



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 02:33 pm BST

PDB ID : 7O1V / pdb_00007o1v
EMDB ID : EMD-12697
Title : Structure of a Minimal Photosystem I
Authors : Nelson, N.; Caspy, I.; Lambrev, P.
Deposited on : 2021-03-30
Resolution : 4.31 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

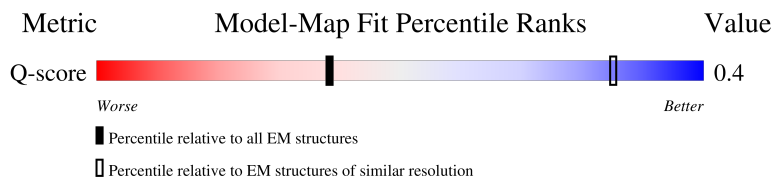
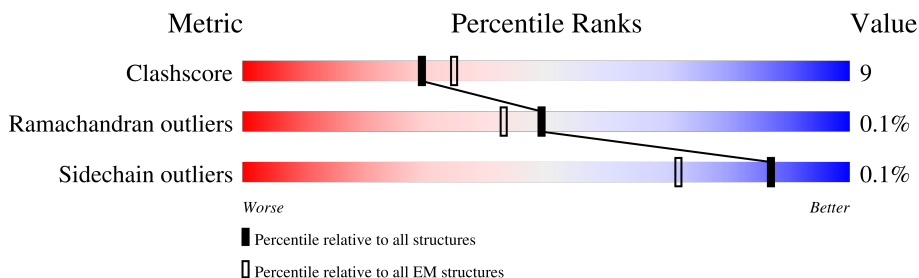
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.31 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3904 (3.81 - 4.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	739	
2	B	729	
3	C	80	
4	D	141	

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Mol	Chain	Length	Quality of chain
5	E	69	 81% 19%
6	K	80	 18% 88% 12%
7	M	31	 23% 84% 16%

2 Entry composition

There are 15 unique types of molecules in this entry. The entry contains 20914 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	739	Total	C	N	O	S	0	0
			5787	3791	984	985	27		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	729	Total	C	N	O	S	0	0
			5770	3798	967	990	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	80	Total	C	N	O	S	0	0
			600	369	103	117	11		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	141	Total	C	N	O	S	0	0
			1102	697	190	211	4		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
5	E	69	Total	C	N	O	0	0
			543	340	96	107		

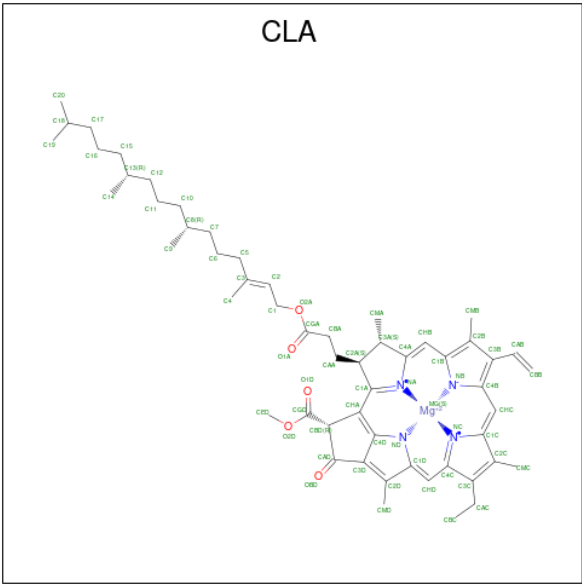
- Molecule 6 is a protein called Photosystem I reaction center subunit Psak 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	80	Total	C	N	O	S	1	0
			579	378	93	102	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	31	Total	C	N	O	S	0	0
			238	159	36	42	1		

- Molecule 8 is CHLOROPHYLL A (CCD ID: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			54	44	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			52	42	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	A	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	

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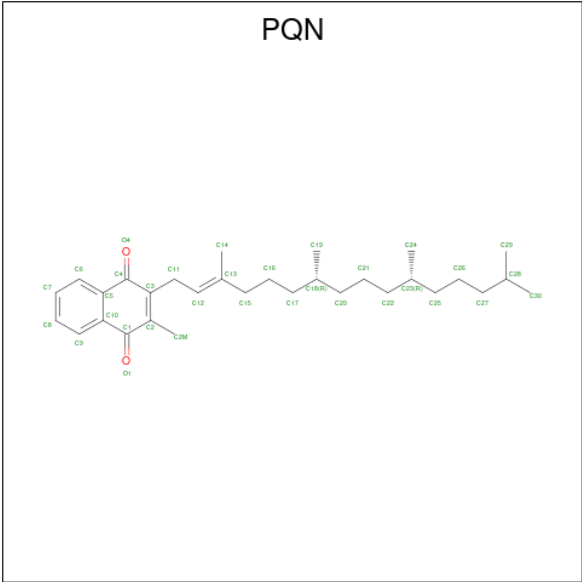
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			46	36	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			57	47	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			62	52	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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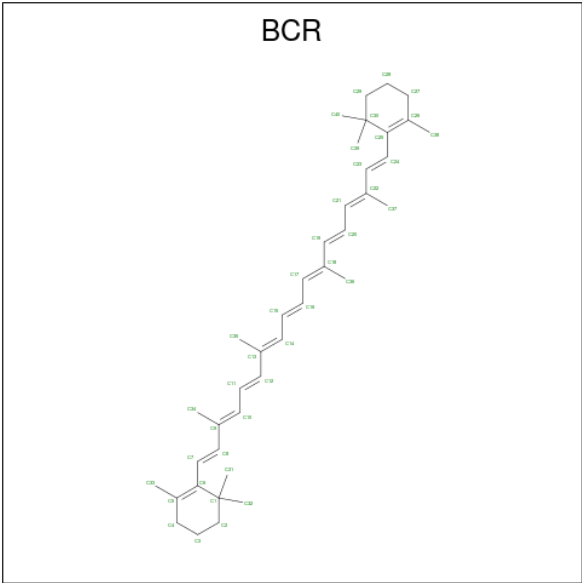
Mol	Chain	Residues	Atoms					AltConf
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	B	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
8	K	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 9 is PHYLLOQUINONE (CCD ID: PQN) (formula: $C_{31}H_{46}O_2$).



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

- Molecule 10 is BETA-CAROTENE (CCD ID: BCR) (formula: C₄₀H₅₆).



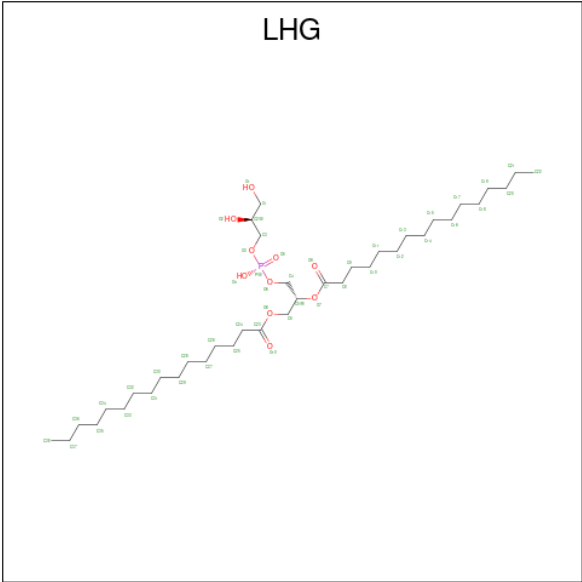
Mol	Chain	Residues	Atoms		AltConf
10	A	1	Total	C	0
			40	40	
10	A	1	Total	C	0
			40	40	

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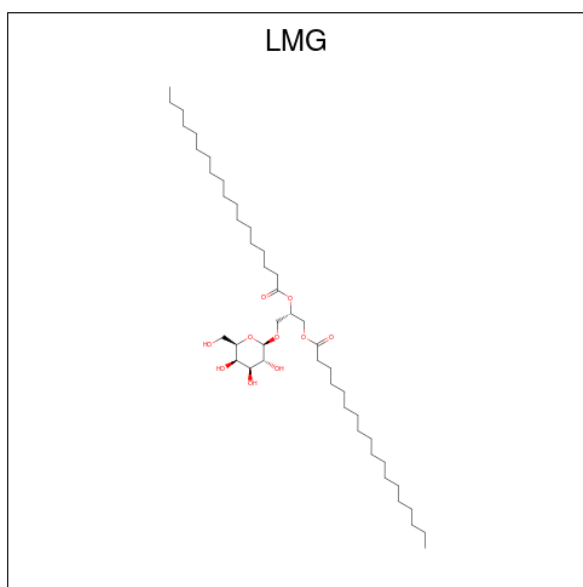
Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total C 40 40	0
10	A	1	Total C 40 40	0
10	A	1	Total C 40 40	0
10	A	1	Total C 40 40	0
10	A	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	B	1	Total C 40 40	0
10	K	1	Total C 40 40	0

- Molecule 11 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: C₃₈H₇₅O₁₀P).



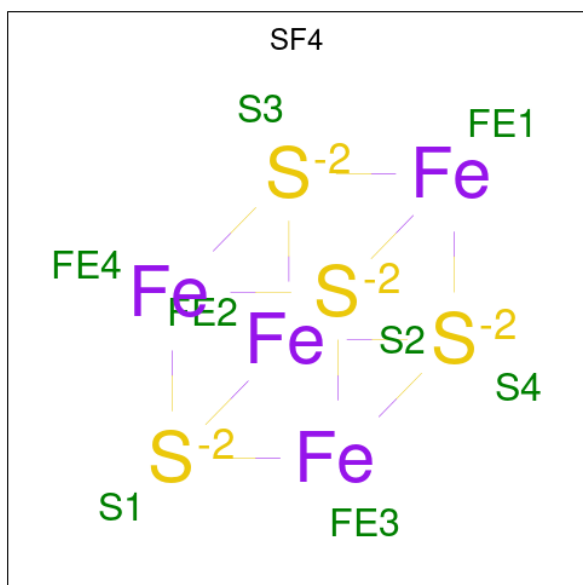
Mol	Chain	Residues	Atoms				AltConf
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	A	1	Total	C	O	P	0
			49	38	10	1	
11	B	1	Total	C	O	P	0
			49	38	10	1	
11	B	1	Total	C	O	P	0
			24	13	10	1	
11	M	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 12 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (CCD ID: LMG) (formula: C₄₅H₈₆O₁₀).



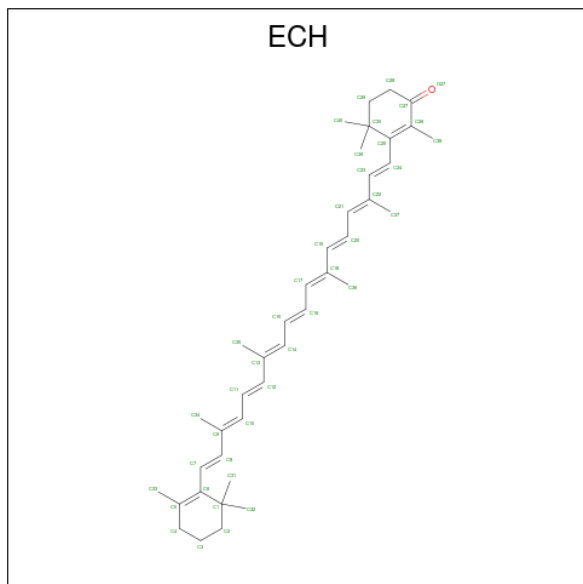
Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total	C	O	0
			50	40	10	
12	B	1	Total	C	O	0
			55	45	10	
12	B	1	Total	C	O	0
			31	21	10	
12	K	1	Total	C	O	0
			55	45	10	

- Molecule 13 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



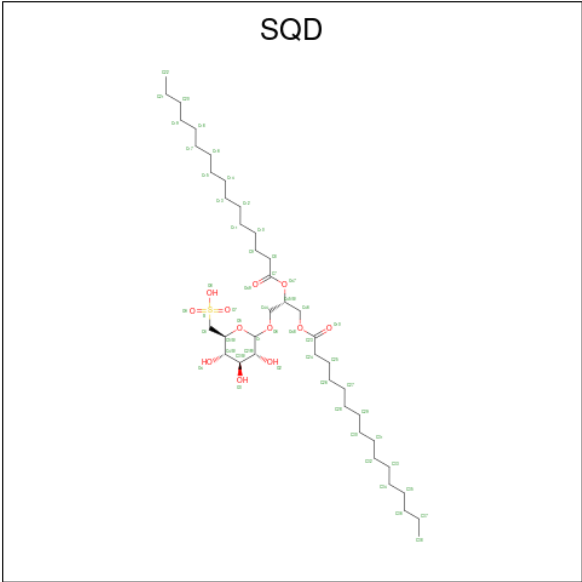
Mol	Chain	Residues	Atoms			AltConf
13	A	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	
13	C	1	Total	Fe	S	0
			8	4	4	

- Molecule 14 is beta,beta-caroten-4-one (CCD ID: ECH) (formula: $C_{40}H_{54}O$).



Mol	Chain	Residues	Atoms			AltConf
14	B	1	Total	C	O	0
			41	40	1	
14	M	1	Total	C	O	0
			41	40	1	

- Molecule 15 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).

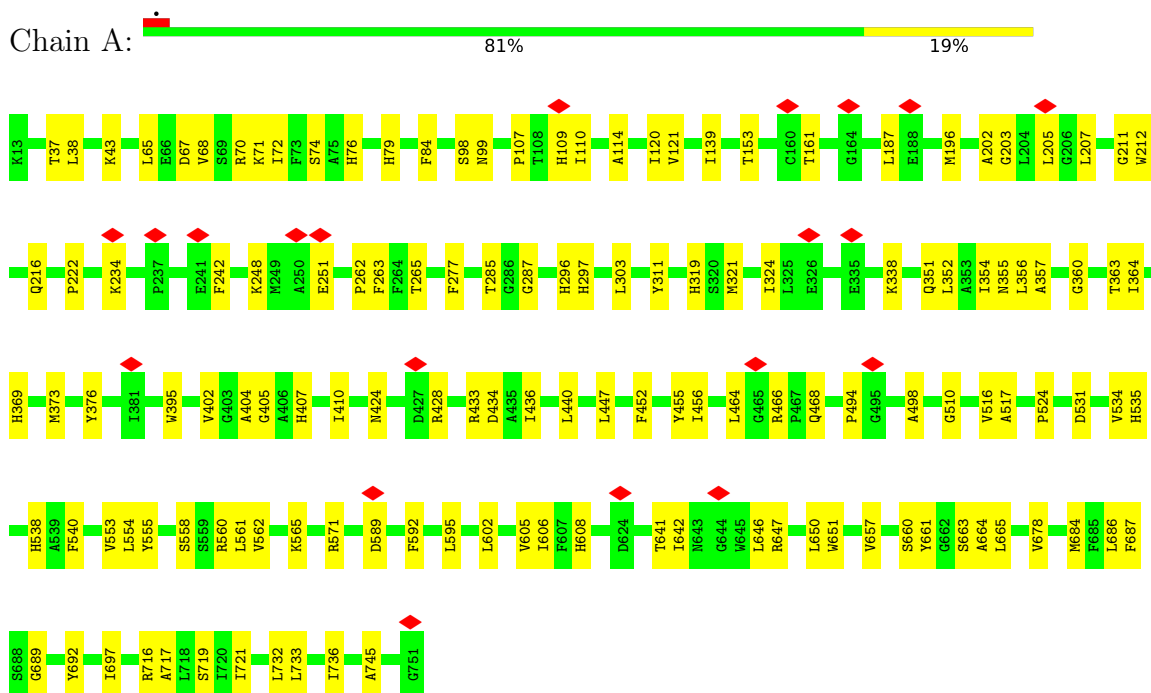


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
15	B	1	54	41	12	1	0

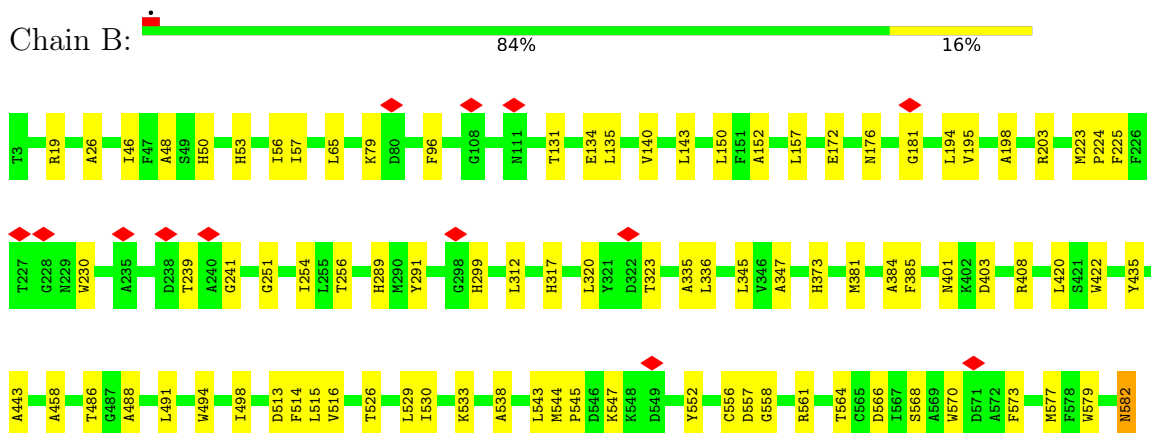
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Photosystem I P700 chlorophyll a apoprotein A1

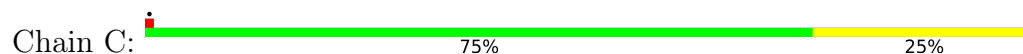


- Molecule 2: Photosystem I P700 chlorophyll a apoprotein A2

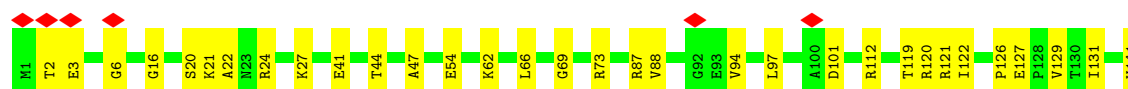
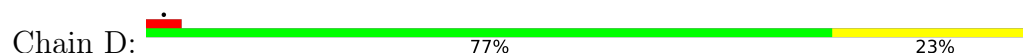




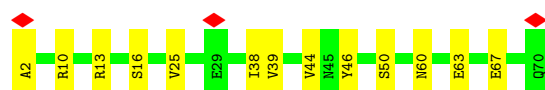
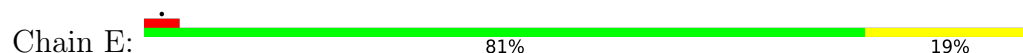
- Molecule 3: Photosystem I iron-sulfur center



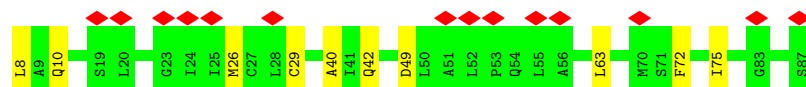
- Molecule 4: Photosystem I reaction center subunit II



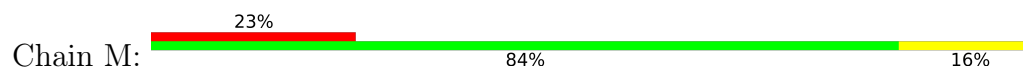
- Molecule 5: Photosystem I reaction center subunit IV



- Molecule 6: Photosystem I reaction center subunit PsaK 2



- Molecule 7: Photosystem I reaction center subunit XII



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	74303	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.088	Depositor
Minimum map value	-0.033	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.008	Depositor
Map size ($\text{\AA}$)	233.18399, 233.18399, 233.18399	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.8328, 0.8328, 0.8328	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/5985	0.53	0/8158
2	B	0.24	0/5981	0.54	3/8178 (0.0%)
3	C	0.26	0/610	0.78	0/826
4	D	0.21	0/1126	0.55	0/1517
5	E	0.20	0/552	0.53	0/745
6	K	0.22	0/590	0.58	0/797
7	M	0.22	0/241	0.63	0/326
All	All	0.24	0/15085	0.55	3/20547 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	533	LYS	CB-CG-CD	5.96	125.00	111.30
2	B	614	MET	CG-SD-CE	-5.78	88.18	100.90
2	B	659	MET	CB-CA-C	-5.34	99.78	110.42

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5787	0	5646	112	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5770	0	5547	103	0
3	C	600	0	581	18	0
4	D	1102	0	1101	20	0
5	E	543	0	525	10	0
6	K	579	0	601	7	0
7	M	238	0	260	4	0
8	A	2446	0	2250	87	0
8	B	2482	0	2461	88	0
8	K	130	0	142	2	0
9	A	33	0	46	3	0
9	B	33	0	46	1	0
10	A	280	0	370	23	0
10	B	280	0	371	23	0
10	K	40	0	53	4	0
11	A	98	0	148	12	0
11	B	73	0	92	5	0
11	M	49	0	74	1	0
12	A	50	0	73	0	0
12	B	86	0	118	9	0
12	K	55	0	86	0	0
13	A	8	0	0	1	0
13	C	16	0	0	1	0
14	B	41	0	54	5	0
14	M	41	0	54	2	0
15	B	54	0	77	0	0
All	All	20914	0	20776	384	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 9.

The worst 5 of 384 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)
3:C:58:CYS:HB2	13:C:3003:SF4:S4	2.03	0.98
2:B:582:ASN:C	2:B:582:ASN:HD22	1.82	0.87
8:B:1220:CLA:HAB	8:B:1227:CLA:HAC1	1.59	0.84
1:A:72:ILE:HG22	1:A:76:HIS:CE1	2.14	0.82
8:B:1236:CLA:H43	10:B:4010:BCR:H10C	1.61	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	737/739 (100%)	693 (94%)	43 (6%)	1 (0%)	48	83
2	B	727/729 (100%)	695 (96%)	32 (4%)	0	100	100
3	C	78/80 (98%)	76 (97%)	2 (3%)	0	100	100
4	D	139/141 (99%)	133 (96%)	6 (4%)	0	100	100
5	E	67/69 (97%)	62 (92%)	5 (8%)	0	100	100
6	K	79/80 (99%)	67 (85%)	12 (15%)	0	100	100
7	M	29/31 (94%)	29 (100%)	0	0	100	100
All	All	1856/1869 (99%)	1755 (95%)	100 (5%)	1 (0%)	49	83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	593/593 (100%)	593 (100%)	0	100	100
2	B	582/582 (100%)	581 (100%)	1 (0%)	87	85
3	C	68/68 (100%)	68 (100%)	0	100	100
4	D	116/116 (100%)	116 (100%)	0	100	100
5	E	58/58 (100%)	58 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	K	60/60 (100%)	60 (100%)	0	100	100
7	M	25/25 (100%)	25 (100%)	0	100	100
All	All	1502/1502 (100%)	1501 (100%)	1 (0%)	87	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	582	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	639	ASN
6	K	30	ASN
7	M	7	GLN
4	D	124	GLN
2	B	289	HIS

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](#)

120 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	LHG	B	5004	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
8	CLA	B	1230	-	69,73,73	1.37	7 (10%)	83,113,113	2.00	19 (22%)
8	CLA	A	1117	-	69,73,73	1.37	6 (8%)	83,113,113	1.99	18 (21%)
8	CLA	A	1103	-	64,68,73	1.42	7 (10%)	77,107,113	2.01	19 (24%)
8	CLA	A	1111	-	59,63,73	1.48	6 (10%)	71,101,113	2.11	19 (26%)
8	CLA	B	1207	-	59,63,73	1.47	7 (11%)	71,101,113	2.01	19 (26%)
8	CLA	B	1206	-	59,63,73	1.49	6 (10%)	71,101,113	2.16	20 (28%)
8	CLA	B	1205	-	59,63,73	1.49	7 (11%)	71,101,113	2.12	18 (25%)
8	CLA	B	1237	-	69,73,73	1.36	7 (10%)	83,113,113	2.04	22 (26%)
8	CLA	B	1203	-	69,73,73	1.37	7 (10%)	83,113,113	1.88	18 (21%)
10	BCR	B	4017	-	41,41,41	1.86	5 (12%)	56,56,56	4.52	19 (33%)
8	CLA	B	1211	-	50,54,73	1.61	8 (16%)	60,90,113	2.02	15 (25%)
8	CLA	A	1011	-	64,68,73	1.44	7 (10%)	77,107,113	2.00	18 (23%)
14	ECH	M	4021	-	42,42,42	0.78	0	55,58,58	2.09	16 (29%)
8	CLA	B	1220	-	61,65,73	1.45	7 (11%)	73,103,113	2.06	20 (27%)
8	CLA	A	1124	-	59,63,73	1.49	7 (11%)	71,101,113	2.03	16 (22%)
8	CLA	B	1022	-	64,68,73	1.44	7 (10%)	77,107,113	1.95	21 (27%)
10	BCR	B	4014	-	41,41,41	1.90	4 (9%)	56,56,56	4.51	18 (32%)
8	CLA	A	1127	-	69,73,73	1.40	6 (8%)	83,113,113	1.84	19 (22%)
8	CLA	A	1136	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	19 (22%)
8	CLA	B	1021	-	64,68,73	1.41	7 (10%)	77,107,113	2.12	21 (27%)
8	CLA	B	1225	-	69,73,73	1.39	7 (10%)	83,113,113	1.92	18 (21%)
11	LHG	M	5001	-	48,48,48	0.40	0	51,54,54	1.05	3 (5%)
8	CLA	A	1107	-	54,58,73	1.55	6 (11%)	65,95,113	2.18	17 (26%)
8	CLA	A	1801	-	50,54,73	1.61	7 (14%)	60,90,113	2.05	15 (25%)
8	CLA	B	1219	-	69,73,73	1.36	6 (8%)	83,113,113	1.93	19 (22%)
8	CLA	A	1125	-	56,60,73	1.54	8 (14%)	67,97,113	2.11	22 (32%)
8	CLA	B	1214	-	69,73,73	1.37	8 (11%)	83,113,113	1.93	18 (21%)
8	CLA	A	1112	-	54,58,73	1.53	6 (11%)	65,95,113	2.14	17 (26%)
8	CLA	B	1239	-	69,73,73	1.38	7 (10%)	83,113,113	1.96	18 (21%)
8	CLA	A	1113	-	49,53,73	1.58	6 (12%)	59,89,113	2.13	17 (28%)
14	ECH	B	4006	-	42,42,42	0.86	1 (2%)	55,58,58	2.19	16 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	BCR	B	4004	-	41,41,41	1.85	4 (9%)	56,56,56	4.38	17 (30%)
10	BCR	A	4012	-	41,41,41	1.86	4 (9%)	56,56,56	4.35	16 (28%)
8	CLA	A	1110	-	64,68,73	1.42	7 (10%)	77,107,113	2.04	19 (24%)
8	CLA	A	1133	-	69,73,73	1.36	8 (11%)	83,113,113	1.94	16 (19%)
8	CLA	B	1213	-	69,73,73	1.36	7 (10%)	83,113,113	2.10	22 (26%)
8	CLA	B	1238	-	69,73,73	1.35	6 (8%)	83,113,113	1.90	21 (25%)
8	CLA	B	1023	-	64,68,73	1.41	6 (9%)	77,107,113	1.97	18 (23%)
8	CLA	K	1401	-	69,73,73	1.35	6 (8%)	83,113,113	1.96	21 (25%)
11	LHG	A	5003	-	48,48,48	0.40	0	51,54,54	1.04	3 (5%)
8	CLA	A	1119	-	69,73,73	1.38	7 (10%)	83,113,113	1.90	18 (21%)
13	SF4	A	3001	1,2	0,12,12	-	-	-	-	-
8	CLA	A	1120	-	53,57,73	1.55	7 (13%)	62,93,113	2.22	17 (27%)
9	PQN	B	2002	-	34,34,34	0.36	0	42,45,45	1.17	3 (7%)
10	BCR	A	4008	-	41,41,41	1.80	4 (9%)	56,56,56	4.23	14 (25%)
10	BCR	B	4005	-	41,41,41	1.83	4 (9%)	56,56,56	4.38	15 (26%)
10	BCR	A	4001	-	41,41,41	1.87	4 (9%)	56,56,56	4.36	17 (30%)
11	LHG	B	5006	-	23,23,48	0.53	0	26,29,54	1.37	3 (11%)
8	CLA	B	1231	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	19 (22%)
13	SF4	C	3003	3	0,12,12	-	-	-	-	-
8	CLA	B	1229	-	69,73,73	1.37	7 (10%)	83,113,113	1.94	19 (22%)
8	CLA	A	1135	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	17 (20%)
8	CLA	B	1202	-	69,73,73	1.37	8 (11%)	83,113,113	1.88	16 (19%)
11	LHG	A	5001	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
8	CLA	A	1137	-	54,58,73	1.55	7 (12%)	65,95,113	2.13	20 (30%)
8	CLA	A	1106	-	64,68,73	1.42	8 (12%)	77,107,113	1.96	17 (22%)
8	CLA	B	1228	-	69,73,73	1.39	7 (10%)	83,113,113	1.87	19 (22%)
8	CLA	A	1102	-	59,63,73	1.48	7 (11%)	71,101,113	2.17	20 (28%)
8	CLA	B	1221	-	59,63,73	1.48	7 (11%)	71,101,113	2.07	19 (26%)
8	CLA	B	1212	-	49,53,73	1.60	8 (16%)	59,89,113	2.13	18 (30%)
8	CLA	A	1114	-	49,53,73	1.61	7 (14%)	59,89,113	2.13	17 (28%)
8	CLA	A	1101	-	69,73,73	1.36	6 (8%)	83,113,113	1.96	20 (24%)
8	CLA	A	1121	-	54,58,73	1.54	7 (12%)	65,95,113	2.22	19 (29%)
8	CLA	A	1118	-	50,54,73	1.60	7 (14%)	60,90,113	2.11	14 (23%)
8	CLA	B	1234	-	69,73,73	1.37	7 (10%)	83,113,113	1.95	19 (22%)
10	BCR	A	4007	-	41,41,41	1.82	4 (9%)	56,56,56	4.30	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLA	B	1218	-	54,58,73	1.53	7 (12%)	65,95,113	2.16	18 (27%)
8	CLA	B	1236	-	54,58,73	1.57	6 (11%)	65,95,113	2.10	19 (29%)
12	LMG	B	5002	-	55,55,55	1.13	6 (10%)	63,63,63	1.04	3 (4%)
8	CLA	A	1115	-	50,54,73	1.59	8 (16%)	60,90,113	2.08	14 (23%)
10	BCR	B	4010	-	41,41,41	1.83	4 (9%)	56,56,56	4.41	21 (37%)
8	CLA	B	1222	-	59,63,73	1.46	6 (10%)	71,101,113	2.05	18 (25%)
8	CLA	A	1123	-	69,73,73	1.41	9 (13%)	83,113,113	2.00	15 (18%)
10	BCR	B	4011	-	41,41,41	1.88	4 (9%)	56,56,56	4.36	17 (30%)
8	CLA	A	1129	-	50,54,73	1.62	8 (16%)	60,90,113	2.09	13 (21%)
13	SF4	C	3002	3	0,12,12	-	-	-	-	-
15	SQD	B	5008	-	53,54,54	0.79	0	62,65,65	0.90	2 (3%)
8	CLA	B	1224	-	66,70,73	1.42	7 (10%)	79,109,113	1.93	18 (22%)
8	CLA	B	1232	-	54,58,73	1.55	7 (12%)	65,95,113	2.17	20 (30%)
8	CLA	B	1223	-	64,68,73	1.44	9 (14%)	77,107,113	2.05	18 (23%)
8	CLA	A	1116	-	58,62,73	1.51	8 (13%)	69,99,113	2.07	20 (28%)
8	CLA	B	1210	-	69,73,73	1.37	7 (10%)	83,113,113	1.97	20 (24%)
8	CLA	A	1132	-	54,58,73	1.53	7 (12%)	65,95,113	2.14	17 (26%)
12	LMG	K	5009	-	55,55,55	1.14	6 (10%)	63,63,63	1.03	2 (3%)
8	CLA	B	1227	-	59,63,73	1.48	7 (11%)	71,101,113	1.99	17 (23%)
8	CLA	A	1013	-	59,63,73	1.48	6 (10%)	71,101,113	2.10	20 (28%)
10	BCR	A	4003	-	41,41,41	1.79	4 (9%)	56,56,56	3.95	16 (28%)
8	CLA	A	1126	-	64,68,73	1.43	8 (12%)	77,107,113	2.00	19 (24%)
9	PQN	A	2001	-	34,34,34	0.37	0	42,45,45	1.11	5 (11%)
8	CLA	A	1130	-	59,63,73	1.48	7 (11%)	71,101,113	2.03	19 (26%)
8	CLA	A	1139	-	50,54,73	1.61	7 (14%)	60,90,113	2.13	17 (28%)
12	LMG	B	5005	-	31,31,55	0.54	0	39,39,63	1.10	2 (5%)
8	CLA	A	1108	-	49,53,73	1.63	8 (16%)	59,89,113	2.08	16 (27%)
8	CLA	B	1217	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	18 (21%)
8	CLA	B	1204	-	50,54,73	1.59	8 (16%)	60,90,113	2.10	17 (28%)
8	CLA	A	1131	-	59,63,73	1.47	7 (11%)	71,101,113	2.07	19 (26%)
8	CLA	B	1226	-	69,73,73	1.38	7 (10%)	83,113,113	1.99	17 (20%)
8	CLA	K	1402	-	69,73,73	1.36	7 (10%)	83,113,113	1.97	21 (25%)
10	BCR	K	4001	-	41,41,41	1.83	4 (9%)	56,56,56	4.26	14 (25%)
10	BCR	A	4019	-	41,41,41	1.85	4 (9%)	56,56,56	4.40	16 (28%)
8	CLA	B	1240	-	69,73,73	1.37	7 (10%)	83,113,113	1.96	19 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	CLA	B	1216	-	59,63,73	1.49	7 (11%)	71,101,113	2.04	19 (26%)
10	BCR	B	4018	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	18 (32%)
8	CLA	A	1122	-	64,68,73	1.41	7 (10%)	77,107,113	2.06	18 (23%)
8	CLA	A	1128	-	64,68,73	1.42	7 (10%)	77,107,113	1.99	18 (23%)
10	BCR	A	4002	-	41,41,41	1.82	4 (9%)	56,56,56	4.40	17 (30%)
8	CLA	B	1209	-	69,73,73	1.36	7 (10%)	83,113,113	1.99	18 (21%)
8	CLA	B	1201	-	50,54,73	1.58	7 (14%)	60,90,113	2.10	15 (25%)
8	CLA	A	1104	-	69,73,73	1.36	7 (10%)	83,113,113	1.94	20 (24%)
8	CLA	A	1134	-	50,54,73	1.60	8 (16%)	60,90,113	2.14	17 (28%)
8	CLA	B	1208	-	49,53,73	1.61	7 (14%)	59,89,113	2.06	16 (27%)
8	CLA	A	1105	-	54,58,73	1.54	7 (12%)	65,95,113	2.13	18 (27%)
8	CLA	A	1012	-	59,63,73	1.52	7 (11%)	71,101,113	1.96	20 (28%)
8	CLA	A	1138	-	69,73,73	1.36	6 (8%)	83,113,113	1.98	20 (24%)
8	CLA	A	1109	-	64,68,73	1.41	6 (9%)	77,107,113	2.05	21 (27%)
8	CLA	B	1215	-	69,73,73	1.38	6 (8%)	83,113,113	1.98	17 (20%)
8	CLA	B	1235	-	64,68,73	1.42	9 (14%)	77,107,113	1.98	23 (29%)
12	LMG	A	5002	-	50,50,55	1.03	5 (10%)	58,58,63	1.08	2 (3%)
8	CLA	A	1140	-	69,73,73	1.37	7 (10%)	83,113,113	1.93	17 (20%)

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
11	LHG	B	5004	-	-	28/53/53/53	-
8	CLA	B	1230	-	-	20/39/115/115	-
8	CLA	A	1117	-	-	20/39/115/115	-
8	CLA	A	1103	-	-	17/33/109/115	-
8	CLA	A	1111	-	-	12/27/103/115	-
8	CLA	B	1207	-	-	9/27/103/115	-
8	CLA	B	1206	-	-	11/27/103/115	-
8	CLA	B	1205	-	-	12/27/103/115	-
8	CLA	B	1237	-	-	18/39/115/115	-
8	CLA	B	1203	-	-	18/39/115/115	-
10	BCR	B	4017	-	-	10/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	B	1211	-	-	3/17/93/115	-
8	CLA	A	1011	-	-	18/33/109/115	-
14	ECH	M	4021	-	-	17/29/66/66	0/2/2/2
8	CLA	B	1220	-	-	11/30/106/115	-
8	CLA	A	1124	-	-	7/27/103/115	-
8	CLA	B	1022	-	-	14/33/109/115	-
10	BCR	B	4014	-	-	12/29/63/63	0/2/2/2
8	CLA	A	1127	-	-	22/39/115/115	-
8	CLA	A	1136	-	-	19/39/115/115	-
8	CLA	B	1021	-	-	19/33/109/115	-
8	CLA	B	1225	-	-	13/39/115/115	-
11	LHG	M	5001	-	-	34/53/53/53	-
8	CLA	A	1107	-	-	6/21/97/115	-
8	CLA	A	1801	-	-	9/17/93/115	-
8	CLA	B	1219	-	-	22/39/115/115	-
8	CLA	A	1125	-	-	9/24/100/115	-
8	CLA	B	1214	-	-	18/39/115/115	-
8	CLA	A	1112	-	-	11/21/97/115	-
8	CLA	B	1239	-	-	14/39/115/115	-
8	CLA	A	1113	-	-	8/15/91/115	-
14	ECH	B	4006	-	-	10/29/66/66	0/2/2/2
10	BCR	B	4004	-	-	12/29/63/63	0/2/2/2
10	BCR	A	4012	-	-	11/29/63/63	0/2/2/2
8	CLA	A	1110	-	-	18/33/109/115	-
8	CLA	A	1133	-	-	17/39/115/115	-
8	CLA	B	1213	-	-	14/39/115/115	-
8	CLA	B	1238	-	-	17/39/115/115	-
8	CLA	B	1023	-	-	15/33/109/115	-
8	CLA	K	1401	-	-	18/39/115/115	-
11	LHG	A	5003	-	-	29/53/53/53	-
8	CLA	A	1119	-	-	16/39/115/115	-
13	SF4	A	3001	1,2	-	-	0/6/5/5
8	CLA	A	1120	-	-	10/20/96/115	-
9	PQN	B	2002	-	-	9/23/43/43	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	BCR	A	4008	-	-	17/29/63/63	0/2/2/2
10	BCR	B	4005	-	-	8/29/63/63	0/2/2/2
10	BCR	A	4001	-	-	11/29/63/63	0/2/2/2
11	LHG	B	5006	-	-	17/28/28/53	-
8	CLA	B	1231	-	-	14/39/115/115	-
13	SF4	C	3003	3	-	-	0/6/5/5
8	CLA	B	1229	-	-	18/39/115/115	-
8	CLA	A	1135	-	-	17/39/115/115	-
8	CLA	B	1202	-	-	15/39/115/115	-
11	LHG	A	5001	-	-	30/53/53/53	-
8	CLA	A	1137	-	-	10/21/97/115	-
8	CLA	A	1106	-	-	13/33/109/115	-
8	CLA	B	1228	-	-	23/39/115/115	-
8	CLA	A	1102	-	-	9/27/103/115	-
8	CLA	B	1221	-	-	9/27/103/115	-
8	CLA	B	1212	-	-	7/15/91/115	-
8	CLA	A	1114	-	-	7/15/91/115	-
8	CLA	A	1101	-	-	15/39/115/115	-
8	CLA	A	1121	-	-	9/21/97/115	-
8	CLA	A	1118	-	-	10/17/93/115	-
8	CLA	B	1234	-	-	21/39/115/115	-
10	BCR	A	4007	-	-	7/29/63/63	0/2/2/2
8	CLA	B	1218	-	-	12/21/97/115	-
8	CLA	B	1236	-	-	10/21/97/115	-
12	LMG	B	5002	-	-	13/50/70/70	0/1/1/1
8	CLA	A	1115	-	-	6/17/93/115	-
10	BCR	B	4010	-	-	12/29/63/63	0/2/2/2
8	CLA	B	1222	-	-	9/27/103/115	-
8	CLA	A	1123	-	-	24/39/115/115	-
10	BCR	B	4011	-	-	16/29/63/63	0/2/2/2
8	CLA	A	1129	-	-	9/17/93/115	-
13	SF4	C	3002	3	-	-	0/6/5/5
15	SQD	B	5008	-	-	10/49/69/69	0/1/1/1
8	CLA	B	1224	-	-	21/36/112/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	B	1232	-	-	11/21/97/115	-
8	CLA	B	1223	-	-	17/33/109/115	-
8	CLA	A	1116	-	-	14/26/102/115	-
8	CLA	B	1210	-	-	25/39/115/115	-
8	CLA	A	1132	-	-	10/21/97/115	-
12	LMG	K	5009	-	-	16/50/70/70	0/1/1/1
8	CLA	B	1227	-	-	16/27/103/115	-
8	CLA	A	1013	-	-	13/27/103/115	-
10	BCR	A	4003	-	-	13/29/63/63	0/2/2/2
8	CLA	A	1126	-	-	18/33/109/115	-
9	PQN	A	2001	-	-	8/23/43/43	0/2/2/2
8	CLA	A	1130	-	-	13/27/103/115	-
8	CLA	A	1139	-	-	8/17/93/115	-
12	LMG	B	5005	-	-	6/26/46/70	0/1/1/1
8	CLA	A	1108	-	-	11/15/91/115	-
8	CLA	B	1217	-	-	19/39/115/115	-
8	CLA	B	1204	-	-	8/17/93/115	-
8	CLA	A	1131	-	-	15/27/103/115	-
8	CLA	B	1226	-	-	15/39/115/115	-
8	CLA	K	1402	-	-	20/39/115/115	-
10	BCR	K	4001	-	-	8/29/63/63	0/2/2/2
10	BCR	A	4019	-	-	9/29/63/63	0/2/2/2
8	CLA	B	1240	-	-	17/39/115/115	-
8	CLA	B	1216	-	-	17/27/103/115	-
10	BCR	B	4018	-	-	9/29/63/63	0/2/2/2
8	CLA	A	1122	-	-	16/33/109/115	-
8	CLA	A	1128	-	-	17/33/109/115	-
10	BCR	A	4002	-	-	11/29/63/63	0/2/2/2
8	CLA	B	1209	-	-	25/39/115/115	-
8	CLA	B	1201	-	-	15/17/93/115	-
8	CLA	A	1104	-	-	20/39/115/115	-
8	CLA	A	1134	-	-	13/17/93/115	-
8	CLA	B	1208	-	-	5/15/91/115	-
8	CLA	A	1105	-	-	9/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	CLA	A	1012	-	-	10/27/103/115	-
8	CLA	A	1138	-	-	19/39/115/115	-
8	CLA	A	1109	-	-	16/33/109/115	-
8	CLA	B	1215	-	-	21/39/115/115	-
8	CLA	B	1235	-	-	16/33/109/115	-
12	LMG	A	5002	-	-	19/45/65/70	0/1/1/1
8	CLA	A	1140	-	-	16/39/115/115	-

The worst 5 of 696 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	4014	BCR	C10-C9	7.60	1.45	1.35
10	B	4011	BCR	C10-C9	7.41	1.45	1.35
10	A	4012	BCR	C10-C9	7.35	1.45	1.35
10	A	4019	BCR	C10-C9	7.23	1.45	1.35
10	B	4018	BCR	C10-C9	7.23	1.45	1.35

The worst 5 of 1932 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	4017	BCR	C10-C11-C12	18.17	179.92	123.22
10	A	4008	BCR	C10-C11-C12	17.82	178.84	123.22
10	A	4001	BCR	C10-C11-C12	17.71	178.50	123.22
10	B	4011	BCR	C10-C11-C12	17.58	178.09	123.22
10	A	4019	BCR	C10-C11-C12	17.52	177.90	123.22

There are no chirality outliers.

5 of 1670 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1011	CLA	C2A-CAA-CBA-CGA
8	A	1011	CLA	CHA-CBD-CGD-O1D
8	A	1011	CLA	CHA-CBD-CGD-O2D
8	A	1011	CLA	CBD-CGD-O2D-CED
8	A	1101	CLA	CHA-CBD-CGD-O1D

There are no ring outliers.

99 monomers are involved in 219 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	5004	LHG	5	0
8	B	1230	CLA	2	0
8	A	1117	CLA	5	0
8	A	1103	CLA	5	0
8	A	1111	CLA	2	0
8	B	1206	CLA	2	0
8	B	1205	CLA	1	0
8	B	1203	CLA	1	0
10	B	4017	BCR	4	0
8	B	1211	CLA	2	0
8	A	1011	CLA	2	0
14	M	4021	ECH	2	0
8	B	1220	CLA	2	0
8	A	1124	CLA	4	0
8	B	1022	CLA	2	0
10	B	4014	BCR	3	0
8	A	1127	CLA	4	0
8	A	1136	CLA	3	0
8	B	1021	CLA	5	0
8	B	1225	CLA	4	0
11	M	5001	LHG	1	0
8	A	1107	CLA	2	0
8	B	1219	CLA	4	0
8	B	1214	CLA	2	0
8	A	1112	CLA	6	0
8	B	1239	CLA	3	0
14	B	4006	ECH	5	0
10	B	4004	BCR	4	0
10	A	4012	BCR	3	0
8	A	1133	CLA	3	0
8	B	1213	CLA	4	0
8	B	1238	CLA	3	0
8	B	1023	CLA	1	0
8	K	1401	CLA	1	0
11	A	5003	LHG	4	0
8	A	1119	CLA	2	0
13	A	3001	SF4	1	0
8	A	1120	CLA	1	0
9	B	2002	PQN	1	0
10	A	4008	BCR	5	0
10	B	4005	BCR	3	0
10	A	4001	BCR	3	0
8	B	1231	CLA	3	0

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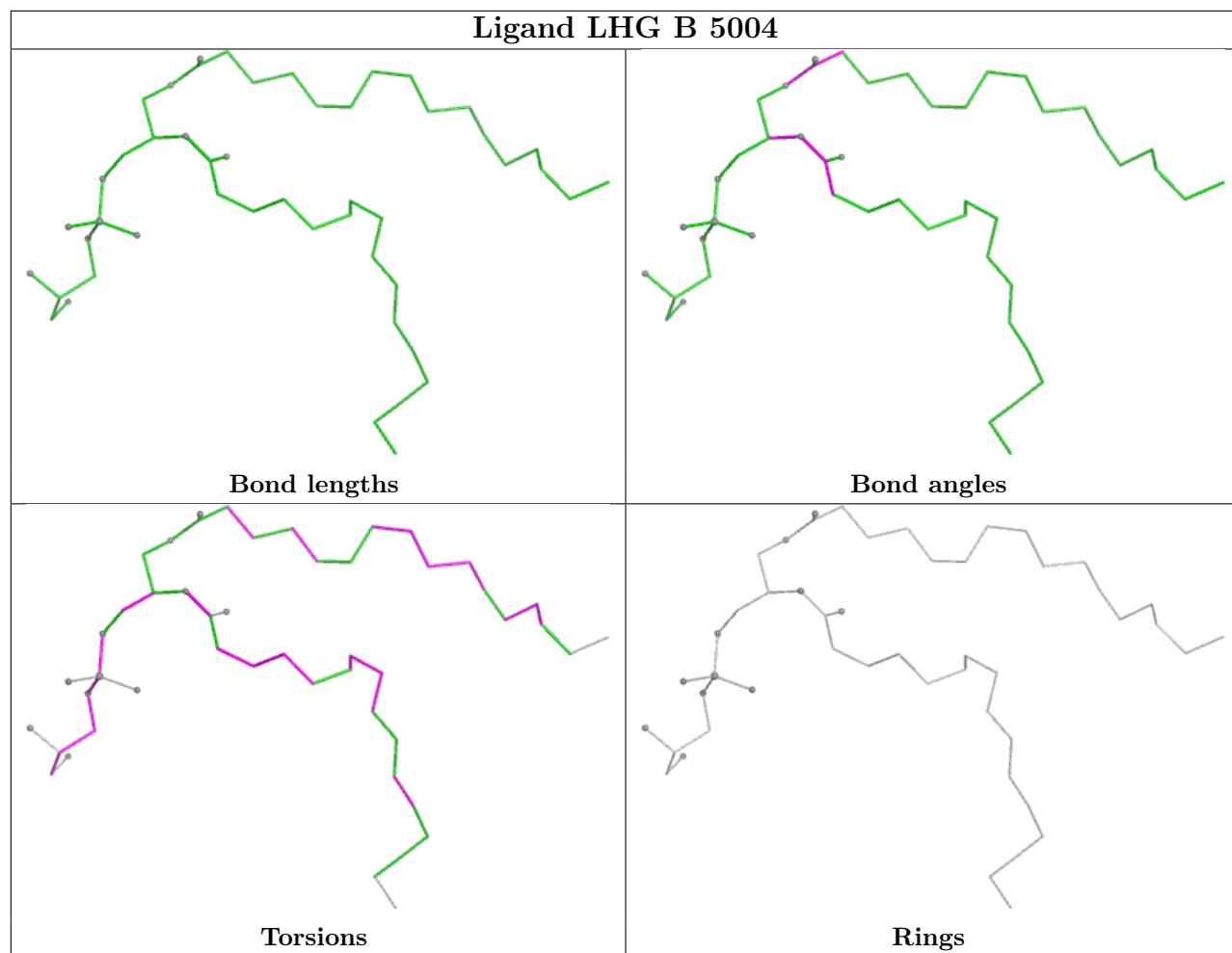
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	C	3003	SF4	1	0
8	B	1229	CLA	2	0
8	A	1135	CLA	2	0
8	B	1202	CLA	6	0
11	A	5001	LHG	8	0
8	A	1137	CLA	1	0
8	A	1106	CLA	3	0
8	B	1228	CLA	2	0
8	A	1102	CLA	1	0
8	B	1221	CLA	2	0
8	A	1114	CLA	1	0
8	A	1118	CLA	2	0
8	B	1234	CLA	4	0
10	A	4007	BCR	3	0
8	B	1218	CLA	1	0
8	B	1236	CLA	4	0
12	B	5002	LMG	9	0
8	A	1115	CLA	1	0
10	B	4010	BCR	4	0
8	B	1222	CLA	6	0
8	A	1123	CLA	2	0
10	B	4011	BCR	2	0
8	A	1129	CLA	2	0
8	B	1224	CLA	2	0
8	B	1223	CLA	2	0
8	A	1116	CLA	6	0
8	B	1210	CLA	2	0
8	A	1132	CLA	1	0
8	B	1227	CLA	7	0
8	A	1013	CLA	3	0
10	A	4003	BCR	2	0
8	A	1126	CLA	4	0
9	A	2001	PQN	3	0
8	A	1130	CLA	1	0
8	A	1139	CLA	1	0
8	A	1108	CLA	1	0
8	B	1217	CLA	4	0
8	B	1226	CLA	4	0
8	K	1402	CLA	1	0
10	K	4001	BCR	4	0
10	A	4019	BCR	2	0
8	B	1240	CLA	1	0

