



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:26 AM UTC

PDB ID : 2PPS / pdb\_00002pps  
Title : PHOTOSYNTHETIC REACTION CENTER AND CORE ANTENNA SYSTEM (TRIMERIC), ALPHA CARBON ONLY  
Authors : Krauss, N.; Schubert, W.-D.; Klukas, O.; Fromme, P.; Witt, H.T.; Saenger, W.  
Deposited on : 1997-05-27  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

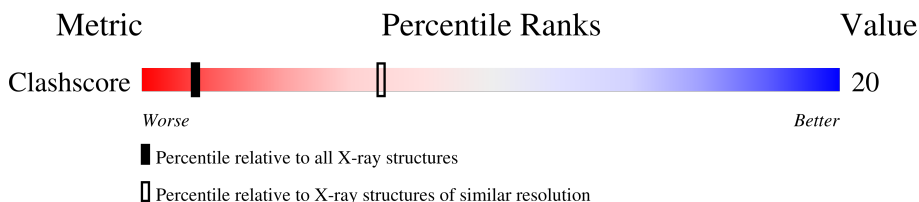
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

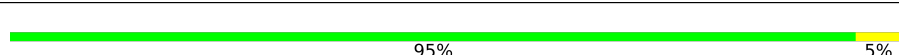
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1129 (4.20-3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	478	 96%
2	B	503	 96%
3	L	111	 100%
4	K	64	 95% 5%
5	F	130	 99%
6	C	80	 92% 8%

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
7	CLA	A	2001	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLA	A	2006	X	-	-	-
7	CLA	A	2502	X	-	-	-
7	CLA	A	3005	X	-	-	-
7	CLA	A	3007	X	-	-	-
7	CLA	A	3009	X	-	-	-
7	CLA	A	3013	X	-	-	-
7	CLA	A	3016	X	-	-	-
7	CLA	A	3017	X	-	-	-
7	CLA	A	3018	X	-	-	-
7	CLA	A	3021	X	-	-	-
7	CLA	A	3024	X	-	-	-
7	CLA	A	3026	X	-	-	-
7	CLA	A	3027	X	-	-	-
7	CLA	A	3029	X	-	-	-
7	CLA	A	3030	X	-	-	-
7	CLA	A	3032	X	-	-	-
7	CLA	A	3039	X	-	-	-
7	CLA	A	3040	X	-	-	-
7	CLA	A	3041	X	-	-	-
7	CLA	A	3043	X	-	-	-
7	CLA	A	3045	X	-	-	-
7	CLA	A	3047	X	-	-	-
7	CLA	A	3048	X	-	-	-
7	CLA	A	3052	X	-	-	-
7	CLA	A	3053	X	-	-	-
7	CLA	A	3056	X	-	-	-
7	CLA	A	3057	X	-	-	-
7	CLA	A	3058	X	-	-	-
7	CLA	A	3062	X	-	-	-
7	CLA	A	3065	X	-	-	-
7	CLA	A	3067	X	-	-	-
7	CLA	A	3068	X	-	-	-
7	CLA	A	3071	X	-	-	-
7	CLA	A	3072	X	-	-	-
7	CLA	A	3073	X	-	-	-
7	CLA	A	3077	X	-	-	-
7	CLA	A	3078	X	-	-	-
7	CLA	A	3079	X	-	-	-
7	CLA	B	2002	X	-	-	-
7	CLA	B	2003	X	-	-	-
7	CLA	B	2004	X	-	-	-
7	CLA	B	2005	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLA	B	2501	X	-	-	-
7	CLA	B	3001	X	-	-	-
7	CLA	B	3003	X	-	-	-
7	CLA	B	3006	X	-	-	-
7	CLA	B	3008	X	-	-	-
7	CLA	B	3010	X	-	-	-
7	CLA	B	3011	X	-	-	-
7	CLA	B	3015	X	-	-	-
7	CLA	B	3019	X	-	-	-
7	CLA	B	3020	X	-	-	-
7	CLA	B	3023	X	-	-	-
7	CLA	B	3025	X	-	-	-
7	CLA	B	3028	X	-	-	-
7	CLA	B	3034	X	-	-	-
7	CLA	B	3035	X	-	-	-
7	CLA	B	3037	X	-	-	-
7	CLA	B	3042	X	-	-	-
7	CLA	B	3044	X	-	-	-
7	CLA	B	3046	X	-	-	-
7	CLA	B	3055	X	-	-	-
7	CLA	B	3060	X	-	-	-
7	CLA	B	3063	X	-	-	-
7	CLA	B	3066	X	-	-	-
7	CLA	B	3069	X	-	-	-
7	CLA	B	3070	X	-	-	-
7	CLA	B	3074	X	-	-	-
7	CLA	B	3075	X	-	-	-
7	CLA	B	3076	X	-	-	-
7	CLA	B	3080	X	-	-	-
7	CLA	B	3081	X	-	-	-
7	CLA	F	3002	X	-	-	-
7	CLA	F	3004	X	-	-	-
7	CLA	F	3012	X	-	-	-
7	CLA	F	3022	X	-	-	-
7	CLA	F	3031	X	-	-	-
7	CLA	F	3033	X	-	-	-
7	CLA	F	3054	X	-	-	-
7	CLA	F	3059	X	-	-	-
7	CLA	F	3061	X	-	-	-
7	CLA	K	3050	X	-	-	-
7	CLA	K	3051	X	-	-	-
7	CLA	L	3036	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	CLA	L	3038	X	-	-	-
7	CLA	L	3049	X	-	-	-
9	SF4	B	2008	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3616 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
1	A	478	Total C 478 478	0	0	478

- Molecule 2 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	503	Total C 503 503	0	0	503

- Molecule 3 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	L	111	Total C 111 111	0	0	111

- Molecule 4 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
4	K	64	Total C 64 64	0	0	64

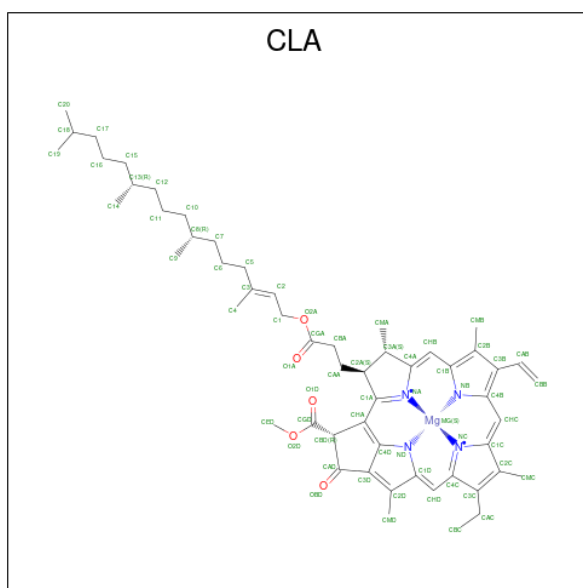
- Molecule 5 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	130	Total C 130 130	0	0	130

- Molecule 6 is a protein called PHOTOSYSTEM I.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
6	C	80	Total C 80 80	0	0	80

- Molecule 7 is CHLOROPHYLL A (CCD ID: CLA) (formula:  $C_{55}H_{72}MgN_4O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	A	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		

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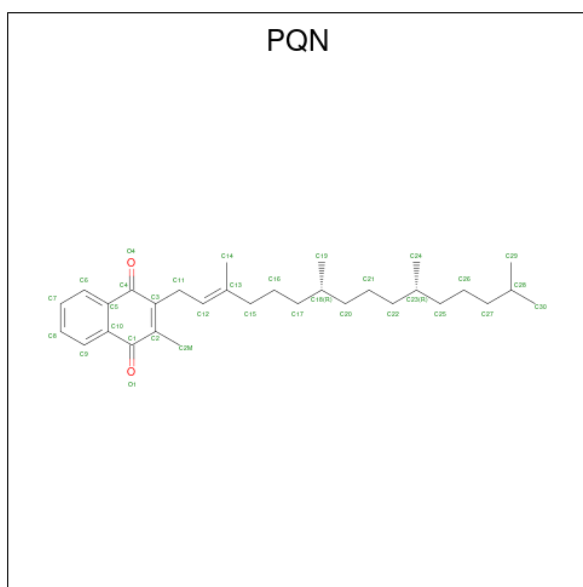
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	B	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		

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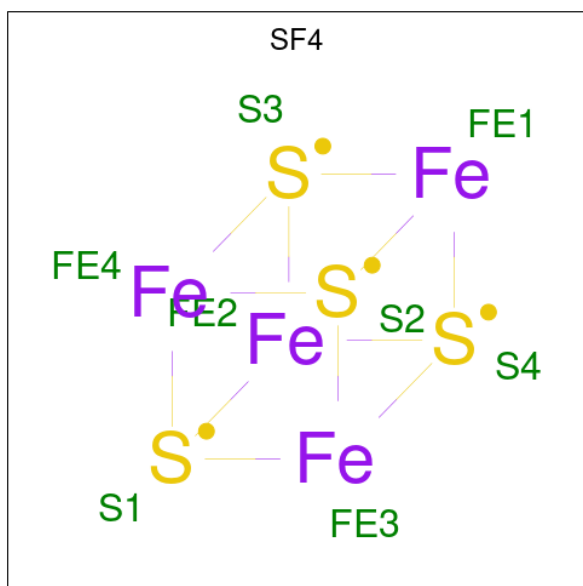
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	L	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	K	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		
7	F	1	Total	C	Mg	N	0	0
			25	20	1	4		

- Molecule 8 is PHYLLOQUINONE (CCD ID: PQN) (formula:  $C_{31}H_{46}O_2$ ).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C 1 1	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe<sub>4</sub>S<sub>4</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	0
9	C	1	Total Fe S 8 4 4	0	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.

Note EDS was not executed.

- Molecule 1: PHOTOSYSTEM I

Chain A:  96%



- Molecule 2: PHOTOSYSTEM I

Chain B:  96%



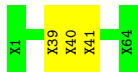
- Molecule 3: PHOTOSYSTEM I

Chain L:  100%

There are no outlier residues recorded for this chain.

- Molecule 4: PHOTOSYSTEM I

Chain K:  95% 5%



- Molecule 5: PHOTOSYSTEM I

Chain F:  99%



- Molecule 6: PHOTOSYSTEM I

Chain C:  92% 8%



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	286.00Å 286.00Å 167.00Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 4.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-4.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.10	Depositor
Refinement program		Depositor
R, $R_{free}$	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3616	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	20.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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).

There are no protein, RNA or DNA chains available to summarize Z scores of covalent bonds and angles.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	478	0	0	16	0
2	B	503	0	0	16	0
3	L	111	0	0	0	0
4	K	64	0	0	2	0
5	F	130	0	0	1	0
6	C	80	0	0	4	0
7	A	1000	0	120	41	0
7	B	850	0	102	12	0
7	F	225	0	27	8	0
7	K	50	0	6	0	0
7	L	100	0	12	0	0
8	B	1	0	0	0	0
9	B	8	0	0	3	0
9	C	16	0	0	0	0
All	All	3616	0	267	78	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 20.

All (78) 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)
7:A:3014:CLA:HHC	7:A:3029:CLA:C3D	1.61	1.31
1:A:94:UNK:CA	1:A:107:UNK:CA	2.11	1.29
2:B:470:UNK:CA	2:B:474:UNK:CA	2.12	1.27
1:A:295:UNK:CA	7:A:3016:CLA:C3C	2.19	1.20
2:B:428:UNK:CA	7:B:2005:CLA:C3A	2.20	1.20
7:A:3014:CLA:CHC	7:A:3029:CLA:C3D	2.21	1.17
7:A:3024:CLA:C3A	7:A:3027:CLA:CHD	2.39	1.00
1:A:45:UNK:CA	7:A:3071:CLA:C1A	2.38	1.00
2:B:343:UNK:CA	9:B:2008:SF4:S2	2.56	0.94
6:C:6:UNK:CA	6:C:68:UNK:CA	2.46	0.93
7:A:3024:CLA:C3A	7:A:3027:CLA:C4C	2.47	0.93
2:B:344:UNK:CA	9:B:2008:SF4:S1	2.57	0.92
7:A:3024:CLA:C2C	7:A:3030:CLA:C2A	2.48	0.91
7:A:3056:CLA:HHD	7:A:3057:CLA:C2A	2.01	0.91
1:A:362:UNK:CA	1:A:363:UNK:CA	2.50	0.90
2:B:428:UNK:CA	7:B:2005:CLA:C4A	2.50	0.89
1:A:45:UNK:CA	7:A:3071:CLA:CHA	2.51	0.88
7:A:3056:CLA:CHD	7:A:3057:CLA:C2A	2.51	0.87
1:A:44:UNK:CA	7:A:3071:CLA:C3D	2.55	0.85
1:A:326:UNK:CA	9:B:2008:SF4:S4	2.66	0.84
2:B:428:UNK:CA	7:B:2005:CLA:CHB	2.54	0.84
7:A:3007:CLA:C2C	7:F:3002:CLA:C3A	2.59	0.80
1:A:287:UNK:CA	1:A:288:UNK:CA	2.59	0.80
2:B:32:UNK:CA	7:B:3069:CLA:C2B	2.59	0.80
2:B:428:UNK:CA	7:B:2005:CLA:HHB	2.14	0.77
7:A:3027:CLA:C2A	7:A:3039:CLA:C2A	2.62	0.77
7:A:3014:CLA:C1C	7:A:3029:CLA:C3D	2.63	0.76
7:A:3056:CLA:C2D	7:A:3057:CLA:CHA	2.64	0.75
7:A:3007:CLA:CHC	7:F:3002:CLA:C2A	2.66	0.73
2:B:221:UNK:CA	2:B:222:UNK:CA	2.66	0.72
7:B:3001:CLA:C2D	7:F:3012:CLA:C2A	2.67	0.72
7:B:3001:CLA:C3D	7:F:3012:CLA:C2A	2.69	0.70
1:A:45:UNK:CA	7:A:3071:CLA:C2A	2.68	0.70
7:A:3016:CLA:C2A	7:A:3029:CLA:C3C	2.71	0.68
2:B:466:UNK:CA	2:B:467:UNK:CA	2.71	0.68
1:A:398:UNK:CA	1:A:460:UNK:CA	2.71	0.68
7:A:3014:CLA:C2C	7:A:3029:CLA:C3D	2.73	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:3014:CLA:HHC	7:A:3029:CLA:C2D	2.25	0.67
2:B:457:UNK:CA	2:B:458:UNK:CA	2.74	0.65
2:B:139:UNK:CA	2:B:140:UNK:CA	2.74	0.64
1:A:140:UNK:CA	1:A:141:UNK:CA	2.75	0.64
6:C:7:UNK:CA	6:C:68:UNK:CA	2.77	0.63
1:A:431:UNK:CA	1:A:432:UNK:CA	2.79	0.60
7:A:3016:CLA:C2A	7:A:3029:CLA:C2C	2.79	0.60
1:A:185:UNK:CA	7:A:3016:CLA:CHB	2.80	0.60
6:C:9:UNK:CA	6:C:67:UNK:CA	2.81	0.59
7:A:3005:CLA:C3B	7:A:3017:CLA:CHA	2.82	0.58
2:B:282:UNK:CA	7:B:3020:CLA:C2D	2.82	0.57
7:A:3024:CLA:C2A	7:A:3027:CLA:CHD	2.81	0.57
7:A:3024:CLA:HHC	7:A:3027:CLA:C3C	2.35	0.57
1:A:17:UNK:CA	7:A:3079:CLA:HHD	2.35	0.56
7:A:3024:CLA:C2A	7:A:3027:CLA:C1D	2.83	0.56
7:B:3003:CLA:C1B	7:B:3006:CLA:CHA	2.83	0.56
5:F:114:UNK:CA	7:F:3031:CLA:C2A	2.88	0.52
7:A:3014:CLA:C2C	7:A:3029:CLA:C2D	2.87	0.52
4:K:39:UNK:CA	4:K:40:UNK:CA	2.89	0.51
7:B:3003:CLA:C4B	7:B:3006:CLA:C2A	2.89	0.51
7:A:3005:CLA:C3A	7:A:3014:CLA:CHB	2.89	0.51
1:A:163:UNK:CA	7:A:3026:CLA:C3A	2.90	0.50
7:A:3024:CLA:CHB	7:A:3027:CLA:C3C	2.90	0.49
2:B:255:UNK:CA	2:B:256:UNK:CA	2.91	0.49
7:A:3016:CLA:C1A	7:A:3029:CLA:C3C	2.91	0.48
2:B:305:UNK:CA	2:B:306:UNK:CA	2.91	0.48
6:C:7:UNK:CA	6:C:8:UNK:CA	2.92	0.48
7:A:3005:CLA:C2A	7:A:3014:CLA:C3A	2.92	0.47
2:B:172:UNK:CA	2:B:173:UNK:CA	2.92	0.47
7:A:3016:CLA:C3A	7:A:3029:CLA:C3C	2.92	0.47
7:A:3024:CLA:C3A	7:A:3027:CLA:C1D	2.91	0.47
7:A:3027:CLA:C2A	7:A:3039:CLA:CHA	2.93	0.46
7:B:3011:CLA:C3D	7:B:3034:CLA:C2A	2.93	0.46
7:A:3007:CLA:C1C	7:F:3002:CLA:C2A	2.96	0.44
7:A:3027:CLA:C3A	7:A:3039:CLA:C2A	2.96	0.44
1:A:240:UNK:CA	1:A:241:UNK:CA	2.96	0.43
7:A:3007:CLA:HHC	7:F:3002:CLA:C2A	2.47	0.42
7:B:3011:CLA:C3D	7:B:3034:CLA:C3A	2.97	0.42
7:A:3007:CLA:HHC	7:F:3002:CLA:C1A	2.51	0.41
7:A:3018:CLA:C2D	7:A:3024:CLA:C2A	2.99	0.41
4:K:39:UNK:CA	4:K:41:UNK:CA	2.99	0.40

There are no symmetry-related clashes.

### 5.3 Torsion angles [i](#)

#### 5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

#### 5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

#### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 93 ligands modelled in this entry, 1 is modelled with single atom - leaving 92 for Mogul analysis.

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
7	CLA	F	3031	-	24,32,73	2.86	7 (29%)	31,54,113	2.32	8 (25%)
7	CLA	A	3067	-	24,32,73	2.87	7 (29%)	31,54,113	2.33	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	A	3068	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	B	2003	-	24,32,73	3.02	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3048	-	24,32,73	2.90	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	B	3060	-	24,32,73	2.88	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	F	3002	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	3028	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3058	-	24,32,73	2.90	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	2004	-	24,32,73	2.95	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	F	3004	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3046	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3069	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	B	3037	-	24,32,73	2.88	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	3027	-	24,32,73	2.88	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	3044	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	B	3081	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3024	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3026	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	3019	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3025	-	24,32,73	2.87	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3035	-	24,32,73	2.87	7 (29%)	31,54,113	2.34	8 (25%)
7	CLA	B	3070	-	24,32,73	2.89	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3045	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3065	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3032	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3015	-	24,32,73	2.88	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	3078	-	24,32,73	2.86	7 (29%)	31,54,113	2.32	8 (25%)
7	CLA	A	3077	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	2005	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3047	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	2006	-	24,32,73	2.87	8 (33%)	31,54,113	2.34	8 (25%)
9	SF4	B	2008	-	0,12,12	-	-	-	-	-
7	CLA	B	3011	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3014	-	24,32,73	3.08	9 (37%)	31,54,113	2.38	8 (25%)
7	CLA	F	3059	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3073	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	A	3017	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3057	-	24,32,73	2.88	7 (29%)	31,54,113	2.34	8 (25%)
7	CLA	L	3038	-	24,32,73	2.86	7 (29%)	31,54,113	2.33	8 (25%)
7	CLA	B	2501	-	24,32,73	2.90	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	3041	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	F	3061	-	24,32,73	2.90	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	B	3020	-	24,32,73	2.89	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	F	3033	-	24,32,73	2.87	8 (33%)	31,54,113	2.33	8 (25%)
7	CLA	F	3022	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	2502	-	24,32,73	2.88	7 (29%)	31,54,113	2.34	8 (25%)
7	CLA	B	3080	-	24,32,73	2.88	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	B	2002	-	24,32,73	2.90	8 (33%)	31,54,113	2.33	8 (25%)
7	CLA	A	3040	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3010	-	24,32,73	2.90	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	3016	-	24,32,73	2.88	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	A	3007	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	2001	-	24,32,73	3.02	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3062	-	24,32,73	2.89	8 (33%)	31,54,113	2.33	8 (25%)
7	CLA	K	3050	-	24,32,73	2.87	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3006	-	24,32,73	2.88	8 (33%)	31,54,113	2.36	8 (25%)
9	SF4	C	2009	-	0,12,12	-	-	-	-	-
7	CLA	A	3005	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3030	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3021	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	F	3054	-	24,32,73	2.89	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	B	3075	-	24,32,73	2.87	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3056	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	A	3039	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
9	SF4	C	2010	-	0,12,12	-	-	-	-	-
7	CLA	B	3008	-	24,32,73	2.87	7 (29%)	31,54,113	2.34	8 (25%)
7	CLA	B	3042	-	24,32,73	2.87	7 (29%)	31,54,113	2.33	8 (25%)
7	CLA	L	3064	-	24,32,73	3.07	9 (37%)	31,54,113	2.38	8 (25%)
7	CLA	L	3036	-	24,32,73	2.89	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3052	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3053	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	CLA	K	3051	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	F	3012	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3055	-	24,32,73	2.88	8 (33%)	31,54,113	2.33	8 (25%)
7	CLA	A	3009	-	24,32,73	2.87	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3079	-	24,32,73	2.88	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3074	-	24,32,73	2.89	7 (29%)	31,54,113	2.36	8 (25%)
7	CLA	L	3049	-	24,32,73	2.87	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3029	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	3023	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3034	-	24,32,73	2.87	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3013	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3001	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3072	-	24,32,73	2.89	8 (33%)	31,54,113	2.36	8 (25%)
7	CLA	B	3003	-	24,32,73	2.89	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	B	3066	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	A	3018	-	24,32,73	2.87	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	A	3071	-	24,32,73	2.88	8 (33%)	31,54,113	2.35	8 (25%)
7	CLA	A	3043	-	24,32,73	2.88	7 (29%)	31,54,113	2.35	8 (25%)
7	CLA	B	3076	-	24,32,73	2.87	8 (33%)	31,54,113	2.34	8 (25%)
7	CLA	B	3063	-	24,32,73	2.89	8 (33%)	31,54,113	2.34	8 (25%)

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
7	CLA	F	3031	-	1/1/4/20	-	-
7	CLA	A	3067	-	1/1/4/20	-	-
7	CLA	A	3068	-	1/1/4/20	-	-
7	CLA	B	2003	-	1/1/4/20	-	-
7	CLA	A	3048	-	1/1/4/20	-	-
7	CLA	B	3060	-	1/1/4/20	-	-
7	CLA	F	3002	-	1/1/4/20	-	-
7	CLA	B	3028	-	1/1/4/20	-	-
7	CLA	A	3058	-	1/1/4/20	-	-
7	CLA	B	2004	-	1/1/4/20	-	-
7	CLA	F	3004	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	B	3046	-	1/1/4/20	-	-
7	CLA	B	3069	-	1/1/4/20	-	-
7	CLA	B	3037	-	1/1/4/20	-	-
7	CLA	A	3027	-	1/1/4/20	-	-
7	CLA	B	3044	-	1/1/4/20	-	-
7	CLA	B	3081	-	1/1/4/20	-	-
7	CLA	A	3024	-	1/1/4/20	-	-
7	CLA	A	3026	-	1/1/4/20	-	-
7	CLA	B	3019	-	1/1/4/20	-	-
7	CLA	B	3025	-	1/1/4/20	-	-
7	CLA	B	3035	-	1/1/4/20	-	-
7	CLA	B	3070	-	1/1/4/20	-	-
7	CLA	A	3045	-	1/1/4/20	-	-
7	CLA	A	3065	-	1/1/4/20	-	-
7	CLA	A	3032	-	1/1/4/20	-	-
7	CLA	B	3015	-	1/1/4/20	-	-
7	CLA	A	3078	-	1/1/4/20	-	-
7	CLA	A	3077	-	1/1/4/20	-	-
7	CLA	B	2005	-	1/1/4/20	-	-
7	CLA	A	3047	-	1/1/4/20	-	-
7	CLA	A	2006	-	1/1/4/20	-	-
9	SF4	B	2008	-	-	-	0/6/5/5
7	CLA	B	3011	-	1/1/4/20	-	-
7	CLA	F	3059	-	1/1/4/20	-	-
7	CLA	A	3073	-	1/1/4/20	-	-
7	CLA	A	3017	-	1/1/4/20	-	-
7	CLA	A	3057	-	1/1/4/20	-	-
7	CLA	L	3038	-	1/1/4/20	-	-
7	CLA	B	2501	-	1/1/4/20	-	-
7	CLA	A	3041	-	1/1/4/20	-	-
7	CLA	F	3061	-	1/1/4/20	-	-
7	CLA	B	3020	-	1/1/4/20	-	-
7	CLA	F	3033	-	1/1/4/20	-	-
7	CLA	F	3022	-	1/1/4/20	-	-
7	CLA	A	2502	-	1/1/4/20	-	-
7	CLA	B	3080	-	1/1/4/20	-	-
7	CLA	B	2002	-	1/1/4/20	-	-
7	CLA	A	3040	-	1/1/4/20	-	-
7	CLA	B	3010	-	1/1/4/20	-	-
7	CLA	A	3016	-	1/1/4/20	-	-
7	CLA	A	3007	-	1/1/4/20	-	-
7	CLA	A	2001	-	1/1/4/20	-	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	CLA	A	3062	-	1/1/4/20	-	-
7	CLA	K	3050	-	1/1/4/20	-	-
7	CLA	B	3006	-	1/1/4/20	-	-
9	SF4	C	2009	-	-	-	0/6/5/5
7	CLA	A	3005	-	1/1/4/20	-	-
7	CLA	A	3030	-	1/1/4/20	-	-
7	CLA	A	3021	-	1/1/4/20	-	-
7	CLA	F	3054	-	1/1/4/20	-	-
7	CLA	B	3075	-	1/1/4/20	-	-
7	CLA	A	3056	-	1/1/4/20	-	-
7	CLA	A	3039	-	1/1/4/20	-	-
9	SF4	C	2010	-	-	-	0/6/5/5
7	CLA	B	3008	-	1/1/4/20	-	-
7	CLA	B	3042	-	1/1/4/20	-	-
7	CLA	L	3036	-	1/1/4/20	-	-
7	CLA	A	3052	-	1/1/4/20	-	-
7	CLA	A	3053	-	1/1/4/20	-	-
7	CLA	K	3051	-	1/1/4/20	-	-
7	CLA	F	3012	-	1/1/4/20	-	-
7	CLA	B	3055	-	1/1/4/20	-	-
7	CLA	A	3009	-	1/1/4/20	-	-
7	CLA	A	3079	-	1/1/4/20	-	-
7	CLA	B	3074	-	1/1/4/20	-	-
7	CLA	L	3049	-	1/1/4/20	-	-
7	CLA	A	3029	-	1/1/4/20	-	-
7	CLA	B	3023	-	1/1/4/20	-	-
7	CLA	B	3034	-	1/1/4/20	-	-
7	CLA	A	3013	-	1/1/4/20	-	-
7	CLA	B	3001	-	1/1/4/20	-	-
7	CLA	A	3072	-	1/1/4/20	-	-
7	CLA	B	3003	-	1/1/4/20	-	-
7	CLA	B	3066	-	1/1/4/20	-	-
7	CLA	A	3018	-	1/1/4/20	-	-
7	CLA	A	3071	-	1/1/4/20	-	-
7	CLA	A	3043	-	1/1/4/20	-	-
7	CLA	B	3076	-	1/1/4/20	-	-
7	CLA	B	3063	-	1/1/4/20	-	-

All (687) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3014	CLA	C3D-C2D	8.93	1.55	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	3064	CLA	C3D-C2D	8.87	1.55	1.35
7	B	2003	CLA	MG-NB	7.08	2.19	2.05
7	A	2001	CLA	MG-NB	6.85	2.19	2.05
7	B	2501	CLA	C3A-C2A	-6.76	1.35	1.52
7	A	3041	CLA	C3A-C2A	-6.75	1.35	1.52
7	A	3062	CLA	C3A-C2A	-6.74	1.35	1.52
7	F	3059	CLA	C3A-C2A	-6.74	1.35	1.52
7	F	3022	CLA	C3A-C2A	-6.74	1.36	1.52
7	A	3079	CLA	C3A-C2A	-6.74	1.36	1.52
7	F	3054	CLA	C3A-C2A	-6.74	1.36	1.52
7	B	3010	CLA	C3A-C2A	-6.73	1.36	1.52
7	B	3037	CLA	C3A-C2A	-6.73	1.36	1.52
7	B	3011	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3077	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3007	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3057	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3027	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3026	CLA	C3A-C2A	-6.73	1.36	1.52
7	B	2002	CLA	C3A-C2A	-6.73	1.36	1.52
7	B	3020	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3039	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	3067	CLA	C3A-C2A	-6.73	1.36	1.52
7	A	2001	CLA	C3A-C2A	-6.73	1.36	1.52
7	B	2004	CLA	C3A-C2A	-6.72	1.36	1.52
7	F	3061	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	2502	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3013	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3014	CLA	C3A-C2A	-6.72	1.36	1.52
7	B	3023	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3071	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3065	CLA	C3A-C2A	-6.72	1.36	1.52
7	B	3074	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3056	CLA	C3A-C2A	-6.72	1.36	1.52
7	B	3001	CLA	C3A-C2A	-6.72	1.36	1.52
7	B	3015	CLA	C3A-C2A	-6.72	1.36	1.52
7	A	3032	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	3019	CLA	C3A-C2A	-6.71	1.36	1.52
7	A	3052	CLA	C3A-C2A	-6.71	1.36	1.52
7	F	3004	CLA	C3A-C2A	-6.71	1.36	1.52
7	A	3030	CLA	C3A-C2A	-6.71	1.36	1.52
7	A	3040	CLA	C3A-C2A	-6.71	1.36	1.52
7	K	3051	CLA	C3A-C2A	-6.71	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3078	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	2005	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	3044	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	3080	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	3025	CLA	C3A-C2A	-6.71	1.36	1.52
7	F	3002	CLA	C3A-C2A	-6.71	1.36	1.52
7	B	3066	CLA	C3A-C2A	-6.71	1.36	1.52
7	A	3045	CLA	C3A-C2A	-6.70	1.36	1.52
7	A	3048	CLA	C3A-C2A	-6.70	1.36	1.52
7	B	3063	CLA	C3A-C2A	-6.70	1.36	1.52
7	A	3021	CLA	C3A-C2A	-6.70	1.36	1.52
7	K	3050	CLA	C3A-C2A	-6.70	1.36	1.52
7	B	3055	CLA	C3A-C2A	-6.70	1.36	1.52
7	B	3042	CLA	C3A-C2A	-6.70	1.36	1.52
7	A	3024	CLA	C3A-C2A	-6.70	1.36	1.52
7	B	2003	CLA	C3A-C2A	-6.70	1.36	1.52
7	A	3047	CLA	C3A-C2A	-6.69	1.36	1.52
7	L	3036	CLA	C3A-C2A	-6.69	1.36	1.52
7	B	3070	CLA	C3A-C2A	-6.69	1.36	1.52
7	B	3076	CLA	C3A-C2A	-6.69	1.36	1.52
7	A	3072	CLA	C3A-C2A	-6.69	1.36	1.52
7	B	3046	CLA	C3A-C2A	-6.69	1.36	1.52
7	B	3034	CLA	C3A-C2A	-6.69	1.36	1.52
7	B	3069	CLA	C3A-C2A	-6.69	1.36	1.52
7	A	3053	CLA	C3A-C2A	-6.69	1.36	1.52
7	L	3064	CLA	C3A-C2A	-6.68	1.36	1.52
7	A	3043	CLA	C3A-C2A	-6.68	1.36	1.52
7	B	3035	CLA	C3A-C2A	-6.68	1.36	1.52
7	B	3081	CLA	C3A-C2A	-6.68	1.36	1.52
7	A	3005	CLA	C3A-C2A	-6.68	1.36	1.52
7	B	3006	CLA	C3A-C2A	-6.68	1.36	1.52
7	A	3018	CLA	C3A-C2A	-6.68	1.36	1.52
7	A	3029	CLA	C3A-C2A	-6.67	1.36	1.52
7	B	3075	CLA	C3A-C2A	-6.67	1.36	1.52
7	F	3012	CLA	C3A-C2A	-6.67	1.36	1.52
7	B	3008	CLA	C3A-C2A	-6.67	1.36	1.52
7	B	3003	CLA	C3A-C2A	-6.67	1.36	1.52
7	B	3028	CLA	C3A-C2A	-6.67	1.36	1.52
7	A	3073	CLA	C3A-C2A	-6.66	1.36	1.52
7	L	3049	CLA	C3A-C2A	-6.66	1.36	1.52
7	A	3068	CLA	C3A-C2A	-6.66	1.36	1.52
7	F	3031	CLA	C3A-C2A	-6.66	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3058	CLA	C3A-C2A	-6.65	1.36	1.52
7	A	2006	CLA	C3A-C2A	-6.64	1.36	1.52
7	A	3009	CLA	C3A-C2A	-6.64	1.36	1.52
7	B	3060	CLA	C3A-C2A	-6.64	1.36	1.52
7	A	3017	CLA	C3A-C2A	-6.63	1.36	1.52
7	A	3016	CLA	C3A-C2A	-6.63	1.36	1.52
7	F	3033	CLA	C3A-C2A	-6.62	1.36	1.52
7	L	3038	CLA	C3A-C2A	-6.61	1.36	1.52
7	F	3061	CLA	MG-NB	6.59	2.18	2.05
7	A	3068	CLA	MG-NB	6.58	2.18	2.05
7	B	2501	CLA	MG-NB	6.57	2.18	2.05
7	A	3048	CLA	MG-NB	6.55	2.18	2.05
7	B	3010	CLA	MG-NB	6.55	2.18	2.05
7	B	3063	CLA	MG-NB	6.55	2.18	2.05
7	B	3020	CLA	MG-NB	6.54	2.18	2.05
7	B	3003	CLA	MG-NB	6.54	2.18	2.05
7	A	3029	CLA	MG-NB	6.54	2.18	2.05
7	A	3058	CLA	MG-NB	6.53	2.18	2.05
7	A	3026	CLA	MG-NB	6.53	2.18	2.05
7	A	3073	CLA	MG-NB	6.52	2.18	2.05
7	B	3070	CLA	MG-NB	6.52	2.18	2.05
7	B	3028	CLA	MG-NB	6.52	2.18	2.05
7	B	3060	CLA	MG-NB	6.52	2.18	2.05
7	A	3021	CLA	MG-NB	6.52	2.18	2.05
7	F	3022	CLA	MG-NB	6.51	2.18	2.05
7	A	3047	CLA	MG-NB	6.51	2.18	2.05
7	B	3001	CLA	MG-NB	6.51	2.18	2.05
7	B	3006	CLA	MG-NB	6.50	2.18	2.05
7	A	3040	CLA	MG-NB	6.50	2.18	2.05
7	A	3016	CLA	MG-NB	6.50	2.18	2.05
7	A	3072	CLA	MG-NB	6.50	2.18	2.05
7	A	3053	CLA	MG-NB	6.50	2.18	2.05
7	A	3039	CLA	MG-NB	6.50	2.18	2.05
7	A	3056	CLA	MG-NB	6.50	2.18	2.05
7	B	3046	CLA	MG-NB	6.50	2.18	2.05
7	A	3014	CLA	MG-ND	6.50	2.18	2.05
7	B	3069	CLA	MG-NB	6.50	2.18	2.05
7	A	3077	CLA	MG-NB	6.49	2.18	2.05
7	A	3043	CLA	MG-NB	6.49	2.18	2.05
7	B	3066	CLA	MG-NB	6.49	2.18	2.05
7	A	3007	CLA	MG-NB	6.49	2.18	2.05
7	B	3015	CLA	MG-NB	6.49	2.18	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3017	CLA	MG-NB	6.49	2.18	2.05
7	B	3034	CLA	MG-NB	6.49	2.18	2.05
7	B	3074	CLA	MG-NB	6.49	2.18	2.05
7	A	3009	CLA	MG-NB	6.49	2.18	2.05
7	L	3064	CLA	MG-ND	6.49	2.18	2.05
7	B	3044	CLA	MG-NB	6.48	2.18	2.05
7	F	3002	CLA	MG-NB	6.48	2.18	2.05
7	A	3045	CLA	MG-NB	6.48	2.18	2.05
7	B	3011	CLA	MG-NB	6.48	2.18	2.05
7	K	3051	CLA	MG-NB	6.48	2.18	2.05
7	A	2502	CLA	MG-NB	6.48	2.18	2.05
7	A	3005	CLA	MG-NB	6.48	2.18	2.05
7	A	3041	CLA	MG-NB	6.48	2.18	2.05
7	A	3027	CLA	MG-NB	6.48	2.18	2.05
7	B	3023	CLA	MG-NB	6.48	2.18	2.05
7	B	3080	CLA	MG-NB	6.47	2.18	2.05
7	B	3055	CLA	MG-NB	6.47	2.18	2.05
7	F	3012	CLA	MG-NB	6.47	2.18	2.05
7	B	3075	CLA	MG-NB	6.47	2.18	2.05
7	L	3049	CLA	MG-NB	6.46	2.18	2.05
7	A	3052	CLA	MG-NB	6.46	2.18	2.05
7	B	3008	CLA	MG-NB	6.46	2.18	2.05
7	A	3024	CLA	MG-NB	6.46	2.18	2.05
7	B	3081	CLA	MG-NB	6.45	2.18	2.05
7	L	3036	CLA	MG-NB	6.45	2.18	2.05
7	A	3065	CLA	MG-NB	6.45	2.18	2.05
7	B	3076	CLA	MG-NB	6.45	2.18	2.05
7	A	3018	CLA	MG-NB	6.44	2.18	2.05
7	B	3037	CLA	MG-NB	6.44	2.18	2.05
7	A	3013	CLA	MG-NB	6.44	2.18	2.05
7	B	3025	CLA	MG-NB	6.44	2.18	2.05
7	F	3054	CLA	MG-NB	6.44	2.18	2.05
7	A	3032	CLA	MG-NB	6.43	2.18	2.05
7	A	3057	CLA	MG-NB	6.43	2.18	2.05
7	A	3062	CLA	MG-NB	6.43	2.18	2.05
7	B	3019	CLA	MG-NB	6.43	2.18	2.05
7	A	3030	CLA	MG-NB	6.43	2.18	2.05
7	F	3033	CLA	MG-NB	6.42	2.18	2.05
7	B	2005	CLA	MG-NB	6.41	2.18	2.05
7	B	3035	CLA	MG-NB	6.41	2.18	2.05
7	F	3059	CLA	MG-NB	6.41	2.18	2.05
7	L	3038	CLA	MG-NB	6.40	2.18	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	3004	CLA	MG-NB	6.40	2.18	2.05
7	A	3067	CLA	MG-NB	6.40	2.18	2.05
7	B	2004	CLA	MG-NB	6.40	2.18	2.05
7	B	3042	CLA	MG-NB	6.39	2.18	2.05
7	F	3031	CLA	MG-NB	6.39	2.18	2.05
7	A	3078	CLA	MG-NB	6.38	2.18	2.05
7	K	3050	CLA	MG-NB	6.38	2.18	2.05
7	A	2006	CLA	MG-NB	6.37	2.18	2.05
7	A	3079	CLA	MG-NB	6.37	2.18	2.05
7	A	3071	CLA	MG-NB	6.36	2.18	2.05
7	F	3054	CLA	C3B-C4B	5.80	1.52	1.40
7	A	3048	CLA	C3B-C4B	5.80	1.52	1.40
7	B	3028	CLA	C3B-C4B	5.77	1.52	1.40
7	A	2001	CLA	C3B-C4B	5.76	1.52	1.40
7	A	3065	CLA	C3B-C4B	5.76	1.52	1.40
7	A	3057	CLA	C3B-C4B	5.76	1.52	1.40
7	B	3060	CLA	C3B-C4B	5.76	1.52	1.40
7	A	3079	CLA	C3B-C4B	5.76	1.52	1.40
7	A	3013	CLA	C3B-C4B	5.76	1.52	1.40
7	F	3002	CLA	C3B-C4B	5.76	1.52	1.40
7	A	3062	CLA	C3B-C4B	5.75	1.52	1.40
7	B	3011	CLA	C3B-C4B	5.74	1.52	1.40
7	B	3006	CLA	C3B-C4B	5.74	1.52	1.40
7	B	3037	CLA	C3B-C4B	5.74	1.52	1.40
7	B	3074	CLA	C3B-C4B	5.74	1.52	1.40
7	A	3072	CLA	C3B-C4B	5.74	1.52	1.40
7	A	3005	CLA	C3B-C4B	5.74	1.52	1.40
7	A	3056	CLA	C3B-C4B	5.74	1.52	1.40
7	F	3059	CLA	C3B-C4B	5.74	1.52	1.40
7	F	3061	CLA	C3B-C4B	5.74	1.52	1.40
7	B	3010	CLA	C3B-C4B	5.74	1.52	1.40
7	F	3022	CLA	C3B-C4B	5.73	1.52	1.40
7	A	3071	CLA	C3B-C4B	5.73	1.52	1.40
7	B	2004	CLA	C3B-C4B	5.73	1.52	1.40
7	A	3058	CLA	C3B-C4B	5.73	1.52	1.40
7	A	3073	CLA	C3B-C4B	5.73	1.52	1.40
7	A	3021	CLA	C3B-C4B	5.72	1.52	1.40
7	A	3043	CLA	C3B-C4B	5.72	1.52	1.40
7	A	3007	CLA	C3B-C4B	5.72	1.52	1.40
7	A	3024	CLA	C3B-C4B	5.72	1.52	1.40
7	B	3001	CLA	C3B-C4B	5.72	1.52	1.40
7	B	3023	CLA	C3B-C4B	5.72	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3081	CLA	C3B-C4B	5.72	1.52	1.40
7	B	2501	CLA	C3B-C4B	5.72	1.52	1.40
7	A	2502	CLA	C3B-C4B	5.72	1.52	1.40
7	B	3019	CLA	C3B-C4B	5.72	1.52	1.40
7	L	3038	CLA	C3B-C4B	5.71	1.52	1.40
7	A	3016	CLA	C3B-C4B	5.71	1.52	1.40
7	B	3020	CLA	C3B-C4B	5.71	1.52	1.40
7	A	3017	CLA	C3B-C4B	5.71	1.52	1.40
7	A	3053	CLA	C3B-C4B	5.71	1.52	1.40
7	F	3004	CLA	C3B-C4B	5.71	1.52	1.40
7	A	3077	CLA	C3B-C4B	5.71	1.52	1.40
7	B	3015	CLA	C3B-C4B	5.71	1.52	1.40
7	B	3066	CLA	C3B-C4B	5.70	1.52	1.40
7	K	3050	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3067	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3039	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3045	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3041	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3052	CLA	C3B-C4B	5.70	1.52	1.40
7	A	3068	CLA	C3B-C4B	5.70	1.52	1.40
7	B	2003	CLA	C3B-C4B	5.70	1.52	1.40
7	F	3033	CLA	C3B-C4B	5.70	1.52	1.40
7	B	3008	CLA	C3B-C4B	5.70	1.52	1.40
7	B	3044	CLA	C3B-C4B	5.69	1.52	1.40
7	B	3075	CLA	C3B-C4B	5.69	1.52	1.40
7	A	3078	CLA	C3B-C4B	5.69	1.52	1.40
7	B	2005	CLA	C3B-C4B	5.69	1.52	1.40
7	L	3036	CLA	C3B-C4B	5.69	1.52	1.40
7	B	3003	CLA	C3B-C4B	5.69	1.52	1.40
7	B	3076	CLA	C3B-C4B	5.69	1.52	1.40
7	B	3069	CLA	C3B-C4B	5.69	1.52	1.40
7	A	3032	CLA	C3B-C4B	5.69	1.52	1.40
7	B	3042	CLA	C3B-C4B	5.69	1.52	1.40
7	A	3026	CLA	C3B-C4B	5.68	1.52	1.40
7	F	3012	CLA	C3B-C4B	5.68	1.52	1.40
7	A	3029	CLA	C3B-C4B	5.68	1.52	1.40
7	B	3046	CLA	C3B-C4B	5.68	1.52	1.40
7	B	3070	CLA	C3B-C4B	5.68	1.52	1.40
7	B	3025	CLA	C3B-C4B	5.68	1.52	1.40
7	A	3027	CLA	C3B-C4B	5.68	1.52	1.40
7	A	3030	CLA	C3B-C4B	5.67	1.52	1.40
7	A	3040	CLA	C3B-C4B	5.67	1.52	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3055	CLA	C3B-C4B	5.67	1.52	1.40
7	A	2006	CLA	C3B-C4B	5.67	1.52	1.40
7	B	3034	CLA	C3B-C4B	5.67	1.52	1.40
7	B	3080	CLA	C3B-C4B	5.67	1.52	1.40
7	B	3063	CLA	C3B-C4B	5.66	1.52	1.40
7	K	3051	CLA	C3B-C4B	5.66	1.52	1.40
7	B	3035	CLA	C3B-C4B	5.66	1.52	1.40
7	A	3018	CLA	C3B-C4B	5.66	1.52	1.40
7	F	3031	CLA	C3B-C4B	5.65	1.52	1.40
7	A	3047	CLA	C3B-C4B	5.63	1.52	1.40
7	B	2002	CLA	C3B-C4B	5.62	1.52	1.40
7	A	3009	CLA	C3B-C4B	5.60	1.52	1.40
7	L	3049	CLA	C3B-C4B	5.59	1.52	1.40
7	B	2002	CLA	MG-NB	5.52	2.16	2.05
7	A	2006	CLA	C2B-C1B	5.30	1.51	1.40
7	F	3002	CLA	C2B-C1B	5.29	1.51	1.40
7	B	3003	CLA	C2B-C1B	5.29	1.51	1.40
7	B	3060	CLA	C2B-C1B	5.29	1.51	1.40
7	A	3043	CLA	C2B-C1B	5.28	1.51	1.40
7	B	3010	CLA	C2B-C1B	5.27	1.51	1.40
7	A	3030	CLA	C2B-C1B	5.27	1.51	1.40
7	A	3071	CLA	C2B-C1B	5.27	1.51	1.40
7	A	3016	CLA	C2B-C1B	5.27	1.51	1.40
7	F	3004	CLA	C2B-C1B	5.27	1.51	1.40
7	B	3080	CLA	C2B-C1B	5.27	1.51	1.40
7	B	3070	CLA	C2B-C1B	5.26	1.51	1.40
7	B	3081	CLA	C2B-C1B	5.26	1.51	1.40
7	B	2501	CLA	C2B-C1B	5.26	1.51	1.40
7	A	3041	CLA	C2B-C1B	5.26	1.51	1.40
7	B	3015	CLA	C2B-C1B	5.26	1.51	1.40
7	A	3062	CLA	C2B-C1B	5.26	1.51	1.40
7	A	3048	CLA	C2B-C1B	5.26	1.51	1.40
7	A	3053	CLA	C2B-C1B	5.25	1.51	1.40
7	B	3028	CLA	C2B-C1B	5.25	1.51	1.40
7	A	3027	CLA	C2B-C1B	5.25	1.51	1.40
7	F	3033	CLA	C2B-C1B	5.25	1.51	1.40
7	F	3061	CLA	C2B-C1B	5.25	1.51	1.40
7	L	3036	CLA	C2B-C1B	5.25	1.51	1.40
7	A	3065	CLA	C2B-C1B	5.25	1.51	1.40
7	A	3047	CLA	C2B-C1B	5.25	1.51	1.40
7	A	3079	CLA	C2B-C1B	5.25	1.51	1.40
7	B	2003	CLA	C2B-C1B	5.25	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3034	CLA	C2B-C1B	5.25	1.51	1.40
7	A	3018	CLA	C2B-C1B	5.25	1.51	1.40
7	B	3063	CLA	C2B-C1B	5.25	1.51	1.40
7	B	3011	CLA	C2B-C1B	5.24	1.51	1.40
7	F	3059	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3056	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3072	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3017	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3026	CLA	C2B-C1B	5.24	1.51	1.40
7	B	3001	CLA	C2B-C1B	5.24	1.51	1.40
7	B	3042	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3057	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3039	CLA	C2B-C1B	5.24	1.51	1.40
7	B	3046	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3058	CLA	C2B-C1B	5.24	1.51	1.40
7	A	3007	CLA	C2B-C1B	5.23	1.51	1.40
7	B	3074	CLA	C2B-C1B	5.23	1.51	1.40
7	B	3023	CLA	C2B-C1B	5.23	1.51	1.40
7	B	3069	CLA	C2B-C1B	5.23	1.51	1.40
7	B	3019	CLA	C2B-C1B	5.23	1.51	1.40
7	B	3035	CLA	C2B-C1B	5.23	1.51	1.40
7	A	3073	CLA	C2B-C1B	5.23	1.51	1.40
7	F	3054	CLA	C2B-C1B	5.23	1.51	1.40
7	A	2001	CLA	C2B-C1B	5.23	1.51	1.40
7	A	3024	CLA	C2B-C1B	5.23	1.51	1.40
7	B	2005	CLA	C2B-C1B	5.22	1.51	1.40
7	B	3025	CLA	C2B-C1B	5.22	1.51	1.40
7	A	3029	CLA	C2B-C1B	5.22	1.51	1.40
7	A	3032	CLA	C2B-C1B	5.22	1.51	1.40
7	F	3022	CLA	C2B-C1B	5.22	1.51	1.40
7	B	3020	CLA	C2B-C1B	5.22	1.51	1.40
7	A	3067	CLA	C2B-C1B	5.22	1.51	1.40
7	B	2002	CLA	C2B-C1B	5.22	1.51	1.40
7	A	3040	CLA	C2B-C1B	5.22	1.51	1.40
7	A	3068	CLA	C2B-C1B	5.22	1.51	1.40
7	B	3037	CLA	C2B-C1B	5.21	1.51	1.40
7	A	2502	CLA	C2B-C1B	5.21	1.51	1.40
7	A	3045	CLA	C2B-C1B	5.21	1.51	1.40
7	B	3055	CLA	C2B-C1B	5.21	1.51	1.40
7	A	3077	CLA	C2B-C1B	5.21	1.51	1.40
7	B	3006	CLA	C2B-C1B	5.21	1.51	1.40
7	A	3078	CLA	C2B-C1B	5.21	1.51	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3052	CLA	C2B-C1B	5.20	1.51	1.40
7	B	3076	CLA	C2B-C1B	5.20	1.51	1.40
7	A	3021	CLA	C2B-C1B	5.20	1.51	1.40
7	F	3012	CLA	C2B-C1B	5.20	1.51	1.40
7	K	3051	CLA	C2B-C1B	5.20	1.51	1.40
7	K	3050	CLA	C2B-C1B	5.20	1.51	1.40
7	B	3044	CLA	C2B-C1B	5.20	1.51	1.40
7	A	3005	CLA	C2B-C1B	5.20	1.51	1.40
7	B	3066	CLA	C2B-C1B	5.20	1.51	1.40
7	A	3009	CLA	C2B-C1B	5.19	1.51	1.40
7	B	3075	CLA	C2B-C1B	5.17	1.51	1.40
7	A	3013	CLA	C2B-C1B	5.17	1.51	1.40
7	F	3031	CLA	C2B-C1B	5.16	1.51	1.40
7	L	3049	CLA	C2B-C1B	5.16	1.51	1.40
7	B	3008	CLA	C2B-C1B	5.14	1.51	1.40
7	B	2004	CLA	C2B-C1B	5.13	1.51	1.40
7	L	3038	CLA	C2B-C1B	5.12	1.51	1.40
7	L	3049	CLA	C3B-C2B	4.83	1.55	1.39
7	B	2005	CLA	C3B-C2B	4.82	1.55	1.39
7	B	3035	CLA	C3B-C2B	4.81	1.55	1.39
7	B	3066	CLA	C3B-C2B	4.80	1.55	1.39
7	L	3036	CLA	C3B-C2B	4.80	1.55	1.39
7	B	3055	CLA	C3B-C2B	4.80	1.55	1.39
7	A	3024	CLA	C3B-C2B	4.80	1.55	1.39
7	A	3027	CLA	C3B-C2B	4.80	1.55	1.39
7	B	3028	CLA	C3B-C2B	4.80	1.55	1.39
7	K	3050	CLA	C3B-C2B	4.80	1.55	1.39
7	B	3069	CLA	C3B-C2B	4.80	1.55	1.39
7	B	2002	CLA	C3B-C2B	4.79	1.55	1.39
7	A	2006	CLA	C3B-C2B	4.79	1.55	1.39
7	A	3009	CLA	C3B-C2B	4.79	1.55	1.39
7	B	3019	CLA	C3B-C2B	4.79	1.55	1.39
7	F	3031	CLA	C3B-C2B	4.79	1.55	1.39
7	B	3034	CLA	C3B-C2B	4.79	1.55	1.39
7	B	3006	CLA	C3B-C2B	4.79	1.55	1.39
7	L	3038	CLA	C3B-C2B	4.79	1.55	1.39
7	B	3042	CLA	C3B-C2B	4.79	1.55	1.39
7	A	3039	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3075	CLA	C3B-C2B	4.78	1.55	1.39
7	A	3058	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3046	CLA	C3B-C2B	4.78	1.55	1.39
7	F	3012	CLA	C3B-C2B	4.78	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3048	CLA	C3B-C2B	4.78	1.55	1.39
7	A	3052	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3044	CLA	C3B-C2B	4.78	1.55	1.39
7	F	3004	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3020	CLA	C3B-C2B	4.78	1.55	1.39
7	A	2502	CLA	C3B-C2B	4.78	1.55	1.39
7	A	3007	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3060	CLA	C3B-C2B	4.78	1.55	1.39
7	K	3051	CLA	C3B-C2B	4.78	1.55	1.39
7	B	3081	CLA	C3B-C2B	4.78	1.55	1.39
7	F	3061	CLA	C3B-C2B	4.78	1.55	1.39
7	A	3053	CLA	C3B-C2B	4.78	1.55	1.39
7	A	3068	CLA	C3B-C2B	4.77	1.55	1.39
7	B	3010	CLA	C3B-C2B	4.77	1.55	1.39
7	F	3033	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3072	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3005	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3018	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3026	CLA	C3B-C2B	4.77	1.55	1.39
7	B	3011	CLA	C3B-C2B	4.77	1.55	1.39
7	A	2001	CLA	C3B-C2B	4.77	1.55	1.39
7	B	3025	CLA	C3B-C2B	4.77	1.55	1.39
7	B	3080	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3041	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3043	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3045	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3056	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3073	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3040	CLA	C3B-C2B	4.77	1.55	1.39
7	B	2501	CLA	C3B-C2B	4.77	1.55	1.39
7	A	3032	CLA	C3B-C2B	4.76	1.55	1.39
7	B	2004	CLA	C3B-C2B	4.76	1.55	1.39
7	A	3017	CLA	C3B-C2B	4.76	1.55	1.39
7	B	3001	CLA	C3B-C2B	4.76	1.55	1.39
7	B	3070	CLA	C3B-C2B	4.76	1.55	1.39
7	A	3021	CLA	C3B-C2B	4.76	1.55	1.39
7	B	3074	CLA	C3B-C2B	4.76	1.55	1.39
7	A	3016	CLA	C3B-C2B	4.76	1.55	1.39
7	A	3029	CLA	C3B-C2B	4.76	1.55	1.39
7	F	3022	CLA	C3B-C2B	4.76	1.55	1.39
7	B	3008	CLA	C3B-C2B	4.75	1.55	1.39
7	B	3076	CLA	C3B-C2B	4.75	1.55	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3037	CLA	C3B-C2B	4.75	1.55	1.39
7	F	3054	CLA	C3B-C2B	4.75	1.55	1.39
7	A	3030	CLA	C3B-C2B	4.75	1.55	1.39
7	A	3047	CLA	C3B-C2B	4.75	1.55	1.39
7	A	3077	CLA	C3B-C2B	4.75	1.55	1.39
7	B	2003	CLA	C3B-C2B	4.75	1.55	1.39
7	A	3013	CLA	C3B-C2B	4.74	1.55	1.39
7	A	3071	CLA	C3B-C2B	4.74	1.55	1.39
7	B	3063	CLA	C3B-C2B	4.74	1.55	1.39
7	B	3015	CLA	C3B-C2B	4.74	1.55	1.39
7	F	3002	CLA	C3B-C2B	4.74	1.55	1.39
7	A	3057	CLA	C3B-C2B	4.74	1.55	1.39
7	B	3023	CLA	C3B-C2B	4.74	1.55	1.39
7	B	3003	CLA	C3B-C2B	4.74	1.55	1.39
7	A	3079	CLA	C3B-C2B	4.73	1.55	1.39
7	F	3059	CLA	C3B-C2B	4.73	1.55	1.39
7	A	3067	CLA	C3B-C2B	4.72	1.55	1.39
7	A	3062	CLA	C3B-C2B	4.72	1.55	1.39
7	A	3078	CLA	C3B-C2B	4.72	1.55	1.39
7	A	3065	CLA	C3B-C2B	4.69	1.54	1.39
7	B	2002	CLA	MG-NC	-4.28	1.96	2.06
7	A	2001	CLA	MG-NC	-4.21	1.96	2.06
7	B	2003	CLA	MG-NC	-4.02	1.96	2.06
7	B	2004	CLA	MG-NC	-3.88	1.97	2.06
7	A	3058	CLA	C3C-C2C	3.38	1.42	1.35
7	A	3007	CLA	C3C-C2C	3.36	1.42	1.35
7	F	3054	CLA	C3C-C2C	3.35	1.42	1.35
7	F	3061	CLA	C3C-C2C	3.34	1.42	1.35
7	B	2002	CLA	C3C-C2C	3.34	1.42	1.35
7	B	3063	CLA	C3C-C2C	3.32	1.42	1.35
7	A	3071	CLA	C3C-C2C	3.32	1.42	1.35
7	B	3010	CLA	C3C-C2C	3.32	1.42	1.35
7	A	3079	CLA	C3C-C2C	3.32	1.42	1.35
7	B	3020	CLA	C3C-C2C	3.31	1.42	1.35
7	B	3008	CLA	C3C-C2C	3.31	1.42	1.35
7	F	3002	CLA	C3C-C2C	3.31	1.42	1.35
7	A	3045	CLA	C3C-C2C	3.31	1.42	1.35
7	A	3039	CLA	C3C-C2C	3.31	1.42	1.35
7	B	3044	CLA	C3C-C2C	3.31	1.42	1.35
7	B	3019	CLA	C3C-C2C	3.31	1.42	1.35
7	B	3028	CLA	C3C-C2C	3.30	1.42	1.35
7	A	3052	CLA	C3C-C2C	3.30	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3077	CLA	C3C-C2C	3.30	1.42	1.35
7	B	2501	CLA	C3C-C2C	3.30	1.42	1.35
7	A	3009	CLA	C3C-C2C	3.30	1.42	1.35
7	A	3048	CLA	C3C-C2C	3.30	1.42	1.35
7	B	3070	CLA	C3C-C2C	3.30	1.42	1.35
7	B	3001	CLA	C3C-C2C	3.30	1.42	1.35
7	B	2004	CLA	C3C-C2C	3.30	1.42	1.35
7	A	3005	CLA	C3C-C2C	3.30	1.42	1.35
7	B	3074	CLA	C3C-C2C	3.29	1.42	1.35
7	B	3080	CLA	C3C-C2C	3.29	1.42	1.35
7	A	3013	CLA	C3C-C2C	3.29	1.42	1.35
7	A	3067	CLA	C3C-C2C	3.29	1.42	1.35
7	A	2502	CLA	C3C-C2C	3.29	1.42	1.35
7	A	3053	CLA	C3C-C2C	3.29	1.42	1.35
7	B	3055	CLA	C3C-C2C	3.29	1.42	1.35
7	A	3024	CLA	C3C-C2C	3.29	1.42	1.35
7	A	3062	CLA	C3C-C2C	3.29	1.42	1.35
7	B	2003	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3015	CLA	C3C-C2C	3.28	1.42	1.35
7	A	2001	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3073	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3040	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3068	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3046	CLA	C3C-C2C	3.28	1.42	1.35
7	F	3059	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3076	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3026	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3011	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3069	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3021	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3072	CLA	C3C-C2C	3.28	1.42	1.35
7	A	3047	CLA	C3C-C2C	3.28	1.42	1.35
7	B	3066	CLA	C3C-C2C	3.28	1.42	1.35
7	B	2005	CLA	C3C-C2C	3.27	1.42	1.35
7	A	3016	CLA	C3C-C2C	3.27	1.42	1.35
7	A	3078	CLA	C3C-C2C	3.27	1.42	1.35
7	A	3065	CLA	C3C-C2C	3.27	1.42	1.35
7	L	3038	CLA	C3C-C2C	3.27	1.42	1.35
7	A	3014	CLA	C2D-C1D	3.27	1.52	1.44
7	A	3014	CLA	C3C-C2C	3.27	1.42	1.35
7	A	3029	CLA	C3C-C2C	3.27	1.42	1.35
7	F	3012	CLA	C3C-C2C	3.27	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3018	CLA	C3C-C2C	3.26	1.42	1.35
7	F	3033	CLA	C3C-C2C	3.26	1.42	1.35
7	F	3031	CLA	C3C-C2C	3.26	1.42	1.35
7	F	3004	CLA	C3C-C2C	3.26	1.42	1.35
7	B	3006	CLA	C3C-C2C	3.26	1.42	1.35
7	A	3041	CLA	C3C-C2C	3.26	1.42	1.35
7	L	3064	CLA	C2D-C1D	3.26	1.52	1.44
7	A	3056	CLA	C3C-C2C	3.26	1.42	1.35
7	A	3030	CLA	C3C-C2C	3.25	1.42	1.35
7	A	3017	CLA	C3C-C2C	3.25	1.42	1.35
7	K	3051	CLA	C3C-C2C	3.25	1.42	1.35
7	B	3003	CLA	C3C-C2C	3.25	1.42	1.35
7	L	3036	CLA	C3C-C2C	3.25	1.42	1.35
7	A	2006	CLA	C3C-C2C	3.25	1.42	1.35
7	L	3064	CLA	C3C-C2C	3.24	1.42	1.35
7	K	3050	CLA	C3C-C2C	3.24	1.42	1.35
7	L	3049	CLA	C3C-C2C	3.24	1.42	1.35
7	B	3034	CLA	C3C-C2C	3.24	1.42	1.35
7	A	3043	CLA	C3C-C2C	3.24	1.42	1.35
7	L	3064	CLA	C2B-C1B	3.24	1.47	1.40
7	B	3037	CLA	C3C-C2C	3.24	1.42	1.35
7	B	3042	CLA	C3C-C2C	3.24	1.42	1.35
7	A	3032	CLA	C3C-C2C	3.23	1.42	1.35
7	B	3035	CLA	C3C-C2C	3.23	1.42	1.35
7	B	3060	CLA	C3C-C2C	3.22	1.42	1.35
7	B	3075	CLA	C3C-C2C	3.22	1.42	1.35
7	F	3022	CLA	C3C-C2C	3.22	1.42	1.35
7	B	3081	CLA	C3C-C2C	3.22	1.42	1.35
7	B	3023	CLA	C3C-C2C	3.22	1.42	1.35
7	A	3014	CLA	C2B-C1B	3.21	1.47	1.40
7	B	3025	CLA	C3C-C2C	3.21	1.42	1.35
7	A	3027	CLA	C3C-C2C	3.21	1.42	1.35
7	A	3057	CLA	C3C-C2C	3.19	1.42	1.35
7	L	3064	CLA	C3D-C4D	2.85	1.51	1.44
7	A	3014	CLA	C3D-C4D	2.85	1.51	1.44
7	L	3064	CLA	C3B-C4B	2.60	1.45	1.40
7	A	3014	CLA	C3B-C4B	2.56	1.45	1.40
7	L	3036	CLA	MG-ND	2.28	2.10	2.05
7	A	3030	CLA	MG-ND	2.28	2.10	2.05
7	A	3057	CLA	MG-ND	2.27	2.10	2.05
7	K	3050	CLA	MG-ND	2.27	2.10	2.05
7	F	3033	CLA	MG-ND	2.27	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	3038	CLA	MG-ND	2.26	2.10	2.05
7	A	3032	CLA	MG-ND	2.26	2.10	2.05
7	L	3049	CLA	MG-ND	2.25	2.10	2.05
7	F	3054	CLA	MG-ND	2.25	2.10	2.05
7	A	3062	CLA	MG-ND	2.25	2.10	2.05
7	F	3059	CLA	MG-ND	2.25	2.10	2.05
7	B	3008	CLA	MG-ND	2.25	2.10	2.05
7	B	2005	CLA	MG-ND	2.25	2.10	2.05
7	F	3012	CLA	MG-ND	2.25	2.10	2.05
7	A	2006	CLA	MG-ND	2.25	2.10	2.05
7	B	3069	CLA	MG-ND	2.24	2.10	2.05
7	A	3072	CLA	MG-ND	2.24	2.10	2.05
7	A	3079	CLA	MG-ND	2.24	2.10	2.05
7	A	3067	CLA	MG-ND	2.24	2.10	2.05
7	A	3071	CLA	MG-ND	2.24	2.10	2.05
7	B	3042	CLA	MG-ND	2.24	2.10	2.05
7	A	3065	CLA	MG-ND	2.24	2.10	2.05
7	A	3078	CLA	MG-ND	2.23	2.10	2.05
7	L	3064	CLA	MG-NB	2.23	2.10	2.05
7	F	3004	CLA	MG-ND	2.23	2.10	2.05
7	A	3007	CLA	MG-ND	2.22	2.10	2.05
7	B	3019	CLA	MG-ND	2.22	2.10	2.05
7	B	3075	CLA	MG-ND	2.22	2.10	2.05
7	A	3029	CLA	MG-ND	2.22	2.10	2.05
7	B	3023	CLA	MG-ND	2.22	2.10	2.05
7	B	3037	CLA	MG-ND	2.21	2.10	2.05
7	A	3013	CLA	MG-ND	2.21	2.10	2.05
7	A	3073	CLA	MG-ND	2.21	2.10	2.05
7	A	3047	CLA	MG-ND	2.21	2.10	2.05
7	B	3080	CLA	MG-ND	2.21	2.10	2.05
7	A	3045	CLA	MG-ND	2.21	2.10	2.05
7	B	3020	CLA	MG-ND	2.21	2.10	2.05
7	B	3011	CLA	MG-ND	2.20	2.10	2.05
7	A	3009	CLA	MG-ND	2.20	2.10	2.05
7	A	3024	CLA	MG-ND	2.20	2.10	2.05
7	B	3034	CLA	MG-ND	2.20	2.10	2.05
7	A	3018	CLA	MG-ND	2.20	2.10	2.05
7	B	3035	CLA	MG-ND	2.20	2.10	2.05
7	A	3014	CLA	MG-NB	2.20	2.10	2.05
7	B	3081	CLA	MG-ND	2.20	2.10	2.05
7	B	3025	CLA	MG-ND	2.19	2.10	2.05
7	A	3058	CLA	MG-ND	2.19	2.10	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3074	CLA	MG-ND	2.19	2.10	2.05
7	F	3002	CLA	MG-ND	2.19	2.10	2.05
7	F	3031	CLA	MG-ND	2.19	2.10	2.05
7	A	3068	CLA	MG-ND	2.19	2.10	2.05
7	B	3066	CLA	MG-ND	2.19	2.10	2.05
7	A	3021	CLA	MG-ND	2.19	2.10	2.05
7	A	3017	CLA	MG-ND	2.19	2.10	2.05
7	K	3051	CLA	MG-ND	2.19	2.10	2.05
7	A	3016	CLA	MG-ND	2.18	2.10	2.05
7	B	3003	CLA	MG-ND	2.18	2.10	2.05
7	B	3044	CLA	MG-ND	2.18	2.10	2.05
7	F	3022	CLA	MG-ND	2.18	2.10	2.05
7	B	3001	CLA	MG-ND	2.18	2.10	2.05
7	B	3046	CLA	MG-ND	2.18	2.10	2.05
7	B	3076	CLA	MG-ND	2.18	2.10	2.05
7	A	3077	CLA	MG-ND	2.18	2.10	2.05
7	F	3061	CLA	MG-ND	2.18	2.10	2.05
7	A	3040	CLA	MG-ND	2.18	2.10	2.05
7	A	2502	CLA	MG-ND	2.18	2.10	2.05
7	B	3006	CLA	MG-ND	2.17	2.10	2.05
7	A	3039	CLA	MG-ND	2.17	2.10	2.05
7	A	3041	CLA	MG-ND	2.17	2.10	2.05
7	A	3056	CLA	MG-ND	2.17	2.10	2.05
7	A	3027	CLA	MG-ND	2.17	2.10	2.05
7	A	3043	CLA	MG-ND	2.17	2.10	2.05
7	B	3028	CLA	MG-ND	2.16	2.10	2.05
7	A	3052	CLA	MG-ND	2.16	2.10	2.05
7	B	3063	CLA	MG-ND	2.16	2.10	2.05
7	B	3015	CLA	MG-ND	2.16	2.10	2.05
7	B	3055	CLA	MG-ND	2.15	2.10	2.05
7	A	3053	CLA	MG-ND	2.15	2.10	2.05
7	B	3070	CLA	MG-ND	2.15	2.10	2.05
7	B	3010	CLA	MG-ND	2.15	2.10	2.05
7	B	3060	CLA	MG-ND	2.15	2.10	2.05
7	A	3026	CLA	MG-ND	2.15	2.10	2.05
7	A	3005	CLA	MG-ND	2.14	2.10	2.05
7	A	3048	CLA	MG-ND	2.14	2.10	2.05
7	B	2501	CLA	MG-ND	2.13	2.10	2.05
7	A	3013	CLA	C1C-NC	-2.08	1.33	1.38
7	L	3049	CLA	C1C-NC	-2.08	1.33	1.38
7	K	3050	CLA	C1C-NC	-2.08	1.33	1.38
7	A	3047	CLA	C1C-NC	-2.07	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	3003	CLA	C1C-NC	-2.07	1.33	1.38
7	B	3010	CLA	C1C-NC	-2.07	1.33	1.38
7	A	3009	CLA	C1C-NC	-2.07	1.33	1.38
7	B	2004	CLA	C1C-NC	-2.07	1.33	1.38
7	A	3065	CLA	C1C-NC	-2.06	1.33	1.38
7	A	3058	CLA	C1C-NC	-2.06	1.33	1.38
7	A	3072	CLA	C1C-NC	-2.06	1.33	1.38
7	B	2501	CLA	C1C-NC	-2.06	1.33	1.38
7	A	3071	CLA	C1C-NC	-2.06	1.33	1.38
7	F	3059	CLA	C1C-NC	-2.06	1.33	1.38
7	A	3062	CLA	C1C-NC	-2.05	1.33	1.38
7	A	3027	CLA	C1C-NC	-2.05	1.33	1.38
7	A	3077	CLA	C1C-NC	-2.05	1.33	1.38
7	A	3041	CLA	C1C-NC	-2.05	1.33	1.38
7	A	3039	CLA	C1C-NC	-2.05	1.33	1.38
7	A	3005	CLA	C1C-NC	-2.04	1.33	1.38
7	B	3076	CLA	C1C-NC	-2.04	1.33	1.38
7	B	3075	CLA	C1C-NC	-2.04	1.33	1.38
7	L	3036	CLA	C1C-NC	-2.04	1.33	1.38
7	B	3019	CLA	C1C-NC	-2.04	1.33	1.38
7	B	2002	CLA	C1C-NC	-2.04	1.33	1.38
7	B	3037	CLA	C1C-NC	-2.04	1.33	1.38
7	A	3007	CLA	C1C-NC	-2.03	1.33	1.38
7	A	3026	CLA	C1C-NC	-2.03	1.33	1.38
7	A	3052	CLA	C1C-NC	-2.03	1.33	1.38
7	F	3012	CLA	C1C-NC	-2.03	1.33	1.38
7	B	3025	CLA	C1C-NC	-2.03	1.33	1.38
7	B	3001	CLA	C1C-NC	-2.03	1.33	1.38
7	F	3002	CLA	C1C-NC	-2.03	1.33	1.38
7	A	3056	CLA	C1C-NC	-2.03	1.33	1.38
7	B	2005	CLA	C1C-NC	-2.03	1.33	1.38
7	A	2006	CLA	C1C-NC	-2.02	1.33	1.38
7	A	3032	CLA	C1C-NC	-2.02	1.33	1.38
7	B	3028	CLA	C1C-NC	-2.02	1.33	1.38
7	B	3063	CLA	C1C-NC	-2.02	1.33	1.38
7	B	3015	CLA	C1C-NC	-2.02	1.33	1.38
7	B	3055	CLA	C1C-NC	-2.02	1.33	1.38
7	F	3033	CLA	C1C-NC	-2.02	1.33	1.38
7	A	3030	CLA	C1C-NC	-2.02	1.33	1.38
7	B	3046	CLA	C1C-NC	-2.02	1.33	1.38
7	A	3029	CLA	C1C-NC	-2.02	1.33	1.38
7	A	3040	CLA	C1C-NC	-2.02	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	3079	CLA	C1C-NC	-2.02	1.33	1.38
7	F	3004	CLA	C1C-NC	-2.01	1.33	1.38
7	K	3051	CLA	C1C-NC	-2.01	1.33	1.38
7	A	3024	CLA	C1C-NC	-2.01	1.33	1.38
7	B	3011	CLA	C1C-NC	-2.01	1.33	1.38
7	B	3023	CLA	C1C-NC	-2.01	1.33	1.38
7	A	3053	CLA	C1C-NC	-2.01	1.33	1.38
7	A	3017	CLA	C1C-NC	-2.01	1.33	1.38
7	B	3006	CLA	C1C-NC	-2.01	1.33	1.38
7	A	3018	CLA	C1C-NC	-2.01	1.33	1.38
7	A	3073	CLA	C1C-NC	-2.00	1.33	1.38
7	B	3081	CLA	C1C-NC	-2.00	1.33	1.38
7	A	3021	CLA	C1C-NC	-2.00	1.33	1.38
7	F	3022	CLA	C1C-NC	-2.00	1.33	1.38

