



Full wwPDB EM Validation Report ⓘ

Aug 1, 2024 – 04:14 PM JST

PDB ID : 8WGH
EMDB ID : EMD-37513
Title : Cryo-EM structure of the red-shifted *Fittonia albivenis* PSI-LHCI
Authors : Huang, G.Q.; Li, X.X.; Sui, S.F.; Qin, X.C.
Deposited on : 2023-09-21
Resolution : 2.40 Å (reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

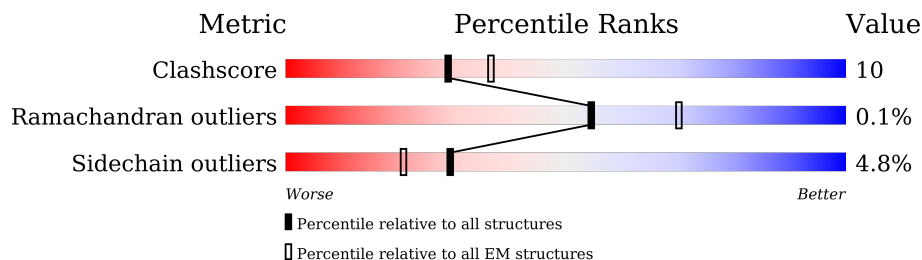
EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.40 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.








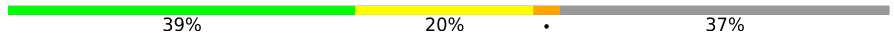


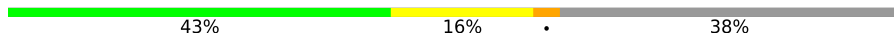
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	1	246	61% 18% 19%
2	2	265	62% 16% 21%
3	3	272	63% 17% 19%
4	4	248	61% 18% 21%
5	A	750	81% 17% ..
6	B	734	86% 13% .
7	C	81	89% 9% ..
8	D	190	61% 12% 26%
9	E	151	34% 7% 58%

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Mol	Chain	Length	Quality of chain
10	F	221	
11	G	145	
12	H	145	
13	I	36	
14	J	44	
15	K	132	
16	L	217	
17	N	173	
18	O	144	

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	CHL	1	301	X	-	-	-
19	CHL	1	306	X	-	-	-
19	CHL	2	301	X	-	-	-
19	CHL	2	305	X	-	-	-
19	CHL	2	306	X	-	-	-
19	CHL	2	307	X	-	-	-
19	CHL	2	314	X	-	-	-
19	CHL	3	306	X	-	-	-
19	CHL	4	305	X	-	-	-
19	CHL	4	306	X	-	-	-
19	CHL	4	307	X	-	-	-
19	CHL	4	315	X	-	-	-
20	CLA	1	302	X	-	-	-
20	CLA	1	303	X	-	-	-
20	CLA	1	304	X	-	-	-
20	CLA	1	305	X	-	-	-
20	CLA	1	307	X	-	-	-
20	CLA	1	308	X	-	-	-
20	CLA	1	309	X	-	-	-
20	CLA	1	310	X	-	-	-
20	CLA	1	311	X	-	-	-
20	CLA	1	312	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	1	313	X	-	-	-
20	CLA	1	314	X	-	-	-
20	CLA	1	321	X	-	-	-
20	CLA	2	302	X	-	-	-
20	CLA	2	303	X	-	-	-
20	CLA	2	304	X	-	-	-
20	CLA	2	308	X	-	-	-
20	CLA	2	309	X	-	-	-
20	CLA	2	310	X	-	-	-
20	CLA	2	311	X	-	-	-
20	CLA	2	312	X	-	-	-
20	CLA	2	313	X	-	-	-
20	CLA	3	301	X	-	-	-
20	CLA	3	302	X	-	-	-
20	CLA	3	303	X	-	-	-
20	CLA	3	304	X	-	-	-
20	CLA	3	305	X	-	-	-
20	CLA	3	307	X	-	-	-
20	CLA	3	308	X	-	-	-
20	CLA	3	310	X	-	-	-
20	CLA	3	311	X	-	-	-
20	CLA	3	312	X	-	-	-
20	CLA	3	313	X	-	-	-
20	CLA	3	314	X	-	-	-
20	CLA	4	301	X	-	-	-
20	CLA	4	302	X	-	-	-
20	CLA	4	303	X	-	-	-
20	CLA	4	304	X	-	-	-
20	CLA	4	308	X	-	-	-
20	CLA	4	309	X	-	-	-
20	CLA	4	310	X	-	-	-
20	CLA	4	311	X	-	-	-
20	CLA	4	312	X	-	-	-
20	CLA	4	313	X	-	-	-
20	CLA	4	314	X	-	-	-
20	CLA	A	801	X	-	-	-
20	CLA	A	802	X	-	-	-
20	CLA	A	803	X	-	-	-
20	CLA	A	804	X	-	-	-
20	CLA	A	805	X	-	-	-
20	CLA	A	806	X	-	-	-
20	CLA	A	807	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	A	808	X	-	-	-
20	CLA	A	809	X	-	-	-
20	CLA	A	810	X	-	-	-
20	CLA	A	811	X	-	-	-
20	CLA	A	812	X	-	-	-
20	CLA	A	813	X	-	-	-
20	CLA	A	814	X	-	-	-
20	CLA	A	815	X	-	-	-
20	CLA	A	816	X	-	-	-
20	CLA	A	817	X	-	-	-
20	CLA	A	818	X	-	-	-
20	CLA	A	819	X	-	-	-
20	CLA	A	820	X	-	-	-
20	CLA	A	821	X	-	-	-
20	CLA	A	822	X	-	-	-
20	CLA	A	823	X	-	-	-
20	CLA	A	824	X	-	-	-
20	CLA	A	825	X	-	-	-
20	CLA	A	826	X	-	-	-
20	CLA	A	827	X	-	-	-
20	CLA	A	828	X	-	-	-
20	CLA	A	829	X	-	-	-
20	CLA	A	830	X	-	-	-
20	CLA	A	831	X	-	-	-
20	CLA	A	832	X	-	-	-
20	CLA	A	833	X	-	-	-
20	CLA	A	834	X	-	-	-
20	CLA	A	835	X	-	-	-
20	CLA	A	836	X	-	-	-
20	CLA	A	837	X	-	-	-
20	CLA	A	838	X	-	-	-
20	CLA	A	839	X	-	-	-
20	CLA	A	840	X	-	-	-
20	CLA	A	841	X	-	-	-
20	CLA	A	851	X	-	-	-
20	CLA	A	853	X	-	-	-
20	CLA	B	801	X	-	-	-
20	CLA	B	802	X	-	-	-
20	CLA	B	803	X	-	-	-
20	CLA	B	804	X	-	-	-
20	CLA	B	805	X	-	-	-
20	CLA	B	806	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	B	807	X	-	-	-
20	CLA	B	808	X	-	-	-
20	CLA	B	809	X	-	-	-
20	CLA	B	810	X	-	-	-
20	CLA	B	811	X	-	-	-
20	CLA	B	812	X	-	-	-
20	CLA	B	813	X	-	-	-
20	CLA	B	814	X	-	-	-
20	CLA	B	815	X	-	-	-
20	CLA	B	816	X	-	-	-
20	CLA	B	817	X	-	-	-
20	CLA	B	818	X	-	-	-
20	CLA	B	819	X	-	-	-
20	CLA	B	820	X	-	-	-
20	CLA	B	821	X	-	-	-
20	CLA	B	822	X	-	-	-
20	CLA	B	823	X	-	-	-
20	CLA	B	824	X	-	-	-
20	CLA	B	825	X	-	-	-
20	CLA	B	826	X	-	-	-
20	CLA	B	827	X	-	-	-
20	CLA	B	828	X	-	-	-
20	CLA	B	829	X	-	-	-
20	CLA	B	830	X	-	-	-
20	CLA	B	831	X	-	-	-
20	CLA	B	832	X	-	-	-
20	CLA	B	833	X	-	-	-
20	CLA	B	834	X	-	-	-
20	CLA	B	835	X	-	-	-
20	CLA	B	836	X	-	-	-
20	CLA	B	837	X	-	-	-
20	CLA	B	838	X	-	-	-
20	CLA	B	839	X	-	-	-
20	CLA	F	802	X	-	-	-
20	CLA	F	804	X	-	-	-
20	CLA	F	805	X	-	-	-
20	CLA	G	603	X	-	-	-
20	CLA	G	604	X	-	-	-
20	CLA	G	605	X	-	-	-
20	CLA	H	201	X	-	-	-
20	CLA	J	101	X	-	-	-
20	CLA	J	103	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	CLA	K	201	X	-	-	-
20	CLA	K	202	X	-	-	-
20	CLA	K	203	X	-	-	-
20	CLA	K	205	X	-	-	-
20	CLA	L	302	X	-	-	-
20	CLA	L	303	X	-	-	-
20	CLA	L	304	X	-	-	-
20	CLA	L	307	X	-	-	-
20	CLA	N	202	X	-	-	-
20	CLA	N	203	X	-	-	-
20	CLA	O	201	X	-	-	-
20	CLA	O	202	X	-	-	-
20	CLA	O	203	X	-	-	-

2 Entry composition i

There are 30 unique types of molecules in this entry. The entry contains 38187 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	1	199	1559	1016	261	278	4	0	0

- Molecule 2 is a protein called Chlorophyll a-b binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	2	209	1626	1068	264	289	5	0	0

- Molecule 3 is a protein called Chlorophyll a-b binding protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	3	220	1727	1139	277	305	6	0	0

- Molecule 4 is a protein called Chlorophyll a-b binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	4	197	1568	1027	253	283	5	0	0

- Molecule 5 is a protein called Photosystem I P700 chlorophyll a apoprotein A1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	742	5831	3820	989	1003	19	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	248	SER	VAL	conflict	UNP A0A8A0WPY6

- Molecule 6 is a protein called Photosystem I P700 chlorophyll a apoprotein A2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	733	5854	3843	996	1002	13	0	0

- Molecule 7 is a protein called Photosystem I iron-sulfur center.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	141	1116	714	193	206	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
9	E	63	511	324	92	95	0	0

- Molecule 10 is a protein called Photosystem I reaction center subunit III, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	153	1216	793	208	212	3	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
11	G	98	768	498	126	144	0	0

- Molecule 12 is a protein called Photosystem I reaction center subunit VI.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
12	H	90	681	444	109	128	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	29	Total	C	N	O	S	0	0
			221	151	35	34	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	J	40	Total	C	N	O	S	0	0
			318	215	49	53	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	K	83	Total	C	N	O	S	0	0
			588	378	100	108	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	L	162	Total	C	N	O	S	0	0
			1225	812	195	217	1		

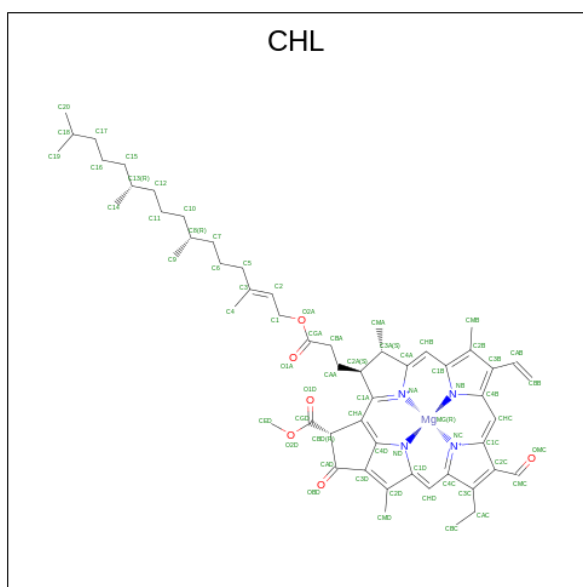
- Molecule 17 is a protein called Photosystem I reaction center subunit N.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	84	Total	C	N	O	S	0	0
			686	440	111	131	4		

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

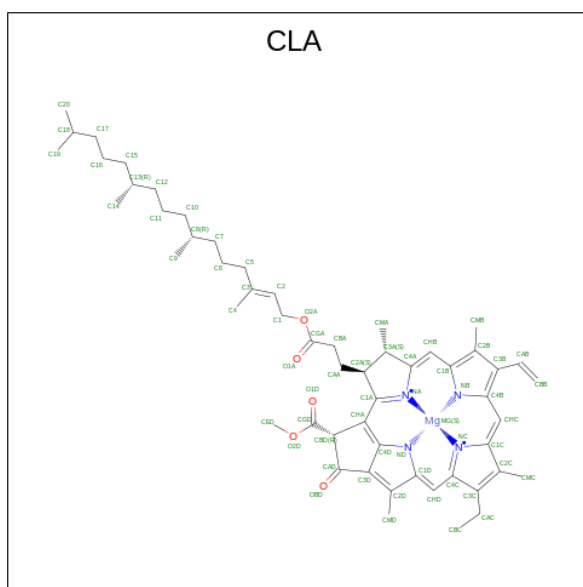
Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	89	Total	C	N	O	S	0	0
			705	475	112	117	1		

- Molecule 19 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	Mg	N		O
19	1	1	52	41	1	4	6	0
19	1	1	48	37	1	4	6	0
19	2	1	53	42	1	4	6	0
19	2	1	43	34	1	4	4	0
19	2	1	48	37	1	4	6	0
19	2	1	51	40	1	4	6	0
19	2	1	43	34	1	4	4	0
19	3	1	47	36	1	4	6	0
19	4	1	53	42	1	4	6	0
19	4	1	51	40	1	4	6	0
19	4	1	51	40	1	4	6	0
19	4	1	43	34	1	4	4	0

- Molecule 20 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			61	51	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			41	33	1	4	3	
20	1	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	2	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	2	1	49	39	1	4	5	0
20	2	1	60	50	1	4	5	0
20	2	1	50	40	1	4	5	0
20	2	1	60	50	1	4	5	0
20	2	1	41	33	1	4	3	0
20	2	1	52	42	1	4	5	0
20	2	1	65	55	1	4	5	0
20	2	1	43	35	1	4	3	0
20	3	1	60	50	1	4	5	0
20	3	1	50	40	1	4	5	0
20	3	1	45	35	1	4	5	0
20	3	1	42	34	1	4	3	0
20	3	1	47	37	1	4	5	0
20	3	1	50	40	1	4	5	0
20	3	1	50	40	1	4	5	0
20	3	1	46	36	1	4	5	0
20	3	1	52	42	1	4	5	0
20	3	1	55	45	1	4	5	0
20	3	1	45	35	1	4	5	0
20	3	1	45	35	1	4	5	0
20	3	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	4	1	46	36	1	4	5	0
20	4	1	60	50	1	4	5	0
20	4	1	60	50	1	4	5	0
20	4	1	50	40	1	4	5	0
20	4	1	50	40	1	4	5	0
20	4	1	60	50	1	4	5	0
20	4	1	55	45	1	4	5	0
20	4	1	52	42	1	4	5	0
20	4	1	65	55	1	4	5	0
20	4	1	45	35	1	4	5	0
20	4	1	50	40	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	55	45	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0

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

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	45	35	1	4	5	0
20	A	1	51	41	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	A	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	45	35	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	55	45	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
20	B	1	54	44	1	4	5	0
20	B	1	55	45	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	60	50	1	4	5	0
20	B	1	55	45	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	60	50	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	50	40	1	4	5	0
20	B	1	56	46	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	60	50	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	50	40	1	4	5	0

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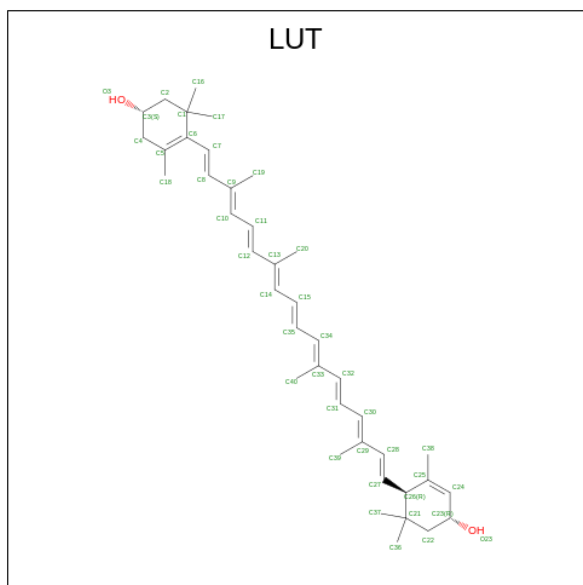
Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	B	1	65	55	1	4	5	0
20	B	1	58	48	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	45	35	1	4	5	0
20	B	1	51	41	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	47	37	1	4	5	0
20	B	1	65	55	1	4	5	0
20	B	1	65	55	1	4	5	0
20	F	1	65	55	1	4	5	0
20	F	1	45	35	1	4	5	0
20	F	1	46	36	1	4	5	0
20	G	1	45	35	1	4	5	0
20	G	1	50	40	1	4	5	0
20	G	1	46	36	1	4	5	0
20	H	1	56	46	1	4	5	0
20	J	1	65	55	1	4	5	0
20	J	1	42	34	1	4	3	0
20	K	1	46	36	1	4	5	0
20	K	1	60	50	1	4	5	0
20	K	1	46	36	1	4	5	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Mg	N	O	
20	K	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	L	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	N	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
20	O	1	Total	C	Mg	N	O	0
			60	50	1	4	5	

- Molecule 21 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



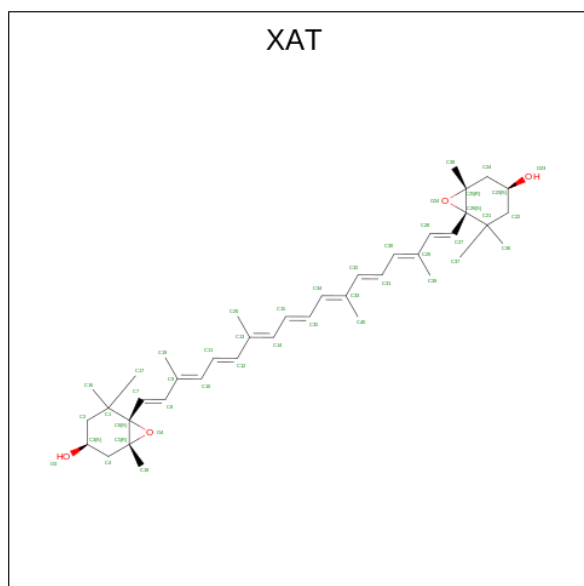
Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
21	1	1	Total	C	O	0
			42	40	2	

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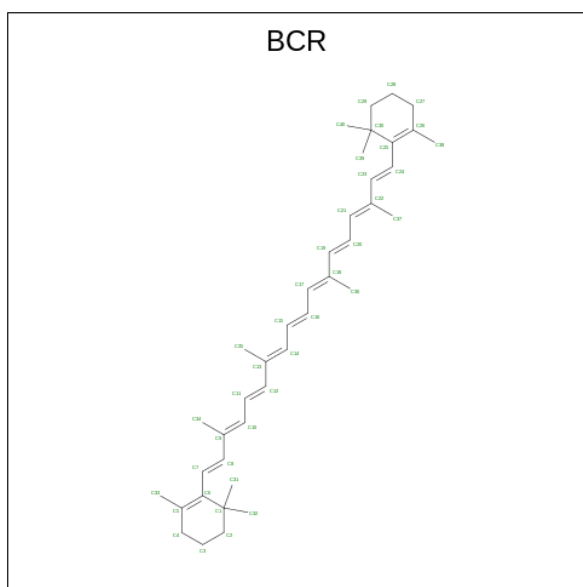
Mol	Chain	Residues	Atoms			AltConf
21	1	1	Total	C	O	0
			42	40	2	
21	2	1	Total	C	O	0
			42	40	2	
21	3	1	Total	C	O	0
			42	40	2	
21	4	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	
21	O	1	Total	C	O	0
			42	40	2	

- Molecule 22 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'-TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



Mol	Chain	Residues	Atoms			AltConf
22	1	1	Total	C	O	0
			44	40	4	
22	2	1	Total	C	O	0
			44	40	4	
22	3	1	Total	C	O	0
			44	40	4	
22	4	1	Total	C	O	0
			44	40	4	

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



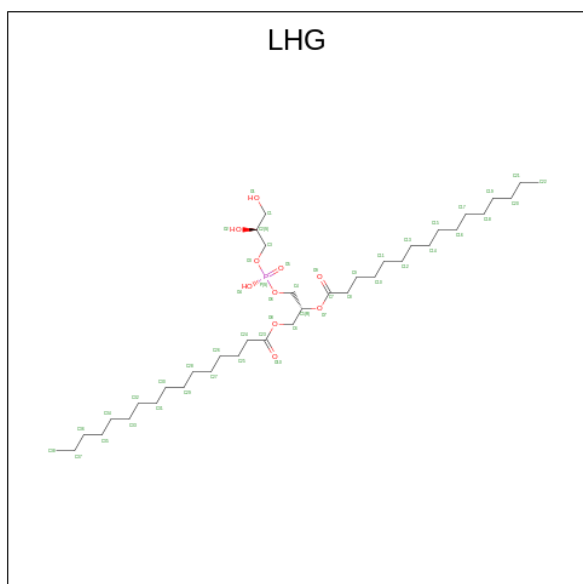
Mol	Chain	Residues	Atoms	AltConf
23	1	1	Total C 40 40	0
23	2	1	Total C 40 40	0
23	3	1	Total C 40 40	0
23	4	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	A	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0

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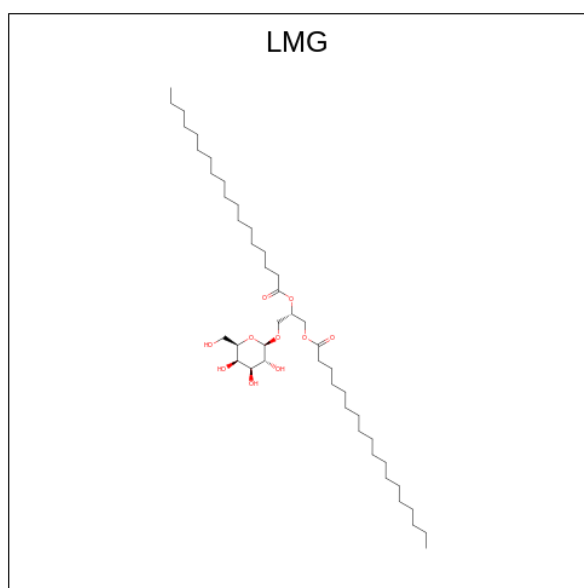
Mol	Chain	Residues	Atoms	AltConf
23	B	1	Total C 40 40	0
23	B	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	F	1	Total C 40 40	0
23	G	1	Total C 40 40	0
23	I	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	J	1	Total C 40 40	0
23	K	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0
23	L	1	Total C 40 40	0

- Molecule 24 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: $C_{38}H_{75}O_{10}P$) (labeled as "Ligand of Interest" by depositor).



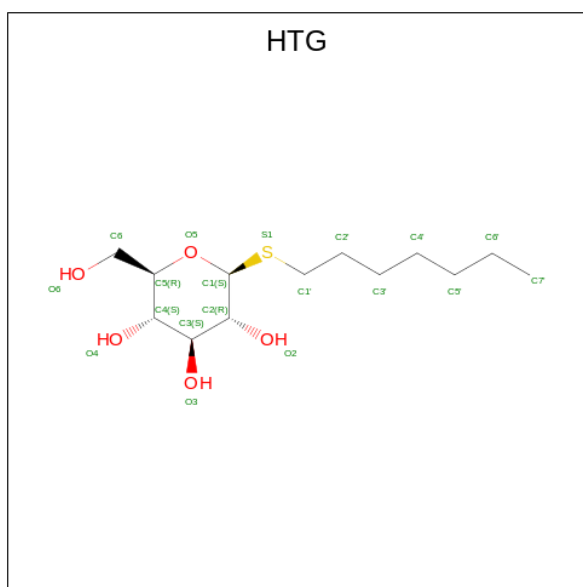
Mol	Chain	Residues	Atoms				AltConf
24	1	1	Total	C	O	P	0
			49	38	10	1	
24	2	1	Total	C	O	P	0
			37	26	10	1	
24	A	1	Total	C	O	P	0
			49	38	10	1	
24	A	1	Total	C	O	P	0
			27	16	10	1	
24	B	1	Total	C	O	P	0
			23	12	10	1	

- Molecule 25 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: $C_{45}H_{86}O_{10}$) (labeled as "Ligand of Interest" by depositor).



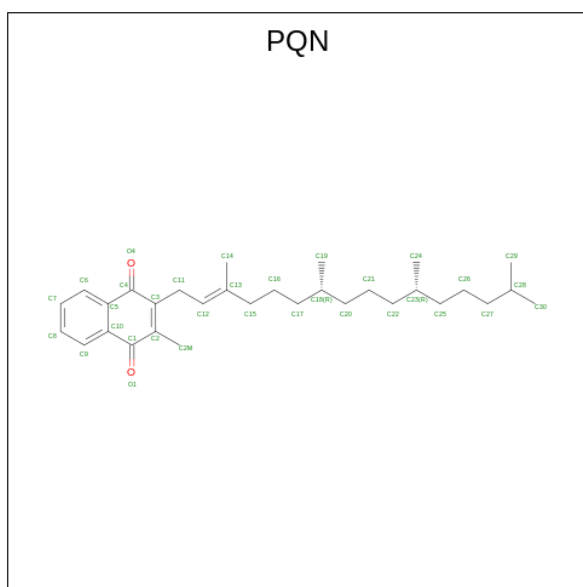
Mol	Chain	Residues	Atoms			AltConf
25	1	1	Total	C	O	0
			49	39	10	
25	1	1	Total	C	O	0
			44	34	10	
25	4	1	Total	C	O	0
			44	34	10	

- Molecule 26 is heptyl 1-thio-beta-D-glucopyranoside (three-letter code: HTG) (formula: $C_{13}H_{26}O_5S$).



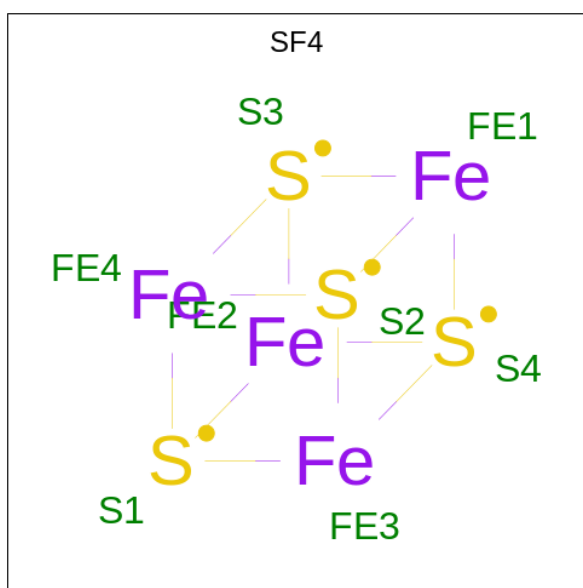
Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
26	1	1	Total 19	C 13	O 5	S 1	0
26	4	1	Total 19	C 13	O 5	S 1	0
26	A	1	Total 19	C 13	O 5	S 1	0
26	B	1	Total 19	C 13	O 5	S 1	0
26	B	1	Total 19	C 13	O 5	S 1	0
26	F	1	Total 19	C 13	O 5	S 1	0
26	F	1	Total 19	C 13	O 5	S 1	0
26	G	1	Total 19	C 13	O 5	S 1	0
26	J	1	Total 19	C 13	O 5	S 1	0
26	N	1	Total 19	C 13	O 5	S 1	0

- Molecule 27 is PHYLLOQUINONE (three-letter code: PQN) (formula: C₃₁H₄₆O₂).



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

- Molecule 28 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe₄S₄).



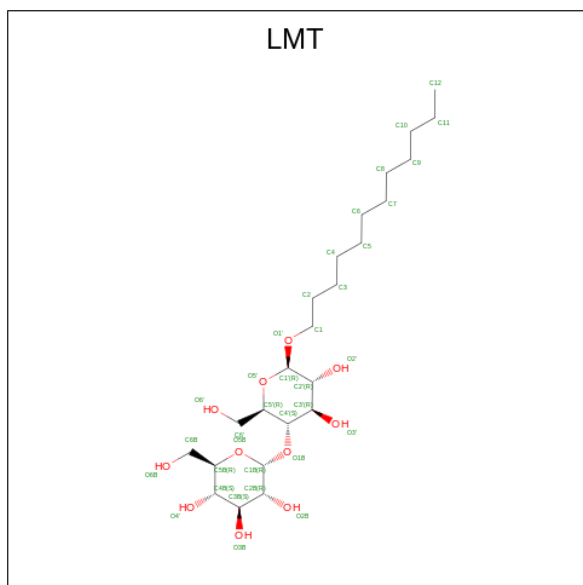
Mol	Chain	Residues	Atoms			AltConf
28	A	1	Total	Fe	S	0
			8	4	4	
28	C	1	Total	Fe	S	0
			8	4	4	

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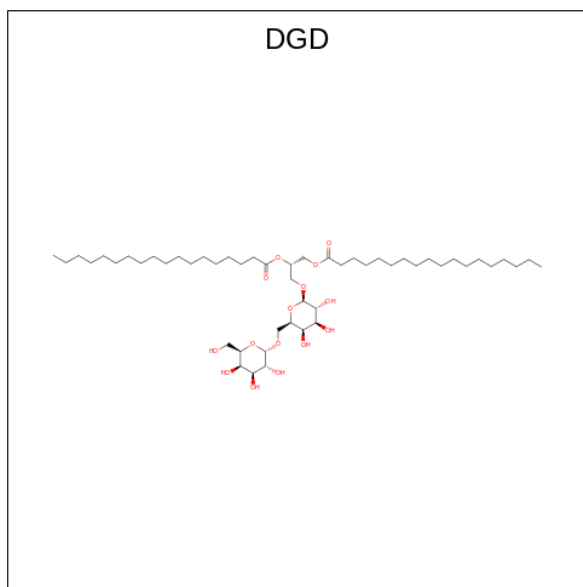
Mol	Chain	Residues	Atoms			AltConf
			Total	Fe	S	
28	C	1	8	4	4	0

- Molecule 29 is DODECYL-BETA-D-MALTOSE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
29	B	1	35	24	11	0
29	G	1	35	24	11	0

- Molecule 30 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).

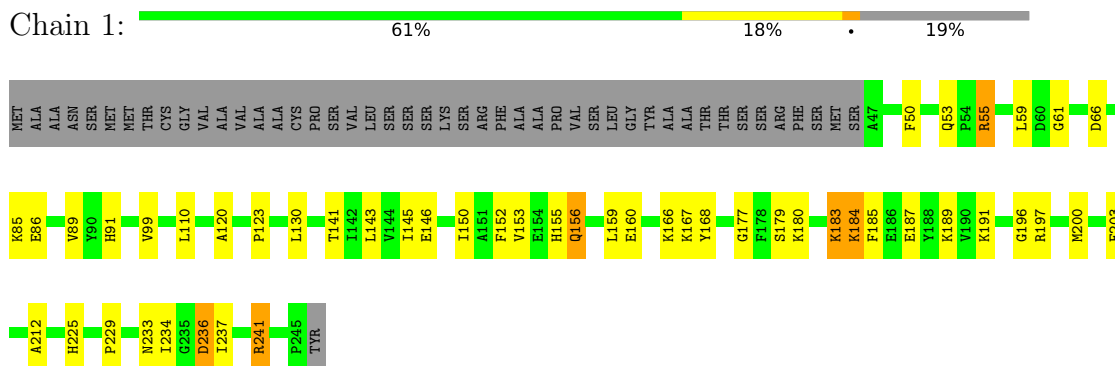


Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
30	B	1	66	51	15	0

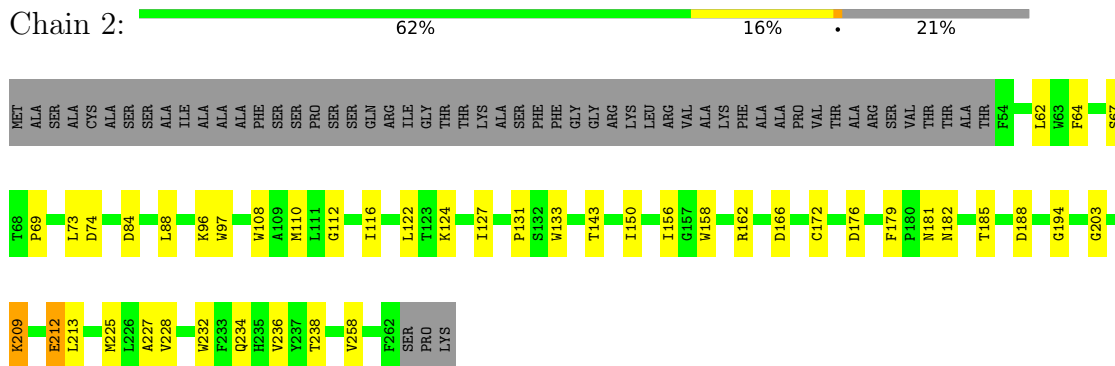
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

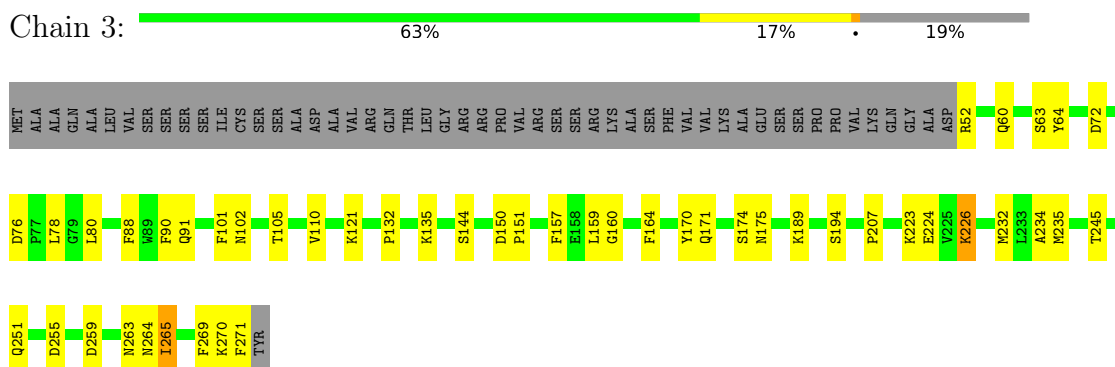
- Molecule 1: Chlorophyll a-b binding protein 1



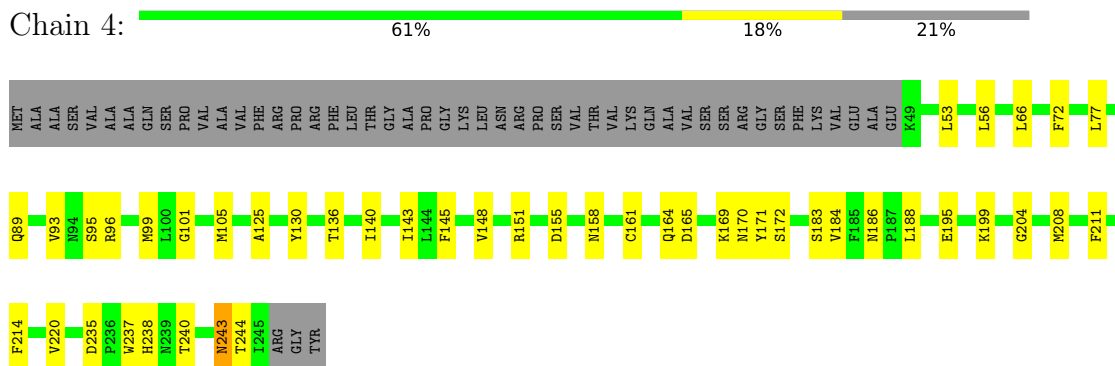
- Molecule 2: Chlorophyll a-b binding protein 2



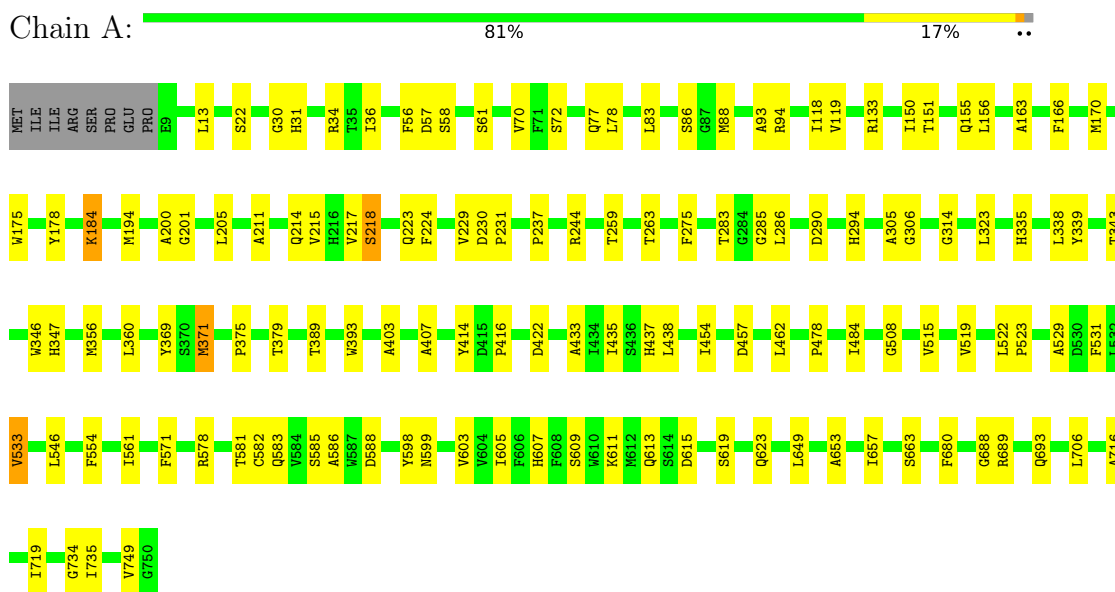
- Molecule 3: Chlorophyll a-b binding protein 3



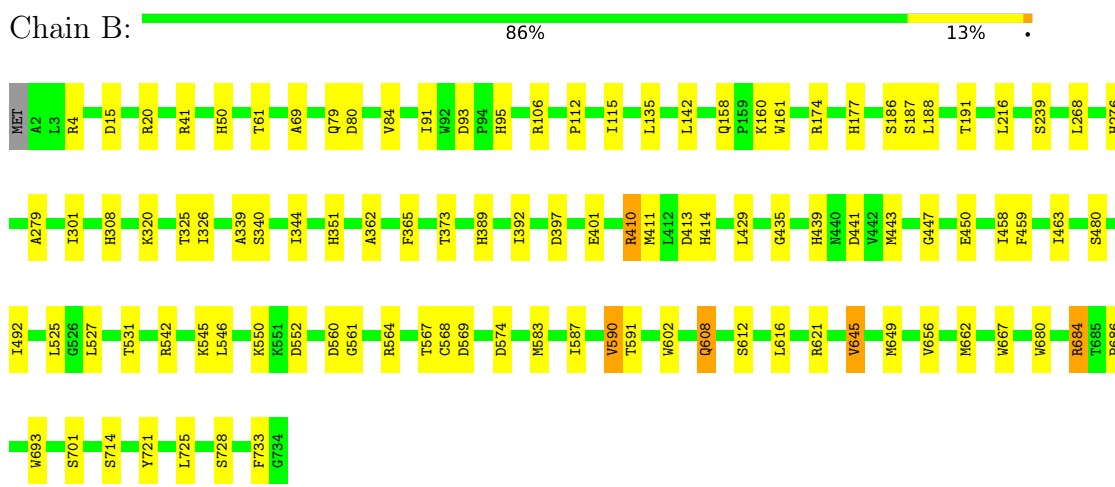
• Molecule 4: Chlorophyll a-b binding protein 4




• Molecule 5: Photosystem I P700 chlorophyll a apoprotein A1



• Molecule 6: Photosystem I P700 chlorophyll a apoprotein A2



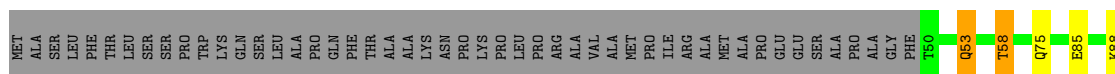
• Molecule 7: Photosystem I iron-sulfur center

Chain C:  89% 9% ..



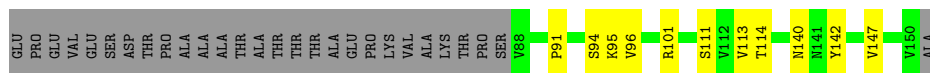
- Molecule 8: Photosystem I reaction center subunit II

Chain D:  61% 12% • 26%



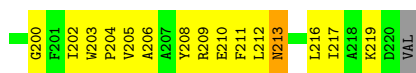
- Molecule 9: Photosystem I reaction center subunit IV

Chain E:  34% 7% 58%



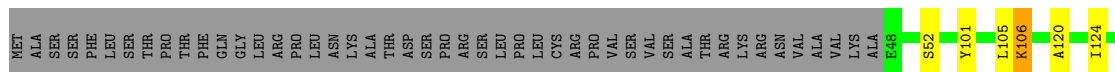
- Molecule 10: Photosystem I reaction center subunit III, chloroplastic

Chain F:  48% 19% • 31%



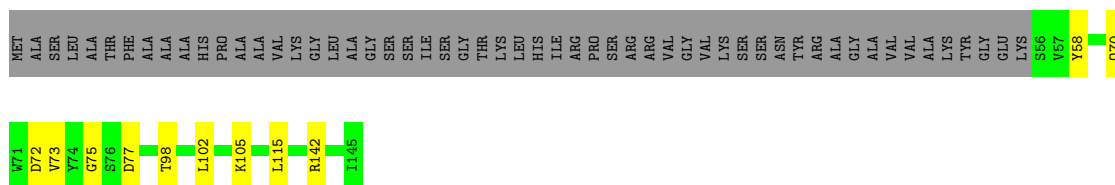
- Molecule 11: Photosystem I reaction center subunit VIII

Chain G:  61% 6% • 32%



- Molecule 12: Photosystem I reaction center subunit VI

Chain H:  54% 8% 38%



- Molecule 13: Photosystem I reaction center subunit VIII

Chain I:  64% 17% 19%



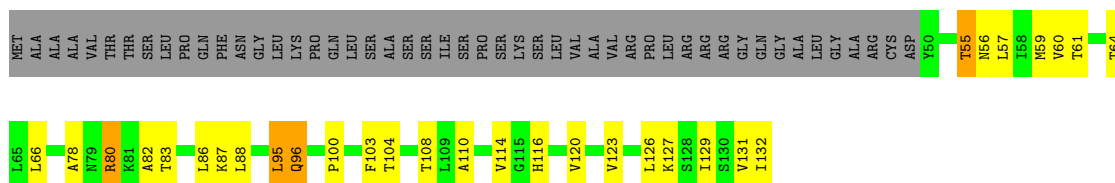
- Molecule 14: Photosystem I reaction center subunit IX

Chain J:  66% 25% 9%



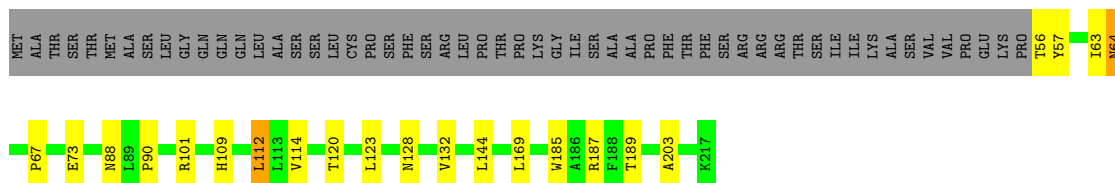
- Molecule 15: Photosystem I reaction center subunit psaK

Chain K:  39% 20% 37%




- Molecule 16: Photosystem I reaction center subunit XI

Chain L:  65% 9% 25%



- Molecule 17: Photosystem I reaction center subunit N

Chain N:  35% 11% 51%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157342	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k 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: BCR, XAT, CLA, LMG, LMT, PQN, CHL, HTG, LUT, DGD, SF4, LHG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.26	0/1610	0.45	0/2195
2	2	0.34	0/1687	0.52	1/2313 (0.0%)
3	3	0.31	0/1791	0.47	1/2435 (0.0%)
4	4	0.27	0/1621	0.43	0/2215
5	A	0.26	0/6029	0.44	0/8223
6	B	0.26	0/6066	0.45	0/8285
7	C	0.25	0/628	0.50	0/852
8	D	0.27	0/1143	0.52	0/1546
9	E	0.27	0/522	0.51	0/710
10	F	0.27	0/1246	0.49	0/1681
11	G	0.52	0/788	0.49	0/1070
12	H	0.26	0/701	0.45	0/955
13	I	0.27	0/227	0.44	0/310
14	J	0.26	0/327	0.51	0/446
15	K	0.27	0/596	0.54	0/809
16	L	0.27	0/1263	0.45	0/1731
17	N	0.38	0/701	0.48	0/942
18	O	0.29	0/733	0.50	0/1001
All	All	0.28	0/27679	0.47	2/37719 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	3	226	LYS	CD-CE-NZ	-5.68	98.64	111.70
2	2	74	ASP	CB-CG-OD2	5.14	122.92	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	1	1559	0	1536	38	0
2	2	1626	0	1570	37	0
3	3	1727	0	1651	36	0
4	4	1568	0	1517	36	0
5	A	5831	0	5683	94	0
6	B	5854	0	5635	69	0
7	C	615	0	600	3	0
8	D	1116	0	1122	13	0
9	E	511	0	510	6	0
10	F	1216	0	1245	37	0
11	G	768	0	740	7	0
12	H	681	0	671	7	0
13	I	221	0	237	3	0
14	J	318	0	331	9	0
15	K	588	0	619	21	0
16	L	1225	0	1240	15	0
17	N	686	0	664	18	0
18	O	705	0	686	19	0
19	1	100	0	72	6	0
19	2	238	0	169	23	0
19	3	47	0	30	3	0
19	4	198	0	143	12	0
20	1	744	0	720	32	0
20	2	485	0	445	21	0
20	3	633	0	499	24	0
20	4	593	0	524	35	0
20	A	2610	0	2708	132	0
20	B	2361	0	2424	96	0
20	F	156	0	138	7	0
20	G	141	0	105	0	0
20	H	56	0	51	3	0
20	J	107	0	103	2	0
20	K	197	0	158	8	0
20	L	206	0	177	8	0
20	N	95	0	69	2	0
20	O	157	0	135	16	0
21	1	84	0	112	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
21	2	42	0	56	2	0
21	3	42	0	56	4	0
21	4	42	0	56	5	0
21	O	84	0	112	8	0
22	1	44	0	56	2	0
22	2	44	0	56	2	0
22	3	44	0	56	6	0
22	4	44	0	56	8	0
23	1	40	0	56	4	0
23	2	40	0	56	6	0
23	3	40	0	56	4	0
23	4	40	0	56	5	0
23	A	240	0	336	18	0
23	B	240	0	336	22	0
23	F	80	0	112	7	0
23	G	40	0	56	3	0
23	I	40	0	56	6	0
23	J	80	0	112	10	0
23	K	40	0	56	4	0
23	L	120	0	168	9	0
24	1	49	0	74	7	0
24	2	37	0	44	1	0
24	A	76	0	98	3	0
24	B	23	0	16	2	0
25	1	93	0	132	6	0
25	4	44	0	61	4	0
26	1	19	0	26	2	0
26	4	19	0	26	0	0
26	A	19	0	26	0	0
26	B	38	0	52	1	0
26	F	38	0	52	1	0
26	G	19	0	26	0	0
26	J	19	0	26	0	0
26	N	19	0	26	1	0
27	A	33	0	46	3	0
27	B	33	0	46	1	0
28	A	8	0	0	0	0
28	C	16	0	0	0	0
29	B	35	0	46	0	0
29	G	35	0	46	0	0
30	B	66	0	96	2	0
All	All	38187	0	37964	787	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (787) 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)
10:F:217:ILE:HG13	20:F:802:CLA:O1A	1.45	1.16
20:1:309:CLA:HAB	21:1:315:LUT:H32	1.42	0.98
19:2:306:CHL:HMB1	19:2:306:CHL:HBB1	1.49	0.93
20:3:309:CLA:HBC2	20:3:309:CLA:HHD	1.50	0.93
19:2:307:CHL:HBB1	19:2:307:CHL:HMB1	1.51	0.93
20:B:831:CLA:HBB1	23:F:801:BCR:HC8	1.53	0.91
20:O:202:CLA:HHC	20:O:202:CLA:HBB1	1.53	0.90
1:1:156:GLN:HA	1:1:159:LEU:HD12	1.53	0.89
19:4:305:CHL:O1A	23:4:318:BCR:H21C	1.75	0.87
20:3:308:CLA:HAB	21:3:315:LUT:H32	1.58	0.86
3:3:105:THR:HG22	19:3:306:CHL:CED	2.10	0.81
10:F:217:ILE:CG1	20:F:802:CLA:O1A	2.27	0.81
20:3:309:CLA:HBC2	20:3:309:CLA:CHD	2.08	0.79
20:4:303:CLA:HMD2	20:4:308:CLA:CHD	2.13	0.78
20:B:823:CLA:HAB	20:B:830:CLA:HMD2	1.63	0.78
20:1:303:CLA:HHC	20:1:303:CLA:HBB1	1.67	0.76
5:A:371:MET:HE1	20:A:826:CLA:HHC	1.67	0.76
20:O:202:CLA:HBC3	20:O:202:CLA:HHD	1.68	0.75
20:4:309:CLA:HAB	21:4:316:LUT:H32	1.68	0.75
20:A:821:CLA:H12	20:K:205:CLA:HMB2	1.67	0.75
20:B:831:CLA:HAB	20:B:832:CLA:HMB2	1.68	0.74
23:A:849:BCR:H362	20:A:851:CLA:H42	1.70	0.73
6:B:106:ARG:HH11	6:B:115:ILE:HG12	1.54	0.72
20:B:827:CLA:HHC	20:B:827:CLA:HBB1	1.72	0.72
18:O:94:PHE:HA	18:O:97:ILE:HD12	1.72	0.72
23:2:317:BCR:HC42	25:4:319:LMG:H301	1.71	0.72
19:2:305:CHL:O1D	19:2:305:CHL:H2A	1.90	0.71
4:4:95:SER:HB2	4:4:204:GLY:HA3	1.73	0.71
2:2:64:PHE:CE1	19:2:301:CHL:HED2	2.25	0.71
20:B:825:CLA:HMA1	23:B:845:BCR:H14C	1.71	0.71
19:2:306:CHL:H2A	19:2:306:CHL:HED2	1.73	0.71
17:N:134:GLN:O	17:N:138:LYS:NZ	2.24	0.70
20:A:806:CLA:H62	20:A:808:CLA:H61	1.72	0.70
20:A:810:CLA:H202	23:J:102:BCR:H24C	1.74	0.69
5:A:706:LEU:HD23	10:F:217:ILE:CD1	2.22	0.69
20:4:303:CLA:HMD2	20:4:308:CLA:C1D	2.22	0.69
19:4:305:CHL:CGA	23:4:318:BCR:H21C	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:411:MET:HE2	23:B:844:BCR:H271	1.75	0.69
20:4:312:CLA:H92	20:4:312:CLA:HMC2	1.75	0.69
5:A:214:GLN:HA	5:A:218:SER:HB2	1.72	0.69
20:3:309:CLA:HHC	20:3:309:CLA:HBB1	1.74	0.68
1:1:99:VAL:HG11	21:1:315:LUT:H12	1.76	0.68
20:K:201:CLA:HHC	20:K:201:CLA:HBB1	1.75	0.68
5:A:175:TRP:HB2	20:A:810:CLA:HMC3	1.76	0.68
2:2:112:GLY:O	2:2:116:ILE:HG13	1.94	0.67
20:H:201:CLA:HMB2	20:L:302:CLA:HAA1	1.77	0.67
3:3:259:ASP:O	3:3:263:ASN:ND2	2.27	0.67
2:2:112:GLY:HA2	22:2:316:XAT:H181	1.78	0.66
20:A:831:CLA:H43	20:L:303:CLA:H43	1.77	0.66
5:A:657:ILE:HD12	6:B:621:ARG:HG3	1.76	0.66
5:A:508:GLY:HA2	5:A:523:PRO:HB3	1.79	0.65
14:J:31:ARG:HD3	23:J:102:BCR:H312	1.79	0.65
2:2:122:LEU:HD22	2:2:127:ILE:HD12	1.79	0.65
5:A:230:ASP:OD1	17:N:105:ARG:NH2	2.30	0.65
1:1:91:HIS:HB3	1:1:200:MET:HE3	1.78	0.64
5:A:706:LEU:CD2	10:F:217:ILE:CD1	2.75	0.64
2:2:156:ILE:HG21	20:2:308:CLA:HMC3	1.78	0.64
6:B:463:ILE:HD11	20:B:835:CLA:H2	1.79	0.64
20:O:203:CLA:H3A	20:O:203:CLA:H11	1.79	0.64
19:2:305:CHL:HAB	19:2:306:CHL:HMC	1.79	0.63
5:A:57:ASP:OD2	5:A:347:HIS:NE2	2.30	0.63
9:E:113:VAL:HG12	9:E:114:THR:HG23	1.80	0.63
20:H:201:CLA:HBB2	23:L:306:BCR:H311	1.80	0.63
16:L:88:ASN:HB3	20:L:302:CLA:HAC1	1.81	0.62
6:B:340:SER:HB3	20:B:824:CLA:H42	1.82	0.62
20:B:828:CLA:HHC	20:B:828:CLA:HBB1	1.82	0.62
5:A:583:GLN:HA	5:A:588:ASP:OD2	1.98	0.62
5:A:403:ALA:HB2	23:A:848:BCR:H323	1.82	0.62
20:B:801:CLA:H122	23:B:846:BCR:H12C	1.82	0.61
20:B:801:CLA:HBB1	20:B:801:CLA:HMB1	1.82	0.61
6:B:492:ILE:HD11	11:G:140:TYR:CE1	2.35	0.61
23:B:841:BCR:H372	23:G:606:BCR:HC42	1.82	0.61
5:A:166:PHE:O	5:A:170:MET:HG2	2.00	0.61
20:B:805:CLA:H92	20:B:813:CLA:H2	1.83	0.61
20:A:820:CLA:H12	20:A:823:CLA:HBA2	1.81	0.61
8:D:93:GLU:O	8:D:123:ARG:NH1	2.33	0.61
16:L:109:HIS:HA	16:L:112:LEU:HD23	1.82	0.61
8:D:89:GLU:HA	8:D:102:MET:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:69:ALA:HB2	6:B:135:LEU:HB2	1.82	0.60
1:1:150:ILE:HG21	20:1:308:CLA:HMC3	1.84	0.59
3:3:52:ARG:NH1	3:3:72:ASP:OD2	2.34	0.59
10:F:128:LEU:HD21	14:J:38:THR:HG21	1.83	0.59
5:A:283:THR:HG22	5:A:285:GLY:H	1.67	0.59
20:A:853:CLA:H91	10:F:197:ILE:HD11	1.85	0.59
20:B:815:CLA:H93	23:B:841:BCR:H23C	1.85	0.59
20:A:841:CLA:H143	23:L:301:BCR:H17C	1.84	0.59
4:4:165:ASP:HB3	19:4:315:CHL:C4C	2.33	0.59
5:A:706:LEU:HD23	10:F:217:ILE:HD13	1.85	0.59
20:B:805:CLA:H112	20:B:805:CLA:HBD	1.85	0.58
3:3:226:LYS:HE3	20:3:309:CLA:O1D	2.03	0.58
1:1:212:ALA:HB1	1:1:237:ILE:HD13	1.84	0.58
20:B:806:CLA:H151	20:B:828:CLA:HBB2	1.85	0.58
6:B:301:ILE:HG21	20:B:824:CLA:HAC1	1.85	0.58
12:H:115:LEU:HD21	13:I:16:LEU:HD13	1.85	0.58
2:2:64:PHE:HE1	19:2:301:CHL:HED2	1.67	0.58
20:1:311:CLA:HBB1	20:1:311:CLA:HMB1	1.86	0.58
5:A:561:ILE:HD11	5:A:581:THR:HG21	1.84	0.58
1:1:196:GLY:O	1:1:200:MET:HG3	2.03	0.58
15:K:100:PRO:HG2	20:K:201:CLA:HBC2	1.85	0.58
19:1:301:CHL:HBB1	20:1:302:CLA:HMD2	1.85	0.58
20:A:851:CLA:H11	6:B:616:LEU:HD12	1.84	0.58
4:4:101:GLY:O	4:4:105:MET:HG3	2.04	0.57
6:B:389:HIS:HA	6:B:392:ILE:HD12	1.86	0.57
20:A:828:CLA:HBB1	20:A:828:CLA:HMB1	1.86	0.57
6:B:527:LEU:O	6:B:531:THR:HG23	2.04	0.57
20:B:819:CLA:H203	20:B:824:CLA:H141	1.85	0.57
10:F:76:LYS:NZ	10:F:124:GLY:O	2.36	0.57
20:A:836:CLA:HBB1	20:A:836:CLA:HMB1	1.85	0.57
24:1:318:LHG:HC81	23:4:318:BCR:HC21	1.86	0.57
19:4:306:CHL:HBB1	22:4:317:XAT:H161	1.85	0.57
5:A:151:THR:H	5:A:155:GLN:HE22	1.52	0.57
5:A:211:ALA:O	5:A:215:VAL:HG13	2.04	0.57
8:D:137:VAL:HG22	8:D:143:VAL:HG22	1.85	0.57
20:1:310:CLA:C1D	20:1:311:CLA:HMD2	2.34	0.57
20:3:304:CLA:HMB1	20:3:304:CLA:HBB1	1.86	0.57
5:A:438:LEU:HD22	20:A:838:CLA:HBB1	1.85	0.57
20:A:806:CLA:HBB1	20:A:806:CLA:HMB1	1.86	0.57
2:2:62:LEU:HD11	2:2:69:PRO:HD3	1.87	0.56
20:4:303:CLA:HMD2	20:4:308:CLA:C4C	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:4:303:CLA:H12	10:F:205:VAL:HG13	1.87	0.56
5:A:118:ILE:HD13	23:J:102:BCR:H313	1.87	0.56
5:A:688:GLY:HA3	6:B:568:CYS:HB2	1.86	0.56
20:B:822:CLA:HBA1	20:B:822:CLA:HBD	1.87	0.56
13:I:26:LEU:O	13:I:30:VAL:HG22	2.05	0.56
19:2:301:CHL:HHD	23:3:317:BCR:HC31	1.86	0.56
20:B:828:CLA:H193	23:B:843:BCR:H17C	1.86	0.56
21:1:319:LUT:H392	20:4:308:CLA:H2	1.88	0.56
4:4:105:MET:HE2	22:4:317:XAT:H8	1.88	0.56
5:A:379:THR:HG21	5:A:515:VAL:HB	1.87	0.56
1:1:110:LEU:HD11	1:1:130:LEU:HD23	1.88	0.56
2:2:64:PHE:O	2:2:67:SER:OG	2.21	0.56
20:A:801:CLA:HAB	20:B:802:CLA:NA	2.21	0.56
6:B:439:HIS:O	6:B:443:MET:HG2	2.05	0.56
20:A:825:CLA:H171	18:O:123:LEU:HD22	1.88	0.55
15:K:66:LEU:HD11	20:K:205:CLA:HAB	1.88	0.55
1:1:203:PHE:CD2	22:1:316:XAT:H14	2.41	0.55
3:3:105:THR:HG22	19:3:306:CHL:HED3	1.86	0.55
13:I:19:PRO:HG3	23:I:101:BCR:H12C	1.89	0.55
20:B:834:CLA:HMB1	20:B:834:CLA:HBB1	1.88	0.55
8:D:118:LEU:O	8:D:122:THR:HG23	2.07	0.55
20:A:803:CLA:H43	20:A:810:CLA:HMC2	1.88	0.55
6:B:410:ARG:O	6:B:414:HIS:ND1	2.37	0.55
4:4:204:GLY:O	4:4:208:MET:HG3	2.07	0.55
1:1:152:PHE:CE2	23:1:317:BCR:H10C	2.42	0.55
1:1:236:ASP:OD1	1:1:236:ASP:N	2.28	0.55
5:A:454:ILE:HG22	20:A:833:CLA:HBC2	1.88	0.55
20:3:307:CLA:CHB	20:3:314:CLA:HBB1	2.36	0.55
20:A:827:CLA:H171	23:J:104:BCR:H17C	1.88	0.55
20:B:812:CLA:H8	20:B:812:CLA:HBB1	1.89	0.55
20:1:313:CLA:HED1	4:4:136:THR:HG23	1.89	0.55
4:4:145:PHE:HA	4:4:148:VAL:HG22	1.89	0.55
20:A:820:CLA:HMB2	20:A:824:CLA:HMA3	1.89	0.55
20:A:841:CLA:H152	16:L:144:LEU:HD21	1.89	0.55
2:2:96:LYS:NZ	2:2:96:LYS:HB3	2.22	0.54
19:2:305:CHL:HHC	19:2:306:CHL:HMC	1.89	0.54
5:A:30:GLY:HA3	5:A:36:ILE:HG22	1.88	0.54
25:1:320:LMG:H192	25:1:320:LMG:H351	1.89	0.54
20:A:802:CLA:CGA	20:A:802:CLA:H3A	2.37	0.54
6:B:268:LEU:HD23	20:B:817:CLA:HMA2	1.88	0.54
1:1:91:HIS:HB3	1:1:200:MET:CE	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:837:CLA:HBB1	20:A:837:CLA:HMB1	1.87	0.54
20:2:310:CLA:NC	24:2:318:LHG:HC42	2.22	0.54
20:3:301:CLA:HAB	22:3:316:XAT:H32	1.89	0.54
20:4:302:CLA:HBB1	20:4:302:CLA:HMB1	1.89	0.54
6:B:560:ASP:OD2	6:B:564:ARG:NH2	2.40	0.54
5:A:360:LEU:HD11	20:A:818:CLA:H71	1.90	0.54
6:B:542:ARG:NH2	8:D:176:ASN:OD1	2.34	0.54
20:B:822:CLA:HBC2	20:B:823:CLA:HBA2	1.90	0.54
26:B:850:HTG:H1'1	26:B:850:HTG:O2	2.04	0.54
1:1:55:ARG:HD3	1:1:59:LEU:O	2.08	0.54
1:1:86:GLU:HB2	1:1:167:LYS:HG2	1.89	0.54
1:1:229:PRO:O	1:1:233:ASN:ND2	2.34	0.54
5:A:598:TYR:OH	20:A:801:CLA:HED2	2.08	0.54
20:A:829:CLA:HBB1	20:A:829:CLA:HMB1	1.90	0.54
23:2:317:BCR:HC31	20:4:301:CLA:CHD	2.38	0.53
20:B:808:CLA:HMB2	20:B:808:CLA:H142	1.89	0.53
20:B:801:CLA:H171	20:B:810:CLA:HMC2	1.91	0.53
10:F:167:VAL:HG13	10:F:196:ILE:HG22	1.90	0.53
20:A:807:CLA:HMC3	20:A:808:CLA:HMD2	1.91	0.53
1:1:155:HIS:O	1:1:156:GLN:HG2	2.09	0.53
1:1:225:HIS:CG	20:1:312:CLA:HAA2	2.44	0.53
20:B:832:CLA:H51	23:F:801:BCR:H312	1.90	0.53
19:1:301:CHL:CBB	20:1:302:CLA:HMD2	2.38	0.53
24:1:318:LHG:H182	4:4:143:ILE:HG12	1.90	0.53
20:4:311:CLA:HBC1	20:4:312:CLA:H201	1.89	0.53
6:B:91:ILE:HB	6:B:112:PRO:HB2	1.91	0.53
18:O:124:GLY:O	18:O:128:THR:HG23	2.08	0.53
3:3:265:ILE:HG12	20:3:311:CLA:H43	1.91	0.53
20:3:307:CLA:HMB2	20:3:314:CLA:C4B	2.39	0.53
1:1:156:GLN:HG3	20:1:307:CLA:HMC3	1.90	0.53
20:2:310:CLA:C1D	20:2:311:CLA:HMD2	2.39	0.53
4:4:158:ASN:HB2	4:4:161:CYS:SG	2.48	0.52
6:B:276:HIS:HB2	20:B:817:CLA:C1B	2.39	0.52
10:F:206:ALA:O	10:F:210:GLU:HG3	2.08	0.52
4:4:165:ASP:HB3	19:4:315:CHL:NC	2.24	0.52
20:4:304:CLA:HMB1	20:4:304:CLA:HBB1	1.91	0.52
24:1:318:LHG:H291	24:1:318:LHG:HC91	1.92	0.52
18:O:87:ASN:ND2	18:O:88:SER:H	2.06	0.52
4:4:183:SER:OG	4:4:184:VAL:N	2.40	0.52
20:A:814:CLA:C3B	23:A:854:BCR:H333	2.40	0.52
6:B:279:ALA:HA	20:B:816:CLA:HMC3	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:2:232:TRP:O	2:2:236:VAL:HG23	2.09	0.52
5:A:529:ALA:O	5:A:533:VAL:HG22	2.10	0.52
3:3:60:GLN:O	3:3:63:SER:OG	2.27	0.52
4:4:171:TYR:CE1	19:4:315:CHL:HAA2	2.45	0.52
4:4:211:PHE:CD2	22:4:317:XAT:H14	2.45	0.52
14:J:31:ARG:NH2	20:J:103:CLA:O1D	2.42	0.52
5:A:389:THR:HG23	5:A:605:ILE:HG21	1.92	0.52
1:1:141:THR:O	1:1:145:ILE:HG13	2.10	0.52
20:4:303:CLA:H42	10:F:208:TYR:CD1	2.45	0.52
1:1:168:TYR:CZ	1:1:189:LYS:HD3	2.45	0.52
3:3:235:MET:CE	22:3:316:XAT:H10	2.40	0.52
5:A:231:PRO:HD2	17:N:105:ARG:HH21	1.75	0.52
20:A:801:CLA:HAB	20:B:802:CLA:C1A	2.40	0.52
5:A:294:HIS:HB2	20:A:817:CLA:C1B	2.40	0.51
20:H:201:CLA:O1A	20:H:201:CLA:H3A	2.10	0.51
14:J:12:PRO:HB2	23:J:102:BCR:H401	1.92	0.51
16:L:90:PRO:O	16:L:101:ARG:HD2	2.11	0.51
1:1:187:GLU:O	1:1:191:LYS:HG3	2.09	0.51
2:2:158:TRP:CH2	23:2:317:BCR:HC8	2.45	0.51
3:3:64:TYR:OH	3:3:76:ASP:OD1	2.22	0.51
20:3:309:CLA:CHD	20:3:309:CLA:CBC	2.86	0.51
6:B:546:LEU:O	6:B:564:ARG:NH1	2.44	0.51
20:A:853:CLA:H42	14:J:15:SER:HA	1.93	0.51
17:N:142:VAL:HG21	17:N:145:LEU:HD12	1.92	0.51
17:N:148:ASP:O	17:N:152:GLU:HB2	2.10	0.51
2:2:108:TRP:CE2	19:2:307:CHL:HED2	2.46	0.51
19:2:306:CHL:CED	19:2:306:CHL:HAA1	2.40	0.51
5:A:77:GLN:HE21	20:A:804:CLA:HMA1	1.76	0.51
18:O:76:LEU:O	18:O:80:SER:OG	2.21	0.51
19:2:301:CHL:H42	3:3:160:GLY:HA2	1.91	0.51
6:B:561:GLY:O	6:B:567:THR:OG1	2.29	0.51
15:K:66:LEU:CD2	15:K:114:VAL:HG13	2.40	0.51
20:B:834:CLA:HBB1	23:B:845:BCR:HC21	1.93	0.51
1:1:234:ILE:HD13	20:1:312:CLA:H42	1.92	0.51
5:A:283:THR:HG23	5:A:375:PRO:HA	1.93	0.51
16:L:185:TRP:O	16:L:189:THR:HG22	2.11	0.51
6:B:450:GLU:OE1	10:F:119:ARG:NH1	2.44	0.51
20:1:321:CLA:HBA1	24:B:849:LHG:HC42	1.93	0.50
4:4:165:ASP:HB3	19:4:315:CHL:C1C	2.42	0.50
20:A:805:CLA:H151	20:A:828:CLA:HBB2	1.94	0.50
20:B:821:CLA:HMD2	23:B:841:BCR:HC7	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:835:CLA:HMB1	20:B:835:CLA:HBB1	1.93	0.50
20:B:818:CLA:HBB2	20:B:824:CLA:H203	1.93	0.50
5:A:13:LEU:HB3	5:A:184:LYS:HG3	1.93	0.50
6:B:15:ASP:HB3	6:B:20:ARG:HB2	1.93	0.50
6:B:80:ASP:HB3	6:B:84:VAL:HG23	1.93	0.50
20:O:202:CLA:HBC3	20:O:202:CLA:CHD	2.39	0.50
1:1:85:LYS:O	1:1:89:VAL:HG23	2.12	0.50
2:2:110:MET:SD	20:2:309:CLA:HAB	2.51	0.50
19:2:305:CHL:CHC	19:2:306:CHL:HMC	2.41	0.50
3:3:251:GLN:NE2	3:3:255:ASP:OD1	2.45	0.50
8:D:75:GLN:HG2	12:H:70:GLN:HG3	1.94	0.50
14:J:10:VAL:HG13	14:J:12:PRO:HD2	1.93	0.50
2:2:181:ASN:ND2	2:2:182:ASN:OD1	2.45	0.50
5:A:484:ILE:HD13	20:A:834:CLA:HBB1	1.93	0.50
20:A:851:CLA:HMB1	20:A:851:CLA:HBB1	1.92	0.50
5:A:86:SER:HB2	5:A:163:ALA:HB3	1.93	0.50
5:A:582:CYS:HB3	6:B:667:TRP:HE3	1.77	0.50
20:A:825:CLA:H193	23:A:848:BCR:H382	1.92	0.50
23:B:841:BCR:H321	11:G:120:ALA:HB1	1.94	0.50
10:F:217:ILE:CD1	20:F:802:CLA:O1A	2.60	0.50
20:2:312:CLA:H92	20:2:312:CLA:HMC2	1.92	0.50
5:A:338:LEU:HD13	20:A:823:CLA:HMD3	1.94	0.50
5:A:356:MET:HG3	20:A:824:CLA:HHB	1.94	0.50
14:J:12:PRO:O	14:J:16:THR:HG22	2.12	0.50
5:A:680:PHE:HZ	20:A:840:CLA:HBC2	1.76	0.49
20:B:803:CLA:H143	23:B:846:BCR:H362	1.94	0.49
20:A:820:CLA:H2	20:A:824:CLA:HMB1	1.94	0.49
20:B:817:CLA:HAC2	20:B:824:CLA:H201	1.93	0.49
7:C:61:ASP:H	9:E:140:ASN:HD21	1.60	0.49
20:1:303:CLA:HBC1	20:1:308:CLA:HAC1	1.94	0.49
6:B:680:TRP:CE2	6:B:684:ARG:HG3	2.47	0.49
20:B:819:CLA:HMB2	20:B:824:CLA:HMA3	1.93	0.49
15:K:116:HIS:O	15:K:120:VAL:HG23	2.13	0.49
15:K:126:LEU:HB3	15:K:132:ILE:HG13	1.93	0.49
2:2:150:ILE:HG21	20:4:313:CLA:HED1	1.93	0.49
5:A:57:ASP:OD1	5:A:57:ASP:N	2.44	0.49
5:A:283:THR:HG22	5:A:285:GLY:N	2.27	0.49
20:A:804:CLA:H152	20:A:812:CLA:H51	1.95	0.49
20:A:816:CLA:CHD	20:A:817:CLA:HBB2	2.43	0.49
20:B:816:CLA:O1A	11:G:138:ASN:ND2	2.45	0.49
10:F:208:TYR:O	10:F:212:LEU:HD22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:2:306:CHL:HAA1	19:2:306:CHL:HED3	1.94	0.49
6:B:187:SER:O	6:B:191:THR:HG22	2.12	0.49
23:B:841:BCR:H362	23:G:606:BCR:H312	1.94	0.49
4:4:99:MET:SD	20:4:309:CLA:HMC3	2.53	0.49
23:A:845:BCR:H402	23:A:854:BCR:HC8	1.94	0.49
20:4:303:CLA:HMC2	22:4:317:XAT:C12	2.42	0.49
20:3:309:CLA:HBB1	20:3:309:CLA:CHC	2.37	0.49
5:A:72:SER:OG	5:A:178:TYR:HB2	2.12	0.49
5:A:217:VAL:HG13	5:A:237:PRO:HB3	1.95	0.49
20:B:808:CLA:O1A	20:B:827:CLA:HBD	2.13	0.49
6:B:93:ASP:OD1	6:B:95:HIS:ND1	2.33	0.49
25:1:320:LMG:H132	25:1:320:LMG:H301	1.95	0.48
25:1:320:LMG:H312	25:1:320:LMG:H152	1.94	0.48
2:2:97:TRP:CZ2	20:2:308:CLA:HAA2	2.48	0.48
1:1:120:ALA:HB3	19:1:306:CHL:HMD3	1.95	0.48
2:2:116:ILE:HG23	2:2:133:TRP:CG	2.49	0.48
5:A:438:LEU:HG	5:A:546:LEU:HB2	1.93	0.48
1:1:146:GLU:OE2	19:1:306:CHL:OMC	2.31	0.48
19:1:301:CHL:HED3	4:4:151:ARG:HD2	1.95	0.48
5:A:231:PRO:HD2	17:N:105:ARG:NH2	2.28	0.48
9:E:95:LYS:NZ	9:E:111:SER:OG	2.46	0.48
18:O:59:ASP:O	18:O:59:ASP:OD2	2.32	0.48
4:4:186:ASN:OD1	21:4:316:LUT:O23	2.22	0.48
4:4:238:HIS:O	4:4:243:ASN:ND2	2.46	0.48
6:B:410:ARG:HA	6:B:413:ASP:HB2	1.95	0.48
20:B:829:CLA:H161	20:B:839:CLA:HMA2	1.94	0.48
3:3:223:LYS:HD3	20:3:310:CLA:HBD	1.96	0.48
1:1:184:LYS:HA	1:1:187:GLU:HG2	1.95	0.48
4:4:89:GLN:O	4:4:93:VAL:HG22	2.14	0.48
5:A:151:THR:H	5:A:155:GLN:NE2	2.12	0.48
20:A:822:CLA:HBB1	18:O:131:PHE:CE2	2.48	0.48
6:B:340:SER:O	6:B:344:ILE:HG23	2.14	0.48
15:K:83:THR:N	15:K:86:LEU:O	2.47	0.48
3:3:101:PHE:O	3:3:105:THR:HG23	2.13	0.48
3:3:269:PHE:O	5:A:259:THR:OG1	2.23	0.48
6:B:174:ARG:HB2	20:B:813:CLA:HBC2	1.96	0.48
6:B:397:ASP:OD1	8:D:181:LYS:NZ	2.44	0.48
23:F:806:BCR:H11C	23:F:806:BCR:H341	1.70	0.48
3:3:105:THR:HG22	19:3:306:CHL:HED1	1.91	0.47
6:B:339:ALA:HB2	23:B:845:BCR:H372	1.95	0.47
6:B:344:ILE:HG21	20:B:824:CLA:H43	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:K:202:CLA:HBA1	20:K:202:CLA:HBD	1.96	0.47
16:L:114:VAL:HG21	16:L:203:ALA:HB3	1.95	0.47
20:1:304:CLA:H41	20:1:304:CLA:H61	1.54	0.47
20:4:304:CLA:CHA	20:4:304:CLA:HBA1	2.42	0.47
20:4:312:CLA:HBA1	20:4:312:CLA:HBD	1.95	0.47
20:A:853:CLA:O1D	10:F:185:GLU:HG2	2.14	0.47
20:B:801:CLA:OBD	20:B:802:CLA:HMB3	2.13	0.47
20:B:813:CLA:H112	20:B:813:CLA:H143	1.66	0.47
8:D:53:GLN:H	8:D:53:GLN:HG2	1.50	0.47
9:E:91:PRO:O	9:E:94:SER:OG	2.27	0.47
15:K:66:LEU:HD21	15:K:114:VAL:HG13	1.96	0.47
16:L:63:ILE:HA	16:L:73:GLU:HG3	1.96	0.47
20:1:303:CLA:HED2	20:1:303:CLA:H43	1.97	0.47
20:A:810:CLA:H122	20:J:101:CLA:HBB2	1.97	0.47
19:2:301:CHL:HMB1	19:2:301:CHL:HBB1	1.96	0.47
20:B:812:CLA:H51	20:B:812:CLA:H11	1.74	0.47
21:O:205:LUT:H191	21:O:205:LUT:H11	1.77	0.47
3:3:132:PRO:HD2	3:3:135:LYS:HE3	1.97	0.47
20:A:831:CLA:H111	20:A:831:CLA:H152	1.62	0.47
6:B:458:ILE:HG21	10:F:141:ASN:HD22	1.78	0.47
20:B:813:CLA:H151	20:B:828:CLA:HMD2	1.97	0.47
20:O:202:CLA:HBB1	20:O:202:CLA:CHC	2.33	0.47
20:1:307:CLA:H72	20:1:307:CLA:H112	1.75	0.47
19:4:306:CHL:HBA1	19:4:306:CHL:H3A	1.60	0.47
5:A:735:ILE:HG21	20:A:827:CLA:HMC2	1.96	0.47
20:B:825:CLA:HBA2	20:B:825:CLA:H3A	1.70	0.47
17:N:167:TRP:HA	17:N:167:TRP:CE3	2.49	0.47
5:A:118:ILE:HG13	5:A:119:VAL:HG13	1.96	0.47
20:B:805:CLA:H141	20:B:805:CLA:H162	1.68	0.47
20:B:810:CLA:H43	20:B:810:CLA:HED2	1.96	0.47
20:B:831:CLA:H202	20:F:802:CLA:HAB	1.96	0.47
16:L:123:LEU:HD12	16:L:132:VAL:HG11	1.96	0.47
20:3:307:CLA:HMB1	20:3:307:CLA:HBB1	1.97	0.47
5:A:305:ALA:HB2	20:A:820:CLA:HBC2	1.97	0.47
6:B:365:PHE:HB3	6:B:602:TRP:CZ3	2.49	0.47
20:1:313:CLA:CED	4:4:136:THR:HG23	2.45	0.47
19:2:301:CHL:HMD2	23:3:317:BCR:H323	1.97	0.47
5:A:133:ARG:HB2	17:N:113:PHE:CE2	2.50	0.47
5:A:693:GLN:NE2	5:A:716:ALA:H	2.12	0.47
23:A:849:BCR:H361	23:A:849:BCR:H20C	1.69	0.47
6:B:177:HIS:CG	20:B:813:CLA:HMC2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:188:LEU:HD21	23:B:841:BCR:H383	1.96	0.47
15:K:129:ILE:HG22	15:K:131:VAL:HG23	1.96	0.47
17:N:167:TRP:HA	17:N:167:TRP:HE3	1.79	0.47
20:2:310:CLA:CAB	23:3:317:BCR:H312	2.45	0.46
3:3:80:LEU:HD22	3:3:90:PHE:HE2	1.80	0.46
3:3:102:ASN:ND2	20:3:307:CLA:OBD	2.48	0.46
3:3:170:TYR:HD2	20:3:307:CLA:HMA2	1.80	0.46
4:4:235:ASP:OD2	4:4:238:HIS:ND1	2.38	0.46
5:A:224:PHE:O	5:A:229:VAL:HG13	2.15	0.46
20:A:801:CLA:HBB1	20:A:851:CLA:HED1	1.96	0.46
20:B:835:CLA:HMB2	20:B:837:CLA:HED1	1.96	0.46
5:A:583:GLN:HB3	5:A:588:ASP:HB3	1.97	0.46
20:B:818:CLA:H3A	20:B:818:CLA:HBA2	1.46	0.46
20:B:827:CLA:H3A	20:B:827:CLA:HBA2	1.50	0.46
15:K:104:THR:O	15:K:108:THR:HG23	2.15	0.46
20:4:303:CLA:CMD	20:4:308:CLA:C1D	2.93	0.46
20:A:831:CLA:H92	20:A:831:CLA:H61	1.72	0.46
6:B:733:PHE:HB3	12:H:142:ARG:HE	1.79	0.46
20:B:805:CLA:HBA1	20:B:805:CLA:H3A	1.36	0.46
20:B:806:CLA:H193	20:B:806:CLA:H161	1.67	0.46
20:O:203:CLA:H3A	20:O:203:CLA:HBA2	1.44	0.46
1:1:160:GLU:O	1:1:166:LYS:NZ	2.38	0.46
20:B:825:CLA:HAA2	20:B:826:CLA:OBD	2.16	0.46
9:E:96:VAL:HB	9:E:147:VAL:HG13	1.98	0.46
23:2:317:BCR:H11C	23:2:317:BCR:H341	1.76	0.46
5:A:118:ILE:HB	23:J:102:BCR:H322	1.96	0.46
20:A:811:CLA:HHC	20:A:811:CLA:HBB1	1.98	0.46
6:B:429:LEU:HB3	6:B:525:LEU:HB2	1.98	0.46
10:F:147:TRP:HZ2	20:F:805:CLA:HBA1	1.79	0.46
10:F:192:LEU:O	10:F:196:ILE:HG12	2.16	0.46
5:A:607:HIS:CE1	20:A:836:CLA:HBC3	2.51	0.46
20:A:803:CLA:HAB	20:A:810:CLA:H142	1.96	0.46
20:B:812:CLA:H3A	20:B:812:CLA:HBA2	1.54	0.46
4:4:243:ASN:OD1	4:4:243:ASN:N	2.49	0.46
5:A:582:CYS:HB2	6:B:667:TRP:HB3	1.96	0.46
1:1:197:ARG:HG2	20:1:302:CLA:C3C	2.45	0.46
19:2:301:CHL:HAB	19:2:301:CHL:HHC	1.82	0.46
3:3:78:LEU:HD23	20:A:811:CLA:H2	1.98	0.46
20:3:313:CLA:HHC	20:3:313:CLA:HBB1	1.97	0.46
4:4:125:ALA:O	4:4:130:TYR:OH	2.29	0.46
6:B:326:ILE:HD12	20:B:824:CLA:HMC2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:O:201:CLA:H11	20:O:201:CLA:H52	1.78	0.46
4:4:188:LEU:HD12	21:4:316:LUT:H222	1.97	0.46
6:B:569:ASP:HA	6:B:574:ASP:OD2	2.16	0.46
20:L:303:CLA:H72	20:L:303:CLA:H112	1.59	0.46
18:O:115:TRP:O	18:O:119:VAL:HG23	2.16	0.46
20:O:202:CLA:HHC	20:O:202:CLA:CBB	2.37	0.46
20:4:301:CLA:HMB2	25:4:319:LMG:H182	1.97	0.46
20:A:806:CLA:H202	20:A:806:CLA:H162	1.76	0.46
23:B:845:BCR:H341	23:B:845:BCR:H11C	1.80	0.46
10:F:203:TRP:CD1	10:F:204:PRO:HD3	2.51	0.46
5:A:653:ALA:O	5:A:657:ILE:HG12	2.15	0.45
20:4:308:CLA:HBB	20:4:314:CLA:HBC2	1.98	0.45
5:A:435:ILE:HG13	5:A:554:PHE:HE2	1.81	0.45
23:A:849:BCR:H24C	23:A:849:BCR:H371	1.76	0.45
20:B:818:CLA:H112	20:B:818:CLA:H71	1.59	0.45
21:1:315:LUT:H35	21:1:315:LUT:H401	1.76	0.45
3:3:110:VAL:HG11	21:3:315:LUT:H10	1.98	0.45
5:A:339:TYR:O	5:A:343:THR:OG1	2.28	0.45
20:A:823:CLA:HBB2	24:A:844:LHG:H101	1.98	0.45
20:A:827:CLA:HBA1	20:A:827:CLA:HBD	1.97	0.45
6:B:401:GLU:OE1	6:B:401:GLU:N	2.45	0.45
20:B:828:CLA:H3A	20:B:828:CLA:HBA2	1.59	0.45
23:B:841:BCR:HC8	11:G:124:ILE:HD11	1.98	0.45
11:G:106:LYS:O	11:G:106:LYS:HD3	2.16	0.45
4:4:155:ASP:OD1	19:4:307:CHL:HBC1	2.16	0.45
5:A:88:MET:HE1	20:A:807:CLA:HMA2	1.98	0.45
23:A:854:BCR:H351	23:A:854:BCR:H15C	1.69	0.45
20:A:811:CLA:H62	20:A:811:CLA:H41	1.90	0.45
20:B:817:CLA:H202	20:B:817:CLA:H162	1.77	0.45
12:H:73:VAL:HG13	16:L:169:LEU:HD11	1.98	0.45
15:K:56:ASN:ND2	20:K:203:CLA:OBD	2.43	0.45
18:O:118:MET:SD	20:O:202:CLA:O2A	2.75	0.45
23:2:317:BCR:HC42	25:4:319:LMG:H321	1.98	0.45
20:A:823:CLA:HMA1	20:O:201:CLA:HBB2	1.98	0.45
20:A:837:CLA:H202	20:L:303:CLA:H102	1.99	0.45
20:A:839:CLA:H2A	20:A:839:CLA:HED3	1.98	0.45
6:B:160:LYS:HE3	6:B:160:LYS:HB2	1.63	0.45
20:B:832:CLA:H91	20:B:832:CLA:H111	1.72	0.45
15:K:82:ALA:HB2	15:K:88:LEU:HD23	1.97	0.45
21:O:205:LUT:H201	21:O:205:LUT:H15	1.79	0.45
20:1:304:CLA:HMB3	22:1:316:XAT:H162	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:3:121:LYS:HB2	3:3:121:LYS:HE2	1.73	0.45
20:3:309:CLA:HHC	20:3:309:CLA:CBB	2.42	0.45
23:4:318:BCR:H11C	23:4:318:BCR:H341	1.82	0.45
5:A:56:PHE:CD2	20:A:804:CLA:HMC2	2.52	0.45
5:A:201:GLY:O	5:A:205:LEU:HB2	2.16	0.45
5:A:599:ASN:O	5:A:603:VAL:HG23	2.17	0.45
10:F:85:GLU:HB2	10:F:120:PHE:CD2	2.52	0.45
1:1:241:ARG:HA	1:1:241:ARG:HD2	1.77	0.45
5:A:194:MET:HE2	20:A:812:CLA:HBC2	1.97	0.45
5:A:346:TRP:HB3	20:A:804:CLA:HAC1	1.99	0.45
20:A:826:CLA:H61	20:A:826:CLA:H2	1.72	0.45
20:B:829:CLA:HBB1	20:B:829:CLA:HMB1	1.98	0.45
20:B:831:CLA:HBB2	23:F:801:BCR:HC41	1.97	0.45
17:N:167:TRP:CE3	17:N:167:TRP:O	2.70	0.45
23:2:317:BCR:H24C	23:2:317:BCR:H371	1.80	0.45
5:A:393:TRP:HB3	20:A:827:CLA:HMC3	1.99	0.45
20:A:853:CLA:H93	20:A:853:CLA:H61	1.77	0.45
10:F:83:LYS:NZ	10:F:83:LYS:HB2	2.32	0.45
23:J:102:BCR:H15C	23:J:102:BCR:H351	1.76	0.45
5:A:414:TYR:CE2	5:A:416:PRO:HD3	2.52	0.44
20:1:303:CLA:HMD2	20:1:308:CLA:C1D	2.47	0.44
3:3:88:PHE:O	3:3:91:GLN:NE2	2.47	0.44
5:A:314:GLY:HA3	15:K:78:ALA:HA	1.99	0.44
15:K:60:VAL:O	15:K:64:THR:HG23	2.18	0.44
21:O:204:LUT:H15	21:O:204:LUT:H201	1.81	0.44
20:1:303:CLA:HMA2	20:1:303:CLA:H11	2.00	0.44
20:4:301:CLA:H3A	20:4:301:CLA:HBA2	1.76	0.44
20:4:312:CLA:O1A	20:4:313:CLA:C2D	2.65	0.44
20:A:821:CLA:HBA2	20:A:821:CLA:H3A	1.25	0.44
20:A:823:CLA:H12	20:A:838:CLA:H142	1.99	0.44
20:A:825:CLA:HBA2	20:A:825:CLA:H3A	1.77	0.44
21:O:205:LUT:H31	21:O:205:LUT:H391	1.70	0.44
21:O:205:LUT:H361	21:O:205:LUT:H28	2.00	0.44
1:1:150:ILE:HA	1:1:153:VAL:HG22	1.99	0.44
3:3:207:PRO:HD2	21:3:315:LUT:H23	1.99	0.44
4:4:72:PHE:HE2	22:4:317:XAT:H383	1.82	0.44
9:E:140:ASN:HB3	9:E:142:TYR:CE1	2.52	0.44
10:F:209:ARG:O	10:F:213:ASN:ND2	2.50	0.44
15:K:55:THR:O	15:K:59:MET:HG2	2.16	0.44
16:L:64:ASN:O	16:L:64:ASN:ND2	2.51	0.44
17:N:156:LYS:HB2	17:N:156:LYS:HE2	1.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:204:LUT:H35	21:O:204:LUT:H401	1.80	0.44
2:2:209:LYS:O	2:2:212:GLU:HG3	2.17	0.44
2:2:234:GLN:O	2:2:238:THR:OG1	2.22	0.44
20:A:805:CLA:H43	24:A:843:LHG:H261	1.99	0.44
20:A:818:CLA:H141	20:A:826:CLA:H193	2.00	0.44
27:A:842:PQN:H141	27:A:842:PQN:H161	1.59	0.44
6:B:645:VAL:HG11	20:B:809:CLA:HMD2	1.99	0.44
23:B:844:BCR:H11C	23:B:844:BCR:H341	1.81	0.44
23:L:301:BCR:H24C	23:L:301:BCR:H371	1.81	0.44
18:O:87:ASN:HD22	18:O:88:SER:H	1.66	0.44
1:1:123:PRO:O	25:1:323:LMG:O3	2.26	0.44
24:1:318:LHG:H321	20:4:314:CLA:HED1	2.00	0.44
5:A:259:THR:O	5:A:263:THR:OG1	2.27	0.44
20:A:808:CLA:H62	20:A:808:CLA:H92	1.84	0.44
20:B:802:CLA:H102	20:B:802:CLA:H62	1.82	0.44
20:B:807:CLA:H62	20:B:807:CLA:H2	1.77	0.44
1:1:152:PHE:CE2	23:1:317:BCR:H12C	2.53	0.44
20:4:302:CLA:H72	22:4:317:XAT:H28	1.99	0.44
20:A:807:CLA:H3A	20:A:807:CLA:HBA2	1.31	0.44
6:B:608:GLN:O	6:B:612:SER:HB2	2.17	0.44
20:1:312:CLA:H91	20:1:312:CLA:H112	1.67	0.44
20:A:803:CLA:HBA1	20:A:803:CLA:H3A	1.57	0.44
6:B:351:HIS:ND1	20:B:817:CLA:OBD	2.48	0.44
6:B:458:ILE:HG21	10:F:141:ASN:ND2	2.32	0.44
18:O:79:SER:OG	18:O:90:THR:CG2	2.66	0.44
5:A:360:LEU:HB2	20:A:826:CLA:H41	2.00	0.44
5:A:578:ARG:NH2	8:D:115:GLU:OE1	2.47	0.44
20:A:825:CLA:H191	23:A:848:BCR:H393	2.00	0.44
10:F:102:GLU:O	17:N:144:PHE:HZ	2.01	0.44
20:K:202:CLA:H93	20:K:202:CLA:H111	1.87	0.44
20:1:321:CLA:HBC1	26:1:322:HTG:H5	2.00	0.43
20:4:302:CLA:HAB	22:4:317:XAT:H32	2.00	0.43
20:A:853:CLA:HED3	10:F:185:GLU:HA	1.99	0.43
20:B:805:CLA:H122	20:B:813:CLA:HBD	1.99	0.43
20:1:312:CLA:H152	24:1:318:LHG:H132	1.99	0.43
20:2:312:CLA:CHB	20:2:313:CLA:HMD3	2.48	0.43
5:A:335:HIS:HB3	5:A:338:LEU:HD12	2.00	0.43
20:A:806:CLA:H72	20:A:806:CLA:H112	1.73	0.43
7:C:2:SER:N	7:C:71:HIS:O	2.50	0.43
20:3:311:CLA:CHB	21:3:315:LUT:H42	2.49	0.43
5:A:290:ASP:HB3	20:A:817:CLA:HMA1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:A:842:PQN:H292	27:A:842:PQN:H261	1.83	0.43
20:B:808:CLA:H122	20:B:827:CLA:H13	1.99	0.43
20:N:203:CLA:H2A	20:N:203:CLA:HED2	2.01	0.43
1:1:152:PHE:CZ	23:1:317:BCR:H10C	2.53	0.43
20:B:803:CLA:CGA	20:B:803:CLA:H3A	2.48	0.43
20:B:833:CLA:H72	20:B:833:CLA:H112	1.93	0.43
20:2:310:CLA:HBD	20:2:311:CLA:OBD	2.18	0.43
5:A:407:ALA:HB1	5:A:586:ALA:HB1	2.01	0.43
20:A:821:CLA:O1A	20:K:205:CLA:HHB	2.18	0.43
20:A:827:CLA:HBA1	20:A:827:CLA:H12	1.67	0.43
23:I:101:BCR:H11C	23:I:101:BCR:H341	1.79	0.43
23:I:101:BCR:H20C	23:I:101:BCR:H361	1.85	0.43
18:O:104:PHE:CG	18:O:105:PRO:HA	2.54	0.43
19:1:306:CHL:H3A	19:1:306:CHL:HBA2	1.56	0.43
2:2:185:THR:HG23	2:2:194:GLY:HA2	2.00	0.43
19:4:305:CHL:CGA	23:4:318:BCR:H19C	2.48	0.43
5:A:286:LEU:HD21	5:A:371:MET:HB3	1.99	0.43
23:A:849:BCR:H15C	23:A:849:BCR:H351	1.85	0.43
6:B:435:GLY:HA3	20:B:832:CLA:HAB	2.00	0.43
6:B:714:SER:HB2	30:B:848:DGD:HBF1	2.00	0.43
14:J:25:LEU:O	14:J:29:ILE:HG13	2.19	0.43
17:N:119:VAL:HG23	26:N:201:HTG:O4	2.19	0.43
20:A:825:CLA:HAA2	20:A:826:CLA:OBD	2.19	0.43
21:O:205:LUT:H35	21:O:205:LUT:H401	1.71	0.43
24:1:318:LHG:O3	24:1:318:LHG:O1	2.24	0.43
20:3:307:CLA:HBA2	20:3:307:CLA:H3A	1.35	0.43
20:A:809:CLA:HAB	20:A:812:CLA:H111	2.01	0.43
2:2:88:LEU:HD13	20:2:302:CLA:H42	2.00	0.43
2:2:227:ALA:HA	20:2:312:CLA:HBB1	2.01	0.43
3:3:159:LEU:HD22	20:3:307:CLA:HBB2	2.01	0.43
3:3:235:MET:HE2	22:3:316:XAT:H10	1.99	0.43
21:4:316:LUT:H31	21:4:316:LUT:H391	1.93	0.43
5:A:433:ALA:O	5:A:437:HIS:ND1	2.49	0.43
5:A:719:ILE:HG12	6:B:568:CYS:SG	2.59	0.43
20:A:805:CLA:H61	20:A:805:CLA:H92	1.72	0.43
20:A:817:CLA:H141	20:A:817:CLA:H162	1.76	0.43
20:B:823:CLA:HBD	20:B:823:CLA:HBA1	2.01	0.43
10:F:203:TRP:CG	10:F:204:PRO:HD3	2.54	0.43
23:L:306:BCR:H351	23:L:306:BCR:H15C	1.77	0.43
1:1:185:PHE:CZ	20:1:309:CLA:HED3	2.54	0.43
20:1:307:CLA:H2	21:1:315:LUT:H383	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:1:313:CLA:HAA1	4:4:140:ILE:HG12	2.00	0.43
5:A:519:VAL:HG11	5:A:522:LEU:HD23	2.00	0.43
5:A:706:LEU:HD21	10:F:217:ILE:CD1	2.49	0.43
20:A:823:CLA:HBB	20:O:201:CLA:CBB	2.48	0.43
23:B:841:BCR:H15C	23:B:841:BCR:H351	1.70	0.43
23:B:845:BCR:H351	23:B:845:BCR:H15C	1.67	0.43
10:F:70:SER:O	10:F:70:SER:OG	2.25	0.43
20:L:302:CLA:CHA	20:L:302:CLA:HBA1	2.49	0.43
20:A:833:CLA:H62	20:A:833:CLA:H2	1.79	0.42
23:A:854:BCR:C11	23:K:204:BCR:H333	2.49	0.42
10:F:163:TRP:O	10:F:167:VAL:HG23	2.18	0.42
12:H:72:ASP:OD1	12:H:75:GLY:HA3	2.19	0.42
17:N:99:GLU:HG2	17:N:103:LYS:HZ3	1.84	0.42
21:1:319:LUT:H35	21:1:319:LUT:H401	1.85	0.42
20:3:311:CLA:H61	20:3:311:CLA:H2	1.84	0.42
20:A:817:CLA:H3A	20:A:817:CLA:HBA2	1.61	0.42
20:A:831:CLA:H91	20:A:831:CLA:H112	1.72	0.42
6:B:583:MET:O	6:B:587:ILE:HG12	2.20	0.42
23:B:843:BCR:H24C	23:B:843:BCR:H371	1.66	0.42
23:B:846:BCR:H20C	23:B:846:BCR:H361	1.91	0.42
8:D:58:THR:HB	8:D:106:PRO:HB2	2.01	0.42
23:L:305:BCR:H15C	23:L:305:BCR:H351	1.78	0.42
17:N:167:TRP:CE3	17:N:167:TRP:CA	3.02	0.42
2:2:225:MET:HE3	20:2:302:CLA:HMC3	2.00	0.42
19:4:315:CHL:HHC	19:4:315:CHL:HBB1	1.99	0.42
5:A:462:LEU:HG	20:B:809:CLA:HMC3	2.00	0.42
20:A:805:CLA:H161	20:A:805:CLA:H193	1.76	0.42
20:A:851:CLA:O1D	20:A:851:CLA:H2A	2.20	0.42
6:B:645:VAL:HG13	20:B:809:CLA:HAC1	2.00	0.42
20:B:803:CLA:H202	20:B:803:CLA:H162	1.81	0.42
20:B:833:CLA:H71	20:B:834:CLA:HMB2	2.00	0.42
19:4:305:CHL:HAB	19:4:306:CHL:OMC	2.20	0.42
20:B:807:CLA:H2	23:I:101:BCR:HC31	2.01	0.42
20:B:830:CLA:H3A	20:B:830:CLA:HBA2	1.30	0.42
15:K:80:ARG:HG2	15:K:88:LEU:HB3	2.01	0.42
18:O:68:ILE:HD11	21:O:204:LUT:H26	2.01	0.42
20:1:308:CLA:HBA2	20:1:308:CLA:H3A	1.33	0.42
5:A:194:MET:HB2	20:A:812:CLA:HBC2	2.00	0.42
5:A:611:LYS:HE2	5:A:615:ASP:OD2	2.20	0.42
20:A:808:CLA:H111	23:J:102:BCR:H373	2.00	0.42
30:B:848:DGD:HAW1	30:B:848:DGD:HAN2	1.80	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:101:TYR:O	11:G:105:LEU:HG	2.19	0.42
15:K:110:ALA:O	15:K:114:VAL:HG12	2.19	0.42
20:2:311:CLA:H52	20:2:311:CLA:H12	1.75	0.42
4:4:96:ARG:HG2	20:4:309:CLA:C3C	2.49	0.42
6:B:587:ILE:HA	6:B:590:VAL:HG13	2.00	0.42
20:B:823:CLA:H51	20:B:824:CLA:H142	2.02	0.42
20:B:838:CLA:HBB2	27:B:840:PQN:H141	2.02	0.42
20:B:838:CLA:H18	23:I:101:BCR:H362	2.02	0.42
20:F:805:CLA:C2D	26:F:807:HTG:H3'2	2.50	0.42
12:H:98:THR:HG22	16:L:187:ARG:HA	2.02	0.42
14:J:1:MET:O	14:J:5:LYS:HG3	2.19	0.42
15:K:103:PHE:CE2	15:K:108:THR:HG22	2.55	0.42
23:K:204:BCR:H20C	23:K:204:BCR:H361	1.81	0.42
16:L:144:LEU:HD22	23:L:305:BCR:H401	2.02	0.42
17:N:100:LEU:HD22	17:N:104:LYS:HE2	2.01	0.42
20:1:321:CLA:HMD1	6:B:308:HIS:HA	2.01	0.42
19:2:301:CHL:HED1	3:3:171:GLN:HG3	2.01	0.42
4:4:164:GLN:NE2	4:4:169:LYS:O	2.53	0.42
20:4:302:CLA:H93	20:4:302:CLA:H112	1.80	0.42
20:A:822:CLA:HBB2	20:A:838:CLA:H172	2.01	0.42
20:A:827:CLA:HBB1	20:A:827:CLA:HMB1	2.02	0.42
20:A:834:CLA:H11	20:A:834:CLA:H52	1.77	0.42
23:F:806:BCR:H371	23:F:806:BCR:H24C	1.81	0.42
23:K:204:BCR:H15C	23:K:204:BCR:H351	1.84	0.42
1:1:197:ARG:HB3	24:1:318:LHG:H252	2.00	0.42
2:2:203:GLY:HA2	20:2:309:CLA:CAA	2.49	0.42
19:2:305:CHL:HAB	19:2:306:CHL:CMC	2.48	0.42
20:4:312:CLA:HAA1	20:4:312:CLA:HED3	2.01	0.42
20:A:801:CLA:H122	20:A:801:CLA:H161	1.58	0.42
20:A:823:CLA:HMA1	20:O:201:CLA:CBB	2.50	0.42
20:A:831:CLA:HBA1	6:B:686:PRO:HD3	2.02	0.42
20:A:833:CLA:HAA2	16:L:120:THR:OG1	2.19	0.42
23:A:854:BCR:H24C	23:A:854:BCR:H371	1.80	0.42
8:D:110:LYS:NZ	12:H:58:TYR:O	2.52	0.42
1:1:61:GLY:HA2	1:1:66:ASP:HB3	2.02	0.42
23:A:848:BCR:H15C	23:A:848:BCR:H351	1.79	0.42
23:A:854:BCR:H403	15:K:110:ALA:HB1	2.02	0.42
20:L:303:CLA:H142	20:L:303:CLA:H111	1.73	0.42
21:1:319:LUT:H15	21:1:319:LUT:H201	1.74	0.42
5:A:31:HIS:CE1	20:A:810:CLA:HAA1	2.54	0.42
5:A:649:LEU:HD11	20:A:801:CLA:H72	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:A:818:CLA:H162	20:A:818:CLA:H122	1.87	0.42
25:1:323:LMG:HC61	11:G:136:SER:HA	2.02	0.41
20:4:301:CLA:CBB	20:4:302:CLA:HMD2	2.50	0.41
20:A:809:CLA:H121	20:A:809:CLA:H162	1.71	0.41
15:K:57:LEU:O	15:K:61:THR:HG22	2.20	0.41
15:K:95:LEU:O	15:K:96:GLN:HB3	2.20	0.41
23:L:306:BCR:H11C	23:L:306:BCR:H341	1.83	0.41
20:A:802:CLA:H192	20:A:802:CLA:H162	1.72	0.41
20:B:808:CLA:HMC3	20:B:809:CLA:C3D	2.51	0.41
20:B:825:CLA:H42	20:B:836:CLA:HBA1	2.01	0.41
23:K:204:BCR:H11C	23:K:204:BCR:H341	1.85	0.41
23:L:305:BCR:H20C	23:L:305:BCR:H361	1.87	0.41
2:2:143:THR:CG2	4:4:237:TRP:HB3	2.50	0.41
2:2:228:VAL:HG11	22:2:316:XAT:H12	2.03	0.41
3:3:224:GLU:HB2	20:3:308:CLA:C1B	2.50	0.41
4:4:240:THR:O	4:4:244:THR:HG23	2.21	0.41
20:4:311:CLA:H12	20:4:311:CLA:H52	1.76	0.41
5:A:689:ARG:HH12	5:A:693:GLN:HE21	1.67	0.41
20:A:834:CLA:H171	20:O:203:CLA:H112	2.01	0.41
6:B:373:THR:HG23	6:B:591:THR:HG21	2.02	0.41
23:1:317:BCR:H15C	23:1:317:BCR:H351	1.76	0.41
2:2:213:LEU:HD12	2:2:213:LEU:HA	1.89	0.41
25:4:319:LMG:H222	25:4:319:LMG:H251	1.89	0.41
20:A:809:CLA:H41	20:A:809:CLA:H62	1.69	0.41
20:A:812:CLA:H202	20:A:812:CLA:H161	1.84	0.41
20:A:812:CLA:H61	20:A:812:CLA:H92	1.79	0.41
20:A:832:CLA:HMD3	20:L:303:CLA:H18	2.02	0.41
20:A:841:CLA:H101	20:A:841:CLA:H13	1.50	0.41
6:B:61:THR:HB	6:B:142:LEU:HD13	2.02	0.41
6:B:662:MET:HB2	20:B:803:CLA:C1C	2.50	0.41
20:B:836:CLA:HMB2	20:B:837:CLA:C2D	2.50	0.41
20:2:308:CLA:H3A	20:2:308:CLA:HBA2	1.42	0.41
3:3:235:MET:HE1	22:3:316:XAT:H10	2.03	0.41
6:B:721:TYR:HB2	20:B:802:CLA:HED3	2.02	0.41
23:B:844:BCR:H351	23:B:844:BCR:H15C	1.76	0.41
7:C:2:SER:O	7:C:70:TRP:HB3	2.20	0.41
16:L:144:LEU:HB3	23:L:305:BCR:H401	2.02	0.41
20:N:203:CLA:H3A	20:N:203:CLA:HBA2	1.71	0.41
18:O:73:ILE:HD13	18:O:73:ILE:HA	1.69	0.41
21:2:315:LUT:H401	21:2:315:LUT:H35	1.78	0.41
5:A:323:LEU:O	5:A:335:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:571:PHE:CE1	5:A:585:SER:HB3	2.55	0.41
6:B:552:ASP:OD1	8:D:187:VAL:HG21	2.21	0.41
20:B:813:CLA:H43	23:B:842:BCR:H19C	2.03	0.41
10:F:172:LEU:HD23	10:F:172:LEU:HA	1.89	0.41
1:1:183:LYS:HE2	1:1:183:LYS:HB2	1.75	0.41
21:1:319:LUT:H382	20:4:308:CLA:HBA1	2.03	0.41
3:3:80:LEU:HD21	20:A:811:CLA:H2	2.02	0.41
3:3:234:ALA:HA	20:3:311:CLA:HBB1	2.03	0.41
23:J:104:BCR:H351	23:J:104:BCR:H15C	1.78	0.41
17:N:141:LYS:HE3	17:N:141:LYS:HB2	1.71	0.41
18:O:104:PHE:CD1	18:O:105:PRO:HA	2.55	0.41
18:O:131:PHE:HD1	20:O:203:CLA:HBB1	1.84	0.41
20:O:203:CLA:H11	20:O:203:CLA:HBA2	1.66	0.41
1:1:177:GLY:O	1:1:180:LYS:HG3	2.20	0.41
20:1:321:CLA:HBB1	24:B:849:LHG:HC11	2.02	0.41
20:1:321:CLA:HBC2	26:1:322:HTG:H1'1	2.02	0.41
2:2:166:ASP:OD2	19:2:307:CHL:HBC1	2.21	0.41
21:2:315:LUT:H15	21:2:315:LUT:H201	1.88	0.41
4:4:53:LEU:HD23	4:4:56:LEU:HB2	2.03	0.41
20:A:810:CLA:H61	20:A:810:CLA:H41	1.91	0.41
20:A:836:CLA:H11	20:A:837:CLA:O1A	2.21	0.41
6:B:50:HIS:HE1	20:B:805:CLA:H172	1.86	0.41
6:B:693:TRP:HE3	20:B:838:CLA:HMD3	1.85	0.41
8:D:178:ILE:H	8:D:178:ILE:HG13	1.36	0.41
15:K:123:VAL:O	15:K:127:LYS:HG2	2.21	0.41
18:O:130:THR:HG22	18:O:134:ILE:HD12	2.02	0.41
1:1:143:LEU:HD23	1:1:143:LEU:HA	1.87	0.41
2:2:131:PRO:HG2	20:2:304:CLA:HED2	2.03	0.41
19:2:301:CHL:H11	3:3:160:GLY:HA2	2.03	0.41
20:2:304:CLA:H62	20:2:304:CLA:H92	1.79	0.41
23:3:317:BCR:H351	23:3:317:BCR:H15C	1.72	0.41
4:4:77:LEU:HD21	10:F:202:ILE:HD13	2.01	0.41
20:4:304:CLA:C2B	22:4:317:XAT:H183	2.50	0.41
5:A:93:ALA:HB2	5:A:156:LEU:HB2	2.02	0.41
5:A:200:ALA:HB2	5:A:306:GLY:HA3	2.02	0.41
5:A:609:SER:O	5:A:613:GLN:HG3	2.21	0.41
20:A:805:CLA:H201	24:A:843:LHG:H221	2.03	0.41
20:A:833:CLA:H61	20:A:833:CLA:H92	1.85	0.41
6:B:158:GLN:HB2	6:B:161:TRP:HE3	1.85	0.41
6:B:447:GLY:O	10:F:88:GLN:NE2	2.37	0.41
20:B:804:CLA:H3A	20:B:804:CLA:HBA2	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:B:831:CLA:H142	23:F:806:BCR:HC8	2.03	0.41
10:F:157:PHE:HB2	23:F:801:BCR:H321	2.01	0.41
23:I:101:BCR:H15C	23:I:101:BCR:H351	1.79	0.41
16:L:56:THR:HB	16:L:57:TYR:H	1.66	0.41
2:2:64:PHE:CD1	19:2:301:CHL:HMA3	2.56	0.41
3:3:270:LYS:HB3	3:3:270:LYS:HE2	1.56	0.41
22:3:316:XAT:H35	22:3:316:XAT:H401	1.81	0.41
4:4:195:GLU:OE2	4:4:199:LYS:NZ	2.54	0.41
5:A:78:LEU:HD22	20:A:804:CLA:H92	2.03	0.41
23:A:847:BCR:H15C	23:A:847:BCR:H351	1.81	0.41
6:B:459:PHE:CZ	20:F:805:CLA:HBB1	2.56	0.41
6:B:656:VAL:HG22	20:B:839:CLA:HMB3	2.03	0.41
23:J:102:BCR:H361	23:J:102:BCR:H20C	1.87	0.41
17:N:93:LYS:HZ3	17:N:93:LYS:HB2	1.85	0.41
25:1:323:LMG:H152	25:1:323:LMG:H181	1.79	0.40
2:2:162:ARG:NH1	20:4:301:CLA:OBD	2.54	0.40
2:2:162:ARG:NE	19:2:314:CHL:HMC	2.37	0.40
2:2:176:ASP:HB3	2:2:179:PHE:O	2.20	0.40
20:2:303:CLA:HMD2	20:2:308:CLA:C1D	2.51	0.40
3:3:78:LEU:HD23	20:A:811:CLA:C2	2.51	0.40
4:4:214:PHE:HE1	21:4:316:LUT:H41	1.87	0.40
5:A:734:GLY:O	20:A:801:CLA:HED1	2.21	0.40
20:A:835:CLA:HBC1	18:O:84:ILE:HG23	2.03	0.40
20:B:829:CLA:H202	20:B:839:CLA:H3A	2.03	0.40
23:G:606:BCR:H24C	23:G:606:BCR:H371	1.79	0.40
5:A:478:PRO:HG3	5:A:531:PHE:HB2	2.02	0.40
20:A:818:CLA:HAB	20:A:818:CLA:H8	2.02	0.40
20:A:822:CLA:HBA1	20:O:203:CLA:HBA1	2.04	0.40
23:A:847:BCR:H20C	23:A:847:BCR:H361	1.87	0.40
2:2:258:VAL:HG22	20:2:312:CLA:C3D	2.51	0.40
3:3:232:MET:HG2	22:3:316:XAT:C34	2.51	0.40
4:4:53:LEU:HD13	20:4:301:CLA:HMA3	2.02	0.40
20:A:804:CLA:H3A	20:A:804:CLA:HBA1	1.48	0.40
20:A:807:CLA:HBB1	20:A:808:CLA:O1A	2.21	0.40
20:A:816:CLA:H61	20:A:816:CLA:H41	1.73	0.40
20:A:824:CLA:H172	20:A:824:CLA:H13	1.95	0.40
20:A:825:CLA:H202	18:O:123:LEU:HD22	2.03	0.40
20:A:838:CLA:H112	20:A:838:CLA:H151	1.79	0.40
27:A:842:PQN:H261	27:A:842:PQN:H222	1.92	0.40
23:A:846:BCR:H351	23:A:846:BCR:H15C	1.76	0.40
10:F:68:ASP:N	10:F:72:LEU:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:163:TRP:CD1	10:F:200:GLY:HA3	2.56	0.40
2:2:73:LEU:HD11	2:2:84:ASP:HB2	2.03	0.40
2:2:97:TRP:CH2	20:2:308:CLA:HAA2	2.57	0.40
2:2:108:TRP:CE2	20:2:308:CLA:HBC3	2.56	0.40
3:3:150:ASP:OD1	3:3:151:PRO:HD2	2.22	0.40
5:A:150:ILE:HG23	5:A:155:GLN:HE21	1.85	0.40
20:A:802:CLA:H41	20:A:802:CLA:H62	1.90	0.40
10:F:68:ASP:HB3	10:F:69:ILE:H	1.50	0.40
20:1:303:CLA:CBC	20:1:308:CLA:HAC1	2.50	0.40
20:4:303:CLA:H41	20:4:303:CLA:H61	1.75	0.40
23:A:845:BCR:H361	23:A:845:BCR:H20C	1.84	0.40
20:B:810:CLA:H91	20:B:810:CLA:H111	1.84	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	1	197/246 (80%)	194 (98%)	3 (2%)	0	100	100
2	2	207/265 (78%)	203 (98%)	3 (1%)	1 (0%)	29	41
3	3	218/272 (80%)	206 (94%)	12 (6%)	0	100	100
4	4	195/248 (79%)	189 (97%)	6 (3%)	0	100	100
5	A	740/750 (99%)	722 (98%)	18 (2%)	0	100	100
6	B	731/734 (100%)	716 (98%)	14 (2%)	1 (0%)	51	68
7	C	78/81 (96%)	75 (96%)	3 (4%)	0	100	100
8	D	139/190 (73%)	135 (97%)	4 (3%)	0	100	100
9	E	61/151 (40%)	59 (97%)	2 (3%)	0	100	100
10	F	151/221 (68%)	150 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	G	96/145 (66%)	95 (99%)	1 (1%)	0	100	100
12	H	88/145 (61%)	87 (99%)	1 (1%)	0	100	100
13	I	27/36 (75%)	27 (100%)	0	0	100	100
14	J	38/44 (86%)	38 (100%)	0	0	100	100
15	K	81/132 (61%)	75 (93%)	5 (6%)	1 (1%)	13	19
16	L	160/217 (74%)	157 (98%)	3 (2%)	0	100	100
17	N	82/173 (47%)	76 (93%)	5 (6%)	1 (1%)	13	19
18	O	87/144 (60%)	85 (98%)	2 (2%)	0	100	100
All	All	3376/4194 (80%)	3289 (97%)	83 (2%)	4 (0%)	54	68

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	2	172	CYS
6	B	362	ALA
17	N	167	TRP
15	K	96	GLN

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	1	162/198 (82%)	153 (94%)	9 (6%)	21	34
2	2	168/208 (81%)	164 (98%)	4 (2%)	49	68
3	3	175/217 (81%)	164 (94%)	11 (6%)	18	28
4	4	168/207 (81%)	163 (97%)	5 (3%)	41	61
5	A	600/608 (99%)	579 (96%)	21 (4%)	36	55
6	B	598/599 (100%)	577 (96%)	21 (4%)	36	55
7	C	70/71 (99%)	65 (93%)	5 (7%)	14	23
8	D	121/159 (76%)	110 (91%)	11 (9%)	9	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	E	57/124 (46%)	56 (98%)	1 (2%)	59	76
10	F	126/185 (68%)	112 (89%)	14 (11%)	6	8
11	G	84/125 (67%)	82 (98%)	2 (2%)	49	68
12	H	72/110 (66%)	69 (96%)	3 (4%)	30	47
13	I	25/31 (81%)	23 (92%)	2 (8%)	12	18
14	J	34/38 (90%)	33 (97%)	1 (3%)	42	62
15	K	61/99 (62%)	57 (93%)	4 (7%)	16	26
16	L	129/176 (73%)	125 (97%)	4 (3%)	40	60
17	N	74/139 (53%)	65 (88%)	9 (12%)	5	6
18	O	73/114 (64%)	65 (89%)	8 (11%)	6	8
All	All	2797/3408 (82%)	2662 (95%)	135 (5%)	29	41

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	50	PHE
1	1	53	GLN
1	1	55	ARG
1	1	156	GLN
1	1	179	SER
1	1	183	LYS
1	1	184	LYS
1	1	236	ASP
1	1	241	ARG
2	2	124	LYS
2	2	188	ASP
2	2	209	LYS
2	2	212	GLU
3	3	144	SER
3	3	157	PHE
3	3	164	PHE
3	3	174	SER
3	3	175	ASN
3	3	189	LYS
3	3	194	SER
3	3	245	THR
3	3	264	ASN
3	3	265	ILE

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Mol	Chain	Res	Type
3	3	271	PHE
4	4	66	LEU
4	4	170	ASN
4	4	172	SER
4	4	220	VAL
4	4	243	ASN
5	A	22	SER
5	A	34	ARG
5	A	58	SER
5	A	61	SER
5	A	70	VAL
5	A	83	LEU
5	A	94	ARG
5	A	184	LYS
5	A	218	SER
5	A	223	GLN
5	A	244	ARG
5	A	275	PHE
5	A	369	TYR
5	A	371	MET
5	A	422	ASP
5	A	457	ASP
5	A	533	VAL
5	A	619	SER
5	A	623	GLN
5	A	663	SER
5	A	749	VAL
6	B	4	ARG
6	B	41	ARG
6	B	79	GLN
6	B	186	SER
6	B	216	LEU
6	B	239	SER
6	B	320	LYS
6	B	325	THR
6	B	410	ARG
6	B	441	ASP
6	B	480	SER
6	B	545	LYS
6	B	550	LYS
6	B	590	VAL
6	B	608	GLN

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Mol	Chain	Res	Type
6	B	645	VAL
6	B	649	MET
6	B	684	ARG
6	B	701	SER
6	B	725	LEU
6	B	728	SER
7	C	2	SER
7	C	41	SER
7	C	58	CYS
7	C	64	SER
7	C	66	ARG
8	D	53	GLN
8	D	58	THR
8	D	85	GLU
8	D	88	LYS
8	D	94	MET
8	D	104	GLU
8	D	125	ARG
8	D	126	SER
8	D	129	LYS
8	D	150	ASP
8	D	178	ILE
9	E	101	ARG
10	F	68	ASP
10	F	76	LYS
10	F	89	ILE
10	F	121	ASP
10	F	132	SER
10	F	137	HIS
10	F	170	SER
10	F	176	SER
10	F	194	SER
10	F	195	ARG
10	F	211	PHE
10	F	213	ASN
10	F	216	LEU
10	F	219	LYS
11	G	52	SER
11	G	106	LYS
12	H	77	ASP
12	H	102	LEU
12	H	105	LYS

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Mol	Chain	Res	Type
13	I	8	SER
13	I	13	LEU
14	J	4	LEU
15	K	55	THR
15	K	80	ARG
15	K	87	LYS
15	K	95	LEU
16	L	64	ASN
16	L	67	PRO
16	L	112	LEU
16	L	128	ASN
17	N	93	LYS
17	N	138	LYS
17	N	140	LYS
17	N	142	VAL
17	N	151	ILE
17	N	158	ILE
17	N	163	SER
17	N	165	VAL
17	N	167	TRP
18	O	58	ARG
18	O	59	ASP
18	O	61	LEU
18	O	65	LEU
18	O	73	ILE
18	O	87	ASN
18	O	131	PHE
18	O	139	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	112	ASN
1	1	126	GLN
1	1	156	GLN
1	1	209	GLN
1	1	221	ASN
2	2	174	ASN
2	2	181	ASN
2	2	234	GLN
2	2	245	ASN
3	3	175	ASN

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Mol	Chain	Res	Type
3	3	182	GLN
3	3	241	GLN
3	3	252	ASN
4	4	164	GLN
4	4	170	ASN
5	A	77	GLN
5	A	155	GLN
5	A	223	GLN
5	A	599	ASN
5	A	607	HIS
5	A	623	GLN
5	A	693	GLN
5	A	721	GLN
6	B	98	GLN
6	B	218	HIS
6	B	236	ASN
6	B	266	GLN
6	B	327	ASN
6	B	704	GLN
7	C	38	GLN
8	D	131	ASN
8	D	144	GLN
8	D	167	ASN
9	E	140	ASN
10	F	213	ASN
11	G	50	ASN
11	G	72	ASN
12	H	83	ASN
16	L	58	GLN
16	L	64	ASN
16	L	128	ASN
18	O	87	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

