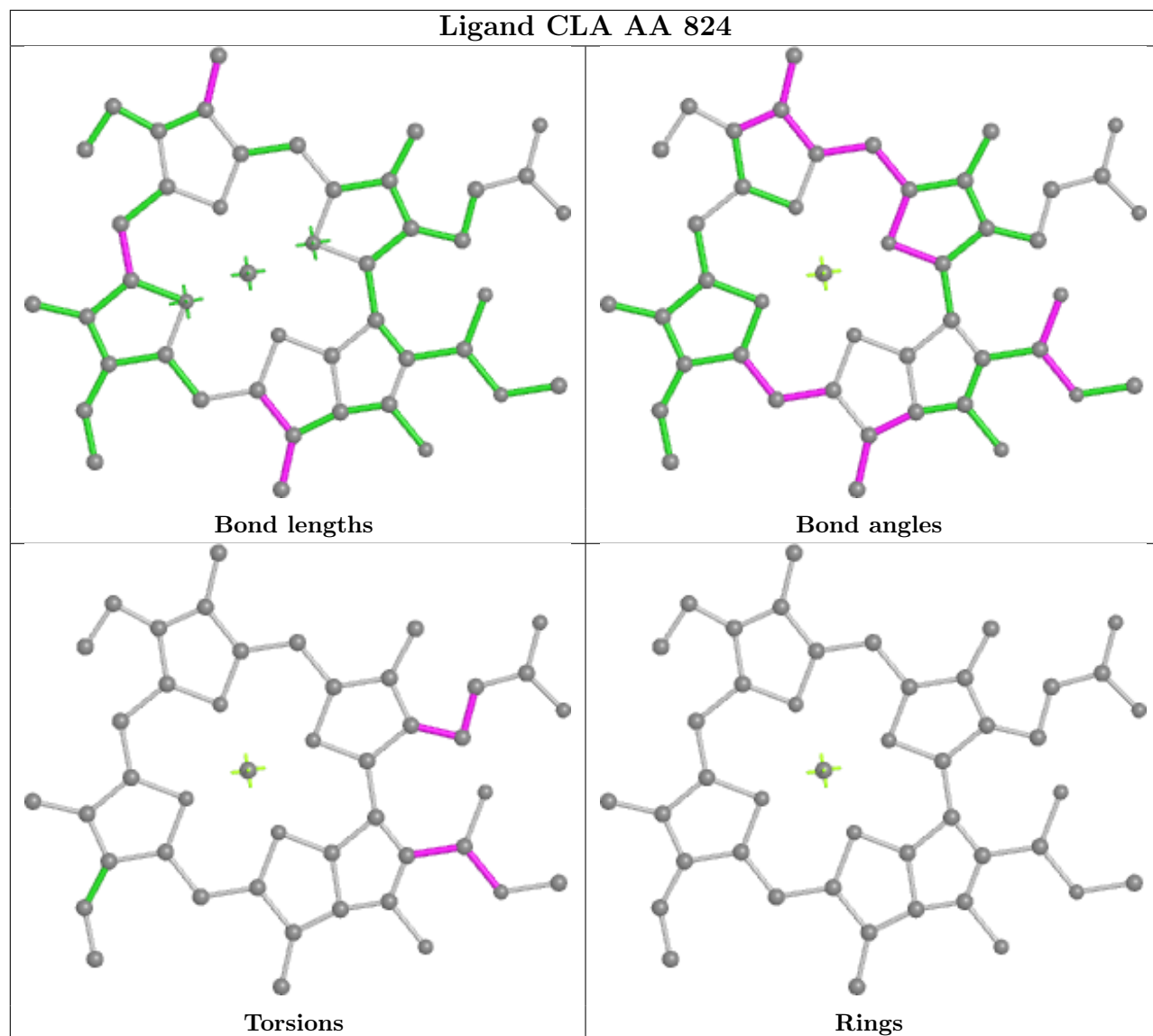
Torsions

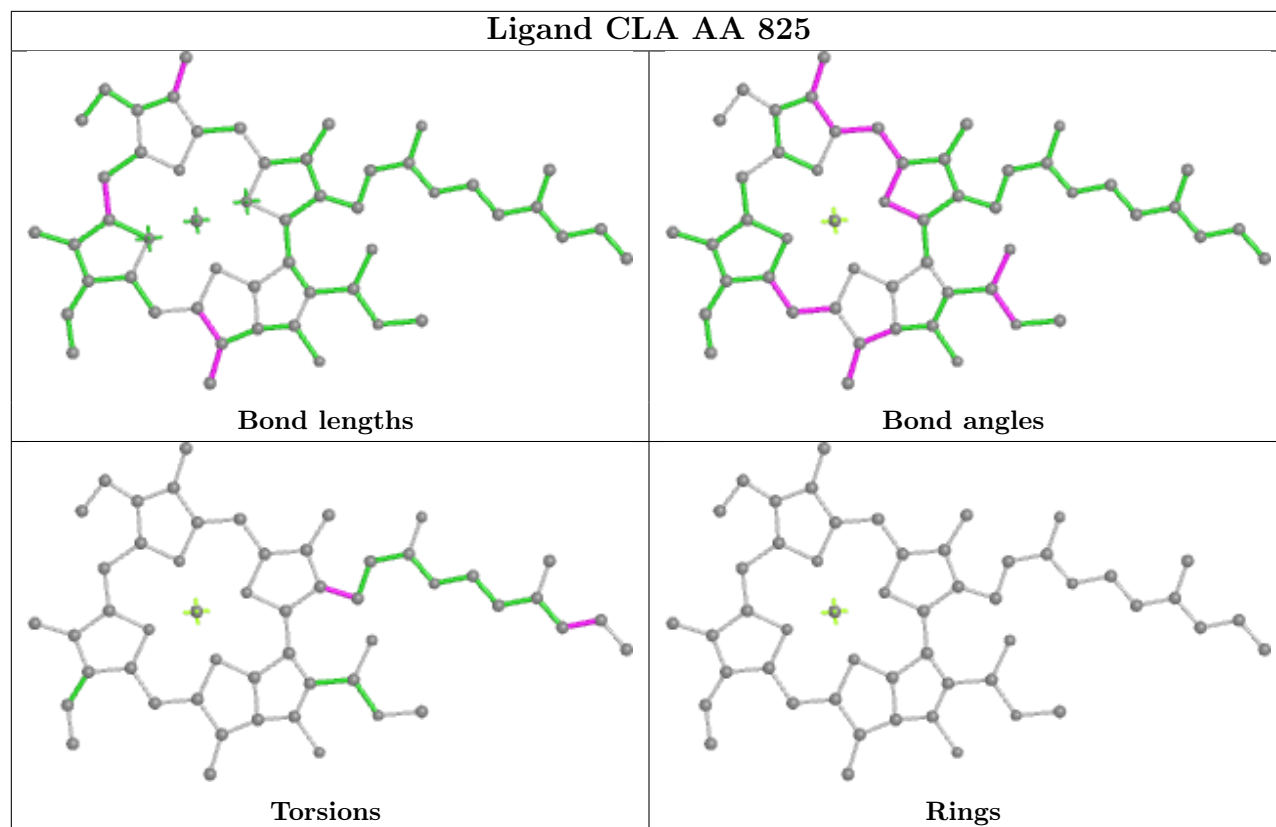


Rings

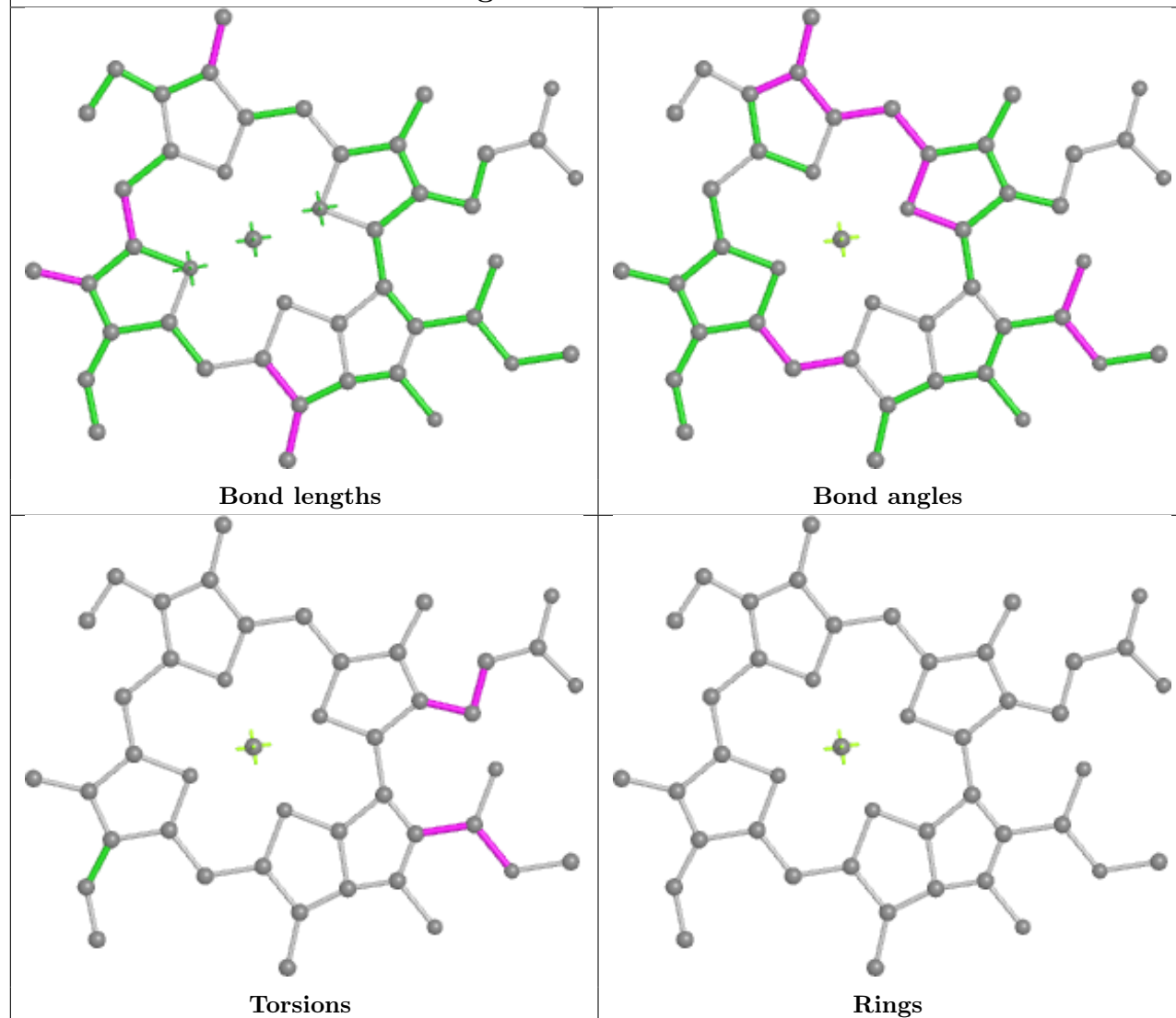


Ligand CLA AA 824

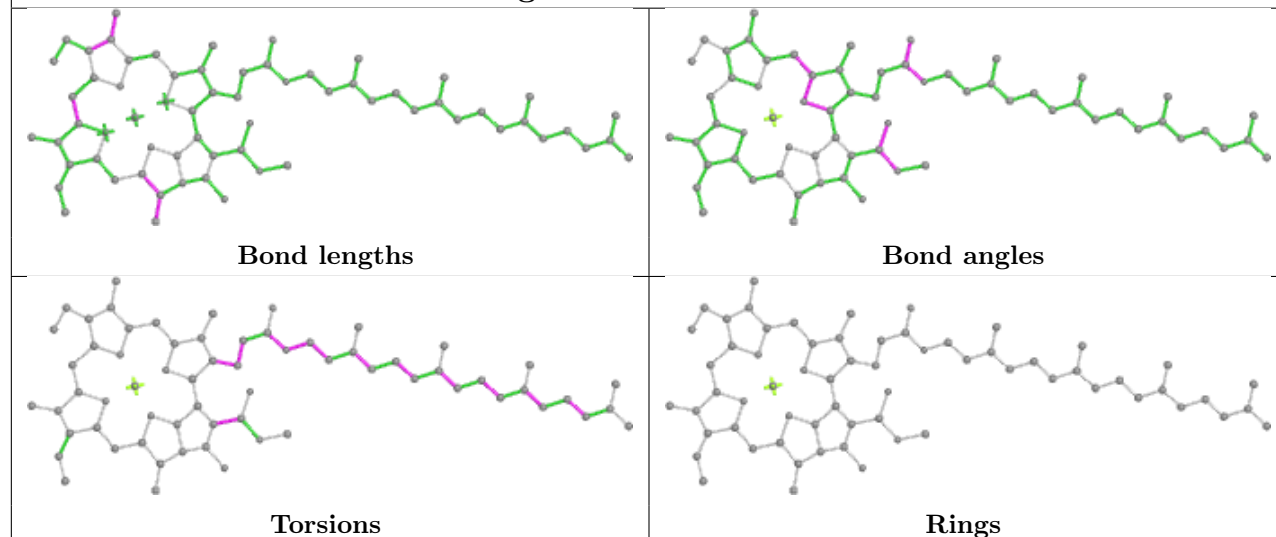




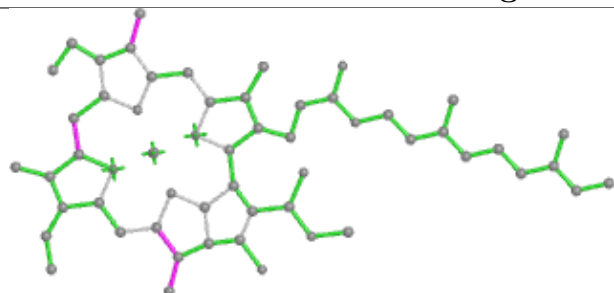
Ligand CLA AA 826



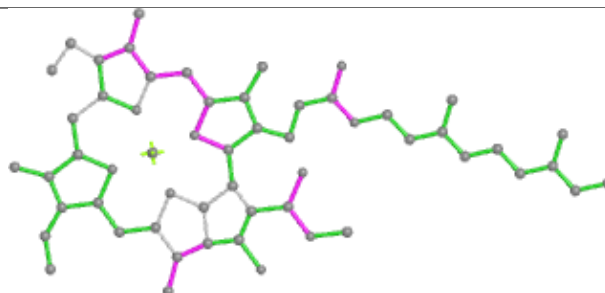
Ligand CLA AA 827



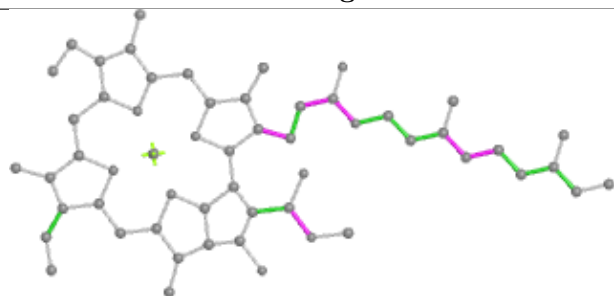
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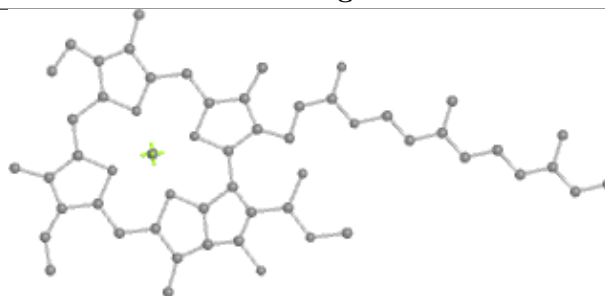
Bond lengths



Bond angles

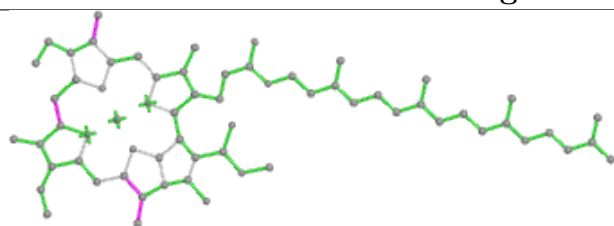


Torsions

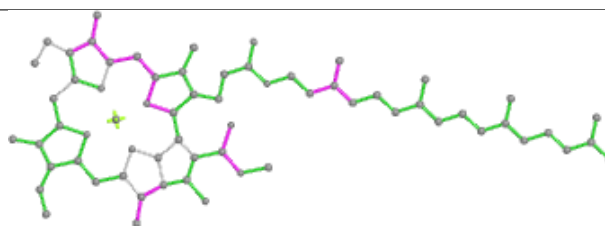


Rings

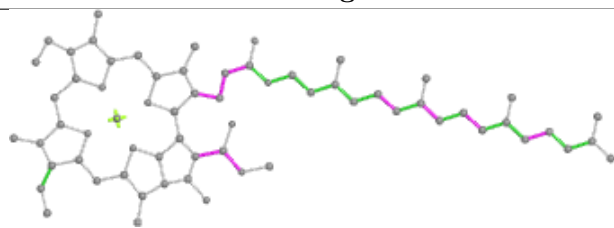
Ligand CLA AA 829



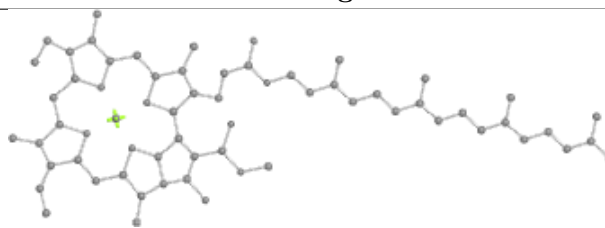
Bond lengths



Bond angles

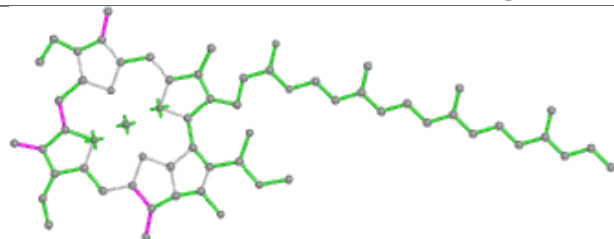


Torsions

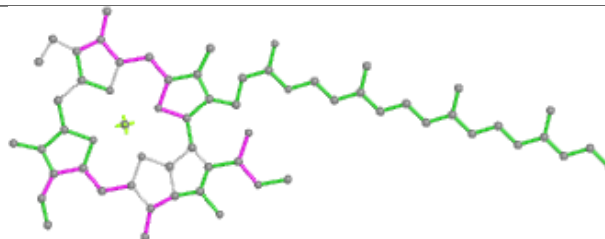


Rings

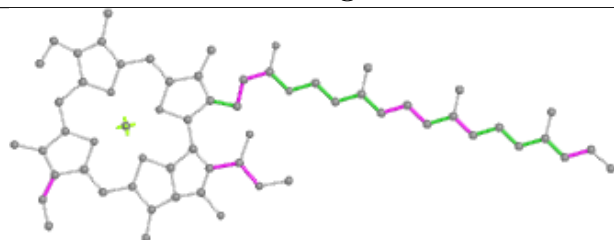
Ligand CLA AA 830



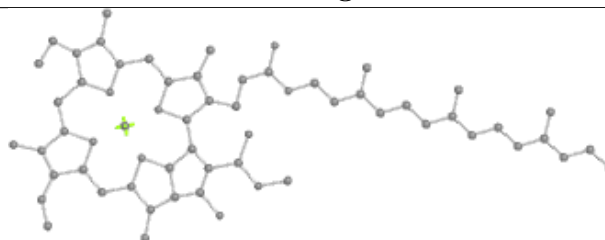
Bond lengths



Bond angles

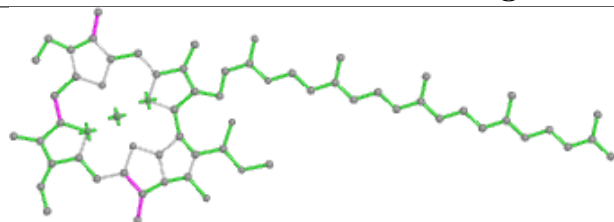


Torsions

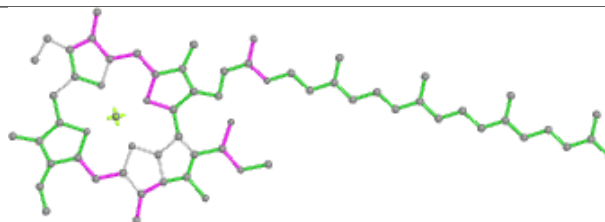


Rings

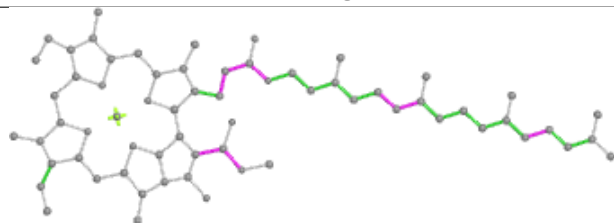
Ligand CLA AA 831



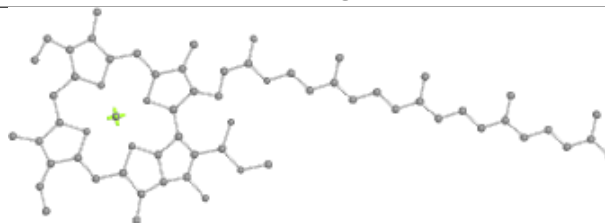
Bond lengths



Bond angles

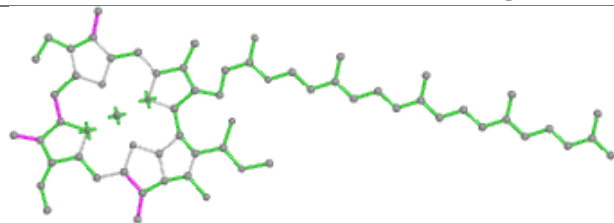


Torsions

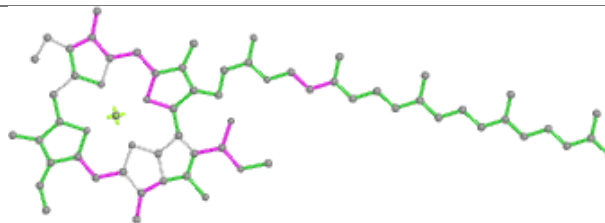


Rings

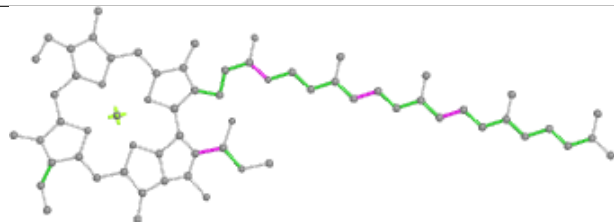
Ligand CLA AA 832



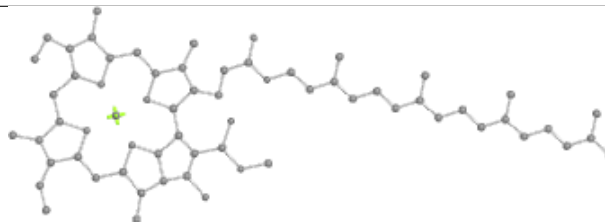
Bond lengths



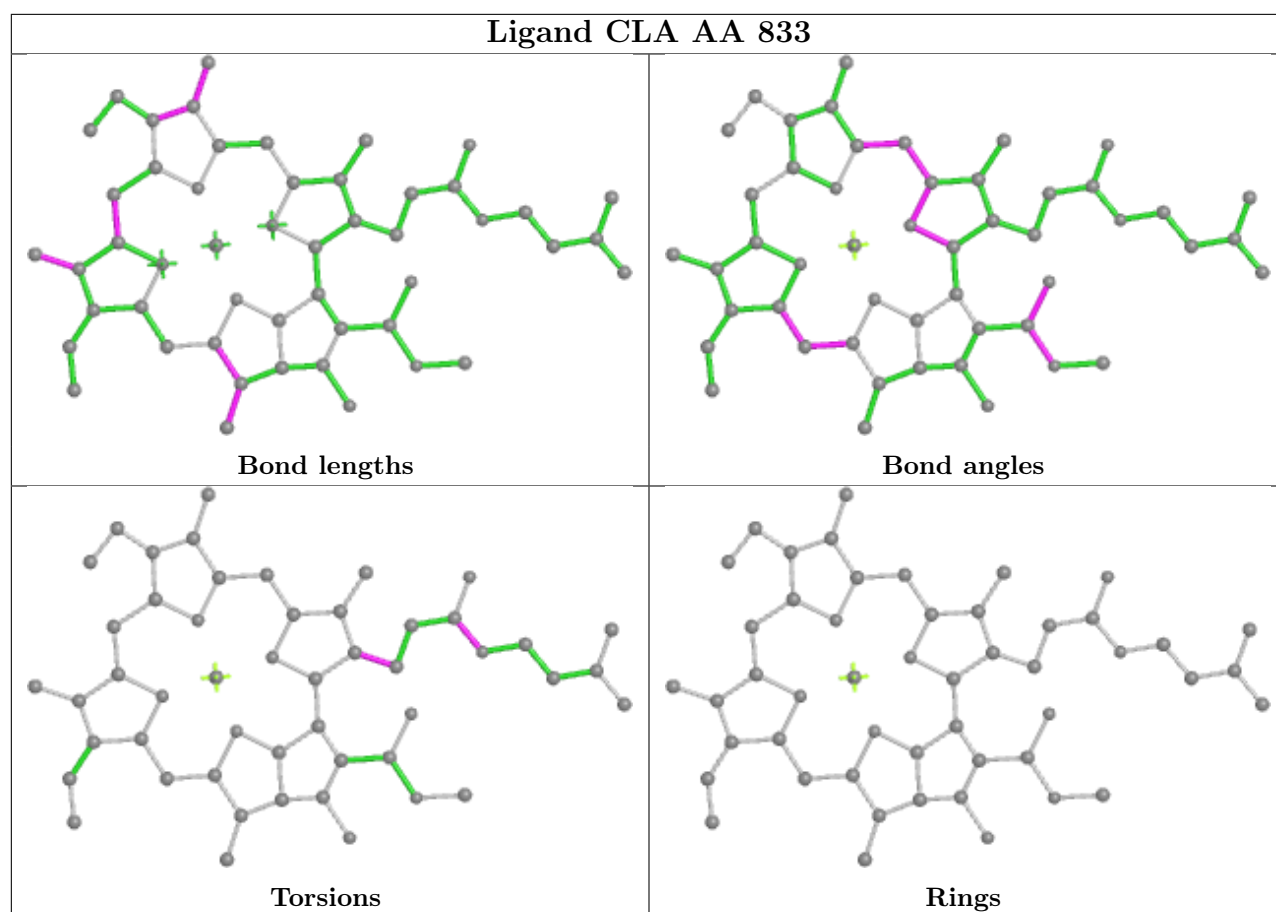
Bond angles



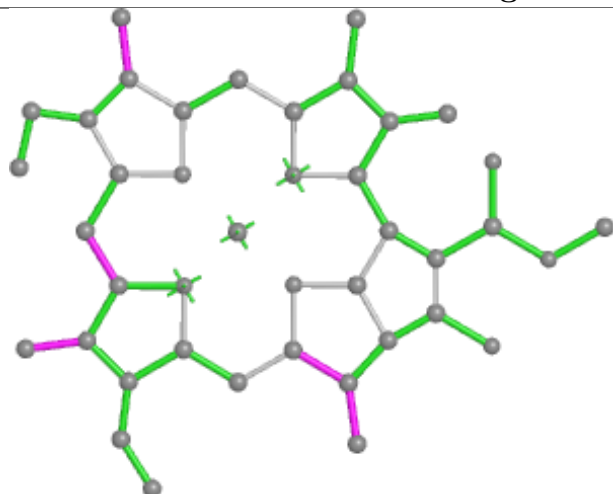
Torsions



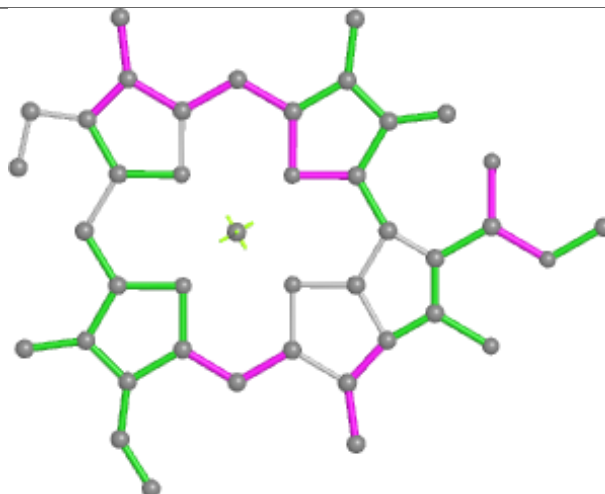
Rings



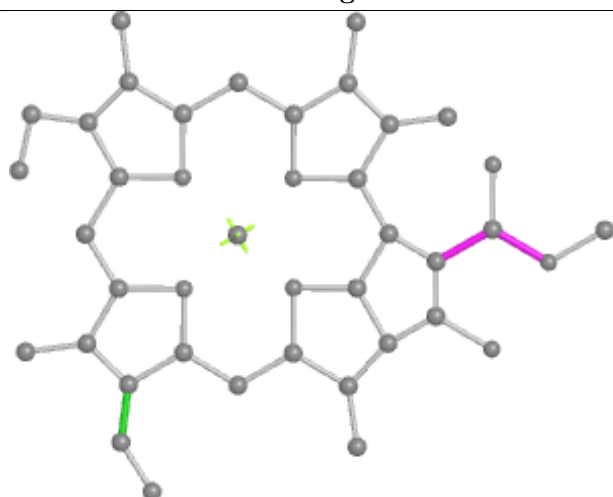
Ligand CLA AA 834



Bond lengths



Bond angles

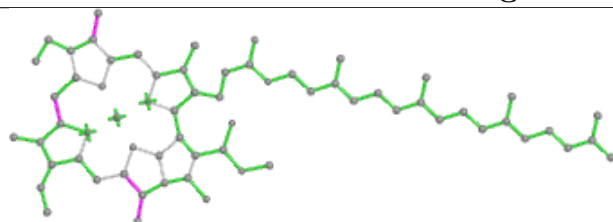


Torsions

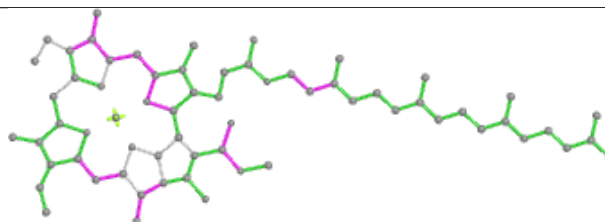


Rings

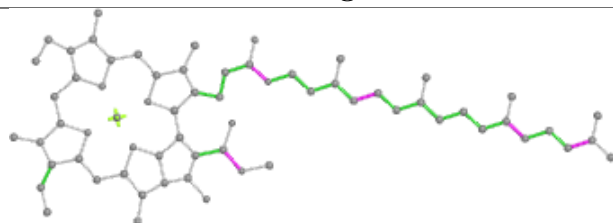
Ligand CLA AA 835



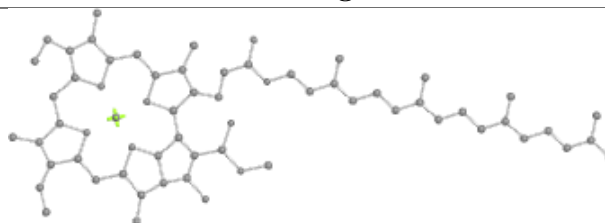
Bond lengths



Bond angles

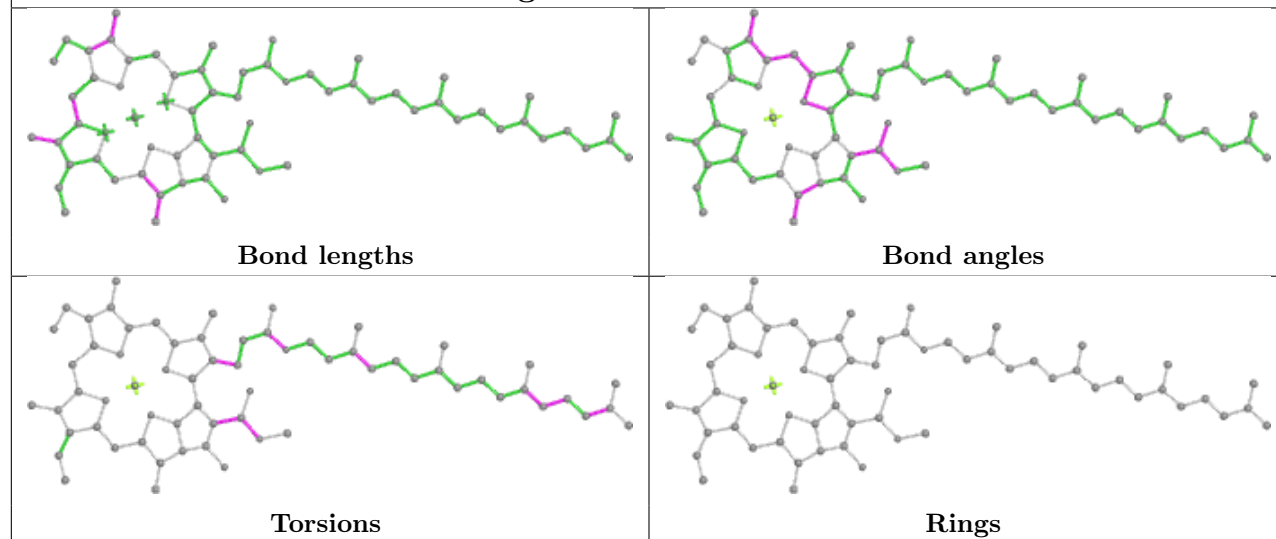


Torsions

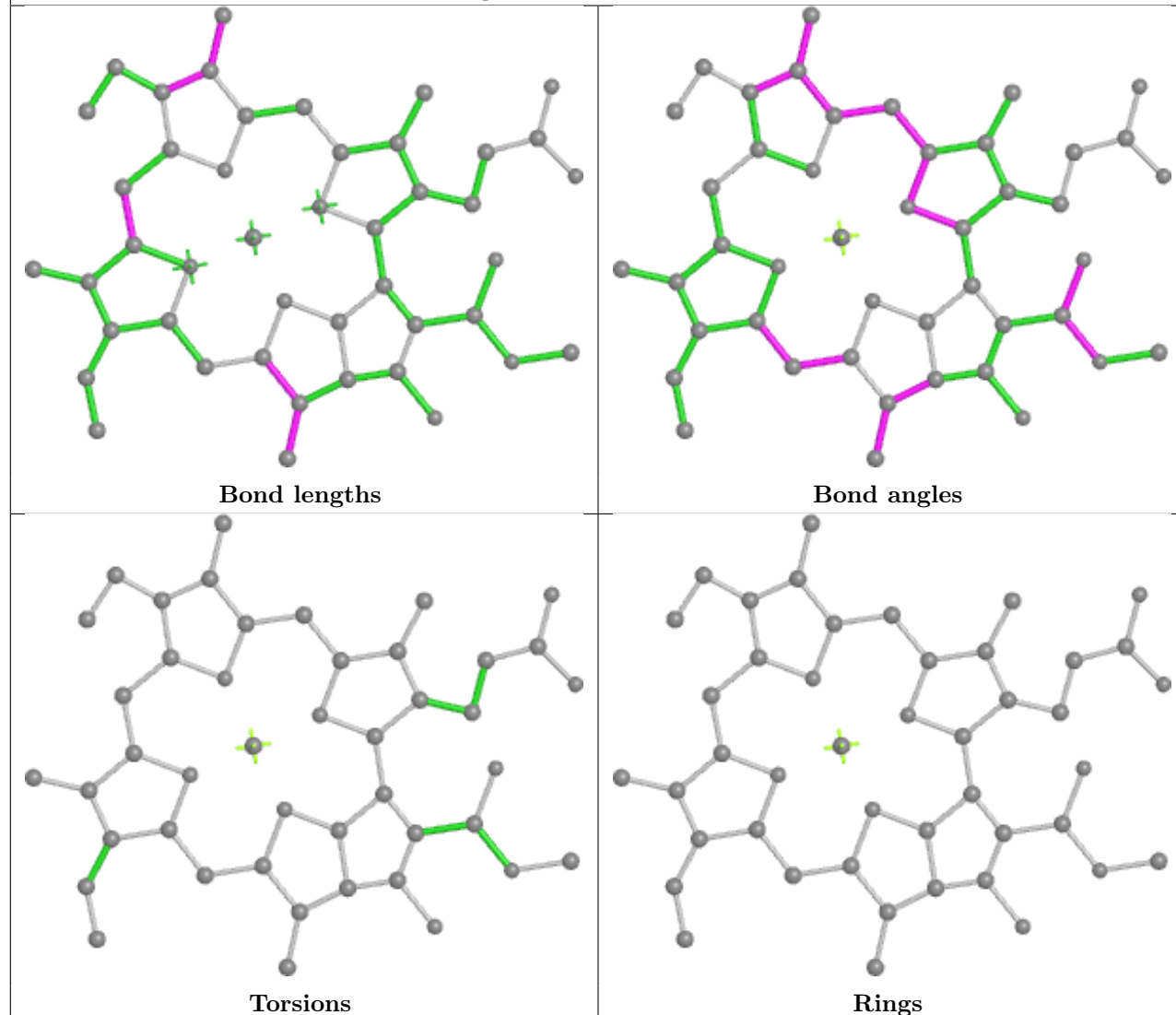


Rings

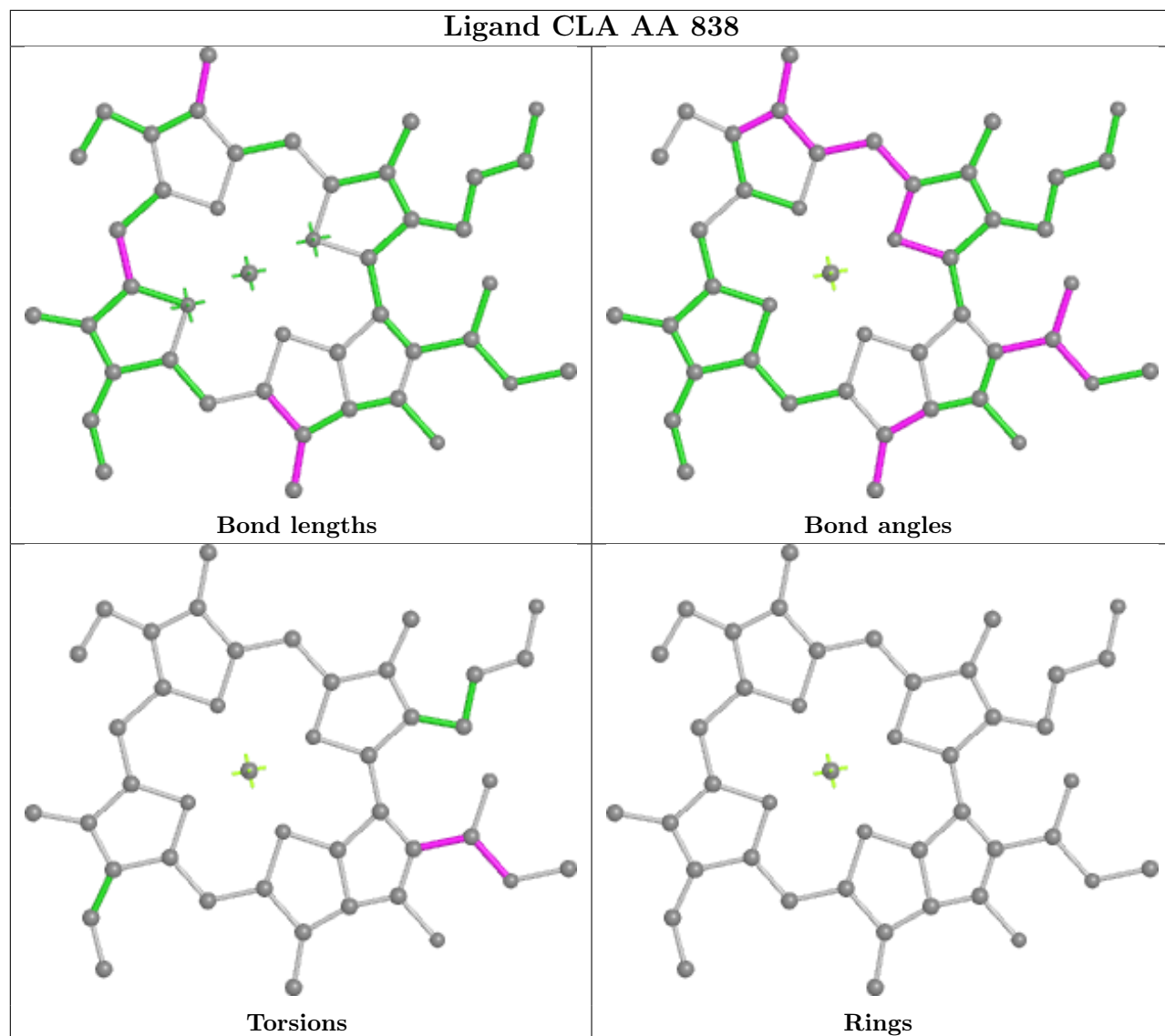
Ligand CLA AA 836



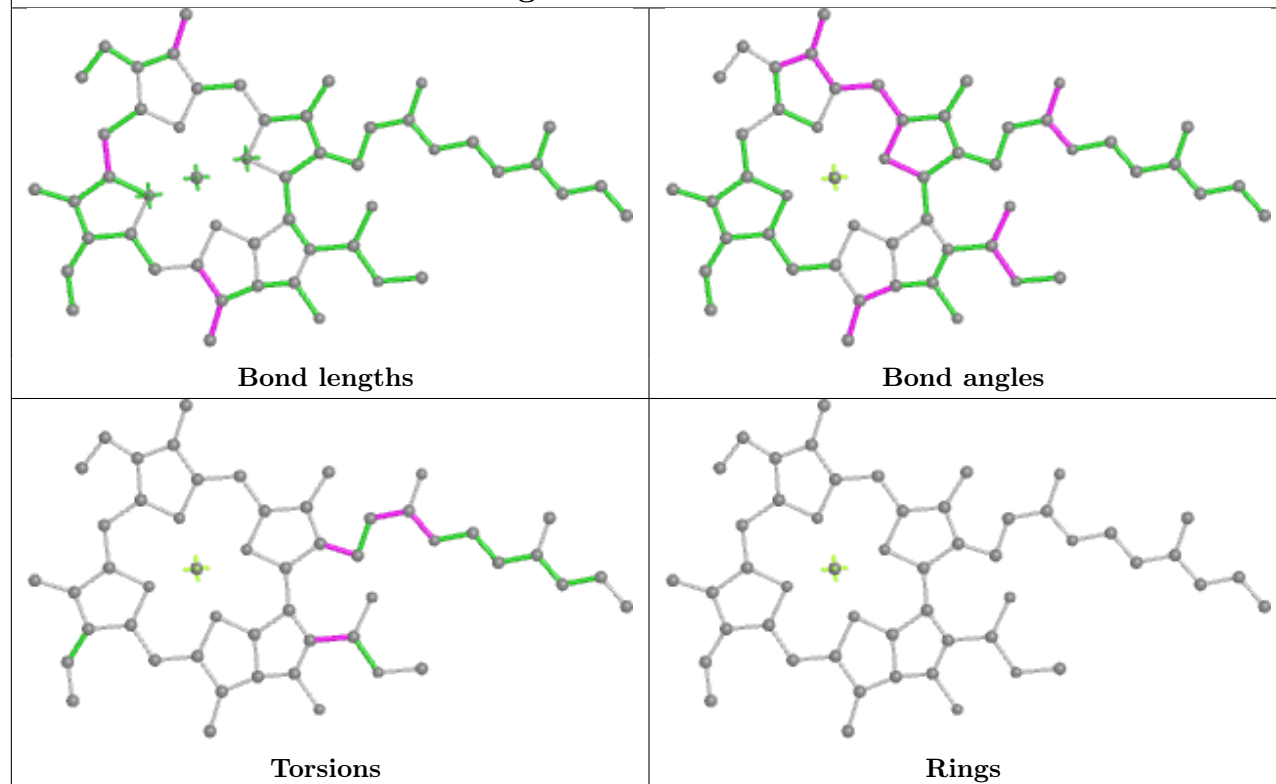
Ligand CLA AA 837



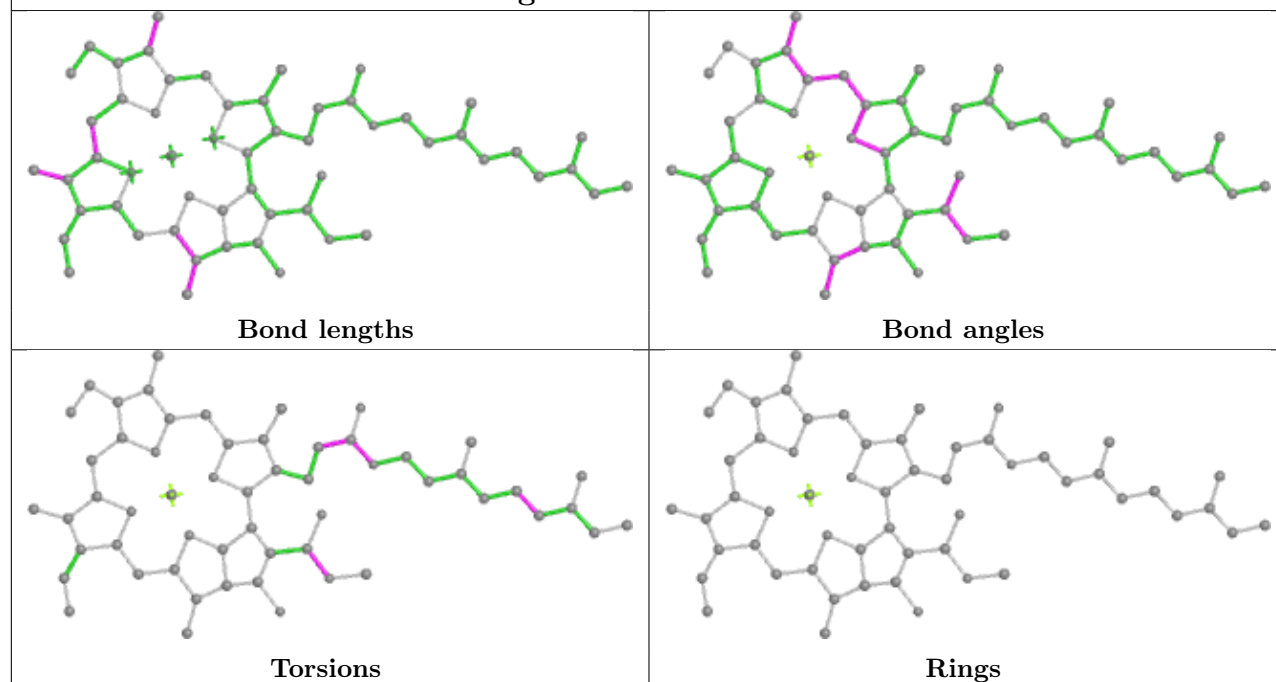
Ligand CLA AA 838



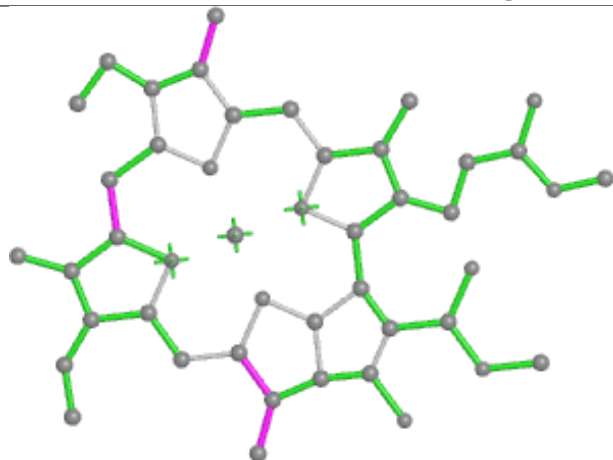
Ligand CLA AA 839



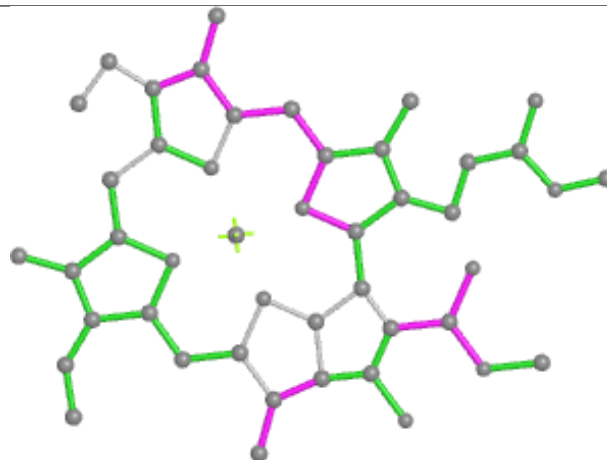
Ligand CLA AA 840



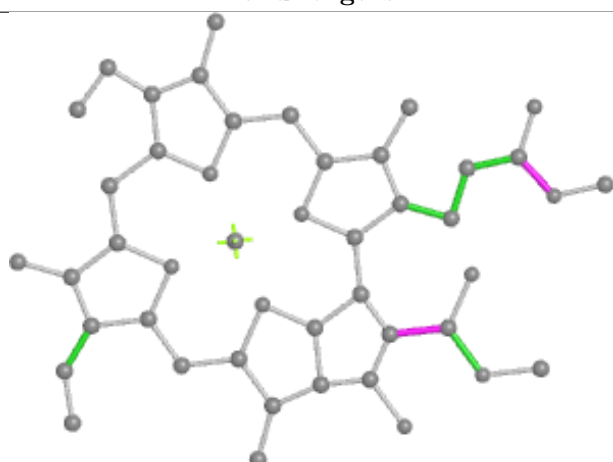
Ligand CLA AA 841



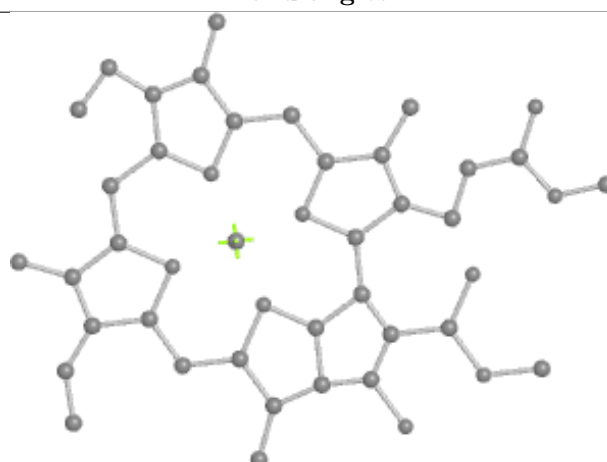
Bond lengths



Bond angles

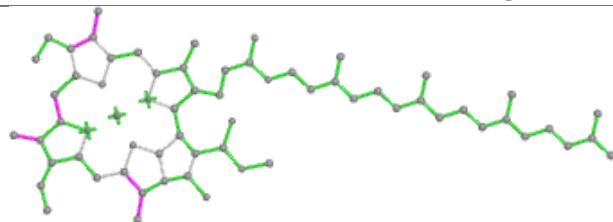


Torsions

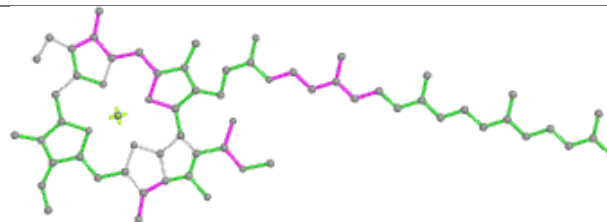


Rings

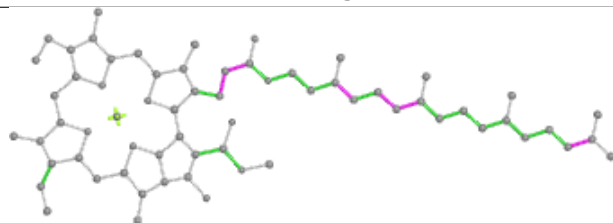
Ligand CLA AA 842



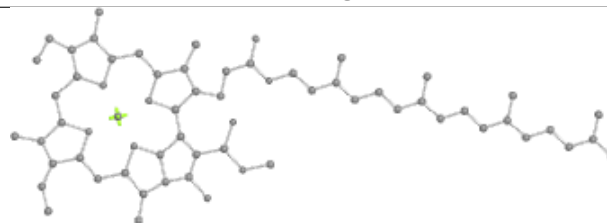
Bond lengths



Bond angles

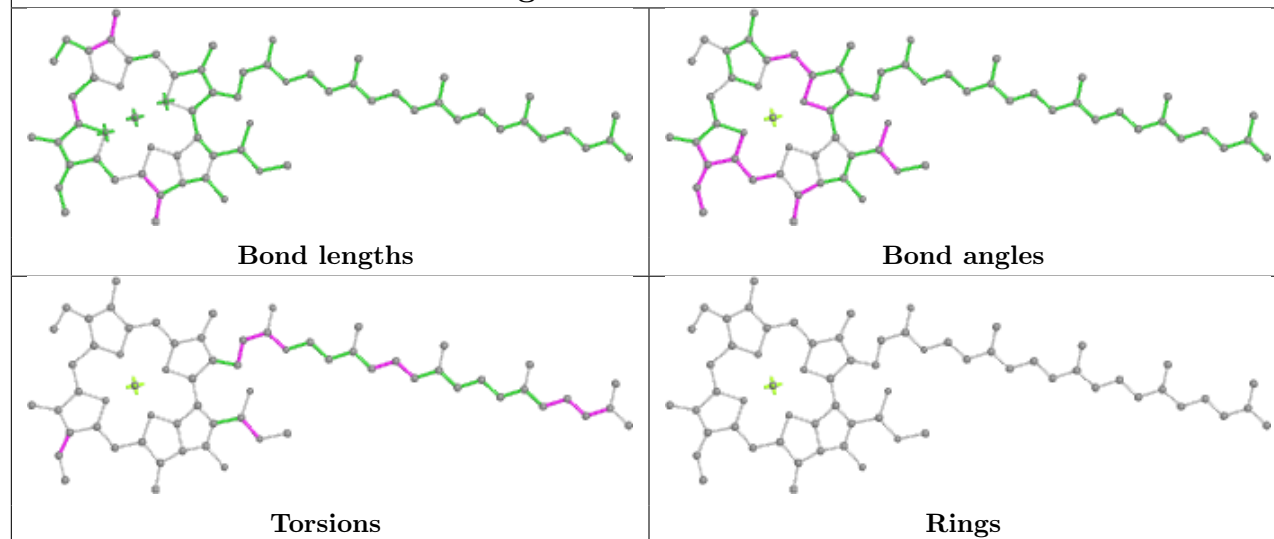


Torsions

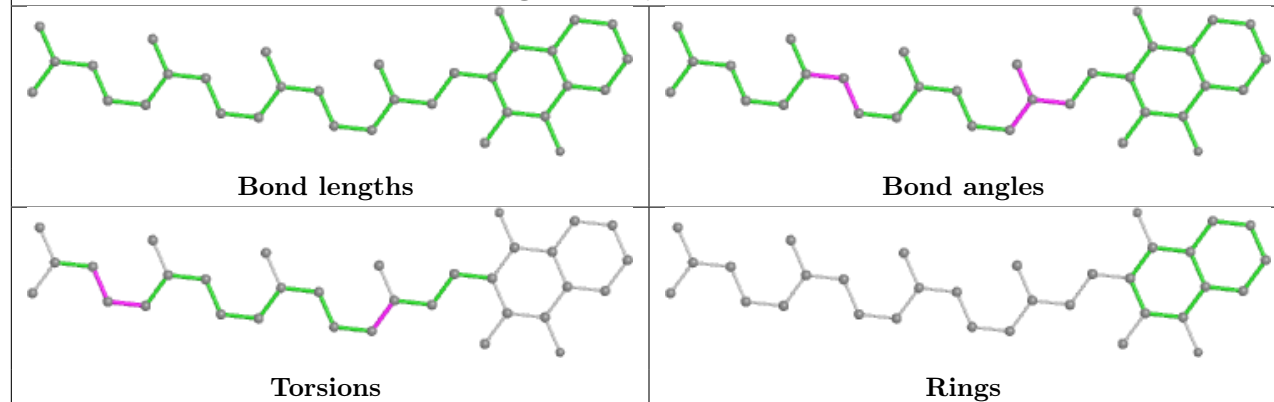


Rings

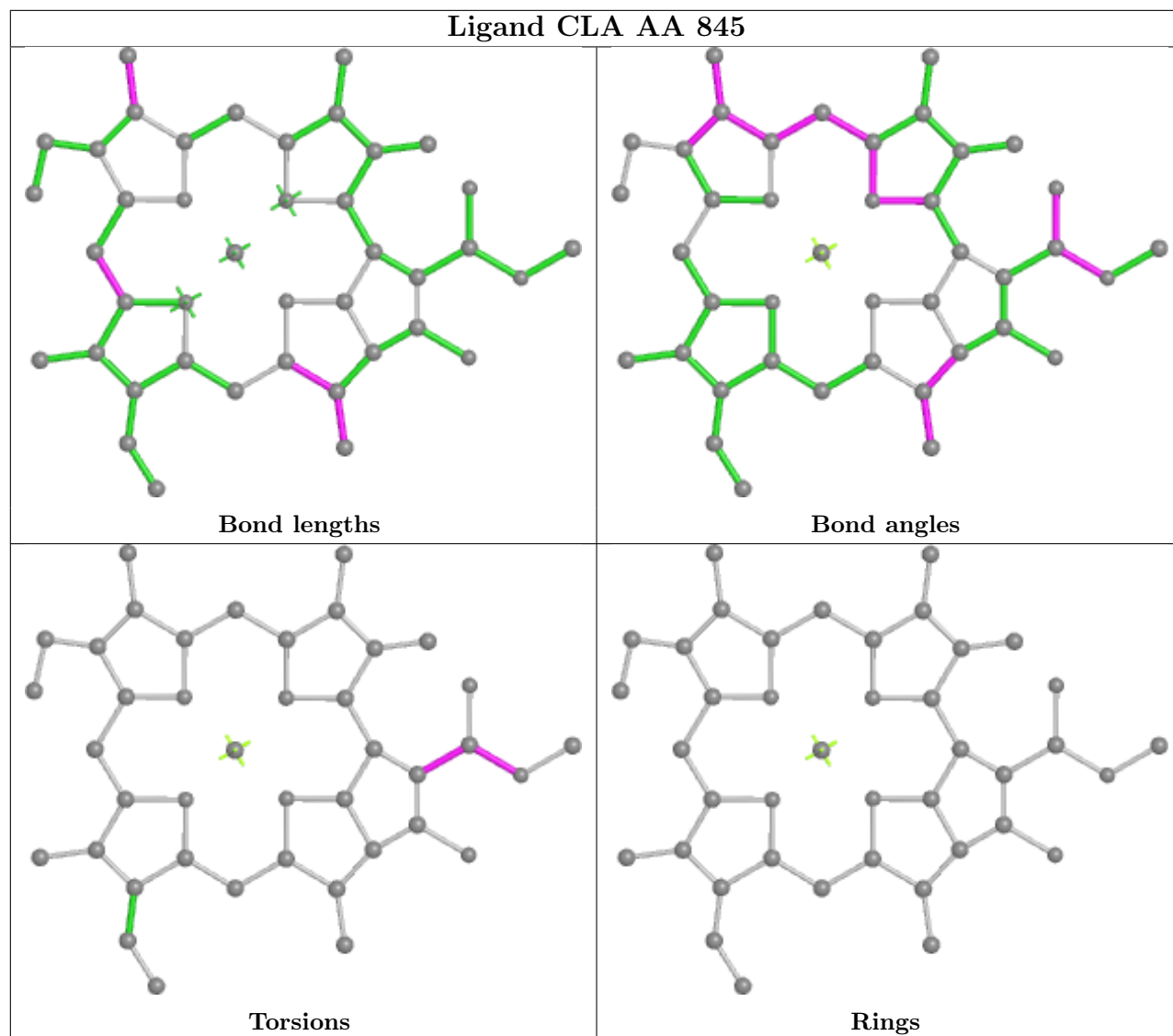
Ligand CLA AA 843

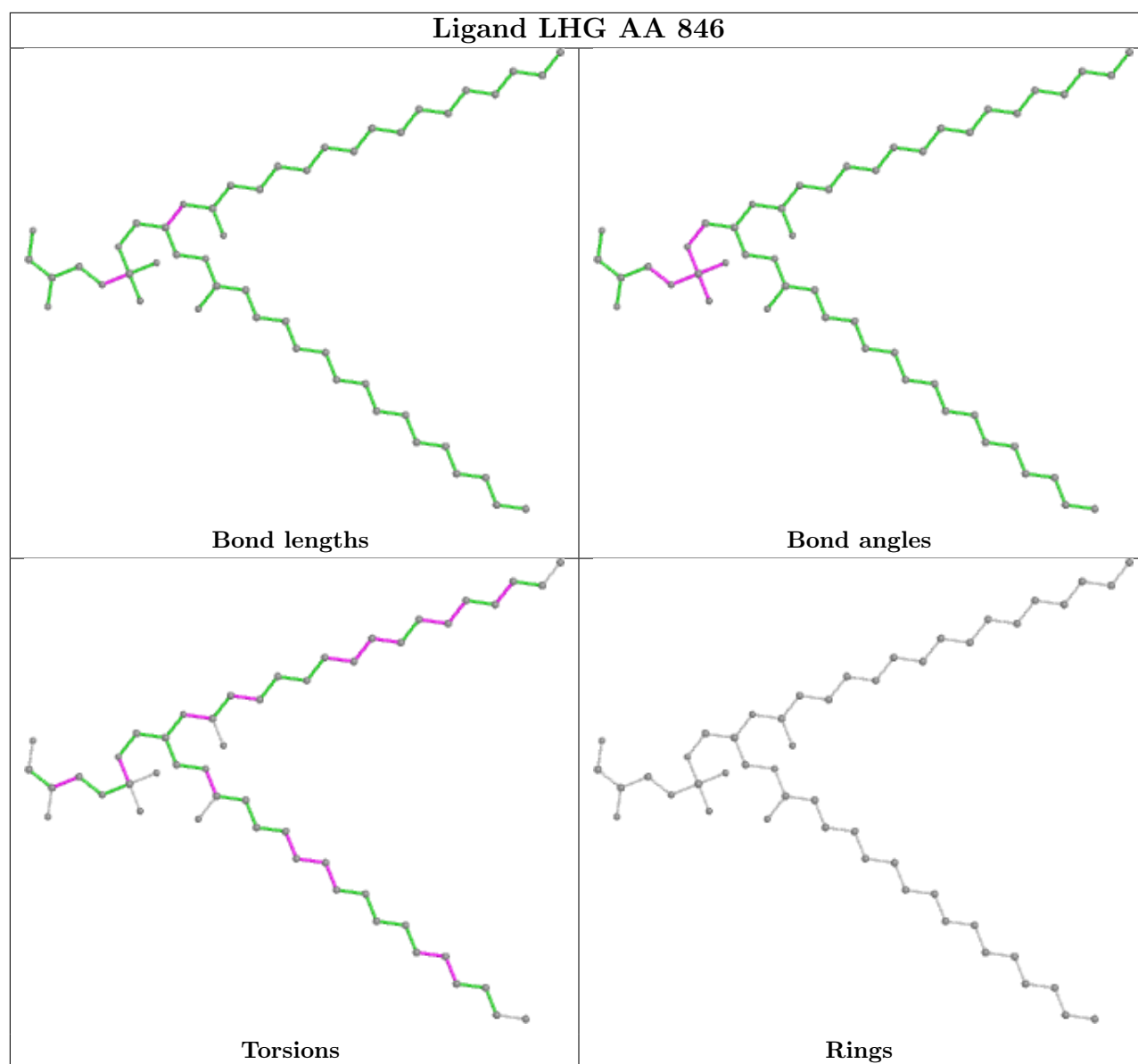


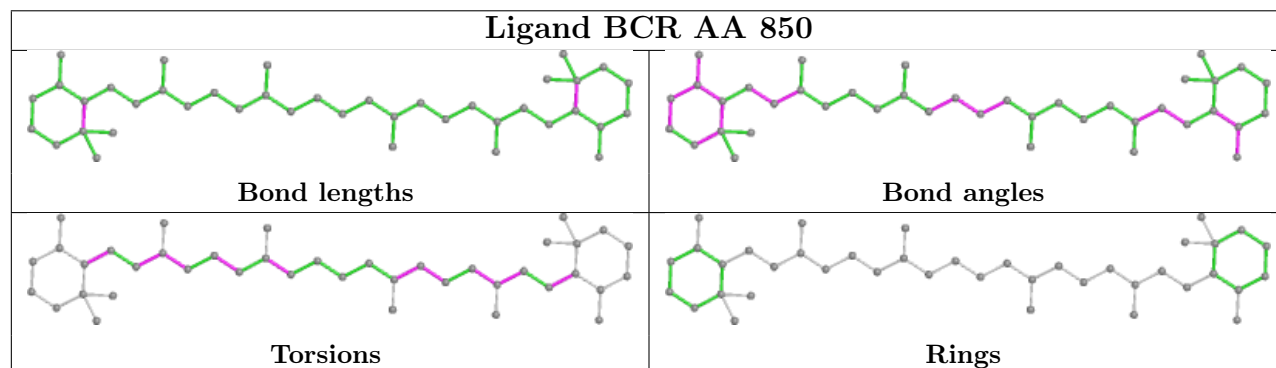
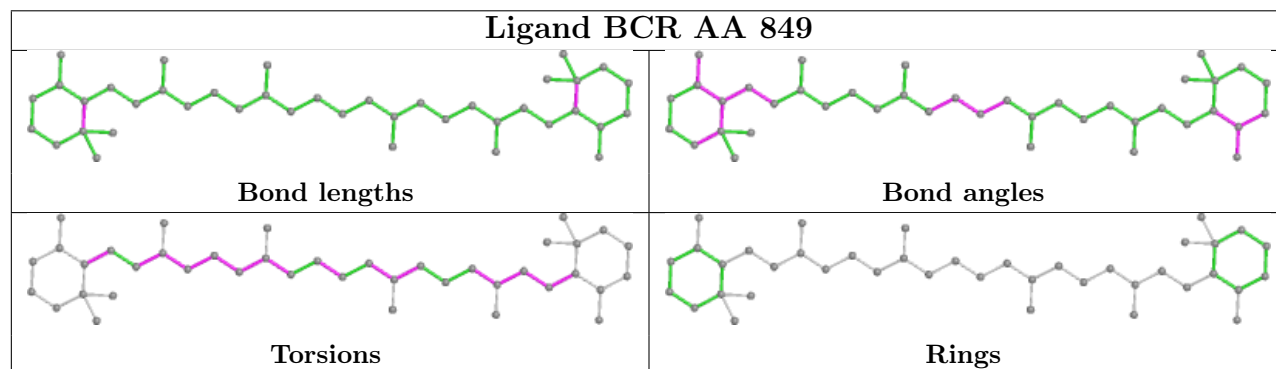
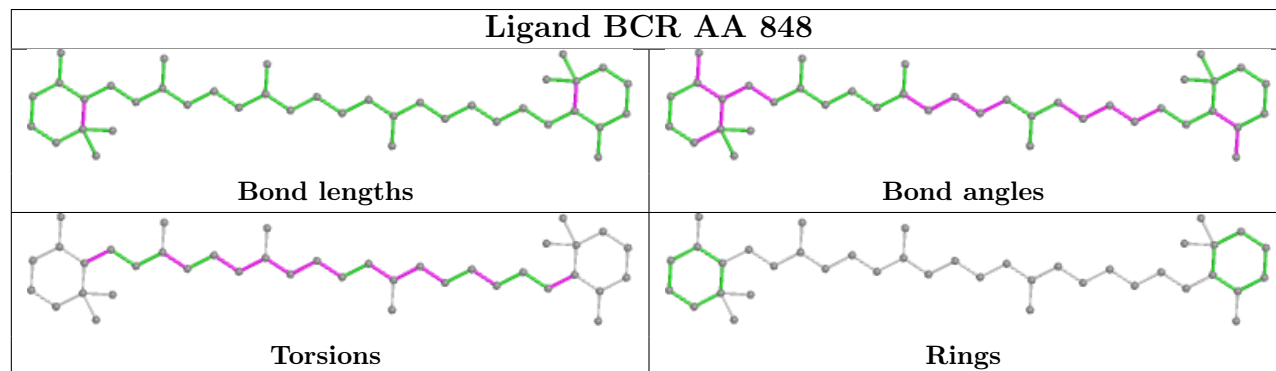
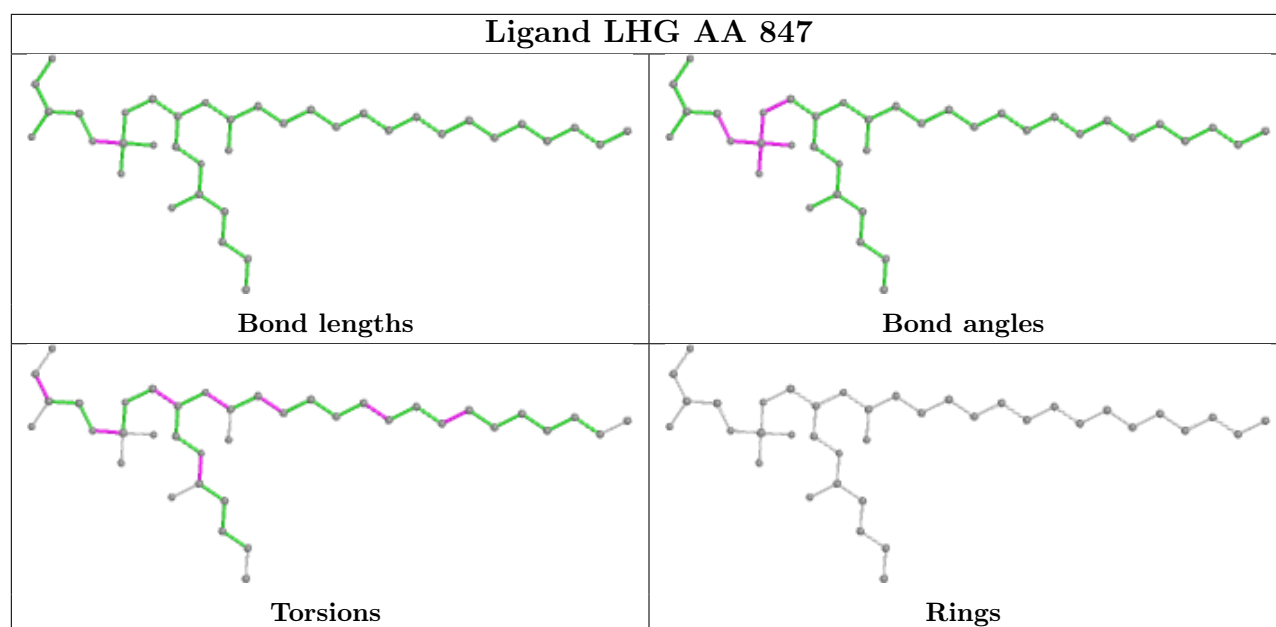
Ligand PQN AA 844

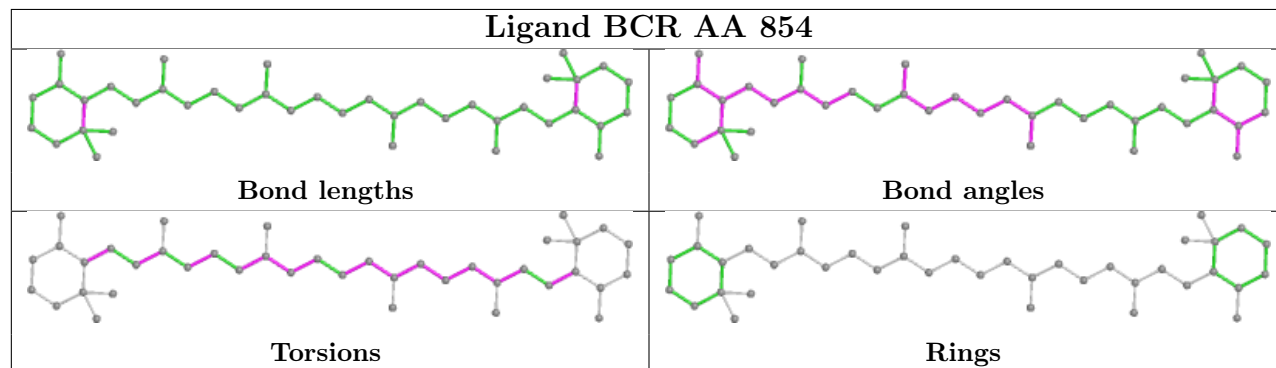
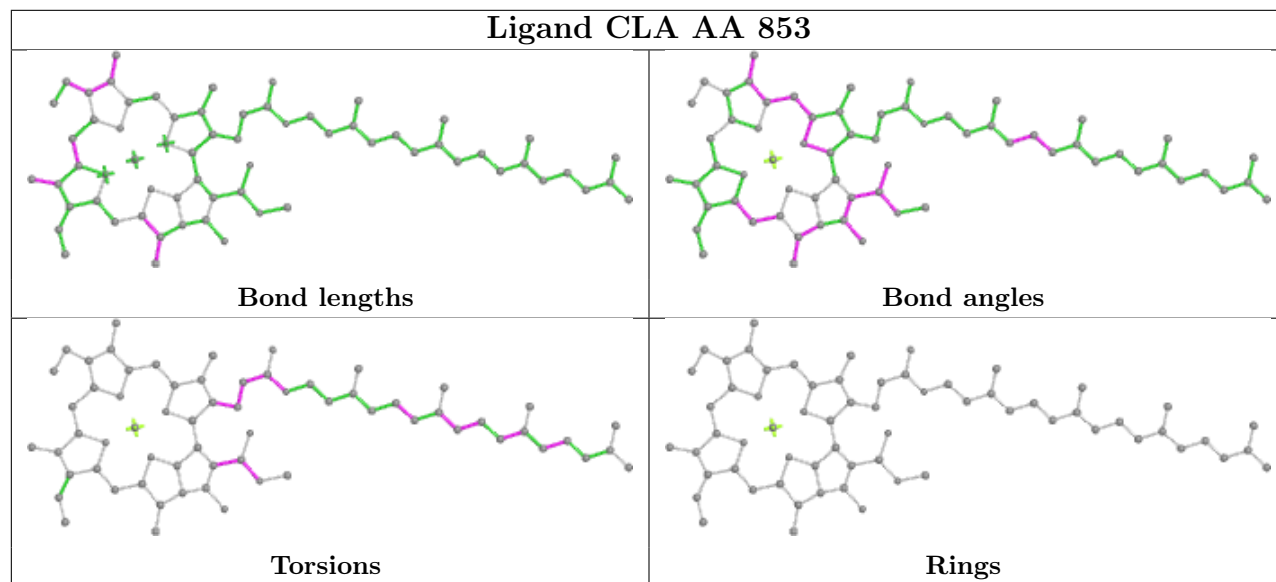
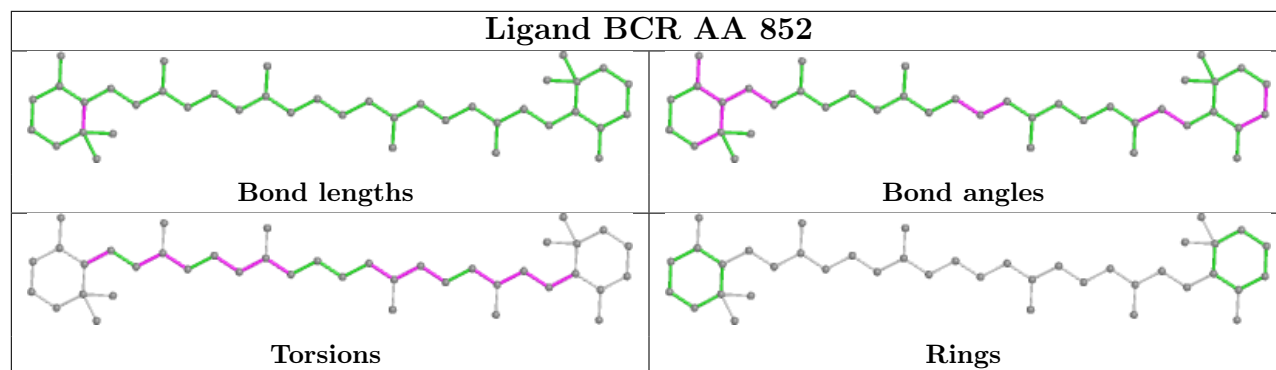
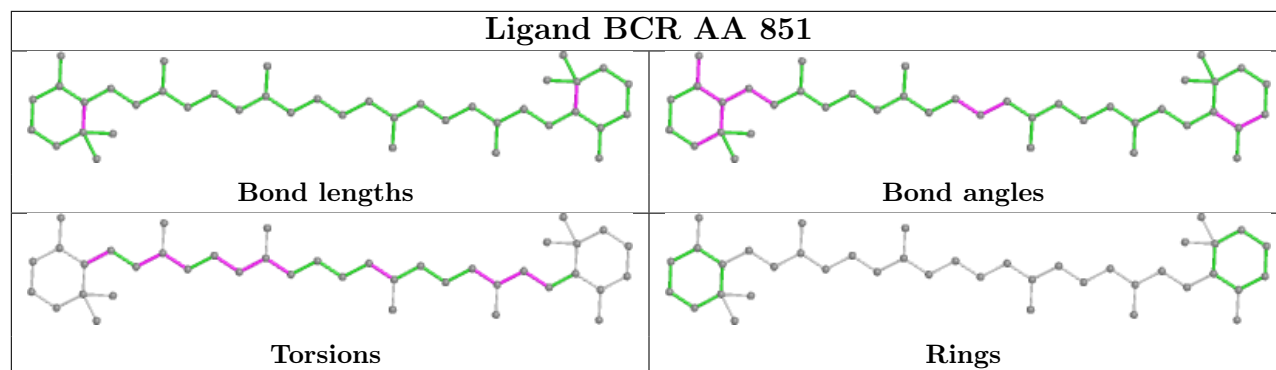