All (712) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3061	CLA	C1B-NB-C4B	6.81	111.09	106.31
7	B	3003	CLA	C1B-NB-C4B	6.81	111.09	106.31
7	F	3054	CLA	C1B-NB-C4B	6.80	111.08	106.31
7	B	3060	CLA	C1B-NB-C4B	6.77	111.06	106.31
7	A	3068	CLA	C1B-NB-C4B	6.77	111.06	106.31
7	B	2501	CLA	C1B-NB-C4B	6.77	111.06	106.31
7	B	3010	CLA	C1B-NB-C4B	6.76	111.06	106.31
7	F	3002	CLA	C1B-NB-C4B	6.76	111.06	106.31
7	B	3074	CLA	C1B-NB-C4B	6.76	111.06	106.31
7	A	3048	CLA	C1B-NB-C4B	6.76	111.05	106.31
7	B	3020	CLA	C1B-NB-C4B	6.76	111.05	106.31
7	A	3058	CLA	C1B-NB-C4B	6.75	111.05	106.31
7	A	3007	CLA	C1B-NB-C4B	6.75	111.05	106.31
7	B	3028	CLA	C1B-NB-C4B	6.75	111.05	106.31
7	F	3022	CLA	C1B-NB-C4B	6.74	111.04	106.31
7	A	3073	CLA	C1B-NB-C4B	6.74	111.04	106.31
7	B	3006	CLA	C1B-NB-C4B	6.73	111.04	106.31
7	A	3065	CLA	C1B-NB-C4B	6.73	111.03	106.31
7	A	3039	CLA	C1B-NB-C4B	6.73	111.03	106.31
7	B	3069	CLA	C1B-NB-C4B	6.72	111.03	106.31
7	A	2001	CLA	C1B-NB-C4B	6.72	111.03	106.31
7	A	3072	CLA	C1B-NB-C4B	6.72	111.03	106.31
7	A	3021	CLA	C1B-NB-C4B	6.72	111.03	106.31
7	A	3077	CLA	C1B-NB-C4B	6.72	111.02	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3056	CLA	C1B-NB-C4B	6.71	111.02	106.31
7	A	3014	CLA	C4D-ND-C1D	6.71	111.02	106.31
7	B	3001	CLA	C1B-NB-C4B	6.71	111.02	106.31
7	L	3064	CLA	C4D-ND-C1D	6.71	111.02	106.31
7	B	3063	CLA	C1B-NB-C4B	6.70	111.02	106.31
7	B	3015	CLA	C1B-NB-C4B	6.70	111.01	106.31
7	A	3043	CLA	C1B-NB-C4B	6.70	111.01	106.31
7	B	3070	CLA	C1B-NB-C4B	6.69	111.00	106.31
7	A	3016	CLA	C1B-NB-C4B	6.69	111.00	106.31
7	B	3034	CLA	C1B-NB-C4B	6.68	111.00	106.31
7	A	3045	CLA	C1B-NB-C4B	6.68	111.00	106.31
7	A	3071	CLA	C1B-NB-C4B	6.68	111.00	106.31
7	A	2502	CLA	C1B-NB-C4B	6.68	111.00	106.31
7	B	2003	CLA	C1B-NB-C4B	6.67	111.00	106.31
7	A	3041	CLA	C1B-NB-C4B	6.67	110.99	106.31
7	A	3062	CLA	C1B-NB-C4B	6.67	110.99	106.31
7	F	3004	CLA	C1B-NB-C4B	6.67	110.99	106.31
7	B	3046	CLA	C1B-NB-C4B	6.66	110.99	106.31
7	B	3044	CLA	C1B-NB-C4B	6.66	110.98	106.31
7	B	3080	CLA	C1B-NB-C4B	6.65	110.98	106.31
7	F	3059	CLA	C1B-NB-C4B	6.65	110.98	106.31
7	B	3011	CLA	C1B-NB-C4B	6.65	110.98	106.31
7	A	3057	CLA	C1B-NB-C4B	6.64	110.97	106.31
7	A	3029	CLA	C1B-NB-C4B	6.64	110.97	106.31
7	A	3053	CLA	C1B-NB-C4B	6.63	110.96	106.31
7	A	3079	CLA	C1B-NB-C4B	6.63	110.96	106.31
7	A	3030	CLA	C1B-NB-C4B	6.62	110.96	106.31
7	A	3047	CLA	C1B-NB-C4B	6.62	110.96	106.31
7	B	3023	CLA	C1B-NB-C4B	6.62	110.96	106.31
7	B	3037	CLA	C1B-NB-C4B	6.61	110.95	106.31
7	A	3027	CLA	C1B-NB-C4B	6.61	110.95	106.31
7	A	3017	CLA	C1B-NB-C4B	6.61	110.95	106.31
7	L	3036	CLA	C1B-NB-C4B	6.61	110.95	106.31
7	K	3051	CLA	C1B-NB-C4B	6.60	110.94	106.31
7	B	3066	CLA	C1B-NB-C4B	6.60	110.94	106.31
7	B	3081	CLA	C1B-NB-C4B	6.60	110.94	106.31
7	A	3040	CLA	C1B-NB-C4B	6.60	110.94	106.31
7	A	3026	CLA	C1B-NB-C4B	6.59	110.94	106.31
7	A	3032	CLA	C1B-NB-C4B	6.59	110.94	106.31
7	B	2005	CLA	C1B-NB-C4B	6.59	110.94	106.31
7	A	3005	CLA	C1B-NB-C4B	6.59	110.93	106.31
7	F	3012	CLA	C1B-NB-C4B	6.59	110.93	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3008	CLA	C1B-NB-C4B	6.58	110.93	106.31
7	A	3027	CLA	CHC-C1C-NC	6.57	133.99	124.33
7	F	3033	CLA	C1B-NB-C4B	6.57	110.92	106.31
7	A	3078	CLA	CHC-C1C-NC	6.57	133.98	124.33
7	A	3065	CLA	CHC-C1C-NC	6.57	133.98	124.33
7	A	3013	CLA	C1B-NB-C4B	6.56	110.92	106.31
7	F	3059	CLA	CHC-C1C-NC	6.56	133.98	124.33
7	A	3071	CLA	CHC-C1C-NC	6.56	133.97	124.33
7	A	3067	CLA	CHC-C1C-NC	6.55	133.96	124.33
7	A	3052	CLA	C1B-NB-C4B	6.55	110.91	106.31
7	A	3062	CLA	CHC-C1C-NC	6.55	133.95	124.33
7	A	3018	CLA	C1B-NB-C4B	6.55	110.91	106.31
7	B	3060	CLA	CHC-C1C-NC	6.55	133.95	124.33
7	A	3021	CLA	CHC-C1C-NC	6.54	133.95	124.33
7	A	2006	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	B	3035	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	A	3077	CLA	CHC-C1C-NC	6.54	133.95	124.33
7	B	3006	CLA	CHC-C1C-NC	6.54	133.95	124.33
7	B	2004	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	B	3076	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	A	3024	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	B	3034	CLA	CHC-C1C-NC	6.54	133.94	124.33
7	K	3050	CLA	CHC-C1C-NC	6.54	133.94	124.33
7	A	3067	CLA	C1B-NB-C4B	6.54	110.90	106.31
7	F	3002	CLA	CHC-C1C-NC	6.53	133.93	124.33
7	A	2006	CLA	CHC-C1C-NC	6.53	133.93	124.33
7	B	3001	CLA	CHC-C1C-NC	6.53	133.92	124.33
7	F	3004	CLA	CHC-C1C-NC	6.53	133.92	124.33
7	B	3025	CLA	C1B-NB-C4B	6.53	110.89	106.31
7	A	3009	CLA	CHC-C1C-NC	6.53	133.92	124.33
7	L	3049	CLA	CHC-C1C-NC	6.53	133.92	124.33
7	B	3074	CLA	CHC-C1C-NC	6.53	133.92	124.33
7	A	3045	CLA	CHC-C1C-NC	6.52	133.92	124.33
7	A	3048	CLA	CHC-C1C-NC	6.52	133.92	124.33
7	A	3072	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	B	3025	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	L	3049	CLA	C1B-NB-C4B	6.52	110.89	106.31
7	B	3081	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	A	3024	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	A	3043	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	B	3019	CLA	C1B-NB-C4B	6.52	110.89	106.31
7	A	3016	CLA	CHC-C1C-NC	6.52	133.91	124.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3017	CLA	CHC-C1C-NC	6.52	133.91	124.33
7	A	3009	CLA	C1B-NB-C4B	6.52	110.88	106.31
7	B	3075	CLA	C1B-NB-C4B	6.52	110.88	106.31
7	B	3069	CLA	CHC-C1C-NC	6.51	133.90	124.33
7	A	3007	CLA	CHC-C1C-NC	6.51	133.90	124.33
7	A	3079	CLA	CHC-C1C-NC	6.51	133.89	124.33
7	L	3038	CLA	CHC-C1C-NC	6.51	133.89	124.33
7	F	3022	CLA	CHC-C1C-NC	6.51	133.89	124.33
7	A	3026	CLA	CHC-C1C-NC	6.51	133.89	124.33
7	B	3046	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	B	2005	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	B	3023	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	B	3008	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	A	3073	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	F	3012	CLA	CHC-C1C-NC	6.50	133.88	124.33
7	A	3032	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	A	2001	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	K	3050	CLA	C1B-NB-C4B	6.49	110.87	106.31
7	A	3041	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	F	3033	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	A	3040	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	A	3056	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	B	3055	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	A	3052	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	B	3044	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	A	3013	CLA	CHC-C1C-NC	6.49	133.87	124.33
7	B	3070	CLA	CHC-C1C-NC	6.49	133.86	124.33
7	A	3058	CLA	CHC-C1C-NC	6.49	133.86	124.33
7	L	3038	CLA	C1B-NB-C4B	6.48	110.86	106.31
7	B	3066	CLA	CHC-C1C-NC	6.48	133.86	124.33
7	B	3042	CLA	C1B-NB-C4B	6.48	110.86	106.31
7	A	3078	CLA	C1B-NB-C4B	6.48	110.86	106.31
7	A	3068	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	K	3051	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	B	3080	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	F	3054	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	A	2502	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	A	3018	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	B	3011	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	B	3063	CLA	CHC-C1C-NC	6.48	133.85	124.33
7	B	2501	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3037	CLA	CHC-C1C-NC	6.47	133.84	124.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3003	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3035	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3010	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3019	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3076	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	3015	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	B	2003	CLA	CHC-C1C-NC	6.47	133.84	124.33
7	F	3031	CLA	CHC-C1C-NC	6.47	133.83	124.33
7	B	3028	CLA	CHC-C1C-NC	6.46	133.83	124.33
7	A	3030	CLA	CHC-C1C-NC	6.46	133.82	124.33
7	A	3053	CLA	CHC-C1C-NC	6.46	133.82	124.33
7	B	3075	CLA	CHC-C1C-NC	6.46	133.82	124.33
7	B	2002	CLA	CHC-C1C-NC	6.45	133.81	124.33
7	B	3020	CLA	CHC-C1C-NC	6.45	133.81	124.33
7	L	3036	CLA	CHC-C1C-NC	6.45	133.81	124.33
7	F	3061	CLA	CHC-C1C-NC	6.44	133.80	124.33
7	A	3039	CLA	CHC-C1C-NC	6.44	133.79	124.33
7	A	3047	CLA	CHC-C1C-NC	6.43	133.78	124.33
7	B	3042	CLA	CHC-C1C-NC	6.43	133.78	124.33
7	A	3005	CLA	CHC-C1C-NC	6.43	133.77	124.33
7	A	3029	CLA	CHC-C1C-NC	6.42	133.77	124.33
7	B	2004	CLA	CHC-C1C-NC	6.42	133.76	124.33
7	A	3057	CLA	CHC-C1C-NC	6.41	133.75	124.33
7	B	3055	CLA	C1B-NB-C4B	6.41	110.81	106.31
7	F	3031	CLA	C1B-NB-C4B	6.40	110.81	106.31
7	A	3014	CLA	CHD-C4C-NC	6.34	133.88	124.24
7	B	2002	CLA	C1B-NB-C4B	6.34	110.76	106.31
7	L	3064	CLA	CHD-C4C-NC	6.33	133.87	124.24
7	A	3009	CLA	C2C-C1C-CHC	-4.36	114.40	125.84
7	F	3033	CLA	C2C-C1C-CHC	-4.36	114.42	125.84
7	A	3027	CLA	C2C-C1C-CHC	-4.35	114.43	125.84
7	F	3002	CLA	C2C-C1C-CHC	-4.35	114.43	125.84
7	A	3077	CLA	C2C-C1C-CHC	-4.35	114.44	125.84
7	A	3071	CLA	C2C-C1C-CHC	-4.35	114.44	125.84
7	B	2002	CLA	C2C-C1C-CHC	-4.35	114.44	125.84
7	F	3059	CLA	C2C-C1C-CHC	-4.35	114.45	125.84
7	B	3001	CLA	C2C-C1C-CHC	-4.35	114.45	125.84
7	A	3007	CLA	C2C-C1C-CHC	-4.35	114.45	125.84
7	A	2006	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	A	3041	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	A	3065	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	L	3049	CLA	C2C-C1C-CHC	-4.34	114.47	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3026	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	K	3050	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	B	3010	CLA	C2C-C1C-CHC	-4.34	114.47	125.84
7	A	3078	CLA	C2C-C1C-CHC	-4.34	114.48	125.84
7	A	3062	CLA	C2C-C1C-CHC	-4.34	114.48	125.84
7	B	3008	CLA	C2C-C1C-CHC	-4.33	114.48	125.84
7	B	3055	CLA	C2C-C1C-CHC	-4.33	114.48	125.84
7	A	3045	CLA	C2C-C1C-CHC	-4.33	114.48	125.84
7	A	3058	CLA	C2C-C1C-CHC	-4.33	114.48	125.84
7	A	3018	CLA	C2C-C1C-CHC	-4.33	114.49	125.84
7	B	3028	CLA	C2C-C1C-CHC	-4.33	114.49	125.84
7	A	3067	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	2501	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	A	3013	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	A	3079	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	3019	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	A	3040	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	3074	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	3063	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	A	3021	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	3046	CLA	C2C-C1C-CHC	-4.33	114.50	125.84
7	B	3006	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	F	3012	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	B	3076	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	A	3056	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	A	2502	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	B	3023	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	A	3024	CLA	C2C-C1C-CHC	-4.32	114.51	125.84
7	A	3072	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	B	3020	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	B	3044	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	F	3061	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	B	3003	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	A	3052	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	B	2004	CLA	C2C-C1C-CHC	-4.32	114.52	125.84
7	B	3025	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	A	3048	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	B	2005	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	B	3011	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	B	3034	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	B	3037	CLA	C2C-C1C-CHC	-4.32	114.53	125.84
7	L	3036	CLA	C2C-C1C-CHC	-4.32	114.53	125.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3004	CLA	C2C-C1C-CHC	-4.31	114.53	125.84
7	A	3017	CLA	C2C-C1C-CHC	-4.31	114.53	125.84
7	A	3030	CLA	C2C-C1C-CHC	-4.31	114.53	125.84
7	A	3005	CLA	C2C-C1C-CHC	-4.31	114.53	125.84
7	B	3070	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	B	3075	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	F	3022	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	A	3016	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	L	3038	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	B	3035	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	B	3060	CLA	C2C-C1C-CHC	-4.31	114.54	125.84
7	A	3039	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	B	3015	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	A	3073	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	F	3054	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	K	3051	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	F	3031	CLA	C2C-C1C-CHC	-4.31	114.55	125.84
7	A	3043	CLA	C2C-C1C-CHC	-4.31	114.56	125.84
7	B	3069	CLA	C2C-C1C-CHC	-4.31	114.56	125.84
7	B	3081	CLA	C2C-C1C-CHC	-4.30	114.56	125.84
7	A	3047	CLA	C2C-C1C-CHC	-4.30	114.56	125.84
7	B	3066	CLA	C2C-C1C-CHC	-4.30	114.56	125.84
7	A	3053	CLA	C2C-C1C-CHC	-4.30	114.57	125.84
7	A	3068	CLA	C2C-C1C-CHC	-4.30	114.58	125.84
7	B	3042	CLA	C2C-C1C-CHC	-4.30	114.58	125.84
7	A	3032	CLA	C2C-C1C-CHC	-4.29	114.59	125.84
7	B	3080	CLA	C2C-C1C-CHC	-4.29	114.59	125.84
7	B	2003	CLA	C2C-C1C-CHC	-4.29	114.61	125.84
7	A	3029	CLA	C2C-C1C-CHC	-4.29	114.61	125.84
7	A	2001	CLA	C2C-C1C-CHC	-4.28	114.62	125.84
7	A	3057	CLA	C2C-C1C-CHC	-4.26	114.68	125.84
7	A	3014	CLA	C3C-C4C-CHD	-4.14	114.48	125.23
7	L	3064	CLA	C3C-C4C-CHD	-4.12	114.53	125.23
7	A	3014	CLA	C2D-C3D-C4D	-3.70	102.85	107.35
7	B	2002	CLA	C3B-C2B-C1B	-3.64	102.76	106.81
7	A	2006	CLA	C3B-C2B-C1B	-3.64	102.76	106.81
7	L	3064	CLA	C2D-C3D-C4D	-3.62	102.96	107.35
7	A	3024	CLA	C3B-C2B-C1B	-3.61	102.79	106.81
7	B	3055	CLA	C3B-C2B-C1B	-3.59	102.81	106.81
7	A	3009	CLA	C3B-C2B-C1B	-3.59	102.82	106.81
7	A	3027	CLA	C3B-C2B-C1B	-3.59	102.82	106.81
7	A	3047	CLA	C3B-C2B-C1B	-3.58	102.82	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3042	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	A	3056	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	B	3015	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	A	3043	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	B	3035	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	F	3031	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	B	3080	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	L	3049	CLA	C3B-C2B-C1B	-3.58	102.82	106.81
7	A	3039	CLA	C3B-C2B-C1B	-3.58	102.83	106.81
7	F	3033	CLA	C3B-C2B-C1B	-3.58	102.83	106.81
7	A	3053	CLA	C3B-C2B-C1B	-3.58	102.83	106.81
7	F	3012	CLA	C3B-C2B-C1B	-3.57	102.83	106.81
7	B	3069	CLA	C3B-C2B-C1B	-3.57	102.83	106.81
7	A	3041	CLA	C3B-C2B-C1B	-3.57	102.84	106.81
7	B	2005	CLA	C3B-C2B-C1B	-3.57	102.84	106.81
7	A	3005	CLA	C3B-C2B-C1B	-3.57	102.84	106.81
7	A	3057	CLA	C3B-C2B-C1B	-3.57	102.84	106.81
7	A	3029	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	A	3052	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	B	3028	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	A	3017	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	B	2501	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	K	3050	CLA	C3B-C2B-C1B	-3.56	102.85	106.81
7	A	3018	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3076	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	A	3048	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3034	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3010	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3011	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3046	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3066	CLA	C3B-C2B-C1B	-3.55	102.86	106.81
7	B	3019	CLA	C3B-C2B-C1B	-3.54	102.86	106.81
7	A	3058	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	B	3075	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	L	3064	CLA	C3D-C2D-C1D	-3.54	103.05	107.35
7	A	3026	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	A	3040	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	B	3060	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	A	3032	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	B	3023	CLA	C3B-C2B-C1B	-3.54	102.87	106.81
7	A	3030	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	K	3051	CLA	C3B-C2B-C1B	-3.53	102.88	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3016	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	2004	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3001	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3044	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3070	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	L	3036	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3025	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3003	CLA	C3B-C2B-C1B	-3.53	102.88	106.81
7	B	3008	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
7	B	2003	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
7	F	3061	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
7	A	3068	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
7	F	3004	CLA	C3B-C2B-C1B	-3.52	102.89	106.81
7	A	3072	CLA	C3B-C2B-C1B	-3.52	102.90	106.81
7	B	3037	CLA	C3B-C2B-C1B	-3.52	102.90	106.81
7	B	3081	CLA	C3B-C2B-C1B	-3.52	102.90	106.81
7	B	3063	CLA	C3B-C2B-C1B	-3.52	102.90	106.81
7	A	3045	CLA	C3B-C2B-C1B	-3.51	102.90	106.81
7	F	3022	CLA	C3B-C2B-C1B	-3.51	102.90	106.81
7	A	2502	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	A	3021	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	B	3006	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	F	3002	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	B	3020	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	A	3073	CLA	C3B-C2B-C1B	-3.50	102.91	106.81
7	A	3014	CLA	C3D-C2D-C1D	-3.50	103.10	107.35
7	A	3007	CLA	C3B-C2B-C1B	-3.50	102.92	106.81
7	A	3062	CLA	C3B-C2B-C1B	-3.48	102.94	106.81
7	B	3074	CLA	C3B-C2B-C1B	-3.48	102.94	106.81
7	L	3038	CLA	C3B-C2B-C1B	-3.47	102.94	106.81
7	A	3067	CLA	C3B-C2B-C1B	-3.47	102.95	106.81
7	A	3013	CLA	C3B-C2B-C1B	-3.46	102.95	106.81
7	F	3059	CLA	C3B-C2B-C1B	-3.46	102.95	106.81
7	A	3065	CLA	C3B-C2B-C1B	-3.46	102.96	106.81
7	F	3054	CLA	C3B-C2B-C1B	-3.45	102.97	106.81
7	L	3038	CLA	C2B-C3B-C4B	-3.44	102.98	106.81
7	A	3079	CLA	C3B-C2B-C1B	-3.44	102.98	106.81
7	A	2001	CLA	C3B-C2B-C1B	-3.43	103.00	106.81
7	A	3071	CLA	C3B-C2B-C1B	-3.42	103.00	106.81
7	B	3075	CLA	C2B-C3B-C4B	-3.42	103.00	106.81
7	A	3077	CLA	C3B-C2B-C1B	-3.42	103.01	106.81
7	A	3078	CLA	C3B-C2B-C1B	-3.42	103.01	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3066	CLA	C2B-C3B-C4B	-3.41	103.01	106.81
7	B	3081	CLA	C2B-C3B-C4B	-3.41	103.02	106.81
7	A	2001	CLA	C2B-C3B-C4B	-3.40	103.02	106.81
7	B	3028	CLA	C2B-C3B-C4B	-3.40	103.02	106.81
7	B	2004	CLA	C2B-C3B-C4B	-3.40	103.03	106.81
7	L	3036	CLA	C2B-C3B-C4B	-3.39	103.03	106.81
7	B	3037	CLA	C2B-C3B-C4B	-3.39	103.04	106.81
7	B	3019	CLA	C2B-C3B-C4B	-3.39	103.04	106.81
7	B	2005	CLA	C2B-C3B-C4B	-3.39	103.04	106.81
7	A	3013	CLA	C2B-C3B-C4B	-3.38	103.04	106.81
7	A	3077	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	F	3033	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	A	3007	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	A	3024	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	A	3021	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	A	3068	CLA	C2B-C3B-C4B	-3.38	103.05	106.81
7	A	3073	CLA	C2B-C3B-C4B	-3.37	103.05	106.81
7	B	3006	CLA	C2B-C3B-C4B	-3.37	103.05	106.81
7	A	3072	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	F	3031	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	A	3048	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	B	3025	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	B	3060	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	L	3049	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	F	3012	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	K	3050	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	A	2502	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	B	3042	CLA	C2B-C3B-C4B	-3.37	103.06	106.81
7	A	3040	CLA	C2B-C3B-C4B	-3.36	103.06	106.81
7	B	3063	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	K	3051	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	B	3070	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	B	3074	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	F	3061	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	A	3026	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	B	3076	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	A	3009	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	B	3020	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	F	3054	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	B	3046	CLA	C2B-C3B-C4B	-3.36	103.07	106.81
7	A	3016	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	A	3017	CLA	C2B-C3B-C4B	-3.35	103.08	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	3008	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	A	3052	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	A	3029	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	B	3011	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	B	3001	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	A	3078	CLA	C2B-C3B-C4B	-3.35	103.08	106.81
7	A	3027	CLA	C4A-NA-C1A	3.35	108.21	106.68
7	B	3037	CLA	C4A-NA-C1A	3.35	108.21	106.68
7	B	3044	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3071	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	B	2003	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	F	3004	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3018	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3045	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	B	3069	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	F	3002	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	B	3055	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3005	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3041	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3030	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	B	3035	CLA	C2B-C3B-C4B	-3.34	103.09	106.81
7	A	3067	CLA	C2B-C3B-C4B	-3.33	103.10	106.81
7	A	3027	CLA	C2B-C3B-C4B	-3.33	103.10	106.81
7	B	2002	CLA	C2B-C3B-C4B	-3.33	103.10	106.81
7	A	3053	CLA	C2B-C3B-C4B	-3.33	103.10	106.81
7	A	3032	CLA	C2B-C3B-C4B	-3.33	103.11	106.81
7	B	2501	CLA	C2B-C3B-C4B	-3.33	103.11	106.81
7	A	3079	CLA	C2B-C3B-C4B	-3.32	103.11	106.81
7	B	3010	CLA	C2B-C3B-C4B	-3.32	103.11	106.81
7	A	3058	CLA	C2B-C3B-C4B	-3.32	103.11	106.81
7	F	3059	CLA	C2B-C3B-C4B	-3.32	103.12	106.81
7	B	2004	CLA	C4A-NA-C1A	3.32	108.19	106.68
7	F	3022	CLA	C2B-C3B-C4B	-3.32	103.12	106.81
7	B	3080	CLA	C2B-C3B-C4B	-3.31	103.12	106.81
7	A	3047	CLA	C2B-C3B-C4B	-3.31	103.12	106.81
7	A	3029	CLA	C4A-NA-C1A	3.31	108.19	106.68
7	A	3043	CLA	C2B-C3B-C4B	-3.31	103.12	106.81
7	B	3034	CLA	C2B-C3B-C4B	-3.31	103.12	106.81
7	B	3003	CLA	C2B-C3B-C4B	-3.31	103.13	106.81
7	A	2006	CLA	C2B-C3B-C4B	-3.31	103.13	106.81
7	A	3056	CLA	C2B-C3B-C4B	-3.31	103.13	106.81
7	B	3023	CLA	C2B-C3B-C4B	-3.30	103.13	106.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3057	CLA	C2B-C3B-C4B	-3.30	103.13	106.81
7	A	3039	CLA	C2B-C3B-C4B	-3.30	103.14	106.81
7	A	3062	CLA	C2B-C3B-C4B	-3.30	103.14	106.81
7	B	3075	CLA	C4A-NA-C1A	3.29	108.18	106.68
7	B	3015	CLA	C2B-C3B-C4B	-3.28	103.15	106.81
7	A	3065	CLA	C2B-C3B-C4B	-3.28	103.16	106.81
7	A	3026	CLA	C4A-NA-C1A	3.28	108.18	106.68
7	B	2002	CLA	C4A-NA-C1A	3.25	108.16	106.68
7	F	3031	CLA	C4A-NA-C1A	3.25	108.16	106.68
7	A	3047	CLA	C4A-NA-C1A	3.24	108.16	106.68
7	K	3050	CLA	C4A-NA-C1A	3.24	108.16	106.68
7	B	3080	CLA	C4A-NA-C1A	3.22	108.15	106.68
7	A	3041	CLA	C4A-NA-C1A	3.20	108.14	106.68
7	A	3072	CLA	C4A-NA-C1A	3.20	108.14	106.68
7	A	2001	CLA	C4A-NA-C1A	3.20	108.14	106.68
7	A	3057	CLA	C4A-NA-C1A	3.20	108.14	106.68
7	A	3052	CLA	C4A-NA-C1A	3.18	108.13	106.68
7	A	3053	CLA	C4A-NA-C1A	3.18	108.13	106.68
7	B	3042	CLA	C4A-NA-C1A	3.18	108.13	106.68
7	B	3035	CLA	C4A-NA-C1A	3.16	108.12	106.68
7	B	3076	CLA	C4A-NA-C1A	3.15	108.12	106.68
7	B	3023	CLA	C4A-NA-C1A	3.15	108.12	106.68
7	B	3015	CLA	C4A-NA-C1A	3.15	108.11	106.68
7	B	3011	CLA	C4A-NA-C1A	3.14	108.11	106.68
7	B	3066	CLA	C4A-NA-C1A	3.14	108.11	106.68
7	K	3051	CLA	C4A-NA-C1A	3.14	108.11	106.68
7	L	3049	CLA	C4A-NA-C1A	3.13	108.11	106.68
7	A	3009	CLA	C4A-NA-C1A	3.12	108.10	106.68
7	B	2005	CLA	C4A-NA-C1A	3.12	108.10	106.68
7	L	3036	CLA	C4A-NA-C1A	3.12	108.10	106.68
7	A	3024	CLA	C4A-NA-C1A	3.11	108.10	106.68
7	B	2501	CLA	C4A-NA-C1A	3.11	108.10	106.68
7	A	3056	CLA	C4A-NA-C1A	3.11	108.10	106.68
7	A	3073	CLA	C4A-NA-C1A	3.11	108.10	106.68
7	B	3010	CLA	C4A-NA-C1A	3.10	108.09	106.68
7	B	3019	CLA	C4A-NA-C1A	3.10	108.09	106.68
7	B	2003	CLA	C4A-NA-C1A	3.10	108.09	106.68
7	B	3006	CLA	C4A-NA-C1A	3.10	108.09	106.68
7	A	3048	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	B	3025	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	A	3016	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	A	3032	CLA	C4A-NA-C1A	3.09	108.09	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	3012	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	A	3068	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	F	3004	CLA	C4A-NA-C1A	3.09	108.09	106.68
7	A	3013	CLA	C4A-NA-C1A	3.08	108.08	106.68
7	B	3046	CLA	C4A-NA-C1A	3.08	108.08	106.68
7	A	3005	CLA	C4A-NA-C1A	3.07	108.08	106.68
7	L	3038	CLA	C4A-NA-C1A	3.07	108.08	106.68
7	B	3055	CLA	C4A-NA-C1A	3.06	108.07	106.68
7	B	3008	CLA	C4A-NA-C1A	3.05	108.07	106.68
7	B	3081	CLA	C4A-NA-C1A	3.05	108.07	106.68
7	A	3040	CLA	C4A-NA-C1A	3.05	108.07	106.68
7	F	3002	CLA	C4A-NA-C1A	3.05	108.07	106.68
7	A	3014	CLA	C4A-NA-C1A	3.04	108.07	106.68
7	A	3043	CLA	C4A-NA-C1A	3.03	108.06	106.68
7	A	3045	CLA	C4A-NA-C1A	3.03	108.06	106.68
7	A	3058	CLA	C4A-NA-C1A	3.03	108.06	106.68
7	F	3054	CLA	C4A-NA-C1A	3.03	108.06	106.68
7	B	3060	CLA	C4A-NA-C1A	3.02	108.06	106.68
7	F	3022	CLA	C4A-NA-C1A	3.02	108.06	106.68
7	B	3070	CLA	C4A-NA-C1A	3.01	108.05	106.68
7	A	3030	CLA	C4A-NA-C1A	3.01	108.05	106.68
7	A	3039	CLA	C4A-NA-C1A	3.01	108.05	106.68
7	F	3061	CLA	C4A-NA-C1A	3.01	108.05	106.68
7	A	3017	CLA	C4A-NA-C1A	3.00	108.05	106.68
7	B	3069	CLA	C4A-NA-C1A	3.00	108.05	106.68
7	B	3074	CLA	C4A-NA-C1A	3.00	108.05	106.68
7	A	3007	CLA	C4A-NA-C1A	2.99	108.04	106.68
7	B	3003	CLA	C4A-NA-C1A	2.99	108.04	106.68
7	A	2502	CLA	C4A-NA-C1A	2.99	108.04	106.68
7	A	3018	CLA	C4A-NA-C1A	2.99	108.04	106.68
7	B	3044	CLA	C4A-NA-C1A	2.99	108.04	106.68
7	A	3021	CLA	C4A-NA-C1A	2.98	108.04	106.68
7	B	3020	CLA	C4A-NA-C1A	2.98	108.04	106.68
7	L	3064	CLA	C4A-NA-C1A	2.97	108.03	106.68
7	A	2006	CLA	C4A-NA-C1A	2.94	108.02	106.68
7	B	3028	CLA	C4A-NA-C1A	2.93	108.02	106.68
7	B	3001	CLA	C4A-NA-C1A	2.93	108.01	106.68
7	B	3063	CLA	C4A-NA-C1A	2.92	108.01	106.68
7	B	3034	CLA	C4A-NA-C1A	2.92	108.01	106.68
7	F	3033	CLA	C4A-NA-C1A	2.88	107.99	106.68
7	A	3079	CLA	C4A-NA-C1A	2.85	107.98	106.68
7	A	3071	CLA	C4A-NA-C1A	2.78	107.95	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3077	CLA	C4A-NA-C1A	2.76	107.94	106.68
7	A	3067	CLA	C4A-NA-C1A	2.74	107.93	106.68
7	B	3034	CLA	C3A-C4A-CHB	2.74	127.27	123.91
7	B	3044	CLA	C3A-C4A-CHB	2.74	127.27	123.91
7	A	3005	CLA	C3A-C4A-CHB	2.72	127.25	123.91
7	A	3007	CLA	C3A-C4A-CHB	2.72	127.24	123.91
7	B	3074	CLA	C3A-C4A-CHB	2.72	127.24	123.91
7	B	3046	CLA	C3A-C4A-CHB	2.71	127.24	123.91
7	K	3051	CLA	C3A-C4A-CHB	2.71	127.23	123.91
7	A	3016	CLA	C3A-C4A-CHB	2.71	127.23	123.91
7	A	3056	CLA	C3A-C4A-CHB	2.70	127.22	123.91
7	A	3013	CLA	C3A-C4A-CHB	2.70	127.22	123.91
7	F	3054	CLA	C3A-C4A-CHB	2.70	127.22	123.91
7	B	3015	CLA	C3A-C4A-CHB	2.69	127.21	123.91
7	A	3045	CLA	C3A-C4A-CHB	2.69	127.21	123.91
7	B	2501	CLA	C3A-C4A-CHB	2.69	127.21	123.91
7	B	3019	CLA	C3A-C4A-CHB	2.69	127.21	123.91
7	B	3003	CLA	C3A-C4A-CHB	2.68	127.20	123.91
7	B	3011	CLA	C3A-C4A-CHB	2.68	127.19	123.91
7	A	3048	CLA	C3A-C4A-CHB	2.68	127.19	123.91
7	B	3060	CLA	C3A-C4A-CHB	2.68	127.19	123.91
7	B	3028	CLA	C3A-C4A-CHB	2.68	127.19	123.91
7	A	3039	CLA	C3A-C4A-CHB	2.67	127.19	123.91
7	A	3077	CLA	C3A-C4A-CHB	2.67	127.19	123.91
7	F	3004	CLA	C3A-C4A-CHB	2.67	127.19	123.91
7	A	3078	CLA	C4A-NA-C1A	2.67	107.90	106.68
7	A	3043	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	B	3020	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	B	3006	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	L	3049	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	F	3012	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	A	2502	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	A	3017	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	B	2005	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	B	3001	CLA	C3A-C4A-CHB	2.67	127.18	123.91
7	F	3059	CLA	C3A-C4A-CHB	2.66	127.18	123.91
7	B	3069	CLA	C3A-C4A-CHB	2.66	127.17	123.91
7	A	3052	CLA	C3A-C4A-CHB	2.66	127.17	123.91
7	A	3067	CLA	C3A-C4A-CHB	2.66	127.17	123.91
7	F	3061	CLA	C3A-C4A-CHB	2.66	127.17	123.91
7	L	3064	CLA	C2A-C1A-CHA	2.66	127.17	122.63
7	B	2004	CLA	C3A-C4A-CHB	2.65	127.16	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2003	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	B	3042	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	B	3063	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	A	3072	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	B	3010	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	F	3002	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	F	3022	CLA	C3A-C4A-CHB	2.65	127.16	123.91
7	A	3027	CLA	C3A-C4A-CHB	2.65	127.15	123.91
7	A	3041	CLA	C3A-C4A-CHB	2.65	127.15	123.91
7	A	3057	CLA	C3A-C4A-CHB	2.65	127.15	123.91
7	A	3073	CLA	C3A-C4A-CHB	2.65	127.15	123.91
7	B	3037	CLA	C3A-C4A-CHB	2.65	127.15	123.91
7	A	3062	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	A	3079	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	A	3029	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	A	3014	CLA	C2A-C1A-CHA	2.64	127.14	122.63
7	A	2006	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	A	3030	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	B	3008	CLA	C3A-C4A-CHB	2.64	127.15	123.91
7	B	3080	CLA	C3A-C4A-CHB	2.64	127.14	123.91
7	A	3078	CLA	C3A-C4A-CHB	2.64	127.14	123.91
7	A	3058	CLA	C3A-C4A-CHB	2.63	127.14	123.91
7	B	3023	CLA	C3A-C4A-CHB	2.63	127.14	123.91
7	B	3055	CLA	C3A-C4A-CHB	2.63	127.14	123.91
7	B	2002	CLA	C3A-C4A-CHB	2.63	127.14	123.91
7	A	3047	CLA	C3A-C4A-CHB	2.63	127.14	123.91
7	A	3068	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	A	3026	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	A	3009	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	A	3040	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	A	3021	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	B	3066	CLA	C3A-C4A-CHB	2.63	127.13	123.91
7	A	3053	CLA	C3A-C4A-CHB	2.62	127.12	123.91
7	A	3071	CLA	C3A-C4A-CHB	2.62	127.12	123.91
7	B	3025	CLA	C3A-C4A-CHB	2.62	127.12	123.91
7	A	3065	CLA	C3A-C4A-CHB	2.62	127.12	123.91
7	F	3031	CLA	C3A-C4A-CHB	2.61	127.11	123.91
7	A	3018	CLA	C3A-C4A-CHB	2.61	127.11	123.91
7	F	3059	CLA	C4A-NA-C1A	2.61	107.87	106.68
7	B	3076	CLA	C3A-C4A-CHB	2.61	127.11	123.91
7	B	3075	CLA	C3A-C4A-CHB	2.61	127.11	123.91
7	F	3033	CLA	C3A-C4A-CHB	2.61	127.11	123.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3032	CLA	C3A-C4A-CHB	2.60	127.10	123.91
7	K	3050	CLA	C3A-C4A-CHB	2.60	127.10	123.91
7	B	3070	CLA	C3A-C4A-CHB	2.60	127.09	123.91
7	L	3036	CLA	C3A-C4A-CHB	2.60	127.09	123.91
7	L	3038	CLA	C3A-C4A-CHB	2.60	127.09	123.91
7	B	3035	CLA	C3A-C4A-CHB	2.59	127.09	123.91
7	B	3081	CLA	C3A-C4A-CHB	2.59	127.08	123.91
7	A	2001	CLA	C3A-C4A-CHB	2.58	127.08	123.91
7	A	3065	CLA	C4A-NA-C1A	2.57	107.85	106.68
7	A	3062	CLA	C4A-NA-C1A	2.56	107.85	106.68
7	A	3024	CLA	C3A-C4A-CHB	2.56	127.04	123.91
7	A	3029	CLA	C2C-C3C-C4C	-2.53	104.03	107.24
7	A	3047	CLA	C2C-C3C-C4C	-2.52	104.06	107.24
7	B	3044	CLA	C2C-C3C-C4C	-2.51	104.06	107.24
7	B	2003	CLA	C2C-C3C-C4C	-2.50	104.08	107.24
7	A	3024	CLA	C2C-C3C-C4C	-2.48	104.10	107.24
7	B	3063	CLA	C2C-C3C-C4C	-2.48	104.10	107.24
7	A	3072	CLA	C2C-C3C-C4C	-2.48	104.11	107.24
7	B	3080	CLA	C2C-C3C-C4C	-2.48	104.11	107.24
7	A	3052	CLA	C2C-C3C-C4C	-2.48	104.11	107.24
7	B	3011	CLA	C2C-C3C-C4C	-2.47	104.11	107.24
7	B	3028	CLA	C2C-C3C-C4C	-2.47	104.11	107.24
7	B	3055	CLA	C2C-C3C-C4C	-2.47	104.12	107.24
7	L	3036	CLA	C2C-C3C-C4C	-2.47	104.12	107.24
7	F	3031	CLA	C2C-C3C-C4C	-2.47	104.12	107.24
7	A	3077	CLA	C2C-C3C-C4C	-2.47	104.12	107.24
7	A	3073	CLA	C2C-C3C-C4C	-2.47	104.12	107.24
7	A	3032	CLA	C2C-C3C-C4C	-2.46	104.12	107.24
7	B	3015	CLA	C2C-C3C-C4C	-2.46	104.12	107.24
7	F	3022	CLA	C2C-C3C-C4C	-2.46	104.12	107.24
7	L	3038	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	A	3013	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	A	3009	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	A	3026	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	B	3037	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	A	3005	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	B	3070	CLA	C2C-C3C-C4C	-2.46	104.13	107.24
7	A	3053	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	B	3019	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	B	3001	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	B	3034	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	B	3076	CLA	C2C-C3C-C4C	-2.45	104.14	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3048	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	A	3071	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	L	3049	CLA	C2C-C3C-C4C	-2.45	104.14	107.24
7	B	3060	CLA	C2C-C3C-C4C	-2.44	104.15	107.24
7	A	3067	CLA	C2C-C3C-C4C	-2.44	104.15	107.24
7	A	3068	CLA	C2C-C3C-C4C	-2.44	104.15	107.24
7	A	3078	CLA	C2C-C3C-C4C	-2.44	104.15	107.24
7	F	3061	CLA	C2C-C3C-C4C	-2.44	104.15	107.24
7	F	3002	CLA	C2C-C3C-C4C	-2.44	104.16	107.24
7	A	3057	CLA	C2C-C3C-C4C	-2.44	104.16	107.24
7	B	2004	CLA	C2C-C3C-C4C	-2.43	104.16	107.24
7	B	3010	CLA	C2C-C3C-C4C	-2.43	104.16	107.24
7	B	3074	CLA	C2C-C3C-C4C	-2.43	104.16	107.24
7	A	3045	CLA	C2C-C3C-C4C	-2.43	104.16	107.24
7	B	3066	CLA	C2C-C3C-C4C	-2.43	104.17	107.24
7	F	3054	CLA	C2C-C3C-C4C	-2.43	104.17	107.24
7	A	3058	CLA	C2C-C3C-C4C	-2.43	104.17	107.24
7	B	3046	CLA	C2C-C3C-C4C	-2.43	104.17	107.24
7	A	3065	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	B	2005	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	B	3023	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	A	3043	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	F	3033	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	A	3007	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	K	3050	CLA	C2C-C3C-C4C	-2.42	104.17	107.24
7	K	3051	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	B	3006	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	A	3039	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	B	2002	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	A	3021	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	B	3081	CLA	C2C-C3C-C4C	-2.42	104.18	107.24
7	B	3075	CLA	C2C-C3C-C4C	-2.41	104.18	107.24
7	B	3020	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	A	3079	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	B	3069	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	A	3040	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	B	2501	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	A	3018	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	B	3008	CLA	C2C-C3C-C4C	-2.41	104.19	107.24
7	A	3062	CLA	C2C-C3C-C4C	-2.41	104.20	107.24
7	B	3025	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	L	3064	CLA	C3C-C2C-C1C	-2.40	104.20	107.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	3056	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	F	3059	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	A	3014	CLA	C3C-C2C-C1C	-2.40	104.20	107.24
7	F	3012	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	A	3030	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	A	2001	CLA	C2C-C3C-C4C	-2.40	104.20	107.24
7	A	3041	CLA	C2C-C3C-C4C	-2.40	104.21	107.24
7	F	3004	CLA	C2C-C3C-C4C	-2.40	104.21	107.24
7	A	2502	CLA	C2C-C3C-C4C	-2.39	104.21	107.24
7	A	2006	CLA	C2C-C3C-C4C	-2.39	104.21	107.24
7	B	3042	CLA	C2C-C3C-C4C	-2.39	104.22	107.24
7	A	3016	CLA	C2C-C3C-C4C	-2.38	104.22	107.24
7	A	3017	CLA	C2C-C3C-C4C	-2.38	104.23	107.24
7	B	3003	CLA	C2C-C3C-C4C	-2.36	104.25	107.24
7	B	3035	CLA	C2C-C3C-C4C	-2.36	104.25	107.24
7	A	3027	CLA	C2C-C3C-C4C	-2.36	104.25	107.24

All (87) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	2001	CLA	ND
7	A	2006	CLA	ND
7	A	2502	CLA	ND
7	A	3005	CLA	ND
7	A	3007	CLA	ND
7	A	3009	CLA	ND
7	A	3013	CLA	ND
7	A	3016	CLA	ND
7	A	3017	CLA	ND
7	A	3018	CLA	ND
7	A	3021	CLA	ND
7	A	3024	CLA	ND
7	A	3026	CLA	ND
7	A	3027	CLA	ND
7	A	3029	CLA	ND
7	A	3030	CLA	ND
7	A	3032	CLA	ND
7	A	3039	CLA	ND
7	A	3040	CLA	ND
7	A	3041	CLA	ND
7	A	3043	CLA	ND
7	A	3045	CLA	ND

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Atom</b>
7	A	3047	CLA	ND
7	A	3048	CLA	ND
7	A	3052	CLA	ND
7	A	3053	CLA	ND
7	A	3056	CLA	ND
7	A	3057	CLA	ND
7	A	3058	CLA	ND
7	A	3062	CLA	ND
7	A	3065	CLA	ND
7	A	3067	CLA	ND
7	A	3068	CLA	ND
7	A	3071	CLA	ND
7	A	3072	CLA	ND
7	A	3073	CLA	ND
7	A	3077	CLA	ND
7	A	3078	CLA	ND
7	A	3079	CLA	ND
7	B	2002	CLA	ND
7	B	2003	CLA	ND
7	B	2004	CLA	ND
7	B	2005	CLA	ND
7	B	2501	CLA	ND
7	B	3001	CLA	ND
7	B	3003	CLA	ND
7	B	3006	CLA	ND
7	B	3008	CLA	ND
7	B	3010	CLA	ND
7	B	3011	CLA	ND
7	B	3015	CLA	ND
7	B	3019	CLA	ND
7	B	3020	CLA	ND
7	B	3023	CLA	ND
7	B	3025	CLA	ND
7	B	3028	CLA	ND
7	B	3034	CLA	ND
7	B	3035	CLA	ND
7	B	3037	CLA	ND
7	B	3042	CLA	ND
7	B	3044	CLA	ND
7	B	3046	CLA	ND
7	B	3055	CLA	ND
7	B	3060	CLA	ND

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Mol	Chain	Res	Type	Atom
7	B	3063	CLA	ND
7	B	3066	CLA	ND
7	B	3069	CLA	ND
7	B	3070	CLA	ND
7	B	3074	CLA	ND
7	B	3075	CLA	ND
7	B	3076	CLA	ND
7	B	3080	CLA	ND
7	B	3081	CLA	ND
7	L	3036	CLA	ND
7	L	3038	CLA	ND
7	L	3049	CLA	ND
7	K	3050	CLA	ND
7	K	3051	CLA	ND
7	F	3002	CLA	ND
7	F	3004	CLA	ND
7	F	3012	CLA	ND
7	F	3022	CLA	ND
7	F	3031	CLA	ND
7	F	3033	CLA	ND
7	F	3054	CLA	ND
7	F	3059	CLA	ND
7	F	3061	CLA	ND

There are no torsion outliers.

