



wwPDB EM Validation Summary Report ⓘ

Nov 16, 2022 – 12:27 PM JST

PDB ID : 6KGX
EMDB ID : EMD-9976
Title : Structure of the phycobilisome from the red alga *Porphyridium purpureum*
Authors : Sui, S.F.; Ma, J.F.; You, X.; Sun, S.
Deposited on : 2019-07-12
Resolution : 2.80 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:

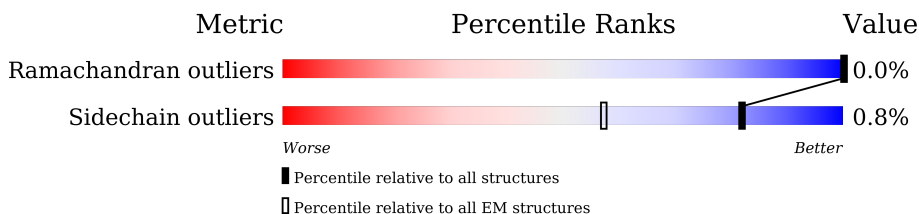
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 2.80 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A1	164	99% 99% .
1	A3	164	100% 99% .
1	A4	164	100% 99% .
1	AD	164	100% 99% .
1	AE	164	32% 100% .
1	AG	164	34% 99% .
1	B9	164	78% 99% .
1	BJ	164	79% 100% .
1	C1	164	100% 99% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	C3	164	100%
1	C4	164	99%
1	C8	164	24% 98%
1	CA	164	26% 100%
1	CD	164	100% 100%
1	CE	164	41% 99%
1	CG	164	38% 98%
1	D9	164	29% 98%
1	DJ	164	27% 99%
1	E1	164	100% 99%
1	E3	164	100% 99%
1	E4	164	100% 99%
1	E8	164	67% 100%
1	EA	164	65% 100%
1	ED	164	100% 99%
1	EE	164	17% 99%
1	EG	164	18% 98%
1	F9	164	49% 99%
1	FJ	164	48% 99%
1	G1	164	96% 96%
1	G3	164	99% 99%
1	G4	164	96% 99%
1	G8	164	77% 99%
1	GA	164	76% 99%
1	GD	164	99% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	GE	164	98%
1	GG	164	98%
1	H9	164	79%
1	HJ	164	100%
1	I1	164	77%
1	I3	164	99%
1	I4	164	95%
1	I8	164	99%
1	IA	164	30%
1	ID	164	31%
1	IE	164	99%
1	IG	164	100%
1	J5	164	98%
1	J9	164	99%
1	JC	164	97%
1	JJ	164	100%
1	K1	164	100%
1	K3	164	98%
1	K4	164	98%
1	K8	164	99%
1	KA	164	9%
1	KD	164	100%
1	KE	164	99%
1	KG	164	9%
1	L9	164	7%
1	L9	164	90%
1	L9	164	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	LJ	164	90% 99%
1	M3	164	38% 100%
1	M8	164	100%
1	MA	164	100%
1	MD	164	39% 99%
1	ME	164	62% 99%
1	MG	164	65% 100%
1	N1	164	99%
1	N4	164	99%
1	N9	164	100% 99%
1	NJ	164	100% 98%
1	O2	164	100%
1	O3	164	99%
1	O6	164	99%
1	O7	164	97% 99%
1	O8	164	37% 99%
1	OA	164	40% 99%
1	OB	164	100%
1	OD	164	98%
1	OE	164	35% 100%
1	OF	164	96% 99%
1	OG	164	37% 100%
1	OI	164	100%
1	P1	164	24% 99%
1	P4	164	25% 99%

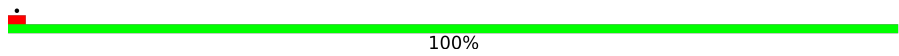
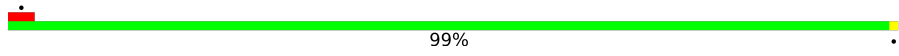
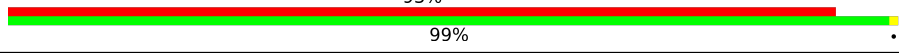
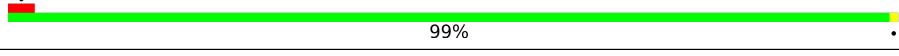
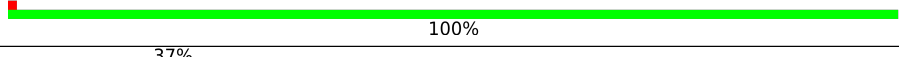
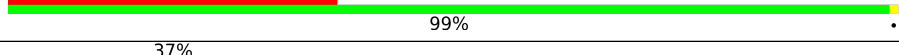
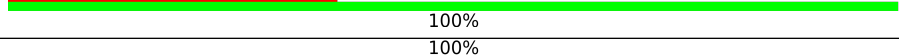
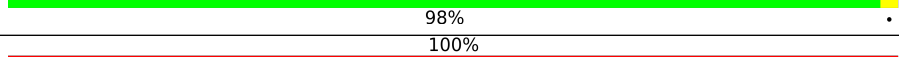
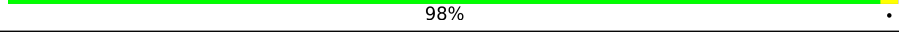
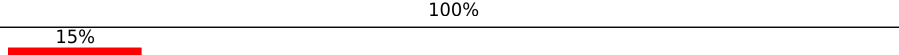
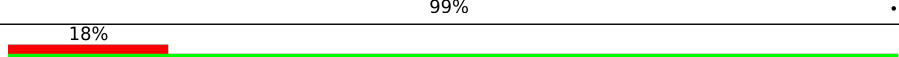
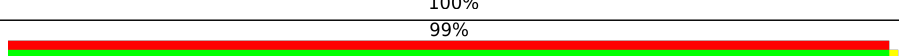
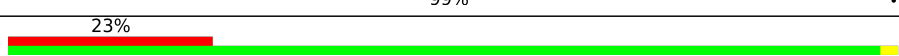
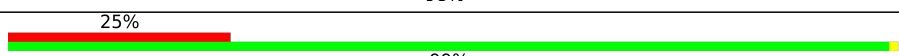
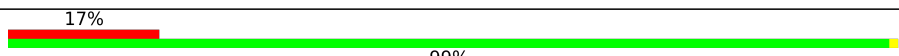
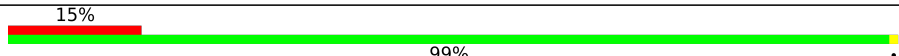
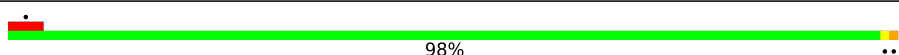
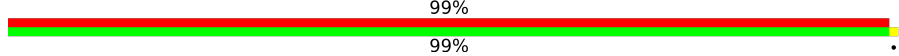
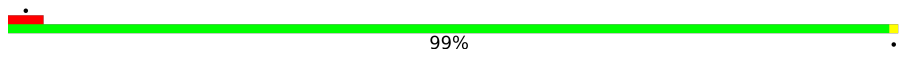

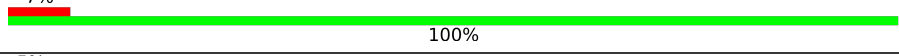
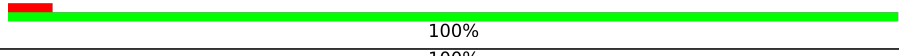
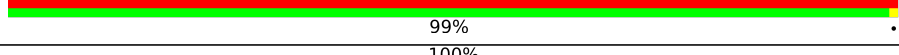
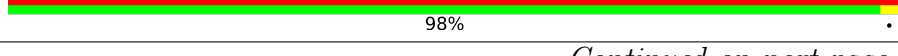

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	P9	164	100%
1	PJ	164	100%
1	Q2	164	99%
1	Q3	164	99%
1	Q6	164	99%
1	Q7	164	99%
1	Q8	164	100%
1	QA	164	100%
1	QB	164	99%
1	QD	164	99%
1	QE	164	98%
1	QF	164	99%
1	QG	164	99%
1	QI	164	99%
1	R1	164	99%
1	R4	164	99%
1	R9	164	100%
1	RJ	164	99%
1	S2	164	100%
1	S3	164	99%
1	S6	164	99%
1	S7	164	100%
1	S8	164	99%
1	SA	164	99%
1	SB	164	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	SD	164	 100%
1	SE	164	 99%
1	SF	164	 93% 99%
1	SG	164	 99%
1	SI	164	 100%
1	T1	164	 37% 99%
1	T4	164	 37% 100%
1	T9	164	 100% 98%
1	TJ	164	 100% 98%
1	U2	164	 100%
1	U3	164	 15% 99%
1	U6	164	 18% 100%
1	U7	164	 99% 99%
1	U8	164	 23% 98%
1	UA	164	 25% 99%
1	UB	164	 17% 99%
1	UD	164	 15% 99%
1	UE	164	 98% 99%
1	UF	164	 99% 99%
1	UG	164	 99%
1	UI	164	 100%
1	V1	164	 7% 100%
1	V4	164	 5% 100%
1	V9	164	 100% 99%
1	VJ	164	 100% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	W2	164	99%
1	W3	164	29% 100%
1	W6	164	6% 100%
1	W7	164	98% 100%
1	W8	164	5% 100%
1	WA	164	5% 99%
1	WB	164	6% 100%
1	WD	164	29% 100%
1	WE	164	29% 100%
1	WF	164	98% 99%
1	WG	164	30% 99%
1	WI	164	99%
1	X1	164	99%
1	X4	164	99%
1	X9	164	100%
1	XJ	164	98% 100%
1	Y8	164	9% 99%
1	YA	164	8% 98%
1	YE	164	96% 100%
1	YG	164	98% 100%
1	Z2	164	100%
1	Z6	164	100%
1	Z7	164	99%
1	ZB	164	100%
1	ZF	164	100%
1	ZF	164	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	ZI	164	100%
1	a8	164	76%
1	aA	164	78%
1	aE	164	83%
1	aG	164	84%
1	b2	164	40%
1	b6	164	61%
1	b7	164	100%
1	bB	164	58%
1	bF	164	100%
1	bI	164	39%
1	c1	164	100%
1	c4	164	100%
1	cE	164	84%
1	cG	164	83%
1	d2	164	28%
1	d6	164	90%
1	d7	164	100%
1	d8	164	88%
1	dA	164	87%
1	dB	164	93%
1	dF	164	100%
1	dI	164	32%
1	e1	164	100%
1	e4	164	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	eE	164	79% 99%
1	eG	164	79% 98%
1	f2	164	45% 99%
1	f6	164	94% 99%
1	f7	164	100% 99%
1	f8	164	96% 99%
1	fA	164	95% 99%
1	fB	164	96% 99%
1	fF	164	100% 98%
1	fI	164	46% 100%
1	g1	164	100% 98%
1	g4	164	100% 99%
1	gE	164	76% 99%
1	gG	164	71% 100%
1	h2	164	20% 100%
1	h6	164	98% 99%
1	h7	164	100% 99%
1	h8	164	98% 98%
1	hA	164	98% 99%
1	hB	164	96% 99%
1	hF	164	100% 98%
1	hI	164	21% 100%
1	i1	164	100% 99%
1	i4	164	100% 99%
1	iE	164	82% 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	iG	164	83% 98%
1	j2	164	29% 100%
1	j6	164	82% 100%
1	j7	164	100% 99%
1	j8	164	93% 99%
1	jA	164	95% 100%
1	jB	164	83% 100%
1	jF	164	100% 98%
1	jI	164	32% 100%
1	k1	164	100% 99%
1	k4	164	100% 99%
1	kE	164	100% 97%
1	kG	164	100% 99%
1	l2	164	22% 100%
1	l6	164	78% 99%
1	l7	164	100% 100%
1	l8	164	51% 94% 6%
1	lA	164	52% 98%
1	lB	164	78% 100%
1	lF	164	100% 96%
1	lI	164	22% 100%
1	m1	164	100% 99%
1	m4	164	100% 99%
1	mE	164	99% 95%
1	mG	164	99% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	oE	164	100%
1	oG	164	100%
1	p1	164	100%
1	p4	164	100%
1	qE	164	100%
1	qG	164	98%
1	r1	164	99%
1	r4	164	98%
1	sE	164	100%
1	sG	164	99%
1	t1	164	100%
1	t4	164	98%
1	uE	164	100%
1	uG	164	99%
1	v1	164	100%
1	v4	164	99%
1	x1	164	100%
1	x4	164	96%
1	z1	164	100%
1	z4	164	99%
2	11	177	100%
2	14	177	99%
2	A5	177	82%
2	AC	177	81%
2	B1	177	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B3	177	100%
2	B4	177	99%
2	B5	177	82%
2	BC	177	81%
2	BD	177	82%
2	BE	177	76%
2	BG	177	100%
2	C5	177	97%
2	C9	177	38%
2	CC	177	99%
2	CJ	177	82%
2	D1	177	80%
2	D3	177	62%
2	D4	177	99%
2	D8	177	99%
2	DA	177	98%
2	DD	177	100%
2	DE	177	99%
2	DG	177	28%
2	E9	177	27%
2	EJ	177	99%
2	F1	177	44%
2	F3	177	98%
2	F4	177	92%
2	F5	177	99%
2	F5	177	93%
2	F5	177	36%
2	F5	177	82%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F8	177	24% 99%
2	FA	177	21% 99%
2	FC	177	37% 82% 18%
2	FD	177	100% 98%
2	FE	177	98%
2	FG	177	99%
2	G5	177	81% 81% 18%
2	G9	177	90% 99%
2	GC	177	81% 82% 18%
2	GJ	177	88% 99%
2	H1	177	99% 98%
2	H3	177	99% 98%
2	H4	177	100% 99%
2	H5	177	10% 81% 18%
2	H8	177	50% 99%
2	HA	177	50% 99%
2	HC	177	10% 82% 18%
2	HD	177	99% 98%
2	HE	177	6% 99%
2	HG	177	5% 99%
2	I5	177	22% 97%
2	I9	177	21% 98%
2	IC	177	23% 99%
2	IJ	177	20% 99%
2	J1	177	98% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J3	177	100%
2	J4	177	98% 99%
2	J8	177	58% 99%
2	JA	177	58% 99%
2	JD	177	100% 99%
2	JE	177	98%
2	JG	177	98%
2	K5	177	10% 97%
2	K9	177	94% 99%
2	KC	177	10% 97%
2	KJ	177	93% 99%
2	L1	177	99% 98%
2	L3	177	99% 99%
2	L4	177	99% 99%
2	L5	177	11% 77% 6% 18%
2	L8	177	7% 99%
2	LA	177	7% 99%
2	LC	177	10% 79% 18%
2	LD	177	99% 99%
2	LE	177	99%
2	LG	177	98%
2	M9	177	84% 99%
2	MJ	177	84% 99%
2	N3	177	19% 99%
2	N8	177	5% 97%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	NA	177	5% 98%
2	ND	177	19% 99%
2	NE	177	56% 99%
2	NG	177	55% 99%
2	O1	177	5% 99%
2	O4	177	6% 98%
2	O9	177	100% 98%
2	OJ	177	100% 97%
2	P2	177	100%
2	P3	177	12% 98%
2	P6	177	7% 98%
2	P7	177	64% 99%
2	P8	177	69% 99%
2	PA	177	72% 98%
2	PB	177	6% 99%
2	PD	177	12% 98%
2	PE	177	38% 99%
2	PF	177	64% 98%
2	PG	177	38% 99%
2	PI	177	100%
2	Q1	177	7% 99%
2	Q4	177	6% 99%
2	Q9	177	100% 97%
2	QJ	177	99% 99%
2	R2	177	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	R3	177	8% 99%
2	R6	177	19% 99%
2	R7	177	98% 99%
2	R8	177	33% 99%
2	RA	177	33% 98%
2	RB	177	18% 99%
2	RD	177	10% 99%
2	RE	177	14% 98%
2	RF	177	98% 99%
2	RG	177	14% 99%
2	RI	177	99%
2	S1	177	24% 98%
2	S4	177	27% 98%
2	S9	177	100% 99%
2	SJ	177	100% 98%
2	T2	177	5% 98%
2	T3	177	99%
2	T6	177	7% 99%
2	T7	177	95% 99%
2	T8	177	30% 99%
2	TA	177	30% 99%
2	TB	177	6% 99%
2	TD	177	99%
2	TE	177	8% 99%
2	TF	177	96% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	TG	177	8% 99%
2	TI	177	5% 99%
2	U1	177	36% 98%
2	U4	177	36% 99%
2	U9	177	100% 98%
2	UJ	177	100% 99%
2	V2	177	98%
2	V3	177	45% 99%
2	V6	177	45% 98%
2	V7	177	99% 97%
2	V8	177	52% 99%
2	VA	177	55% 99%
2	VB	177	46% 98%
2	VD	177	44% 99%
2	VE	177	23% 97%
2	VF	177	98%
2	VG	177	23% 98%
2	VI	177	97%
2	W1	177	99%
2	W4	177	98%
2	W9	177	100% 96%
2	WJ	177	100% 99%
2	X3	177	11% 99%
2	X8	177	12% 98%
2	XA	177	12% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	XD	177	12% 99%
2	XE	177	8% 98%
2	XG	177	7% 99%
2	Y1	177	7% 98%
2	Y2	177	99%
2	Y4	177	6% 97%
2	Y6	177	99%
2	Y7	177	98%
2	Y9	177	99%
2	YB	177	99%
2	YF	177	98%
2	YI	177	99%
2	YJ	177	100%
2	Z1	177	50% 82% 18%
2	Z4	177	49% 81% 18%
2	Z8	177	5% 99%
2	ZA	177	5% 99%
2	ZE	177	93% 98%
2	ZG	177	93% 97%
2	a1	177	79% 81% 18%
2	a2	177	97%
2	a4	177	79% 81% 18%
2	a6	177	18% 99%
2	a7	177	100% 99%
2	aB	177	19% 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	aF	177	100% 99%
2	aI	177	97%
2	bE	177	77% 98%
2	bG	177	76% 99%
2	c2	177	56% 99%
2	c6	177	74% 99%
2	c7	177	100% 99%
2	c8	177	96% 99%
2	cA	177	95% 99%
2	cB	177	73% 100%
2	cF	177	100% 98%
2	cI	177	57% 99%
2	d1	177	100% 99%
2	d4	177	100% 98%
2	dE	177	80% 99%
2	dG	177	79% 98%
2	e2	177	17% 99%
2	e6	177	85% 99%
2	e7	177	100% 99%
2	e8	177	44% 99%
2	eA	177	42% 99%
2	eB	177	85% 99%
2	eF	177	100% 98%
2	eI	177	18% 99%
2	fI	177	100% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	f4	177	100% 98% ..
2	fE	177	69% 98% .
2	fG	177	68% 99% .
2	g2	177	51% 99% .
2	g6	177	77% 98% .
2	g7	177	100% 99% .
2	g8	177	98% 99% .
2	gA	177	98% 99% .
2	gB	177	77% 98% .
2	gF	177	100% 99% .
2	gI	177	47% 99% .
2	h1	177	100% 98% .
2	h4	177	100% 99% .
2	hE	177	92% 99% .
2	hG	177	91% 99% .
2	i2	177	11% 99% .
2	i6	177	98% 99% .
2	i7	177	100% 99% .
2	i8	177	90% 99% .
2	iA	177	89% 99% .
2	iB	177	98% 99% .
2	iF	177	100% 97% .
2	iI	177	14% 99% .
2	j1	177	100% 97% ..
2	j4	177	100% 99% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	jE	177	54% 99%
2	jG	177	53% 99%
2	k2	177	44% 98%
2	k6	177	41% 99%
2	k7	177	100% 99%
2	k8	177	89% 99%
2	kA	177	88% 99%
2	kB	177	42% 99%
2	kF	177	100% 98%
2	kI	177	42% 98%
2	l1	177	100% 98%
2	l4	177	100% 98%
2	lE	177	100% 99%
2	lG	177	100% 97%
2	m2	177	14% 99%
2	m6	177	94% 99%
2	m7	177	100% 99%
2	m8	177	79% 98%
2	mA	177	80% 98%
2	mB	177	93% 98%
2	mF	177	100% 97%
2	mI	177	12% 99%
2	n1	177	98% 98%
2	n4	177	98% 99%
2	nE	177	100% 98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	nG	177	100%
2	pE	177	100% 97%
2	pG	177	100% 98%
2	q1	177	100% 97%
2	q4	177	100% 97%
2	rE	177	100% 98%
2	rG	177	100% 97%
2	s1	177	100% 97%
2	s4	177	100% 98%
2	tE	177	100% 98%
2	tG	177	100% 99%
2	u1	177	99% 98%
2	u4	177	99% 98%
2	vE	177	99% 98%
2	vG	177	98% 98%
2	w1	177	100% 99%
2	w4	177	100% 98%
2	y1	177	100% 98%
2	y4	177	100% 99%
3	21	333	71% 68%
3	24	333	71% 68%
3	M1	333	69% 69%
3	M4	333	69% 69%
4	b1	405	16% 75%
4	b4	405	18% 76%

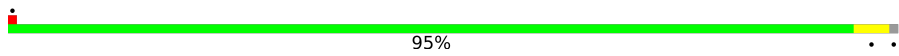
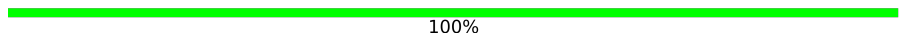
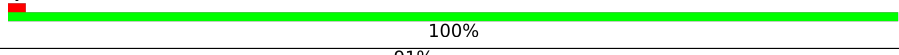
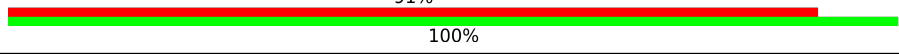
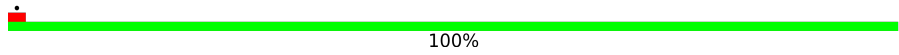
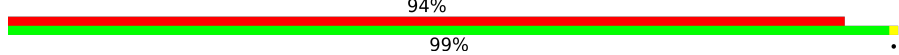
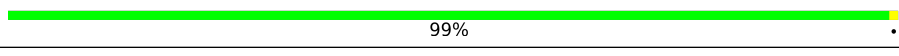
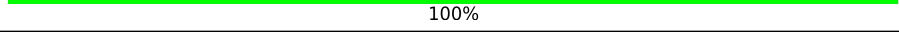
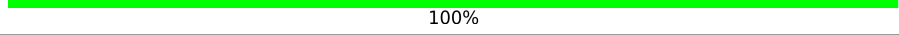
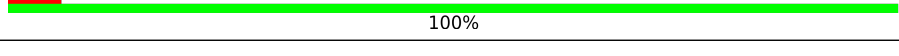
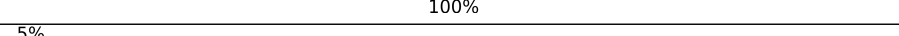
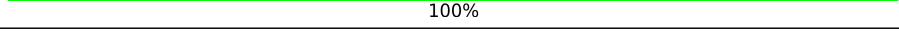
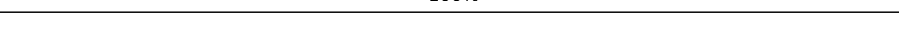
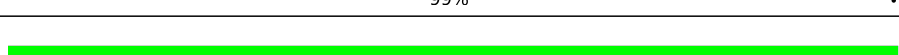

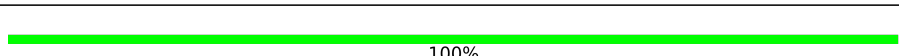

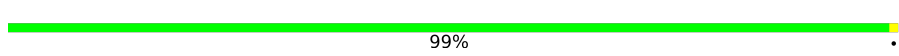
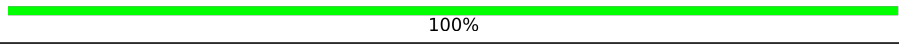
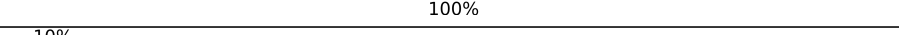
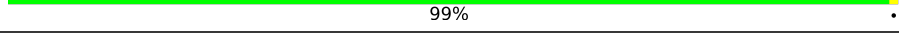
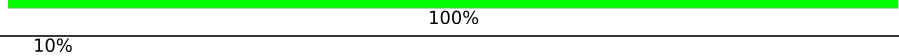
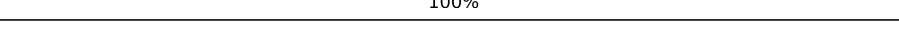
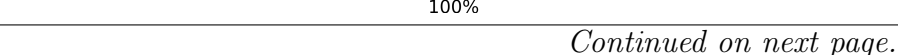

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	o1	405	52% 51% 48%
4	o4	405	52% 50% 48%
5	31	288	95%
5	34	288	95%
6	X2	363	88% 11%
6	X6	363	88% 11%
6	X7	363	78% 88% 11%
6	XB	363	88% 11%
6	XF	363	77% 88% 11%
6	XI	363	88% 11%
7	A2	290	18% 88% 11%
7	A6	290	70% 88% 11%
7	A7	290	89% 88% 11%
7	A9	290	88% 87% 12%
7	AB	290	68% 88% 11%
7	AF	290	89% 88% 11%
7	AI	290	17% 89% 11%
7	AJ	290	88% 88% 12%
7	Y3	290	81% 80% 18%
7	YD	290	81% 81% 18%
8	B2	232	96%
8	B6	232	6% 97%
8	B7	232	27% 97%
8	BB	232	6% 95%
8	BF	232	27% 96%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	BI	232	 95%
9	C2	162	 100%
9	C6	162	 100%
9	C7	162	 91% 100%
9	CB	162	 100%
9	CF	162	 94% 99%
9	CI	162	 99%
9	E2	162	 100%
9	E6	162	 100%
9	E7	162	 6% 100%
9	EB	162	 100%
9	EF	162	 5% 100%
9	EI	162	 100%
9	G2	162	 99%
9	G6	162	 100%
9	G7	162	 72% 99%
9	GB	162	 100%
9	GF	162	 71% 99%
9	GI	162	 99%
9	I2	162	 100%
9	I6	162	 100%
9	I7	162	 10% 99%
9	IB	162	 100%
9	IF	162	 10% 100%
9	II	162	 100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
9	K2	162	99%
9	K6	162	100%
9	K7	162	44% 99%
9	KB	162	100%
9	KF	162	43% 99%
9	KI	162	99%
9	M2	162	99%
9	M6	162	100%
9	M7	162	91% 99%
9	MB	162	100%
9	MF	162	90% 99%
9	MI	162	99%
10	D2	172	99%
10	D6	172	99%
10	D7	172	94% 99%
10	DB	172	99%
10	DF	172	94% 99%
10	DI	172	98%
10	F2	172	99%
10	F6	172	98%
10	F7	172	49% 98%
10	FB	172	99%
10	FF	172	49% 99%
10	FI	172	98%
10	H2	172	98%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
10	H6	172	99%
10	H7	172	33% 99%
10	HB	172	99%
10	HF	172	33% 98%
10	HI	172	98%
10	J2	172	98%
10	J6	172	97%
10	J7	172	36% 98%
10	JB	172	98%
10	JF	172	37% 98%
10	JI	172	99%
10	L2	172	98%
10	L6	172	98%
10	L7	172	5% 99%
10	LB	172	99%
10	LF	172	5% 99%
10	LI	172	98%
10	N2	172	98%
10	N6	172	99%
10	N7	172	72% 99%
10	NB	172	98%
10	NF	172	76% 99%
10	NI	172	98%
11	e3	303	9% 82% 18%
11	eD	303	8% 82% 18%

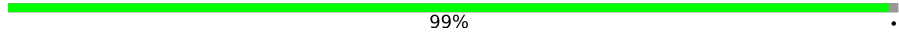
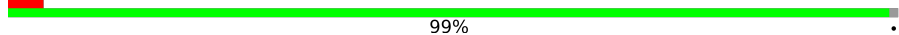
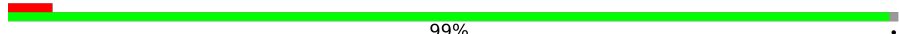
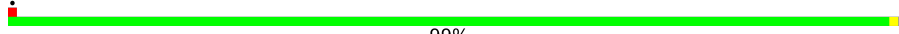


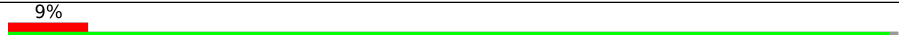
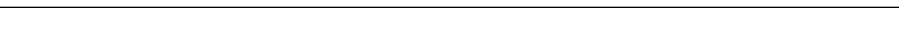
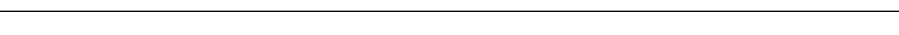
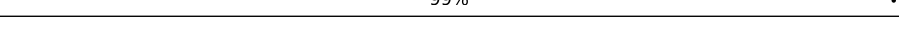
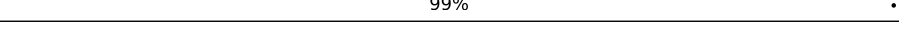
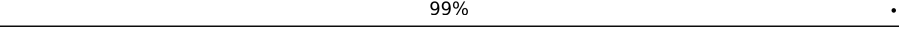
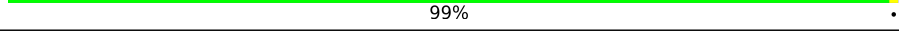
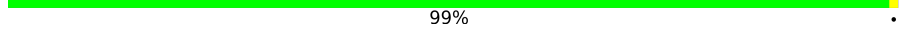
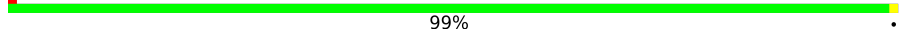
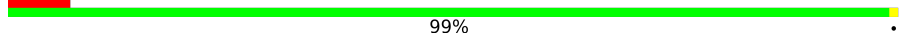
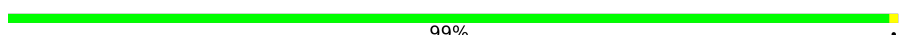
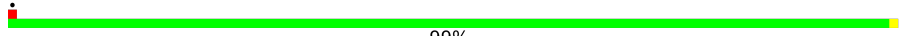





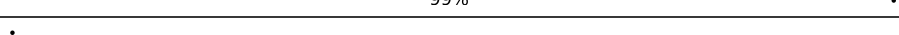
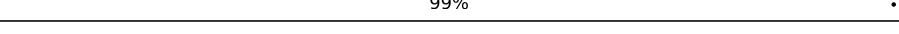
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
12	b8	490	11% 74% 22%
12	bA	490	11% 75% 22%
13	A8	273	76% 86% 13%
13	AA	273	76% 87% 13%
13	wE	273	55% 85% 13%
13	wG	273	57% 87% 13%
13	xE	273	87% 86% 13%
13	xG	273	87% 87% 13%
14	B8	290	30% 86% 14%
14	BA	290	32% 86% 14%
14	yE	290	7% 86% 14%
14	yG	290	9% 86% 14%
15	d9	342	34% 79% 17%
15	dJ	342	34% 80% 17%
16	zE	498	6% 73% 26%
16	zG	498	6% 74% 26%
17	AH	161	5% 99%
17	CH	161	99%
17	EH	161	99%
17	GH	161	99%
17	JH	161	99%
17	KH	161	8% 99%
17	NH	161	99%
17	PH	161	99%
17	RH	161	99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
17	TH	161	 99%
17	cH	161	 99%
17	eH	161	 99%
17	gH	161	 99%
17	iH	161	 99%
17	lH	161	 98%
17	mH	161	 99%
17	pH	161	 99%
17	rH	161	 99%
17	tH	161	 99%
17	vH	161	 99%
18	BH	161	 99%
18	DH	161	 99%
18	FH	161	 99%
18	HH	161	 99%
18	IH	161	 99%
18	LH	161	 99%
18	MH	161	 98%
18	OH	161	 99%
18	QH	161	 99%
18	SH	161	 99%
18	UH	161	 99%
18	dH	161	 99%
18	fH	161	 99%
18	hH	161	 99%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
18	jH	161	5% 99%
18	kH	161	99%
18	nH	161	99%
18	oH	161	96%
18	qH	161	10% 99%
18	sH	161	99%
18	uH	161	99%
18	wH	161	99%
19	VH	161	8% 99%
19	xH	161	17% 99%
20	WH	173	5% 100%
20	yH	173	5% 100%
21	XH	93	99%
21	zH	93	99%
22	1H	879	7% 95%
22	YH	879	7% 95%
23	2H	159	11% 83% 17%
23	ZH	159	11% 83% 17%
24	3H	288	5% 85% 12%
24	aH	288	5% 85% 12%
25	4H	253	5% 80% 19%
25	bH	253	5% 80% 19%

2 Entry composition [i](#)

There are 28 unique types of molecules in this entry. The entry contains 1014295 atoms, of which 1824 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 Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A1	164	1250	779	219	245	7	0	0
1	C1	164	1250	779	219	245	7	0	0
1	E1	164	1250	779	219	245	7	0	0
1	G1	164	1250	779	219	245	7	0	0
1	I1	164	1250	779	219	245	7	0	0
1	K1	164	1250	779	219	245	7	0	0
1	N1	164	1250	779	219	245	7	0	0
1	P1	164	1250	779	219	245	7	0	0
1	R1	164	1250	779	219	245	7	0	0
1	T1	164	1250	779	219	245	7	0	0
1	V1	164	1250	779	219	245	7	0	0
1	X1	164	1250	779	219	245	7	0	0
1	c1	164	1250	779	219	245	7	0	0
1	e1	164	1250	779	219	245	7	0	0
1	g1	164	1250	779	219	245	7	0	0
1	i1	164	1250	779	219	245	7	0	0
1	k1	164	1250	779	219	245	7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	m1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	p1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	r1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	t1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	v1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	x1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	z1	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	O2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Q2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	S2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	U2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	W2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Z2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	b2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	d2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	f2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	h2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	j2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	l2	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	A3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	C3	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	E3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	G3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	I3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	K3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	M3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	O3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Q3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	S3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	U3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	W3	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	A4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	C4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	E4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	G4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	I4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	K4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	N4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	P4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	R4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	T4	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	V4	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	X4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	c4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	e4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	g4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	i4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	k4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	m4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	p4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	r4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	t4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	v4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	x4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	z4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	J5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	O6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Q6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	S6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	U6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	W6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	Z6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	b6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	d6	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	f6	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	h6	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	j6	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	l6	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	O7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Q7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	S7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	U7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	W7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Z7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	b7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	d7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	f7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	h7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	j7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	l7	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	C8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	E8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	G8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	I8	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	K8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	M8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	O8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Q8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	S8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	U8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	W8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	Y8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	a8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	d8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	f8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	h8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	j8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	l8	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	B9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	D9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	F9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	H9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	J9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	L9	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	N9	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	P9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	R9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	T9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	V9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	X9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	dA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	fA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	hA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	jA	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	lA	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ZB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	bB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	dB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	fB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	hB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	jB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	lB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	JC	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	AD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	CD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ED	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	GD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ID	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	KD	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	MD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WD	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	AE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	CE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	EE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	GE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	IE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	KE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ME	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	YE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	aE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	cE	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	eE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	gE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	iE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	kE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	mE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	oE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	qE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	sE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	uE	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ZF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	bF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	dF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	fF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	hF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	jF	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	lF	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	CG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	EG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	GG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	IG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	KG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	MG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	OG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	QG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	SG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	UG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	WG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	YG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	aG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	cG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	eG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	gG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	iG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	kG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	mG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	oG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	qG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	sG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	uG	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	OI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	QI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	SI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	UI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	WI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	ZI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	bI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	dI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	fI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	hI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	jI	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	II	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	BJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	DJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	FJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	HJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	JJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0
1	LJ	164	Total 1250	C 779	N 219	O 245	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
1	NJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	PJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	RJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	TJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	VJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
1	XJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 2 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	D1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	F1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	H1	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	J1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	L1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	O1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Q1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	S1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	U1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	W1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Z1	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	a1	146	Total	C	N	O	S	0	0
			1065	654	187	213	11		
2	d1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	f1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	h1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	j1	177	Total	C	N	O	S	1	0
			1297	802	225	258	12		
2	l1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	n1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	q1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	s1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	u1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	w1	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	y1	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	11	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	P2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	R2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	T2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	V2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	Y2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	a2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	c2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	e2	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	g2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i2	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	k2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	B3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H3	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	N3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	R3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	T3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	V3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X3	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	B4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J4	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	L4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	O4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Q4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	S4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	U4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	W4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Y4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Z4	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	a4	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	d4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	f4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	h4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	j4	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	l4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	n4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	q4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	s4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	u4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	w4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	y4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	14	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	B5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	C5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	F5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	G5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	H5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	I5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	K5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	P6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	T6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V6	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Y6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	a6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	c6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	e6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	g6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i6	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	k6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m6	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	P7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	T7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V7	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Y7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	a7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	c7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	e7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	g7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i7	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	k7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	m7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	F8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	H8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	J8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	L8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	N8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R8	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	T8	177	Total 1303	C 806	N 225	O 260	S 12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	V8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Z8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	c8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	e8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	g8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	i8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	k8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	m8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	C9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	E9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	G9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	I9	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	K9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	M9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	O9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Q9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	S9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	U9	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	W9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Y9	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	DA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	LA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RA	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	TA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	ZA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	cA	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	eA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	gA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	iA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	kA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	mA	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TB	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	VB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	AC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	BC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	CC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	FC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	GC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	HC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	IC	176	Total 1286	C 795	N 224	O 256	S 11	0	0
2	KC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LC	146	Total 1065	C 654	N 187	O 213	S 11	0	0
2	BD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	DD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	FD	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HD	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	JD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	ND	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	TD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XD	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	BE	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	DE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	LE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	TE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	VE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	XE	177	Total 1303	C 806	N 225	O 260	S 12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	ZE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	bE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	dE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	fE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	hE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	jE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	lE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	nE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	pE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	rE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	tE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	vE	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gF	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	iF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	BG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	DG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	LG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	TG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	VG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	XG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	ZG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	bG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	dG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	fG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	hG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	jG	177	Total 1303	C 806	N 225	O 260	S 12	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	lG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	nG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	pG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	rG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	tG	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	vG	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iI	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	kI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	CJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	EJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	GJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
2	IJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	KJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	MJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	OJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	QJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	SJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	UJ	177	Total	C	N	O	S	2	0
			1300	804	225	259	12		
2	WJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		
2	YJ	177	Total	C	N	O	S	0	0
			1294	800	225	257	12		

- Molecule 3 is a protein called LR7.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	M1	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	21	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	M4	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		
3	24	238	Total	C	N	O	S	0	0
			1846	1137	347	347	15		

- Molecule 4 is a protein called LR2_Hb.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b1	323	Total	C	N	O	S	0	0
			2485	1566	422	486	11		
4	o1	212	Total	C	N	O	S	0	0
			1645	1036	283	319	7		
4	b4	323	Total	C	N	O	S	0	0
			2485	1566	422	486	11		
4	o4	212	Total	C	N	O	S	0	0
			1645	1036	283	319	7		

- Molecule 5 is a protein called LR9.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	31	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		
5	34	285	Total	C	N	O	S	0	0
			2182	1399	369	404	10		

- Molecule 6 is a protein called LR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	X2	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	X6	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	X7	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XB	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XF	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
6	XI	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		

- Molecule 7 is a protein called LR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	A2	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	Y3	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
7	A6	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	A7	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	A9	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
7	AB	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	YD	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
7	AF	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
7	AI	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	AJ	256	1979	1220	367	377	15	0	0

- Molecule 8 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	B2	230	1889	1206	331	348	4	0	0
8	B6	231	1897	1212	332	349	4	0	0
8	B7	227	1874	1197	328	345	4	0	0
8	BB	231	1897	1212	332	349	4	0	0
8	BF	227	1874	1197	328	345	4	0	0
8	BI	230	1889	1206	331	348	4	0	0

- Molecule 9 is a protein called C-phycoyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	C2	162	1228	773	209	240	6	0	0
9	E2	162	1228	773	209	240	6	0	0
9	G2	162	1228	773	209	240	6	0	0
9	I2	162	1228	773	209	240	6	0	0
9	K2	162	1228	773	209	240	6	0	0
9	M2	162	1228	773	209	240	6	0	0
9	C6	162	1228	773	209	240	6	0	0
9	E6	162	1228	773	209	240	6	0	0
9	G6	162	1228	773	209	240	6	0	0
9	I6	162	1228	773	209	240	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	K6	162	1228	773	209	240	6	0	0
9	M6	162	1228	773	209	240	6	0	0
9	C7	162	1228	773	209	240	6	0	0
9	E7	162	1228	773	209	240	6	0	0
9	G7	162	1228	773	209	240	6	0	0
9	I7	162	1228	773	209	240	6	0	0
9	K7	162	1228	773	209	240	6	0	0
9	M7	162	1228	773	209	240	6	0	0
9	CB	162	1228	773	209	240	6	0	0
9	EB	162	1228	773	209	240	6	0	0
9	GB	162	1228	773	209	240	6	0	0
9	IB	162	1228	773	209	240	6	0	0
9	KB	162	1228	773	209	240	6	0	0
9	MB	162	1228	773	209	240	6	0	0
9	CF	162	1228	773	209	240	6	0	0
9	EF	162	1228	773	209	240	6	0	0
9	GF	162	1228	773	209	240	6	0	0
9	IF	162	1228	773	209	240	6	0	0
9	KF	162	1228	773	209	240	6	0	0
9	MF	162	1228	773	209	240	6	0	0
9	CI	162	1228	773	209	240	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
9	EI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	GI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	II	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	KI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
9	MI	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

- Molecule 10 is a protein called C-phycoyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	D2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	H6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	J6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	L6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	N6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	D7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
10	F7	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	H7	172	1272	786	224	253	9	0	0
10	J7	172	1272	786	224	253	9	0	0
10	L7	172	1272	786	224	253	9	0	0
10	N7	172	1272	786	224	253	9	0	0
10	DB	172	1272	786	224	253	9	0	0
10	FB	172	1272	786	224	253	9	0	0
10	HB	172	1272	786	224	253	9	0	0
10	JB	172	1272	786	224	253	9	0	0
10	LB	172	1272	786	224	253	9	0	0
10	NB	172	1272	786	224	253	9	0	0
10	DF	172	1272	786	224	253	9	0	0
10	FF	172	1272	786	224	253	9	0	0
10	HF	172	1272	786	224	253	9	0	0
10	JF	172	1272	786	224	253	9	0	0
10	LF	172	1272	786	224	253	9	0	0
10	NF	172	1272	786	224	253	9	0	0
10	DI	172	1272	786	224	253	9	0	0
10	FI	172	1272	786	224	253	9	0	0
10	HI	172	1272	786	224	253	9	0	0
10	JI	172	1272	786	224	253	9	0	0
10	LI	172	1272	786	224	253	9	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	NI	172	1272	786	224	253	9	0	0

- Molecule 11 is a protein called LR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	e3	248	1932	1217	336	369	10	0	0
11	eD	248	1932	1217	336	369	10	0	0

- Molecule 12 is a protein called LRC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	b8	380	2961	1867	514	565	15	0	0
12	bA	380	2961	1867	514	565	15	0	0

- Molecule 13 is a protein called LR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	A8	238	1814	1122	335	342	15	0	0
13	AA	238	1814	1122	335	342	15	0	0
13	wE	238	1814	1122	335	342	15	0	0
13	xE	238	1814	1122	335	342	15	0	0
13	wG	238	1814	1122	335	342	15	0	0
13	xG	238	1814	1122	335	342	15	0	0

- Molecule 14 is a protein called LR8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	B8	250	1902	1184	346	358	14	0	0
14	BA	250	1902	1184	346	358	14	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
14	yE	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
14	yG	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		

- Molecule 15 is a protein called LR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	d9	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		
15	dJ	285	Total	C	N	O	S	0	0
			2203	1367	390	435	11		

- Molecule 16 is a protein called LRC3.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	zE	370	Total	C	N	O	S	0	0
			2901	1833	514	540	14		
16	zG	370	Total	C	N	O	S	0	0
			2901	1833	514	540	14		

- Molecule 17 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	AH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	CH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	EH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	GH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	JH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	KH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	NH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	PH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
17	RH	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	TH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	cH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	eH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	gH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	iH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	lH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	mH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	pH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	rH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	tH	160	Total 1225	C 768	N 211	O 239	S 7	0	0
17	vH	160	Total 1225	C 768	N 211	O 239	S 7	0	0

- Molecule 18 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	DH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	FH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	BH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	HH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	IH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	LH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	MH	161	Total 1219	C 767	N 206	O 239	S 7	0	0
18	OH	161	Total 1219	C 767	N 206	O 239	S 7	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
18	QH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	SH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	UH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	dH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	fH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	hH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	jH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	kH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	nH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	oH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	qH	161	Total	C	N	O	S	0	0
			1219	767	206	239	7		
18	sH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	uH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
18	wH	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 19 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	VH	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
19	xH	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 20 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	WH	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
20	yH	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 21 is a protein called LC.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	XH	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
21	zH	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 22 is a protein called Phycobilisome linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	YH	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		
22	1H	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		

- Molecule 23 is a protein called LRC4.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	ZH	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		
23	2H	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		

- Molecule 24 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	aH	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		
24	3H	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		

- Molecule 25 is a protein called LRC6.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	bH	206	Total	C	N	O	S	0	0
			1532	982	259	286	5		
25	4H	206	Total	C	N	O	S	0	0
			1532	982	259	286	5		

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	F1	1	129	99	12	18	0
26	F1	1	129	99	12	18	0
26	G1	1	86	66	8	12	0
26	G1	1	86	66	8	12	0
26	H1	1	129	99	12	18	0
26	H1	1	129	99	12	18	0
26	H1	1	129	99	12	18	0
26	I1	1	86	66	8	12	0
26	I1	1	86	66	8	12	0
26	J1	1	129	99	12	18	0
26	J1	1	129	99	12	18	0
26	J1	1	129	99	12	18	0
26	K1	1	86	66	8	12	0
26	K1	1	86	66	8	12	0
26	L1	1	129	99	12	18	0
26	L1	1	129	99	12	18	0
26	L1	1	129	99	12	18	0
26	M1	1	129	99	12	18	0
26	M1	1	129	99	12	18	0
26	M1	1	129	99	12	18	0
26	N1	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	N1	1	129	99	12	18	0
26	N1	1	129	99	12	18	0
26	O1	1	86	66	8	12	0
26	O1	1	86	66	8	12	0
26	P1	1	129	99	12	18	0
26	P1	1	129	99	12	18	0
26	P1	1	129	99	12	18	0
26	Q1	1	86	66	8	12	0
26	Q1	1	86	66	8	12	0
26	R1	1	129	99	12	18	0
26	R1	1	129	99	12	18	0
26	R1	1	129	99	12	18	0
26	S1	1	86	66	8	12	0
26	S1	1	86	66	8	12	0
26	T1	1	129	99	12	18	0
26	T1	1	129	99	12	18	0
26	T1	1	129	99	12	18	0
26	U1	1	86	66	8	12	0
26	U1	1	86	66	8	12	0
26	V1	1	129	99	12	18	0
26	V1	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	V1	1	Total 129	C 99	N 12	O 18	0
26	W1	1	Total 86	C 66	N 8	O 12	0
26	W1	1	Total 86	C 66	N 8	O 12	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	X1	1	Total 129	C 99	N 12	O 18	0
26	Y1	1	Total 86	C 66	N 8	O 12	0
26	Y1	1	Total 86	C 66	N 8	O 12	0
26	Z1	1	Total 86	C 66	N 8	O 12	0
26	Z1	1	Total 86	C 66	N 8	O 12	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	a1	1	Total 129	C 99	N 12	O 18	0
26	b1	1	Total 43	C 33	N 4	O 6	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	c1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	d1	1	Total 129	C 99	N 12	O 18	0
26	e1	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	e1	1	Total 86	C 66	N 8	O 12	0
26	f1	1	Total 86	C 66	N 8	O 12	0
26	f1	1	Total 86	C 66	N 8	O 12	0
26	g1	1	Total 129	C 99	N 12	O 18	0
26	g1	1	Total 129	C 99	N 12	O 18	0
26	g1	1	Total 129	C 99	N 12	O 18	0
26	h1	1	Total 86	C 66	N 8	O 12	0
26	h1	1	Total 86	C 66	N 8	O 12	0
26	i1	1	Total 129	C 99	N 12	O 18	0
26	i1	1	Total 129	C 99	N 12	O 18	0
26	i1	1	Total 129	C 99	N 12	O 18	0
26	j1	1	Total 86	C 66	N 8	O 12	0
26	j1	1	Total 86	C 66	N 8	O 12	0
26	k1	1	Total 129	C 99	N 12	O 18	0
26	k1	1	Total 129	C 99	N 12	O 18	0
26	k1	1	Total 129	C 99	N 12	O 18	0
26	l1	1	Total 86	C 66	N 8	O 12	0
26	l1	1	Total 86	C 66	N 8	O 12	0
26	m1	1	Total 129	C 99	N 12	O 18	0
26	m1	1	Total 129	C 99	N 12	O 18	0
26	m1	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	n1	1	43	33	4	6	0
26	o1	1	43	33	4	6	0
26	p1	1	86	66	8	12	0
26	p1	1	86	66	8	12	0
26	q1	1	129	99	12	18	0
26	q1	1	129	99	12	18	0
26	q1	1	129	99	12	18	0
26	r1	1	86	66	8	12	0
26	r1	1	86	66	8	12	0
26	s1	1	129	99	12	18	0
26	s1	1	129	99	12	18	0
26	s1	1	129	99	12	18	0
26	t1	1	86	66	8	12	0
26	t1	1	86	66	8	12	0
26	u1	1	129	99	12	18	0
26	u1	1	129	99	12	18	0
26	u1	1	129	99	12	18	0
26	v1	1	86	66	8	12	0
26	v1	1	86	66	8	12	0
26	w1	1	129	99	12	18	0
26	w1	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	w1	1	Total 129	C 99	N 12	O 18	0
26	x1	1	Total 86	C 66	N 8	O 12	0
26	x1	1	Total 86	C 66	N 8	O 12	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	y1	1	Total 129	C 99	N 12	O 18	0
26	z1	1	Total 86	C 66	N 8	O 12	0
26	z1	1	Total 86	C 66	N 8	O 12	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	11	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	21	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	A2	1	Total 129	C 99	N 12	O 18	0
26	D2	1	Total 43	C 33	N 4	O 6	0
26	F2	1	Total 43	C 33	N 4	O 6	0
26	H2	1	Total 43	C 33	N 4	O 6	0
26	J2	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	L2	1	43	33	4	6	0
26	N2	1	43	33	4	6	0
26	O2	1	86	66	8	12	0
26	O2	1	86	66	8	12	0
26	P2	1	129	99	12	18	0
26	P2	1	129	99	12	18	0
26	P2	1	129	99	12	18	0
26	Q2	1	86	66	8	12	0
26	Q2	1	86	66	8	12	0
26	R2	1	129	99	12	18	0
26	R2	1	129	99	12	18	0
26	R2	1	129	99	12	18	0
26	S2	1	86	66	8	12	0
26	S2	1	86	66	8	12	0
26	T2	1	129	99	12	18	0
26	T2	1	129	99	12	18	0
26	T2	1	129	99	12	18	0
26	U2	1	86	66	8	12	0
26	U2	1	86	66	8	12	0
26	V2	1	129	99	12	18	0
26	V2	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	V2	1	Total 129	C 99	N 12	O 18	0
26	W2	1	Total 43	C 33	N 4	O 6	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Y2	1	Total 129	C 99	N 12	O 18	0
26	Z2	1	Total 86	C 66	N 8	O 12	0
26	Z2	1	Total 86	C 66	N 8	O 12	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	a2	1	Total 129	C 99	N 12	O 18	0
26	b2	1	Total 86	C 66	N 8	O 12	0
26	b2	1	Total 86	C 66	N 8	O 12	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	c2	1	Total 129	C 99	N 12	O 18	0
26	d2	1	Total 86	C 66	N 8	O 12	0
26	d2	1	Total 86	C 66	N 8	O 12	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	e2	1	Total 129	C 99	N 12	O 18	0
26	f2	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	f2	1	Total 86	C 66	N 8	O 12	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	g2	1	Total 129	C 99	N 12	O 18	0
26	h2	1	Total 86	C 66	N 8	O 12	0
26	h2	1	Total 86	C 66	N 8	O 12	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	i2	1	Total 129	C 99	N 12	O 18	0
26	j2	1	Total 86	C 66	N 8	O 12	0
26	j2	1	Total 86	C 66	N 8	O 12	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	k2	1	Total 129	C 99	N 12	O 18	0
26	l2	1	Total 86	C 66	N 8	O 12	0
26	l2	1	Total 86	C 66	N 8	O 12	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	m2	1	Total 129	C 99	N 12	O 18	0
26	e3	1	Total 43	C 33	N 4	O 6	0
26	A3	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A3	1	86	66	8	12	0
26	B3	1	129	99	12	18	0
26	B3	1	129	99	12	18	0
26	B3	1	129	99	12	18	0
26	C3	1	86	66	8	12	0
26	C3	1	86	66	8	12	0
26	D3	1	129	99	12	18	0
26	D3	1	129	99	12	18	0
26	D3	1	129	99	12	18	0
26	E3	1	86	66	8	12	0
26	E3	1	86	66	8	12	0
26	F3	1	129	99	12	18	0
26	F3	1	129	99	12	18	0
26	F3	1	129	99	12	18	0
26	G3	1	86	66	8	12	0
26	G3	1	86	66	8	12	0
26	H3	1	129	99	12	18	0
26	H3	1	129	99	12	18	0
26	H3	1	129	99	12	18	0
26	I3	1	86	66	8	12	0
26	I3	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	J3	1	Total 129	C 99	N 12	O 18	0
26	J3	1	Total 129	C 99	N 12	O 18	0
26	J3	1	Total 129	C 99	N 12	O 18	0
26	K3	1	Total 86	C 66	N 8	O 12	0
26	K3	1	Total 86	C 66	N 8	O 12	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	L3	1	Total 129	C 99	N 12	O 18	0
26	M3	1	Total 86	C 66	N 8	O 12	0
26	M3	1	Total 86	C 66	N 8	O 12	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	N3	1	Total 129	C 99	N 12	O 18	0
26	O3	1	Total 86	C 66	N 8	O 12	0
26	O3	1	Total 86	C 66	N 8	O 12	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	P3	1	Total 129	C 99	N 12	O 18	0
26	Q3	1	Total 86	C 66	N 8	O 12	0
26	Q3	1	Total 86	C 66	N 8	O 12	0
26	R3	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	R3	1	129	99	12	18	0
26	R3	1	129	99	12	18	0
26	S3	1	86	66	8	12	0
26	S3	1	86	66	8	12	0
26	T3	1	129	99	12	18	0
26	T3	1	129	99	12	18	0
26	T3	1	129	99	12	18	0
26	U3	1	86	66	8	12	0
26	U3	1	86	66	8	12	0
26	V3	1	129	99	12	18	0
26	V3	1	129	99	12	18	0
26	V3	1	129	99	12	18	0
26	W3	1	86	66	8	12	0
26	W3	1	86	66	8	12	0
26	X3	1	129	99	12	18	0
26	X3	1	129	99	12	18	0
26	X3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	Y3	1	129	99	12	18	0
26	A4	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A4	1	86	66	8	12	0
26	B4	1	129	99	12	18	0
26	B4	1	129	99	12	18	0
26	B4	1	129	99	12	18	0
26	C4	1	86	66	8	12	0
26	C4	1	86	66	8	12	0
26	D4	1	129	99	12	18	0
26	D4	1	129	99	12	18	0
26	D4	1	129	99	12	18	0
26	E4	1	86	66	8	12	0
26	E4	1	86	66	8	12	0
26	F4	1	129	99	12	18	0
26	F4	1	129	99	12	18	0
26	F4	1	129	99	12	18	0
26	G4	1	86	66	8	12	0
26	G4	1	86	66	8	12	0
26	H4	1	129	99	12	18	0
26	H4	1	129	99	12	18	0
26	H4	1	129	99	12	18	0
26	I4	1	86	66	8	12	0
26	I4	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	J4	1	Total 129	C 99	N 12	O 18	0
26	J4	1	Total 129	C 99	N 12	O 18	0
26	J4	1	Total 129	C 99	N 12	O 18	0
26	K4	1	Total 86	C 66	N 8	O 12	0
26	K4	1	Total 86	C 66	N 8	O 12	0
26	L4	1	Total 129	C 99	N 12	O 18	0
26	L4	1	Total 129	C 99	N 12	O 18	0
26	L4	1	Total 129	C 99	N 12	O 18	0
26	M4	1	Total 129	C 99	N 12	O 18	0
26	M4	1	Total 129	C 99	N 12	O 18	0
26	M4	1	Total 129	C 99	N 12	O 18	0
26	N4	1	Total 129	C 99	N 12	O 18	0
26	N4	1	Total 129	C 99	N 12	O 18	0
26	N4	1	Total 129	C 99	N 12	O 18	0
26	O4	1	Total 86	C 66	N 8	O 12	0
26	O4	1	Total 86	C 66	N 8	O 12	0
26	P4	1	Total 129	C 99	N 12	O 18	0
26	P4	1	Total 129	C 99	N 12	O 18	0
26	P4	1	Total 129	C 99	N 12	O 18	0
26	Q4	1	Total 86	C 66	N 8	O 12	0
26	Q4	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	R4	1	Total 129	C 99	N 12	O 18	0
26	R4	1	Total 129	C 99	N 12	O 18	0
26	R4	1	Total 129	C 99	N 12	O 18	0
26	S4	1	Total 86	C 66	N 8	O 12	0
26	S4	1	Total 86	C 66	N 8	O 12	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	T4	1	Total 129	C 99	N 12	O 18	0
26	U4	1	Total 86	C 66	N 8	O 12	0
26	U4	1	Total 86	C 66	N 8	O 12	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	V4	1	Total 129	C 99	N 12	O 18	0
26	W4	1	Total 86	C 66	N 8	O 12	0
26	W4	1	Total 86	C 66	N 8	O 12	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	X4	1	Total 129	C 99	N 12	O 18	0
26	Y4	1	Total 86	C 66	N 8	O 12	0
26	Y4	1	Total 86	C 66	N 8	O 12	0
26	Z4	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	Z4	1	Total 86	C 66	N 8	O 12	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	a4	1	Total 129	C 99	N 12	O 18	0
26	b4	1	Total 43	C 33	N 4	O 6	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	c4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	d4	1	Total 129	C 99	N 12	O 18	0
26	e4	1	Total 86	C 66	N 8	O 12	0
26	e4	1	Total 86	C 66	N 8	O 12	0
26	f4	1	Total 86	C 66	N 8	O 12	0
26	f4	1	Total 86	C 66	N 8	O 12	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	g4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0
26	h4	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	i4	1	Total 86	C 66	N 8	O 12	0
26	i4	1	Total 86	C 66	N 8	O 12	0
26	j4	1	Total 86	C 66	N 8	O 12	0
26	j4	1	Total 86	C 66	N 8	O 12	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	k4	1	Total 129	C 99	N 12	O 18	0
26	l4	1	Total 86	C 66	N 8	O 12	0
26	l4	1	Total 86	C 66	N 8	O 12	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	m4	1	Total 129	C 99	N 12	O 18	0
26	n4	1	Total 86	C 66	N 8	O 12	0
26	n4	1	Total 86	C 66	N 8	O 12	0
26	p4	1	Total 86	C 66	N 8	O 12	0
26	p4	1	Total 86	C 66	N 8	O 12	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	q4	1	Total 129	C 99	N 12	O 18	0
26	r4	1	Total 86	C 66	N 8	O 12	0
26	r4	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	s4	1	Total 129	C 99	N 12	O 18	0
26	s4	1	Total 129	C 99	N 12	O 18	0
26	s4	1	Total 129	C 99	N 12	O 18	0
26	t4	1	Total 86	C 66	N 8	O 12	0
26	t4	1	Total 86	C 66	N 8	O 12	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	u4	1	Total 129	C 99	N 12	O 18	0
26	v4	1	Total 86	C 66	N 8	O 12	0
26	v4	1	Total 86	C 66	N 8	O 12	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	w4	1	Total 172	C 132	N 16	O 24	0
26	x4	1	Total 86	C 66	N 8	O 12	0
26	x4	1	Total 86	C 66	N 8	O 12	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	y4	1	Total 129	C 99	N 12	O 18	0
26	z4	1	Total 86	C 66	N 8	O 12	0
26	z4	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	14	1	Total 129	C 99	N 12	O 18	0
26	14	1	Total 129	C 99	N 12	O 18	0
26	14	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	24	1	Total 129	C 99	N 12	O 18	0
26	A5	1	Total 86	C 66	N 8	O 12	0
26	A5	1	Total 86	C 66	N 8	O 12	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	B5	1	Total 129	C 99	N 12	O 18	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	C5	1	Total 172	C 132	N 16	O 24	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	F5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0
26	G5	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	H5	1	129	99	12	18	0
26	H5	1	129	99	12	18	0
26	H5	1	129	99	12	18	0
26	I5	1	129	99	12	18	0
26	I5	1	129	99	12	18	0
26	I5	1	129	99	12	18	0
26	J5	1	86	66	8	12	0
26	J5	1	86	66	8	12	0
26	K5	1	129	99	12	18	0
26	K5	1	129	99	12	18	0
26	K5	1	129	99	12	18	0
26	L5	1	129	99	12	18	0
26	L5	1	129	99	12	18	0
26	L5	1	129	99	12	18	0
26	A6	1	86	66	8	12	0
26	A6	1	86	66	8	12	0
26	D6	1	43	33	4	6	0
26	G6	1	43	33	4	6	0
26	H6	1	43	33	4	6	0
26	K6	1	43	33	4	6	0
26	L6	1	43	33	4	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	N6	1	43	33	4	6	0
26	O6	1	129	99	12	18	0
26	O6	1	129	99	12	18	0
26	O6	1	129	99	12	18	0
26	P6	1	86	66	8	12	0
26	P6	1	86	66	8	12	0
26	Q6	1	129	99	12	18	0
26	Q6	1	129	99	12	18	0
26	Q6	1	129	99	12	18	0
26	R6	1	86	66	8	12	0
26	R6	1	86	66	8	12	0
26	S6	1	129	99	12	18	0
26	S6	1	129	99	12	18	0
26	S6	1	129	99	12	18	0
26	T6	1	86	66	8	12	0
26	T6	1	86	66	8	12	0
26	U6	1	129	99	12	18	0
26	U6	1	129	99	12	18	0
26	U6	1	129	99	12	18	0
26	V6	1	86	66	8	12	0
26	V6	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	W6	1	Total 129	C 99	N 12	O 18	0
26	W6	1	Total 129	C 99	N 12	O 18	0
26	W6	1	Total 129	C 99	N 12	O 18	0
26	Y6	1	Total 86	C 66	N 8	O 12	0
26	Y6	1	Total 86	C 66	N 8	O 12	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	Z6	1	Total 129	C 99	N 12	O 18	0
26	a6	1	Total 86	C 66	N 8	O 12	0
26	a6	1	Total 86	C 66	N 8	O 12	0
26	b6	1	Total 86	C 66	N 8	O 12	0
26	b6	1	Total 86	C 66	N 8	O 12	0
26	c6	1	Total 86	C 66	N 8	O 12	0
26	c6	1	Total 86	C 66	N 8	O 12	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	d6	1	Total 172	C 132	N 16	O 24	0
26	e6	1	Total 129	C 99	N 12	O 18	0
26	e6	1	Total 129	C 99	N 12	O 18	0
26	e6	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	f6	1	Total 129	C 99	N 12	O 18	0
26	f6	1	Total 129	C 99	N 12	O 18	0
26	f6	1	Total 129	C 99	N 12	O 18	0
26	g6	1	Total 86	C 66	N 8	O 12	0
26	g6	1	Total 86	C 66	N 8	O 12	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	h6	1	Total 129	C 99	N 12	O 18	0
26	i6	1	Total 86	C 66	N 8	O 12	0
26	i6	1	Total 86	C 66	N 8	O 12	0
26	j6	1	Total 86	C 66	N 8	O 12	0
26	j6	1	Total 86	C 66	N 8	O 12	0
26	k6	1	Total 86	C 66	N 8	O 12	0
26	k6	1	Total 86	C 66	N 8	O 12	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	l6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	m6	1	Total 129	C 99	N 12	O 18	0
26	A7	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	A7	1	Total 129	C 99	N 12	O 18	0
26	A7	1	Total 129	C 99	N 12	O 18	0
26	D7	1	Total 43	C 33	N 4	O 6	0
26	F7	1	Total 43	C 33	N 4	O 6	0
26	H7	1	Total 43	C 33	N 4	O 6	0
26	J7	1	Total 43	C 33	N 4	O 6	0
26	L7	1	Total 43	C 33	N 4	O 6	0
26	N7	1	Total 43	C 33	N 4	O 6	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	O7	1	Total 129	C 99	N 12	O 18	0
26	P7	1	Total 86	C 66	N 8	O 12	0
26	P7	1	Total 86	C 66	N 8	O 12	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	Q7	1	Total 129	C 99	N 12	O 18	0
26	R7	1	Total 86	C 66	N 8	O 12	0
26	R7	1	Total 86	C 66	N 8	O 12	0
26	S7	1	Total 129	C 99	N 12	O 18	0
26	S7	1	Total 129	C 99	N 12	O 18	0
26	S7	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	T7	1	86	66	8	12	0
26	T7	1	86	66	8	12	0
26	U7	1	129	99	12	18	0
26	U7	1	129	99	12	18	0
26	U7	1	129	99	12	18	0
26	V7	1	86	66	8	12	0
26	V7	1	86	66	8	12	0
26	W7	1	129	99	12	18	0
26	W7	1	129	99	12	18	0
26	W7	1	129	99	12	18	0
26	Y7	1	86	66	8	12	0
26	Y7	1	86	66	8	12	0
26	Z7	1	129	99	12	18	0
26	Z7	1	129	99	12	18	0
26	Z7	1	129	99	12	18	0
26	a7	1	86	66	8	12	0
26	a7	1	86	66	8	12	0
26	b7	1	129	99	12	18	0
26	b7	1	129	99	12	18	0
26	b7	1	129	99	12	18	0
26	c7	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	c7	1	Total 86	C 66	N 8	O 12	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	d7	1	Total 129	C 99	N 12	O 18	0
26	e7	1	Total 86	C 66	N 8	O 12	0
26	e7	1	Total 86	C 66	N 8	O 12	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	f7	1	Total 129	C 99	N 12	O 18	0
26	g7	1	Total 86	C 66	N 8	O 12	0
26	g7	1	Total 86	C 66	N 8	O 12	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	h7	1	Total 129	C 99	N 12	O 18	0
26	i7	1	Total 86	C 66	N 8	O 12	0
26	i7	1	Total 86	C 66	N 8	O 12	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	j7	1	Total 129	C 99	N 12	O 18	0
26	k7	1	Total 86	C 66	N 8	O 12	0
26	k7	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	l7	1	Total 129	C 99	N 12	O 18	0
26	l7	1	Total 129	C 99	N 12	O 18	0
26	l7	1	Total 129	C 99	N 12	O 18	0
26	m7	1	Total 86	C 66	N 8	O 12	0
26	m7	1	Total 86	C 66	N 8	O 12	0
26	A8	1	Total 86	C 66	N 8	O 12	0
26	A8	1	Total 86	C 66	N 8	O 12	0
26	B8	1	Total 43	C 33	N 4	O 6	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	C8	1	Total 129	C 99	N 12	O 18	0
26	D8	1	Total 86	C 66	N 8	O 12	0
26	D8	1	Total 86	C 66	N 8	O 12	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	E8	1	Total 129	C 99	N 12	O 18	0
26	F8	1	Total 86	C 66	N 8	O 12	0
26	F8	1	Total 86	C 66	N 8	O 12	0
26	G8	1	Total 129	C 99	N 12	O 18	0
26	G8	1	Total 129	C 99	N 12	O 18	0
26	G8	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	H8	1	86	66	8	12	0
26	H8	1	86	66	8	12	0
26	I8	1	129	99	12	18	0
26	I8	1	129	99	12	18	0
26	I8	1	129	99	12	18	0
26	J8	1	86	66	8	12	0
26	J8	1	86	66	8	12	0
26	K8	1	129	99	12	18	0
26	K8	1	129	99	12	18	0
26	K8	1	129	99	12	18	0
26	L8	1	86	66	8	12	0
26	L8	1	86	66	8	12	0
26	M8	1	129	99	12	18	0
26	M8	1	129	99	12	18	0
26	M8	1	129	99	12	18	0
26	N8	1	86	66	8	12	0
26	N8	1	86	66	8	12	0
26	O8	1	129	99	12	18	0
26	O8	1	129	99	12	18	0
26	O8	1	129	99	12	18	0
26	P8	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	P8	1	Total 86	C 66	N 8	O 12	0
26	Q8	1	Total 129	C 99	N 12	O 18	0
26	Q8	1	Total 129	C 99	N 12	O 18	0
26	Q8	1	Total 129	C 99	N 12	O 18	0
26	R8	1	Total 86	C 66	N 8	O 12	0
26	R8	1	Total 86	C 66	N 8	O 12	0
26	S8	1	Total 129	C 99	N 12	O 18	0
26	S8	1	Total 129	C 99	N 12	O 18	0
26	S8	1	Total 129	C 99	N 12	O 18	0
26	T8	1	Total 86	C 66	N 8	O 12	0
26	T8	1	Total 86	C 66	N 8	O 12	0
26	U8	1	Total 129	C 99	N 12	O 18	0
26	U8	1	Total 129	C 99	N 12	O 18	0
26	U8	1	Total 129	C 99	N 12	O 18	0
26	V8	1	Total 86	C 66	N 8	O 12	0
26	V8	1	Total 86	C 66	N 8	O 12	0
26	W8	1	Total 129	C 99	N 12	O 18	0
26	W8	1	Total 129	C 99	N 12	O 18	0
26	W8	1	Total 129	C 99	N 12	O 18	0
26	X8	1	Total 86	C 66	N 8	O 12	0
26	X8	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Y8	1	Total 129	C 99	N 12	O 18	0
26	Z8	1	Total 86	C 66	N 8	O 12	0
26	Z8	1	Total 86	C 66	N 8	O 12	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	a8	1	Total 172	C 132	N 16	O 24	0
26	c8	1	Total 86	C 66	N 8	O 12	0
26	c8	1	Total 86	C 66	N 8	O 12	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	d8	1	Total 129	C 99	N 12	O 18	0
26	e8	1	Total 86	C 66	N 8	O 12	0
26	e8	1	Total 86	C 66	N 8	O 12	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	f8	1	Total 129	C 99	N 12	O 18	0
26	g8	1	Total 86	C 66	N 8	O 12	0
26	g8	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	h8	1	Total 129	C 99	N 12	O 18	0
26	h8	1	Total 129	C 99	N 12	O 18	0
26	h8	1	Total 129	C 99	N 12	O 18	0
26	i8	1	Total 86	C 66	N 8	O 12	0
26	i8	1	Total 86	C 66	N 8	O 12	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	j8	1	Total 129	C 99	N 12	O 18	0
26	k8	1	Total 86	C 66	N 8	O 12	0
26	k8	1	Total 86	C 66	N 8	O 12	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	l8	1	Total 129	C 99	N 12	O 18	0
26	m8	1	Total 86	C 66	N 8	O 12	0
26	m8	1	Total 86	C 66	N 8	O 12	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	A9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0
26	B9	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	C9	1	86	66	8	12	0
26	C9	1	86	66	8	12	0
26	D9	1	129	99	12	18	0
26	D9	1	129	99	12	18	0
26	D9	1	129	99	12	18	0
26	E9	1	86	66	8	12	0
26	E9	1	86	66	8	12	0
26	F9	1	129	99	12	18	0
26	F9	1	129	99	12	18	0
26	F9	1	129	99	12	18	0
26	G9	1	86	66	8	12	0
26	G9	1	86	66	8	12	0
26	H9	1	129	99	12	18	0
26	H9	1	129	99	12	18	0
26	H9	1	129	99	12	18	0
26	I9	1	86	66	8	12	0
26	I9	1	86	66	8	12	0
26	J9	1	129	99	12	18	0
26	J9	1	129	99	12	18	0
26	J9	1	129	99	12	18	0
26	K9	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	K9	1	Total 86	C 66	N 8	O 12	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	L9	1	Total 129	C 99	N 12	O 18	0
26	M9	1	Total 86	C 66	N 8	O 12	0
26	M9	1	Total 86	C 66	N 8	O 12	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	N9	1	Total 129	C 99	N 12	O 18	0
26	O9	1	Total 86	C 66	N 8	O 12	0
26	O9	1	Total 86	C 66	N 8	O 12	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	P9	1	Total 129	C 99	N 12	O 18	0
26	Q9	1	Total 86	C 66	N 8	O 12	0
26	Q9	1	Total 86	C 66	N 8	O 12	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	R9	1	Total 129	C 99	N 12	O 18	0
26	S9	1	Total 86	C 66	N 8	O 12	0
26	S9	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	T9	1	Total 129	C 99	N 12	O 18	0
26	T9	1	Total 129	C 99	N 12	O 18	0
26	T9	1	Total 129	C 99	N 12	O 18	0
26	U9	1	Total 86	C 66	N 8	O 12	0
26	U9	1	Total 86	C 66	N 8	O 12	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	V9	1	Total 129	C 99	N 12	O 18	0
26	W9	1	Total 86	C 66	N 8	O 12	0
26	W9	1	Total 86	C 66	N 8	O 12	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	X9	1	Total 129	C 99	N 12	O 18	0
26	Y9	1	Total 86	C 66	N 8	O 12	0
26	Y9	1	Total 86	C 66	N 8	O 12	0
26	AA	1	Total 86	C 66	N 8	O 12	0
26	AA	1	Total 86	C 66	N 8	O 12	0
26	BA	1	Total 43	C 33	N 4	O 6	0
26	CA	1	Total 129	C 99	N 12	O 18	0
26	CA	1	Total 129	C 99	N 12	O 18	0
26	CA	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	DA	1	86	66	8	12	0
26	DA	1	86	66	8	12	0
26	EA	1	129	99	12	18	0
26	EA	1	129	99	12	18	0
26	EA	1	129	99	12	18	0
26	FA	1	86	66	8	12	0
26	FA	1	86	66	8	12	0
26	GA	1	129	99	12	18	0
26	GA	1	129	99	12	18	0
26	GA	1	129	99	12	18	0
26	HA	1	86	66	8	12	0
26	HA	1	86	66	8	12	0
26	IA	1	129	99	12	18	0
26	IA	1	129	99	12	18	0
26	IA	1	129	99	12	18	0
26	JA	1	86	66	8	12	0
26	JA	1	86	66	8	12	0
26	KA	1	129	99	12	18	0
26	KA	1	129	99	12	18	0
26	KA	1	129	99	12	18	0
26	LA	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	LA	1	86	66	8	12	0
26	MA	1	129	99	12	18	0
26	MA	1	129	99	12	18	0
26	MA	1	129	99	12	18	0
26	NA	1	86	66	8	12	0
26	NA	1	86	66	8	12	0
26	OA	1	129	99	12	18	0
26	OA	1	129	99	12	18	0
26	OA	1	129	99	12	18	0
26	PA	1	86	66	8	12	0
26	PA	1	86	66	8	12	0
26	QA	1	129	99	12	18	0
26	QA	1	129	99	12	18	0
26	QA	1	129	99	12	18	0
26	RA	1	86	66	8	12	0
26	RA	1	86	66	8	12	0
26	SA	1	129	99	12	18	0
26	SA	1	129	99	12	18	0
26	SA	1	129	99	12	18	0
26	TA	1	86	66	8	12	0
26	TA	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	UA	1	Total 129	C 99	N 12	O 18	0
26	UA	1	Total 129	C 99	N 12	O 18	0
26	UA	1	Total 129	C 99	N 12	O 18	0
26	VA	1	Total 86	C 66	N 8	O 12	0
26	VA	1	Total 86	C 66	N 8	O 12	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	WA	1	Total 129	C 99	N 12	O 18	0
26	XA	1	Total 86	C 66	N 8	O 12	0
26	XA	1	Total 86	C 66	N 8	O 12	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	YA	1	Total 129	C 99	N 12	O 18	0
26	ZA	1	Total 86	C 66	N 8	O 12	0
26	ZA	1	Total 86	C 66	N 8	O 12	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	aA	1	Total 172	C 132	N 16	O 24	0
26	cA	1	Total 129	C 99	N 12	O 18	0
26	cA	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	cA	1	Total 129	C 99	N 12	O 18	0
26	dA	1	Total 43	C 33	N 4	O 6	0
26	eA	1	Total 86	C 66	N 8	O 12	0
26	eA	1	Total 86	C 66	N 8	O 12	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	fA	1	Total 129	C 99	N 12	O 18	0
26	gA	1	Total 86	C 66	N 8	O 12	0
26	gA	1	Total 86	C 66	N 8	O 12	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	hA	1	Total 129	C 99	N 12	O 18	0
26	iA	1	Total 86	C 66	N 8	O 12	0
26	iA	1	Total 86	C 66	N 8	O 12	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	jA	1	Total 129	C 99	N 12	O 18	0
26	kA	1	Total 86	C 66	N 8	O 12	0
26	kA	1	Total 86	C 66	N 8	O 12	0
26	lA	1	Total 129	C 99	N 12	O 18	0
26	lA	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	lA	1	Total 129	C 99	N 12	O 18	0
26	mA	1	Total 86	C 66	N 8	O 12	0
26	mA	1	Total 86	C 66	N 8	O 12	0
26	AB	1	Total 86	C 66	N 8	O 12	0
26	AB	1	Total 86	C 66	N 8	O 12	0
26	DB	1	Total 43	C 33	N 4	O 6	0
26	GB	1	Total 43	C 33	N 4	O 6	0
26	HB	1	Total 43	C 33	N 4	O 6	0
26	KB	1	Total 43	C 33	N 4	O 6	0
26	LB	1	Total 43	C 33	N 4	O 6	0
26	NB	1	Total 43	C 33	N 4	O 6	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	OB	1	Total 129	C 99	N 12	O 18	0
26	PB	1	Total 86	C 66	N 8	O 12	0
26	PB	1	Total 86	C 66	N 8	O 12	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	QB	1	Total 129	C 99	N 12	O 18	0
26	RB	1	Total 86	C 66	N 8	O 12	0
26	RB	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SB	1	Total 129	C 99	N 12	O 18	0
26	SB	1	Total 129	C 99	N 12	O 18	0
26	SB	1	Total 129	C 99	N 12	O 18	0
26	TB	1	Total 86	C 66	N 8	O 12	0
26	TB	1	Total 86	C 66	N 8	O 12	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	UB	1	Total 129	C 99	N 12	O 18	0
26	VB	1	Total 86	C 66	N 8	O 12	0
26	VB	1	Total 86	C 66	N 8	O 12	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	WB	1	Total 129	C 99	N 12	O 18	0
26	YB	1	Total 86	C 66	N 8	O 12	0
26	YB	1	Total 86	C 66	N 8	O 12	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	ZB	1	Total 129	C 99	N 12	O 18	0
26	aB	1	Total 86	C 66	N 8	O 12	0
26	aB	1	Total 86	C 66	N 8	O 12	0
26	bB	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	bB	1	86	66	8	12	0
26	cB	1	86	66	8	12	0
26	cB	1	86	66	8	12	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	dB	1	172	132	16	24	0
26	eB	1	129	99	12	18	0
26	eB	1	129	99	12	18	0
26	eB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	fB	1	129	99	12	18	0
26	gB	1	86	66	8	12	0
26	gB	1	86	66	8	12	0
26	hB	1	129	99	12	18	0
26	hB	1	129	99	12	18	0
26	hB	1	129	99	12	18	0
26	iB	1	86	66	8	12	0
26	iB	1	86	66	8	12	0
26	jB	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jB	1	Total 86	C 66	N 8	O 12	0
26	kB	1	Total 86	C 66	N 8	O 12	0
26	kB	1	Total 86	C 66	N 8	O 12	0
26	lB	1	Total 129	C 99	N 12	O 18	0
26	lB	1	Total 129	C 99	N 12	O 18	0
26	lB	1	Total 129	C 99	N 12	O 18	0
26	mB	1	Total 129	C 99	N 12	O 18	0
26	mB	1	Total 129	C 99	N 12	O 18	0
26	mB	1	Total 129	C 99	N 12	O 18	0
26	AC	1	Total 129	C 99	N 12	O 18	0
26	AC	1	Total 129	C 99	N 12	O 18	0
26	AC	1	Total 129	C 99	N 12	O 18	0
26	BC	1	Total 129	C 99	N 12	O 18	0
26	BC	1	Total 129	C 99	N 12	O 18	0
26	BC	1	Total 129	C 99	N 12	O 18	0
26	CC	1	Total 129	C 99	N 12	O 18	0
26	CC	1	Total 129	C 99	N 12	O 18	0
26	CC	1	Total 129	C 99	N 12	O 18	0
26	FC	1	Total 129	C 99	N 12	O 18	0
26	FC	1	Total 129	C 99	N 12	O 18	0
26	FC	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	GC	1	Total 129	C 99	N 12	O 18	0
26	GC	1	Total 129	C 99	N 12	O 18	0
26	GC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	HC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	IC	1	Total 129	C 99	N 12	O 18	0
26	JC	1	Total 86	C 66	N 8	O 12	0
26	JC	1	Total 86	C 66	N 8	O 12	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	KC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	LC	1	Total 129	C 99	N 12	O 18	0
26	eD	1	Total 43	C 33	N 4	O 6	0
26	AD	1	Total 86	C 66	N 8	O 12	0
26	AD	1	Total 86	C 66	N 8	O 12	0
26	BD	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	BD	1	Total 129	C 99	N 12	O 18	0
26	BD	1	Total 129	C 99	N 12	O 18	0
26	CD	1	Total 86	C 66	N 8	O 12	0
26	CD	1	Total 86	C 66	N 8	O 12	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	DD	1	Total 129	C 99	N 12	O 18	0
26	ED	1	Total 86	C 66	N 8	O 12	0
26	ED	1	Total 86	C 66	N 8	O 12	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	FD	1	Total 129	C 99	N 12	O 18	0
26	GD	1	Total 86	C 66	N 8	O 12	0
26	GD	1	Total 86	C 66	N 8	O 12	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	HD	1	Total 129	C 99	N 12	O 18	0
26	ID	1	Total 86	C 66	N 8	O 12	0
26	ID	1	Total 86	C 66	N 8	O 12	0
26	JD	1	Total 129	C 99	N 12	O 18	0
26	JD	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	JD	1	Total 129	C 99	N 12	O 18	0
26	KD	1	Total 86	C 66	N 8	O 12	0
26	KD	1	Total 86	C 66	N 8	O 12	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	LD	1	Total 129	C 99	N 12	O 18	0
26	MD	1	Total 86	C 66	N 8	O 12	0
26	MD	1	Total 86	C 66	N 8	O 12	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	ND	1	Total 129	C 99	N 12	O 18	0
26	OD	1	Total 86	C 66	N 8	O 12	0
26	OD	1	Total 86	C 66	N 8	O 12	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	PD	1	Total 129	C 99	N 12	O 18	0
26	QD	1	Total 86	C 66	N 8	O 12	0
26	QD	1	Total 86	C 66	N 8	O 12	0
26	RD	1	Total 129	C 99	N 12	O 18	0
26	RD	1	Total 129	C 99	N 12	O 18	0
26	RD	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SD	1	86	66	8	12	0
26	SD	1	86	66	8	12	0
26	TD	1	129	99	12	18	0
26	TD	1	129	99	12	18	0
26	TD	1	129	99	12	18	0
26	UD	1	86	66	8	12	0
26	UD	1	86	66	8	12	0
26	VD	1	129	99	12	18	0
26	VD	1	129	99	12	18	0
26	VD	1	129	99	12	18	0
26	WD	1	86	66	8	12	0
26	WD	1	86	66	8	12	0
26	XD	1	129	99	12	18	0
26	XD	1	129	99	12	18	0
26	XD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	YD	1	129	99	12	18	0
26	AE	1	86	66	8	12	0
26	AE	1	86	66	8	12	0
26	BE	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	BE	1	86	66	8	12	0
26	CE	1	129	99	12	18	0
26	CE	1	129	99	12	18	0
26	CE	1	129	99	12	18	0
26	DE	1	129	99	12	18	0
26	DE	1	129	99	12	18	0
26	DE	1	129	99	12	18	0
26	EE	1	86	66	8	12	0
26	EE	1	86	66	8	12	0
26	FE	1	86	66	8	12	0
26	FE	1	86	66	8	12	0
26	GE	1	129	99	12	18	0
26	GE	1	129	99	12	18	0
26	GE	1	129	99	12	18	0
26	HE	1	86	66	8	12	0
26	HE	1	86	66	8	12	0
26	IE	1	129	99	12	18	0
26	IE	1	129	99	12	18	0
26	IE	1	129	99	12	18	0
26	JE	1	86	66	8	12	0
26	JE	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	KE	1	Total 129	C 99	N 12	O 18	0
26	KE	1	Total 129	C 99	N 12	O 18	0
26	KE	1	Total 129	C 99	N 12	O 18	0
26	LE	1	Total 86	C 66	N 8	O 12	0
26	LE	1	Total 86	C 66	N 8	O 12	0
26	ME	1	Total 129	C 99	N 12	O 18	0
26	ME	1	Total 129	C 99	N 12	O 18	0
26	ME	1	Total 129	C 99	N 12	O 18	0
26	NE	1	Total 86	C 66	N 8	O 12	0
26	NE	1	Total 86	C 66	N 8	O 12	0
26	OE	1	Total 129	C 99	N 12	O 18	0
26	OE	1	Total 129	C 99	N 12	O 18	0
26	OE	1	Total 129	C 99	N 12	O 18	0
26	PE	1	Total 86	C 66	N 8	O 12	0
26	PE	1	Total 86	C 66	N 8	O 12	0
26	QE	1	Total 129	C 99	N 12	O 18	0
26	QE	1	Total 129	C 99	N 12	O 18	0
26	QE	1	Total 129	C 99	N 12	O 18	0
26	RE	1	Total 86	C 66	N 8	O 12	0
26	RE	1	Total 86	C 66	N 8	O 12	0
26	SE	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	SE	1	Total 129	C 99	N 12	O 18	0
26	SE	1	Total 129	C 99	N 12	O 18	0
26	TE	1	Total 86	C 66	N 8	O 12	0
26	TE	1	Total 86	C 66	N 8	O 12	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	UE	1	Total 129	C 99	N 12	O 18	0
26	VE	1	Total 86	C 66	N 8	O 12	0
26	VE	1	Total 86	C 66	N 8	O 12	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	WE	1	Total 129	C 99	N 12	O 18	0
26	XE	1	Total 86	C 66	N 8	O 12	0
26	XE	1	Total 86	C 66	N 8	O 12	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	YE	1	Total 129	C 99	N 12	O 18	0
26	ZE	1	Total 86	C 66	N 8	O 12	0
26	ZE	1	Total 86	C 66	N 8	O 12	0
26	aE	1	Total 129	C 99	N 12	O 18	0
26	aE	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	aE	1	Total 129	C 99	N 12	O 18	0
26	bE	1	Total 86	C 66	N 8	O 12	0
26	bE	1	Total 86	C 66	N 8	O 12	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	cE	1	Total 129	C 99	N 12	O 18	0
26	dE	1	Total 86	C 66	N 8	O 12	0
26	dE	1	Total 86	C 66	N 8	O 12	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	eE	1	Total 129	C 99	N 12	O 18	0
26	fE	1	Total 86	C 66	N 8	O 12	0
26	fE	1	Total 86	C 66	N 8	O 12	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	gE	1	Total 129	C 99	N 12	O 18	0
26	hE	1	Total 86	C 66	N 8	O 12	0
26	hE	1	Total 86	C 66	N 8	O 12	0
26	iE	1	Total 129	C 99	N 12	O 18	0
26	iE	1	Total 129	C 99	N 12	O 18	0
26	iE	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jE	1	86	66	8	12	0
26	jE	1	86	66	8	12	0
26	kE	1	129	99	12	18	0
26	kE	1	129	99	12	18	0
26	kE	1	129	99	12	18	0
26	lE	1	86	66	8	12	0
26	lE	1	86	66	8	12	0
26	mE	1	129	99	12	18	0
26	mE	1	129	99	12	18	0
26	mE	1	129	99	12	18	0
26	nE	1	86	66	8	12	0
26	nE	1	86	66	8	12	0
26	oE	1	129	99	12	18	0
26	oE	1	129	99	12	18	0
26	oE	1	129	99	12	18	0
26	pE	1	86	66	8	12	0
26	pE	1	86	66	8	12	0
26	qE	1	129	99	12	18	0
26	qE	1	129	99	12	18	0
26	qE	1	129	99	12	18	0
26	rE	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	rE	1	86	66	8	12	0
26	sE	1	129	99	12	18	0
26	sE	1	129	99	12	18	0
26	sE	1	129	99	12	18	0
26	tE	1	86	66	8	12	0
26	tE	1	86	66	8	12	0
26	uE	1	129	99	12	18	0
26	uE	1	129	99	12	18	0
26	uE	1	129	99	12	18	0
26	vE	1	86	66	8	12	0
26	vE	1	86	66	8	12	0
26	wE	1	129	99	12	18	0
26	wE	1	129	99	12	18	0
26	wE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	xE	1	129	99	12	18	0
26	yE	1	43	33	4	6	0
26	zE	1	43	33	4	6	0
26	AF	1	129	99	12	18	0
26	AF	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	AF	1	Total 129	C 99	N 12	O 18	0
26	DF	1	Total 43	C 33	N 4	O 6	0
26	FF	1	Total 43	C 33	N 4	O 6	0
26	HF	1	Total 43	C 33	N 4	O 6	0
26	JF	1	Total 43	C 33	N 4	O 6	0
26	LF	1	Total 43	C 33	N 4	O 6	0
26	NF	1	Total 43	C 33	N 4	O 6	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	OF	1	Total 129	C 99	N 12	O 18	0
26	PF	1	Total 86	C 66	N 8	O 12	0
26	PF	1	Total 86	C 66	N 8	O 12	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	QF	1	Total 129	C 99	N 12	O 18	0
26	RF	1	Total 86	C 66	N 8	O 12	0
26	RF	1	Total 86	C 66	N 8	O 12	0
26	SF	1	Total 86	C 66	N 8	O 12	0
26	SF	1	Total 86	C 66	N 8	O 12	0
26	TF	1	Total 86	C 66	N 8	O 12	0
26	TF	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	UF	1	Total 129	C 99	N 12	O 18	0
26	UF	1	Total 129	C 99	N 12	O 18	0
26	UF	1	Total 129	C 99	N 12	O 18	0
26	VF	1	Total 129	C 99	N 12	O 18	0
26	VF	1	Total 129	C 99	N 12	O 18	0
26	VF	1	Total 129	C 99	N 12	O 18	0
26	WF	1	Total 129	C 99	N 12	O 18	0
26	WF	1	Total 129	C 99	N 12	O 18	0
26	WF	1	Total 129	C 99	N 12	O 18	0
26	YF	1	Total 86	C 66	N 8	O 12	0
26	YF	1	Total 86	C 66	N 8	O 12	0
26	ZF	1	Total 129	C 99	N 12	O 18	0
26	ZF	1	Total 129	C 99	N 12	O 18	0
26	ZF	1	Total 129	C 99	N 12	O 18	0
26	aF	1	Total 86	C 66	N 8	O 12	0
26	aF	1	Total 86	C 66	N 8	O 12	0
26	bF	1	Total 129	C 99	N 12	O 18	0
26	bF	1	Total 129	C 99	N 12	O 18	0
26	bF	1	Total 129	C 99	N 12	O 18	0
26	cF	1	Total 86	C 66	N 8	O 12	0
26	cF	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	dF	1	Total 129	C 99	N 12	O 18	0
26	dF	1	Total 129	C 99	N 12	O 18	0
26	dF	1	Total 129	C 99	N 12	O 18	0
26	eF	1	Total 86	C 66	N 8	O 12	0
26	eF	1	Total 86	C 66	N 8	O 12	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	fF	1	Total 129	C 99	N 12	O 18	0
26	gF	1	Total 86	C 66	N 8	O 12	0
26	gF	1	Total 86	C 66	N 8	O 12	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	hF	1	Total 129	C 99	N 12	O 18	0
26	iF	1	Total 86	C 66	N 8	O 12	0
26	iF	1	Total 86	C 66	N 8	O 12	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	jF	1	Total 129	C 99	N 12	O 18	0
26	kF	1	Total 86	C 66	N 8	O 12	0
26	kF	1	Total 86	C 66	N 8	O 12	0
26	lF	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	lF	1	Total 129	C 99	N 12	O 18	0
26	lF	1	Total 129	C 99	N 12	O 18	0
26	mF	1	Total 86	C 66	N 8	O 12	0
26	mF	1	Total 86	C 66	N 8	O 12	0
26	AG	1	Total 86	C 66	N 8	O 12	0
26	AG	1	Total 86	C 66	N 8	O 12	0
26	BG	1	Total 86	C 66	N 8	O 12	0
26	BG	1	Total 86	C 66	N 8	O 12	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	CG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	DG	1	Total 129	C 99	N 12	O 18	0
26	EG	1	Total 86	C 66	N 8	O 12	0
26	EG	1	Total 86	C 66	N 8	O 12	0
26	FG	1	Total 86	C 66	N 8	O 12	0
26	FG	1	Total 86	C 66	N 8	O 12	0
26	GG	1	Total 129	C 99	N 12	O 18	0
26	GG	1	Total 129	C 99	N 12	O 18	0
26	GG	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	HG	1	86	66	8	12	0
26	HG	1	86	66	8	12	0
26	IG	1	129	99	12	18	0
26	IG	1	129	99	12	18	0
26	IG	1	129	99	12	18	0
26	JG	1	86	66	8	12	0
26	JG	1	86	66	8	12	0
26	KG	1	129	99	12	18	0
26	KG	1	129	99	12	18	0
26	KG	1	129	99	12	18	0
26	LG	1	86	66	8	12	0
26	LG	1	86	66	8	12	0
26	MG	1	129	99	12	18	0
26	MG	1	129	99	12	18	0
26	MG	1	129	99	12	18	0
26	NG	1	86	66	8	12	0
26	NG	1	86	66	8	12	0
26	OG	1	129	99	12	18	0
26	OG	1	129	99	12	18	0
26	OG	1	129	99	12	18	0
26	PG	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	PG	1	86	66	8	12	0
26	QG	1	129	99	12	18	0
26	QG	1	129	99	12	18	0
26	QG	1	129	99	12	18	0
26	RG	1	86	66	8	12	0
26	RG	1	86	66	8	12	0
26	SG	1	129	99	12	18	0
26	SG	1	129	99	12	18	0
26	SG	1	129	99	12	18	0
26	TG	1	86	66	8	12	0
26	TG	1	86	66	8	12	0
26	UG	1	86	66	8	12	0
26	UG	1	86	66	8	12	0
26	VG	1	86	66	8	12	0
26	VG	1	86	66	8	12	0
26	WG	1	129	99	12	18	0
26	WG	1	129	99	12	18	0
26	WG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0
26	XG	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	YG	1	Total 129	C 99	N 12	O 18	0
26	YG	1	Total 129	C 99	N 12	O 18	0
26	YG	1	Total 129	C 99	N 12	O 18	0
26	ZG	1	Total 86	C 66	N 8	O 12	0
26	ZG	1	Total 86	C 66	N 8	O 12	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	aG	1	Total 129	C 99	N 12	O 18	0
26	bG	1	Total 86	C 66	N 8	O 12	0
26	bG	1	Total 86	C 66	N 8	O 12	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	cG	1	Total 129	C 99	N 12	O 18	0
26	dG	1	Total 86	C 66	N 8	O 12	0
26	dG	1	Total 86	C 66	N 8	O 12	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	eG	1	Total 129	C 99	N 12	O 18	0
26	fG	1	Total 86	C 66	N 8	O 12	0
26	fG	1	Total 86	C 66	N 8	O 12	0
26	gG	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	gG	1	129	99	12	18	0
26	gG	1	129	99	12	18	0
26	hG	1	86	66	8	12	0
26	hG	1	86	66	8	12	0
26	iG	1	129	99	12	18	0
26	iG	1	129	99	12	18	0
26	iG	1	129	99	12	18	0
26	jG	1	86	66	8	12	0
26	jG	1	86	66	8	12	0
26	kG	1	129	99	12	18	0
26	kG	1	129	99	12	18	0
26	kG	1	129	99	12	18	0
26	lG	1	86	66	8	12	0
26	lG	1	86	66	8	12	0
26	mG	1	129	99	12	18	0
26	mG	1	129	99	12	18	0
26	mG	1	129	99	12	18	0
26	nG	1	86	66	8	12	0
26	nG	1	86	66	8	12	0
26	oG	1	129	99	12	18	0
26	oG	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	oG	1	Total 129	C 99	N 12	O 18	0
26	pG	1	Total 86	C 66	N 8	O 12	0
26	pG	1	Total 86	C 66	N 8	O 12	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	qG	1	Total 129	C 99	N 12	O 18	0
26	rG	1	Total 86	C 66	N 8	O 12	0
26	rG	1	Total 86	C 66	N 8	O 12	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	sG	1	Total 129	C 99	N 12	O 18	0
26	tG	1	Total 86	C 66	N 8	O 12	0
26	tG	1	Total 86	C 66	N 8	O 12	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	uG	1	Total 129	C 99	N 12	O 18	0
26	vG	1	Total 86	C 66	N 8	O 12	0
26	vG	1	Total 86	C 66	N 8	O 12	0
26	wG	1	Total 129	C 99	N 12	O 18	0
26	wG	1	Total 129	C 99	N 12	O 18	0
26	wG	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	xG	1	Total 129	C 99	N 12	O 18	0
26	xG	1	Total 129	C 99	N 12	O 18	0
26	xG	1	Total 129	C 99	N 12	O 18	0
26	yG	1	Total 43	C 33	N 4	O 6	0
26	zG	1	Total 43	C 33	N 4	O 6	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	AI	1	Total 129	C 99	N 12	O 18	0
26	DI	1	Total 43	C 33	N 4	O 6	0
26	FI	1	Total 43	C 33	N 4	O 6	0
26	HI	1	Total 43	C 33	N 4	O 6	0
26	JI	1	Total 43	C 33	N 4	O 6	0
26	LI	1	Total 43	C 33	N 4	O 6	0
26	NI	1	Total 43	C 33	N 4	O 6	0
26	OI	1	Total 86	C 66	N 8	O 12	0
26	OI	1	Total 86	C 66	N 8	O 12	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	PI	1	Total 129	C 99	N 12	O 18	0
26	QI	1	Total 86	C 66	N 8	O 12	0
26	QI	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	RI	1	Total 129	C 99	N 12	O 18	0
26	RI	1	Total 129	C 99	N 12	O 18	0
26	RI	1	Total 129	C 99	N 12	O 18	0
26	SI	1	Total 86	C 66	N 8	O 12	0
26	SI	1	Total 86	C 66	N 8	O 12	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	TI	1	Total 129	C 99	N 12	O 18	0
26	UI	1	Total 86	C 66	N 8	O 12	0
26	UI	1	Total 86	C 66	N 8	O 12	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	VI	1	Total 129	C 99	N 12	O 18	0
26	WI	1	Total 43	C 33	N 4	O 6	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	YI	1	Total 129	C 99	N 12	O 18	0
26	ZI	1	Total 86	C 66	N 8	O 12	0
26	ZI	1	Total 86	C 66	N 8	O 12	0
26	aI	1	Total 129	C 99	N 12	O 18	0
26	aI	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	aI	1	Total 129	C 99	N 12	O 18	0
26	bI	1	Total 86	C 66	N 8	O 12	0
26	bI	1	Total 86	C 66	N 8	O 12	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	cI	1	Total 129	C 99	N 12	O 18	0
26	dI	1	Total 86	C 66	N 8	O 12	0
26	dI	1	Total 86	C 66	N 8	O 12	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	eI	1	Total 129	C 99	N 12	O 18	0
26	fI	1	Total 86	C 66	N 8	O 12	0
26	fI	1	Total 86	C 66	N 8	O 12	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	gI	1	Total 129	C 99	N 12	O 18	0
26	hI	1	Total 86	C 66	N 8	O 12	0
26	hI	1	Total 86	C 66	N 8	O 12	0
26	iI	1	Total 129	C 99	N 12	O 18	0
26	iI	1	Total 129	C 99	N 12	O 18	0
26	iI	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	jI	1	86	66	8	12	0
26	jI	1	86	66	8	12	0
26	kI	1	129	99	12	18	0
26	kI	1	129	99	12	18	0
26	kI	1	129	99	12	18	0
26	lI	1	86	66	8	12	0
26	lI	1	86	66	8	12	0
26	mI	1	129	99	12	18	0
26	mI	1	129	99	12	18	0
26	mI	1	129	99	12	18	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	AJ	1	172	132	16	24	0
26	BJ	1	129	99	12	18	0
26	BJ	1	129	99	12	18	0
26	BJ	1	129	99	12	18	0
26	CJ	1	86	66	8	12	0
26	CJ	1	86	66	8	12	0
26	DJ	1	129	99	12	18	0
26	DJ	1	129	99	12	18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	DJ	1	Total 129	C 99	N 12	O 18	0
26	EJ	1	Total 86	C 66	N 8	O 12	0
26	EJ	1	Total 86	C 66	N 8	O 12	0
26	FJ	1	Total 86	C 66	N 8	O 12	0
26	FJ	1	Total 86	C 66	N 8	O 12	0
26	GJ	1	Total 86	C 66	N 8	O 12	0
26	GJ	1	Total 86	C 66	N 8	O 12	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	HJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	IJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	JJ	1	Total 129	C 99	N 12	O 18	0
26	KJ	1	Total 86	C 66	N 8	O 12	0
26	KJ	1	Total 86	C 66	N 8	O 12	0
26	LJ	1	Total 129	C 99	N 12	O 18	0
26	LJ	1	Total 129	C 99	N 12	O 18	0
26	LJ	1	Total 129	C 99	N 12	O 18	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
26	MJ	1	Total 86	C 66	N 8	O 12	0
26	MJ	1	Total 86	C 66	N 8	O 12	0
26	NJ	1	Total 129	C 99	N 12	O 18	0
26	NJ	1	Total 129	C 99	N 12	O 18	0
26	NJ	1	Total 129	C 99	N 12	O 18	0
26	OJ	1	Total 43	C 33	N 4	O 6	0
26	PJ	1	Total 129	C 99	N 12	O 18	0
26	PJ	1	Total 129	C 99	N 12	O 18	0
26	PJ	1	Total 129	C 99	N 12	O 18	0
26	QJ	1	Total 86	C 66	N 8	O 12	0
26	QJ	1	Total 86	C 66	N 8	O 12	0
26	RJ	1	Total 129	C 99	N 12	O 18	0
26	RJ	1	Total 129	C 99	N 12	O 18	0
26	RJ	1	Total 129	C 99	N 12	O 18	0
26	SJ	1	Total 86	C 66	N 8	O 12	0
26	SJ	1	Total 86	C 66	N 8	O 12	0
26	TJ	1	Total 129	C 99	N 12	O 18	0
26	TJ	1	Total 129	C 99	N 12	O 18	0
26	TJ	1	Total 129	C 99	N 12	O 18	0
26	UJ	1	Total 86	C 66	N 8	O 12	0
26	UJ	1	Total 86	C 66	N 8	O 12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	K1	1	Total 43	C 33	N 4	O 6	0
27	21	1	Total 86	C 66	N 8	O 12	0
27	21	1	Total 86	C 66	N 8	O 12	0
27	A2	1	Total 86	C 66	N 8	O 12	0
27	A2	1	Total 86	C 66	N 8	O 12	0
27	K3	1	Total 43	C 33	N 4	O 6	0
27	Y3	1	Total 43	C 33	N 4	O 6	0
27	A4	1	Total 43	C 33	N 4	O 6	0
27	K4	1	Total 43	C 33	N 4	O 6	0
27	24	1	Total 86	C 66	N 8	O 12	0
27	24	1	Total 86	C 66	N 8	O 12	0
27	A6	1	Total 86	C 66	N 8	O 12	0
27	A6	1	Total 86	C 66	N 8	O 12	0
27	A7	1	Total 86	C 66	N 8	O 12	0
27	A7	1	Total 86	C 66	N 8	O 12	0
27	A8	1	Total 86	C 66	N 8	O 12	0
27	A8	1	Total 86	C 66	N 8	O 12	0
27	B8	1	Total 43	C 33	N 4	O 6	0
27	Q8	1	Total 43	C 33	N 4	O 6	0
27	A9	1	Total 43	C 33	N 4	O 6	0
27	N9	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