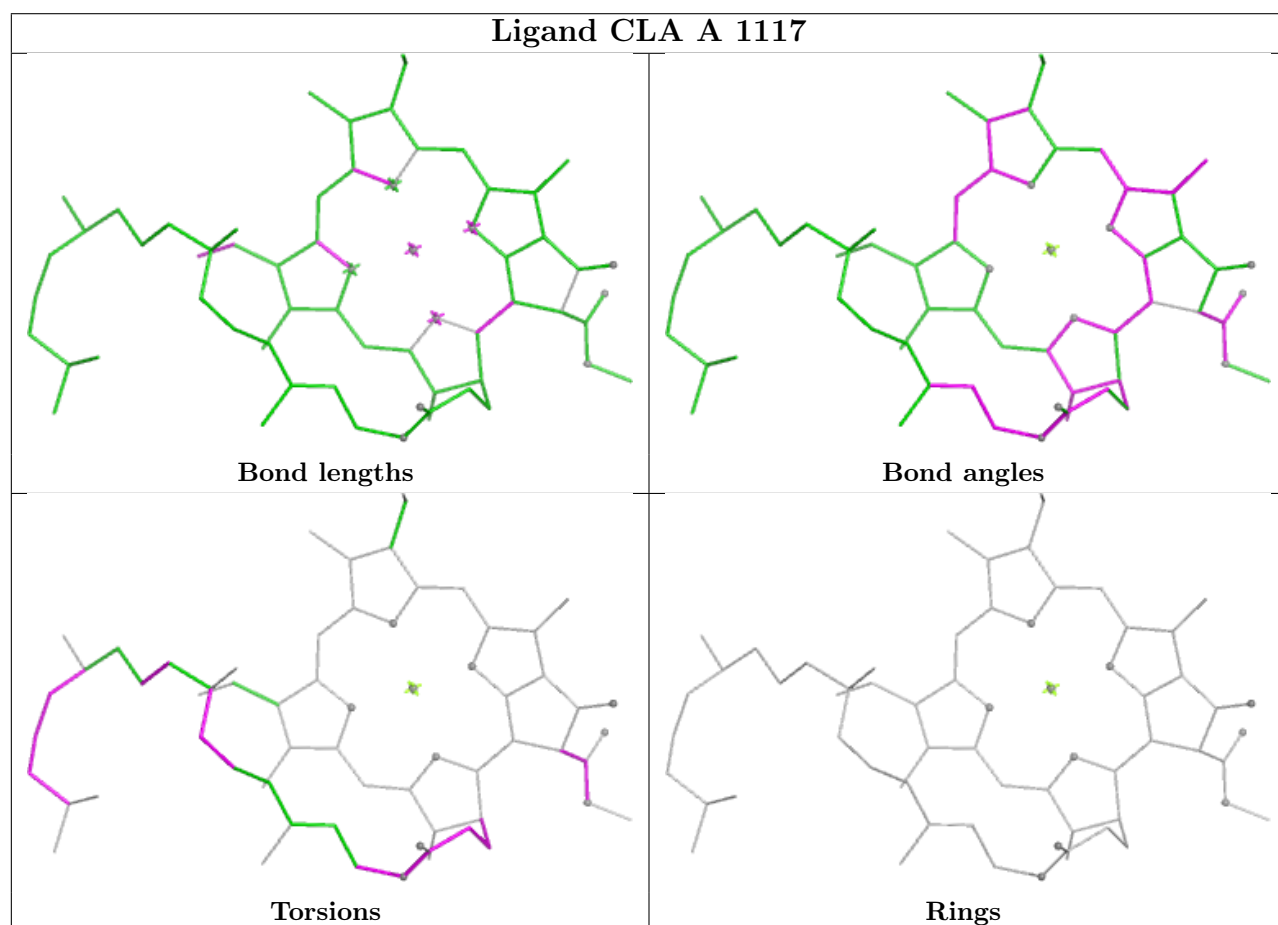
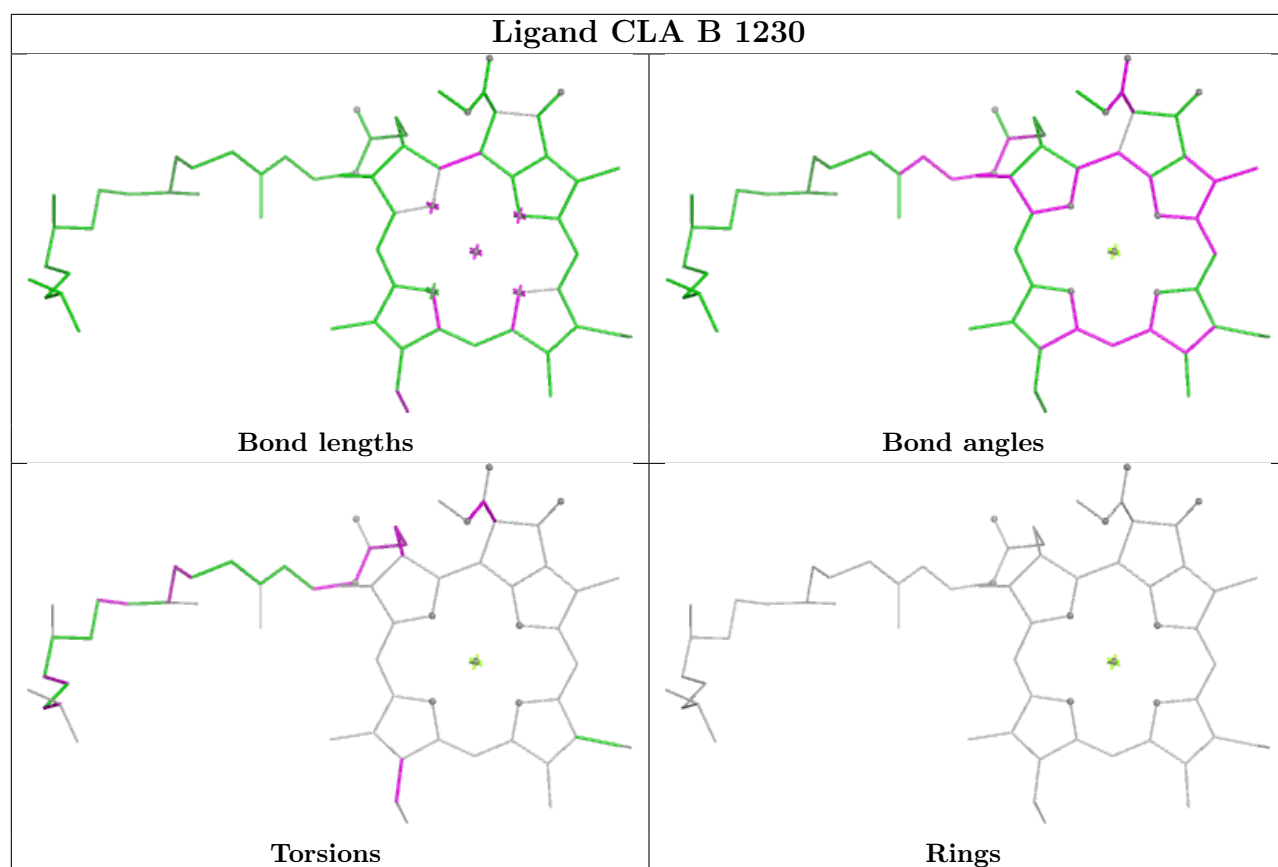
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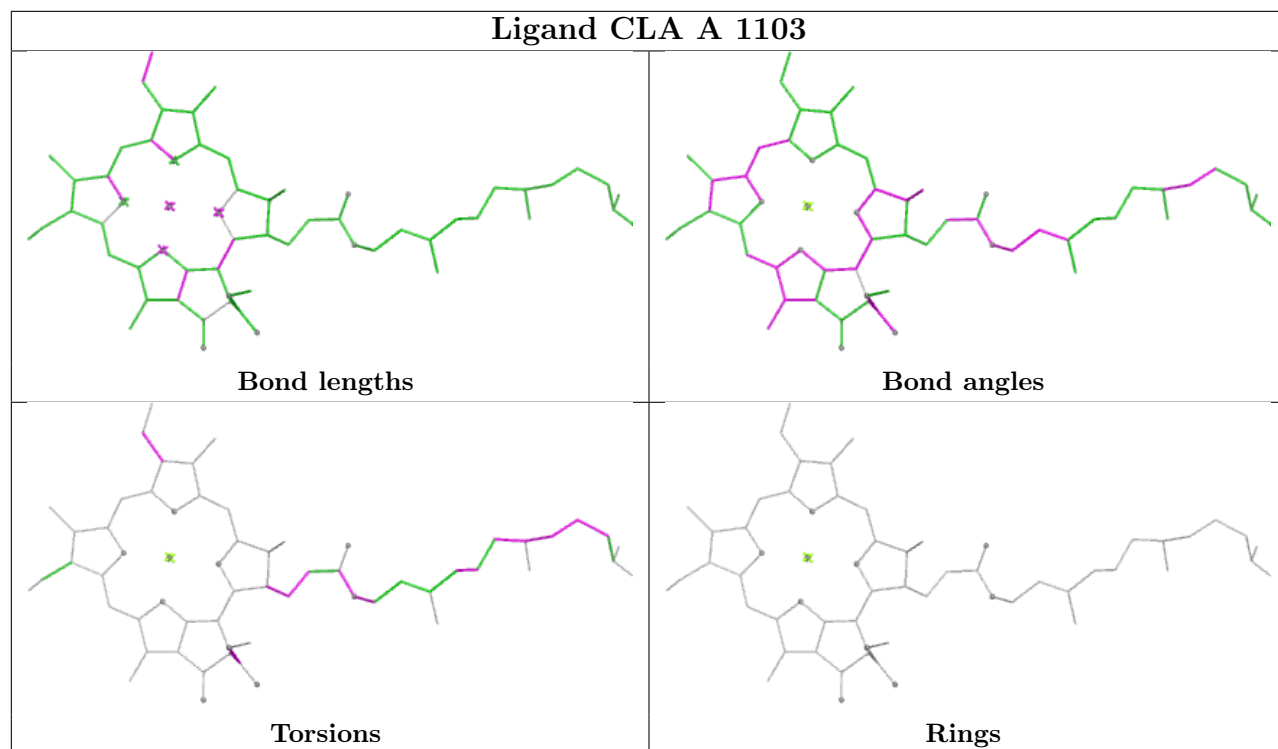
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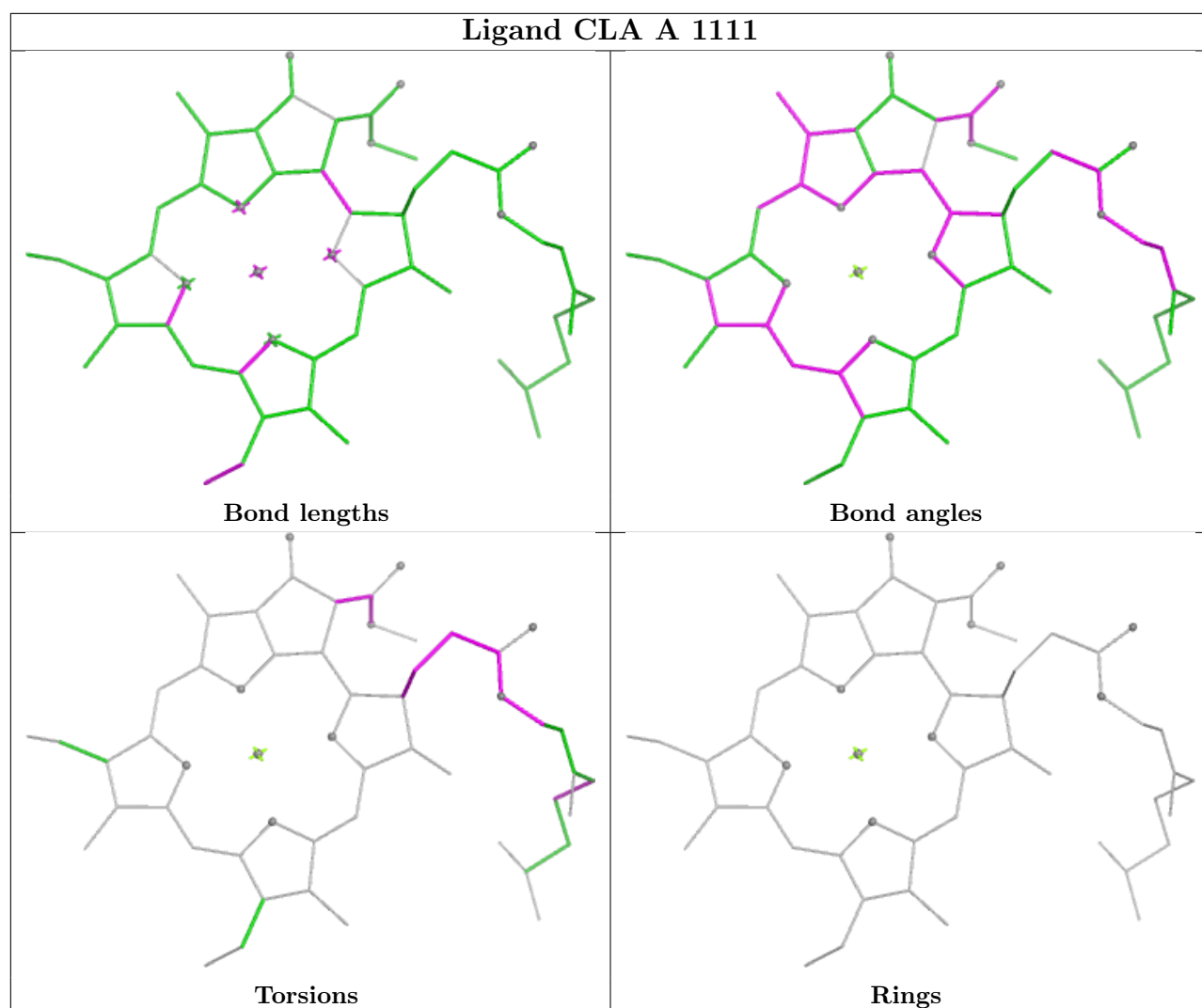
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	1216	CLA	4	0
10	B	4018	BCR	4	0
8	A	1122	CLA	3	0
8	A	1128	CLA	3	0
10	A	4002	BCR	5	0
8	B	1209	CLA	1	0
8	B	1208	CLA	1	0
8	A	1105	CLA	2	0
8	A	1012	CLA	3	0
8	A	1138	CLA	3	0
8	A	1109	CLA	4	0
8	B	1215	CLA	2	0
8	B	1235	CLA	4	0
8	A	1140	CLA	4	0

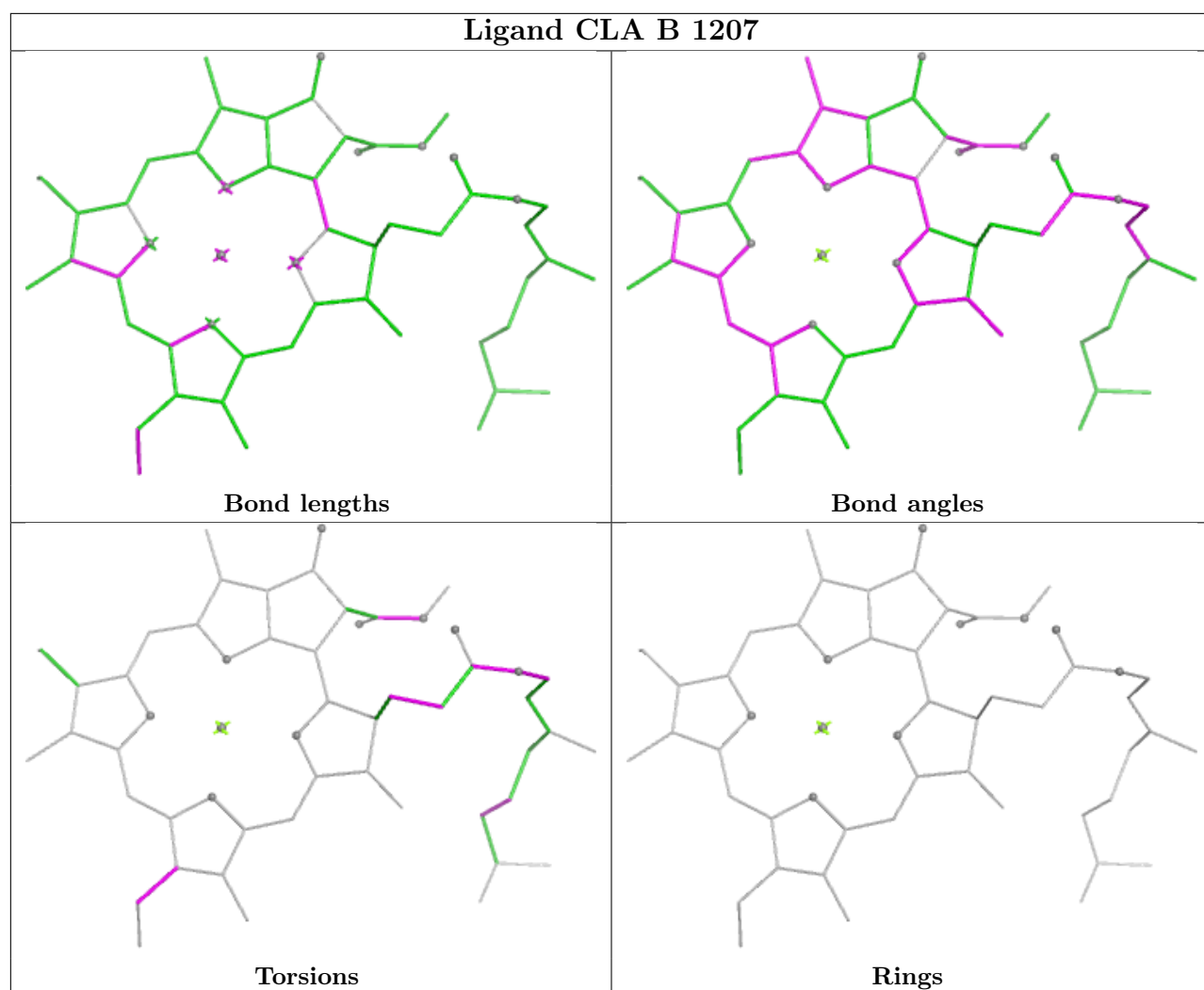
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

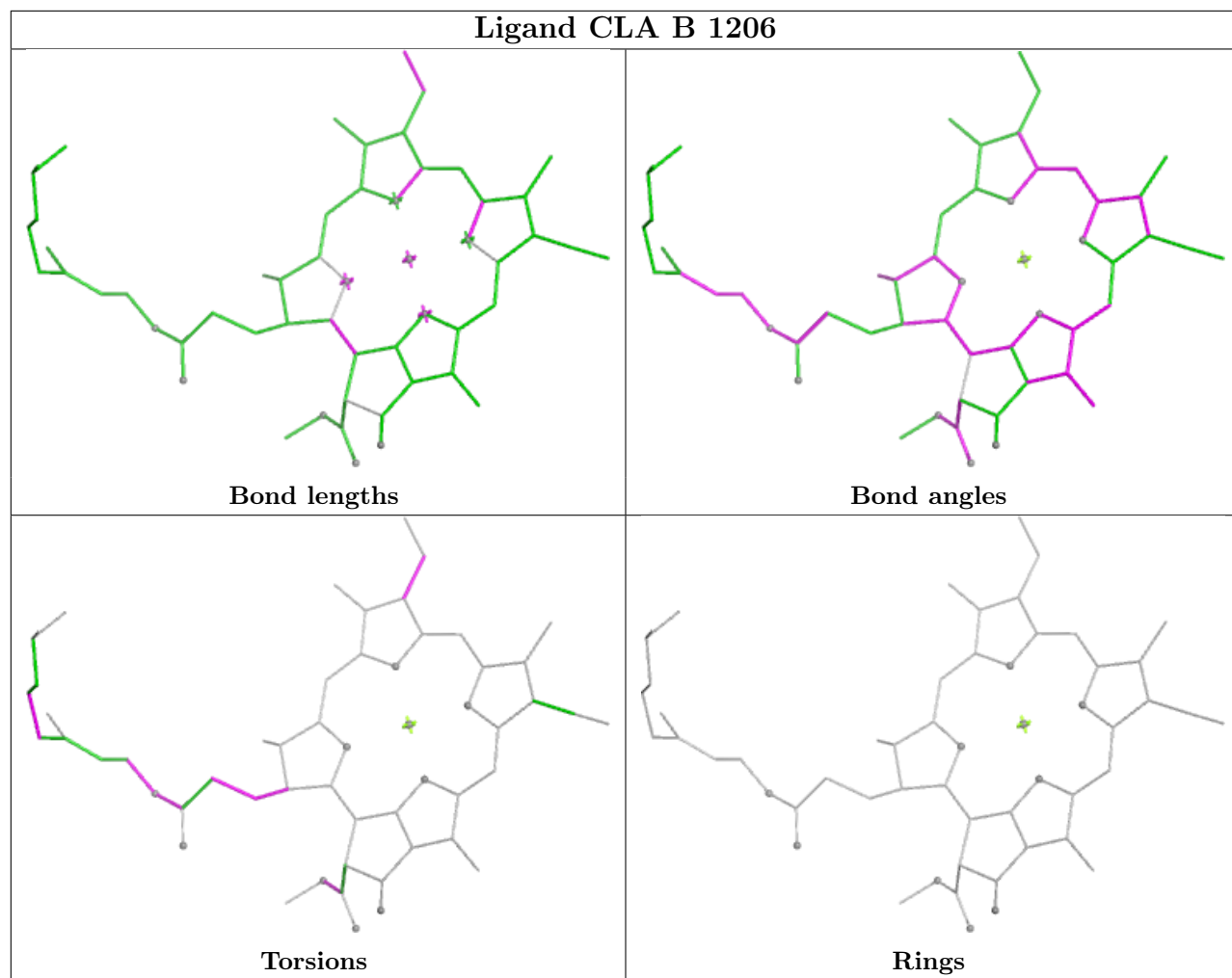


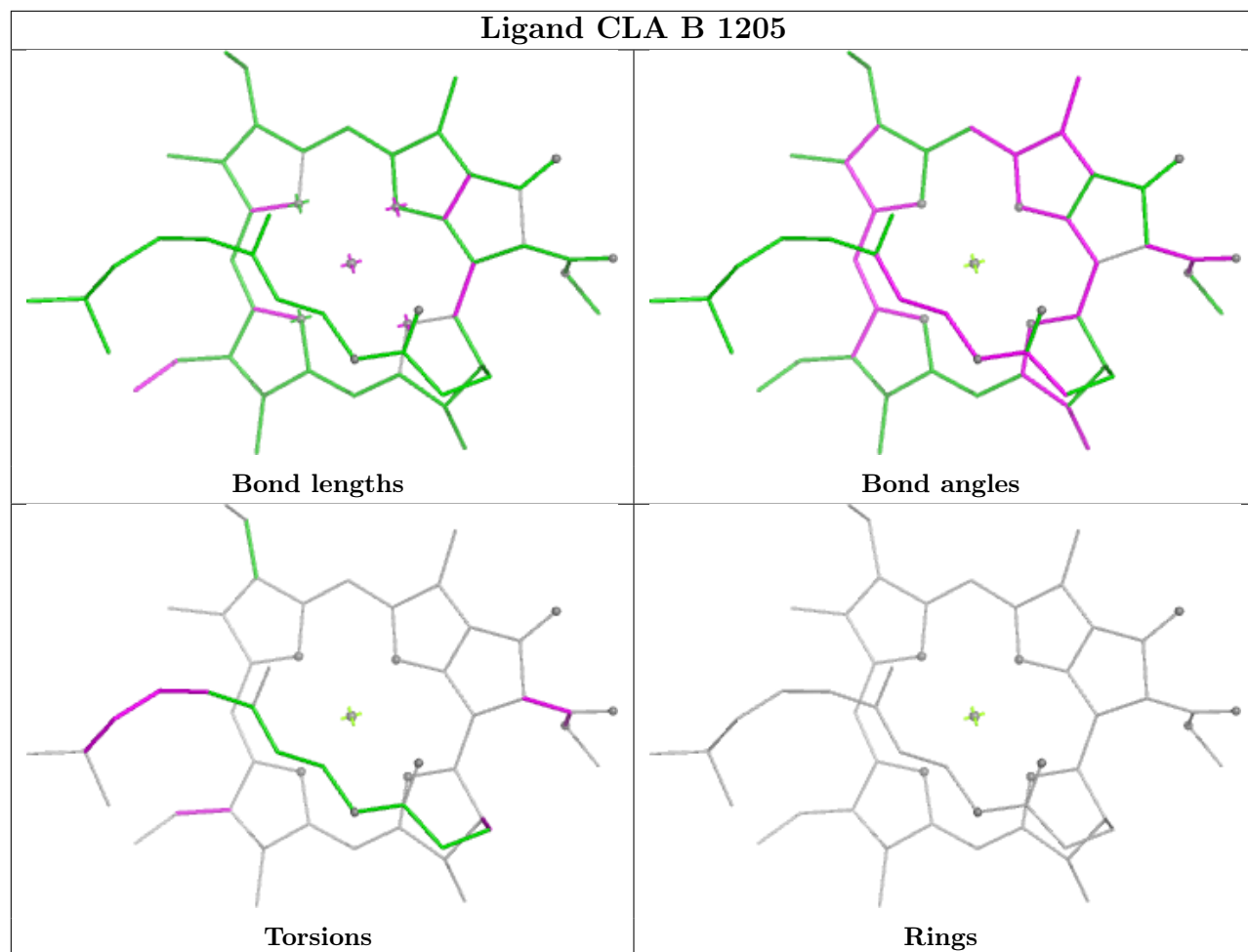


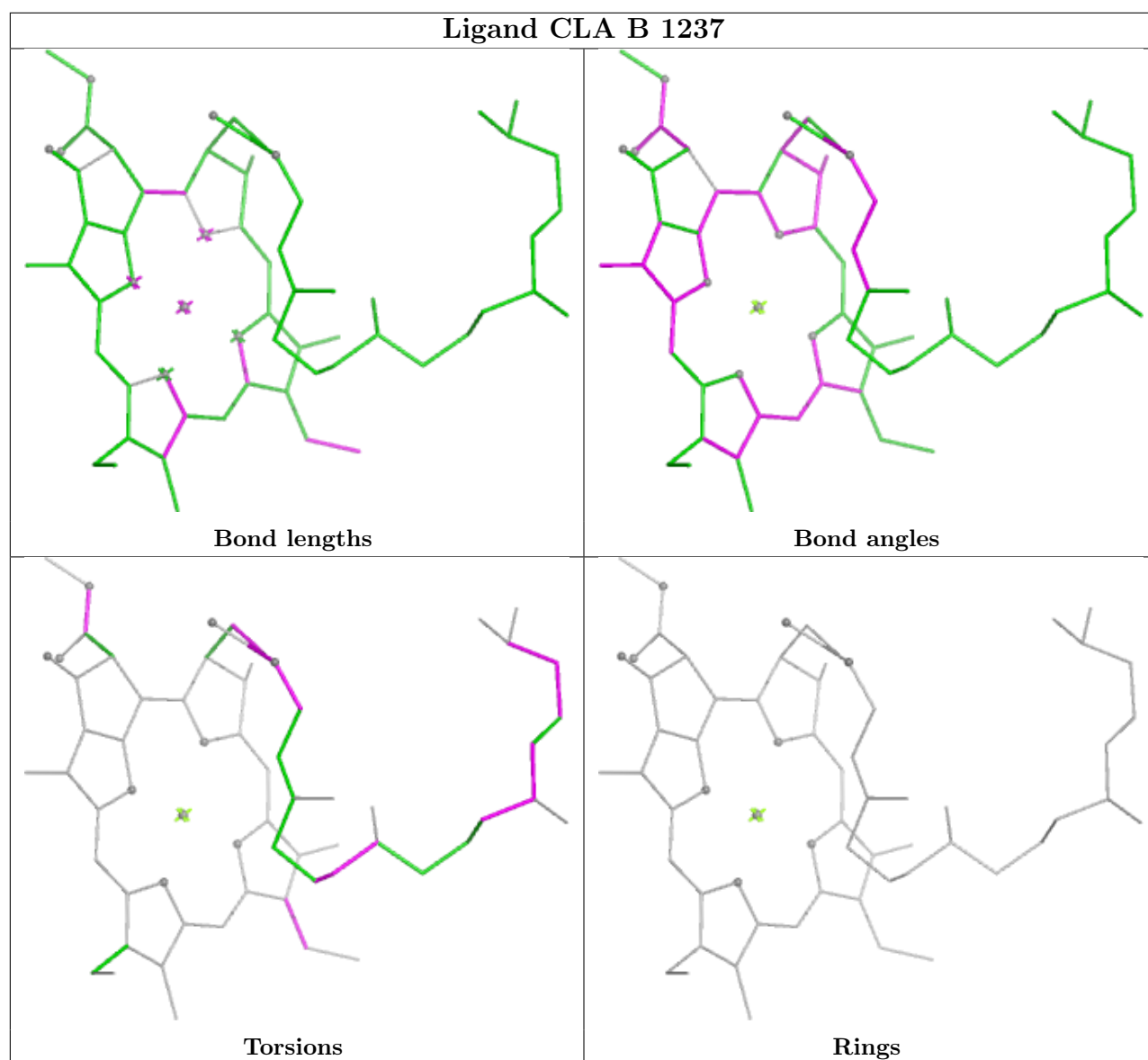


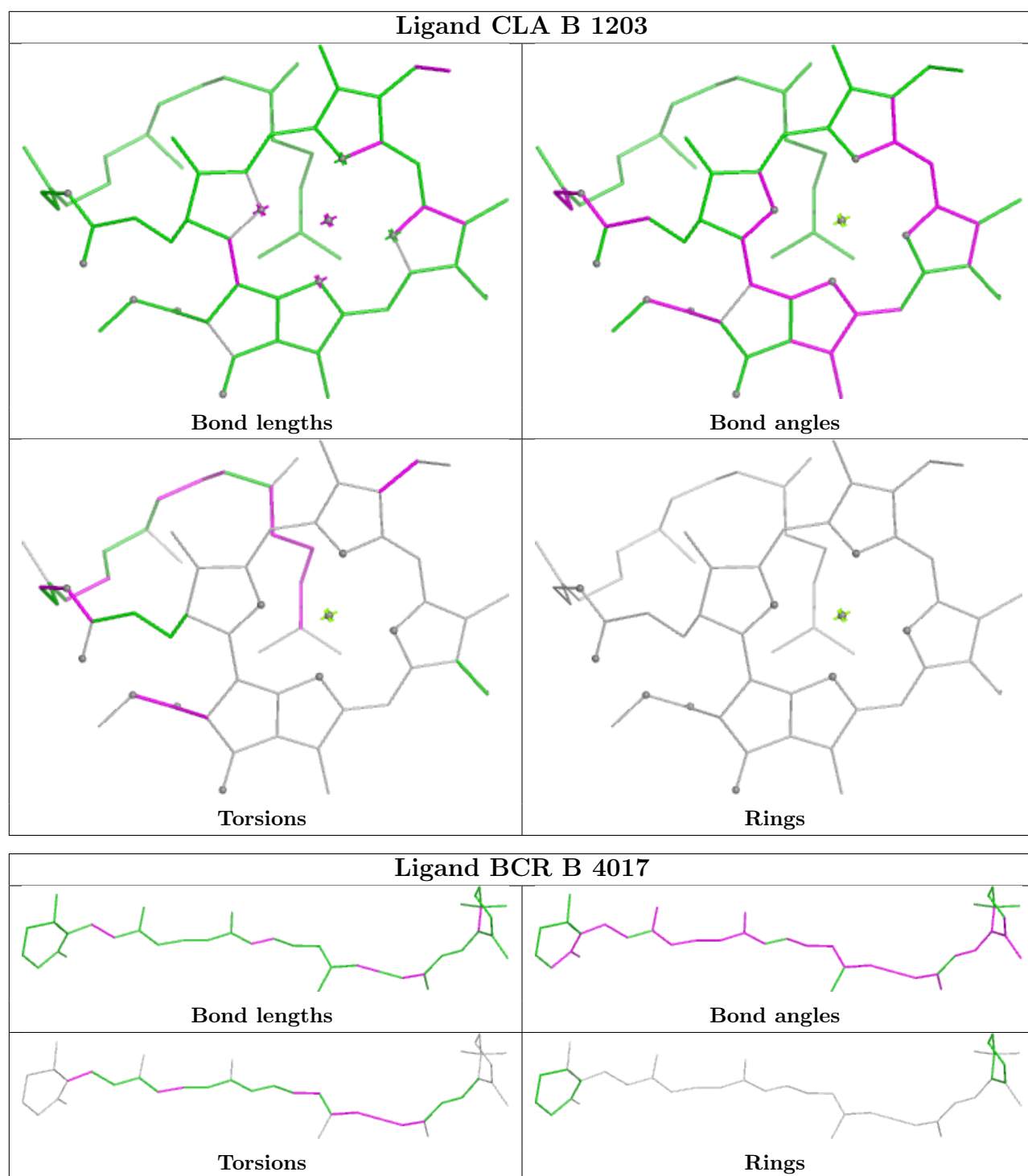


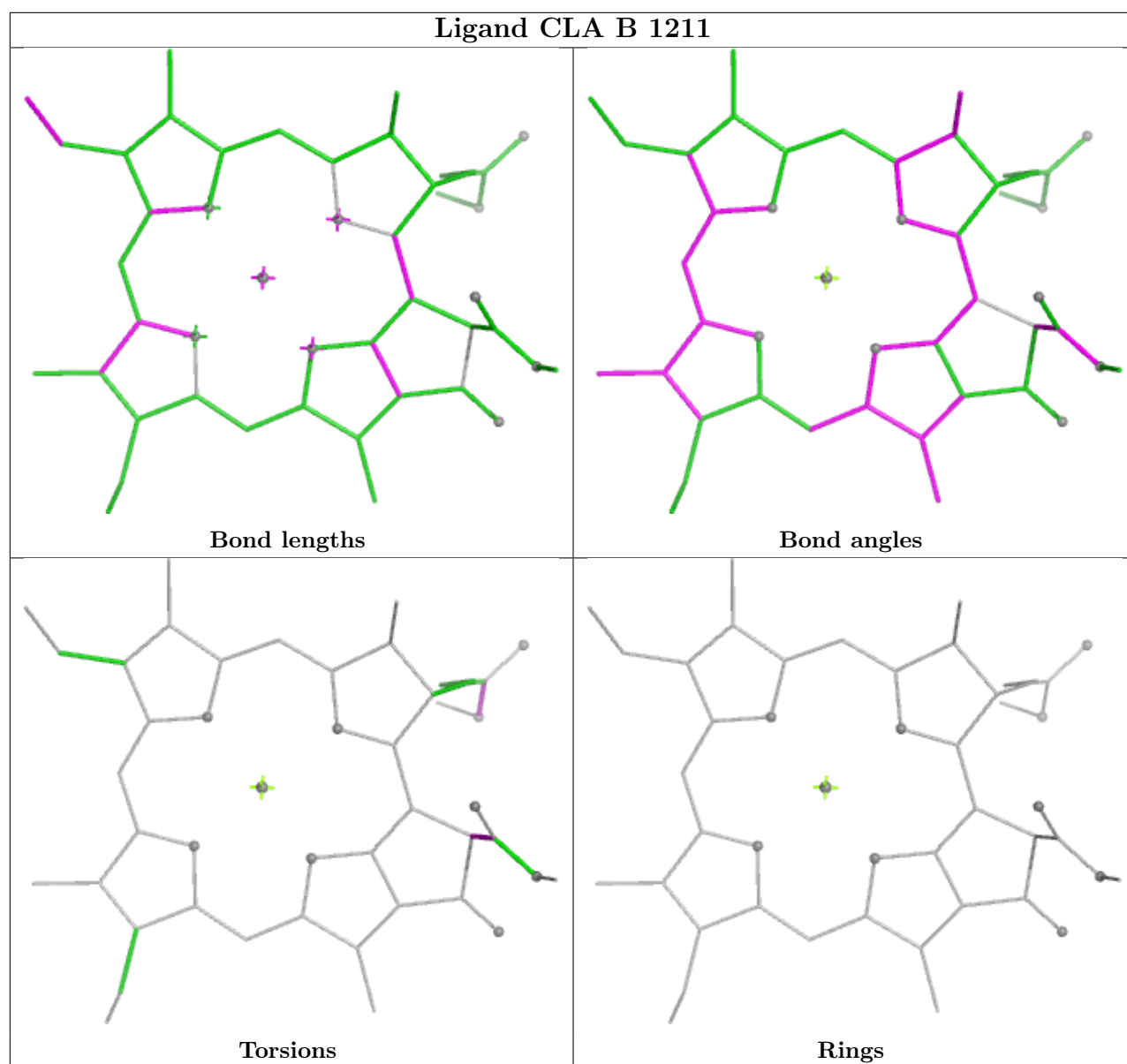


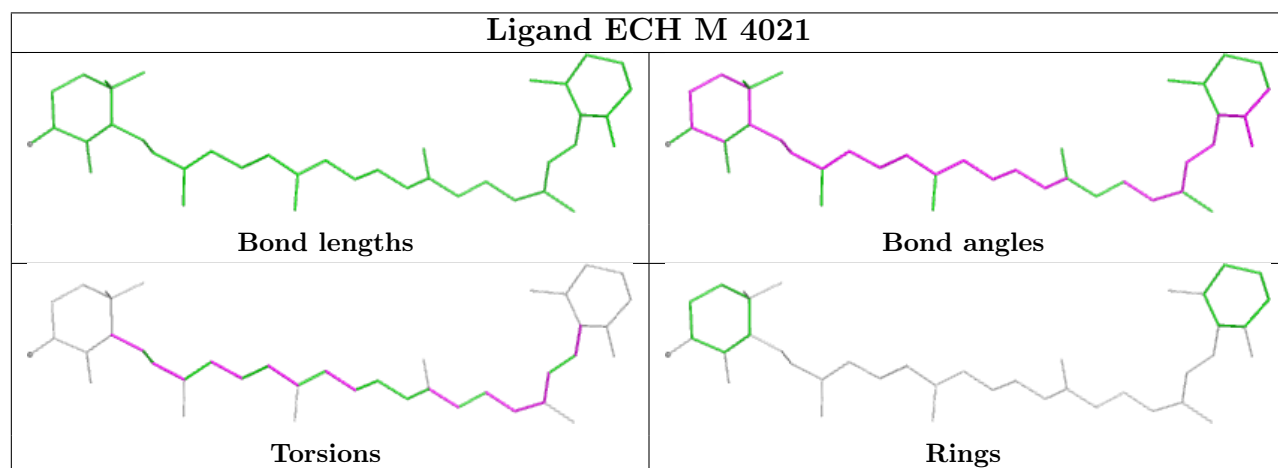
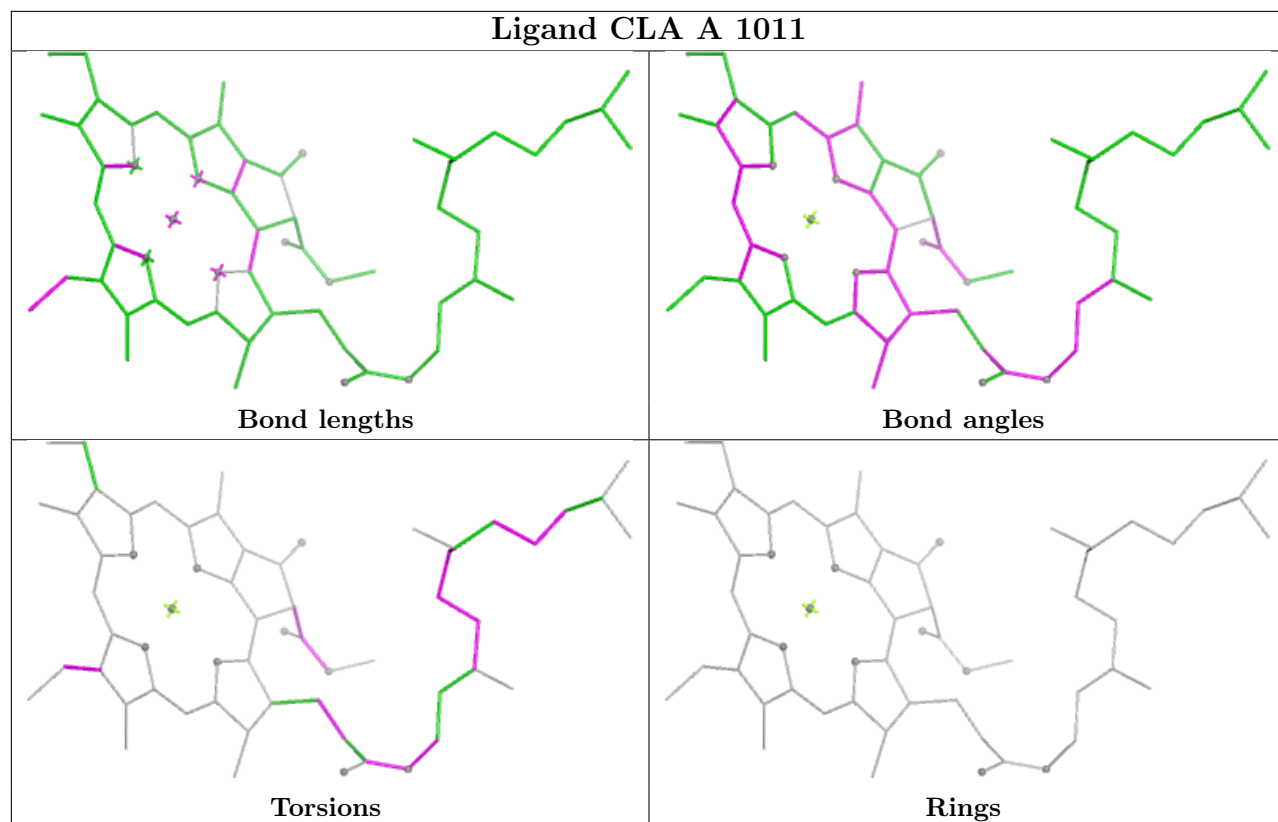


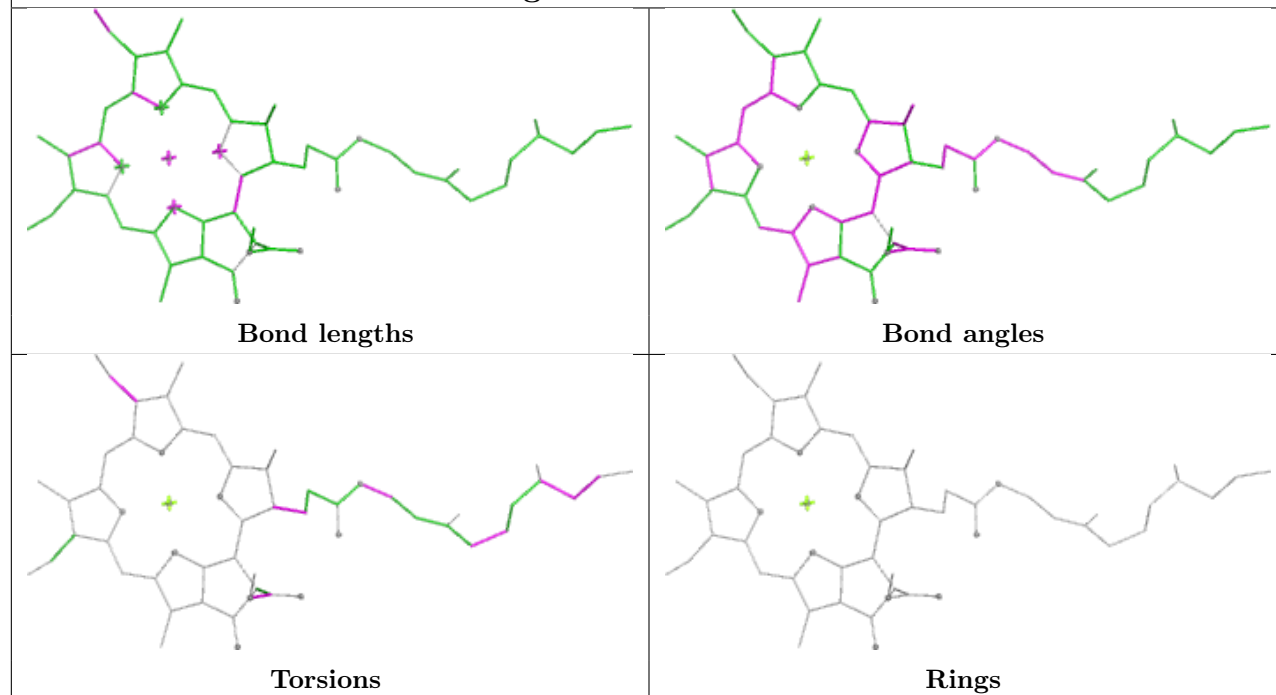
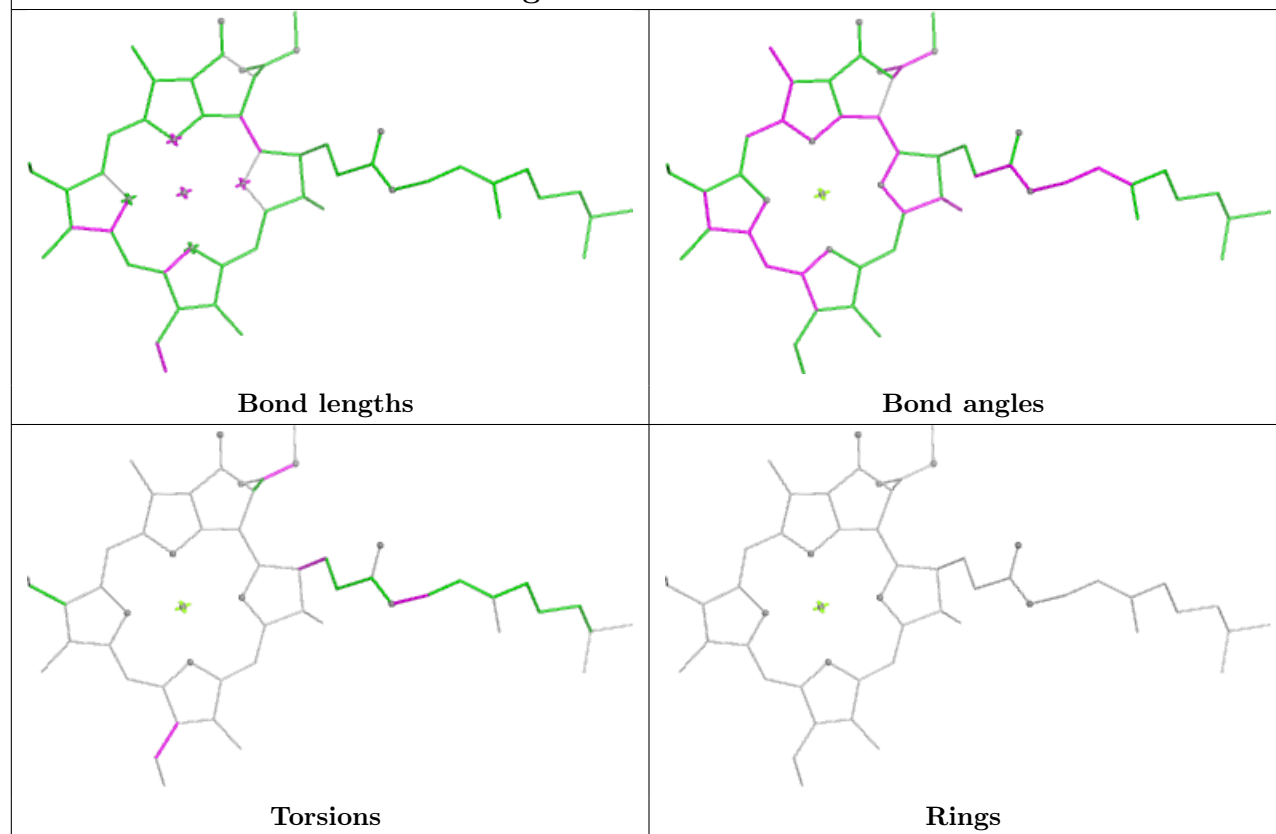


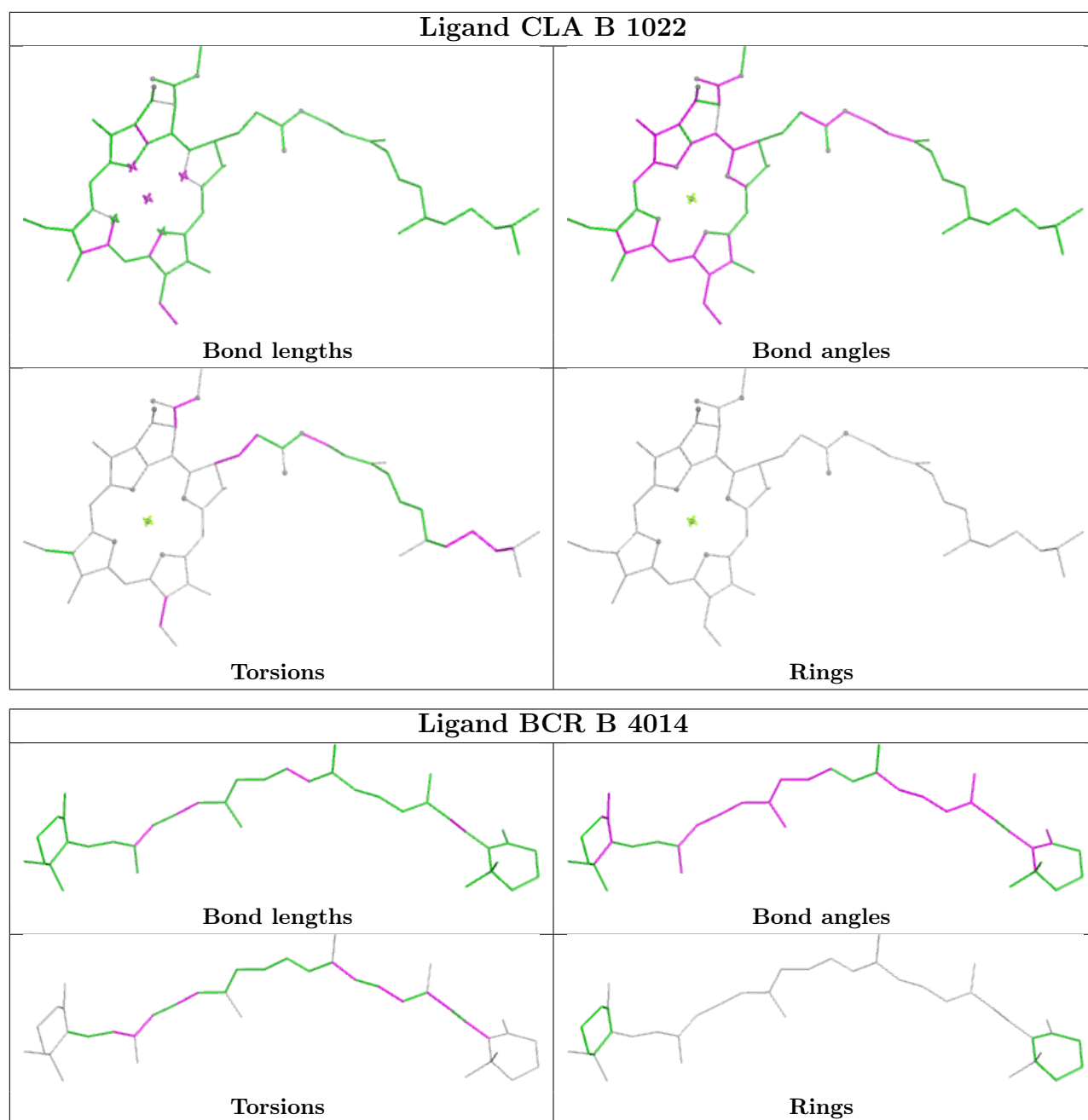




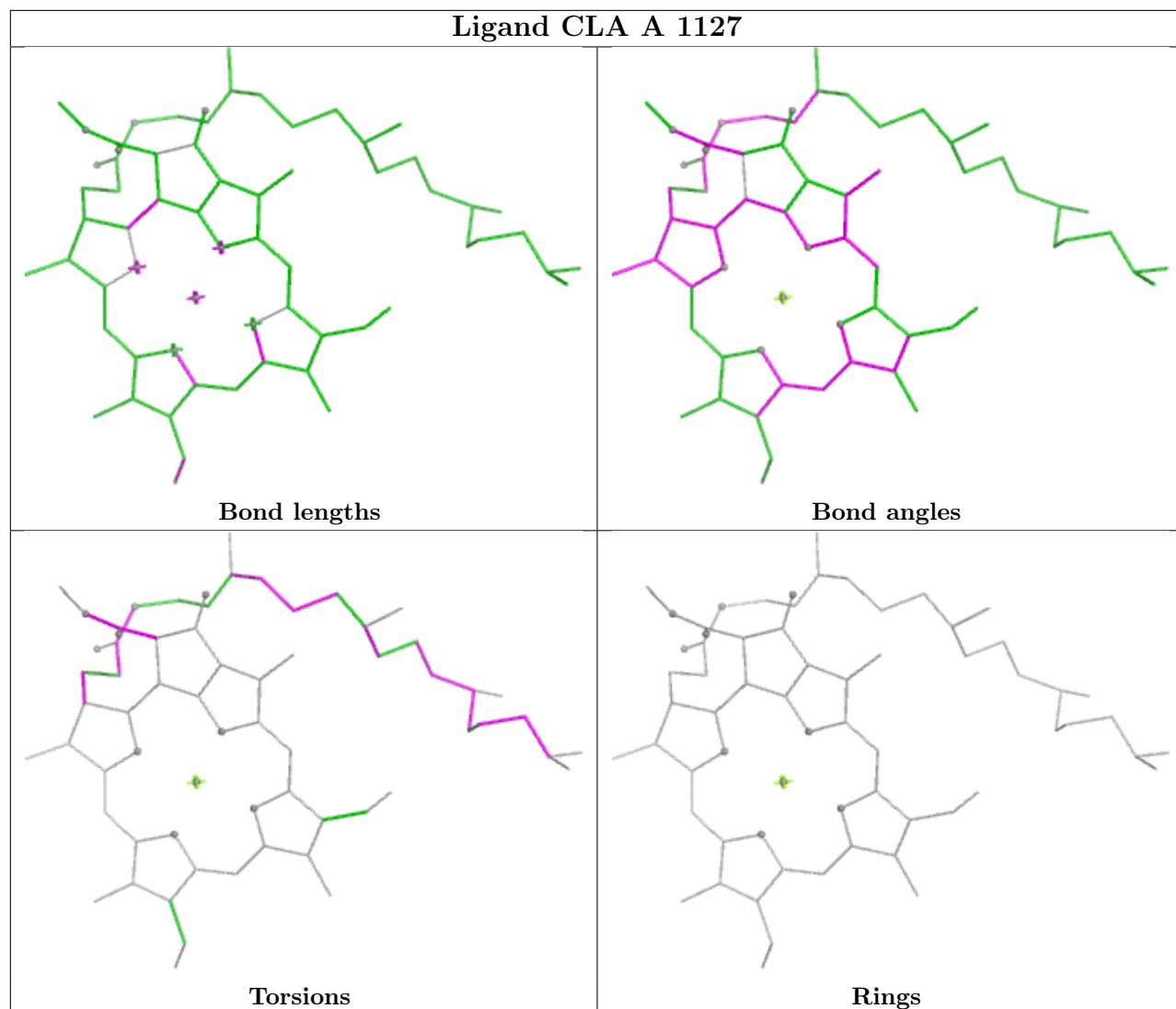


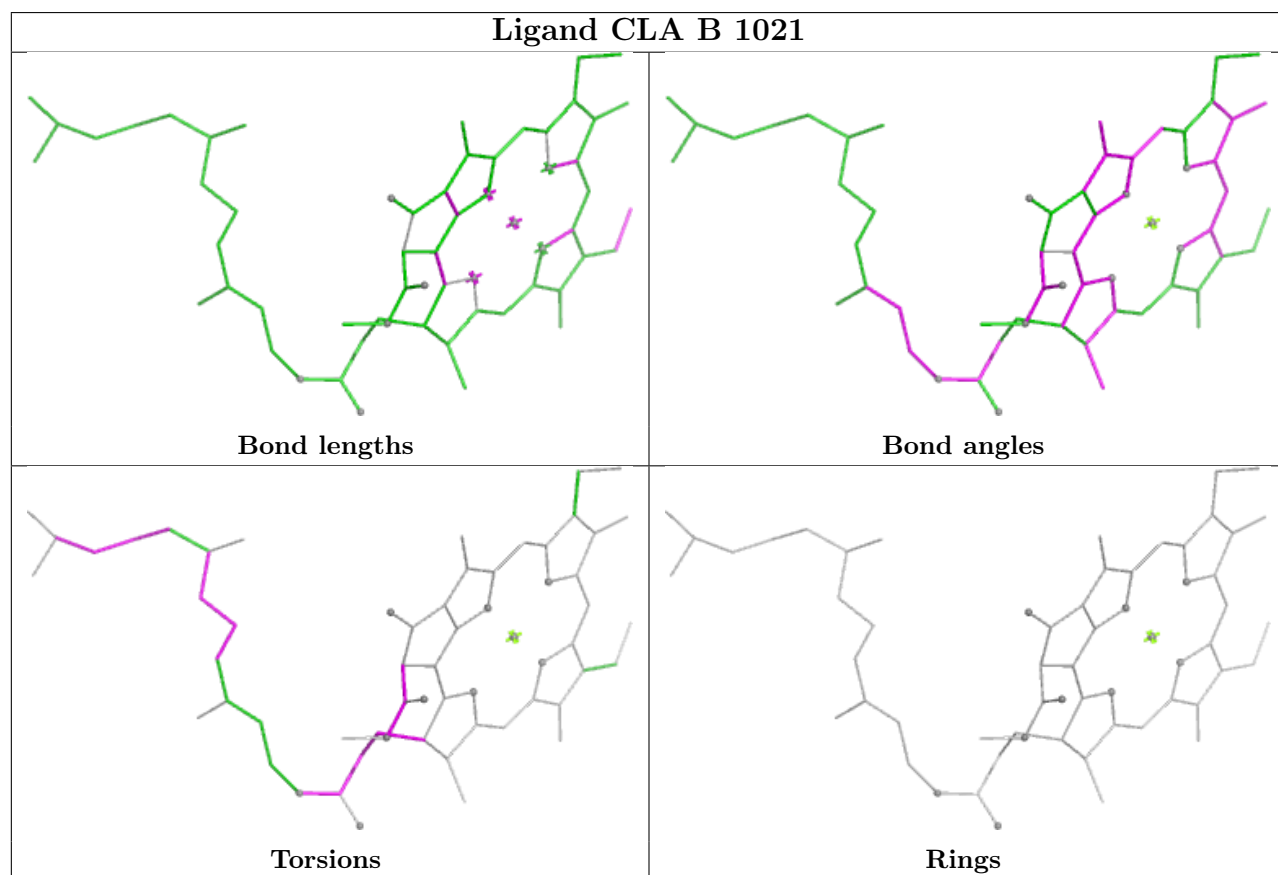
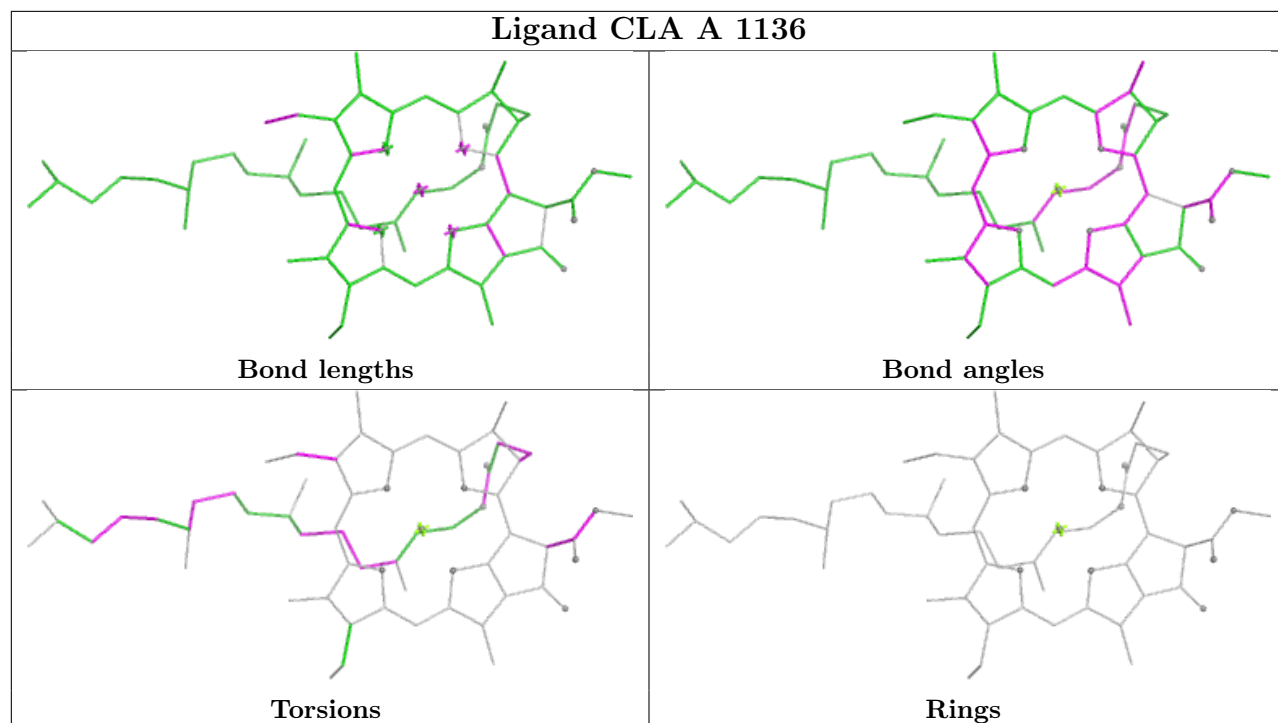