There are no ring outliers.

28 monomers are involved in 57 short contacts:

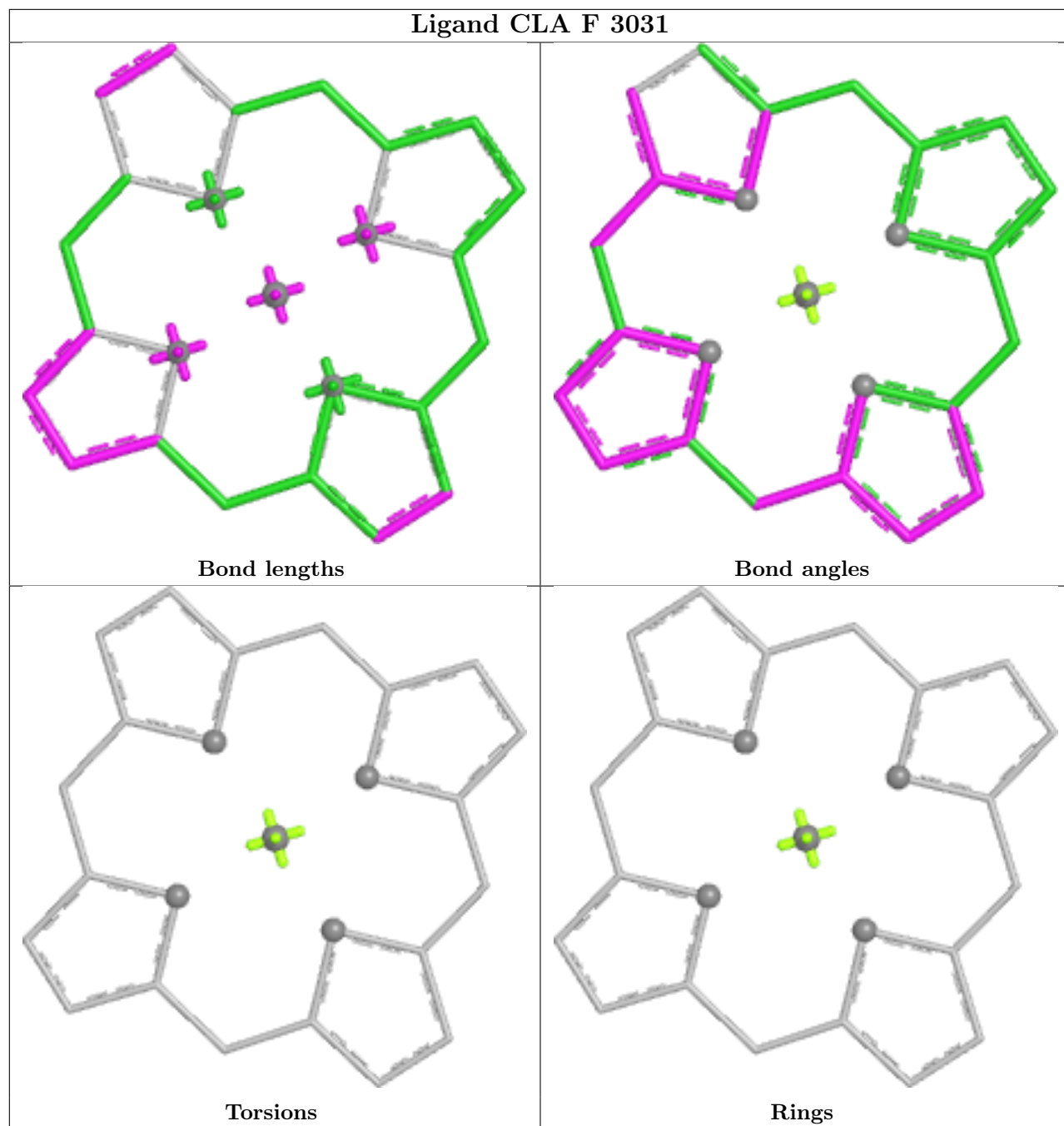
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	3031	CLA	1	0
7	F	3002	CLA	5	0
7	B	3069	CLA	1	0
7	A	3027	CLA	10	0
7	A	3024	CLA	9	0
7	A	3026	CLA	1	0
7	B	2005	CLA	4	0
9	B	2008	SF4	3	0
7	B	3011	CLA	2	0
7	A	3014	CLA	8	0
7	A	3017	CLA	1	0
7	A	3057	CLA	3	0
7	B	3020	CLA	1	0

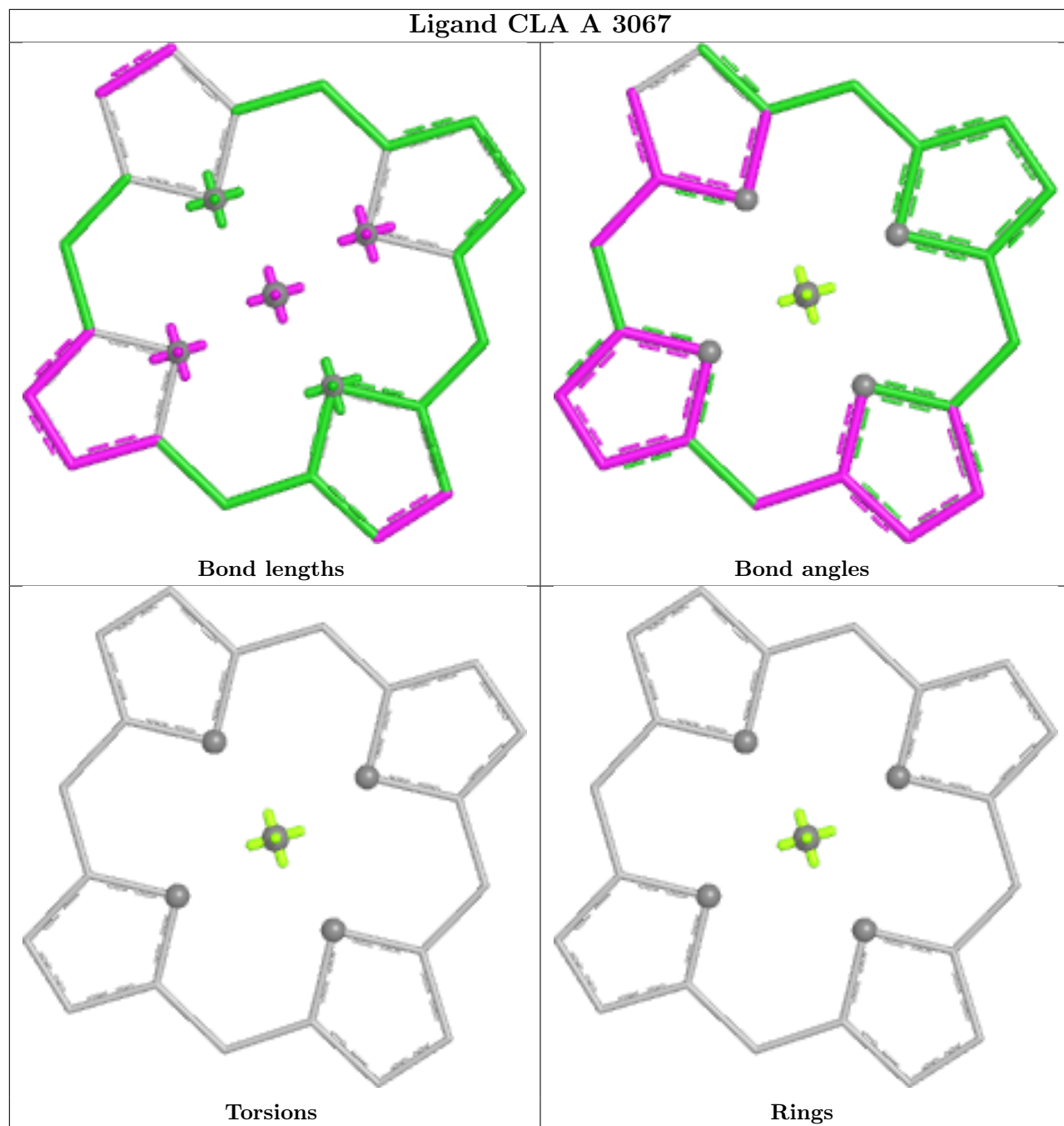
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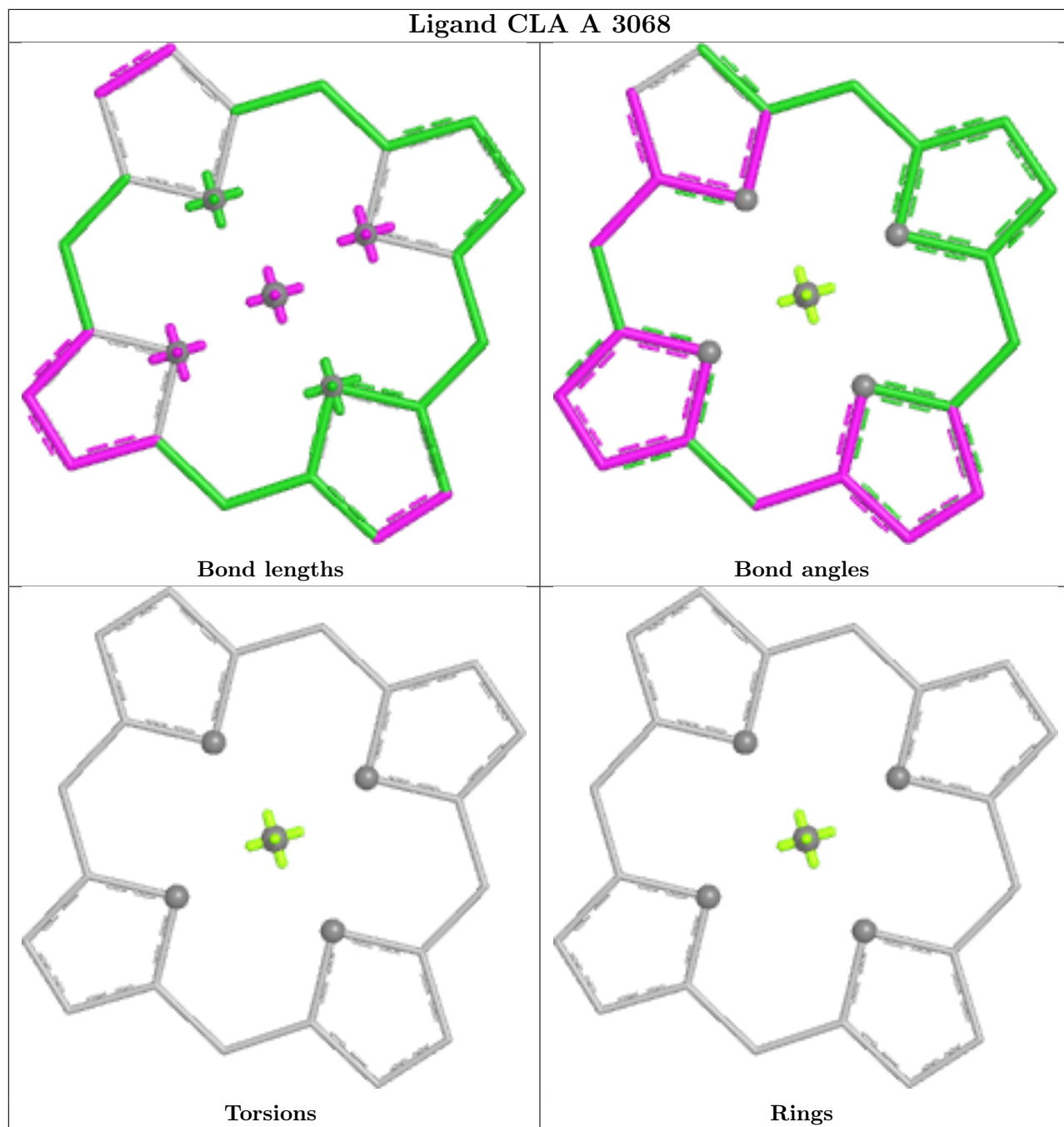
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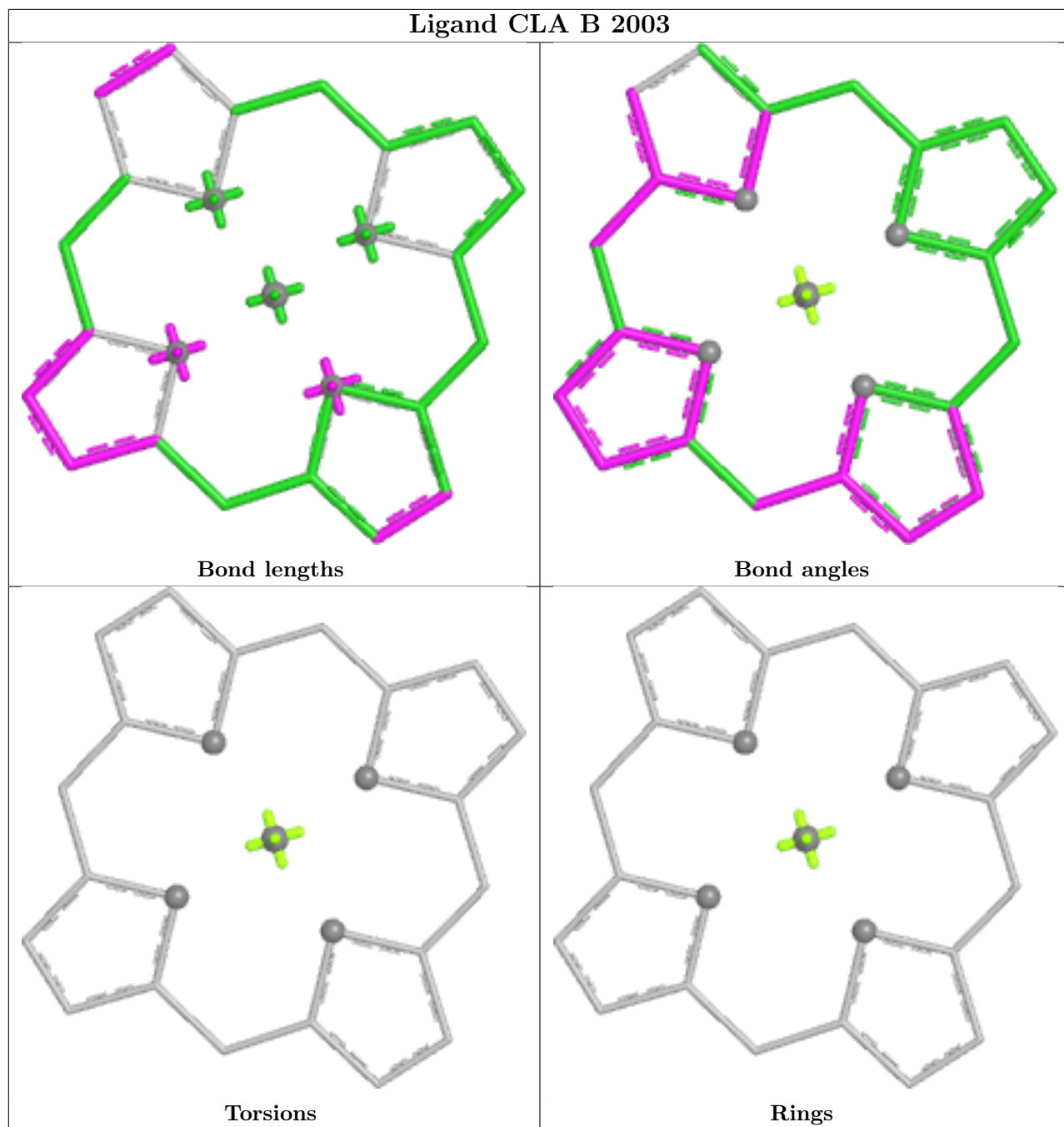
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3016	CLA	6	0
7	A	3007	CLA	5	0
7	B	3006	CLA	2	0
7	A	3005	CLA	3	0
7	A	3030	CLA	1	0
7	A	3056	CLA	3	0
7	A	3039	CLA	3	0
7	F	3012	CLA	2	0
7	A	3079	CLA	1	0
7	A	3029	CLA	10	0
7	B	3034	CLA	2	0
7	B	3001	CLA	2	0
7	B	3003	CLA	2	0
7	A	3018	CLA	1	0
7	A	3071	CLA	4	0

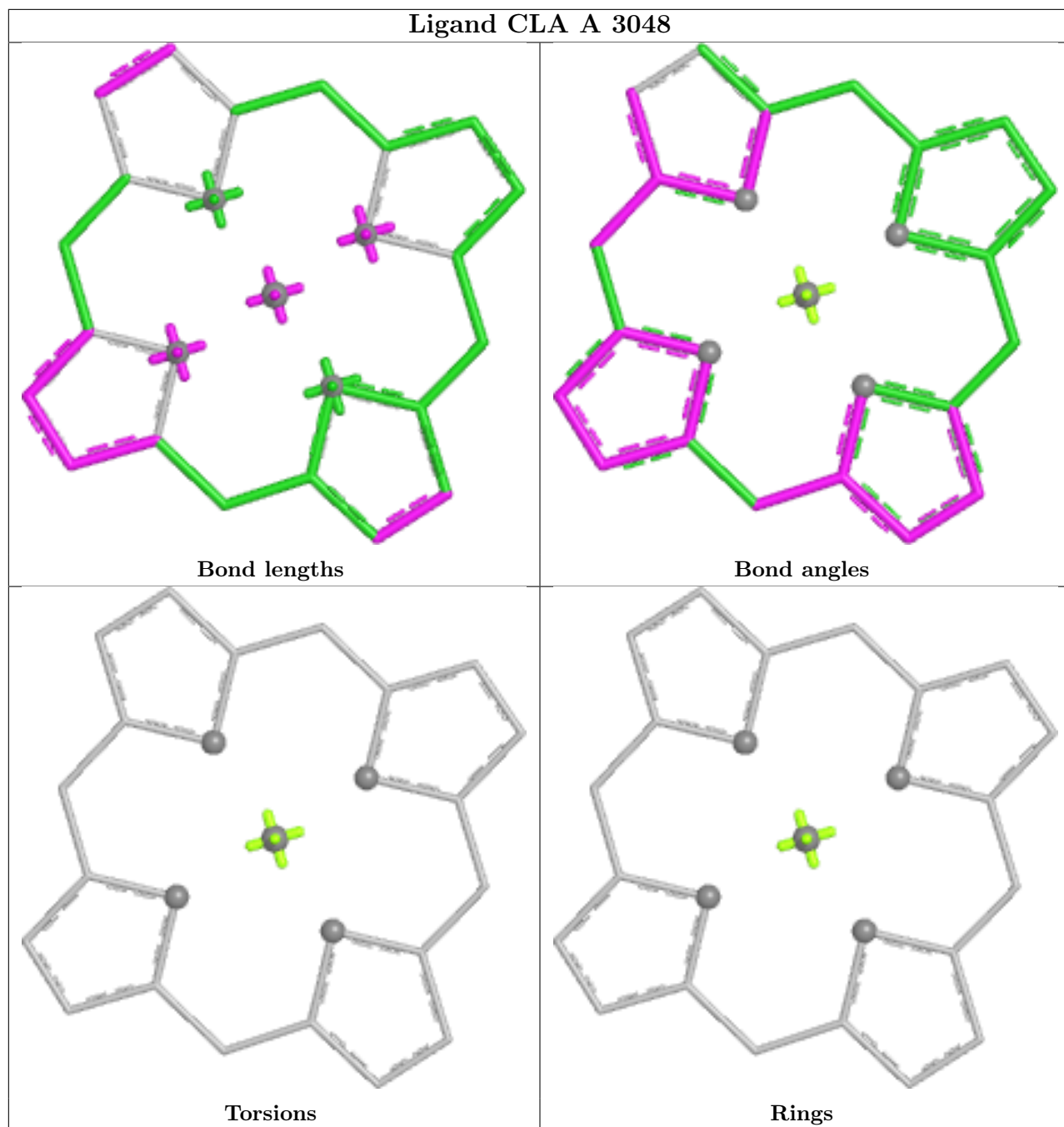
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