Ligand CLA AA 845

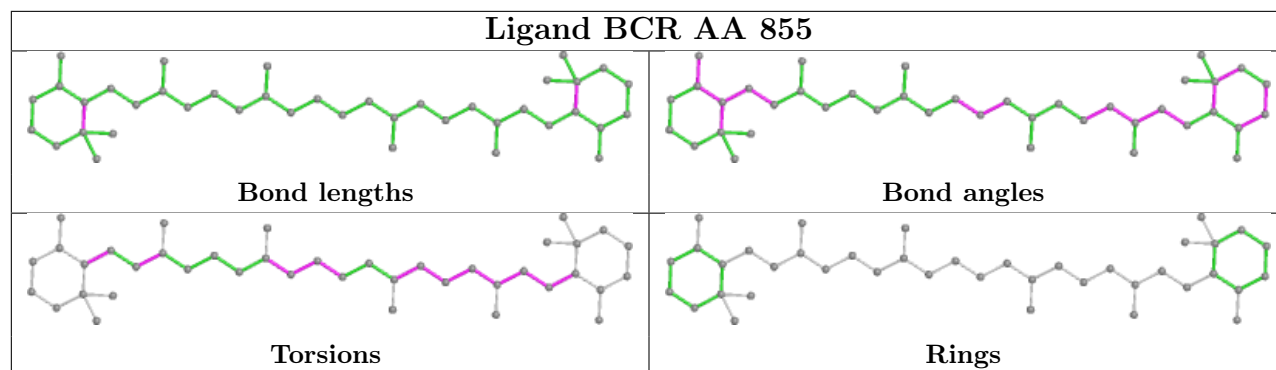




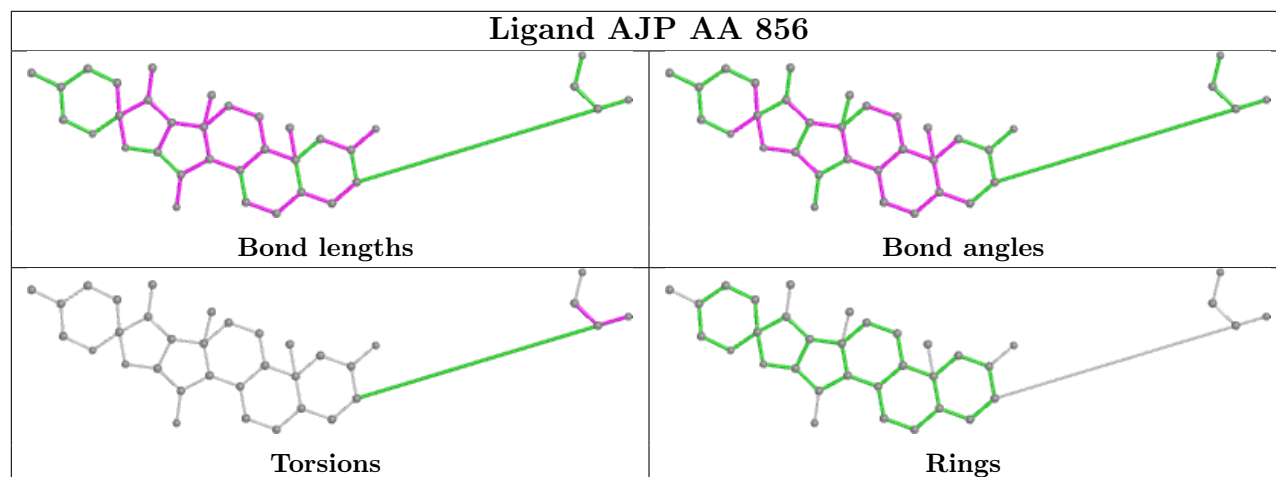




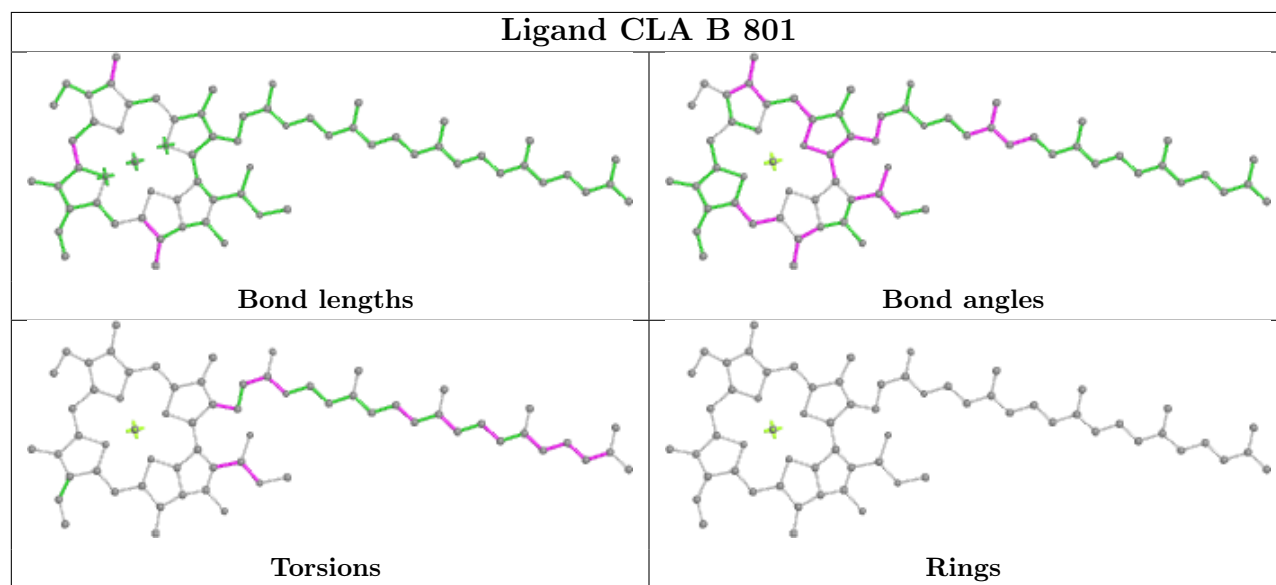
Ligand BCR AA 855



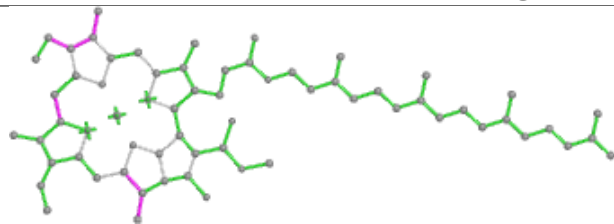
Ligand AJP AA 856



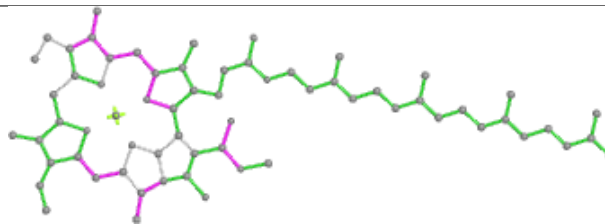
Ligand CLA B 801



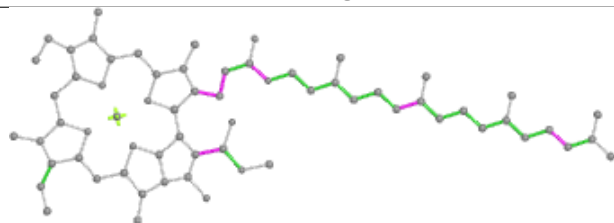
Ligand CLA B 802



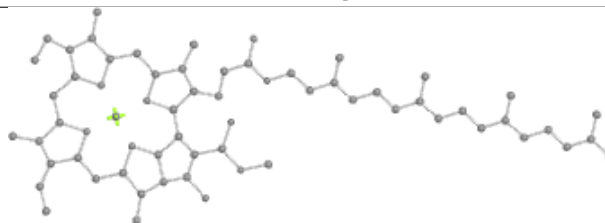
Bond lengths



Bond angles

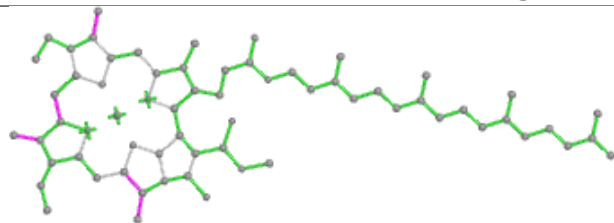


Torsions

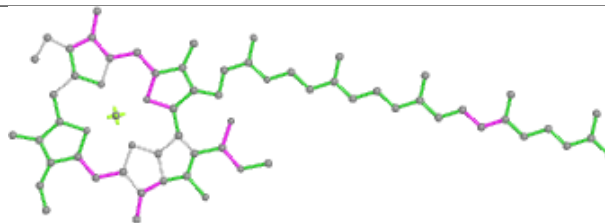


Rings

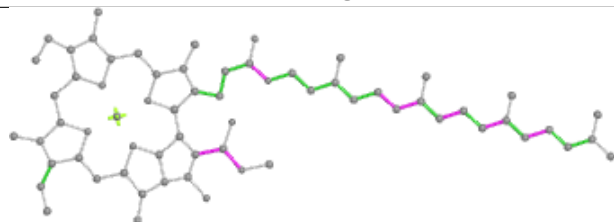
Ligand CLA B 803



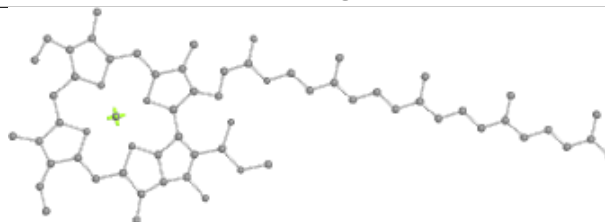
Bond lengths



Bond angles

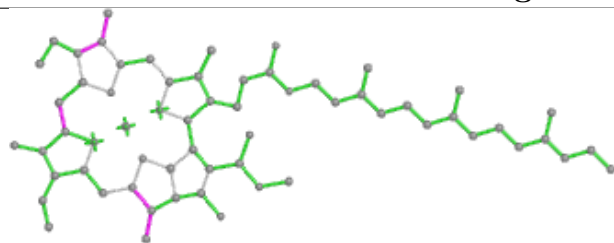


Torsions

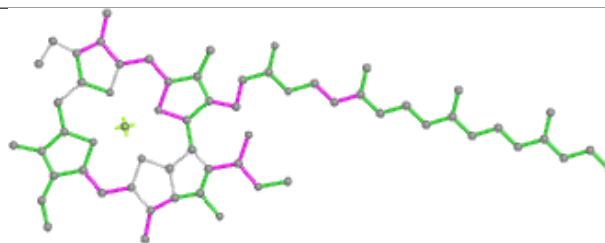


Rings

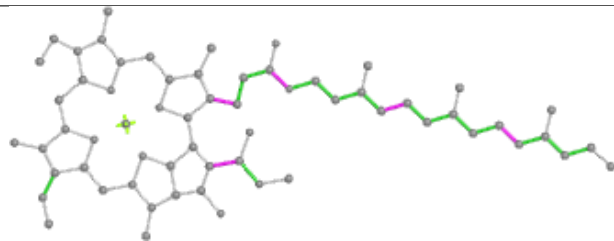
Ligand CLA B 804



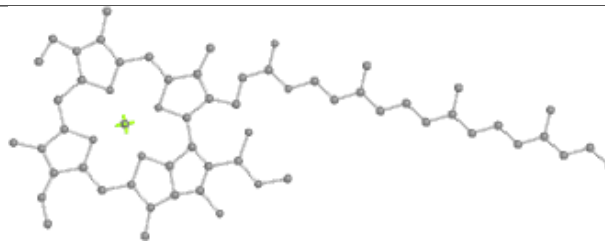
Bond lengths



Bond angles

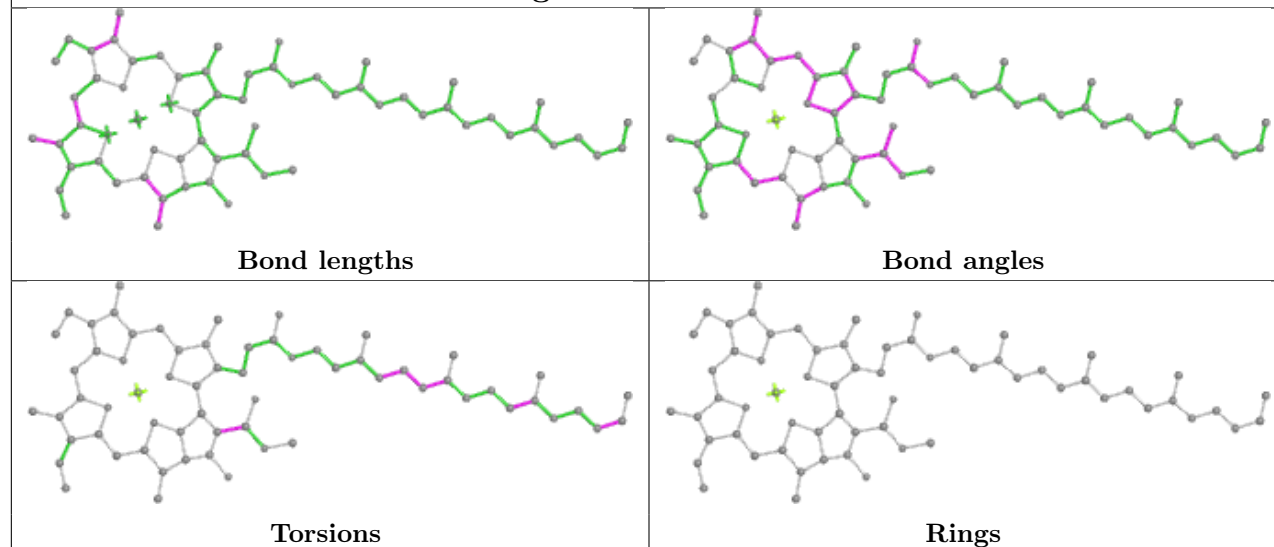


Torsions

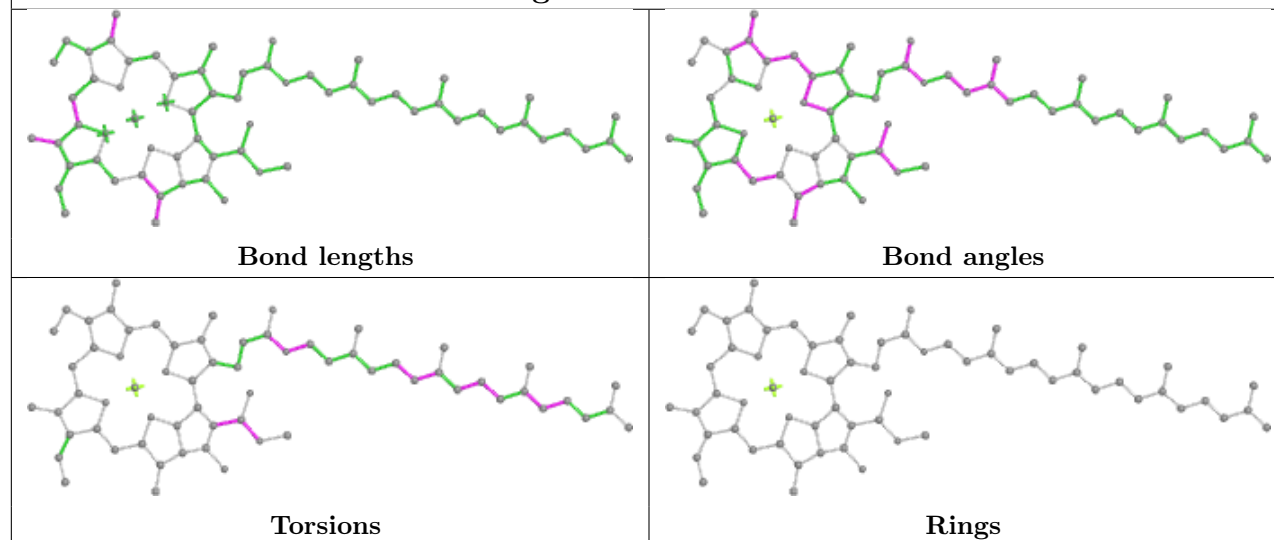


Rings

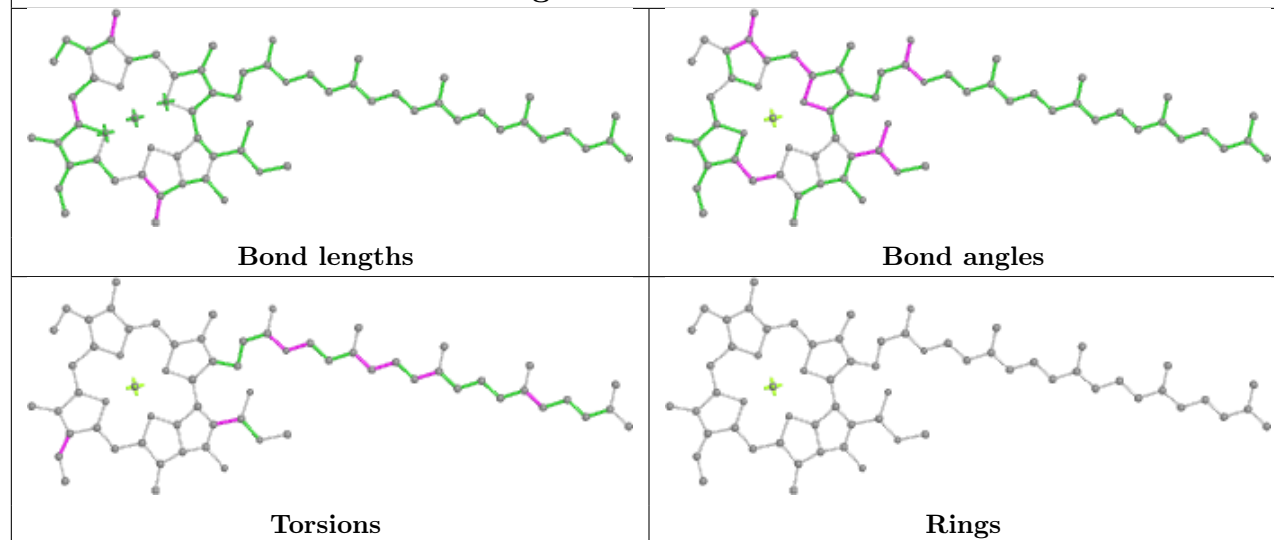
Ligand CLA B 805



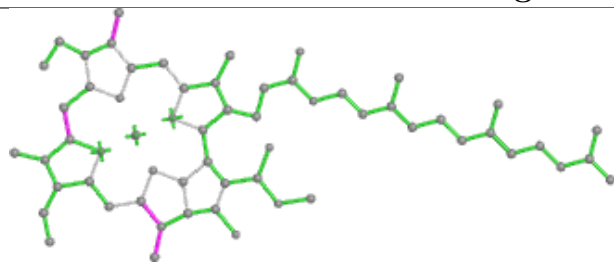
Ligand CLA B 806



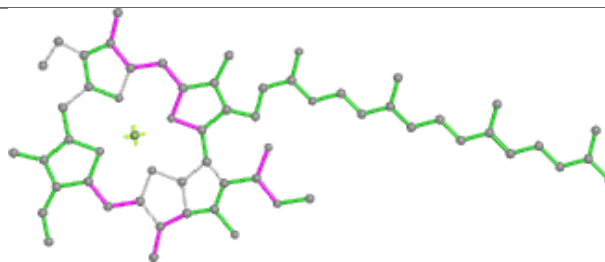
Ligand CLA B 807



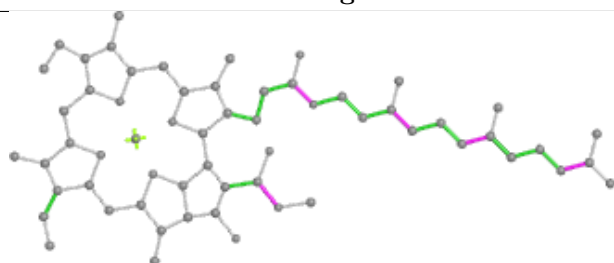
Ligand CLA B 808



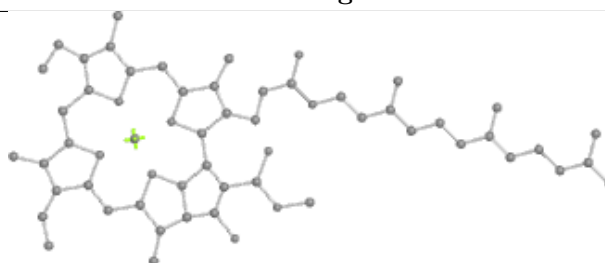
Bond lengths



Bond angles

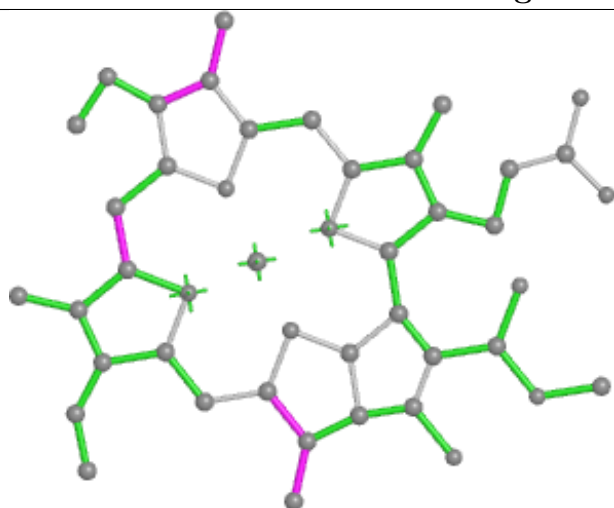


Torsions

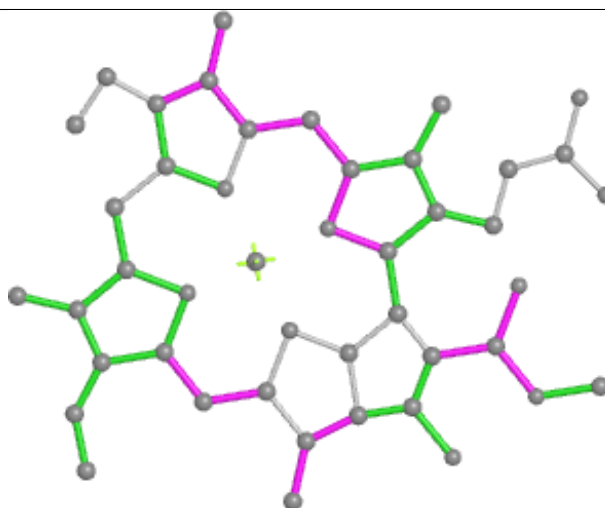


Rings

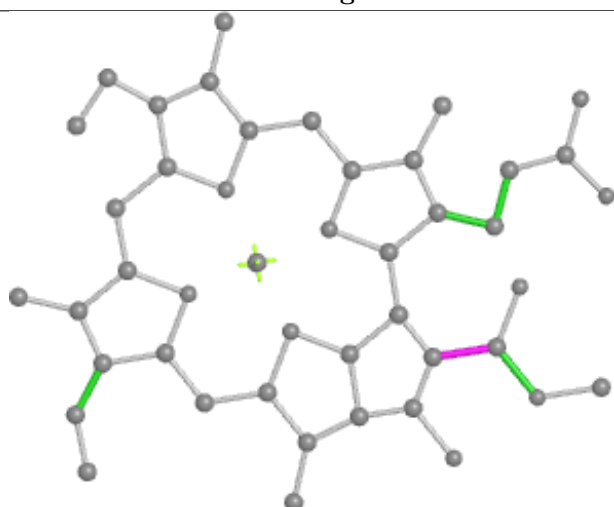
Ligand CLA B 809



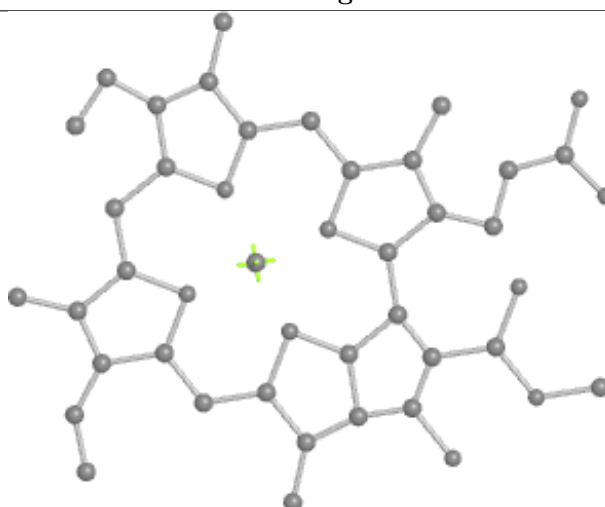
Bond lengths



Bond angles

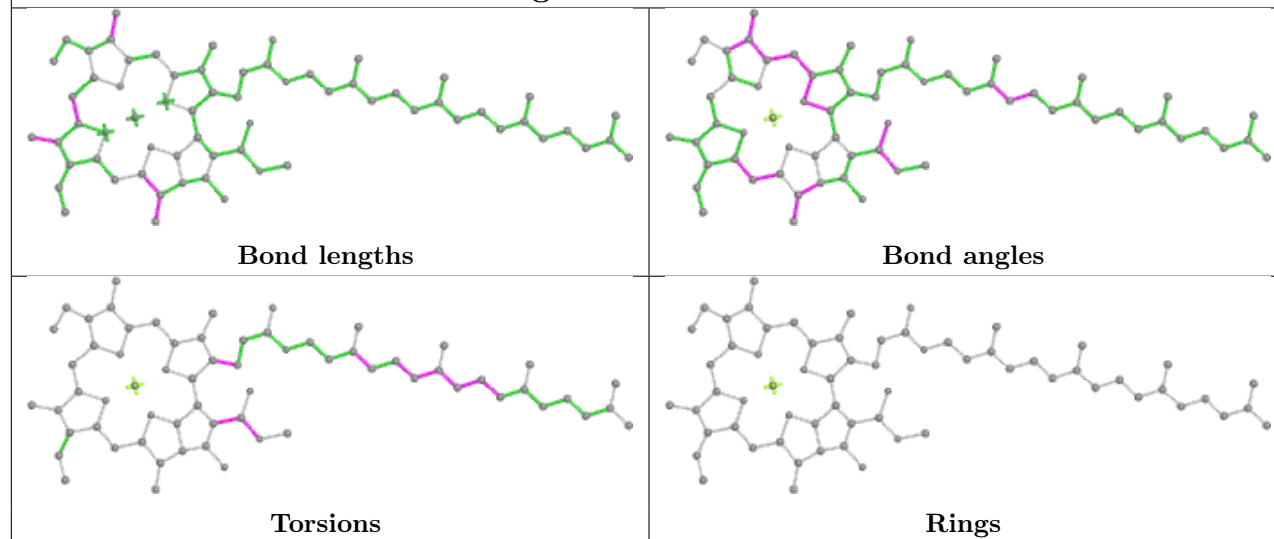


Torsions

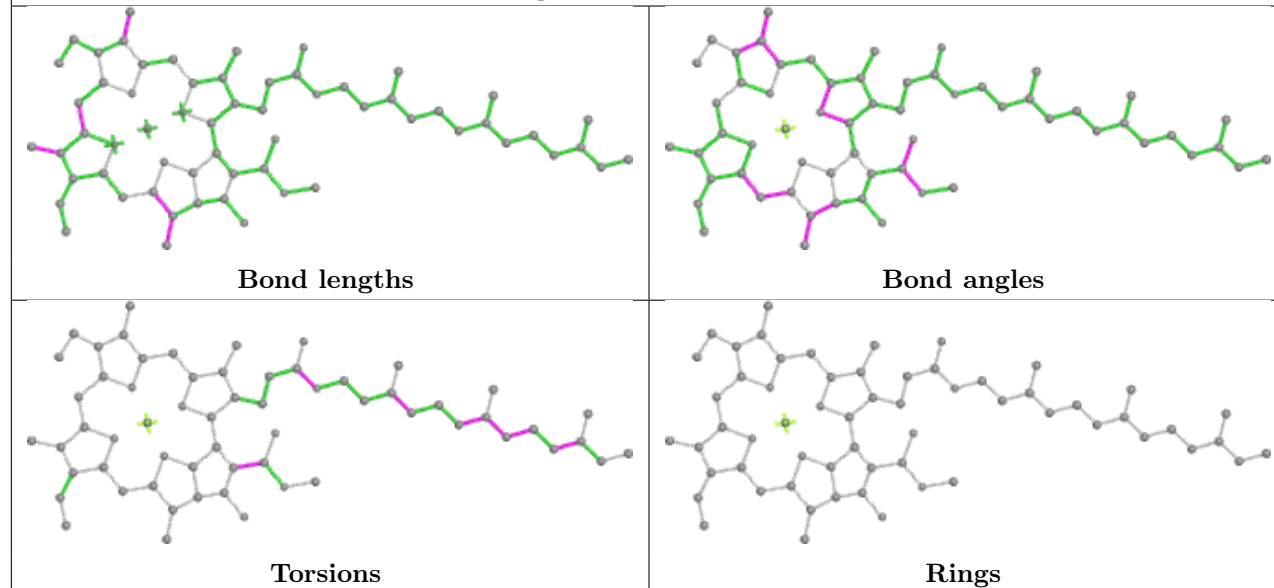


Rings

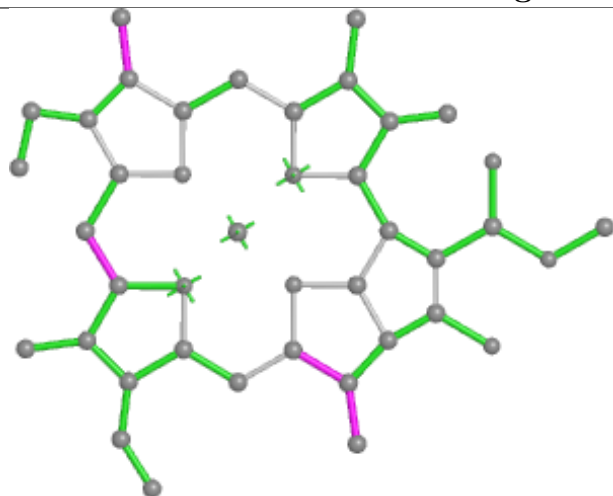
Ligand CLA B 810



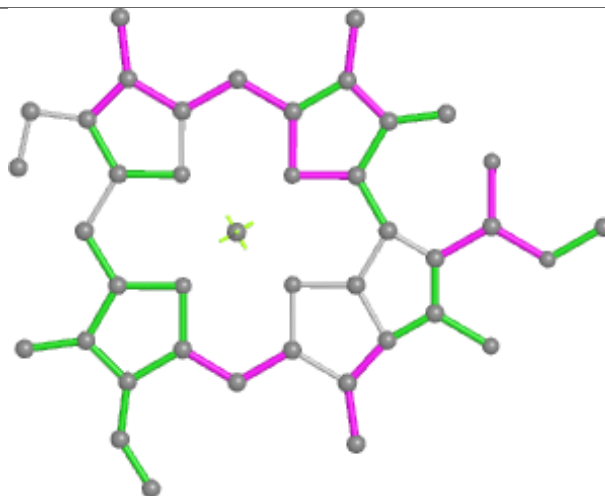
Ligand CLA B 811



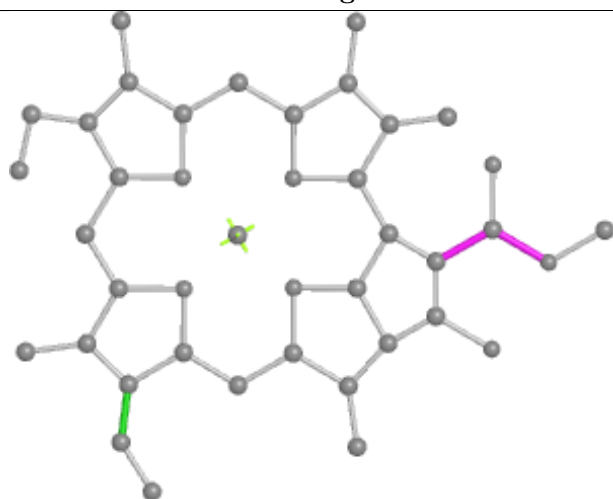
Ligand CLA B 812



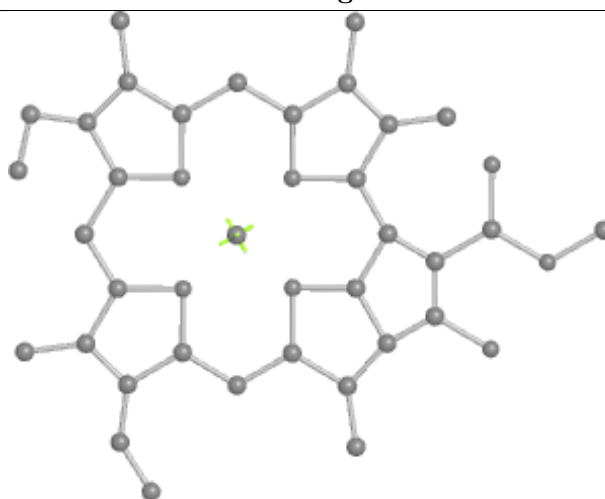
Bond lengths



Bond angles

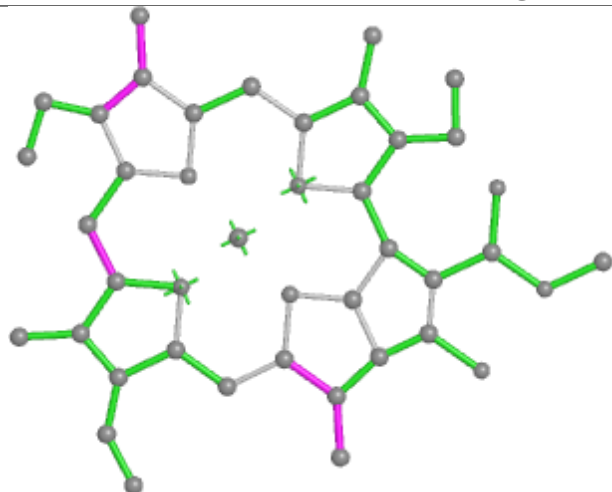


Torsions

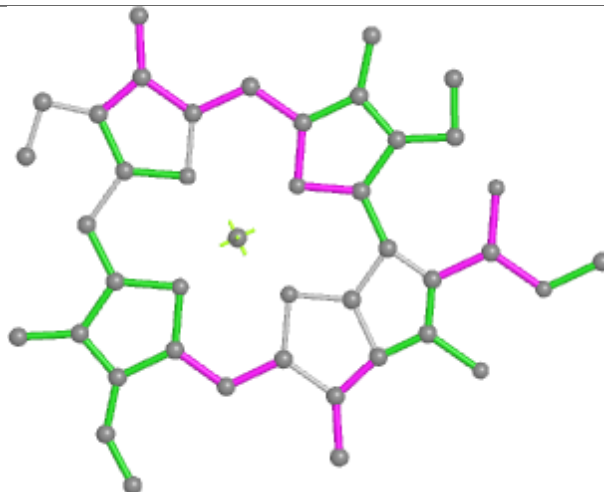


Rings

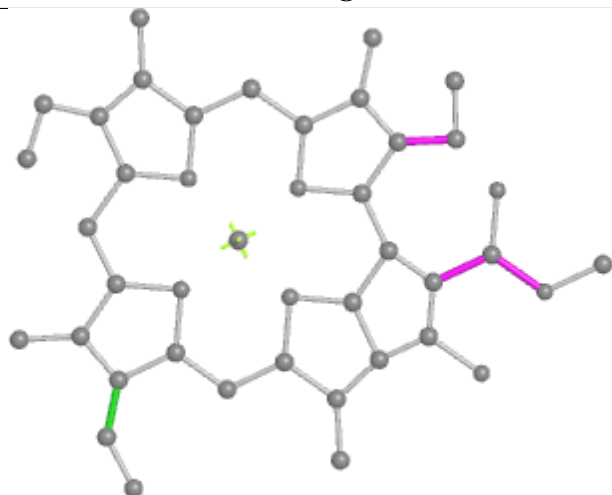
Ligand CLA B 813



Bond lengths



Bond angles

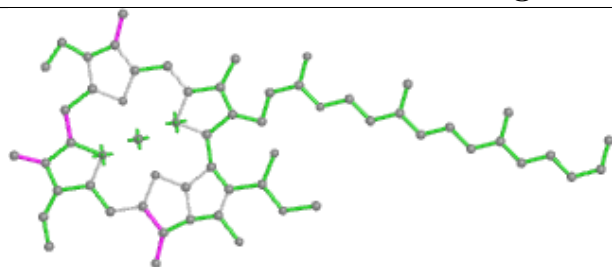


Torsions

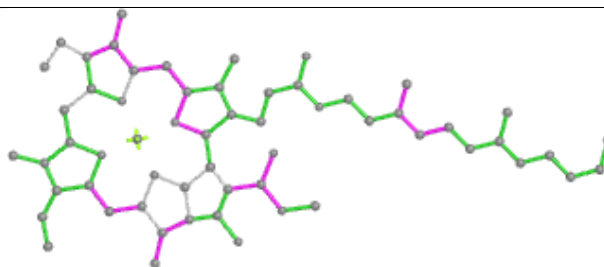


Rings

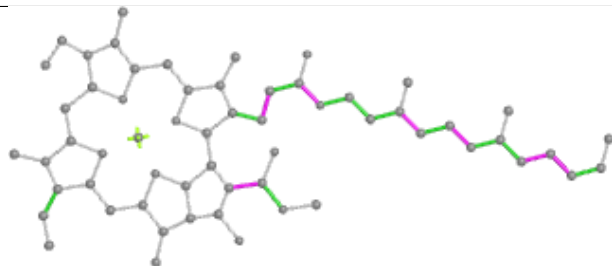
Ligand CLA B 814



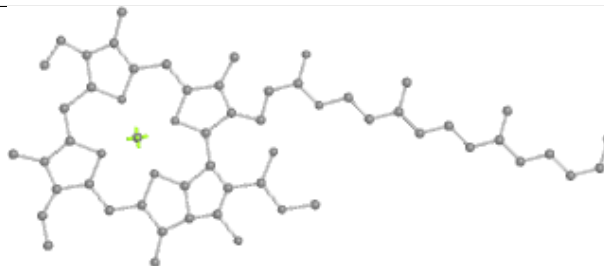
Bond lengths



Bond angles

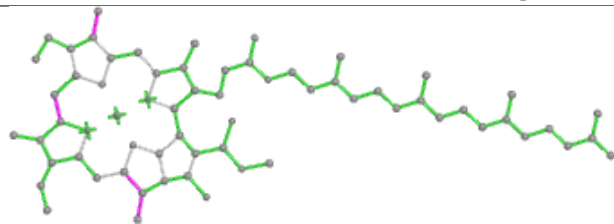


Torsions

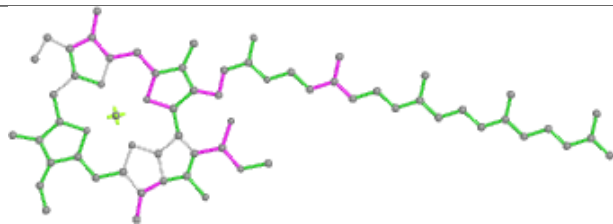


Rings

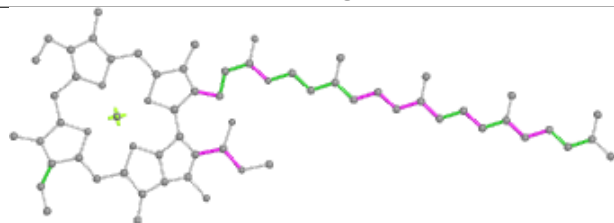
Ligand CLA B 815



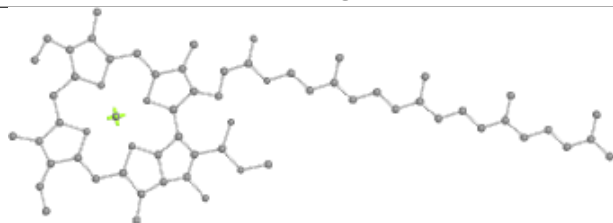
Bond lengths



Bond angles

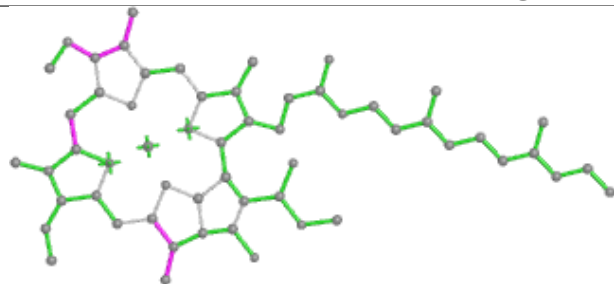


Torsions

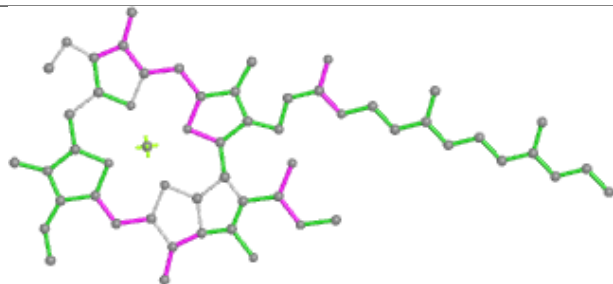


Rings

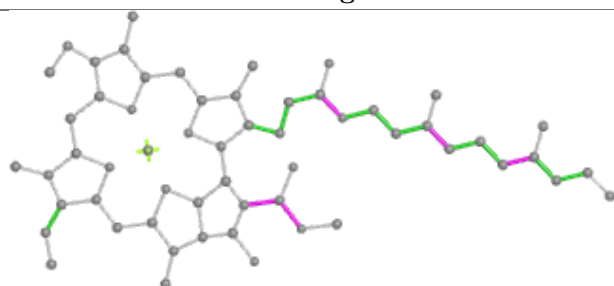
Ligand CLA B 816



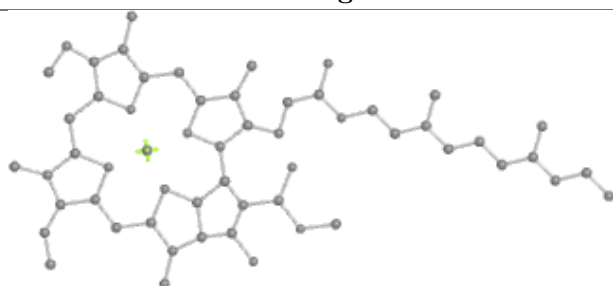
Bond lengths



Bond angles

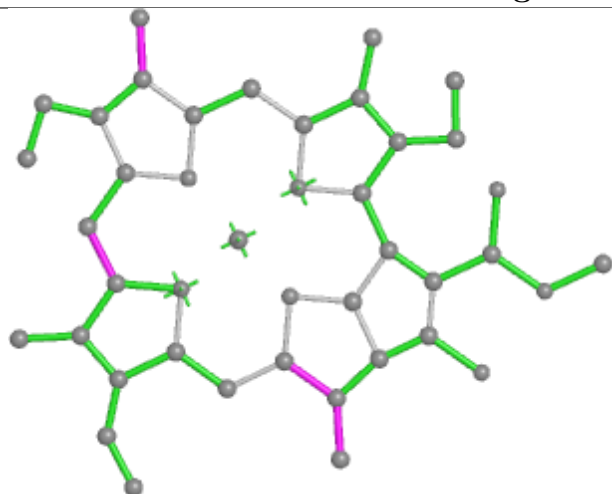


Torsions

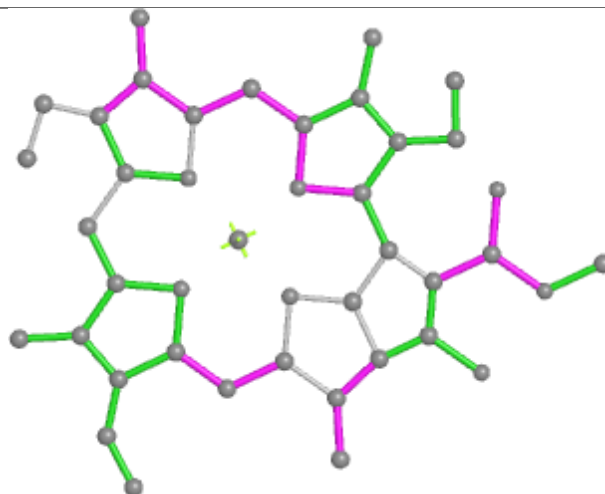


Rings

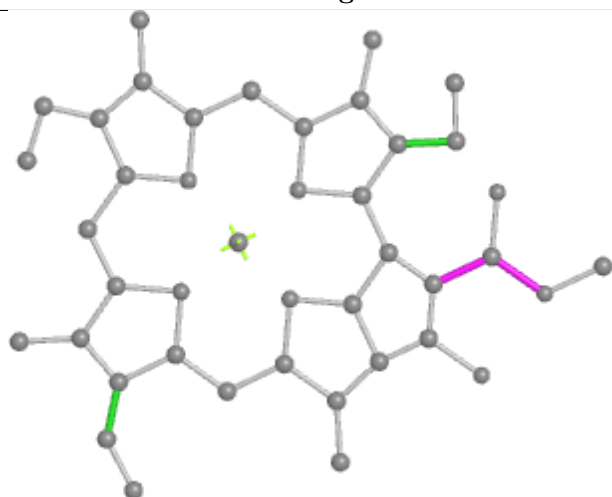
Ligand CLA B 817



Bond lengths



Bond angles

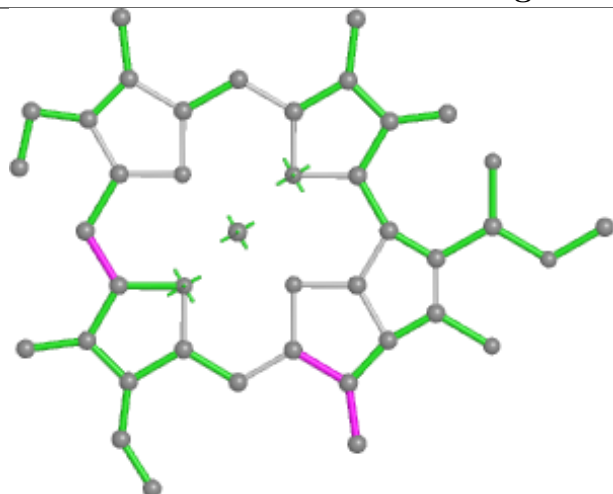


Torsions

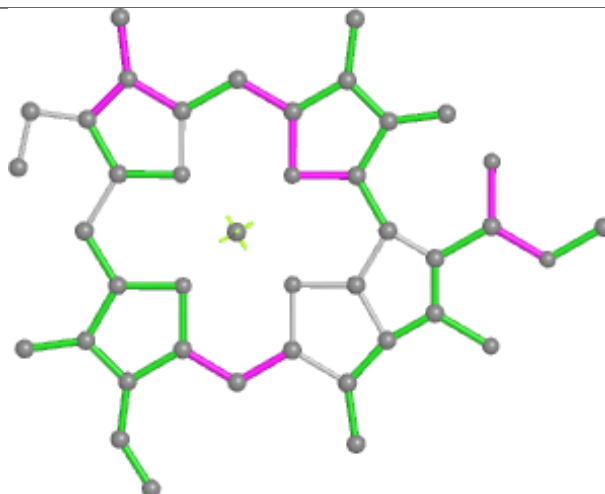


Rings

Ligand CLA B 818



Bond lengths



Bond angles

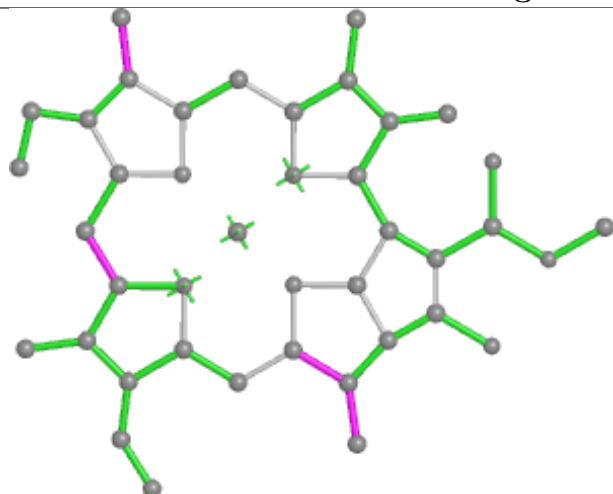


Torsions

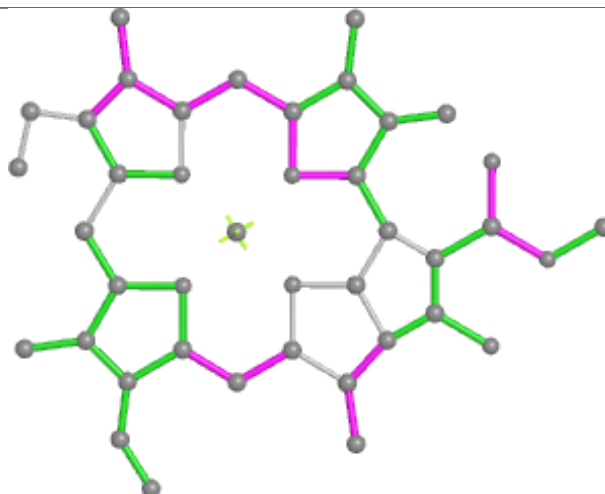


Rings

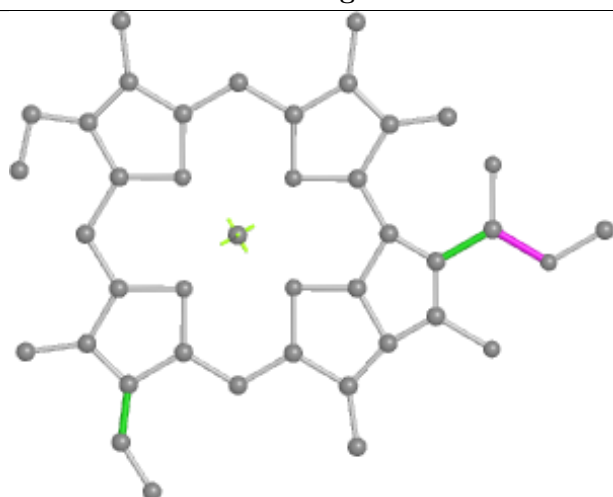
Ligand CLA B 819



Bond lengths



Bond angles

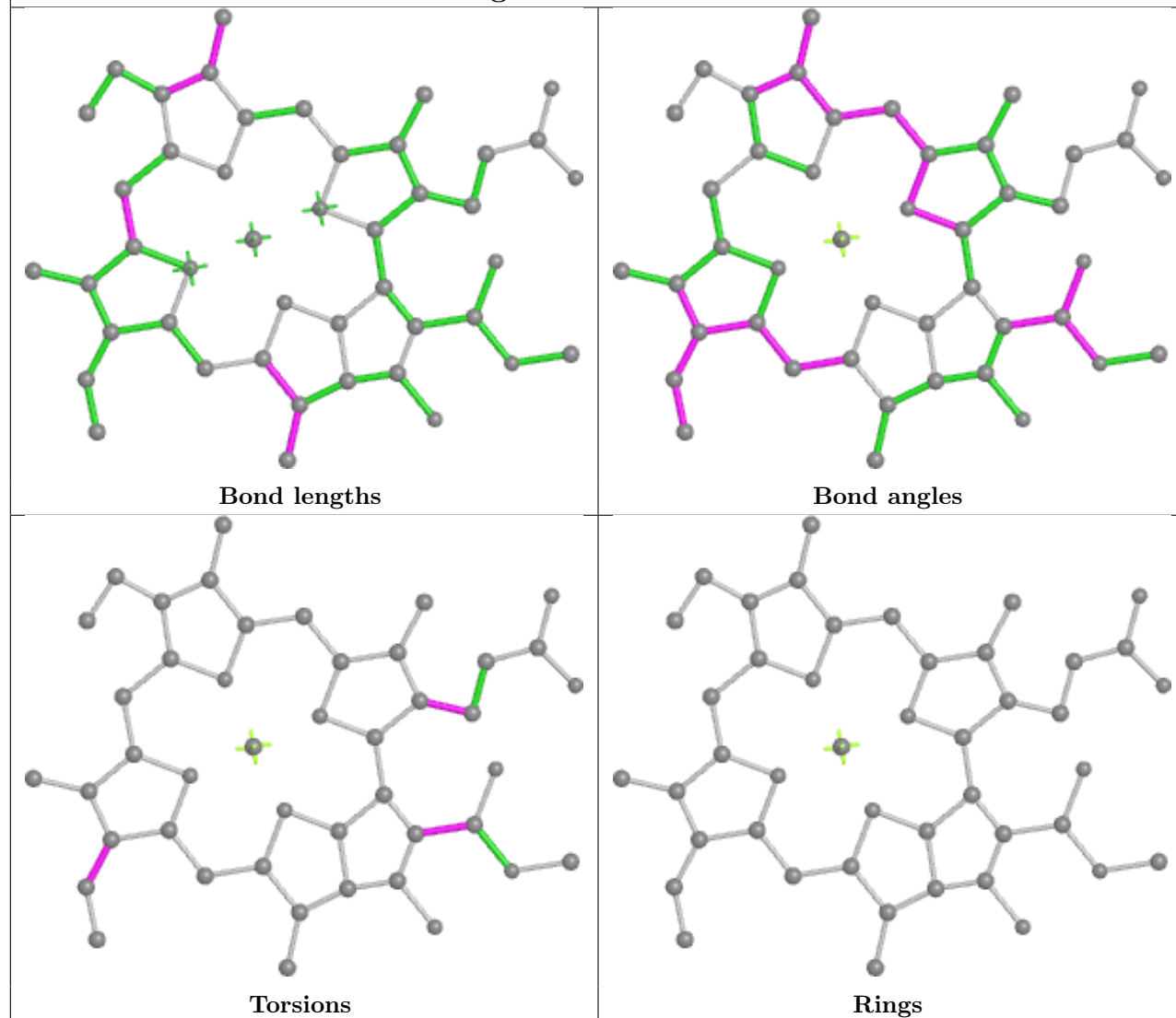


Torsions

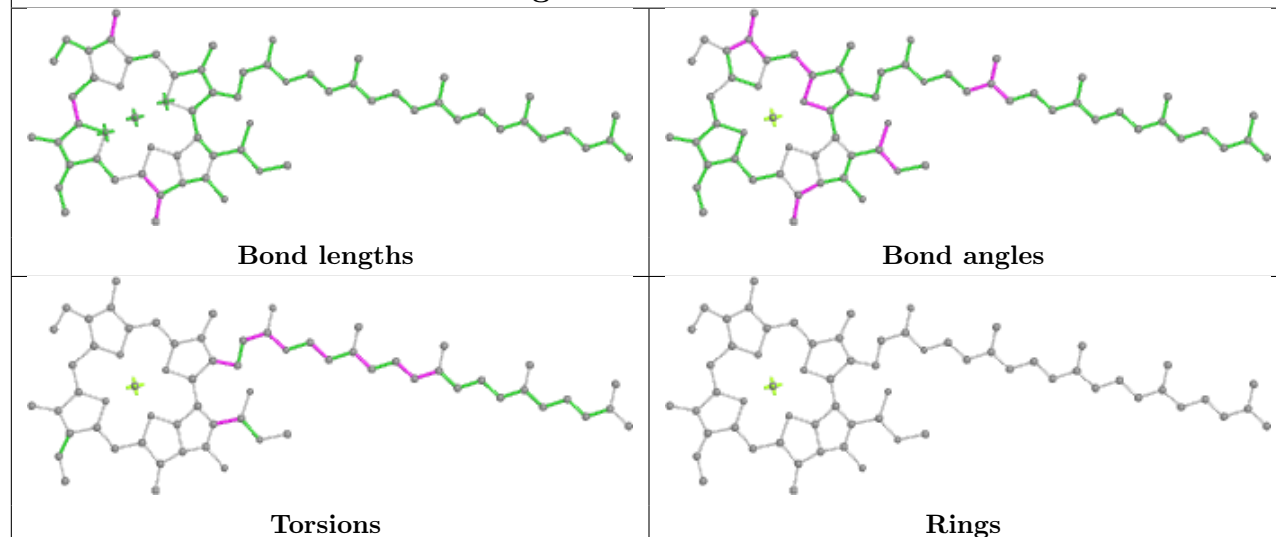


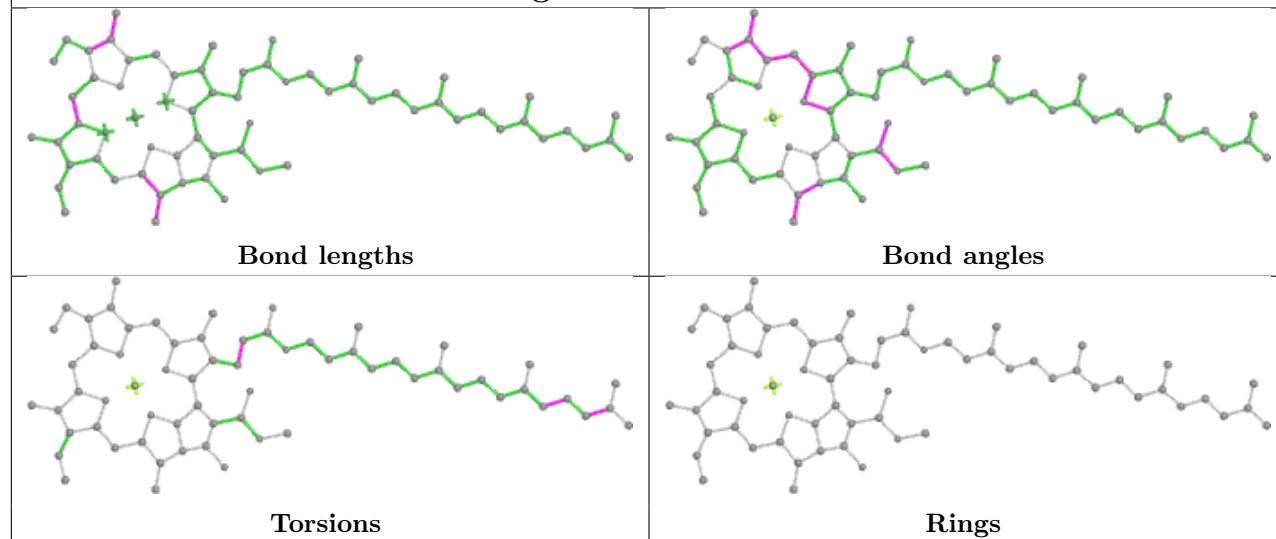
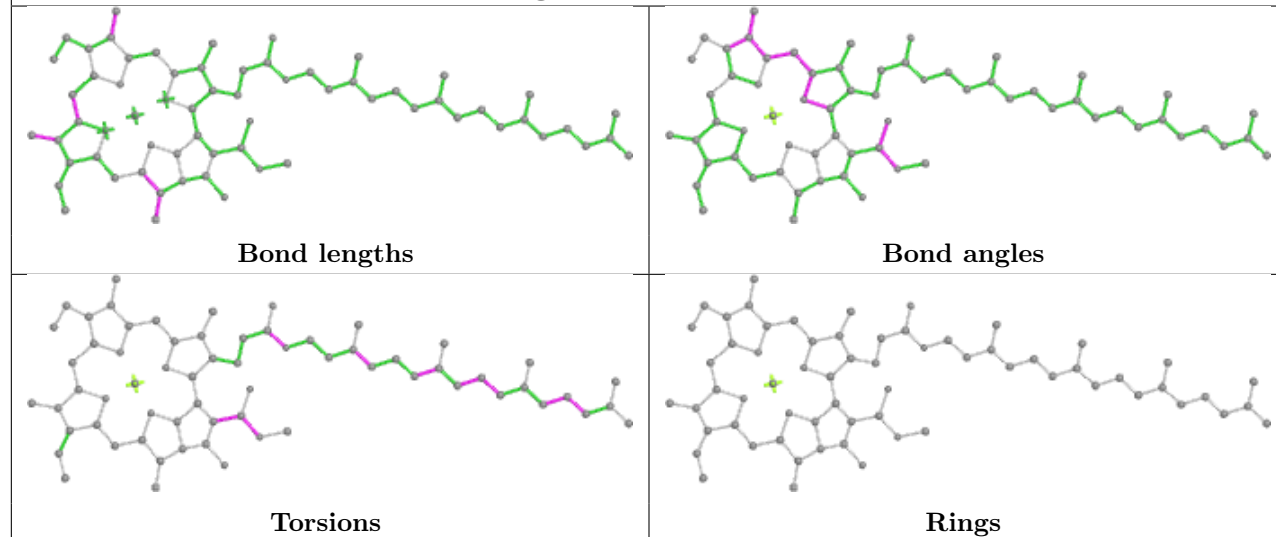
Rings

Ligand CLA B 820

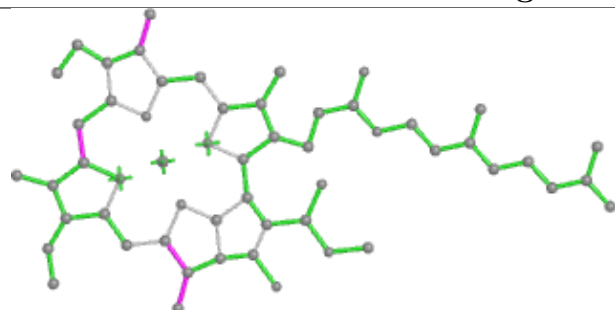


Ligand CLA B 821

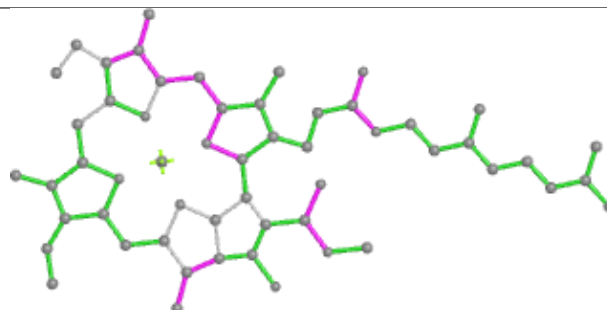


Ligand CLA B 822**Ligand CLA B 823**

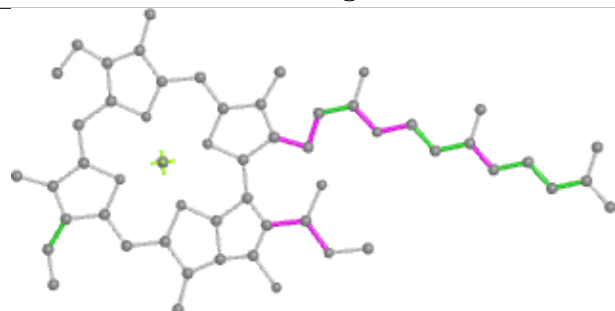
Ligand CLA B 824



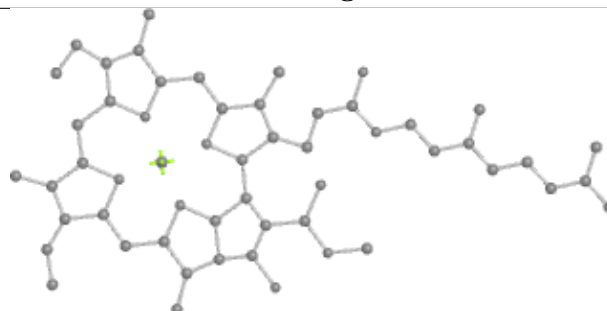
Bond lengths



Bond angles

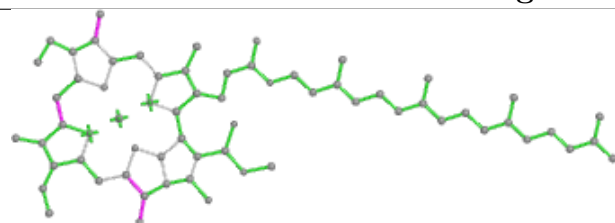


Torsions

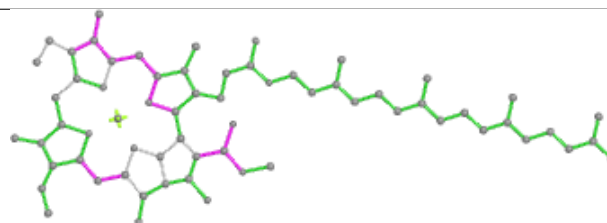


Rings

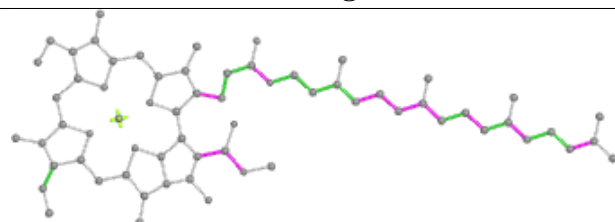
Ligand CLA B 825



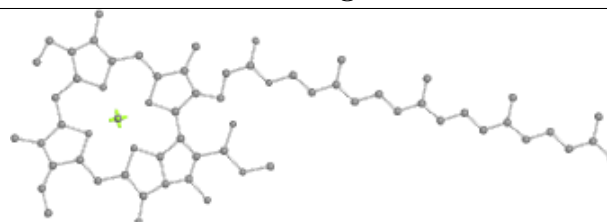
Bond lengths



Bond angles

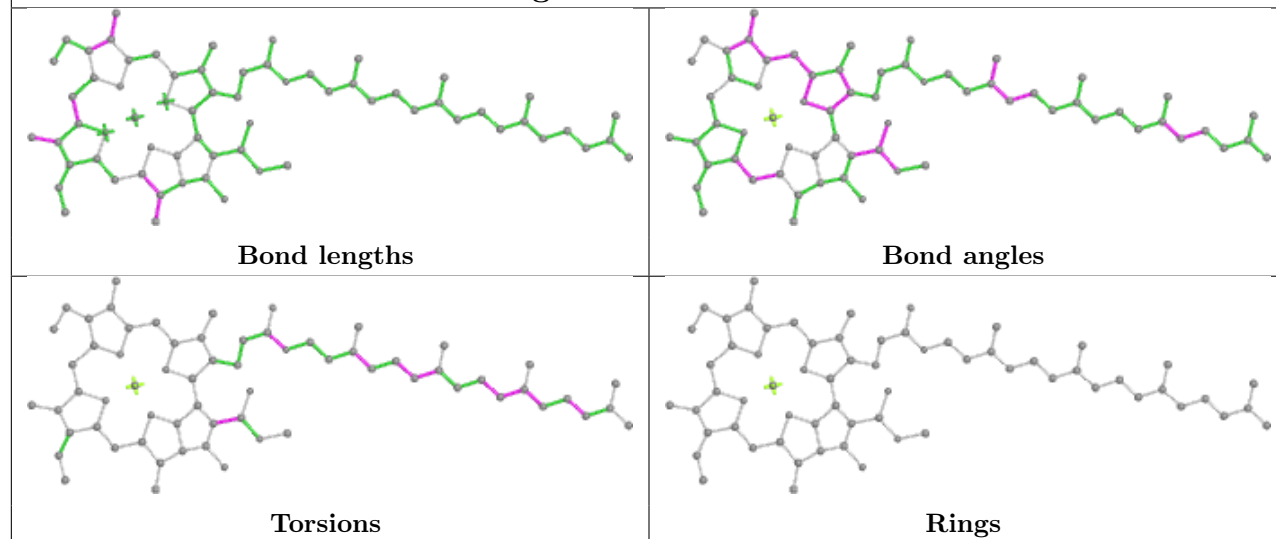


Torsions

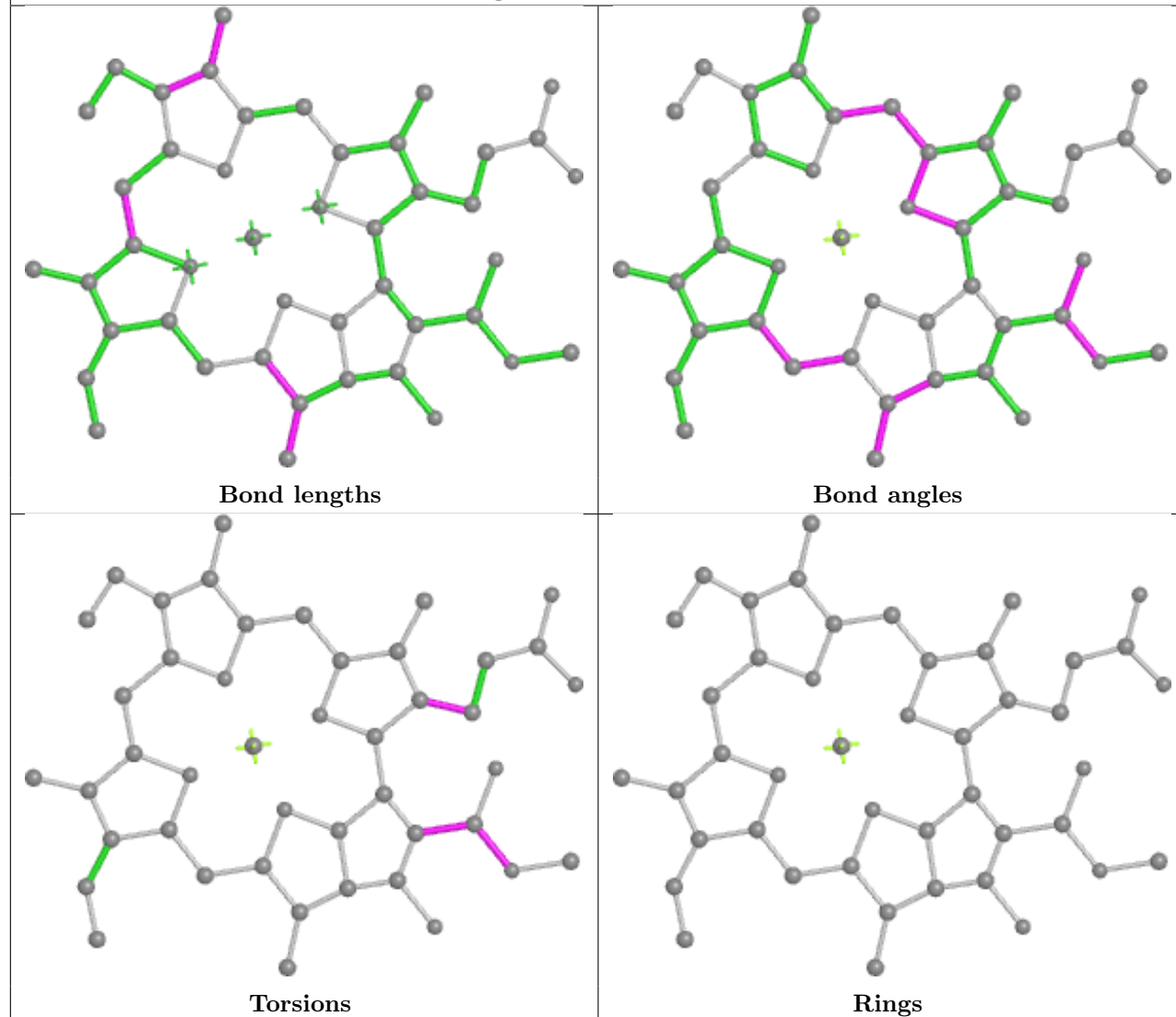


Rings

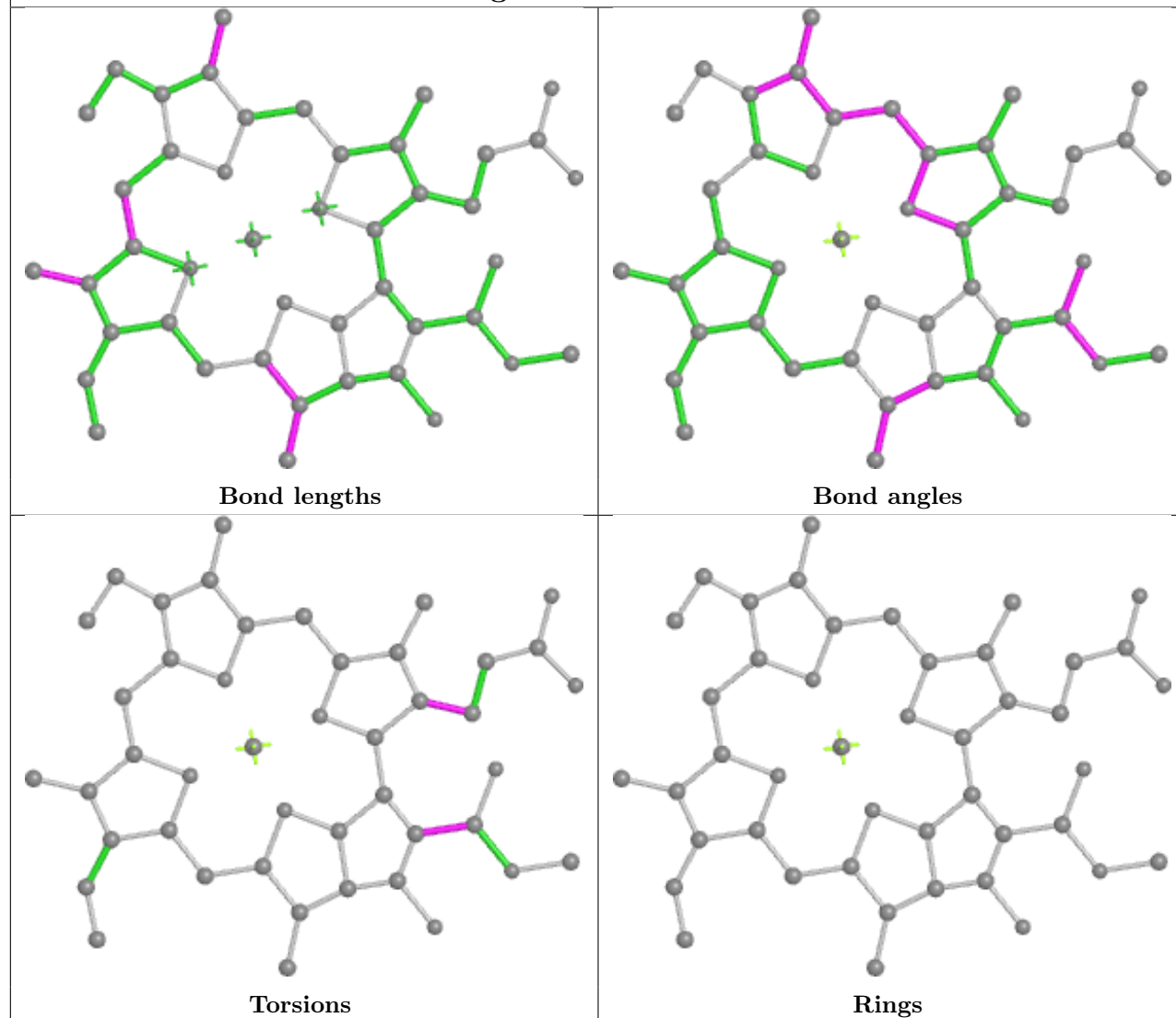
Ligand CLA B 826



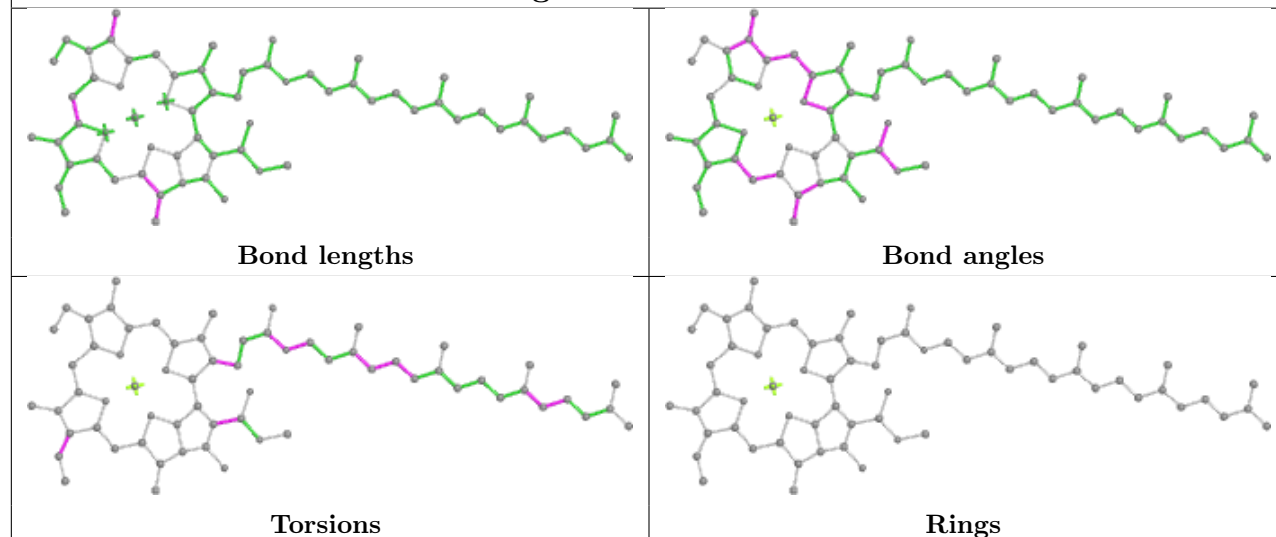
Ligand CLA B 827



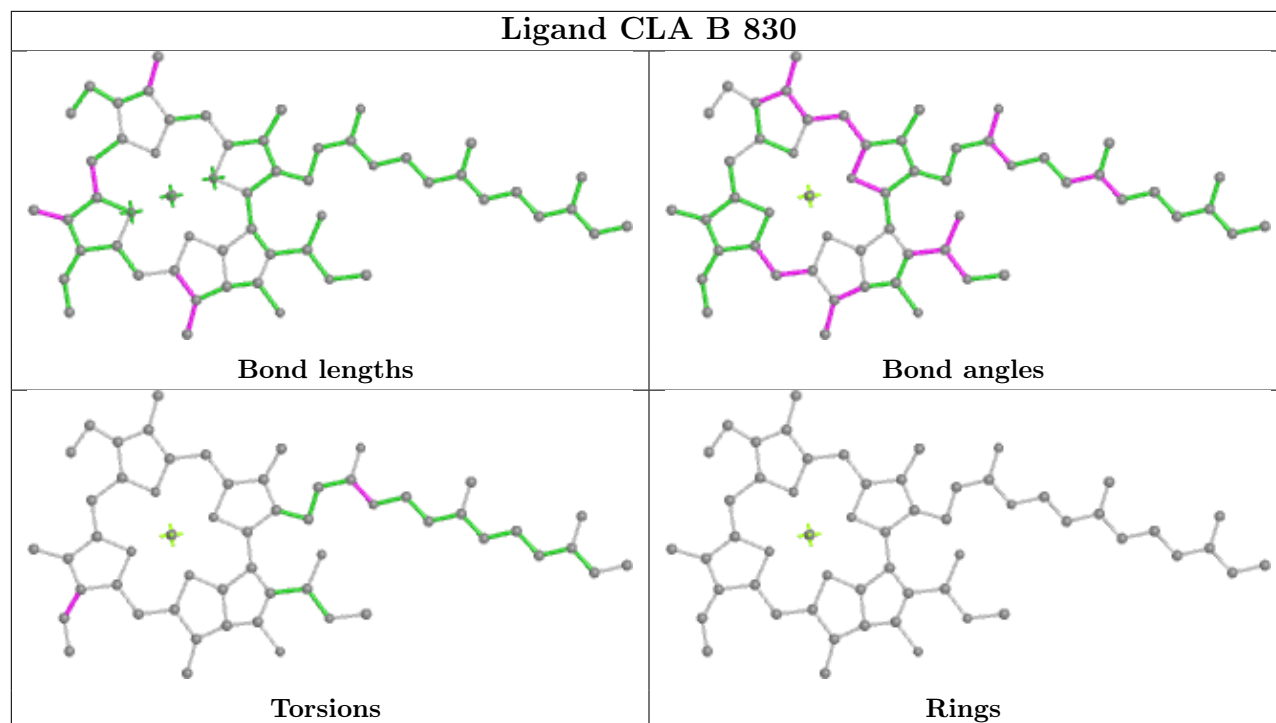
Ligand CLA B 828



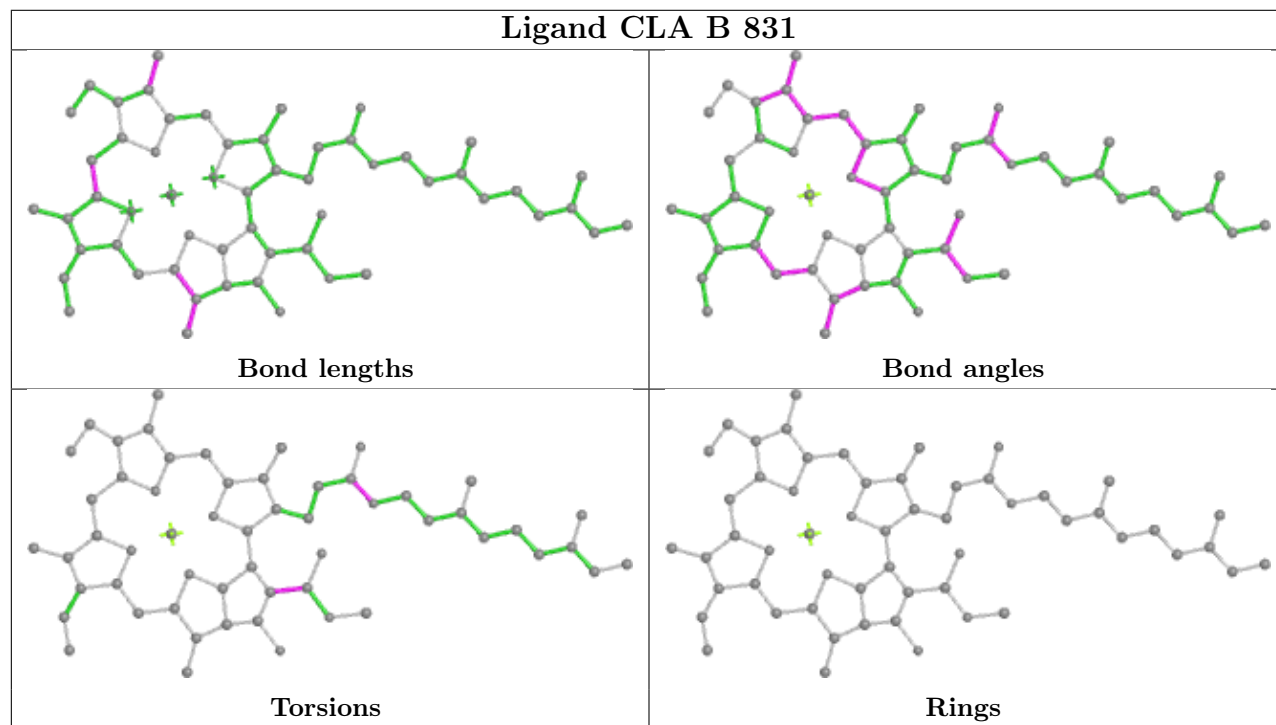
Ligand CLA B 829



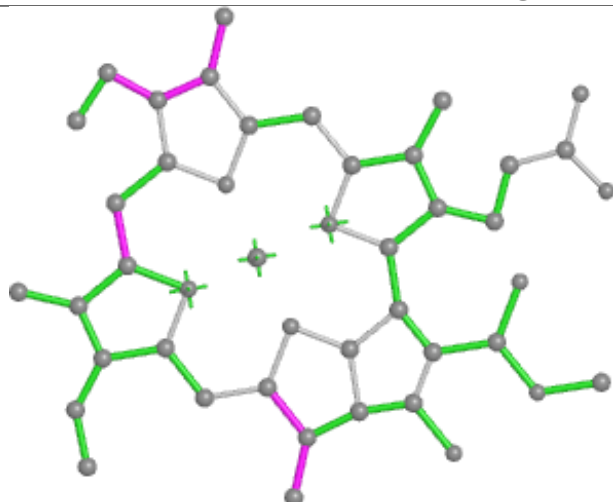
Ligand CLA B 830



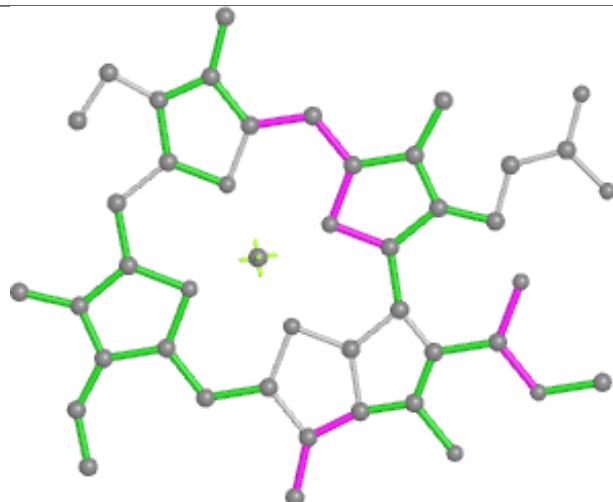
Ligand CLA B 831



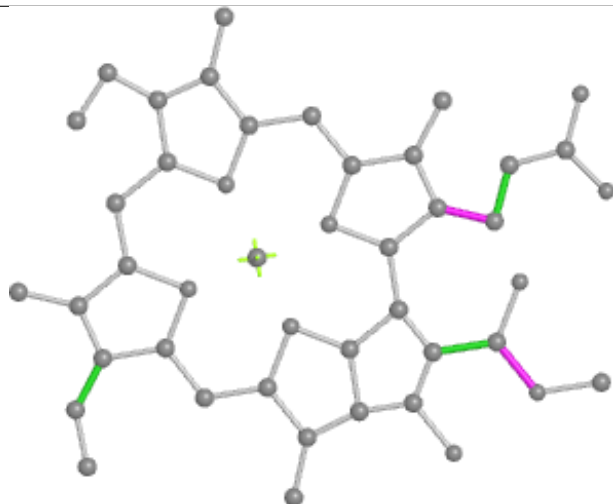
Ligand CLA B 832



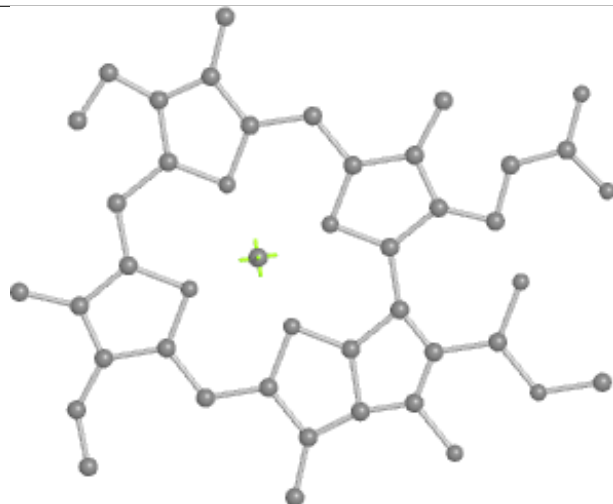
Bond lengths



Bond angles

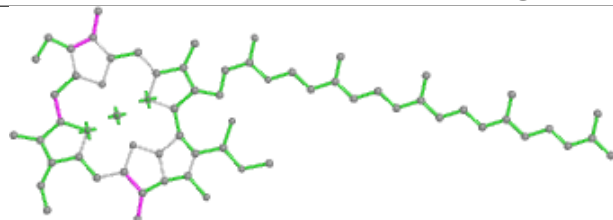


Torsions

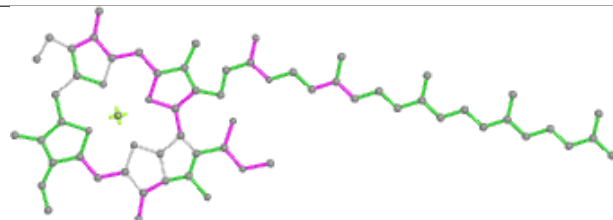


Rings

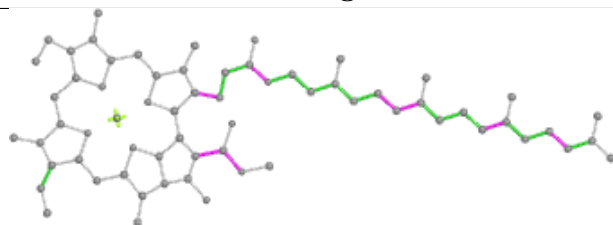
Ligand CLA B 833



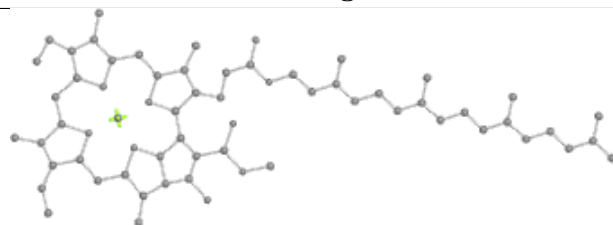
Bond lengths



Bond angles

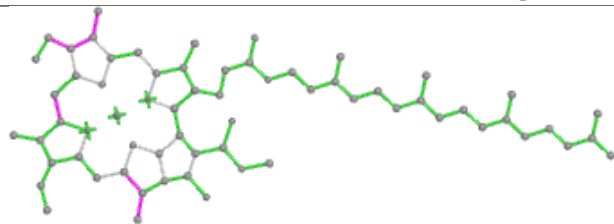


Torsions

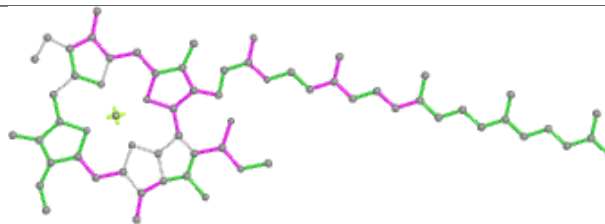


Rings

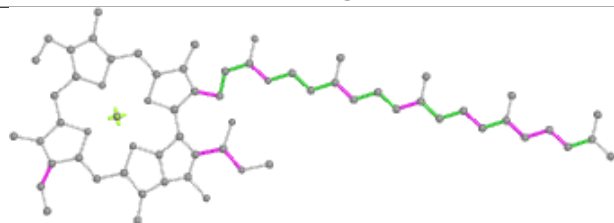
Ligand CLA B 834



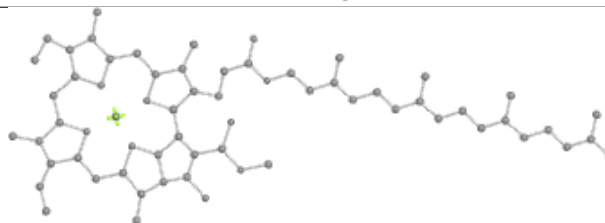
Bond lengths



Bond angles

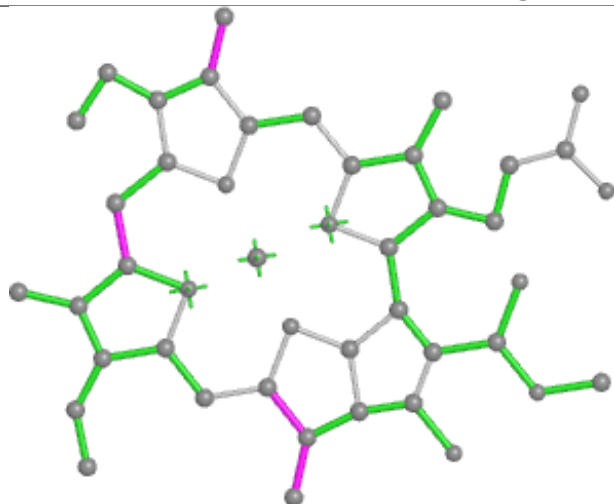


Torsions

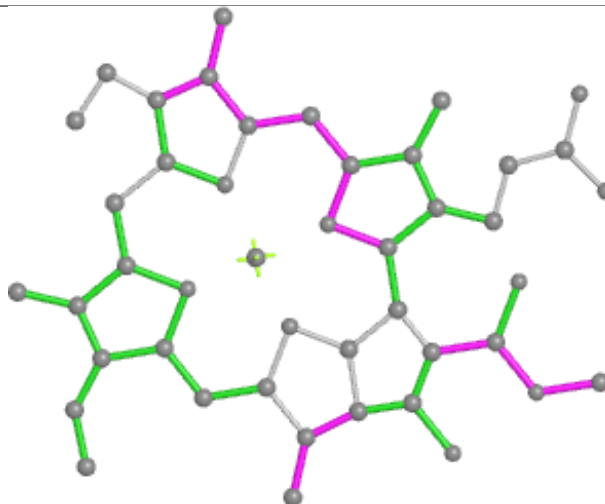


Rings

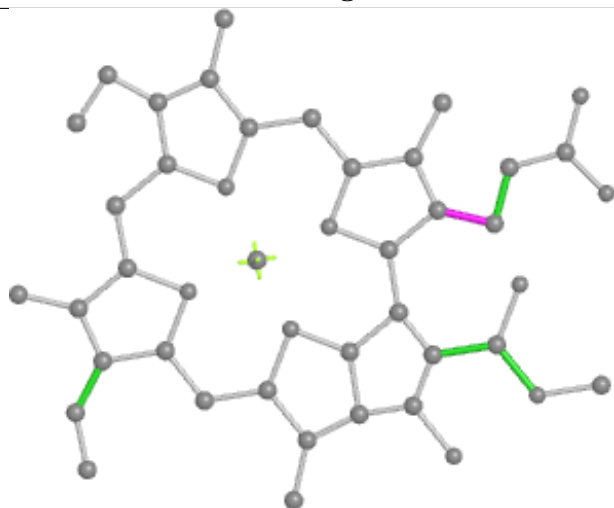
Ligand CLA B 835



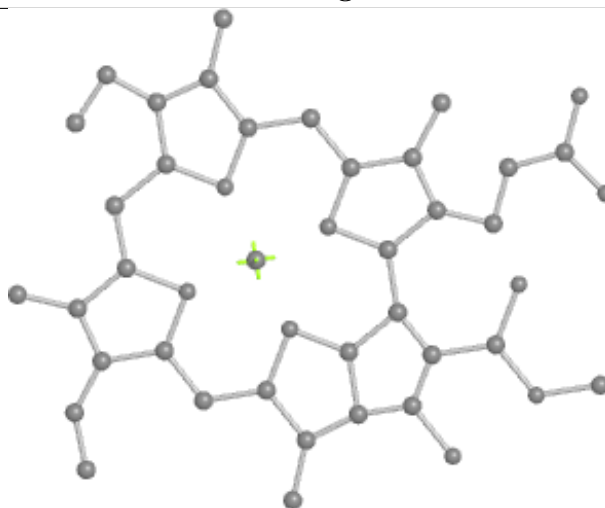
Bond lengths



Bond angles

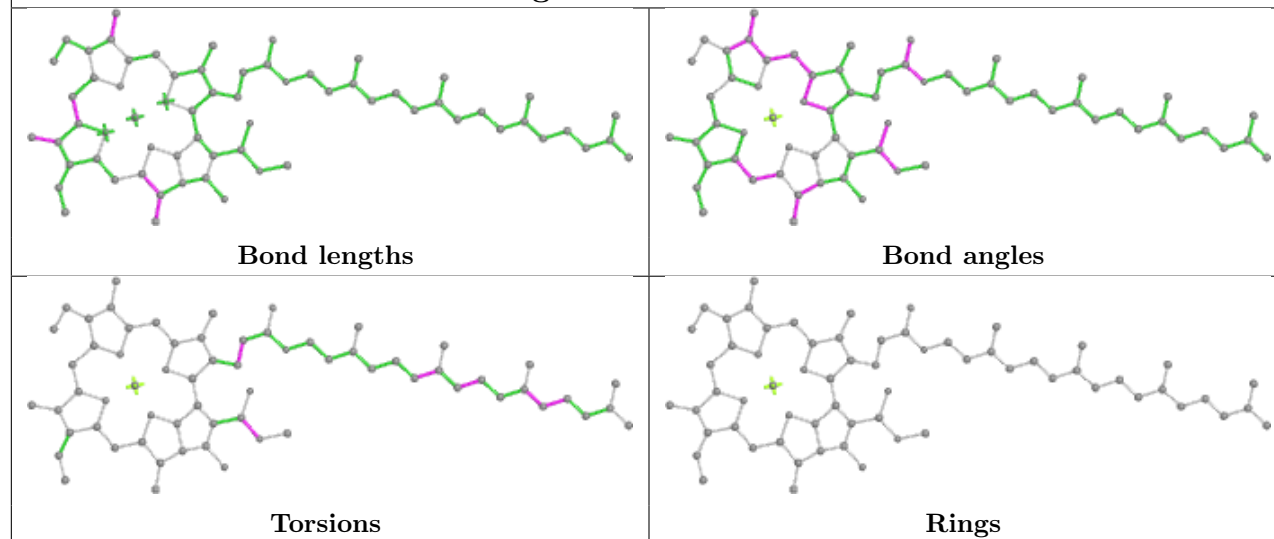


Torsions

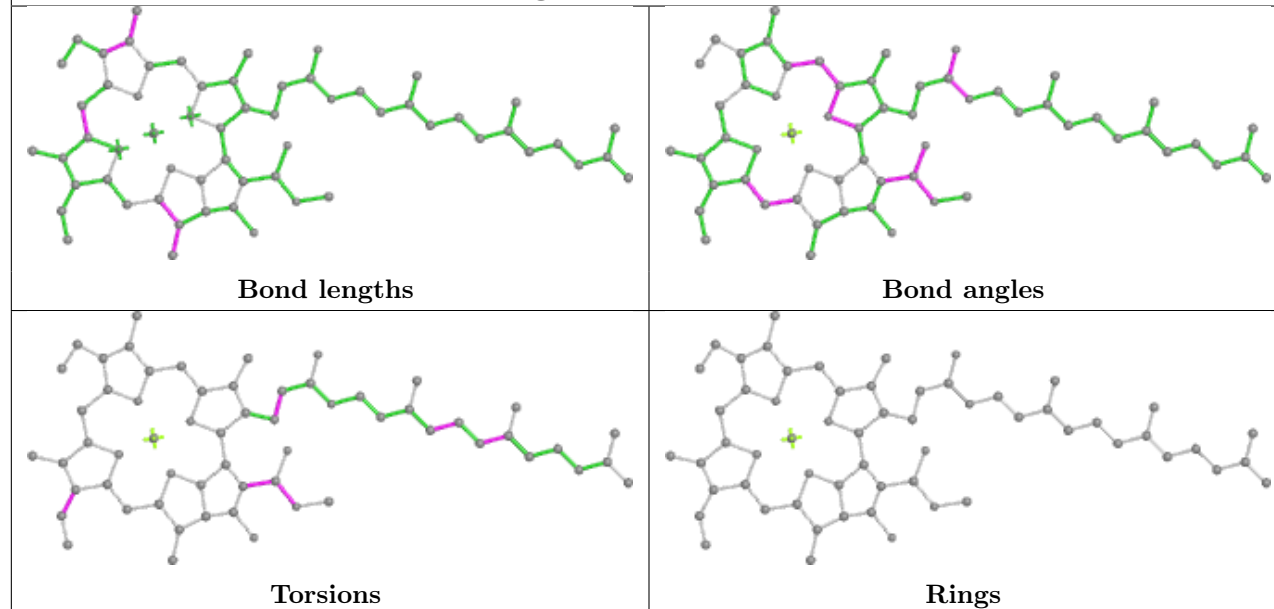


Rings

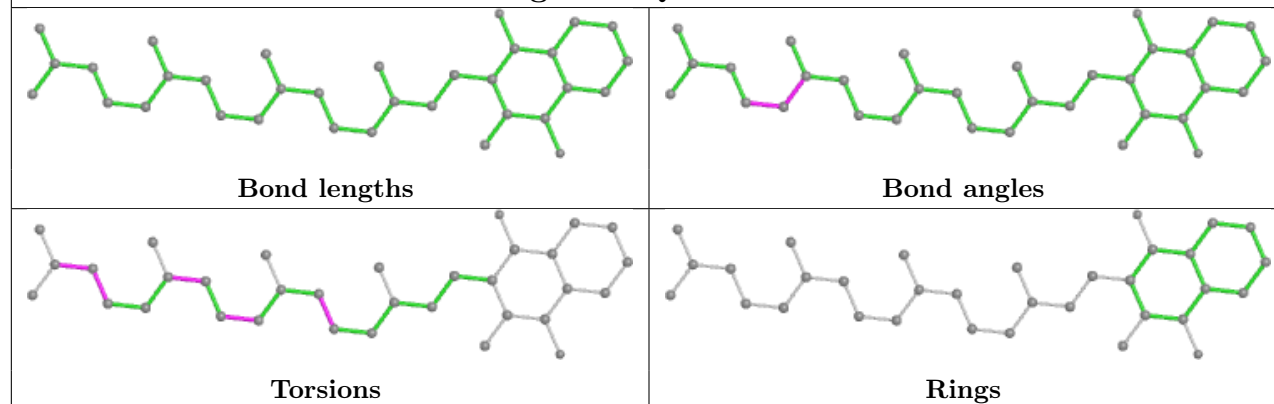
Ligand CLA B 836

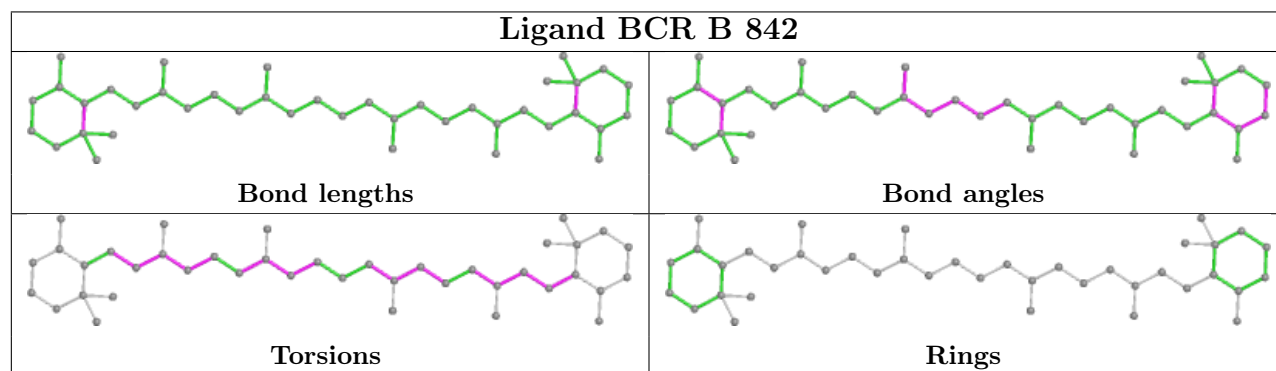
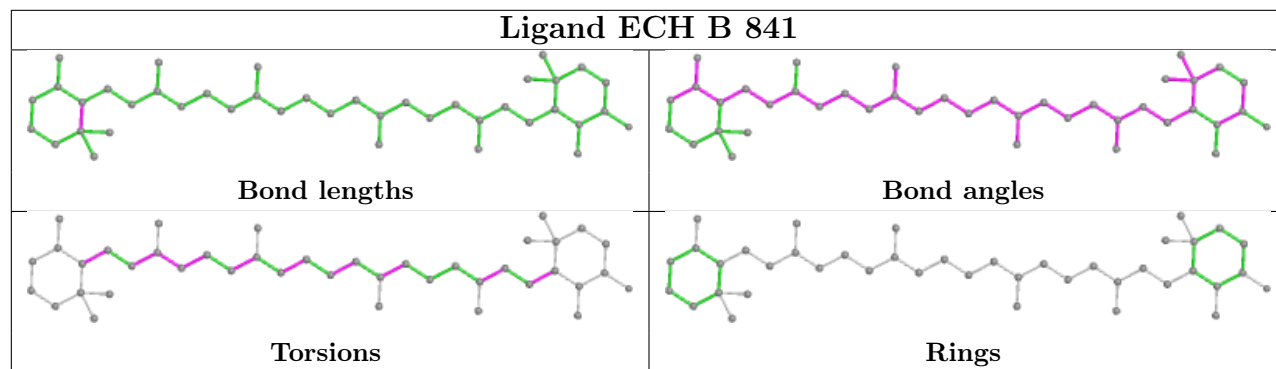
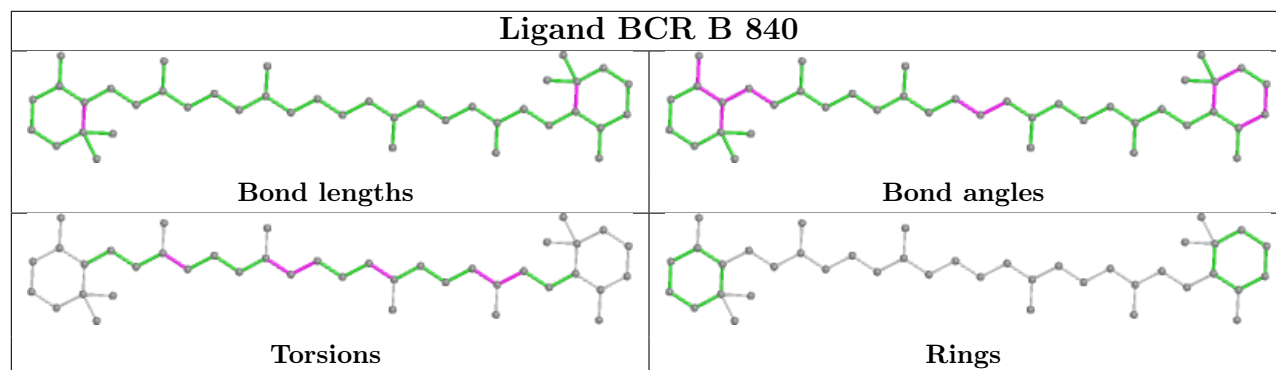
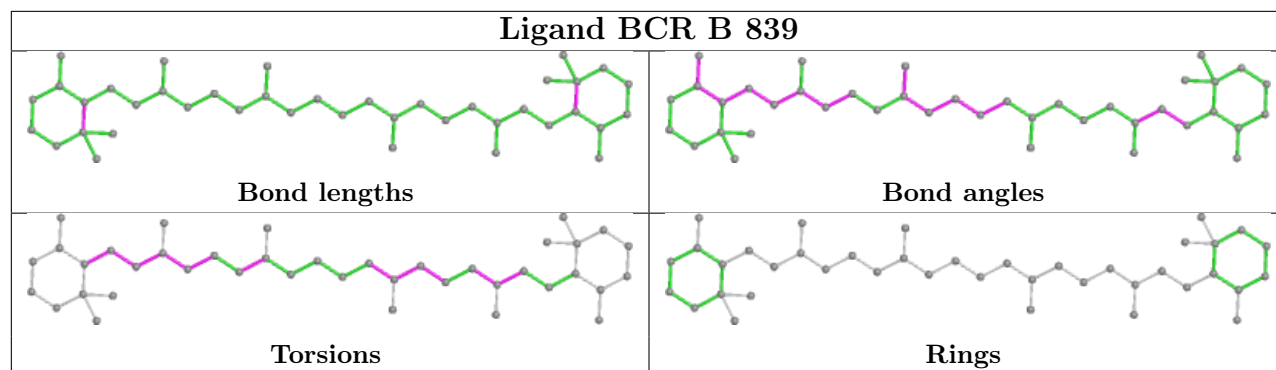


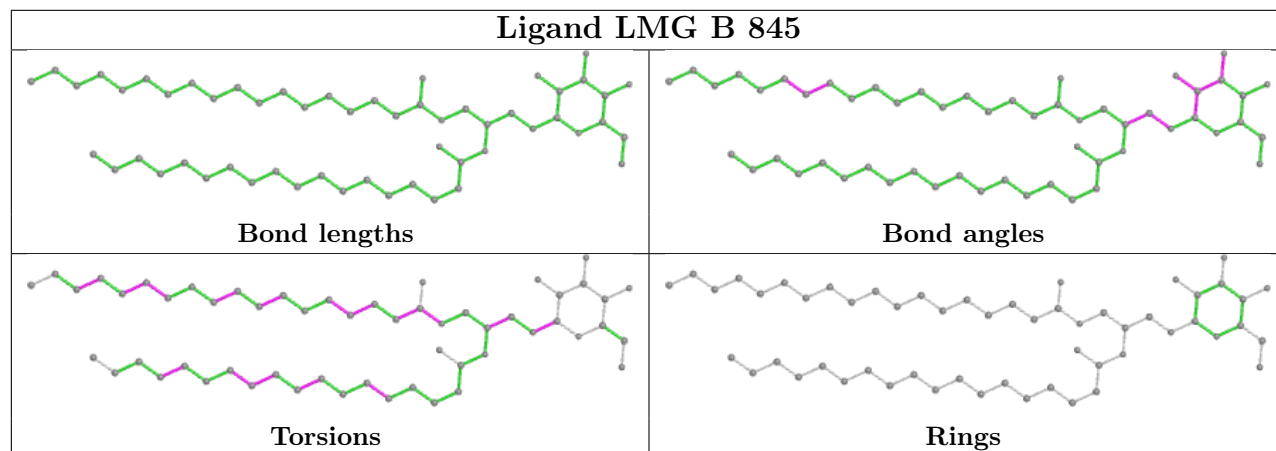
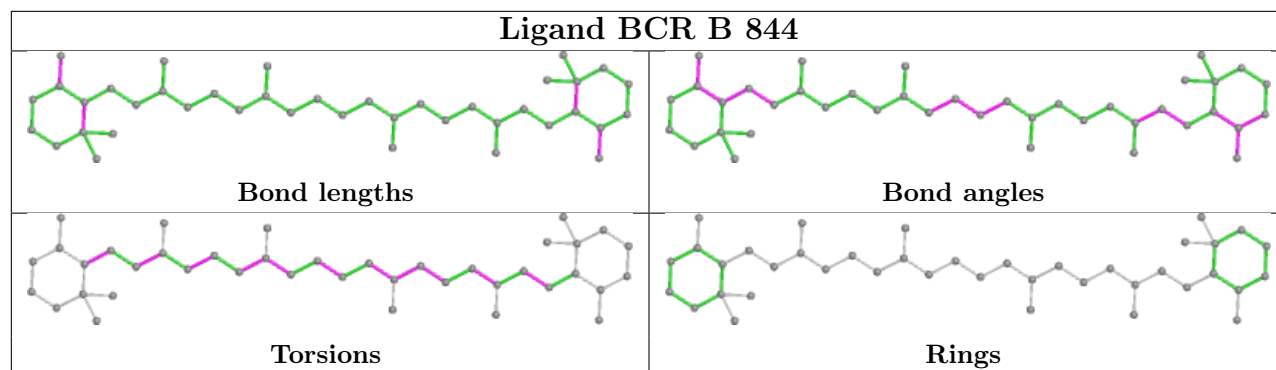
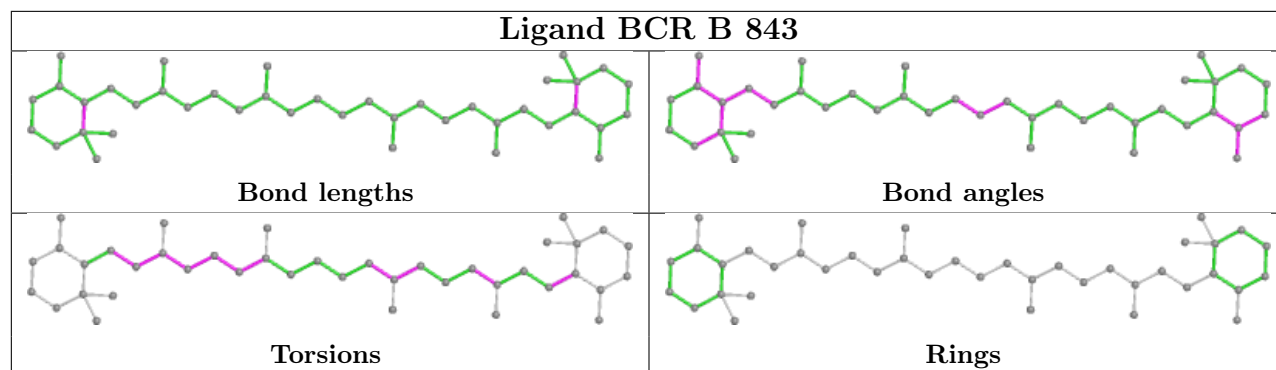
Ligand CLA B 837



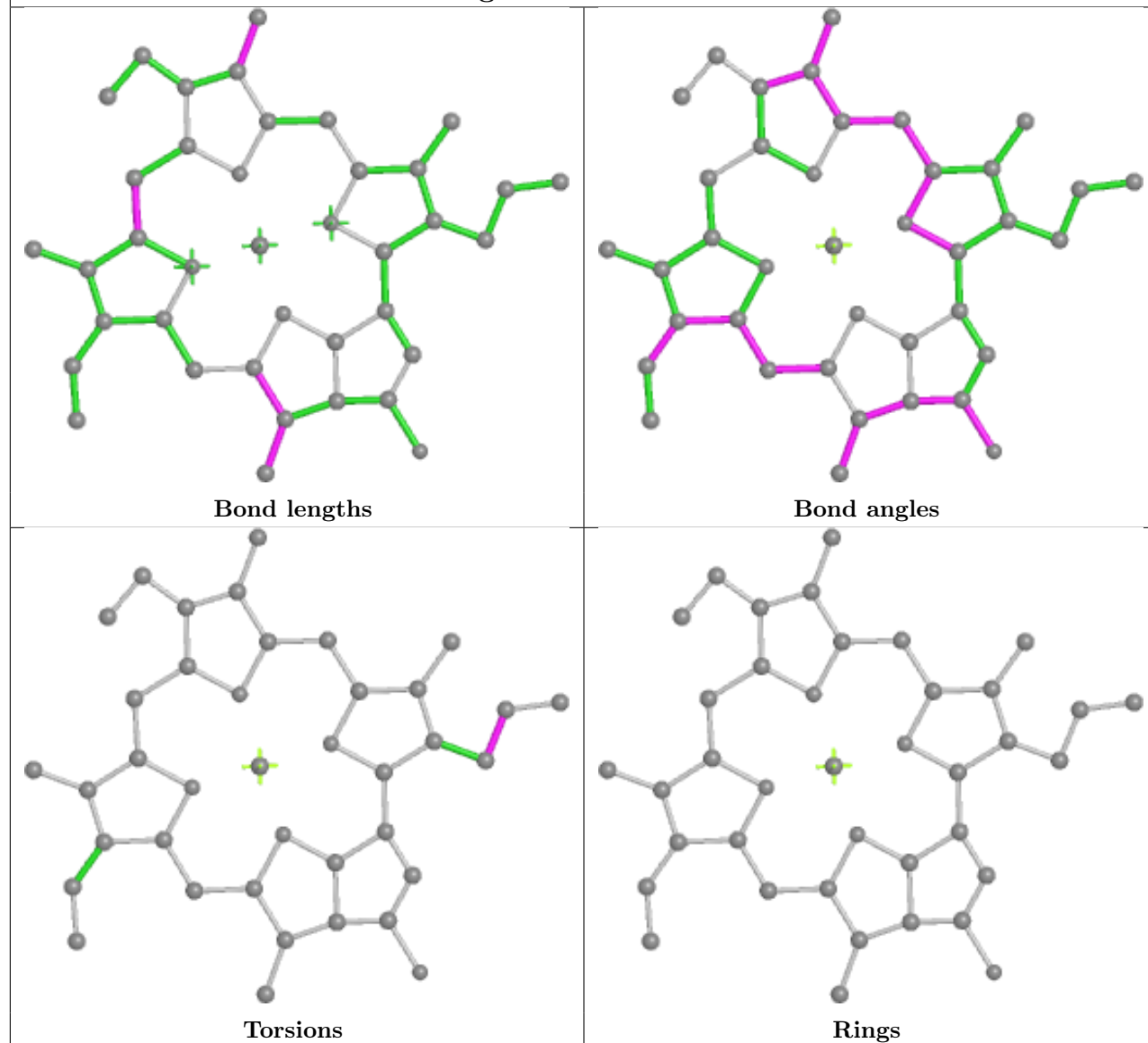
Ligand PQN B 838



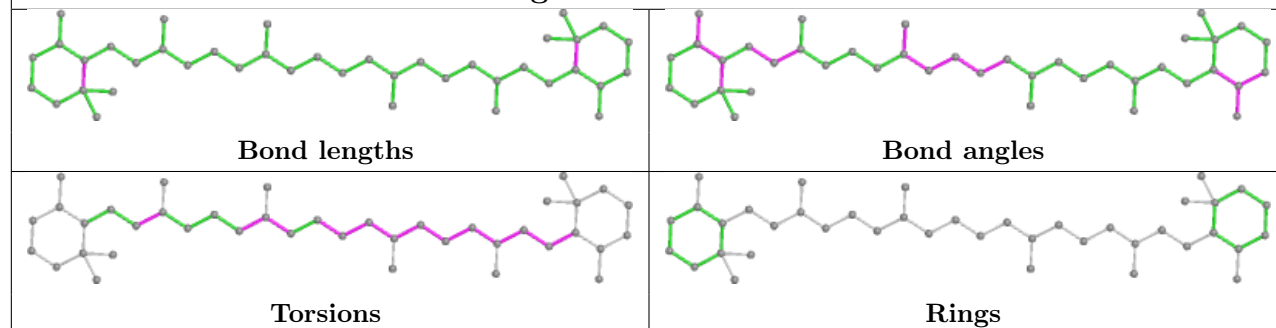




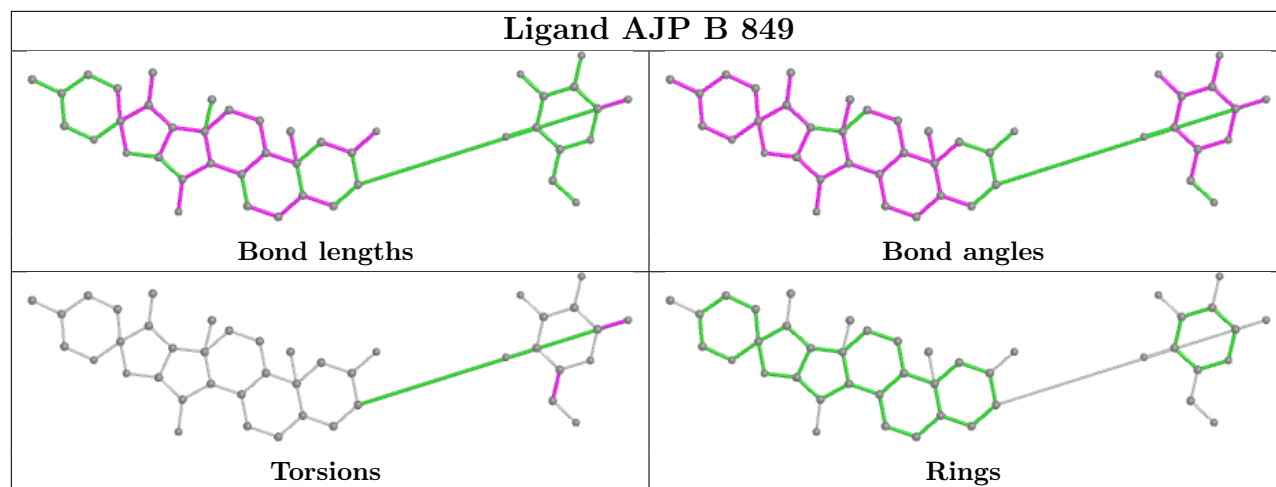
Ligand CLA B 846



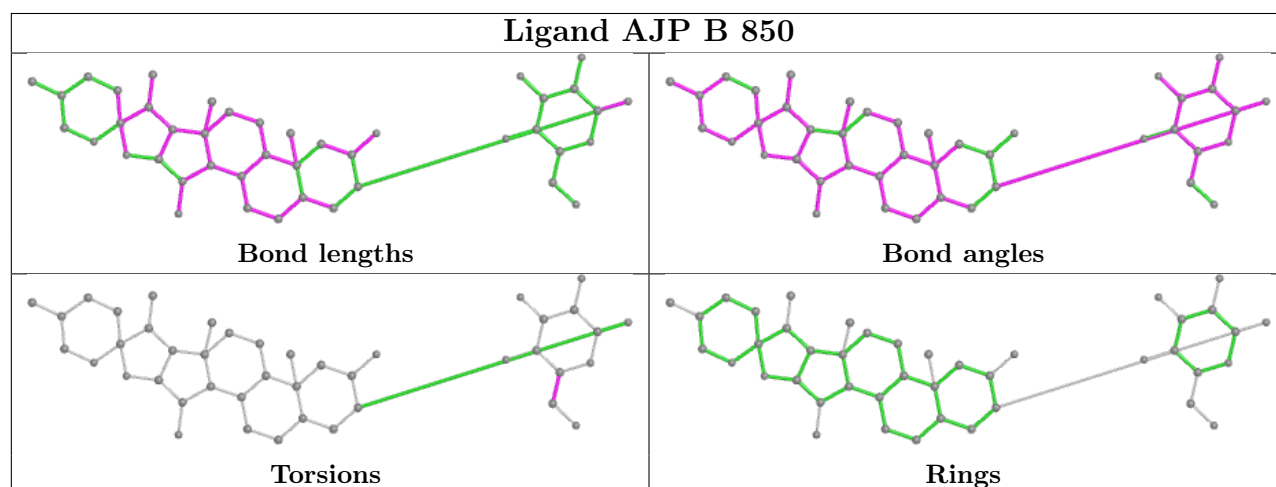
Ligand BCR B 848



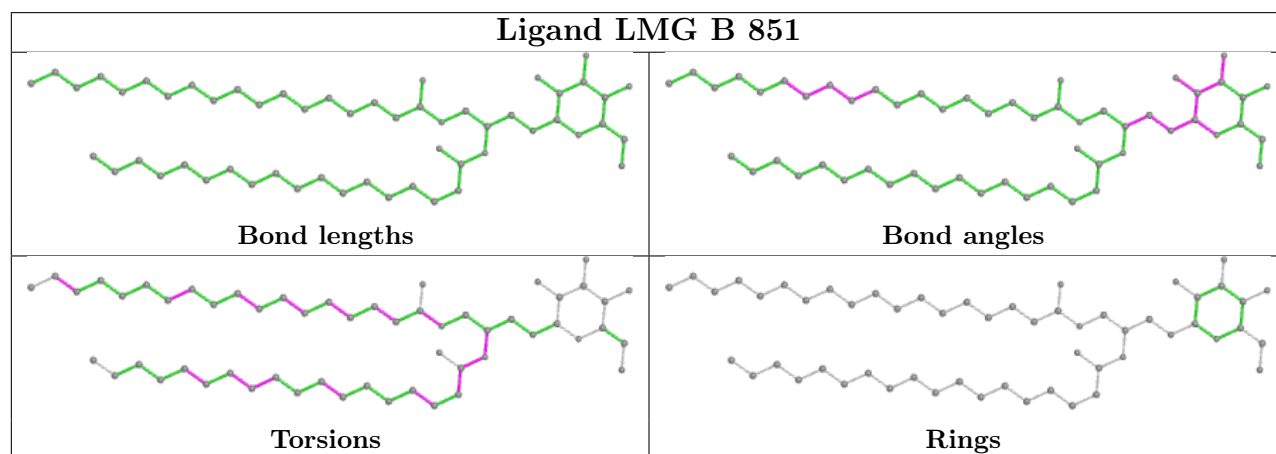
Ligand AJP B 849

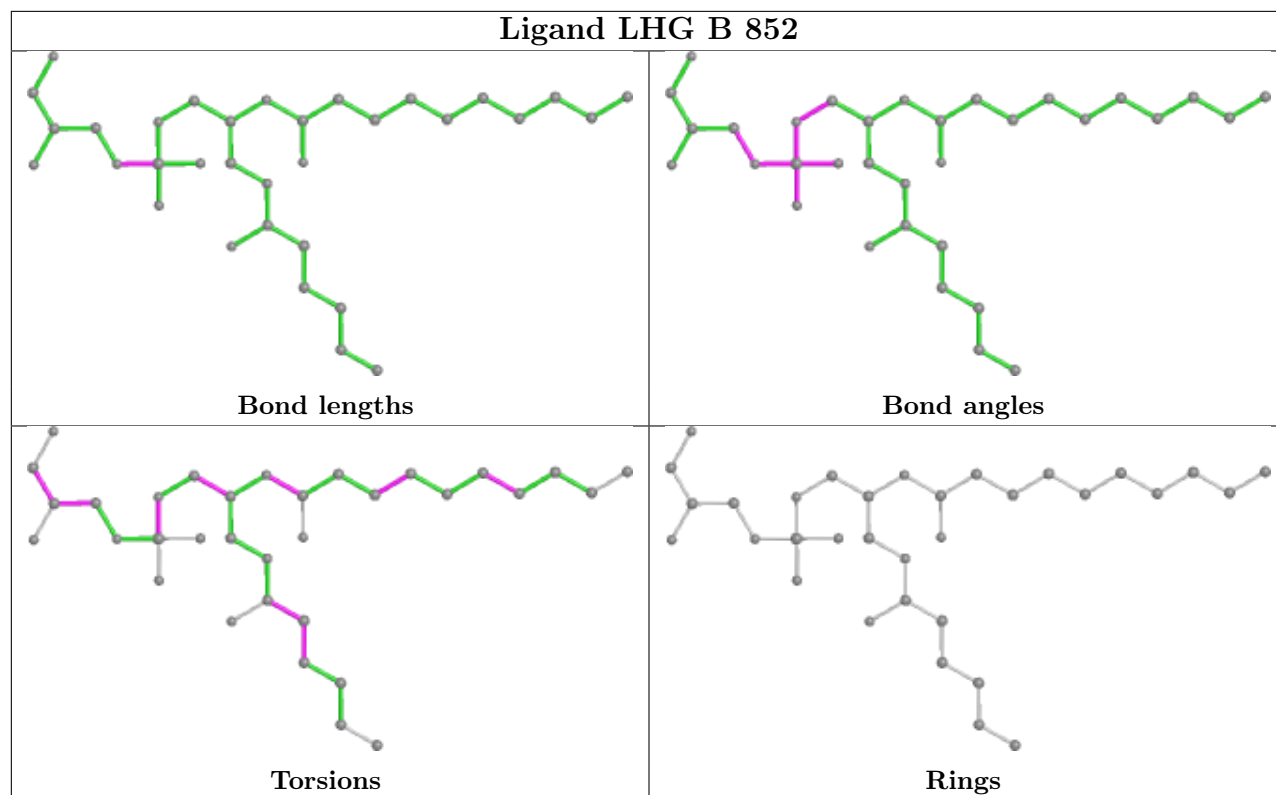


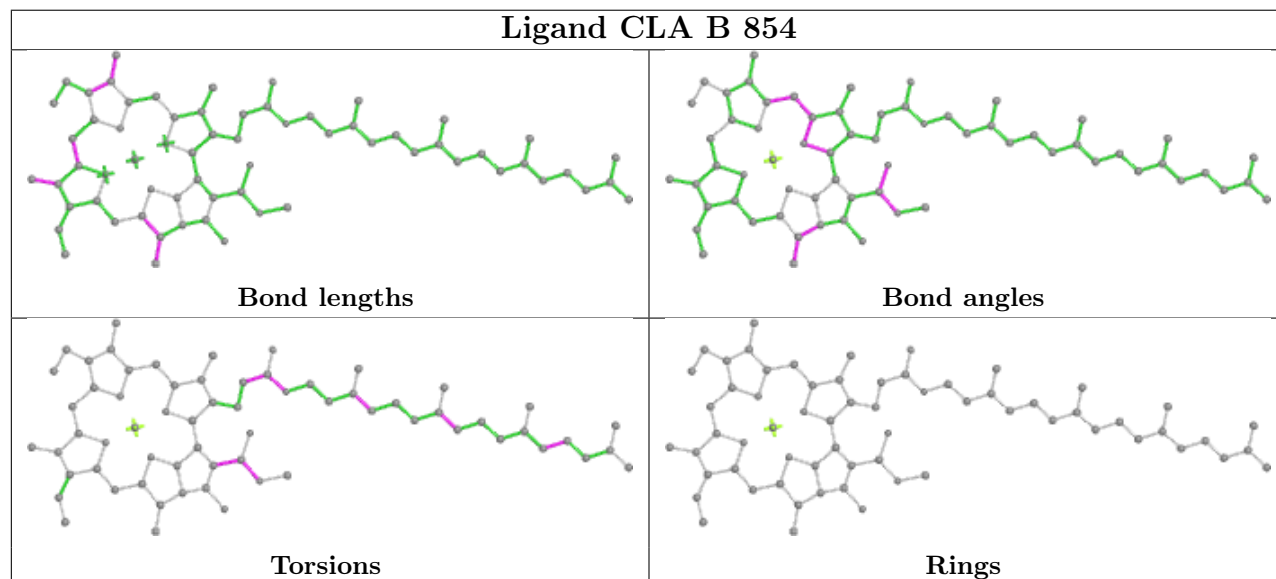
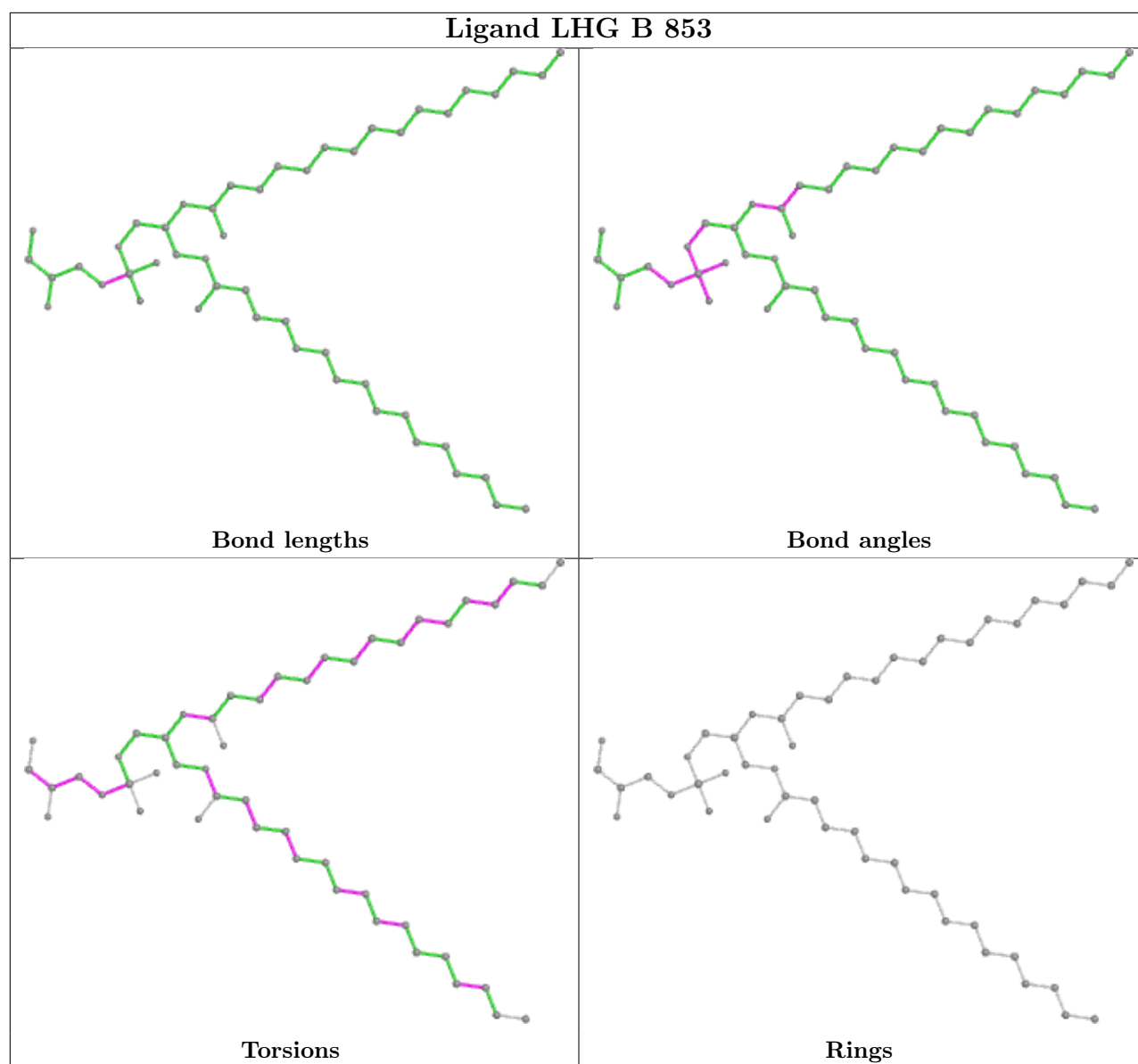
Ligand AJP B 850