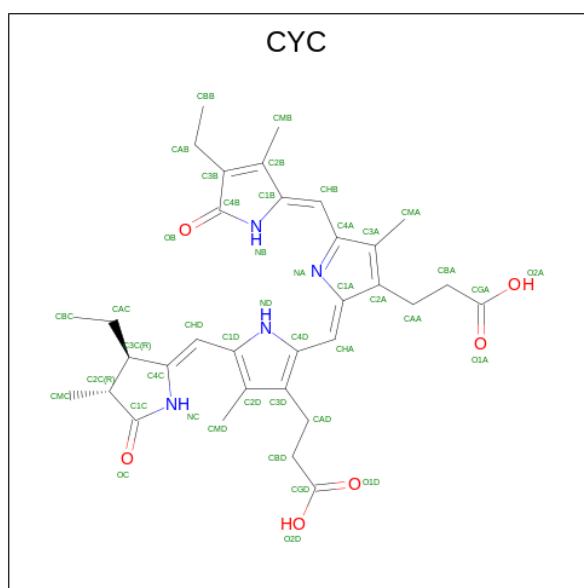
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	AA	1	86	66	8	12	0
27	AA	1	86	66	8	12	0
27	BA	1	43	33	4	6	0
27	QA	1	43	33	4	6	0
27	AB	1	86	66	8	12	0
27	AB	1	86	66	8	12	0
27	KD	1	43	33	4	6	0
27	YD	1	43	33	4	6	0
27	wE	1	43	33	4	6	0
27	xE	1	129	99	12	18	0
27	xE	1	129	99	12	18	0
27	xE	1	129	99	12	18	0
27	yE	1	86	66	8	12	0
27	yE	1	86	66	8	12	0
27	AF	1	86	66	8	12	0
27	AF	1	86	66	8	12	0
27	wG	1	43	33	4	6	0
27	xG	1	129	99	12	18	0
27	xG	1	129	99	12	18	0
27	xG	1	129	99	12	18	0
27	yG	1	86	66	8	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
27	yG	1	Total 86	C 66	N 8	O 12	0
27	AI	1	Total 86	C 66	N 8	O 12	0
27	AI	1	Total 86	C 66	N 8	O 12	0
27	AJ	1	Total 43	C 33	N 4	O 6	0
27	NJ	1	Total 43	C 33	N 4	O 6	0

- Molecule 28 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	C2	1	Total 43	C 33	N 4	O 6	0
28	D2	1	Total 43	C 33	N 4	O 6	0
28	E2	1	Total 43	C 33	N 4	O 6	0
28	F2	1	Total 43	C 33	N 4	O 6	0
28	G2	1	Total 43	C 33	N 4	O 6	0
28	H2	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	I2	1	43	33	4	6	0
28	J2	1	43	33	4	6	0
28	K2	1	43	33	4	6	0
28	L2	1	43	33	4	6	0
28	M2	1	43	33	4	6	0
28	N2	1	43	33	4	6	0
28	B6	1	86	66	8	12	0
28	B6	1	86	66	8	12	0
28	C6	1	43	33	4	6	0
28	D6	1	43	33	4	6	0
28	E6	1	43	33	4	6	0
28	F6	1	43	33	4	6	0
28	G6	1	43	33	4	6	0
28	H6	1	43	33	4	6	0
28	I6	1	43	33	4	6	0
28	K6	1	43	33	4	6	0
28	L6	1	43	33	4	6	0
28	M6	1	43	33	4	6	0
28	C7	1	43	33	4	6	0
28	D7	1	43	33	4	6	0
28	E7	1	43	33	4	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	F7	1	43	33	4	6	0
28	G7	1	43	33	4	6	0
28	H7	1	43	33	4	6	0
28	I7	1	43	33	4	6	0
28	J7	1	86	66	8	12	0
28	J7	1	86	66	8	12	0
28	K7	1	43	33	4	6	0
28	L7	1	43	33	4	6	0
28	N7	1	43	33	4	6	0
28	BB	1	43	33	4	6	0
28	CB	1	43	33	4	6	0
28	DB	1	43	33	4	6	0
28	EB	1	43	33	4	6	0
28	FB	1	43	33	4	6	0
28	GB	1	43	33	4	6	0
28	HB	1	43	33	4	6	0
28	IB	1	43	33	4	6	0
28	KB	1	43	33	4	6	0
28	LB	1	43	33	4	6	0
28	MB	1	43	33	4	6	0
28	NB	1	43	33	4	6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	
28	CF	1	Total	C	N	O	0	
			43	33	4	6		
28	DF	1	Total	C	N	O	0	
			86	66	8	12		
28	DF	1	Total	C	N	O	0	
			86	66	8	12		
28	EF	1	Total	C	N	O	0	
			43	33	4	6		
28	FF	1	Total	C	N	O	0	
			43	33	4	6		
28	HF	1	Total	C	N	O	0	
			43	33	4	6		
28	IF	1	Total	C	N	O	0	
			43	33	4	6		
28	JF	1	Total	C	N	O	0	
			86	66	8	12		
28	JF	1	Total	C	N	O	0	
			86	66	8	12		
28	KF	1	Total	C	N	O	0	
			43	33	4	6		
28	LF	1	Total	C	N	O	0	
			43	33	4	6		
28	NF	1	Total	C	N	O	0	
			43	33	4	6		
28	AH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	CH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	FH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	EH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	GH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	IH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	JH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	KH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	LH	1	Total	C	H	N	O	0
			81	33	38	4	6	

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf	
28	MH	1	Total 81	C 33	H 38	N 4	O 6	0
28	NH	1	Total 81	C 33	H 38	N 4	O 6	0
28	OH	1	Total 81	C 33	H 38	N 4	O 6	0
28	PH	1	Total 81	C 33	H 38	N 4	O 6	0
28	QH	1	Total 81	C 33	H 38	N 4	O 6	0
28	RH	1	Total 81	C 33	H 38	N 4	O 6	0
28	SH	1	Total 81	C 33	H 38	N 4	O 6	0
28	TH	1	Total 81	C 33	H 38	N 4	O 6	0
28	UH	1	Total 81	C 33	H 38	N 4	O 6	0
28	VH	1	Total 81	C 33	H 38	N 4	O 6	0
28	WH	1	Total 81	C 33	H 38	N 4	O 6	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	YH	1	Total 324	C 132	H 152	N 16	O 24	0
28	cH	1	Total 81	C 33	H 38	N 4	O 6	0
28	dH	1	Total 81	C 33	H 38	N 4	O 6	0
28	eH	1	Total 81	C 33	H 38	N 4	O 6	0
28	fH	1	Total 81	C 33	H 38	N 4	O 6	0
28	gH	1	Total 81	C 33	H 38	N 4	O 6	0
28	hH	1	Total 81	C 33	H 38	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
28	iH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	jH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	kH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	lH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	mH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	nH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	oH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	pH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	qH	1	Total	C	H	N	O	0
			162	66	76	8	12	
28	qH	1	Total	C	H	N	O	0
			162	66	76	8	12	
28	rH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	sH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	tH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	uH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	vH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	wH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	yH	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	1H	1	Total	C	H	N	O	0
			81	33	38	4	6	
28	CI	1	Total	C	N	O		0
			43	33	4	6		
28	DI	1	Total	C	N	O		0
			43	33	4	6		
28	EI	1	Total	C	N	O		0
			43	33	4	6		

Continued on next page...

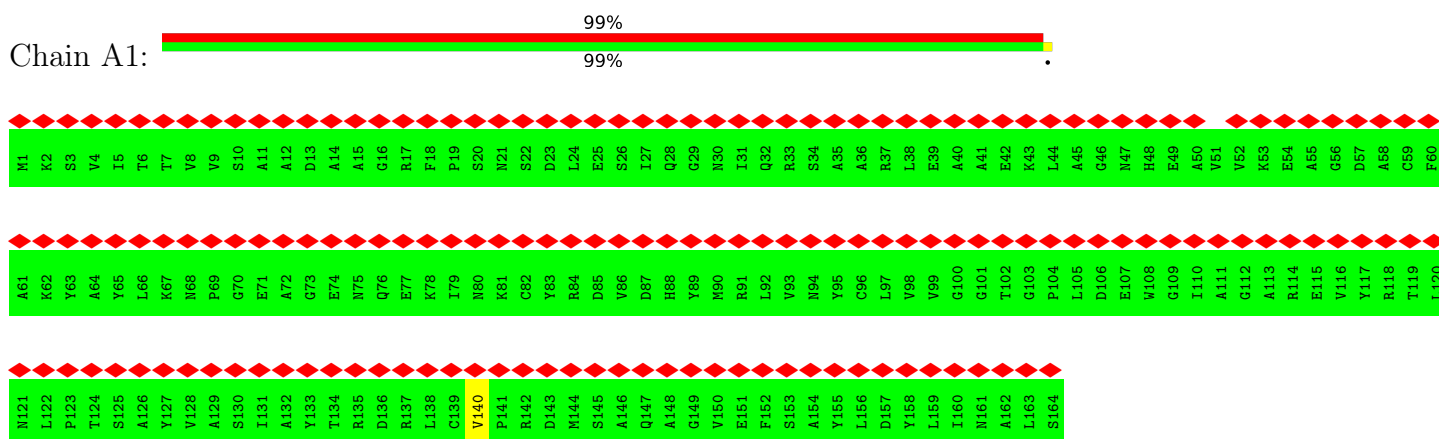
Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
28	FI	1	Total 43	C 33	N 4	O 6	0
28	GI	1	Total 43	C 33	N 4	O 6	0
28	HI	1	Total 43	C 33	N 4	O 6	0
28	II	1	Total 43	C 33	N 4	O 6	0
28	JI	1	Total 43	C 33	N 4	O 6	0
28	KI	1	Total 43	C 33	N 4	O 6	0
28	LI	1	Total 43	C 33	N 4	O 6	0
28	MI	1	Total 43	C 33	N 4	O 6	0
28	NI	1	Total 43	C 33	N 4	O 6	0

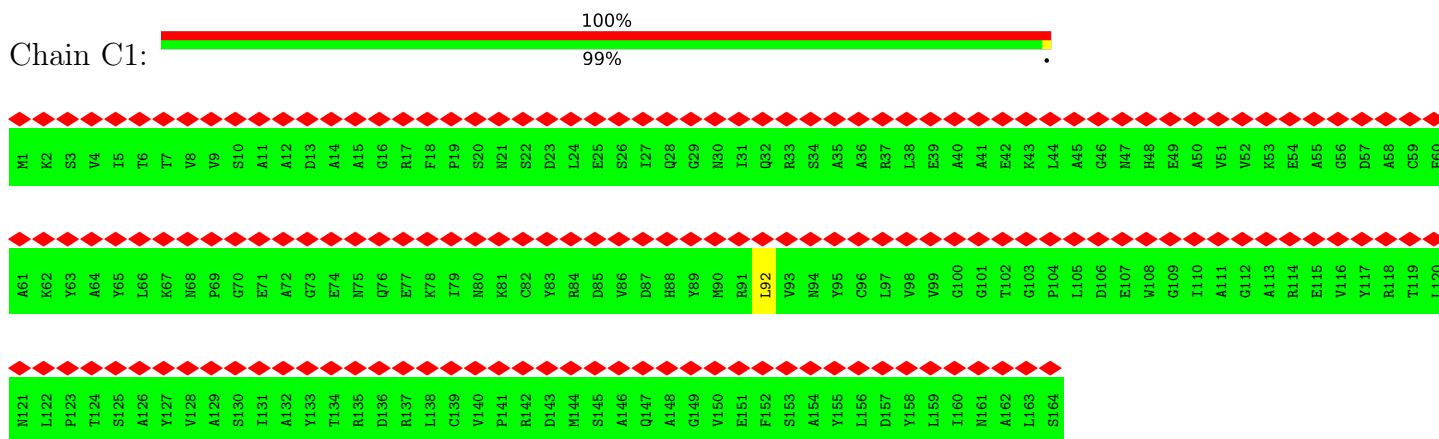
3 Residue-property plots [i](#)

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 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.

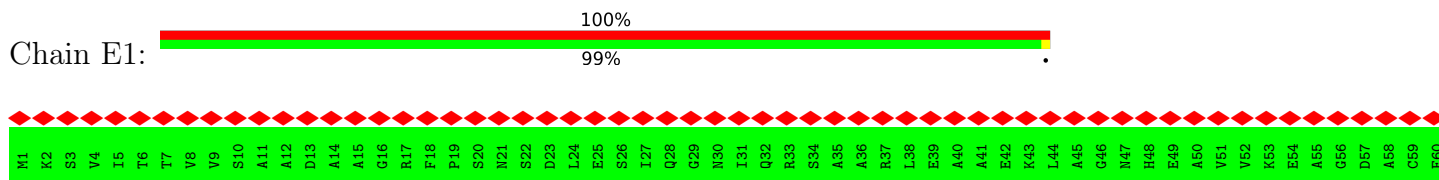
- Molecule 1: Phycoerythrin alpha subunit

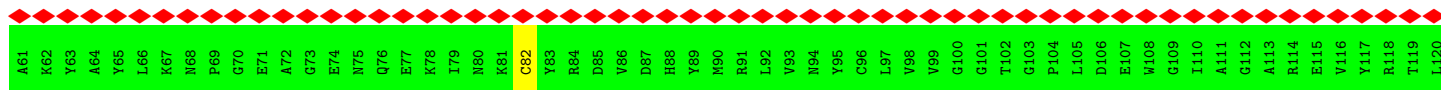


- Molecule 1: Phycoerythrin alpha subunit

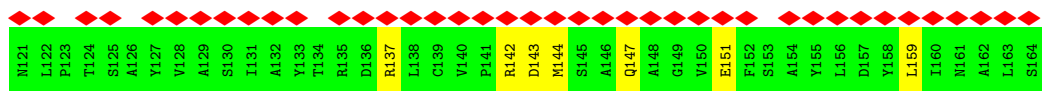
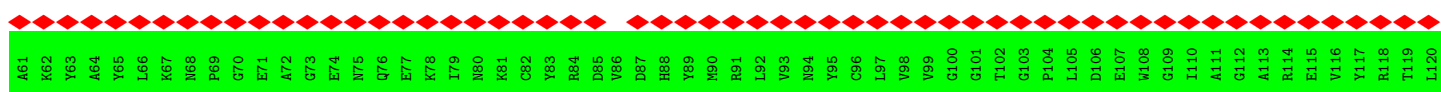
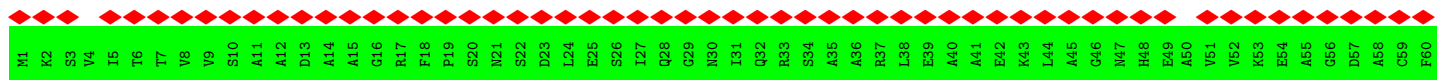


- Molecule 1: Phycoerythrin alpha subunit

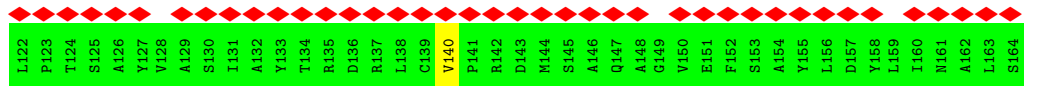
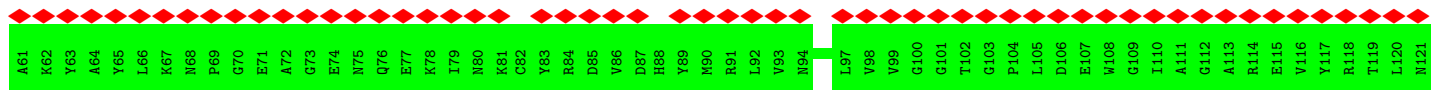
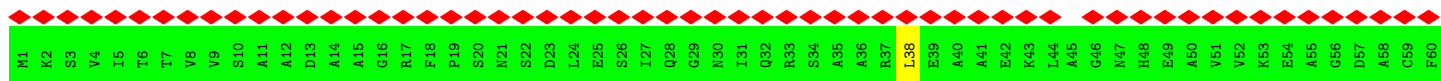




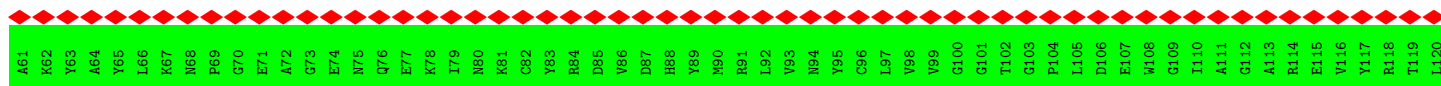
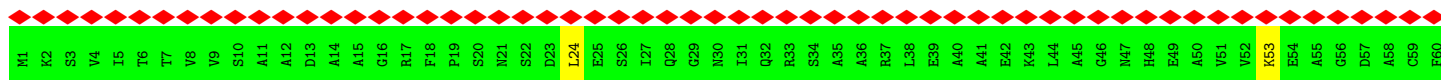
• Molecule 1: Phycoerythrin alpha subunit



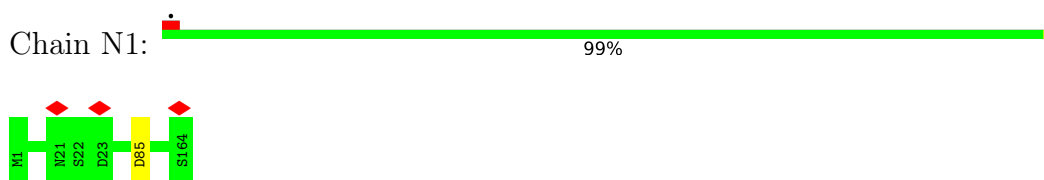
• Molecule 1: Phycoerythrin alpha subunit



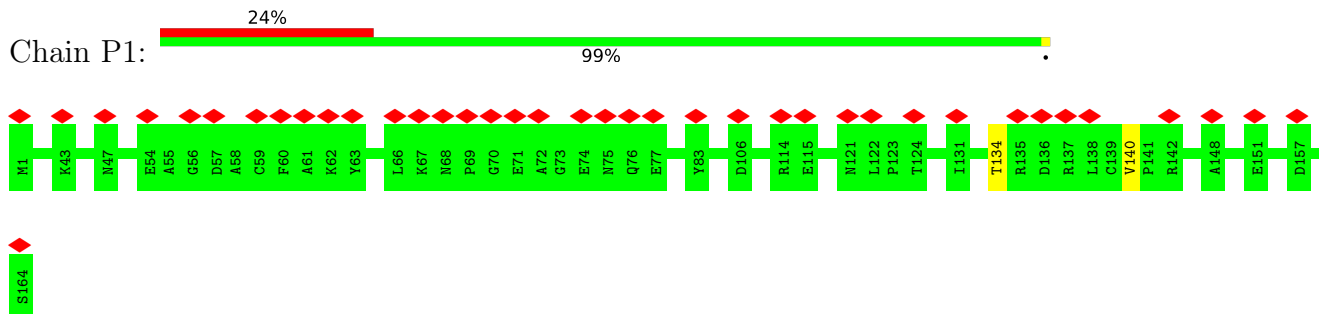
• Molecule 1: Phycoerythrin alpha subunit



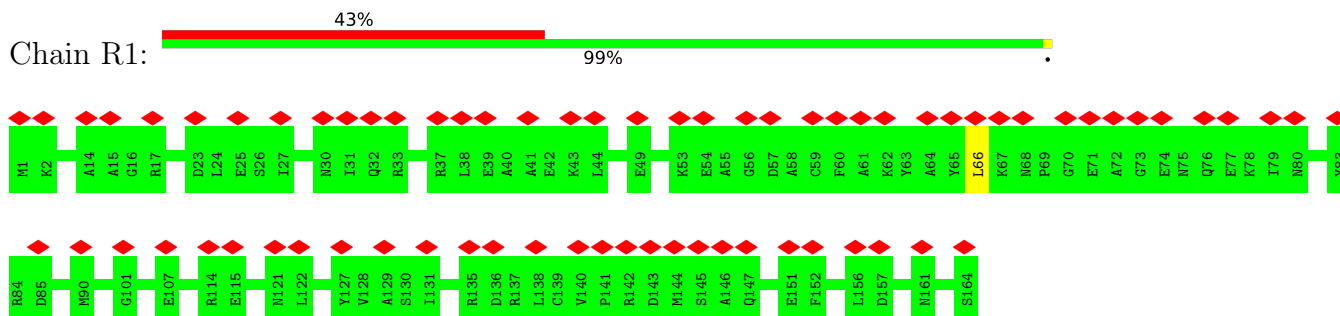
- Molecule 1: Phycoerythrin alpha subunit



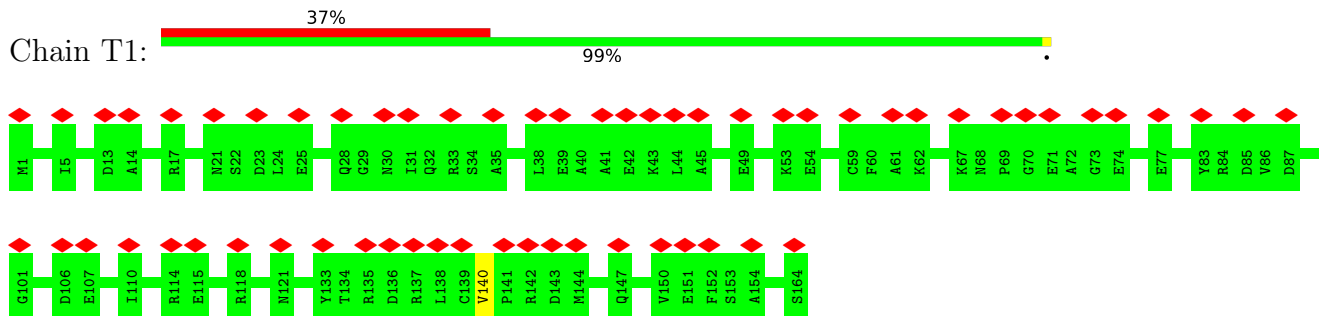
- Molecule 1: Phycoerythrin alpha subunit



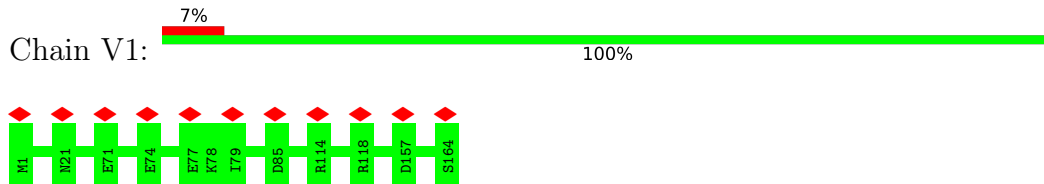
- Molecule 1: Phycoerythrin alpha subunit



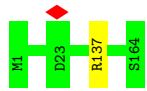
- Molecule 1: Phycoerythrin alpha subunit



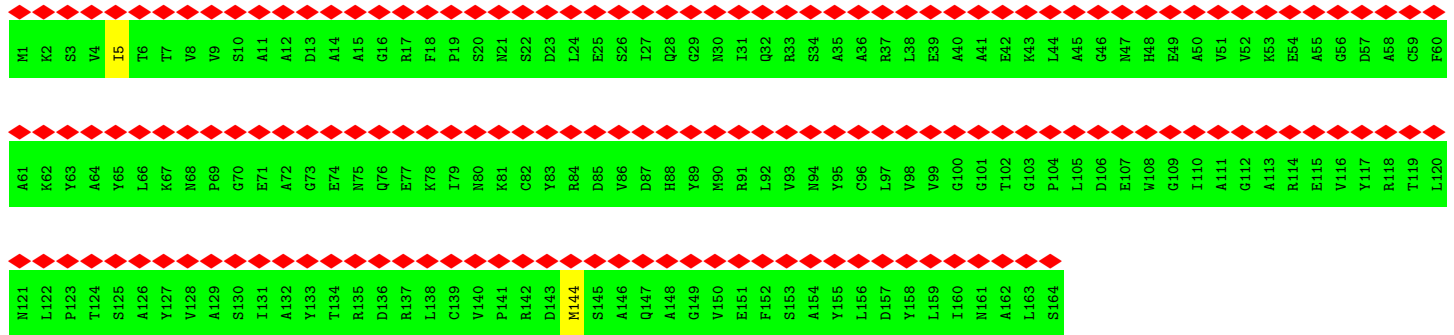
- Molecule 1: Phycoerythrin alpha subunit



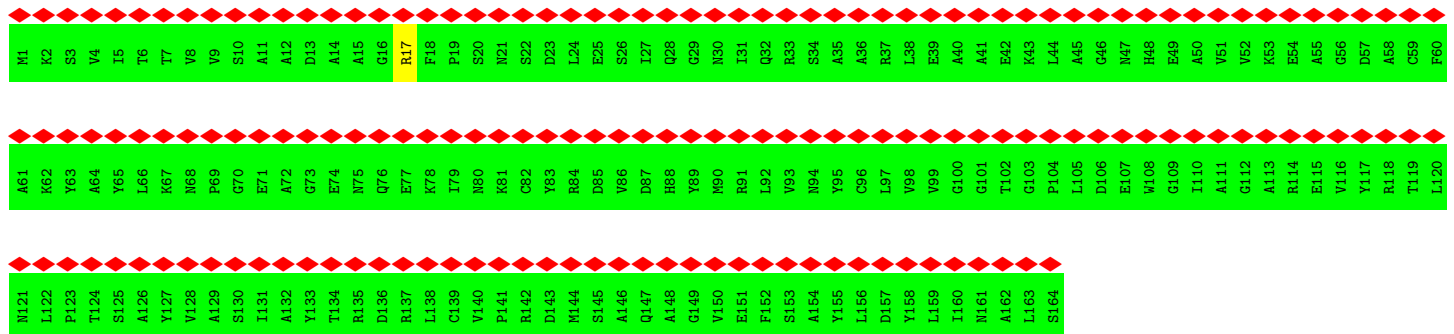
- Molecule 1: Phycoerythrin alpha subunit



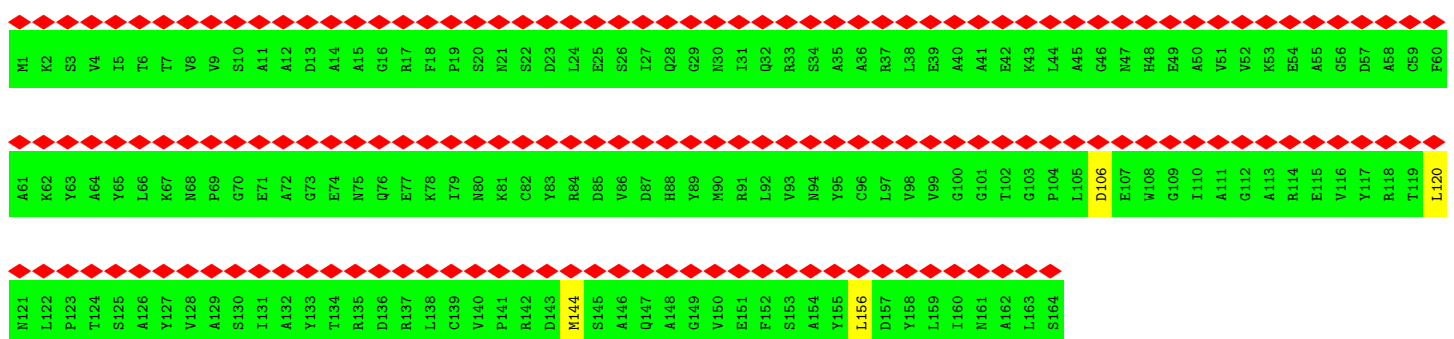
• Molecule 1: Phycoerythrin alpha subunit



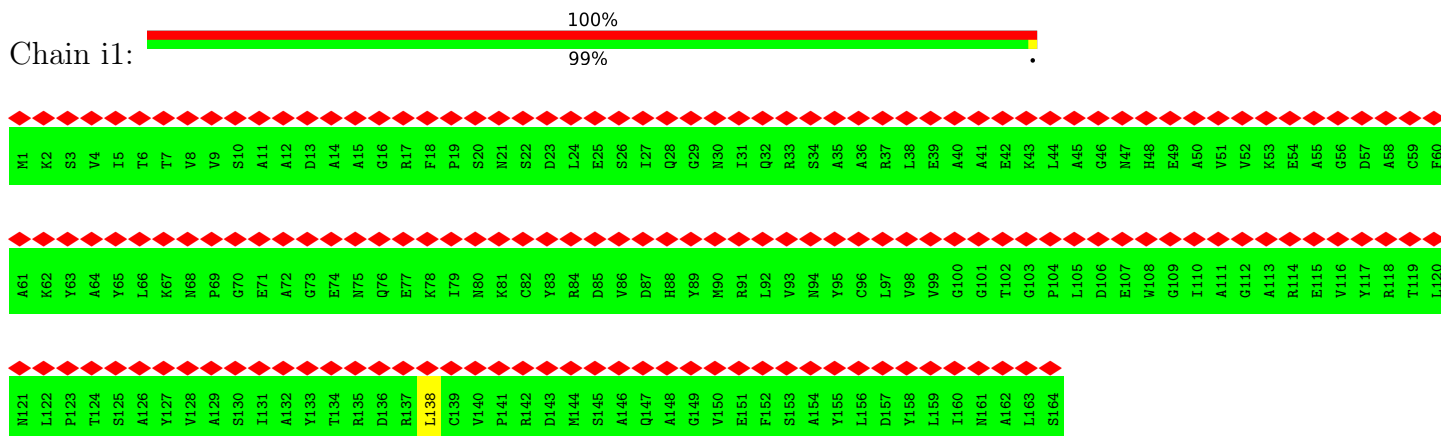
• Molecule 1: Phycoerythrin alpha subunit



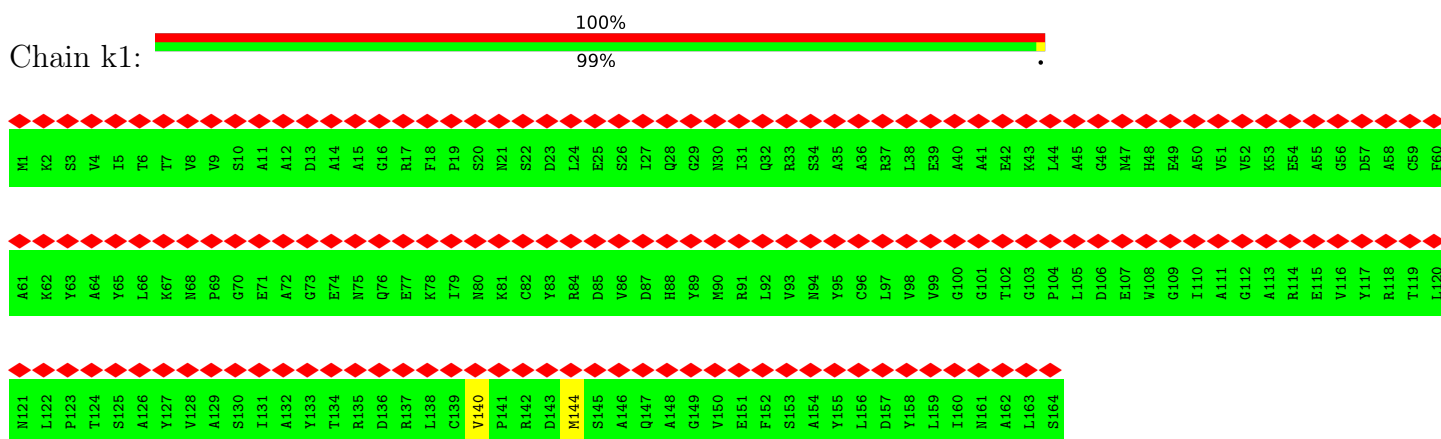
• Molecule 1: Phycoerythrin alpha subunit



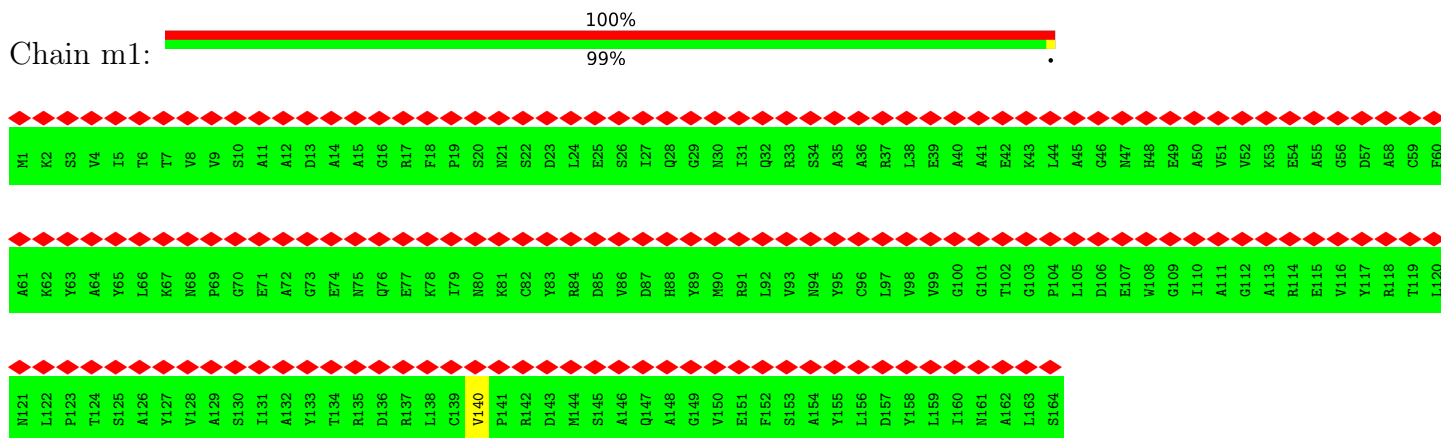
• Molecule 1: Phycoerythrin alpha subunit



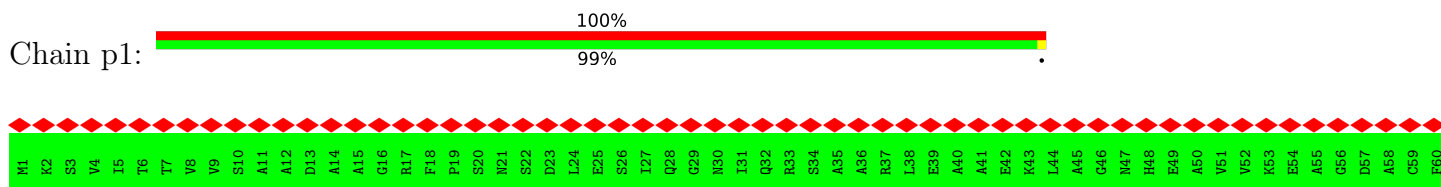
• Molecule 1: Phycoerythrin alpha subunit

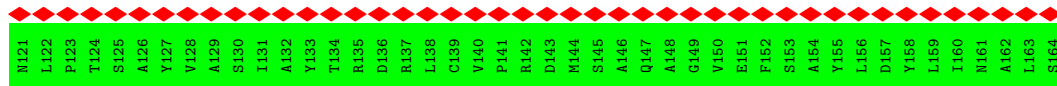
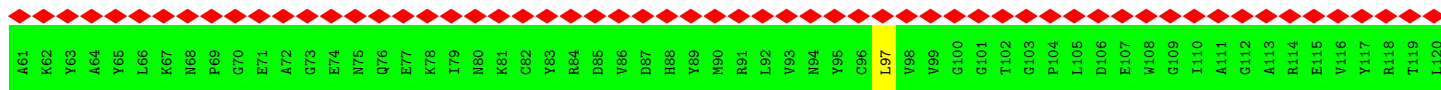


• Molecule 1: Phycoerythrin alpha subunit

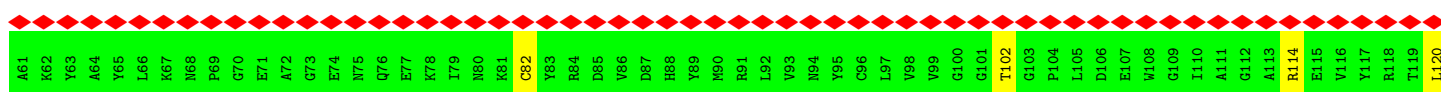
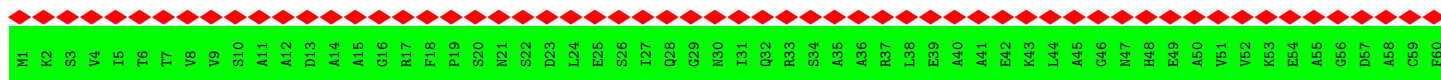


• Molecule 1: Phycoerythrin alpha subunit

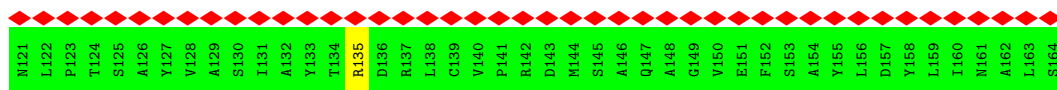
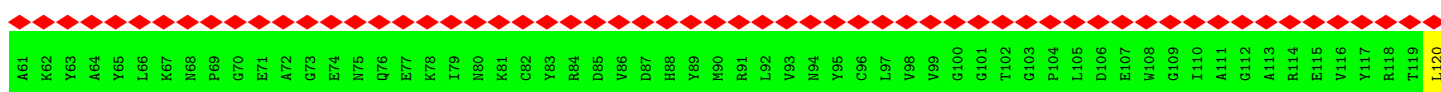
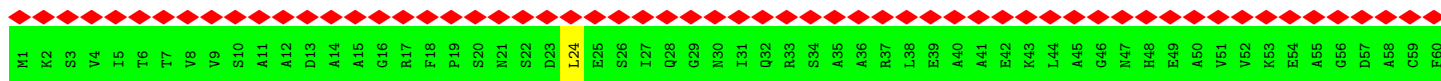




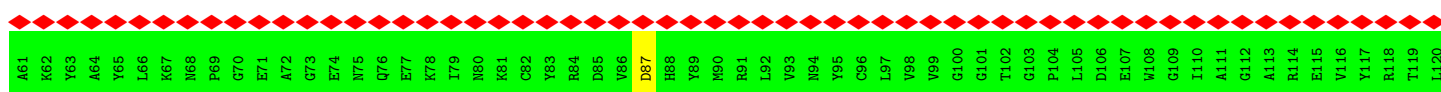
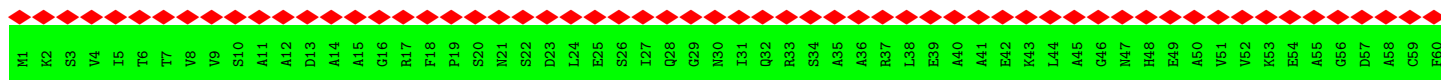
• Molecule 1: Phycoerythrin alpha subunit

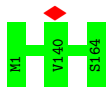


• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit





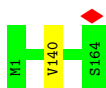
- Molecule 1: Phycoerythrin alpha subunit

Chain U2: 100%

There are no outlier residues recorded for this chain.

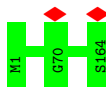
- Molecule 1: Phycoerythrin alpha subunit

Chain W2: 99%



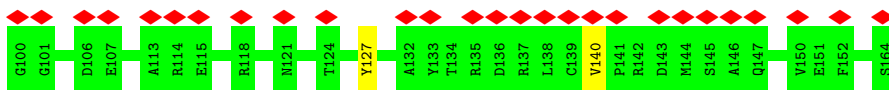
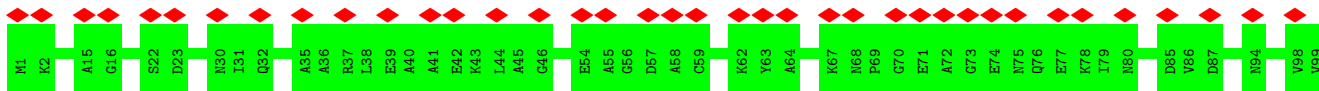
- Molecule 1: Phycoerythrin alpha subunit

Chain Z2: 100%



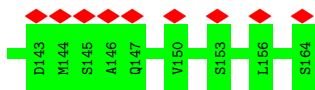
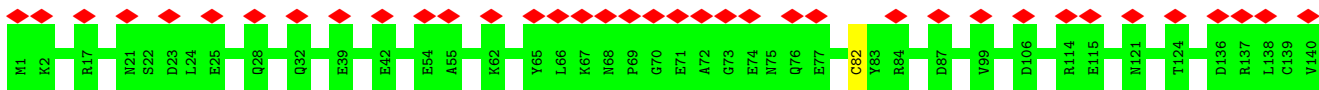
- Molecule 1: Phycoerythrin alpha subunit

Chain b2: 40% 99%



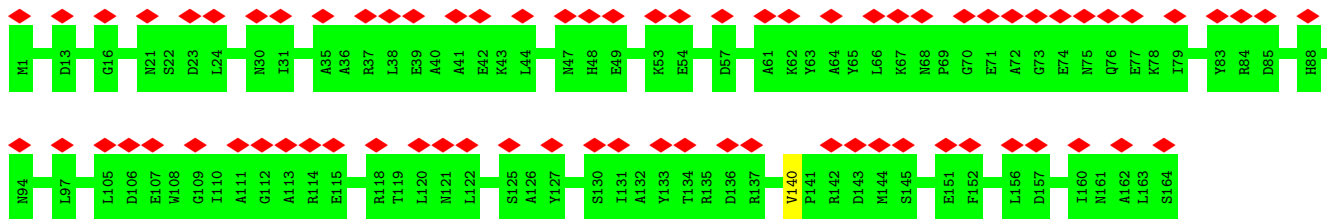
- Molecule 1: Phycoerythrin alpha subunit

Chain d2: 28% 99%

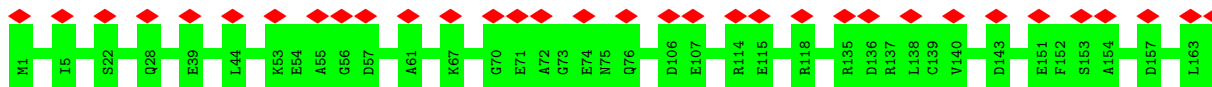


- Molecule 1: Phycoerythrin alpha subunit

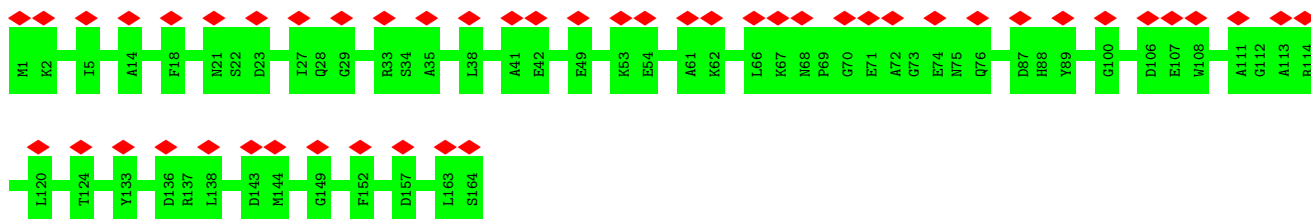
Chain f2: 45% 99%



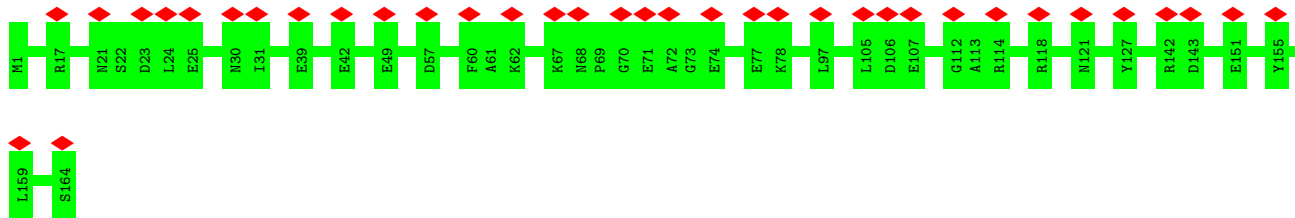
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

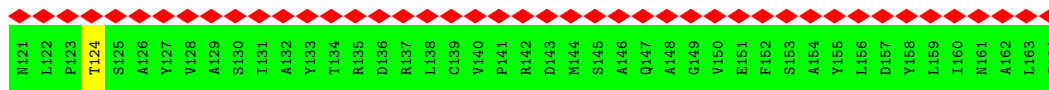


• Molecule 1: Phycoerythrin alpha subunit

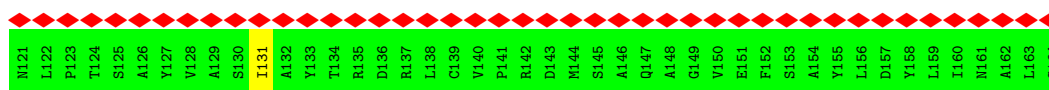
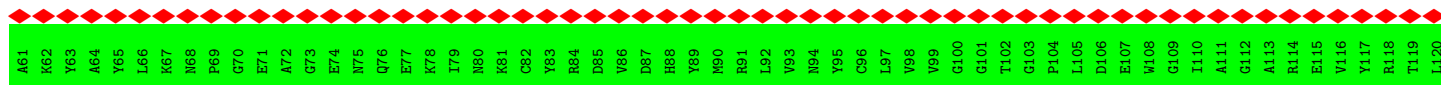
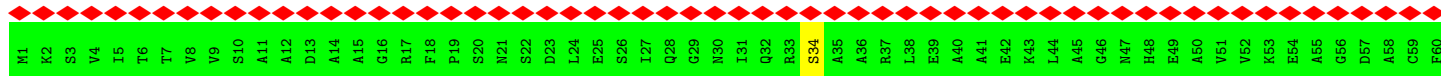


• Molecule 1: Phycoerythrin alpha subunit

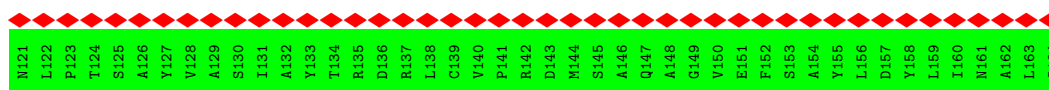
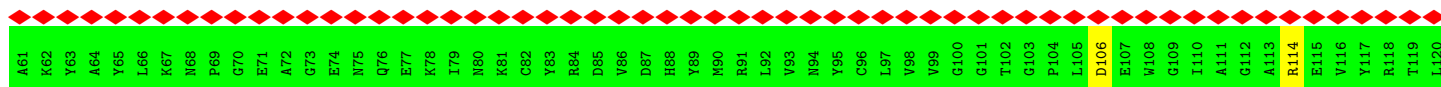
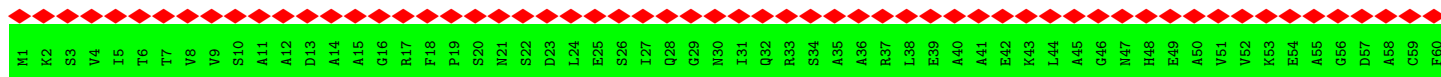




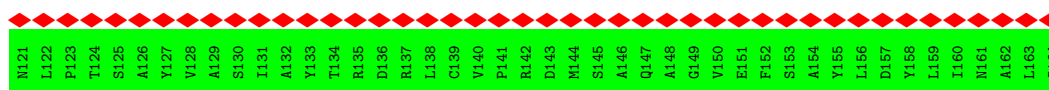
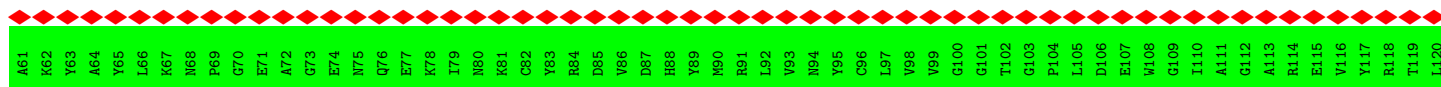
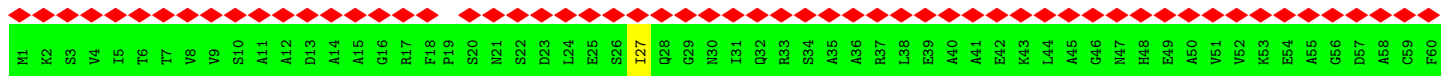
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

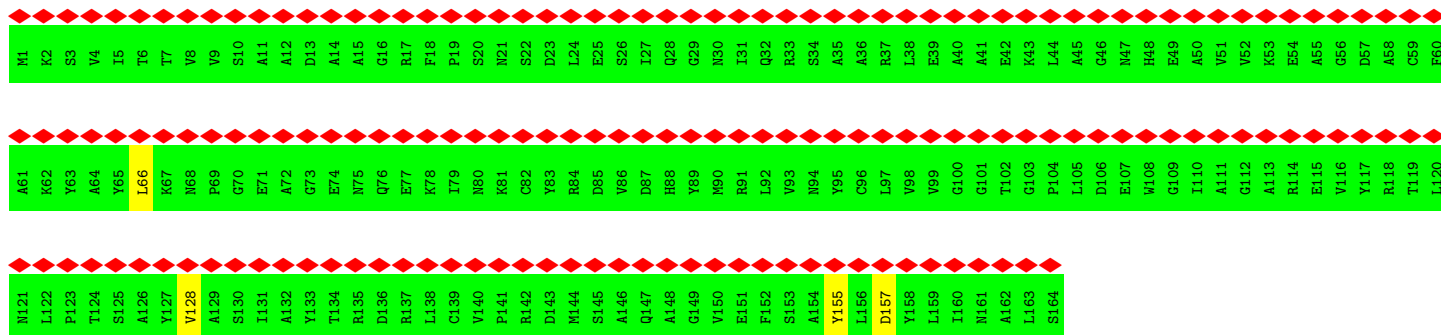


• Molecule 1: Phycoerythrin alpha subunit

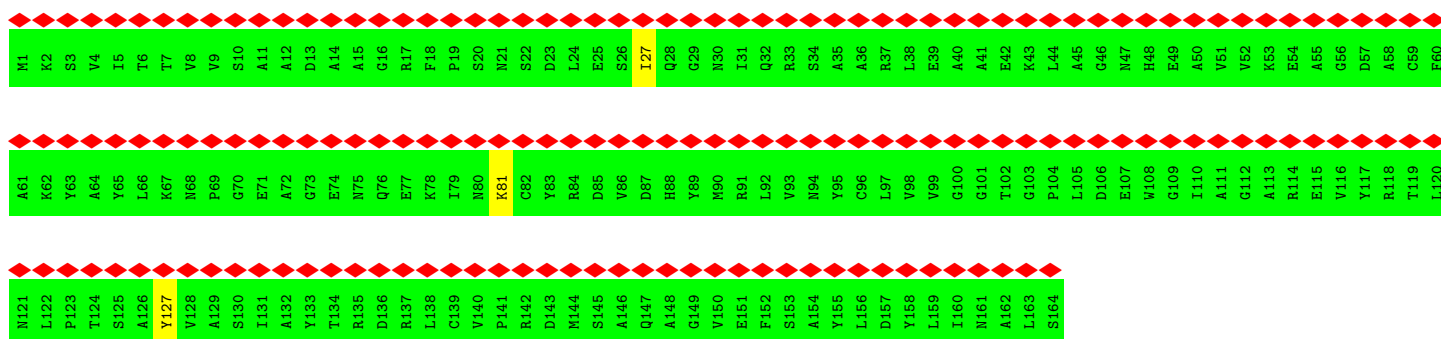


• Molecule 1: Phycoerythrin alpha subunit

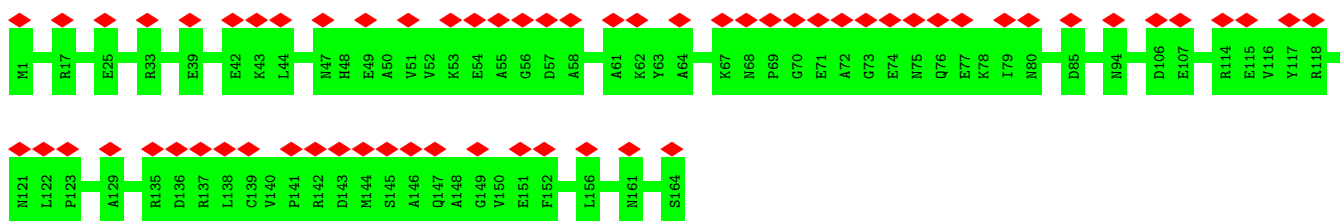
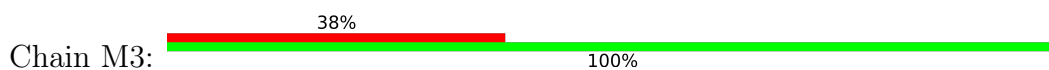




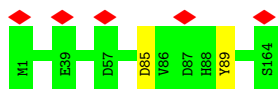
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

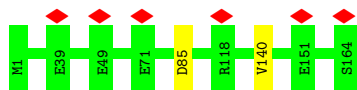


• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

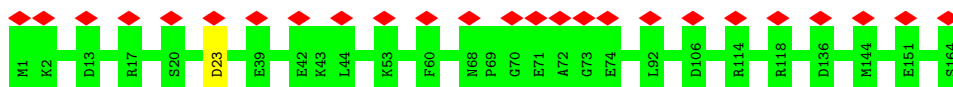




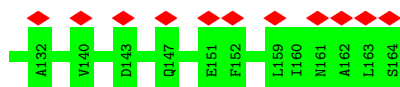
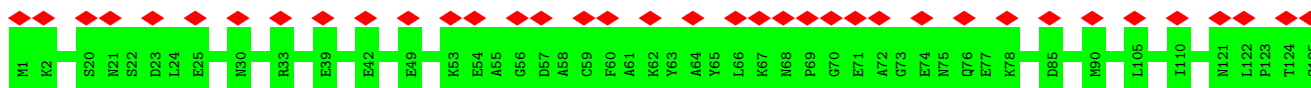
- Molecule 1: Phycoerythrin alpha subunit



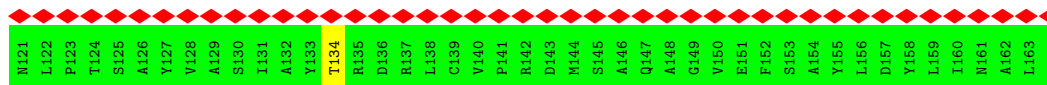
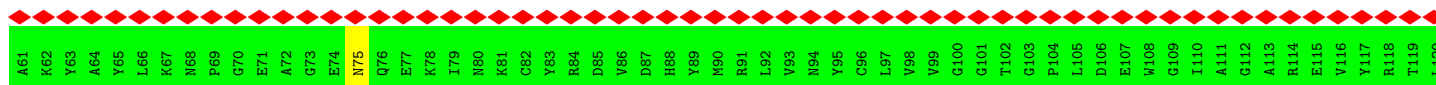
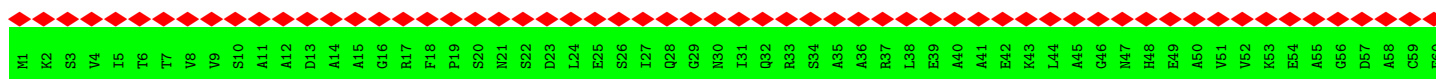
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit

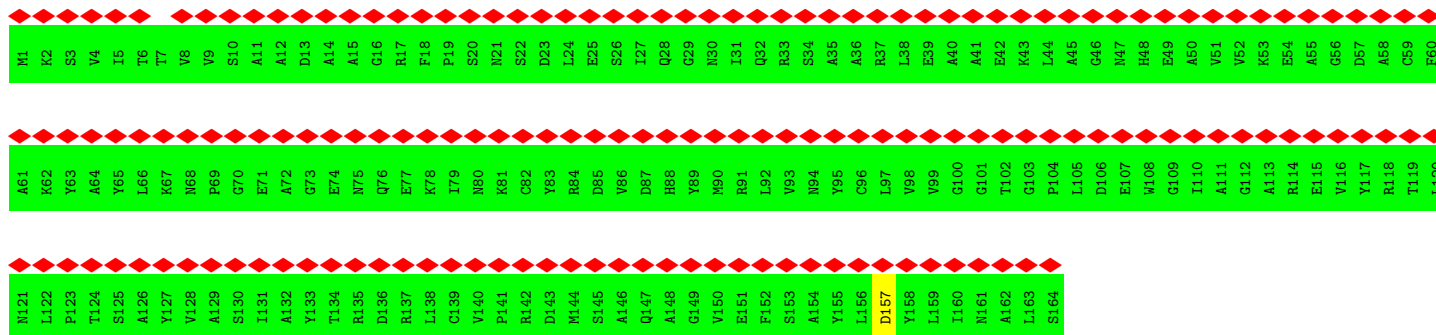


- Molecule 1: Phycoerythrin alpha subunit

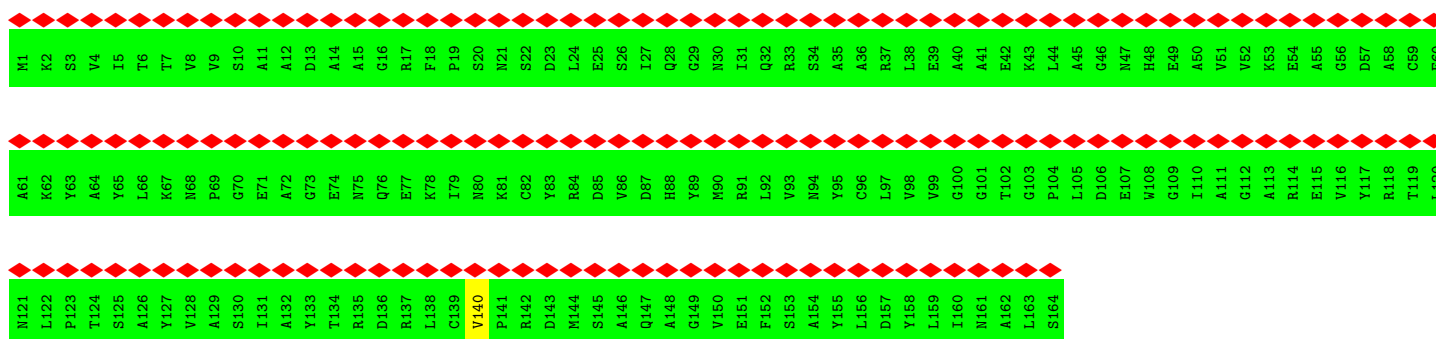


- Molecule 1: Phycoerythrin alpha subunit

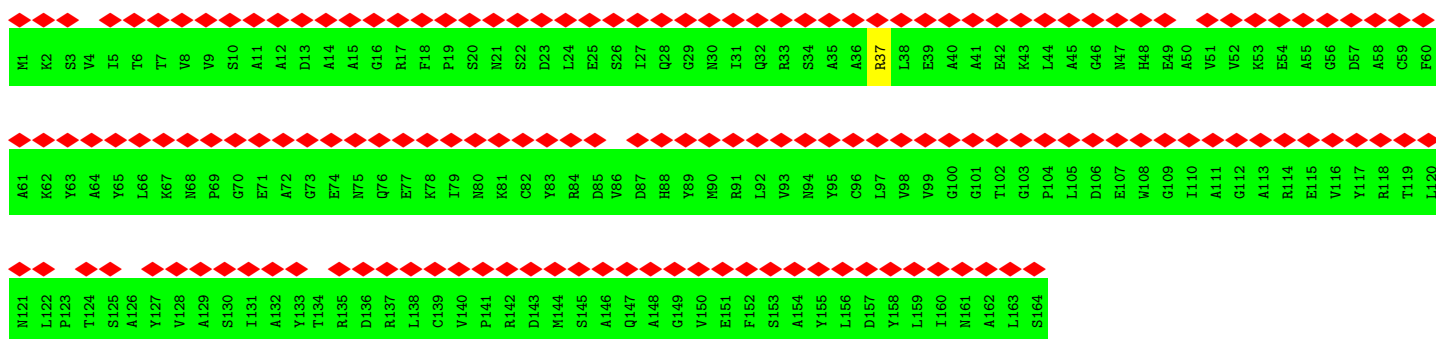




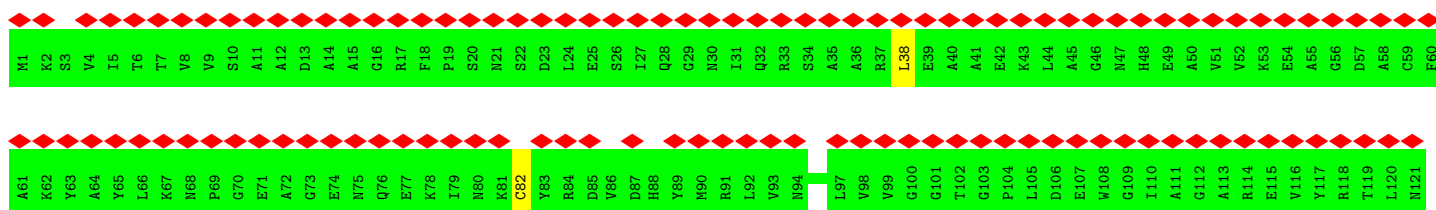
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

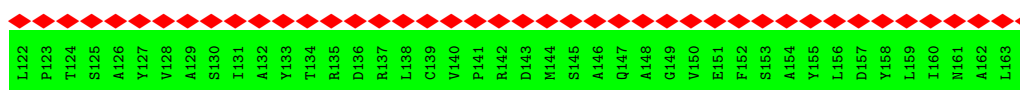
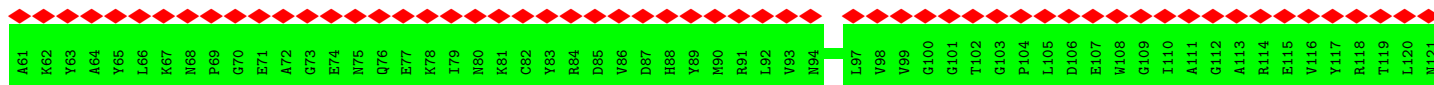
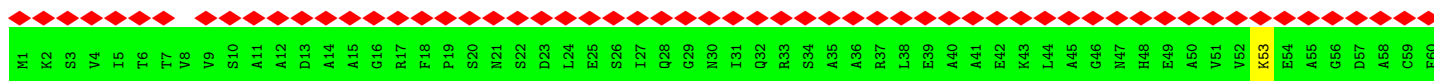


• Molecule 1: Phycoerythrin alpha subunit





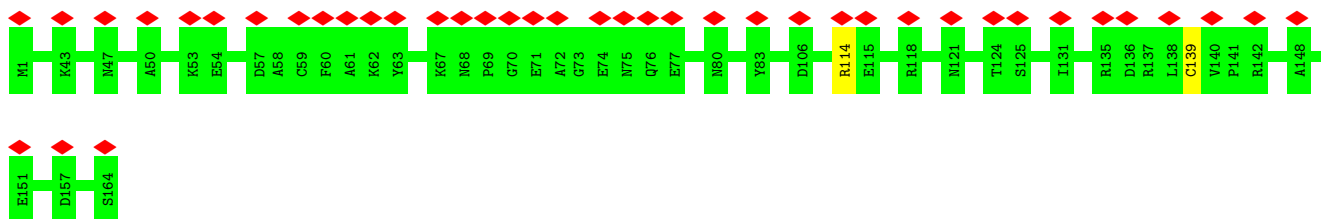
• Molecule 1: Phycoerythrin alpha subunit



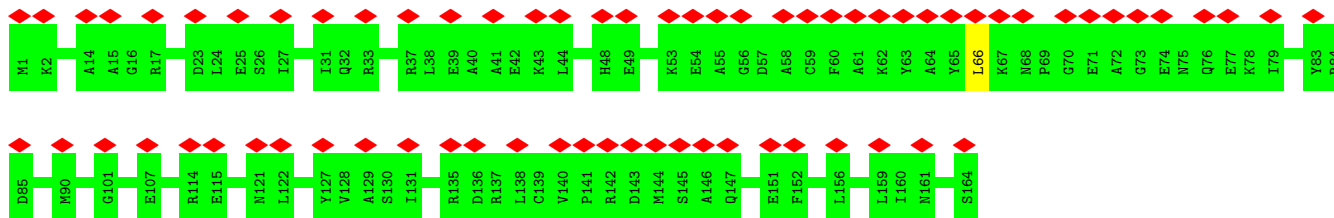
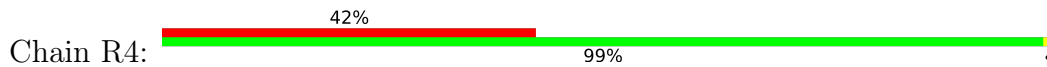
• Molecule 1: Phycoerythrin alpha subunit



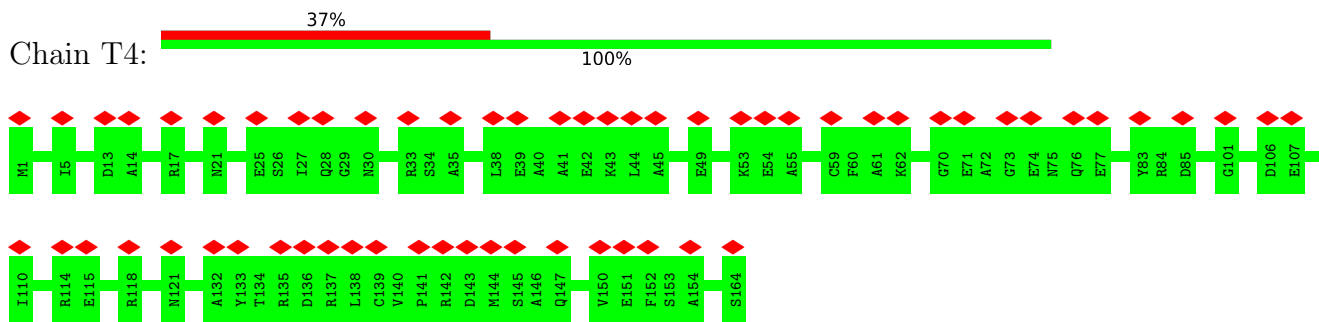
• Molecule 1: Phycoerythrin alpha subunit



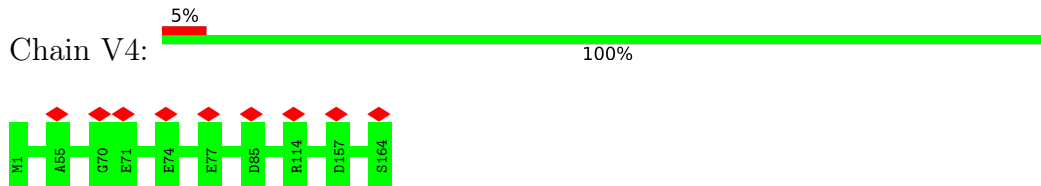
• Molecule 1: Phycoerythrin alpha subunit



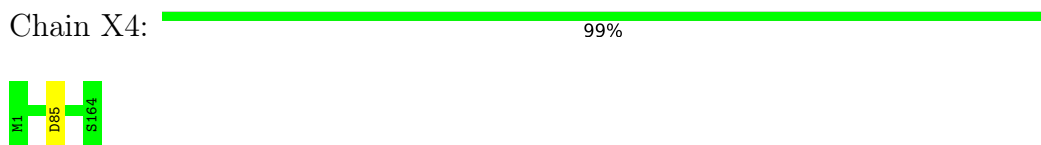
• Molecule 1: Phycoerythrin alpha subunit



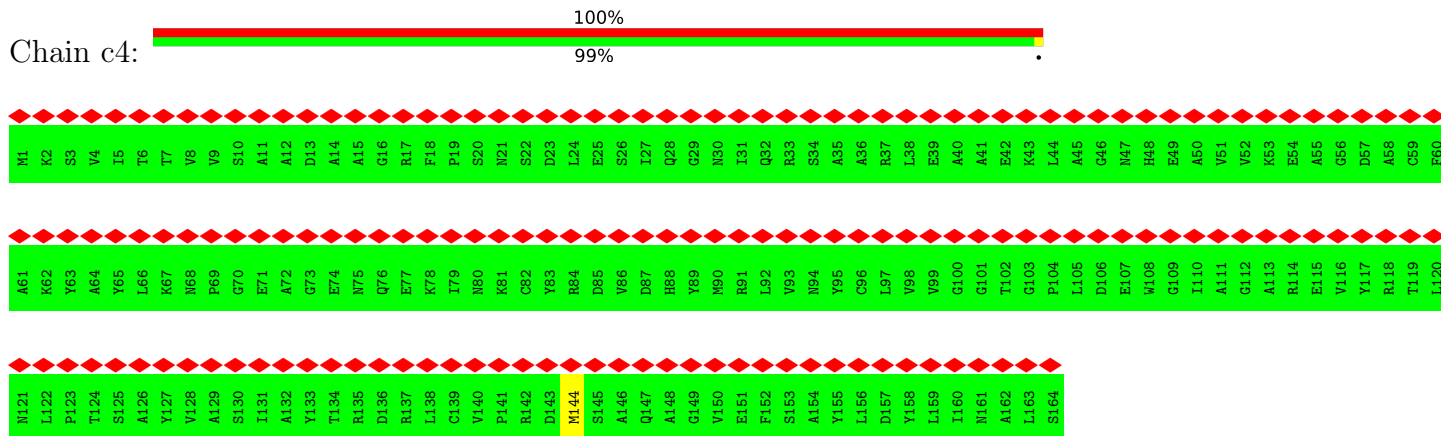
• Molecule 1: Phycoerythrin alpha subunit



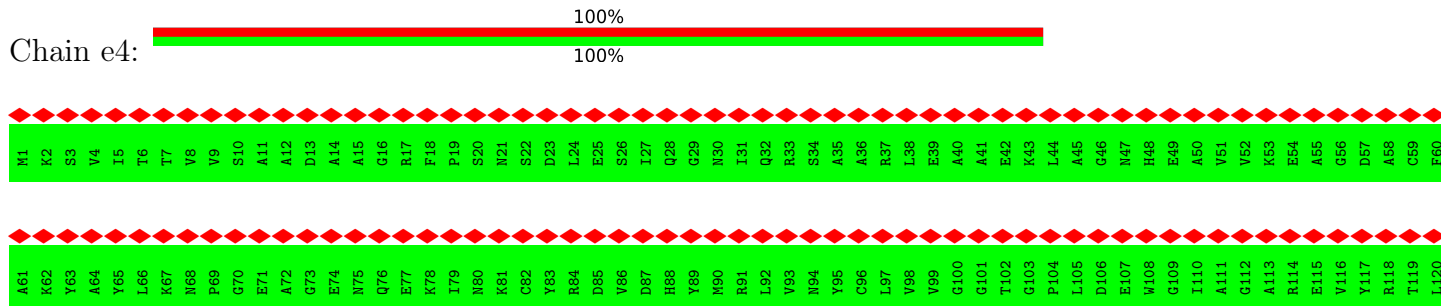
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

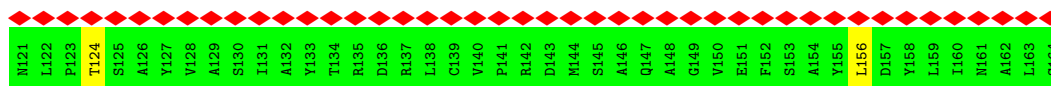
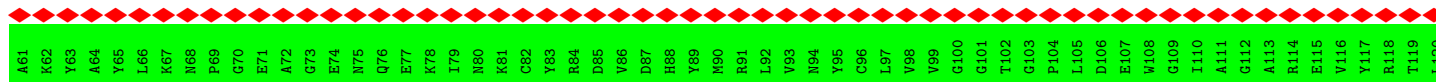
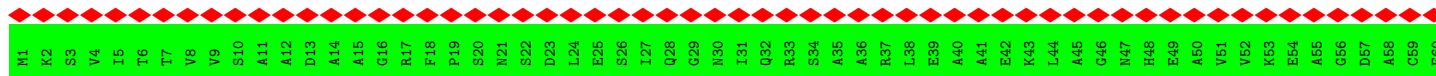


• Molecule 1: Phycoerythrin alpha subunit

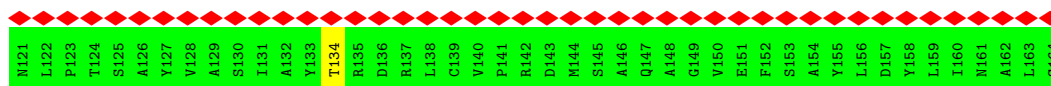
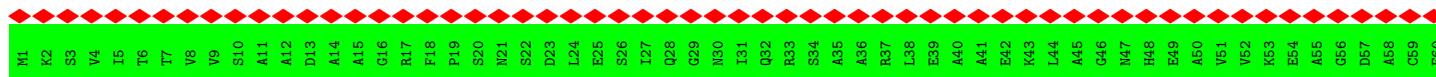




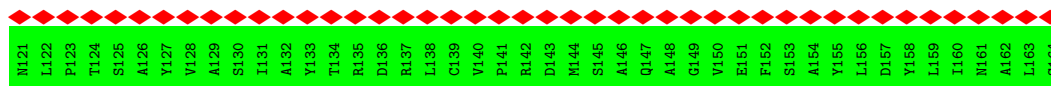
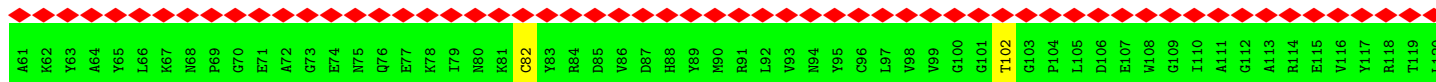
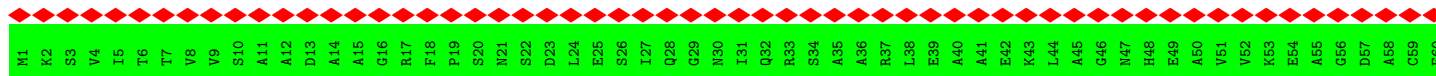
• Molecule 1: Phycoerythrin alpha subunit