225 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
20	CLA	A	826	-	65,73,73	1.49	6 (9%)	76,113,113	1.37	7 (9%)
23	BCR	2	317	-	41,41,41	0.74	0	56,56,56	2.13	17 (30%)
20	CLA	3	301	3	60,68,73	1.54	7 (11%)	70,107,113	1.42	7 (10%)
28	SF4	C	101	-	0,12,12	-	-	-		
20	CLA	A	814	-	50,58,73	1.67	5 (10%)	58,95,113	1.59	9 (15%)
20	CLA	1	305	-	52,60,73	1.66	6 (11%)	60,97,113	1.48	7 (11%)
20	CLA	1	321	-	65,73,73	1.49	6 (9%)	76,113,113	1.36	9 (11%)
20	CLA	A	807	5	65,73,73	1.45	5 (7%)	76,113,113	1.42	9 (11%)
20	CLA	B	813	-	65,73,73	1.48	6 (9%)	76,113,113	1.37	7 (9%)
23	BCR	A	848	-	41,41,41	0.75	1 (2%)	56,56,56	1.88	15 (26%)
20	CLA	B	817	-	65,73,73	1.49	6 (9%)	76,113,113	1.39	7 (9%)
20	CLA	K	203	-	46,54,73	1.72	7 (15%)	53,90,113	1.61	6 (11%)
20	CLA	A	810	20	65,73,73	1.48	6 (9%)	76,113,113	1.35	7 (9%)
20	CLA	B	820	-	50,58,73	1.68	5 (10%)	58,95,113	1.56	7 (12%)
20	CLA	B	812	-	55,63,73	1.61	5 (9%)	64,101,113	1.45	8 (12%)
20	CLA	B	822	-	65,73,73	1.49	6 (9%)	76,113,113	1.42	8 (10%)
20	CLA	B	823	-	60,68,73	1.54	7 (11%)	70,107,113	1.47	10 (14%)
20	CLA	3	309	-	46,54,73	2.15	11 (23%)	53,90,113	2.36	16 (30%)
26	HTG	F	807	-	19,19,19	1.06	2 (10%)	23,24,24	0.52	0
20	CLA	B	808	-	65,73,73	1.46	6 (9%)	76,113,113	1.42	9 (11%)
20	CLA	B	827	-	65,73,73	1.53	6 (9%)	76,113,113	1.33	9 (11%)
26	HTG	B	851	-	19,19,19	1.08	2 (10%)	23,24,24	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
23	BCR	A	847	-	41,41,41	0.68	0	56,56,56	2.00	16 (28%)
23	BCR	G	606	-	41,41,41	0.68	0	56,56,56	1.95	16 (28%)
23	BCR	F	801	-	41,41,41	0.68	0	56,56,56	1.79	14 (25%)
21	LUT	2	315	-	42,43,43	0.75	0	51,60,60	1.69	15 (29%)
26	HTG	B	850	-	19,19,19	1.06	2 (10%)	23,24,24	0.84	0
20	CLA	1	311	1	52,60,73	1.64	6 (11%)	60,97,113	1.57	7 (11%)
23	BCR	A	845	-	41,41,41	0.72	0	56,56,56	1.94	16 (28%)
20	CLA	B	837	-	47,55,73	1.73	6 (12%)	54,91,113	1.56	7 (12%)
24	LHG	B	849	-	22,22,48	1.19	2 (9%)	25,28,54	1.01	1 (4%)
20	CLA	4	313	-	45,53,73	1.79	5 (11%)	52,89,113	1.59	8 (15%)
20	CLA	A	828	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	7 (9%)
25	LMG	1	323	-	44,44,55	0.99	2 (4%)	52,52,63	1.04	3 (5%)
20	CLA	3	313	-	45,53,73	1.80	5 (11%)	52,89,113	1.54	6 (11%)
20	CLA	A	812	-	65,73,73	1.47	5 (7%)	76,113,113	1.38	6 (7%)
20	CLA	4	311	4	52,60,73	1.64	6 (11%)	60,97,113	1.53	6 (10%)
20	CLA	B	829	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	6 (7%)
20	CLA	1	310	24	41,49,73	1.81	6 (14%)	47,84,113	1.69	8 (17%)
20	CLA	A	802	-	65,73,73	1.46	5 (7%)	76,113,113	1.39	7 (9%)
23	BCR	K	204	-	41,41,41	0.68	0	56,56,56	2.02	18 (32%)
20	CLA	A	801	-	65,73,73	1.48	5 (7%)	76,113,113	1.49	10 (13%)
23	BCR	L	305	-	41,41,41	0.70	0	56,56,56	2.09	13 (23%)
23	BCR	A	846	-	41,41,41	0.73	0	56,56,56	1.97	15 (26%)
20	CLA	A	829	-	65,73,73	1.46	6 (9%)	76,113,113	1.45	7 (9%)
20	CLA	2	304	-	60,68,73	1.55	6 (10%)	70,107,113	1.40	7 (10%)
20	CLA	A	804	-	65,73,73	1.47	7 (10%)	76,113,113	1.42	6 (7%)
23	BCR	A	854	-	41,41,41	0.69	0	56,56,56	1.94	12 (21%)
20	CLA	2	309	2	60,68,73	1.53	6 (10%)	70,107,113	1.40	8 (11%)
20	CLA	A	819	-	45,53,73	1.77	6 (13%)	52,89,113	1.59	7 (13%)
20	CLA	1	313	-	55,63,73	1.61	5 (9%)	64,101,113	1.47	7 (10%)
20	CLA	3	308	3	50,58,73	1.66	6 (12%)	58,95,113	1.54	8 (13%)
20	CLA	K	202	-	60,68,73	1.55	6 (10%)	70,107,113	1.45	11 (15%)
20	CLA	L	304	-	50,58,73	1.67	6 (12%)	58,95,113	1.54	9 (15%)
20	CLA	A	818	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	9 (11%)
23	BCR	L	301	-	41,41,41	0.72	0	56,56,56	1.96	13 (23%)
24	LHG	1	318	20	48,48,48	0.93	2 (4%)	51,54,54	1.04	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	2	306	-	48,56,74	2.32	16 (33%)	51,92,114	3.24	23 (45%)
20	CLA	1	304	-	52,60,73	1.65	6 (11%)	60,97,113	1.52	8 (13%)
20	CLA	F	804	-	45,53,73	1.79	6 (13%)	52,89,113	1.55	7 (13%)
20	CLA	A	809	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
20	CLA	1	309	1	60,68,73	1.50	5 (8%)	70,107,113	1.43	8 (11%)
20	CLA	2	310	24	41,49,73	1.81	5 (12%)	47,84,113	1.68	8 (17%)
19	CHL	2	307	-	51,59,74	2.33	21 (41%)	55,96,114	3.45	28 (50%)
20	CLA	A	841	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	9 (11%)
20	CLA	N	202	17	44,53,73	1.77	6 (13%)	50,89,113	1.58	7 (14%)
24	LHG	2	318	20	36,36,48	1.07	2 (5%)	39,42,54	1.13	3 (7%)
30	DGD	B	848	-	67,67,67	0.84	2 (2%)	81,81,81	0.94	4 (4%)
23	BCR	3	317	-	41,41,41	0.66	0	56,56,56	1.99	16 (28%)
21	LUT	O	205	-	42,43,43	0.85	1 (2%)	51,60,60	2.00	14 (27%)
20	CLA	B	804	-	45,53,73	1.76	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	1	314	1	46,54,73	1.73	6 (13%)	53,90,113	1.56	6 (11%)
26	HTG	A	852	-	19,19,19	1.27	2 (10%)	23,24,24	1.49	4 (17%)
20	CLA	1	302	1	65,73,73	1.48	7 (10%)	76,113,113	1.38	7 (9%)
20	CLA	O	201	24	52,60,73	1.66	6 (11%)	60,97,113	1.45	7 (11%)
19	CHL	2	305	-	43,51,74	2.42	19 (44%)	45,86,114	3.72	24 (53%)
27	PQN	A	842	-	34,34,34	1.62	2 (5%)	42,45,45	1.05	3 (7%)
20	CLA	B	821	-	56,64,73	1.61	6 (10%)	65,102,113	1.45	8 (12%)
20	CLA	J	103	14	42,50,73	1.83	6 (14%)	48,85,113	1.59	7 (14%)
20	CLA	A	827	-	65,73,73	1.46	6 (9%)	76,113,113	1.40	8 (10%)
20	CLA	4	302	4	60,68,73	1.51	6 (10%)	70,107,113	1.46	7 (10%)
21	LUT	1	319	-	42,43,43	0.71	0	51,60,60	1.73	12 (23%)
20	CLA	B	835	-	51,59,73	1.64	6 (11%)	59,96,113	1.53	7 (11%)
20	CLA	B	803	-	65,73,73	1.47	7 (10%)	76,113,113	1.40	8 (10%)
20	CLA	L	303	-	65,73,73	1.48	5 (7%)	76,113,113	1.39	9 (11%)
20	CLA	O	202	-	45,53,73	2.01	8 (17%)	52,89,113	1.94	7 (13%)
23	BCR	B	845	-	41,41,41	0.69	0	56,56,56	1.99	17 (30%)
23	BCR	J	104	-	41,41,41	0.67	0	56,56,56	1.98	15 (26%)
20	CLA	B	838	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
22	XAT	3	316	-	39,47,47	0.88	0	54,74,74	2.72	21 (38%)
20	CLA	3	312	-	45,53,73	1.78	5 (11%)	52,89,113	1.58	7 (13%)
20	CLA	1	307	-	61,69,73	1.53	5 (8%)	71,108,113	1.40	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	4	305	-	53,61,74	2.23	16 (30%)	57,98,114	3.06	26 (45%)
20	CLA	A	839	-	65,73,73	1.47	5 (7%)	76,113,113	1.39	8 (10%)
20	CLA	B	805	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
20	CLA	B	811	-	54,62,73	1.67	7 (12%)	67,100,113	1.51	9 (13%)
20	CLA	B	815	-	60,68,73	1.51	5 (8%)	70,107,113	1.45	7 (10%)
20	CLA	B	828	-	65,73,73	1.50	5 (7%)	76,113,113	1.33	9 (11%)
20	CLA	N	203	-	50,58,73	1.70	5 (10%)	58,95,113	1.54	9 (15%)
21	LUT	O	204	-	42,43,43	0.76	0	51,60,60	1.73	12 (23%)
23	BCR	I	101	-	41,41,41	0.76	0	56,56,56	2.08	17 (30%)
26	HTG	1	322	-	19,19,19	1.06	2 (10%)	23,24,24	1.05	3 (13%)
20	CLA	B	807	-	55,63,73	1.59	6 (10%)	64,101,113	1.47	9 (14%)
20	CLA	3	314	-	46,54,73	1.78	5 (10%)	53,90,113	1.51	6 (11%)
22	XAT	4	317	-	39,47,47	0.88	0	54,74,74	2.65	19 (35%)
20	CLA	B	831	-	65,73,73	1.47	5 (7%)	76,113,113	1.34	7 (9%)
20	CLA	3	305	3	47,55,73	1.74	5 (10%)	54,91,113	1.52	7 (12%)
20	CLA	1	312	1	65,73,73	1.50	5 (7%)	76,113,113	1.34	7 (9%)
22	XAT	2	316	-	39,47,47	0.88	0	54,74,74	2.64	20 (37%)
20	CLA	A	815	-	45,53,73	1.78	6 (13%)	52,89,113	1.56	6 (11%)
20	CLA	A	833	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
21	LUT	4	316	-	42,43,43	0.76	0	51,60,60	1.61	13 (25%)
20	CLA	A	823	-	55,63,73	1.61	5 (9%)	64,101,113	1.43	9 (14%)
20	CLA	B	818	-	60,68,73	1.53	6 (10%)	70,107,113	1.42	7 (10%)
27	PQN	B	840	-	34,34,34	1.60	2 (5%)	42,45,45	1.12	3 (7%)
20	CLA	1	303	-	65,73,73	1.51	6 (9%)	76,113,113	1.37	8 (10%)
20	CLA	A	824	-	65,73,73	1.48	6 (9%)	76,113,113	1.40	7 (9%)
20	CLA	A	813	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	A	817	-	65,73,73	1.49	7 (10%)	76,113,113	1.35	9 (11%)
20	CLA	A	835	5	45,53,73	1.80	5 (11%)	52,89,113	1.56	7 (13%)
24	LHG	A	844	20	26,26,48	1.25	2 (7%)	29,32,54	1.34	3 (10%)
20	CLA	2	313	-	43,51,73	1.78	6 (13%)	49,86,113	1.63	7 (14%)
20	CLA	A	822	-	51,59,73	1.67	6 (11%)	59,96,113	1.46	8 (13%)
21	LUT	3	315	-	42,43,43	0.75	0	51,60,60	1.59	12 (23%)
20	CLA	1	308	1	65,73,73	1.49	5 (7%)	76,113,113	1.36	7 (9%)
20	CLA	A	825	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	10 (13%)
29	LMT	B	847	-	36,36,36	0.40	0	47,47,47	0.68	1 (2%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	2	311	2	52,60,73	1.63	6 (11%)	60,97,113	1.56	7 (11%)
20	CLA	A	808	5	65,73,73	1.49	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	4	303	-	60,68,73	1.53	7 (11%)	70,107,113	1.46	7 (10%)
20	CLA	B	832	-	58,66,73	1.56	6 (10%)	67,104,113	1.49	10 (14%)
23	BCR	F	806	-	41,41,41	0.71	0	56,56,56	2.03	17 (30%)
20	CLA	3	302	-	50,58,73	1.72	5 (10%)	58,95,113	1.50	8 (13%)
20	CLA	4	310	-	55,63,73	1.63	5 (9%)	64,101,113	1.41	8 (12%)
20	CLA	F	802	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	8 (10%)
20	CLA	A	820	-	65,73,73	1.48	5 (7%)	76,113,113	1.37	8 (10%)
20	CLA	B	816	-	55,63,73	1.59	6 (10%)	64,101,113	1.45	8 (12%)
29	LMT	G	601	-	36,36,36	0.41	0	47,47,47	0.64	1 (2%)
21	LUT	1	315	-	42,43,43	0.76	0	51,60,60	1.64	14 (27%)
20	CLA	A	811	-	54,62,73	1.65	6 (11%)	62,99,113	1.44	8 (12%)
26	HTG	F	803	-	19,19,19	1.09	2 (10%)	23,24,24	0.55	0
20	CLA	A	806	-	65,73,73	1.45	5 (7%)	76,113,113	1.42	8 (10%)
20	CLA	B	810	-	65,73,73	1.47	6 (9%)	76,113,113	1.41	8 (10%)
20	CLA	L	302	16	45,53,73	1.76	6 (13%)	52,89,113	1.66	7 (13%)
19	CHL	4	307	-	51,59,74	2.31	24 (47%)	55,96,114	3.13	24 (43%)
20	CLA	A	821	-	49,57,73	1.67	6 (12%)	55,93,113	1.58	7 (12%)
20	CLA	B	824	-	65,73,73	1.47	6 (9%)	76,113,113	1.44	8 (10%)
20	CLA	O	203	-	60,68,73	1.53	6 (10%)	70,107,113	1.43	8 (11%)
23	BCR	1	317	-	41,41,41	0.68	0	56,56,56	1.91	18 (32%)
20	CLA	H	201	-	56,64,73	1.60	6 (10%)	65,102,113	1.45	7 (10%)
20	CLA	A	831	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	B	834	-	45,53,73	1.75	5 (11%)	52,89,113	1.62	7 (13%)
20	CLA	3	310	-	52,60,73	1.67	6 (11%)	60,97,113	1.49	8 (13%)
23	BCR	A	849	-	41,41,41	0.72	0	56,56,56	1.97	15 (26%)
20	CLA	2	302	2	65,73,73	1.45	6 (9%)	76,113,113	1.39	8 (10%)
20	CLA	A	816	-	65,73,73	1.48	6 (9%)	76,113,113	1.33	8 (10%)
20	CLA	3	311	3	55,63,73	1.63	6 (10%)	64,101,113	1.45	8 (12%)
20	CLA	B	836	-	65,73,73	1.47	5 (7%)	76,113,113	1.40	8 (10%)
20	CLA	K	205	15	45,53,73	1.78	6 (13%)	52,89,113	1.56	6 (11%)
20	CLA	B	806	6	65,73,73	1.45	5 (7%)	76,113,113	1.38	8 (10%)
28	SF4	A	850	-	0,12,12	-	-	-	-	-
20	CLA	A	834	-	65,73,73	1.50	5 (7%)	76,113,113	1.36	7 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
19	CHL	4	315	-	43,51,74	2.35	18 (41%)	45,86,114	3.22	21 (46%)
20	CLA	G	605	11	46,54,73	1.76	5 (10%)	53,90,113	1.51	6 (11%)
19	CHL	3	306	-	47,55,74	2.40	21 (44%)	50,91,114	3.55	26 (52%)
26	HTG	G	602	-	19,19,19	1.08	2 (10%)	23,24,24	0.56	0
20	CLA	A	836	-	51,59,73	1.64	5 (9%)	59,96,113	1.57	9 (15%)
20	CLA	3	304	-	42,50,73	1.80	5 (11%)	48,85,113	1.67	6 (12%)
20	CLA	A	851	-	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
28	SF4	C	102	-	0,12,12	-	-	-	-	-
20	CLA	F	805	-	46,54,73	1.76	6 (13%)	53,90,113	1.55	6 (11%)
20	CLA	A	803	20	55,63,73	1.62	6 (10%)	64,101,113	1.49	9 (14%)
20	CLA	4	308	4	50,58,73	1.67	6 (12%)	58,95,113	1.52	9 (15%)
19	CHL	1	301	1	52,60,74	2.23	16 (30%)	56,97,114	2.70	23 (41%)
20	CLA	B	809	6	65,73,73	1.46	5 (7%)	76,113,113	1.41	8 (10%)
19	CHL	2	301	2	53,61,74	2.50	25 (47%)	57,98,114	3.86	30 (52%)
23	BCR	B	842	-	41,41,41	0.71	0	56,56,56	2.03	19 (33%)
19	CHL	1	306	1	48,56,74	2.33	19 (39%)	51,92,114	3.21	26 (50%)
20	CLA	L	307	-	45,53,73	1.80	6 (13%)	52,89,113	1.59	7 (13%)
20	CLA	3	303	-	45,53,73	1.77	5 (11%)	52,89,113	1.60	8 (15%)
20	CLA	3	307	3	50,58,73	1.65	6 (12%)	58,95,113	1.57	8 (13%)
20	CLA	B	819	-	65,73,73	1.48	7 (10%)	76,113,113	1.35	8 (10%)
20	CLA	4	301	4	46,54,73	1.76	5 (10%)	53,90,113	1.53	6 (11%)
24	LHG	A	843	-	48,48,48	0.92	2 (4%)	51,54,54	1.00	3 (5%)
23	BCR	B	843	-	41,41,41	0.70	0	56,56,56	2.06	14 (25%)
26	HTG	4	320	-	19,19,19	1.12	2 (10%)	23,24,24	0.57	0
20	CLA	A	853	-	65,73,73	1.49	6 (9%)	76,113,113	1.34	8 (10%)
20	CLA	J	101	-	65,73,73	1.47	6 (9%)	76,113,113	1.42	9 (11%)
20	CLA	B	802	-	65,73,73	1.48	6 (9%)	76,113,113	1.31	7 (9%)
25	LMG	1	320	-	49,49,55	0.94	2 (4%)	57,57,63	1.02	3 (5%)
20	CLA	B	839	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	8 (10%)
20	CLA	G	604	-	50,58,73	1.69	5 (10%)	58,95,113	1.53	8 (13%)
20	CLA	B	825	-	65,73,73	1.47	6 (9%)	76,113,113	1.43	9 (11%)
20	CLA	G	603	-	45,53,73	1.79	5 (11%)	52,89,113	1.58	7 (13%)
23	BCR	4	318	-	41,41,41	0.67	0	56,56,56	3.33	22 (39%)
19	CHL	4	306	-	51,59,74	2.42	23 (45%)	55,96,114	3.03	26 (47%)
20	CLA	B	830	-	50,58,73	1.67	6 (12%)	58,95,113	1.53	8 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
20	CLA	K	201	15	46,54,73	1.76	6 (13%)	53,90,113	1.53	6 (11%)
22	XAT	1	316	-	39,47,47	0.88	0	54,74,74	2.58	18 (33%)
20	CLA	B	833	-	65,73,73	1.48	6 (9%)	76,113,113	1.36	9 (11%)
20	CLA	A	840	-	65,73,73	1.49	6 (9%)	76,113,113	1.35	8 (10%)
23	BCR	B	841	-	41,41,41	0.71	0	56,56,56	1.89	16 (28%)
20	CLA	A	838	-	65,73,73	1.50	6 (9%)	76,113,113	1.39	7 (9%)
20	CLA	A	832	-	65,73,73	1.49	5 (7%)	76,113,113	1.34	7 (9%)
23	BCR	J	102	-	41,41,41	0.68	0	56,56,56	1.97	17 (30%)
20	CLA	4	314	-	50,58,73	1.69	5 (10%)	58,95,113	1.51	9 (15%)
20	CLA	A	805	-	65,73,73	1.47	6 (9%)	76,113,113	1.40	7 (9%)
26	HTG	N	201	-	19,19,19	1.08	2 (10%)	23,24,24	0.61	0
25	LMG	4	319	-	44,44,55	0.98	2 (4%)	52,52,63	1.01	3 (5%)
20	CLA	2	308	2	50,58,73	1.65	6 (12%)	58,95,113	1.55	8 (13%)
23	BCR	B	844	-	41,41,41	0.71	0	56,56,56	1.85	15 (26%)
20	CLA	A	837	-	65,73,73	1.45	6 (9%)	76,113,113	1.43	8 (10%)
20	CLA	4	312	-	65,73,73	1.48	6 (9%)	76,113,113	1.39	6 (7%)
23	BCR	L	306	-	41,41,41	0.72	0	56,56,56	2.09	13 (23%)
19	CHL	2	314	2	43,51,74	2.25	12 (27%)	45,86,114	2.96	18 (40%)
20	CLA	2	312	2	65,73,73	1.49	5 (7%)	76,113,113	1.36	9 (11%)
20	CLA	B	801	-	65,73,73	1.49	5 (7%)	76,113,113	1.40	7 (9%)
20	CLA	A	830	-	50,58,73	1.66	6 (12%)	58,95,113	1.58	7 (12%)
20	CLA	4	304	-	50,58,73	2.02	13 (26%)	58,95,113	3.47	22 (37%)
23	BCR	B	846	-	41,41,41	0.71	0	56,56,56	1.76	14 (25%)
20	CLA	4	309	4	60,68,73	1.51	6 (10%)	70,107,113	1.42	9 (12%)
20	CLA	B	826	-	65,73,73	1.47	5 (7%)	76,113,113	1.42	8 (10%)
26	HTG	J	105	-	19,19,19	1.11	2 (10%)	23,24,24	0.56	0
20	CLA	B	814	-	65,73,73	1.47	6 (9%)	76,113,113	1.38	7 (9%)
20	CLA	2	303	-	49,57,73	1.70	6 (12%)	55,93,113	1.55	7 (12%)

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
20	CLA	A	826	-	1/1/15/20	5/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
23	BCR	2	317	-	-	2/29/63/63	0/2/2/2
20	CLA	3	301	3	1/1/14/20	6/31/109/115	-
28	SF4	C	101	-	-	-	0/6/5/5
20	CLA	A	814	-	1/1/12/20	7/19/97/115	-
20	CLA	1	305	-	1/1/12/20	3/22/100/115	-
20	CLA	1	321	-	1/1/15/20	7/37/115/115	-
20	CLA	A	807	5	1/1/15/20	10/37/115/115	-
20	CLA	B	813	-	1/1/15/20	14/37/115/115	-
23	BCR	A	848	-	-	0/29/63/63	0/2/2/2
20	CLA	B	817	-	1/1/15/20	13/37/115/115	-
20	CLA	K	203	-	1/1/11/20	6/15/93/115	-
20	CLA	A	810	20	1/1/15/20	16/37/115/115	-
20	CLA	B	820	-	1/1/12/20	1/19/97/115	-
20	CLA	B	812	-	1/1/13/20	6/25/103/115	-
20	CLA	B	822	-	1/1/15/20	12/37/115/115	-
20	CLA	B	823	-	1/1/14/20	12/31/109/115	-
20	CLA	3	309	-	-	4/15/93/115	-
26	HTG	F	807	-	-	2/10/30/30	0/1/1/1
20	CLA	B	808	-	1/1/15/20	5/37/115/115	-
20	CLA	B	827	-	1/1/15/20	14/37/115/115	-
26	HTG	B	851	-	-	2/10/30/30	0/1/1/1
23	BCR	A	847	-	-	2/29/63/63	0/2/2/2
23	BCR	G	606	-	-	0/29/63/63	0/2/2/2
23	BCR	F	801	-	-	3/29/63/63	0/2/2/2
21	LUT	2	315	-	-	2/29/67/67	0/2/2/2
26	HTG	B	850	-	-	8/10/30/30	0/1/1/1
20	CLA	1	311	1	1/1/12/20	7/22/100/115	-
23	BCR	A	845	-	-	6/29/63/63	0/2/2/2
20	CLA	B	837	-	1/1/11/20	2/16/94/115	-
24	LHG	B	849	-	-	7/26/26/53	-
20	CLA	4	313	-	1/1/11/20	1/13/91/115	-
20	CLA	A	828	-	1/1/15/20	11/37/115/115	-
25	LMG	1	323	-	-	10/39/59/70	0/1/1/1
20	CLA	3	313	-	1/1/11/20	3/13/91/115	-
20	CLA	A	812	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	4	311	4	1/1/12/20	5/22/100/115	-
20	CLA	B	829	-	1/1/15/20	6/37/115/115	-
20	CLA	1	310	24	1/1/10/20	2/8/86/115	-
20	CLA	A	802	-	1/1/15/20	15/37/115/115	-
23	BCR	K	204	-	-	6/29/63/63	0/2/2/2
20	CLA	A	801	-	1/1/15/20	11/37/115/115	-
23	BCR	L	305	-	-	4/29/63/63	0/2/2/2
23	BCR	A	846	-	-	0/29/63/63	0/2/2/2
20	CLA	A	829	-	1/1/15/20	9/37/115/115	-
20	CLA	2	304	-	1/1/14/20	10/31/109/115	-
20	CLA	A	804	-	1/1/15/20	10/37/115/115	-
23	BCR	A	854	-	-	0/29/63/63	0/2/2/2
20	CLA	2	309	2	1/1/14/20	6/31/109/115	-
20	CLA	A	819	-	1/1/11/20	2/13/91/115	-
20	CLA	1	313	-	1/1/13/20	11/25/103/115	-
20	CLA	3	308	3	1/1/12/20	1/19/97/115	-
20	CLA	K	202	-	1/1/14/20	7/31/109/115	-
20	CLA	L	304	-	1/1/12/20	2/19/97/115	-
20	CLA	A	818	-	1/1/15/20	9/37/115/115	-
23	BCR	L	301	-	-	4/29/63/63	0/2/2/2
24	LHG	1	318	20	-	13/53/53/53	-
19	CHL	2	306	-	3/3/16/26	10/18/116/137	-
20	CLA	1	304	-	1/1/12/20	5/22/100/115	-
20	CLA	F	804	-	1/1/11/20	3/13/91/115	-
20	CLA	A	809	-	1/1/15/20	14/37/115/115	-
20	CLA	1	309	1	1/1/14/20	4/31/109/115	-
20	CLA	2	310	24	1/1/10/20	4/8/86/115	-
19	CHL	2	307	-	3/3/17/26	9/21/119/137	-
20	CLA	A	841	-	1/1/15/20	23/37/115/115	-
20	CLA	N	202	17	1/1/11/20	4/13/91/115	-
24	LHG	2	318	20	-	12/41/41/53	-
30	DGD	B	848	-	-	10/55/95/95	0/2/2/2
23	BCR	3	317	-	-	4/29/63/63	0/2/2/2
21	LUT	O	205	-	-	6/29/67/67	0/2/2/2
20	CLA	B	804	-	1/1/11/20	5/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	1	314	1	1/1/11/20	3/15/93/115	-
26	HTG	A	852	-	-	2/10/30/30	0/1/1/1
20	CLA	1	302	1	1/1/15/20	10/37/115/115	-
20	CLA	O	201	24	1/1/12/20	9/22/100/115	-
19	CHL	2	305	-	3/3/15/26	3/12/110/137	-
27	PQN	A	842	-	-	7/23/43/43	0/2/2/2
20	CLA	B	821	-	1/1/13/20	9/27/105/115	-
20	CLA	J	103	14	1/1/10/20	4/10/88/115	-
20	CLA	A	827	-	1/1/15/20	16/37/115/115	-
20	CLA	4	302	4	1/1/14/20	8/31/109/115	-
21	LUT	1	319	-	-	2/29/67/67	0/2/2/2
20	CLA	B	835	-	1/1/12/20	3/21/99/115	-
20	CLA	B	803	-	1/1/15/20	10/37/115/115	-
20	CLA	L	303	-	1/1/15/20	12/37/115/115	-
20	CLA	O	202	-	1/1/11/20	7/13/91/115	-
23	BCR	B	845	-	-	2/29/63/63	0/2/2/2
23	BCR	J	104	-	-	2/29/63/63	0/2/2/2
20	CLA	B	838	-	1/1/15/20	5/37/115/115	-
22	XAT	3	316	-	-	0/31/93/93	0/4/4/4
20	CLA	3	312	-	1/1/11/20	3/13/91/115	-
20	CLA	1	307	-	1/1/14/20	12/33/111/115	-
19	CHL	4	305	-	3/3/17/26	5/24/122/137	-
20	CLA	A	839	-	1/1/15/20	16/37/115/115	-
20	CLA	B	805	-	1/1/15/20	15/37/115/115	-
20	CLA	B	811	-	1/1/13/20	8/25/101/115	-
20	CLA	B	815	-	1/1/14/20	9/31/109/115	-
20	CLA	B	828	-	1/1/15/20	15/37/115/115	-
20	CLA	N	203	-	1/1/12/20	8/19/97/115	-
21	LUT	O	204	-	-	1/29/67/67	0/2/2/2
23	BCR	I	101	-	-	8/29/63/63	0/2/2/2
26	HTG	1	322	-	-	0/10/30/30	0/1/1/1
20	CLA	B	807	-	1/1/13/20	8/25/103/115	-
20	CLA	3	314	-	1/1/11/20	4/15/93/115	-
22	XAT	4	317	-	-	0/31/93/93	0/4/4/4
20	CLA	B	831	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	3	305	3	1/1/11/20	7/16/94/115	-
20	CLA	1	312	1	1/1/15/20	15/37/115/115	-
22	XAT	2	316	-	-	0/31/93/93	0/4/4/4
20	CLA	A	815	-	1/1/11/20	0/13/91/115	-
20	CLA	A	833	-	1/1/15/20	10/37/115/115	-
21	LUT	4	316	-	-	2/29/67/67	0/2/2/2
20	CLA	A	823	-	1/1/13/20	4/25/103/115	-
20	CLA	B	818	-	1/1/14/20	11/31/109/115	-
27	PQN	B	840	-	-	1/23/43/43	0/2/2/2
20	CLA	1	303	-	1/1/15/20	10/37/115/115	-
20	CLA	A	824	-	1/1/15/20	11/37/115/115	-
20	CLA	A	813	-	1/1/11/20	2/13/91/115	-
20	CLA	A	817	-	1/1/15/20	14/37/115/115	-
20	CLA	A	835	5	1/1/11/20	9/13/91/115	-
24	LHG	A	844	20	-	12/31/31/53	-
20	CLA	2	313	-	1/1/10/20	4/11/89/115	-
20	CLA	A	822	-	1/1/12/20	7/21/99/115	-
21	LUT	3	315	-	-	2/29/67/67	0/2/2/2
20	CLA	1	308	1	1/1/15/20	12/37/115/115	-
20	CLA	A	825	-	1/1/15/20	3/37/115/115	-
29	LMT	B	847	-	-	6/21/61/61	0/2/2/2
20	CLA	2	311	2	1/1/12/20	8/22/100/115	-
20	CLA	A	808	5	1/1/15/20	16/37/115/115	-
20	CLA	4	303	-	1/1/14/20	9/31/109/115	-
20	CLA	B	832	-	1/1/13/20	2/29/107/115	-
23	BCR	F	806	-	-	2/29/63/63	0/2/2/2
20	CLA	3	302	-	1/1/12/20	4/19/97/115	-
20	CLA	4	310	-	1/1/13/20	7/25/103/115	-
20	CLA	F	802	-	1/1/15/20	9/37/115/115	-
20	CLA	A	820	-	1/1/15/20	8/37/115/115	-
20	CLA	B	816	-	1/1/13/20	6/25/103/115	-
29	LMT	G	601	-	-	4/21/61/61	0/2/2/2
21	LUT	1	315	-	-	2/29/67/67	0/2/2/2
20	CLA	A	811	-	1/1/12/20	5/24/102/115	-
26	HTG	F	803	-	-	2/10/30/30	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	806	-	1/1/15/20	10/37/115/115	-
20	CLA	B	810	-	1/1/15/20	11/37/115/115	-
20	CLA	L	302	16	1/1/11/20	6/13/91/115	-
19	CHL	4	307	-	3/3/17/26	3/21/119/137	-
20	CLA	A	821	-	1/1/11/20	9/18/96/115	-
20	CLA	B	824	-	1/1/15/20	14/37/115/115	-
20	CLA	O	203	-	1/1/14/20	7/31/109/115	-
23	BCR	1	317	-	-	2/29/63/63	0/2/2/2
20	CLA	H	201	-	1/1/13/20	11/27/105/115	-
20	CLA	A	831	-	1/1/15/20	15/37/115/115	-
20	CLA	B	834	-	1/1/11/20	1/13/91/115	-
20	CLA	3	310	-	1/1/12/20	0/22/100/115	-
23	BCR	A	849	-	-	4/29/63/63	0/2/2/2
20	CLA	2	302	2	1/1/15/20	7/37/115/115	-
20	CLA	A	816	-	1/1/15/20	10/37/115/115	-
20	CLA	3	311	3	1/1/13/20	1/25/103/115	-
20	CLA	B	836	-	1/1/15/20	6/37/115/115	-
20	CLA	K	205	15	1/1/11/20	0/13/91/115	-
20	CLA	B	806	6	1/1/15/20	13/37/115/115	-
28	SF4	A	850	-	-	-	0/6/5/5
20	CLA	A	834	-	1/1/15/20	11/37/115/115	-
19	CHL	4	315	-	3/3/15/26	4/12/110/137	-
20	CLA	G	605	11	1/1/11/20	6/15/93/115	-
19	CHL	3	306	-	3/3/16/26	5/17/115/137	-
26	HTG	G	602	-	-	0/10/30/30	0/1/1/1
20	CLA	A	836	-	1/1/12/20	6/21/99/115	-
20	CLA	3	304	-	1/1/10/20	0/10/88/115	-
20	CLA	A	851	-	1/1/15/20	15/37/115/115	-
28	SF4	C	102	-	-	-	0/6/5/5
20	CLA	F	805	-	1/1/11/20	6/15/93/115	-
20	CLA	A	803	20	1/1/13/20	6/25/103/115	-
20	CLA	4	308	4	1/1/12/20	4/19/97/115	-
19	CHL	1	301	1	3/3/17/26	10/23/121/137	-
20	CLA	B	809	6	1/1/15/20	4/37/115/115	-
19	CHL	2	301	2	3/3/17/26	8/24/122/137	-
23	BCR	B	842	-	-	6/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
19	CHL	1	306	1	3/3/16/26	11/18/116/137	-
20	CLA	L	307	-	1/1/11/20	7/13/91/115	-
20	CLA	3	303	-	1/1/11/20	4/13/91/115	-
20	CLA	3	307	3	1/1/12/20	6/19/97/115	-
20	CLA	B	819	-	1/1/15/20	7/37/115/115	-
20	CLA	4	301	4	1/1/11/20	7/15/93/115	-
24	LHG	A	843	-	-	9/53/53/53	-
23	BCR	B	843	-	-	4/29/63/63	0/2/2/2
26	HTG	4	320	-	-	3/10/30/30	0/1/1/1
20	CLA	A	853	-	1/1/15/20	14/37/115/115	-
20	CLA	J	101	-	1/1/15/20	5/37/115/115	-
20	CLA	B	802	-	1/1/15/20	8/37/115/115	-
25	LMG	1	320	-	-	9/44/64/70	0/1/1/1
20	CLA	B	839	-	1/1/15/20	6/37/115/115	-
20	CLA	G	604	-	1/1/12/20	4/19/97/115	-
20	CLA	B	825	-	1/1/15/20	15/37/115/115	-
20	CLA	G	603	-	1/1/11/20	2/13/91/115	-
23	BCR	4	318	-	-	6/29/63/63	0/2/2/2
19	CHL	4	306	-	3/3/17/26	10/21/119/137	-
20	CLA	B	830	-	1/1/12/20	5/19/97/115	-
20	CLA	K	201	15	1/1/11/20	2/15/93/115	-
22	XAT	1	316	-	-	1/31/93/93	0/4/4/4
20	CLA	B	833	-	1/1/15/20	11/37/115/115	-
20	CLA	A	840	-	1/1/15/20	6/37/115/115	-
23	BCR	B	841	-	-	3/29/63/63	0/2/2/2
20	CLA	A	838	-	1/1/15/20	12/37/115/115	-
20	CLA	A	832	-	1/1/15/20	8/37/115/115	-
23	BCR	J	102	-	-	7/29/63/63	0/2/2/2
20	CLA	4	314	-	1/1/12/20	7/19/97/115	-
20	CLA	A	805	-	1/1/15/20	17/37/115/115	-
26	HTG	N	201	-	-	2/10/30/30	0/1/1/1
25	LMG	4	319	-	-	6/39/59/70	0/1/1/1
20	CLA	2	308	2	1/1/12/20	5/19/97/115	-
23	BCR	B	844	-	-	2/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
20	CLA	A	837	-	1/1/15/20	12/37/115/115	-
20	CLA	4	312	-	1/1/15/20	12/37/115/115	-
23	BCR	L	306	-	-	0/29/63/63	0/2/2/2
19	CHL	2	314	2	3/3/15/26	2/12/110/137	-
20	CLA	2	312	2	1/1/15/20	9/37/115/115	-
20	CLA	B	801	-	1/1/15/20	5/37/115/115	-
20	CLA	A	830	-	1/1/12/20	3/19/97/115	-
20	CLA	4	304	-	1/1/12/20	8/19/97/115	-
23	BCR	B	846	-	-	2/29/63/63	0/2/2/2
20	CLA	4	309	4	1/1/14/20	6/31/109/115	-
20	CLA	B	826	-	1/1/15/20	2/37/115/115	-
26	HTG	J	105	-	-	1/10/30/30	0/1/1/1
20	CLA	B	814	-	1/1/15/20	7/37/115/115	-
20	CLA	2	303	-	1/1/11/20	8/18/96/115	-

All (1148) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	827	CLA	C4B-NB	8.01	1.42	1.35
20	1	303	CLA	C4B-NB	7.81	1.42	1.35
20	3	314	CLA	C4B-NB	7.77	1.42	1.35
20	3	309	CLA	C4B-NB	7.74	1.42	1.35
27	A	842	PQN	C3-C2	7.73	1.49	1.35
20	B	828	CLA	C4B-NB	7.72	1.42	1.35
20	A	811	CLA	C4B-NB	7.70	1.42	1.35
20	3	302	CLA	C4B-NB	7.68	1.42	1.35
20	K	201	CLA	C4B-NB	7.67	1.42	1.35
20	4	310	CLA	C4B-NB	7.64	1.42	1.35
27	B	840	PQN	C3-C2	7.62	1.49	1.35
20	L	307	CLA	C4B-NB	7.61	1.42	1.35
20	3	313	CLA	C4B-NB	7.57	1.42	1.35
20	A	835	CLA	C4B-NB	7.57	1.42	1.35
20	1	312	CLA	C4B-NB	7.54	1.41	1.35
20	4	301	CLA	C4B-NB	7.54	1.41	1.35
20	J	103	CLA	C4B-NB	7.54	1.41	1.35
20	F	805	CLA	C4B-NB	7.53	1.41	1.35
20	3	311	CLA	C4B-NB	7.53	1.41	1.35
20	A	838	CLA	C4B-NB	7.53	1.41	1.35
20	G	604	CLA	C4B-NB	7.53	1.41	1.35
20	1	321	CLA	C4B-NB	7.53	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	821	CLA	C4B-NB	7.53	1.41	1.35
20	3	310	CLA	C4B-NB	7.52	1.41	1.35
20	A	803	CLA	C4B-NB	7.50	1.41	1.35
20	A	853	CLA	C4B-NB	7.50	1.41	1.35
20	A	834	CLA	C4B-NB	7.50	1.41	1.35
20	N	203	CLA	C4B-NB	7.50	1.41	1.35
20	A	840	CLA	C4B-NB	7.49	1.41	1.35
20	G	605	CLA	C4B-NB	7.48	1.41	1.35
20	B	837	CLA	C4B-NB	7.46	1.41	1.35
20	3	305	CLA	C4B-NB	7.46	1.41	1.35
20	1	308	CLA	C4B-NB	7.46	1.41	1.35
20	A	832	CLA	C4B-NB	7.45	1.41	1.35
20	O	202	CLA	C4B-NB	7.45	1.41	1.35
20	4	314	CLA	C4B-NB	7.45	1.41	1.35
20	4	312	CLA	C4B-NB	7.45	1.41	1.35
20	B	801	CLA	C4B-NB	7.44	1.41	1.35
20	1	307	CLA	C4B-NB	7.44	1.41	1.35
20	2	304	CLA	C4B-NB	7.42	1.41	1.35
20	B	811	CLA	C4B-NB	7.41	1.41	1.35
20	B	833	CLA	C4B-NB	7.41	1.41	1.35
20	B	836	CLA	C4B-NB	7.41	1.41	1.35
20	A	817	CLA	C4B-NB	7.41	1.41	1.35
20	4	313	CLA	C4B-NB	7.40	1.41	1.35
20	A	815	CLA	C4B-NB	7.40	1.41	1.35
20	K	202	CLA	C4B-NB	7.40	1.41	1.35
20	1	305	CLA	C4B-NB	7.39	1.41	1.35
20	A	826	CLA	C4B-NB	7.39	1.41	1.35
20	G	603	CLA	C4B-NB	7.39	1.41	1.35
20	A	808	CLA	C4B-NB	7.39	1.41	1.35
20	O	201	CLA	C4B-NB	7.39	1.41	1.35
20	L	303	CLA	C4B-NB	7.39	1.41	1.35
20	A	810	CLA	C4B-NB	7.39	1.41	1.35
20	H	201	CLA	C4B-NB	7.39	1.41	1.35
20	B	822	CLA	C4B-NB	7.38	1.41	1.35
20	A	823	CLA	C4B-NB	7.38	1.41	1.35
20	2	312	CLA	C4B-NB	7.38	1.41	1.35
20	3	312	CLA	C4B-NB	7.36	1.41	1.35
20	B	812	CLA	C4B-NB	7.36	1.41	1.35
20	B	838	CLA	C4B-NB	7.36	1.41	1.35
20	B	820	CLA	C4B-NB	7.36	1.41	1.35
20	F	804	CLA	C4B-NB	7.36	1.41	1.35
20	4	304	CLA	C4B-NB	7.36	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	816	CLA	C4B-NB	7.36	1.41	1.35
20	2	303	CLA	C4B-NB	7.35	1.41	1.35
20	B	825	CLA	C4B-NB	7.35	1.41	1.35
20	2	313	CLA	C4B-NB	7.34	1.41	1.35
20	B	802	CLA	C4B-NB	7.34	1.41	1.35
20	A	819	CLA	C4B-NB	7.34	1.41	1.35
20	A	813	CLA	C4B-NB	7.34	1.41	1.35
20	B	817	CLA	C4B-NB	7.34	1.41	1.35
20	B	818	CLA	C4B-NB	7.33	1.41	1.35
20	A	841	CLA	C4B-NB	7.33	1.41	1.35
20	B	830	CLA	C4B-NB	7.33	1.41	1.35
20	A	818	CLA	C4B-NB	7.32	1.41	1.35
20	K	205	CLA	C4B-NB	7.32	1.41	1.35
20	3	301	CLA	C4B-NB	7.32	1.41	1.35
20	A	831	CLA	C4B-NB	7.31	1.41	1.35
20	B	810	CLA	C4B-NB	7.31	1.41	1.35
20	A	812	CLA	C4B-NB	7.31	1.41	1.35
20	B	839	CLA	C4B-NB	7.31	1.41	1.35
20	B	805	CLA	C4B-NB	7.31	1.41	1.35
20	1	313	CLA	C4B-NB	7.31	1.41	1.35
20	1	310	CLA	C4B-NB	7.30	1.41	1.35
20	1	314	CLA	C4B-NB	7.30	1.41	1.35
20	L	304	CLA	C4B-NB	7.30	1.41	1.35
20	A	824	CLA	C4B-NB	7.30	1.41	1.35
20	A	830	CLA	C4B-NB	7.30	1.41	1.35
20	A	804	CLA	C4B-NB	7.30	1.41	1.35
20	B	829	CLA	C4B-NB	7.30	1.41	1.35
20	N	202	CLA	C4B-NB	7.29	1.41	1.35
20	A	839	CLA	C4B-NB	7.29	1.41	1.35
20	A	825	CLA	C4B-NB	7.29	1.41	1.35
20	B	831	CLA	C4B-NB	7.28	1.41	1.35
20	A	820	CLA	C4B-NB	7.28	1.41	1.35
20	F	802	CLA	C4B-NB	7.28	1.41	1.35
20	1	311	CLA	C4B-NB	7.27	1.41	1.35
20	A	809	CLA	C4B-NB	7.27	1.41	1.35
20	B	813	CLA	C4B-NB	7.27	1.41	1.35
20	3	303	CLA	C4B-NB	7.26	1.41	1.35
20	A	851	CLA	C4B-NB	7.26	1.41	1.35
20	L	302	CLA	C4B-NB	7.25	1.41	1.35
20	B	824	CLA	C4B-NB	7.25	1.41	1.35
20	B	826	CLA	C4B-NB	7.25	1.41	1.35
20	A	814	CLA	C4B-NB	7.25	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	822	CLA	C4B-NB	7.25	1.41	1.35
20	B	816	CLA	C4B-NB	7.25	1.41	1.35
20	3	304	CLA	C4B-NB	7.25	1.41	1.35
20	A	802	CLA	C4B-NB	7.24	1.41	1.35
20	A	805	CLA	C4B-NB	7.24	1.41	1.35
20	B	823	CLA	C4B-NB	7.24	1.41	1.35
20	O	203	CLA	C4B-NB	7.24	1.41	1.35
20	1	304	CLA	C4B-NB	7.24	1.41	1.35
20	A	827	CLA	C4B-NB	7.24	1.41	1.35
20	B	814	CLA	C4B-NB	7.24	1.41	1.35
20	1	302	CLA	C4B-NB	7.23	1.41	1.35
20	B	832	CLA	C4B-NB	7.23	1.41	1.35
20	B	804	CLA	C4B-NB	7.23	1.41	1.35
20	4	309	CLA	C4B-NB	7.23	1.41	1.35
20	B	834	CLA	C4B-NB	7.23	1.41	1.35
20	B	819	CLA	C4B-NB	7.23	1.41	1.35
20	4	311	CLA	C4B-NB	7.22	1.41	1.35
20	J	101	CLA	C4B-NB	7.22	1.41	1.35
20	B	803	CLA	C4B-NB	7.21	1.41	1.35
20	A	833	CLA	C4B-NB	7.21	1.41	1.35
20	A	829	CLA	C4B-NB	7.21	1.41	1.35
20	3	307	CLA	C4B-NB	7.20	1.41	1.35
20	B	807	CLA	C4B-NB	7.20	1.41	1.35
20	4	308	CLA	C4B-NB	7.20	1.41	1.35
20	A	837	CLA	C4B-NB	7.20	1.41	1.35
20	B	808	CLA	C4B-NB	7.19	1.41	1.35
20	B	815	CLA	C4B-NB	7.19	1.41	1.35
20	A	821	CLA	C4B-NB	7.18	1.41	1.35
20	2	311	CLA	C4B-NB	7.18	1.41	1.35
20	A	828	CLA	C4B-NB	7.18	1.41	1.35
20	A	801	CLA	C4B-NB	7.18	1.41	1.35
20	A	836	CLA	C4B-NB	7.18	1.41	1.35
20	4	302	CLA	C4B-NB	7.17	1.41	1.35
20	4	303	CLA	C4B-NB	7.17	1.41	1.35
20	B	809	CLA	C4B-NB	7.17	1.41	1.35
20	3	308	CLA	C4B-NB	7.15	1.41	1.35
20	B	835	CLA	C4B-NB	7.13	1.41	1.35
20	2	308	CLA	C4B-NB	7.12	1.41	1.35
20	B	806	CLA	C4B-NB	7.12	1.41	1.35
20	2	310	CLA	C4B-NB	7.12	1.41	1.35
20	K	203	CLA	C4B-NB	7.12	1.41	1.35
20	A	807	CLA	C4B-NB	7.09	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	309	CLA	C4B-NB	7.07	1.41	1.35
20	1	309	CLA	C4B-NB	7.00	1.41	1.35
20	A	806	CLA	C4B-NB	7.00	1.41	1.35
20	2	302	CLA	C4B-NB	6.99	1.41	1.35
19	2	301	CHL	O1D-CGD	-5.70	1.06	1.21
19	1	301	CHL	CHC-C1C	5.28	1.48	1.35
20	3	309	CLA	CAA-C2A	-5.21	1.44	1.54
19	4	306	CHL	CHC-C1C	5.21	1.48	1.35
19	2	314	CHL	O2D-CGD	5.13	1.45	1.33
19	1	301	CHL	O2D-CGD	5.09	1.45	1.33
19	1	306	CHL	CHC-C1C	5.02	1.47	1.35
19	4	305	CHL	CHC-C1C	4.98	1.47	1.35
19	4	305	CHL	O2A-CGA	4.96	1.47	1.33
19	3	306	CHL	CHC-C1C	4.93	1.47	1.35
19	4	307	CHL	CHC-C1C	4.93	1.47	1.35
27	B	840	PQN	C10-C5	4.93	1.48	1.40
27	A	842	PQN	C10-C5	4.92	1.48	1.40
19	2	305	CHL	CHC-C1C	4.91	1.47	1.35
19	2	301	CHL	CHC-C1C	4.89	1.47	1.35
19	1	306	CHL	C3B-C2B	4.88	1.47	1.40
19	2	307	CHL	CHC-C1C	4.85	1.47	1.35
19	4	315	CHL	CHC-C1C	4.84	1.47	1.35
19	2	314	CHL	CHC-C1C	4.83	1.47	1.35
19	1	301	CHL	C2C-C3C	4.81	1.47	1.36
19	2	306	CHL	CHC-C1C	4.79	1.47	1.35
20	O	202	CLA	O2D-CGD	4.79	1.44	1.33
19	4	306	CHL	C3D-C4D	-4.77	1.33	1.44
19	1	306	CHL	C3D-C4D	-4.74	1.33	1.44
19	2	306	CHL	C3D-C4D	-4.71	1.33	1.44
19	3	306	CHL	C3D-C4D	-4.71	1.33	1.44
19	2	307	CHL	C3D-C4D	-4.71	1.33	1.44
19	4	307	CHL	C3B-C2B	4.70	1.46	1.40
19	1	301	CHL	C3D-C4D	-4.70	1.33	1.44
19	4	307	CHL	C3D-C4D	-4.68	1.33	1.44
19	4	305	CHL	C3D-C4D	-4.67	1.33	1.44
19	1	301	CHL	C3B-C2B	4.67	1.46	1.40
19	4	315	CHL	C3B-C2B	4.66	1.46	1.40
19	1	306	CHL	C2C-C3C	4.66	1.46	1.36
19	4	306	CHL	C2C-C3C	4.62	1.46	1.36
19	2	305	CHL	C3D-C4D	-4.62	1.33	1.44
19	2	301	CHL	C3B-C2B	4.62	1.46	1.40
19	2	305	CHL	C3B-C2B	4.61	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	314	CHL	C3B-C2B	4.60	1.46	1.40
19	4	315	CHL	C3D-C4D	-4.60	1.33	1.44
19	1	301	CHL	CHD-C1D	4.59	1.47	1.38
19	2	306	CHL	C3B-C2B	4.59	1.46	1.40
19	3	306	CHL	C3B-C2B	4.59	1.46	1.40
19	2	314	CHL	C3D-C4D	-4.59	1.33	1.44
19	4	315	CHL	C2C-C3C	4.59	1.46	1.36
19	4	306	CHL	CAA-C2A	-4.58	1.45	1.54
19	2	301	CHL	C3D-C4D	-4.57	1.33	1.44
19	2	301	CHL	C2C-C3C	4.57	1.46	1.36
19	4	306	CHL	OMC-CMC	-4.56	1.11	1.22
19	4	305	CHL	C2C-C3C	4.55	1.46	1.36
19	4	306	CHL	C3B-C2B	4.54	1.46	1.40
19	2	314	CHL	C2C-C3C	4.53	1.46	1.36
19	4	306	CHL	CHD-C1D	4.52	1.47	1.38
19	1	306	CHL	CHD-C1D	4.51	1.47	1.38
26	A	852	HTG	C1 ¹ -S1	-4.50	1.75	1.81
20	4	304	CLA	O1D-CGD	-4.47	1.10	1.21
19	2	306	CHL	C2C-C3C	4.46	1.46	1.36
19	3	306	CHL	C2C-C3C	4.43	1.46	1.36
19	2	305	CHL	C2C-C3C	4.43	1.46	1.36
19	4	307	CHL	C2C-C3C	4.42	1.46	1.36
19	3	306	CHL	CHD-C1D	4.40	1.46	1.38
20	O	202	CLA	O2A-CGA	4.40	1.45	1.30
19	2	307	CHL	C2C-C3C	4.39	1.46	1.36
19	2	301	CHL	OMC-CMC	-4.39	1.11	1.22
19	4	307	CHL	CHD-C1D	4.37	1.46	1.38
19	2	306	CHL	CHD-C1D	4.37	1.46	1.38
24	B	849	LHG	O7-C7	4.32	1.46	1.34
19	2	307	CHL	CHD-C1D	4.30	1.46	1.38
19	4	315	CHL	CHD-C1D	4.30	1.46	1.38
19	4	305	CHL	CHD-C1D	4.29	1.46	1.38
19	2	301	CHL	OBD-CAD	-4.28	1.15	1.22
19	2	301	CHL	CHD-C1D	4.25	1.46	1.38
20	3	309	CLA	C1D-ND	4.24	1.43	1.37
19	1	301	CHL	O2A-CGA	4.24	1.45	1.33
25	4	319	LMG	O8-C28	4.23	1.45	1.33
19	2	314	CHL	CHD-C1D	4.22	1.46	1.38
19	2	305	CHL	CHD-C1D	4.22	1.46	1.38
25	1	323	LMG	O8-C28	4.21	1.45	1.33
20	A	801	CLA	C1D-ND	4.21	1.43	1.37
19	4	305	CHL	C3B-C2B	4.19	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	844	LHG	O8-C23	4.18	1.45	1.33
25	1	320	LMG	O8-C28	4.17	1.45	1.33
24	2	318	LHG	O8-C23	4.16	1.45	1.33
19	2	307	CHL	C3B-C2B	4.15	1.46	1.40
24	A	843	LHG	O8-C23	4.15	1.45	1.33
19	1	301	CHL	CHD-C4C	4.15	1.48	1.39
24	1	318	LHG	O8-C23	4.14	1.45	1.33
30	B	848	DGD	O1G-C1A	4.14	1.45	1.33
25	1	320	LMG	O7-C10	4.09	1.45	1.34
24	1	318	LHG	O7-C7	4.09	1.45	1.34
19	2	301	CHL	CAA-C2A	-4.08	1.46	1.54
24	A	844	LHG	O7-C7	4.08	1.45	1.34
19	4	306	CHL	CHD-C4C	4.07	1.48	1.39
19	2	305	CHL	O1D-CGD	-4.06	1.11	1.21
30	B	848	DGD	O2G-C1B	4.06	1.45	1.34
25	1	323	LMG	O7-C10	4.06	1.45	1.34
24	2	318	LHG	O7-C7	4.05	1.45	1.34
25	4	319	LMG	O7-C10	4.03	1.45	1.34
19	1	306	CHL	CHD-C4C	4.01	1.48	1.39
19	2	307	CHL	CAA-C2A	-3.99	1.46	1.54
19	4	305	CHL	CHD-C4C	3.99	1.48	1.39
24	A	843	LHG	O7-C7	3.99	1.45	1.34
19	4	315	CHL	CHD-C4C	3.97	1.48	1.39
26	4	320	HTG	C1'-S1	-3.95	1.76	1.81
19	3	306	CHL	CHD-C4C	3.95	1.48	1.39
26	J	105	HTG	C1'-S1	-3.95	1.76	1.81
20	O	202	CLA	C1D-ND	3.93	1.42	1.37
19	2	306	CHL	CHD-C4C	3.93	1.48	1.39
19	1	306	CHL	O2D-CGD	3.92	1.42	1.33
20	G	603	CLA	C1D-ND	3.92	1.42	1.37
20	N	203	CLA	C1D-ND	3.91	1.42	1.37
19	3	306	CHL	OMC-CMC	-3.90	1.13	1.22
26	F	803	HTG	C1'-S1	-3.90	1.76	1.81
20	1	308	CLA	C1D-ND	3.89	1.42	1.37
20	4	313	CLA	C1D-ND	3.88	1.42	1.37
19	2	305	CHL	CHD-C4C	3.88	1.48	1.39
19	4	307	CHL	CHD-C4C	3.87	1.48	1.39
20	1	312	CLA	C1D-ND	3.87	1.42	1.37
20	3	313	CLA	C1D-ND	3.86	1.42	1.37
20	1	302	CLA	C1D-ND	3.86	1.42	1.37
19	2	307	CHL	OMC-CMC	-3.86	1.13	1.22
26	B	851	HTG	C1'-S1	-3.85	1.76	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	305	CHL	C1B-NB	-3.85	1.31	1.35
19	2	301	CHL	CHD-C4C	3.85	1.48	1.39
20	2	309	CLA	C1D-ND	3.85	1.42	1.37
26	N	201	HTG	C1'-S1	-3.85	1.76	1.81
20	B	804	CLA	C1D-ND	3.85	1.42	1.37
20	3	304	CLA	C1D-ND	3.84	1.42	1.37
19	2	314	CHL	CHD-C4C	3.84	1.48	1.39
20	O	203	CLA	C1D-ND	3.84	1.42	1.37
20	3	310	CLA	C1D-ND	3.84	1.42	1.37
20	2	311	CLA	C1D-ND	3.84	1.42	1.37
20	4	314	CLA	C1D-ND	3.83	1.42	1.37
20	2	312	CLA	C1D-ND	3.83	1.42	1.37
20	A	834	CLA	C1D-ND	3.83	1.42	1.37
20	4	303	CLA	C1D-ND	3.83	1.42	1.37
20	G	605	CLA	C1D-ND	3.83	1.42	1.37
20	A	820	CLA	C1D-ND	3.83	1.42	1.37
20	A	814	CLA	C1D-ND	3.83	1.42	1.37
20	A	824	CLA	C1D-ND	3.83	1.42	1.37
20	B	824	CLA	C1D-ND	3.83	1.42	1.37
20	1	304	CLA	C1D-ND	3.83	1.42	1.37
20	A	840	CLA	C1D-ND	3.83	1.42	1.37
26	G	602	HTG	C1'-S1	-3.82	1.76	1.81
20	B	837	CLA	C1D-ND	3.82	1.42	1.37
20	B	801	CLA	C1D-ND	3.82	1.42	1.37
20	B	813	CLA	C1D-ND	3.82	1.42	1.37
20	B	820	CLA	C1D-ND	3.81	1.42	1.37
20	L	307	CLA	C1D-ND	3.81	1.42	1.37
20	A	835	CLA	C1D-ND	3.81	1.42	1.37
20	3	308	CLA	C1D-ND	3.81	1.42	1.37
20	A	829	CLA	C1D-ND	3.81	1.42	1.37
20	A	805	CLA	C1D-ND	3.81	1.42	1.37
20	A	810	CLA	C1D-ND	3.81	1.42	1.37
20	J	101	CLA	C1D-ND	3.80	1.42	1.37
19	2	307	CHL	CHD-C4C	3.80	1.47	1.39
20	B	819	CLA	C1D-ND	3.80	1.42	1.37
20	3	311	CLA	C1D-ND	3.80	1.42	1.37
20	N	202	CLA	C1D-ND	3.80	1.42	1.37
20	H	201	CLA	C1D-ND	3.80	1.42	1.37
20	K	201	CLA	C1D-ND	3.80	1.42	1.37
20	L	302	CLA	C1D-ND	3.79	1.42	1.37
20	3	302	CLA	C1D-ND	3.79	1.42	1.37
20	A	838	CLA	C1D-ND	3.79	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	802	CLA	C1D-ND	3.79	1.42	1.37
20	4	311	CLA	C1D-ND	3.79	1.42	1.37
20	1	313	CLA	C1D-ND	3.79	1.42	1.37
20	1	303	CLA	C1D-ND	3.79	1.42	1.37
20	A	819	CLA	C1D-ND	3.79	1.42	1.37
20	3	305	CLA	C1D-ND	3.79	1.42	1.37
26	F	807	HTG	C1'-S1	-3.79	1.76	1.81
20	2	302	CLA	C1D-ND	3.78	1.42	1.37
20	1	307	CLA	C1D-ND	3.78	1.42	1.37
20	B	822	CLA	C1D-ND	3.78	1.42	1.37
20	G	604	CLA	C1D-ND	3.78	1.42	1.37
20	B	826	CLA	C1D-ND	3.78	1.42	1.37
20	A	808	CLA	C1D-ND	3.78	1.42	1.37
19	3	306	CHL	O2D-CGD	3.77	1.42	1.33
20	4	308	CLA	C1D-ND	3.77	1.42	1.37
20	J	103	CLA	C1D-ND	3.77	1.42	1.37
20	B	829	CLA	C1D-ND	3.77	1.42	1.37
20	3	314	CLA	C1D-ND	3.77	1.42	1.37
20	K	205	CLA	C1D-ND	3.77	1.42	1.37
20	1	311	CLA	C1D-ND	3.76	1.42	1.37
20	B	836	CLA	C1D-ND	3.76	1.42	1.37
20	A	803	CLA	C1D-ND	3.76	1.42	1.37
20	B	812	CLA	C1D-ND	3.76	1.42	1.37
20	A	839	CLA	C1D-ND	3.76	1.42	1.37
20	B	805	CLA	C1D-ND	3.76	1.42	1.37
20	A	806	CLA	C1D-ND	3.76	1.42	1.37
26	B	850	HTG	C1'-S1	-3.76	1.76	1.81
20	B	823	CLA	C1D-ND	3.76	1.42	1.37
20	3	312	CLA	C1D-ND	3.76	1.42	1.37
20	A	841	CLA	C1D-ND	3.75	1.42	1.37
20	A	812	CLA	C1D-ND	3.75	1.42	1.37
20	B	838	CLA	C1D-ND	3.75	1.42	1.37
20	2	310	CLA	C1D-ND	3.75	1.42	1.37
20	A	802	CLA	C1D-ND	3.75	1.42	1.37
20	A	818	CLA	C1D-ND	3.75	1.42	1.37
20	A	809	CLA	C1D-ND	3.75	1.42	1.37
20	A	828	CLA	C1D-ND	3.75	1.42	1.37
20	B	821	CLA	C1D-ND	3.74	1.42	1.37
20	B	814	CLA	C1D-ND	3.74	1.42	1.37
20	O	201	CLA	C1D-ND	3.74	1.42	1.37
20	4	301	CLA	C1D-ND	3.74	1.42	1.37
20	B	834	CLA	C1D-ND	3.74	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	301	CLA	C1D-ND	3.74	1.42	1.37
20	B	832	CLA	C1D-ND	3.74	1.42	1.37
20	K	203	CLA	C1D-ND	3.74	1.42	1.37
20	F	805	CLA	C1D-ND	3.73	1.42	1.37
20	A	823	CLA	C1D-ND	3.73	1.42	1.37
20	1	314	CLA	C1D-ND	3.73	1.42	1.37
20	B	835	CLA	C1D-ND	3.73	1.42	1.37
20	A	825	CLA	C1D-ND	3.73	1.42	1.37
20	A	833	CLA	C1D-ND	3.73	1.42	1.37
20	A	832	CLA	C1D-ND	3.73	1.42	1.37
20	A	813	CLA	C1D-ND	3.73	1.42	1.37
20	B	811	CLA	C1D-ND	3.73	1.42	1.37
20	B	816	CLA	C1D-ND	3.73	1.42	1.37
20	A	830	CLA	C1D-ND	3.72	1.42	1.37
20	K	202	CLA	C1D-ND	3.72	1.42	1.37
20	A	837	CLA	C1D-ND	3.72	1.42	1.37
20	A	851	CLA	C1D-ND	3.72	1.42	1.37
20	B	806	CLA	C1D-ND	3.72	1.42	1.37
20	B	808	CLA	C1D-ND	3.72	1.42	1.37
20	1	309	CLA	C1D-ND	3.72	1.42	1.37
20	2	308	CLA	C1D-ND	3.72	1.42	1.37
20	A	853	CLA	C1D-ND	3.72	1.42	1.37
20	4	302	CLA	C1D-ND	3.71	1.42	1.37
20	B	825	CLA	C1D-ND	3.71	1.42	1.37
20	B	839	CLA	C1D-ND	3.71	1.42	1.37
20	F	804	CLA	C1D-ND	3.71	1.42	1.37
20	A	836	CLA	C1D-ND	3.71	1.42	1.37
20	B	827	CLA	C1D-ND	3.71	1.42	1.37
20	2	313	CLA	C1D-ND	3.71	1.42	1.37
20	4	304	CLA	C1D-ND	3.71	1.42	1.37
20	A	807	CLA	C1D-ND	3.71	1.42	1.37
20	B	815	CLA	C1D-ND	3.71	1.42	1.37
20	L	303	CLA	C1D-ND	3.71	1.42	1.37
20	A	826	CLA	C1D-ND	3.70	1.42	1.37
26	1	322	HTG	C1'-S1	-3.70	1.76	1.81
20	A	827	CLA	C1D-ND	3.70	1.42	1.37
20	A	811	CLA	C1D-ND	3.70	1.42	1.37
20	A	831	CLA	C1D-ND	3.70	1.42	1.37
20	A	815	CLA	C1D-ND	3.70	1.42	1.37
20	B	807	CLA	C1D-ND	3.70	1.42	1.37
20	B	833	CLA	C1D-ND	3.69	1.42	1.37
20	2	303	CLA	C1D-ND	3.69	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	830	CLA	C1D-ND	3.69	1.42	1.37
20	A	804	CLA	C1D-ND	3.69	1.42	1.37
20	A	822	CLA	C1D-ND	3.69	1.42	1.37
20	B	810	CLA	C1D-ND	3.69	1.42	1.37
20	B	802	CLA	C1D-ND	3.69	1.42	1.37
20	L	304	CLA	C1D-ND	3.69	1.42	1.37
20	A	817	CLA	C1D-ND	3.68	1.42	1.37
20	B	828	CLA	C1D-ND	3.68	1.42	1.37
20	1	321	CLA	C1D-ND	3.68	1.42	1.37
20	O	202	CLA	C1C-NC	3.68	1.43	1.37
20	3	303	CLA	C1D-ND	3.67	1.42	1.37
20	2	304	CLA	C1D-ND	3.67	1.42	1.37
20	B	818	CLA	C1D-ND	3.67	1.42	1.37
20	3	307	CLA	C1D-ND	3.67	1.42	1.37
19	2	314	CHL	OBD-CAD	3.67	1.28	1.22
20	B	817	CLA	C1D-ND	3.66	1.42	1.37
19	1	301	CHL	OBD-CAD	3.65	1.28	1.22
20	1	310	CLA	C1D-ND	3.65	1.42	1.37
20	1	305	CLA	C1D-ND	3.65	1.42	1.37
20	4	310	CLA	C1D-ND	3.64	1.42	1.37
19	4	307	CHL	O2A-CGA	3.63	1.44	1.33
20	4	312	CLA	C1D-ND	3.63	1.42	1.37
20	B	803	CLA	C1D-ND	3.63	1.42	1.37
20	4	309	CLA	C1D-ND	3.62	1.42	1.37
20	A	821	CLA	C1D-ND	3.60	1.42	1.37
19	1	306	CHL	O2A-CGA	3.60	1.43	1.33
20	4	304	CLA	O2A-C1	-3.59	1.36	1.46
20	B	831	CLA	C1D-ND	3.59	1.42	1.37
20	B	809	CLA	C1D-ND	3.57	1.42	1.37
20	B	811	CLA	CAB-C3B	-3.53	1.44	1.51
20	A	816	CLA	C1D-ND	3.53	1.42	1.37
19	2	306	CHL	OMC-CMC	-3.52	1.13	1.22
19	2	306	CHL	O2A-CGA	3.51	1.43	1.33
19	4	315	CHL	O2D-CGD	3.50	1.41	1.33
19	4	305	CHL	CMB-C2B	-3.47	1.44	1.51
19	2	307	CHL	CBA-CGA	-3.41	1.40	1.50
19	2	306	CHL	O2D-CED	-3.39	1.37	1.45
19	4	307	CHL	OBD-CAD	-3.37	1.16	1.22
19	2	307	CHL	O2D-CGD	3.33	1.41	1.33
19	1	306	CHL	O2D-CED	-3.32	1.37	1.45
19	4	306	CHL	CMD-C2D	-3.32	1.43	1.50
19	4	307	CHL	OMC-CMC	-3.31	1.14	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	2	301	CHL	O2D-CED	-3.30	1.37	1.45
20	2	309	CLA	CHC-C1C	3.28	1.43	1.35
20	4	309	CLA	CHC-C1C	3.27	1.43	1.35
20	A	826	CLA	CHC-C1C	3.26	1.43	1.35
19	3	306	CHL	CAA-C2A	-3.26	1.48	1.54
20	B	825	CLA	CHC-C1C	3.26	1.43	1.35
19	2	307	CHL	C1B-NB	-3.24	1.32	1.35
19	4	315	CHL	CAA-C2A	-3.22	1.47	1.54
20	B	823	CLA	CHC-C1C	3.21	1.43	1.35
20	B	827	CLA	CHC-C1C	3.20	1.43	1.35
20	A	817	CLA	CHC-C1C	3.20	1.43	1.35
20	A	825	CLA	CHC-C1C	3.20	1.43	1.35
20	A	831	CLA	CHC-C1C	3.20	1.43	1.35
20	4	302	CLA	CHC-C1C	3.20	1.43	1.35
20	1	321	CLA	CHC-C1C	3.20	1.43	1.35
20	L	304	CLA	CHC-C1C	3.20	1.43	1.35
20	A	851	CLA	CHC-C1C	3.19	1.43	1.35
20	2	308	CLA	CHC-C1C	3.19	1.43	1.35
20	B	811	CLA	CHC-C1C	3.19	1.43	1.35
20	B	805	CLA	CHC-C1C	3.19	1.43	1.35
20	4	311	CLA	CHC-C1C	3.18	1.43	1.35
20	3	301	CLA	CHC-C1C	3.18	1.43	1.35
20	N	203	CLA	CHC-C1C	3.18	1.43	1.35
20	1	305	CLA	CHC-C1C	3.18	1.43	1.35
20	3	308	CLA	CHC-C1C	3.18	1.43	1.35
20	A	803	CLA	CHC-C1C	3.18	1.43	1.35
20	A	839	CLA	CHC-C1C	3.18	1.43	1.35
20	1	302	CLA	CHC-C1C	3.18	1.43	1.35
20	O	201	CLA	CHC-C1C	3.18	1.43	1.35
20	A	804	CLA	CHC-C1C	3.18	1.43	1.35
20	A	824	CLA	CHC-C1C	3.18	1.43	1.35
20	F	804	CLA	CHC-C1C	3.18	1.43	1.35
19	4	315	CHL	OMC-CMC	-3.18	1.14	1.22
20	B	836	CLA	CHC-C1C	3.17	1.43	1.35
20	1	309	CLA	CHC-C1C	3.17	1.43	1.35
20	A	816	CLA	CHC-C1C	3.17	1.43	1.35
20	3	305	CLA	CHC-C1C	3.17	1.43	1.35
20	A	807	CLA	CHC-C1C	3.17	1.43	1.35
20	A	802	CLA	CHC-C1C	3.17	1.43	1.35
20	K	203	CLA	CHC-C1C	3.17	1.43	1.35
20	2	312	CLA	CHC-C1C	3.17	1.43	1.35
20	L	303	CLA	CHC-C1C	3.16	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	F	802	CLA	CHC-C1C	3.16	1.43	1.35
20	B	801	CLA	CHC-C1C	3.16	1.43	1.35
20	G	605	CLA	CHC-C1C	3.16	1.43	1.35
20	O	202	CLA	CHC-C1C	3.16	1.43	1.35
20	3	307	CLA	CHC-C1C	3.16	1.43	1.35
20	A	806	CLA	CHC-C1C	3.16	1.43	1.35
20	B	803	CLA	CHC-C1C	3.16	1.43	1.35
20	K	202	CLA	CHC-C1C	3.16	1.43	1.35
20	B	821	CLA	CHC-C1C	3.16	1.43	1.35
20	B	819	CLA	CHC-C1C	3.16	1.43	1.35
20	2	303	CLA	CHC-C1C	3.16	1.43	1.35
20	3	310	CLA	CHC-C1C	3.16	1.43	1.35
20	A	818	CLA	CHC-C1C	3.15	1.43	1.35
20	A	828	CLA	CHC-C1C	3.15	1.43	1.35
20	A	809	CLA	CHC-C1C	3.15	1.43	1.35
20	4	308	CLA	CHC-C1C	3.15	1.43	1.35
20	A	810	CLA	CHC-C1C	3.15	1.43	1.35
20	B	833	CLA	CHC-C1C	3.15	1.43	1.35
20	B	835	CLA	CHC-C1C	3.15	1.43	1.35
20	B	837	CLA	CHC-C1C	3.15	1.43	1.35
20	F	805	CLA	CHC-C1C	3.15	1.43	1.35
20	A	813	CLA	CHC-C1C	3.15	1.43	1.35
20	B	834	CLA	CHC-C1C	3.15	1.43	1.35
20	O	203	CLA	CHC-C1C	3.15	1.43	1.35
20	A	834	CLA	CHC-C1C	3.14	1.43	1.35
20	3	304	CLA	CHC-C1C	3.14	1.43	1.35
20	1	312	CLA	CHC-C1C	3.14	1.43	1.35
20	1	314	CLA	CHC-C1C	3.14	1.43	1.35
20	4	312	CLA	CHC-C1C	3.14	1.43	1.35
20	A	814	CLA	CHC-C1C	3.14	1.43	1.35
20	N	202	CLA	CHC-C1C	3.14	1.43	1.35
20	A	822	CLA	CHC-C1C	3.14	1.43	1.35
20	A	821	CLA	CHC-C1C	3.14	1.43	1.35
20	2	304	CLA	CHC-C1C	3.13	1.43	1.35
20	L	307	CLA	CHC-C1C	3.13	1.43	1.35
20	1	304	CLA	CHC-C1C	3.13	1.43	1.35
20	A	815	CLA	CHC-C1C	3.13	1.43	1.35
20	A	833	CLA	CHC-C1C	3.13	1.43	1.35
20	B	820	CLA	CHC-C1C	3.13	1.43	1.35
20	A	841	CLA	CHC-C1C	3.13	1.43	1.35
20	A	837	CLA	CHC-C1C	3.13	1.43	1.35
20	J	101	CLA	CHC-C1C	3.13	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	311	CLA	CHC-C1C	3.13	1.43	1.35
20	B	802	CLA	CHC-C1C	3.13	1.43	1.35
20	B	830	CLA	CHC-C1C	3.13	1.43	1.35
20	J	103	CLA	CHC-C1C	3.13	1.43	1.35
19	2	301	CHL	CMB-C2B	-3.13	1.45	1.51
20	A	830	CLA	CHC-C1C	3.13	1.43	1.35
20	A	812	CLA	CHC-C1C	3.13	1.43	1.35
20	A	840	CLA	CHC-C1C	3.13	1.43	1.35
20	B	818	CLA	CHC-C1C	3.13	1.43	1.35
20	A	811	CLA	CHC-C1C	3.13	1.43	1.35
20	3	312	CLA	CHC-C1C	3.13	1.43	1.35
20	1	308	CLA	CHC-C1C	3.12	1.43	1.35
20	3	313	CLA	CHC-C1C	3.12	1.43	1.35
20	A	823	CLA	CHC-C1C	3.12	1.43	1.35
20	G	604	CLA	CHC-C1C	3.12	1.43	1.35
20	3	314	CLA	CHC-C1C	3.12	1.43	1.35
20	A	820	CLA	CHC-C1C	3.12	1.43	1.35
20	B	804	CLA	CHC-C1C	3.12	1.43	1.35
20	B	838	CLA	CHC-C1C	3.12	1.43	1.35
20	1	311	CLA	CHC-C1C	3.12	1.43	1.35
20	A	801	CLA	CHC-C1C	3.12	1.43	1.35
20	B	812	CLA	CHC-C1C	3.12	1.43	1.35
20	2	302	CLA	CHC-C1C	3.12	1.43	1.35
20	A	853	CLA	CHC-C1C	3.12	1.43	1.35
20	B	815	CLA	CHC-C1C	3.12	1.43	1.35
20	A	836	CLA	CHC-C1C	3.12	1.43	1.35
20	B	822	CLA	CHC-C1C	3.12	1.43	1.35
20	G	603	CLA	CHC-C1C	3.12	1.43	1.35
20	H	201	CLA	CHC-C1C	3.12	1.43	1.35
20	4	314	CLA	CHC-C1C	3.12	1.43	1.35
20	B	826	CLA	CHC-C1C	3.12	1.43	1.35
20	1	307	CLA	CHC-C1C	3.12	1.43	1.35
20	K	201	CLA	CHC-C1C	3.11	1.42	1.35
20	K	205	CLA	CHC-C1C	3.11	1.42	1.35
20	B	816	CLA	CHC-C1C	3.11	1.42	1.35
20	B	828	CLA	CHC-C1C	3.11	1.42	1.35
20	B	814	CLA	CHC-C1C	3.11	1.42	1.35
20	B	813	CLA	CHC-C1C	3.11	1.42	1.35
20	A	805	CLA	CHC-C1C	3.11	1.42	1.35
20	A	826	CLA	C4D-ND	-3.11	1.33	1.37
20	B	821	CLA	C4D-ND	-3.11	1.33	1.37
20	4	310	CLA	CHC-C1C	3.11	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	819	CLA	CHC-C1C	3.11	1.42	1.35
20	4	301	CLA	CHC-C1C	3.10	1.42	1.35
20	B	829	CLA	CHC-C1C	3.10	1.42	1.35
20	A	835	CLA	CHC-C1C	3.10	1.42	1.35
20	A	808	CLA	CHC-C1C	3.10	1.42	1.35
20	4	304	CLA	CHC-C1C	3.10	1.42	1.35
20	B	806	CLA	CHC-C1C	3.10	1.42	1.35
20	B	832	CLA	CHC-C1C	3.10	1.42	1.35
20	A	832	CLA	CHC-C1C	3.10	1.42	1.35
20	4	313	CLA	CHC-C1C	3.09	1.42	1.35
20	1	313	CLA	CHC-C1C	3.09	1.42	1.35
20	A	838	CLA	CHC-C1C	3.09	1.42	1.35
20	A	827	CLA	CHC-C1C	3.09	1.42	1.35
20	3	302	CLA	CHC-C1C	3.09	1.42	1.35
20	4	304	CLA	CAA-C2A	-3.09	1.48	1.54
20	B	839	CLA	CHC-C1C	3.09	1.42	1.35
20	3	303	CLA	CHC-C1C	3.09	1.42	1.35
20	2	313	CLA	CHC-C1C	3.09	1.42	1.35
20	B	835	CLA	C4D-ND	-3.09	1.33	1.37
20	L	302	CLA	CHC-C1C	3.09	1.42	1.35
19	1	301	CHL	C3D-C2D	3.09	1.47	1.39
20	B	807	CLA	CHC-C1C	3.09	1.42	1.35
20	1	310	CLA	CHC-C1C	3.08	1.42	1.35
20	B	817	CLA	CHC-C1C	3.08	1.42	1.35
20	A	829	CLA	CHC-C1C	3.08	1.42	1.35
20	B	831	CLA	CHC-C1C	3.08	1.42	1.35
20	3	311	CLA	CHC-C1C	3.08	1.42	1.35
20	3	309	CLA	CHC-C1C	3.08	1.42	1.35
20	B	824	CLA	CHC-C1C	3.08	1.42	1.35
20	A	806	CLA	C4D-ND	-3.07	1.33	1.37
20	B	810	CLA	CHC-C1C	3.06	1.42	1.35
20	B	808	CLA	CHC-C1C	3.06	1.42	1.35
20	2	310	CLA	CHC-C1C	3.06	1.42	1.35
20	B	809	CLA	CHC-C1C	3.06	1.42	1.35
20	L	303	CLA	C4D-ND	-3.06	1.33	1.37
20	K	202	CLA	C4D-ND	-3.06	1.33	1.37
20	4	303	CLA	CHC-C1C	3.05	1.42	1.35
19	3	306	CHL	O1D-CGD	-3.05	1.13	1.21
20	B	826	CLA	C4D-ND	-3.05	1.33	1.37
19	4	306	CHL	C1D-C2D	3.04	1.51	1.45
20	A	804	CLA	C4D-ND	-3.04	1.33	1.37
20	B	810	CLA	C4D-ND	-3.03	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	807	CLA	C4D-ND	-3.03	1.33	1.37
20	A	823	CLA	C4D-ND	-3.03	1.33	1.37
20	2	302	CLA	C4D-ND	-3.02	1.33	1.37
20	B	814	CLA	C4D-ND	-3.02	1.33	1.37
20	1	313	CLA	C4D-ND	-3.02	1.33	1.37
20	2	303	CLA	C4D-ND	-3.02	1.33	1.37
20	A	825	CLA	C4D-ND	-3.02	1.33	1.37
20	1	303	CLA	CHC-C1C	3.02	1.42	1.35
20	L	302	CLA	C4D-ND	-3.02	1.33	1.37
20	A	803	CLA	C4D-ND	-3.01	1.33	1.37
20	O	202	CLA	C4D-ND	-3.01	1.33	1.37
20	A	833	CLA	C4D-ND	-3.01	1.33	1.37
20	L	304	CLA	C4D-ND	-3.01	1.33	1.37
20	A	837	CLA	C4D-ND	-3.00	1.33	1.37
20	A	822	CLA	C4D-ND	-3.00	1.33	1.37
20	B	831	CLA	C4D-ND	-3.00	1.33	1.37
20	A	816	CLA	C4D-ND	-2.99	1.33	1.37
20	A	853	CLA	C4D-ND	-2.99	1.33	1.37
20	4	303	CLA	C4D-ND	-2.98	1.33	1.37
20	4	310	CLA	C4D-ND	-2.98	1.33	1.37
19	4	306	CHL	CBD-CGD	-2.98	1.43	1.52
20	A	827	CLA	C4D-ND	-2.98	1.33	1.37
20	B	816	CLA	C4D-ND	-2.98	1.33	1.37
19	1	301	CHL	C1D-C2D	2.98	1.51	1.45
20	1	304	CLA	C4D-ND	-2.98	1.33	1.37
20	3	305	CLA	C4D-ND	-2.98	1.33	1.37
20	1	314	CLA	C4D-ND	-2.98	1.33	1.37
20	A	815	CLA	C4D-ND	-2.97	1.33	1.37
20	A	821	CLA	C4D-ND	-2.97	1.33	1.37
20	A	813	CLA	C4D-ND	-2.97	1.33	1.37
20	O	201	CLA	C4D-ND	-2.97	1.33	1.37
20	K	203	CLA	C4D-ND	-2.97	1.33	1.37
20	A	836	CLA	C4D-ND	-2.97	1.33	1.37
20	3	312	CLA	C4D-ND	-2.97	1.33	1.37
20	A	805	CLA	C4D-ND	-2.97	1.33	1.37
20	B	809	CLA	C4D-ND	-2.97	1.33	1.37
20	1	321	CLA	C4D-ND	-2.97	1.33	1.37
20	A	841	CLA	C4D-ND	-2.96	1.33	1.37
20	B	818	CLA	C4D-ND	-2.96	1.33	1.37
26	A	852	HTG	C1-S1	-2.96	1.76	1.80
20	B	830	CLA	C4D-ND	-2.96	1.33	1.37
20	O	203	CLA	C4D-ND	-2.96	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	304	CLA	C4D-ND	-2.96	1.33	1.37
20	B	805	CLA	C4D-ND	-2.96	1.33	1.37
20	A	818	CLA	C4D-ND	-2.96	1.33	1.37
19	1	306	CHL	C1D-C2D	2.96	1.51	1.45
20	A	809	CLA	C4D-ND	-2.95	1.33	1.37
20	G	605	CLA	C4D-ND	-2.95	1.33	1.37
20	1	309	CLA	C4D-ND	-2.95	1.33	1.37
20	2	310	CLA	C4D-ND	-2.95	1.33	1.37
20	A	810	CLA	C4D-ND	-2.95	1.33	1.37
20	B	813	CLA	C4D-ND	-2.95	1.33	1.37
19	1	306	CHL	C3D-C2D	2.95	1.47	1.39
19	4	315	CHL	C3D-C2D	2.95	1.47	1.39
20	B	807	CLA	C4D-ND	-2.95	1.33	1.37
20	A	814	CLA	C4D-ND	-2.95	1.33	1.37
20	A	835	CLA	C4D-ND	-2.95	1.33	1.37
20	B	822	CLA	C4D-ND	-2.95	1.33	1.37
19	2	305	CHL	OMC-CMC	-2.95	1.15	1.22
20	1	311	CLA	C4D-ND	-2.95	1.33	1.37
20	B	819	CLA	C4D-ND	-2.95	1.33	1.37
20	2	311	CLA	C4D-ND	-2.95	1.33	1.37
20	3	301	CLA	C4D-ND	-2.94	1.33	1.37
20	1	302	CLA	C4D-ND	-2.94	1.33	1.37
20	B	836	CLA	C4D-ND	-2.94	1.33	1.37
19	4	315	CHL	C1D-C2D	2.94	1.51	1.45
20	B	801	CLA	C4D-ND	-2.94	1.33	1.37
20	A	811	CLA	C4D-ND	-2.94	1.33	1.37
20	B	823	CLA	C4D-ND	-2.94	1.33	1.37
20	A	817	CLA	C4D-ND	-2.94	1.33	1.37
20	4	308	CLA	C4D-ND	-2.94	1.33	1.37
20	4	313	CLA	C4D-ND	-2.94	1.33	1.37
20	A	834	CLA	C4D-ND	-2.94	1.33	1.37
20	3	303	CLA	C4D-ND	-2.94	1.33	1.37
20	A	832	CLA	C4D-ND	-2.94	1.33	1.37
20	F	804	CLA	C4D-ND	-2.94	1.33	1.37
20	B	838	CLA	C4D-ND	-2.94	1.33	1.37
20	3	309	CLA	O2D-CGD	2.94	1.40	1.33
20	A	824	CLA	C4D-ND	-2.93	1.33	1.37
20	A	828	CLA	C4D-ND	-2.93	1.33	1.37
20	B	827	CLA	C4D-ND	-2.93	1.33	1.37
20	B	839	CLA	C4D-ND	-2.93	1.33	1.37
20	B	837	CLA	C4D-ND	-2.93	1.33	1.37
20	A	820	CLA	C4D-ND	-2.93	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	A	839	CLA	C4D-ND	-2.93	1.33	1.37
20	B	815	CLA	C4D-ND	-2.93	1.33	1.37
20	3	302	CLA	C4D-ND	-2.93	1.33	1.37
20	K	205	CLA	C4D-ND	-2.93	1.33	1.37
20	F	802	CLA	C4D-ND	-2.93	1.33	1.37
20	4	311	CLA	C4D-ND	-2.93	1.33	1.37
20	A	838	CLA	C4D-ND	-2.93	1.33	1.37
20	B	829	CLA	C4D-ND	-2.92	1.33	1.37
19	4	305	CHL	C3D-C2D	2.92	1.47	1.39
20	3	307	CLA	C4D-ND	-2.92	1.33	1.37
20	A	812	CLA	C4D-ND	-2.92	1.33	1.37
20	B	806	CLA	C4D-ND	-2.92	1.33	1.37
20	J	101	CLA	C4D-ND	-2.92	1.33	1.37
20	A	851	CLA	C4D-ND	-2.92	1.33	1.37
20	3	310	CLA	C4D-ND	-2.92	1.33	1.37
20	4	301	CLA	C4D-ND	-2.92	1.33	1.37
19	3	306	CHL	C1D-C2D	2.92	1.51	1.45
19	4	307	CHL	C3D-C2D	2.91	1.47	1.39
19	4	305	CHL	C1D-C2D	2.91	1.51	1.45
20	1	305	CLA	C4D-ND	-2.91	1.33	1.37
20	A	808	CLA	C4D-ND	-2.91	1.33	1.37
20	B	803	CLA	C4D-ND	-2.91	1.33	1.37
20	B	832	CLA	C4D-ND	-2.91	1.33	1.37
20	4	314	CLA	C4D-ND	-2.91	1.33	1.37
20	A	829	CLA	C4D-ND	-2.91	1.33	1.37
20	B	834	CLA	C4D-ND	-2.91	1.33	1.37
20	3	311	CLA	C4D-ND	-2.90	1.33	1.37
20	4	302	CLA	C4D-ND	-2.90	1.33	1.37
20	B	828	CLA	C4D-ND	-2.90	1.33	1.37
20	2	304	CLA	C4D-ND	-2.90	1.33	1.37
20	1	310	CLA	C4D-ND	-2.90	1.33	1.37
20	B	820	CLA	C4D-ND	-2.89	1.33	1.37
19	4	306	CHL	C3D-C2D	2.89	1.47	1.39
20	B	817	CLA	C4D-ND	-2.89	1.33	1.37
19	2	305	CHL	C1D-C2D	2.89	1.51	1.45
20	J	103	CLA	C4D-ND	-2.89	1.33	1.37
20	F	805	CLA	C4D-ND	-2.89	1.33	1.37
19	2	306	CHL	C3D-C2D	2.89	1.47	1.39
19	2	306	CHL	CAA-C2A	-2.89	1.48	1.54
19	2	314	CHL	C3D-C2D	2.89	1.47	1.39
19	2	301	CHL	C1D-C2D	2.89	1.51	1.45
20	2	308	CLA	C4D-ND	-2.89	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	2	312	CLA	C4D-ND	-2.89	1.33	1.37
19	2	314	CHL	C1D-C2D	2.88	1.51	1.45
20	3	314	CLA	C4D-ND	-2.88	1.33	1.37
20	1	312	CLA	C4D-ND	-2.88	1.33	1.37
19	2	301	CHL	O1A-CGA	-2.88	1.14	1.22
19	3	306	CHL	C3D-C2D	2.87	1.47	1.39
20	B	812	CLA	C4D-ND	-2.87	1.33	1.37
19	4	307	CHL	O2D-CED	-2.87	1.38	1.45
20	A	830	CLA	C4D-ND	-2.87	1.33	1.37
19	2	305	CHL	C3D-C2D	2.87	1.47	1.39
20	4	309	CLA	C4D-ND	-2.87	1.33	1.37
20	B	824	CLA	C4D-ND	-2.87	1.33	1.37
20	G	603	CLA	C4D-ND	-2.87	1.33	1.37
20	3	308	CLA	C4D-ND	-2.86	1.33	1.37
20	B	804	CLA	C4D-ND	-2.86	1.33	1.37
20	4	304	CLA	C4D-ND	-2.86	1.33	1.37
20	A	802	CLA	C4D-ND	-2.86	1.33	1.37
20	1	307	CLA	C4D-ND	-2.86	1.33	1.37
20	4	312	CLA	C4D-ND	-2.86	1.33	1.37
20	A	819	CLA	C4D-ND	-2.86	1.33	1.37
20	B	825	CLA	C4D-ND	-2.86	1.33	1.37
20	A	840	CLA	C4D-ND	-2.86	1.33	1.37
19	2	306	CHL	C1D-C2D	2.86	1.51	1.45
20	A	831	CLA	C4D-ND	-2.86	1.33	1.37
20	K	201	CLA	C4D-ND	-2.85	1.33	1.37
19	2	307	CHL	C3D-C2D	2.85	1.46	1.39
19	2	301	CHL	C3D-C2D	2.85	1.46	1.39
20	B	833	CLA	C4D-ND	-2.84	1.33	1.37
20	B	811	CLA	C4D-ND	-2.84	1.33	1.37
20	H	201	CLA	C4D-ND	-2.84	1.33	1.37
20	L	307	CLA	C4D-ND	-2.84	1.33	1.37
20	3	313	CLA	C4D-ND	-2.84	1.33	1.37
19	3	306	CHL	O2A-CGA	2.83	1.42	1.33
20	3	309	CLA	C4D-ND	-2.83	1.33	1.37
20	2	313	CLA	C4D-ND	-2.83	1.33	1.37
20	B	808	CLA	C4D-ND	-2.83	1.33	1.37
20	1	308	CLA	C4D-ND	-2.83	1.33	1.37
20	4	304	CLA	CMA-C3A	-2.83	1.47	1.53
20	B	802	CLA	C4D-ND	-2.83	1.33	1.37
20	1	303	CLA	C4D-ND	-2.82	1.33	1.37
20	2	309	CLA	C4D-ND	-2.82	1.33	1.37
20	3	309	CLA	C1C-NC	2.82	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	G	604	CLA	C4D-ND	-2.82	1.33	1.37
20	O	202	CLA	OBD-CAD	2.81	1.27	1.22
19	3	306	CHL	O1A-CGA	-2.81	1.14	1.22
19	4	307	CHL	C1D-C2D	2.80	1.50	1.45
19	4	305	CHL	CAA-C2A	-2.79	1.48	1.54
20	N	202	CLA	C4D-ND	-2.79	1.33	1.37
19	2	307	CHL	O2A-CGA	2.79	1.41	1.33
19	2	307	CHL	C1D-C2D	2.79	1.50	1.45
20	N	203	CLA	C4D-ND	-2.77	1.33	1.37
19	2	307	CHL	O2D-CED	-2.74	1.38	1.45
20	A	801	CLA	C4D-ND	-2.73	1.33	1.37
19	4	306	CHL	O2A-CGA	2.70	1.41	1.33
19	4	306	CHL	O2D-CGD	2.69	1.39	1.33
19	2	305	CHL	O2D-CGD	2.69	1.39	1.33
19	2	306	CHL	CMD-C2D	-2.68	1.45	1.50
19	4	305	CHL	O1D-CGD	-2.68	1.14	1.21
20	3	309	CLA	O2A-CGA	2.65	1.41	1.33
26	4	320	HTG	C1-S1	-2.64	1.76	1.80
19	4	305	CHL	CBD-CGD	-2.64	1.44	1.52
26	J	105	HTG	C1-S1	-2.61	1.76	1.80
20	B	819	CLA	CMB-C2B	-2.59	1.46	1.51
19	2	307	CHL	O2A-C1	-2.58	1.38	1.46
20	B	829	CLA	CMB-C2B	-2.58	1.46	1.51
20	A	835	CLA	CMB-C2B	-2.58	1.46	1.51
20	B	809	CLA	CMB-C2B	-2.57	1.46	1.51
19	2	306	CHL	CMB-C2B	-2.57	1.46	1.51
19	4	307	CHL	O1A-CGA	-2.56	1.14	1.22
20	A	841	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	839	CLA	CMB-C2B	-2.56	1.46	1.51
20	B	817	CLA	CMB-C2B	-2.55	1.46	1.51
19	2	301	CHL	CMA-C3A	-2.55	1.47	1.53
26	G	602	HTG	C1-S1	-2.55	1.76	1.80
20	A	820	CLA	CMB-C2B	-2.54	1.46	1.51
20	2	304	CLA	CMB-C2B	-2.54	1.46	1.51
19	4	306	CHL	C1B-NB	-2.54	1.32	1.35
19	1	301	CHL	MG-NA	-2.53	2.00	2.06
20	F	804	CLA	CMB-C2B	-2.53	1.46	1.51
26	F	803	HTG	C1-S1	-2.53	1.76	1.80
20	3	302	CLA	CMB-C2B	-2.53	1.46	1.51
20	A	834	CLA	CMB-C2B	-2.52	1.46	1.51
20	H	201	CLA	CMB-C2B	-2.52	1.46	1.51
20	B	828	CLA	CMB-C2B	-2.52	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	303	CLA	CMB-C2B	-2.51	1.46	1.51
20	B	838	CLA	CMB-C2B	-2.51	1.46	1.51
20	2	309	CLA	CMB-C2B	-2.51	1.46	1.51
19	1	301	CHL	C4B-CHC	2.51	1.48	1.41
20	A	818	CLA	CMB-C2B	-2.51	1.46	1.51
20	A	816	CLA	CMB-C2B	-2.50	1.46	1.51
20	A	823	CLA	CMB-C2B	-2.50	1.46	1.51
20	B	830	CLA	CMB-C2B	-2.50	1.46	1.51
19	2	307	CHL	O1A-CGA	-2.50	1.15	1.22
20	3	311	CLA	CMB-C2B	-2.50	1.46	1.51
20	K	205	CLA	CMB-C2B	-2.50	1.46	1.51
20	A	829	CLA	CMB-C2B	-2.49	1.46	1.51
20	4	308	CLA	CMB-C2B	-2.49	1.46	1.51
20	A	832	CLA	CMB-C2B	-2.49	1.46	1.51
20	B	812	CLA	CMB-C2B	-2.49	1.46	1.51
24	B	849	LHG	O8-C23	2.49	1.45	1.33
20	4	310	CLA	CMB-C2B	-2.49	1.46	1.51
20	B	822	CLA	CMB-C2B	-2.49	1.46	1.51
20	A	801	CLA	CMB-C2B	-2.49	1.46	1.51
20	3	312	CLA	CMB-C2B	-2.48	1.46	1.51
20	A	840	CLA	CMB-C2B	-2.48	1.46	1.51
20	B	831	CLA	CMB-C2B	-2.48	1.46	1.51
19	4	306	CHL	C4B-NB	-2.48	1.33	1.35
26	N	201	HTG	C1-S1	-2.48	1.76	1.80
20	B	832	CLA	CMB-C2B	-2.48	1.46	1.51
19	4	315	CHL	CMB-C2B	-2.48	1.46	1.51
20	3	313	CLA	CMB-C2B	-2.47	1.46	1.51
20	1	309	CLA	CMB-C2B	-2.47	1.46	1.51
20	A	817	CLA	CMB-C2B	-2.47	1.46	1.51
19	2	305	CHL	C3B-CAB	-2.47	1.42	1.47
20	1	312	CLA	CMB-C2B	-2.47	1.46	1.51
20	2	312	CLA	CMB-C2B	-2.47	1.46	1.51
19	2	306	CHL	C4C-C3C	2.47	1.49	1.45
20	B	808	CLA	CMB-C2B	-2.47	1.46	1.51
20	A	822	CLA	CMB-C2B	-2.47	1.46	1.51
20	G	603	CLA	CMB-C2B	-2.47	1.46	1.51
26	1	322	HTG	C1-S1	-2.47	1.76	1.80
20	A	836	CLA	CMB-C2B	-2.46	1.46	1.51
20	L	302	CLA	CMB-C2B	-2.46	1.46	1.51
20	A	831	CLA	CMB-C2B	-2.46	1.46	1.51
26	B	850	HTG	C1-S1	-2.46	1.76	1.80
20	F	805	CLA	CMB-C2B	-2.46	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	3	310	CLA	CMB-C2B	-2.46	1.46	1.51
20	A	811	CLA	CMB-C2B	-2.46	1.46	1.51
20	A	810	CLA	CMB-C2B	-2.46	1.46	1.51
20	B	811	CLA	CMB-C2B	-2.46	1.46	1.51
20	A	853	CLA	CMB-C2B	-2.45	1.46	1.51
20	G	604	CLA	CMB-C2B	-2.45	1.46	1.51
20	J	103	CLA	CMB-C2B	-2.45	1.46	1.51
20	A	808	CLA	CMB-C2B	-2.45	1.46	1.51
20	K	202	CLA	CMB-C2B	-2.45	1.46	1.51
20	A	830	CLA	CMB-C2B	-2.45	1.46	1.51
20	1	308	CLA	CMB-C2B	-2.45	1.46	1.51
20	A	838	CLA	CMB-C2B	-2.45	1.46	1.51
20	2	303	CLA	CMB-C2B	-2.45	1.46	1.51
20	1	307	CLA	CMB-C2B	-2.45	1.46	1.51
20	A	815	CLA	CMB-C2B	-2.45	1.46	1.51
20	4	309	CLA	CMB-C2B	-2.45	1.46	1.51
20	B	821	CLA	CMB-C2B	-2.45	1.46	1.51
20	K	201	CLA	CMB-C2B	-2.44	1.46	1.51
19	1	306	CHL	CMB-C2B	-2.44	1.46	1.51
20	A	805	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	824	CLA	CMB-C2B	-2.44	1.46	1.51
20	L	307	CLA	CMB-C2B	-2.44	1.46	1.51
20	4	312	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	819	CLA	CMB-C2B	-2.44	1.46	1.51
20	O	201	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	803	CLA	CMB-C2B	-2.44	1.46	1.51
26	B	851	HTG	C1-S1	-2.44	1.77	1.80
20	G	605	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	839	CLA	CMB-C2B	-2.44	1.46	1.51
20	A	826	CLA	CMB-C2B	-2.43	1.46	1.51
20	4	301	CLA	CMB-C2B	-2.43	1.46	1.51
20	B	814	CLA	CMB-C2B	-2.43	1.46	1.51
20	B	807	CLA	CMB-C2B	-2.43	1.46	1.51
20	1	303	CLA	CMB-C2B	-2.43	1.46	1.51
20	B	824	CLA	CMB-C2B	-2.43	1.46	1.51
20	1	313	CLA	CMB-C2B	-2.43	1.46	1.51
20	L	303	CLA	CMB-C2B	-2.43	1.46	1.51
20	B	804	CLA	CMB-C2B	-2.43	1.46	1.51
20	4	304	CLA	O2D-CGD	2.43	1.39	1.33
20	B	833	CLA	CMB-C2B	-2.43	1.46	1.51
20	2	310	CLA	CMB-C2B	-2.42	1.46	1.51
20	B	820	CLA	CMB-C2B	-2.42	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	826	CLA	CMB-C2B	-2.42	1.46	1.51
19	2	305	CHL	CMB-C2B	-2.42	1.46	1.51
20	B	802	CLA	CMB-C2B	-2.42	1.46	1.51
20	B	813	CLA	CMB-C2B	-2.42	1.46	1.51
20	B	823	CLA	CMB-C2B	-2.42	1.46	1.51
20	1	310	CLA	CMB-C2B	-2.42	1.46	1.51
20	A	809	CLA	CMB-C2B	-2.42	1.46	1.51
20	B	827	CLA	CMB-C2B	-2.42	1.46	1.51
19	4	306	CHL	C4B-CHC	2.42	1.47	1.41
20	4	302	CLA	CMB-C2B	-2.42	1.46	1.51
20	A	828	CLA	CMB-C2B	-2.42	1.46	1.51
20	3	305	CLA	CMB-C2B	-2.42	1.46	1.51
20	3	314	CLA	CMB-C2B	-2.41	1.46	1.51
20	4	314	CLA	CMB-C2B	-2.41	1.46	1.51
20	4	311	CLA	CMB-C2B	-2.41	1.46	1.51
20	B	815	CLA	CMB-C2B	-2.41	1.46	1.51
20	B	836	CLA	CMB-C2B	-2.41	1.46	1.51
20	3	308	CLA	CMB-C2B	-2.41	1.46	1.51
20	F	802	CLA	CMB-C2B	-2.41	1.46	1.51
20	A	833	CLA	CMB-C2B	-2.41	1.46	1.51
19	4	307	CHL	C4-C3	-2.41	1.43	1.50
20	3	307	CLA	CMB-C2B	-2.41	1.46	1.51
20	A	814	CLA	CMB-C2B	-2.41	1.46	1.51
20	B	837	CLA	CMB-C2B	-2.41	1.46	1.51
20	L	304	CLA	CMB-C2B	-2.41	1.46	1.51
20	B	816	CLA	CMB-C2B	-2.40	1.46	1.51
19	3	306	CHL	O2D-CED	-2.40	1.39	1.45
20	A	804	CLA	CMB-C2B	-2.40	1.46	1.51
20	3	301	CLA	CMB-C2B	-2.40	1.46	1.51
20	A	851	CLA	CMB-C2B	-2.40	1.46	1.51
20	B	803	CLA	CMB-C2B	-2.40	1.46	1.51
20	B	834	CLA	CMB-C2B	-2.40	1.46	1.51
19	1	306	CHL	C4C-C3C	2.40	1.49	1.45
20	1	305	CLA	CMB-C2B	-2.40	1.46	1.51
20	B	835	CLA	CMB-C2B	-2.40	1.46	1.51
20	2	308	CLA	CMB-C2B	-2.40	1.46	1.51
20	1	304	CLA	CMB-C2B	-2.40	1.46	1.51
20	1	321	CLA	CMB-C2B	-2.40	1.46	1.51
20	J	101	CLA	CMB-C2B	-2.39	1.46	1.51
19	1	306	CHL	C4B-CHC	2.39	1.47	1.41
20	A	825	CLA	CMB-C2B	-2.39	1.46	1.51
20	B	805	CLA	CMB-C2B	-2.39	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	825	CLA	CMB-C2B	-2.39	1.46	1.51
20	A	807	CLA	CMB-C2B	-2.39	1.46	1.51
20	4	313	CLA	CMB-C2B	-2.39	1.46	1.51
19	4	315	CHL	CMC-C2C	-2.39	1.40	1.45
20	B	818	CLA	CMB-C2B	-2.38	1.46	1.51
20	N	203	CLA	CMB-C2B	-2.38	1.46	1.51
20	K	203	CLA	CMB-C2B	-2.38	1.46	1.51
20	A	821	CLA	CMB-C2B	-2.38	1.46	1.51
20	A	806	CLA	CMB-C2B	-2.38	1.46	1.51
20	2	302	CLA	CMB-C2B	-2.38	1.46	1.51
20	3	304	CLA	CMB-C2B	-2.37	1.46	1.51
20	A	813	CLA	CMB-C2B	-2.37	1.46	1.51
20	A	837	CLA	CMB-C2B	-2.37	1.46	1.51
20	4	304	CLA	CAA-CBA	-2.37	1.45	1.52
20	B	801	CLA	CMB-C2B	-2.37	1.46	1.51
20	N	202	CLA	CMB-C2B	-2.37	1.46	1.51
20	A	812	CLA	CMB-C2B	-2.37	1.46	1.51
20	2	313	CLA	CMB-C2B	-2.37	1.46	1.51
20	B	810	CLA	CMB-C2B	-2.37	1.46	1.51
26	F	807	HTG	C1-S1	-2.36	1.77	1.80
20	1	302	CLA	CMB-C2B	-2.36	1.46	1.51
20	1	314	CLA	CMB-C2B	-2.36	1.46	1.51
19	4	306	CHL	C4C-C3C	2.36	1.49	1.45
20	1	311	CLA	CMB-C2B	-2.36	1.46	1.51
20	4	303	CLA	CMB-C2B	-2.36	1.46	1.51
20	O	203	CLA	CMB-C2B	-2.36	1.46	1.51
20	A	827	CLA	CMB-C2B	-2.35	1.46	1.51
20	A	802	CLA	CMB-C2B	-2.35	1.46	1.51
20	B	806	CLA	CMB-C2B	-2.35	1.46	1.51
19	4	307	CHL	O1D-CGD	-2.35	1.15	1.21
19	4	315	CHL	C4C-C3C	2.34	1.49	1.45
19	3	306	CHL	C4B-CHC	2.34	1.47	1.41
19	4	315	CHL	CMD-C2D	-2.33	1.45	1.50
20	2	311	CLA	CMB-C2B	-2.32	1.46	1.51
19	4	307	CHL	CMA-C3A	-2.32	1.48	1.53
19	2	301	CHL	C4C-C3C	2.31	1.49	1.45
19	2	305	CHL	C4B-CHC	2.30	1.47	1.41
19	2	314	CHL	C4C-C3C	2.29	1.49	1.45
19	1	306	CHL	CBD-CGD	-2.28	1.45	1.52
20	1	305	CLA	CMD-C2D	-2.28	1.46	1.50
19	2	305	CHL	C4C-C3C	2.27	1.49	1.45
19	1	306	CHL	MG-NA	-2.26	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	4	304	CLA	CMD-C2D	-2.26	1.46	1.50
19	2	301	CHL	C4B-CHC	2.26	1.47	1.41
19	4	307	CHL	CMD-C2D	-2.25	1.46	1.50
19	4	305	CHL	C4B-CHC	2.25	1.47	1.41
19	4	305	CHL	C4C-C3C	2.24	1.48	1.45
19	4	307	CHL	MG-NA	-2.24	2.00	2.06
20	B	803	CLA	CMC-C2C	-2.24	1.46	1.50
19	4	307	CHL	CAC-C3C	-2.24	1.45	1.51
19	4	307	CHL	C4B-CHC	2.24	1.47	1.41
19	4	315	CHL	C4B-CHC	2.23	1.47	1.41
19	2	307	CHL	CMD-C2D	-2.23	1.46	1.50
20	3	309	CLA	CBD-CGD	-2.23	1.45	1.52
19	1	306	CHL	C1B-CHB	2.23	1.47	1.41
20	4	304	CLA	O1A-CGA	-2.23	1.15	1.22
19	1	301	CHL	C1D-ND	-2.22	1.35	1.37
19	2	314	CHL	C4B-CHC	2.22	1.47	1.41
19	2	301	CHL	CMC-C2C	-2.22	1.40	1.45
19	2	305	CHL	CMD-C2D	-2.21	1.46	1.50
19	3	306	CHL	CMD-C2D	-2.21	1.46	1.50
21	O	205	LUT	C26-C27	2.21	1.53	1.50
19	1	301	CHL	C1B-CHB	2.19	1.47	1.41
19	1	301	CHL	C4C-C3C	2.19	1.48	1.45
19	4	307	CHL	CBD-CGD	-2.19	1.45	1.52
19	2	306	CHL	C4B-CHC	2.18	1.47	1.41
19	2	307	CHL	C4B-CHC	2.18	1.47	1.41
19	2	301	CHL	O2A-CGA	2.18	1.39	1.33
19	2	301	CHL	CMD-C2D	-2.17	1.46	1.50
19	3	306	CHL	MG-NA	-2.17	2.01	2.06
19	4	306	CHL	MG-NA	-2.17	2.01	2.06
19	4	315	CHL	MG-NA	-2.16	2.01	2.06
20	A	822	CLA	CMD-C2D	-2.16	1.46	1.50
19	2	301	CHL	MG-NA	-2.14	2.01	2.06
19	4	305	CHL	MG-NA	-2.12	2.01	2.06
19	2	307	CHL	C4C-C3C	2.12	1.48	1.45
19	1	306	CHL	OMC-CMC	-2.12	1.17	1.22
20	4	303	CLA	CMD-C2D	-2.11	1.46	1.50
20	A	841	CLA	CMD-C2D	-2.11	1.46	1.50
20	B	838	CLA	CMD-C2D	-2.11	1.46	1.50
19	3	306	CHL	CMA-C3A	-2.11	1.48	1.53
20	B	802	CLA	CMD-C2D	-2.10	1.46	1.50
20	A	808	CLA	CMD-C2D	-2.10	1.46	1.50
20	4	304	CLA	CBD-CGD	-2.10	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	823	CLA	CMD-C2D	-2.10	1.46	1.50
19	1	306	CHL	O1D-CGD	-2.10	1.16	1.21
19	4	315	CHL	C1B-CHB	2.09	1.46	1.41
20	B	808	CLA	CMD-C2D	-2.09	1.46	1.50
19	4	306	CHL	O2D-CED	-2.09	1.40	1.45
20	1	303	CLA	CMD-C2D	-2.08	1.46	1.50
19	3	306	CHL	C4C-C3C	2.08	1.48	1.45
20	A	831	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	309	CLA	C3B-CAB	-2.07	1.43	1.47
20	1	302	CLA	CMD-C2D	-2.07	1.46	1.50
20	F	805	CLA	CMD-C2D	-2.07	1.46	1.50
20	A	810	CLA	CMD-C2D	-2.07	1.46	1.50
20	3	309	CLA	CBA-CGA	-2.06	1.44	1.50
20	B	822	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	814	CLA	CMD-C2D	-2.06	1.46	1.50
20	K	203	CLA	CMD-C2D	-2.06	1.46	1.50
20	B	825	CLA	CMD-C2D	-2.06	1.46	1.50
20	1	302	CLA	CMC-C2C	-2.05	1.46	1.50
19	4	307	CHL	C4C-C3C	2.05	1.48	1.45
19	2	301	CHL	O2D-CGD	2.05	1.38	1.33
20	A	804	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	830	CLA	CMD-C2D	-2.05	1.46	1.50
20	3	301	CLA	CMC-C2C	-2.05	1.46	1.50
19	4	306	CHL	C1B-CHB	2.05	1.46	1.41
20	2	302	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	824	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	817	CLA	CMD-C2D	-2.05	1.46	1.50
20	B	835	CLA	CMD-C2D	-2.05	1.46	1.50
19	2	301	CHL	C1B-CHB	2.05	1.46	1.41
20	2	304	CLA	CMD-C2D	-2.05	1.46	1.50
20	N	202	CLA	CMD-C2D	-2.05	1.46	1.50
20	A	817	CLA	CMC-C2C	-2.04	1.46	1.50
20	L	302	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	804	CLA	CMC-C2C	-2.04	1.46	1.50
20	B	833	CLA	CMD-C2D	-2.04	1.46	1.50
20	A	819	CLA	CMD-C2D	-2.04	1.46	1.50
20	H	201	CLA	CMD-C2D	-2.04	1.46	1.50
19	4	307	CHL	C1B-CHB	2.04	1.46	1.41
20	A	816	CLA	CMD-C2D	-2.04	1.46	1.50
19	2	305	CHL	MG-NA	-2.04	2.01	2.06
20	B	807	CLA	CMD-C2D	-2.04	1.46	1.50
20	B	832	CLA	CMD-C2D	-2.03	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	K	203	CLA	CMC-C2C	-2.03	1.46	1.50
20	3	310	CLA	CMD-C2D	-2.03	1.46	1.50
20	J	103	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	837	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	839	CLA	CMD-C2D	-2.03	1.46	1.50
20	1	311	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	817	CLA	CMD-C2D	-2.03	1.46	1.50
19	4	307	CHL	C1D-ND	-2.03	1.35	1.37
20	4	311	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	827	CLA	CMD-C2D	-2.03	1.46	1.50
20	1	310	CLA	CMD-C2D	-2.03	1.46	1.50
20	2	303	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	838	CLA	CMD-C2D	-2.03	1.46	1.50
20	4	303	CLA	CMC-C2C	-2.03	1.46	1.50
20	B	830	CLA	CMD-C2D	-2.03	1.46	1.50
20	L	304	CLA	CMD-C2D	-2.03	1.46	1.50
20	4	302	CLA	CMD-C2D	-2.03	1.46	1.50
20	4	309	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	821	CLA	CMD-C2D	-2.03	1.46	1.50
20	B	829	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	809	CLA	CMD-C2D	-2.03	1.46	1.50
20	A	827	CLA	CMD-C2D	-2.02	1.46	1.50
20	1	321	CLA	CMD-C2D	-2.02	1.46	1.50
20	2	313	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	815	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	826	CLA	CMC-C2C	-2.02	1.46	1.50
20	3	301	CLA	CMD-C2D	-2.02	1.46	1.50
20	4	308	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	853	CLA	CMD-C2D	-2.02	1.46	1.50
20	B	819	CLA	CMC-C2C	-2.02	1.46	1.50
20	B	821	CLA	CMD-C2D	-2.02	1.46	1.50
20	1	304	CLA	CMD-C2D	-2.02	1.46	1.50
20	F	802	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	833	CLA	CMD-C2D	-2.02	1.46	1.50
20	2	308	CLA	CMD-C2D	-2.02	1.46	1.50
20	F	804	CLA	CMD-C2D	-2.02	1.46	1.50
20	K	205	CLA	CMD-C2D	-2.02	1.46	1.50
20	A	803	CLA	CMD-C2D	-2.02	1.46	1.50
19	2	305	CHL	C1B-CHB	2.02	1.46	1.41
20	2	311	CLA	CMD-C2D	-2.02	1.46	1.50
19	2	307	CHL	MG-NA	-2.02	2.01	2.06
20	A	837	CLA	CMD-C2D	-2.02	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	B	810	CLA	CMD-C2D	-2.02	1.46	1.50
20	1	314	CLA	CMD-C2D	-2.01	1.46	1.50
20	2	309	CLA	CMD-C2D	-2.01	1.46	1.50
19	2	301	CHL	C1D-ND	-2.01	1.35	1.37
20	A	825	CLA	CMD-C2D	-2.01	1.46	1.50
20	O	203	CLA	CMD-C2D	-2.01	1.46	1.50
20	K	202	CLA	CMD-C2D	-2.01	1.46	1.50
19	3	306	CHL	C1B-CHB	2.01	1.46	1.41
20	B	818	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	818	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	840	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	803	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	813	CLA	CMD-C2D	-2.01	1.46	1.50
20	3	307	CLA	CMD-C2D	-2.01	1.46	1.50
20	J	101	CLA	CMD-C2D	-2.01	1.46	1.50
20	3	308	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	824	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	828	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	829	CLA	CMC-C2C	-2.01	1.46	1.50
20	A	805	CLA	CMD-C2D	-2.01	1.46	1.50
20	4	312	CLA	CMD-C2D	-2.01	1.46	1.50
20	B	811	CLA	CMD-C2D	-2.01	1.46	1.50
19	4	306	CHL	C2C-C1C	2.01	1.48	1.44
20	B	819	CLA	CMD-C2D	-2.01	1.46	1.50
20	L	307	CLA	CMD-C2D	-2.01	1.46	1.50
20	A	811	CLA	CMD-C2D	-2.00	1.46	1.50
20	K	201	CLA	CMD-C2D	-2.00	1.46	1.50
19	4	306	CHL	C1D-ND	-2.00	1.35	1.37
20	O	201	CLA	CMD-C2D	-2.00	1.46	1.50
20	B	823	CLA	CMC-C2C	-2.00	1.46	1.50
20	3	311	CLA	CMD-C2D	-2.00	1.46	1.50
20	A	851	CLA	CMD-C2D	-2.00	1.46	1.50
20	B	816	CLA	CMC-C2C	-2.00	1.46	1.50
23	A	848	BCR	C1-C6	-2.00	1.51	1.53