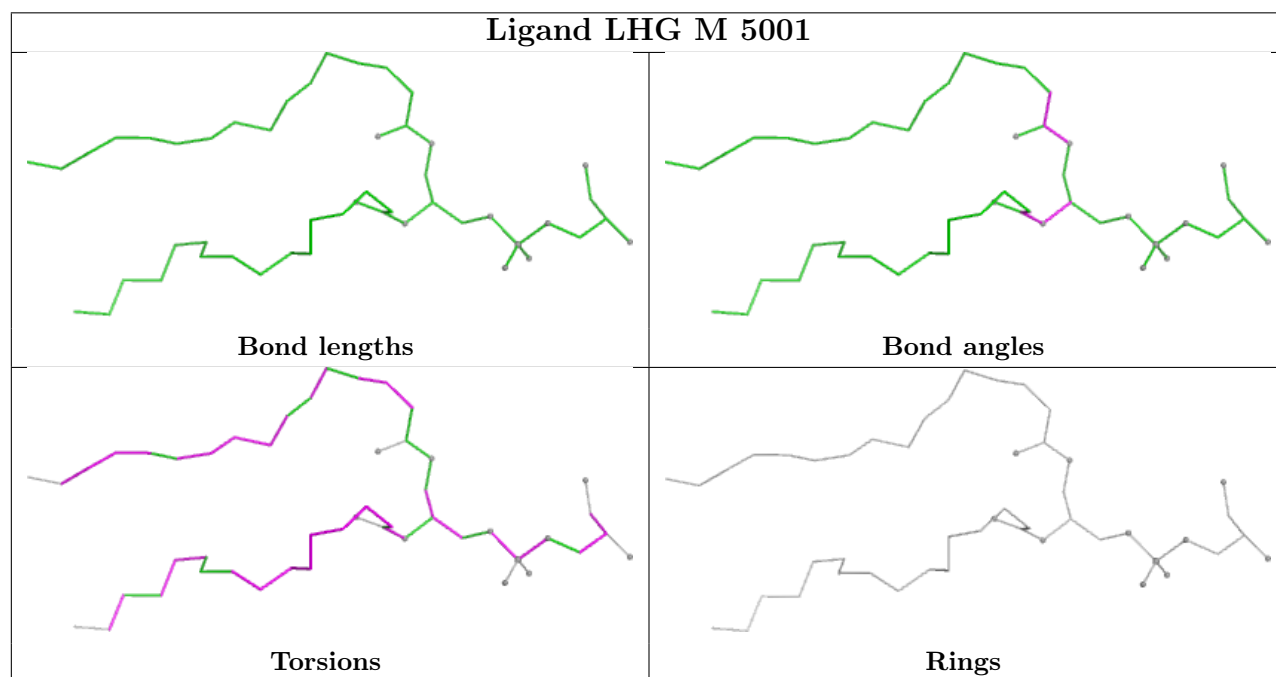
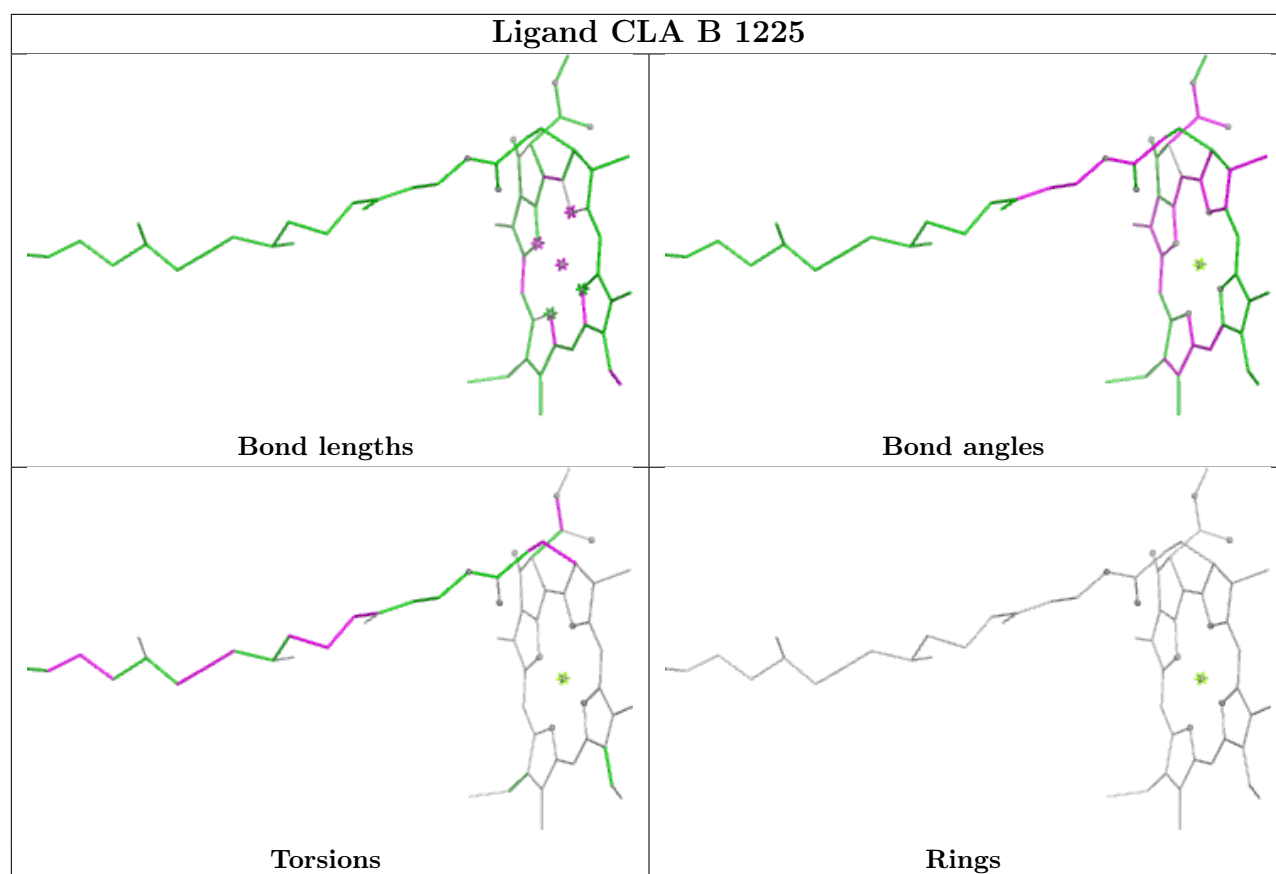
Ligand CLA B 1220**Ligand CLA A 1124**

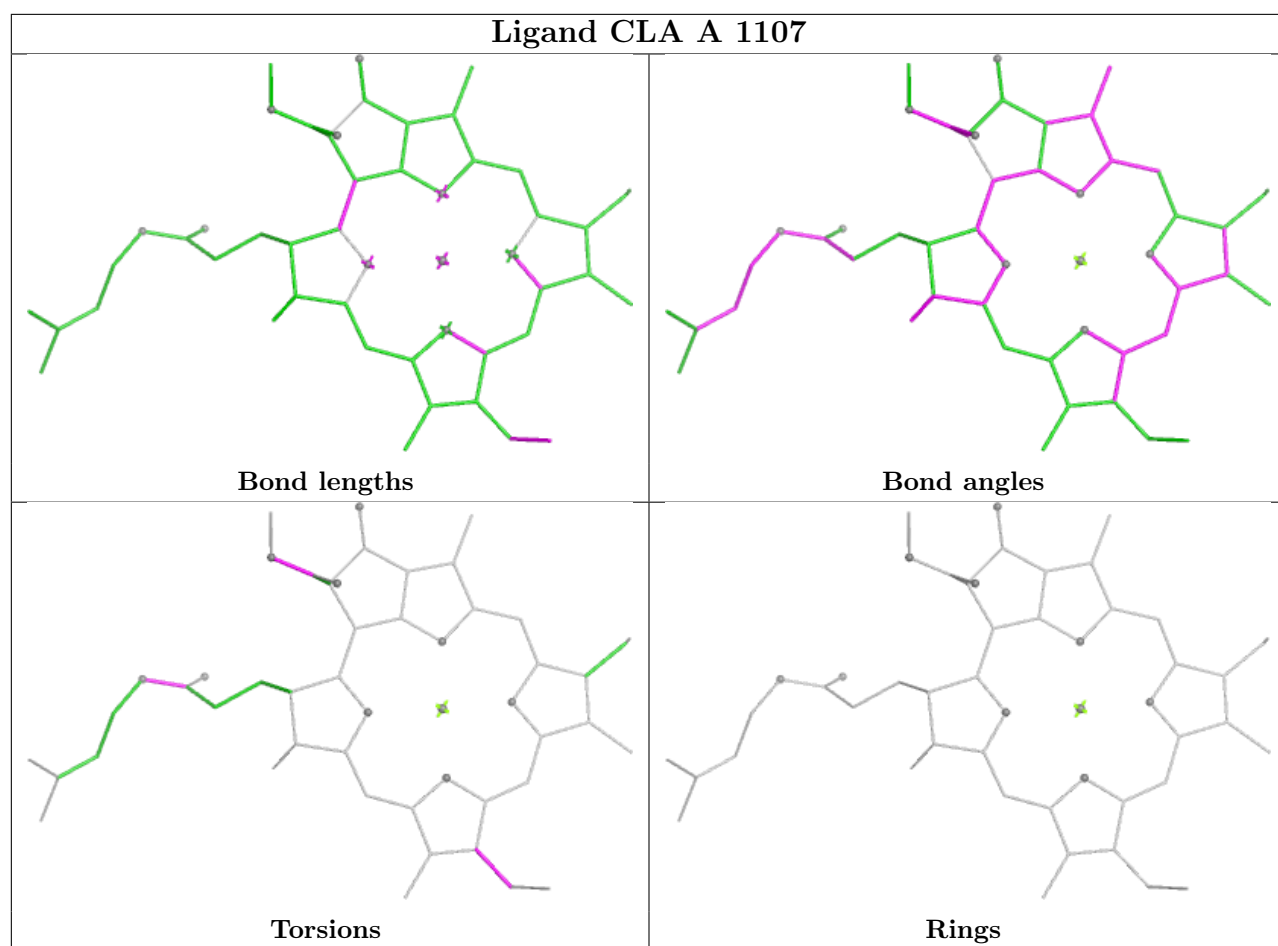


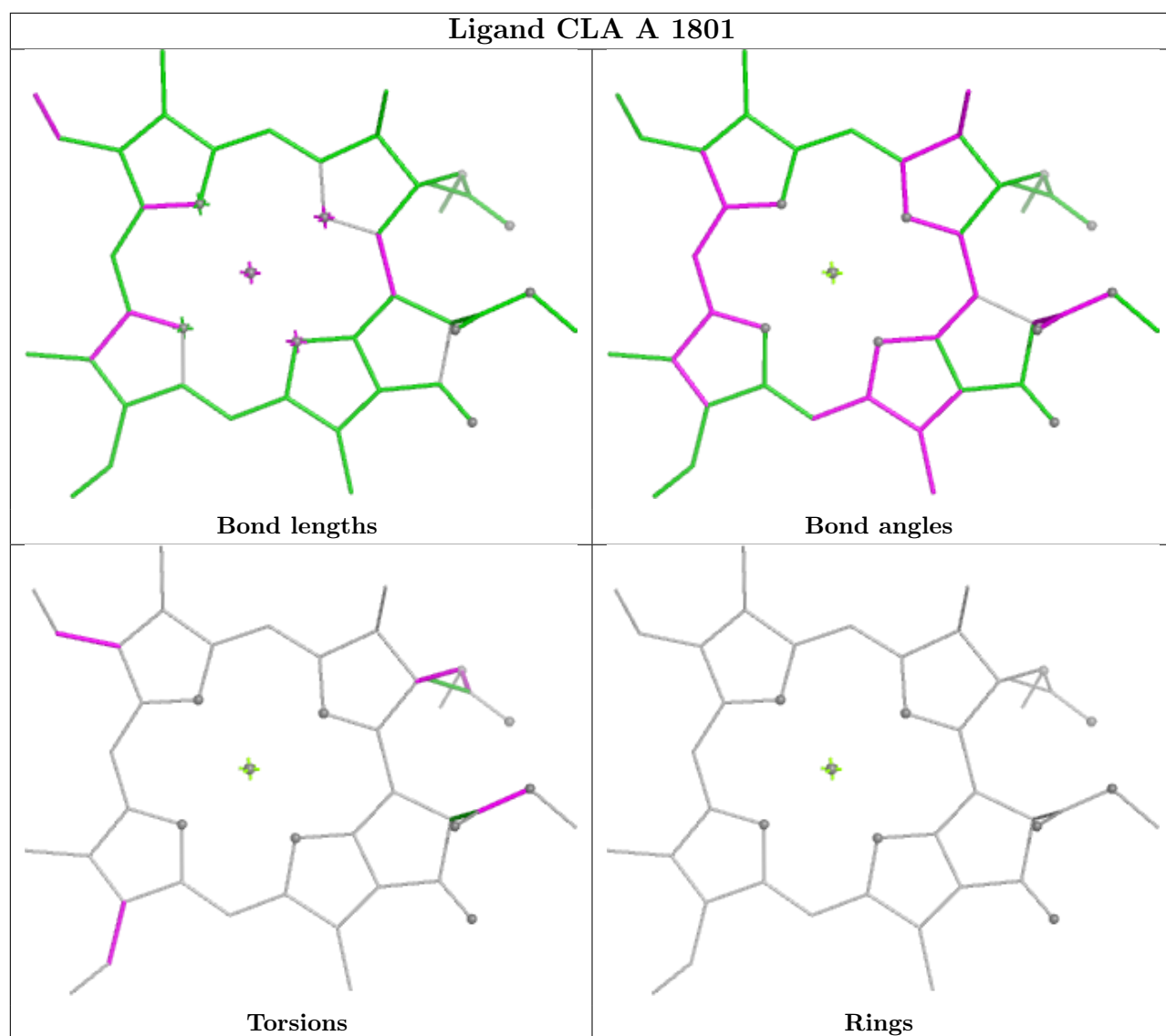
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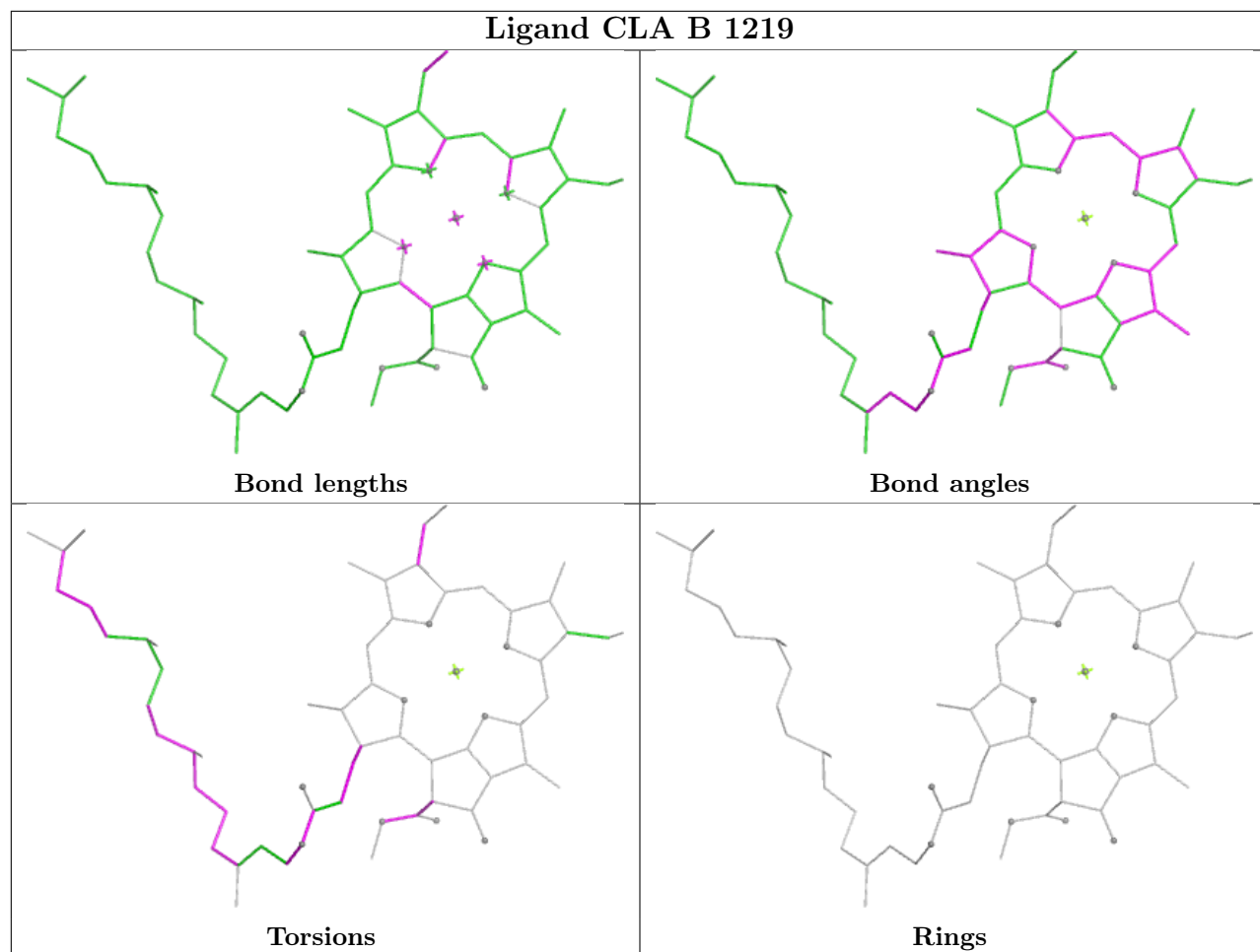


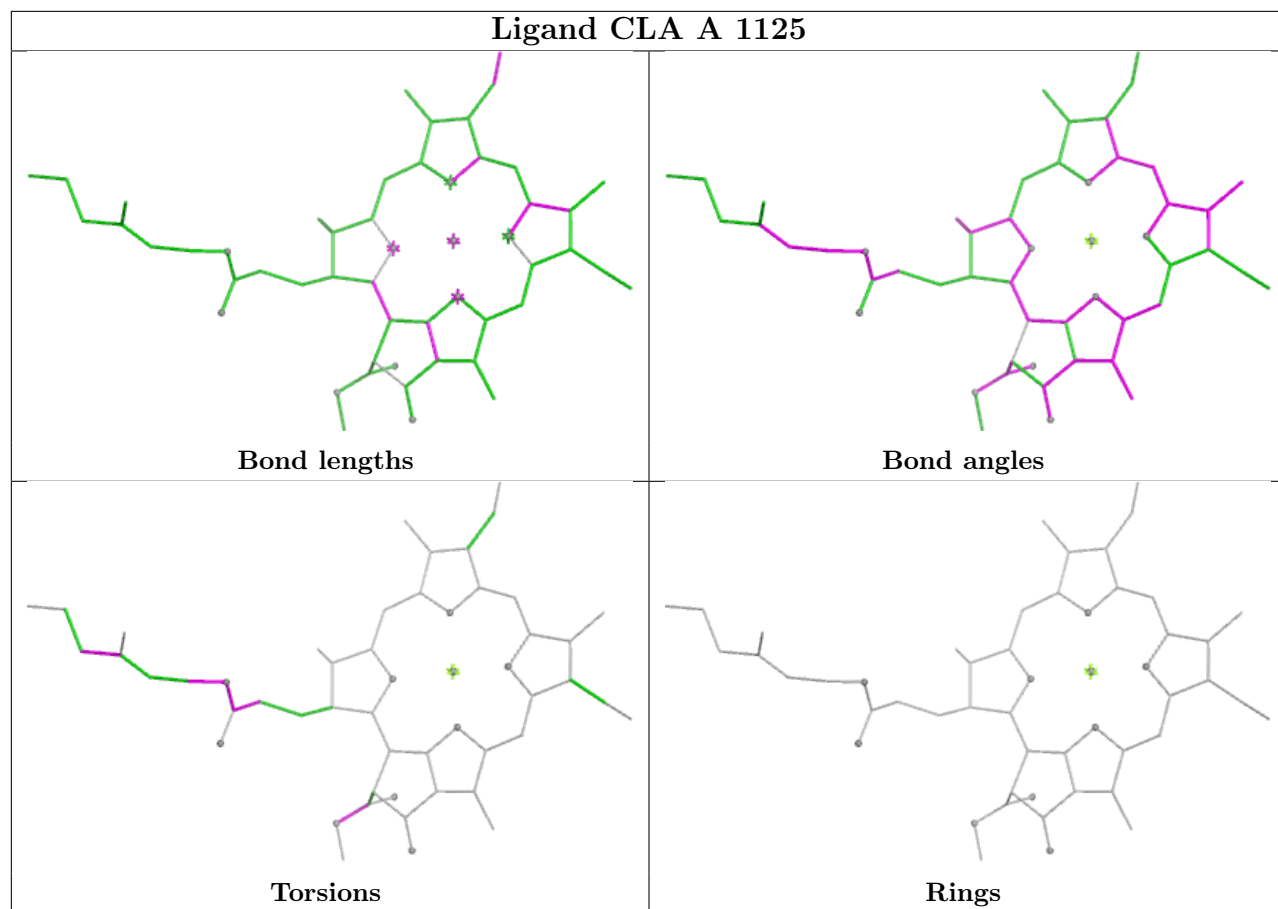


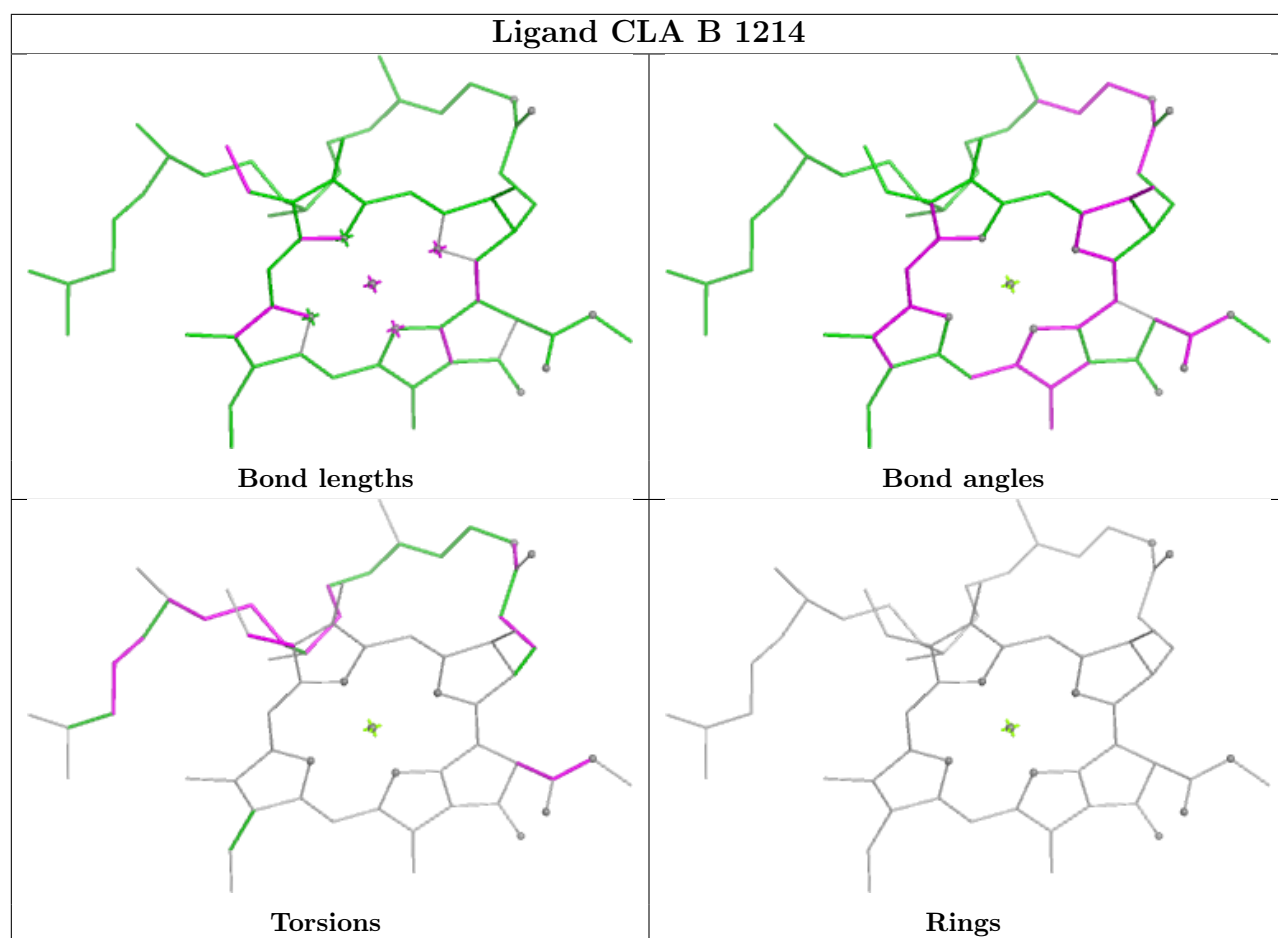




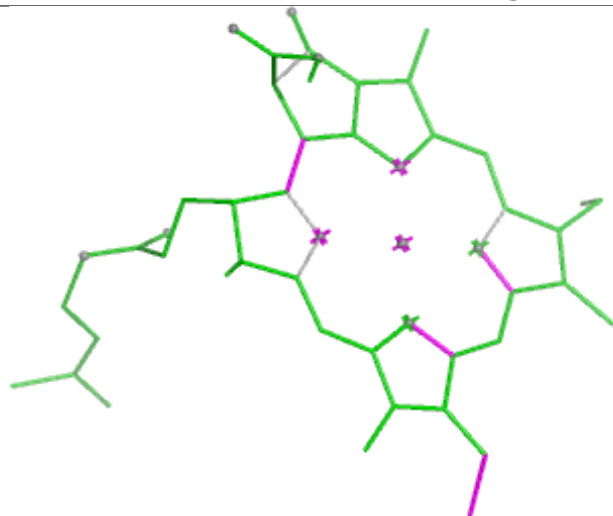




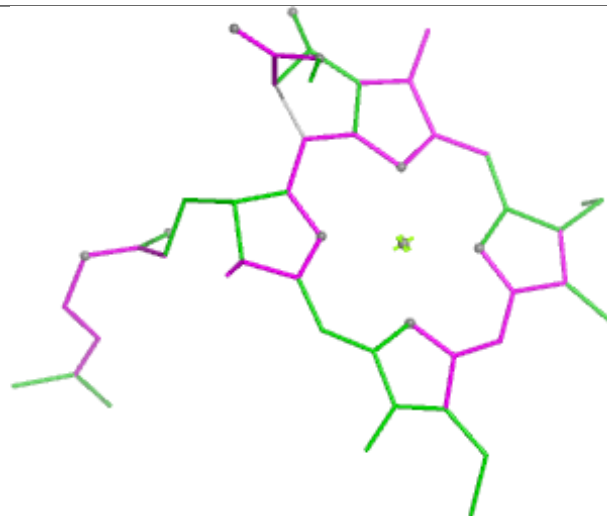




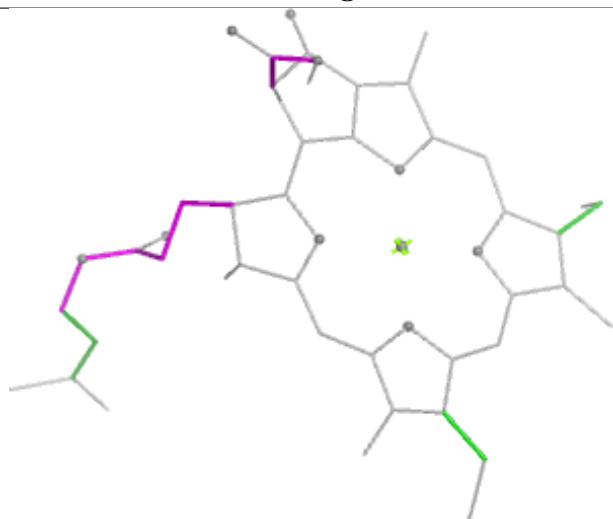
Ligand CLA A 1112



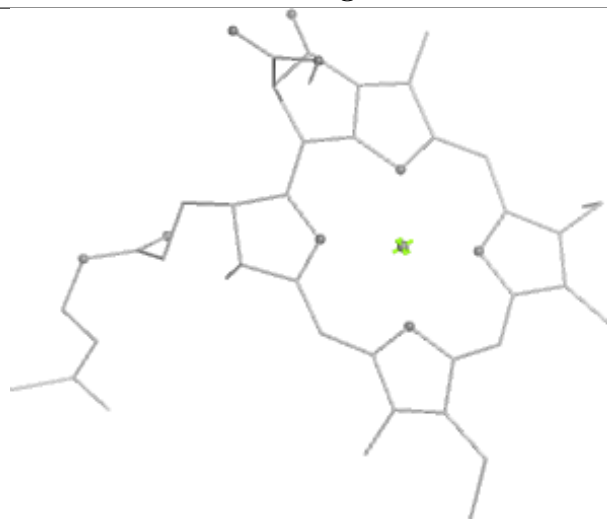
Bond lengths



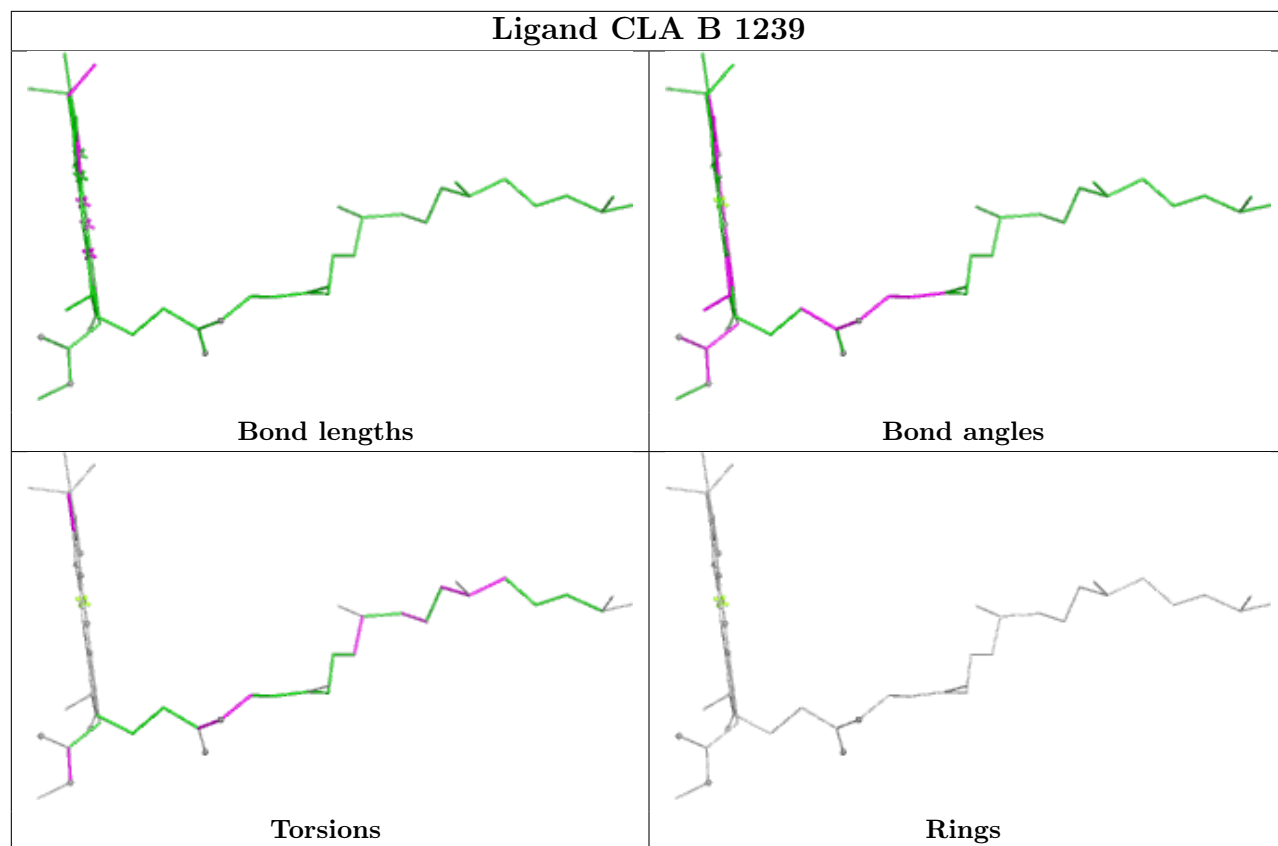
Bond angles



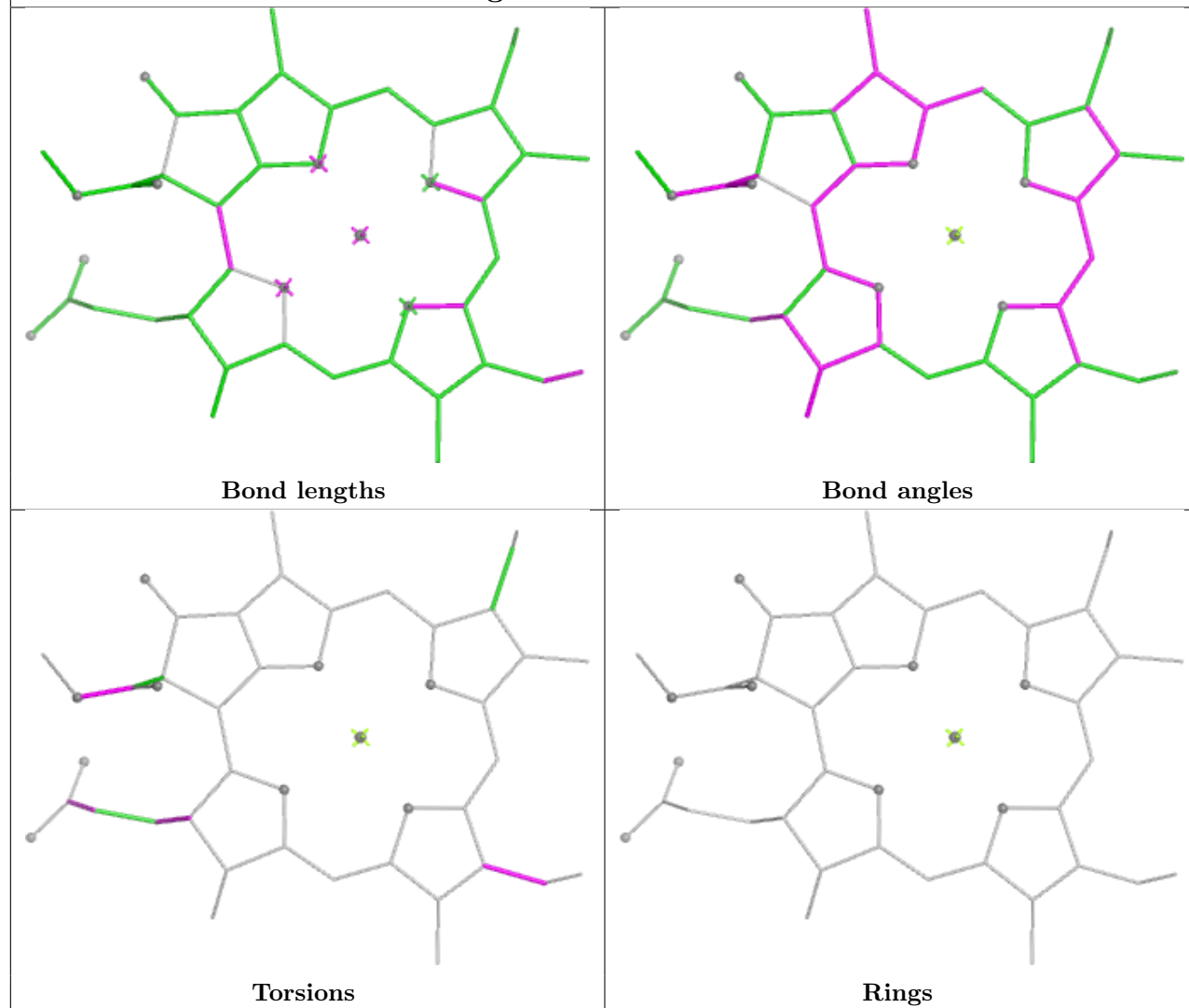
Torsions



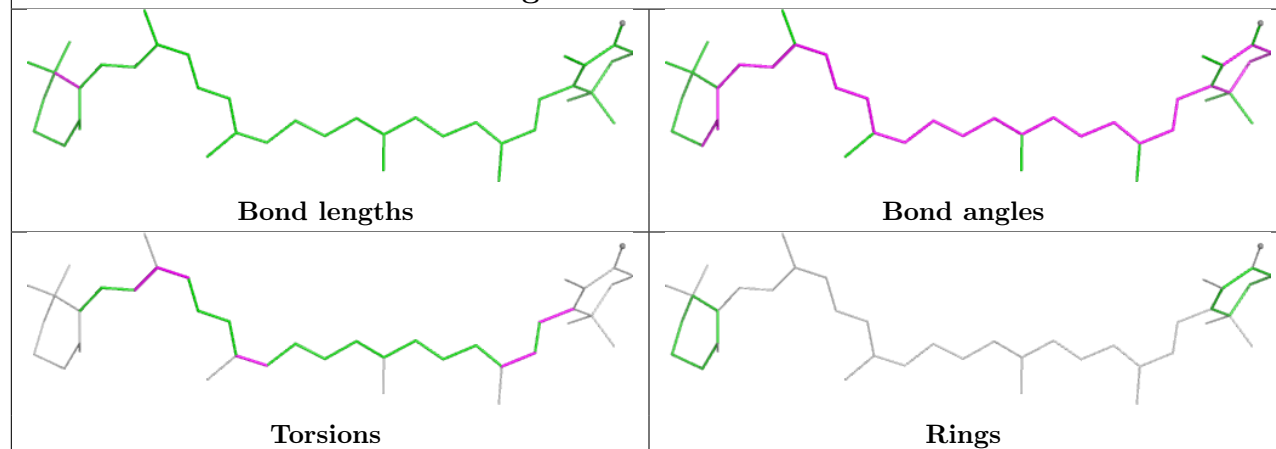
Rings

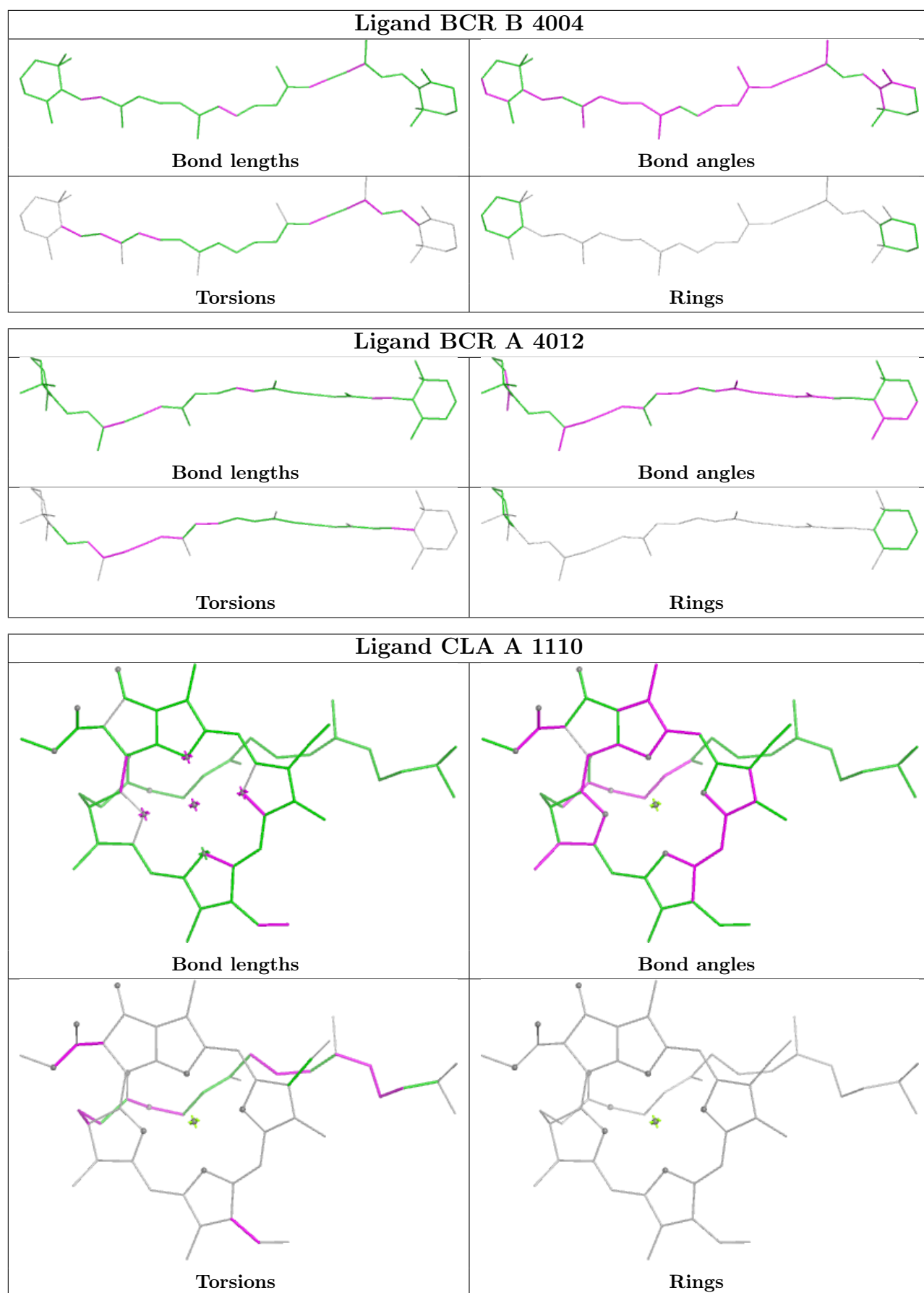


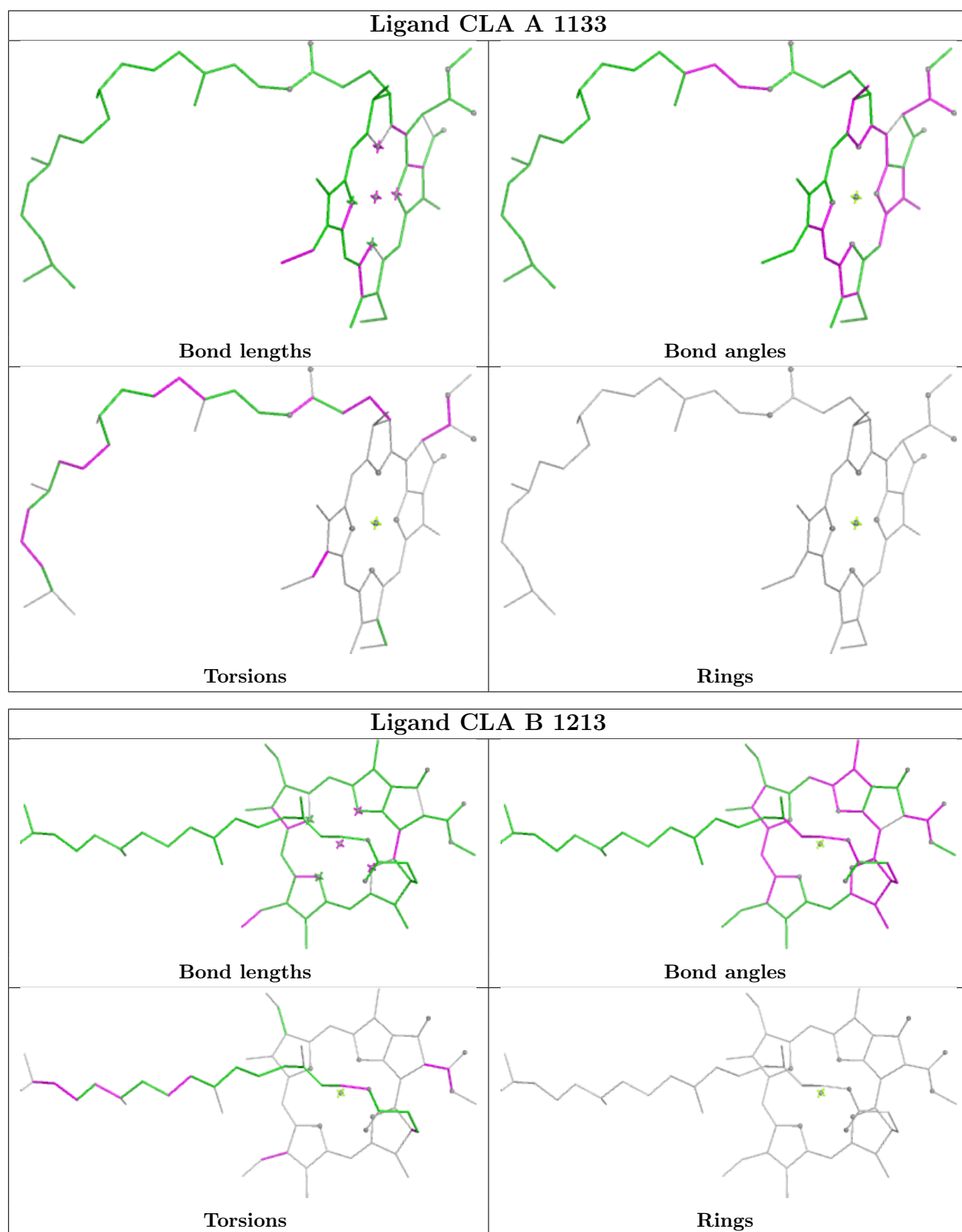
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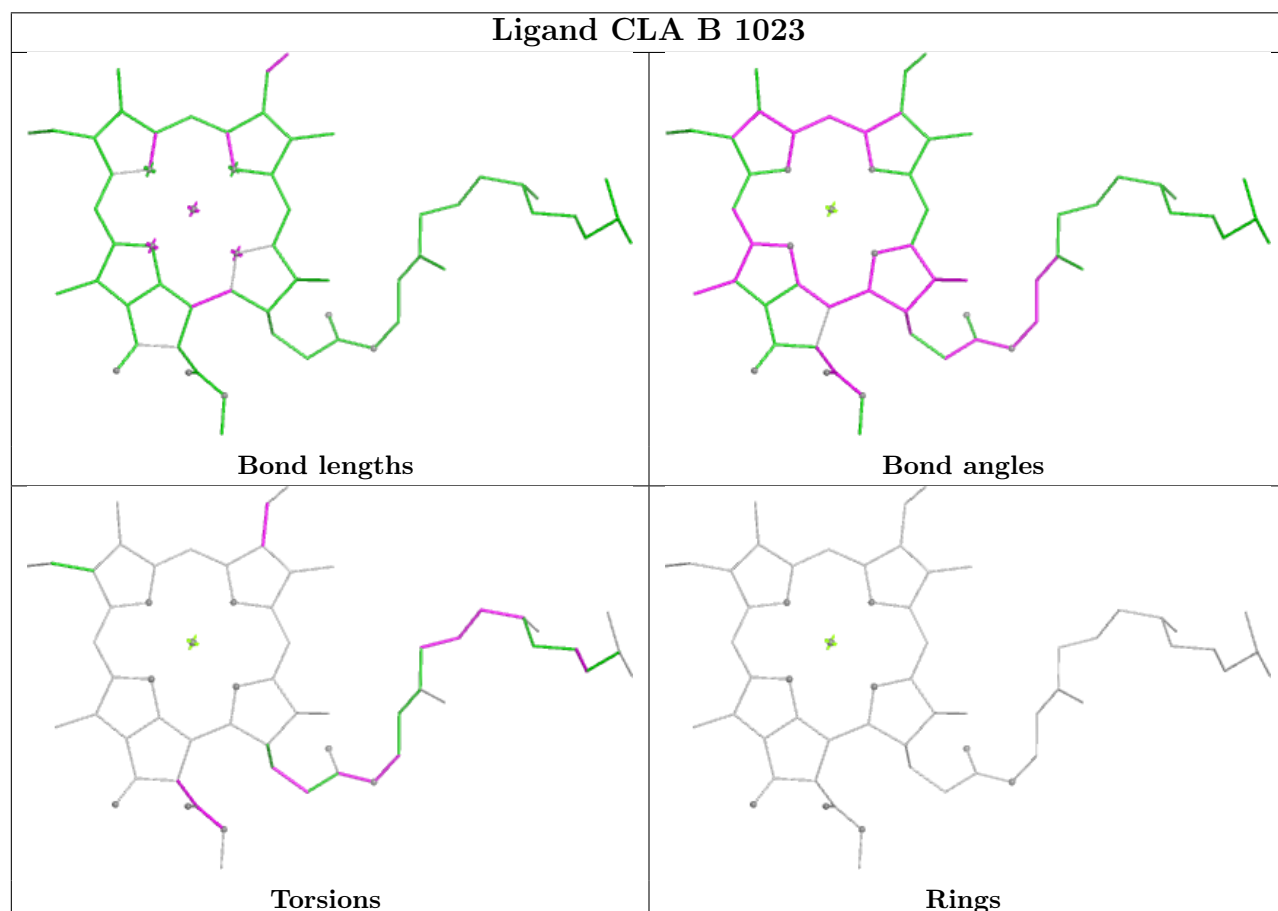
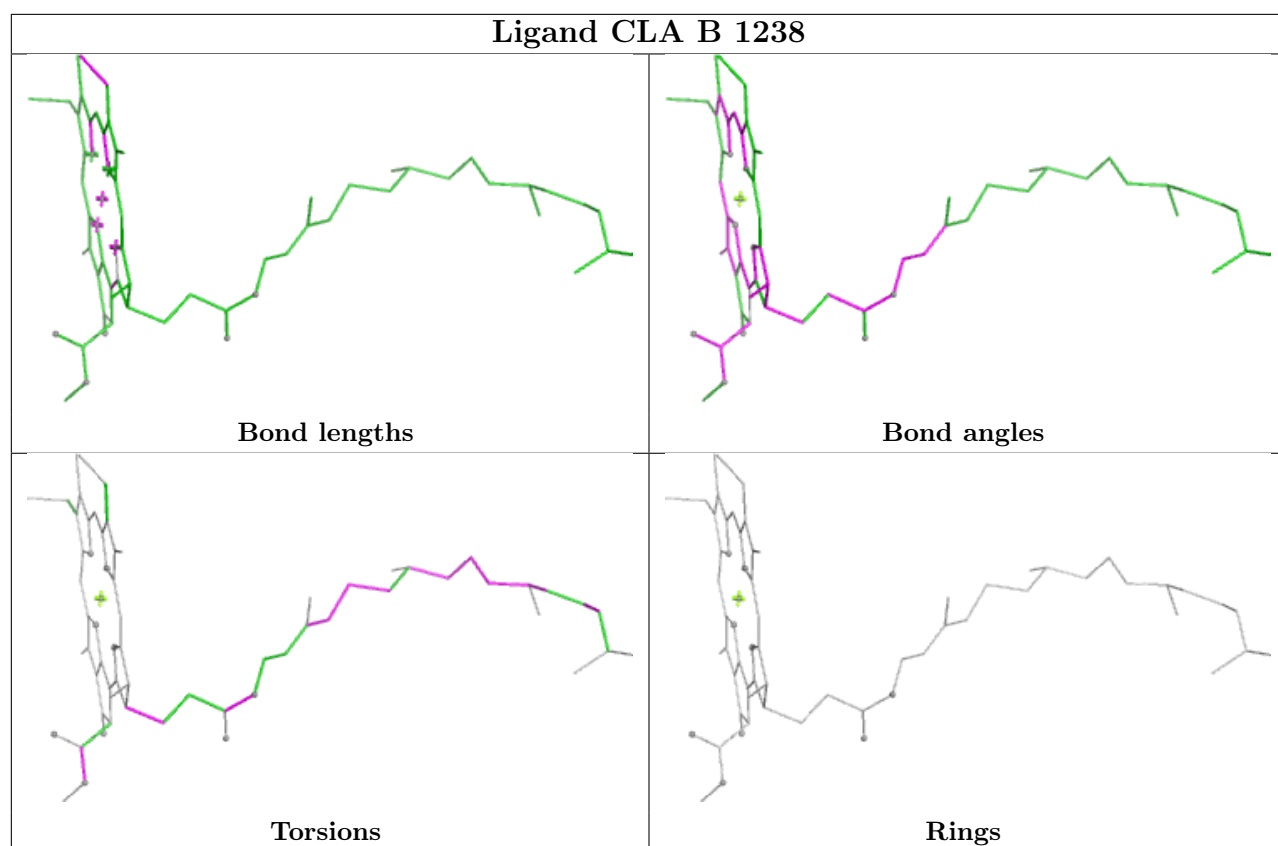