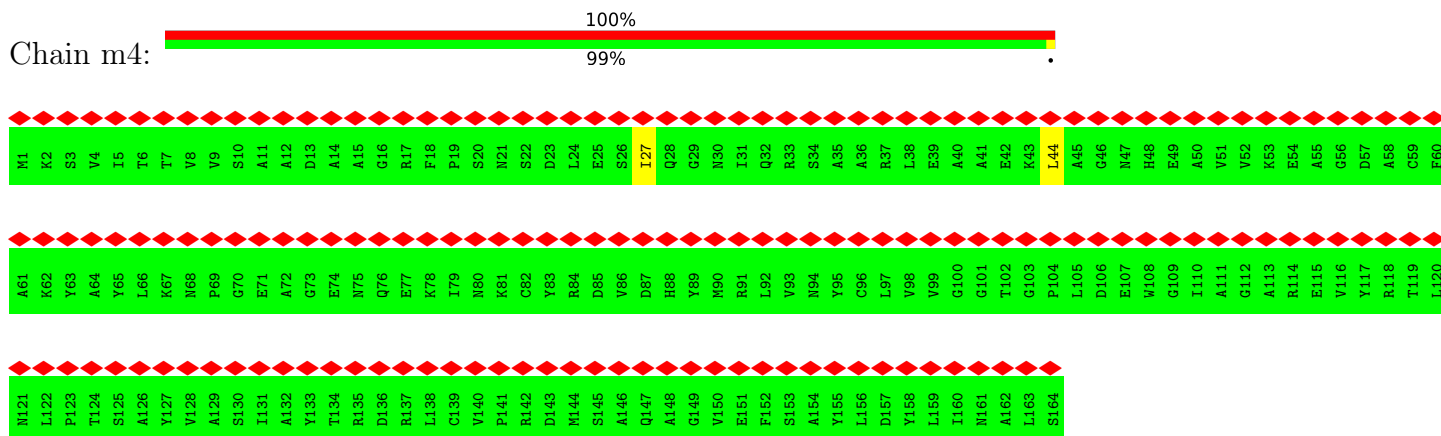
• Molecule 1: Phycoerythrin alpha subunit



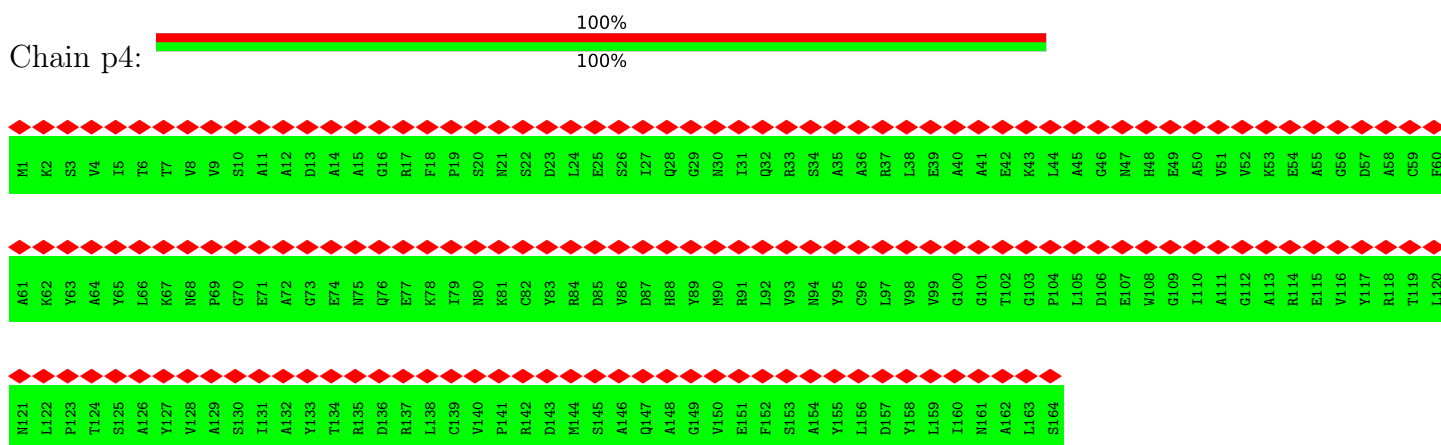
• Molecule 1: Phycoerythrin alpha subunit



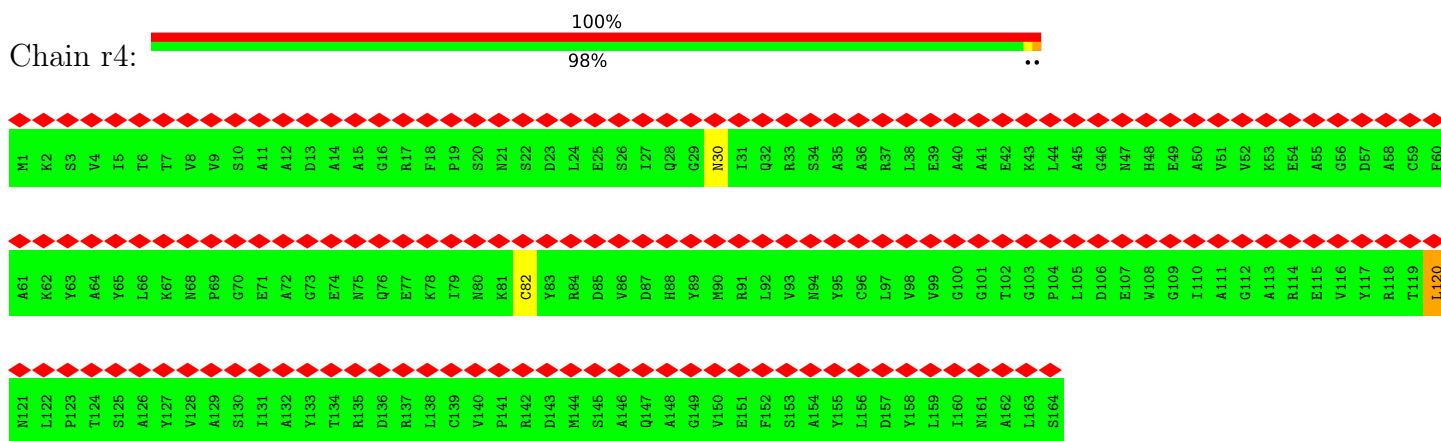
• Molecule 1: Phycoerythrin alpha subunit



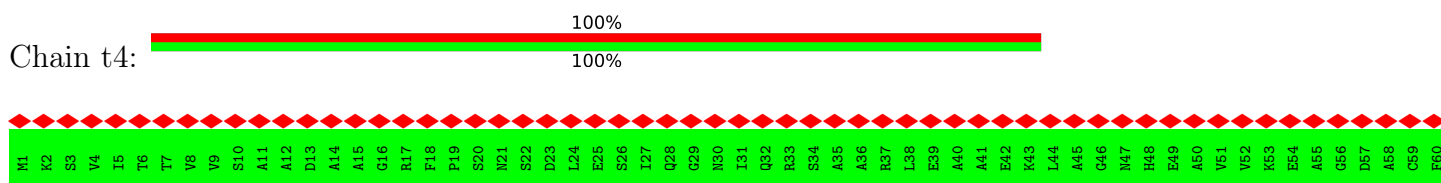
• Molecule 1: Phycoerythrin alpha subunit

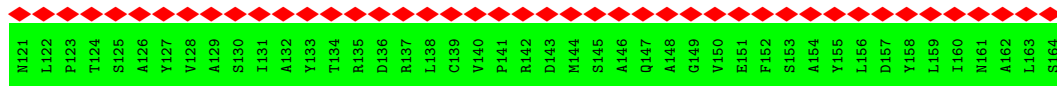
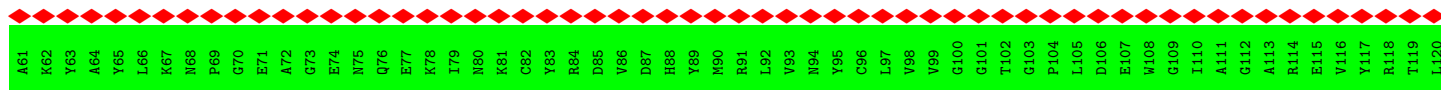


• Molecule 1: Phycoerythrin alpha subunit

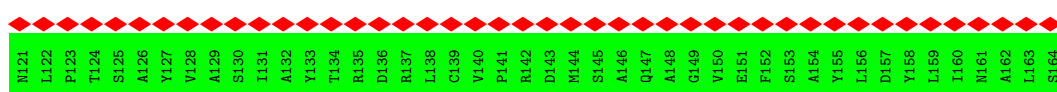
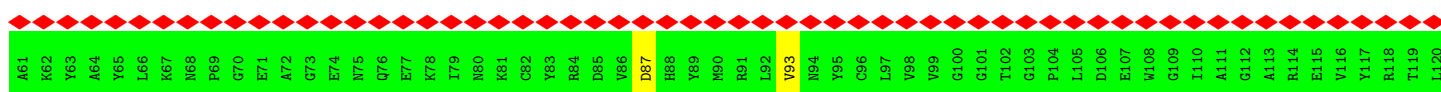
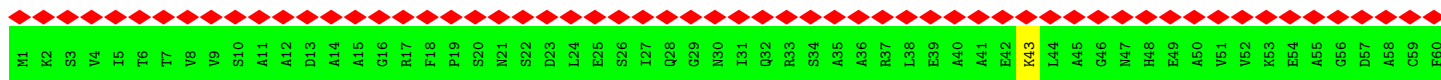


• Molecule 1: Phycoerythrin alpha subunit

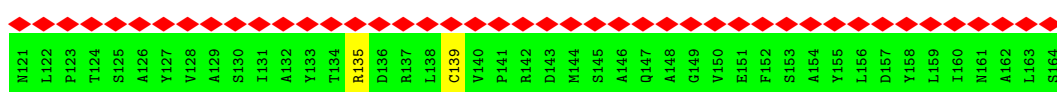
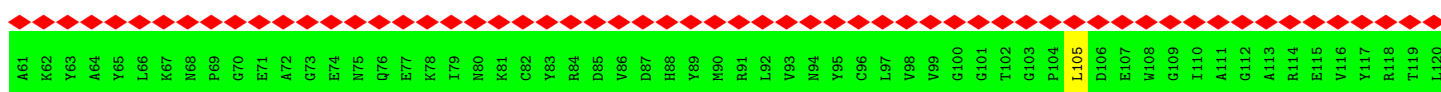
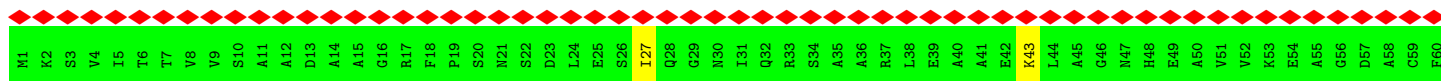




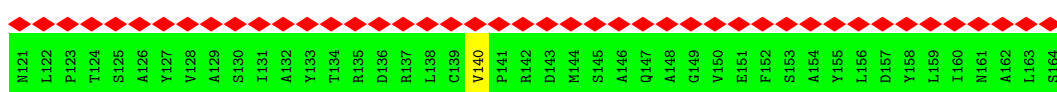
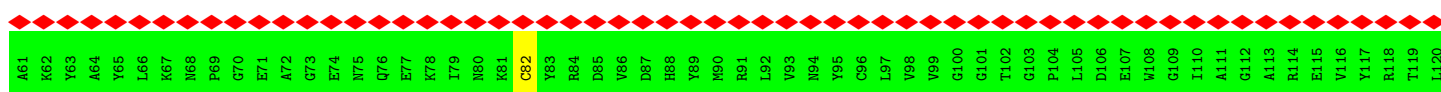
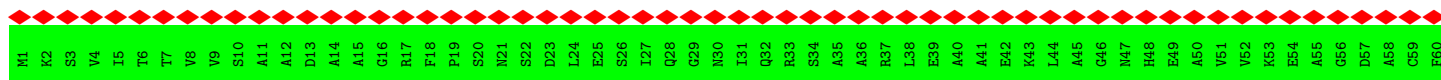
• Molecule 1: Phycoerythrin alpha subunit



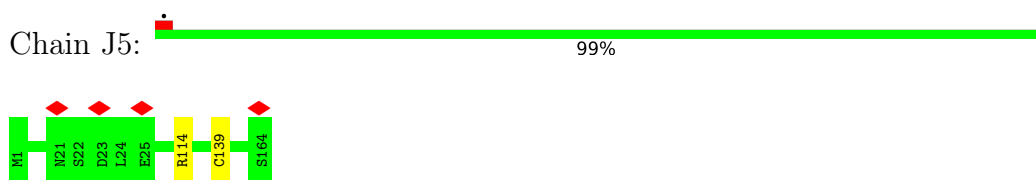
• Molecule 1: Phycoerythrin alpha subunit



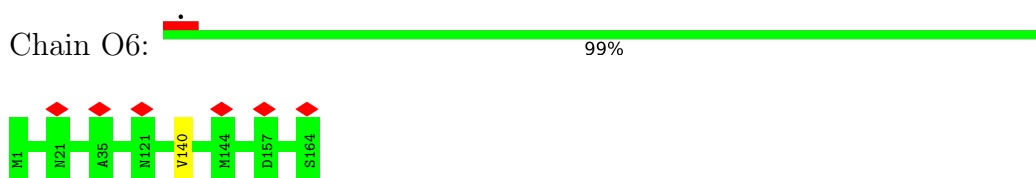
• Molecule 1: Phycoerythrin alpha subunit



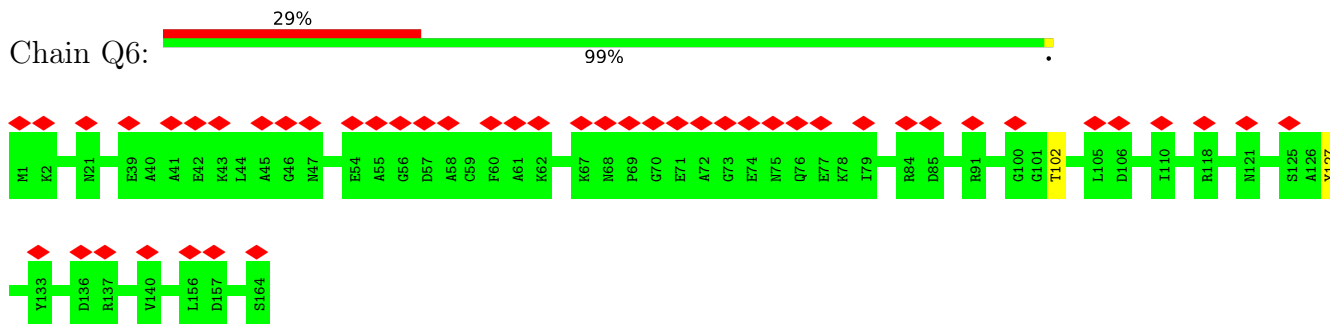
- Molecule 1: Phycoerythrin alpha subunit



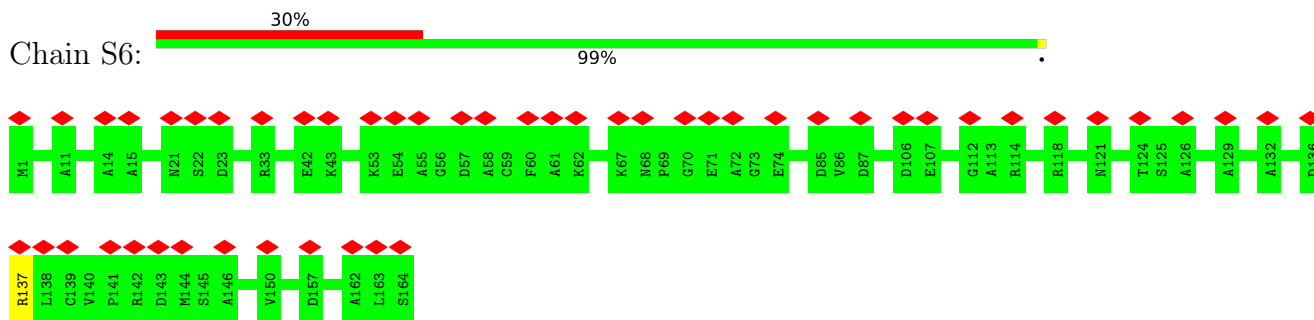
- Molecule 1: Phycoerythrin alpha subunit



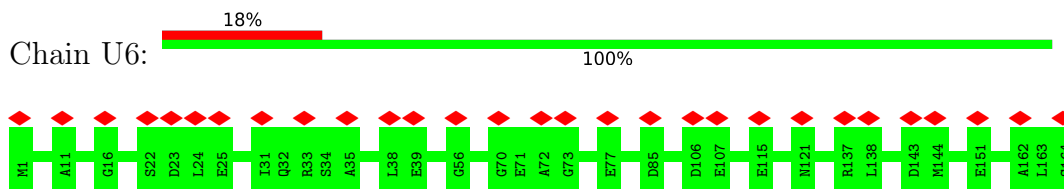
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit

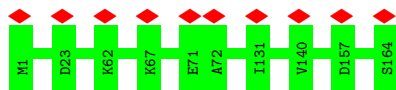


- Molecule 1: Phycoerythrin alpha subunit

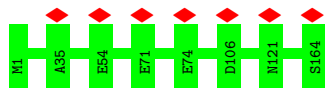


- Molecule 1: Phycoerythrin alpha subunit

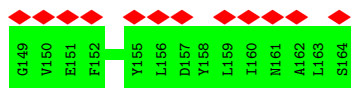
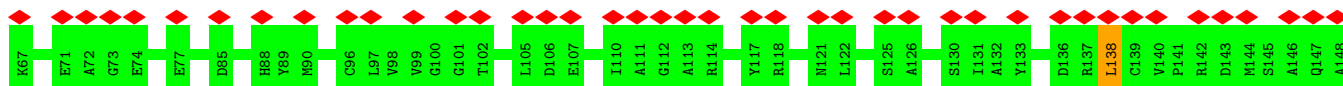
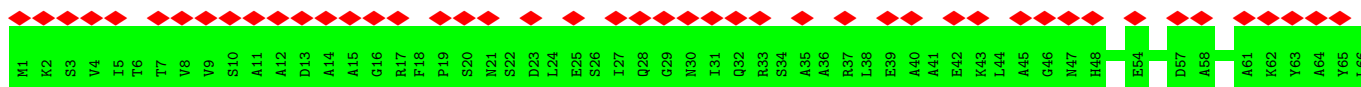




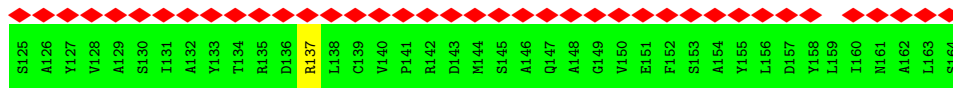
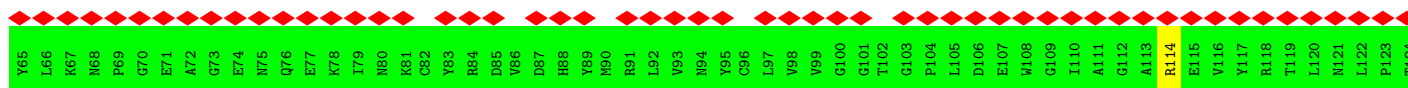
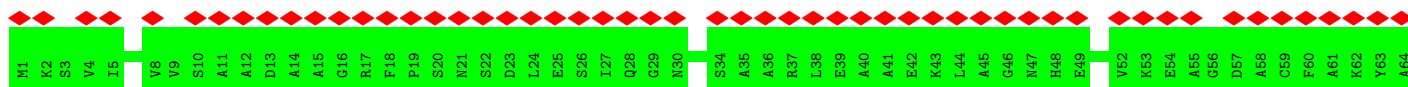
• Molecule 1: Phycoerythrin alpha subunit



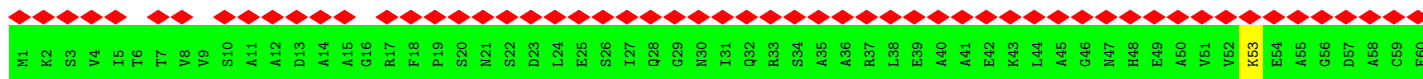
• Molecule 1: Phycoerythrin alpha subunit

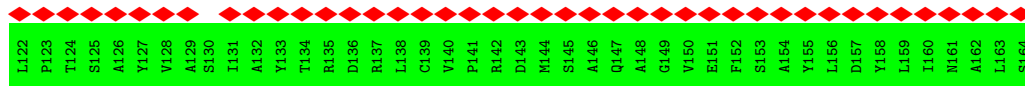
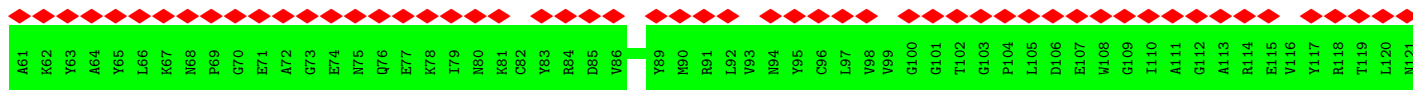


• Molecule 1: Phycoerythrin alpha subunit

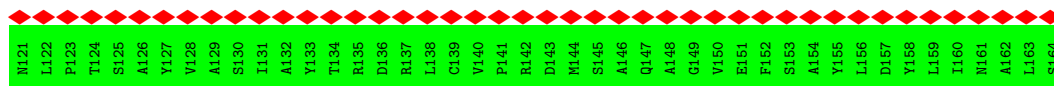
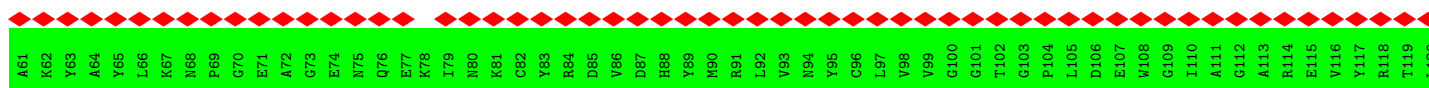
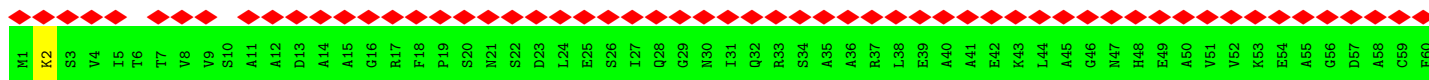


• Molecule 1: Phycoerythrin alpha subunit

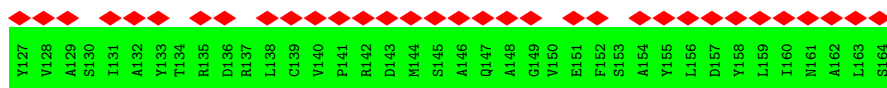
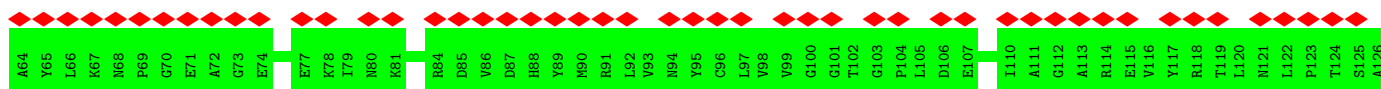
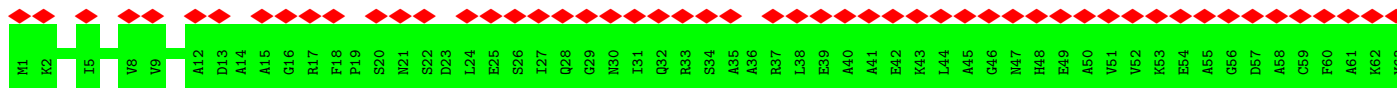
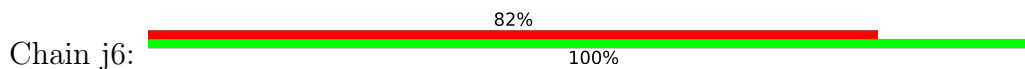




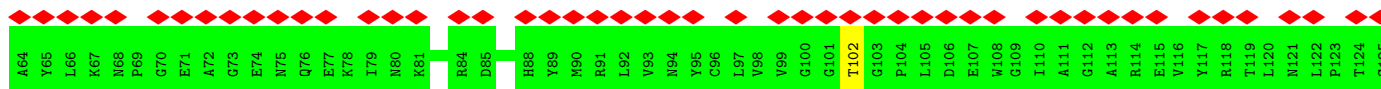
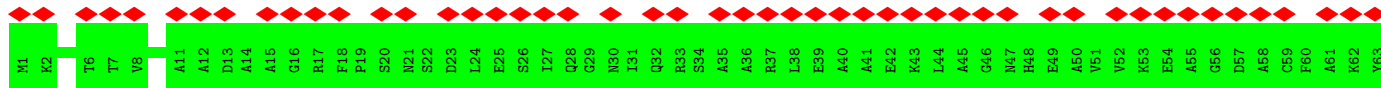
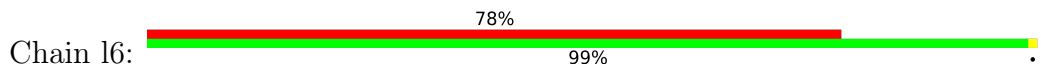
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

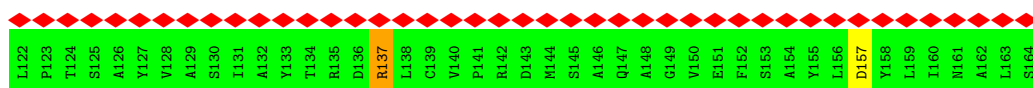
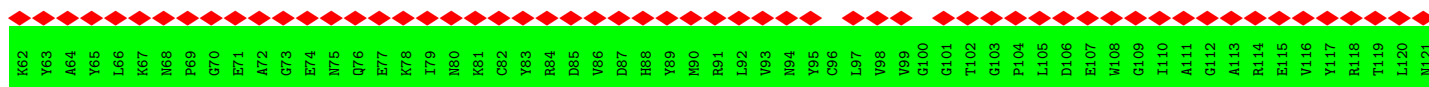
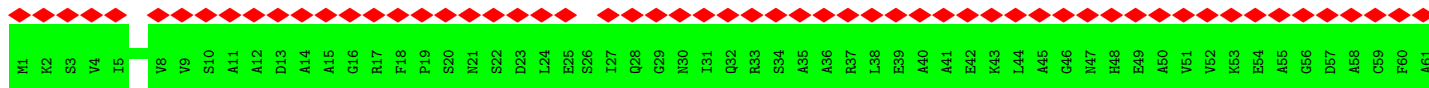


• Molecule 1: Phycoerythrin alpha subunit

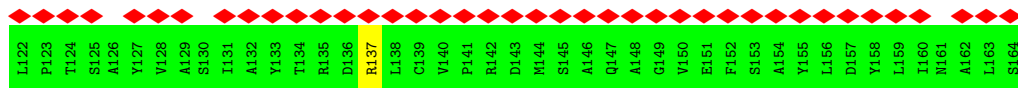
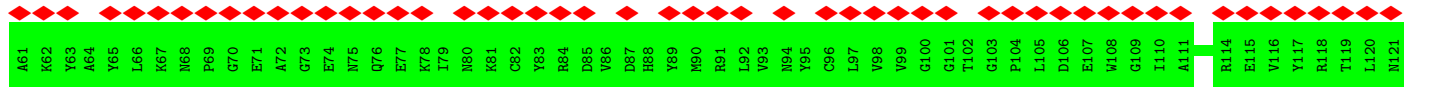
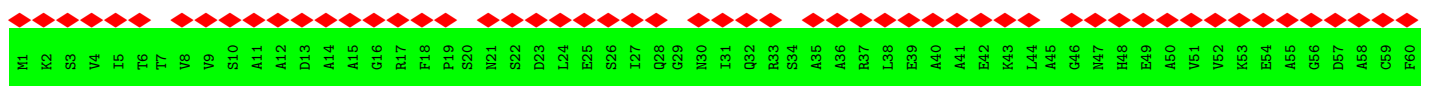
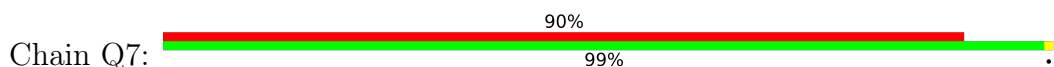




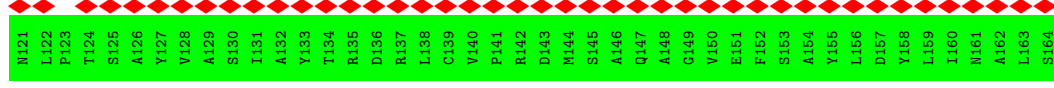
• Molecule 1: Phycoerythrin alpha subunit



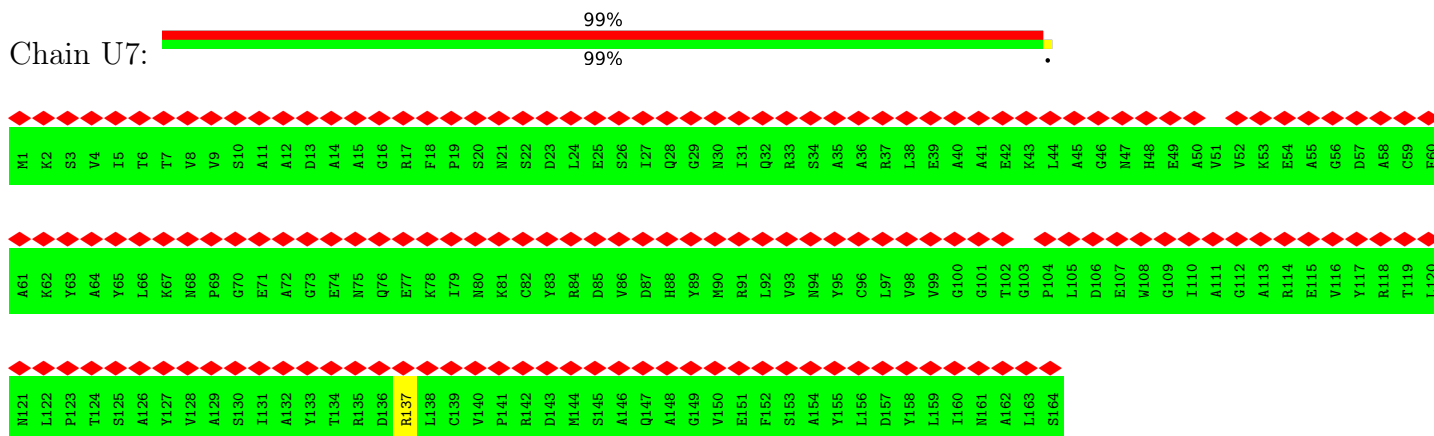
• Molecule 1: Phycoerythrin alpha subunit



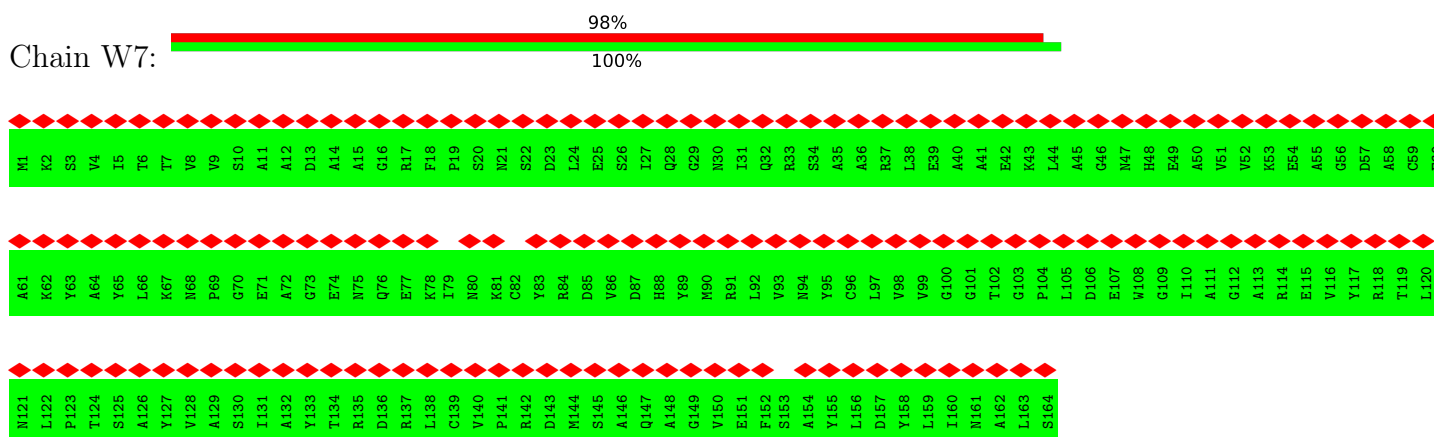
• Molecule 1: Phycoerythrin alpha subunit



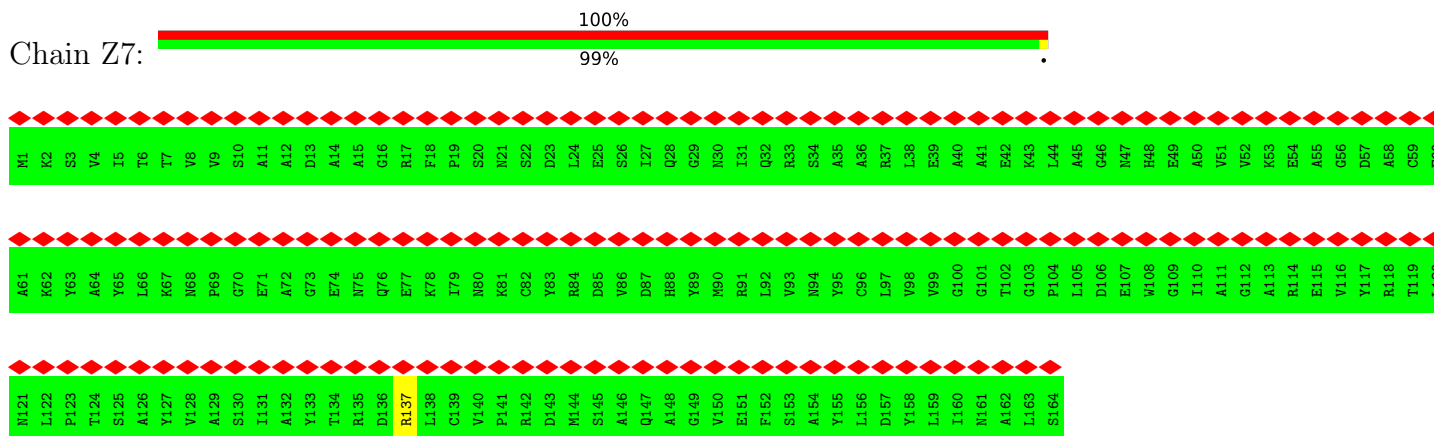
• Molecule 1: Phycoerythrin alpha subunit



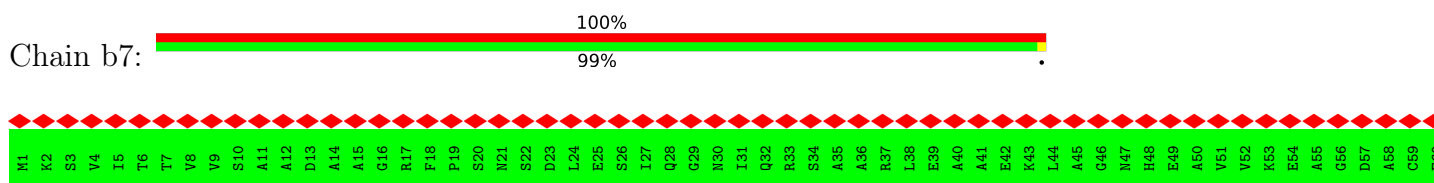
• Molecule 1: Phycoerythrin alpha subunit

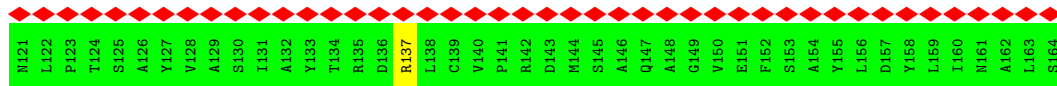
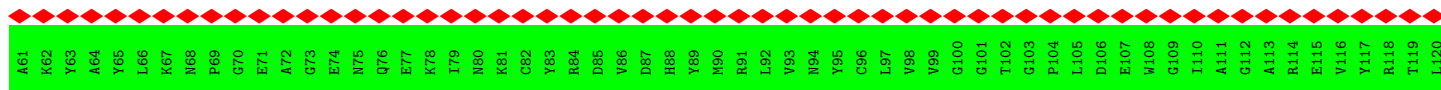


• Molecule 1: Phycoerythrin alpha subunit

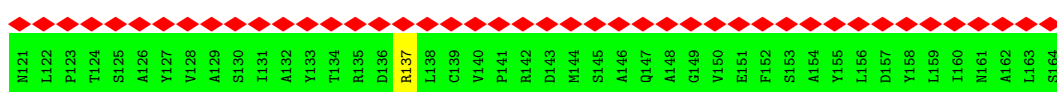
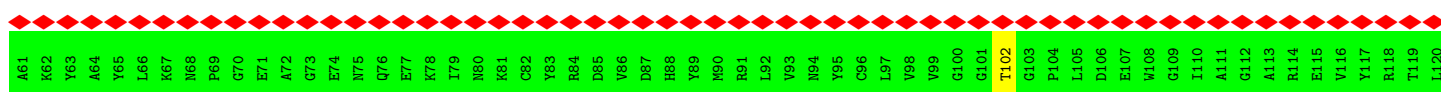
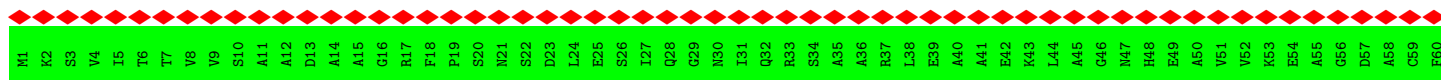


• Molecule 1: Phycoerythrin alpha subunit

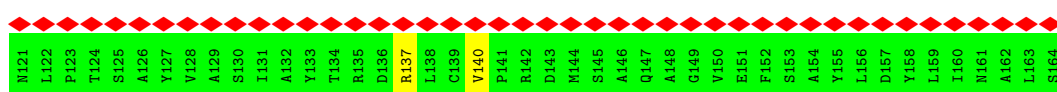
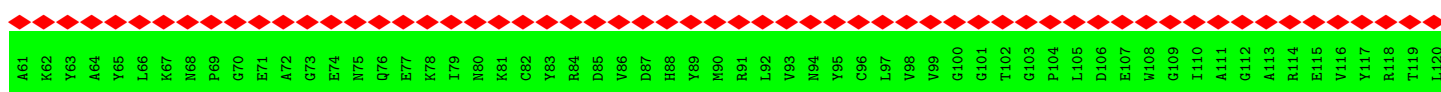
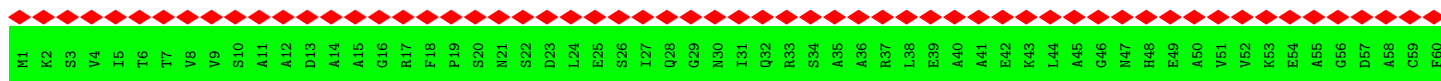




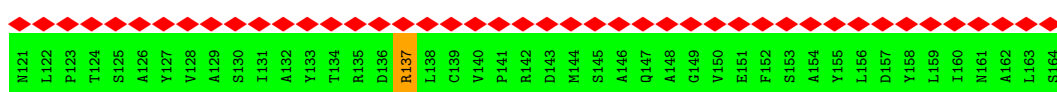
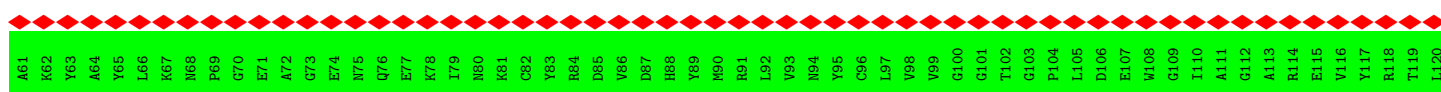
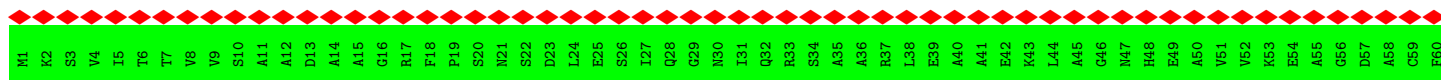
• Molecule 1: Phycoerythrin alpha subunit



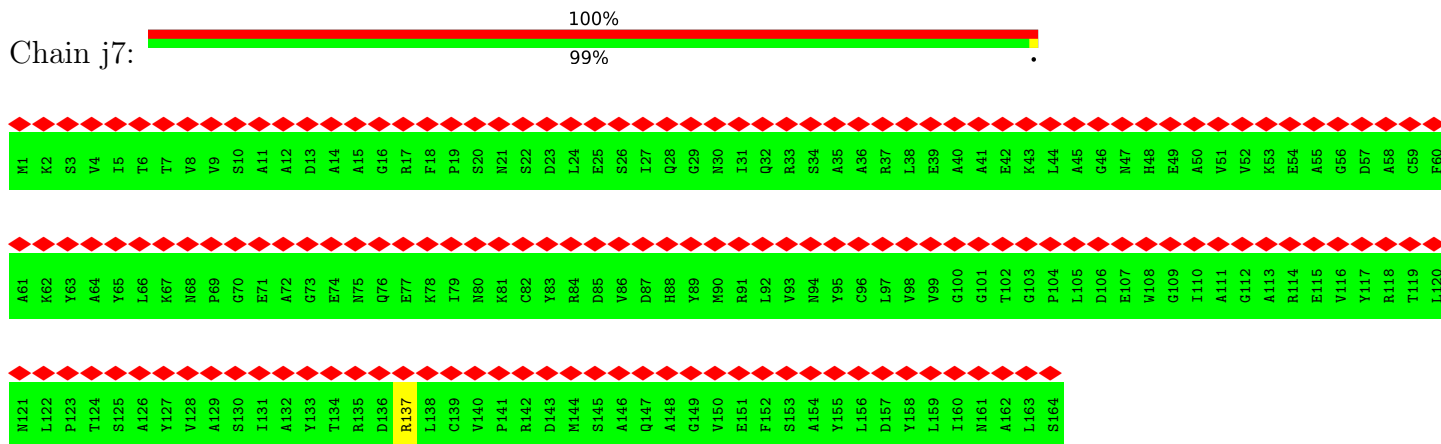
• Molecule 1: Phycoerythrin alpha subunit



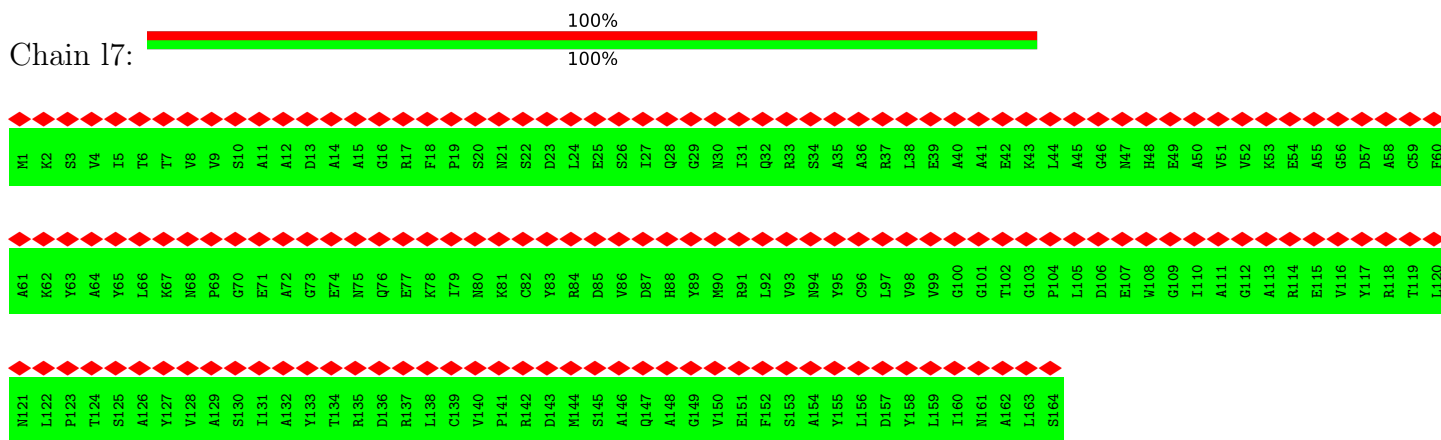
• Molecule 1: Phycoerythrin alpha subunit



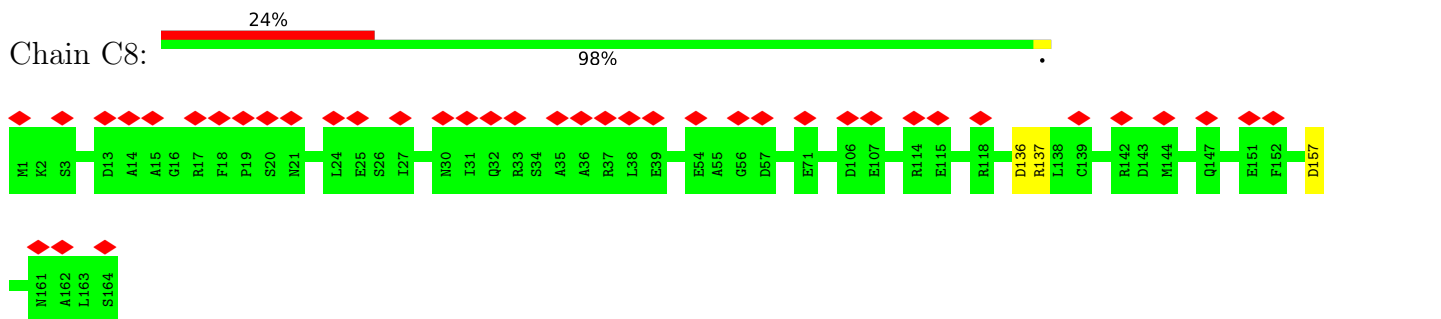
• Molecule 1: Phycoerythrin alpha subunit



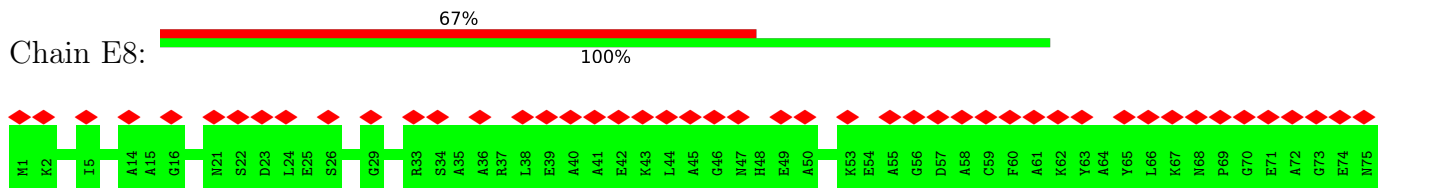
• Molecule 1: Phycoerythrin alpha subunit

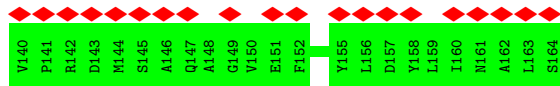
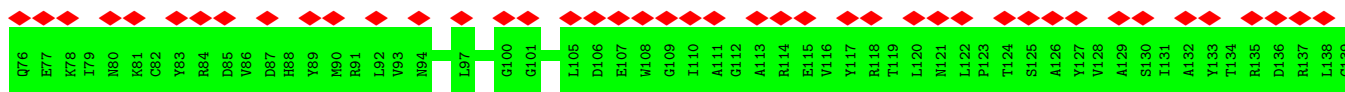


• Molecule 1: Phycoerythrin alpha subunit

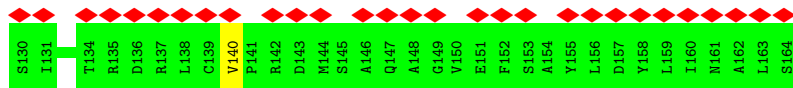
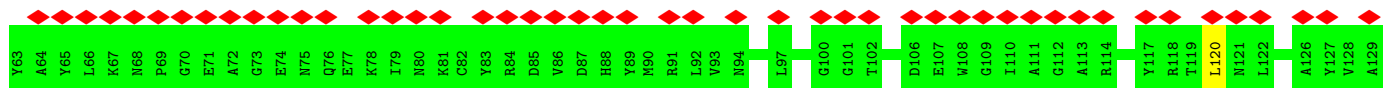
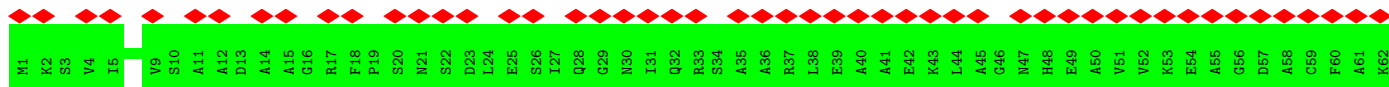
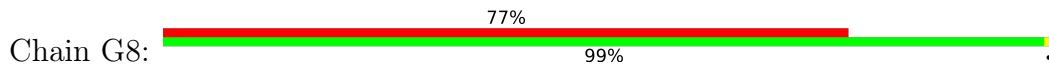


• Molecule 1: Phycoerythrin alpha subunit

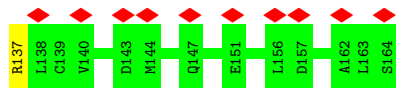
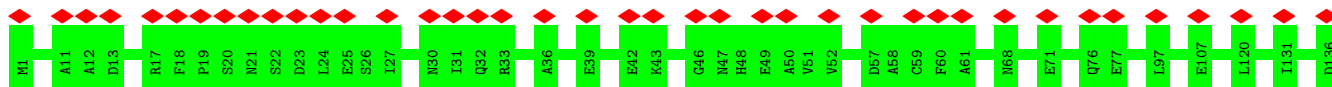




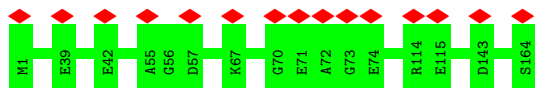
• Molecule 1: Phycoerythrin alpha subunit



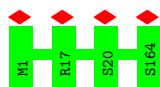
• Molecule 1: Phycoerythrin alpha subunit



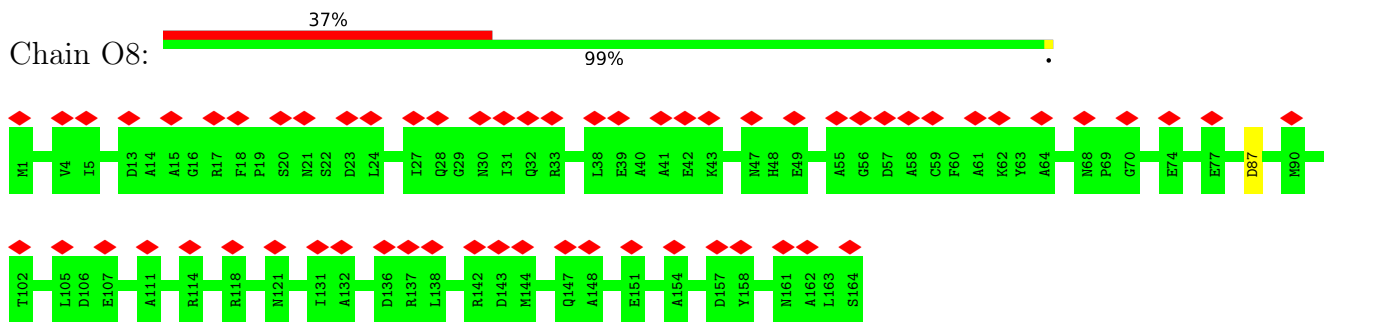
• Molecule 1: Phycoerythrin alpha subunit



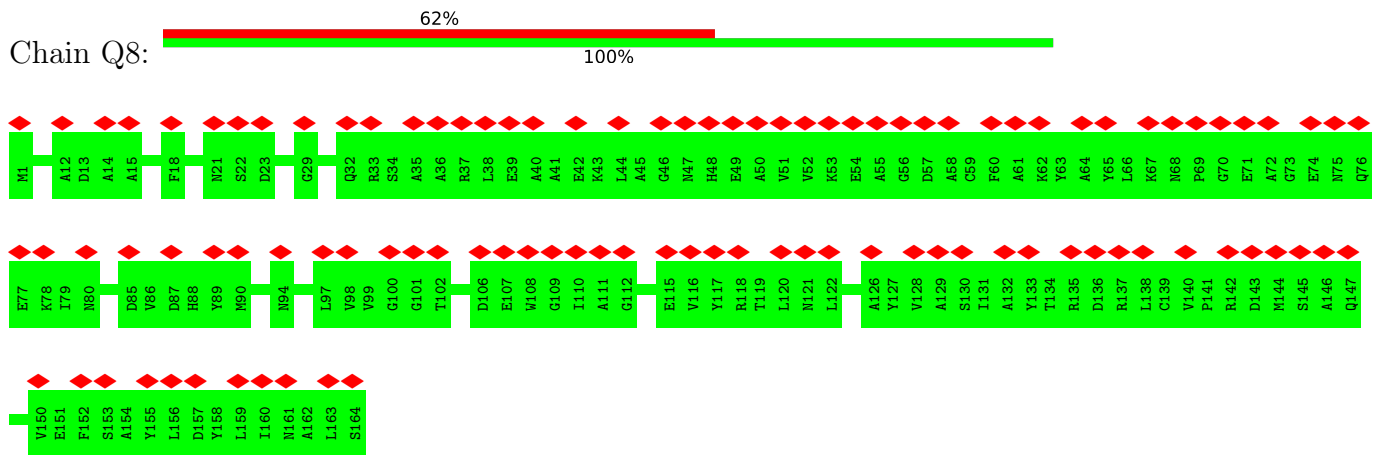
• Molecule 1: Phycoerythrin alpha subunit



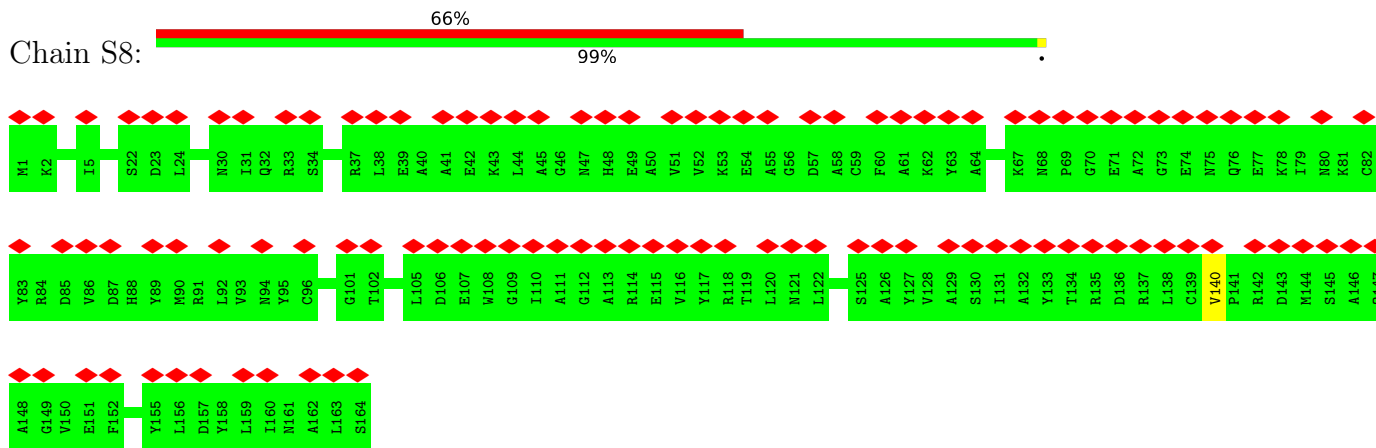
• Molecule 1: Phycoerythrin alpha subunit



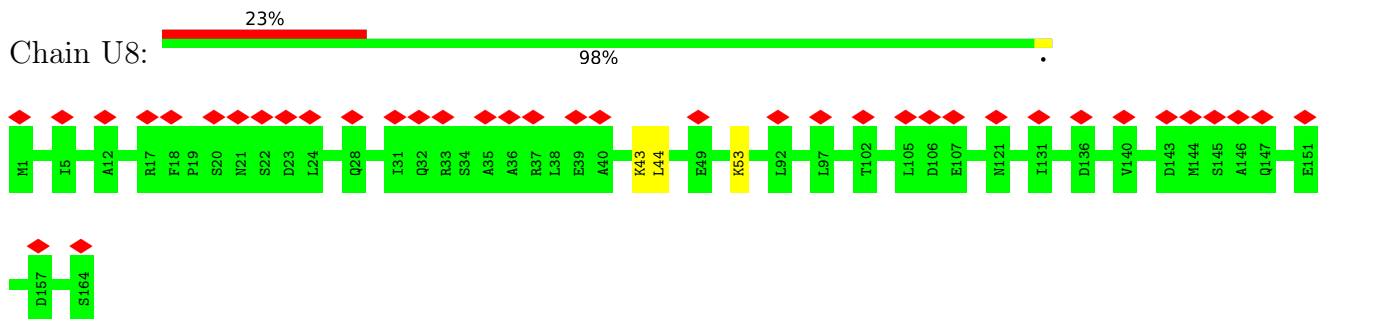
• Molecule 1: Phycoerythrin alpha subunit



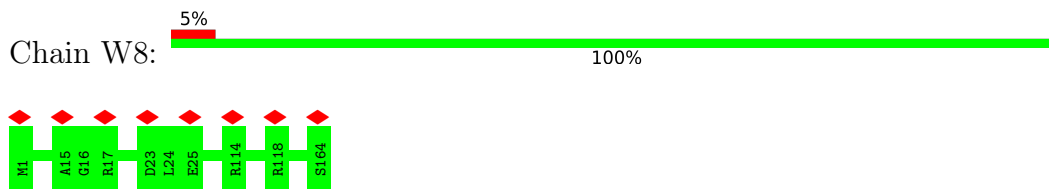
• Molecule 1: Phycoerythrin alpha subunit



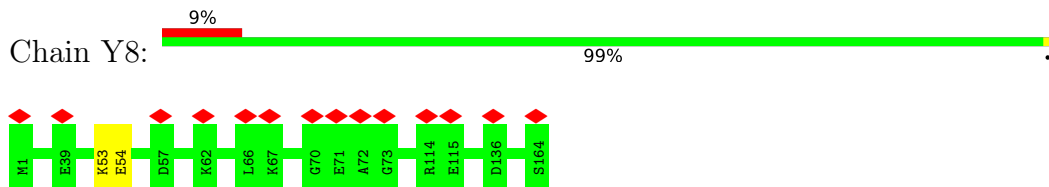
• Molecule 1: Phycoerythrin alpha subunit



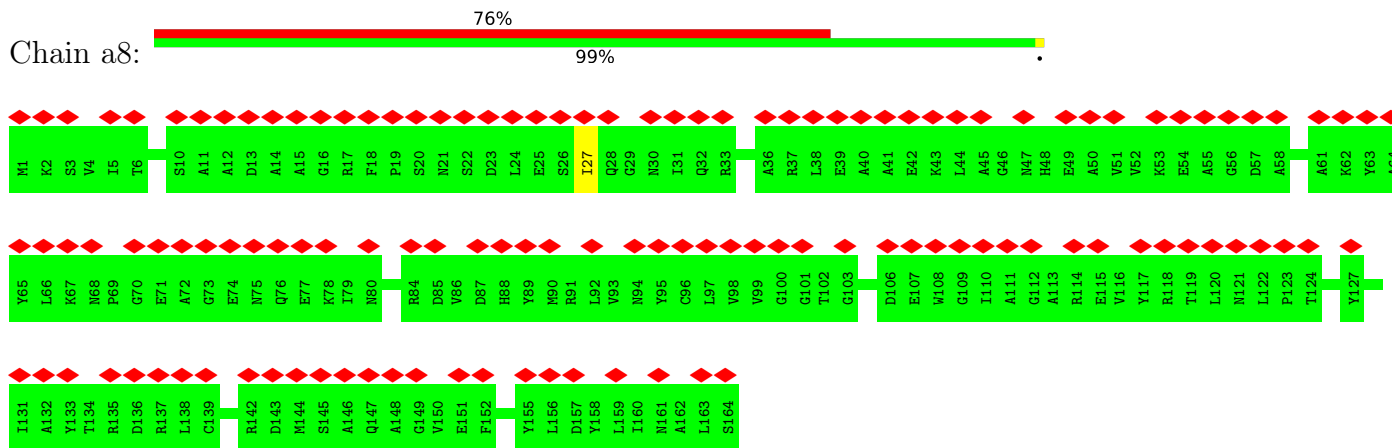
• Molecule 1: Phycoerythrin alpha subunit



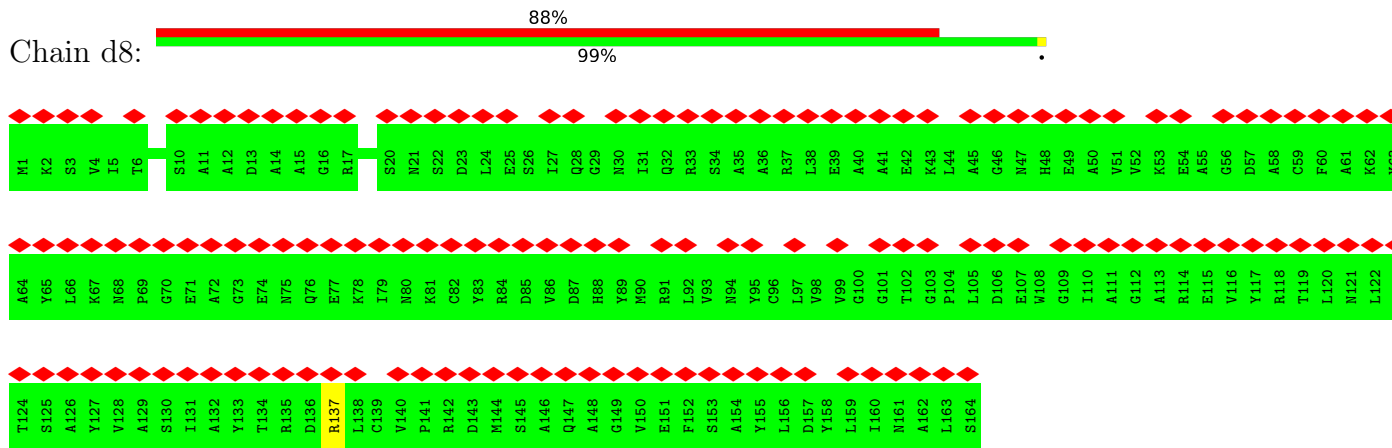
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

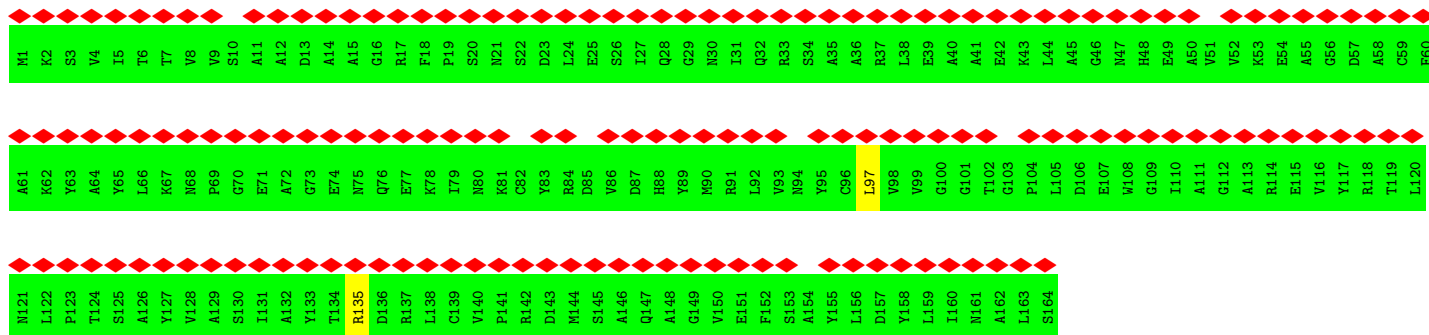


• Molecule 1: Phycoerythrin alpha subunit

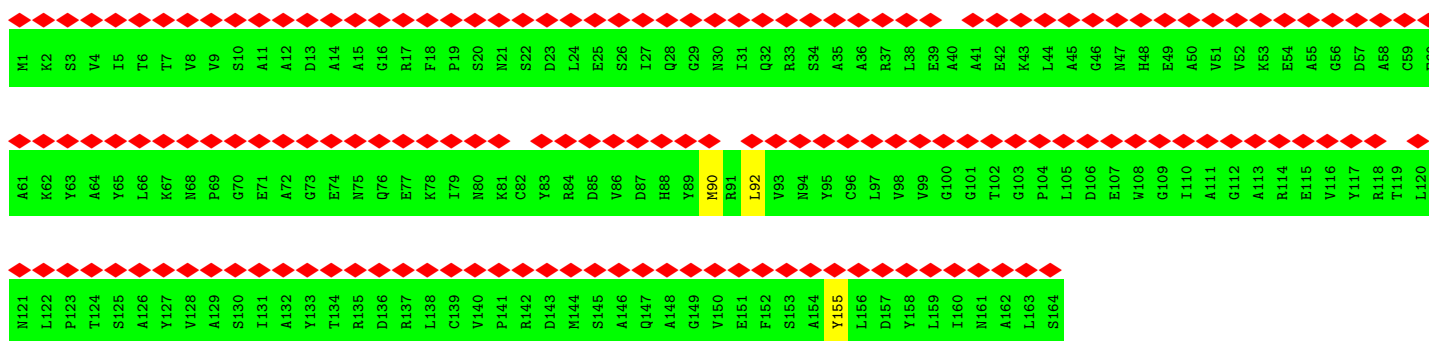


• Molecule 1: Phycoerythrin alpha subunit

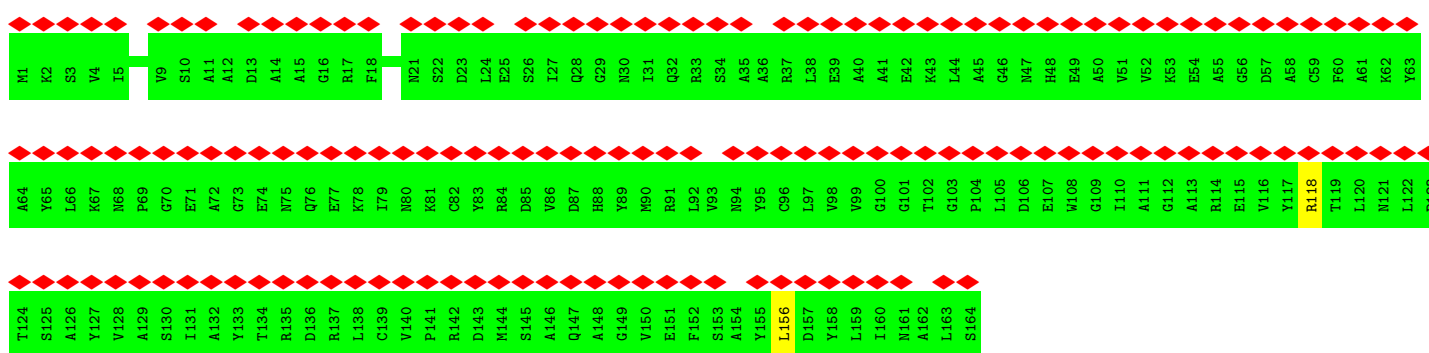




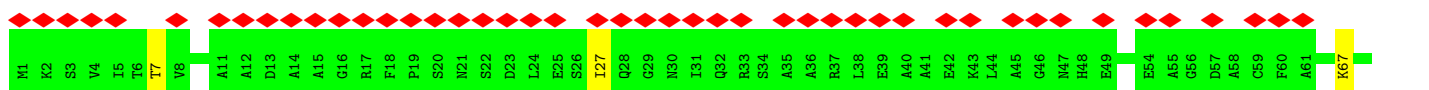
• Molecule 1: Phycoerythrin alpha subunit

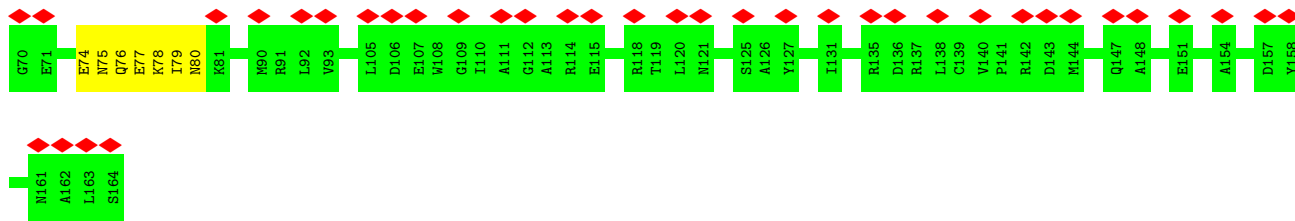


• Molecule 1: Phycoerythrin alpha subunit

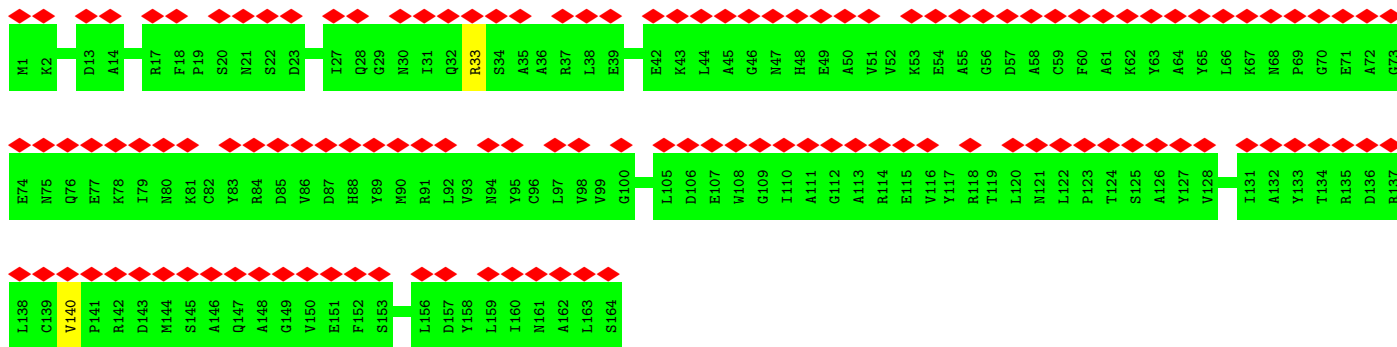
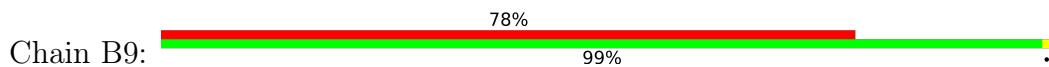


• Molecule 1: Phycoerythrin alpha subunit

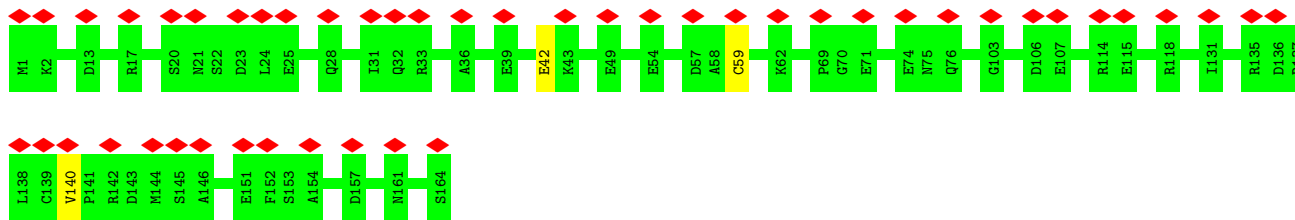




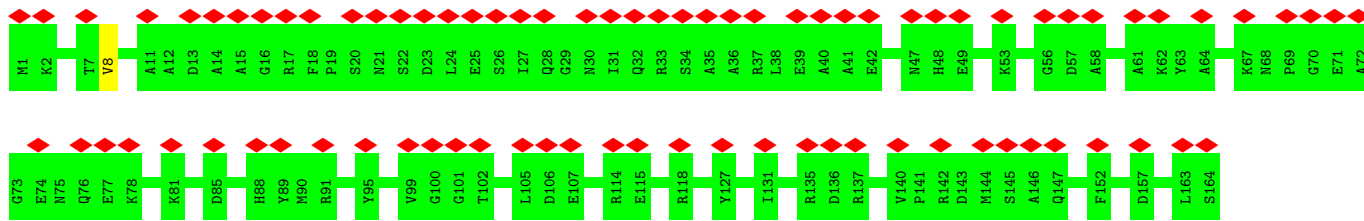
• Molecule 1: Phycoerythrin alpha subunit



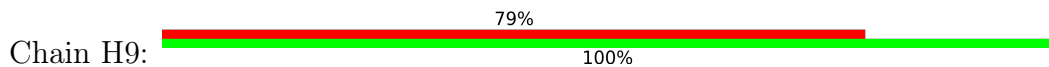
• Molecule 1: Phycoerythrin alpha subunit

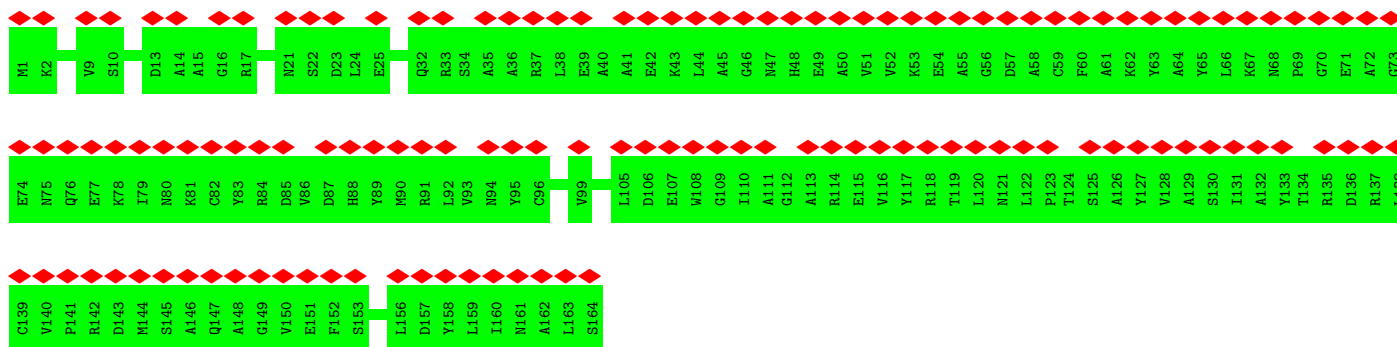


• Molecule 1: Phycoerythrin alpha subunit

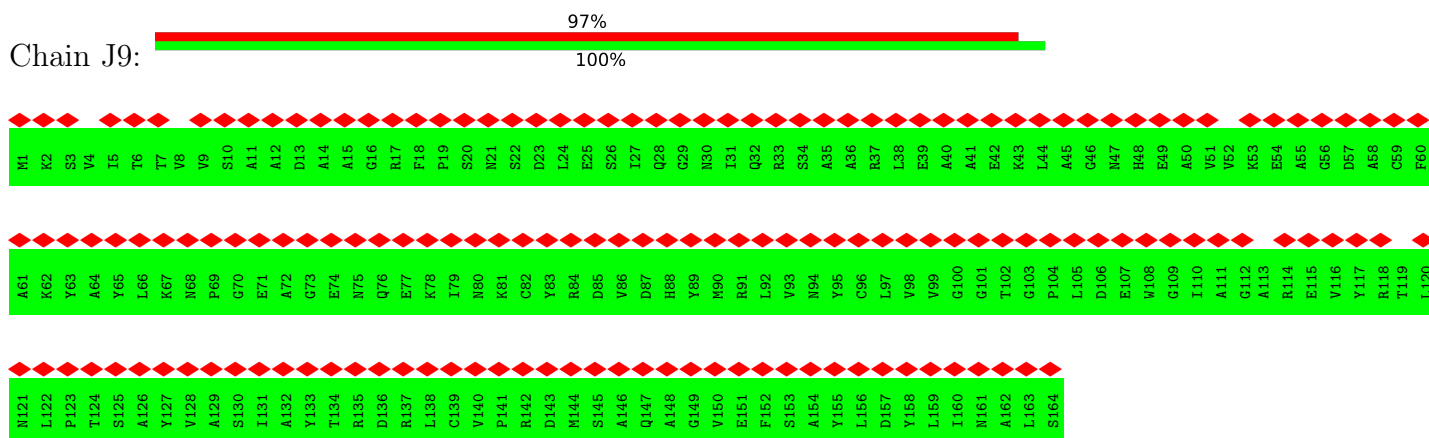


• Molecule 1: Phycoerythrin alpha subunit

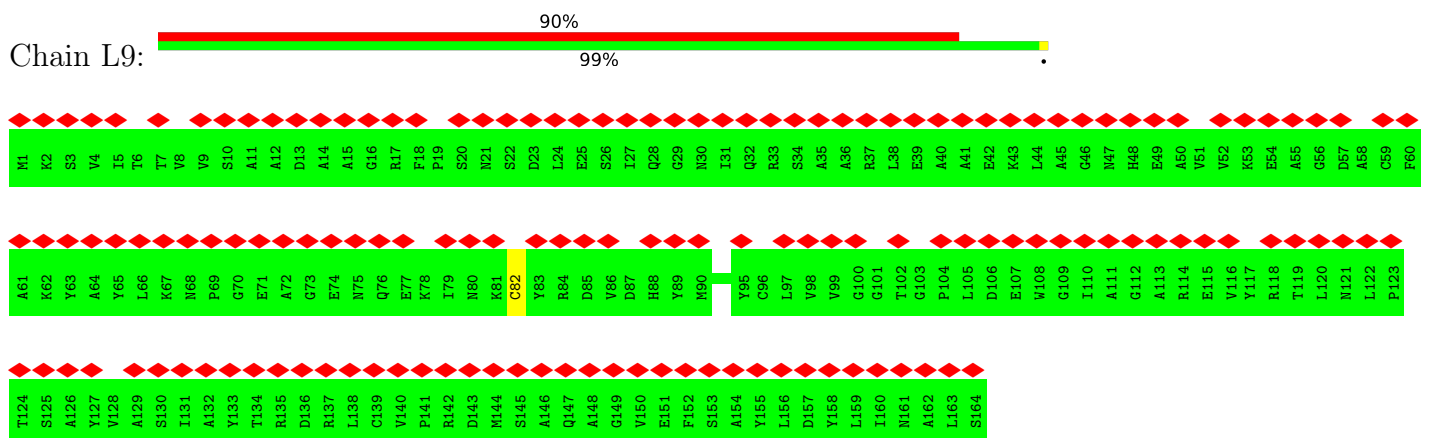




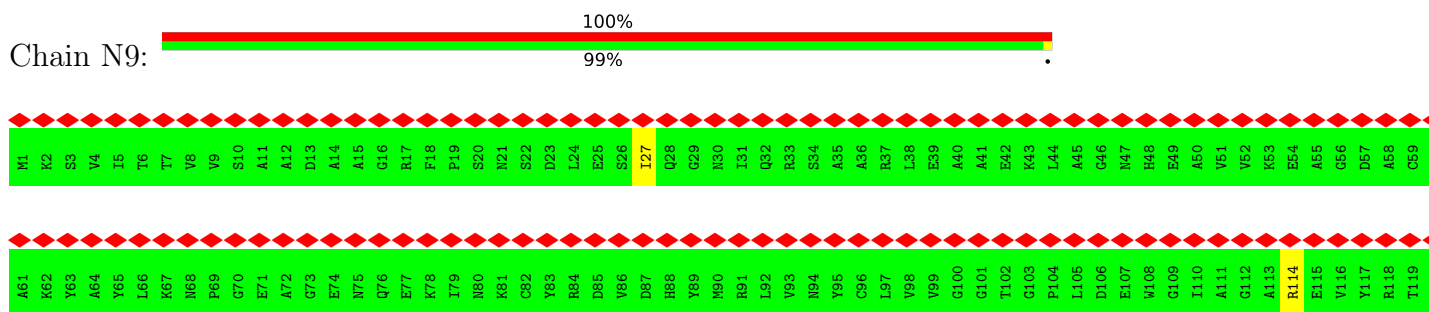
• Molecule 1: Phycoerythrin alpha subunit

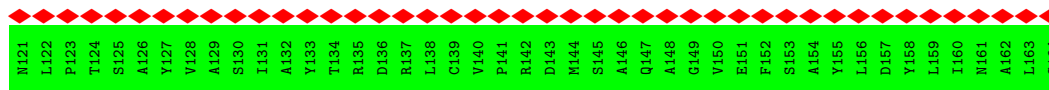


• Molecule 1: Phycoerythrin alpha subunit

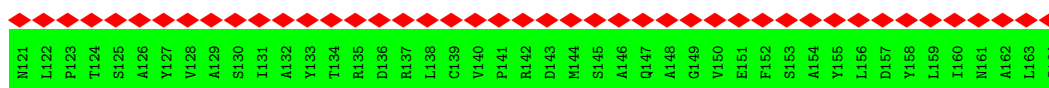
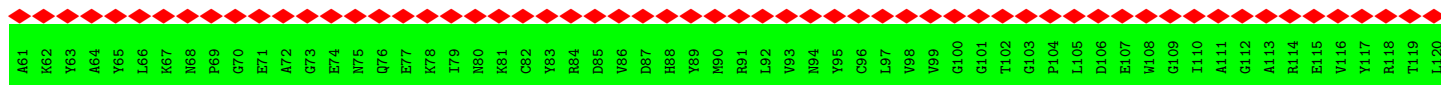
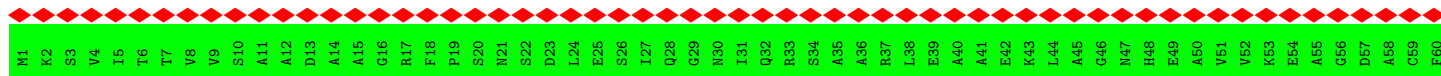


• Molecule 1: Phycoerythrin alpha subunit

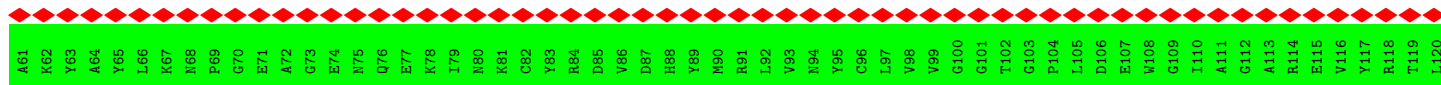
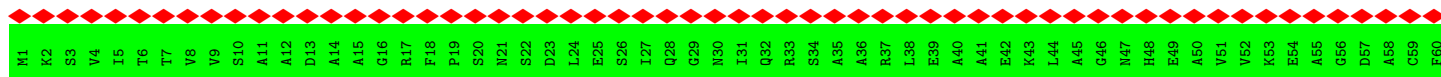




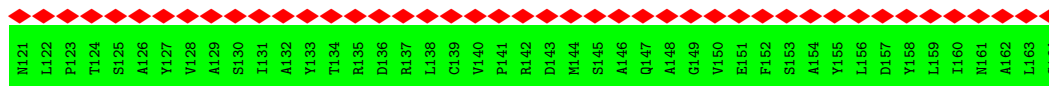
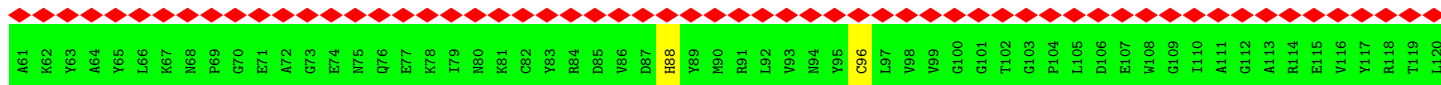
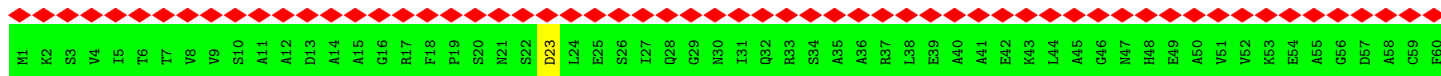
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

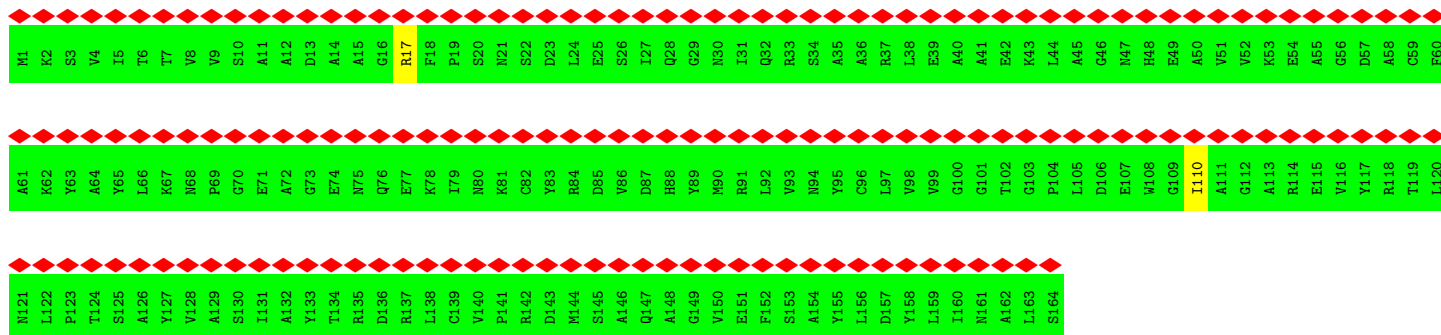


• Molecule 1: Phycoerythrin alpha subunit

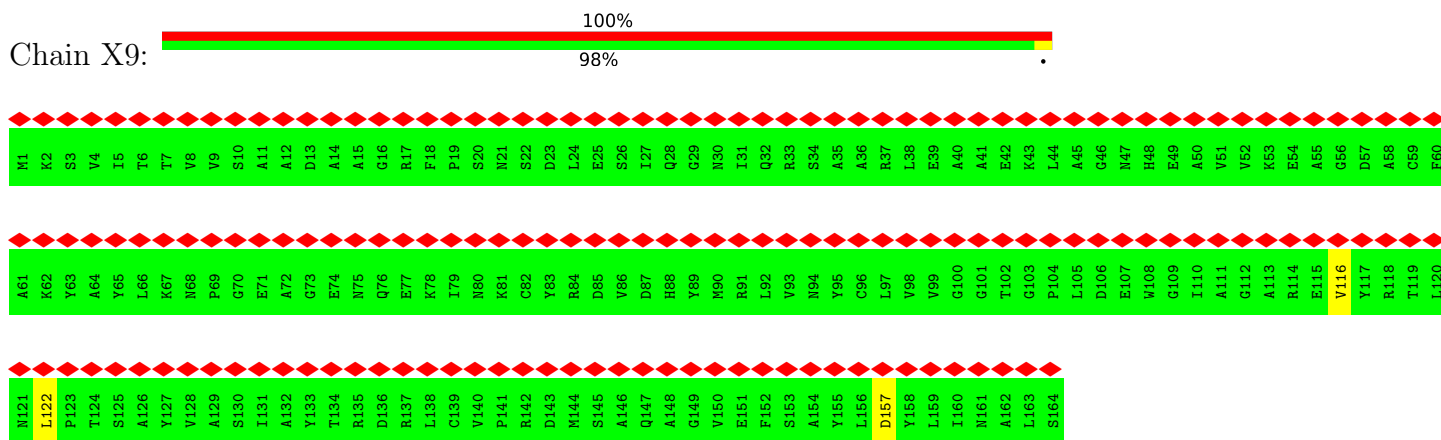


• Molecule 1: Phycoerythrin alpha subunit

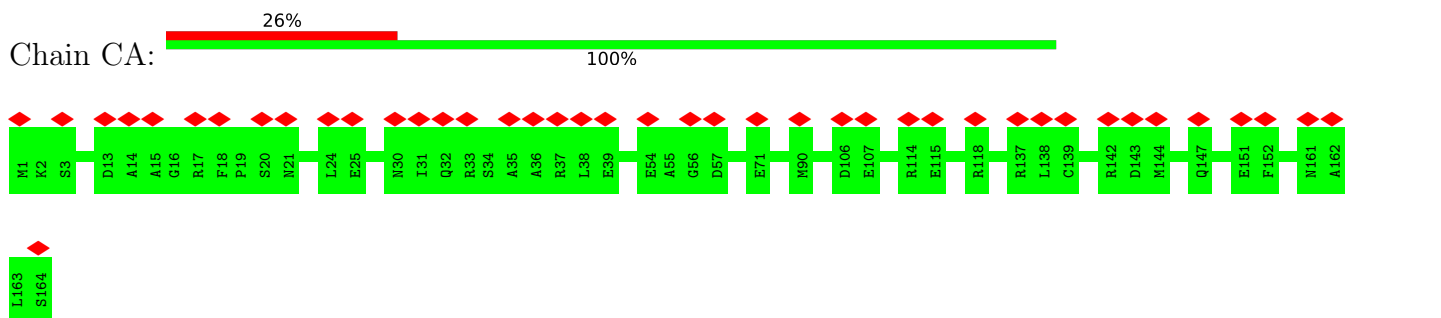




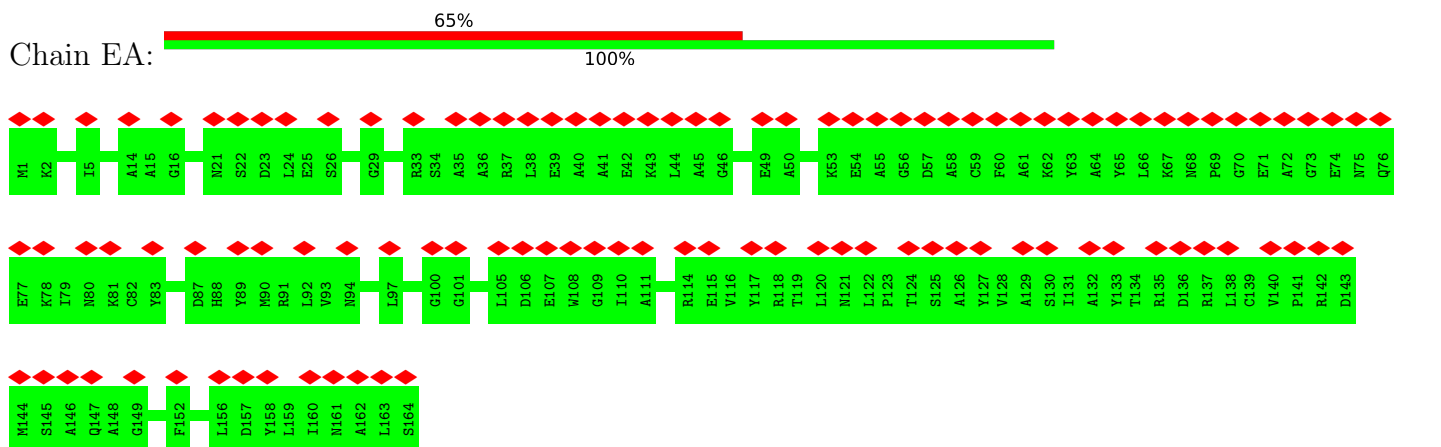
• Molecule 1: Phycoerythrin alpha subunit