All (2091) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	4	318	BCR	C32-C1-C6	-15.04	85.90	110.30
20	4	304	CLA	O2D-CGD-CBD	14.88	137.72	111.27
19	2	301	CHL	O2D-CGD-CBD	14.22	136.54	111.27
19	2	305	CHL	O2D-CGD-CBD	12.66	133.77	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	304	CLA	O2D-CGD-O1D	-9.88	104.53	123.84
19	2	305	CHL	O2D-CGD-O1D	-9.81	104.66	123.84
19	3	306	CHL	O2D-CGD-CBD	9.48	128.11	111.27
19	4	307	CHL	O2D-CGD-CBD	9.30	127.79	111.27
19	2	301	CHL	OMC-CMC-C2C	-9.28	104.70	125.69
19	2	306	CHL	O2D-CGD-O1D	-8.73	106.78	123.84
19	1	306	CHL	CMD-C2D-C1D	8.63	139.93	124.71
19	4	306	CHL	CMD-C2D-C1D	8.49	139.67	124.71
23	4	318	BCR	C32-C1-C31	-8.31	83.03	108.53
19	2	314	CHL	CMD-C2D-C1D	8.24	139.23	124.71
19	2	306	CHL	O2D-CGD-CBD	8.16	125.77	111.27
19	2	307	CHL	CAC-C3C-C4C	8.15	135.38	124.81
19	3	306	CHL	CMB-C2B-C1B	8.12	140.94	128.46
20	4	304	CLA	CAA-C2A-C3A	-8.11	90.58	112.78
19	4	305	CHL	CMD-C2D-C1D	7.98	138.78	124.71
19	1	301	CHL	CMD-C2D-C1D	7.94	138.70	124.71
19	2	301	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
22	4	317	XAT	O4-C5-C4	7.64	119.12	113.38
19	4	305	CHL	O2D-CGD-CBD	7.62	124.80	111.27
19	2	307	CHL	O2D-CGD-CBD	7.59	124.76	111.27
19	4	306	CHL	C2C-C3C-C4C	-7.57	101.09	106.49
19	4	315	CHL	O2D-CGD-CBD	7.54	124.67	111.27
22	2	316	XAT	O24-C25-C24	7.53	119.03	113.38
19	4	305	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
19	1	306	CHL	CMB-C2B-C1B	7.51	140.00	128.46
19	2	305	CHL	C2C-C3C-C4C	-7.50	101.15	106.49
19	2	307	CHL	CMB-C2B-C1B	7.50	139.98	128.46
22	1	316	XAT	O24-C25-C24	7.48	119.00	113.38
19	2	306	CHL	C2C-C3C-C4C	-7.45	101.18	106.49
19	2	314	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
19	2	307	CHL	O2D-CGD-O1D	-7.40	109.36	123.84
19	1	306	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
19	4	315	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
19	2	305	CHL	CMD-C2D-C1D	7.34	137.65	124.71
19	2	307	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
19	1	301	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
22	3	316	XAT	O4-C5-C4	7.11	118.72	113.38
19	1	306	CHL	O2D-CGD-CBD	7.10	123.88	111.27
20	L	302	CLA	C4A-NA-C1A	7.10	109.90	106.71
20	4	304	CLA	C1-C2-C3	-7.09	115.28	126.75
19	4	307	CHL	O2D-CGD-O1D	-7.08	109.99	123.84
19	1	301	CHL	CHD-C1D-ND	-7.08	117.95	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	O2D-CGD-O1D	-7.07	110.02	123.84
19	4	307	CHL	C2C-C3C-C4C	-6.97	101.52	106.49
19	4	306	CHL	CHD-C1D-ND	-6.97	118.05	124.45
20	4	312	CLA	C4A-NA-C1A	6.90	109.81	106.71
20	A	830	CLA	C4A-NA-C1A	6.90	109.81	106.71
20	B	836	CLA	C4A-NA-C1A	6.88	109.80	106.71
19	3	306	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
19	3	306	CHL	CHD-C1D-ND	-6.87	118.14	124.45
20	B	803	CLA	C4A-NA-C1A	6.85	109.79	106.71
20	B	808	CLA	C4A-NA-C1A	6.85	109.79	106.71
20	3	309	CLA	O2D-CGD-CBD	6.84	123.42	111.27
22	4	317	XAT	O24-C25-C24	6.83	118.52	113.38
20	B	831	CLA	C4A-NA-C1A	6.81	109.77	106.71
20	B	815	CLA	C4A-NA-C1A	6.80	109.76	106.71
20	A	815	CLA	C4A-NA-C1A	6.79	109.76	106.71
20	B	810	CLA	C4A-NA-C1A	6.78	109.75	106.71
20	1	308	CLA	C4A-NA-C1A	6.77	109.75	106.71
20	4	304	CLA	C4A-NA-C1A	6.77	109.75	106.71
20	K	203	CLA	C4A-NA-C1A	6.77	109.75	106.71
20	B	824	CLA	C4A-NA-C1A	6.76	109.74	106.71
20	B	826	CLA	C4A-NA-C1A	6.75	109.74	106.71
20	B	820	CLA	C4A-NA-C1A	6.75	109.74	106.71
20	K	205	CLA	C4A-NA-C1A	6.74	109.73	106.71
20	G	603	CLA	C4A-NA-C1A	6.73	109.73	106.71
20	2	311	CLA	C4A-NA-C1A	6.72	109.72	106.71
20	4	303	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	A	829	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	1	313	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	A	804	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	A	813	CLA	C4A-NA-C1A	6.70	109.72	106.71
20	3	311	CLA	C4A-NA-C1A	6.69	109.72	106.71
20	A	805	CLA	C4A-NA-C1A	6.69	109.71	106.71
20	A	839	CLA	C4A-NA-C1A	6.68	109.71	106.71
20	B	818	CLA	C4A-NA-C1A	6.68	109.71	106.71
20	1	311	CLA	C4A-NA-C1A	6.67	109.70	106.71
20	L	307	CLA	C4A-NA-C1A	6.66	109.70	106.71
22	2	316	XAT	C18-C5-C6	-6.66	111.10	122.26
20	4	308	CLA	C4A-NA-C1A	6.66	109.70	106.71
20	A	837	CLA	C4A-NA-C1A	6.65	109.70	106.71
20	3	309	CLA	CMD-C2D-C1D	6.63	136.40	124.71
20	A	831	CLA	C4A-NA-C1A	6.63	109.69	106.71
20	L	303	CLA	C4A-NA-C1A	6.62	109.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	301	CLA	C4A-NA-C1A	6.62	109.68	106.71
20	A	838	CLA	C4A-NA-C1A	6.62	109.68	106.71
20	B	804	CLA	C4A-NA-C1A	6.62	109.68	106.71
20	A	814	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	J	103	CLA	C4A-NA-C1A	6.61	109.68	106.71
20	B	834	CLA	C4A-NA-C1A	6.60	109.67	106.71
20	3	310	CLA	C4A-NA-C1A	6.60	109.67	106.71
20	B	832	CLA	C4A-NA-C1A	6.60	109.67	106.71
20	2	312	CLA	C4A-NA-C1A	6.60	109.67	106.71
19	1	306	CHL	CHD-C1D-ND	-6.59	118.40	124.45
20	4	311	CLA	C4A-NA-C1A	6.59	109.67	106.71
20	A	840	CLA	C4A-NA-C1A	6.59	109.67	106.71
20	3	312	CLA	C4A-NA-C1A	6.59	109.67	106.71
20	A	820	CLA	C4A-NA-C1A	6.59	109.67	106.71
22	1	316	XAT	C18-C5-C6	-6.59	111.22	122.26
20	A	833	CLA	C4A-NA-C1A	6.58	109.67	106.71
20	1	314	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	B	821	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	2	303	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	B	812	CLA	C4A-NA-C1A	6.58	109.66	106.71
20	B	807	CLA	C4A-NA-C1A	6.57	109.66	106.71
20	J	101	CLA	C4A-NA-C1A	6.57	109.66	106.71
20	A	853	CLA	C4A-NA-C1A	6.57	109.66	106.71
19	2	301	CHL	CMB-C2B-C1B	6.57	138.56	128.46
20	2	313	CLA	C4A-NA-C1A	6.57	109.66	106.71
20	A	827	CLA	C4A-NA-C1A	6.56	109.66	106.71
20	B	811	CLA	C4A-NA-C1A	6.56	109.66	106.71
20	2	302	CLA	C4A-NA-C1A	6.56	109.65	106.71
22	3	316	XAT	C38-C25-C26	-6.56	111.27	122.26
20	B	839	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	B	816	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	B	833	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	N	203	CLA	C4A-NA-C1A	6.55	109.65	106.71
20	3	305	CLA	C4A-NA-C1A	6.54	109.65	106.71
20	B	809	CLA	C4A-NA-C1A	6.54	109.65	106.71
22	3	316	XAT	C18-C5-C6	-6.54	111.30	122.26
20	B	806	CLA	C4A-NA-C1A	6.53	109.64	106.71
20	A	808	CLA	C4A-NA-C1A	6.53	109.64	106.71
20	A	821	CLA	C4A-NA-C1A	6.53	109.64	106.71
20	N	202	CLA	C4A-NA-C1A	6.53	109.64	106.71
19	2	307	CHL	C1-C2-C3	-6.52	116.20	126.75
20	3	307	CLA	C4A-NA-C1A	6.52	109.64	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	809	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	1	304	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	A	832	CLA	C4A-NA-C1A	6.51	109.63	106.71
20	H	201	CLA	C4A-NA-C1A	6.50	109.63	106.71
20	3	304	CLA	C4A-NA-C1A	6.50	109.63	106.71
20	A	819	CLA	C4A-NA-C1A	6.50	109.63	106.71
20	B	805	CLA	C4A-NA-C1A	6.50	109.63	106.71
20	A	816	CLA	C4A-NA-C1A	6.49	109.62	106.71
20	K	201	CLA	C4A-NA-C1A	6.48	109.62	106.71
20	A	807	CLA	C4A-NA-C1A	6.48	109.62	106.71
20	A	825	CLA	C4A-NA-C1A	6.48	109.62	106.71
23	4	318	BCR	C31-C1-C6	6.48	120.80	110.30
20	B	835	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	1	307	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	G	604	CLA	C4A-NA-C1A	6.47	109.62	106.71
20	2	304	CLA	C4A-NA-C1A	6.47	109.61	106.71
19	4	315	CHL	OMC-CMC-C2C	-6.47	111.06	125.69
20	F	805	CLA	C4A-NA-C1A	6.46	109.61	106.71
20	A	812	CLA	C4A-NA-C1A	6.46	109.61	106.71
20	F	802	CLA	C4A-NA-C1A	6.45	109.61	106.71
20	A	803	CLA	C4A-NA-C1A	6.45	109.61	106.71
20	A	810	CLA	C4A-NA-C1A	6.45	109.61	106.71
20	3	301	CLA	C4A-NA-C1A	6.44	109.60	106.71
20	3	303	CLA	C4A-NA-C1A	6.44	109.60	106.71
20	B	838	CLA	C4A-NA-C1A	6.43	109.60	106.71
20	B	814	CLA	C4A-NA-C1A	6.43	109.59	106.71
20	4	302	CLA	C4A-NA-C1A	6.41	109.59	106.71
20	A	811	CLA	C4A-NA-C1A	6.41	109.59	106.71
22	4	317	XAT	C18-C5-C6	-6.41	111.52	122.26
20	3	302	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	A	817	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	3	308	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	A	824	CLA	C4A-NA-C1A	6.40	109.58	106.71
20	A	834	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	A	835	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	A	836	CLA	C4A-NA-C1A	6.39	109.58	106.71
20	1	309	CLA	C4A-NA-C1A	6.38	109.58	106.71
20	B	817	CLA	C4A-NA-C1A	6.38	109.58	106.71
20	B	819	CLA	C4A-NA-C1A	6.38	109.58	106.71
20	A	802	CLA	C4A-NA-C1A	6.37	109.57	106.71
19	4	307	CHL	CHD-C1D-ND	-6.37	118.60	124.45
20	1	310	CLA	C4A-NA-C1A	6.37	109.57	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	305	CLA	C4A-NA-C1A	6.36	109.57	106.71
20	A	818	CLA	C4A-NA-C1A	6.36	109.56	106.71
20	B	837	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	G	605	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	2	310	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	F	804	CLA	C4A-NA-C1A	6.35	109.56	106.71
20	1	312	CLA	C4A-NA-C1A	6.35	109.56	106.71
22	4	317	XAT	C38-C25-C26	-6.34	111.63	122.26
20	1	321	CLA	C4A-NA-C1A	6.34	109.56	106.71
19	4	315	CHL	CHD-C1D-ND	-6.34	118.62	124.45
20	1	303	CLA	C4A-NA-C1A	6.34	109.56	106.71
20	A	823	CLA	C4A-NA-C1A	6.34	109.56	106.71
20	O	202	CLA	CMD-C2D-C1D	6.33	135.87	124.71
22	1	316	XAT	C38-C25-C26	-6.32	111.66	122.26
20	O	203	CLA	C4A-NA-C1A	6.32	109.55	106.71
20	2	309	CLA	C4A-NA-C1A	6.31	109.55	106.71
20	B	830	CLA	C4A-NA-C1A	6.31	109.55	106.71
20	4	314	CLA	C4A-NA-C1A	6.31	109.54	106.71
19	3	306	CHL	CMD-C2D-C1D	6.30	135.82	124.71
20	B	828	CLA	C4A-NA-C1A	6.30	109.54	106.71
20	3	314	CLA	C4A-NA-C1A	6.30	109.54	106.71
20	4	313	CLA	C4A-NA-C1A	6.29	109.53	106.71
20	L	304	CLA	C4A-NA-C1A	6.28	109.53	106.71
19	4	315	CHL	CAA-C2A-C1A	-6.28	98.23	112.14
22	2	316	XAT	C38-C25-C26	-6.27	111.75	122.26
20	A	841	CLA	C4A-NA-C1A	6.27	109.52	106.71
20	4	310	CLA	C4A-NA-C1A	6.27	109.52	106.71
19	4	305	CHL	CHD-C1D-ND	-6.26	118.70	124.45
20	B	827	CLA	C4A-NA-C1A	6.25	109.52	106.71
20	A	828	CLA	C4A-NA-C1A	6.25	109.52	106.71
20	A	806	CLA	C4A-NA-C1A	6.25	109.51	106.71
20	1	302	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	B	829	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	2	308	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	4	309	CLA	C4A-NA-C1A	6.24	109.51	106.71
20	3	313	CLA	C4A-NA-C1A	6.21	109.50	106.71
20	A	801	CLA	C4A-NA-C1A	6.19	109.49	106.71
20	B	813	CLA	C4A-NA-C1A	6.18	109.48	106.71
19	4	315	CHL	O2D-CGD-O1D	-6.18	111.75	123.84
20	A	822	CLA	C4A-NA-C1A	6.17	109.48	106.71
20	B	802	CLA	C4A-NA-C1A	6.15	109.47	106.71
20	B	825	CLA	C4A-NA-C1A	6.15	109.47	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	CHD-C1D-ND	-6.14	118.81	124.45
19	2	305	CHL	CHD-C1D-ND	-6.11	118.83	124.45
20	B	823	CLA	C4A-NA-C1A	6.10	109.45	106.71
19	2	307	CHL	CHD-C1D-ND	-6.05	118.89	124.45
20	A	826	CLA	C4A-NA-C1A	6.05	109.43	106.71
19	2	306	CHL	CHD-C1D-ND	-6.05	118.89	124.45
20	B	822	CLA	C4A-NA-C1A	6.03	109.42	106.71
22	3	316	XAT	O24-C25-C24	6.02	117.90	113.38
20	K	202	CLA	C4A-NA-C1A	6.02	109.41	106.71
20	O	201	CLA	C4A-NA-C1A	5.98	109.39	106.71
19	2	314	CHL	CHD-C1D-ND	-5.96	118.98	124.45
22	2	316	XAT	O4-C5-C4	5.96	117.86	113.38
19	4	306	CHL	CAA-CBA-CGA	-5.94	95.88	113.25
19	3	306	CHL	O2D-CGD-O1D	-5.94	112.22	123.84
20	B	801	CLA	C4A-NA-C1A	5.93	109.37	106.71
19	2	301	CHL	CED-O2D-CGD	5.92	129.32	115.94
20	O	202	CLA	O2D-CGD-CBD	5.86	121.68	111.27
19	4	305	CHL	O2A-C1-C2	5.73	123.69	108.64
23	B	843	BCR	C24-C23-C22	-5.73	117.58	126.23
20	A	851	CLA	C4A-NA-C1A	5.72	109.28	106.71
20	O	202	CLA	C4A-NA-C1A	5.72	109.28	106.71
23	B	842	BCR	C7-C8-C9	-5.70	117.62	126.23
23	A	849	BCR	C7-C8-C9	-5.68	117.66	126.23
23	B	845	BCR	C15-C14-C13	-5.64	119.27	127.31
23	B	843	BCR	C7-C8-C9	-5.62	117.75	126.23
19	4	307	CHL	CMD-C2D-C1D	5.55	134.50	124.71
19	2	306	CHL	CMD-C2D-C1D	5.53	134.47	124.71
20	3	309	CLA	C4A-NA-C1A	5.48	109.17	106.71
19	3	306	CHL	CAC-C3C-C4C	5.46	131.89	124.81
23	K	204	BCR	C16-C17-C18	-5.43	119.56	127.31
19	2	301	CHL	O1D-CGD-CBD	-5.43	113.38	124.48
23	L	305	BCR	C24-C23-C22	-5.43	118.03	126.23
23	A	854	BCR	C15-C14-C13	-5.41	119.59	127.31
23	A	854	BCR	C16-C17-C18	-5.35	119.68	127.31
23	2	317	BCR	C15-C14-C13	-5.34	119.69	127.31
19	1	301	CHL	O2D-CGD-CBD	5.32	120.72	111.27
22	3	316	XAT	C26-C27-C28	-5.30	114.78	125.99
23	L	301	BCR	C7-C8-C9	-5.30	118.23	126.23
23	B	841	BCR	C15-C14-C13	-5.28	119.77	127.31
19	2	307	CHL	CMD-C2D-C1D	5.27	134.01	124.71
23	F	806	BCR	C11-C10-C9	-5.24	119.83	127.31
23	A	849	BCR	C16-C17-C18	-5.24	119.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	301	CHL	C3C-C4C-NC	5.22	116.42	110.57
23	L	305	BCR	C3-C4-C5	-5.22	104.76	114.08
19	2	314	CHL	C3C-C4C-NC	5.18	116.38	110.57
19	4	306	CHL	CED-O2D-CGD	5.17	127.63	115.94
19	4	305	CHL	O2A-CGA-CBA	5.16	128.10	111.91
23	4	318	BCR	C32-C1-C2	-5.14	88.36	108.91
22	1	316	XAT	O4-C5-C4	5.13	117.24	113.38
19	3	306	CHL	CMA-C3A-C4A	5.12	125.52	111.77
19	2	305	CHL	C3C-C4C-NC	5.11	116.31	110.57
22	1	316	XAT	C6-C7-C8	-5.10	115.20	125.99
23	L	306	BCR	C28-C27-C26	-5.10	104.98	114.08
23	A	849	BCR	C20-C21-C22	-5.08	120.07	127.31
19	2	307	CHL	C3C-C4C-NC	5.07	116.26	110.57
23	4	318	BCR	C15-C14-C13	-5.06	120.08	127.31
21	O	205	LUT	C31-C30-C29	-5.04	120.12	127.31
23	2	317	BCR	C16-C17-C18	-5.03	120.13	127.31
19	2	306	CHL	C3C-C4C-NC	5.02	116.20	110.57
23	3	317	BCR	C15-C14-C13	-5.02	120.15	127.31
23	L	301	BCR	C15-C14-C13	-4.99	120.18	127.31
19	2	301	CHL	CMD-C2D-C1D	4.98	133.48	124.71
19	3	306	CHL	O2A-CGA-CBA	4.97	131.88	112.23
19	4	305	CHL	C3C-C4C-NC	4.95	116.12	110.57
23	F	806	BCR	C15-C14-C13	-4.95	120.25	127.31
21	O	205	LUT	C35-C34-C33	-4.94	120.26	127.31
22	1	316	XAT	O4-C5-C18	4.93	120.96	115.06
19	4	305	CHL	CMB-C2B-C1B	4.92	136.03	128.46
21	O	205	LUT	C7-C8-C9	-4.92	118.80	126.23
23	4	318	BCR	C2-C1-C6	4.91	118.03	110.48
23	F	801	BCR	C16-C15-C14	-4.90	113.44	123.47
19	2	301	CHL	O2A-CGA-CBA	4.89	127.24	111.91
21	1	319	LUT	C15-C14-C13	-4.88	120.34	127.31
19	4	307	CHL	O2A-CGA-CBA	4.88	127.21	111.91
19	2	314	CHL	O2D-CGD-CBD	4.87	119.93	111.27
19	4	306	CHL	C3C-C4C-NC	4.86	116.02	110.57
19	2	301	CHL	O2A-CGA-O1A	-4.85	111.35	123.59
19	4	307	CHL	C3C-C4C-NC	4.84	116.00	110.57
19	4	315	CHL	C3C-C4C-NC	4.84	116.00	110.57
21	O	205	LUT	C11-C10-C9	-4.84	120.41	127.31
22	2	316	XAT	O4-C5-C18	4.83	120.85	115.06
20	3	309	CLA	CAA-CBA-CGA	-4.82	99.16	113.25
19	2	306	CHL	CAC-C3C-C4C	4.81	131.05	124.81
23	3	317	BCR	C3-C4-C5	-4.80	105.51	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	3	306	CHL	C3C-C4C-NC	4.78	115.94	110.57
19	1	306	CHL	C3C-C4C-NC	4.78	115.93	110.57
23	A	854	BCR	C11-C10-C9	-4.77	120.50	127.31
23	K	204	BCR	C20-C21-C22	-4.76	120.52	127.31
23	A	847	BCR	C16-C17-C18	-4.75	120.53	127.31
22	4	317	XAT	C26-C27-C28	-4.74	115.98	125.99
22	2	316	XAT	C6-C7-C8	-4.72	116.00	125.99
23	I	101	BCR	C24-C23-C22	-4.71	119.12	126.23
19	2	314	CHL	C3D-C2D-C1D	-4.70	99.42	105.83
23	I	101	BCR	C16-C17-C18	-4.70	120.60	127.31
22	3	316	XAT	O24-C25-C38	4.69	120.67	115.06
20	4	304	CLA	CAC-C3C-C4C	4.68	130.88	124.81
23	J	104	BCR	C16-C17-C18	-4.65	120.68	127.31
23	1	317	BCR	C15-C14-C13	-4.62	120.71	127.31
19	4	307	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
23	J	102	BCR	C15-C14-C13	-4.62	120.72	127.31
19	2	305	CHL	C3D-C2D-C1D	-4.61	99.53	105.83
19	4	305	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
19	4	307	CHL	OMC-CMC-C2C	-4.61	115.27	125.69
19	2	301	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
23	B	845	BCR	C24-C23-C22	-4.60	119.28	126.23
23	J	102	BCR	C20-C21-C22	-4.59	120.76	127.31
19	3	306	CHL	C3D-C2D-C1D	-4.59	99.57	105.83
19	2	307	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
19	2	306	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
23	2	317	BCR	C11-C10-C9	-4.57	120.79	127.31
23	B	844	BCR	C28-C27-C26	-4.55	105.95	114.08
19	4	315	CHL	C3D-C2D-C1D	-4.54	99.64	105.83
23	A	846	BCR	C15-C14-C13	-4.53	120.85	127.31
19	1	306	CHL	O2A-CGA-O1A	-4.52	112.17	123.59
22	3	316	XAT	C6-C7-C8	-4.52	116.44	125.99
23	G	606	BCR	C28-C27-C26	-4.51	106.03	114.08
23	F	806	BCR	C7-C8-C9	-4.50	119.43	126.23
23	J	104	BCR	C20-C21-C22	-4.50	120.89	127.31
22	4	317	XAT	C6-C7-C8	-4.49	116.49	125.99
23	B	844	BCR	C15-C14-C13	-4.49	120.90	127.31
19	2	307	CHL	OMC-CMC-C2C	-4.49	115.53	125.69
23	L	306	BCR	C20-C21-C22	-4.48	120.92	127.31
19	3	306	CHL	O2A-CGA-O1A	-4.47	109.11	123.14
23	J	102	BCR	C16-C17-C18	-4.47	120.93	127.31
23	2	317	BCR	C38-C26-C25	-4.47	119.51	124.53
23	A	847	BCR	C28-C27-C26	-4.46	106.11	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	304	CLA	CED-O2D-CGD	4.46	126.02	115.94
23	L	306	BCR	C24-C23-C22	-4.45	119.51	126.23
19	1	301	CHL	C3C-C4C-NC	4.45	115.56	110.57
22	2	316	XAT	C26-C27-C28	-4.44	116.60	125.99
19	4	306	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
20	3	309	CLA	CMD-C2D-C3D	-4.42	117.44	127.61
19	2	306	CHL	CGD-CBD-CAD	-4.41	96.44	110.73
23	B	846	BCR	C16-C17-C18	-4.41	121.02	127.31
21	1	315	LUT	C35-C34-C33	-4.41	121.02	127.31
23	B	842	BCR	C15-C14-C13	-4.40	121.03	127.31
23	J	102	BCR	C38-C26-C25	-4.39	119.59	124.53
19	2	307	CHL	CHD-C4C-C3C	-4.39	118.39	124.84
20	4	302	CLA	CMB-C2B-C1B	-4.39	121.72	128.46
23	A	845	BCR	C16-C17-C18	-4.38	121.05	127.31
21	2	315	LUT	C35-C34-C33	-4.38	121.06	127.31
20	A	828	CLA	CMB-C2B-C1B	-4.37	121.74	128.46
23	I	101	BCR	C11-C10-C9	-4.36	121.08	127.31
23	4	318	BCR	C11-C10-C9	-4.36	121.08	127.31
20	A	806	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
20	B	829	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
23	K	204	BCR	C38-C26-C25	-4.36	119.64	124.53
23	A	848	BCR	C7-C8-C9	-4.35	119.66	126.23
19	2	314	CHL	CHD-C4C-C3C	-4.35	118.45	124.84
23	G	606	BCR	C16-C17-C18	-4.34	121.11	127.31
23	L	306	BCR	C15-C14-C13	-4.33	121.14	127.31
23	A	849	BCR	C24-C23-C22	-4.33	119.70	126.23
23	I	101	BCR	C7-C8-C9	-4.33	119.70	126.23
23	3	317	BCR	C11-C10-C9	-4.32	121.15	127.31
19	1	301	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
19	1	306	CHL	C3D-C2D-C1D	-4.31	99.95	105.83
23	K	204	BCR	C7-C8-C9	-4.30	119.74	126.23
20	4	309	CLA	CMB-C2B-C1B	-4.30	121.86	128.46
23	A	848	BCR	C16-C17-C18	-4.30	121.18	127.31
23	J	104	BCR	C15-C14-C13	-4.29	121.19	127.31
22	3	316	XAT	C15-C14-C13	-4.29	121.19	127.31
24	A	844	LHG	O7-C7-C8	4.28	120.73	111.50
23	G	606	BCR	C20-C21-C22	-4.28	121.20	127.31
20	1	311	CLA	CMB-C2B-C1B	-4.28	121.89	128.46
20	A	837	CLA	CMB-C2B-C1B	-4.27	121.89	128.46
23	B	842	BCR	C3-C4-C5	-4.27	106.45	114.08
19	4	307	CHL	CED-O2D-CGD	4.27	125.60	115.94
20	B	801	CLA	CMB-C2B-C1B	-4.27	121.90	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	304	CLA	C5-C3-C4	4.27	124.03	114.60
20	A	836	CLA	CMB-C2B-C1B	-4.27	121.91	128.46
20	A	801	CLA	O2D-CGD-CBD	4.26	118.84	111.27
23	F	801	BCR	C20-C21-C22	-4.26	121.23	127.31
19	2	305	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
22	4	317	XAT	C35-C34-C33	-4.25	121.25	127.31
23	A	848	BCR	C15-C14-C13	-4.25	121.25	127.31
20	B	835	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
20	3	304	CLA	CMB-C2B-C1B	-4.22	121.98	128.46
19	3	306	CHL	CHD-C4C-C3C	-4.22	118.64	124.84
22	1	316	XAT	O24-C25-C38	4.21	120.11	115.06
23	A	846	BCR	C16-C17-C18	-4.21	121.30	127.31
19	2	301	CHL	CHD-C4C-C3C	-4.21	118.65	124.84
23	B	843	BCR	C15-C14-C13	-4.20	121.31	127.31
19	2	314	CHL	C2D-C1D-ND	4.19	113.19	110.10
23	A	846	BCR	C20-C21-C22	-4.19	121.33	127.31
23	B	841	BCR	C3-C4-C5	-4.19	106.60	114.08
20	A	829	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
19	4	307	CHL	CMB-C2B-C1B	4.17	134.88	128.46
23	L	306	BCR	C16-C17-C18	-4.17	121.36	127.31
23	L	305	BCR	C15-C14-C13	-4.16	121.37	127.31
20	B	834	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
19	4	306	CHL	O2D-CGD-CBD	4.14	118.63	111.27
23	I	101	BCR	C15-C14-C13	-4.14	121.40	127.31
20	A	824	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
19	4	307	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
20	3	307	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
22	4	317	XAT	O24-C25-C38	4.12	119.99	115.06
23	B	845	BCR	C33-C5-C6	-4.11	119.91	124.53
21	O	205	LUT	C15-C14-C13	-4.11	121.45	127.31
20	A	804	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
23	B	845	BCR	C11-C10-C9	-4.10	121.46	127.31
23	L	301	BCR	C33-C5-C6	-4.10	119.93	124.53
20	B	825	CLA	CMB-C2B-C1B	-4.09	122.17	128.46
20	4	304	CLA	CMD-C2D-C1D	4.09	131.93	124.71
19	2	301	CHL	C2D-C1D-ND	4.08	113.11	110.10
20	B	826	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
22	1	316	XAT	C26-C27-C28	-4.08	117.37	125.99
20	B	805	CLA	CMB-C2B-C1B	-4.08	122.20	128.46
23	4	318	BCR	C33-C5-C6	-4.08	119.95	124.53
23	A	845	BCR	C20-C21-C22	-4.07	121.50	127.31
23	I	101	BCR	C20-C21-C22	-4.07	121.51	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	O	202	CLA	CMD-C2D-C3D	-4.06	118.26	127.61
20	K	203	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
23	L	305	BCR	C16-C17-C18	-4.06	121.51	127.31
20	2	311	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
19	4	307	CHL	C2D-C1D-ND	4.06	113.10	110.10
25	1	320	LMG	O7-C10-C11	4.06	120.25	111.50
19	4	305	CHL	CHD-C4C-C3C	-4.06	118.88	124.84
23	2	317	BCR	C33-C5-C6	-4.05	119.98	124.53
22	2	316	XAT	O24-C25-C38	4.04	119.90	115.06
22	3	316	XAT	C35-C34-C33	-4.03	121.56	127.31
20	3	309	CLA	CBC-CAC-C3C	-4.03	101.31	112.43
20	A	821	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
19	2	305	CHL	CAA-C2A-C1A	4.02	121.04	112.14
20	O	203	CLA	CMB-C2B-C1B	-4.02	122.28	128.46
26	A	852	HTG	C1'-S1-C1	4.02	107.61	100.09
20	1	309	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
20	A	807	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
19	4	315	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
23	L	305	BCR	C20-C21-C22	-4.00	121.60	127.31
20	B	809	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
19	4	306	CHL	OMC-CMC-C2C	-4.00	116.65	125.69
20	B	815	CLA	CMB-C2B-C1B	-3.99	122.32	128.46
21	O	204	LUT	C35-C34-C33	-3.99	121.61	127.31
23	4	318	BCR	C16-C17-C18	-3.99	121.61	127.31
19	2	305	CHL	C2D-C1D-ND	3.98	113.04	110.10
19	2	306	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
19	2	306	CHL	C3B-C4B-NB	3.98	114.35	109.21
20	1	310	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
20	A	851	CLA	CMB-C2B-C1B	-3.98	122.35	128.46
19	3	306	CHL	C2D-C1D-ND	3.97	113.03	110.10
22	3	316	XAT	O4-C5-C18	3.97	119.82	115.06
23	A	846	BCR	C24-C23-C22	-3.97	120.23	126.23
20	1	302	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
20	A	802	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
23	L	305	BCR	C38-C26-C25	-3.96	120.09	124.53
24	1	318	LHG	O7-C7-C8	3.95	120.01	111.50
23	L	301	BCR	C38-C26-C25	-3.94	120.10	124.53
19	2	306	CHL	C2D-C1D-ND	3.94	113.01	110.10
20	A	827	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
20	3	301	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
21	O	204	LUT	C15-C14-C13	-3.93	121.70	127.31
23	B	843	BCR	C16-C17-C18	-3.93	121.70	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	4	303	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
20	B	837	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
23	G	606	BCR	C24-C23-C22	-3.92	120.32	126.23
20	2	302	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
23	B	846	BCR	C33-C5-C6	-3.91	120.14	124.53
30	B	848	DGD	O2G-C1B-C2B	3.91	119.92	111.50
20	A	803	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
23	A	847	BCR	C15-C14-C13	-3.89	121.75	127.31
20	3	308	CLA	CMB-C2B-C1B	-3.89	122.48	128.46
20	A	814	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
20	B	810	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
20	N	202	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
20	A	801	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
23	B	843	BCR	C33-C5-C6	-3.88	120.17	124.53
19	2	307	CHL	C2D-C1D-ND	3.88	112.96	110.10
20	A	825	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
23	B	841	BCR	C20-C21-C22	-3.88	121.78	127.31
20	2	308	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
19	4	305	CHL	C1-O2A-CGA	3.87	126.59	116.44
23	B	844	BCR	C11-C10-C9	-3.86	121.80	127.31
20	B	818	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
20	L	304	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
20	4	311	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
19	3	306	CHL	C1D-ND-C4D	-3.85	103.60	106.33
20	A	818	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
19	4	306	CHL	C5-C3-C4	3.84	123.09	114.60
19	4	305	CHL	C2D-C1D-ND	3.84	112.94	110.10
20	2	309	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
23	A	846	BCR	C11-C10-C9	-3.83	121.85	127.31
20	B	814	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
19	2	314	CHL	C1D-ND-C4D	-3.82	103.62	106.33
23	2	317	BCR	C20-C21-C22	-3.82	121.86	127.31
19	4	306	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
20	B	806	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
19	2	314	CHL	C3B-C4B-NB	3.81	114.14	109.21
23	A	845	BCR	C24-C23-C22	-3.81	120.48	126.23
20	A	812	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
20	F	802	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
24	2	318	LHG	O7-C7-C8	3.81	119.71	111.50
20	J	101	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
23	J	104	BCR	C24-C23-C22	-3.80	120.49	126.23
23	A	845	BCR	C15-C14-C13	-3.80	121.89	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	303	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
23	1	317	BCR	C28-C27-C26	-3.79	107.30	114.08
23	A	847	BCR	C33-C5-C6	-3.79	120.27	124.53
19	2	301	CHL	C1-O2A-CGA	3.79	126.38	116.44
20	A	826	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
20	A	805	CLA	CMB-C2B-C1B	-3.79	122.65	128.46
23	4	318	BCR	C28-C27-C26	-3.78	107.33	114.08
19	4	315	CHL	C2D-C1D-ND	3.78	112.89	110.10
19	1	301	CHL	C1-C2-C3	-3.78	119.51	126.04
25	4	319	LMG	O7-C10-C11	3.77	119.64	111.50
21	O	204	LUT	C31-C30-C29	-3.77	121.92	127.31
20	B	836	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
19	2	307	CHL	CED-O2D-CGD	3.77	124.45	115.94
24	A	843	LHG	O7-C7-C8	3.76	119.61	111.50
23	2	317	BCR	C24-C23-C22	-3.76	120.55	126.23
20	B	817	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
20	A	830	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
20	B	801	CLA	CMB-C2B-C3B	3.75	131.69	124.68
22	4	317	XAT	O4-C5-C18	3.74	119.54	115.06
20	B	803	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
23	3	317	BCR	C28-C27-C26	-3.74	107.40	114.08
20	O	202	CLA	O2D-CGD-O1D	-3.74	116.52	123.84
23	L	306	BCR	C7-C8-C9	-3.74	120.58	126.23
20	4	302	CLA	CMB-C2B-C3B	3.74	131.68	124.68
23	3	317	BCR	C7-C8-C9	-3.74	120.58	126.23
20	B	822	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
20	B	823	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
19	1	306	CHL	O2A-CGA-CBA	3.72	123.58	111.91
20	2	310	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
19	2	301	CHL	C4-C3-C5	3.72	121.53	115.27
21	4	316	LUT	C35-C34-C33	-3.72	122.00	127.31
19	2	306	CHL	C1D-ND-C4D	-3.71	103.70	106.33
19	4	305	CHL	O2A-CGA-O1A	-3.71	114.23	123.59
20	A	806	CLA	CMB-C2B-C3B	3.71	131.62	124.68
21	1	319	LUT	C11-C10-C9	-3.71	122.02	127.31
20	B	830	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
19	4	305	CHL	O2D-CGD-O1D	-3.71	116.59	123.84
23	J	104	BCR	C11-C10-C9	-3.71	122.02	127.31
23	A	846	BCR	C33-C5-C6	-3.70	120.37	124.53
23	L	306	BCR	C27-C26-C25	-3.70	117.35	122.73
23	B	841	BCR	C16-C17-C18	-3.70	122.03	127.31
23	J	102	BCR	C33-C5-C6	-3.70	120.37	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	203	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
26	A	852	HTG	C1-O5-C5	3.69	119.39	112.58
20	1	314	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
20	4	304	CLA	C1-O2A-CGA	-3.68	106.78	116.44
20	B	804	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
23	A	854	BCR	C20-C21-C22	-3.68	122.06	127.31
23	L	301	BCR	C24-C23-C22	-3.68	120.68	126.23
20	B	824	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
20	B	816	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
25	1	323	LMG	O7-C10-C11	3.67	119.41	111.50
23	1	317	BCR	C33-C5-C6	-3.67	120.41	124.53
20	A	819	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
20	B	807	CLA	CMB-C2B-C1B	-3.67	122.82	128.46
19	2	306	CHL	CMB-C2B-C1B	3.67	134.10	128.46
20	A	828	CLA	CMB-C2B-C3B	3.66	131.53	124.68
22	2	316	XAT	C35-C34-C33	-3.66	122.09	127.31
20	B	813	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
20	A	809	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
23	A	848	BCR	C11-C10-C9	-3.66	122.09	127.31
19	2	301	CHL	C1D-ND-C4D	-3.65	103.74	106.33
20	1	305	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
19	2	301	CHL	C3B-C4B-NB	3.65	113.92	109.21
19	2	307	CHL	C5-C3-C4	3.65	122.66	114.60
20	3	303	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
20	A	835	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
20	2	313	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
23	G	606	BCR	C15-C14-C13	-3.64	122.12	127.31
20	1	304	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
19	4	307	CHL	C1D-ND-C4D	-3.63	103.75	106.33
20	B	820	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
20	L	302	CLA	CMB-C2B-C1B	-3.62	122.89	128.46
20	A	813	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
19	2	305	CHL	C1D-ND-C4D	-3.62	103.77	106.33
21	3	315	LUT	C35-C34-C33	-3.62	122.15	127.31
20	4	304	CLA	O2A-CGA-O1A	-3.61	114.47	123.59
20	2	303	CLA	CMB-C2B-C1B	-3.61	122.92	128.46
23	F	806	BCR	C24-C23-C22	-3.60	120.80	126.23
23	A	847	BCR	C20-C21-C22	-3.60	122.17	127.31
20	H	201	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
20	4	309	CLA	CMB-C2B-C3B	3.60	131.41	124.68
20	A	833	CLA	CMB-C2B-C1B	-3.59	122.94	128.46
20	B	835	CLA	CMB-C2B-C3B	3.59	131.40	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	311	CLA	CMB-C2B-C3B	3.59	131.40	124.68
20	A	837	CLA	CMB-C2B-C3B	3.59	131.40	124.68
19	4	306	CHL	CBA-CAA-C2A	-3.59	103.26	113.86
20	A	839	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
23	B	845	BCR	C16-C17-C18	-3.59	122.19	127.31
20	3	304	CLA	CMB-C2B-C3B	3.59	131.39	124.68
19	2	306	CHL	O2A-CGA-CBA	3.58	123.16	111.91
20	A	811	CLA	CMB-C2B-C1B	-3.58	122.96	128.46
19	4	315	CHL	C3B-C4B-NB	3.58	113.84	109.21
20	A	836	CLA	CMB-C2B-C3B	3.58	131.38	124.68
19	1	306	CHL	O1D-CGD-CBD	-3.58	117.16	124.48
19	1	306	CHL	CHD-C4C-C3C	-3.58	119.58	124.84
19	2	307	CHL	C1D-ND-C4D	-3.58	103.79	106.33
20	B	811	CLA	CAB-C3B-C4B	-3.58	122.97	128.46
19	4	307	CHL	C3B-C4B-NB	3.57	113.83	109.21
23	L	301	BCR	C16-C17-C18	-3.57	122.22	127.31
20	B	834	CLA	CMB-C2B-C3B	3.56	131.35	124.68
23	B	846	BCR	C24-C23-C22	-3.56	120.85	126.23
20	K	201	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
19	2	301	CHL	CAC-C3C-C4C	3.56	129.43	124.81
23	B	841	BCR	C38-C26-C25	-3.56	120.53	124.53
23	1	317	BCR	C16-C17-C18	-3.56	122.23	127.31
23	F	806	BCR	C20-C21-C22	-3.56	122.23	127.31
20	A	838	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
20	B	829	CLA	CMB-C2B-C3B	3.55	131.33	124.68
23	J	104	BCR	C28-C27-C26	-3.55	107.74	114.08
20	4	313	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
23	K	204	BCR	C11-C10-C9	-3.54	122.26	127.31
20	3	313	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
19	4	315	CHL	C1D-ND-C4D	-3.52	103.83	106.33
23	2	317	BCR	C8-C7-C6	-3.52	117.31	127.20
19	4	315	CHL	CMB-C2B-C1B	3.52	133.87	128.46
19	1	301	CHL	C1B-CHB-C4A	-3.52	123.16	130.12
20	A	820	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
23	F	806	BCR	C33-C5-C6	-3.51	120.58	124.53
20	B	828	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
23	2	317	BCR	C33-C5-C4	3.51	120.35	113.62
23	A	847	BCR	C11-C10-C9	-3.50	122.31	127.31
20	1	303	CLA	CMB-C2B-C1B	-3.50	123.09	128.46
20	B	825	CLA	CMB-C2B-C3B	3.49	131.21	124.68
19	4	306	CHL	C3D-C4D-ND	3.49	115.88	110.24
19	3	306	CHL	C3D-C4D-ND	3.48	115.88	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	307	CHL	CBA-CAA-C2A	-3.48	103.58	113.86
20	3	309	CLA	CBA-CAA-C2A	-3.48	103.58	113.86
20	A	829	CLA	CMB-C2B-C3B	3.48	131.20	124.68
20	A	851	CLA	CMB-C2B-C3B	3.48	131.20	124.68
20	1	321	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
20	2	311	CLA	CMB-C2B-C3B	3.48	131.19	124.68
23	B	844	BCR	C16-C17-C18	-3.48	122.35	127.31
23	K	204	BCR	C15-C14-C13	-3.48	122.35	127.31
19	4	305	CHL	C1D-ND-C4D	-3.47	103.87	106.33
23	A	845	BCR	C33-C5-C6	-3.47	120.63	124.53
23	A	848	BCR	C38-C26-C25	-3.47	120.63	124.53
20	3	314	CLA	CMB-C2B-C1B	-3.47	123.14	128.46
24	B	849	LHG	O7-C7-C8	3.47	118.97	111.50
23	B	841	BCR	C11-C10-C9	-3.47	122.36	127.31
20	3	312	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
20	B	819	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
20	A	834	CLA	CMB-C2B-C1B	-3.45	123.16	128.46
23	A	847	BCR	C24-C23-C22	-3.45	121.02	126.23
23	L	306	BCR	C11-C10-C9	-3.44	122.39	127.31
20	A	817	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
20	J	103	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
20	K	203	CLA	CMB-C2B-C3B	3.44	131.12	124.68
20	A	807	CLA	CMB-C2B-C3B	3.44	131.12	124.68
20	A	824	CLA	CMB-C2B-C3B	3.43	131.10	124.68
20	A	827	CLA	CMB-C2B-C3B	3.43	131.09	124.68
20	B	805	CLA	CMB-C2B-C3B	3.43	131.09	124.68
20	F	805	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
23	A	845	BCR	C28-C27-C26	-3.43	107.96	114.08
23	L	306	BCR	C33-C5-C6	-3.43	120.68	124.53
20	B	826	CLA	CMB-C2B-C3B	3.43	131.09	124.68
19	2	314	CHL	C3D-C4D-ND	3.42	115.77	110.24
19	2	306	CHL	CBA-CAA-C2A	-3.42	103.76	113.86
23	3	317	BCR	C16-C17-C18	-3.42	122.43	127.31
23	A	846	BCR	C38-C26-C25	-3.42	120.69	124.53
20	4	304	CLA	O1D-CGD-CBD	-3.42	117.49	124.48
20	L	307	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
20	A	831	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
20	1	309	CLA	CMB-C2B-C3B	3.41	131.06	124.68
20	B	812	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
20	A	821	CLA	CMB-C2B-C3B	3.41	131.06	124.68
20	3	307	CLA	CMB-C2B-C3B	3.41	131.06	124.68
19	4	306	CHL	C2D-C1D-ND	3.41	112.62	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	4	315	CHL	C3D-C4D-ND	3.41	115.75	110.24
20	A	804	CLA	CMB-C2B-C3B	3.41	131.05	124.68
20	B	838	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
23	L	305	BCR	C11-C10-C9	-3.40	122.45	127.31
20	1	307	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
23	F	801	BCR	C3-C4-C5	-3.40	108.01	114.08
20	G	604	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
20	4	304	CLA	O2A-CGA-CBA	3.40	122.57	111.91
23	L	306	BCR	C38-C26-C27	3.40	120.14	113.62
21	3	315	LUT	C15-C14-C13	-3.39	122.47	127.31
20	2	312	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
20	3	305	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
20	F	804	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
19	2	306	CHL	C3D-C4D-ND	3.39	115.72	110.24
20	K	202	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
23	F	806	BCR	C28-C27-C26	-3.39	108.03	114.08
20	B	811	CLA	CMB-C2B-C1B	-3.39	123.26	128.46
23	A	854	BCR	C15-C16-C17	-3.39	116.54	123.47
23	F	806	BCR	C38-C26-C25	-3.38	120.73	124.53
20	A	829	CLA	O2D-CGD-O1D	-3.38	117.22	123.84
20	B	833	CLA	CMB-C2B-C1B	-3.38	123.26	128.46
20	B	832	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
20	A	841	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
21	4	316	LUT	C18-C5-C6	-3.38	120.73	124.53
23	1	317	BCR	C7-C8-C9	-3.38	121.13	126.23
20	O	203	CLA	CMB-C2B-C3B	3.38	131.00	124.68
20	2	313	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
20	2	304	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
20	A	802	CLA	CMB-C2B-C3B	3.38	131.00	124.68
20	4	314	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
20	O	201	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
19	4	315	CHL	CAC-C3C-C4C	3.37	129.18	124.81
20	4	310	CLA	CMB-C2B-C1B	-3.37	123.29	128.46
20	B	837	CLA	CMB-C2B-C3B	3.36	130.97	124.68
19	3	306	CHL	CMB-C2B-C3B	-3.36	118.39	124.68
19	1	306	CHL	C3D-C4D-ND	3.36	115.67	110.24
19	2	305	CHL	CAC-C3C-C4C	3.36	129.17	124.81
20	3	310	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
19	2	307	CHL	C3D-C4D-ND	3.36	115.67	110.24
19	4	306	CHL	C1D-ND-C4D	-3.36	103.95	106.33
21	1	319	LUT	C35-C34-C33	-3.36	122.52	127.31
20	A	840	CLA	CMB-C2B-C1B	-3.36	123.31	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	1	301	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
20	B	821	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
20	3	311	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
20	G	605	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
23	4	318	BCR	C38-C26-C25	-3.35	120.77	124.53
21	4	316	LUT	C15-C14-C13	-3.35	122.53	127.31
23	1	317	BCR	C3-C4-C5	-3.35	108.10	114.08
20	3	302	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
19	4	307	CHL	C3D-C4D-ND	3.35	115.65	110.24
27	A	842	PQN	C14-C13-C15	3.35	120.90	115.27
19	4	305	CHL	C3D-C4D-ND	3.35	115.65	110.24
20	B	839	CLA	CMB-C2B-C1B	-3.34	123.32	128.46
19	4	305	CHL	C3B-C4B-NB	3.34	113.53	109.21
20	1	313	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
20	A	810	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
20	B	825	CLA	O2D-CGD-O1D	-3.34	117.31	123.84
20	A	815	CLA	CMB-C2B-C1B	-3.34	123.34	128.46
20	4	301	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
19	2	314	CHL	CAC-C3C-C4C	3.33	129.13	124.81
23	A	854	BCR	C24-C23-C22	-3.33	121.21	126.23
20	A	853	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
20	A	803	CLA	O2D-CGD-O1D	-3.33	117.33	123.84
20	4	312	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
19	1	306	CHL	OMC-CMC-C2C	-3.32	118.17	125.69
20	B	808	CLA	O2D-CGD-O1D	-3.32	117.34	123.84
20	3	309	CLA	CMA-C3A-C4A	-3.32	102.85	111.77
20	2	302	CLA	CMB-C2B-C3B	3.32	130.88	124.68
19	2	301	CHL	C3D-C4D-ND	3.32	115.60	110.24
19	2	305	CHL	C3D-C4D-ND	3.31	115.60	110.24
20	1	302	CLA	CMB-C2B-C3B	3.31	130.88	124.68
20	B	808	CLA	CMB-C2B-C1B	-3.31	123.38	128.46
20	3	301	CLA	CMB-C2B-C3B	3.31	130.87	124.68
23	F	806	BCR	C16-C17-C18	-3.31	122.59	127.31
23	A	848	BCR	C23-C24-C25	-3.31	117.91	127.20
23	J	104	BCR	C7-C8-C9	-3.31	121.24	126.23
20	1	310	CLA	CMB-C2B-C3B	3.31	130.86	124.68
19	1	301	CHL	C3D-C4D-ND	3.30	115.58	110.24
20	1	308	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
20	B	815	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	A	849	BCR	C15-C14-C13	-3.30	122.60	127.31
20	A	803	CLA	CMB-C2B-C3B	3.30	130.85	124.68
23	B	842	BCR	C16-C17-C18	-3.30	122.61	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	814	CLA	CMB-C2B-C3B	3.29	130.84	124.68
20	1	312	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
21	O	205	LUT	C36-C21-C26	3.29	114.53	109.55
23	A	845	BCR	C7-C8-C9	-3.29	121.26	126.23
23	G	606	BCR	C7-C8-C9	-3.29	121.27	126.23
20	3	308	CLA	CMB-C2B-C3B	3.29	130.83	124.68
20	4	308	CLA	CMB-C2B-C1B	-3.29	123.41	128.46
23	L	305	BCR	C4-C5-C6	-3.29	117.96	122.73
21	1	315	LUT	C15-C14-C13	-3.28	122.62	127.31
20	B	827	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
20	A	825	CLA	CMB-C2B-C3B	3.28	130.82	124.68
23	L	301	BCR	C11-C10-C9	-3.28	122.64	127.31
19	1	306	CHL	CMD-C2D-C3D	-3.27	120.09	127.61
20	A	822	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
20	4	303	CLA	CMB-C2B-C3B	3.27	130.79	124.68
20	4	313	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
19	1	301	CHL	CAC-C3C-C4C	3.26	129.04	124.81
20	L	304	CLA	CMB-C2B-C3B	3.26	130.78	124.68
20	N	202	CLA	CMB-C2B-C3B	3.26	130.77	124.68
23	K	204	BCR	C24-C23-C22	-3.26	121.31	126.23
24	A	844	LHG	O8-C23-C24	3.25	119.91	111.38
23	J	104	BCR	C33-C5-C6	-3.25	120.87	124.53
20	2	308	CLA	CMB-C2B-C3B	3.25	130.77	124.68
23	J	102	BCR	C3-C4-C5	-3.25	108.27	114.08
23	G	606	BCR	C33-C5-C6	-3.25	120.88	124.53
19	1	306	CHL	C3B-C4B-NB	3.25	113.41	109.21
20	A	808	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
20	F	802	CLA	CMB-C2B-C3B	3.25	130.76	124.68
20	B	810	CLA	CMB-C2B-C3B	3.25	130.76	124.68
20	B	809	CLA	CMB-C2B-C3B	3.25	130.75	124.68
20	A	832	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
20	G	603	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
27	B	840	PQN	C11-C12-C13	-3.24	121.41	126.79
22	3	316	XAT	C10-C11-C12	-3.23	113.13	123.22
20	4	311	CLA	CMB-C2B-C3B	3.23	130.72	124.68
20	A	816	CLA	CMB-C2B-C1B	-3.23	123.51	128.46
20	A	818	CLA	CMB-C2B-C3B	3.22	130.71	124.68
20	3	309	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
21	3	315	LUT	C31-C30-C29	-3.21	122.73	127.31
20	K	202	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
20	B	823	CLA	CMB-C2B-C3B	3.21	130.68	124.68
20	B	814	CLA	CMB-C2B-C3B	3.20	130.67	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	818	CLA	CMB-C2B-C3B	3.20	130.67	124.68
20	A	823	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
20	J	101	CLA	CMB-C2B-C3B	3.20	130.67	124.68
20	B	822	CLA	CAA-C2A-C3A	-3.20	104.01	112.78
20	A	851	CLA	O2D-CGD-O1D	-3.20	117.59	123.84
20	B	831	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
21	O	204	LUT	C21-C26-C27	-3.19	108.67	112.70
20	B	806	CLA	CMB-C2B-C3B	3.19	130.65	124.68
23	K	204	BCR	C33-C5-C6	-3.19	120.95	124.53
20	2	309	CLA	CMB-C2B-C3B	3.19	130.64	124.68
23	4	318	BCR	C3-C4-C5	-3.18	108.39	114.08
23	J	104	BCR	C3-C4-C5	-3.18	108.40	114.08
19	2	307	CHL	O2A-CGA-CBA	3.18	121.89	111.91
20	A	812	CLA	CMB-C2B-C3B	3.18	130.63	124.68
22	1	316	XAT	C18-C5-C4	3.18	117.86	114.28
23	B	845	BCR	C15-C16-C17	-3.18	116.97	123.47
20	A	805	CLA	CMB-C2B-C3B	3.18	130.62	124.68
20	2	310	CLA	CMB-C2B-C3B	3.17	130.62	124.68
21	2	315	LUT	C18-C5-C6	-3.17	120.97	124.53
20	J	101	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	A	838	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
20	B	836	CLA	CMB-C2B-C3B	3.17	130.60	124.68
20	B	822	CLA	CMB-C2B-C3B	3.17	130.60	124.68
20	A	826	CLA	CMB-C2B-C3B	3.16	130.60	124.68
20	B	803	CLA	CMB-C2B-C3B	3.16	130.60	124.68
20	L	307	CLA	O2D-CGD-O1D	-3.16	117.66	123.84
20	A	830	CLA	CMB-C2B-C3B	3.16	130.59	124.68
20	L	303	CLA	CMB-C2B-C3B	3.16	130.59	124.68
23	L	305	BCR	C7-C8-C9	-3.15	121.47	126.23
20	4	304	CLA	CAC-C3C-C2C	-3.15	122.14	127.53
19	4	306	CHL	C1-C2-C3	-3.15	121.66	126.75
20	A	825	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
20	A	833	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
23	A	848	BCR	C28-C27-C26	-3.14	108.46	114.08
19	1	301	CHL	O2A-CGA-CBA	3.14	121.77	111.91
20	1	314	CLA	CMB-C2B-C3B	3.14	130.55	124.68
19	1	306	CHL	CMB-C2B-C3B	-3.13	118.81	124.68
20	4	304	CLA	CAA-CBA-CGA	-3.13	104.10	113.25
19	1	306	CHL	CAC-C3C-C4C	3.13	128.88	124.81
22	2	316	XAT	C15-C14-C13	-3.13	122.84	127.31
20	B	802	CLA	CMB-C2B-C1B	-3.13	123.66	128.46
23	A	854	BCR	C28-C27-C26	-3.13	108.50	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	313	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
23	K	204	BCR	C3-C4-C5	-3.12	108.50	114.08
19	1	301	CHL	C4-C3-C5	3.12	119.55	115.98
20	K	205	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
20	B	804	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
21	4	316	LUT	C21-C26-C27	-3.12	108.76	112.70
20	B	804	CLA	CMB-C2B-C3B	3.12	130.51	124.68
20	4	314	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
23	B	842	BCR	C30-C25-C26	-3.11	118.23	122.61
19	4	307	CHL	O2A-CGA-O1A	-3.11	115.74	123.59
23	B	841	BCR	C24-C23-C22	-3.11	121.54	126.23
23	B	842	BCR	C28-C27-C26	-3.10	108.53	114.08
23	A	845	BCR	C38-C26-C27	3.10	119.58	113.62
23	B	845	BCR	C7-C8-C9	-3.10	121.55	126.23
20	B	824	CLA	CMB-C2B-C3B	3.10	130.47	124.68
20	B	816	CLA	CMB-C2B-C3B	3.09	130.46	124.68
20	N	203	CLA	CMB-C2B-C3B	3.09	130.46	124.68
19	2	305	CHL	CMB-C2B-C1B	3.09	133.21	128.46
20	B	824	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
20	A	807	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
20	G	603	CLA	O2D-CGD-O1D	-3.08	117.82	123.84
19	4	306	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
20	L	302	CLA	CMB-C2B-C3B	3.08	130.44	124.68
20	B	817	CLA	CMB-C2B-C3B	3.08	130.44	124.68
21	1	319	LUT	C18-C5-C6	-3.08	121.07	124.53
20	A	838	CLA	CMB-C2B-C3B	3.07	130.43	124.68
23	L	301	BCR	C20-C21-C22	-3.07	122.92	127.31
20	B	807	CLA	CMB-C2B-C3B	3.07	130.43	124.68
20	1	304	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
19	1	306	CHL	C2D-C1D-ND	3.07	112.36	110.10
20	1	305	CLA	CMB-C2B-C3B	3.07	130.41	124.68
19	2	306	CHL	C1-O2A-CGA	3.06	125.63	116.73
23	A	845	BCR	C11-C10-C9	-3.06	122.94	127.31
20	2	310	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
23	B	842	BCR	C34-C9-C10	-3.06	118.64	122.92
20	A	833	CLA	CMB-C2B-C3B	3.06	130.39	124.68
20	A	801	CLA	CMB-C2B-C1B	-3.05	123.77	128.46
19	3	306	CHL	C3B-C4B-NB	3.05	113.16	109.21
23	1	317	BCR	C38-C26-C25	-3.05	121.10	124.53
20	B	813	CLA	CMB-C2B-C3B	3.05	130.39	124.68
23	4	318	BCR	C21-C20-C19	-3.05	113.70	123.22
20	B	830	CLA	CMB-C2B-C3B	3.05	130.38	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	L	303	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
20	B	832	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
23	B	844	BCR	C24-C23-C22	-3.05	121.63	126.23
20	A	818	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
20	2	303	CLA	CMB-C2B-C3B	3.04	130.37	124.68
20	4	313	CLA	CMB-C2B-C3B	3.04	130.37	124.68
20	B	820	CLA	CMB-C2B-C3B	3.04	130.37	124.68
20	A	809	CLA	CMB-C2B-C3B	3.04	130.37	124.68
21	3	315	LUT	C18-C5-C6	-3.04	121.11	124.53
20	2	313	CLA	CMB-C2B-C3B	3.04	130.37	124.68
23	B	845	BCR	C38-C26-C25	-3.04	121.11	124.53
20	F	805	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
27	B	840	PQN	C14-C13-C15	3.04	120.38	115.27
20	1	304	CLA	CMB-C2B-C3B	3.04	130.36	124.68
20	B	836	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
22	3	316	XAT	C24-C23-C22	-3.04	104.91	110.77
21	2	315	LUT	C21-C26-C27	-3.04	108.86	112.70
20	A	819	CLA	CMB-C2B-C3B	3.03	130.36	124.68
21	1	315	LUT	C18-C5-C6	-3.03	121.12	124.53
20	B	807	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	A	830	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
20	1	310	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
20	B	823	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
23	A	847	BCR	C7-C8-C9	-3.03	121.66	126.23
19	4	307	CHL	C5-C3-C4	3.03	121.28	114.60
20	A	831	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
20	A	837	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
19	1	301	CHL	C2D-C1D-ND	3.02	112.33	110.10
20	B	815	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
23	B	843	BCR	C28-C27-C26	-3.02	108.69	114.08
21	2	315	LUT	C15-C14-C13	-3.02	123.00	127.31
19	1	306	CHL	C1B-CHB-C4A	-3.02	124.14	130.12
20	A	839	CLA	CMB-C2B-C3B	3.02	130.32	124.68
23	B	846	BCR	C20-C21-C22	-3.02	123.01	127.31
23	G	606	BCR	C11-C10-C9	-3.01	123.01	127.31
20	B	822	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
23	B	843	BCR	C38-C26-C25	-3.01	121.14	124.53
23	F	801	BCR	C28-C27-C26	-3.01	108.70	114.08
20	A	806	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
20	B	830	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
19	2	314	CHL	CHB-C4A-NA	3.01	128.67	124.51
20	O	203	CLA	O2D-CGD-O1D	-3.01	117.96	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	841	BCR	C2-C1-C6	3.00	115.11	110.48
23	B	842	BCR	C33-C5-C6	-3.00	121.16	124.53
20	3	304	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
20	A	836	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
23	B	846	BCR	C15-C14-C13	-3.00	123.03	127.31
20	B	811	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
20	B	829	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
20	A	813	CLA	CMB-C2B-C3B	3.00	130.28	124.68
20	B	837	CLA	O2D-CGD-O1D	-3.00	117.98	123.84
20	3	303	CLA	CMB-C2B-C3B	3.00	130.28	124.68
20	B	820	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
19	2	306	CHL	CHB-C4A-NA	2.99	128.65	124.51
20	A	814	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
20	B	812	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
20	3	301	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
20	B	818	CLA	O2D-CGD-O1D	-2.99	118.00	123.84
23	B	846	BCR	C7-C8-C9	-2.98	121.73	126.23
20	A	804	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
21	2	315	LUT	C7-C8-C9	-2.98	121.74	126.23
20	A	826	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
20	A	822	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
20	A	819	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
20	L	304	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
21	1	319	LUT	C7-C8-C9	-2.97	121.75	126.23
23	A	854	BCR	C33-C5-C6	-2.97	121.19	124.53
20	G	604	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
20	B	839	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
23	L	305	BCR	C33-C5-C4	2.96	119.30	113.62
20	B	801	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
20	K	203	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
20	H	201	CLA	CMB-C2B-C3B	2.96	130.21	124.68
20	B	814	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
22	3	316	XAT	C38-C25-C24	2.96	117.61	114.28
20	2	308	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
20	B	810	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
20	B	828	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
22	2	316	XAT	C4-C3-C2	-2.95	105.07	110.77
20	A	835	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
20	1	311	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
23	L	301	BCR	C34-C9-C10	-2.95	118.79	122.92
20	4	308	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
20	3	313	CLA	O2D-CGD-O1D	-2.95	118.07	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	204	LUT	C18-C5-C6	-2.95	121.22	124.53
20	L	302	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
20	A	835	CLA	CMB-C2B-C3B	2.95	130.19	124.68
20	1	303	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
20	A	841	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
20	A	823	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
23	B	843	BCR	C33-C5-C4	2.94	119.27	113.62
20	F	804	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
20	4	311	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
20	B	805	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
23	A	849	BCR	C38-C26-C25	-2.94	121.23	124.53
20	B	801	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
20	B	817	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
23	A	847	BCR	C3-C4-C5	-2.93	108.84	114.08
20	A	808	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	K	201	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
23	G	606	BCR	C29-C30-C25	2.93	114.99	110.48
20	B	826	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
20	4	302	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
20	A	810	CLA	O2D-CGD-O1D	-2.93	118.12	123.84
20	3	312	CLA	CMB-C2B-C3B	2.92	130.15	124.68
20	A	801	CLA	CGD-CBD-CAD	2.92	120.20	110.73
23	A	846	BCR	C8-C7-C6	-2.92	119.00	127.20
20	B	835	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	A	812	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
20	B	802	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	3	317	BCR	C38-C26-C25	-2.92	121.25	124.53
20	3	303	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
23	1	317	BCR	C23-C24-C25	-2.91	119.02	127.20
20	3	307	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
20	1	321	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
20	3	312	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
20	4	301	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
20	A	817	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
20	B	819	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
23	A	849	BCR	C34-C9-C10	-2.90	118.85	122.92
23	J	102	BCR	C20-C19-C18	-2.90	118.26	126.42
20	O	201	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
23	B	843	BCR	C34-C9-C10	-2.90	118.86	122.92
20	2	302	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
19	1	306	CHL	C1D-ND-C4D	-2.90	104.27	106.33
23	J	104	BCR	C38-C26-C25	-2.90	121.27	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	831	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	A	839	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
20	4	310	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
20	A	840	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
20	A	824	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
19	4	315	CHL	CBC-CAC-C3C	-2.89	104.45	112.43
23	4	318	BCR	C33-C5-C4	2.89	119.17	113.62
21	O	204	LUT	C11-C10-C9	-2.89	123.18	127.31
20	B	816	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
20	A	813	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
23	L	305	BCR	C2-C1-C6	2.89	114.93	110.48
20	A	820	CLA	CMB-C2B-C3B	2.89	130.08	124.68
20	1	309	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
23	J	102	BCR	C15-C16-C17	-2.88	117.57	123.47
20	F	802	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
20	2	311	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
23	1	317	BCR	C11-C10-C9	-2.88	123.20	127.31
23	2	317	BCR	C3-C4-C5	-2.88	108.93	114.08
23	A	847	BCR	C8-C7-C6	-2.88	119.11	127.20
19	4	305	CHL	O1D-CGD-CBD	-2.88	118.60	124.48
23	F	801	BCR	C24-C23-C22	-2.88	121.89	126.23
20	A	805	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
20	A	811	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
22	1	316	XAT	C31-C30-C29	-2.87	123.22	127.31
20	A	821	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
23	A	847	BCR	C29-C30-C25	2.86	114.89	110.48
23	A	847	BCR	C33-C5-C4	2.86	119.12	113.62
22	2	316	XAT	C10-C11-C12	-2.86	114.28	123.22
20	B	813	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	B	806	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
20	4	312	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
21	2	315	LUT	C35-C15-C14	-2.86	117.61	123.47
23	A	846	BCR	C3-C4-C5	-2.86	108.97	114.08
20	B	834	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	N	203	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	A	831	CLA	CMB-C2B-C3B	2.86	130.02	124.68
20	A	851	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
19	2	307	CHL	CHB-C4A-NA	2.86	128.46	124.51
22	1	316	XAT	C4-C3-C2	-2.86	105.26	110.77
20	A	815	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
20	G	605	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
23	A	849	BCR	C20-C19-C18	-2.85	118.40	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	K	205	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
20	J	103	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
20	3	310	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
20	A	816	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
23	I	101	BCR	C38-C26-C27	2.85	119.08	113.62
20	A	828	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
23	I	101	BCR	C28-C27-C26	-2.84	109.00	114.08
20	2	304	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
20	B	838	CLA	CMB-C2B-C3B	2.84	130.00	124.68
23	A	845	BCR	C30-C25-C26	-2.84	118.61	122.61
20	H	201	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
22	4	317	XAT	C38-C25-C24	2.84	117.47	114.28
20	B	838	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
19	3	306	CHL	CED-O2D-CGD	2.83	122.34	115.94
20	B	832	CLA	CMB-C2B-C3B	2.83	129.97	124.68
22	4	317	XAT	C24-C23-C22	-2.83	105.31	110.77
22	2	316	XAT	C24-C23-C22	-2.83	105.31	110.77
20	3	305	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
23	A	846	BCR	C7-C8-C9	-2.82	121.97	126.23
20	A	817	CLA	CMB-C2B-C3B	2.82	129.96	124.68
20	B	812	CLA	CMB-C2B-C3B	2.82	129.96	124.68
20	1	302	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
20	2	303	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	B	827	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	3	314	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
23	A	846	BCR	C33-C5-C4	2.82	119.03	113.62
20	B	833	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	A	809	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
20	3	311	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
20	F	804	CLA	CMB-C2B-C3B	2.81	129.94	124.68
20	1	321	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	1	317	BCR	C21-C20-C19	-2.81	114.44	123.22
30	B	848	DGD	C2G-O2G-C1B	-2.81	110.87	117.79
20	O	201	CLA	CMB-C2B-C3B	2.81	129.94	124.68
20	B	808	CLA	CMB-C2B-C3B	2.81	129.94	124.68
23	B	843	BCR	C37-C22-C21	-2.81	118.99	122.92
22	4	317	XAT	C10-C11-C12	-2.81	114.46	123.22
21	2	315	LUT	C11-C10-C9	-2.81	123.31	127.31
20	K	202	CLA	CMB-C2B-C3B	2.81	129.93	124.68
23	B	842	BCR	C38-C26-C27	2.81	119.00	113.62
19	4	315	CHL	CMD-C2D-C1D	2.80	129.65	124.71
20	3	305	CLA	CMB-C2B-C3B	2.80	129.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	312	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
21	O	205	LUT	C1-C6-C5	-2.80	118.67	122.61
20	B	823	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
20	2	304	CLA	CMB-C2B-C3B	2.80	129.91	124.68
20	B	809	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	B	821	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
20	B	819	CLA	CMB-C2B-C3B	2.79	129.91	124.68
20	1	313	CLA	CMB-C2B-C3B	2.79	129.90	124.68
20	3	309	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
23	B	844	BCR	C7-C8-C9	-2.79	122.02	126.23
20	K	202	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
23	B	844	BCR	C29-C30-C25	2.79	114.77	110.48
20	1	314	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
19	2	307	CHL	CMB-C2B-C3B	-2.79	119.46	124.68
20	1	307	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
20	4	308	CLA	CMB-C2B-C3B	2.78	129.89	124.68
23	I	101	BCR	C3-C4-C5	-2.78	109.11	114.08
23	F	801	BCR	C33-C5-C6	-2.78	121.40	124.53
20	A	802	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
20	A	834	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	F	805	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	1	307	CLA	CMB-C2B-C3B	2.78	129.88	124.68
20	A	827	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
20	A	834	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
20	4	310	CLA	CMB-C2B-C3B	2.77	129.87	124.68
20	A	811	CLA	CMB-C2B-C3B	2.77	129.87	124.68
20	G	605	CLA	CMB-C2B-C3B	2.77	129.87	124.68
20	3	313	CLA	CMB-C2B-C3B	2.77	129.87	124.68
20	L	307	CLA	CMB-C2B-C3B	2.77	129.86	124.68
20	4	314	CLA	CMB-C2B-C3B	2.77	129.86	124.68
20	2	312	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
23	I	101	BCR	C33-C5-C4	2.77	118.94	113.62
20	4	303	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
23	I	101	BCR	C1-C6-C5	-2.76	118.72	122.61
20	A	832	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
20	A	840	CLA	CMB-C2B-C3B	2.76	129.85	124.68
23	B	843	BCR	C20-C21-C22	-2.76	123.37	127.31
20	2	311	CLA	CHB-C4A-NA	2.76	128.33	124.51
23	B	846	BCR	C16-C15-C14	-2.76	117.82	123.47
20	G	604	CLA	CMB-C2B-C3B	2.76	129.84	124.68
20	A	816	CLA	CMB-C2B-C3B	2.76	129.84	124.68
20	A	841	CLA	CMB-C2B-C3B	2.76	129.84	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	J	103	CLA	CMB-C2B-C3B	2.76	129.84	124.68
23	4	318	BCR	C23-C24-C25	-2.75	119.47	127.20
20	A	810	CLA	CMB-C2B-C3B	2.75	129.83	124.68
20	B	833	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	A	848	BCR	C20-C21-C22	-2.75	123.38	127.31
20	3	310	CLA	CMB-C2B-C3B	2.75	129.83	124.68
23	B	844	BCR	C20-C21-C22	-2.75	123.38	127.31
19	2	305	CHL	CBC-CAC-C3C	-2.75	104.85	112.43
19	1	301	CHL	C3B-C4B-NB	2.75	112.77	109.21
19	2	314	CHL	CMB-C2B-C3B	2.75	129.82	124.68
22	4	317	XAT	C35-C15-C14	-2.75	117.84	123.47
20	3	302	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
23	4	318	BCR	C11-C12-C13	-2.75	118.70	126.42
19	4	306	CHL	CGD-CBD-CAD	-2.75	101.84	110.73
24	1	318	LHG	O8-C23-C24	2.75	120.52	111.91
21	1	319	LUT	C31-C30-C29	-2.74	123.39	127.31
22	1	316	XAT	C10-C11-C12	-2.74	114.66	123.22
20	3	314	CLA	CMB-C2B-C3B	2.74	129.80	124.68
19	3	306	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
22	3	316	XAT	C18-C5-C4	2.74	117.36	114.28
20	A	822	CLA	CMB-C2B-C3B	2.74	129.80	124.68
22	4	317	XAT	C4-C3-C2	-2.74	105.49	110.77
20	B	821	CLA	CMB-C2B-C3B	2.74	129.80	124.68
23	4	318	BCR	C8-C7-C6	-2.73	119.52	127.20
21	3	315	LUT	C21-C26-C27	-2.73	109.25	112.70
20	1	305	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
20	A	820	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
19	1	301	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
19	3	306	CHL	CBC-CAC-C3C	-2.72	104.92	112.43
20	A	808	CLA	CMB-C2B-C3B	2.72	129.77	124.68
19	2	314	CHL	CMD-C2D-C3D	-2.72	121.36	127.61
22	2	316	XAT	C18-C5-C4	2.72	117.34	114.28
22	3	316	XAT	C4-C3-C2	-2.72	105.53	110.77
20	B	811	CLA	CAB-C3B-C2B	2.71	130.00	124.69
19	2	314	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
20	1	308	CLA	CMB-C2B-C3B	2.71	129.75	124.68
20	3	311	CLA	CMB-C2B-C3B	2.71	129.75	124.68
21	1	315	LUT	C8-C7-C6	-2.71	119.59	127.20
20	K	201	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	1	323	LMG	O8-C28-C29	2.71	120.40	111.91
23	3	317	BCR	C33-C5-C4	2.70	118.81	113.62
23	L	306	BCR	C29-C30-C25	2.70	114.64	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	302	CLA	CMB-C2B-C3B	2.70	129.73	124.68
20	B	802	CLA	CMB-C2B-C3B	2.69	129.72	124.68
20	B	839	CLA	CMB-C2B-C3B	2.69	129.72	124.68
20	A	853	CLA	CMB-C2B-C3B	2.69	129.72	124.68
22	4	317	XAT	C18-C5-C4	2.69	117.30	114.28
23	A	849	BCR	C33-C5-C6	-2.69	121.51	124.53
23	A	845	BCR	C38-C26-C25	-2.68	121.51	124.53
20	2	309	CLA	C1B-CHB-C4A	-2.68	124.80	130.12
23	3	317	BCR	C4-C5-C6	-2.68	118.84	122.73
23	G	606	BCR	C3-C4-C5	-2.68	109.29	114.08
20	3	309	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
20	4	301	CLA	CMB-C2B-C3B	2.68	129.69	124.68
20	A	853	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
23	I	101	BCR	C27-C26-C25	-2.68	118.84	122.73
23	B	842	BCR	C24-C23-C22	-2.68	122.19	126.23
23	B	845	BCR	C20-C21-C22	-2.68	123.49	127.31
20	2	312	CLA	CMB-C2B-C3B	2.68	129.68	124.68
20	G	603	CLA	CMB-C2B-C3B	2.67	129.68	124.68
20	3	308	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
20	1	310	CLA	CAA-C2A-C3A	-2.67	109.86	116.10
20	A	801	CLA	C1B-CHB-C4A	-2.67	124.82	130.12
23	G	606	BCR	C27-C26-C25	-2.67	118.85	122.73
23	B	844	BCR	C38-C26-C27	2.67	118.74	113.62
20	L	302	CLA	CHB-C4A-NA	2.67	128.20	124.51
20	B	803	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
20	B	831	CLA	CMB-C2B-C3B	2.66	129.66	124.68
23	B	845	BCR	C3-C4-C5	-2.66	109.32	114.08
19	4	307	CHL	C1B-CHB-C4A	-2.66	124.84	130.12
23	B	843	BCR	C3-C4-C5	-2.66	109.33	114.08
20	A	801	CLA	C1D-ND-C4D	-2.66	104.45	106.33
24	A	844	LHG	C5-O7-C7	-2.66	111.25	117.79
22	1	316	XAT	C24-C23-C22	-2.66	105.64	110.77
20	1	308	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
21	O	204	LUT	C8-C7-C6	-2.65	119.75	127.20
23	4	318	BCR	C31-C1-C2	2.65	119.52	108.91
20	4	304	CLA	CHB-C4A-NA	2.65	128.18	124.51
20	4	312	CLA	CMB-C2B-C3B	2.65	129.64	124.68
20	4	310	CLA	C1B-CHB-C4A	-2.65	124.87	130.12
20	B	824	CLA	CHB-C4A-NA	2.65	128.17	124.51
20	B	817	CLA	CHB-C4A-NA	2.65	128.17	124.51
20	B	811	CLA	CMB-C2B-C3B	2.64	129.87	124.69
20	4	309	CLA	O2D-CGD-O1D	-2.64	118.67	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	815	CLA	CMB-C2B-C3B	2.64	129.62	124.68
23	A	845	BCR	C27-C26-C25	-2.64	118.90	122.73
20	1	312	CLA	CMB-C2B-C3B	2.64	129.62	124.68
20	J	101	CLA	CHB-C4A-NA	2.64	128.16	124.51
21	1	319	LUT	C21-C26-C27	-2.64	109.37	112.70
23	B	845	BCR	C21-C20-C19	-2.64	114.99	123.22
23	J	102	BCR	C11-C10-C9	-2.63	123.55	127.31
20	A	802	CLA	CHB-C4A-NA	2.63	128.15	124.51
19	4	307	CHL	C1C-C2C-C3C	-2.63	105.03	107.11
20	1	303	CLA	CMB-C2B-C3B	2.63	129.60	124.68
20	A	839	CLA	CHB-C4A-NA	2.63	128.15	124.51
23	B	842	BCR	C27-C26-C25	-2.63	118.92	122.73
19	2	307	CHL	C2A-C1A-CHA	-2.63	119.27	123.86
20	G	604	CLA	C1-C2-C3	-2.63	122.50	126.75
20	A	832	CLA	CMB-C2B-C3B	2.62	129.59	124.68
20	1	311	CLA	CHB-C4A-NA	2.62	128.13	124.51
30	B	848	DGD	O1G-C1A-C2A	2.62	120.13	111.91
20	A	823	CLA	CMB-C2B-C3B	2.62	129.58	124.68
21	1	315	LUT	C10-C11-C12	-2.62	115.05	123.22
20	B	808	CLA	CHB-C4A-NA	2.62	128.13	124.51
20	3	307	CLA	CHB-C4A-NA	2.61	128.13	124.51
20	A	820	CLA	CHB-C4A-NA	2.61	128.12	124.51
20	A	830	CLA	CHB-C4A-NA	2.61	128.12	124.51
21	4	316	LUT	C8-C7-C6	-2.61	119.88	127.20
20	B	827	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
20	B	802	CLA	C1B-CHB-C4A	-2.61	124.96	130.12
20	B	828	CLA	CMB-C2B-C3B	2.60	129.54	124.68
25	1	320	LMG	O8-C28-C29	2.60	120.07	111.91
20	1	313	CLA	CHB-C4A-NA	2.60	128.11	124.51
23	B	845	BCR	C8-C7-C6	-2.60	119.91	127.20
20	A	814	CLA	CHB-C4A-NA	2.60	128.10	124.51
23	I	101	BCR	C30-C25-C26	-2.59	118.96	122.61
21	1	319	LUT	C8-C7-C6	-2.59	119.92	127.20
21	1	319	LUT	C15-C35-C34	-2.59	118.16	123.47
20	A	831	CLA	CHB-C4A-NA	2.59	128.10	124.51
23	K	204	BCR	C16-C15-C14	-2.59	118.16	123.47
23	L	301	BCR	C15-C16-C17	-2.59	118.17	123.47
23	A	848	BCR	C33-C5-C6	-2.59	121.62	124.53
20	B	808	CLA	O2A-CGA-O1A	-2.59	117.06	123.59
19	4	306	CHL	C1-O2A-CGA	2.59	123.24	116.44
19	4	305	CHL	CMD-C2D-C3D	-2.59	121.66	127.61
20	N	202	CLA	O2D-CGD-O1D	-2.59	118.22	124.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	823	CLA	CHB-C4A-NA	2.59	128.09	124.51
19	4	315	CHL	C1B-CHB-C4A	-2.59	125.00	130.12
20	1	309	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
21	2	315	LUT	C30-C31-C32	-2.58	115.15	123.22
20	A	827	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
21	O	204	LUT	C7-C8-C9	-2.58	122.33	126.23
23	3	317	BCR	C23-C24-C25	-2.58	119.96	127.20
20	2	309	CLA	CHB-C4A-NA	2.58	128.08	124.51
23	A	846	BCR	C38-C26-C27	2.58	118.57	113.62
23	B	842	BCR	C2-C1-C6	2.58	114.45	110.48
19	4	306	CHL	CAA-C2A-C1A	2.58	120.42	111.97
23	F	801	BCR	C21-C20-C19	-2.58	115.17	123.22
20	1	307	CLA	CHB-C4A-NA	2.57	128.07	124.51
21	3	315	LUT	C7-C8-C9	-2.57	122.35	126.23
20	B	833	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	B	815	CLA	CHB-C4A-NA	2.57	128.07	124.51
20	K	205	CLA	CMB-C2B-C3B	2.57	129.49	124.68
20	4	309	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
20	1	308	CLA	CHB-C4A-NA	2.57	128.06	124.51
21	3	315	LUT	C10-C11-C12	-2.57	115.21	123.22
20	3	309	CLA	CMA-C3A-C2A	-2.57	103.48	113.83
26	A	852	HTG	C4-C3-C2	-2.57	106.34	110.82
20	2	302	CLA	CHB-C4A-NA	2.57	128.06	124.51
20	4	313	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
20	B	820	CLA	CHB-C4A-NA	2.56	128.06	124.51
26	1	322	HTG	O5-C5-C4	2.56	114.35	109.69
20	B	820	CLA	C1-C2-C3	-2.56	122.61	126.75
20	B	822	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	B	823	CLA	C1B-CHB-C4A	-2.56	125.04	130.12
20	B	825	CLA	C1B-CHB-C4A	-2.56	125.05	130.12
23	F	806	BCR	C3-C4-C5	-2.56	109.51	114.08
20	4	302	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	4	308	CLA	CHB-C4A-NA	2.56	128.05	124.51
23	J	102	BCR	C8-C7-C6	-2.56	120.02	127.20
23	A	854	BCR	C11-C12-C13	-2.56	119.23	126.42
20	1	321	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	A	805	CLA	CHB-C4A-NA	2.56	128.05	124.51
20	4	311	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	B	836	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	4	312	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	H	201	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	B	822	CLA	C1B-CHB-C4A	-2.55	125.06	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	2	306	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
20	3	303	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	A	809	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	A	810	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	2	309	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
20	B	806	CLA	CHB-C4A-NA	2.55	128.04	124.51
20	B	824	CLA	O2A-CGA-O1A	-2.55	117.16	123.59
23	A	849	BCR	C11-C10-C9	-2.55	123.67	127.31
20	K	203	CLA	CHB-C4A-NA	2.55	128.03	124.51
23	B	842	BCR	C33-C5-C4	2.54	118.50	113.62
20	3	310	CLA	CHB-C4A-NA	2.54	128.03	124.51
20	2	304	CLA	CHB-C4A-NA	2.54	128.03	124.51
20	A	801	CLA	CMB-C2B-C3B	2.54	129.43	124.68
23	2	317	BCR	C11-C12-C13	-2.54	119.28	126.42
20	B	825	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	N	202	CLA	CHB-C4A-NA	2.54	128.02	124.51
25	1	323	LMG	C8-O7-C10	-2.54	111.55	117.79
20	4	301	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	A	829	CLA	CHB-C4A-NA	2.54	128.02	124.51
20	4	304	CLA	CMD-C2D-C3D	-2.53	121.78	127.61
20	G	603	CLA	CHB-C4A-NA	2.53	128.02	124.51
20	A	804	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	K	205	CLA	CHB-C4A-NA	2.53	128.01	124.51
21	1	315	LUT	C35-C15-C14	-2.53	118.28	123.47
23	A	846	BCR	C28-C27-C26	-2.53	109.56	114.08
19	1	301	CHL	C1D-ND-C4D	-2.53	104.54	106.33
20	B	827	CLA	CMB-C2B-C3B	2.53	129.42	124.68
20	A	807	CLA	CHB-C4A-NA	2.53	128.01	124.51
26	1	322	HTG	O5-C1-C2	-2.53	107.13	110.31
22	3	316	XAT	C19-C9-C8	2.53	122.06	118.08
23	F	806	BCR	C15-C16-C17	-2.53	118.29	123.47
20	2	313	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	A	813	CLA	CHB-C4A-NA	2.53	128.01	124.51
20	3	305	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	1	304	CLA	CHB-C4A-NA	2.52	128.00	124.51
20	B	819	CLA	CHB-C4A-NA	2.52	128.00	124.51
19	2	314	CHL	C2A-C1A-CHA	-2.52	119.45	123.86
23	F	801	BCR	C8-C7-C6	-2.52	120.12	127.20
20	B	826	CLA	CHB-C4A-NA	2.52	127.99	124.51
19	2	307	CHL	C1C-C2C-C3C	-2.52	105.12	107.11
20	A	821	CLA	CHB-C4A-NA	2.52	127.99	124.51
20	4	303	CLA	CHB-C4A-NA	2.51	127.99	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	3	308	CLA	C1-C2-C3	-2.51	122.69	126.75
20	B	804	CLA	CHB-C4A-NA	2.51	127.99	124.51
20	2	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	F	802	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	3	302	CLA	C1B-CHB-C4A	-2.51	125.15	130.12
20	A	836	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	B	832	CLA	CHB-C4A-NA	2.51	127.98	124.51
23	B	844	BCR	C33-C5-C6	-2.51	121.71	124.53
19	1	301	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
20	A	817	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	O	205	LUT	C18-C5-C6	-2.51	121.71	124.53
20	1	314	CLA	CHB-C4A-NA	2.51	127.98	124.51
20	3	312	CLA	CHB-C4A-NA	2.51	127.98	124.51
21	4	316	LUT	C31-C30-C29	-2.50	123.74	127.31
19	2	306	CHL	C2A-C1A-CHA	-2.50	119.49	123.86
20	B	803	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	3	301	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	B	839	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	J	103	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	2	308	CLA	C1-C2-C3	-2.50	122.71	126.75
20	A	834	CLA	CHB-C4A-NA	2.50	127.97	124.51
20	F	805	CLA	CHB-C4A-NA	2.50	127.97	124.51
19	2	306	CHL	O2A-CGA-O1A	-2.50	117.29	123.59
19	1	306	CHL	O2D-CGD-O1D	-2.50	118.96	123.84
21	2	315	LUT	C8-C7-C6	-2.50	120.19	127.20
23	A	848	BCR	C21-C20-C19	-2.50	115.43	123.22
20	2	310	CLA	CAA-C2A-C3A	-2.50	110.28	116.10
19	2	301	CHL	C1B-CHB-C4A	-2.49	125.18	130.12
20	A	818	CLA	C1B-CHB-C4A	-2.49	125.18	130.12
20	B	808	CLA	C1-C2-C3	-2.49	121.73	126.04
20	K	202	CLA	CHB-C4A-NA	2.49	127.96	124.51
24	2	318	LHG	C5-O7-C7	-2.49	111.66	117.79
20	B	830	CLA	C1-C2-C3	-2.49	122.72	126.75
20	B	805	CLA	CHB-C4A-NA	2.49	127.95	124.51
19	4	306	CHL	O1D-CGD-CBD	-2.49	119.39	124.48
20	L	303	CLA	CHB-C4A-NA	2.49	127.95	124.51
23	F	806	BCR	C33-C5-C4	2.49	118.39	113.62
20	A	819	CLA	CHB-C4A-NA	2.49	127.95	124.51
29	B	847	LMT	C1B-O1B-C4'	-2.49	111.81	117.96
20	A	812	CLA	CHB-C4A-NA	2.48	127.95	124.51
20	A	840	CLA	CHB-C4A-NA	2.48	127.95	124.51
19	2	307	CHL	C3B-C4B-NB	2.48	112.42	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	O	205	LUT	C18-C5-C4	2.48	118.95	114.36
20	A	837	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	3	311	CLA	CHB-C4A-NA	2.48	127.94	124.51
27	A	842	PQN	C2M-C2-C3	-2.48	120.35	124.40
23	F	806	BCR	C11-C12-C13	-2.48	119.45	126.42
20	A	802	CLA	C1B-CHB-C4A	-2.48	125.21	130.12
20	A	824	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	2	303	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	A	833	CLA	CHB-C4A-NA	2.48	127.94	124.51
20	1	309	CLA	CHB-C4A-NA	2.47	127.93	124.51
23	F	801	BCR	C36-C18-C19	2.47	121.97	118.08
23	B	846	BCR	C10-C11-C12	-2.47	115.50	123.22
20	N	203	CLA	C1-C2-C3	-2.47	122.75	126.75
20	2	308	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	N	203	CLA	CHB-C4A-NA	2.47	127.93	124.51
27	B	840	PQN	C2M-C2-C3	-2.47	120.36	124.40
23	L	305	BCR	C28-C27-C26	-2.47	109.66	114.08
23	B	842	BCR	C8-C9-C10	2.47	122.74	118.94
20	A	803	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	A	815	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	4	315	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
20	A	808	CLA	CHB-C4A-NA	2.47	127.93	124.51
19	4	305	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
23	K	204	BCR	C20-C19-C18	-2.47	119.48	126.42
20	2	310	CLA	CHB-C4A-NA	2.47	127.93	124.51
20	3	308	CLA	CHB-C4A-NA	2.47	127.92	124.51
23	B	845	BCR	C28-C27-C26	-2.47	109.67	114.08
20	B	816	CLA	CHB-C4A-NA	2.46	127.92	124.51
23	3	317	BCR	C2-C1-C6	2.46	114.27	110.48
20	B	808	CLA	O2D-CGD-CBD	2.46	115.64	111.27
20	B	831	CLA	CHB-C4A-NA	2.46	127.92	124.51
22	3	316	XAT	C35-C15-C14	-2.46	118.43	123.47
20	4	304	CLA	CMB-C2B-C1B	-2.46	124.68	128.46
20	A	841	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	K	201	CLA	CHB-C4A-NA	2.46	127.91	124.51
20	G	604	CLA	CHB-C4A-NA	2.46	127.91	124.51
19	4	306	CHL	O2A-CGA-CBA	2.46	119.61	111.91
20	F	802	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
20	L	307	CLA	CHB-C4A-NA	2.45	127.91	124.51
20	B	812	CLA	CHB-C4A-NA	2.45	127.91	124.51
20	A	807	CLA	C1B-CHB-C4A	-2.45	125.26	130.12
20	B	808	CLA	C1B-CHB-C4A	-2.45	125.26	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	2	316	XAT	C38-C25-C24	2.45	117.04	114.28
20	1	303	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	B	838	CLA	CHB-C4A-NA	2.45	127.90	124.51
20	A	810	CLA	C1B-CHB-C4A	-2.45	125.27	130.12
19	1	301	CHL	CMB-C2B-C3B	2.45	129.26	124.68
20	4	314	CLA	CHB-C4A-NA	2.45	127.90	124.51
23	B	844	BCR	C38-C26-C25	-2.45	121.78	124.53
23	I	101	BCR	C33-C5-C6	-2.45	121.78	124.53
20	4	313	CLA	CHB-C4A-NA	2.45	127.89	124.51
20	A	818	CLA	CHB-C4A-NA	2.45	127.89	124.51
23	3	317	BCR	C15-C16-C17	-2.44	118.47	123.47
20	1	302	CLA	CHB-C4A-NA	2.44	127.89	124.51
23	B	846	BCR	C3-C4-C5	-2.44	109.71	114.08
21	2	315	LUT	C10-C11-C12	-2.44	115.59	123.22
19	4	306	CHL	C2A-C1A-CHA	-2.44	119.59	123.86
20	A	816	CLA	CHB-C4A-NA	2.44	127.89	124.51
19	4	307	CHL	CMA-C3A-C4A	2.44	118.33	111.77
20	3	309	CLA	CHB-C4A-NA	2.44	127.89	124.51
21	O	205	LUT	C38-C25-C24	-2.44	118.34	123.56
20	3	312	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
20	B	803	CLA	C1B-CHB-C4A	-2.44	125.28	130.12
20	B	814	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	F	804	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	O	203	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	B	813	CLA	CHB-C4A-NA	2.44	127.88	124.51
20	L	304	CLA	CHB-C4A-NA	2.44	127.88	124.51
22	4	317	XAT	C31-C30-C29	-2.44	123.83	127.31
20	A	825	CLA	CHB-C4A-NA	2.44	127.88	124.51
23	3	317	BCR	C21-C20-C19	-2.44	115.62	123.22
23	B	842	BCR	C20-C21-C22	-2.43	123.83	127.31
23	1	317	BCR	C37-C22-C23	2.43	121.91	118.08
20	3	307	CLA	C1B-CHB-C4A	-2.43	125.30	130.12
21	4	316	LUT	C10-C11-C12	-2.43	115.63	123.22
20	B	809	CLA	CHB-C4A-NA	2.43	127.87	124.51
20	J	101	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
25	4	319	LMG	O8-C28-C29	2.43	119.52	111.91
20	A	820	CLA	C1B-CHB-C4A	-2.43	125.31	130.12
23	4	318	BCR	C7-C8-C9	-2.43	122.57	126.23
20	B	807	CLA	CHB-C4A-NA	2.42	127.86	124.51
20	B	819	CLA	C1B-CHB-C4A	-2.42	125.32	130.12
20	G	605	CLA	CHB-C4A-NA	2.42	127.86	124.51
20	B	834	CLA	C1B-CHB-C4A	-2.42	125.33	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	845	BCR	C3-C4-C5	-2.41	109.77	114.08
23	I	101	BCR	C4-C5-C6	-2.41	119.23	122.73
21	1	315	LUT	C21-C26-C27	-2.41	109.65	112.70
20	3	308	CLA	C1B-CHB-C4A	-2.41	125.34	130.12
23	1	317	BCR	C33-C5-C4	2.41	118.24	113.62
19	3	306	CHL	C1B-CHB-C4A	-2.41	125.35	130.12
20	2	308	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
20	3	304	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	A	853	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	B	821	CLA	CHB-C4A-NA	2.41	127.84	124.51
20	B	832	CLA	C1B-CHB-C4A	-2.41	125.35	130.12
20	A	806	CLA	CHB-C4A-NA	2.40	127.84	124.51
19	1	306	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
22	4	317	XAT	C15-C14-C13	-2.40	123.88	127.31
21	O	204	LUT	C18-C5-C4	2.40	118.80	114.36
20	A	829	CLA	C1B-CHB-C4A	-2.40	125.36	130.12
20	B	829	CLA	CHB-C4A-NA	2.40	127.83	124.51
23	B	843	BCR	C11-C10-C9	-2.40	123.89	127.31
20	A	825	CLA	C1B-CHB-C4A	-2.40	125.37	130.12
20	1	305	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	B	830	CLA	CHB-C4A-NA	2.40	127.83	124.51
20	B	825	CLA	O2D-CGD-CBD	2.40	115.52	111.27
19	4	306	CHL	C1B-CHB-C4A	-2.39	125.37	130.12
23	B	845	BCR	C33-C5-C4	2.39	118.21	113.62
20	O	202	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	A	838	CLA	C1B-CHB-C4A	-2.39	125.38	130.12
20	1	310	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	B	811	CLA	CHB-C4A-NA	2.39	127.82	124.51
20	A	833	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	B	817	CLA	C1B-CHB-C4A	-2.39	125.39	130.12
20	A	811	CLA	CHB-C4A-NA	2.39	127.81	124.51
19	2	307	CHL	O1A-CGA-CBA	-2.39	114.42	123.73
20	B	834	CLA	CHB-C4A-NA	2.39	127.81	124.51
20	3	314	CLA	CHB-C4A-NA	2.39	127.81	124.51
20	A	830	CLA	C1-C2-C3	-2.39	122.89	126.75
20	B	835	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	B	829	CLA	C1B-CHB-C4A	-2.38	125.39	130.12
23	B	844	BCR	C23-C24-C25	-2.38	120.51	127.20
20	A	826	CLA	CHB-C4A-NA	2.38	127.81	124.51
20	A	803	CLA	O2D-CGD-CBD	2.38	115.50	111.27
20	B	820	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	L	305	BCR	C38-C26-C27	2.38	118.19	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	J	102	BCR	C24-C23-C22	-2.38	122.64	126.23
20	4	310	CLA	CHB-C4A-NA	2.38	127.80	124.51
20	A	809	CLA	C1B-CHB-C4A	-2.38	125.41	130.12
23	1	317	BCR	C29-C30-C25	2.38	114.14	110.48
20	A	832	CLA	CHB-C4A-NA	2.38	127.80	124.51
23	4	318	BCR	C16-C15-C14	-2.38	118.61	123.47
20	B	837	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
30	B	848	DGD	O6D-C5D-C6D	2.37	111.46	106.67
20	3	313	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
20	A	827	CLA	CHB-C4A-NA	2.37	127.79	124.51
20	4	309	CLA	CHB-C4A-NA	2.37	127.79	124.51
19	2	305	CHL	C1C-C2C-C3C	-2.37	105.24	107.11
20	A	829	CLA	O2D-CGD-CBD	2.37	115.47	111.27
20	A	823	CLA	CHB-C4A-NA	2.36	127.78	124.51
23	B	841	BCR	C23-C24-C25	-2.36	120.56	127.20
20	4	308	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
23	1	317	BCR	C38-C26-C27	2.36	118.15	113.62
19	3	306	CHL	O1D-CGD-CBD	-2.36	119.65	124.48
20	4	304	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
20	A	838	CLA	CHB-C4A-NA	2.36	127.78	124.51
20	B	807	CLA	C1B-CHB-C4A	-2.36	125.44	130.12
20	2	304	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
20	A	803	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
20	K	202	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
24	2	318	LHG	O8-C23-C24	2.36	119.31	111.91
20	L	303	CLA	C1B-CHB-C4A	-2.36	125.45	130.12
21	1	315	LUT	C30-C31-C32	-2.36	115.86	123.22
20	B	833	CLA	C1B-CHB-C4A	-2.35	125.45	130.12
20	3	313	CLA	CHB-C4A-NA	2.35	127.77	124.51
23	B	844	BCR	C21-C20-C19	-2.35	115.87	123.22
20	2	303	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	4	302	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	B	815	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
23	G	606	BCR	C10-C11-C12	-2.35	115.88	123.22
19	3	306	CHL	C2A-C1A-CHA	-2.35	119.75	123.86
20	B	809	CLA	C1B-CHB-C4A	-2.35	125.46	130.12
20	B	810	CLA	CHB-C4A-NA	2.35	127.76	124.51
23	A	848	BCR	C16-C15-C14	-2.35	118.67	123.47
20	B	811	CLA	CHD-C1D-ND	-2.35	122.30	124.45
20	B	818	CLA	CHB-C4A-NA	2.34	127.75	124.51
20	A	816	CLA	C1B-CHB-C4A	-2.34	125.49	130.12
20	B	837	CLA	CHB-C4A-NA	2.34	127.74	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	821	CLA	C1B-CHB-C4A	-2.33	125.49	130.12
20	A	828	CLA	CHB-C4A-NA	2.33	127.74	124.51
20	A	832	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	3	303	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	A	835	CLA	CHB-C4A-NA	2.33	127.74	124.51
20	A	828	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	2	302	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	B	827	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
23	B	842	BCR	C11-C10-C9	-2.33	123.99	127.31
20	2	310	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	A	839	CLA	C1B-CHB-C4A	-2.33	125.50	130.12
20	A	835	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
20	A	814	CLA	C1-C2-C3	-2.33	122.99	126.75
21	1	319	LUT	C18-C5-C4	2.33	118.67	114.36
23	B	841	BCR	C20-C19-C18	-2.33	119.88	126.42
23	J	102	BCR	C23-C24-C25	-2.33	120.67	127.20
20	B	816	CLA	C1B-CHB-C4A	-2.33	125.51	130.12
20	B	827	CLA	CHB-C4A-NA	2.32	127.73	124.51
19	2	305	CHL	CAA-C2A-C3A	-2.32	108.45	114.26
22	4	317	XAT	C19-C9-C8	2.32	121.74	118.08
19	2	301	CHL	OBD-CAD-C3D	-2.32	122.93	128.52
23	A	847	BCR	C38-C26-C27	2.32	118.08	113.62
21	1	319	LUT	C30-C31-C32	-2.32	115.97	123.22
20	1	303	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	B	839	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
22	2	316	XAT	C35-C15-C14	-2.32	118.72	123.47
20	3	302	CLA	CHB-C4A-NA	2.32	127.72	124.51
20	B	823	CLA	C1-C2-C3	-2.32	122.03	126.04
20	2	312	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
20	A	834	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
21	4	316	LUT	C35-C15-C14	-2.32	118.72	123.47
20	O	203	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
20	B	821	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
20	O	201	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
20	1	304	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
23	2	317	BCR	C7-C8-C9	-2.32	122.73	126.23
23	K	204	BCR	C2-C1-C6	2.32	114.05	110.48
20	A	822	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	1	321	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
19	2	314	CHL	O2D-CGD-O1D	-2.31	119.31	123.84
20	O	201	CLA	CHB-C4A-NA	2.31	127.71	124.51
20	3	304	CLA	C1B-CHB-C4A	-2.31	125.54	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	813	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
21	O	204	LUT	C10-C11-C12	-2.31	116.00	123.22
23	A	849	BCR	C16-C15-C14	-2.31	118.74	123.47
20	A	806	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
23	K	204	BCR	C28-C27-C26	-2.31	109.95	114.08
23	F	806	BCR	C38-C26-C27	2.31	118.05	113.62
25	4	319	LMG	C8-O7-C10	-2.31	112.11	117.79
20	1	312	CLA	CHB-C4A-NA	2.30	127.70	124.51
20	A	837	CLA	C1B-CHB-C4A	-2.30	125.55	130.12
21	1	315	LUT	C7-C8-C9	-2.30	122.75	126.23
20	B	838	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
19	4	307	CHL	CBC-CAC-C3C	-2.30	106.09	112.43
23	4	318	BCR	C37-C22-C23	2.30	121.70	118.08
20	A	822	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
20	3	302	CLA	C1-C2-C3	-2.30	123.03	126.75
20	A	830	CLA	C1B-CHB-C4A	-2.30	125.56	130.12
27	A	842	PQN	C11-C12-C13	-2.30	122.97	126.79
20	F	804	CLA	C1B-CHB-C4A	-2.30	125.57	130.12
21	1	315	LUT	C31-C30-C29	-2.29	124.03	127.31
20	4	314	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
20	1	305	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
20	A	824	CLA	C1B-CHB-C4A	-2.29	125.57	130.12
21	3	315	LUT	C11-C10-C9	-2.29	124.04	127.31
19	4	307	CHL	CAC-C3C-C4C	2.29	127.79	124.81
20	B	812	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
20	B	804	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	B	845	BCR	C29-C30-C25	2.29	114.01	110.48
20	A	841	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
23	F	806	BCR	C35-C13-C14	-2.29	119.72	122.92
20	3	301	CLA	C1B-CHB-C4A	-2.29	125.58	130.12
20	G	603	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	B	842	BCR	C15-C16-C17	-2.29	118.79	123.47
20	A	817	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
20	A	831	CLA	C1B-CHB-C4A	-2.29	125.59	130.12
23	K	204	BCR	C38-C26-C27	2.28	118.00	113.62
23	A	847	BCR	C27-C26-C25	-2.28	119.42	122.73
20	A	851	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
20	B	836	CLA	CHD-C1D-ND	-2.28	122.36	124.45
20	1	313	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
20	B	814	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
20	G	604	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
20	1	307	CLA	C1B-CHB-C4A	-2.28	125.61	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	B	836	CLA	C1B-CHB-C4A	-2.28	125.61	130.12
20	A	826	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
20	B	828	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
20	K	201	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
20	L	303	CLA	CHD-C1D-ND	-2.27	122.36	124.45
20	4	311	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
20	B	824	CLA	C1B-CHB-C4A	-2.27	125.61	130.12
23	J	102	BCR	C28-C27-C26	-2.27	110.02	114.08
20	3	305	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	4	303	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	N	203	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	L	304	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	1	302	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	B	818	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	B	830	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
22	1	316	XAT	C19-C9-C8	2.27	121.65	118.08
23	J	104	BCR	C20-C19-C18	-2.27	120.04	126.42
20	A	804	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
20	B	821	CLA	CHD-C1D-ND	-2.27	122.37	124.45
23	F	801	BCR	C15-C14-C13	-2.27	124.07	127.31
20	K	202	CLA	CHD-C1D-ND	-2.27	122.37	124.45
19	4	305	CHL	CAA-C2A-C3A	-2.27	106.57	112.78
23	A	847	BCR	C16-C15-C14	-2.27	118.83	123.47
20	3	314	CLA	C1B-CHB-C4A	-2.27	125.63	130.12
20	A	825	CLA	CHD-C1D-ND	-2.26	122.37	124.45
20	H	201	CLA	C1B-CHB-C4A	-2.26	125.63	130.12
20	1	321	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
29	G	601	LMT	C1B-O1B-C4'	-2.26	112.37	117.96
20	L	302	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	B	807	CLA	C1-C2-C3	-2.26	122.14	126.04
20	A	811	CLA	C1B-CHB-C4A	-2.26	125.64	130.12
20	B	827	CLA	C1-C2-C3	-2.26	122.14	126.04
23	B	845	BCR	C11-C12-C13	-2.26	120.08	126.42
20	F	805	CLA	C1B-CHB-C4A	-2.26	125.65	130.12
20	L	304	CLA	C1-C2-C3	-2.26	123.10	126.75
23	B	844	BCR	C27-C26-C25	-2.25	119.46	122.73
23	A	854	BCR	C29-C30-C25	2.25	113.95	110.48
20	K	205	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
19	2	305	CHL	C3B-C4B-NB	2.25	112.12	109.21
20	3	307	CLA	C1-C2-C3	-2.25	123.11	126.75
20	3	310	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
20	A	853	CLA	C1B-CHB-C4A	-2.25	125.66	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	814	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	B	806	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
19	2	301	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
19	2	305	CHL	CHB-C4A-NA	2.25	127.62	124.51
20	1	308	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	K	203	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	L	307	CLA	C1B-CHB-C4A	-2.25	125.67	130.12
20	B	836	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
20	H	201	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
20	1	309	CLA	O2A-CGA-O1A	-2.24	117.94	123.59
20	A	808	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
23	1	317	BCR	C15-C16-C17	-2.24	118.89	123.47
20	1	314	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
19	1	306	CHL	CMA-C3A-C2A	-2.24	104.80	113.83
20	A	840	CLA	C1B-CHB-C4A	-2.24	125.69	130.12
20	B	828	CLA	CHB-C4A-NA	2.24	127.60	124.51
20	K	202	CLA	O2A-CGA-O1A	-2.24	117.95	123.59
23	2	317	BCR	C16-C15-C14	-2.23	118.90	123.47
20	A	836	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
20	3	311	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
20	J	103	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
20	A	823	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
20	A	812	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
21	O	205	LUT	C39-C29-C30	-2.23	119.80	122.92
20	A	805	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
22	3	316	XAT	C31-C30-C29	-2.23	124.13	127.31
23	B	841	BCR	C4-C5-C6	-2.23	119.49	122.73
20	A	813	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
20	A	833	CLA	CHD-C1D-ND	-2.23	122.41	124.45
20	N	202	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
20	B	831	CLA	C1B-CHB-C4A	-2.23	125.70	130.12
20	4	308	CLA	C1-C2-C3	-2.23	123.15	126.75
23	I	101	BCR	C16-C15-C14	-2.23	118.91	123.47
19	4	305	CHL	C1C-C2C-C3C	-2.23	105.35	107.11
23	B	846	BCR	C11-C10-C9	-2.23	124.13	127.31
23	J	102	BCR	C33-C5-C4	2.22	117.89	113.62
20	B	805	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
19	4	306	CHL	CMB-C2B-C1B	2.22	131.88	128.46
20	G	605	CLA	C1B-CHB-C4A	-2.22	125.71	130.12
20	4	303	CLA	O2A-CGA-O1A	-2.22	117.98	123.59
19	2	305	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
23	B	842	BCR	C38-C26-C25	-2.22	122.03	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	B	843	BCR	C8-C9-C10	2.22	122.35	118.94
20	A	819	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
24	A	843	LHG	O8-C23-C24	2.22	118.88	111.91
20	B	835	CLA	C1B-CHB-C4A	-2.22	125.72	130.12
23	1	317	BCR	C8-C7-C6	-2.22	120.97	127.20
23	J	104	BCR	C38-C26-C27	2.22	117.87	113.62
20	1	302	CLA	CHD-C1D-ND	-2.22	122.42	124.45
23	I	101	BCR	C38-C26-C25	-2.21	122.04	124.53
20	2	311	CLA	C1B-CHB-C4A	-2.21	125.73	130.12
22	3	316	XAT	C39-C29-C28	2.21	121.56	118.08
23	B	844	BCR	C15-C16-C17	-2.21	118.94	123.47
23	L	306	BCR	C3-C4-C5	-2.21	110.13	114.08
23	F	801	BCR	C33-C5-C4	2.21	117.86	113.62
19	2	301	CHL	CHB-C4A-NA	2.21	127.56	124.51
20	B	811	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
20	1	312	CLA	C1B-CHB-C4A	-2.21	125.75	130.12
20	4	304	CLA	C5-C3-C2	-2.21	116.27	122.65
23	K	204	BCR	C23-C24-C25	-2.20	121.01	127.20
22	1	316	XAT	C38-C25-C24	2.20	116.76	114.28
20	4	302	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
25	1	320	LMG	C8-O7-C10	-2.20	112.38	117.79
20	B	810	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
20	A	815	CLA	C1B-CHB-C4A	-2.20	125.76	130.12
23	B	842	BCR	C21-C20-C19	-2.20	116.36	123.22
20	4	309	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
20	4	314	CLA	CHD-C1D-ND	-2.20	122.44	124.45
22	1	316	XAT	C35-C34-C33	-2.20	124.17	127.31
20	4	301	CLA	C1B-CHB-C4A	-2.19	125.78	130.12
20	A	838	CLA	O2D-CGD-CBD	2.19	115.16	111.27
20	A	823	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	A	818	CLA	C1-C2-C3	-2.19	122.25	126.04
19	3	306	CHL	CHB-C4A-NA	2.19	127.54	124.51
20	4	314	CLA	C1-C2-C3	-2.19	123.21	126.75
19	2	301	CHL	CAA-CBA-CGA	-2.19	106.85	113.25
20	2	311	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
20	B	828	CLA	CHD-C1D-ND	-2.19	122.44	124.45
23	F	806	BCR	C34-C9-C10	-2.19	119.86	122.92
20	A	810	CLA	CHD-C1D-ND	-2.19	122.44	124.45
20	A	816	CLA	CHD-C1D-ND	-2.19	122.45	124.45
20	A	837	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
23	B	841	BCR	C7-C8-C9	-2.18	122.94	126.23
20	2	313	CLA	C1B-CHB-C4A	-2.18	125.80	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	3	317	BCR	C29-C30-C25	2.18	113.84	110.48
20	2	309	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
19	2	301	CHL	C4-C3-C2	-2.18	118.08	123.68
23	4	318	BCR	C38-C26-C27	2.18	117.81	113.62
20	K	202	CLA	C1-C2-C3	-2.18	122.27	126.04
23	A	849	BCR	C28-C27-C26	-2.18	110.18	114.08
23	1	317	BCR	C39-C30-C25	-2.18	106.76	110.30
21	2	315	LUT	C31-C30-C29	-2.18	124.20	127.31
20	B	825	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
20	B	801	CLA	CHD-C1D-ND	-2.18	122.45	124.45
20	B	826	CLA	C1B-CHB-C4A	-2.18	125.80	130.12
20	1	308	CLA	C1-C2-C3	-2.18	122.28	126.04
22	1	316	XAT	C20-C13-C12	2.18	121.51	118.08
23	F	801	BCR	C2-C1-C6	2.18	113.83	110.48
19	2	305	CHL	CBA-CAA-C2A	-2.17	108.62	113.47
20	A	822	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	J	102	BCR	C38-C26-C27	2.17	117.79	113.62
23	G	606	BCR	C38-C26-C27	2.17	117.79	113.62
20	2	308	CLA	CHD-C1D-ND	-2.17	122.46	124.45
23	A	849	BCR	C8-C9-C10	2.17	122.27	118.94
19	4	305	CHL	CHB-C4A-NA	2.17	127.51	124.51
20	1	310	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
21	3	315	LUT	C8-C7-C6	-2.17	121.11	127.20
21	4	316	LUT	C30-C31-C32	-2.17	116.45	123.22
20	1	311	CLA	C1B-CHB-C4A	-2.17	125.82	130.12
20	2	304	CLA	CHD-C1D-ND	-2.17	122.46	124.45
20	B	828	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
23	A	845	BCR	C16-C15-C14	-2.17	119.03	123.47
19	2	305	CHL	C2A-C1A-CHA	-2.17	120.07	123.86
20	A	837	CLA	CHD-C1D-ND	-2.17	122.46	124.45
21	O	205	LUT	C31-C32-C33	-2.17	120.33	126.42
20	3	308	CLA	O2A-CGA-O1A	-2.17	118.13	123.59
23	A	848	BCR	C38-C26-C27	2.17	117.78	113.62
20	A	831	CLA	CHD-C1D-ND	-2.16	122.47	124.45
20	A	841	CLA	CHD-C1D-ND	-2.16	122.47	124.45
23	B	846	BCR	C21-C20-C19	-2.16	116.47	123.22
20	A	801	CLA	C2A-C1A-CHA	2.16	127.64	123.86
20	B	802	CLA	CHB-C4A-NA	2.16	127.50	124.51
23	A	845	BCR	C10-C11-C12	-2.16	116.48	123.22
23	3	317	BCR	C24-C23-C22	-2.16	122.97	126.23
19	2	307	CHL	C1-O2A-CGA	2.16	122.10	116.44
23	A	848	BCR	C10-C11-C12	-2.16	116.49	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	1	315	LUT	C38-C25-C24	-2.15	118.95	123.56
20	A	807	CLA	C1-C2-C3	-2.15	122.32	126.04
20	3	303	CLA	CHD-C1D-ND	-2.15	122.47	124.45
20	3	309	CLA	CHD-C1D-ND	-2.15	122.47	124.45
20	4	312	CLA	C1B-CHB-C4A	-2.15	125.86	130.12
21	O	205	LUT	C40-C33-C34	-2.15	119.91	122.92
20	4	309	CLA	C1-C2-C3	-2.15	122.33	126.04
23	J	104	BCR	C8-C7-C6	-2.15	121.17	127.20
23	A	854	BCR	C8-C7-C6	-2.15	121.17	127.20
21	1	315	LUT	C18-C5-C4	2.15	118.33	114.36
20	1	312	CLA	CHD-C1D-ND	-2.15	122.48	124.45
20	A	808	CLA	O2A-CGA-O1A	-2.15	118.18	123.59
23	J	104	BCR	C33-C5-C4	2.14	117.74	113.62
23	L	301	BCR	C3-C4-C5	-2.14	110.25	114.08
20	4	313	CLA	O2D-CGD-CBD	2.14	115.08	111.27
20	O	202	CLA	C1B-CHB-C4A	-2.14	125.88	130.12
21	2	315	LUT	C38-C25-C24	-2.14	118.98	123.56
20	B	832	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
20	A	818	CLA	CHD-C1D-ND	-2.14	122.49	124.45
20	A	806	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
19	1	306	CHL	CMA-C3A-C4A	-2.14	106.03	111.77
20	A	816	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
21	4	316	LUT	C38-C25-C24	-2.14	118.99	123.56
20	L	304	CLA	CHD-C1D-ND	-2.14	122.49	124.45
23	A	848	BCR	C15-C16-C17	-2.14	119.10	123.47
23	2	317	BCR	C38-C26-C27	2.13	117.72	113.62
20	A	826	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
20	A	818	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
19	2	306	CHL	OMC-CMC-C2C	-2.13	120.87	125.69
20	B	815	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
20	B	818	CLA	CHD-C1D-ND	-2.13	122.50	124.45
20	B	812	CLA	CHD-C1D-ND	-2.13	122.50	124.45
19	2	305	CHL	C1B-CHB-C4A	-2.13	125.91	130.12
20	O	201	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
20	A	834	CLA	CHD-C1D-ND	-2.13	122.50	124.45
23	A	846	BCR	C15-C16-C17	-2.13	119.12	123.47
20	2	312	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
20	B	828	CLA	C1-C2-C3	-2.12	122.37	126.04
20	1	307	CLA	CHD-C1D-ND	-2.12	122.50	124.45
20	A	821	CLA	CHD-C1D-ND	-2.12	122.50	124.45
23	B	841	BCR	C38-C26-C27	2.12	117.69	113.62
22	2	316	XAT	C19-C9-C8	2.12	121.42	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	1	304	CLA	O2A-CGA-O1A	-2.12	118.24	123.59
20	3	311	CLA	CHD-C1D-ND	-2.12	122.50	124.45
20	G	603	CLA	CHD-C1D-ND	-2.12	122.50	124.45
20	B	833	CLA	CHD-C1D-ND	-2.12	122.51	124.45
23	B	841	BCR	C11-C12-C13	-2.12	120.47	126.42
20	A	836	CLA	C1-C2-C3	-2.12	122.38	126.04
22	1	316	XAT	C35-C15-C14	-2.12	119.14	123.47
20	B	817	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
20	A	825	CLA	CAA-CBA-CGA	-2.12	107.07	113.25
20	A	841	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
20	A	839	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	2	317	BCR	C23-C24-C25	-2.11	121.26	127.20
21	3	315	LUT	C35-C15-C14	-2.11	119.14	123.47
20	A	803	CLA	CHD-C1D-ND	-2.11	122.51	124.45
20	B	804	CLA	O2D-CGD-CBD	2.11	115.02	111.27
20	B	819	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
23	B	846	BCR	C35-C13-C12	2.11	121.41	118.08
20	B	827	CLA	CHD-C1D-ND	-2.11	122.51	124.45
23	F	801	BCR	C29-C30-C25	2.11	113.73	110.48
19	4	305	CHL	CED-O2D-CGD	2.11	120.71	115.94
20	B	809	CLA	CHD-C1D-ND	-2.11	122.52	124.45
23	2	317	BCR	C4-C5-C6	-2.11	119.67	122.73
21	O	204	LUT	C38-C25-C24	-2.11	119.05	123.56
20	A	807	CLA	CHD-C1D-ND	-2.10	122.52	124.45
20	B	802	CLA	O2A-CGA-O1A	-2.10	118.28	123.59
20	F	804	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	F	801	BCR	C35-C13-C12	2.10	121.39	118.08
22	2	316	XAT	C30-C31-C32	-2.10	116.66	123.22
20	B	805	CLA	CHD-C1D-ND	-2.10	122.52	124.45
19	4	315	CHL	C2A-C1A-CHA	-2.10	120.18	123.86
20	1	313	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
20	A	840	CLA	CHD-C1D-ND	-2.10	122.52	124.45
23	G	606	BCR	C16-C15-C14	-2.10	119.17	123.47
19	2	305	CHL	CMD-C2D-C3D	-2.10	122.79	127.61
20	4	313	CLA	CHD-C1D-ND	-2.09	122.53	124.45
19	4	306	CHL	C3B-C4B-NB	2.09	111.92	109.21
24	1	318	LHG	C5-O7-C7	-2.09	112.64	117.79
20	L	307	CLA	O2D-CGD-CBD	2.09	114.99	111.27
23	B	846	BCR	C28-C27-C26	-2.09	110.34	114.08
22	4	317	XAT	C20-C13-C12	2.09	121.37	118.08
22	3	316	XAT	C8-C9-C10	-2.09	115.73	118.94
24	A	843	LHG	C5-O7-C7	-2.09	112.64	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	833	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
20	B	813	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
20	B	833	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
20	F	802	CLA	CHD-C1D-ND	-2.09	122.54	124.45
20	B	805	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
20	B	806	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	A	848	BCR	C37-C22-C23	2.08	121.36	118.08
20	1	311	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
20	2	312	CLA	C1-C2-C3	-2.08	122.44	126.04
23	J	104	BCR	C29-C30-C25	2.08	113.69	110.48
23	B	846	BCR	C8-C7-C6	-2.08	121.35	127.20
20	4	308	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
20	B	823	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
20	A	802	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
20	4	304	CLA	CHD-C1D-ND	-2.08	122.54	124.45
23	3	317	BCR	C38-C26-C27	2.08	117.61	113.62
20	B	832	CLA	CHD-C1D-ND	-2.08	122.54	124.45
20	J	101	CLA	CHD-C1D-ND	-2.08	122.54	124.45
20	B	801	CLA	CHB-C4A-NA	2.08	127.39	124.51
20	B	803	CLA	O1D-CGD-CBD	2.08	128.74	124.48
20	1	304	CLA	CHD-C1D-ND	-2.08	122.55	124.45
21	4	316	LUT	C7-C8-C9	-2.08	123.10	126.23
20	3	309	CLA	CGD-CBD-CAD	-2.08	104.01	110.73
20	2	302	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
20	B	803	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
20	B	823	CLA	CHD-C1D-ND	-2.08	122.55	124.45
20	N	203	CLA	CHD-C1D-ND	-2.08	122.55	124.45
20	B	807	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
19	2	301	CHL	C1-C2-C3	-2.07	122.45	126.04
20	A	820	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	1	315	LUT	C20-C13-C12	2.07	121.34	118.08
20	2	312	CLA	CHD-C1D-ND	-2.07	122.55	124.45
21	2	315	LUT	C18-C5-C4	2.07	118.19	114.36
20	A	823	CLA	C1-C2-C3	-2.07	122.46	126.04
20	1	303	CLA	CHD-C1D-ND	-2.07	122.55	124.45
20	A	806	CLA	CHD-C1D-ND	-2.07	122.55	124.45
23	B	841	BCR	C15-C16-C17	-2.07	119.24	123.47
20	A	853	CLA	O2A-CGA-O1A	-2.07	118.38	123.59
20	4	308	CLA	CHD-C1D-ND	-2.07	122.56	124.45
20	K	202	CLA	O2D-CGD-CBD	2.06	114.94	111.27
22	2	316	XAT	C20-C13-C12	2.06	121.33	118.08
23	L	301	BCR	C21-C20-C19	-2.06	116.77	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	A	845	BCR	C23-C24-C25	-2.06	121.41	127.20
20	3	301	CLA	O2A-CGA-O1A	-2.06	118.39	123.59
20	B	833	CLA	C1-C2-C3	-2.06	122.48	126.04
21	O	205	LUT	C19-C9-C10	-2.06	120.03	122.92
20	A	839	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	A	807	CLA	O2D-CGD-CBD	2.06	114.93	111.27
21	1	319	LUT	C40-C33-C32	2.06	121.32	118.08
20	A	836	CLA	CHD-C1D-ND	-2.06	122.56	124.45
23	G	606	BCR	C8-C7-C6	-2.06	121.42	127.20
20	4	304	CLA	CBC-CAC-C3C	-2.06	106.76	112.43
20	J	101	CLA	O2D-CGD-CBD	2.06	114.92	111.27
21	3	315	LUT	C38-C25-C24	-2.06	119.16	123.56
20	A	827	CLA	C1-C2-C3	-2.06	122.49	126.04
20	B	837	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
20	B	830	CLA	CHD-C1D-ND	-2.06	122.56	124.45
20	B	826	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
20	N	203	CLA	O2A-CGA-O1A	-2.06	118.41	123.59
21	2	315	LUT	C39-C29-C28	2.06	121.31	118.08
20	3	303	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
20	A	814	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
20	G	604	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
21	2	315	LUT	C20-C13-C12	2.05	121.31	118.08
19	4	307	CHL	C2A-C1A-CHA	-2.05	120.27	123.86
19	3	306	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
20	B	824	CLA	O2D-CGD-CBD	2.05	114.92	111.27
23	A	847	BCR	C39-C30-C25	-2.05	106.97	110.30
21	4	316	LUT	C11-C10-C9	-2.05	124.38	127.31
20	A	809	CLA	CHD-C1D-ND	-2.05	122.57	124.45
19	1	301	CHL	O2A-CGA-O1A	-2.05	118.41	123.59
23	G	606	BCR	C35-C13-C12	2.05	121.31	118.08
20	A	825	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
20	A	814	CLA	CHD-C1D-ND	-2.05	122.57	124.45
20	B	839	CLA	CHD-C1D-ND	-2.05	122.57	124.45
23	2	317	BCR	C35-C13-C14	-2.05	120.05	122.92
20	B	832	CLA	CAA-C2A-C1A	-2.05	105.25	111.97
19	1	306	CHL	C2A-C1A-CHA	-2.05	120.27	123.86
26	1	322	HTG	C3-C4-C5	2.05	113.90	110.24
20	2	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
22	2	316	XAT	C39-C29-C28	2.05	121.31	118.08
20	A	823	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
20	A	808	CLA	CHD-C1D-ND	-2.05	122.57	124.45
20	B	825	CLA	CHD-C1D-ND	-2.05	122.57	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	819	CLA	O2A-CGA-O1A	-2.05	118.19	123.30
20	4	310	CLA	CHD-C1D-ND	-2.05	122.57	124.45
20	L	302	CLA	CHD-C1D-ND	-2.05	122.57	124.45
20	A	824	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
20	A	825	CLA	CAA-C2A-C1A	-2.05	105.27	111.97
20	2	303	CLA	CHD-C1D-ND	-2.05	122.57	124.45
21	4	316	LUT	C18-C5-C4	2.05	118.14	114.36
20	B	814	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
19	4	305	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
20	A	801	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
20	A	851	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	J	101	CLA	C1-C2-C3	-2.04	122.51	126.04
19	1	301	CHL	C1C-C2C-C3C	-2.04	105.49	107.11
20	A	840	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	N	202	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	B	821	CLA	C1-C2-C3	-2.04	122.51	126.04
20	B	809	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	A	835	CLA	CHD-C1D-ND	-2.04	122.58	124.45
23	K	204	BCR	C36-C18-C17	-2.04	120.06	122.92
20	1	305	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
20	1	321	CLA	C1-C2-C3	-2.04	122.52	126.04
20	B	826	CLA	C1-C2-C3	-2.04	122.52	126.04
20	A	803	CLA	O2A-CGA-O1A	-2.04	118.45	123.59
19	2	307	CHL	CAA-C2A-C1A	2.04	118.65	111.97
20	L	303	CLA	O2D-CGD-CBD	2.04	114.89	111.27
20	A	811	CLA	CHD-C1D-ND	-2.04	122.58	124.45
20	B	816	CLA	CHD-C1D-ND	-2.04	122.58	124.45
19	2	307	CHL	CGD-CBD-CAD	2.04	117.33	110.73
23	B	845	BCR	C36-C18-C19	2.04	121.28	118.08
20	B	810	CLA	CHD-C1D-ND	-2.04	122.58	124.45
21	1	315	LUT	C11-C10-C9	-2.04	124.41	127.31
20	3	309	CLA	CMC-C2C-C1C	2.03	128.14	125.04
20	L	303	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
23	L	306	BCR	C33-C5-C4	2.03	117.52	113.62
20	B	838	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
22	3	316	XAT	C30-C31-C32	-2.03	116.87	123.22
20	2	302	CLA	CHD-C1D-ND	-2.03	122.59	124.45
20	A	832	CLA	CHD-C1D-ND	-2.03	122.59	124.45
20	A	828	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
23	1	317	BCR	C10-C11-C12	-2.03	116.88	123.22
20	A	822	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	4	310	CLA	O2A-CGA-O1A	-2.03	118.47	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	F	806	BCR	C23-C24-C25	-2.03	121.50	127.20
20	B	816	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
20	L	304	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
19	4	305	CHL	CBC-CAC-C3C	-2.03	106.84	112.43
20	A	820	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	1	303	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	B	819	CLA	C1-C2-C3	-2.03	122.54	126.04
20	3	311	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
19	4	315	CHL	CHB-C4A-NA	2.03	127.31	124.51
20	B	839	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	B	806	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
20	B	822	CLA	C1-C2-C3	-2.02	122.54	126.04
19	1	301	CHL	O1D-CGD-CBD	-2.02	120.34	124.48
20	A	836	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
20	1	309	CLA	C1-C2-C3	-2.02	122.54	126.04
20	A	831	CLA	O2A-CGA-O1A	-2.02	118.48	123.59
19	2	301	CHL	CMB-C2B-C3B	-2.02	120.89	124.68
20	3	305	CLA	CHD-C1D-ND	-2.02	122.59	124.45
20	3	310	CLA	CHD-C1D-ND	-2.02	122.59	124.45
20	1	307	CLA	C1-C2-C3	-2.02	122.55	126.04
20	O	203	CLA	C1-C2-C3	-2.02	122.55	126.04
23	K	204	BCR	C10-C11-C12	-2.02	116.91	123.22
19	2	301	CHL	CBA-CAA-C2A	2.02	119.83	113.86
23	B	841	BCR	C35-C13-C14	-2.02	120.09	122.92
20	3	310	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
23	J	102	BCR	C11-C12-C13	-2.02	120.74	126.42
20	3	302	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
20	B	810	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
20	3	312	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	A	817	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
20	B	832	CLA	O2D-CGD-CBD	2.02	114.86	111.27
20	B	831	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	A	846	BCR	C23-C24-C25	-2.02	121.53	127.20
20	4	314	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	1	301	CHL	CHD-C1D-C2D	2.02	129.71	125.48
20	B	812	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
20	A	813	CLA	O2A-CGA-O1A	-2.02	118.27	123.30
20	B	807	CLA	CHD-C1D-ND	-2.02	122.60	124.45
20	A	841	CLA	C1-C2-C3	-2.02	122.55	126.04
20	B	835	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
23	L	301	BCR	C33-C5-C4	2.02	117.49	113.62
20	4	309	CLA	CHD-C1D-ND	-2.02	122.60	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	A	817	CLA	CHD-C1D-ND	-2.02	122.60	124.45
23	A	849	BCR	C38-C26-C27	2.02	117.49	113.62
20	3	307	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
19	1	306	CHL	C1-O2A-CGA	2.02	122.58	116.73
23	J	102	BCR	C7-C8-C9	-2.02	123.19	126.23
20	1	310	CLA	CHD-C1D-ND	-2.01	122.60	124.45
20	A	813	CLA	CHD-C1D-ND	-2.01	122.60	124.45
20	2	309	CLA	O1D-CGD-CBD	2.01	128.60	124.48
20	B	838	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	2	313	CLA	O2D-CGD-CBD	2.01	114.84	111.27
23	K	204	BCR	C33-C5-C4	2.01	117.48	113.62
20	A	809	CLA	C1-C2-C3	-2.01	122.57	126.04
20	1	321	CLA	CHD-C1D-ND	-2.01	122.61	124.45
20	F	802	CLA	O2A-CGA-O1A	-2.01	118.53	123.59
20	A	851	CLA	CHB-C4A-NA	2.00	127.28	124.51
23	A	849	BCR	C10-C11-C12	-2.00	116.96	123.22
20	A	853	CLA	CHD-C1D-ND	-2.00	122.61	124.45
21	O	204	LUT	C15-C35-C34	-2.00	119.37	123.47
20	B	804	CLA	CHD-C1D-ND	-2.00	122.61	124.45
20	A	827	CLA	C2A-C1A-CHA	2.00	127.36	123.86
20	A	805	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
23	A	854	BCR	C7-C8-C9	-2.00	123.21	126.23
21	3	315	LUT	C19-C9-C8	2.00	121.23	118.08
20	A	817	CLA	C1-C2-C3	-2.00	122.58	126.04
20	B	834	CLA	CHD-C1D-ND	-2.00	122.61	124.45
20	J	103	CLA	CHD-C1D-ND	-2.00	122.61	124.45
26	A	852	HTG	C2'-C1'-S1	-2.00	105.94	112.40
20	A	811	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
20	O	203	CLA	CHD-C1D-ND	-2.00	122.62	124.45