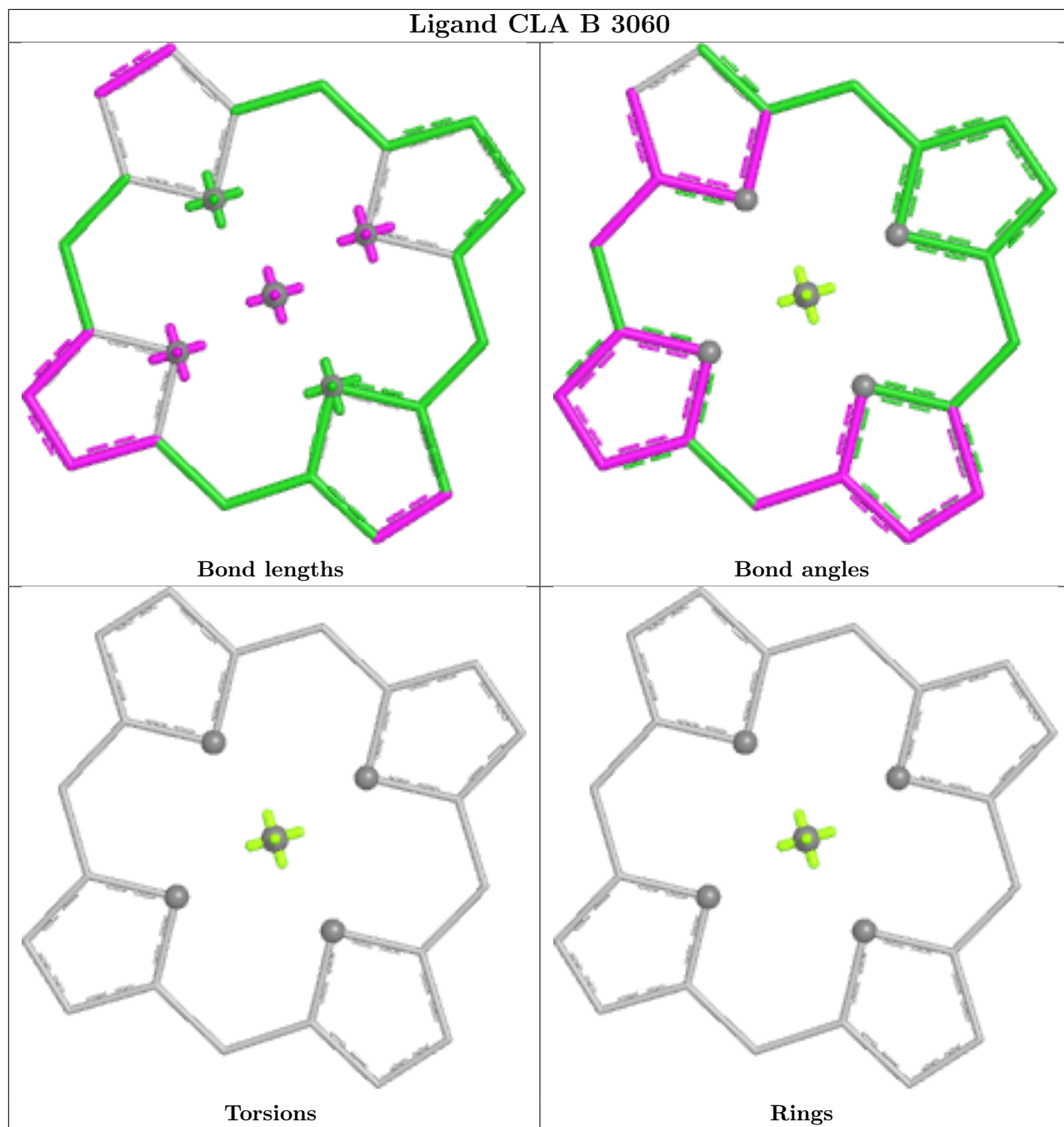


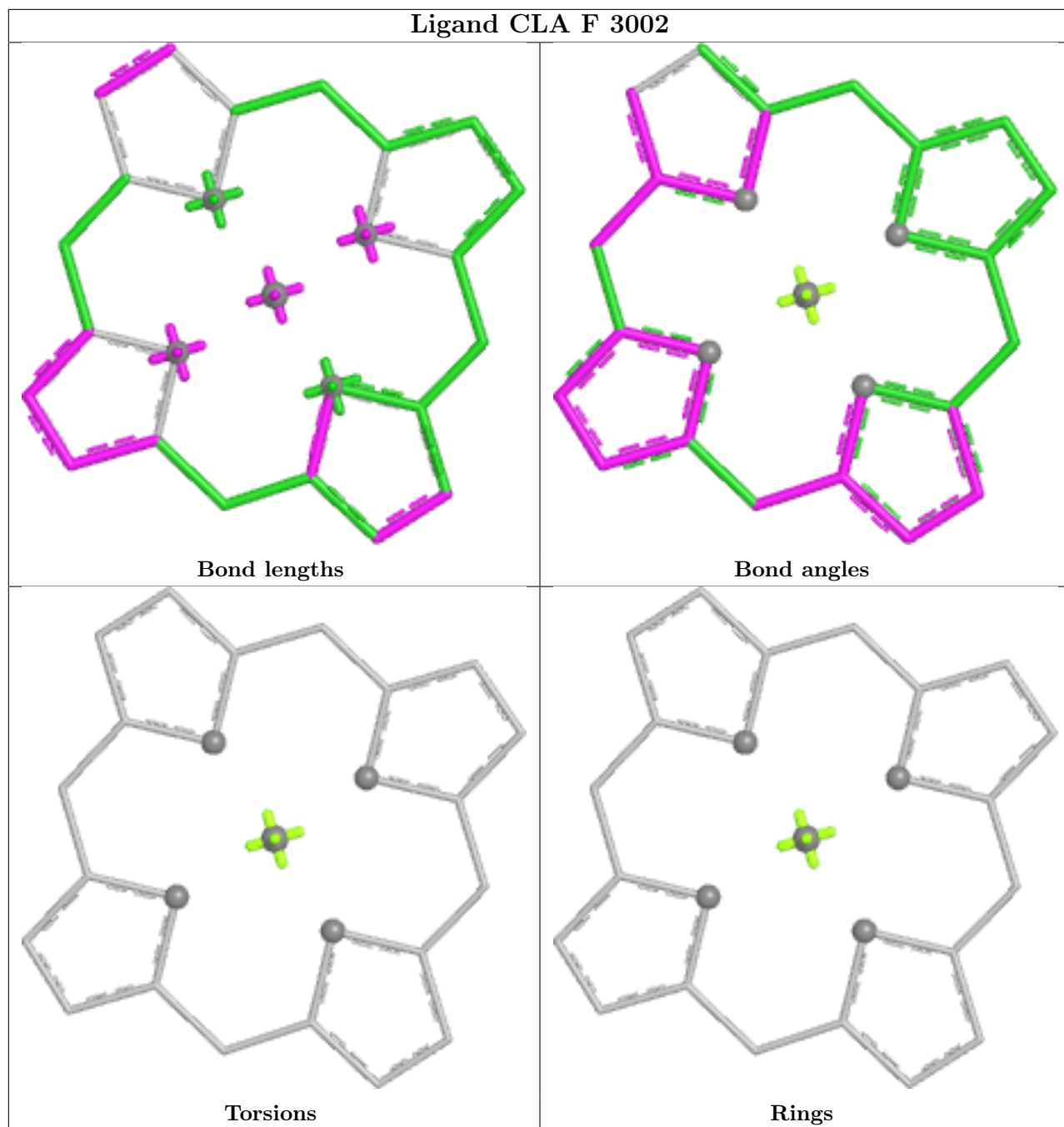


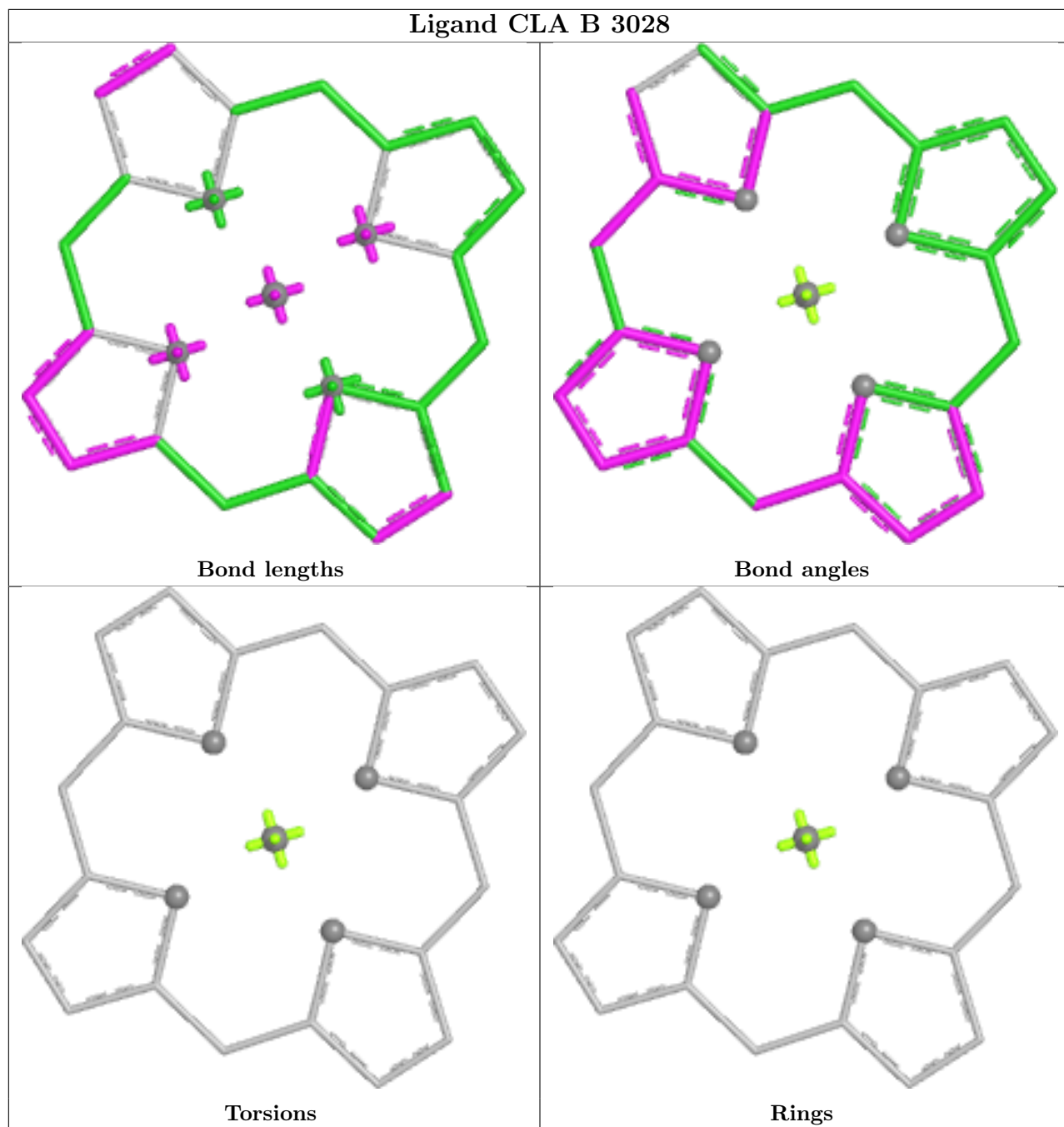


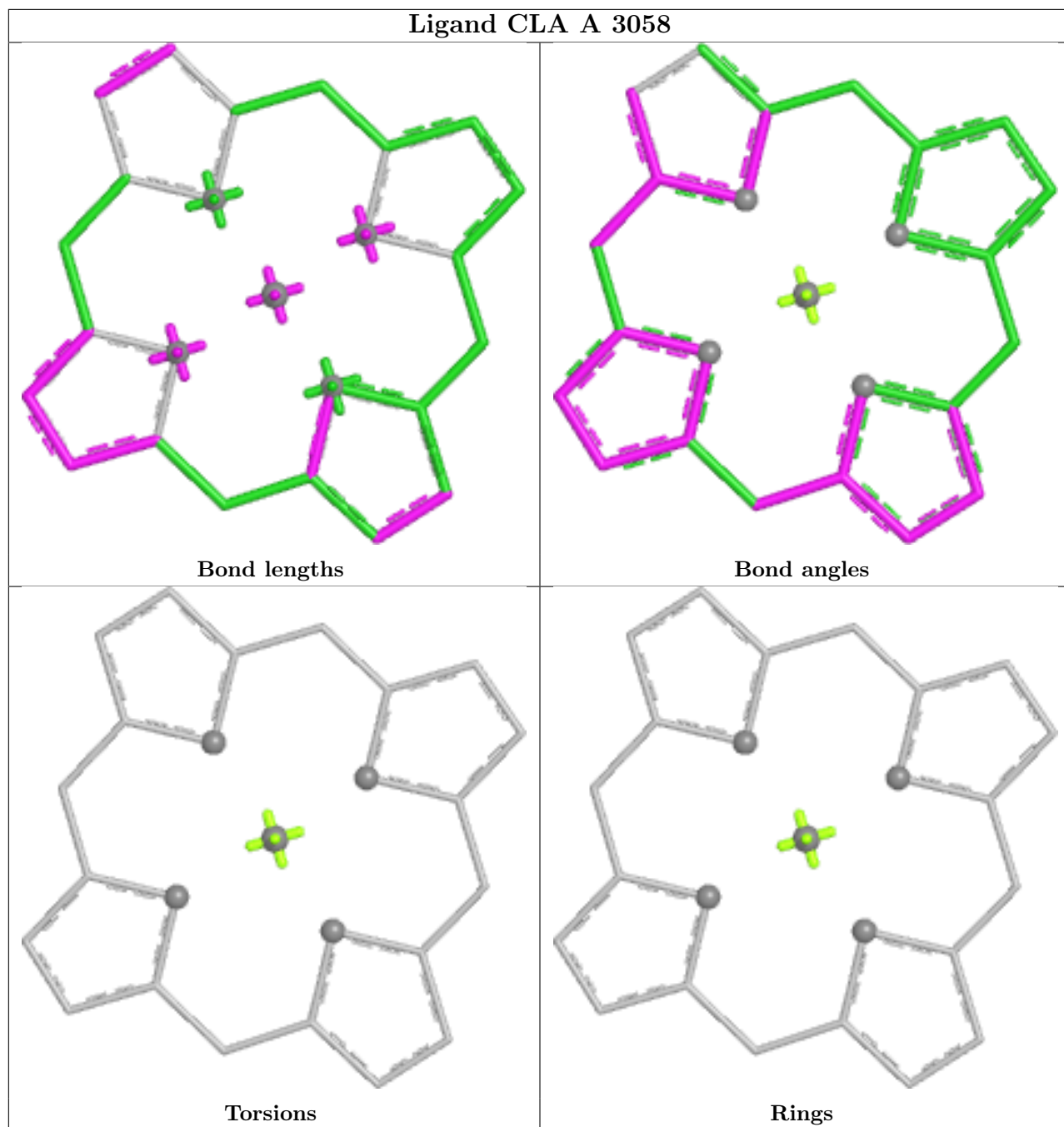


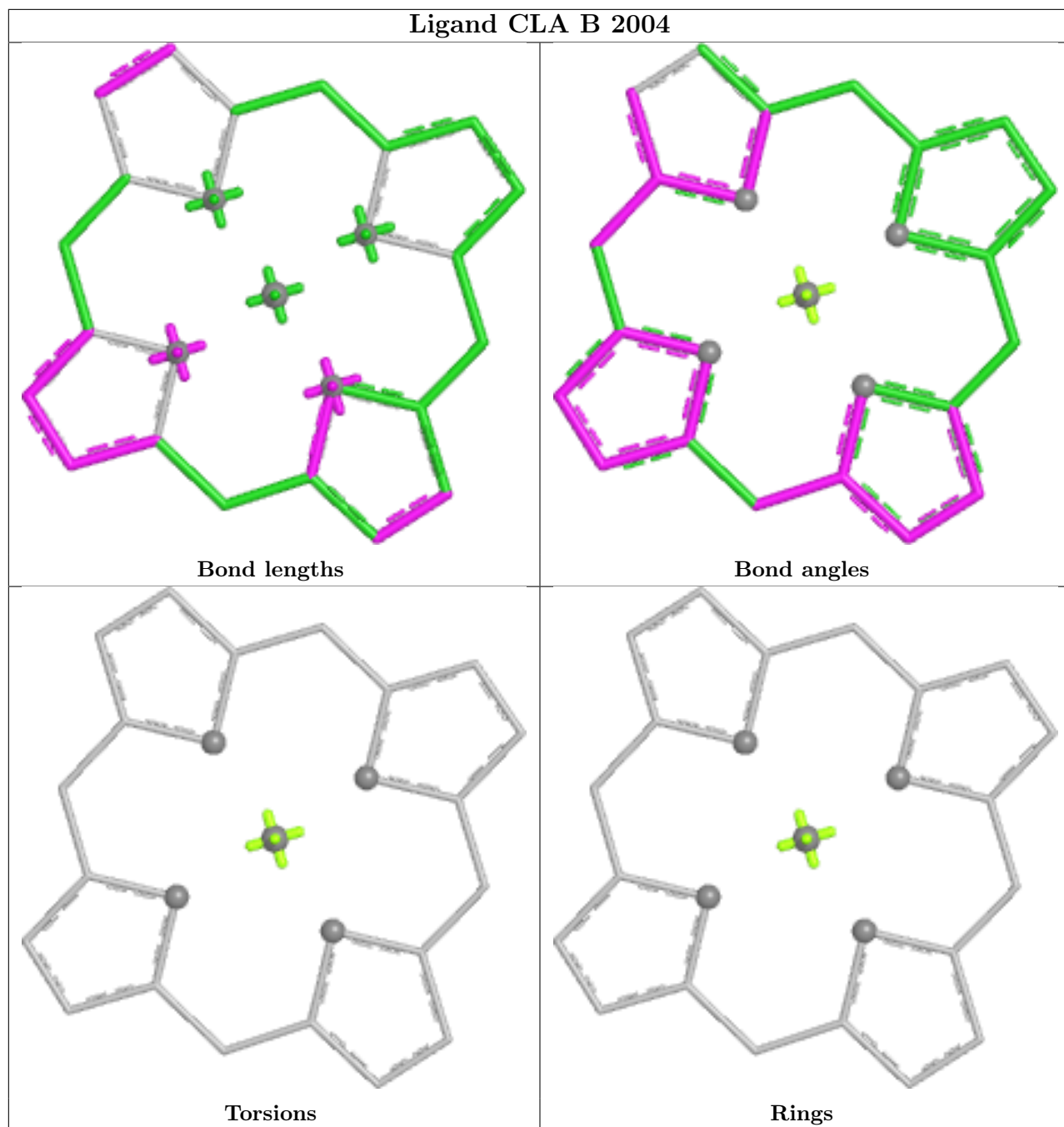


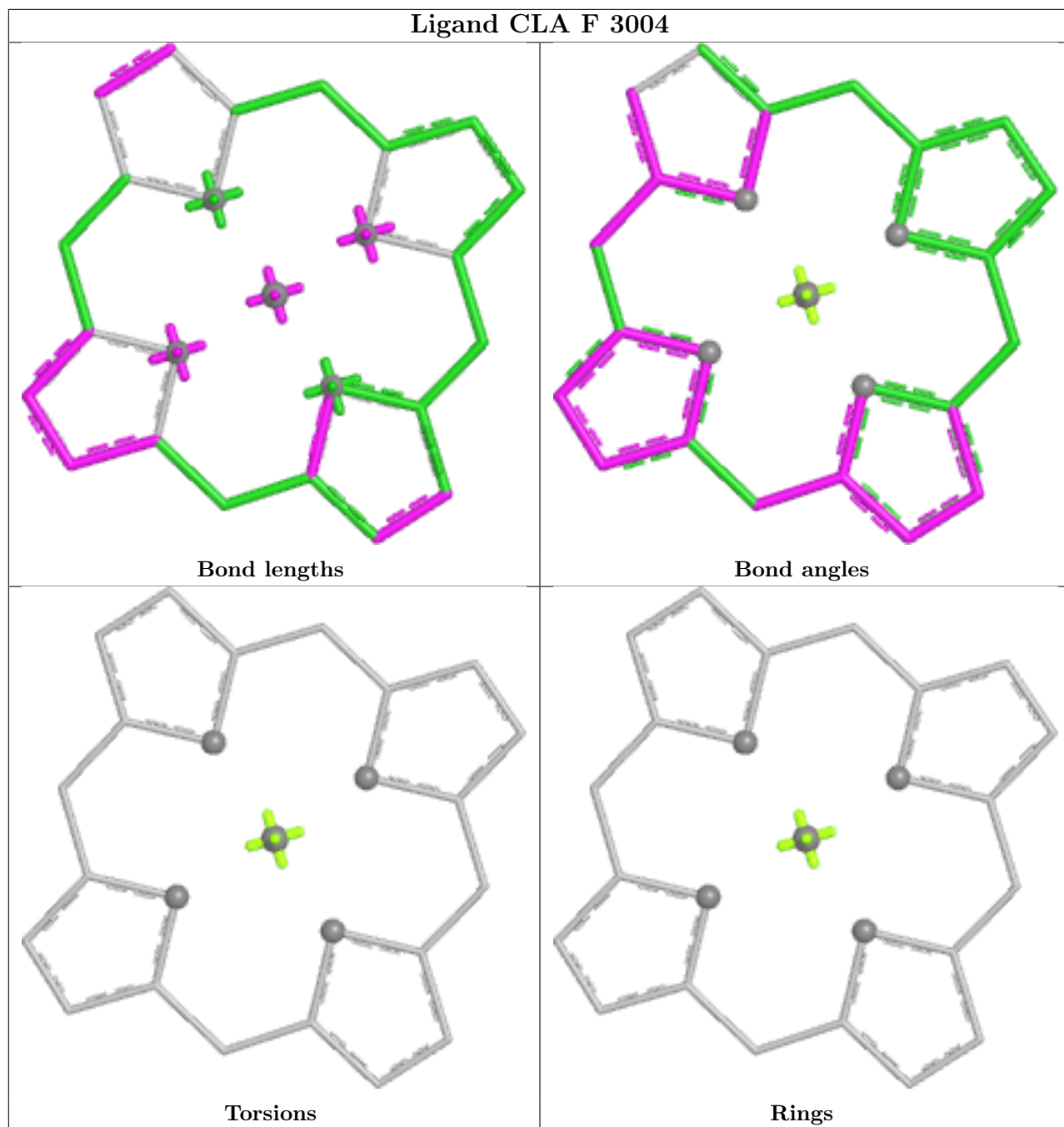


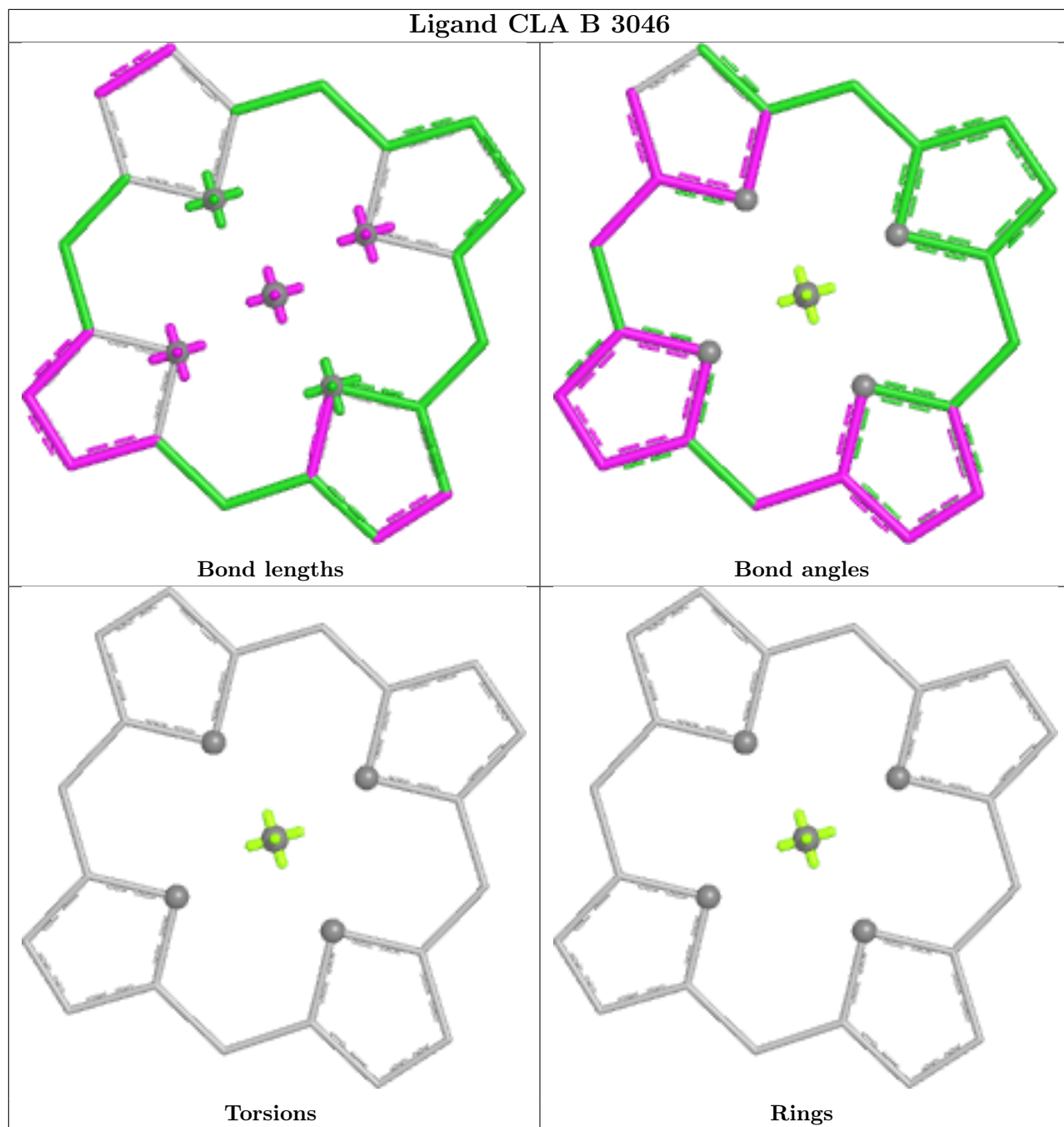


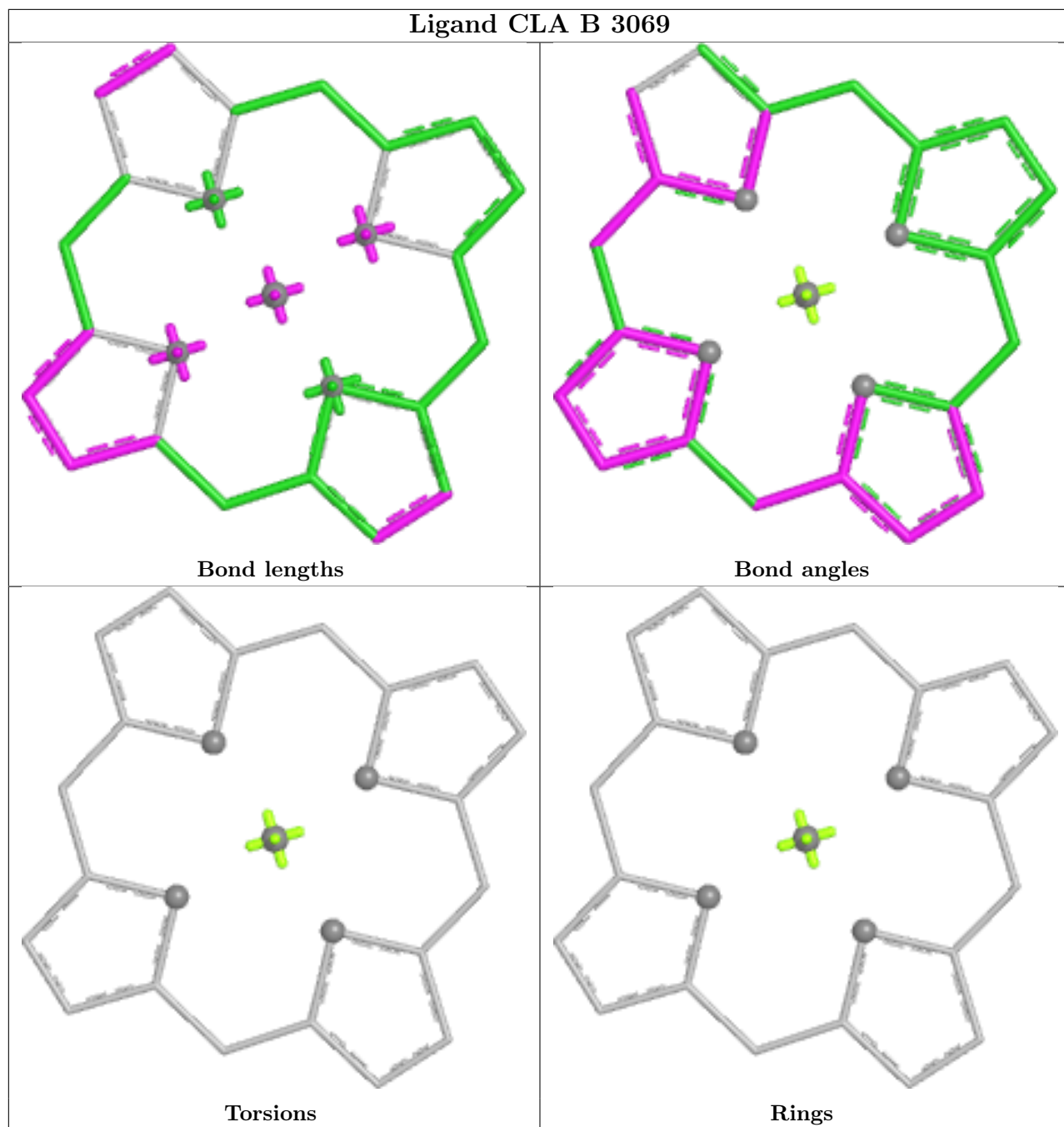


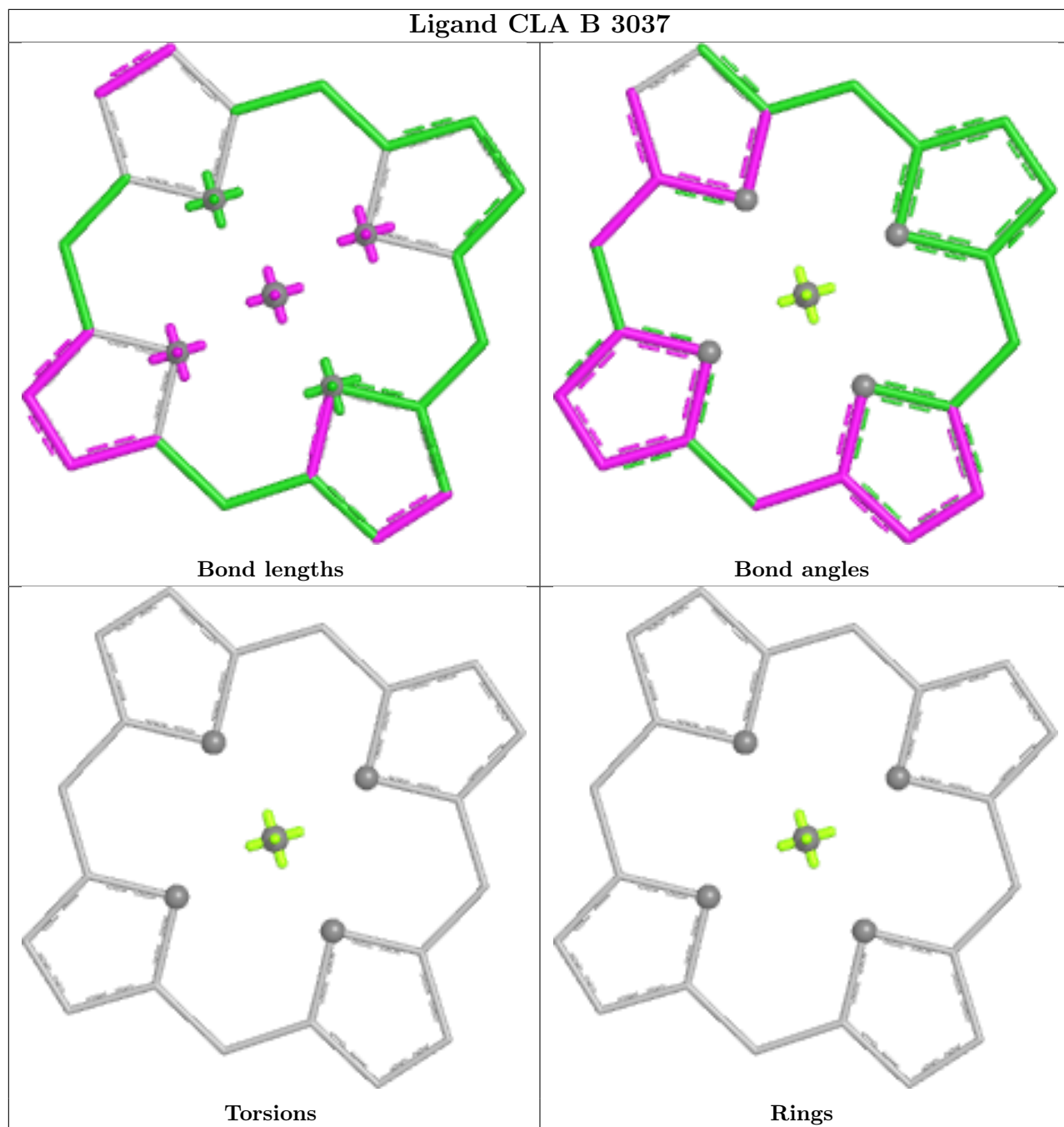


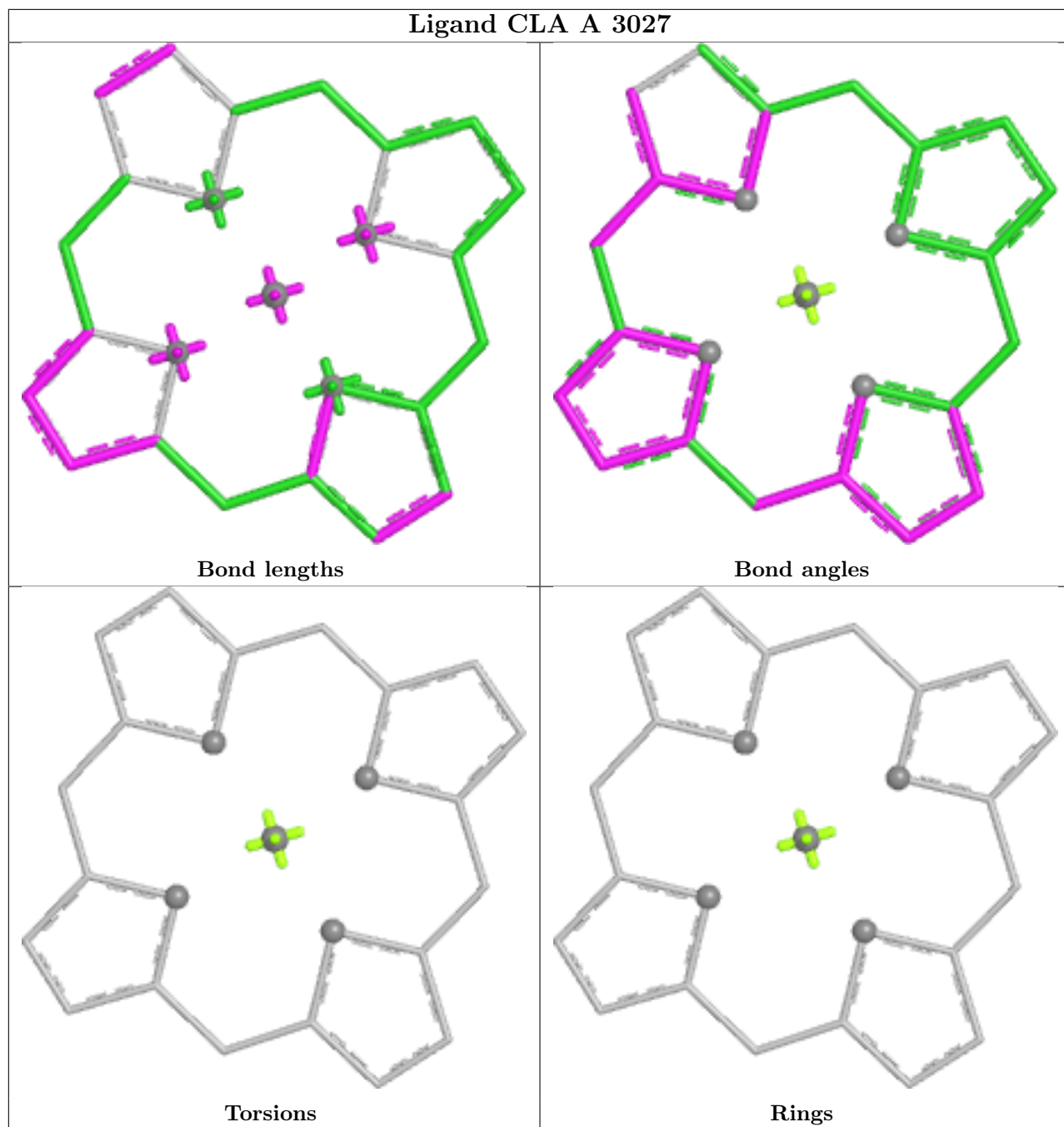


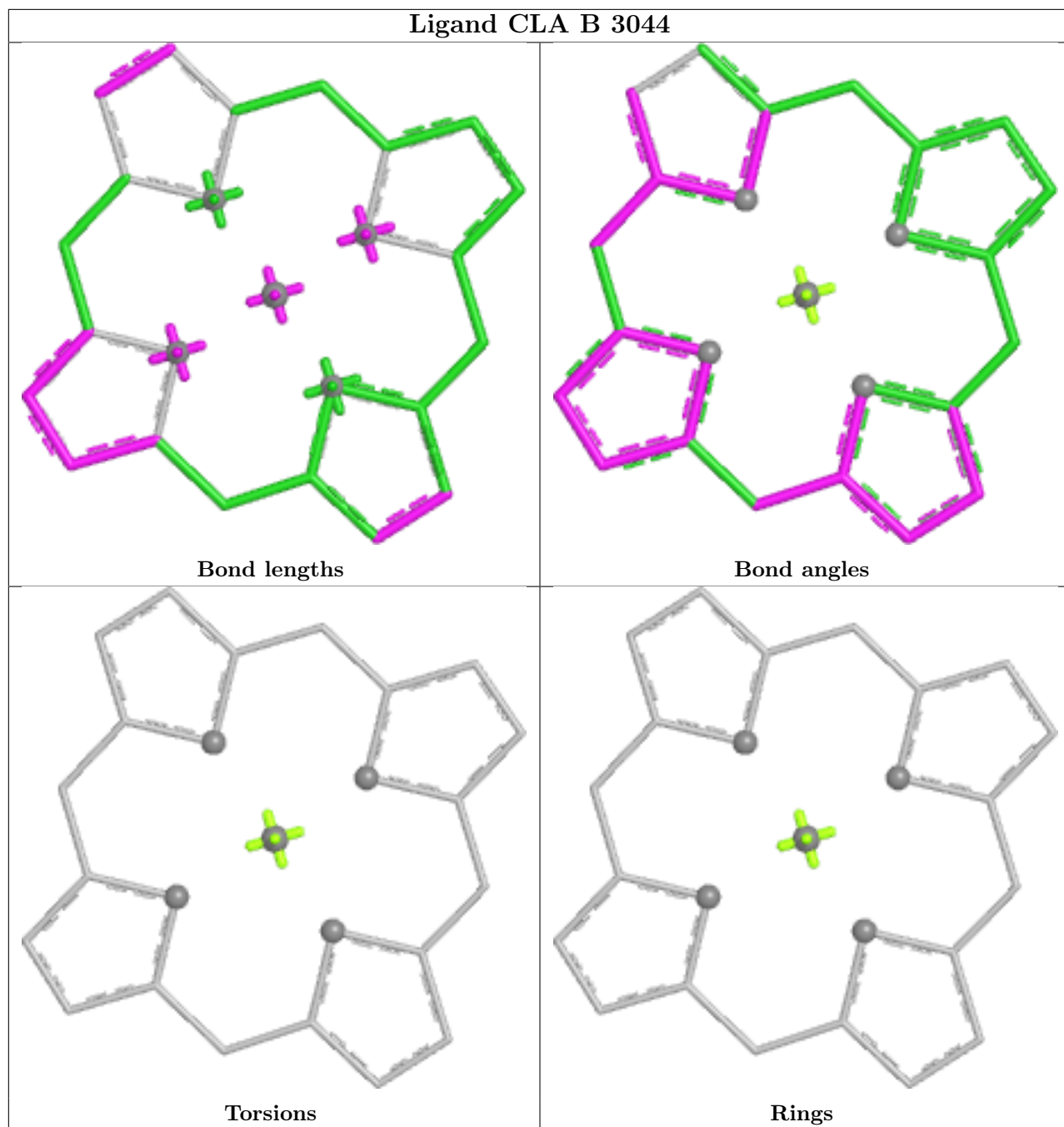


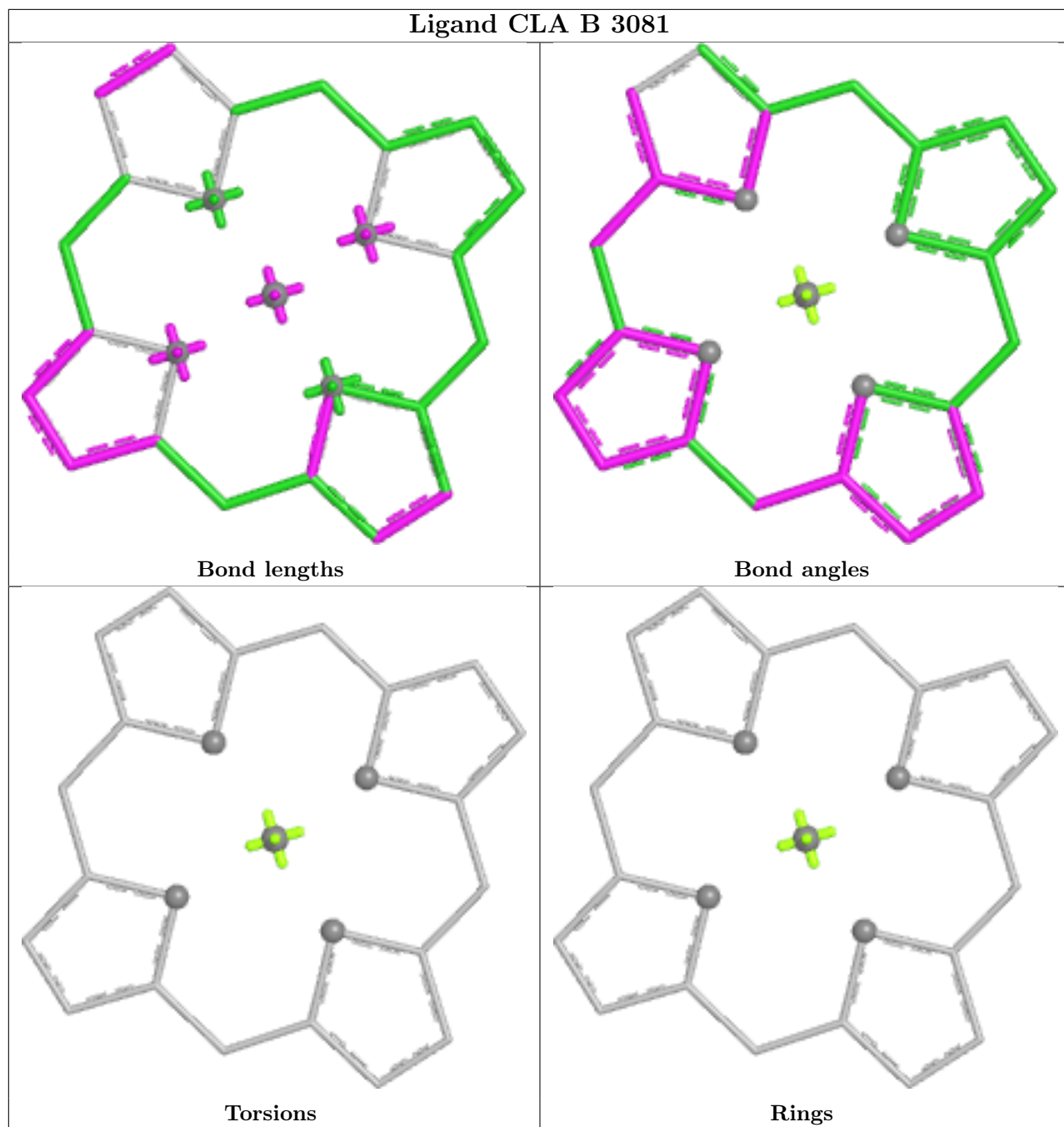


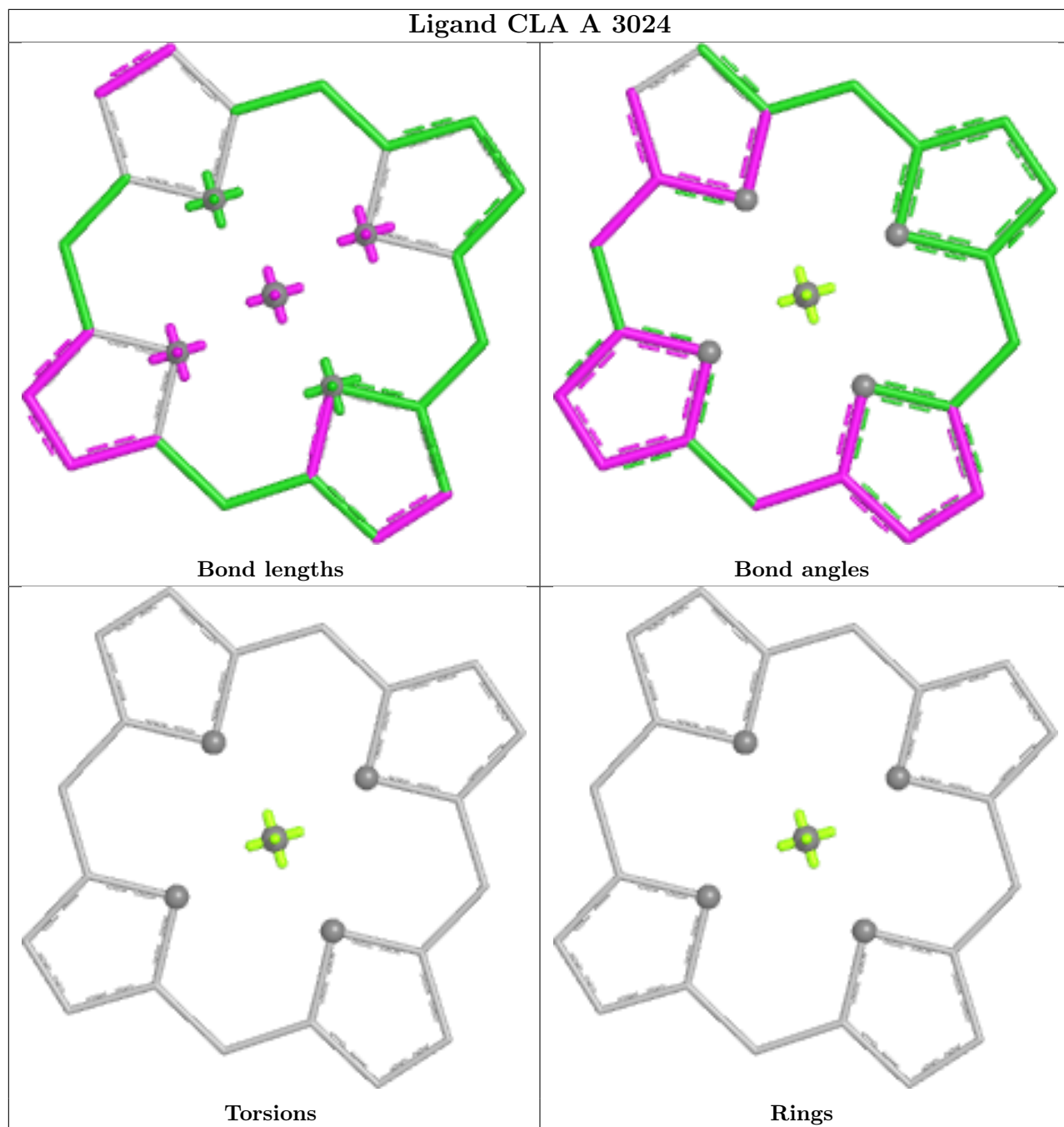


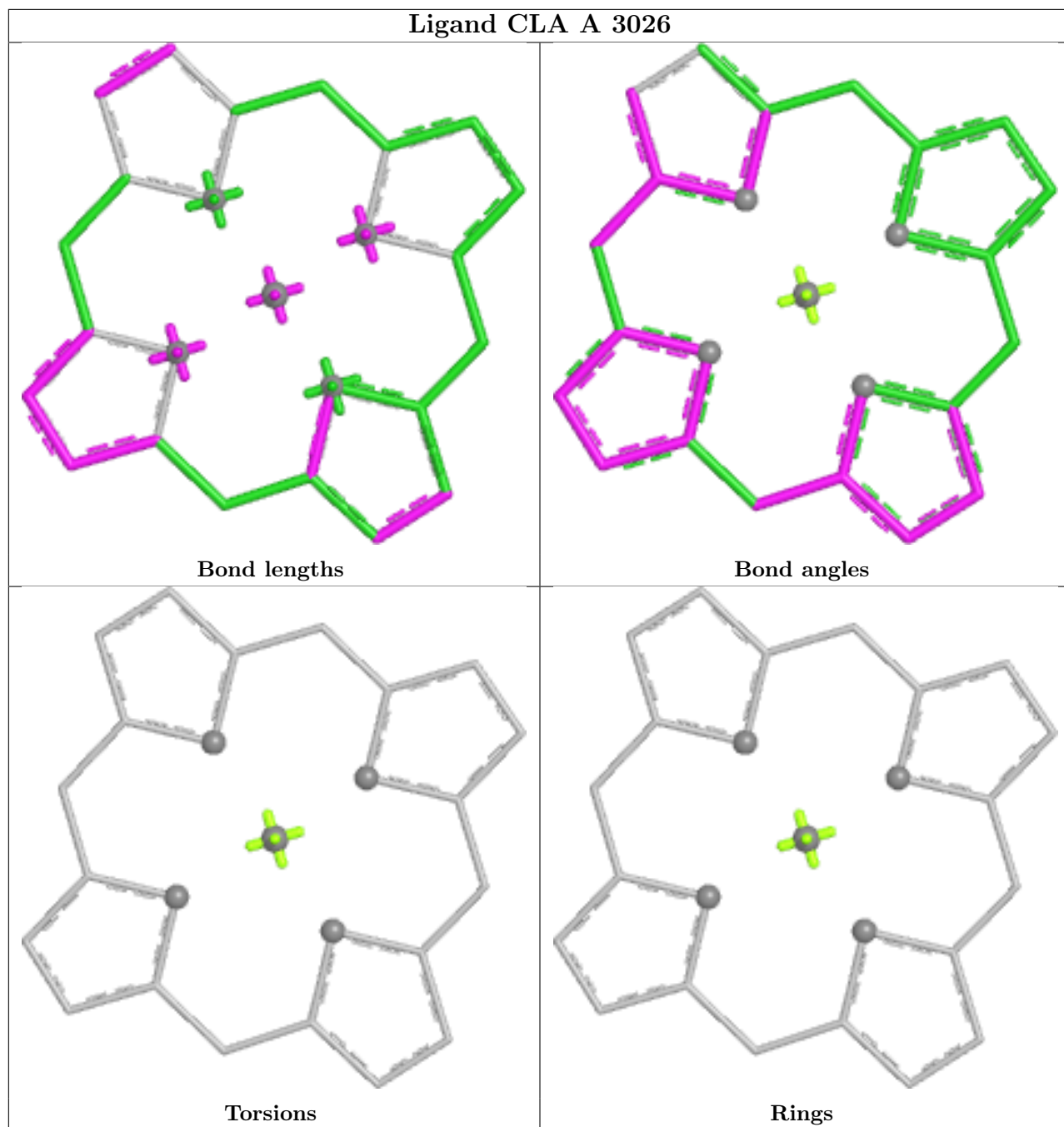


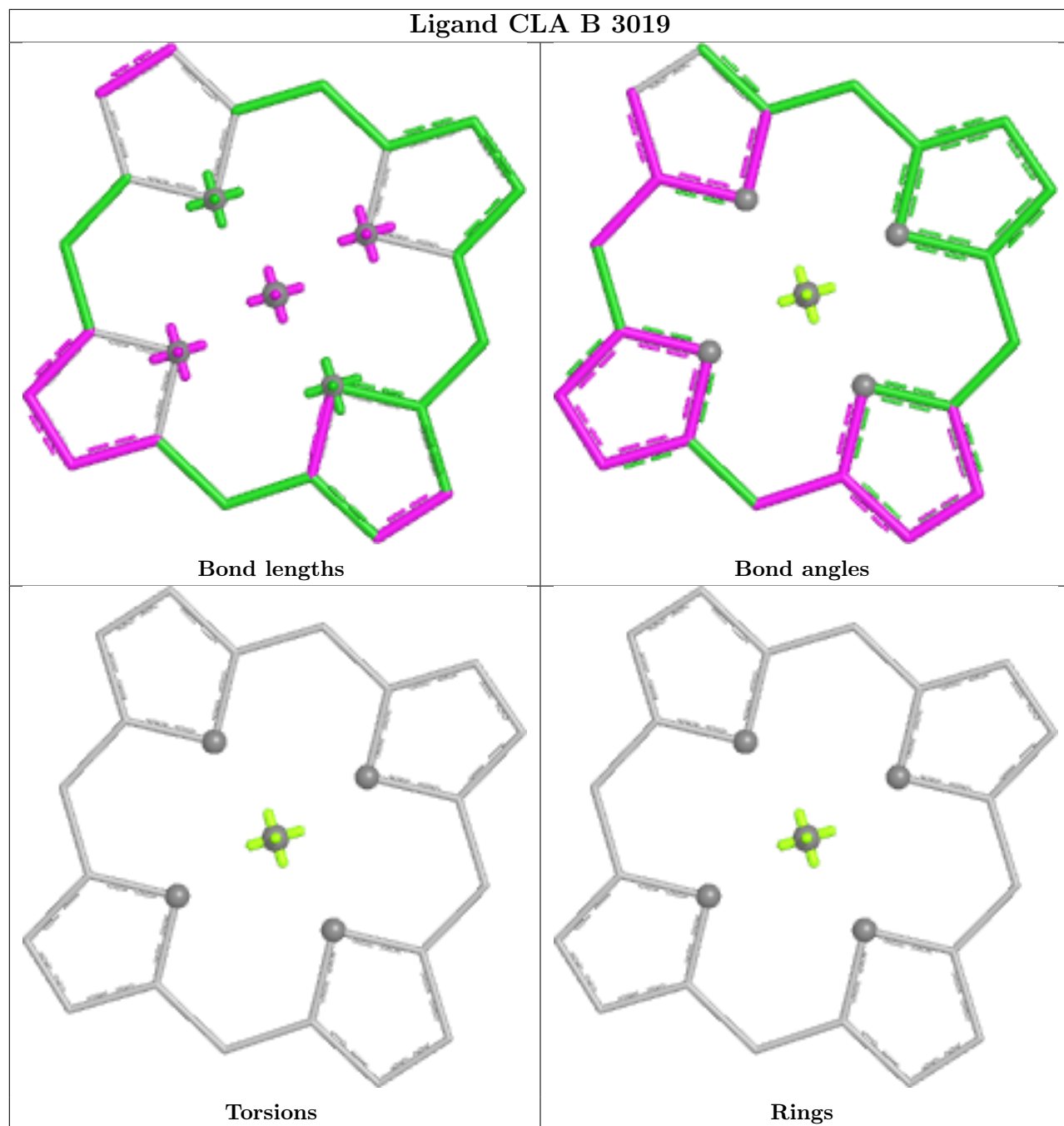


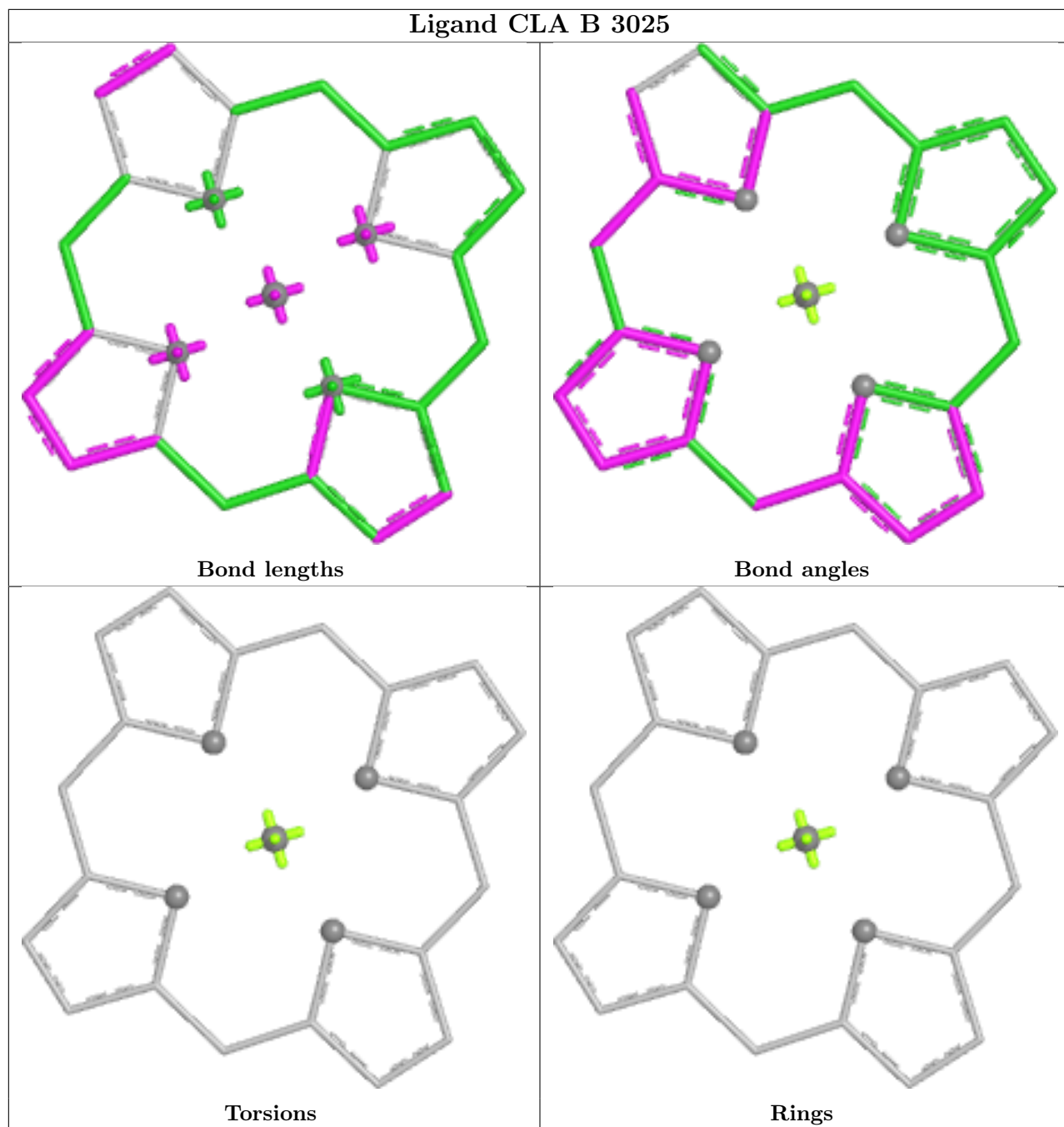


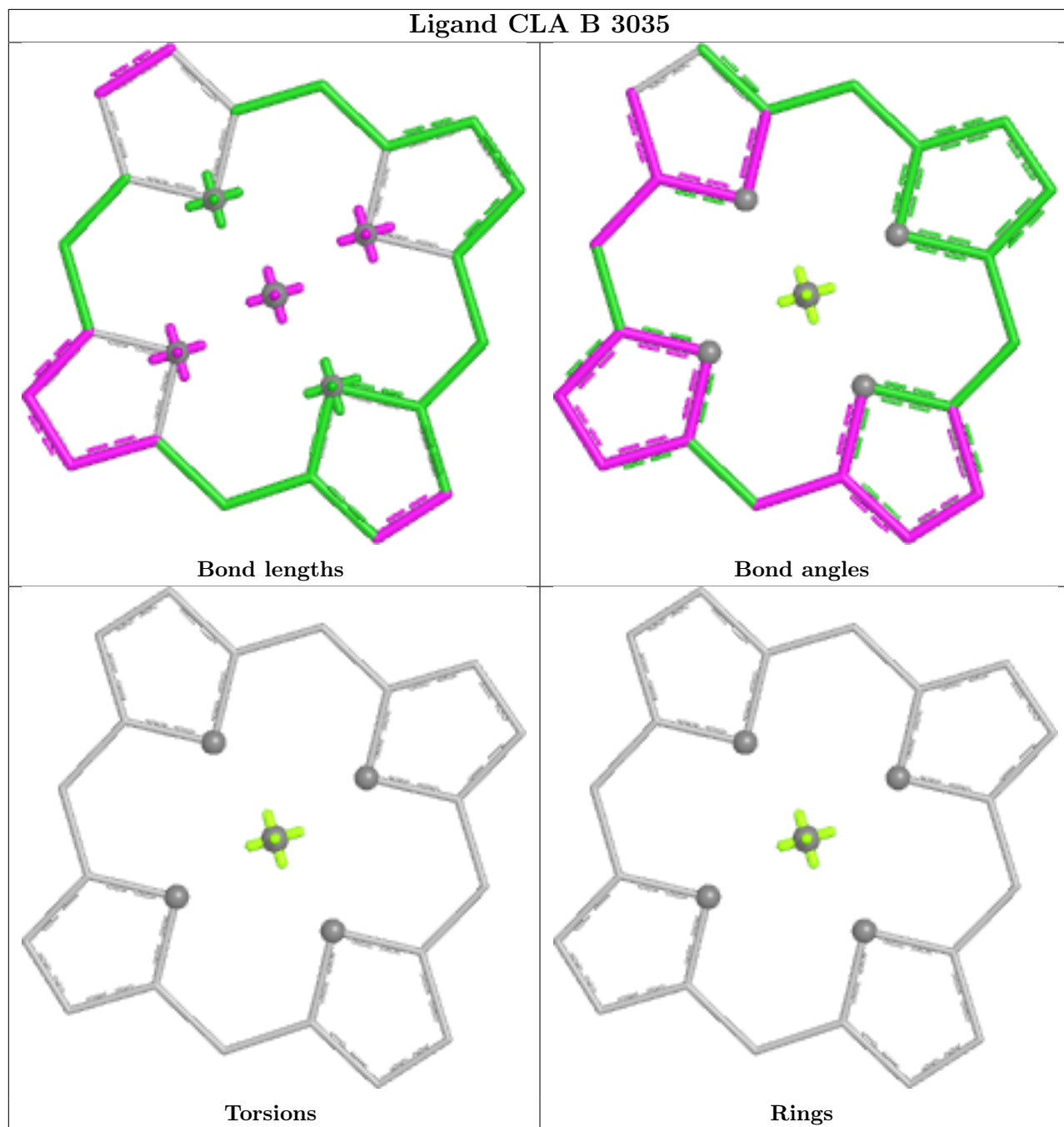