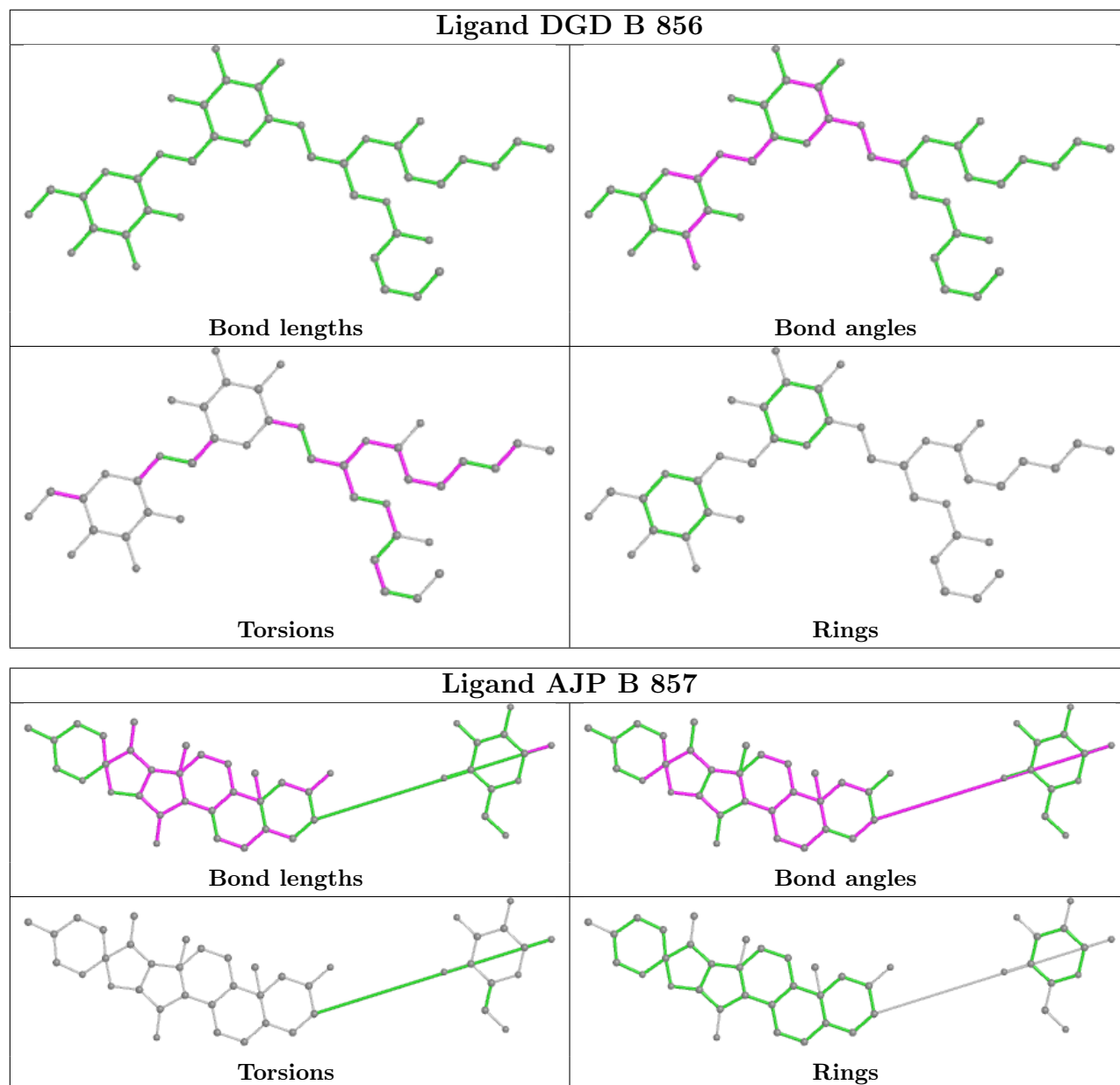


Ligand LMG B 851

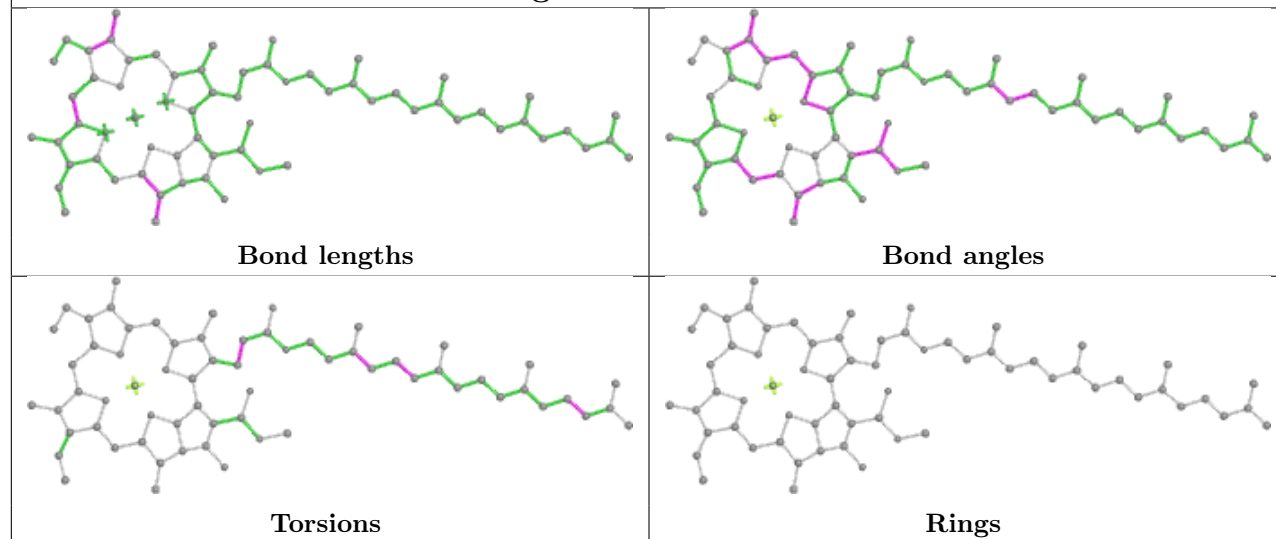




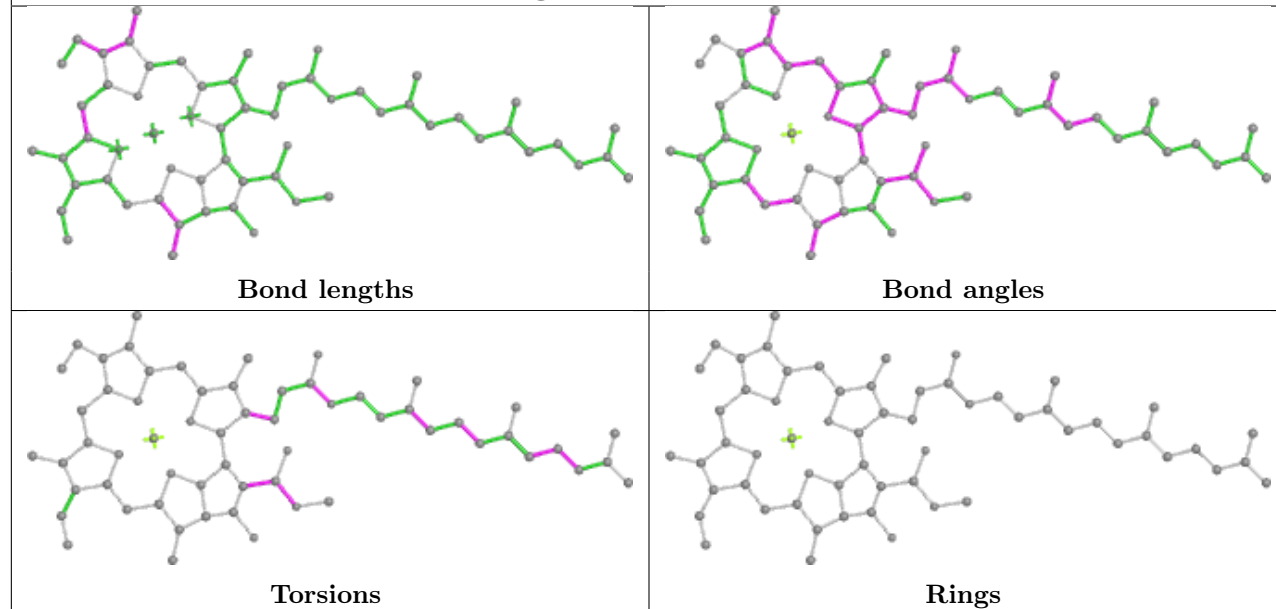




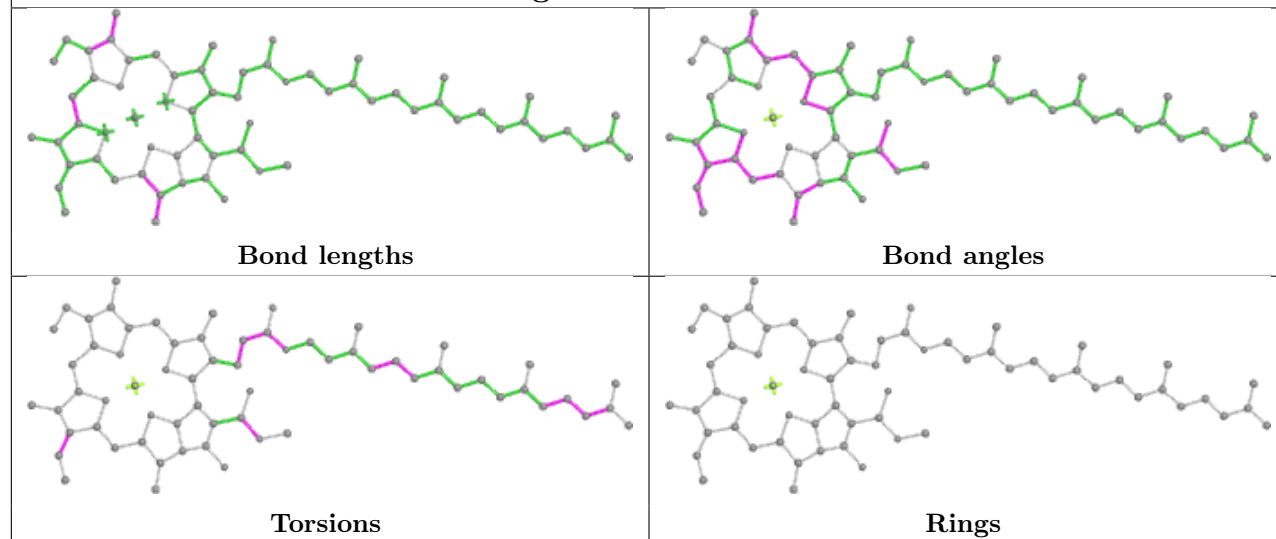
Ligand CLA B 858



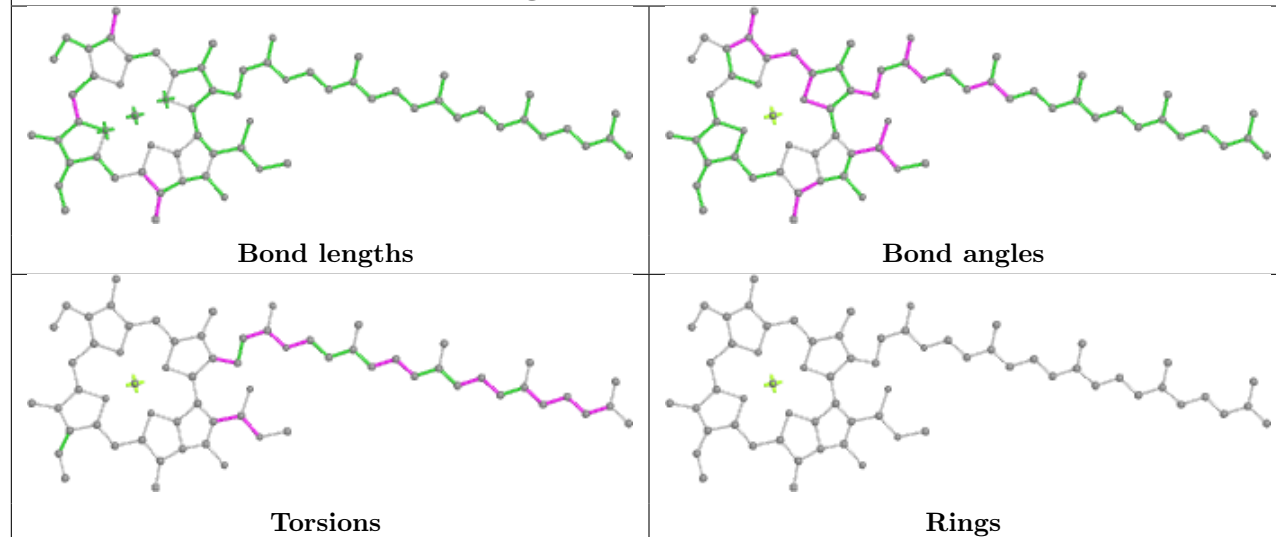
Ligand CLA B 859



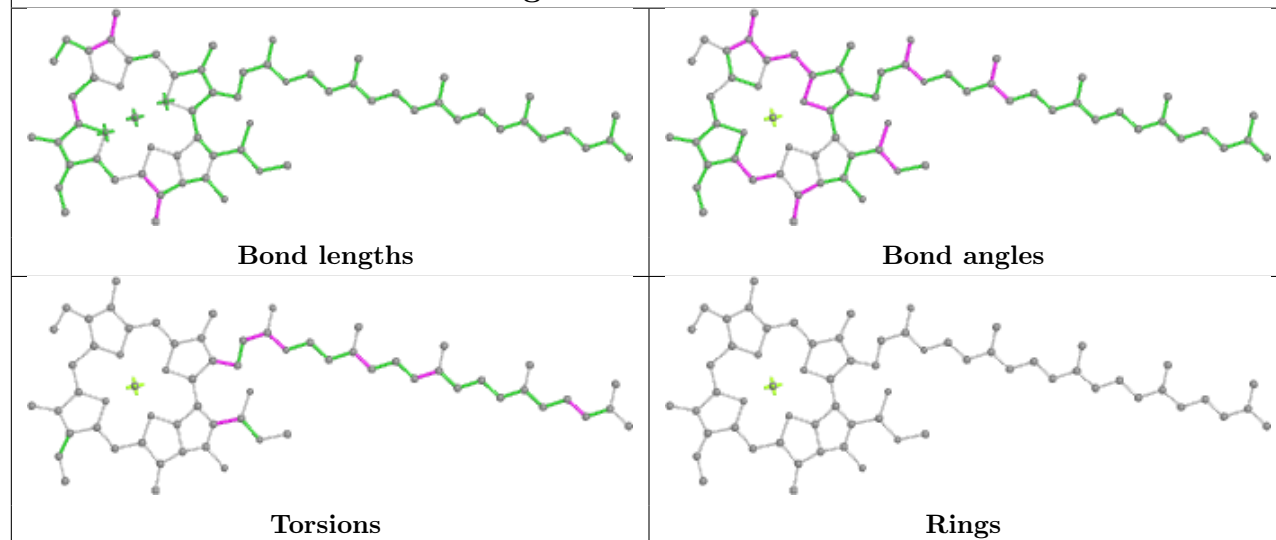
Ligand CLA B 860



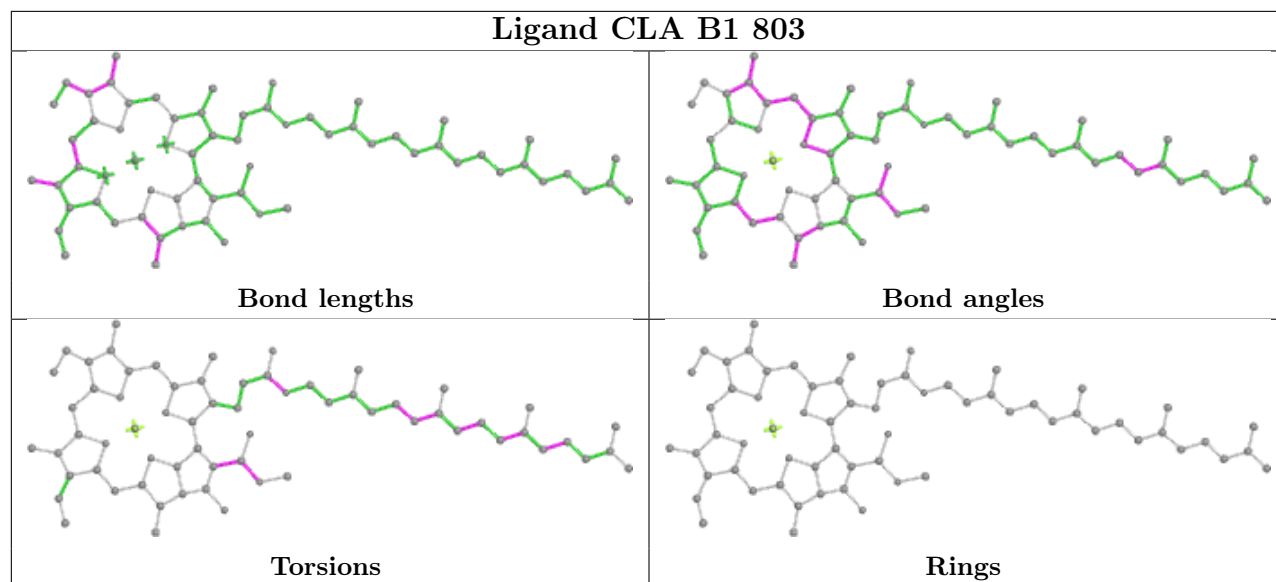
Ligand CLA B1 801



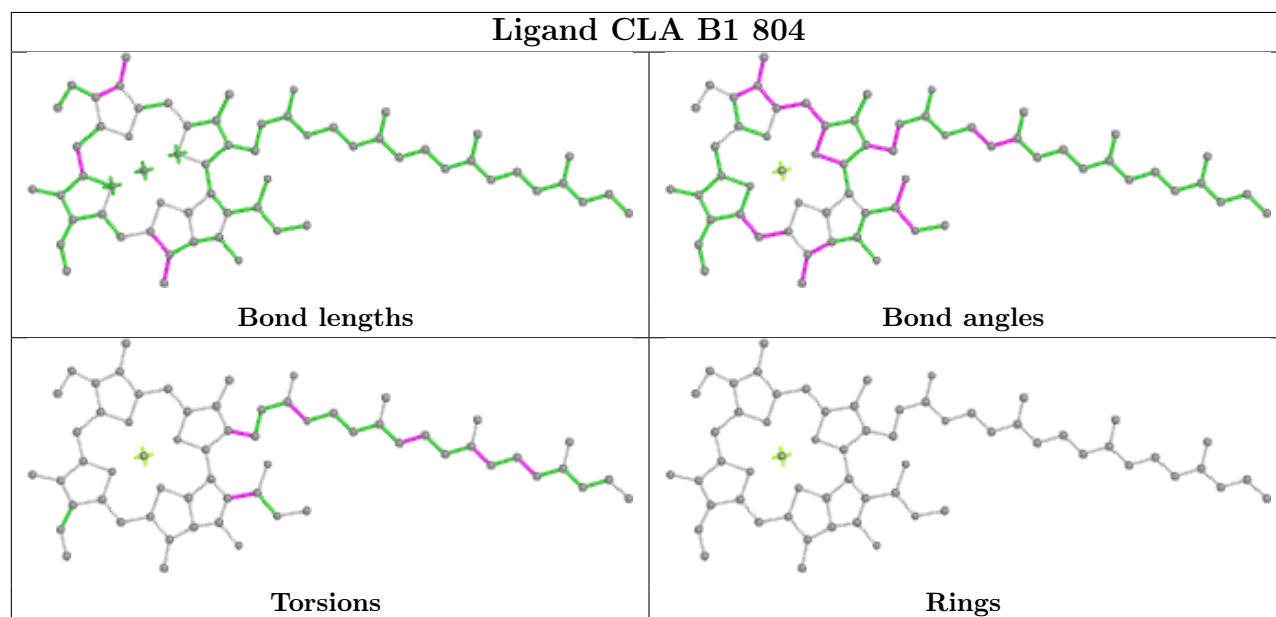
Ligand CLA B1 802

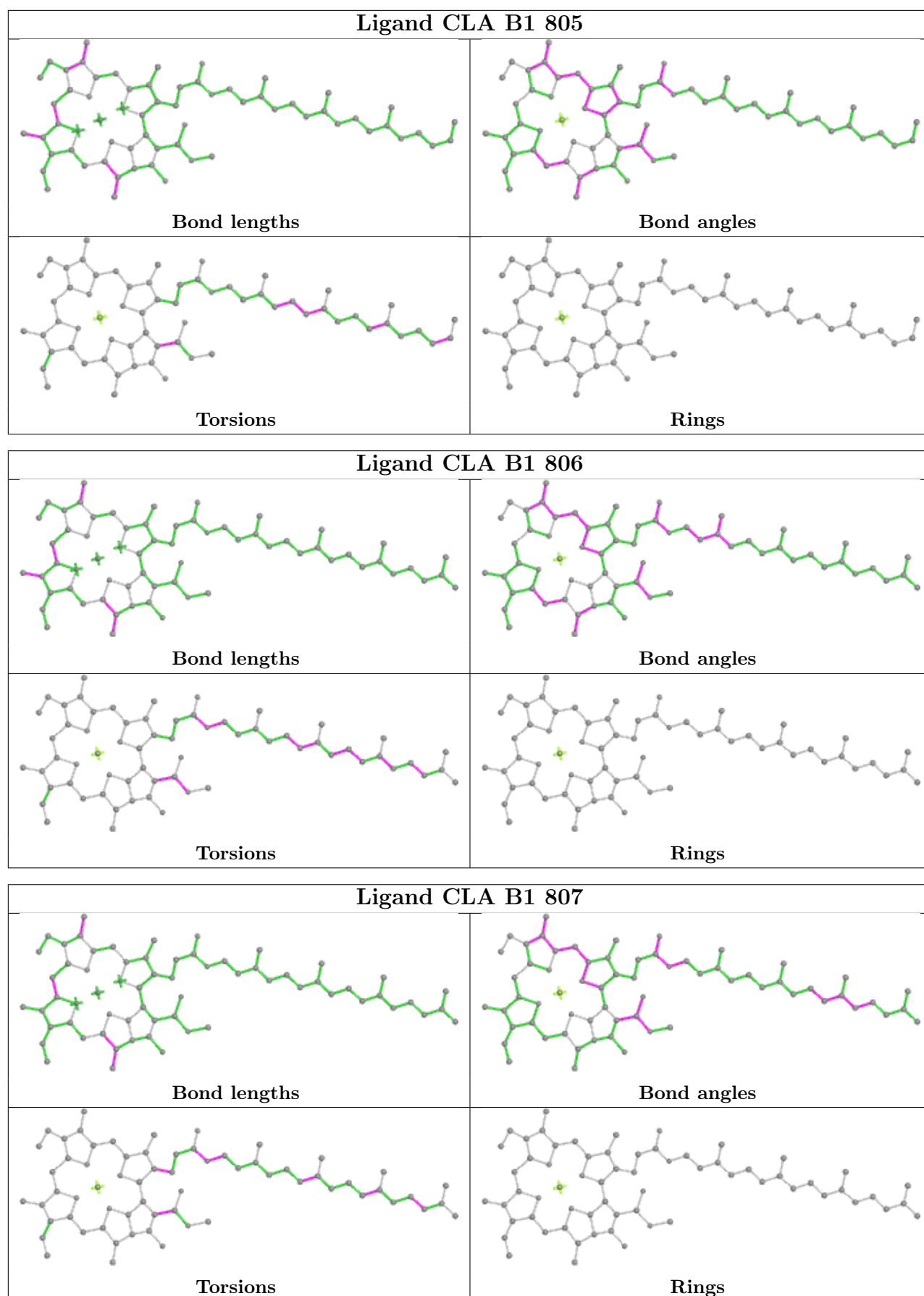


Ligand CLA B1 803

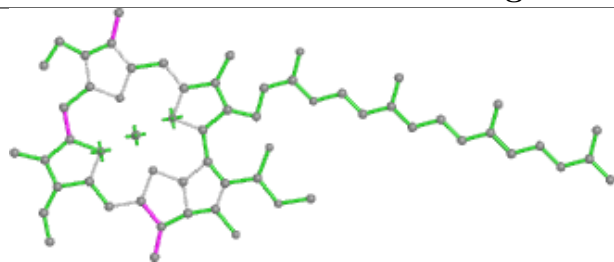


Ligand CLA B1 804

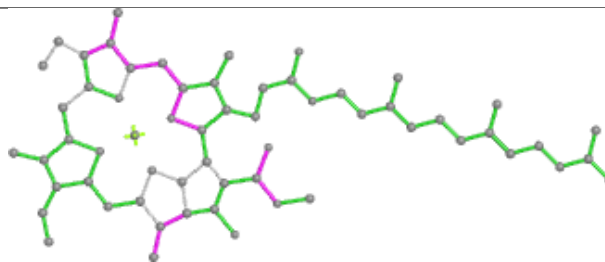




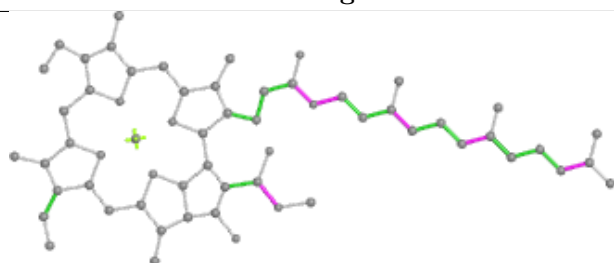
Ligand CLA B1 808



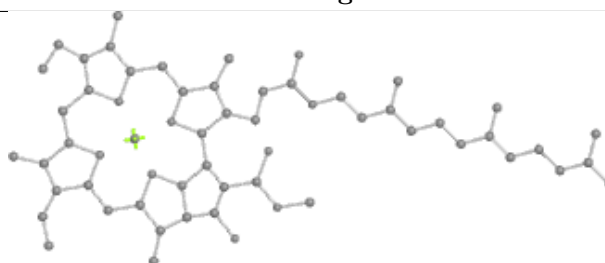
Bond lengths



Bond angles

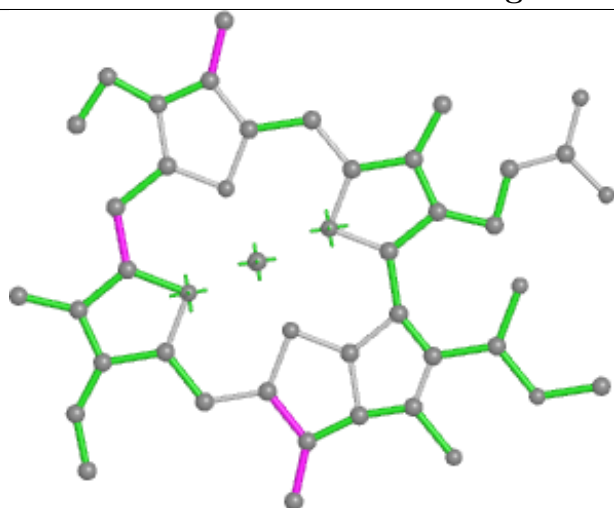


Torsions

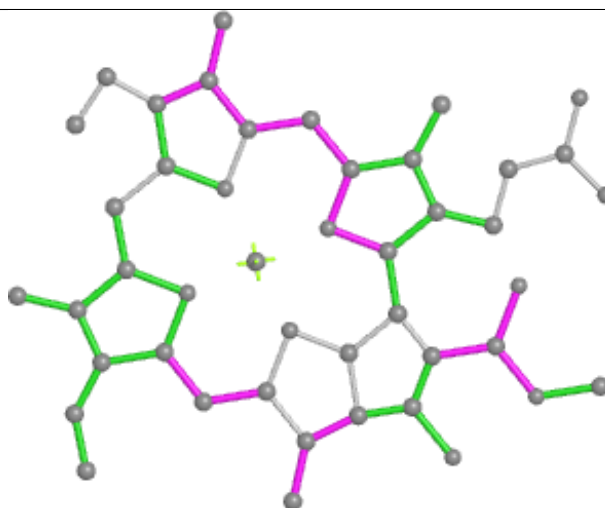


Rings

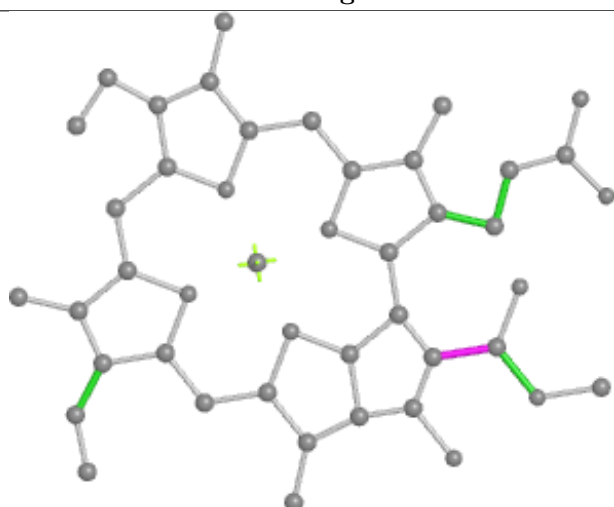
Ligand CLA B1 809



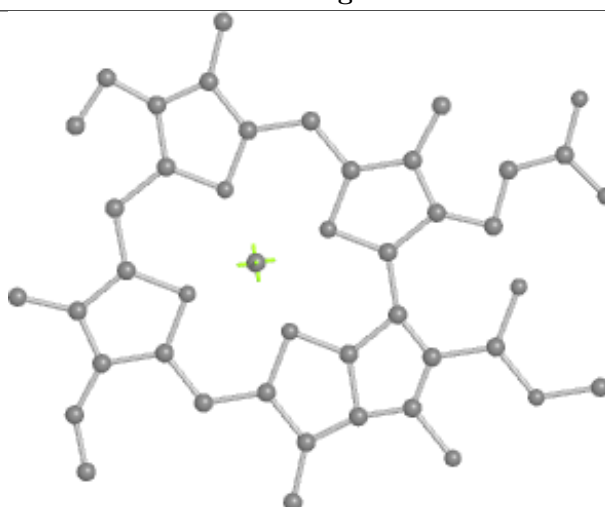
Bond lengths



Bond angles

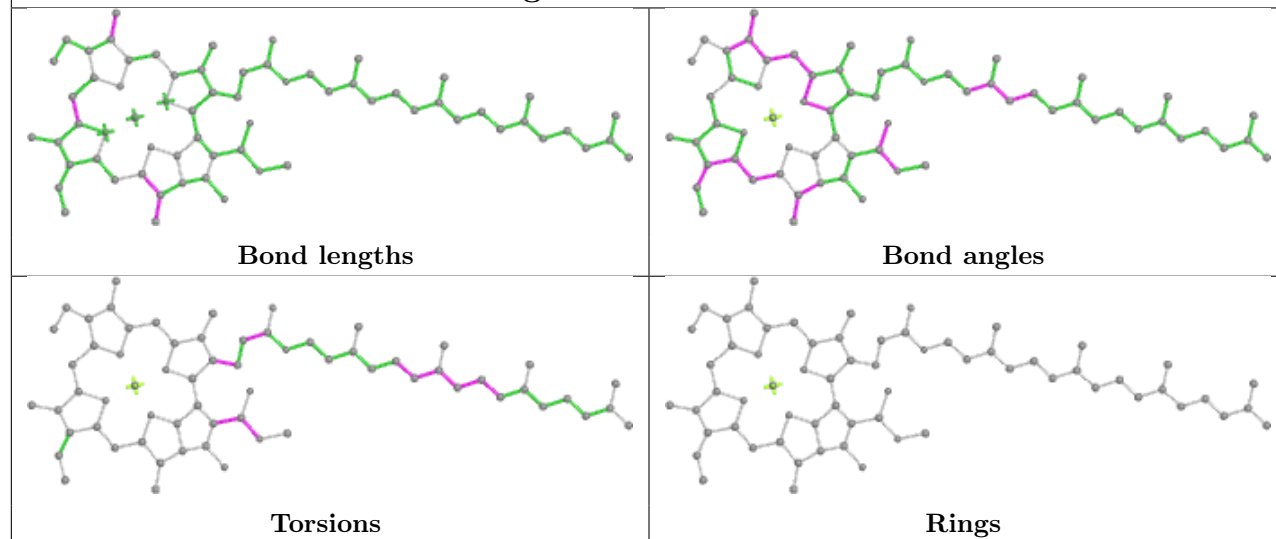


Torsions

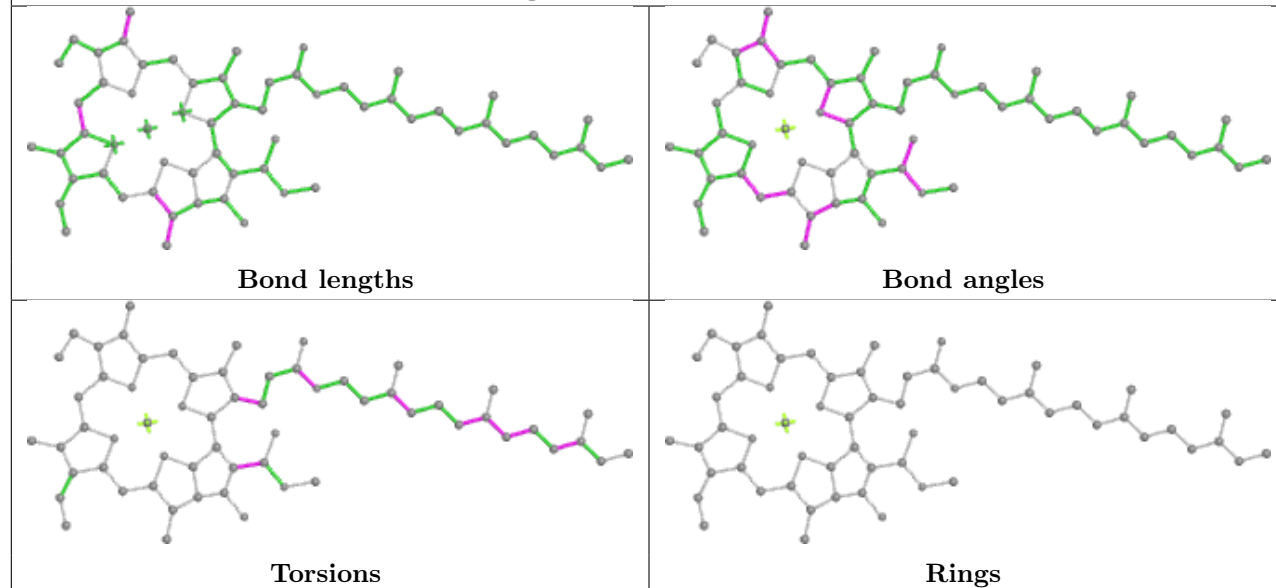


Rings

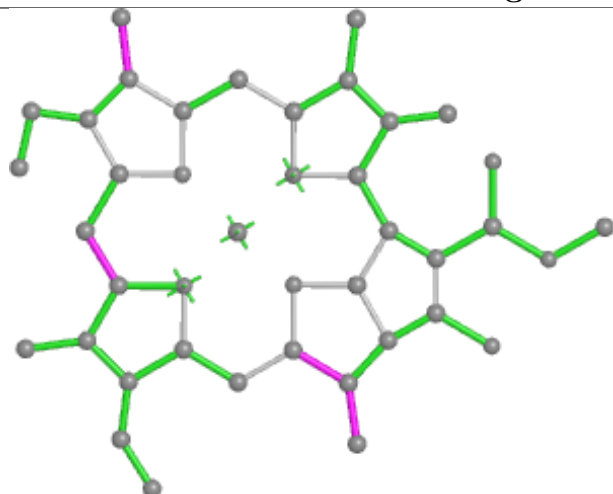
Ligand CLA B1 810



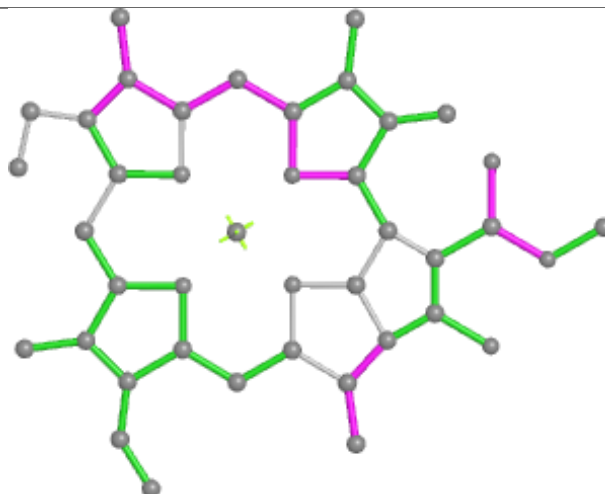
Ligand CLA B1 811



Ligand CLA B1 812



Bond lengths



Bond angles

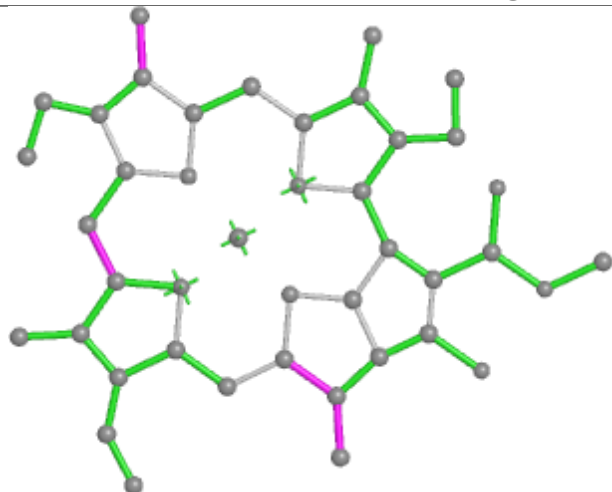


Torsions

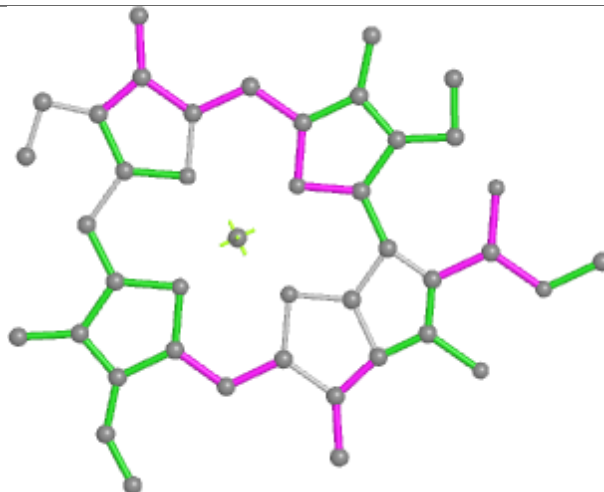


Rings

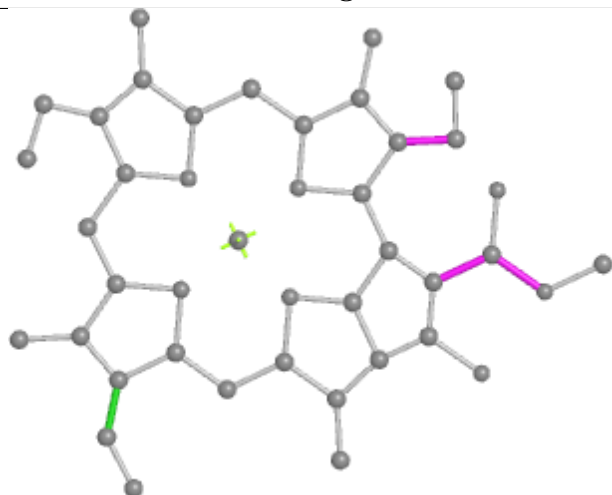
Ligand CLA B1 813



Bond lengths



Bond angles

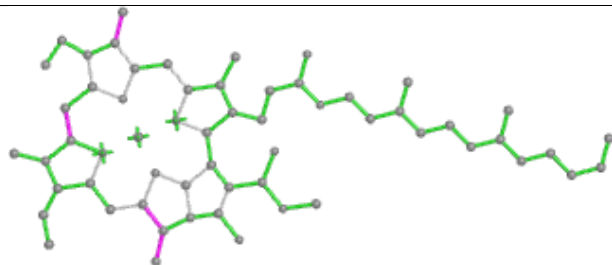


Torsions

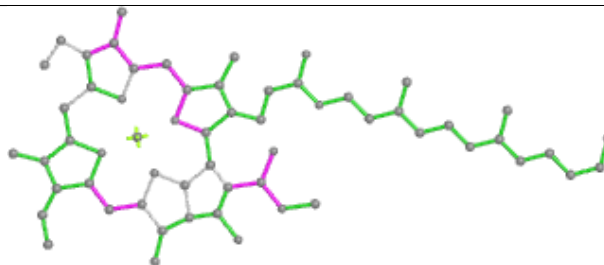


Rings

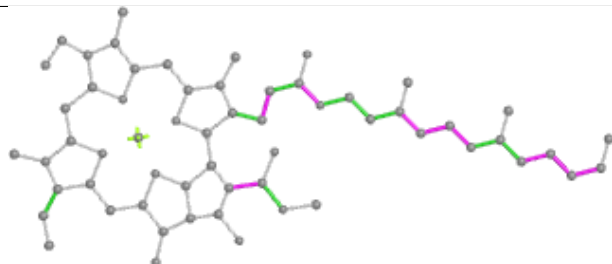
Ligand CLA B1 814



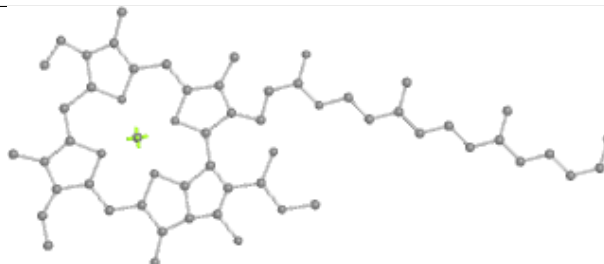
Bond lengths



Bond angles

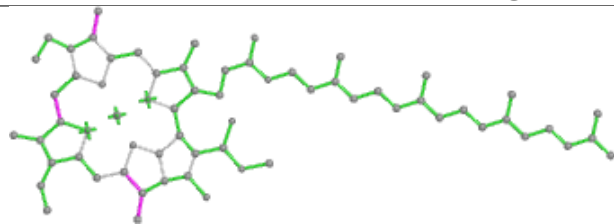


Torsions

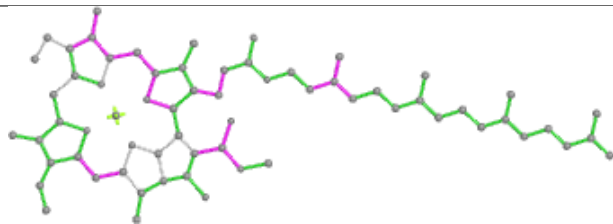


Rings

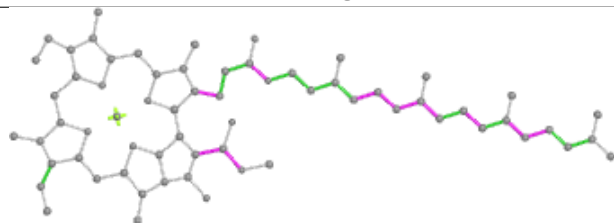
Ligand CLA B1 815



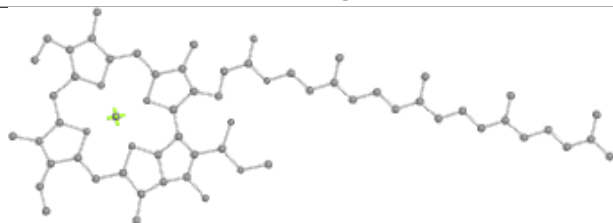
Bond lengths



Bond angles

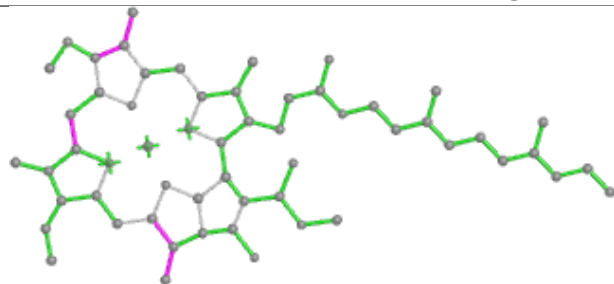


Torsions

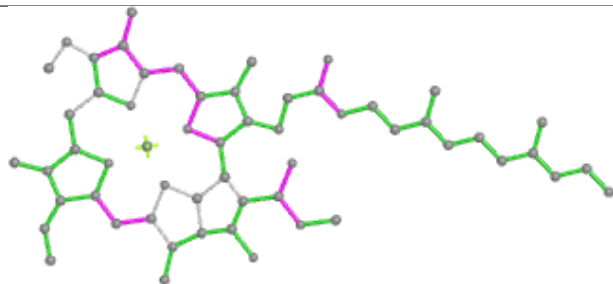


Rings

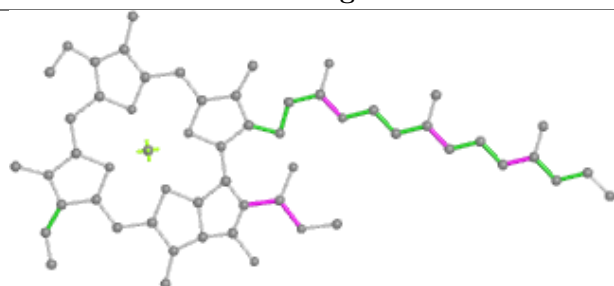
Ligand CLA B1 816



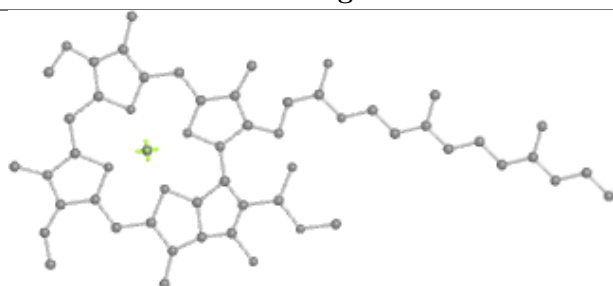
Bond lengths



Bond angles

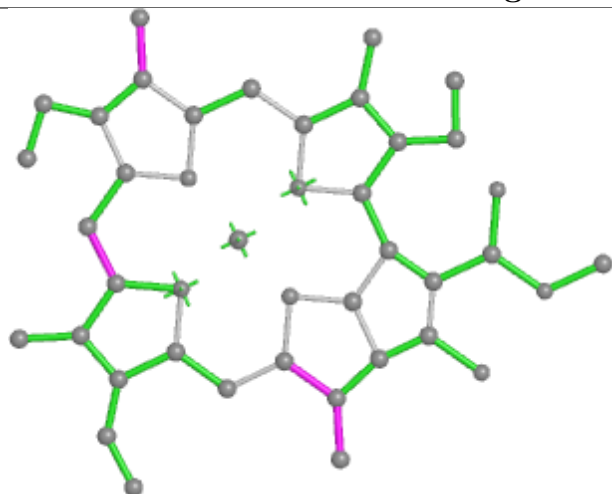


Torsions

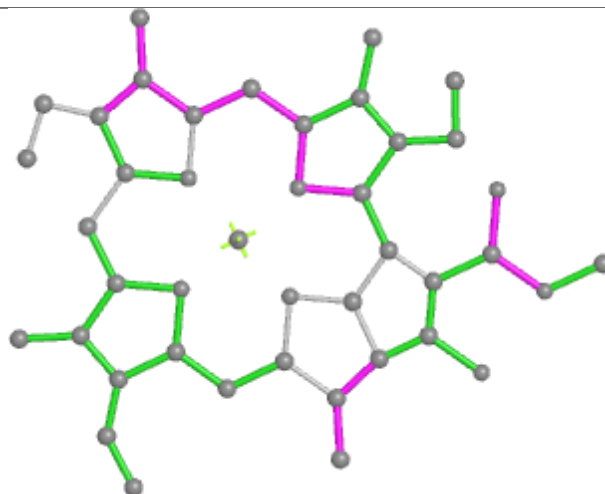


Rings

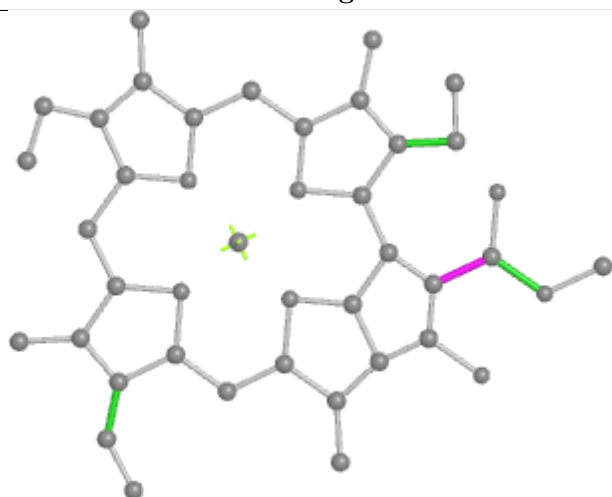
Ligand CLA B1 817



Bond lengths



Bond angles

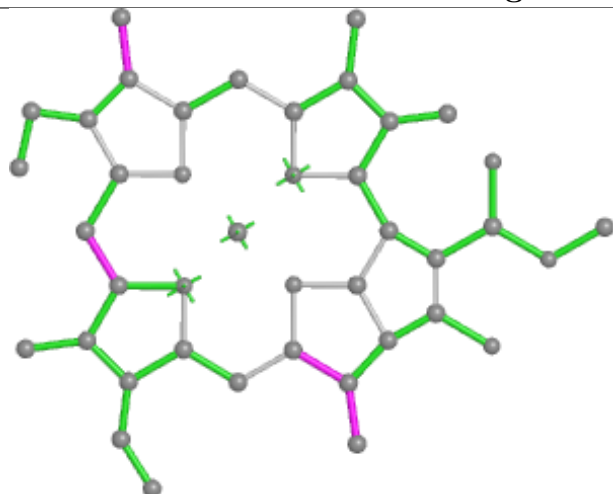


Torsions

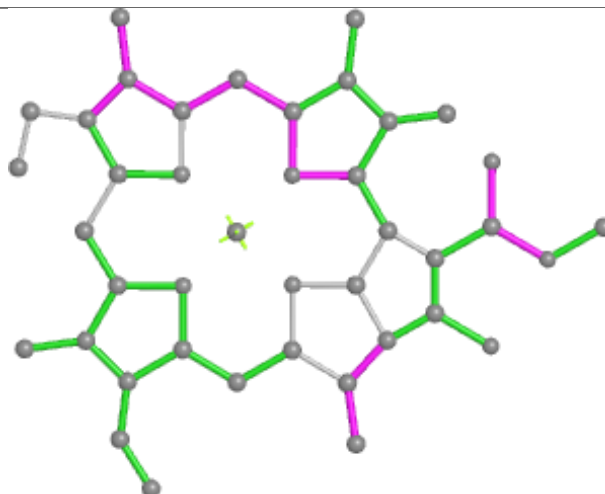


Rings

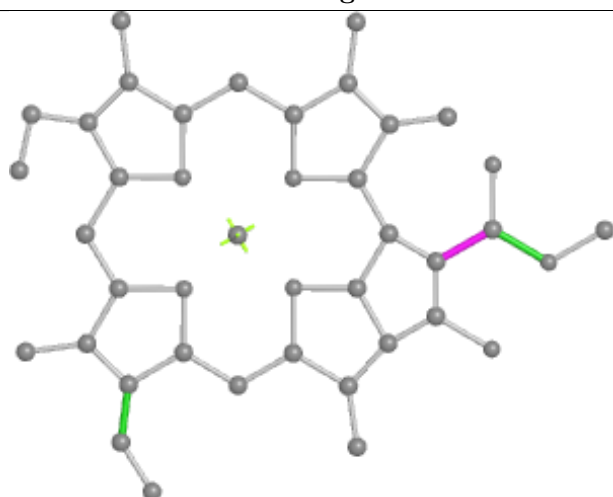
Ligand CLA B1 818



Bond lengths



Bond angles

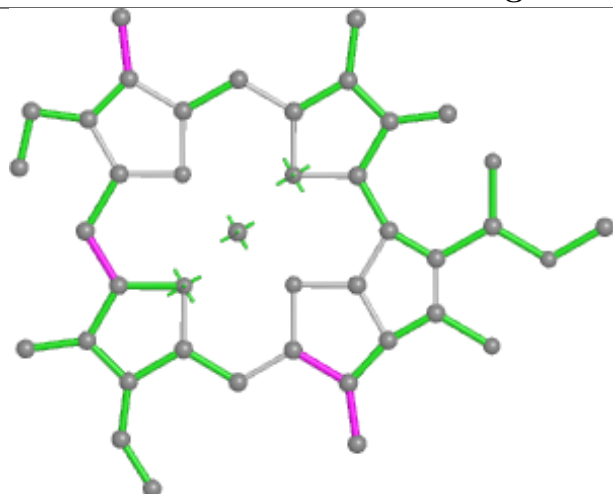


Torsions

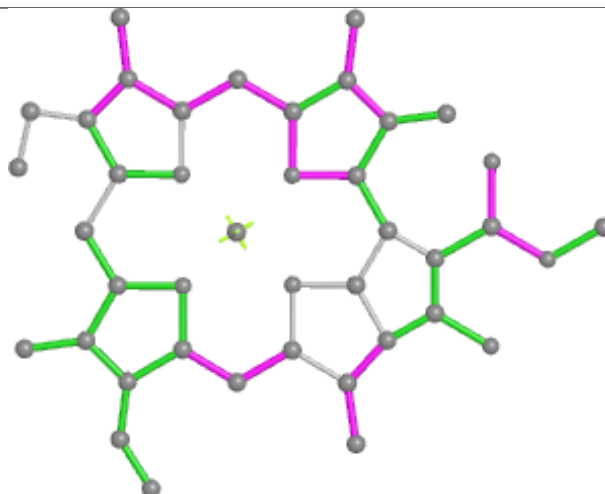


Rings

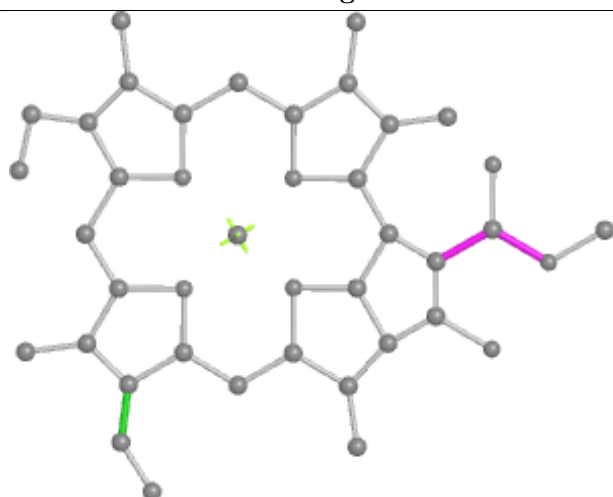
Ligand CLA B1 819



Bond lengths



Bond angles

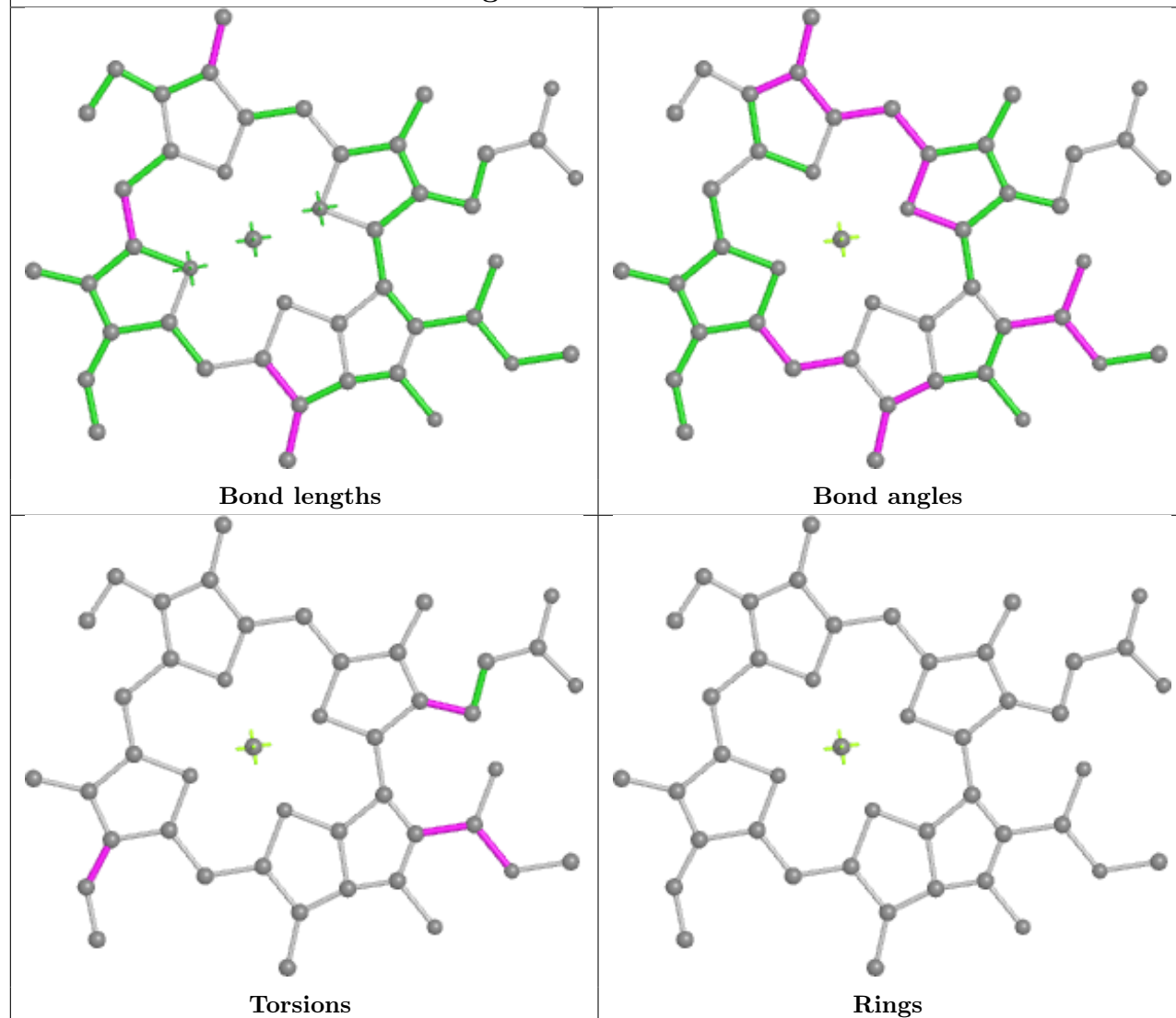


Torsions

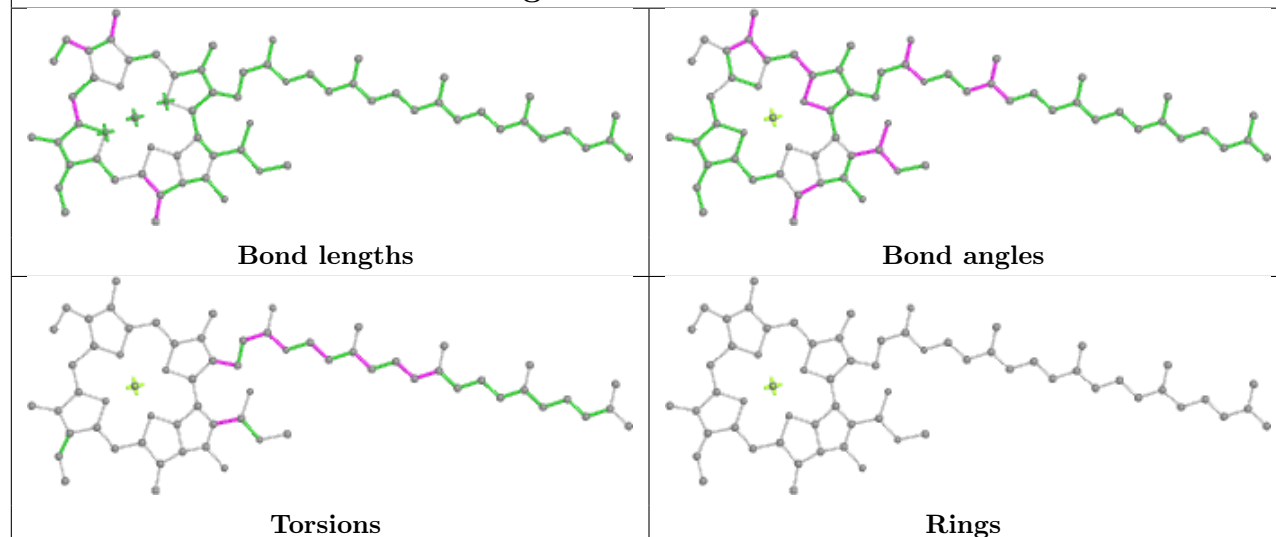


Rings

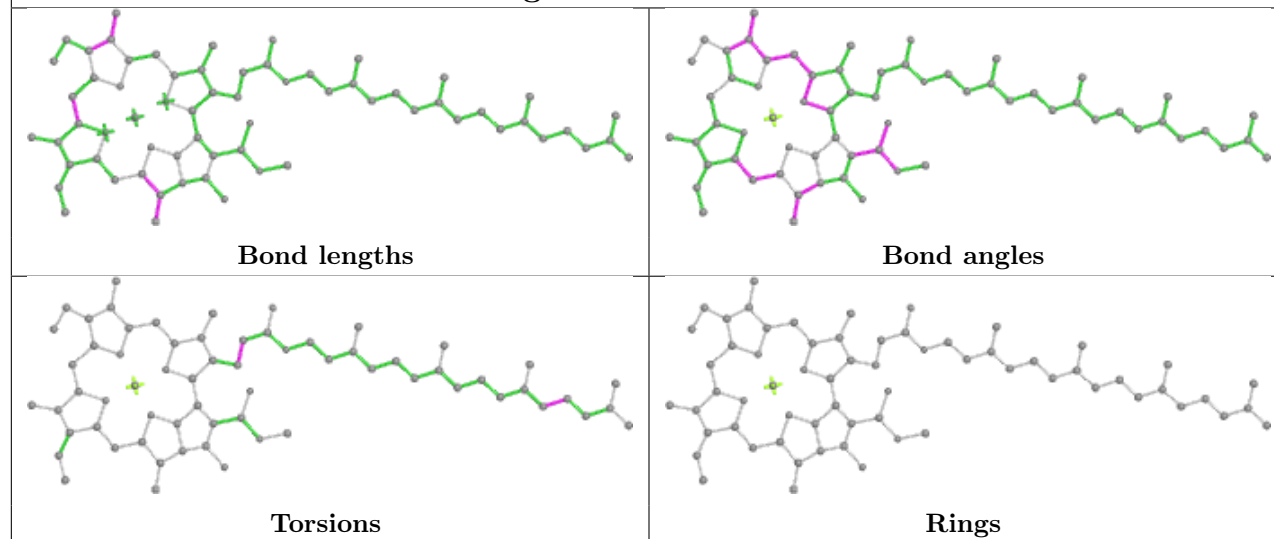
Ligand CLA B1 820



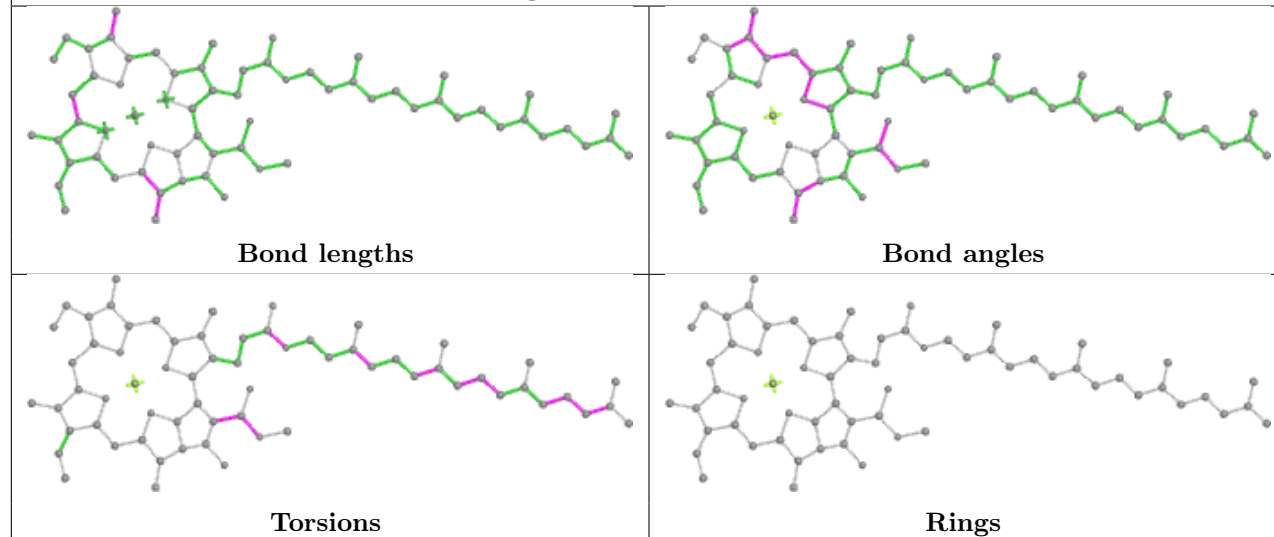
Ligand CLA B1 821

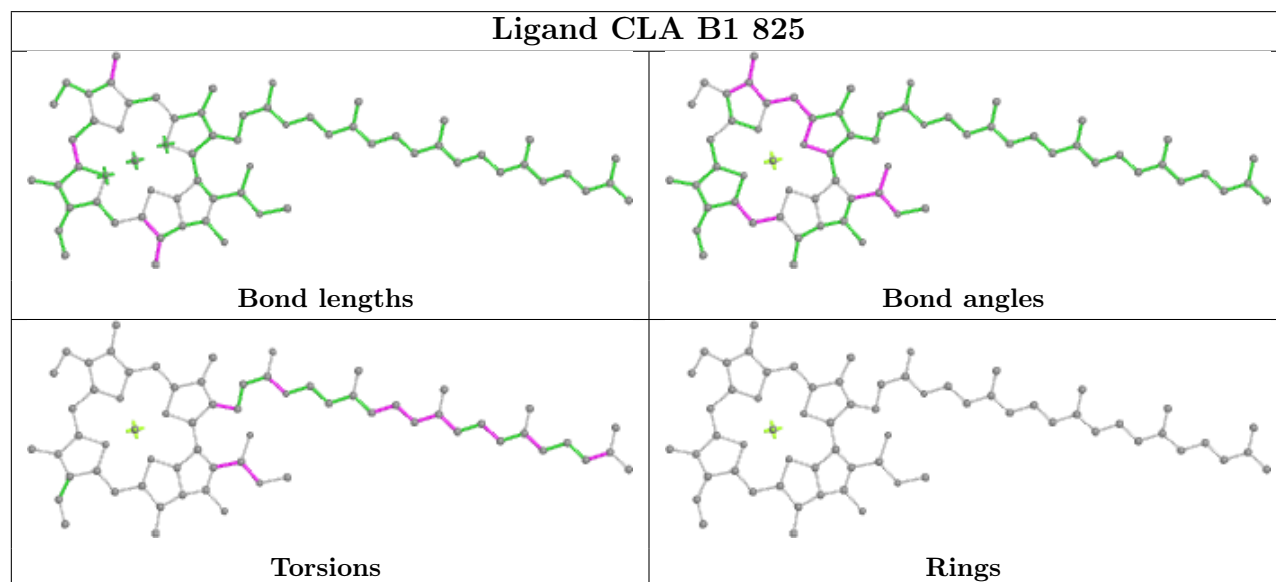
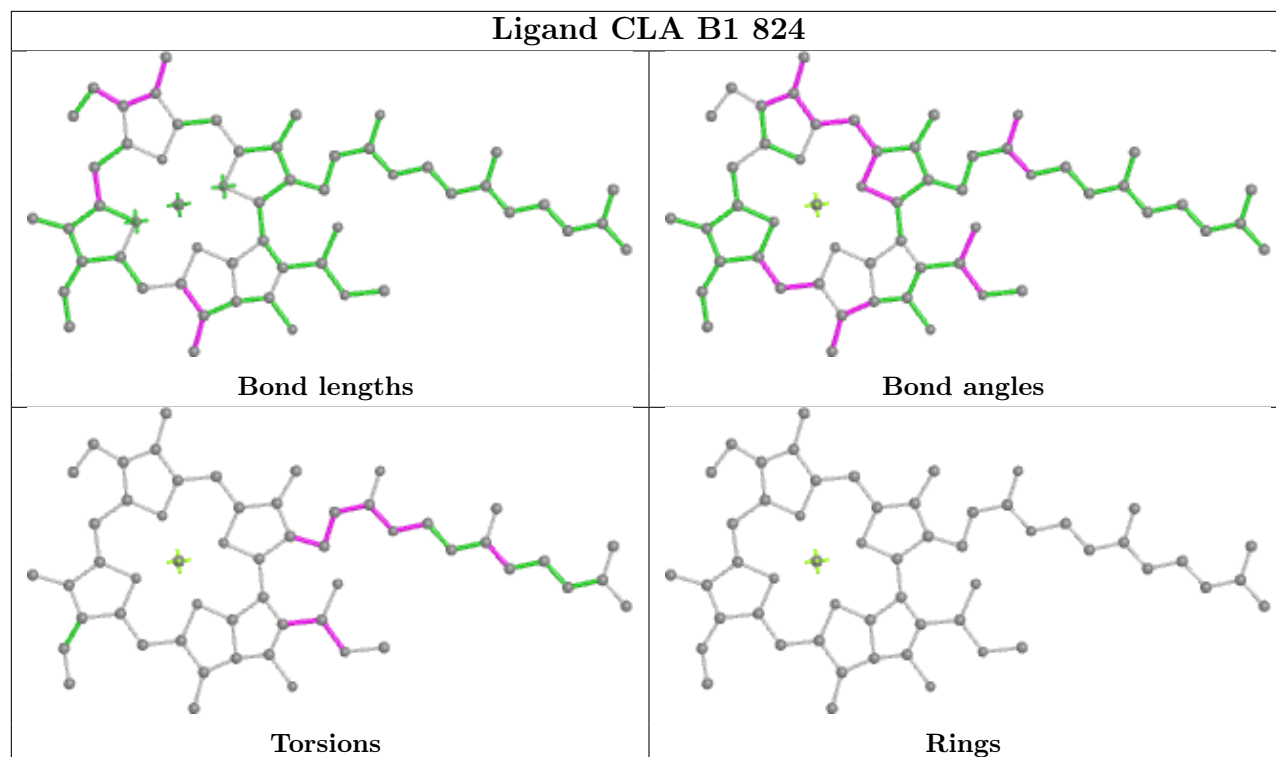


Ligand CLA B1 822

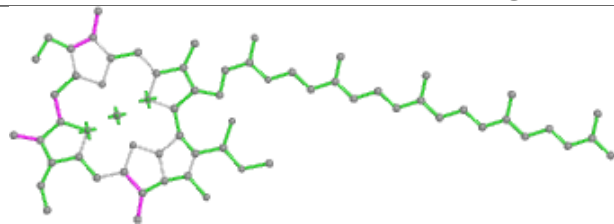


Ligand CLA B1 823

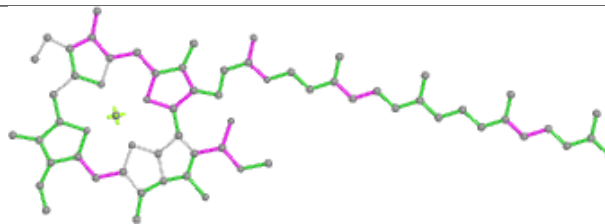




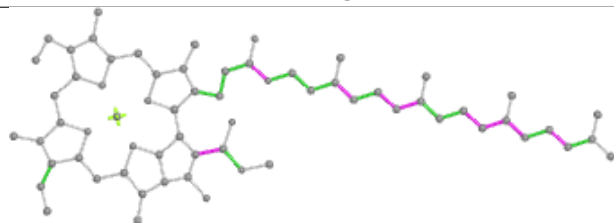
Ligand CLA B1 826



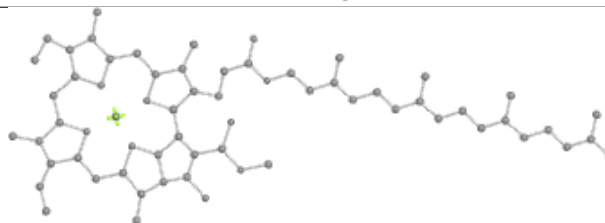
Bond lengths



Bond angles

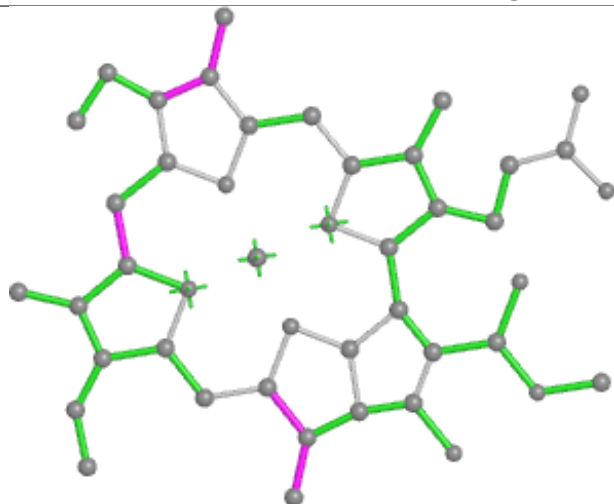


Torsions

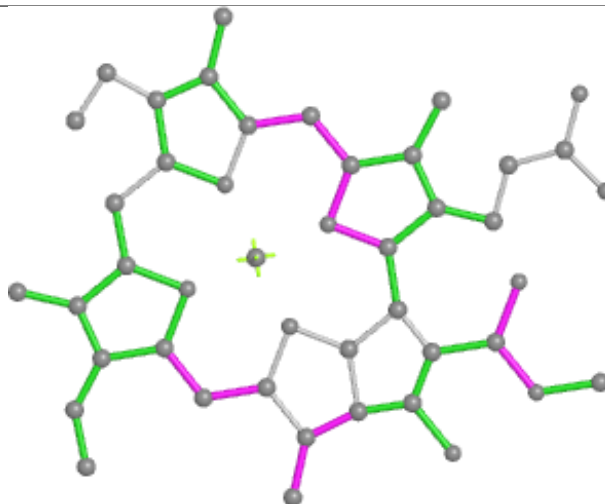


Rings

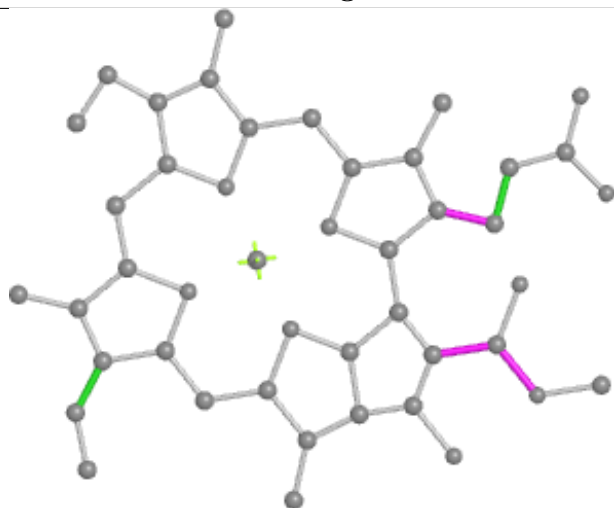
Ligand CLA B1 827



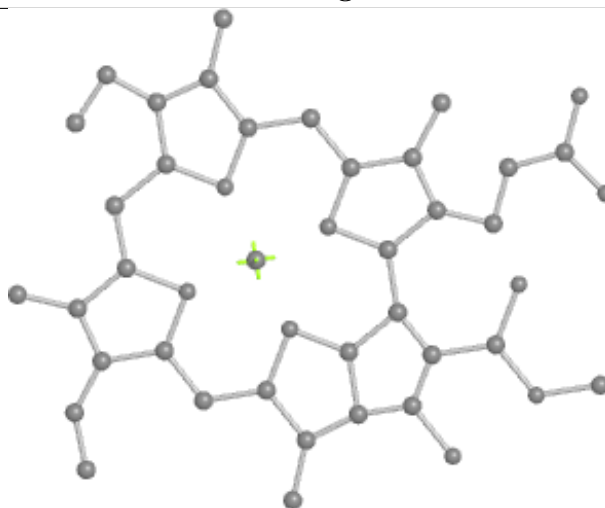
Bond lengths



Bond angles

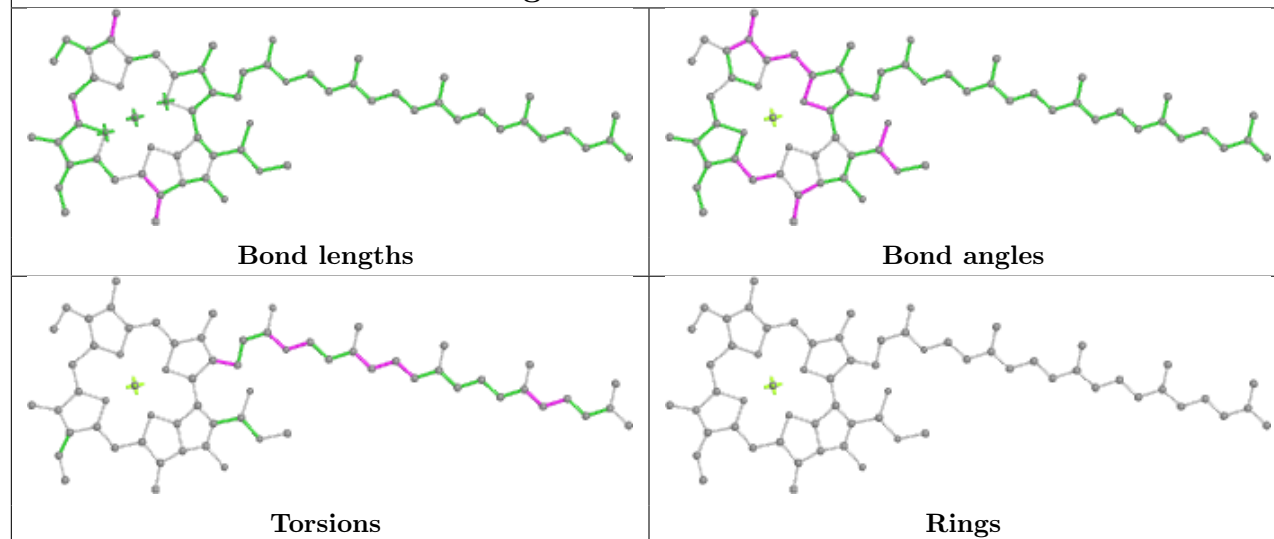


Torsions

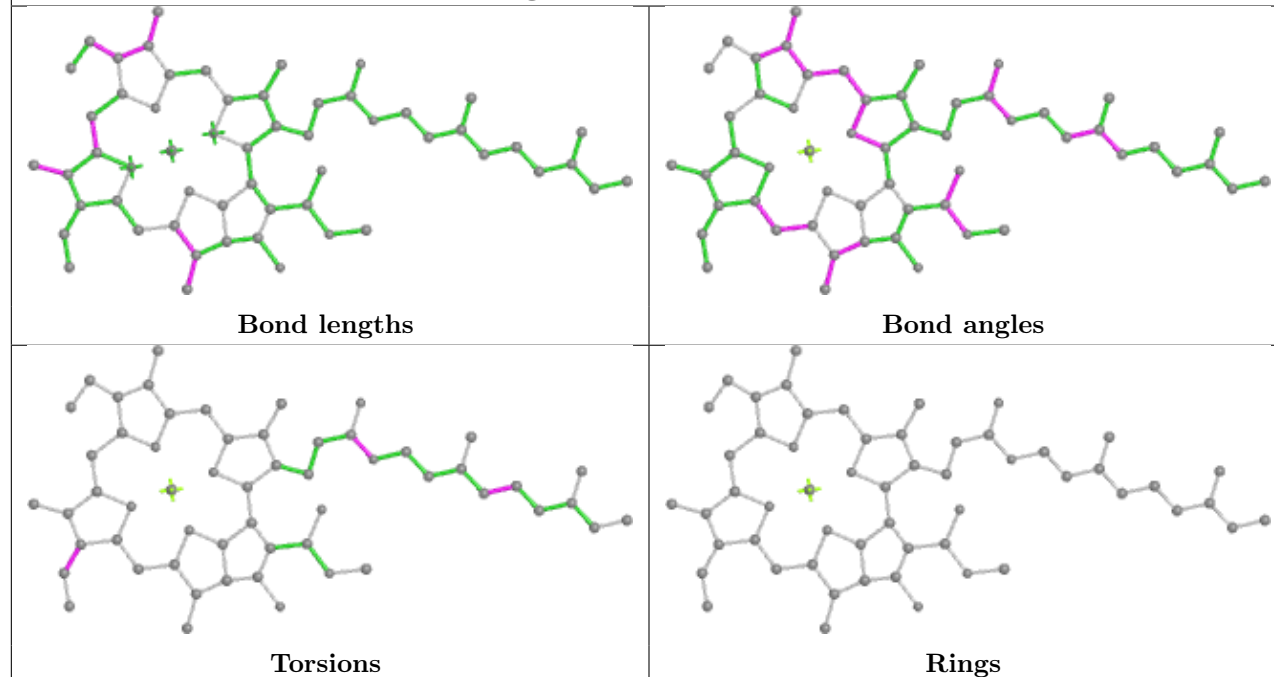


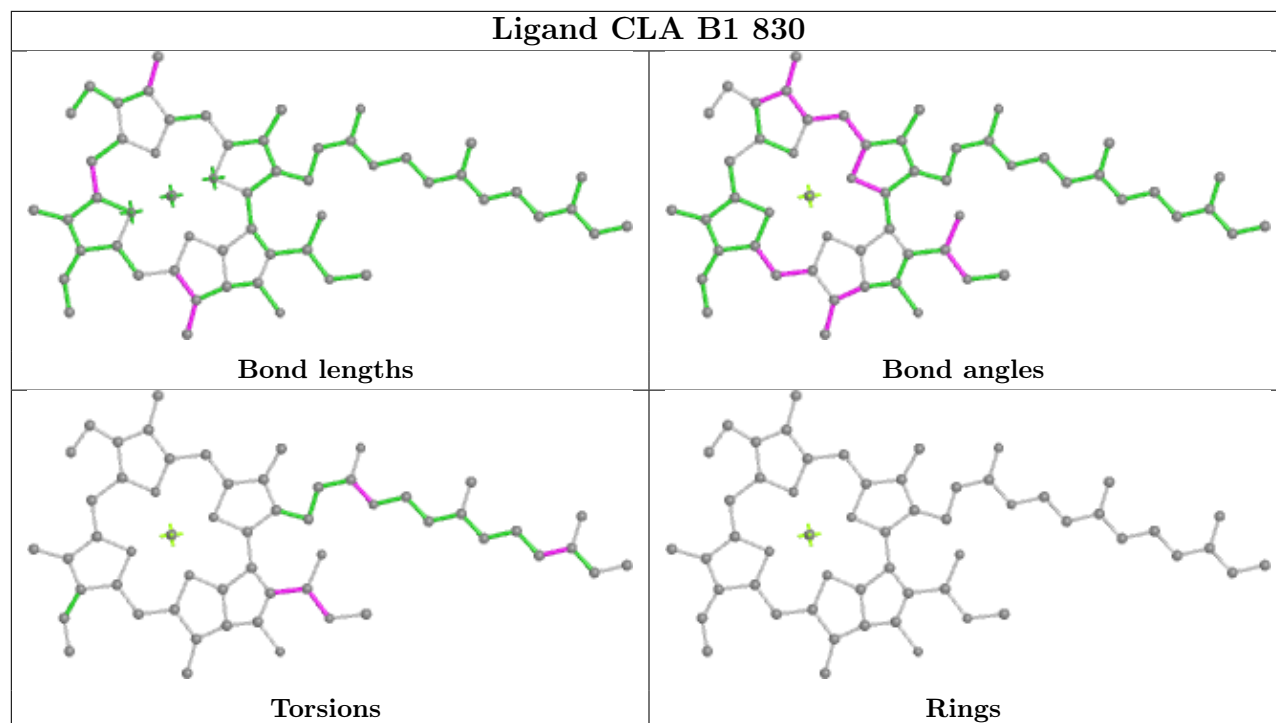
Rings

Ligand CLA B1 828

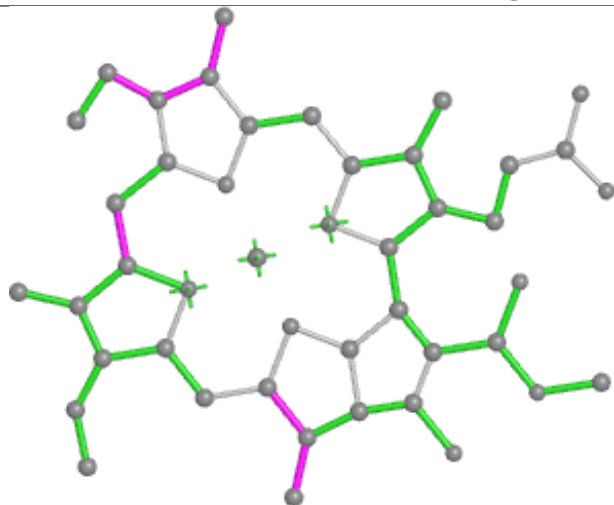


Ligand CLA B1 829

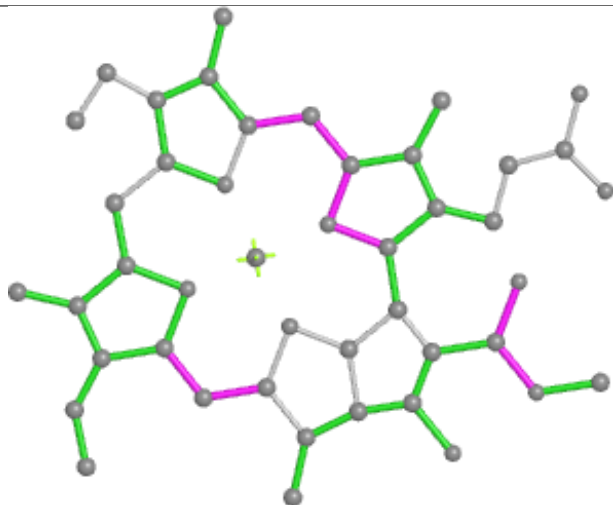




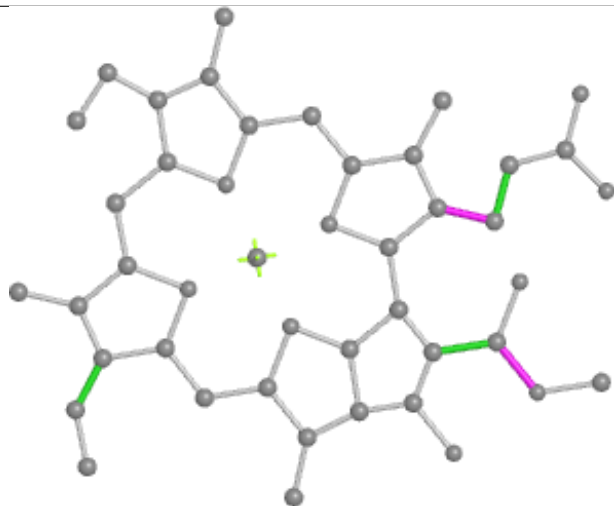
Ligand CLA B1 831



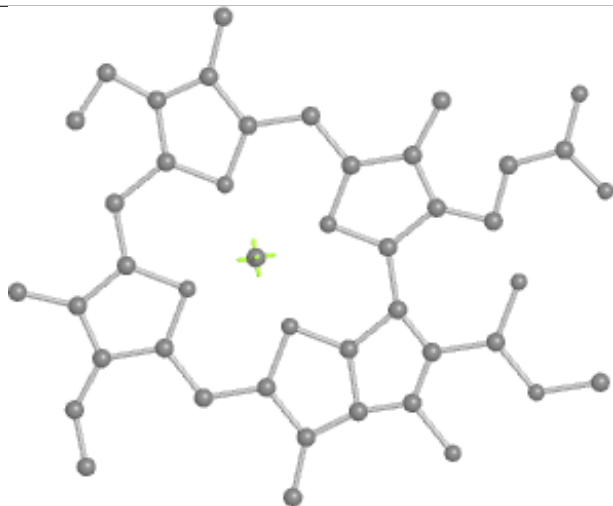
Bond lengths



Bond angles

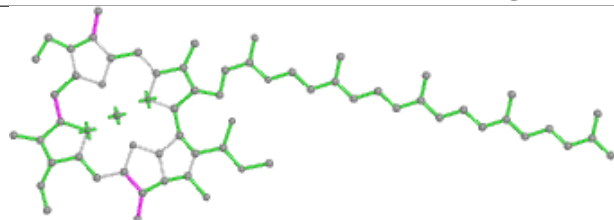


Torsions

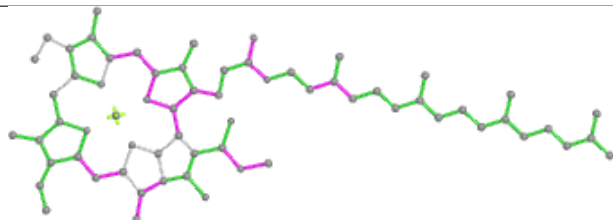


Rings

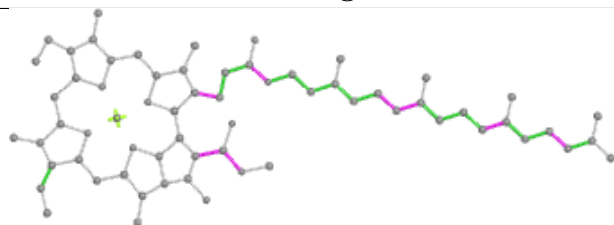
Ligand CLA B1 832



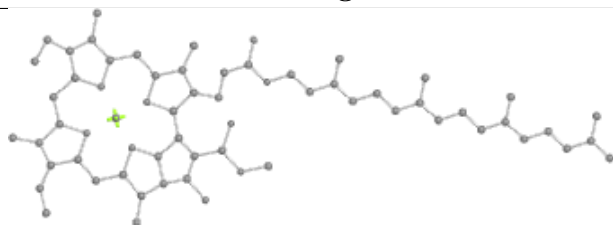
Bond lengths



Bond angles

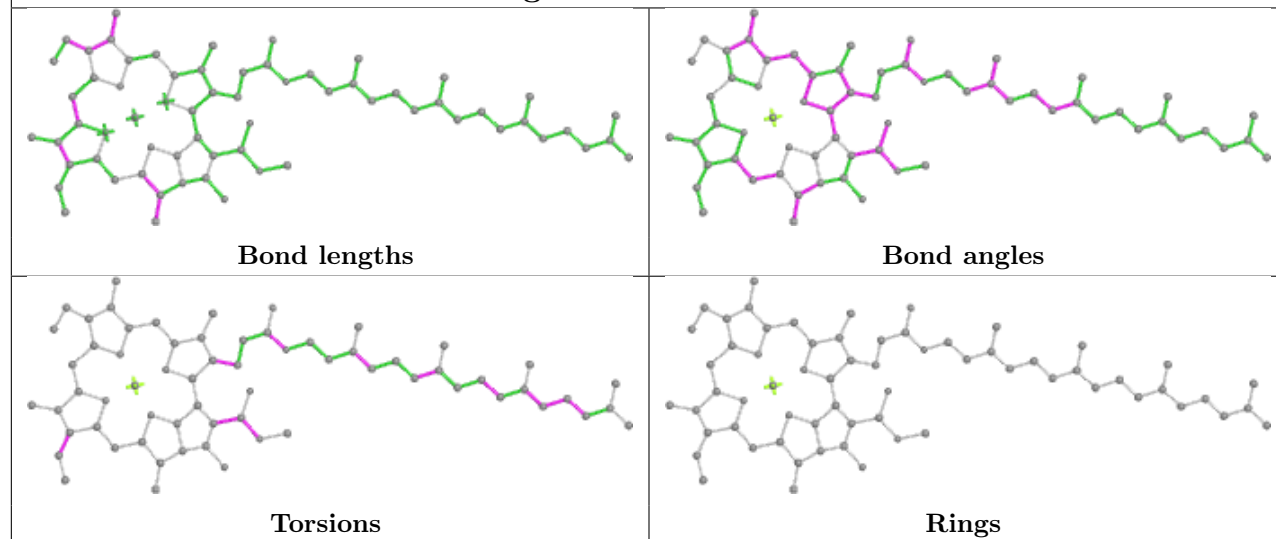


Torsions

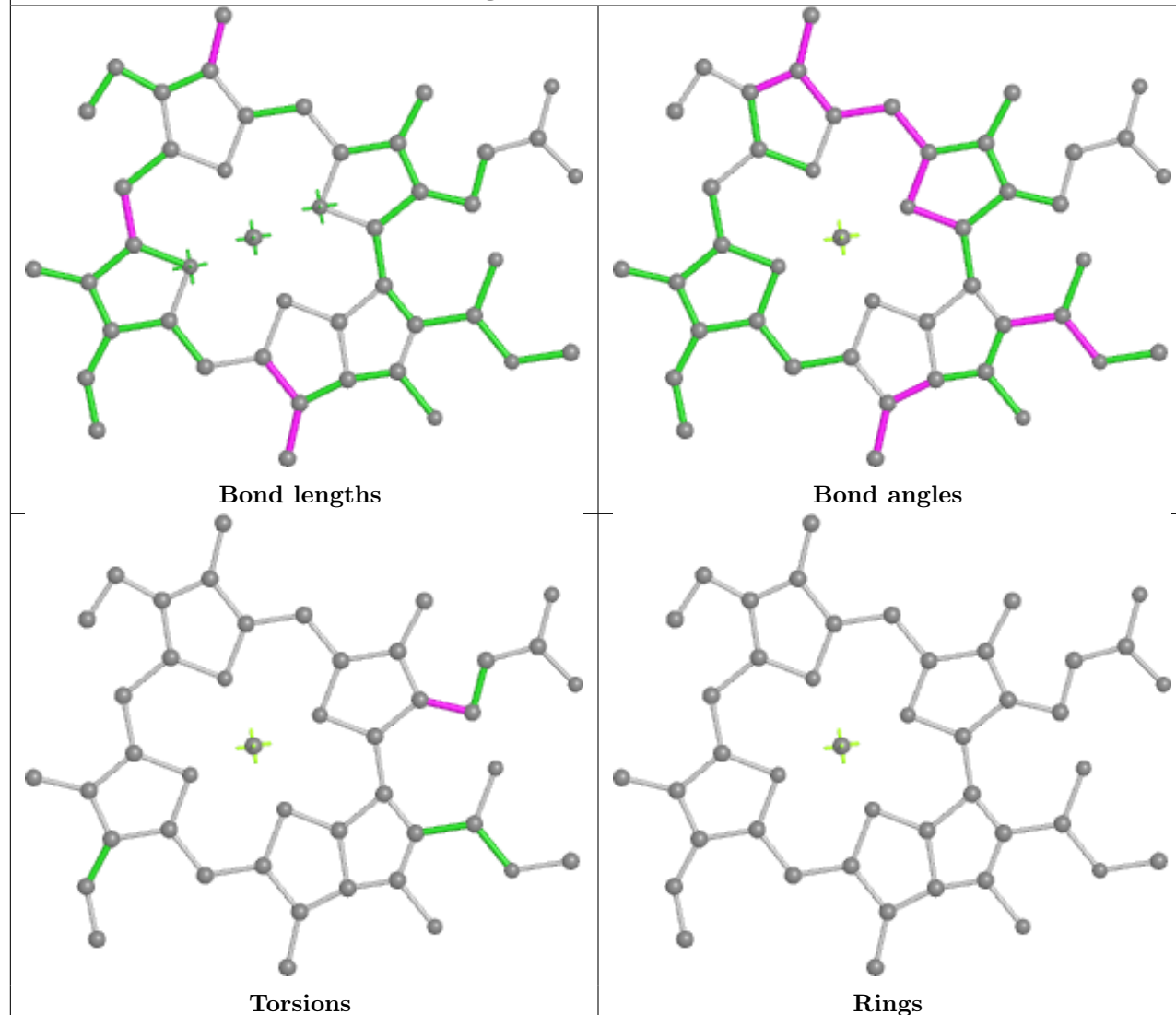


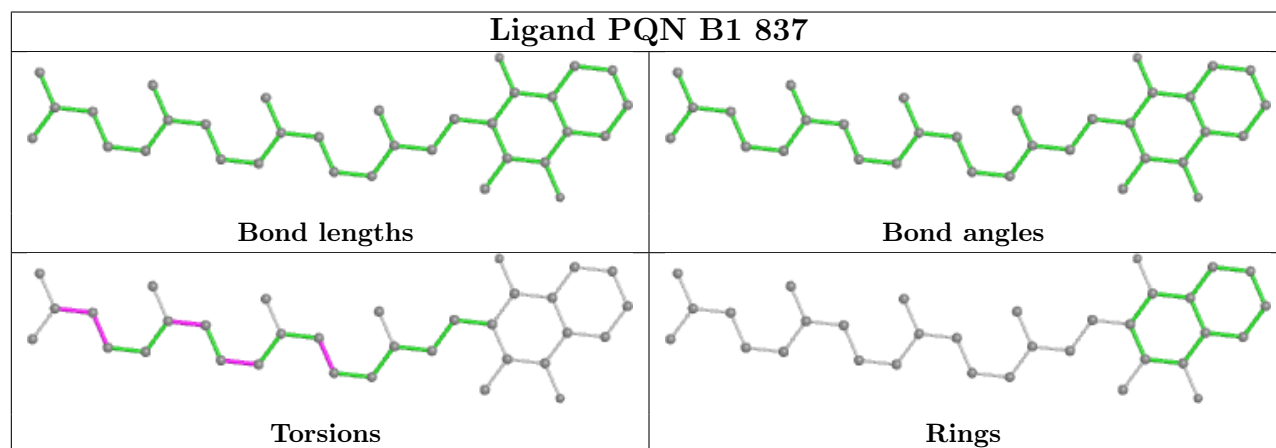
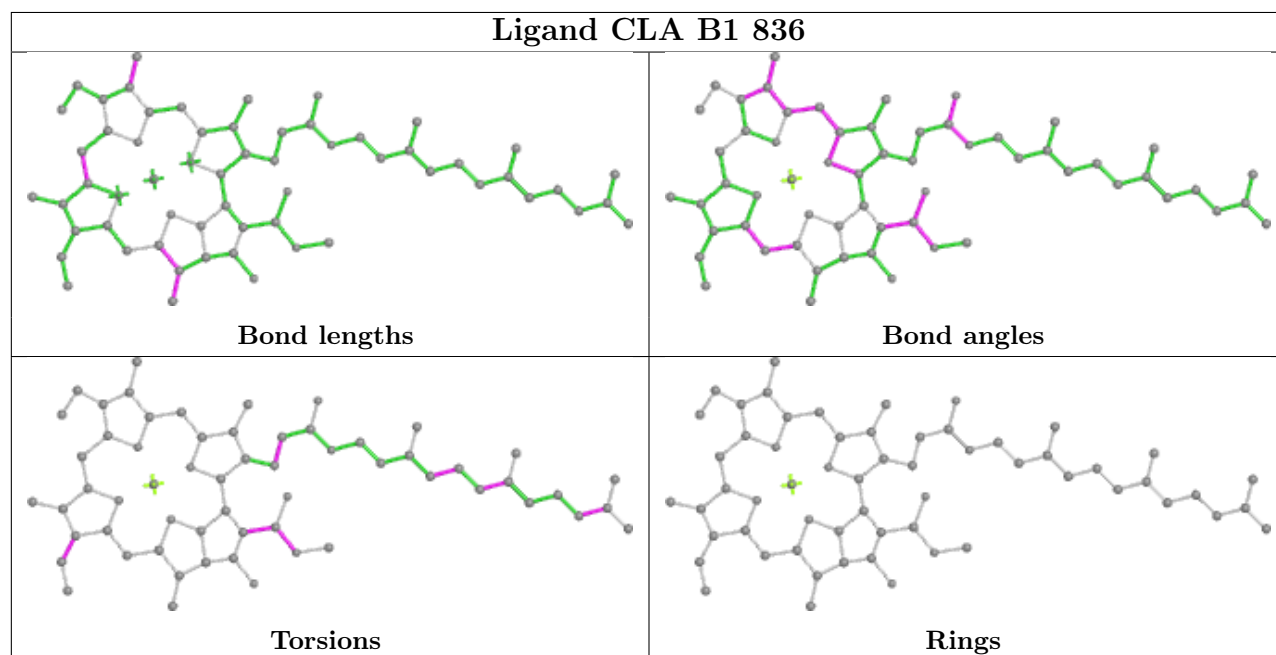
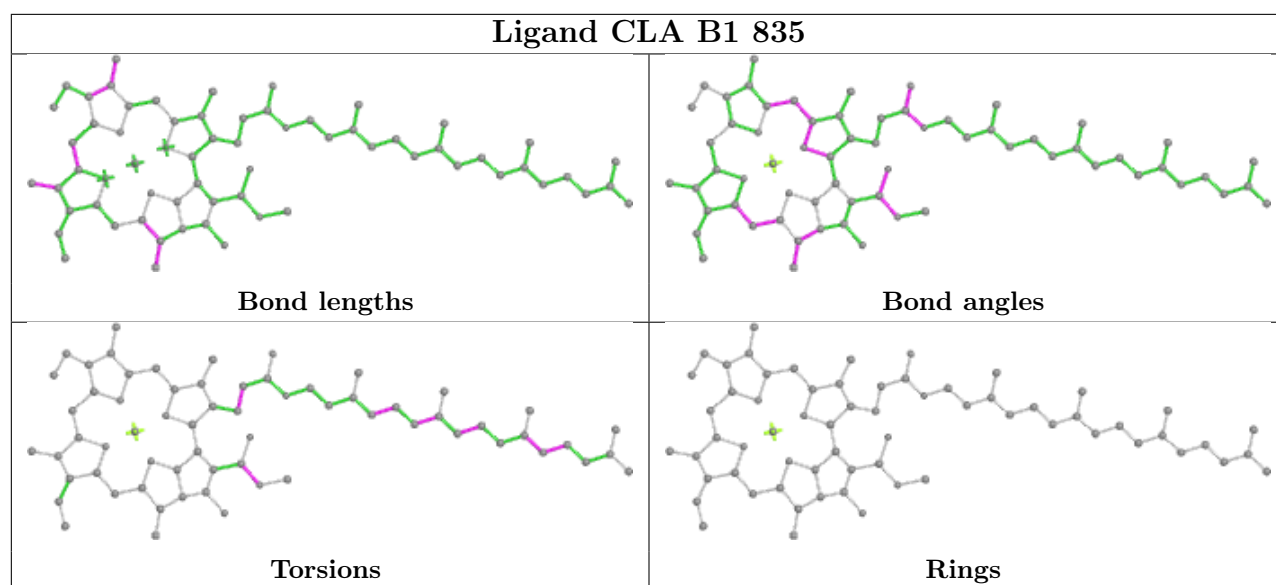
Rings

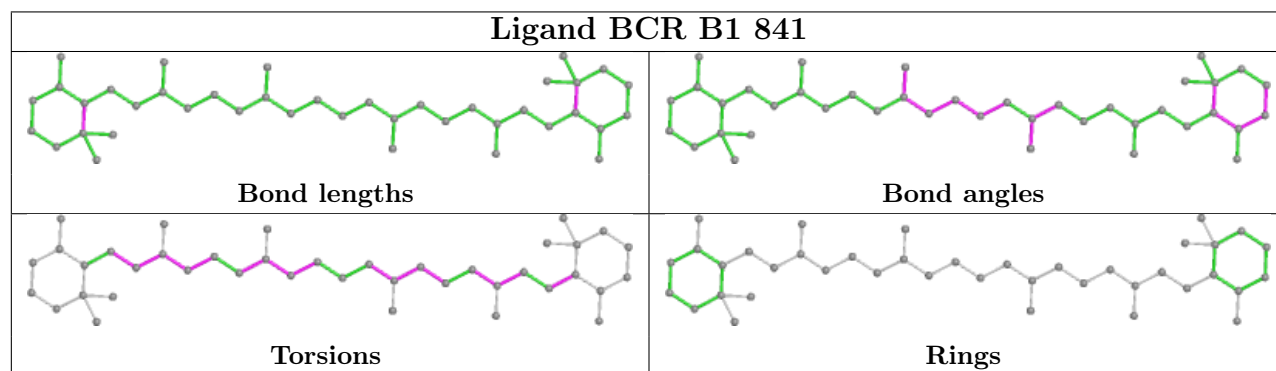
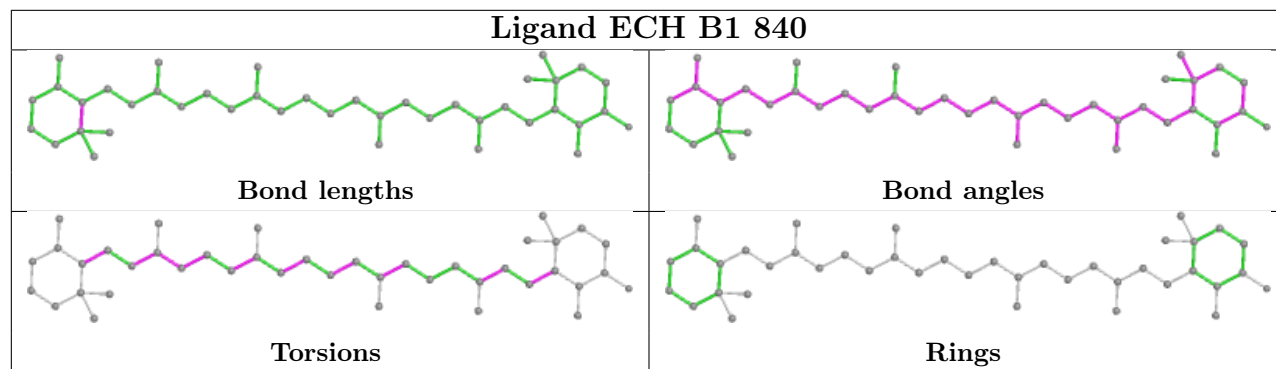
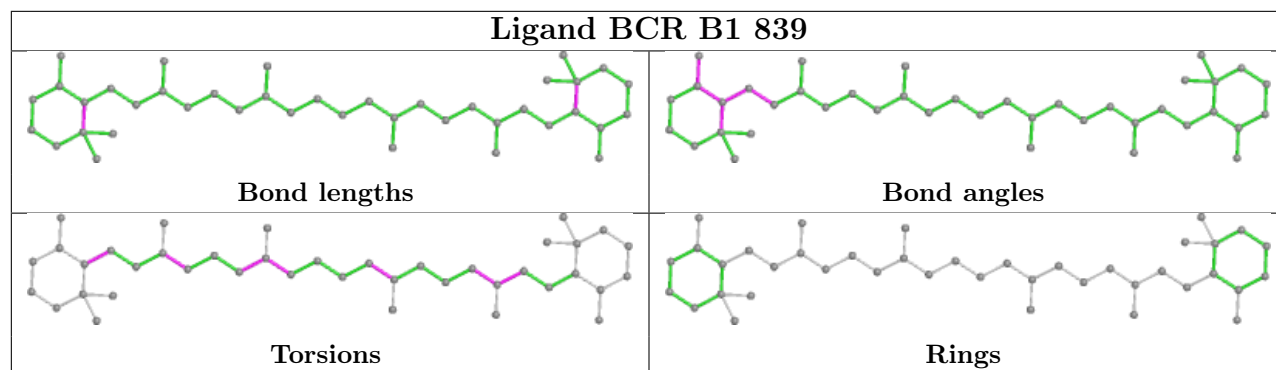
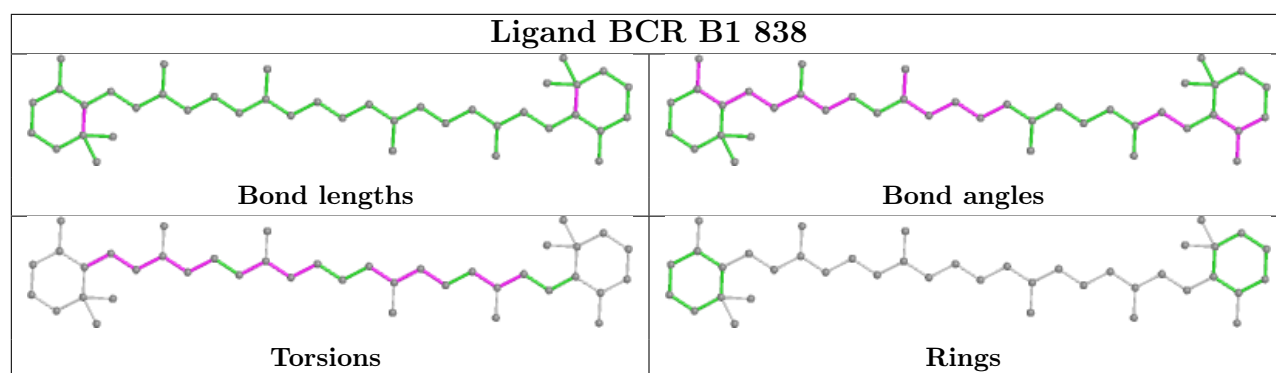
Ligand CLA B1 833

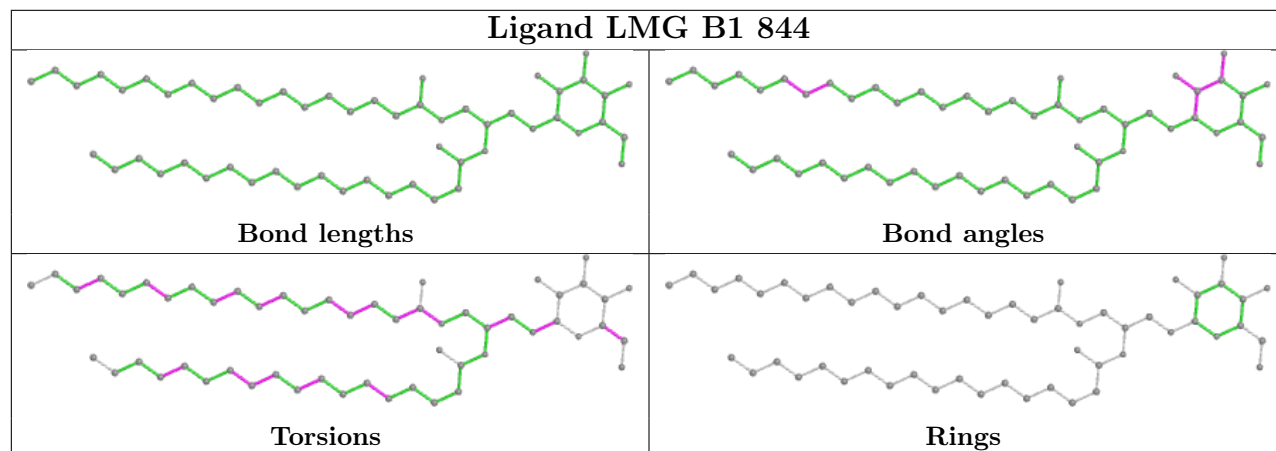
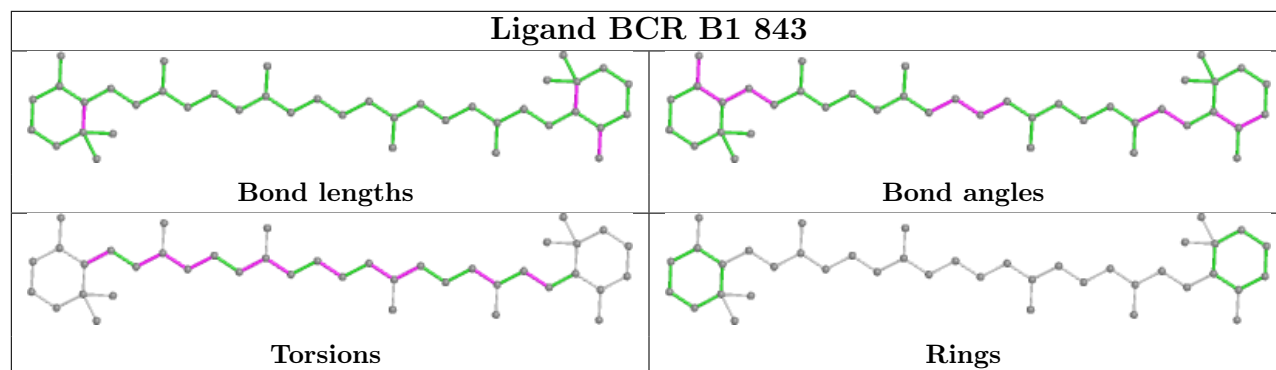
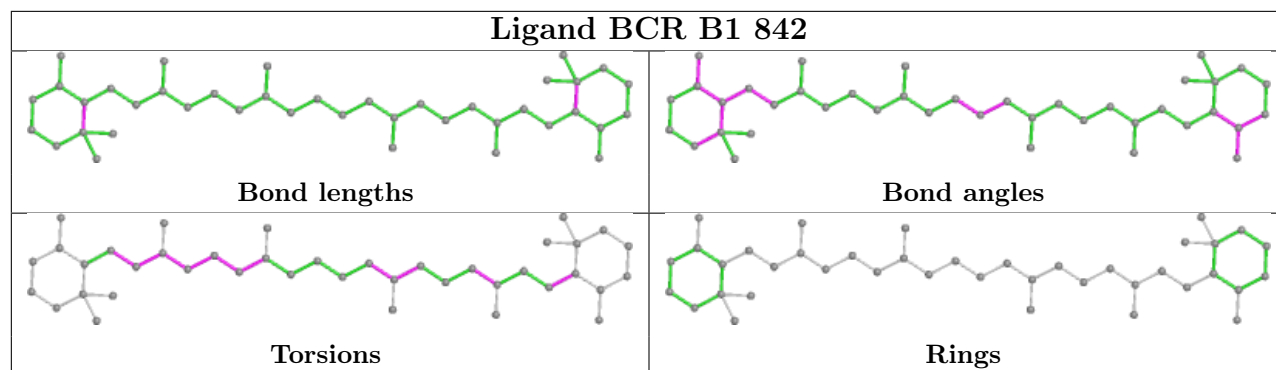