All (185) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
19	1	301	CHL	ND
19	1	301	CHL	NA
19	1	301	CHL	NC
19	1	306	CHL	ND
19	1	306	CHL	NA
19	1	306	CHL	NC
19	2	301	CHL	ND
19	2	301	CHL	NA
19	2	301	CHL	NC

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Mol	Chain	Res	Type	Atom
19	2	305	CHL	ND
19	2	305	CHL	NA
19	2	305	CHL	NC
19	2	306	CHL	ND
19	2	306	CHL	NA
19	2	306	CHL	NC
19	2	307	CHL	ND
19	2	307	CHL	NA
19	2	307	CHL	NC
19	2	314	CHL	ND
19	2	314	CHL	NA
19	2	314	CHL	NC
19	3	306	CHL	ND
19	3	306	CHL	NA
19	3	306	CHL	NC
19	4	305	CHL	ND
19	4	305	CHL	NA
19	4	305	CHL	NC
19	4	306	CHL	ND
19	4	306	CHL	NA
19	4	306	CHL	NC
19	4	307	CHL	ND
19	4	307	CHL	NA
19	4	307	CHL	NC
19	4	315	CHL	ND
19	4	315	CHL	NA
19	4	315	CHL	NC
20	1	302	CLA	ND
20	1	303	CLA	ND
20	1	304	CLA	ND
20	1	305	CLA	ND
20	1	307	CLA	ND
20	1	308	CLA	ND
20	1	309	CLA	ND
20	1	310	CLA	ND
20	1	311	CLA	ND
20	1	312	CLA	ND
20	1	313	CLA	ND
20	1	314	CLA	ND
20	1	321	CLA	ND
20	2	302	CLA	ND
20	2	303	CLA	ND

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Mol	Chain	Res	Type	Atom
20	2	304	CLA	ND
20	2	308	CLA	ND
20	2	309	CLA	ND
20	2	310	CLA	ND
20	2	311	CLA	ND
20	2	312	CLA	ND
20	2	313	CLA	ND
20	3	301	CLA	ND
20	3	302	CLA	ND
20	3	303	CLA	ND
20	3	304	CLA	ND
20	3	305	CLA	ND
20	3	307	CLA	ND
20	3	308	CLA	ND
20	3	310	CLA	ND
20	3	311	CLA	ND
20	3	312	CLA	ND
20	3	313	CLA	ND
20	3	314	CLA	ND
20	4	301	CLA	ND
20	4	302	CLA	ND
20	4	303	CLA	ND
20	4	304	CLA	ND
20	4	308	CLA	ND
20	4	309	CLA	ND
20	4	310	CLA	ND
20	4	311	CLA	ND
20	4	312	CLA	ND
20	4	313	CLA	ND
20	4	314	CLA	ND
20	A	801	CLA	ND
20	A	802	CLA	ND
20	A	803	CLA	ND
20	A	804	CLA	ND
20	A	805	CLA	ND
20	A	806	CLA	ND
20	A	807	CLA	ND
20	A	808	CLA	ND
20	A	809	CLA	ND
20	A	810	CLA	ND
20	A	811	CLA	ND
20	A	812	CLA	ND

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Mol	Chain	Res	Type	Atom
20	A	813	CLA	ND
20	A	814	CLA	ND
20	A	815	CLA	ND
20	A	816	CLA	ND
20	A	817	CLA	ND
20	A	818	CLA	ND
20	A	819	CLA	ND
20	A	820	CLA	ND
20	A	821	CLA	ND
20	A	822	CLA	ND
20	A	823	CLA	ND
20	A	824	CLA	ND
20	A	825	CLA	ND
20	A	826	CLA	ND
20	A	827	CLA	ND
20	A	828	CLA	ND
20	A	829	CLA	ND
20	A	830	CLA	ND
20	A	831	CLA	ND
20	A	832	CLA	ND
20	A	833	CLA	ND
20	A	834	CLA	ND
20	A	835	CLA	ND
20	A	836	CLA	ND
20	A	837	CLA	ND
20	A	838	CLA	ND
20	A	839	CLA	ND
20	A	840	CLA	ND
20	A	841	CLA	ND
20	A	851	CLA	ND
20	A	853	CLA	ND
20	B	801	CLA	ND
20	B	802	CLA	ND
20	B	803	CLA	ND
20	B	804	CLA	ND
20	B	805	CLA	ND
20	B	806	CLA	ND
20	B	807	CLA	ND
20	B	808	CLA	ND
20	B	809	CLA	ND
20	B	810	CLA	ND
20	B	811	CLA	ND

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Mol	Chain	Res	Type	Atom
20	B	812	CLA	ND
20	B	813	CLA	ND
20	B	814	CLA	ND
20	B	815	CLA	ND
20	B	816	CLA	ND
20	B	817	CLA	ND
20	B	818	CLA	ND
20	B	819	CLA	ND
20	B	820	CLA	ND
20	B	821	CLA	ND
20	B	822	CLA	ND
20	B	823	CLA	ND
20	B	824	CLA	ND
20	B	825	CLA	ND
20	B	826	CLA	ND
20	B	827	CLA	ND
20	B	828	CLA	ND
20	B	829	CLA	ND
20	B	830	CLA	ND
20	B	831	CLA	ND
20	B	832	CLA	ND
20	B	833	CLA	ND
20	B	834	CLA	ND
20	B	835	CLA	ND
20	B	836	CLA	ND
20	B	837	CLA	ND
20	B	838	CLA	ND
20	B	839	CLA	ND
20	F	802	CLA	ND
20	F	804	CLA	ND
20	F	805	CLA	ND
20	G	603	CLA	ND
20	G	604	CLA	ND
20	G	605	CLA	ND
20	H	201	CLA	ND
20	J	101	CLA	ND
20	J	103	CLA	ND
20	K	201	CLA	ND
20	K	202	CLA	ND
20	K	203	CLA	ND
20	K	205	CLA	ND
20	L	302	CLA	ND

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Mol	Chain	Res	Type	Atom
20	L	303	CLA	ND
20	L	304	CLA	ND
20	L	307	CLA	ND
20	N	202	CLA	ND
20	N	203	CLA	ND
20	O	201	CLA	ND
20	O	202	CLA	ND
20	O	203	CLA	ND

All (1463) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
19	1	301	CHL	C2-C3-C5-C6
19	1	301	CHL	C4-C3-C5-C6
19	1	306	CHL	C1A-C2A-CAA-CBA
19	1	306	CHL	C3A-C2A-CAA-CBA
19	1	306	CHL	C3C-C2C-CMC-OMC
19	1	306	CHL	CBD-CGD-O2D-CED
19	2	301	CHL	C1C-C2C-CMC-OMC
19	2	301	CHL	C3C-C2C-CMC-OMC
19	2	305	CHL	CAD-CBD-CGD-O1D
19	2	306	CHL	C1C-C2C-CMC-OMC
19	2	306	CHL	C3C-C2C-CMC-OMC
19	2	306	CHL	CBD-CGD-O2D-CED
19	2	307	CHL	C1C-C2C-CMC-OMC
19	2	307	CHL	C3C-C2C-CMC-OMC
19	3	306	CHL	C3C-C2C-CMC-OMC
19	4	305	CHL	C1C-C2C-CMC-OMC
19	4	305	CHL	C3C-C2C-CMC-OMC
19	4	306	CHL	C1A-C2A-CAA-CBA
19	4	306	CHL	C1C-C2C-CMC-OMC
19	4	306	CHL	C3C-C2C-CMC-OMC
20	1	304	CLA	C2-C3-C5-C6
20	1	304	CLA	C4-C3-C5-C6
20	1	308	CLA	C1A-C2A-CAA-CBA
20	1	308	CLA	C3A-C2A-CAA-CBA
20	1	314	CLA	CBA-CGA-O2A-C1
20	1	314	CLA	O1A-CGA-O2A-C1
20	2	308	CLA	C1A-C2A-CAA-CBA
20	2	308	CLA	C3A-C2A-CAA-CBA
20	2	312	CLA	CHA-CBD-CGD-O1D
20	2	313	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	2	313	CLA	CAD-CBD-CGD-O2D
20	3	305	CLA	C1A-C2A-CAA-CBA
20	3	305	CLA	C3A-C2A-CAA-CBA
20	3	307	CLA	C1A-C2A-CAA-CBA
20	3	307	CLA	C3A-C2A-CAA-CBA
20	3	313	CLA	CHA-CBD-CGD-O1D
20	3	313	CLA	CHA-CBD-CGD-O2D
20	3	314	CLA	C2A-CAA-CBA-CGA
20	4	301	CLA	CHA-CBD-CGD-O1D
20	4	301	CLA	CHA-CBD-CGD-O2D
20	4	301	CLA	CAD-CBD-CGD-O1D
20	4	308	CLA	C1A-C2A-CAA-CBA
20	4	308	CLA	C3A-C2A-CAA-CBA
20	4	310	CLA	CHA-CBD-CGD-O1D
20	4	310	CLA	CHA-CBD-CGD-O2D
20	4	312	CLA	C1A-C2A-CAA-CBA
20	4	312	CLA	C3A-C2A-CAA-CBA
20	4	312	CLA	CBD-CGD-O2D-CED
20	4	314	CLA	C2A-CAA-CBA-CGA
20	4	314	CLA	CHA-CBD-CGD-O1D
20	4	314	CLA	CHA-CBD-CGD-O2D
20	A	801	CLA	CHA-CBD-CGD-O1D
20	A	801	CLA	CHA-CBD-CGD-O2D
20	A	803	CLA	C1A-C2A-CAA-CBA
20	A	803	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	C1A-C2A-CAA-CBA
20	A	804	CLA	C3A-C2A-CAA-CBA
20	A	804	CLA	CHA-CBD-CGD-O1D
20	A	804	CLA	CHA-CBD-CGD-O2D
20	A	804	CLA	CAD-CBD-CGD-O1D
20	A	807	CLA	C3A-C2A-CAA-CBA
20	A	809	CLA	C2-C3-C5-C6
20	A	809	CLA	C4-C3-C5-C6
20	A	810	CLA	C1A-C2A-CAA-CBA
20	A	810	CLA	CBD-CGD-O2D-CED
20	A	811	CLA	C2-C3-C5-C6
20	A	811	CLA	C4-C3-C5-C6
20	A	817	CLA	C3A-C2A-CAA-CBA
20	A	821	CLA	C3A-C2A-CAA-CBA
20	A	823	CLA	CHA-CBD-CGD-O1D
20	A	823	CLA	CHA-CBD-CGD-O2D
20	A	827	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	A	827	CLA	CBA-CGA-O2A-C1
20	A	835	CLA	CHA-CBD-CGD-O1D
20	A	835	CLA	CHA-CBD-CGD-O2D
20	A	836	CLA	C3A-C2A-CAA-CBA
20	A	837	CLA	C2-C3-C5-C6
20	A	837	CLA	C4-C3-C5-C6
20	A	837	CLA	C11-C10-C8-C9
20	A	838	CLA	CHA-CBD-CGD-O1D
20	A	838	CLA	CHA-CBD-CGD-O2D
20	A	839	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	CAD-CBD-CGD-O1D
20	A	851	CLA	CAD-CBD-CGD-O2D
20	B	802	CLA	CHA-CBD-CGD-O1D
20	B	802	CLA	CHA-CBD-CGD-O2D
20	B	802	CLA	CBD-CGD-O2D-CED
20	B	804	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C3A-C2A-CAA-CBA
20	B	808	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	CBD-CGD-O2D-CED
20	B	812	CLA	C1A-C2A-CAA-CBA
20	B	812	CLA	C3A-C2A-CAA-CBA
20	B	817	CLA	C2A-CAA-CBA-CGA
20	B	818	CLA	C1A-C2A-CAA-CBA
20	B	818	CLA	C3A-C2A-CAA-CBA
20	B	822	CLA	C2-C3-C5-C6
20	B	822	CLA	C4-C3-C5-C6
20	B	823	CLA	C1A-C2A-CAA-CBA
20	B	823	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	C2-C3-C5-C6
20	B	824	CLA	C4-C3-C5-C6
20	B	825	CLA	CHA-CBD-CGD-O1D
20	B	825	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	C1A-C2A-CAA-CBA
20	B	827	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	C1A-C2A-CAA-CBA
20	B	828	CLA	C3A-C2A-CAA-CBA
20	B	828	CLA	CHA-CBD-CGD-O1D
20	B	828	CLA	CHA-CBD-CGD-O2D
20	B	830	CLA	C1A-C2A-CAA-CBA
20	B	830	CLA	C3A-C2A-CAA-CBA
20	B	839	CLA	C1A-C2A-CAA-CBA
20	B	839	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
20	F	805	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	C6-C7-C8-C9
20	J	103	CLA	CHA-CBD-CGD-O1D
20	J	103	CLA	CHA-CBD-CGD-O2D
20	J	103	CLA	CBD-CGD-O2D-CED
20	K	202	CLA	C1A-C2A-CAA-CBA
20	L	302	CLA	C1A-C2A-CAA-CBA
20	N	202	CLA	CHA-CBD-CGD-O2D
20	O	201	CLA	C1A-C2A-CAA-CBA
20	O	201	CLA	C3A-C2A-CAA-CBA
20	O	201	CLA	CHA-CBD-CGD-O1D
20	O	201	CLA	CHA-CBD-CGD-O2D
20	O	201	CLA	C3-C5-C6-C7
20	O	202	CLA	C1A-C2A-CAA-CBA
20	O	202	CLA	C3A-C2A-CAA-CBA
20	O	203	CLA	C3A-C2A-CAA-CBA
21	1	319	LUT	C1-C6-C7-C8
21	4	316	LUT	C1-C6-C7-C8
21	O	205	LUT	C21-C26-C27-C28
21	O	205	LUT	C25-C26-C27-C28
23	4	318	BCR	C23-C24-C25-C30
23	A	845	BCR	C37-C22-C23-C24
23	B	842	BCR	C1-C6-C7-C8
23	I	101	BCR	C7-C8-C9-C10
23	I	101	BCR	C7-C8-C9-C34
23	I	101	BCR	C21-C22-C23-C24
23	I	101	BCR	C37-C22-C23-C24
23	J	102	BCR	C21-C22-C23-C24
23	J	102	BCR	C37-C22-C23-C24
23	K	204	BCR	C21-C22-C23-C24
23	K	204	BCR	C37-C22-C23-C24
23	L	305	BCR	C37-C22-C23-C24
24	1	318	LHG	C3-O3-P-O5
24	1	318	LHG	C4-O6-P-O4
24	1	318	LHG	C4-O6-P-O5
24	2	318	LHG	O2-C2-C3-O3
24	2	318	LHG	O6-C4-C5-O7
24	A	844	LHG	C3-O3-P-O5
24	A	844	LHG	C3-O3-P-O6
24	A	844	LHG	C4-O6-P-O4
24	B	849	LHG	C3-O3-P-O4
24	B	849	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
26	B	850	HTG	C2-C1-S1-C1'
26	B	850	HTG	C2'-C1'-S1-C1
27	A	842	PQN	C12-C13-C15-C16
27	A	842	PQN	C14-C13-C15-C16
30	B	848	DGD	O6D-C1D-O3G-C3G
19	4	307	CHL	O1D-CGD-O2D-CED
19	2	305	CHL	CBD-CGD-O2D-CED
19	4	307	CHL	CBD-CGD-O2D-CED
19	4	315	CHL	CBD-CGD-O2D-CED
20	1	312	CLA	CBD-CGD-O2D-CED
20	2	303	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	CBD-CGD-O2D-CED
20	3	312	CLA	CBD-CGD-O2D-CED
20	4	303	CLA	CBD-CGD-O2D-CED
20	4	304	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	CBD-CGD-O2D-CED
20	A	851	CLA	CBD-CGD-O2D-CED
20	B	827	CLA	CBD-CGD-O2D-CED
20	K	203	CLA	CBD-CGD-O2D-CED
20	A	827	CLA	O1A-CGA-O2A-C1
20	B	817	CLA	O1A-CGA-O2A-C1
20	O	203	CLA	O1A-CGA-O2A-C1
20	3	309	CLA	O1A-CGA-O2A-C1
20	2	303	CLA	O1D-CGD-O2D-CED
20	A	839	CLA	O1D-CGD-O2D-CED
20	3	309	CLA	CBA-CGA-O2A-C1
19	2	305	CHL	O1D-CGD-O2D-CED
19	2	306	CHL	O1D-CGD-O2D-CED
20	4	303	CLA	O1D-CGD-O2D-CED
20	A	827	CLA	O1D-CGD-O2D-CED
20	B	817	CLA	CBA-CGA-O2A-C1
20	O	203	CLA	CBA-CGA-O2A-C1
20	A	808	CLA	CBD-CGD-O2D-CED
20	A	809	CLA	CBD-CGD-O2D-CED
20	G	603	CLA	CBD-CGD-O2D-CED
20	N	203	CLA	CBD-CGD-O2D-CED
20	1	303	CLA	O1A-CGA-O2A-C1
20	1	305	CLA	O1A-CGA-O2A-C1
20	4	303	CLA	O1A-CGA-O2A-C1
20	A	814	CLA	O1A-CGA-O2A-C1
20	B	812	CLA	O1A-CGA-O2A-C1
20	F	802	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
19	1	306	CHL	O1D-CGD-O2D-CED
20	4	312	CLA	O1D-CGD-O2D-CED
20	B	802	CLA	O1D-CGD-O2D-CED
20	A	810	CLA	O1D-CGD-O2D-CED
20	J	103	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	CBD-CGD-O2D-CED
20	2	311	CLA	CBD-CGD-O2D-CED
20	A	833	CLA	CBD-CGD-O2D-CED
20	B	803	CLA	CBD-CGD-O2D-CED
26	B	850	HTG	S1-C1'-C2'-C3'
20	B	810	CLA	O1D-CGD-O2D-CED
20	A	806	CLA	C3-C5-C6-C7
20	A	809	CLA	C3-C5-C6-C7
20	A	831	CLA	C3-C5-C6-C7
20	A	834	CLA	C3-C5-C6-C7
20	A	837	CLA	C3-C5-C6-C7
20	A	851	CLA	C3-C5-C6-C7
20	B	806	CLA	C3-C5-C6-C7
20	B	818	CLA	C3-C5-C6-C7
20	B	823	CLA	C3-C5-C6-C7
20	H	201	CLA	C3-C5-C6-C7
20	1	303	CLA	CBA-CGA-O2A-C1
20	1	305	CLA	CBA-CGA-O2A-C1
20	3	305	CLA	CBA-CGA-O2A-C1
20	4	303	CLA	CBA-CGA-O2A-C1
20	A	814	CLA	CBA-CGA-O2A-C1
20	B	823	CLA	CBA-CGA-O2A-C1
20	O	201	CLA	CBA-CGA-O2A-C1
20	A	841	CLA	C10-C11-C12-C13
20	1	312	CLA	O1D-CGD-O2D-CED
20	L	307	CLA	CBD-CGD-O2D-CED
20	K	203	CLA	CBA-CGA-O2A-C1
20	1	311	CLA	C3-C5-C6-C7
19	1	306	CHL	C2-C1-O2A-CGA
20	A	822	CLA	CBD-CGD-O2D-CED
20	A	836	CLA	CBD-CGD-O2D-CED
20	4	304	CLA	C2A-CAA-CBA-CGA
20	A	835	CLA	C2A-CAA-CBA-CGA
20	B	838	CLA	C2A-CAA-CBA-CGA
20	A	822	CLA	O1A-CGA-O2A-C1
20	A	805	CLA	C3-C5-C6-C7
20	A	808	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
20	A	832	CLA	C3-C5-C6-C7
19	1	301	CHL	CBA-CGA-O2A-C1
20	4	304	CLA	CBA-CGA-O2A-C1
20	4	312	CLA	CBA-CGA-O2A-C1
20	A	841	CLA	CBA-CGA-O2A-C1
20	B	810	CLA	CBA-CGA-O2A-C1
20	B	812	CLA	CBA-CGA-O2A-C1
20	B	815	CLA	CBA-CGA-O2A-C1
20	B	821	CLA	CBA-CGA-O2A-C1
20	F	802	CLA	CBA-CGA-O2A-C1
20	3	303	CLA	CBD-CGD-O2D-CED
20	3	305	CLA	O1A-CGA-O2A-C1
20	4	312	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	O1A-CGA-O2A-C1
20	B	815	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	O1A-CGA-O2A-C1
20	O	201	CLA	O1A-CGA-O2A-C1
20	F	805	CLA	O1A-CGA-O2A-C1
20	K	203	CLA	O1A-CGA-O2A-C1
19	2	307	CHL	CBD-CGD-O2D-CED
20	2	309	CLA	CBD-CGD-O2D-CED
20	2	313	CLA	CBD-CGD-O2D-CED
20	3	302	CLA	CBD-CGD-O2D-CED
20	A	814	CLA	CBD-CGD-O2D-CED
20	B	806	CLA	CBD-CGD-O2D-CED
20	B	831	CLA	CBD-CGD-O2D-CED
20	2	312	CLA	O1D-CGD-O2D-CED
20	B	827	CLA	O1D-CGD-O2D-CED
24	A	844	LHG	O2-C2-C3-O3
20	2	302	CLA	C3-C5-C6-C7
20	B	815	CLA	C3-C5-C6-C7
20	2	303	CLA	CBA-CGA-O2A-C1
20	B	824	CLA	CBA-CGA-O2A-C1
20	A	851	CLA	O1D-CGD-O2D-CED
20	K	203	CLA	O1D-CGD-O2D-CED
19	3	306	CHL	CBD-CGD-O2D-CED
20	4	310	CLA	CBD-CGD-O2D-CED
20	B	811	CLA	CBD-CGD-O2D-CED
20	3	312	CLA	O1D-CGD-O2D-CED
19	4	315	CHL	O1D-CGD-O2D-CED
20	B	808	CLA	C3-C5-C6-C7
19	2	301	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	822	CLA	CBA-CGA-O2A-C1
20	B	818	CLA	CBA-CGA-O2A-C1
19	1	301	CHL	O1A-CGA-O2A-C1
20	2	303	CLA	O1A-CGA-O2A-C1
20	B	810	CLA	O1A-CGA-O2A-C1
20	B	821	CLA	O1A-CGA-O2A-C1
20	B	824	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	C2A-CAA-CBA-CGA
20	B	804	CLA	C2A-CAA-CBA-CGA
20	B	831	CLA	C2A-CAA-CBA-CGA
20	3	309	CLA	C2C-C3C-CAC-CBC
20	4	304	CLA	O1A-CGA-O2A-C1
20	N	203	CLA	O1D-CGD-O2D-CED
20	A	828	CLA	CBD-CGD-O2D-CED
24	2	318	LHG	C1-C2-C3-O3
20	A	826	CLA	C3-C5-C6-C7
20	4	304	CLA	O1D-CGD-O2D-CED
19	4	306	CHL	CBA-CGA-O2A-C1
20	1	307	CLA	CBA-CGA-O2A-C1
20	4	311	CLA	CBA-CGA-O2A-C1
20	A	803	CLA	CBA-CGA-O2A-C1
20	A	807	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	CBA-CGA-O2A-C1
20	B	822	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	CBA-CGA-O2A-C1
26	F	803	HTG	O5-C5-C6-O6
20	1	307	CLA	O1A-CGA-O2A-C1
20	A	809	CLA	O1D-CGD-O2D-CED
27	A	842	PQN	C18-C20-C21-C22
20	A	801	CLA	C3-C5-C6-C7
19	4	305	CHL	C3-C5-C6-C7
20	1	304	CLA	C3-C5-C6-C7
19	2	301	CHL	O1A-CGA-O2A-C1
19	4	306	CHL	O1A-CGA-O2A-C1
20	2	309	CLA	C11-C10-C8-C9
20	4	302	CLA	C11-C10-C8-C9
20	A	808	CLA	C14-C13-C15-C16
20	A	810	CLA	C14-C13-C15-C16
20	A	824	CLA	C11-C12-C13-C14
20	A	827	CLA	C11-C10-C8-C9
20	A	837	CLA	C11-C12-C13-C14
20	A	841	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
20	A	853	CLA	C6-C7-C8-C9
20	B	803	CLA	C11-C12-C13-C14
20	B	806	CLA	C6-C7-C8-C9
20	B	813	CLA	C11-C12-C13-C14
20	B	819	CLA	C11-C10-C8-C9
20	B	822	CLA	C11-C12-C13-C14
20	B	824	CLA	C6-C7-C8-C9
20	B	836	CLA	C14-C13-C15-C16
20	A	808	CLA	O1D-CGD-O2D-CED
20	A	820	CLA	C5-C6-C7-C8
20	1	314	CLA	C2A-CAA-CBA-CGA
20	B	810	CLA	C2A-CAA-CBA-CGA
20	B	827	CLA	C2A-CAA-CBA-CGA
21	O	205	LUT	C7-C8-C9-C19
23	4	318	BCR	C7-C8-C9-C34
23	B	841	BCR	C7-C8-C9-C34
23	B	845	BCR	C37-C22-C23-C24
23	4	318	BCR	C7-C8-C9-C10
23	L	305	BCR	C21-C22-C23-C24
20	O	202	CLA	C2C-C3C-CAC-CBC
20	4	311	CLA	O1A-CGA-O2A-C1
20	A	807	CLA	O1A-CGA-O2A-C1
20	B	818	CLA	C8-C10-C11-C12
20	F	802	CLA	C8-C10-C11-C12
20	L	303	CLA	C13-C15-C16-C17
20	G	603	CLA	O1D-CGD-O2D-CED
20	4	310	CLA	CBA-CGA-O2A-C1
20	4	314	CLA	CBA-CGA-O2A-C1
20	B	805	CLA	CBA-CGA-O2A-C1
20	A	802	CLA	C15-C16-C17-C18
20	A	817	CLA	C8-C10-C11-C12
20	A	838	CLA	C10-C11-C12-C13
20	B	815	CLA	C5-C6-C7-C8
20	L	303	CLA	C10-C11-C12-C13
20	1	303	CLA	C13-C15-C16-C17
20	1	312	CLA	C10-C11-C12-C13
20	4	302	CLA	C8-C10-C11-C12
20	A	809	CLA	C8-C10-C11-C12
20	A	812	CLA	C15-C16-C17-C18
20	A	829	CLA	C10-C11-C12-C13
20	A	834	CLA	C10-C11-C12-C13
20	B	813	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
20	B	833	CLA	C10-C11-C12-C13
20	L	303	CLA	C8-C10-C11-C12
20	A	817	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	C8-C10-C11-C12
20	A	834	CLA	C13-C15-C16-C17
20	A	853	CLA	C15-C16-C17-C18
20	B	836	CLA	C5-C6-C7-C8
20	H	201	CLA	C5-C6-C7-C8
20	A	814	CLA	C2-C1-O2A-CGA
29	B	847	LMT	C4'-C5'-C6'-O6'
20	3	309	CLA	C4C-C3C-CAC-CBC
20	1	312	CLA	C8-C10-C11-C12
20	A	806	CLA	C10-C11-C12-C13
20	A	810	CLA	C8-C10-C11-C12
20	B	813	CLA	C10-C11-C12-C13
19	2	314	CHL	CBD-CGD-O2D-CED
20	2	310	CLA	CBD-CGD-O2D-CED
20	B	839	CLA	CBD-CGD-O2D-CED
20	A	801	CLA	C8-C10-C11-C12
20	A	833	CLA	O1D-CGD-O2D-CED
20	B	803	CLA	O1D-CGD-O2D-CED
20	1	307	CLA	C11-C12-C13-C15
20	A	801	CLA	C12-C13-C15-C16
20	A	831	CLA	C11-C12-C13-C15
20	A	841	CLA	C11-C10-C8-C7
20	A	851	CLA	C6-C7-C8-C10
20	B	803	CLA	C11-C12-C13-C15
20	B	818	CLA	C11-C10-C8-C7
20	B	838	CLA	C6-C7-C8-C10
20	A	838	CLA	C3-C5-C6-C7
20	A	816	CLA	O1A-CGA-O2A-C1
20	1	313	CLA	C2A-CAA-CBA-CGA
20	3	305	CLA	C2A-CAA-CBA-CGA
20	1	307	CLA	O1D-CGD-O2D-CED
20	2	311	CLA	O1D-CGD-O2D-CED
20	4	309	CLA	C5-C6-C7-C8
20	A	805	CLA	C5-C6-C7-C8
20	B	809	CLA	C13-C15-C16-C17
20	A	803	CLA	O1A-CGA-O2A-C1
20	B	822	CLA	O1A-CGA-O2A-C1
20	B	830	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	A	835	CLA	CBD-CGD-O2D-CED
20	A	831	CLA	C5-C6-C7-C8
20	A	832	CLA	C5-C6-C7-C8
20	B	825	CLA	C10-C11-C12-C13
20	J	101	CLA	C13-C15-C16-C17
20	K	202	CLA	C10-C11-C12-C13
20	A	831	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	CBA-CGA-O2A-C1
20	B	816	CLA	CBA-CGA-O2A-C1
20	A	818	CLA	C15-C16-C17-C18
20	A	831	CLA	C15-C16-C17-C18
20	B	807	CLA	C5-C6-C7-C8
27	A	842	PQN	C15-C16-C17-C18
27	A	842	PQN	C20-C21-C22-C23
27	A	842	PQN	C25-C26-C27-C28
20	H	201	CLA	CBD-CGD-O2D-CED
20	4	310	CLA	O1A-CGA-O2A-C1
20	4	314	CLA	O1A-CGA-O2A-C1
20	B	805	CLA	O1A-CGA-O2A-C1
20	1	303	CLA	C5-C6-C7-C8
20	A	838	CLA	C8-C10-C11-C12
20	A	853	CLA	C5-C6-C7-C8
20	B	813	CLA	C8-C10-C11-C12
20	B	832	CLA	C8-C10-C11-C12
20	B	833	CLA	C5-C6-C7-C8
20	B	839	CLA	C15-C16-C17-C18
24	1	318	LHG	C4-O6-P-O3
24	2	318	LHG	C4-O6-P-O3
24	A	844	LHG	C4-O6-P-O3
24	B	849	LHG	C3-O3-P-O6
24	B	849	LHG	C4-O6-P-O3
20	A	806	CLA	CBA-CGA-O2A-C1
20	A	826	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	CBA-CGA-O2A-C1
20	2	304	CLA	CBD-CGD-O2D-CED
26	B	851	HTG	S1-C1'-C2'-C3'
20	L	307	CLA	O1D-CGD-O2D-CED
20	4	303	CLA	C4-C3-C5-C6
20	A	809	CLA	C13-C15-C16-C17
20	A	839	CLA	C13-C15-C16-C17
20	2	308	CLA	C2A-CAA-CBA-CGA
20	3	312	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	807	CLA	C2A-CAA-CBA-CGA
20	A	851	CLA	C2A-CAA-CBA-CGA
20	B	822	CLA	C2A-CAA-CBA-CGA
20	B	805	CLA	C16-C17-C18-C19
20	B	828	CLA	CBA-CGA-O2A-C1
20	B	831	CLA	CBA-CGA-O2A-C1
20	2	302	CLA	C13-C15-C16-C17
20	A	836	CLA	O1D-CGD-O2D-CED
20	2	304	CLA	C10-C11-C12-C13
20	A	822	CLA	O1D-CGD-O2D-CED
20	B	815	CLA	C11-C12-C13-C14
20	B	822	CLA	C16-C17-C18-C20
20	B	825	CLA	C16-C17-C18-C19
24	1	318	LHG	C9-C10-C11-C12
20	3	303	CLA	O1D-CGD-O2D-CED
24	A	843	LHG	C11-C12-C13-C14
20	A	814	CLA	O1D-CGD-O2D-CED
20	B	833	CLA	C8-C10-C11-C12
20	L	303	CLA	C15-C16-C17-C18
20	H	201	CLA	O1A-CGA-O2A-C1
20	2	304	CLA	C11-C12-C13-C15
20	A	839	CLA	C16-C17-C18-C20
20	B	816	CLA	C6-C7-C8-C9
20	A	805	CLA	C4-C3-C5-C6
20	A	853	CLA	C4-C3-C5-C6
20	B	833	CLA	C4-C3-C5-C6
20	B	838	CLA	C4-C3-C5-C6
20	B	833	CLA	C2-C3-C5-C6
20	1	312	CLA	C6-C7-C8-C9
20	A	810	CLA	C11-C10-C8-C9
20	A	820	CLA	C11-C12-C13-C14
20	4	309	CLA	CBD-CGD-O2D-CED
25	1	320	LMG	C23-C24-C25-C26
20	B	821	CLA	C2A-CAA-CBA-CGA
20	G	605	CLA	C2A-CAA-CBA-CGA
20	A	831	CLA	O1A-CGA-O2A-C1
20	A	837	CLA	O1A-CGA-O2A-C1
20	B	816	CLA	O1A-CGA-O2A-C1
26	4	320	HTG	S1-C1'-C2'-C3'
23	A	845	BCR	C21-C22-C23-C24
20	B	817	CLA	C3-C5-C6-C7
20	2	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	A	852	HTG	C3'-C4'-C5'-C6'
26	B	850	HTG	C3'-C4'-C5'-C6'
29	G	601	LMT	C6-C7-C8-C9
20	1	313	CLA	C6-C7-C8-C10
20	B	807	CLA	C6-C7-C8-C9
20	B	815	CLA	C11-C12-C13-C15
20	B	824	CLA	C5-C6-C7-C8
30	B	848	DGD	CDA-CEA-CFA-CGA
20	G	605	CLA	CBA-CGA-O2A-C1
20	B	806	CLA	O1D-CGD-O2D-CED
25	4	319	LMG	C21-C22-C23-C24
25	1	320	LMG	C10-C11-C12-C13
20	A	806	CLA	O1A-CGA-O2A-C1
19	1	306	CHL	CBA-CGA-O2A-C1
20	A	804	CLA	CBA-CGA-O2A-C1
25	4	319	LMG	C20-C21-C22-C23
20	B	831	CLA	O1D-CGD-O2D-CED
20	4	304	CLA	C3A-C2A-CAA-CBA
20	A	827	CLA	C3A-C2A-CAA-CBA
20	A	832	CLA	C3A-C2A-CAA-CBA
20	B	804	CLA	C3A-C2A-CAA-CBA
20	F	805	CLA	C3A-C2A-CAA-CBA
20	J	101	CLA	C3A-C2A-CAA-CBA
20	L	302	CLA	C3A-C2A-CAA-CBA
20	1	307	CLA	C10-C11-C12-C13
20	3	302	CLA	O1D-CGD-O2D-CED
20	A	853	CLA	C2-C3-C5-C6
20	B	838	CLA	C2-C3-C5-C6
20	1	310	CLA	CBD-CGD-O2D-CED
20	O	202	CLA	C4C-C3C-CAC-CBC
20	G	604	CLA	C2A-CAA-CBA-CGA
20	A	826	CLA	O1A-CGA-O2A-C1
20	B	828	CLA	O1A-CGA-O2A-C1
20	1	313	CLA	C6-C7-C8-C9
20	A	841	CLA	C16-C17-C18-C20
20	B	805	CLA	C16-C17-C18-C20
20	A	811	CLA	C5-C6-C7-C8
20	2	313	CLA	O1D-CGD-O2D-CED
20	1	302	CLA	C15-C16-C17-C18
27	A	842	PQN	C13-C15-C16-C17
20	B	831	CLA	O1A-CGA-O2A-C1
24	A	843	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
19	4	307	CHL	C2-C1-O2A-CGA
20	B	805	CLA	C8-C10-C11-C12
20	B	806	CLA	C15-C16-C17-C18
20	A	804	CLA	O1A-CGA-O2A-C1
20	A	841	CLA	C3-C5-C6-C7
21	1	319	LUT	C5-C6-C7-C8
21	3	315	LUT	C1-C6-C7-C8
21	3	315	LUT	C5-C6-C7-C8
21	O	205	LUT	C1-C6-C7-C8
21	O	205	LUT	C5-C6-C7-C8
23	4	318	BCR	C1-C6-C7-C8
23	4	318	BCR	C5-C6-C7-C8
23	4	318	BCR	C23-C24-C25-C26
23	A	845	BCR	C23-C24-C25-C26
23	A	845	BCR	C23-C24-C25-C30
23	B	842	BCR	C5-C6-C7-C8
23	B	842	BCR	C23-C24-C25-C26
23	B	842	BCR	C23-C24-C25-C30
23	I	101	BCR	C1-C6-C7-C8
23	I	101	BCR	C5-C6-C7-C8
23	I	101	BCR	C23-C24-C25-C26
23	I	101	BCR	C23-C24-C25-C30
23	J	102	BCR	C1-C6-C7-C8
23	J	102	BCR	C5-C6-C7-C8
23	J	102	BCR	C23-C24-C25-C26
23	J	102	BCR	C23-C24-C25-C30
23	K	204	BCR	C23-C24-C25-C26
23	K	204	BCR	C23-C24-C25-C30
23	L	305	BCR	C23-C24-C25-C26
23	L	305	BCR	C23-C24-C25-C30
20	B	811	CLA	O1D-CGD-O2D-CED
20	B	825	CLA	CBA-CGA-O2A-C1
24	B	849	LHG	C8-C7-O7-C5
25	4	319	LMG	C11-C10-O7-C8
24	1	318	LHG	C10-C11-C12-C13
20	B	808	CLA	C4-C3-C5-C6
20	A	801	CLA	C11-C12-C13-C15
20	A	805	CLA	C2-C3-C5-C6
20	A	807	CLA	C11-C12-C13-C15
20	A	810	CLA	C11-C10-C8-C7
20	A	816	CLA	C11-C10-C8-C7
20	A	824	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	827	CLA	C11-C10-C8-C7
20	A	828	CLA	C2-C3-C5-C6
20	A	838	CLA	C6-C7-C8-C10
20	A	841	CLA	C12-C13-C15-C16
20	A	853	CLA	C6-C7-C8-C10
20	B	808	CLA	C2-C3-C5-C6
20	B	813	CLA	C11-C12-C13-C15
20	B	819	CLA	C12-C13-C15-C16
20	B	827	CLA	C6-C7-C8-C10
20	L	303	CLA	C11-C10-C8-C7
20	A	809	CLA	C10-C11-C12-C13
20	B	823	CLA	C8-C10-C11-C12
20	A	809	CLA	C16-C17-C18-C20
20	A	839	CLA	C16-C17-C18-C19
20	B	816	CLA	C6-C7-C8-C10
20	A	828	CLA	CBA-CGA-O2A-C1
20	B	830	CLA	C2A-CAA-CBA-CGA
20	H	201	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	C8-C10-C11-C12
29	B	847	LMT	O5'-C5'-C6'-O6'
20	4	310	CLA	O1D-CGD-O2D-CED
20	A	812	CLA	CBD-CGD-O2D-CED
19	2	307	CHL	O1D-CGD-O2D-CED
20	A	812	CLA	C5-C6-C7-C8
20	2	304	CLA	C11-C12-C13-C14
24	2	318	LHG	C8-C7-O7-C5
25	1	323	LMG	C11-C10-O7-C8
20	A	801	CLA	C13-C15-C16-C17
20	4	301	CLA	CBA-CGA-O2A-C1
19	1	306	CHL	O1A-CGA-O2A-C1
25	4	319	LMG	O9-C10-O7-C8
20	B	822	CLA	C16-C17-C18-C19
20	4	309	CLA	C10-C11-C12-C13
20	A	828	CLA	C4-C3-C5-C6
20	B	823	CLA	C4-C3-C5-C6
20	4	303	CLA	C2-C3-C5-C6
20	1	307	CLA	C11-C12-C13-C14
20	A	805	CLA	C11-C12-C13-C14
20	A	807	CLA	C11-C12-C13-C14
20	A	812	CLA	C6-C7-C8-C9
20	A	816	CLA	C11-C10-C8-C9
20	A	824	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
20	A	829	CLA	C14-C13-C15-C16
20	A	831	CLA	C11-C12-C13-C14
20	A	837	CLA	C6-C7-C8-C9
20	A	841	CLA	C11-C10-C8-C9
20	B	805	CLA	C11-C12-C13-C14
20	B	819	CLA	C14-C13-C15-C16
20	B	827	CLA	C6-C7-C8-C9
20	B	838	CLA	C6-C7-C8-C9
20	A	802	CLA	CBD-CGD-O2D-CED
19	2	307	CHL	C2A-CAA-CBA-CGA
20	1	308	CLA	C2A-CAA-CBA-CGA
20	4	303	CLA	C2A-CAA-CBA-CGA
20	A	820	CLA	C2A-CAA-CBA-CGA
20	B	816	CLA	C2A-CAA-CBA-CGA
26	F	807	HTG	C3'-C4'-C5'-C6'
19	2	306	CHL	O1A-CGA-O2A-C1
20	B	825	CLA	O1A-CGA-O2A-C1
19	2	307	CHL	C1A-C2A-CAA-CBA
20	1	313	CLA	C1A-C2A-CAA-CBA
20	4	304	CLA	C1A-C2A-CAA-CBA
20	A	807	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C1A-C2A-CAA-CBA
20	A	817	CLA	C1A-C2A-CAA-CBA
20	A	821	CLA	C1A-C2A-CAA-CBA
20	A	822	CLA	C1A-C2A-CAA-CBA
20	A	823	CLA	C1A-C2A-CAA-CBA
20	A	832	CLA	C1A-C2A-CAA-CBA
20	A	836	CLA	C1A-C2A-CAA-CBA
20	B	805	CLA	C1A-C2A-CAA-CBA
20	B	821	CLA	C1A-C2A-CAA-CBA
20	F	805	CLA	C1A-C2A-CAA-CBA
20	J	101	CLA	C1A-C2A-CAA-CBA
20	O	203	CLA	C1A-C2A-CAA-CBA
20	A	841	CLA	C16-C17-C18-C19
20	B	825	CLA	C16-C17-C18-C20
24	B	849	LHG	O9-C7-O7-C5
25	1	323	LMG	O9-C10-O7-C8
20	A	828	CLA	O1D-CGD-O2D-CED
20	A	808	CLA	C13-C15-C16-C17
19	3	306	CHL	O1D-CGD-O2D-CED
29	G	601	LMT	C1-C2-C3-C4
20	1	312	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
20	A	808	CLA	C16-C17-C18-C20
25	1	323	LMG	O6-C5-C6-O5
20	B	807	CLA	C3-C5-C6-C7
24	A	844	LHG	C1-C2-C3-O3
24	2	318	LHG	O9-C7-O7-C5
20	2	304	CLA	C5-C6-C7-C8
20	A	802	CLA	C13-C15-C16-C17
30	B	848	DGD	C5B-C6B-C7B-C8B
20	A	828	CLA	C2A-CAA-CBA-CGA
20	A	828	CLA	O1A-CGA-O2A-C1
30	B	848	DGD	CAB-CBB-CCB-CDB
25	4	319	LMG	O6-C5-C6-O5
20	1	307	CLA	C14-C13-C15-C16
25	1	320	LMG	C29-C30-C31-C32
29	B	847	LMT	O5'-C1'-O1'-C1
29	G	601	LMT	O5'-C1'-O1'-C1
20	B	825	CLA	C15-C16-C17-C18
20	1	312	CLA	C13-C15-C16-C17
30	B	848	DGD	O6E-C5E-C6E-O5E
20	A	809	CLA	C16-C17-C18-C19
20	A	812	CLA	CBA-CGA-O2A-C1
20	A	834	CLA	CBA-CGA-O2A-C1
20	A	841	CLA	C15-C16-C17-C18
20	B	822	CLA	C10-C11-C12-C13
20	2	304	CLA	C3-C5-C6-C7
20	4	312	CLA	C3-C5-C6-C7
20	A	817	CLA	C3-C5-C6-C7
19	2	314	CHL	O1D-CGD-O2D-CED
20	B	839	CLA	O1D-CGD-O2D-CED
19	2	306	CHL	CBA-CGA-O2A-C1
20	B	819	CLA	CBA-CGA-O2A-C1
20	2	310	CLA	O1D-CGD-O2D-CED
20	A	817	CLA	O1D-CGD-O2D-CED
25	1	323	LMG	C16-C17-C18-C19
26	F	807	HTG	C1'-C2'-C3'-C4'
25	1	320	LMG	C30-C31-C32-C33
20	A	805	CLA	C10-C11-C12-C13
20	2	312	CLA	C6-C7-C8-C10
20	4	302	CLA	C6-C7-C8-C10
20	4	302	CLA	C11-C10-C8-C7
20	4	312	CLA	C11-C12-C13-C15
20	A	802	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
20	A	805	CLA	C11-C12-C13-C15
20	A	806	CLA	C12-C13-C15-C16
20	A	810	CLA	C11-C12-C13-C15
20	A	817	CLA	C11-C12-C13-C15
20	A	820	CLA	C11-C12-C13-C15
20	A	824	CLA	C11-C12-C13-C15
20	A	829	CLA	C12-C13-C15-C16
20	A	832	CLA	C12-C13-C15-C16
20	A	837	CLA	C6-C7-C8-C10
20	A	837	CLA	C11-C12-C13-C15
20	A	851	CLA	C12-C13-C15-C16
20	A	853	CLA	C12-C13-C15-C16
20	B	805	CLA	C11-C12-C13-C15
20	B	806	CLA	C6-C7-C8-C10
20	B	806	CLA	C12-C13-C15-C16
20	B	813	CLA	C12-C13-C15-C16
20	B	817	CLA	C12-C13-C15-C16
20	B	824	CLA	C12-C13-C15-C16
20	B	831	CLA	C12-C13-C15-C16
20	1	303	CLA	C11-C12-C13-C14
20	1	309	CLA	C11-C10-C8-C9
20	2	312	CLA	C6-C7-C8-C9
20	2	312	CLA	C11-C10-C8-C9
20	4	302	CLA	C6-C7-C8-C9
20	A	801	CLA	C11-C12-C13-C14
20	A	802	CLA	C11-C10-C8-C9
20	A	805	CLA	C6-C7-C8-C9
20	A	805	CLA	C14-C13-C15-C16
20	A	807	CLA	C14-C13-C15-C16
20	A	808	CLA	C11-C12-C13-C14
20	A	810	CLA	C11-C12-C13-C14
20	A	816	CLA	C6-C7-C8-C9
20	A	832	CLA	C14-C13-C15-C16
20	A	839	CLA	C14-C13-C15-C16
20	A	841	CLA	C6-C7-C8-C9
20	A	841	CLA	C11-C12-C13-C14
20	B	803	CLA	C6-C7-C8-C9
20	B	806	CLA	C14-C13-C15-C16
20	B	813	CLA	C14-C13-C15-C16
20	B	817	CLA	C14-C13-C15-C16
20	B	824	CLA	C14-C13-C15-C16
20	4	309	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	A	843	LHG	C24-C25-C26-C27
20	A	818	CLA	O1D-CGD-O2D-CED
20	B	810	CLA	C8-C10-C11-C12
20	A	820	CLA	CBA-CGA-O2A-C1
20	A	837	CLA	C8-C10-C11-C12
20	1	321	CLA	CBD-CGD-O2D-CED
20	B	807	CLA	C6-C7-C8-C10
20	1	313	CLA	CBA-CGA-O2A-C1
20	2	304	CLA	O1D-CGD-O2D-CED
20	A	835	CLA	O1D-CGD-O2D-CED
20	H	201	CLA	O1D-CGD-O2D-CED
20	A	838	CLA	C4-C3-C5-C6
20	B	827	CLA	C4-C3-C5-C6
20	B	823	CLA	C2-C3-C5-C6
20	B	827	CLA	C2-C3-C5-C6
19	4	305	CHL	C2C-C3C-CAC-CBC
20	G	605	CLA	O1A-CGA-O2A-C1
20	B	811	CLA	C6-C7-C8-C9
19	1	306	CHL	C2A-CAA-CBA-CGA
20	1	308	CLA	CBA-CGA-O2A-C1
20	4	308	CLA	CBA-CGA-O2A-C1
20	A	825	CLA	C3A-C2A-CAA-CBA
20	A	831	CLA	C3A-C2A-CAA-CBA
20	B	831	CLA	C3A-C2A-CAA-CBA
20	K	202	CLA	C3A-C2A-CAA-CBA
20	L	303	CLA	C3A-C2A-CAA-CBA
20	L	307	CLA	C3A-C2A-CAA-CBA
20	N	203	CLA	C3A-C2A-CAA-CBA
19	3	306	CHL	CBA-CGA-O2A-C1
20	L	303	CLA	C3-C5-C6-C7
20	2	304	CLA	CBA-CGA-O2A-C1
20	B	829	CLA	CBA-CGA-O2A-C1
20	A	825	CLA	C15-C16-C17-C18
24	2	318	LHG	C4-C5-C6-O8
24	A	844	LHG	C4-C5-C6-O8
20	A	808	CLA	C16-C17-C18-C19
20	A	838	CLA	C2-C3-C5-C6
20	B	835	CLA	CBD-CGD-O2D-CED
20	1	313	CLA	C5-C6-C7-C8
19	4	315	CHL	C3C-C2C-CMC-OMC
20	A	812	CLA	O1A-CGA-O2A-C1
19	2	307	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
20	A	834	CLA	O1A-CGA-O2A-C1
20	B	811	CLA	C6-C7-C8-C10
24	2	318	LHG	O7-C5-C6-O8
24	A	844	LHG	O7-C5-C6-O8
25	1	323	LMG	O1-C7-C8-O7
30	B	848	DGD	O2G-C2G-C3G-O3G
20	A	838	CLA	C16-C17-C18-C20
20	A	841	CLA	C8-C10-C11-C12
20	4	311	CLA	C2-C1-O2A-CGA
20	B	802	CLA	C2-C1-O2A-CGA
20	B	828	CLA	C2-C1-O2A-CGA
20	2	302	CLA	C11-C12-C13-C14
20	4	312	CLA	C11-C10-C8-C9
20	A	817	CLA	C11-C12-C13-C14
20	A	827	CLA	C6-C7-C8-C9
20	A	839	CLA	C6-C7-C8-C9
20	A	839	CLA	C11-C12-C13-C14
20	B	810	CLA	C14-C13-C15-C16
20	B	825	CLA	C11-C10-C8-C9
20	B	828	CLA	C11-C10-C8-C9
20	B	819	CLA	O1A-CGA-O2A-C1
20	A	804	CLA	C2A-CAA-CBA-CGA
20	B	828	CLA	C2A-CAA-CBA-CGA
20	B	813	CLA	C16-C17-C18-C20
21	1	315	LUT	C1-C6-C7-C8
21	1	315	LUT	C5-C6-C7-C8
23	1	317	BCR	C23-C24-C25-C26
23	1	317	BCR	C23-C24-C25-C30
23	3	317	BCR	C1-C6-C7-C8
23	3	317	BCR	C5-C6-C7-C8
23	3	317	BCR	C23-C24-C25-C26
23	A	845	BCR	C1-C6-C7-C8
23	A	845	BCR	C5-C6-C7-C8
23	A	847	BCR	C23-C24-C25-C26
23	B	844	BCR	C5-C6-C7-C8
23	B	846	BCR	C1-C6-C7-C8
23	B	846	BCR	C5-C6-C7-C8
23	J	104	BCR	C23-C24-C25-C26
23	J	104	BCR	C23-C24-C25-C30
23	L	301	BCR	C5-C6-C7-C8
21	O	205	LUT	C7-C8-C9-C10
23	B	845	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
20	A	812	CLA	O1D-CGD-O2D-CED
26	B	850	HTG	C2'-C3'-C4'-C5'
20	B	813	CLA	C16-C17-C18-C19
20	B	821	CLA	C11-C10-C8-C9
20	1	310	CLA	O1D-CGD-O2D-CED
24	2	318	LHG	O6-C4-C5-C6
20	1	302	CLA	C12-C13-C15-C16
20	1	303	CLA	C11-C12-C13-C15
20	1	309	CLA	C11-C10-C8-C7
20	2	302	CLA	C11-C12-C13-C15
20	2	309	CLA	C11-C10-C8-C7
20	2	312	CLA	C11-C10-C8-C7
20	A	805	CLA	C12-C13-C15-C16
20	A	808	CLA	C11-C12-C13-C15
20	A	829	CLA	C11-C10-C8-C7
20	A	839	CLA	C12-C13-C15-C16
20	A	841	CLA	C11-C12-C13-C15
20	B	803	CLA	C6-C7-C8-C10
20	B	810	CLA	C12-C13-C15-C16
20	B	819	CLA	C6-C7-C8-C10
20	B	825	CLA	C6-C7-C8-C10
20	B	833	CLA	C11-C12-C13-C15
20	H	201	CLA	C6-C7-C8-C10
20	A	820	CLA	O1A-CGA-O2A-C1
20	1	321	CLA	C13-C15-C16-C17
23	F	801	BCR	C15-C16-C17-C18
20	K	202	CLA	C11-C12-C13-C14
19	2	306	CHL	C2A-CAA-CBA-CGA
20	A	808	CLA	C2A-CAA-CBA-CGA
20	A	821	CLA	C2A-CAA-CBA-CGA
26	B	850	HTG	O5-C1-S1-C1'
20	A	802	CLA	C16-C17-C18-C20
20	A	853	CLA	C10-C11-C12-C13
20	1	311	CLA	CBA-CGA-O2A-C1
20	A	853	CLA	CBD-CGD-O2D-CED
20	1	305	CLA	CAD-CBD-CGD-O2D
20	4	304	CLA	CAD-CBD-CGD-O2D
20	A	805	CLA	CAD-CBD-CGD-O2D
20	A	806	CLA	CAD-CBD-CGD-O2D
20	A	817	CLA	CAD-CBD-CGD-O2D
20	A	824	CLA	CAD-CBD-CGD-O2D
20	B	820	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	B	833	CLA	CAD-CBD-CGD-O2D
20	K	201	CLA	CAD-CBD-CGD-O2D
24	B	849	LHG	C6-C5-O7-C7
20	1	303	CLA	C15-C16-C17-C18
20	B	803	CLA	C8-C10-C11-C12
20	1	308	CLA	C4-C3-C5-C6
20	A	802	CLA	C16-C17-C18-C19
25	1	320	LMG	O6-C1-O1-C7
20	1	308	CLA	C2-C3-C5-C6
25	1	323	LMG	C7-C8-C9-O8
30	B	848	DGD	C1G-C2G-C3G-O3G
20	1	313	CLA	O1A-CGA-O2A-C1
20	A	821	CLA	O2A-C1-C2-C3
19	2	306	CHL	C2C-C3C-CAC-CBC
20	B	807	CLA	C2A-CAA-CBA-CGA
20	B	814	CLA	C2A-CAA-CBA-CGA
20	A	841	CLA	C13-C15-C16-C17
20	B	801	CLA	CBD-CGD-O2D-CED
20	A	838	CLA	C16-C17-C18-C19
20	B	806	CLA	C16-C17-C18-C19
20	A	802	CLA	O1D-CGD-O2D-CED
19	1	301	CHL	CHA-CBD-CGD-O1D
19	1	301	CHL	CHA-CBD-CGD-O2D
19	2	301	CHL	CHA-CBD-CGD-O1D
19	2	301	CHL	CHA-CBD-CGD-O2D
20	1	313	CLA	CHA-CBD-CGD-O1D
20	1	313	CLA	CHA-CBD-CGD-O2D
20	1	321	CLA	CHA-CBD-CGD-O1D
20	2	312	CLA	CHA-CBD-CGD-O2D
20	A	803	CLA	CHA-CBD-CGD-O1D
20	A	809	CLA	CHA-CBD-CGD-O1D
20	A	809	CLA	CHA-CBD-CGD-O2D
20	A	812	CLA	CHA-CBD-CGD-O1D
20	A	818	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O1D
20	A	829	CLA	CHA-CBD-CGD-O2D
20	B	805	CLA	CHA-CBD-CGD-O1D
20	B	808	CLA	CHA-CBD-CGD-O1D
20	B	824	CLA	CHA-CBD-CGD-O1D
20	B	824	CLA	CHA-CBD-CGD-O2D
20	F	805	CLA	CHA-CBD-CGD-O1D
20	F	805	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	L	307	CLA	CHA-CBD-CGD-O1D
20	L	307	CLA	CHA-CBD-CGD-O2D
20	A	818	CLA	C8-C10-C11-C12
20	A	802	CLA	C3-C5-C6-C7
20	1	308	CLA	O1A-CGA-O2A-C1
20	2	304	CLA	O1A-CGA-O2A-C1
20	4	308	CLA	O1A-CGA-O2A-C1
20	B	829	CLA	O1A-CGA-O2A-C1
20	1	304	CLA	CBA-CGA-O2A-C1
20	1	312	CLA	C14-C13-C15-C16
20	A	834	CLA	C14-C13-C15-C16
29	B	847	LMT	O5B-C5B-C6B-O6B
20	A	840	CLA	C2A-CAA-CBA-CGA
20	B	801	CLA	C2A-CAA-CBA-CGA
20	1	321	CLA	CAA-CBA-CGA-O2A
29	B	847	LMT	C1-C2-C3-C4
24	1	318	LHG	C30-C31-C32-C33
20	3	314	CLA	CBA-CGA-O2A-C1
20	A	813	CLA	C1A-C2A-CAA-CBA
20	A	825	CLA	C1A-C2A-CAA-CBA
20	B	831	CLA	C1A-C2A-CAA-CBA
20	L	307	CLA	C1A-C2A-CAA-CBA
25	1	323	LMG	C18-C19-C20-C21
20	1	311	CLA	O1A-CGA-O2A-C1
24	1	318	LHG	C3-O3-P-O6
20	B	818	CLA	C4-C3-C5-C6
24	2	318	LHG	C4-O6-P-O5
24	A	844	LHG	C4-O6-P-O5
20	A	824	CLA	C16-C17-C18-C19
20	2	303	CLA	O2A-C1-C2-C3
20	4	312	CLA	C8-C10-C11-C12
20	B	809	CLA	C16-C17-C18-C20
26	B	850	HTG	C4'-C5'-C6'-C7'
20	1	321	CLA	O1D-CGD-O2D-CED
19	1	301	CHL	CAD-CBD-CGD-O1D
19	2	301	CHL	CAD-CBD-CGD-O1D
20	3	313	CLA	CAD-CBD-CGD-O1D
20	B	805	CLA	CAD-CBD-CGD-O1D
20	O	201	CLA	CAD-CBD-CGD-O1D
25	1	320	LMG	O7-C10-C11-C12
25	1	320	LMG	C28-C29-C30-C31
30	B	848	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
20	N	203	CLA	CBA-CGA-O2A-C1
20	4	301	CLA	O1A-CGA-O2A-C1
20	A	818	CLA	C4-C3-C5-C6
19	4	306	CHL	C3A-C2A-CAA-CBA
20	1	308	CLA	C11-C10-C8-C7
20	3	301	CLA	C6-C7-C8-C10
20	A	802	CLA	C12-C13-C15-C16
20	A	808	CLA	C12-C13-C15-C16
20	A	831	CLA	C12-C13-C15-C16
20	A	839	CLA	C11-C10-C8-C7
20	A	853	CLA	C11-C10-C8-C7
20	B	815	CLA	C6-C7-C8-C10
20	B	822	CLA	C11-C12-C13-C15
20	B	824	CLA	C6-C7-C8-C10
20	B	803	CLA	C13-C15-C16-C17
20	B	805	CLA	C13-C15-C16-C17
20	1	304	CLA	O1A-CGA-O2A-C1
20	A	817	CLA	C2A-CAA-CBA-CGA
20	A	810	CLA	C16-C17-C18-C20
24	1	318	LHG	C23-C24-C25-C26
19	3	306	CHL	C1C-C2C-CMC-OMC
19	4	315	CHL	C1C-C2C-CMC-OMC
25	1	323	LMG	O1-C7-C8-C9
20	3	301	CLA	C10-C11-C12-C13
20	A	833	CLA	C5-C6-C7-C8
20	B	829	CLA	C5-C6-C7-C8
20	A	806	CLA	C5-C6-C7-C8
20	A	829	CLA	C11-C10-C8-C9
20	A	839	CLA	C11-C10-C8-C9
20	B	818	CLA	C11-C10-C8-C9
20	B	819	CLA	C6-C7-C8-C9
20	B	825	CLA	C6-C7-C8-C9
20	B	831	CLA	C14-C13-C15-C16
20	B	833	CLA	C11-C12-C13-C14
20	F	802	CLA	C11-C12-C13-C14
20	A	853	CLA	O1D-CGD-O2D-CED
19	2	307	CHL	O1A-CGA-O2A-C1
20	B	829	CLA	C3-C5-C6-C7
20	B	817	CLA	C8-C10-C11-C12
20	N	203	CLA	O1A-CGA-O2A-C1
20	4	301	CLA	CAA-CBA-CGA-O2A
20	B	801	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
20	K	202	CLA	C11-C12-C13-C15
30	B	848	DGD	C2A-C3A-C4A-C5A
20	A	839	CLA	C4-C3-C5-C6
20	B	828	CLA	C4-C3-C5-C6
20	A	818	CLA	C2-C3-C5-C6
20	A	824	CLA	C16-C17-C18-C20
20	A	810	CLA	C15-C16-C17-C18
20	A	821	CLA	C1-C2-C3-C4
20	B	833	CLA	C3-C5-C6-C7
19	1	301	CHL	CAA-CBA-CGA-O2A
20	B	835	CLA	O1D-CGD-O2D-CED
20	2	312	CLA	C2A-CAA-CBA-CGA
20	3	311	CLA	C2A-CAA-CBA-CGA
20	B	805	CLA	C2A-CAA-CBA-CGA
20	L	303	CLA	C2A-CAA-CBA-CGA
20	L	304	CLA	CBA-CGA-O2A-C1
19	2	301	CHL	C2-C1-O2A-CGA
20	A	806	CLA	C2-C1-O2A-CGA
25	1	323	LMG	C23-C24-C25-C26
26	N	201	HTG	C2'-C3'-C4'-C5'
20	B	823	CLA	C10-C11-C12-C13
20	L	304	CLA	O1A-CGA-O2A-C1
26	F	803	HTG	C4-C5-C6-O6
20	A	806	CLA	C16-C17-C18-C20
20	4	312	CLA	C10-C11-C12-C13
21	2	315	LUT	C1-C6-C7-C8
21	4	316	LUT	C5-C6-C7-C8
23	3	317	BCR	C23-C24-C25-C30
23	A	847	BCR	C23-C24-C25-C30
23	B	844	BCR	C1-C6-C7-C8
23	L	301	BCR	C1-C6-C7-C8
26	B	851	HTG	C1'-C2'-C3'-C4'
20	4	313	CLA	C2A-CAA-CBA-CGA
20	B	837	CLA	O1A-CGA-O2A-C1
20	A	810	CLA	C10-C11-C12-C13
24	2	318	LHG	C3-O3-P-O6
24	A	843	LHG	C3-O3-P-O6
24	A	843	LHG	C4-O6-P-O3
24	A	843	LHG	C13-C14-C15-C16
20	1	312	CLA	C12-C13-C15-C16
20	A	807	CLA	C12-C13-C15-C16
20	A	834	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
20	A	834	CLA	C12-C13-C15-C16
20	A	839	CLA	C11-C12-C13-C15
20	B	827	CLA	C11-C12-C13-C15
20	B	828	CLA	C11-C10-C8-C7
20	F	802	CLA	C11-C12-C13-C15
24	A	843	LHG	C26-C27-C28-C29
20	B	811	CLA	O1A-CGA-O2A-C1
20	1	302	CLA	C14-C13-C15-C16
20	3	301	CLA	C6-C7-C8-C9
20	4	312	CLA	C11-C12-C13-C14
20	A	801	CLA	C14-C13-C15-C16
20	A	806	CLA	C14-C13-C15-C16
20	A	831	CLA	C14-C13-C15-C16
20	A	838	CLA	C6-C7-C8-C9
20	A	851	CLA	C6-C7-C8-C9
20	A	851	CLA	C14-C13-C15-C16
20	A	853	CLA	C14-C13-C15-C16
20	B	823	CLA	C11-C12-C13-C15
20	B	811	CLA	CBA-CGA-O2A-C1
20	B	837	CLA	CBA-CGA-O2A-C1
20	A	817	CLA	C16-C17-C18-C20
20	A	828	CLA	C16-C17-C18-C20
20	B	809	CLA	C16-C17-C18-C19
20	F	804	CLA	CBD-CGD-O2D-CED
20	B	821	CLA	C11-C10-C8-C7
20	A	817	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	C2-C3-C5-C6
20	A	810	CLA	C16-C17-C18-C19
20	B	836	CLA	CBA-CGA-O2A-C1
20	A	804	CLA	CAA-CBA-CGA-O2A
20	B	807	CLA	CBA-CGA-O2A-C1
20	1	302	CLA	C16-C17-C18-C20
20	B	824	CLA	C16-C17-C18-C20
20	A	820	CLA	C3-C5-C6-C7
20	H	201	CLA	C4-C3-C5-C6
20	L	302	CLA	CAA-CBA-CGA-O1A
20	B	812	CLA	C5-C6-C7-C8
20	B	828	CLA	C5-C6-C7-C8
20	2	311	CLA	O1A-CGA-O2A-C1
20	B	836	CLA	O1A-CGA-O2A-C1
20	4	302	CLA	C10-C11-C12-C13
24	A	843	LHG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
20	A	841	CLA	CBD-CGD-O2D-CED
20	2	304	CLA	C2-C1-O2A-CGA
20	3	307	CLA	C2-C1-O2A-CGA
20	A	805	CLA	C2-C1-O2A-CGA
20	A	851	CLA	C2-C1-O2A-CGA
20	A	853	CLA	C2-C1-O2A-CGA
20	1	303	CLA	C2A-CAA-CBA-CGA
20	1	312	CLA	C2A-CAA-CBA-CGA
20	2	309	CLA	C2A-CAA-CBA-CGA
20	3	307	CLA	C2A-CAA-CBA-CGA
20	A	811	CLA	C2A-CAA-CBA-CGA
20	A	812	CLA	C2A-CAA-CBA-CGA
20	A	816	CLA	C2A-CAA-CBA-CGA
20	A	823	CLA	C2A-CAA-CBA-CGA
20	B	803	CLA	C2A-CAA-CBA-CGA
20	K	201	CLA	C2A-CAA-CBA-CGA
20	2	311	CLA	CBA-CGA-O2A-C1
20	A	840	CLA	CBA-CGA-O2A-C1
20	F	804	CLA	O1D-CGD-O2D-CED
19	2	307	CHL	C3A-C2A-CAA-CBA
20	A	813	CLA	C3A-C2A-CAA-CBA
20	B	811	CLA	C3A-C2A-CAA-CBA
20	B	823	CLA	C3A-C2A-CAA-CBA
20	B	825	CLA	C3A-C2A-CAA-CBA
20	3	301	CLA	C11-C12-C13-C14
20	A	831	CLA	CBD-CGD-O2D-CED
24	1	318	LHG	C27-C28-C29-C30
20	1	312	CLA	C11-C10-C8-C9
20	A	834	CLA	C6-C7-C8-C9
20	B	813	CLA	C11-C10-C8-C9
20	B	817	CLA	C11-C12-C13-C14
20	F	802	CLA	C11-C10-C8-C9
20	O	203	CLA	C6-C7-C8-C9
23	A	849	BCR	C11-C10-C9-C34
23	A	849	BCR	C16-C17-C18-C36
23	B	842	BCR	C11-C10-C9-C34
23	B	843	BCR	C11-C10-C9-C34
23	B	843	BCR	C20-C21-C22-C37
23	F	806	BCR	C35-C13-C14-C15
23	L	301	BCR	C11-C10-C9-C34
20	A	807	CLA	C3-C5-C6-C7
20	A	831	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
19	1	301	CHL	O1D-CGD-O2D-CED
20	A	817	CLA	C10-C11-C12-C13
20	O	202	CLA	CAA-CBA-CGA-O1A
20	A	833	CLA	C13-C15-C16-C17
20	O	203	CLA	C10-C11-C12-C13
20	2	309	CLA	C1A-C2A-CAA-CBA
20	A	831	CLA	C1A-C2A-CAA-CBA
20	B	801	CLA	C1A-C2A-CAA-CBA
20	B	811	CLA	C1A-C2A-CAA-CBA
20	B	813	CLA	C1A-C2A-CAA-CBA
20	B	825	CLA	C1A-C2A-CAA-CBA
20	B	826	CLA	C1A-C2A-CAA-CBA
20	L	303	CLA	C1A-C2A-CAA-CBA
20	N	203	CLA	C1A-C2A-CAA-CBA
20	A	809	CLA	C6-C7-C8-C10
20	A	812	CLA	C11-C10-C8-C7
20	A	824	CLA	C12-C13-C15-C16
20	A	826	CLA	C11-C12-C13-C15
20	A	827	CLA	C6-C7-C8-C10
20	A	827	CLA	C11-C12-C13-C15
20	A	840	CLA	C11-C10-C8-C7
20	A	841	CLA	C6-C7-C8-C10
20	F	802	CLA	C6-C7-C8-C10
20	A	840	CLA	O1A-CGA-O2A-C1
20	B	807	CLA	O1A-CGA-O2A-C1
26	A	852	HTG	S1-C1'-C2'-C3'
20	1	302	CLA	C2A-CAA-CBA-CGA
20	2	302	CLA	C2A-CAA-CBA-CGA
20	4	302	CLA	C2A-CAA-CBA-CGA
20	A	818	CLA	C2A-CAA-CBA-CGA
20	A	839	CLA	C2A-CAA-CBA-CGA
20	N	203	CLA	C2A-CAA-CBA-CGA
20	A	805	CLA	C15-C16-C17-C18
20	A	841	CLA	O1D-CGD-O2D-CED
20	A	801	CLA	C16-C17-C18-C20
20	A	831	CLA	O1D-CGD-O2D-CED
20	1	313	CLA	C4-C3-C5-C6
20	1	303	CLA	C10-C11-C12-C13
23	A	849	BCR	C11-C10-C9-C8
23	A	849	BCR	C16-C17-C18-C19
23	B	842	BCR	C11-C10-C9-C8
23	B	843	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
23	B	843	BCR	C20-C21-C22-C23
23	F	806	BCR	C12-C13-C14-C15
23	L	301	BCR	C11-C10-C9-C8
20	L	302	CLA	CAA-CBA-CGA-O2A
20	A	828	CLA	C16-C17-C18-C19
19	4	306	CHL	C2-C1-O2A-CGA
20	4	310	CLA	C2-C1-O2A-CGA
20	A	810	CLA	C2-C1-O2A-CGA
20	A	811	CLA	C2-C1-O2A-CGA
20	A	830	CLA	C2-C1-O2A-CGA
20	B	806	CLA	C2-C1-O2A-CGA
20	B	812	CLA	C2-C1-O2A-CGA
20	B	817	CLA	C2-C1-O2A-CGA
20	B	839	CLA	C2-C1-O2A-CGA
20	O	201	CLA	C2-C1-O2A-CGA
20	A	839	CLA	C2-C3-C5-C6
20	B	804	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	C11-C10-C8-C9
20	B	814	CLA	C6-C7-C8-C9
20	L	302	CLA	O1D-CGD-O2D-CED
25	1	323	LMG	C22-C23-C24-C25
20	B	809	CLA	C3-C5-C6-C7
21	2	315	LUT	C5-C6-C7-C8
21	O	204	LUT	C1-C6-C7-C8
23	2	317	BCR	C23-C24-C25-C30
23	K	204	BCR	C1-C6-C7-C8
20	B	805	CLA	CAA-CBA-CGA-O2A
24	1	318	LHG	C4-C5-C6-O8
20	A	802	CLA	C8-C10-C11-C12
26	B	850	HTG	C1'-C2'-C3'-C4'
22	1	316	XAT	C33-C34-C35-C15
23	B	841	BCR	C7-C8-C9-C10
23	F	801	BCR	C11-C12-C13-C14
23	J	102	BCR	C17-C18-C19-C20
20	A	817	CLA	C16-C17-C18-C19
20	1	307	CLA	C8-C10-C11-C12
20	B	824	CLA	C15-C16-C17-C18
20	1	302	CLA	C16-C17-C18-C19
20	B	824	CLA	C16-C17-C18-C19
20	A	838	CLA	C15-C16-C17-C18
20	3	314	CLA	O1A-CGA-O2A-C1
20	2	303	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
20	A	836	CLA	C2A-CAA-CBA-CGA
29	B	847	LMT	C5-C6-C7-C8
20	B	804	CLA	CAA-CBA-CGA-O1A
20	O	202	CLA	CAA-CBA-CGA-O2A
20	A	816	CLA	C4-C3-C5-C6
20	B	816	CLA	C4-C3-C5-C6
20	A	805	CLA	C11-C10-C8-C7
20	B	813	CLA	C11-C10-C8-C7
20	B	814	CLA	C6-C7-C8-C10
25	4	319	LMG	C30-C31-C32-C33
20	3	301	CLA	C8-C10-C11-C12
20	1	311	CLA	CAA-CBA-CGA-O2A
20	J	101	CLA	C10-C11-C12-C13
20	B	825	CLA	C13-C15-C16-C17
20	3	307	CLA	CAA-CBA-CGA-O2A
20	B	814	CLA	C8-C10-C11-C12
20	J	101	CLA	C16-C17-C18-C20
26	4	320	HTG	C2'-C1'-S1-C1
26	J	105	HTG	C2'-C1'-S1-C1
20	F	802	CLA	C3-C5-C6-C7
20	B	813	CLA	C4-C3-C5-C6
20	1	313	CLA	C2-C3-C5-C6
20	B	818	CLA	C2-C3-C5-C6
24	A	844	LHG	O7-C7-C8-C9
20	1	307	CLA	C12-C13-C15-C16
20	1	308	CLA	C11-C10-C8-C9
20	A	812	CLA	C11-C10-C8-C9
20	A	853	CLA	C11-C10-C8-C9
20	B	815	CLA	C6-C7-C8-C9
20	F	802	CLA	C6-C7-C8-C9
20	L	303	CLA	C11-C12-C13-C14
20	3	303	CLA	C3A-C2A-CAA-CBA
20	A	835	CLA	C3A-C2A-CAA-CBA
20	B	813	CLA	C3A-C2A-CAA-CBA
20	B	814	CLA	C3A-C2A-CAA-CBA
20	B	817	CLA	C3A-C2A-CAA-CBA
20	B	806	CLA	CAA-CBA-CGA-O2A
20	L	302	CLA	CBD-CGD-O2D-CED
19	1	306	CHL	CAD-CBD-CGD-O2D
20	3	307	CLA	CAD-CBD-CGD-O2D
20	4	301	CLA	CAD-CBD-CGD-O2D
20	4	303	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
20	A	804	CLA	CAD-CBD-CGD-O2D
20	A	814	CLA	CAD-CBD-CGD-O2D
20	A	816	CLA	CAD-CBD-CGD-O2D
20	A	832	CLA	CAD-CBD-CGD-O2D
20	A	836	CLA	CAD-CBD-CGD-O2D
20	A	840	CLA	CAD-CBD-CGD-O2D
20	B	814	CLA	CAD-CBD-CGD-O2D
20	B	818	CLA	CAD-CBD-CGD-O2D
20	B	834	CLA	CAD-CBD-CGD-O2D
20	B	835	CLA	CAD-CBD-CGD-O2D
20	F	804	CLA	CAD-CBD-CGD-O2D
20	G	604	CLA	CAD-CBD-CGD-O2D
20	A	829	CLA	C15-C16-C17-C18
20	A	808	CLA	C2-C1-O2A-CGA
20	A	819	CLA	CAA-CBA-CGA-O2A
20	A	835	CLA	CAA-CBA-CGA-O2A
24	1	318	LHG	C29-C30-C31-C32
25	1	320	LMG	C36-C37-C38-C39
20	1	308	CLA	CAA-CBA-CGA-O2A
23	B	841	BCR	C17-C18-C19-C20
20	1	309	CLA	O1A-CGA-O2A-C1
20	A	805	CLA	CAA-CBA-CGA-O2A
20	A	827	CLA	O2A-C1-C2-C3
20	A	851	CLA	O2A-C1-C2-C3
20	B	831	CLA	O2A-C1-C2-C3
20	B	817	CLA	C10-C11-C12-C13
20	A	819	CLA	CAA-CBA-CGA-O1A
20	A	835	CLA	CAA-CBA-CGA-O1A
20	3	301	CLA	C11-C12-C13-C15
20	1	302	CLA	CHA-CBD-CGD-O1D
20	1	302	CLA	CHA-CBD-CGD-O2D
20	1	311	CLA	CHA-CBD-CGD-O1D
20	1	311	CLA	CHA-CBD-CGD-O2D
20	1	312	CLA	CHA-CBD-CGD-O1D
20	1	312	CLA	CHA-CBD-CGD-O2D
20	1	321	CLA	CHA-CBD-CGD-O2D
20	2	302	CLA	CHA-CBD-CGD-O1D
20	2	310	CLA	CHA-CBD-CGD-O1D
20	2	310	CLA	CHA-CBD-CGD-O2D
20	2	311	CLA	CHA-CBD-CGD-O1D
20	2	311	CLA	CHA-CBD-CGD-O2D
20	4	302	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
20	A	802	CLA	CHA-CBD-CGD-O1D
20	A	802	CLA	CHA-CBD-CGD-O2D
20	A	803	CLA	CHA-CBD-CGD-O2D
20	A	805	CLA	CHA-CBD-CGD-O2D
20	A	812	CLA	CHA-CBD-CGD-O2D
20	A	818	CLA	CHA-CBD-CGD-O2D
20	A	821	CLA	CHA-CBD-CGD-O1D
20	A	821	CLA	CHA-CBD-CGD-O2D
20	A	827	CLA	CHA-CBD-CGD-O1D
20	A	827	CLA	CHA-CBD-CGD-O2D
20	A	828	CLA	CHA-CBD-CGD-O1D
20	A	828	CLA	CHA-CBD-CGD-O2D
20	A	830	CLA	CHA-CBD-CGD-O1D
20	A	830	CLA	CHA-CBD-CGD-O2D
20	A	833	CLA	CHA-CBD-CGD-O1D
20	A	833	CLA	CHA-CBD-CGD-O2D
20	A	851	CLA	CHA-CBD-CGD-O1D
20	A	851	CLA	CHA-CBD-CGD-O2D
20	B	805	CLA	CHA-CBD-CGD-O2D
20	B	810	CLA	CHA-CBD-CGD-O1D
20	B	810	CLA	CHA-CBD-CGD-O2D
20	B	823	CLA	CHA-CBD-CGD-O2D
20	B	827	CLA	CHA-CBD-CGD-O1D
20	B	827	CLA	CHA-CBD-CGD-O2D
20	B	829	CLA	CHA-CBD-CGD-O1D
20	B	832	CLA	CHA-CBD-CGD-O2D
20	G	605	CLA	CHA-CBD-CGD-O1D
20	K	203	CLA	CHA-CBD-CGD-O1D
20	K	203	CLA	CHA-CBD-CGD-O2D
20	L	303	CLA	CHA-CBD-CGD-O1D
20	L	303	CLA	CHA-CBD-CGD-O2D
20	N	203	CLA	CHA-CBD-CGD-O2D
20	O	202	CLA	CHA-CBD-CGD-O2D
20	2	303	CLA	CAA-CBA-CGA-O2A
20	A	834	CLA	CAA-CBA-CGA-O2A
20	3	302	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	CAA-CBA-CGA-O2A
20	A	841	CLA	CAA-CBA-CGA-O2A
24	A	843	LHG	C10-C11-C12-C13
19	1	301	CHL	CBD-CGD-O2D-CED
20	B	822	CLA	C3-C5-C6-C7
20	A	824	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	B	821	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	CAA-CBA-CGA-O2A
20	A	833	CLA	C11-C12-C13-C15
20	A	839	CLA	C6-C7-C8-C10
20	B	825	CLA	C11-C10-C8-C7
20	A	802	CLA	C14-C13-C15-C16
20	A	826	CLA	C11-C12-C13-C14
20	A	840	CLA	C11-C10-C8-C9
20	B	827	CLA	C11-C12-C13-C14
20	4	311	CLA	CAA-CBA-CGA-O2A
20	B	827	CLA	CAA-CBA-CGA-O2A
20	N	202	CLA	CAA-CBA-CGA-O2A
20	A	821	CLA	O1A-CGA-O2A-C1
20	1	309	CLA	CBA-CGA-O2A-C1
24	1	318	LHG	C24-C25-C26-C27
23	F	801	BCR	C11-C12-C13-C35
20	B	806	CLA	CAA-CBA-CGA-O1A
23	K	204	BCR	C7-C8-C9-C10
20	G	604	CLA	CBA-CGA-O2A-C1
20	A	816	CLA	C5-C6-C7-C8
19	4	305	CHL	C4C-C3C-CAC-CBC
20	1	307	CLA	C1A-C2A-CAA-CBA
20	3	303	CLA	C1A-C2A-CAA-CBA
20	4	309	CLA	C1A-C2A-CAA-CBA
20	4	314	CLA	C1A-C2A-CAA-CBA
20	A	808	CLA	C1A-C2A-CAA-CBA
20	A	835	CLA	C1A-C2A-CAA-CBA
20	A	851	CLA	C1A-C2A-CAA-CBA
20	B	802	CLA	C1A-C2A-CAA-CBA
20	B	814	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C1A-C2A-CAA-CBA
20	B	817	CLA	C13-C15-C16-C17
20	A	821	CLA	CBA-CGA-O2A-C1
20	A	805	CLA	CAA-CBA-CGA-O1A
20	B	803	CLA	C15-C16-C17-C18
20	O	203	CLA	C2A-CAA-CBA-CGA
20	B	833	CLA	C16-C17-C18-C20
20	B	802	CLA	C5-C6-C7-C8
20	B	821	CLA	CBD-CGD-O2D-CED
20	3	305	CLA	CAA-CBA-CGA-O2A
20	A	808	CLA	CAA-CBA-CGA-O1A
24	A	844	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	1	320	LMG	C34-C35-C36-C37
20	B	823	CLA	C5-C6-C7-C8
24	2	318	LHG	C3-O3-P-O5
20	A	820	CLA	C16-C17-C18-C20
20	1	308	CLA	CAA-CBA-CGA-O1A
20	B	821	CLA	CAA-CBA-CGA-O1A
23	2	317	BCR	C23-C24-C25-C26
20	1	308	CLA	C8-C10-C11-C12
20	1	311	CLA	CAA-CBA-CGA-O1A
20	4	311	CLA	CAA-CBA-CGA-O1A
20	B	831	CLA	CAA-CBA-CGA-O2A
20	3	308	CLA	C2A-CAA-CBA-CGA
20	4	309	CLA	C2A-CAA-CBA-CGA
20	A	802	CLA	C2A-CAA-CBA-CGA
20	A	834	CLA	CAA-CBA-CGA-O1A
19	2	306	CHL	C4C-C3C-CAC-CBC
20	2	303	CLA	CAA-CBA-CGA-O1A
20	A	827	CLA	C4-C3-C5-C6
20	A	833	CLA	CBA-CGA-O2A-C1
20	H	201	CLA	C2-C3-C5-C6
20	B	806	CLA	C16-C17-C18-C20
19	2	306	CHL	CAD-CBD-CGD-O1D
19	4	306	CHL	CAD-CBD-CGD-O1D
20	1	321	CLA	CAD-CBD-CGD-O1D
20	A	801	CLA	CAD-CBD-CGD-O1D
20	A	812	CLA	CAD-CBD-CGD-O1D
20	A	822	CLA	C2-C3-C5-C6
20	A	841	CLA	CAD-CBD-CGD-O1D
20	B	807	CLA	CAD-CBD-CGD-O1D
20	B	829	CLA	CAD-CBD-CGD-O1D
20	G	605	CLA	CAD-CBD-CGD-O1D
20	G	604	CLA	O1A-CGA-O2A-C1
20	A	824	CLA	CAA-CBA-CGA-O1A
20	A	829	CLA	C5-C6-C7-C8
20	A	824	CLA	C14-C13-C15-C16
20	A	827	CLA	C11-C12-C13-C14
20	A	832	CLA	C11-C10-C8-C9
20	B	802	CLA	C14-C13-C15-C16
20	A	833	CLA	O1A-CGA-O2A-C1
26	4	320	HTG	C2'-C3'-C4'-C5'
19	4	306	CHL	CAA-CBA-CGA-O2A
20	1	302	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
20	1	312	CLA	CAA-CBA-CGA-O2A
20	2	311	CLA	CAA-CBA-CGA-O2A
20	3	314	CLA	CAA-CBA-CGA-O2A
20	B	828	CLA	CAA-CBA-CGA-O1A
20	1	307	CLA	CAA-CBA-CGA-O2A
20	B	810	CLA	CAA-CBA-CGA-O2A
20	K	202	CLA	CAA-CBA-CGA-O2A
27	B	840	PQN	C13-C15-C16-C17
20	A	841	CLA	CAA-CBA-CGA-O1A
20	1	303	CLA	C6-C7-C8-C10
20	4	303	CLA	C11-C10-C8-C7
20	4	314	CLA	C3A-C2A-CAA-CBA
20	A	810	CLA	C3A-C2A-CAA-CBA
20	A	810	CLA	C12-C13-C15-C16
20	A	812	CLA	C12-C13-C15-C16
20	A	837	CLA	C11-C10-C8-C7
20	B	801	CLA	C3A-C2A-CAA-CBA
20	B	822	CLA	C3A-C2A-CAA-CBA
20	B	826	CLA	C3A-C2A-CAA-CBA
20	B	836	CLA	C11-C12-C13-C15
20	B	836	CLA	C12-C13-C15-C16
20	N	202	CLA	CHA-CBD-CGD-O1D
24	A	844	LHG	O6-C4-C5-O7
20	3	302	CLA	CAA-CBA-CGA-O1A
20	K	202	CLA	CAA-CBA-CGA-O1A
30	B	848	DGD	CAA-CBA-CCA-CDA
19	1	306	CHL	CAA-CBA-CGA-O2A
20	2	308	CLA	CAA-CBA-CGA-O2A
20	A	833	CLA	CAA-CBA-CGA-O2A
29	G	601	LMT	C7-C8-C9-C10
20	N	202	CLA	CAA-CBA-CGA-O1A
20	A	814	CLA	CAA-CBA-CGA-O2A
20	2	302	CLA	C10-C11-C12-C13
26	N	201	HTG	C1'-C2'-C3'-C4'
20	1	302	CLA	CAA-CBA-CGA-O1A
20	2	308	CLA	CAA-CBA-CGA-O1A
20	2	311	CLA	CAA-CBA-CGA-O1A
20	L	307	CLA	CAA-CBA-CGA-O2A
20	A	816	CLA	C13-C15-C16-C17
20	B	815	CLA	C8-C10-C11-C12
20	G	605	CLA	CAA-CBA-CGA-O2A
19	4	306	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
20	3	305	CLA	CAA-CBA-CGA-O1A
20	B	831	CLA	CAA-CBA-CGA-O1A
20	A	822	CLA	C2A-CAA-CBA-CGA
20	B	833	CLA	C2A-CAA-CBA-CGA
20	1	312	CLA	CAA-CBA-CGA-O1A

There are no ring outliers.

193 monomers are involved in 527 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	A	826	CLA	5	0
23	2	317	BCR	6	0
20	3	301	CLA	1	0
20	A	814	CLA	1	0
20	1	321	CLA	5	0
20	A	807	CLA	4	0
20	B	813	CLA	7	0
23	A	848	BCR	4	0
20	B	817	CLA	5	0
20	K	203	CLA	1	0
20	A	810	CLA	7	0
20	B	812	CLA	3	0
20	B	822	CLA	2	0
20	B	823	CLA	4	0
20	3	309	CLA	7	0
26	F	807	HTG	1	0
20	B	808	CLA	4	0
20	B	827	CLA	4	0
23	A	847	BCR	2	0
23	G	606	BCR	3	0
23	F	801	BCR	4	0
21	2	315	LUT	2	0
26	B	850	HTG	1	0
20	1	311	CLA	2	0
23	A	845	BCR	2	0
20	B	837	CLA	2	0
24	B	849	LHG	2	0
20	4	313	CLA	2	0
20	A	828	CLA	2	0
25	1	323	LMG	3	0
20	3	313	CLA	1	0
20	A	812	CLA	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	4	311	CLA	2	0
20	B	829	CLA	3	0
20	1	310	CLA	1	0
20	A	802	CLA	3	0
23	K	204	BCR	4	0
20	A	801	CLA	7	0
23	L	305	BCR	4	0
23	A	846	BCR	1	0
20	A	829	CLA	1	0
20	2	304	CLA	2	0
20	A	804	CLA	6	0
23	A	854	BCR	6	0
20	2	309	CLA	2	0
20	1	313	CLA	3	0
20	3	308	CLA	2	0
20	K	202	CLA	2	0
20	A	818	CLA	4	0
23	L	301	BCR	2	0
24	1	318	LHG	7	0
19	2	306	CHL	8	0
20	1	304	CLA	2	0
20	A	809	CLA	3	0
20	1	309	CLA	2	0
20	2	310	CLA	4	0
19	2	307	CHL	3	0
20	A	841	CLA	3	0
24	2	318	LHG	1	0
30	B	848	DGD	2	0
23	3	317	BCR	4	0
21	O	205	LUT	5	0
20	B	804	CLA	1	0
20	1	302	CLA	3	0
20	O	201	CLA	4	0
19	2	305	CHL	5	0
27	A	842	PQN	3	0
20	B	821	CLA	1	0
20	J	103	CLA	1	0
20	A	827	CLA	6	0
20	4	302	CLA	5	0
21	1	319	LUT	4	0
20	B	835	CLA	3	0
20	B	803	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	L	303	CLA	5	0
20	O	202	CLA	6	0
23	B	845	BCR	5	0
23	J	104	BCR	2	0
20	B	838	CLA	3	0
22	3	316	XAT	6	0
20	1	307	CLA	3	0
19	4	305	CHL	4	0
20	A	839	CLA	1	0
20	B	805	CLA	6	0
20	B	815	CLA	1	0
20	B	828	CLA	5	0
20	N	203	CLA	2	0
21	O	204	LUT	3	0
23	I	101	BCR	6	0
26	1	322	HTG	2	0
20	B	807	CLA	2	0
20	3	314	CLA	2	0
22	4	317	XAT	8	0
20	B	831	CLA	5	0
20	1	312	CLA	4	0
22	2	316	XAT	2	0
20	A	833	CLA	4	0
21	4	316	LUT	5	0
20	A	823	CLA	7	0
20	B	818	CLA	3	0
27	B	840	PQN	1	0
20	1	303	CLA	6	0
20	A	824	CLA	4	0
20	A	817	CLA	5	0
20	A	835	CLA	1	0
24	A	844	LHG	1	0
20	2	313	CLA	1	0
20	A	822	CLA	3	0
21	3	315	LUT	4	0
20	1	308	CLA	5	0
20	A	825	CLA	6	0
20	2	311	CLA	3	0
20	A	808	CLA	5	0
20	4	303	CLA	8	0
20	B	832	CLA	4	0
23	F	806	BCR	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
20	F	802	CLA	4	0
20	A	820	CLA	4	0
20	B	816	CLA	2	0
21	1	315	LUT	4	0
20	A	811	CLA	5	0
20	A	806	CLA	4	0
20	B	810	CLA	3	0
20	L	302	CLA	3	0
19	4	307	CHL	1	0
20	A	821	CLA	3	0
20	B	824	CLA	9	0
20	O	203	CLA	6	0
23	1	317	BCR	4	0
20	H	201	CLA	3	0
20	A	831	CLA	5	0
20	B	834	CLA	3	0
20	3	310	CLA	1	0
23	A	849	BCR	4	0
20	2	302	CLA	2	0
20	A	816	CLA	2	0
20	3	311	CLA	4	0
20	B	836	CLA	2	0
20	K	205	CLA	3	0
20	B	806	CLA	2	0
20	A	834	CLA	3	0
19	4	315	CHL	5	0
19	3	306	CHL	3	0
20	A	836	CLA	3	0
20	3	304	CLA	1	0
20	A	851	CLA	5	0
20	F	805	CLA	3	0
20	A	803	CLA	3	0
20	4	308	CLA	7	0
19	1	301	CHL	3	0
20	B	809	CLA	4	0
19	2	301	CHL	10	0
23	B	842	BCR	1	0
19	1	306	CHL	3	0
20	3	307	CLA	7	0
20	B	819	CLA	2	0
20	4	301	CLA	6	0
24	A	843	LHG	2	0

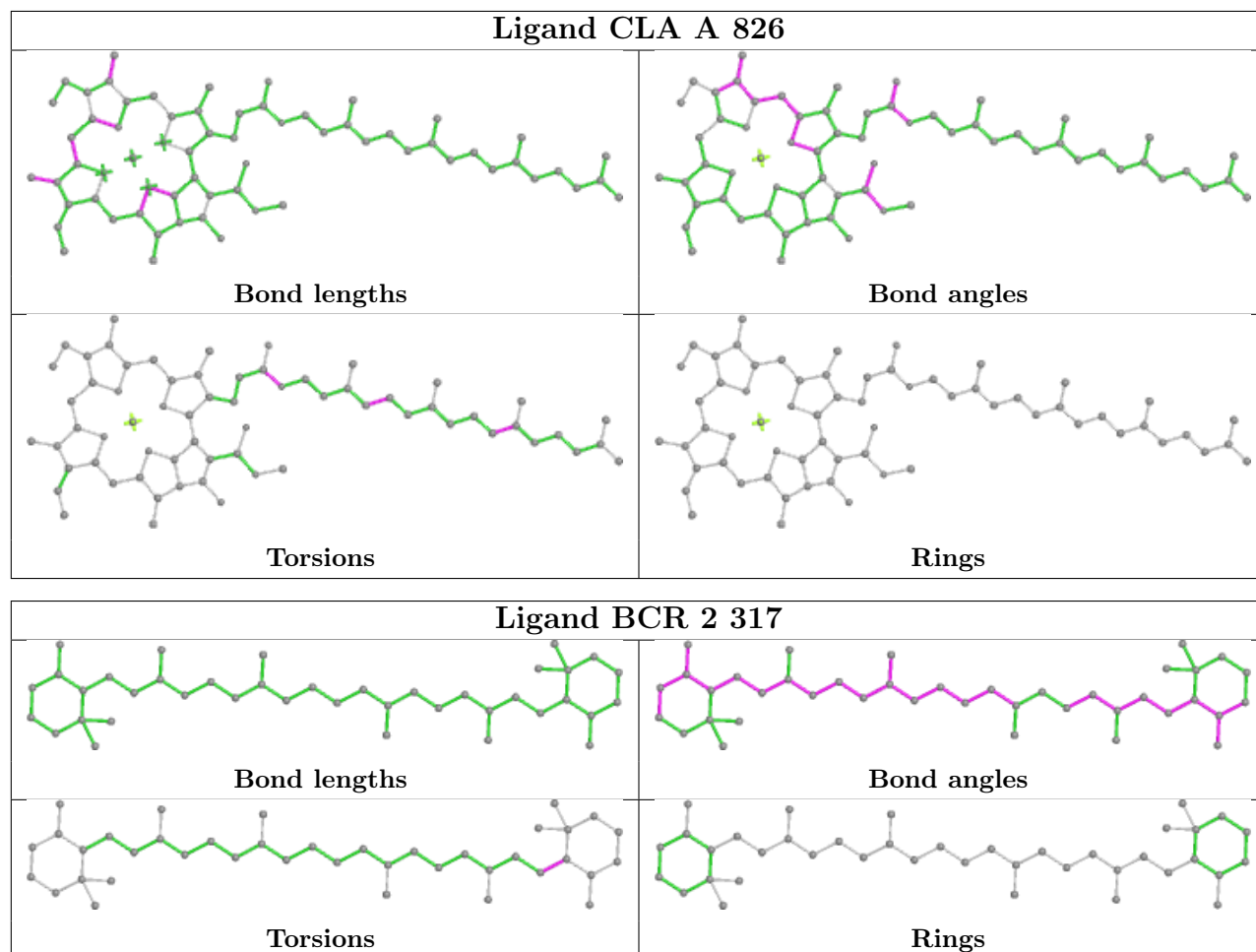
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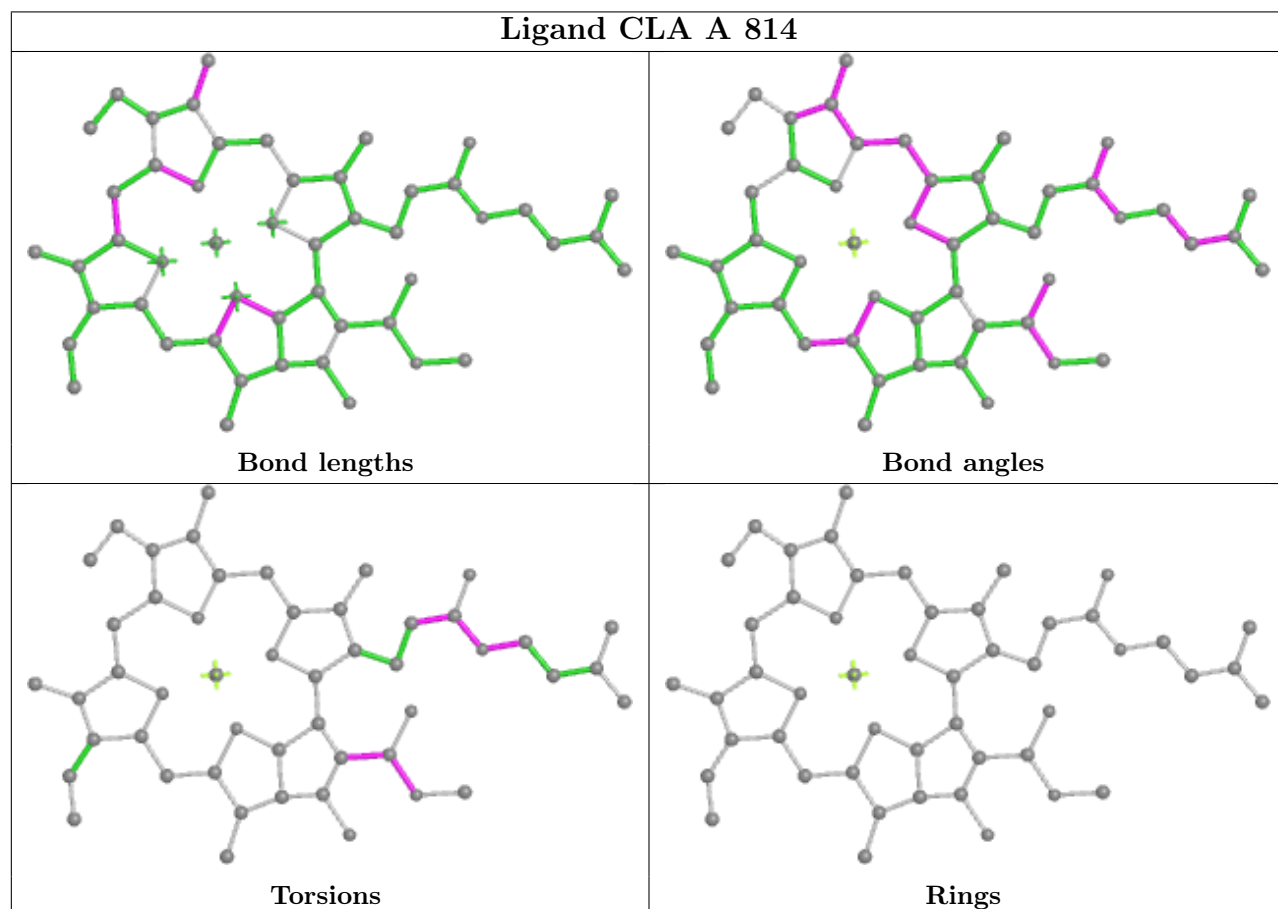
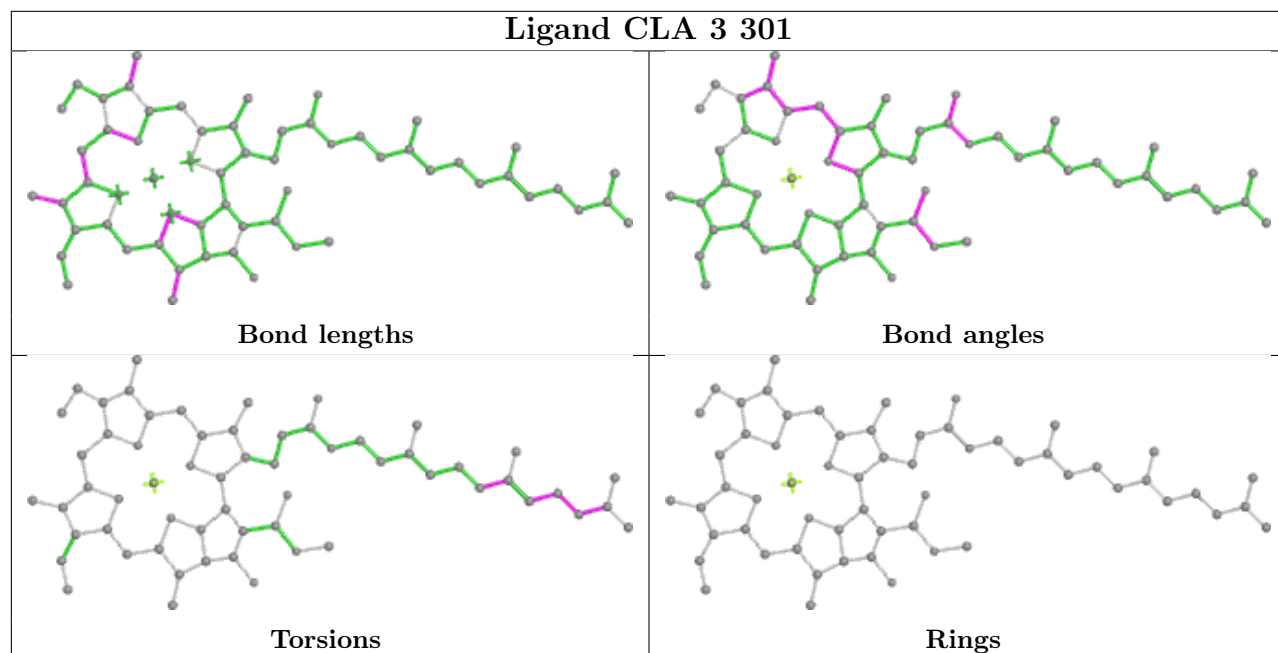
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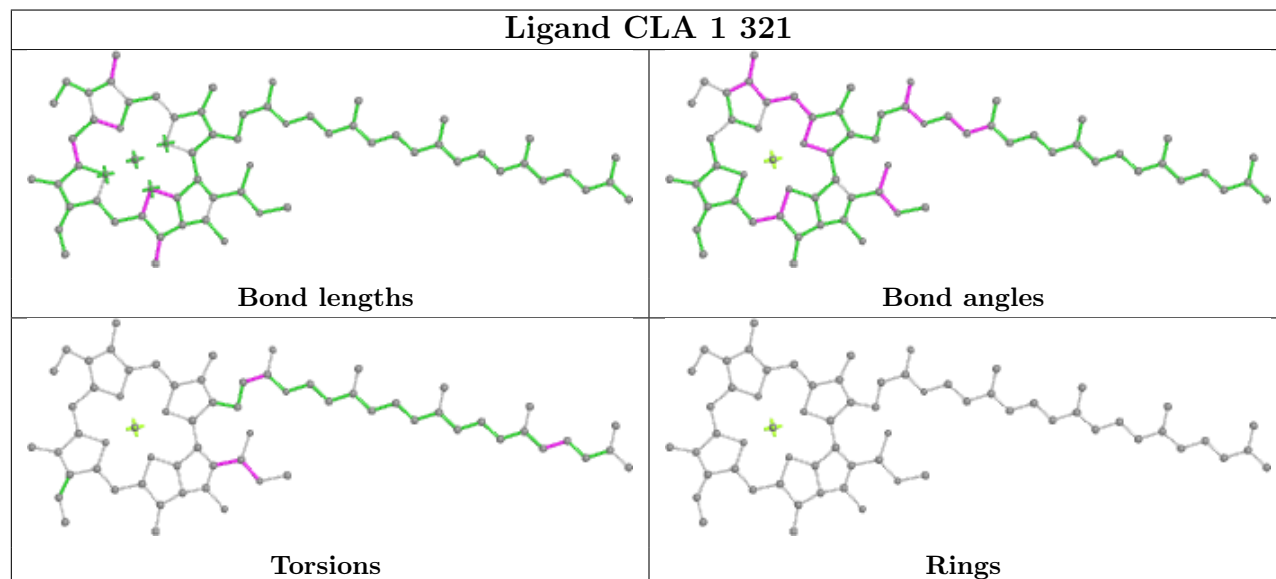
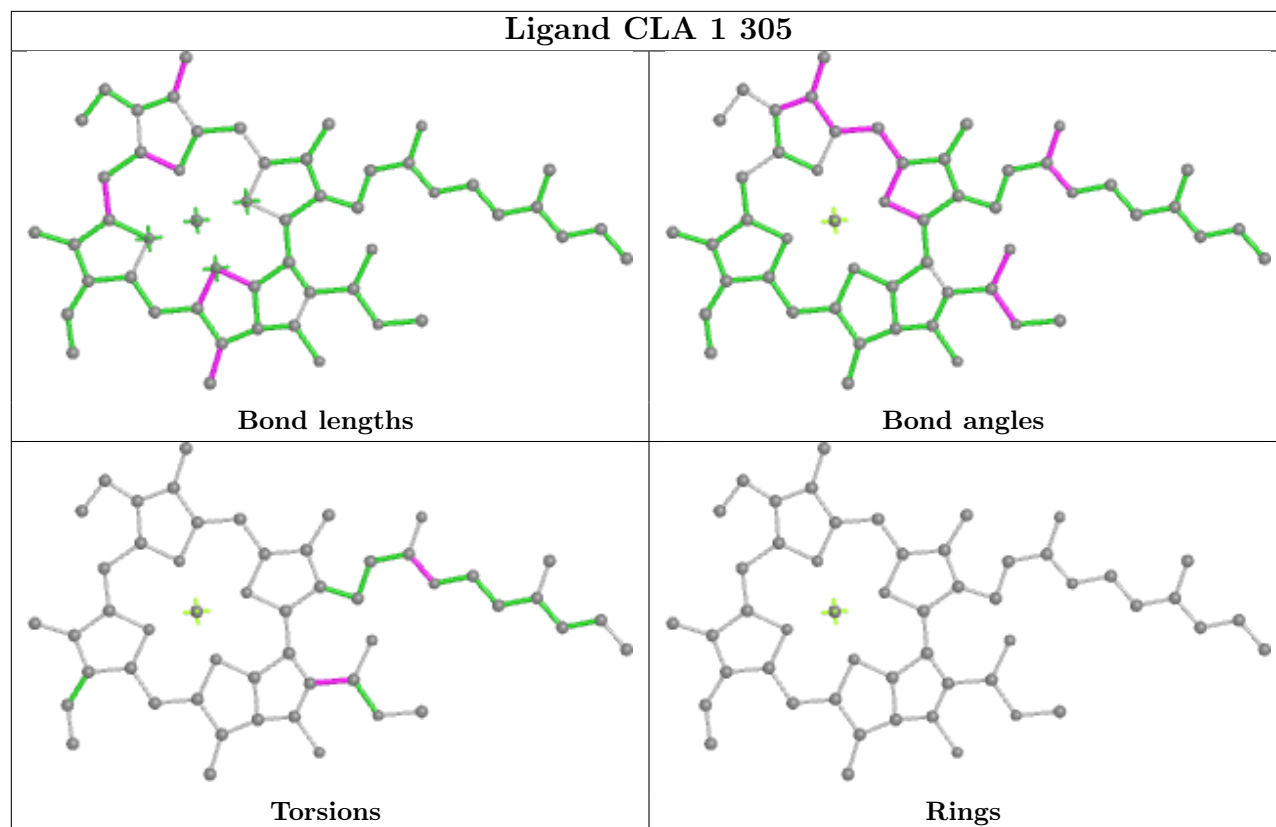
Mol	Chain	Res	Type	Clashes	Symm-Clashes
23	B	843	BCR	2	0
20	A	853	CLA	5	0
20	J	101	CLA	1	0
20	B	802	CLA	5	0
25	1	320	LMG	3	0
20	B	839	CLA	3	0
20	B	825	CLA	4	0
23	4	318	BCR	5	0
19	4	306	CHL	3	0
20	B	830	CLA	2	0
20	K	201	CLA	2	0
22	1	316	XAT	2	0
20	B	833	CLA	2	0
20	A	840	CLA	1	0
23	B	841	BCR	8	0
20	A	838	CLA	4	0
20	A	832	CLA	1	0
23	J	102	BCR	8	0
20	4	314	CLA	2	0
20	A	805	CLA	5	0
26	N	201	HTG	1	0
25	4	319	LMG	4	0
20	2	308	CLA	6	0
23	B	844	BCR	3	0
20	A	837	CLA	3	0
20	4	312	CLA	5	0
23	L	306	BCR	3	0
19	2	314	CHL	1	0
20	2	312	CLA	4	0
20	B	801	CLA	4	0
20	4	304	CLA	3	0
23	B	846	BCR	3	0
20	4	309	CLA	3	0
20	B	826	CLA	1	0
20	2	303	CLA	1	0

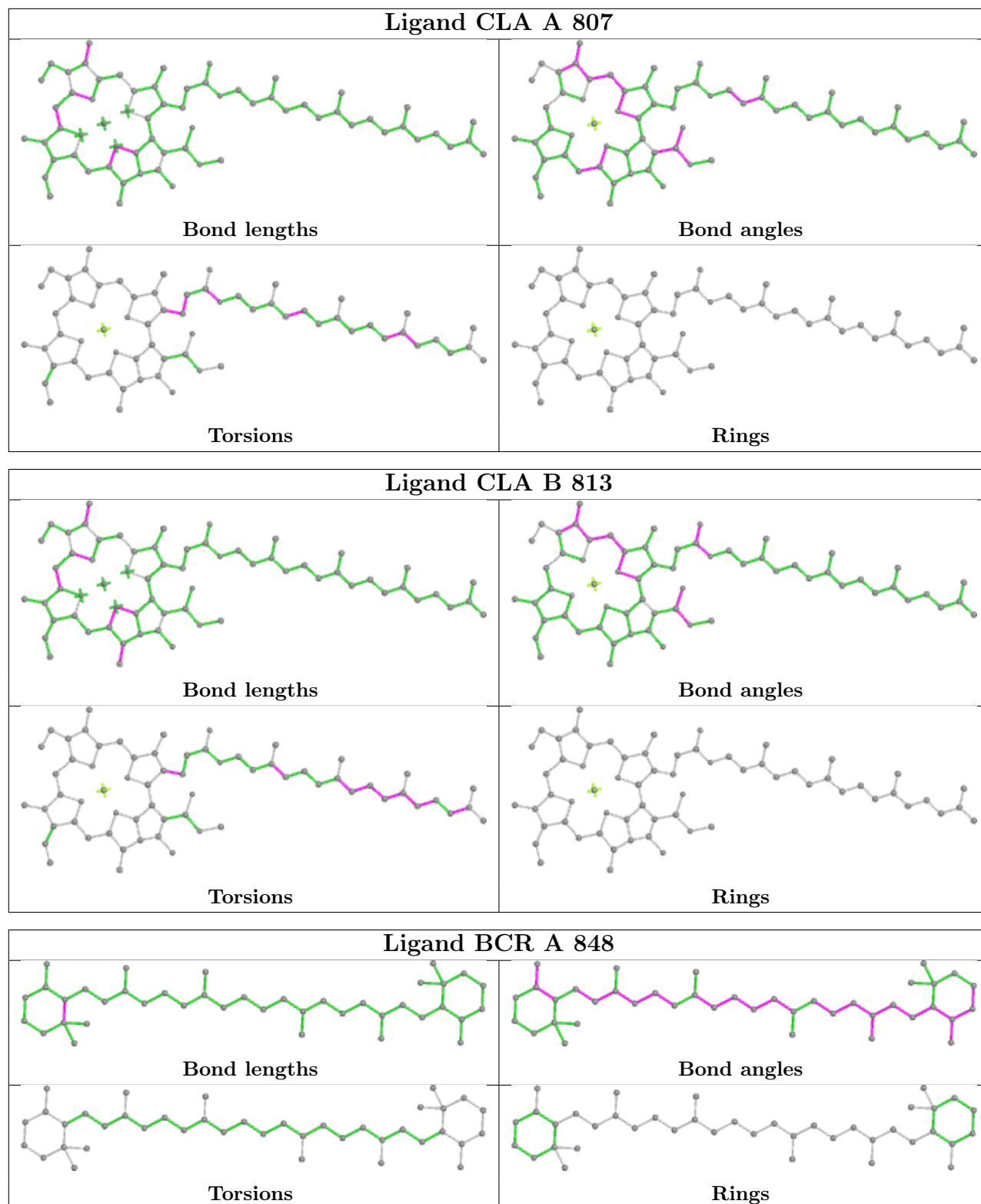
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

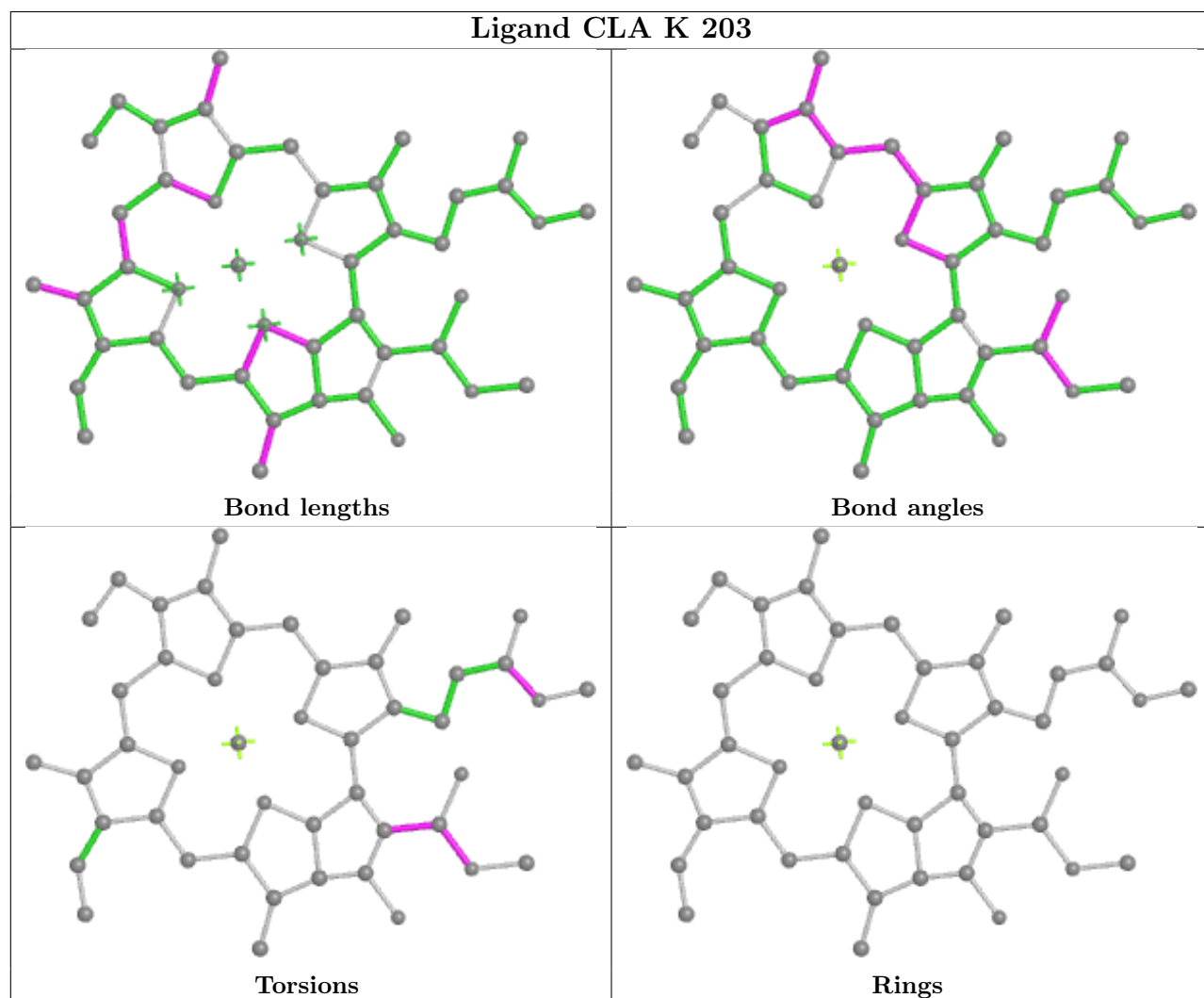
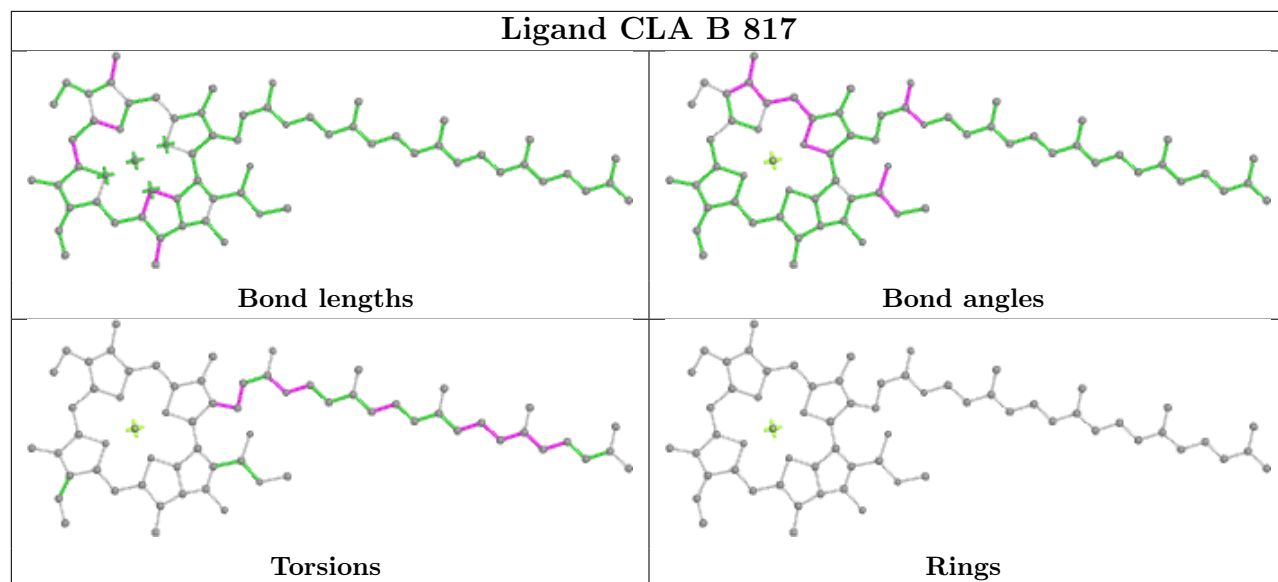
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

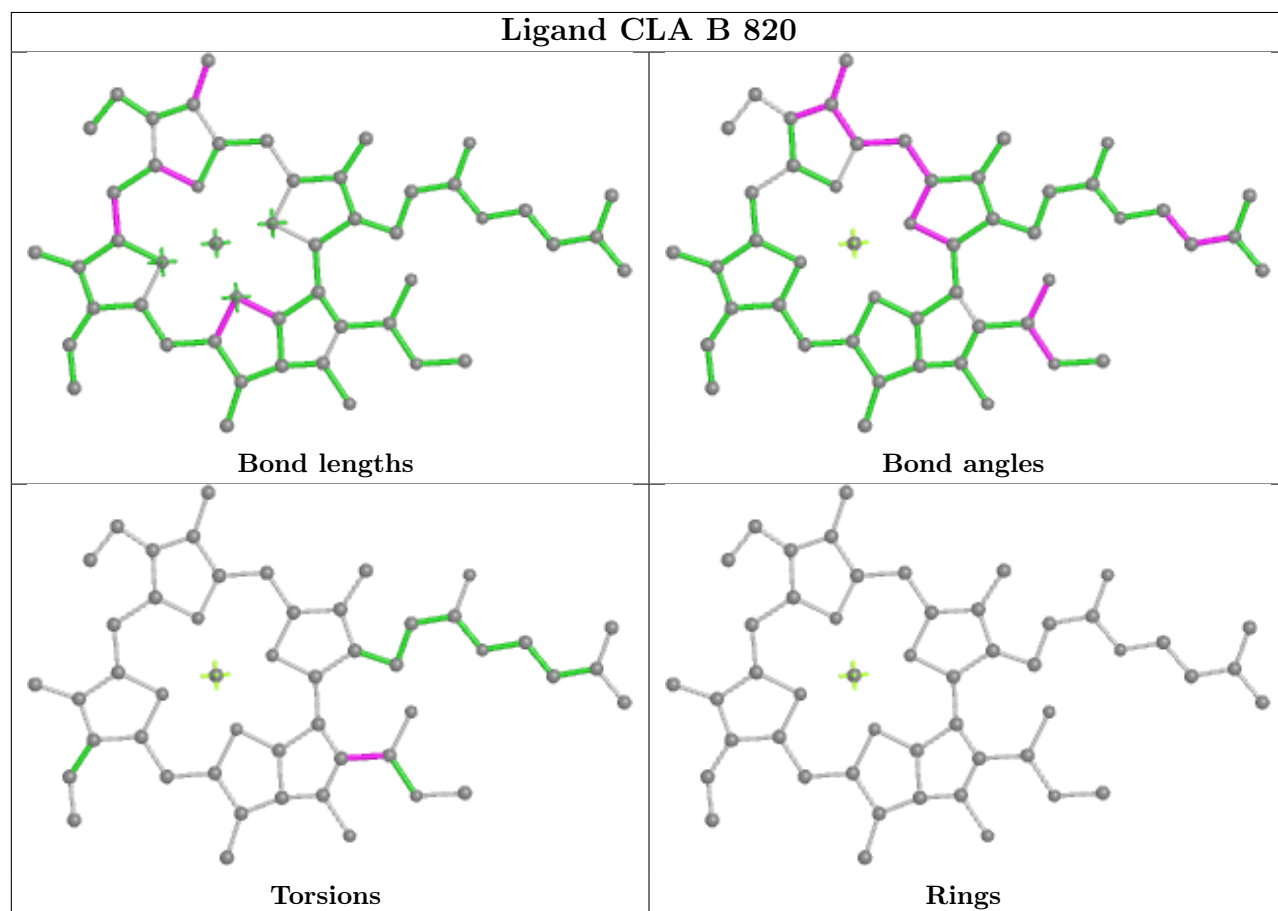
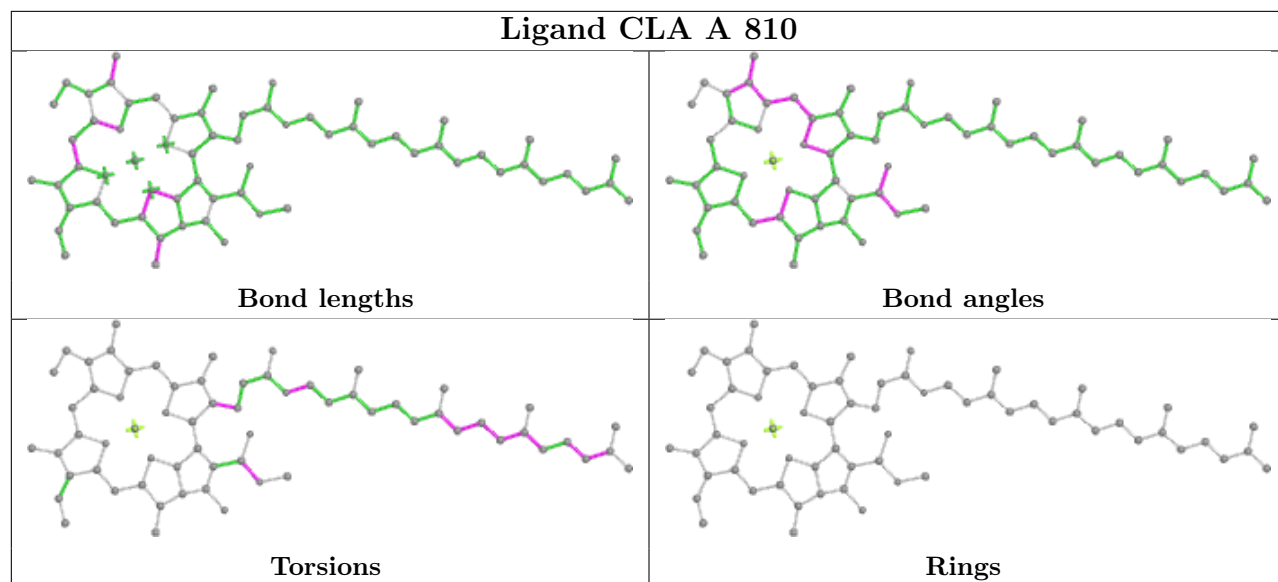