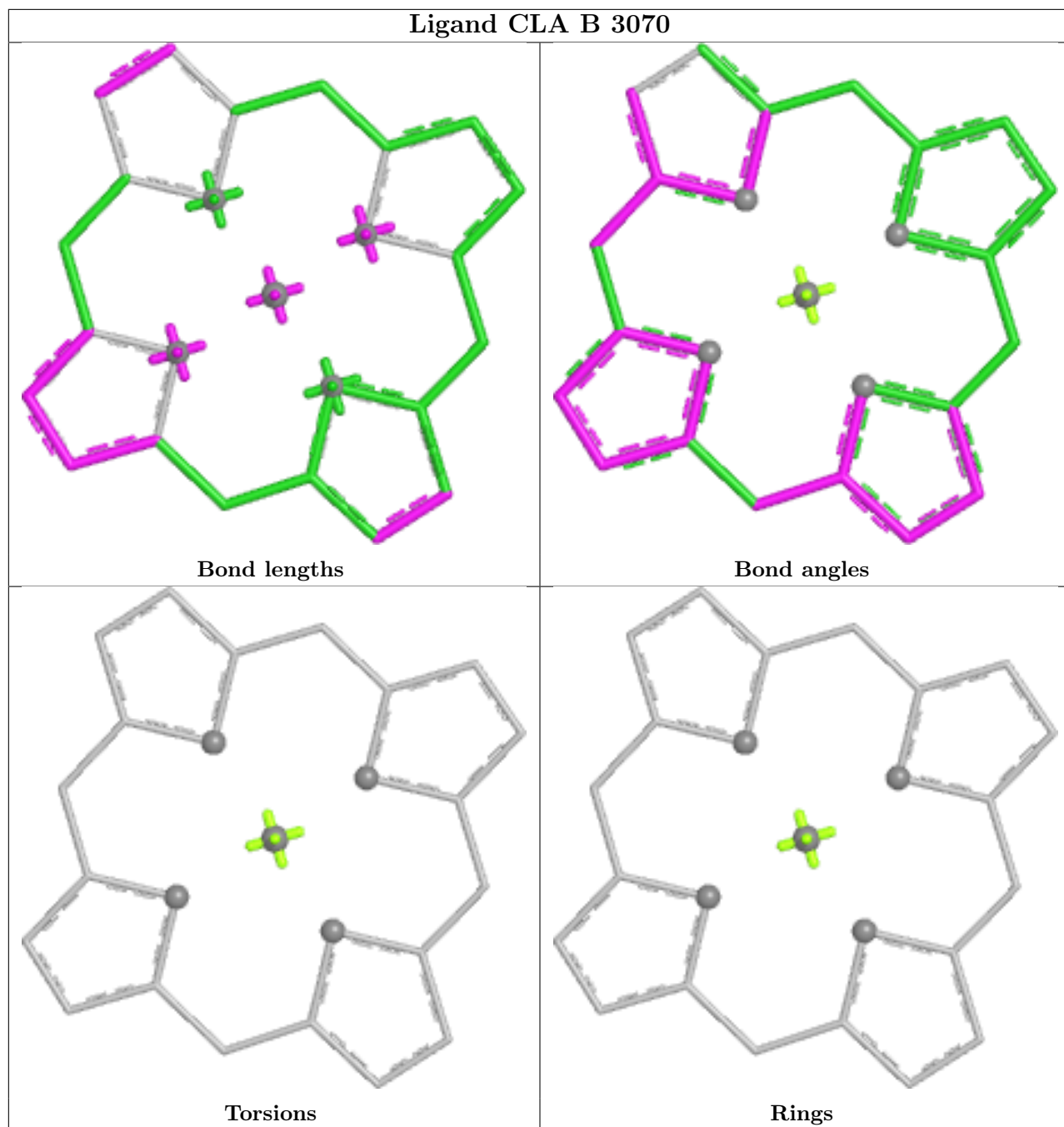


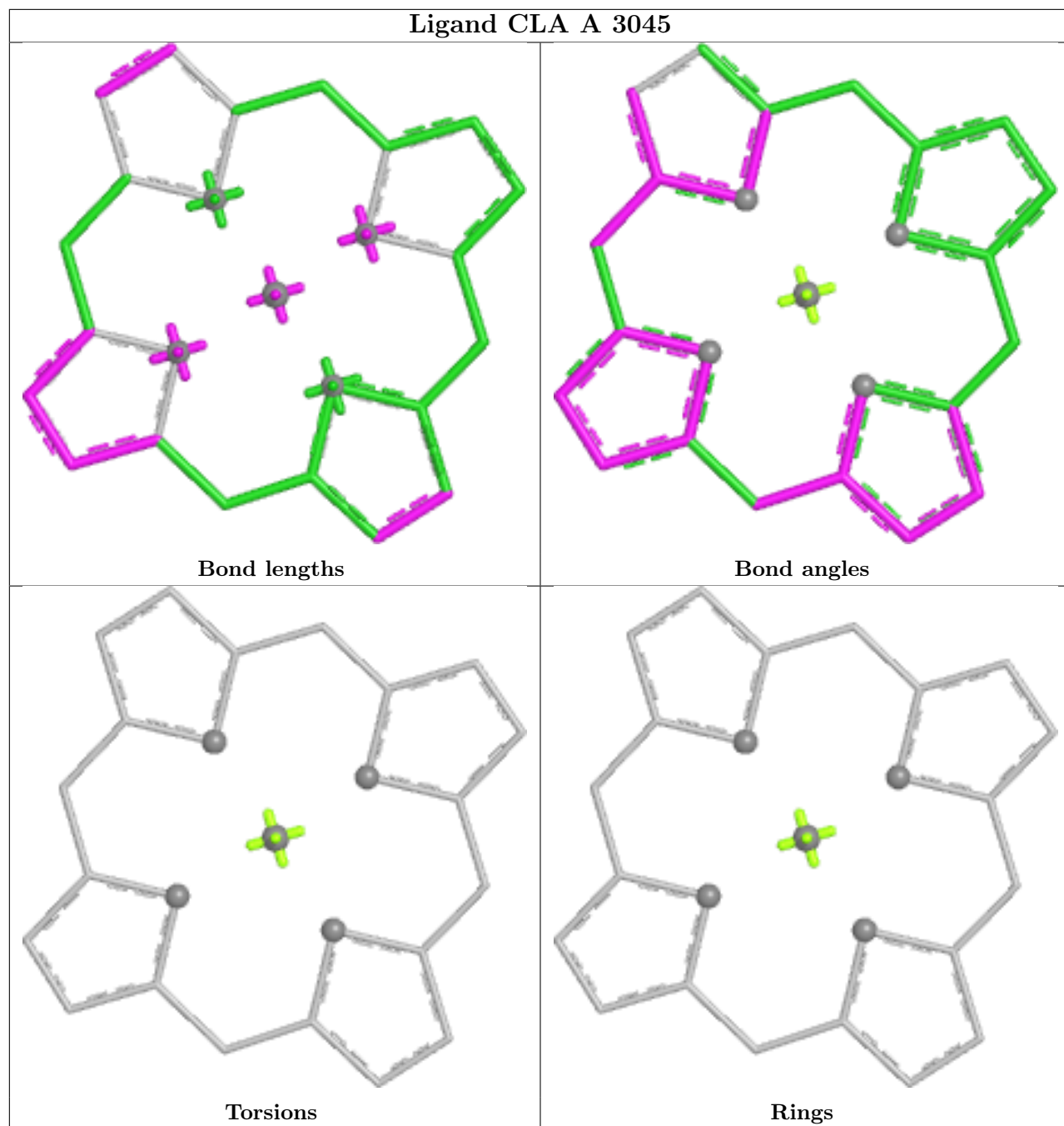


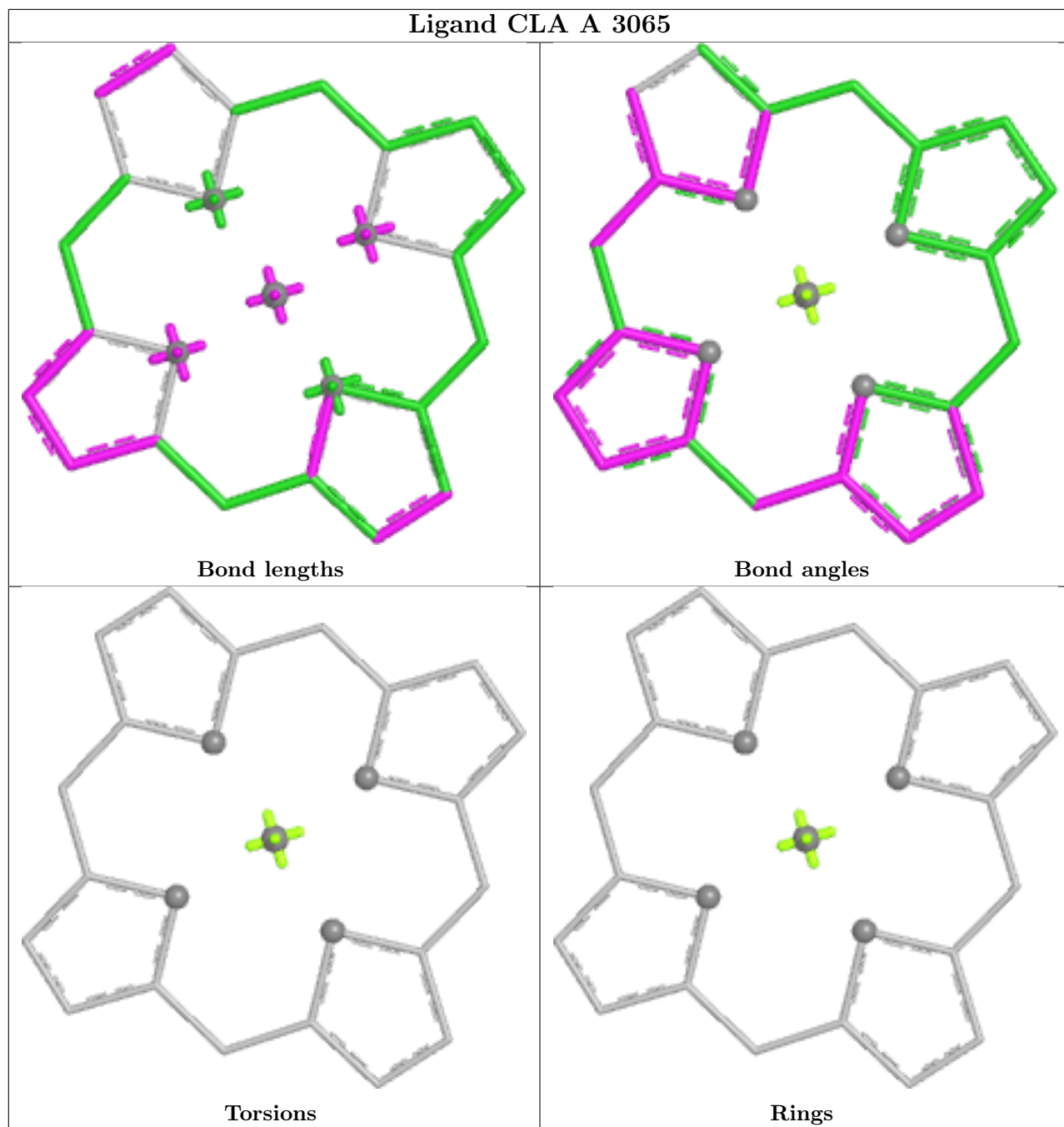


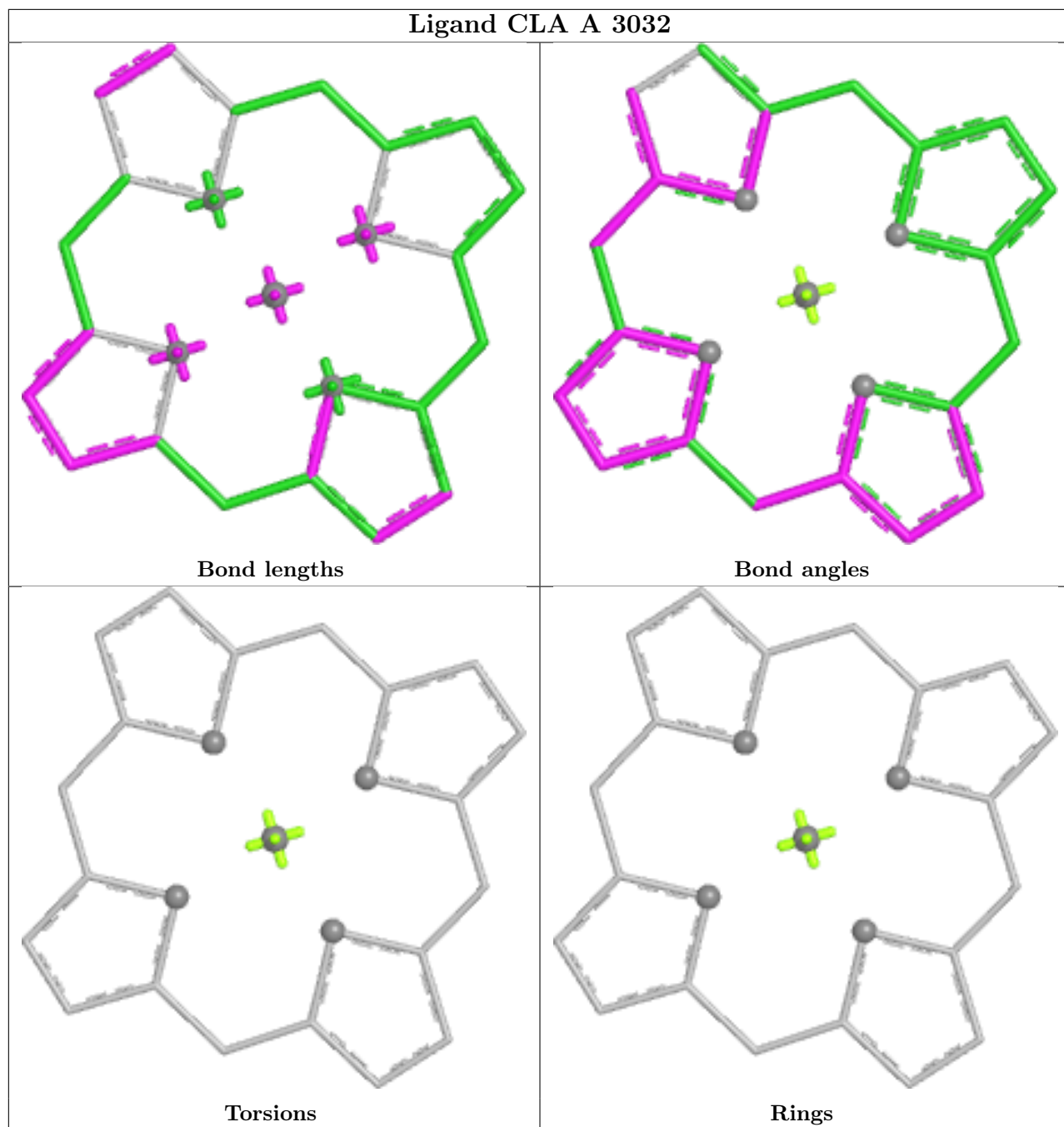


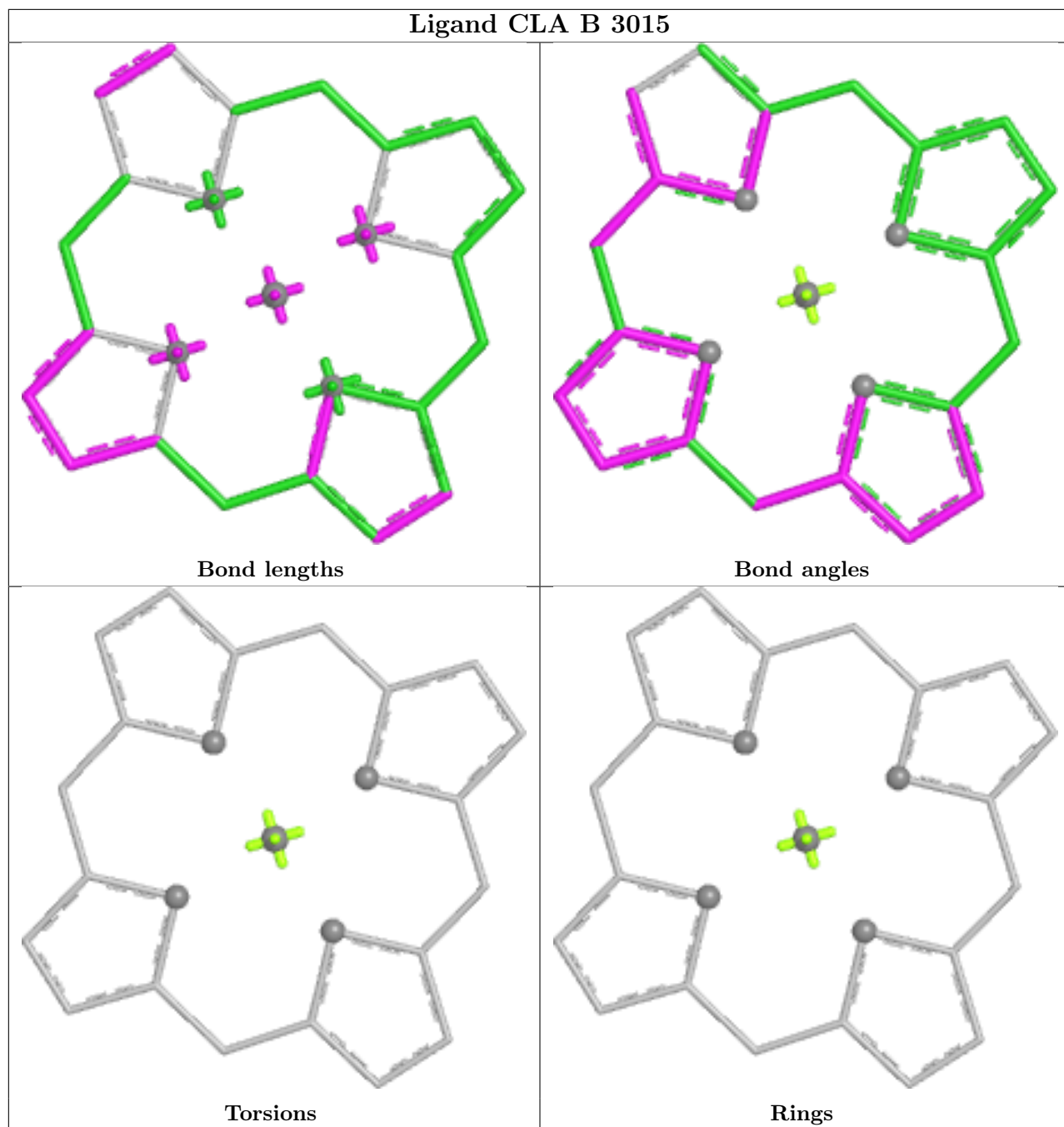


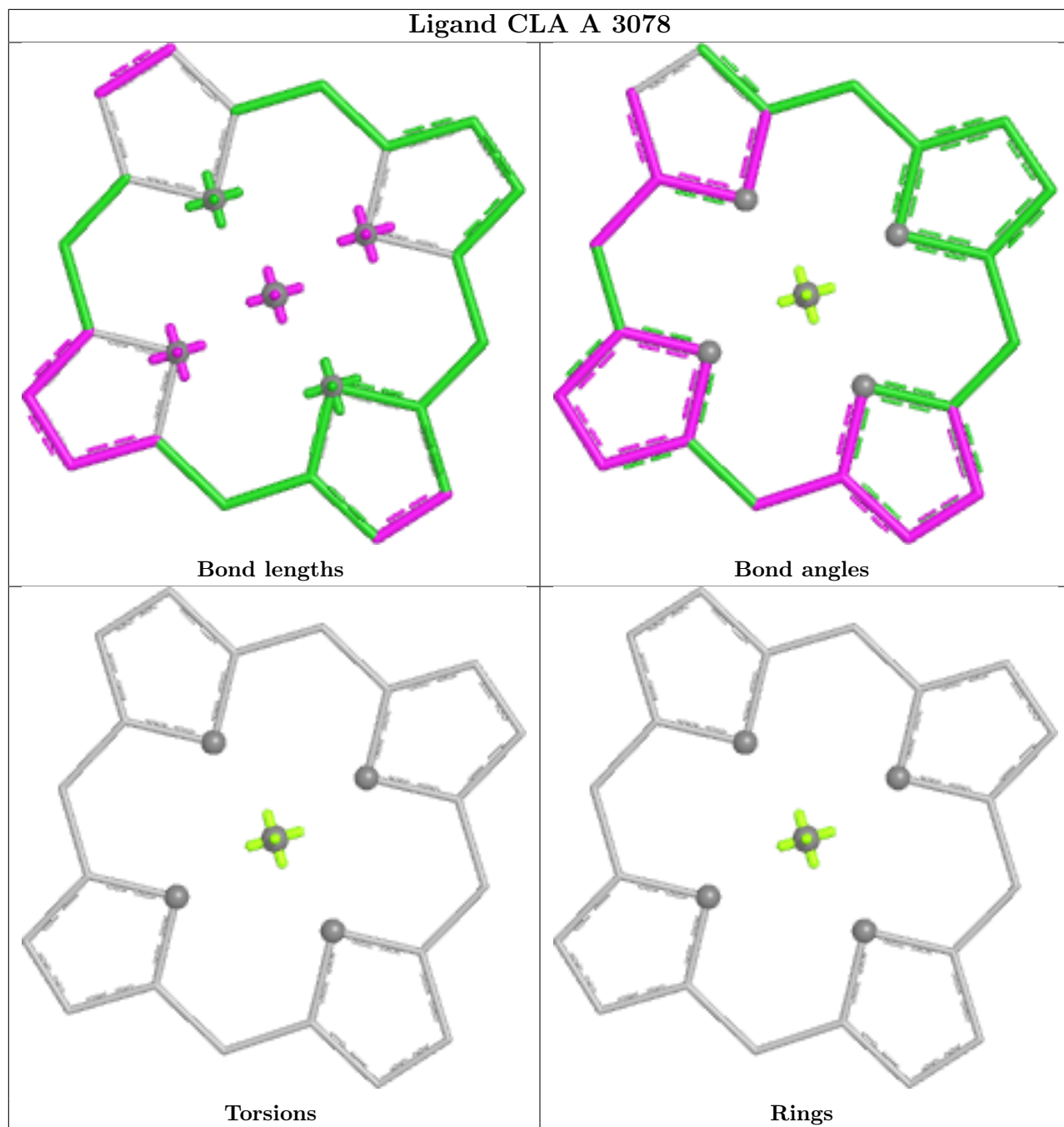


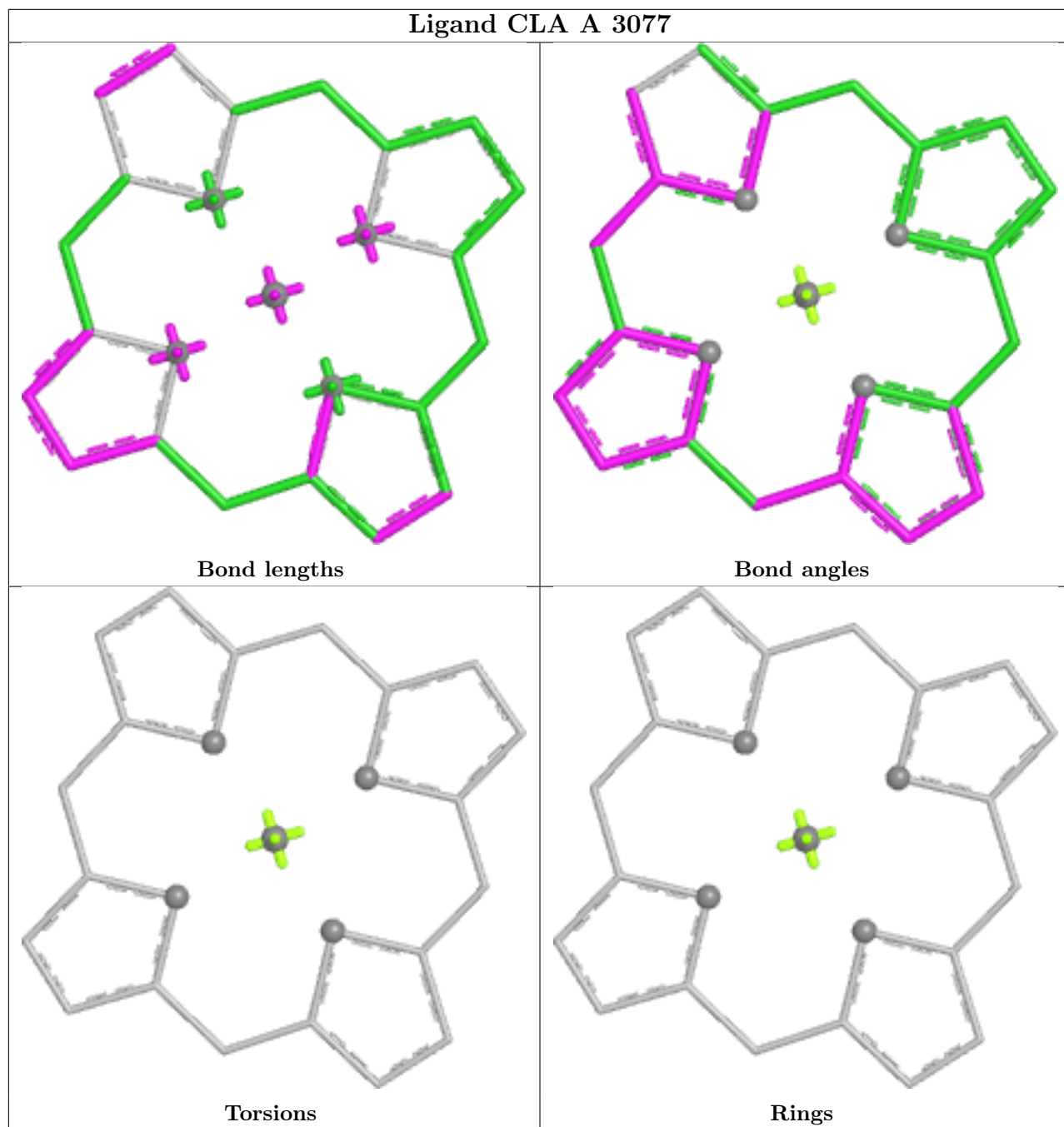


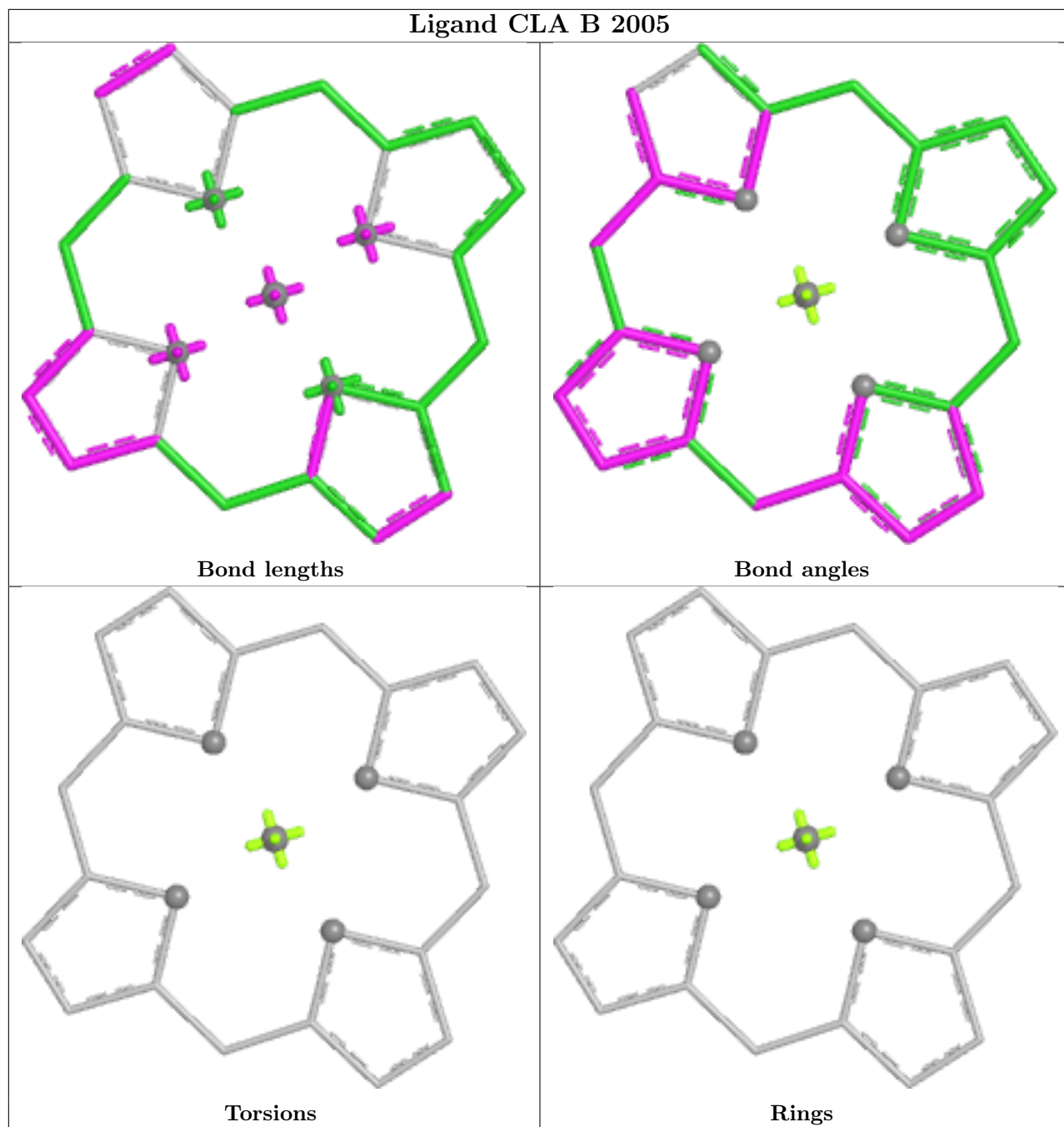


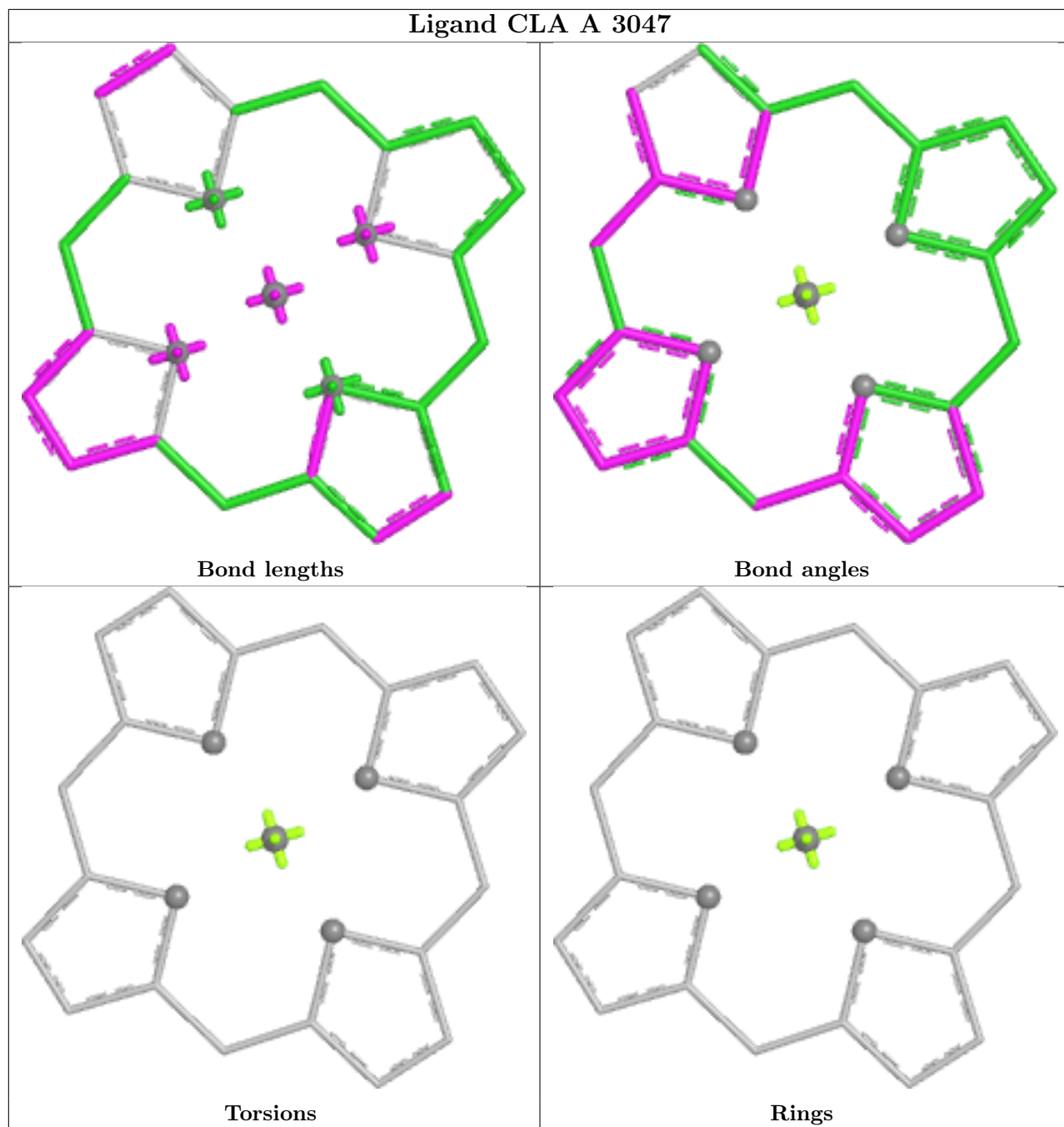


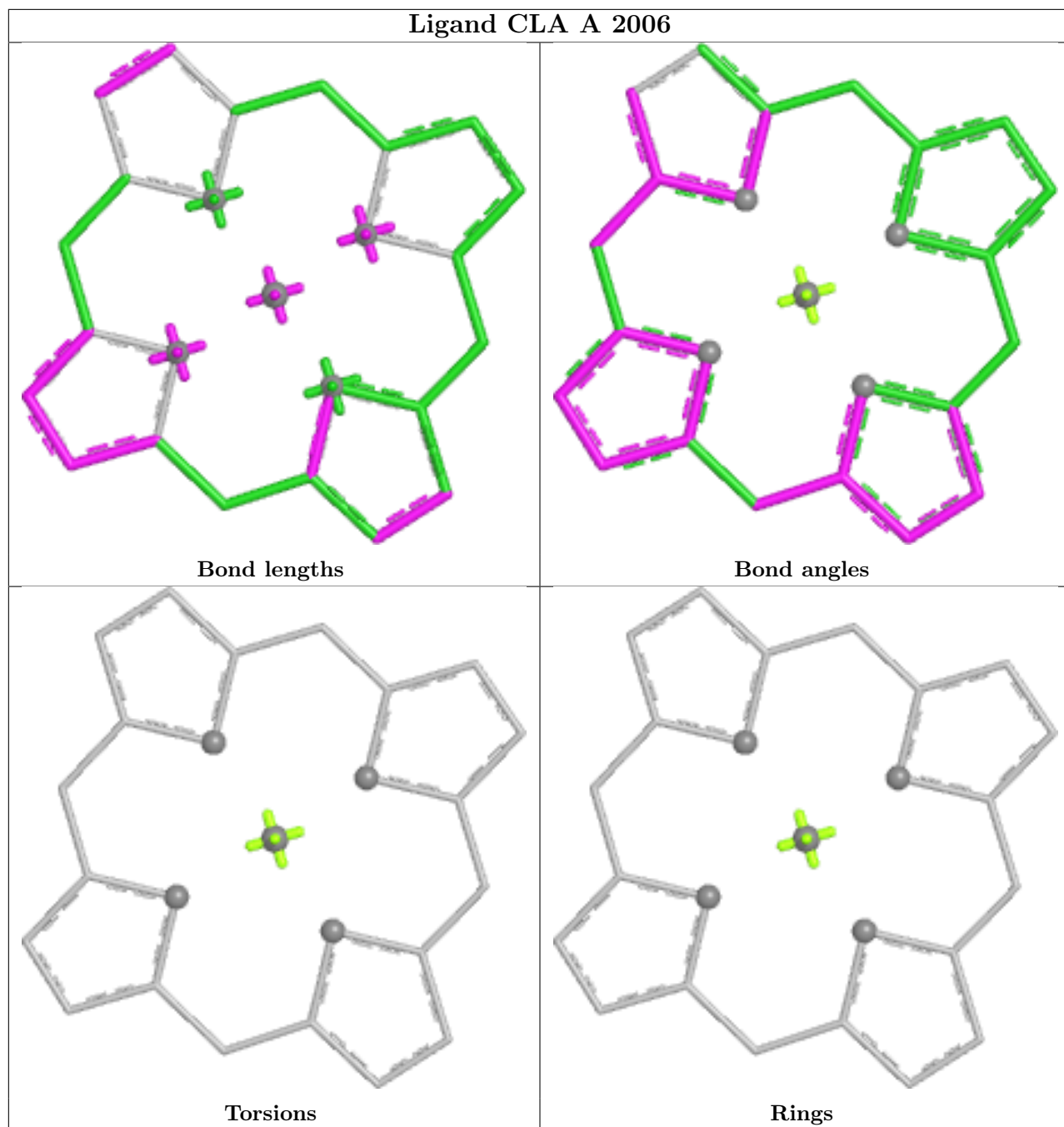


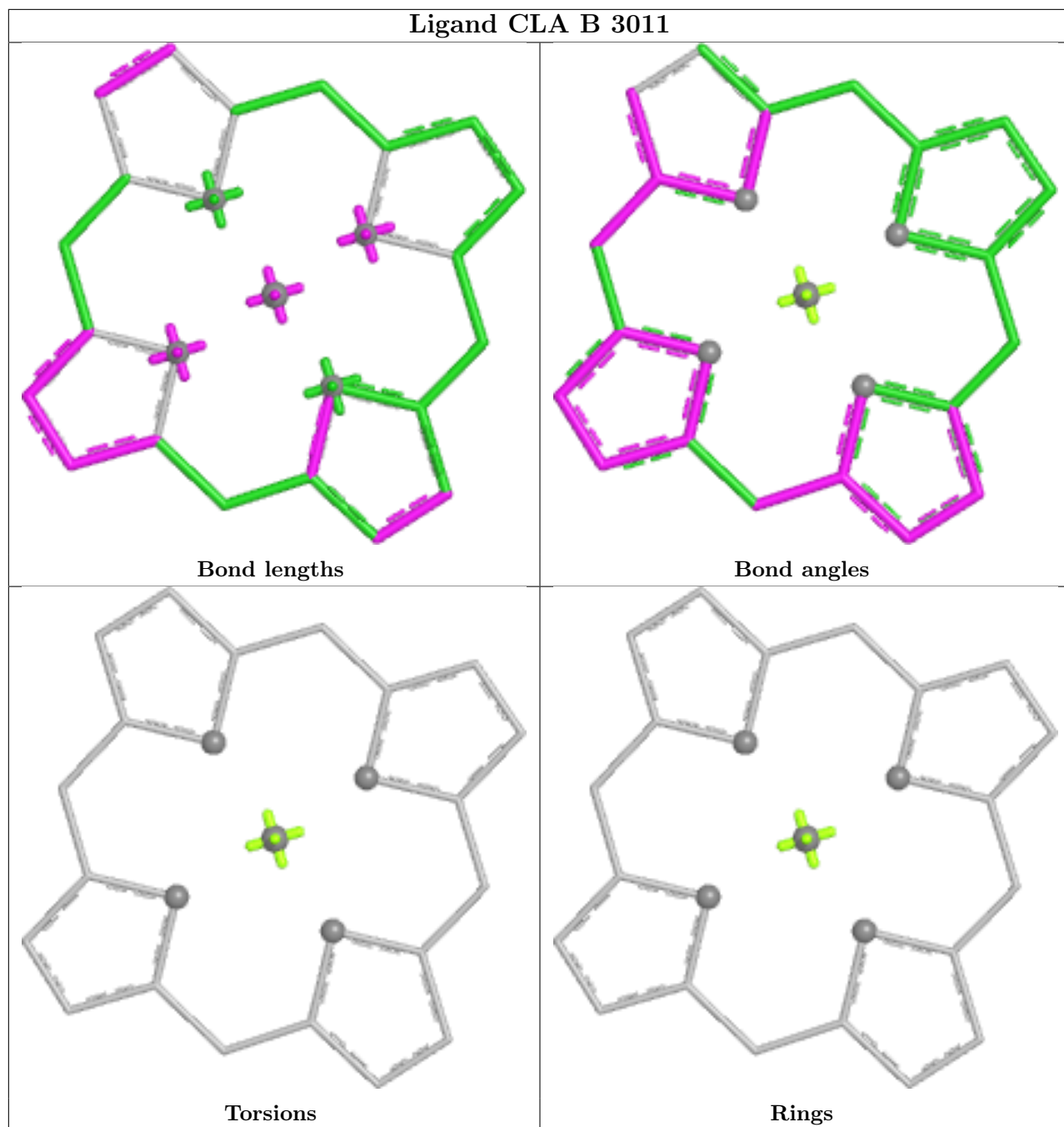


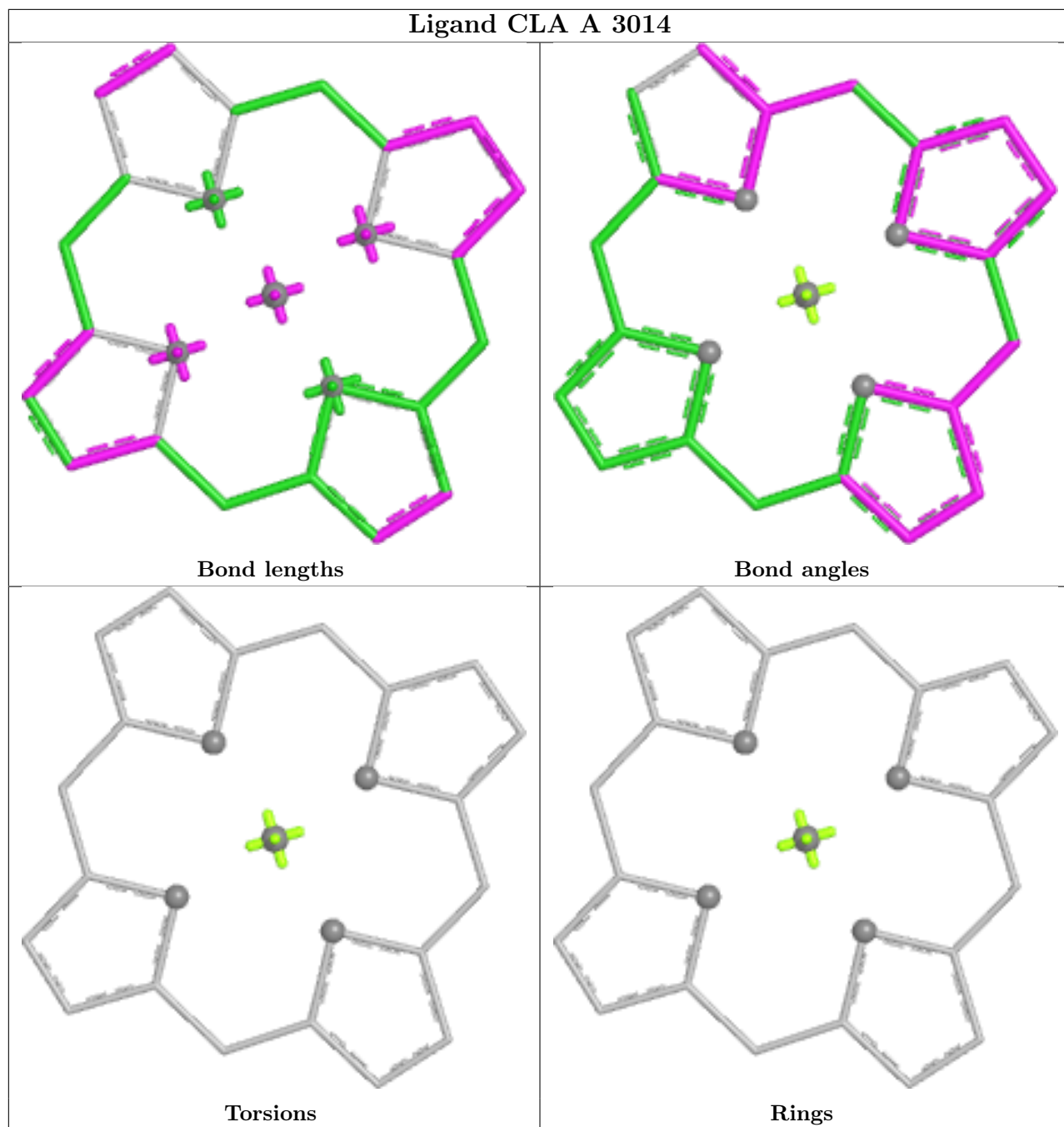


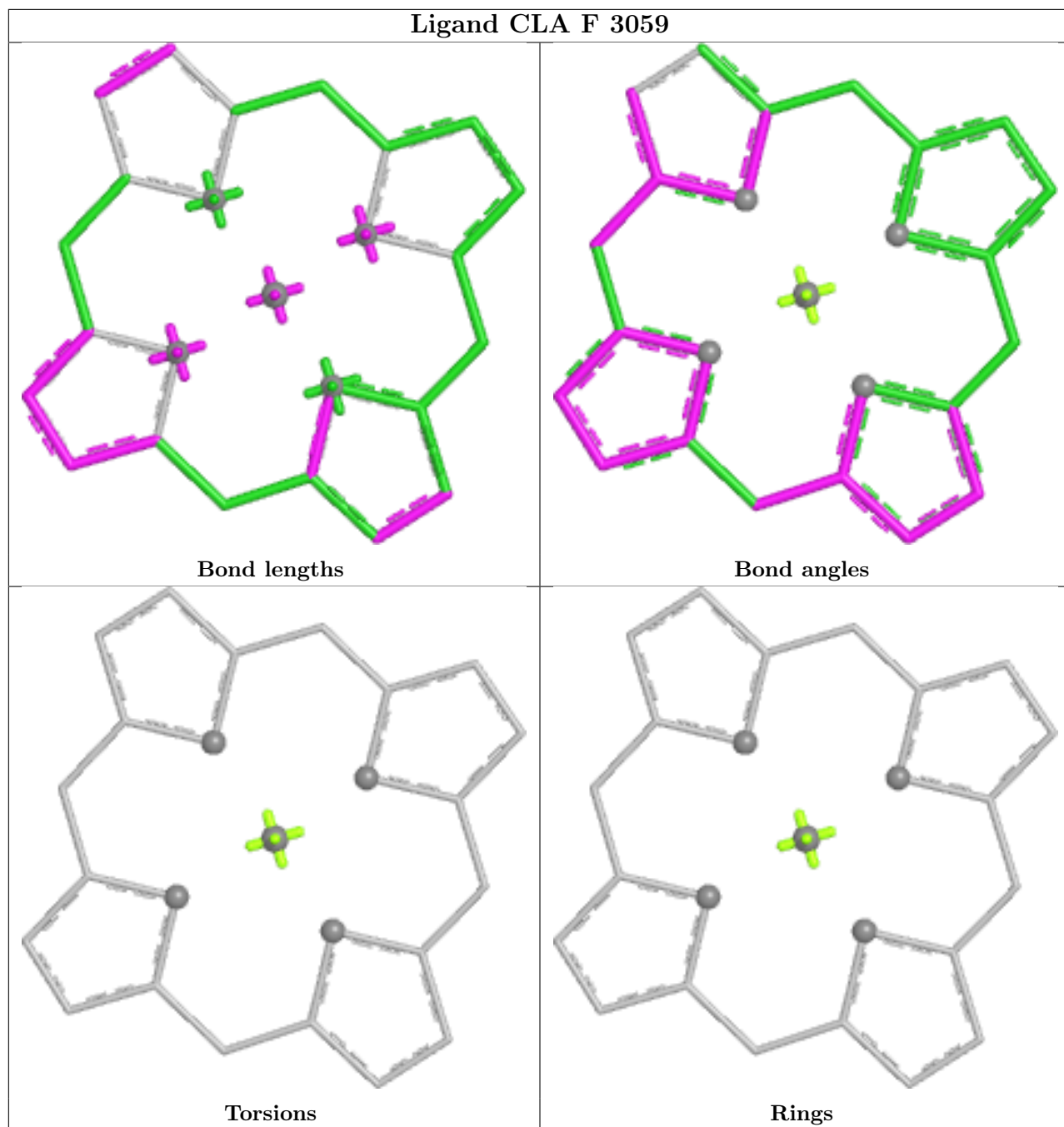


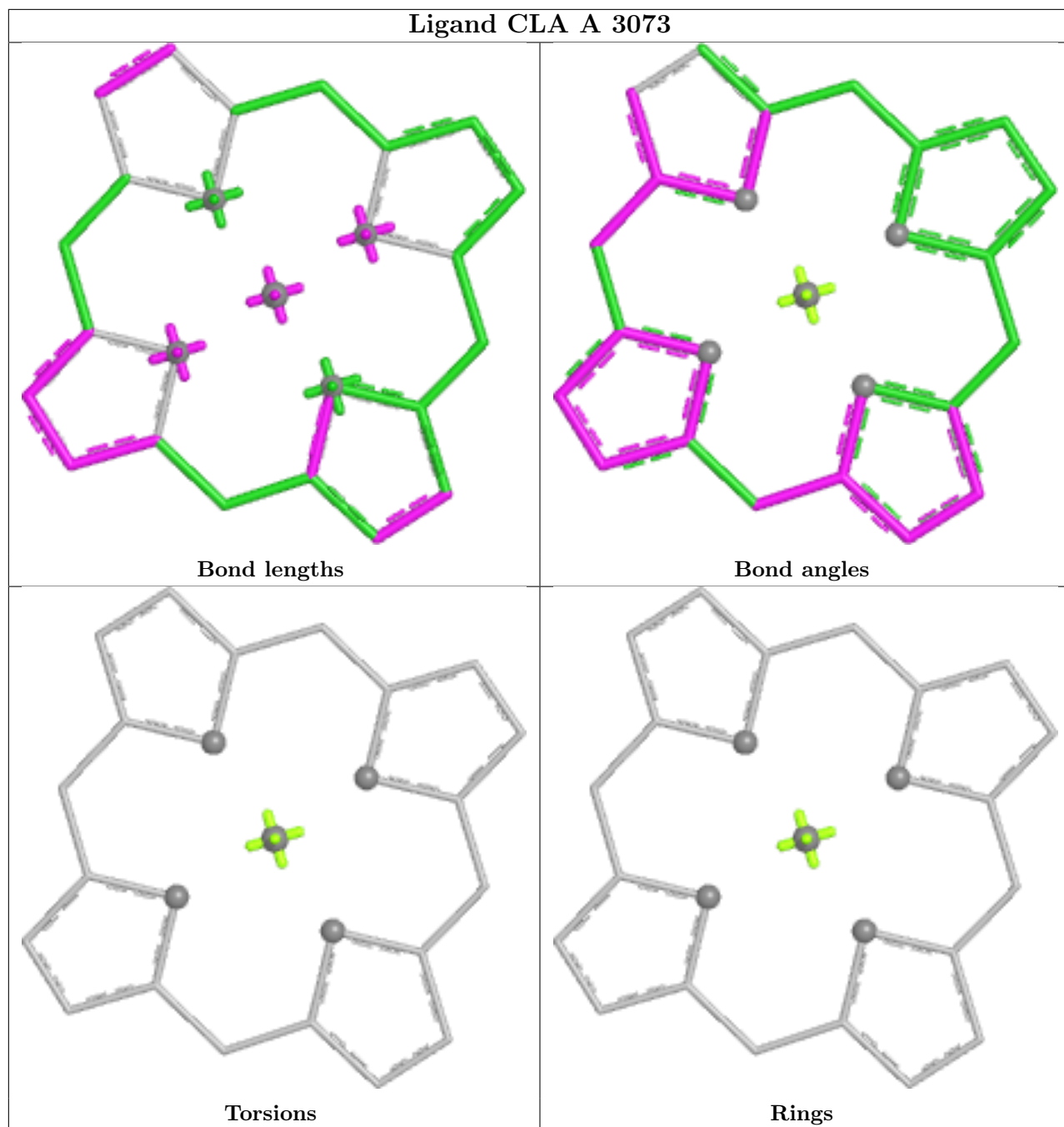


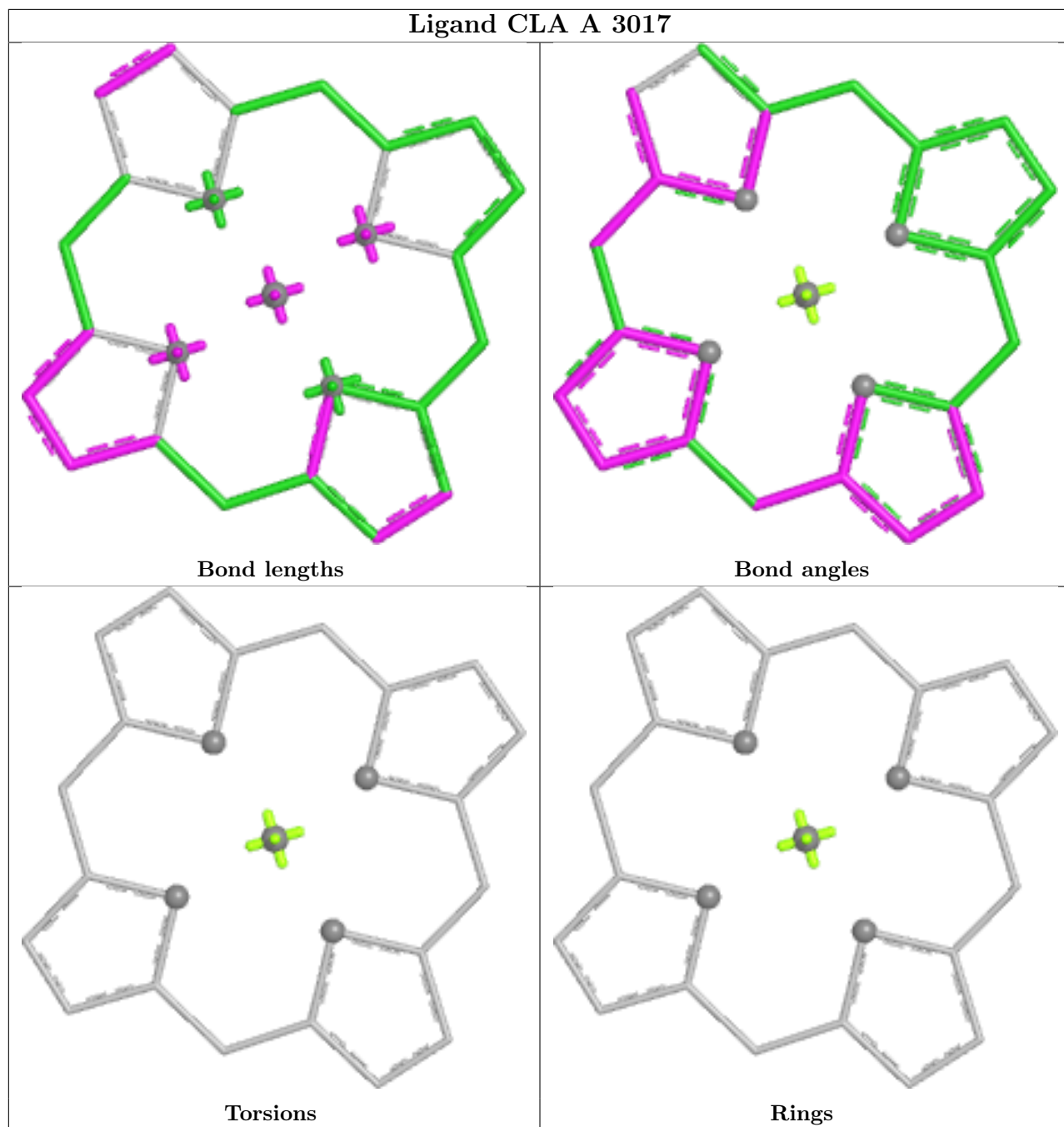


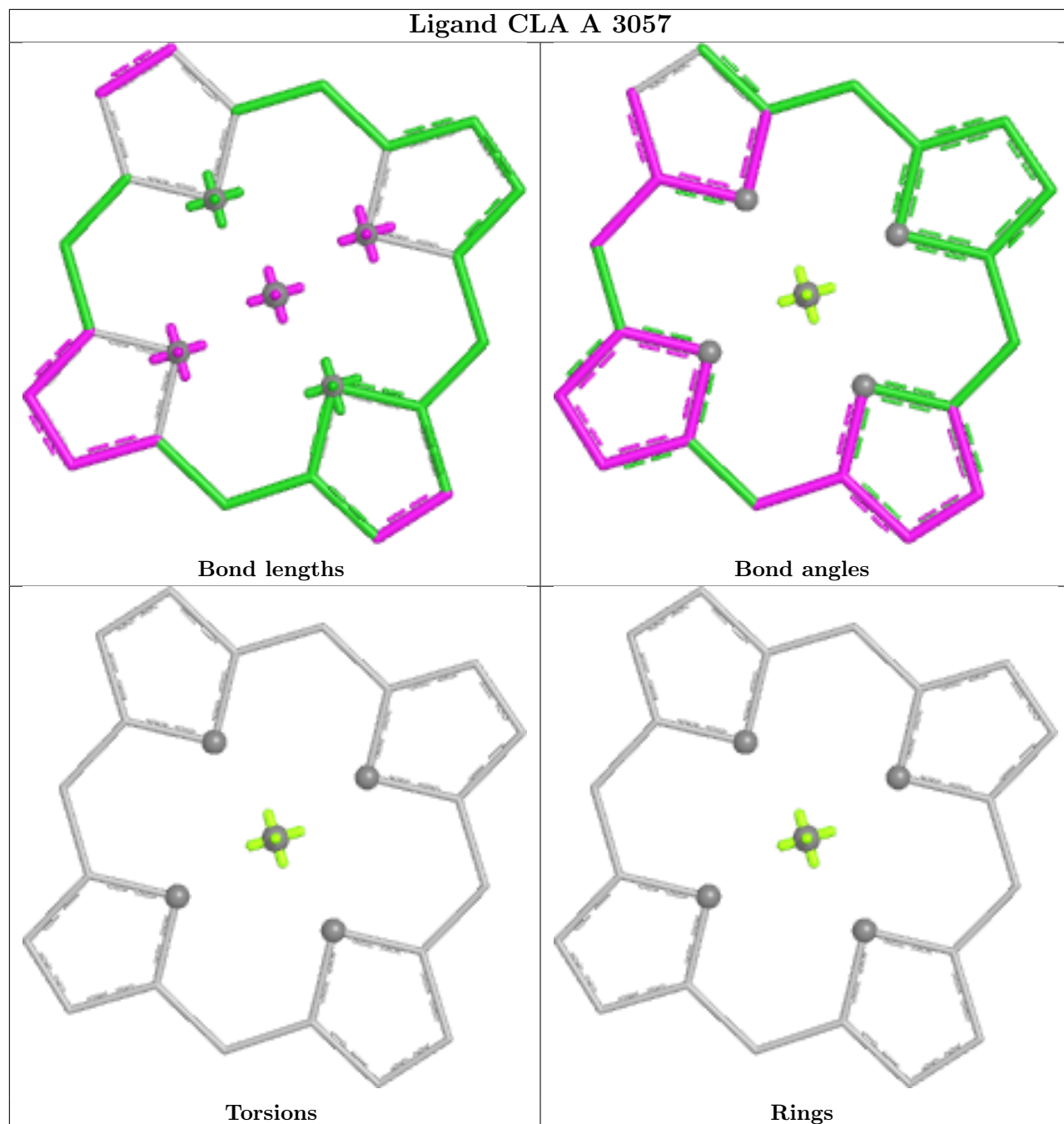


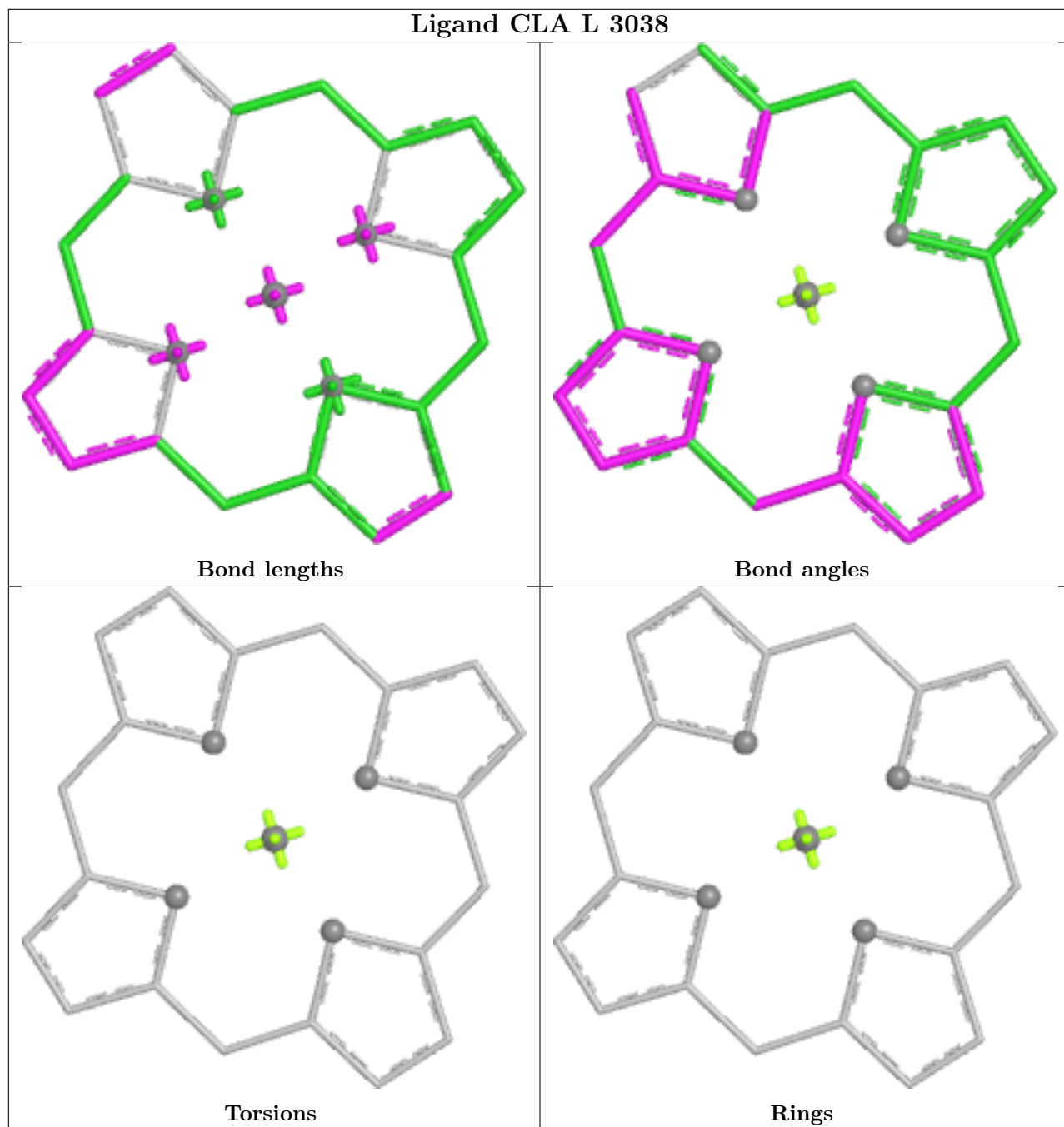