Ligand CLA B1 834

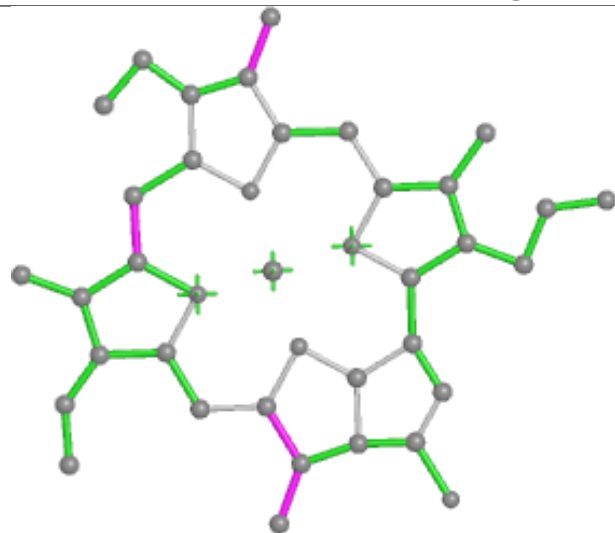




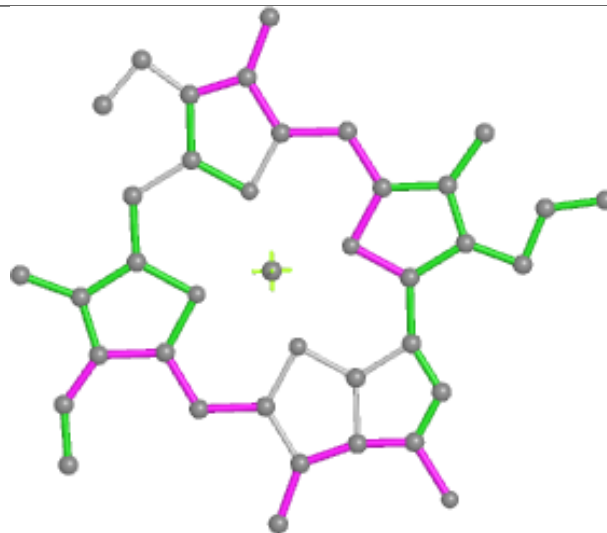




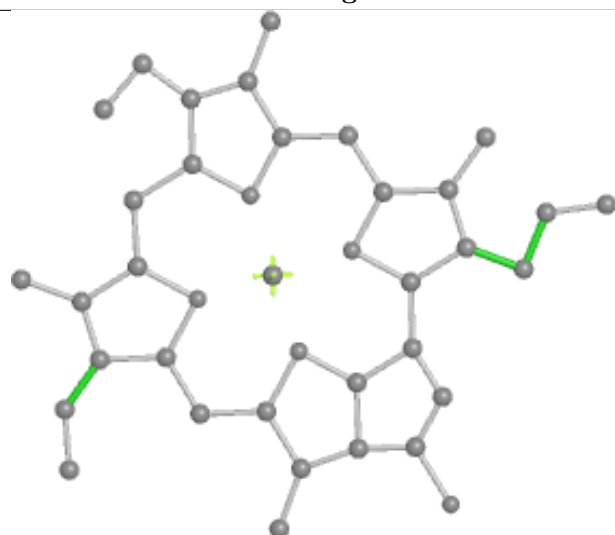
Ligand CLA B1 845



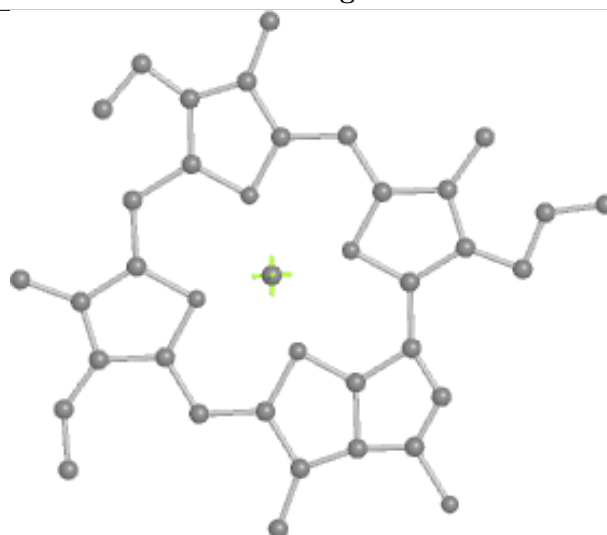
Bond lengths



Bond angles

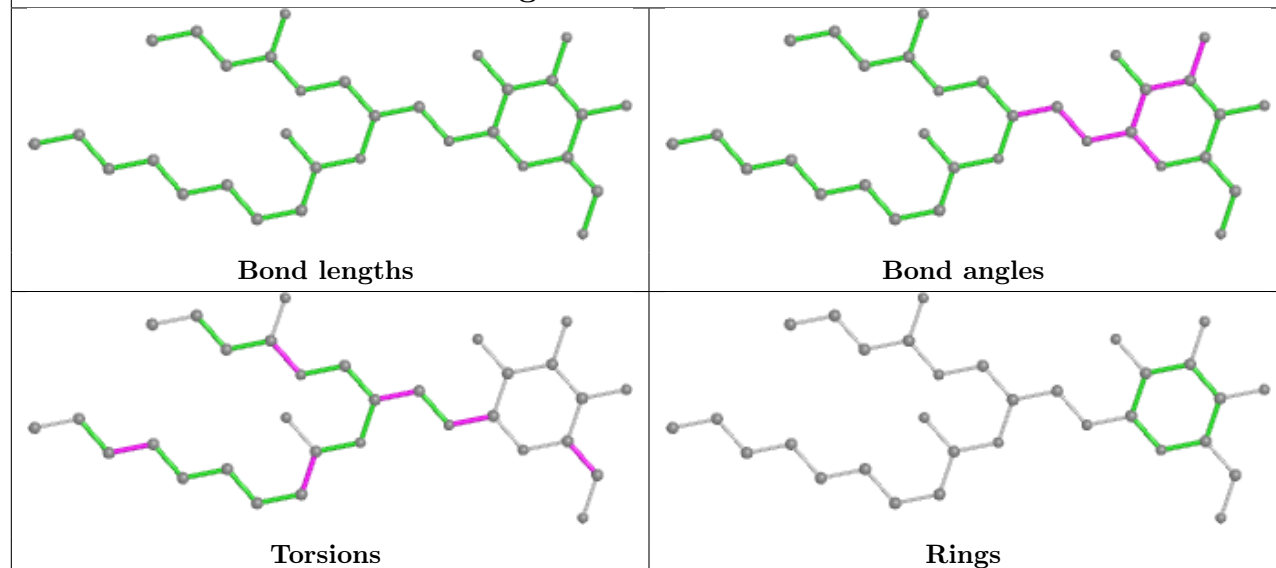


Torsions

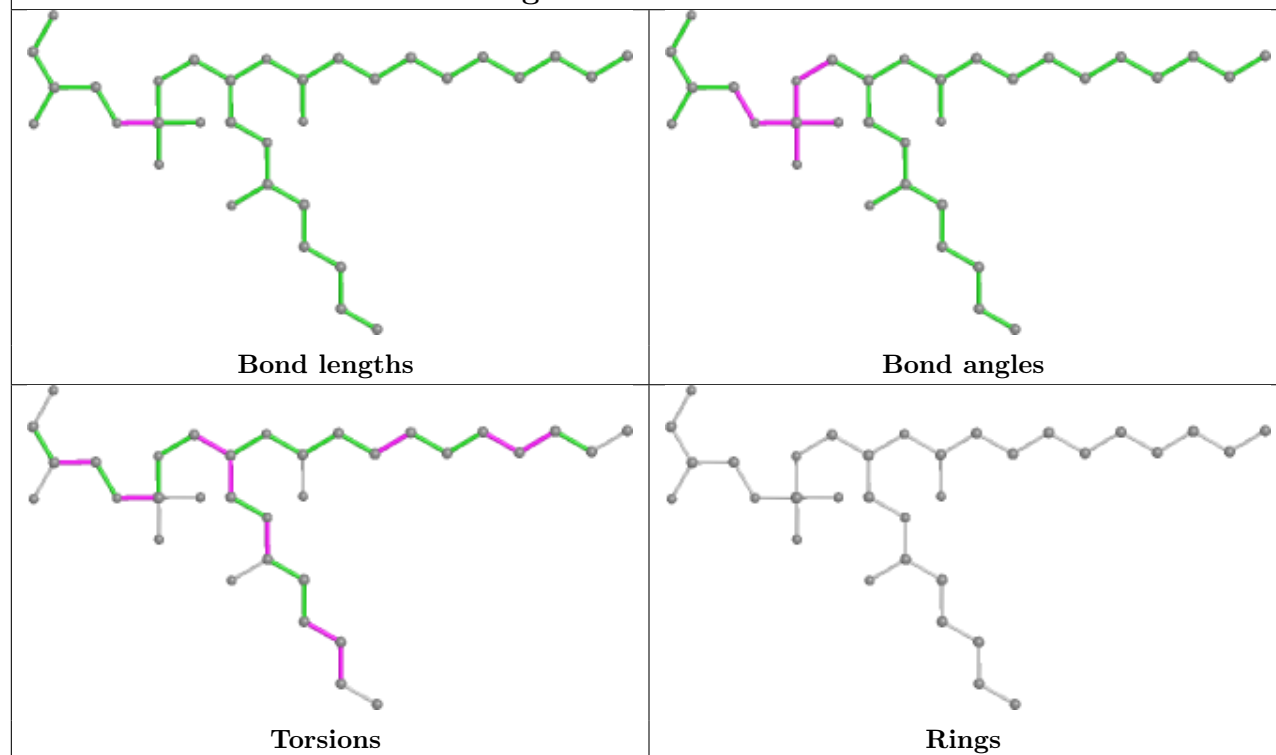


Rings

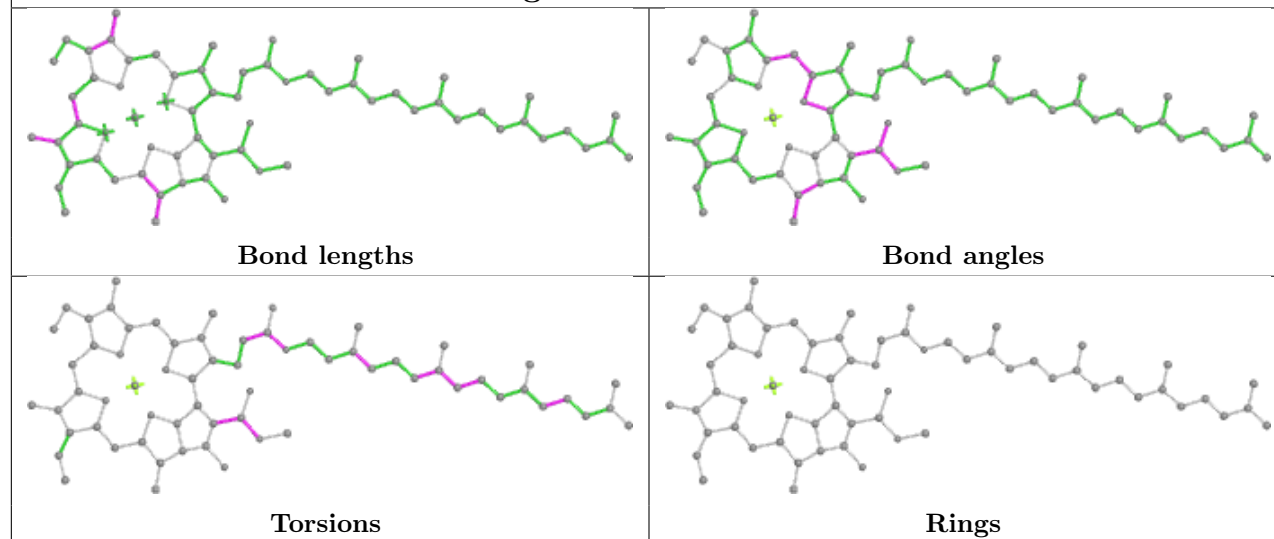
Ligand LMG B1 846



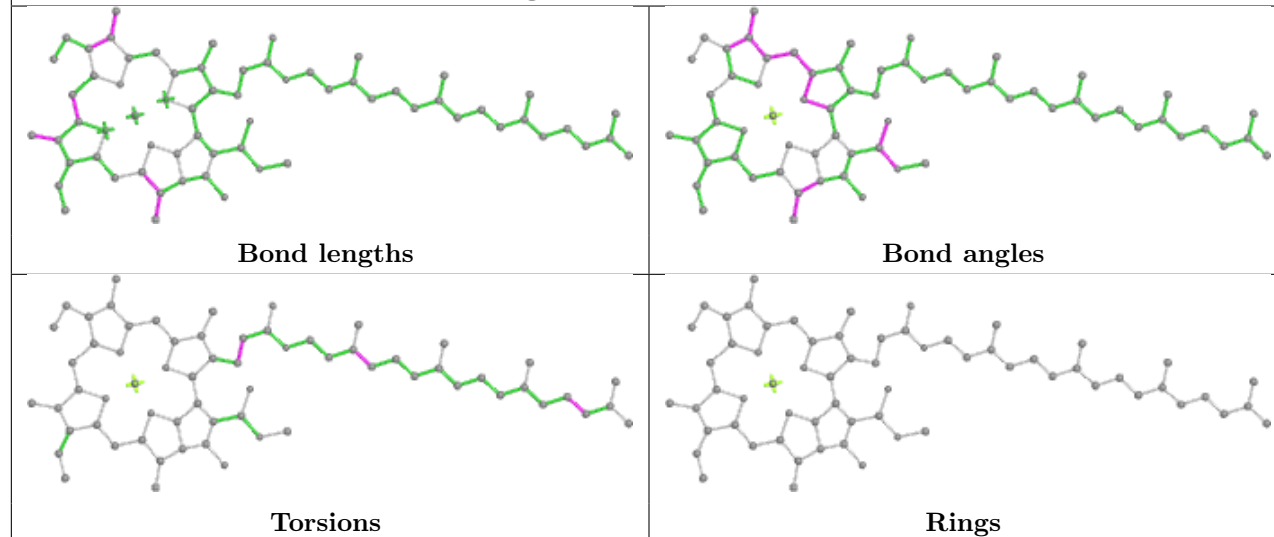
Ligand LHG B1 847

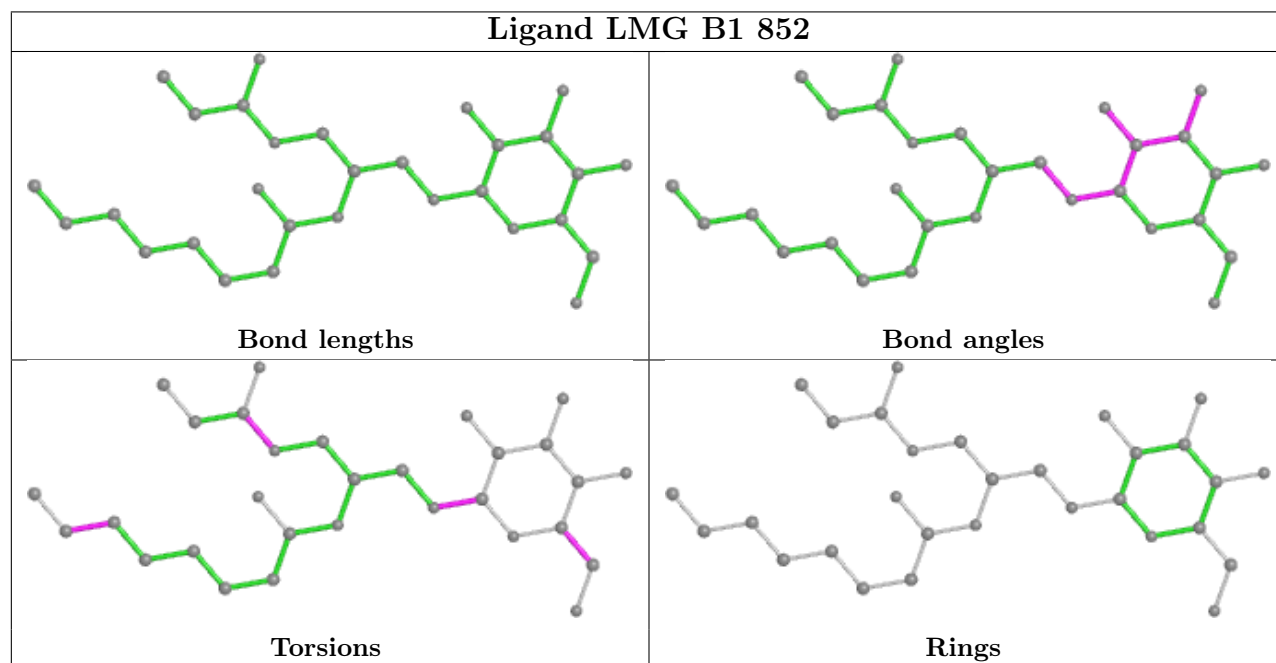
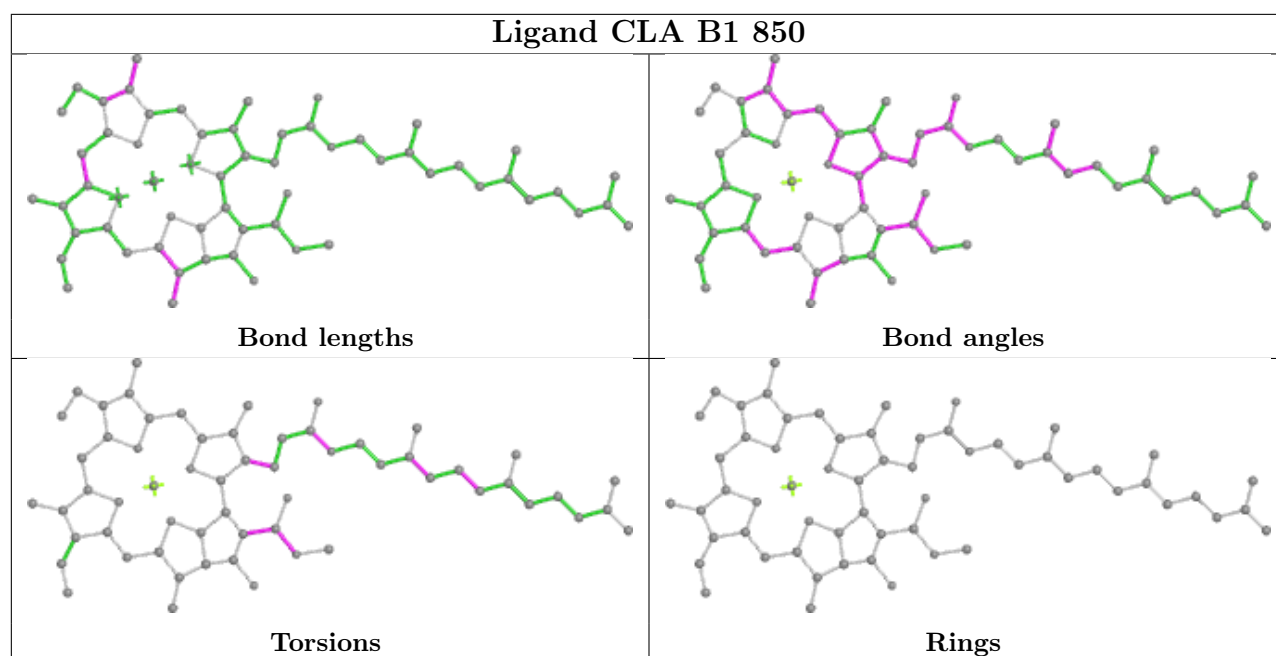


Ligand CLA B1 848

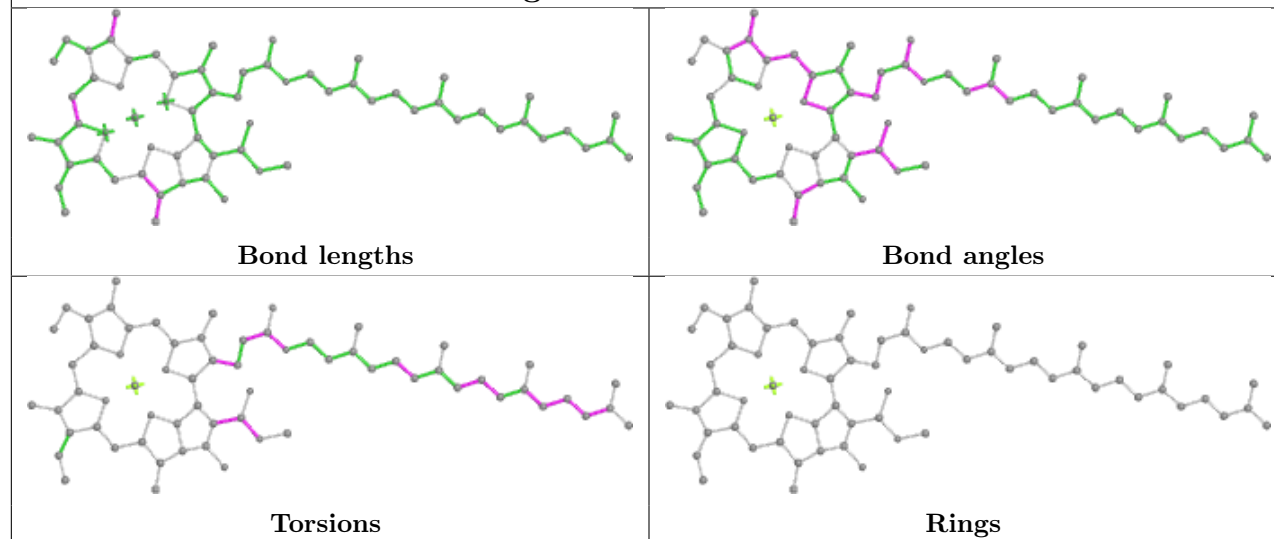


Ligand CLA B1 849

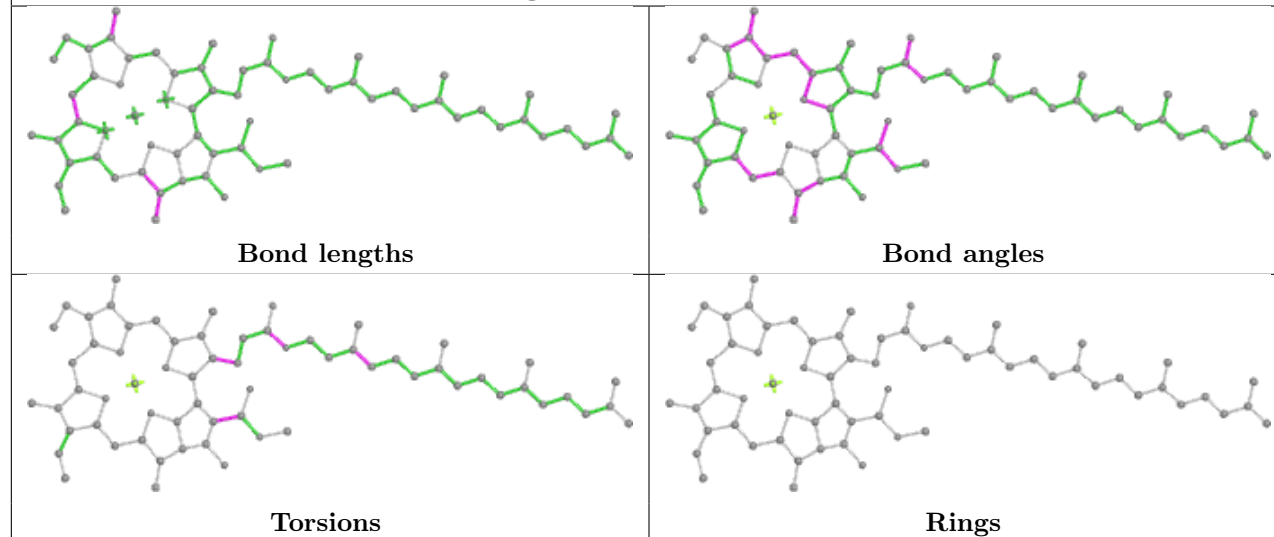




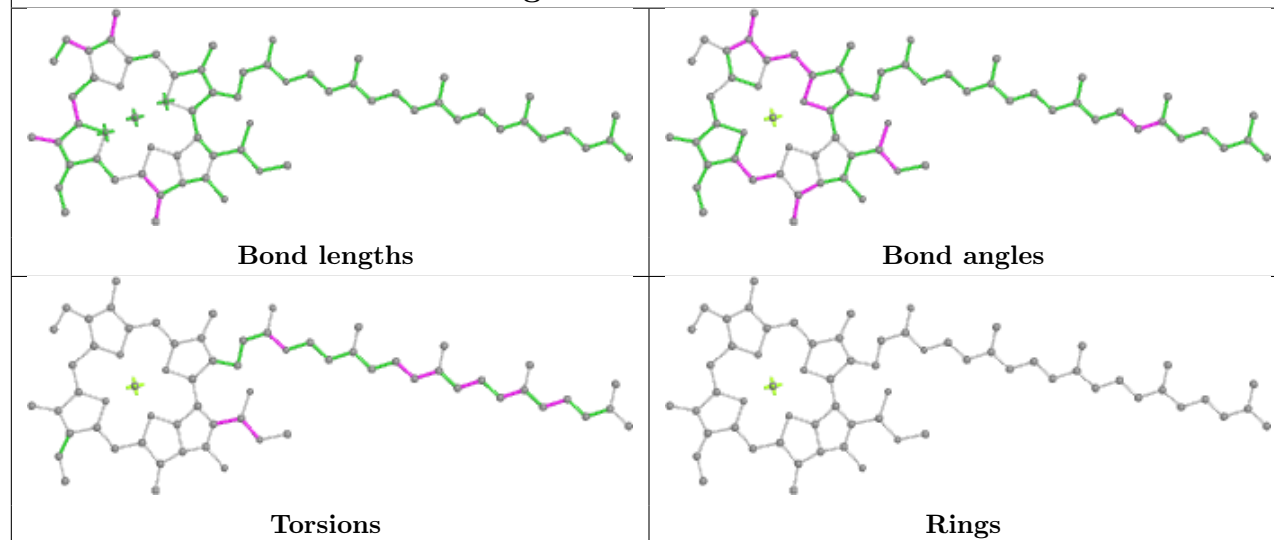
Ligand CLA B2 801

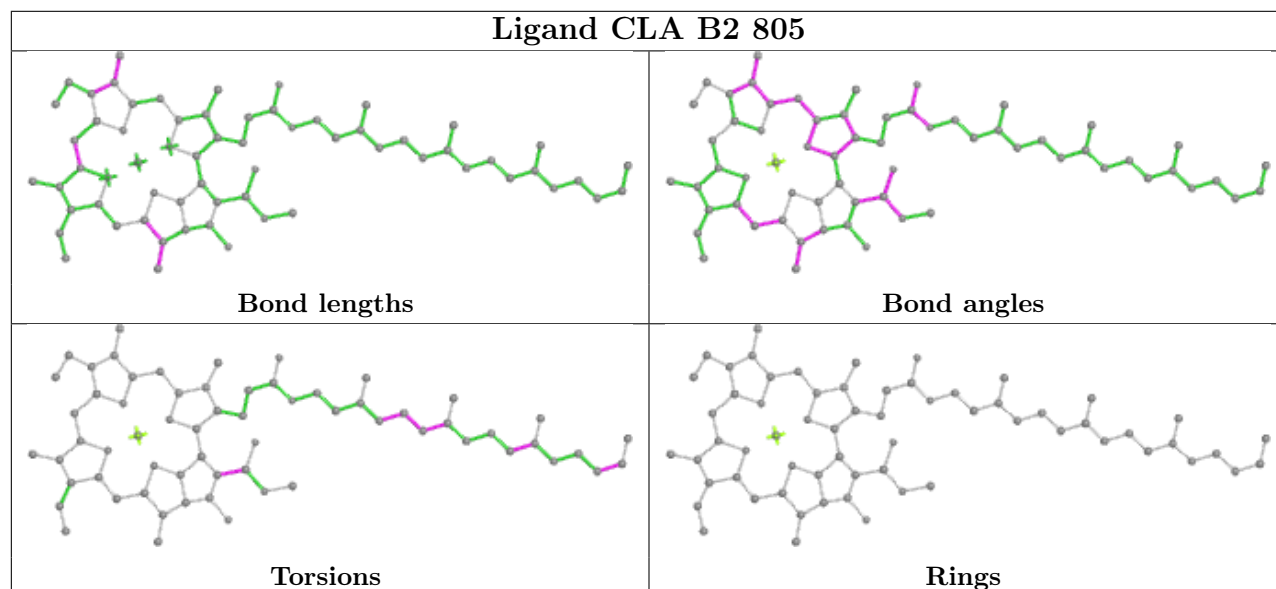
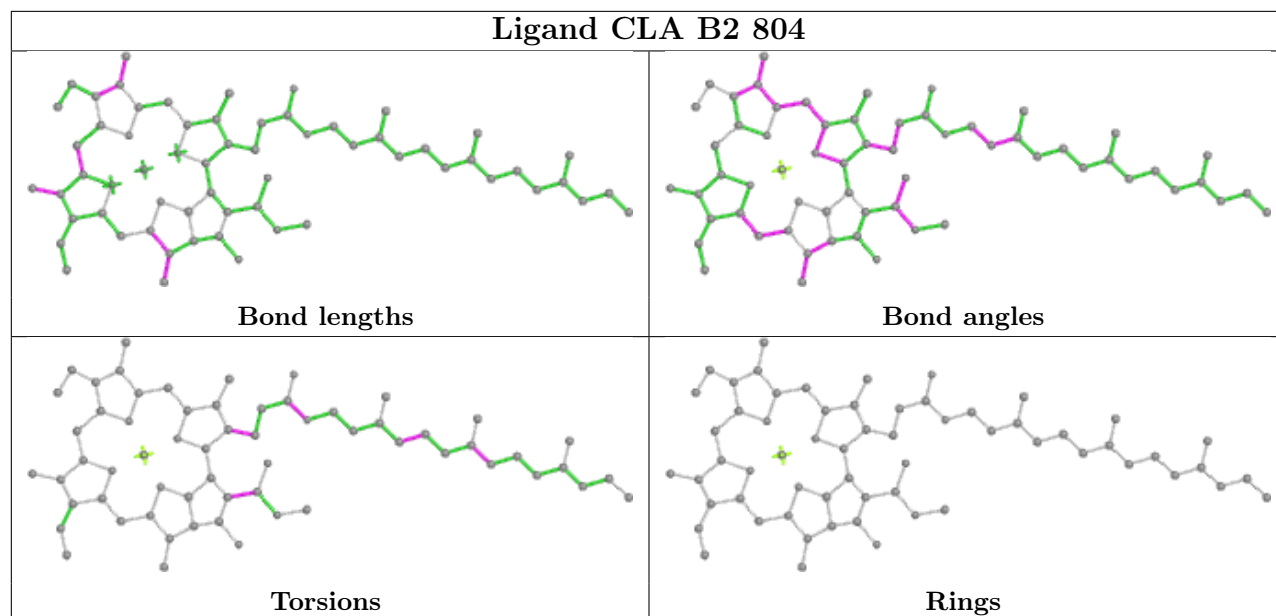


Ligand CLA B2 802

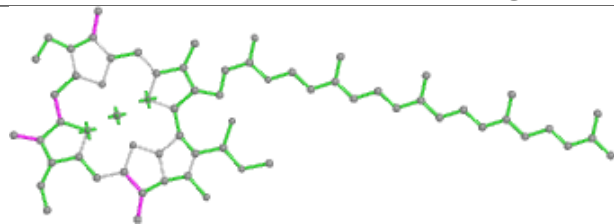


Ligand CLA B2 803

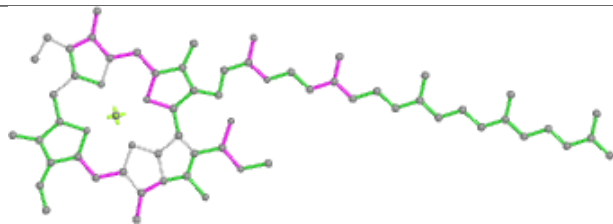




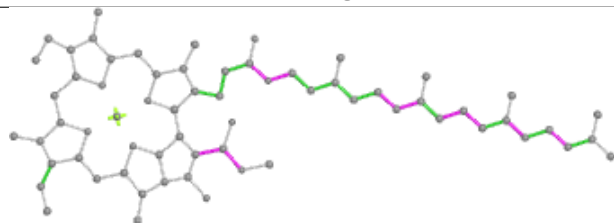
Ligand CLA B2 806



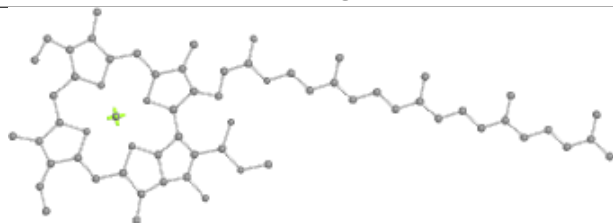
Bond lengths



Bond angles

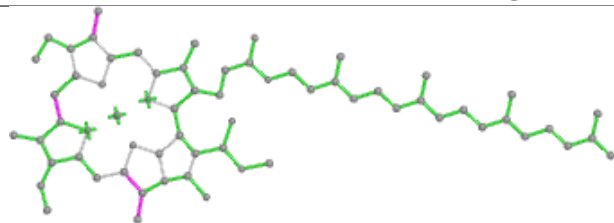


Torsions

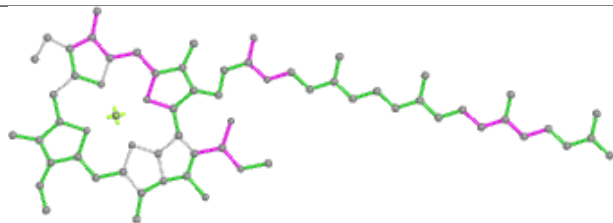


Rings

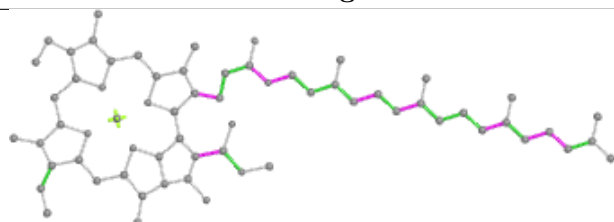
Ligand CLA B2 807



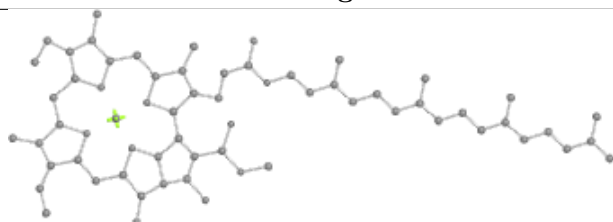
Bond lengths



Bond angles

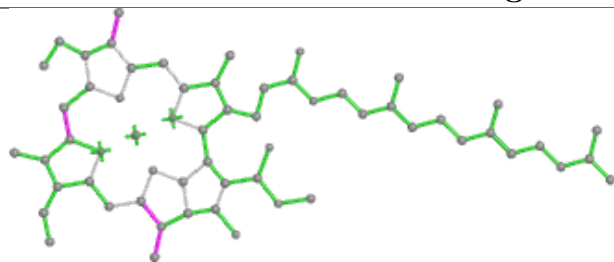


Torsions

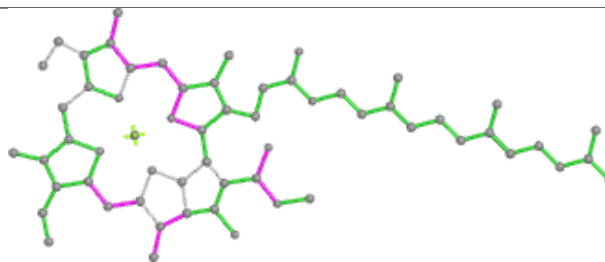


Rings

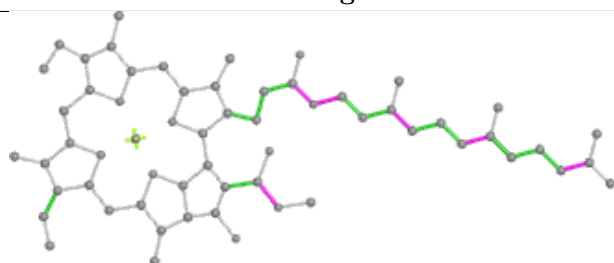
Ligand CLA B2 808



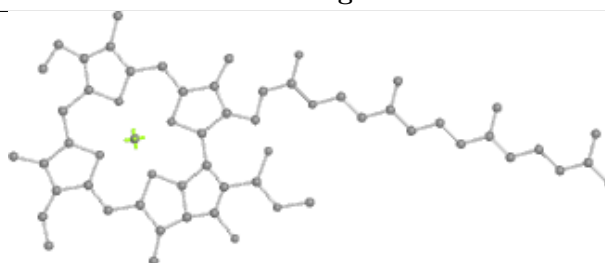
Bond lengths



Bond angles

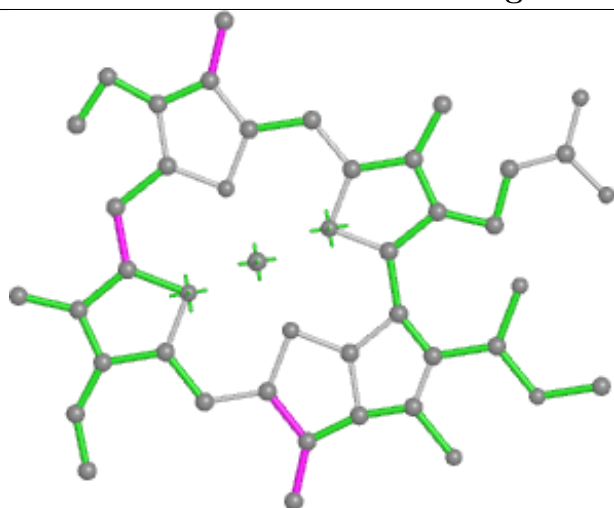


Torsions

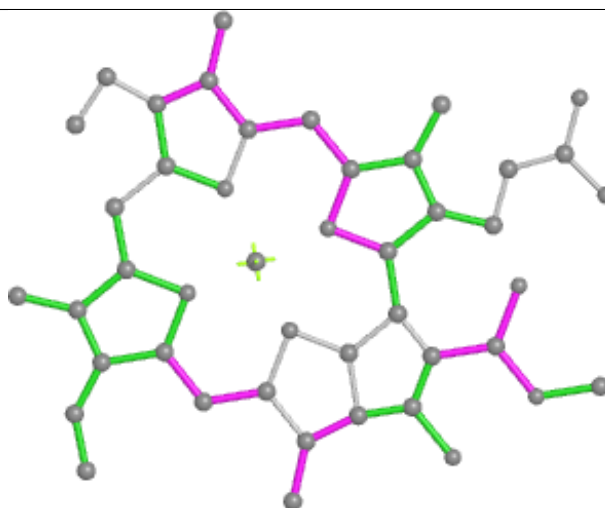


Rings

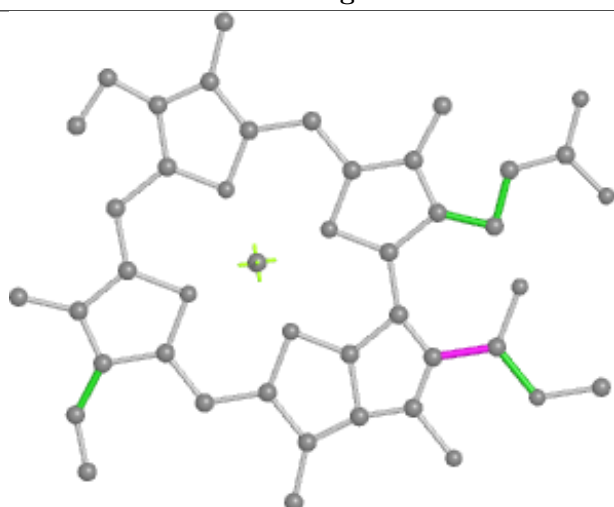
Ligand CLA B2 809



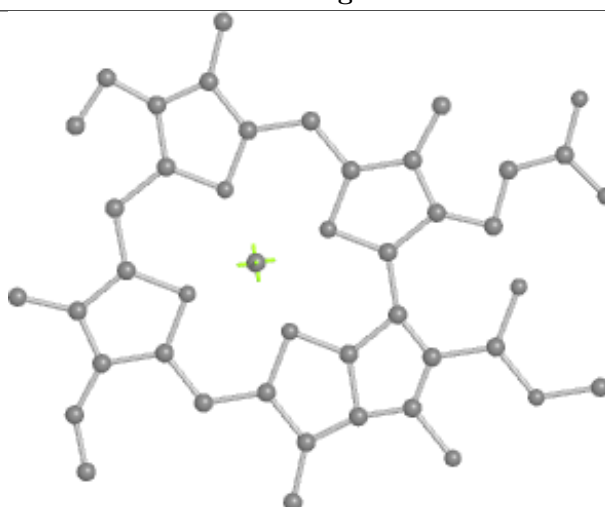
Bond lengths



Bond angles

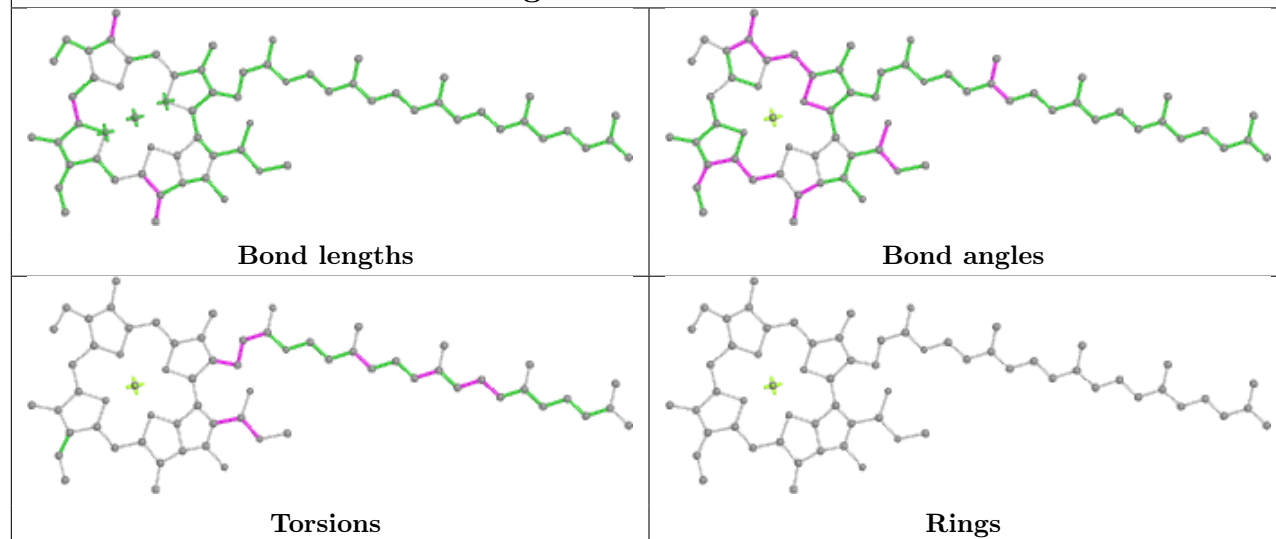


Torsions

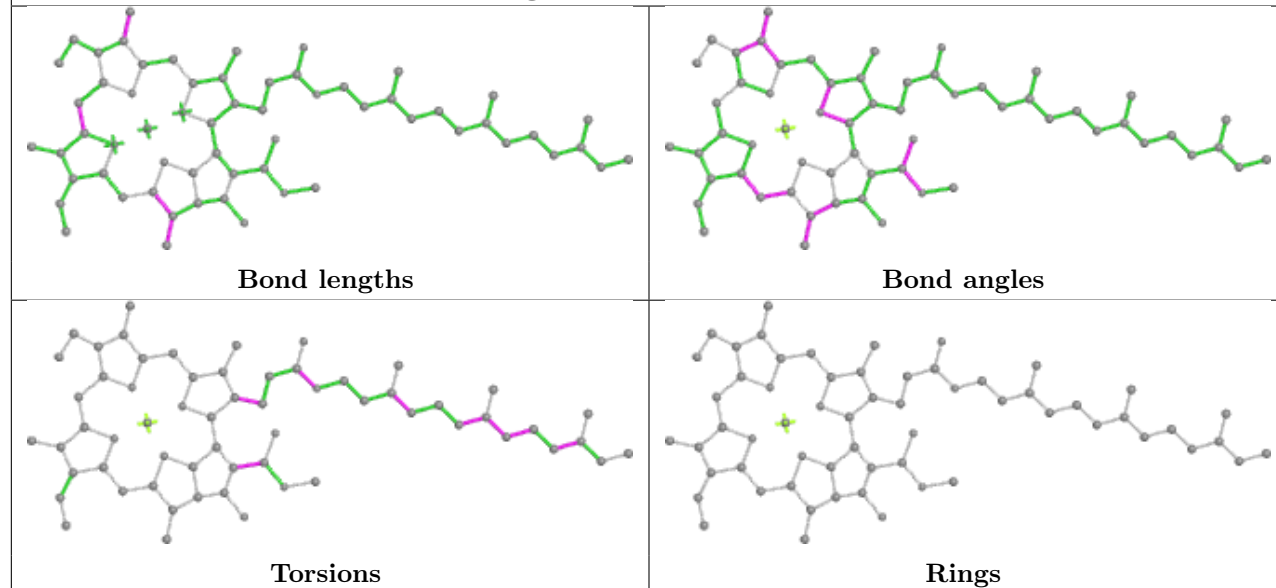


Rings

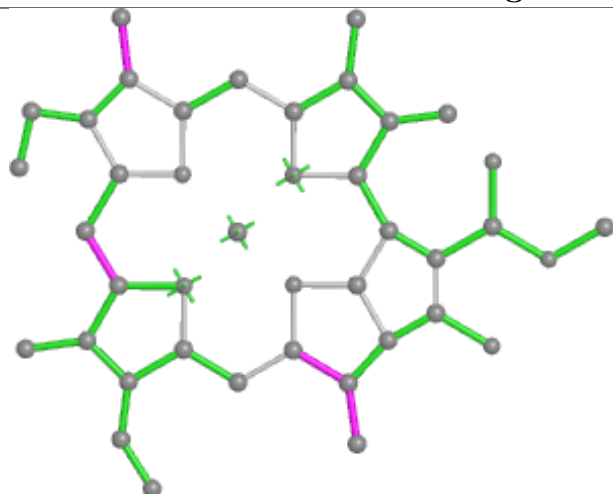
Ligand CLA B2 810



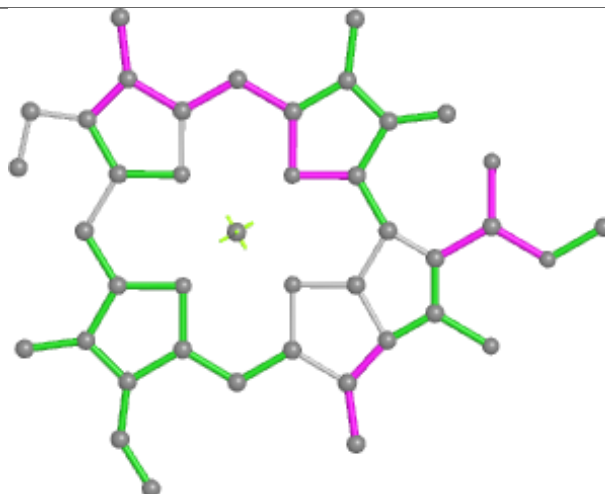
Ligand CLA B2 811



Ligand CLA B2 812



Bond lengths



Bond angles

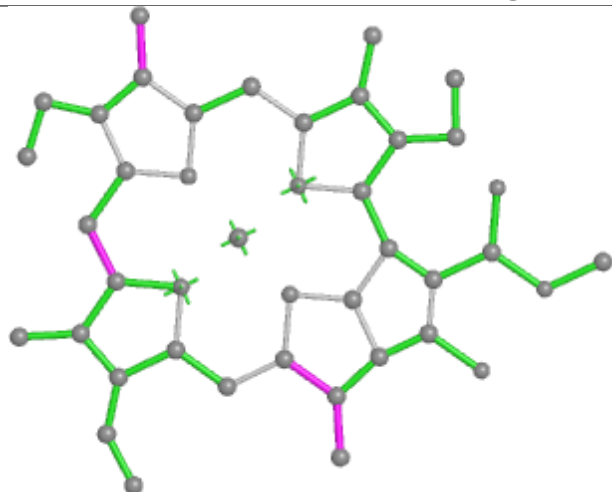


Torsions

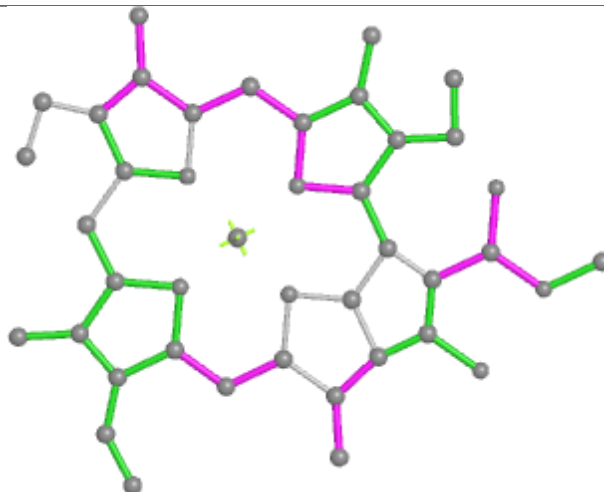


Rings

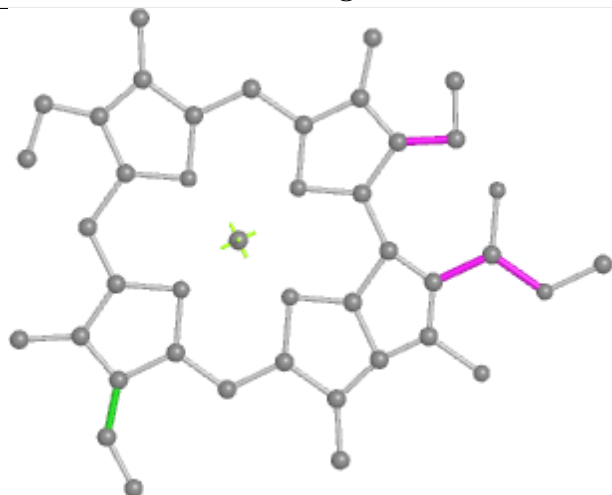
Ligand CLA B2 813



Bond lengths



Bond angles

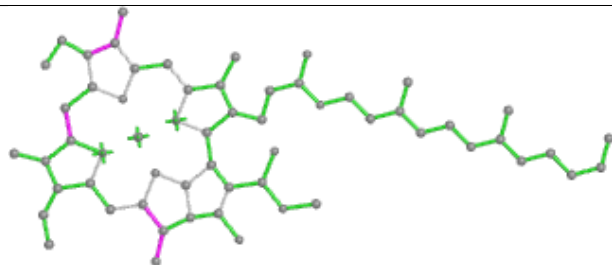


Torsions

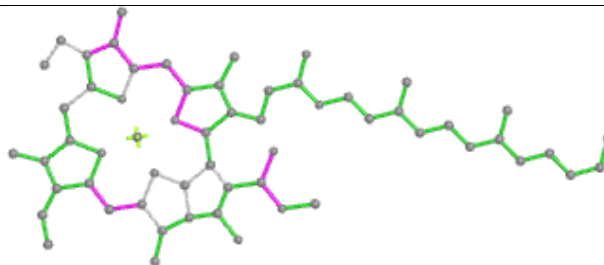


Rings

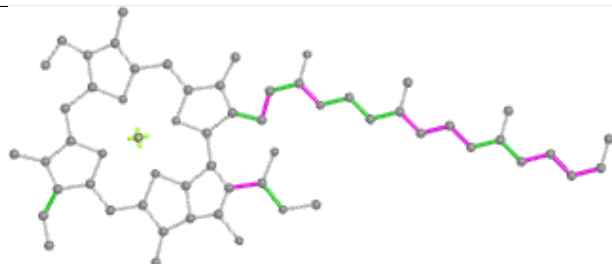
Ligand CLA B2 814



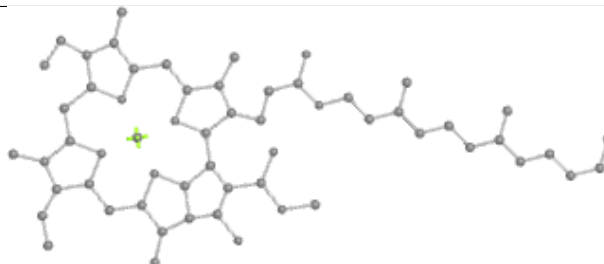
Bond lengths



Bond angles

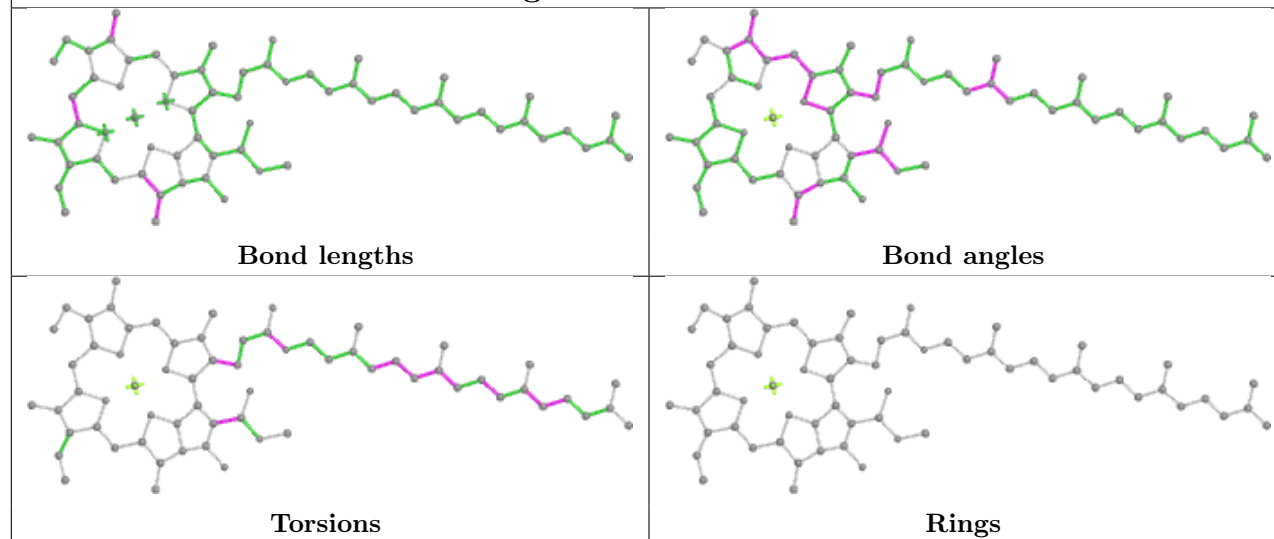


Torsions

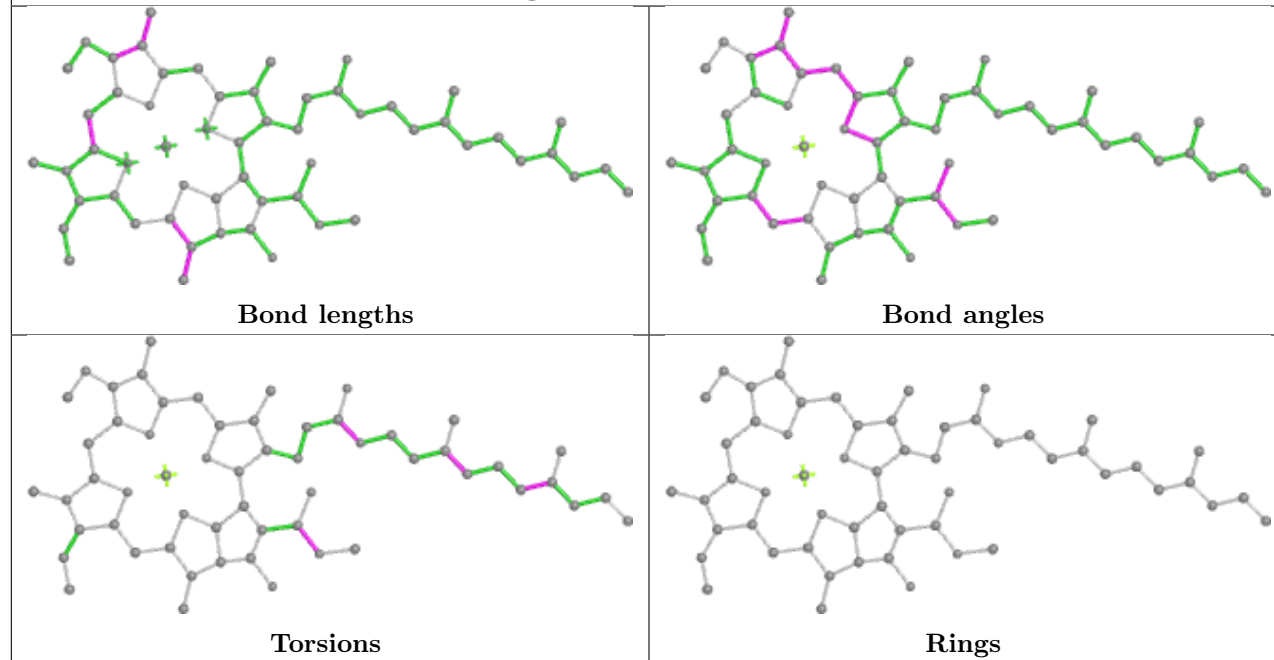


Rings

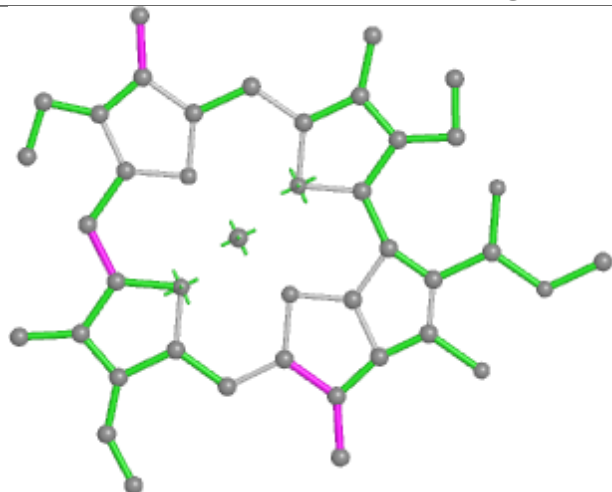
Ligand CLA B2 815



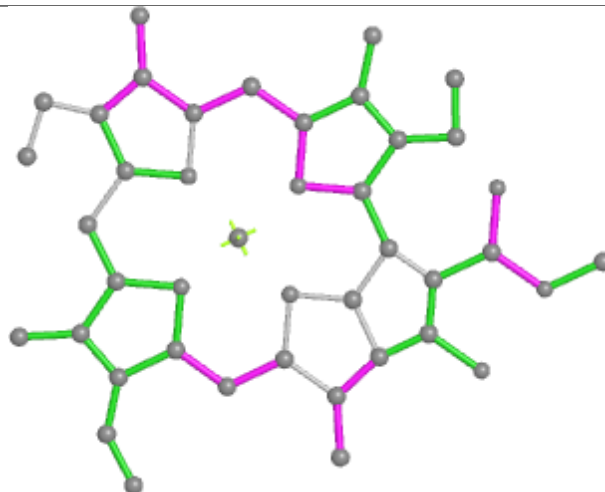
Ligand CLA B2 816



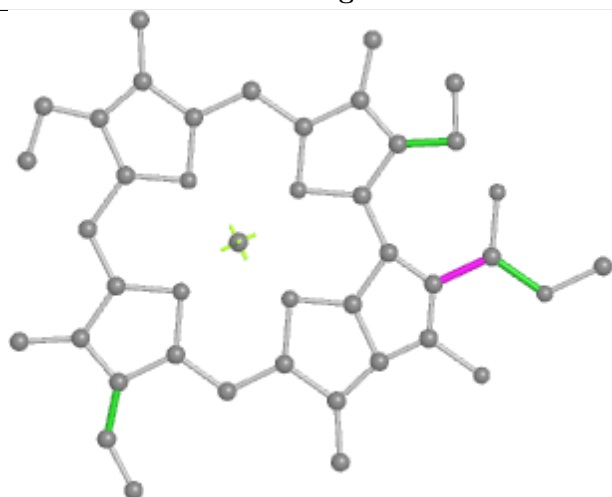
Ligand CLA B2 817



Bond lengths



Bond angles

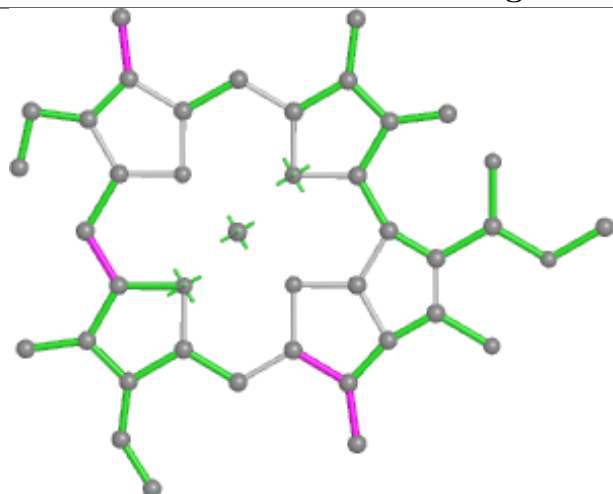


Torsions

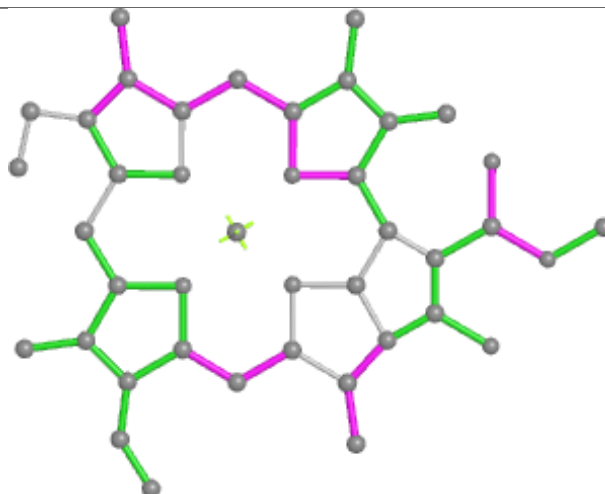


Rings

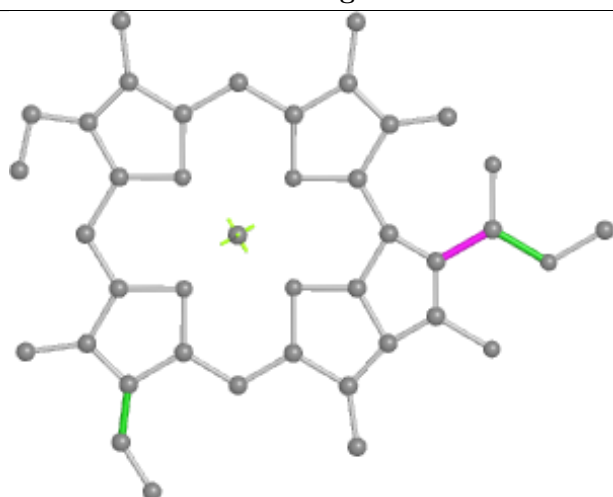
Ligand CLA B2 818



Bond lengths



Bond angles

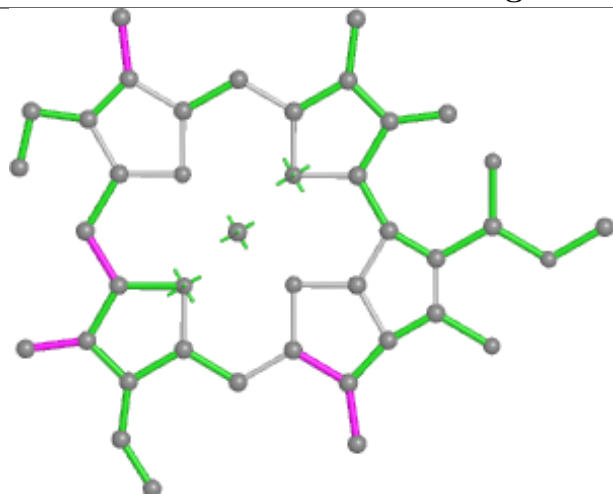


Torsions

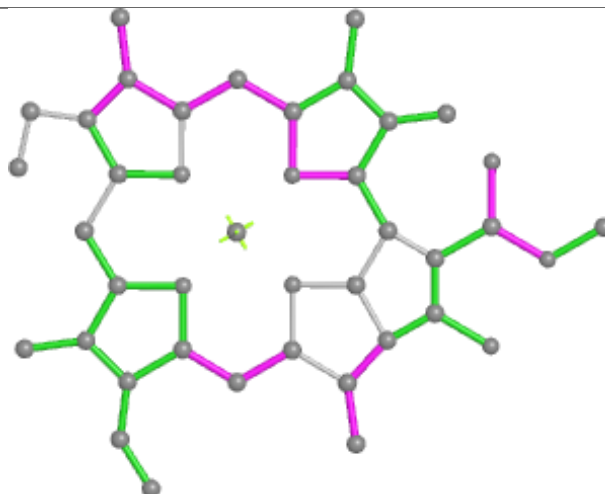


Rings

Ligand CLA B2 819



Bond lengths



Bond angles

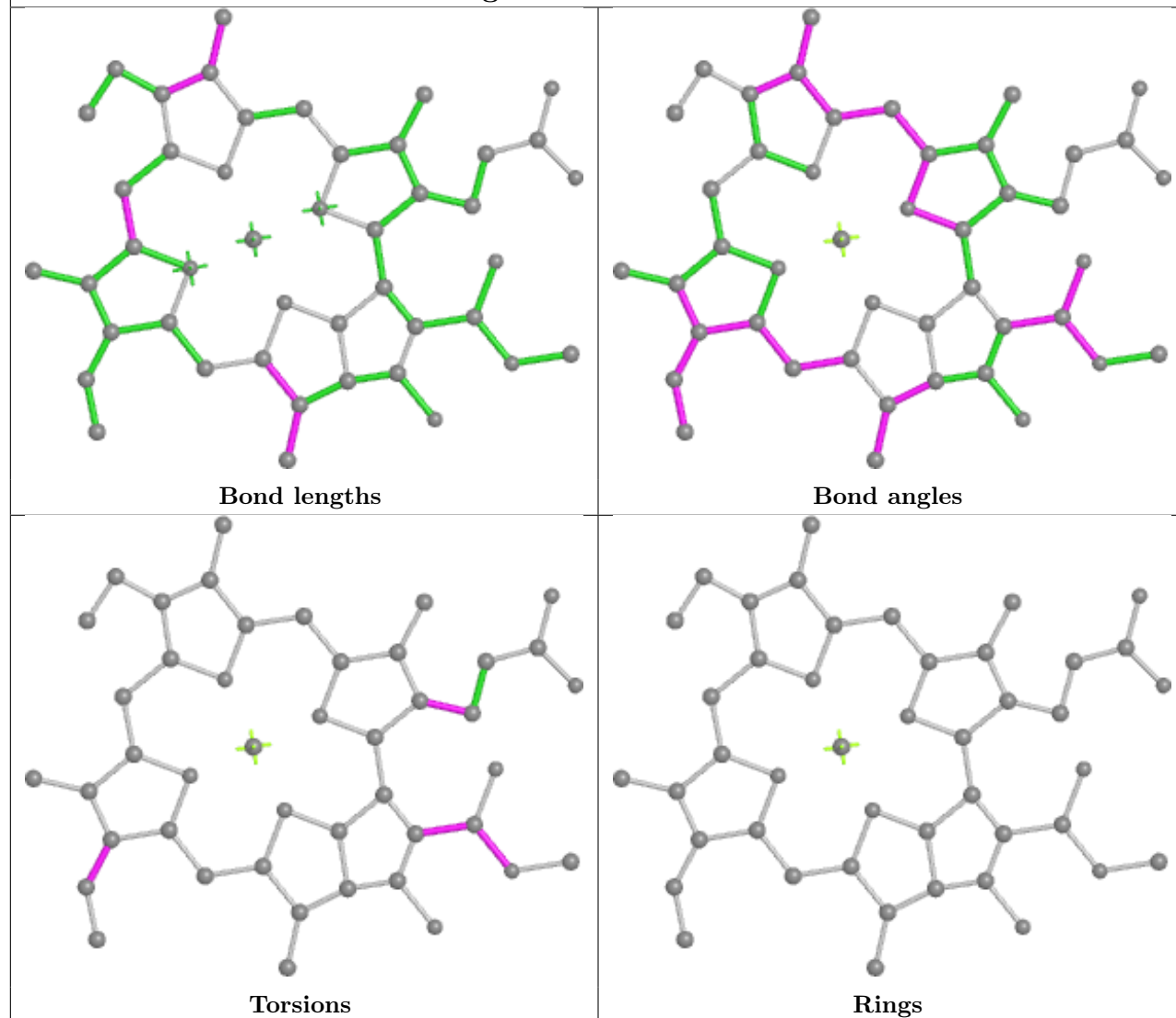


Torsions

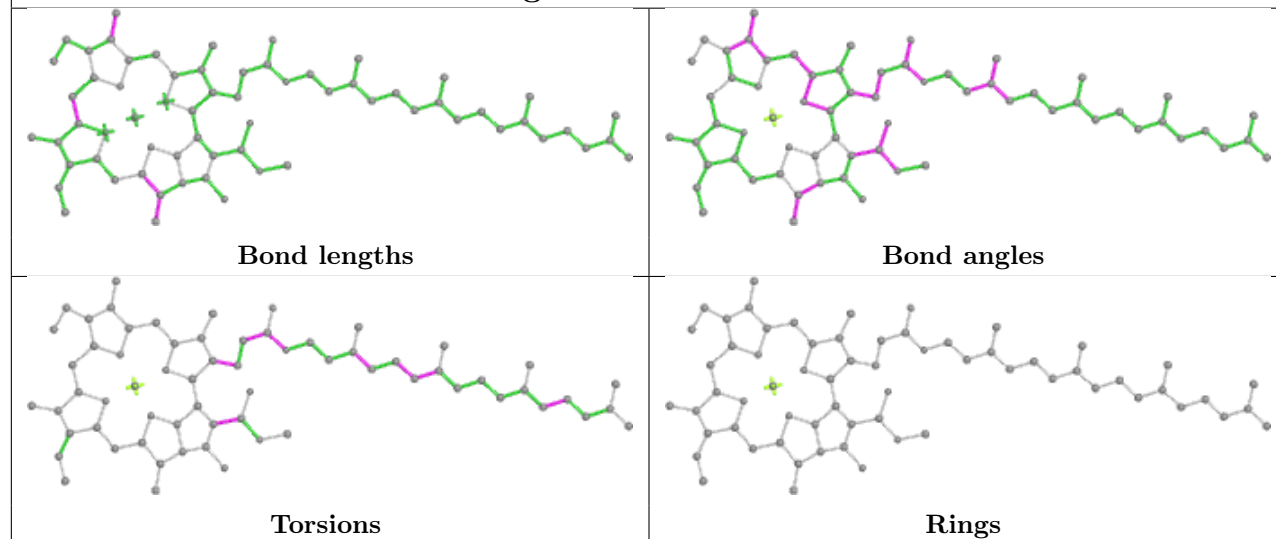


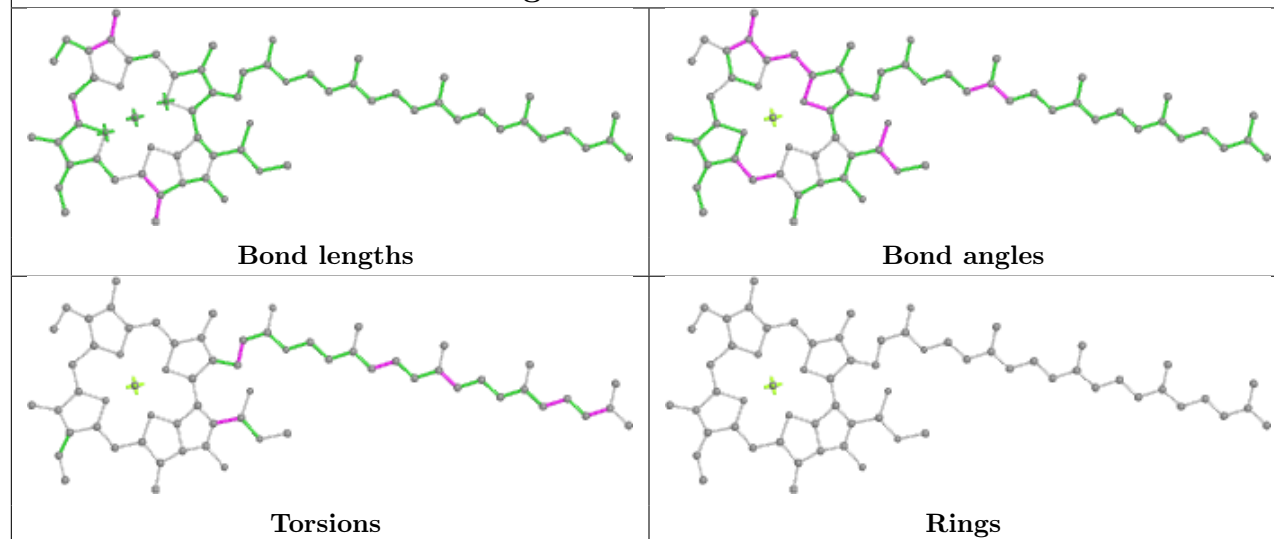
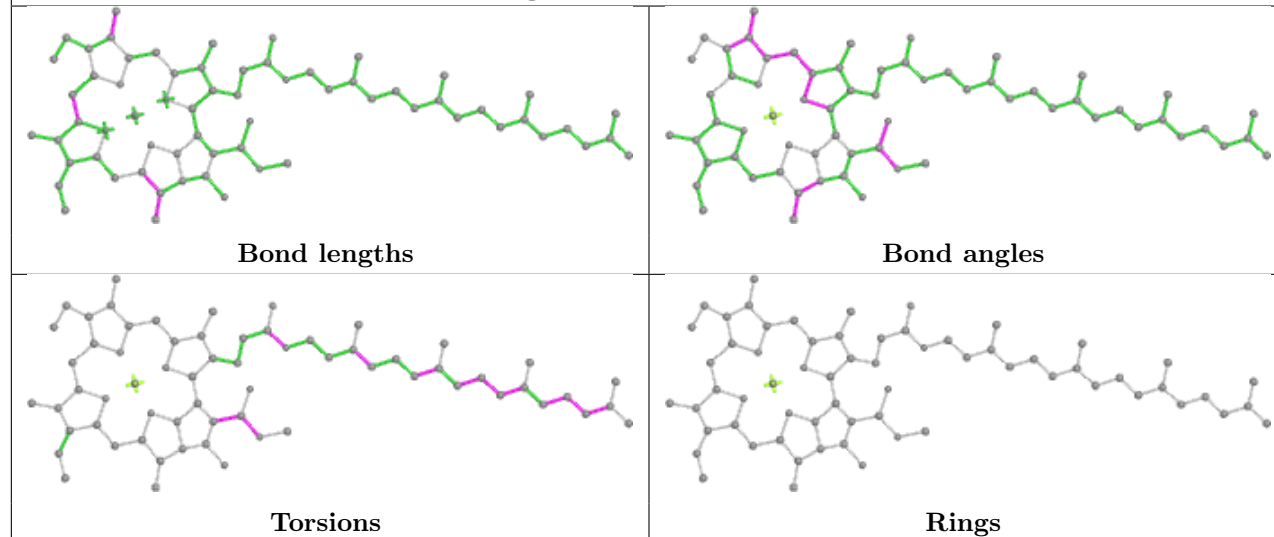
Rings

Ligand CLA B2 820

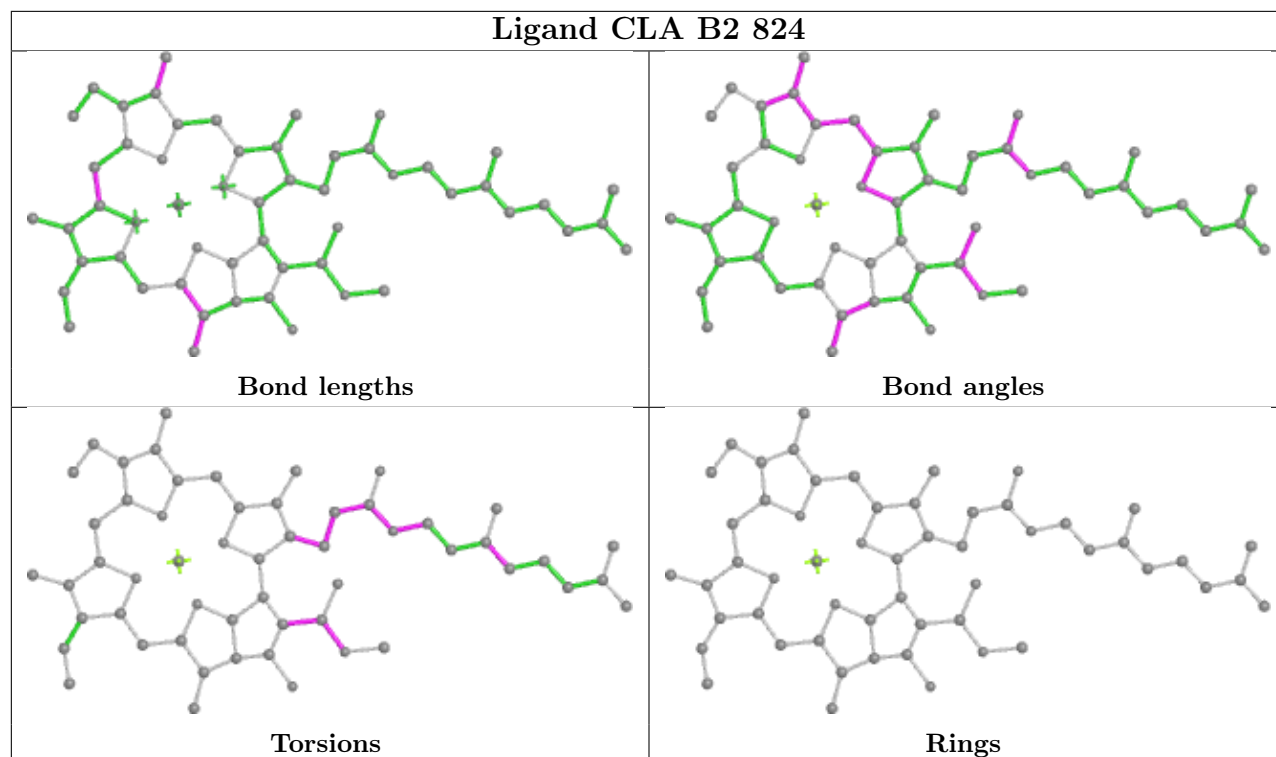


Ligand CLA B2 821

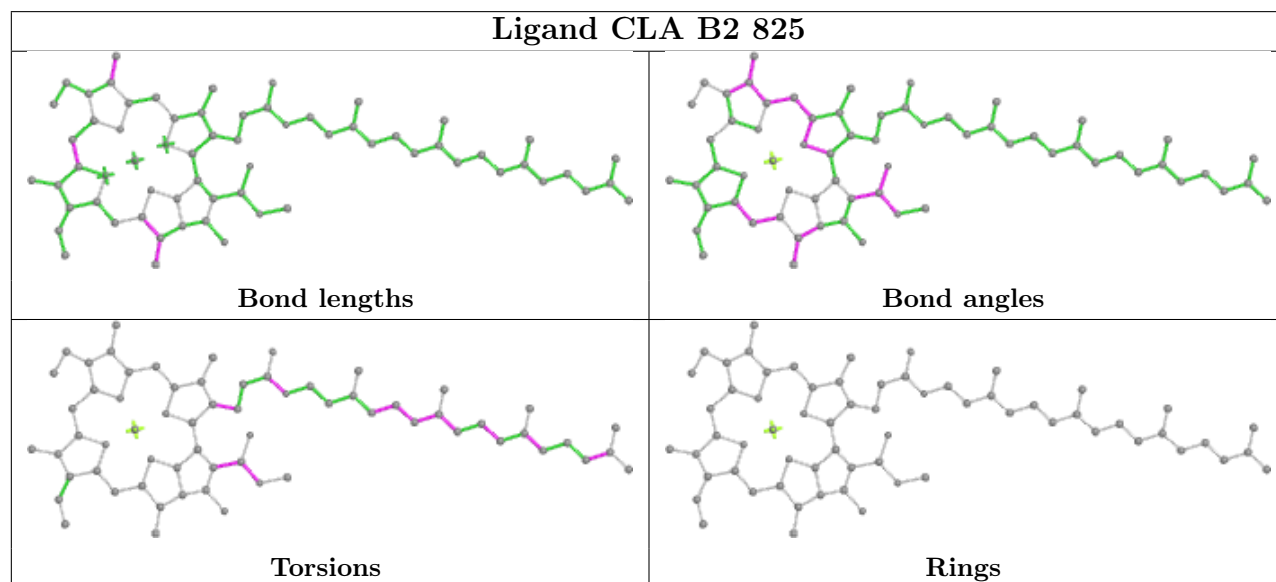


Ligand CLA B2 822**Ligand CLA B2 823**

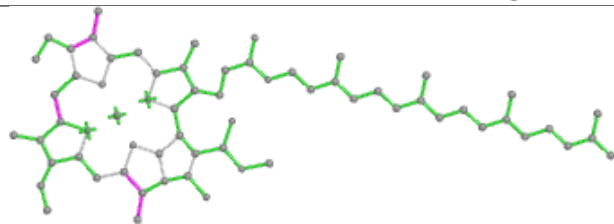
Ligand CLA B2 824



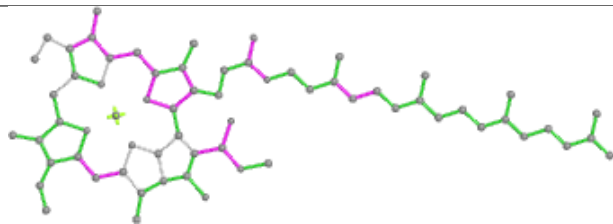
Ligand CLA B2 825



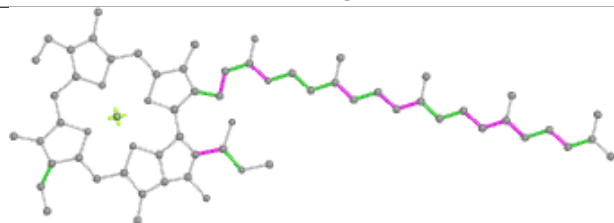
Ligand CLA B2 826



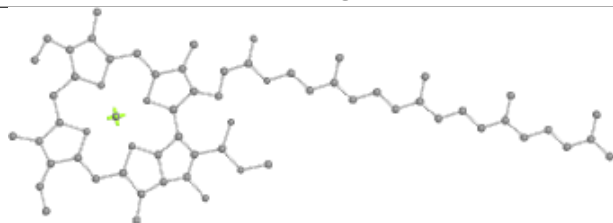
Bond lengths



Bond angles

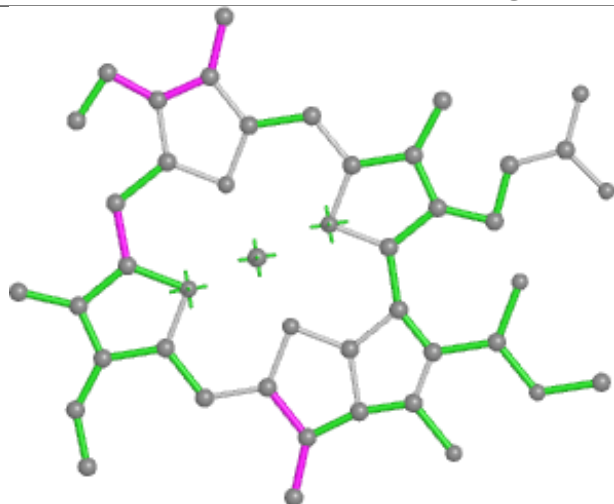


Torsions

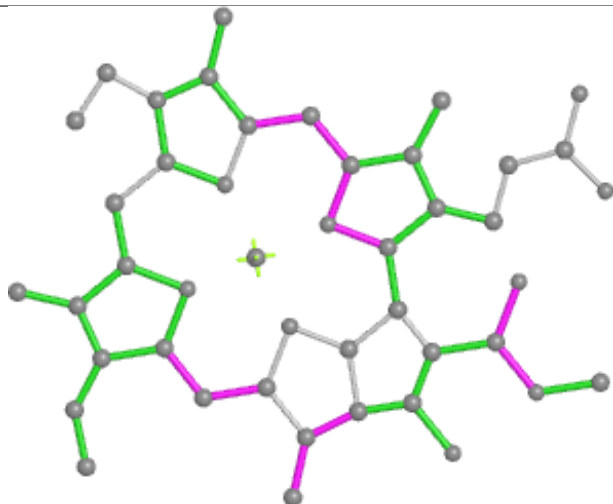


Rings

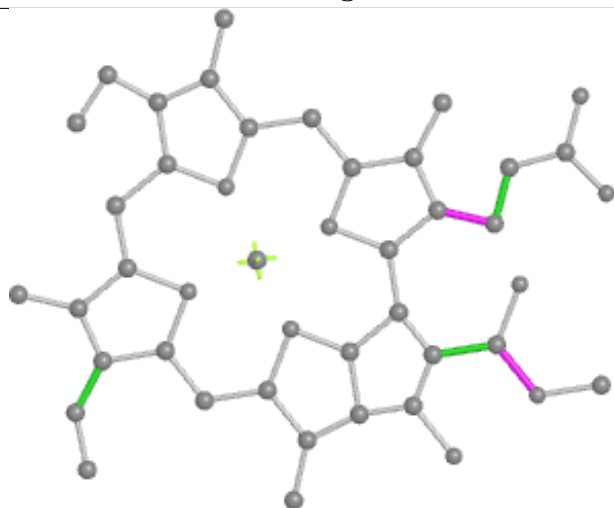
Ligand CLA B2 827



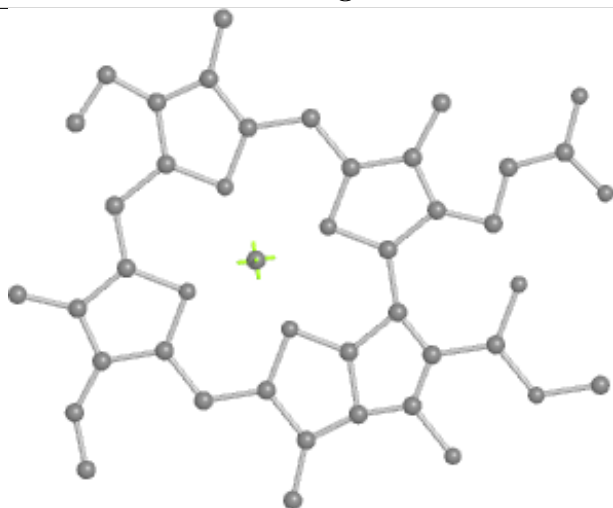
Bond lengths



Bond angles

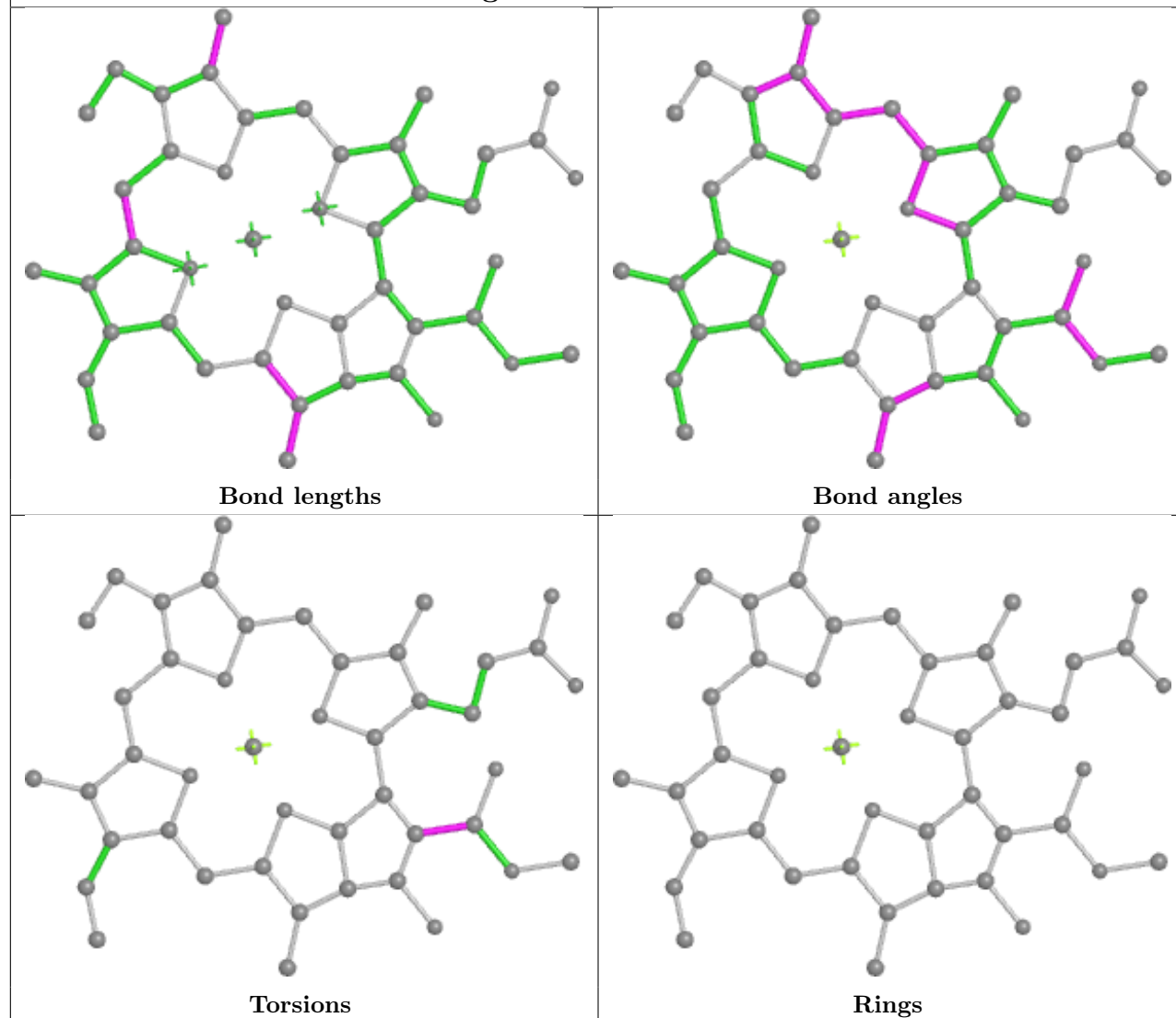


Torsions

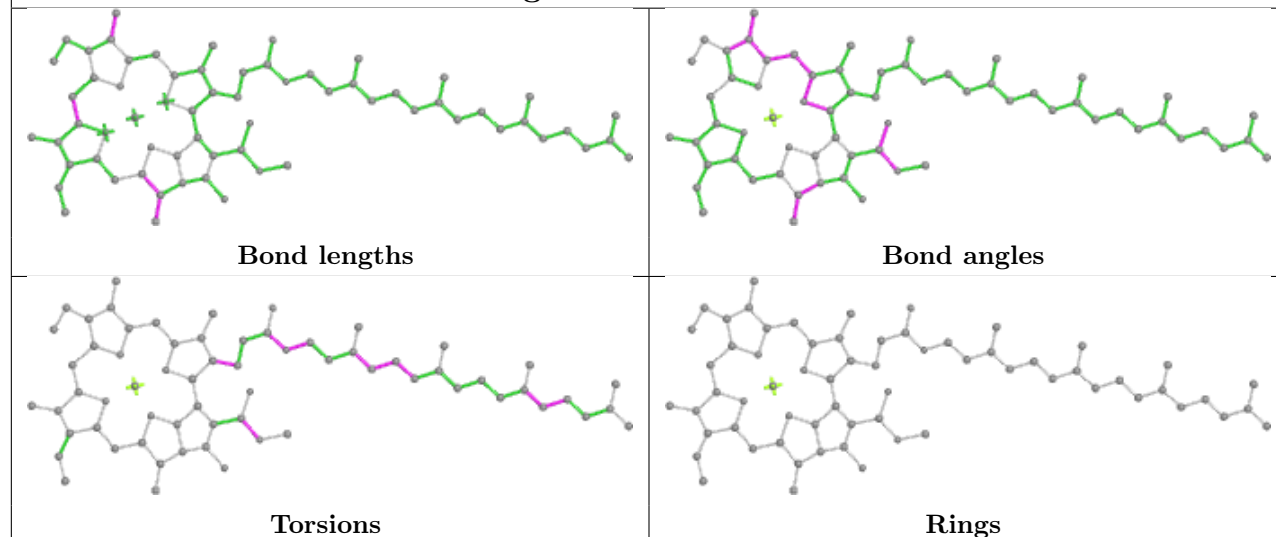


Rings

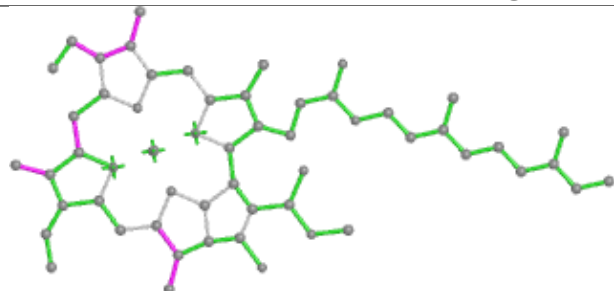
Ligand CLA B2 828



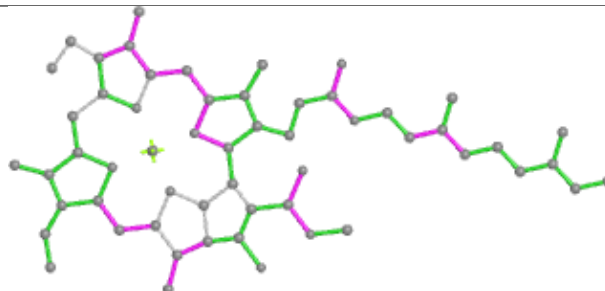
Ligand CLA B2 829



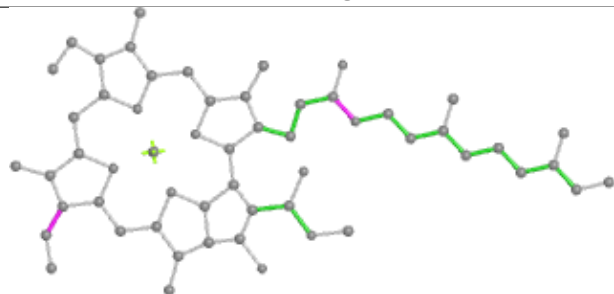
Ligand CLA B2 830



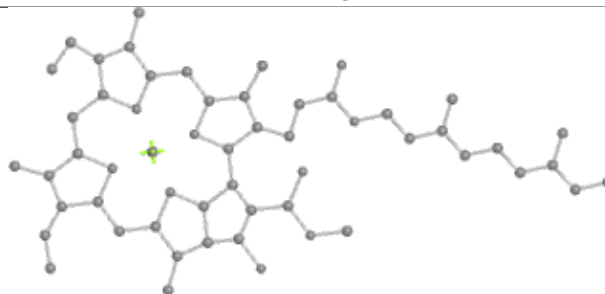
Bond lengths



Bond angles

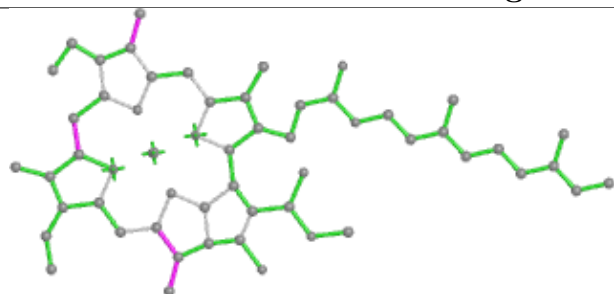


Torsions

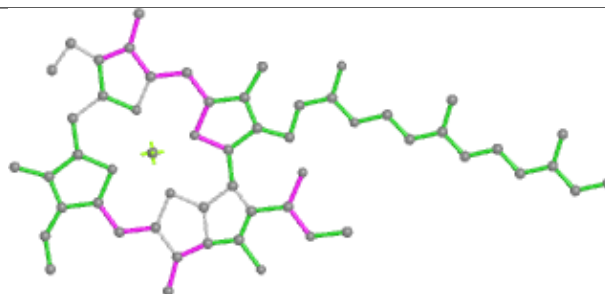


Rings

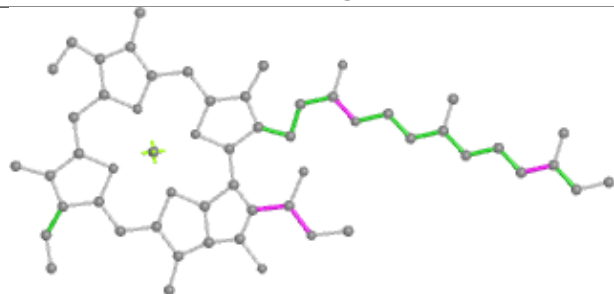
Ligand CLA B2 831



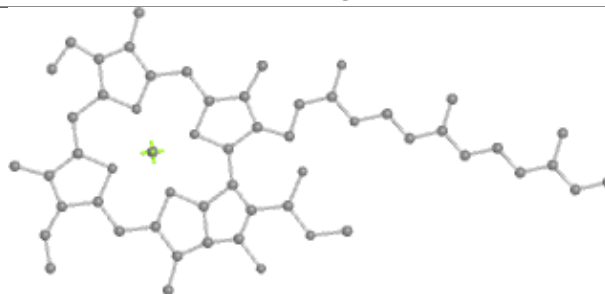
Bond lengths



Bond angles

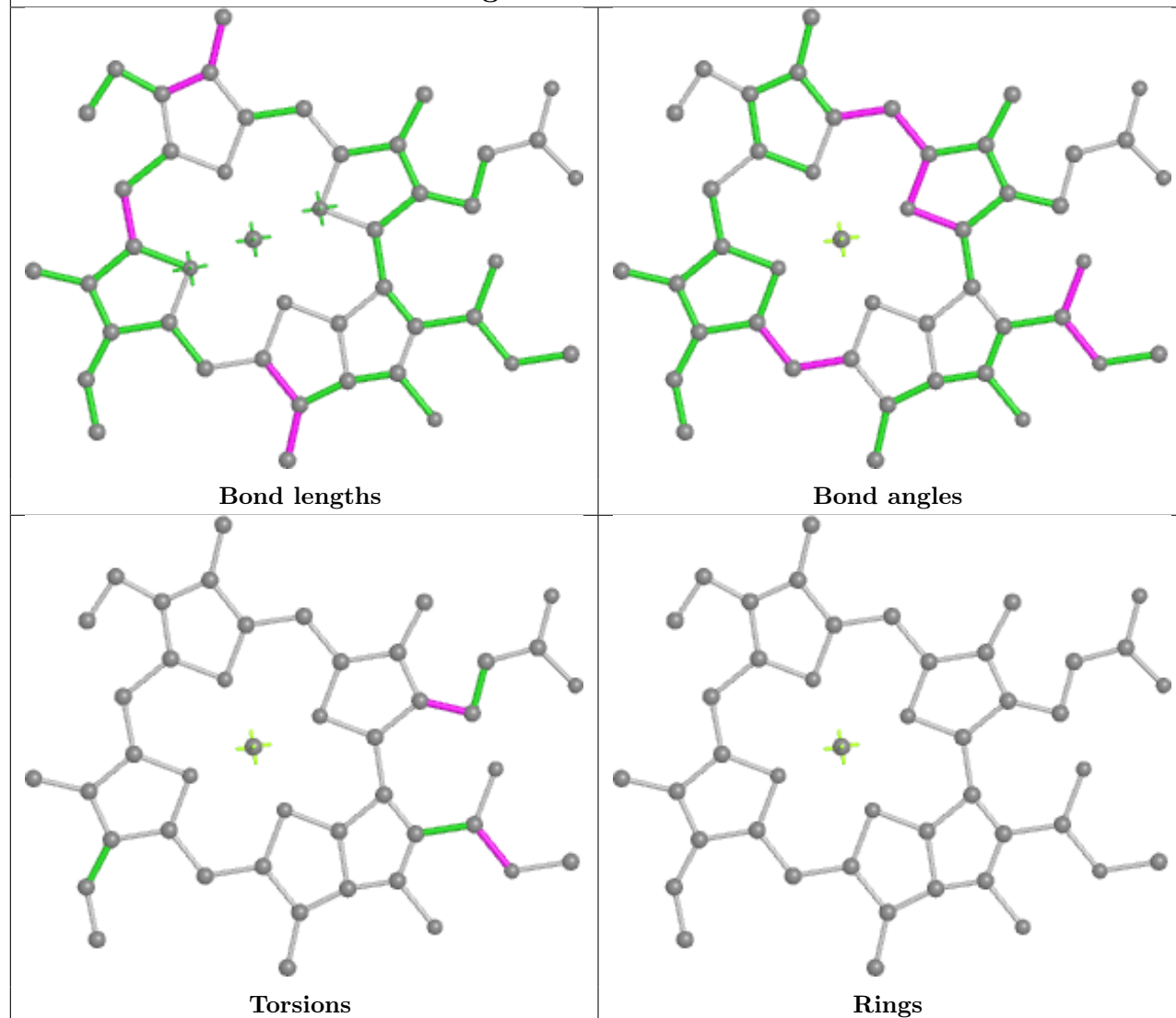


Torsions

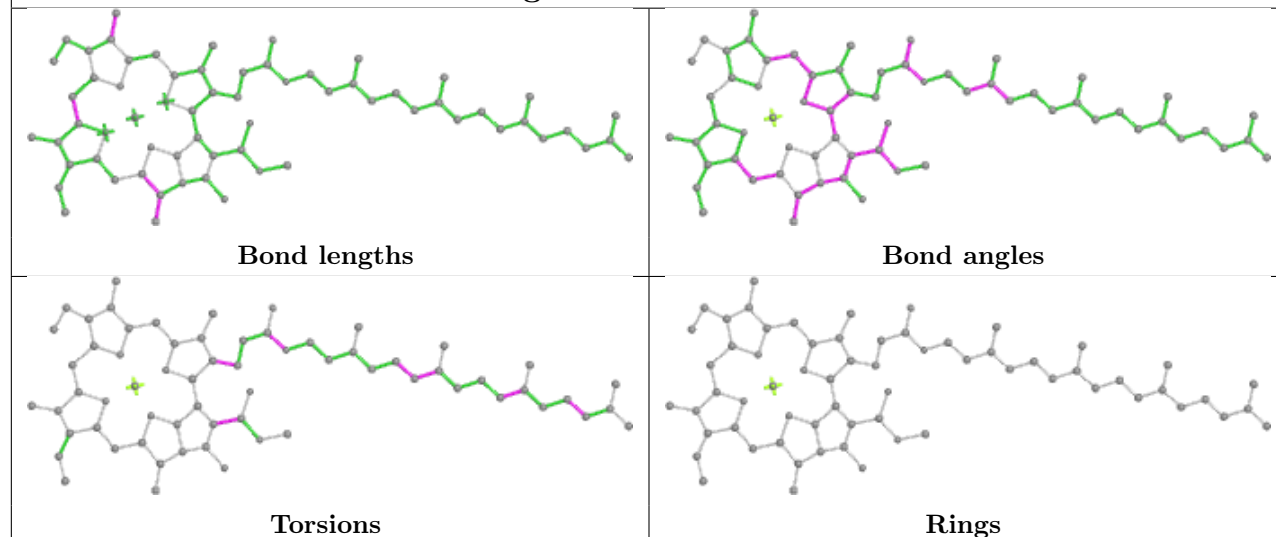


Rings

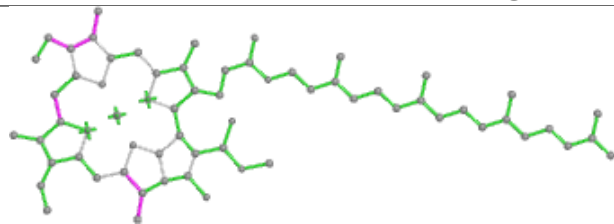
Ligand CLA B2 832



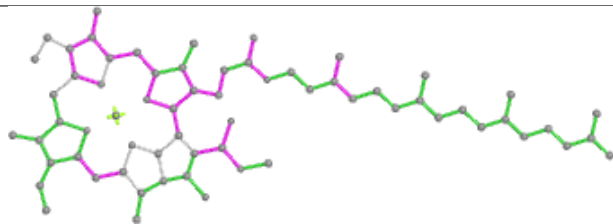
Ligand CLA B2 833



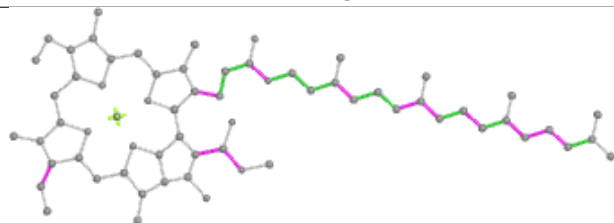
Ligand CLA B2 834



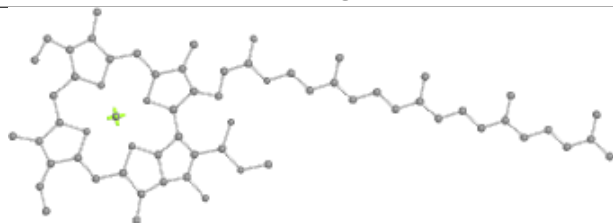
Bond lengths



Bond angles

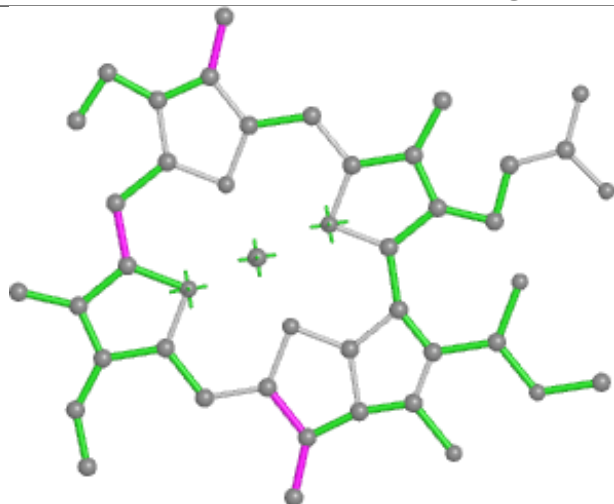


Torsions

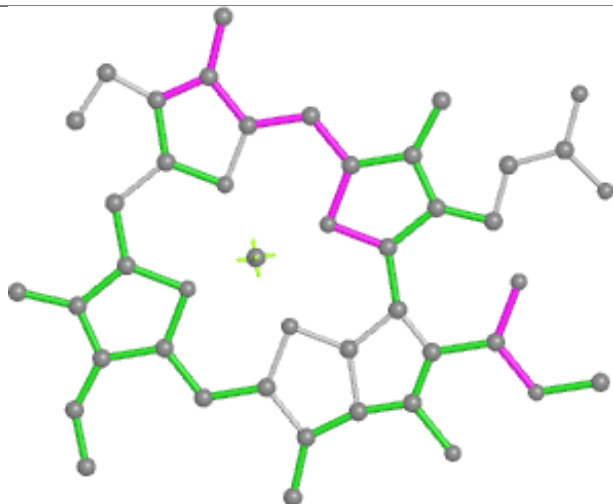


Rings

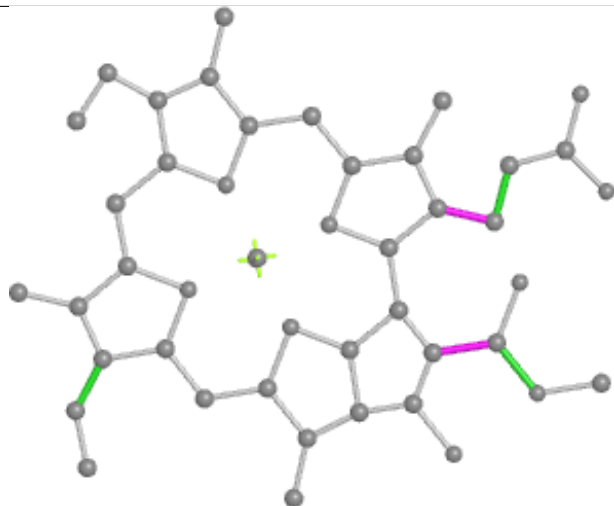
Ligand CLA B2 835



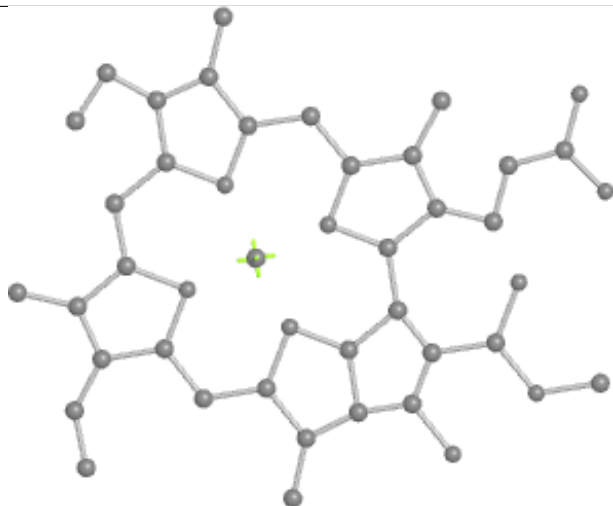
Bond lengths



Bond angles

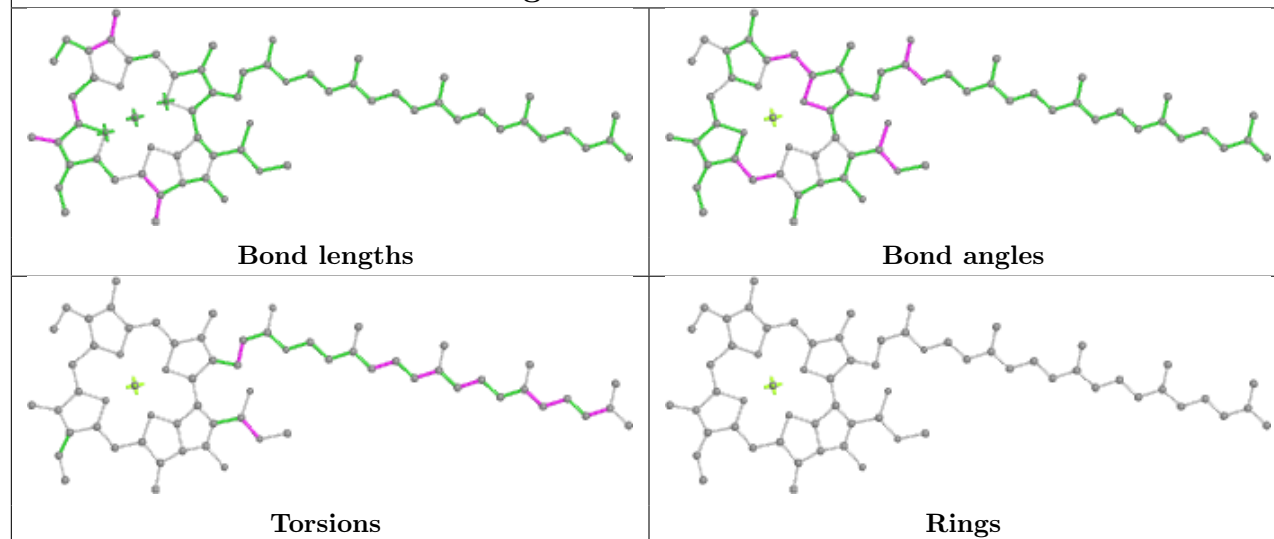


Torsions

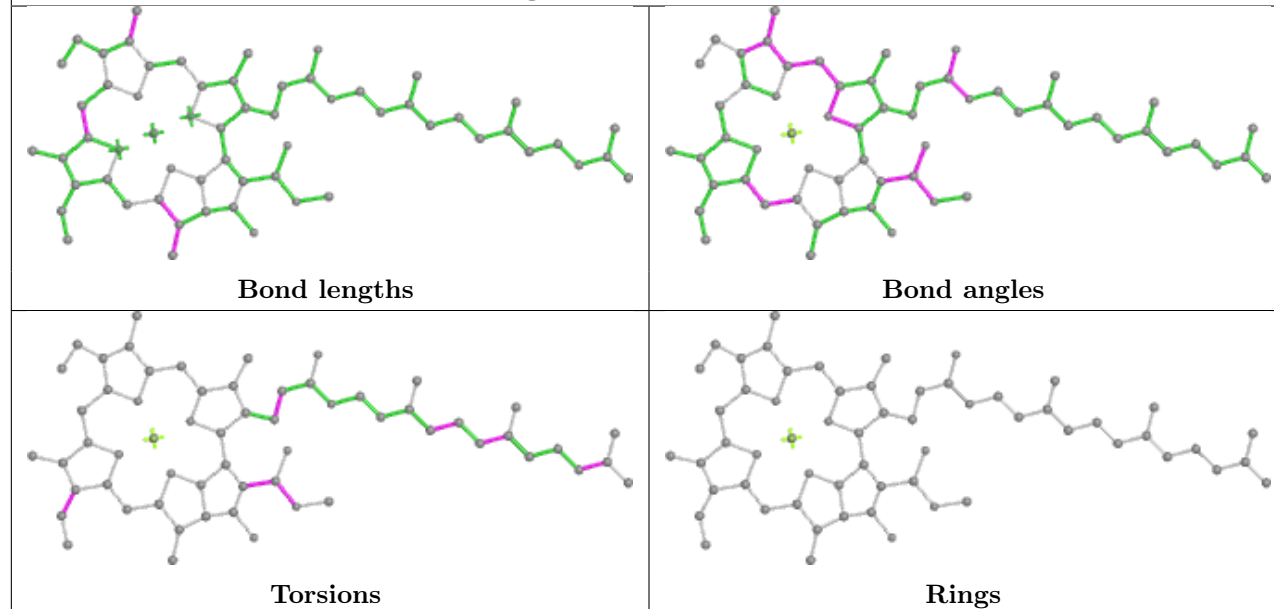


Rings

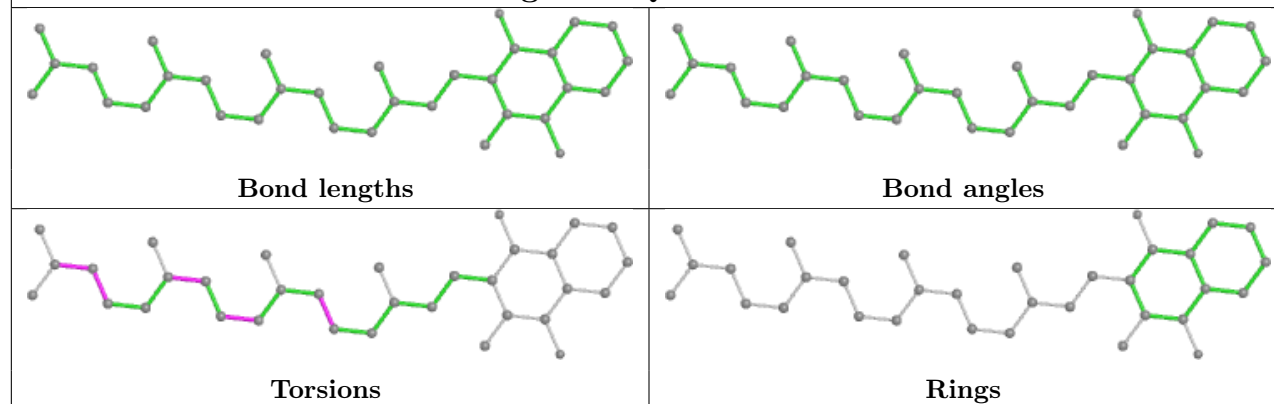
Ligand CLA B2 836

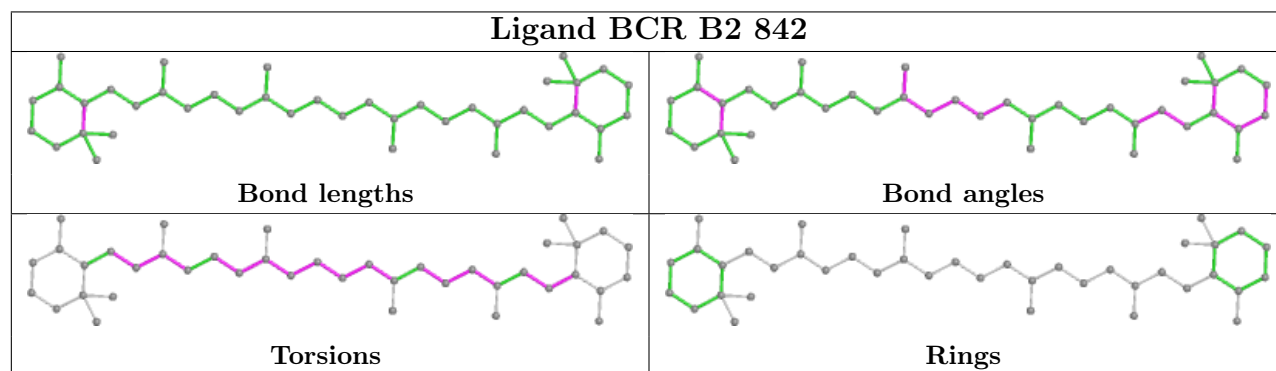
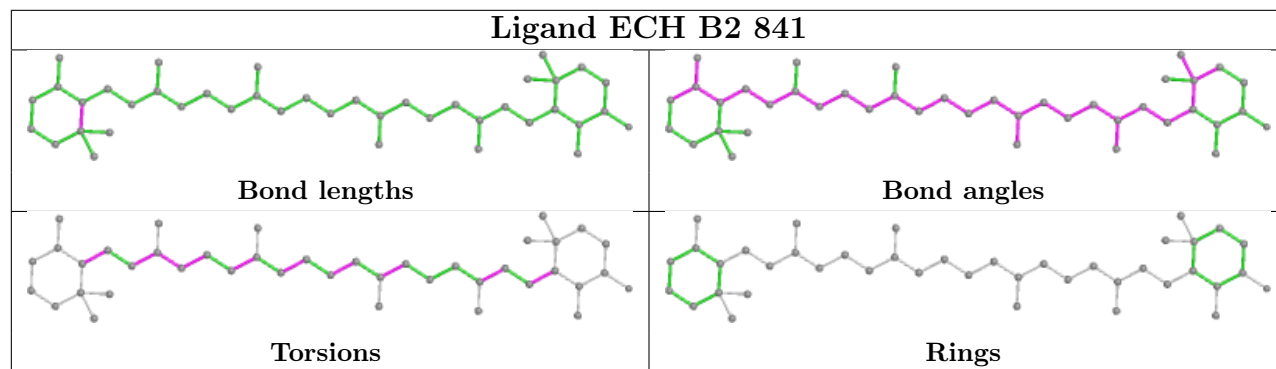
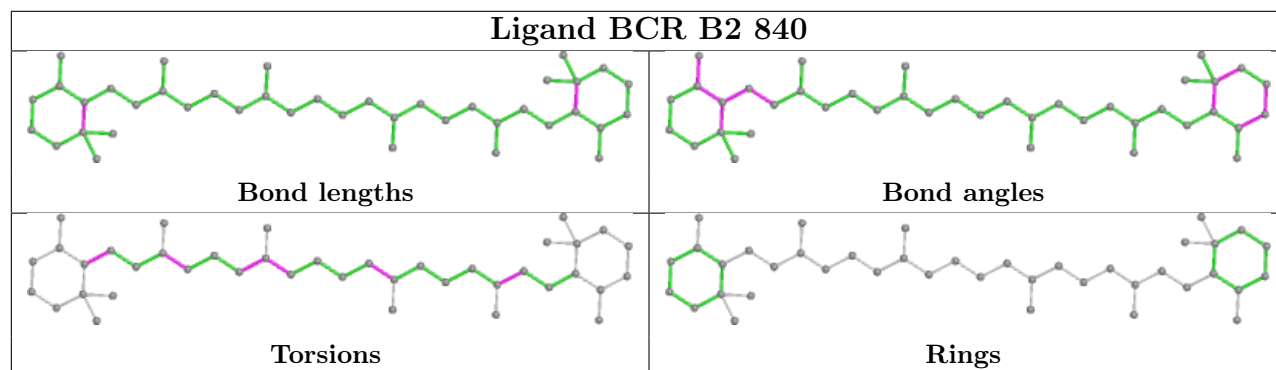
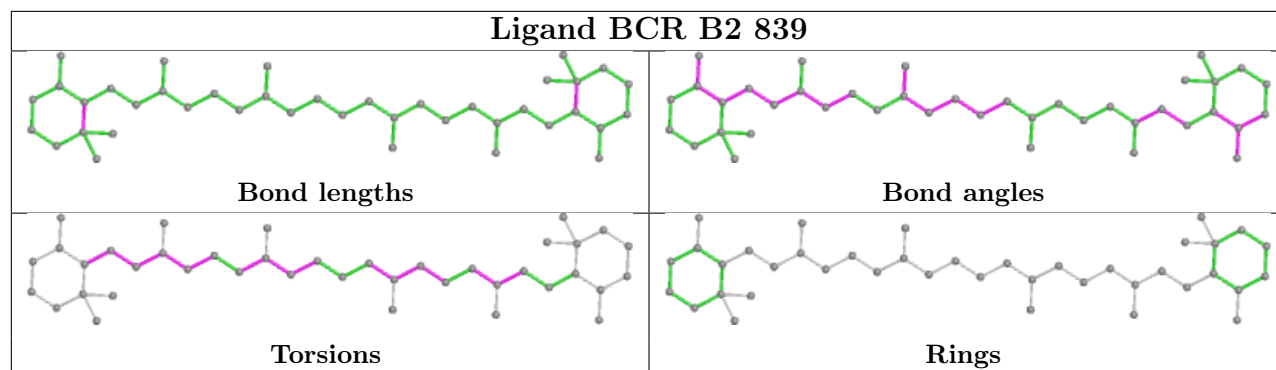