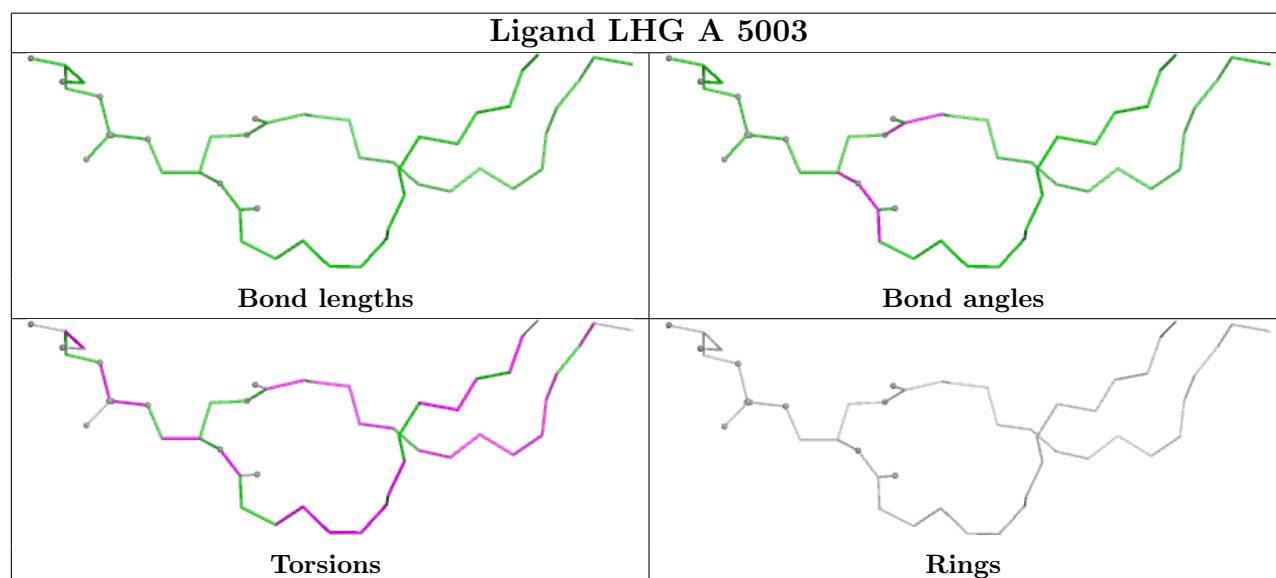
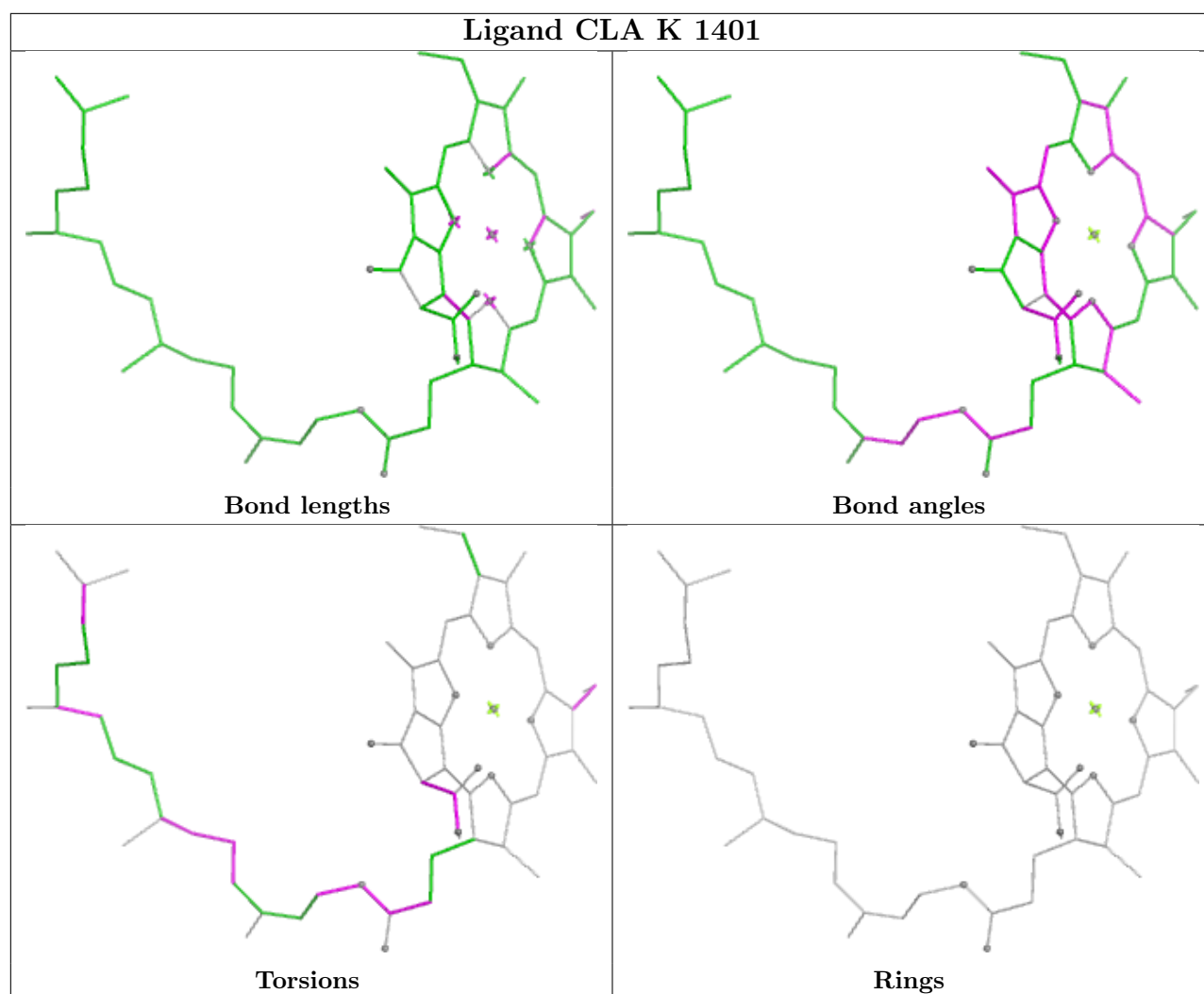
Ligand ECH B 4006

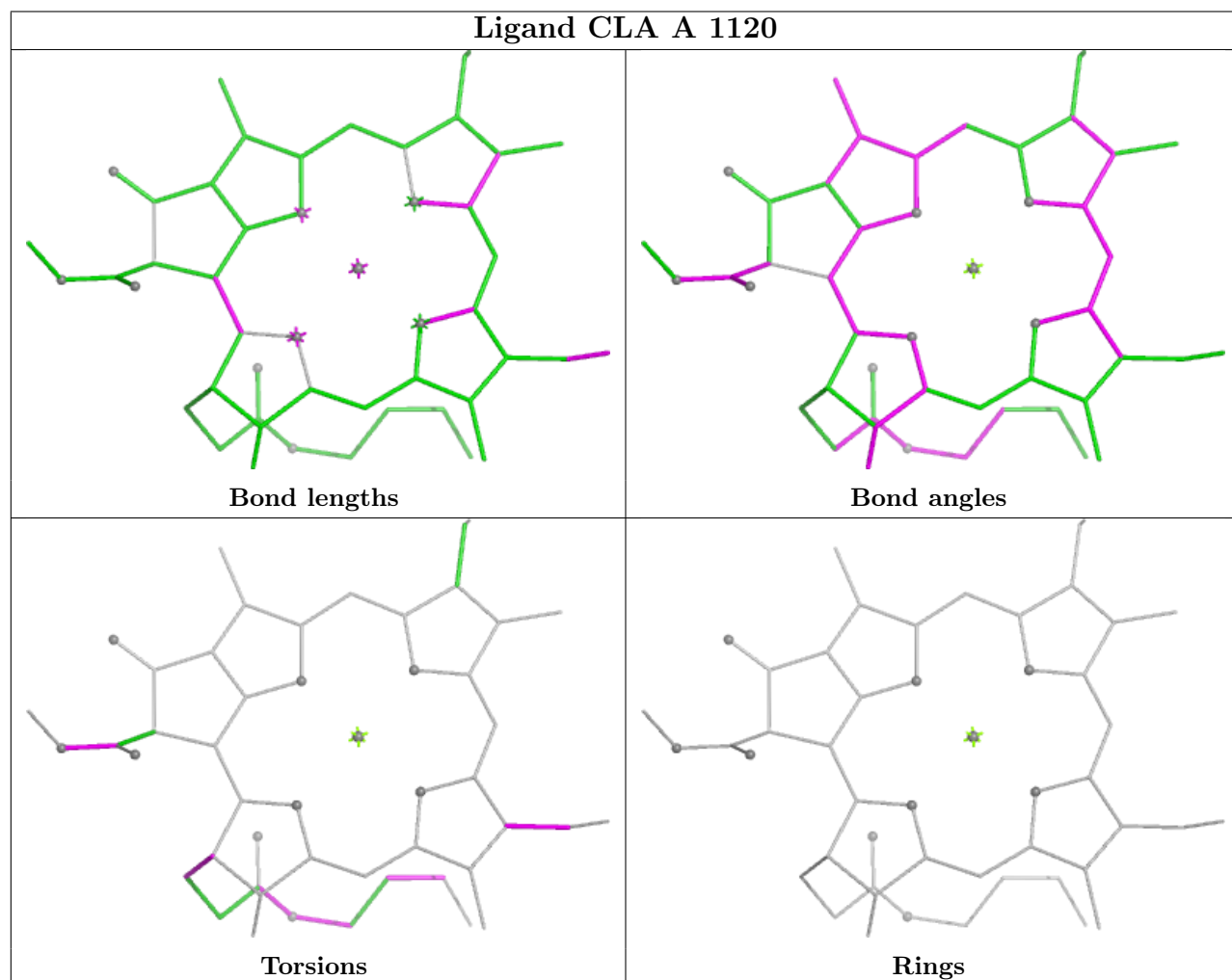
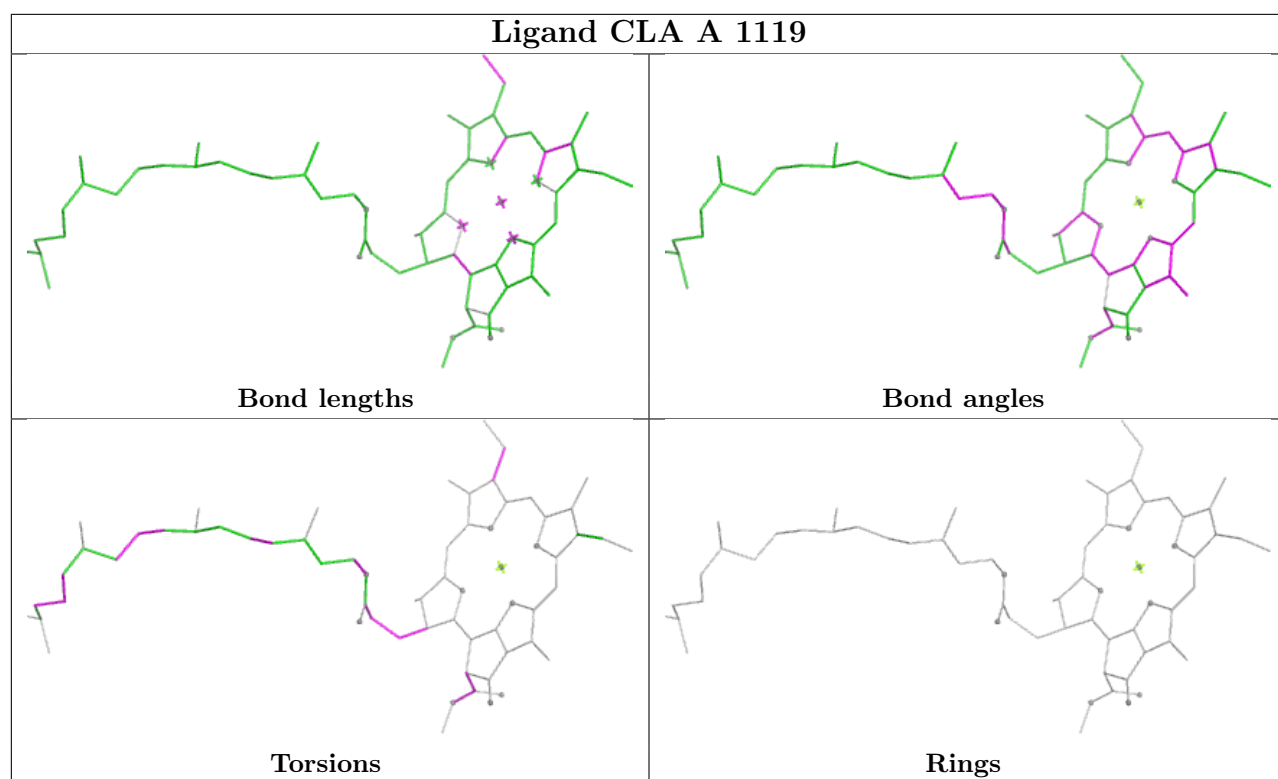


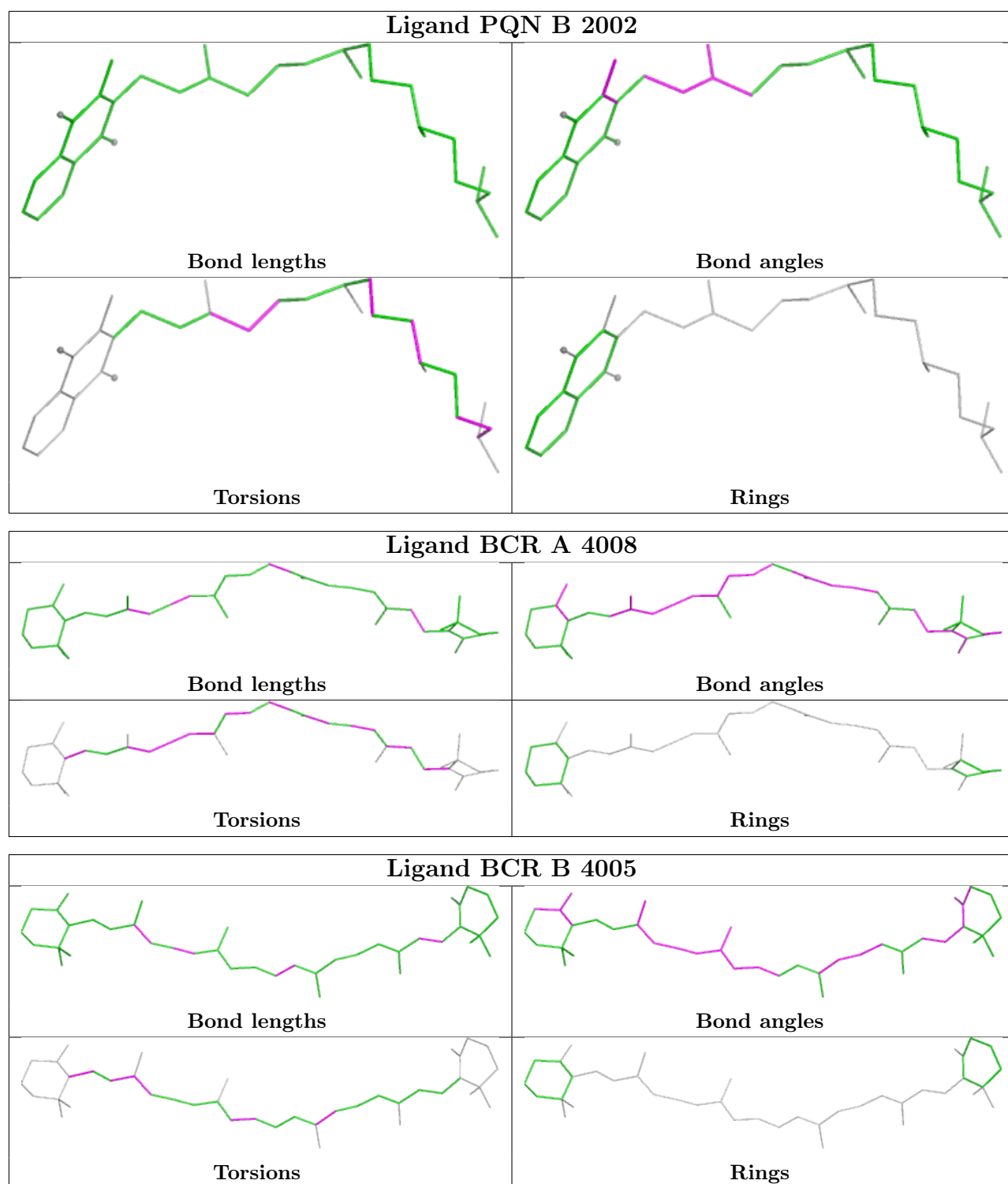


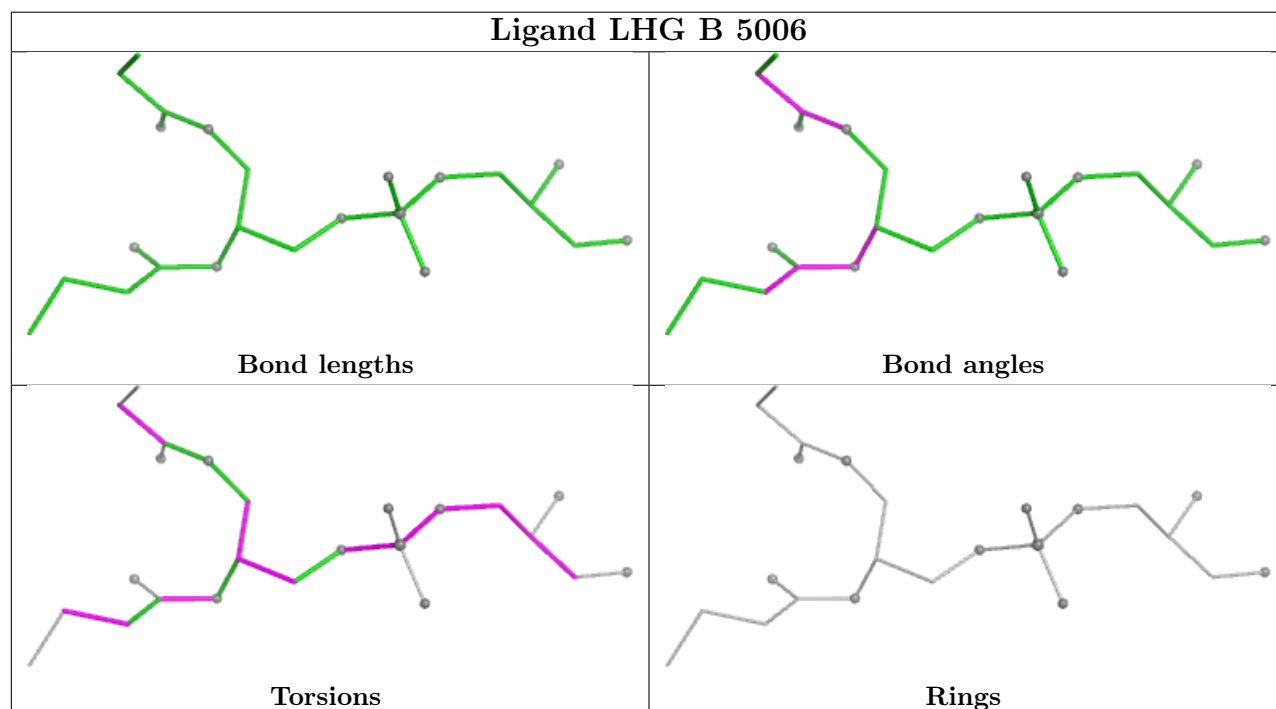
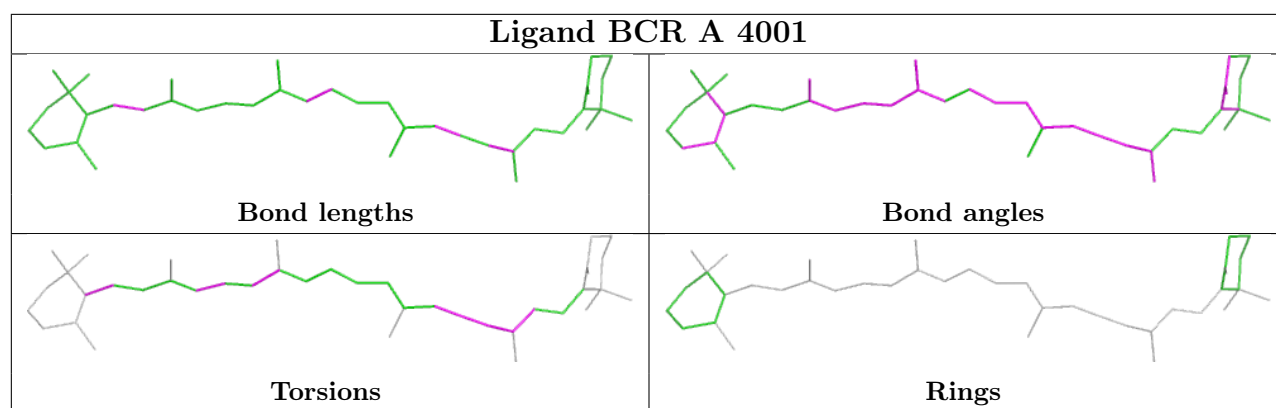


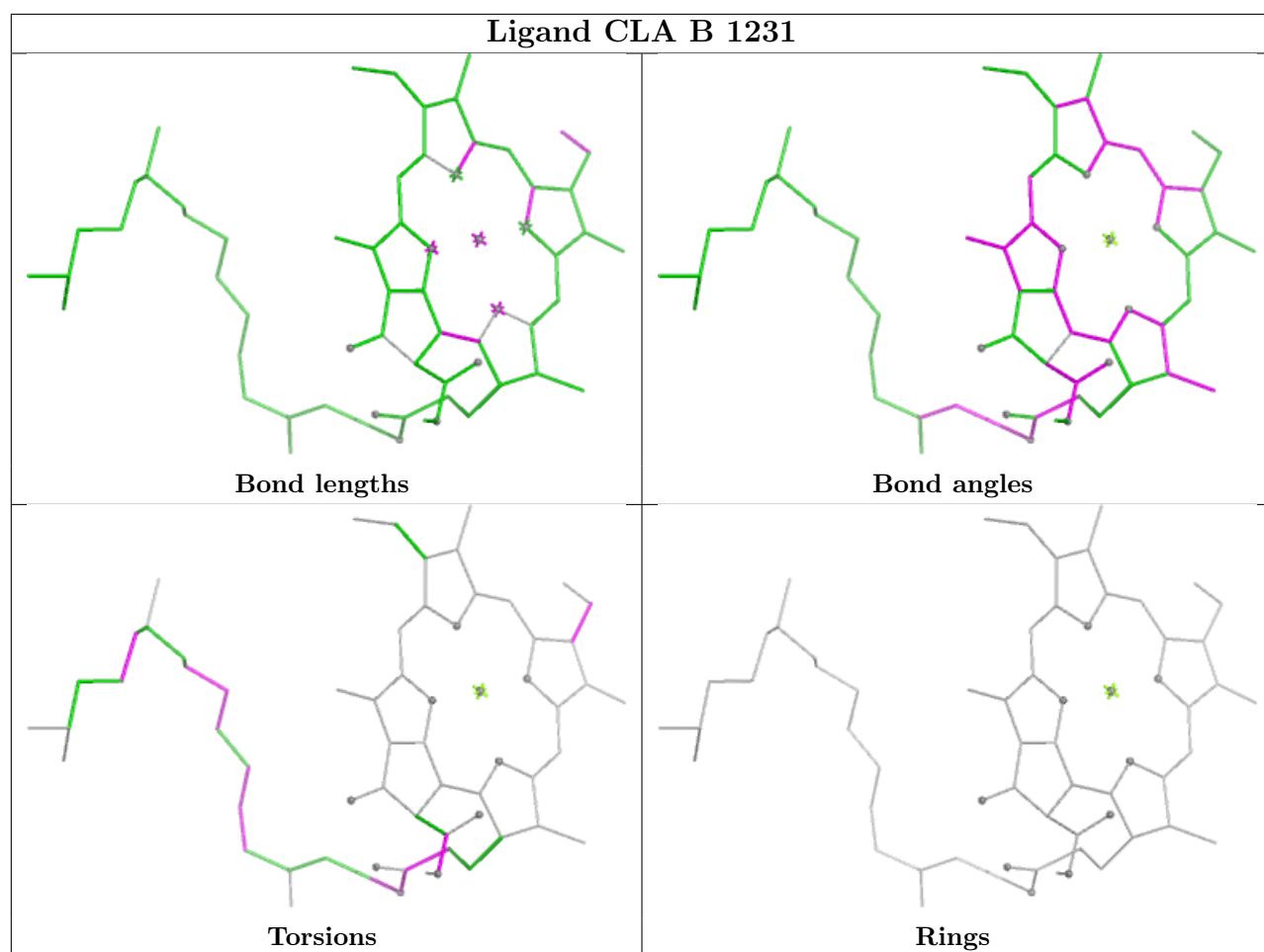


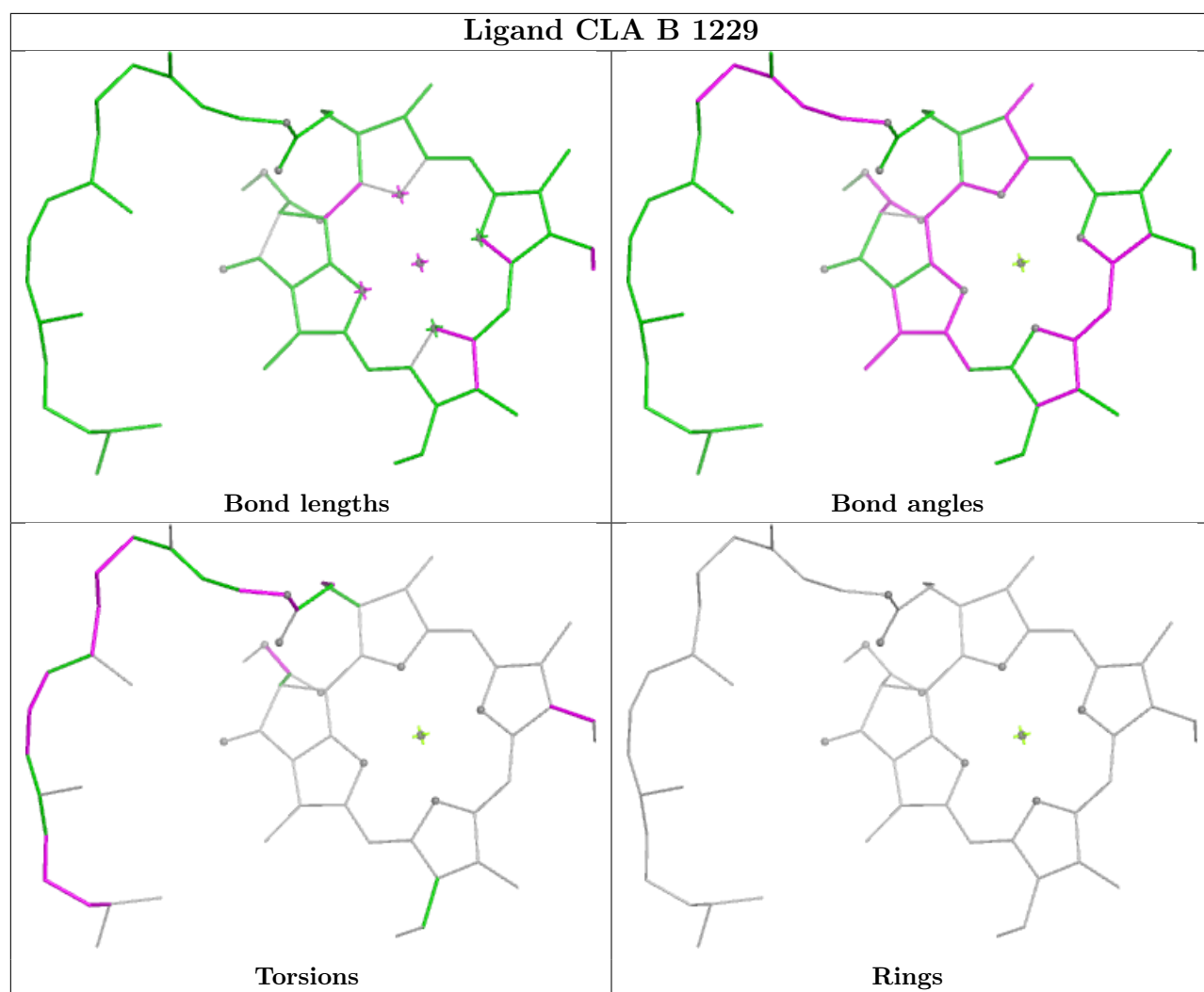


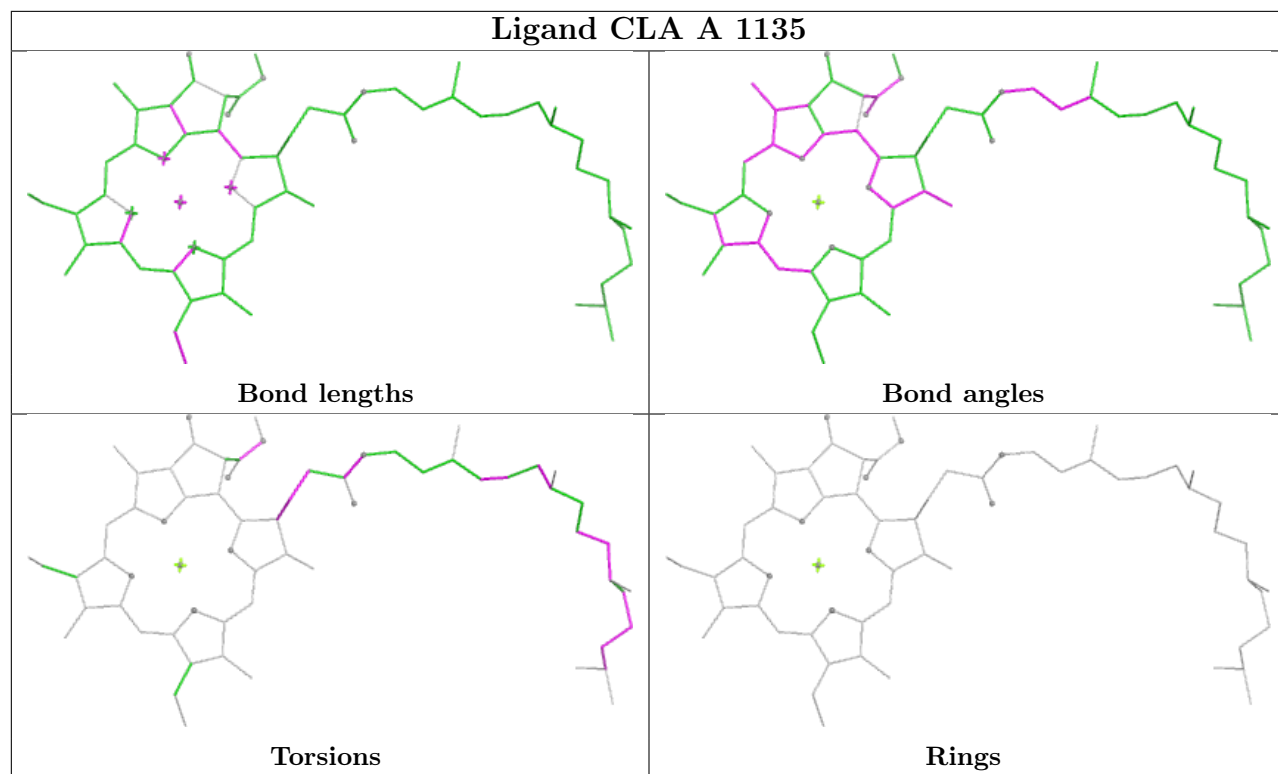
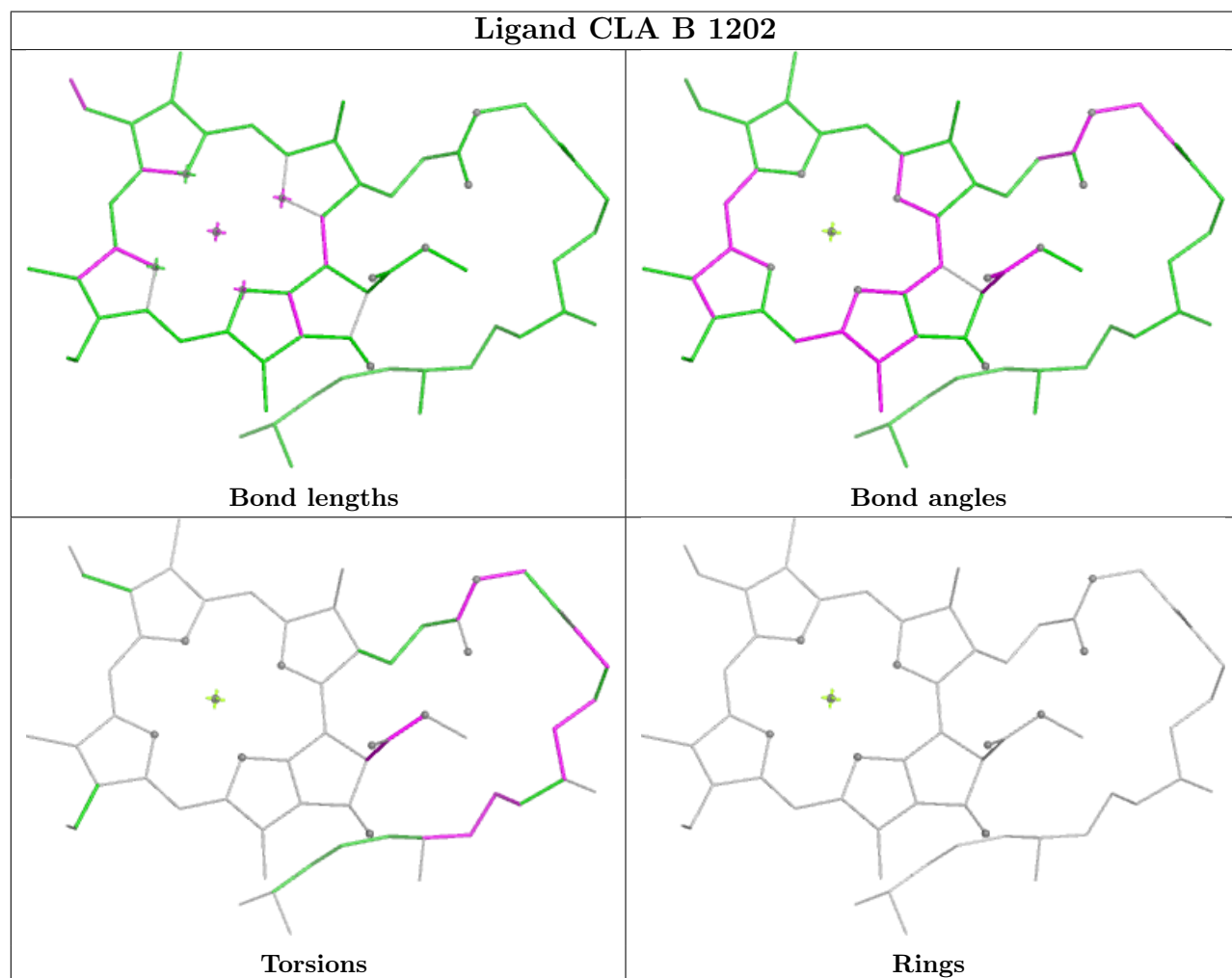


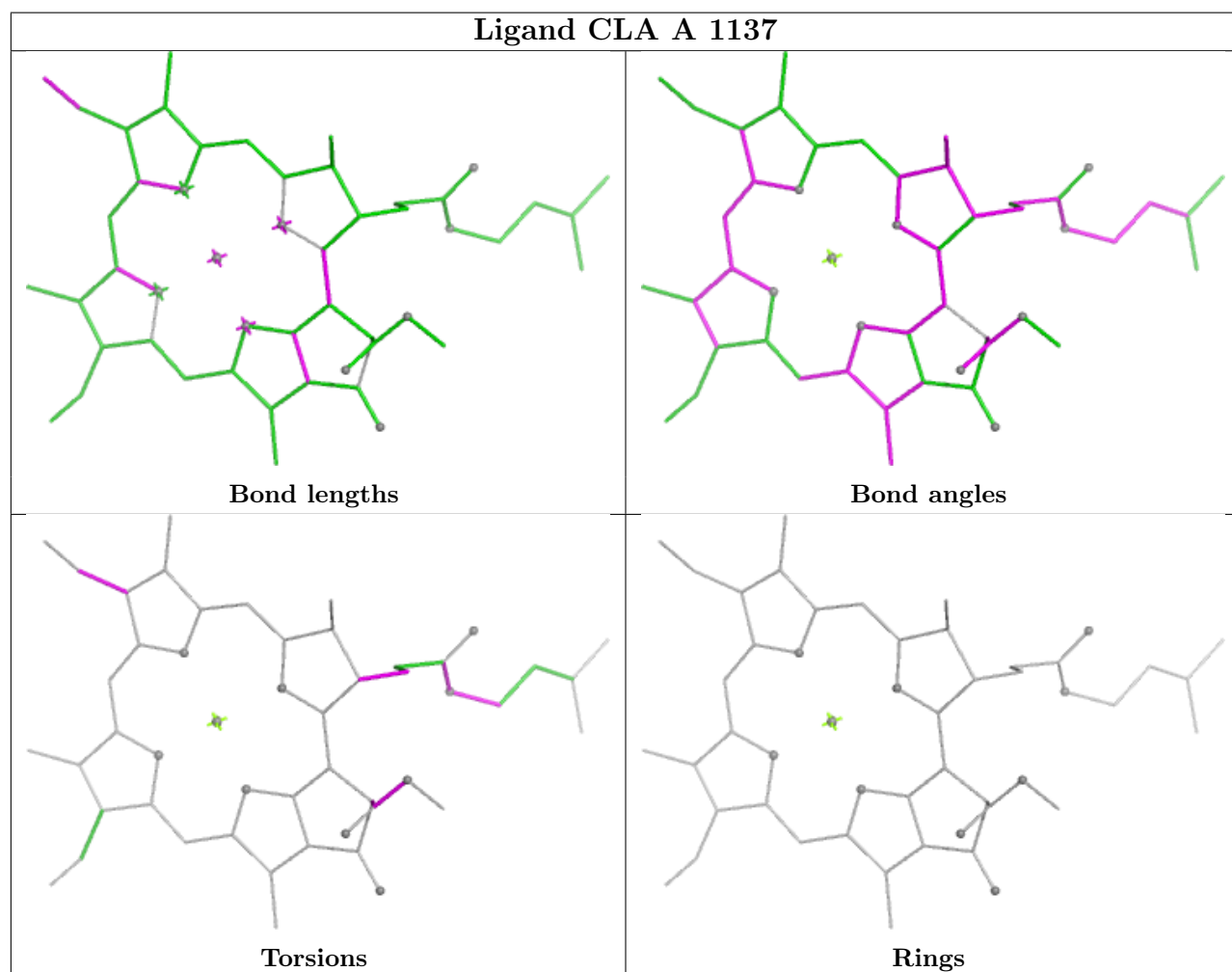
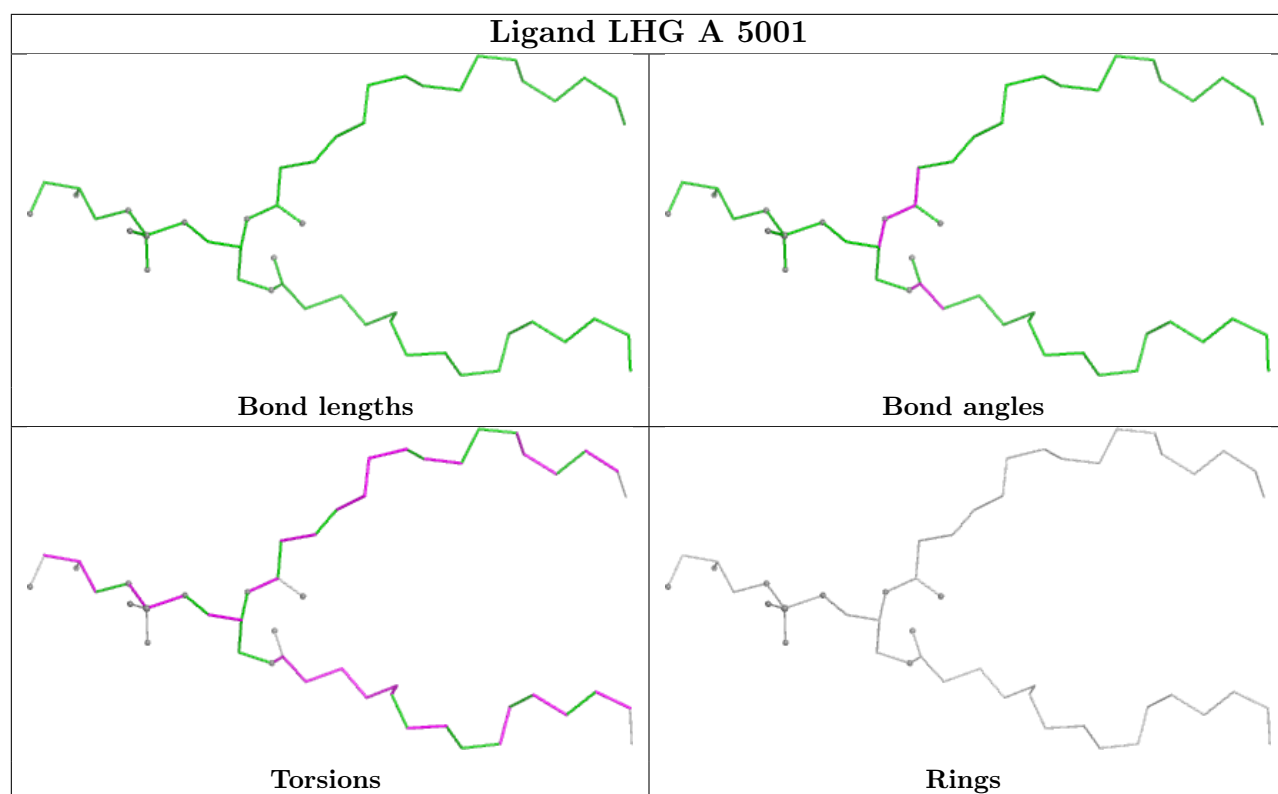