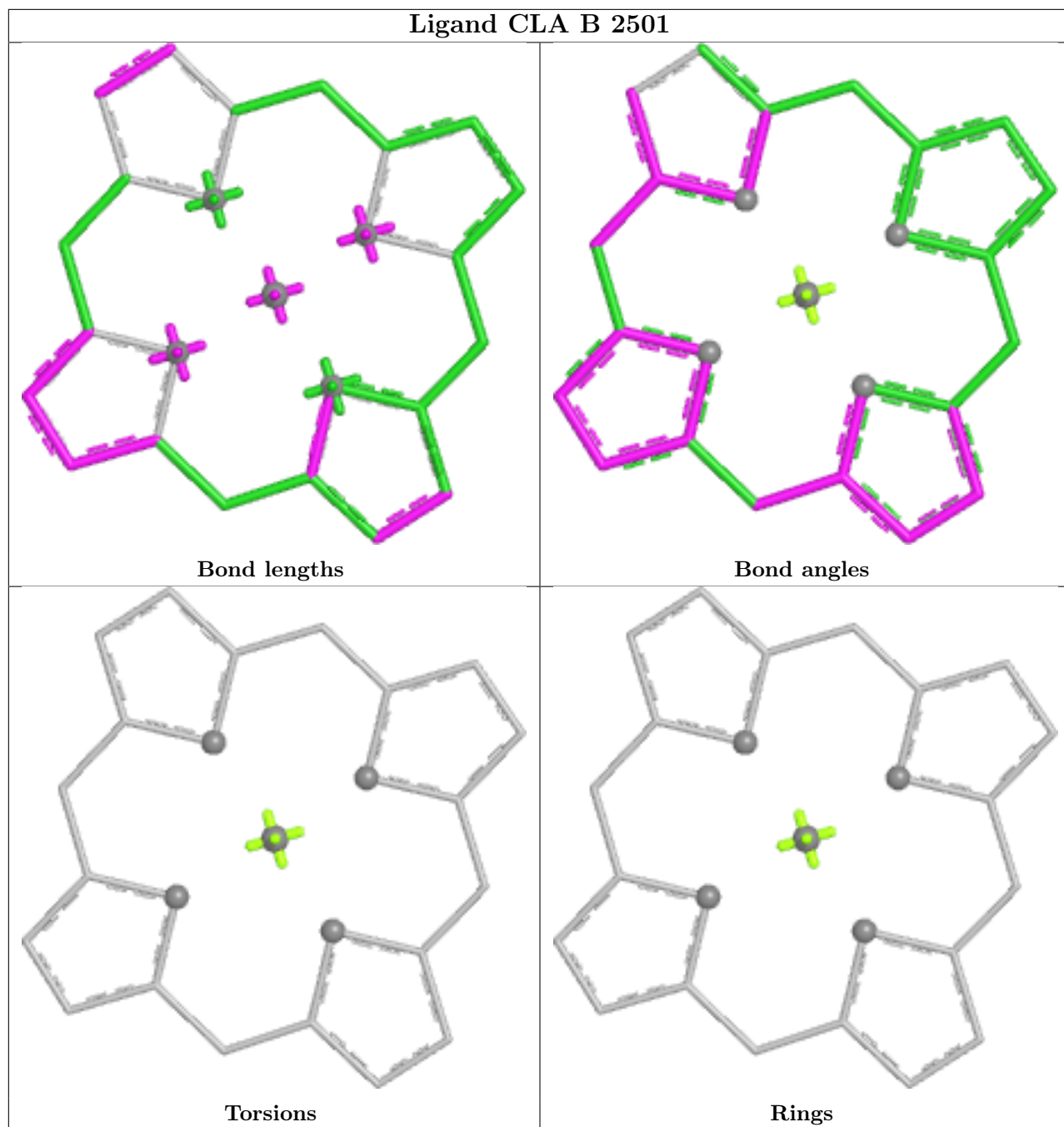


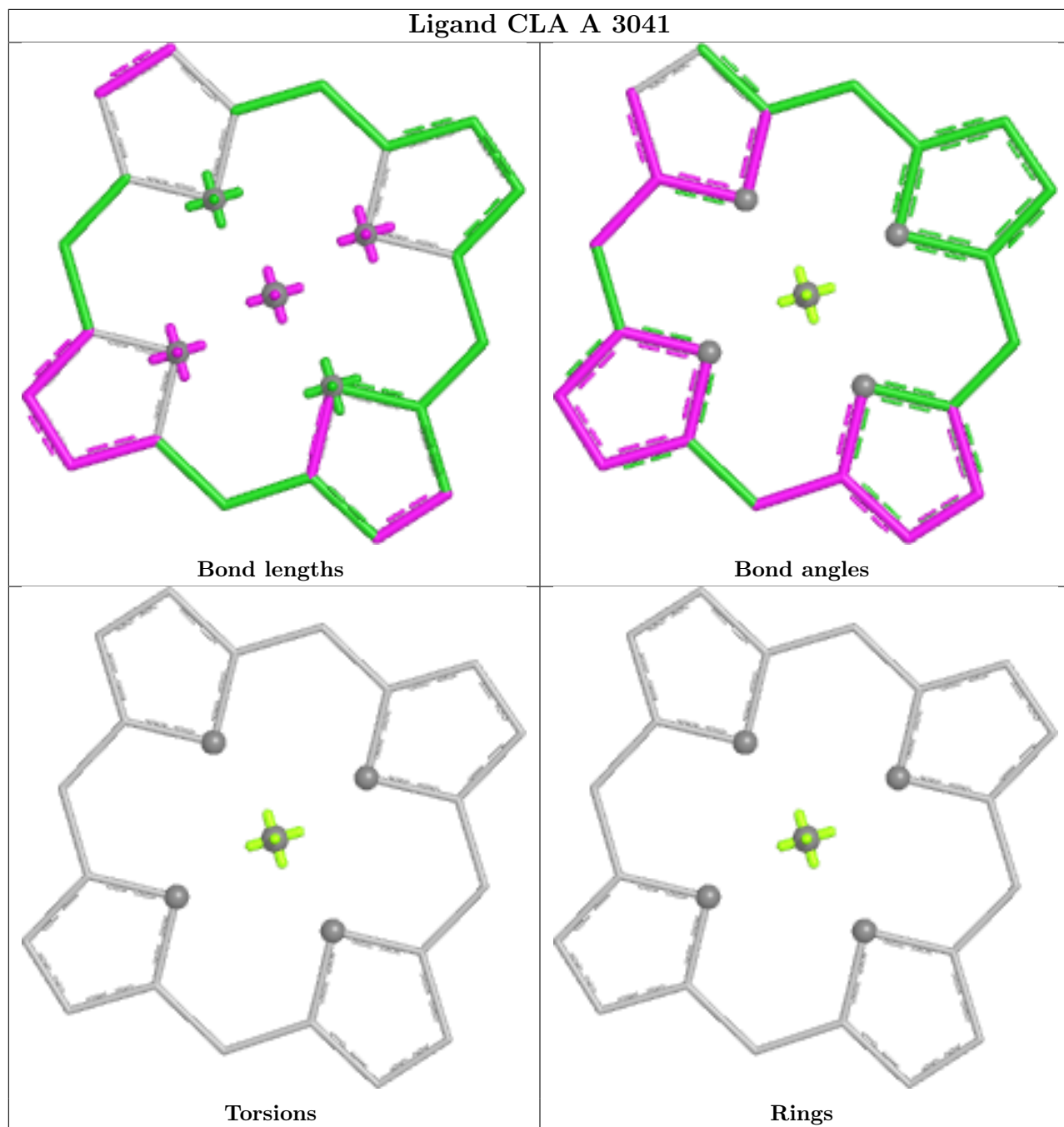


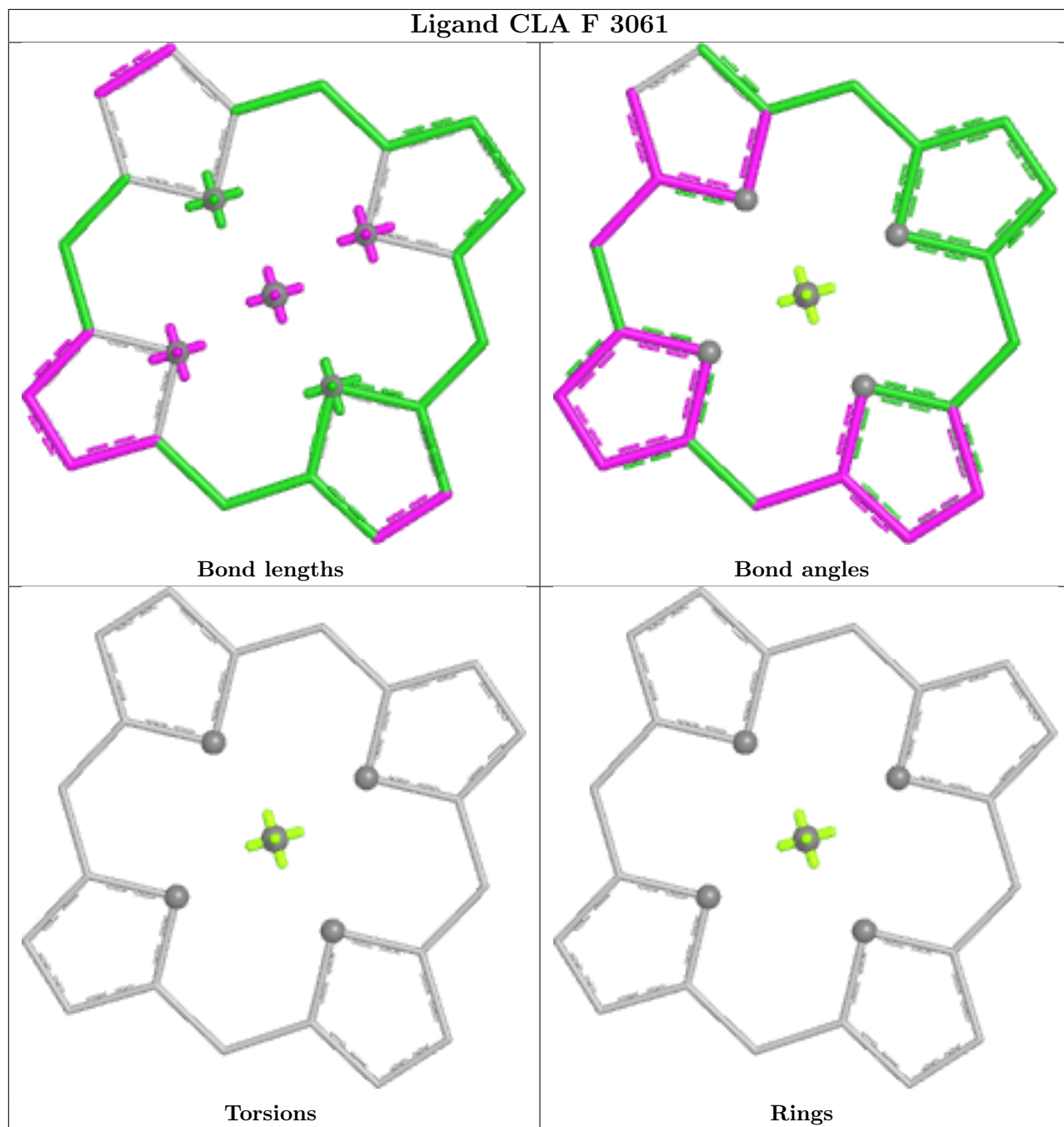


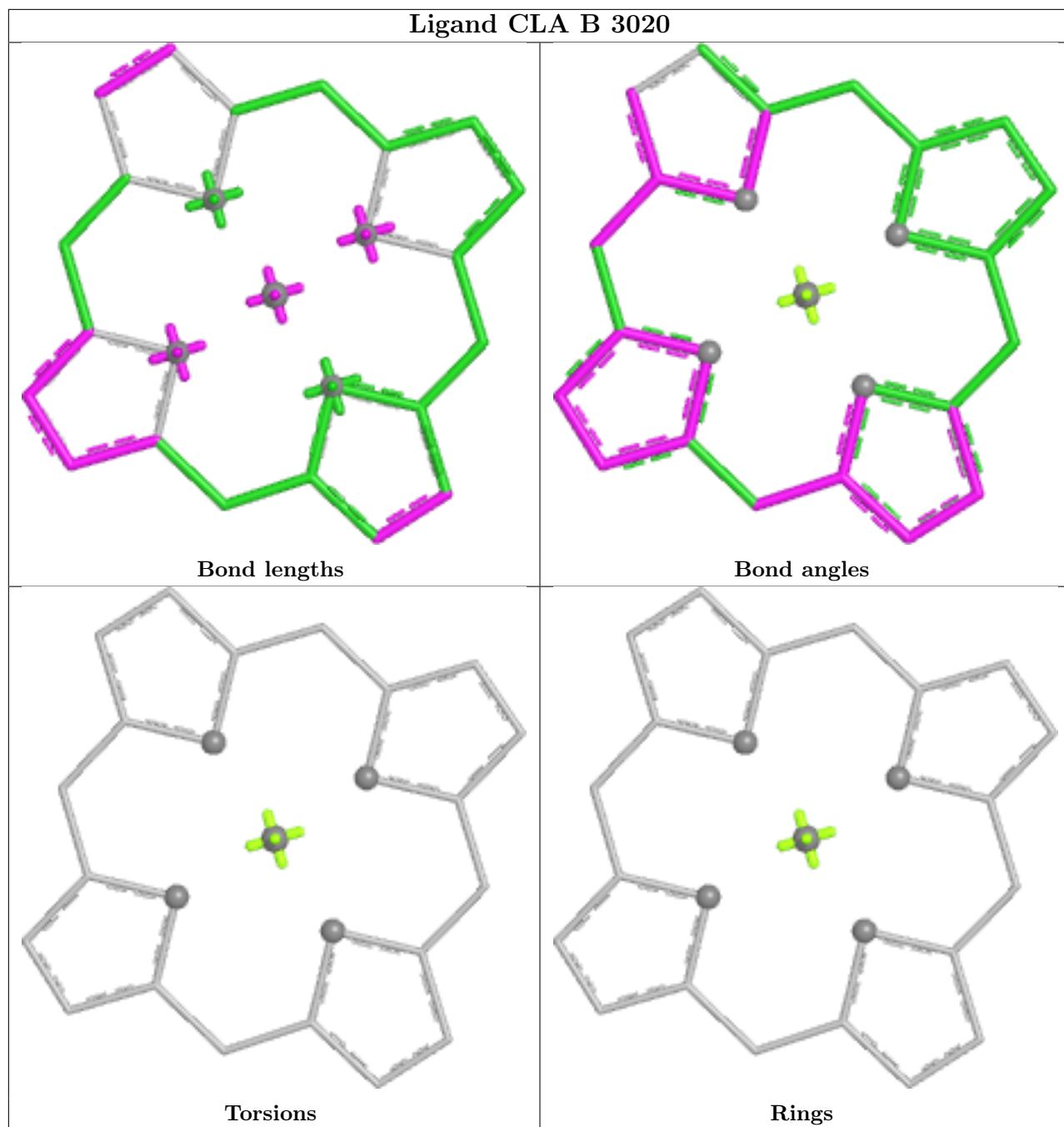


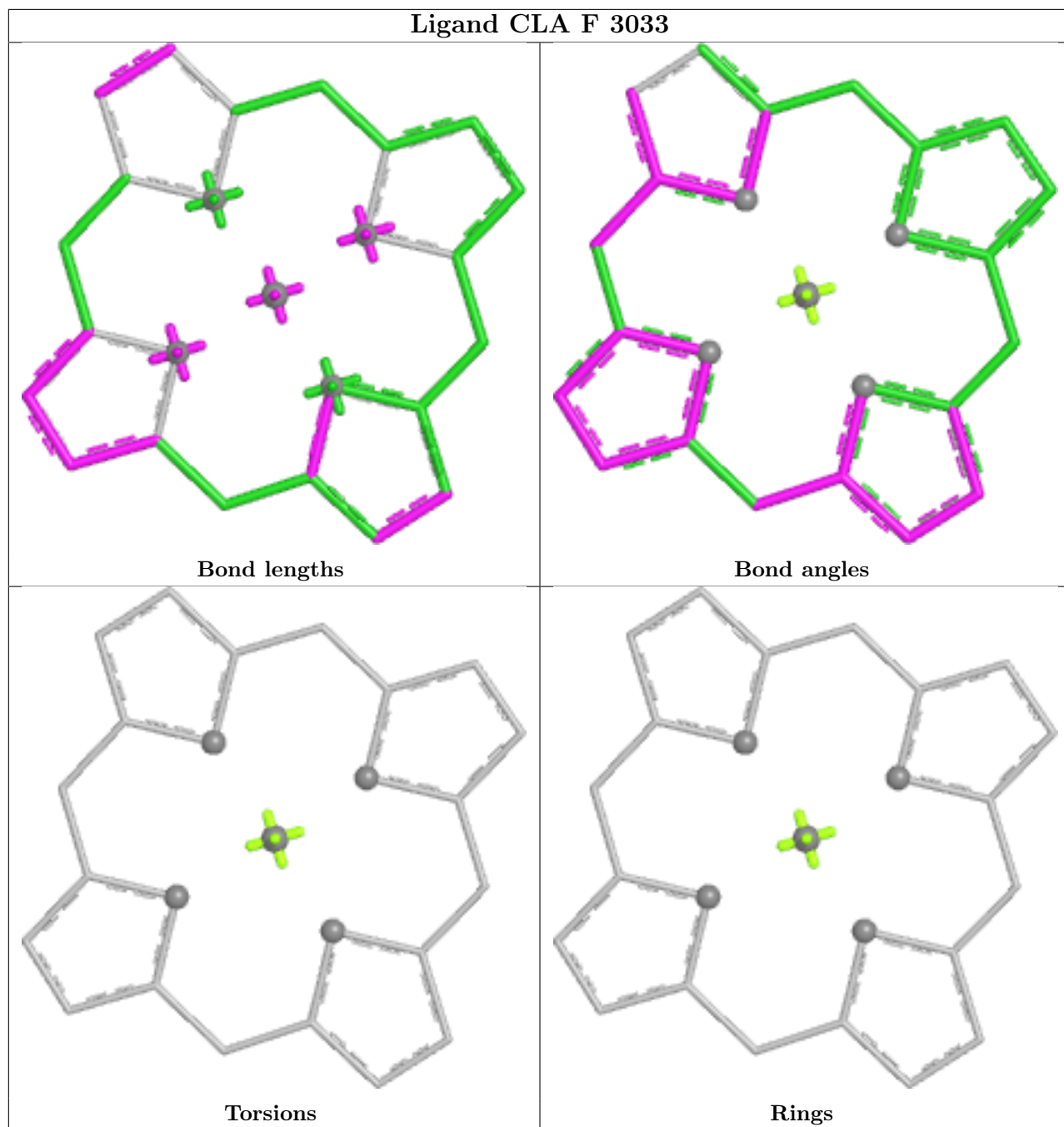


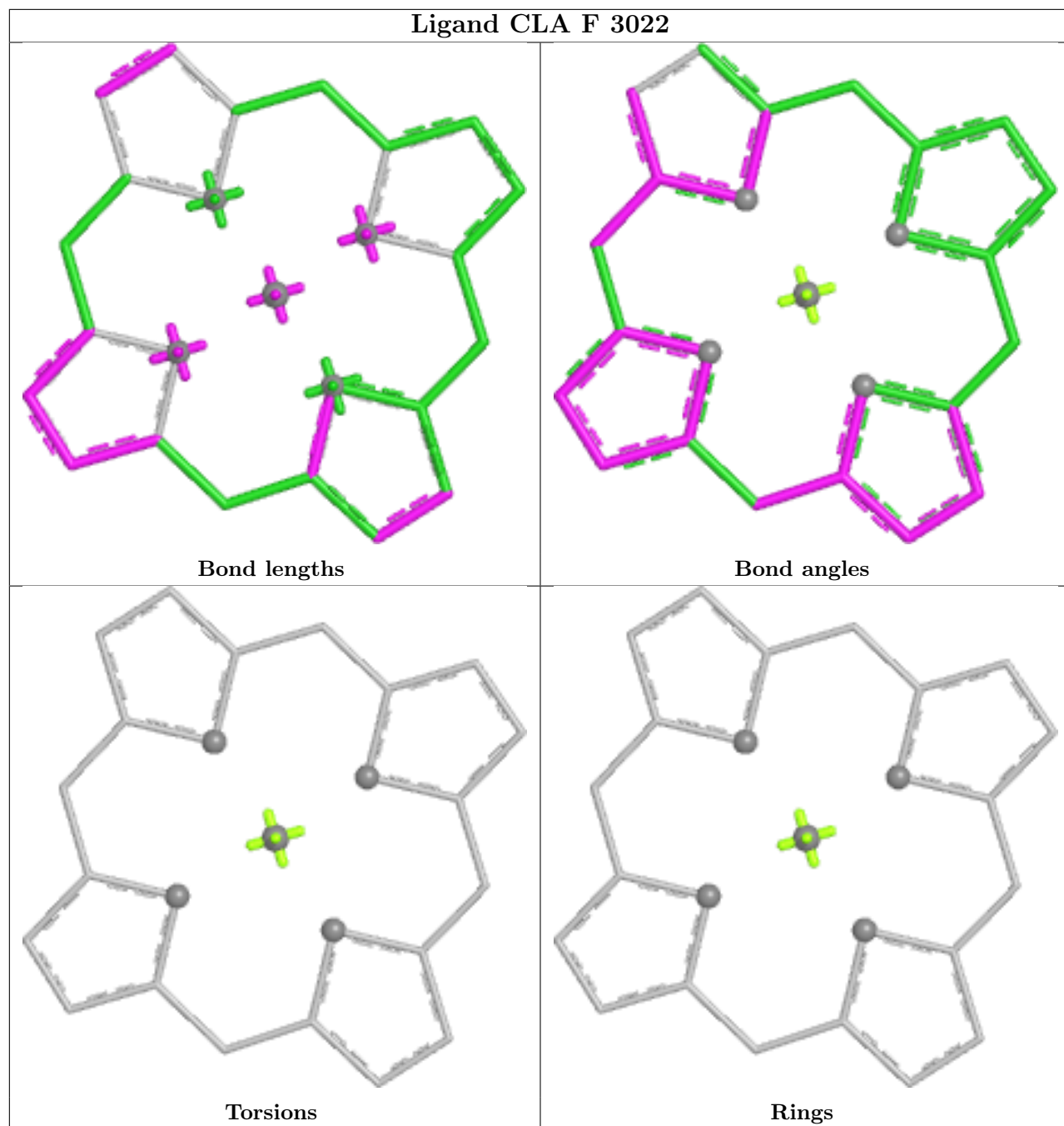


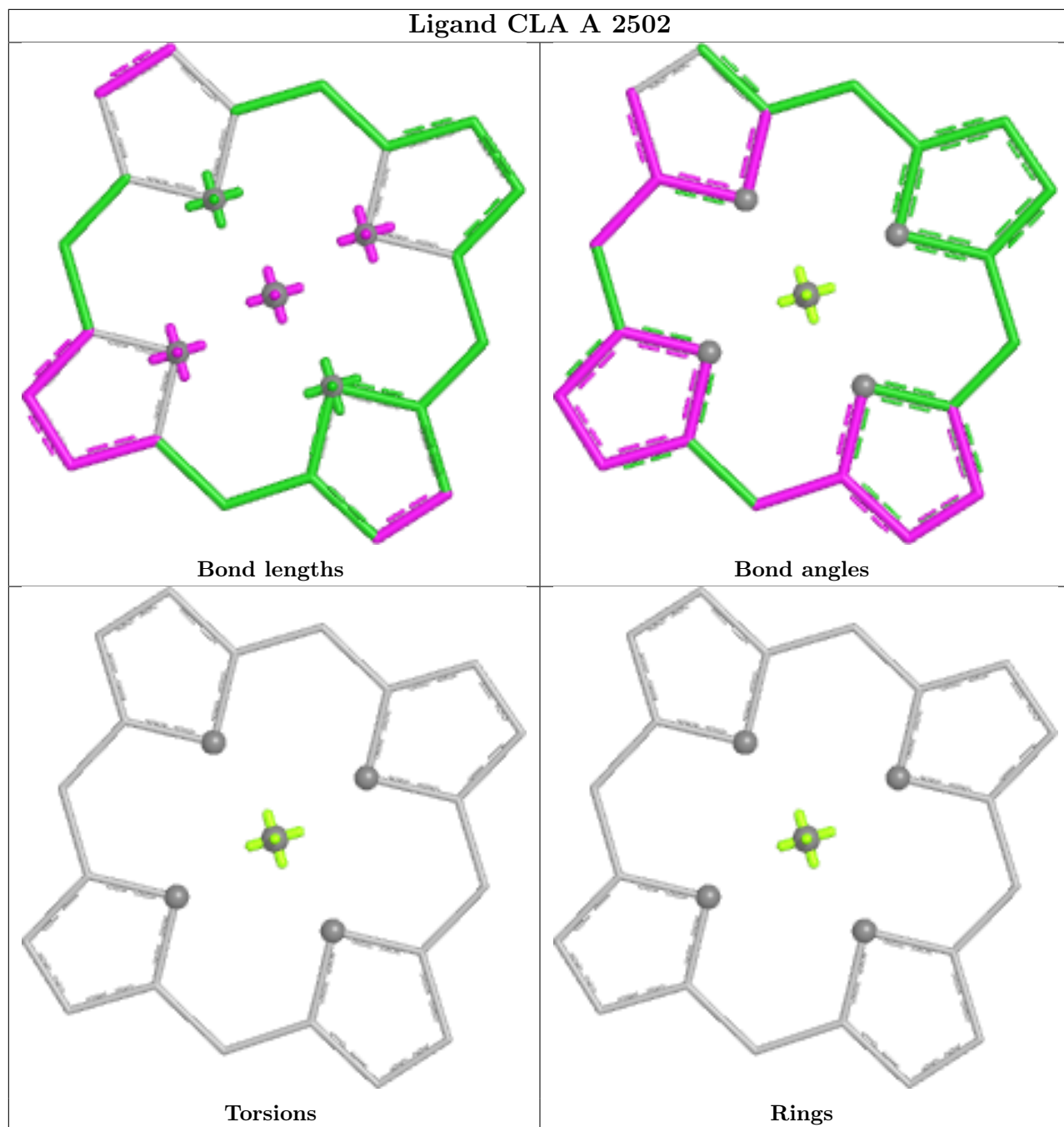


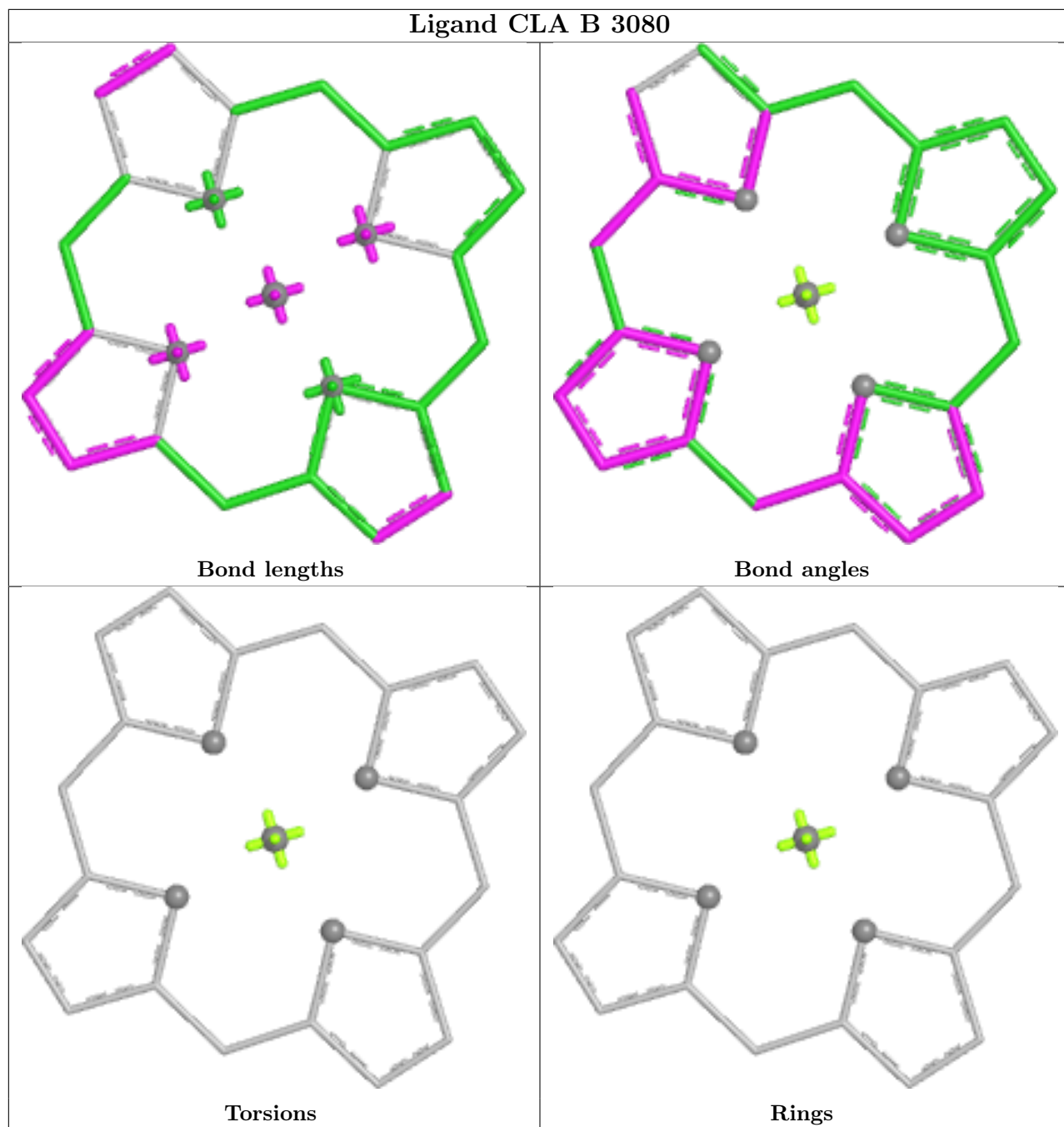


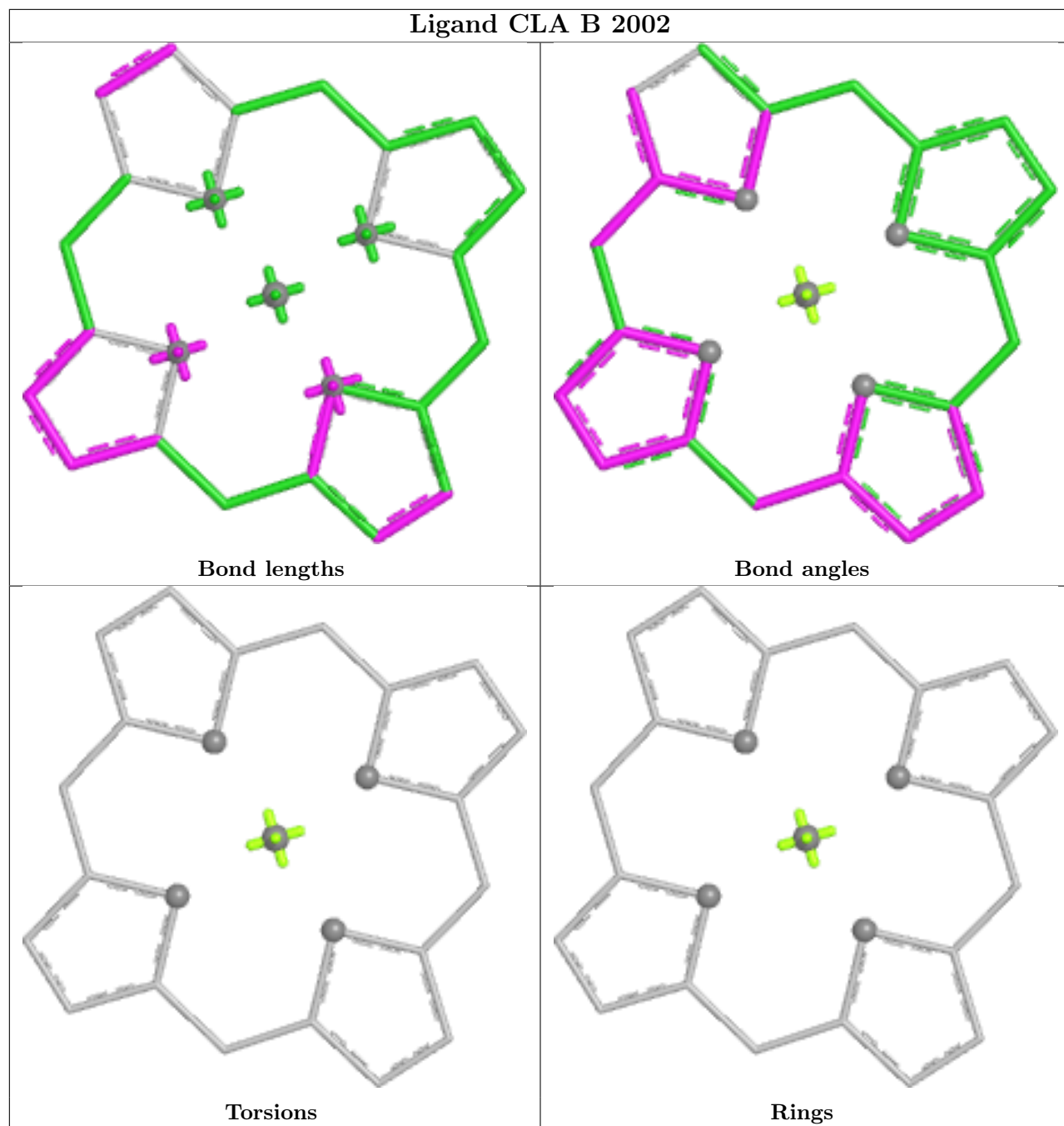


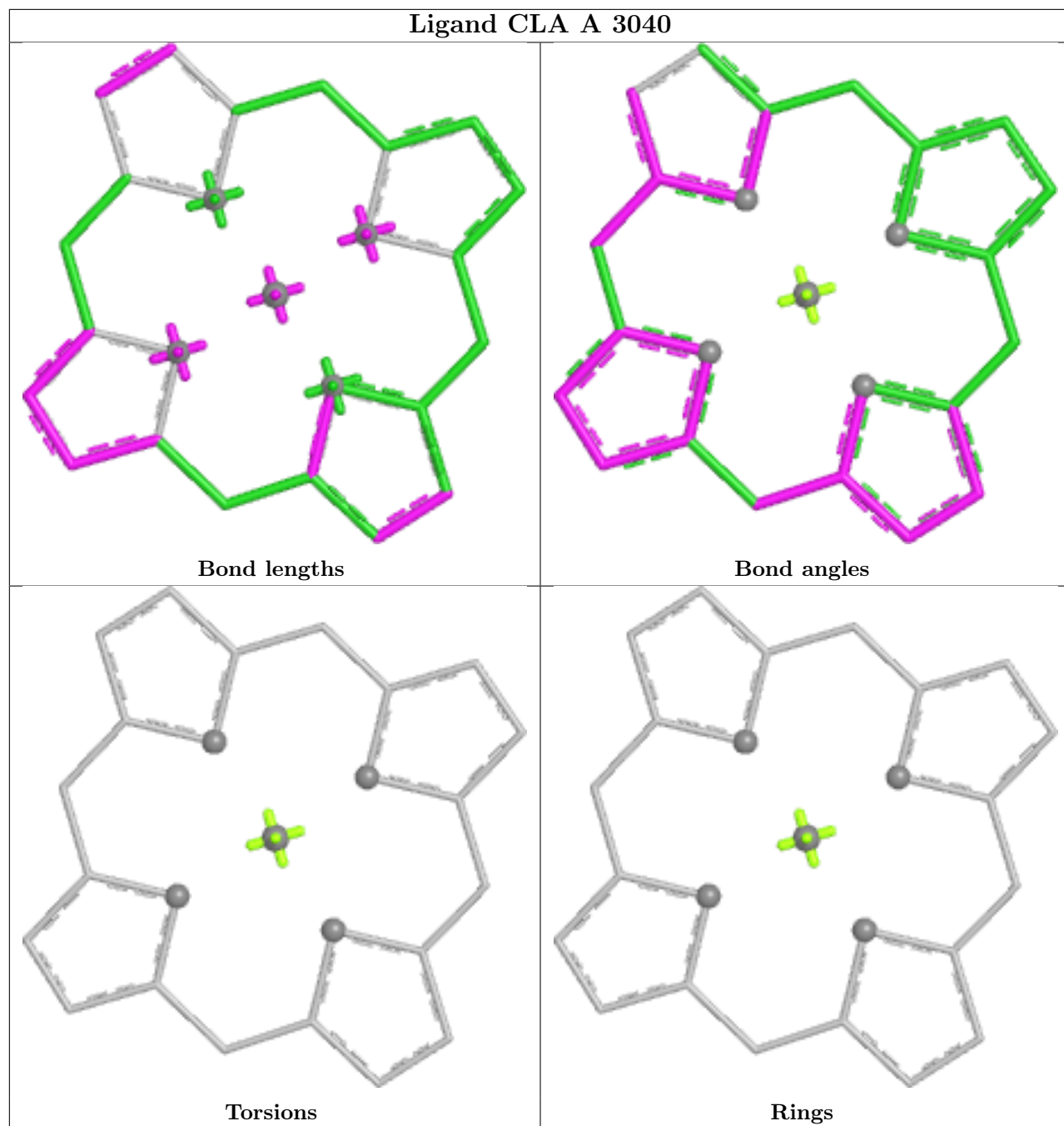


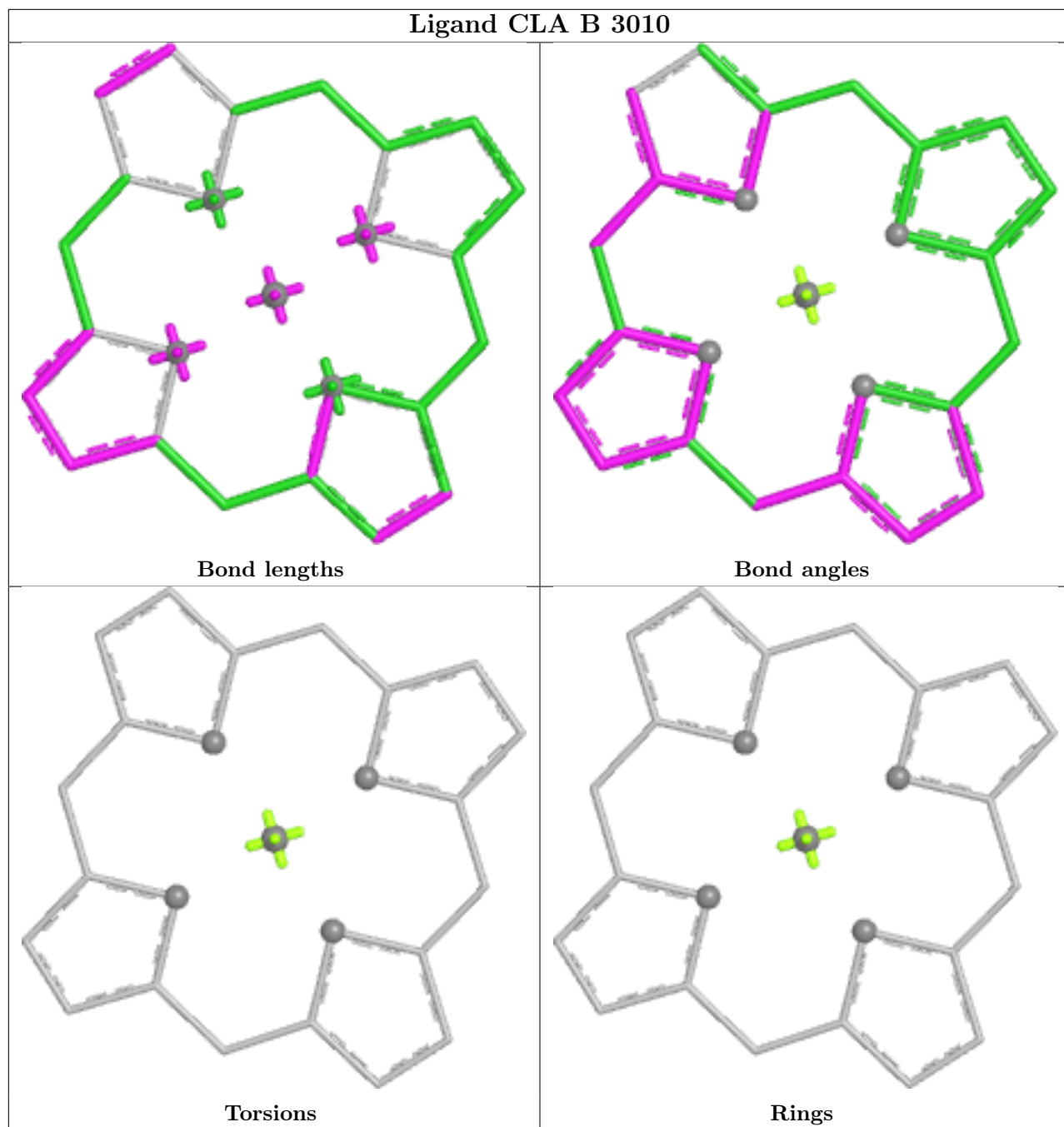


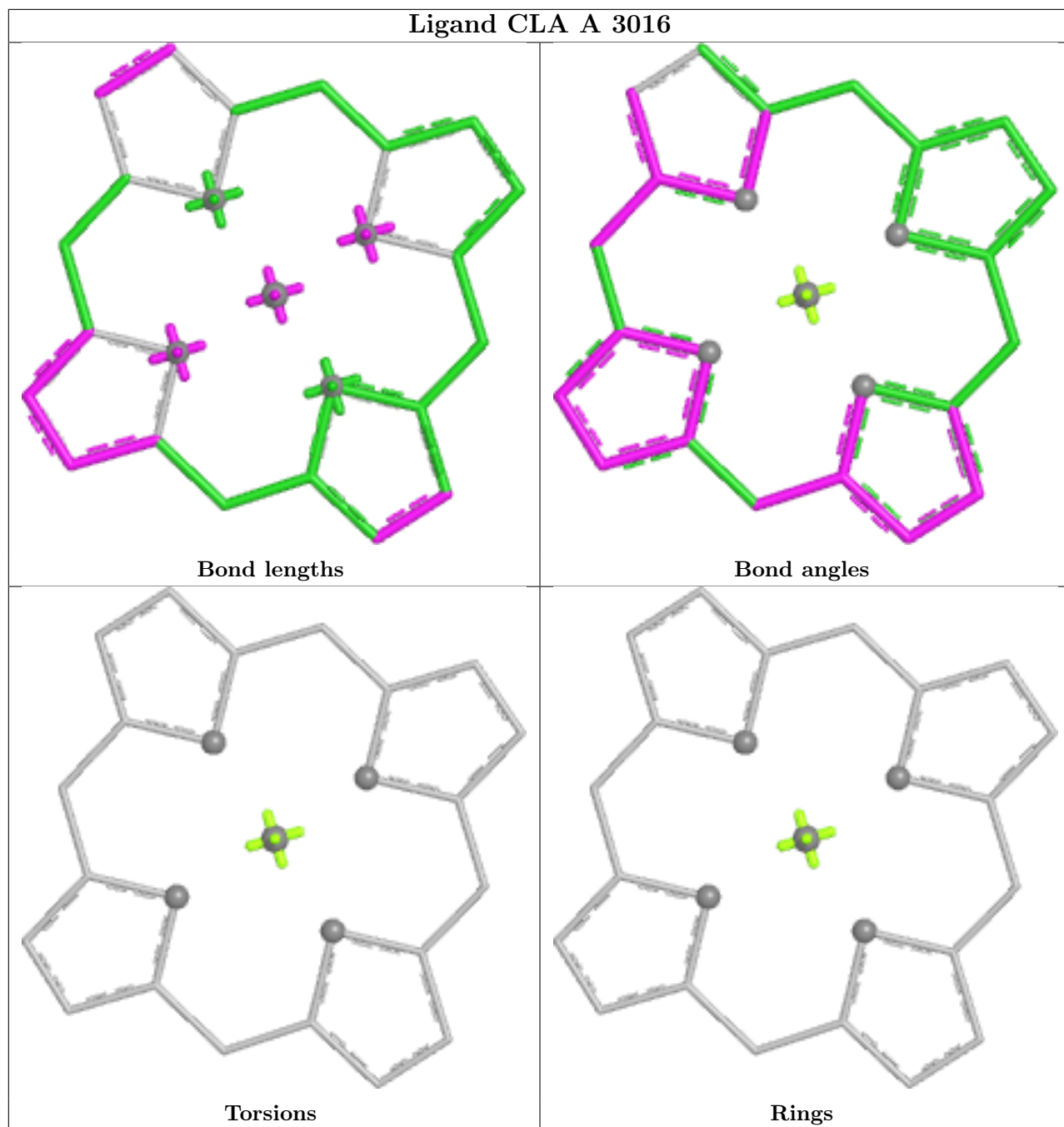


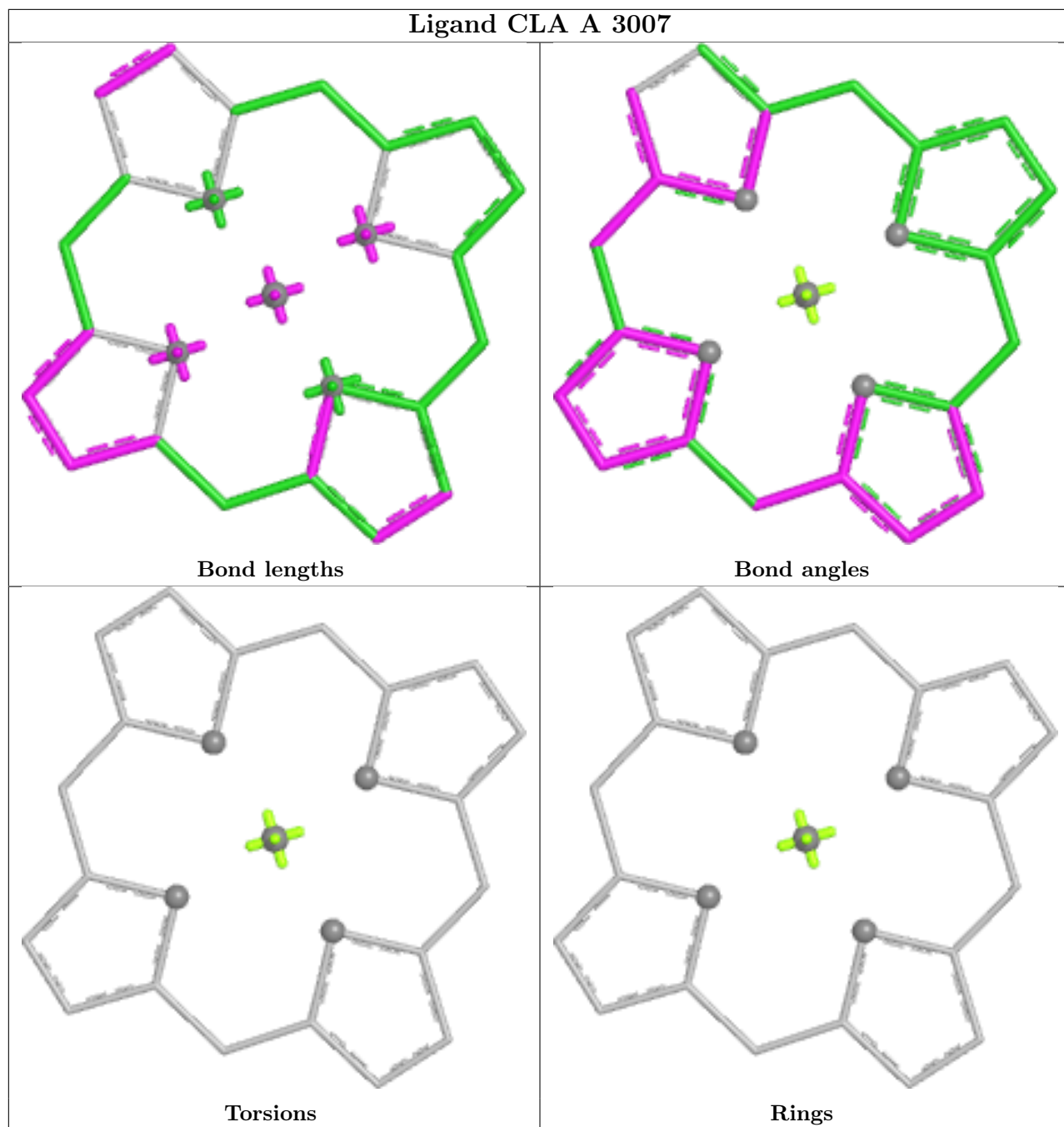


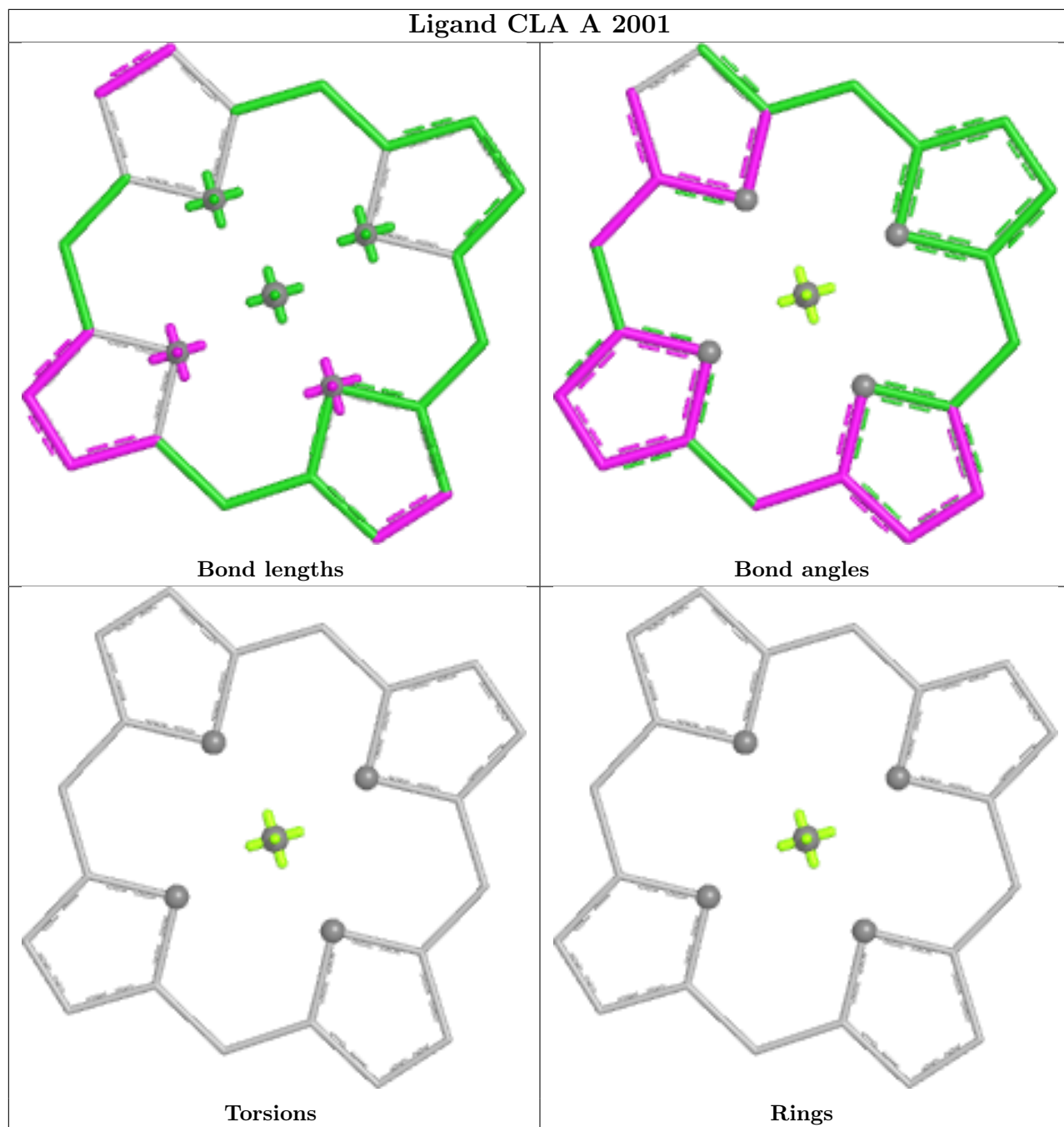


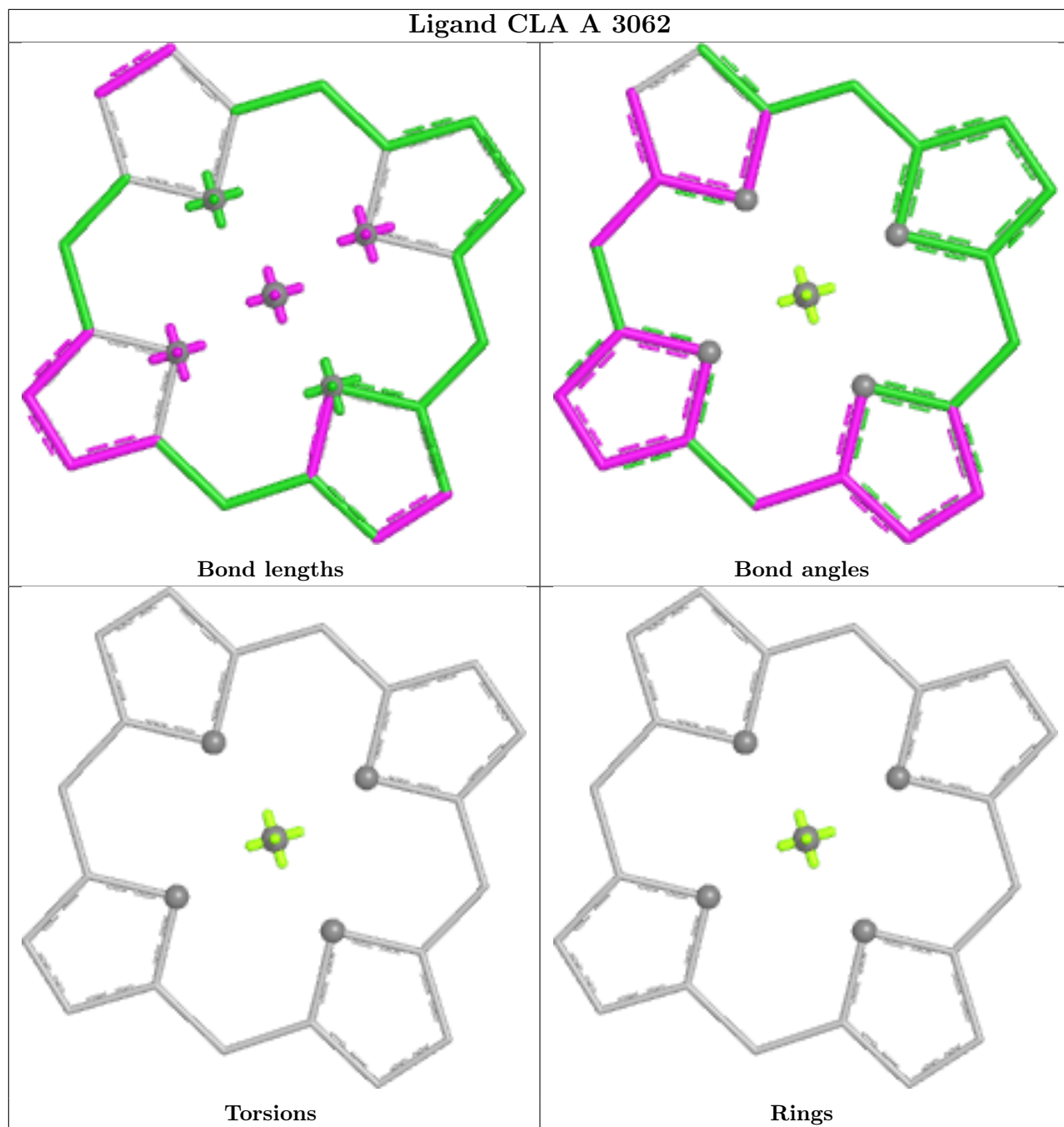


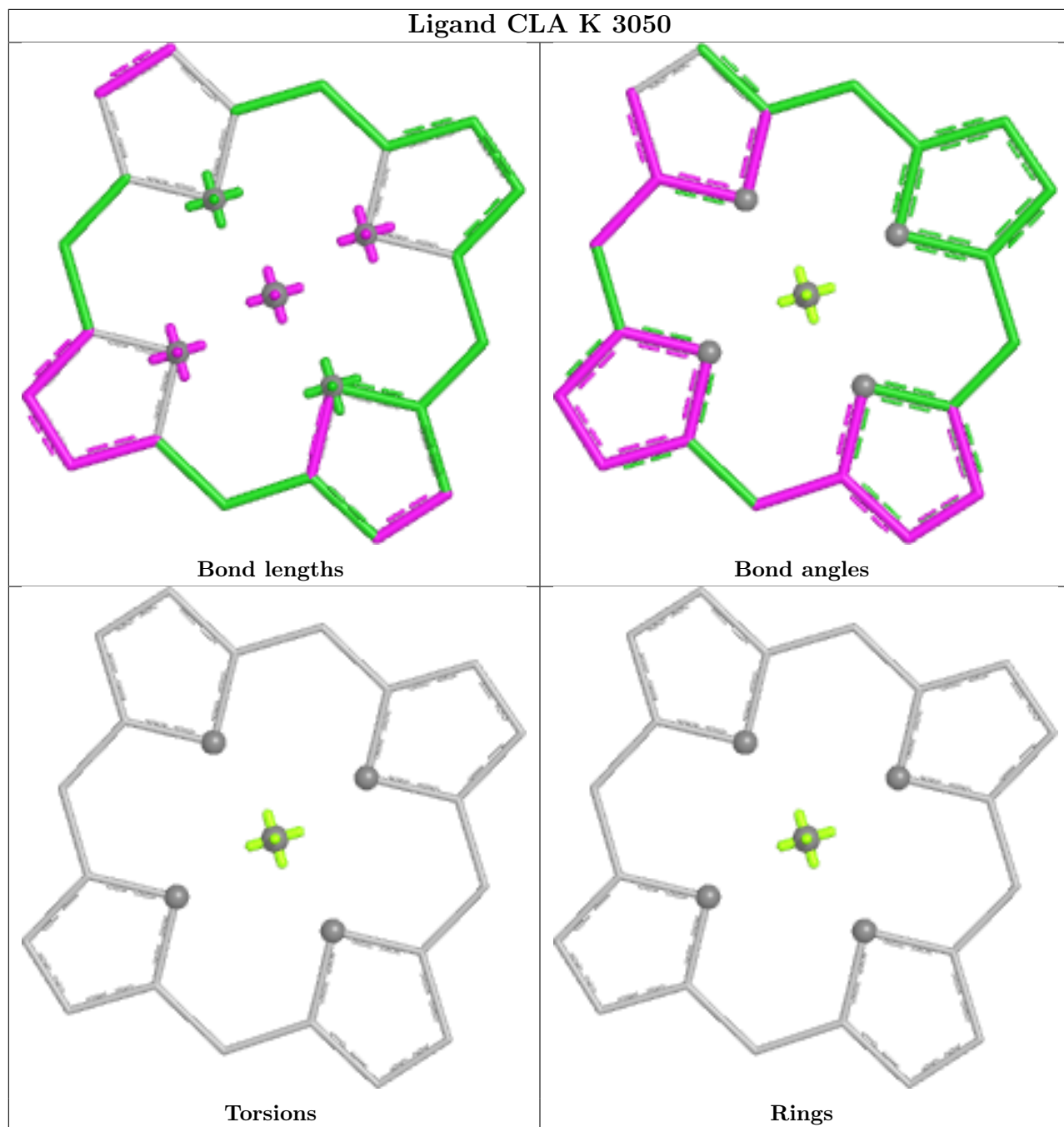


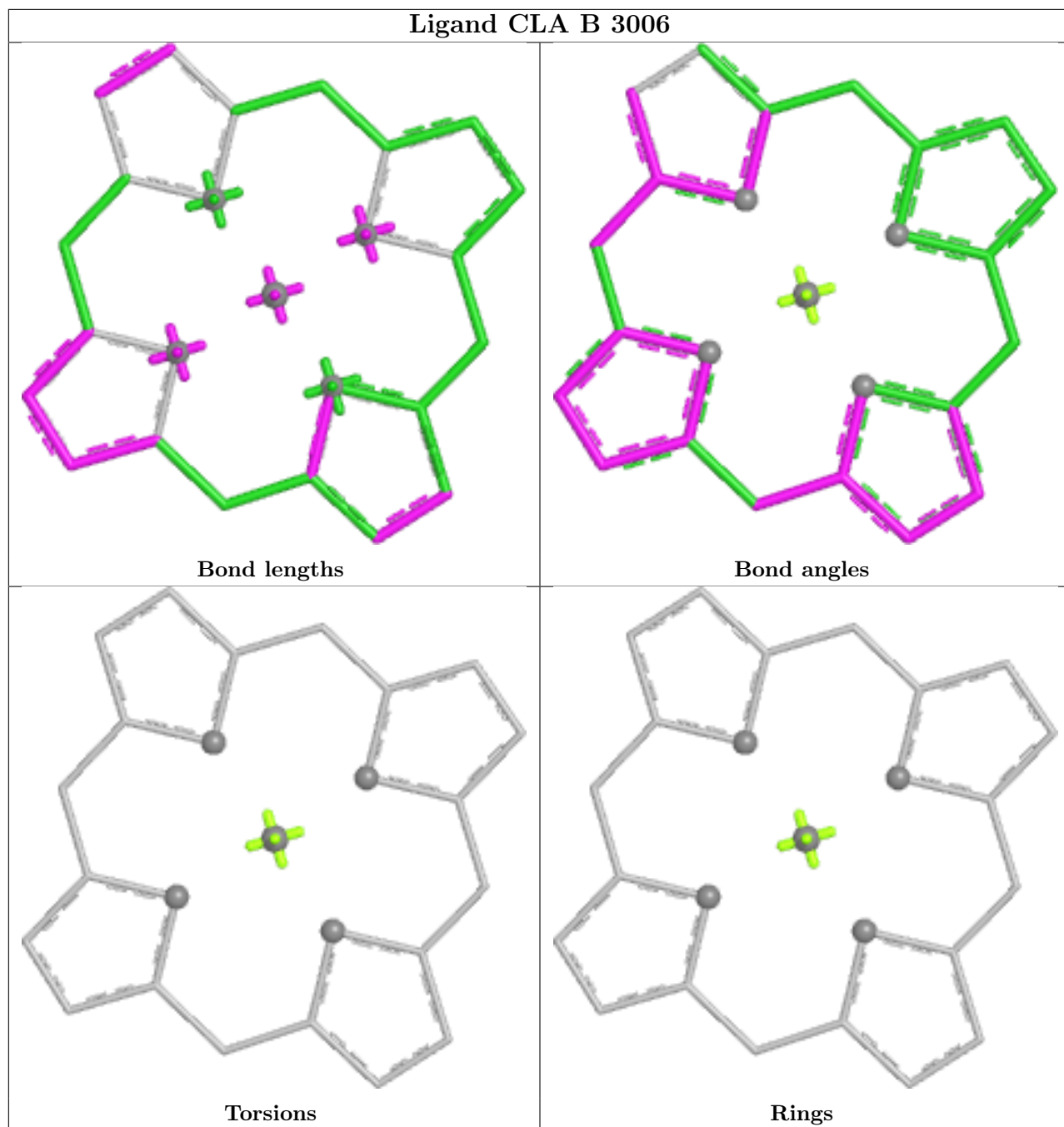


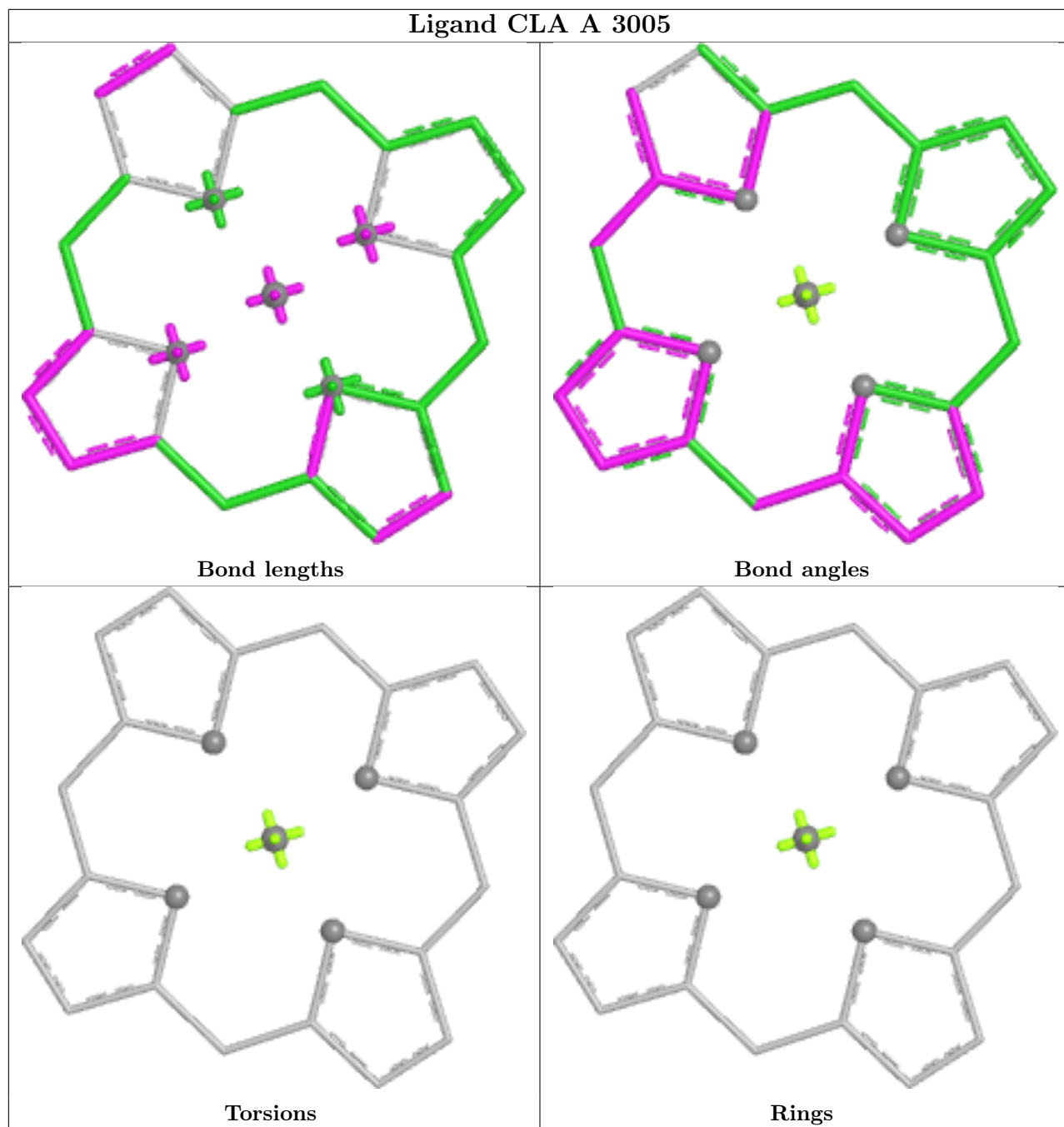