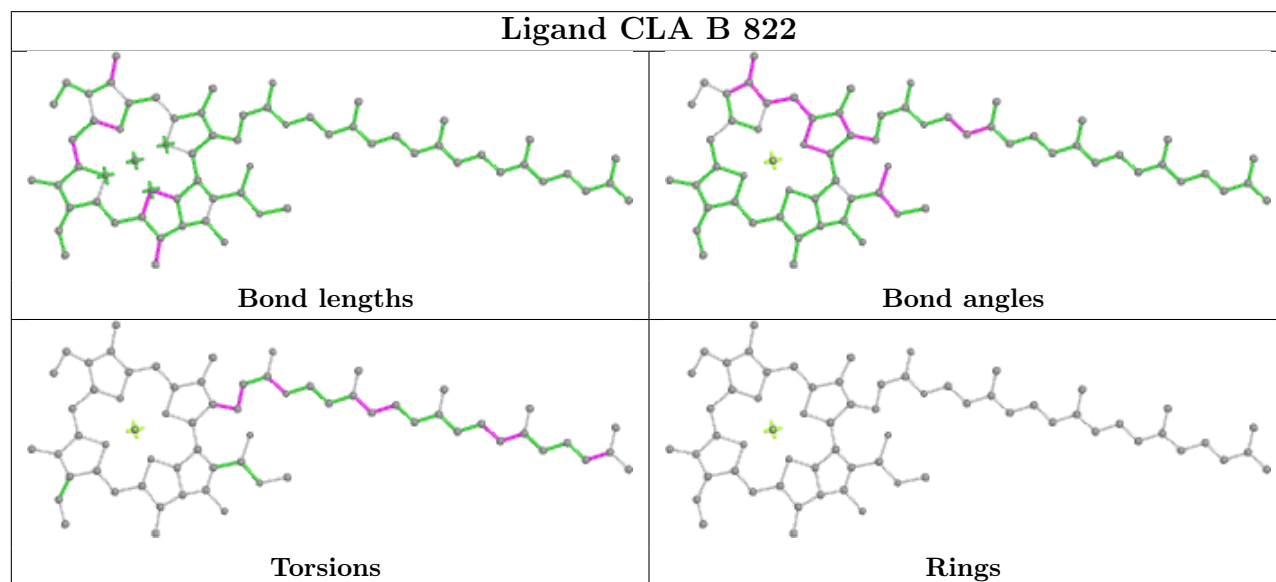
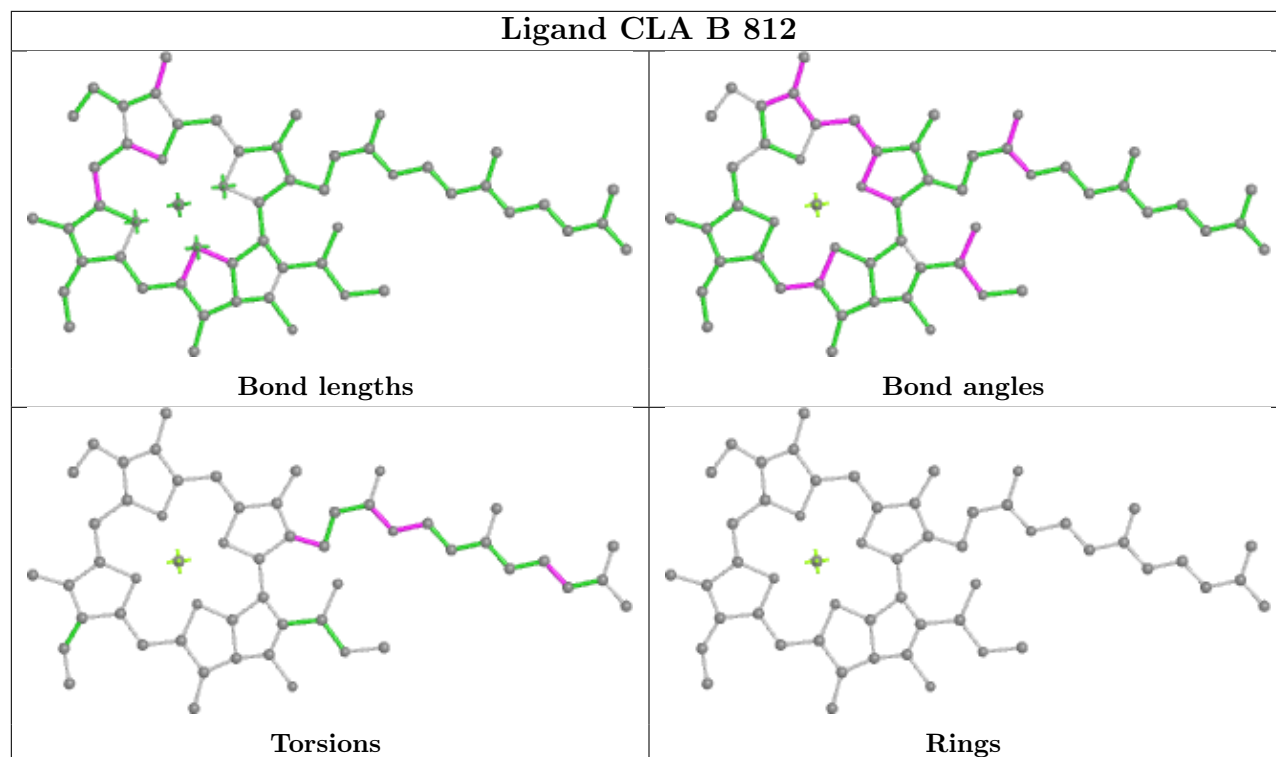


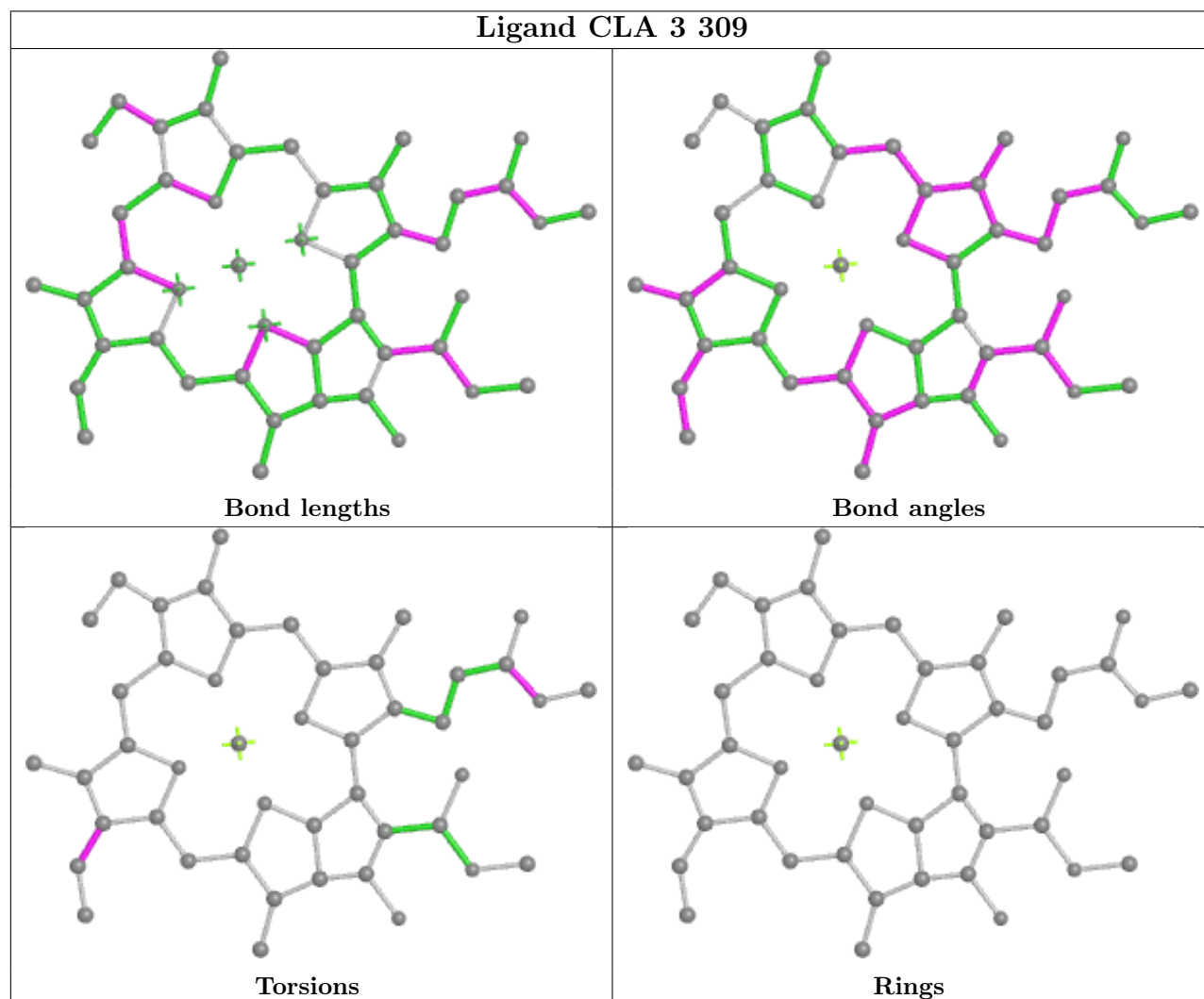
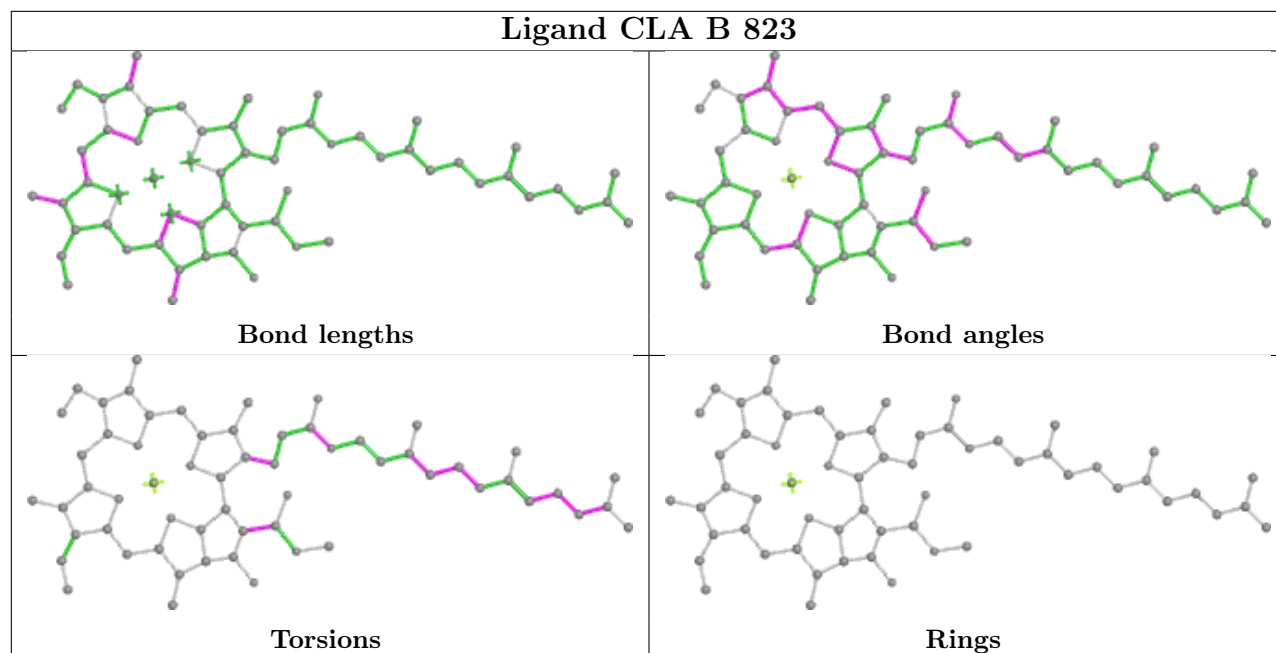


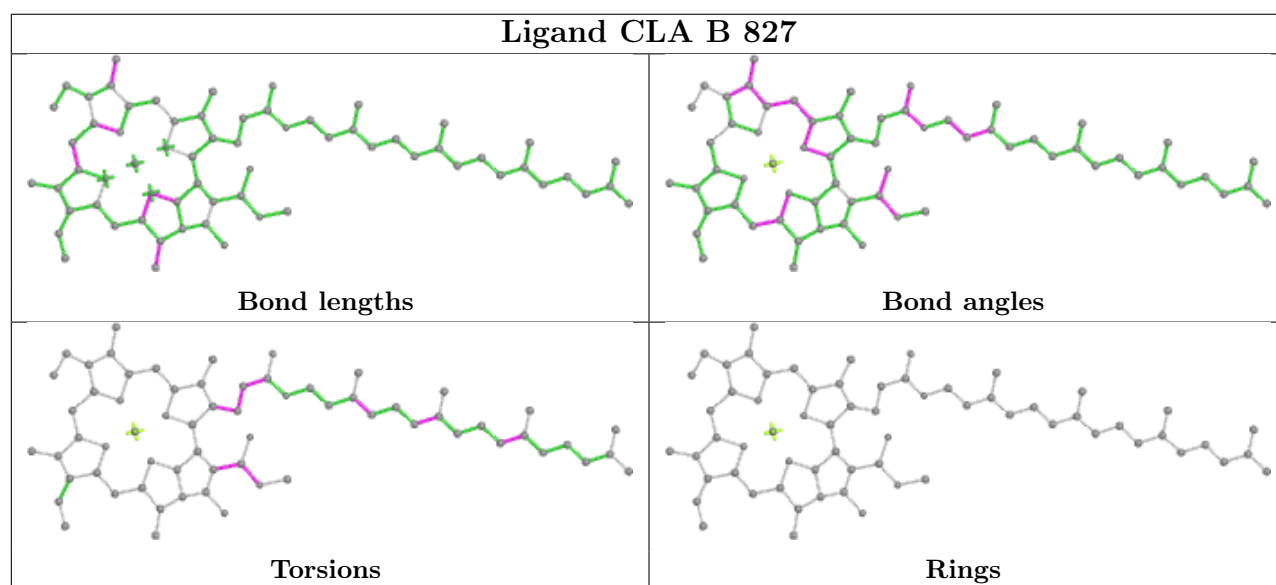
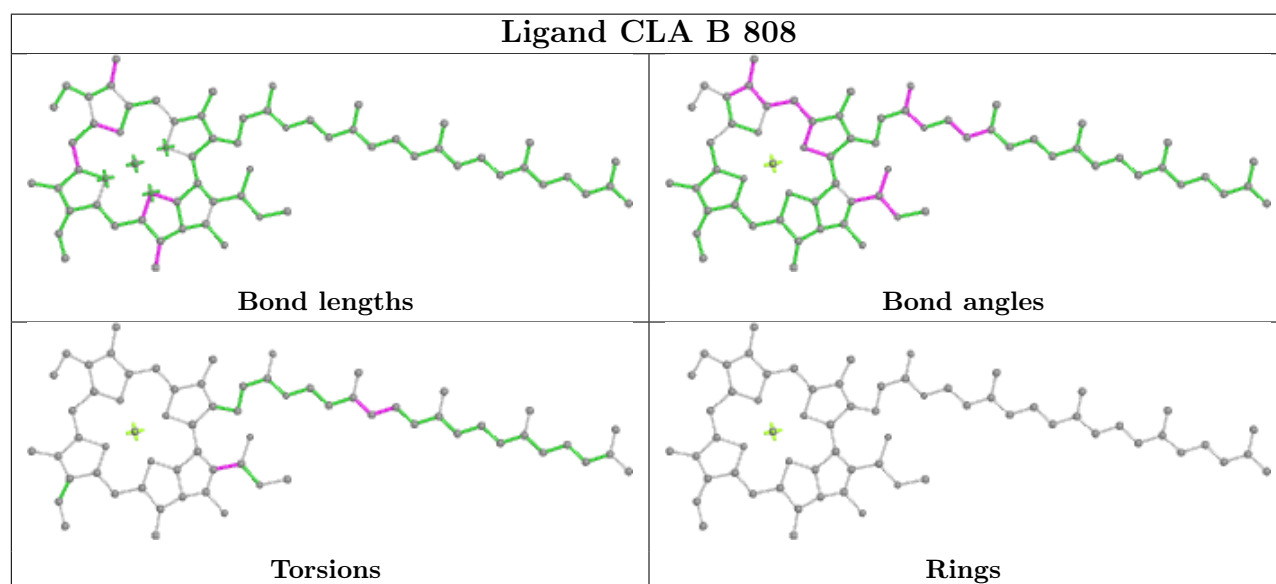
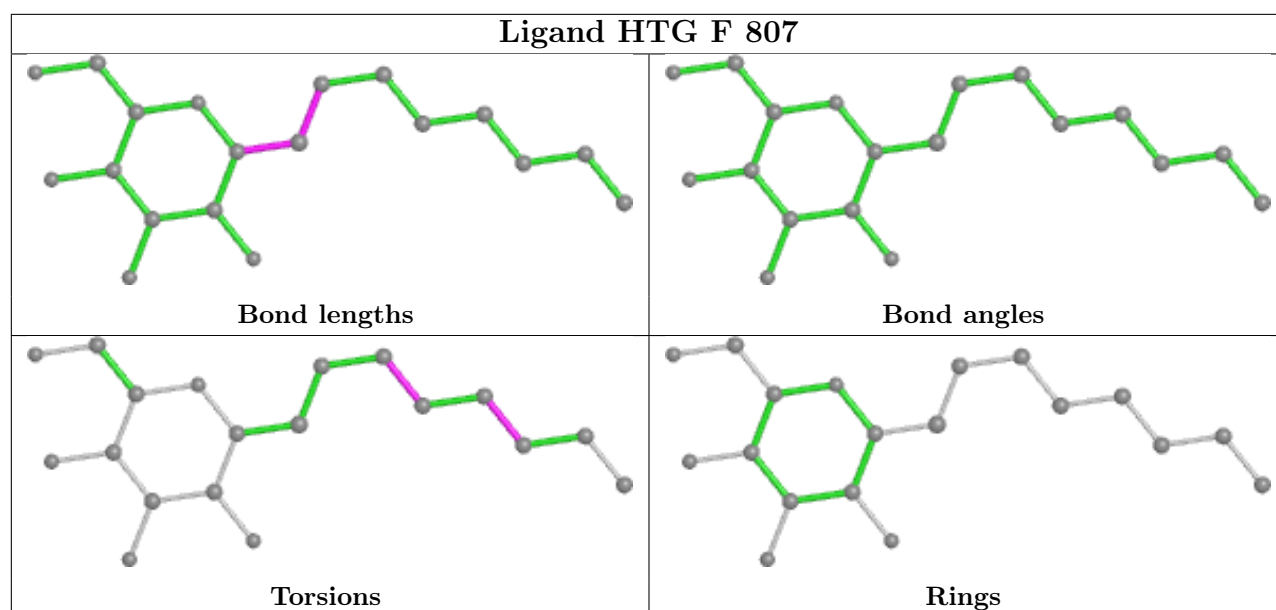


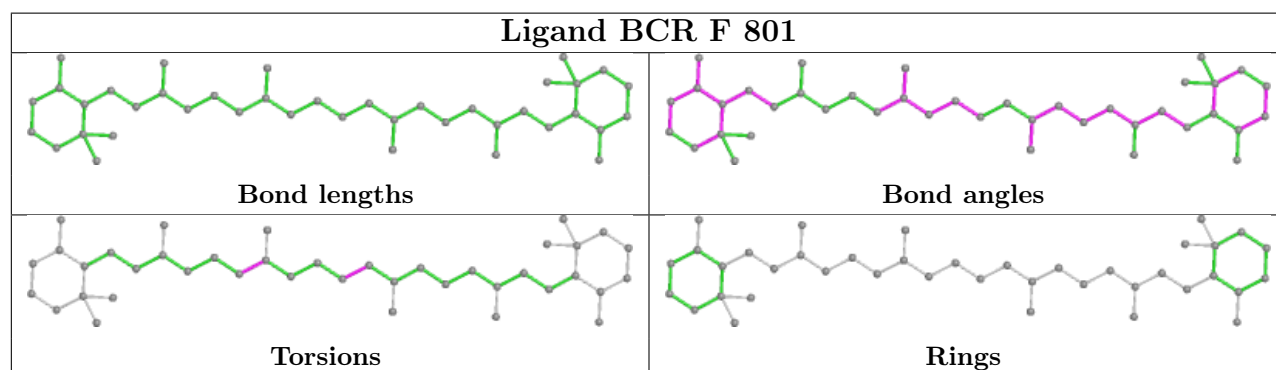
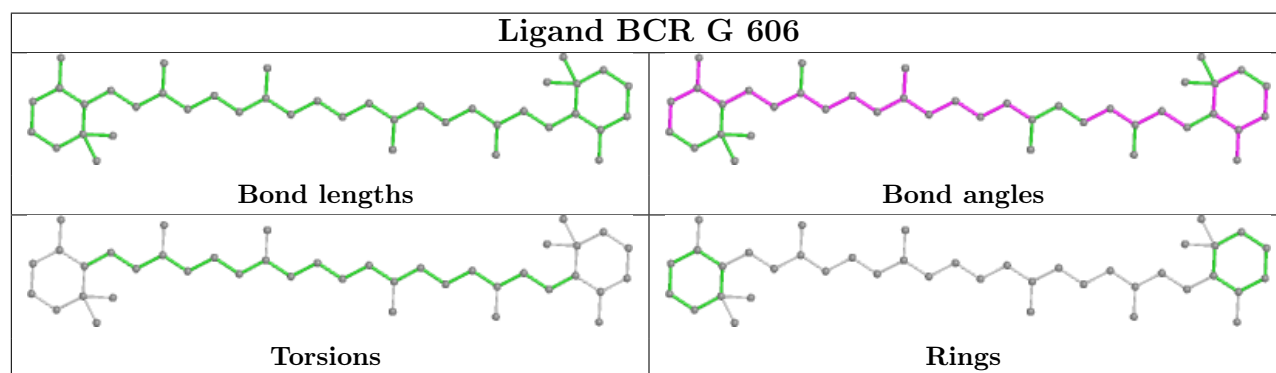
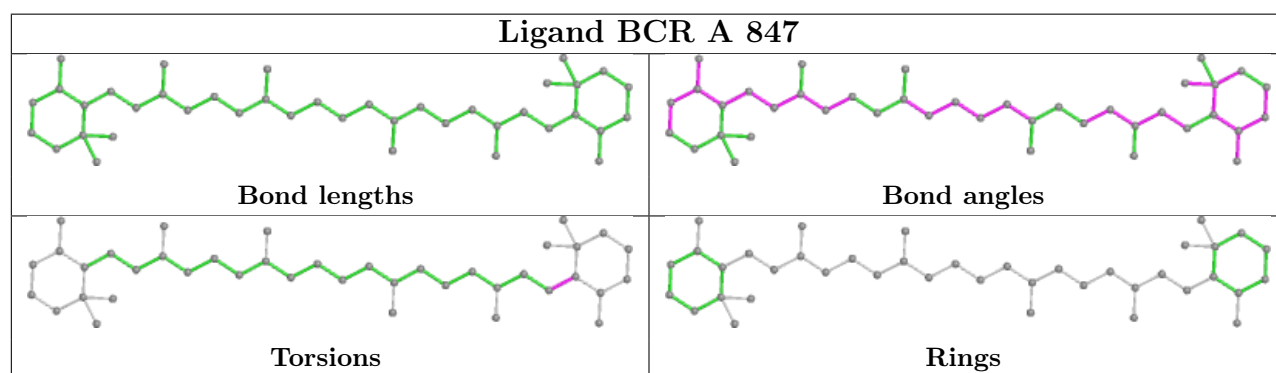
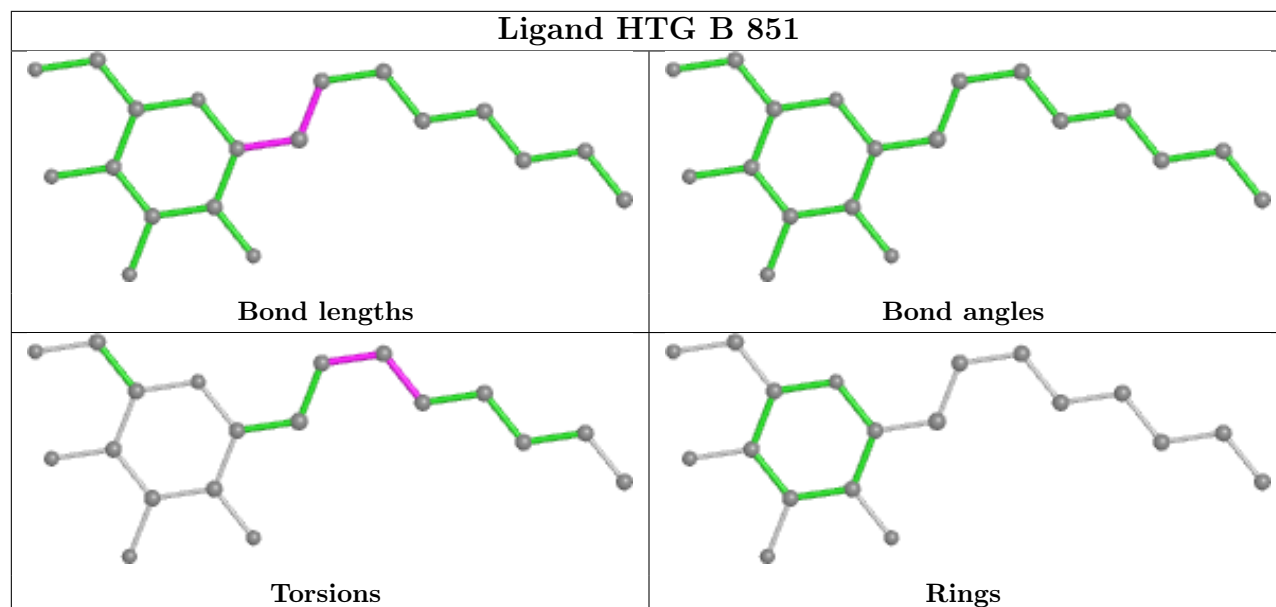


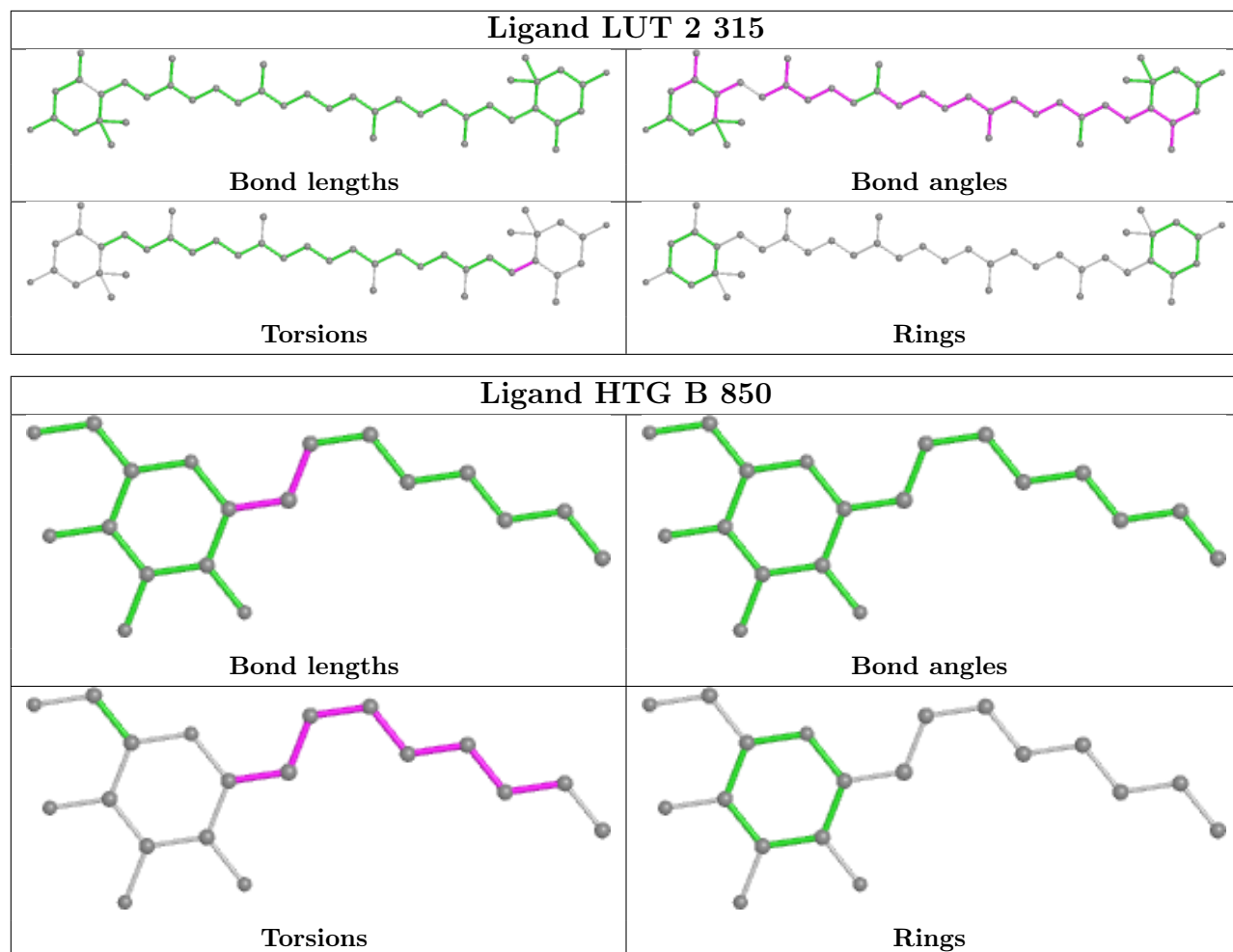


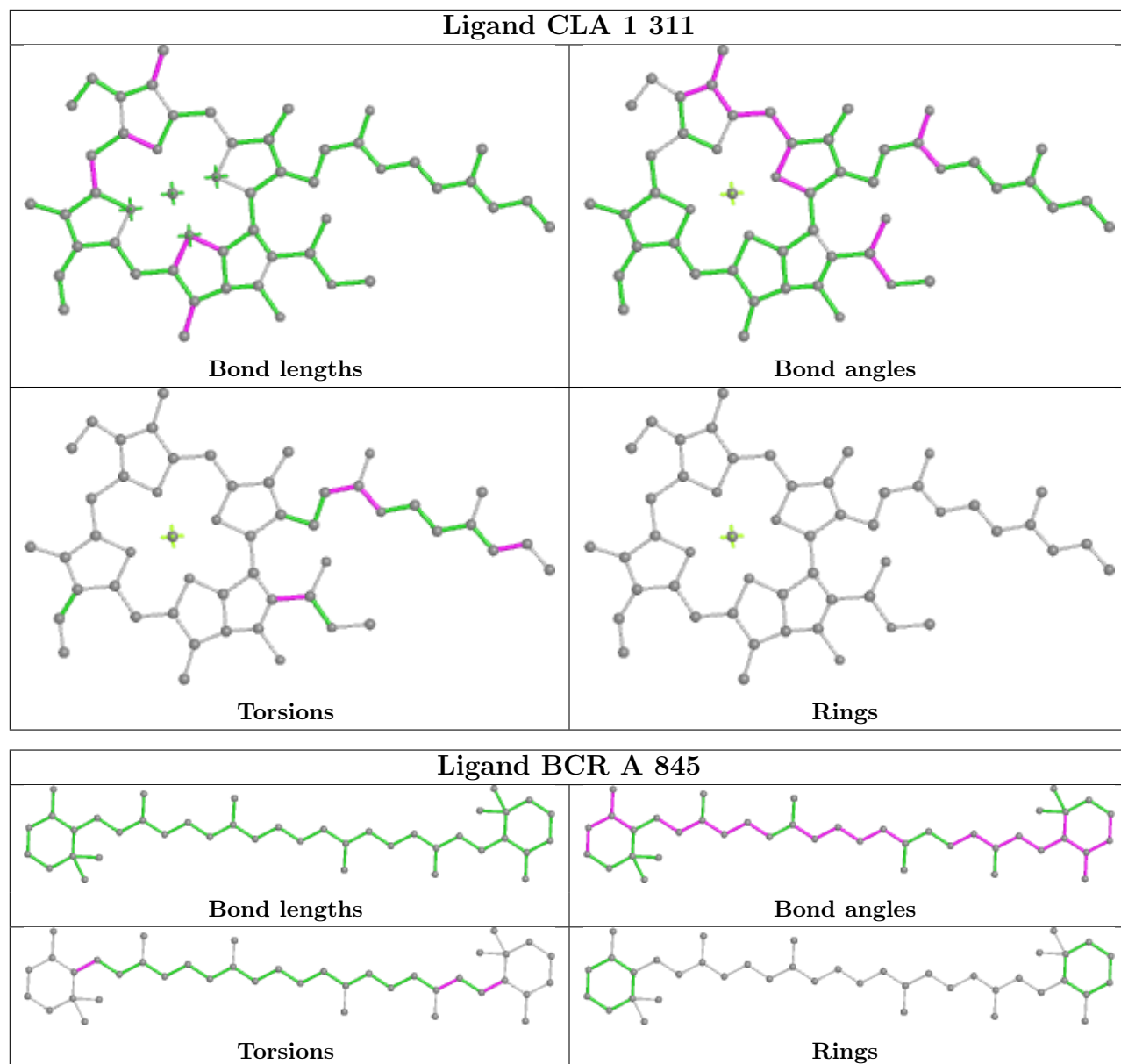


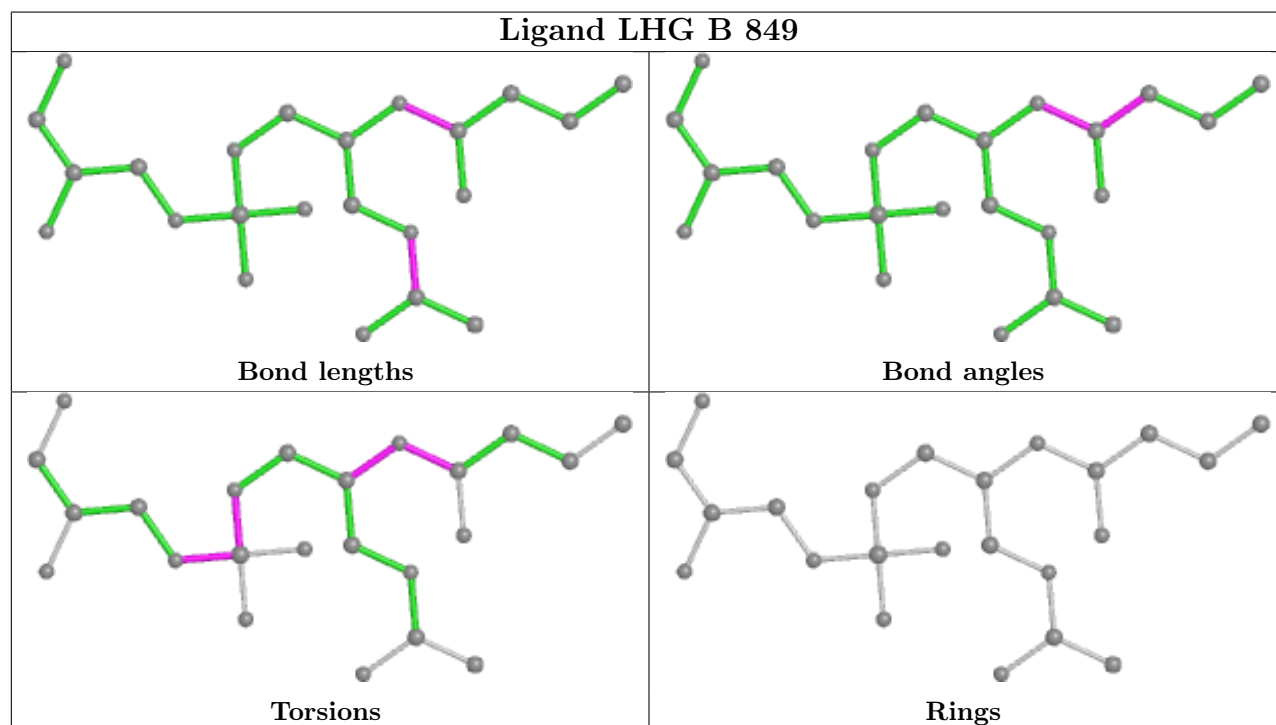
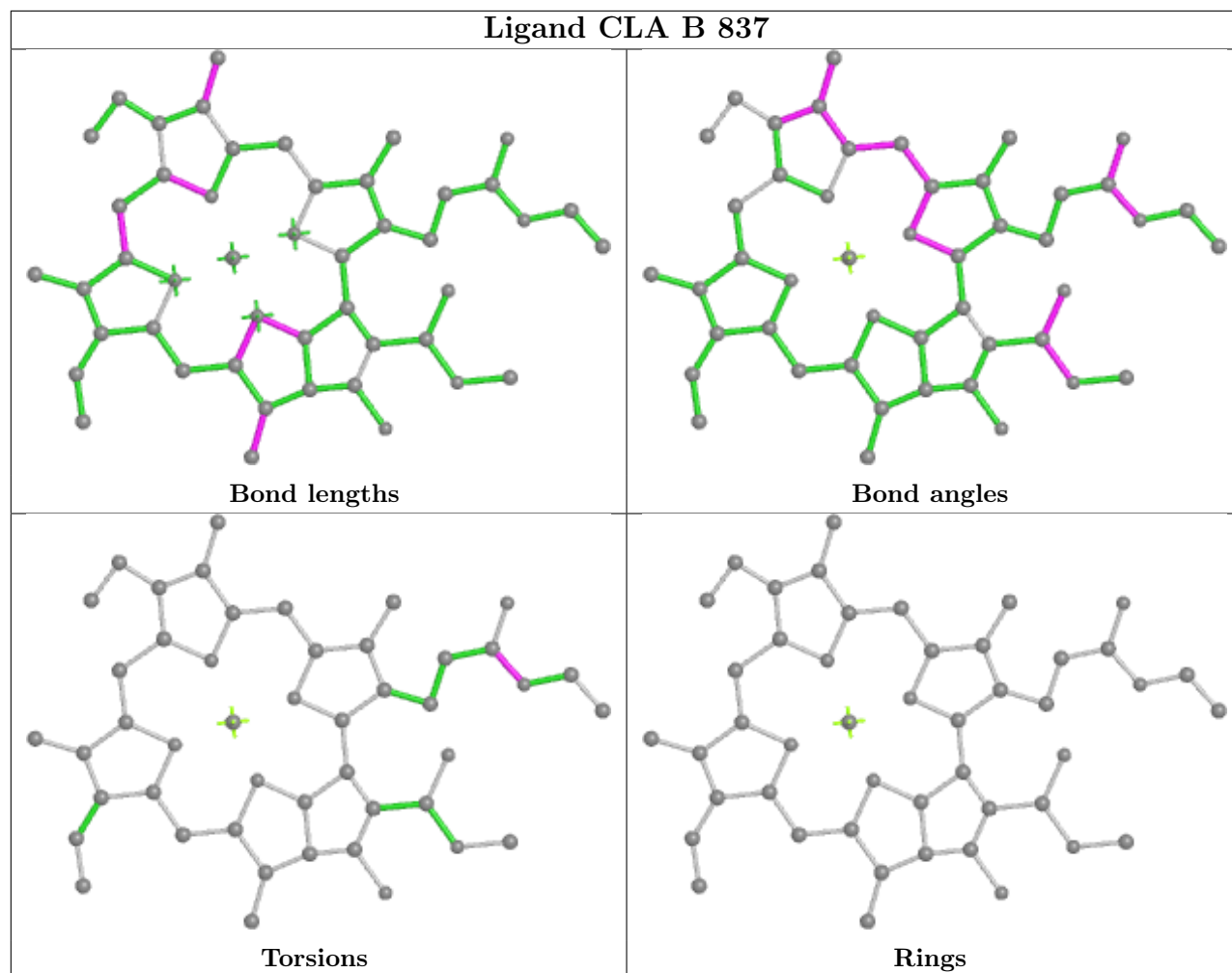


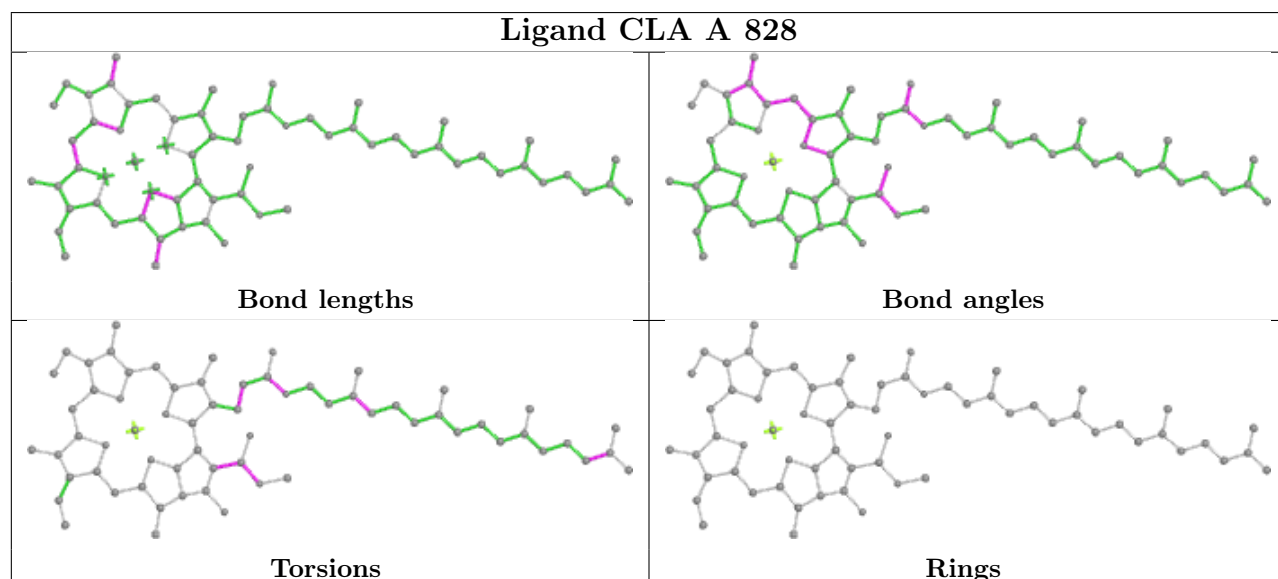
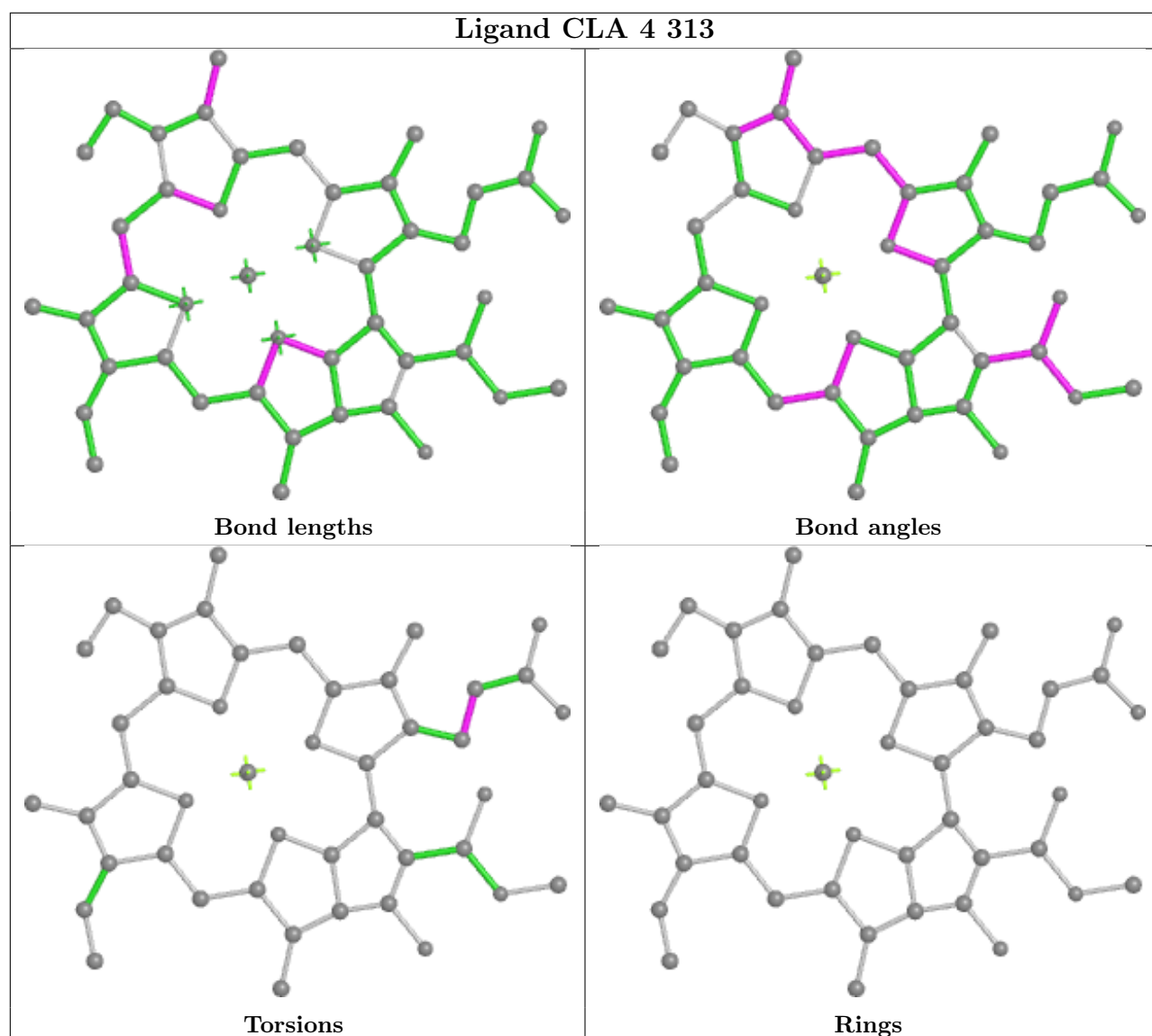


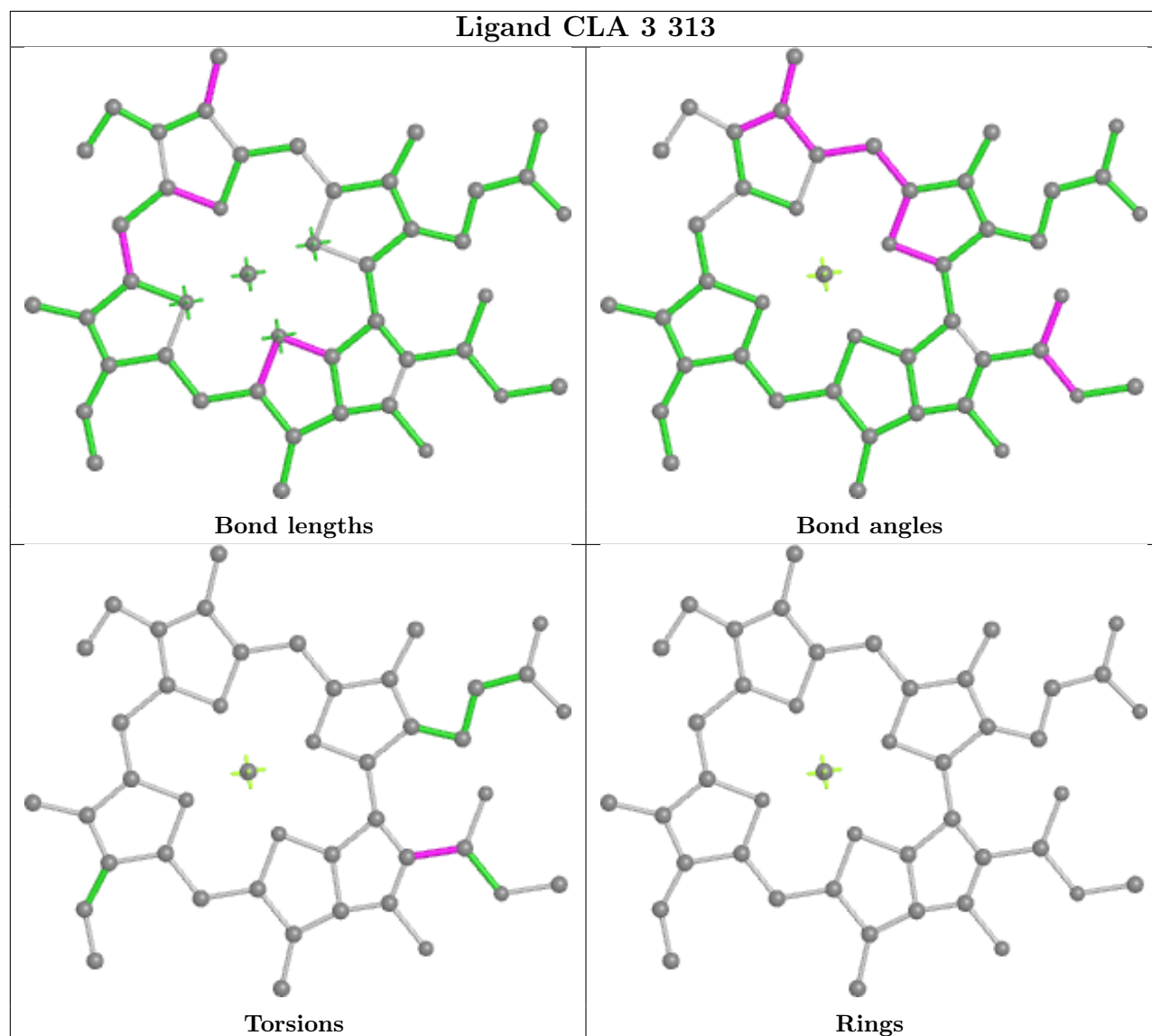
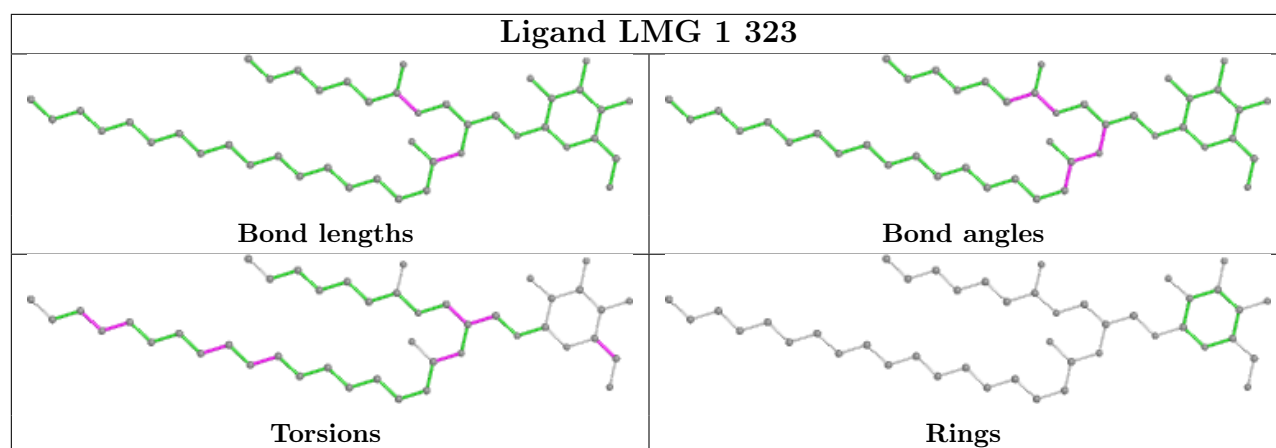


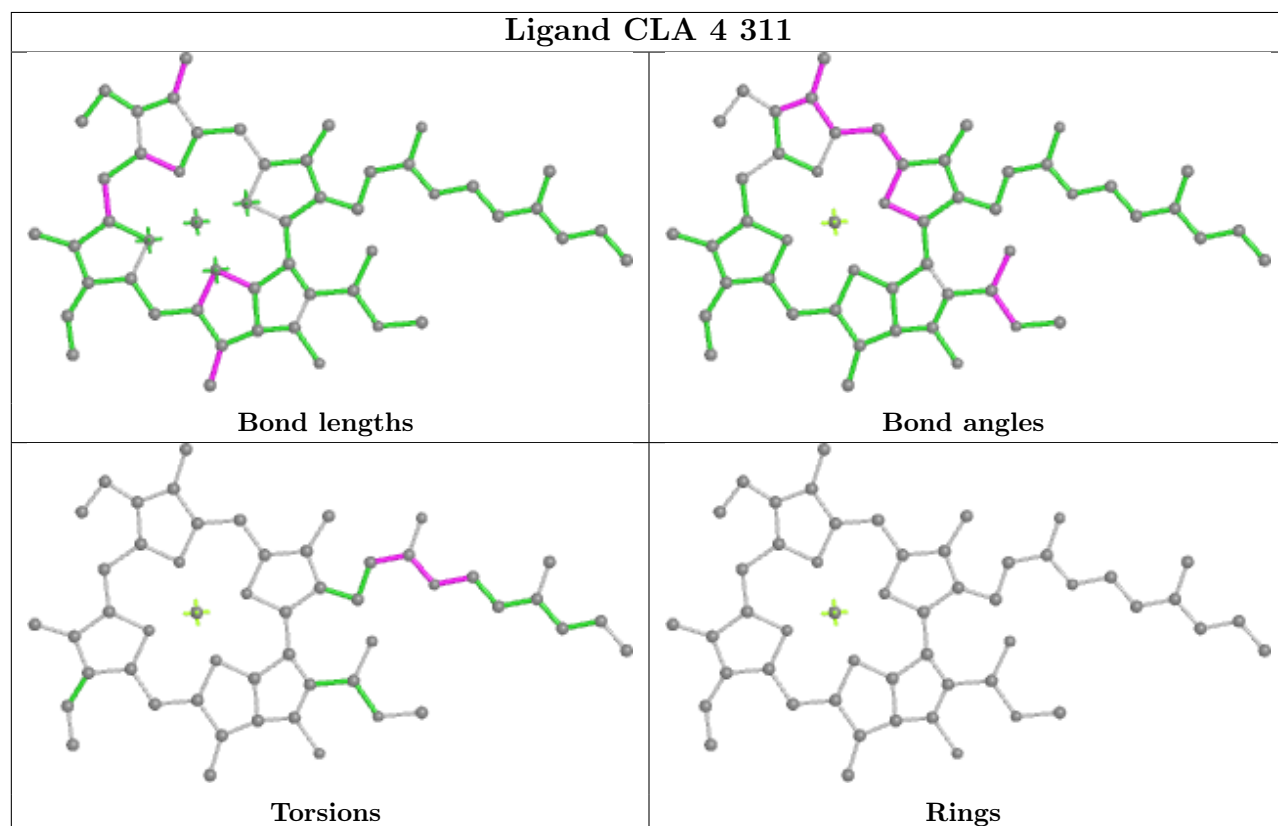
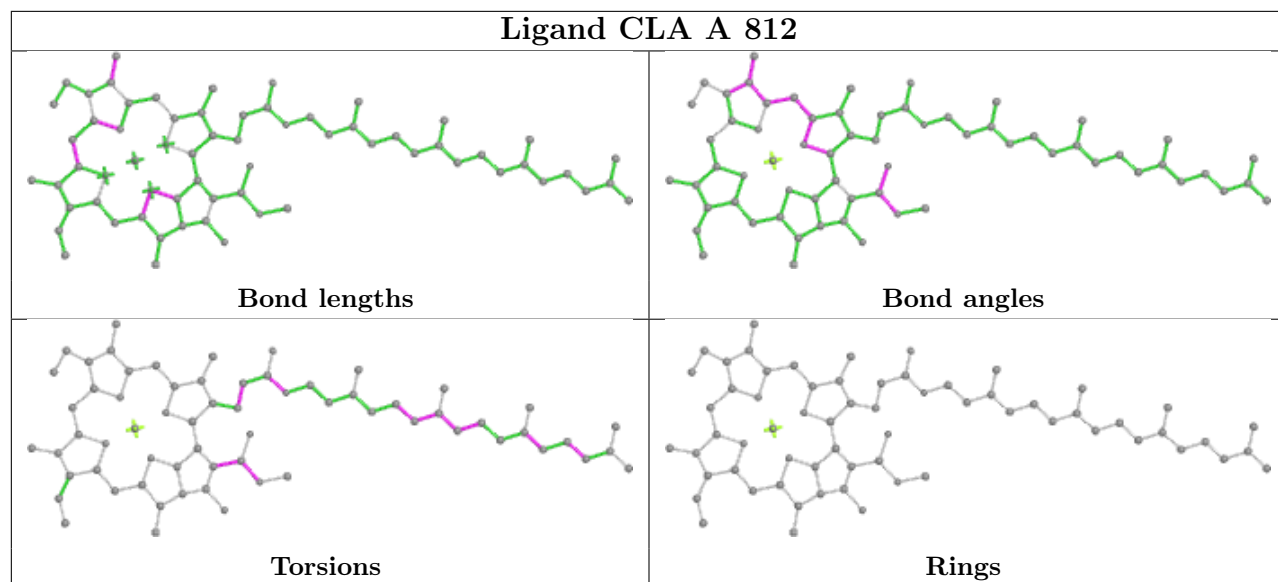


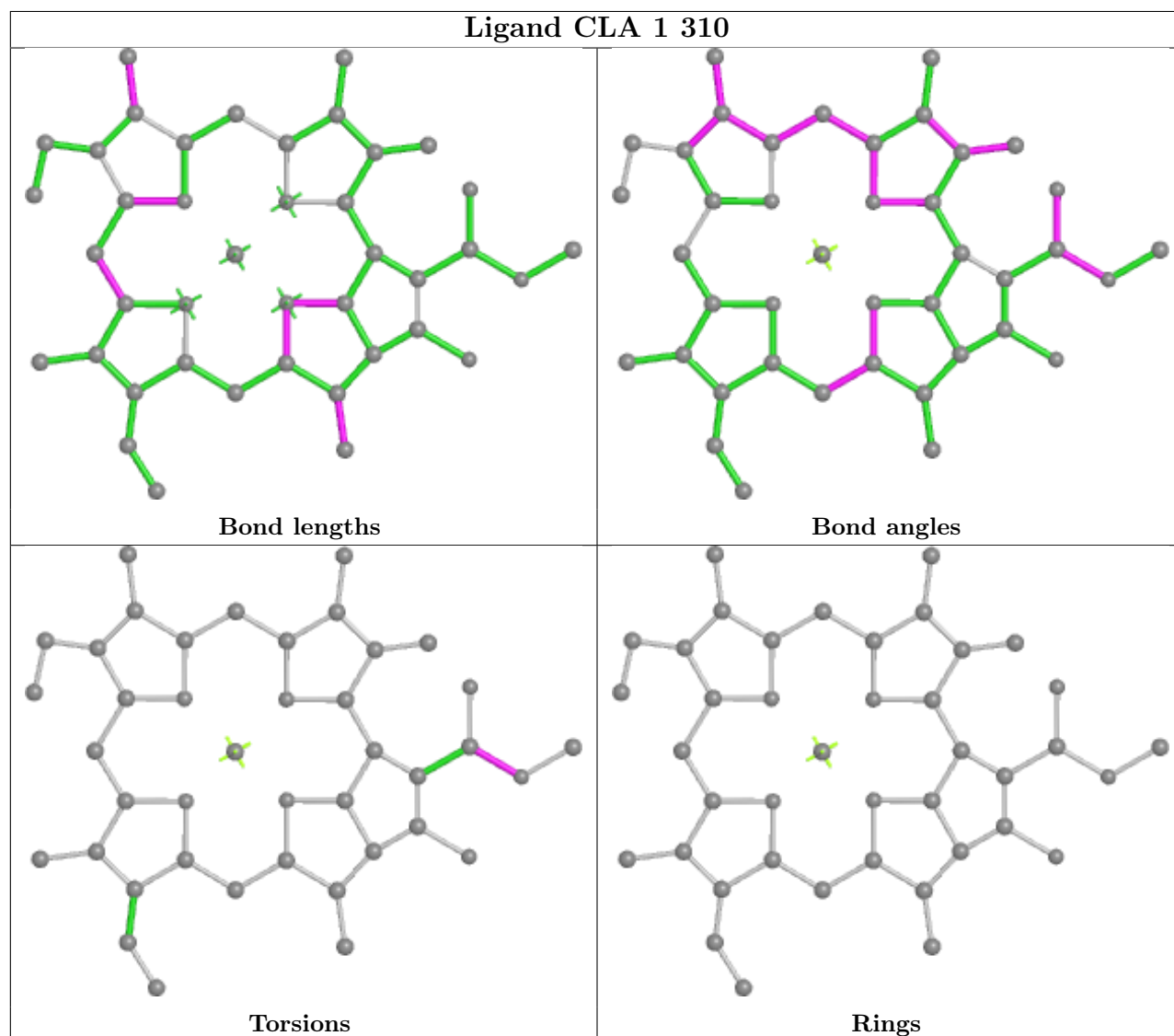
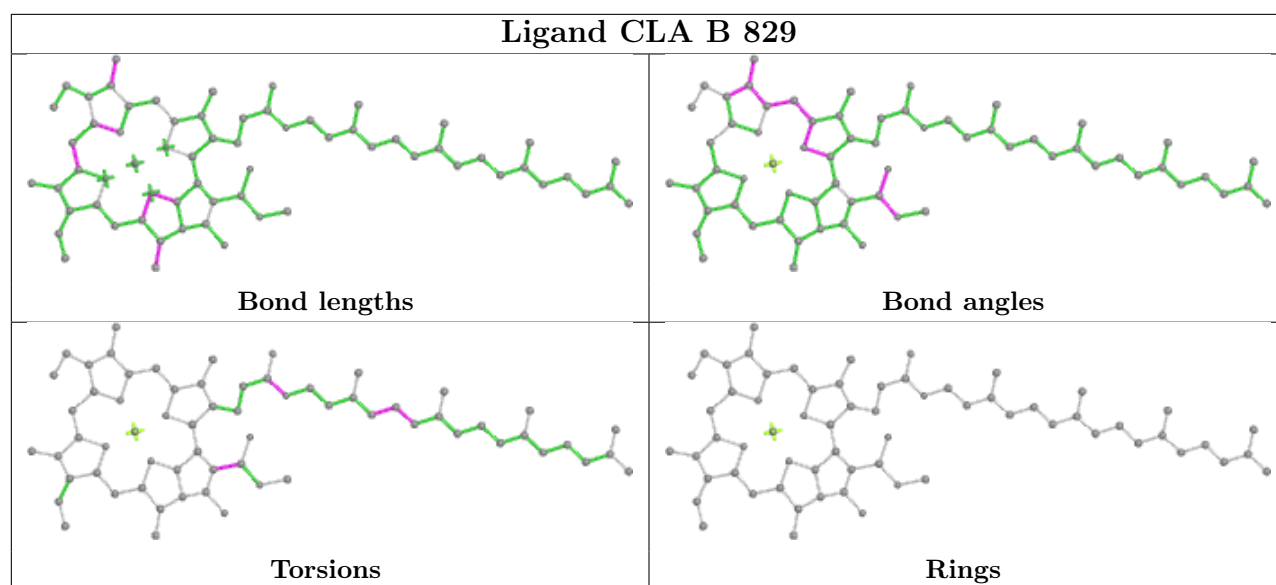


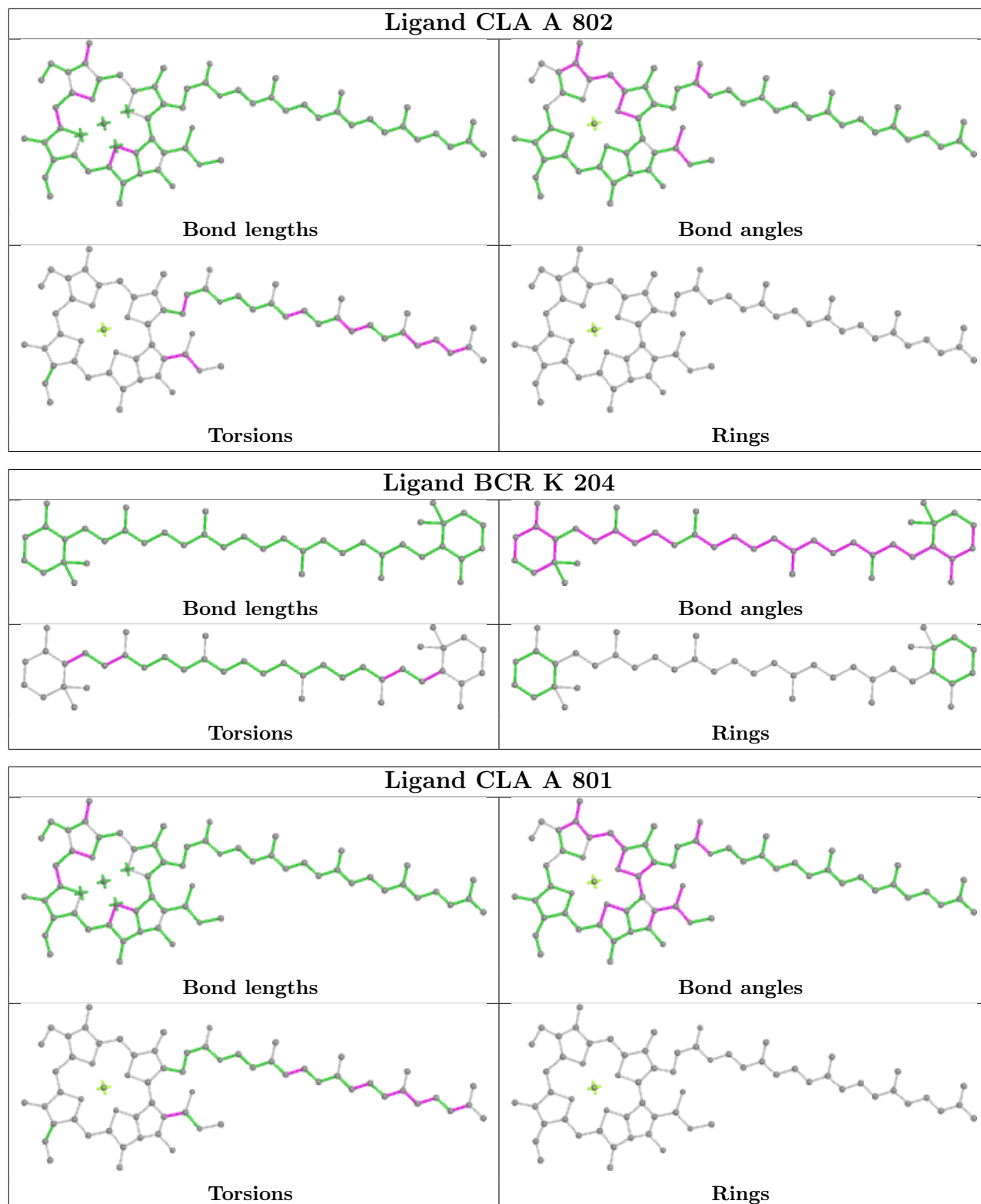


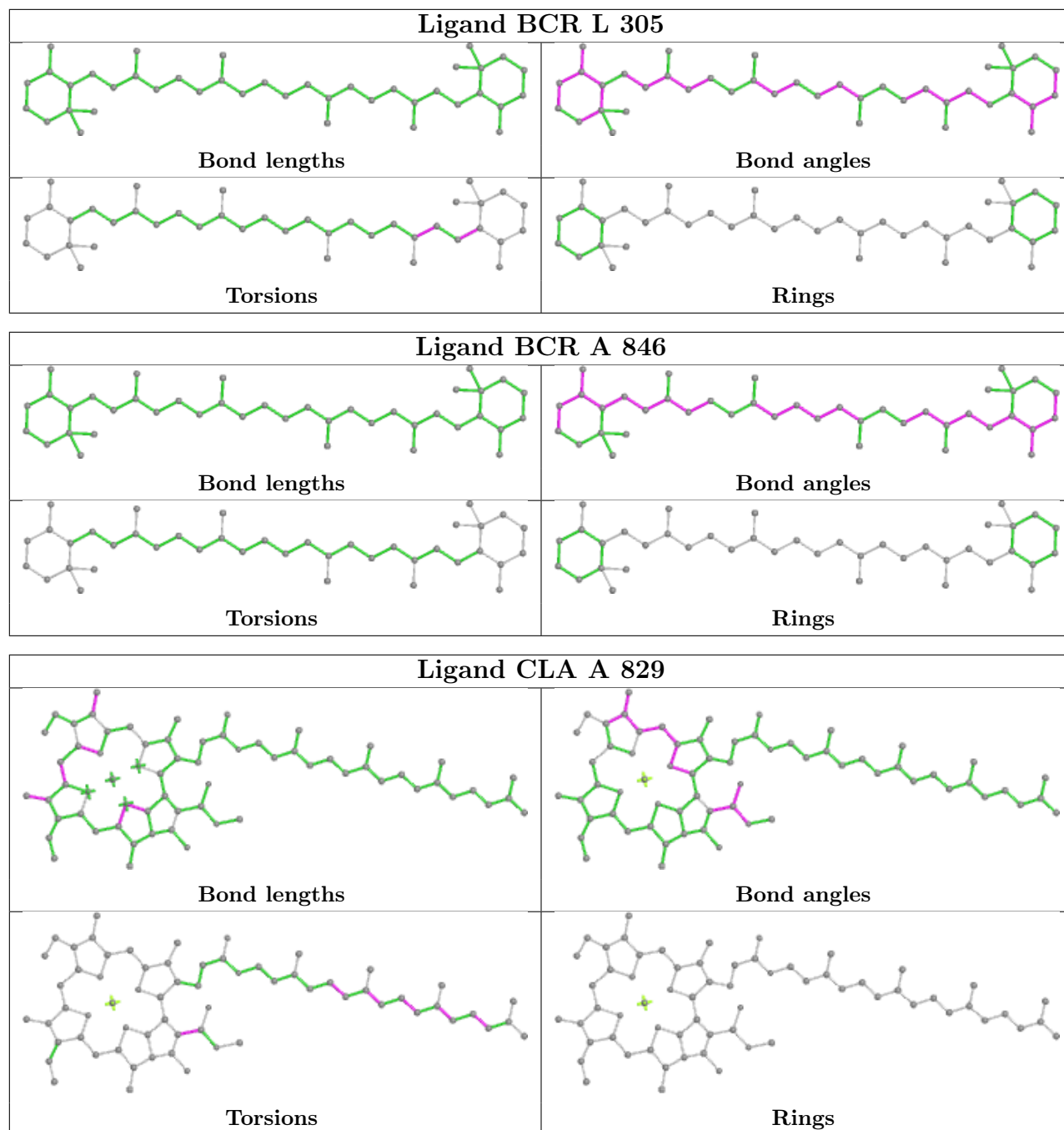


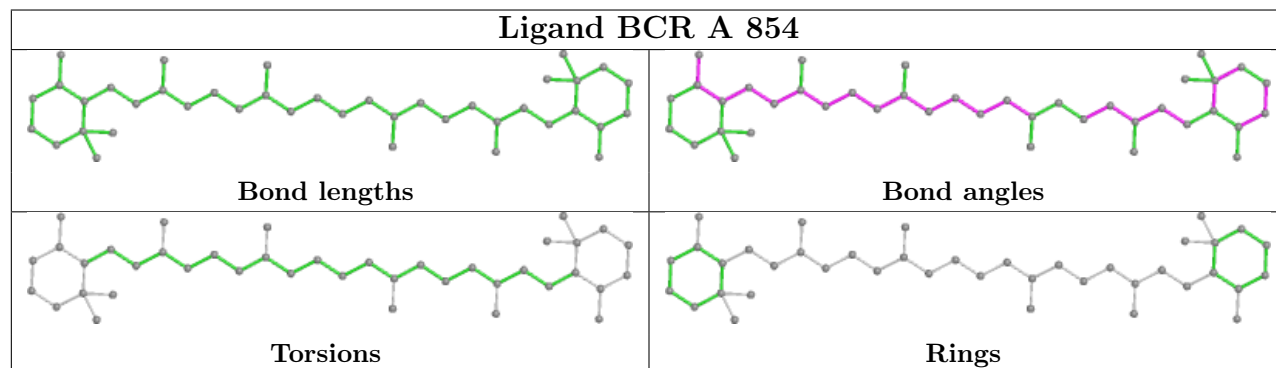
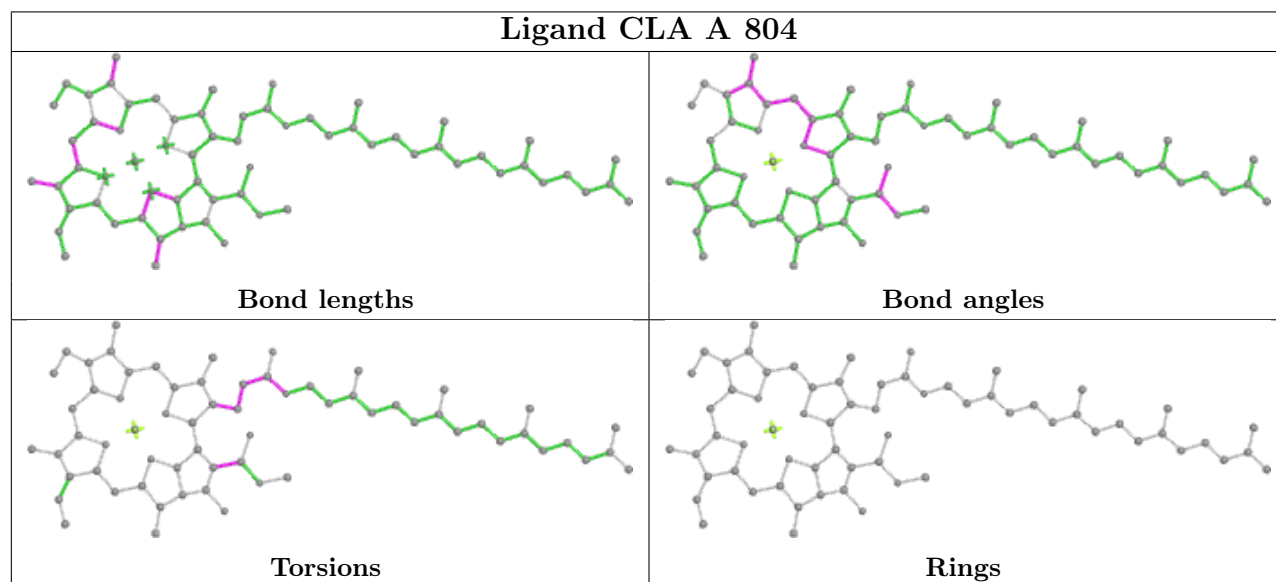
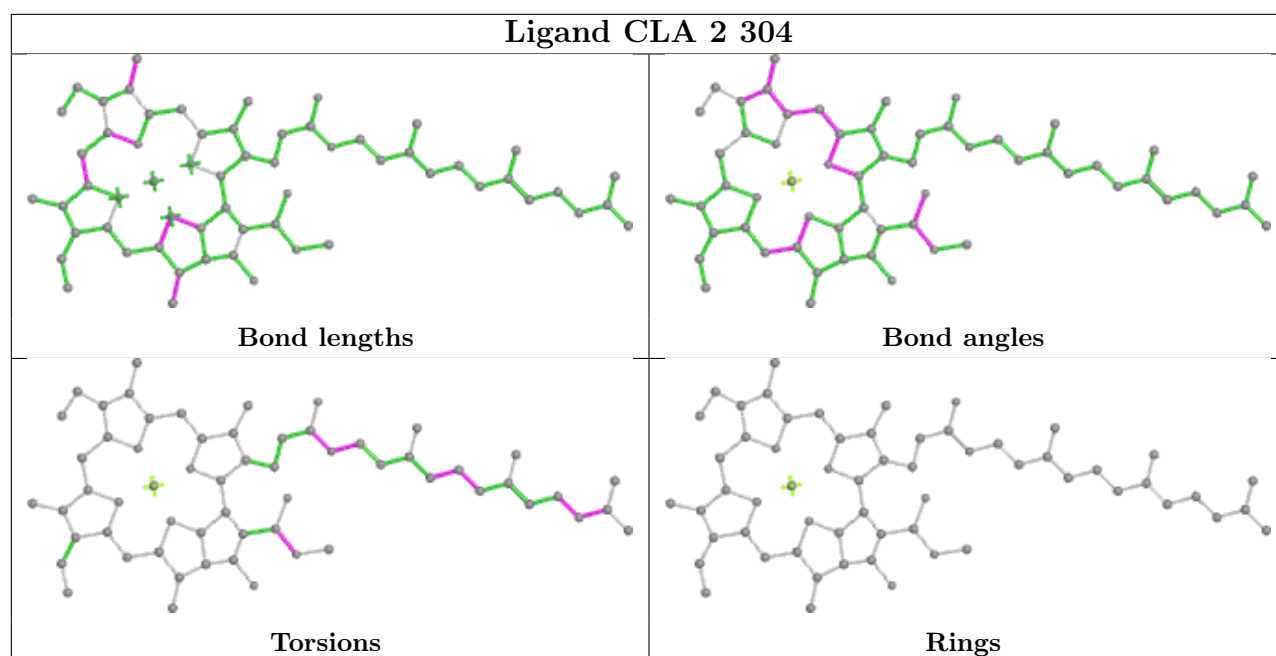


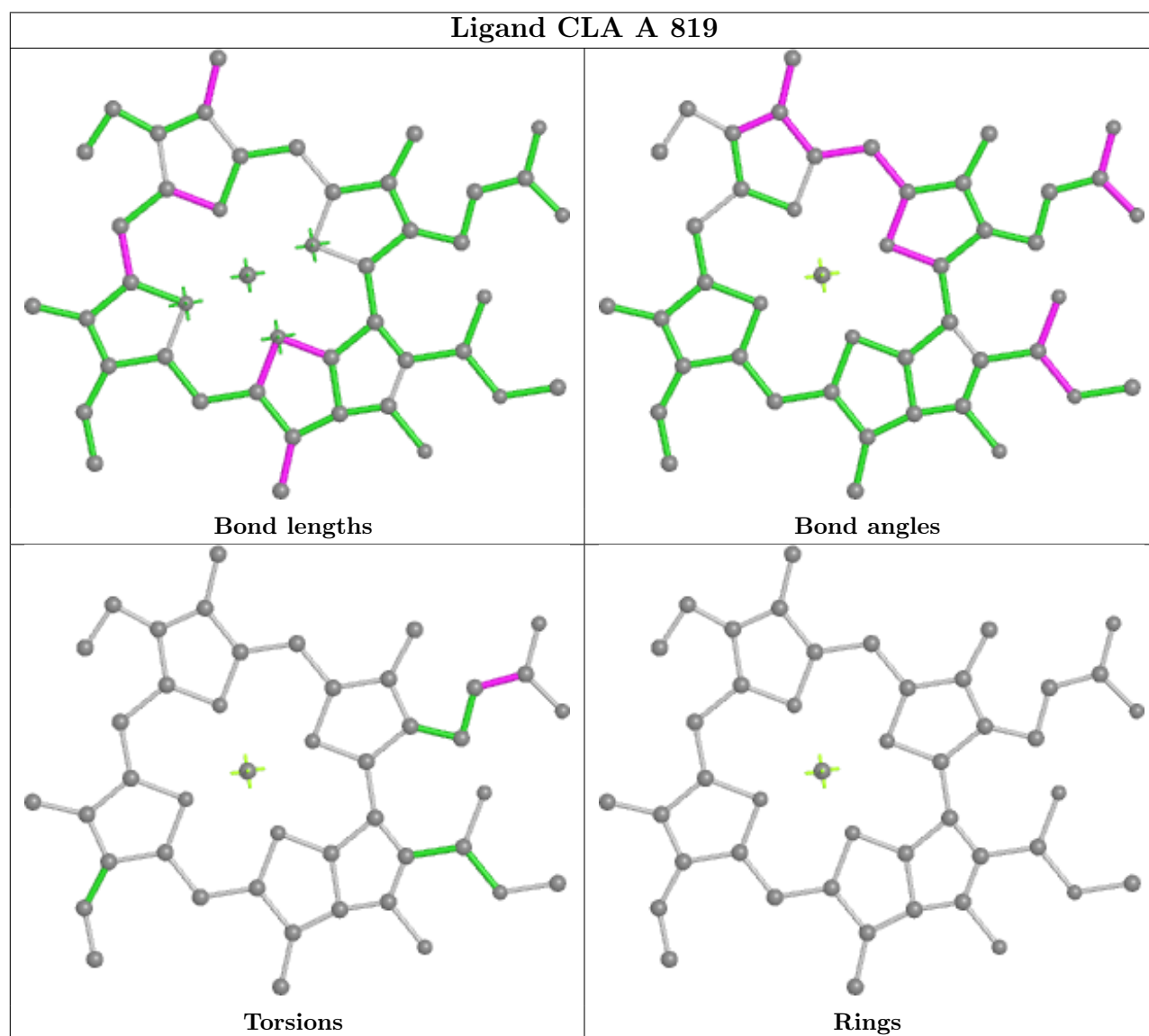
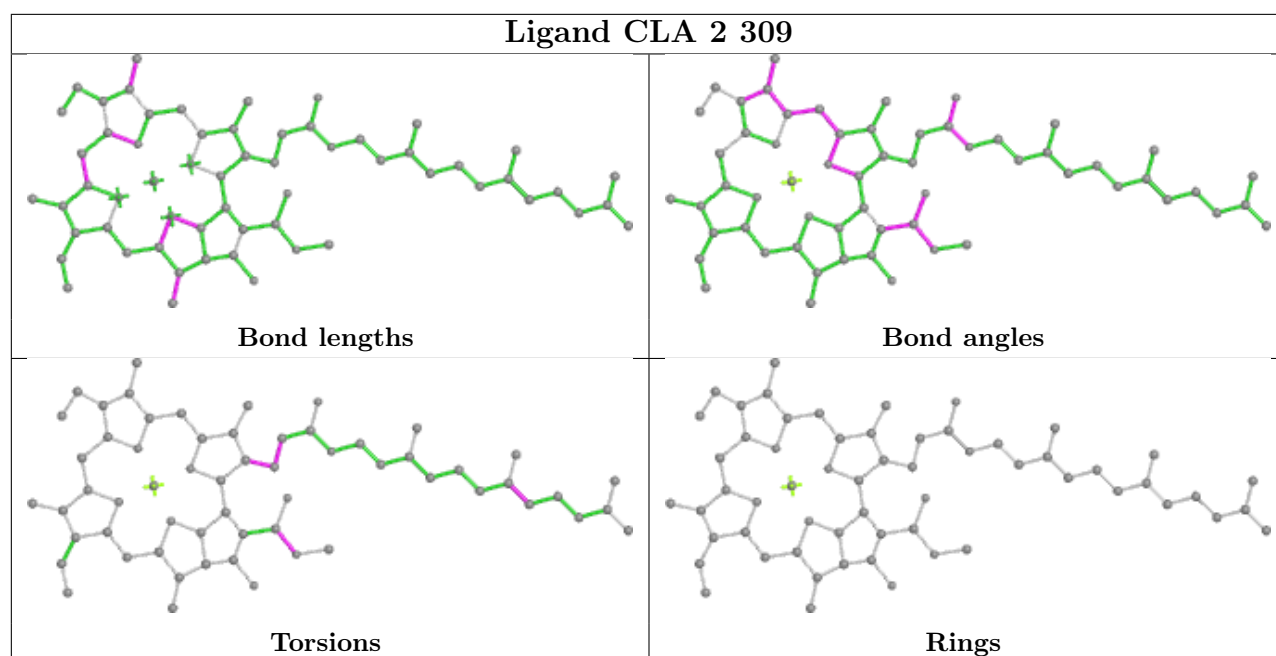




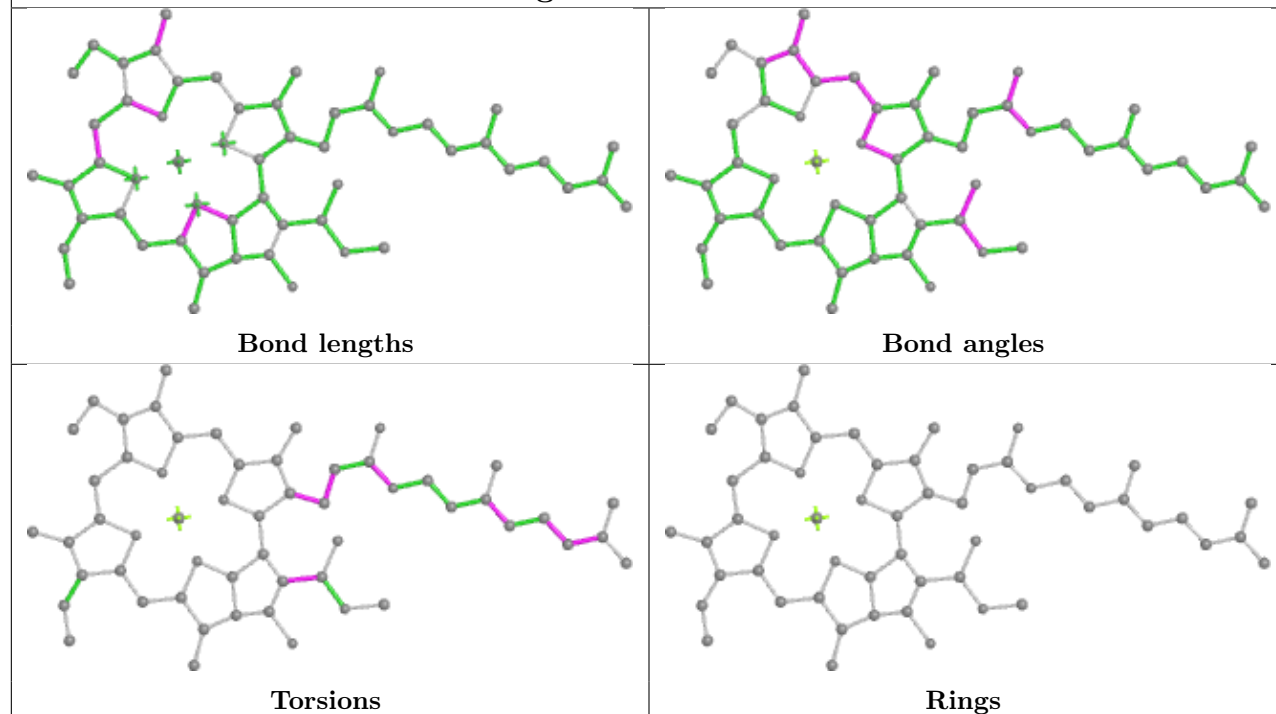




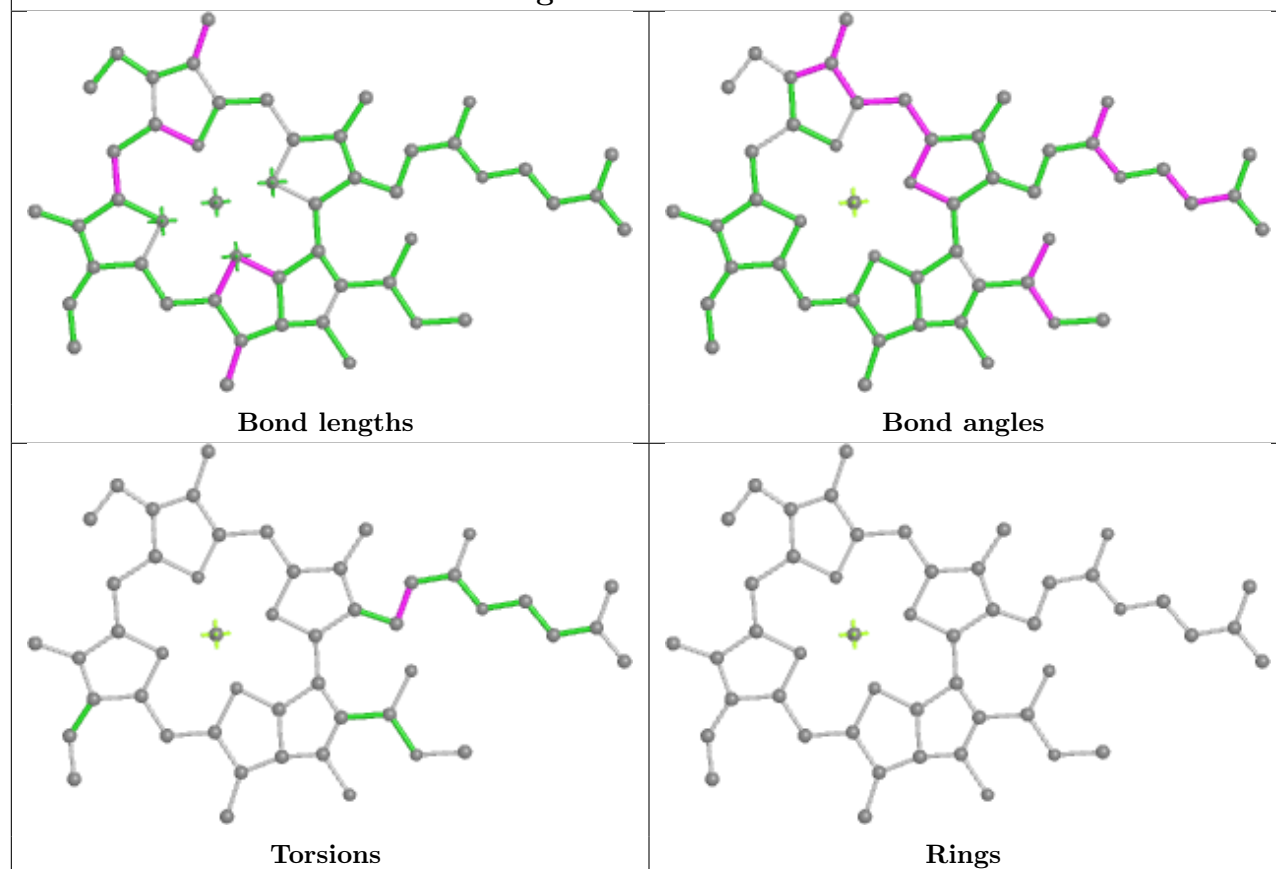


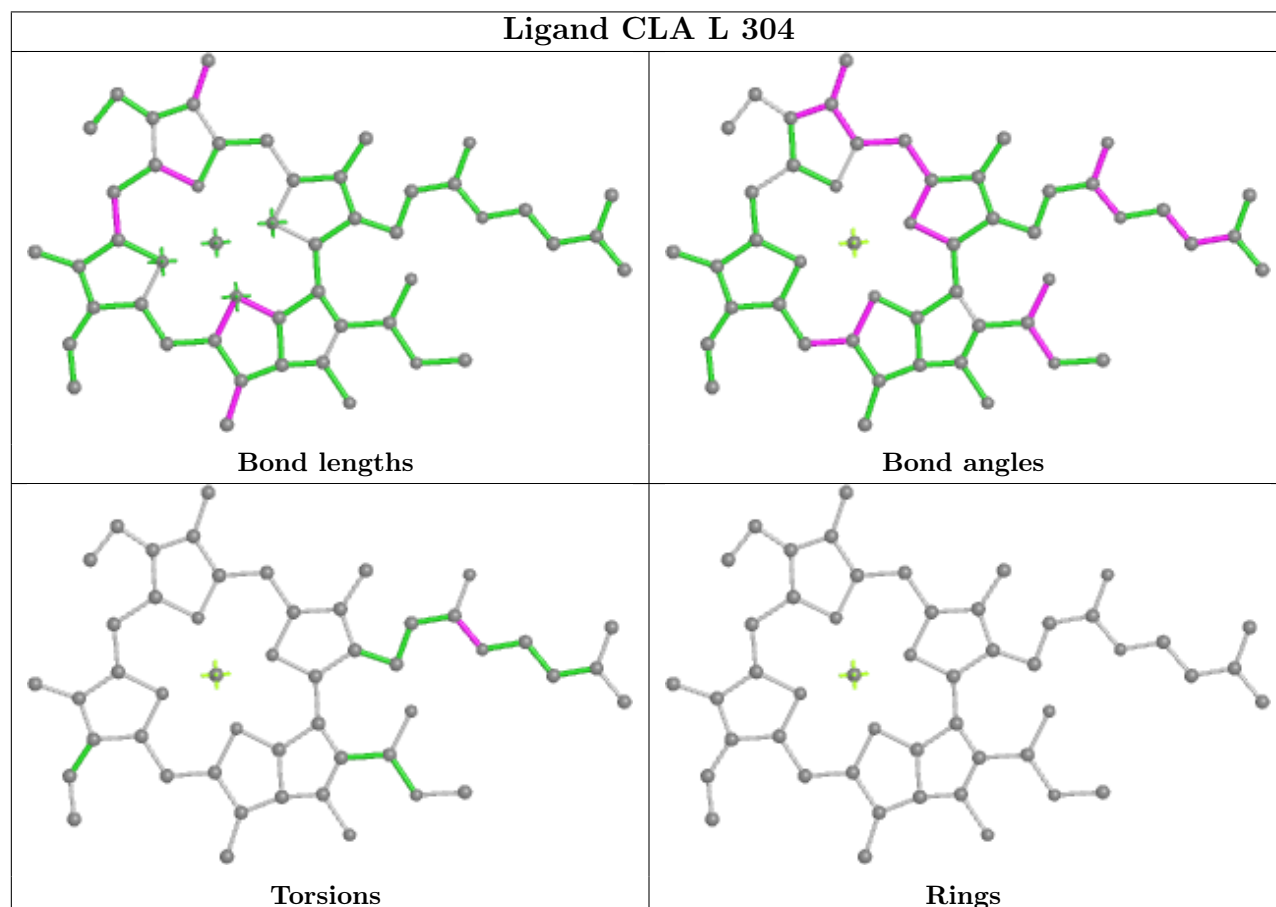
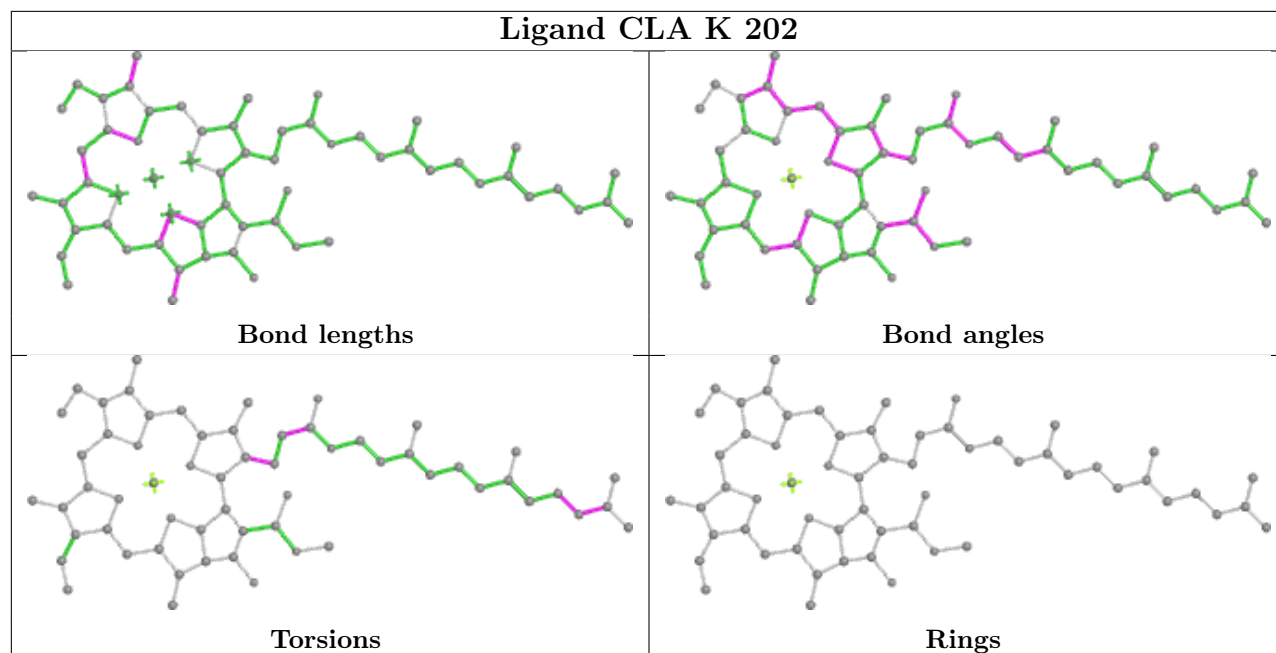


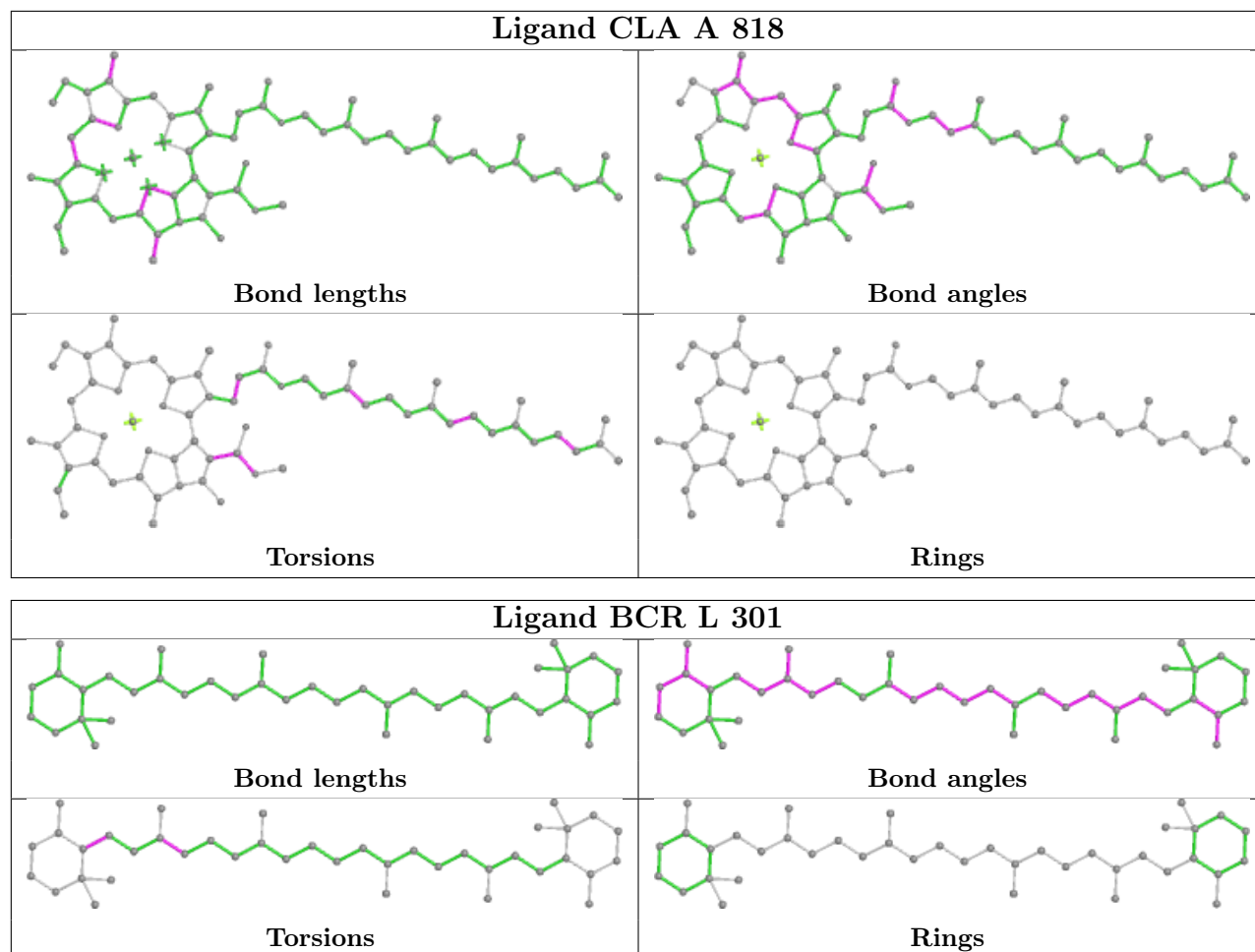
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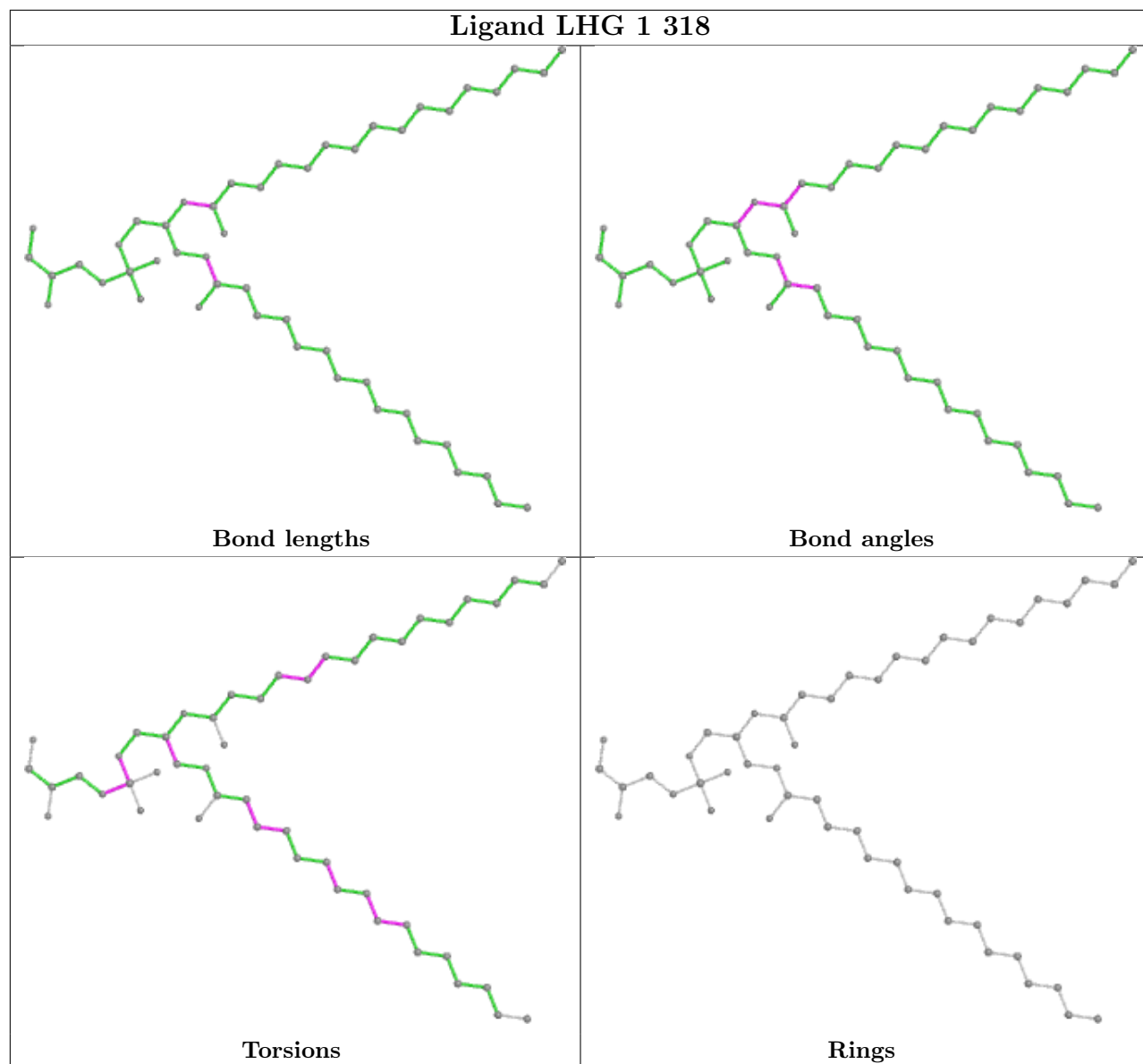


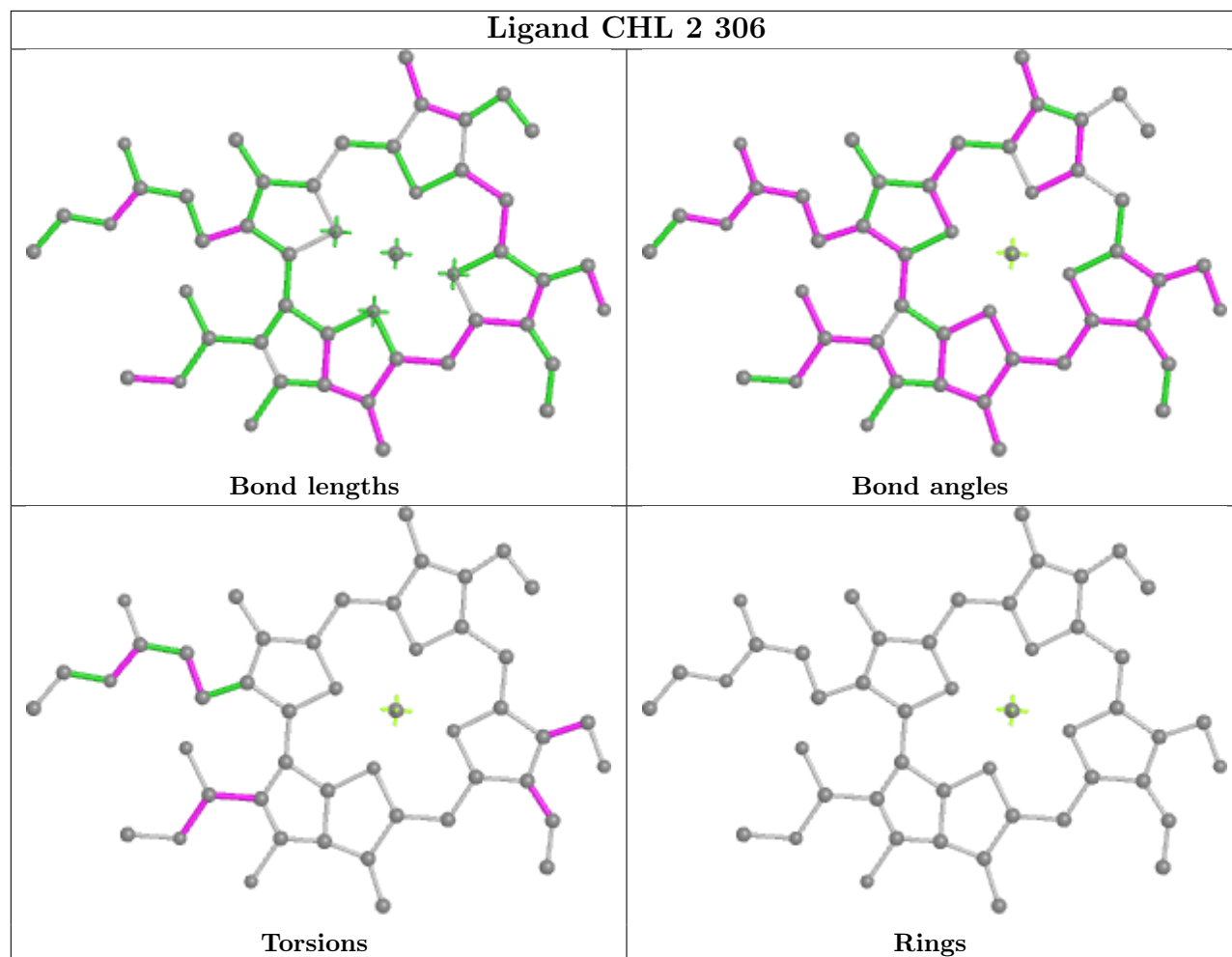
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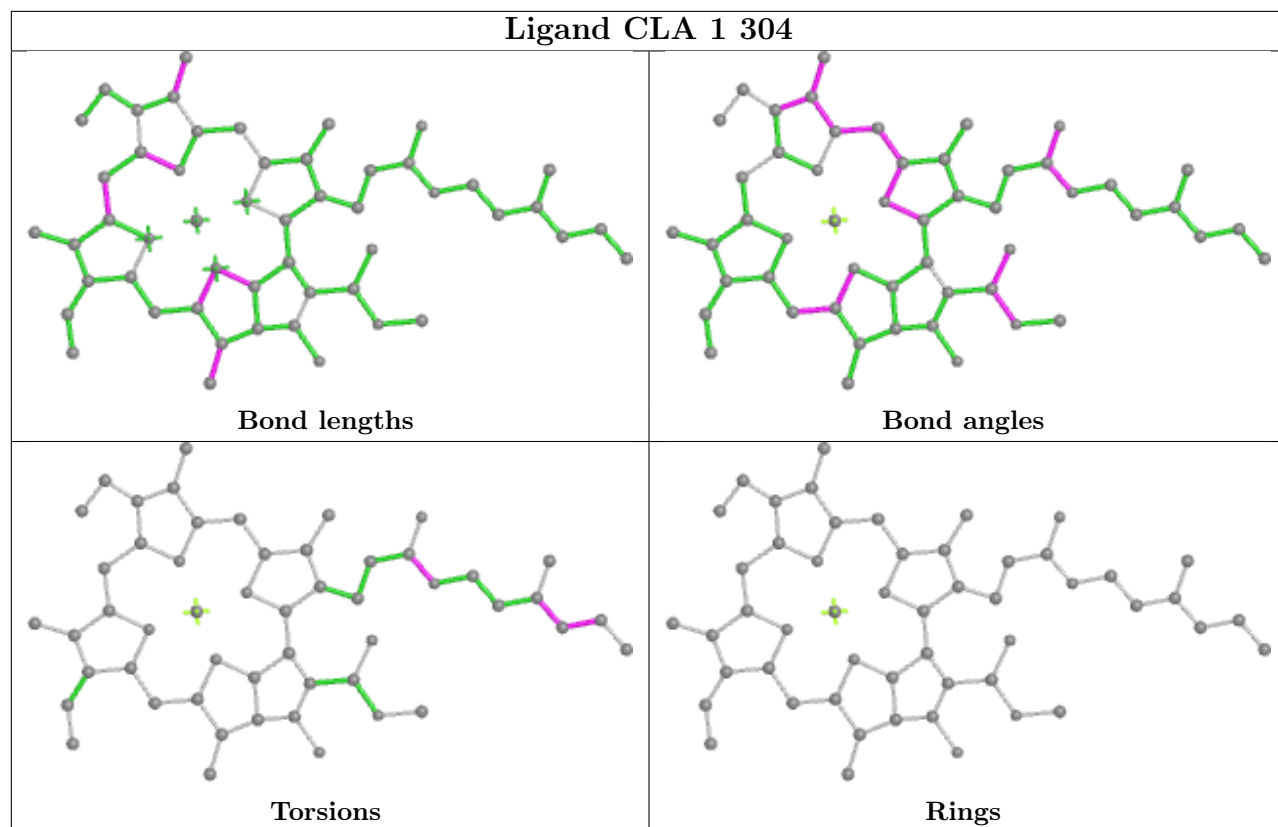


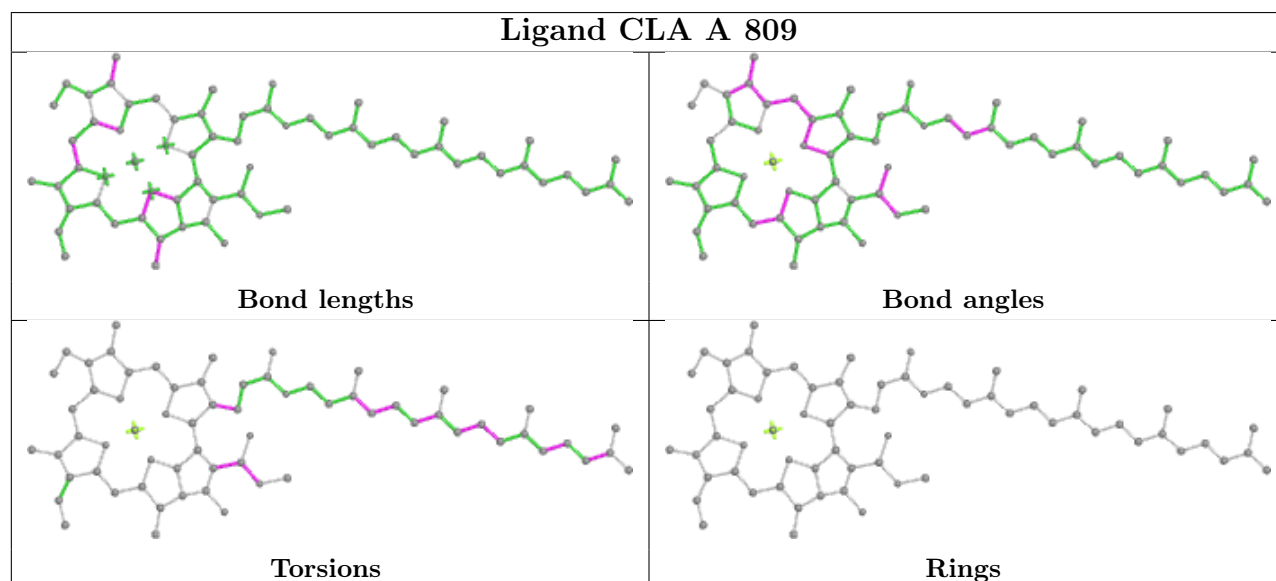
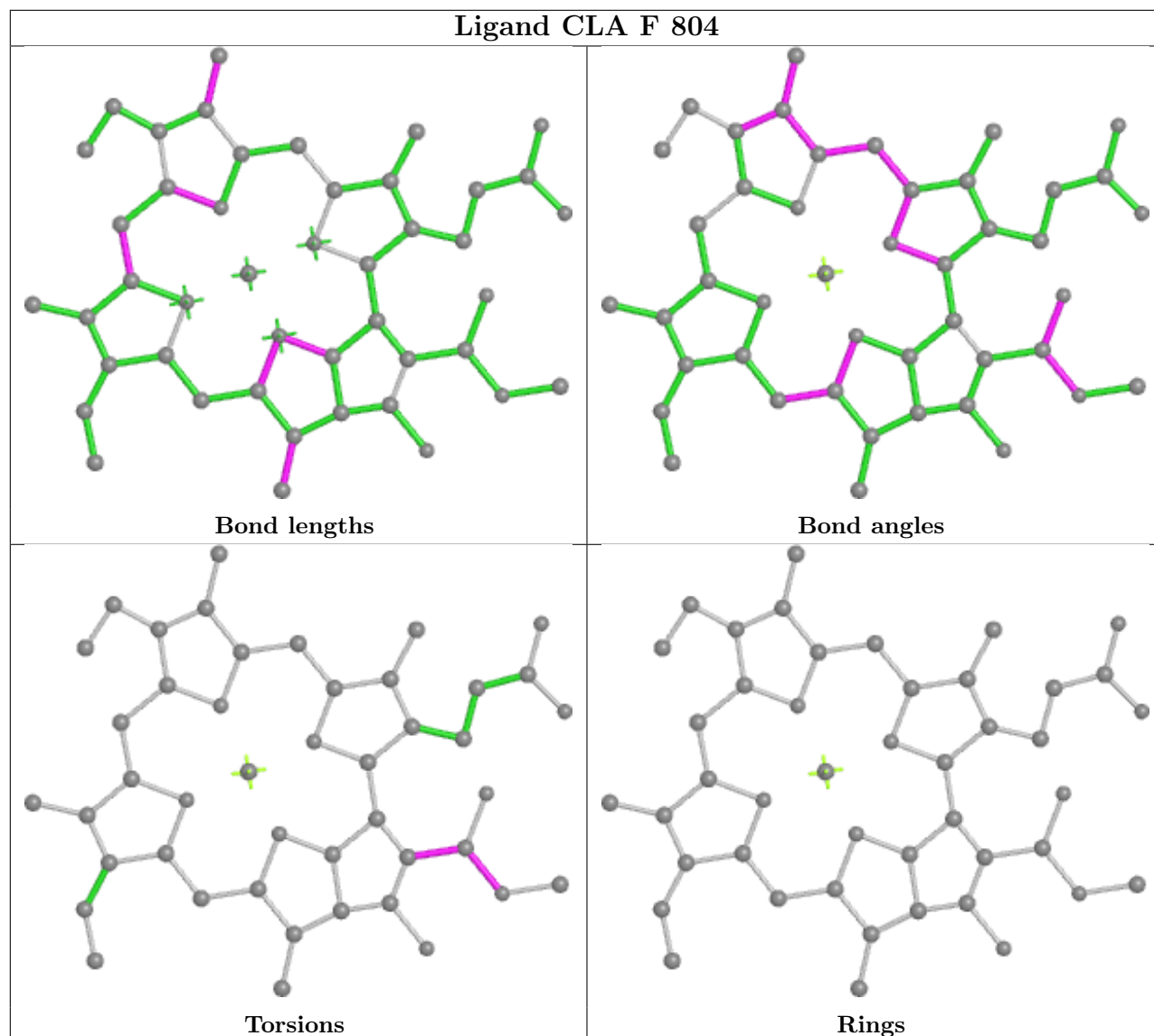


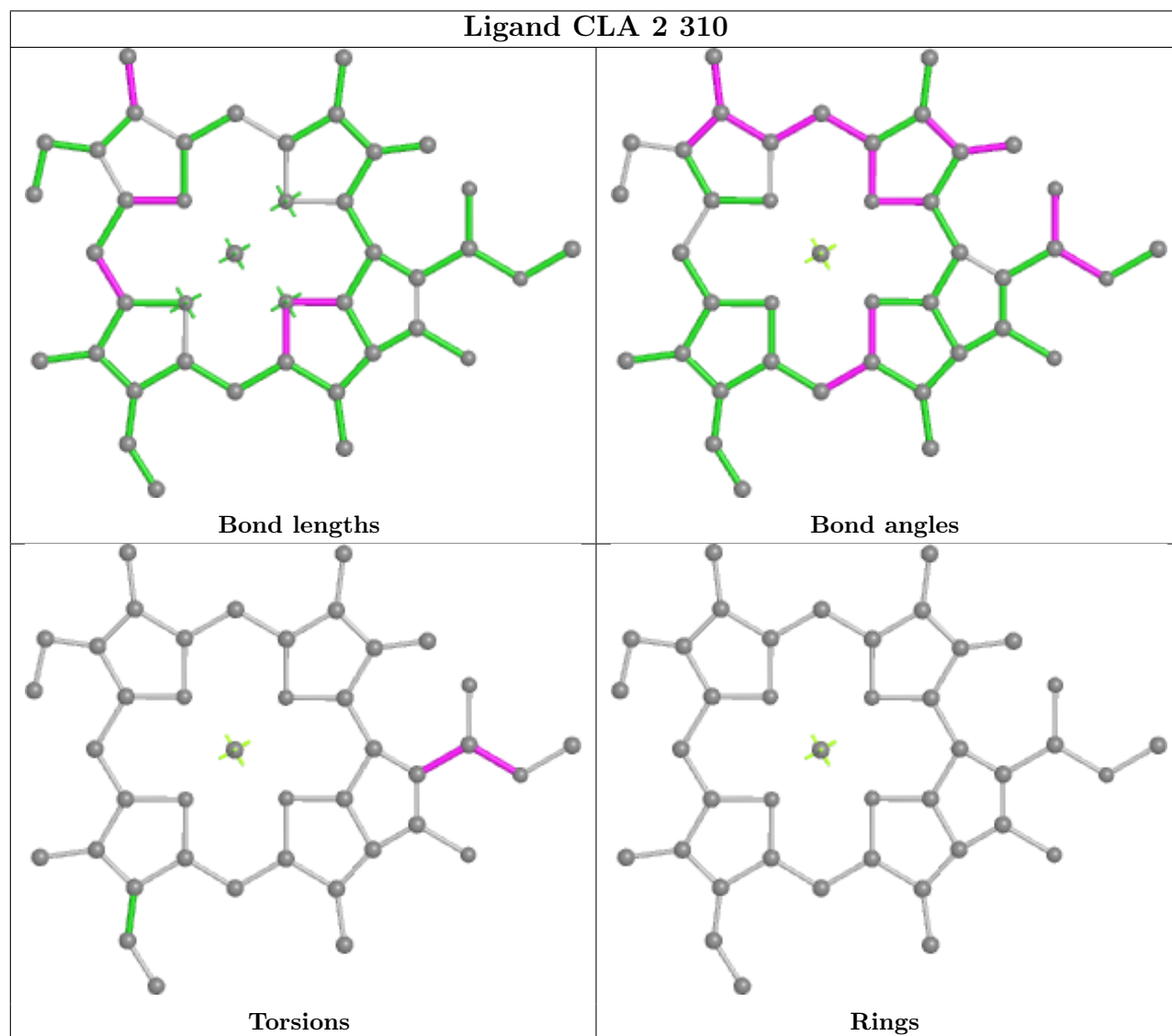
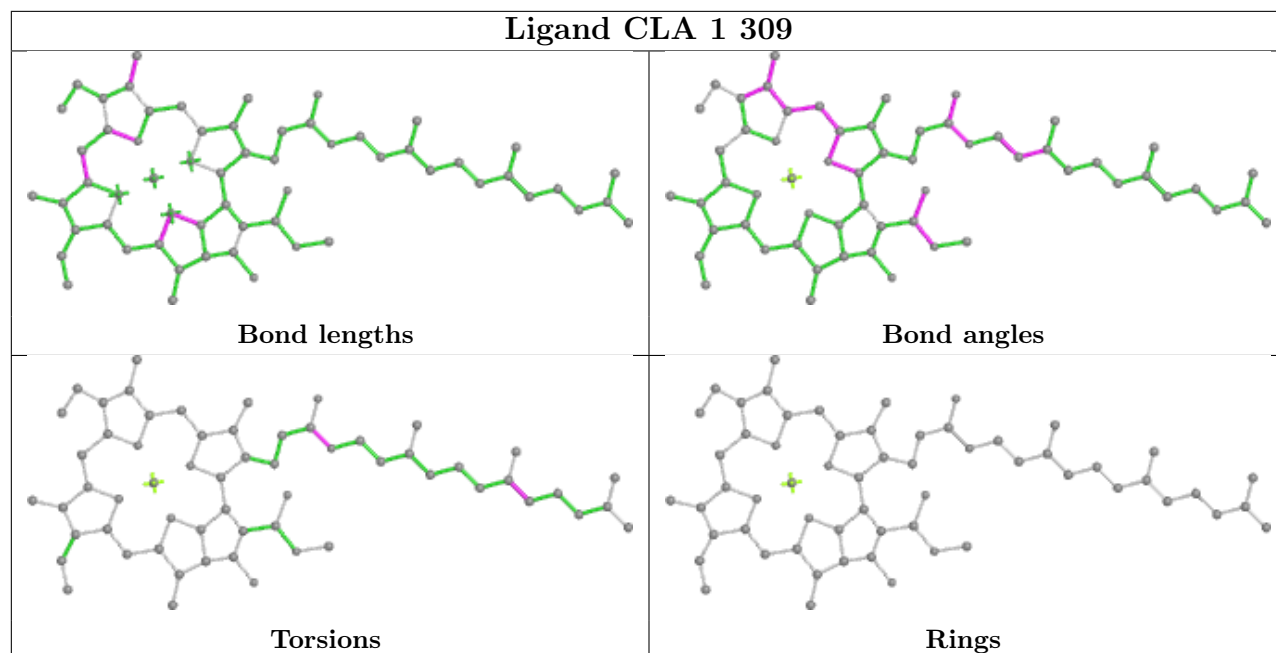