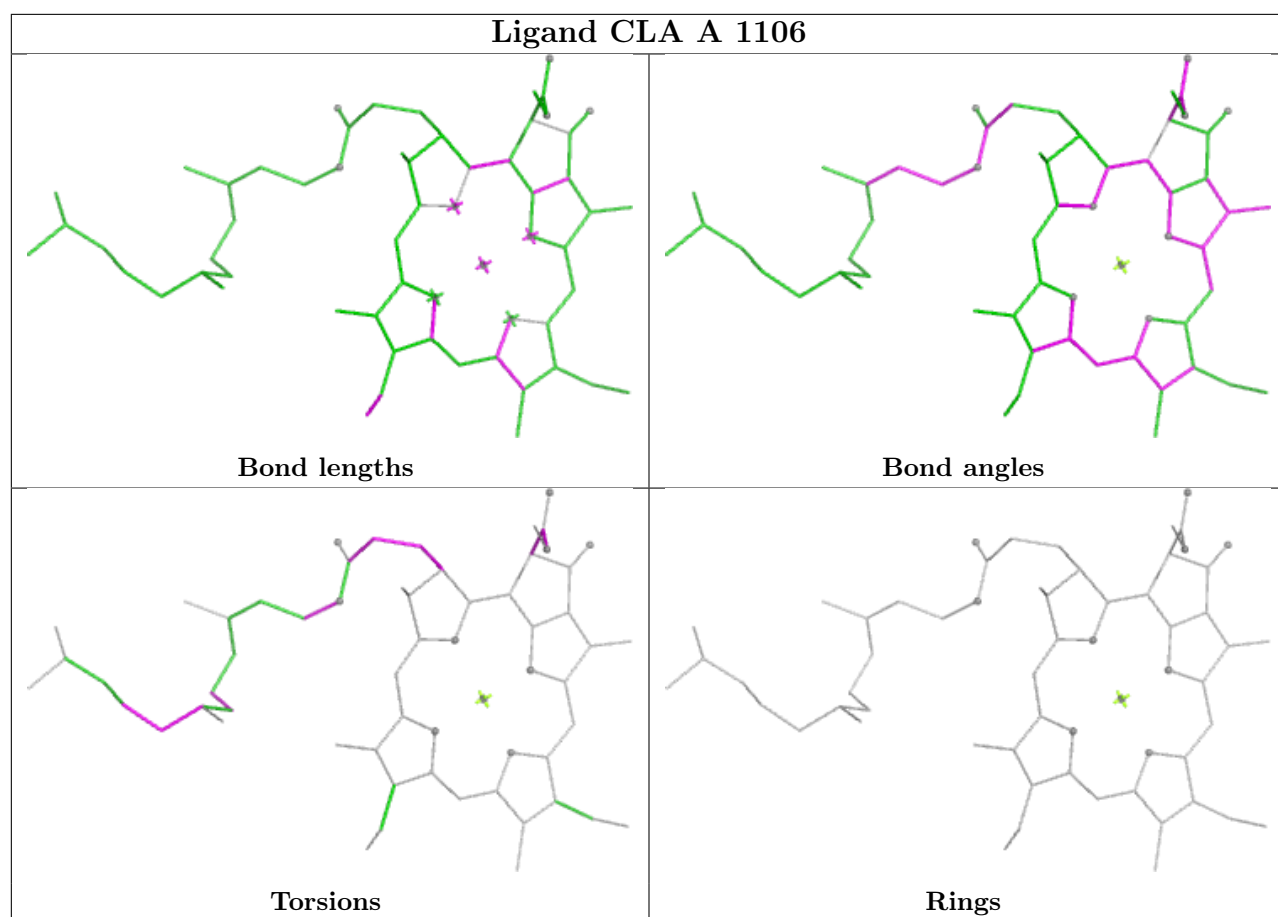


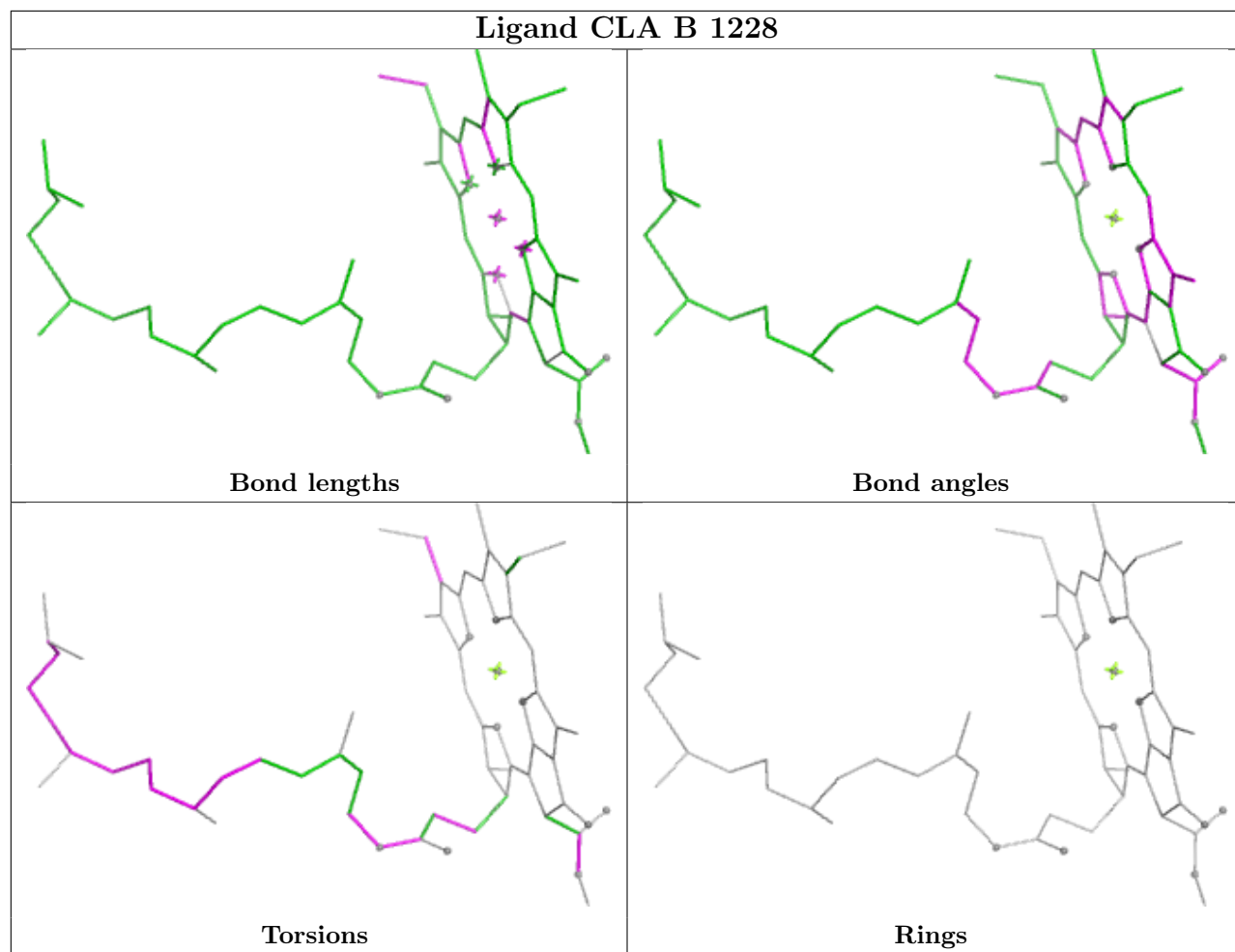


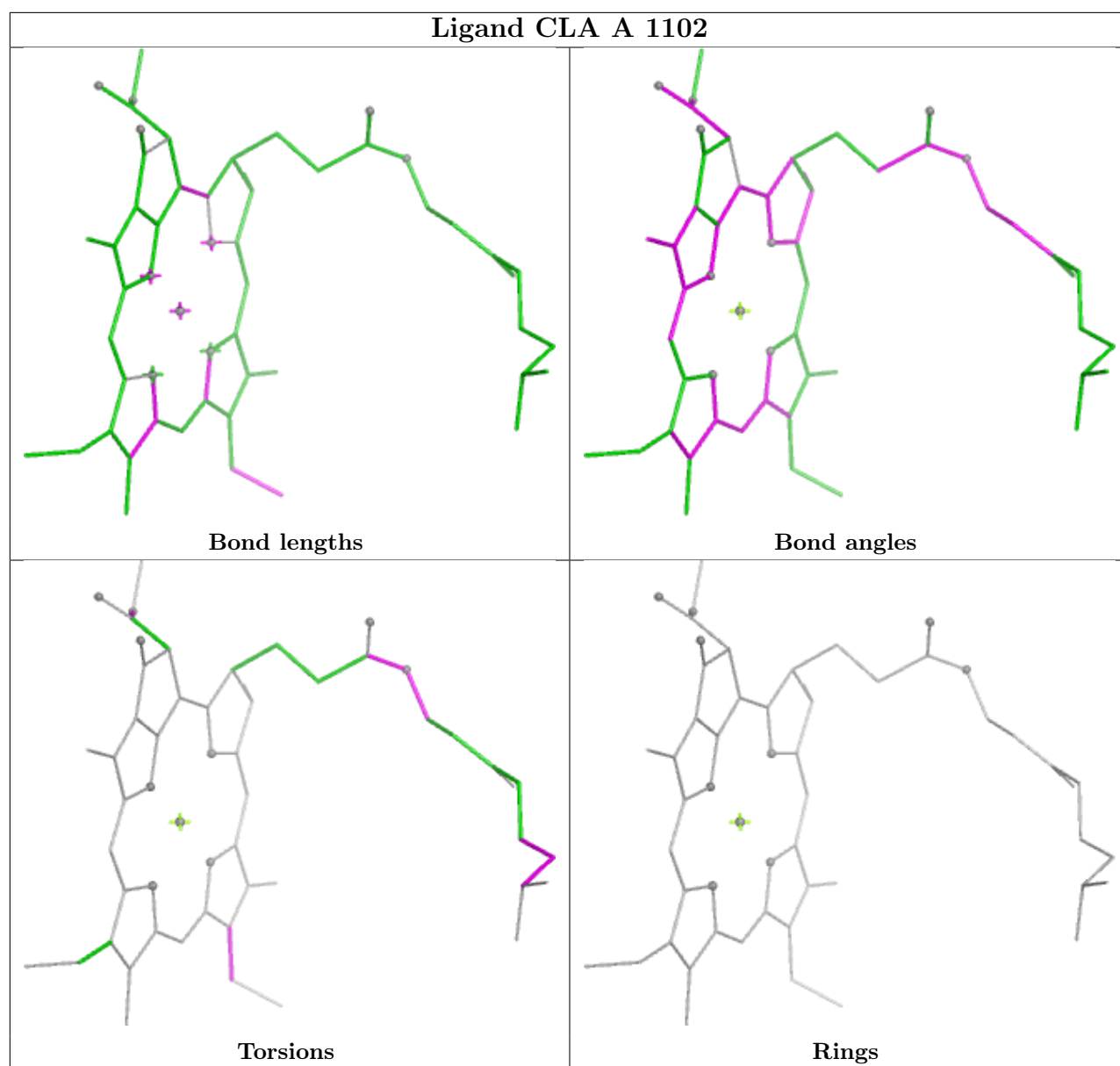


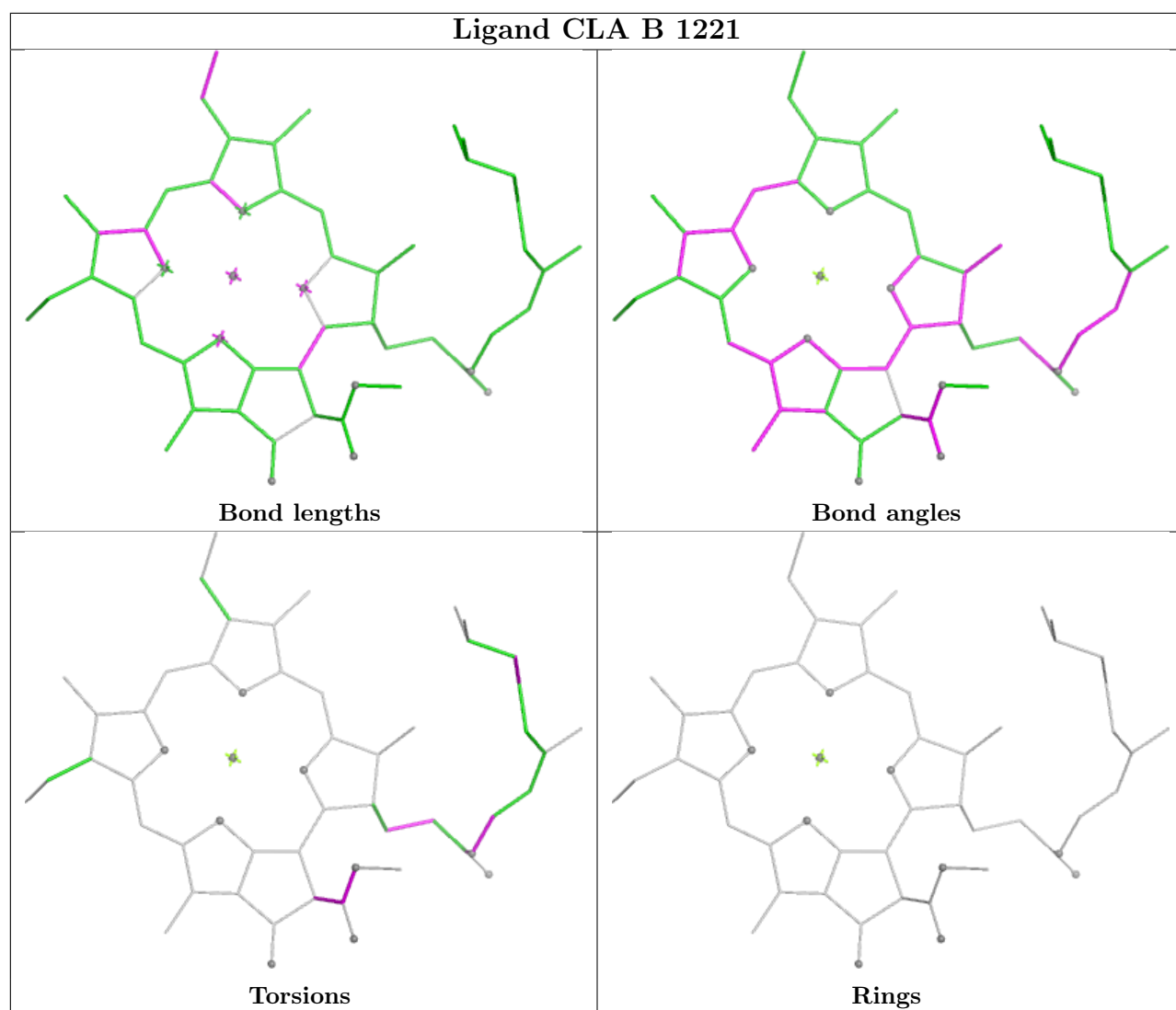
Ligand CLA A 1135**Ligand CLA B 1202**

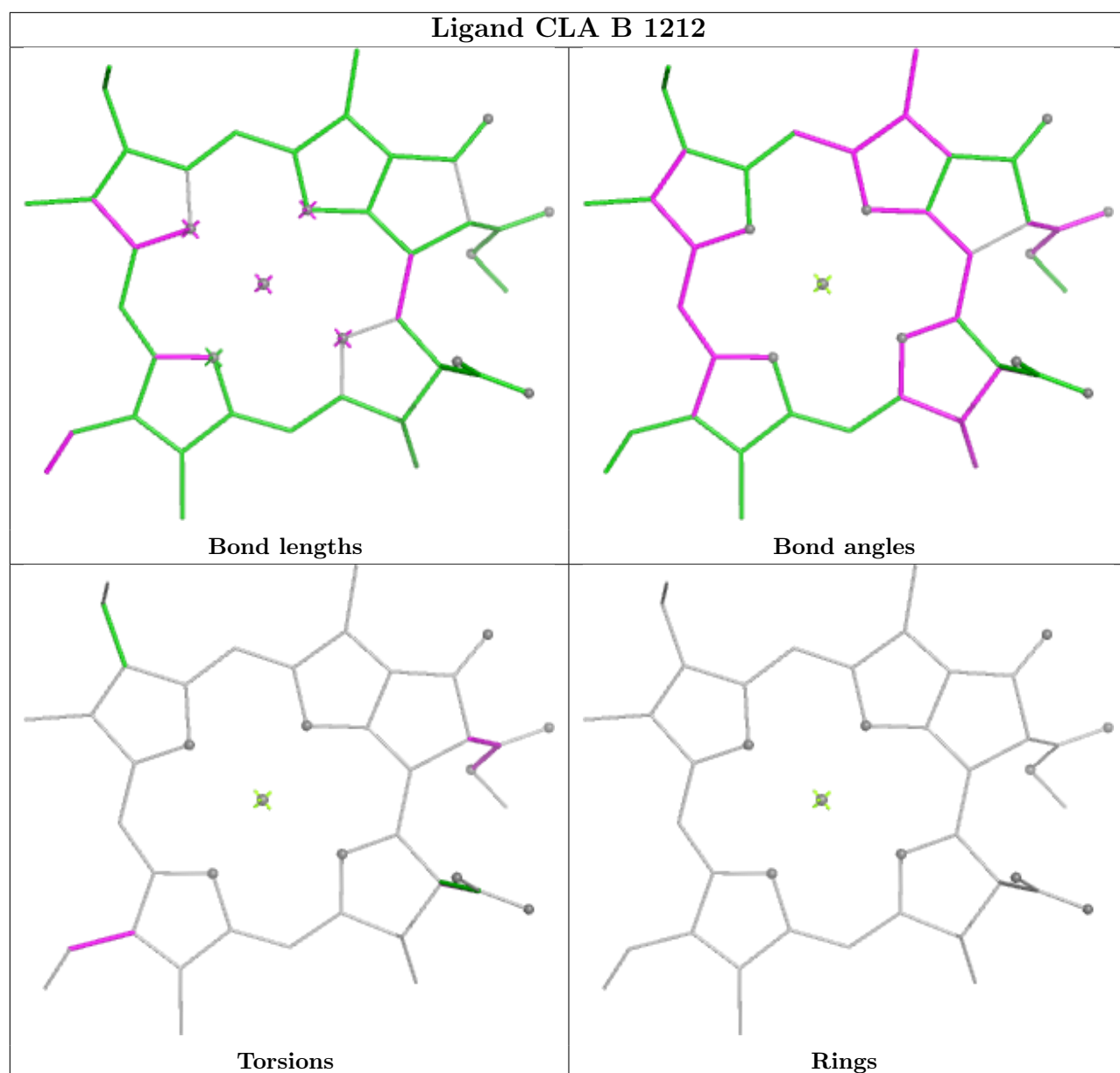


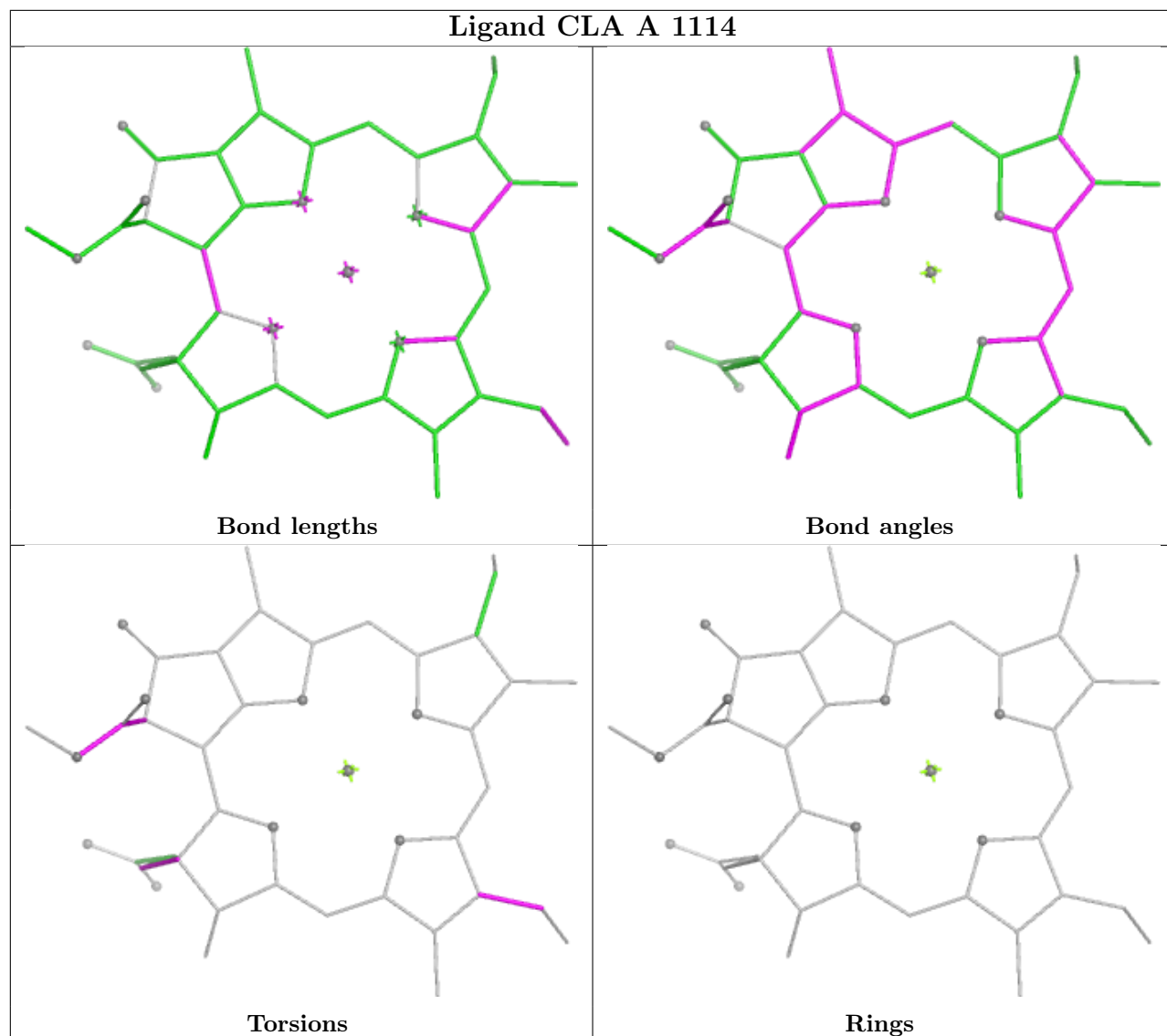


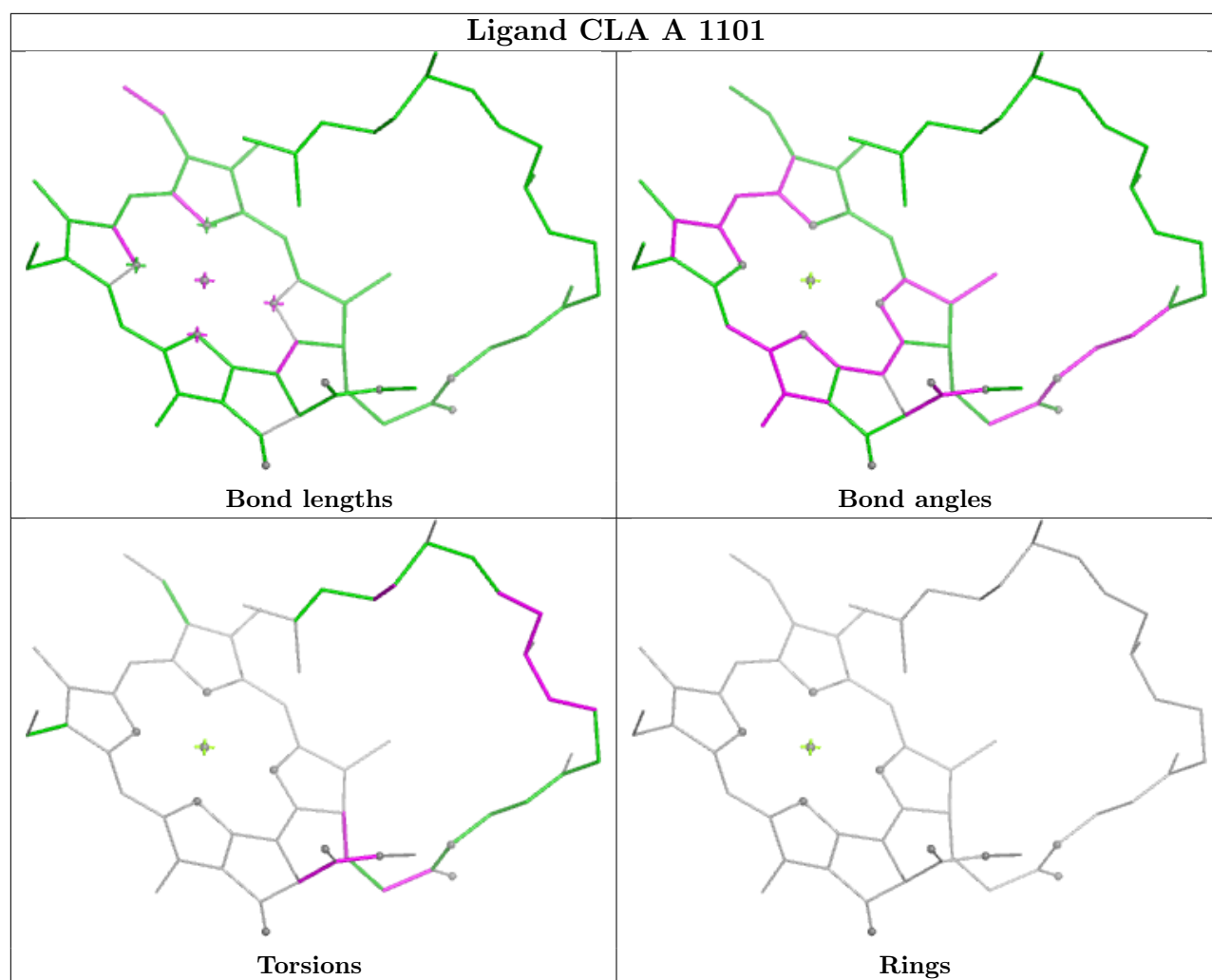




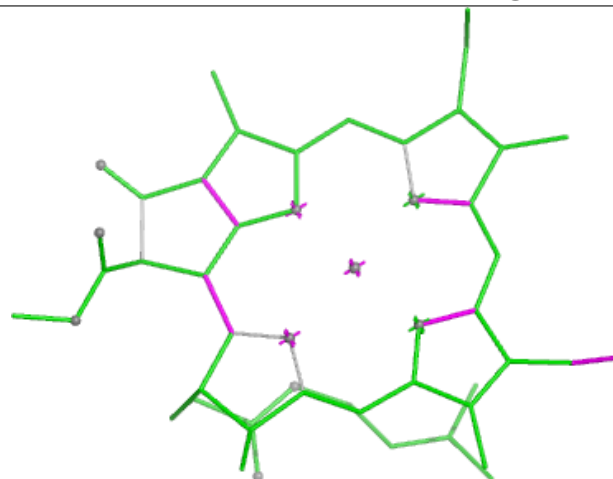




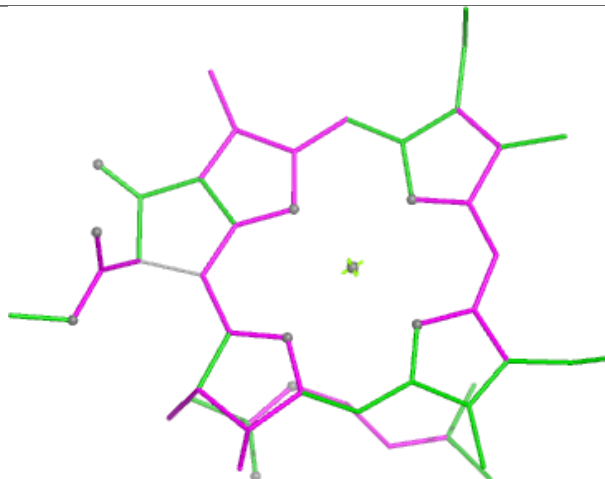




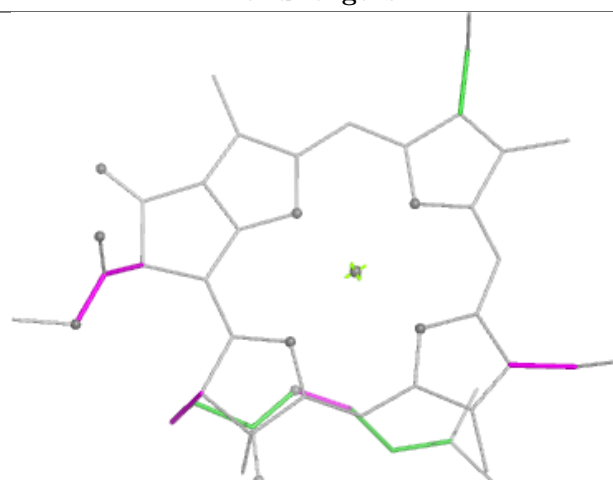
Ligand CLA A 1121



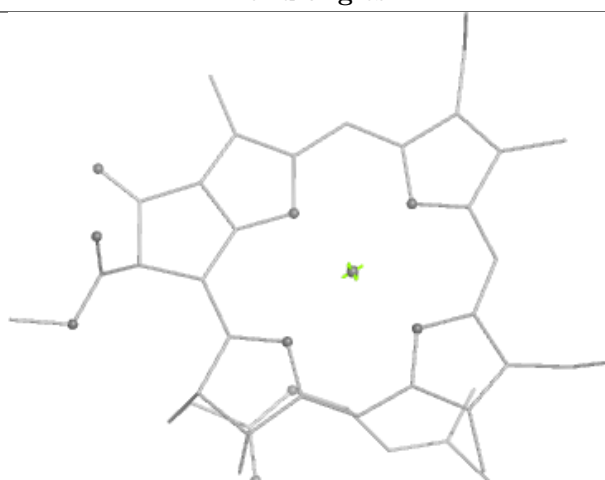
Bond lengths



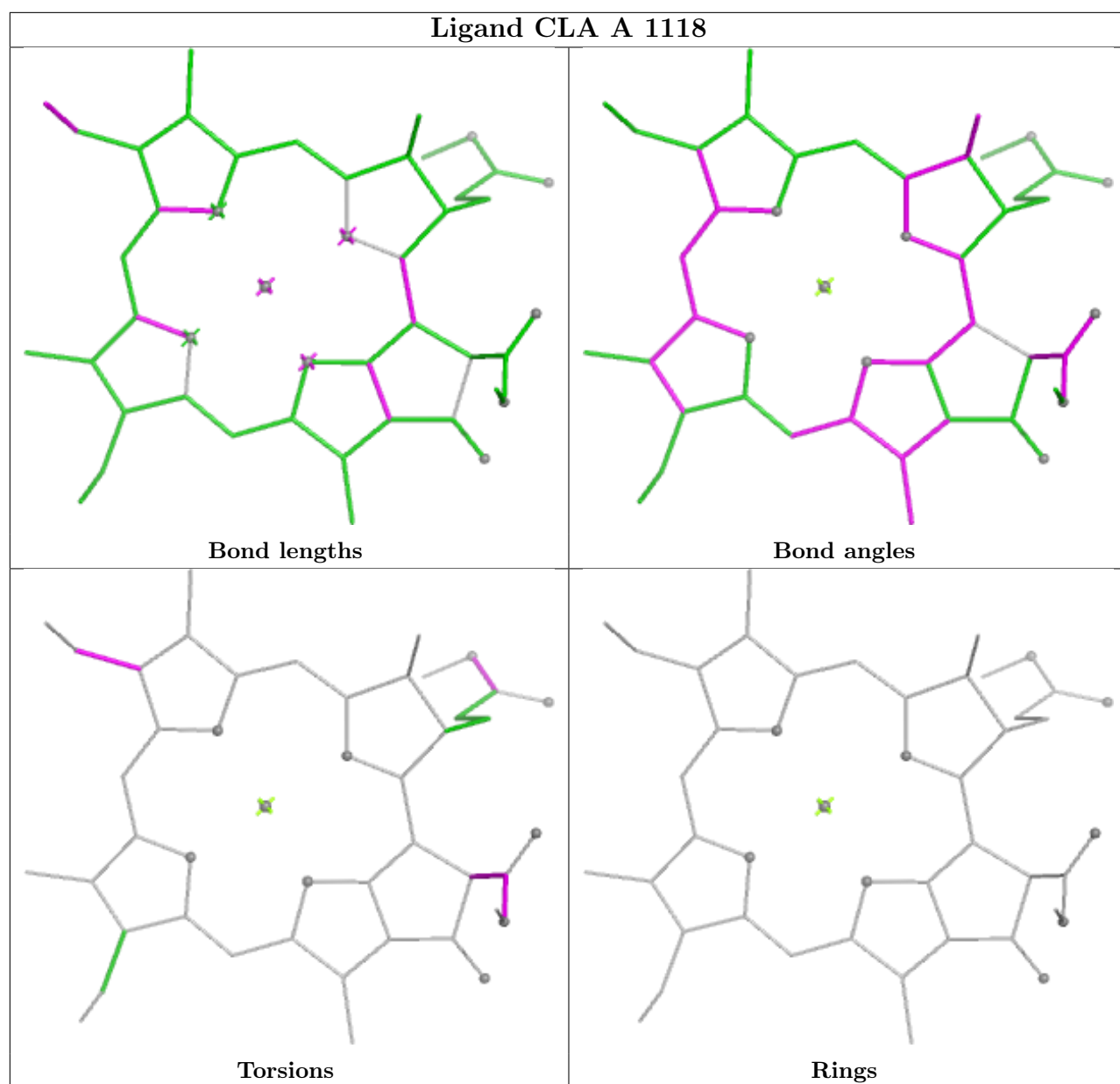
Bond angles

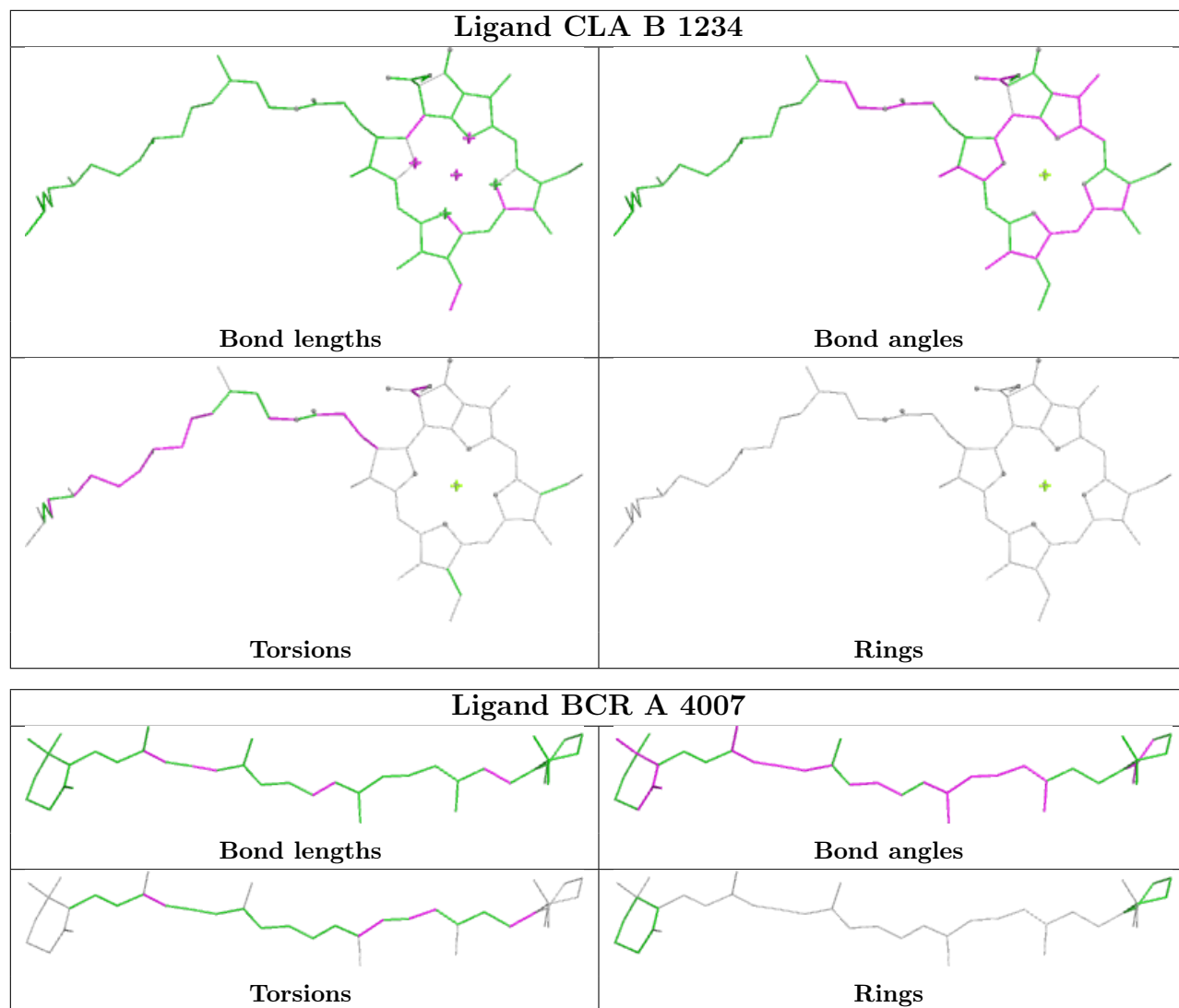


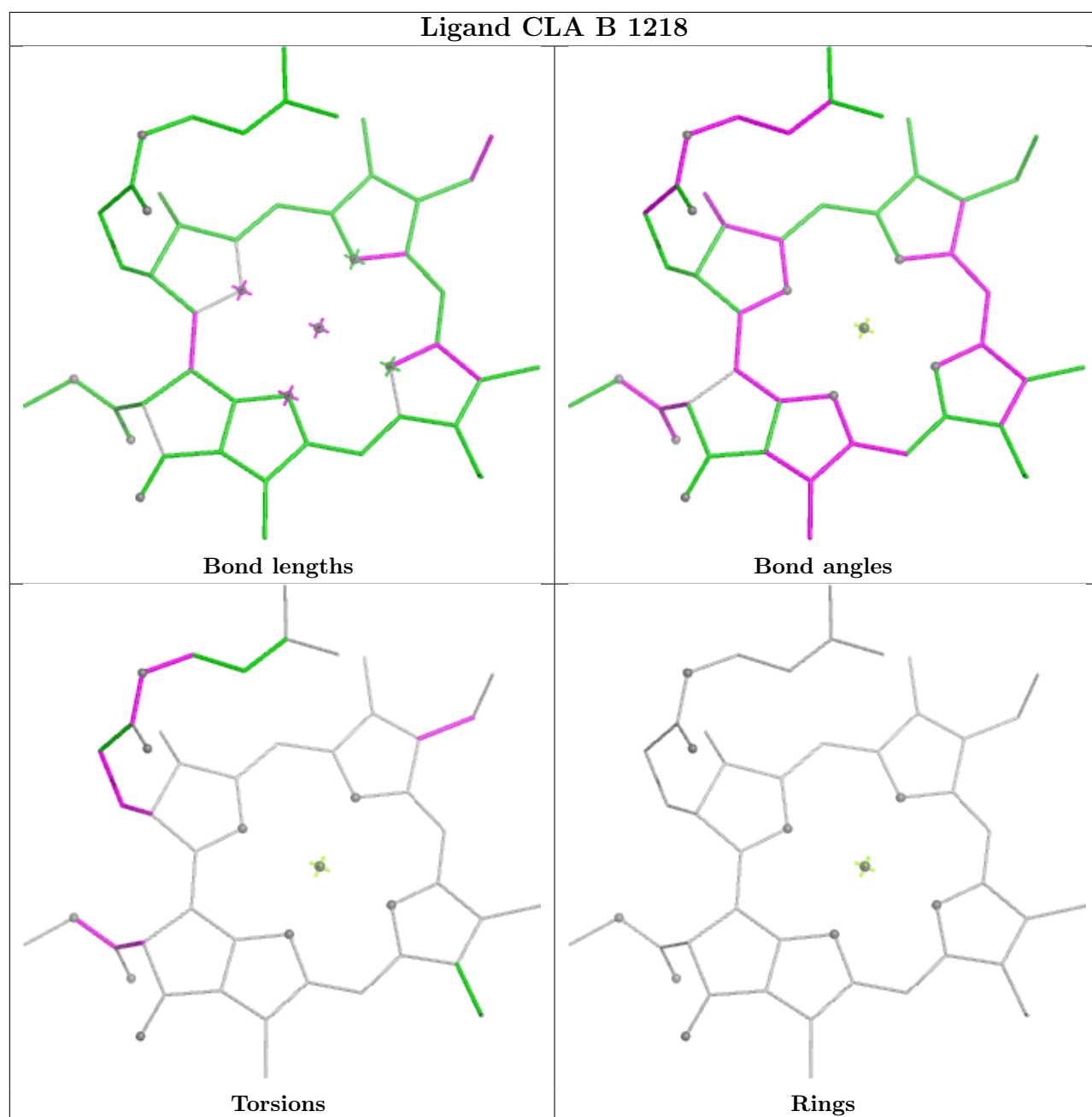
Torsions

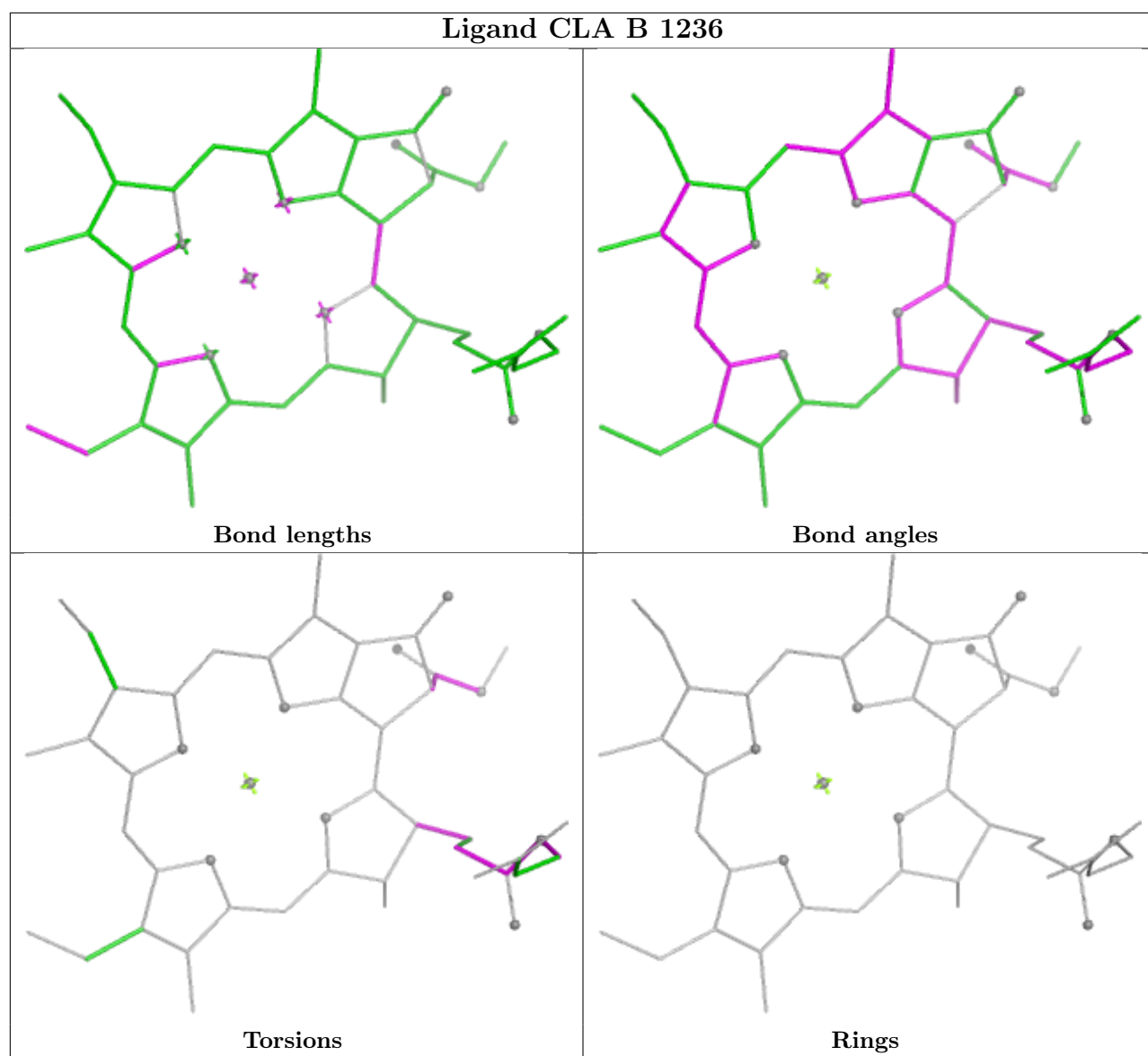


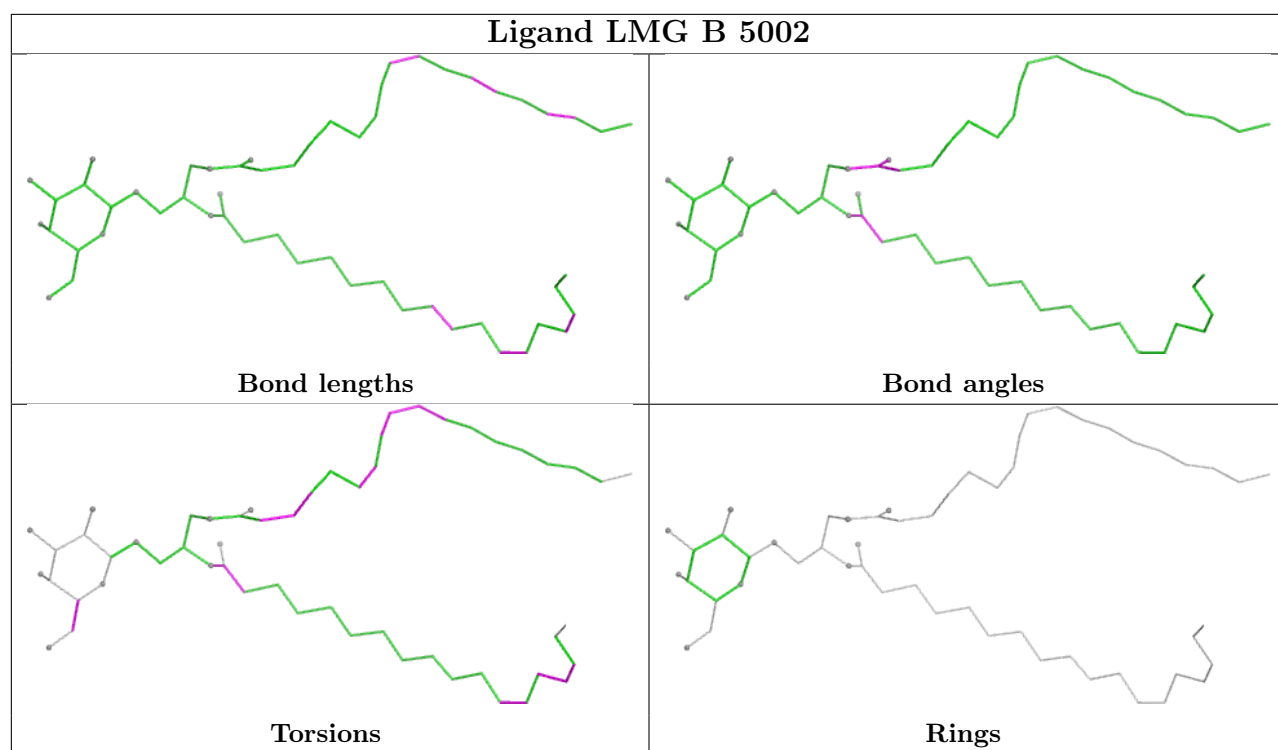
Rings



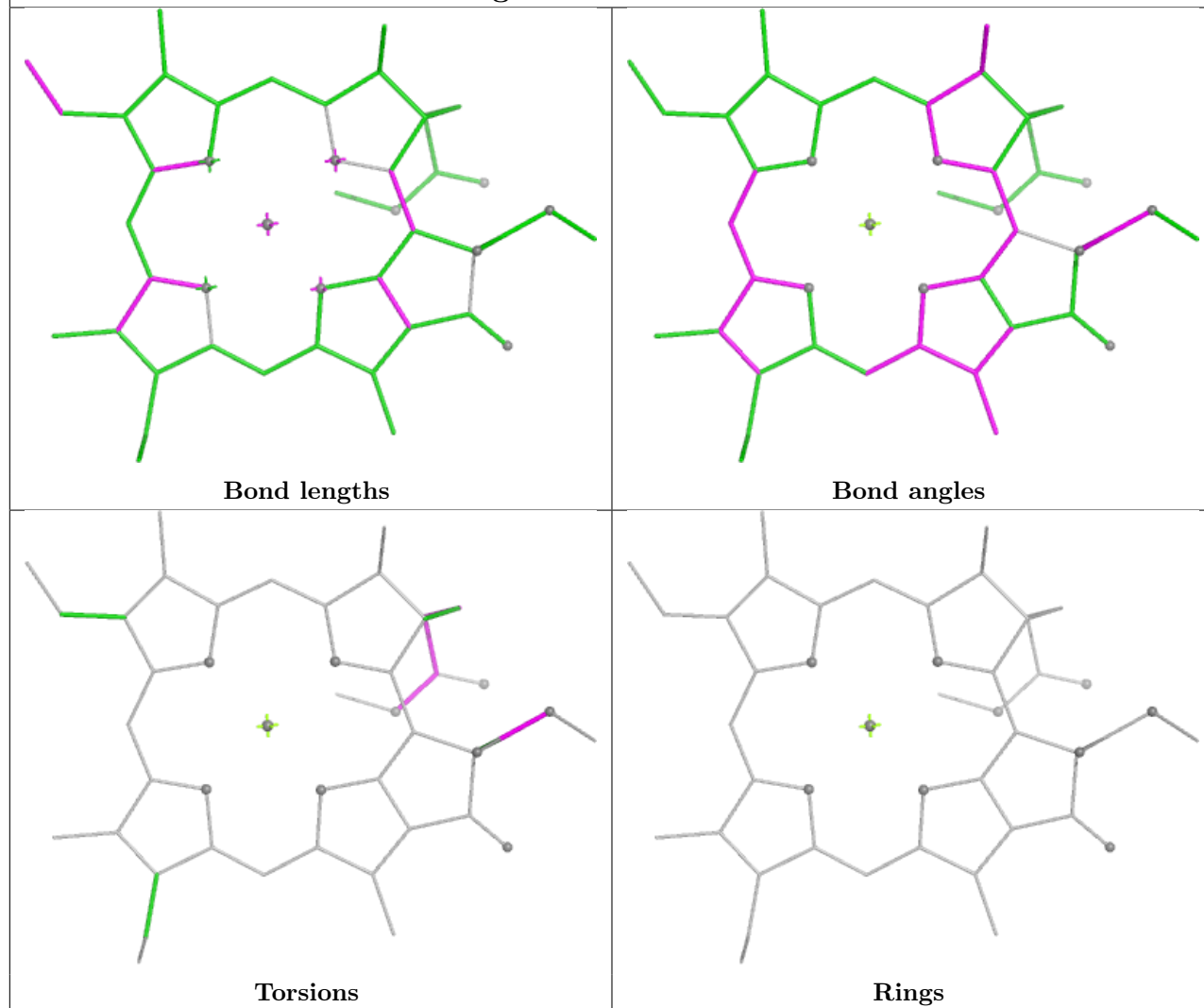




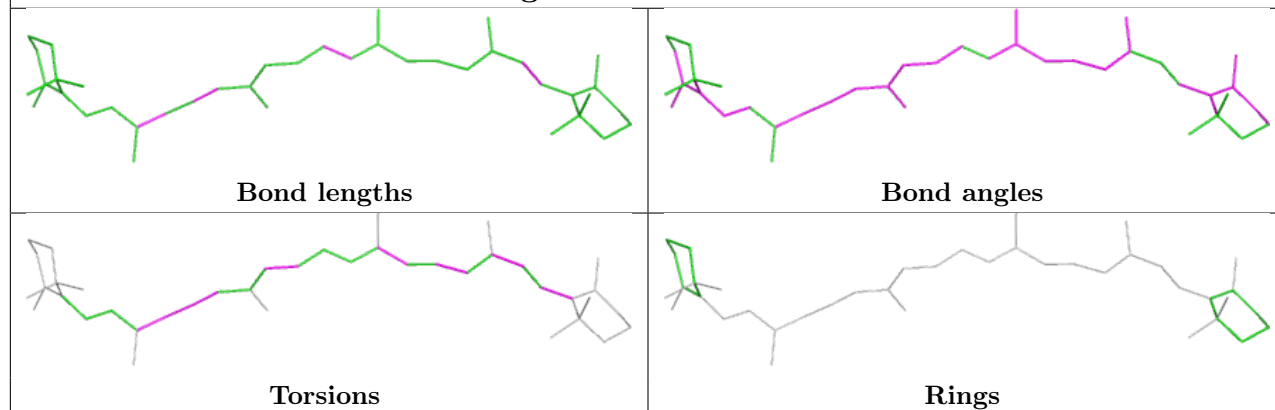


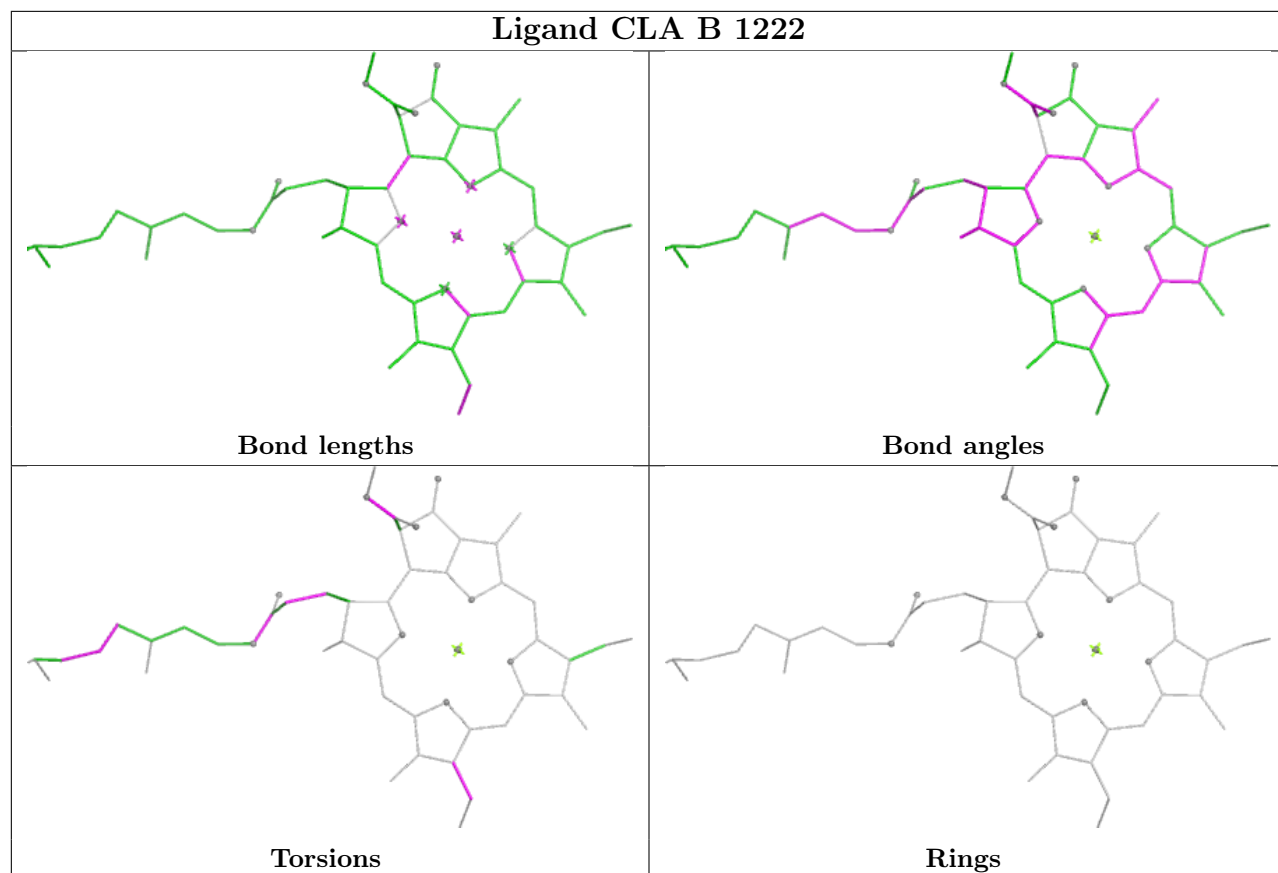


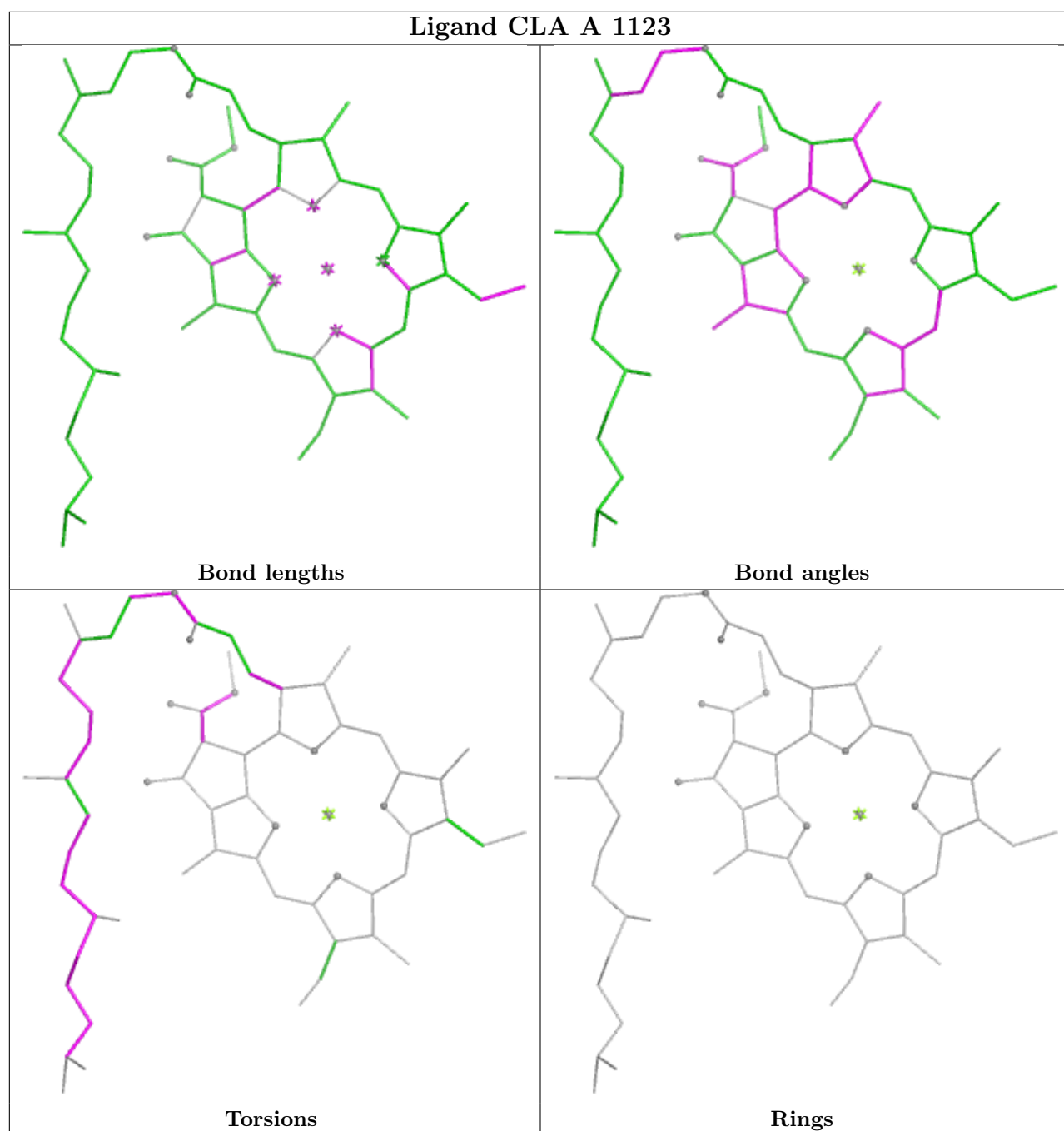
Ligand CLA A 1115

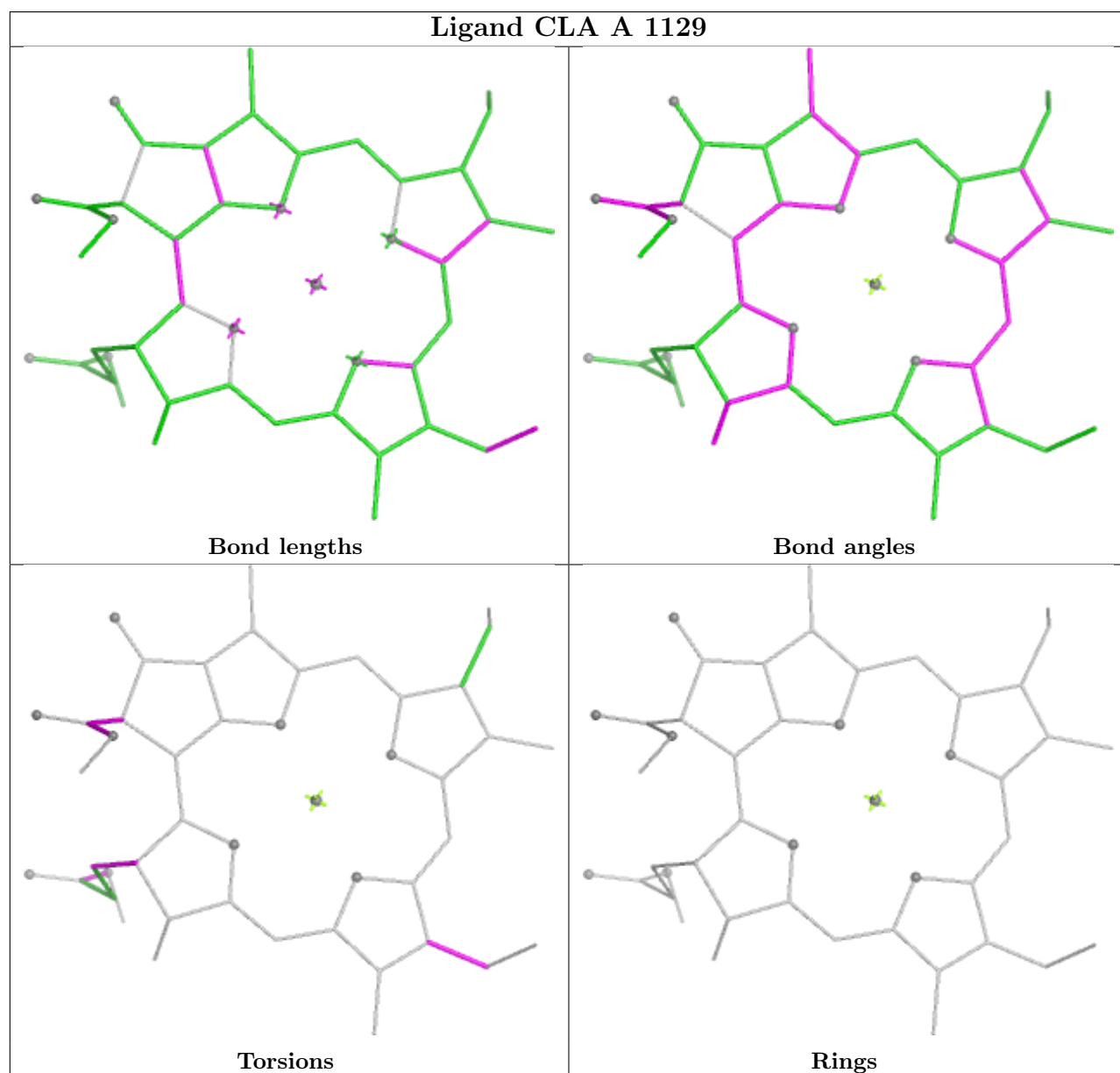
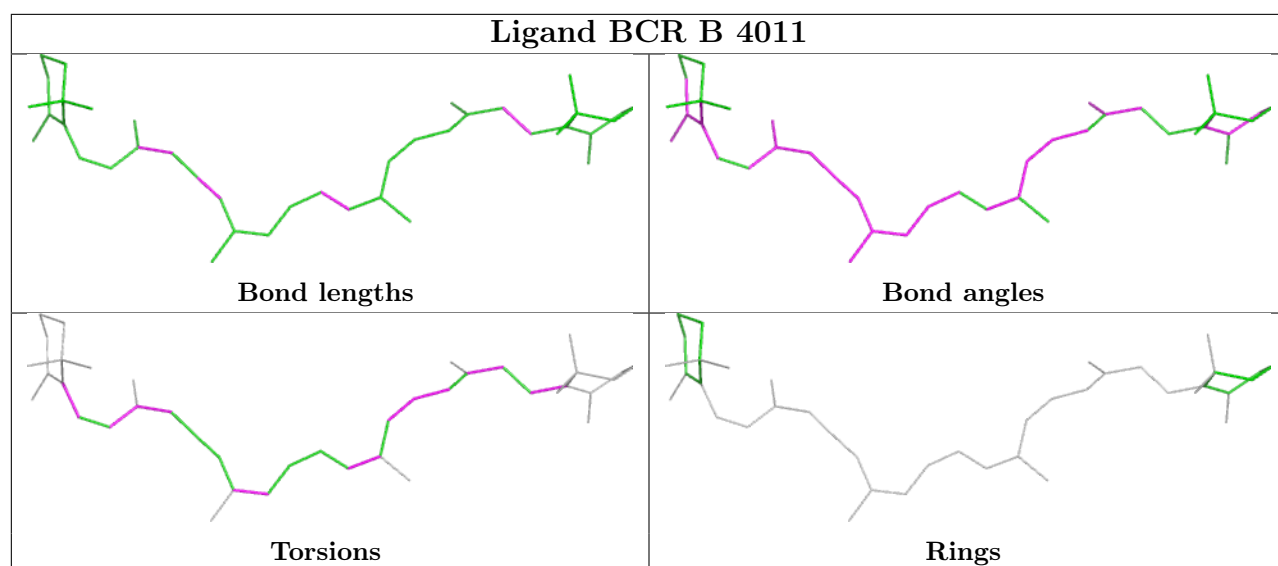