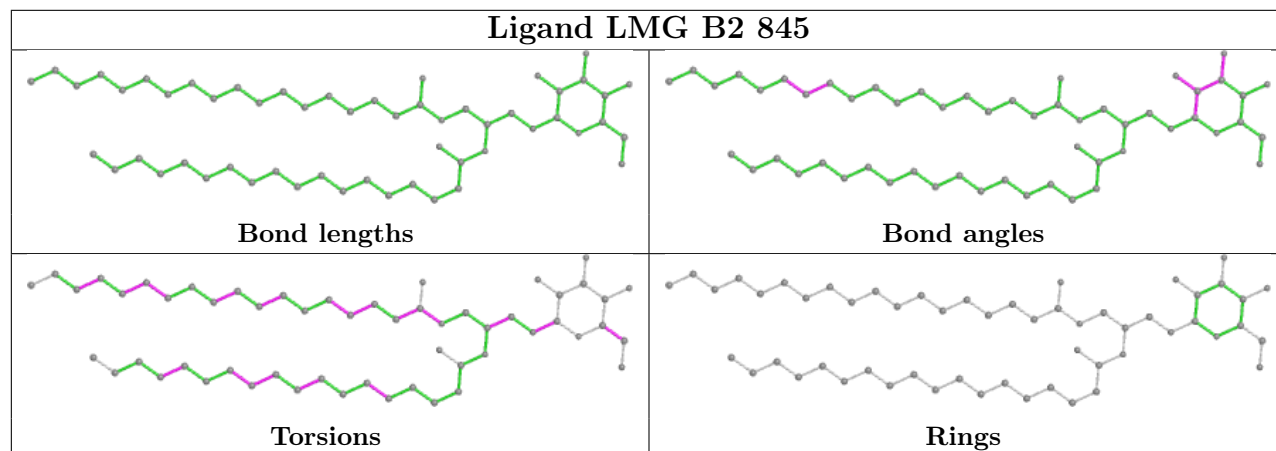
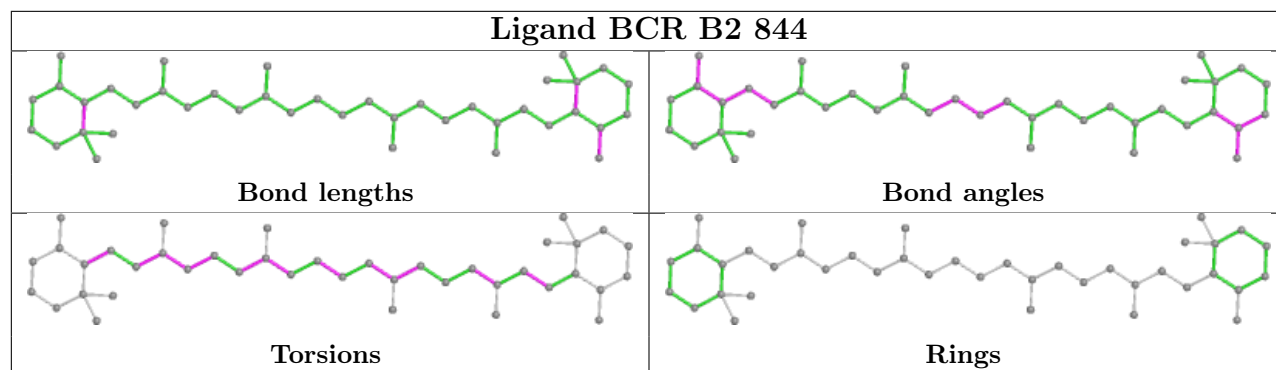
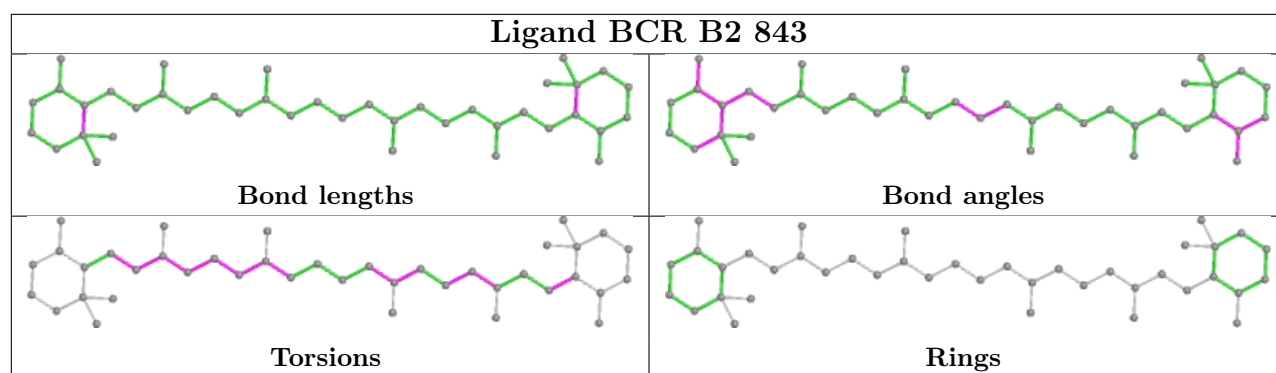
Ligand CLA B2 837



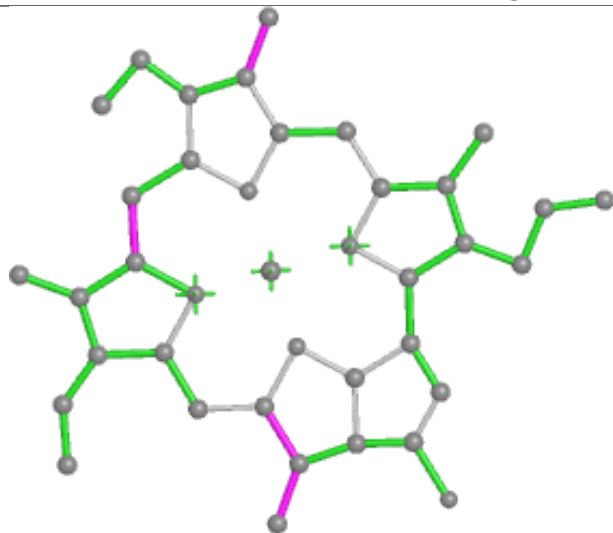
Ligand PQN B2 838



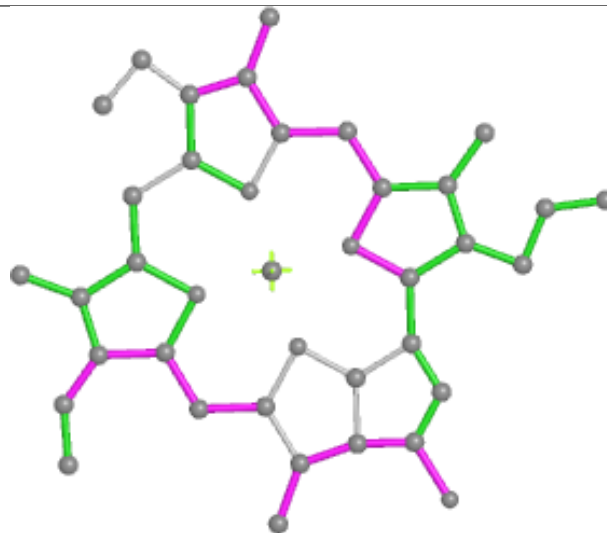




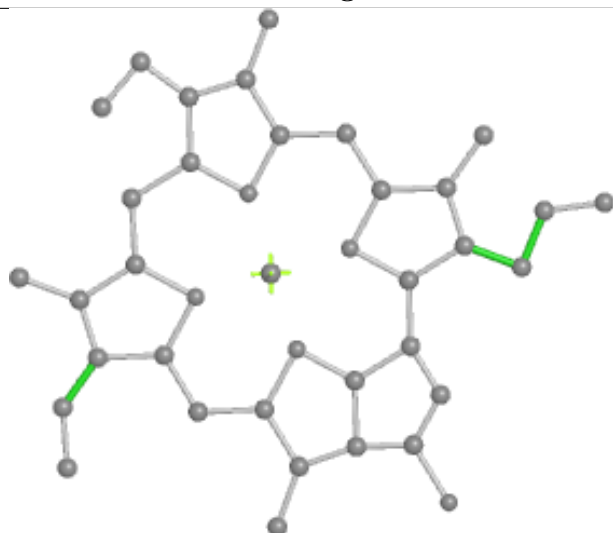
Ligand CLA B2 846



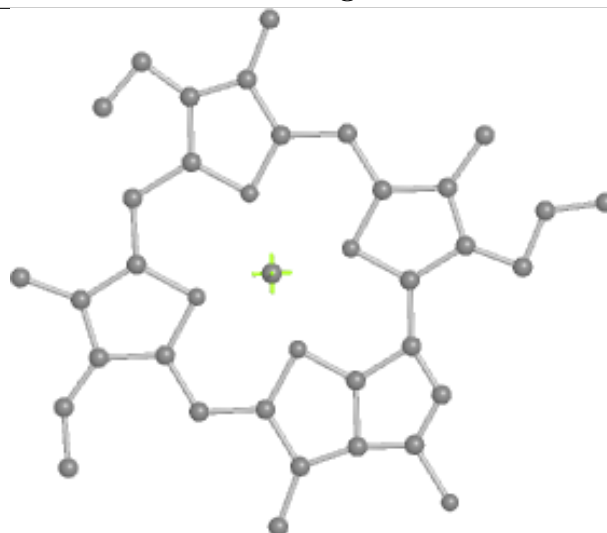
Bond lengths



Bond angles

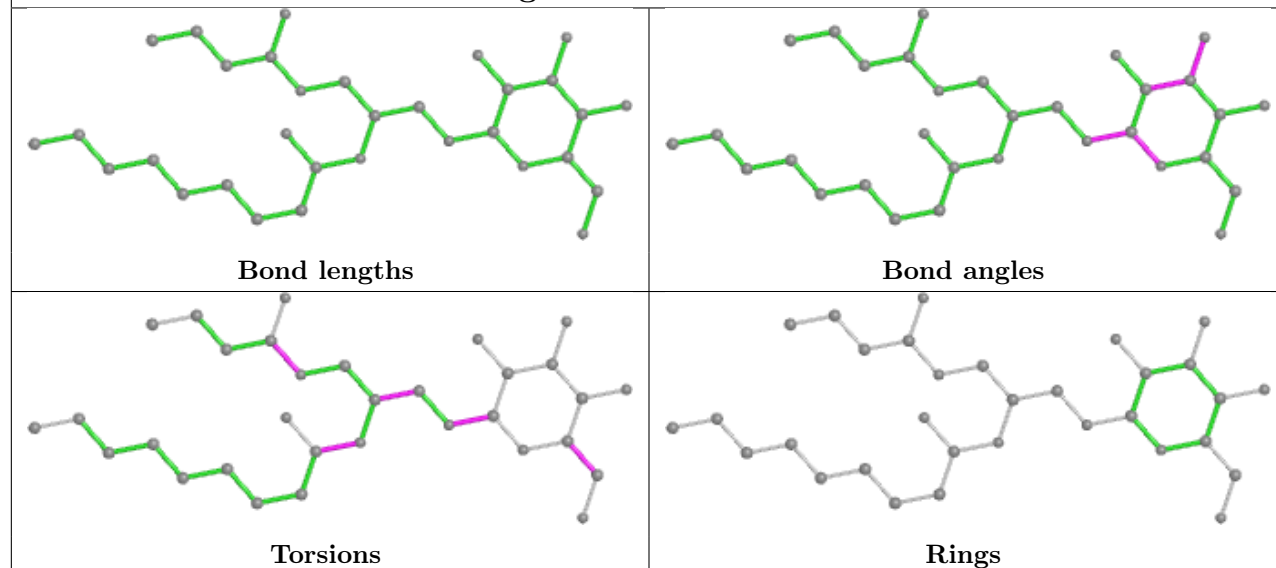


Torsions

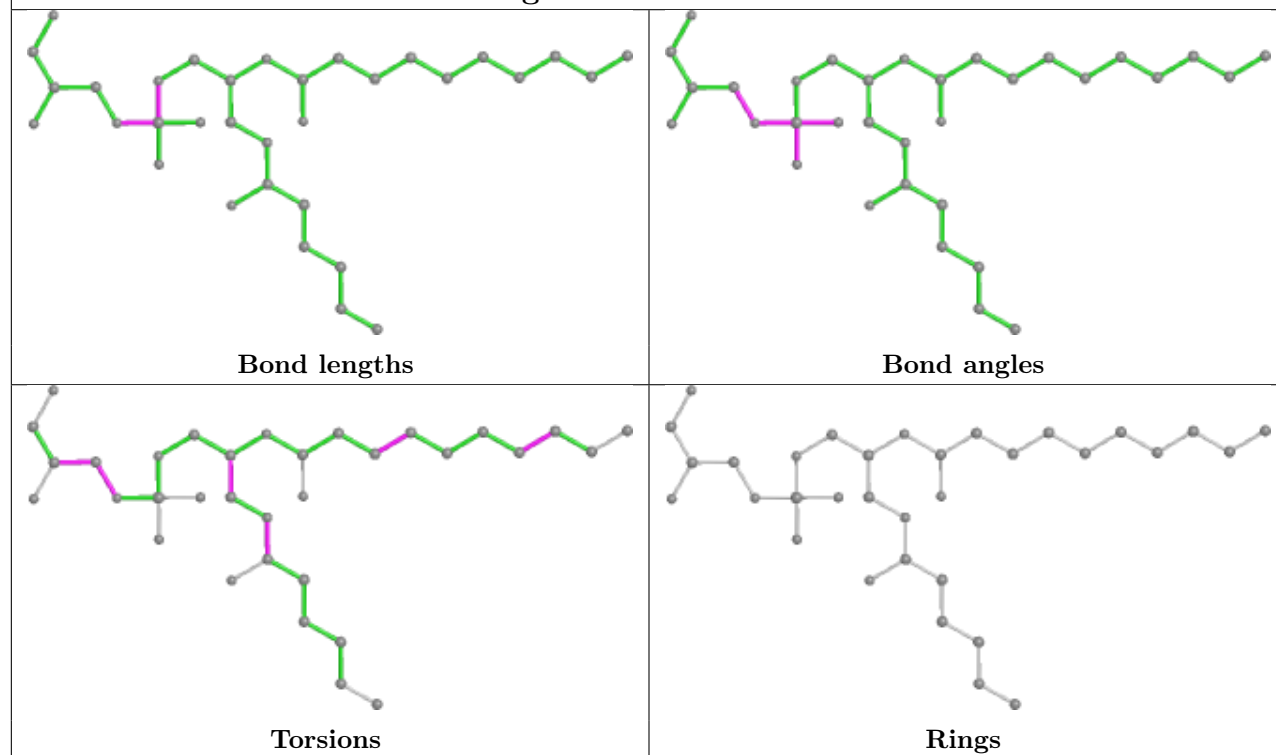


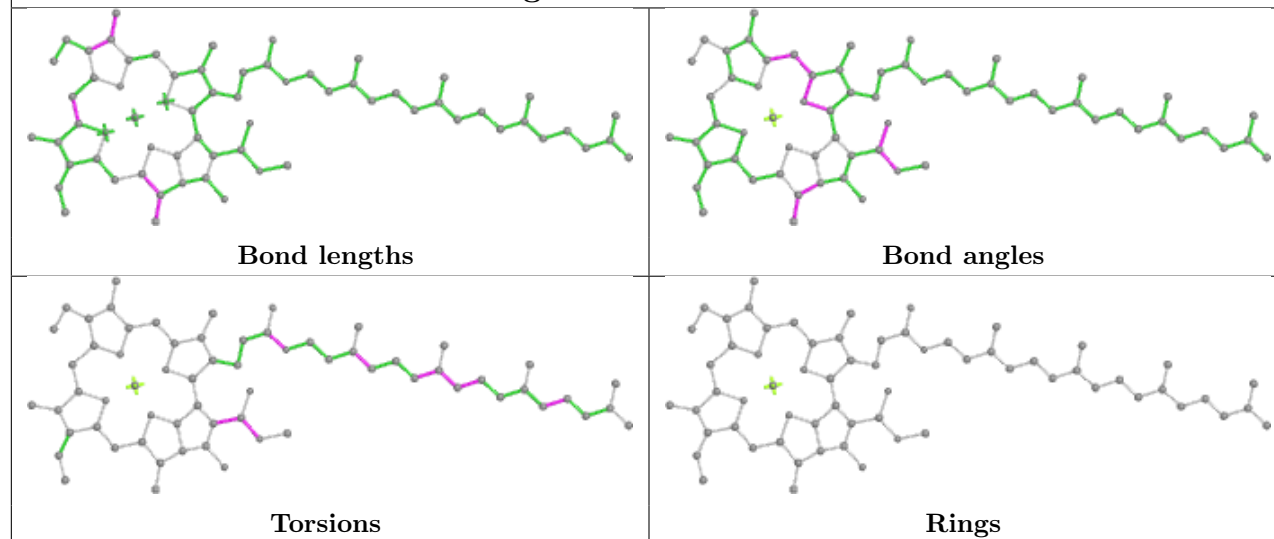
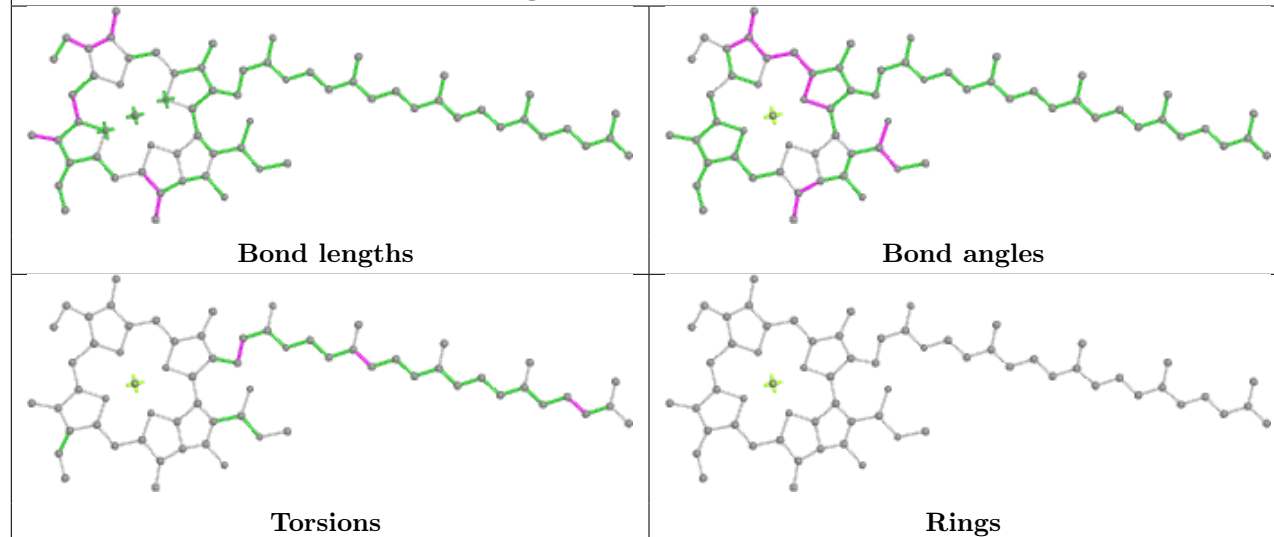
Rings

Ligand LMG B2 847

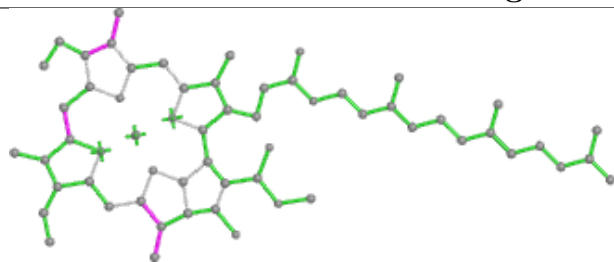


Ligand LHG B2 848

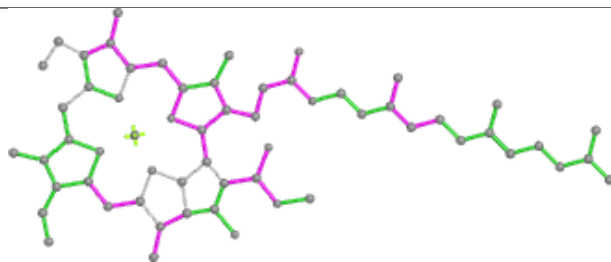


Ligand CLA B2 849**Ligand CLA B2 850**

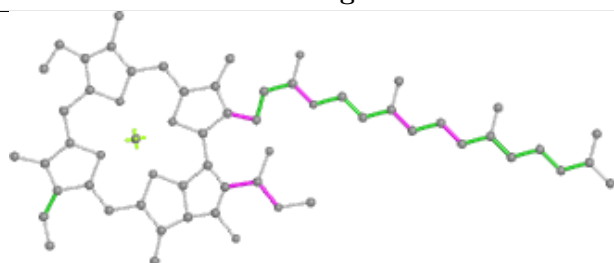
Ligand CLA B2 851



Bond lengths



Bond angles

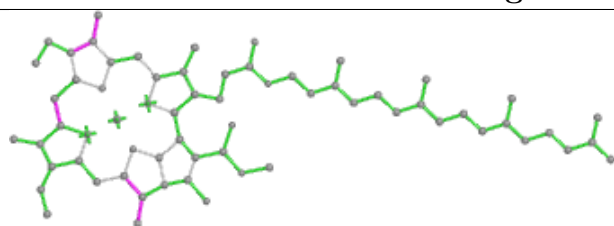


Torsions

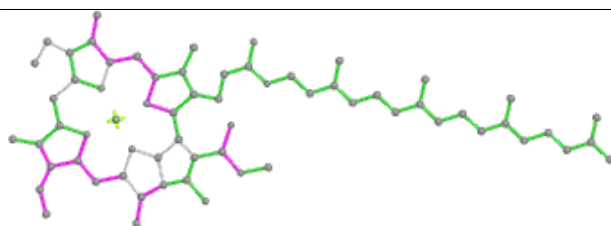


Rings

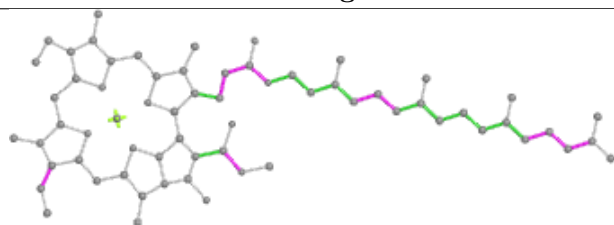
Ligand CLA B2 852



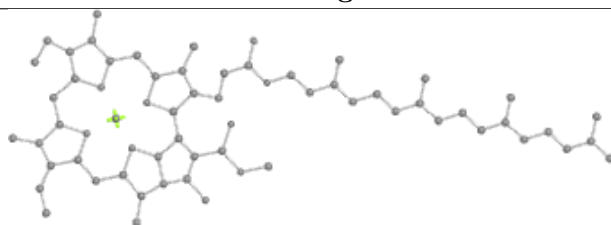
Bond lengths



Bond angles

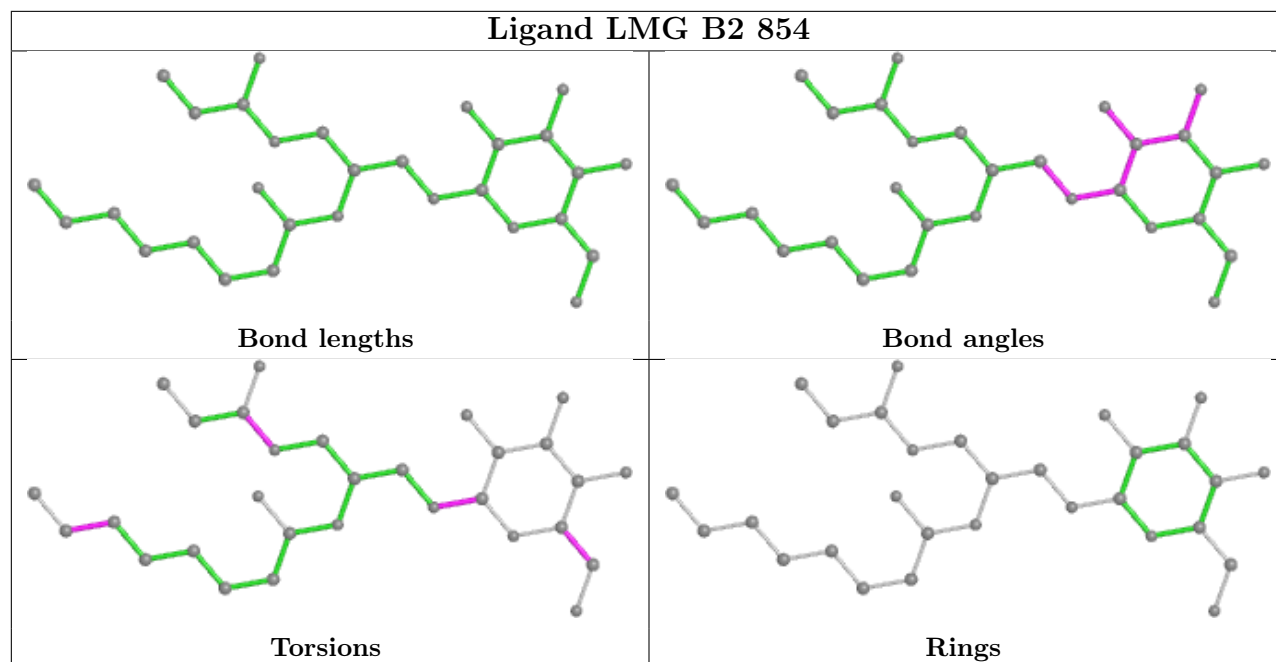


Torsions

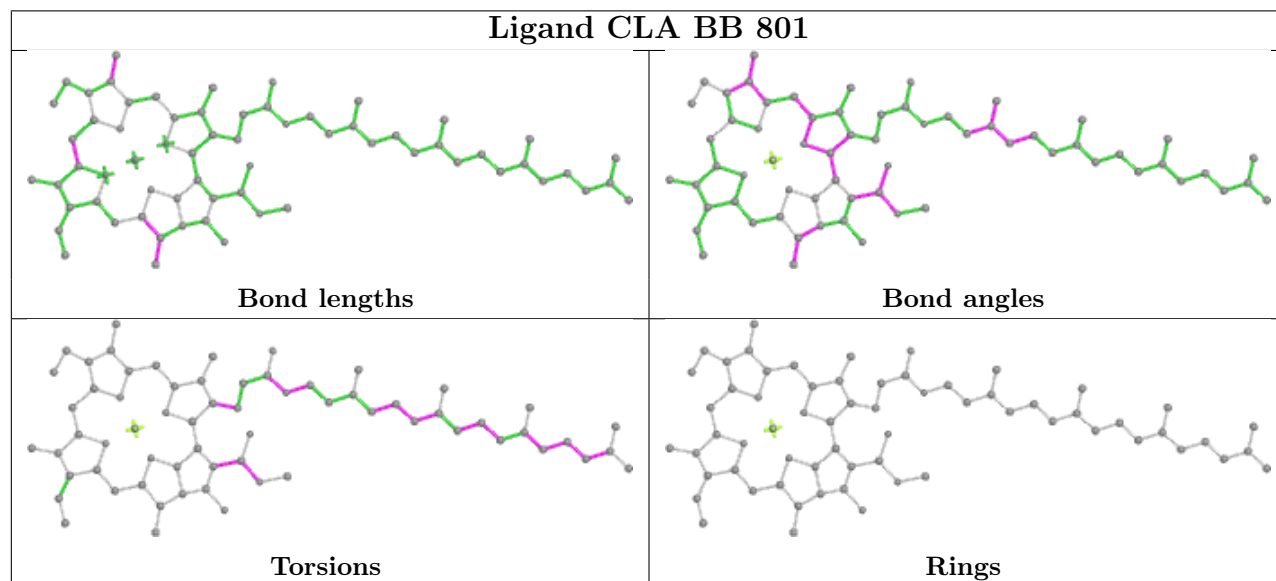


Rings

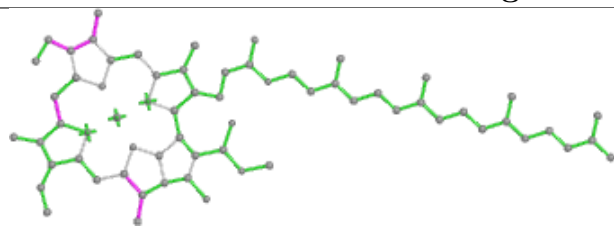
Ligand LMG B2 854



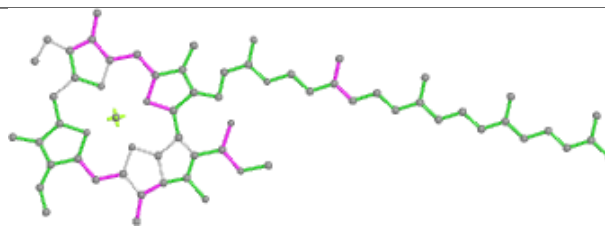
Ligand CLA BB 801



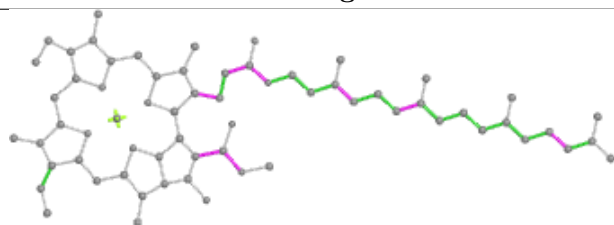
Ligand CLA BB 802



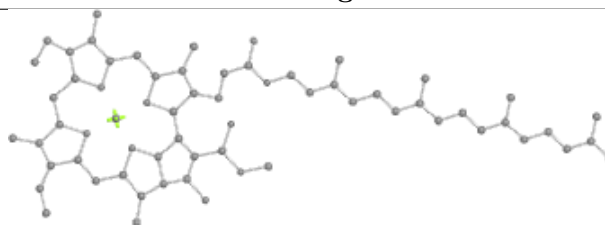
Bond lengths



Bond angles

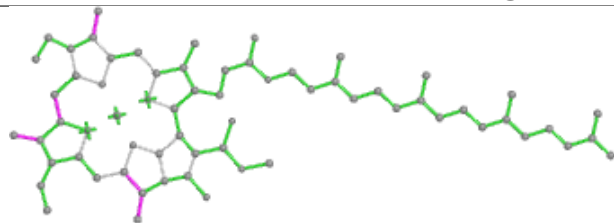


Torsions

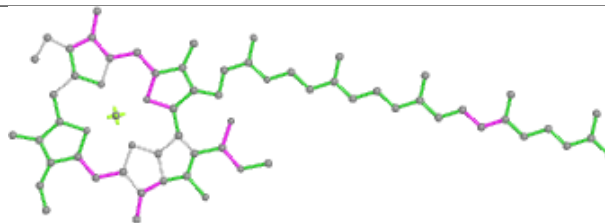


Rings

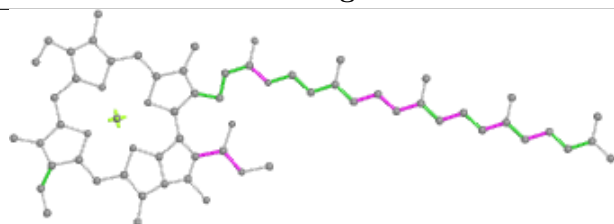
Ligand CLA BB 803



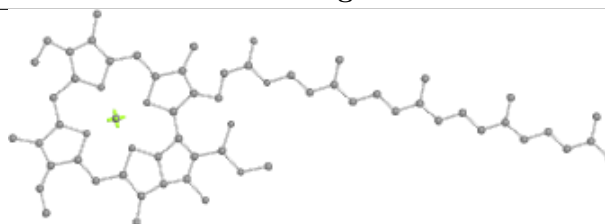
Bond lengths



Bond angles

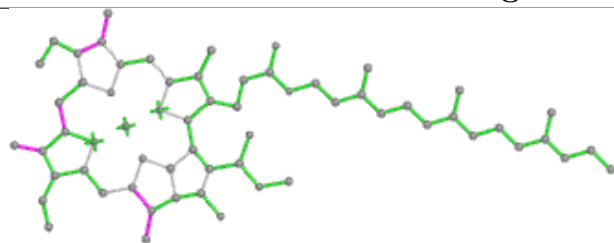


Torsions

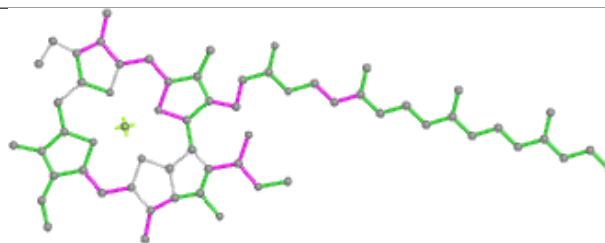


Rings

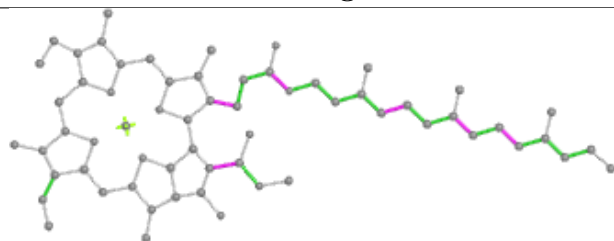
Ligand CLA BB 804



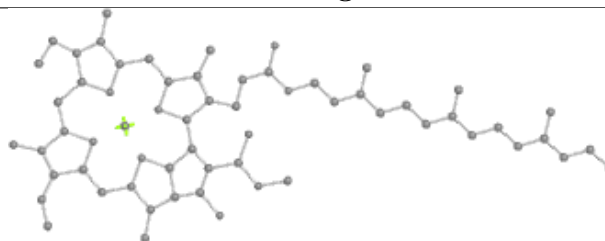
Bond lengths



Bond angles

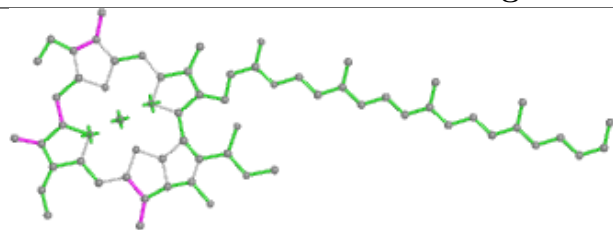


Torsions

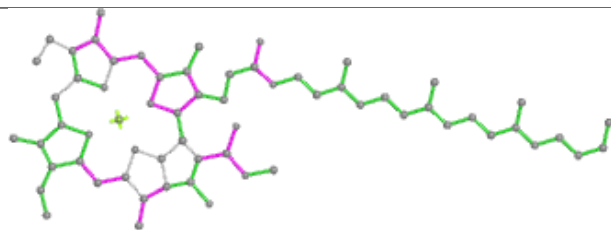


Rings

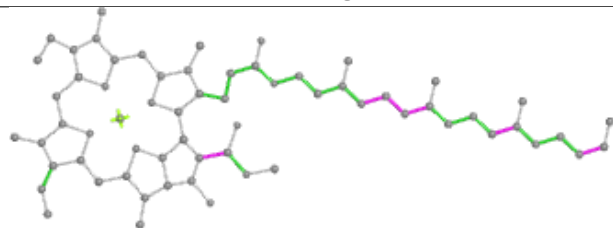
Ligand CLA BB 805



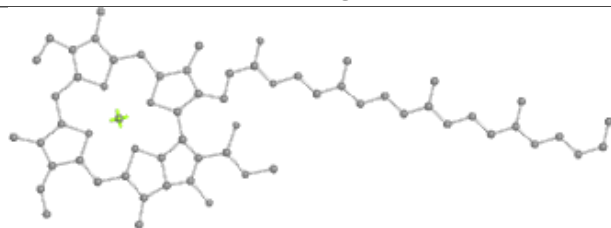
Bond lengths



Bond angles

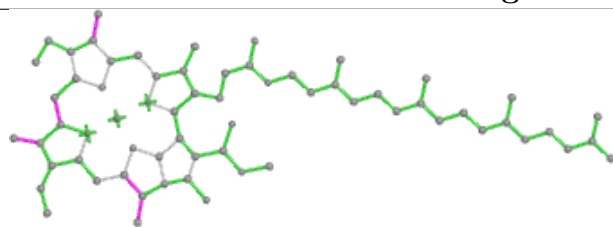


Torsions

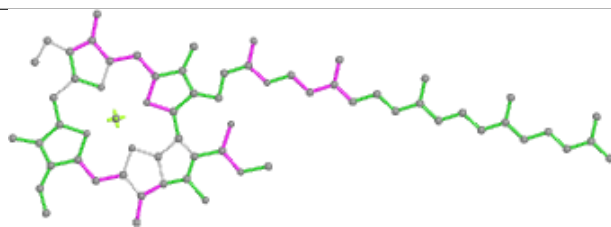


Rings

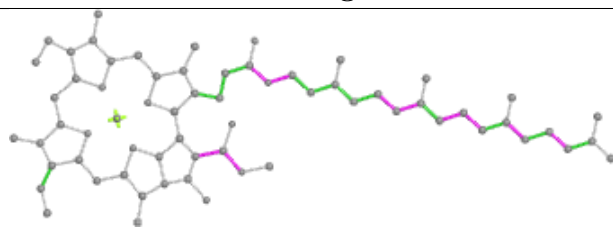
Ligand CLA BB 806



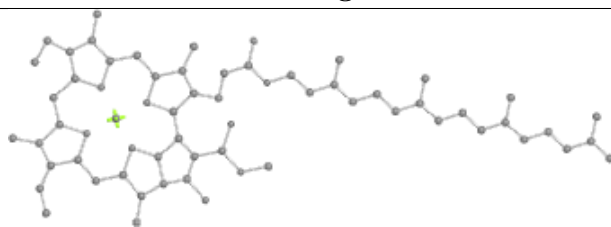
Bond lengths



Bond angles

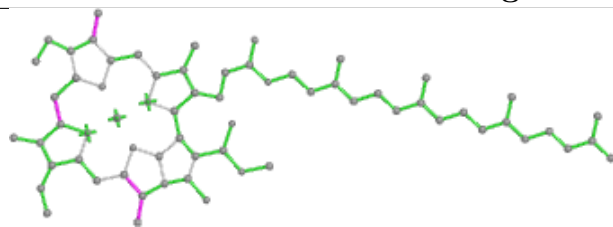


Torsions

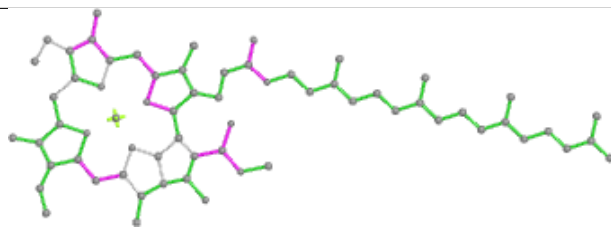


Rings

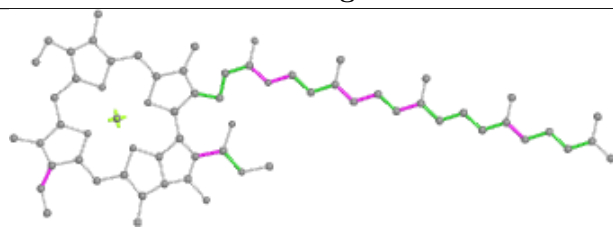
Ligand CLA BB 807



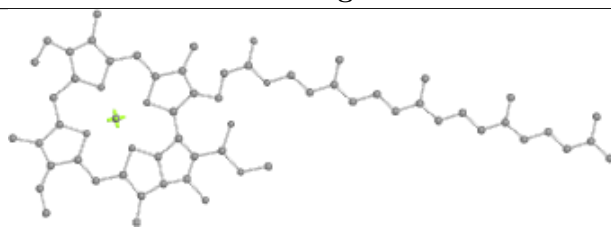
Bond lengths



Bond angles

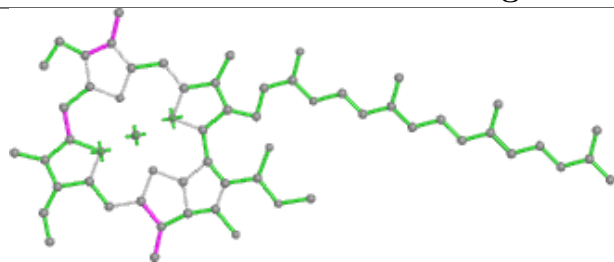


Torsions

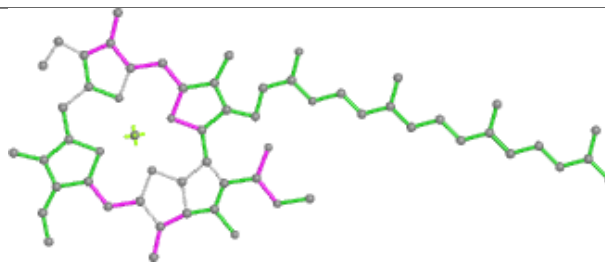


Rings

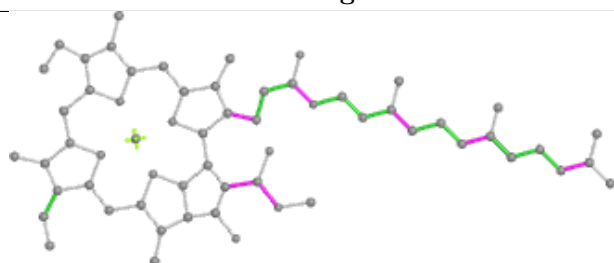
Ligand CLA BB 808



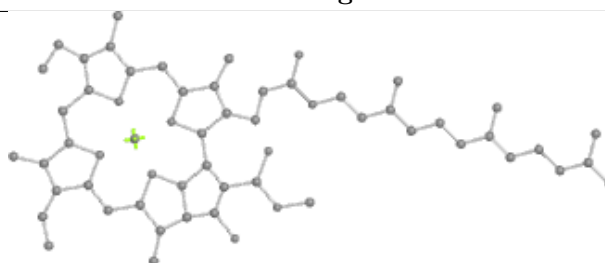
Bond lengths



Bond angles

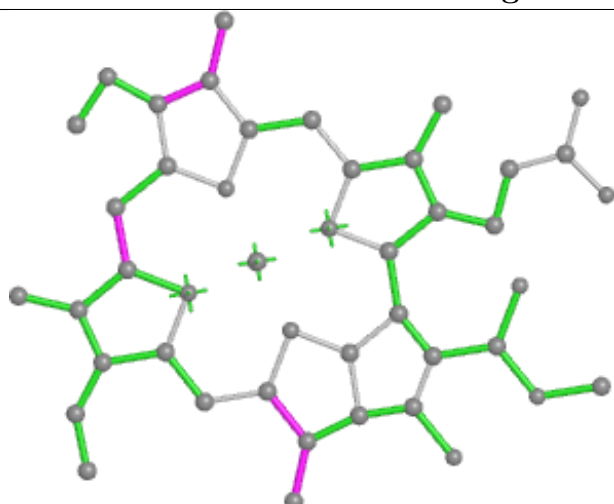


Torsions

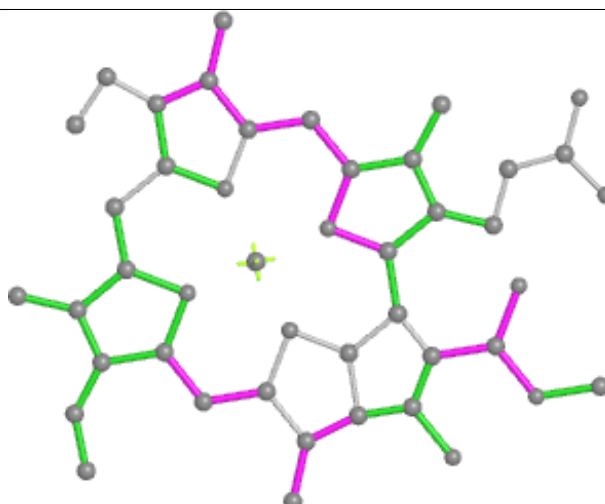


Rings

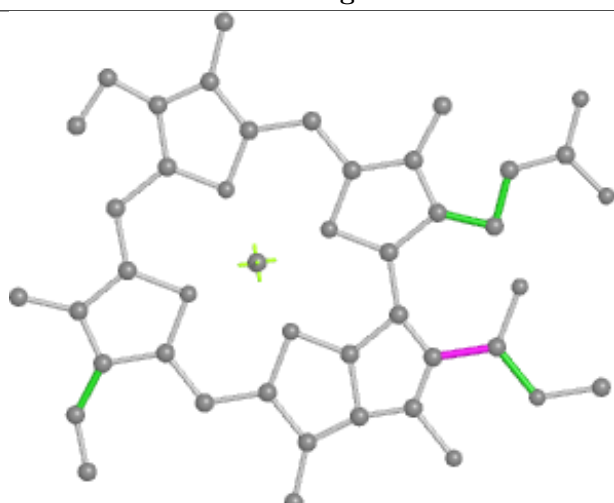
Ligand CLA BB 809



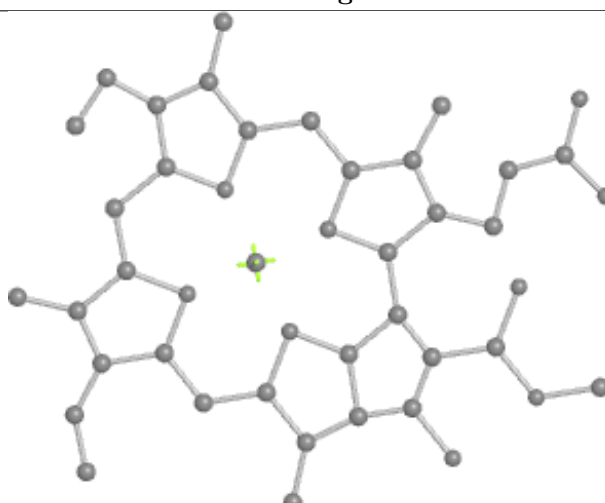
Bond lengths



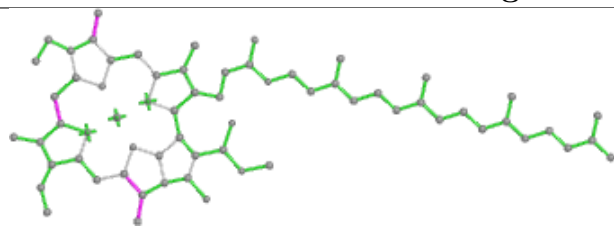
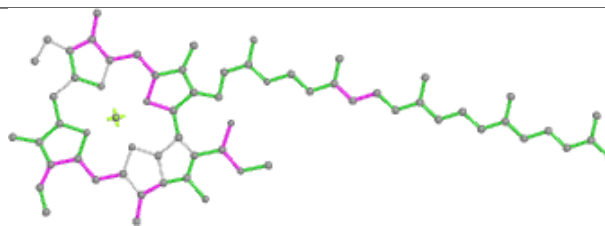
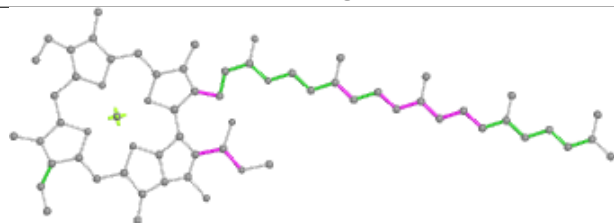
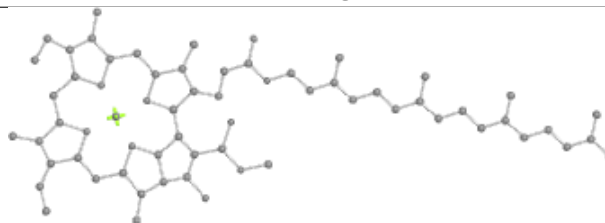
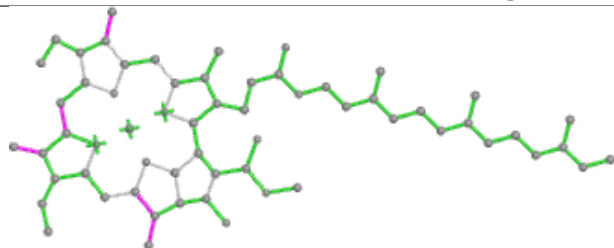
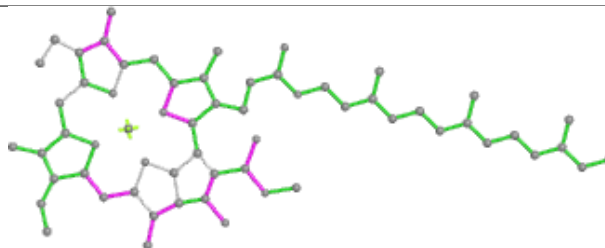
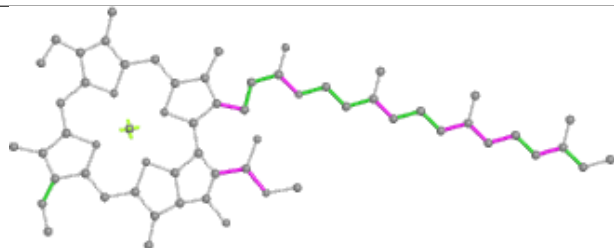
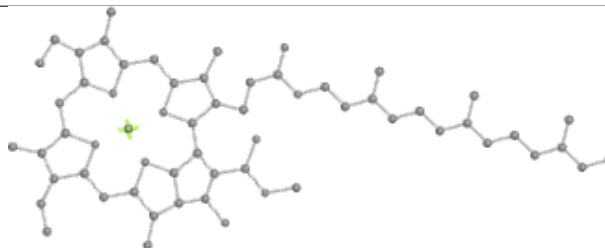
Bond angles



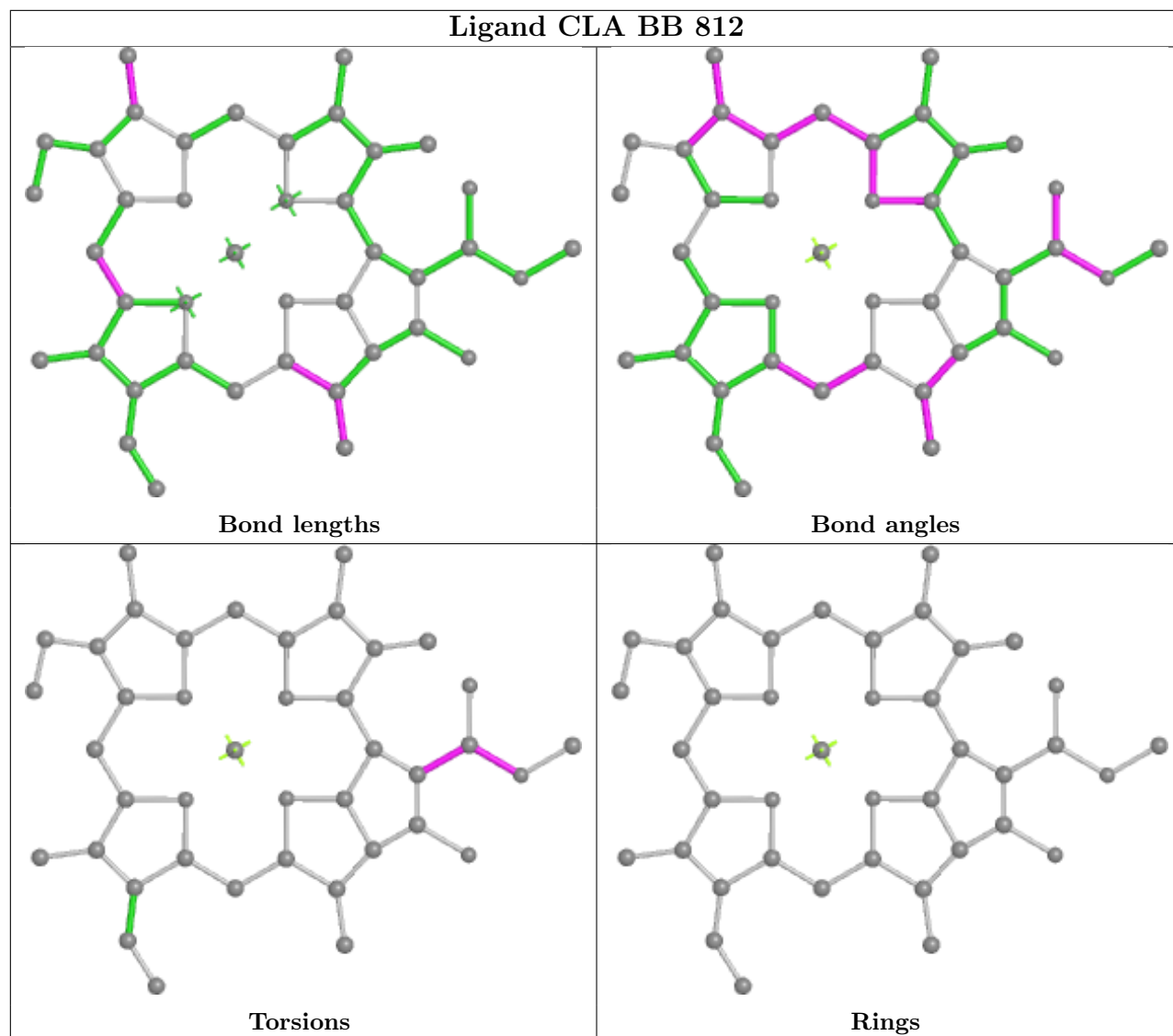
Torsions



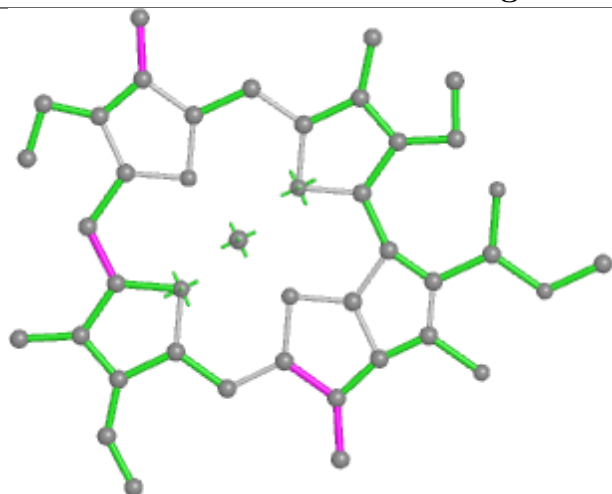
Rings

Ligand CLA BB 810**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA BB 811****Bond lengths****Bond angles****Torsions****Rings**

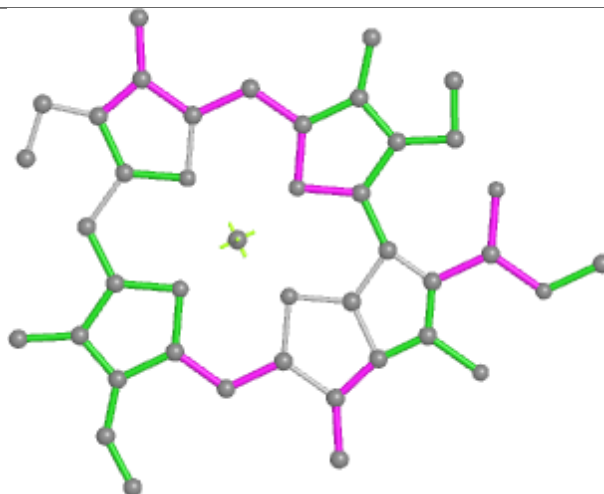
Ligand CLA BB 812



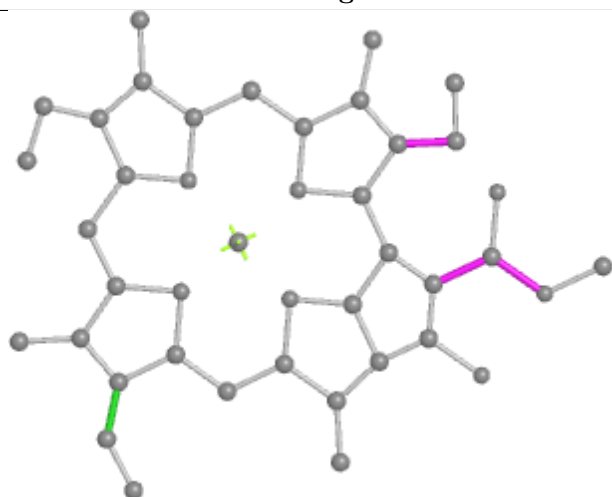
Ligand CLA BB 813



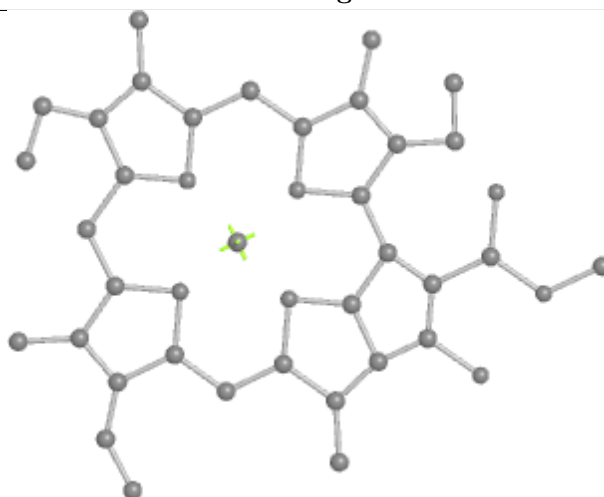
Bond lengths



Bond angles

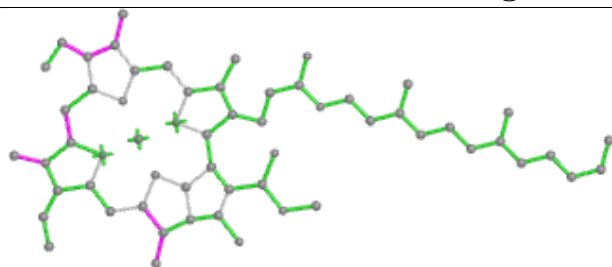


Torsions

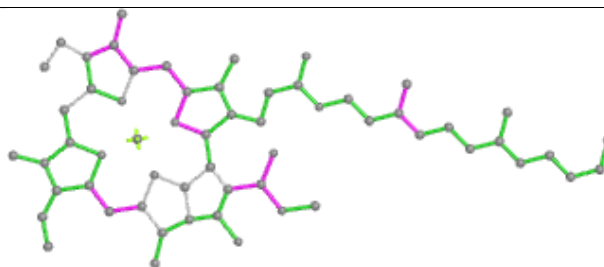


Rings

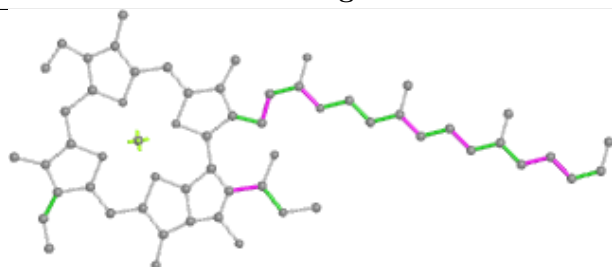
Ligand CLA BB 814



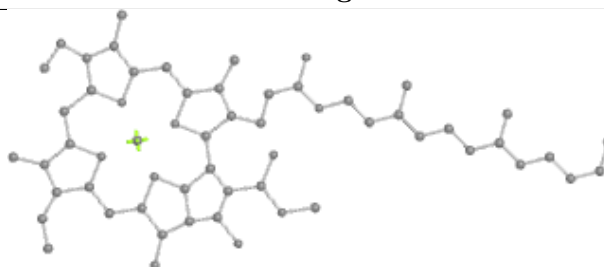
Bond lengths



Bond angles

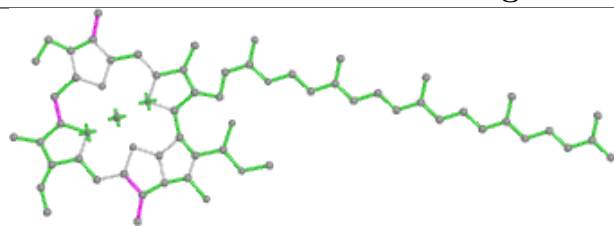


Torsions

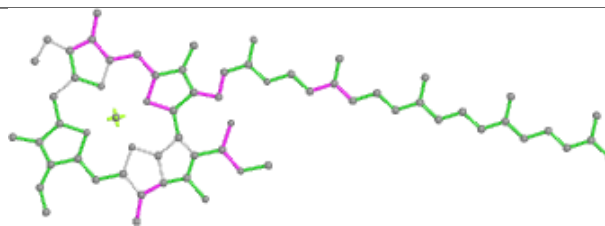


Rings

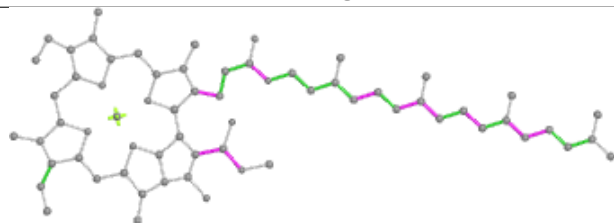
Ligand CLA BB 815



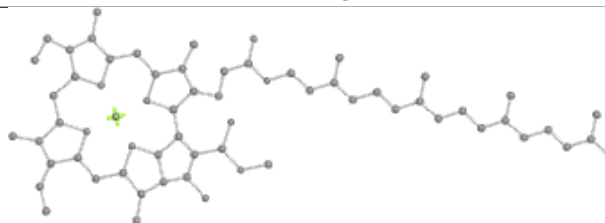
Bond lengths



Bond angles

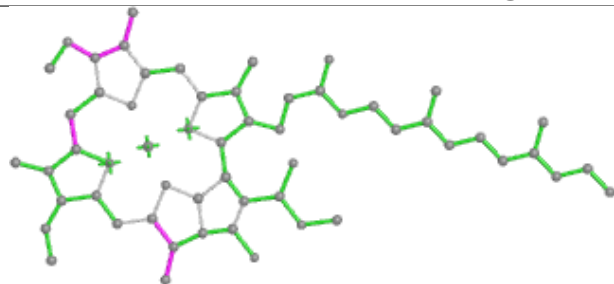


Torsions

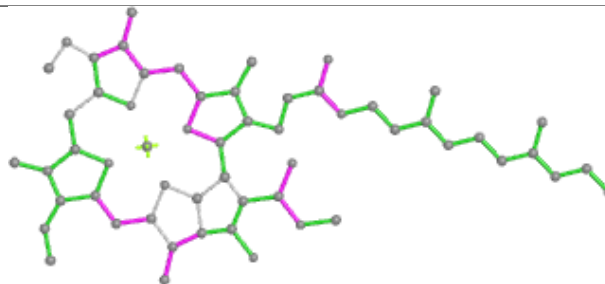


Rings

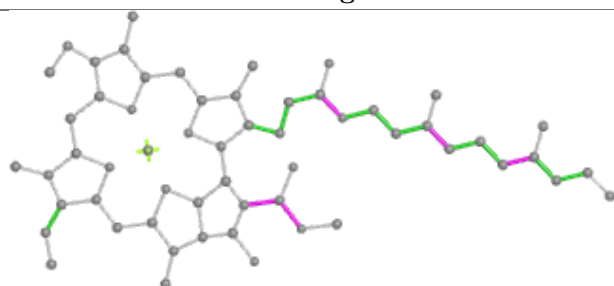
Ligand CLA BB 816



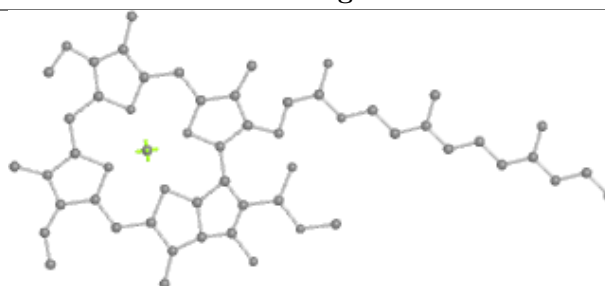
Bond lengths



Bond angles

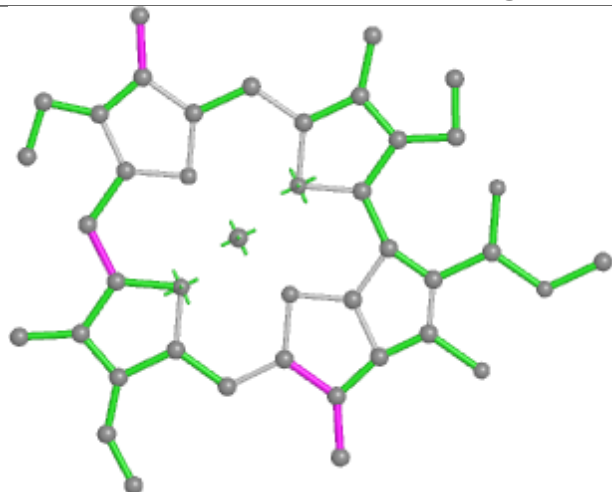


Torsions

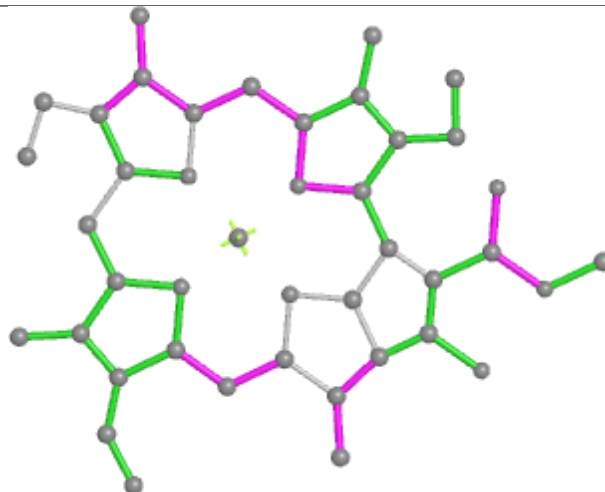


Rings

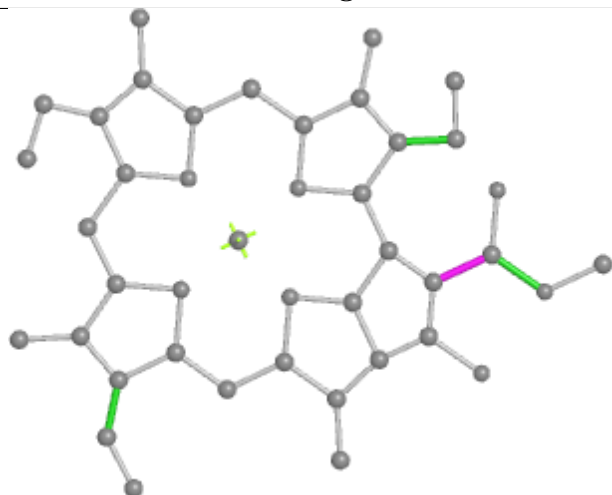
Ligand CLA BB 817



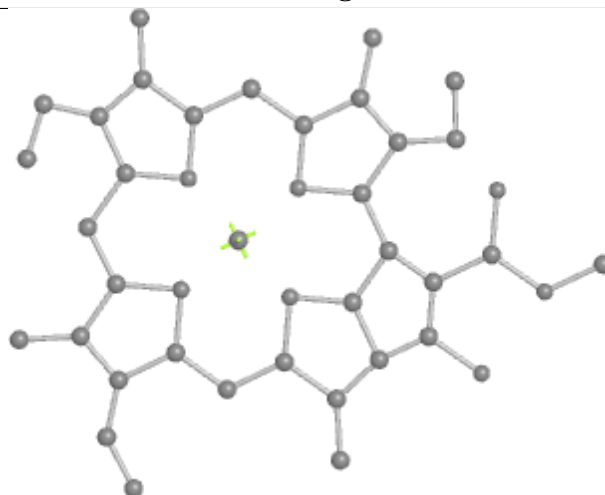
Bond lengths



Bond angles

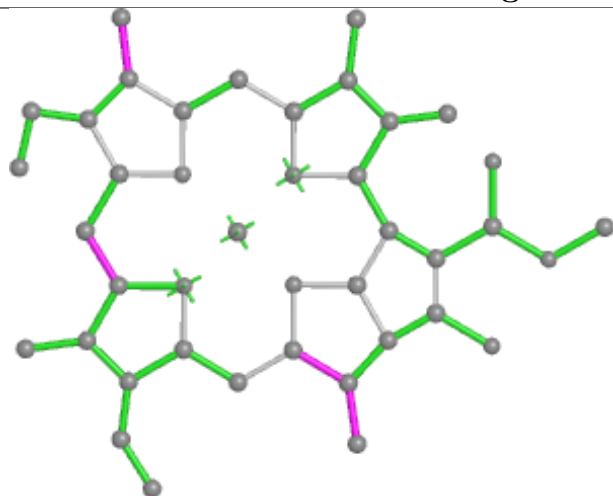


Torsions

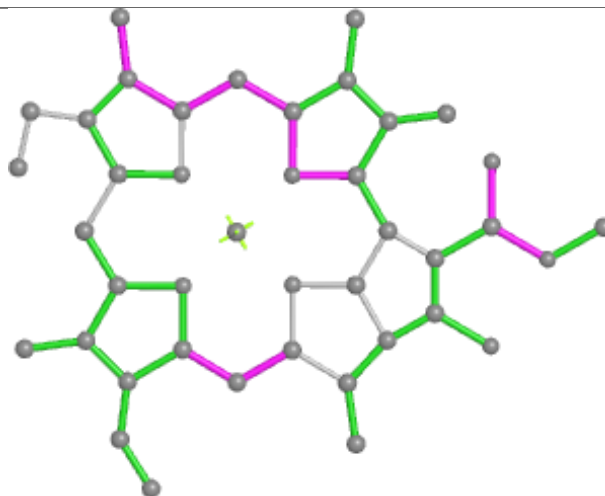


Rings

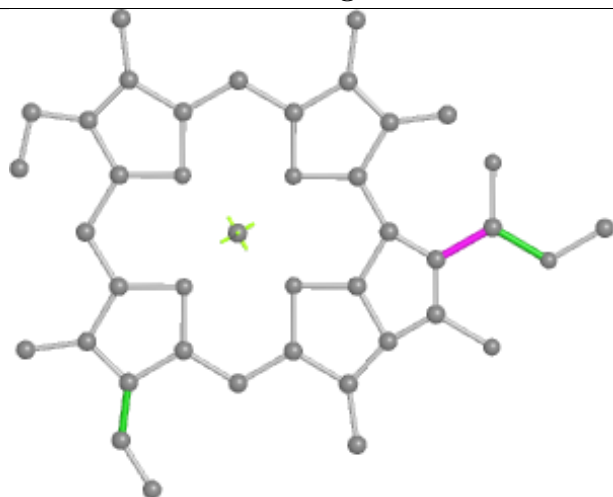
Ligand CLA BB 818



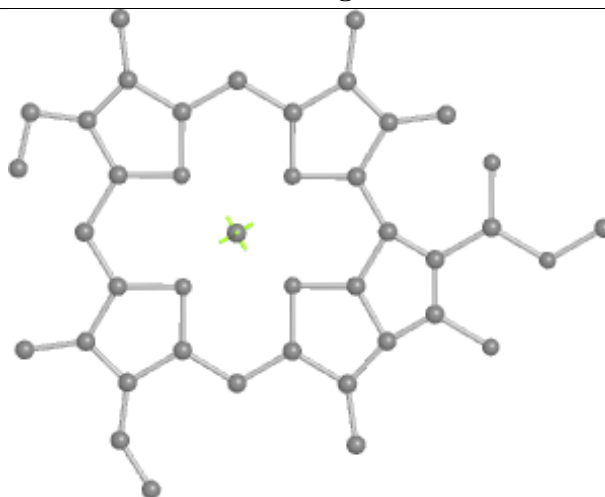
Bond lengths



Bond angles

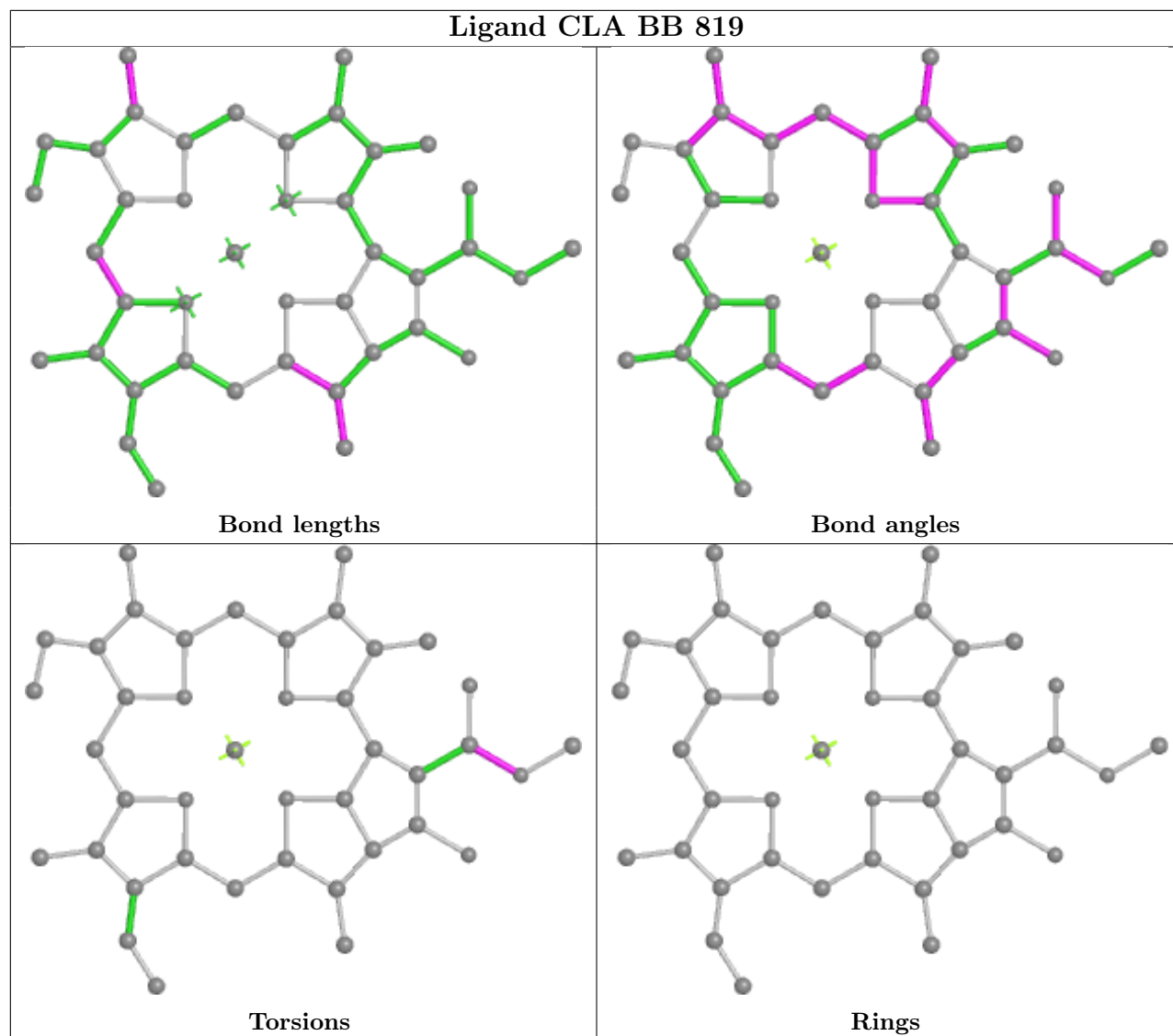


Torsions

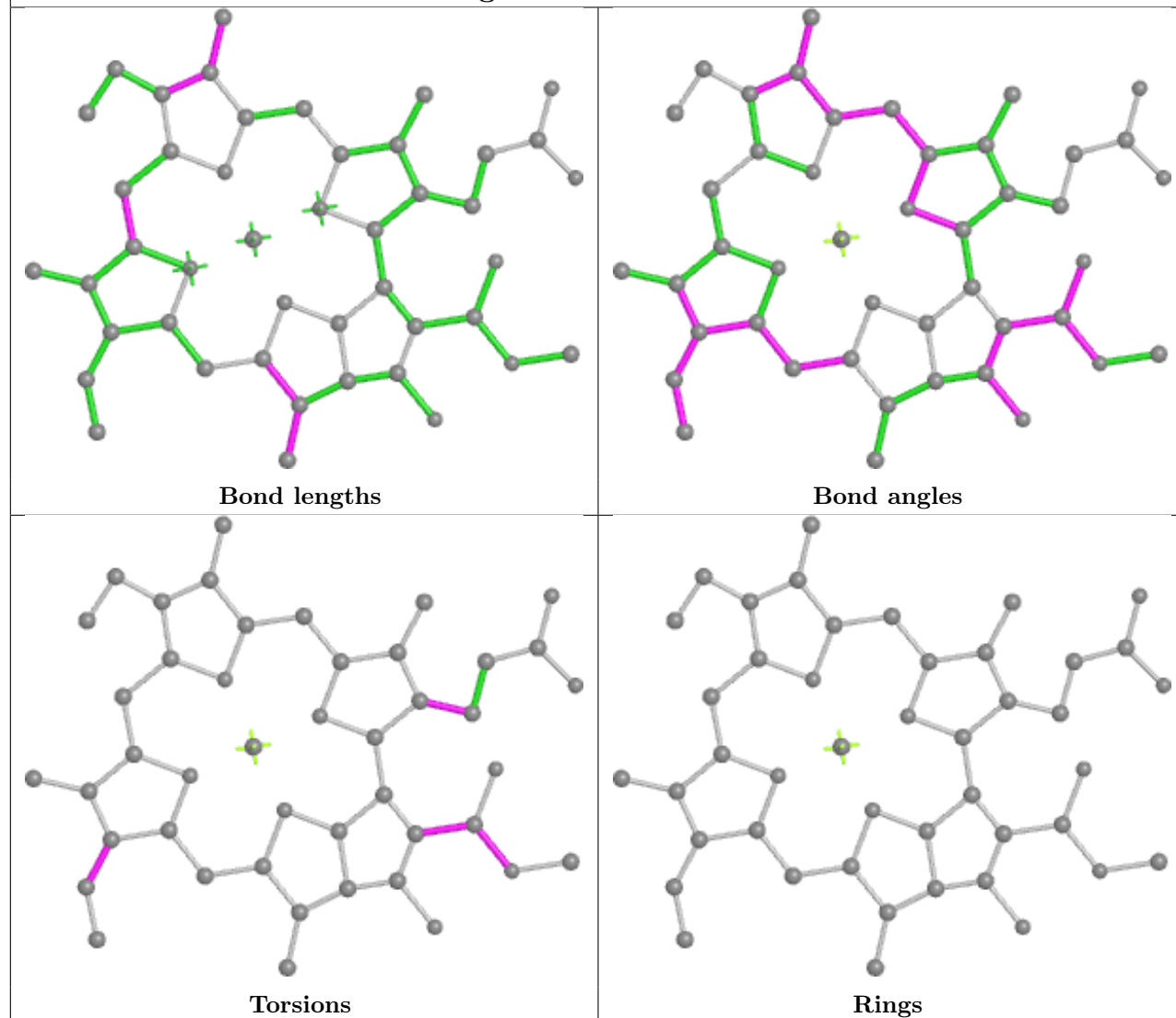


Rings

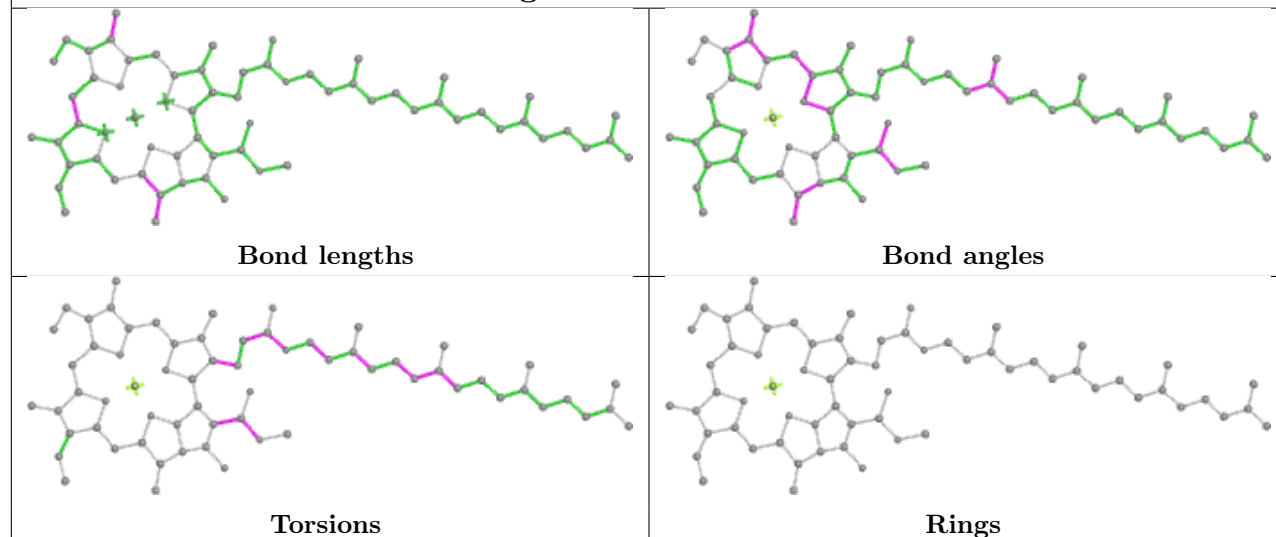
Ligand CLA BB 819

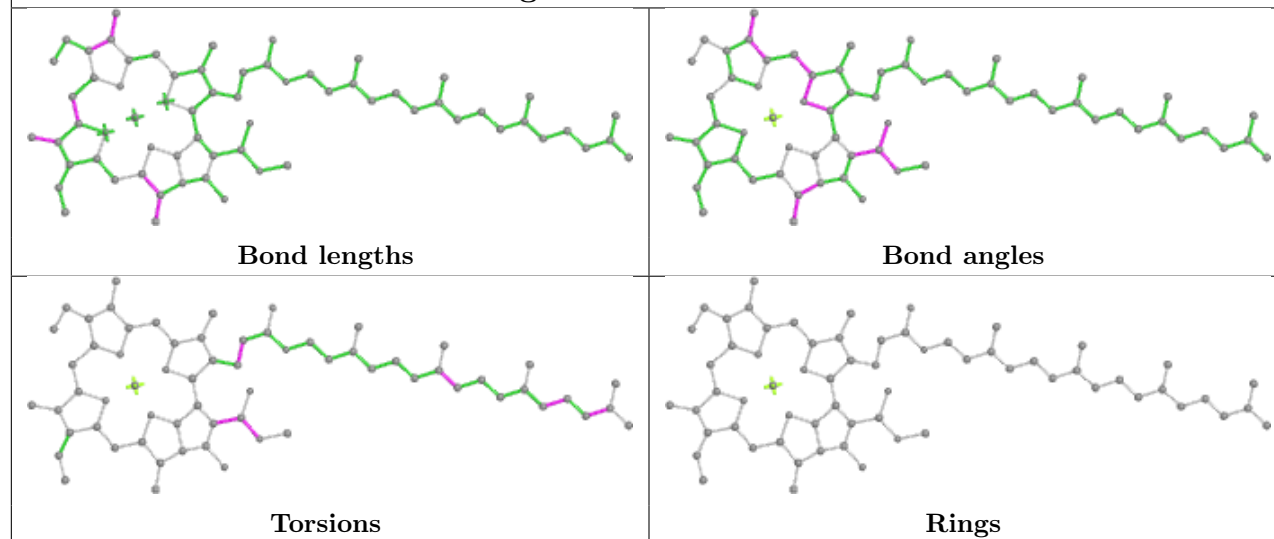
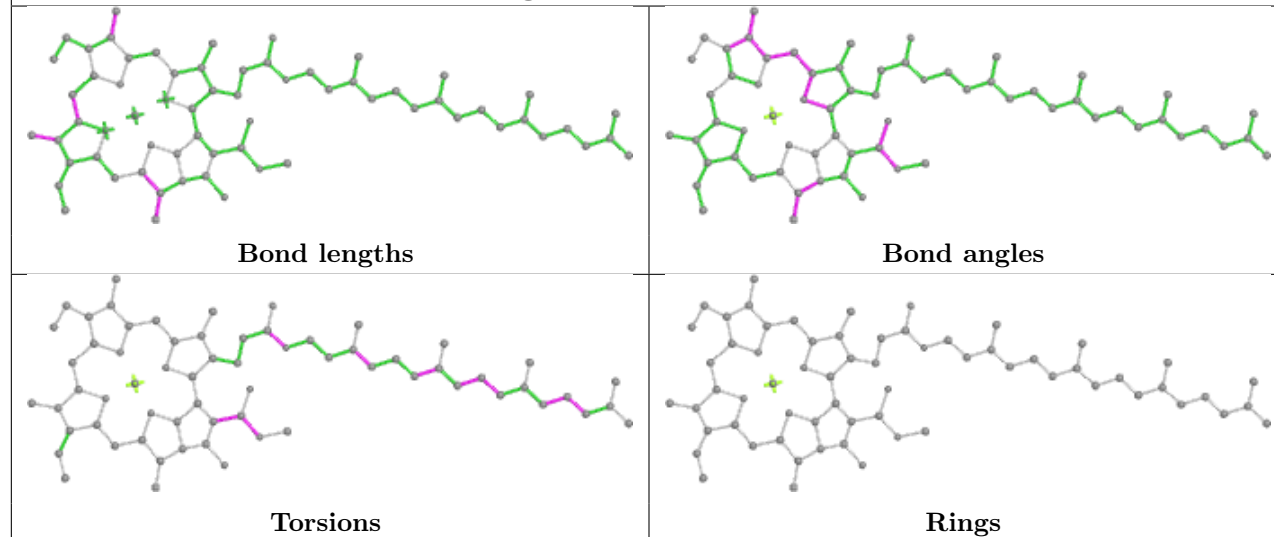