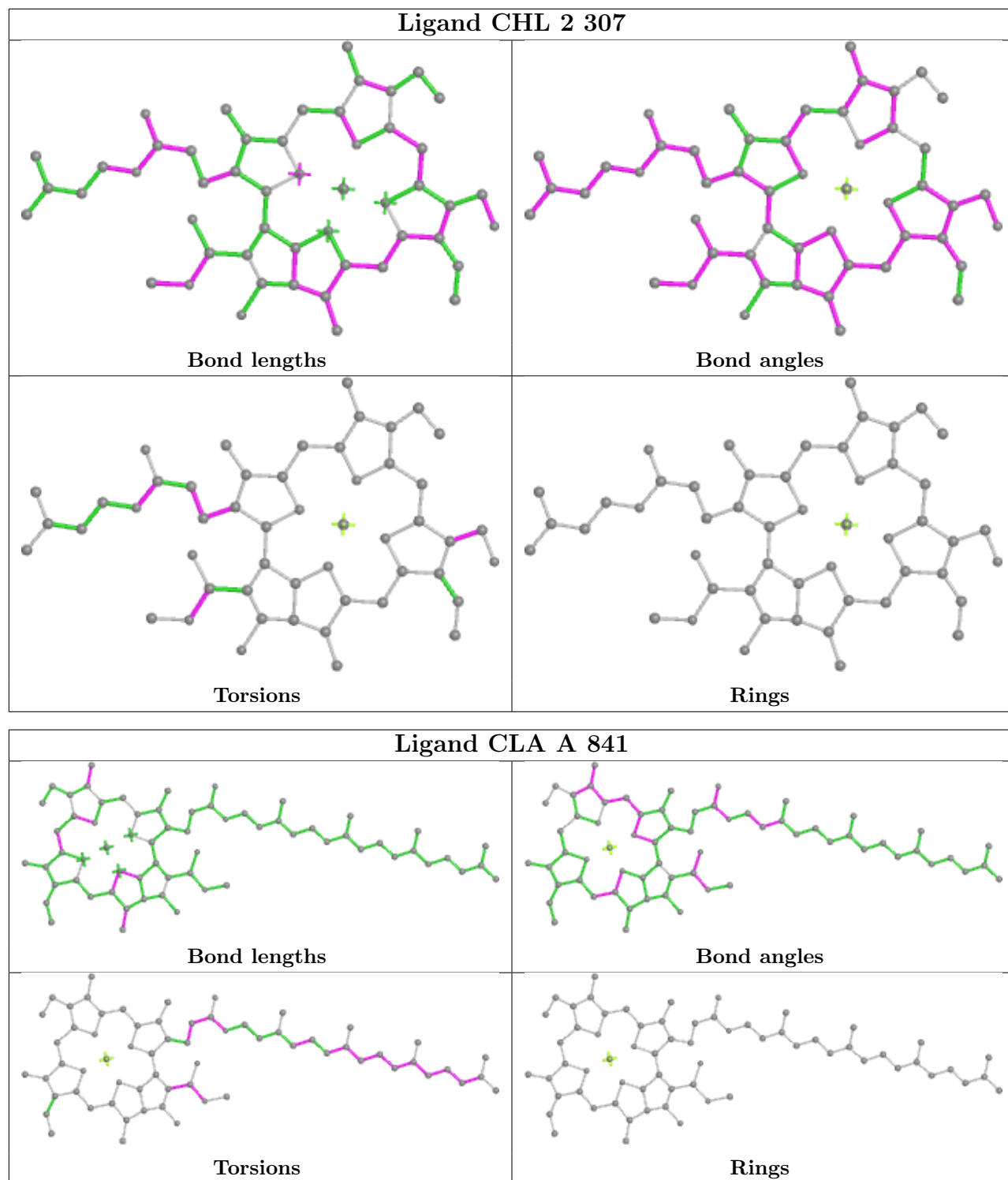


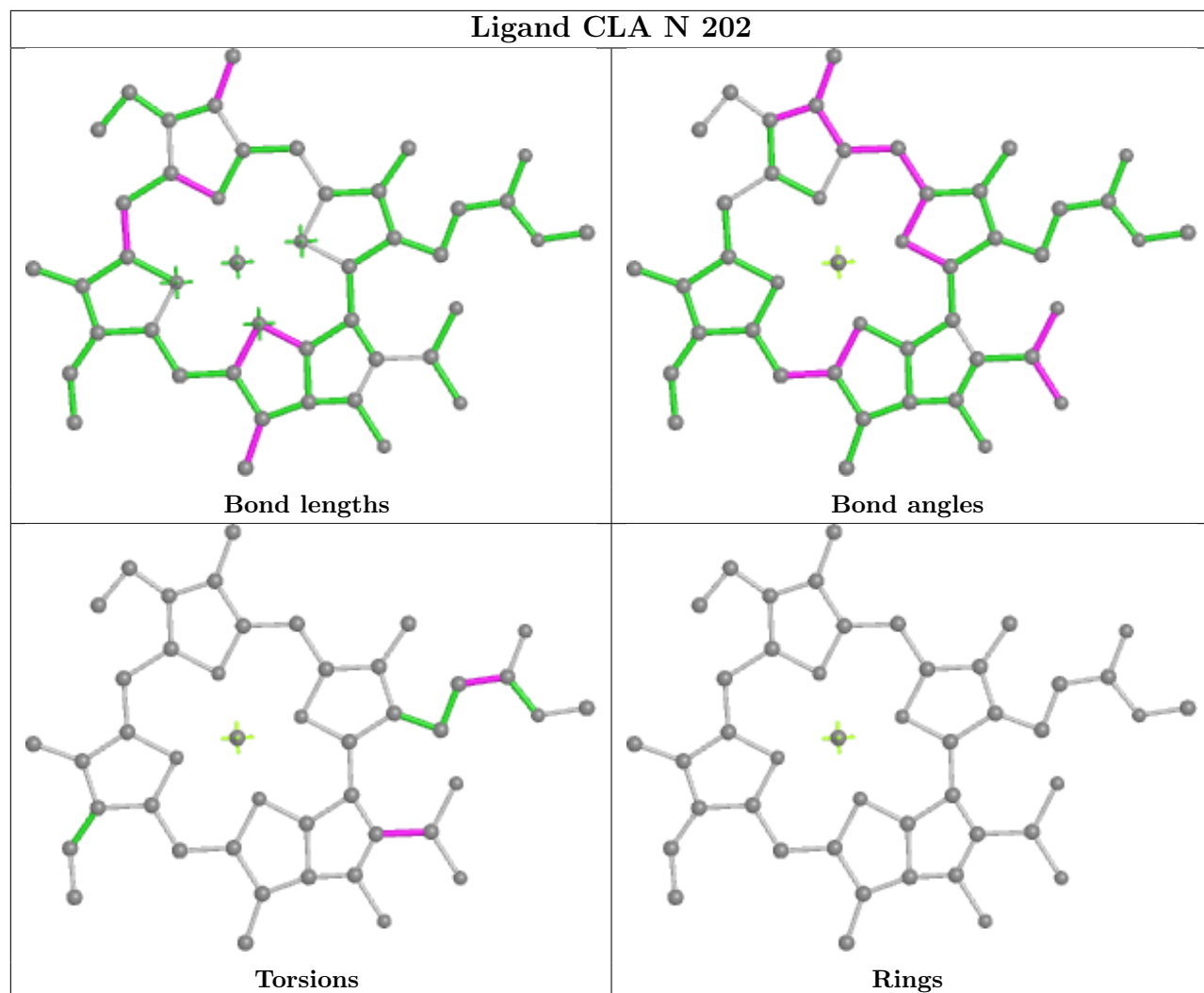


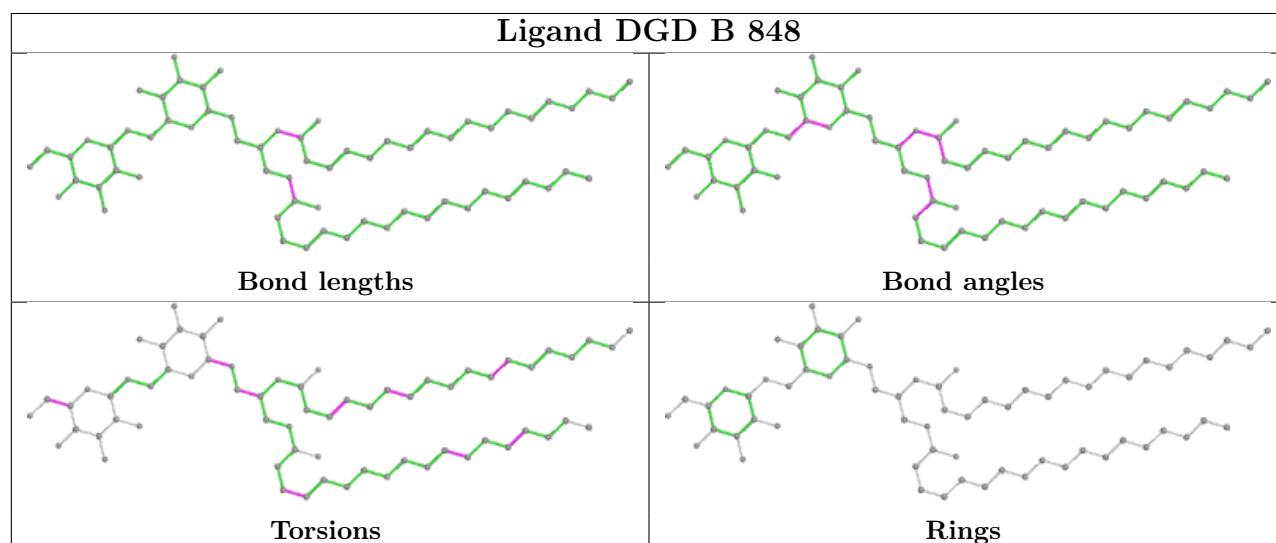
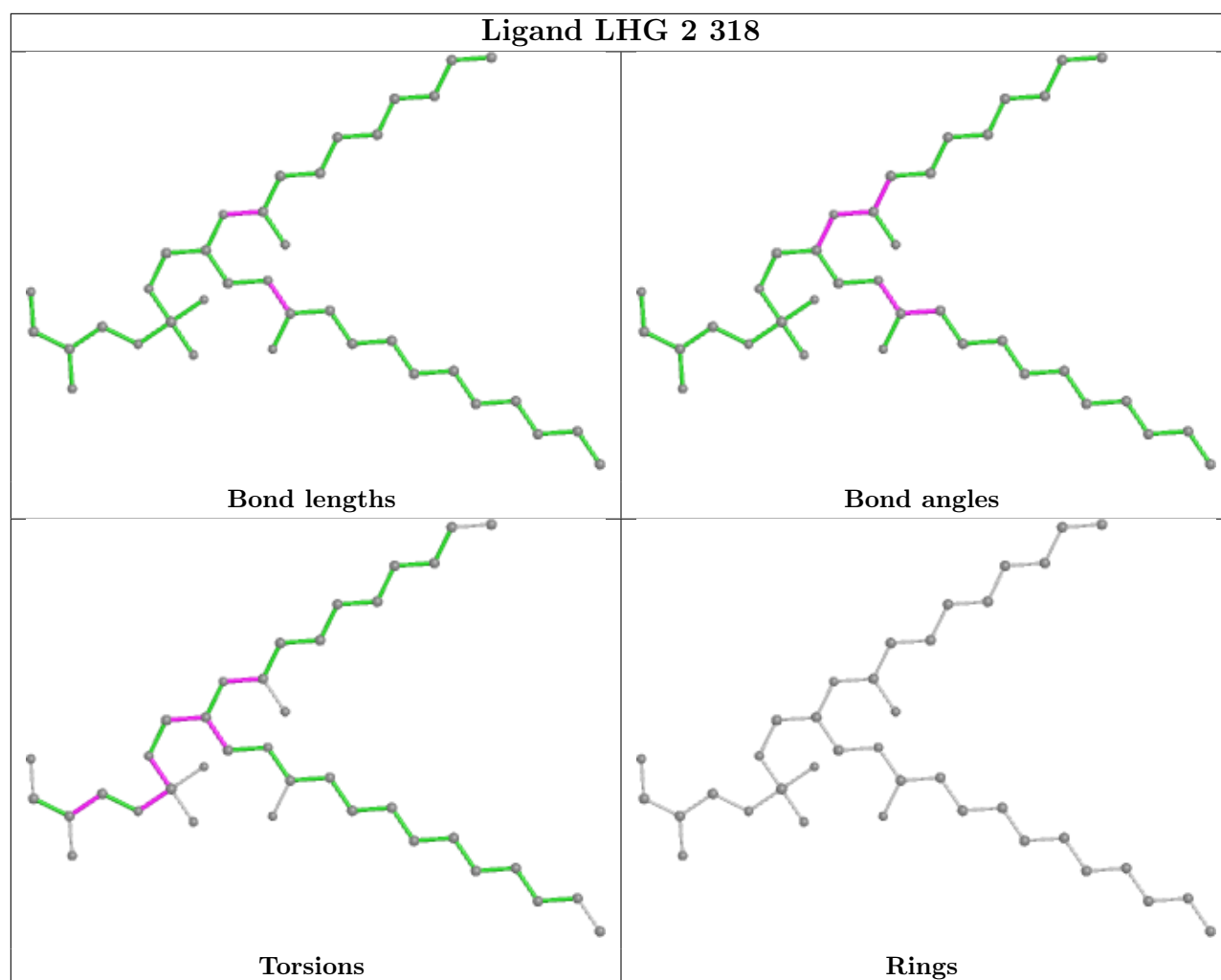


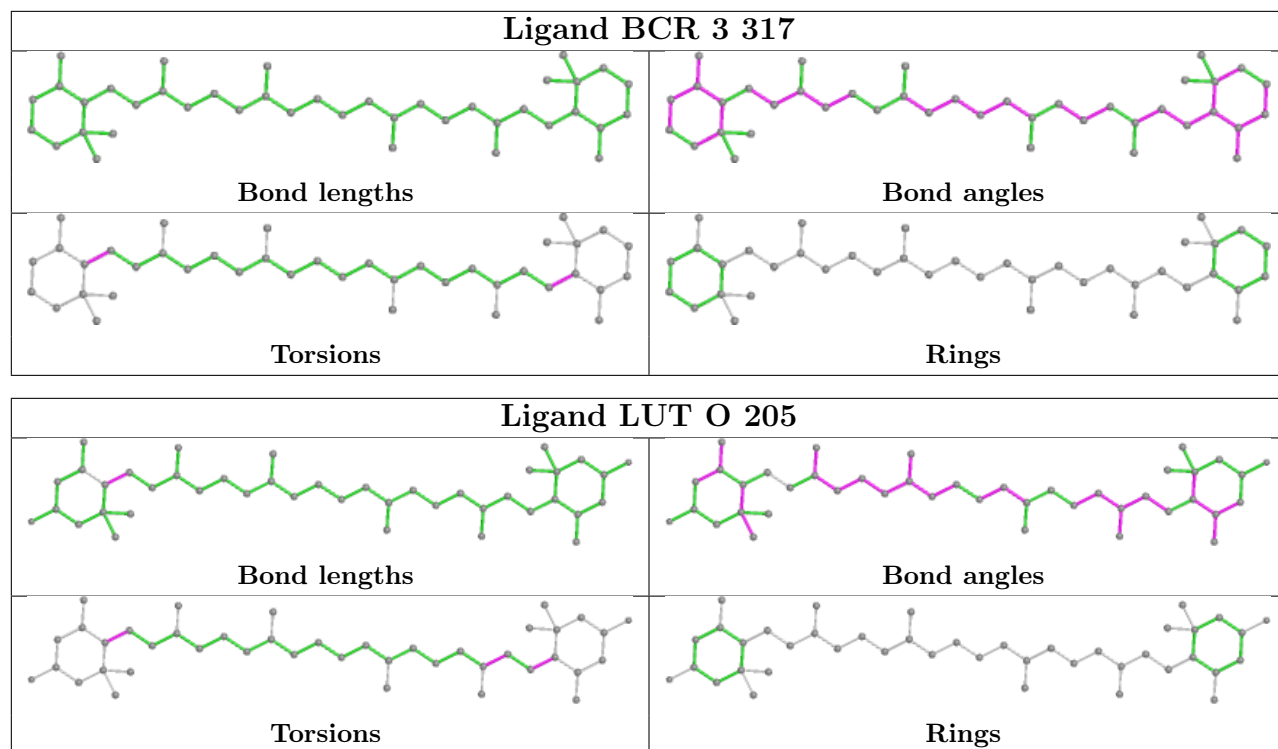


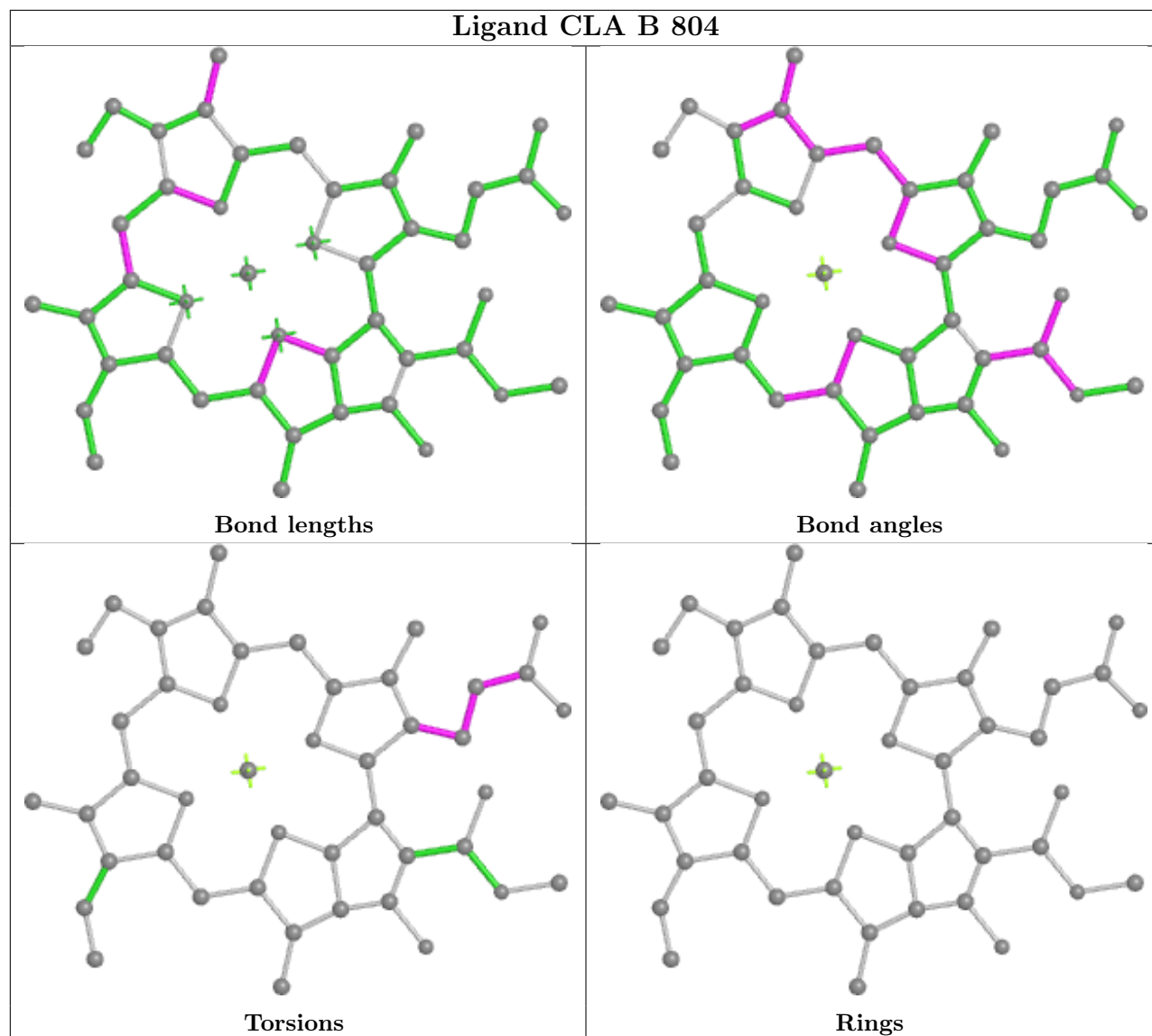


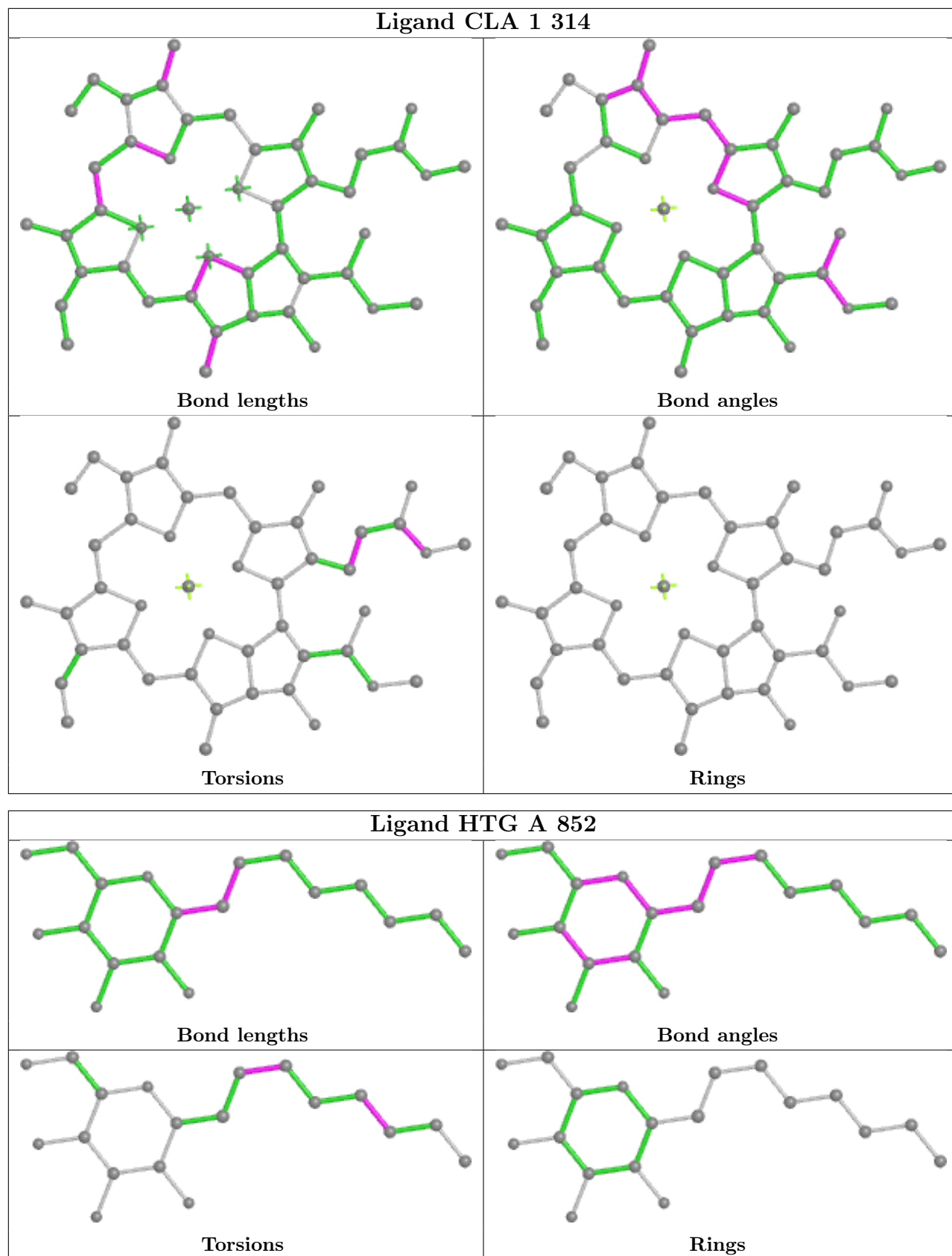


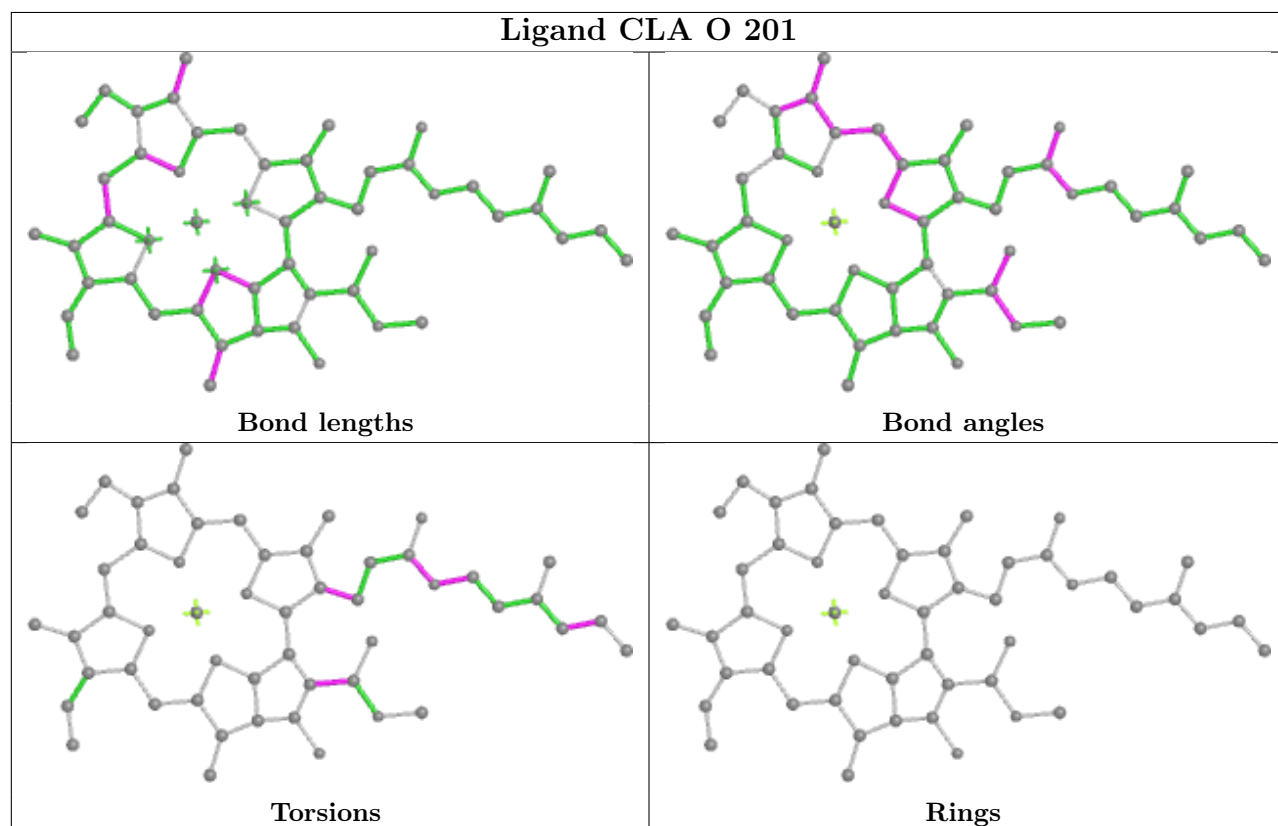
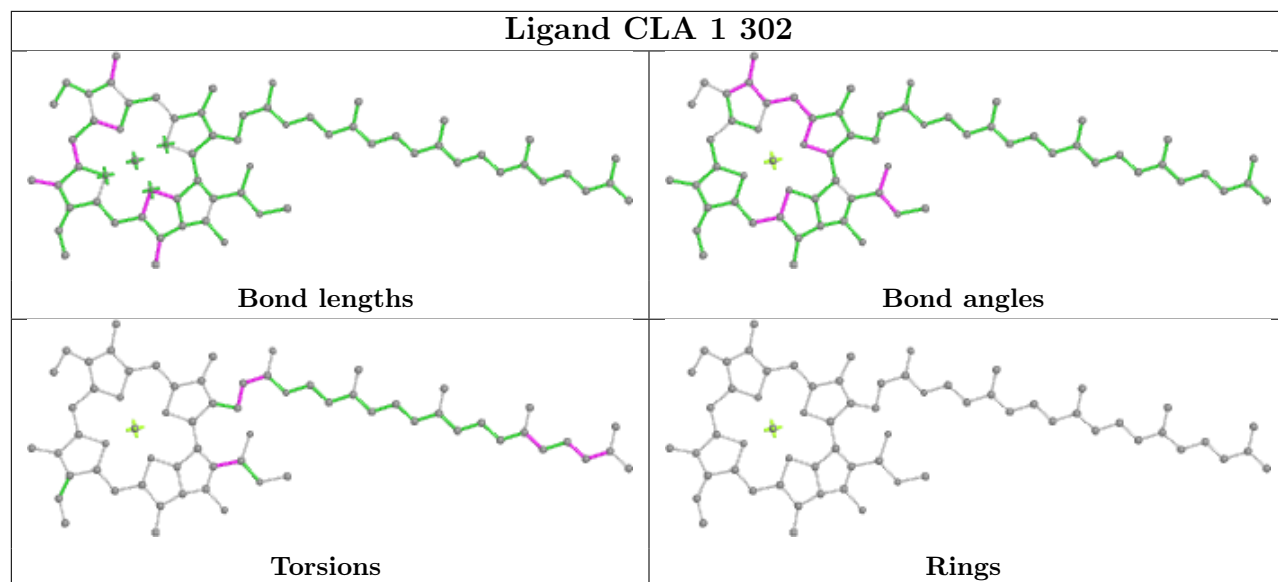


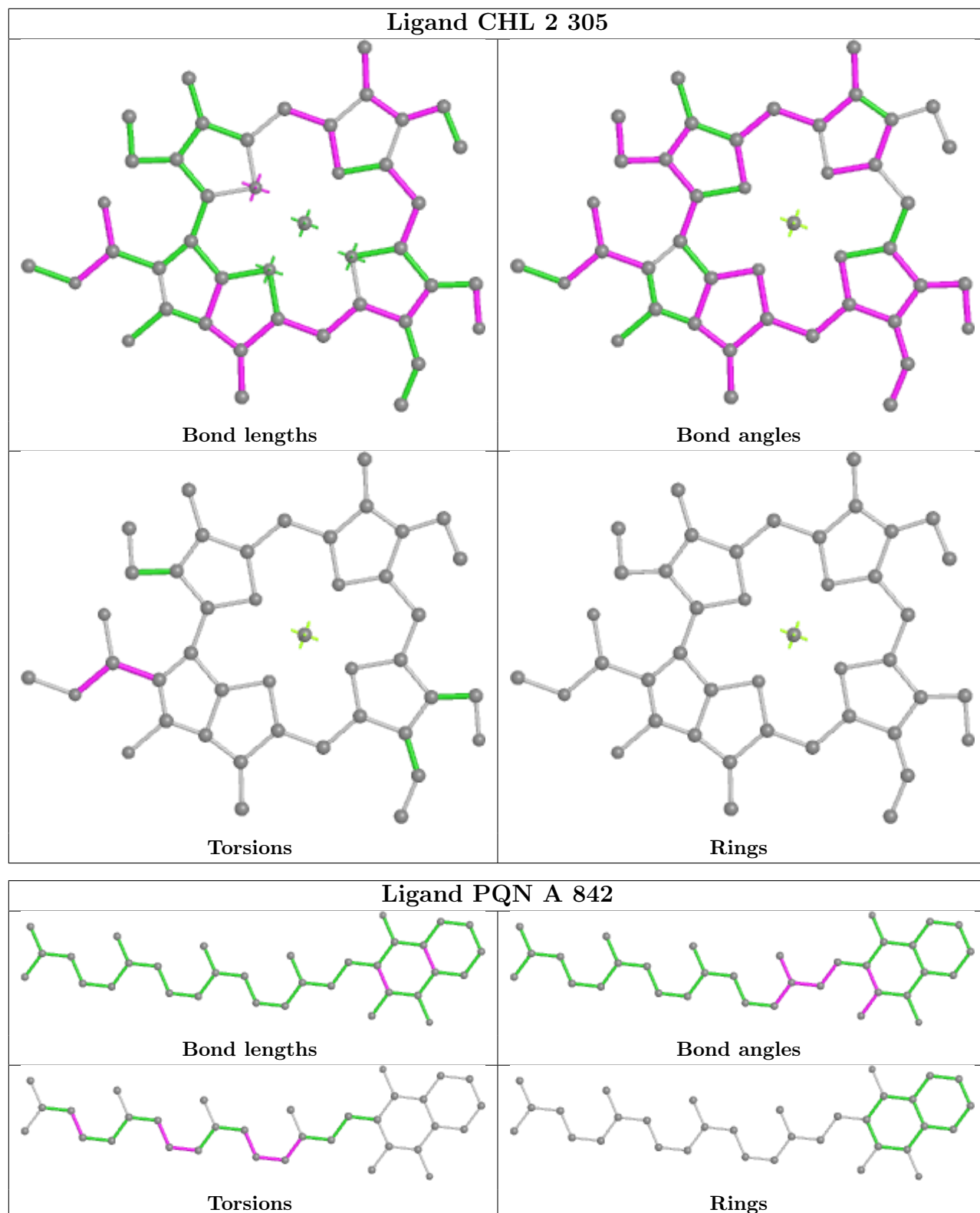


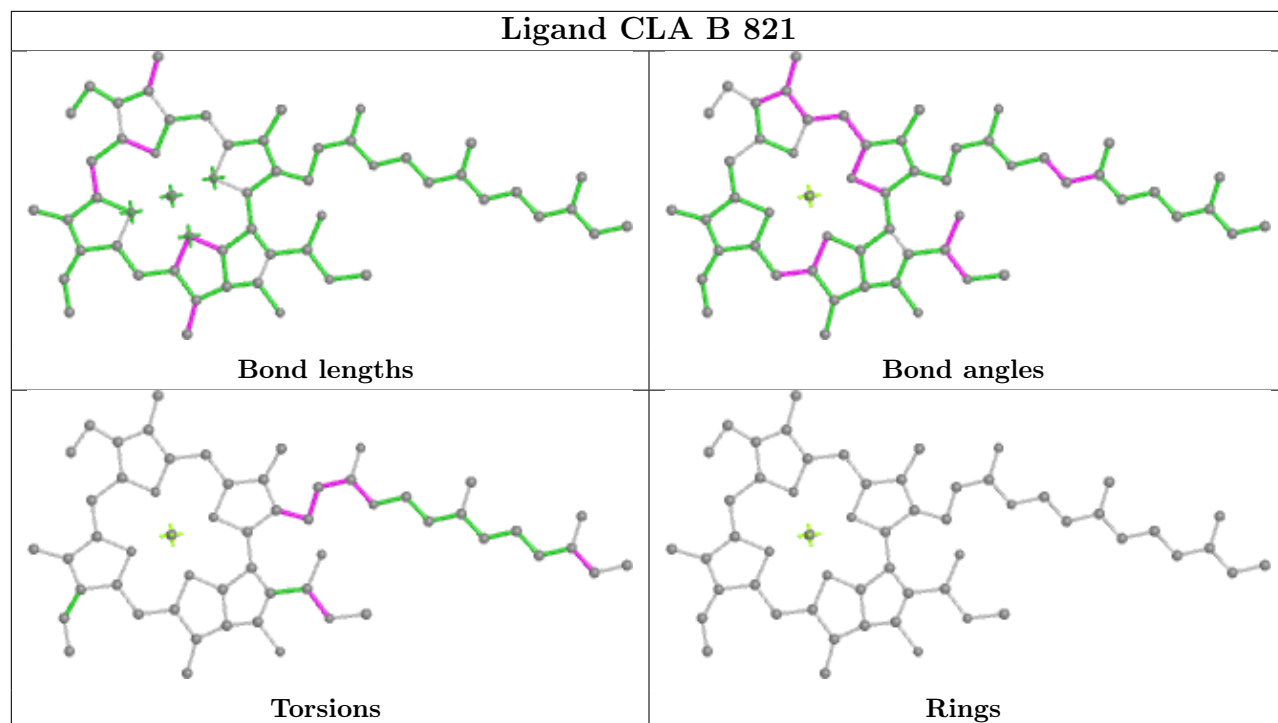




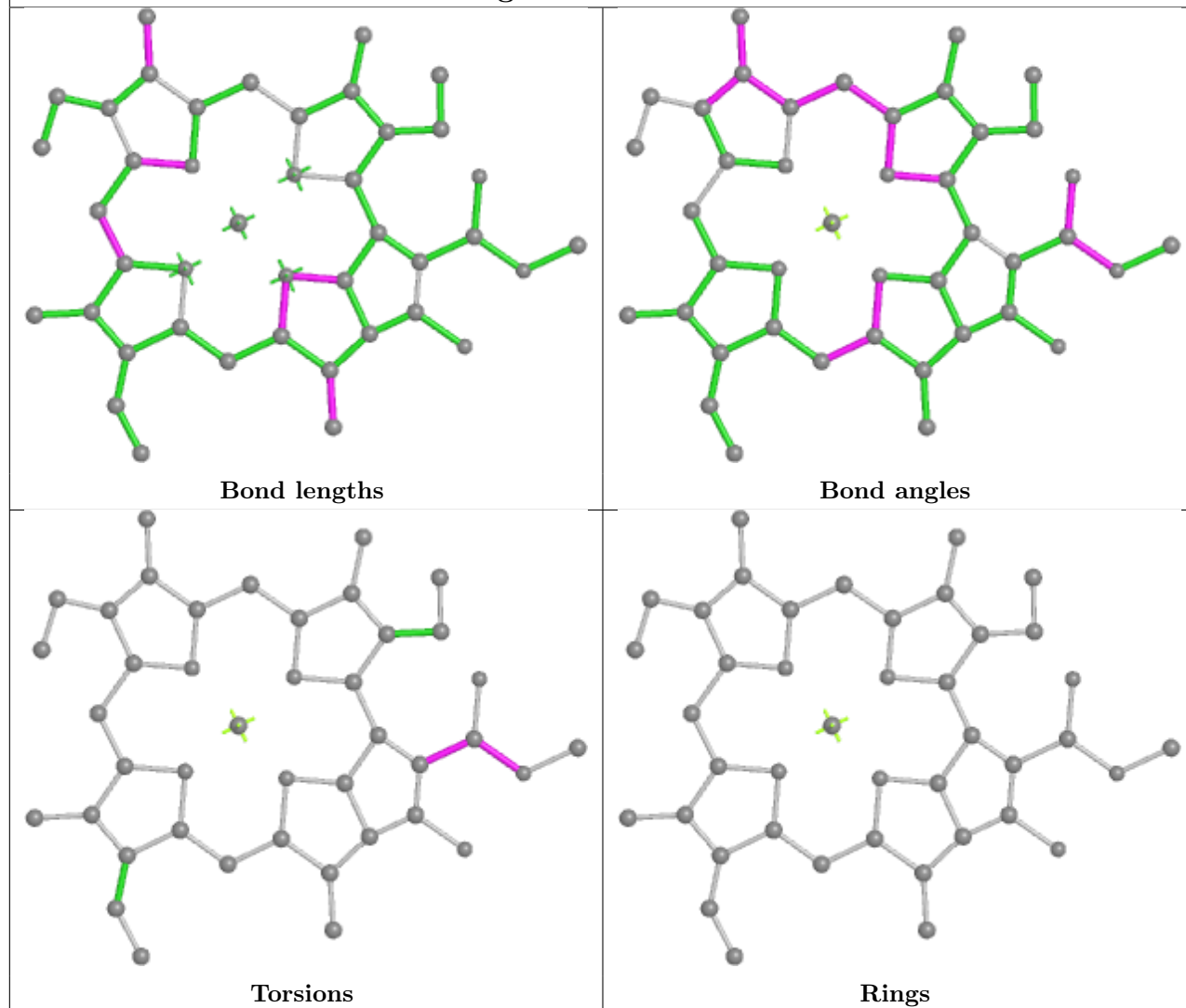




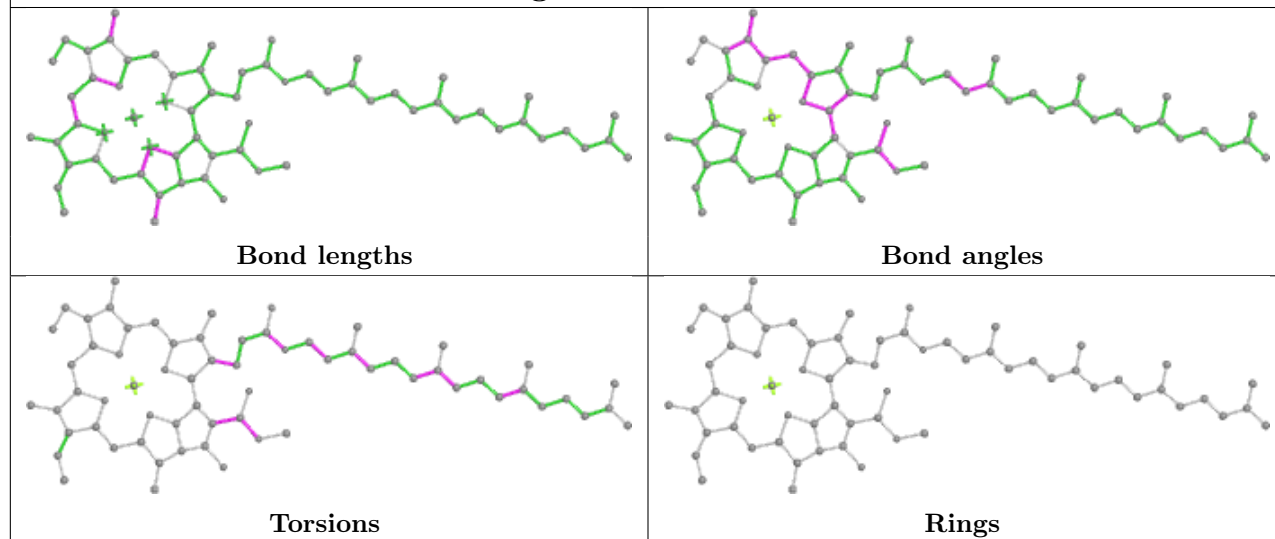


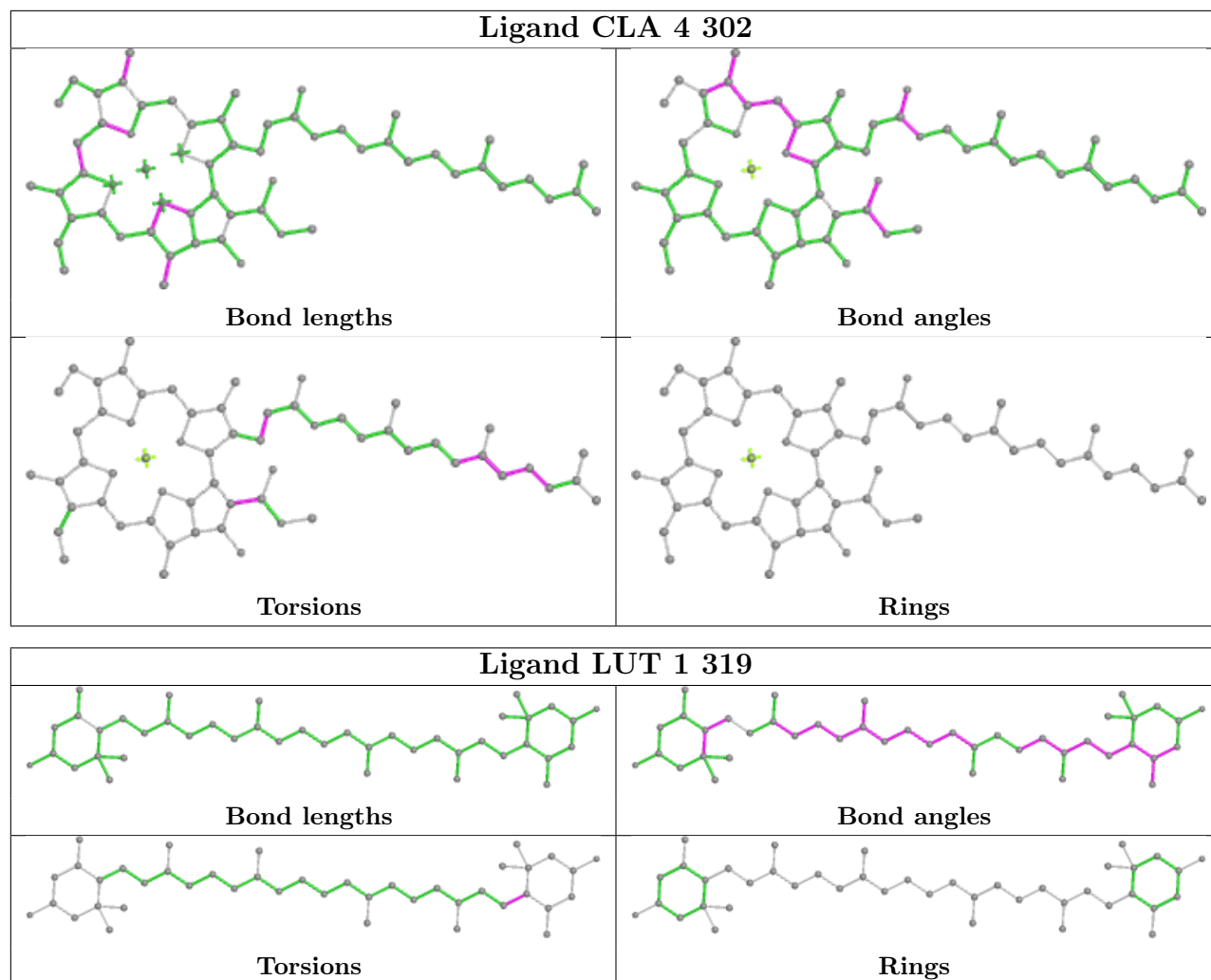


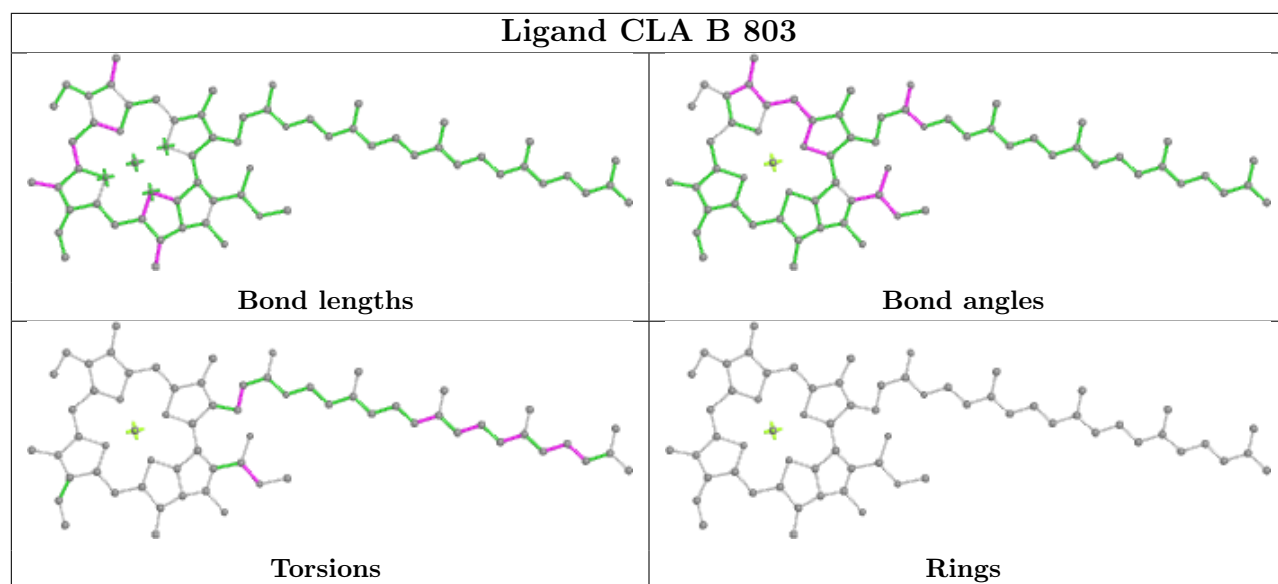
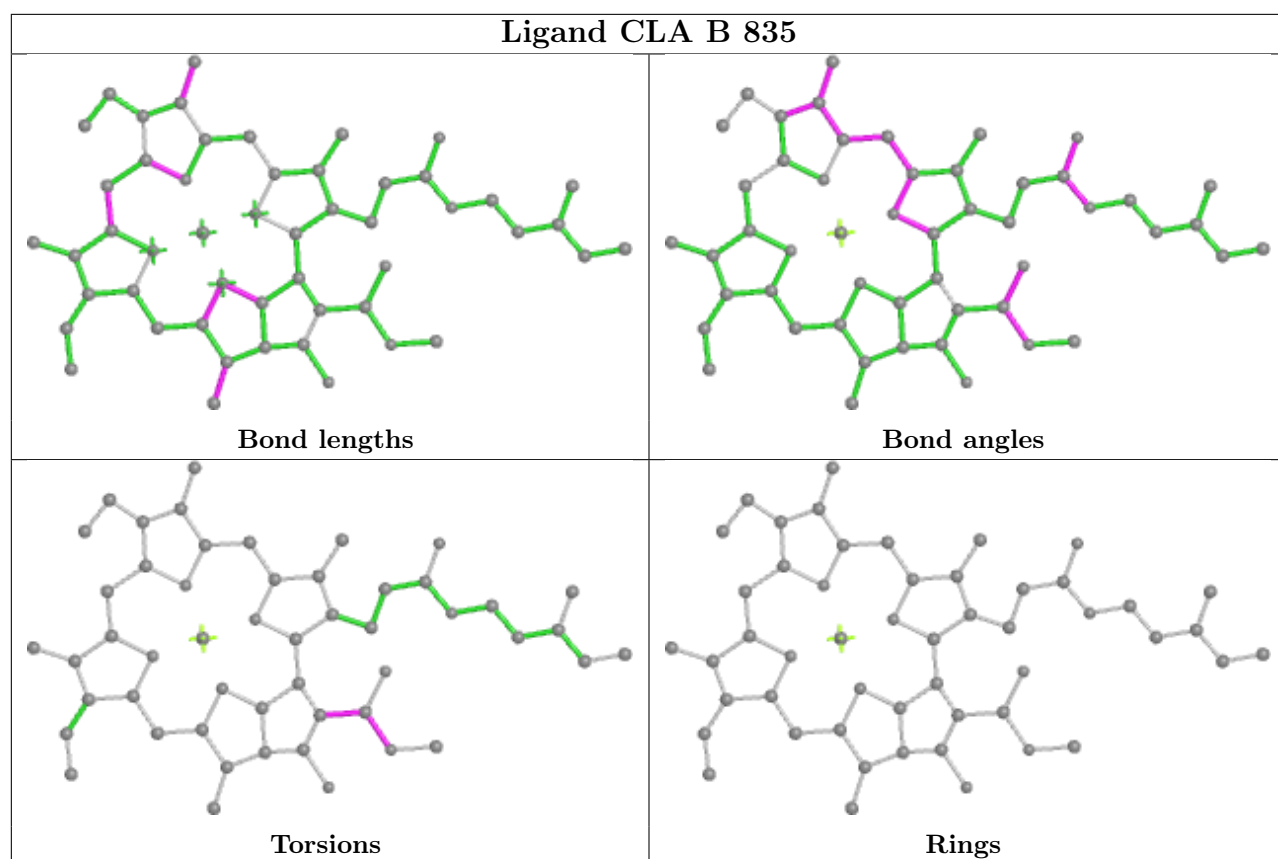
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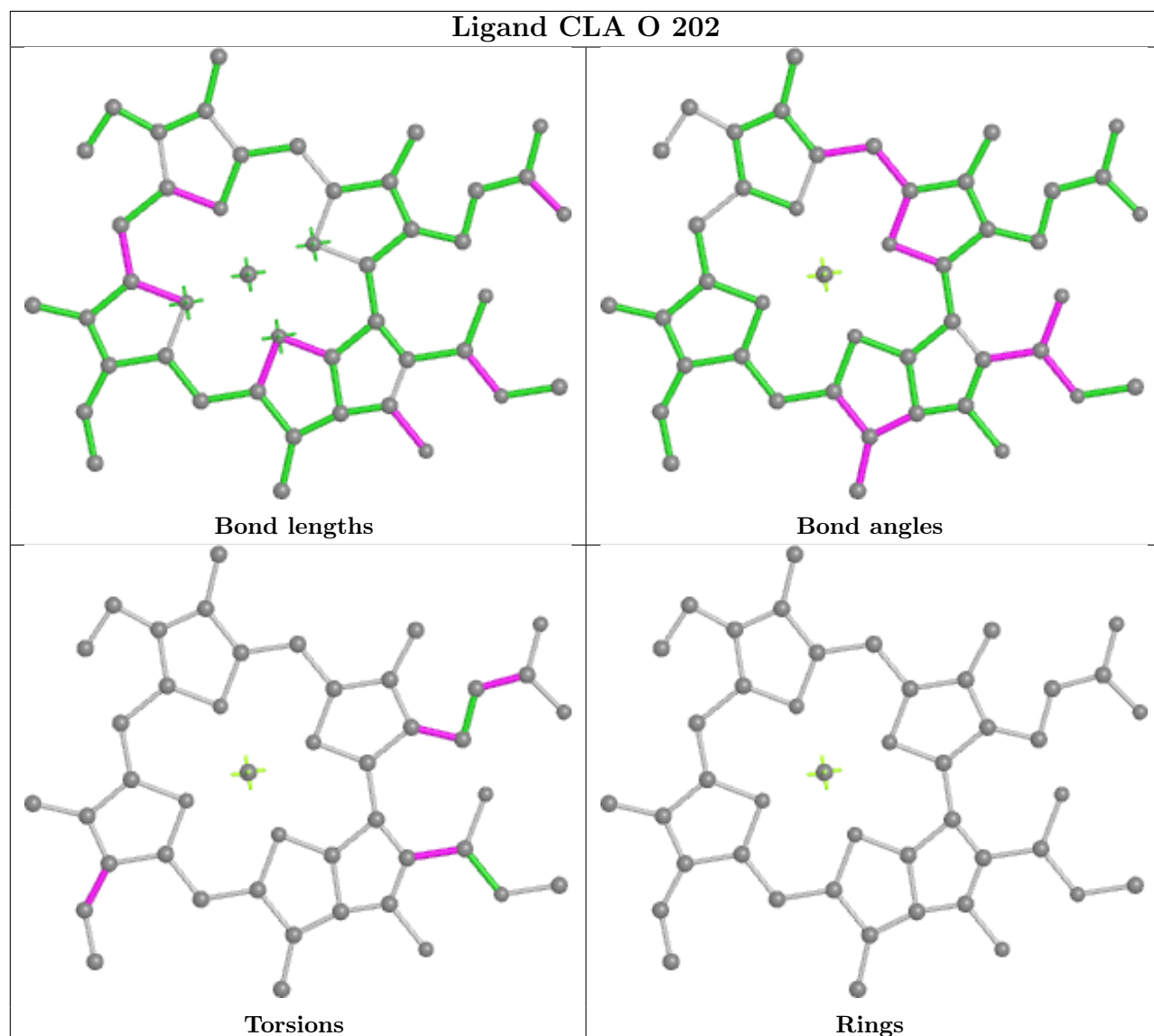
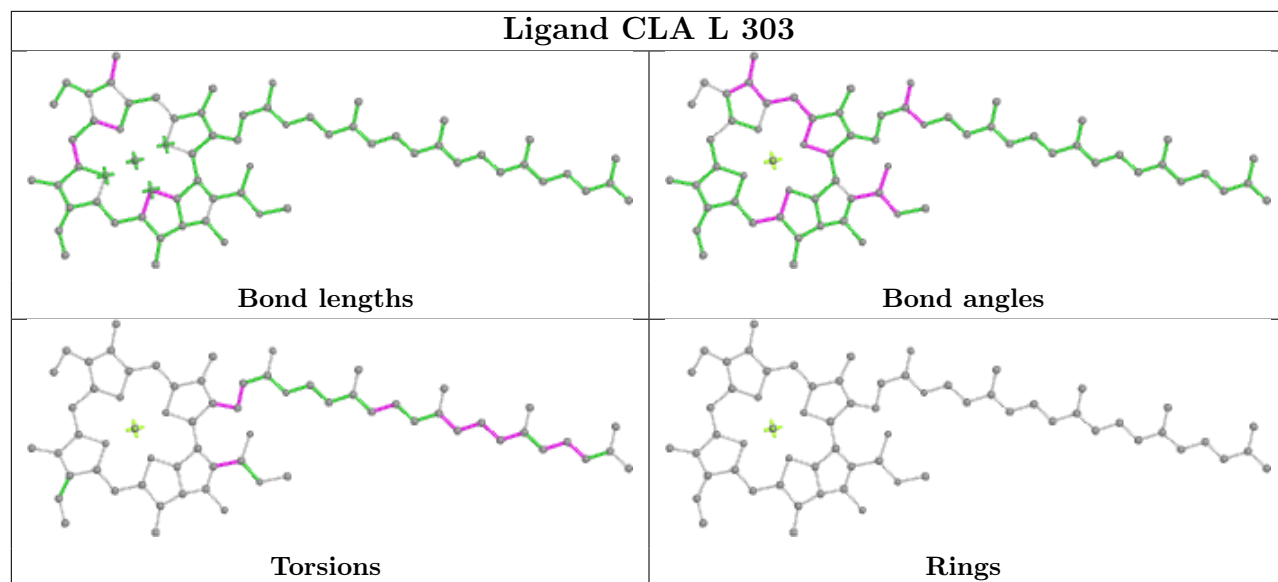


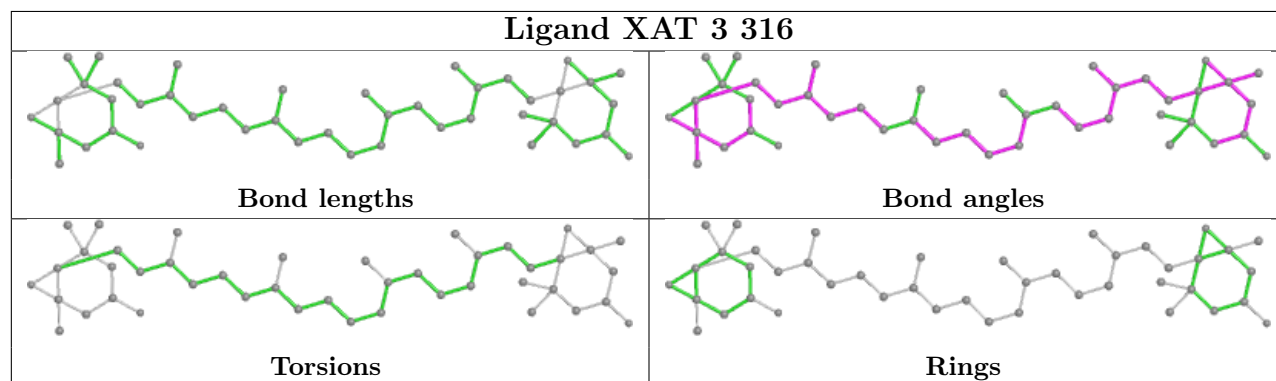
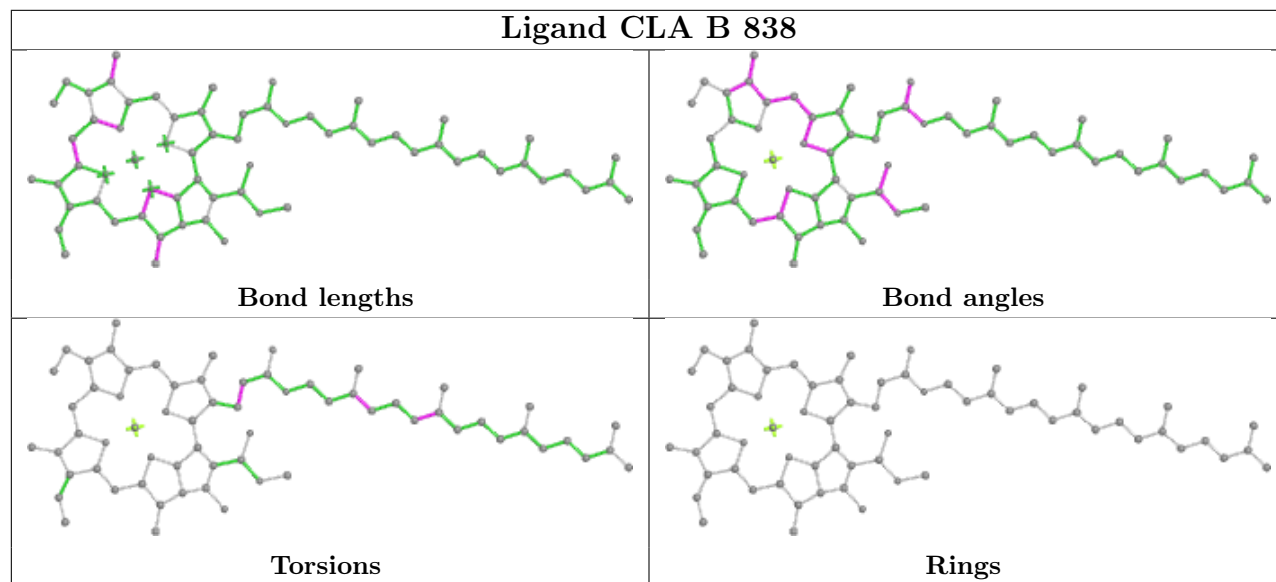
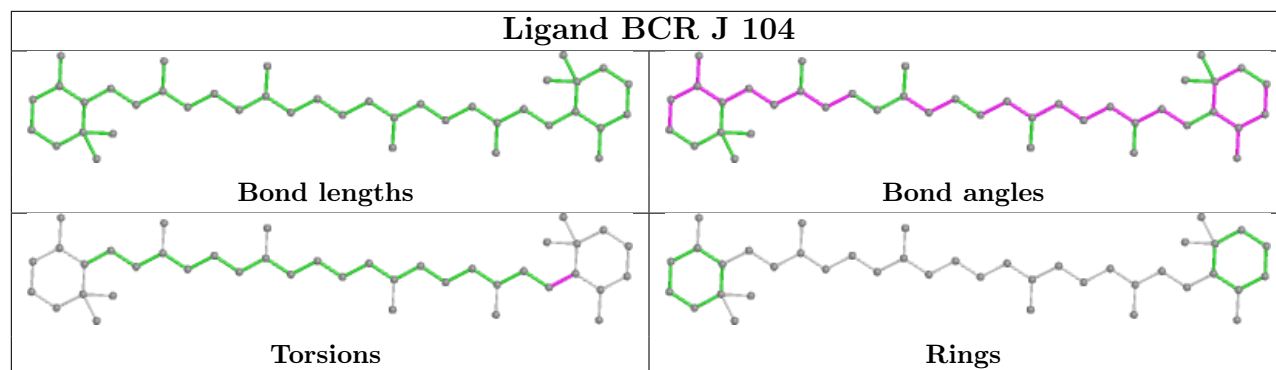
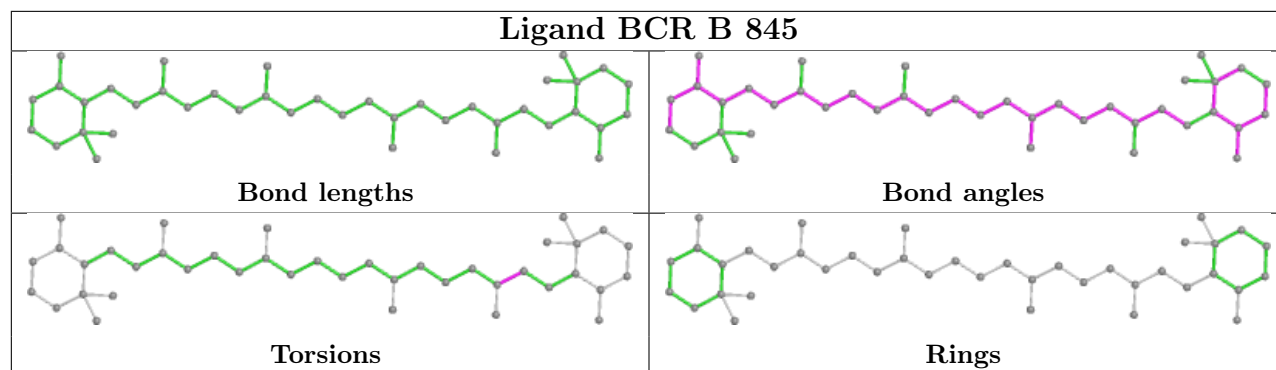
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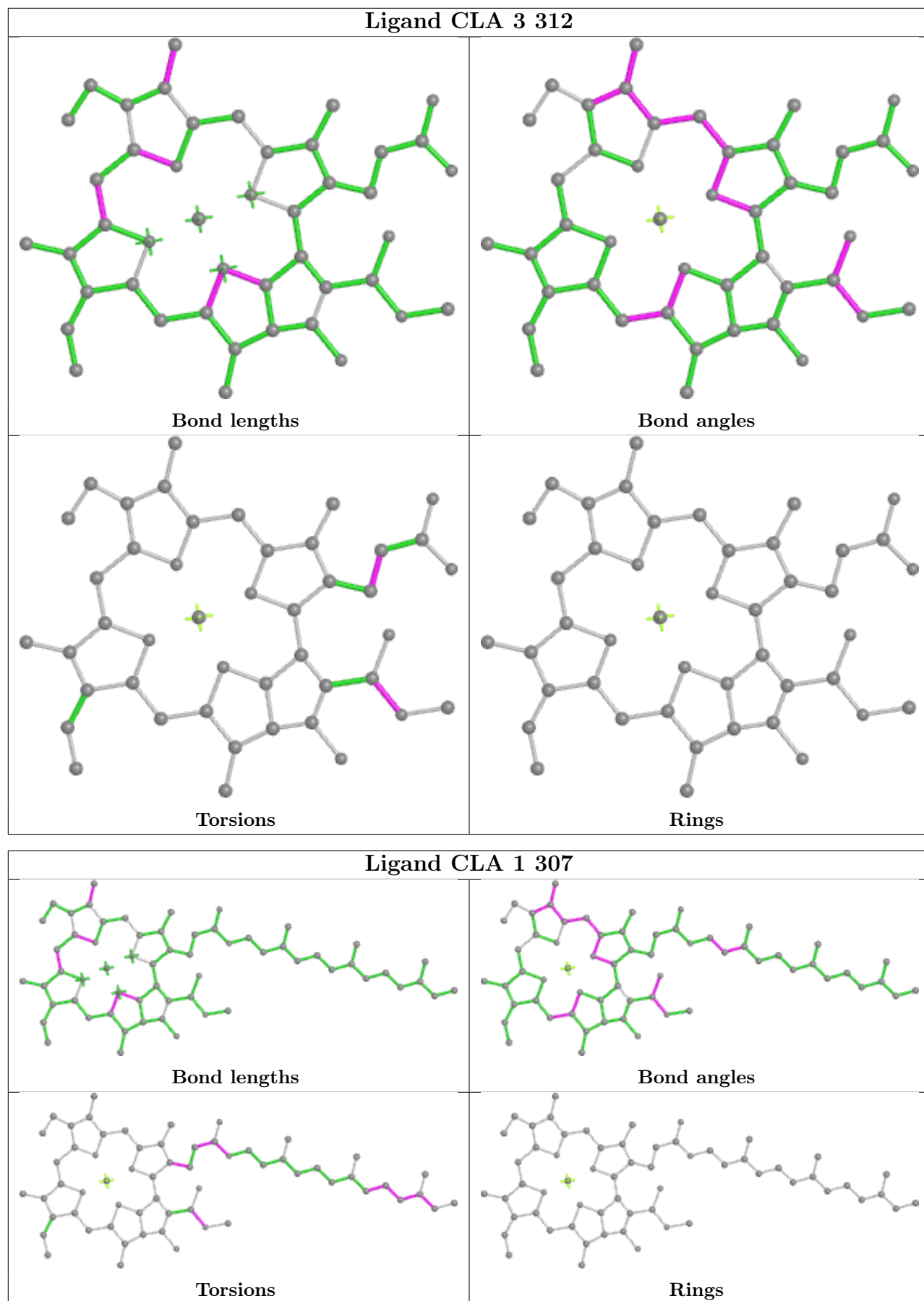


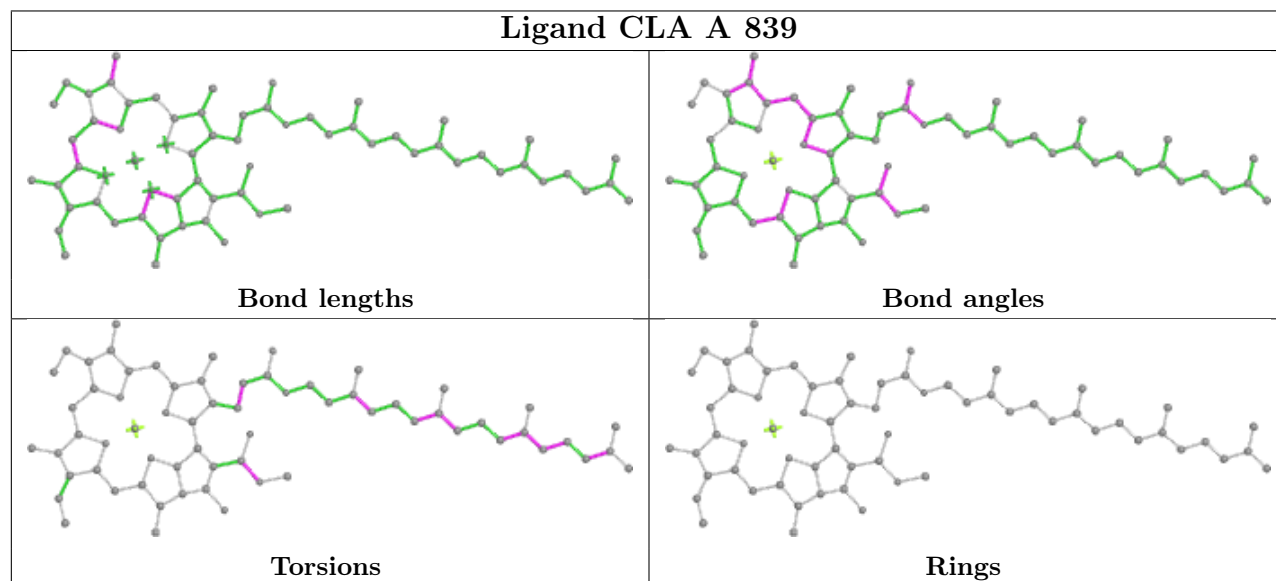
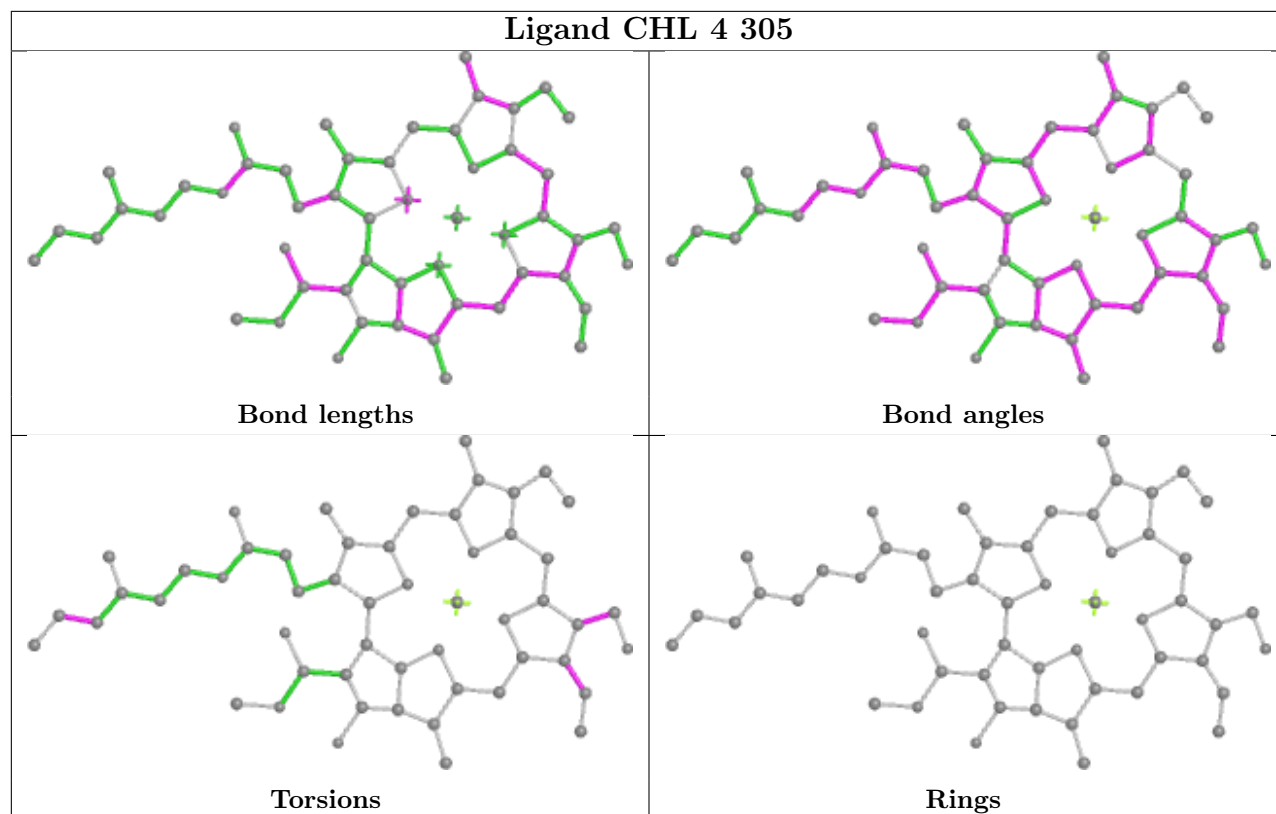


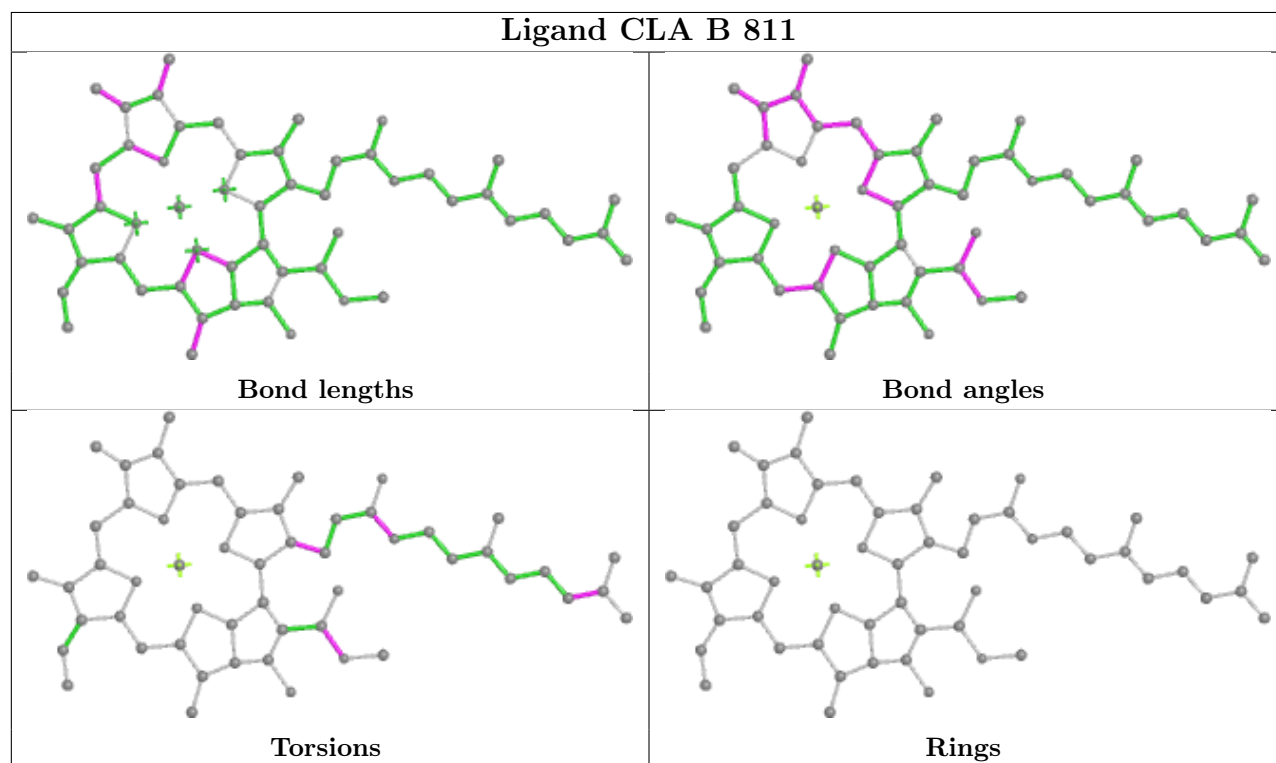
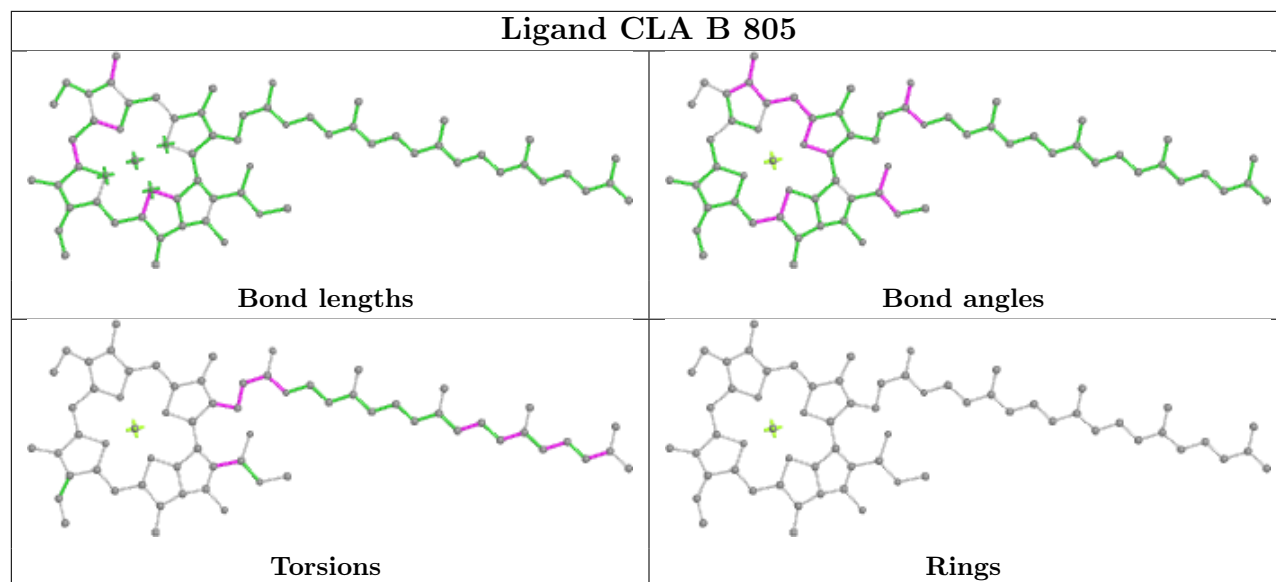


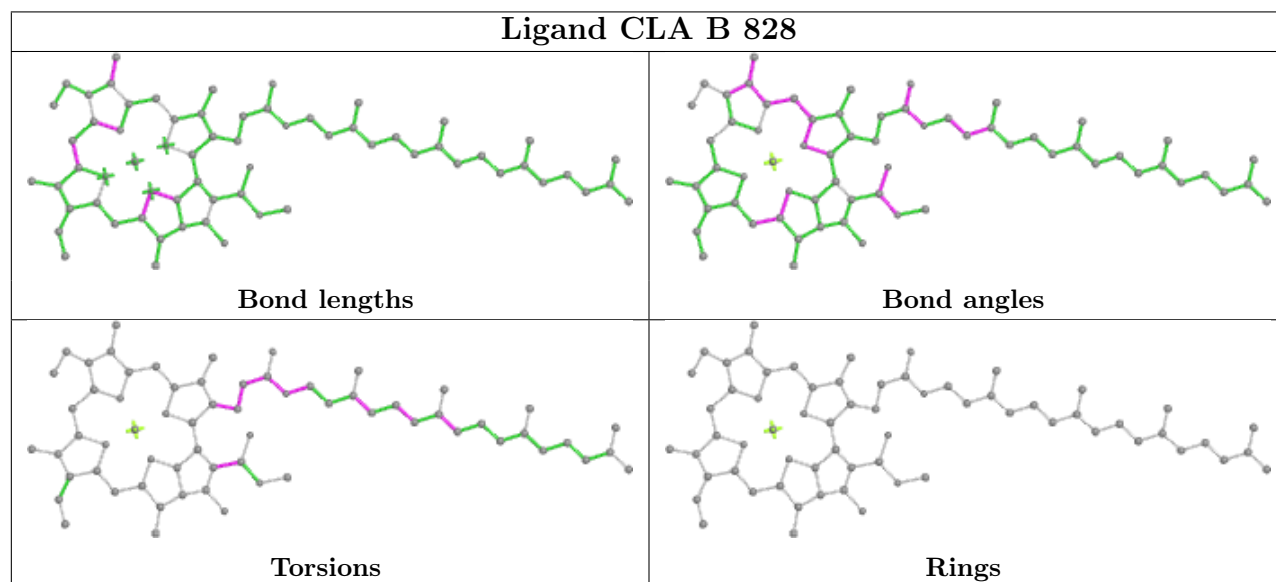
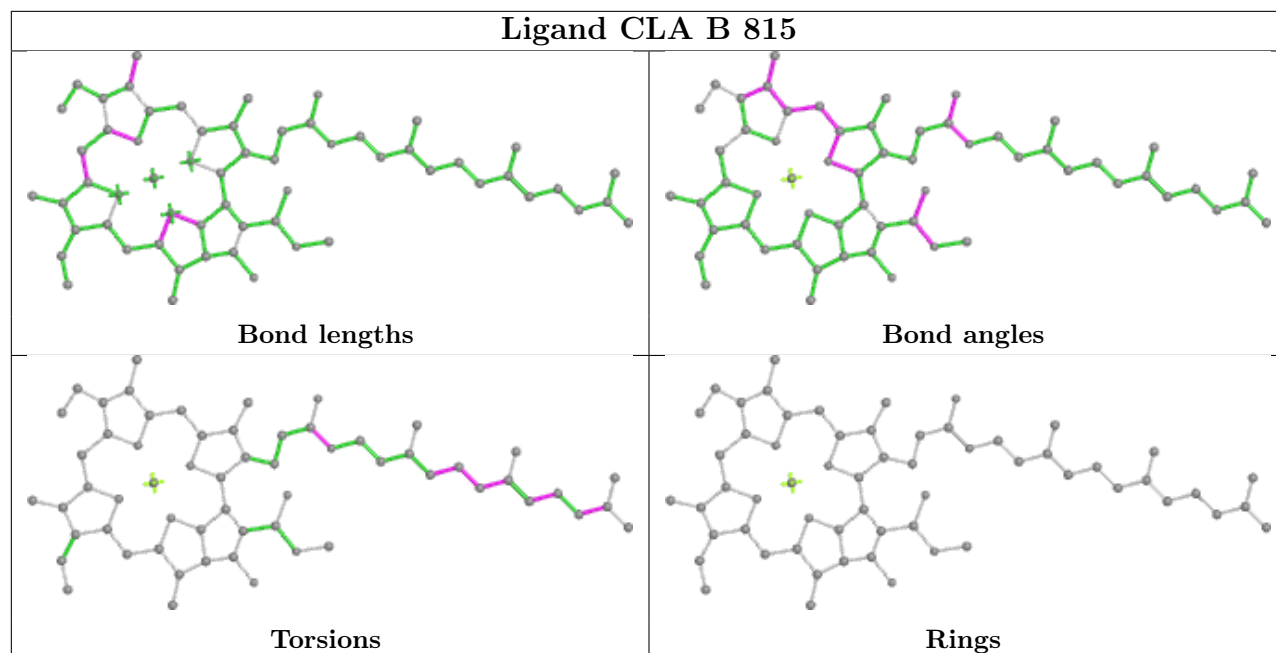


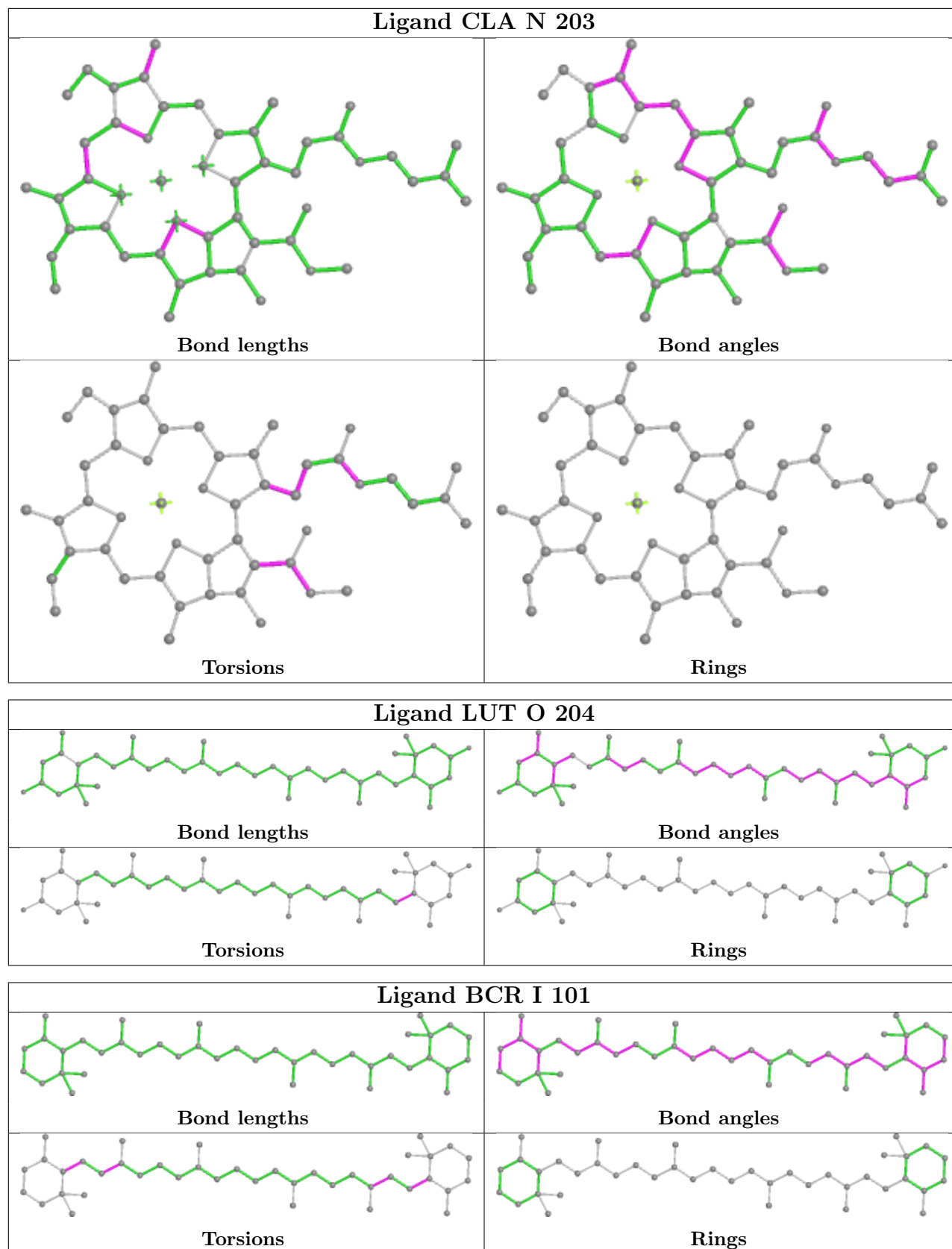


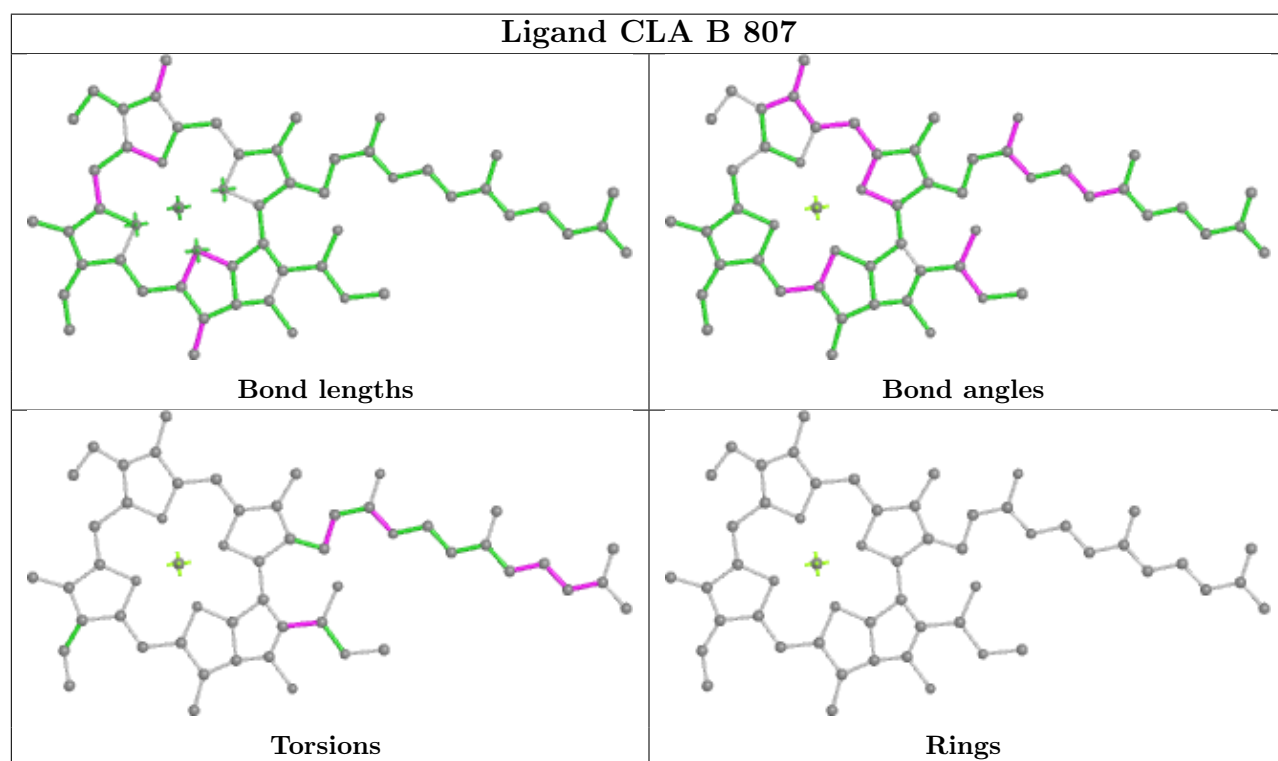
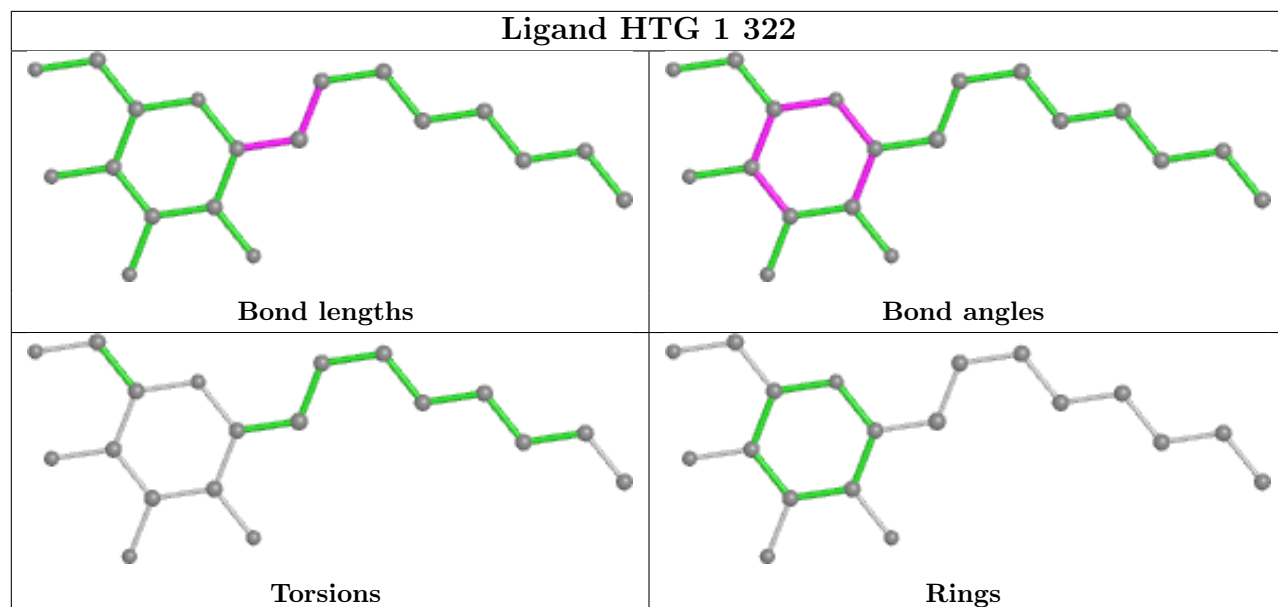


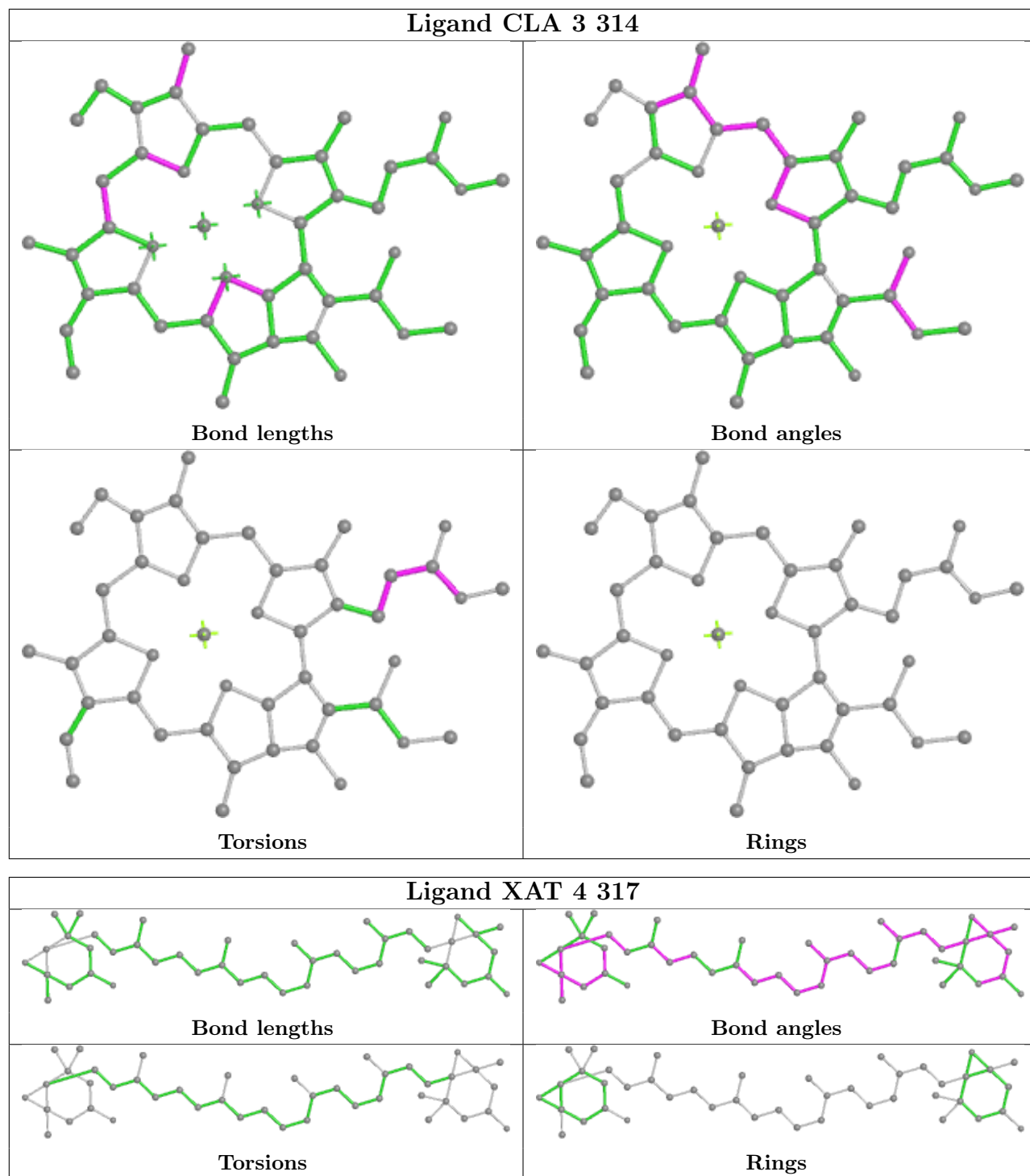


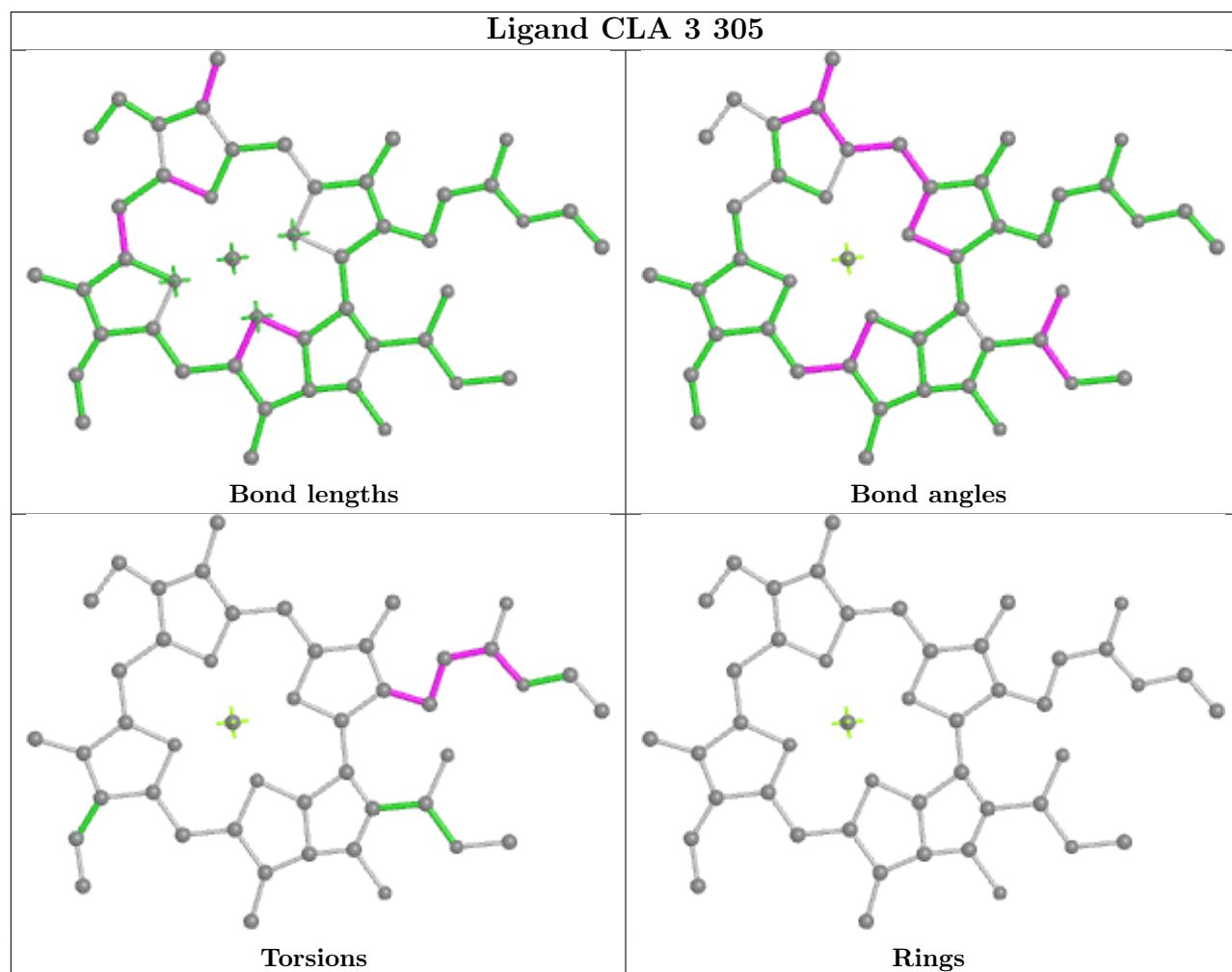
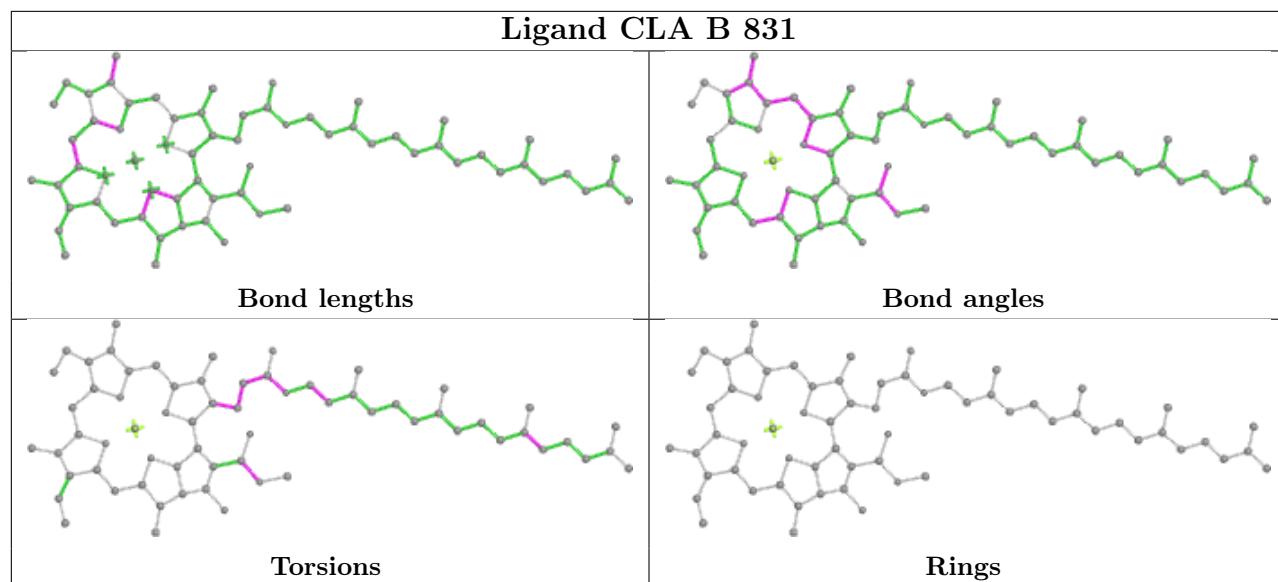


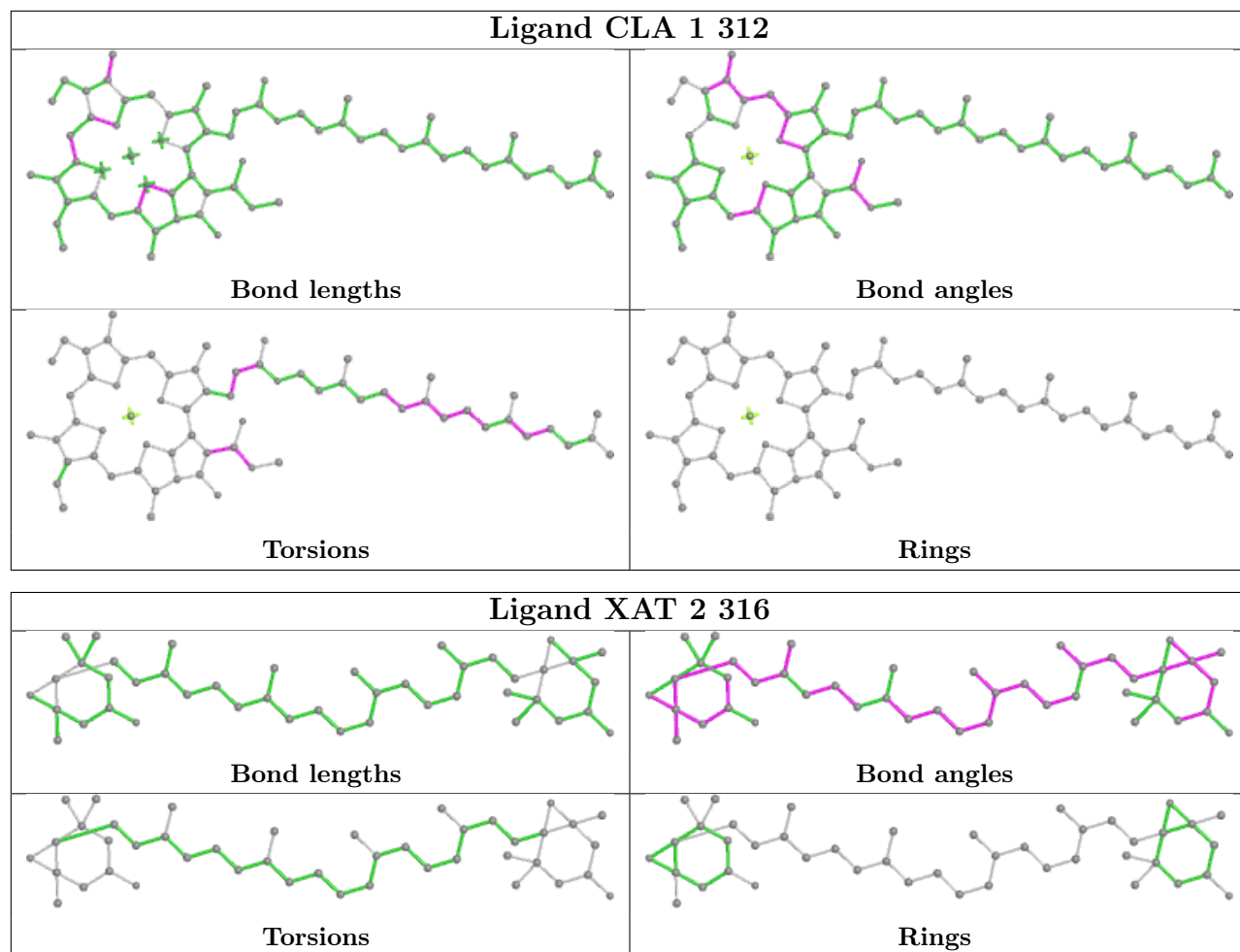


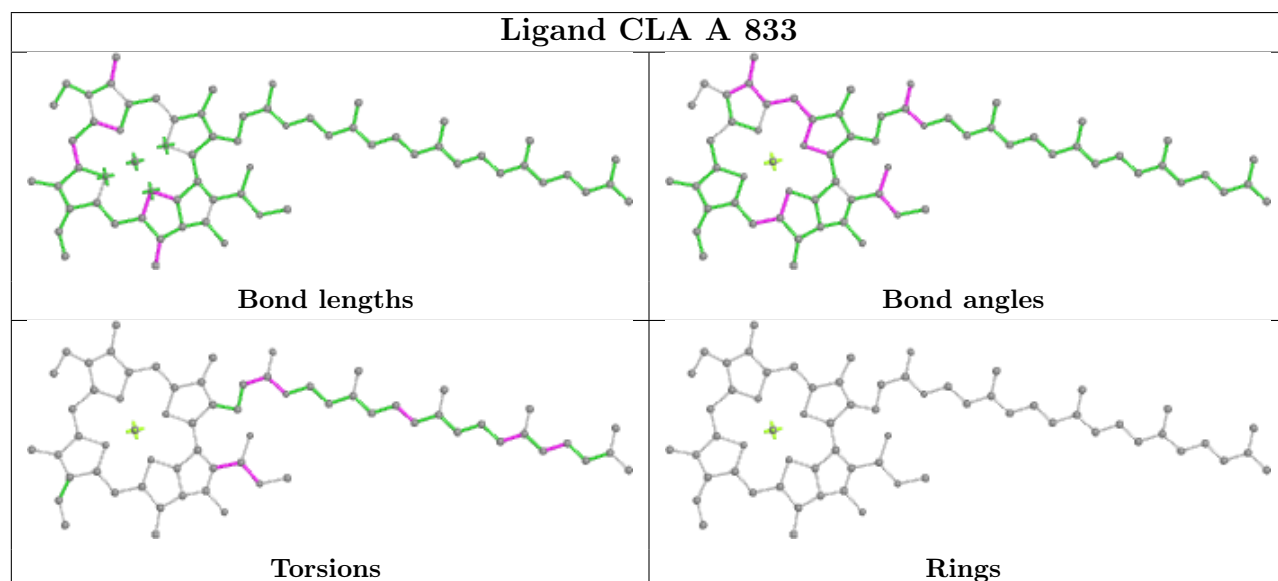
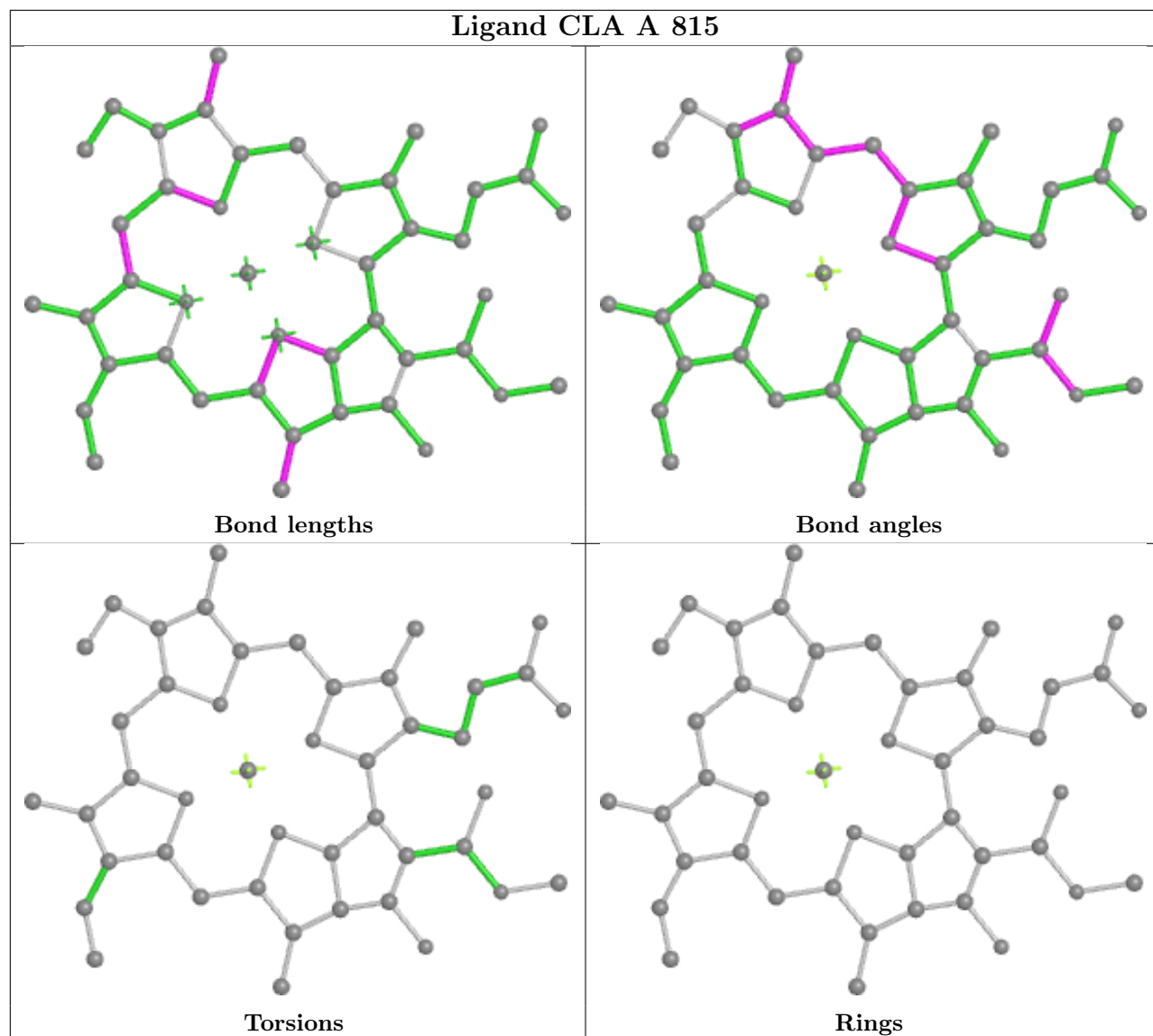


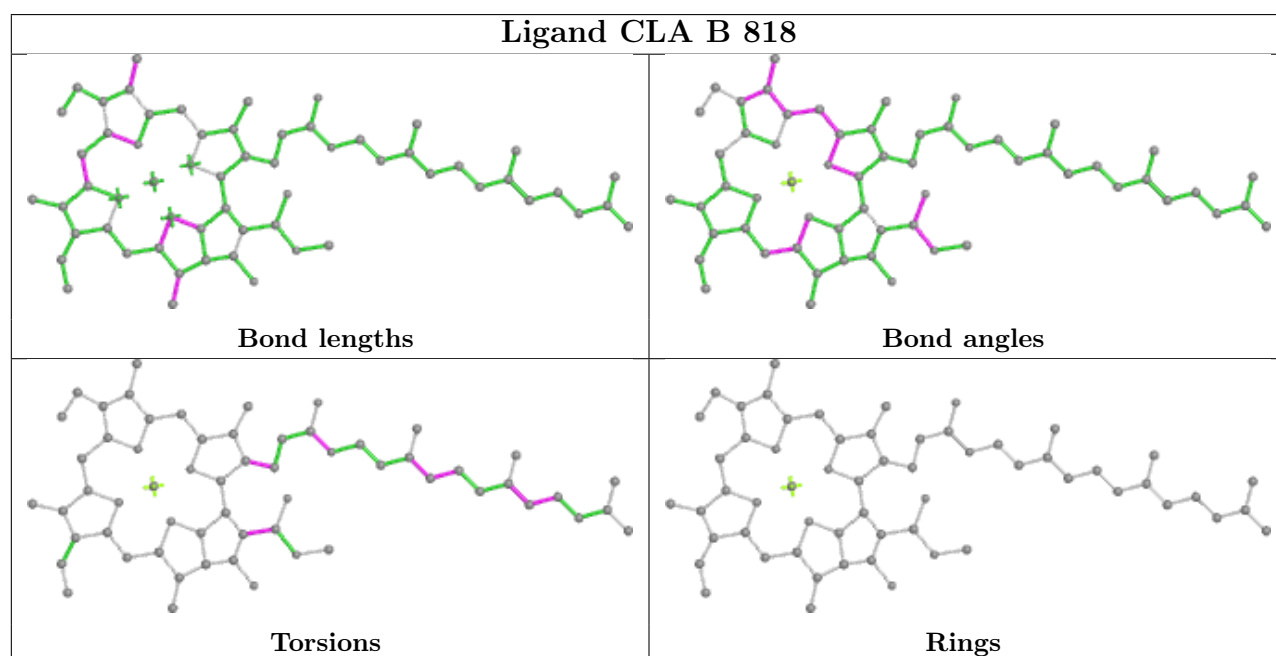
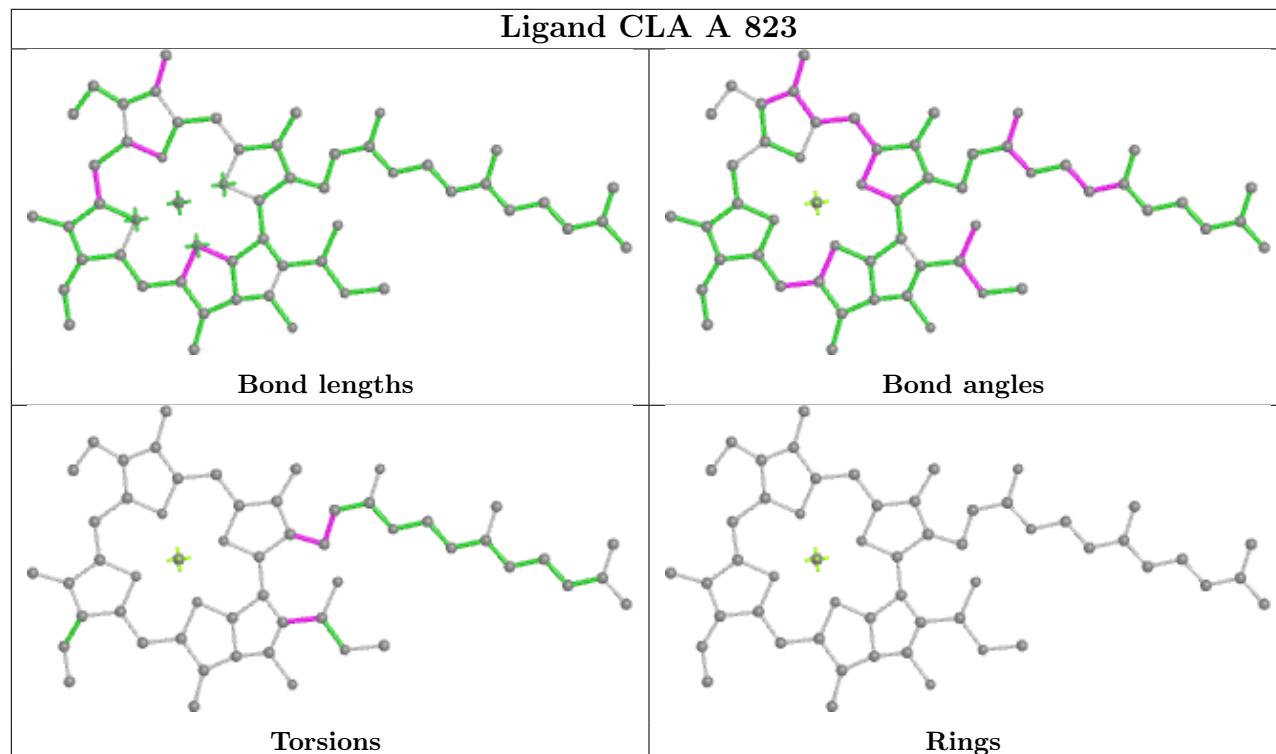
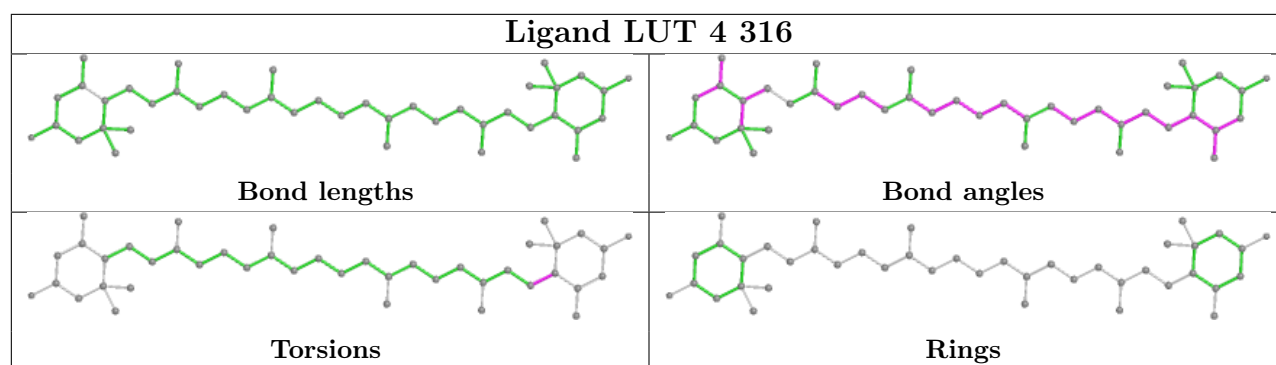


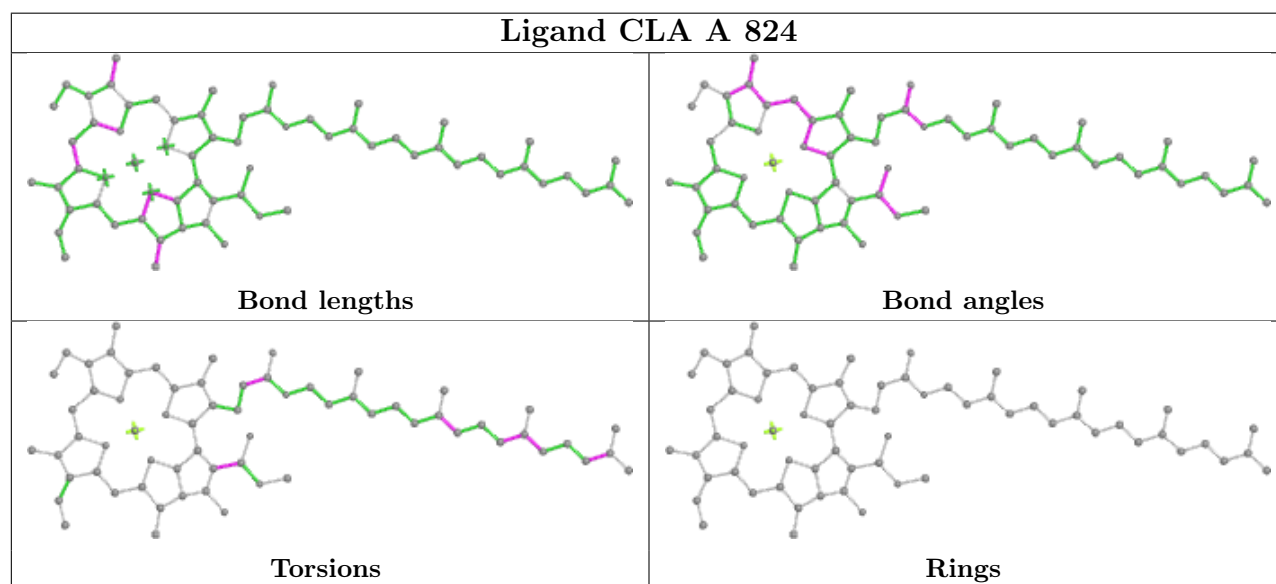
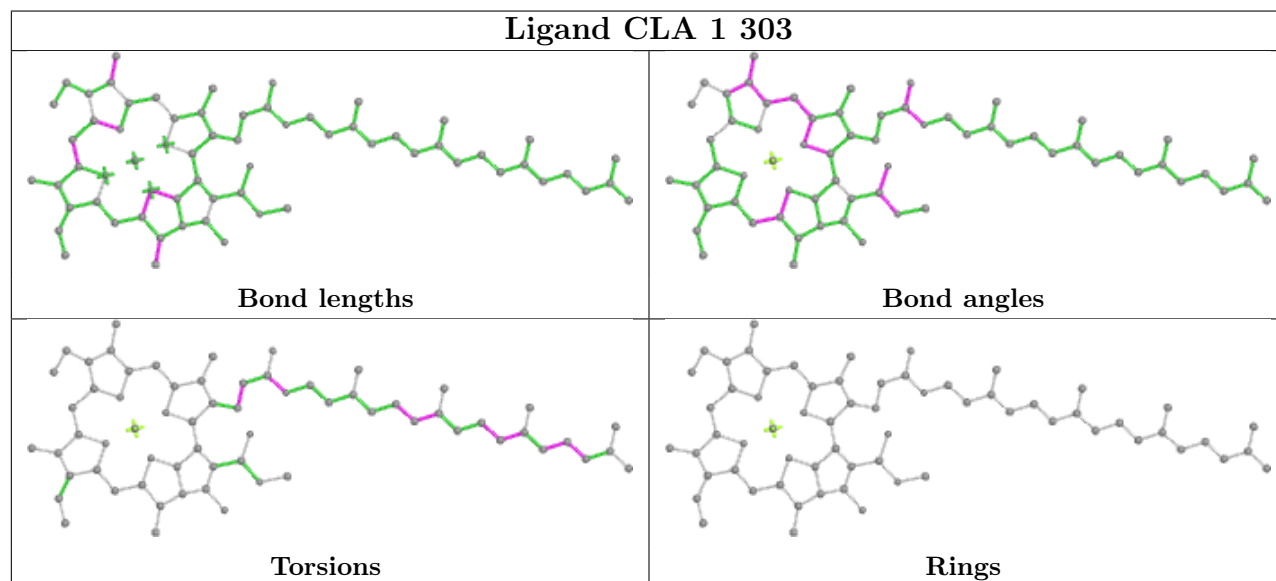
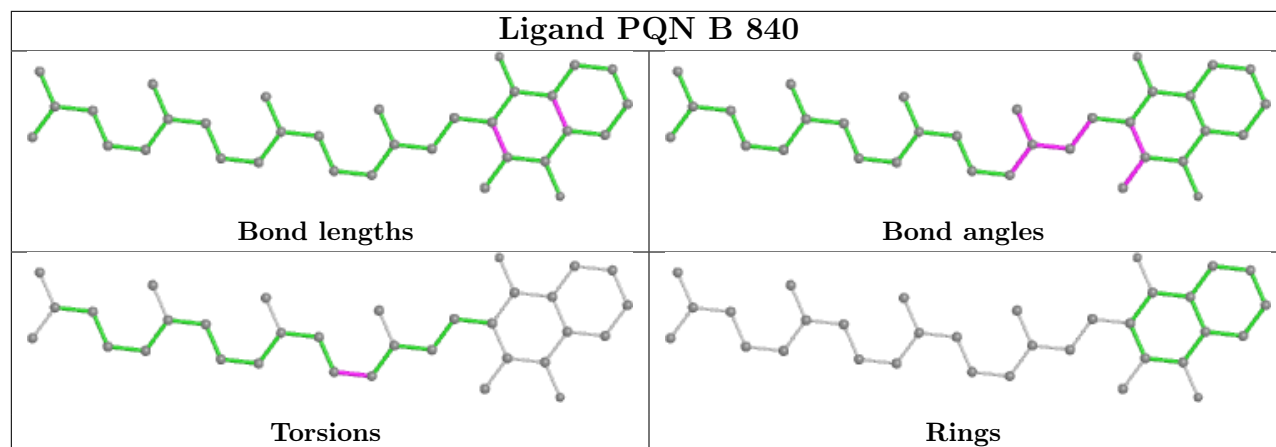