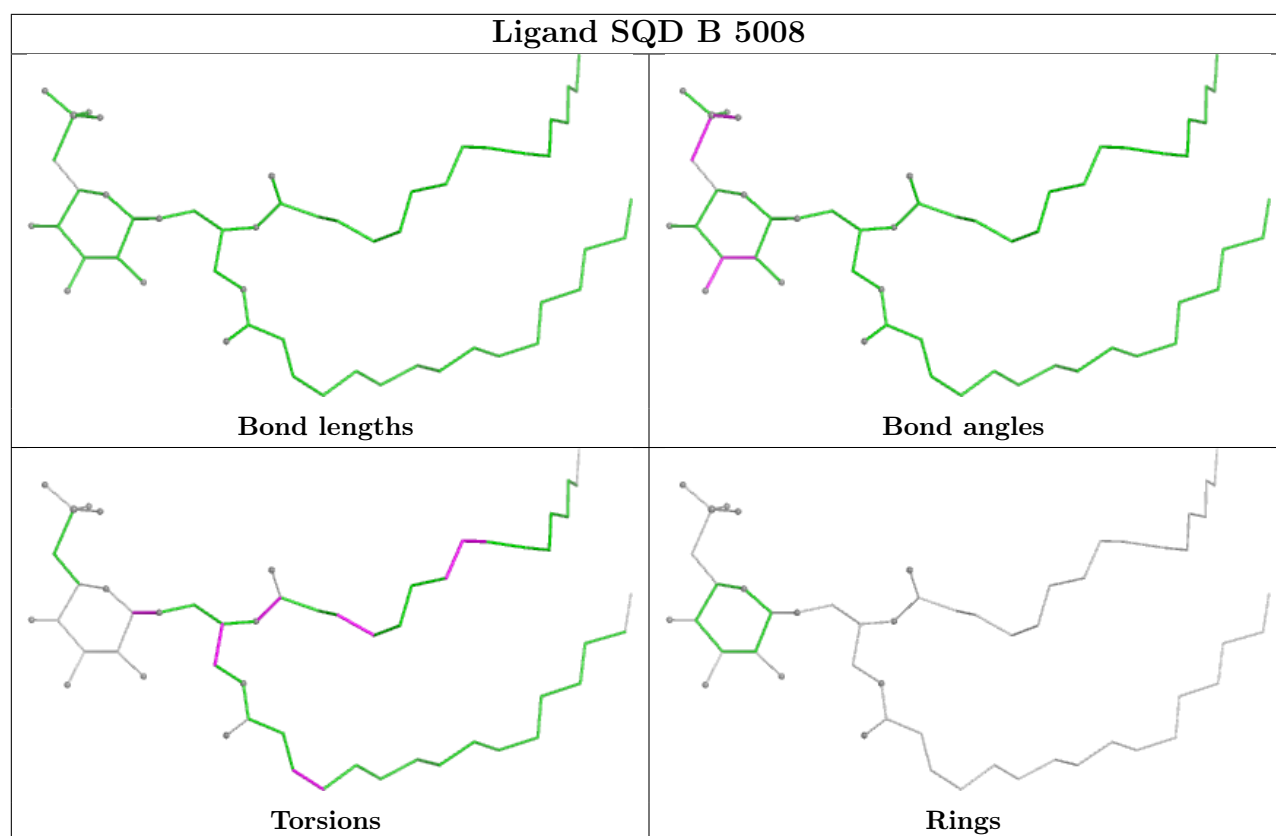
Ligand BCR B 4010

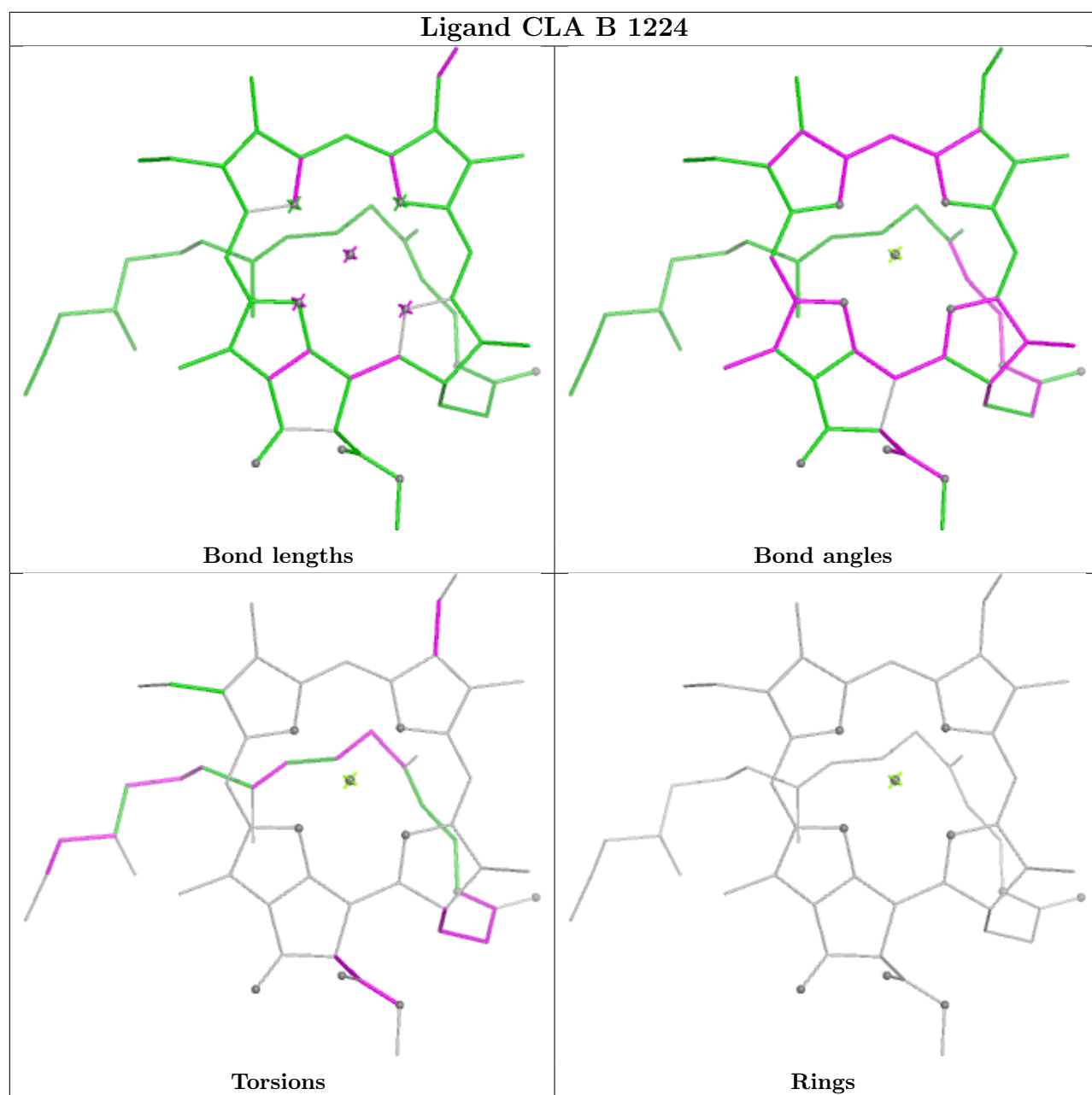


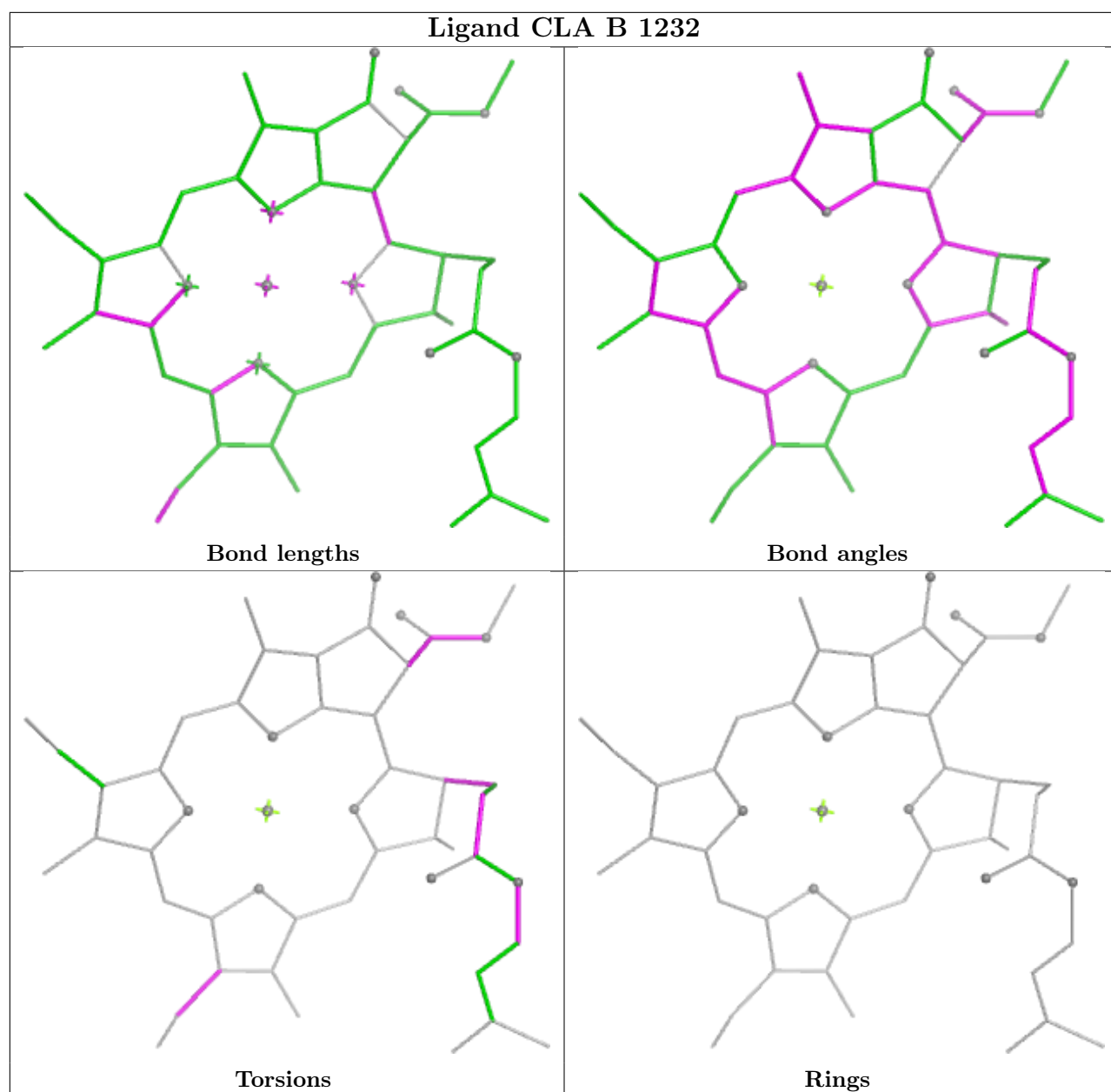


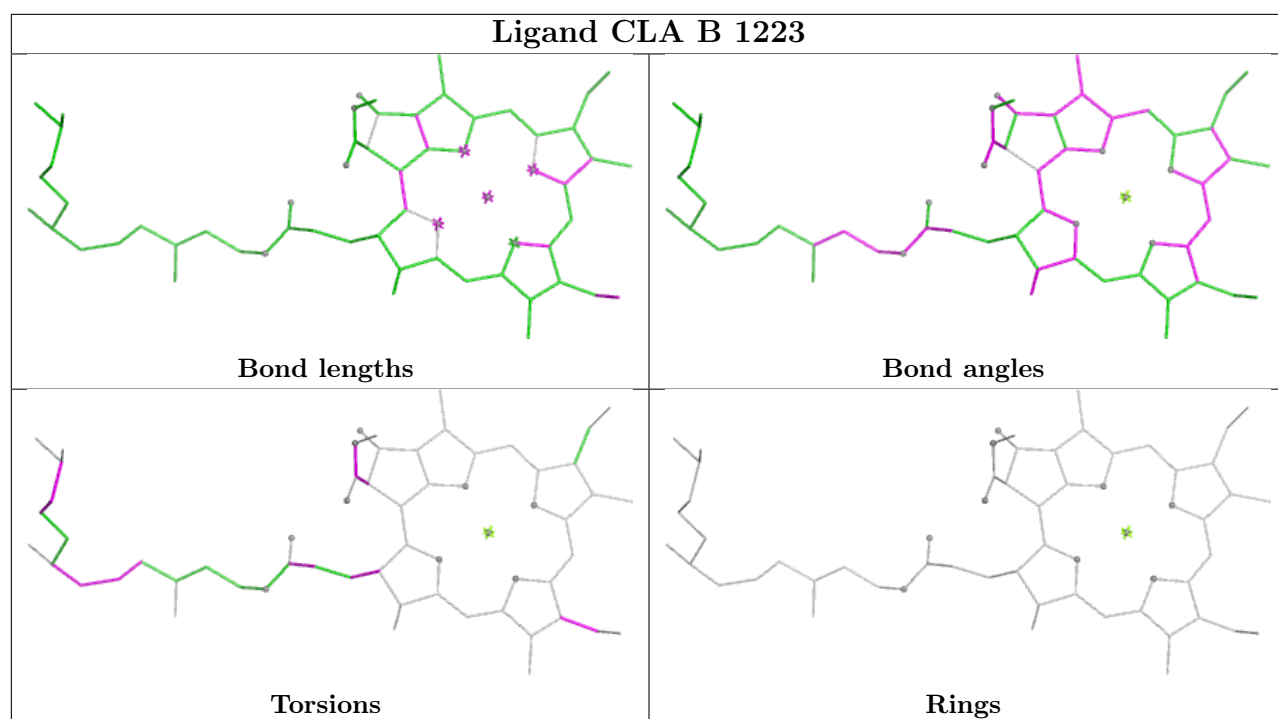


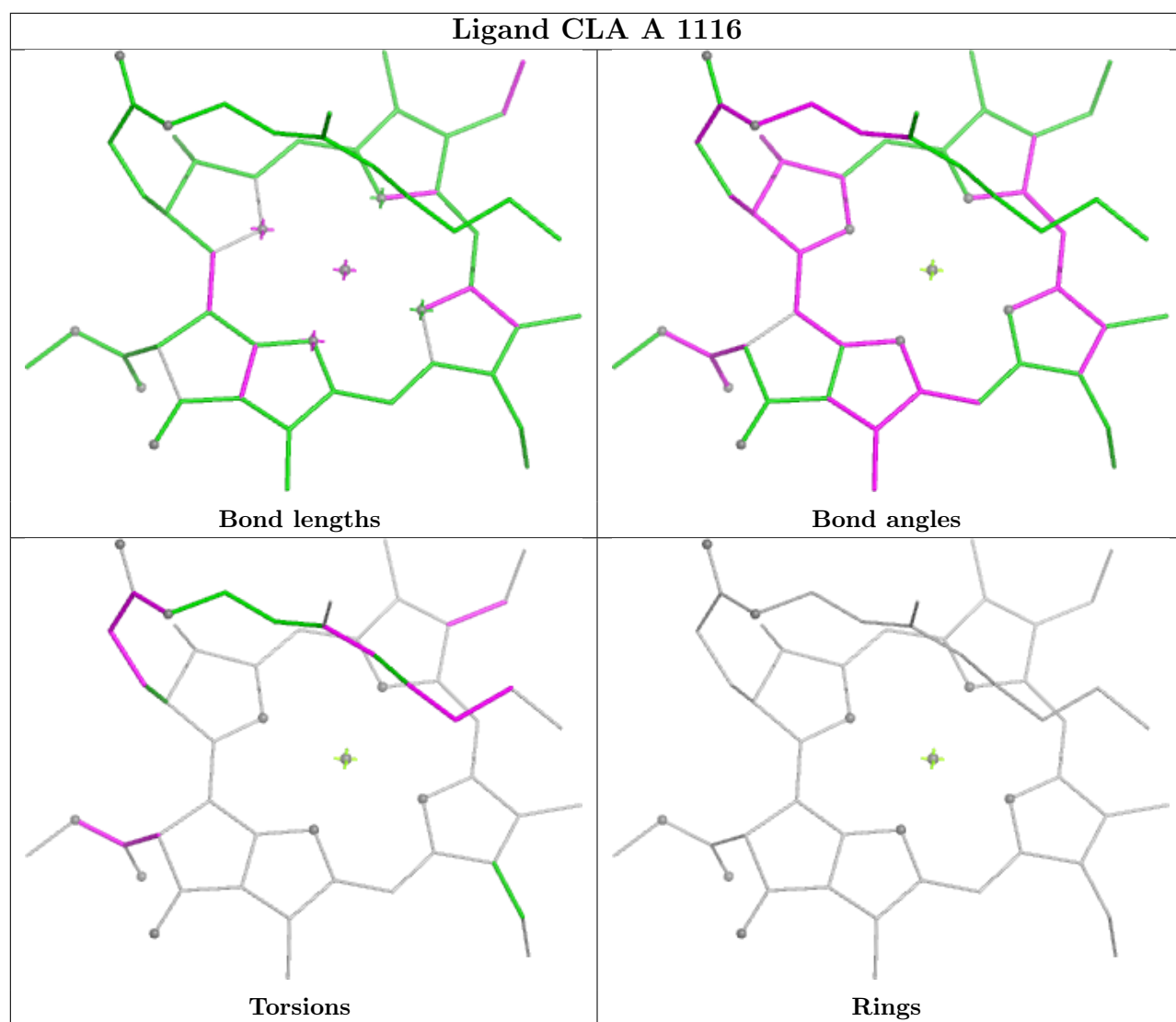


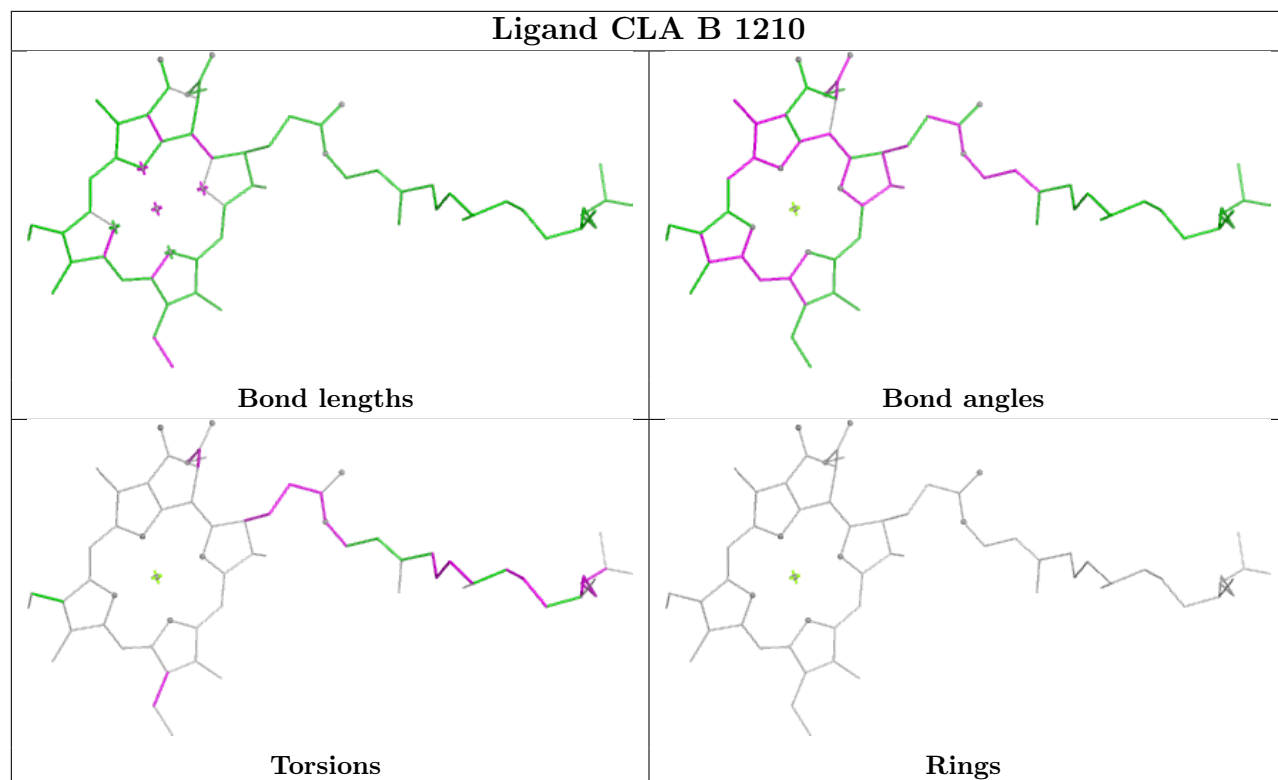




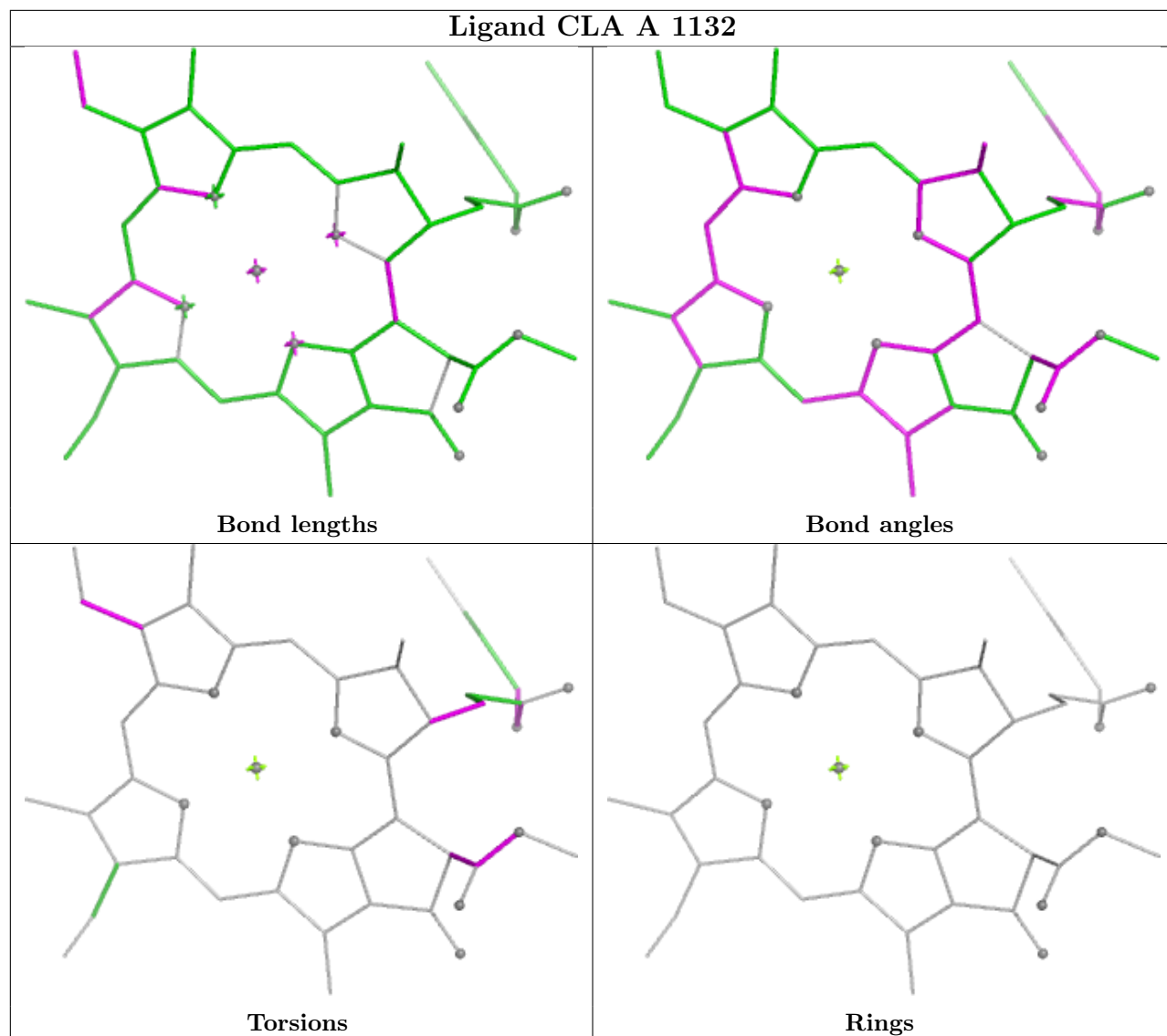


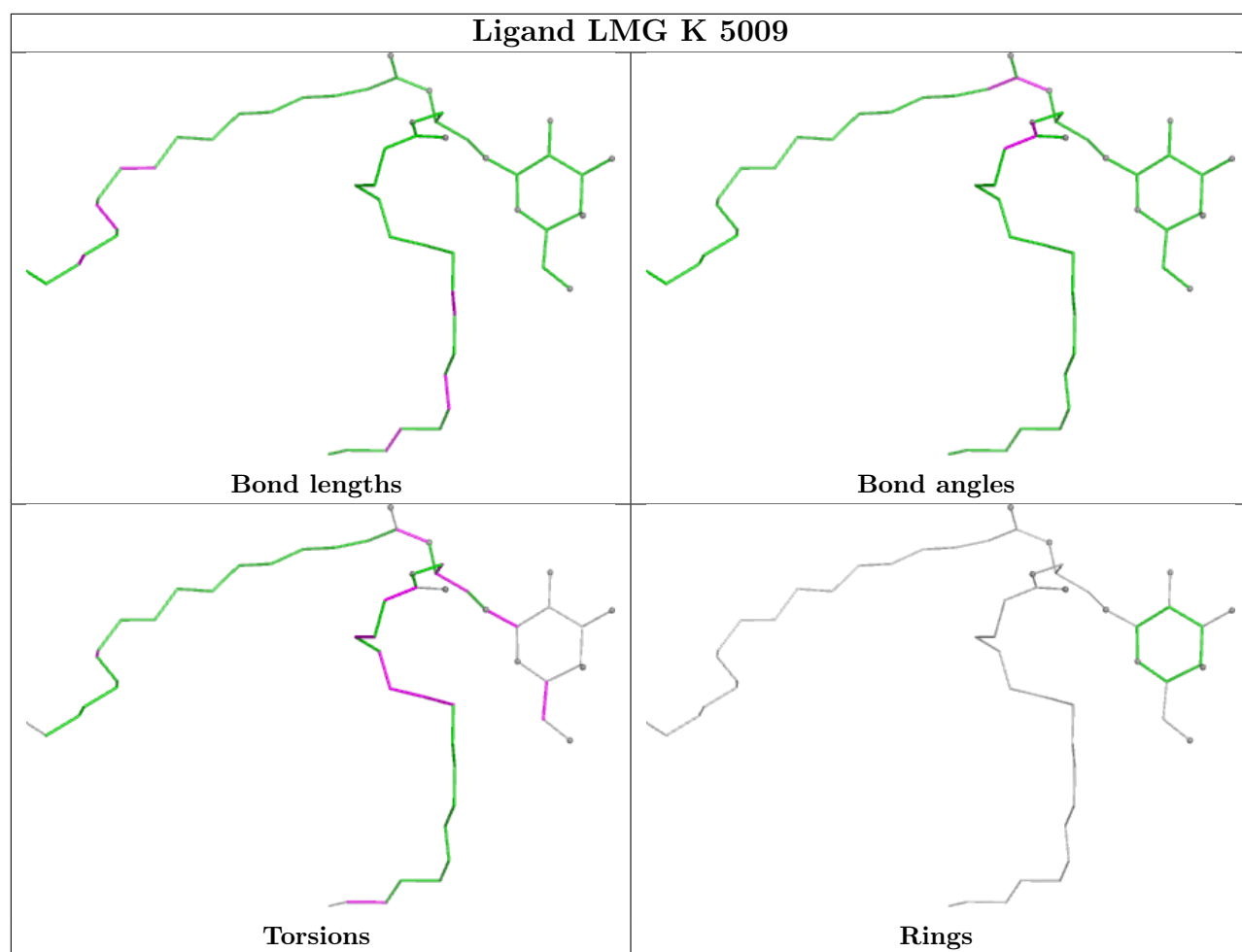


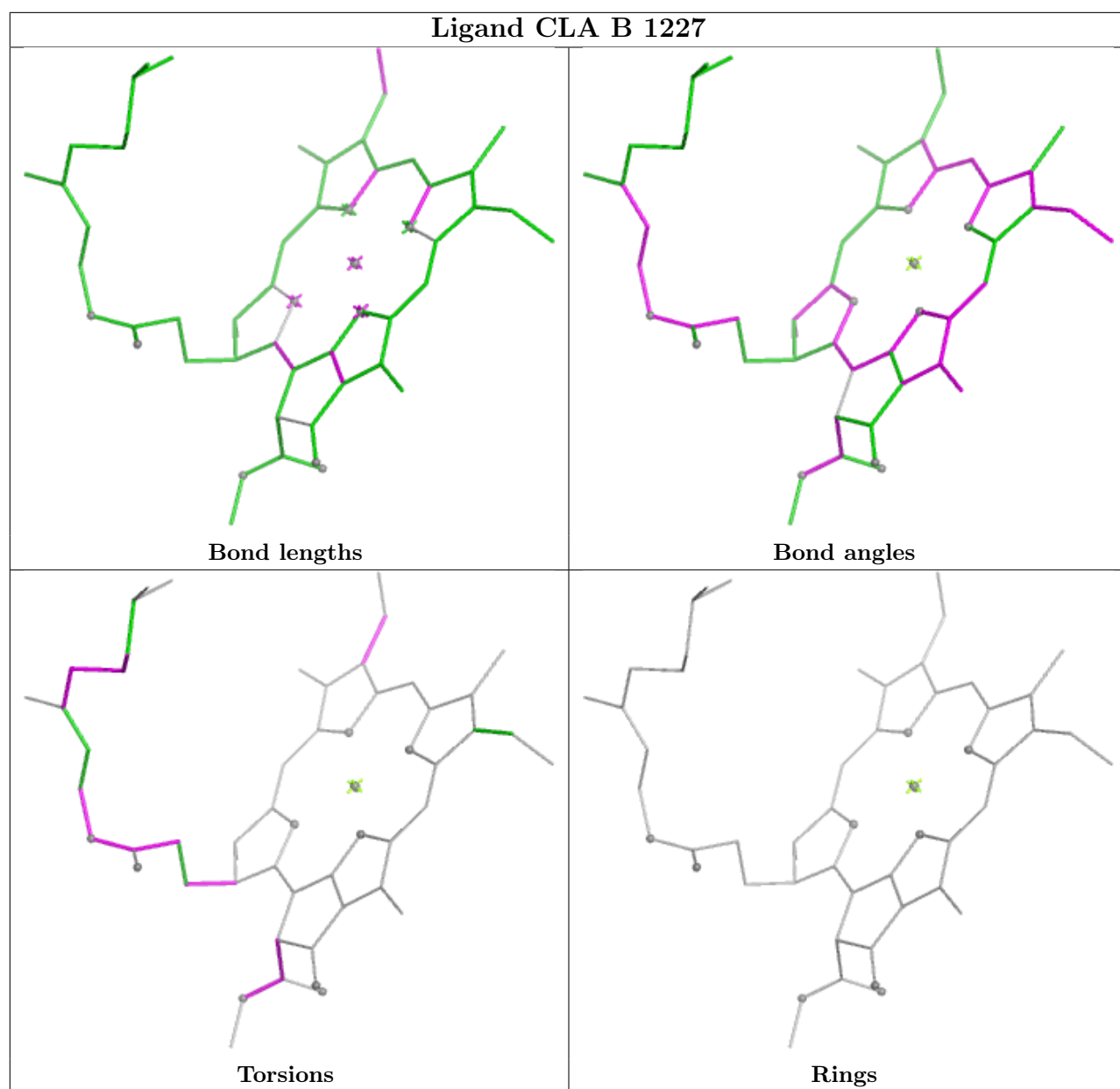


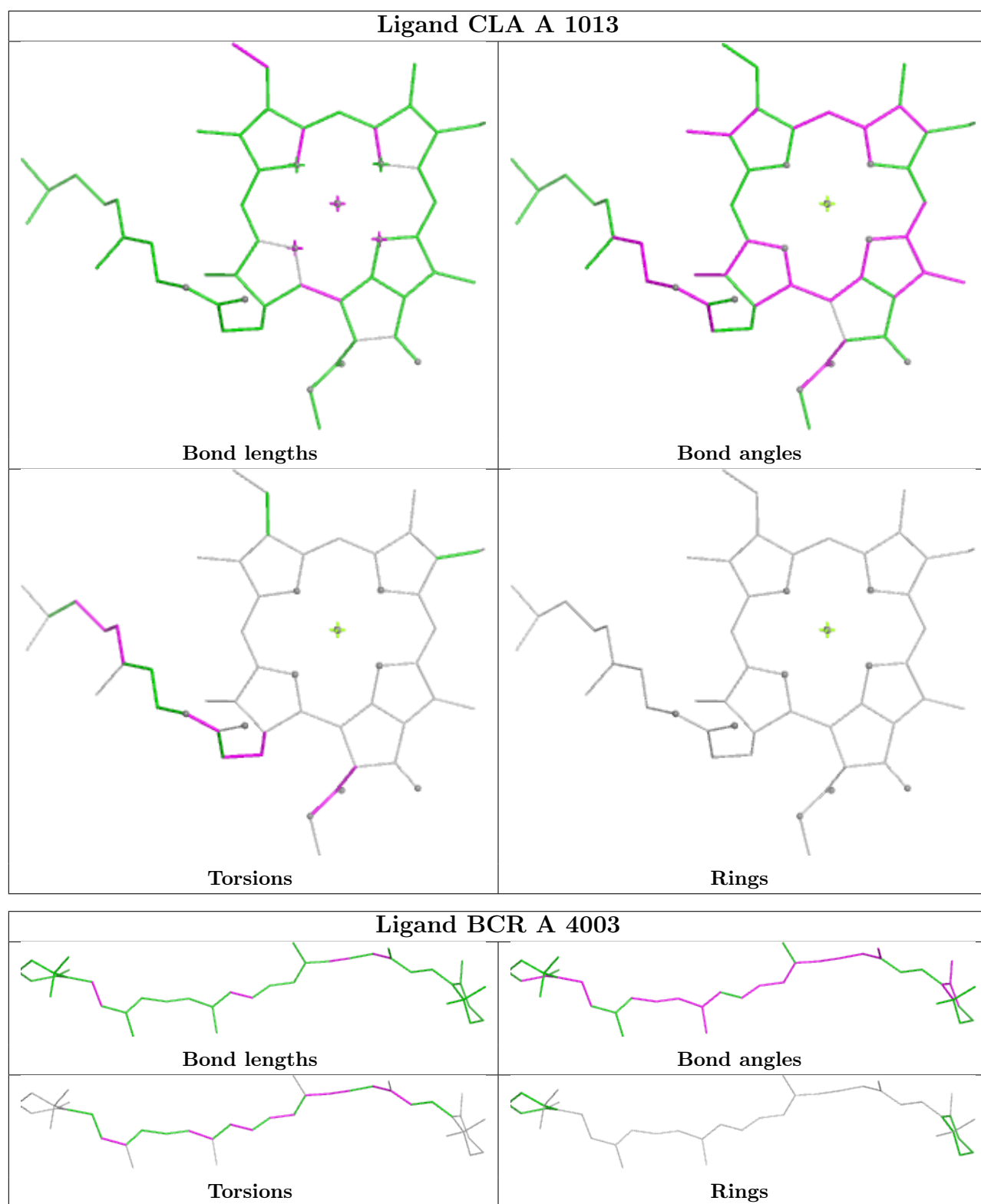


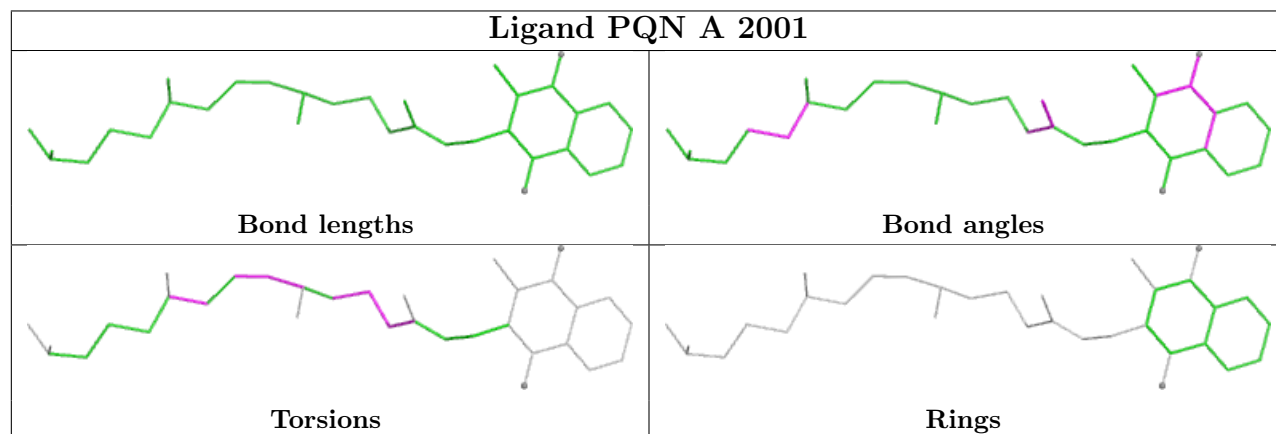
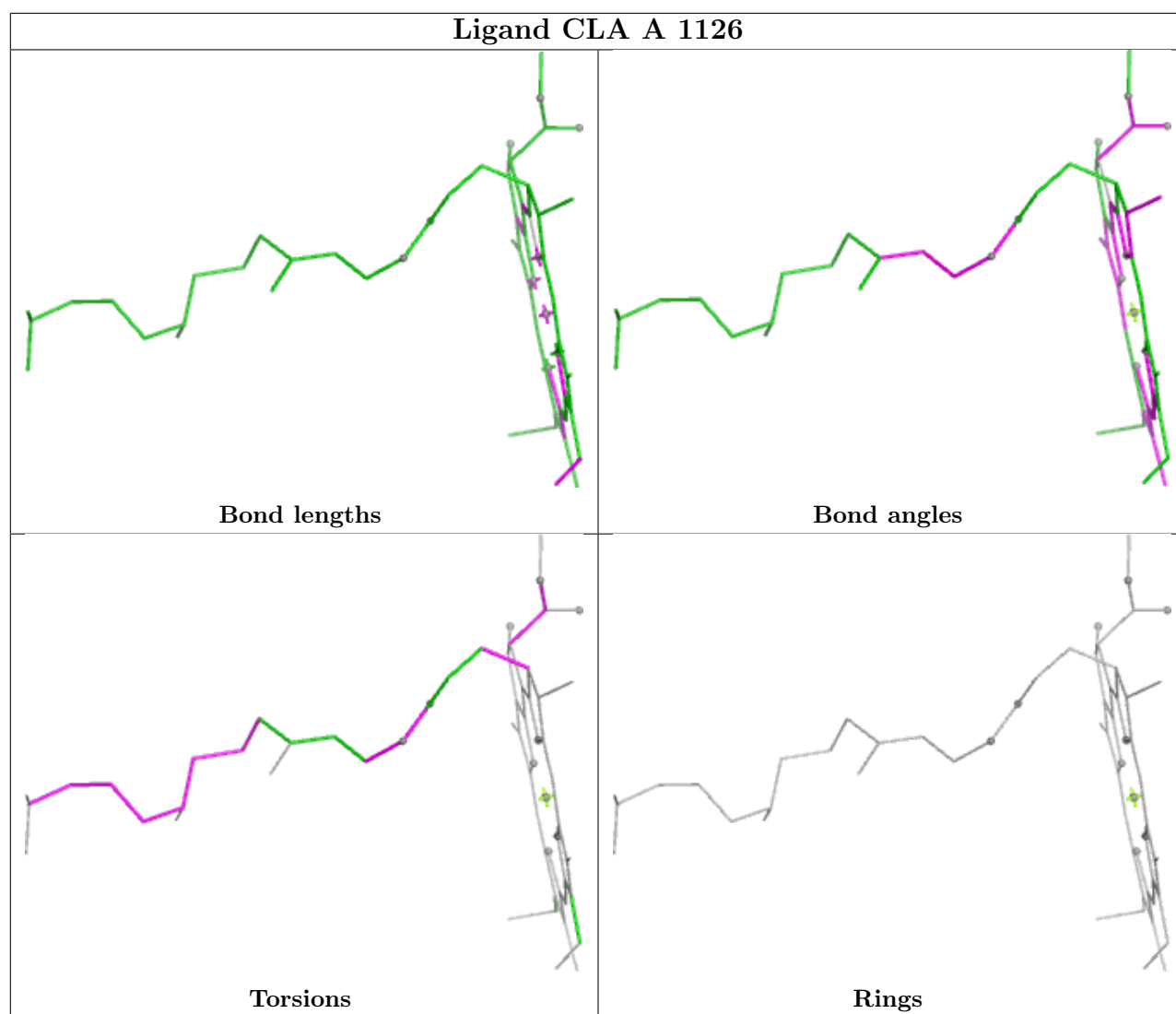
Ligand CLA A 1132