Ligand CLA BB 820

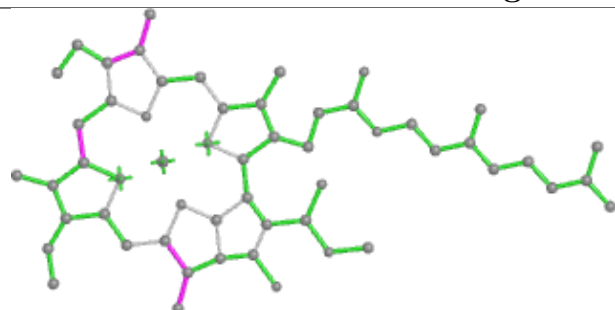


Ligand CLA BB 821

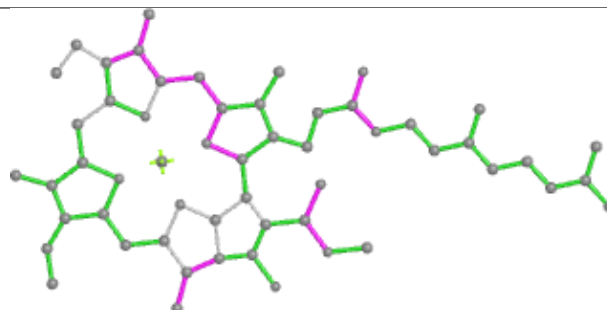


Ligand CLA BB 822**Ligand CLA BB 823**

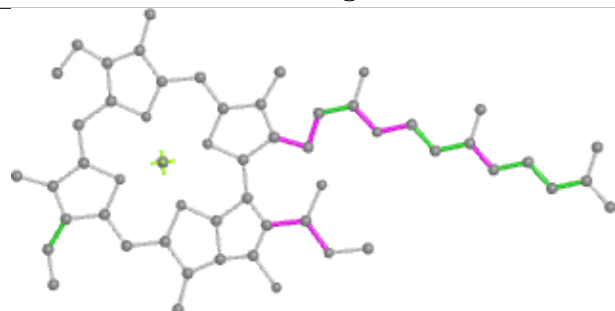
Ligand CLA BB 824



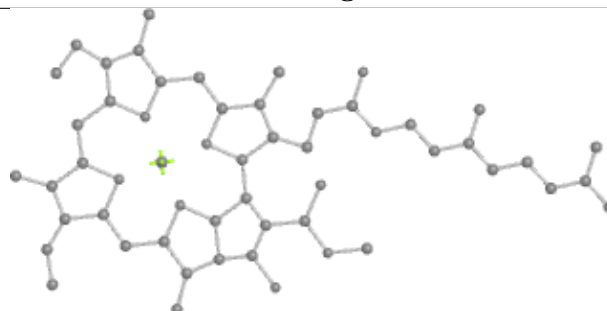
Bond lengths



Bond angles

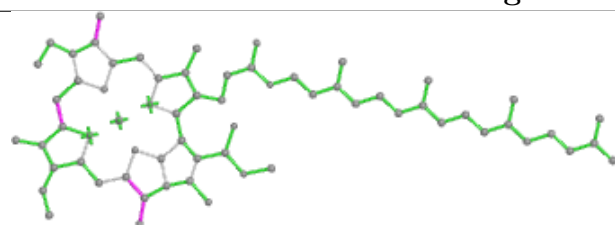


Torsions

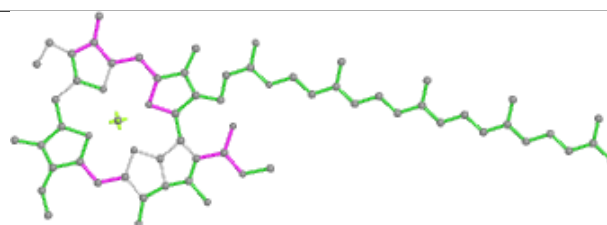


Rings

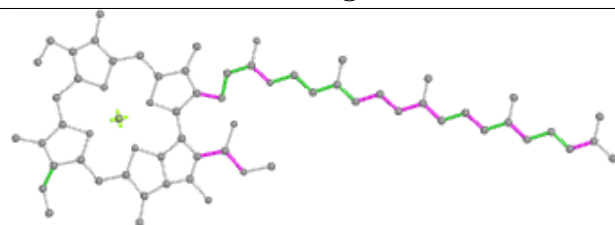
Ligand CLA BB 825



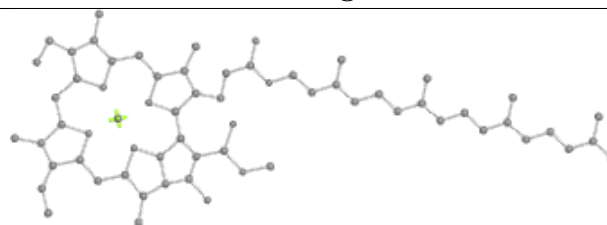
Bond lengths



Bond angles

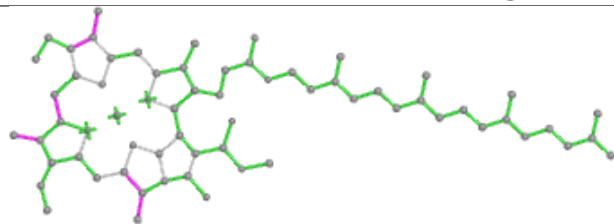


Torsions

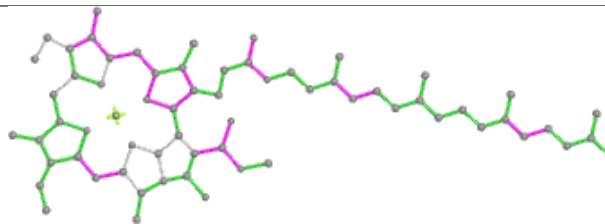


Rings

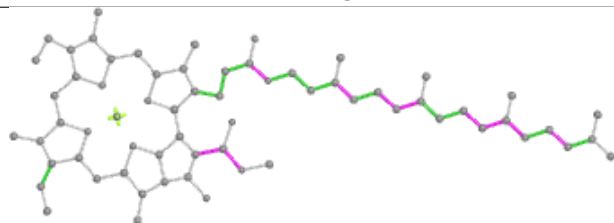
Ligand CLA BB 826



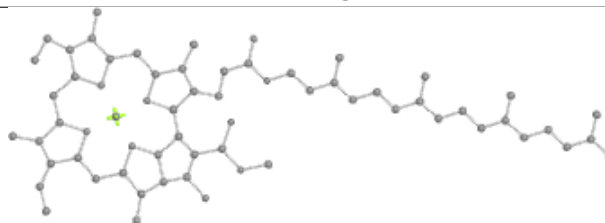
Bond lengths



Bond angles

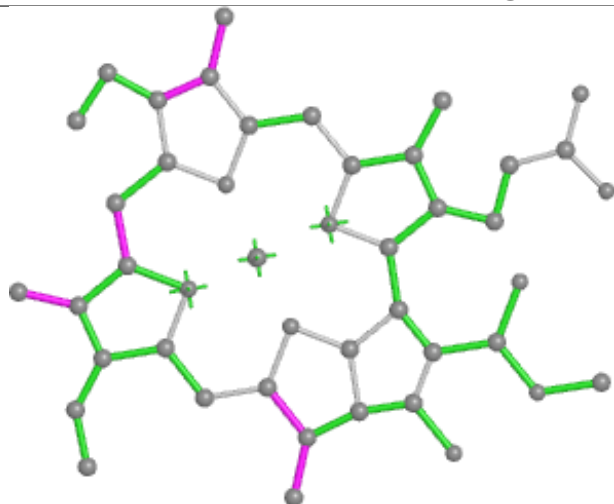


Torsions

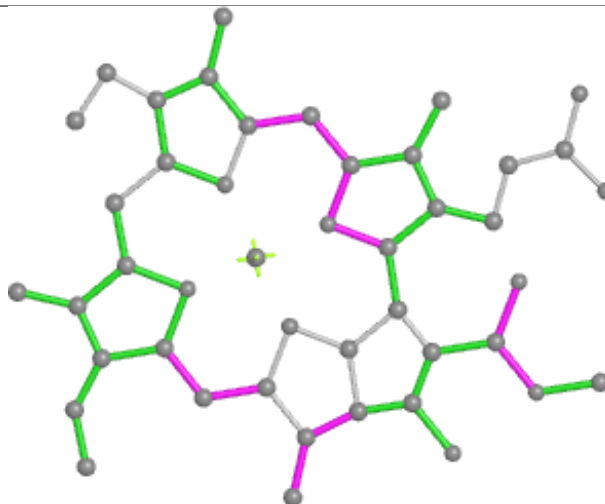


Rings

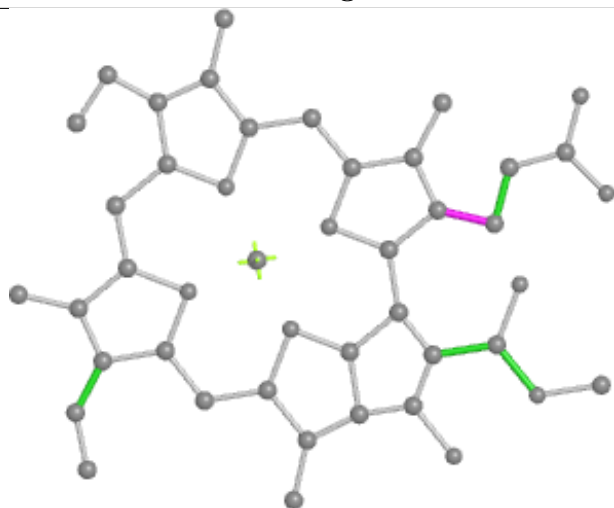
Ligand CLA BB 827



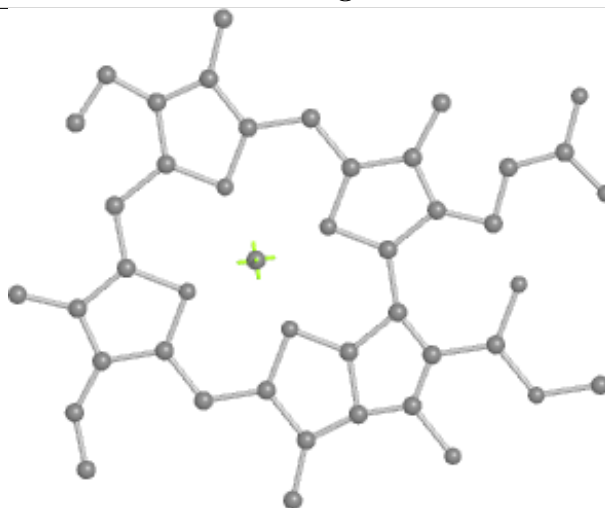
Bond lengths



Bond angles

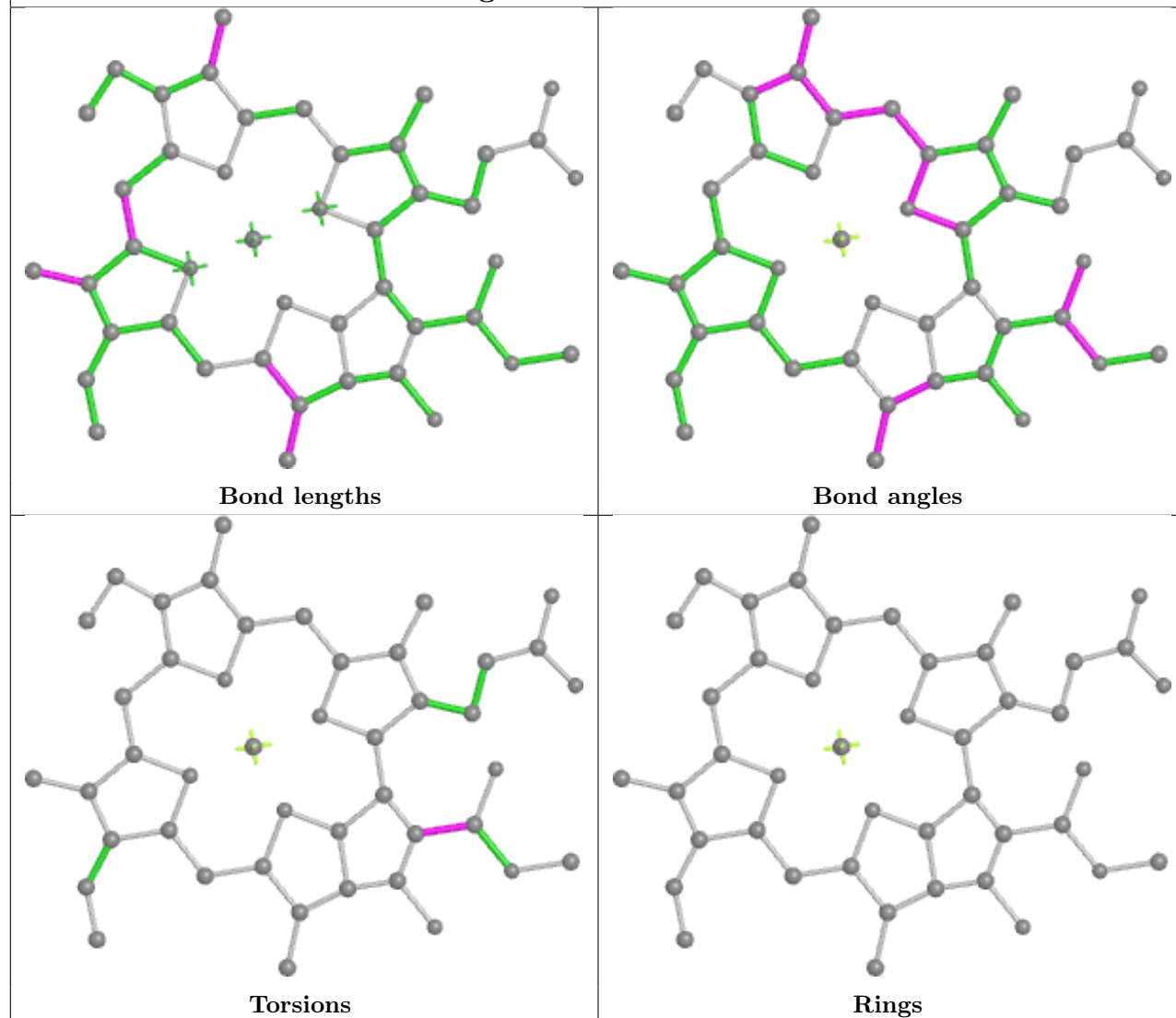


Torsions

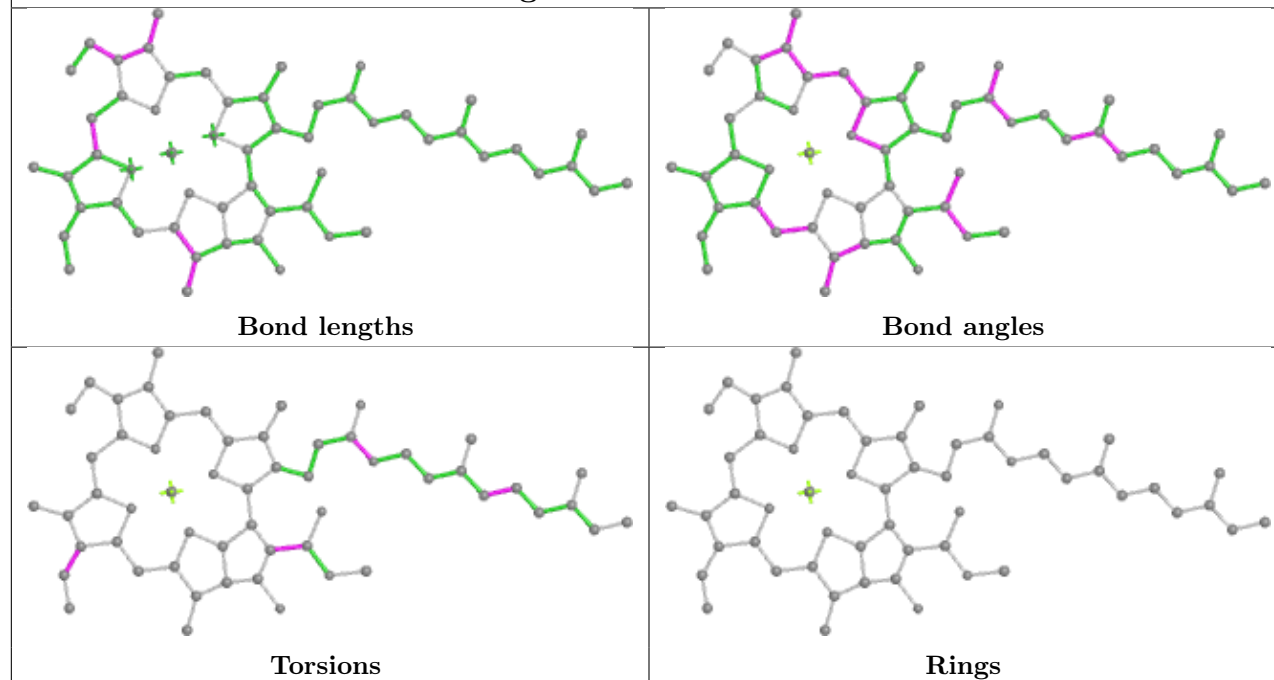


Rings

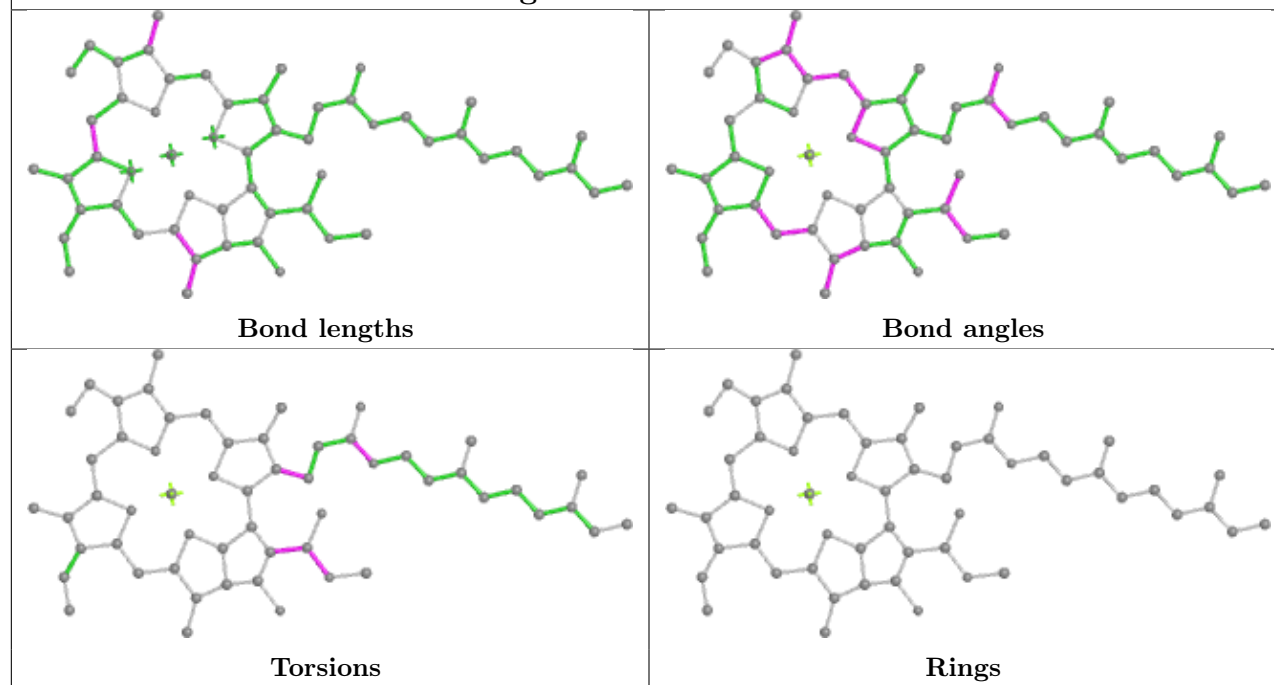
Ligand CLA BB 828



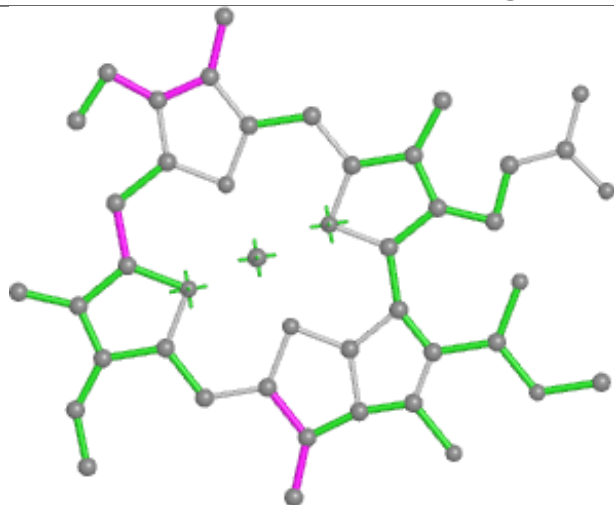
Ligand CLA BB 829



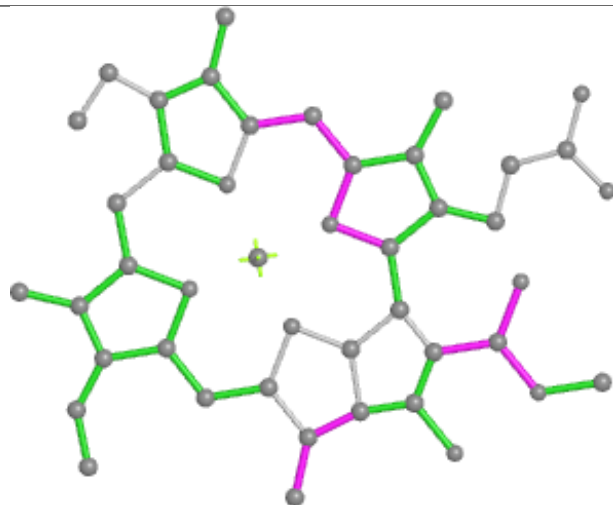
Ligand CLA BB 830



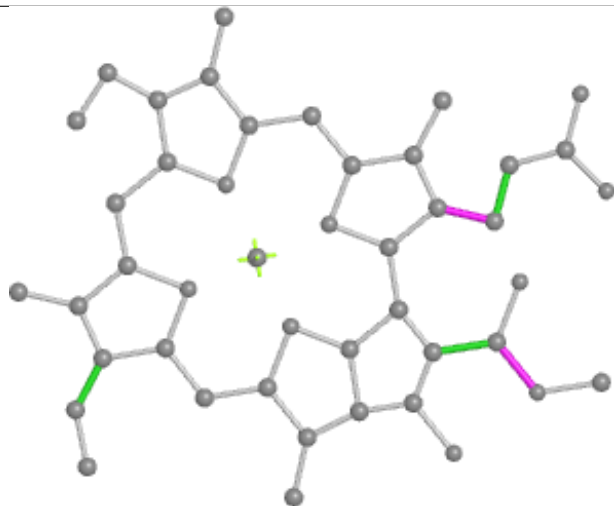
Ligand CLA BB 831



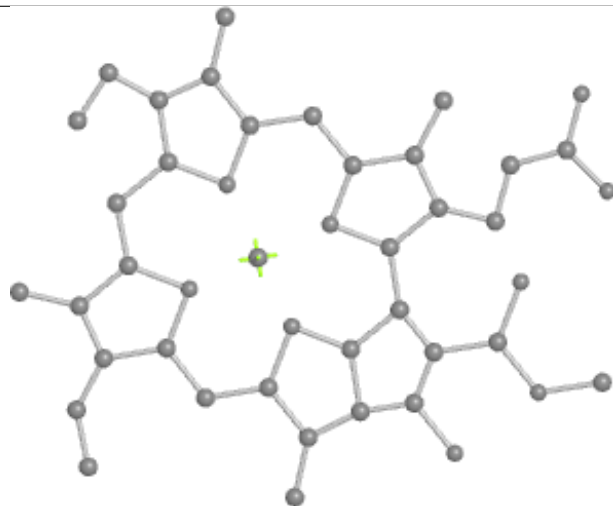
Bond lengths



Bond angles

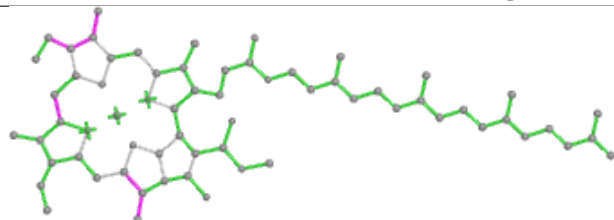


Torsions

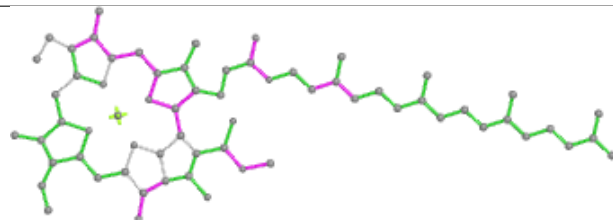


Rings

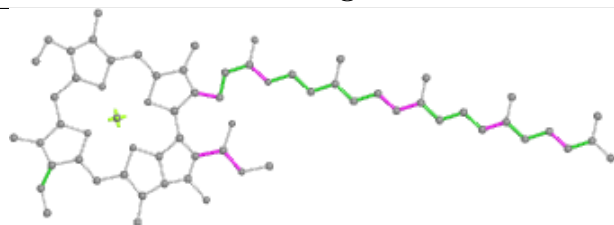
Ligand CLA BB 832



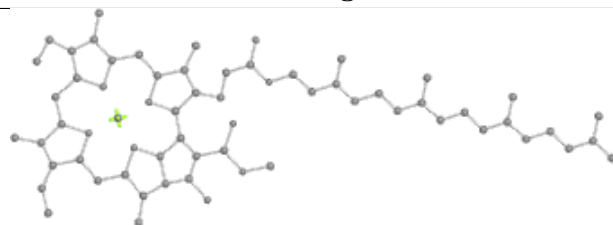
Bond lengths



Bond angles

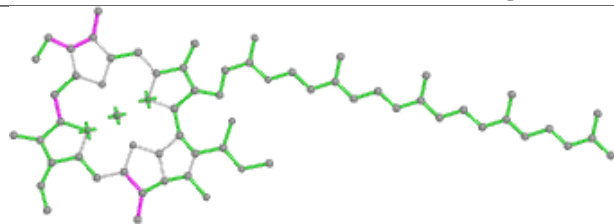


Torsions

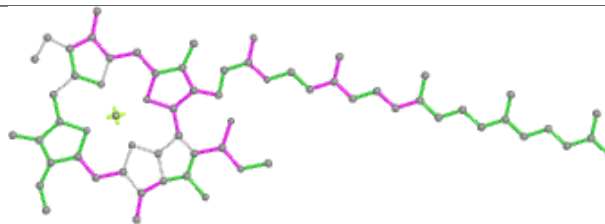


Rings

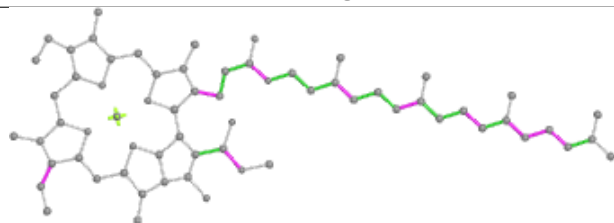
Ligand CLA BB 833



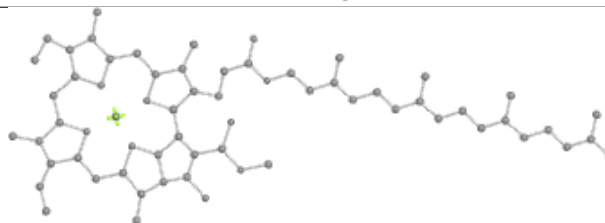
Bond lengths



Bond angles

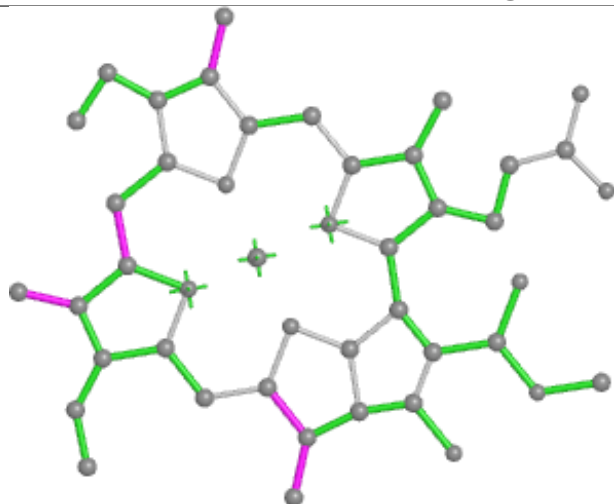


Torsions

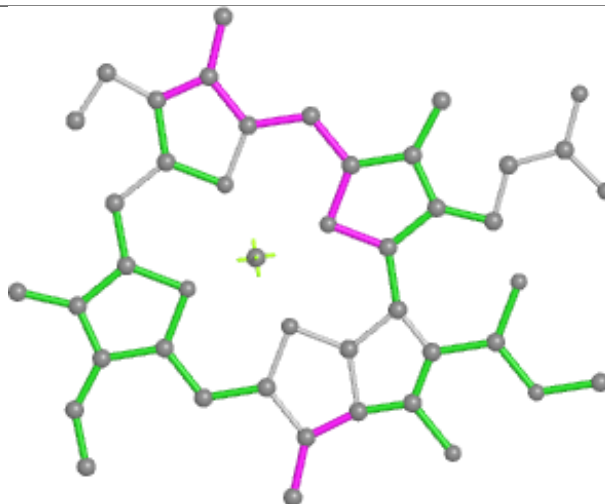


Rings

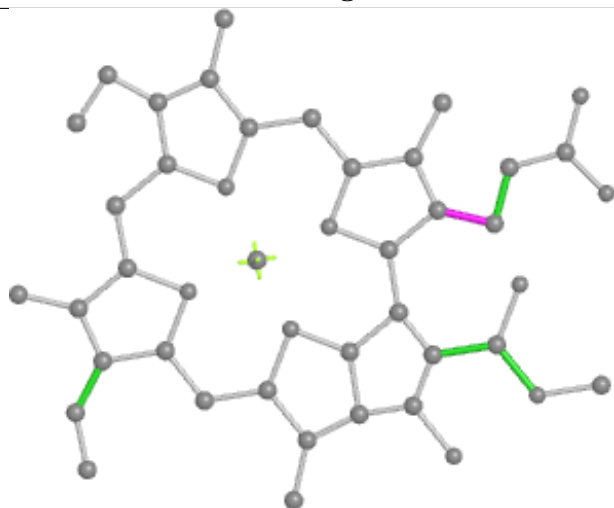
Ligand CLA BB 834



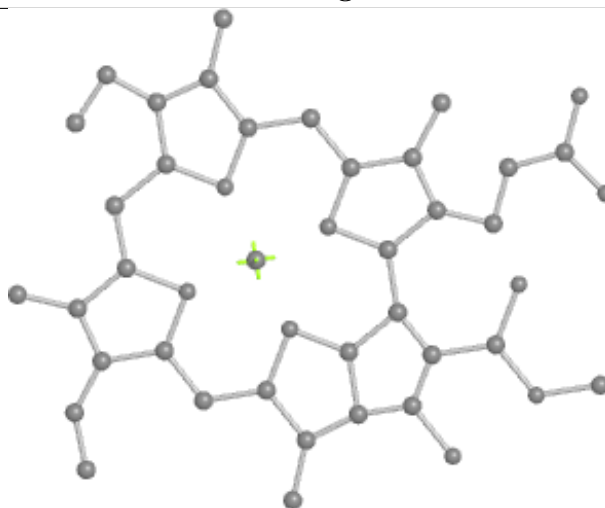
Bond lengths



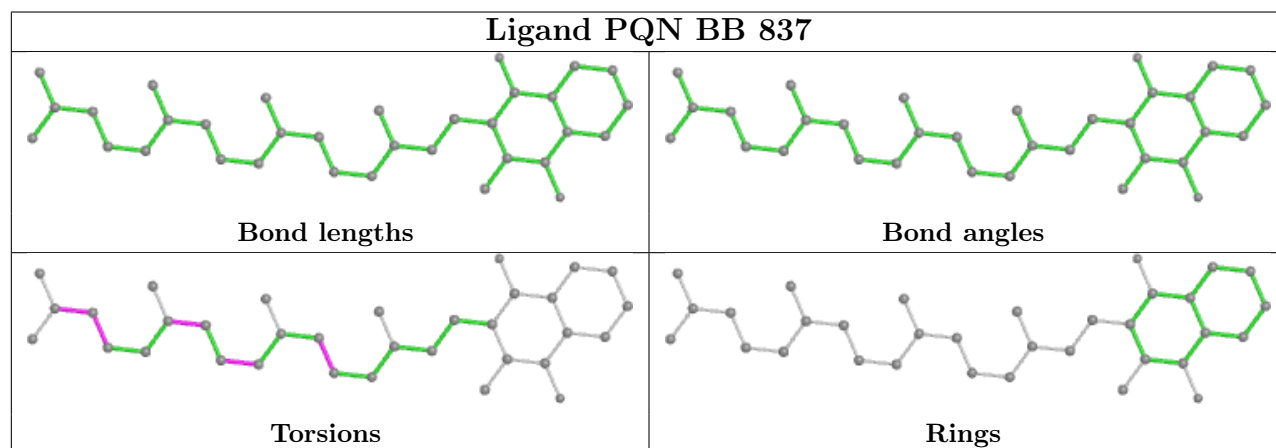
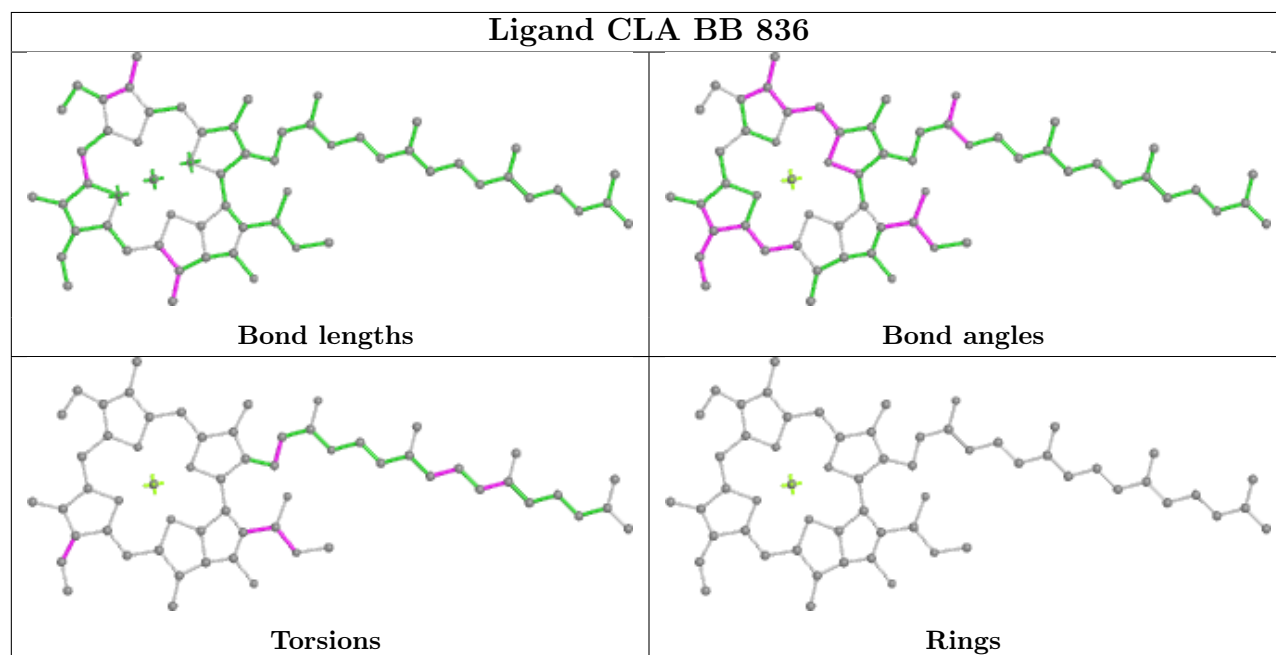
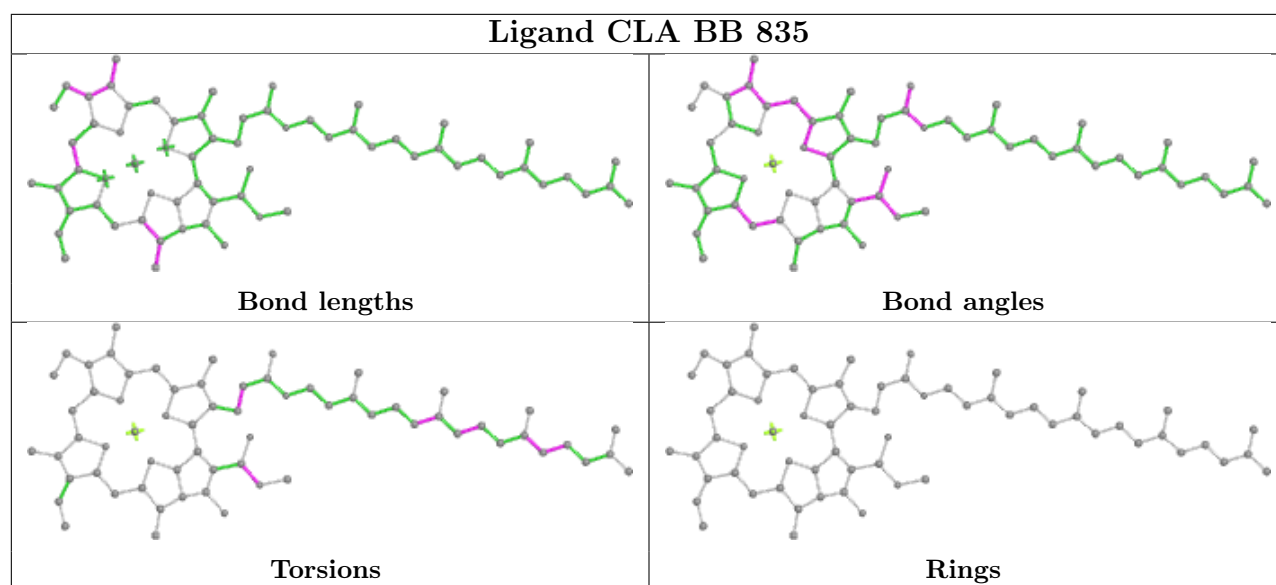
Bond angles

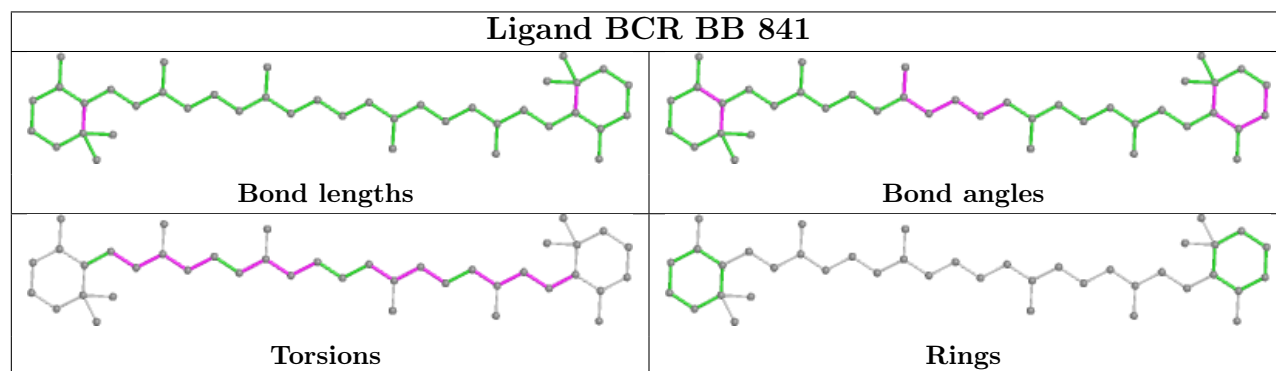
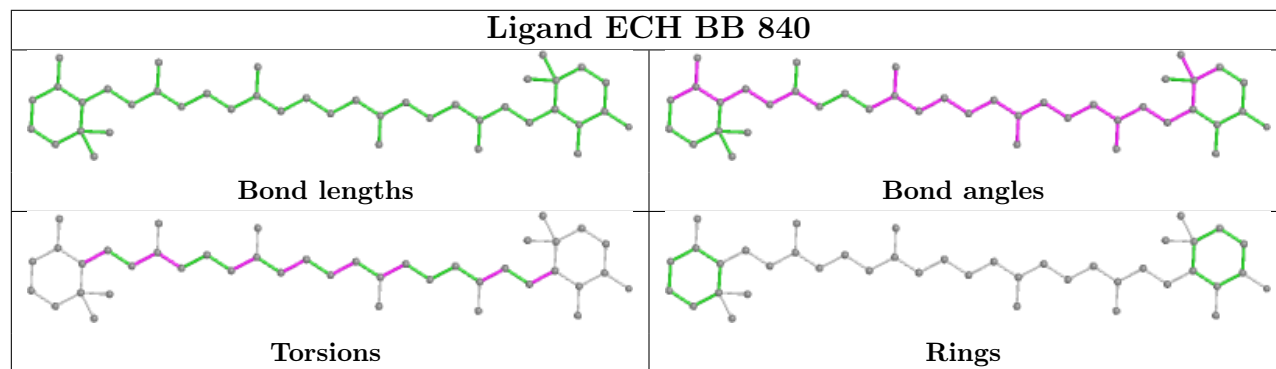
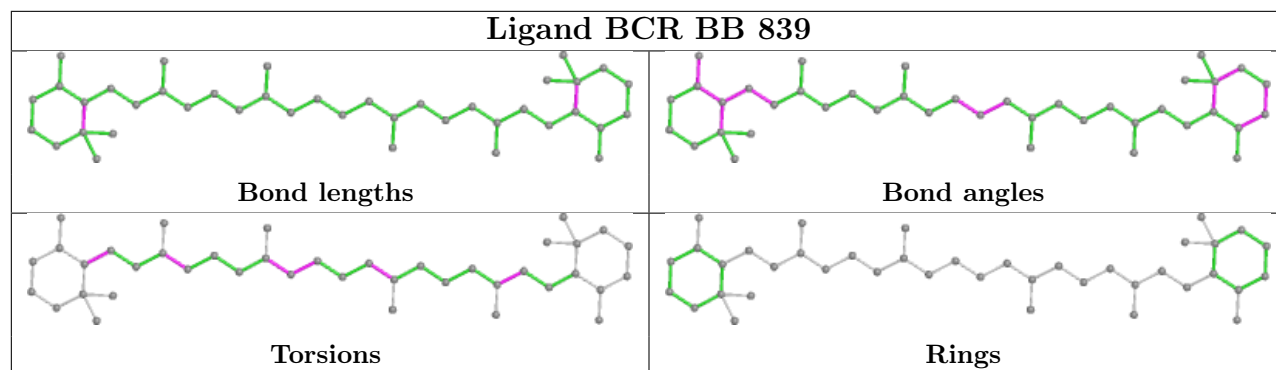
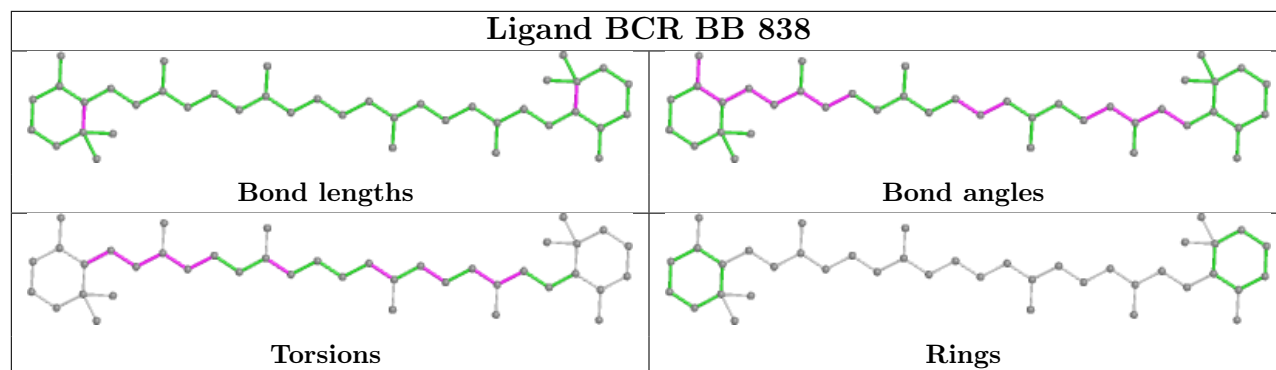


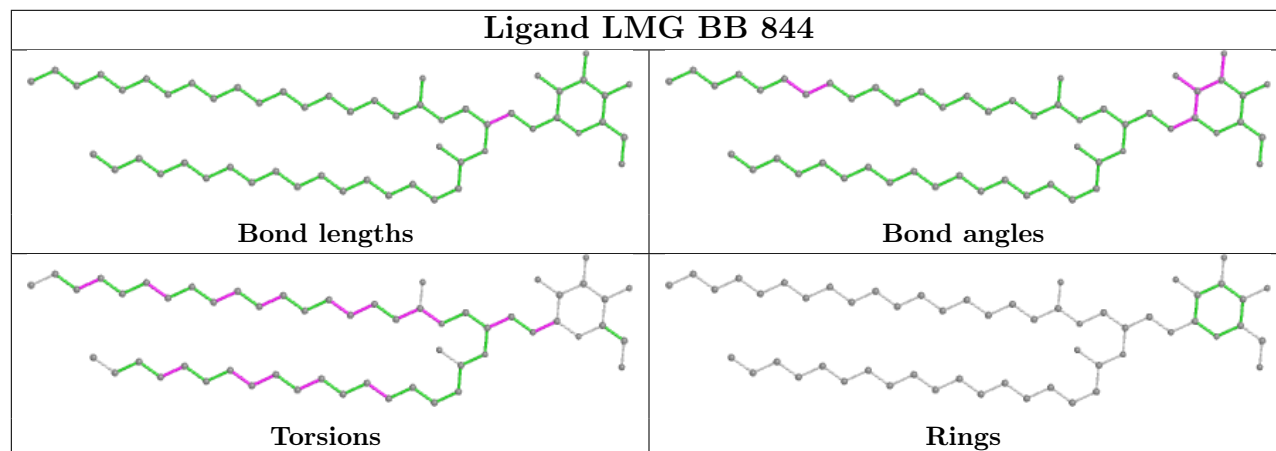
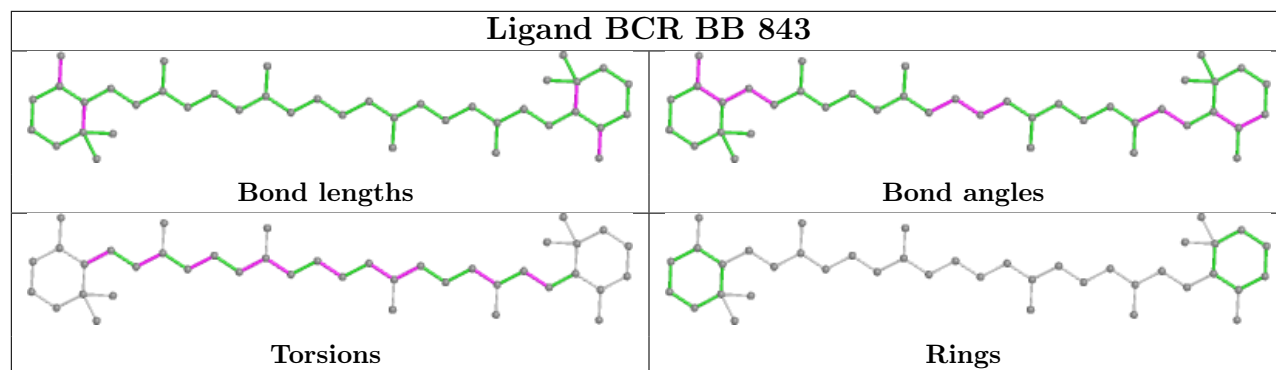
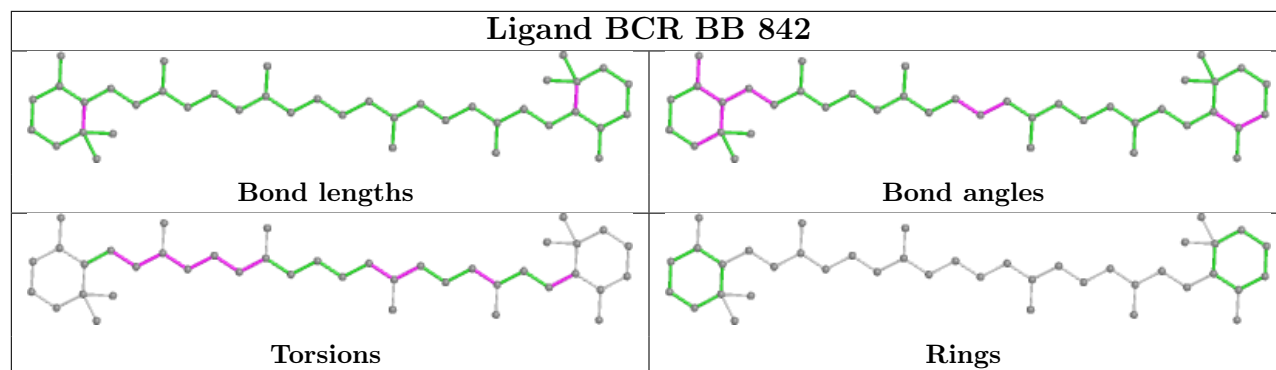
Torsions



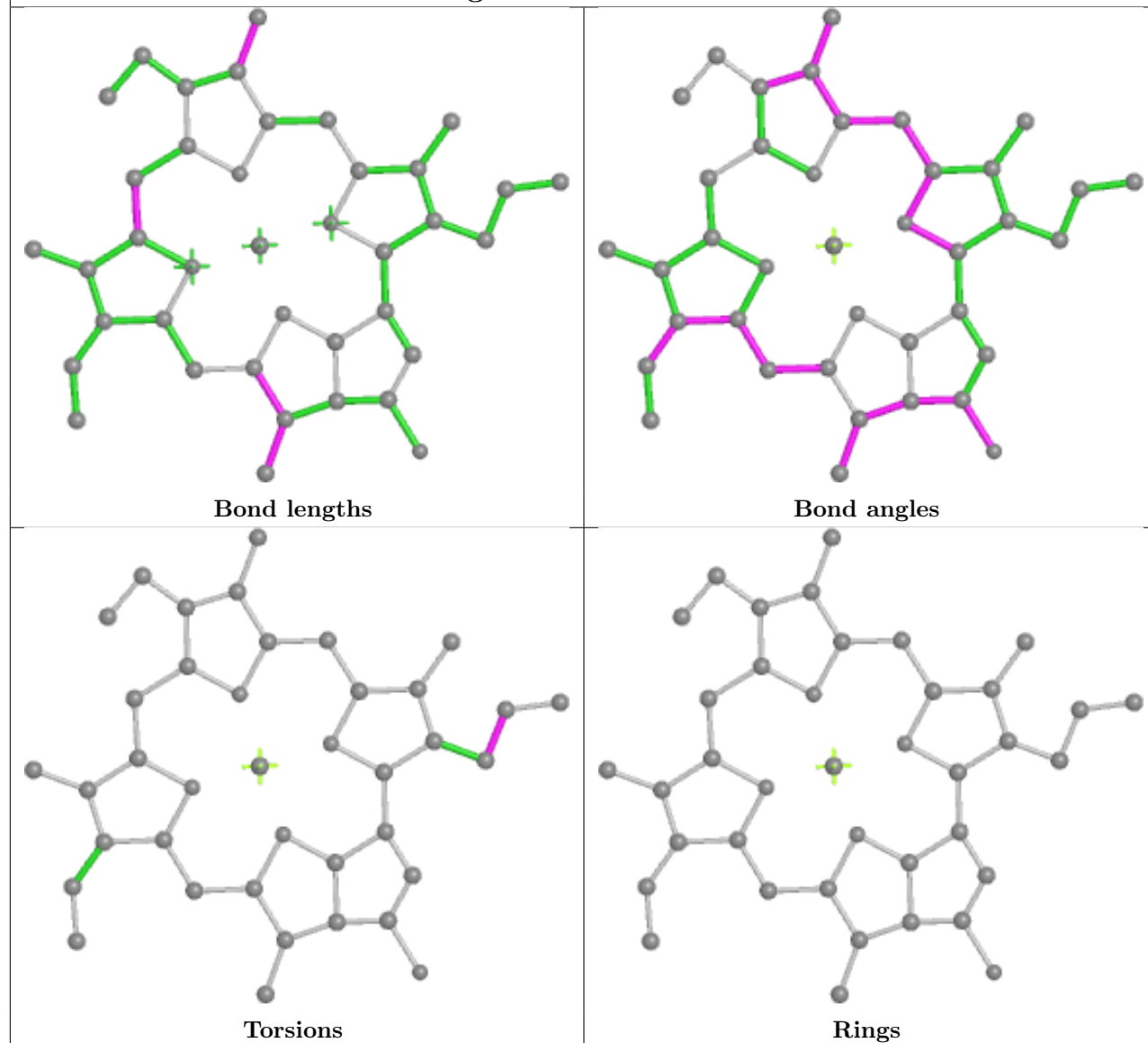
Rings



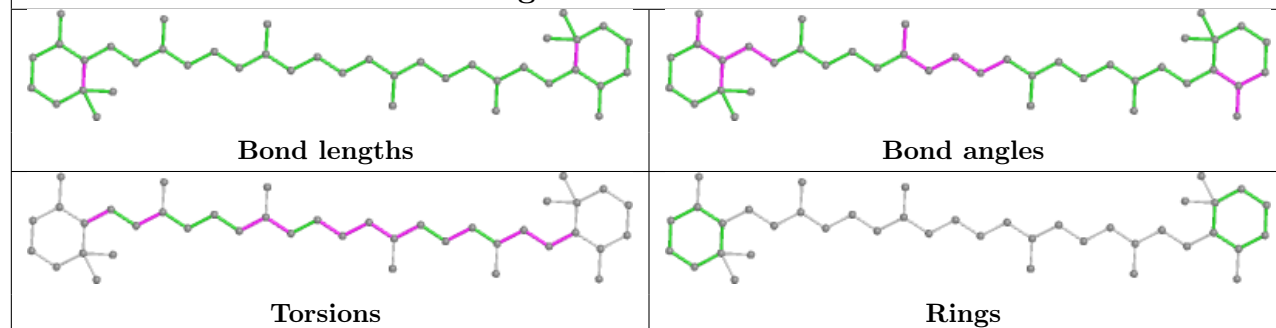


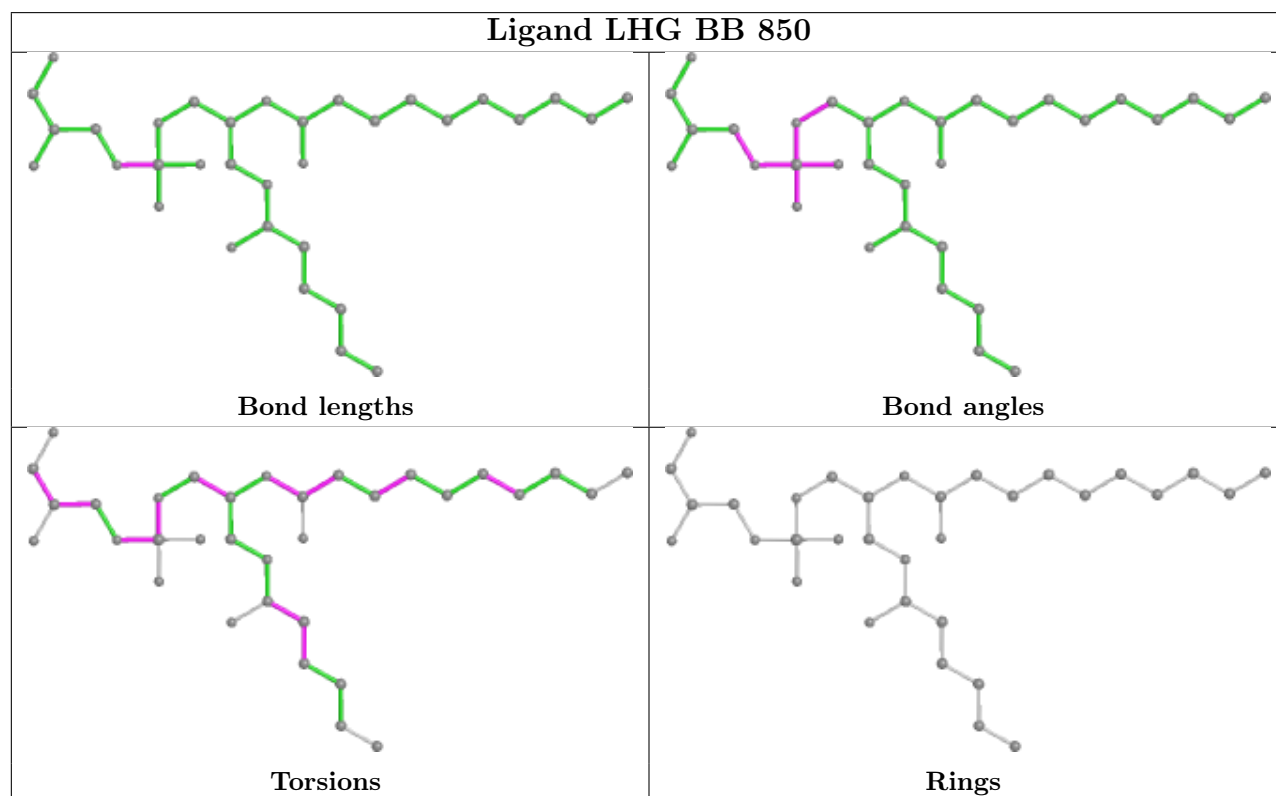
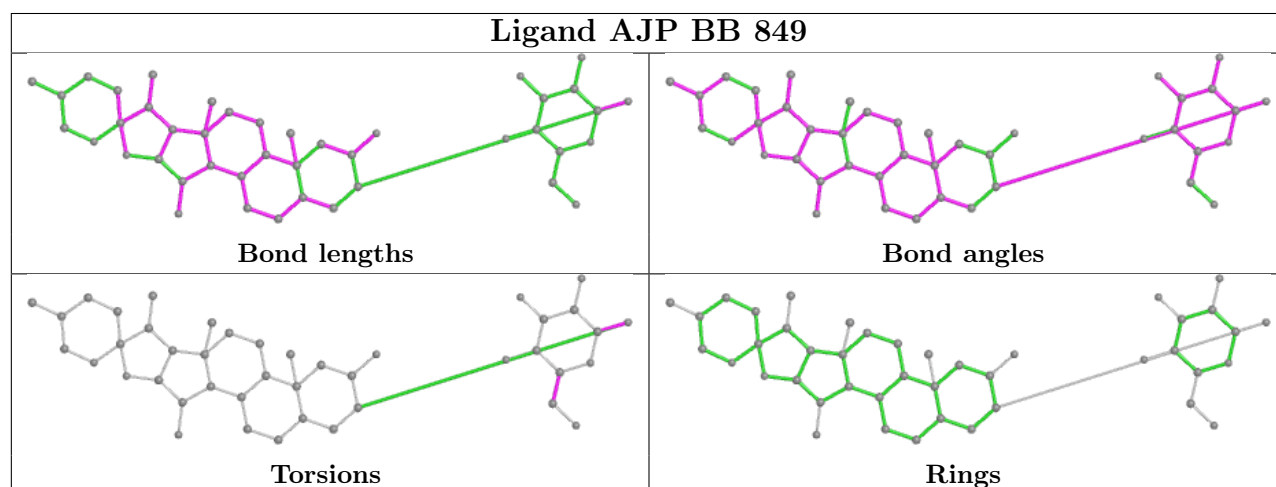
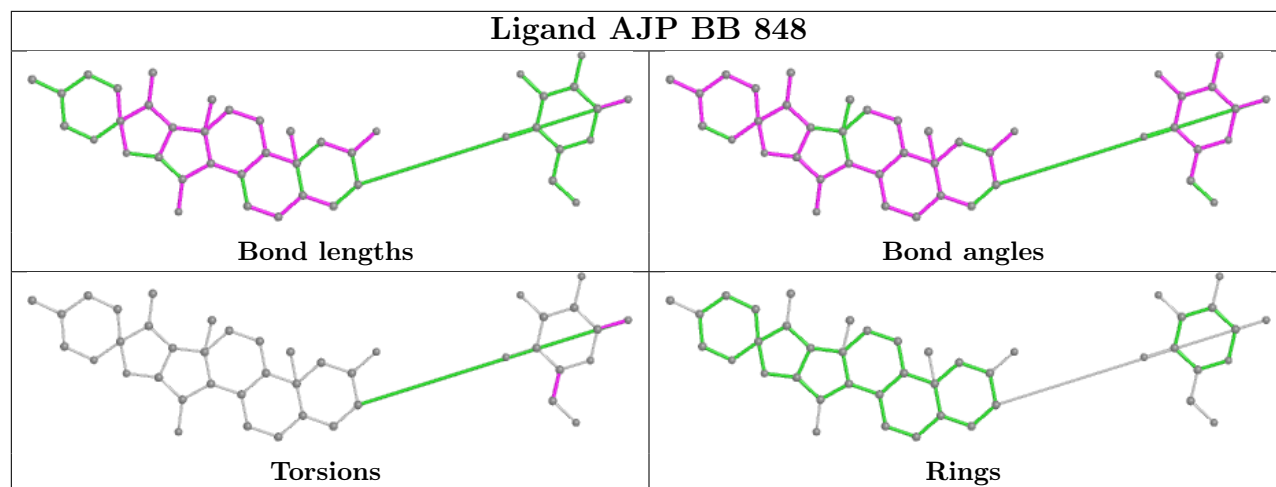


Ligand CLA BB 845

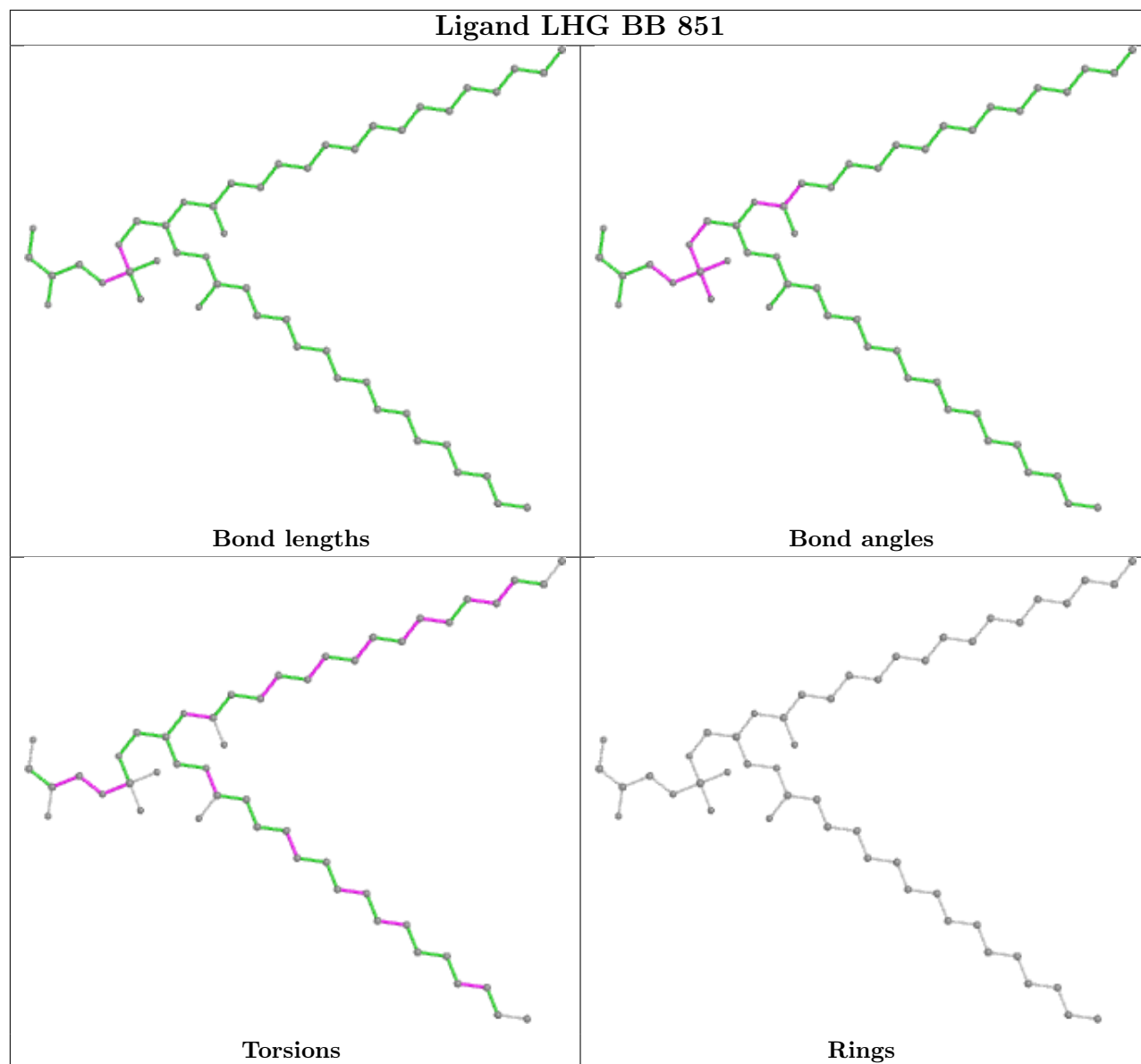


Ligand BCR BB 847

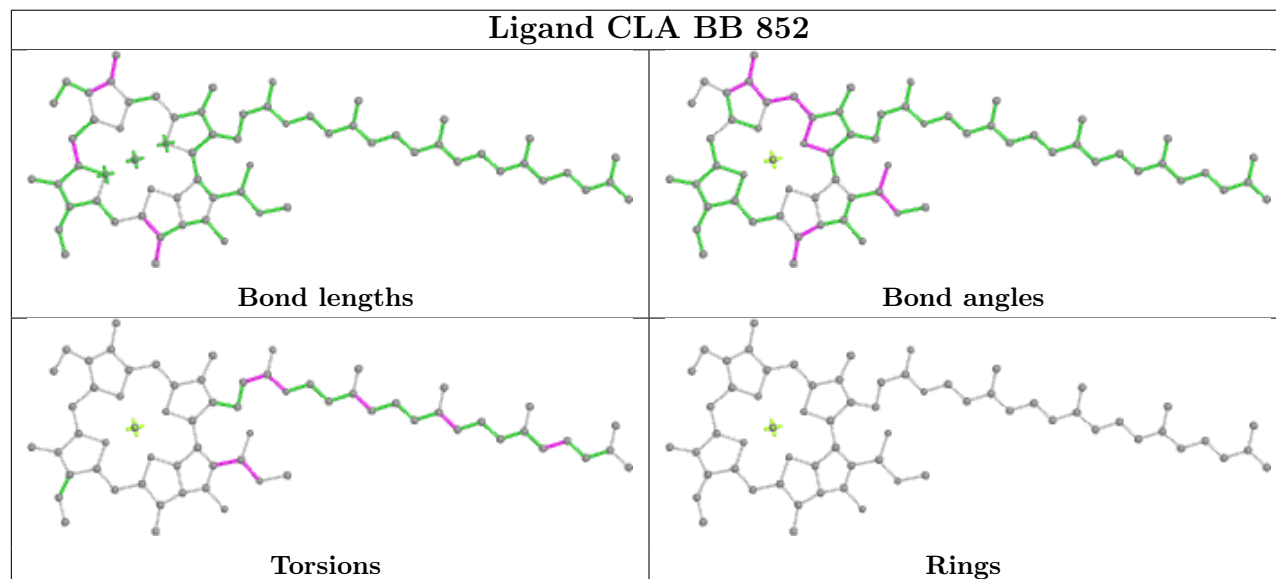




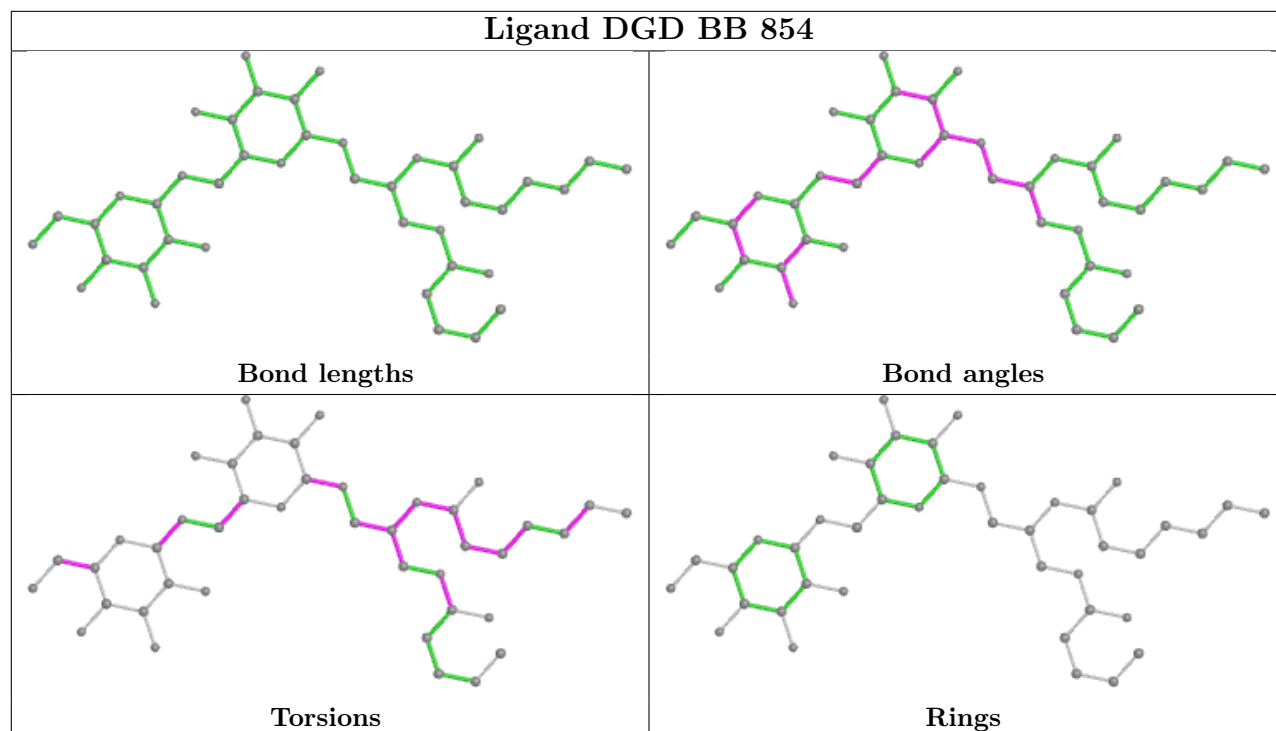
Ligand LHG BB 851



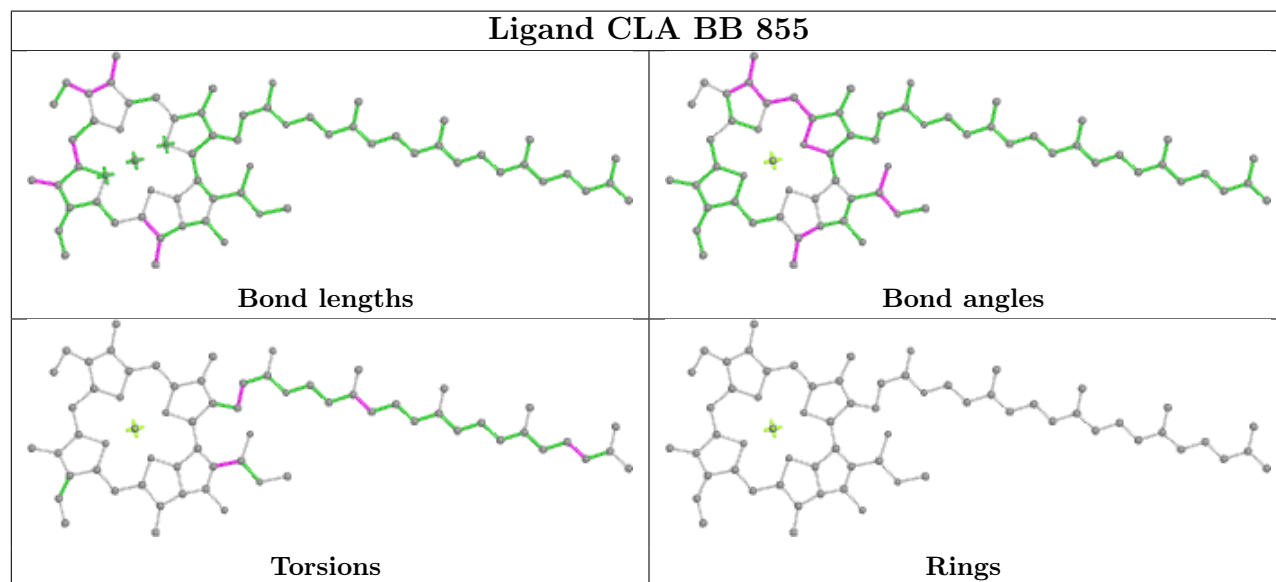
Ligand CLA BB 852



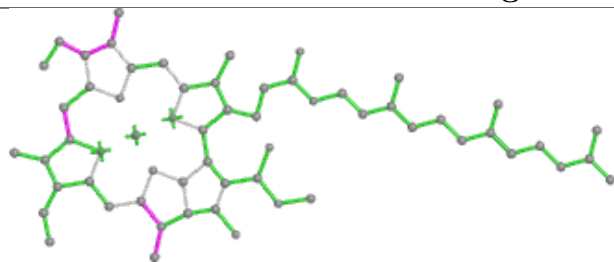
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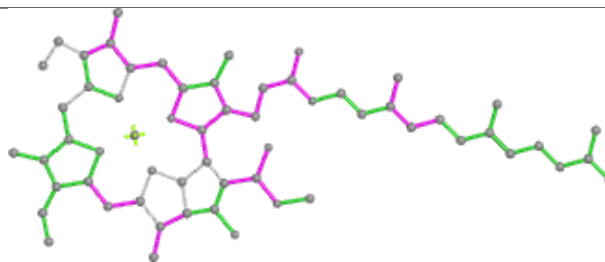
Ligand CLA BB 855



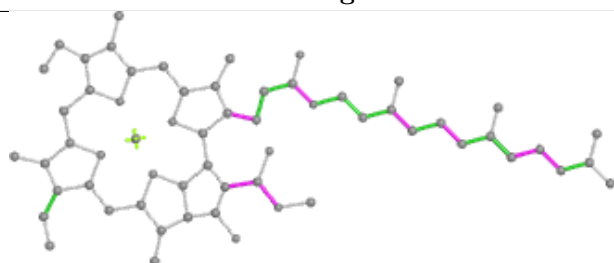
Ligand CLA BB 856



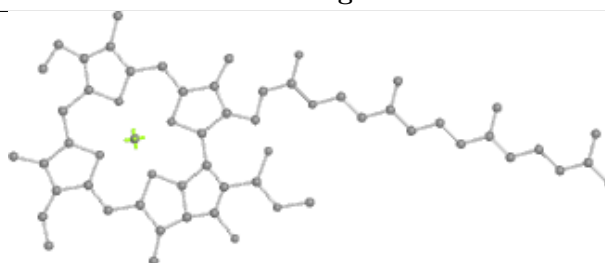
Bond lengths



Bond angles

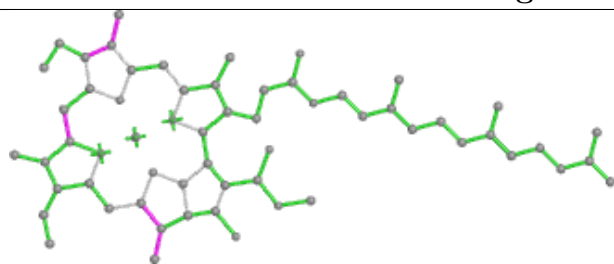


Torsions

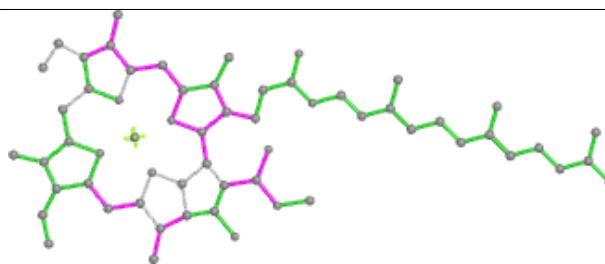


Rings

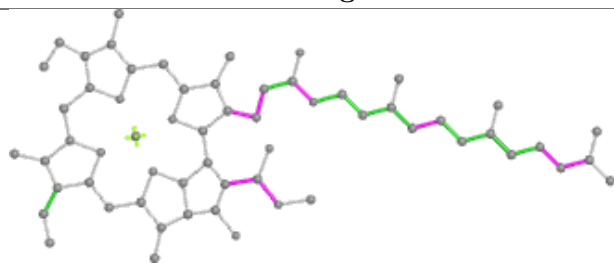
Ligand CLA F 301



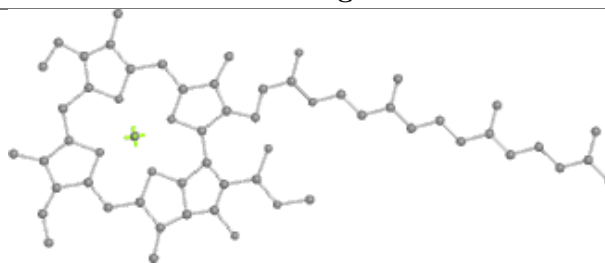
Bond lengths



Bond angles

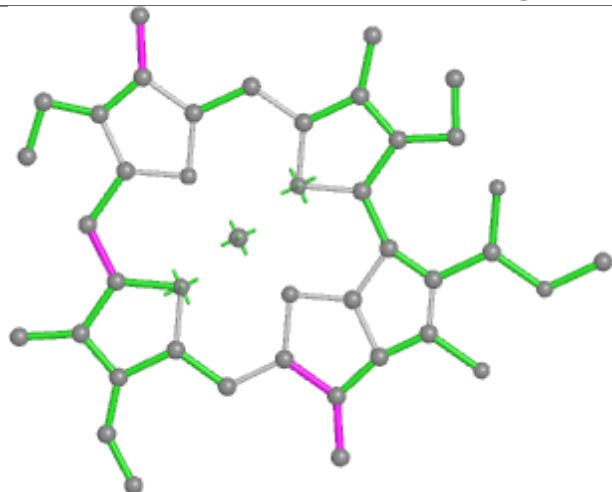


Torsions

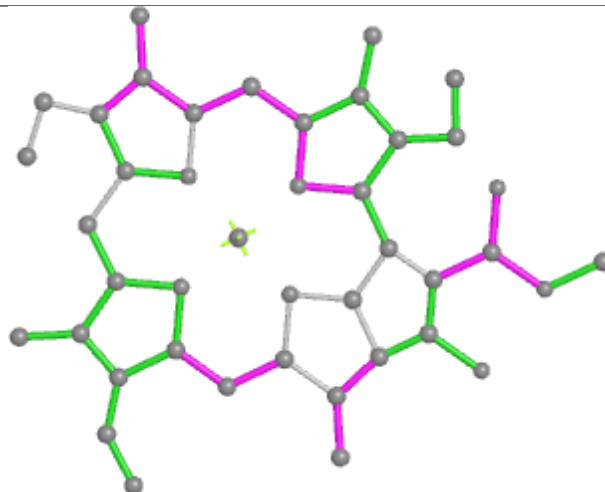


Rings

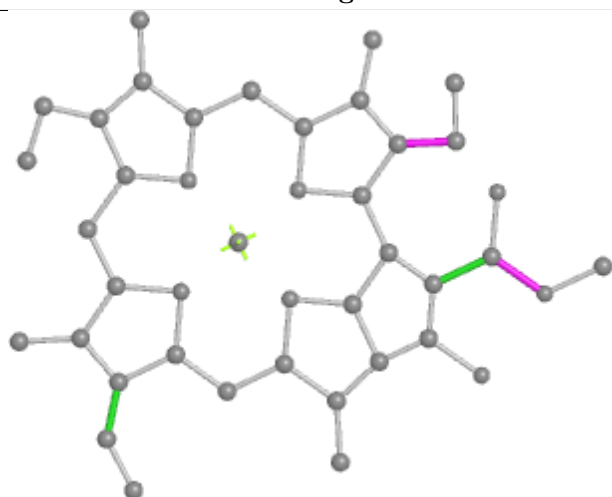
Ligand CLA F 302



Bond lengths



Bond angles

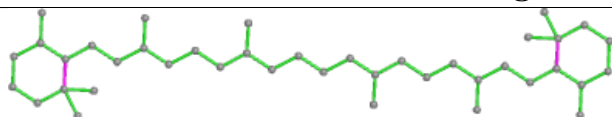


Torsions

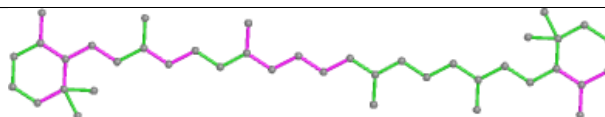


Rings

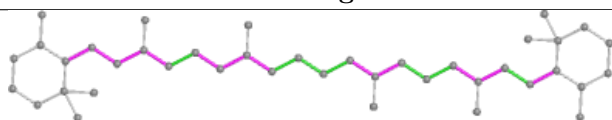
Ligand BCR F 303



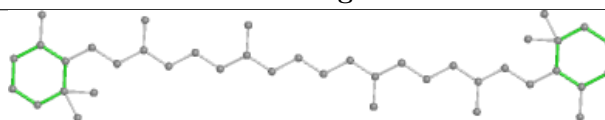
Bond lengths



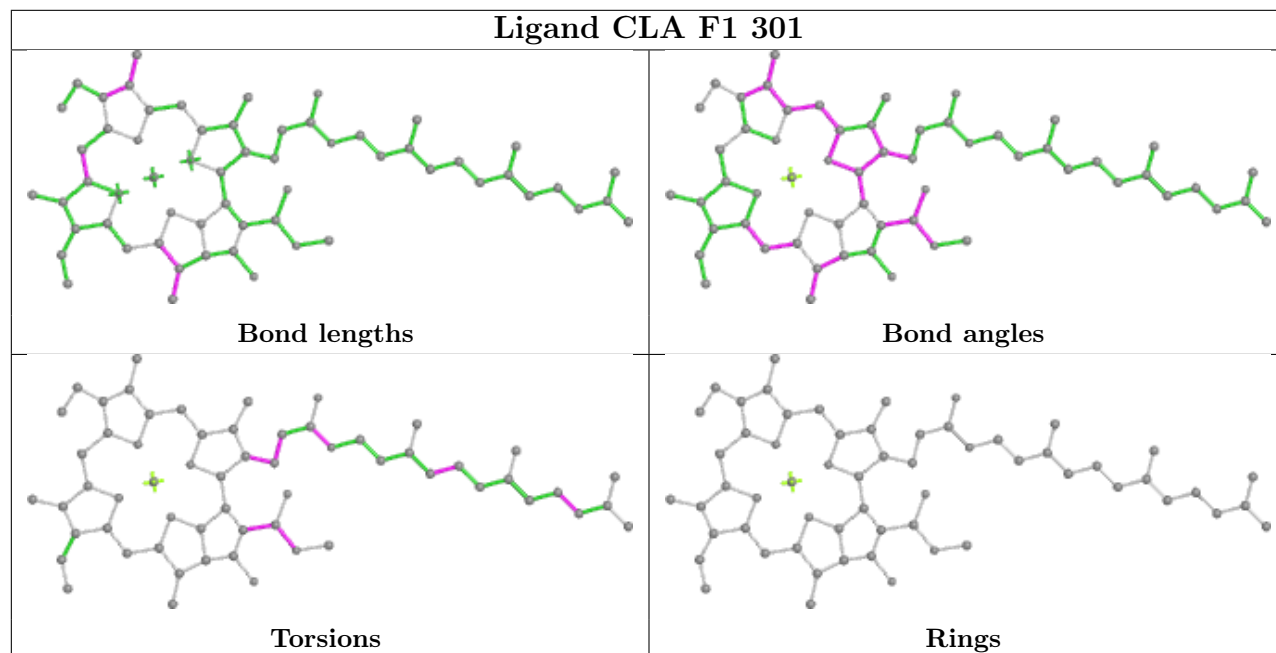
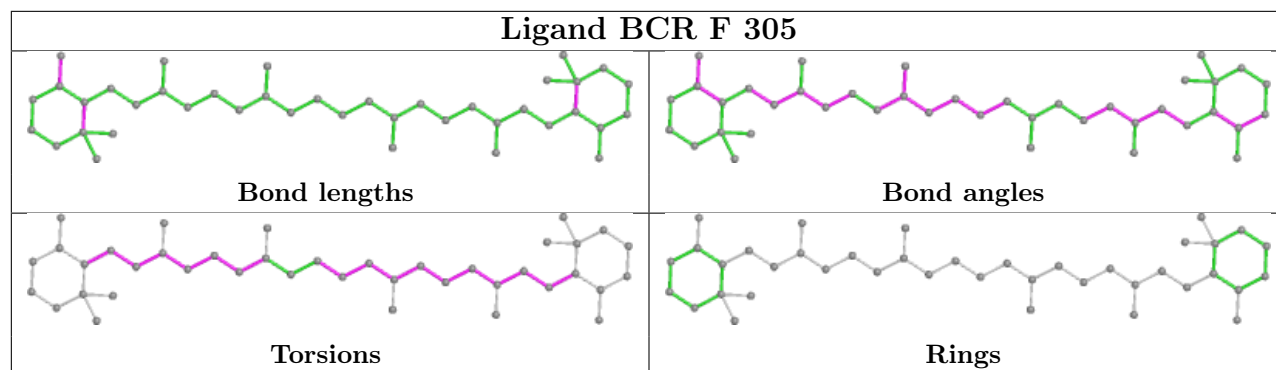
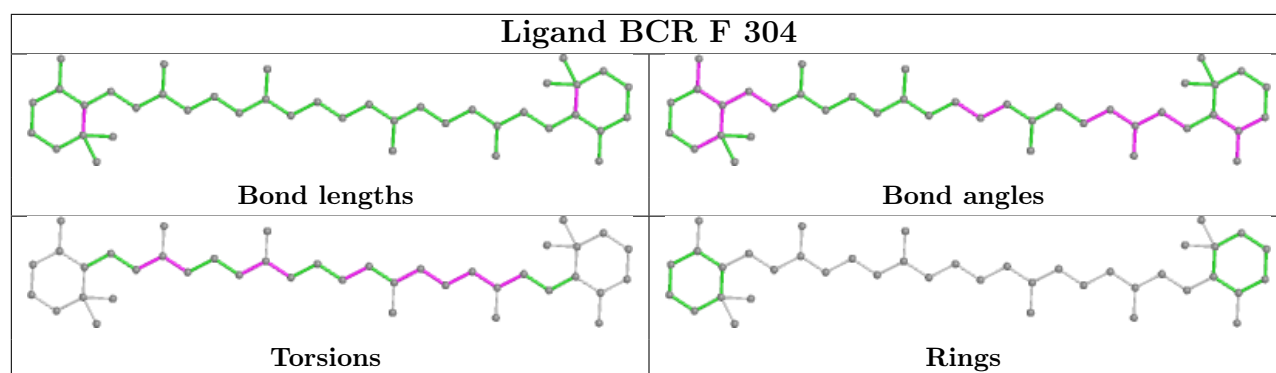
Bond angles

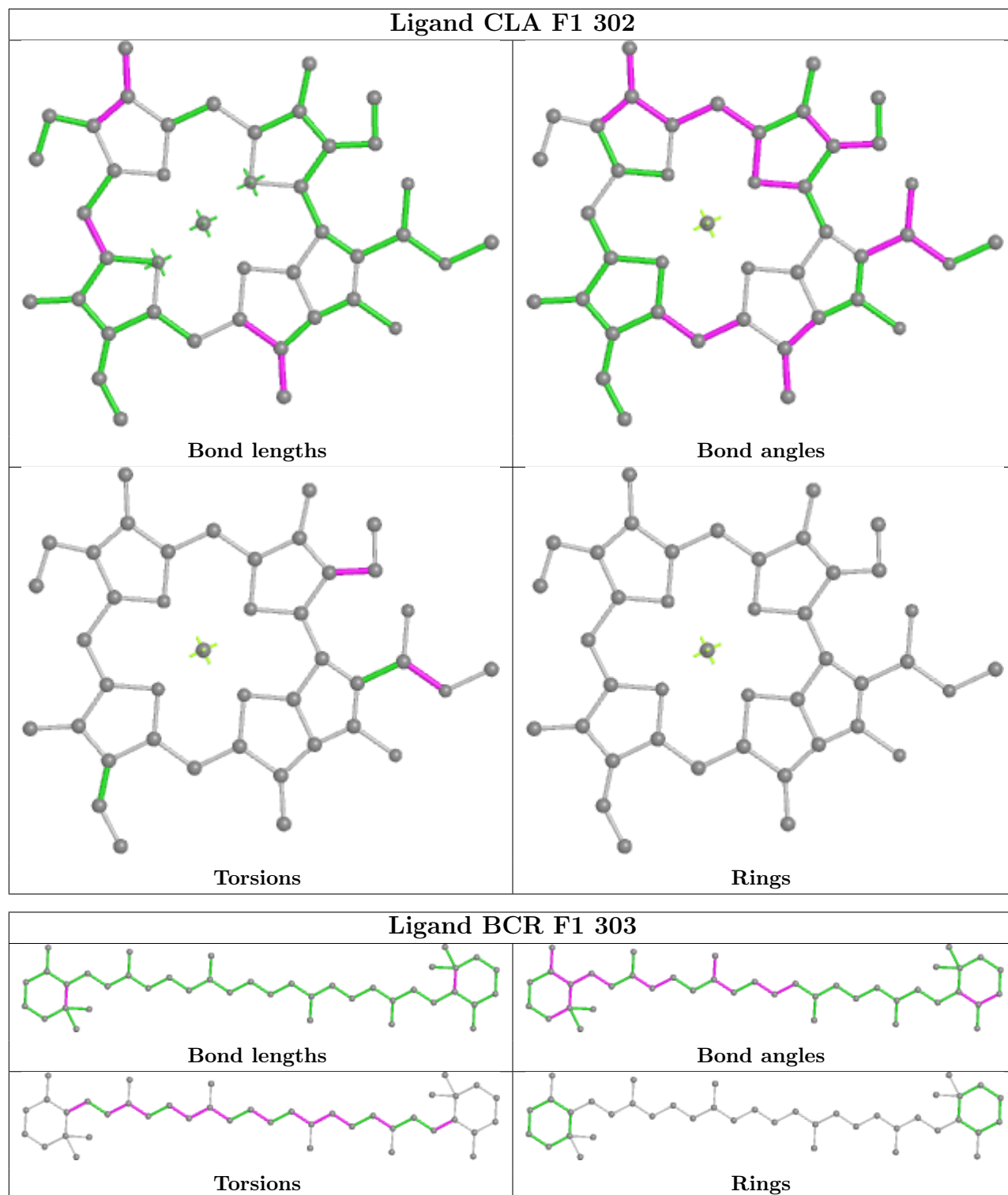


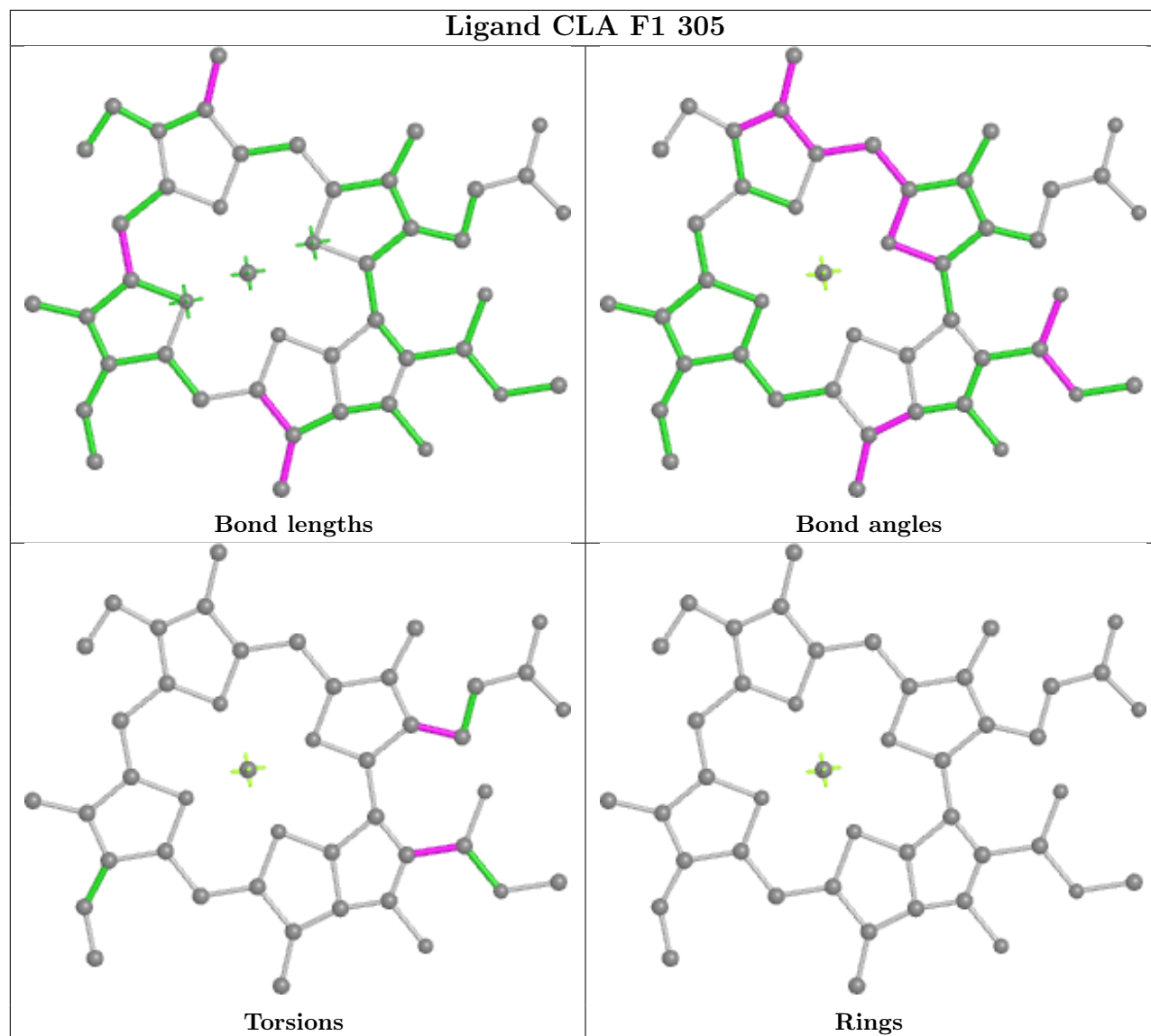
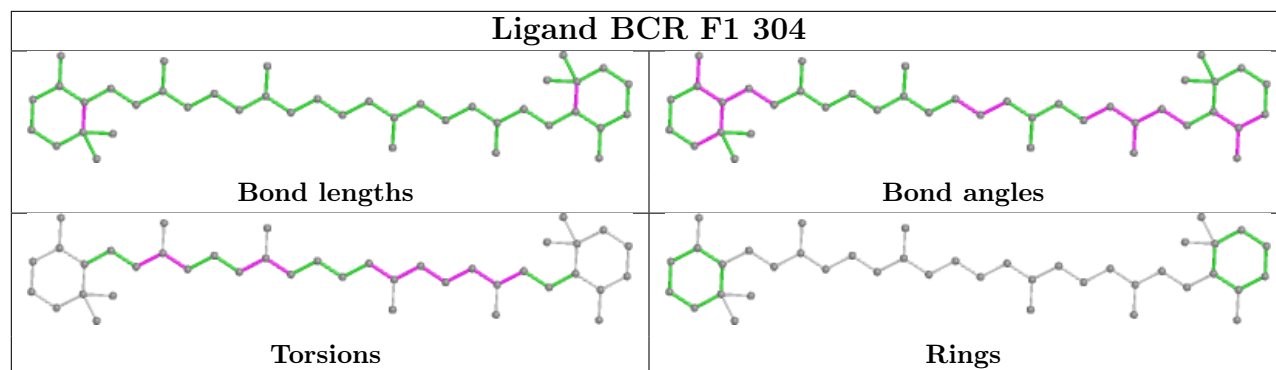
Torsions

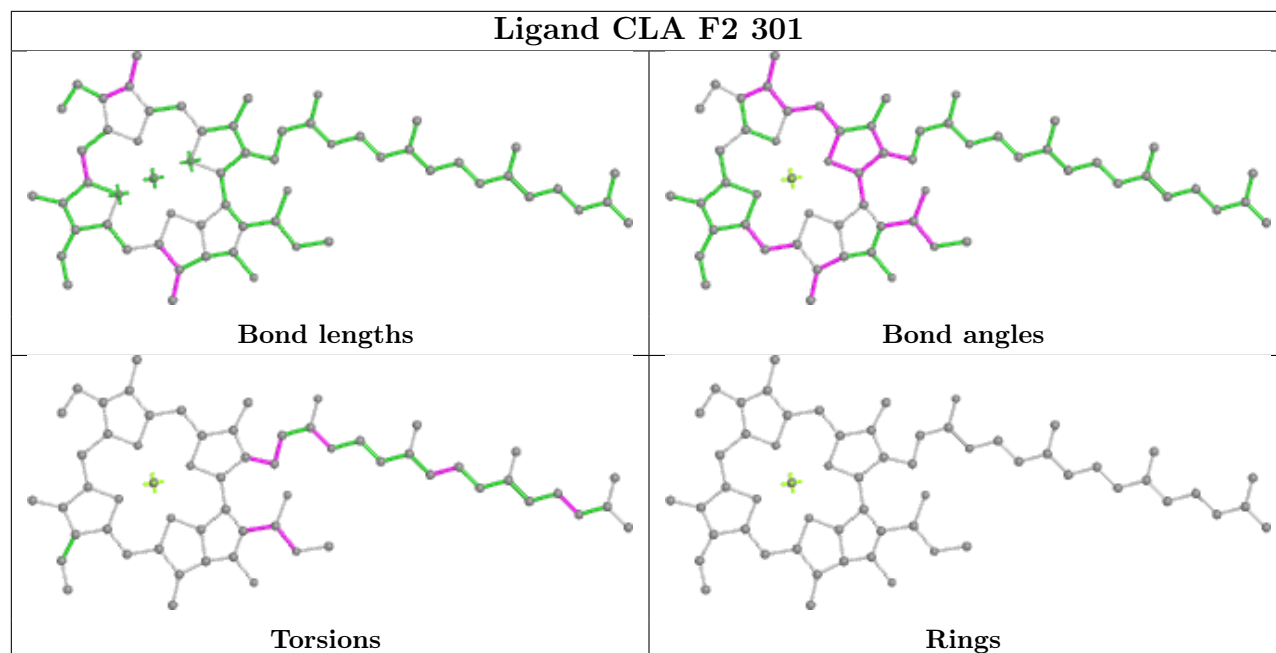
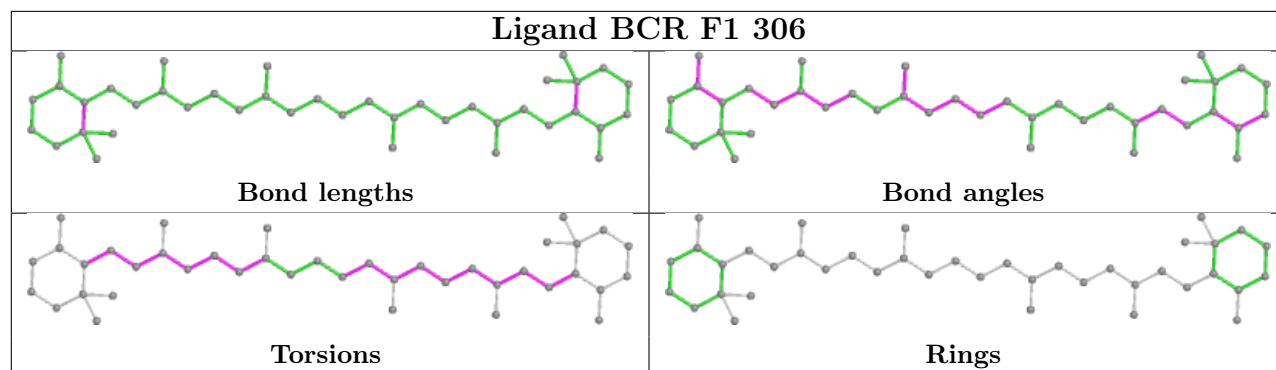


Rings

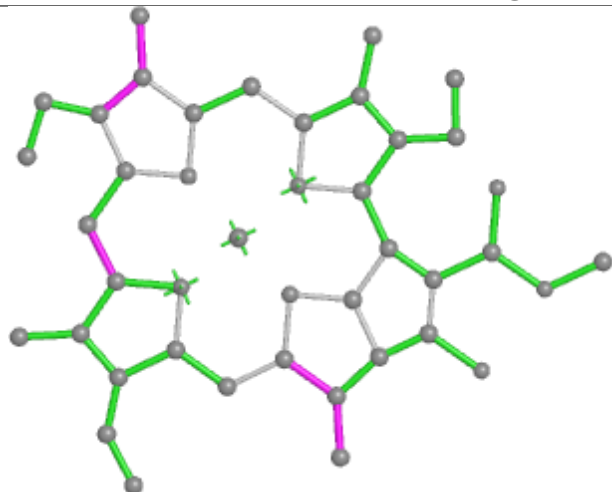




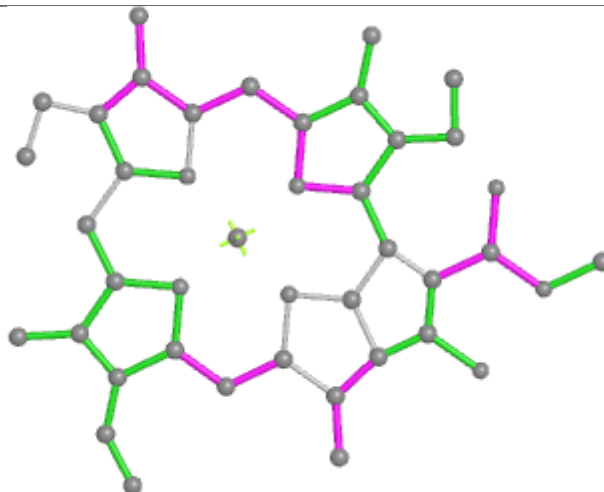




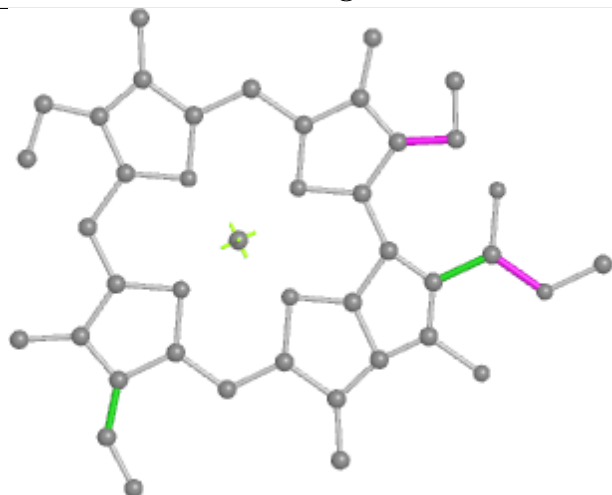
Ligand CLA F2 302



Bond lengths



Bond angles

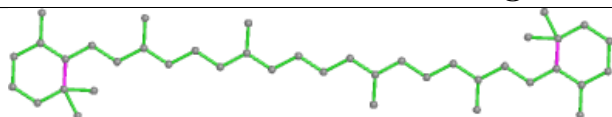


Torsions

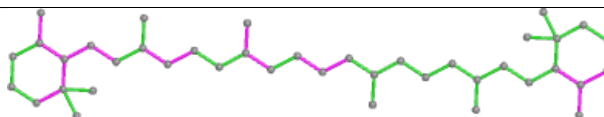


Rings

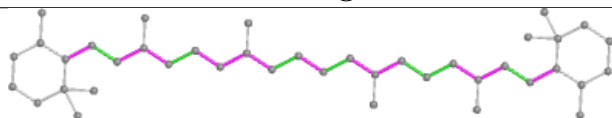
Ligand BCR F2 303



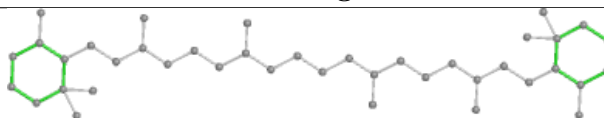
Bond lengths



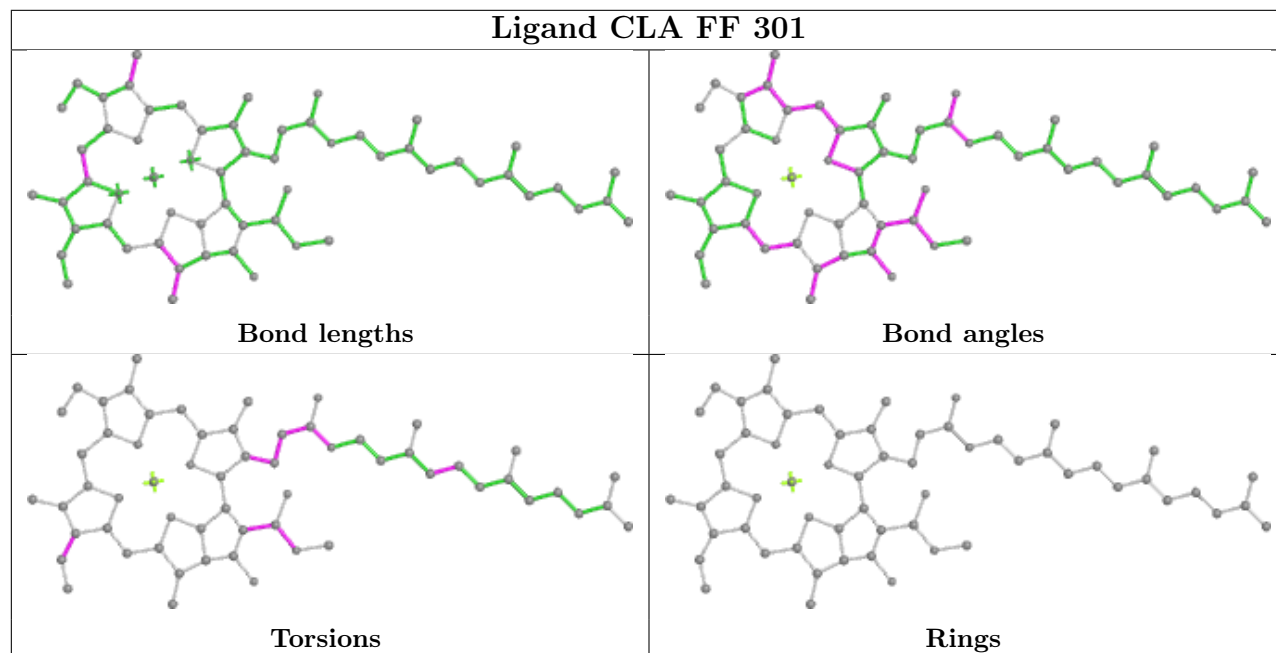
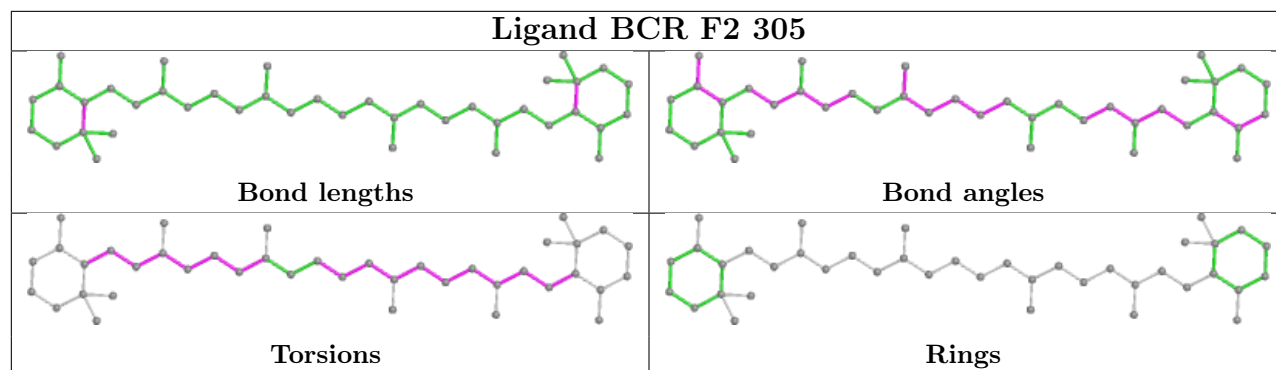
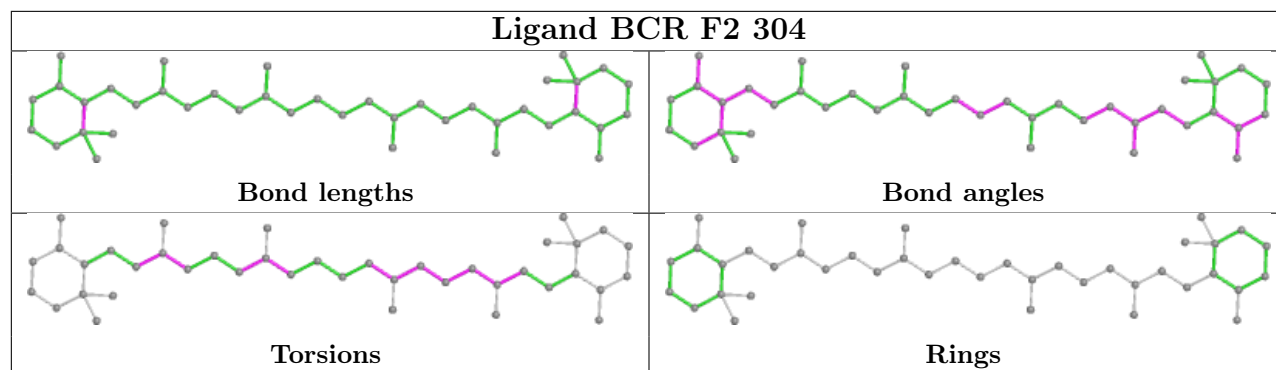
Bond angles



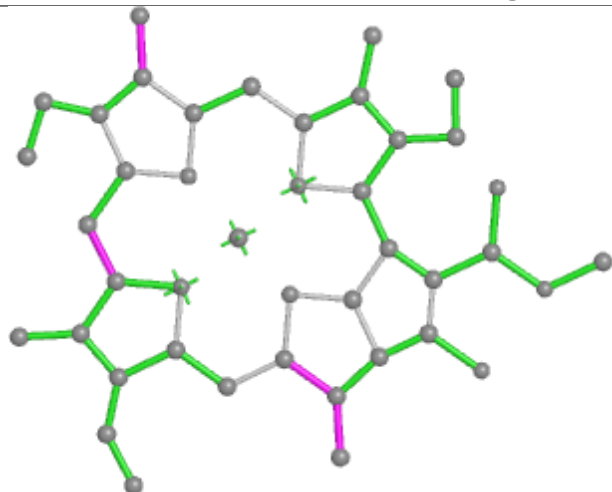
Torsions



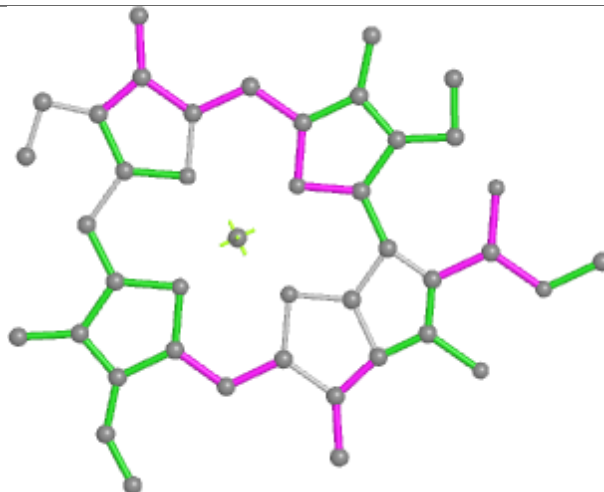
Rings



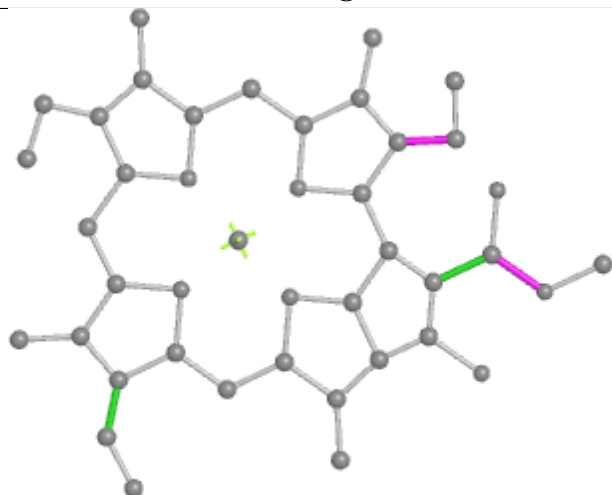
Ligand CLA FF 302



Bond lengths



Bond angles

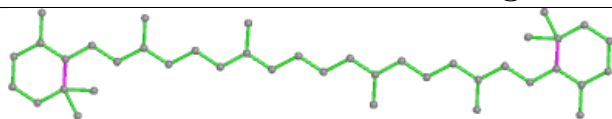


Torsions

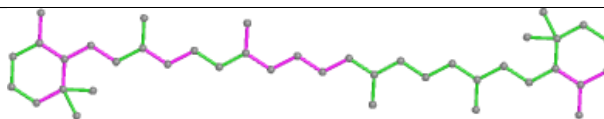


Rings

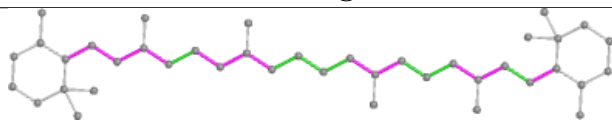
Ligand BCR FF 303



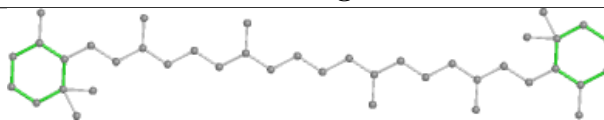
Bond lengths



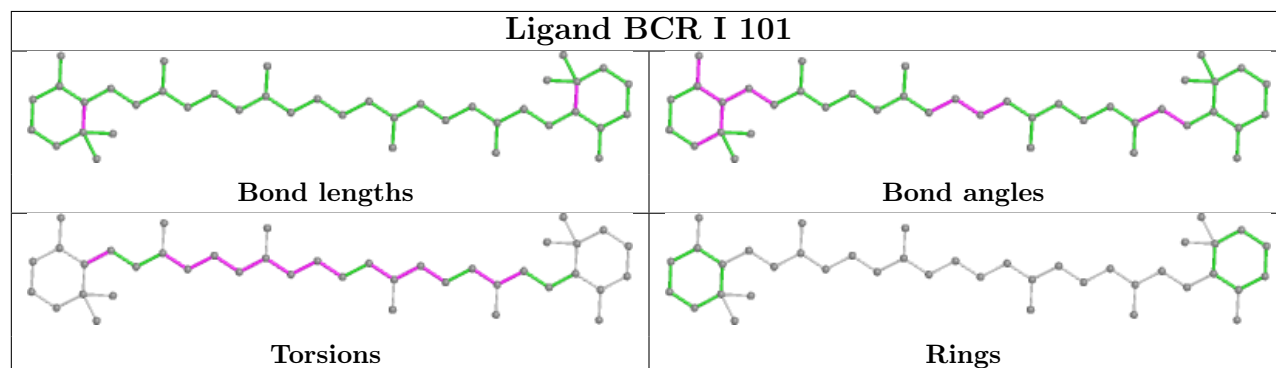
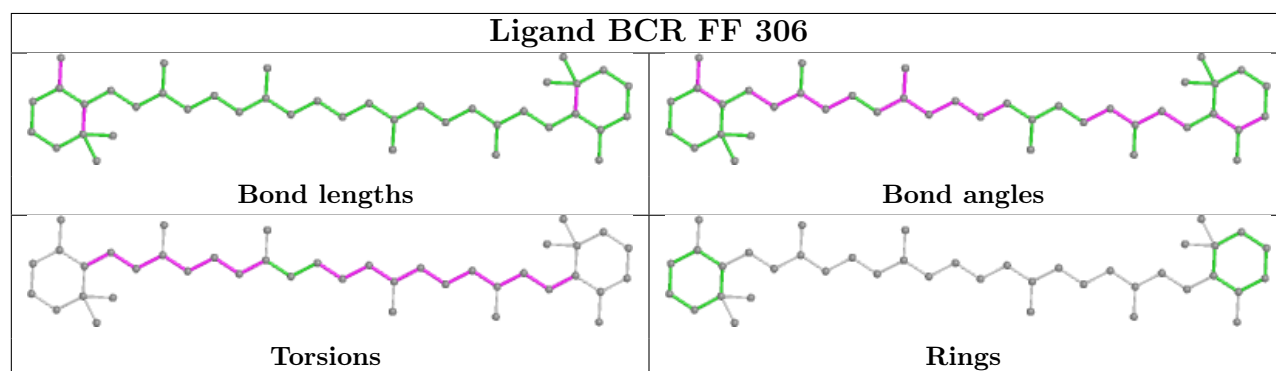
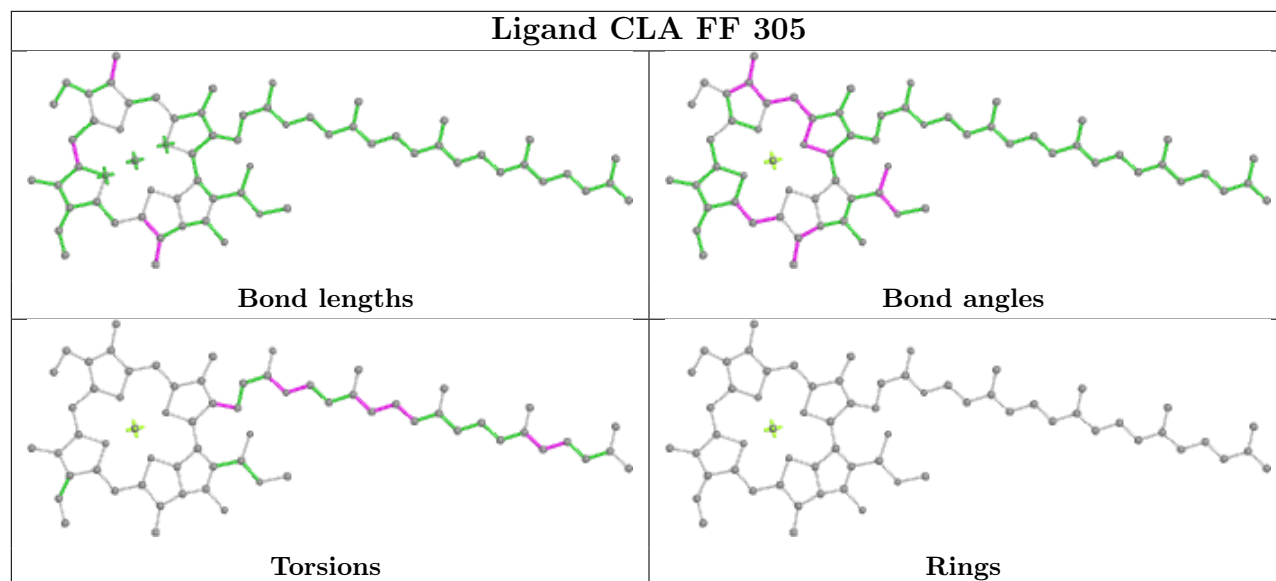
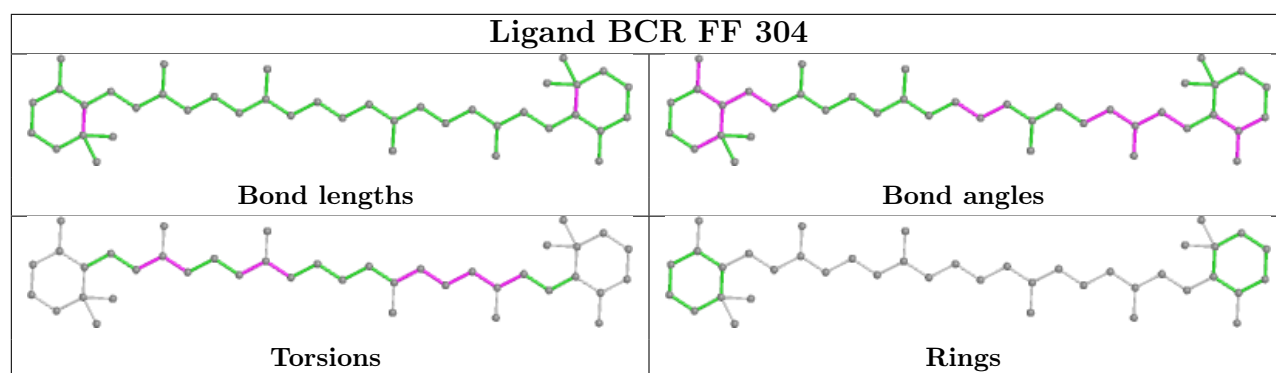
Bond angles