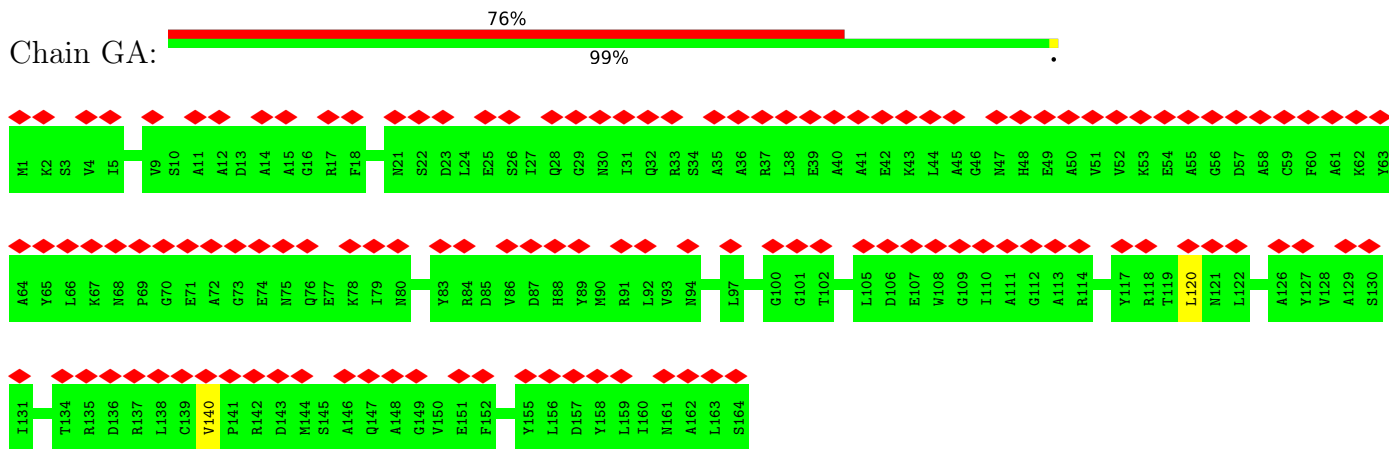
• Molecule 1: Phycoerythrin alpha subunit



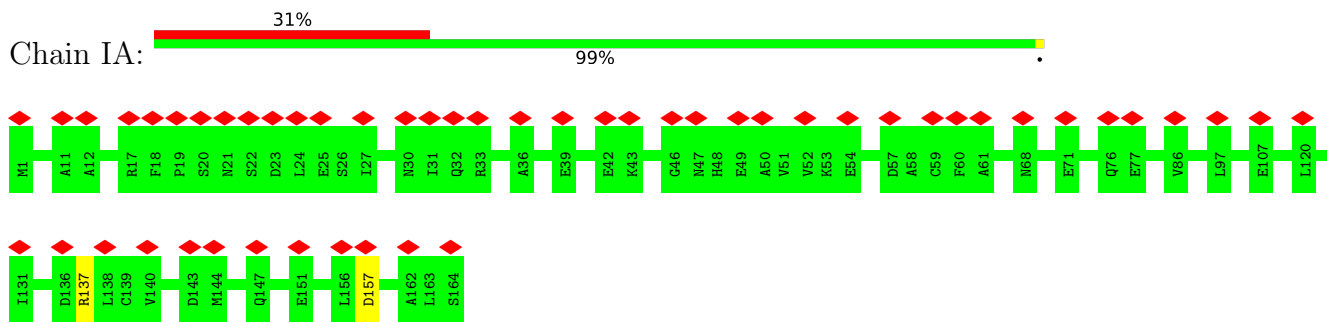
• Molecule 1: Phycoerythrin alpha subunit



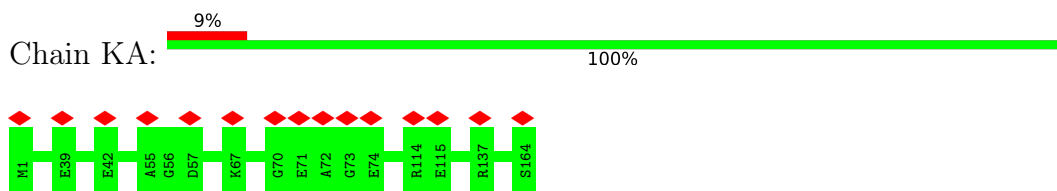
• Molecule 1: Phycoerythrin alpha subunit



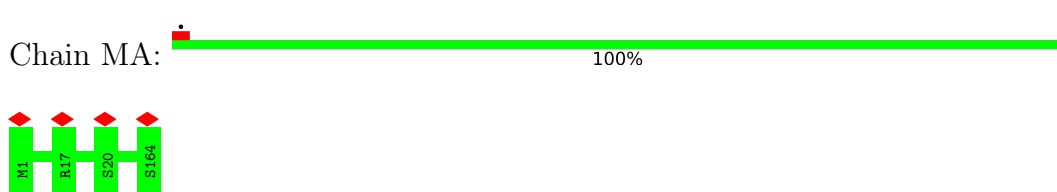
• Molecule 1: Phycoerythrin alpha subunit



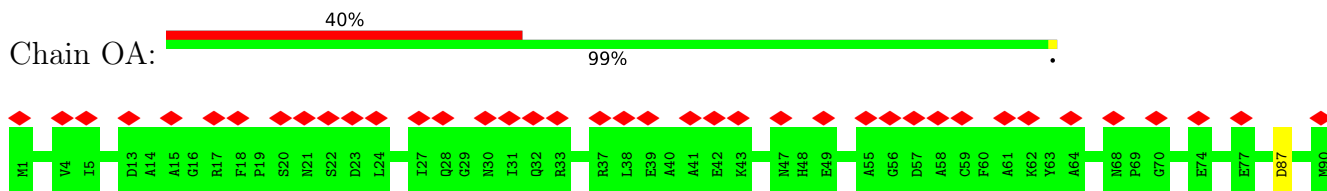
• Molecule 1: Phycoerythrin alpha subunit

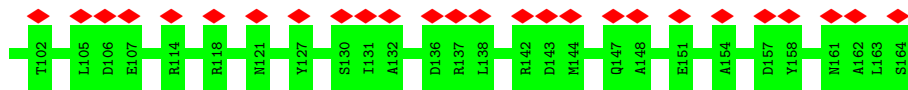


• Molecule 1: Phycoerythrin alpha subunit

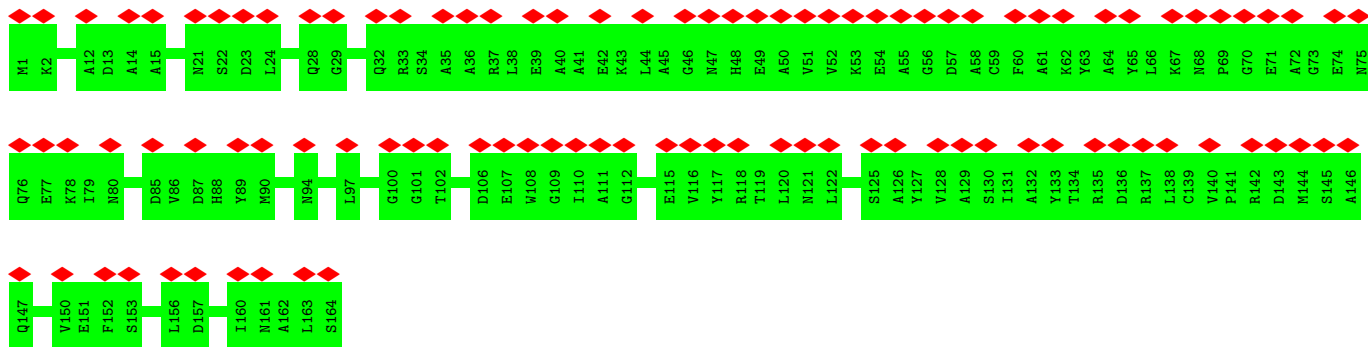


• Molecule 1: Phycoerythrin alpha subunit

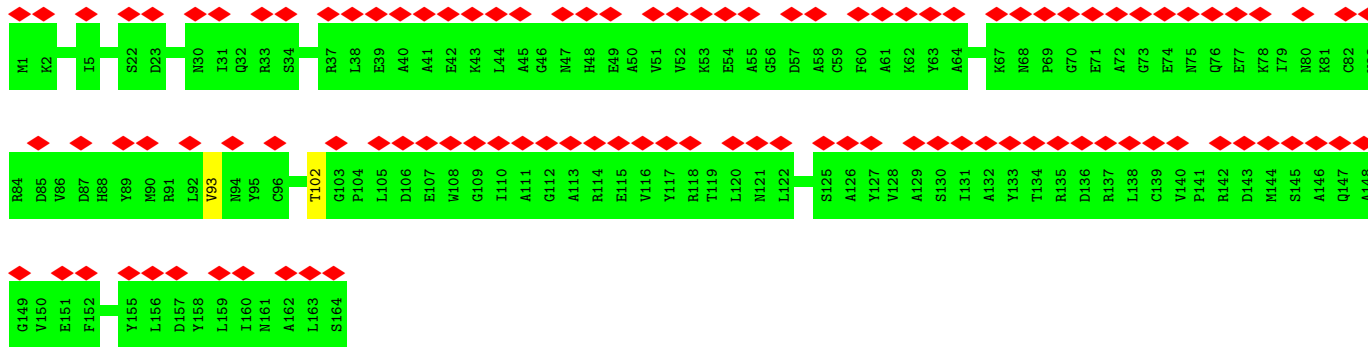




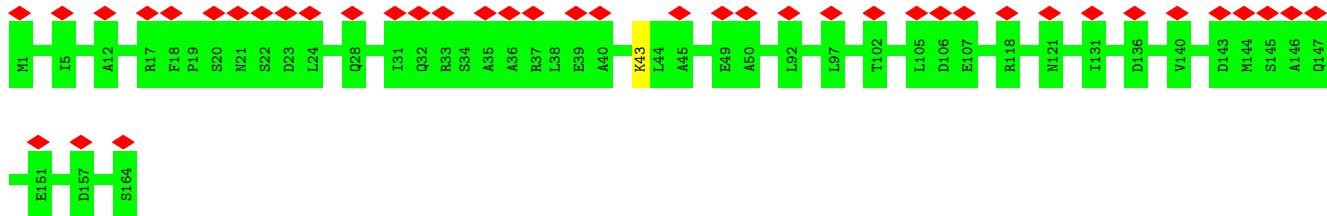
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

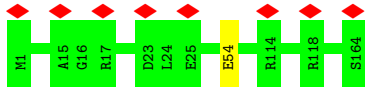


• Molecule 1: Phycoerythrin alpha subunit

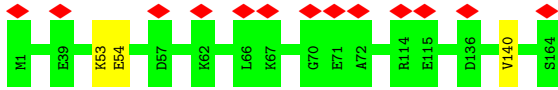


• Molecule 1: Phycoerythrin alpha subunit

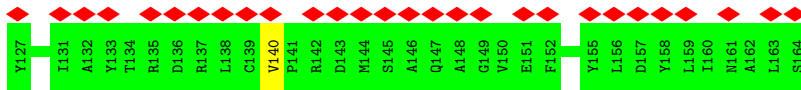
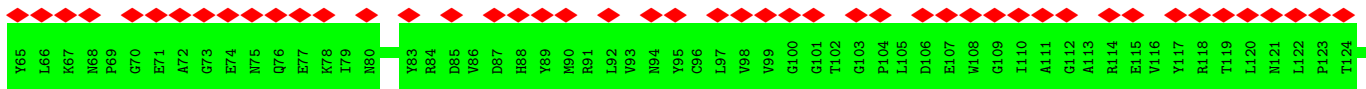
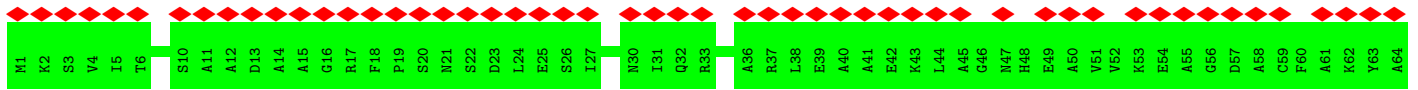
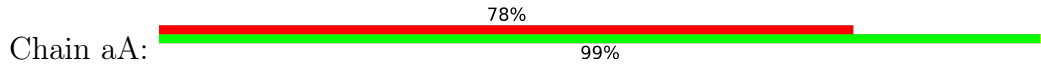




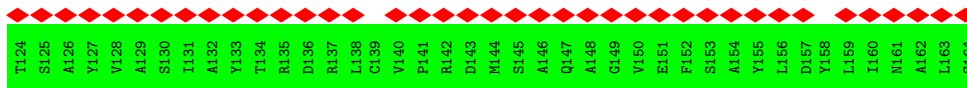
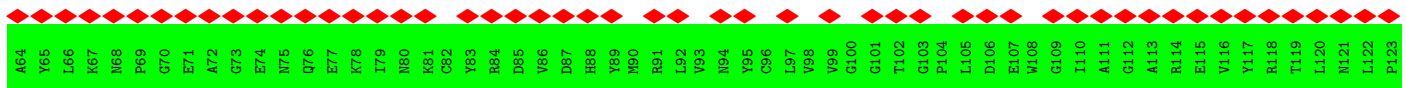
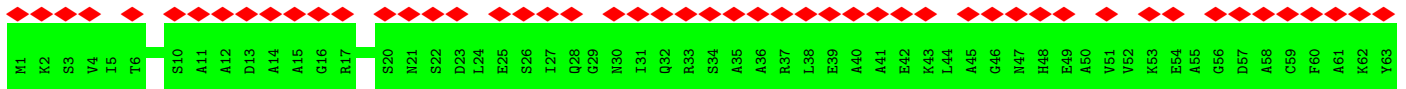
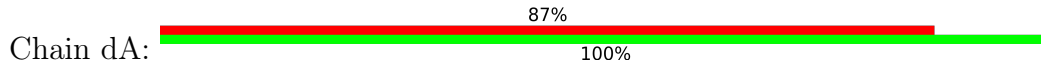
• Molecule 1: Phycoerythrin alpha subunit



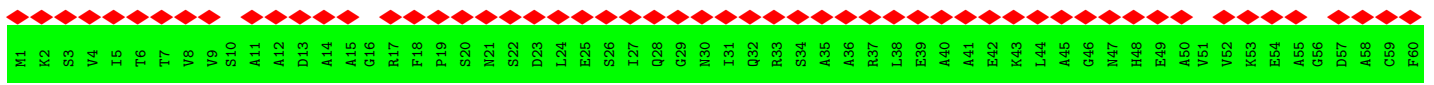
• Molecule 1: Phycoerythrin alpha subunit

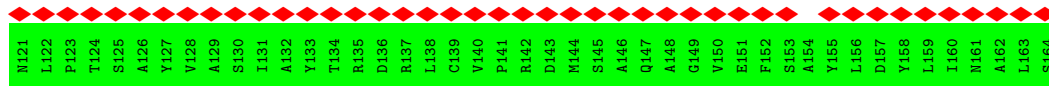
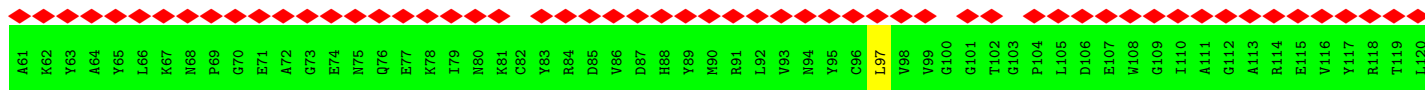


• Molecule 1: Phycoerythrin alpha subunit

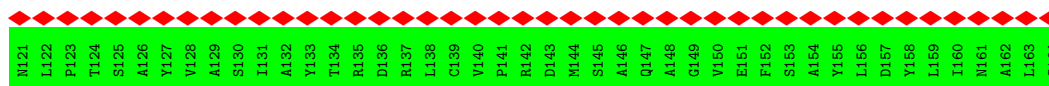
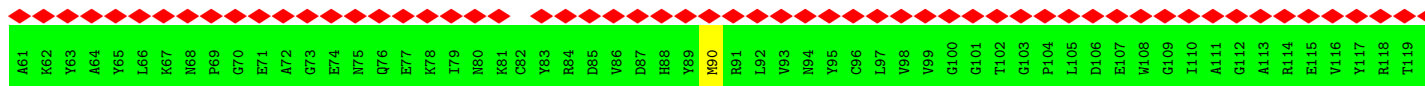
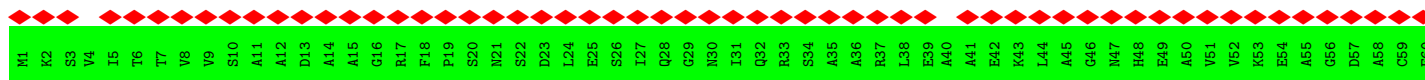


• Molecule 1: Phycoerythrin alpha subunit

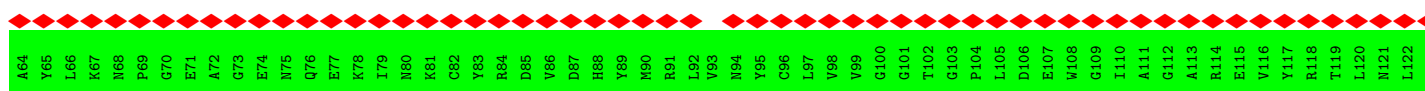




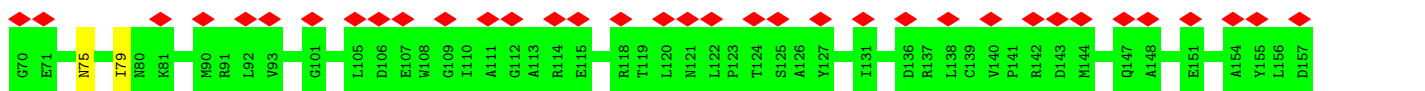
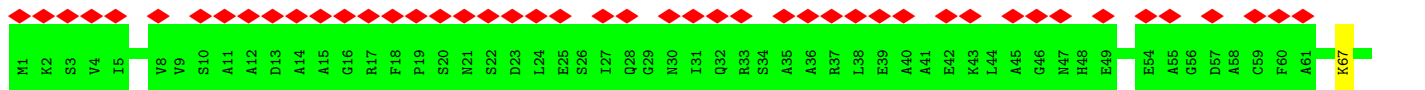
• Molecule 1: Phycoerythrin alpha subunit

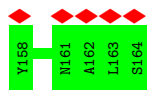


• Molecule 1: Phycoerythrin alpha subunit

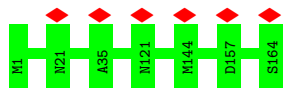


• Molecule 1: Phycoerythrin alpha subunit

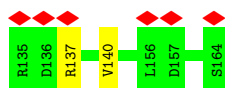
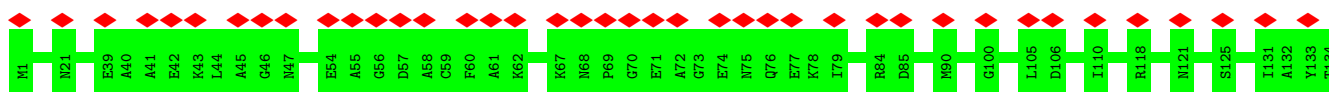




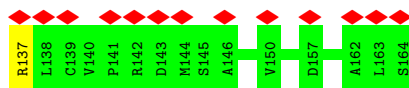
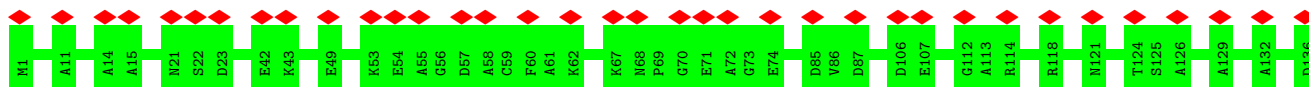
- Molecule 1: Phycoerythrin alpha subunit



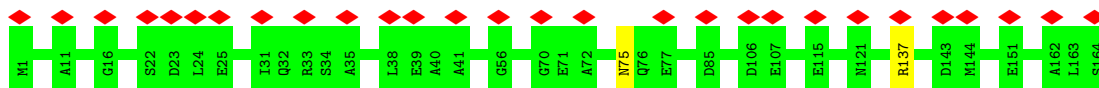
- Molecule 1: Phycoerythrin alpha subunit



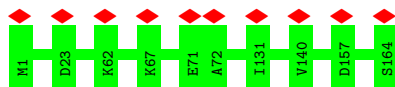
- Molecule 1: Phycoerythrin alpha subunit



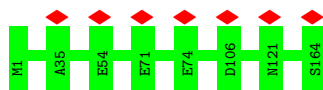
- Molecule 1: Phycoerythrin alpha subunit



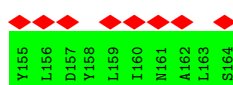
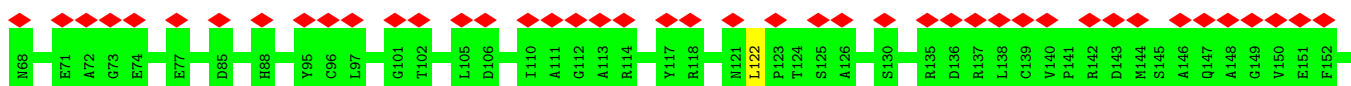
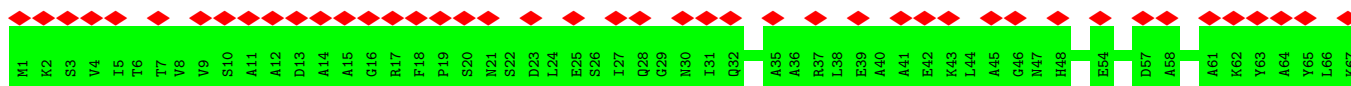
- Molecule 1: Phycoerythrin alpha subunit



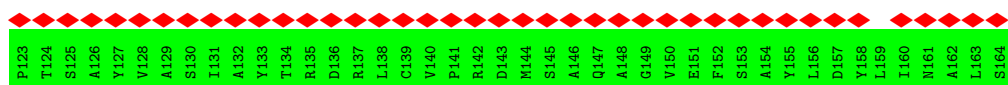
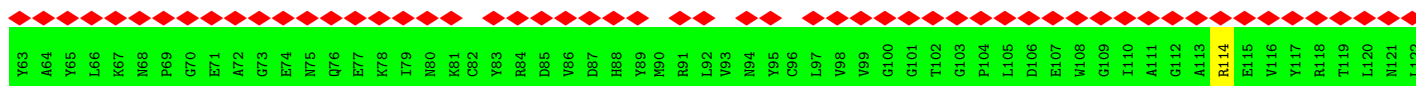
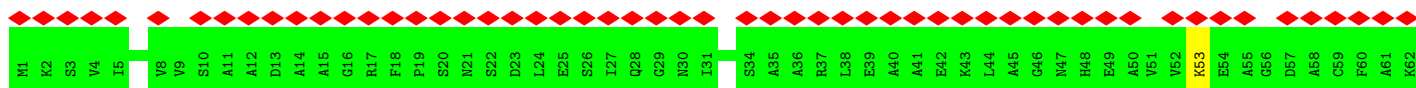
- Molecule 1: Phycoerythrin alpha subunit



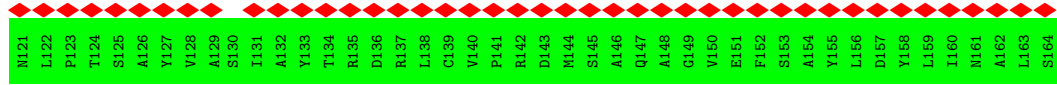
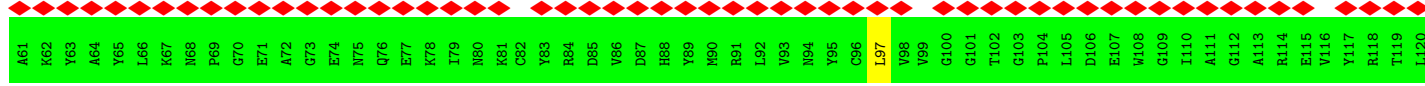
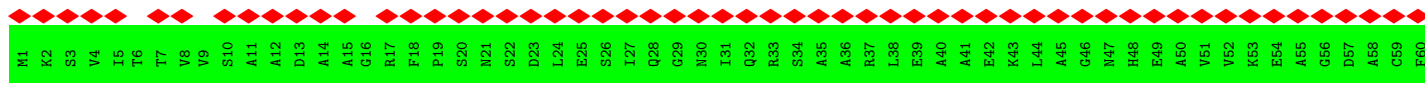
• Molecule 1: Phycoerythrin alpha subunit



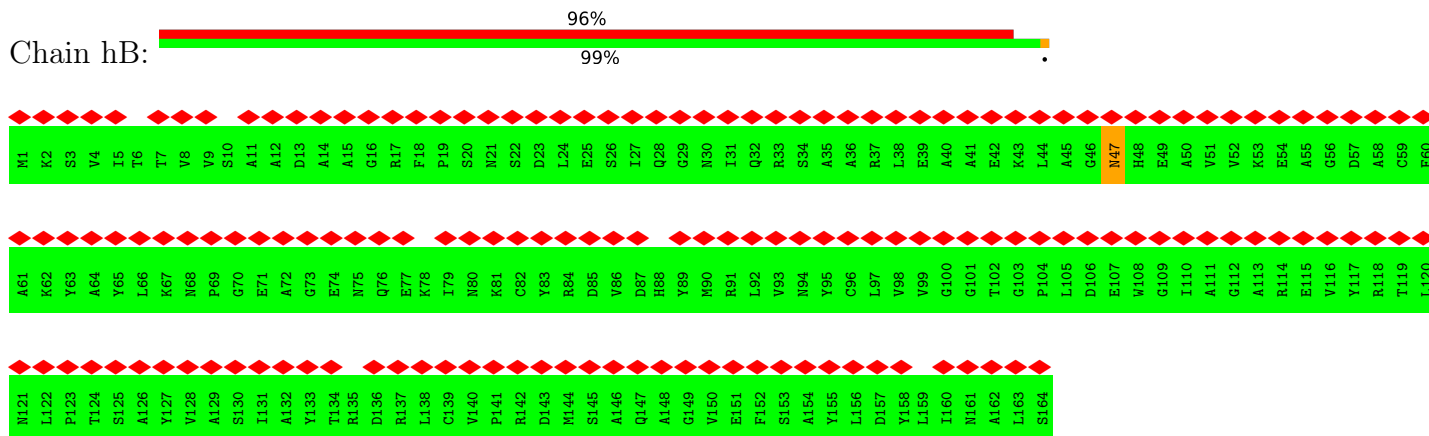
• Molecule 1: Phycoerythrin alpha subunit



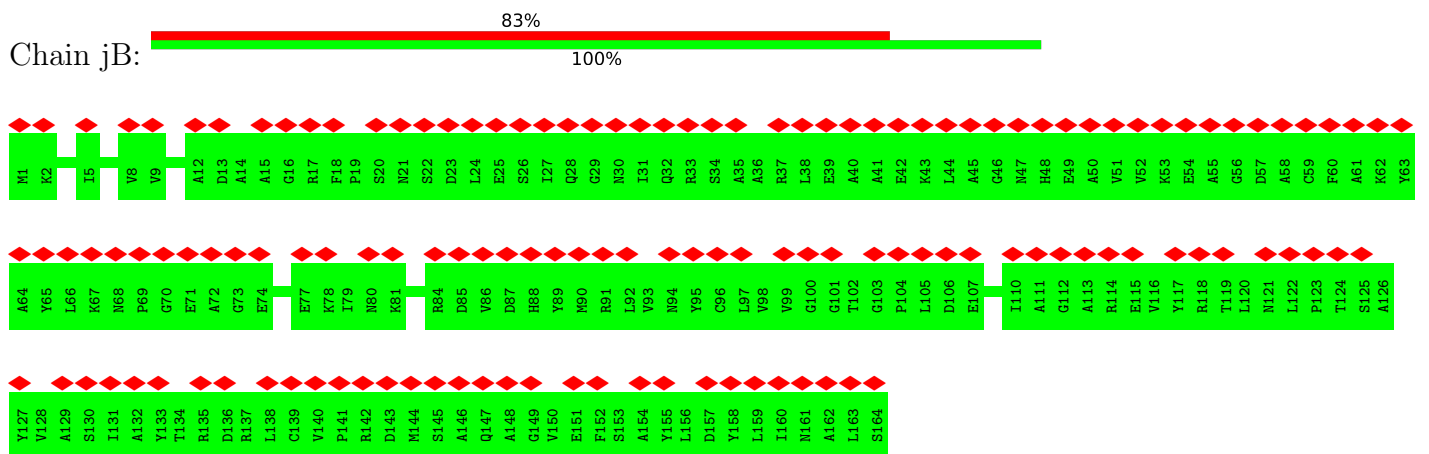
• Molecule 1: Phycoerythrin alpha subunit



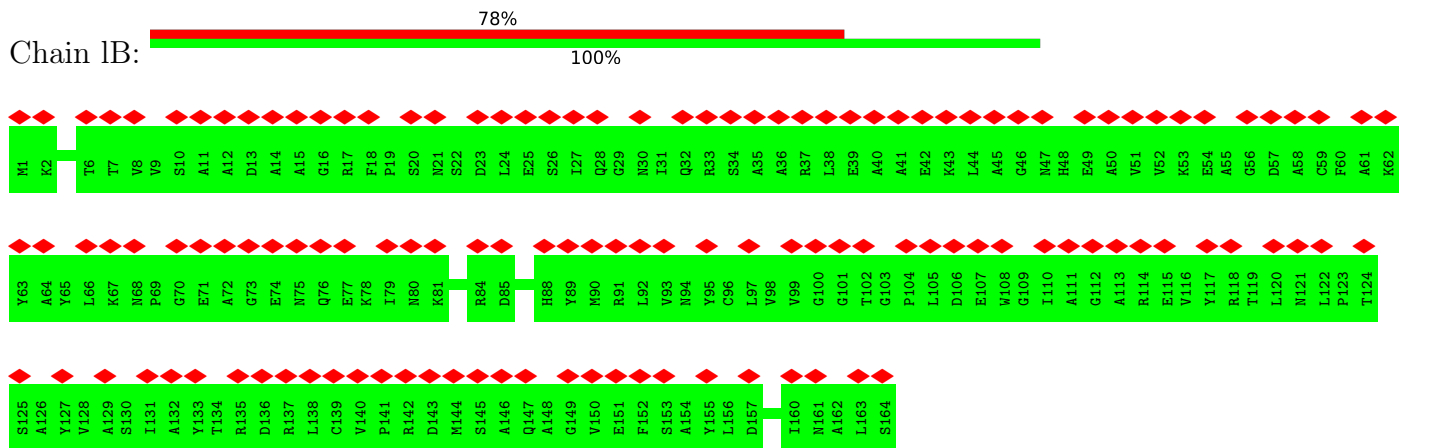
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

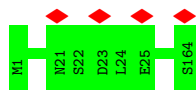


• Molecule 1: Phycoerythrin alpha subunit

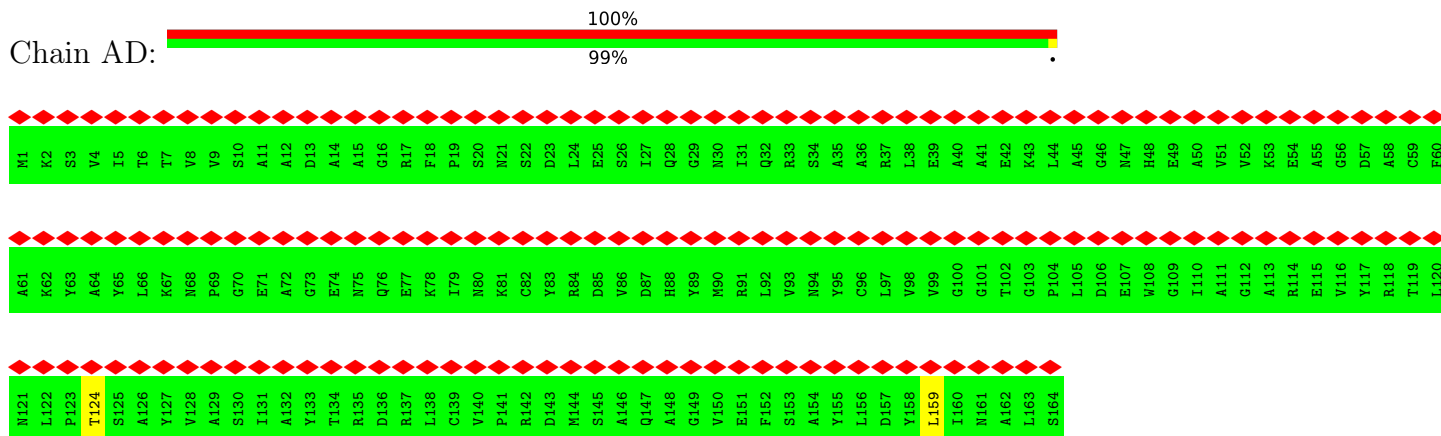


• Molecule 1: Phycoerythrin alpha subunit

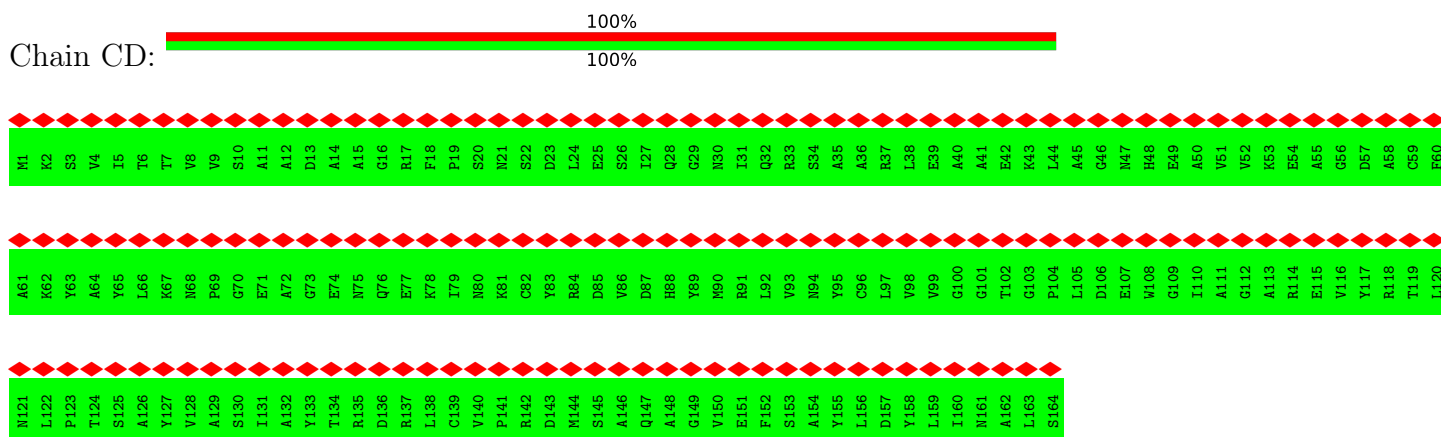




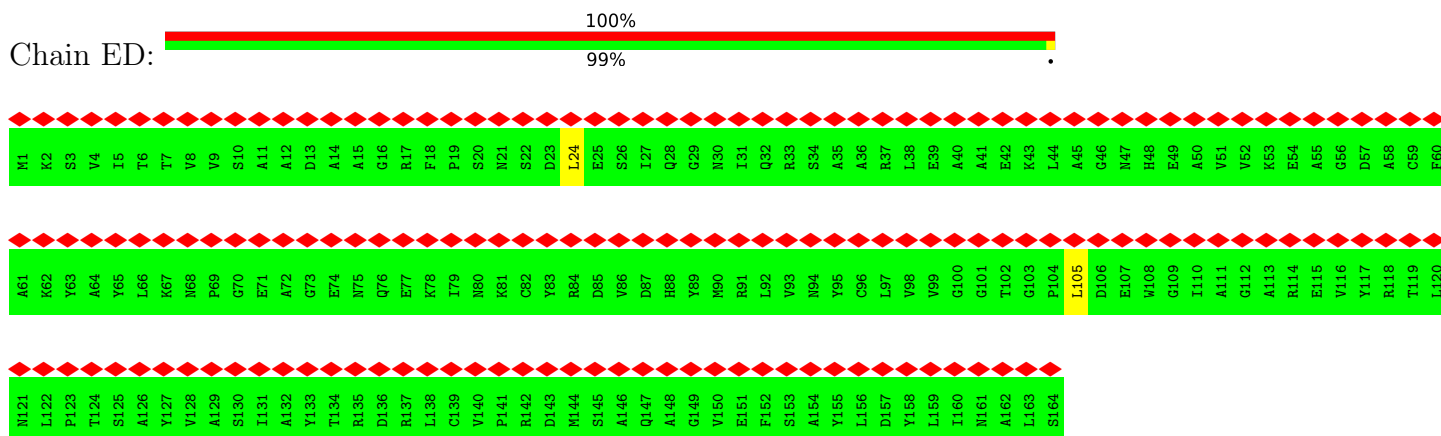
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit

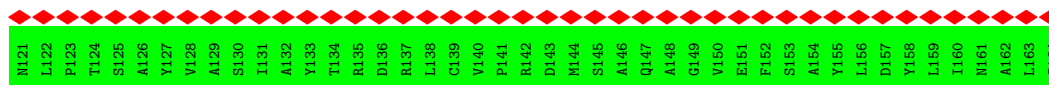
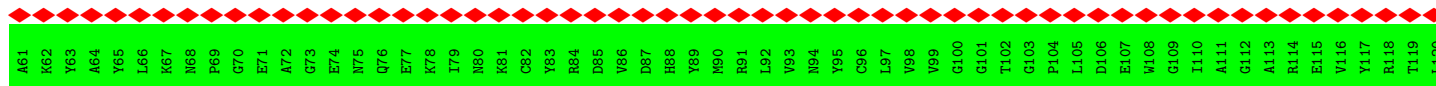
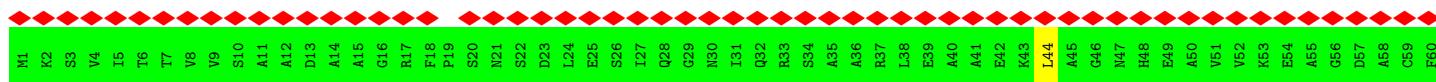


- Molecule 1: Phycoerythrin alpha subunit

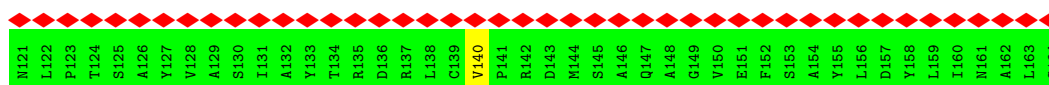
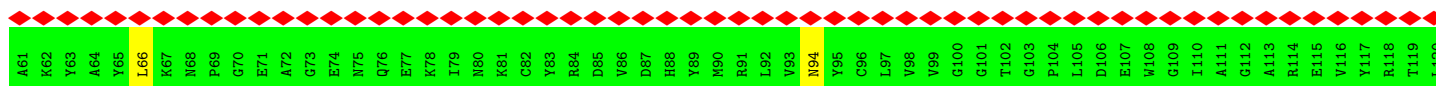


- Molecule 1: Phycoerythrin alpha subunit

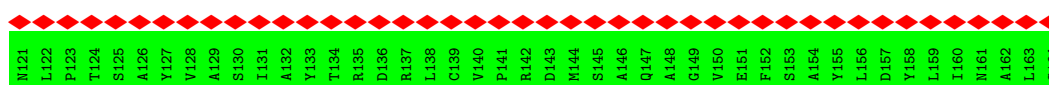
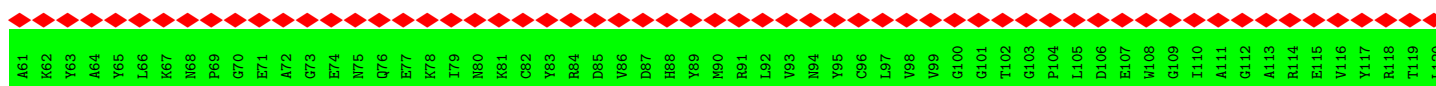
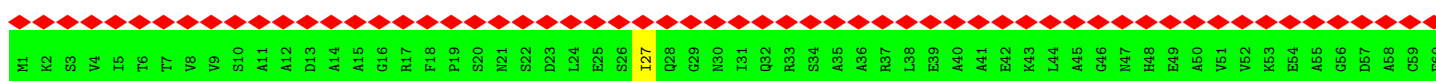




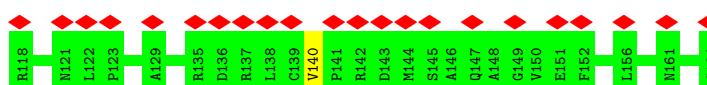
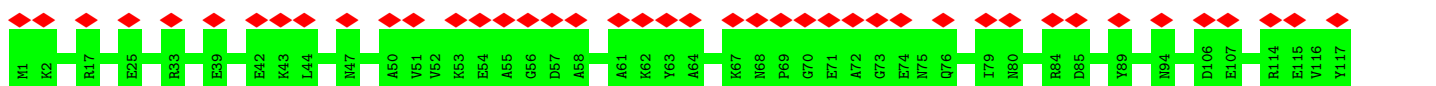
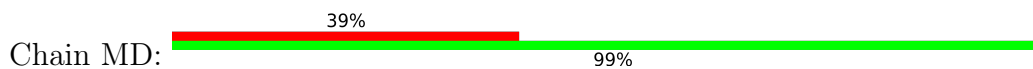
● Molecule 1: Phycoerythrin alpha subunit



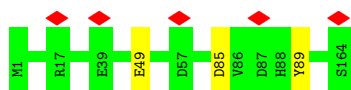
● Molecule 1: Phycoerythrin alpha subunit



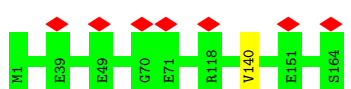
● Molecule 1: Phycoerythrin alpha subunit



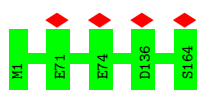
• Molecule 1: Phycoerythrin alpha subunit



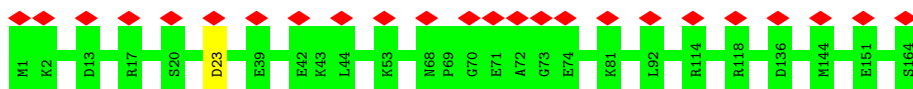
• Molecule 1: Phycoerythrin alpha subunit



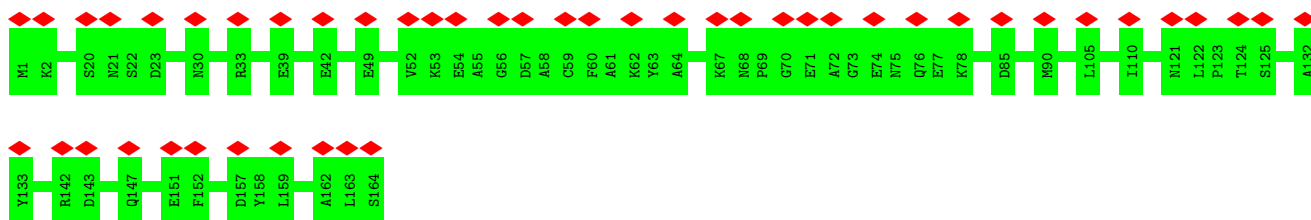
• Molecule 1: Phycoerythrin alpha subunit



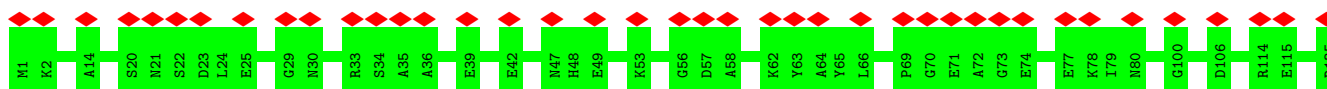
• Molecule 1: Phycoerythrin alpha subunit

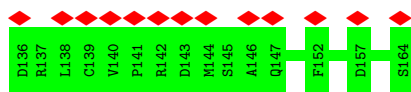


• Molecule 1: Phycoerythrin alpha subunit

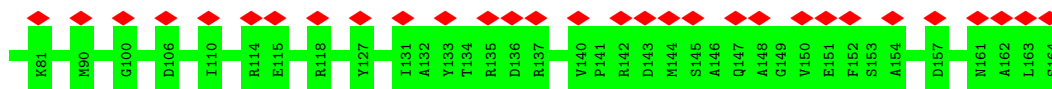
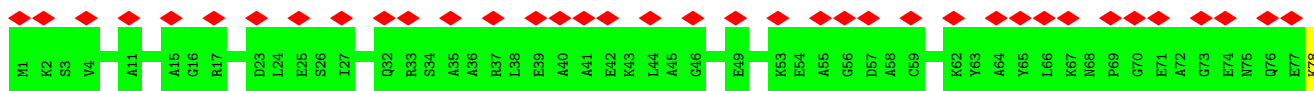
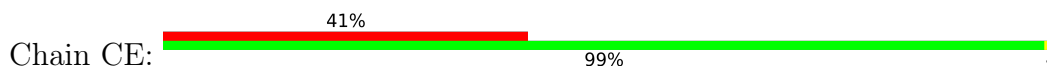


• Molecule 1: Phycoerythrin alpha subunit

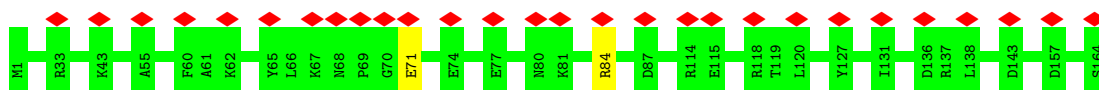




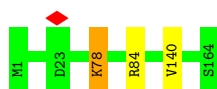
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit

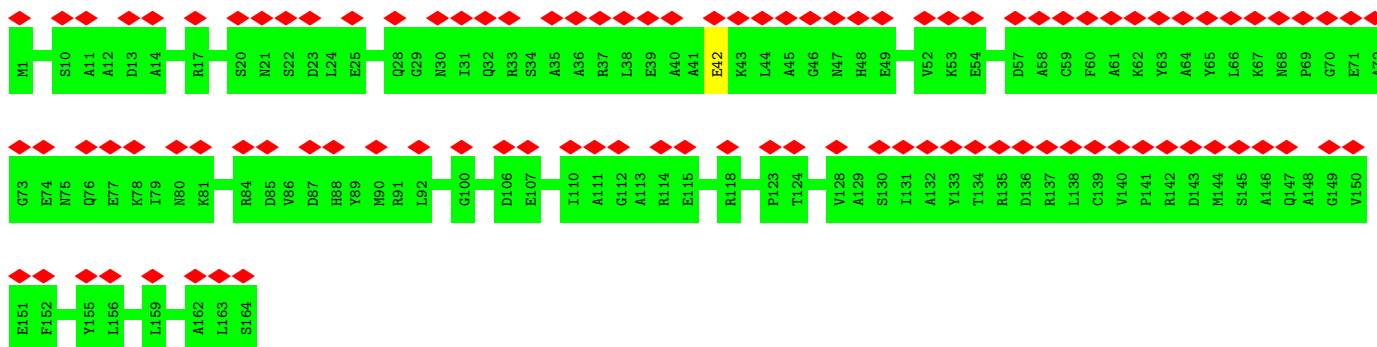


- Molecule 1: Phycoerythrin alpha subunit

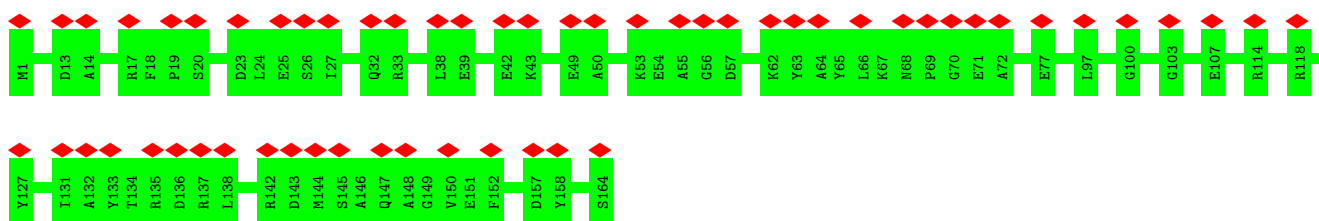


- Molecule 1: Phycoerythrin alpha subunit

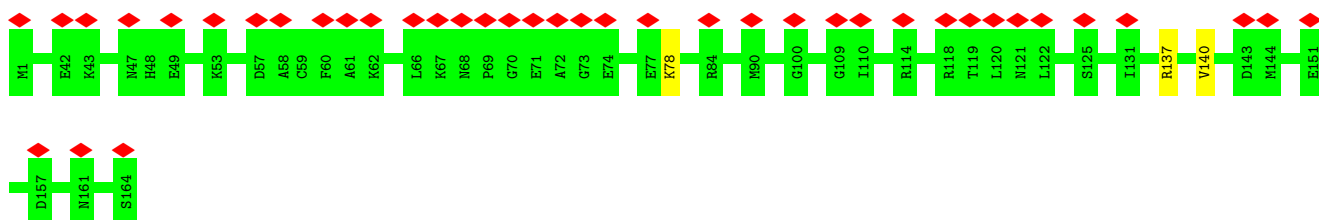




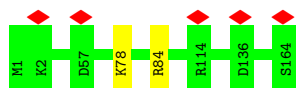
- Molecule 1: Phycoerythrin alpha subunit



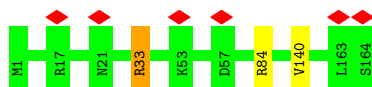
- Molecule 1: Phycoerythrin alpha subunit



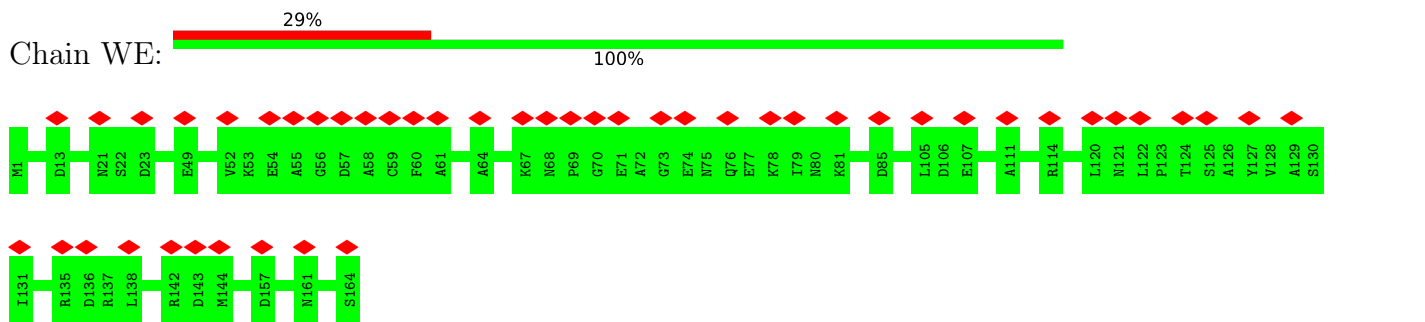
- Molecule 1: Phycoerythrin alpha subunit



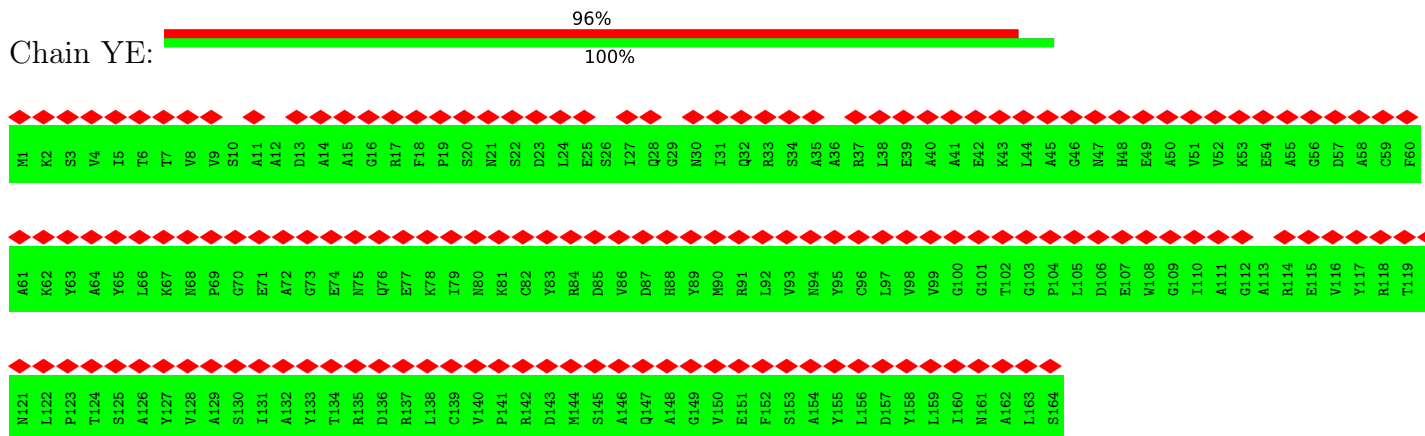
- Molecule 1: Phycoerythrin alpha subunit



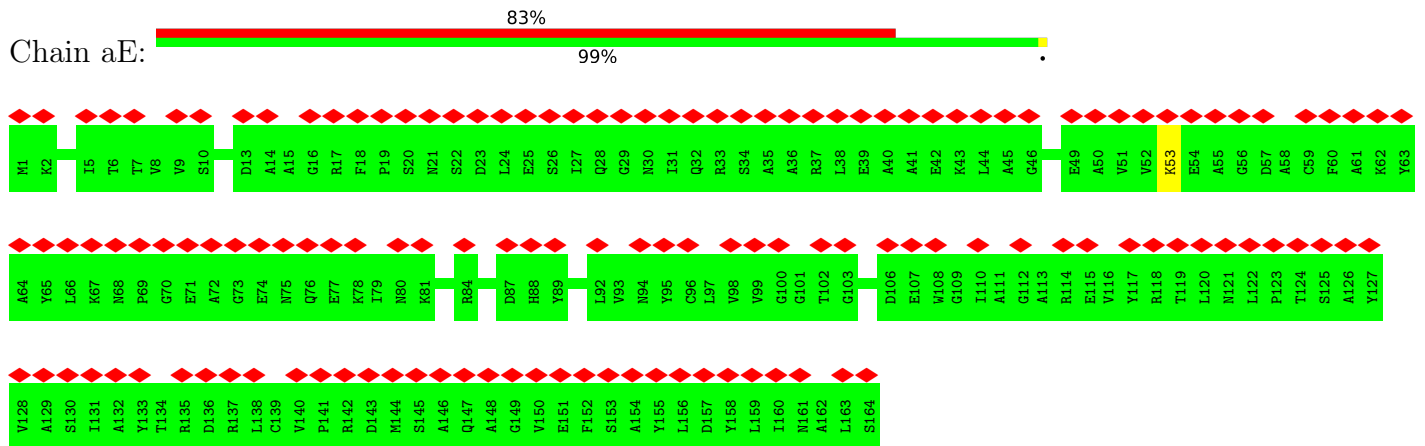
- Molecule 1: Phycoerythrin alpha subunit



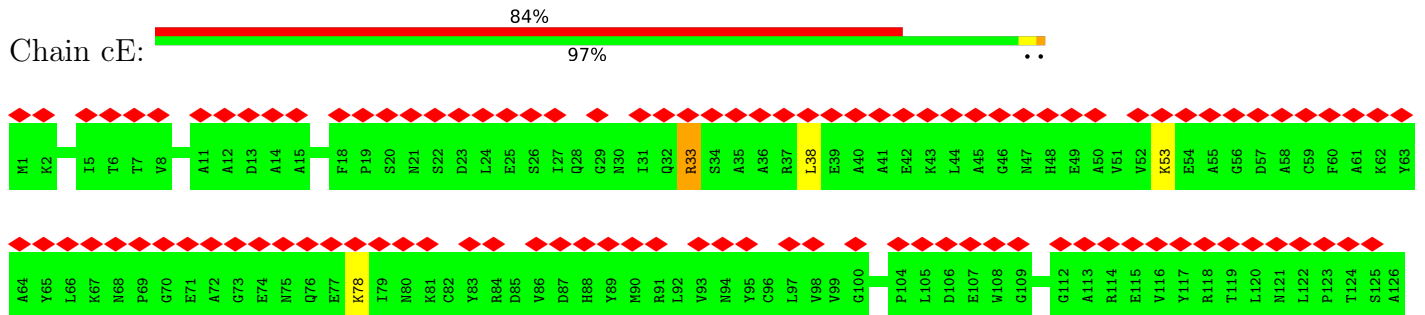
• Molecule 1: Phycoerythrin alpha subunit

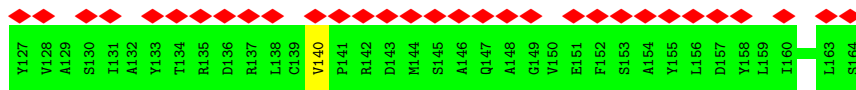


• Molecule 1: Phycoerythrin alpha subunit

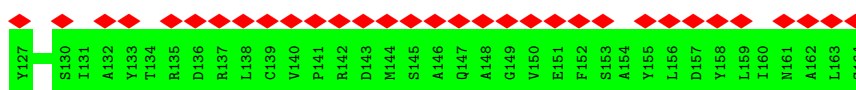
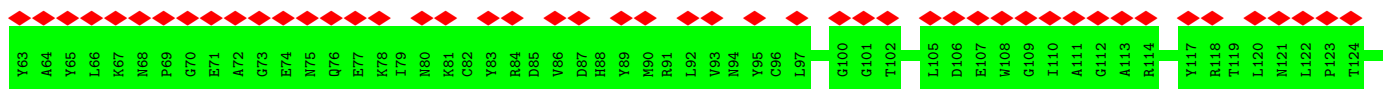
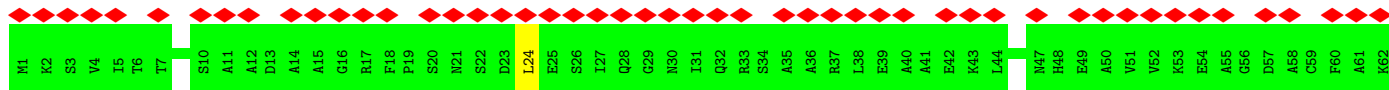
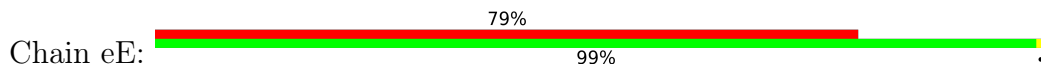


• Molecule 1: Phycoerythrin alpha subunit

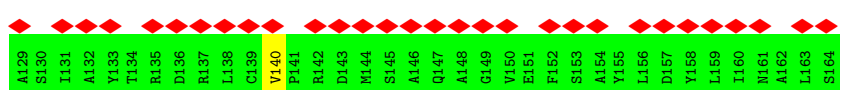
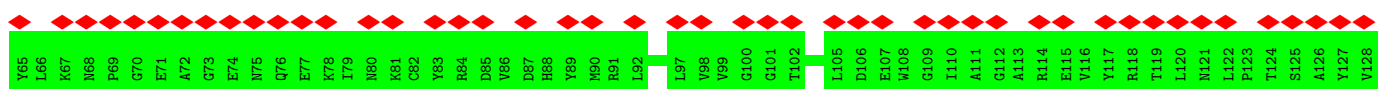
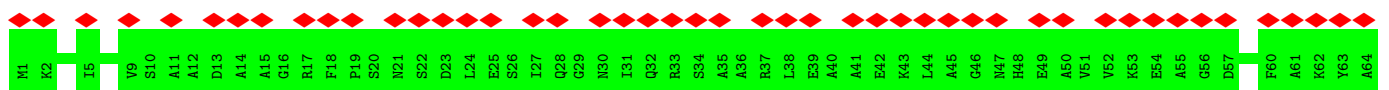
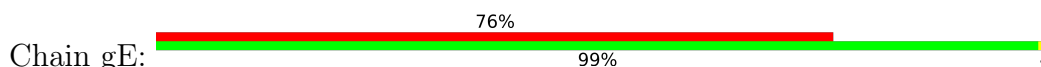




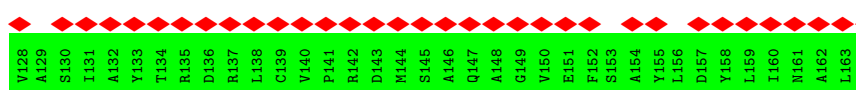
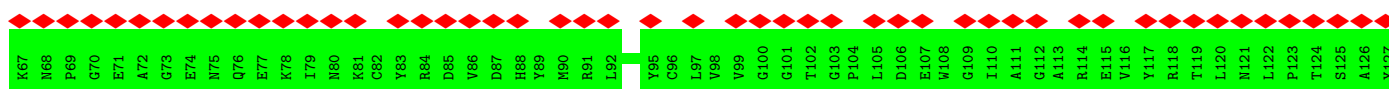
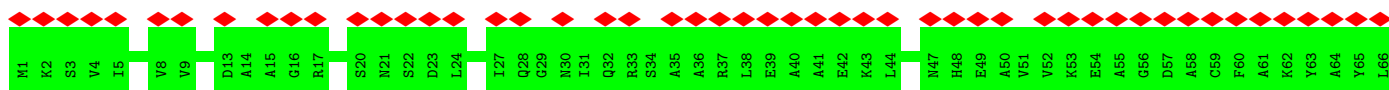
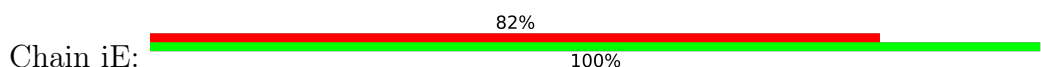
• Molecule 1: Phycoerythrin alpha subunit



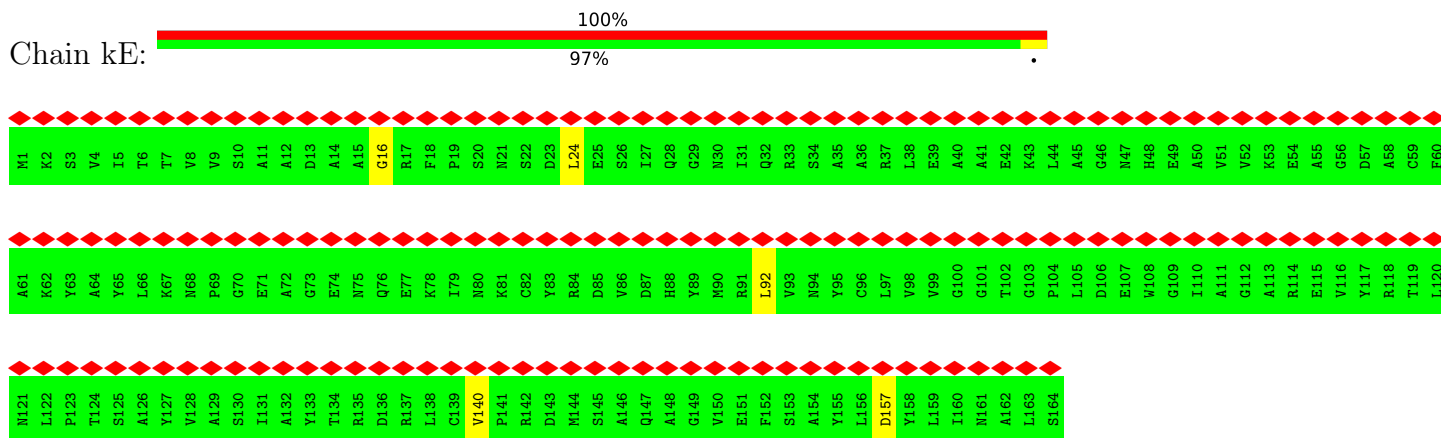
• Molecule 1: Phycoerythrin alpha subunit



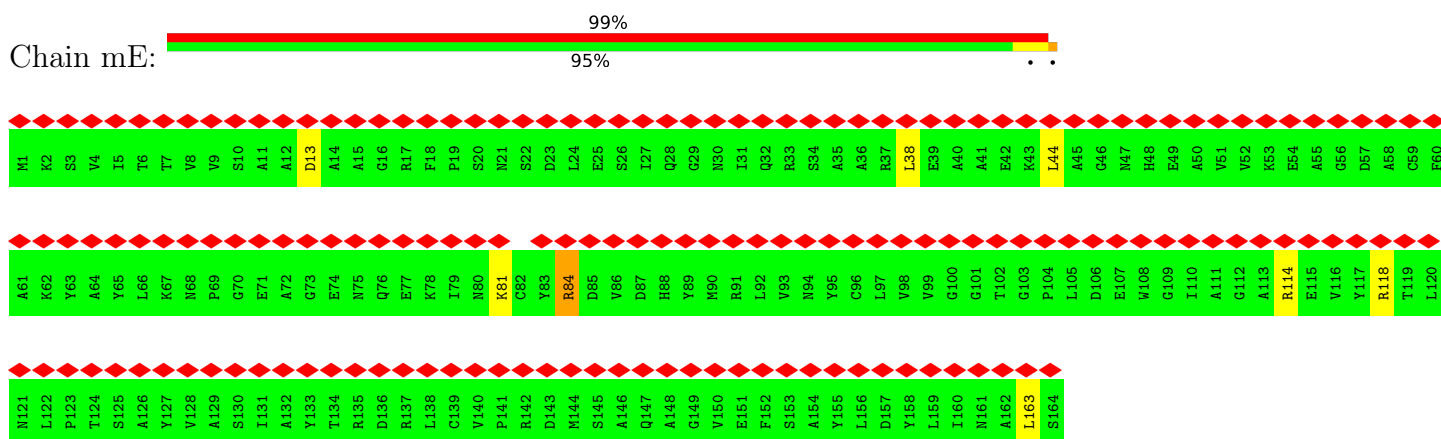
• Molecule 1: Phycoerythrin alpha subunit



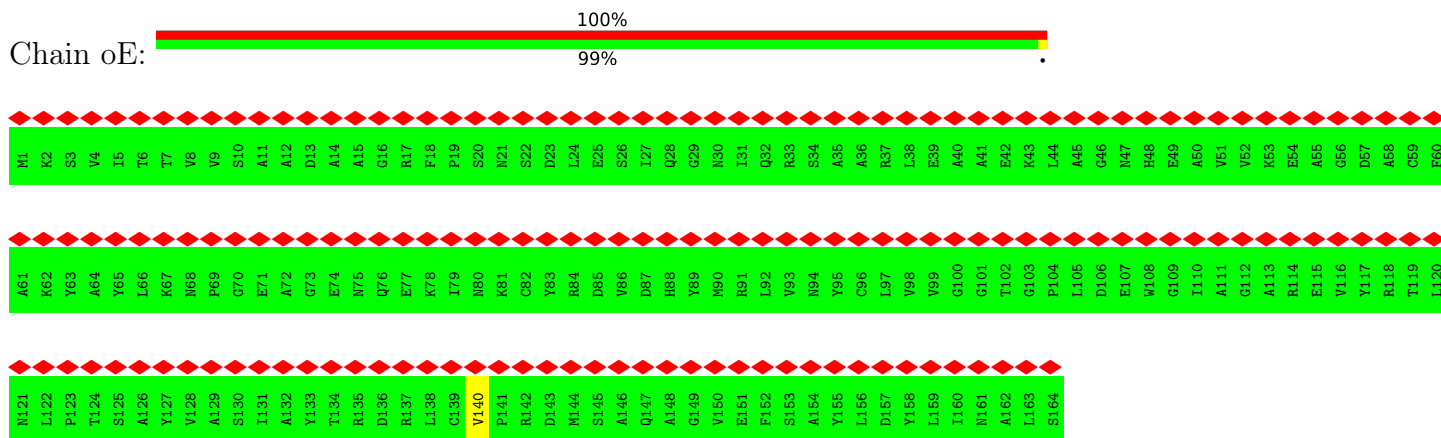
• Molecule 1: Phycoerythrin alpha subunit



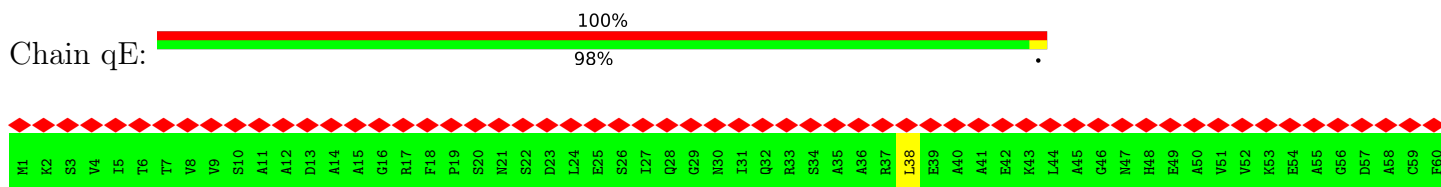
• Molecule 1: Phycoerythrin alpha subunit

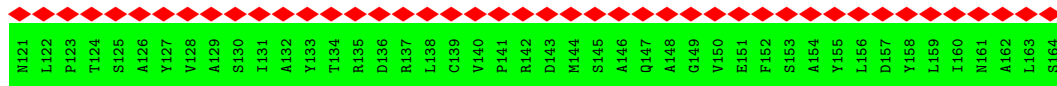
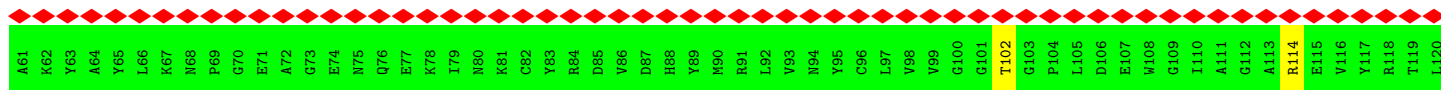


• Molecule 1: Phycoerythrin alpha subunit



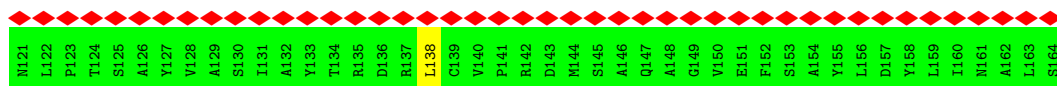
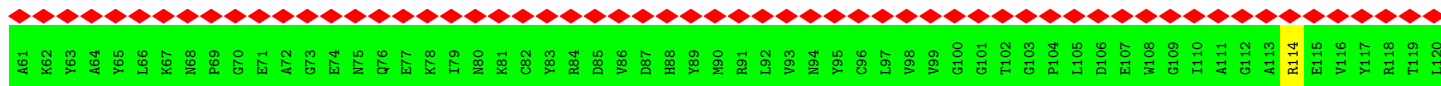
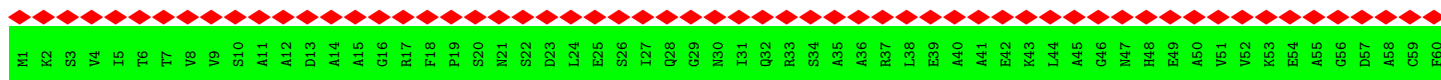
• Molecule 1: Phycoerythrin alpha subunit





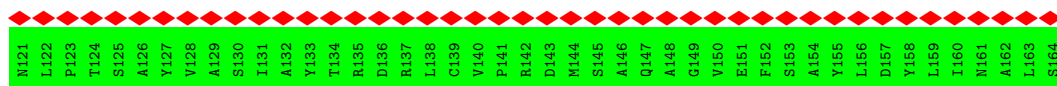
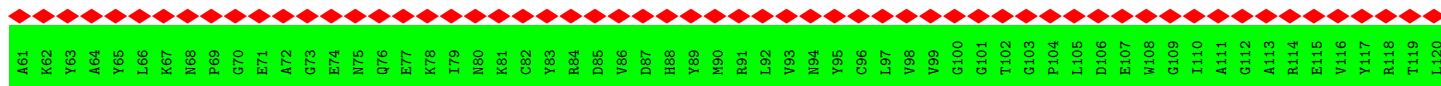
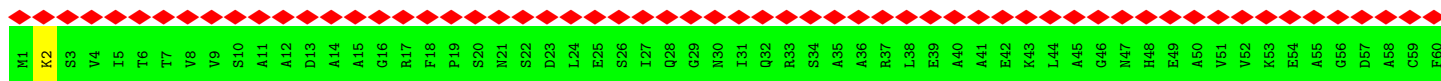
• Molecule 1: Phycoerythrin alpha subunit

Chain sE:



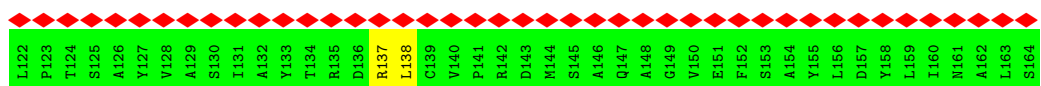
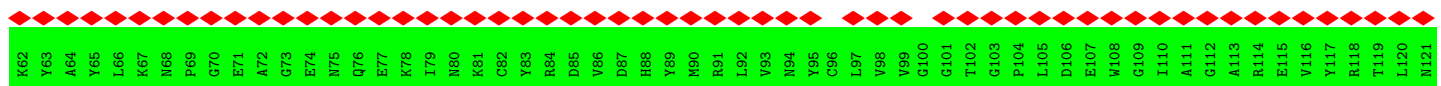
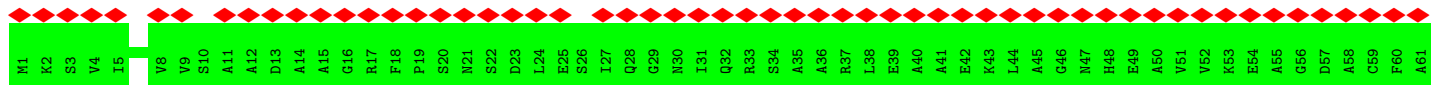
• Molecule 1: Phycoerythrin alpha subunit

Chain uE:

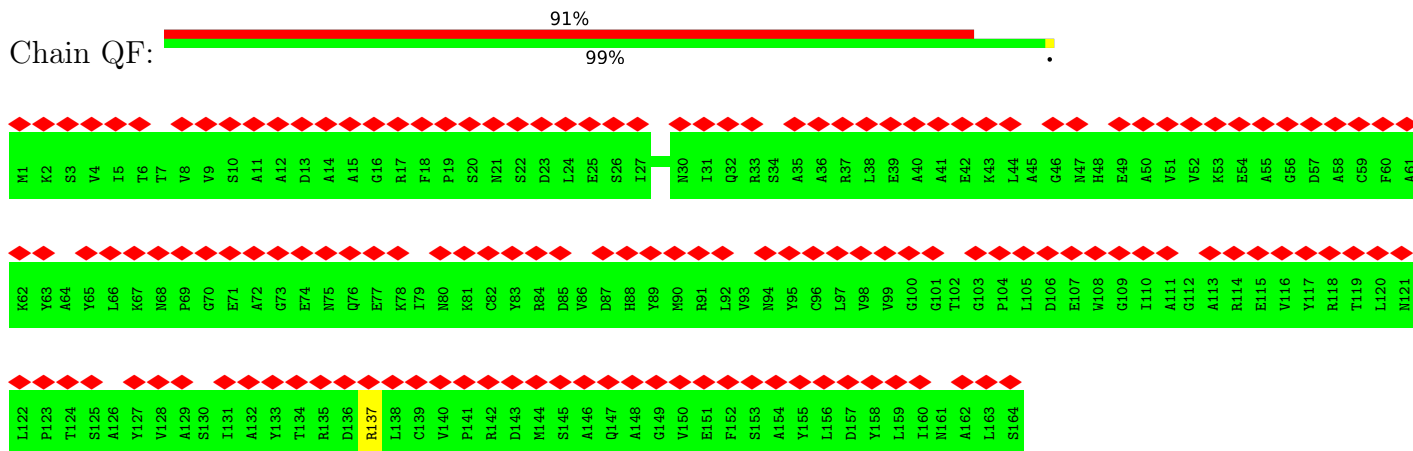


• Molecule 1: Phycoerythrin alpha subunit

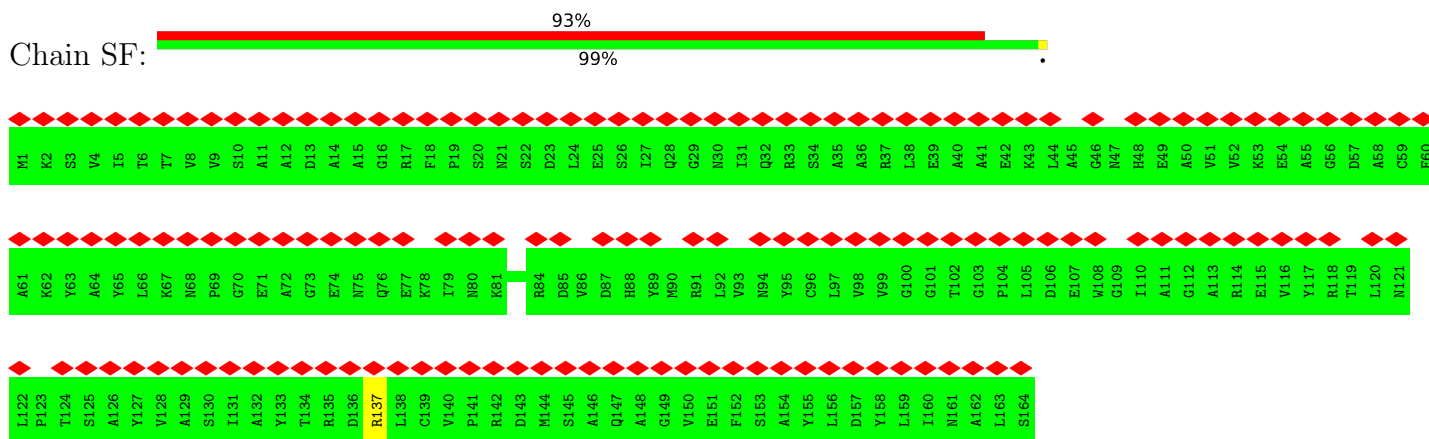
Chain OF:



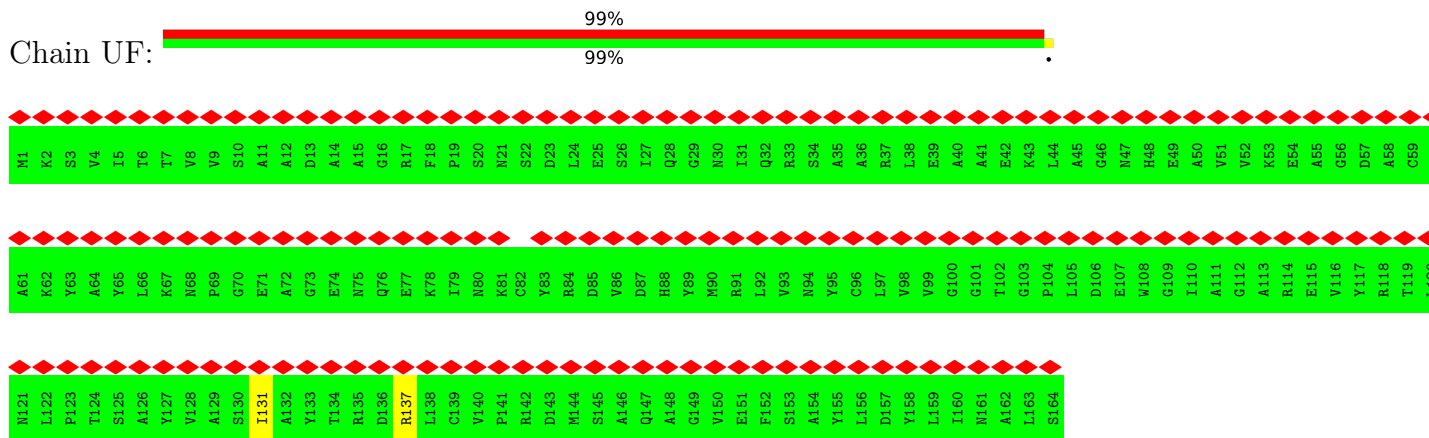
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

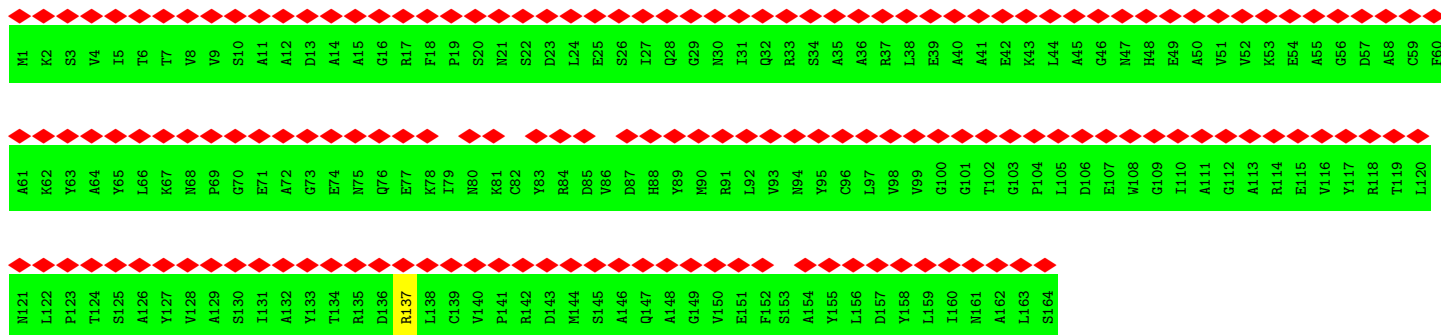


• Molecule 1: Phycoerythrin alpha subunit

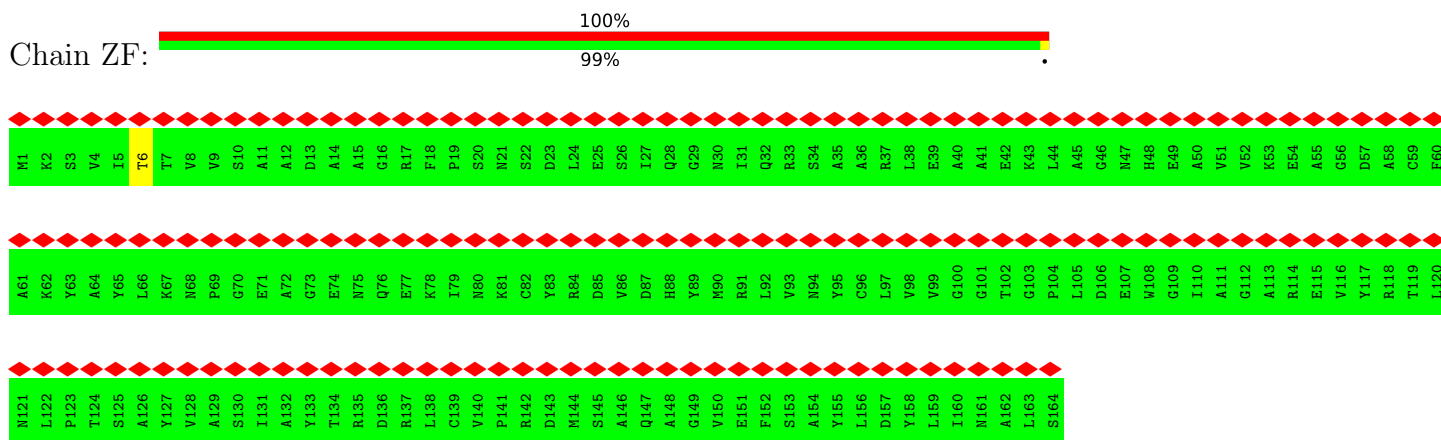


• Molecule 1: Phycoerythrin alpha subunit

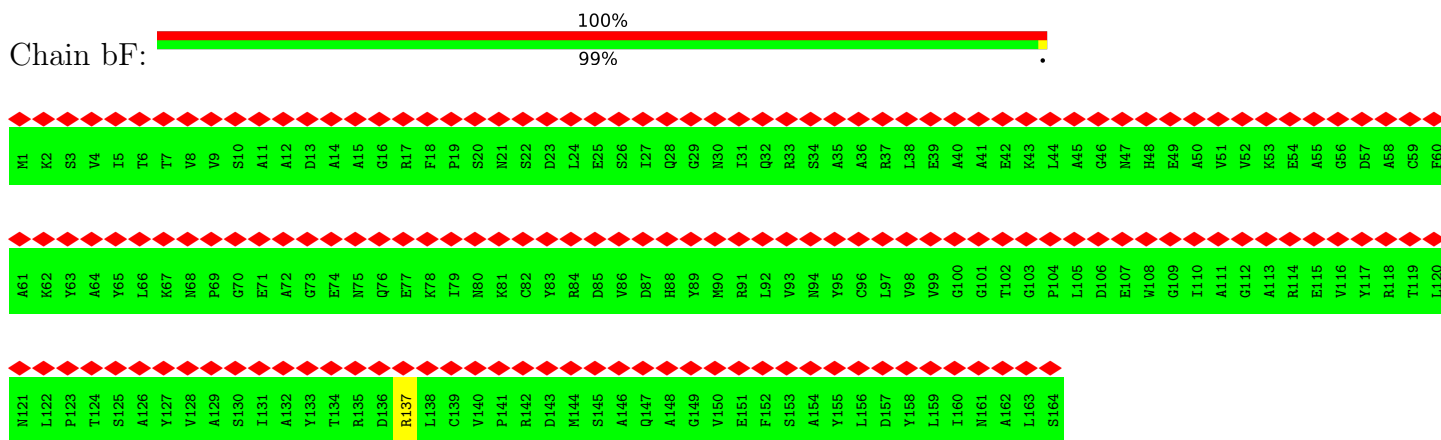




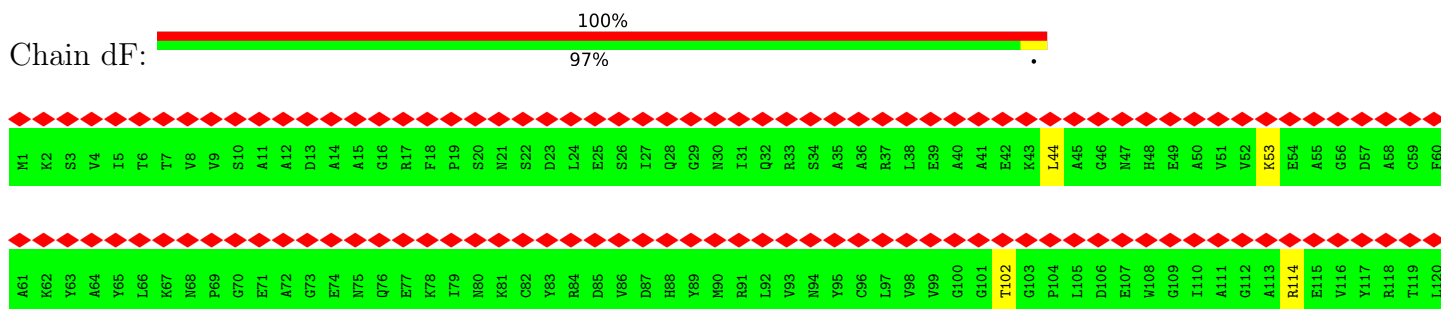
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