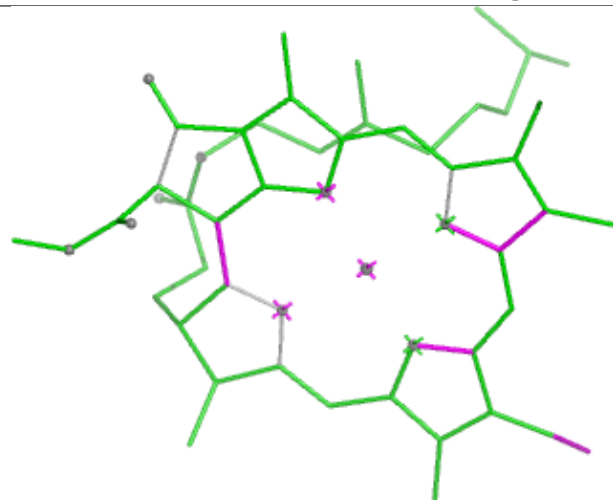




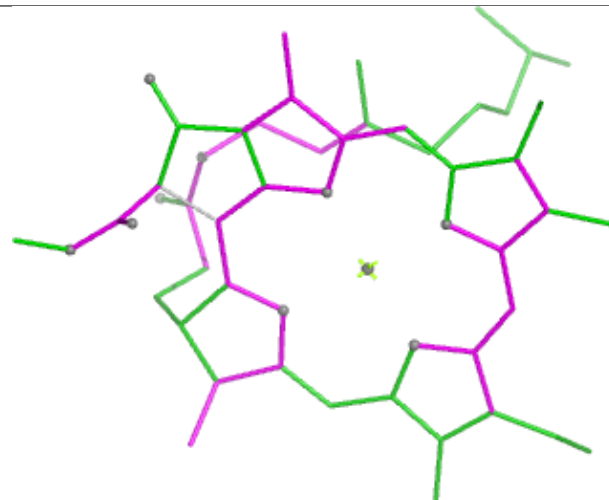




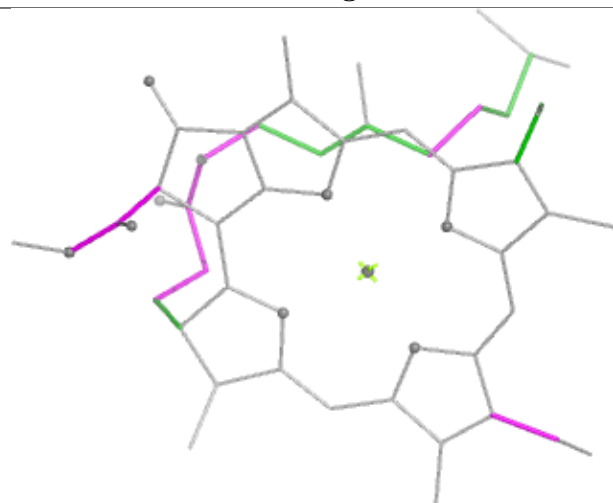
Ligand CLA A 1130



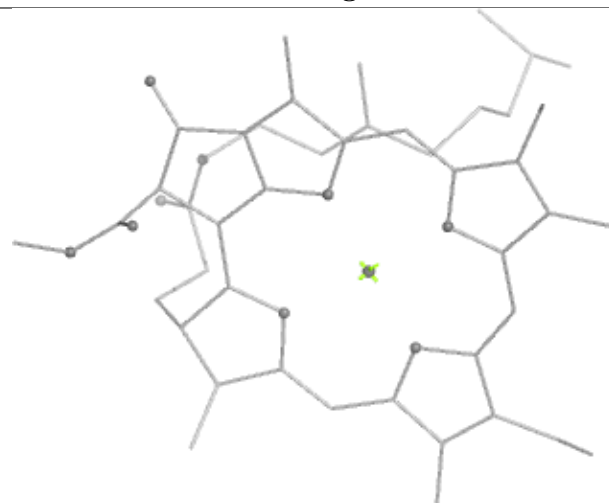
Bond lengths



Bond angles

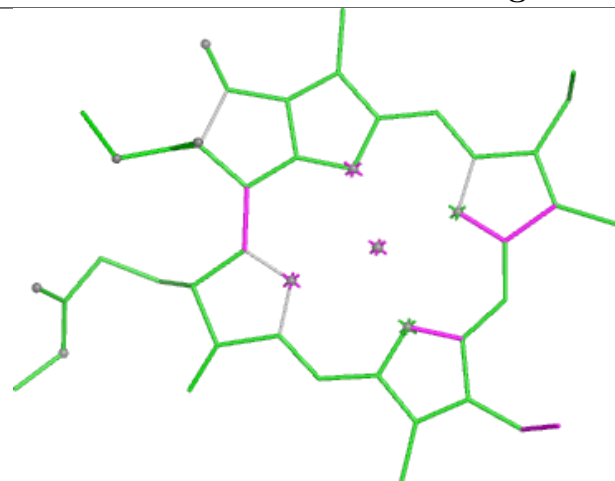


Torsions

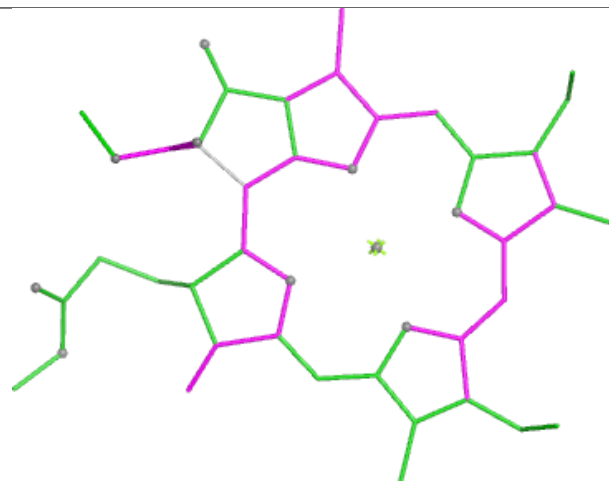


Rings

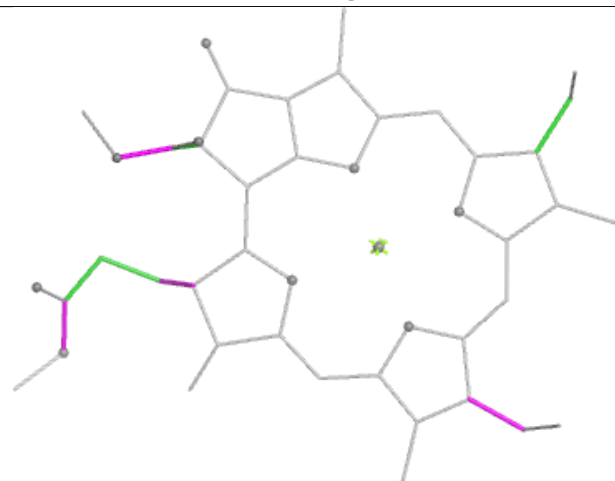
Ligand CLA A 1139



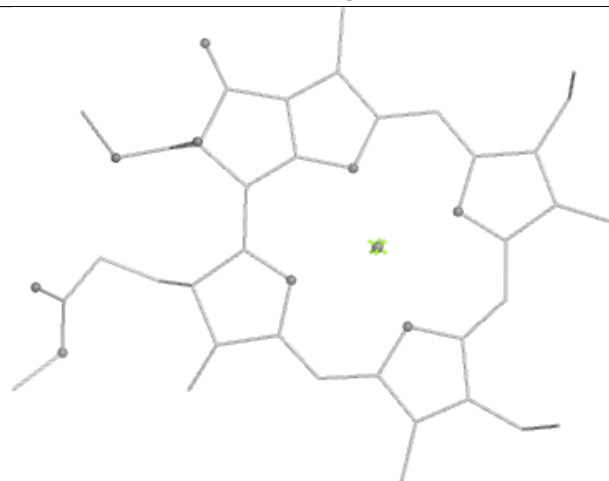
Bond lengths



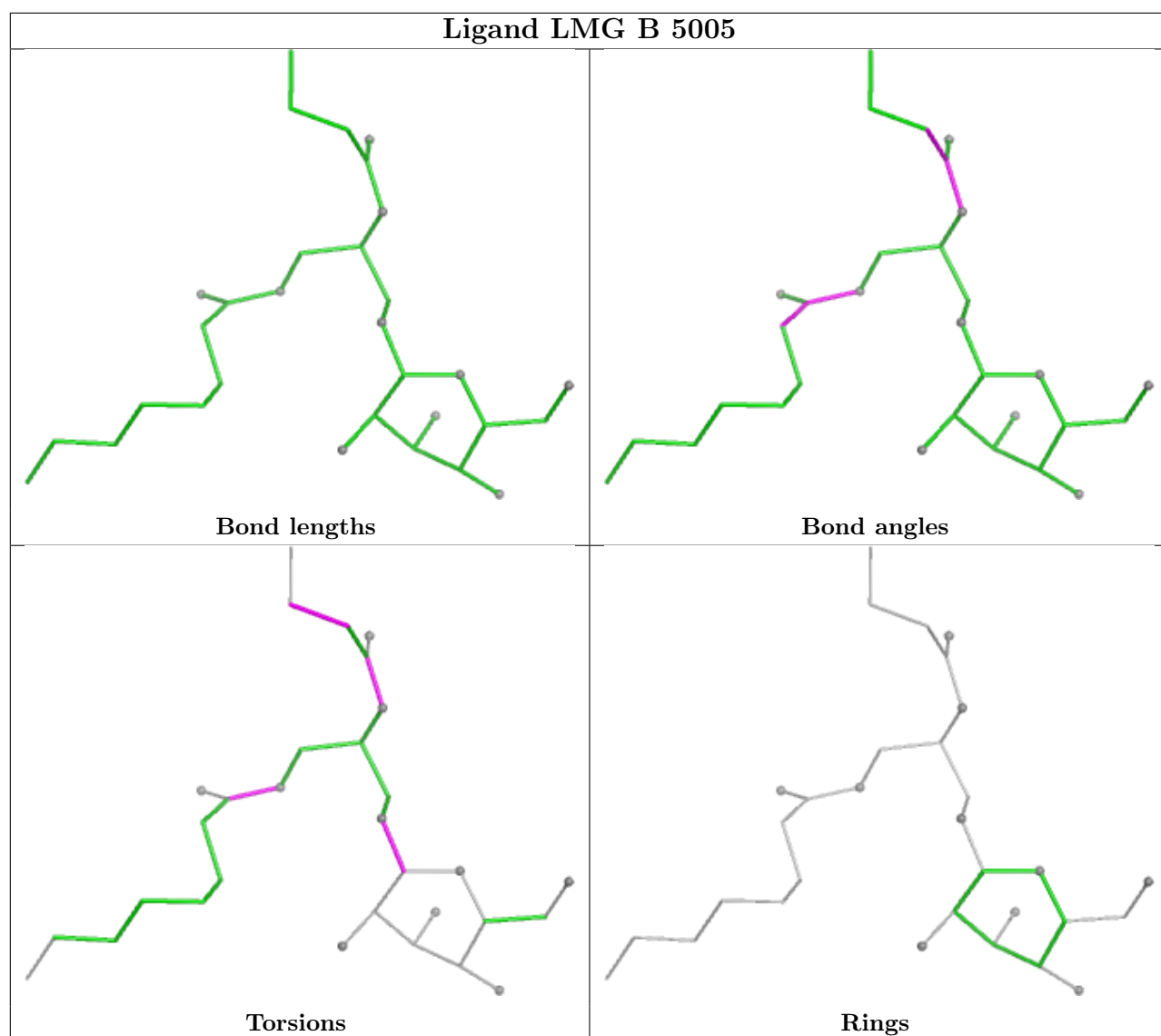
Bond angles

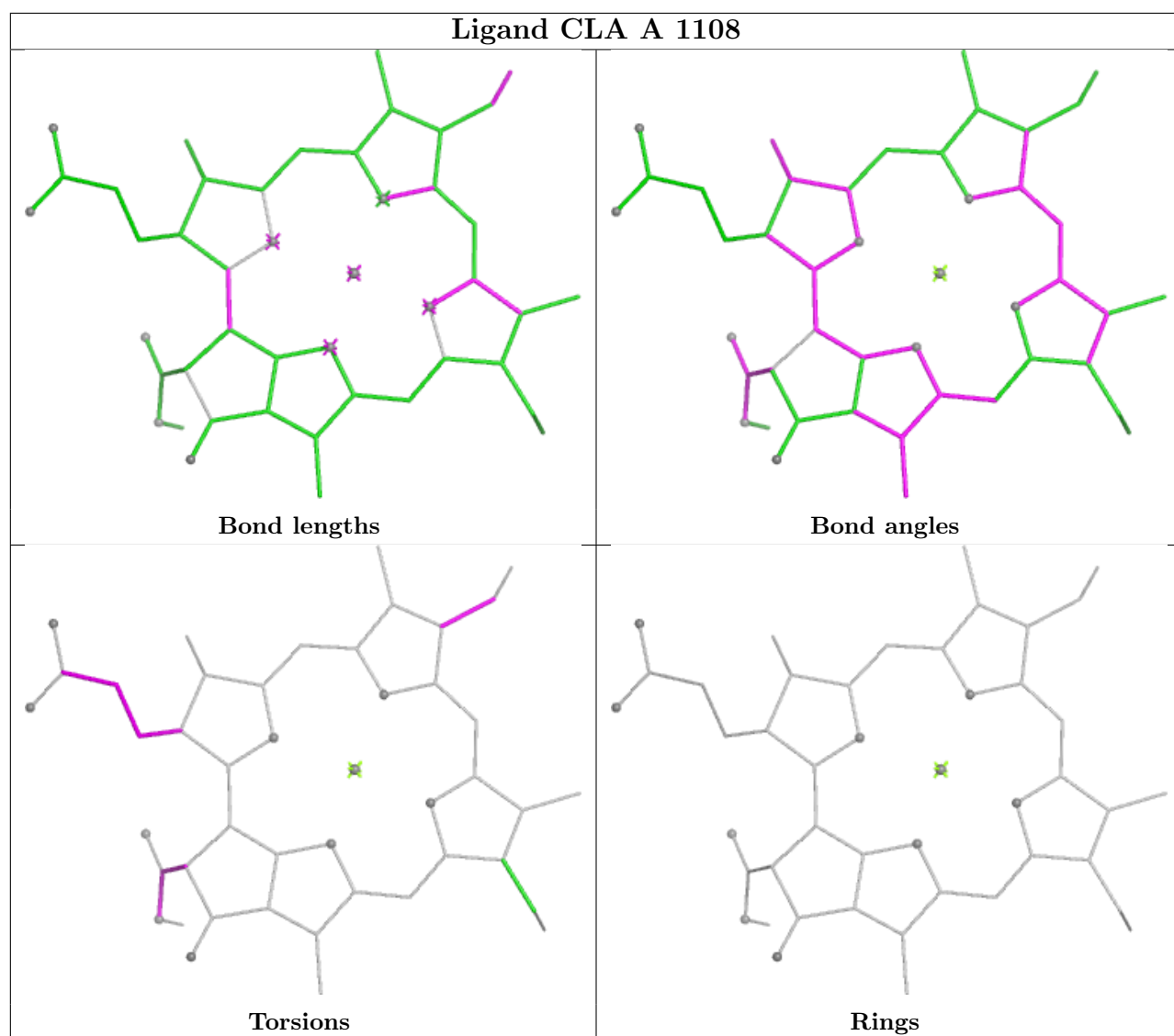


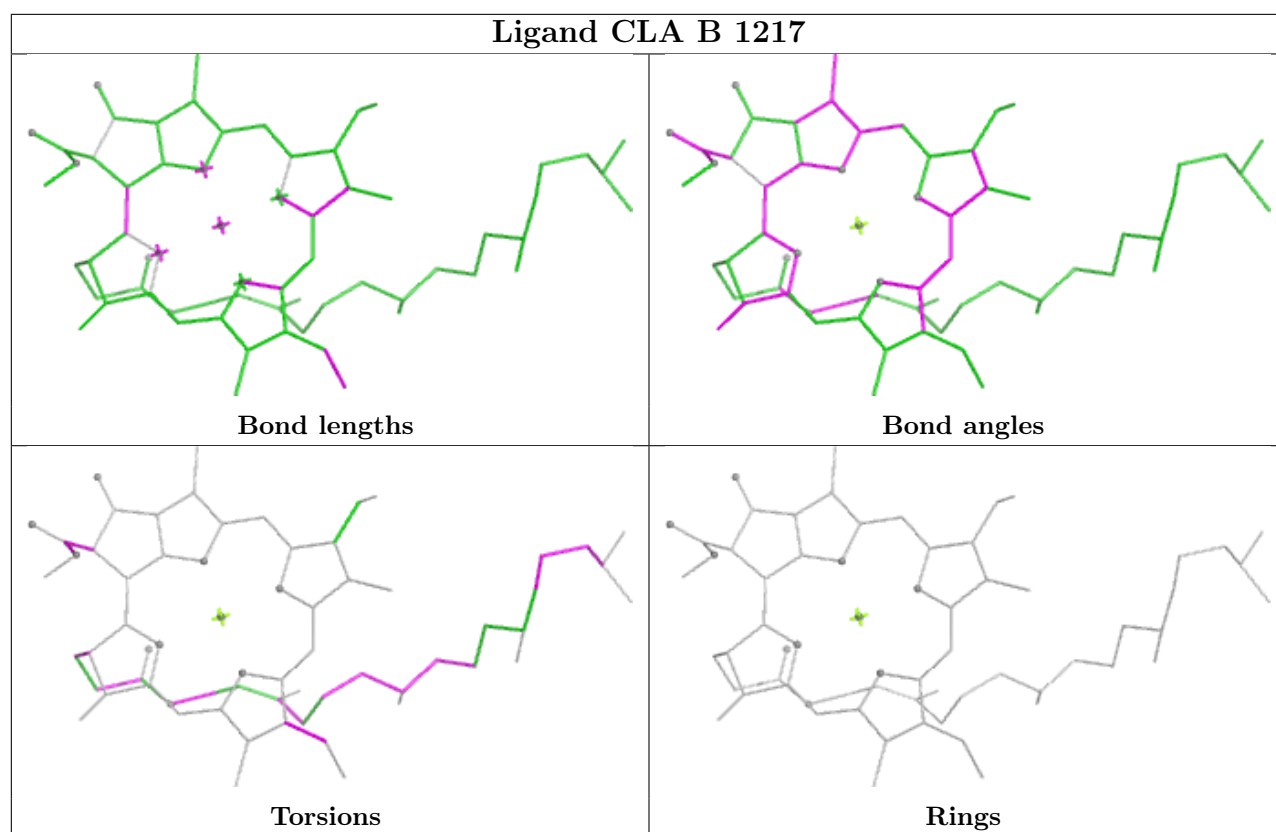
Torsions

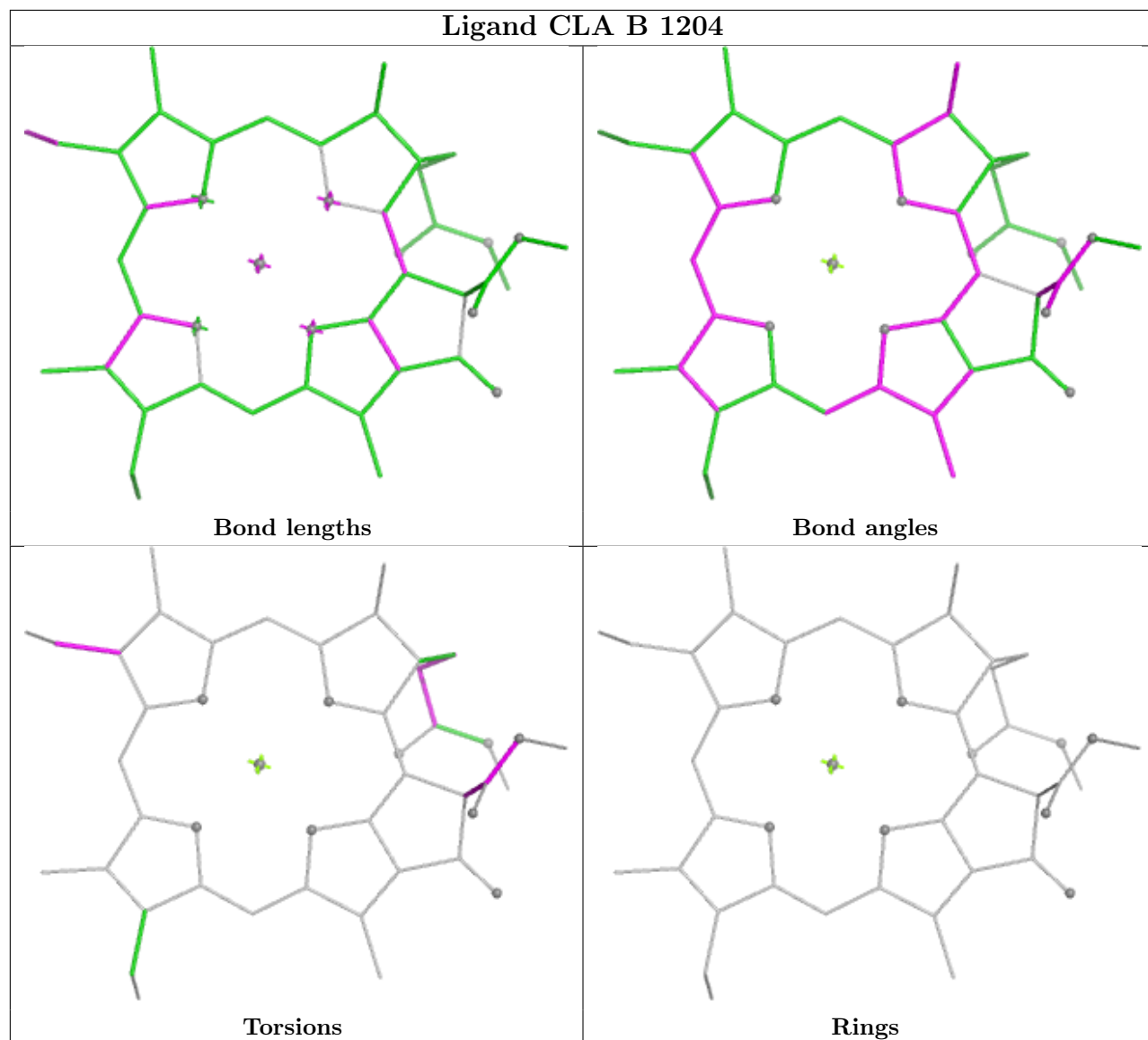


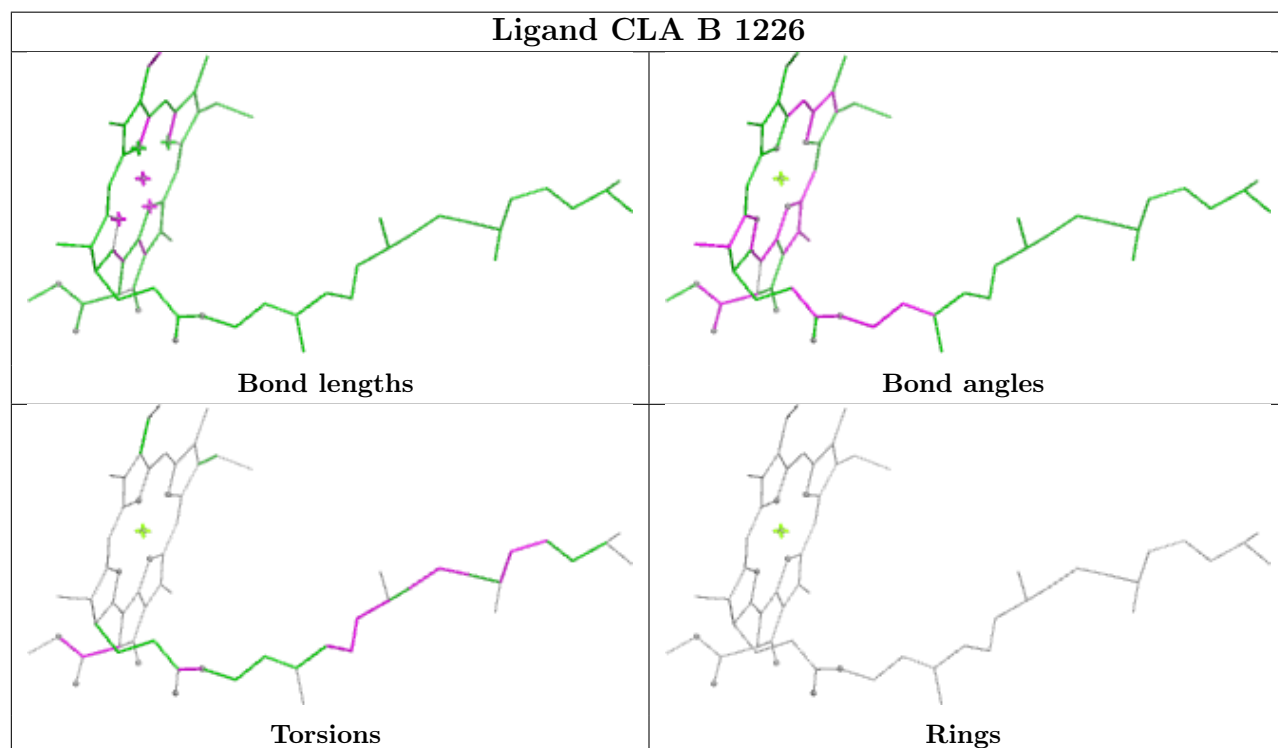
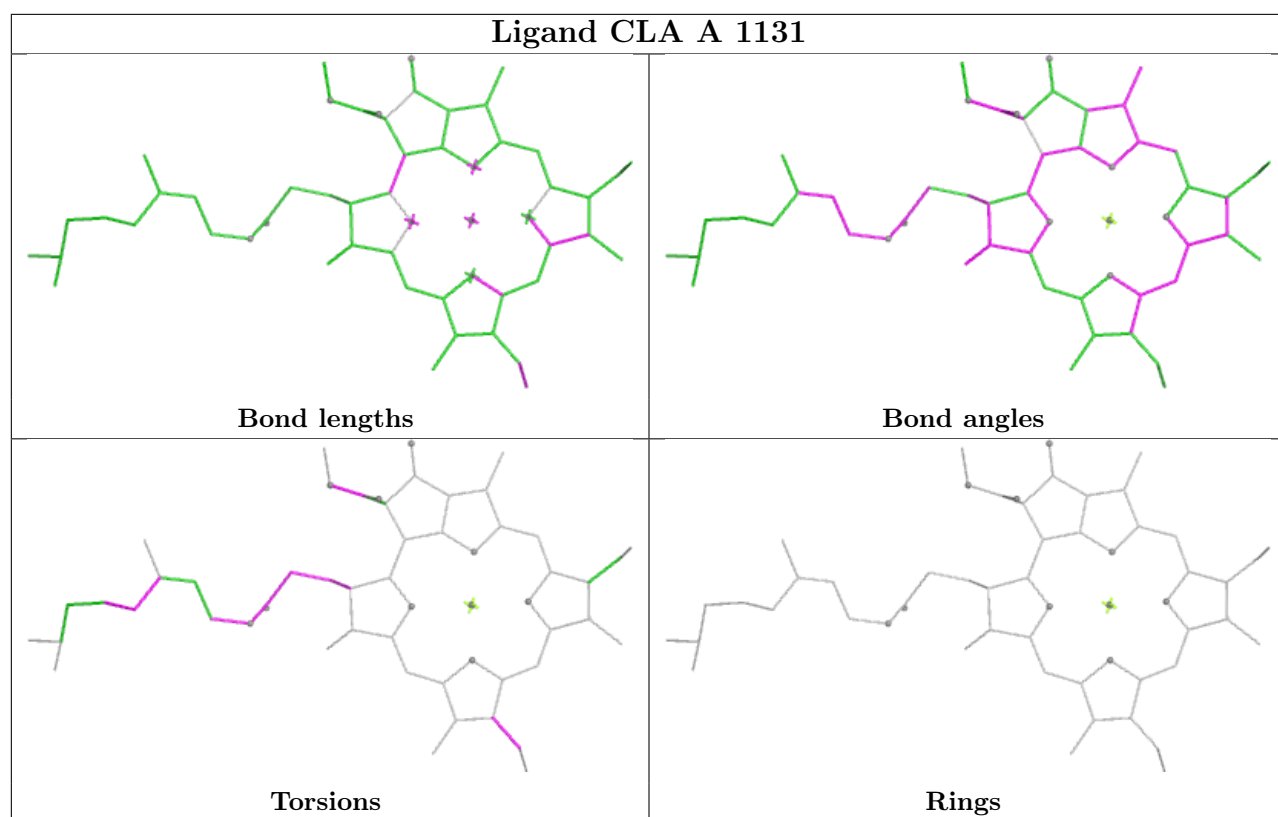
Rings

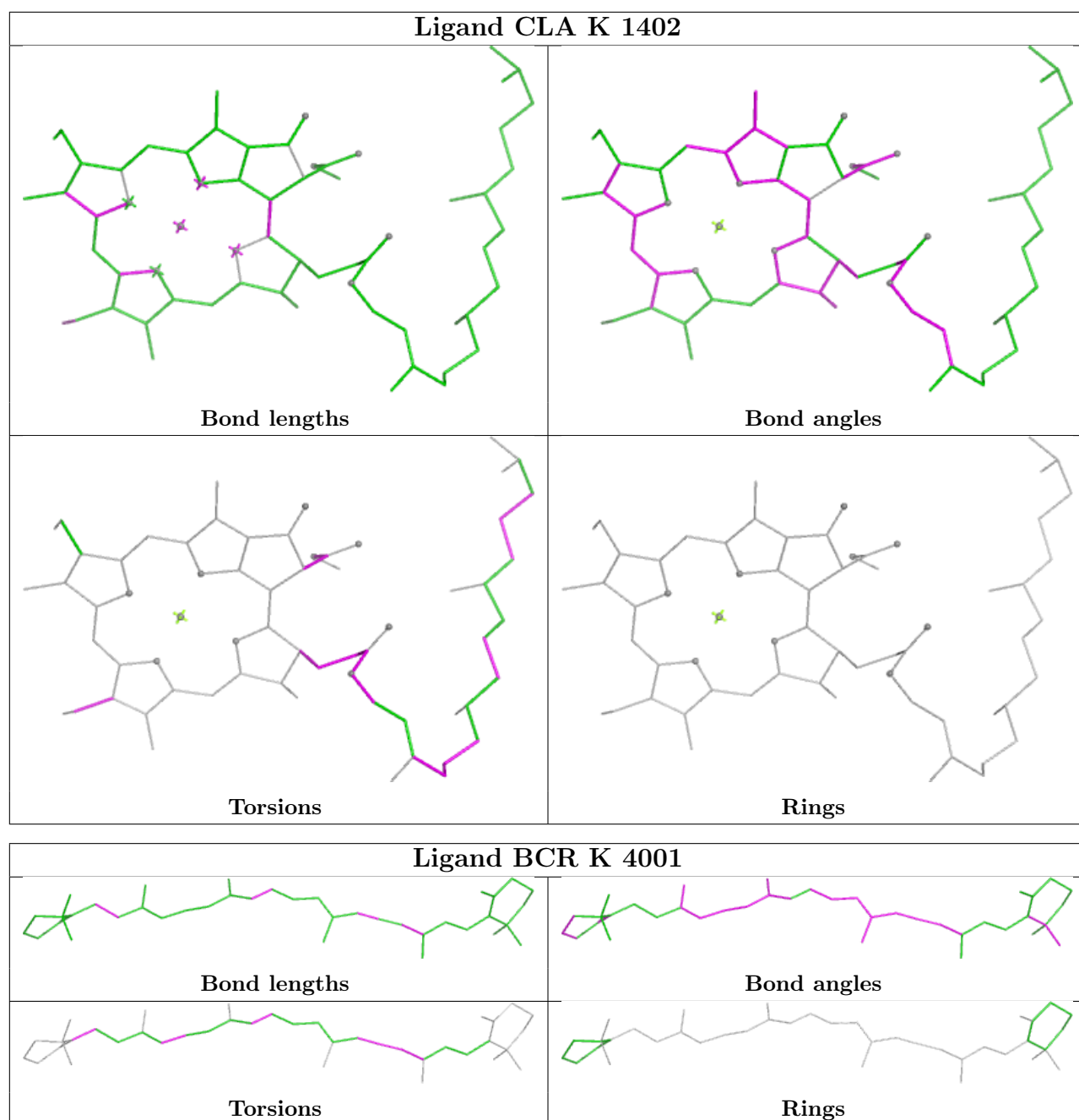


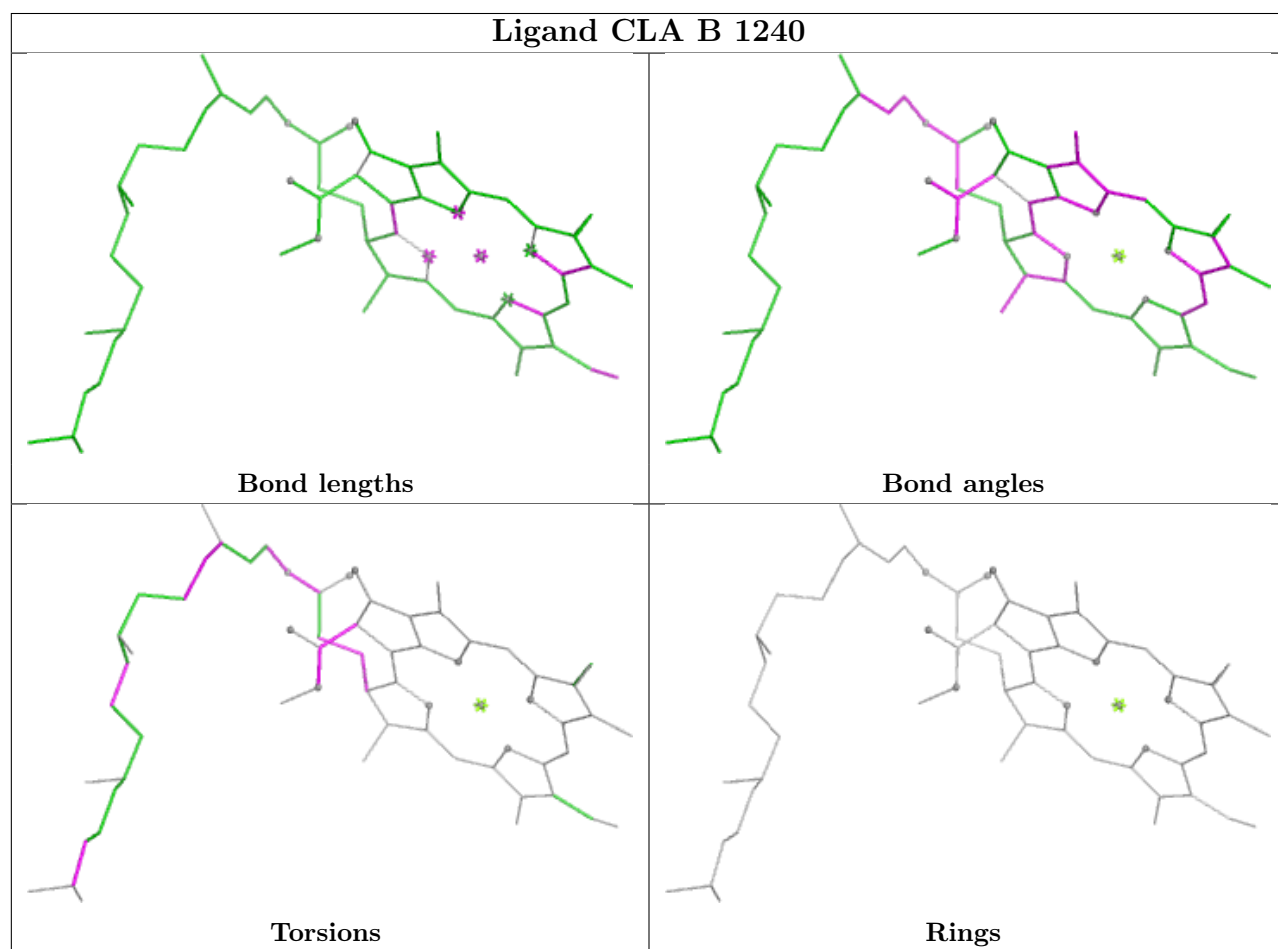
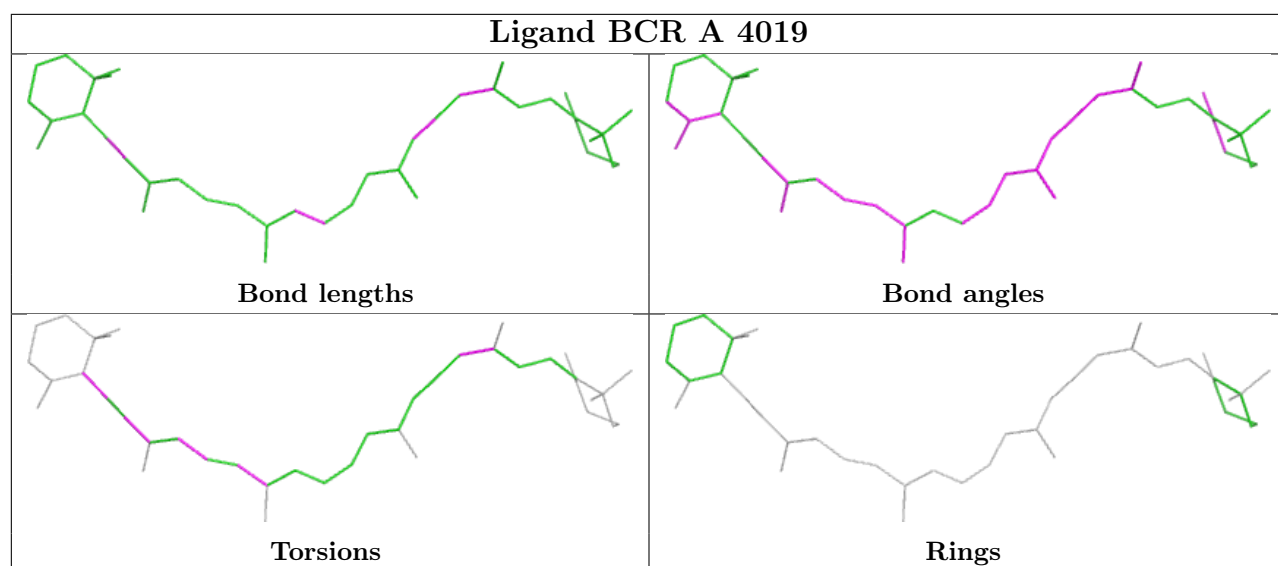


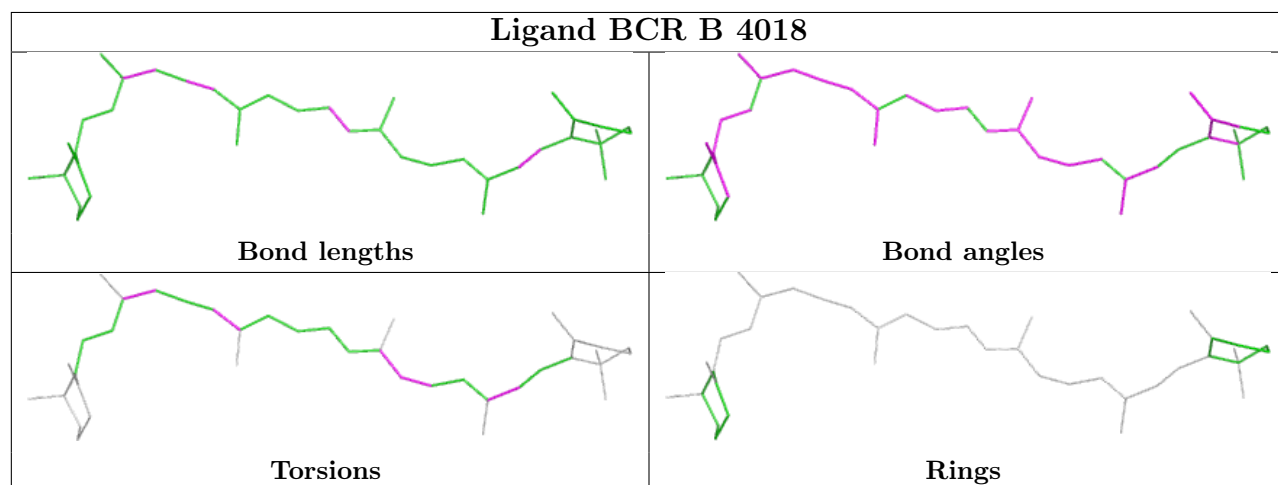
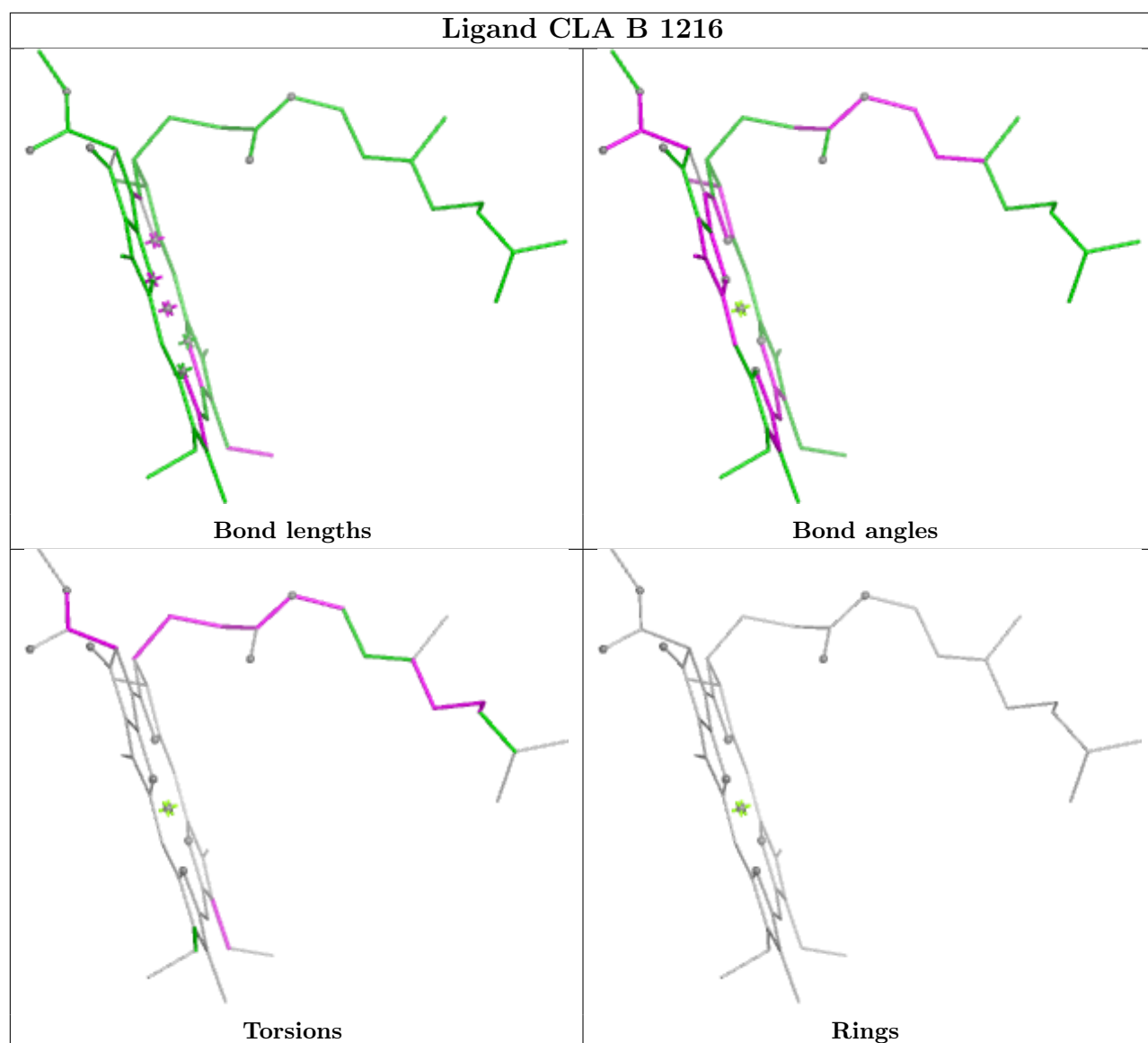


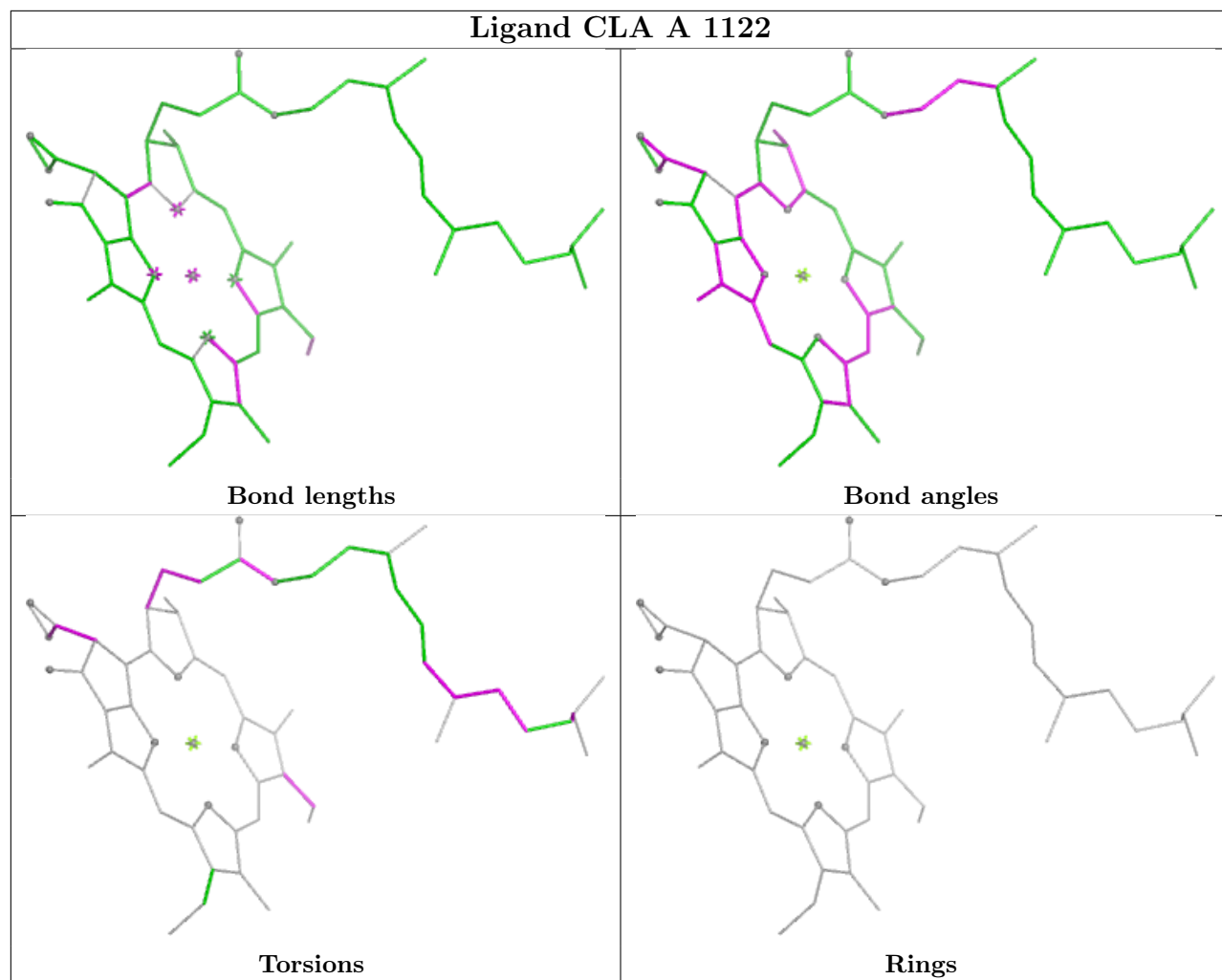


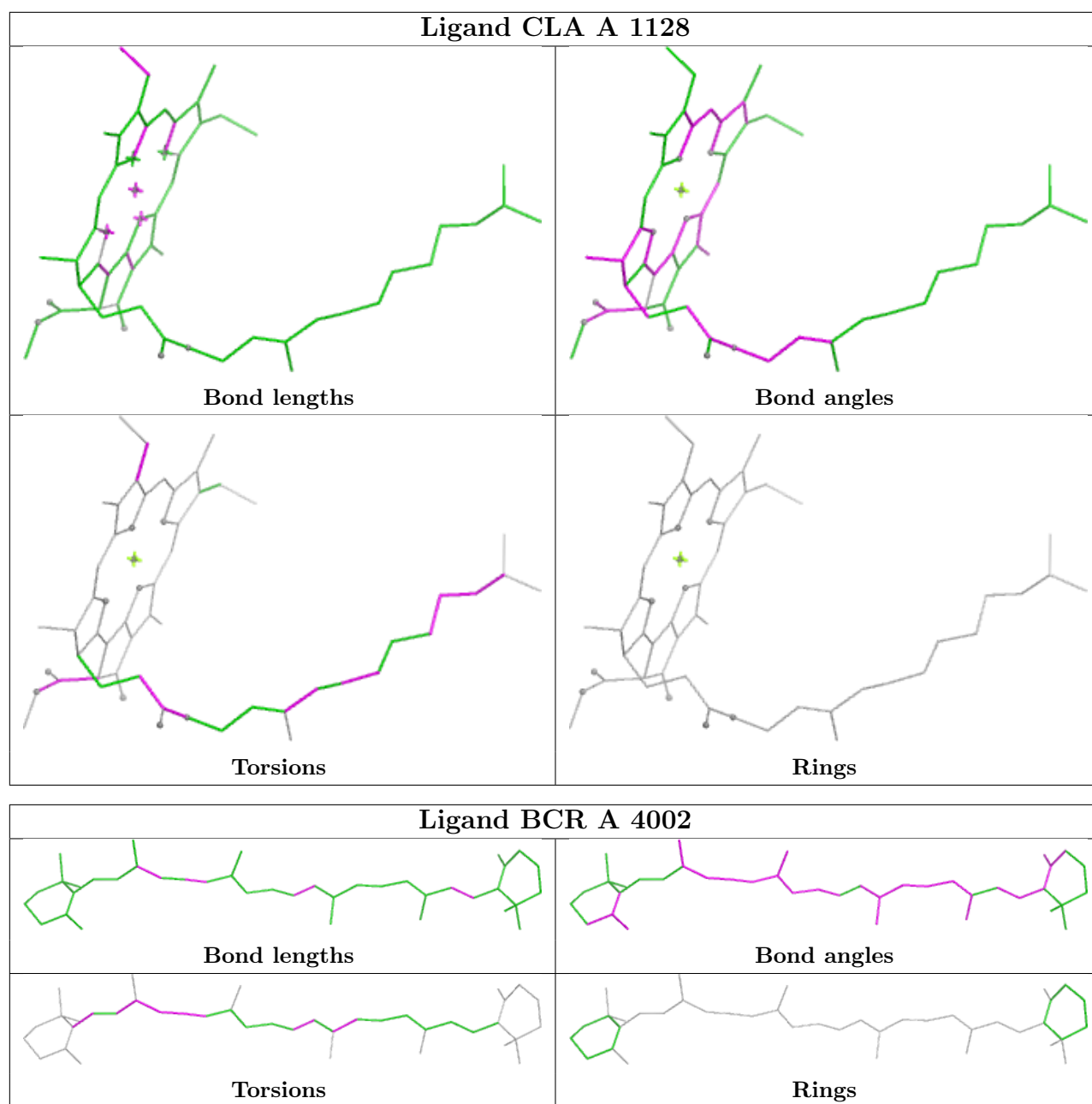


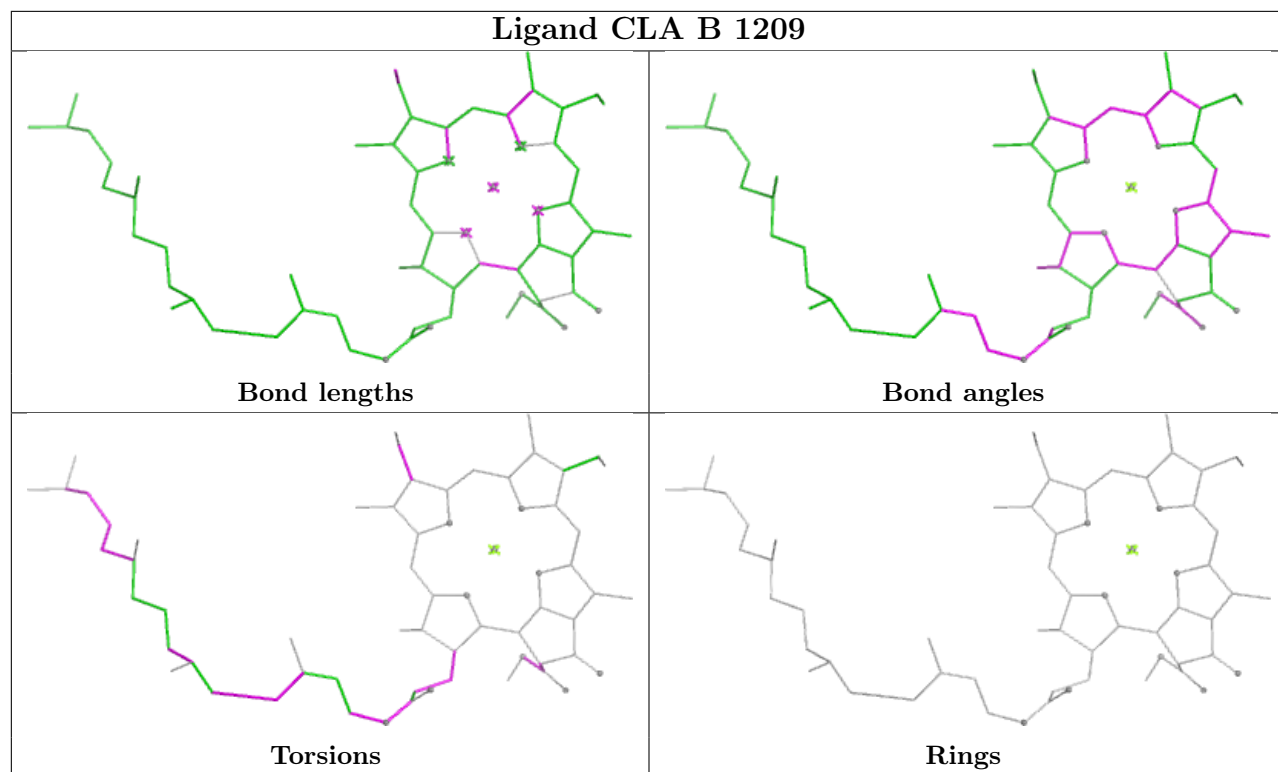


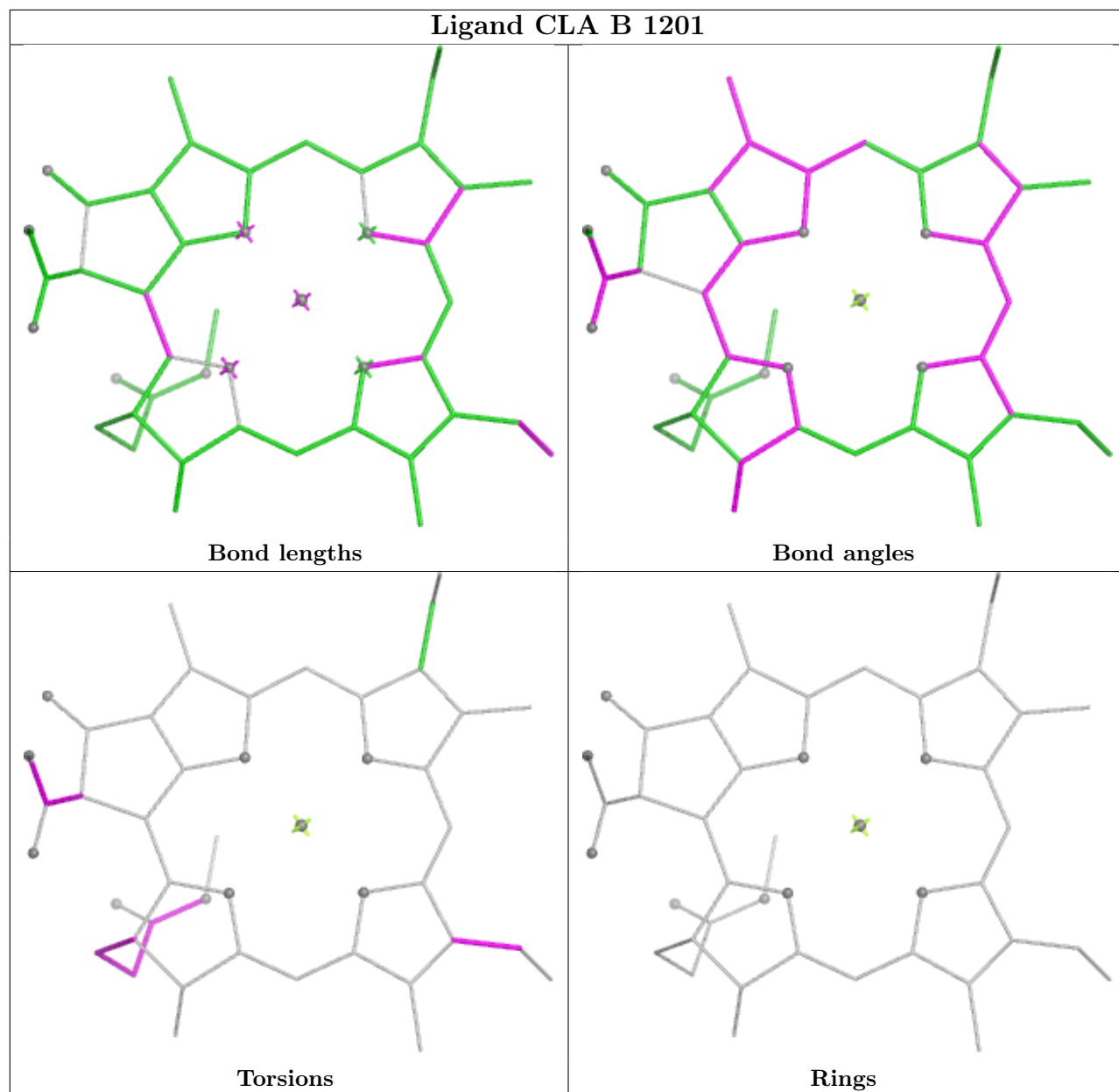


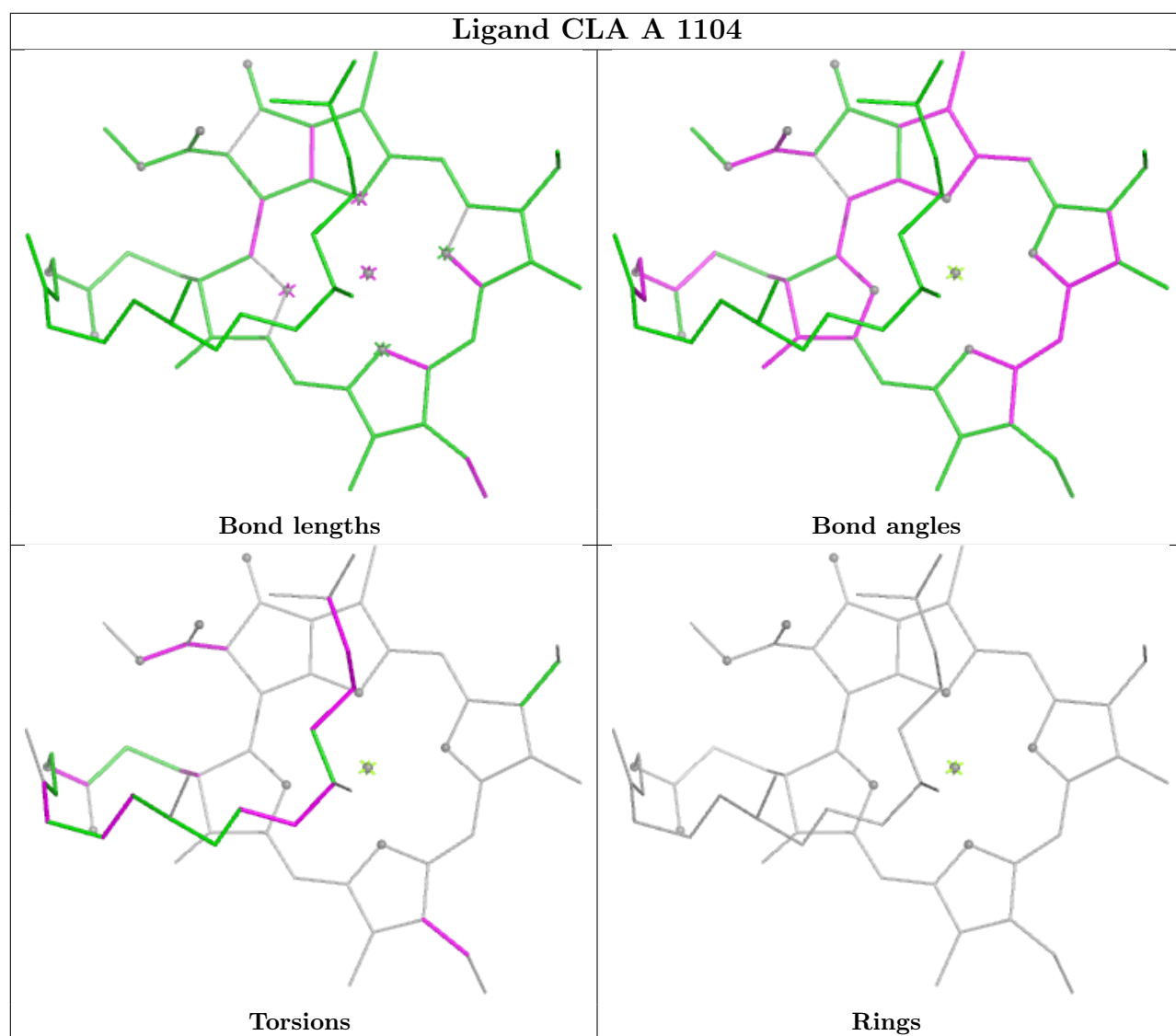


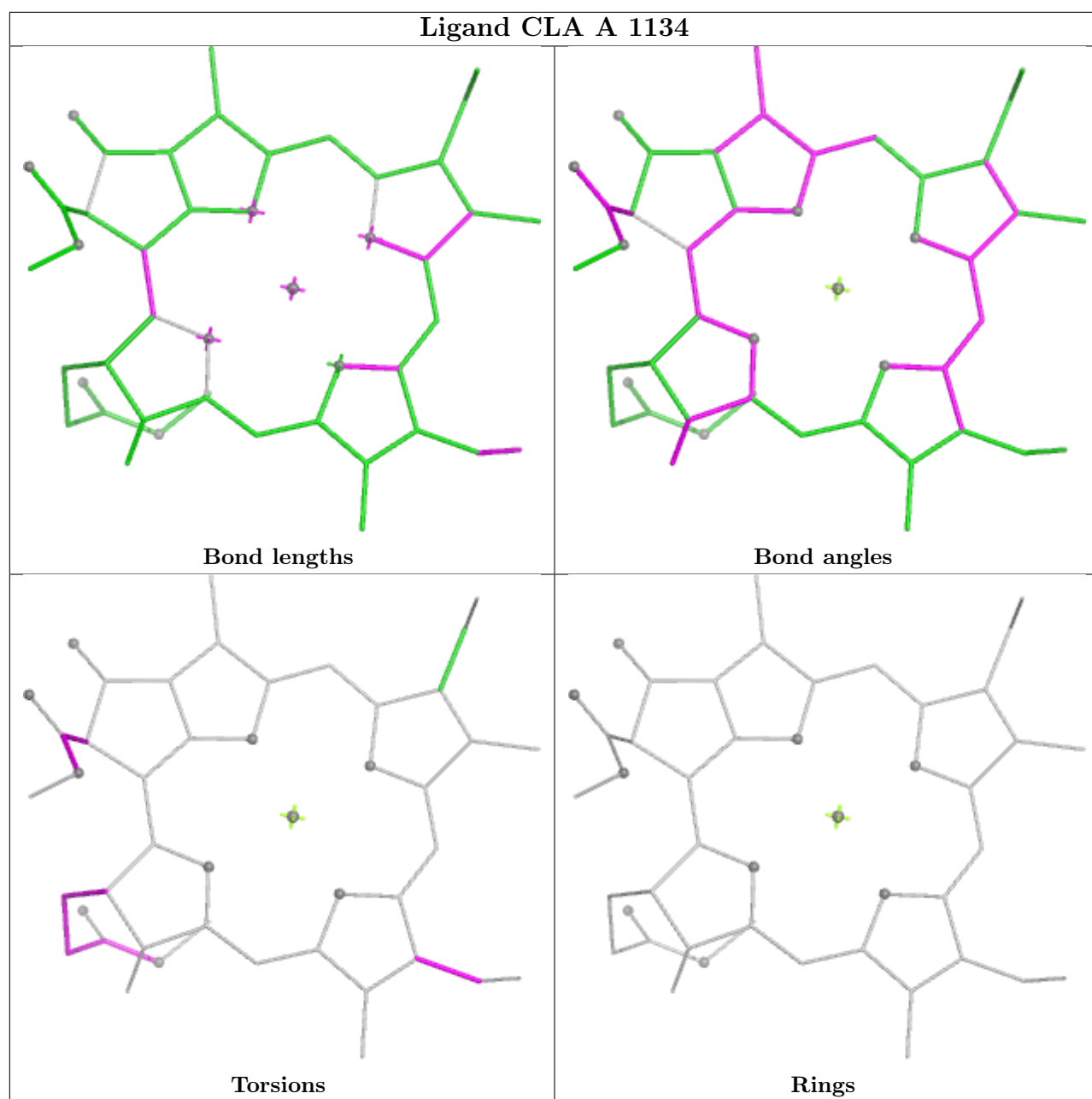


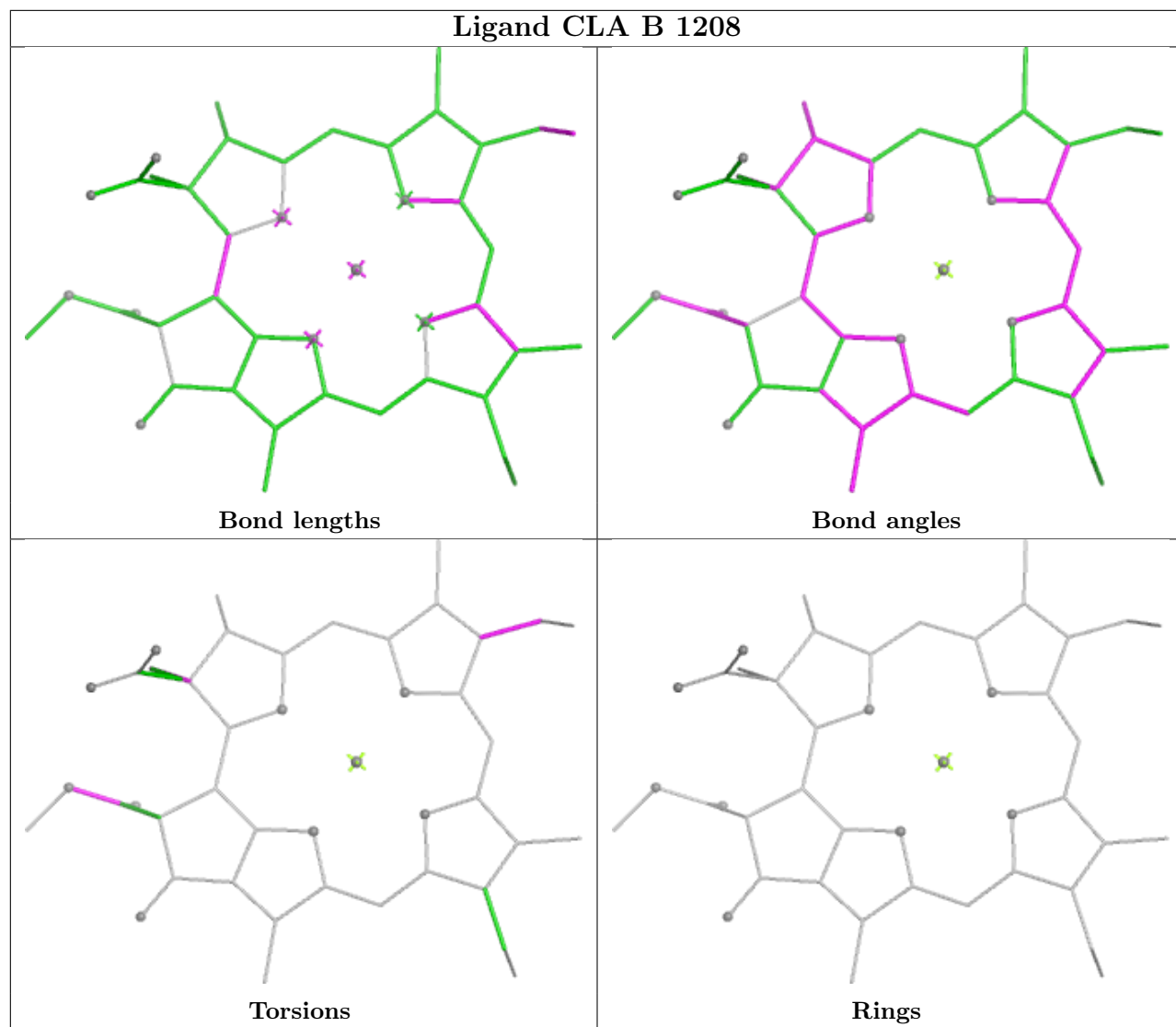




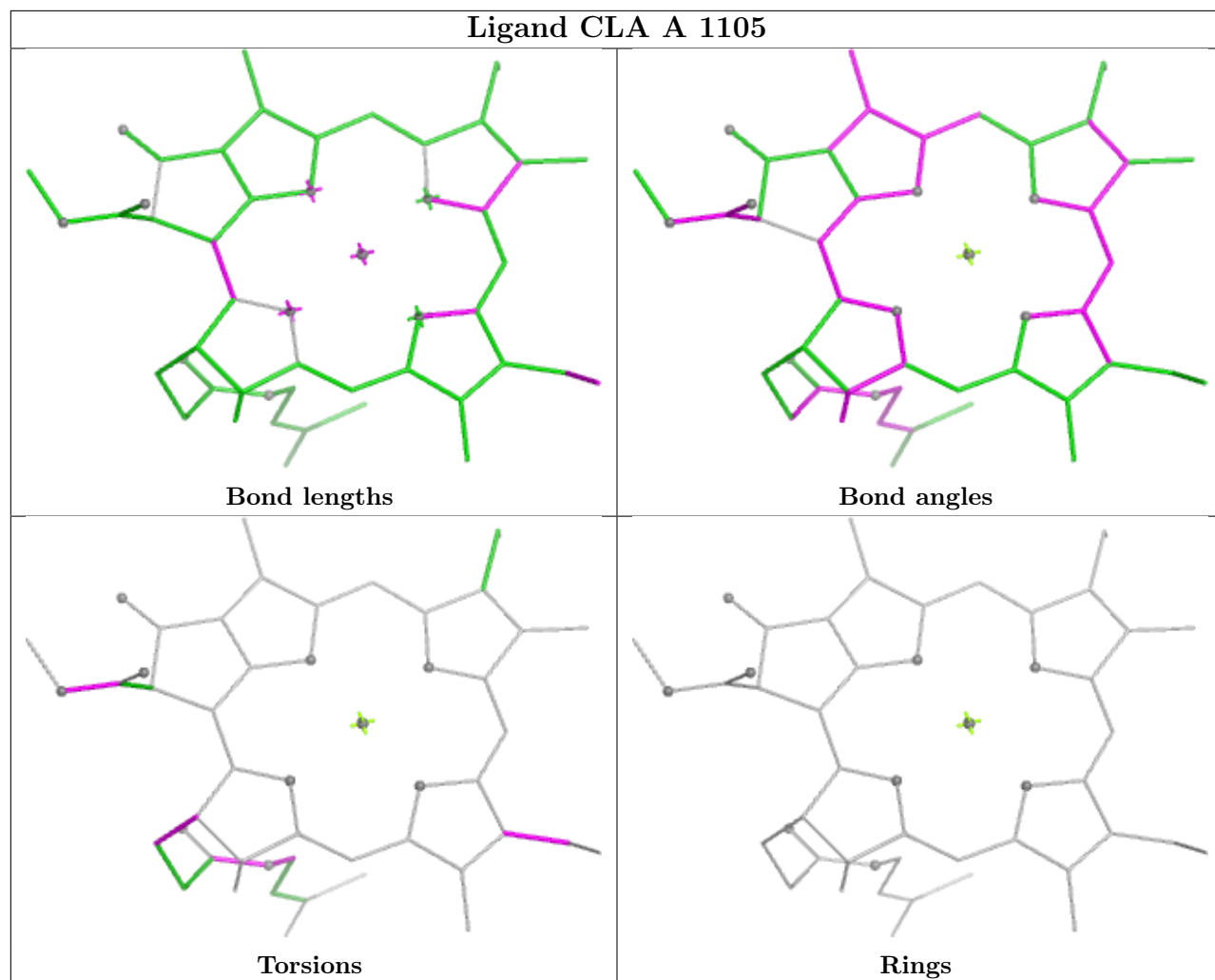


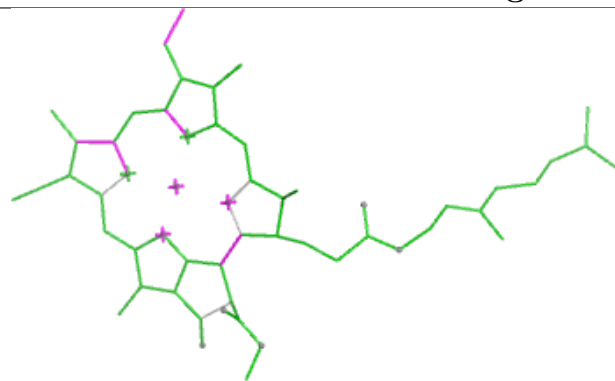
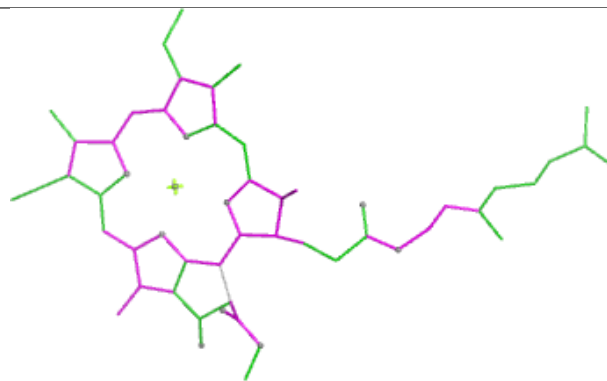
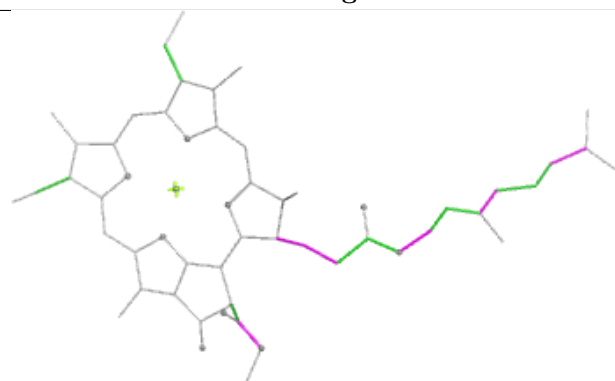
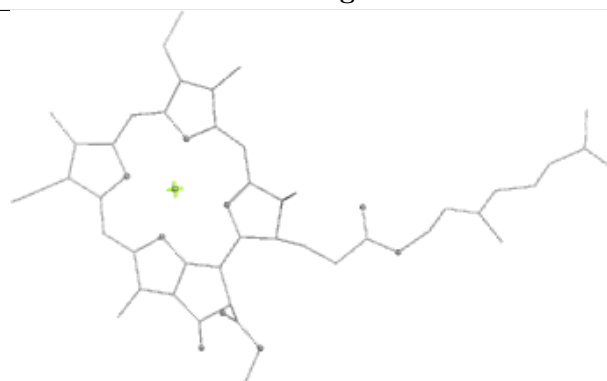
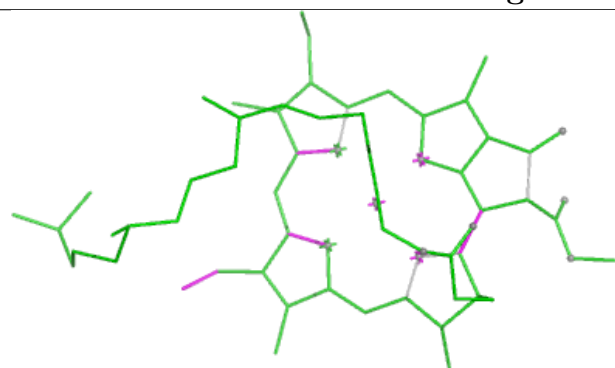
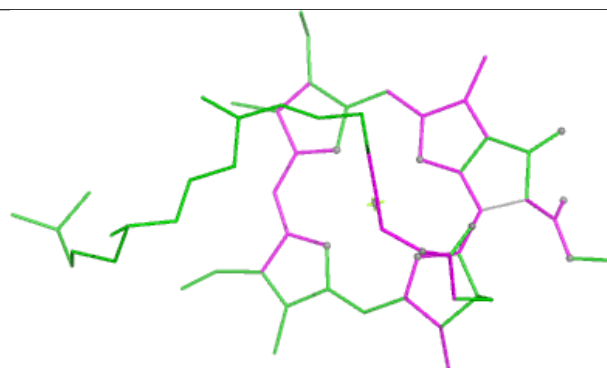
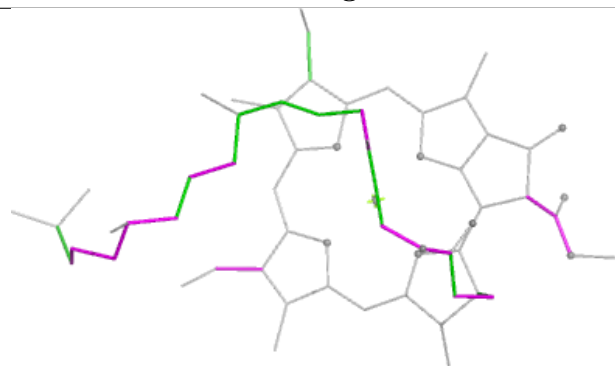
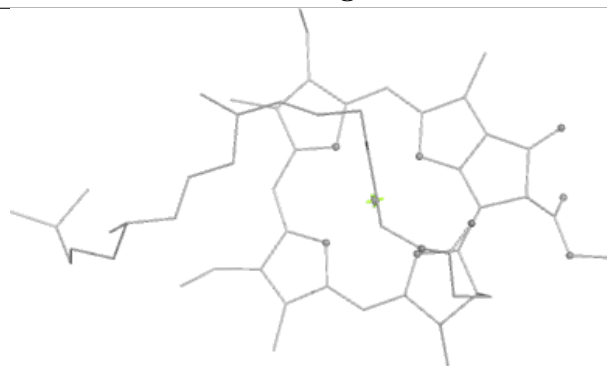