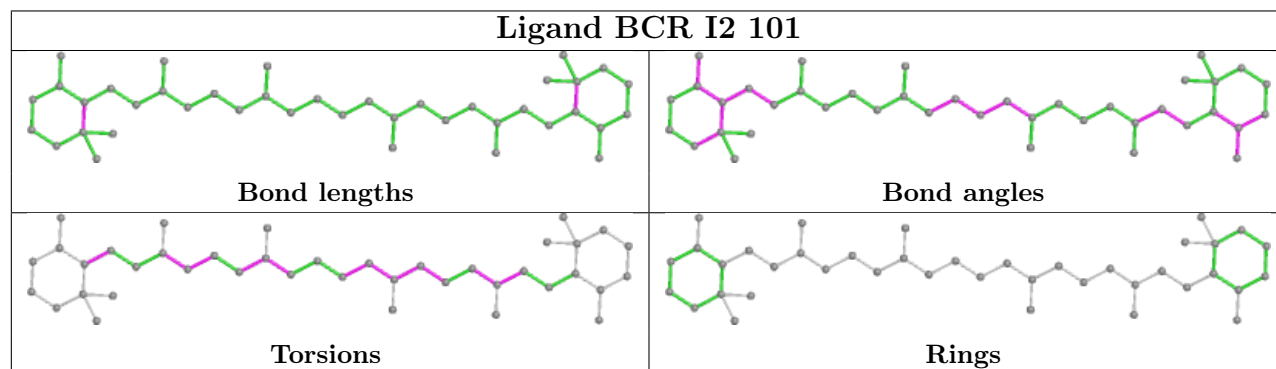
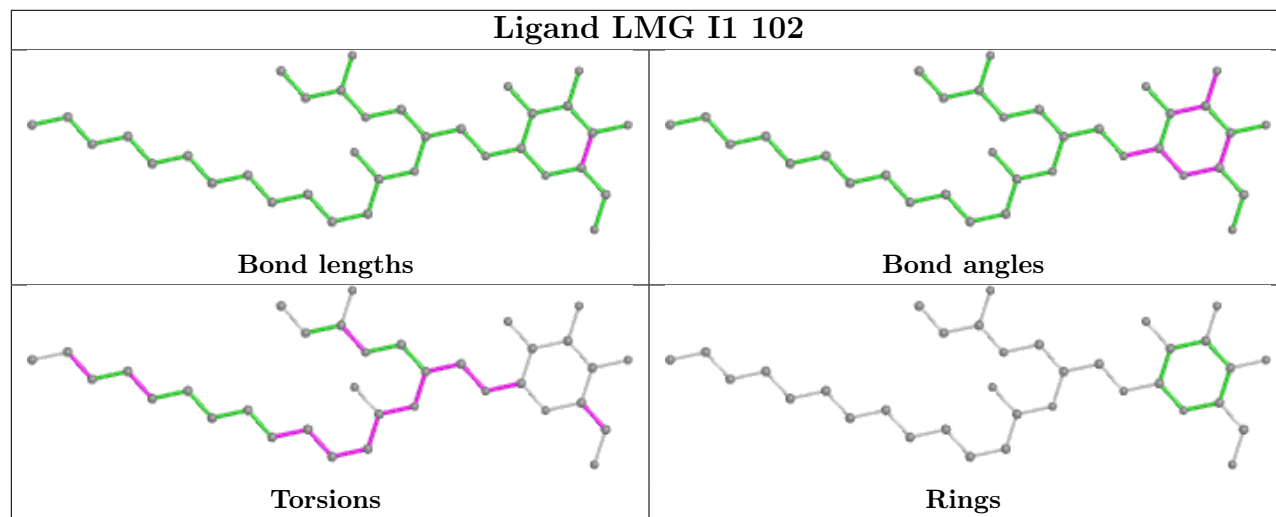
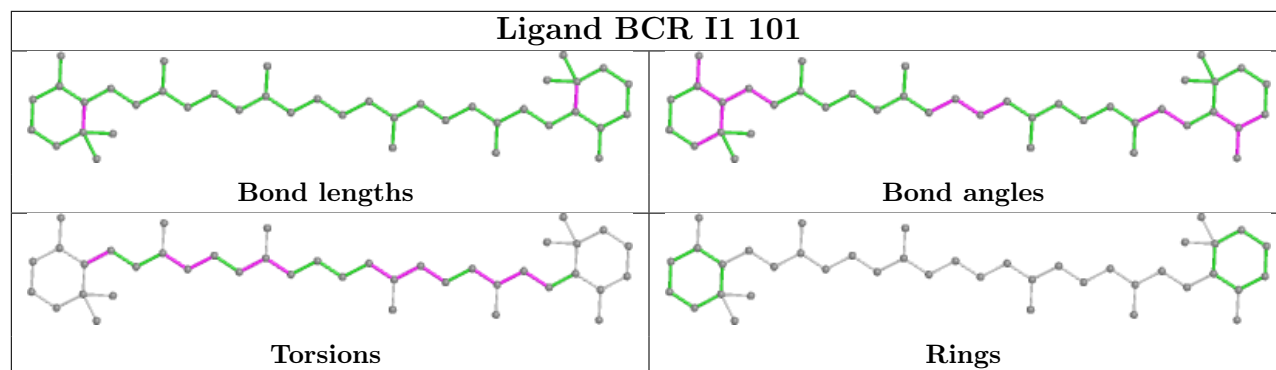
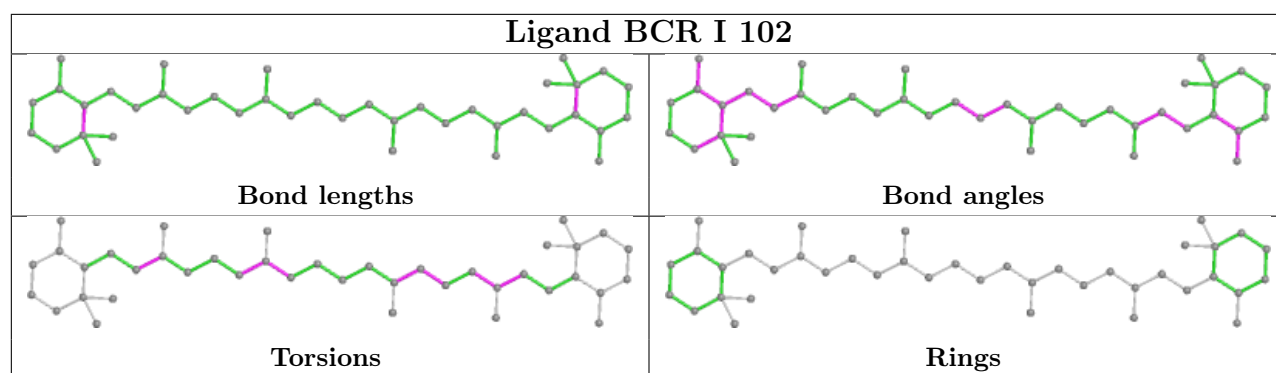


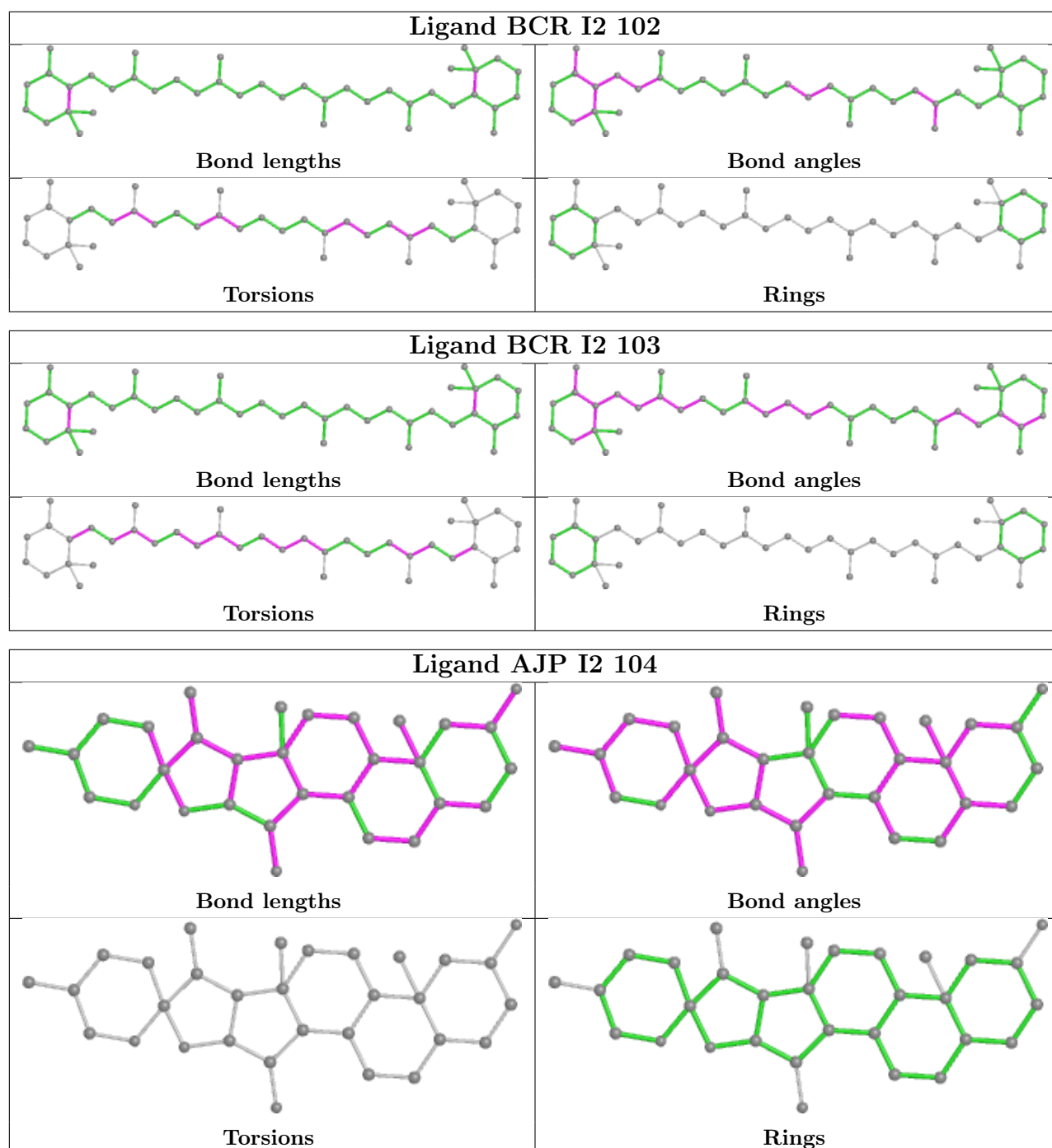
Torsions

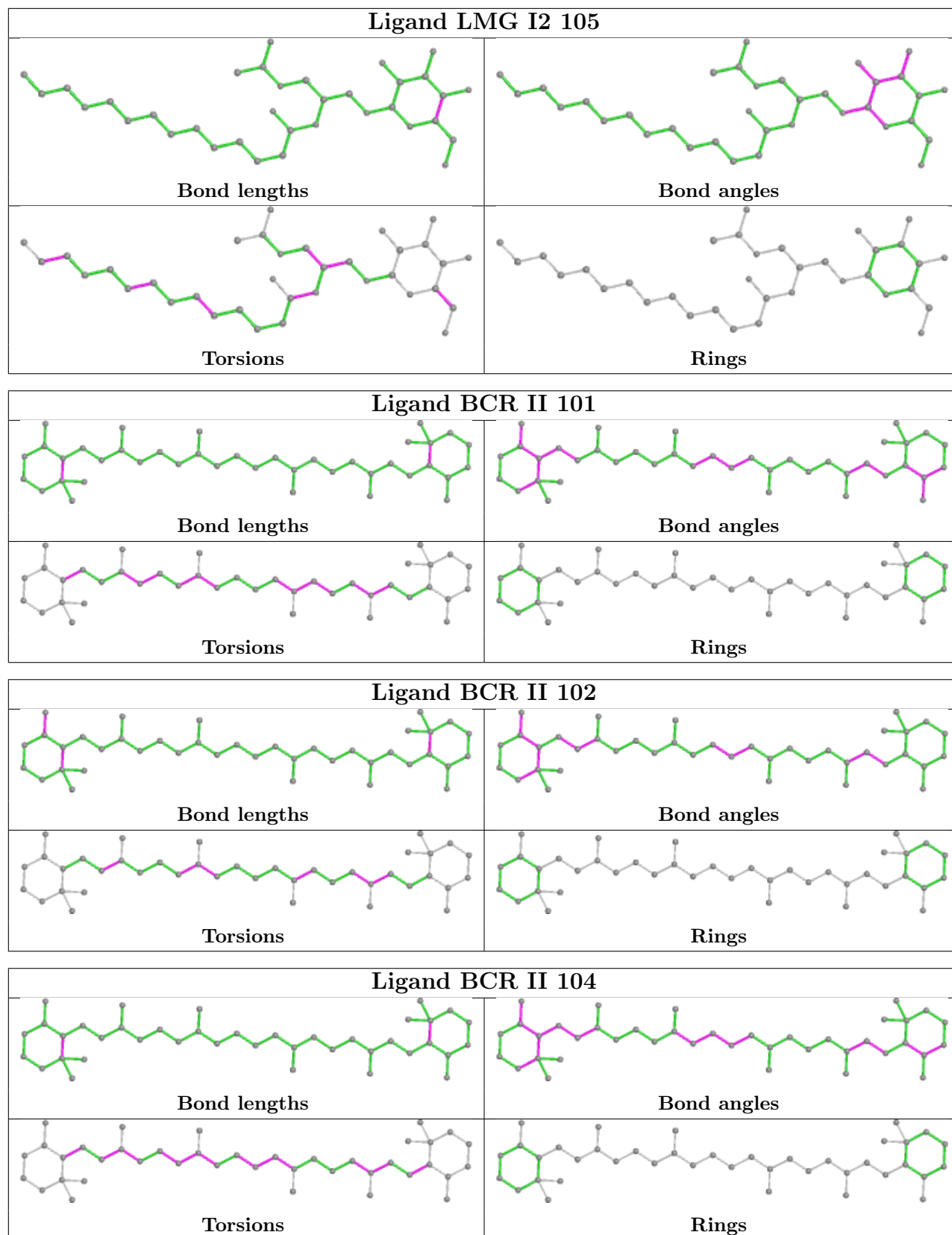


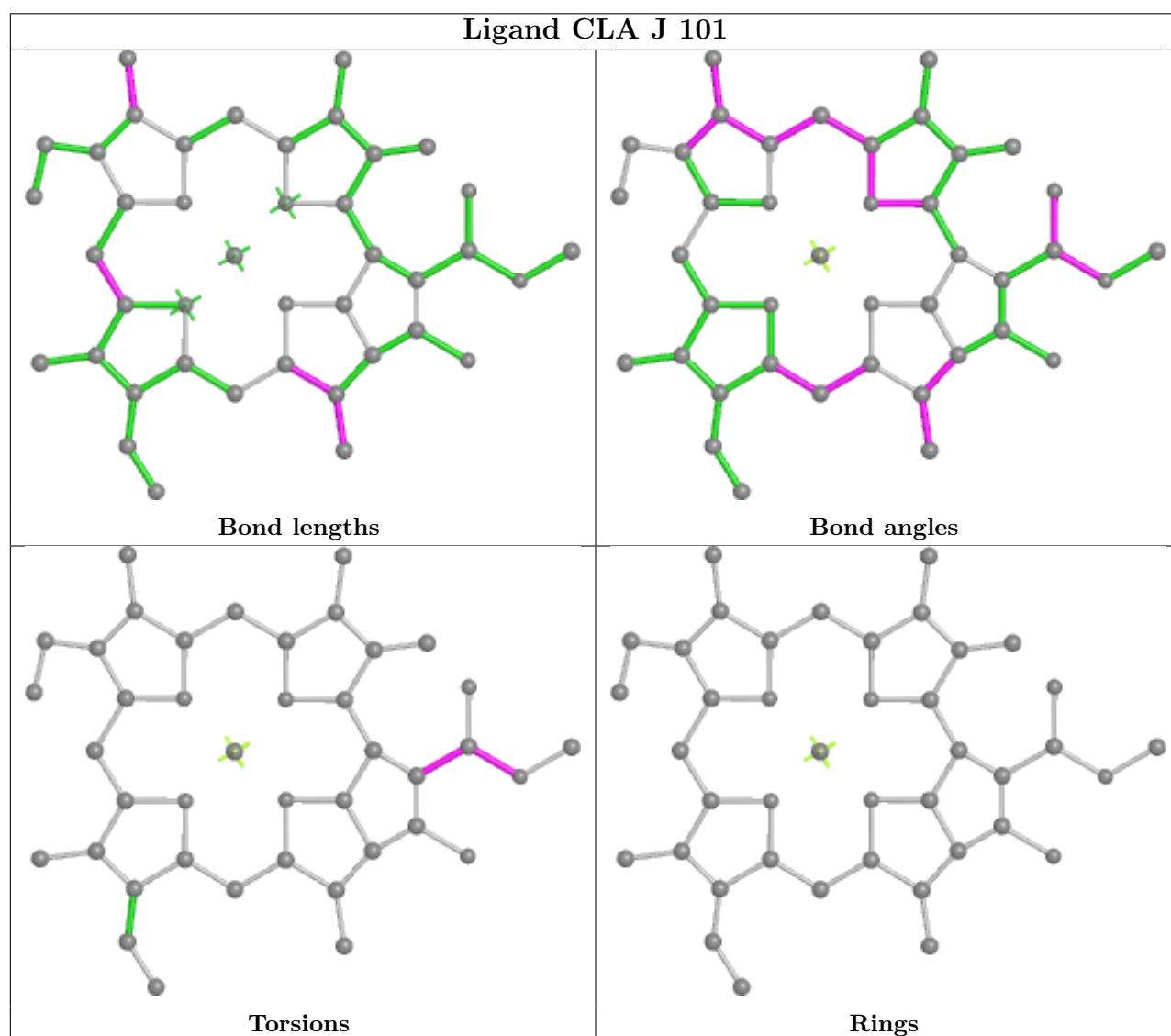
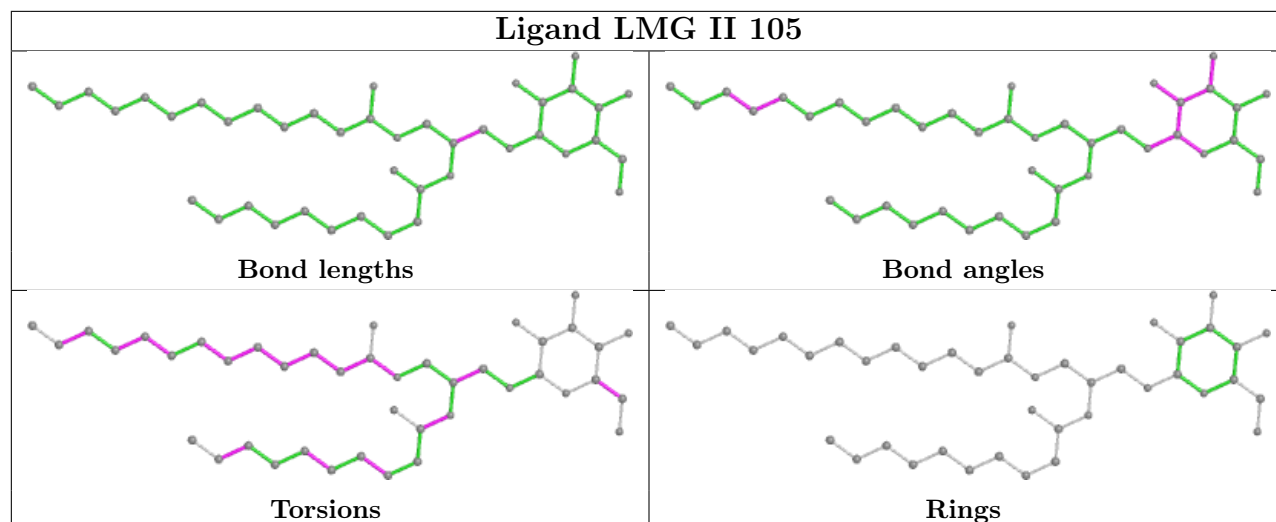
Rings



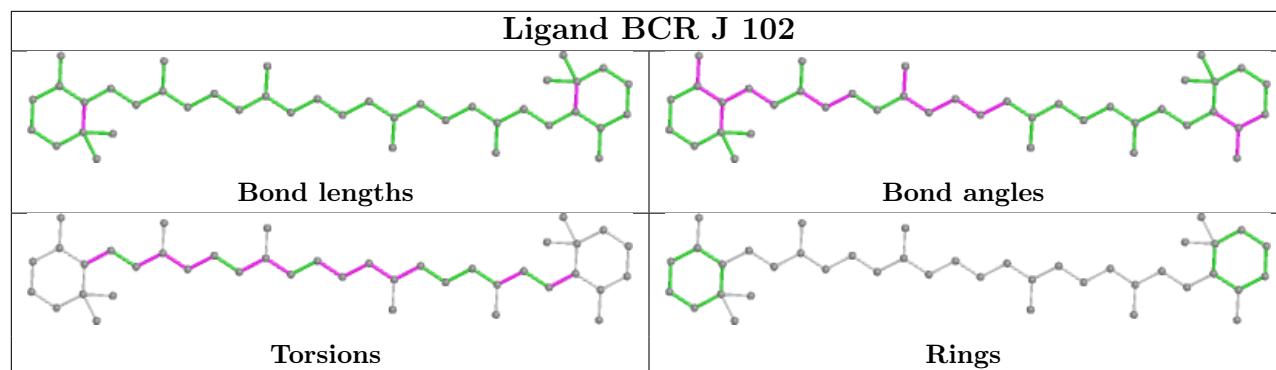




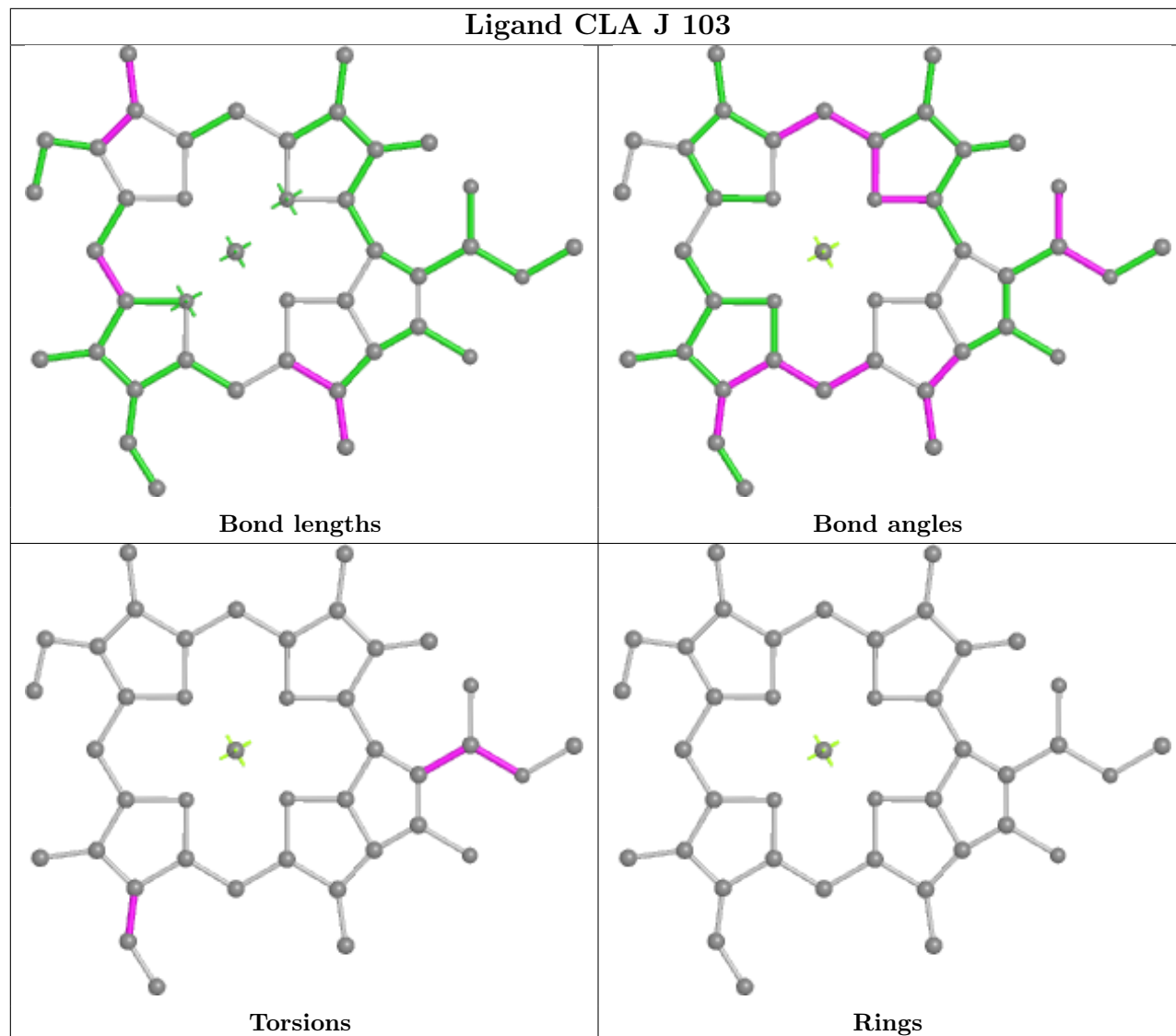




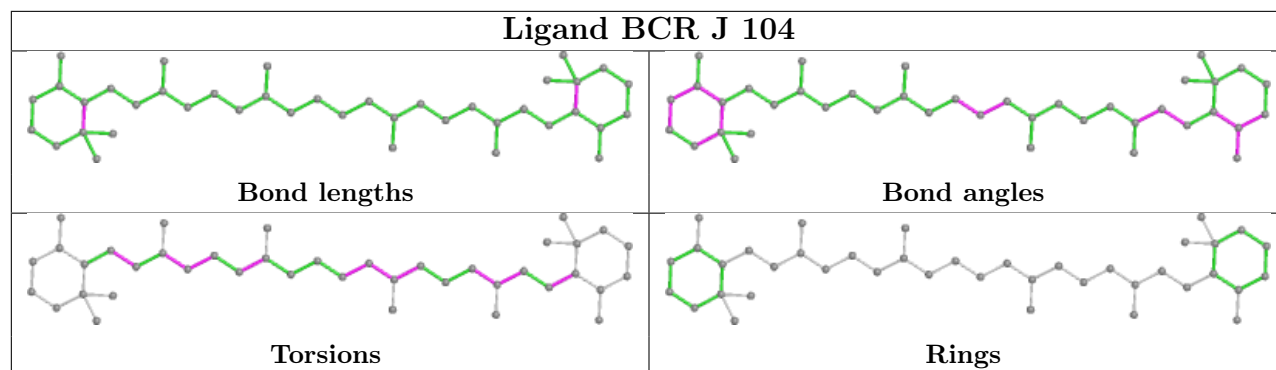
Ligand BCR J 102



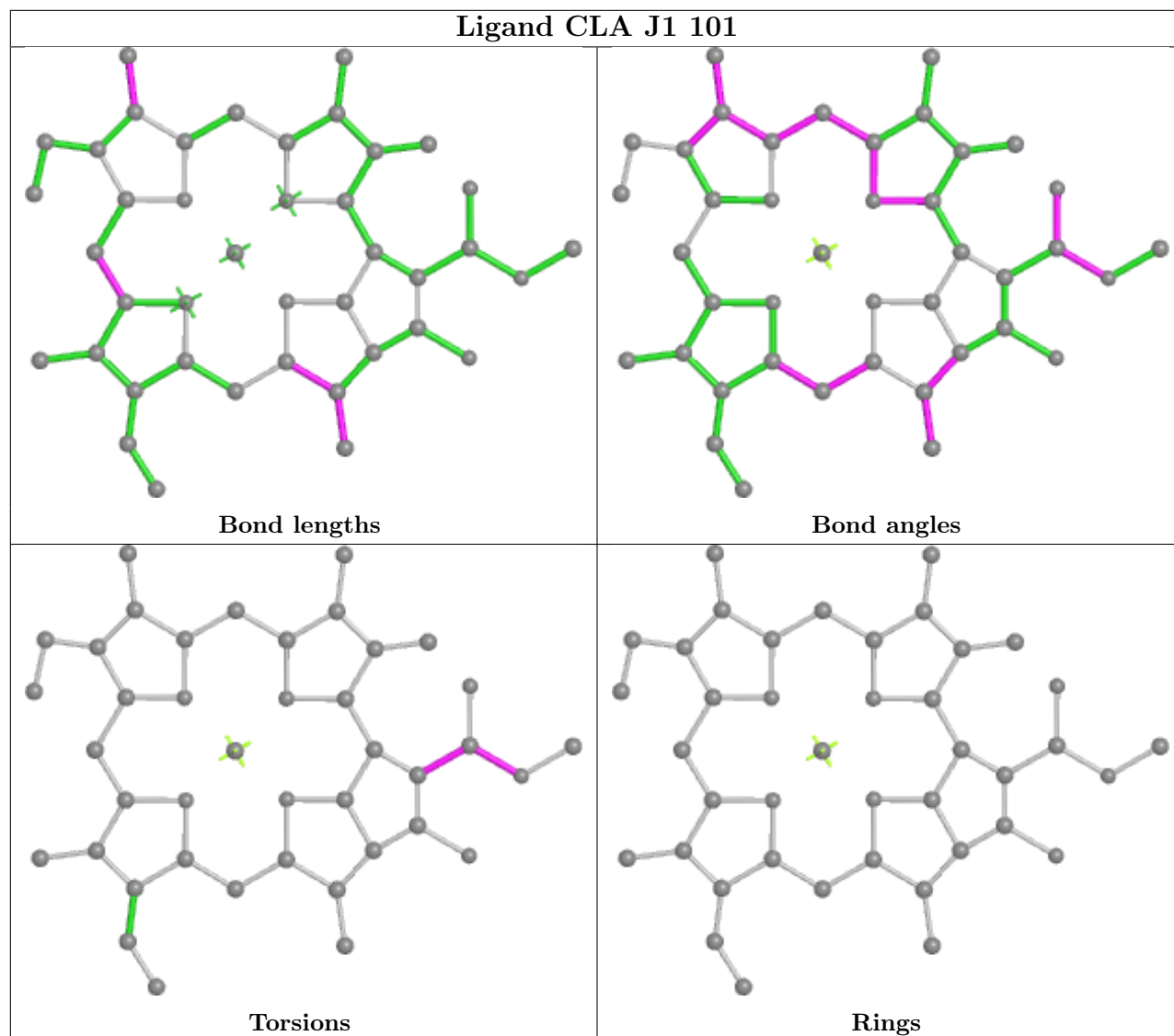
Ligand CLA J 103

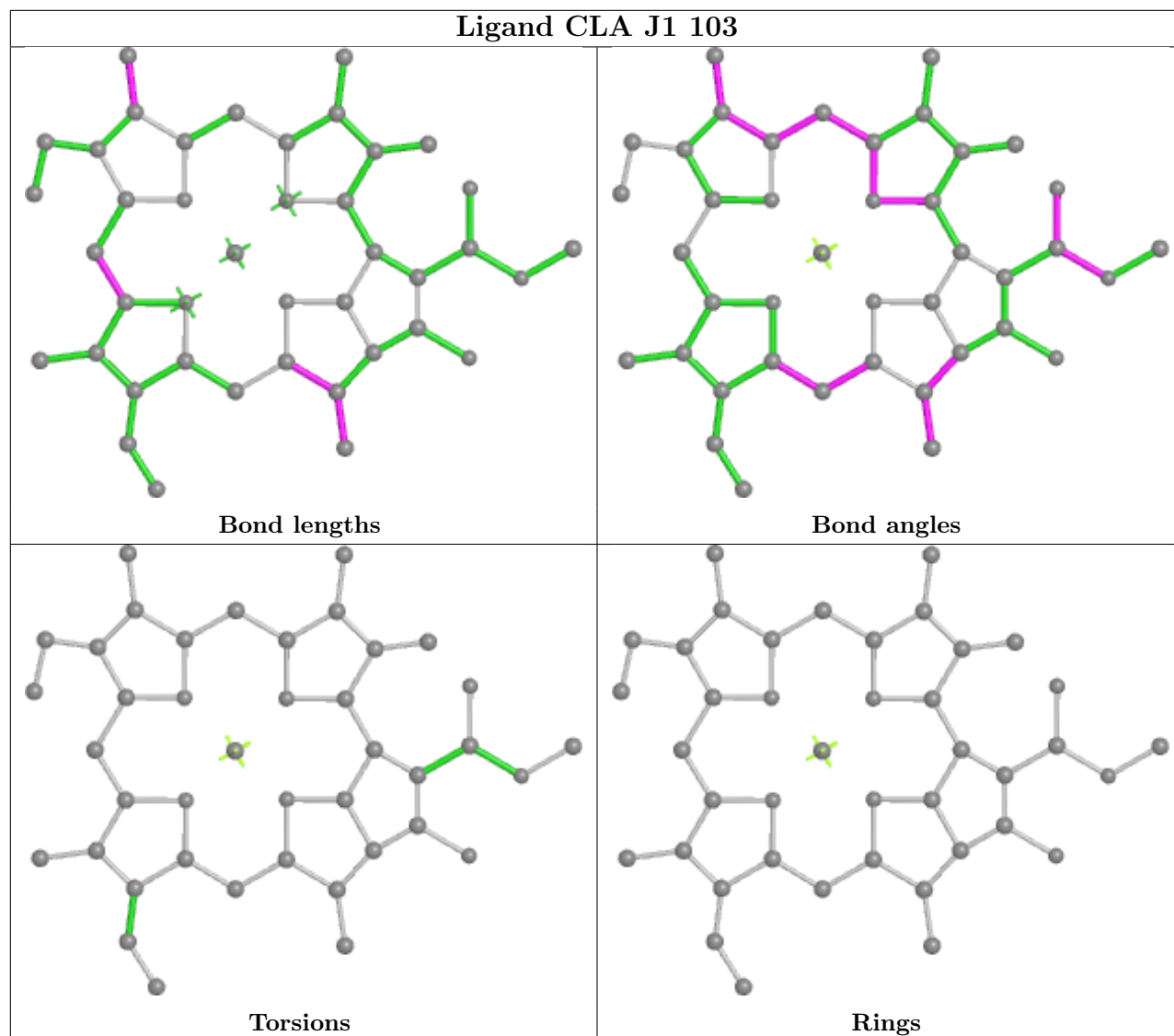
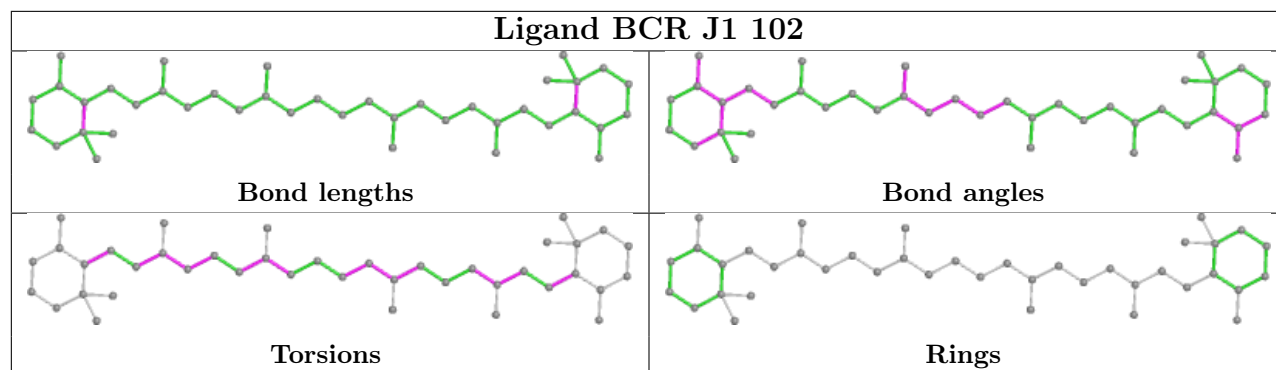


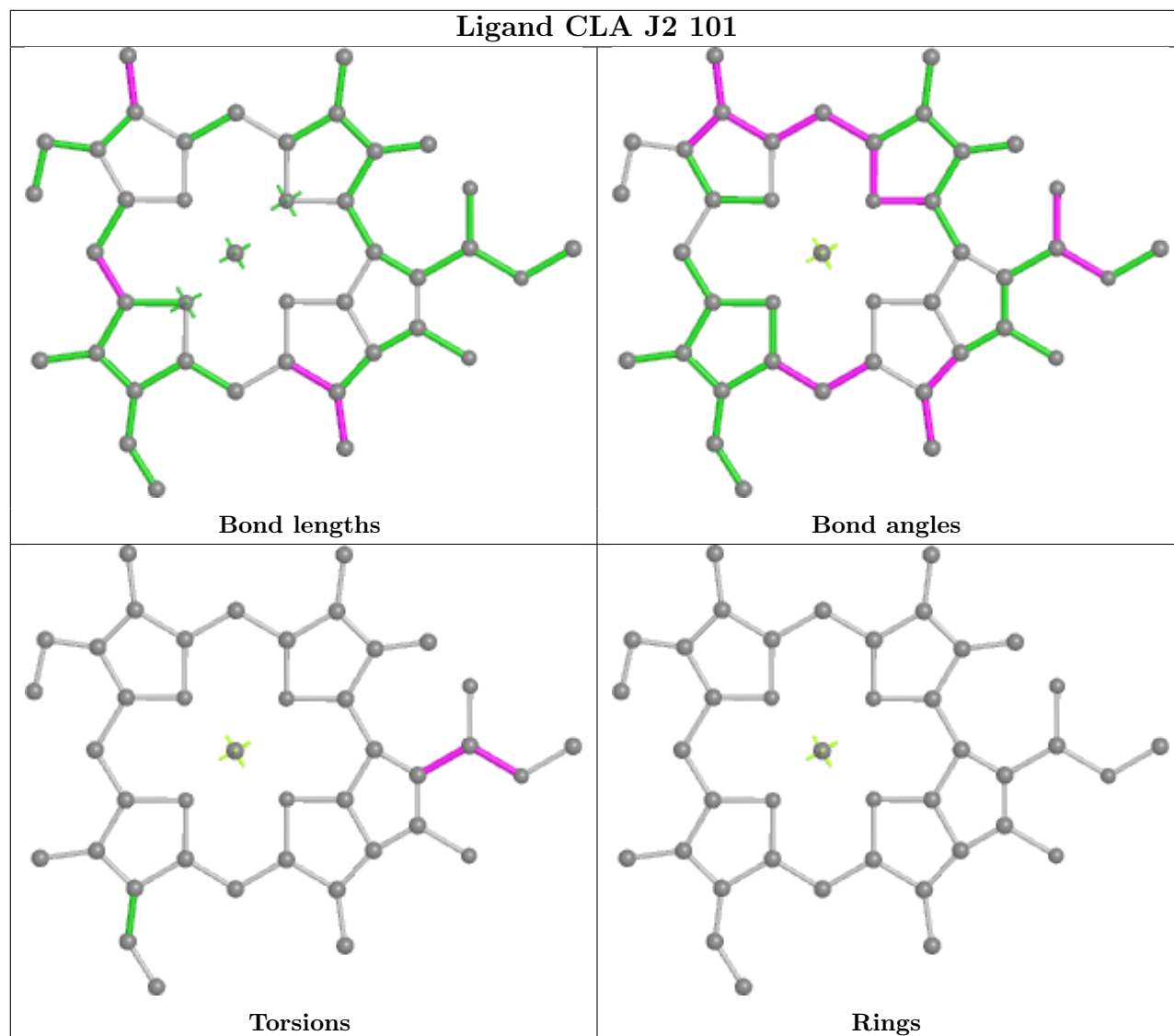
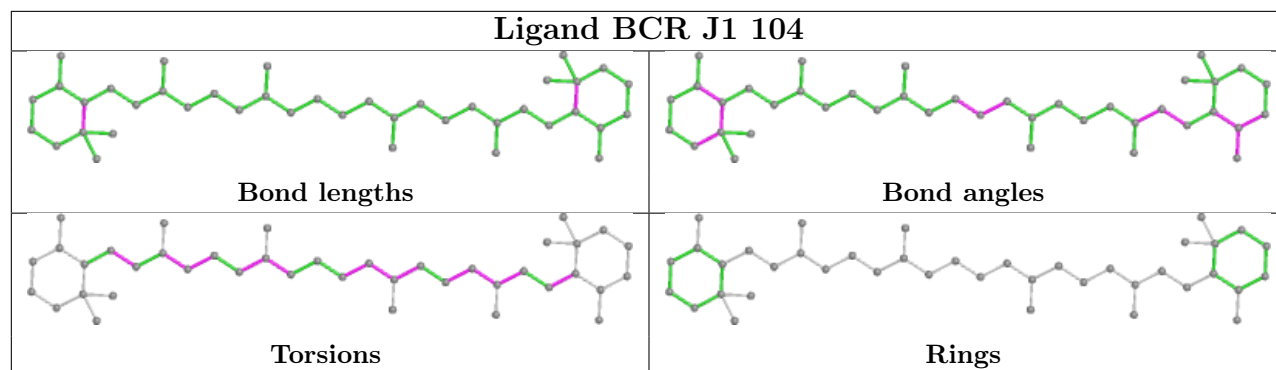
Ligand BCR J 104

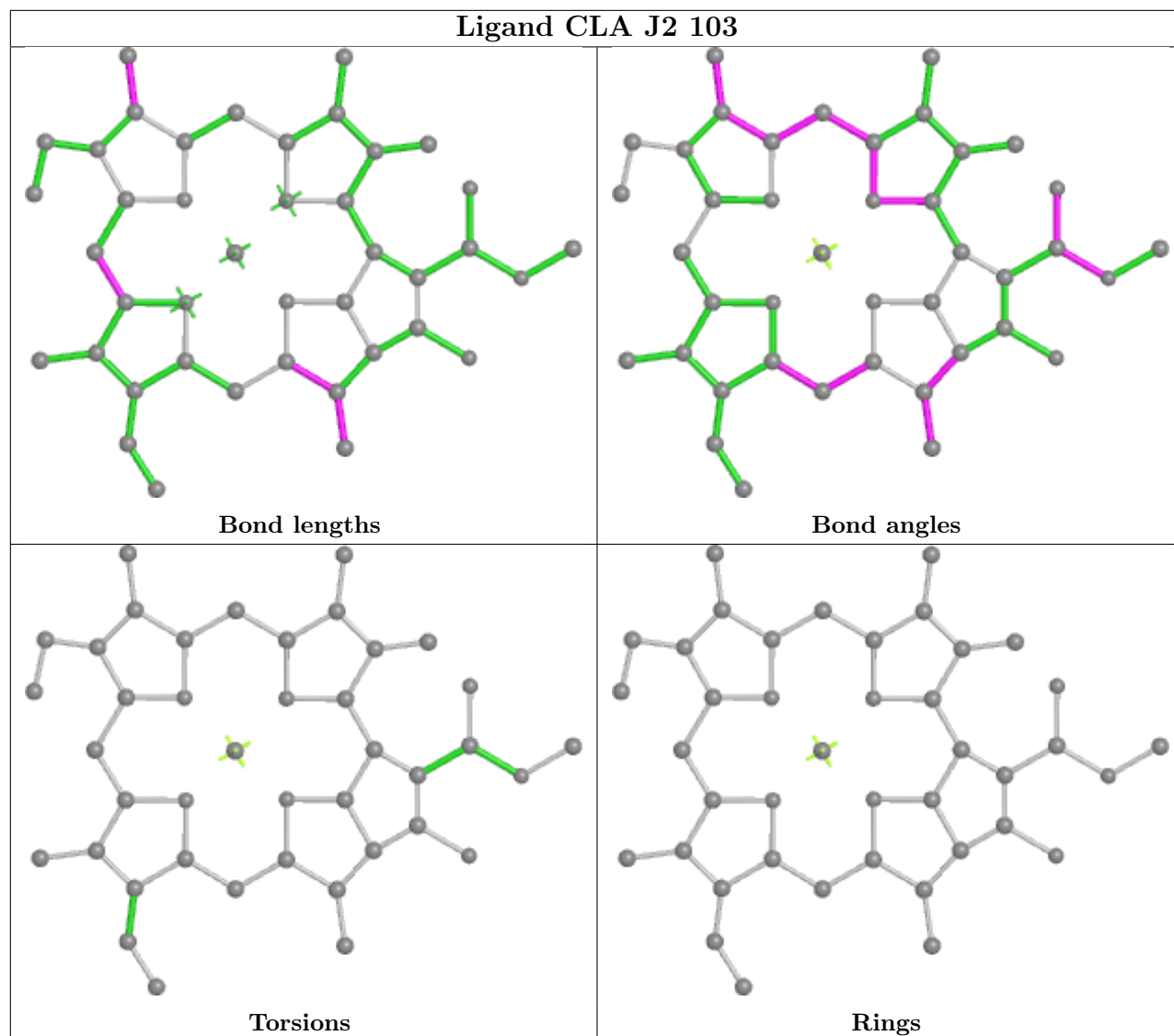
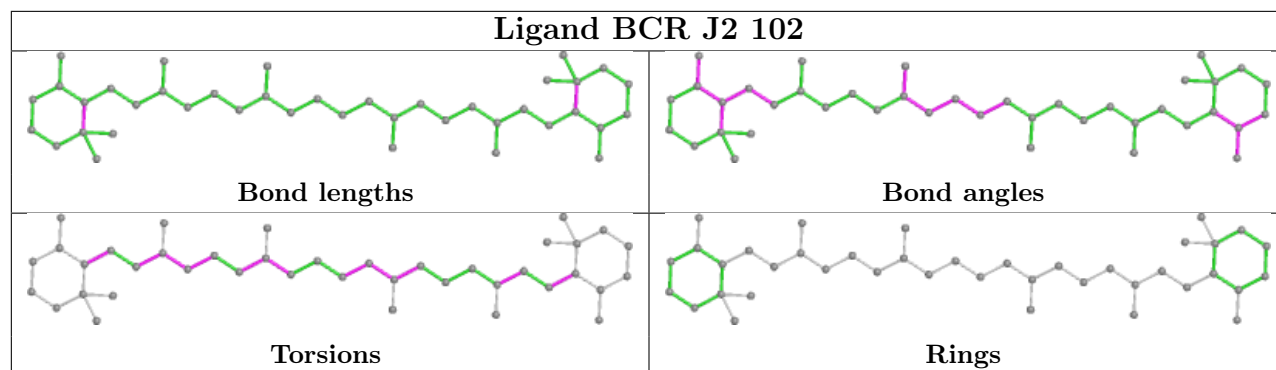


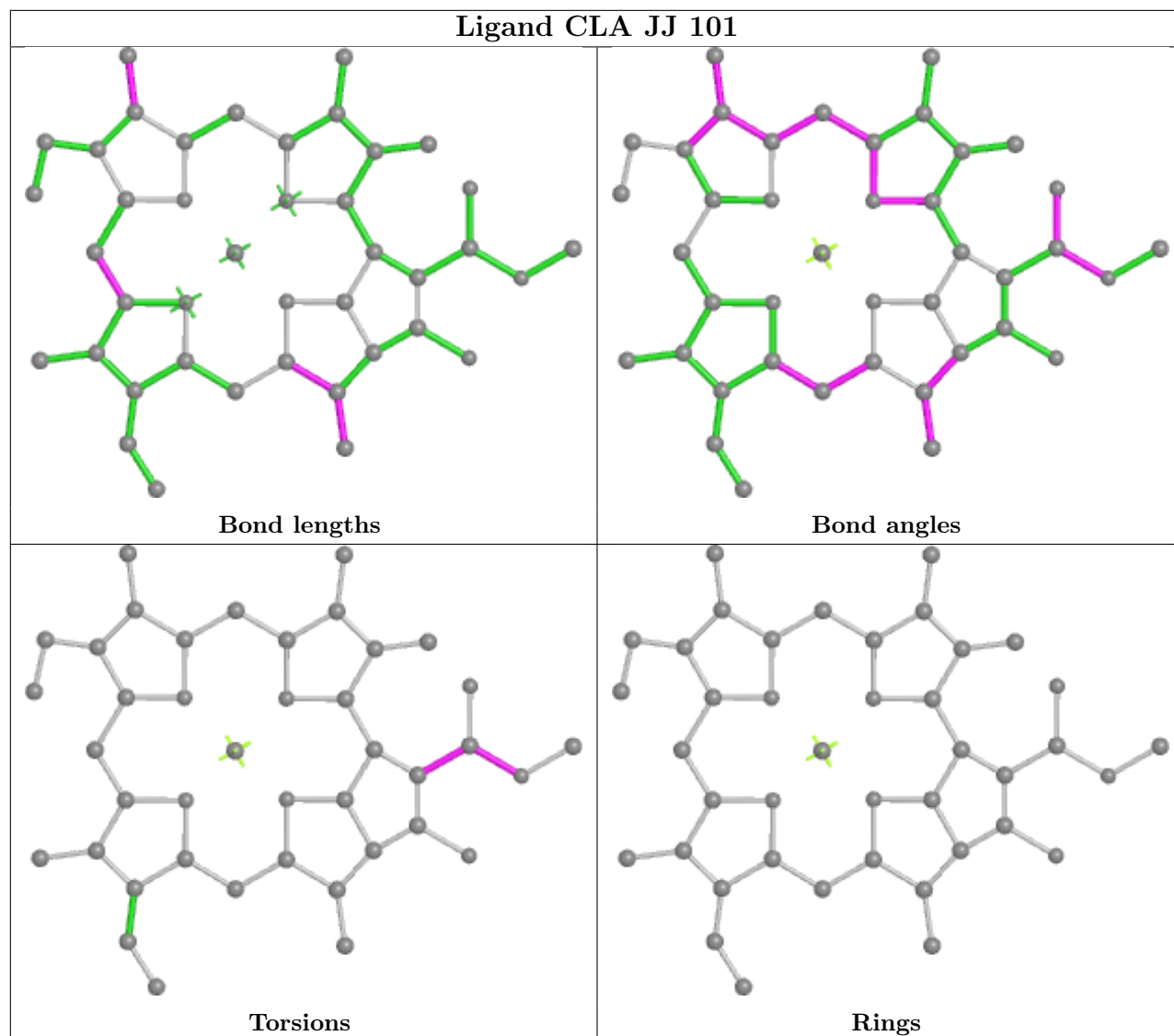
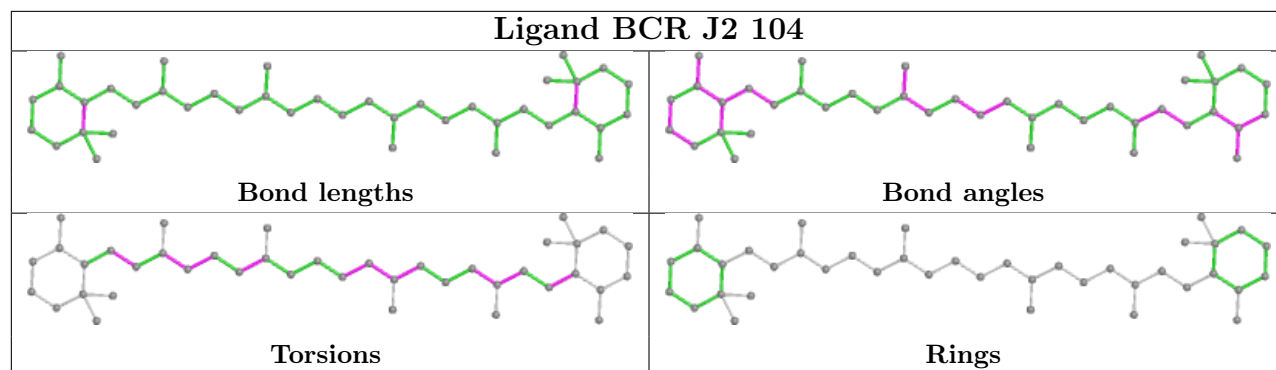
Ligand CLA J1 101

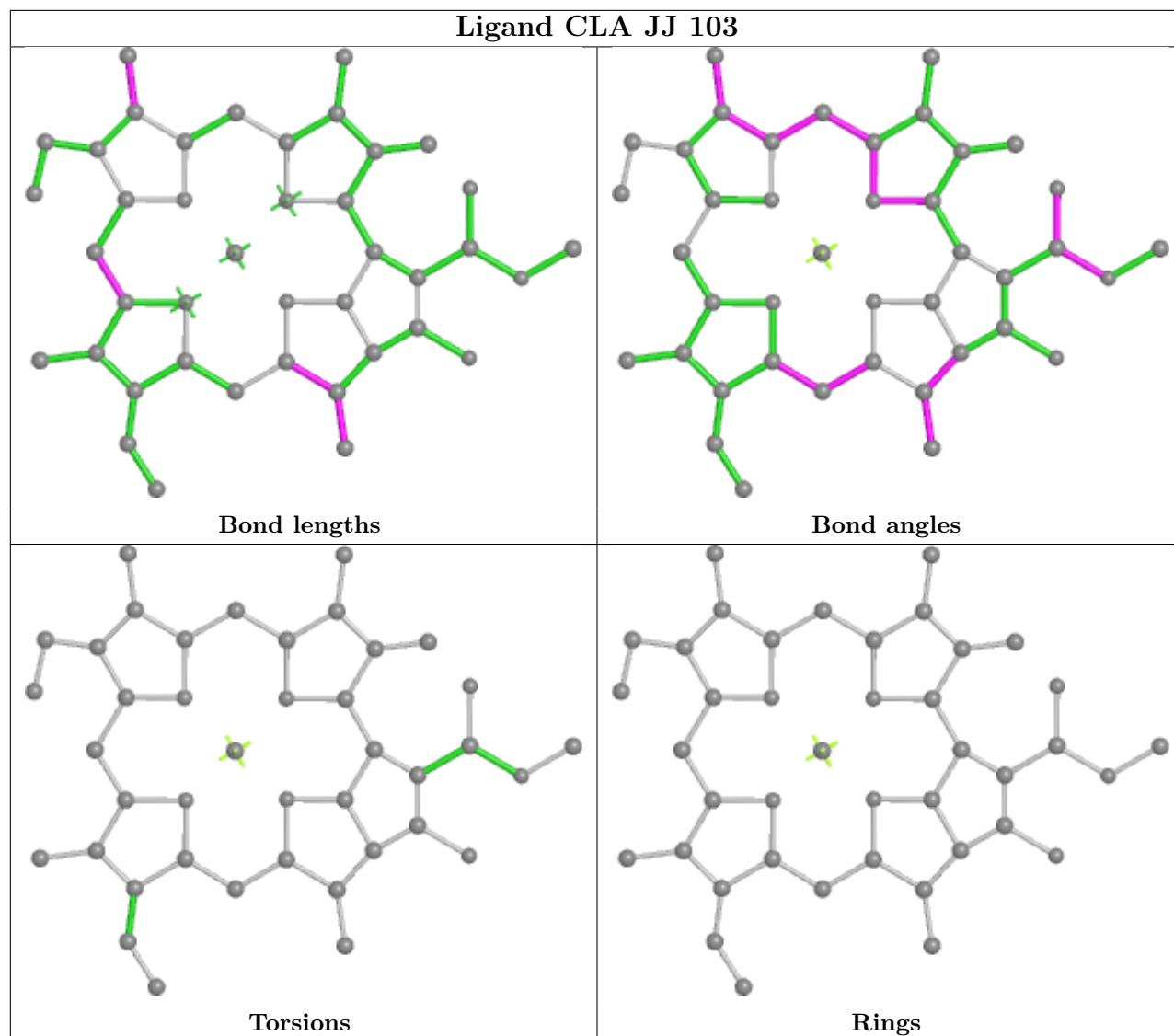
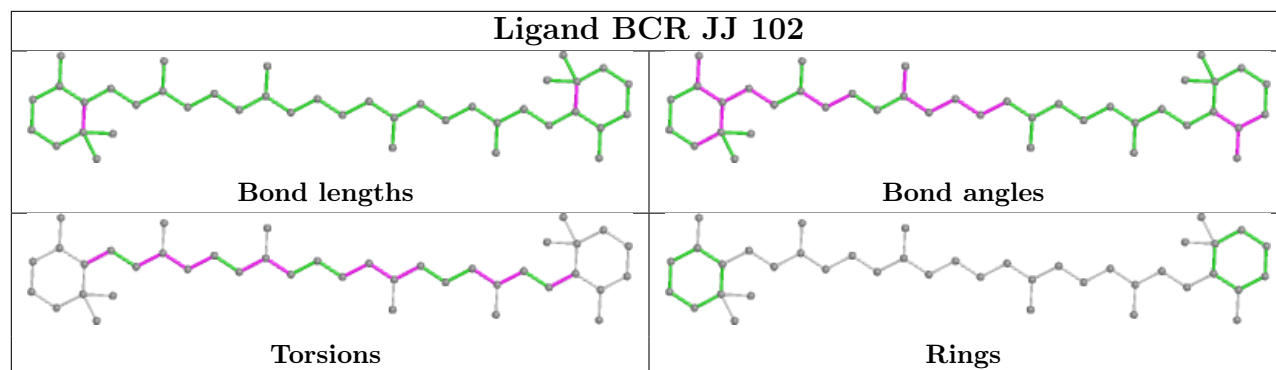




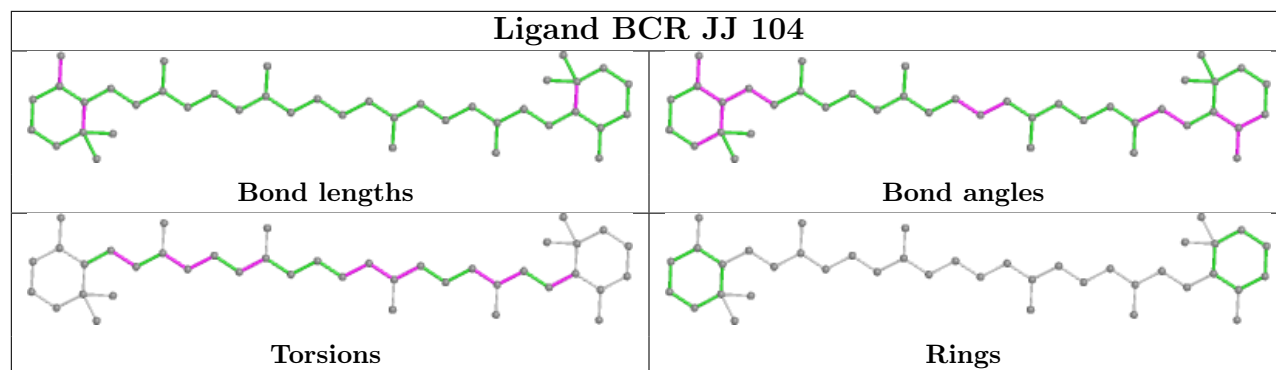




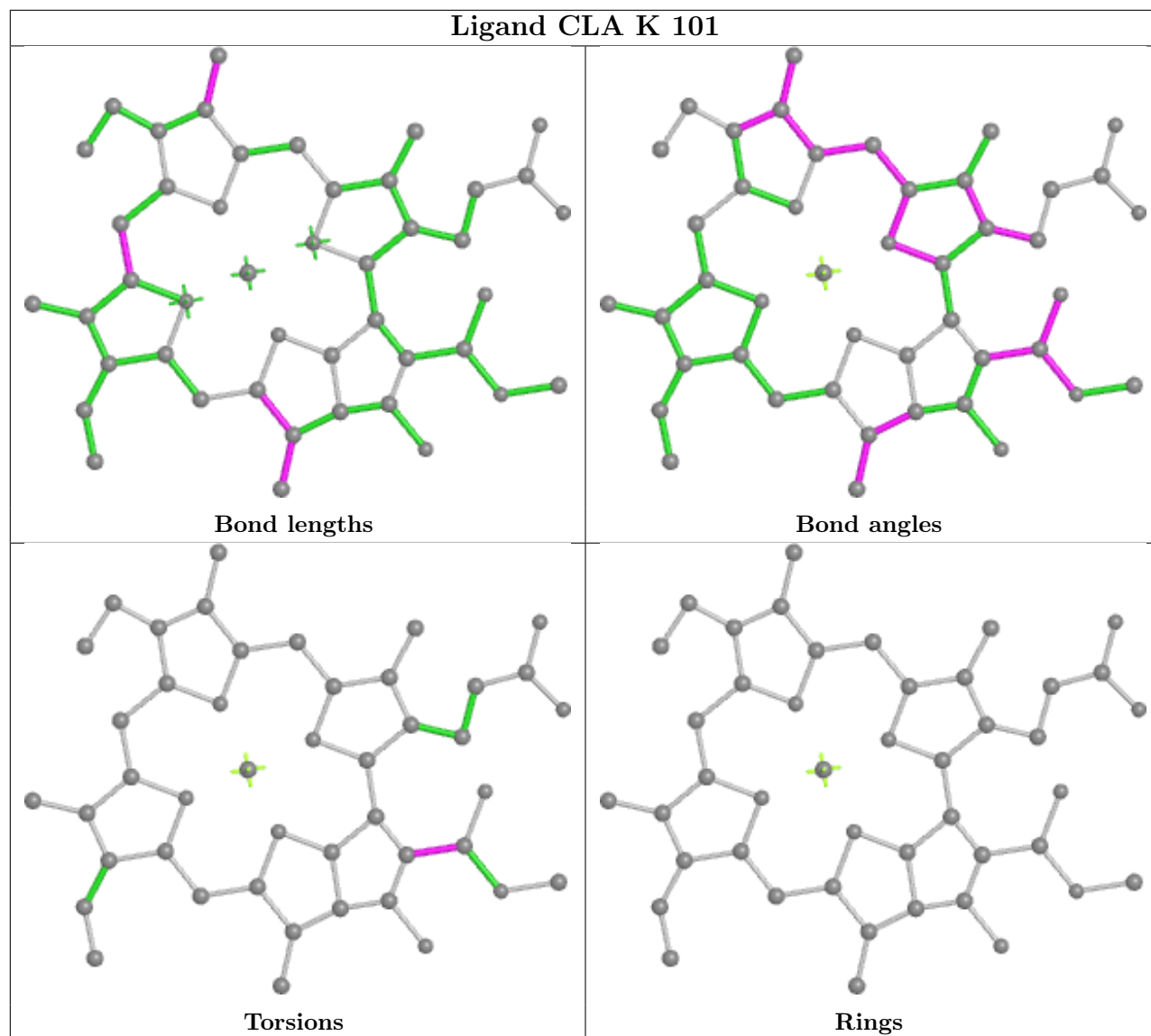




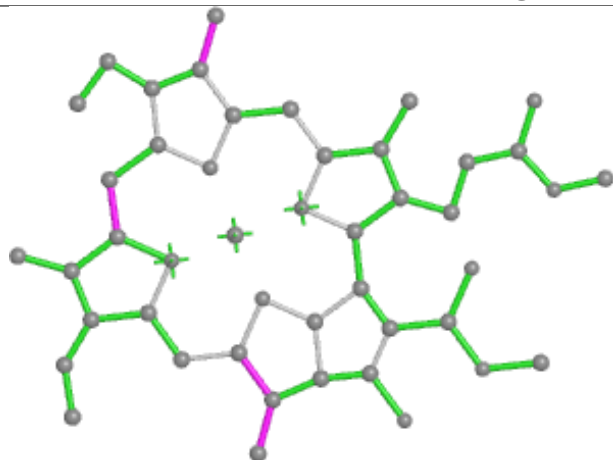
Ligand BCR JJ 104



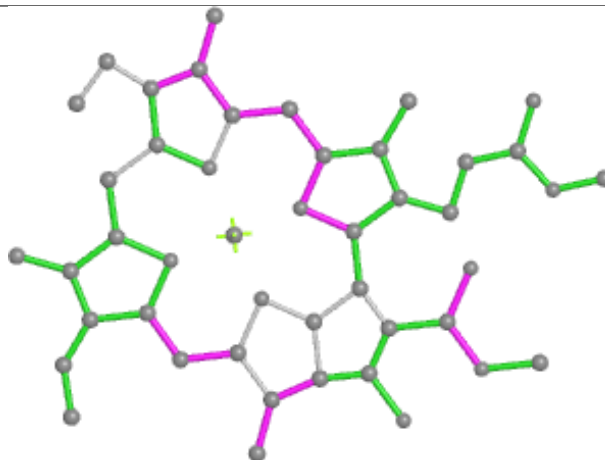
Ligand CLA K 101



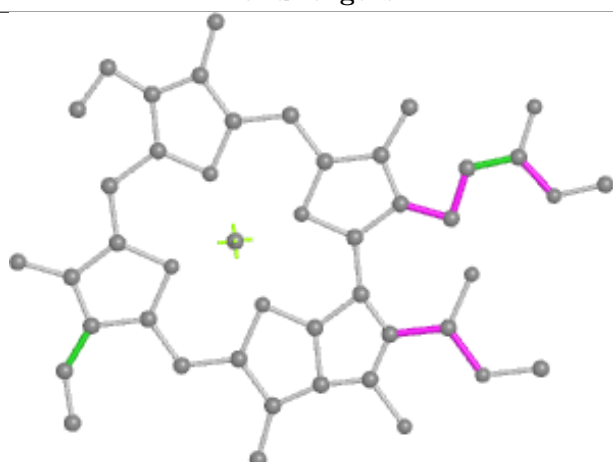
Ligand CLA K 102



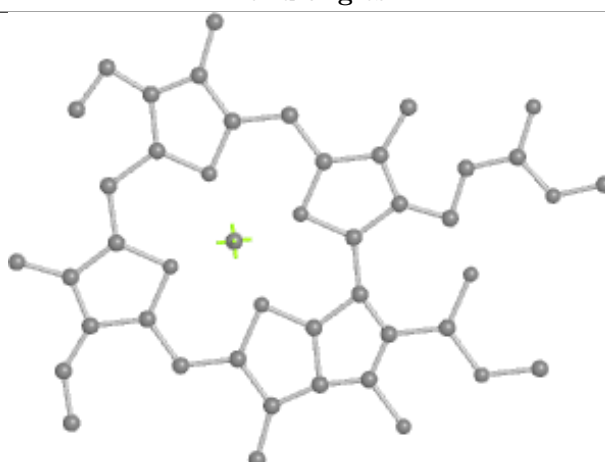
Bond lengths



Bond angles

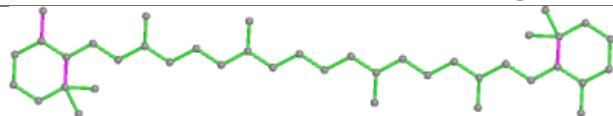


Torsions

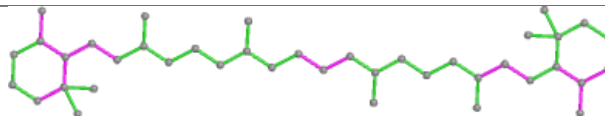


Rings

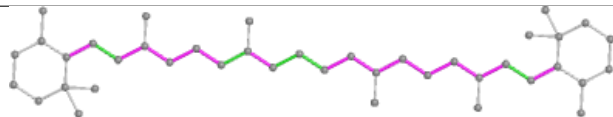
Ligand BCR K 103



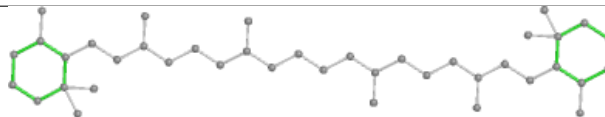
Bond lengths



Bond angles

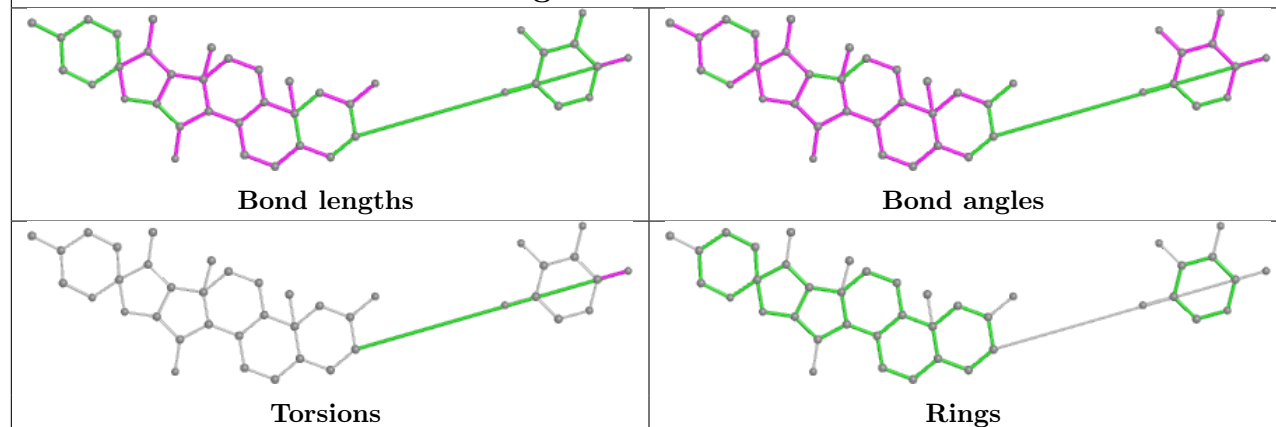


Torsions

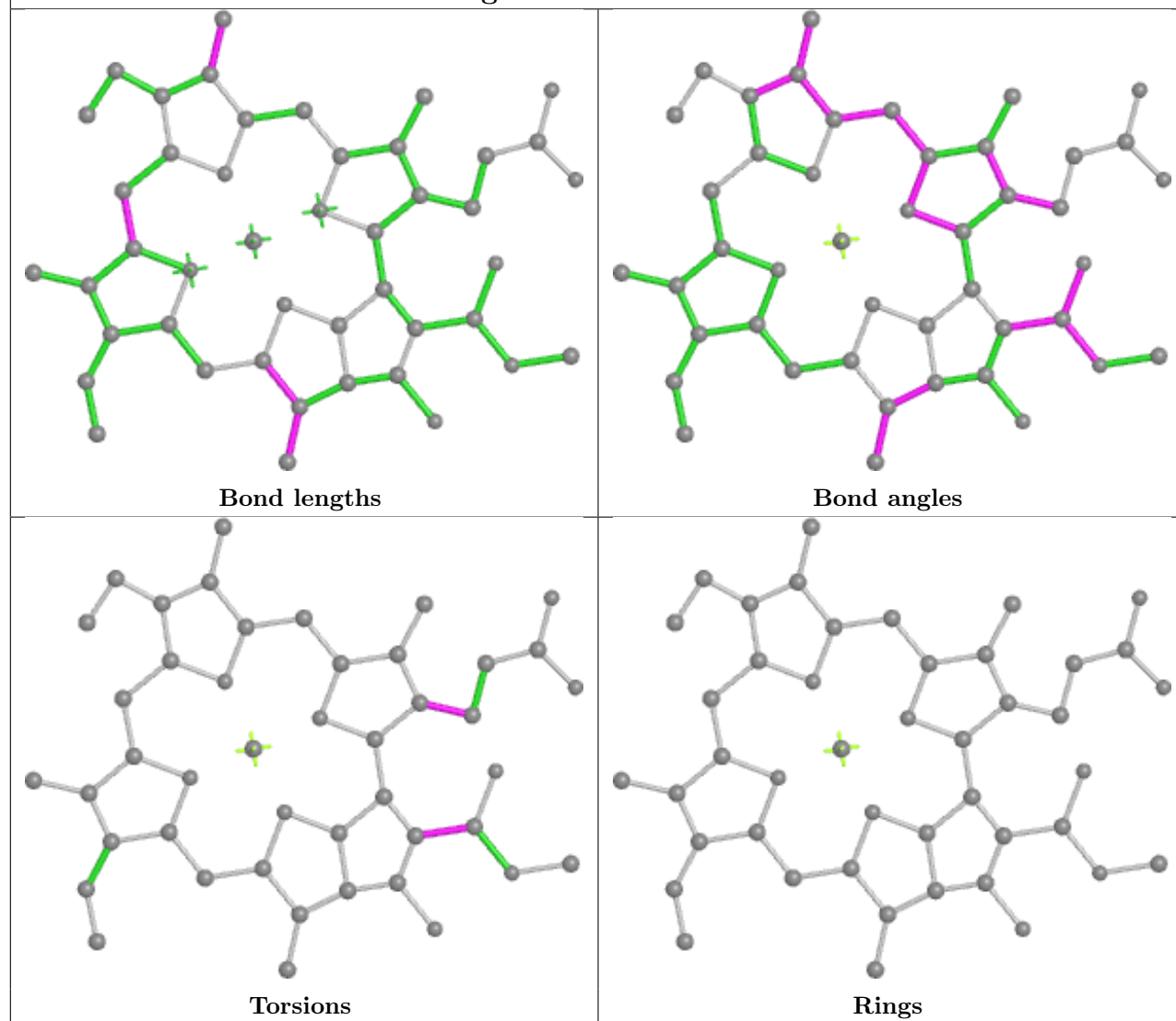


Rings

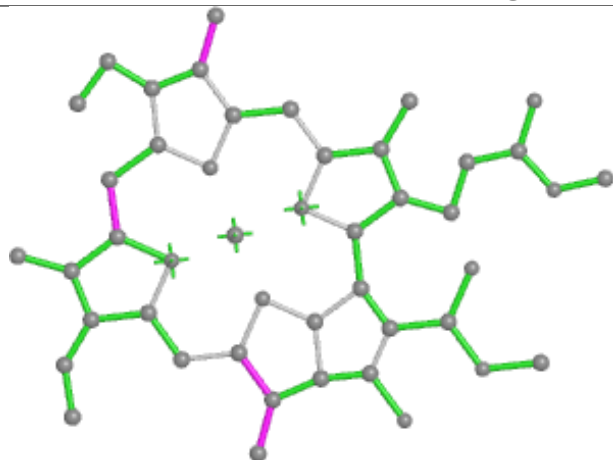
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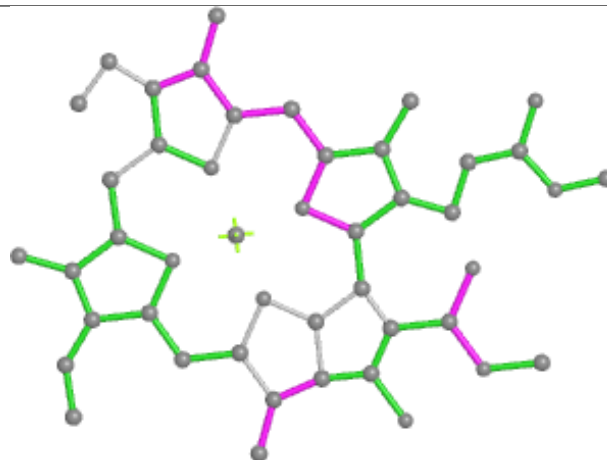
Ligand CLA K1 102



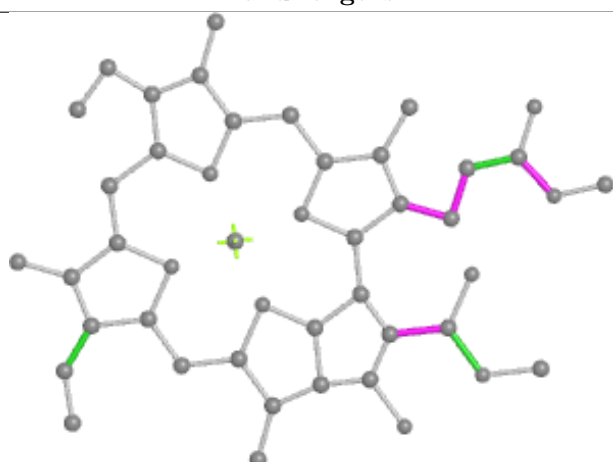
Ligand CLA K1 103



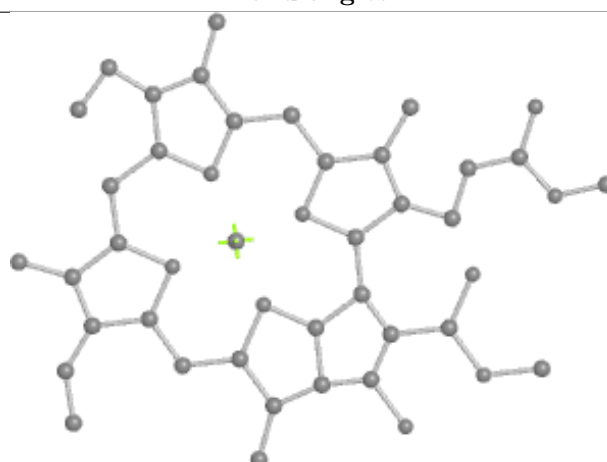
Bond lengths



Bond angles

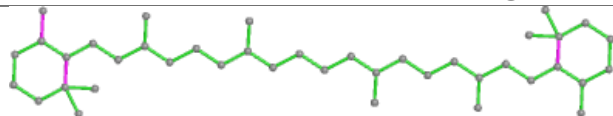


Torsions

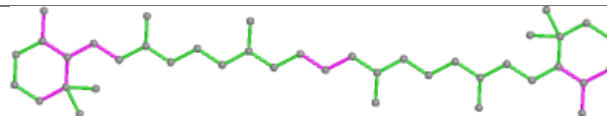


Rings

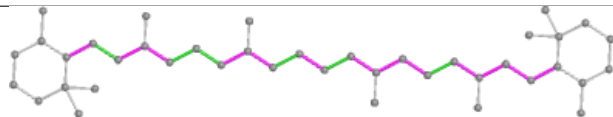
Ligand BCR K1 104



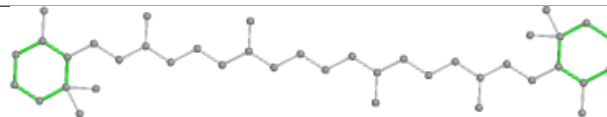
Bond lengths



Bond angles

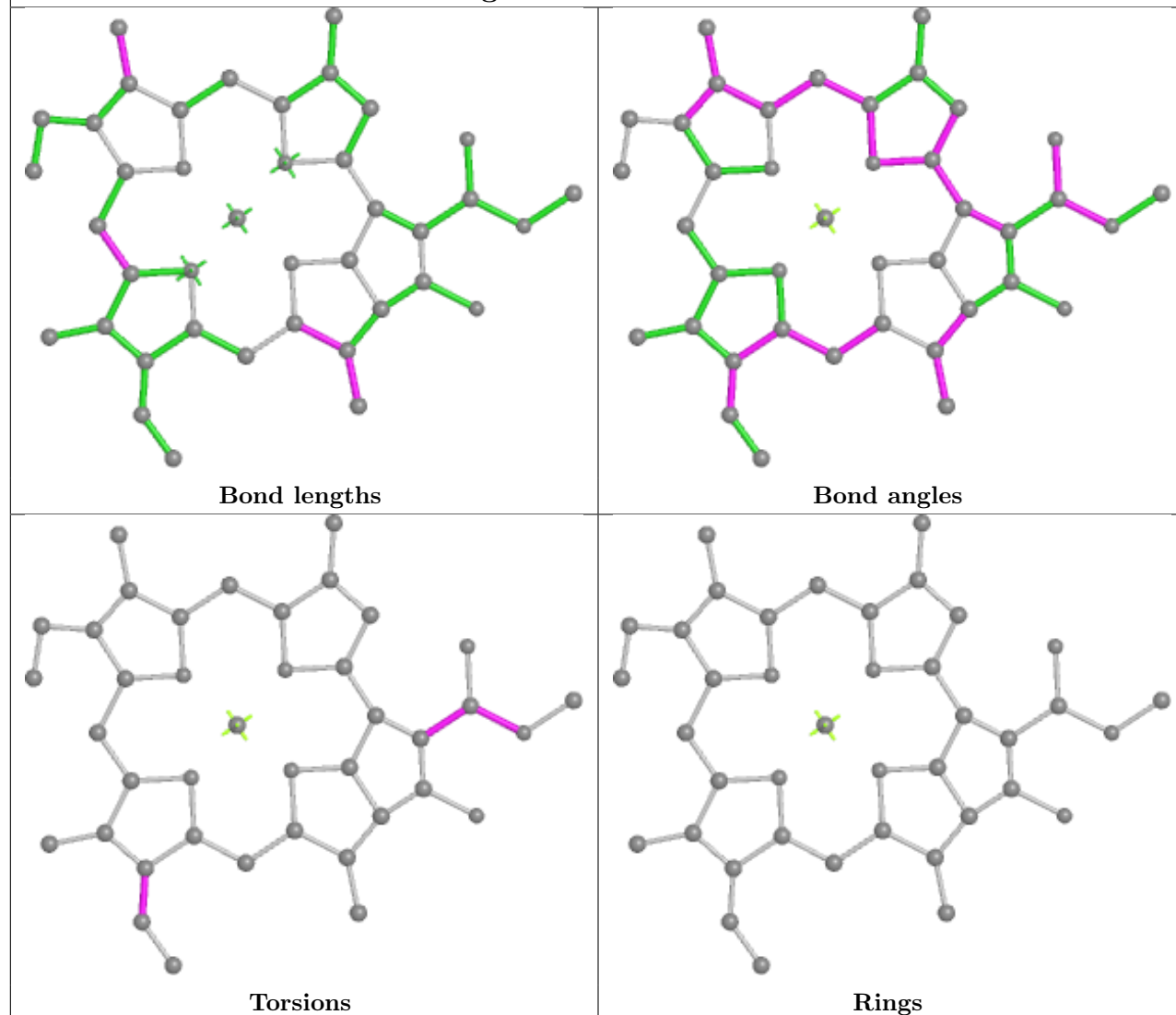


Torsions

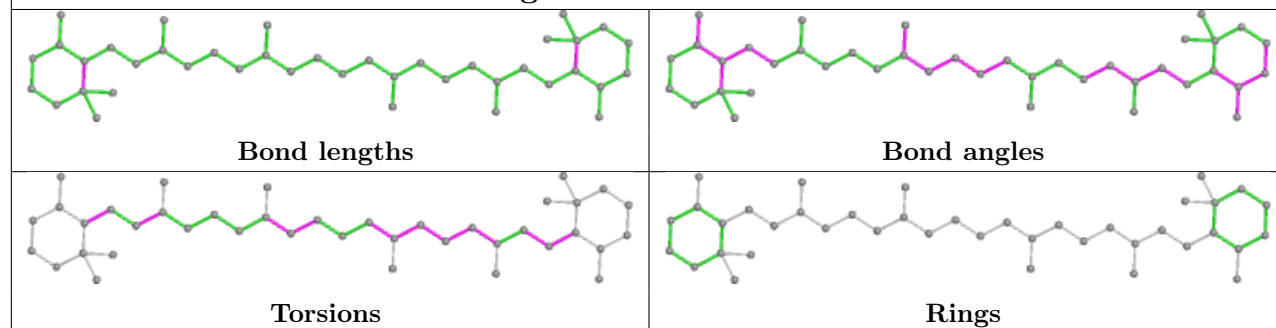


Rings

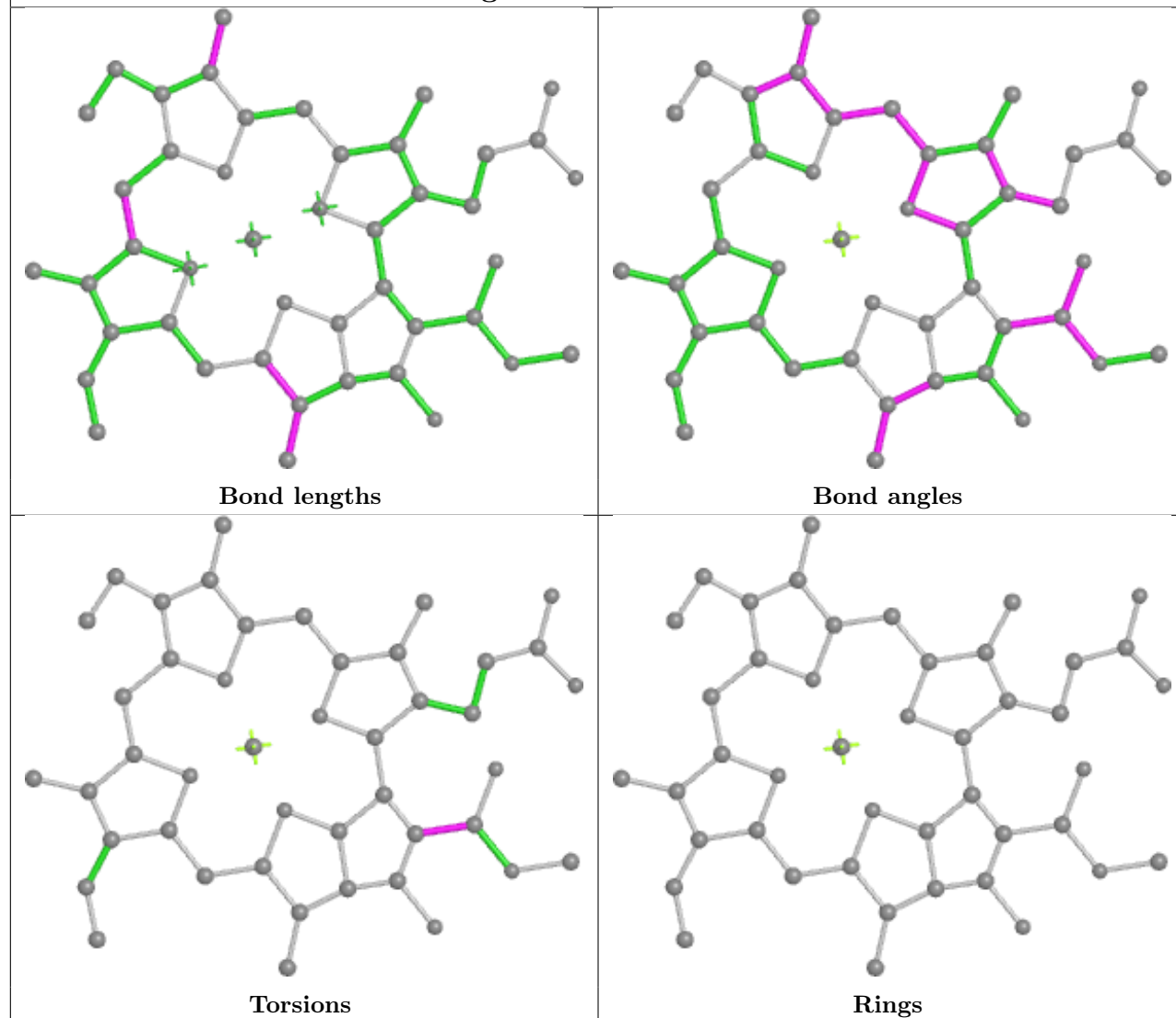
Ligand CLA K1 105



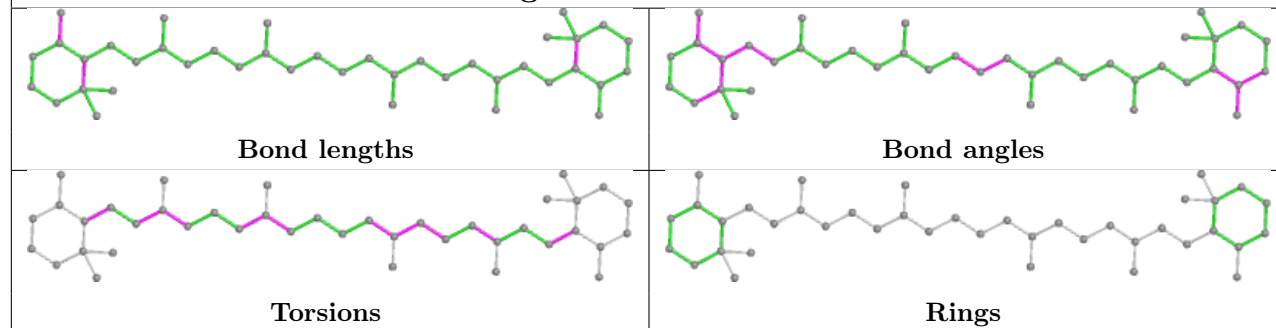
Ligand BCR K1 106



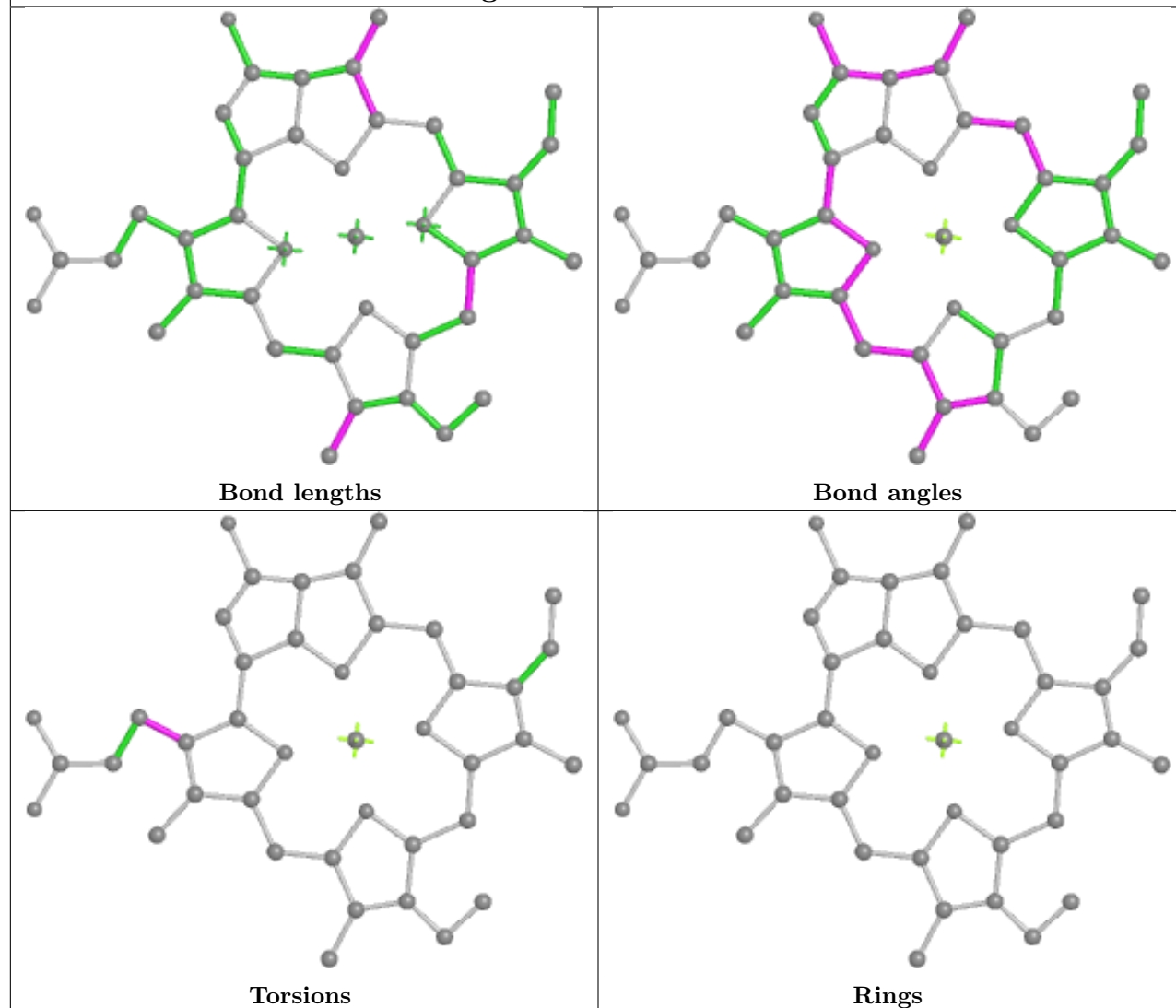
Ligand CLA K2 102



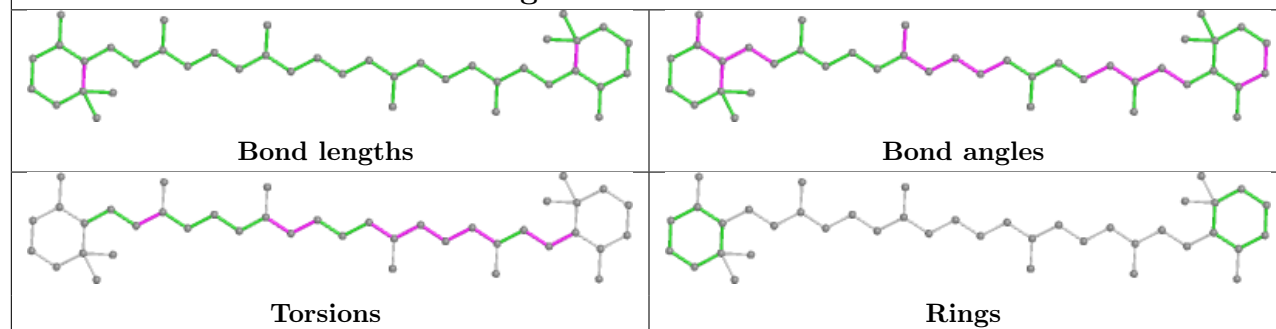
Ligand BCR K2 103



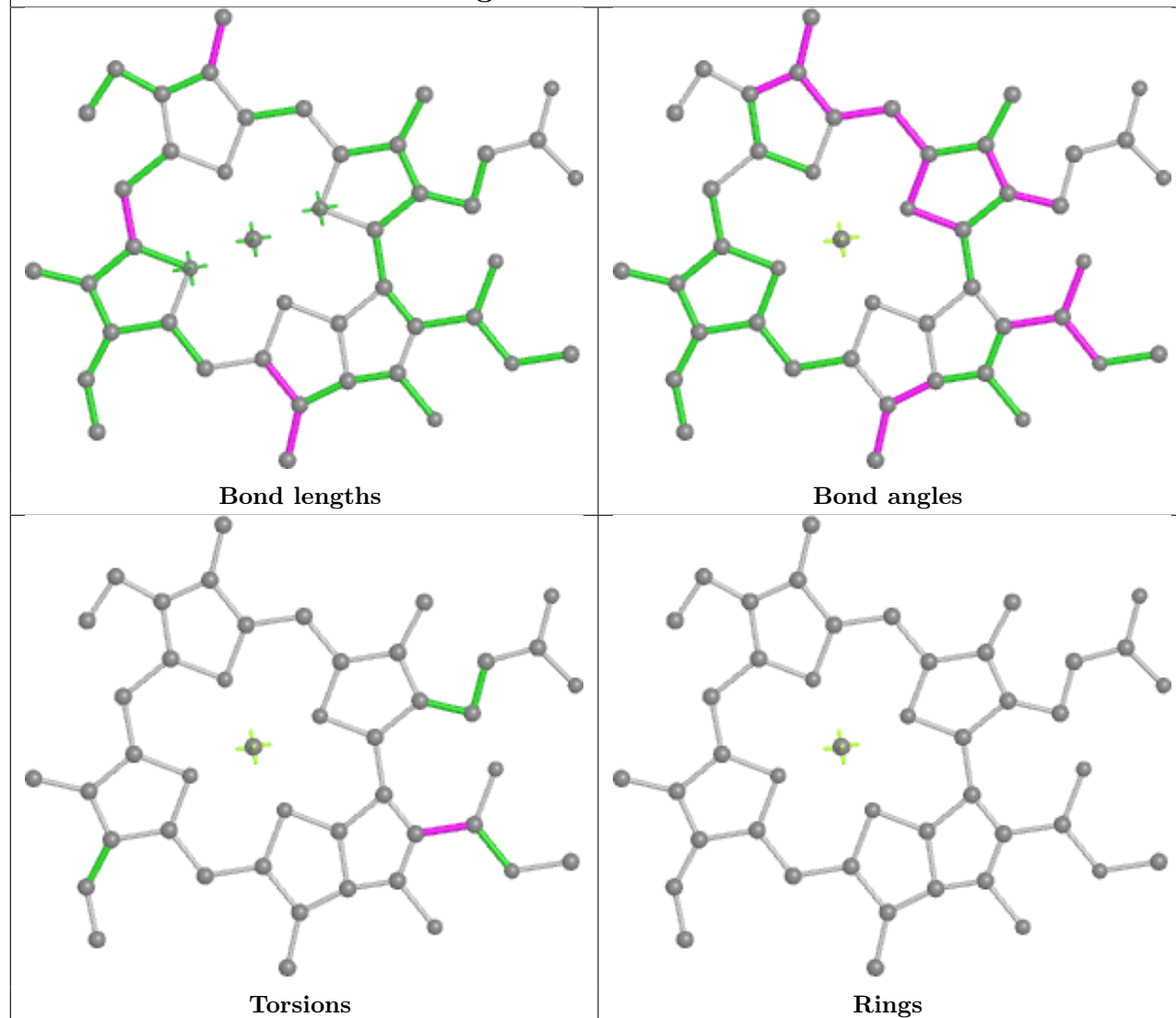
Ligand CLA K2 104



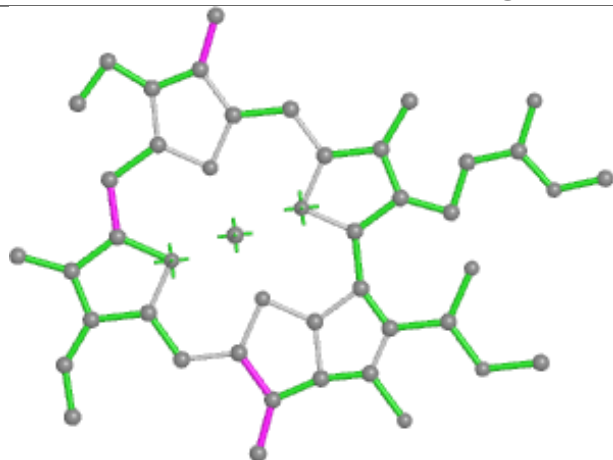
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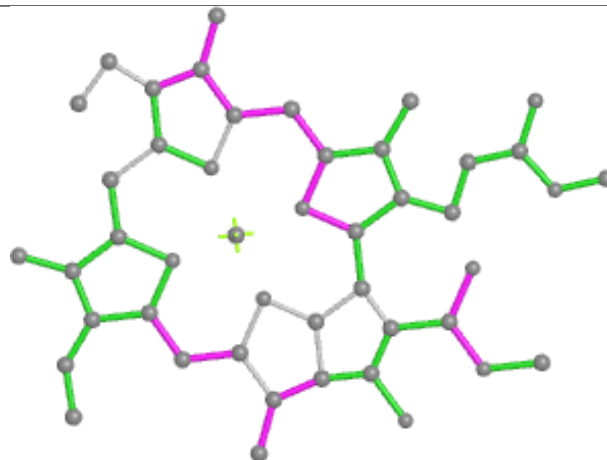
Ligand CLA KK 101



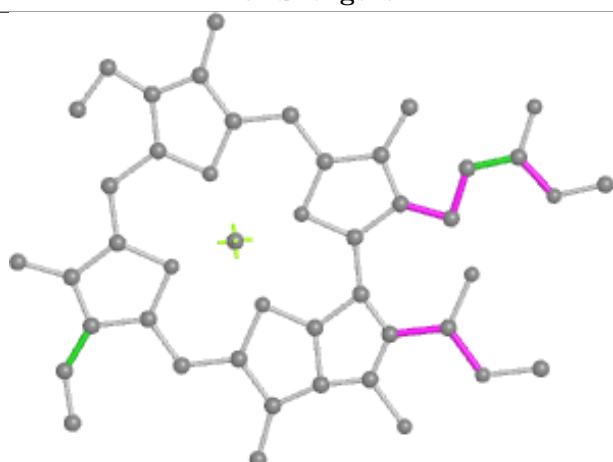
Ligand CLA KK 102



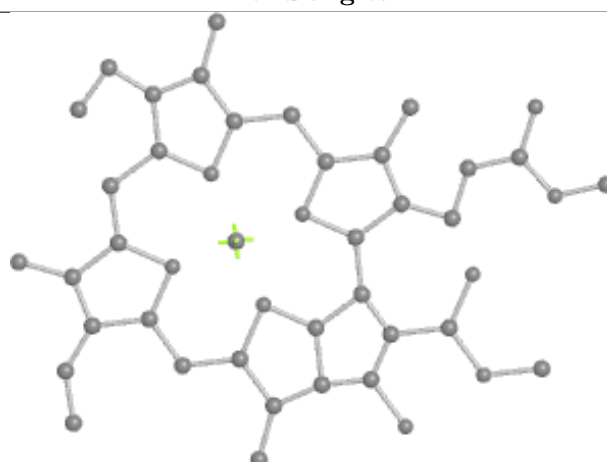
Bond lengths



Bond angles

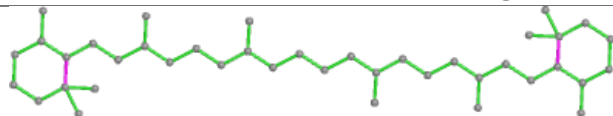


Torsions

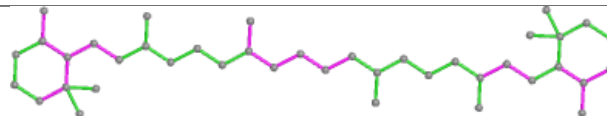


Rings

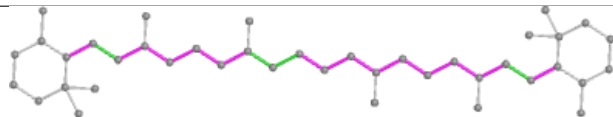
Ligand BCR KK 103



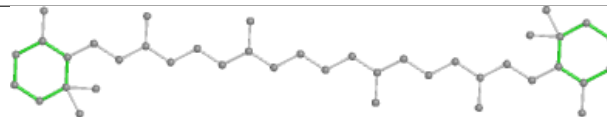
Bond lengths



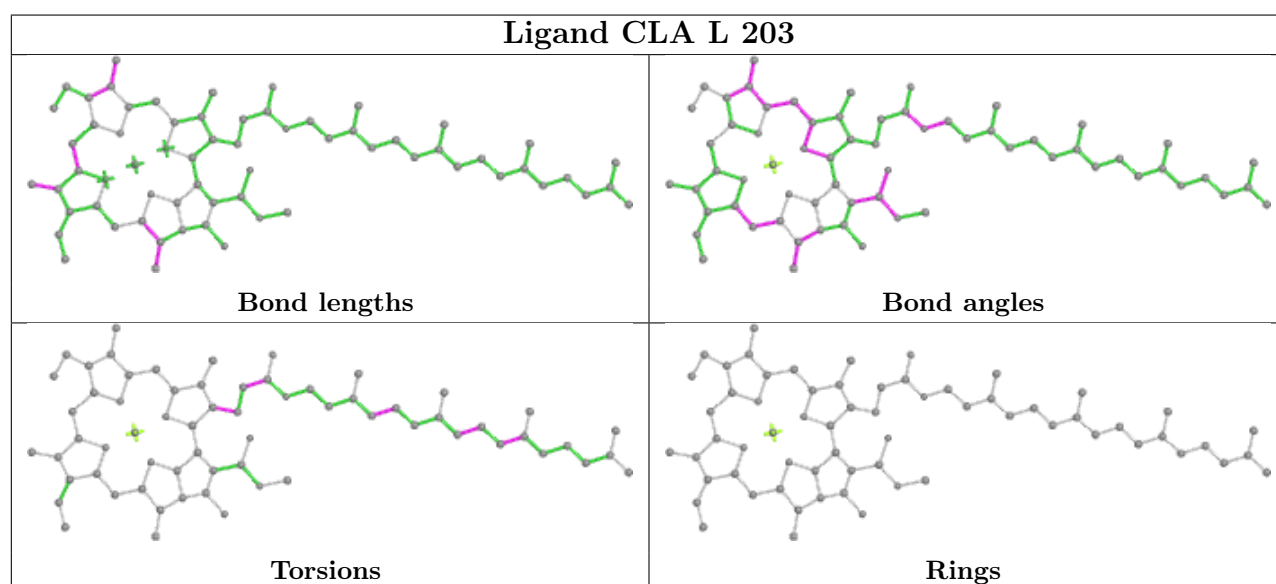
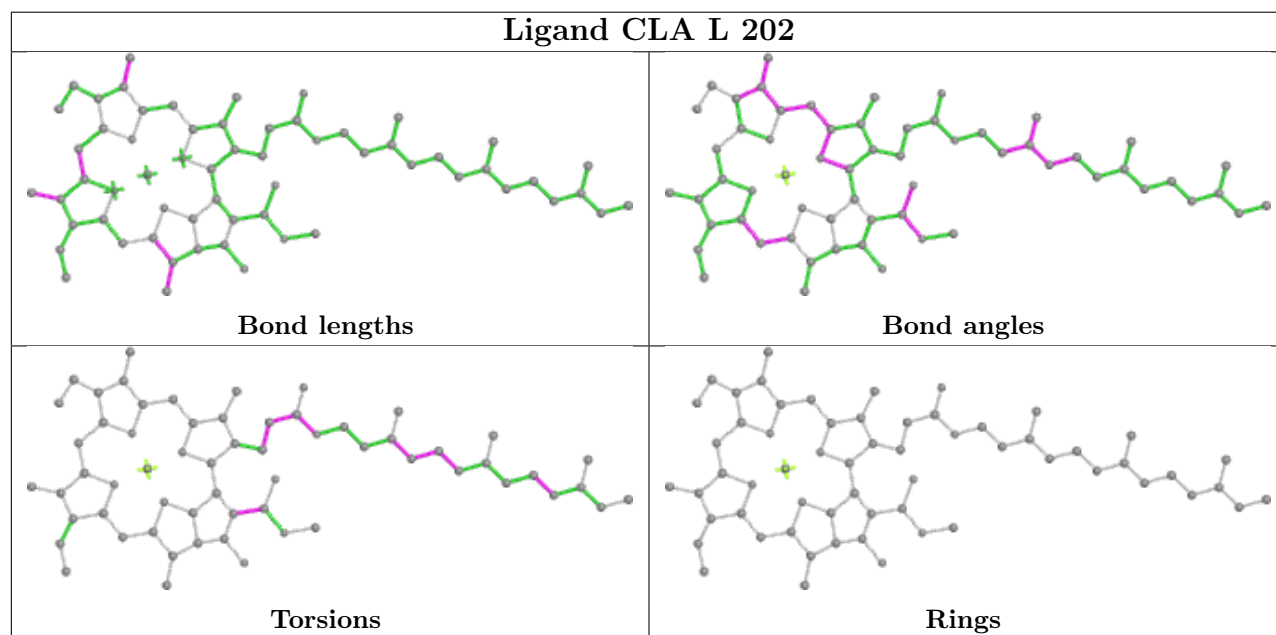
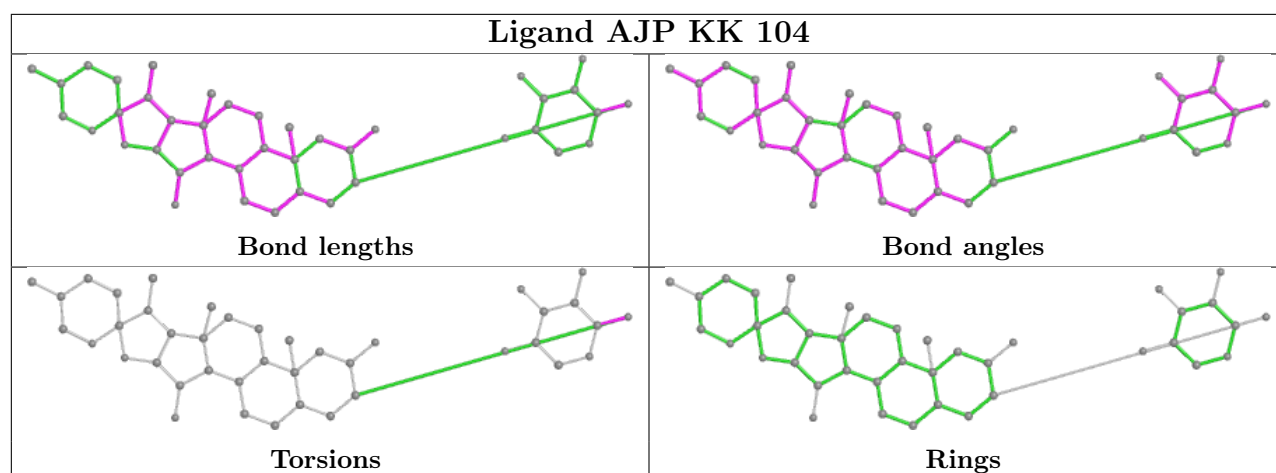
Bond angles