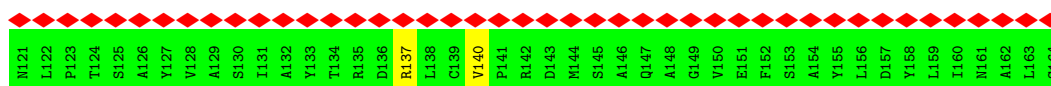
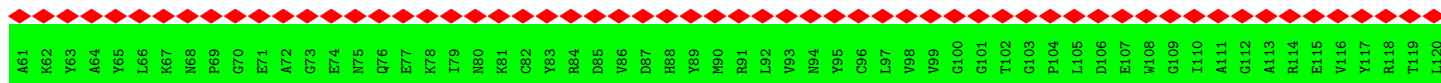
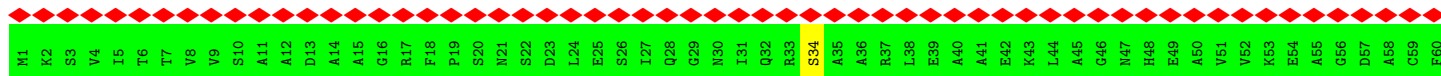


• Molecule 1: Phycoerythrin alpha subunit

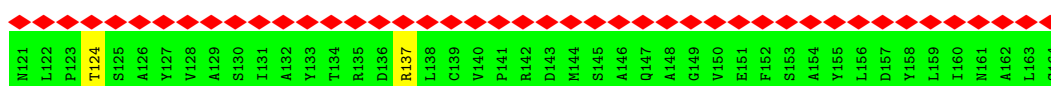
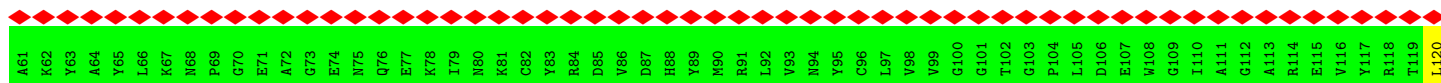
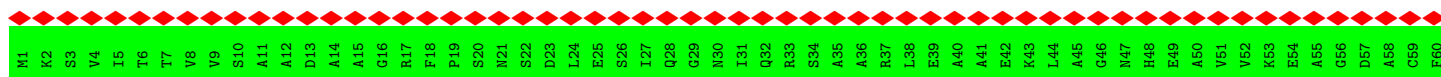




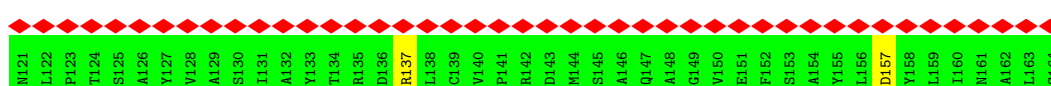
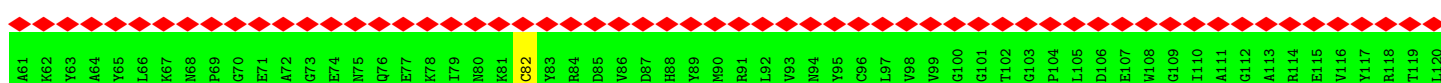
• Molecule 1: Phycoerythrin alpha subunit



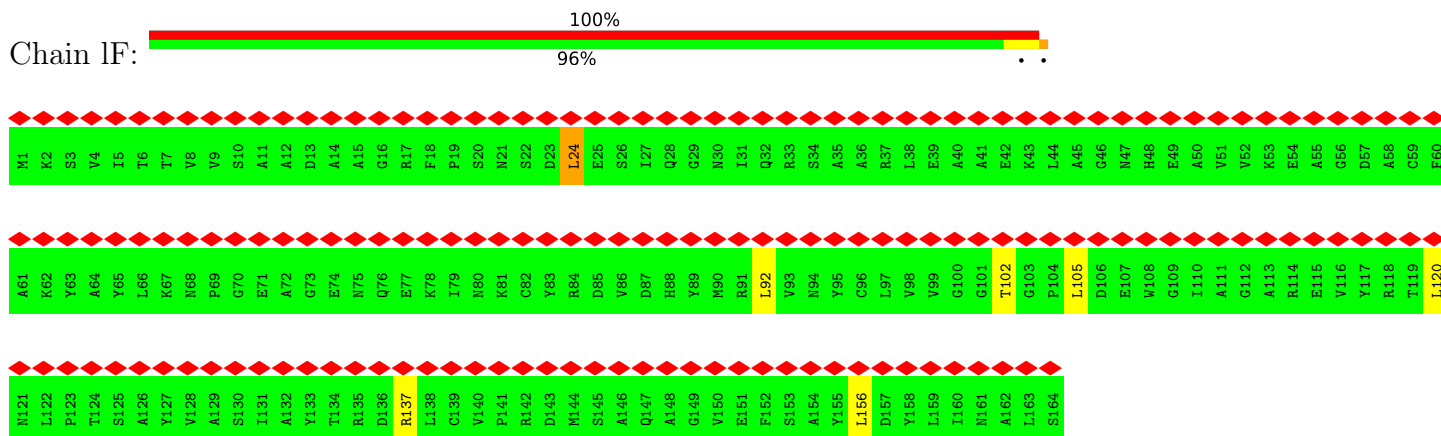
• Molecule 1: Phycoerythrin alpha subunit



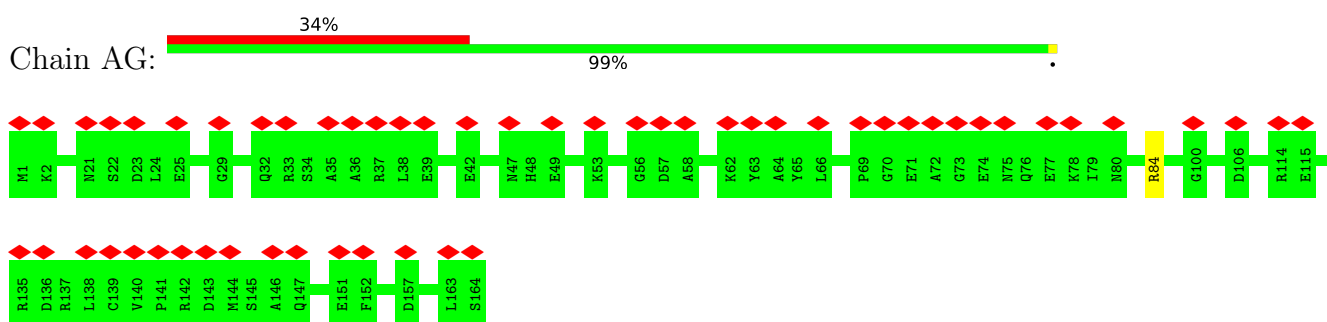
• Molecule 1: Phycoerythrin alpha subunit



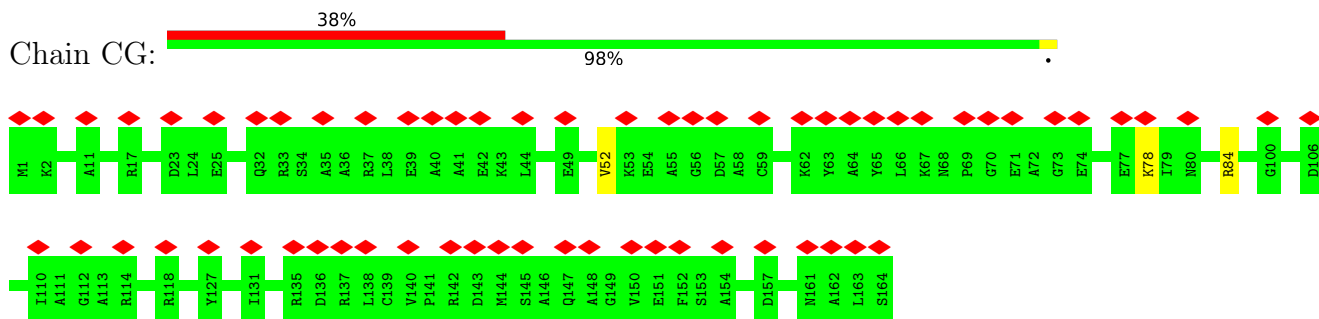
• Molecule 1: Phycoerythrin alpha subunit



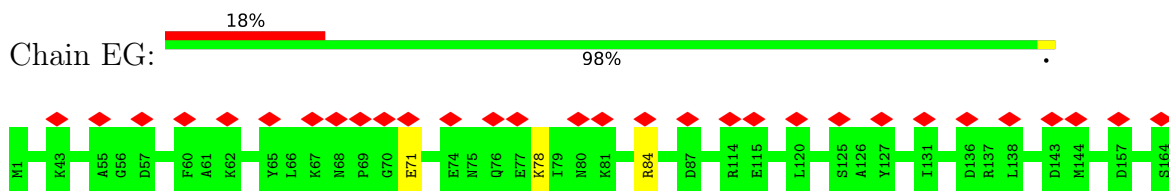
• Molecule 1: Phycoerythrin alpha subunit



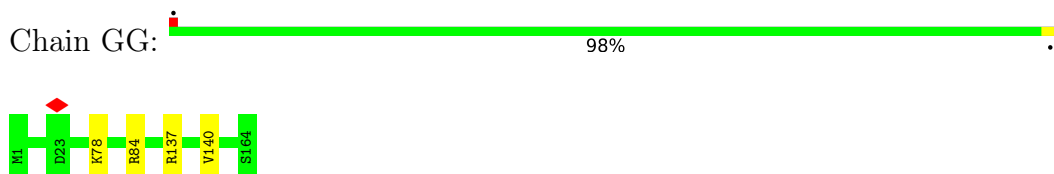
• Molecule 1: Phycoerythrin alpha subunit



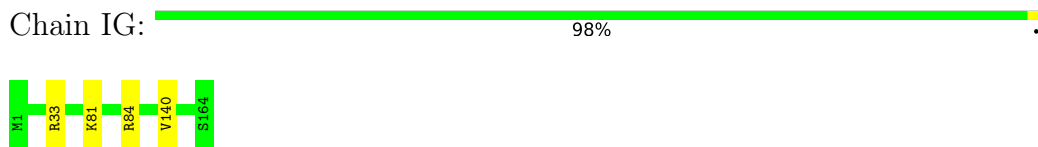
• Molecule 1: Phycoerythrin alpha subunit



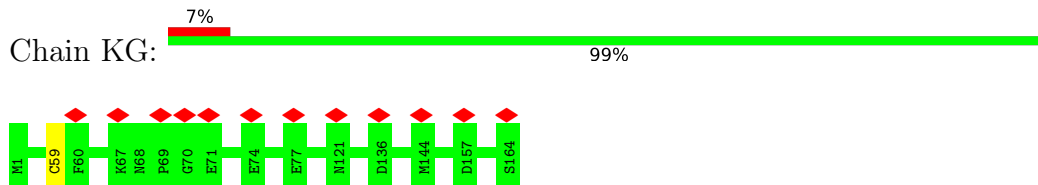
• Molecule 1: Phycoerythrin alpha subunit



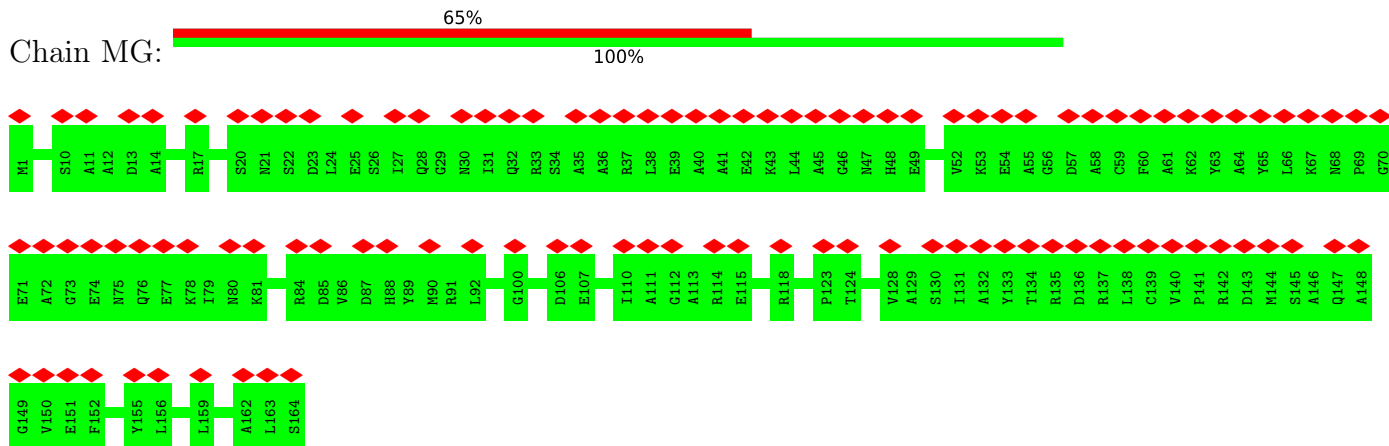
• Molecule 1: Phycoerythrin alpha subunit



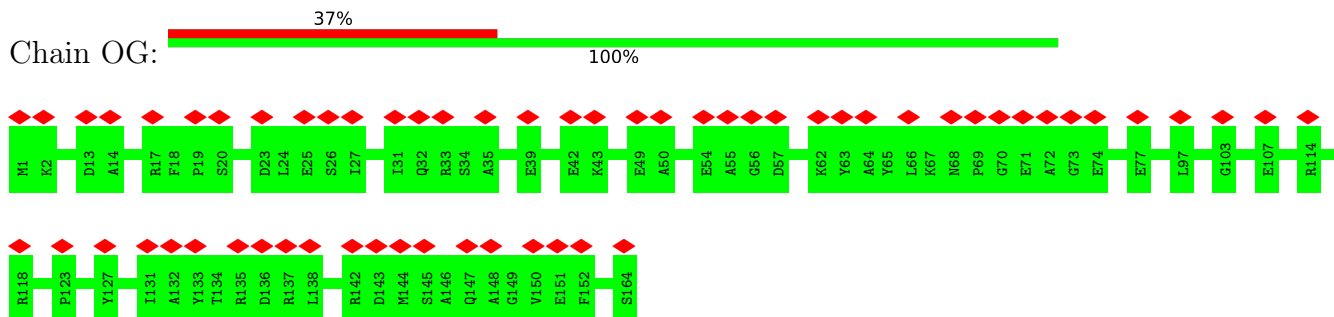
• Molecule 1: Phycoerythrin alpha subunit



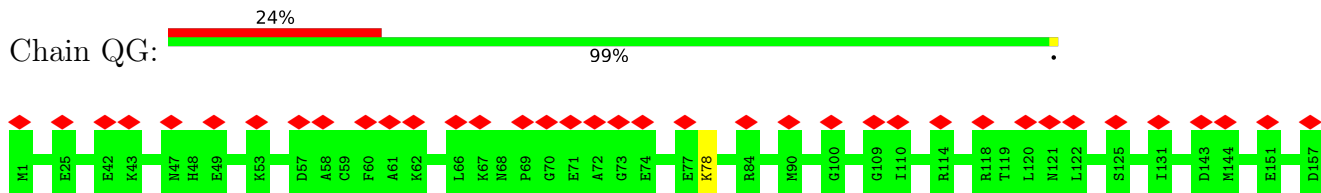
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

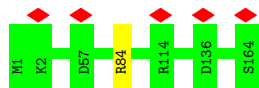


• Molecule 1: Phycoerythrin alpha subunit

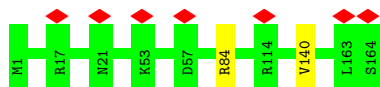




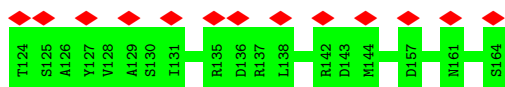
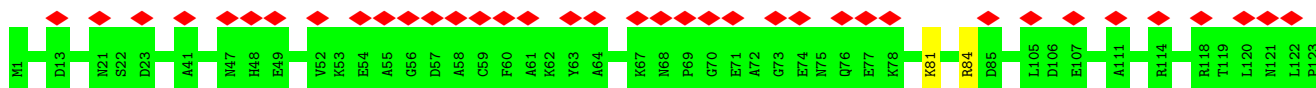
• Molecule 1: Phycoerythrin alpha subunit



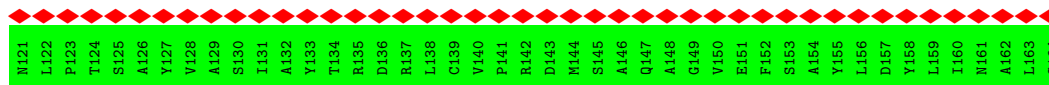
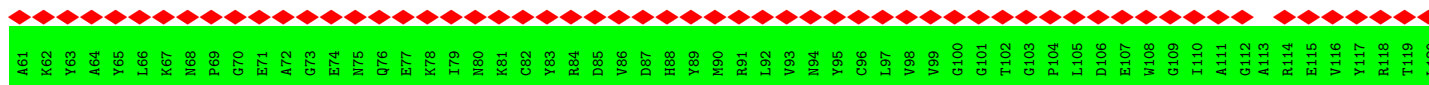
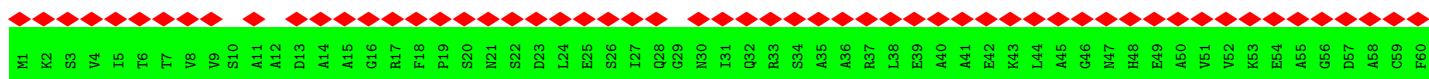
• Molecule 1: Phycoerythrin alpha subunit



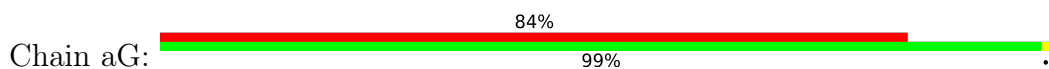
• Molecule 1: Phycoerythrin alpha subunit

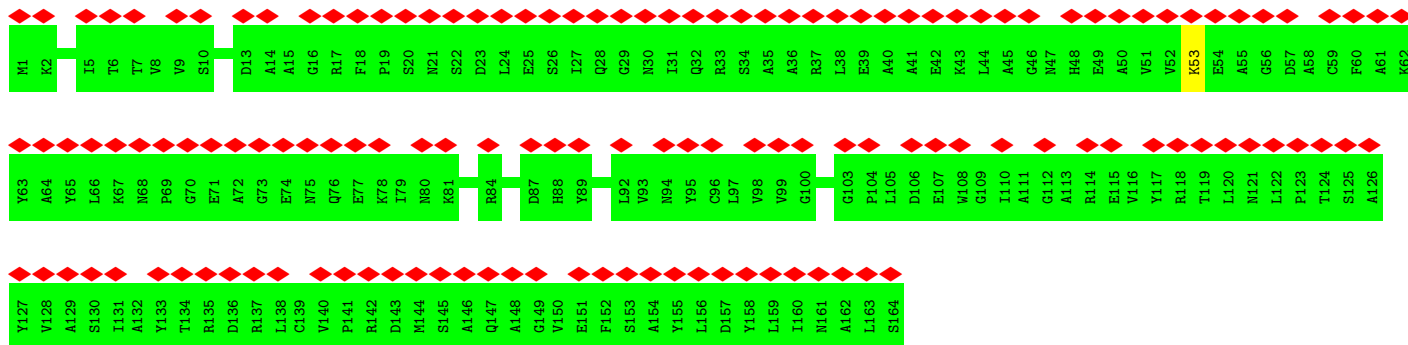


• Molecule 1: Phycoerythrin alpha subunit

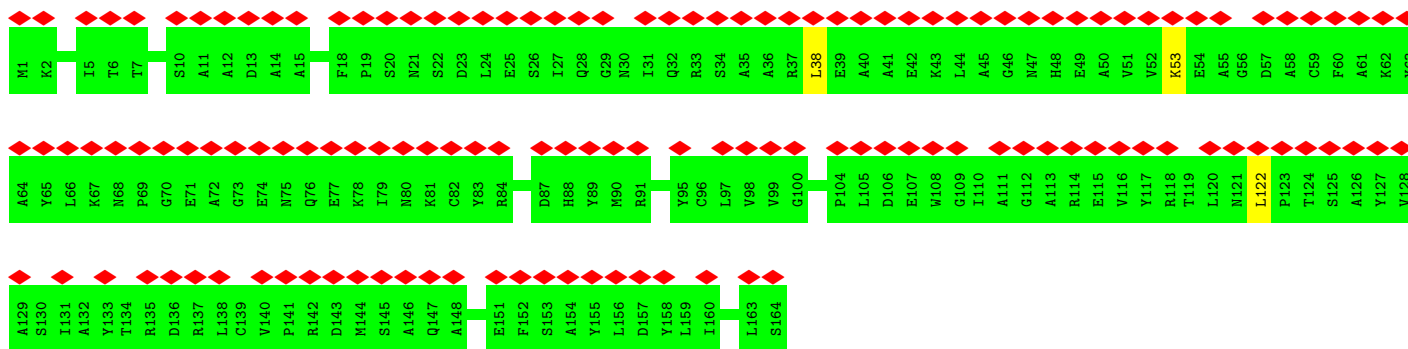
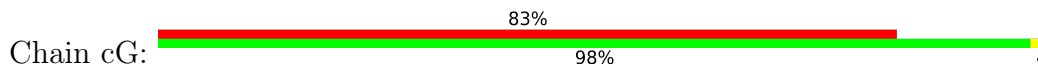


• Molecule 1: Phycoerythrin alpha subunit

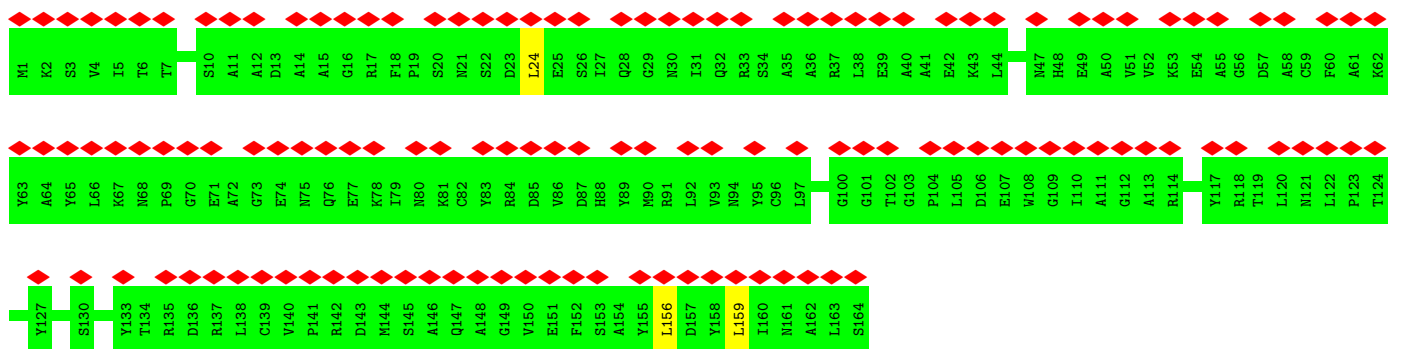
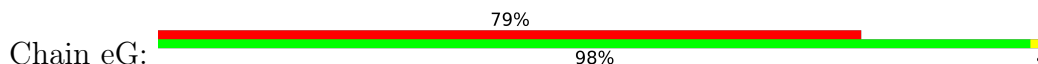




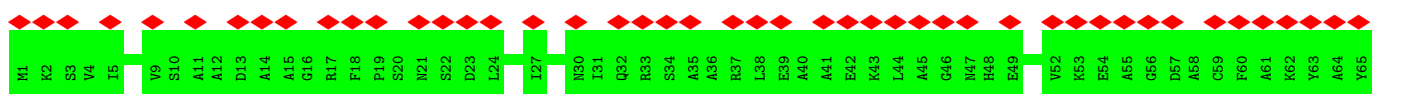
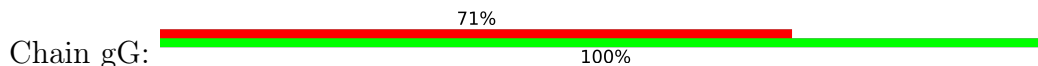
• Molecule 1: Phycoerythrin alpha subunit

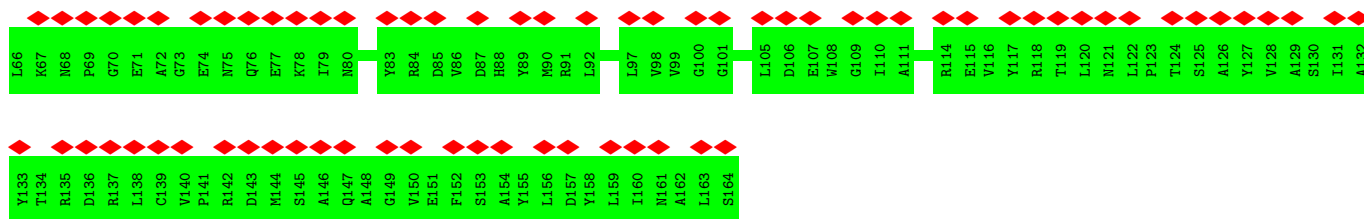


• Molecule 1: Phycoerythrin alpha subunit

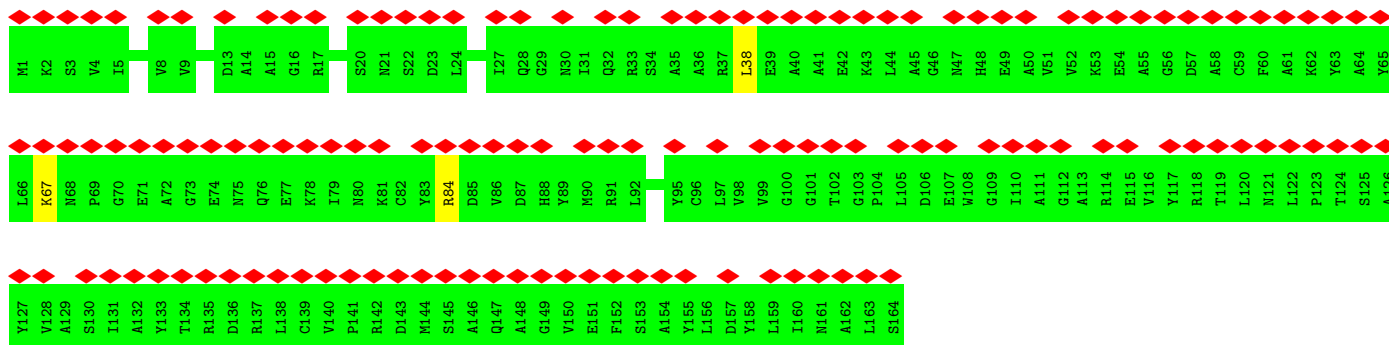
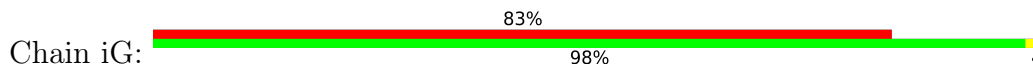


• Molecule 1: Phycoerythrin alpha subunit

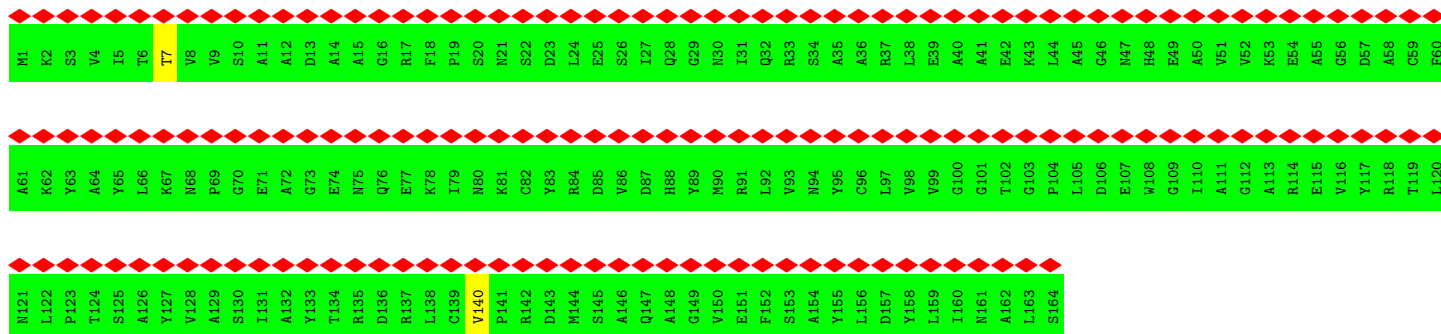




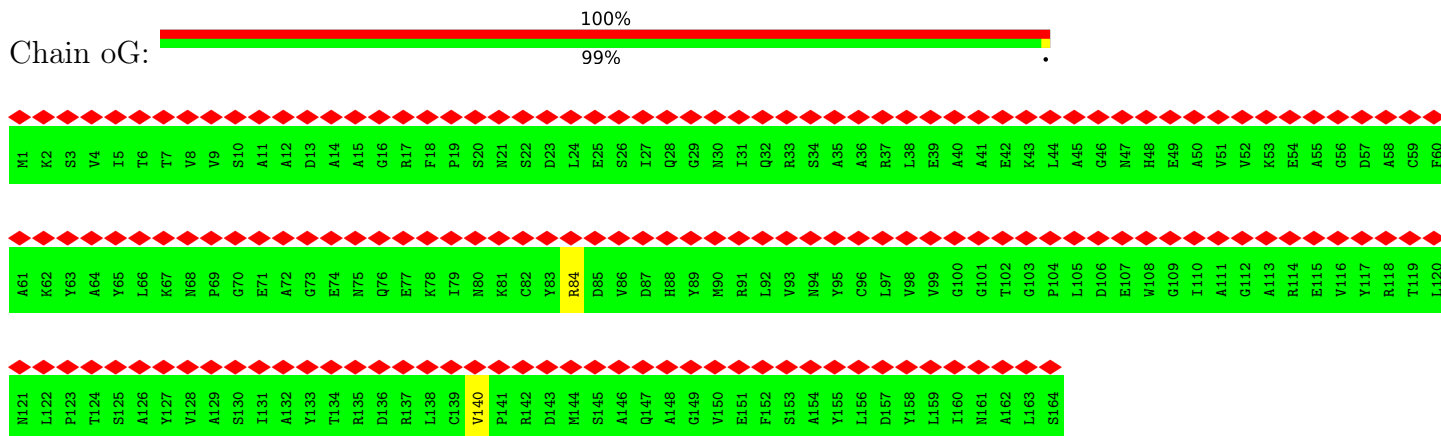
• Molecule 1: Phycoerythrin alpha subunit



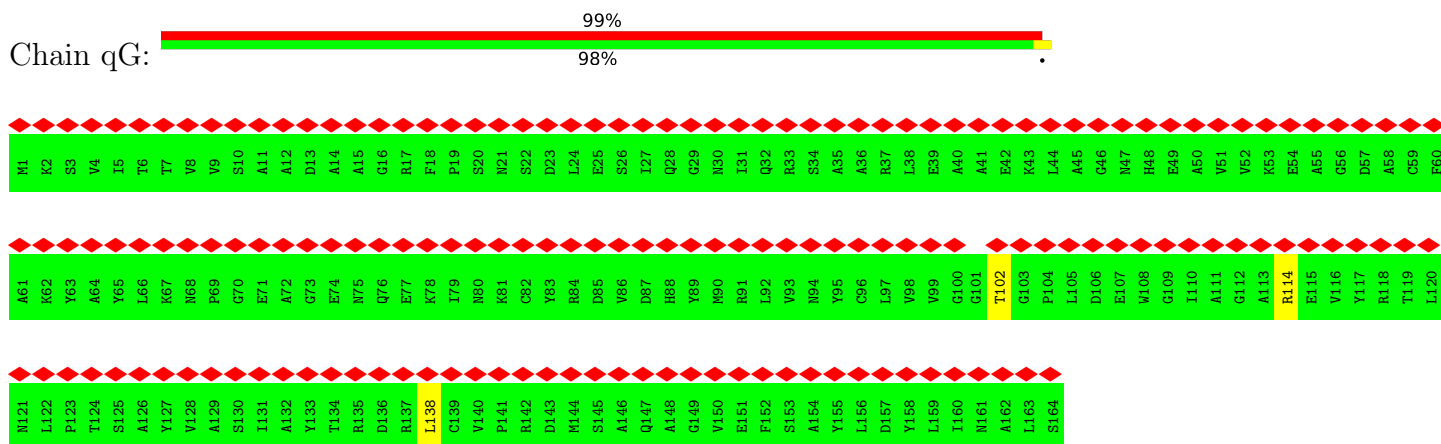
• Molecule 1: Phycoerythrin alpha subunit



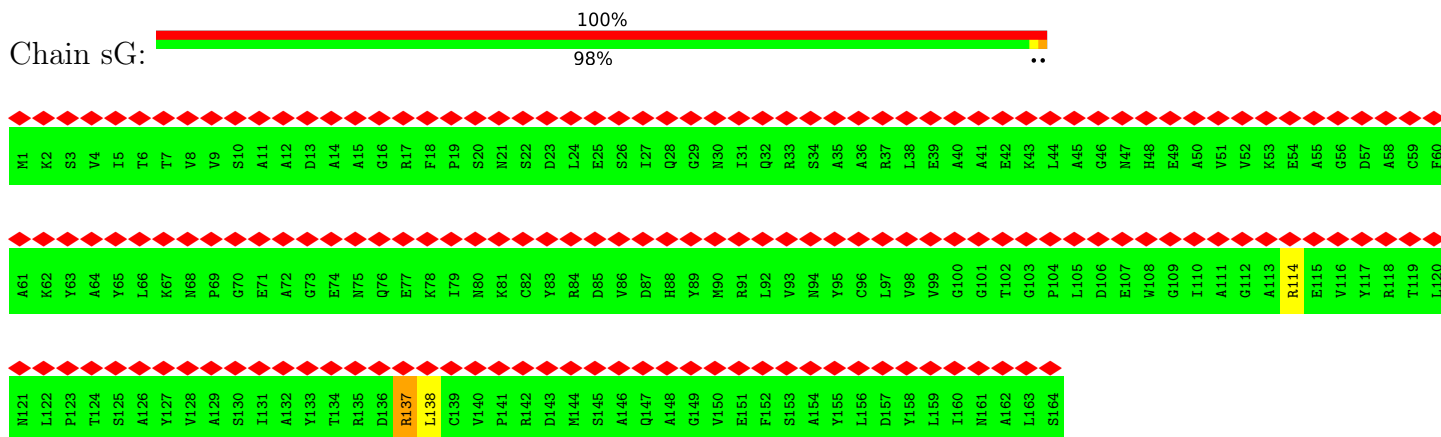
• Molecule 1: Phycoerythrin alpha subunit



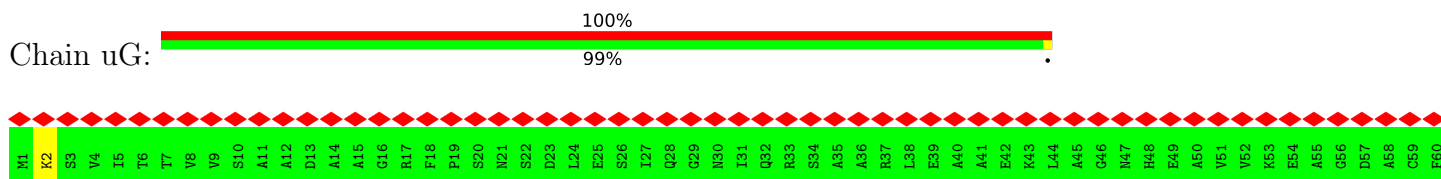
• Molecule 1: Phycoerythrin alpha subunit



• Molecule 1: Phycoerythrin alpha subunit

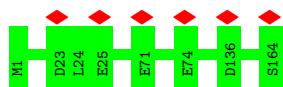


• Molecule 1: Phycoerythrin alpha subunit

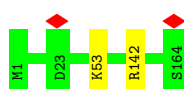




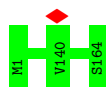
- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit



- Molecule 1: Phycoerythrin alpha subunit

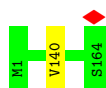


- Molecule 1: Phycoerythrin alpha subunit

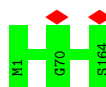


There are no outlier residues recorded for this chain.

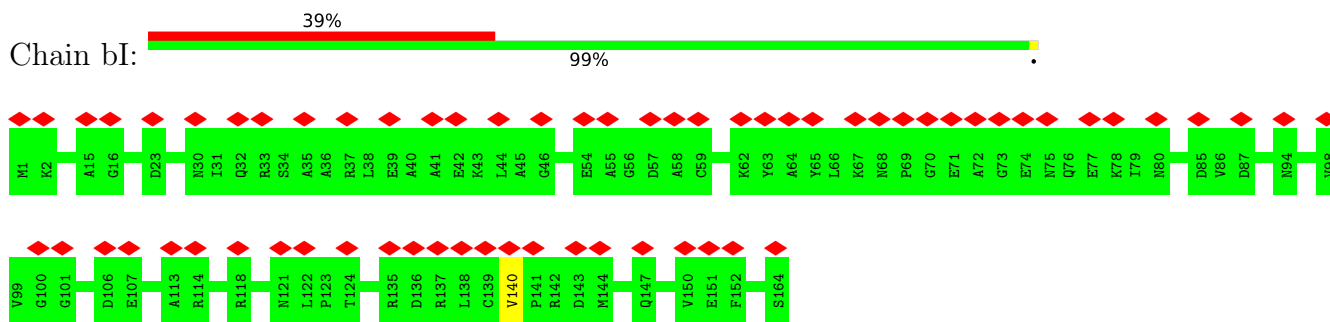
- Molecule 1: Phycoerythrin alpha subunit



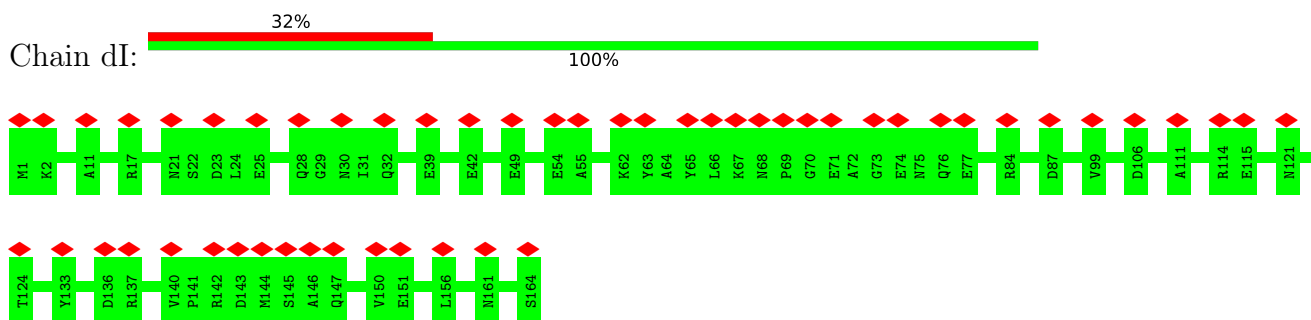
- Molecule 1: Phycoerythrin alpha subunit



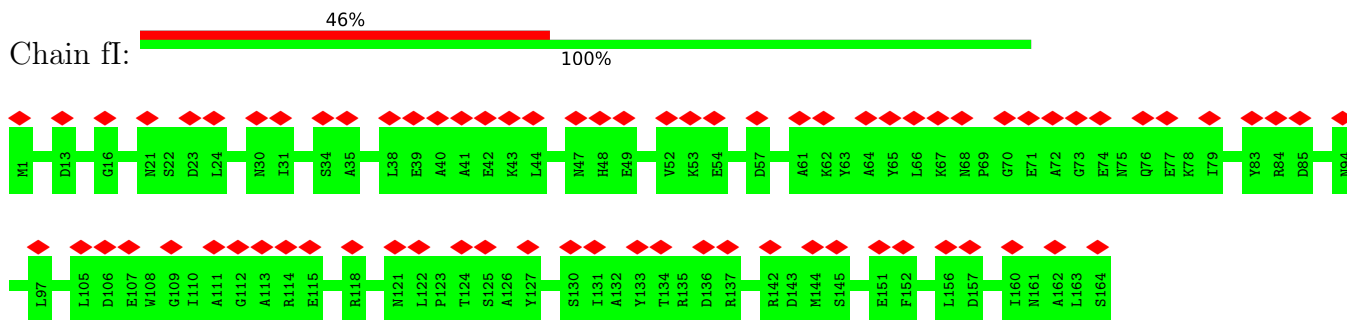
- Molecule 1: Phycoerythrin alpha subunit



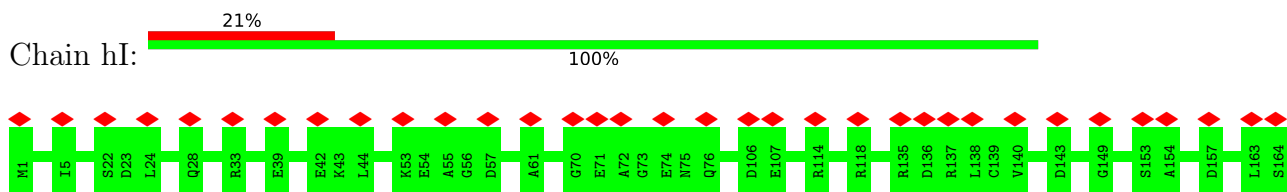
- Molecule 1: Phycoerythrin alpha subunit



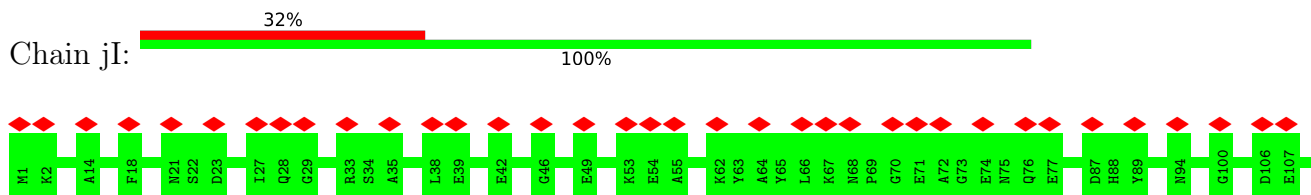
- Molecule 1: Phycoerythrin alpha subunit

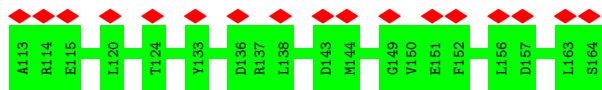


- Molecule 1: Phycoerythrin alpha subunit

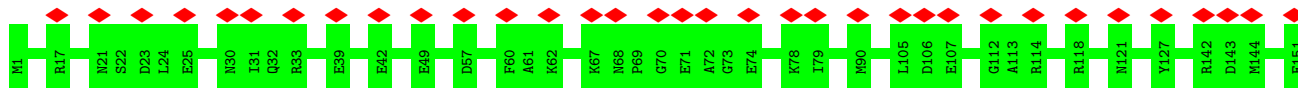


- Molecule 1: Phycoerythrin alpha subunit

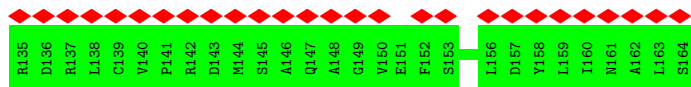
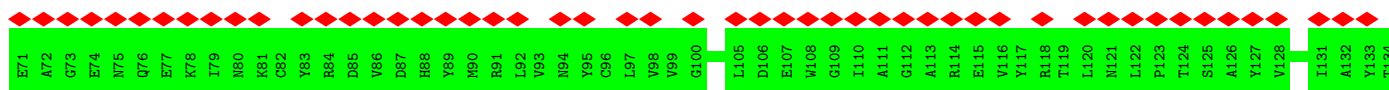
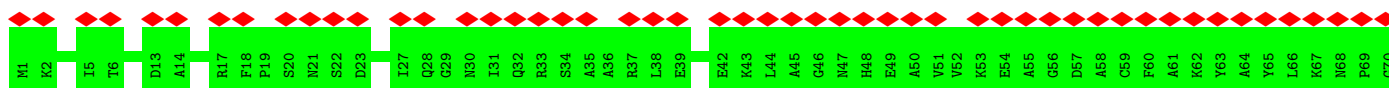
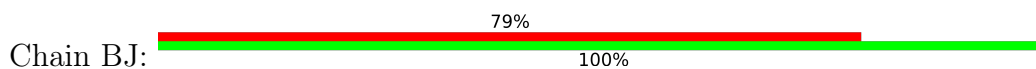




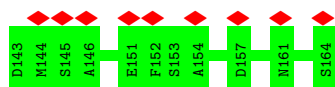
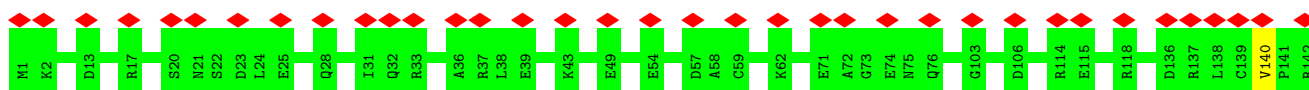
• Molecule 1: Phycoerythrin alpha subunit



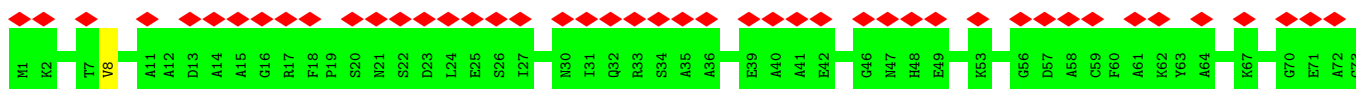
• Molecule 1: Phycoerythrin alpha subunit

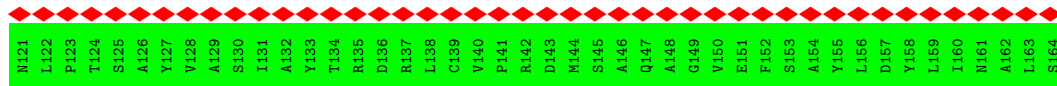
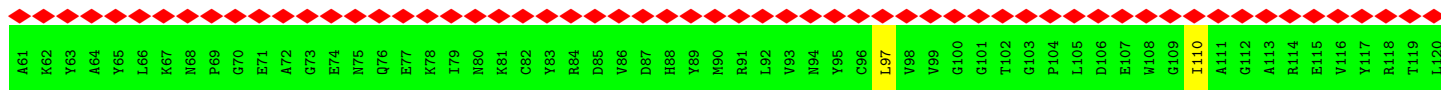


• Molecule 1: Phycoerythrin alpha subunit

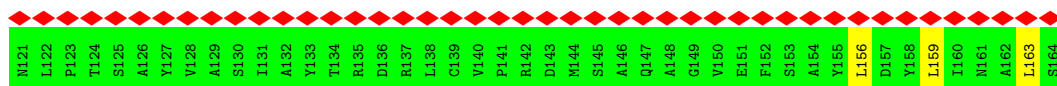
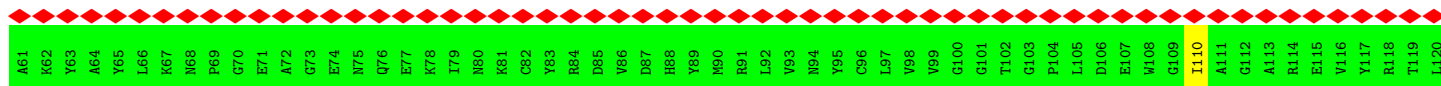
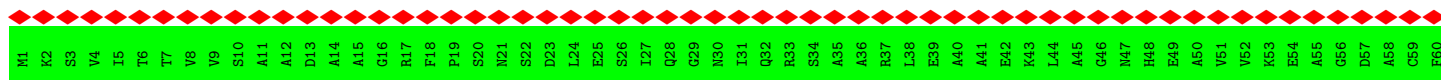


• Molecule 1: Phycoerythrin alpha subunit

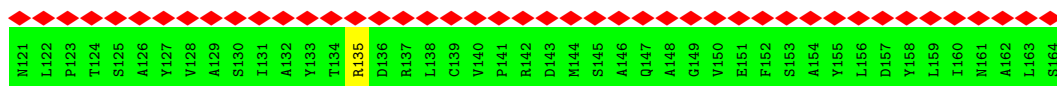
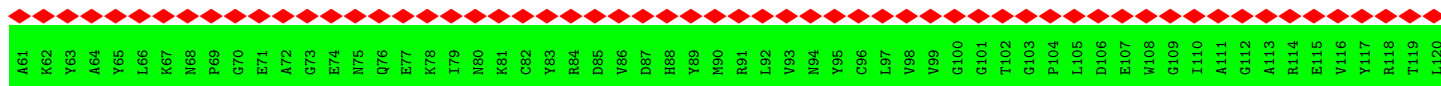
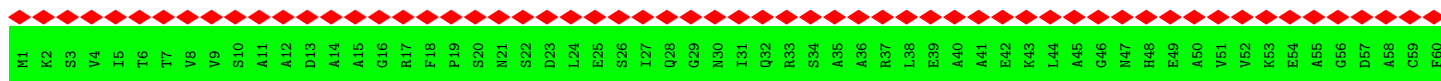




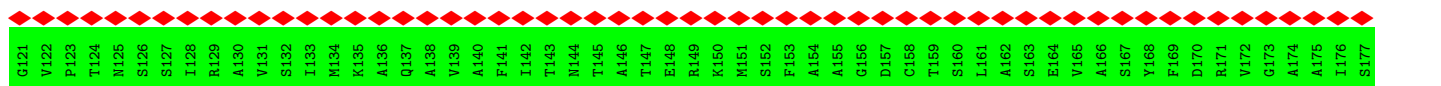
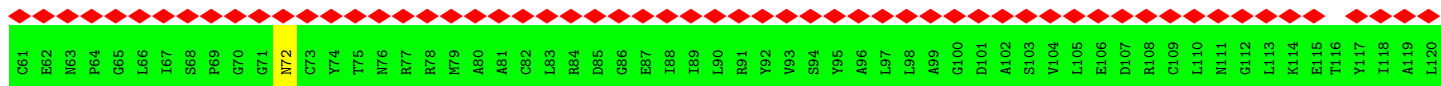
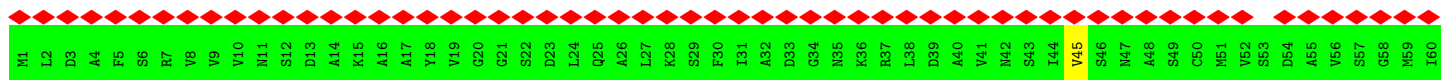
• Molecule 1: Phycoerythrin alpha subunit



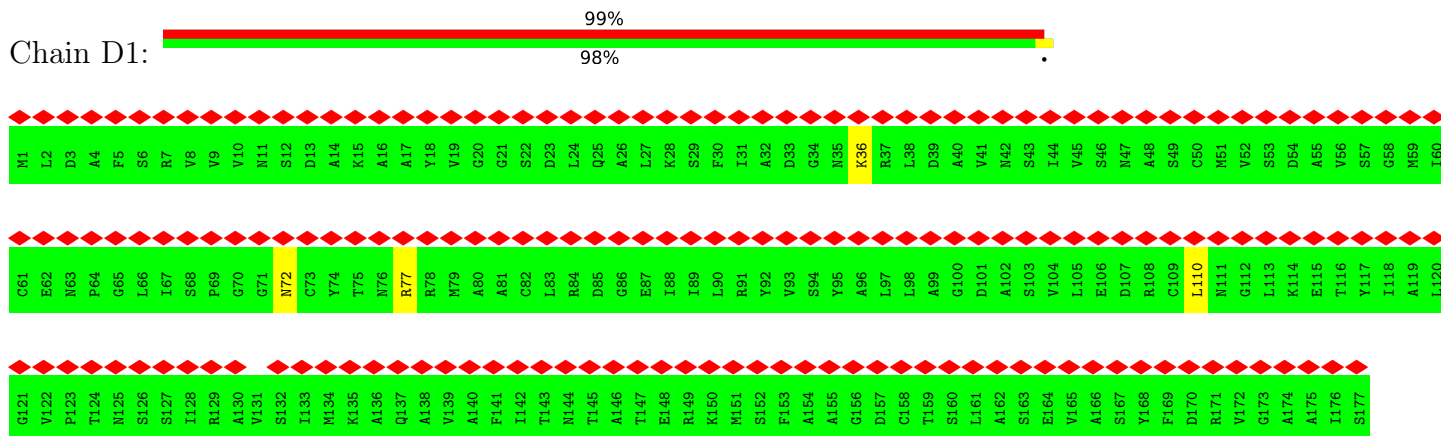
• Molecule 1: Phycoerythrin alpha subunit



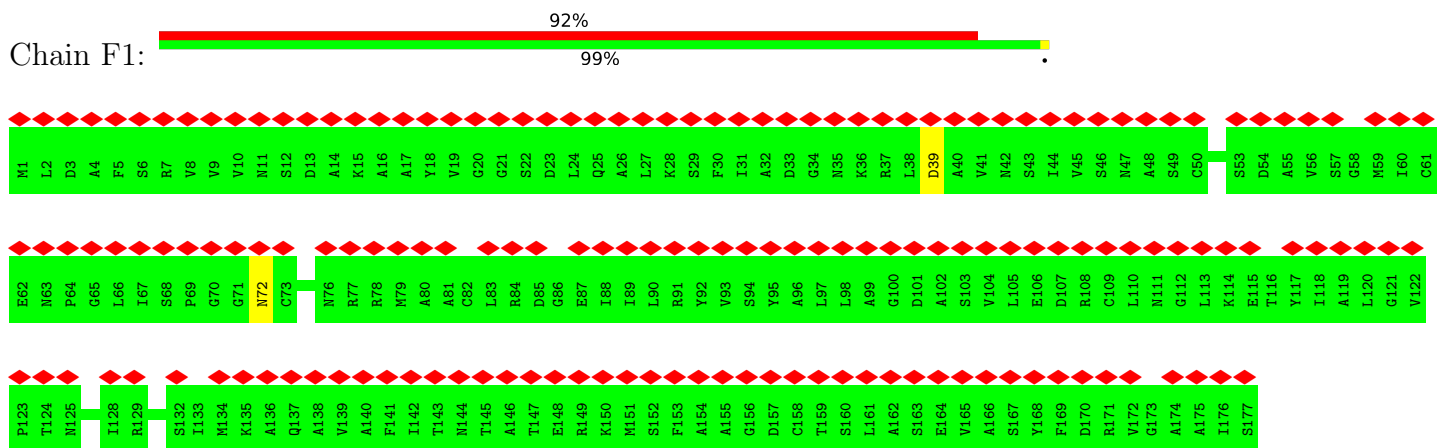
• Molecule 2: B-phycoerythrin beta chain



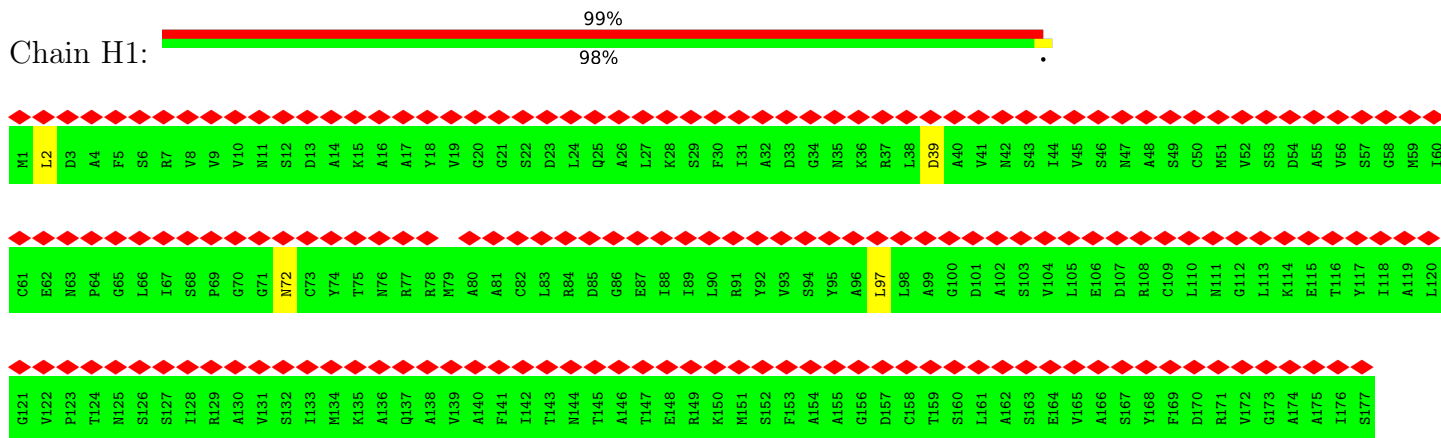
• Molecule 2: B-phycoerythrin beta chain



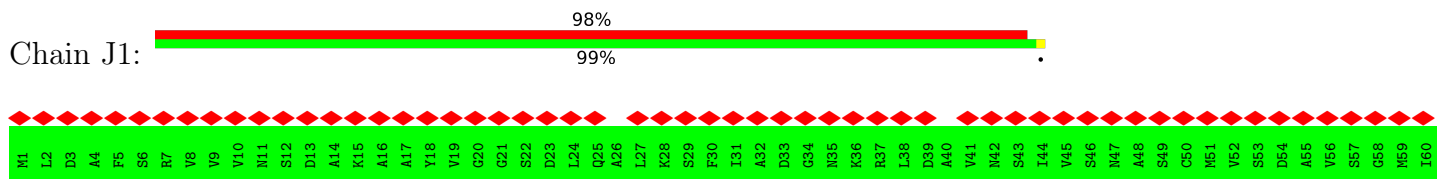
• Molecule 2: B-phycoerythrin beta chain

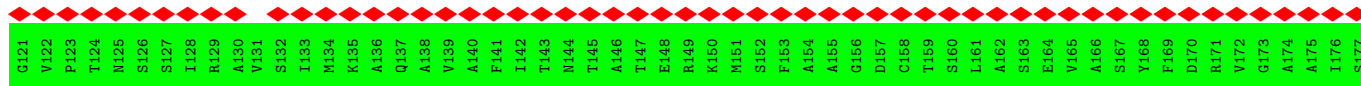
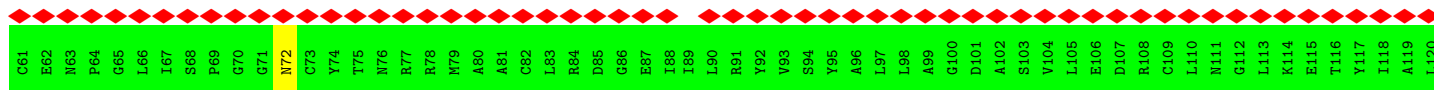


• Molecule 2: B-phycoerythrin beta chain

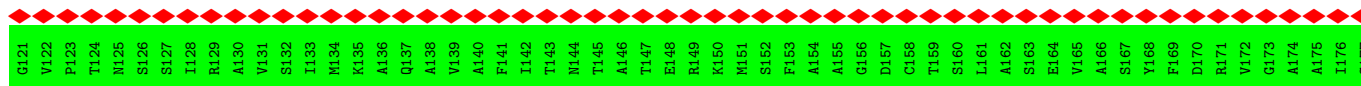
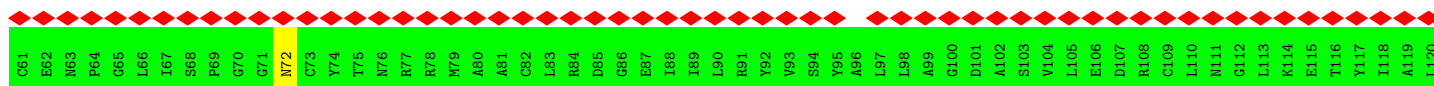
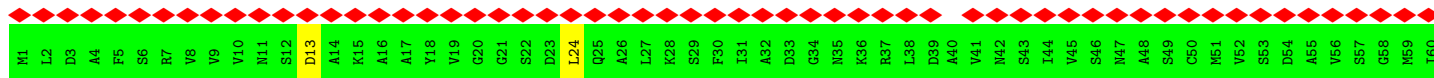


• Molecule 2: B-phycoerythrin beta chain

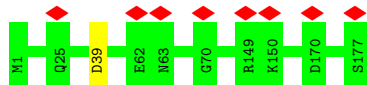




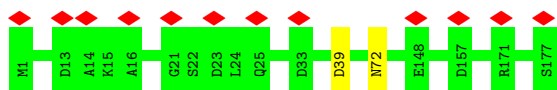
• Molecule 2: B-phycoerythrin beta chain



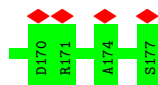
• Molecule 2: B-phycoerythrin beta chain



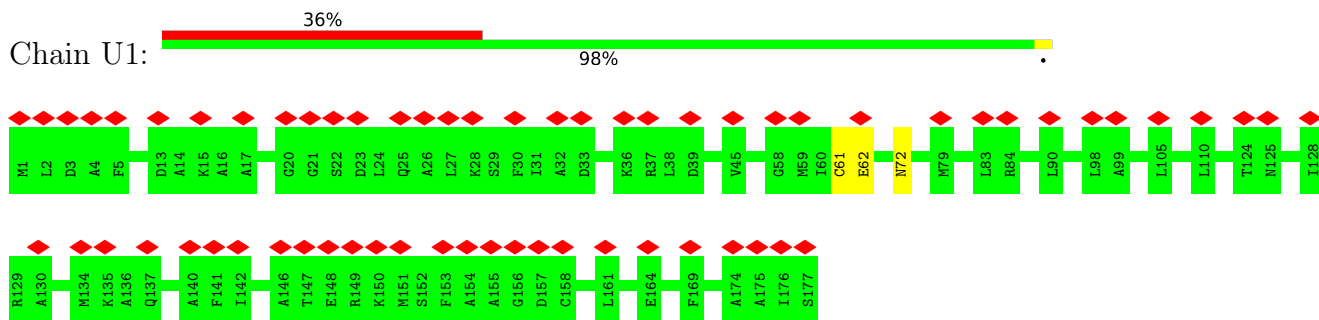
• Molecule 2: B-phycoerythrin beta chain



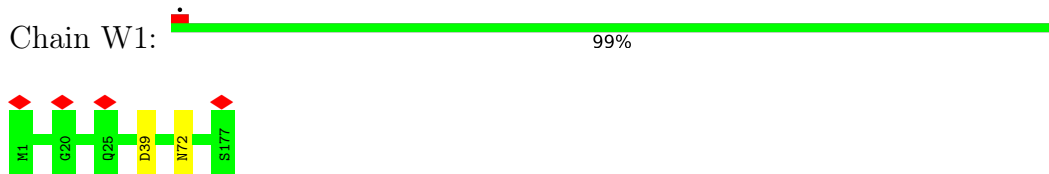
• Molecule 2: B-phycoerythrin beta chain



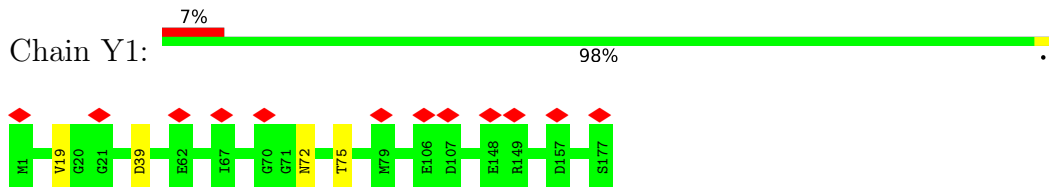
• Molecule 2: B-phycoerythrin beta chain



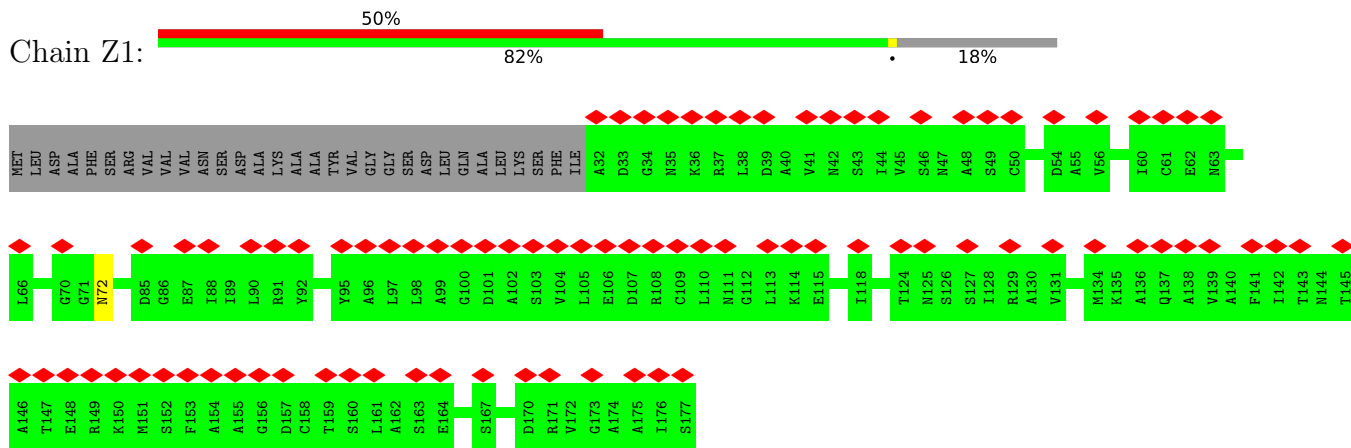
• Molecule 2: B-phycoerythrin beta chain



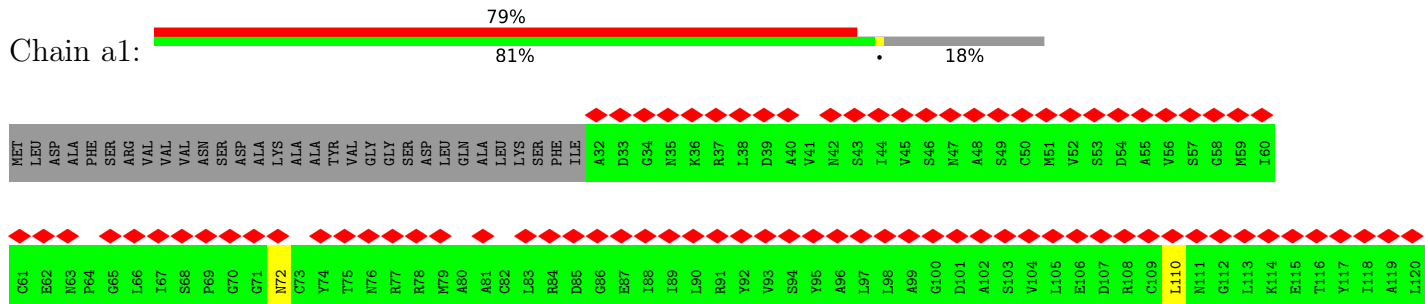
• Molecule 2: B-phycoerythrin beta chain

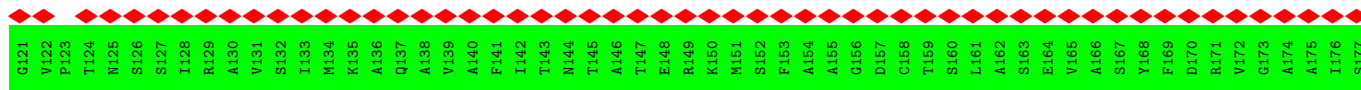


• Molecule 2: B-phycoerythrin beta chain

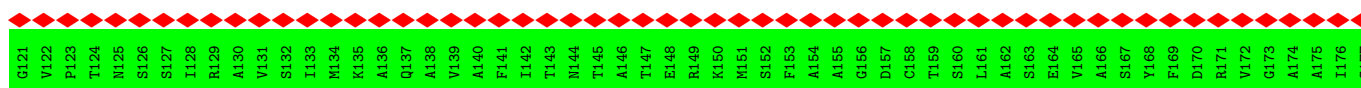
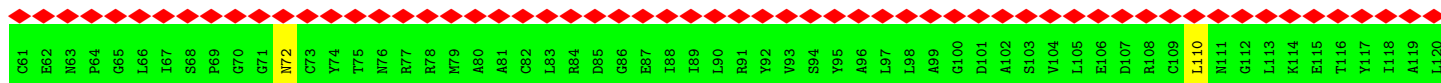
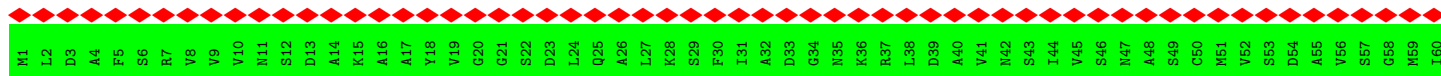


• Molecule 2: B-phycoerythrin beta chain

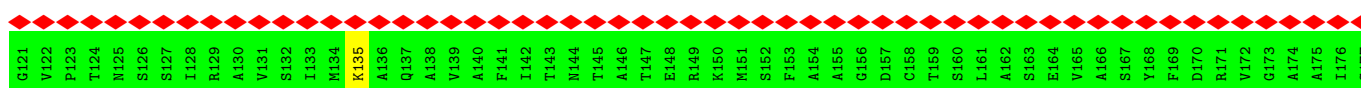
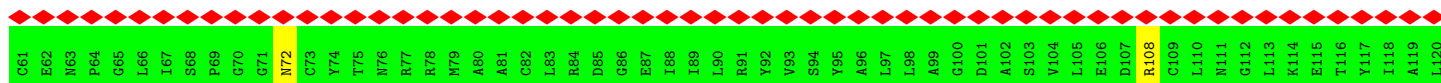




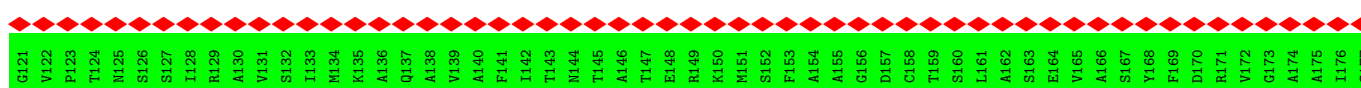
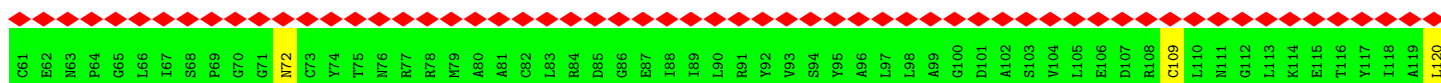
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

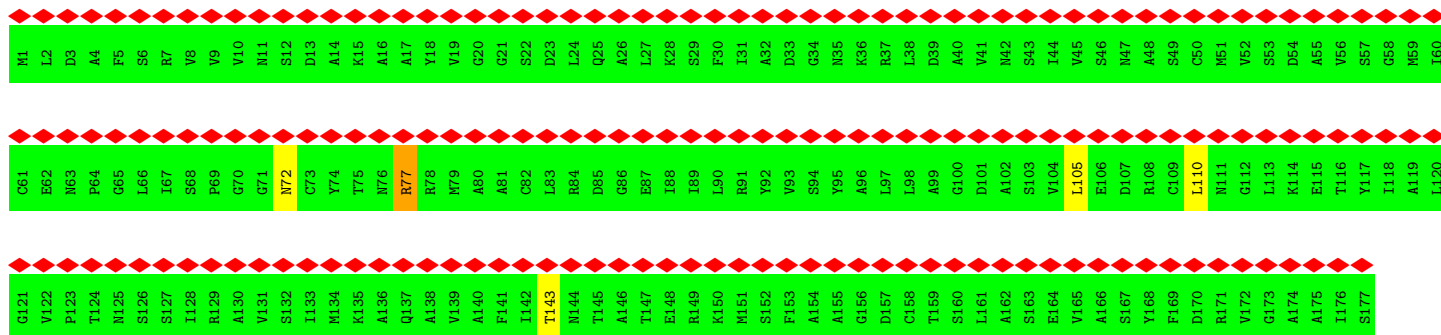


• Molecule 2: B-phycoerythrin beta chain

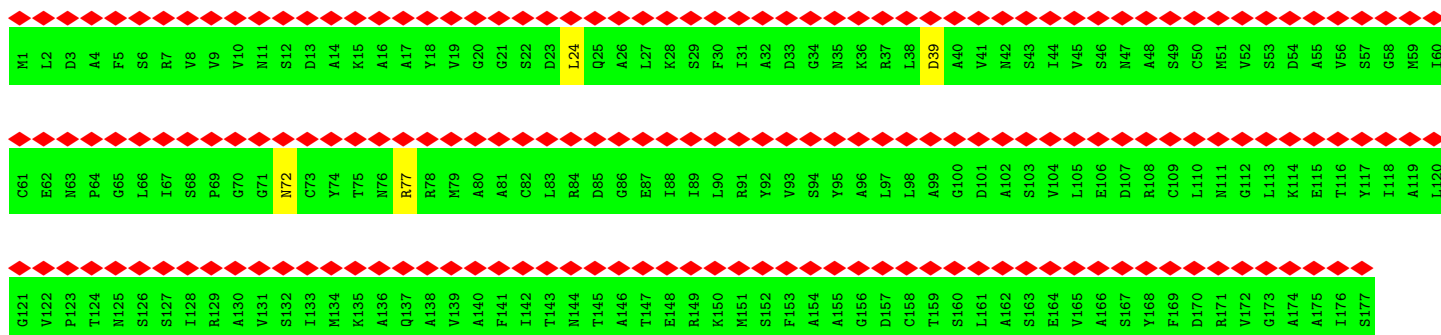


• Molecule 2: B-phycoerythrin beta chain

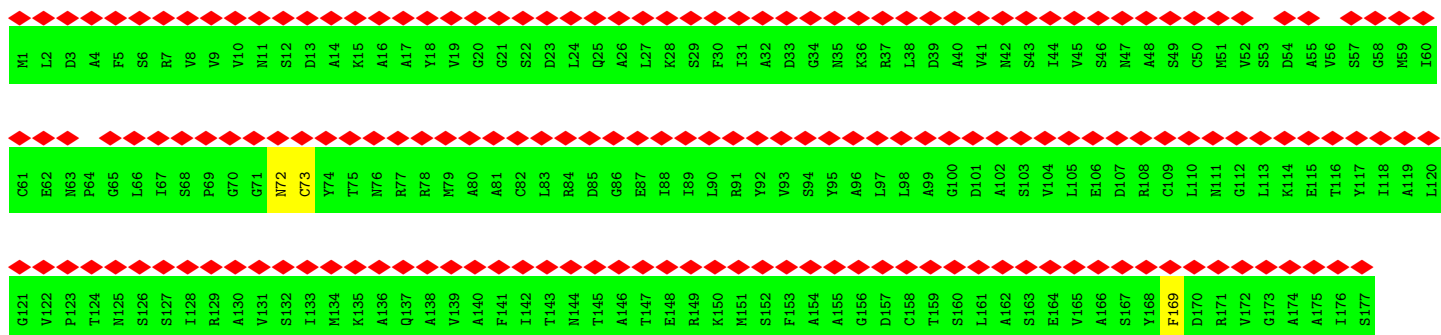




• Molecule 2: B-phycoerythrin beta chain

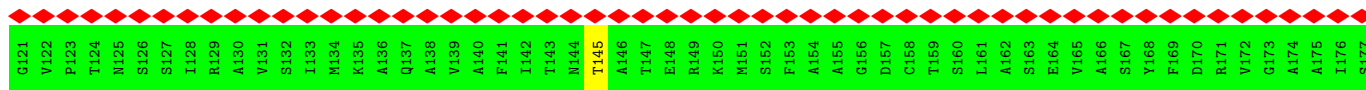


• Molecule 2: B-phycoerythrin beta chain

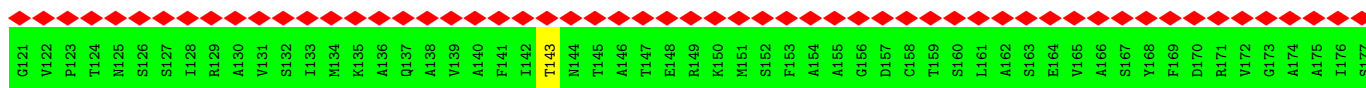
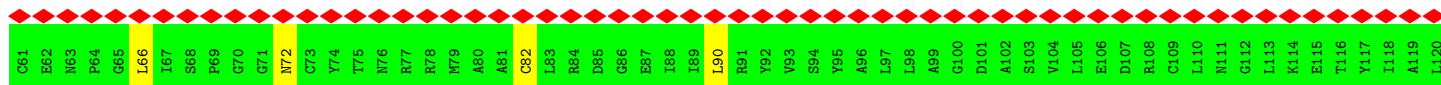


• Molecule 2: B-phycoerythrin beta chain

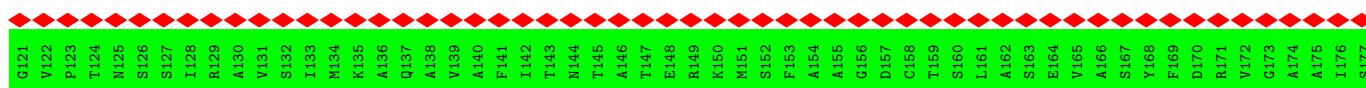
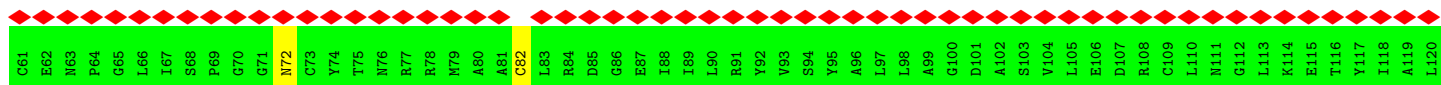




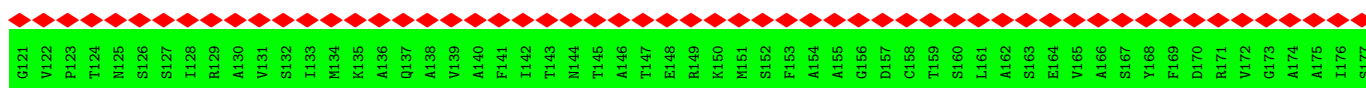
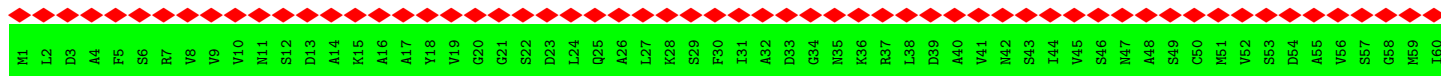
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

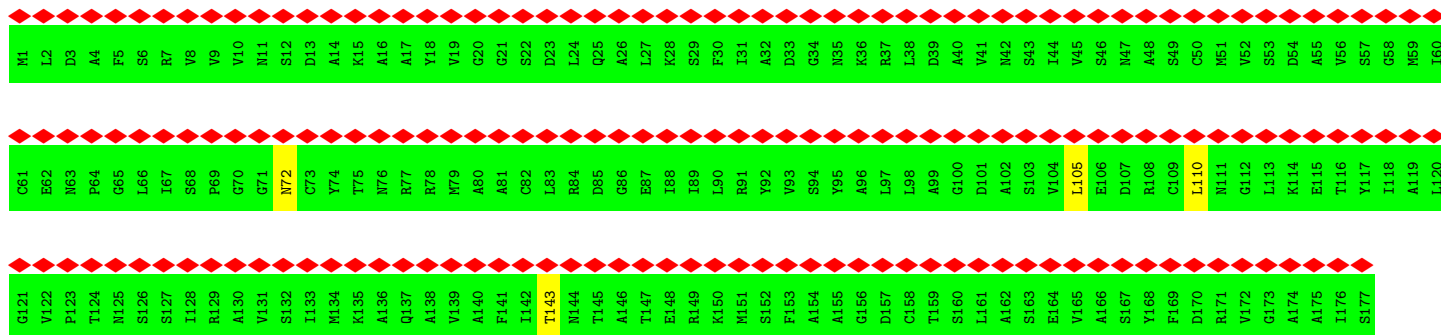


• Molecule 2: B-phycoerythrin beta chain

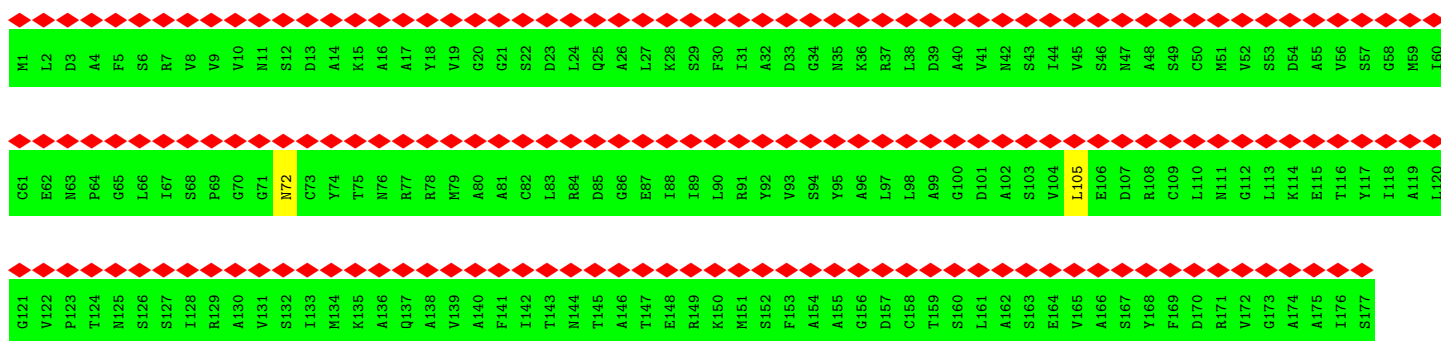


• Molecule 2: B-phycoerythrin beta chain





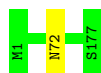
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



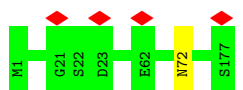
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



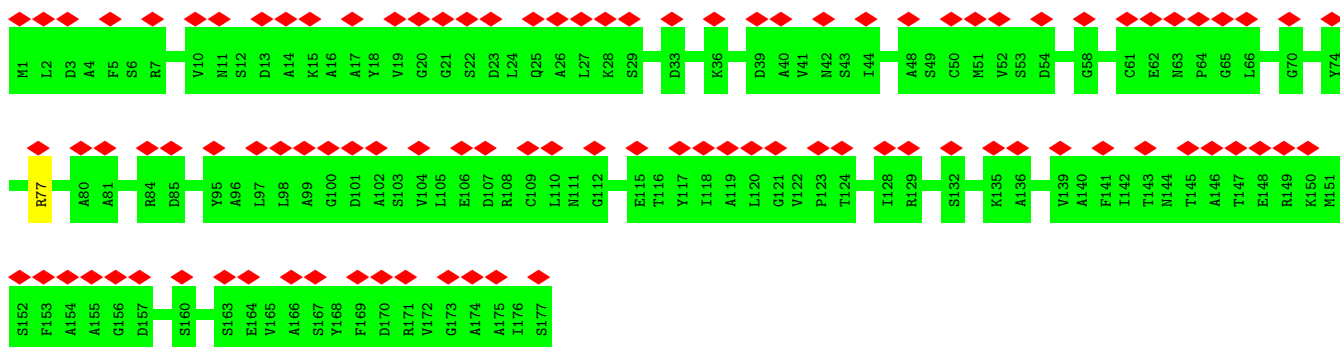
• Molecule 2: B-phycoerythrin beta chain



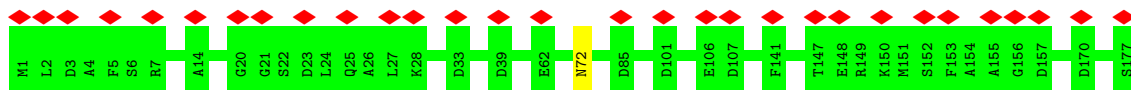
• Molecule 2: B-phycoerythrin beta chain



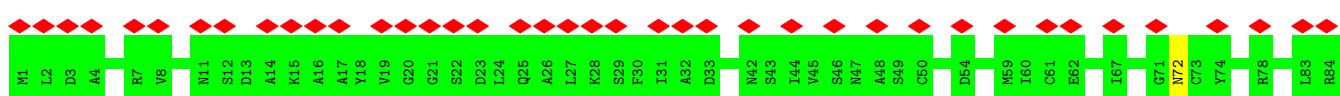
• Molecule 2: B-phycoerythrin beta chain

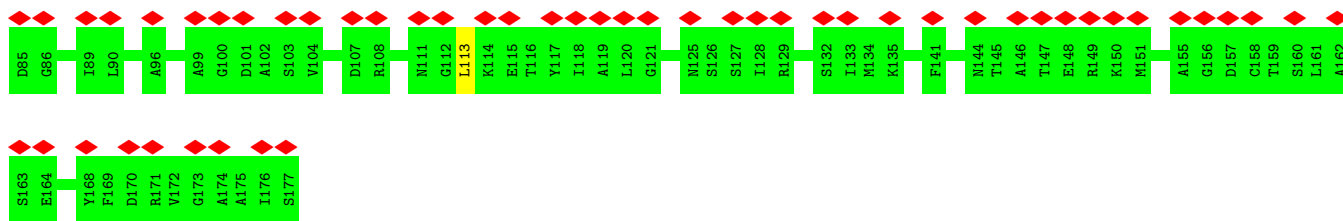


• Molecule 2: B-phycoerythrin beta chain

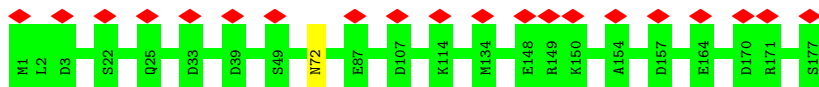


• Molecule 2: B-phycoerythrin beta chain

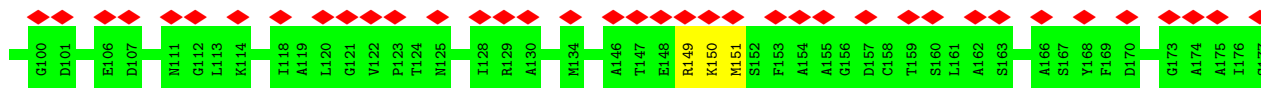
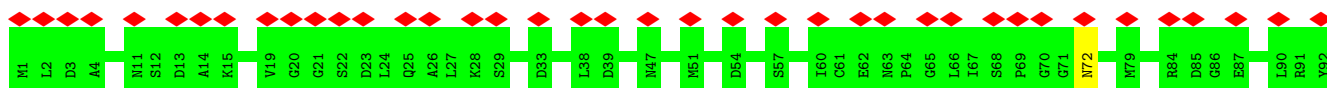




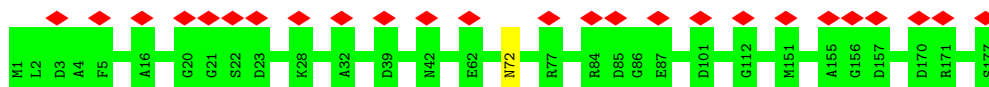
• Molecule 2: B-phycoerythrin beta chain



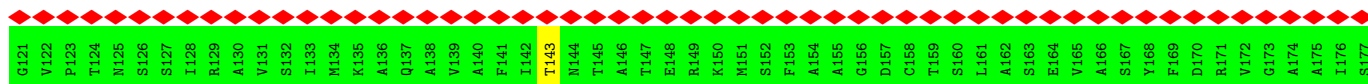
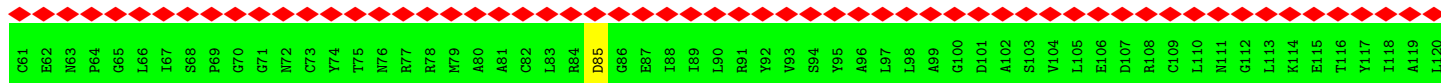
• Molecule 2: B-phycoerythrin beta chain



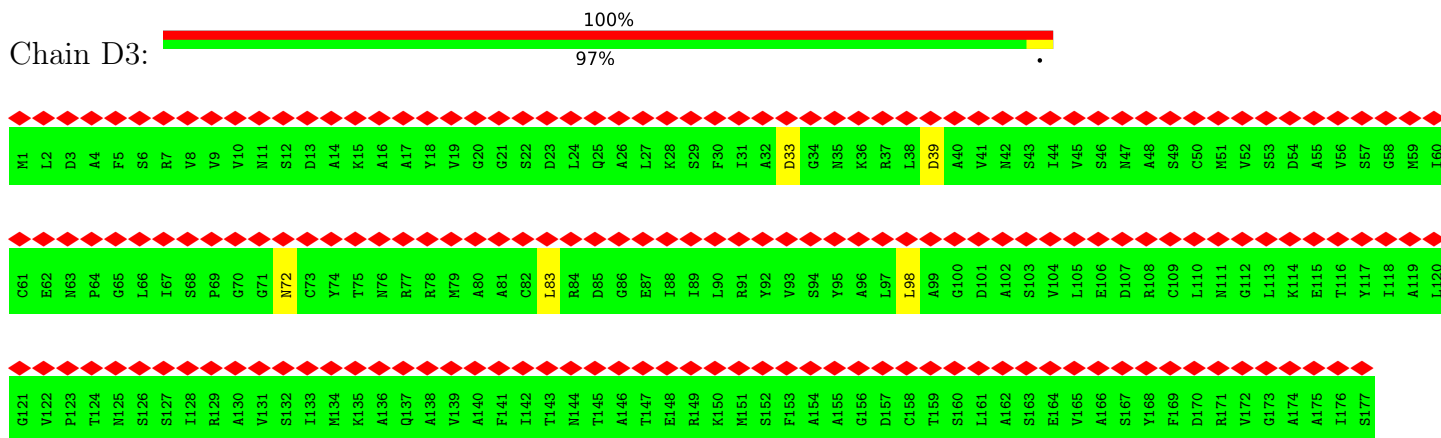
• Molecule 2: B-phycoerythrin beta chain