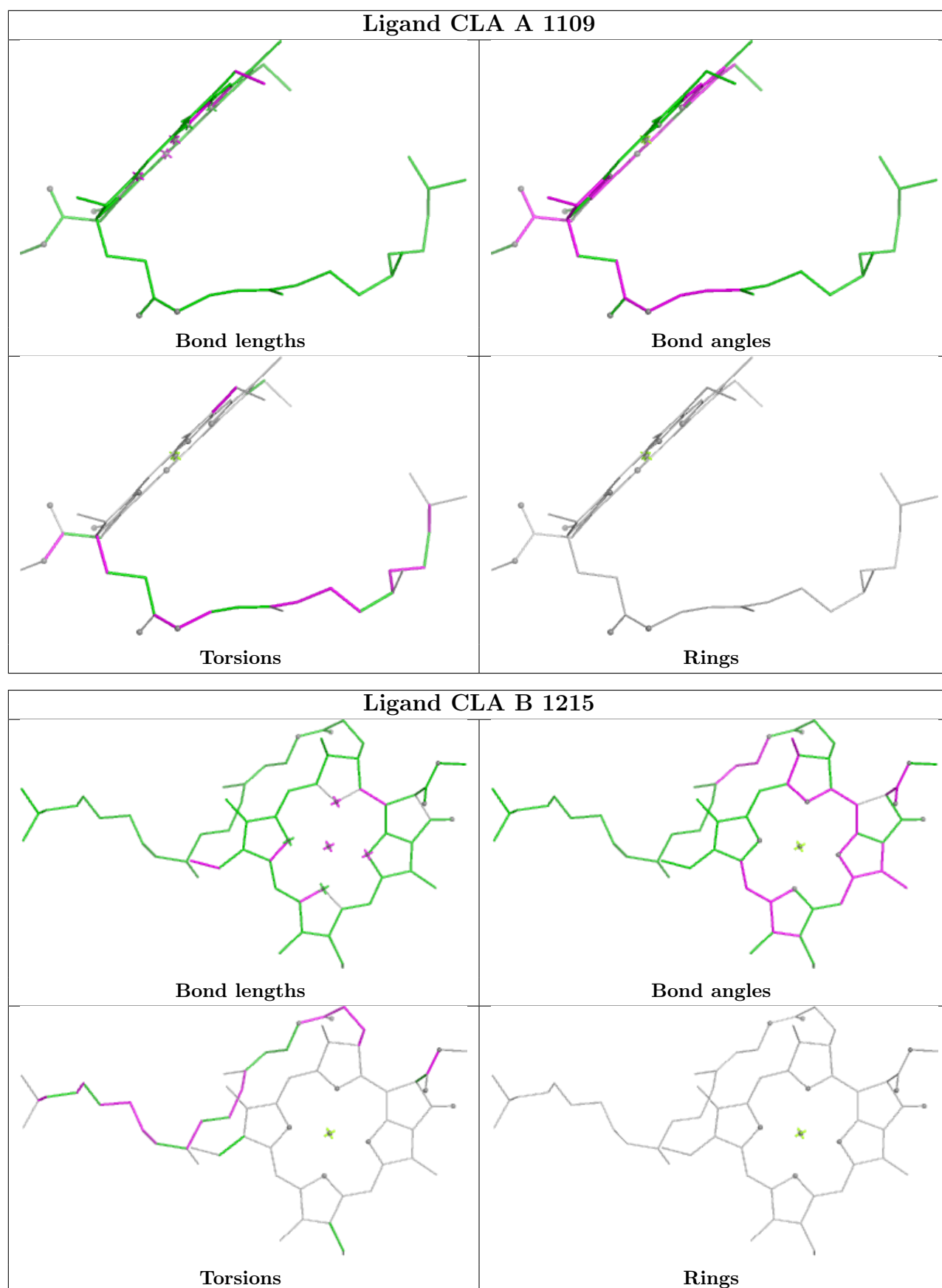


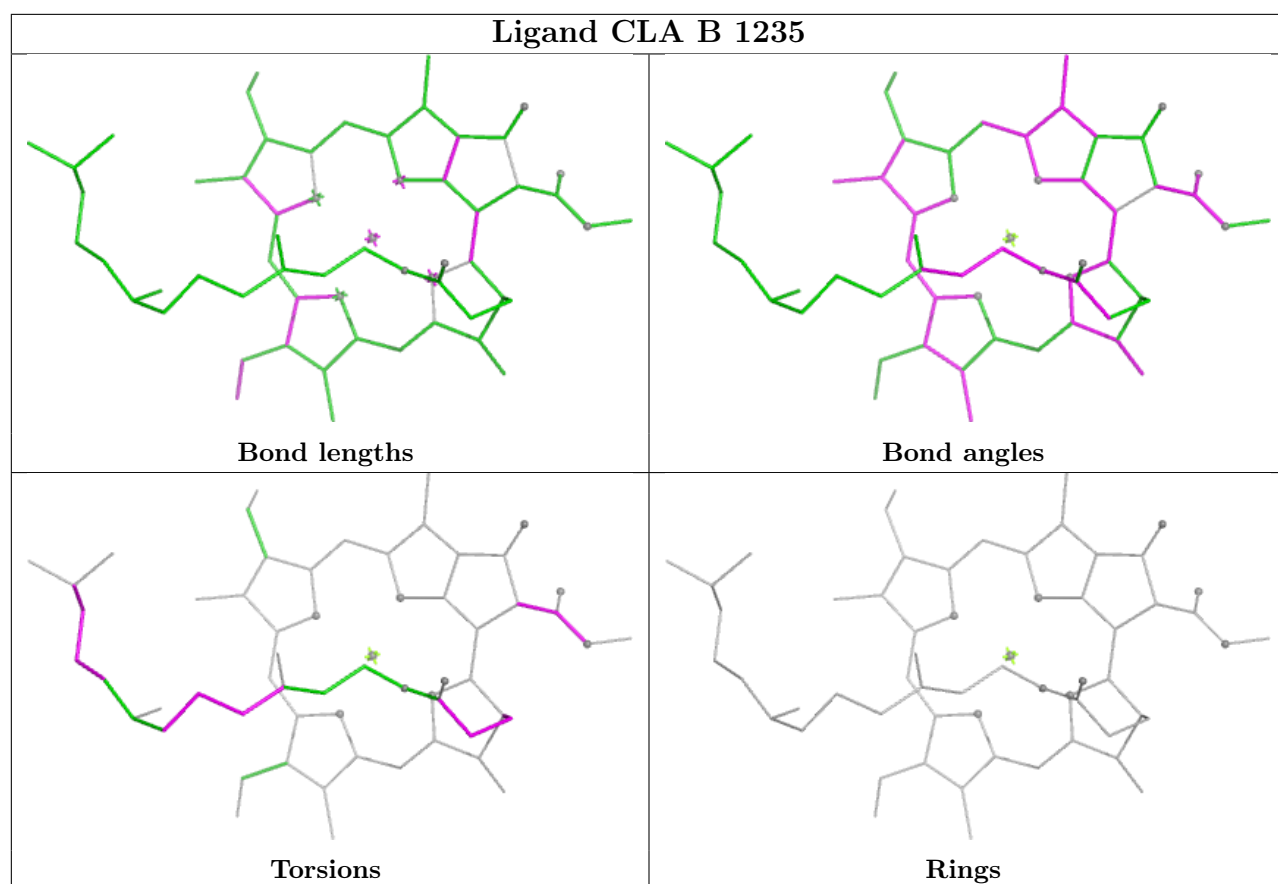


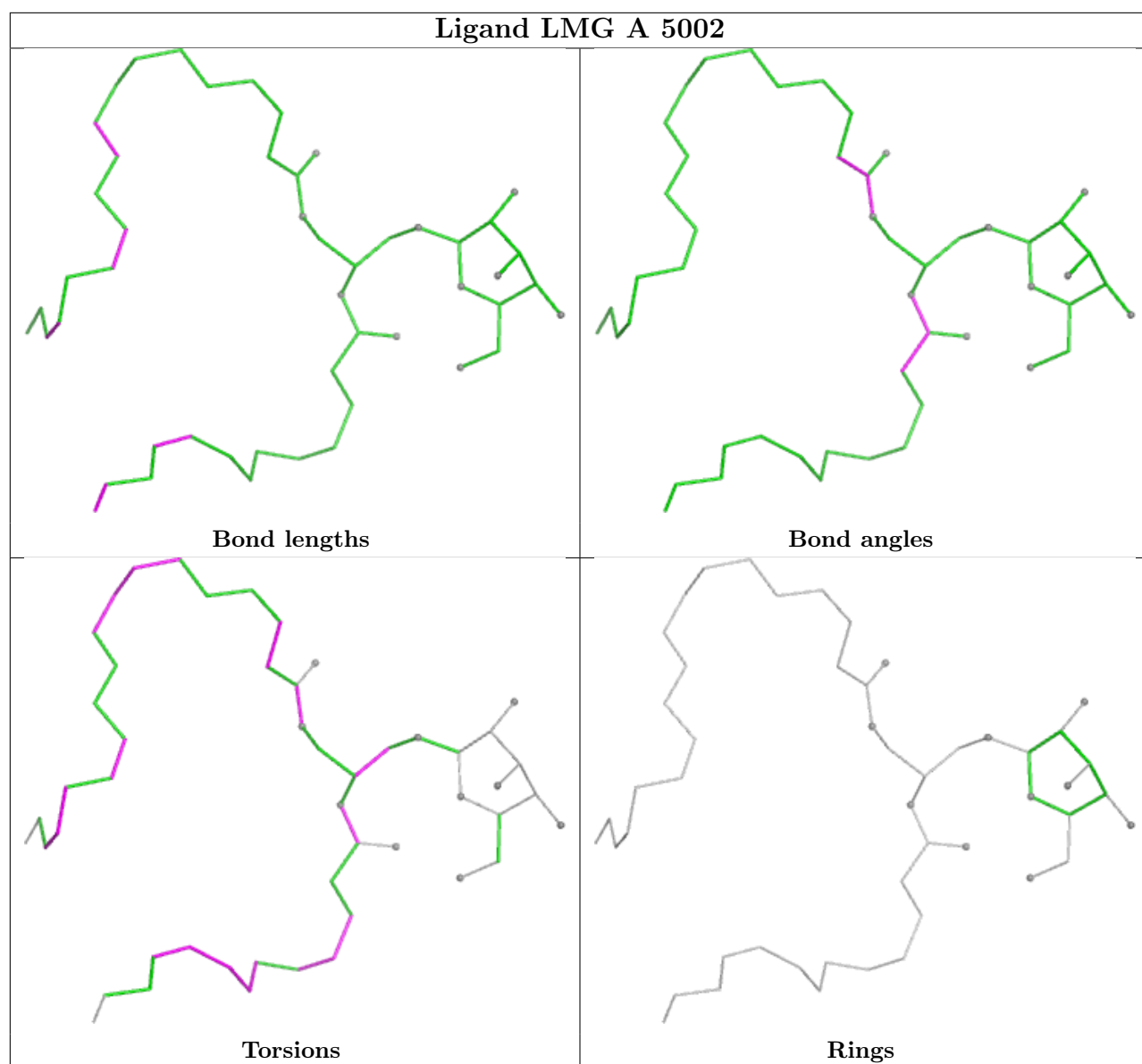
Ligand CLA A 1105

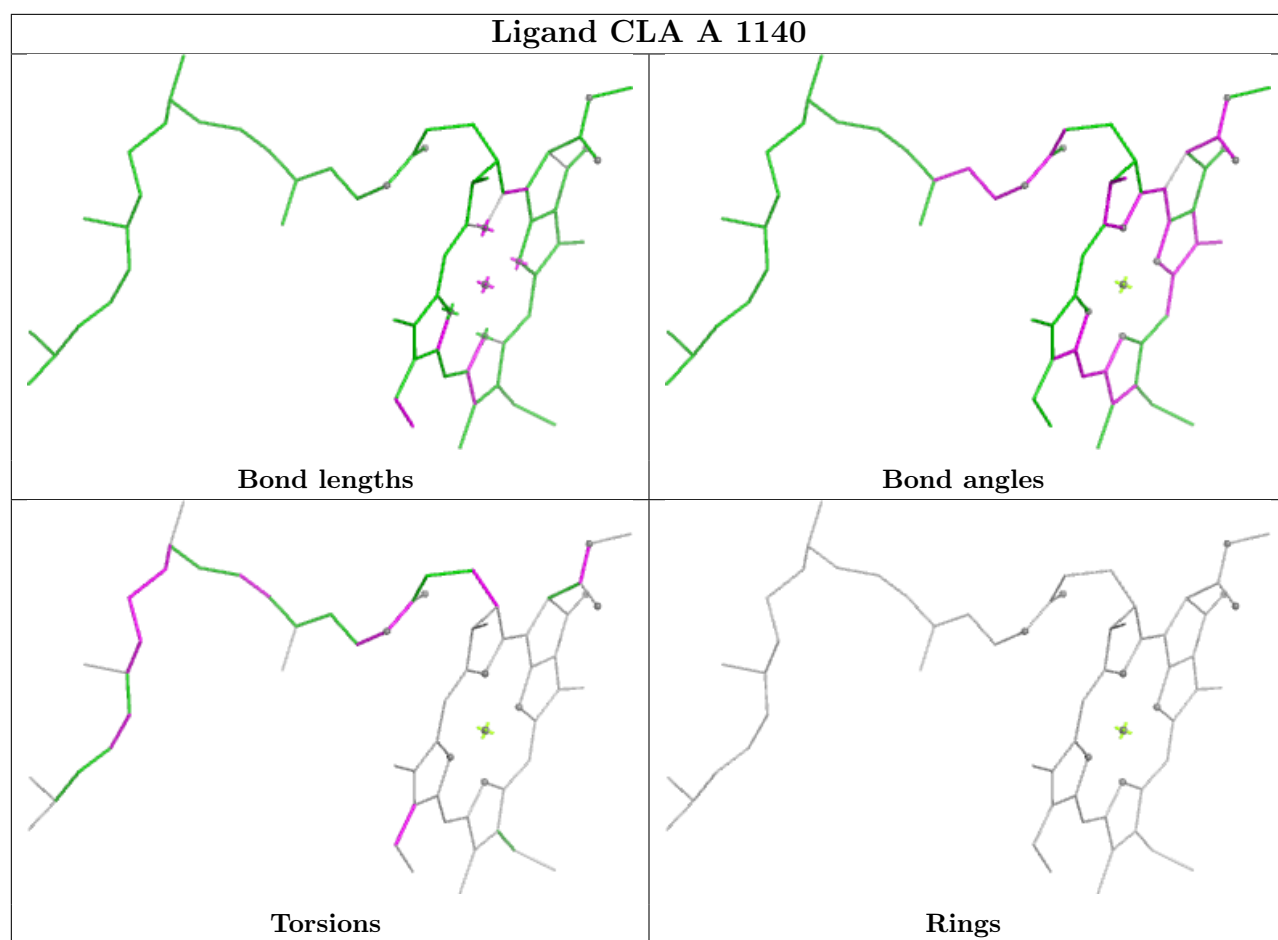


Ligand CLA A 1012**Bond lengths****Bond angles****Torsions****Rings****Ligand CLA A 1138****Bond lengths****Bond angles****Torsions****Rings**









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

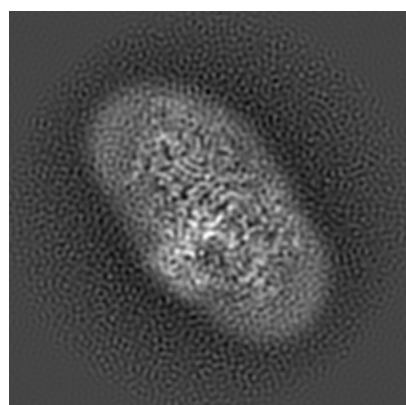
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12697. These allow visual inspection of the internal detail of the map and identification of artifacts.

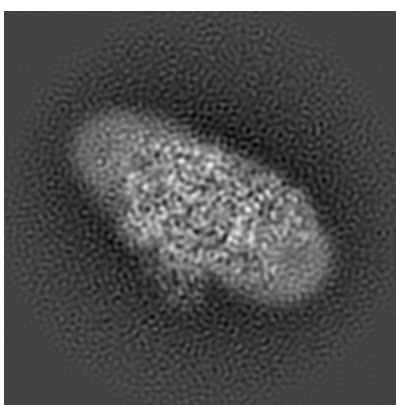
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

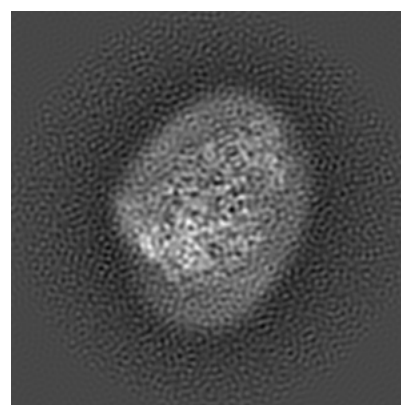
6.1.1 Primary map



X



Y

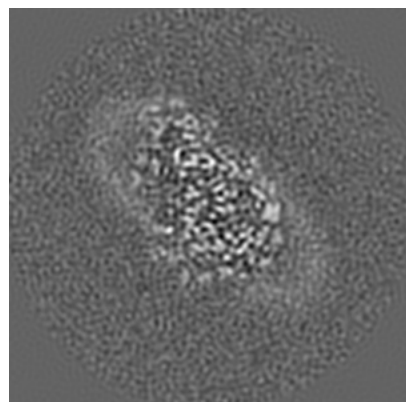


Z

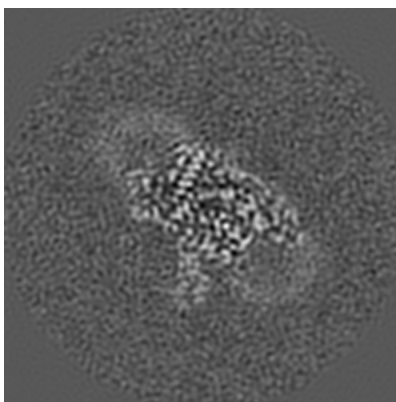
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

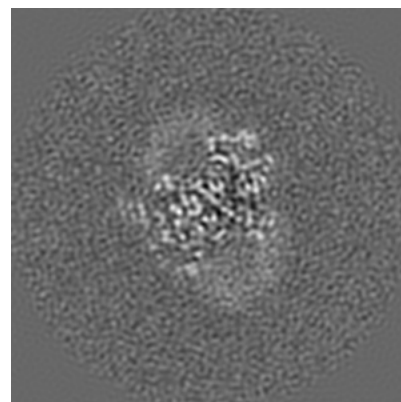
6.2.1 Primary map



X Index: 140



Y Index: 140

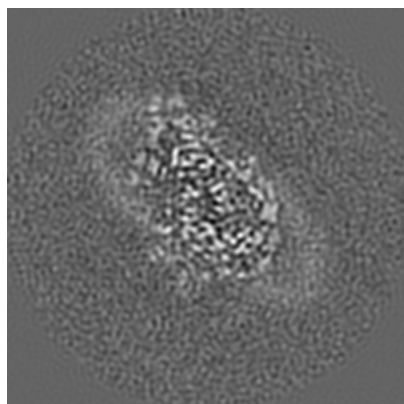


Z Index: 140

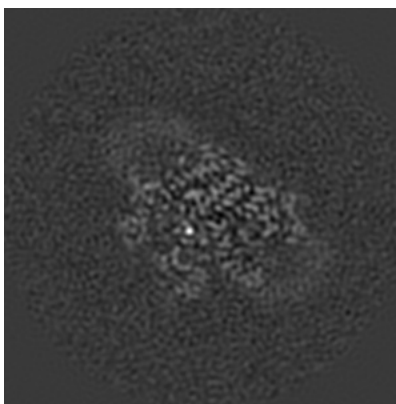
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

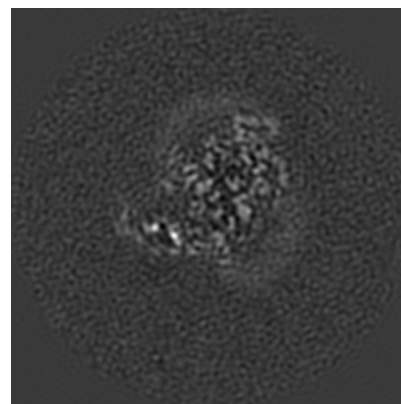
6.3.1 Primary map



X Index: 139



Y Index: 130

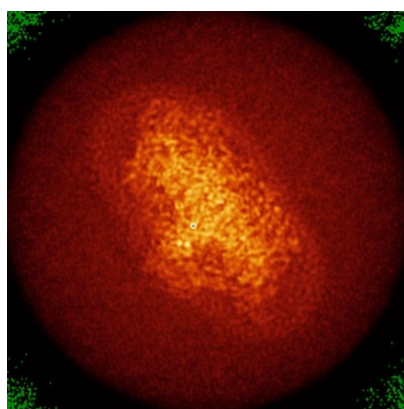


Z Index: 117

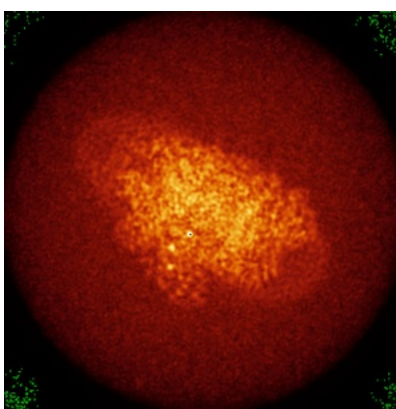
The images above show the largest variance slices of the map in three orthogonal directions.

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

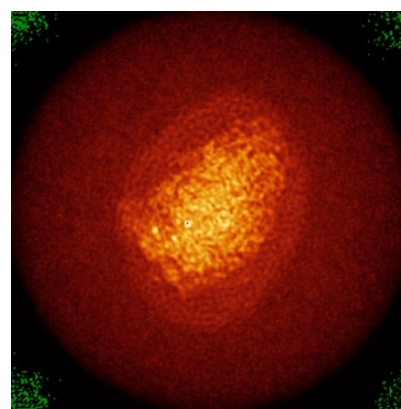
6.4.1 Primary map



X



Y

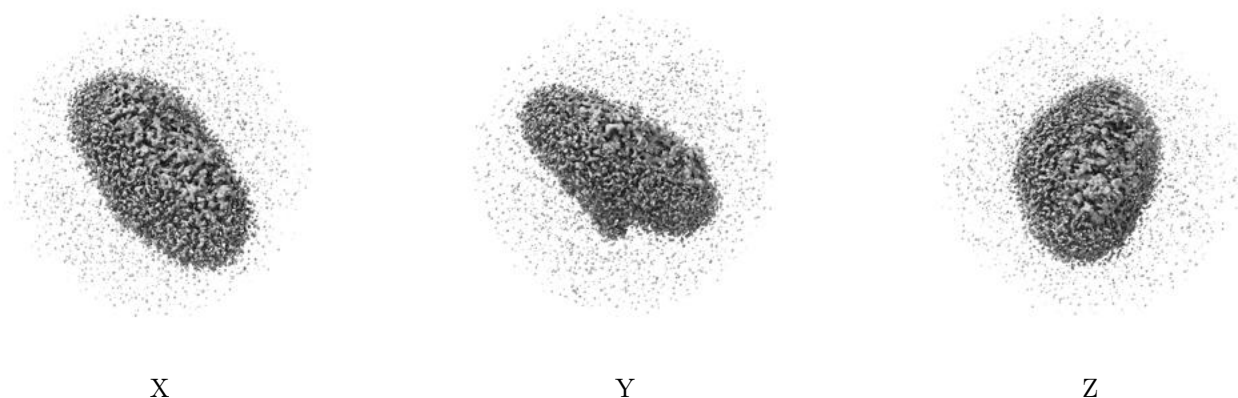


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.008. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

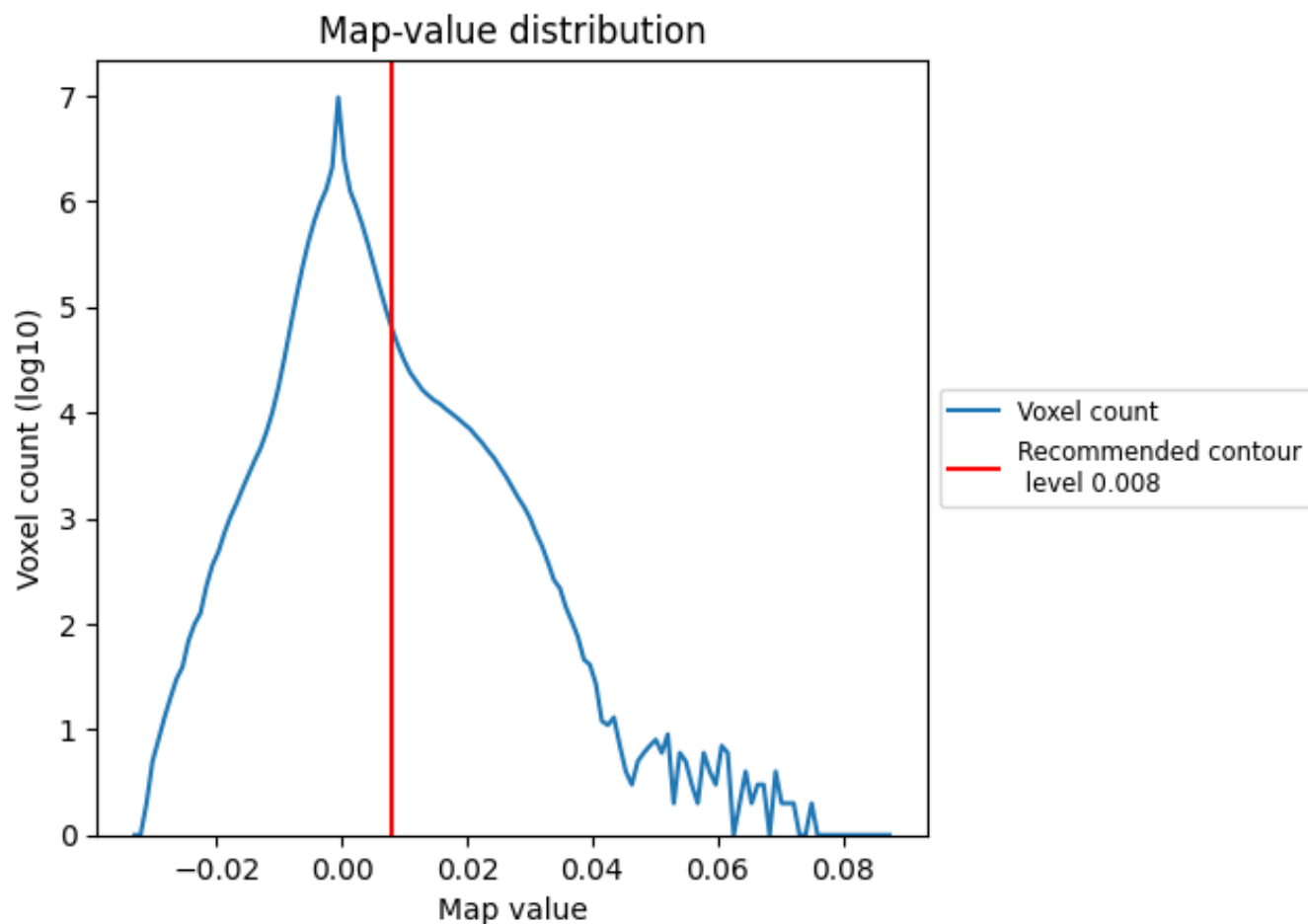
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

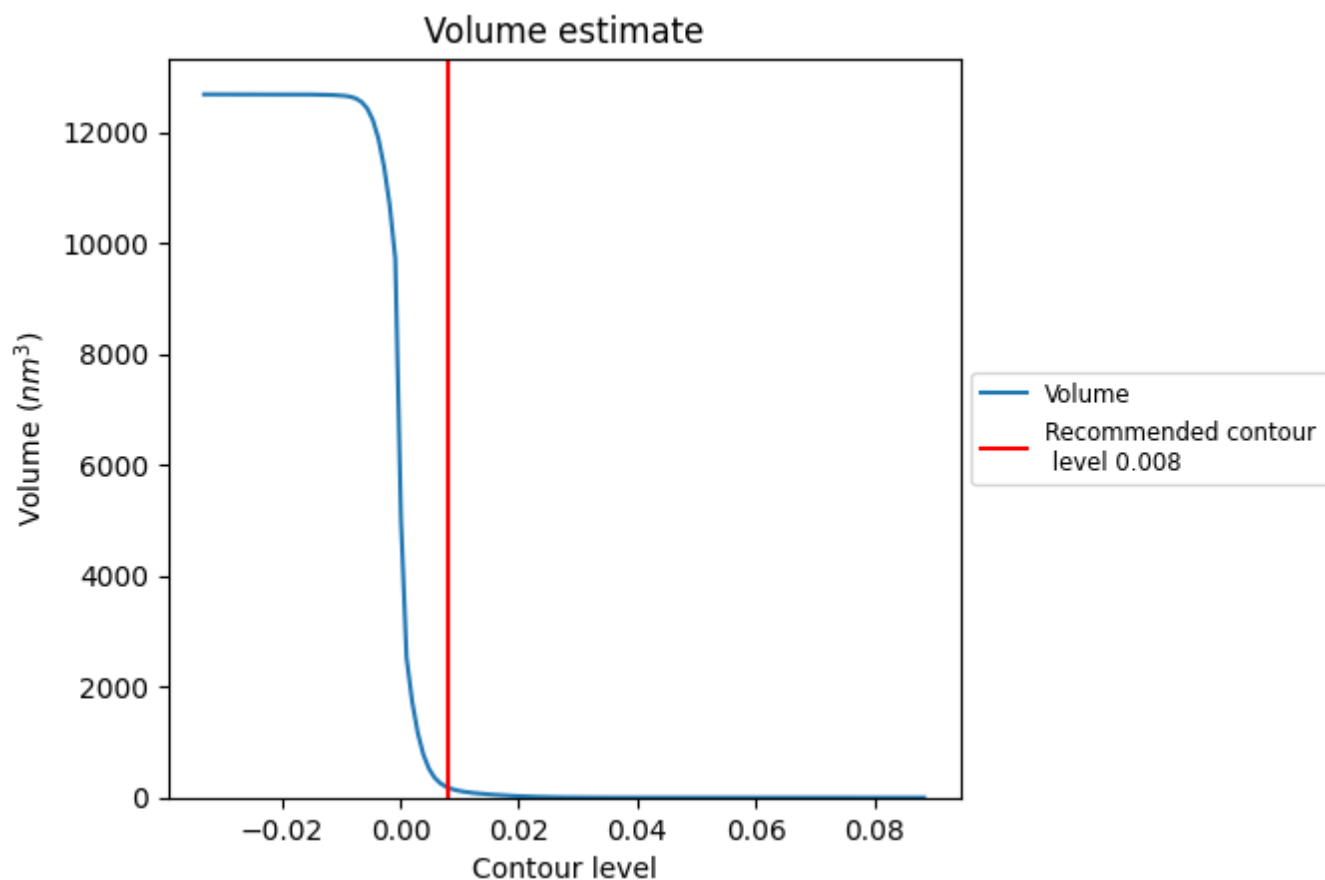
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

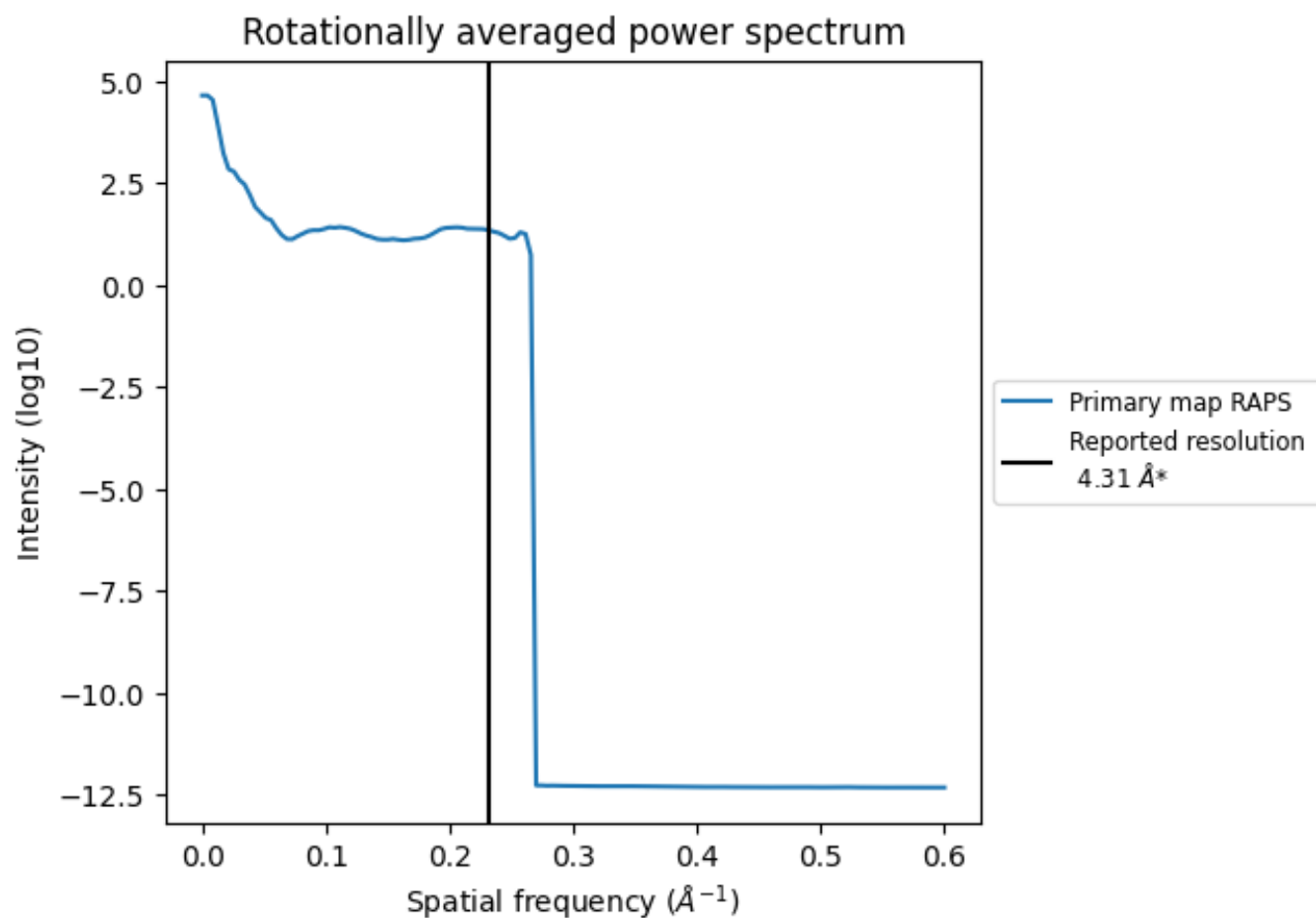
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 185 nm^3 ; this corresponds to an approximate mass of 167 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

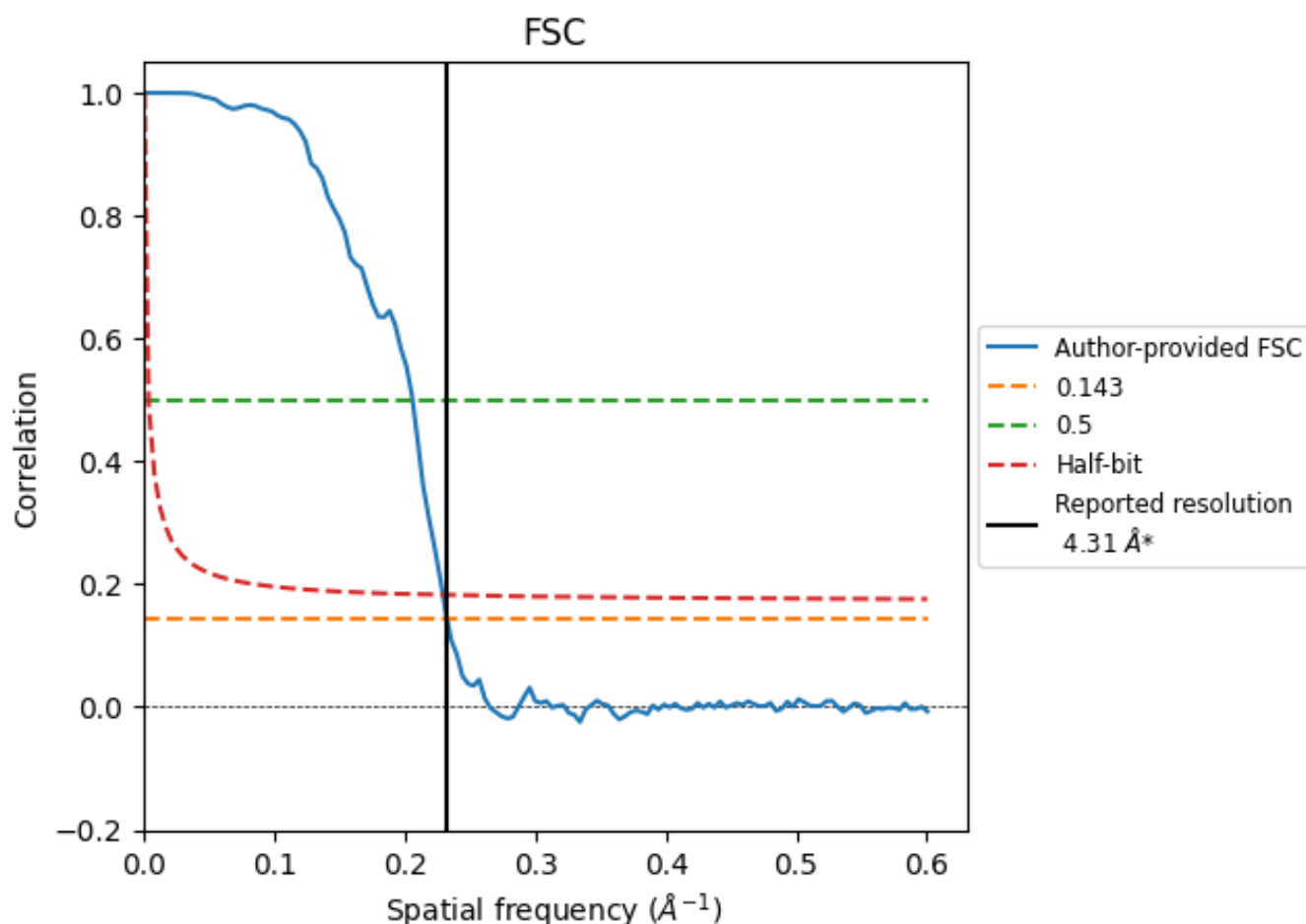


*Reported resolution corresponds to spatial frequency of 0.232 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.232 Å⁻¹

8.2 Resolution estimates [i](#)

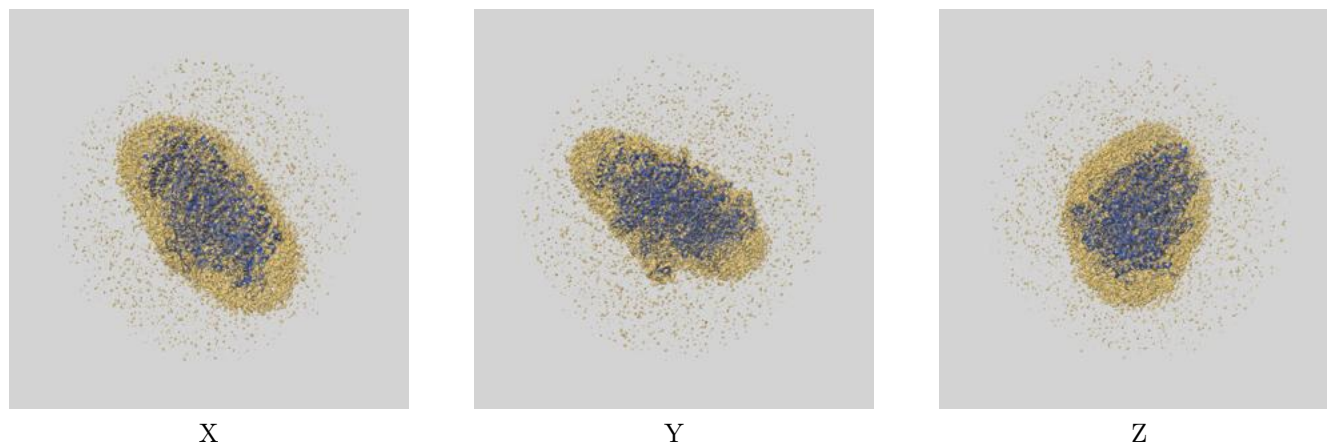
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.31	-	-
Author-provided FSC curve	4.30	4.85	4.36
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

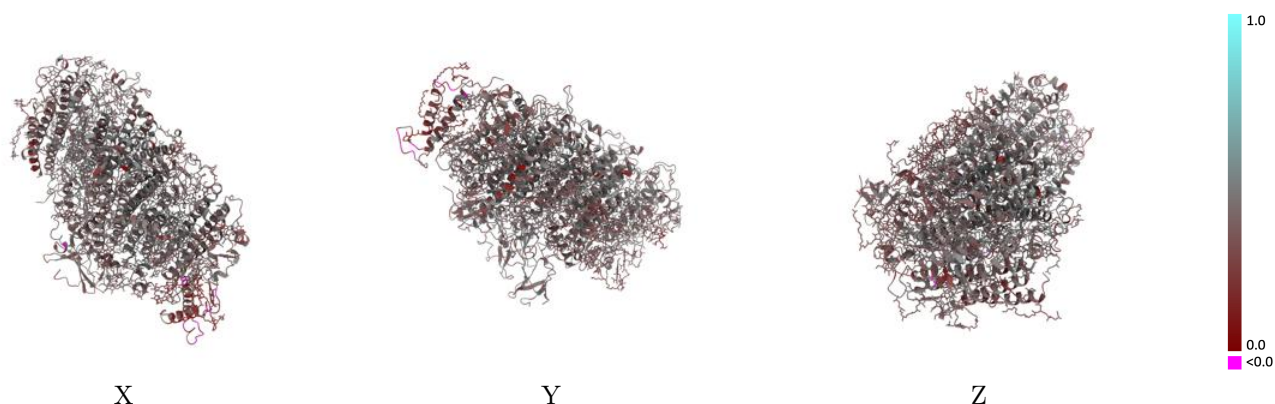
This section contains information regarding the fit between EMDB map EMD-12697 and PDB model 7O1V. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

9.1 Map-model overlay [i](#)



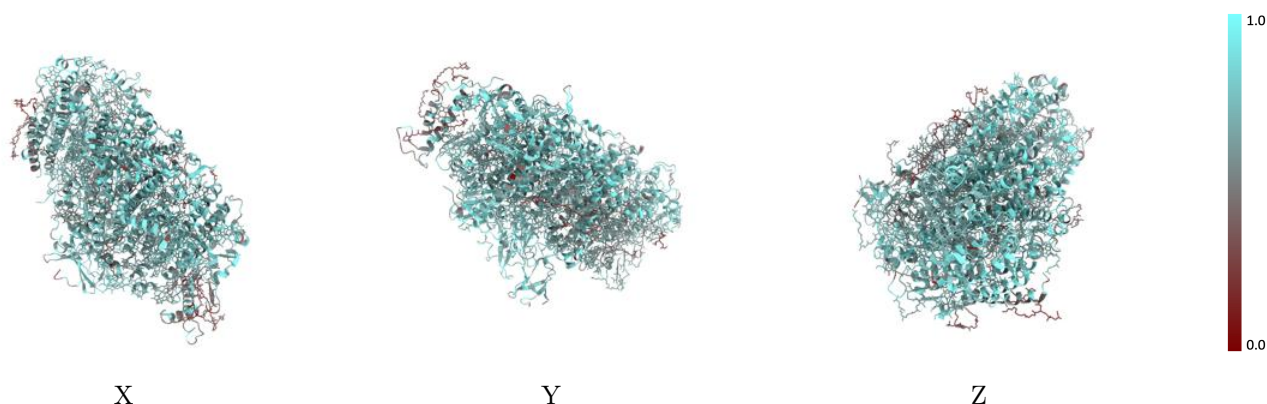
The images above show the 3D surface view of the map at the recommended contour level 0.008 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



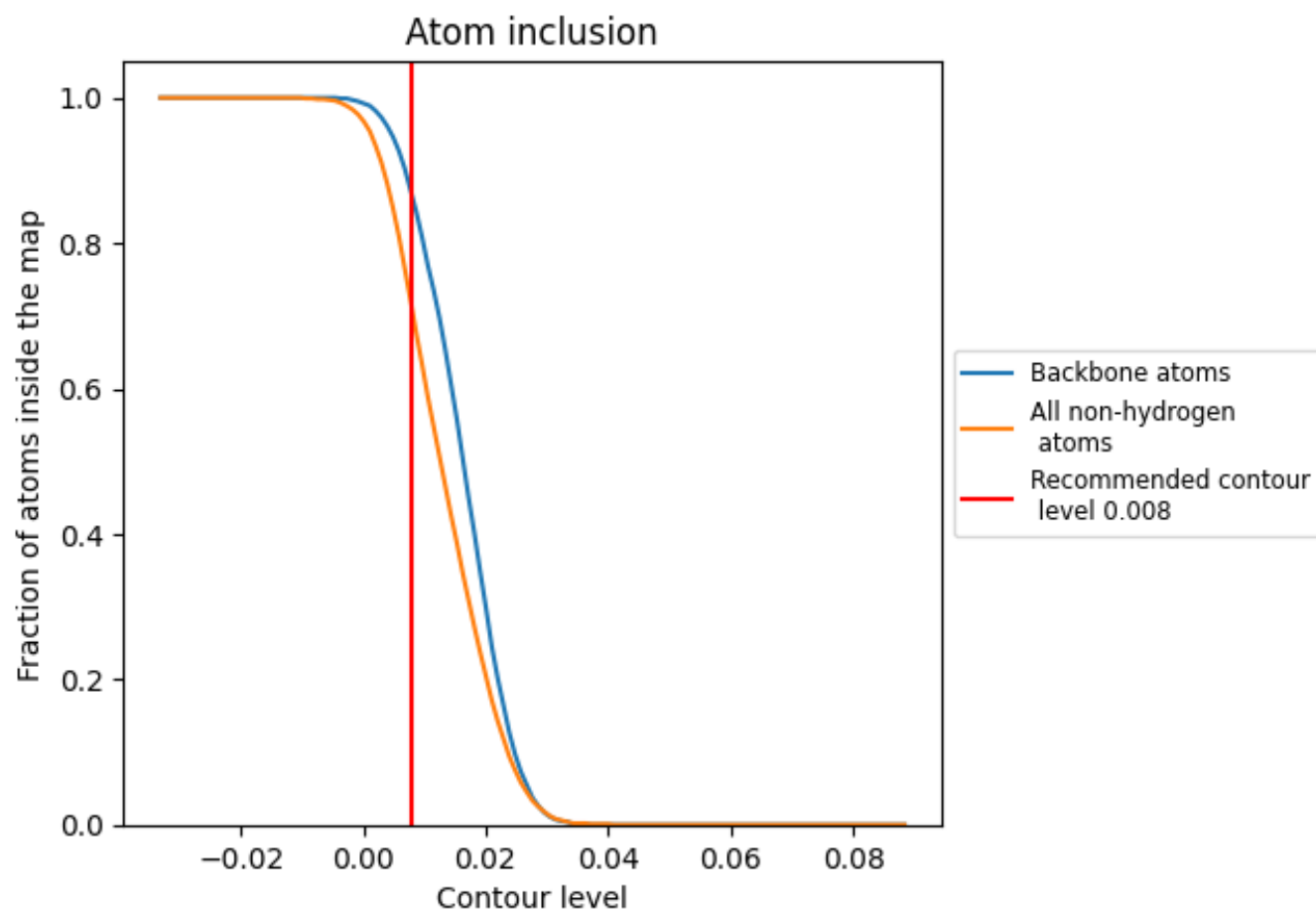
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.008).

9.4 Atom inclusion ⓘ



At the recommended contour level, 86% of all backbone atoms, 71% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.008) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7090	0.4000
A	0.7210	0.4120
B	0.7120	0.4060
C	0.7840	0.3960
D	0.7400	0.3900
E	0.7370	0.4260
K	0.5160	0.2510
M	0.5290	0.3220

1.0

0.0

<0.0