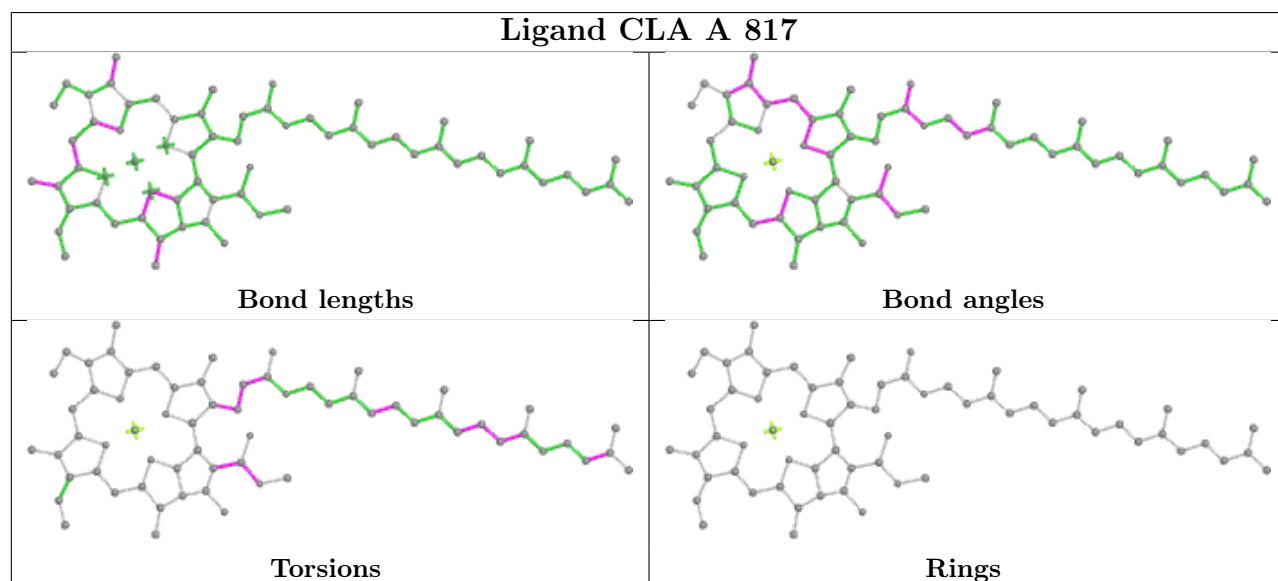
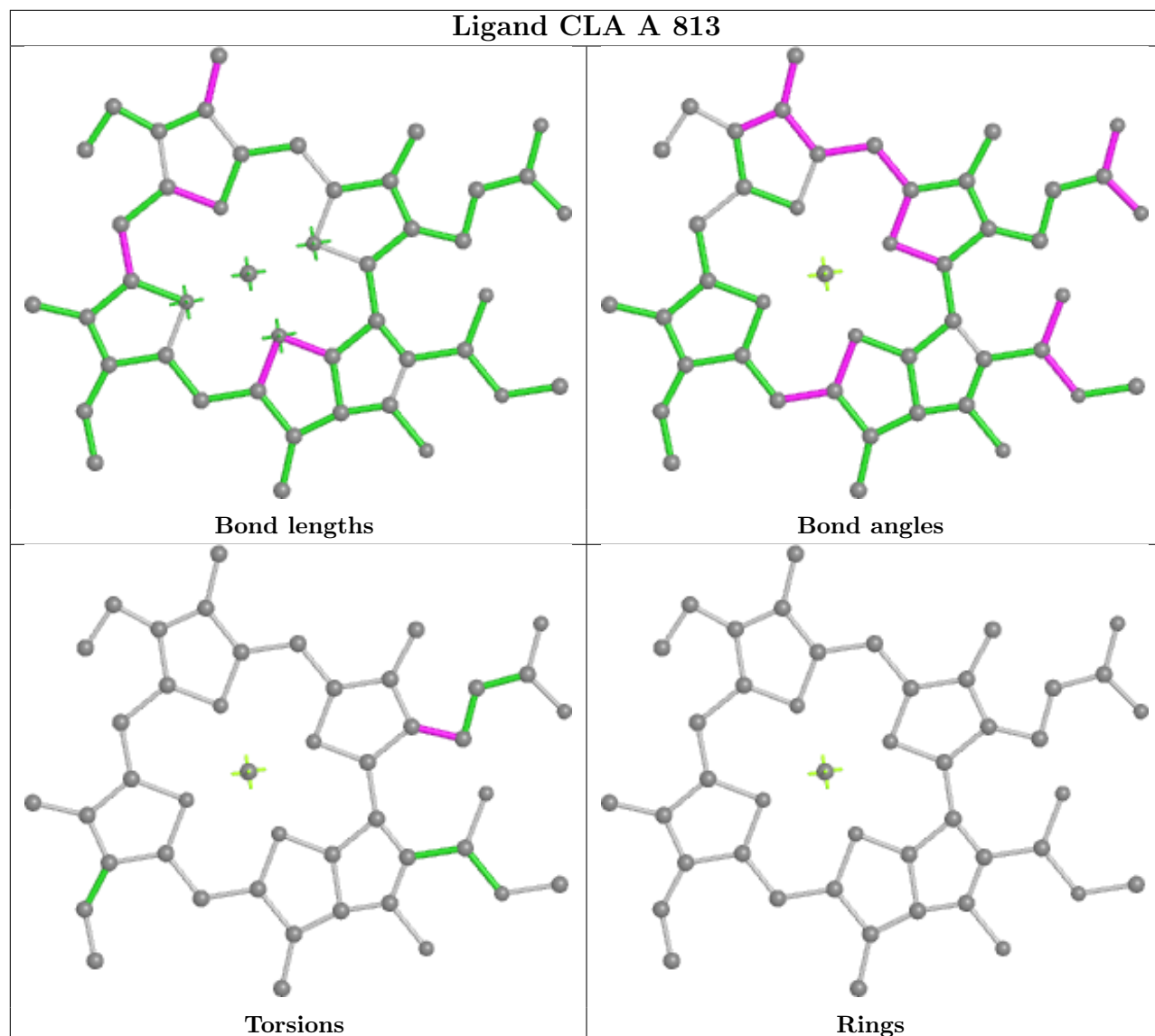


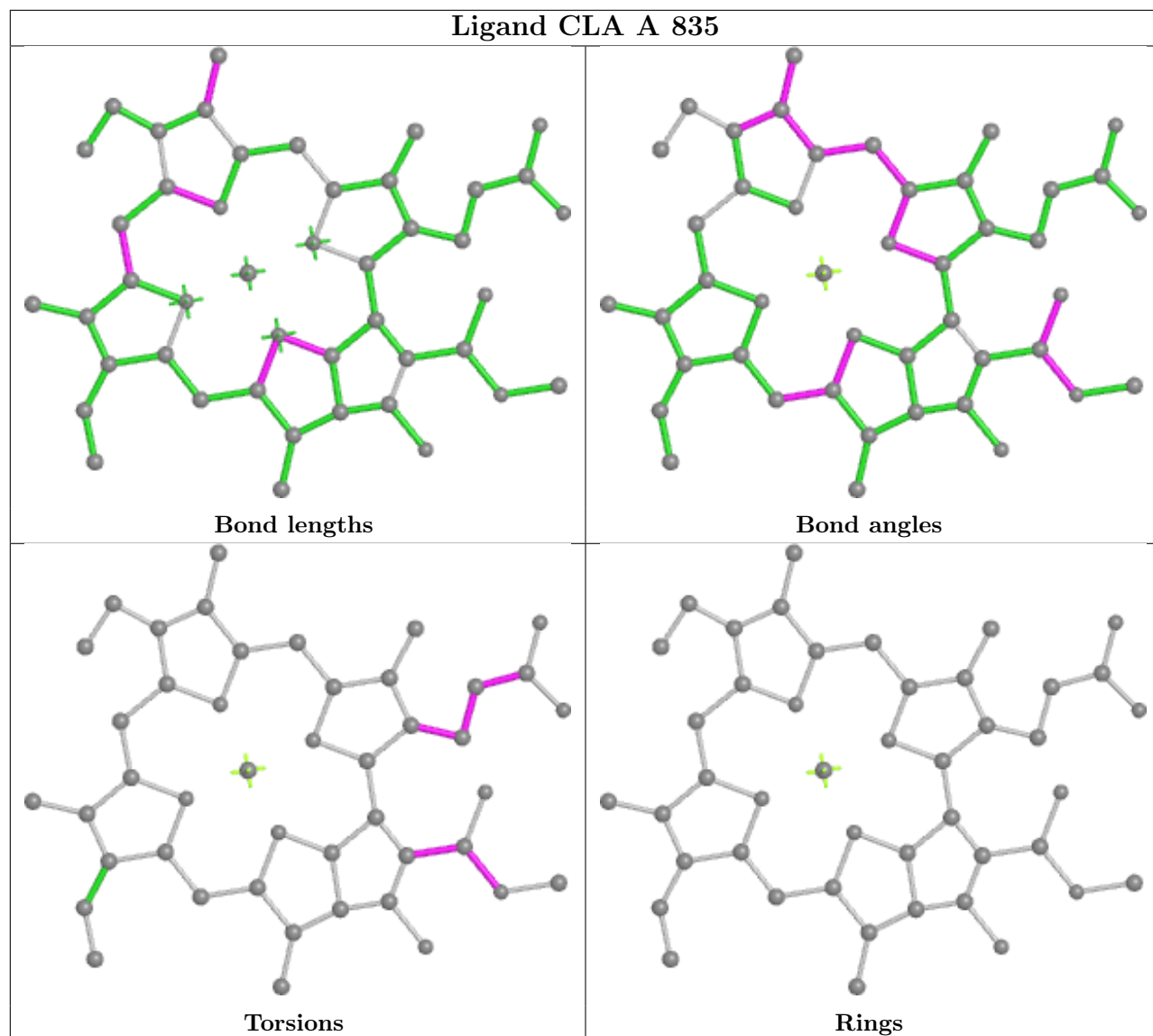


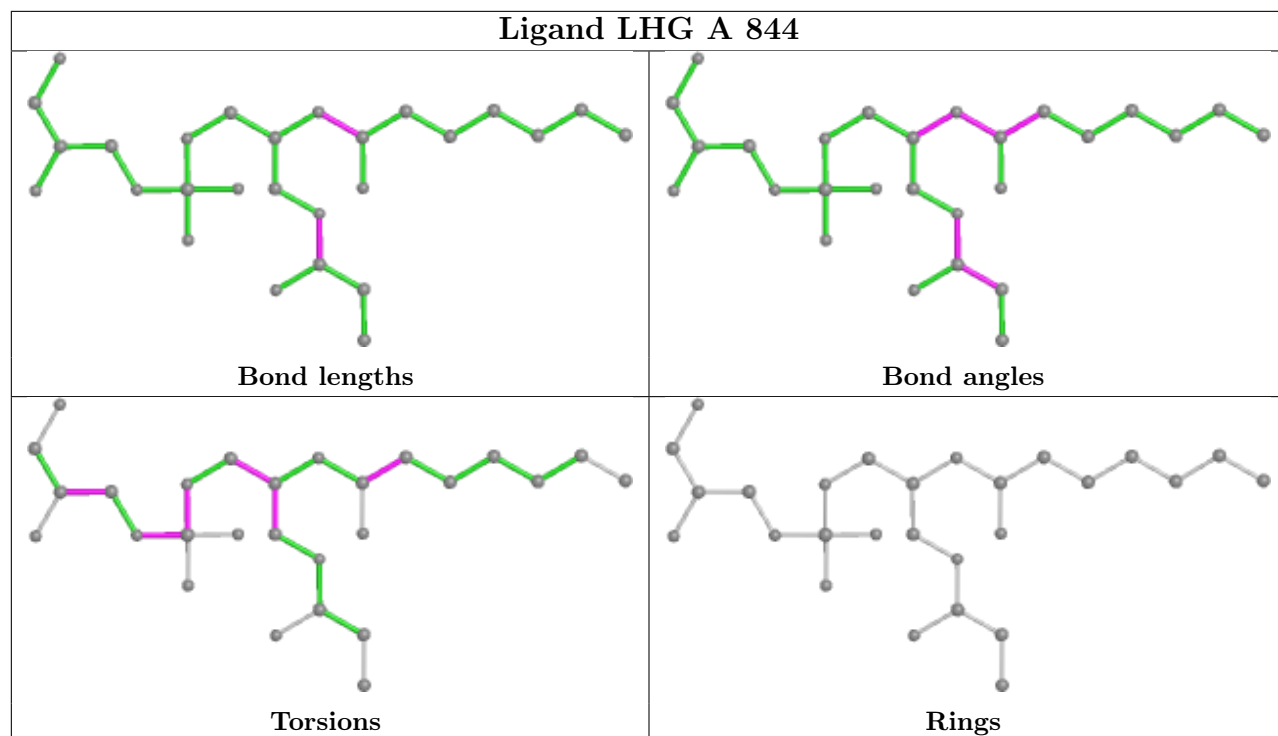


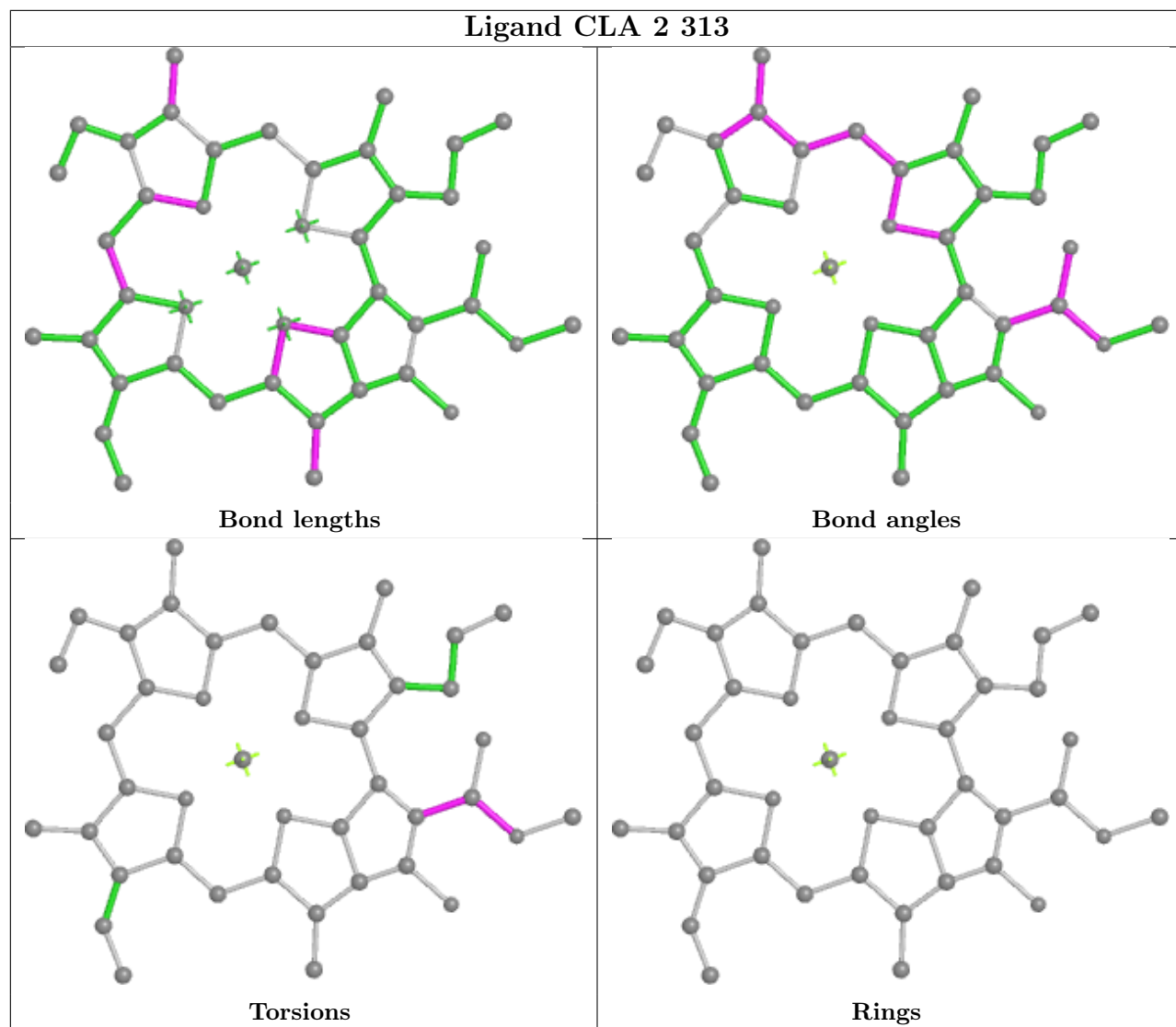


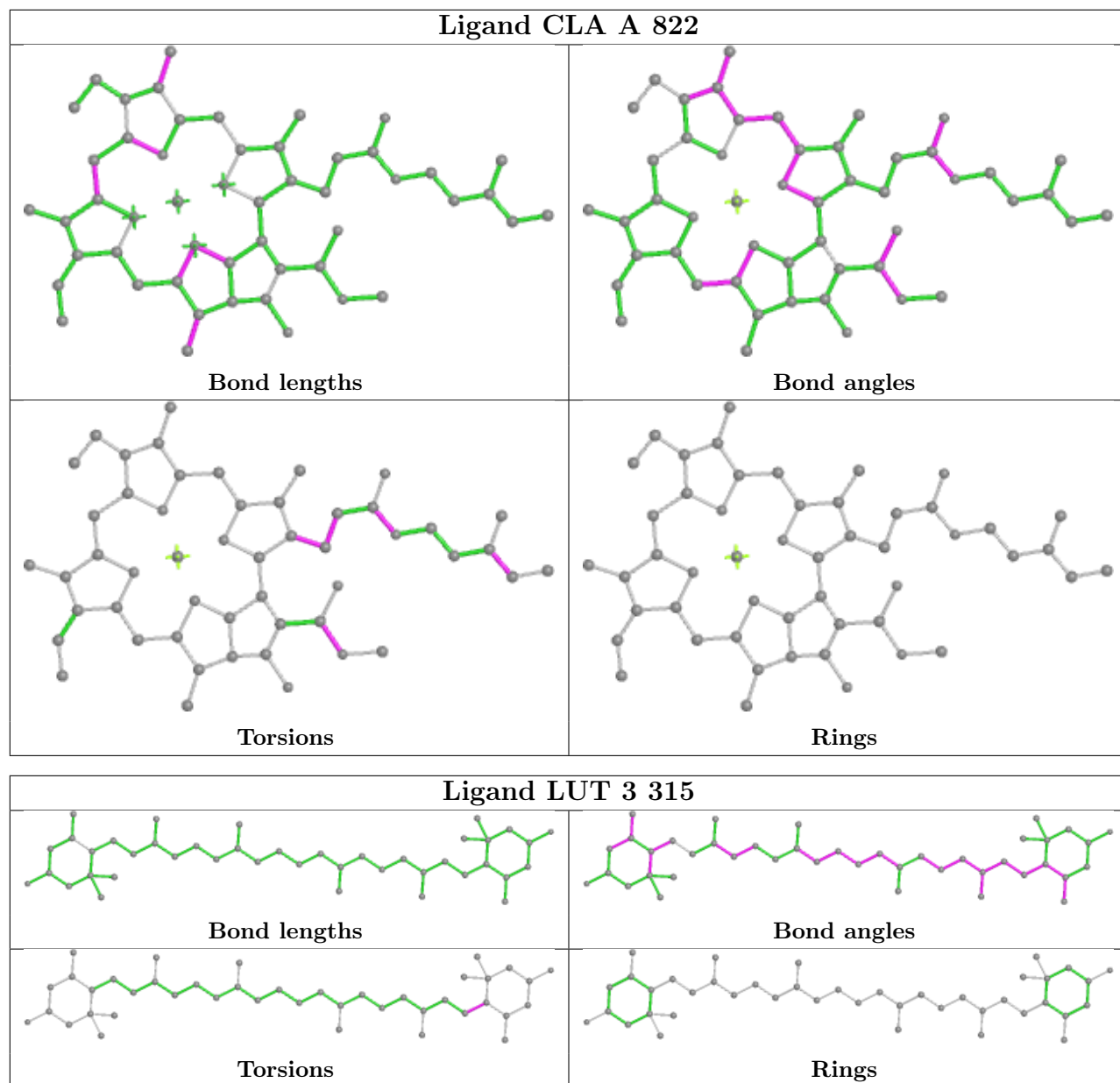


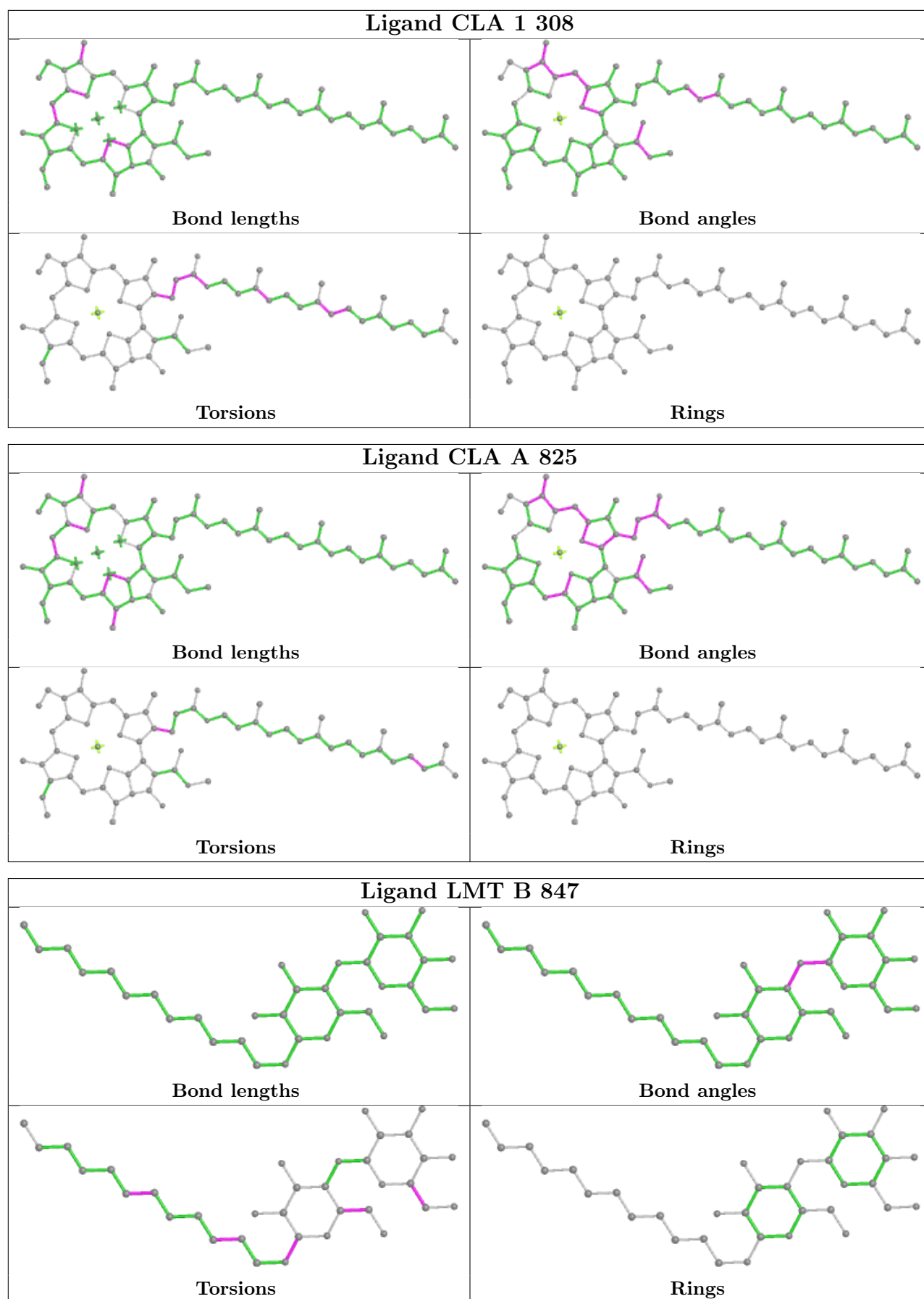


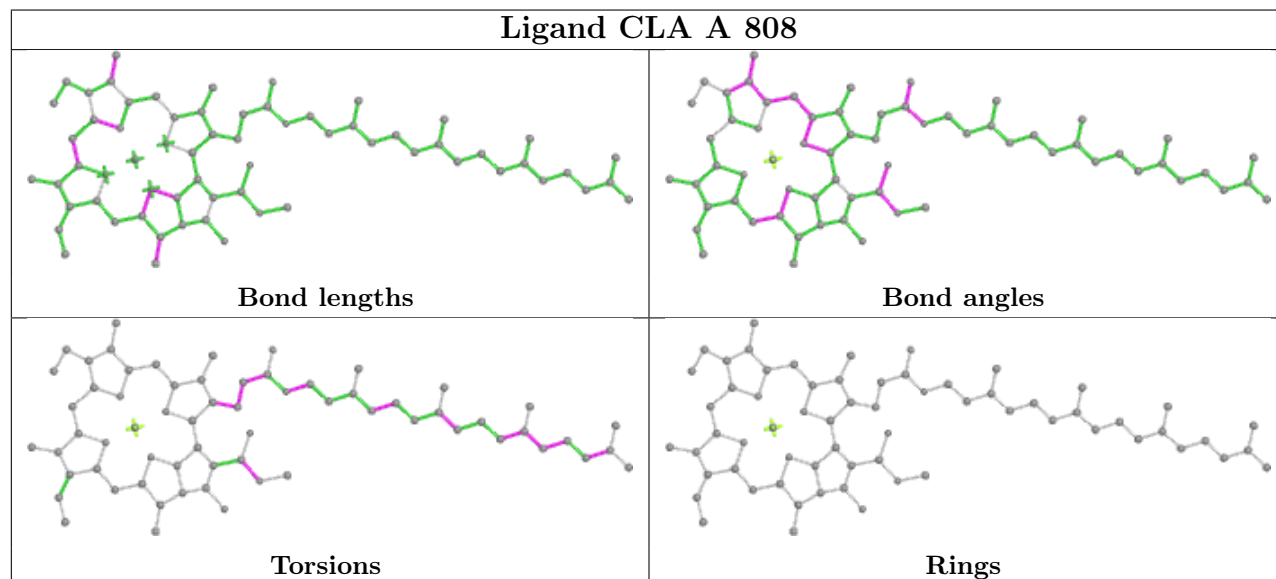
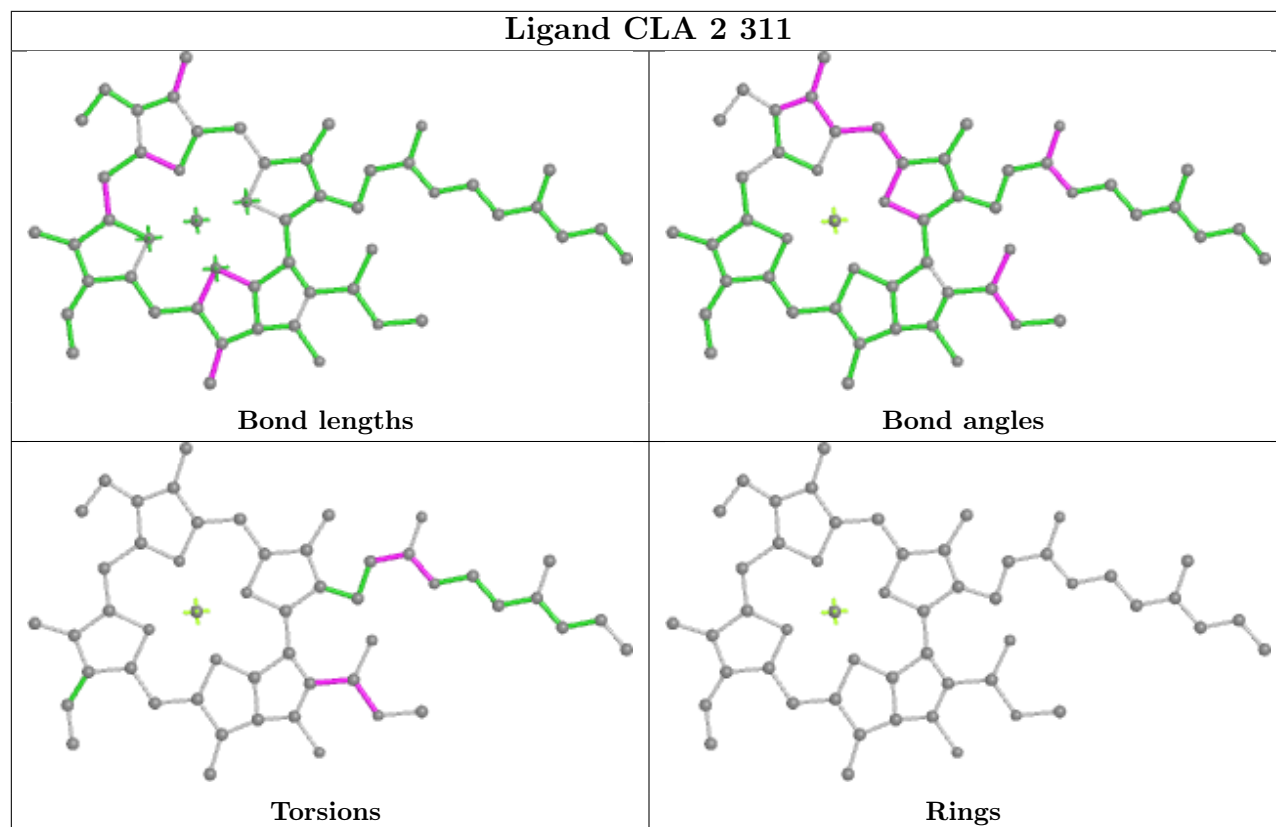


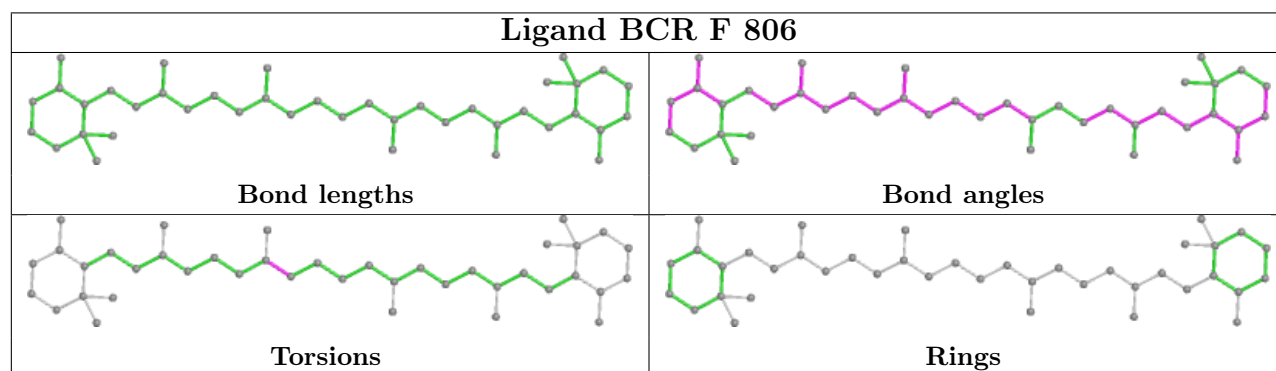
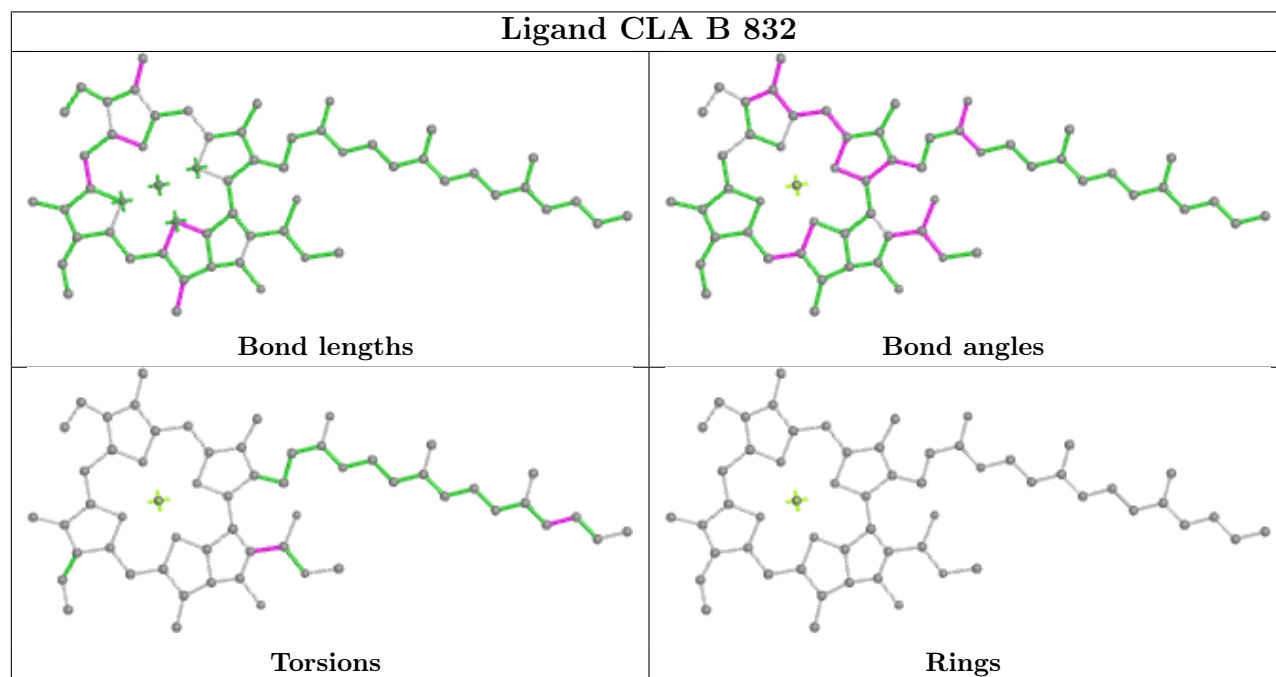
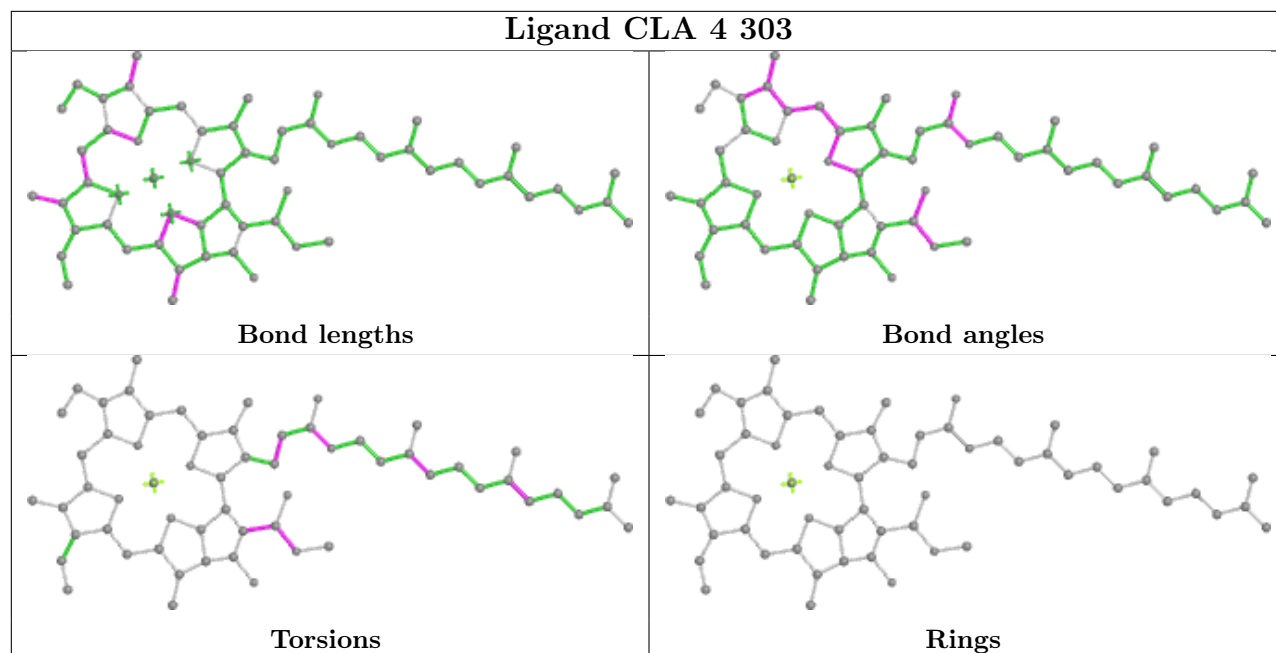


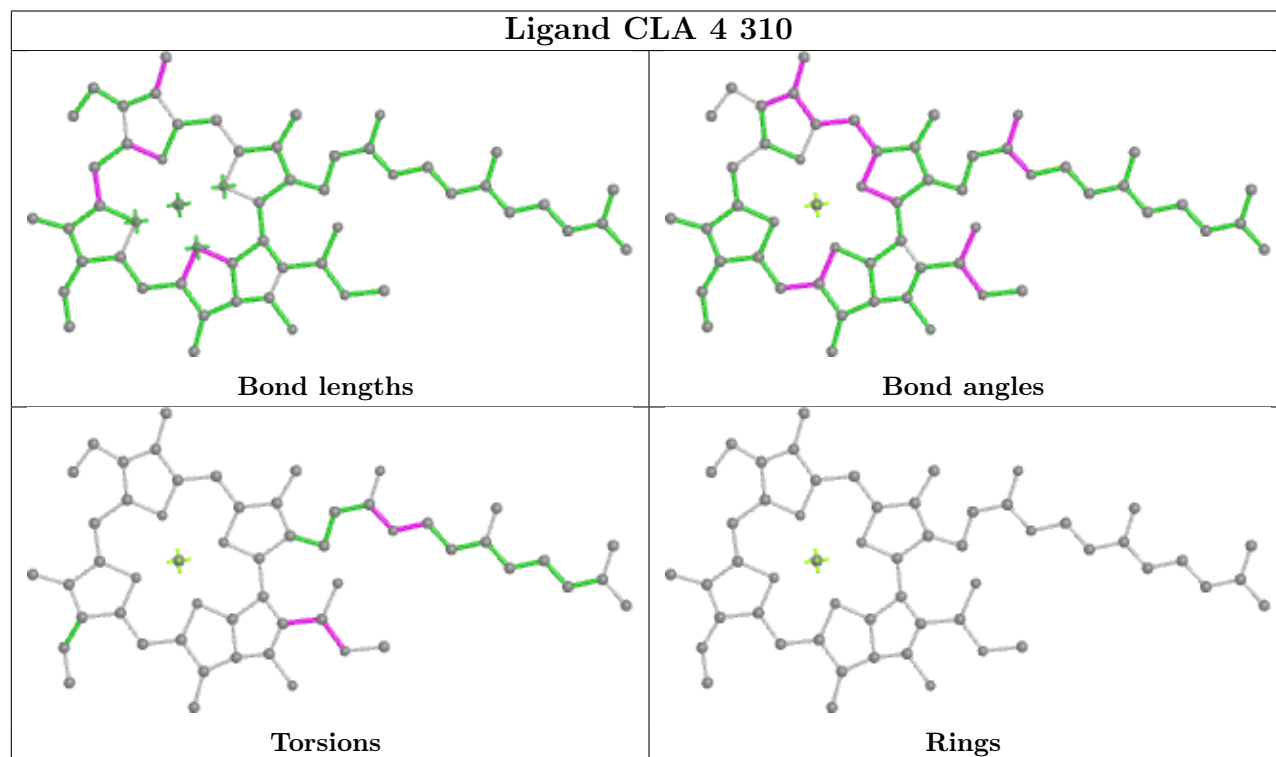
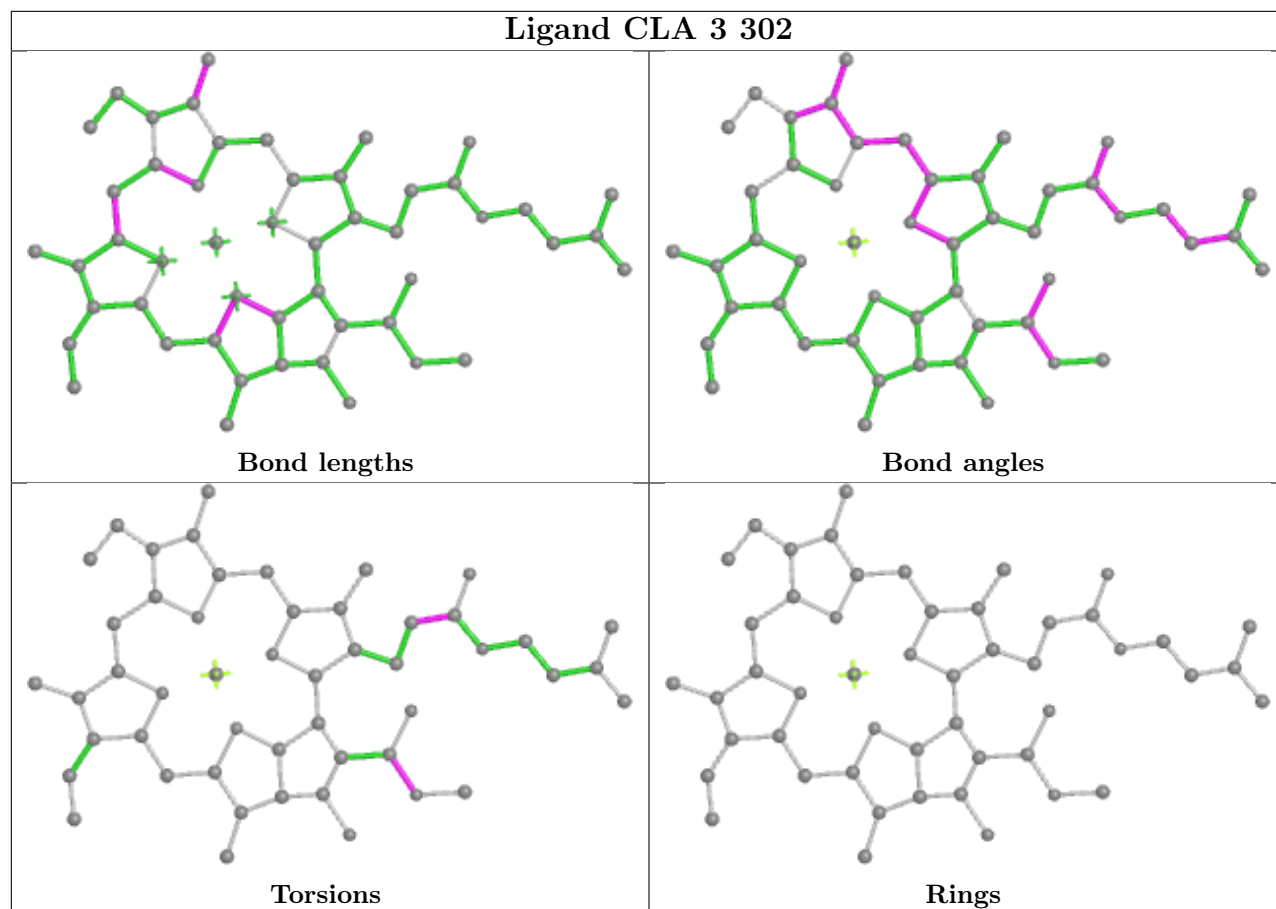


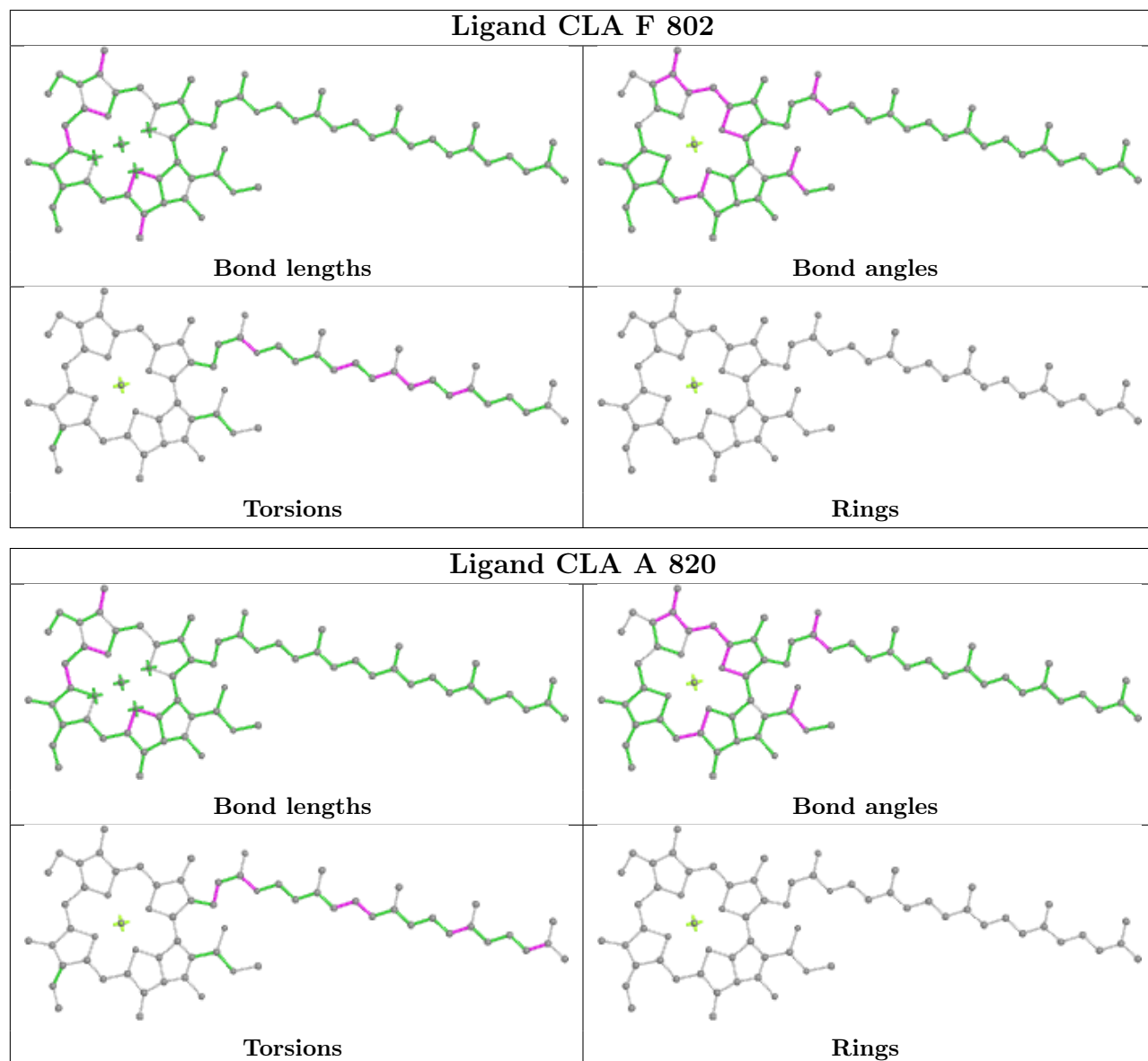


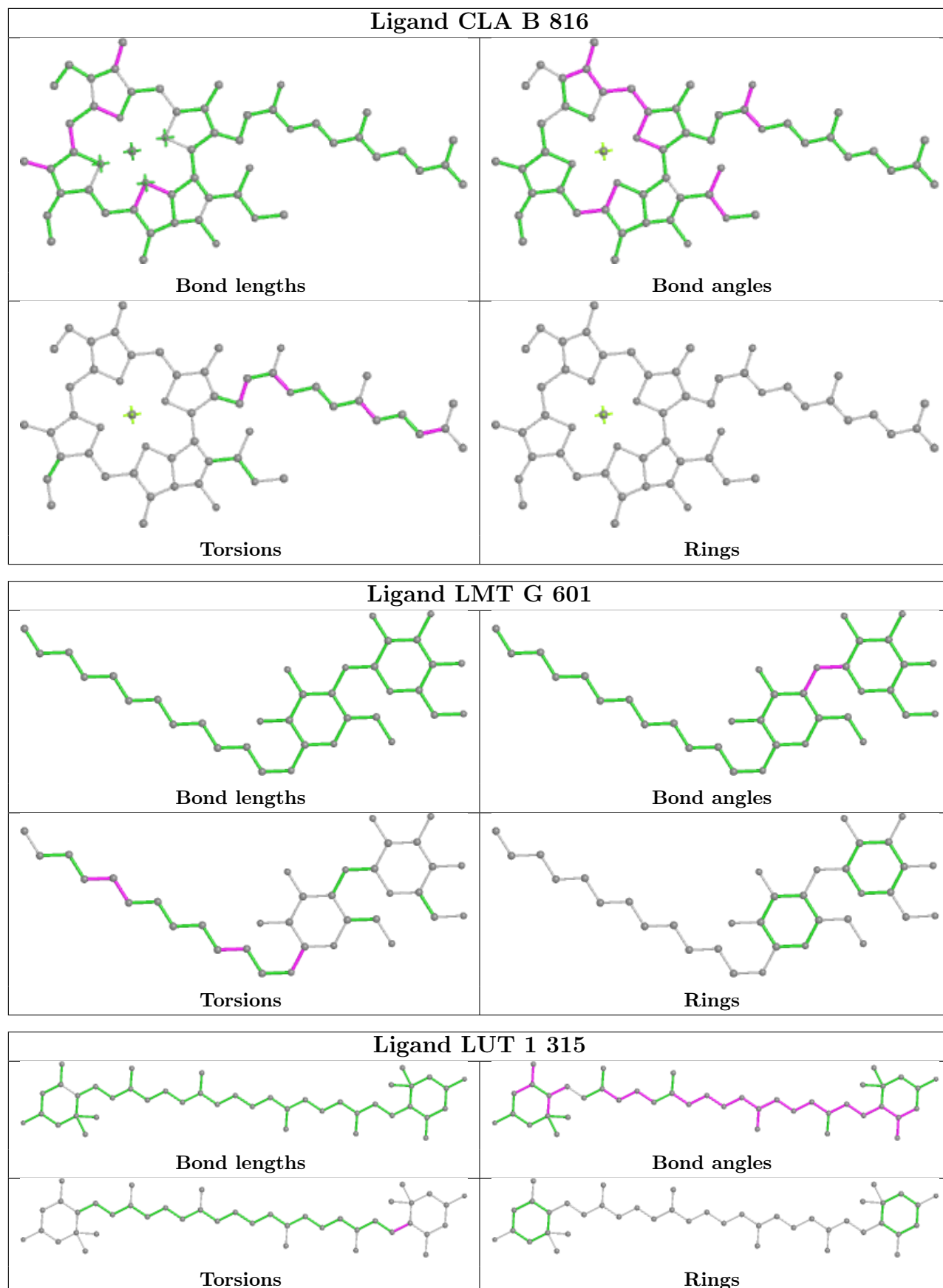


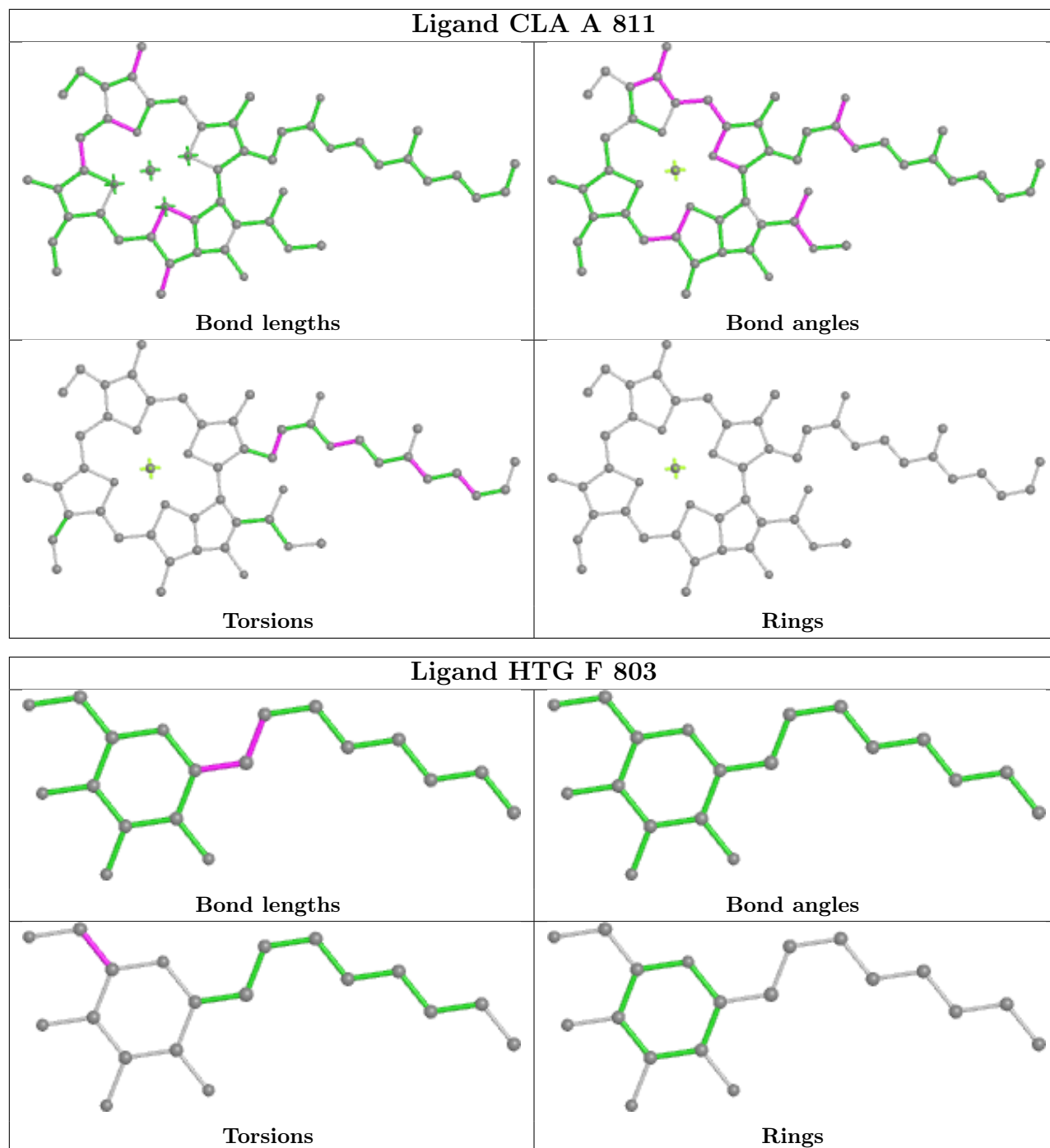


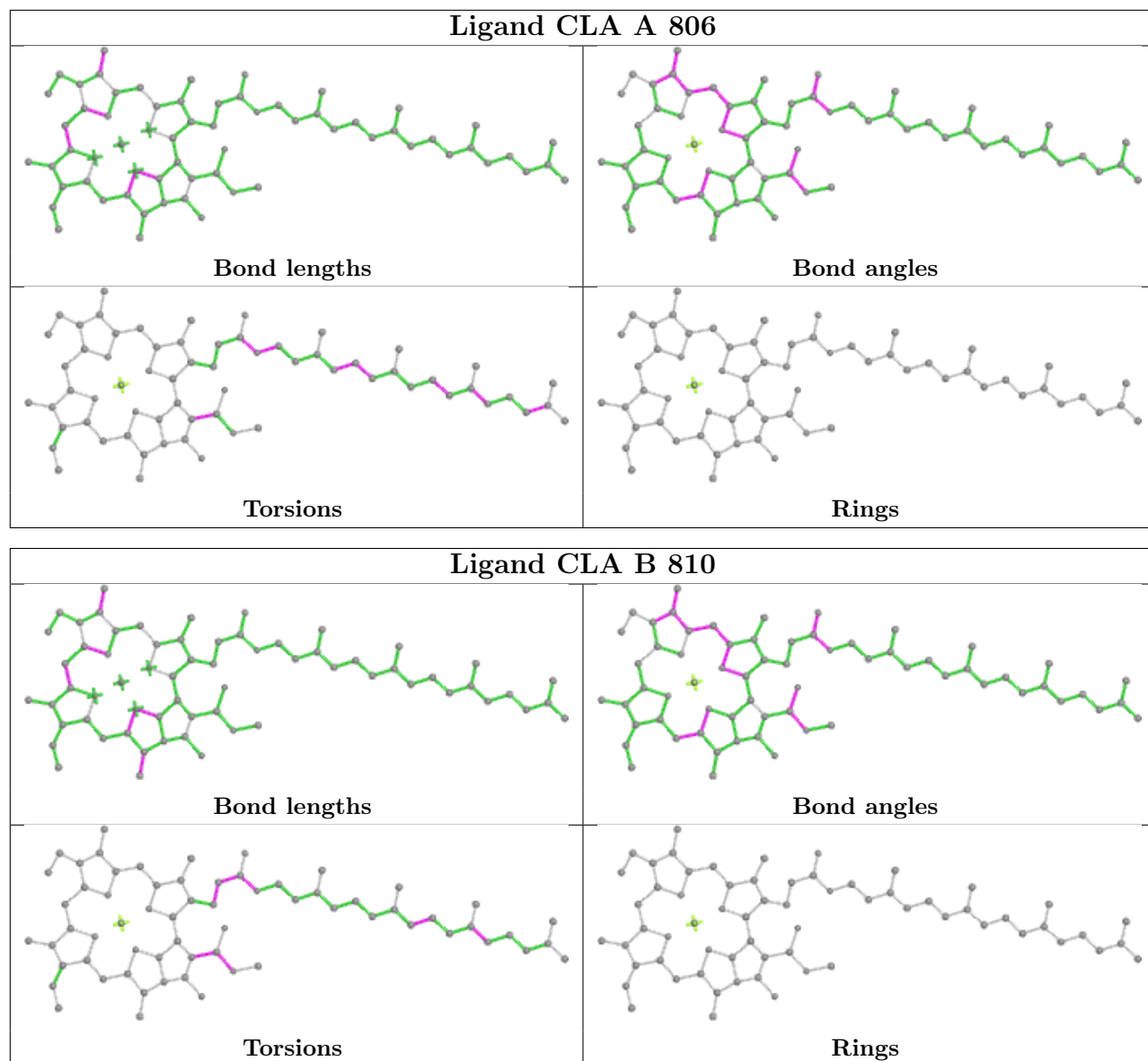


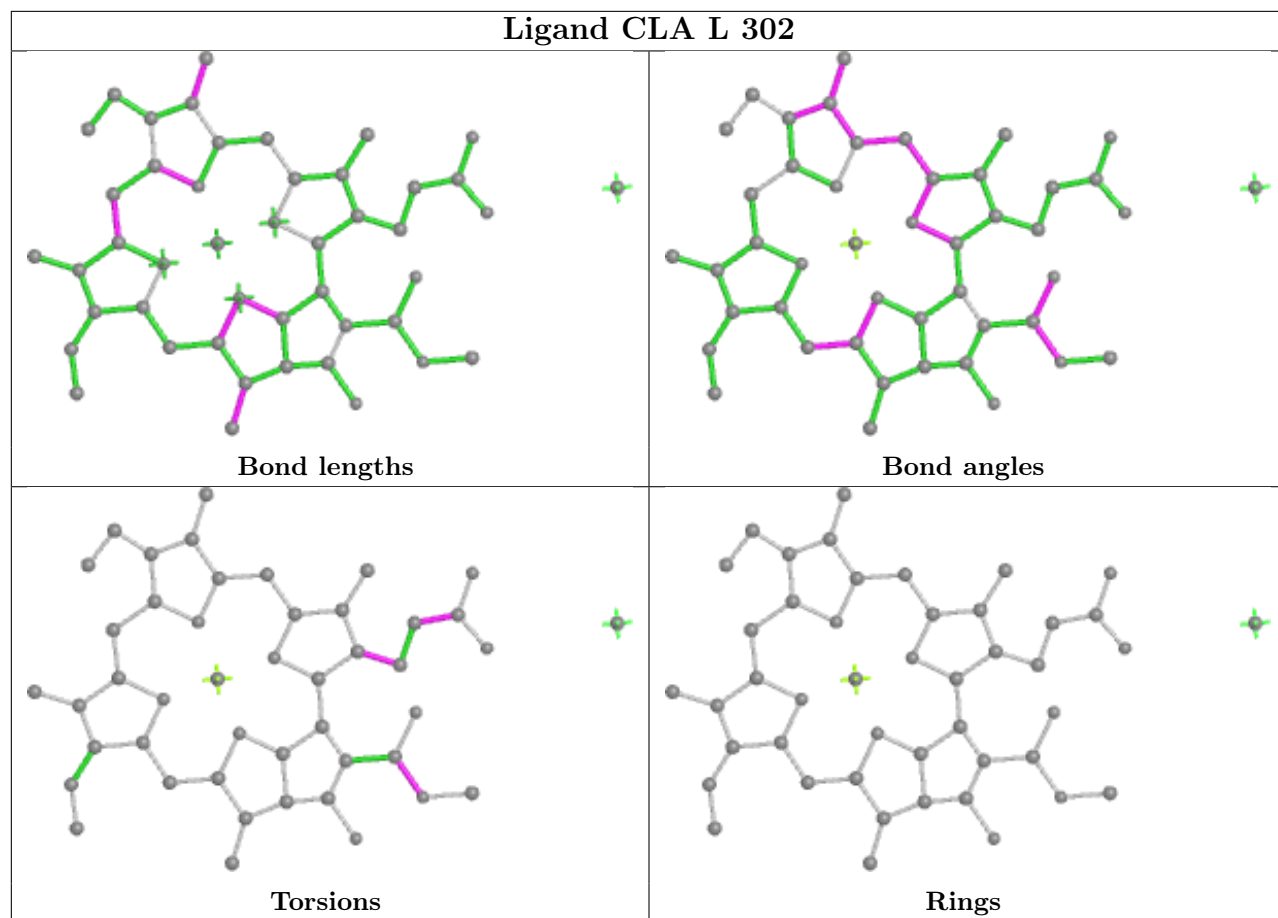


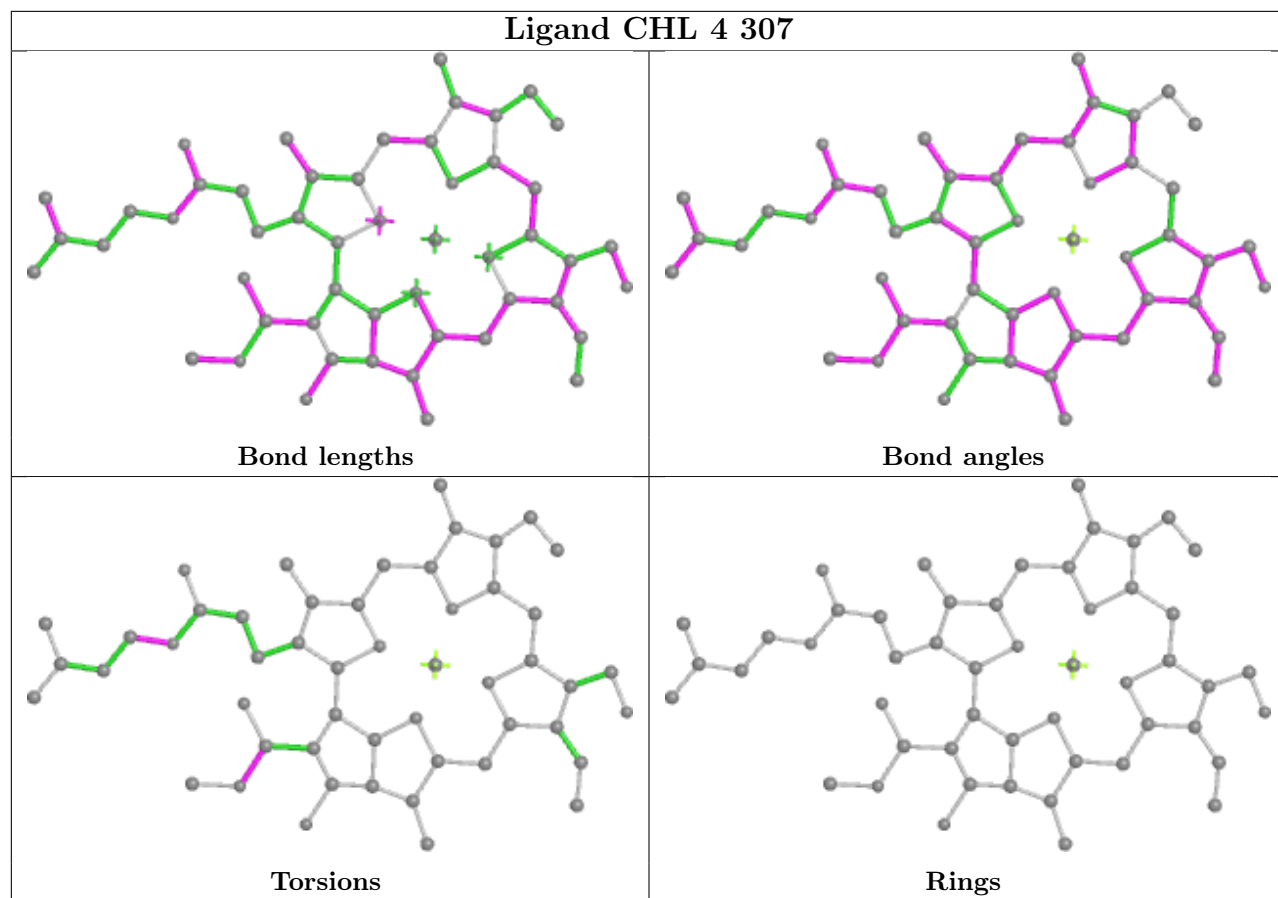


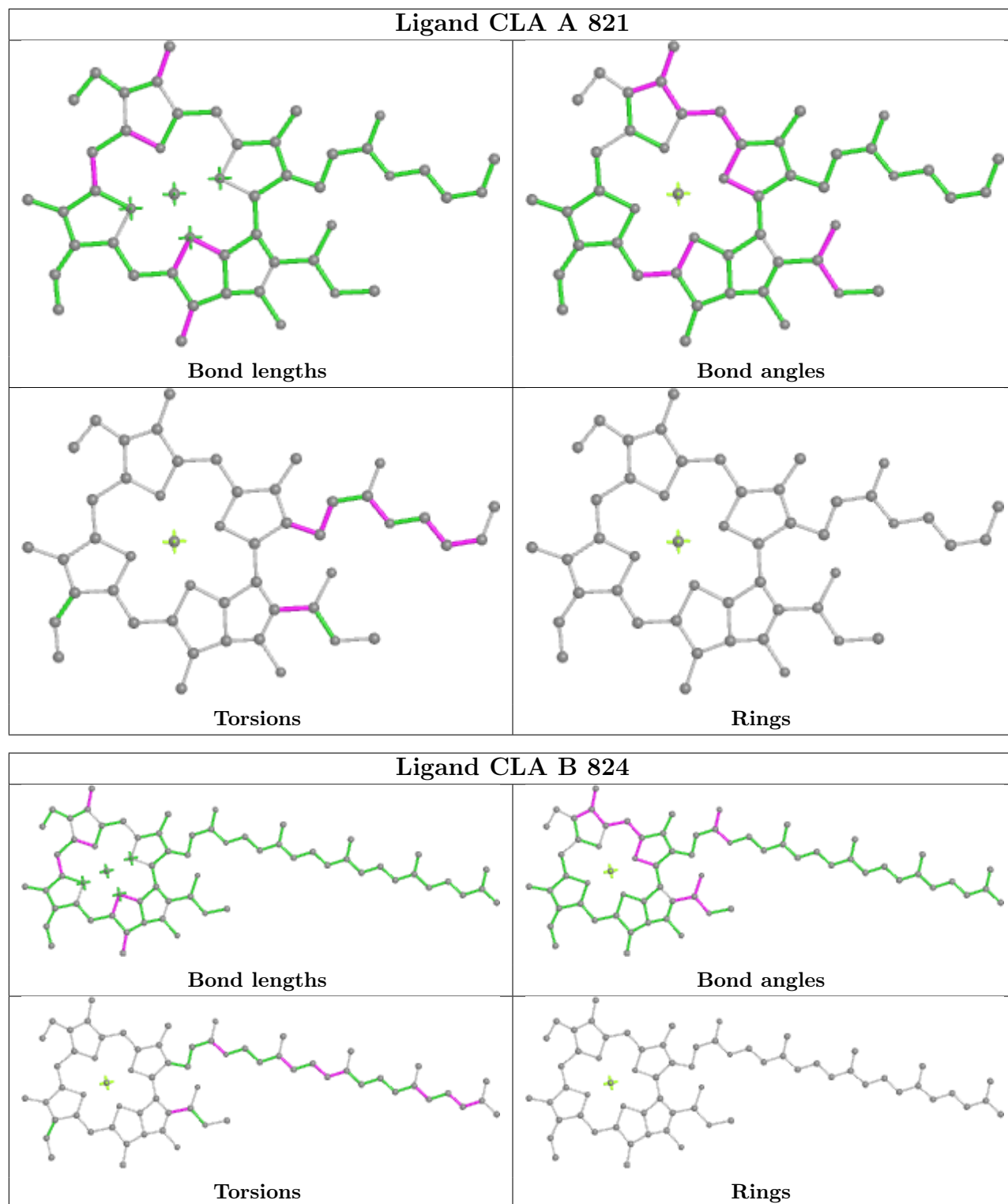


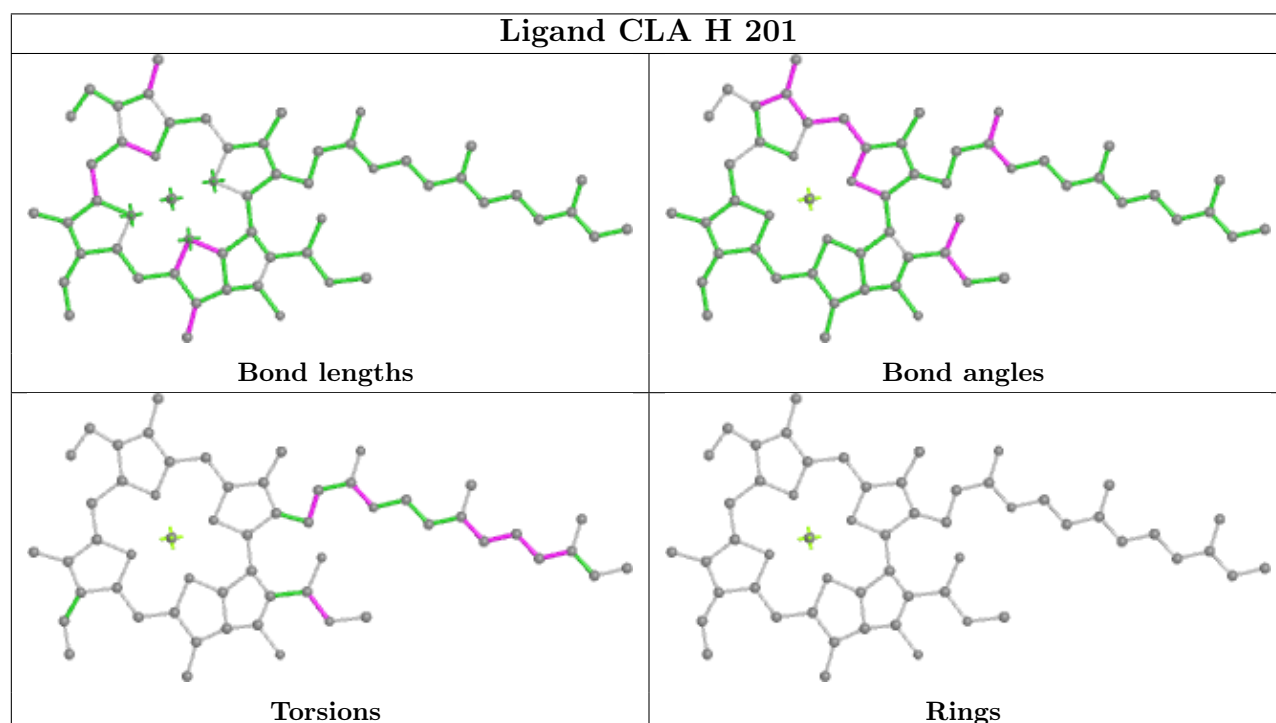
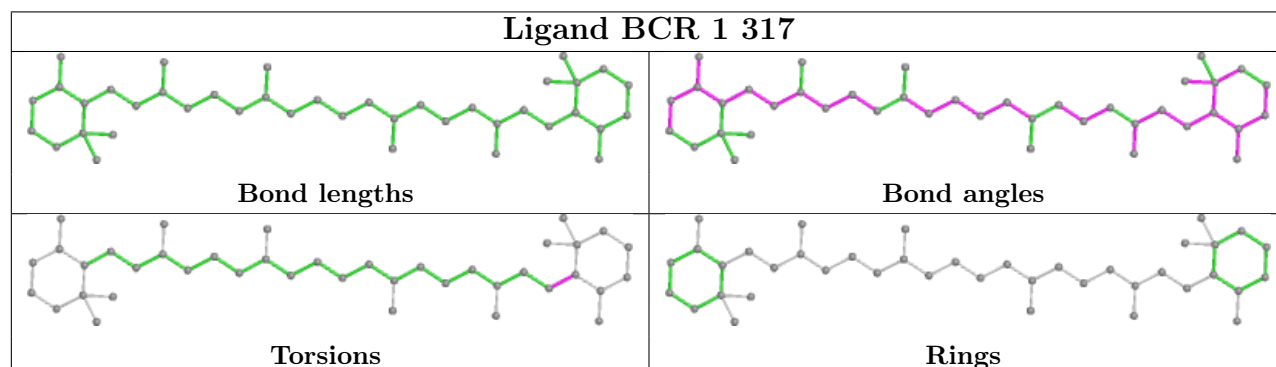
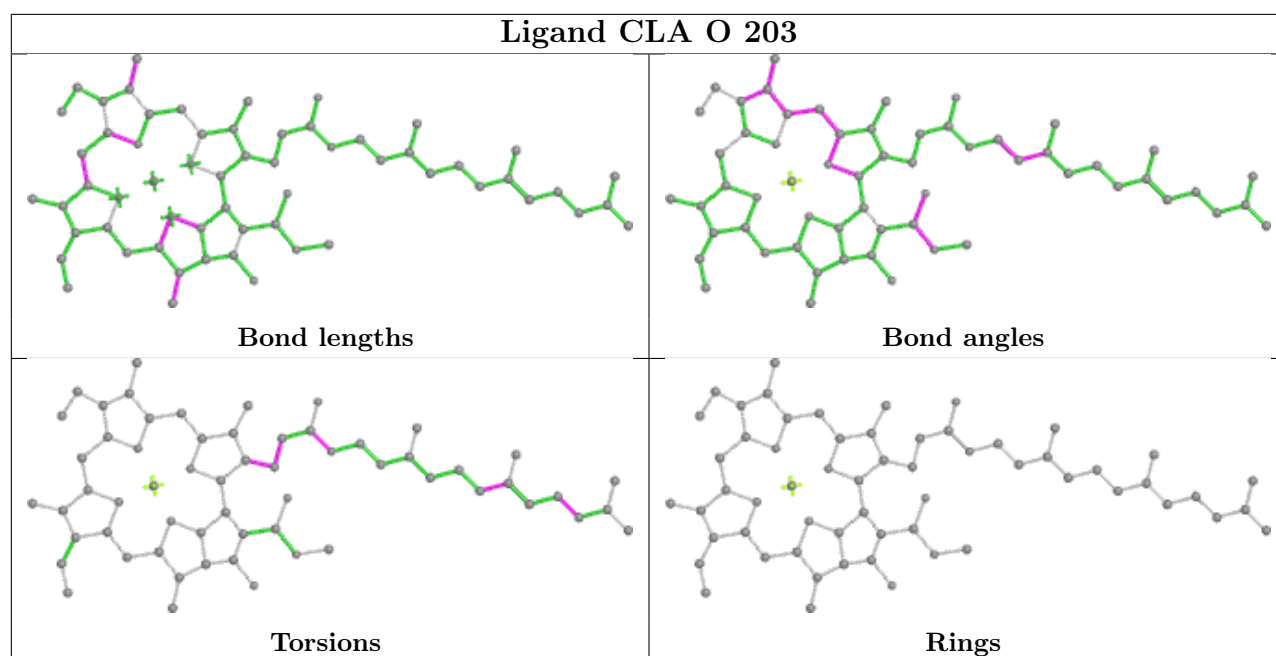


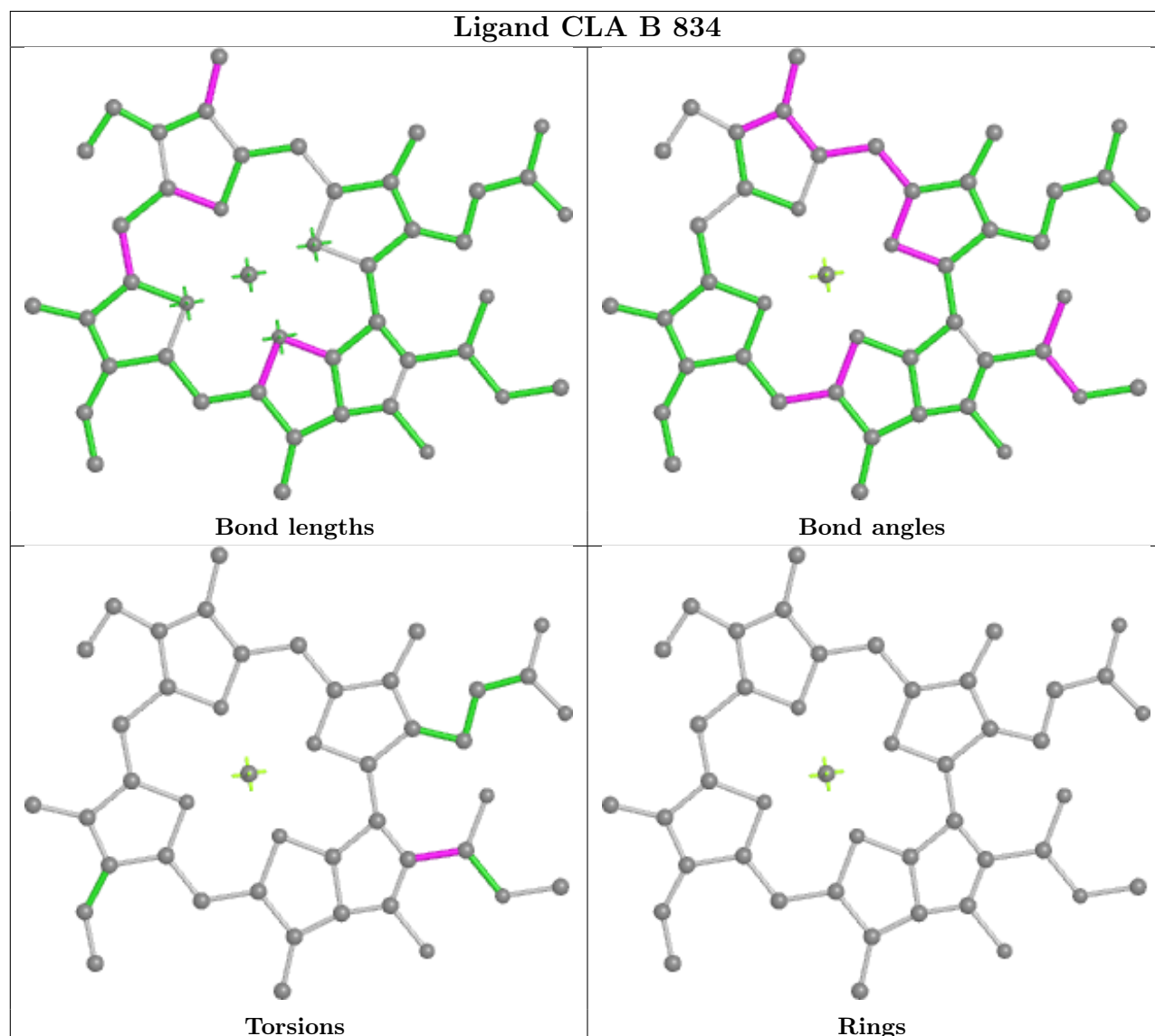
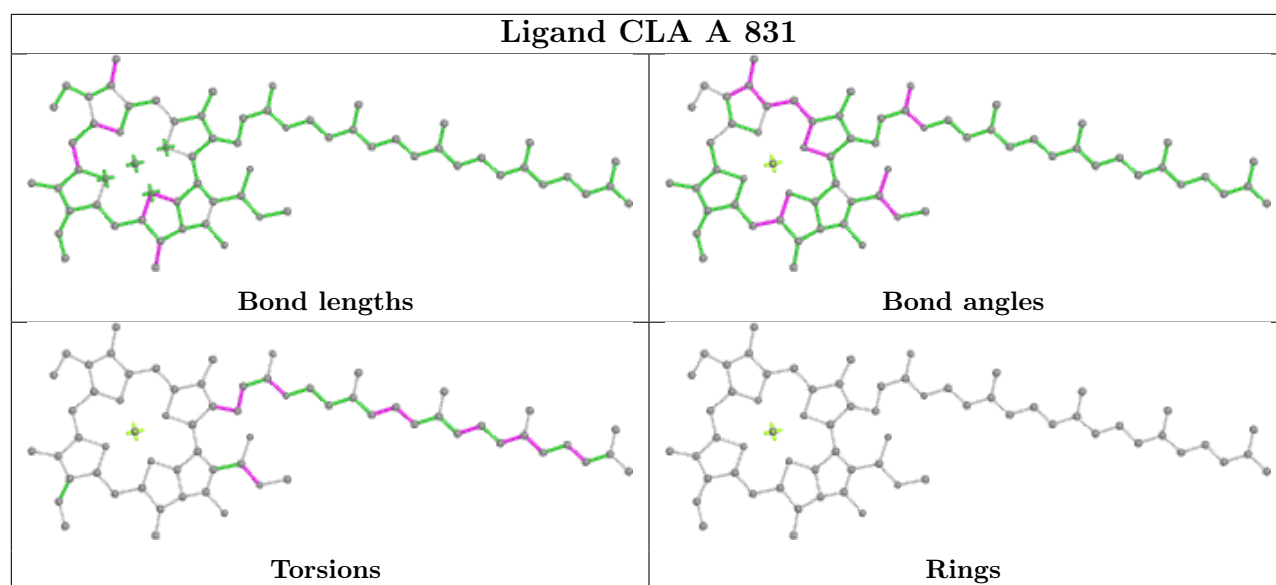


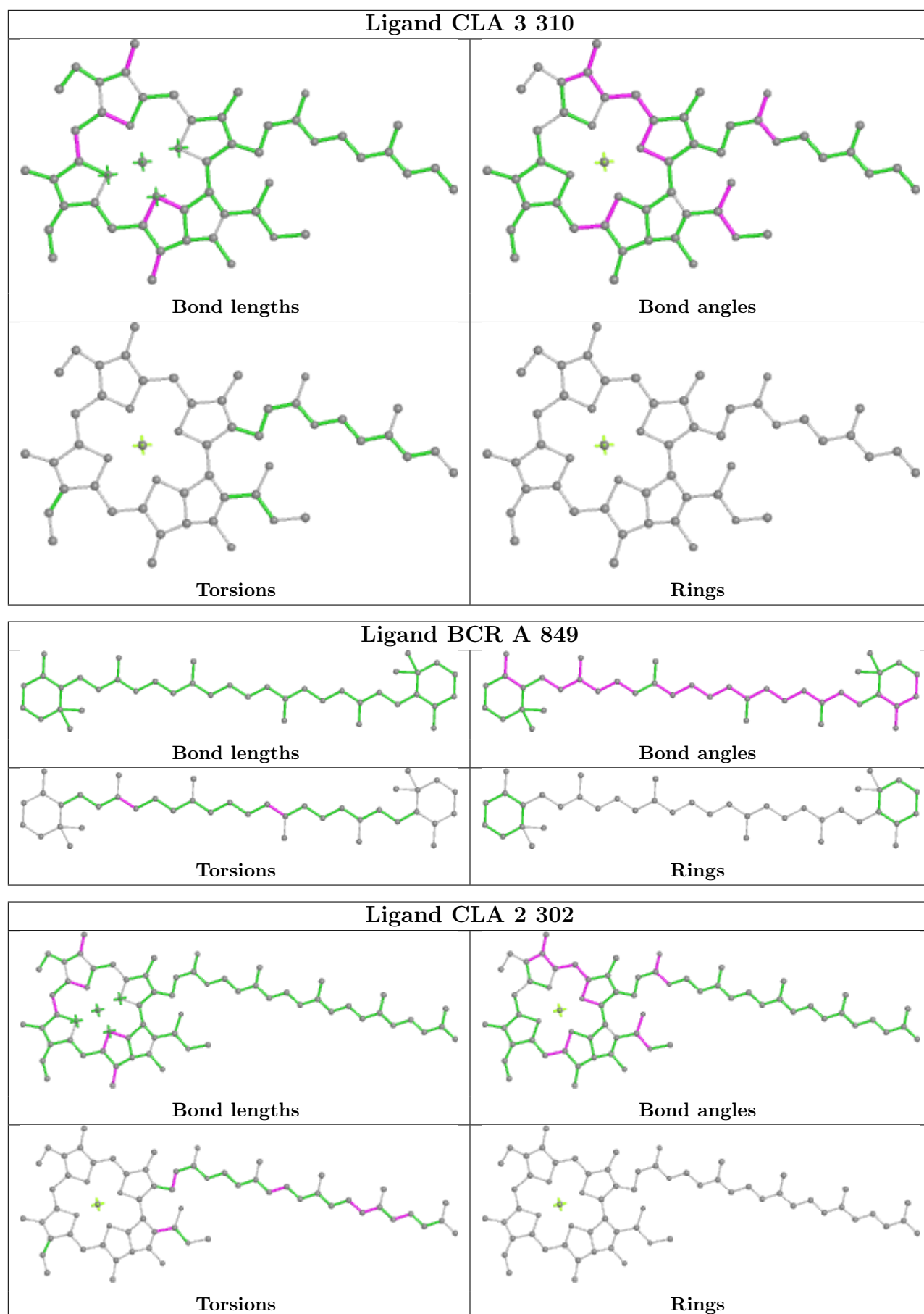


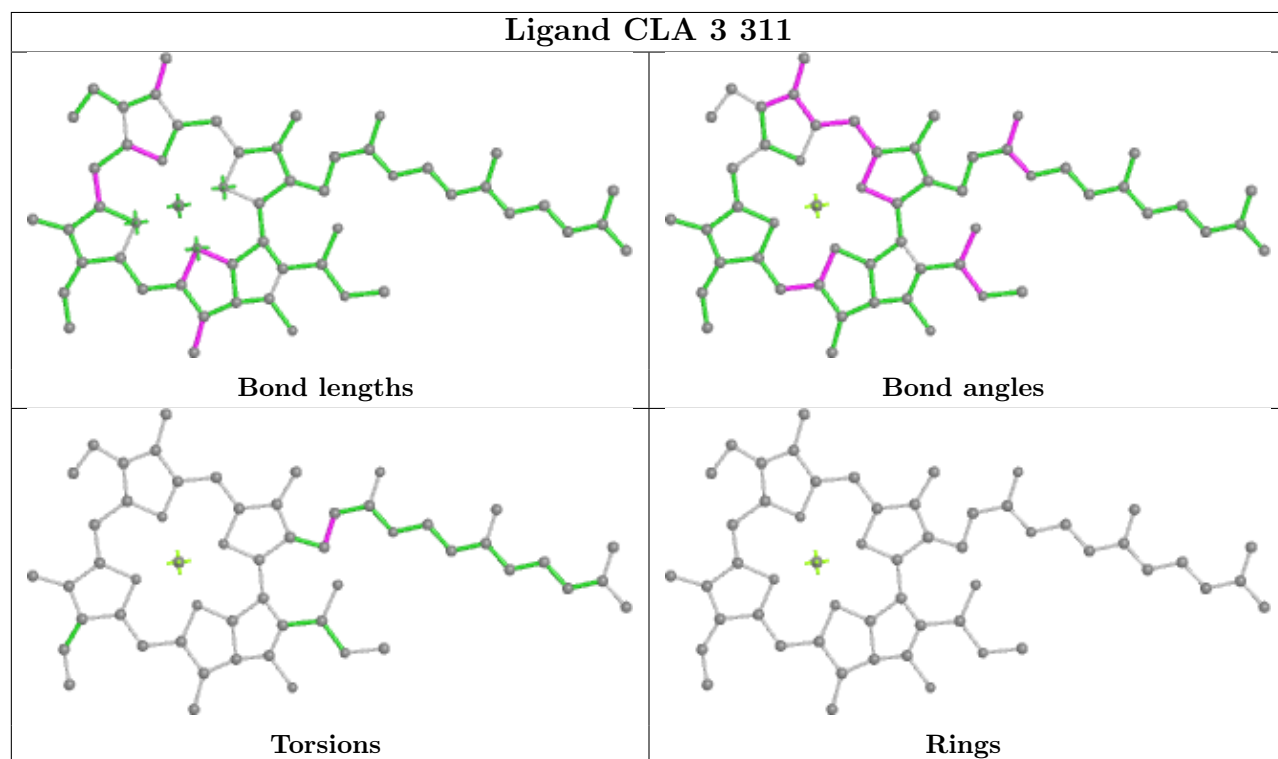
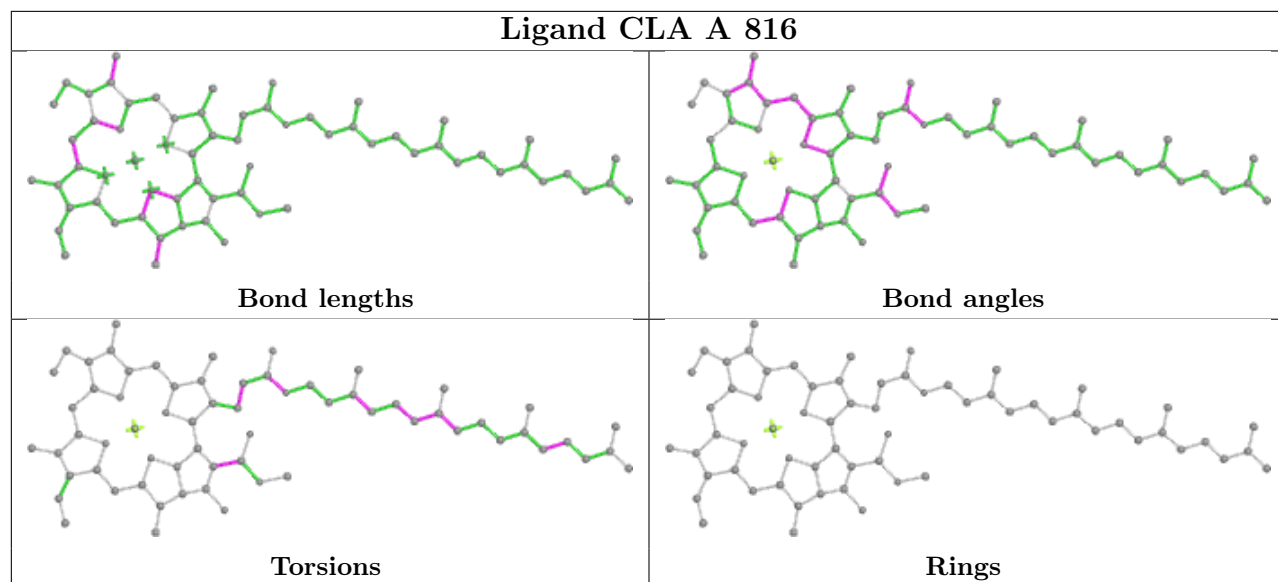


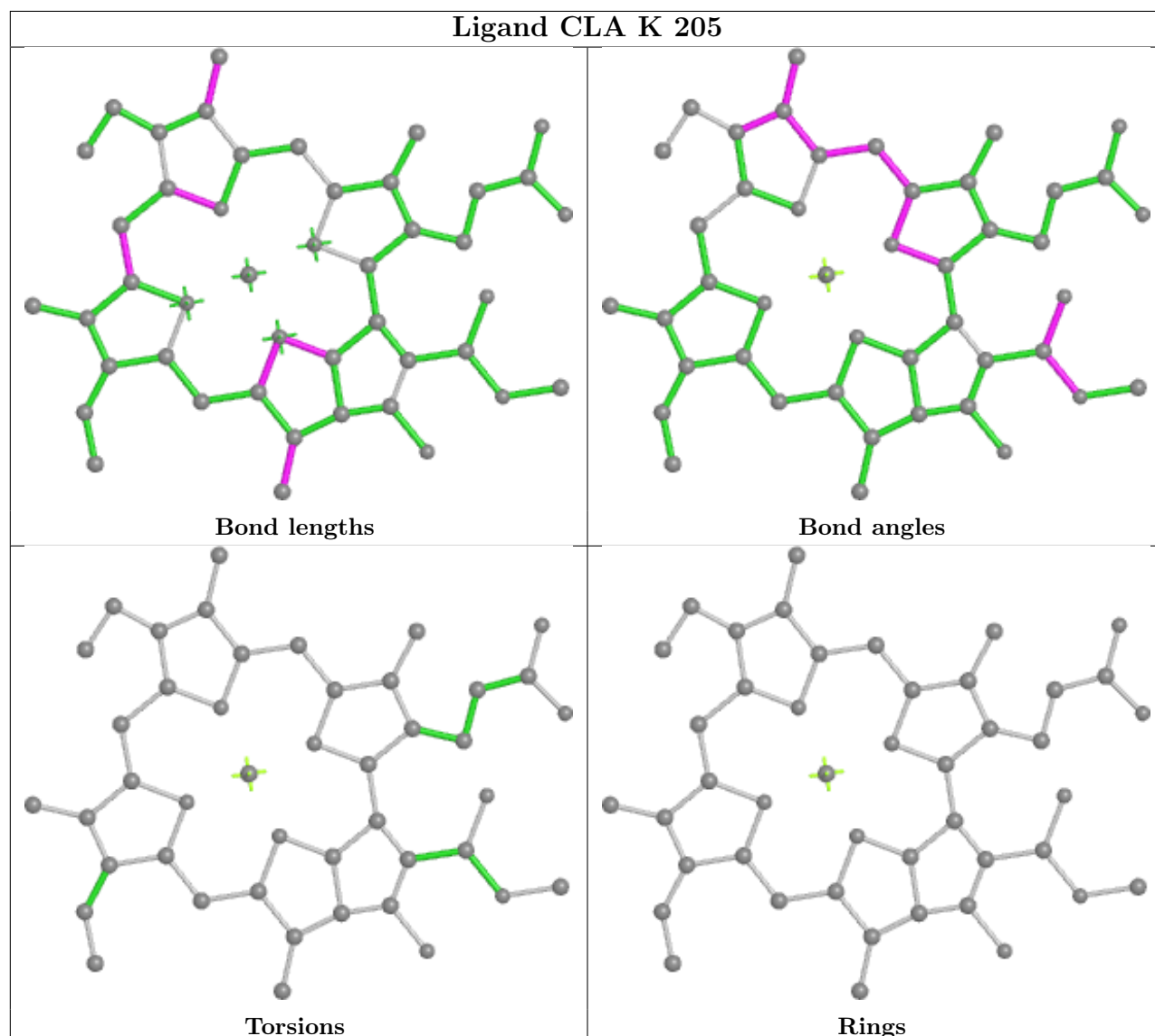
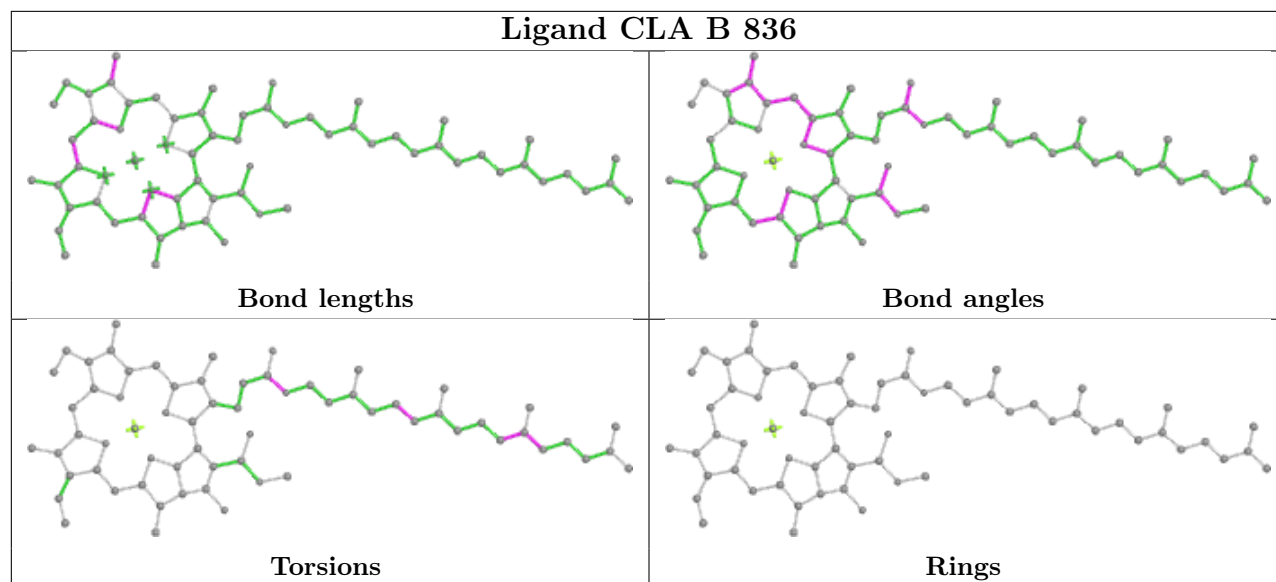


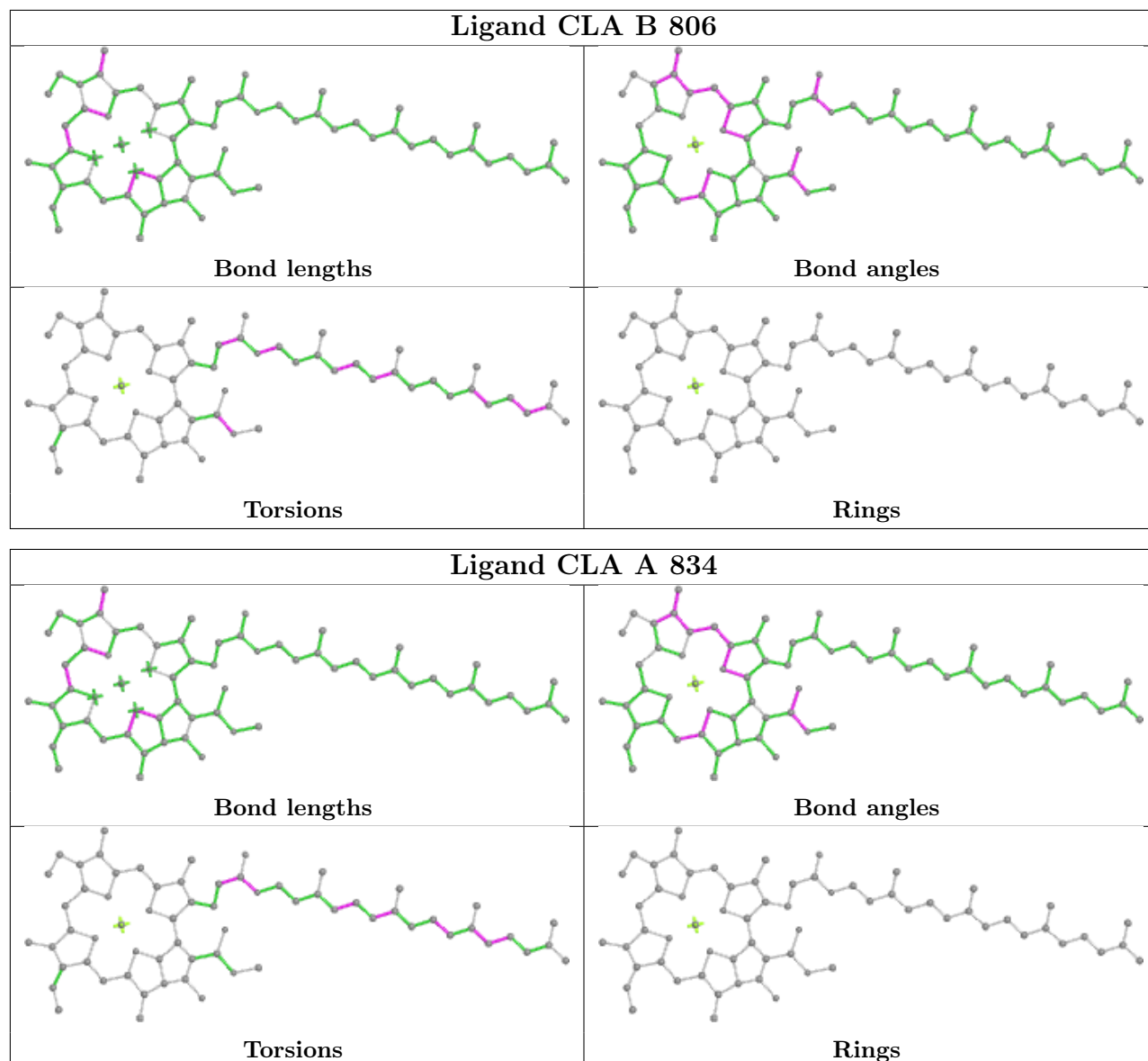


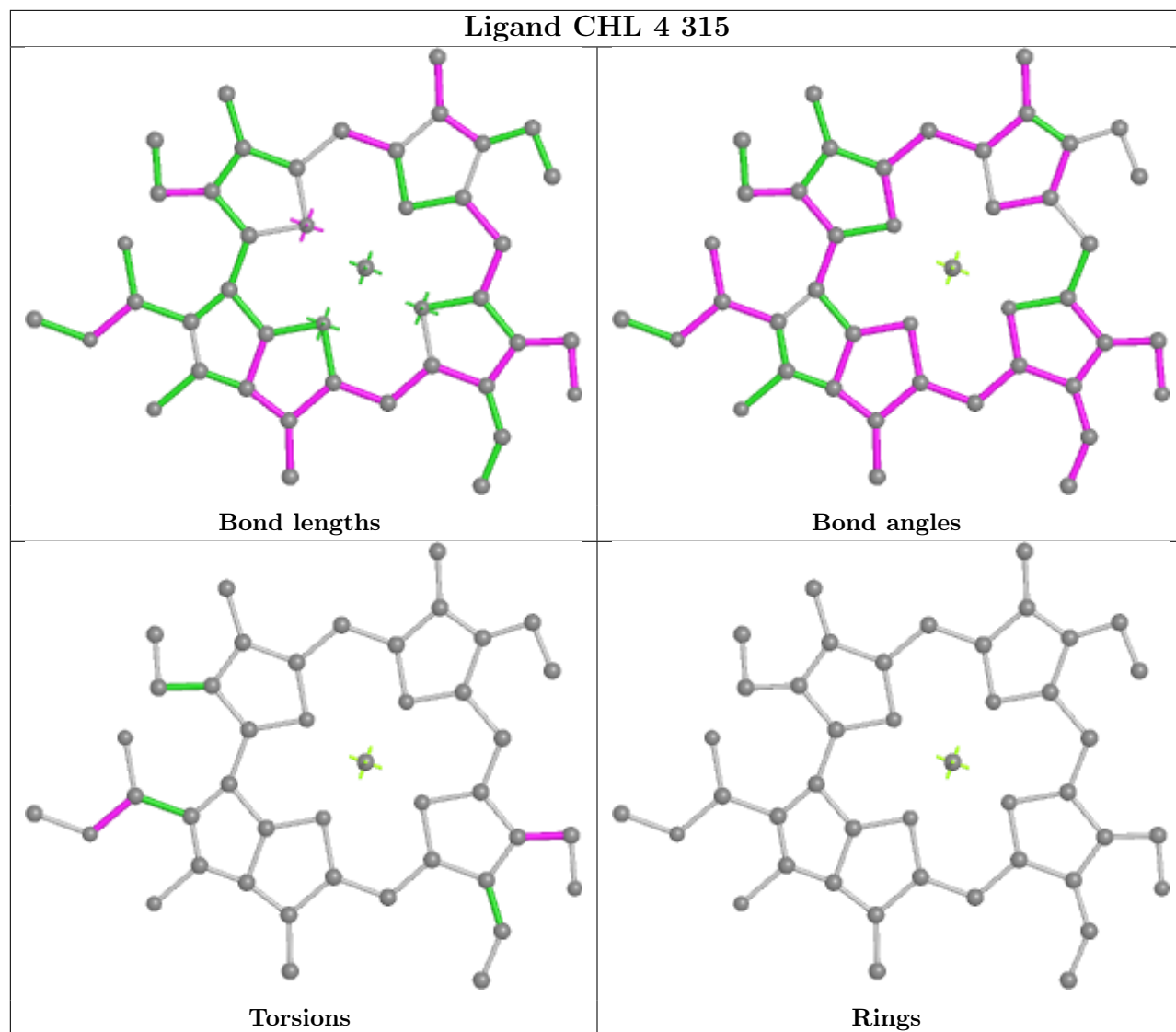


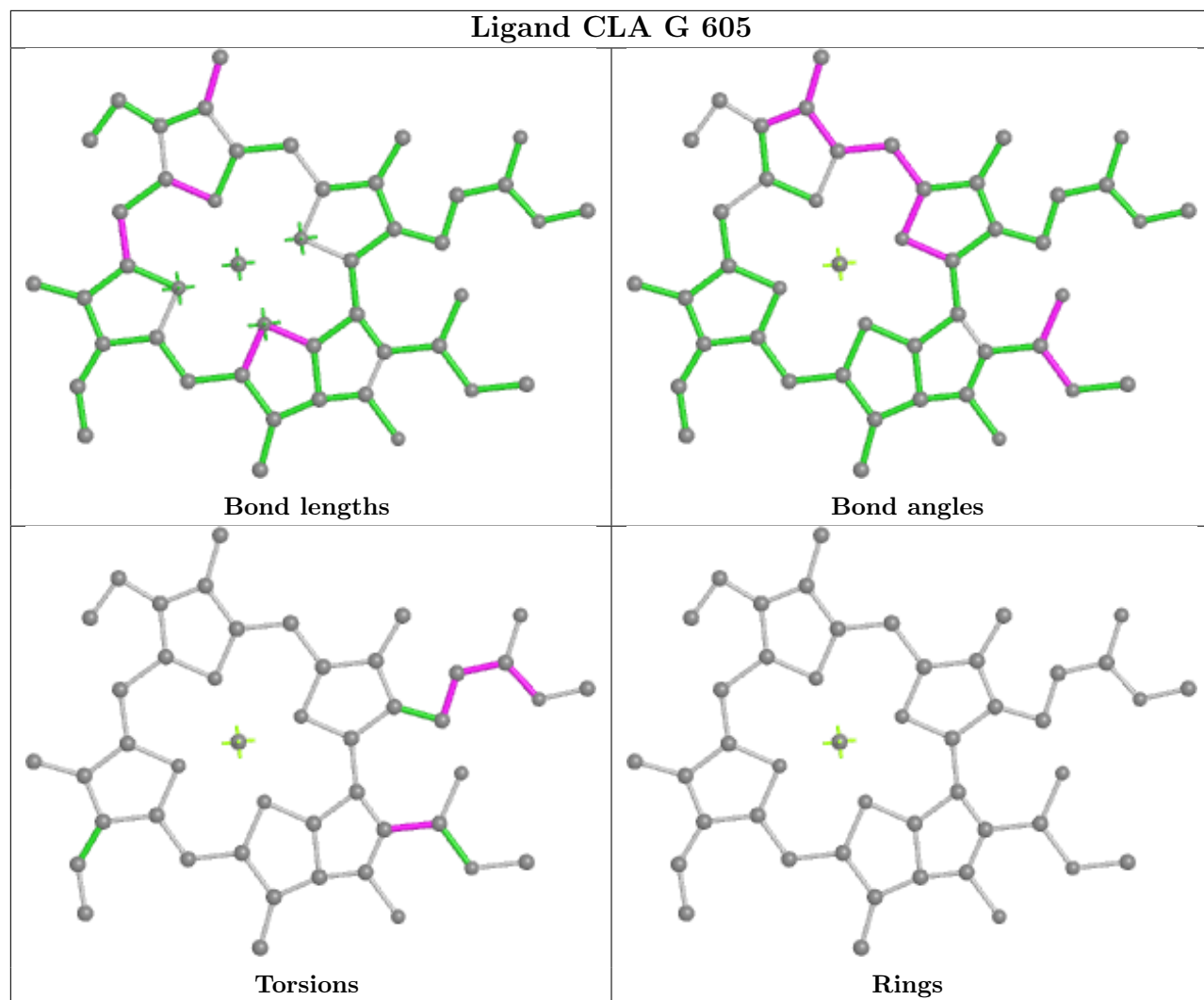


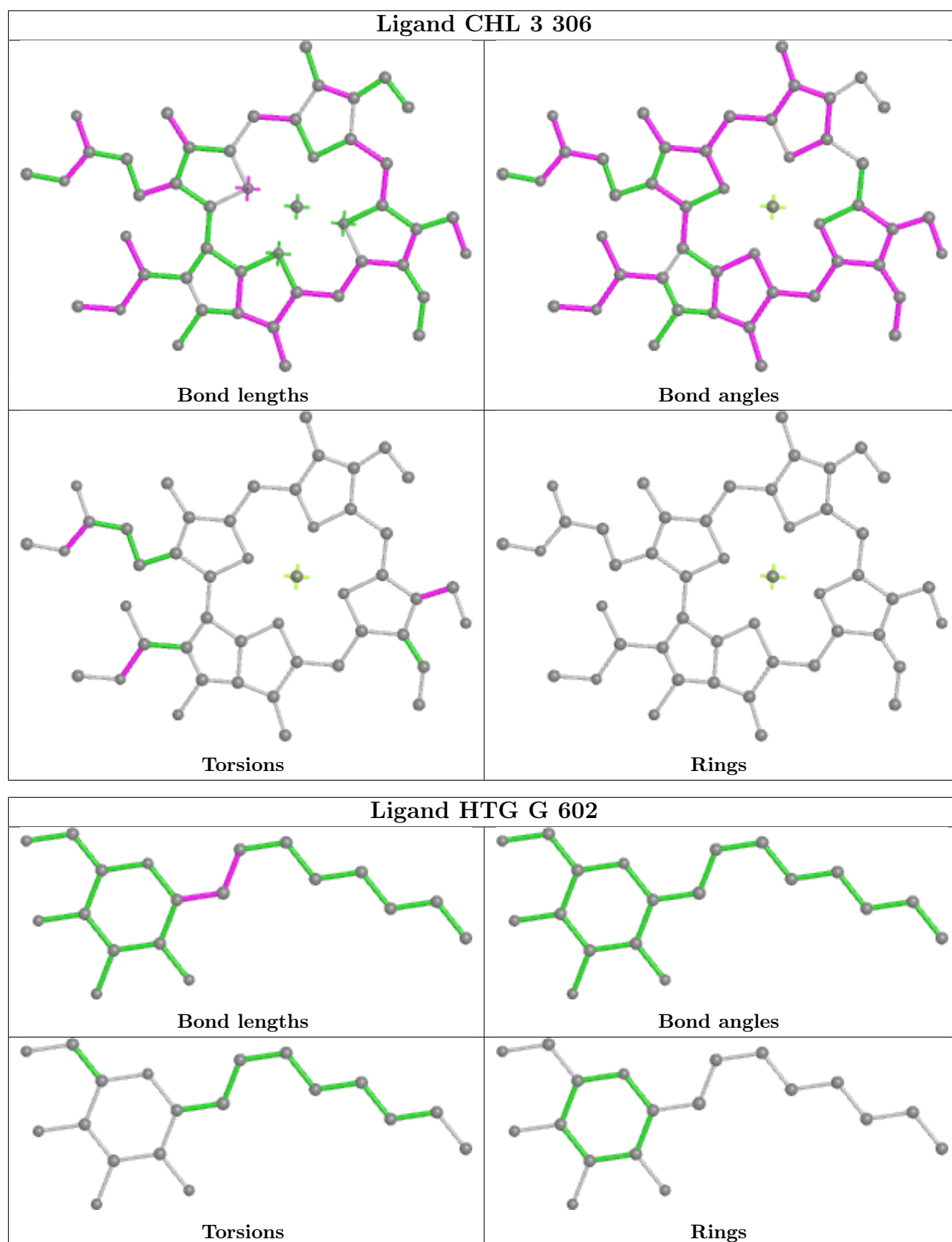


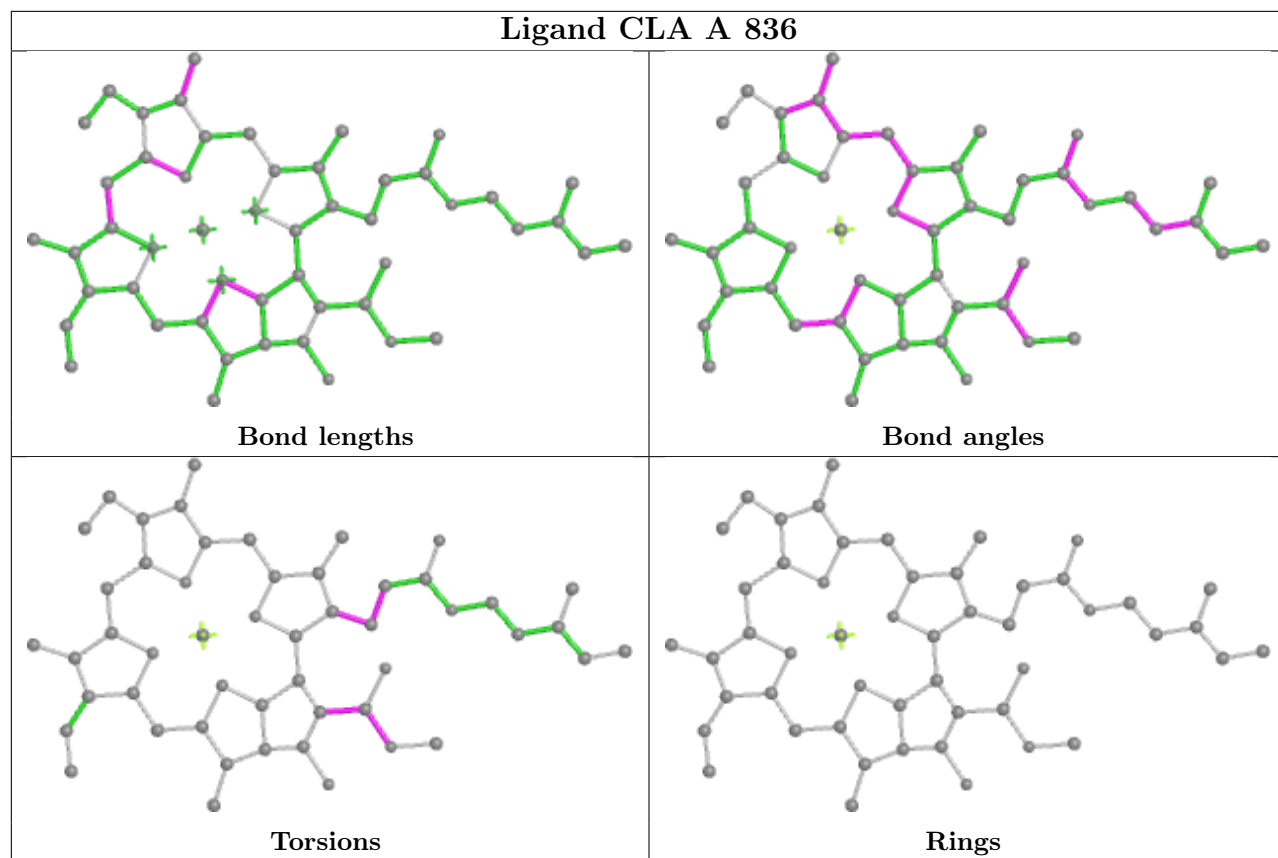


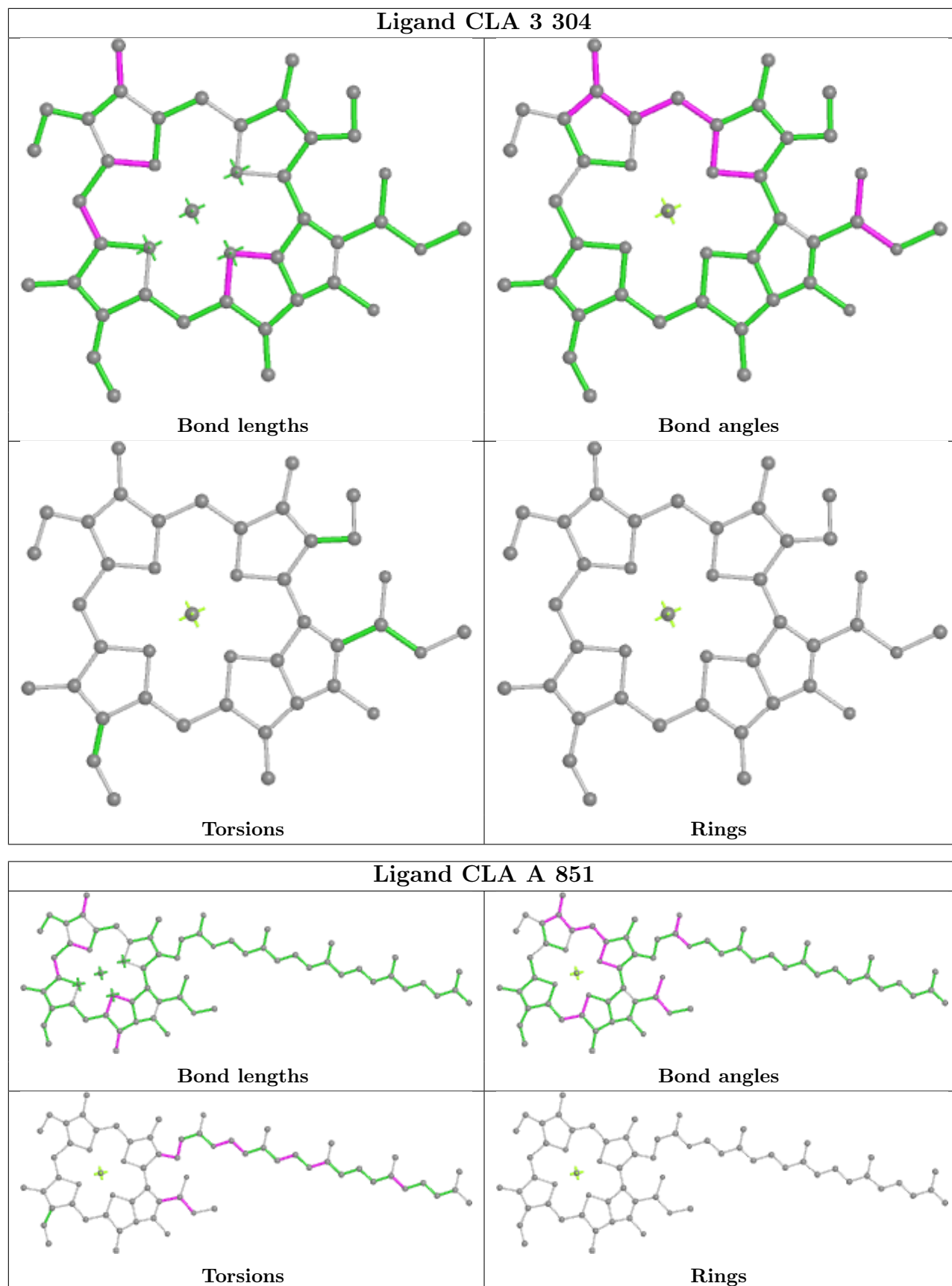


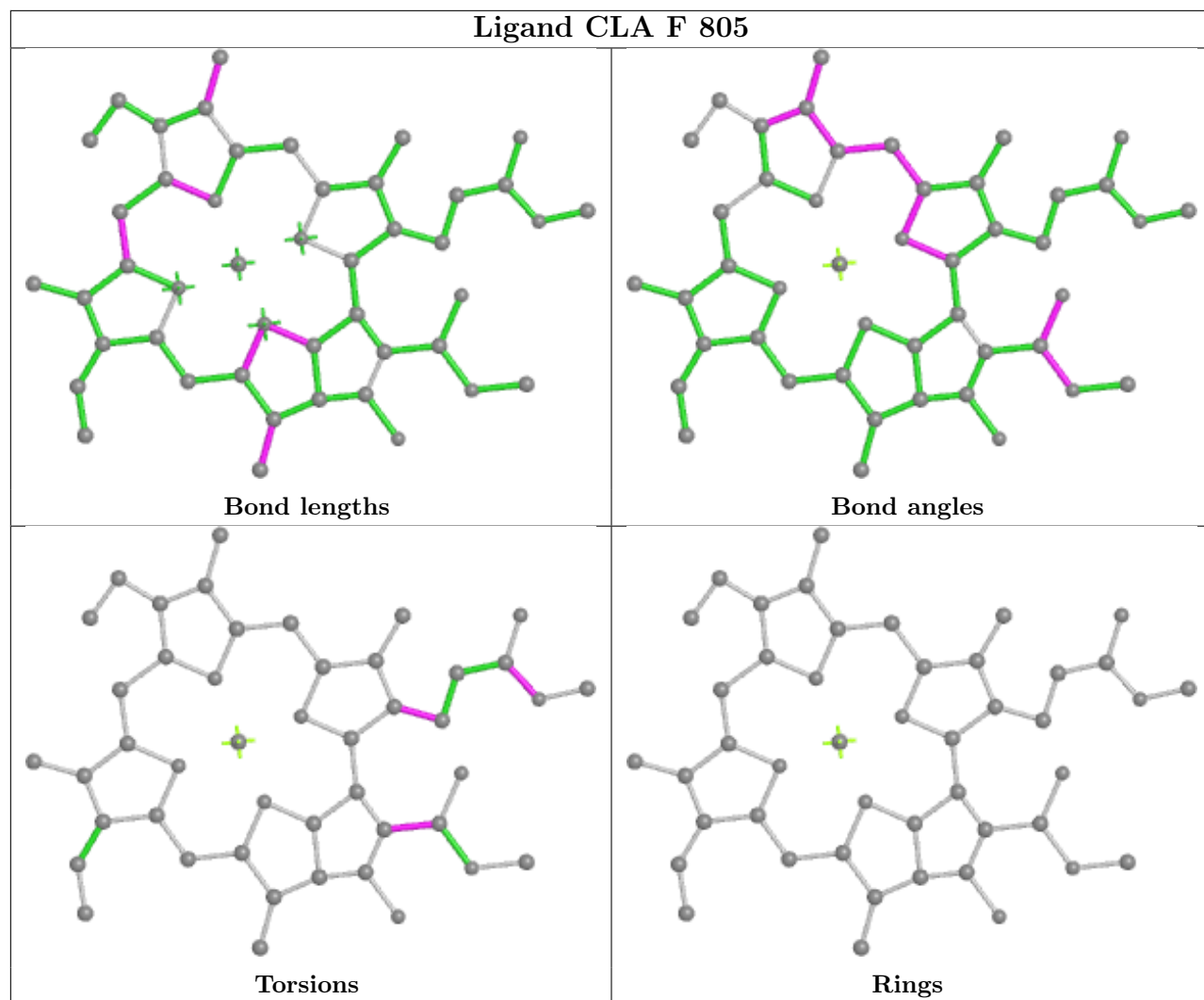


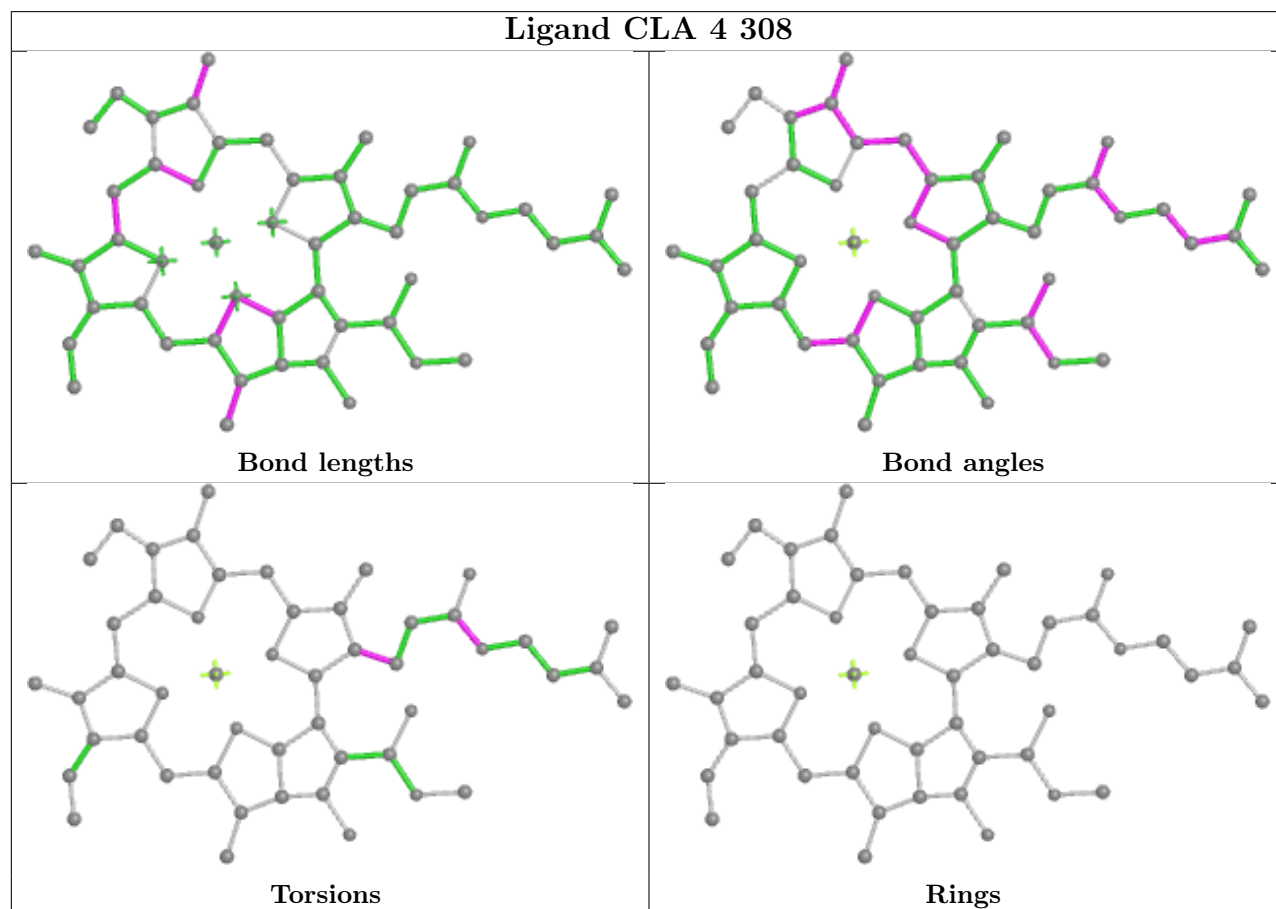
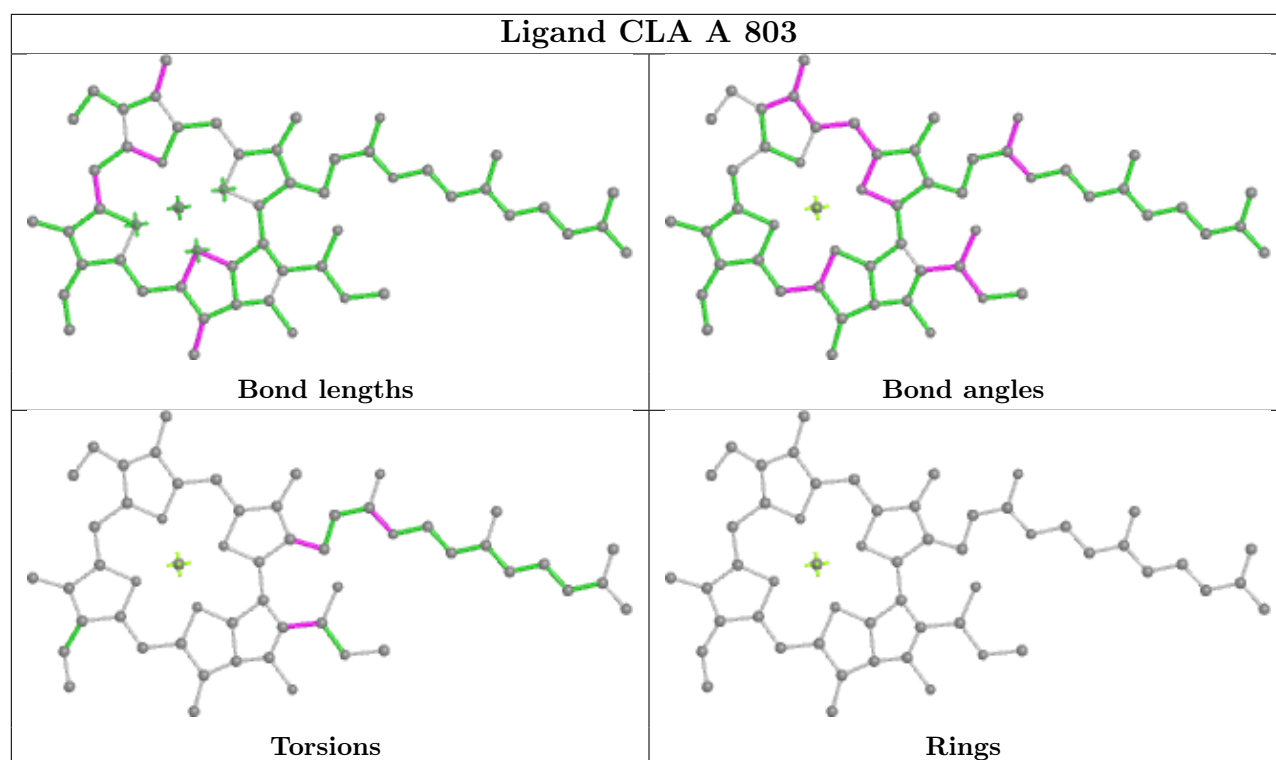