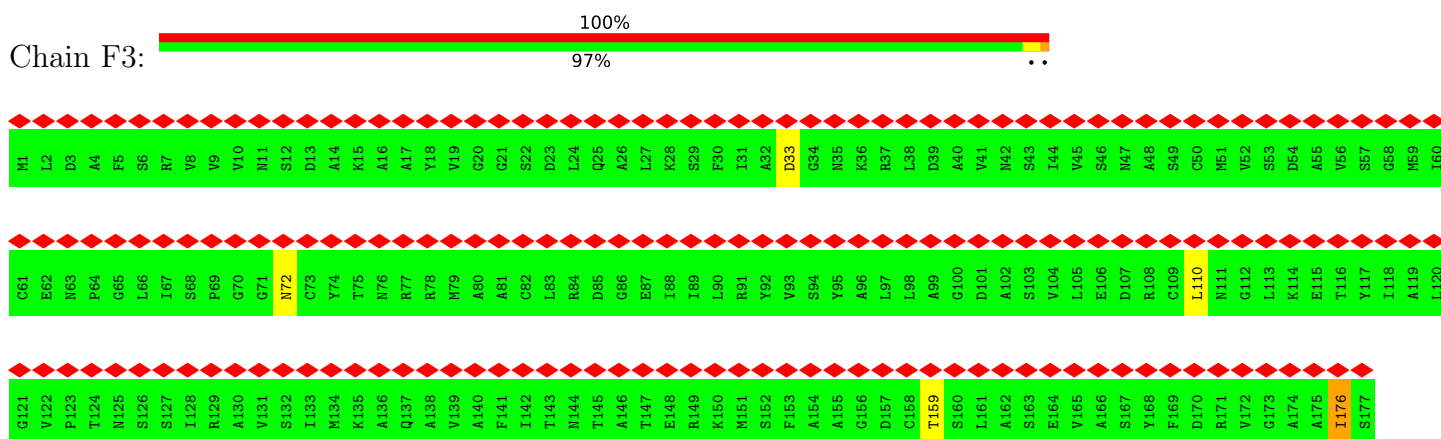
• Molecule 2: B-phycoerythrin beta chain



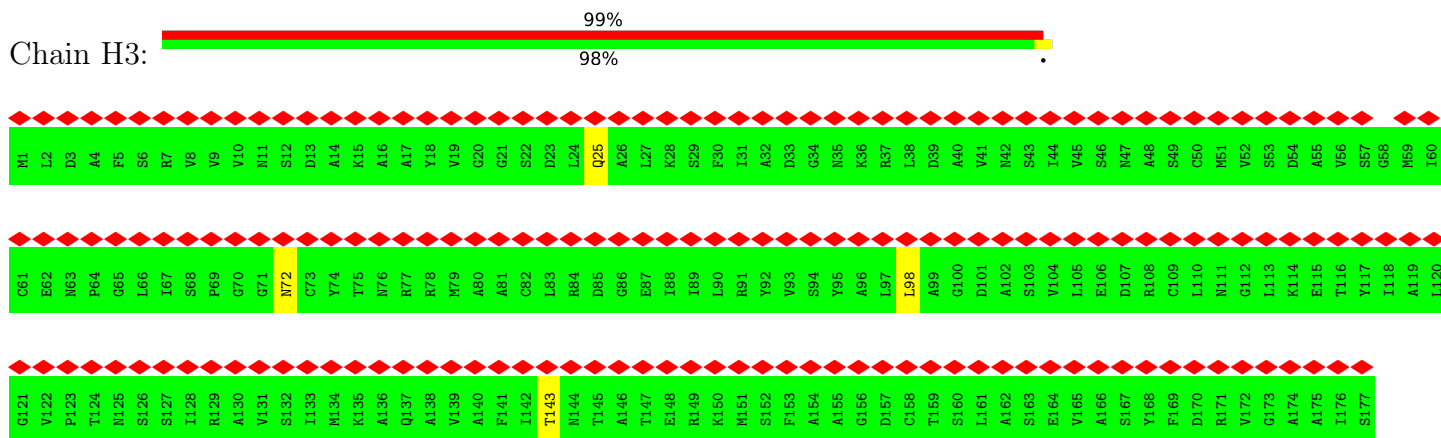
• Molecule 2: B-phycoerythrin beta chain



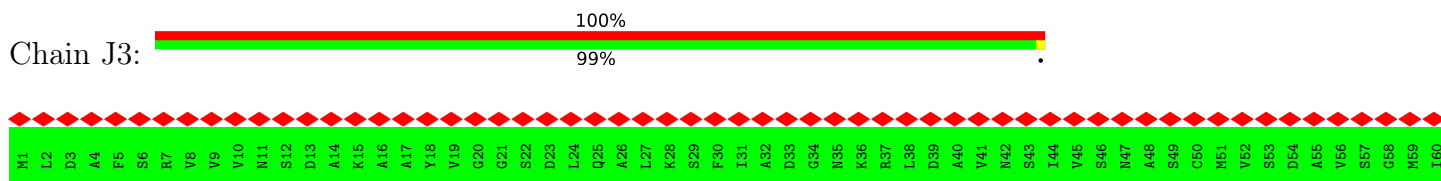
• Molecule 2: B-phycoerythrin beta chain

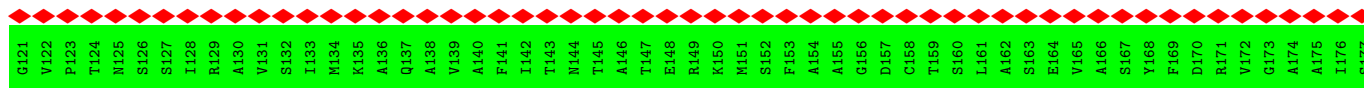
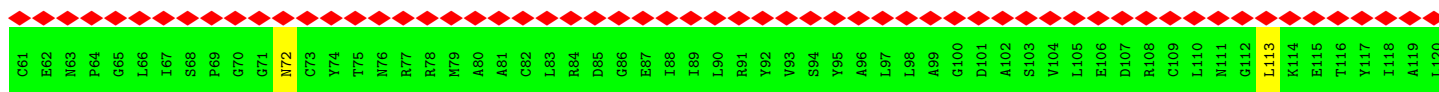


• Molecule 2: B-phycoerythrin beta chain

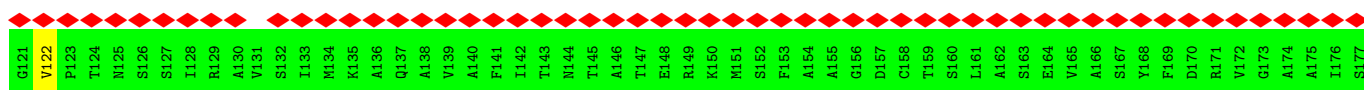
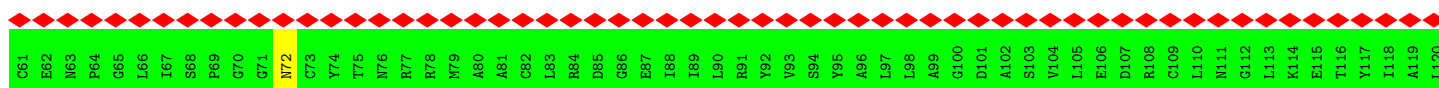
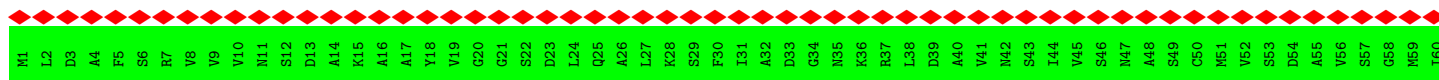


• Molecule 2: B-phycoerythrin beta chain

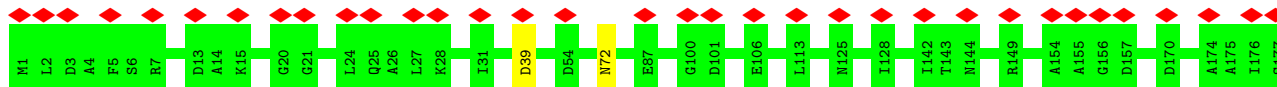




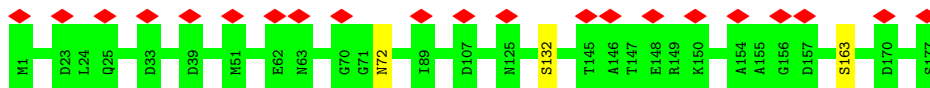
- Molecule 2: B-phycoerythrin beta chain



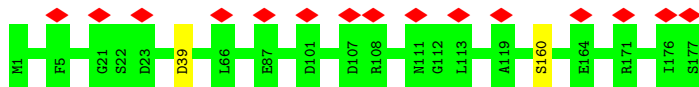
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

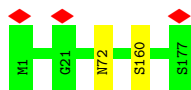


- Molecule 2: B-phycoerythrin beta chain

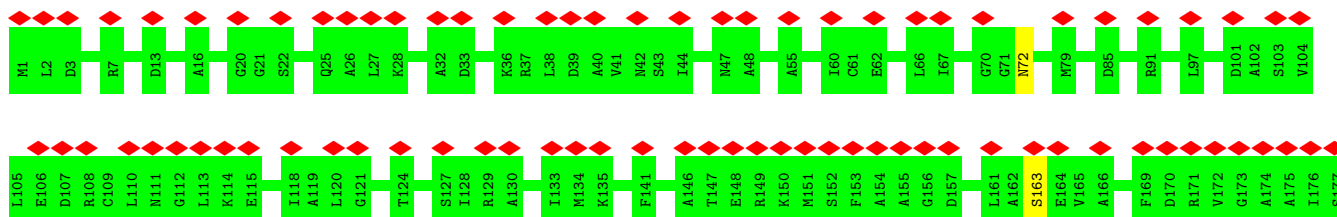


- Molecule 2: B-phycoerythrin beta chain

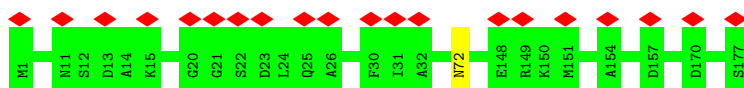




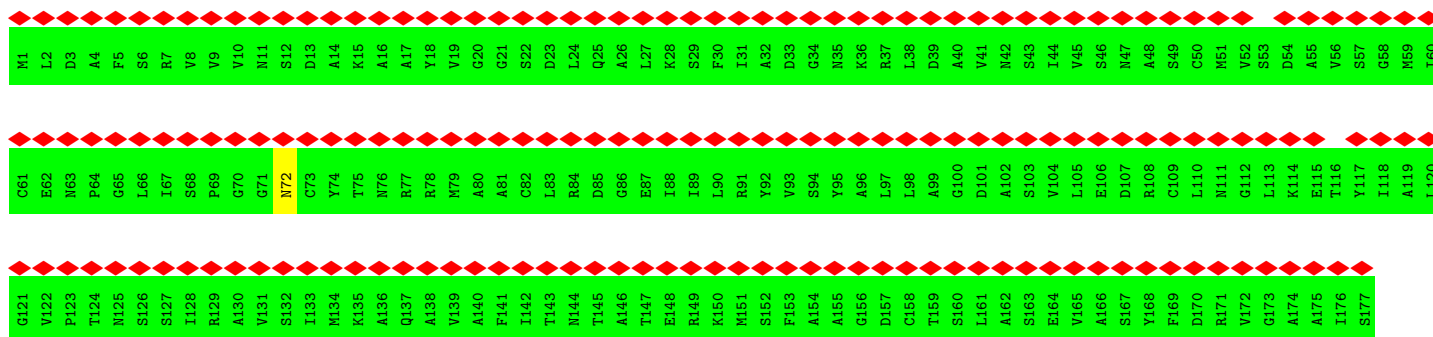
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

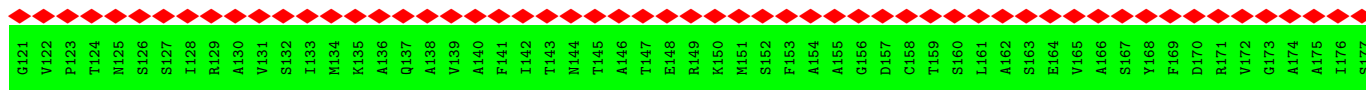


- Molecule 2: B-phycoerythrin beta chain

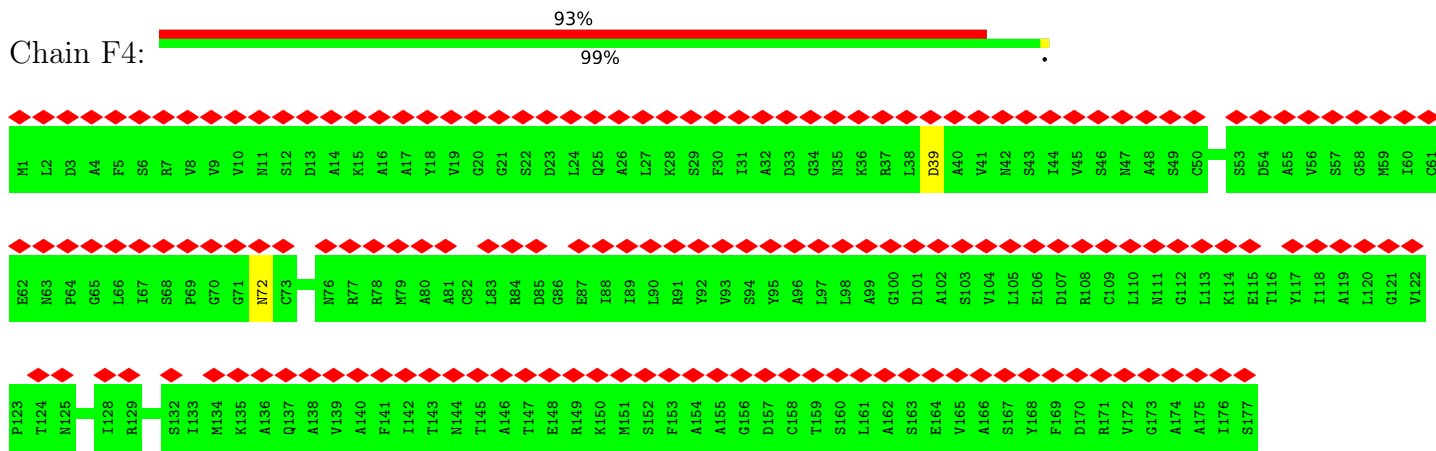


- Molecule 2: B-phycoerythrin beta chain

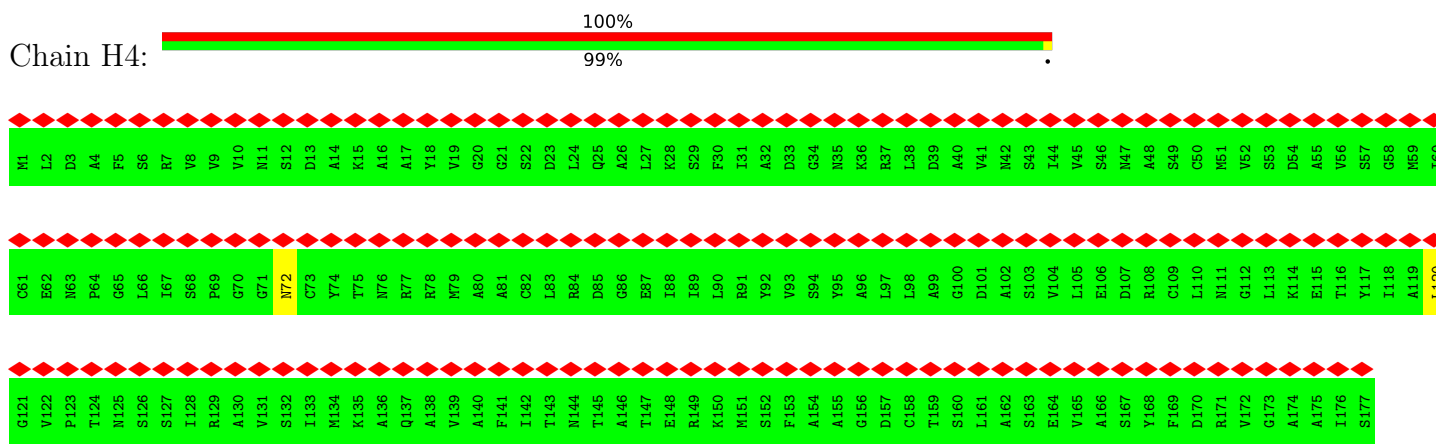




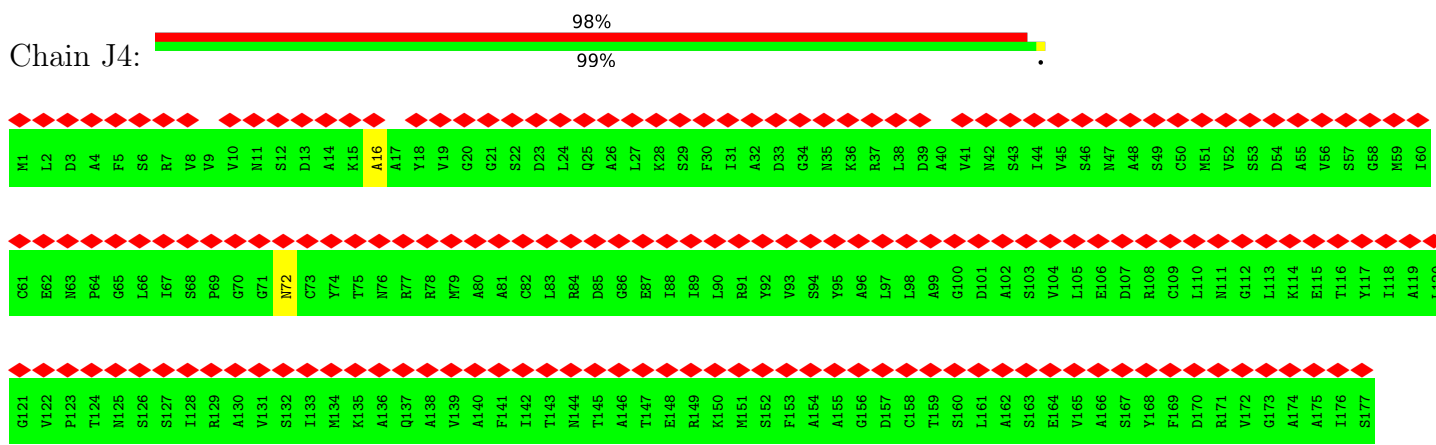
• Molecule 2: B-phycoerythrin beta chain



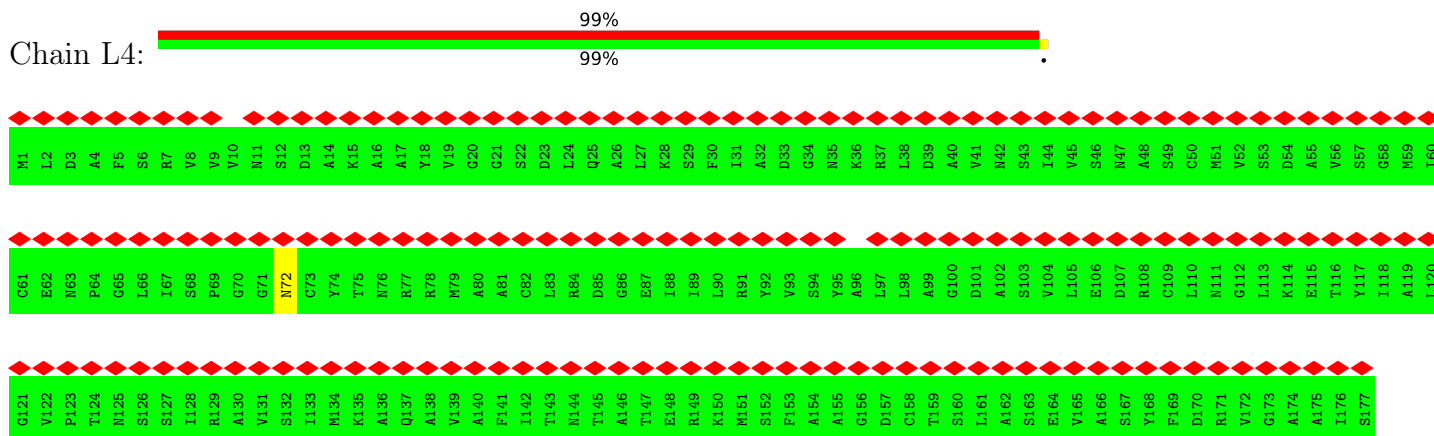
• Molecule 2: B-phycoerythrin beta chain



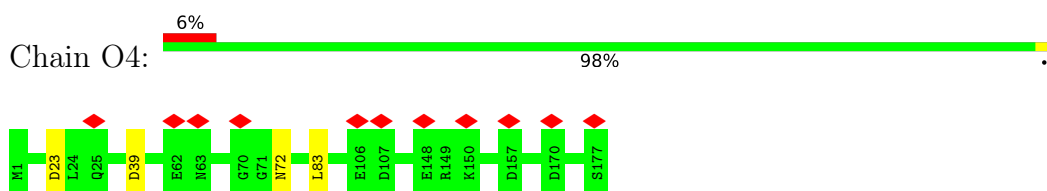
• Molecule 2: B-phycoerythrin beta chain



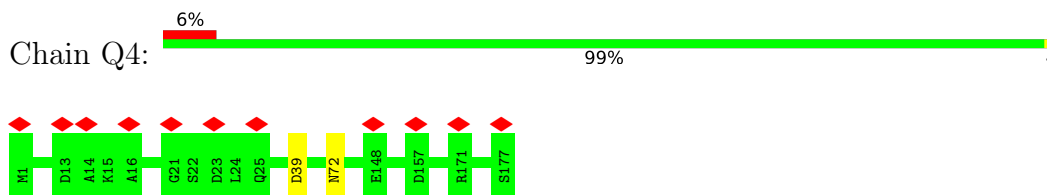
• Molecule 2: B-phycoerythrin beta chain



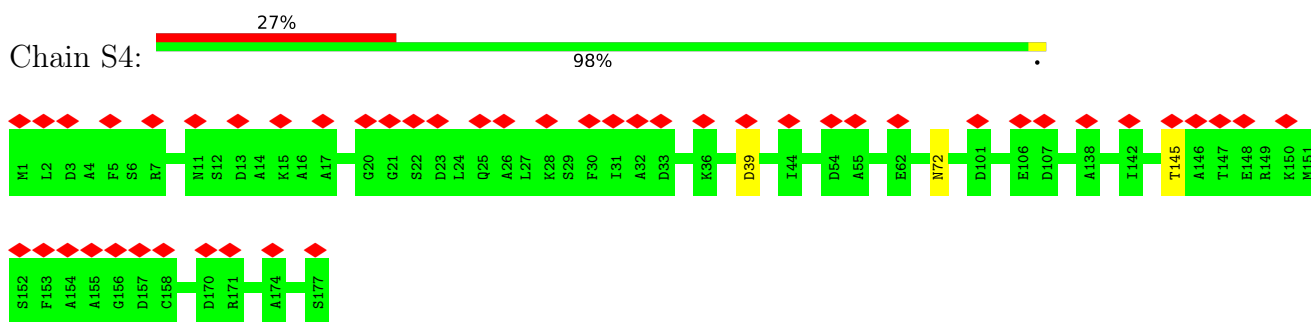
• Molecule 2: B-phycoerythrin beta chain



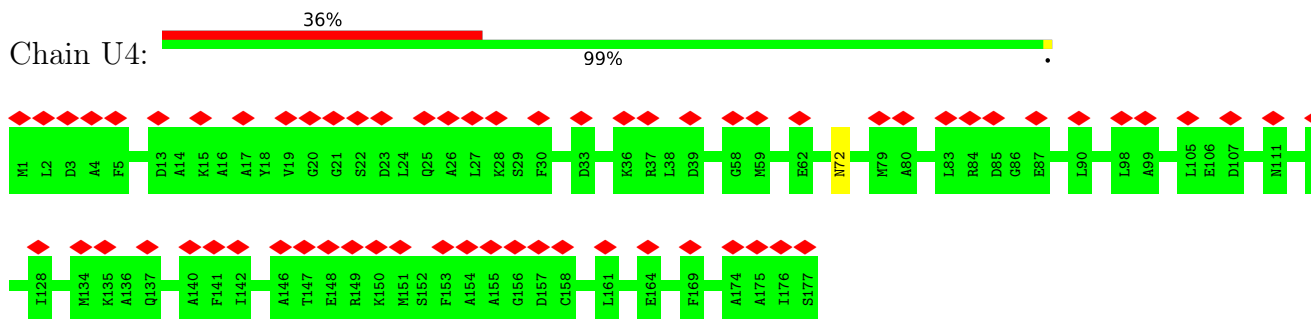
• Molecule 2: B-phycoerythrin beta chain



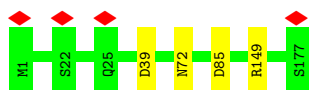
• Molecule 2: B-phycoerythrin beta chain



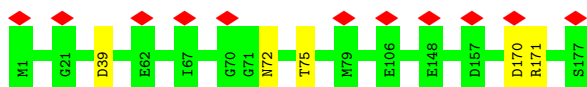
• Molecule 2: B-phycoerythrin beta chain



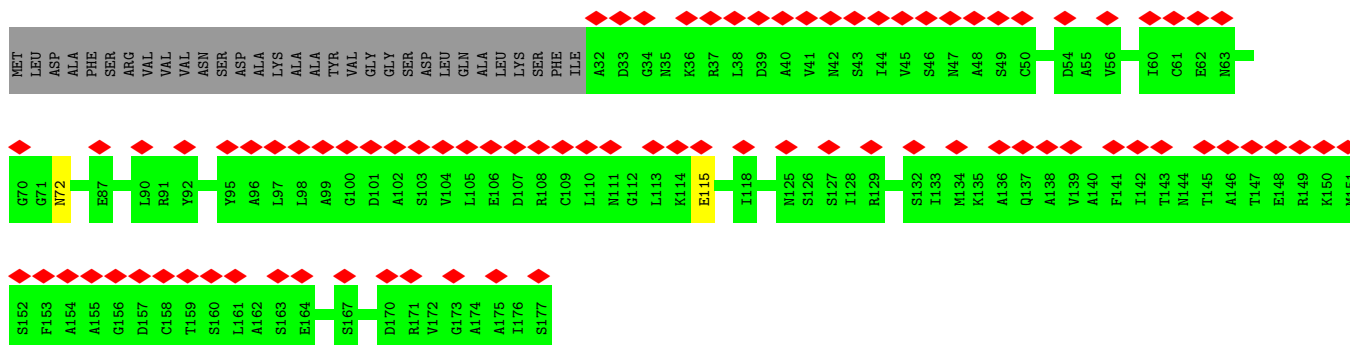
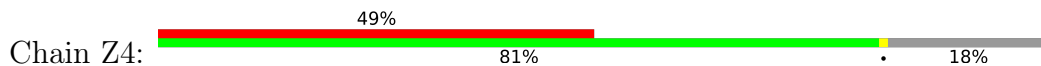
• Molecule 2: B-phycoerythrin beta chain



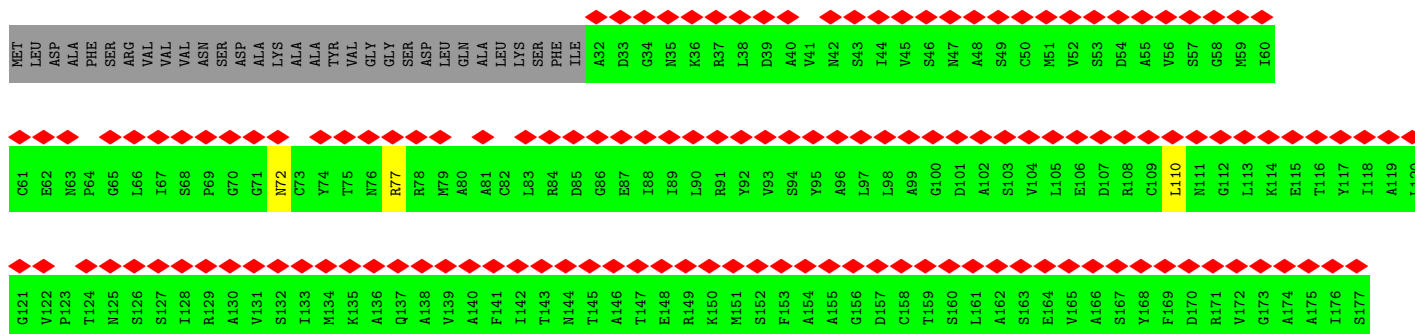
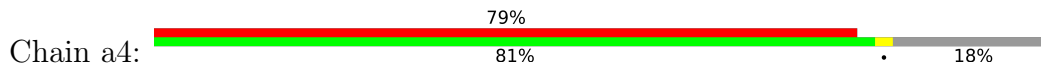
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

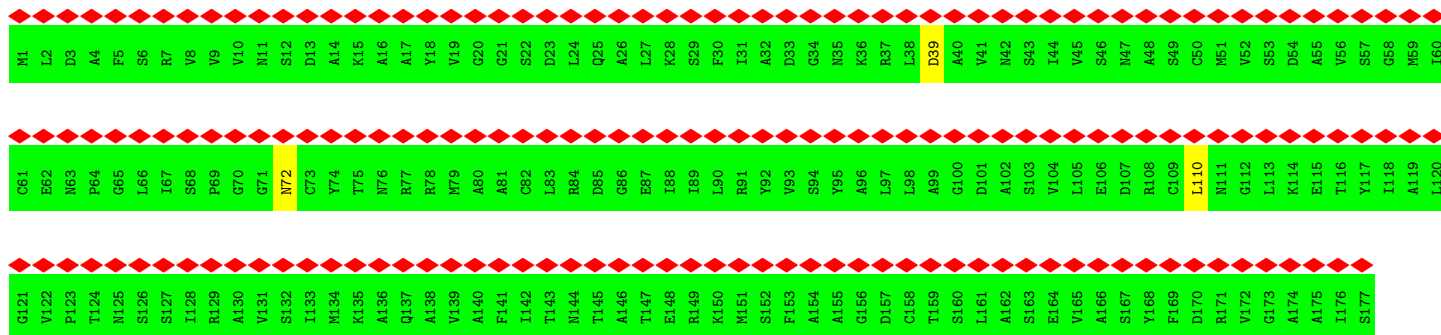


• Molecule 2: B-phycoerythrin beta chain

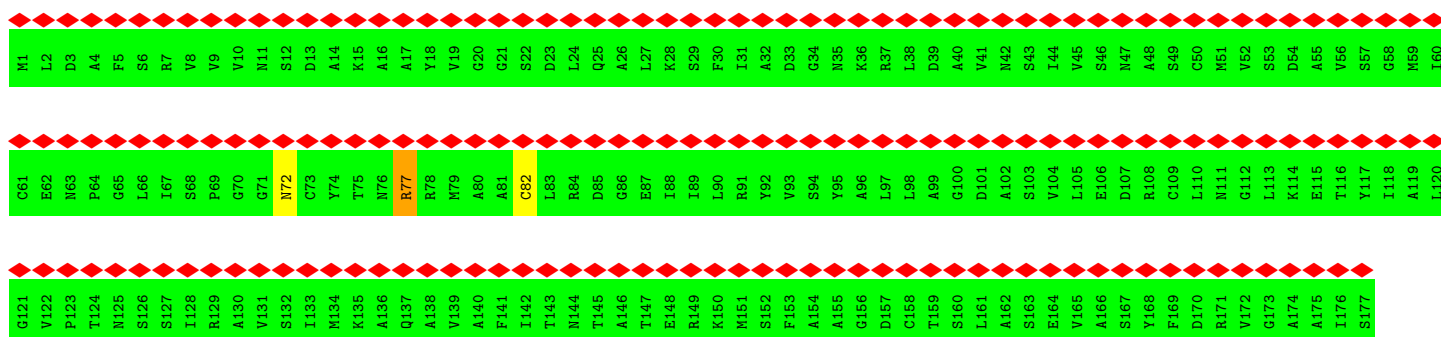


• Molecule 2: B-phycoerythrin beta chain

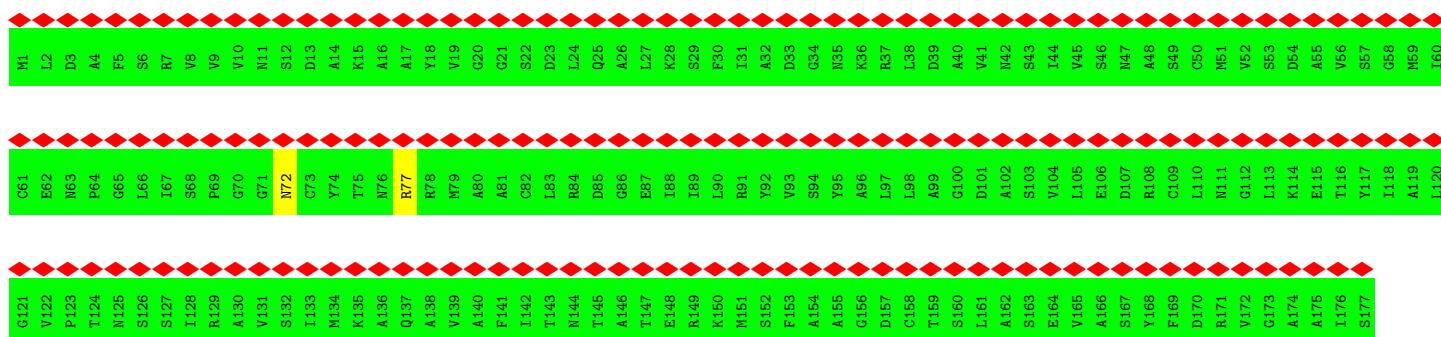




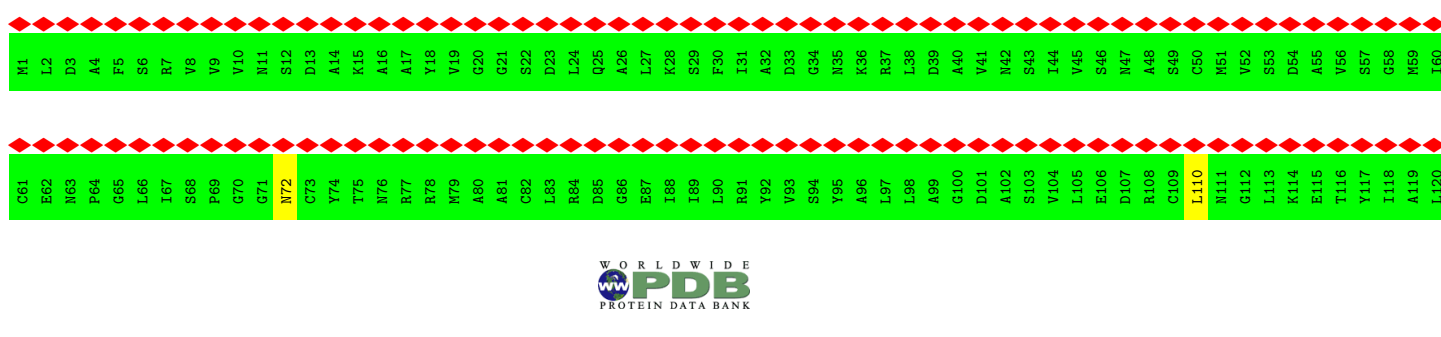
• Molecule 2: B-phycoerythrin beta chain

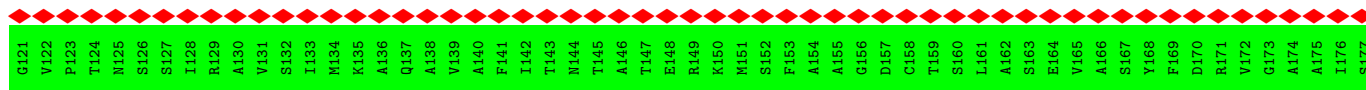


• Molecule 2: B-phycoerythrin beta chain

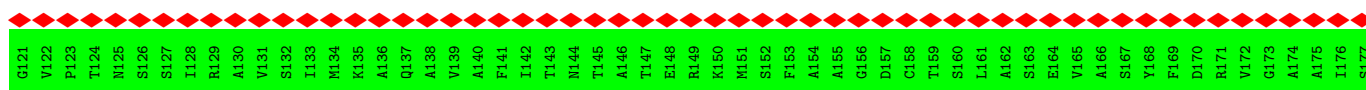
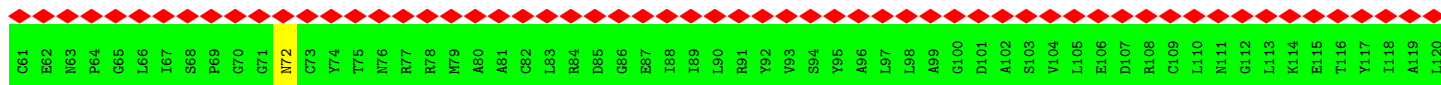


• Molecule 2: B-phycoerythrin beta chain

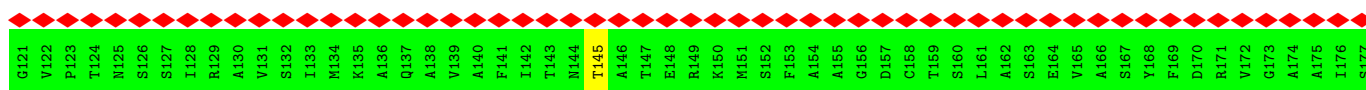
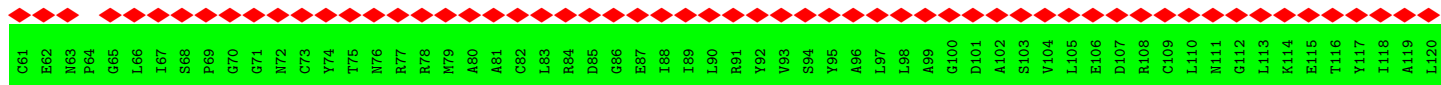




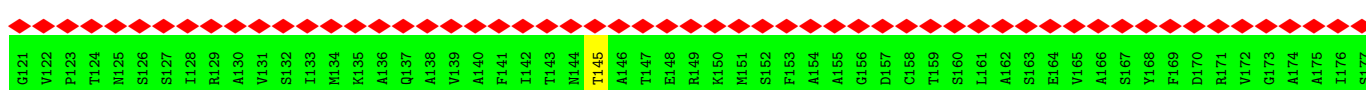
• Molecule 2: B-phycoerythrin beta chain



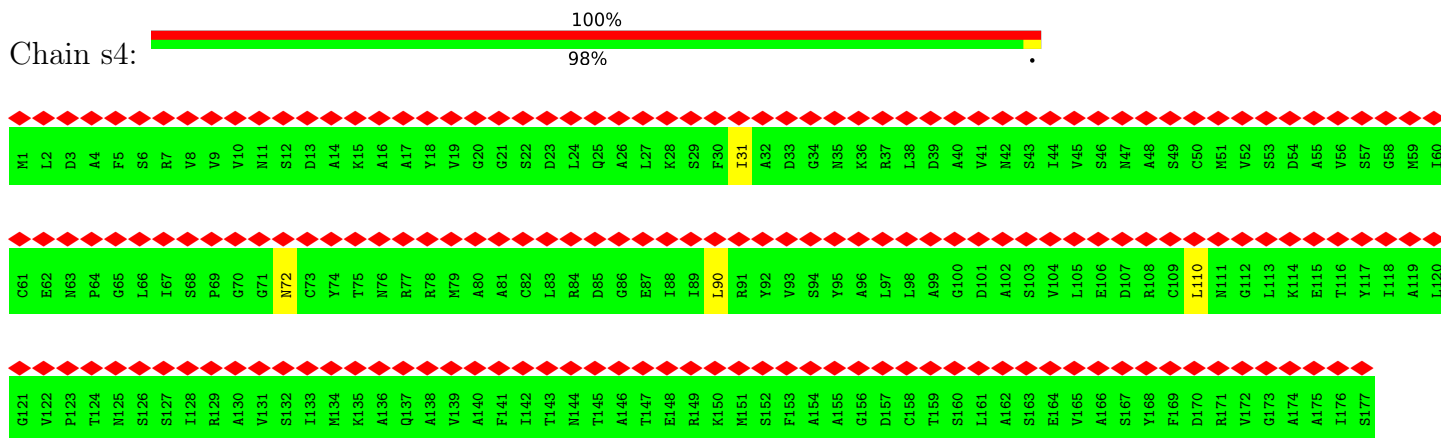
• Molecule 2: B-phycoerythrin beta chain



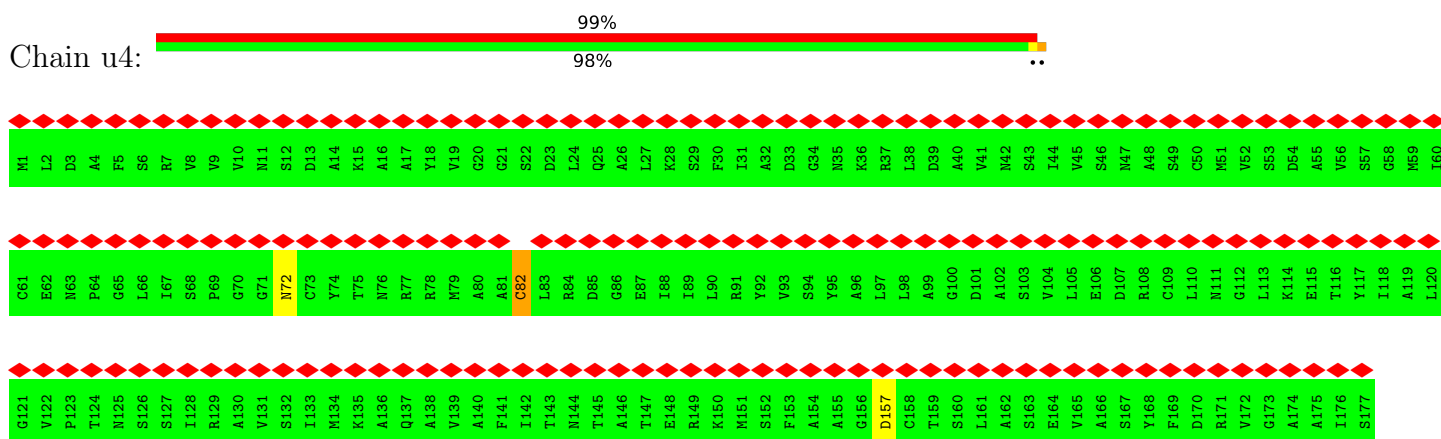
• Molecule 2: B-phycoerythrin beta chain



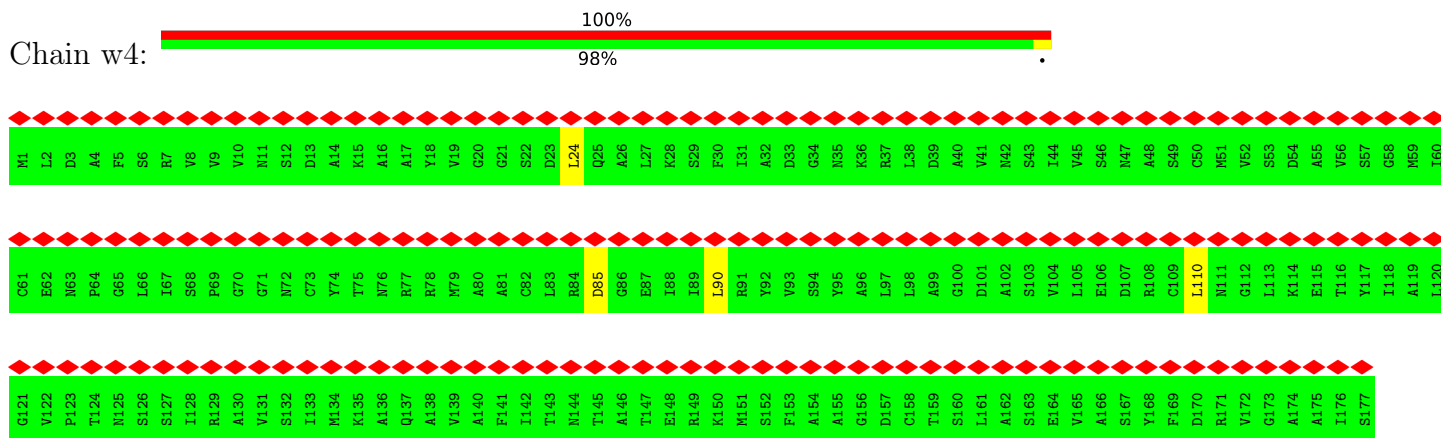
• Molecule 2: B-phycoerythrin beta chain



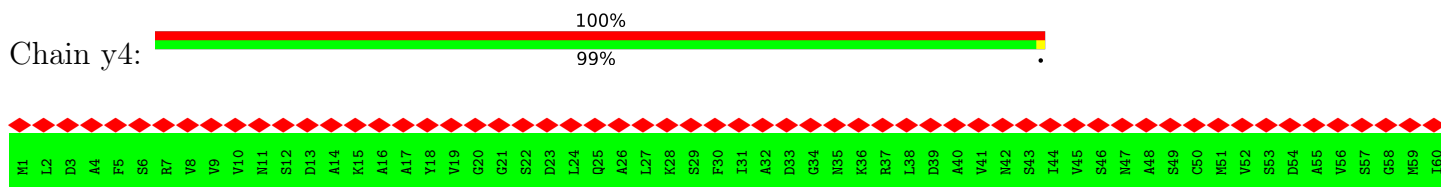
• Molecule 2: B-phycoerythrin beta chain

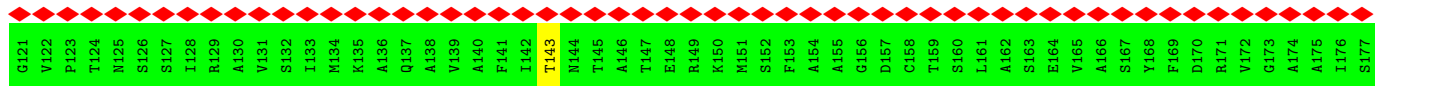
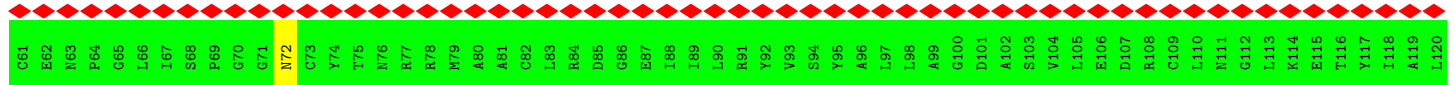


• Molecule 2: B-phycoerythrin beta chain

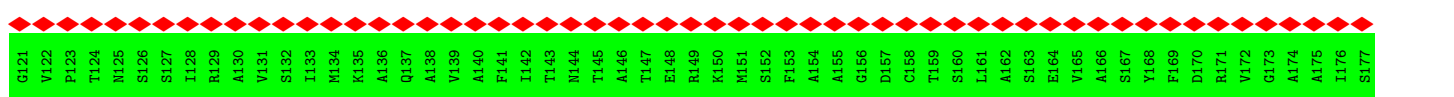
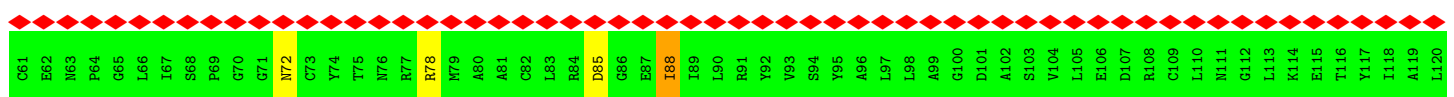
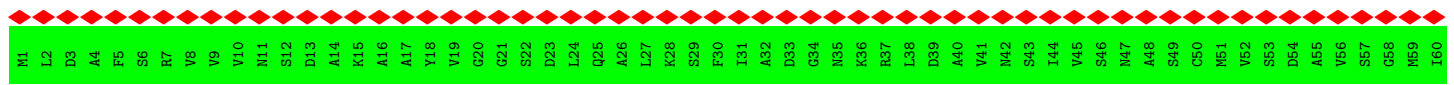


• Molecule 2: B-phycoerythrin beta chain

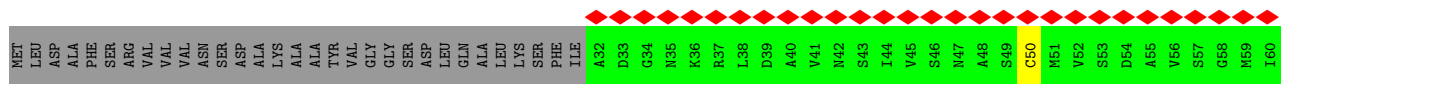
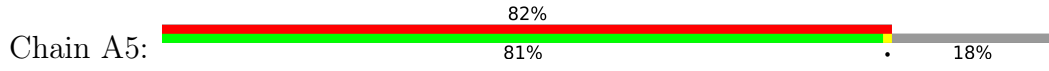




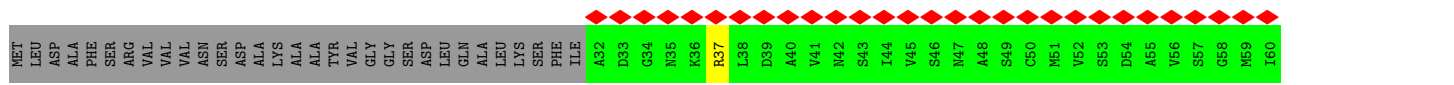
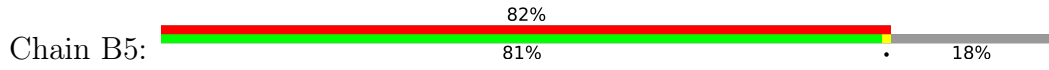
• Molecule 2: B-phycoerythrin beta chain



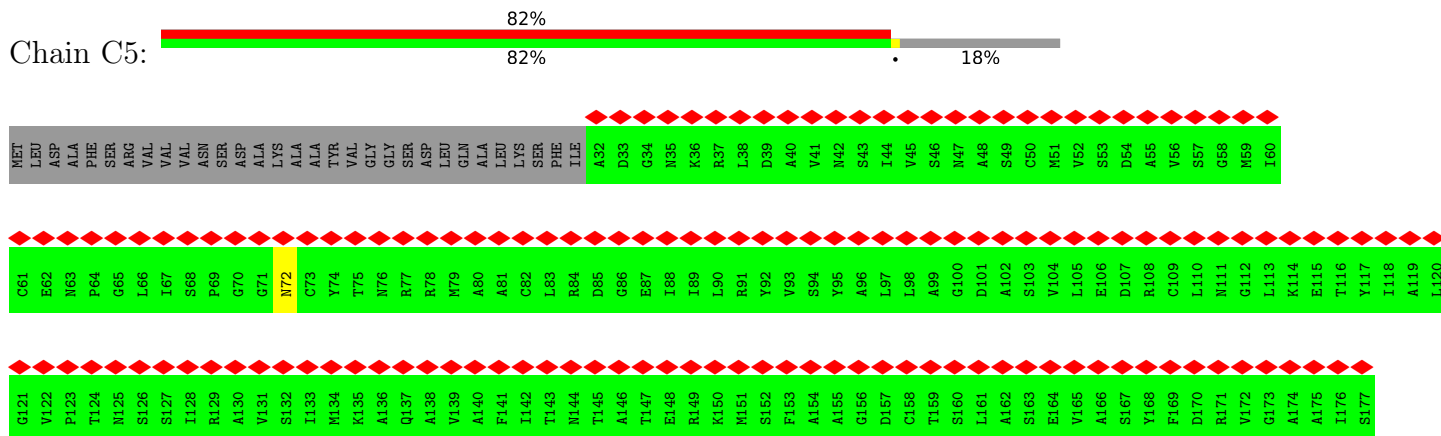
• Molecule 2: B-phycoerythrin beta chain



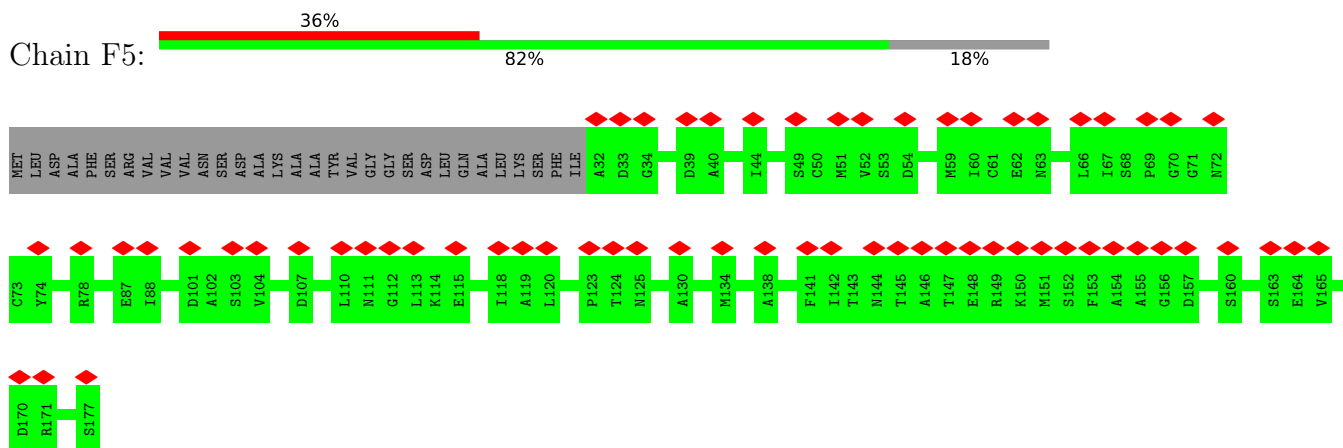
• Molecule 2: B-phycoerythrin beta chain



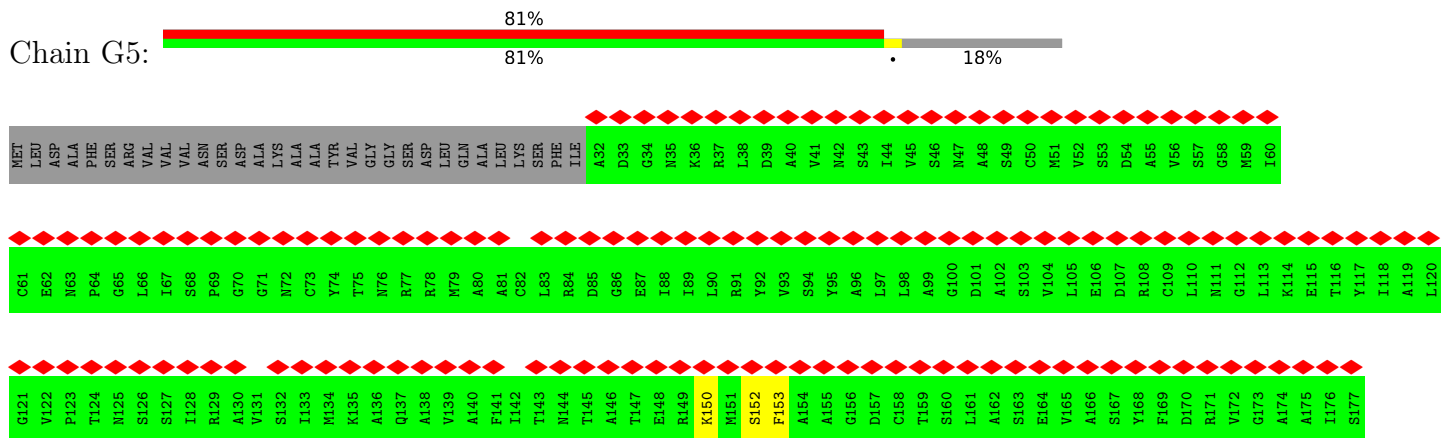
• Molecule 2: B-phycoerythrin beta chain



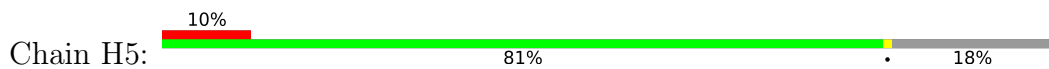
• Molecule 2: B-phycoerythrin beta chain

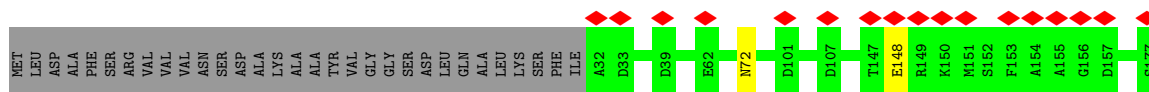


• Molecule 2: B-phycoerythrin beta chain

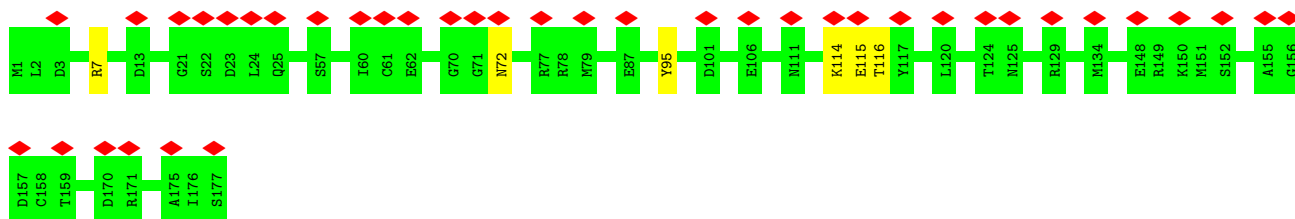


• Molecule 2: B-phycoerythrin beta chain

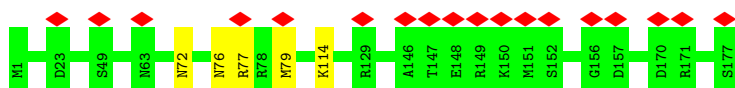




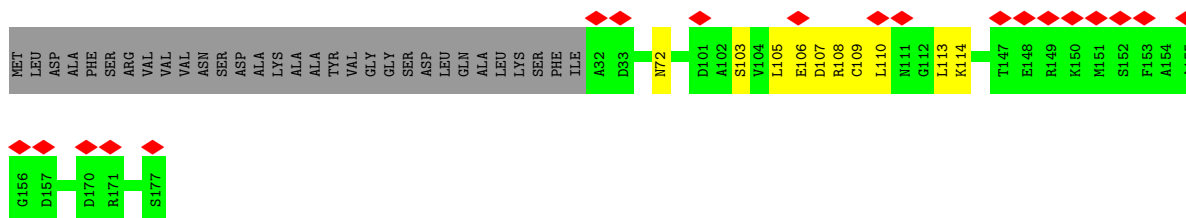
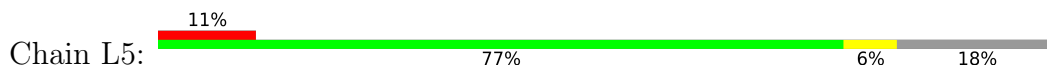
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



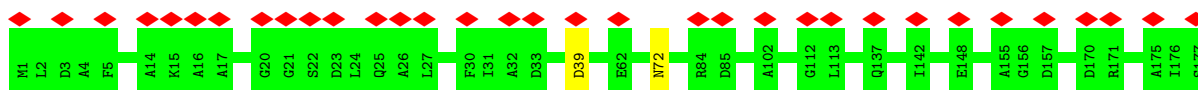
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

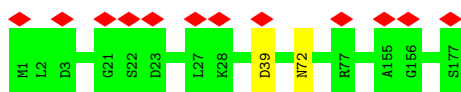


• Molecule 2: B-phycoerythrin beta chain



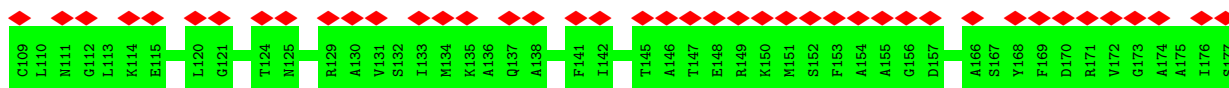
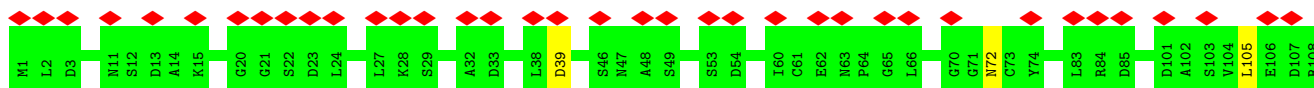
• Molecule 2: B-phycoerythrin beta chain

Chain T6:  7% 99%



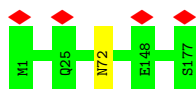
- Molecule 2: B-phycoerythrin beta chain

Chain V6:  45% 98%



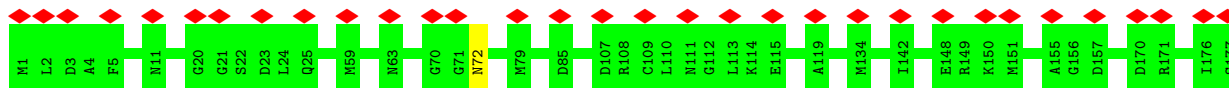
- Molecule 2: B-phycoerythrin beta chain

Chain Y6:  0% 99%

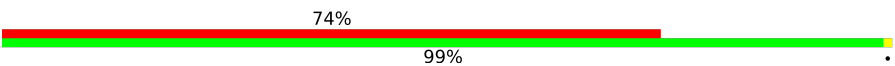


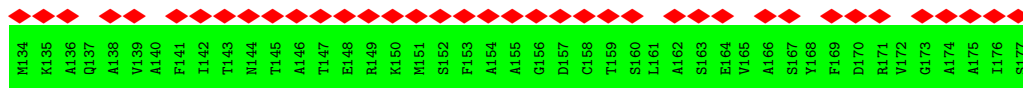
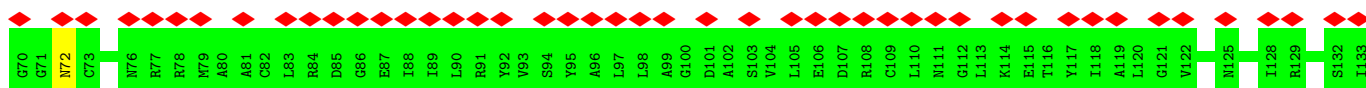
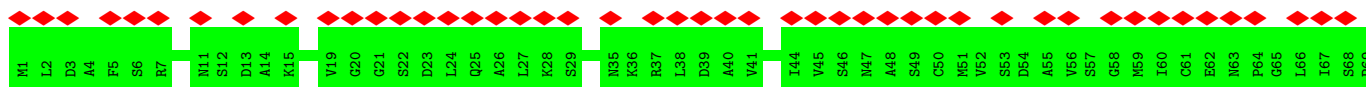
- Molecule 2: B-phycoerythrin beta chain

Chain a6:  18% 99%

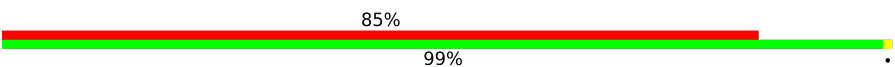


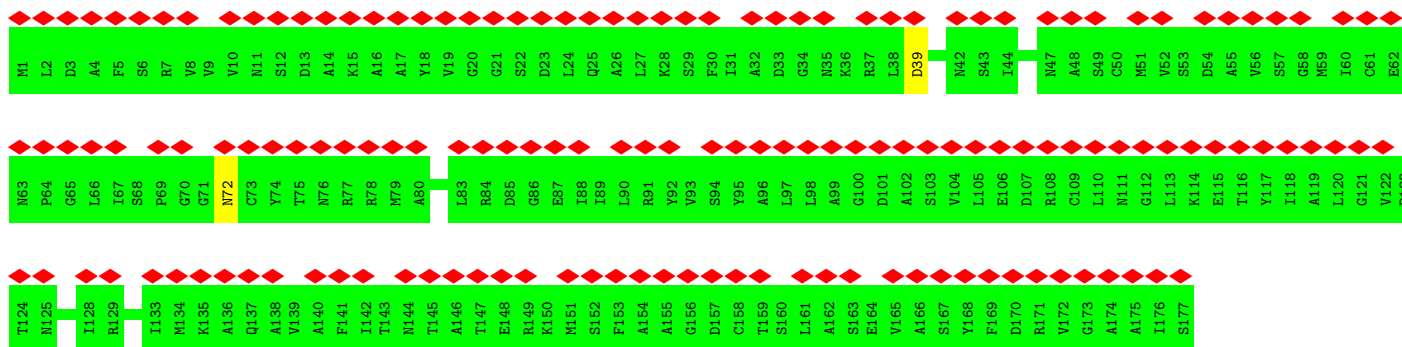
- Molecule 2: B-phycoerythrin beta chain

Chain c6:  74% 99%

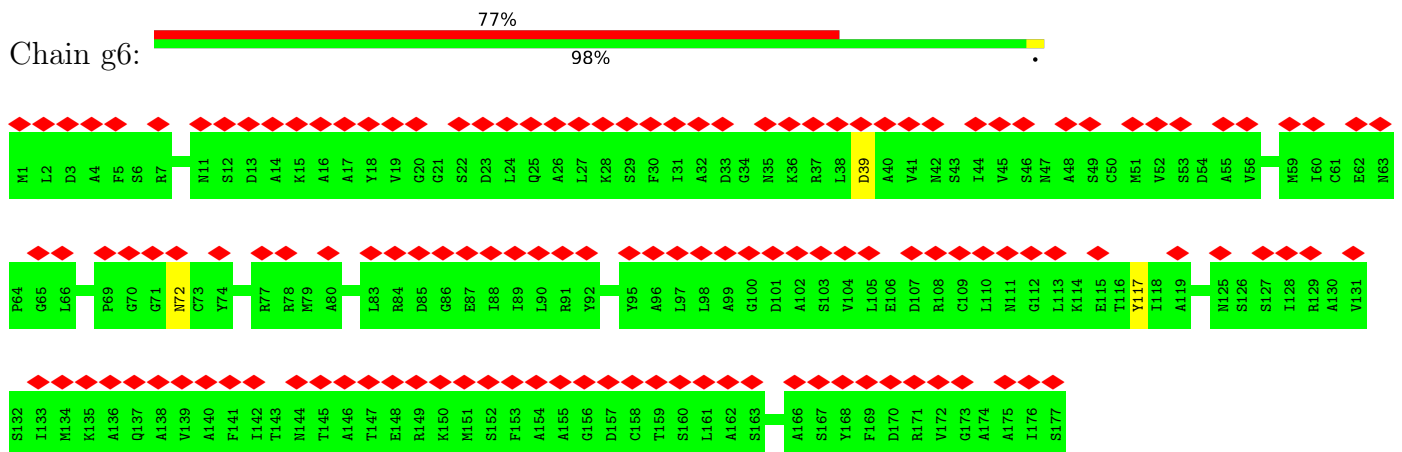


- Molecule 2: B-phycoerythrin beta chain

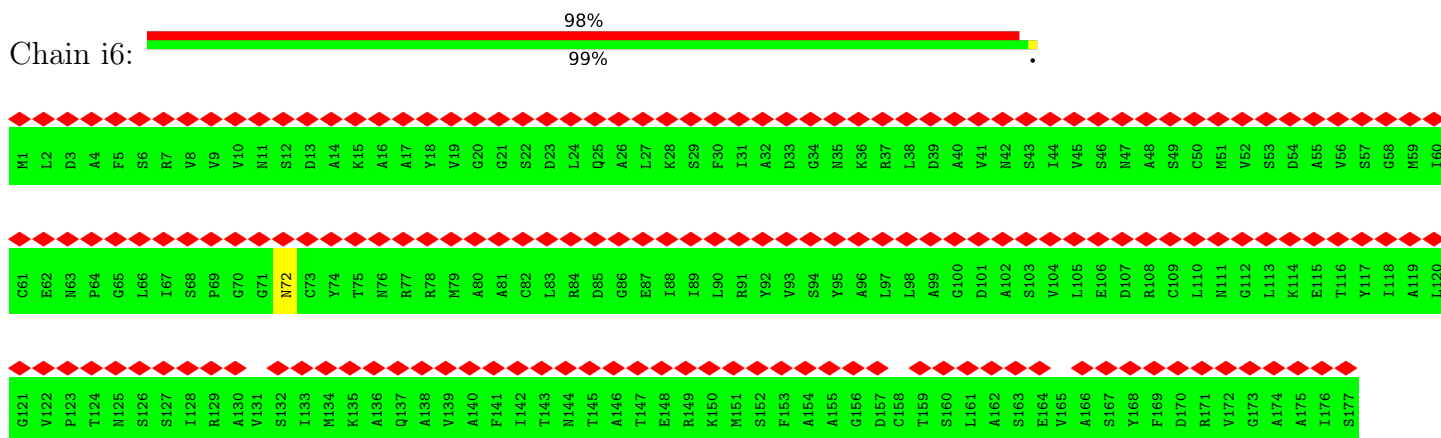
Chain e6:  85% 99%



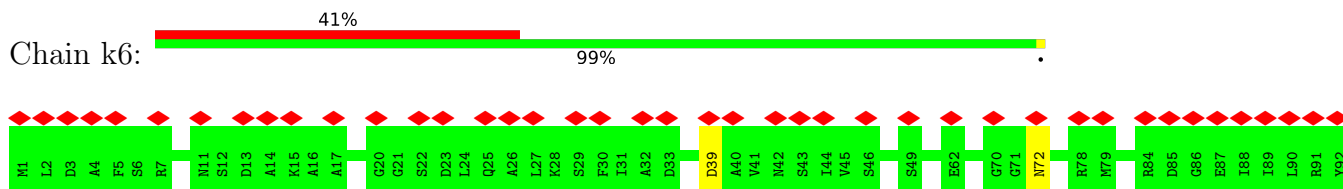
• Molecule 2: B-phycoerythrin beta chain

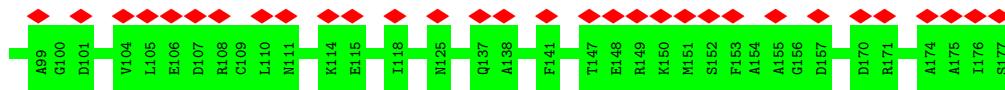


• Molecule 2: B-phycoerythrin beta chain

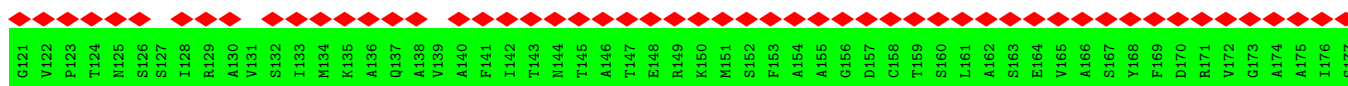
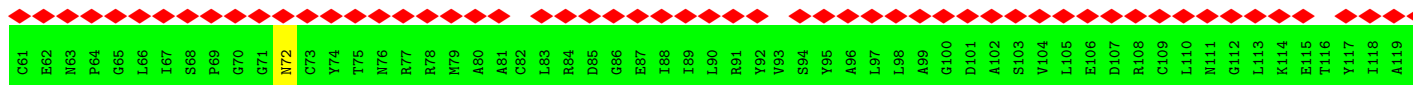
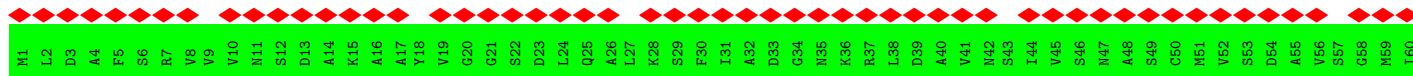


• Molecule 2: B-phycoerythrin beta chain

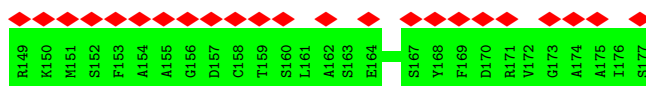
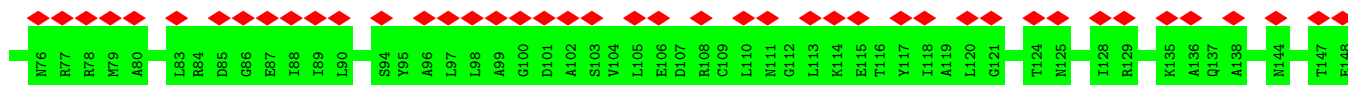
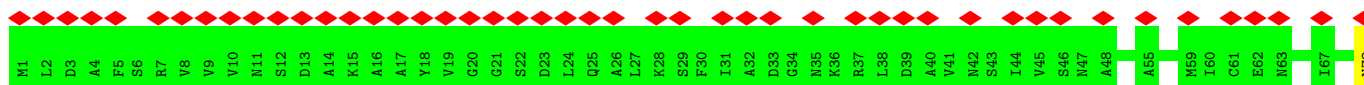




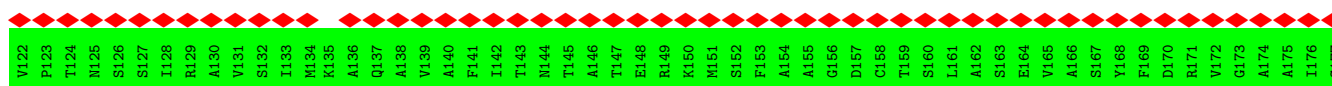
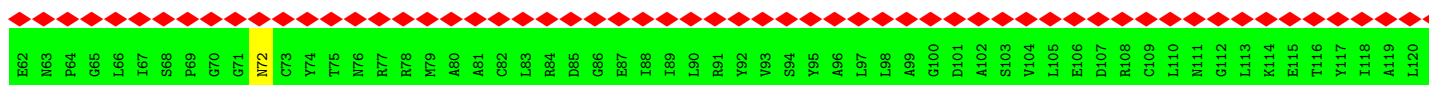
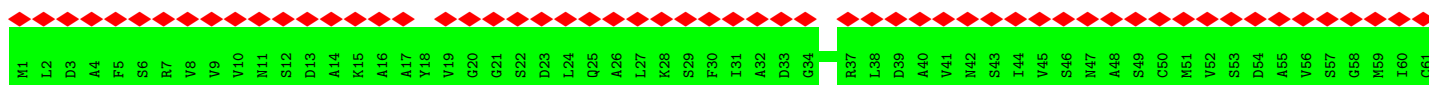
• Molecule 2: B-phycoerythrin beta chain



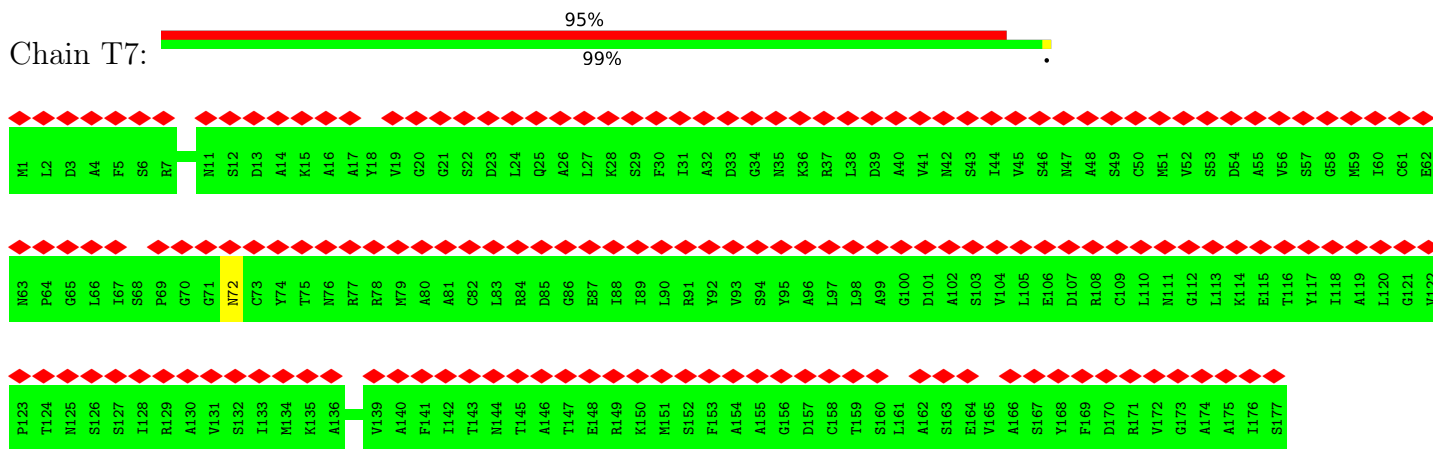
• Molecule 2: B-phycoerythrin beta chain



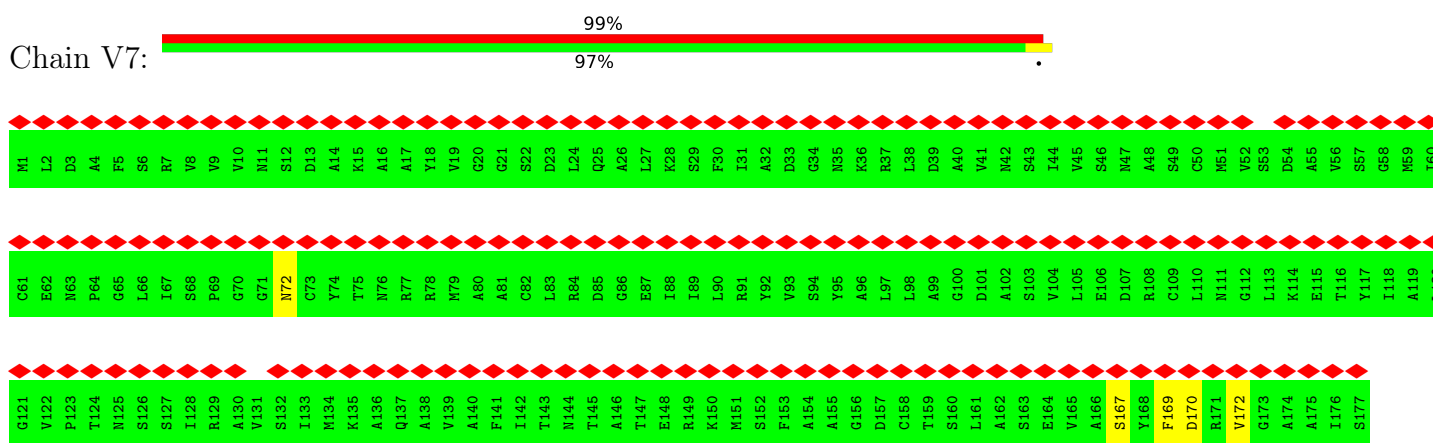
• Molecule 2: B-phycoerythrin beta chain



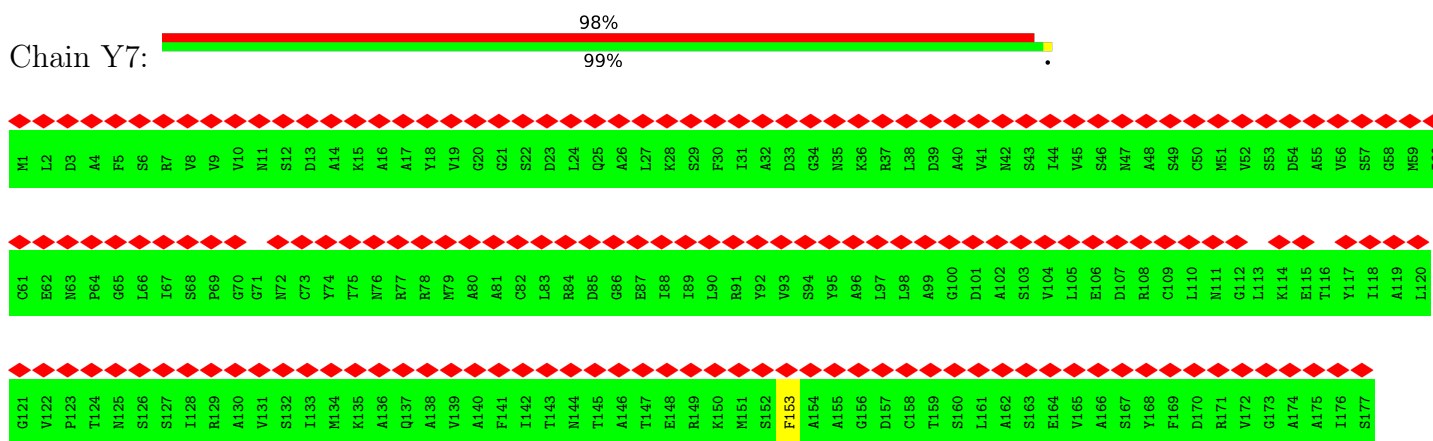
• Molecule 2: B-phycoerythrin beta chain



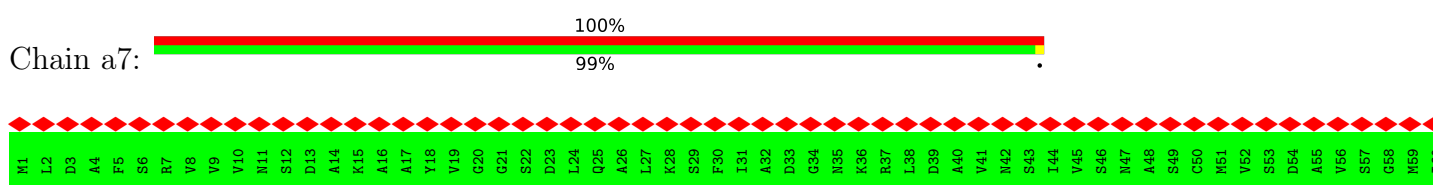
• Molecule 2: B-phycoerythrin beta chain

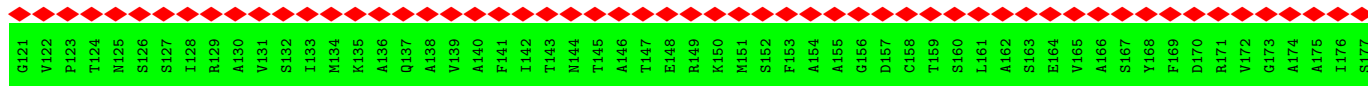
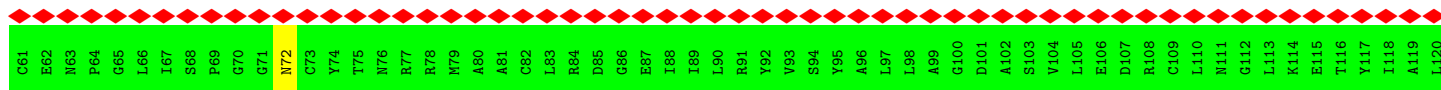


• Molecule 2: B-phycoerythrin beta chain

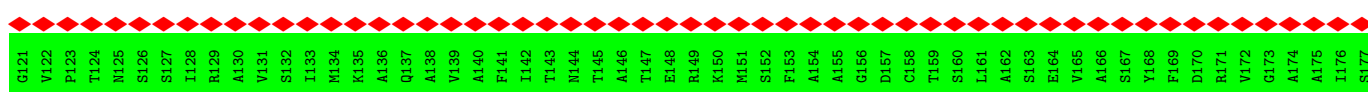
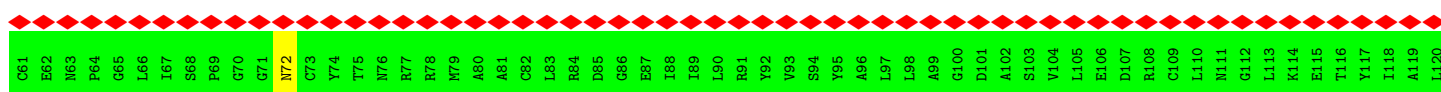


• Molecule 2: B-phycoerythrin beta chain

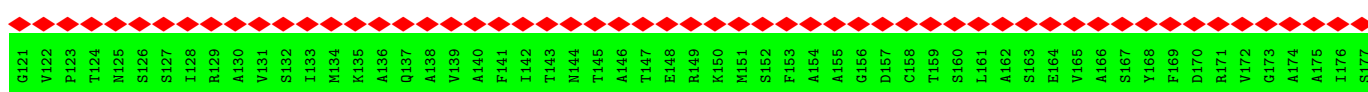
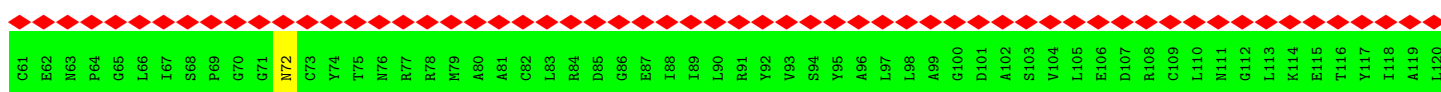
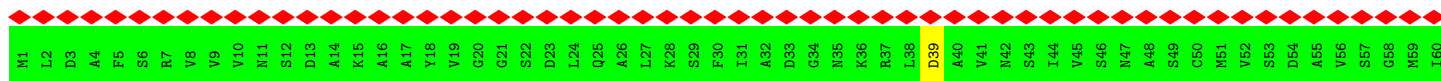




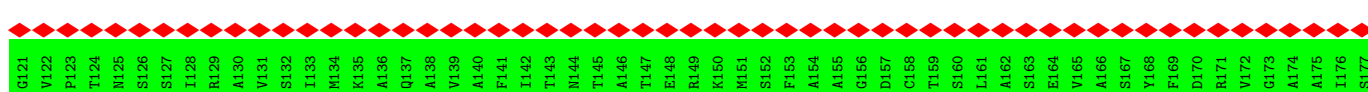
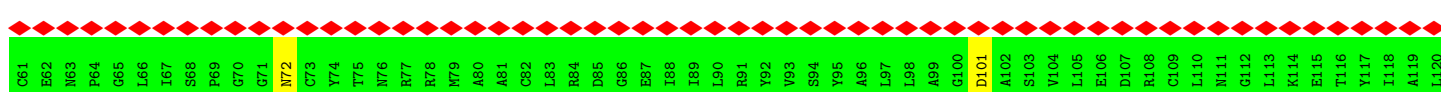
• Molecule 2: B-phycoerythrin beta chain



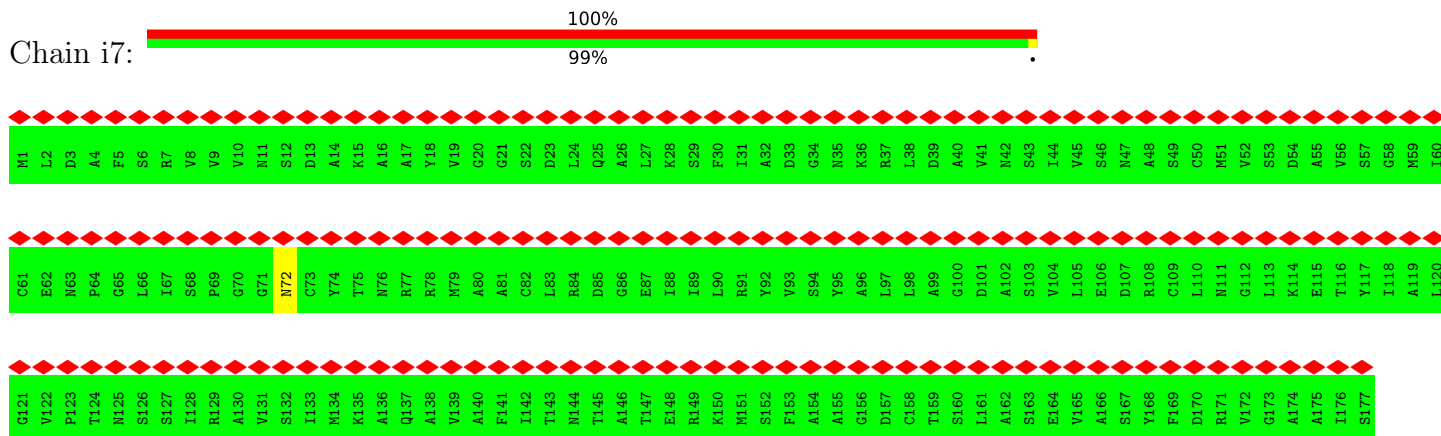
• Molecule 2: B-phycoerythrin beta chain



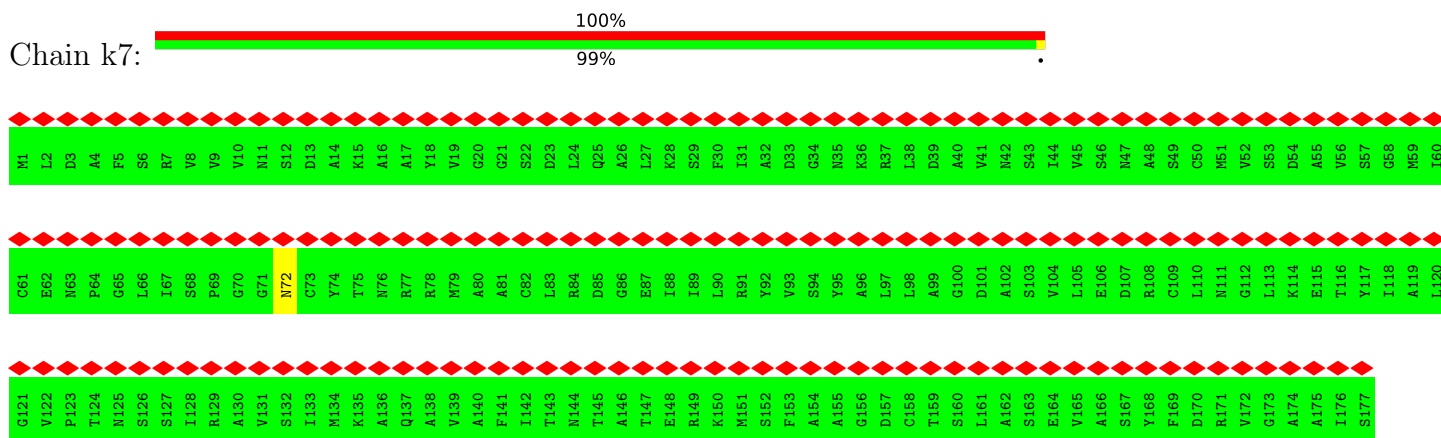
• Molecule 2: B-phycoerythrin beta chain