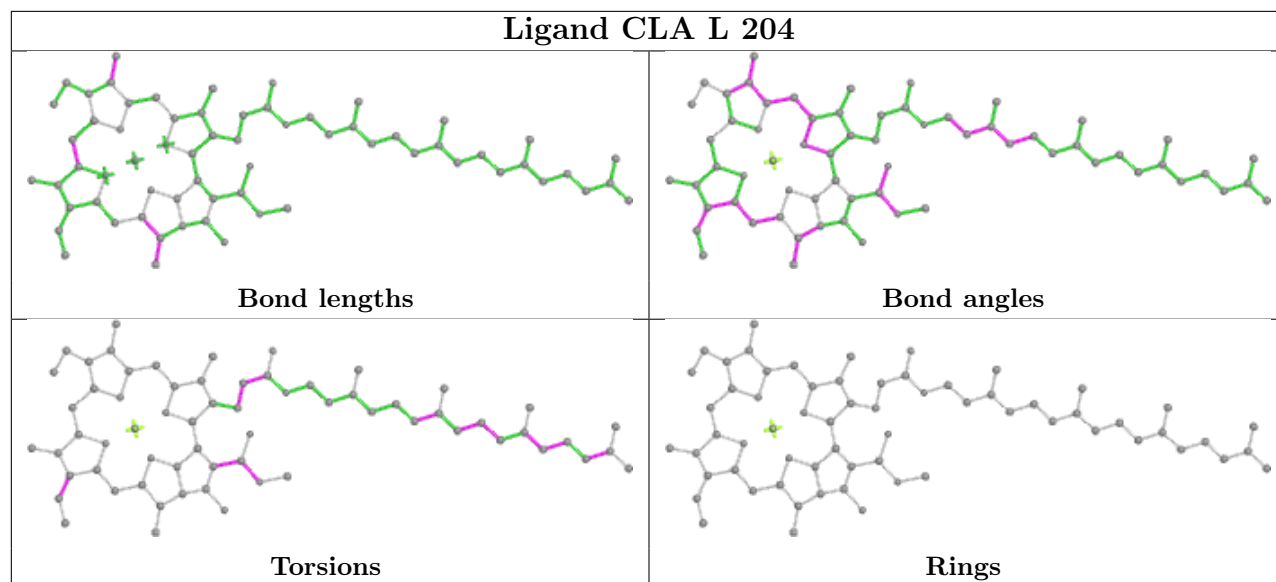
Torsions



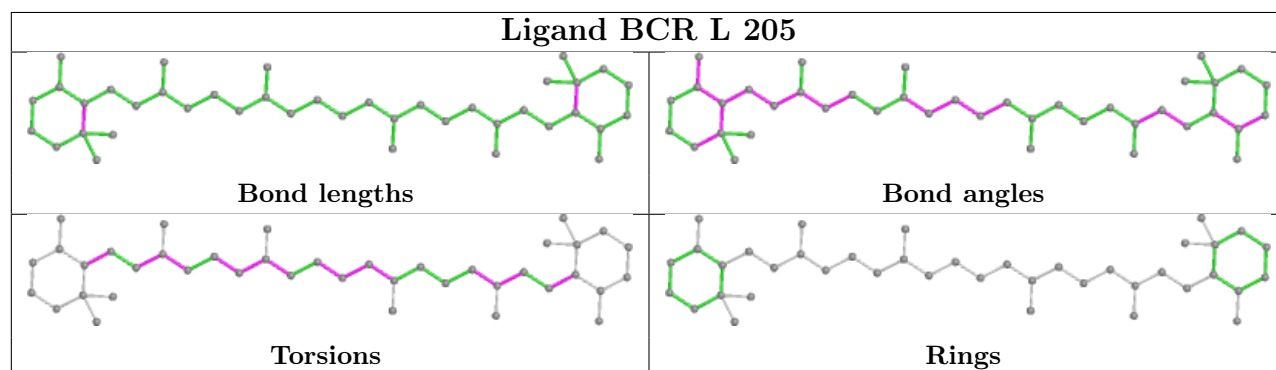
Rings



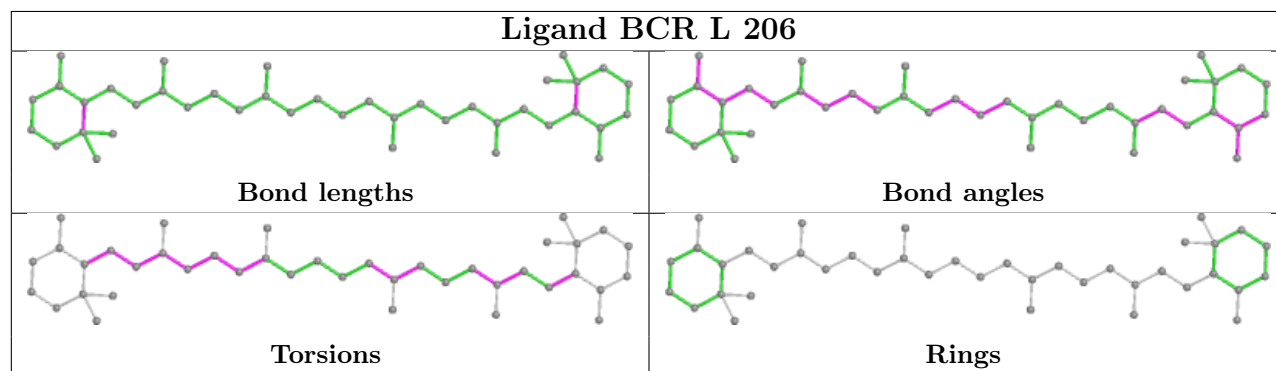
Ligand CLA L 204



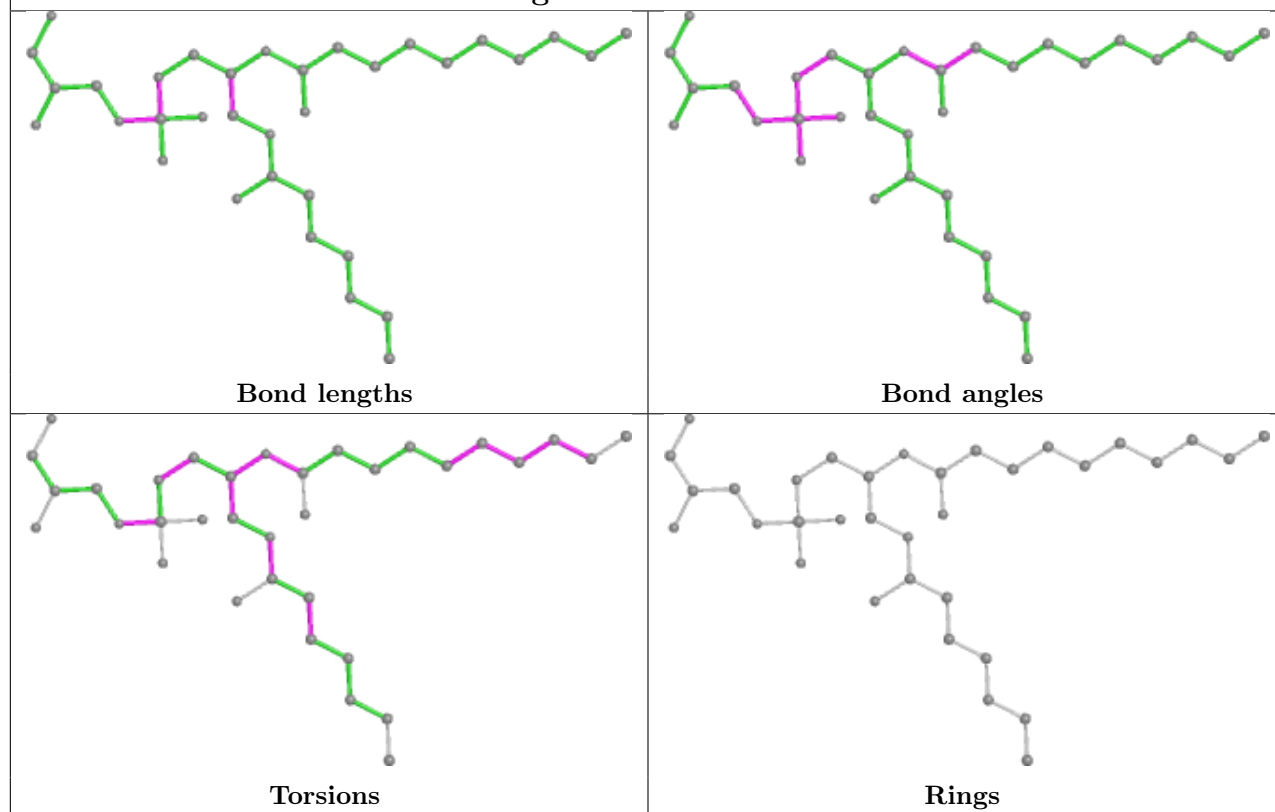
Ligand BCR L 205



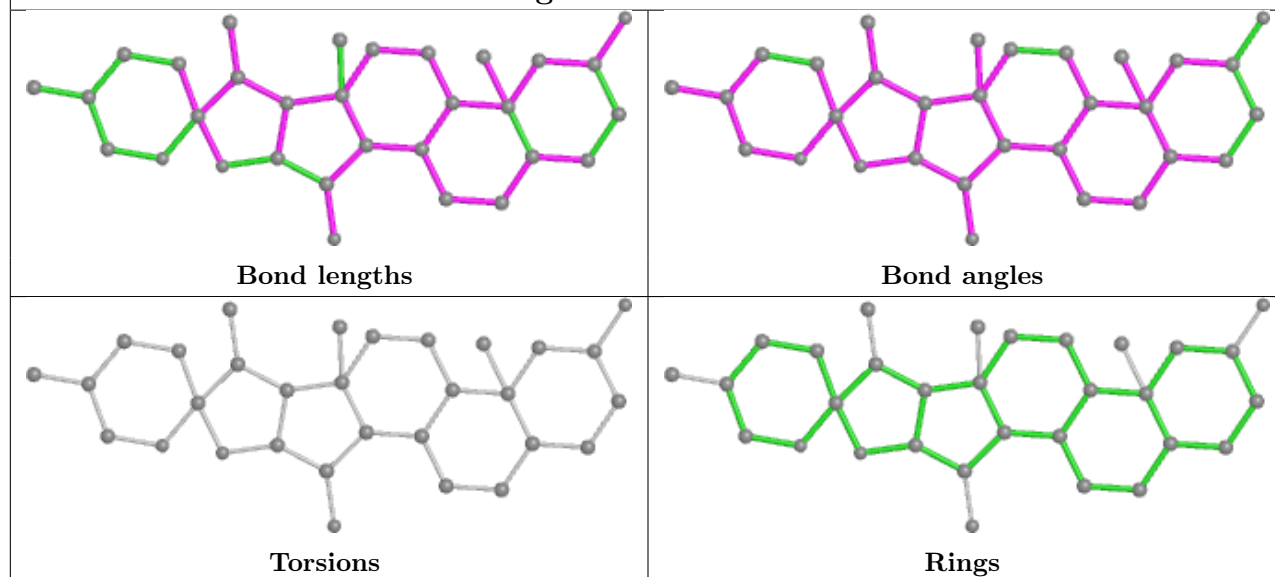
Ligand BCR L 206

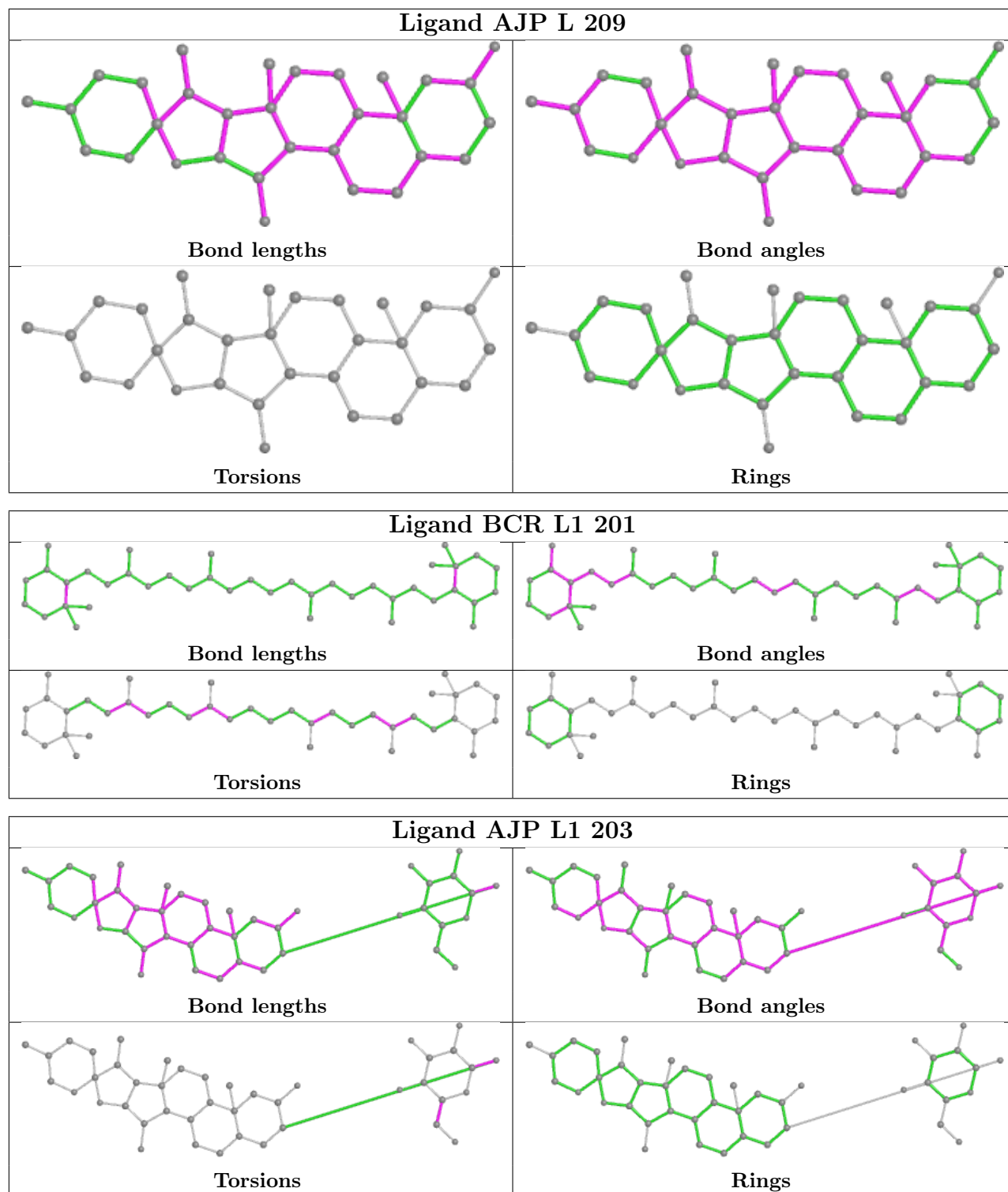


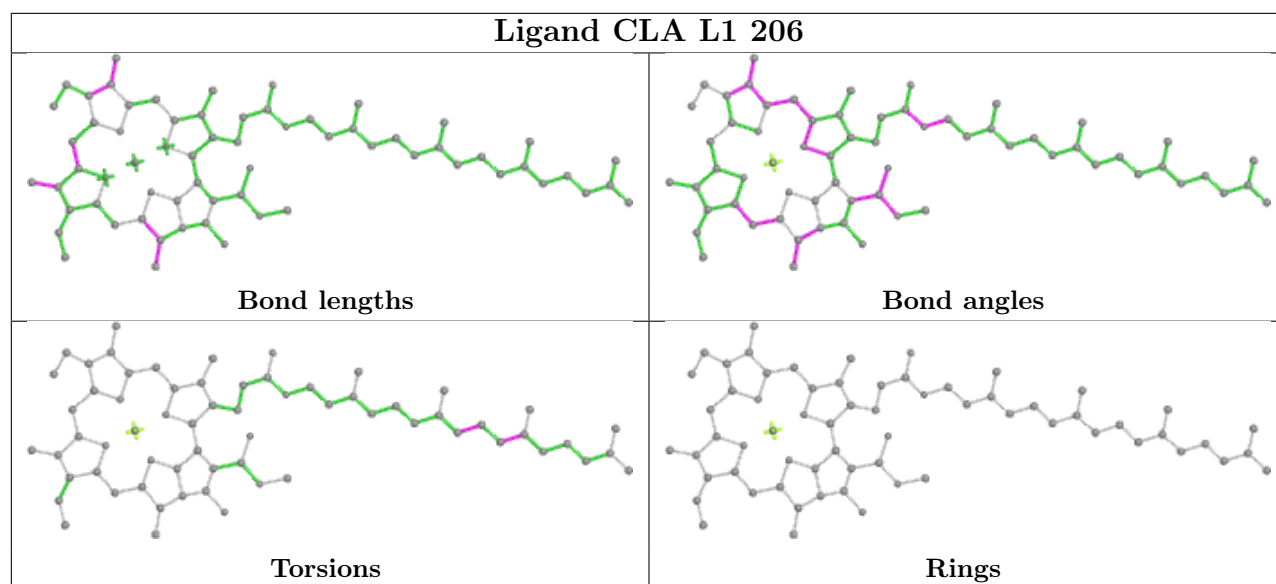
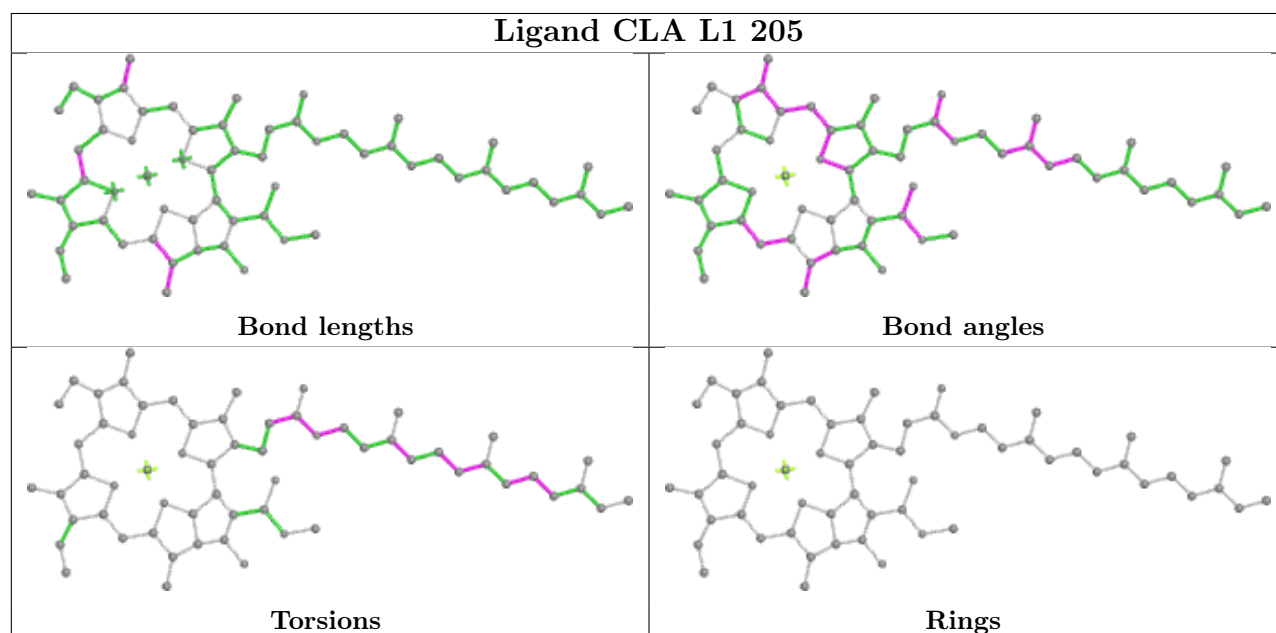
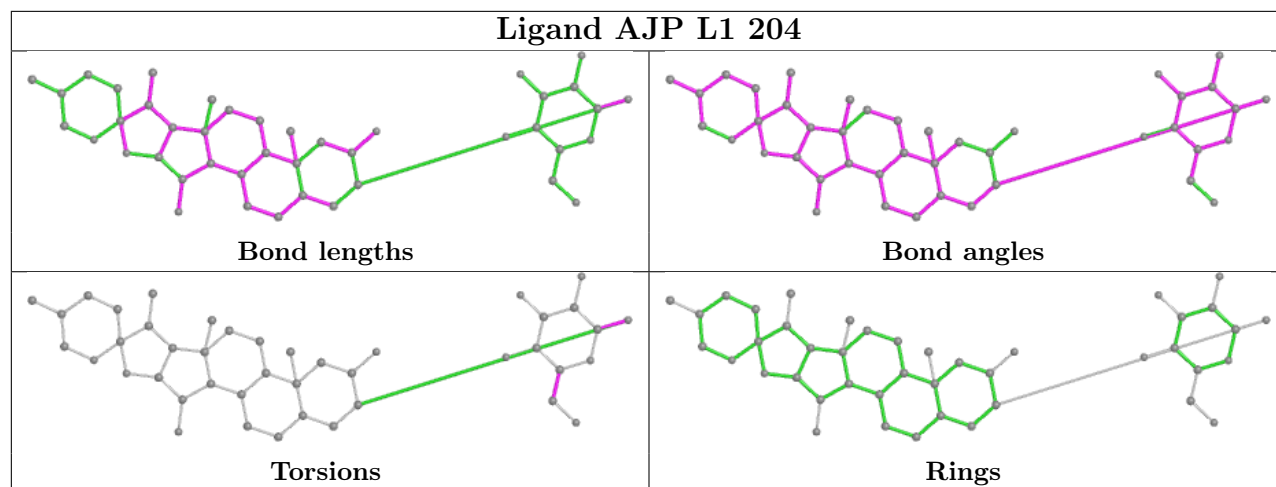
Ligand LHG L 207

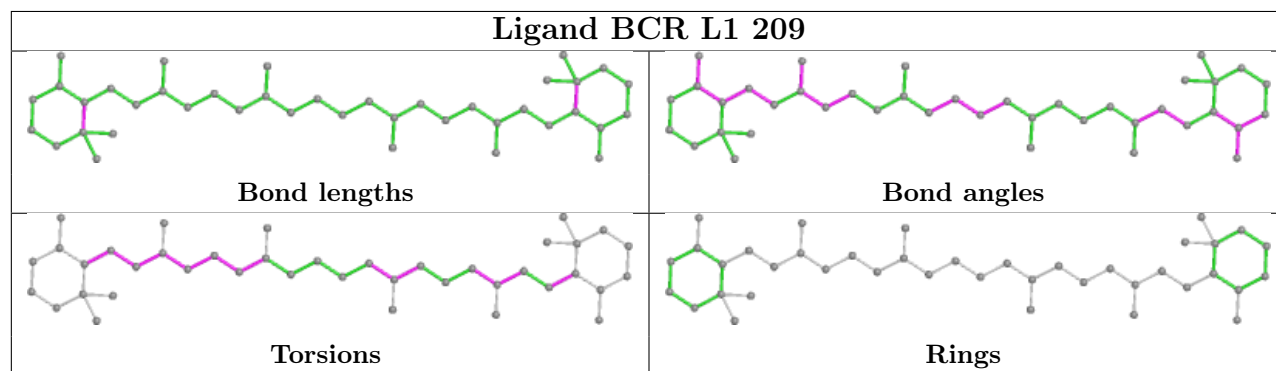
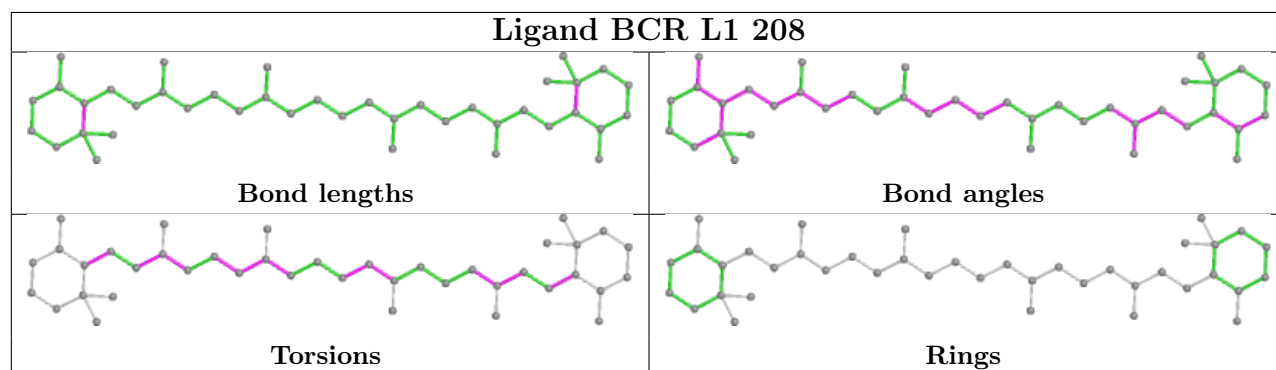
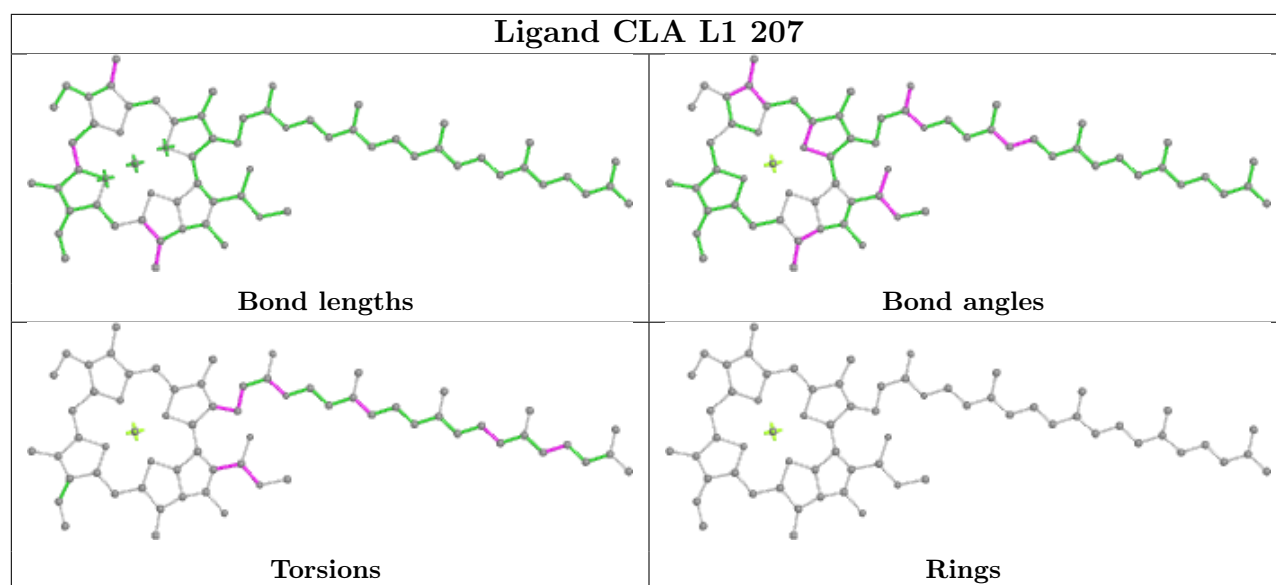


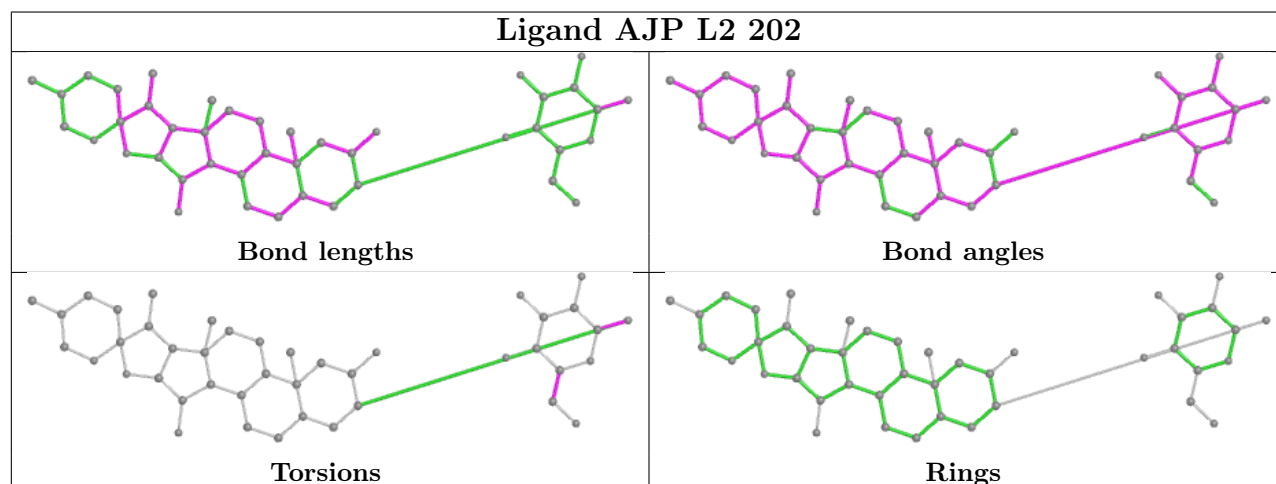
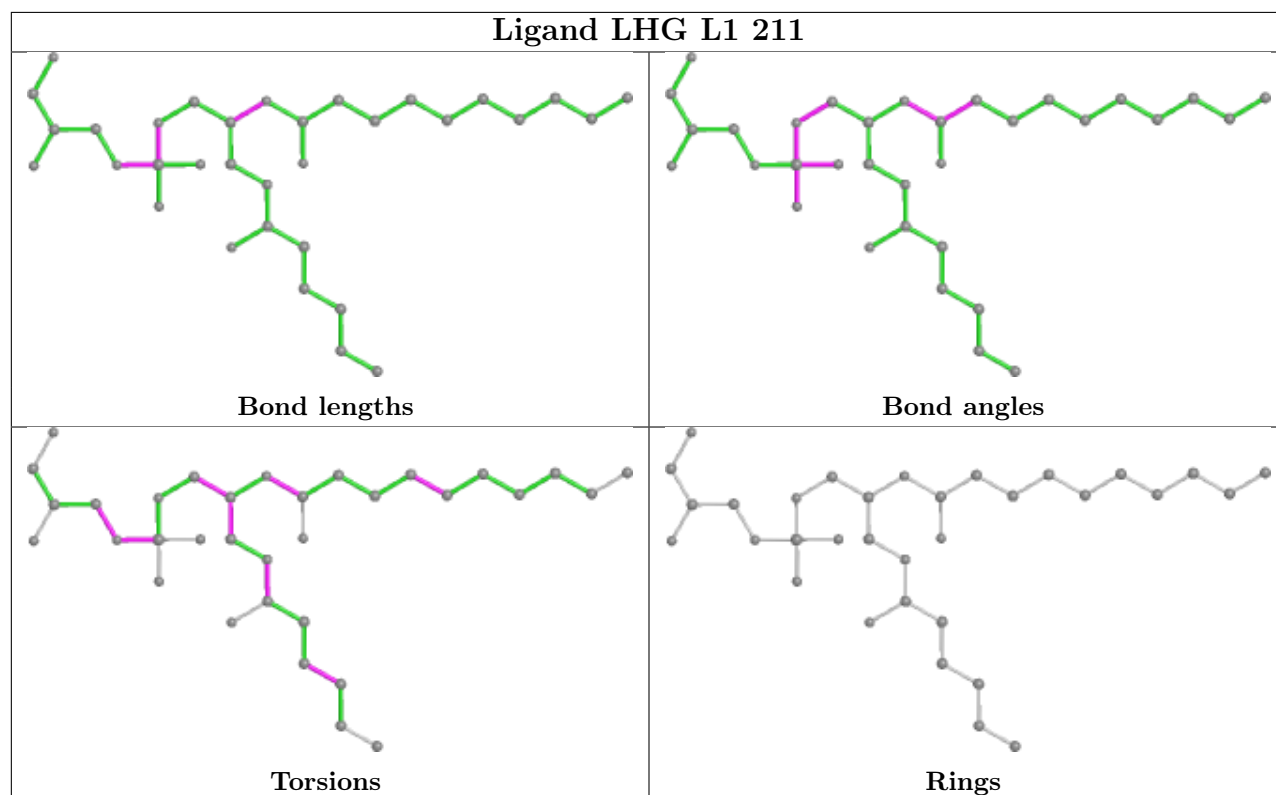
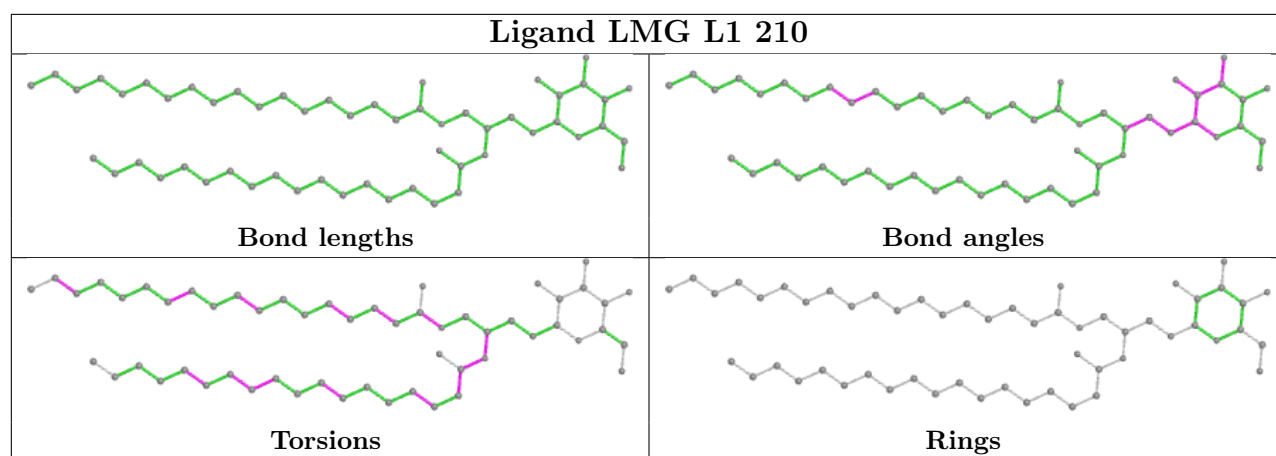
Ligand AJP L 208

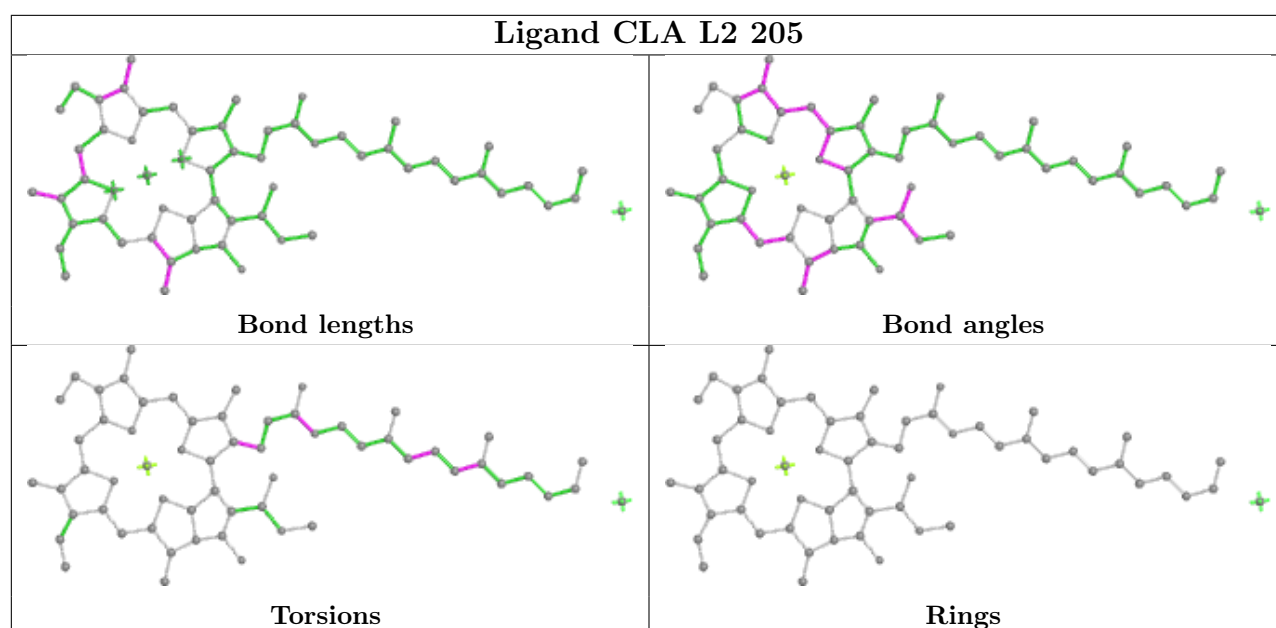
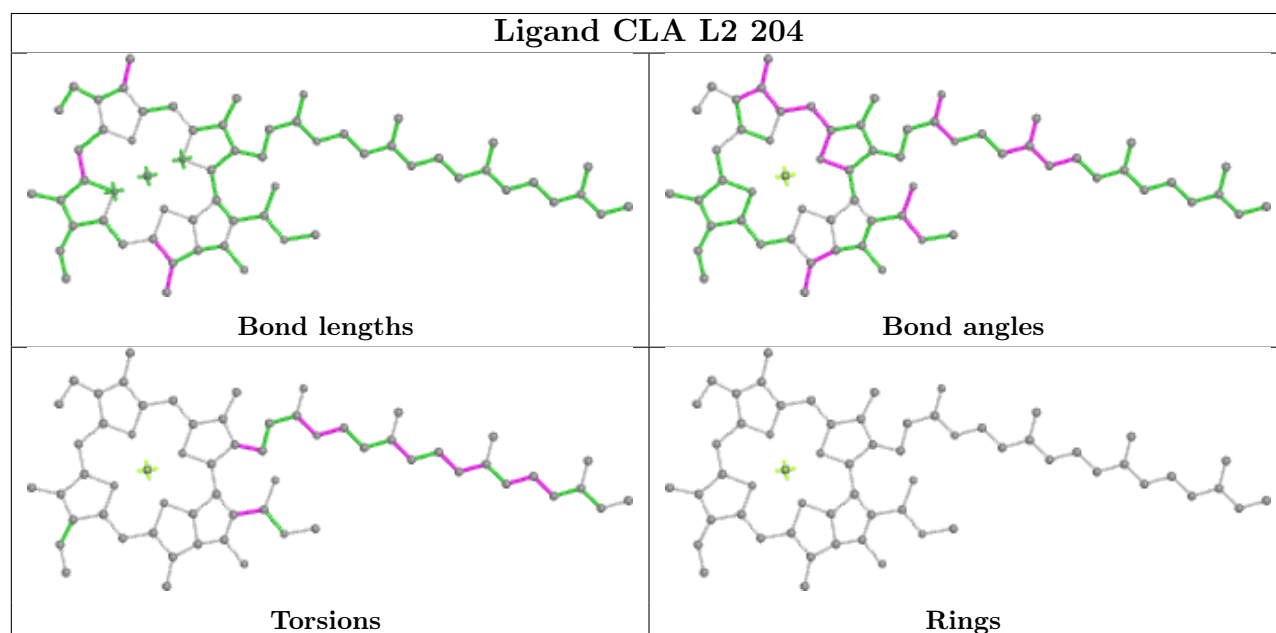
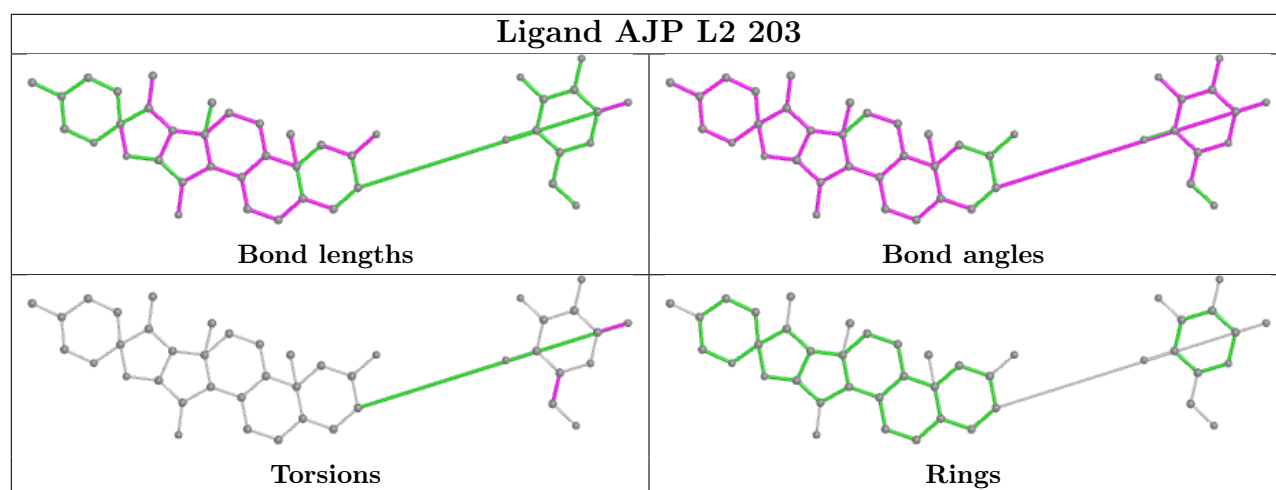


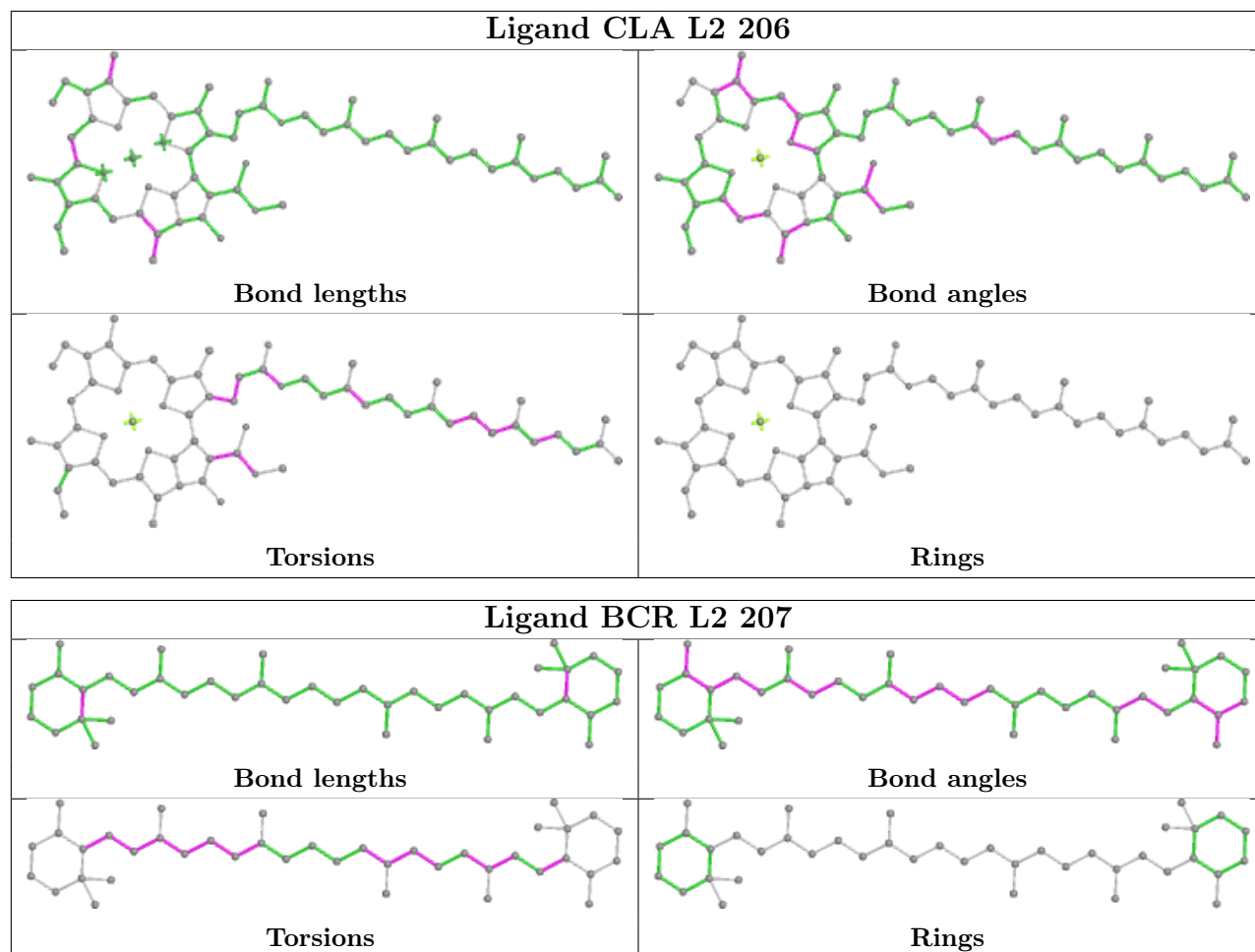


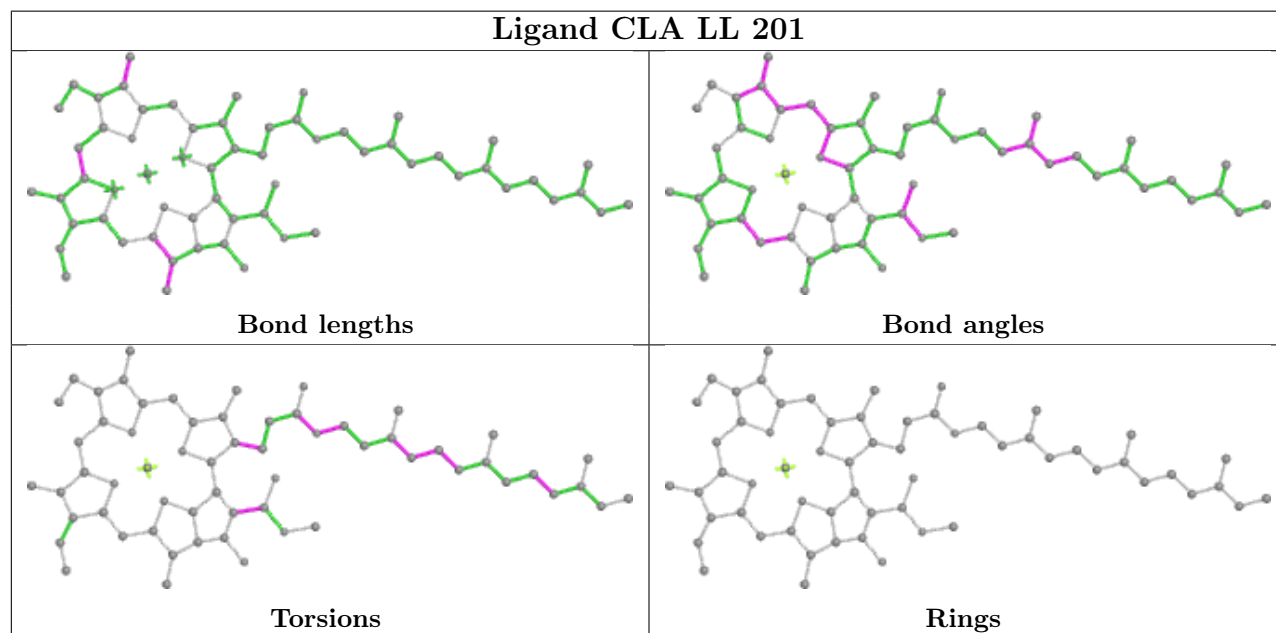
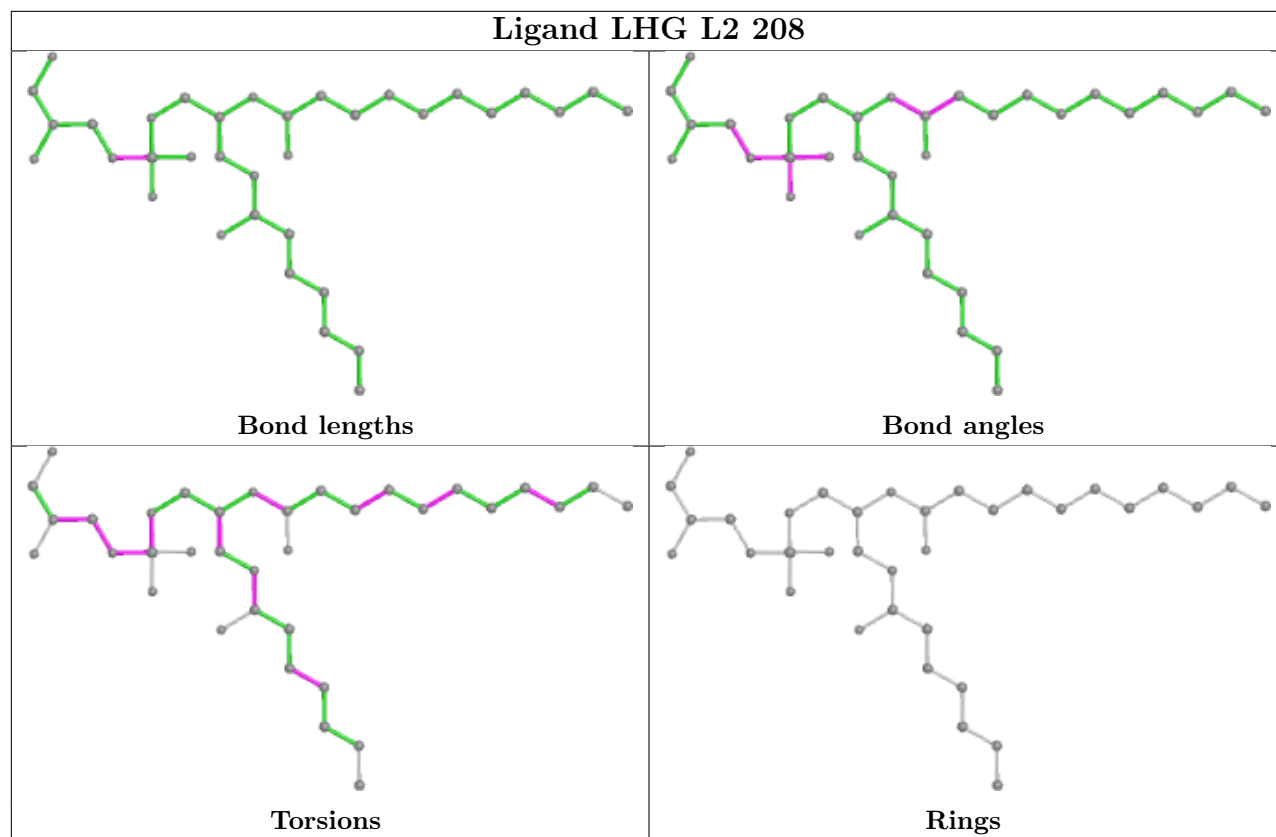




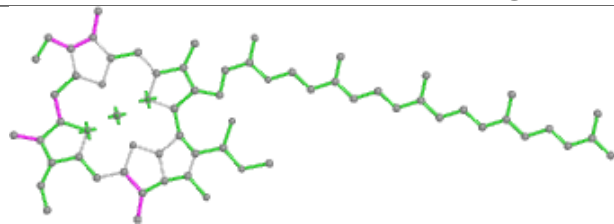




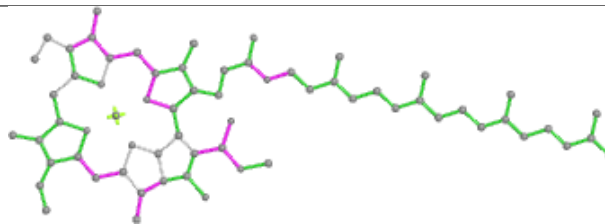




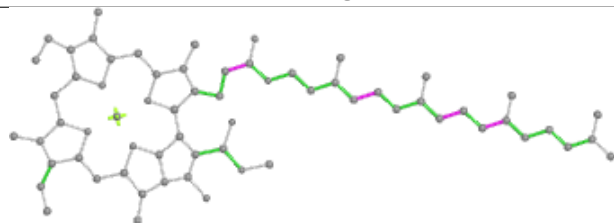
Ligand CLA LL 202



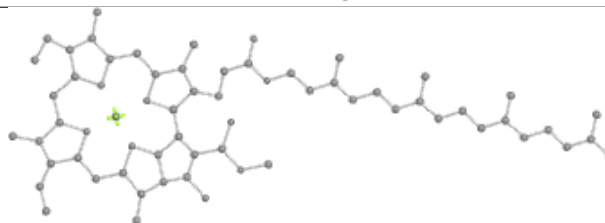
Bond lengths



Bond angles

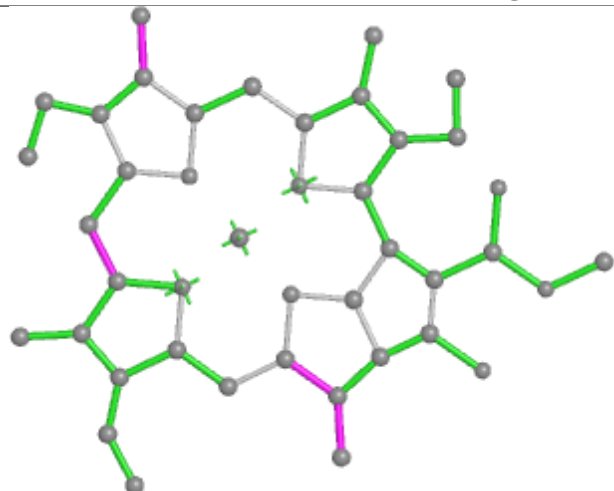


Torsions

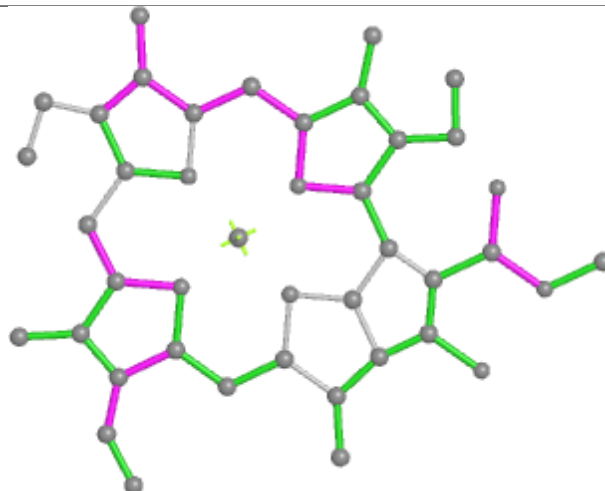


Rings

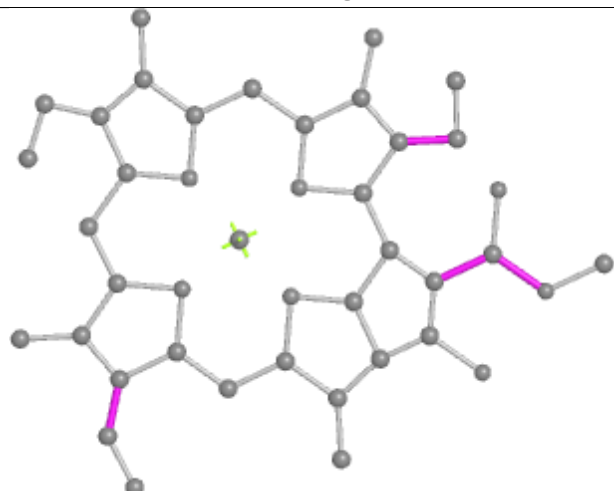
Ligand CLA LL 203



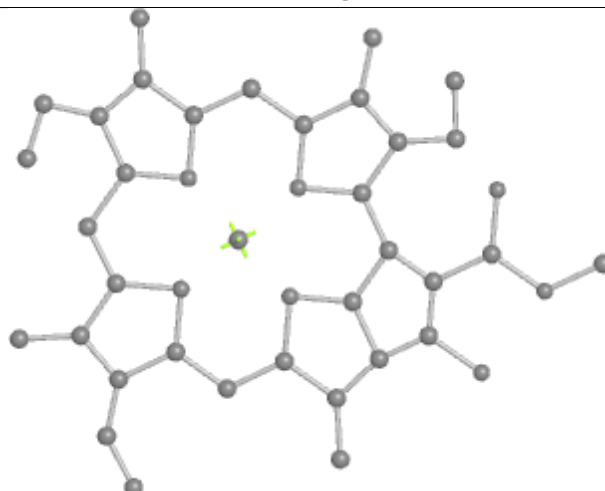
Bond lengths



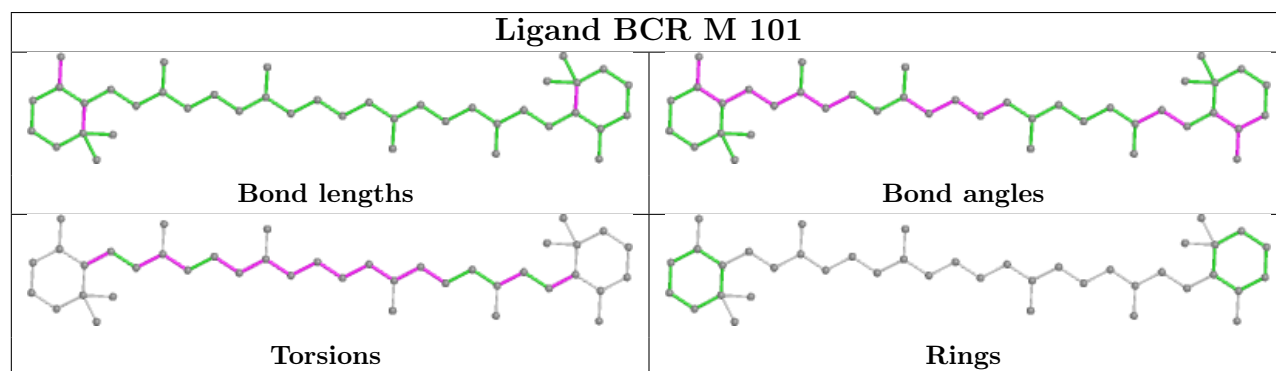
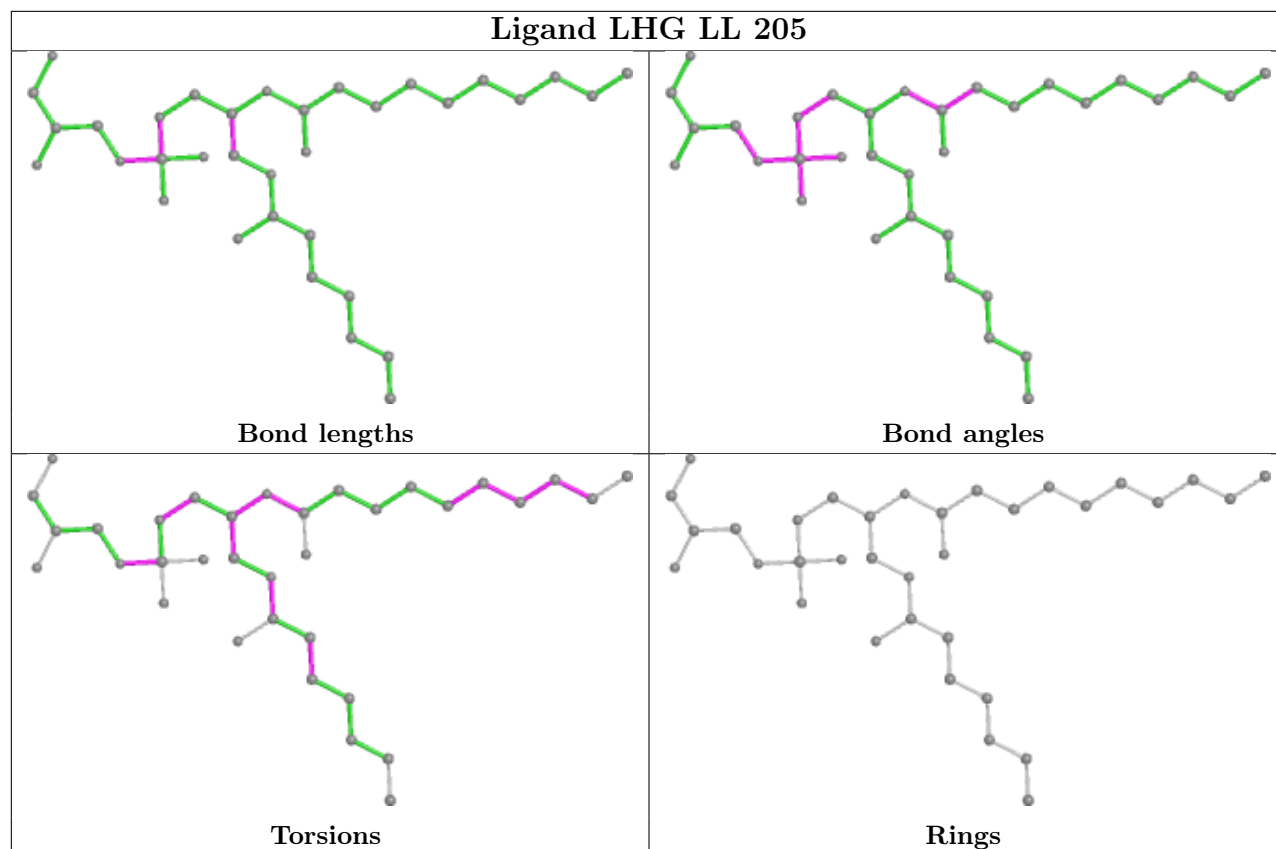
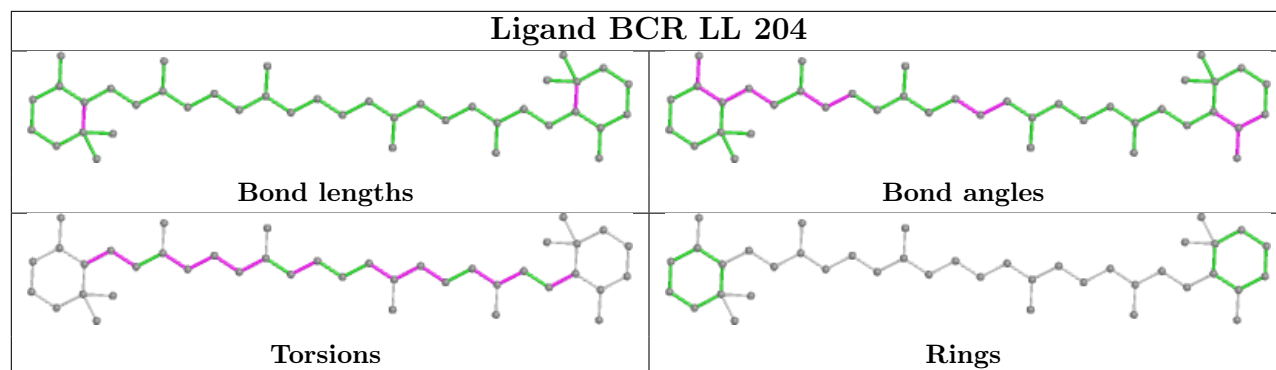
Bond angles

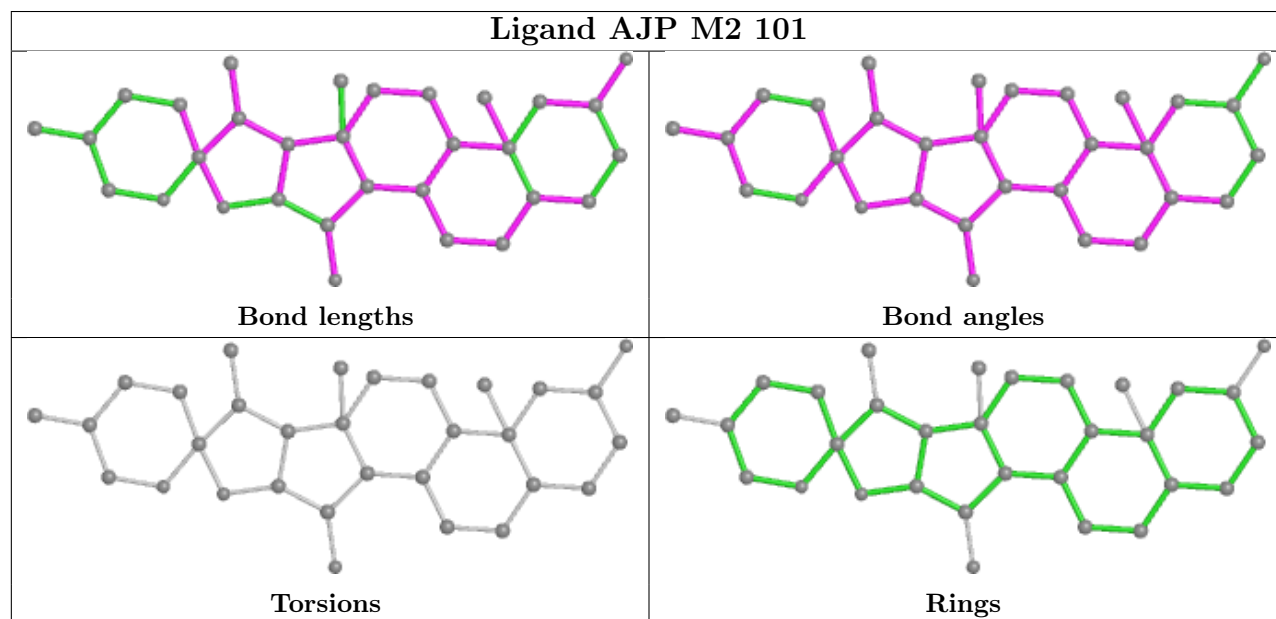
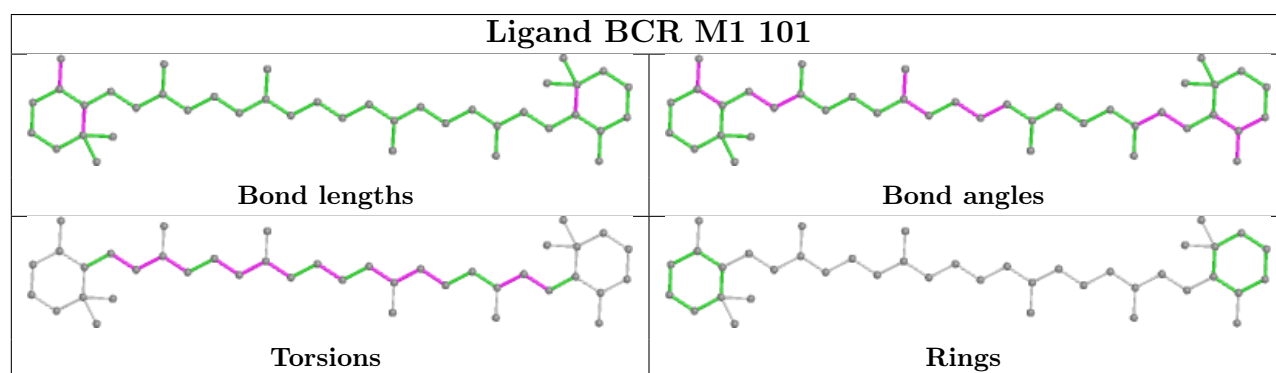
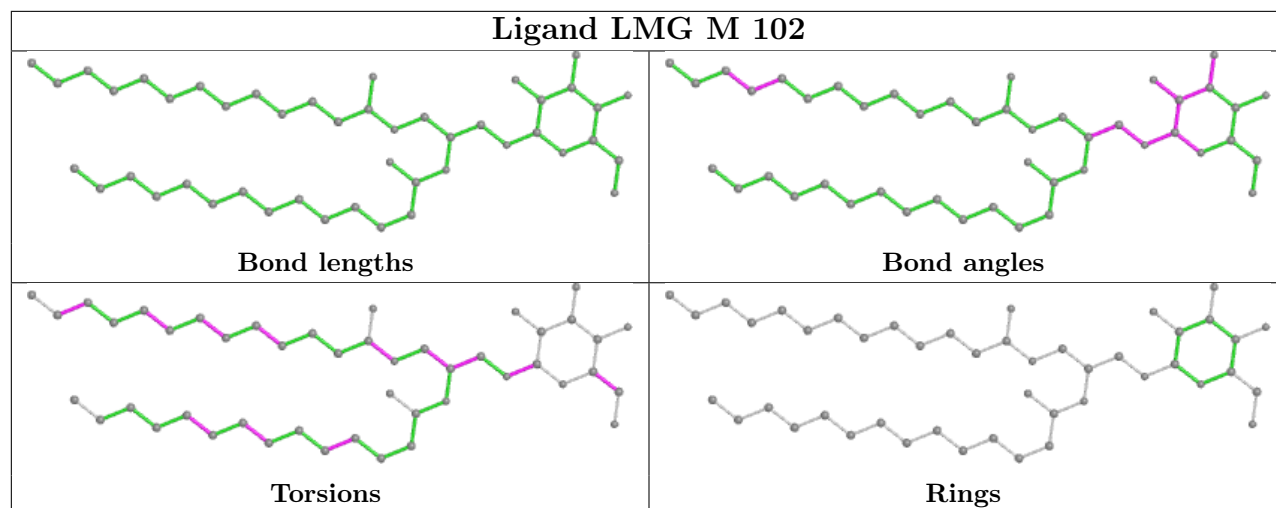


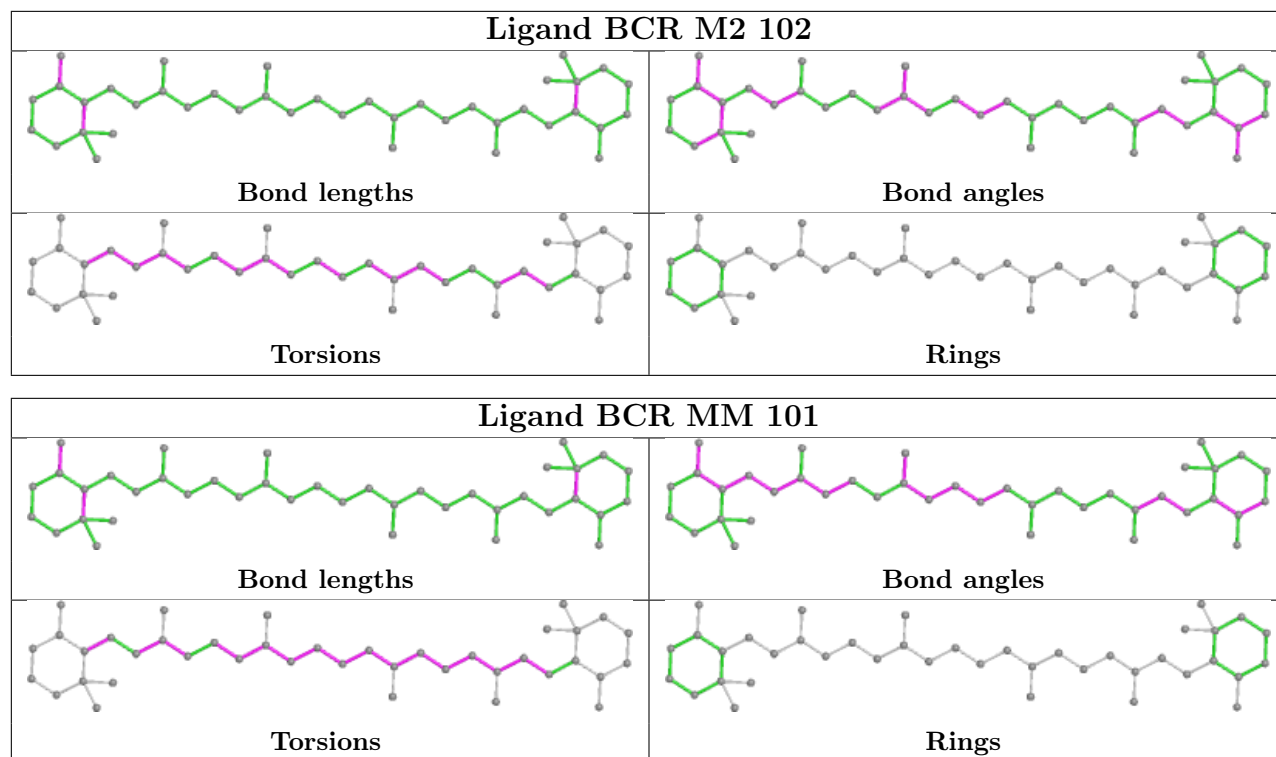
Torsions



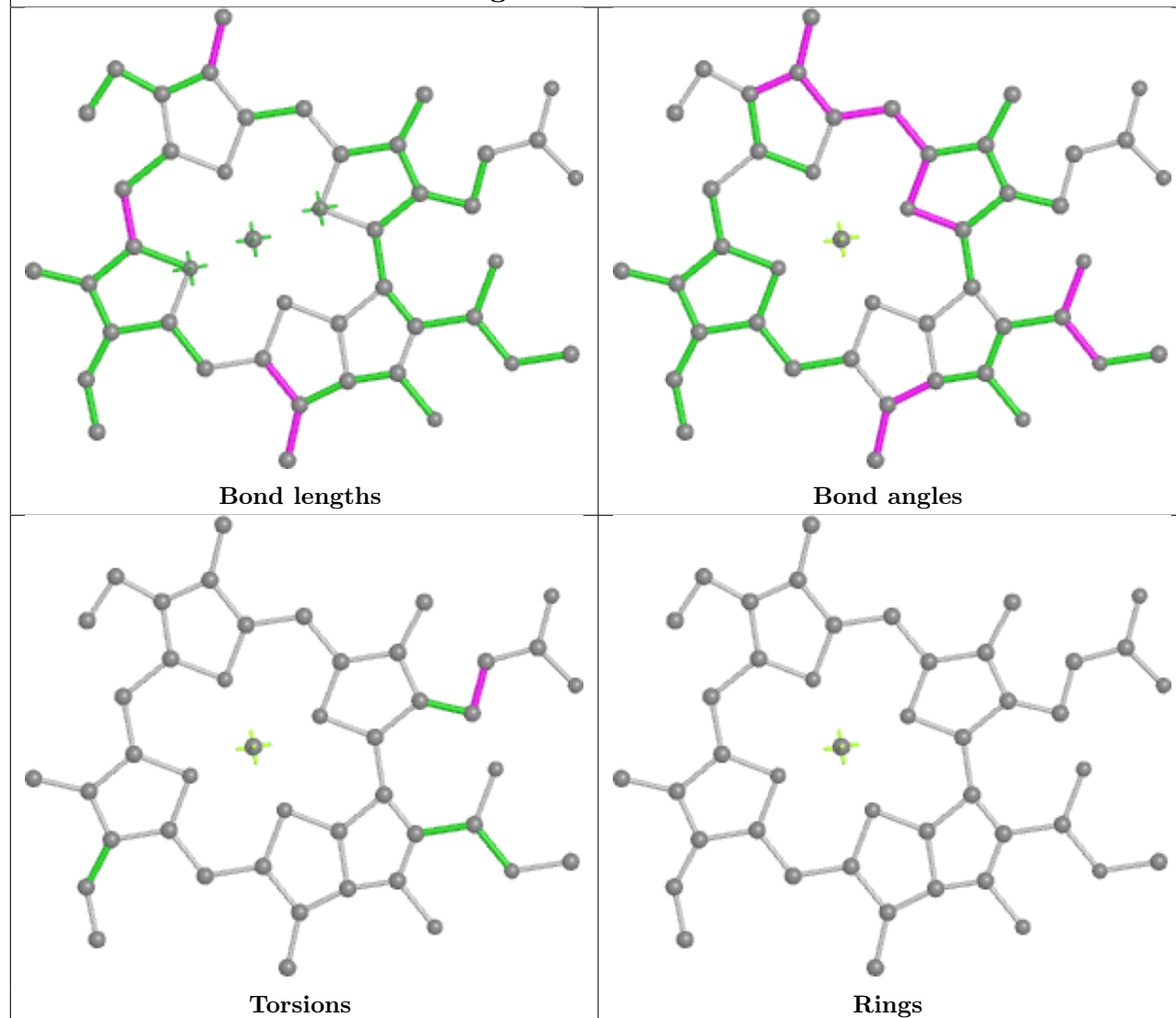
Rings

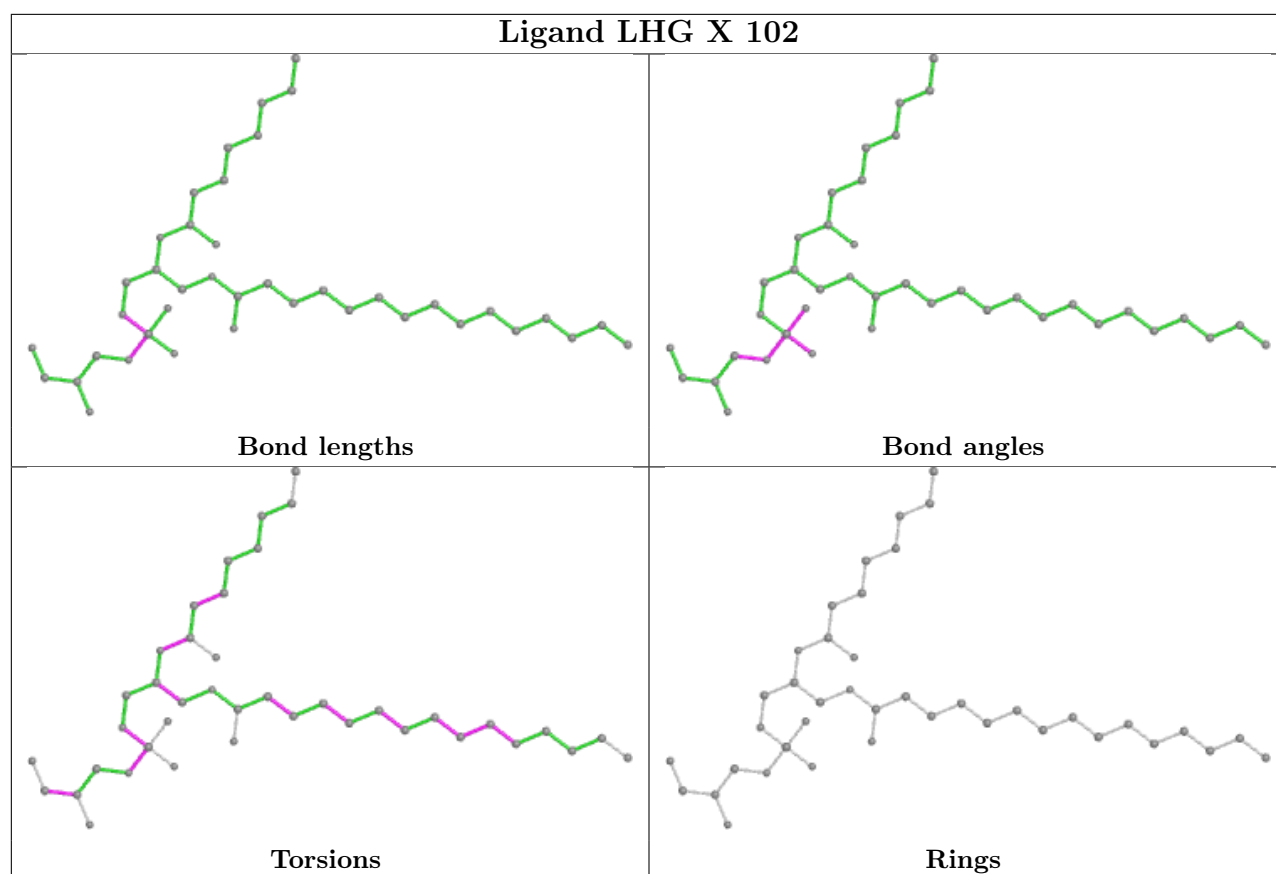




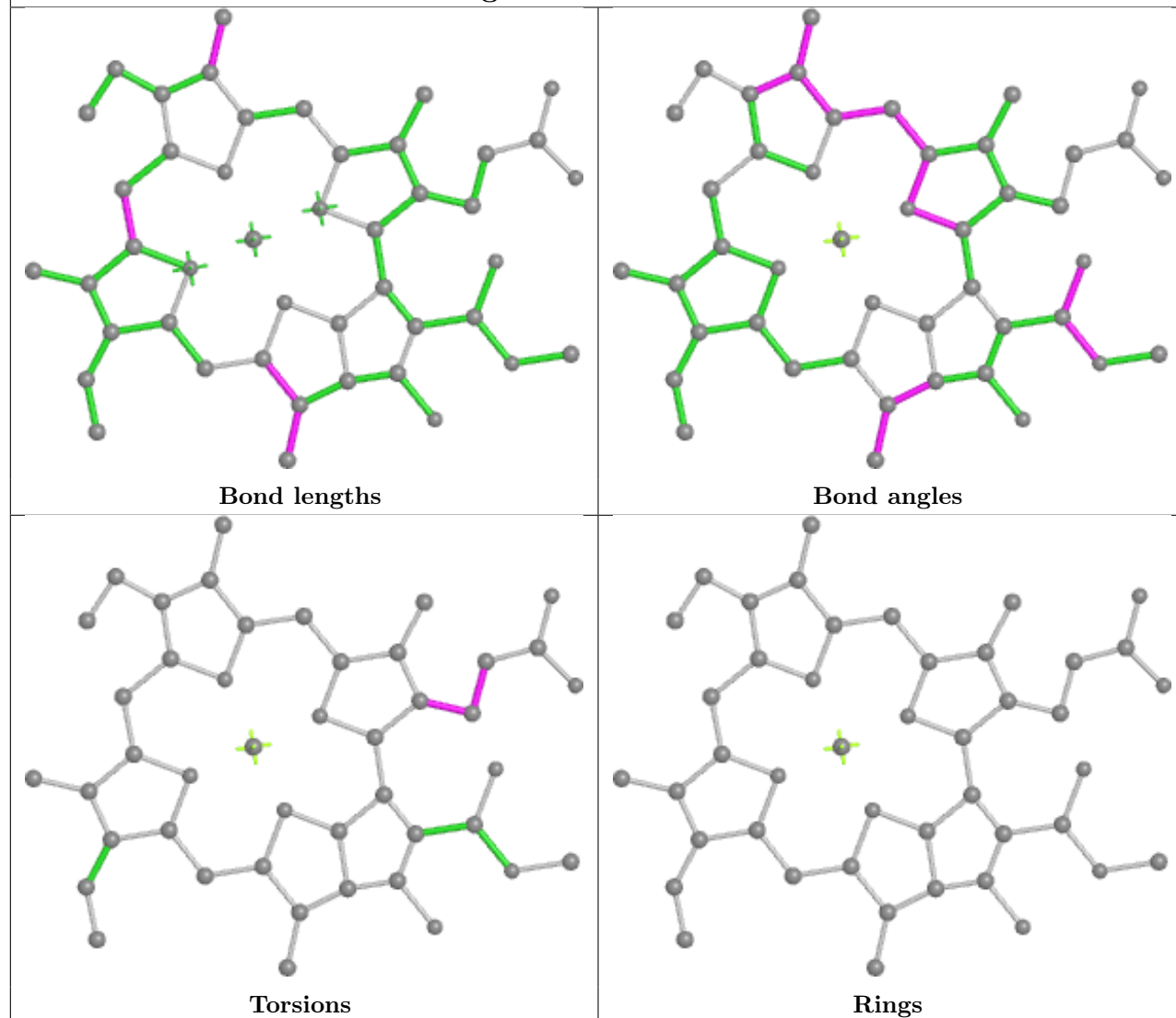


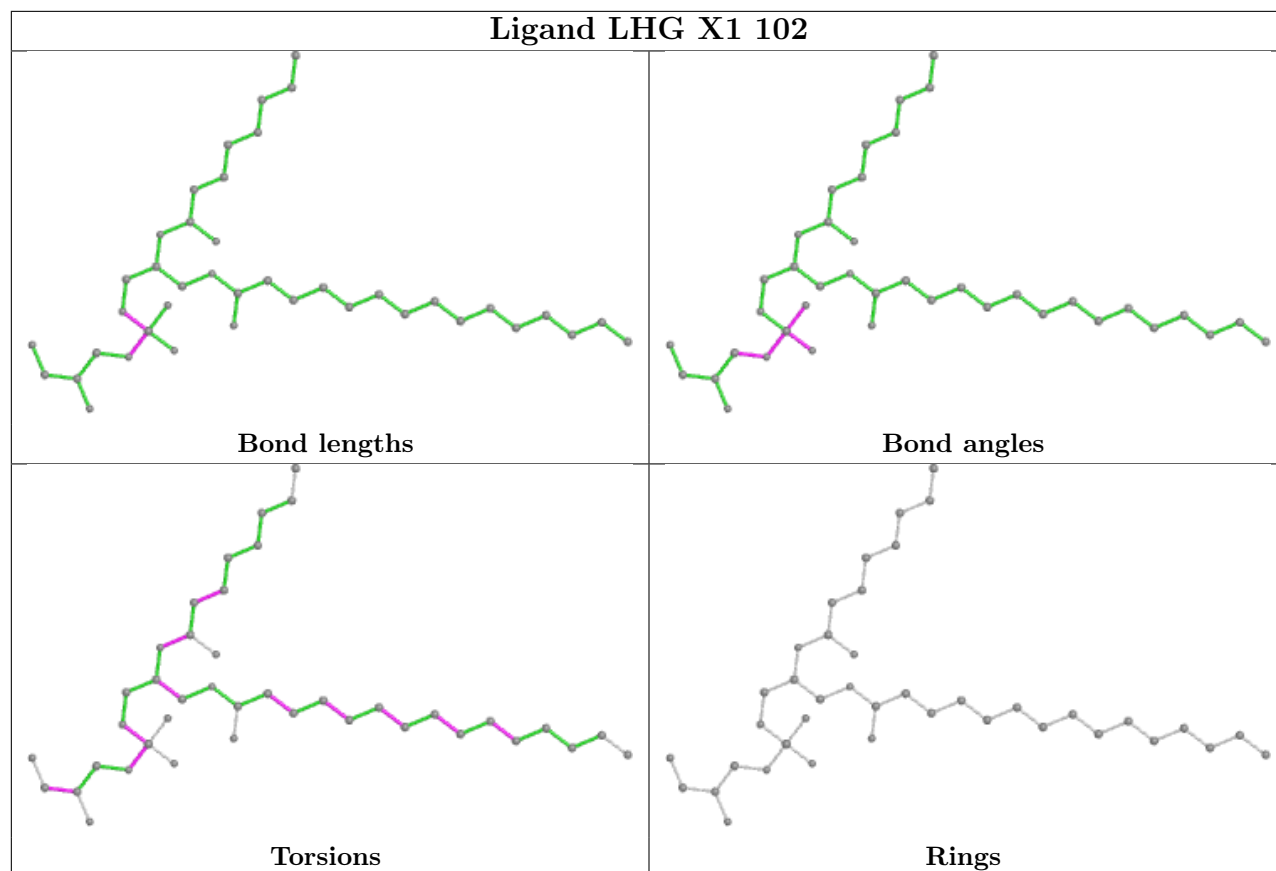
Ligand CLA X 101

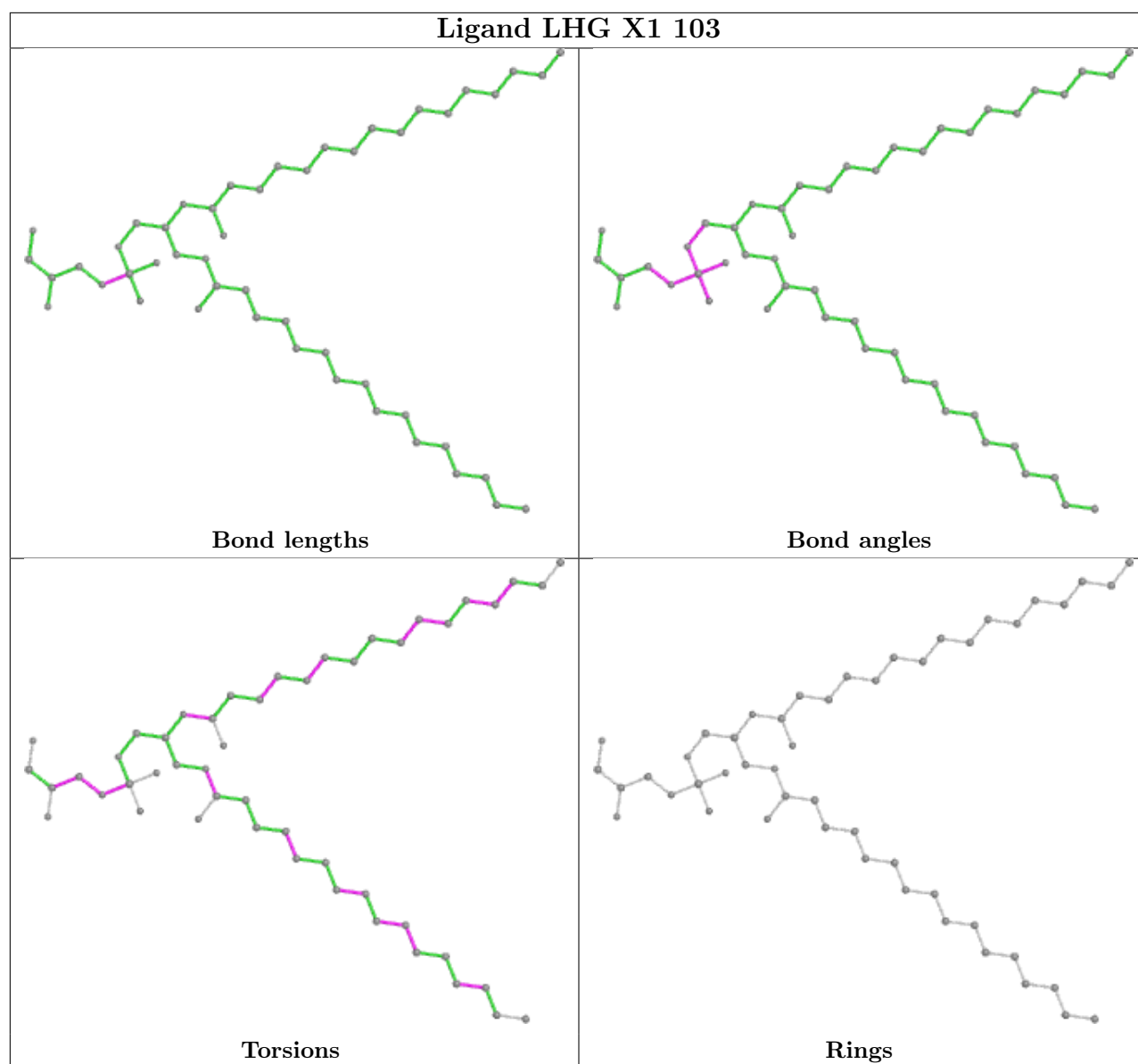




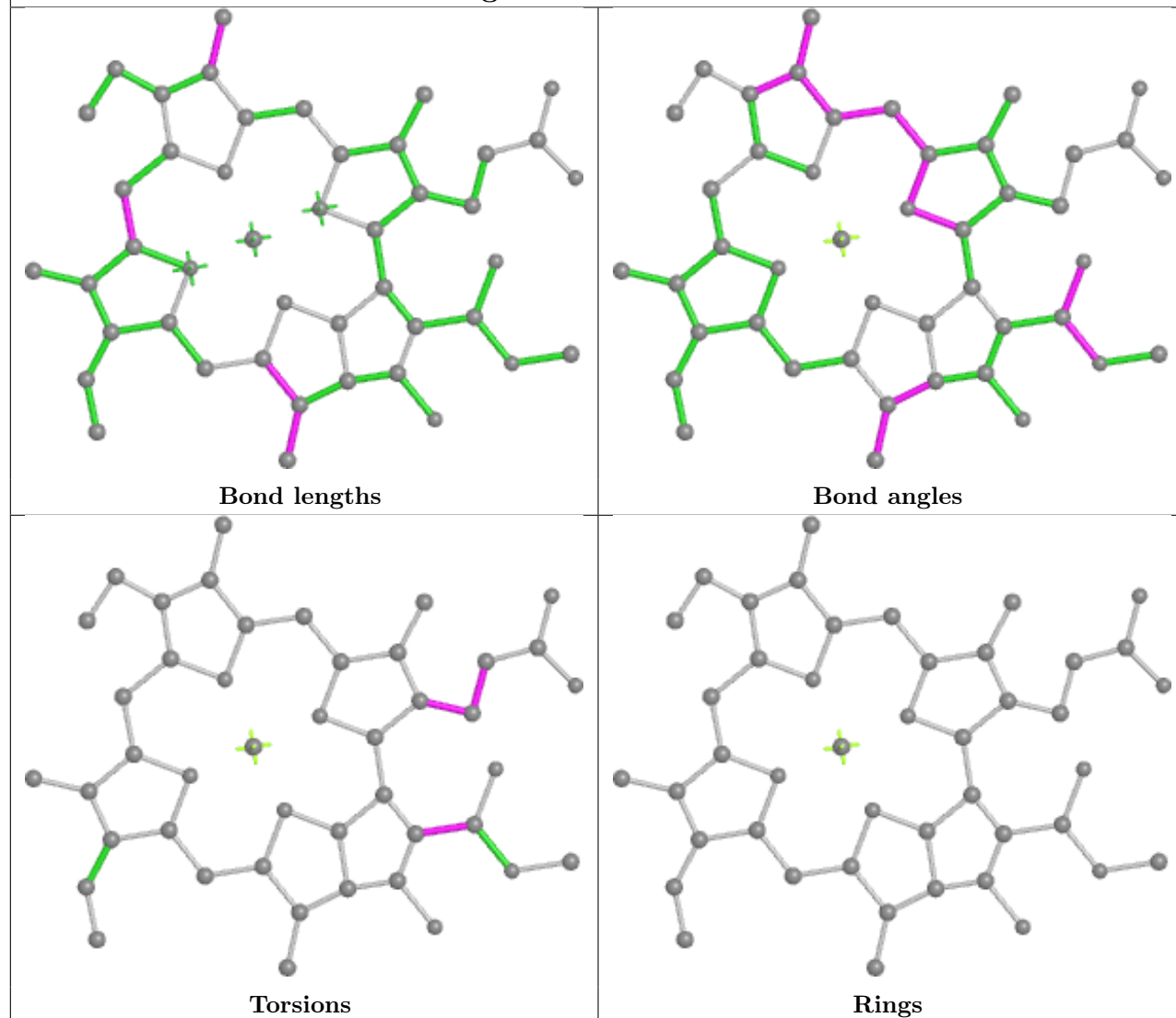
Ligand CLA X1 101

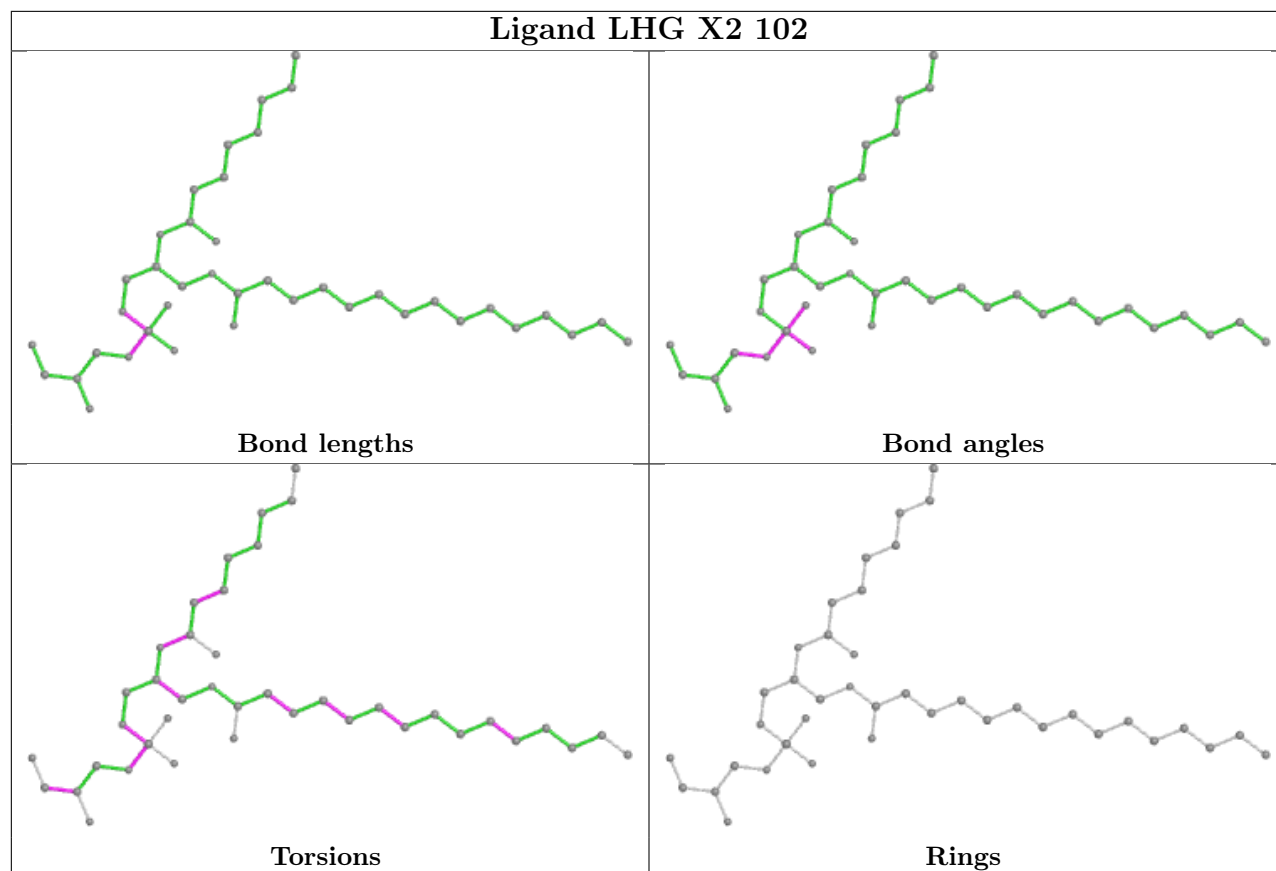


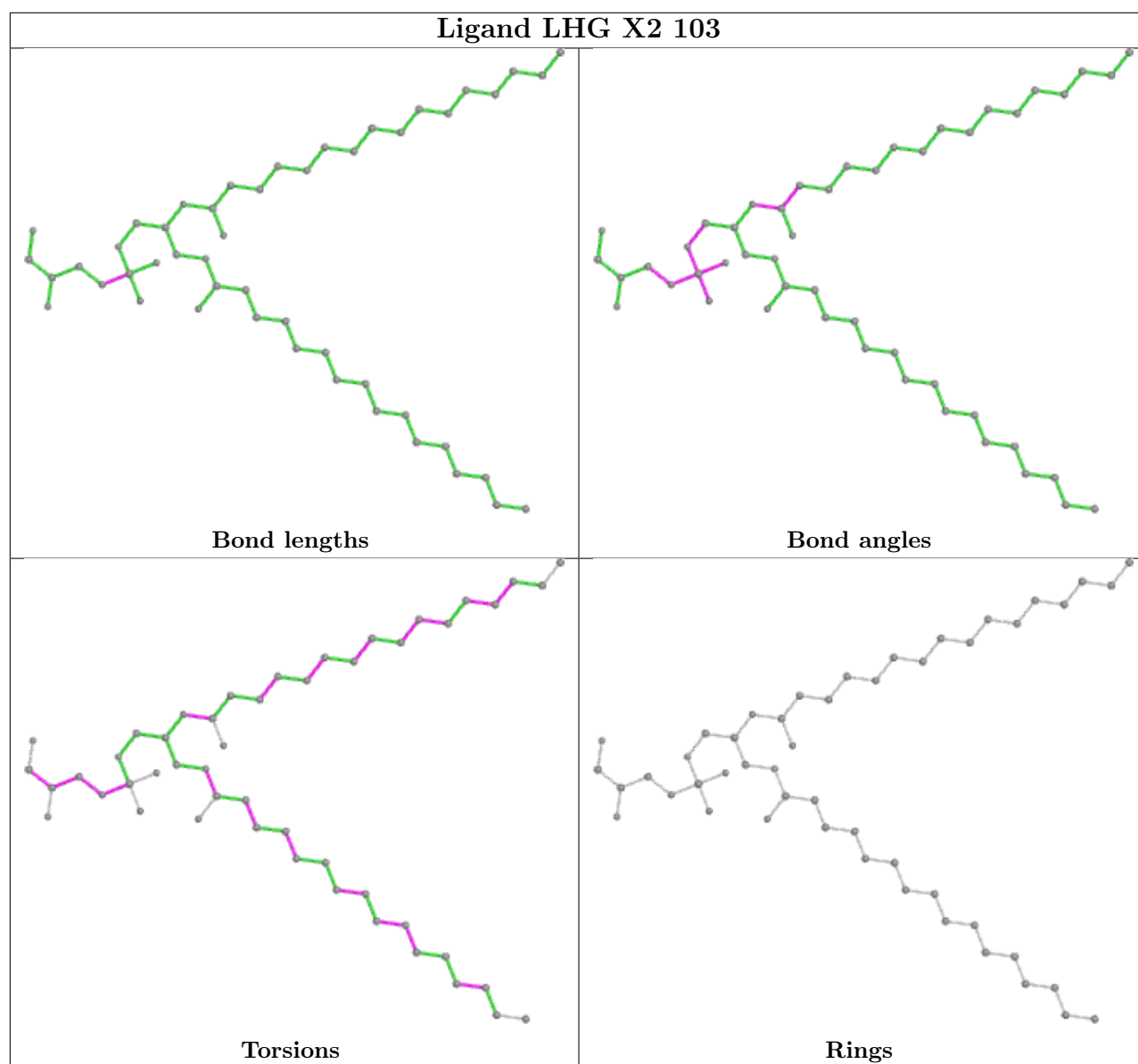




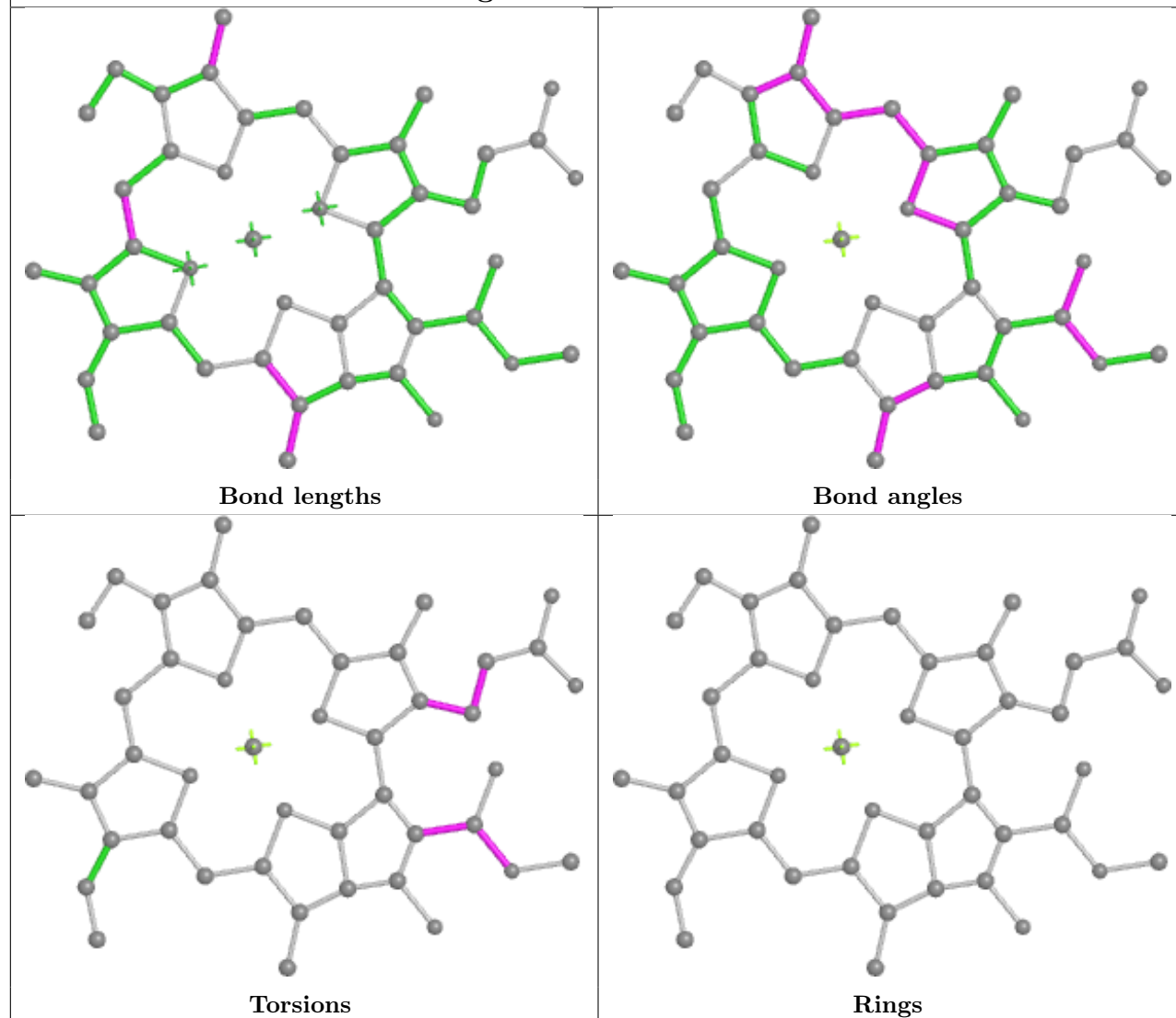
Ligand CLA X2 101

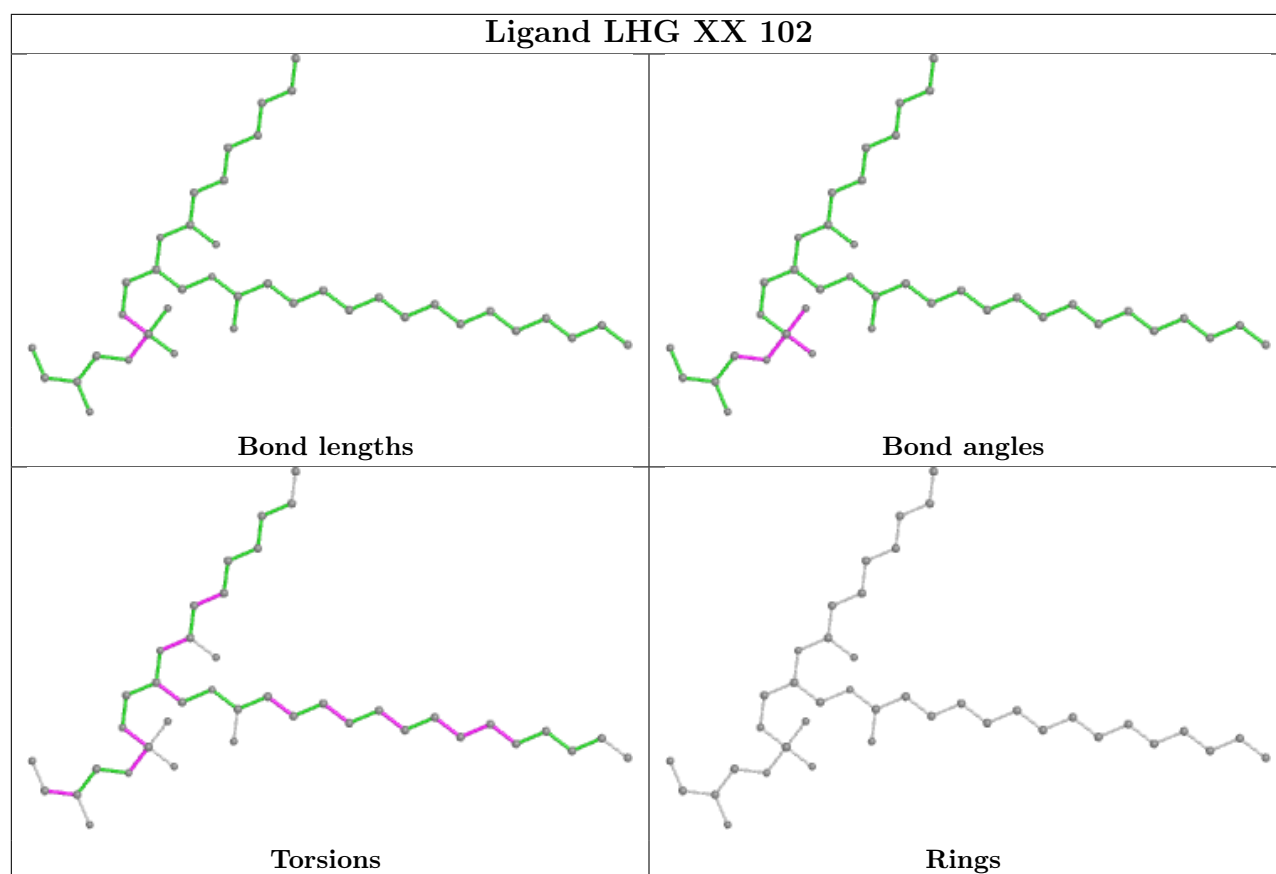






Ligand CLA XX 101





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.