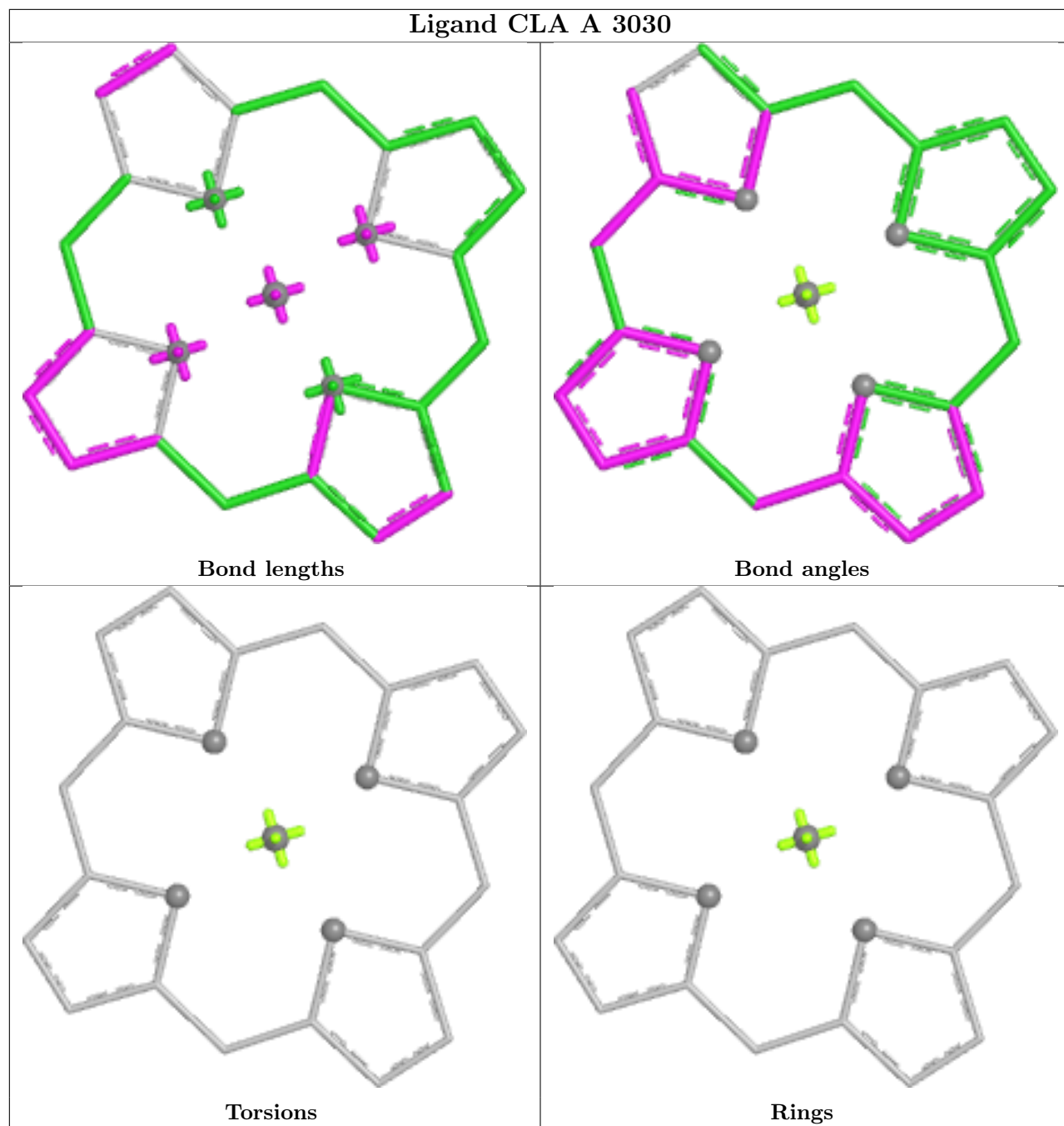


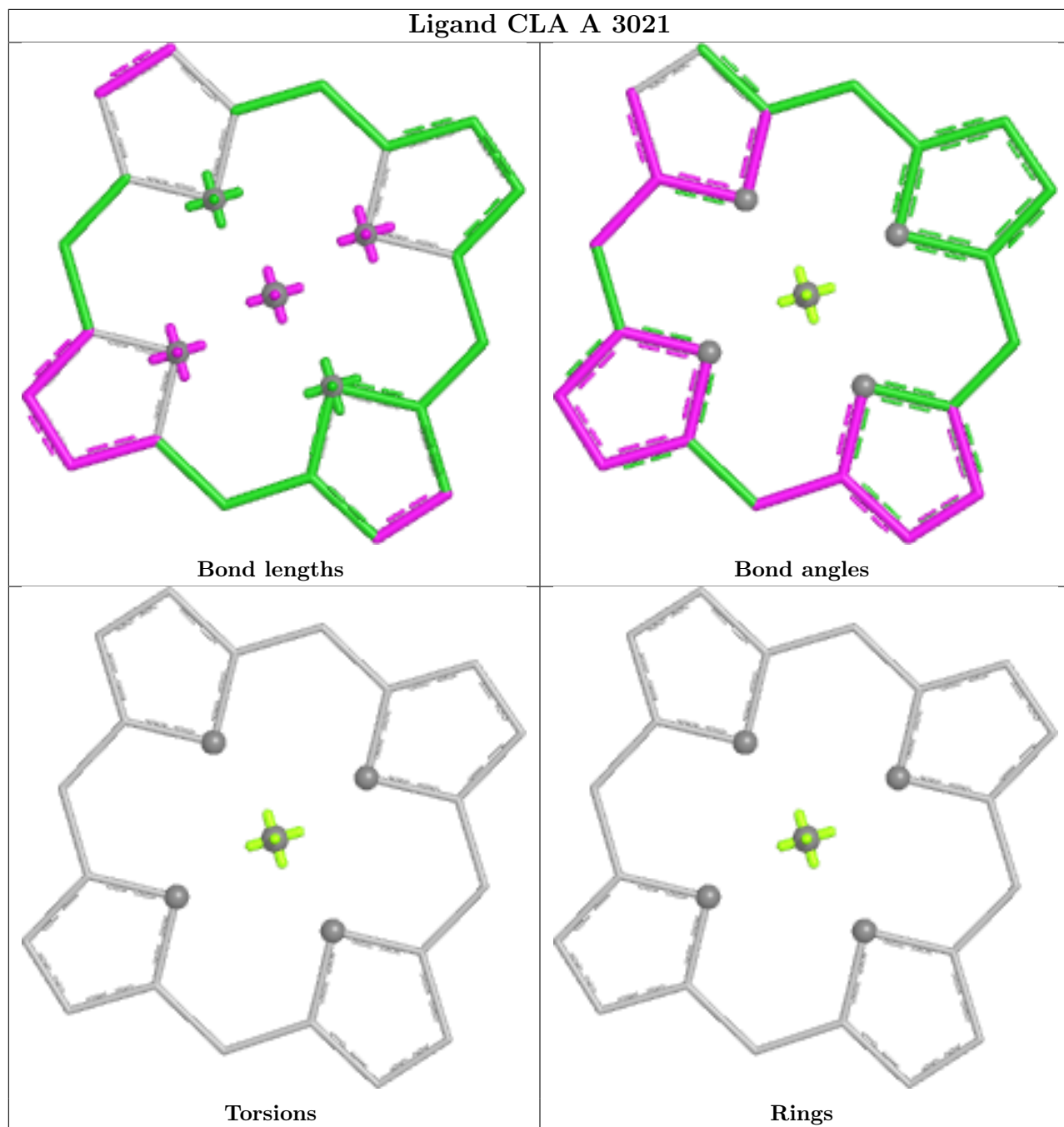


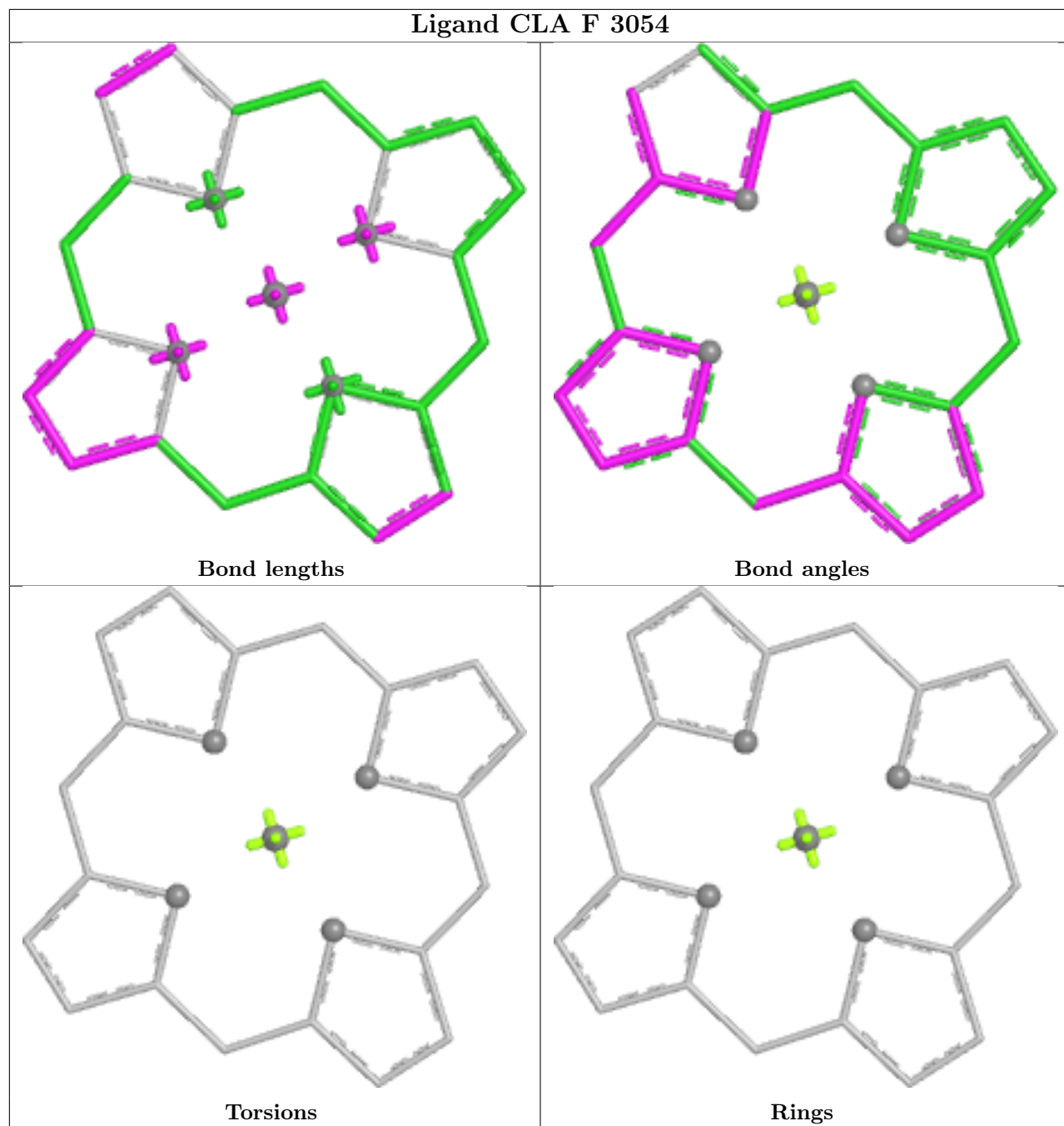


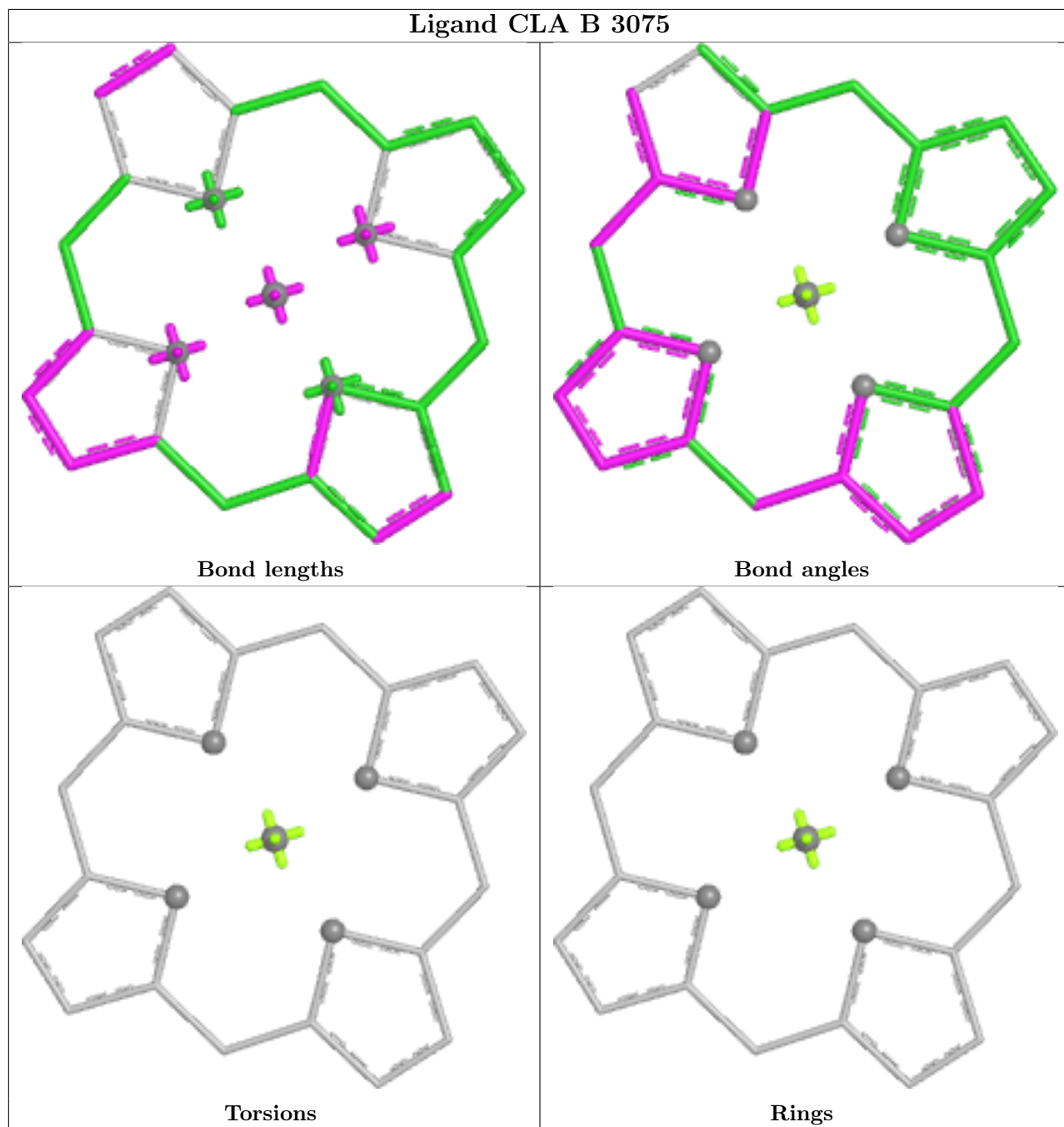


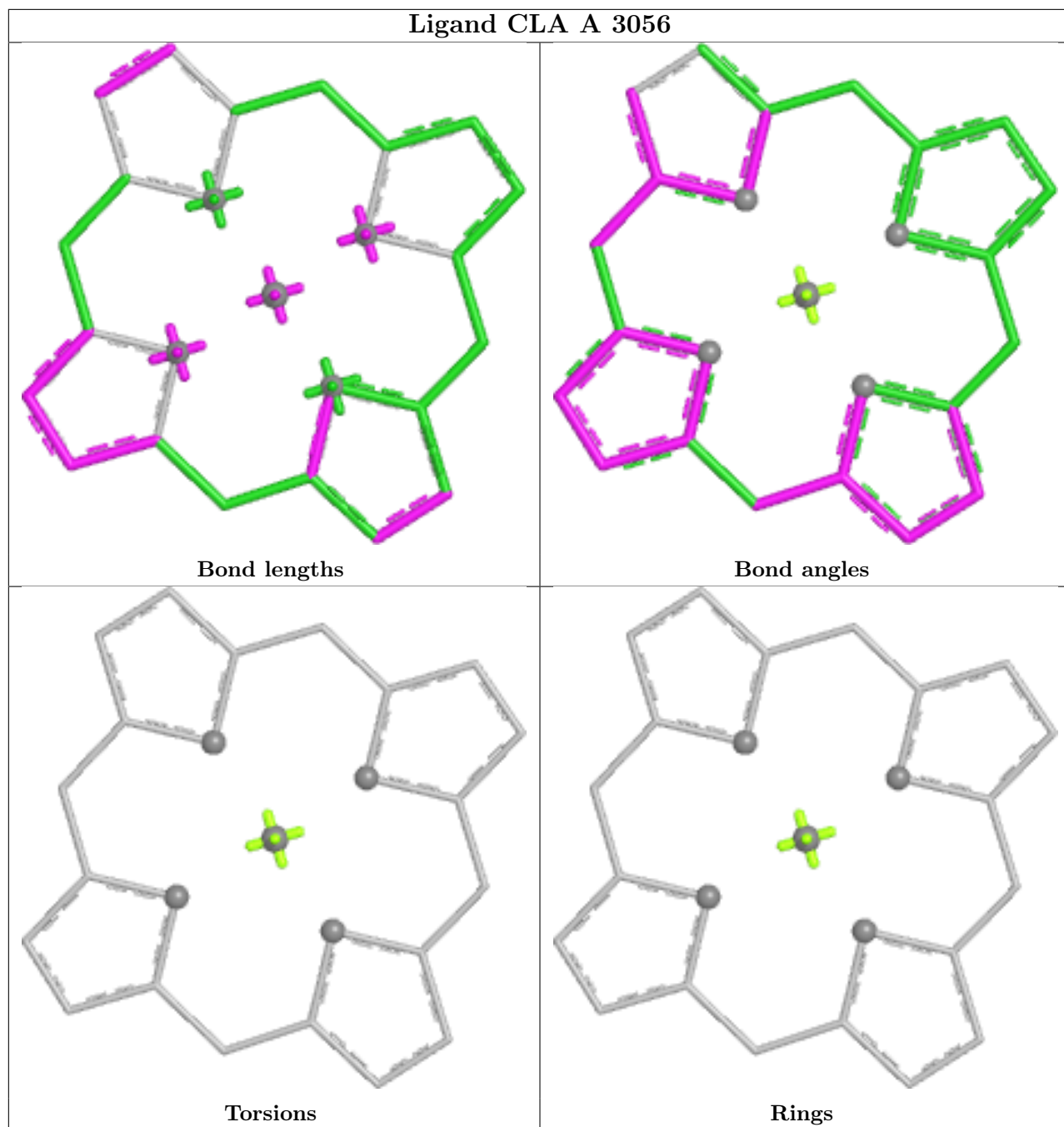


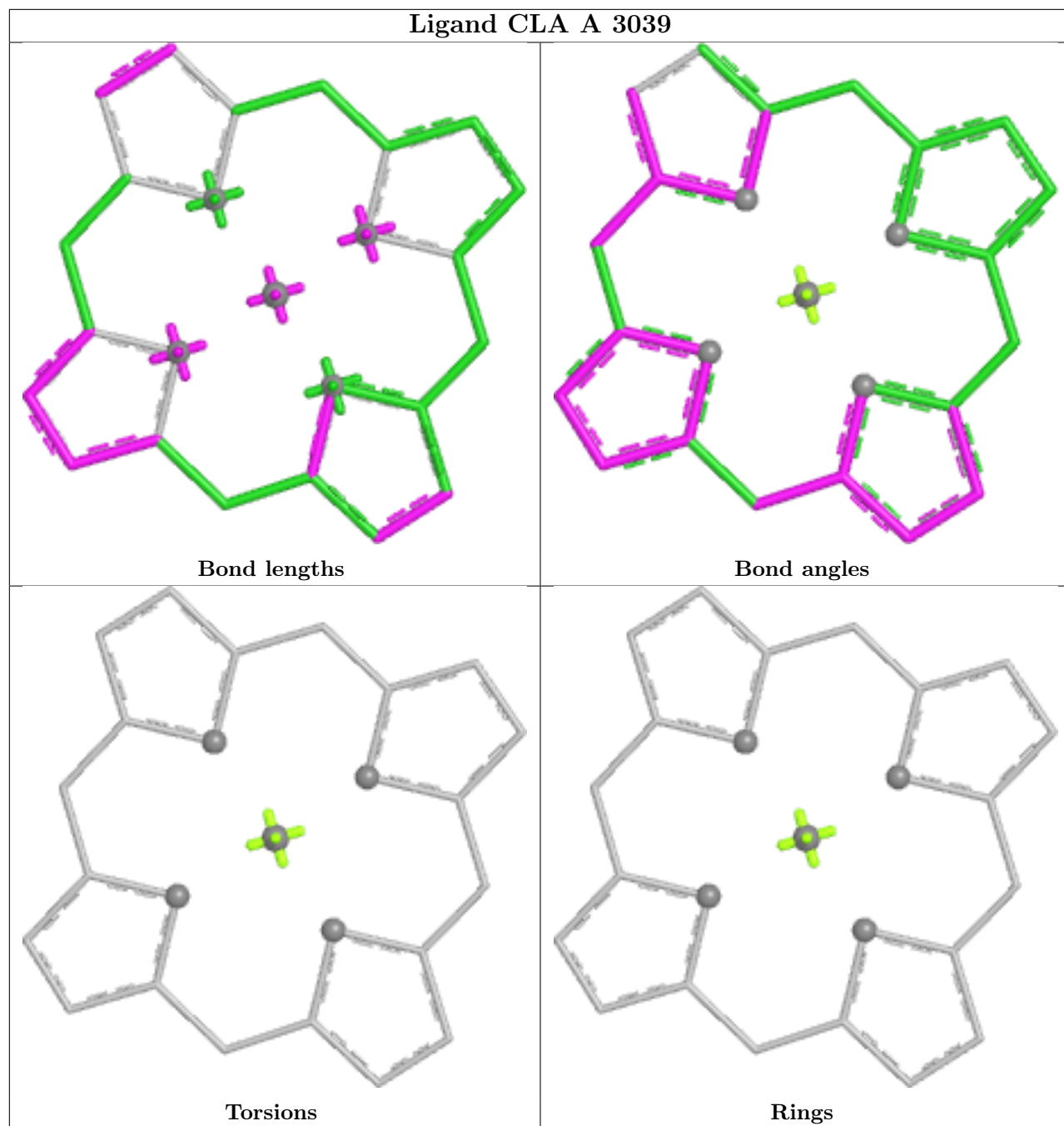


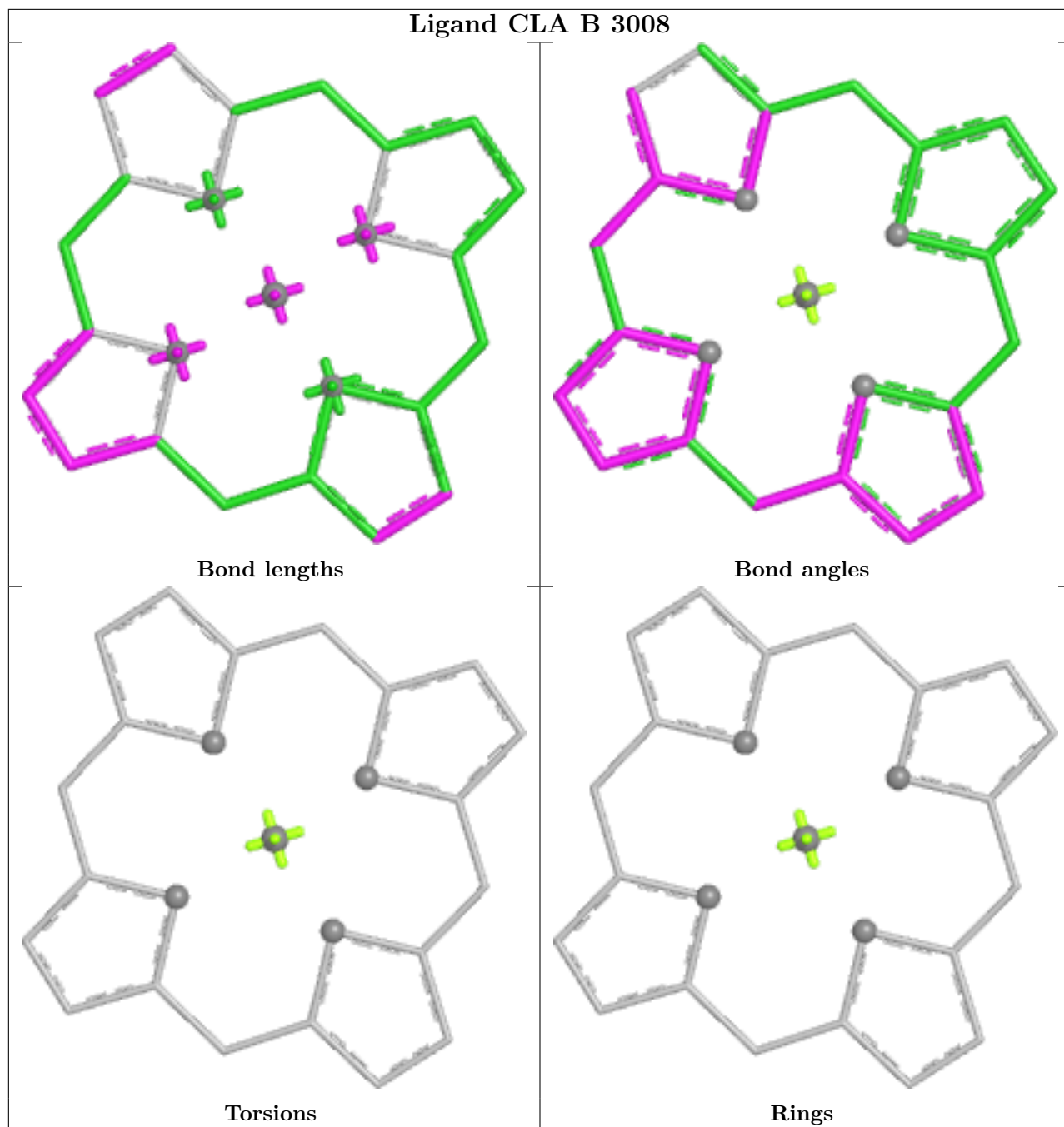


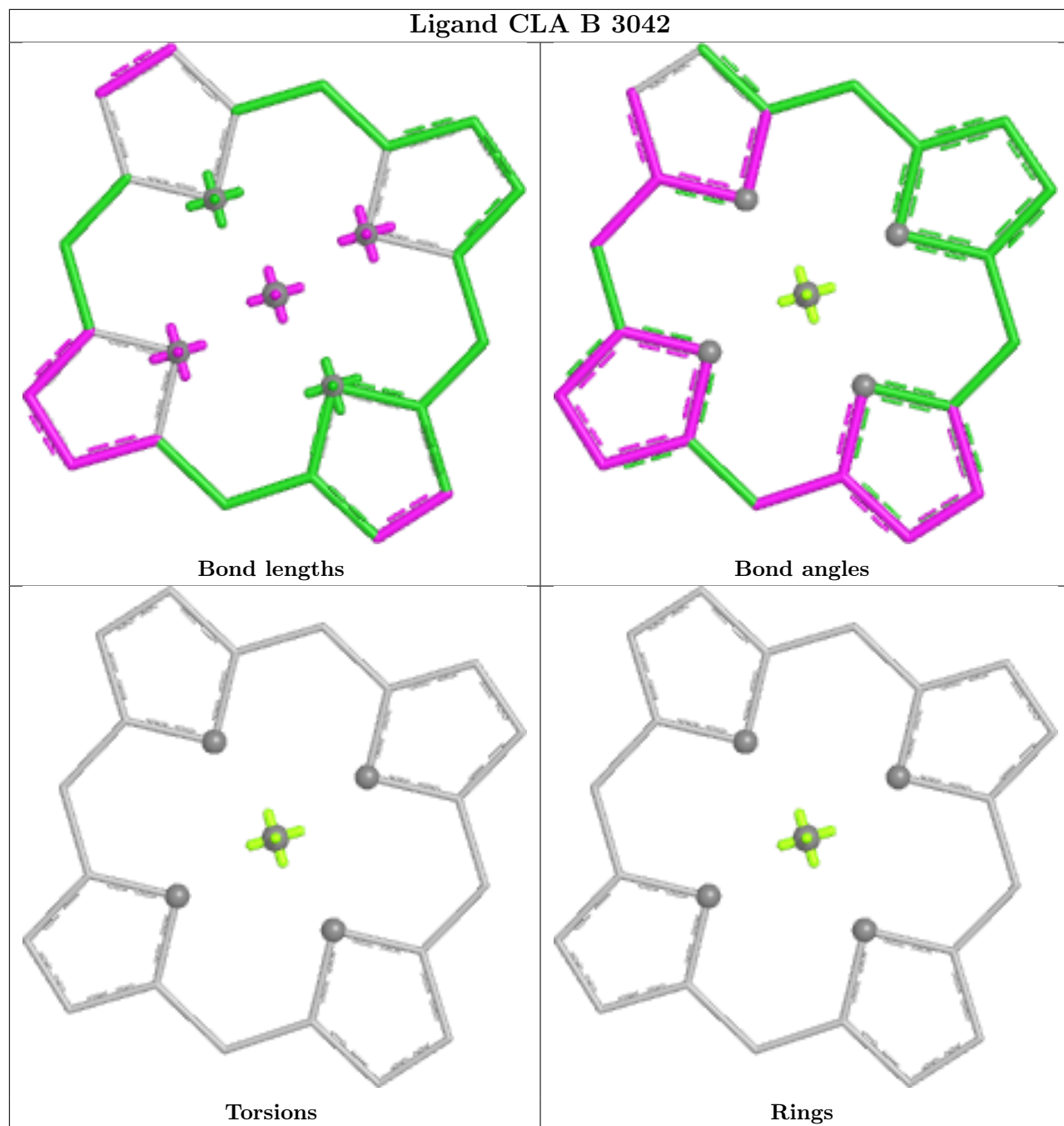


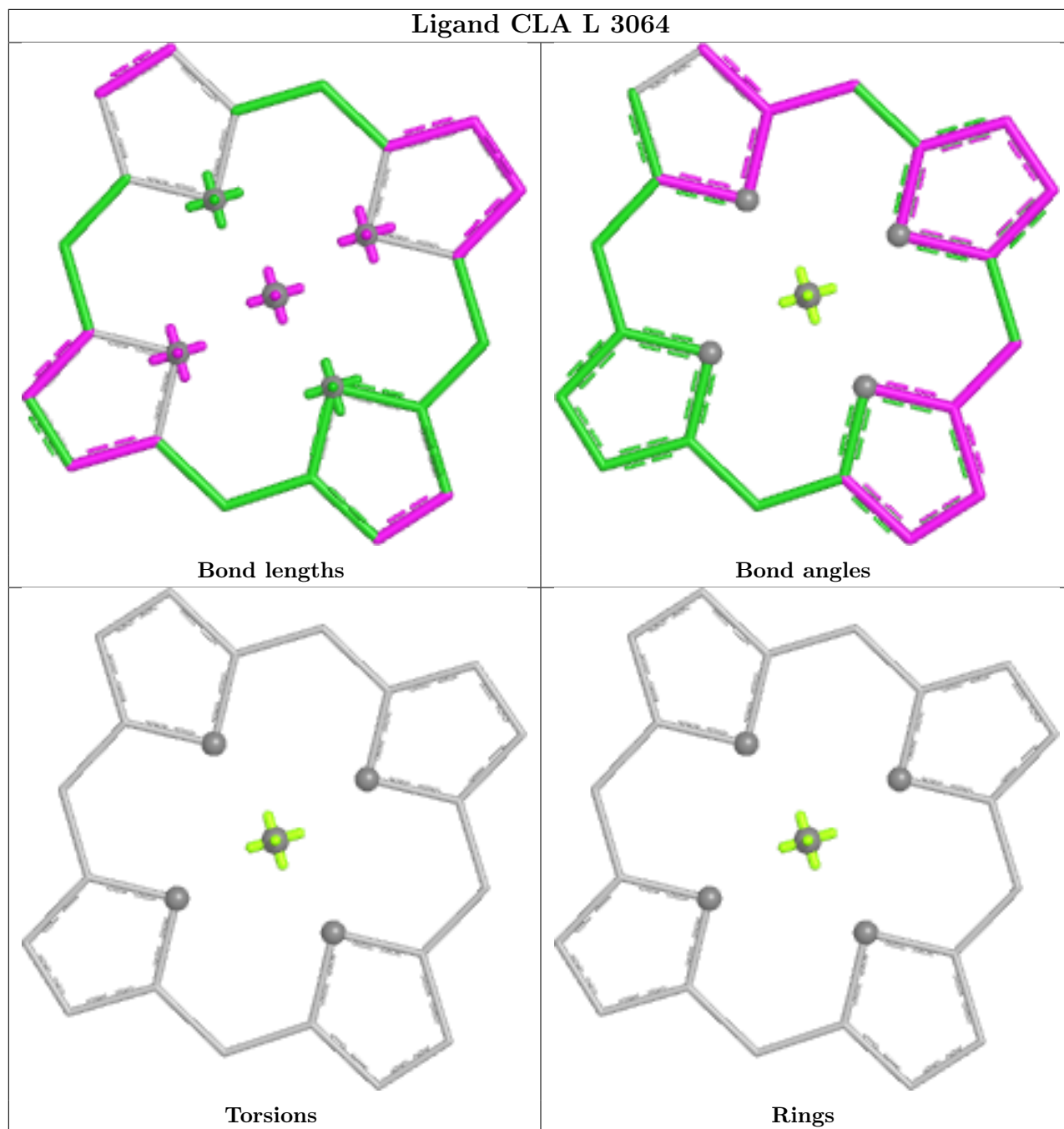


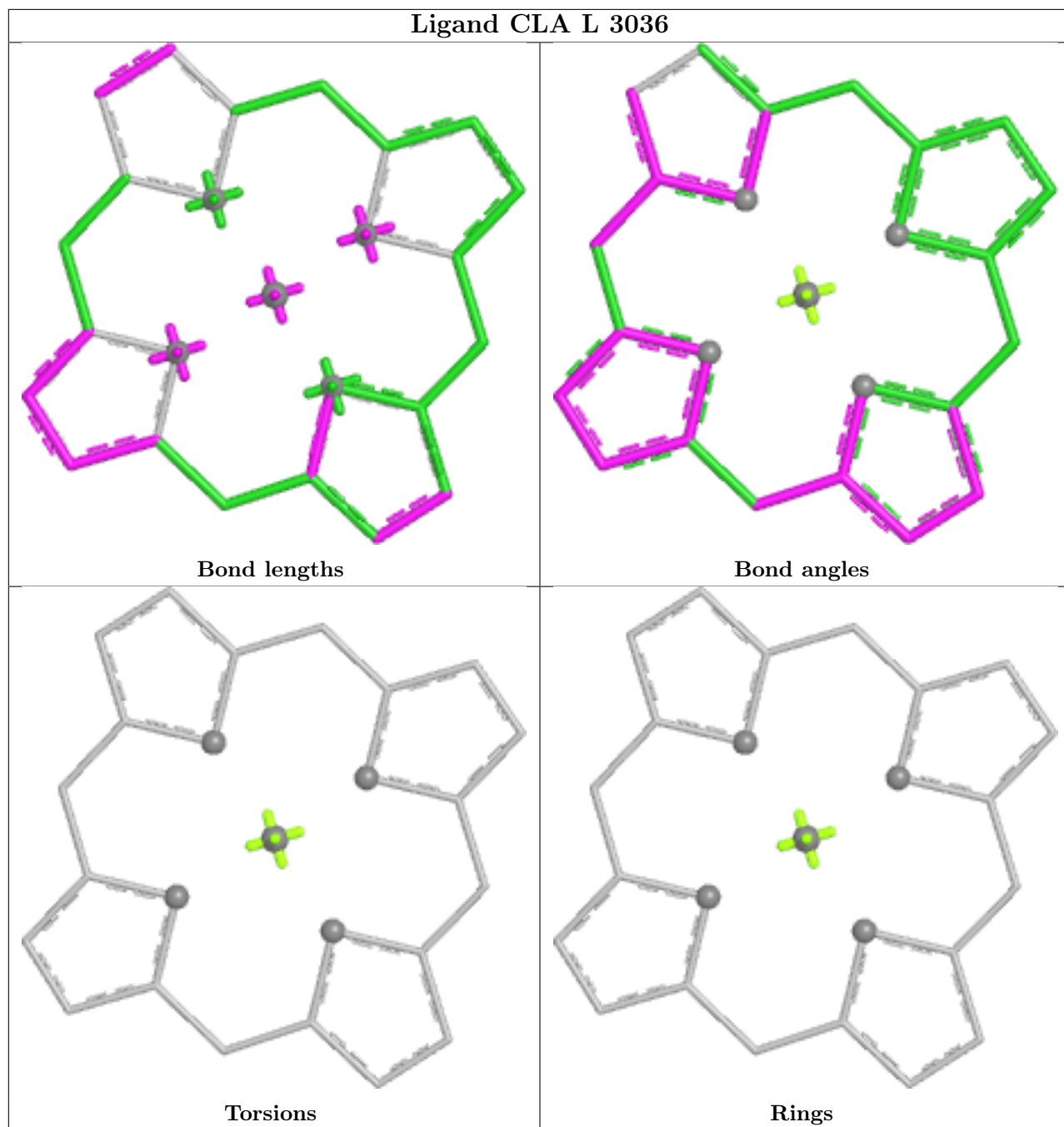


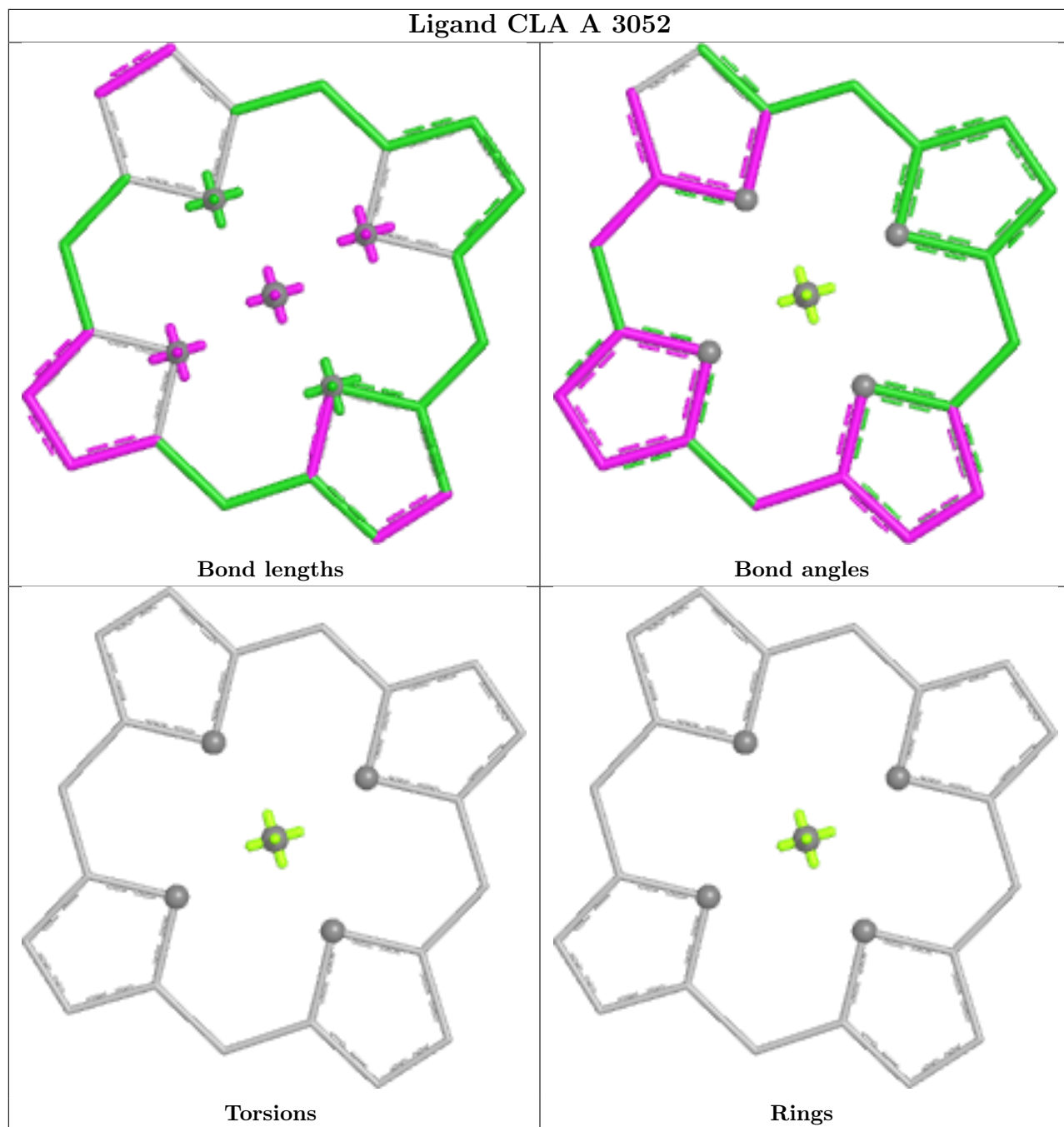


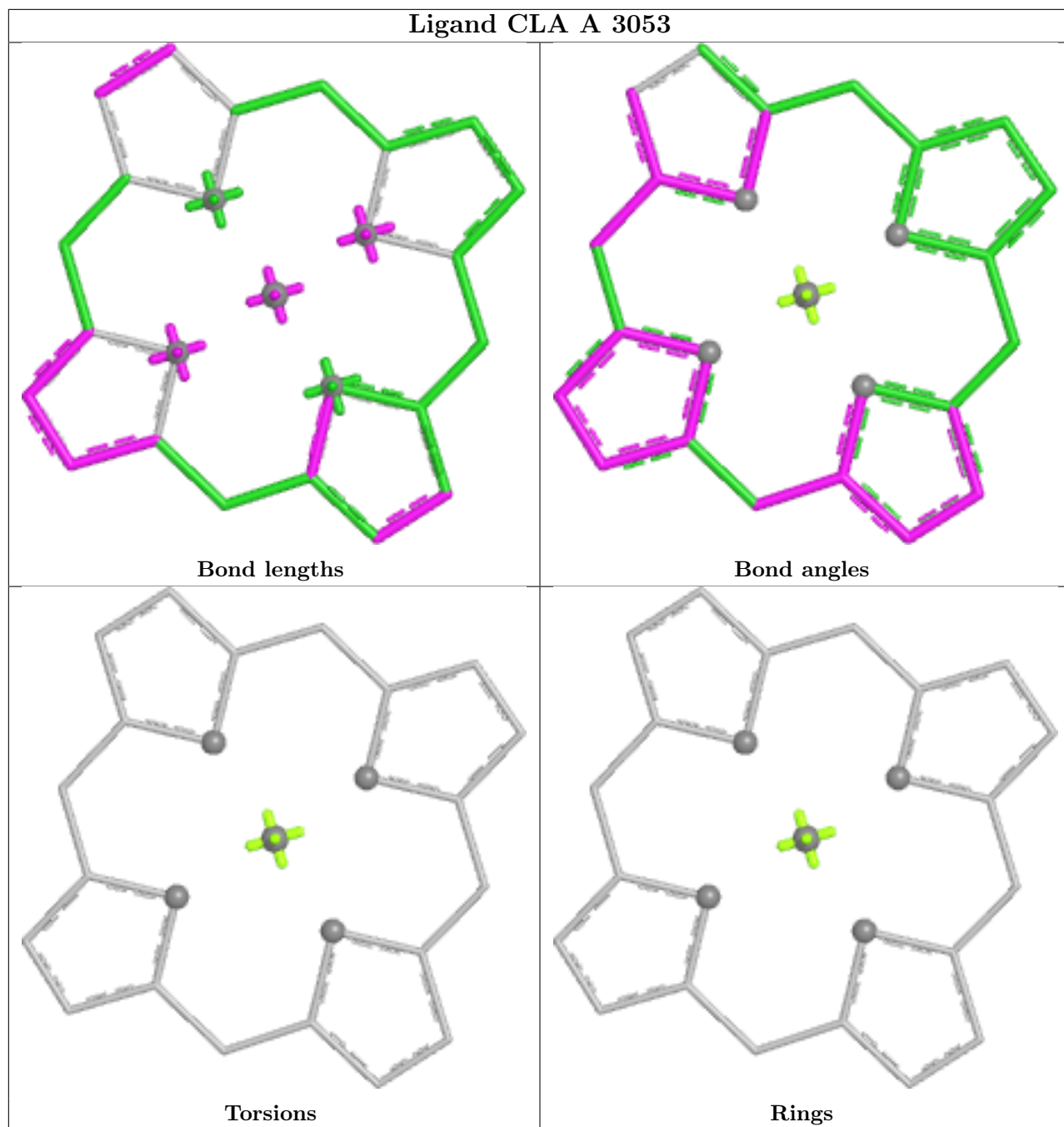


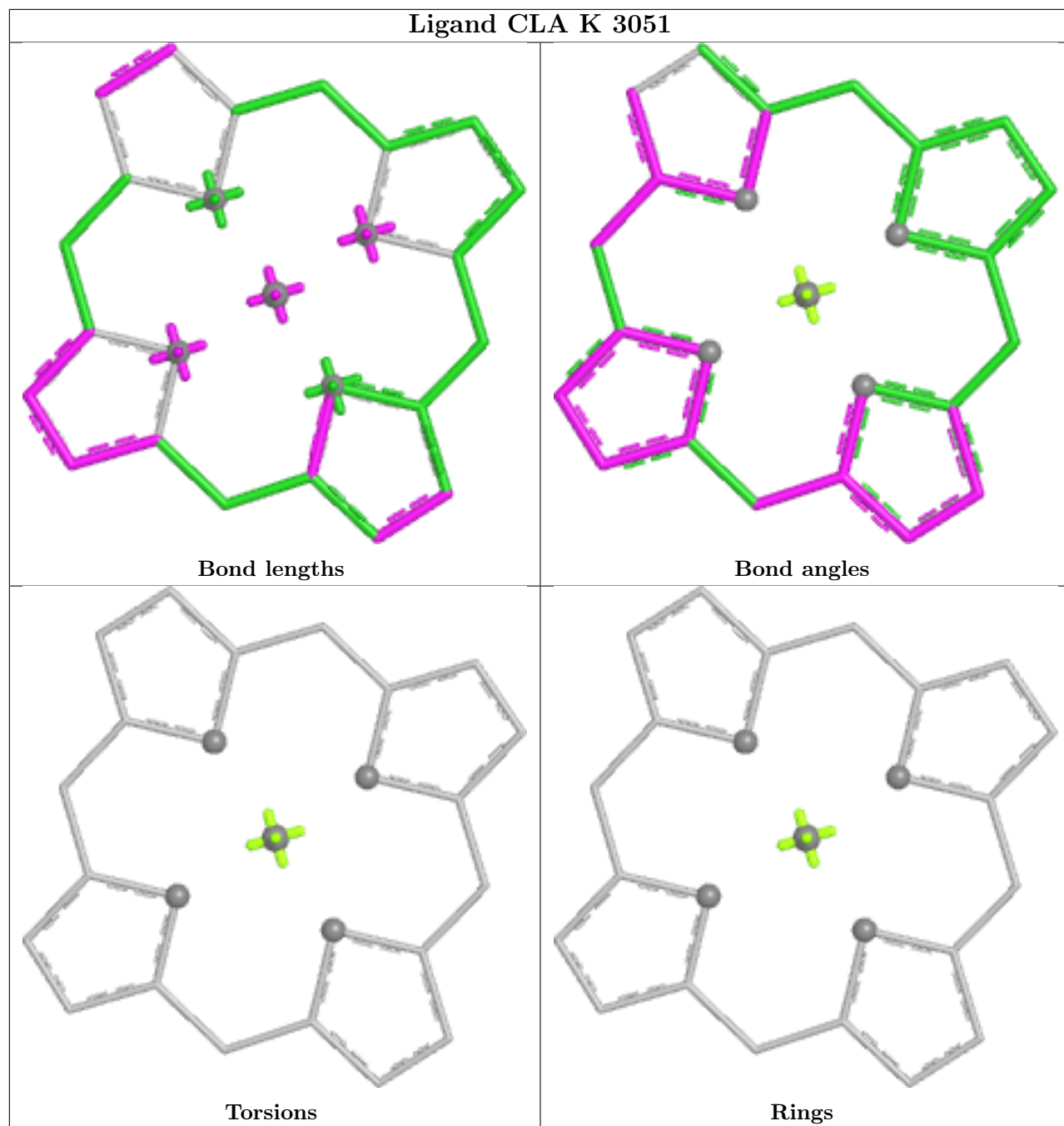


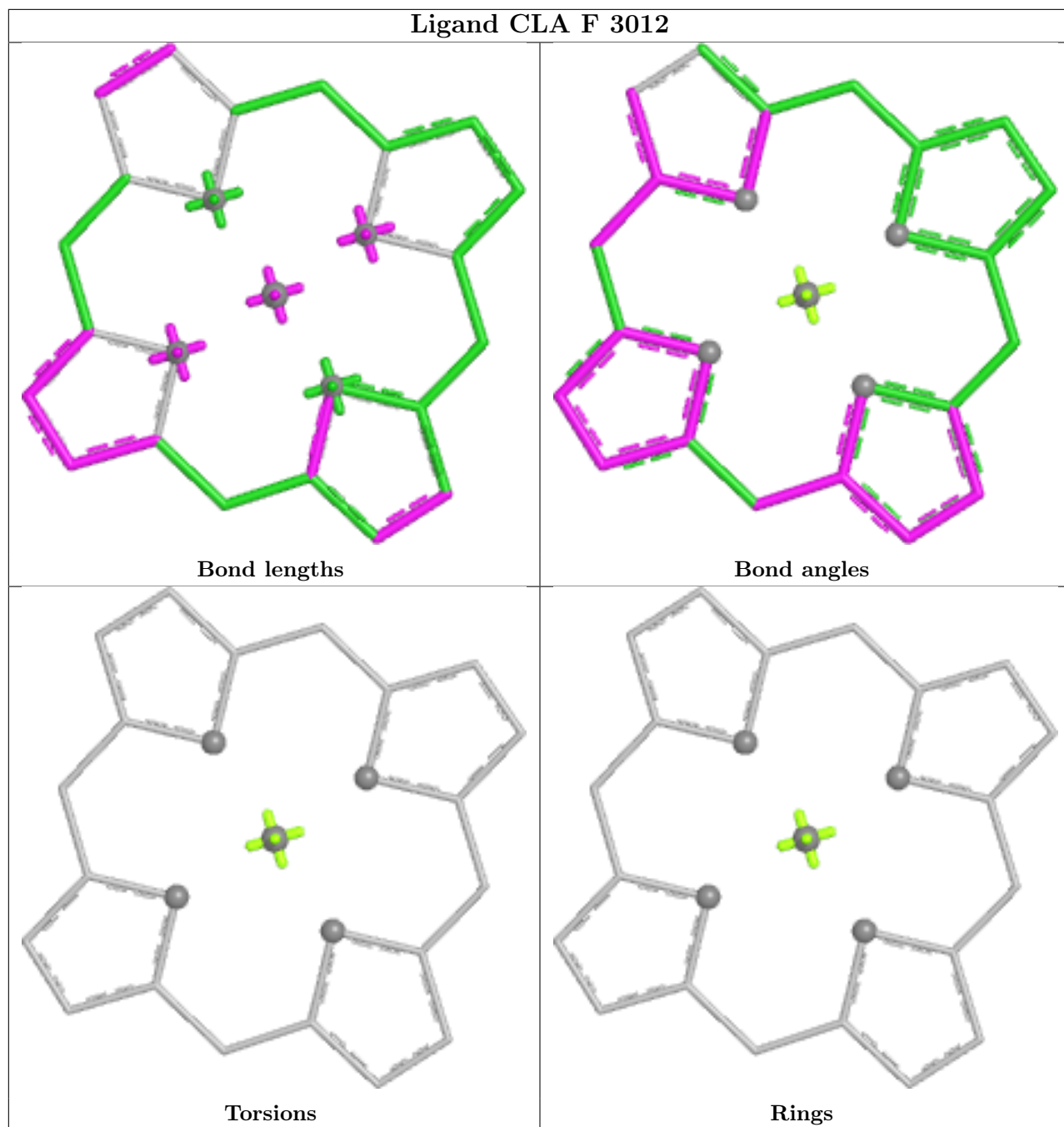


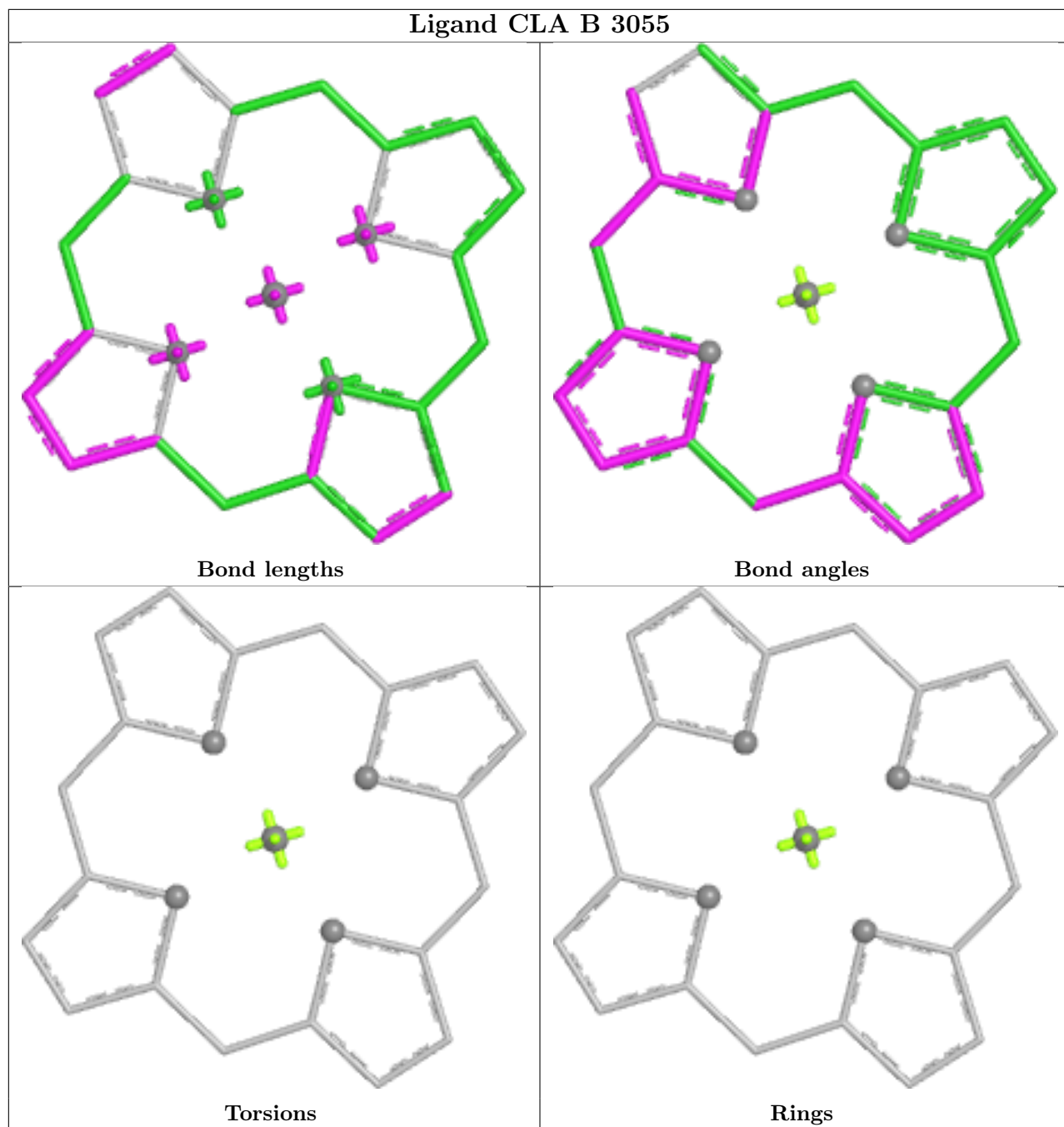


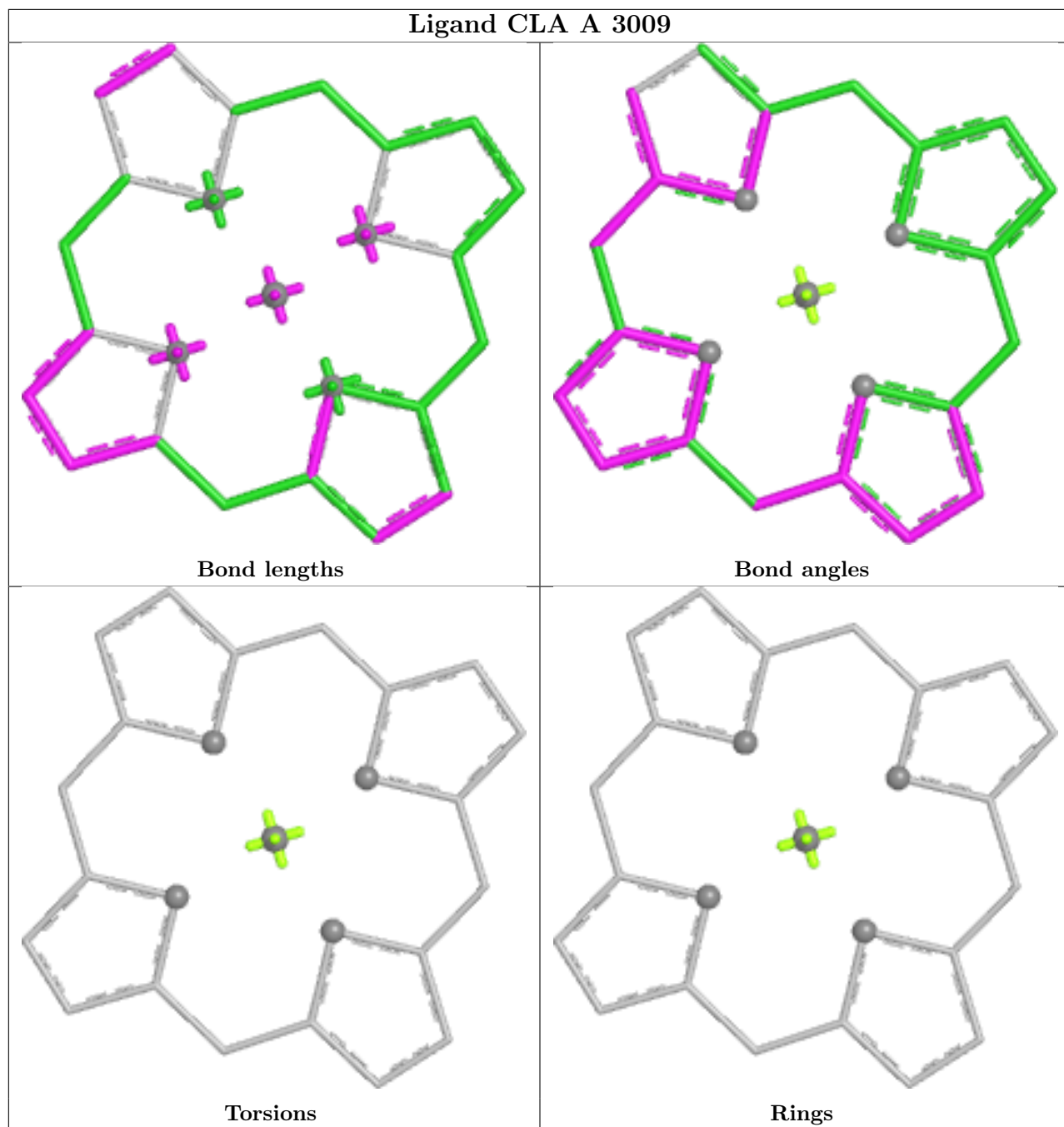




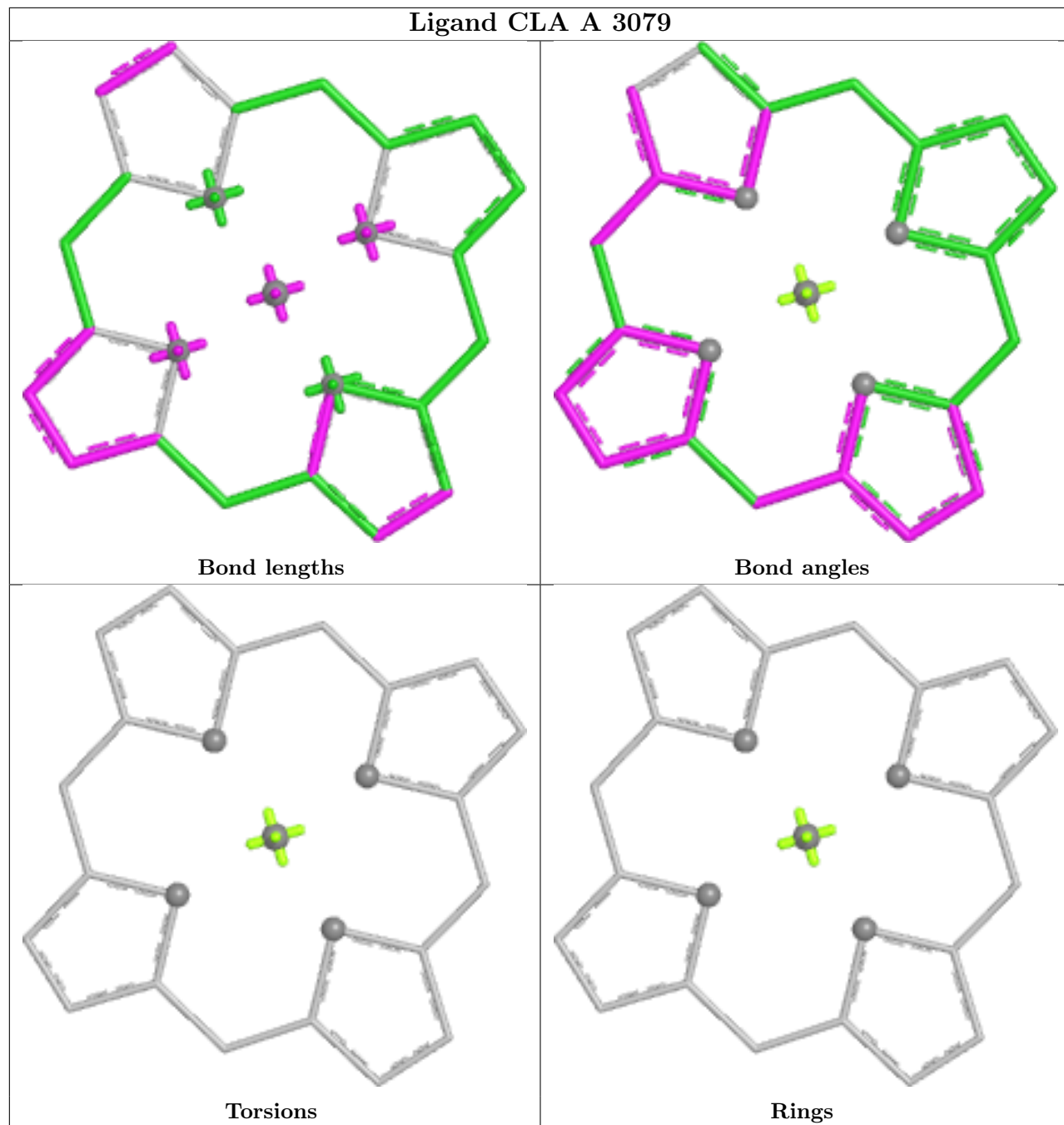