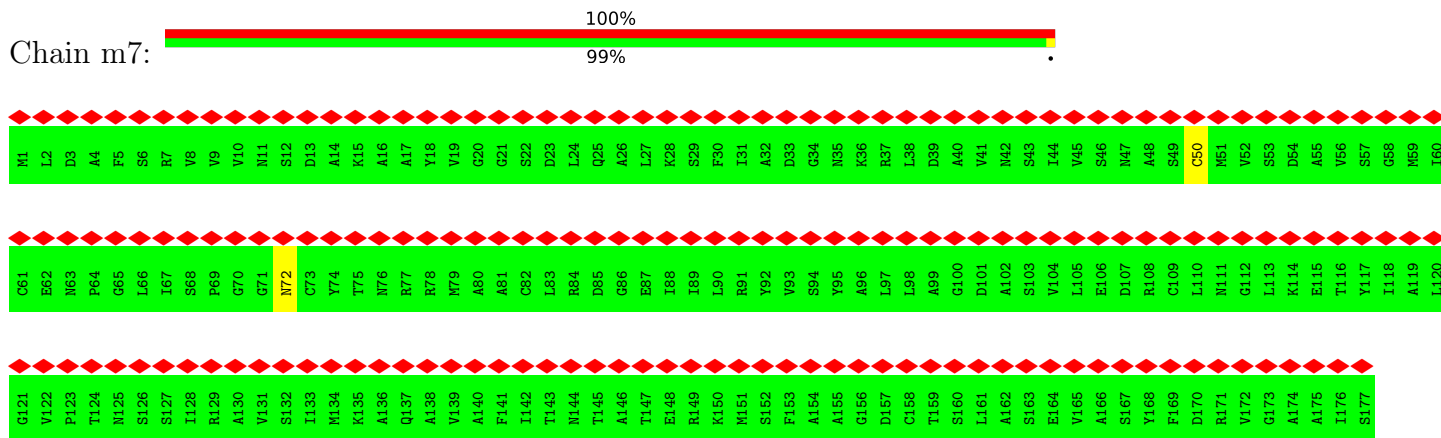
• Molecule 2: B-phycoerythrin beta chain



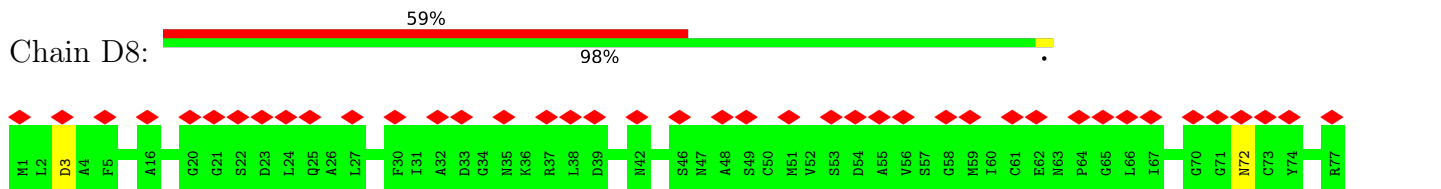
• Molecule 2: B-phycoerythrin beta chain

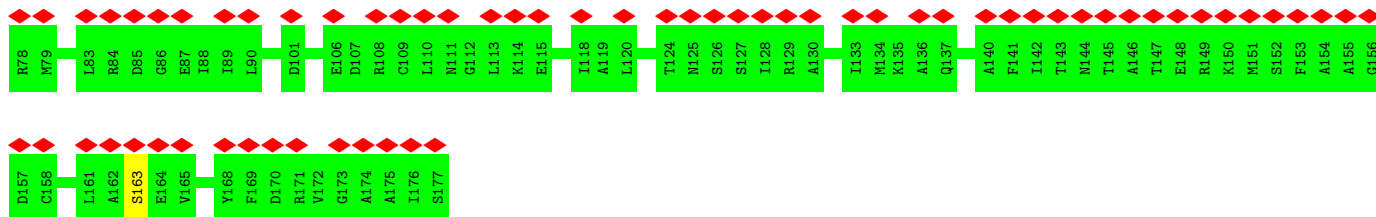


• Molecule 2: B-phycoerythrin beta chain

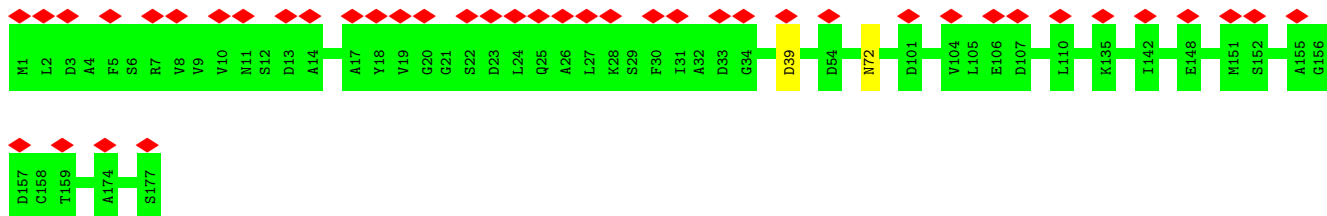


• Molecule 2: B-phycoerythrin beta chain





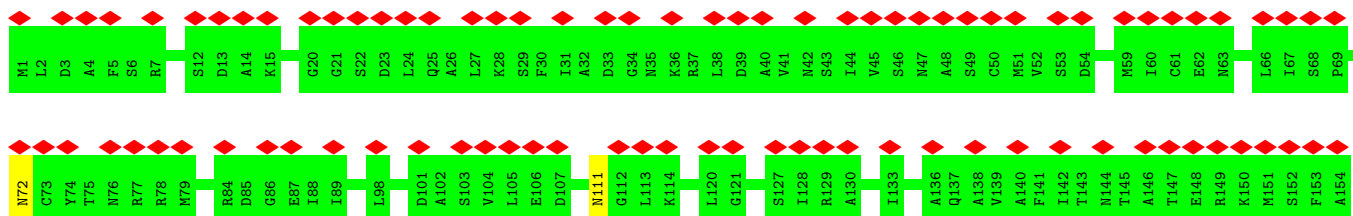
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

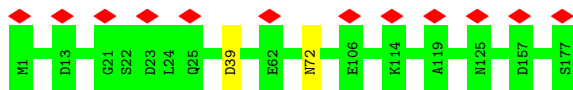


• Molecule 2: B-phycoerythrin beta chain

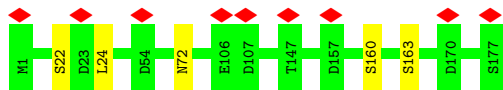


• Molecule 2: B-phycoerythrin beta chain

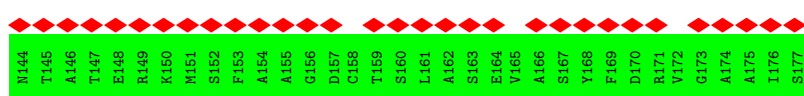
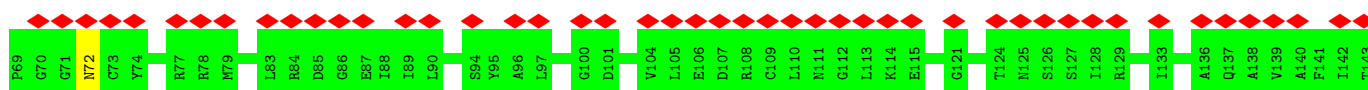
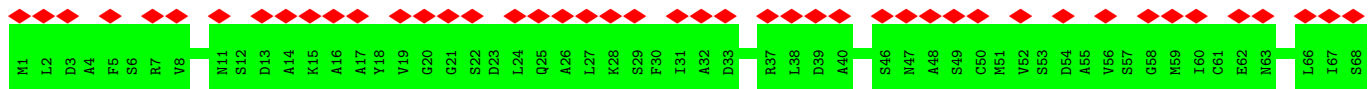




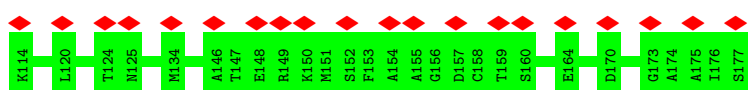
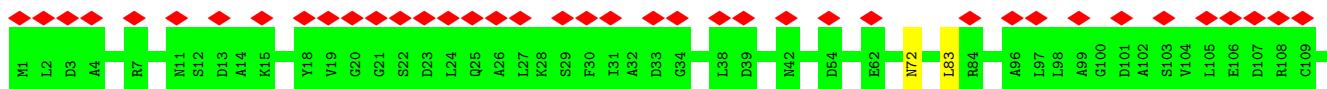
• Molecule 2: B-phycoerythrin beta chain



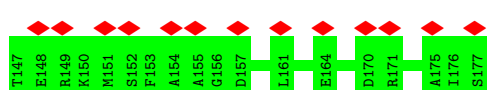
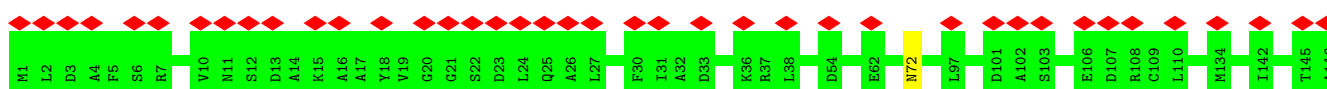
• Molecule 2: B-phycoerythrin beta chain



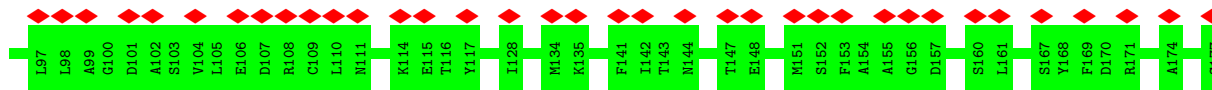
• Molecule 2: B-phycoerythrin beta chain



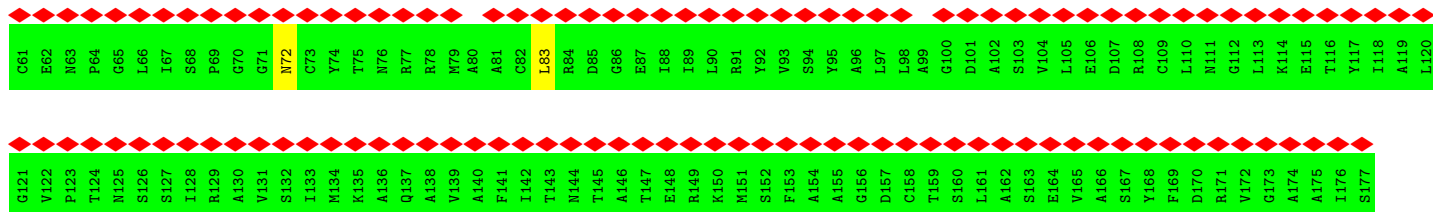
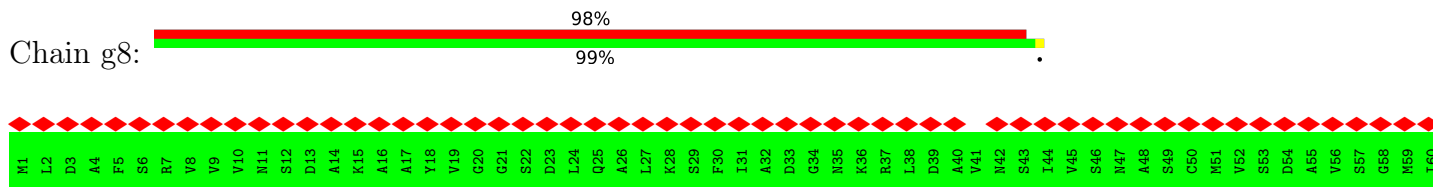
• Molecule 2: B-phycoerythrin beta chain



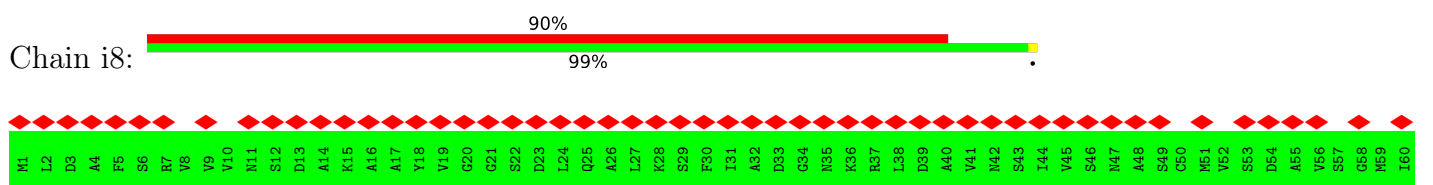
• Molecule 2: B-phycoerythrin beta chain



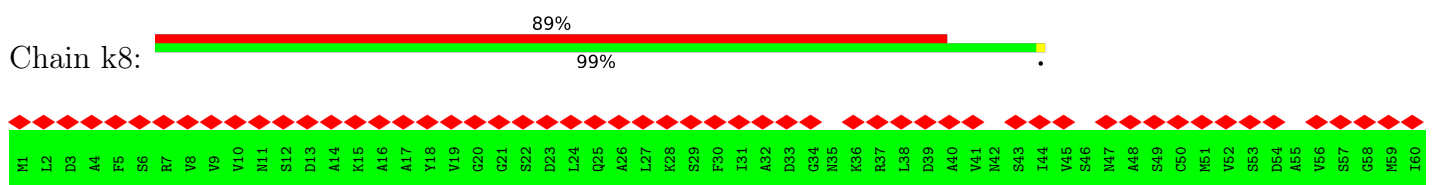
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

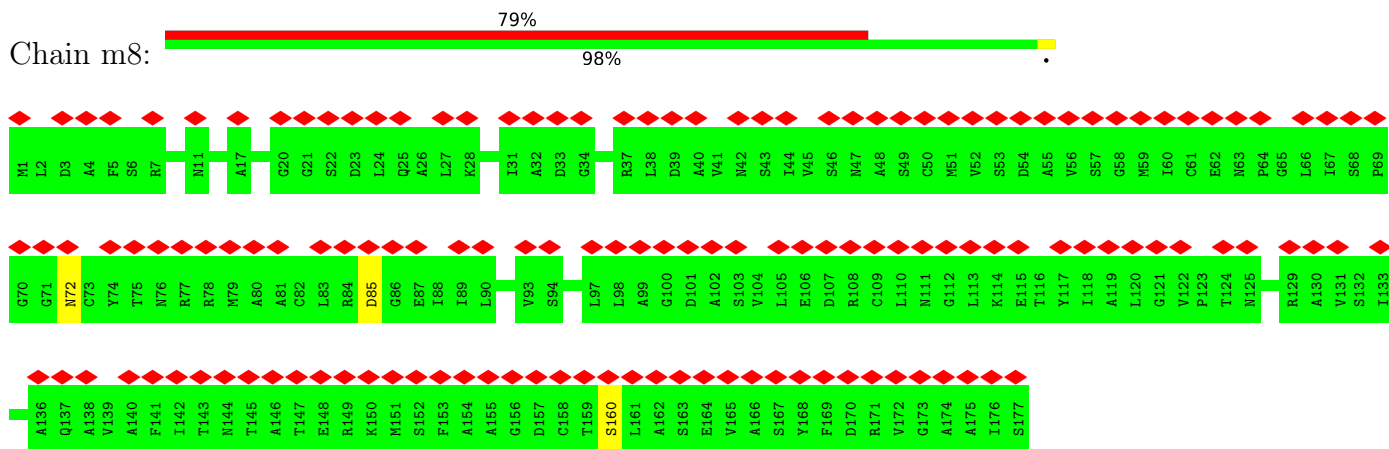


• Molecule 2: B-phycoerythrin beta chain

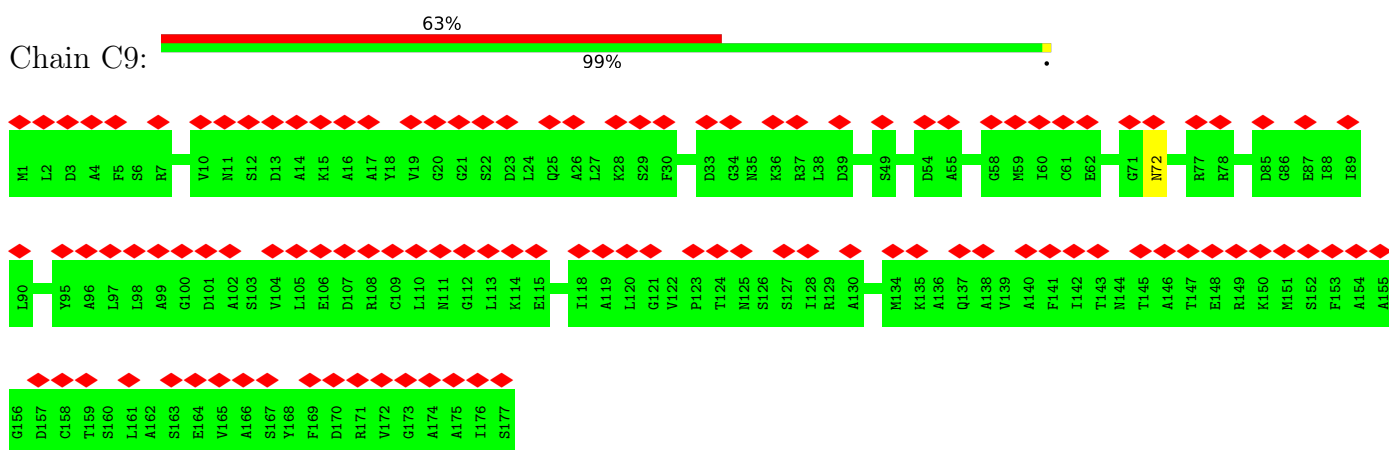


• Molecule 2: B-phycoerythrin beta chain

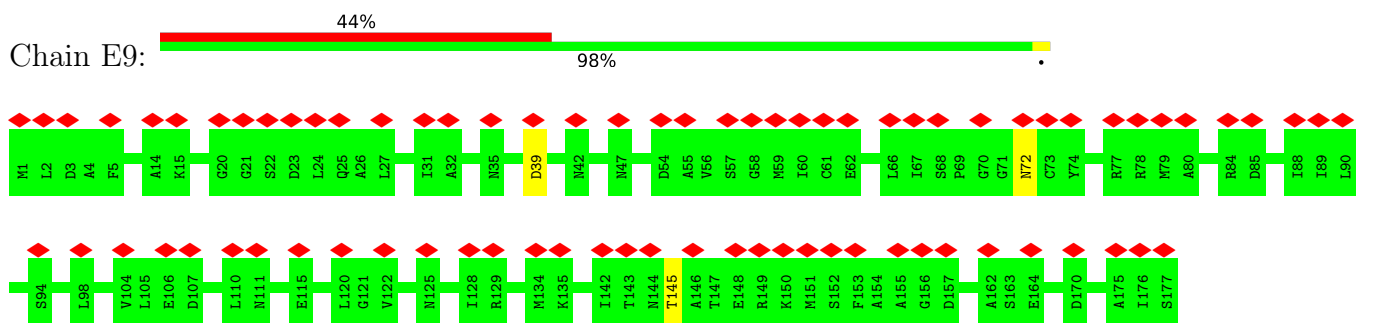




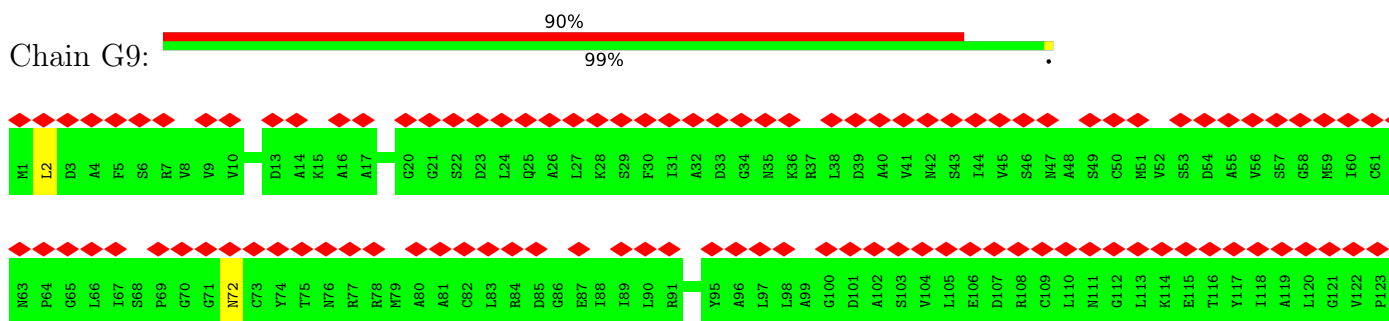
• Molecule 2: B-phycoerythrin beta chain

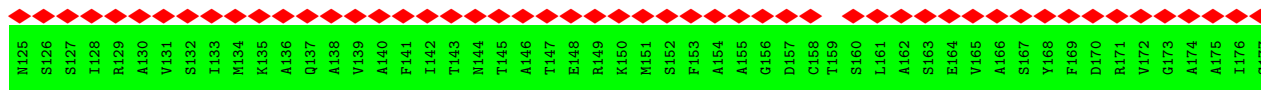


• Molecule 2: B-phycoerythrin beta chain



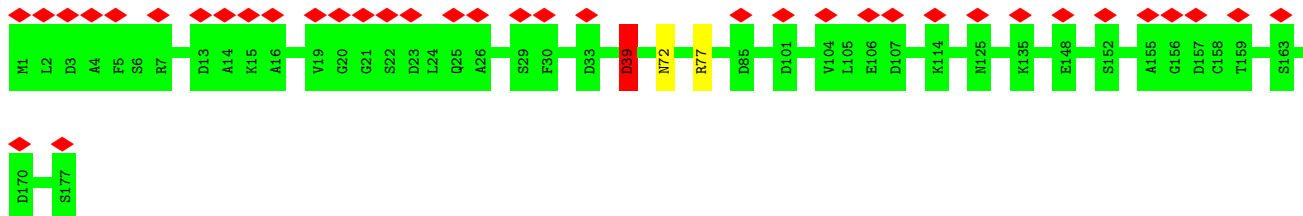
• Molecule 2: B-phycoerythrin beta chain





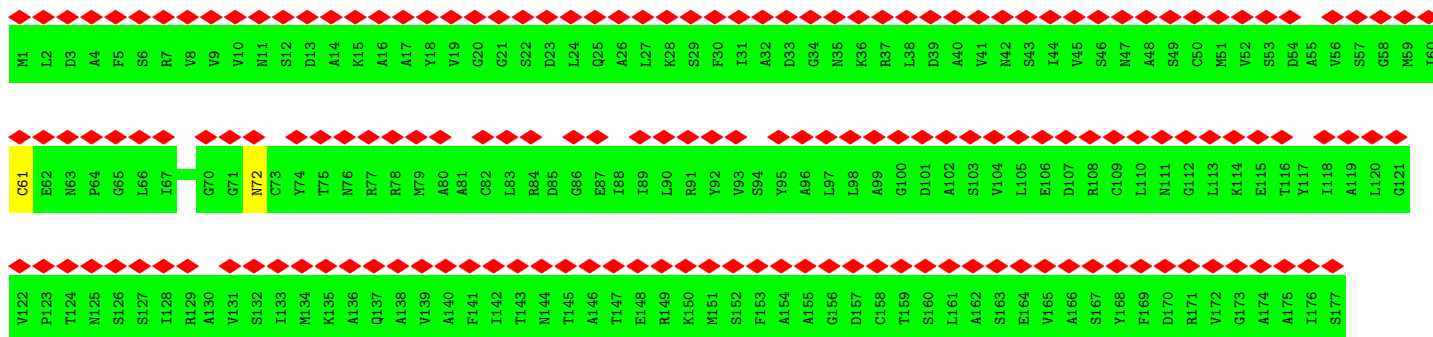
• Molecule 2: B-phycoerythrin beta chain

Chain I9:



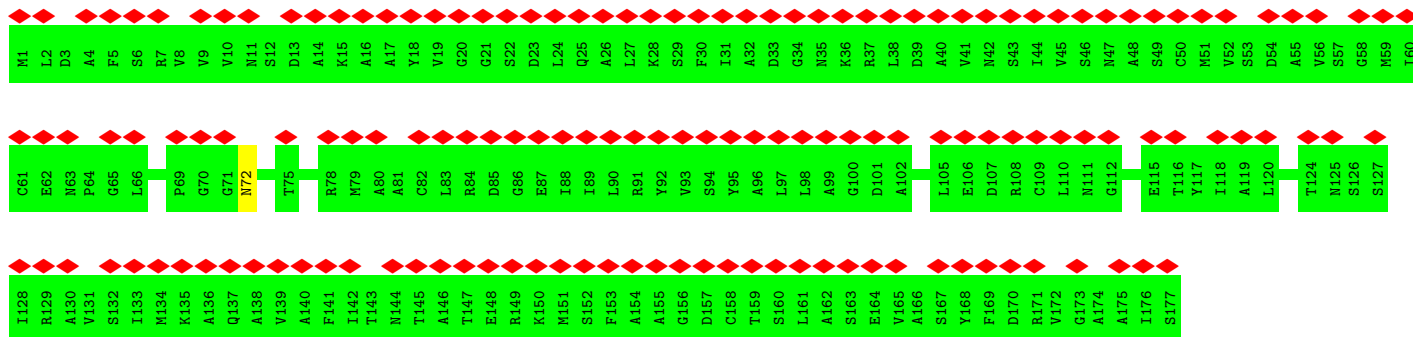
• Molecule 2: B-phycoerythrin beta chain

Chain K9:



• Molecule 2: B-phycoerythrin beta chain

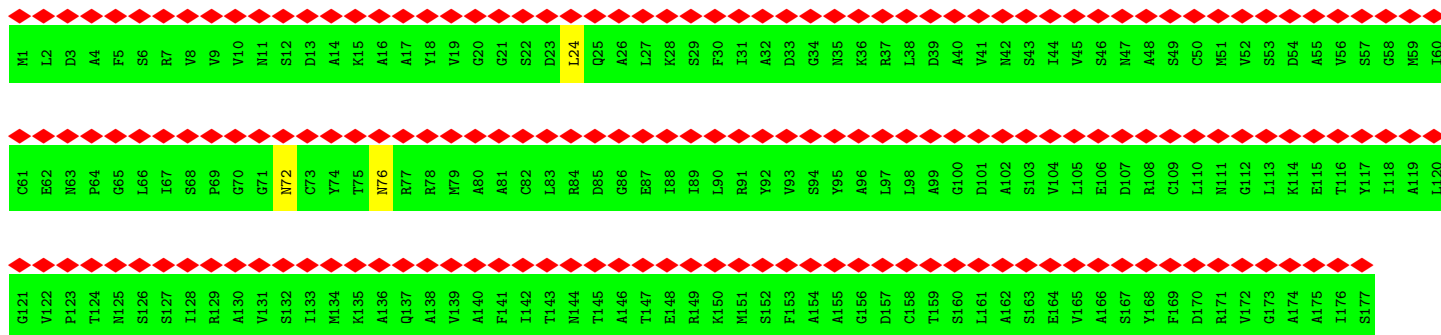
Chain M9:



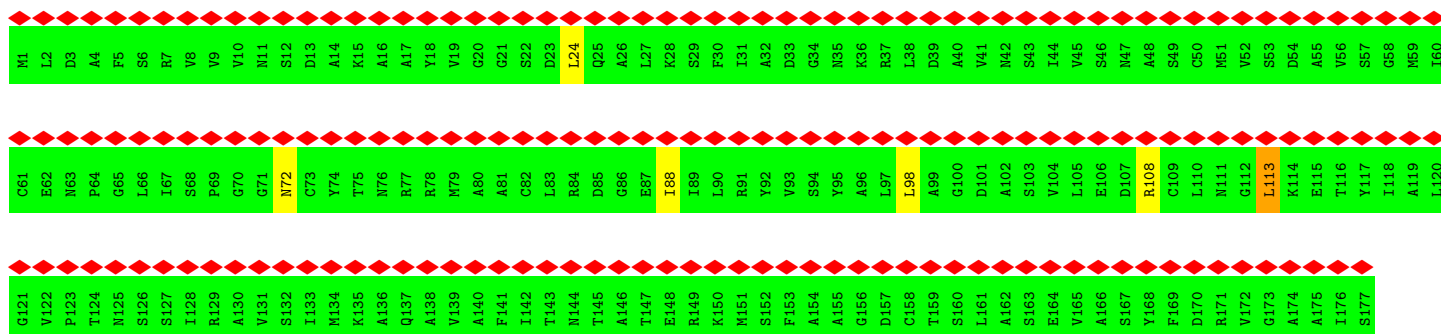
• Molecule 2: B-phycoerythrin beta chain

Chain O9:

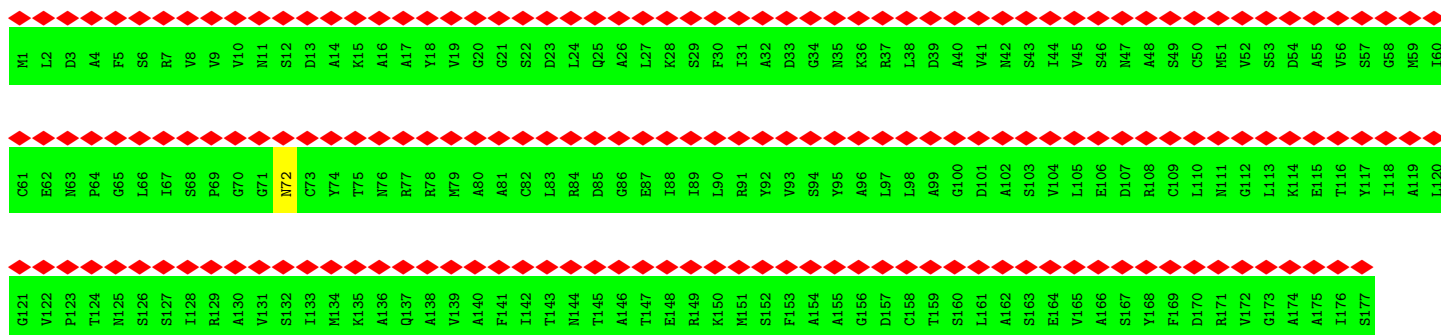




• Molecule 2: B-phycoerythrin beta chain

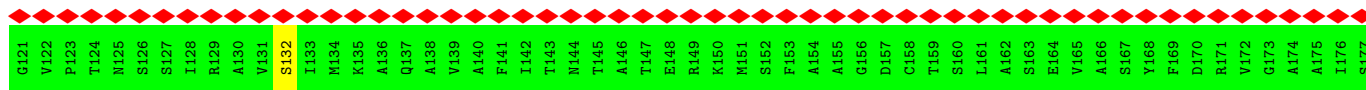


• Molecule 2: B-phycoerythrin beta chain

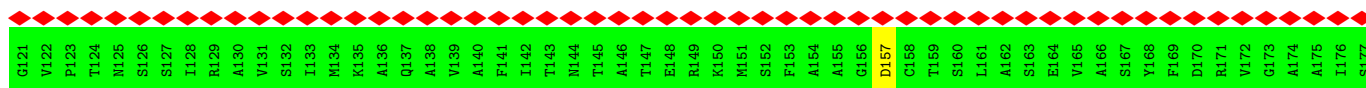
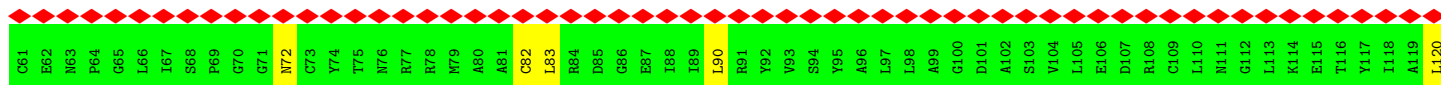
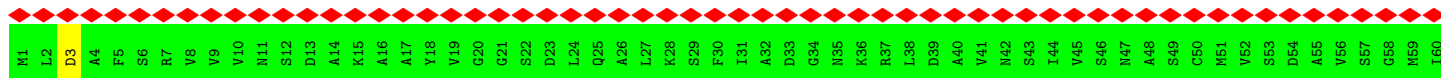


• Molecule 2: B-phycoerythrin beta chain

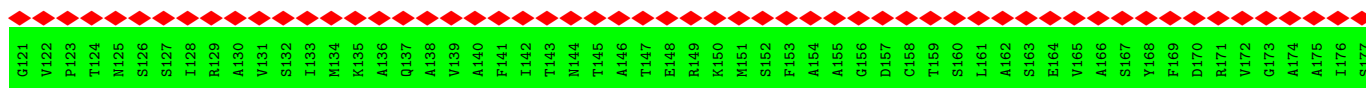
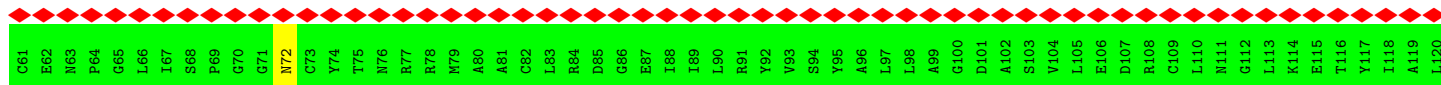




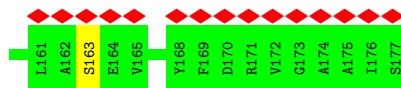
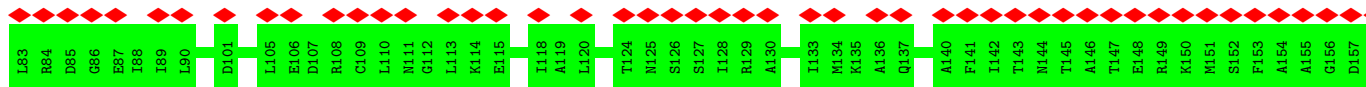
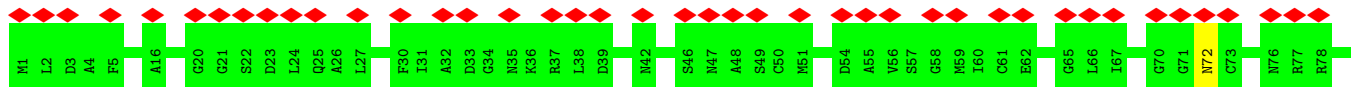
• Molecule 2: B-phycoerythrin beta chain



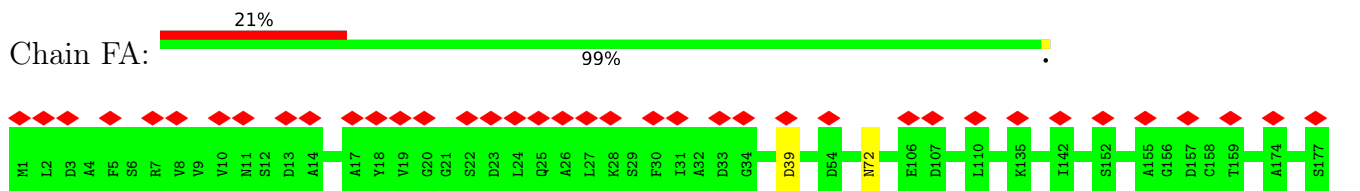
• Molecule 2: B-phycoerythrin beta chain



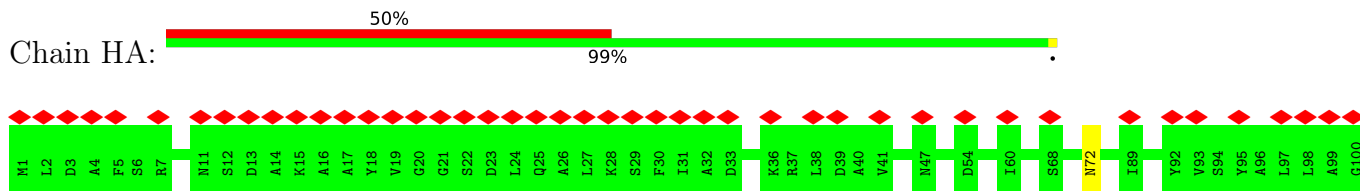
• Molecule 2: B-phycoerythrin beta chain



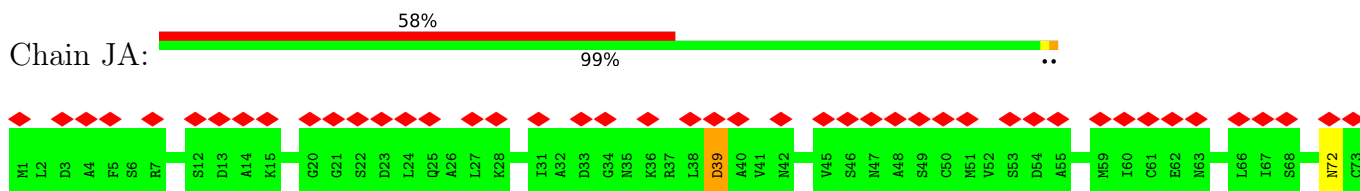
• Molecule 2: B-phycoerythrin beta chain



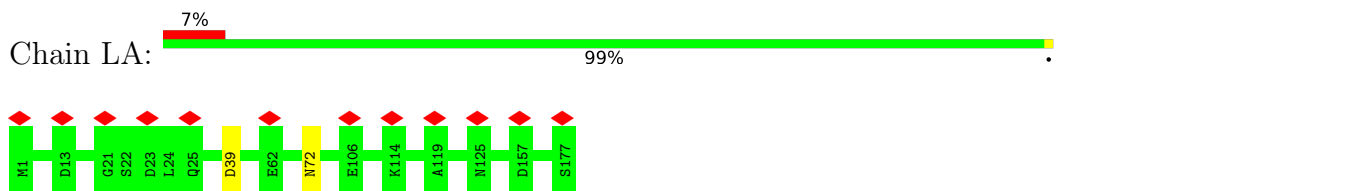
• Molecule 2: B-phycoerythrin beta chain



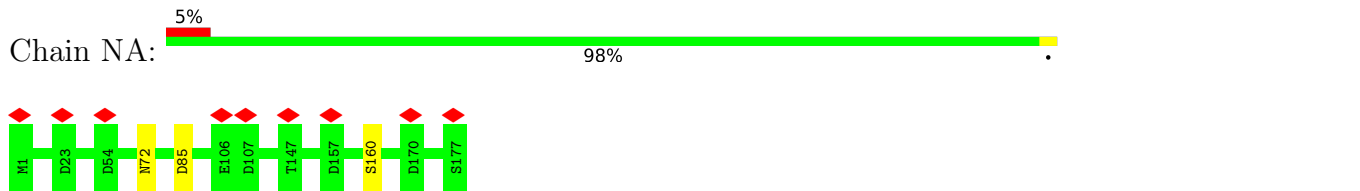
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

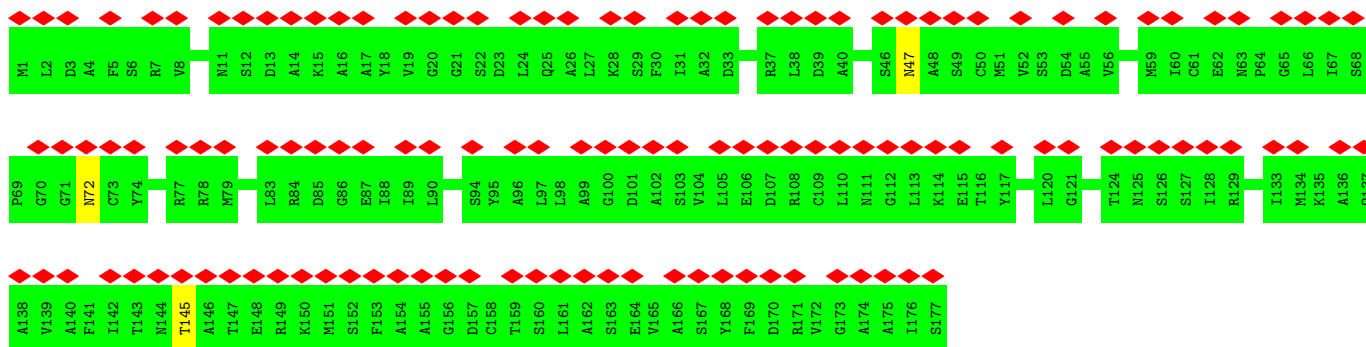


• Molecule 2: B-phycoerythrin beta chain



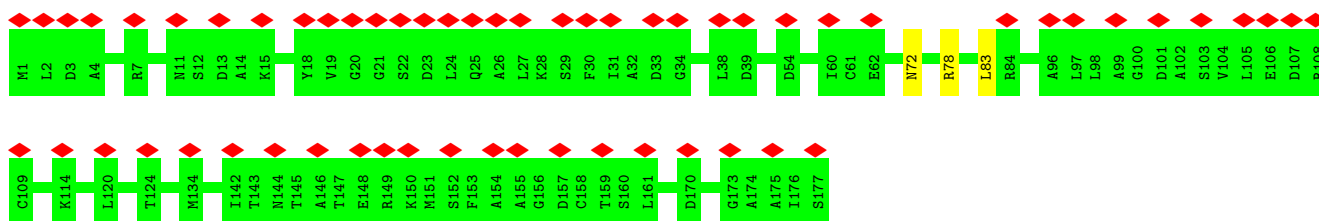
• Molecule 2: B-phycoerythrin beta chain





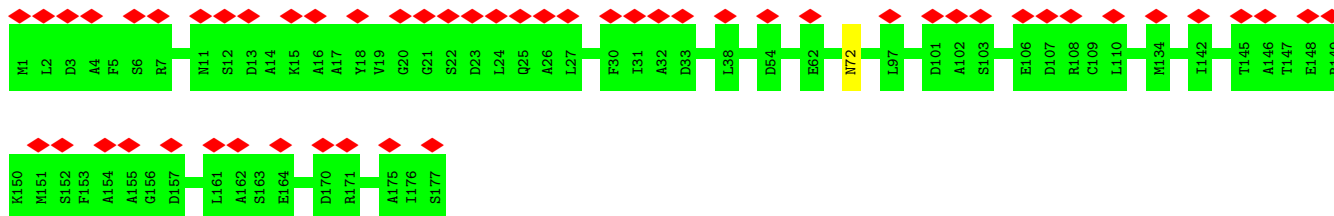
- Molecule 2: B-phycoerythrin beta chain

Chain RA: 98% 33%



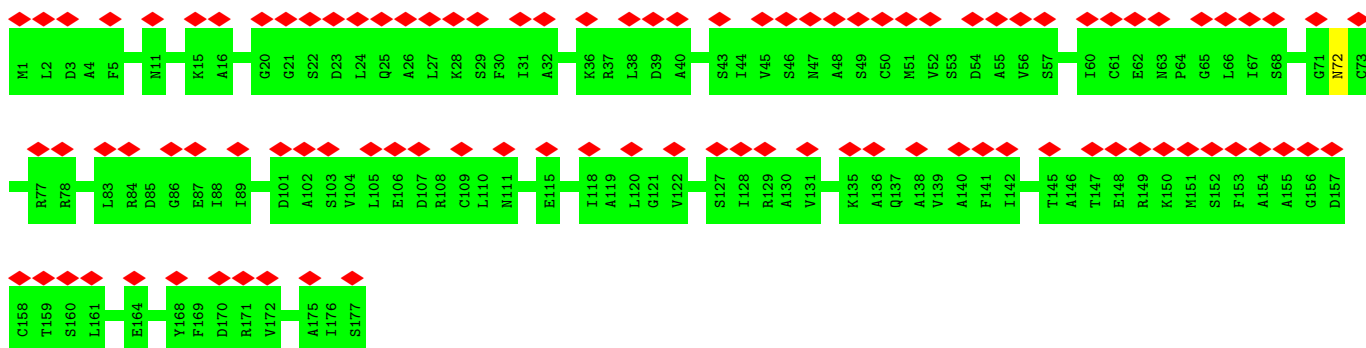
- Molecule 2: B-phycoerythrin beta chain

Chain TA: 99% 30%

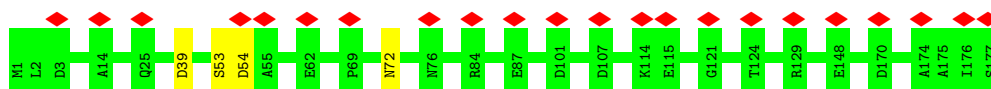


- Molecule 2: B-phycoerythrin beta chain

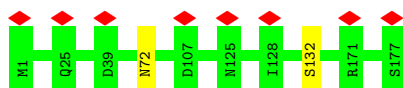
Chain VA: 99% 55%



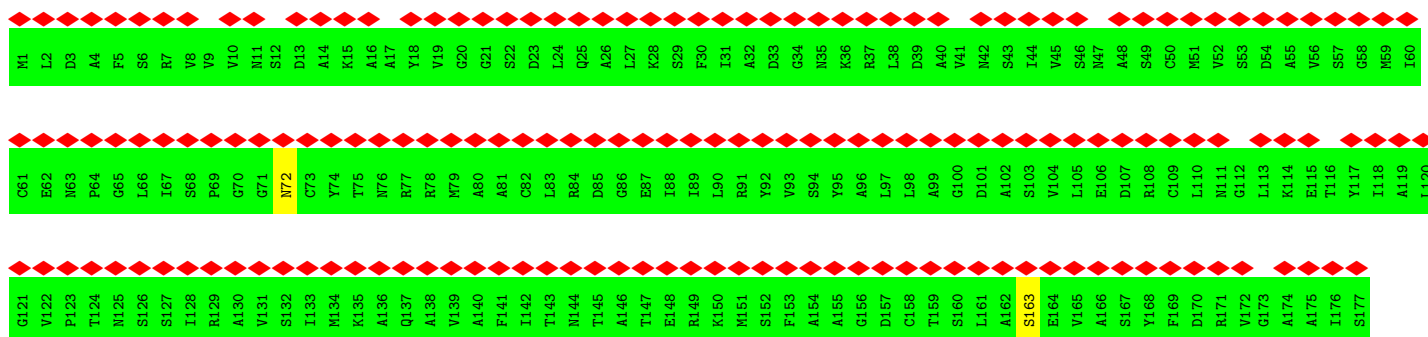
- Molecule 2: B-phycoerythrin beta chain



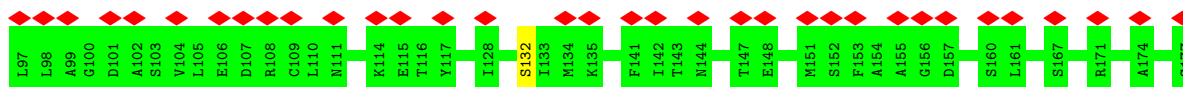
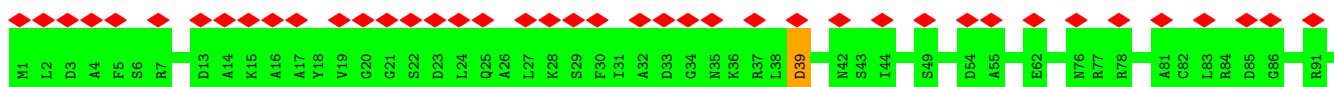
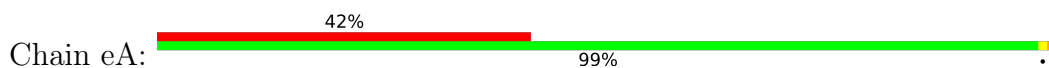
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

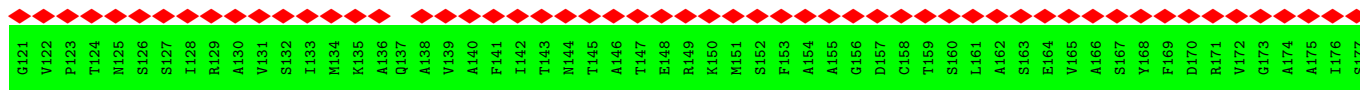


- Molecule 2: B-phycoerythrin beta chain

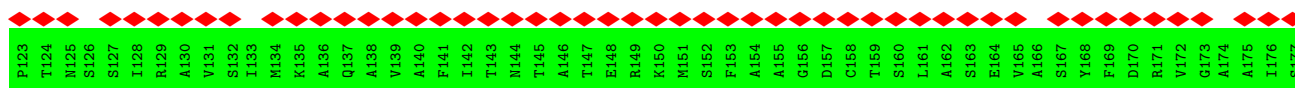
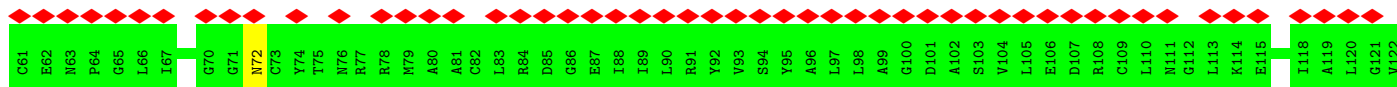
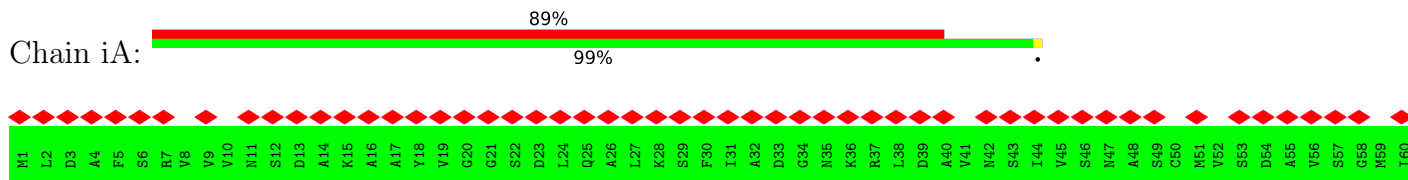


- Molecule 2: B-phycoerythrin beta chain

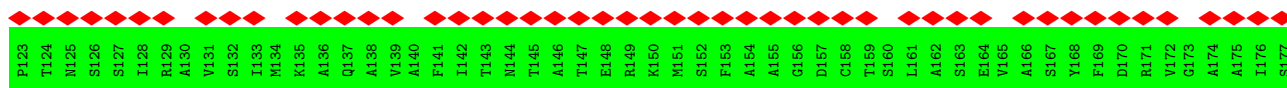
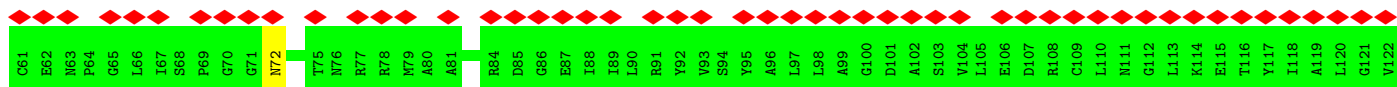
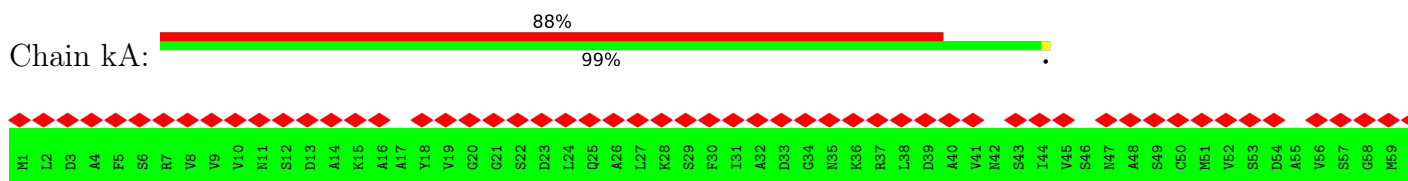




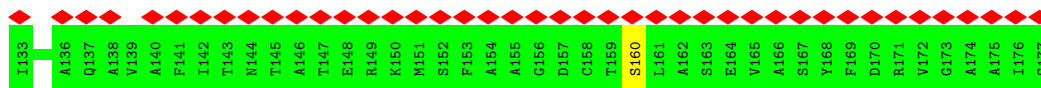
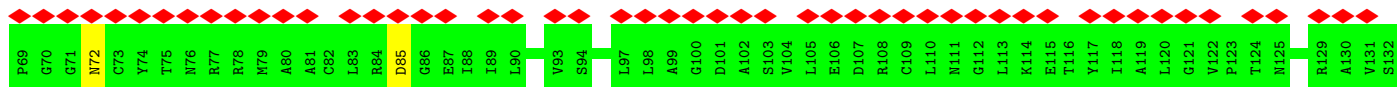
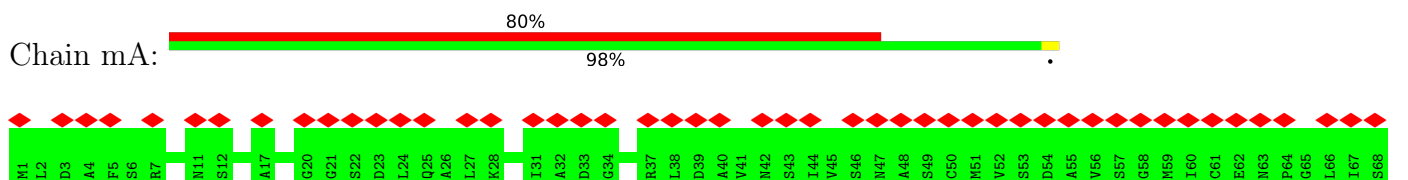
• Molecule 2: B-phycoerythrin beta chain



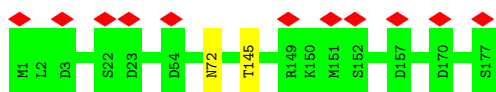
• Molecule 2: B-phycoerythrin beta chain



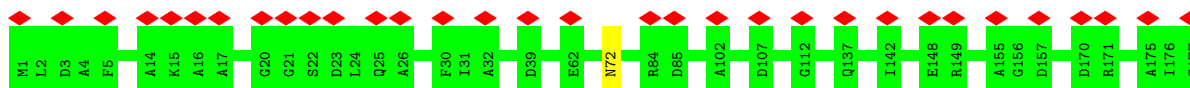
• Molecule 2: B-phycoerythrin beta chain



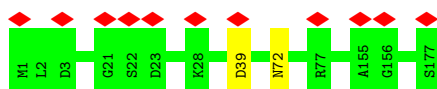
• Molecule 2: B-phycoerythrin beta chain



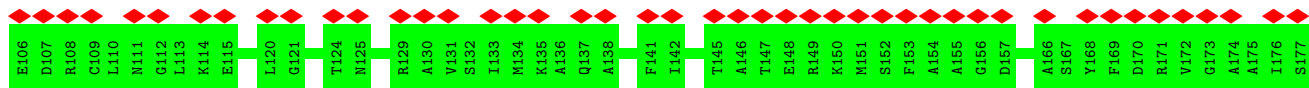
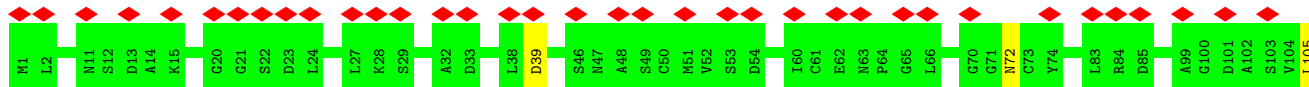
- Molecule 2: B-phycoerythrin beta chain



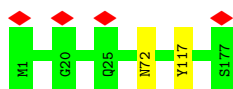
- Molecule 2: B-phycoerythrin beta chain



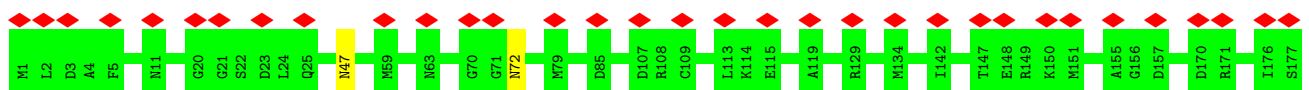
- Molecule 2: B-phycoerythrin beta chain



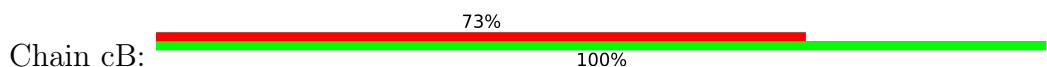
- Molecule 2: B-phycoerythrin beta chain

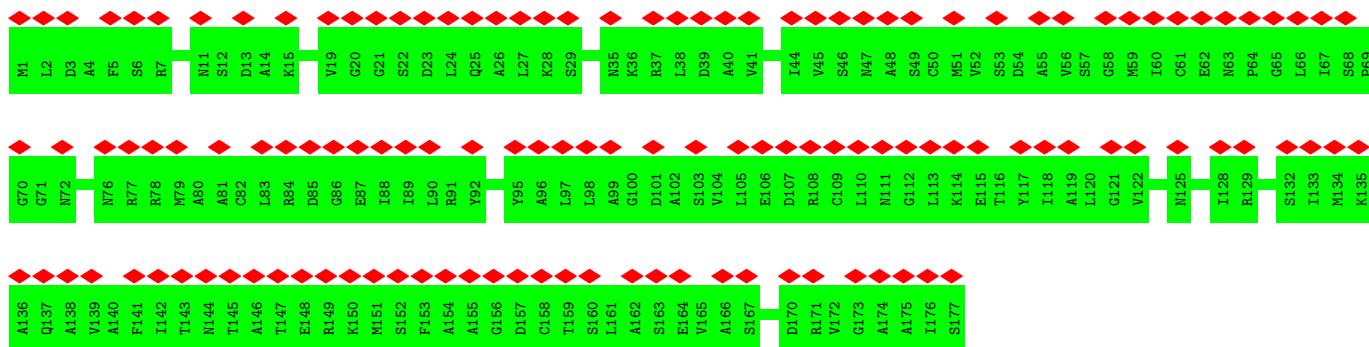


- Molecule 2: B-phycoerythrin beta chain

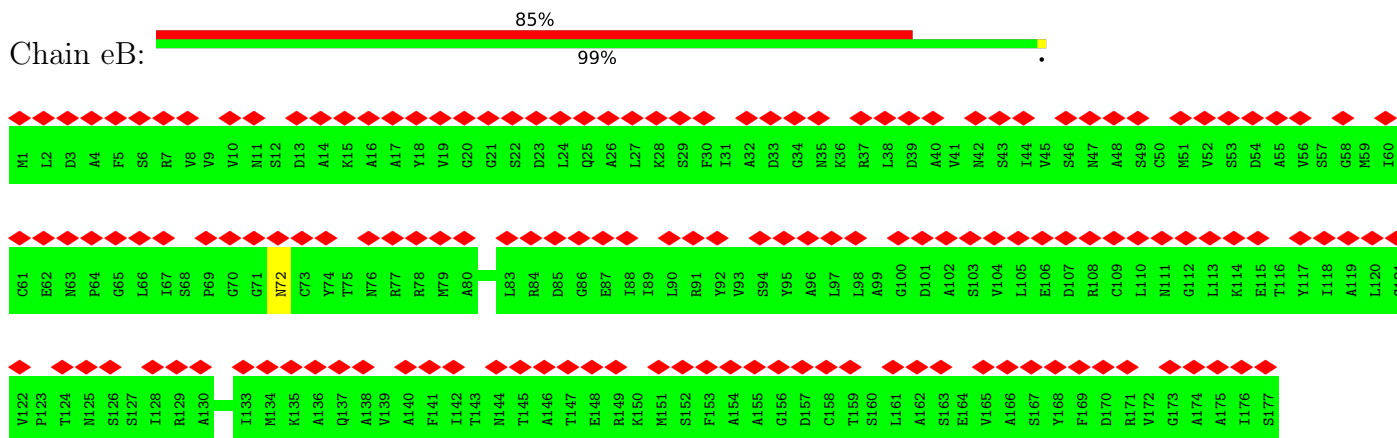


- Molecule 2: B-phycoerythrin beta chain

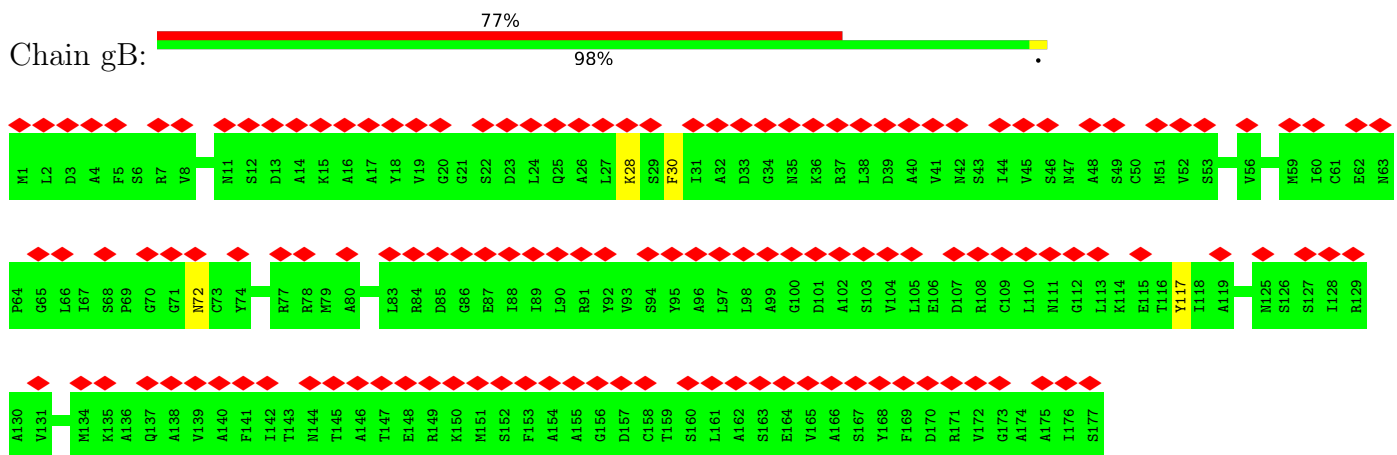




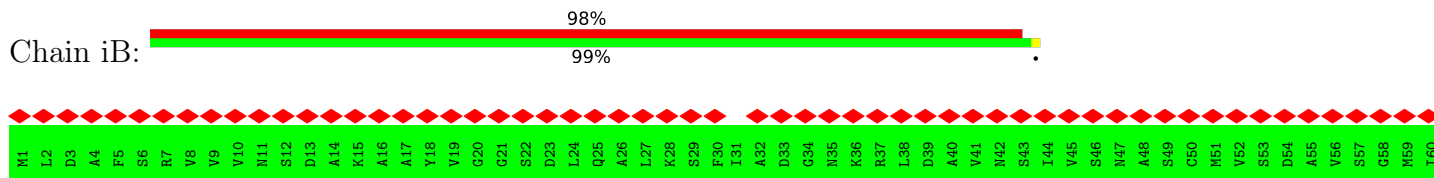
• Molecule 2: B-phycoerythrin beta chain

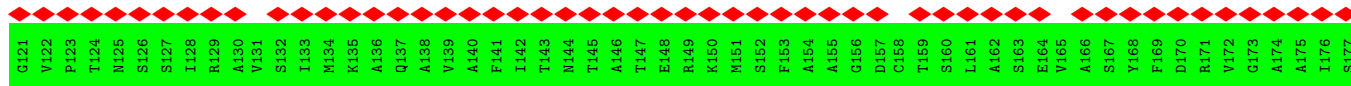
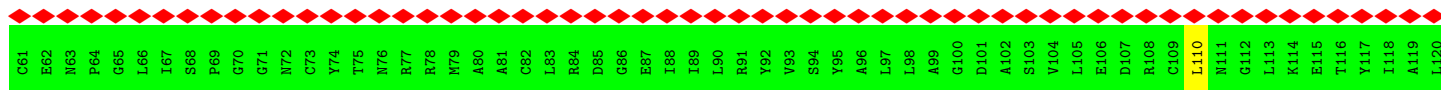


• Molecule 2: B-phycoerythrin beta chain

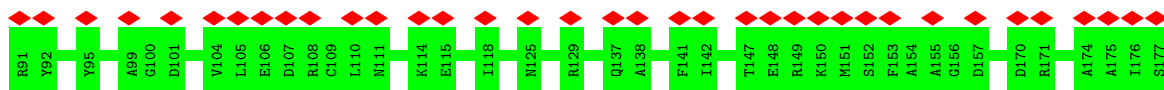
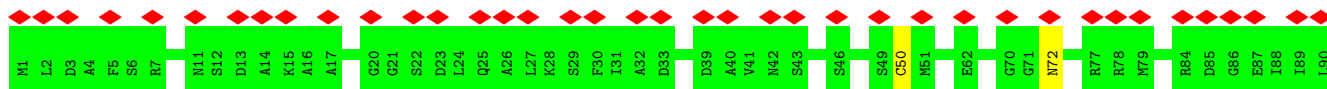
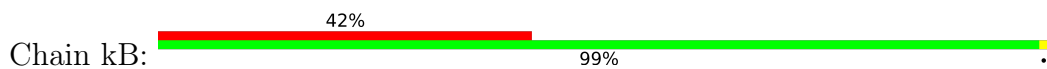


• Molecule 2: B-phycoerythrin beta chain

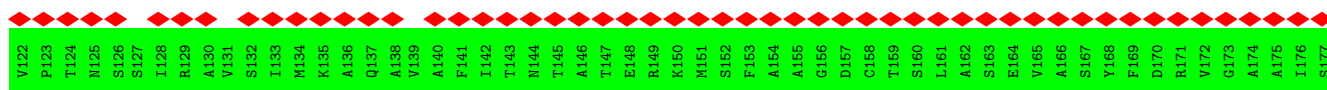
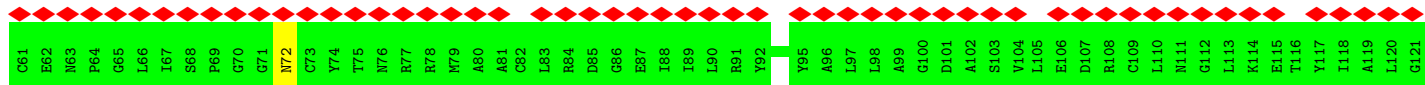
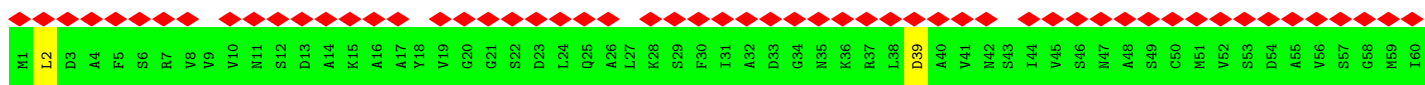




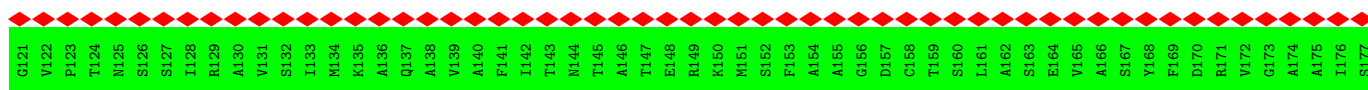
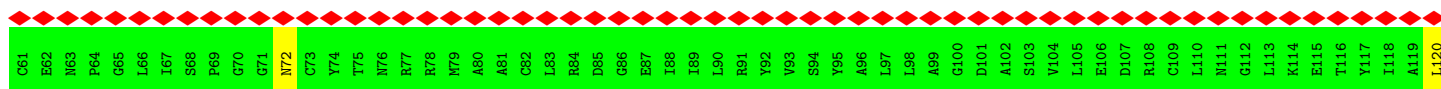
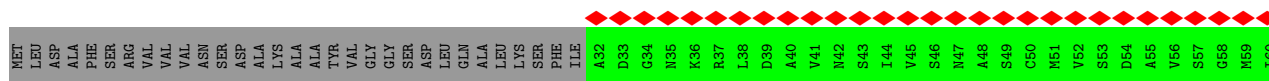
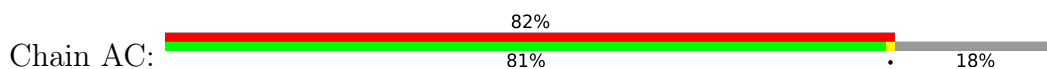
• Molecule 2: B-phycoerythrin beta chain



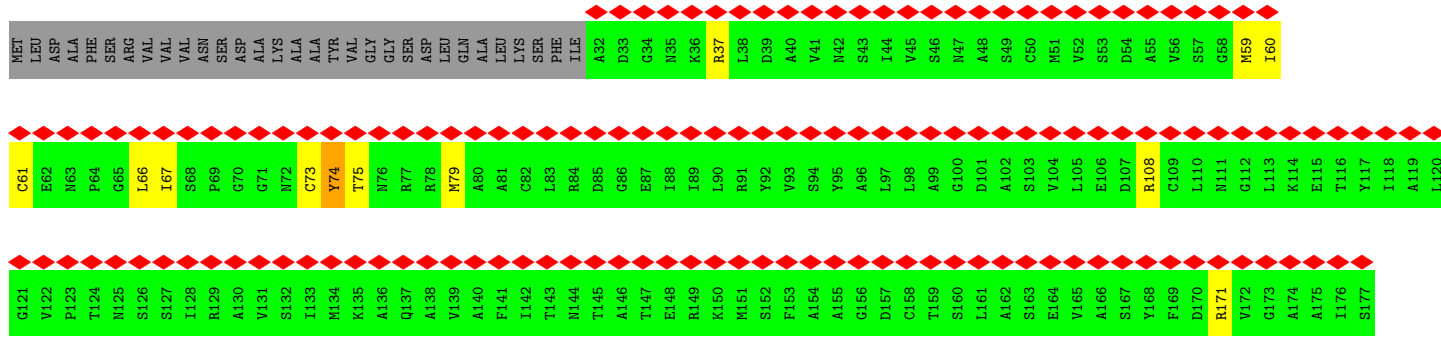
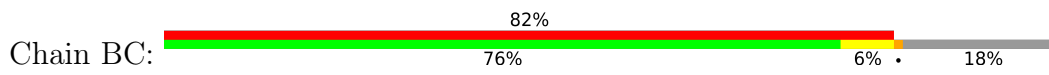
• Molecule 2: B-phycoerythrin beta chain



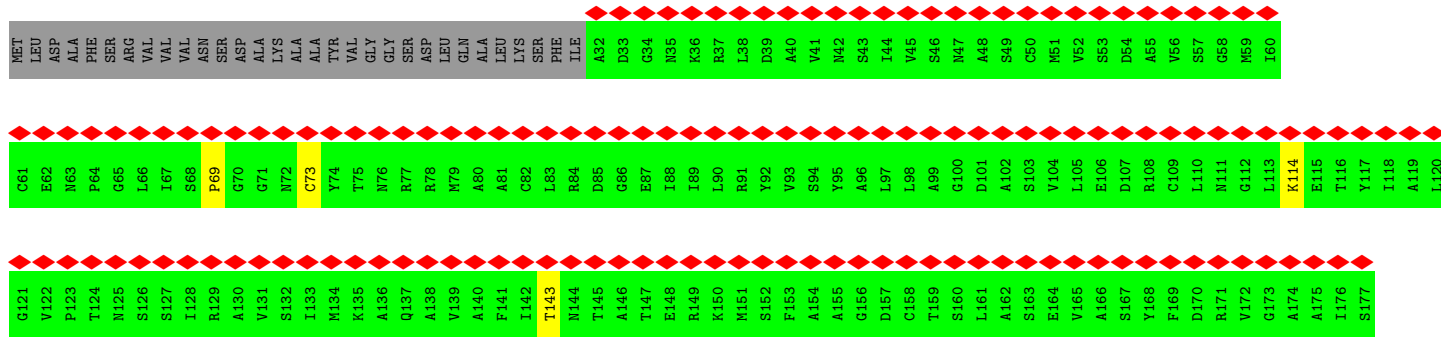
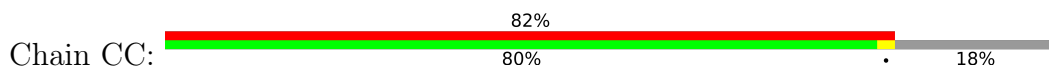
• Molecule 2: B-phycoerythrin beta chain



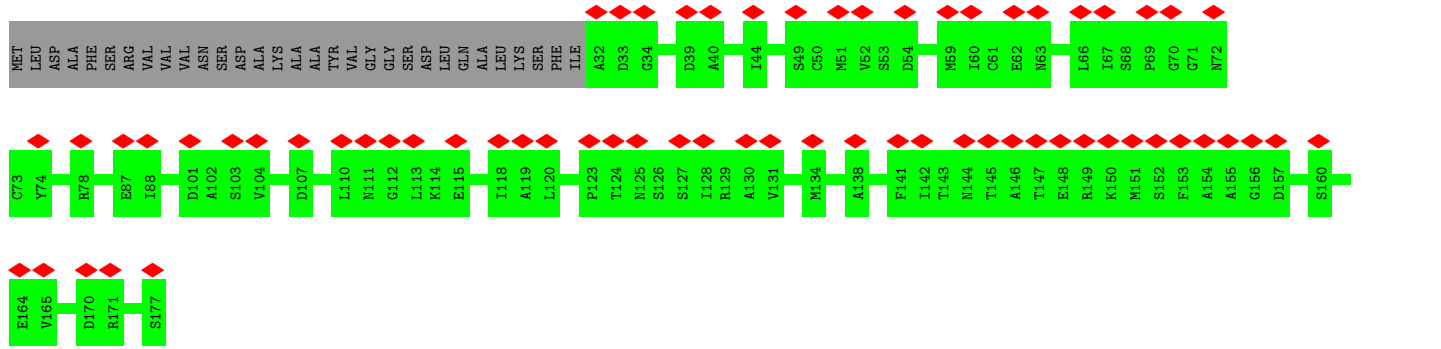
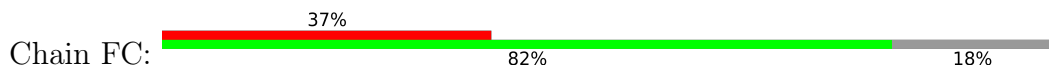
• Molecule 2: B-phycoerythrin beta chain



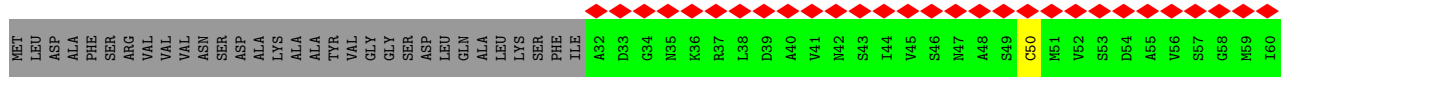
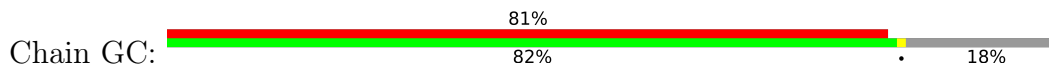
• Molecule 2: B-phycoerythrin beta chain

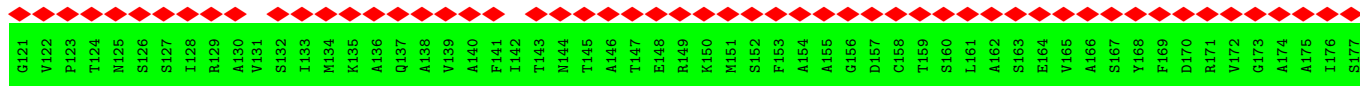
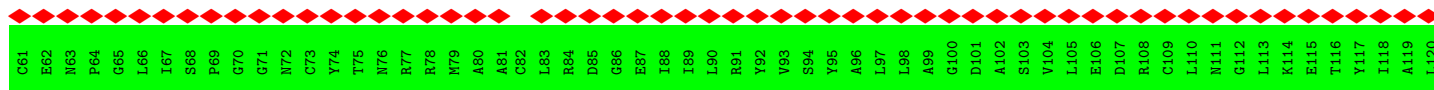


• Molecule 2: B-phycoerythrin beta chain

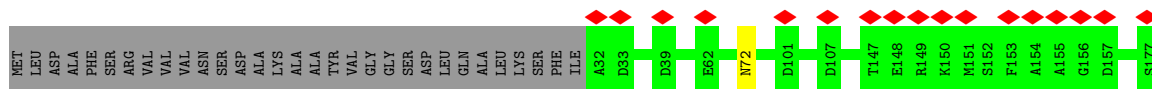
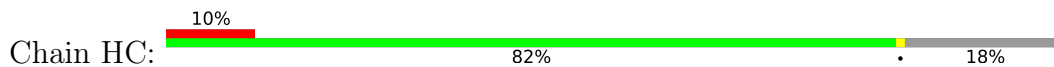


• Molecule 2: B-phycoerythrin beta chain

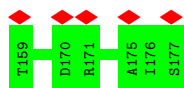
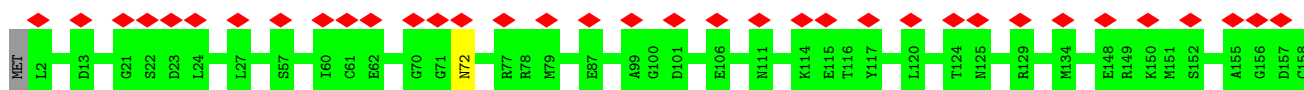




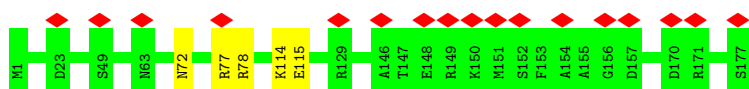
• Molecule 2: B-phycoerythrin beta chain



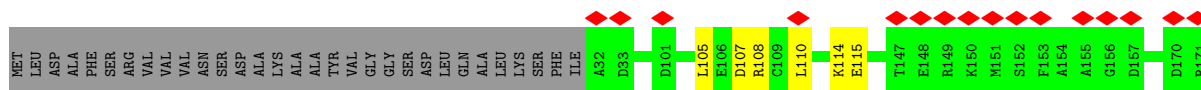
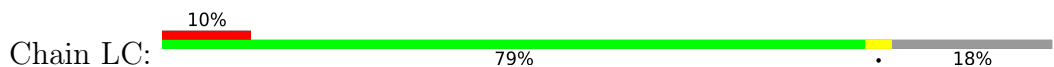
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

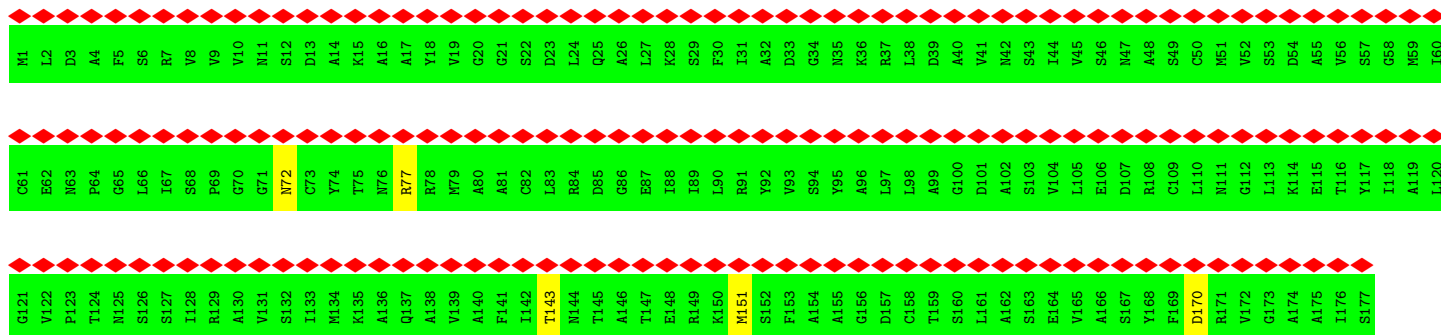


• Molecule 2: B-phycoerythrin beta chain

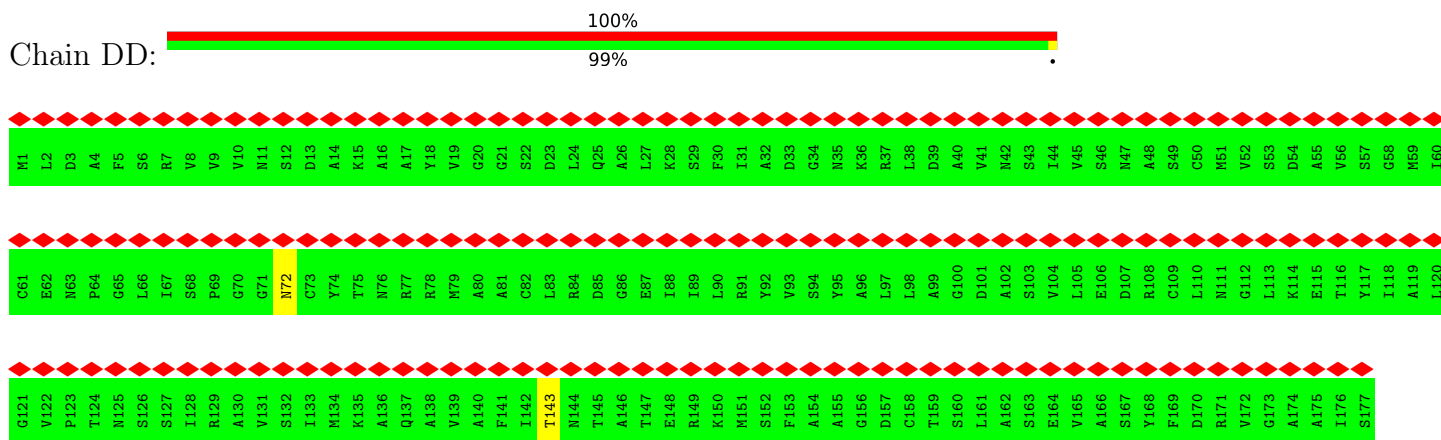


• Molecule 2: B-phycoerythrin beta chain

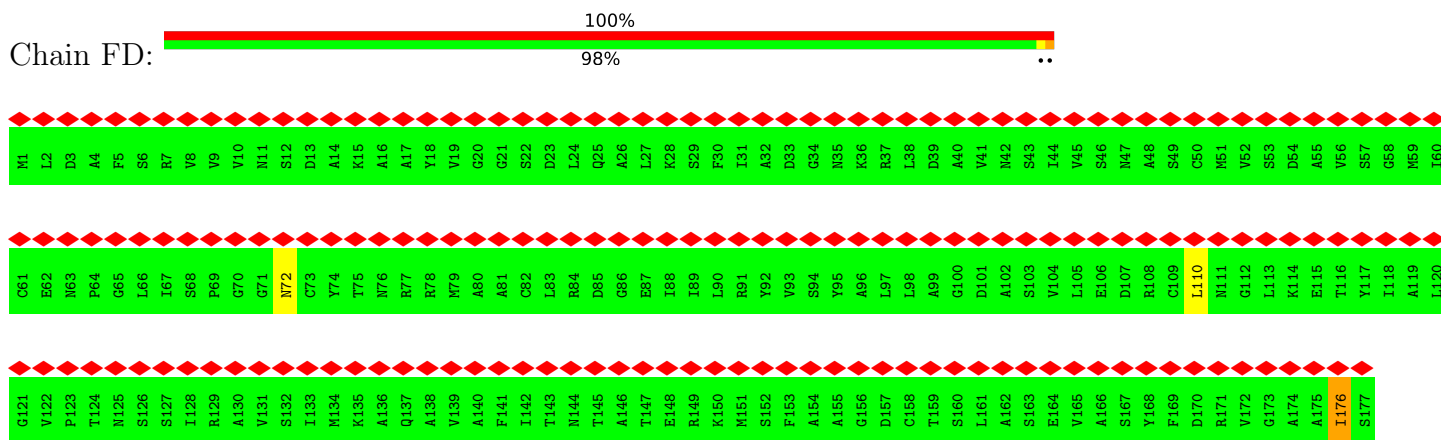




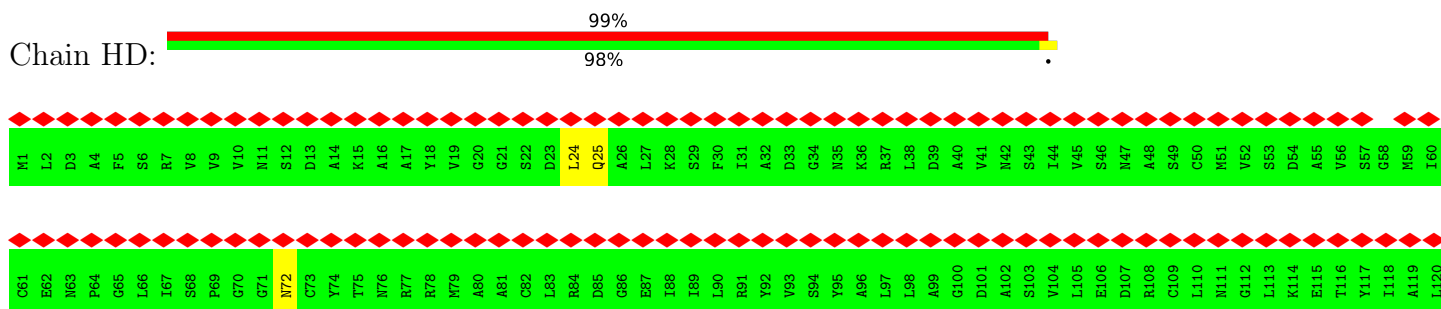
• Molecule 2: B-phycoerythrin beta chain

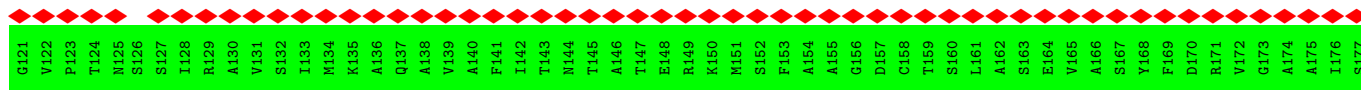


• Molecule 2: B-phycoerythrin beta chain

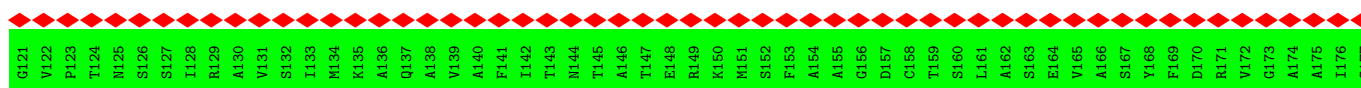
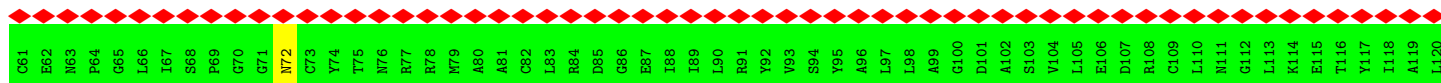
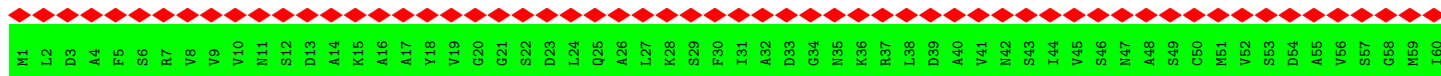


• Molecule 2: B-phycoerythrin beta chain

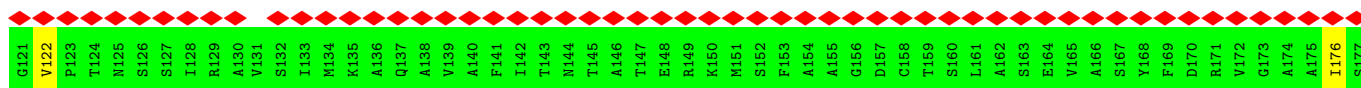
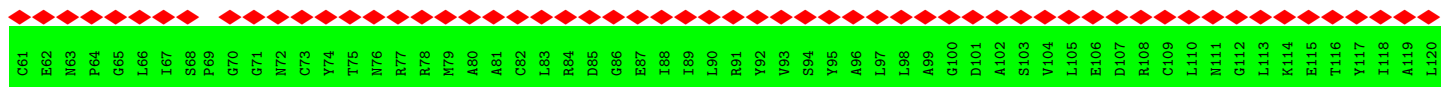




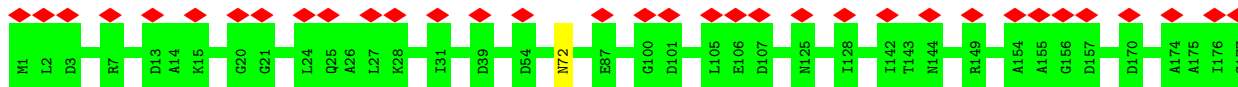
• Molecule 2: B-phycoerythrin beta chain