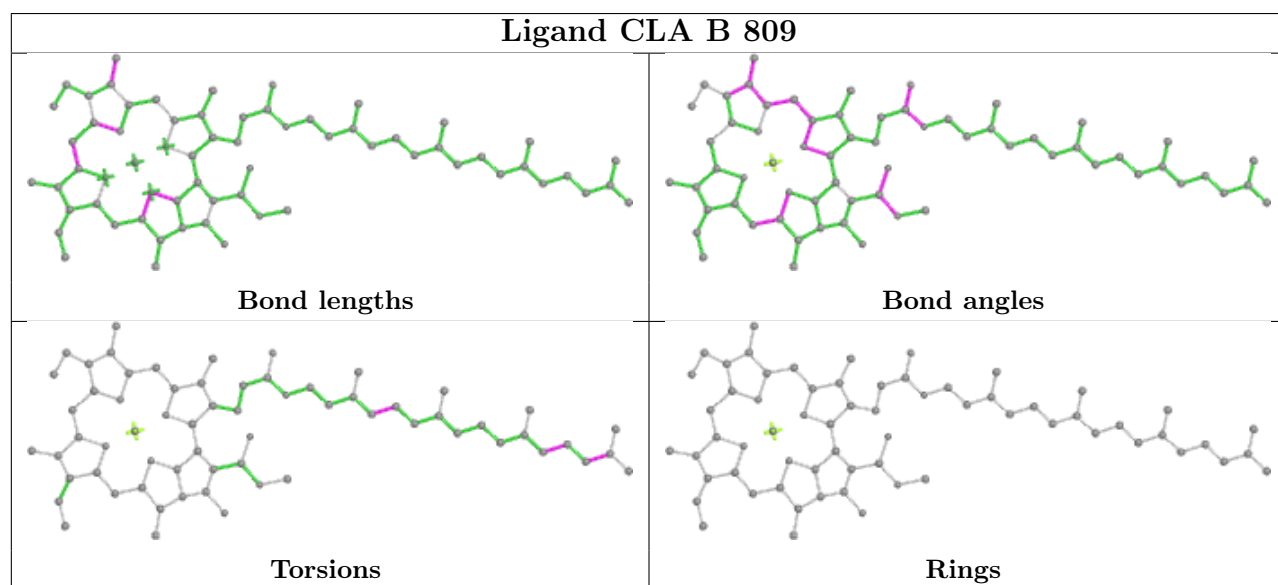
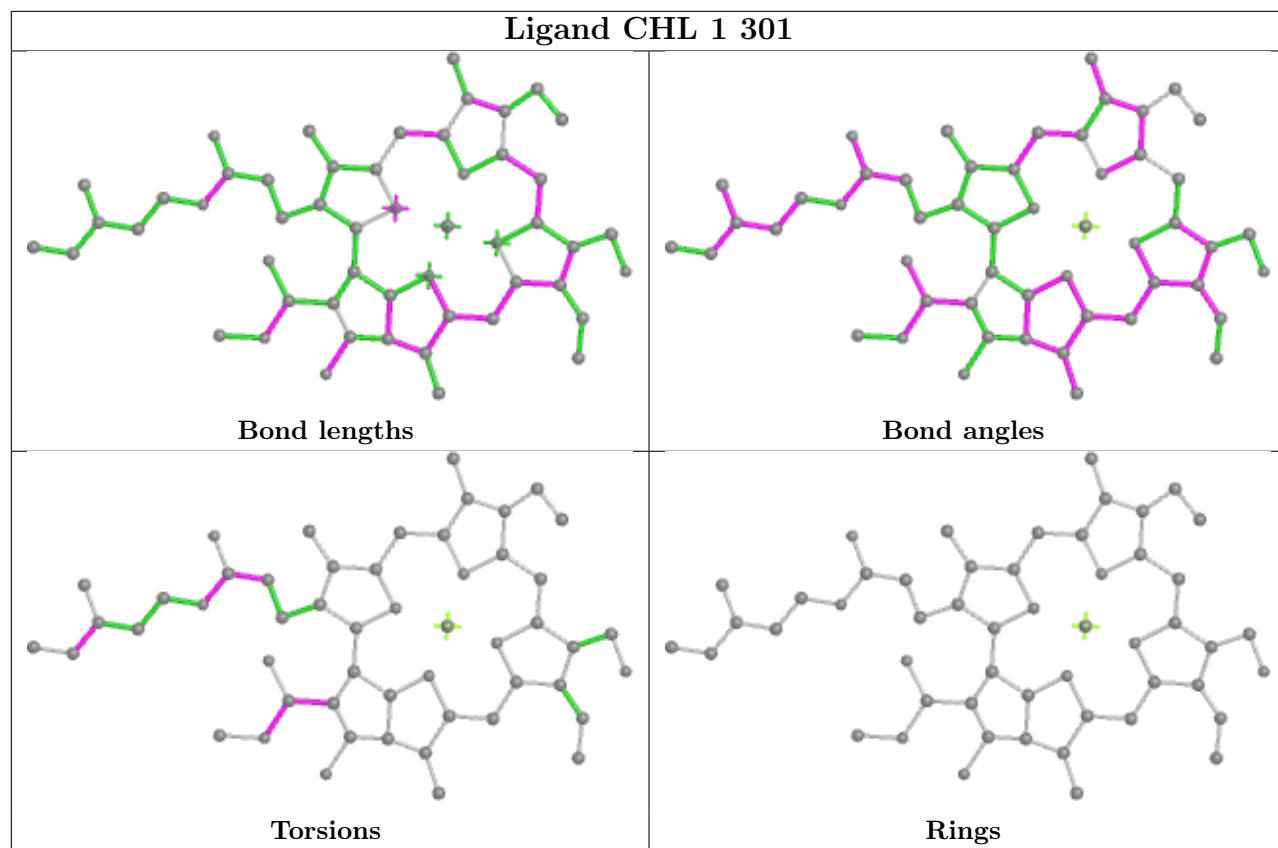


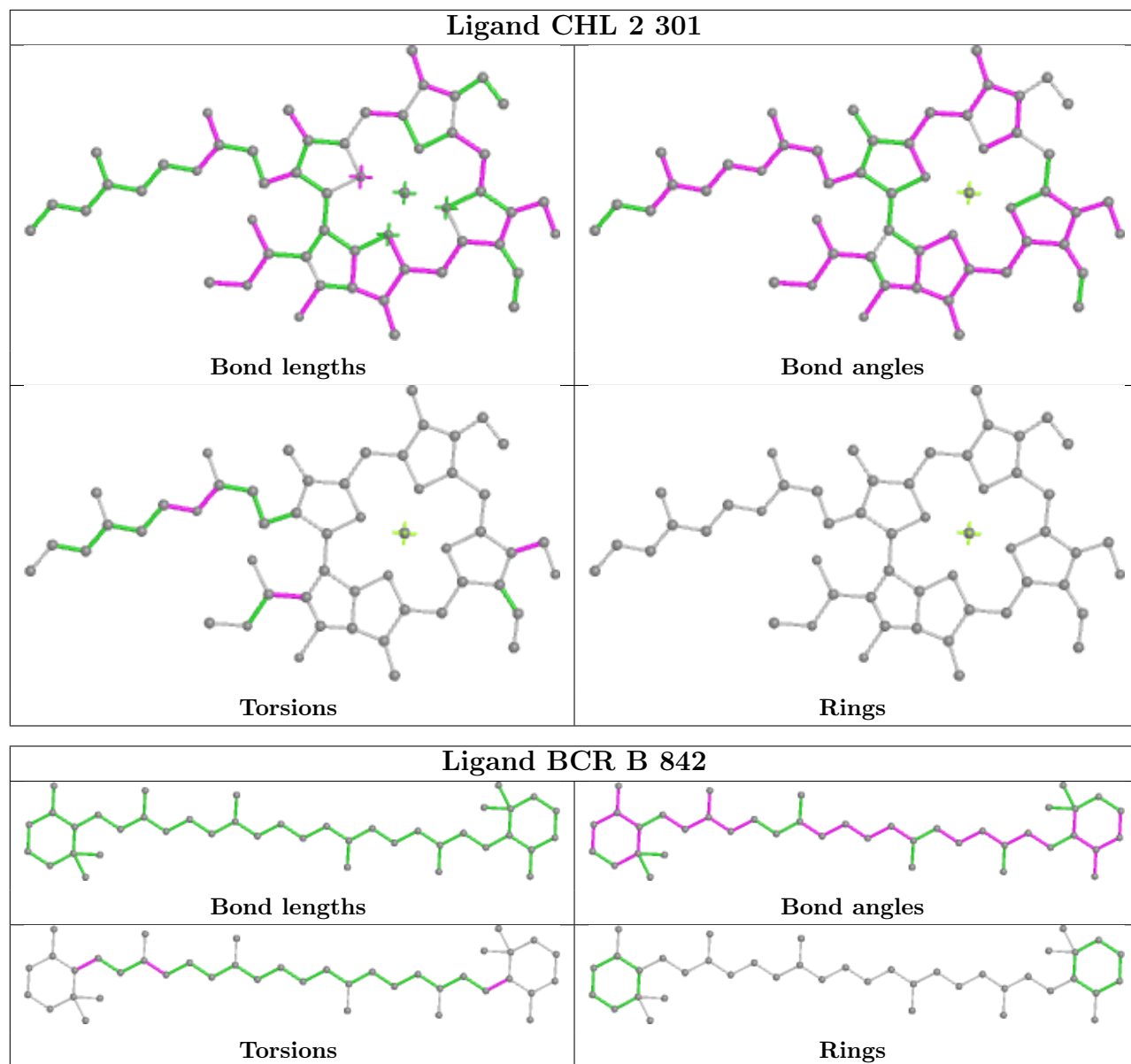


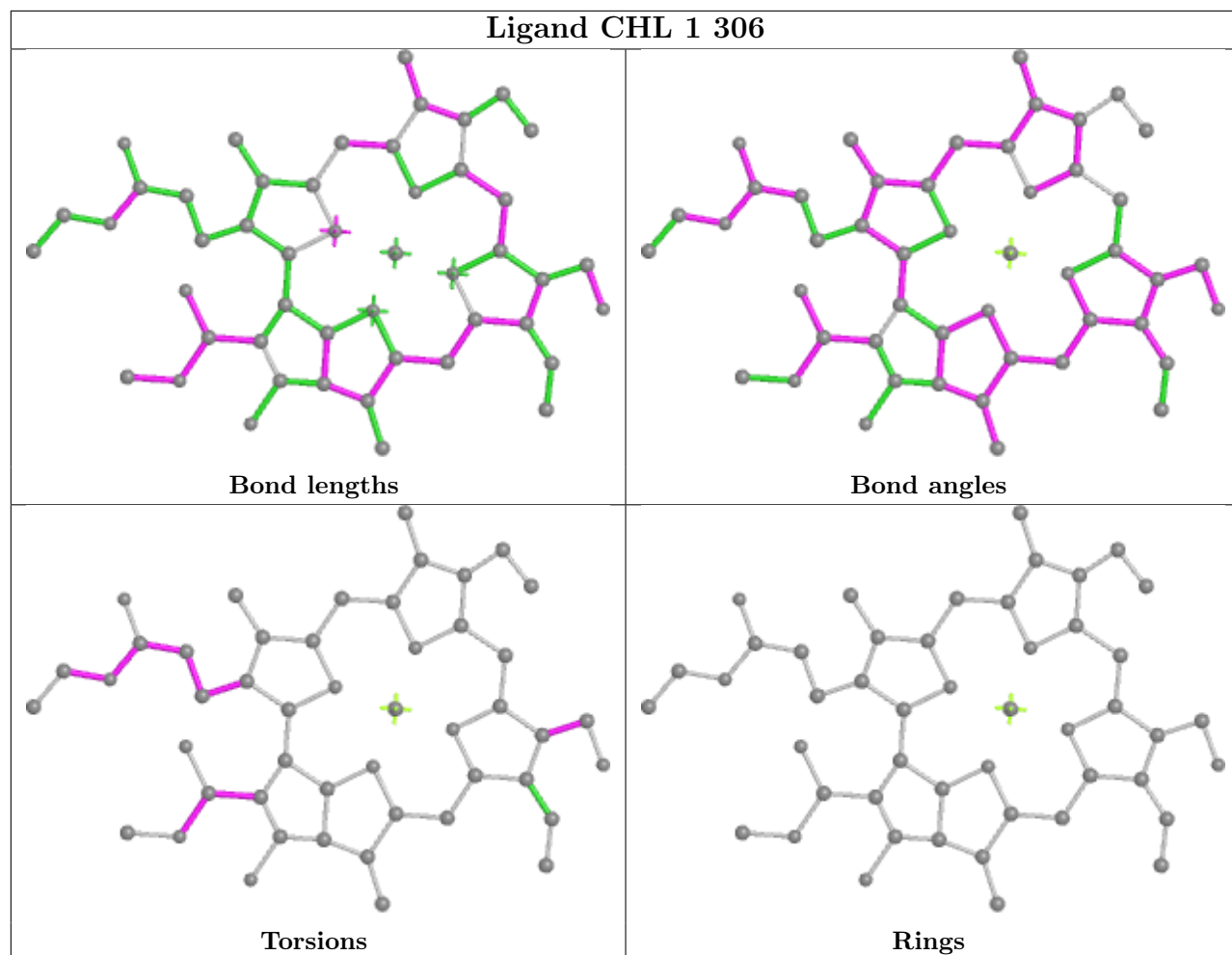


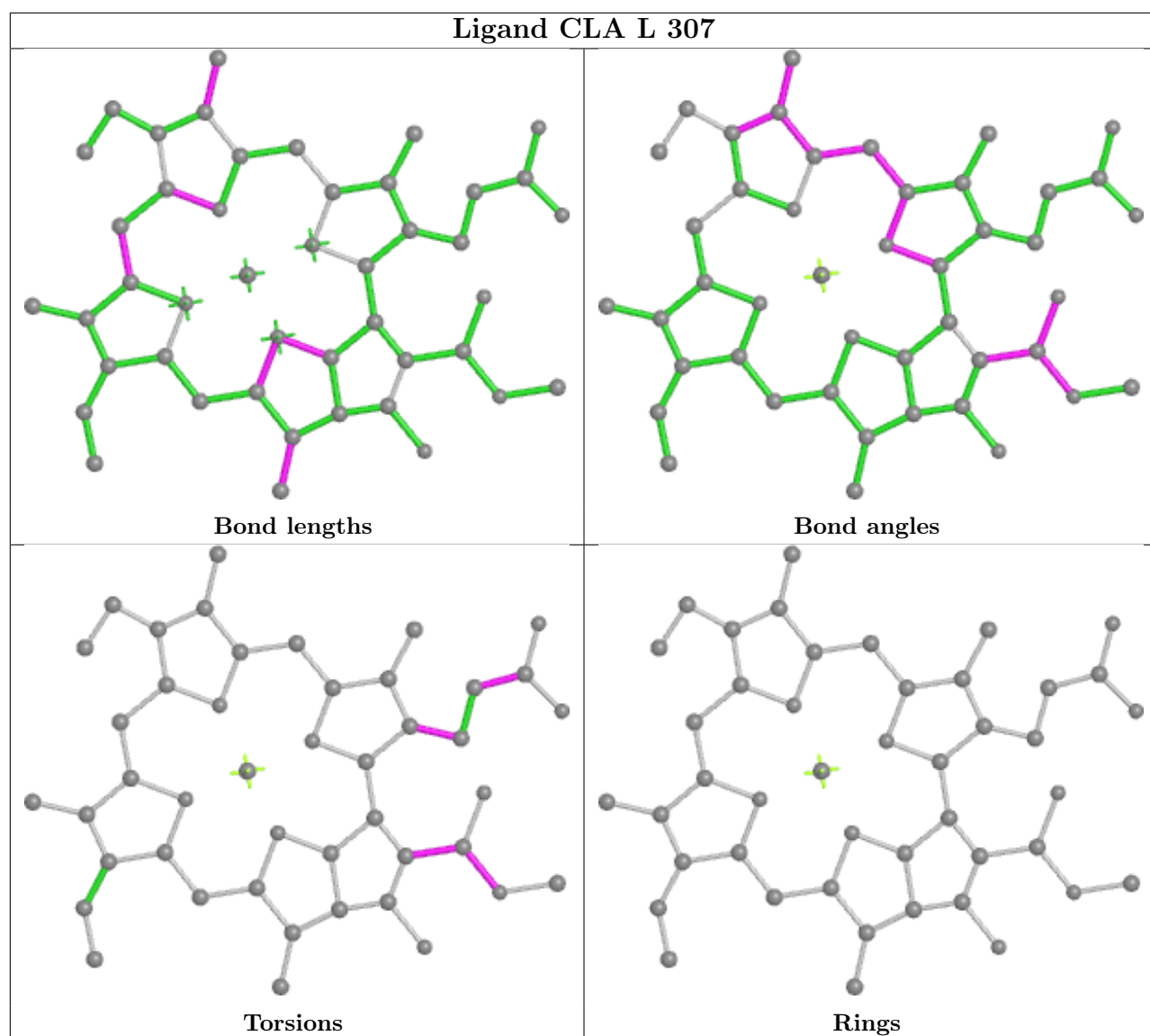


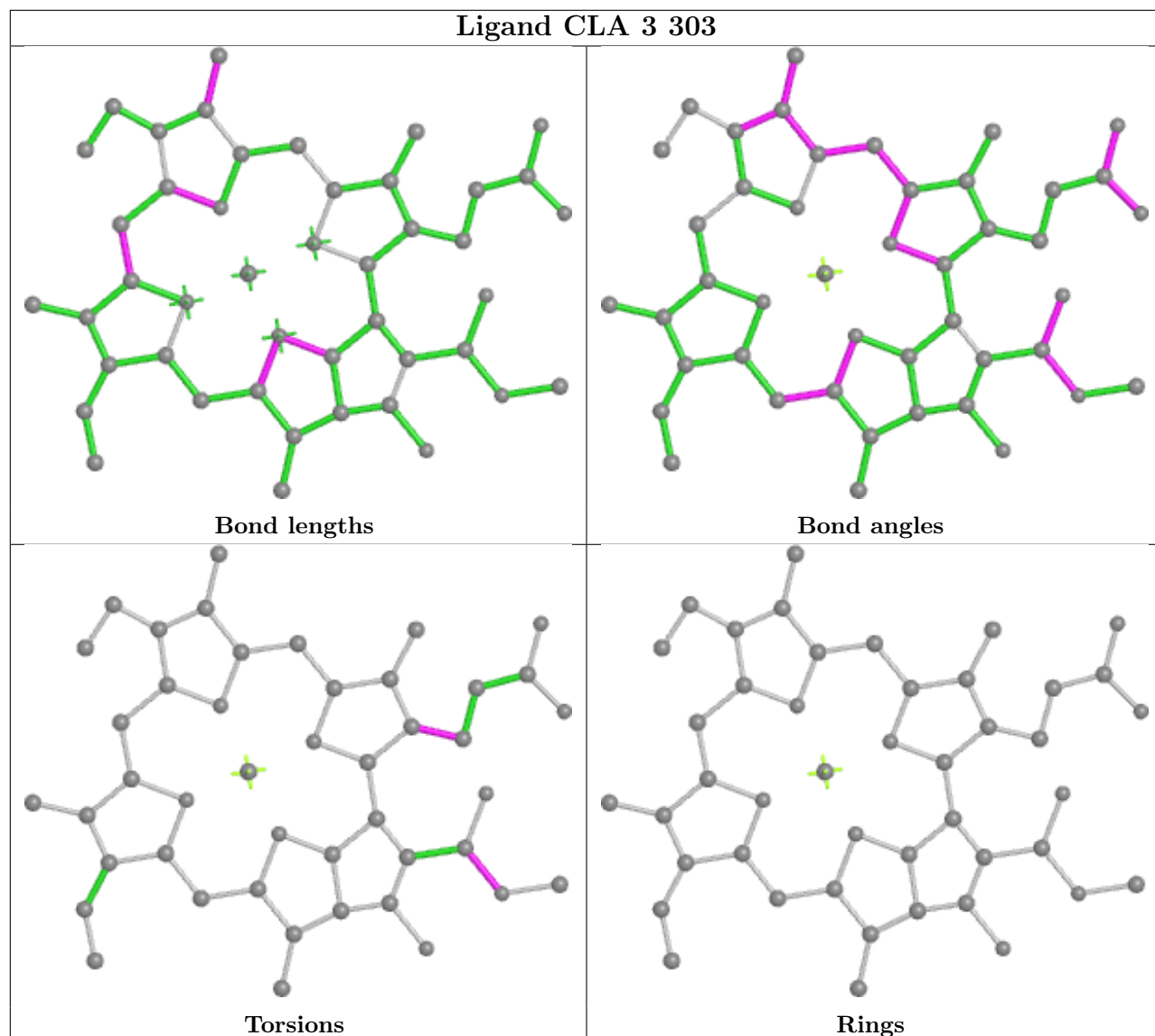


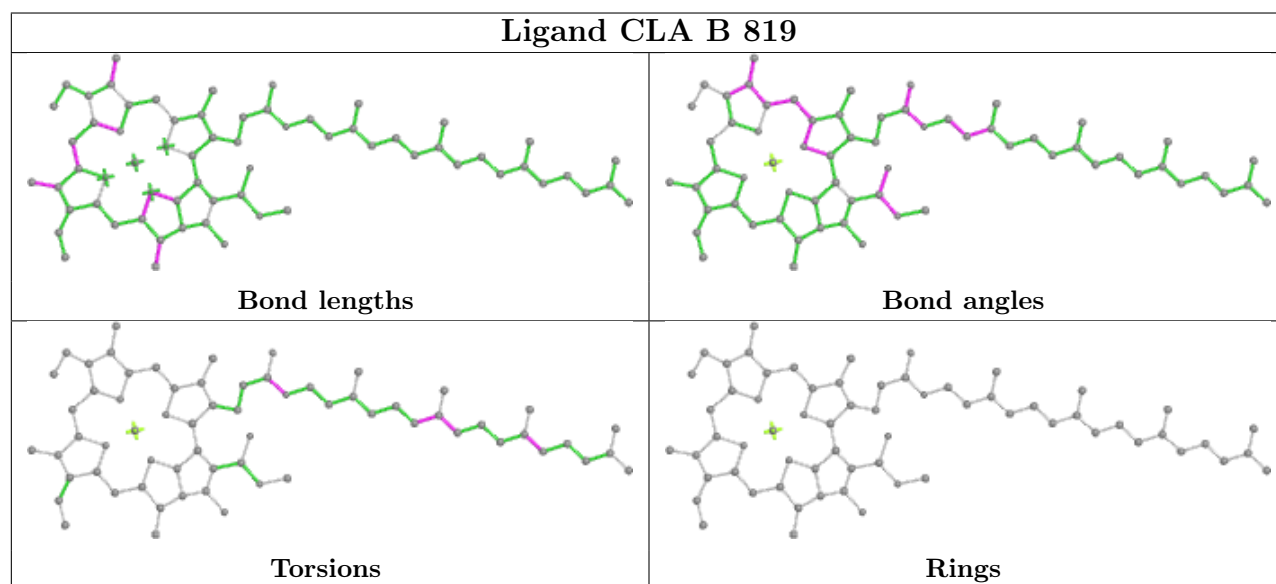
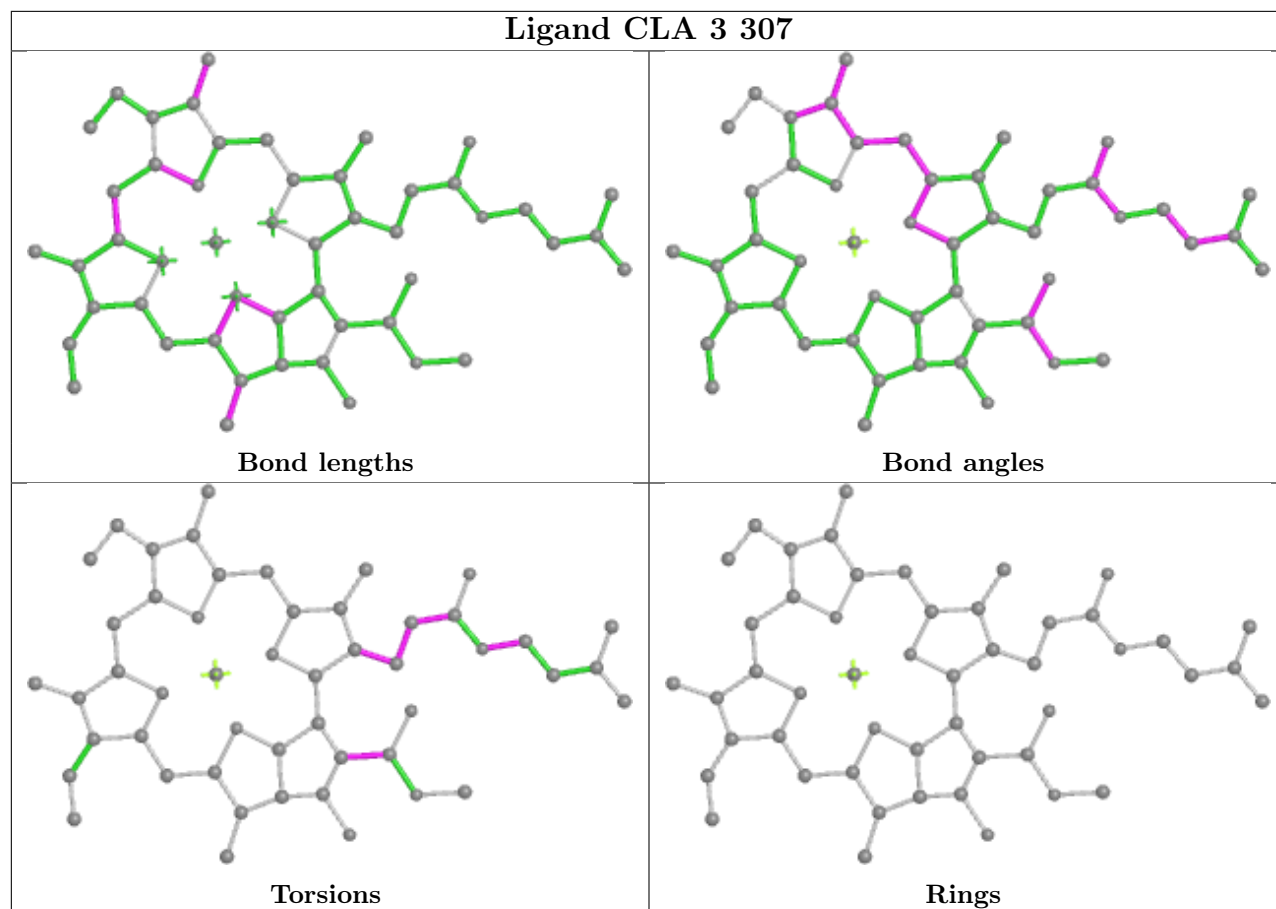


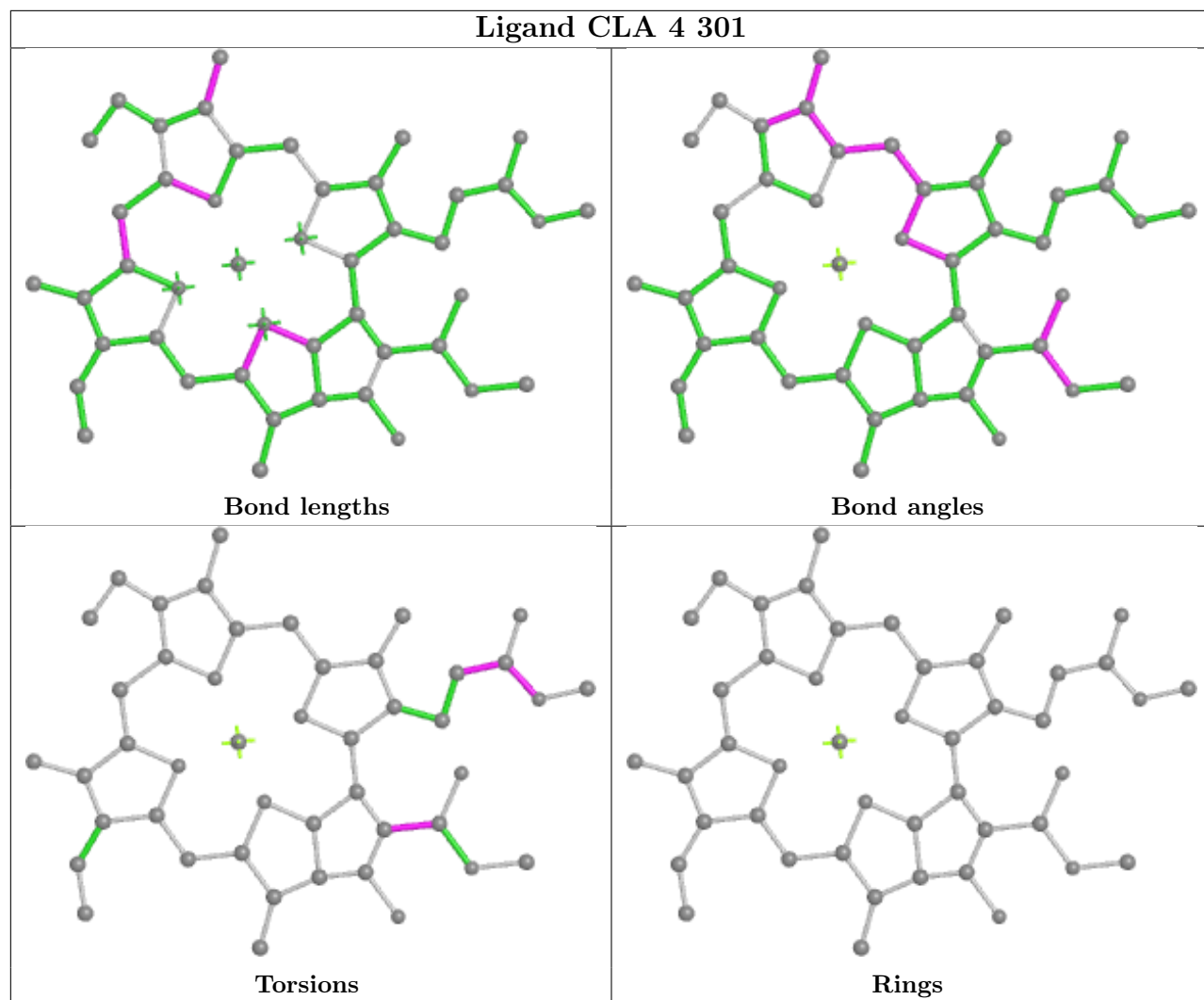


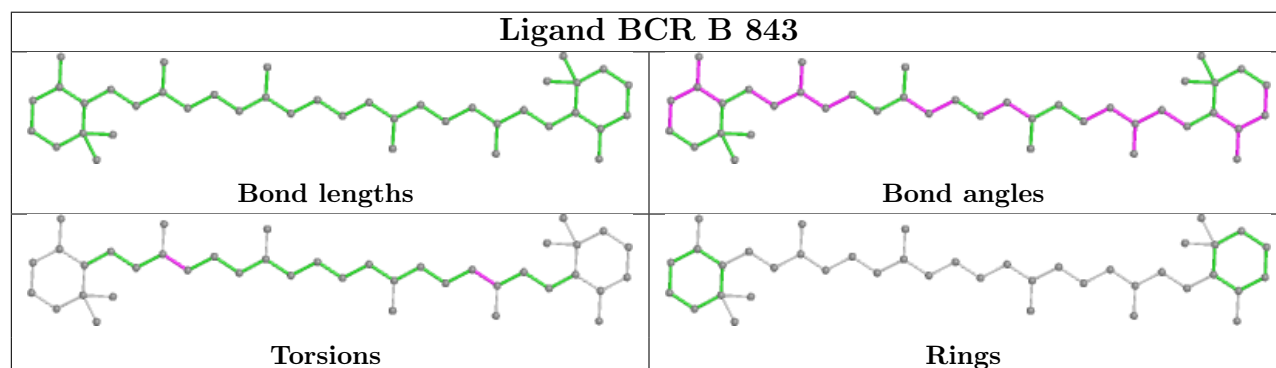
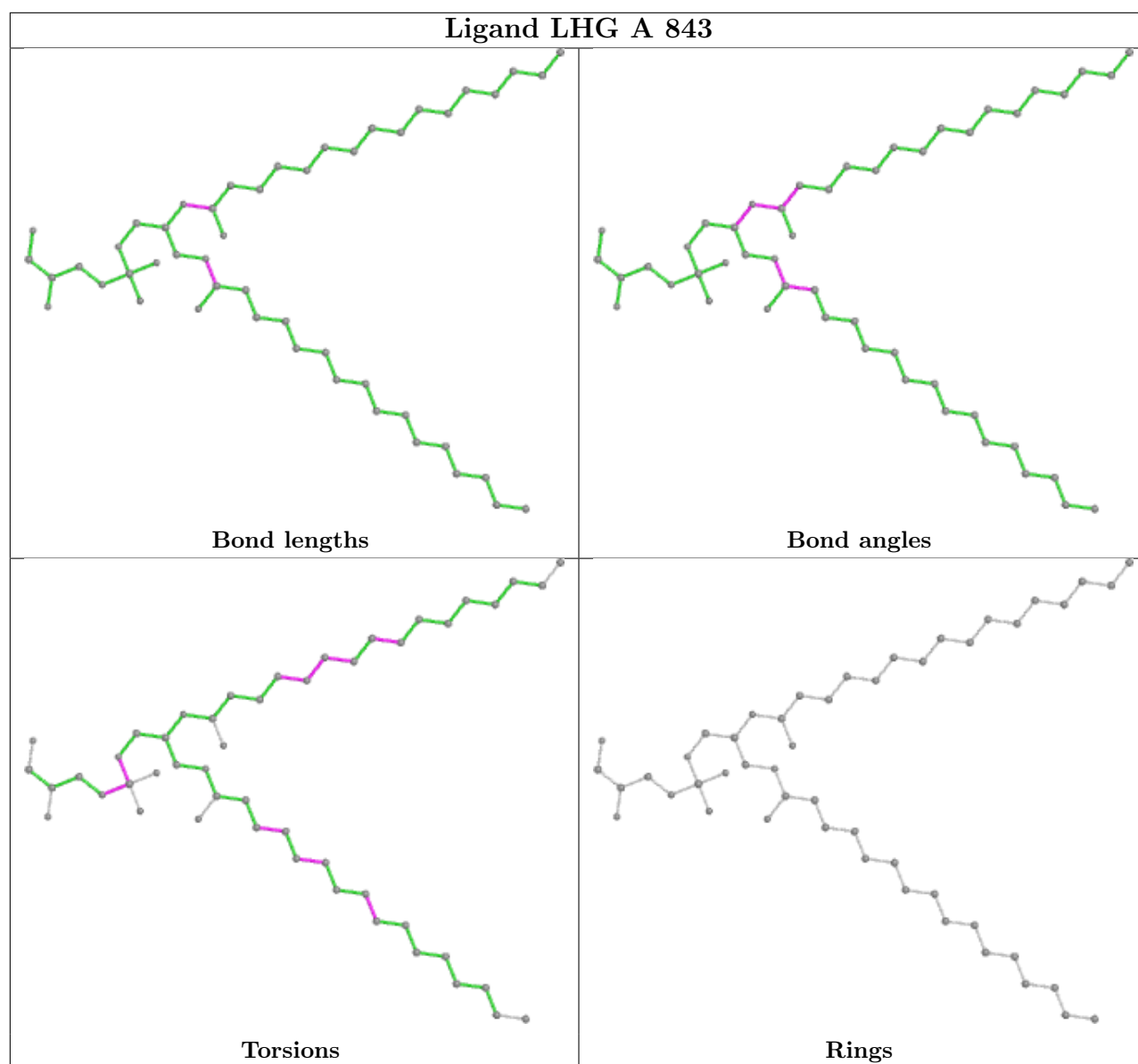


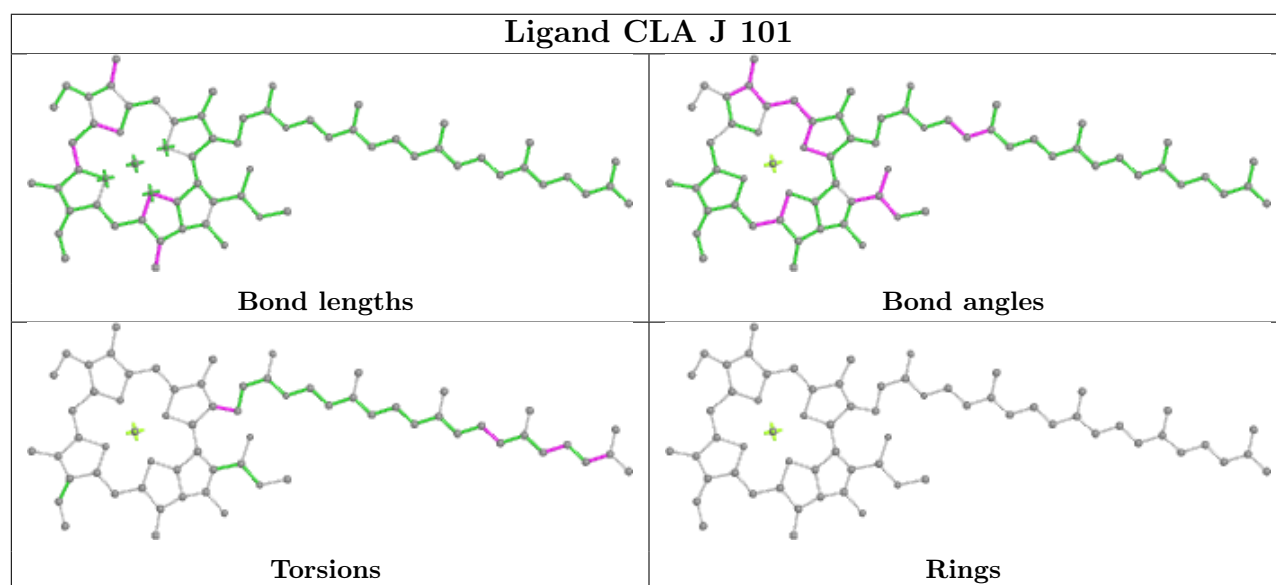
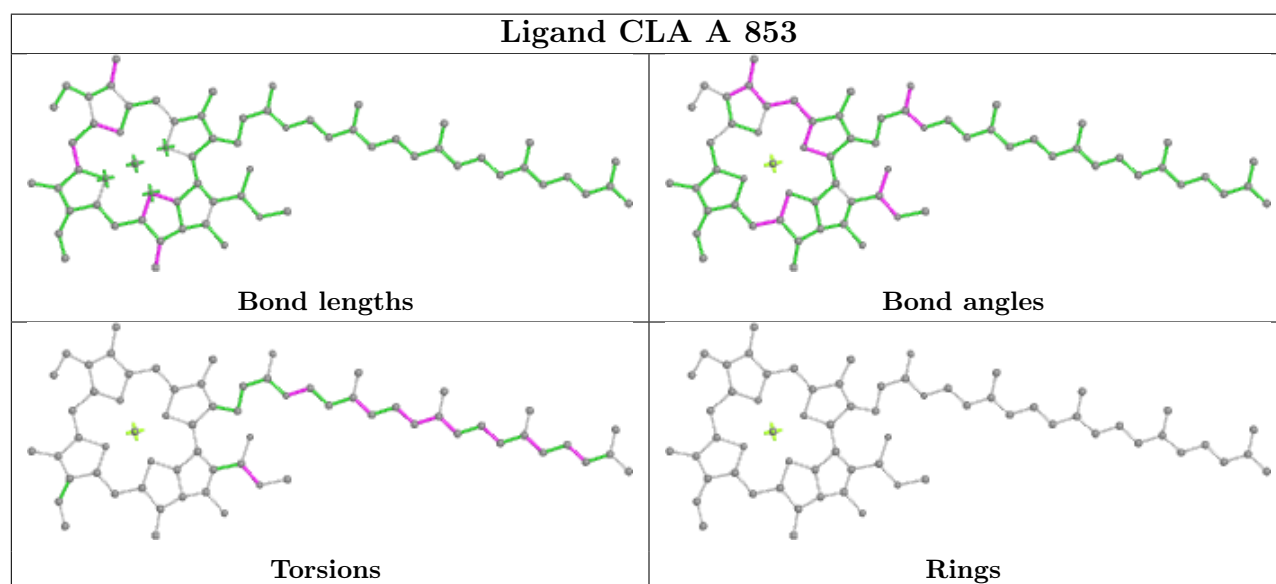
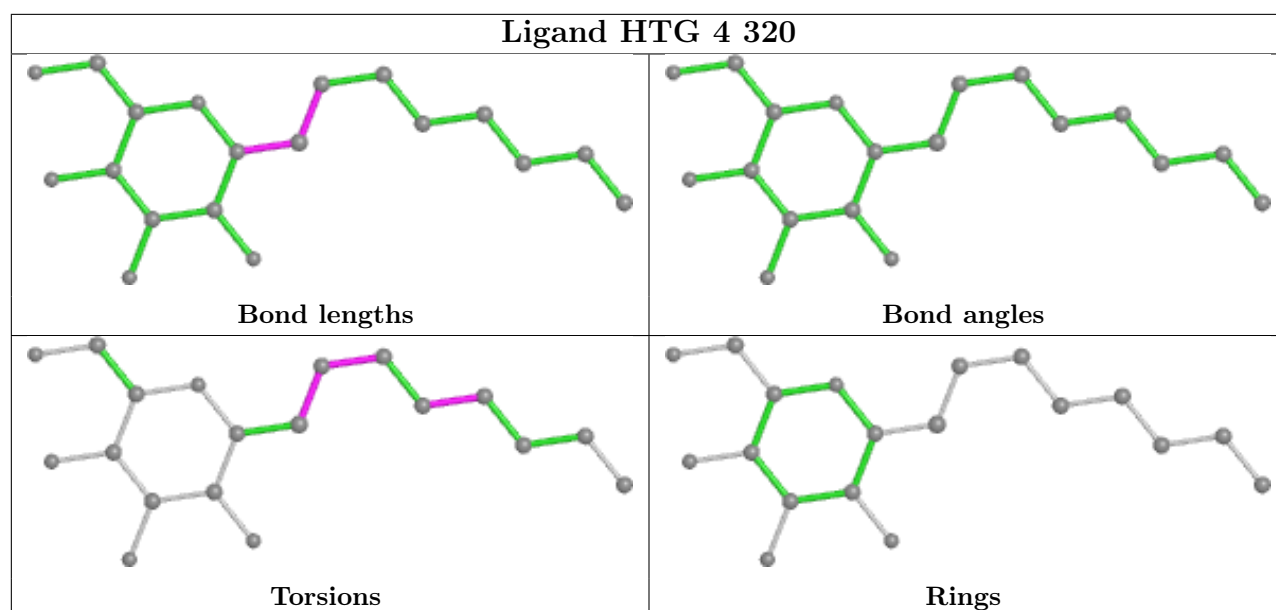


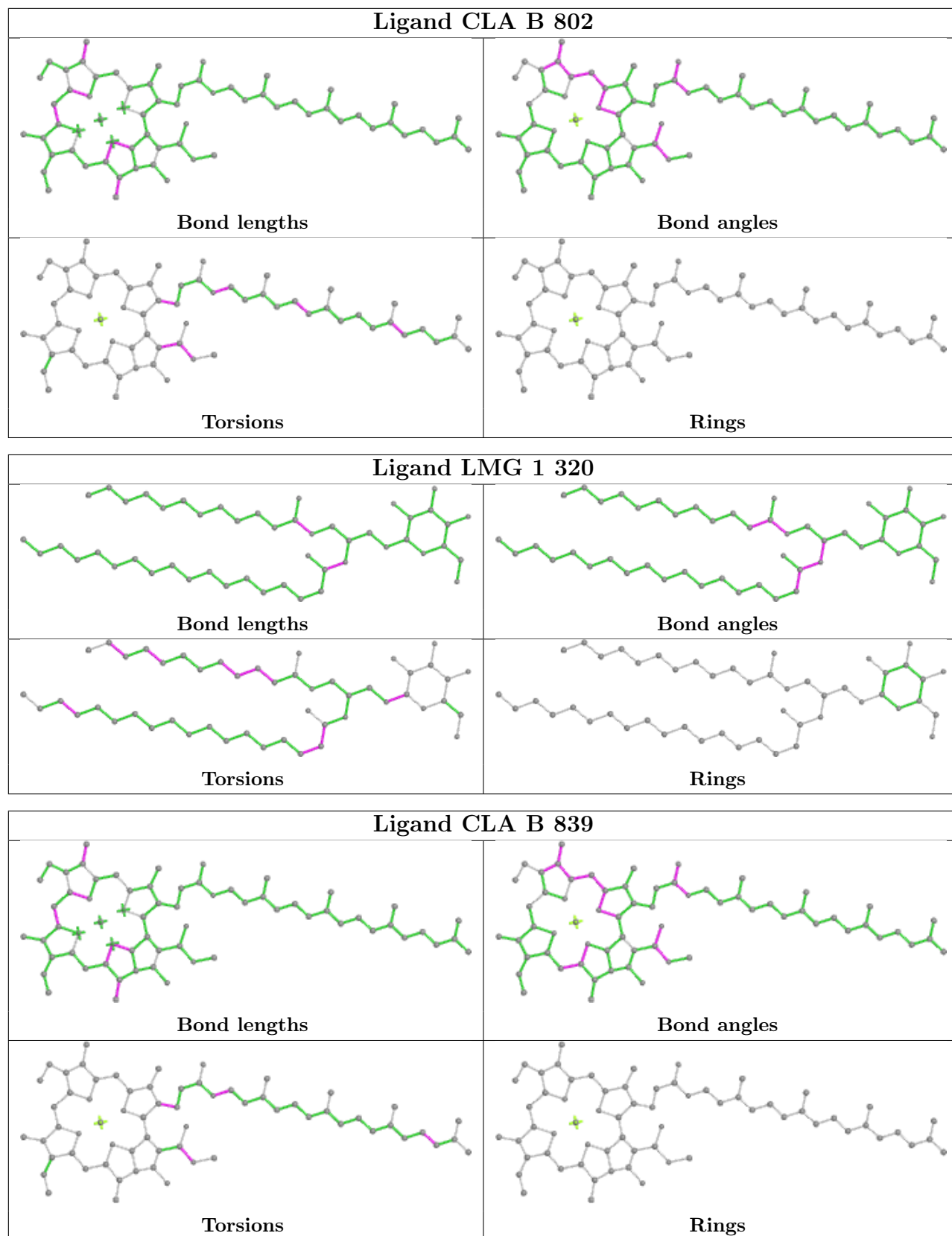


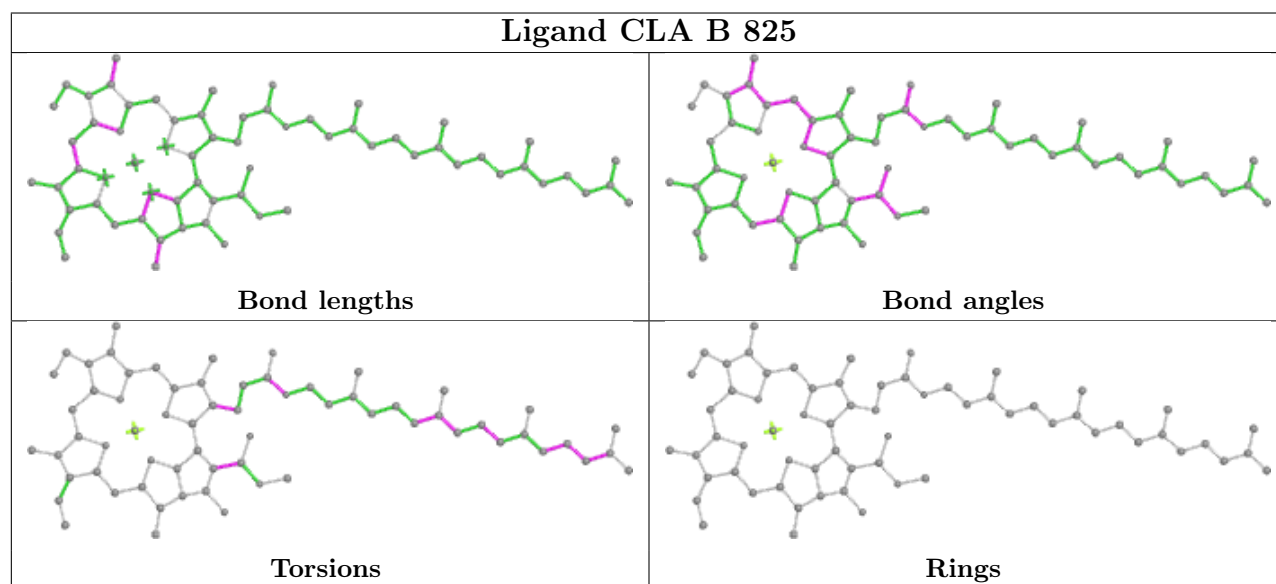
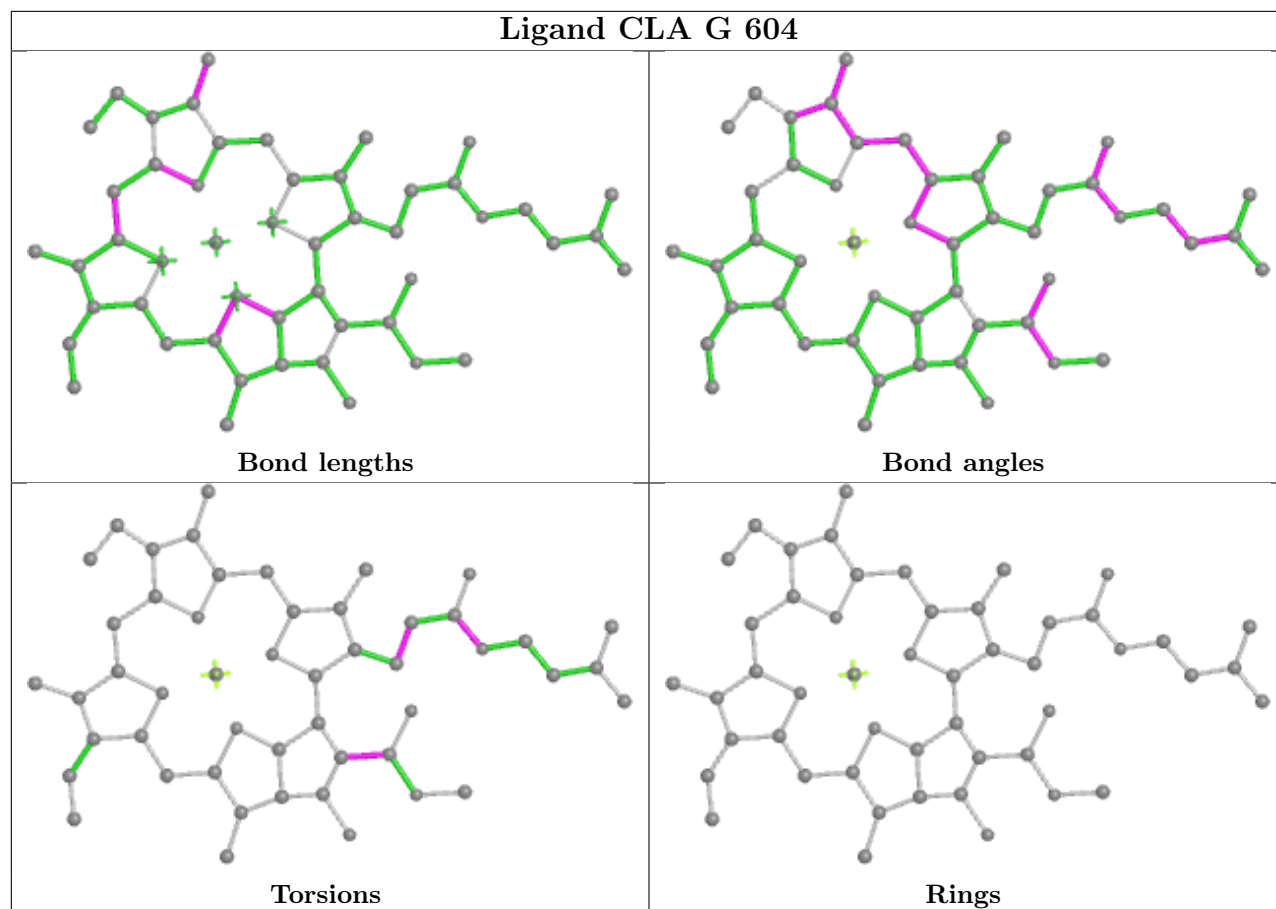


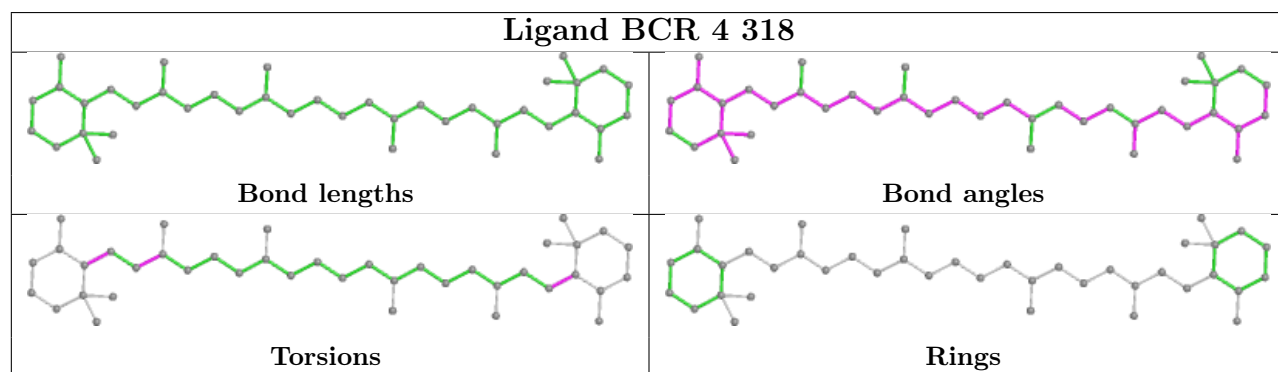
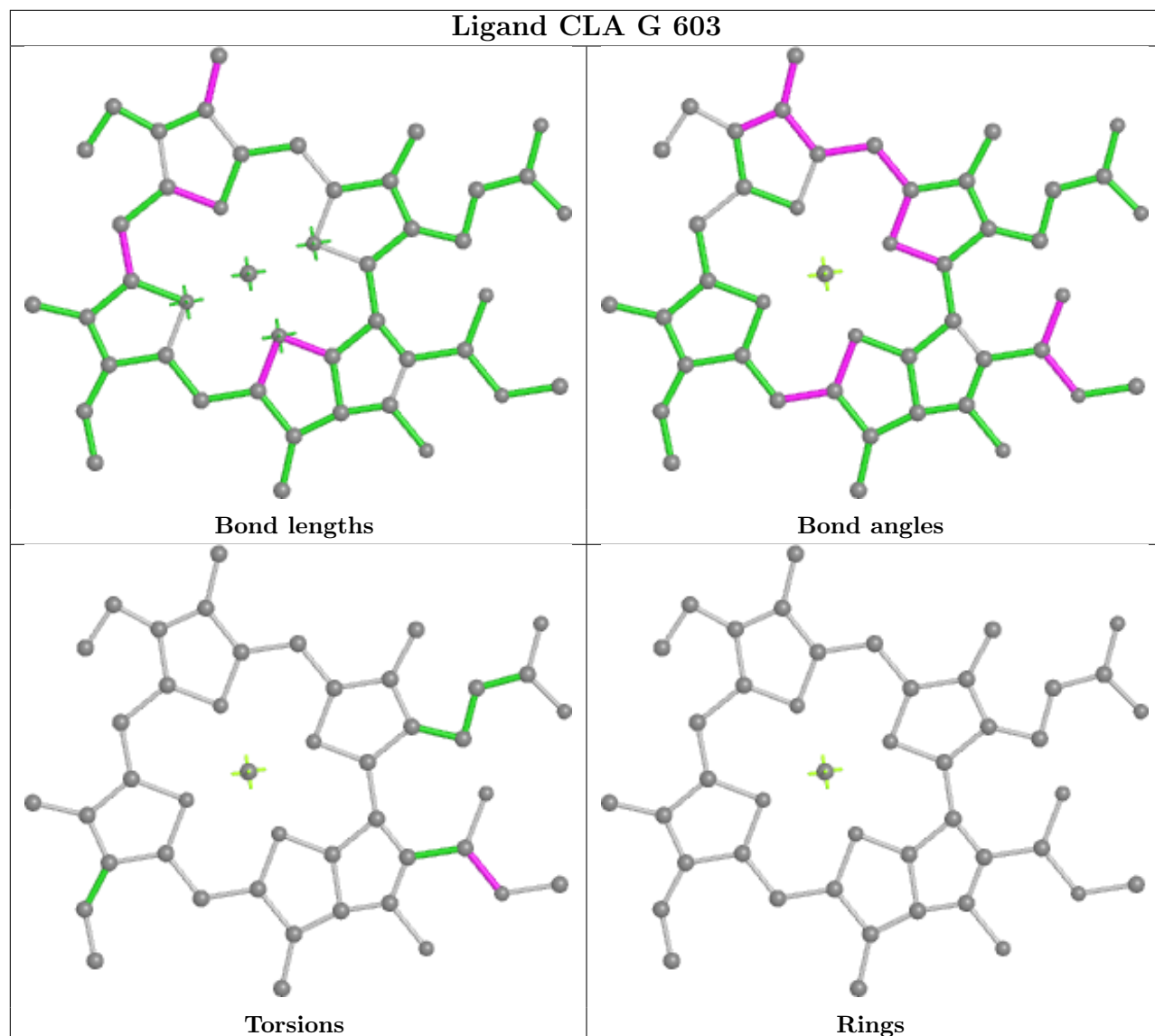


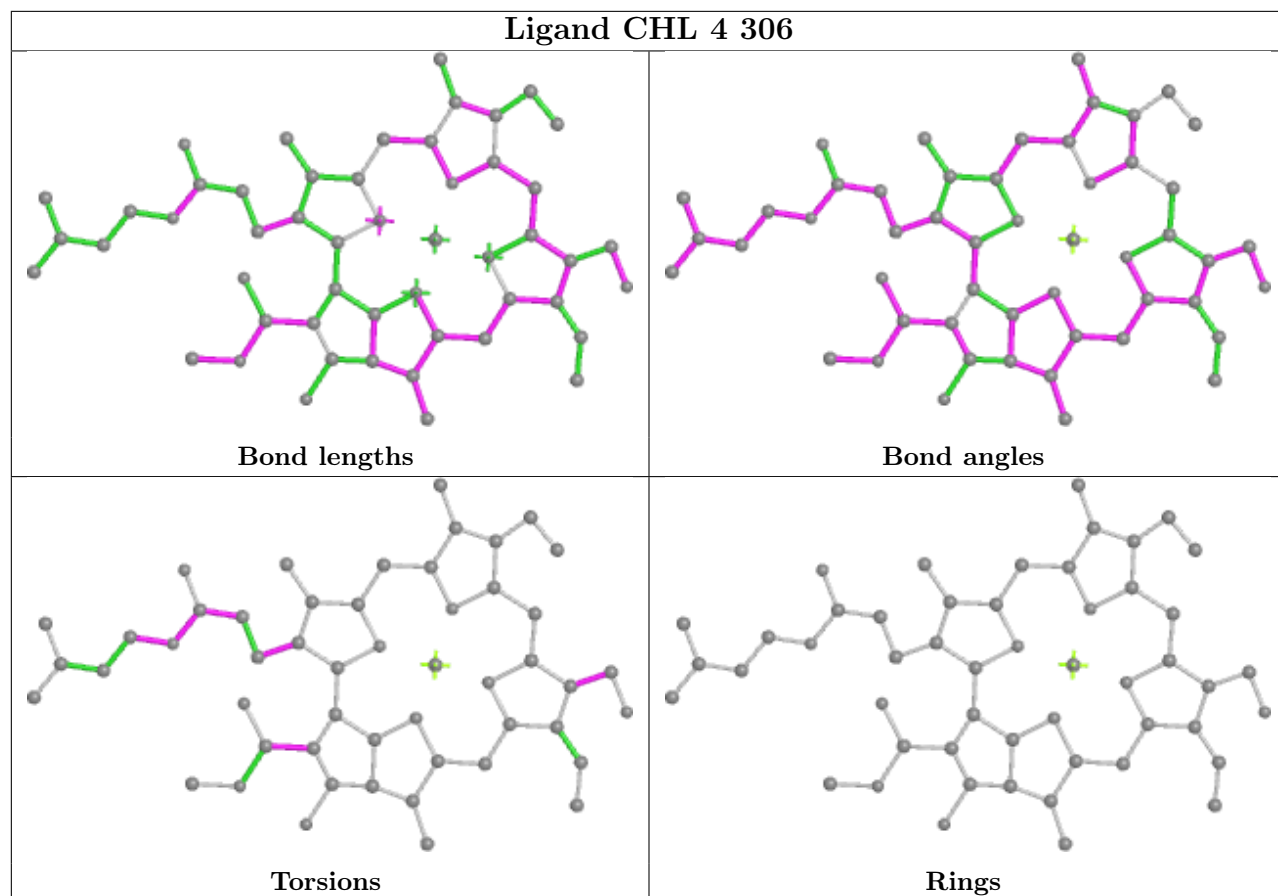


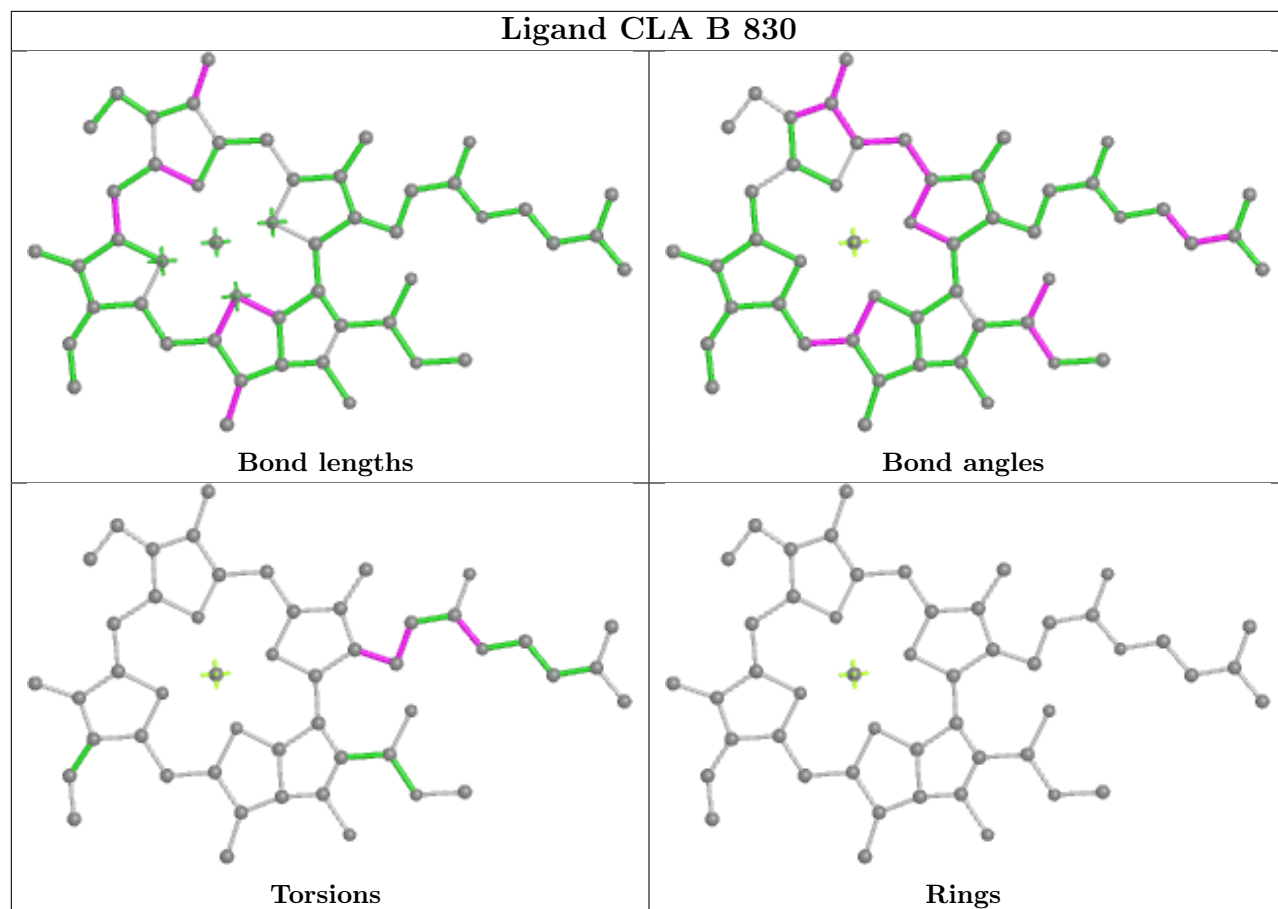


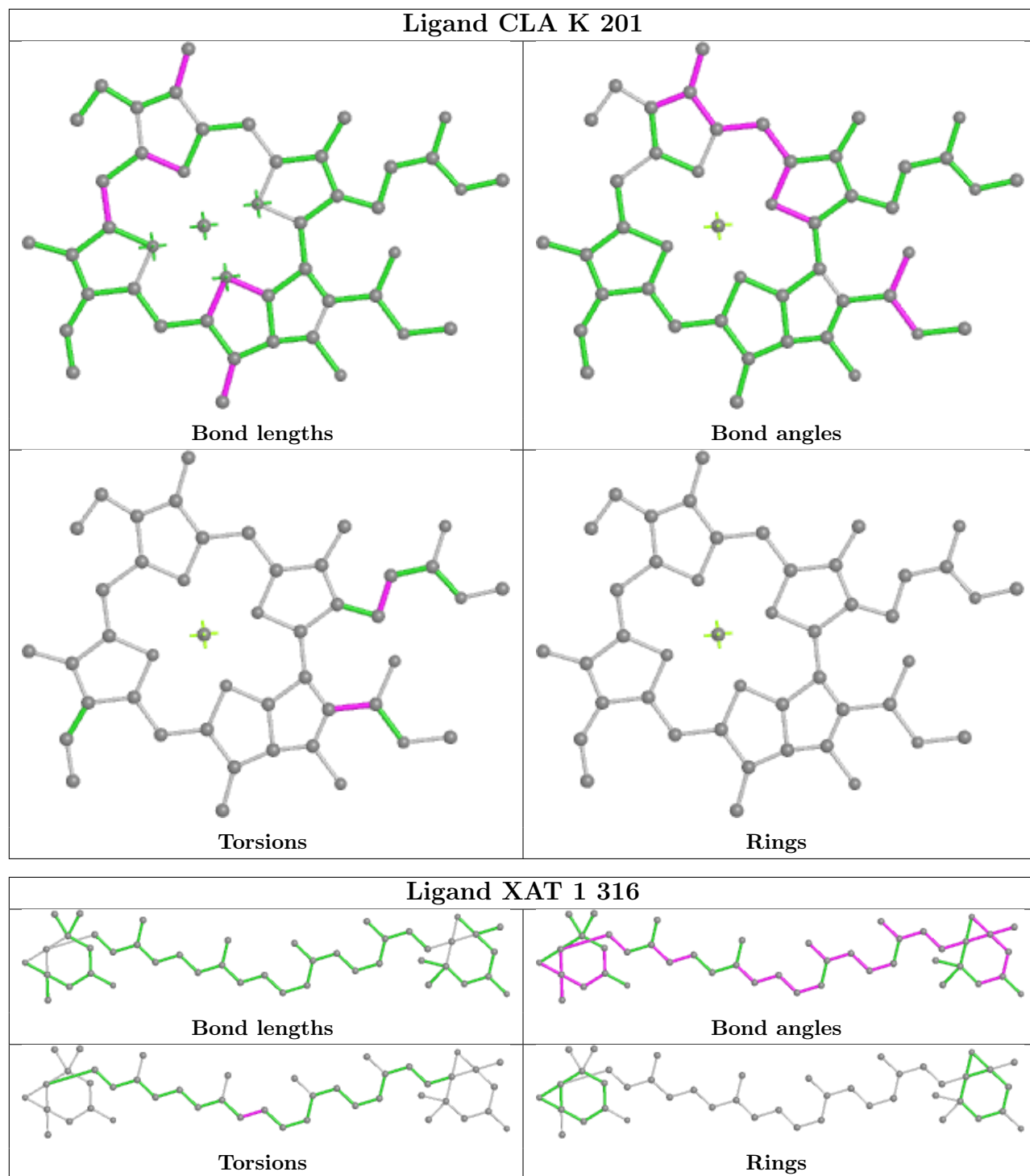


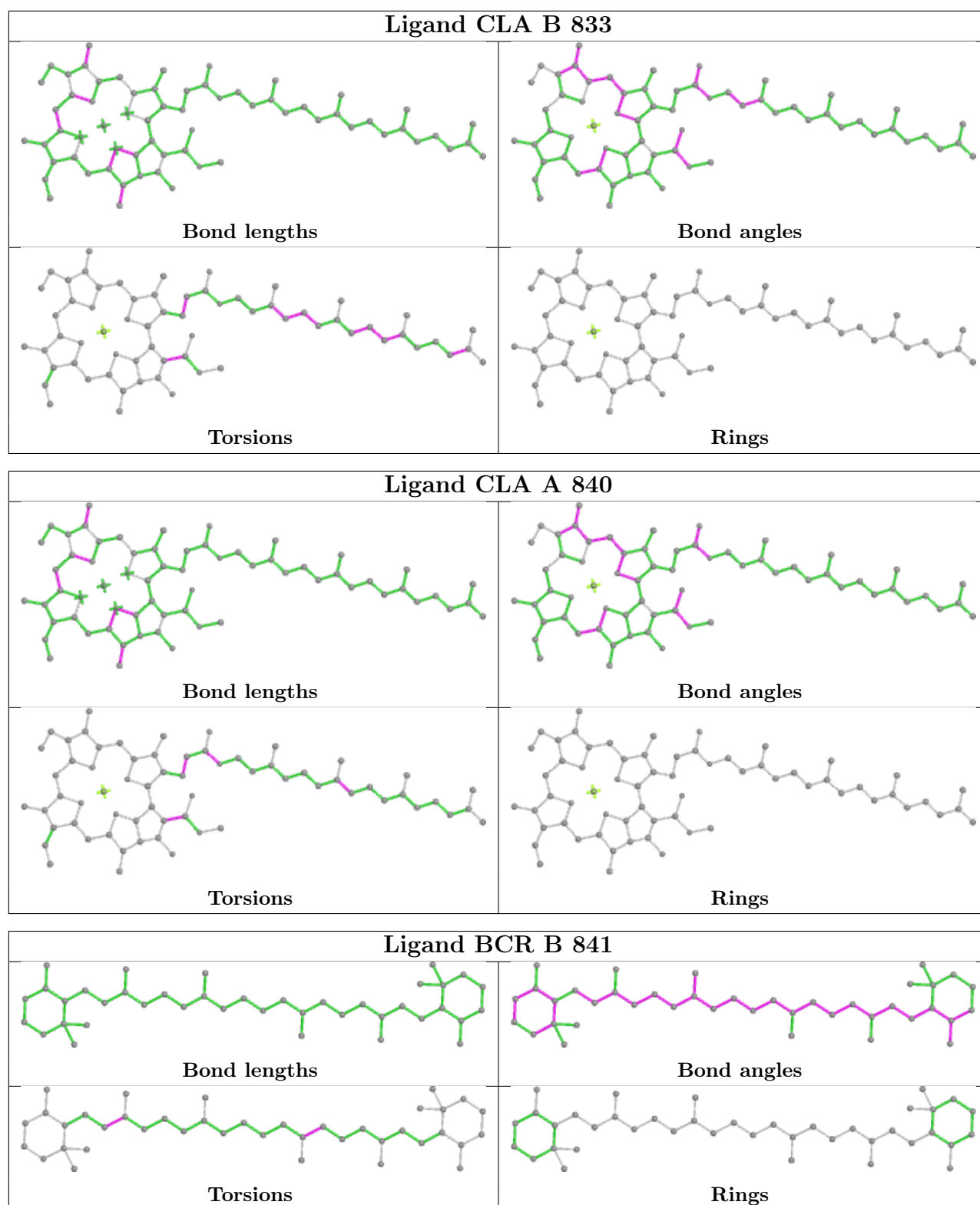


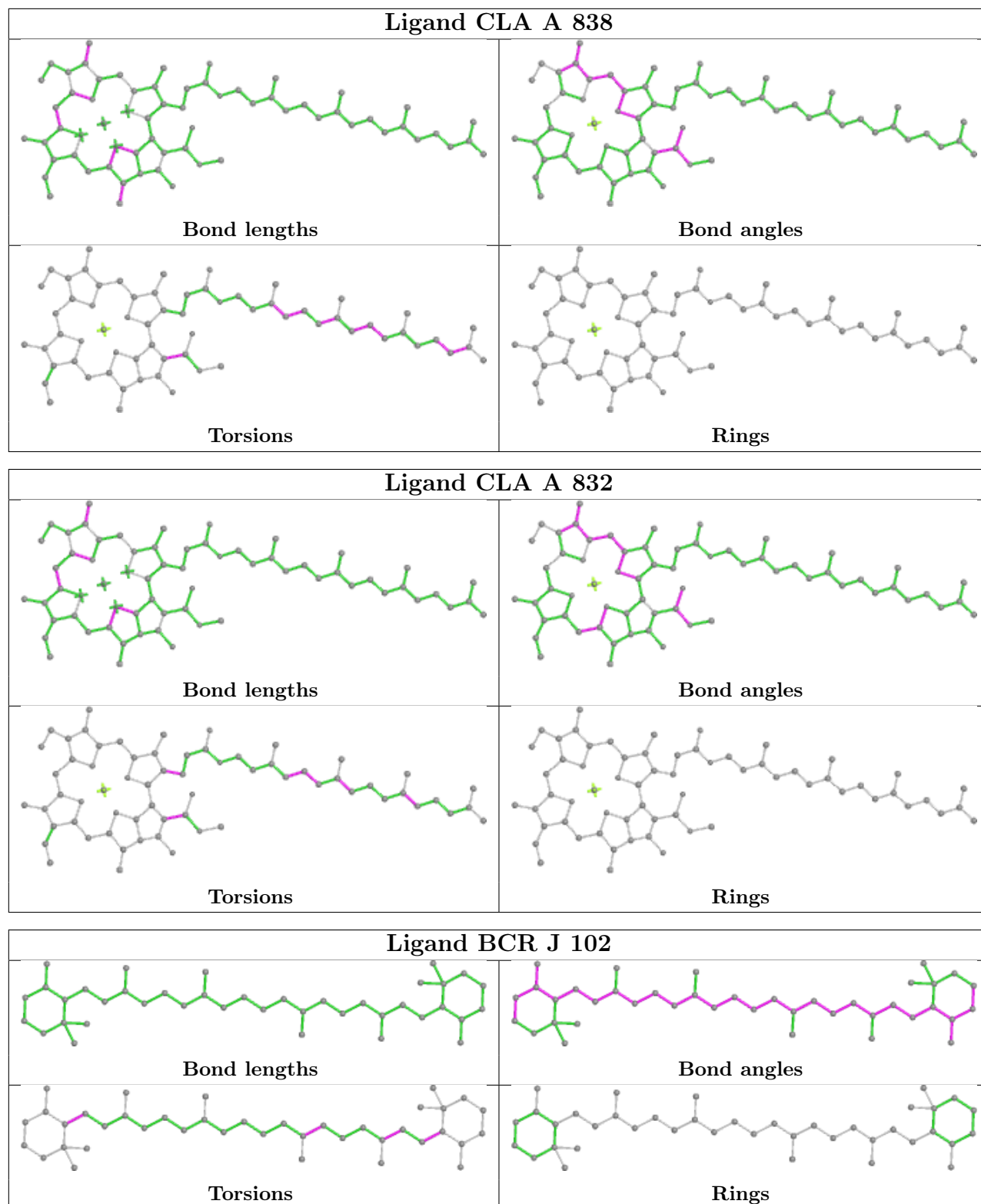


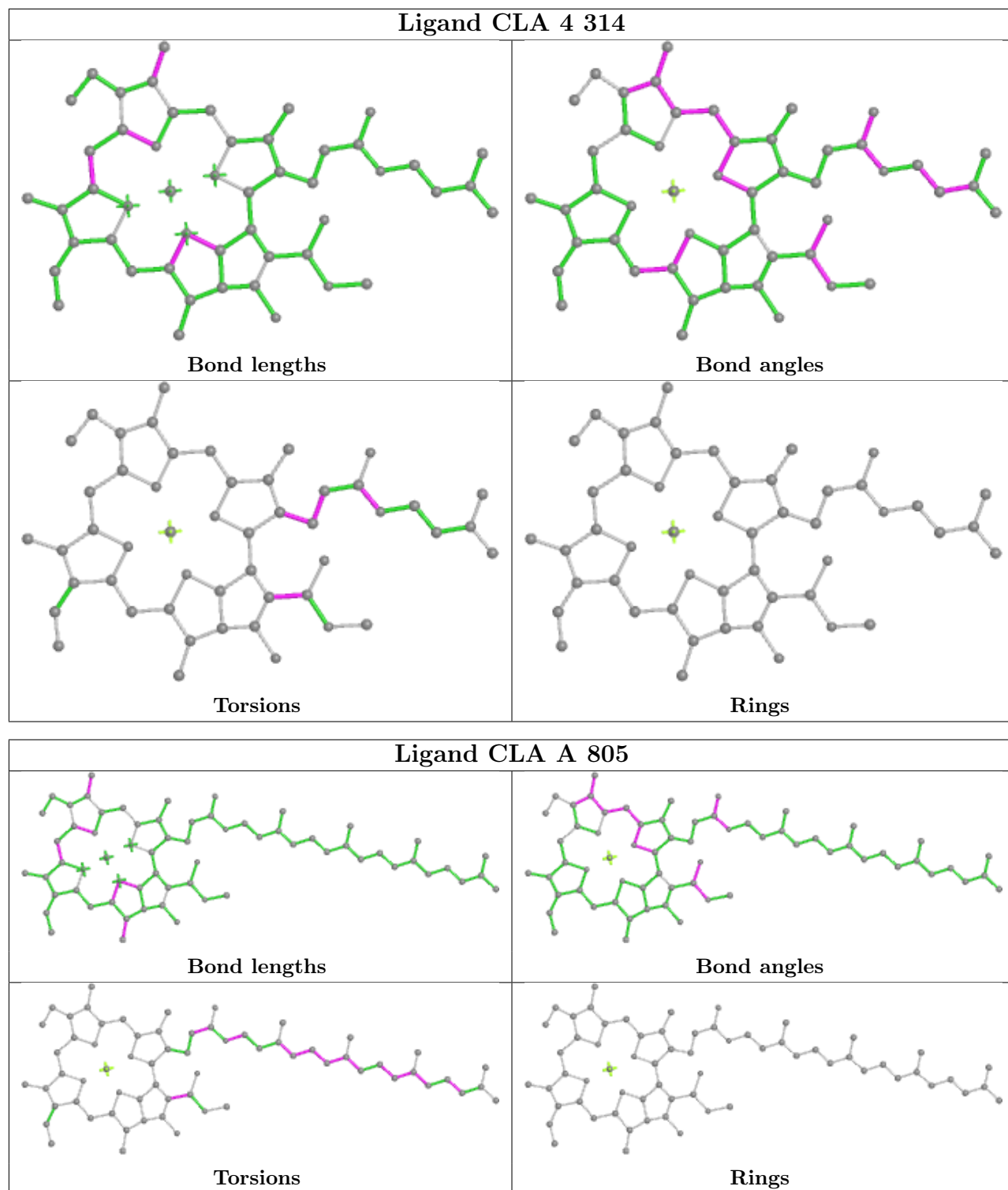


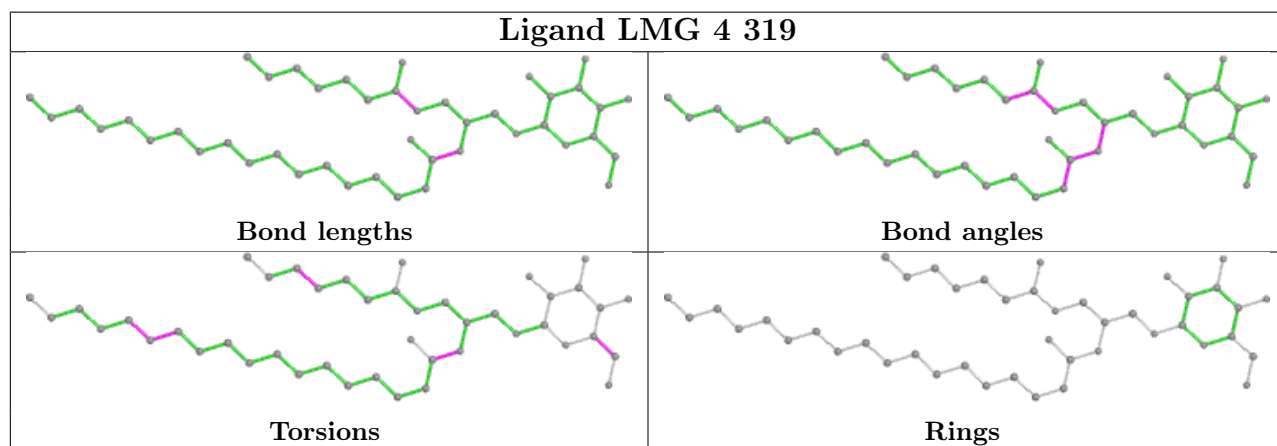
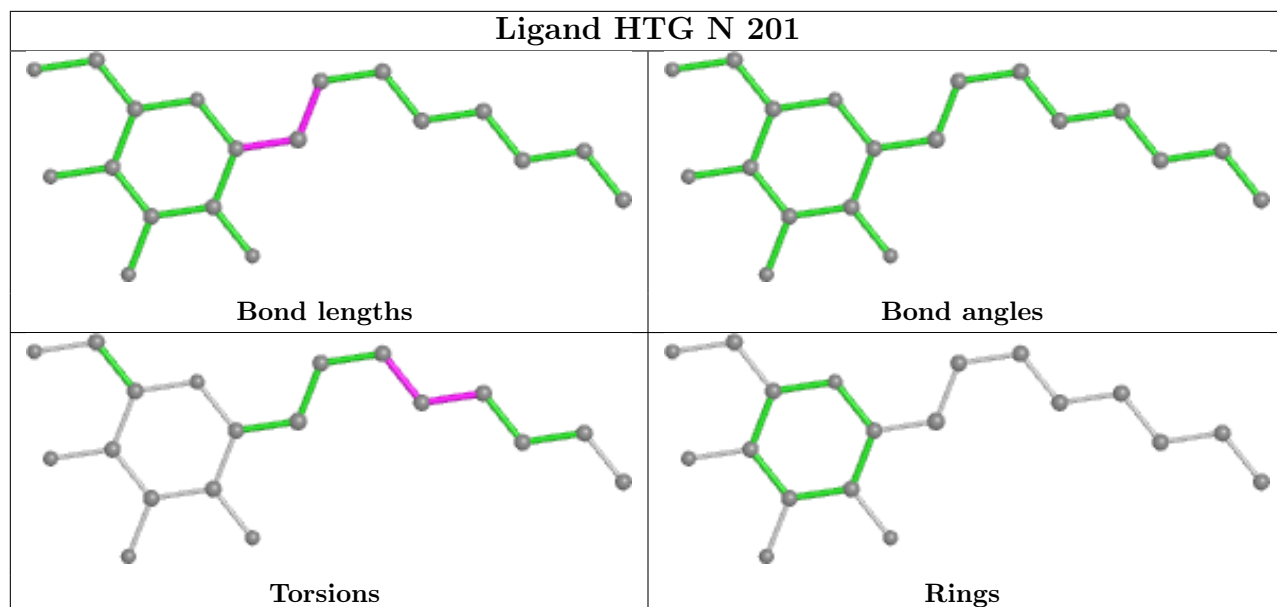


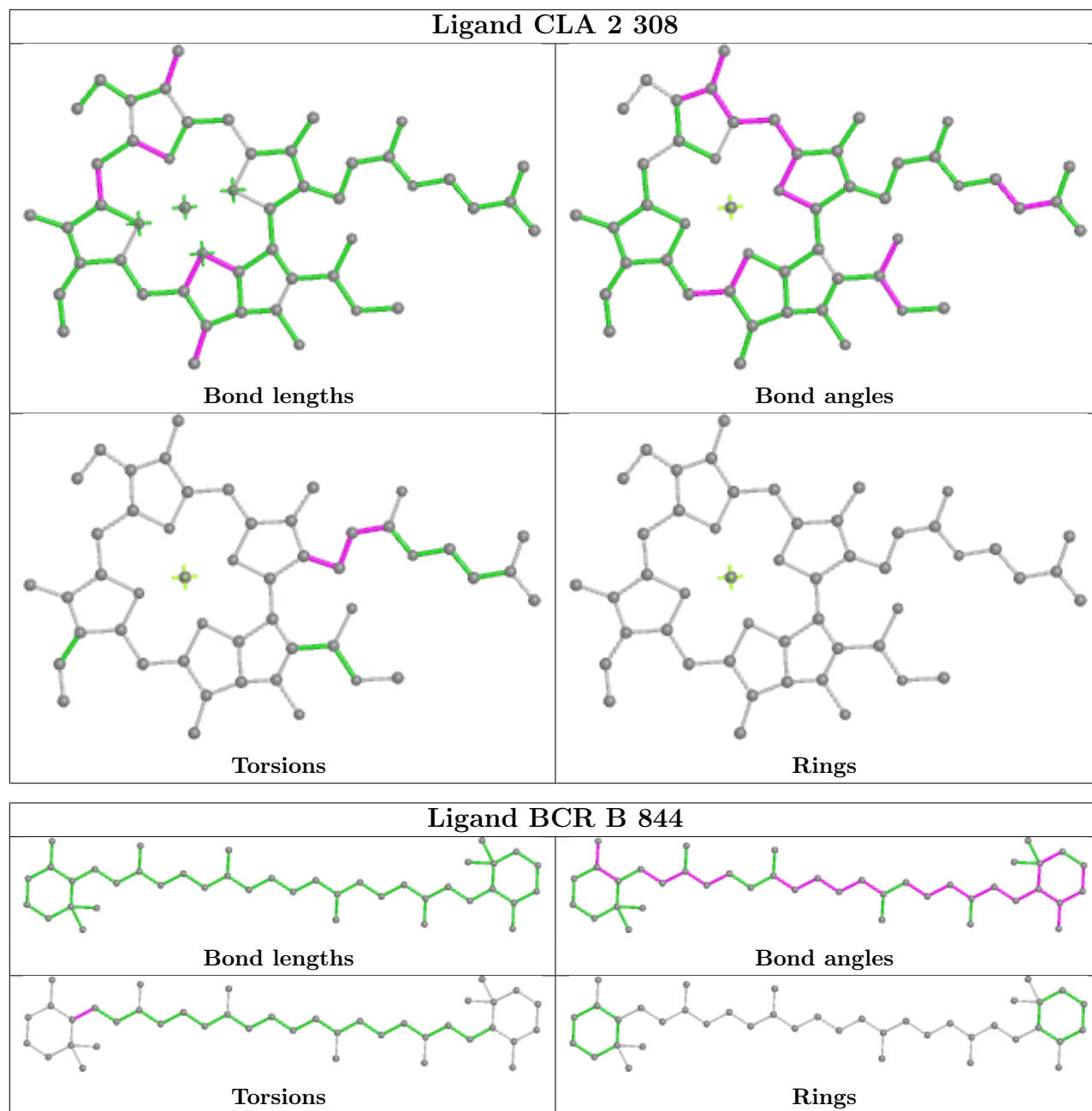


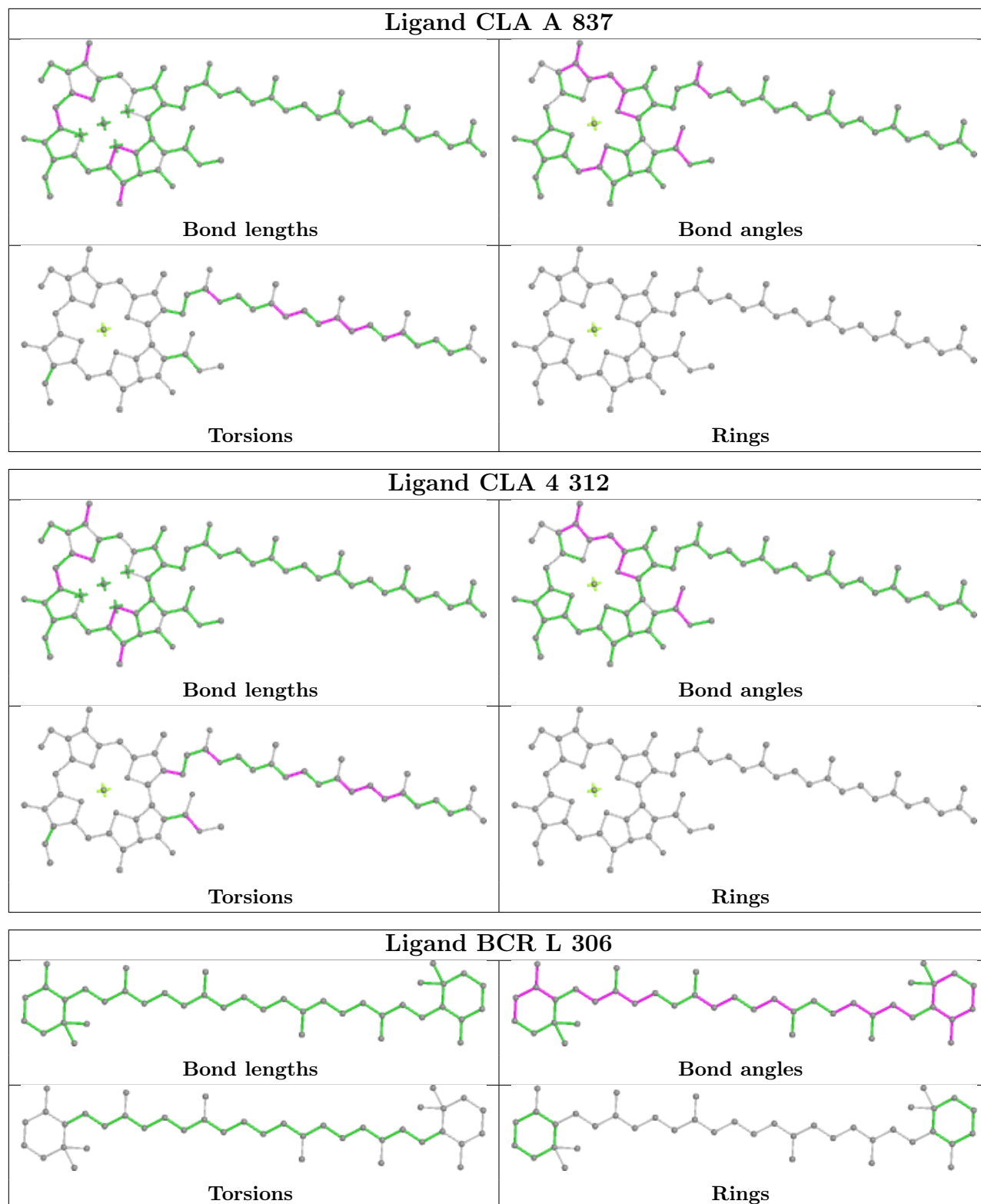


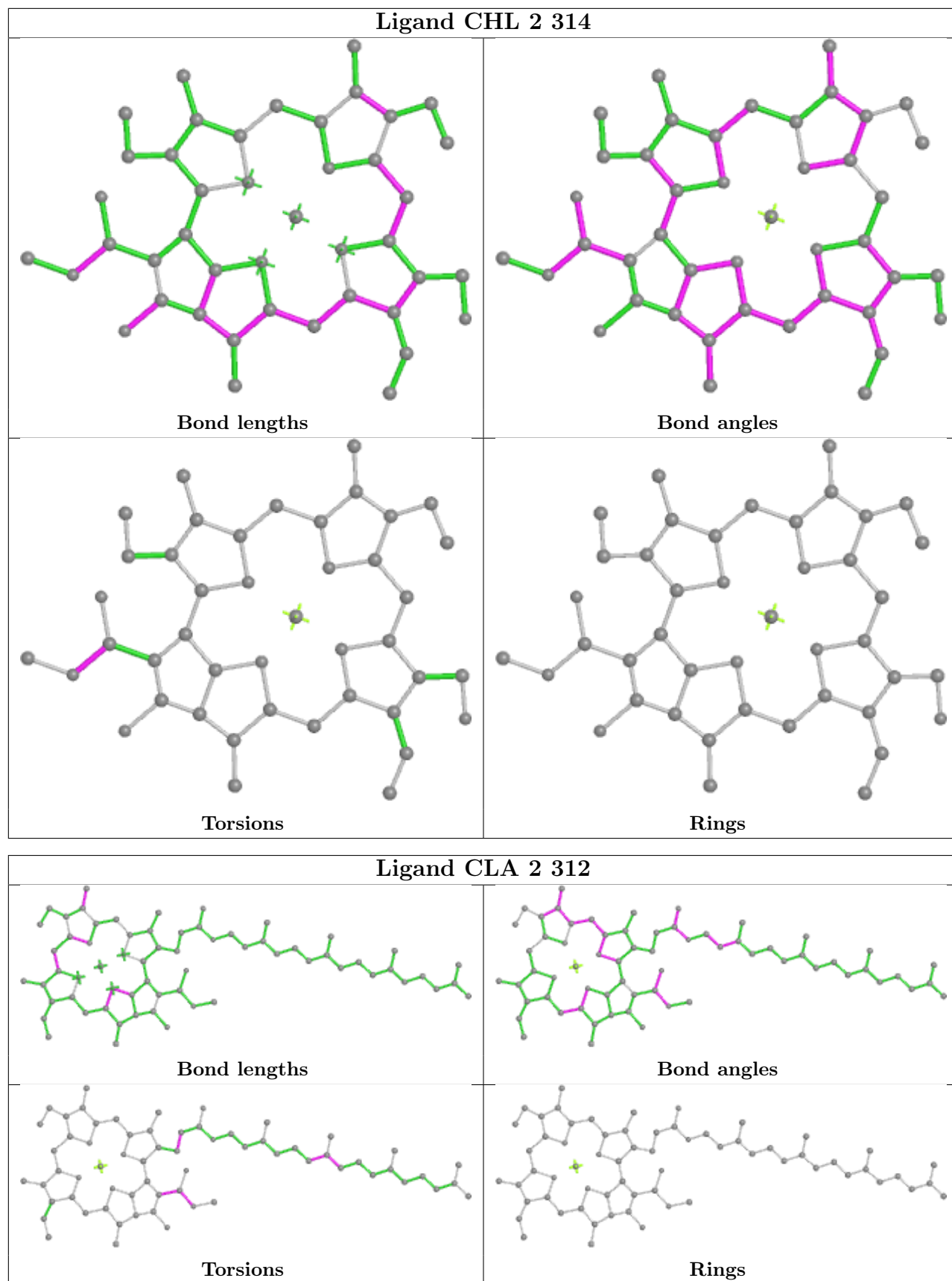


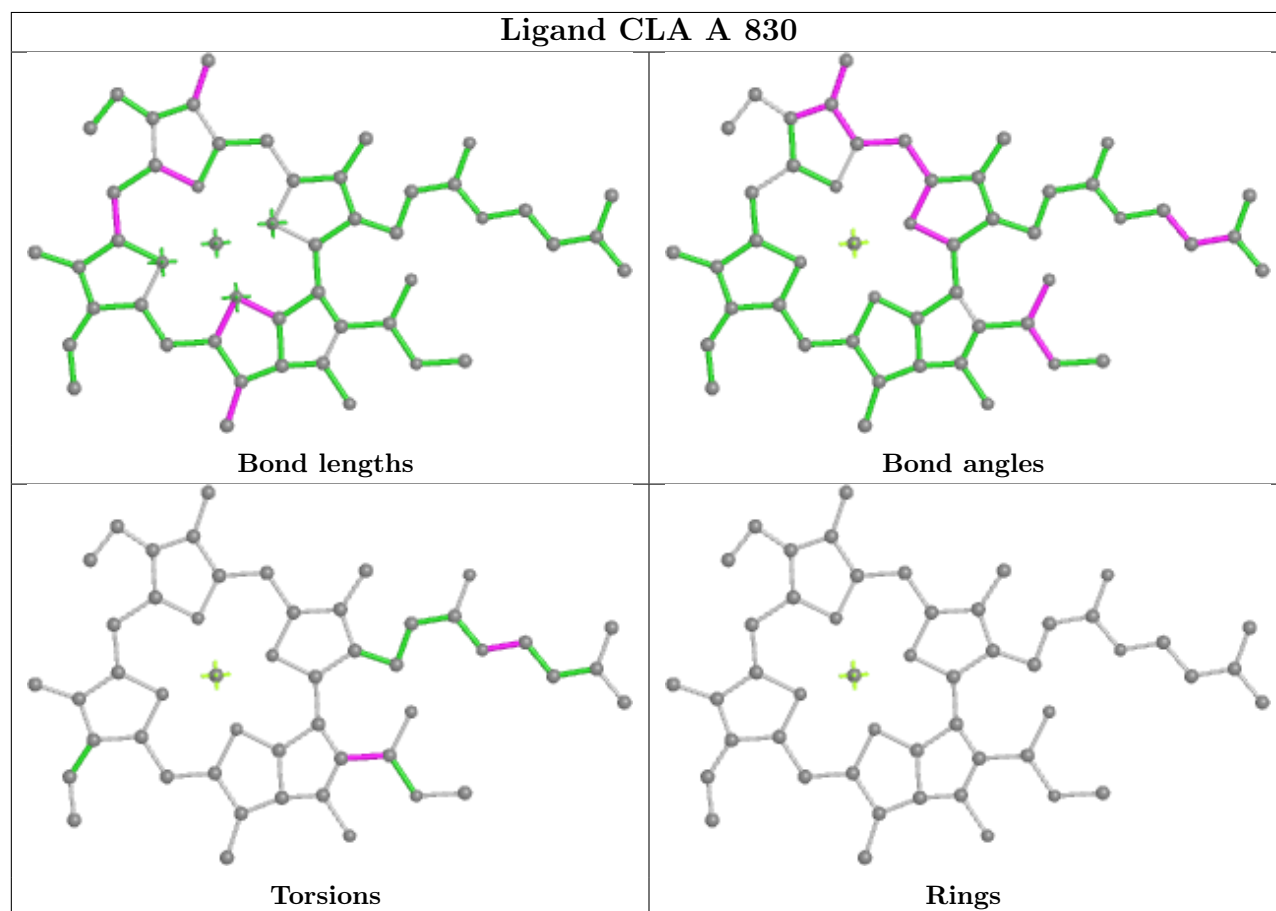
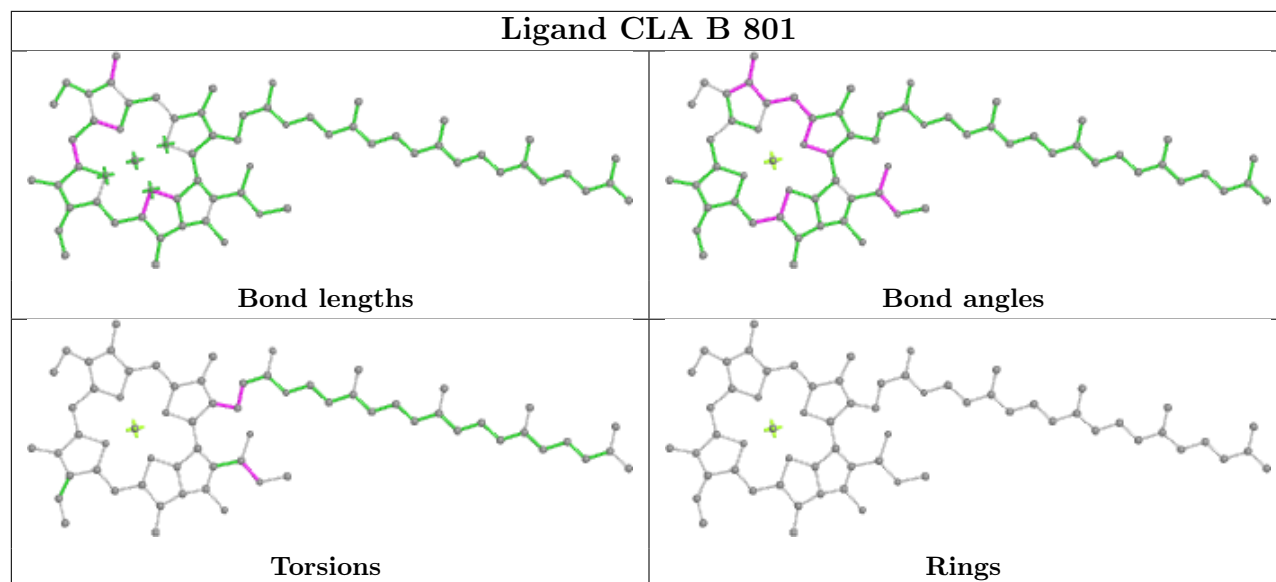


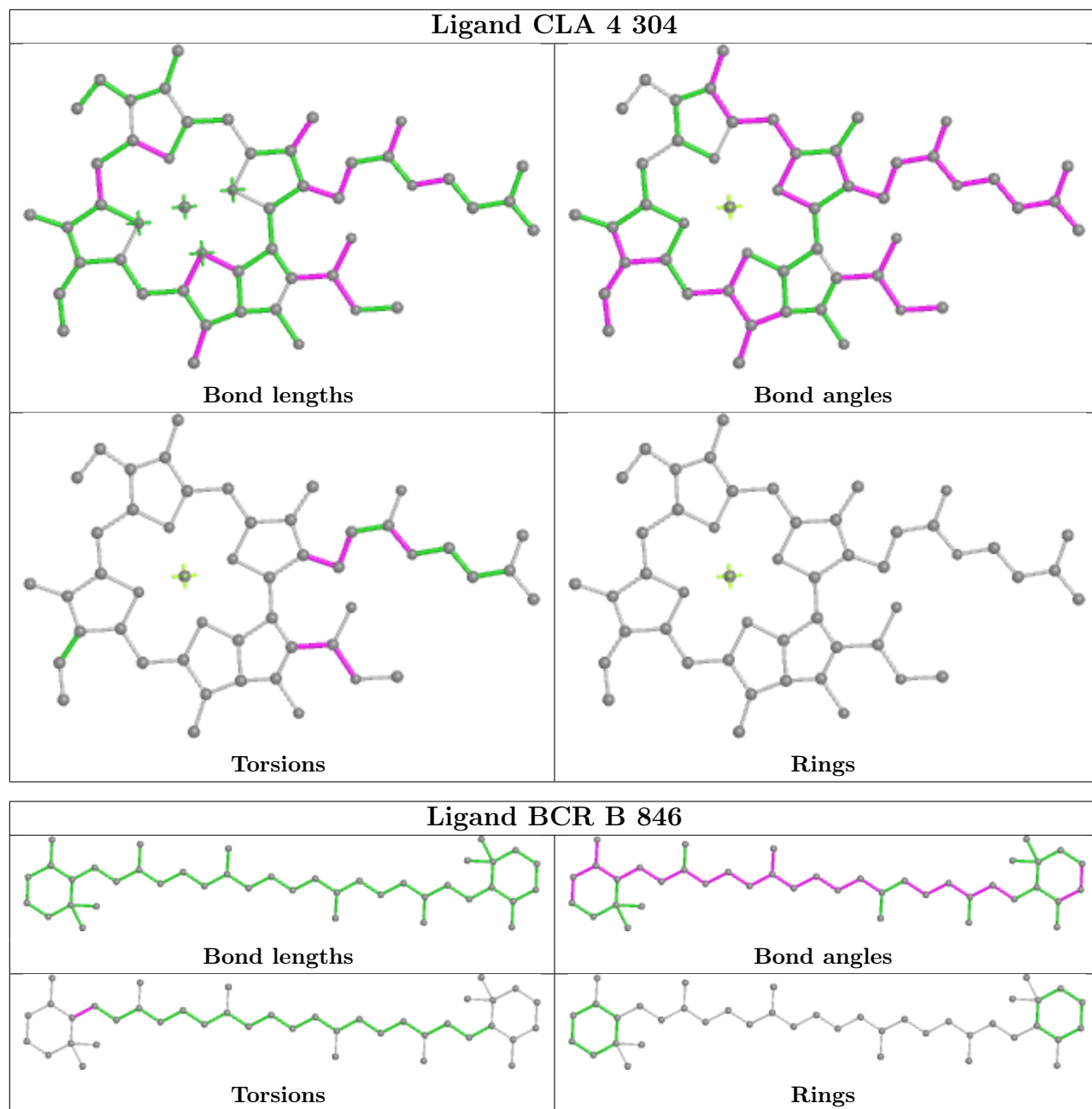


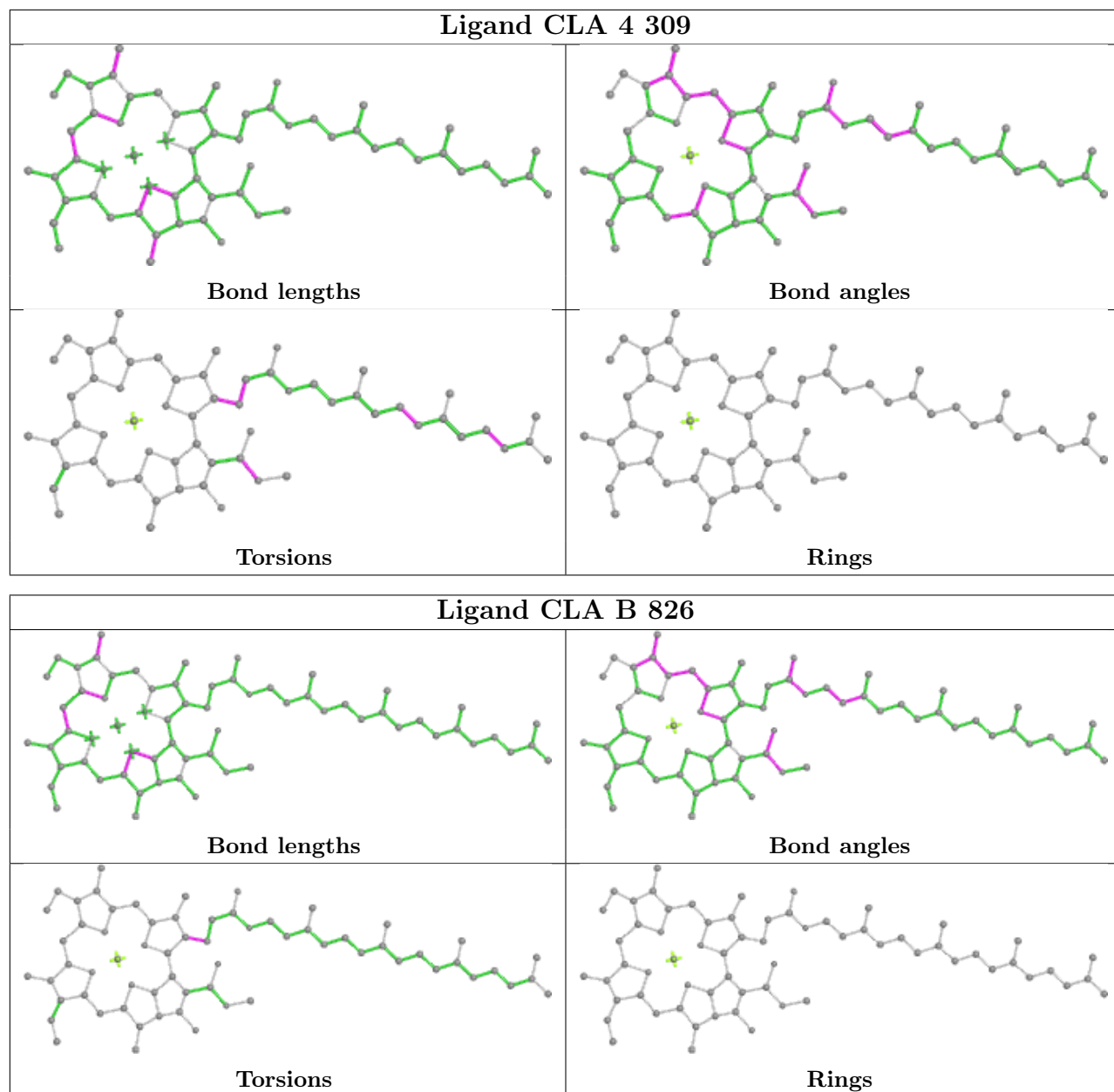


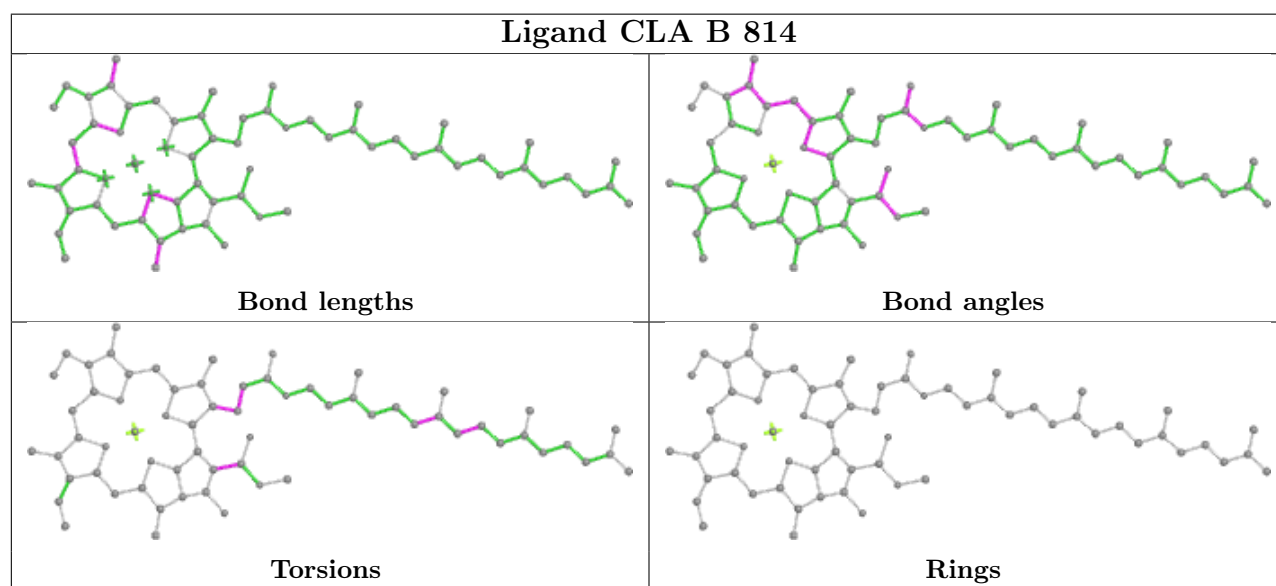
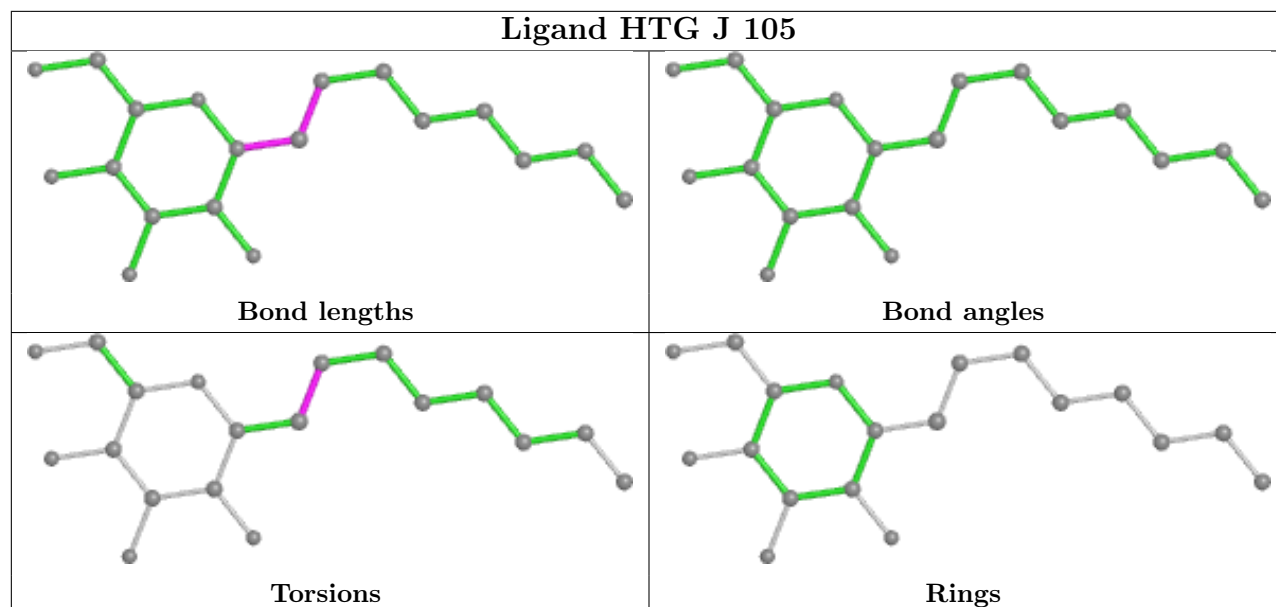


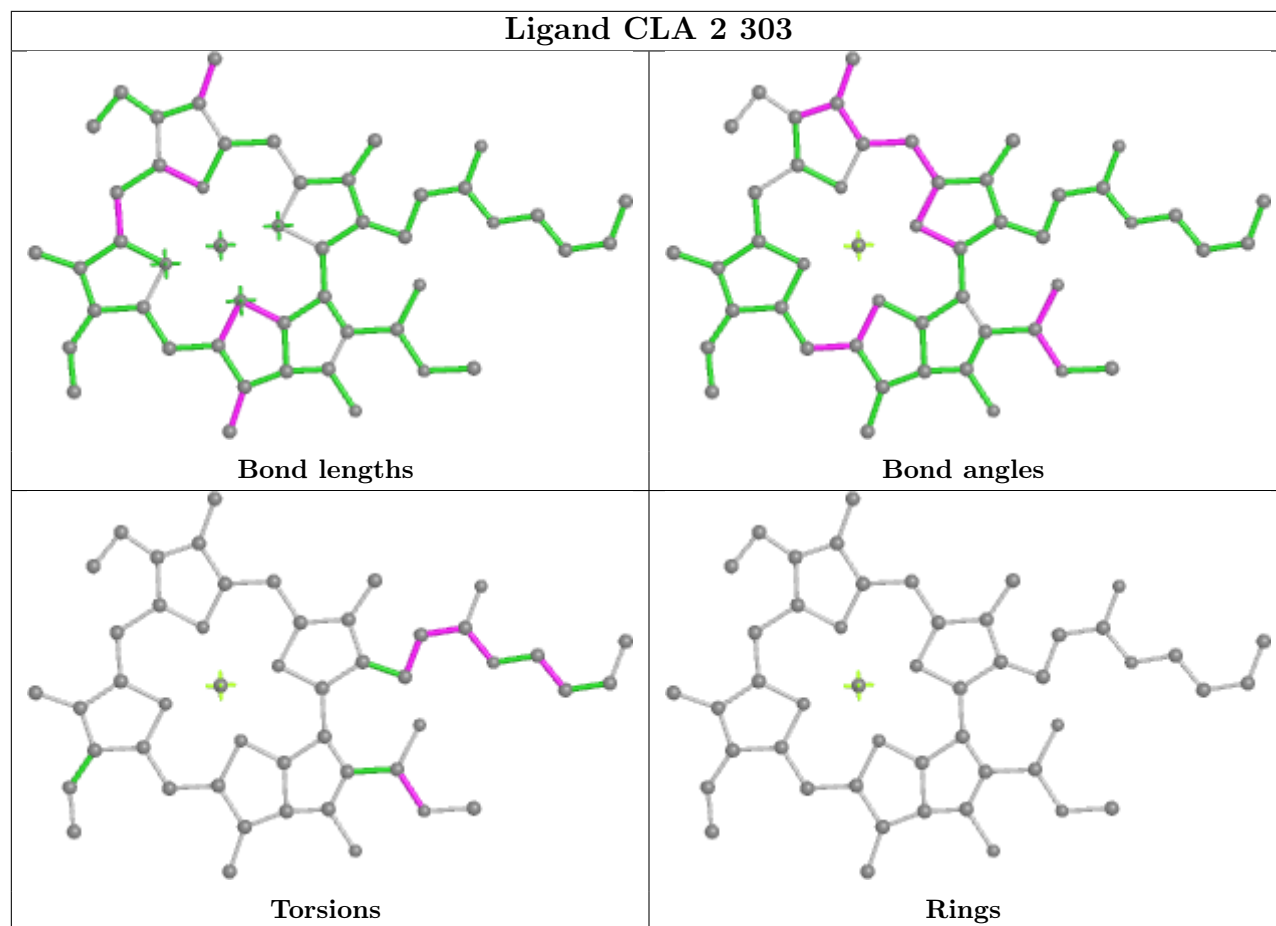












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.