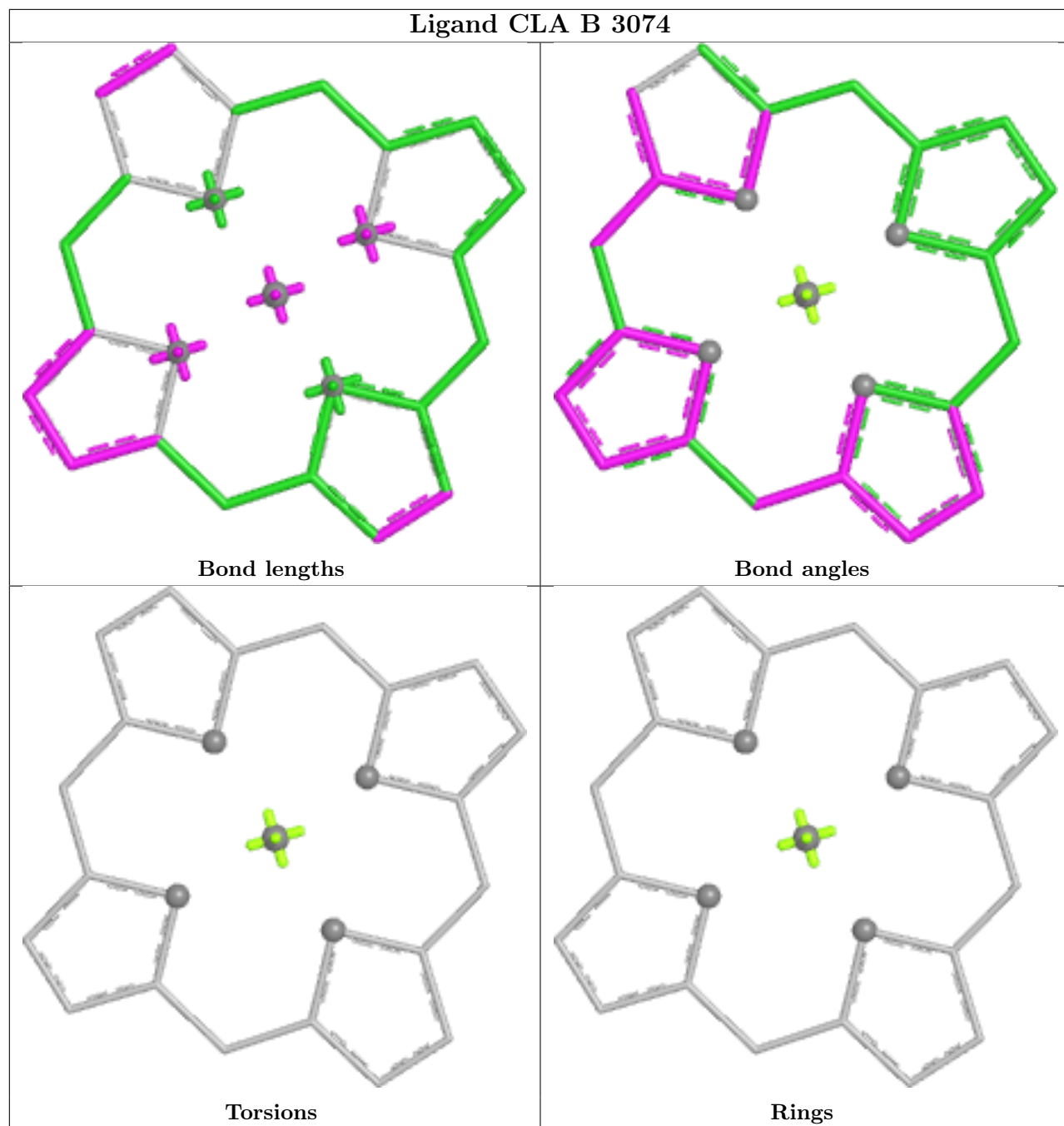


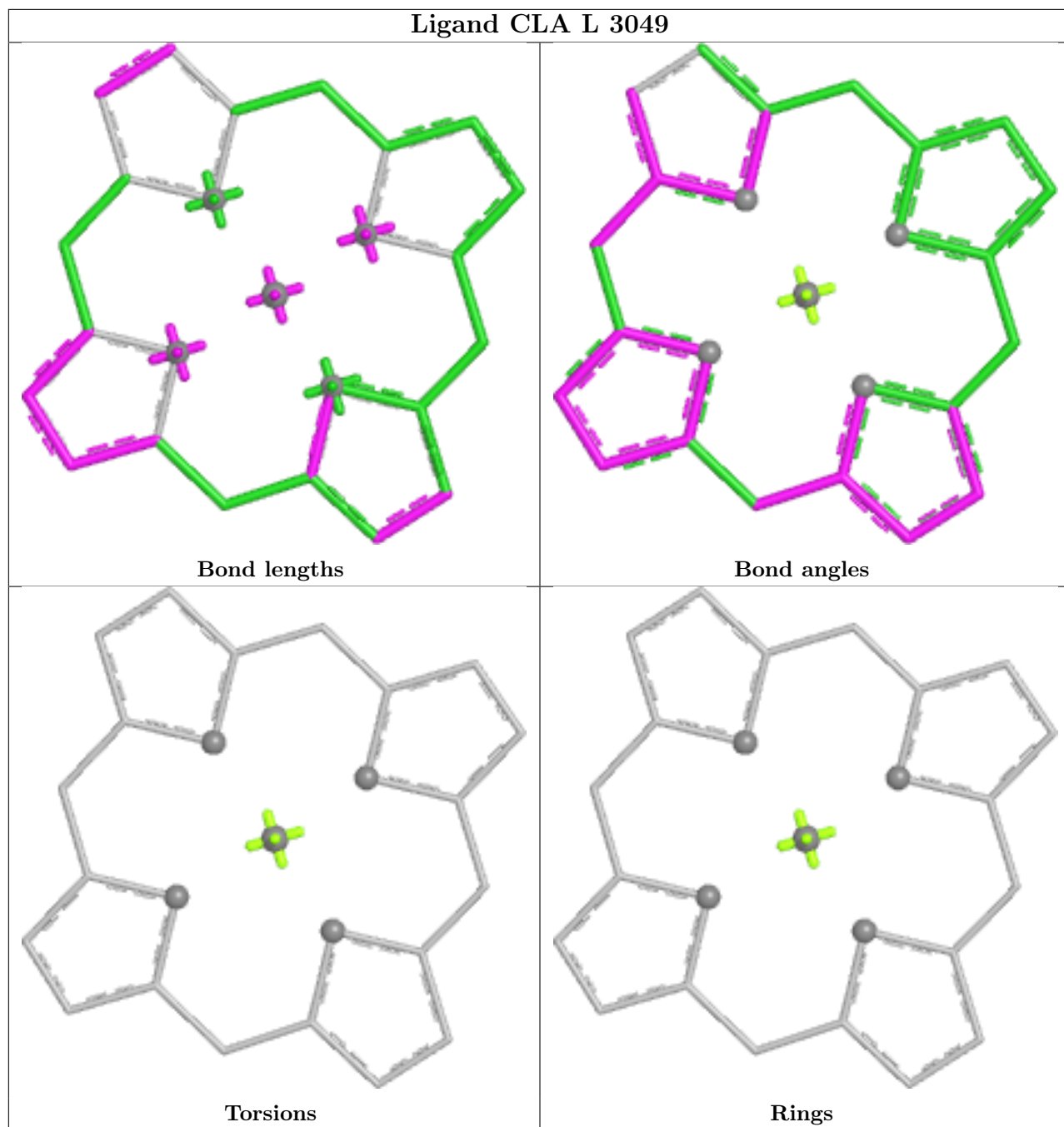


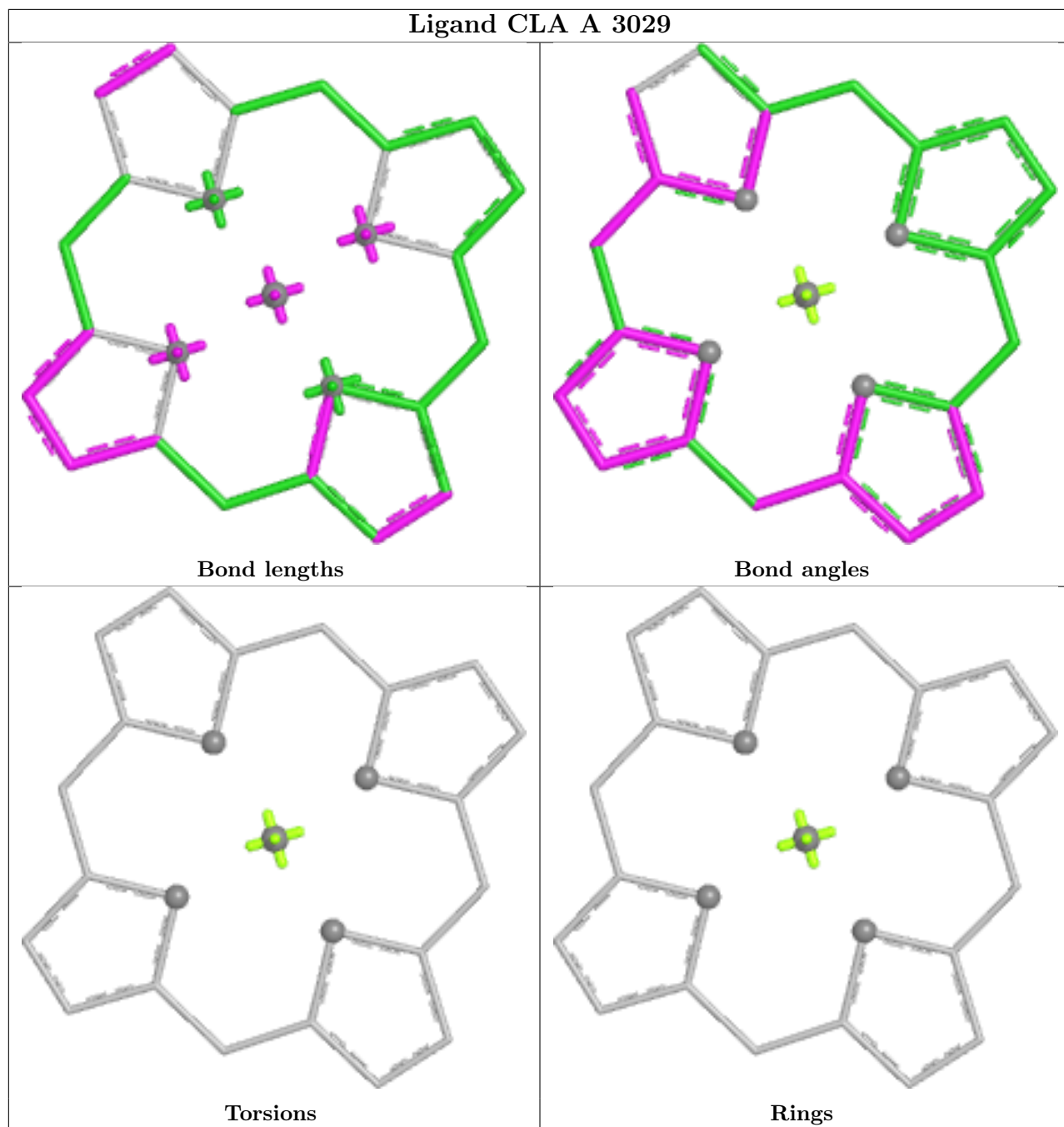


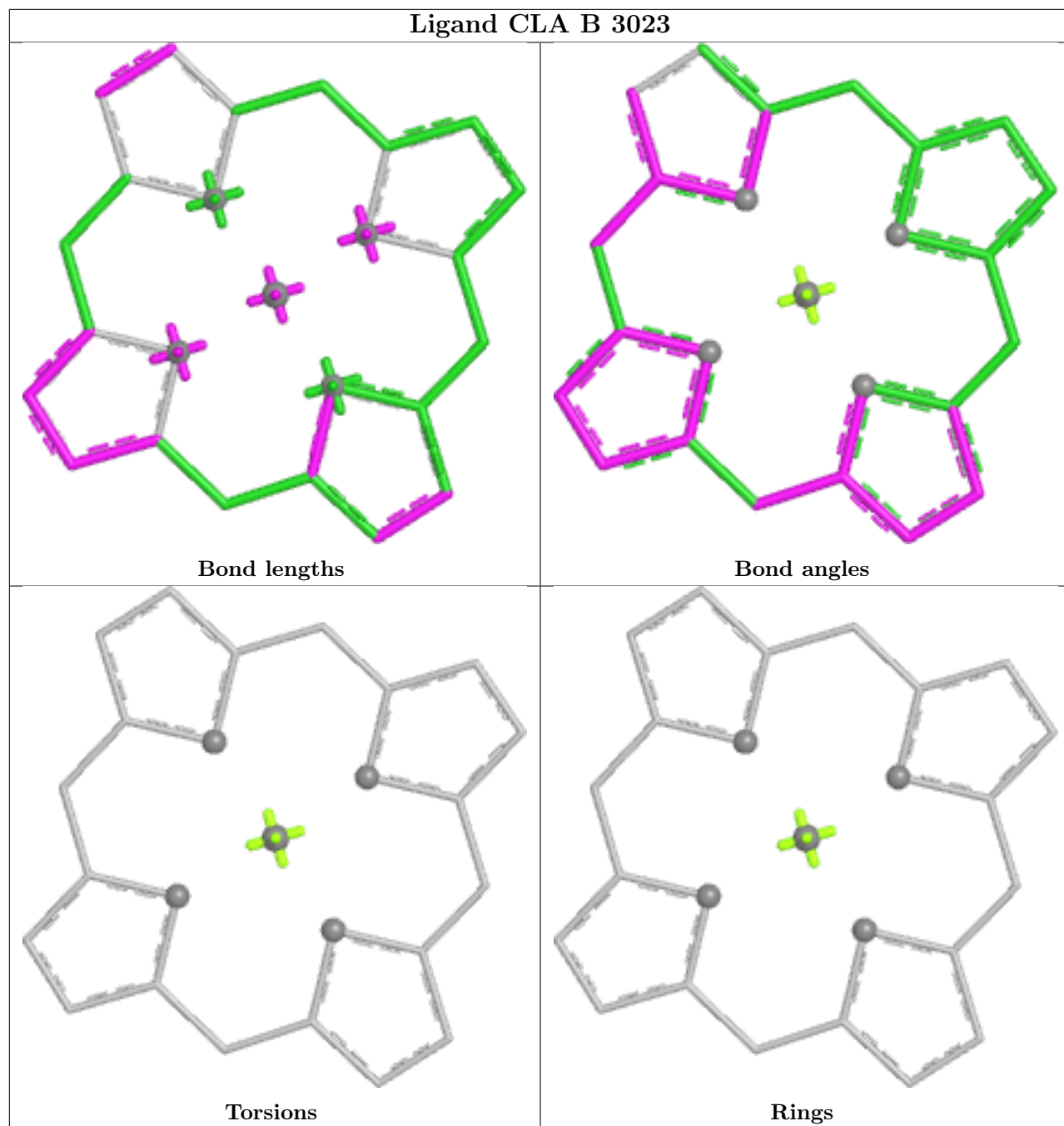
## Ligand CLA A 3079

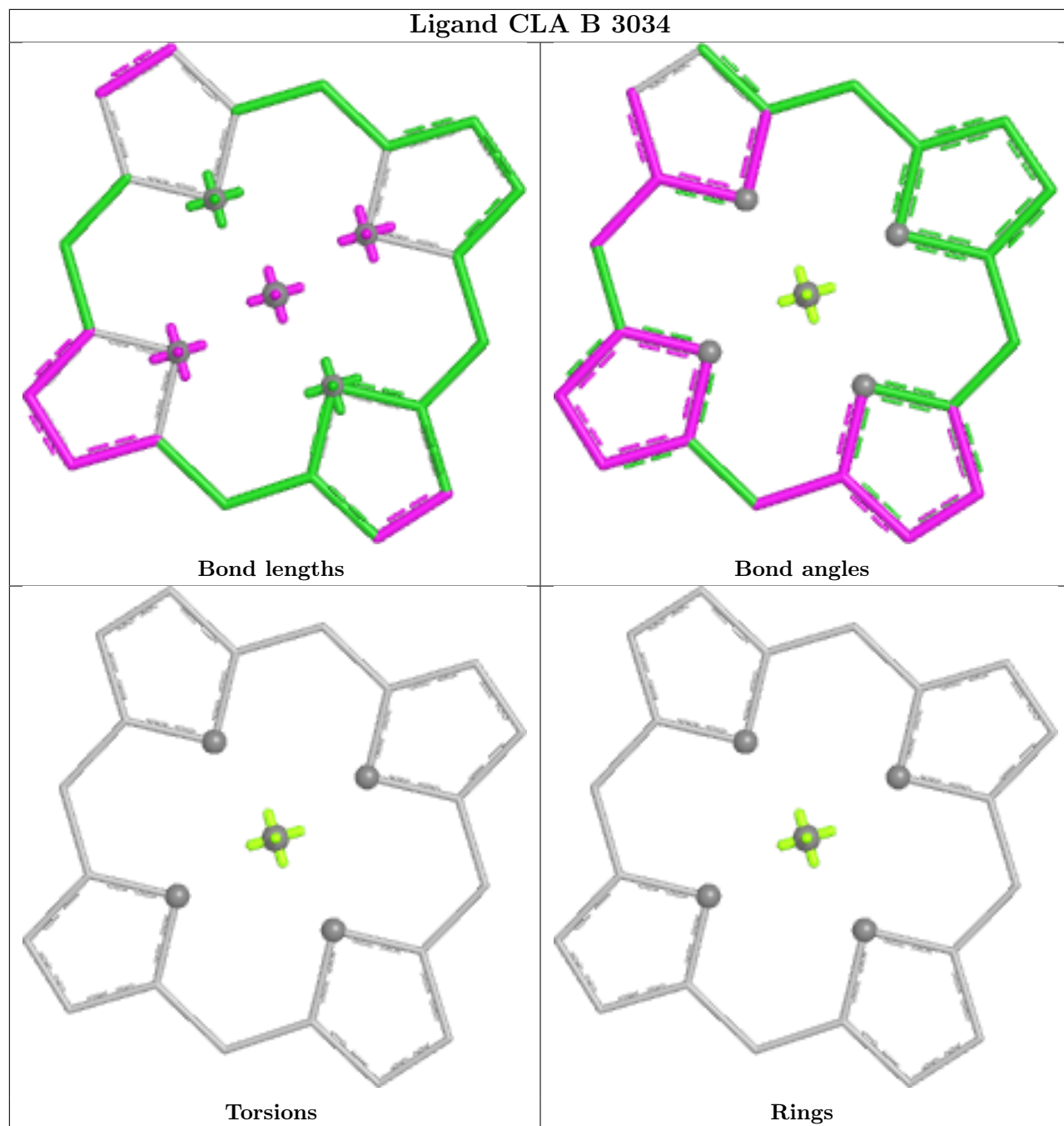


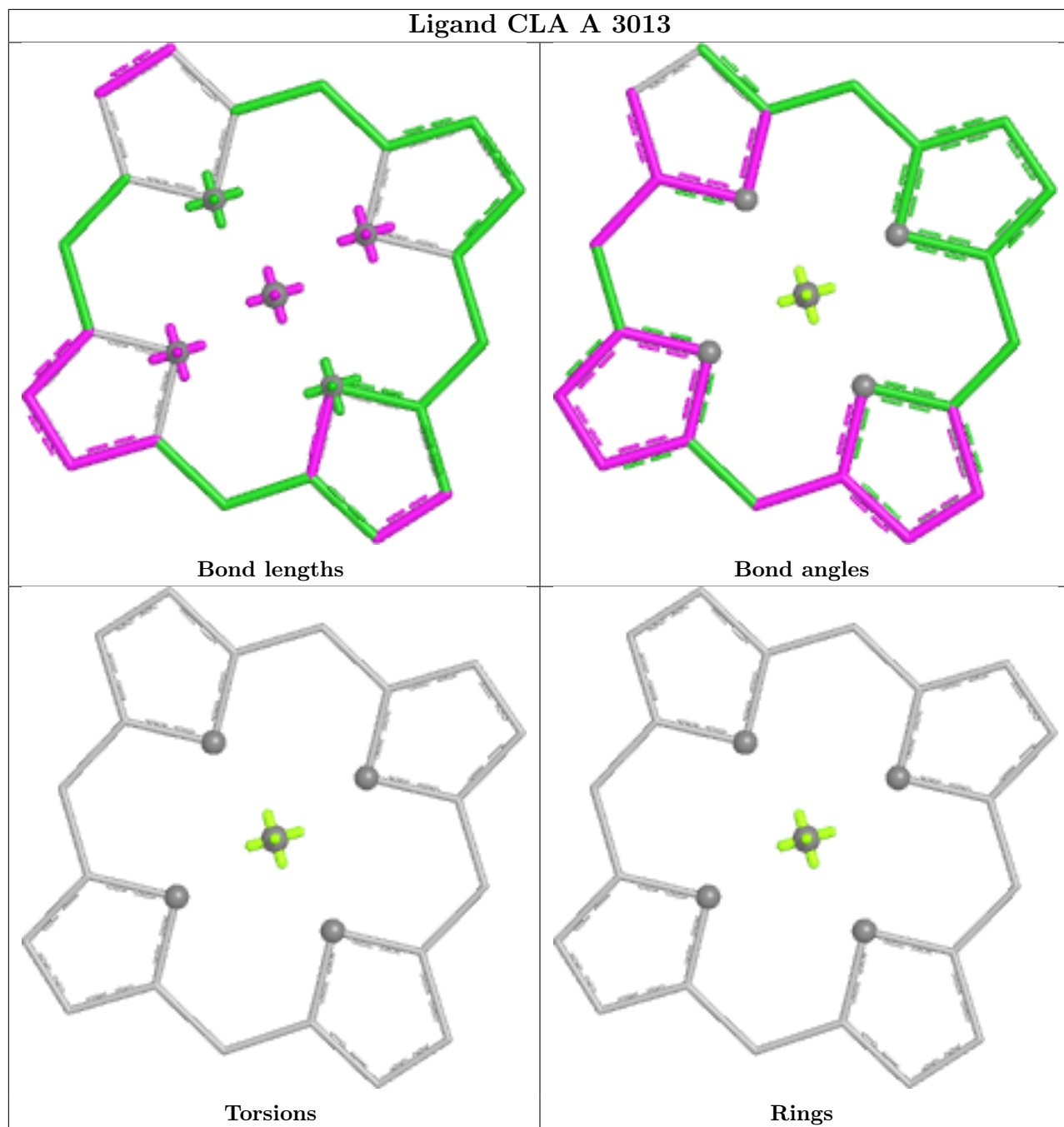


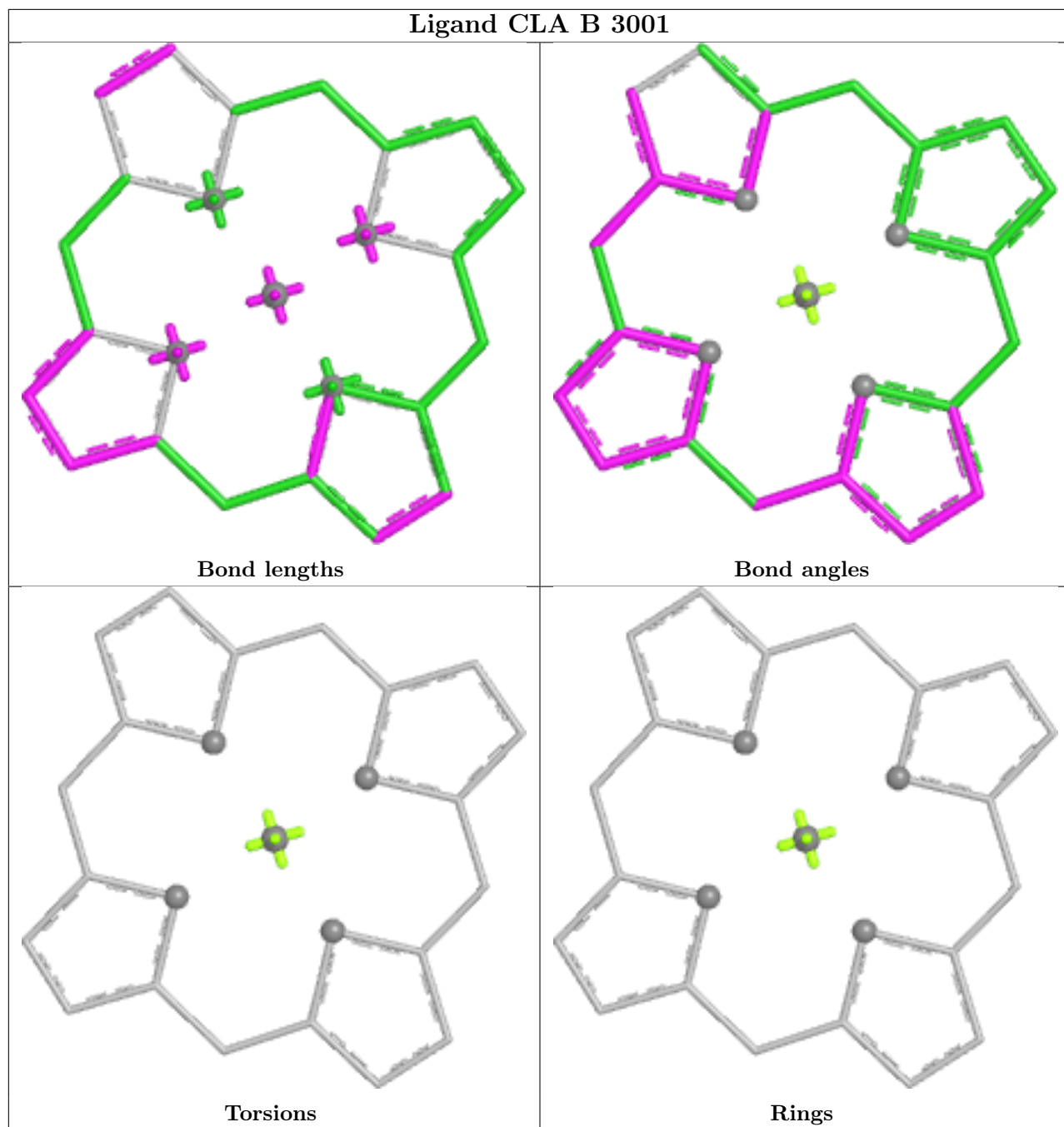


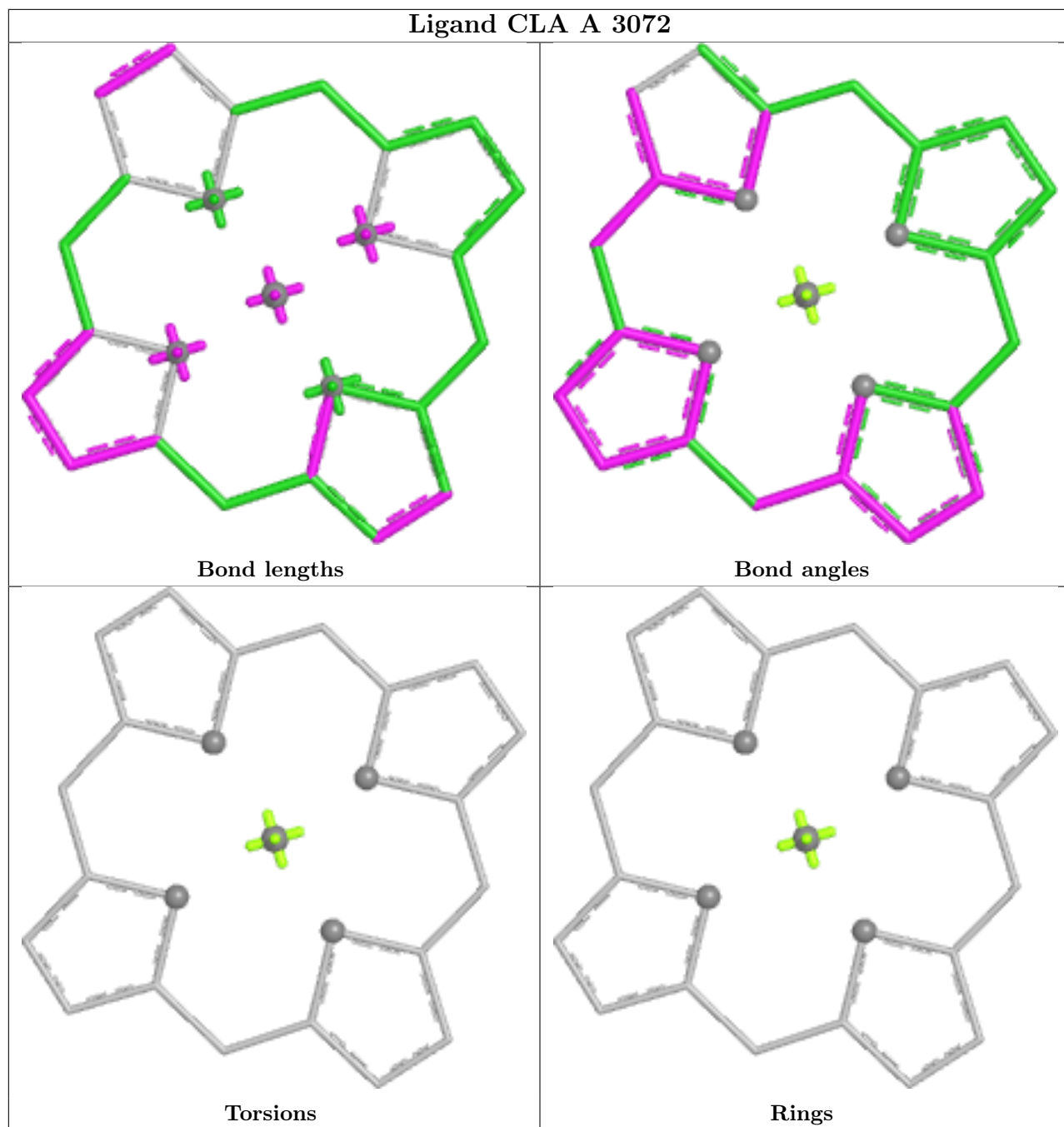


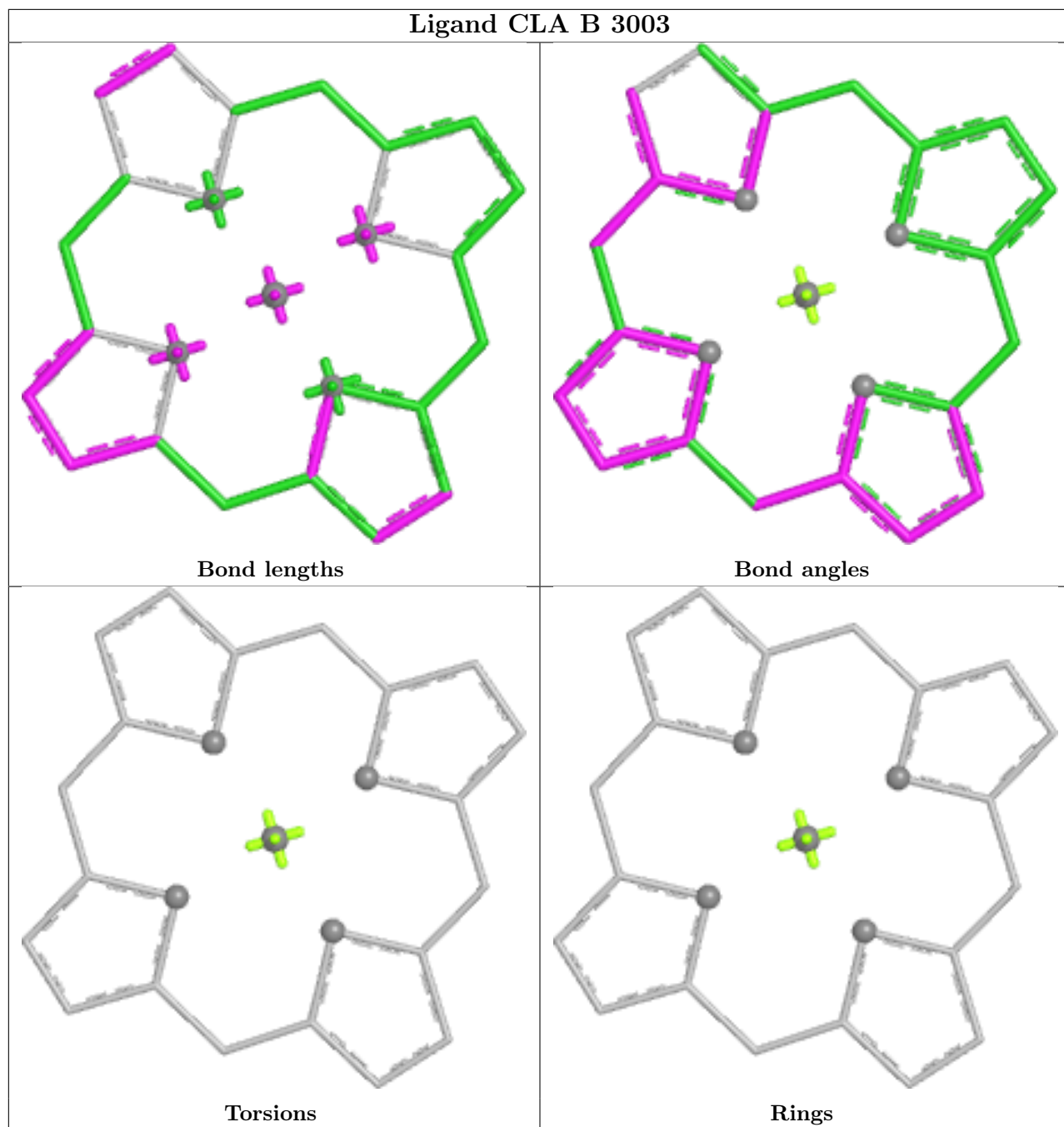


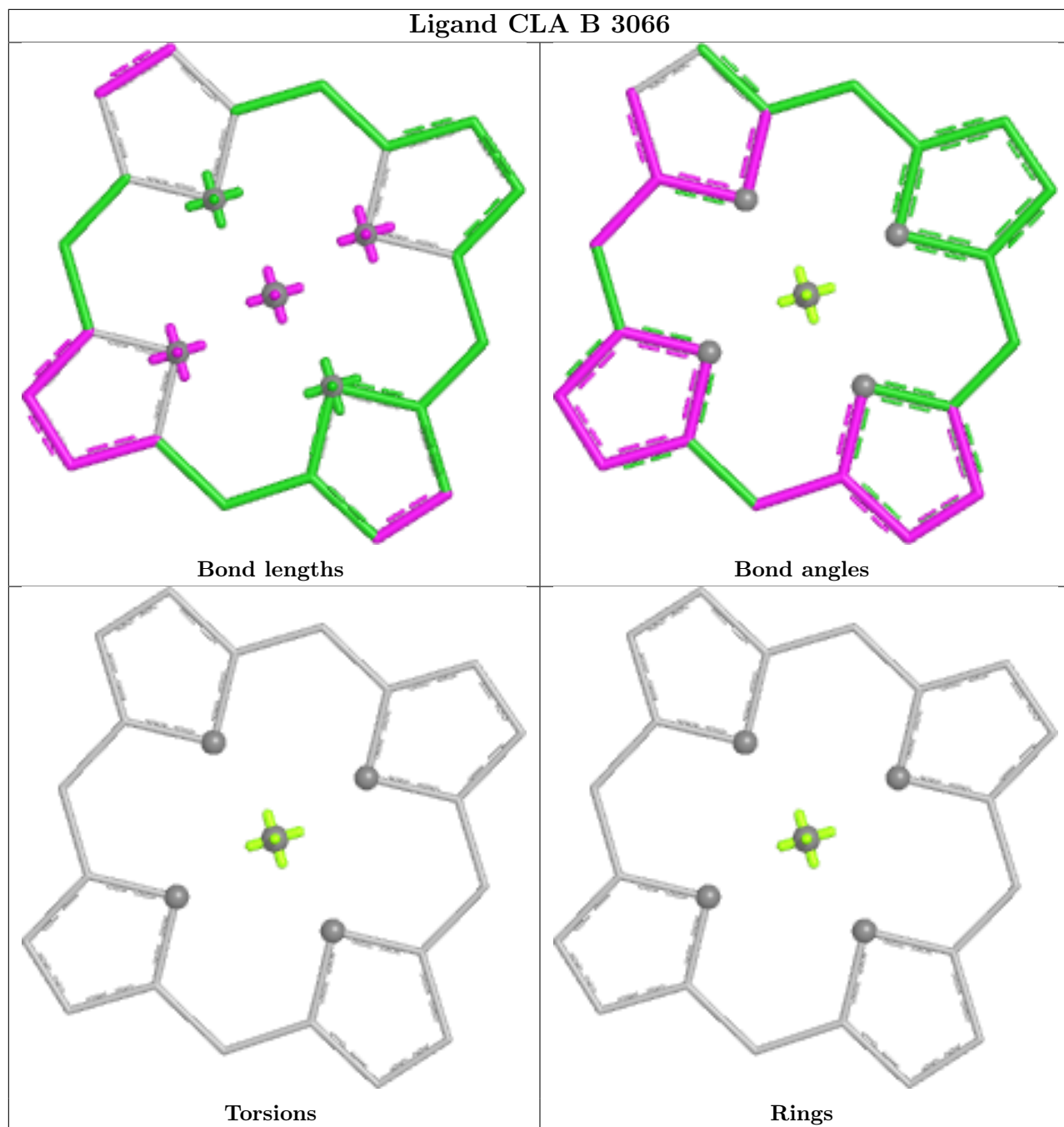


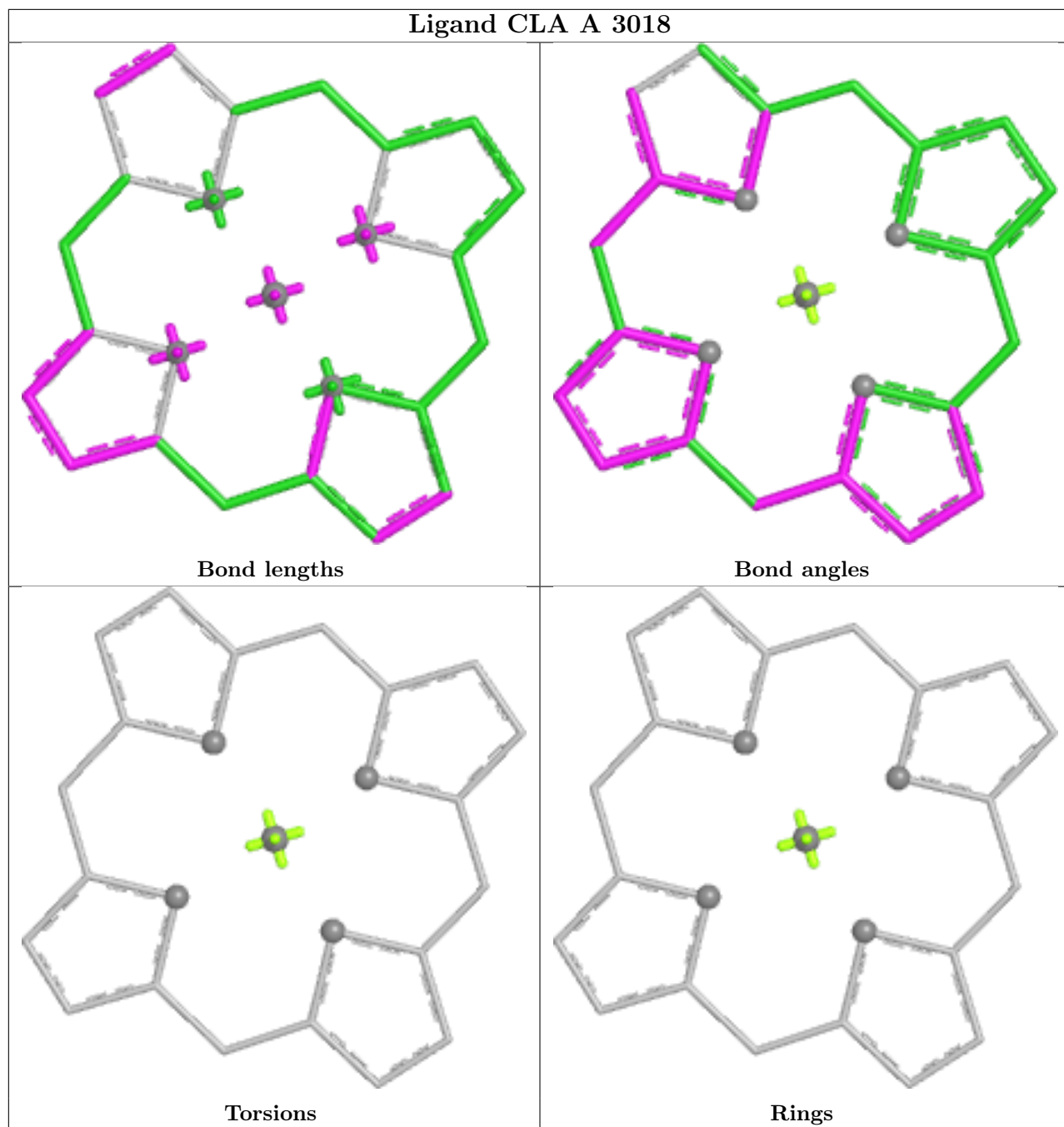


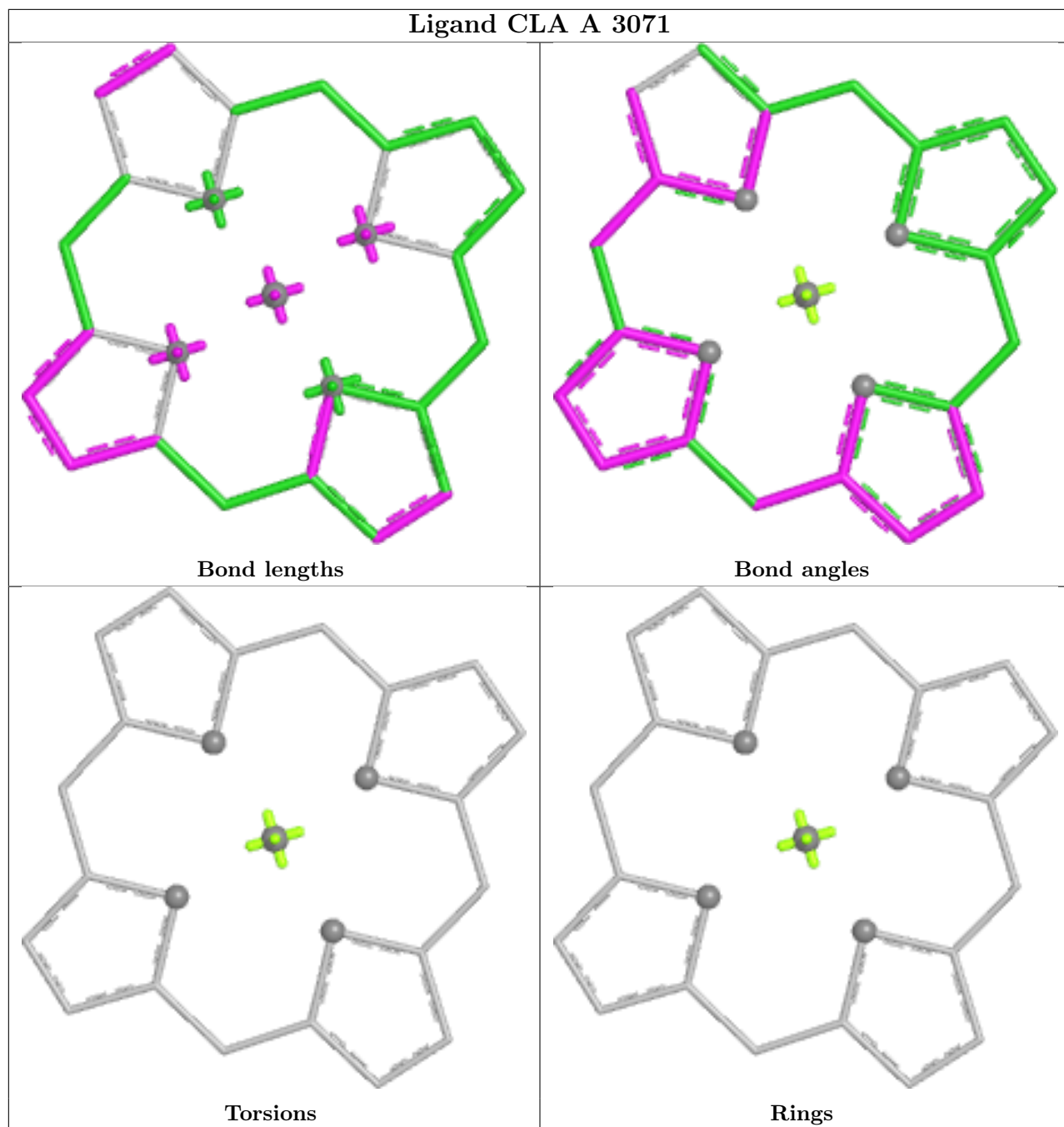


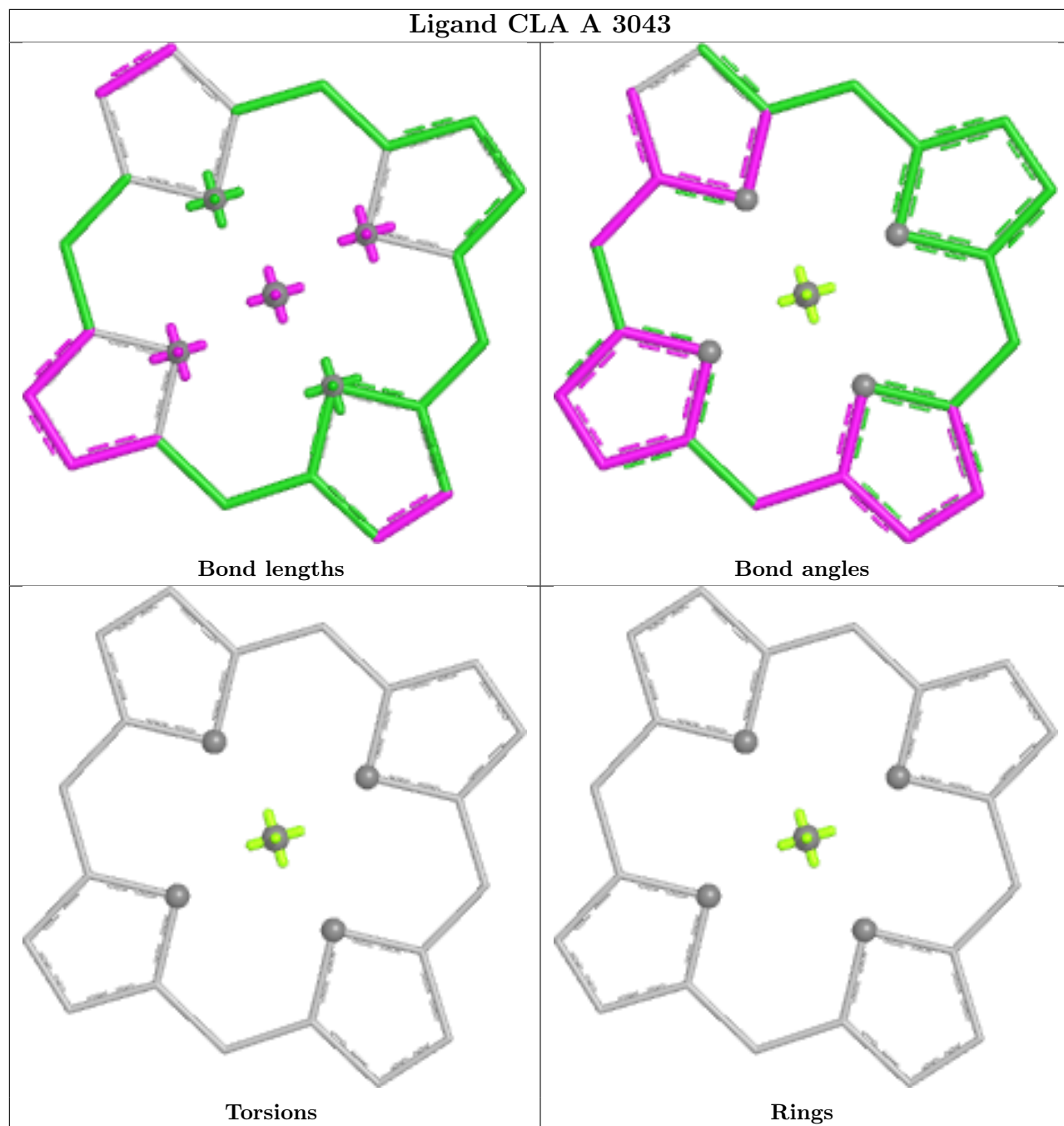


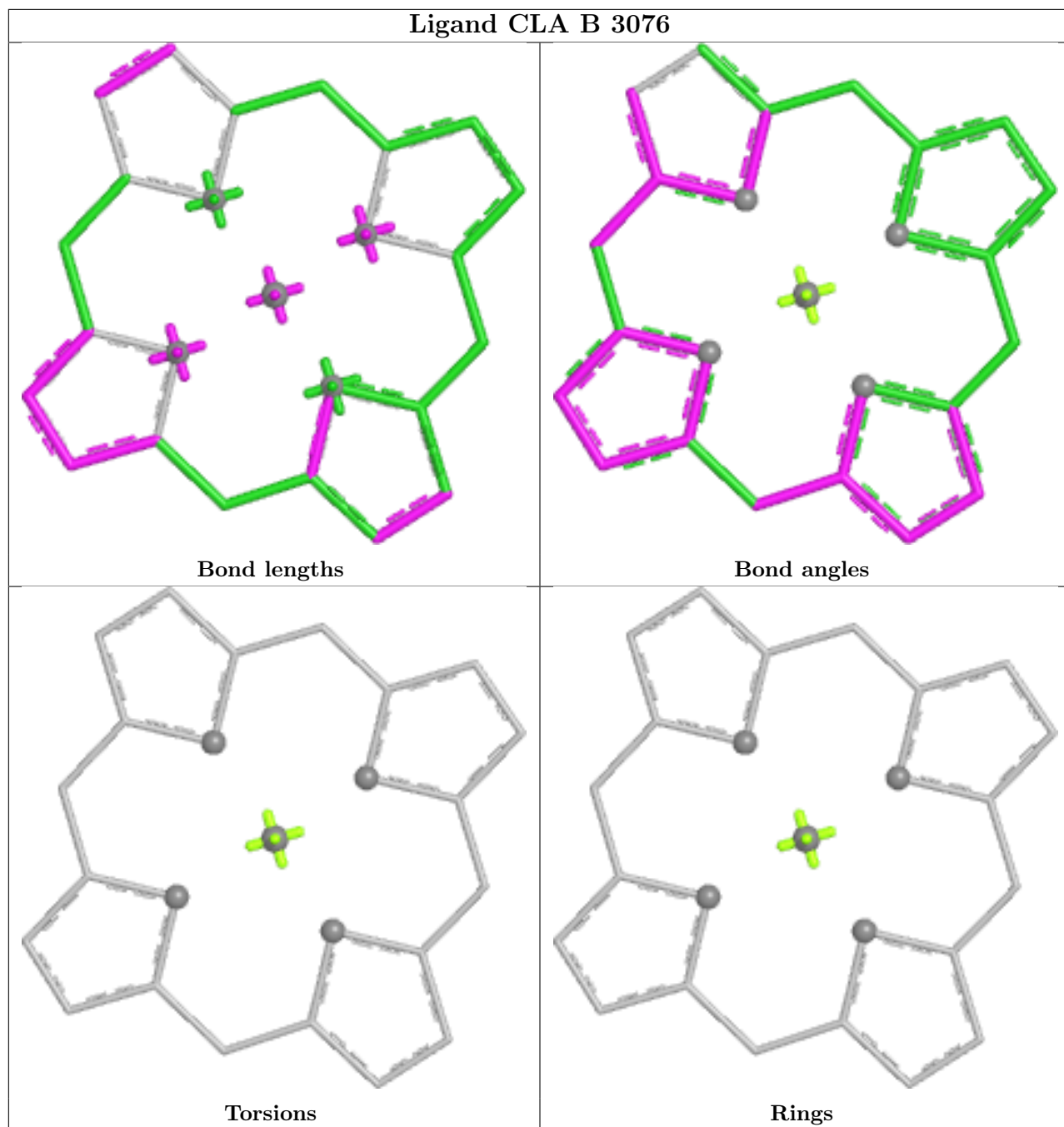


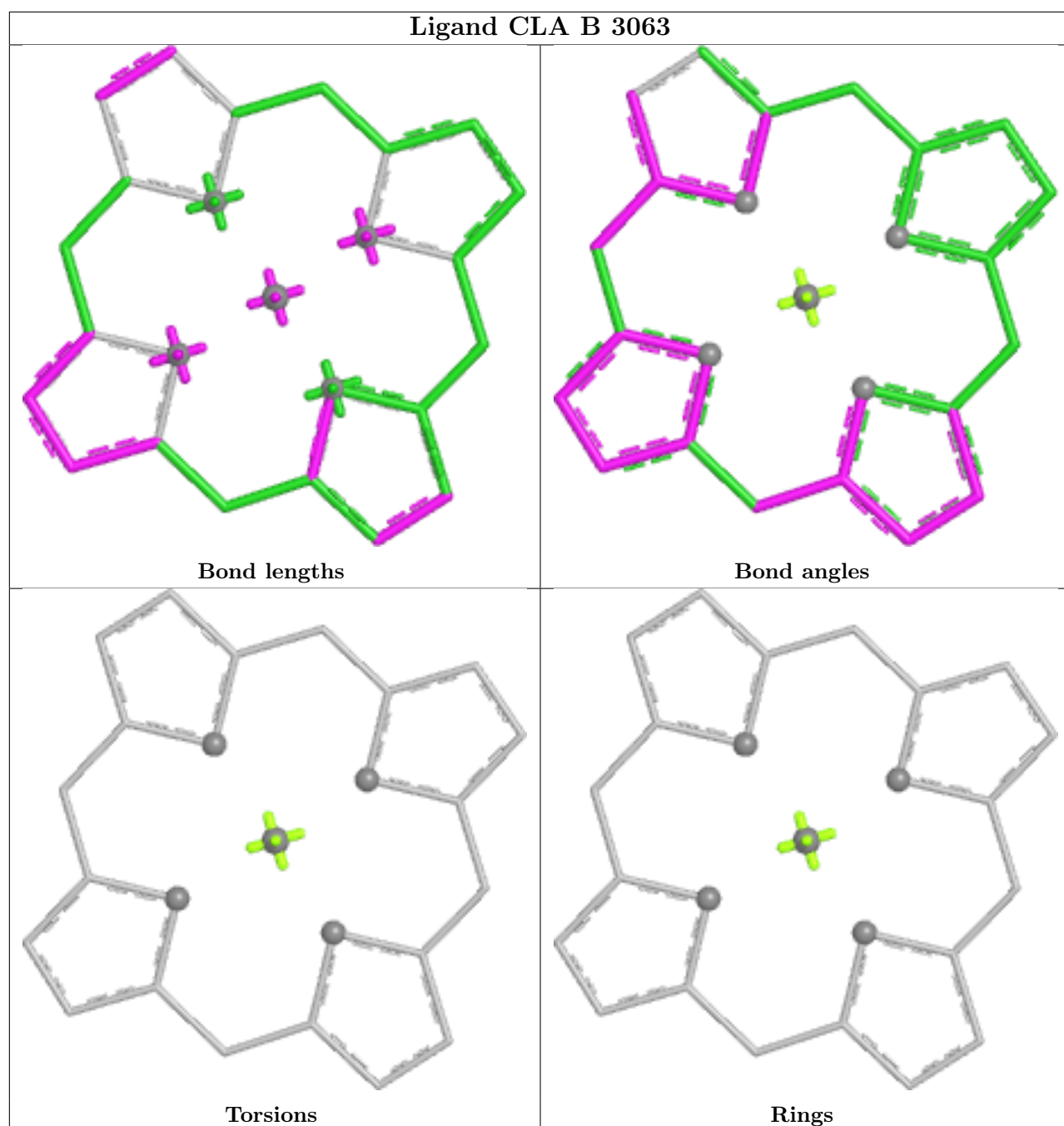












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.