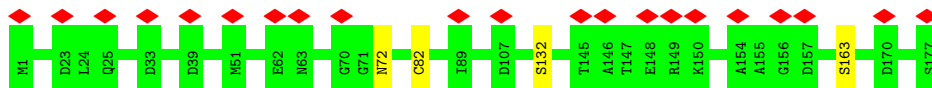
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

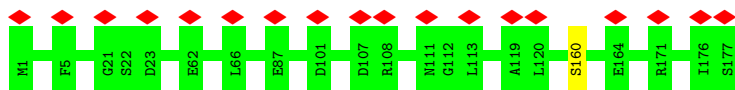


• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

Chain RD:  10% 99%



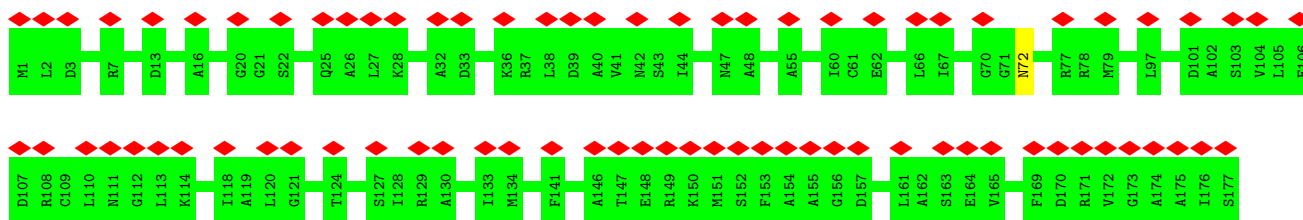
• Molecule 2: B-phycoerythrin beta chain

Chain TD:  99%



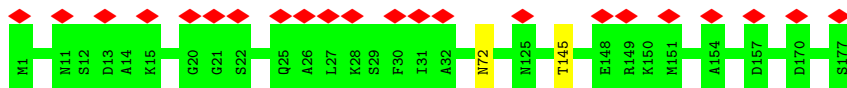
• Molecule 2: B-phycoerythrin beta chain

Chain VD:  44% 99%



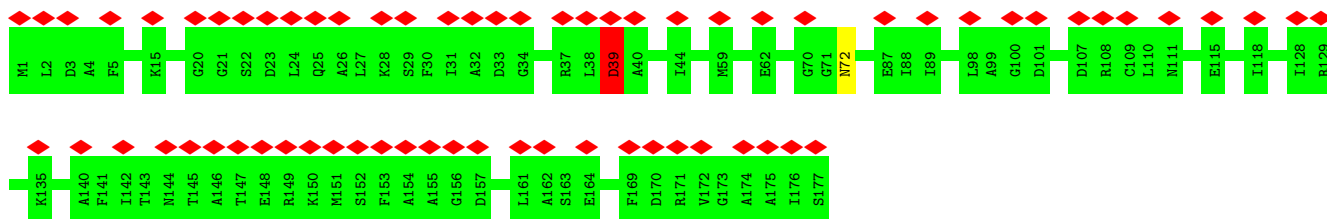
• Molecule 2: B-phycoerythrin beta chain

Chain XD:  12% 99%



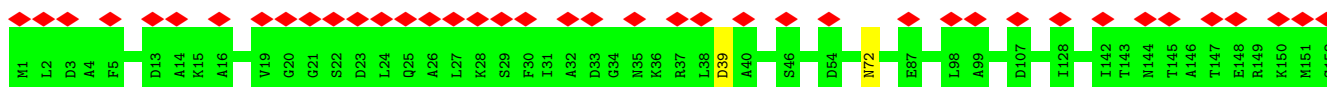
• Molecule 2: B-phycoerythrin beta chain

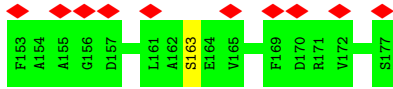
Chain BE:  38% 99%



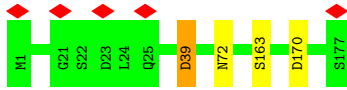
• Molecule 2: B-phycoerythrin beta chain

Chain DE:  28% 98%

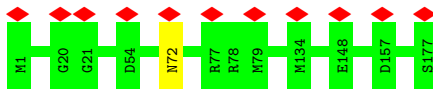




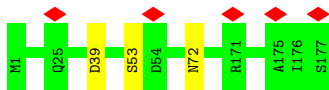
- Molecule 2: B-phycoerythrin beta chain



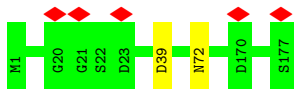
- Molecule 2: B-phycoerythrin beta chain



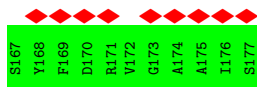
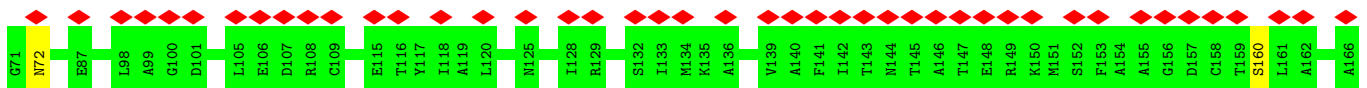
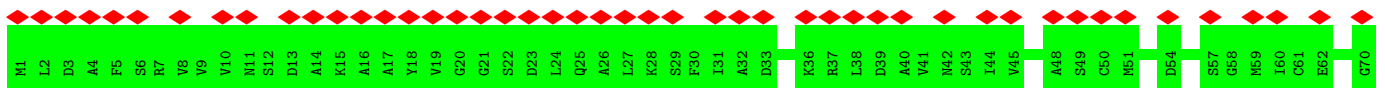
- Molecule 2: B-phycoerythrin beta chain



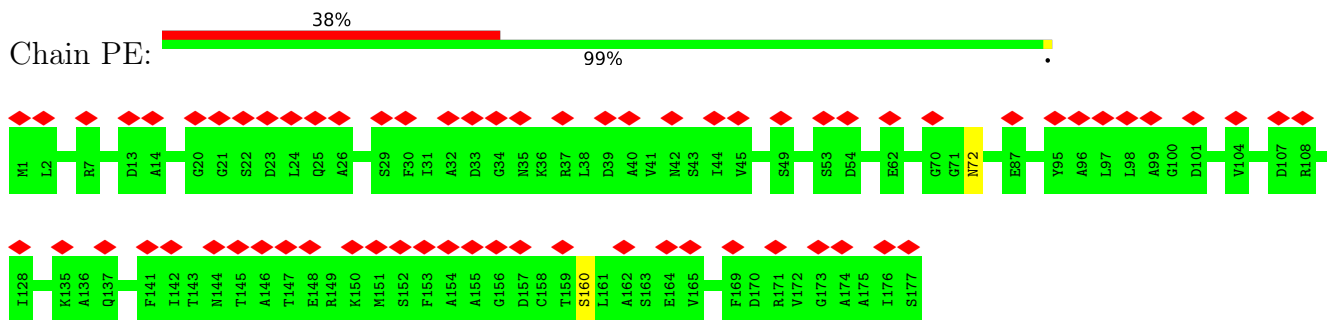
- Molecule 2: B-phycoerythrin beta chain



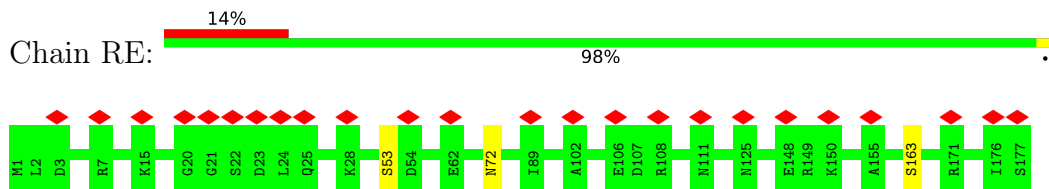
- Molecule 2: B-phycoerythrin beta chain



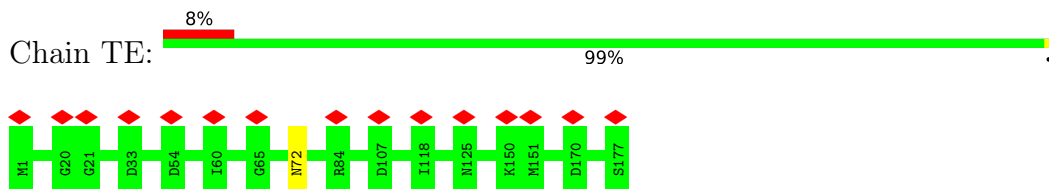
- Molecule 2: B-phycoerythrin beta chain



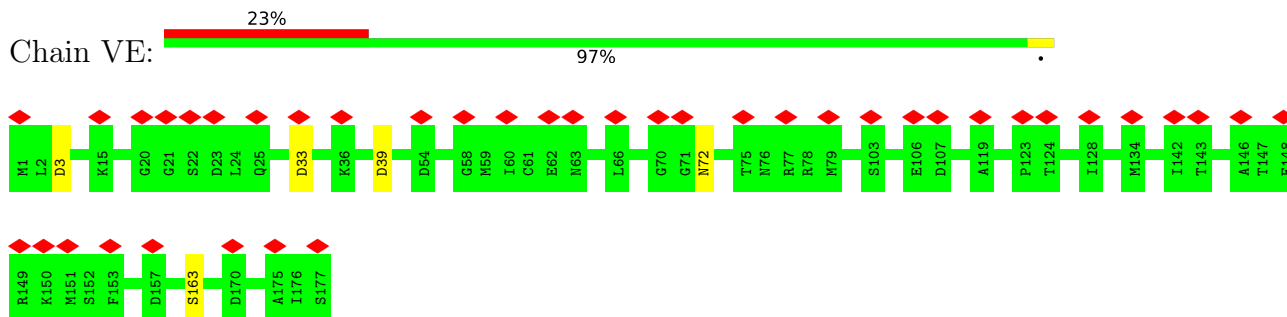
• Molecule 2: B-phycoerythrin beta chain



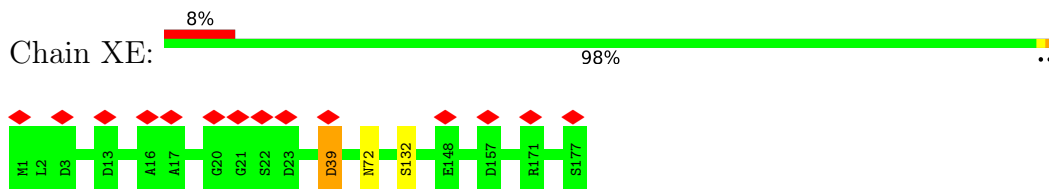
• Molecule 2: B-phycoerythrin beta chain



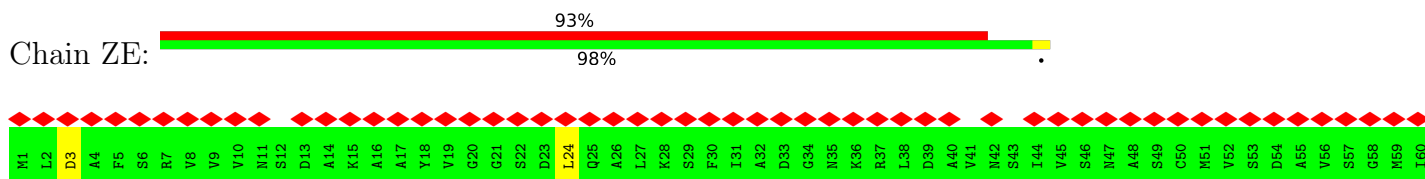
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

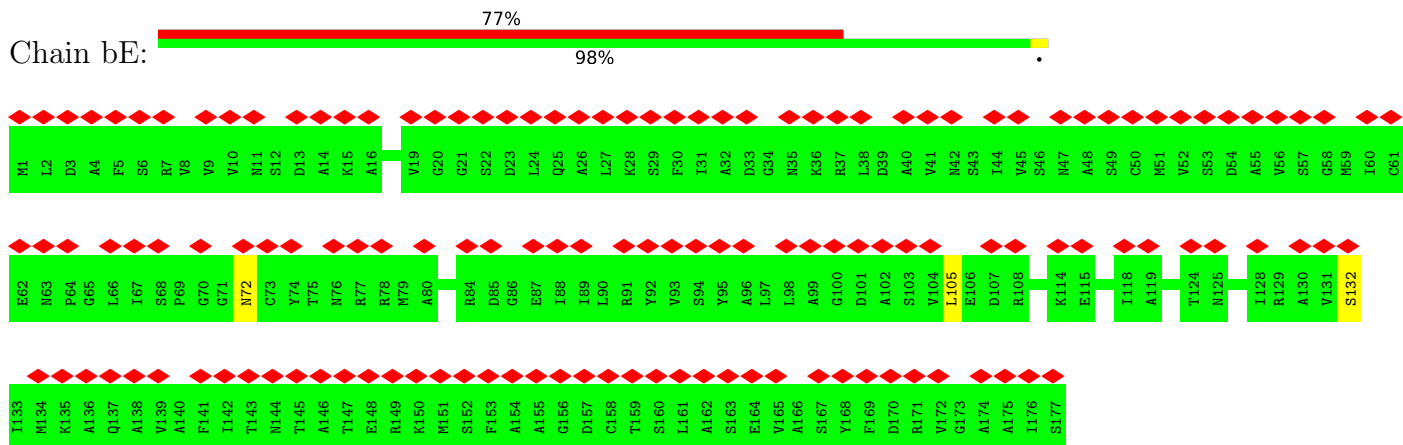


• Molecule 2: B-phycoerythrin beta chain

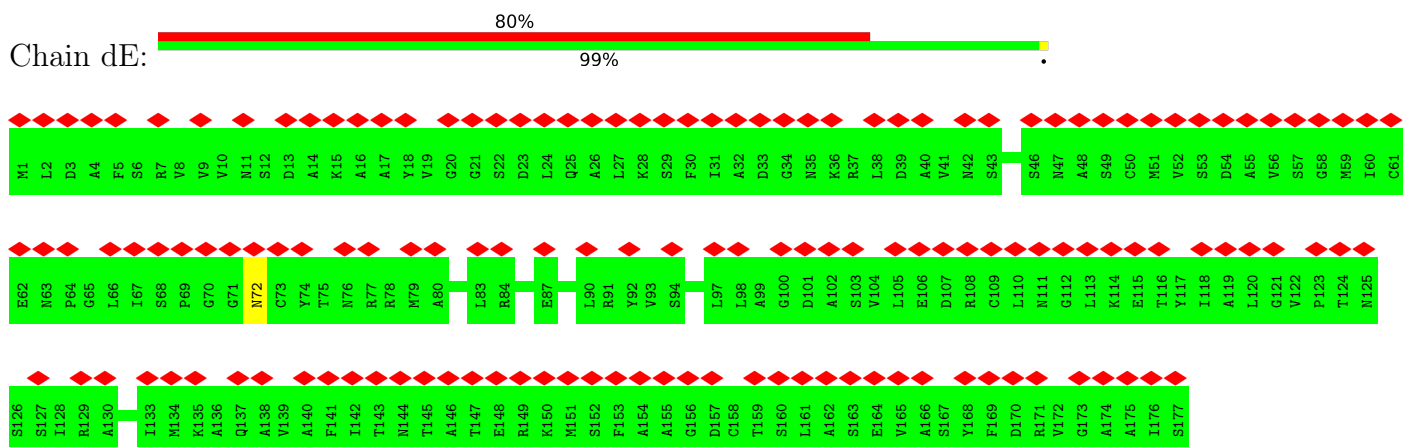




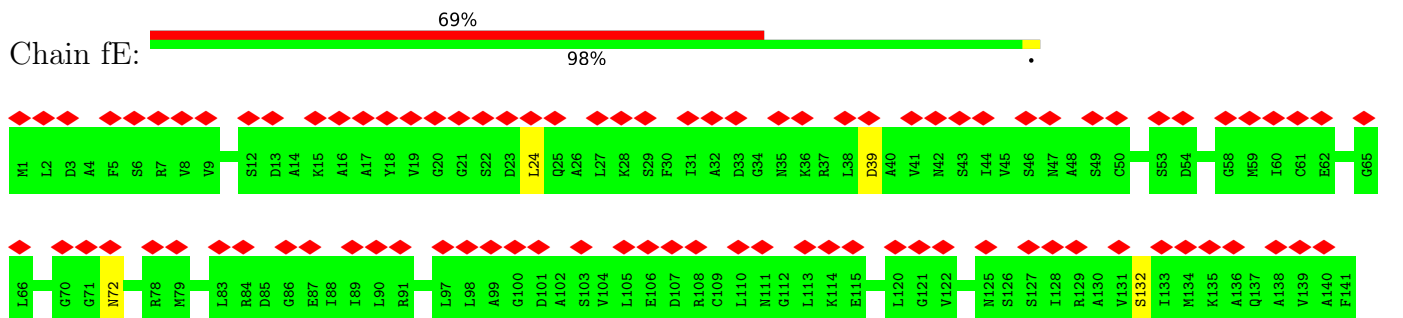
- Molecule 2: B-phycoerythrin beta chain

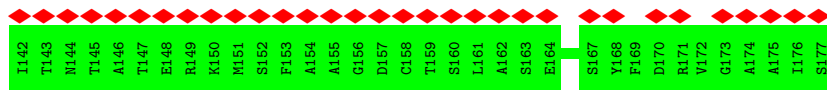


- Molecule 2: B-phycoerythrin beta chain

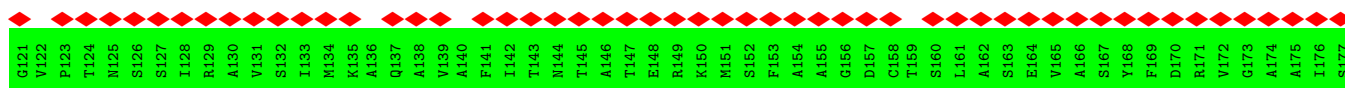
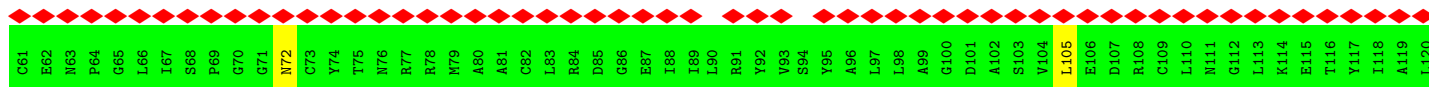


- Molecule 2: B-phycoerythrin beta chain

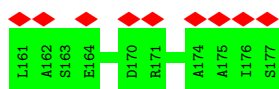
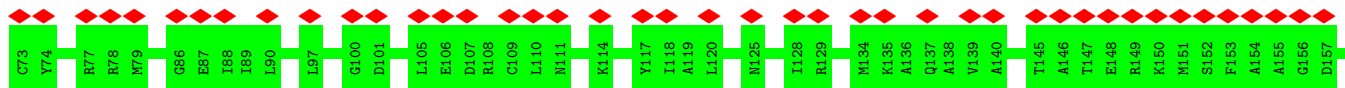




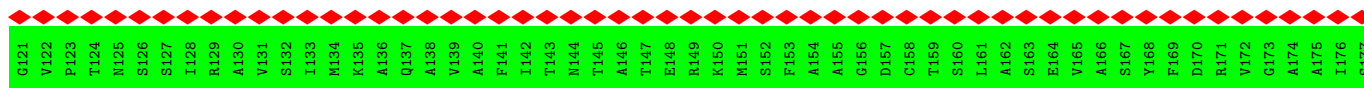
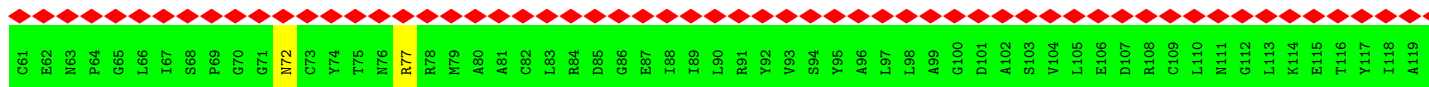
• Molecule 2: B-phycoerythrin beta chain



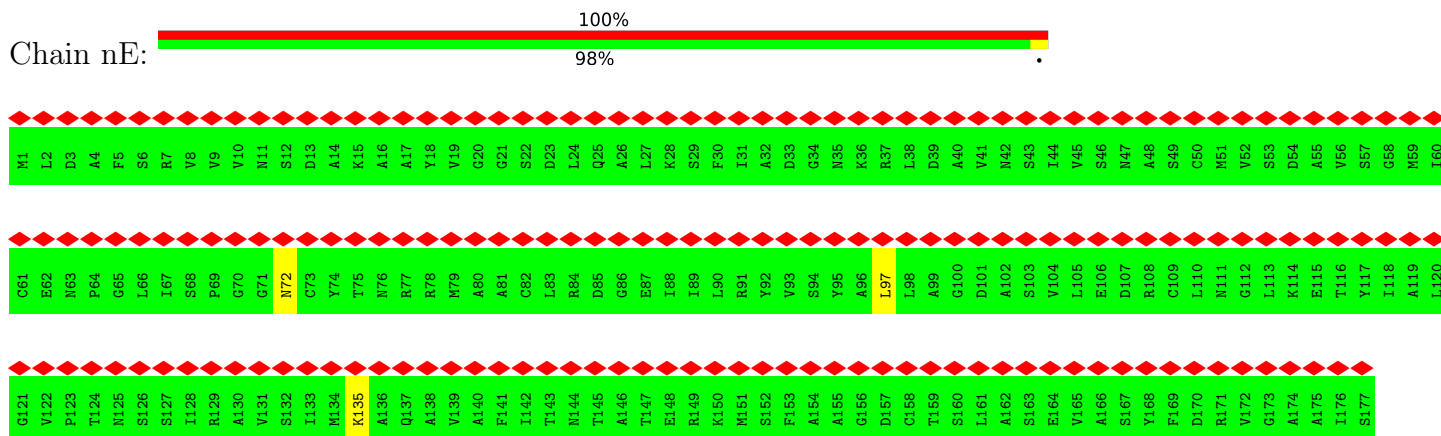
• Molecule 2: B-phycoerythrin beta chain



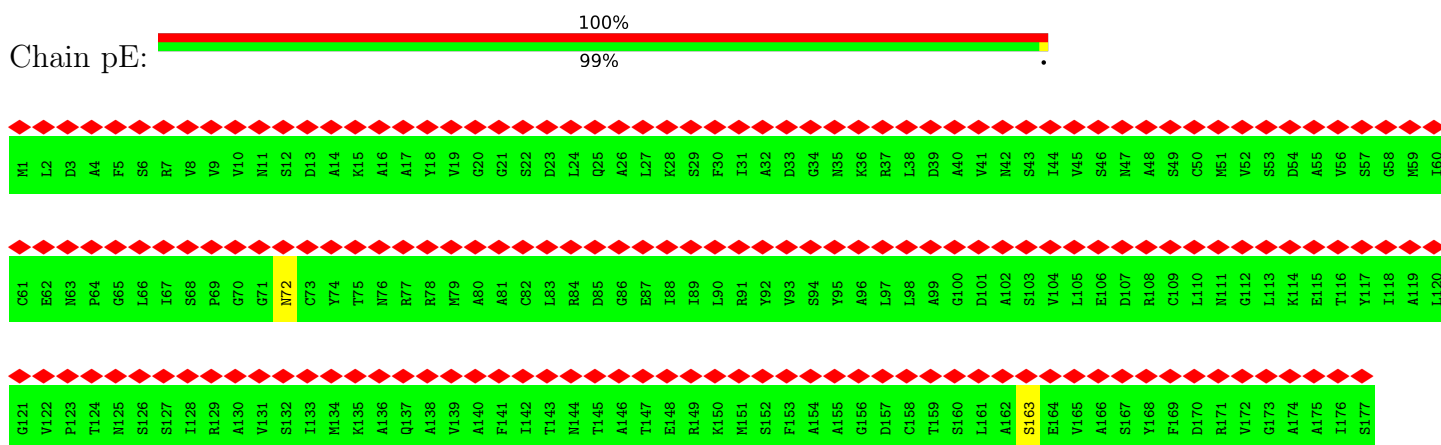
• Molecule 2: B-phycoerythrin beta chain



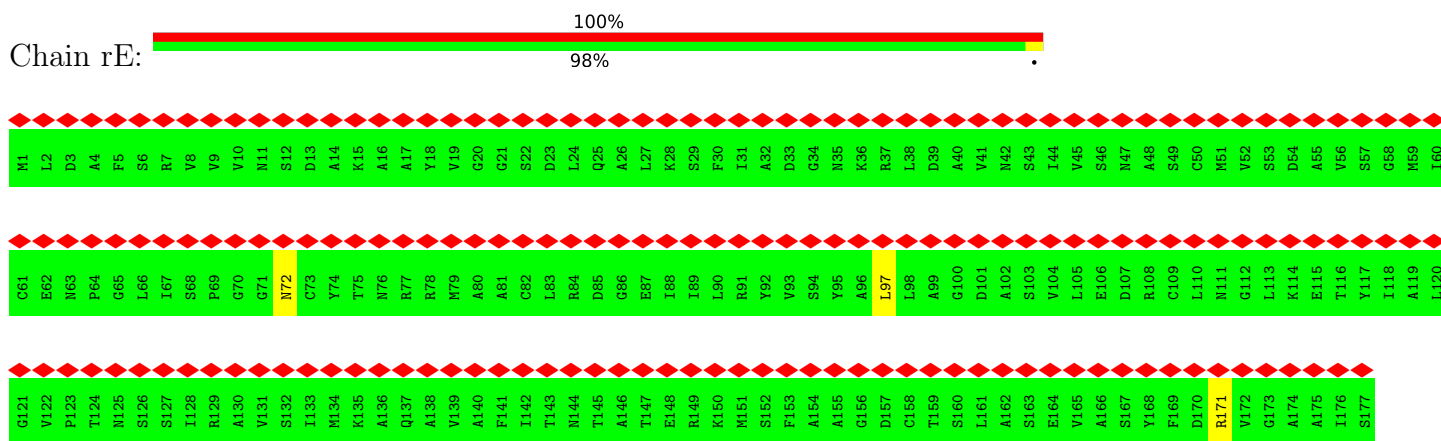
• Molecule 2: B-phycoerythrin beta chain



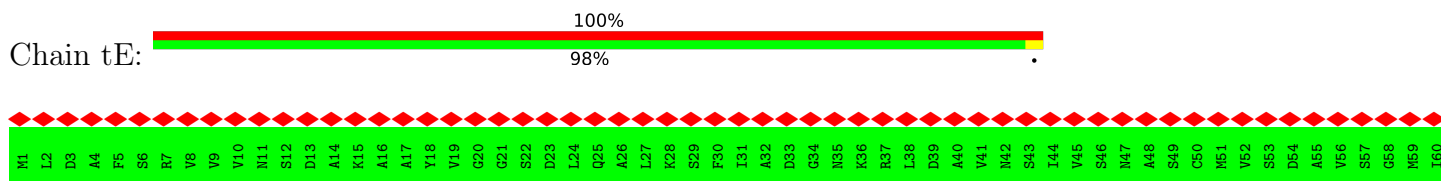
• Molecule 2: B-phycoerythrin beta chain

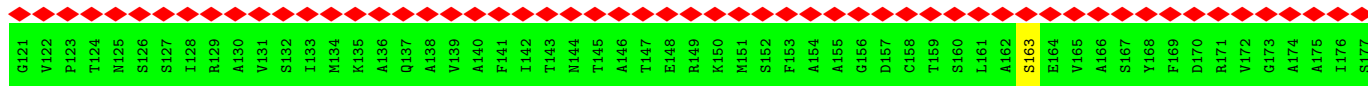
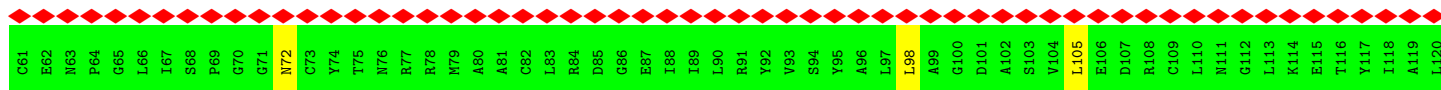


• Molecule 2: B-phycoerythrin beta chain

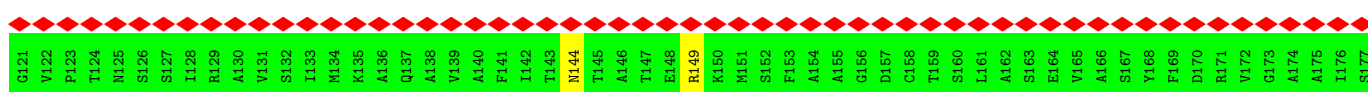


• Molecule 2: B-phycoerythrin beta chain

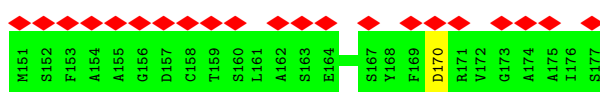
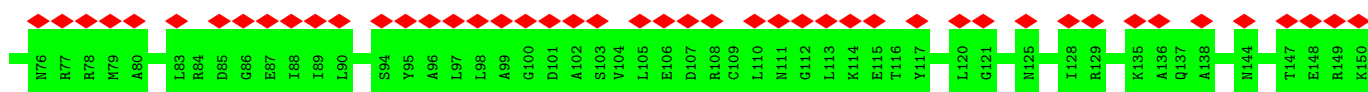
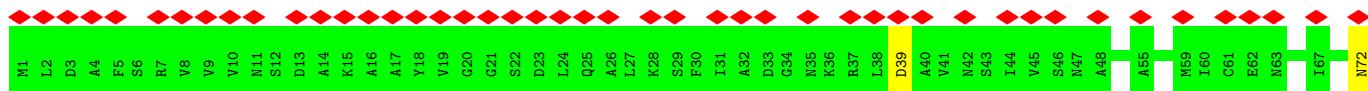




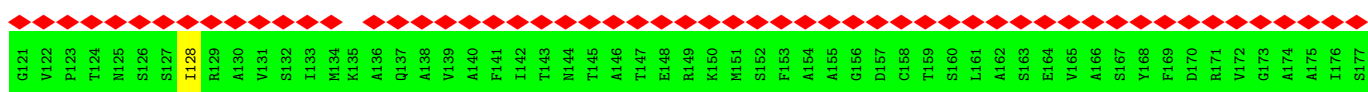
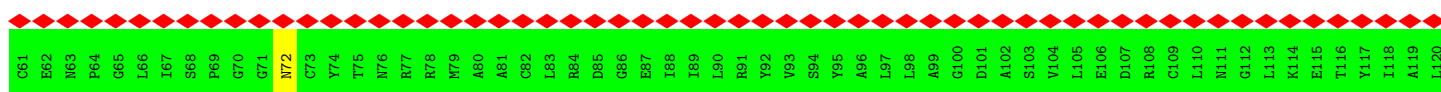
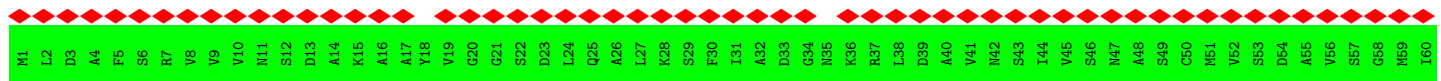
• Molecule 2: B-phycoerythrin beta chain



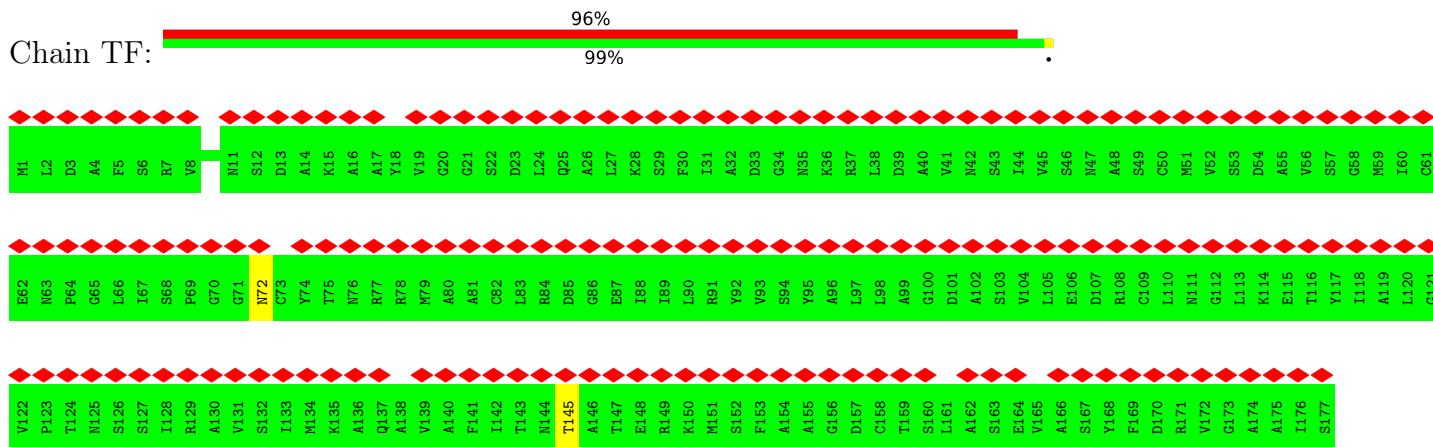
• Molecule 2: B-phycoerythrin beta chain



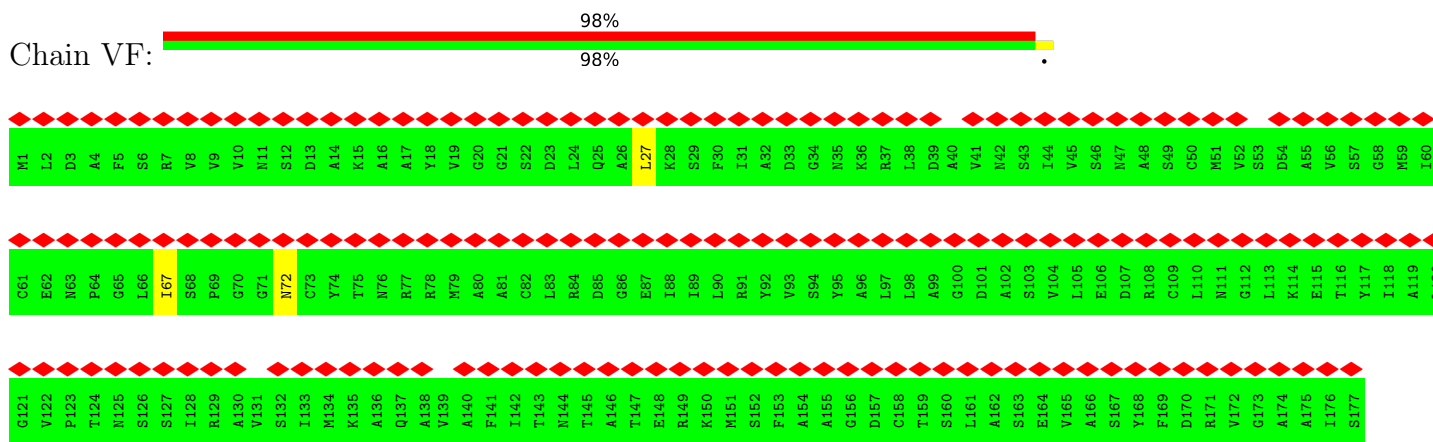
• Molecule 2: B-phycoerythrin beta chain



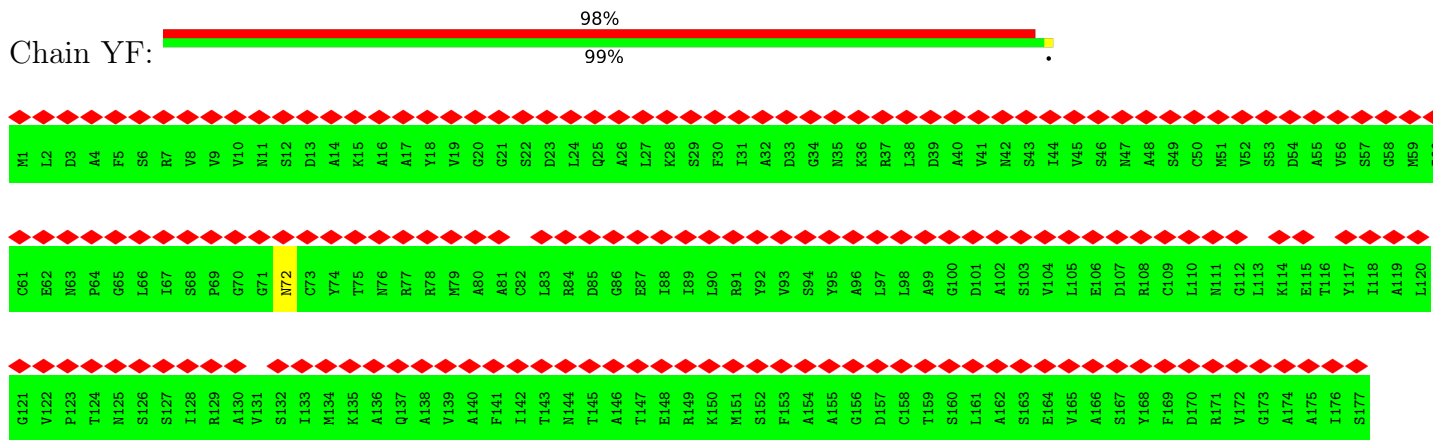
• Molecule 2: B-phycoerythrin beta chain



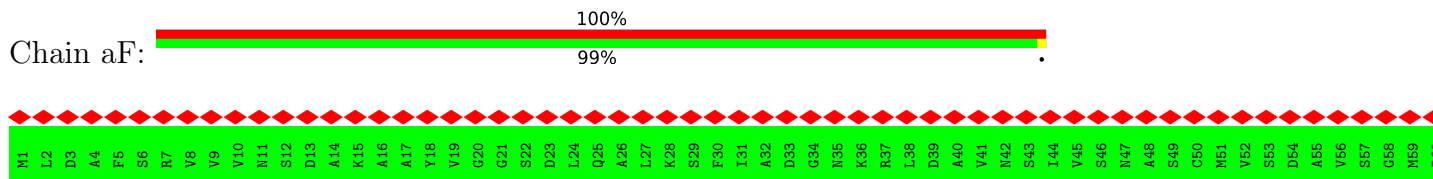
• Molecule 2: B-phycoerythrin beta chain

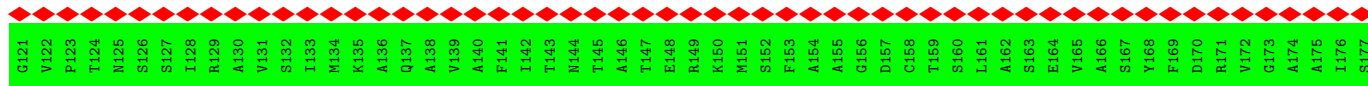
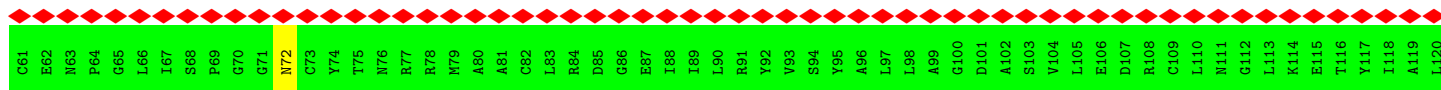


• Molecule 2: B-phycoerythrin beta chain

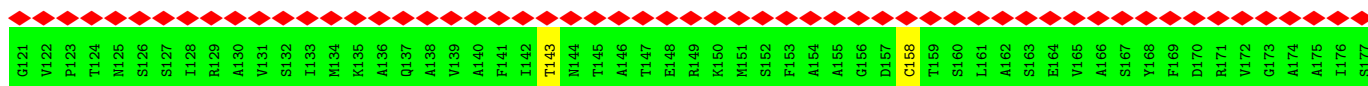


• Molecule 2: B-phycoerythrin beta chain

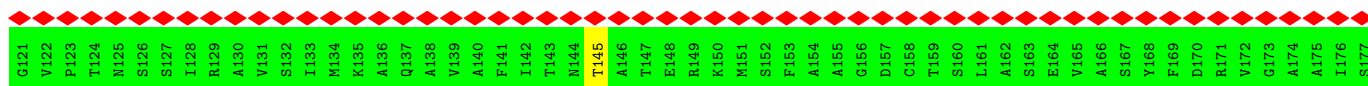
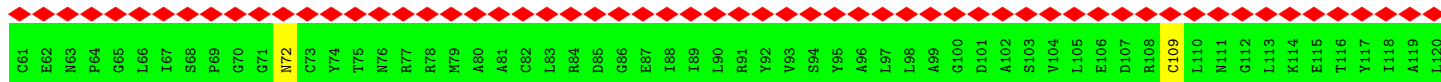




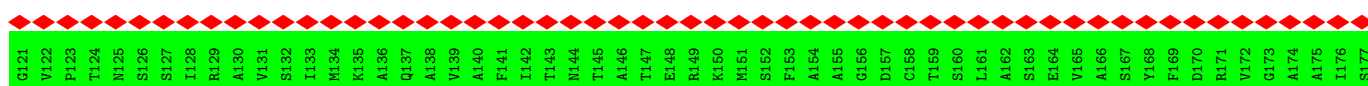
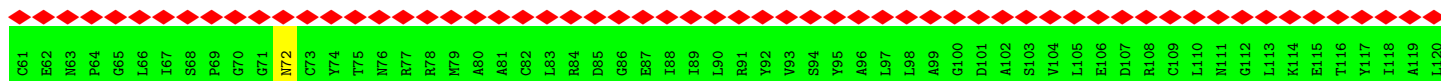
• Molecule 2: B-phycoerythrin beta chain



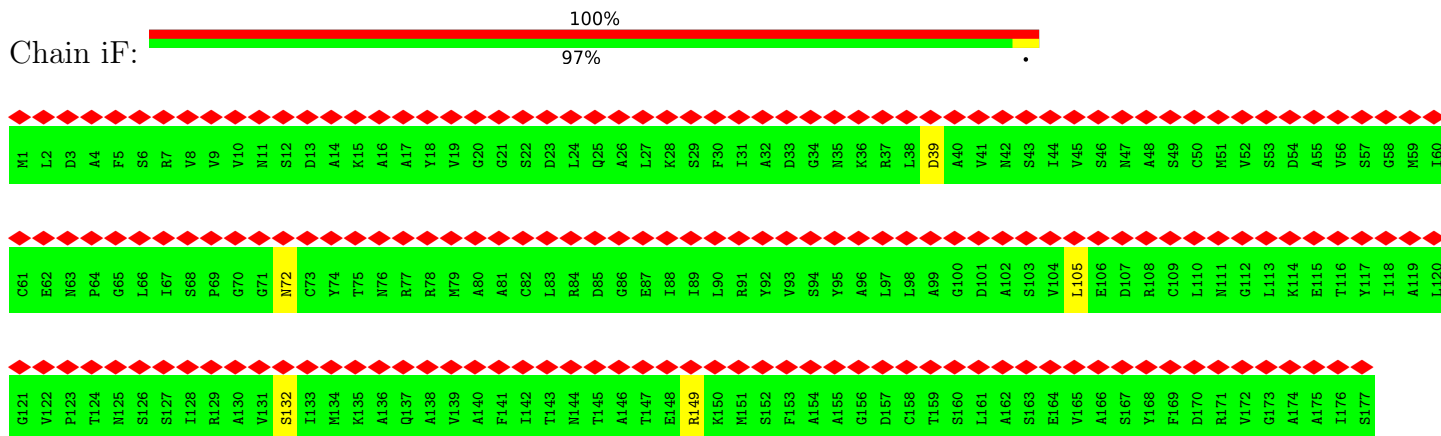
• Molecule 2: B-phycoerythrin beta chain



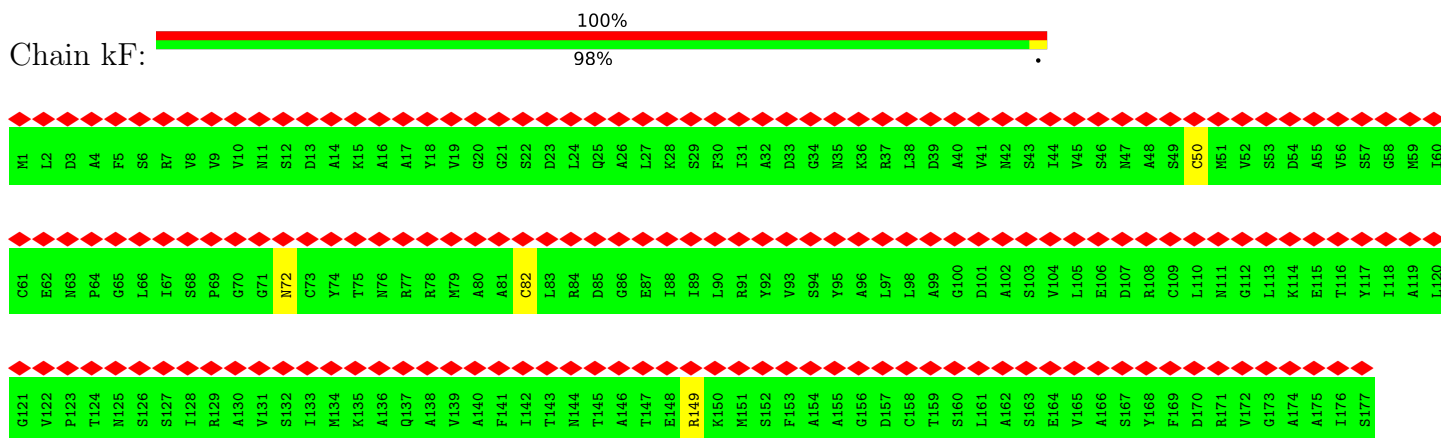
• Molecule 2: B-phycoerythrin beta chain



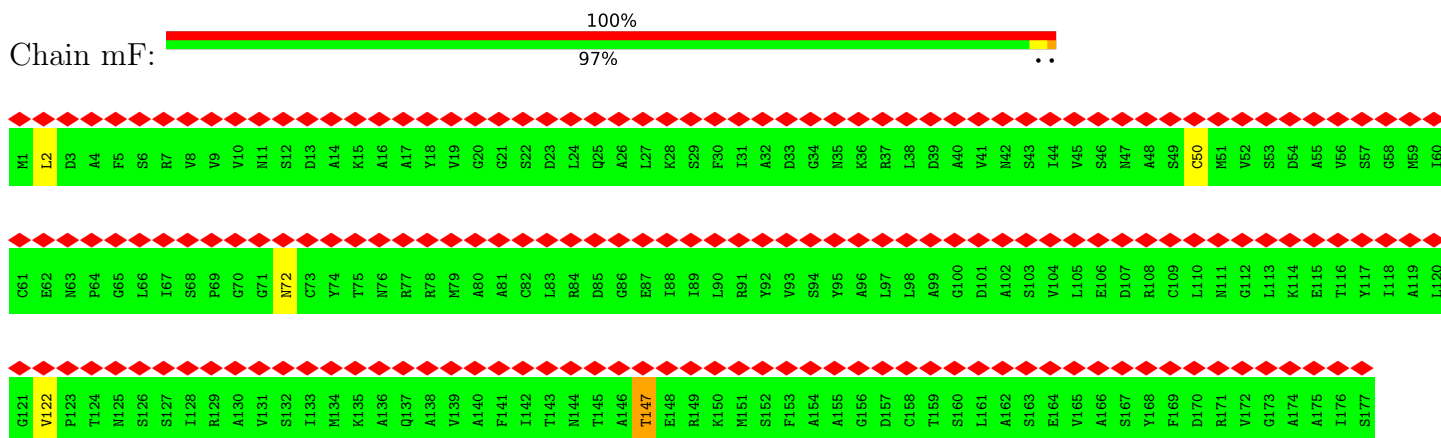
• Molecule 2: B-phycoerythrin beta chain



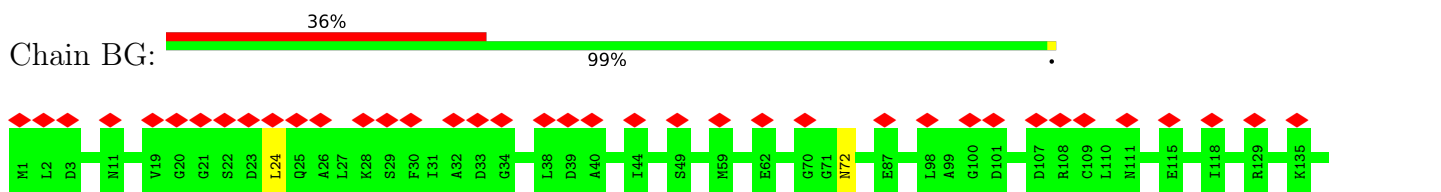
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

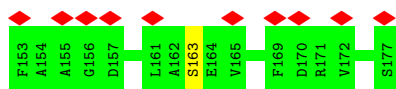
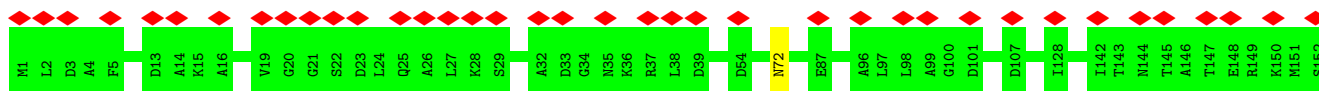


• Molecule 2: B-phycoerythrin beta chain

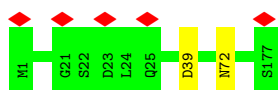




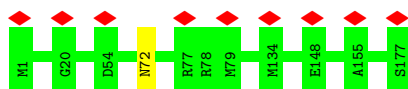
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

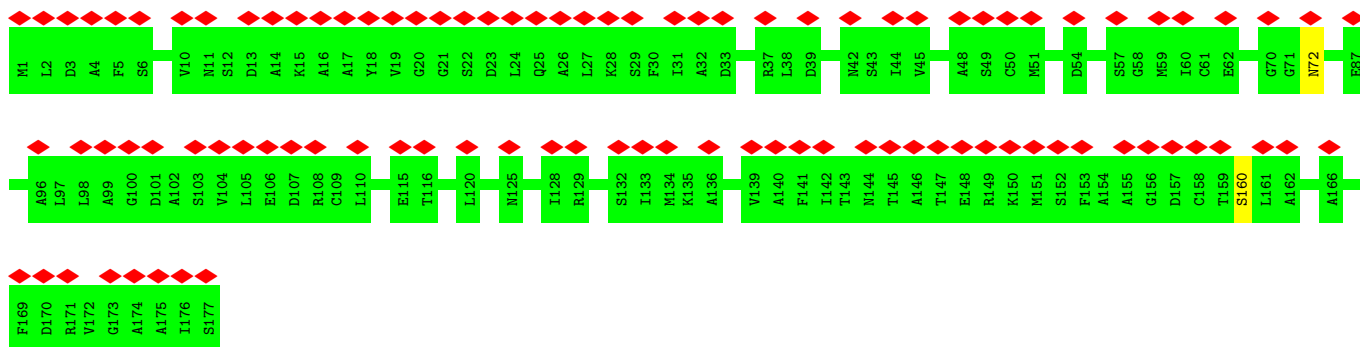


- Molecule 2: B-phycoerythrin beta chain

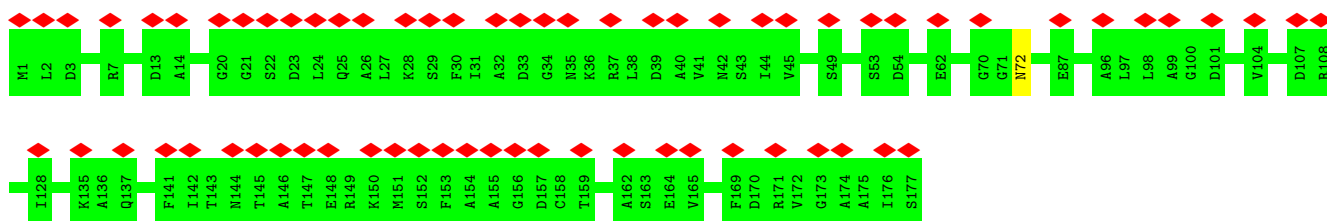
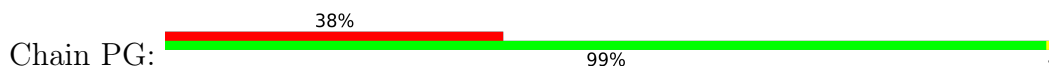


- Molecule 2: B-phycoerythrin beta chain

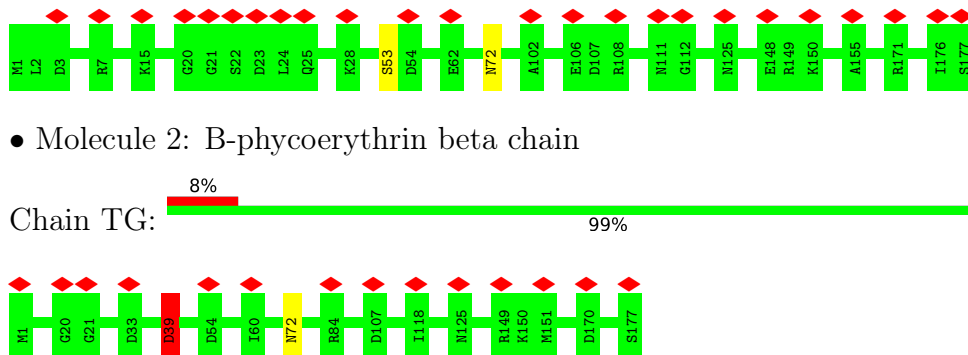




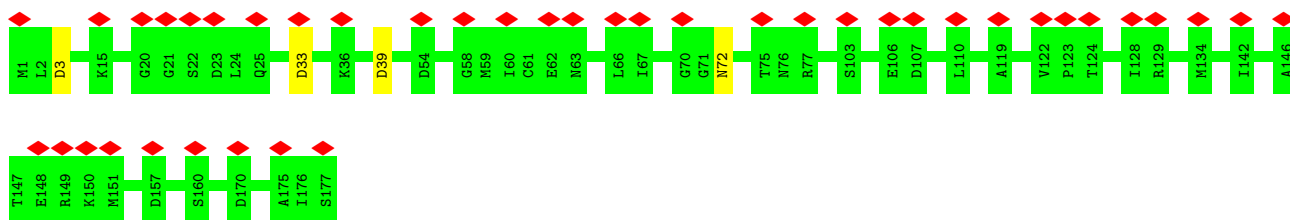
• Molecule 2: B-phycoerythrin beta chain



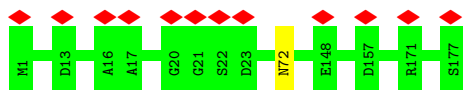
• Molecule 2: B-phycoerythrin beta chain



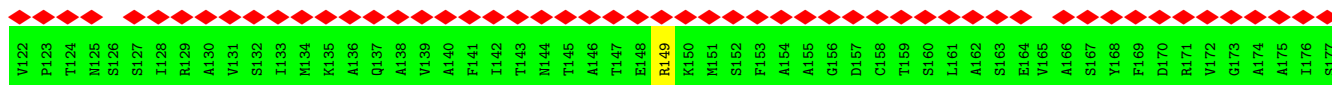
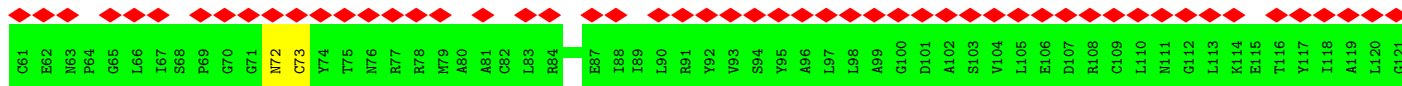
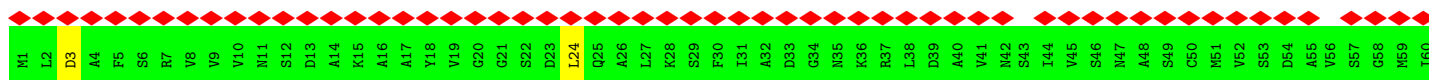
• Molecule 2: B-phycoerythrin beta chain



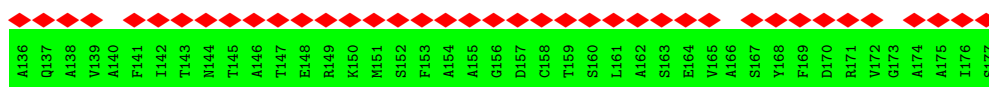
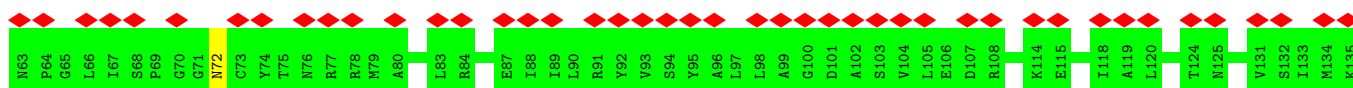
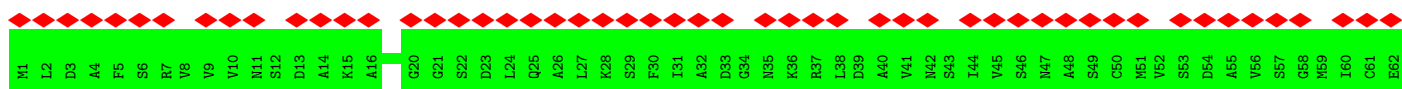
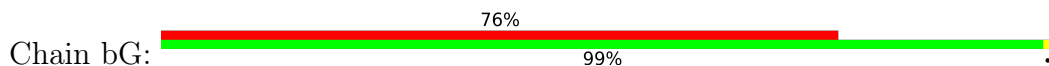
• Molecule 2: B-phycoerythrin beta chain



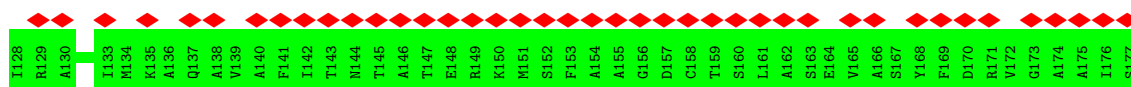
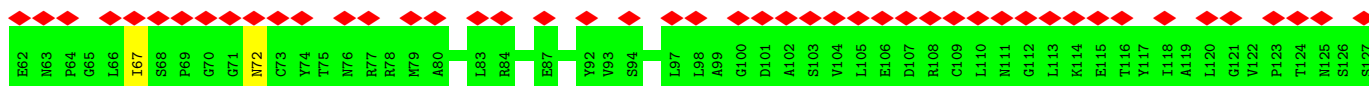
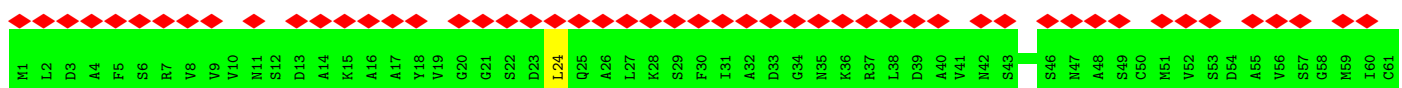
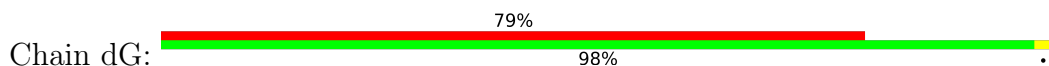
• Molecule 2: B-phycoerythrin beta chain



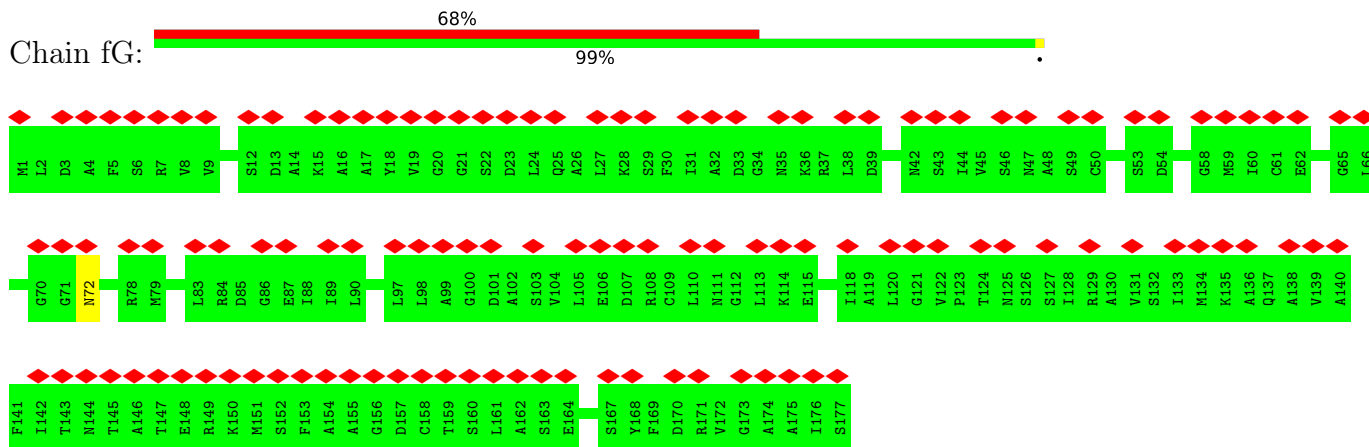
• Molecule 2: B-phycoerythrin beta chain



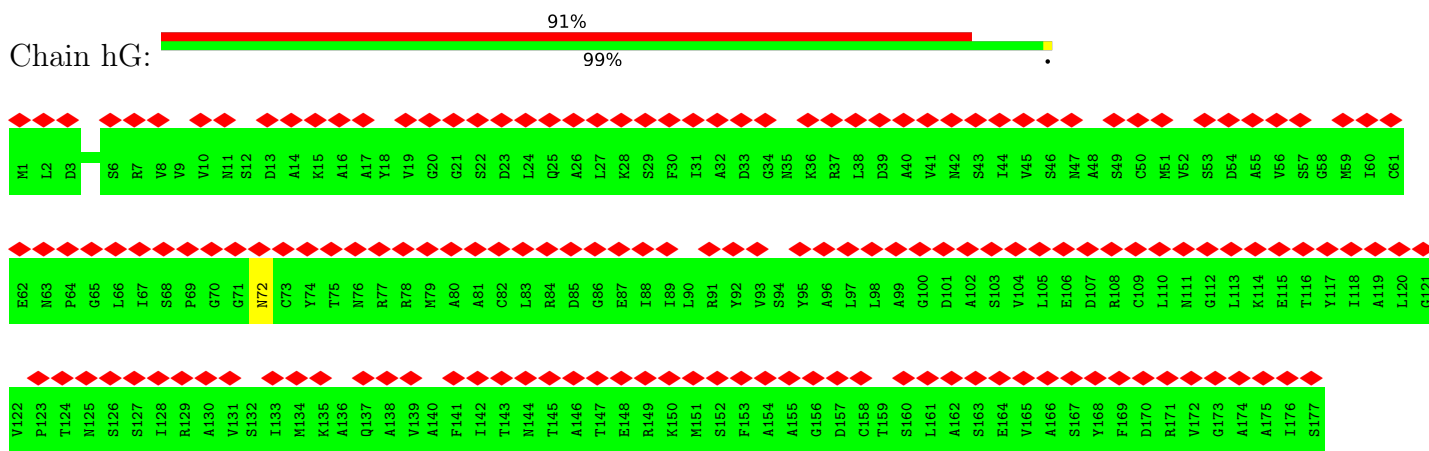
• Molecule 2: B-phycoerythrin beta chain



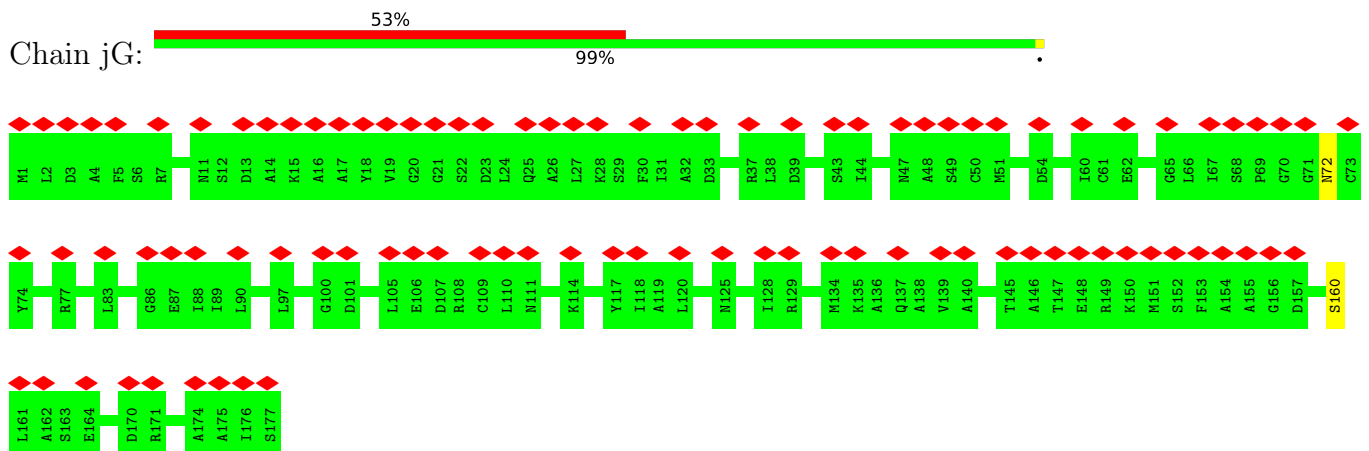
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

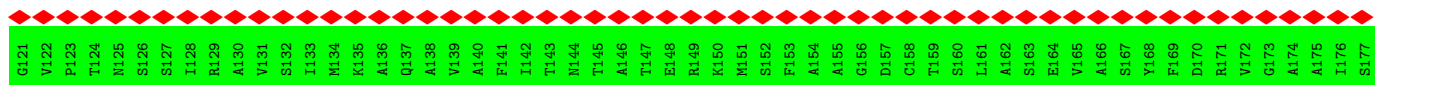
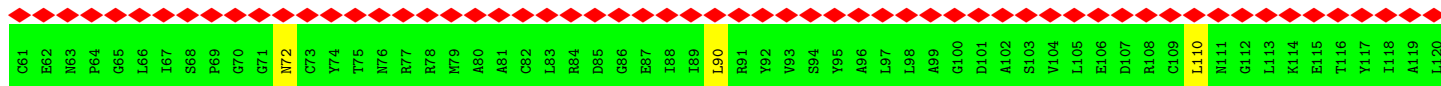
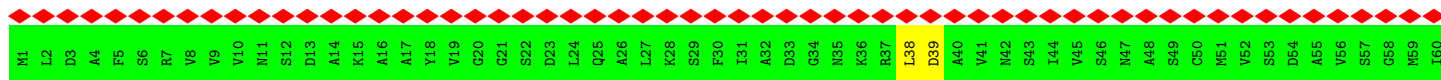


• Molecule 2: B-phycoerythrin beta chain

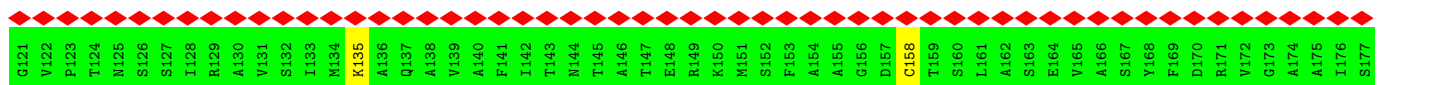
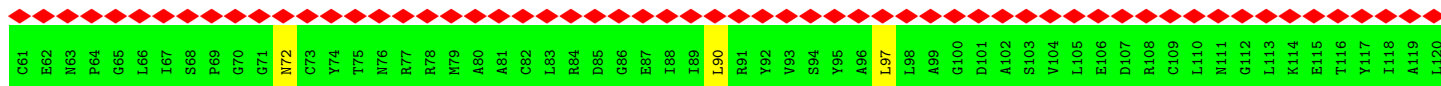
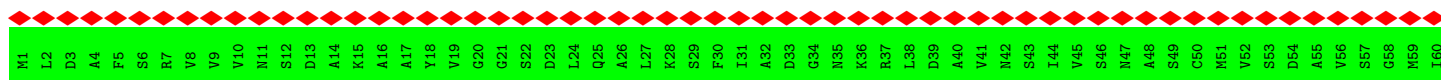


• Molecule 2: B-phycoerythrin beta chain

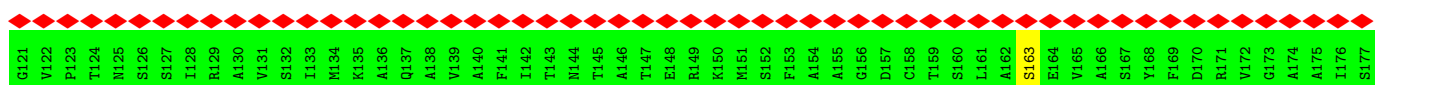
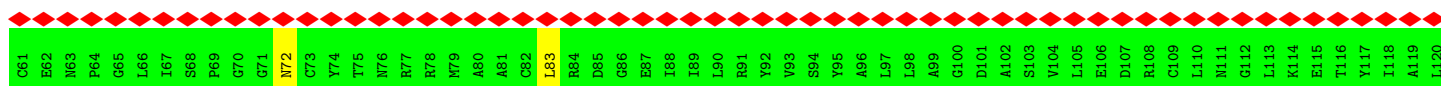
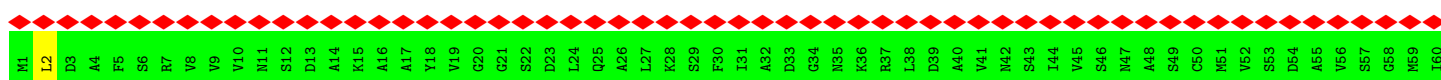




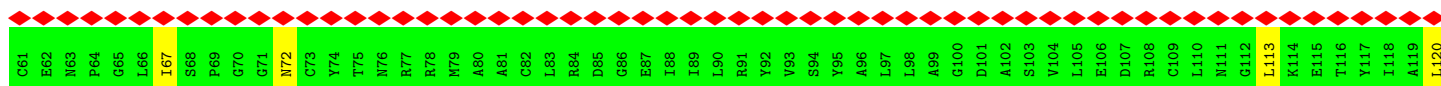
• Molecule 2: B-phycoerythrin beta chain

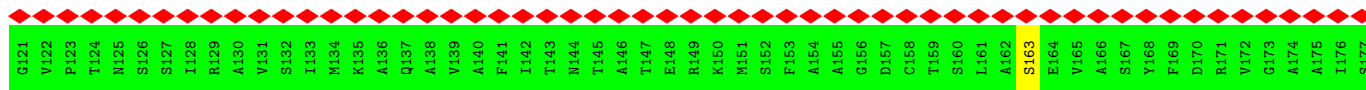


• Molecule 2: B-phycoerythrin beta chain

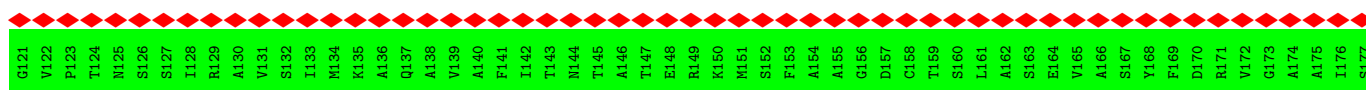
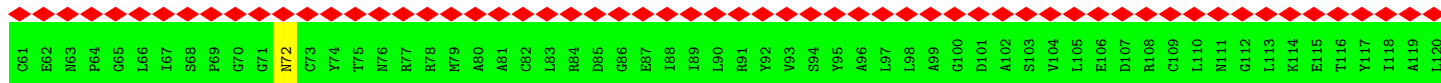
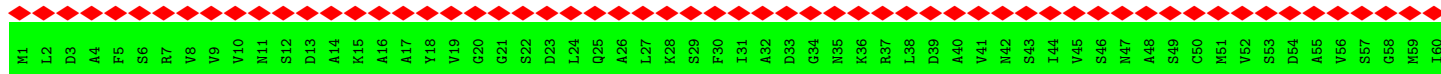


• Molecule 2: B-phycoerythrin beta chain

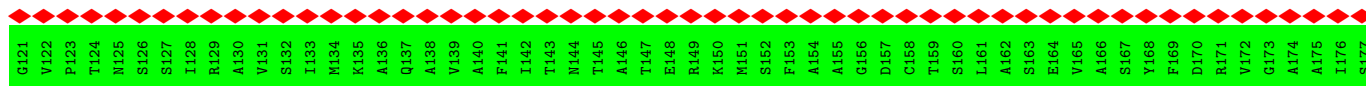
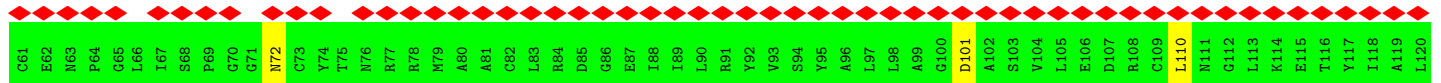
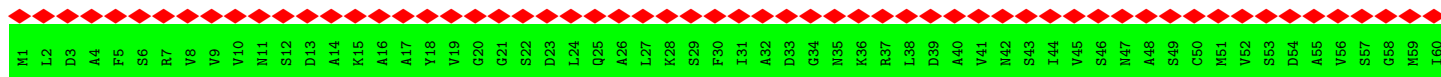




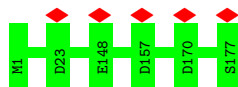
• Molecule 2: B-phycoerythrin beta chain



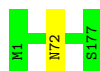
• Molecule 2: B-phycoerythrin beta chain



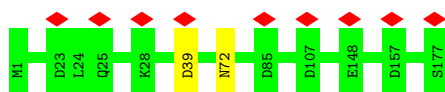
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



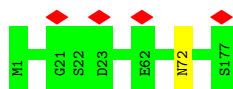
• Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain



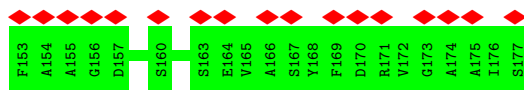
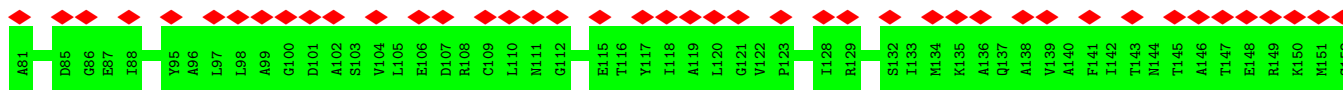
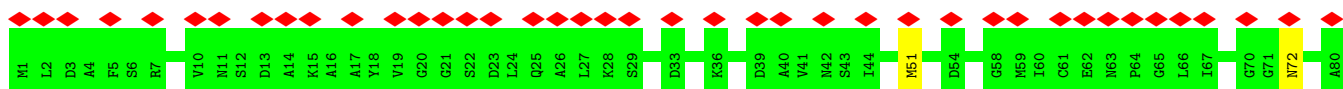
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain



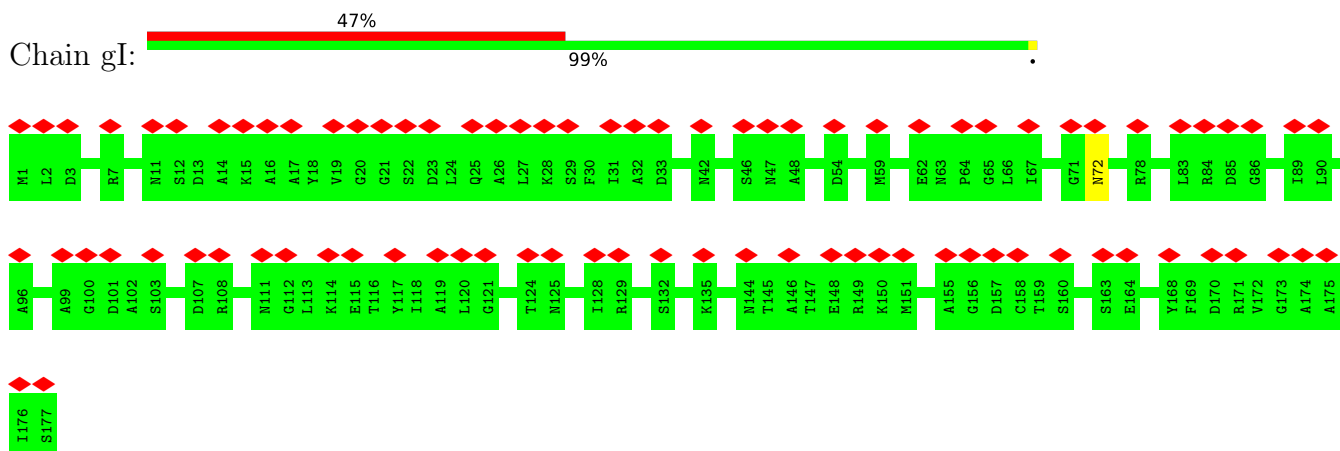
- Molecule 2: B-phycoerythrin beta chain



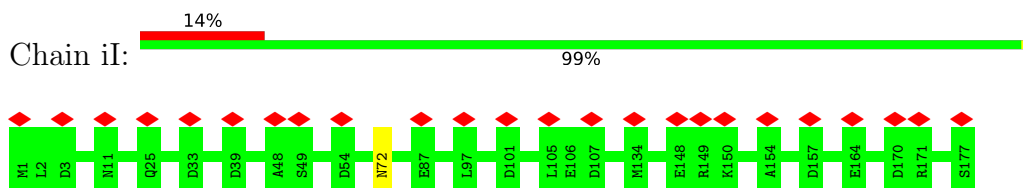
- Molecule 2: B-phycoerythrin beta chain



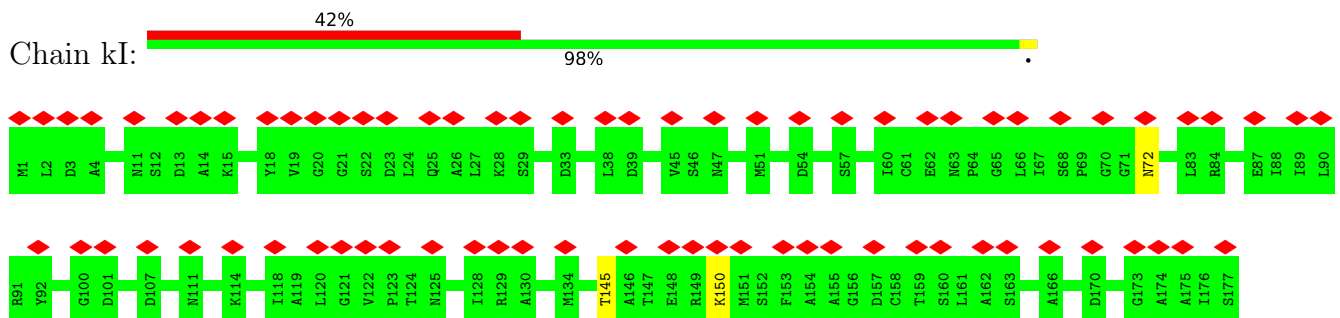
- Molecule 2: B-phycoerythrin beta chain



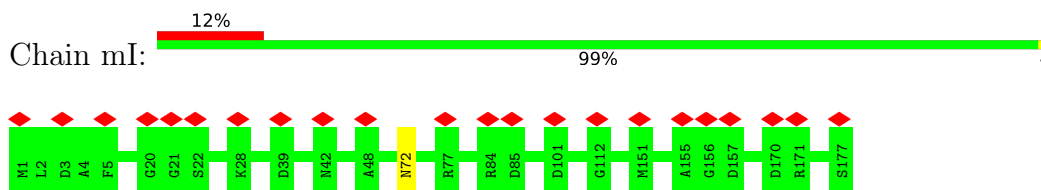
- Molecule 2: B-phycoerythrin beta chain



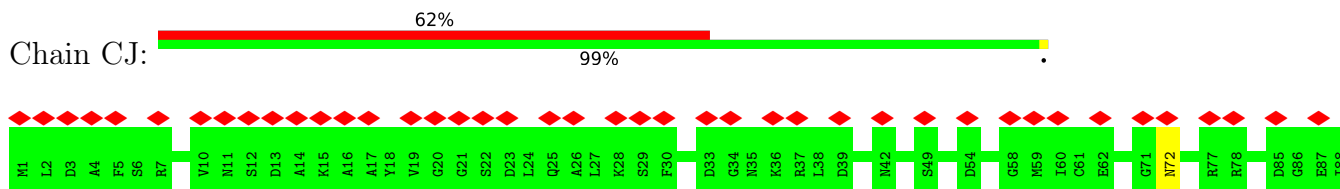
- Molecule 2: B-phycoerythrin beta chain

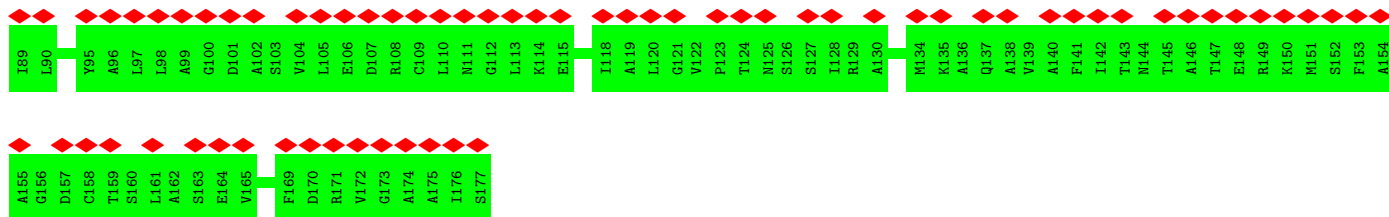


- Molecule 2: B-phycoerythrin beta chain

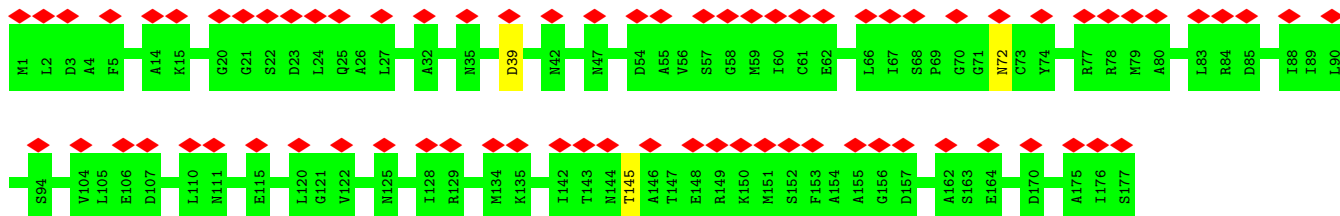
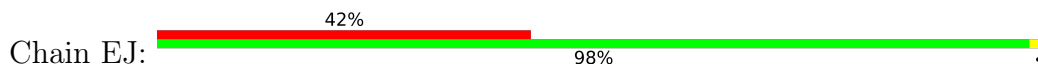


- Molecule 2: B-phycoerythrin beta chain

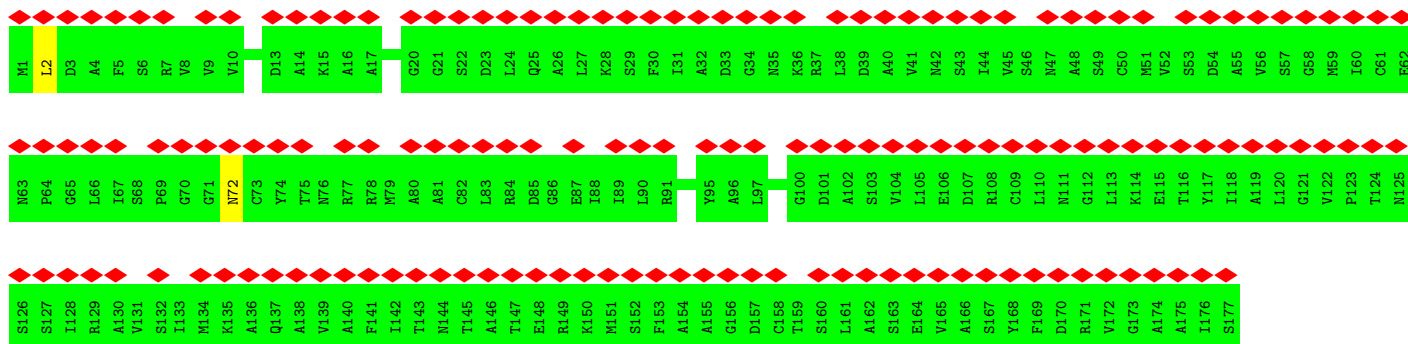
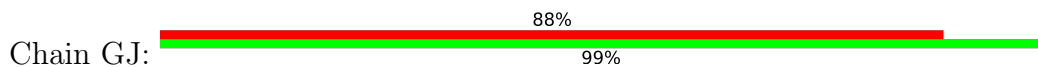




• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

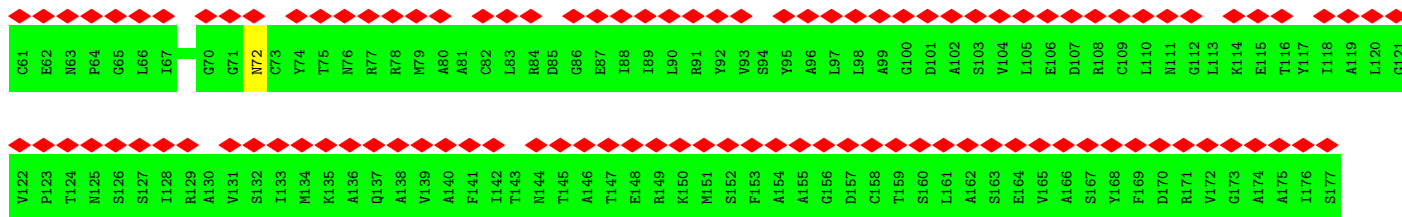


• Molecule 2: B-phycoerythrin beta chain



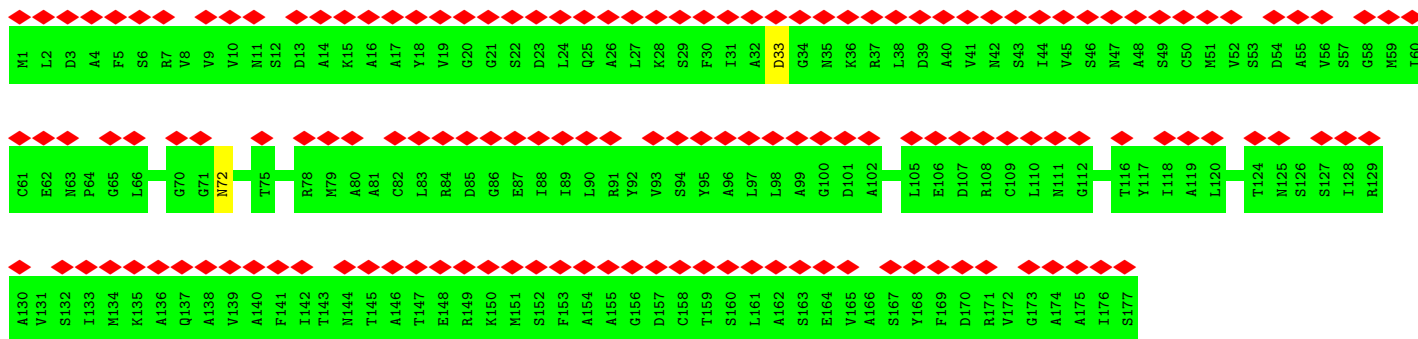
• Molecule 2: B-phycoerythrin beta chain





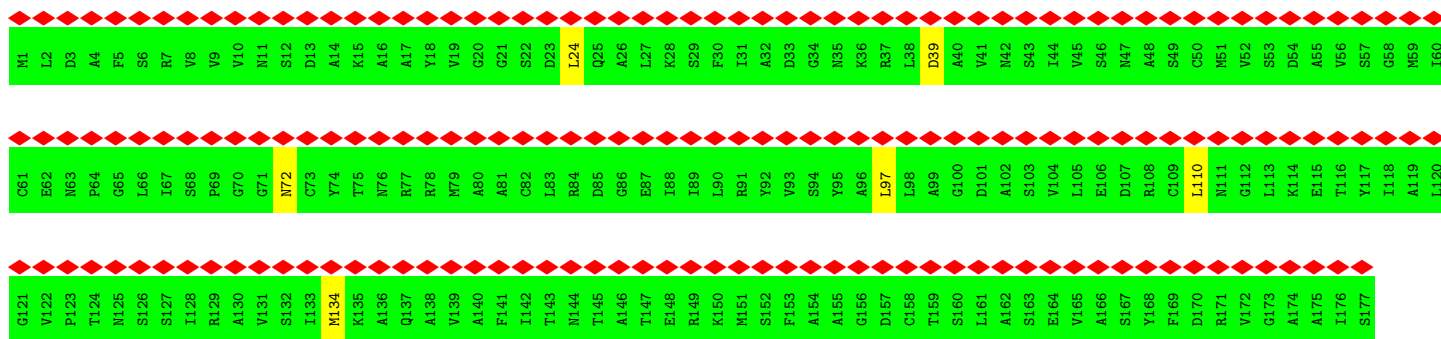
• Molecule 2: B-phycoerythrin beta chain

Chain MJ:



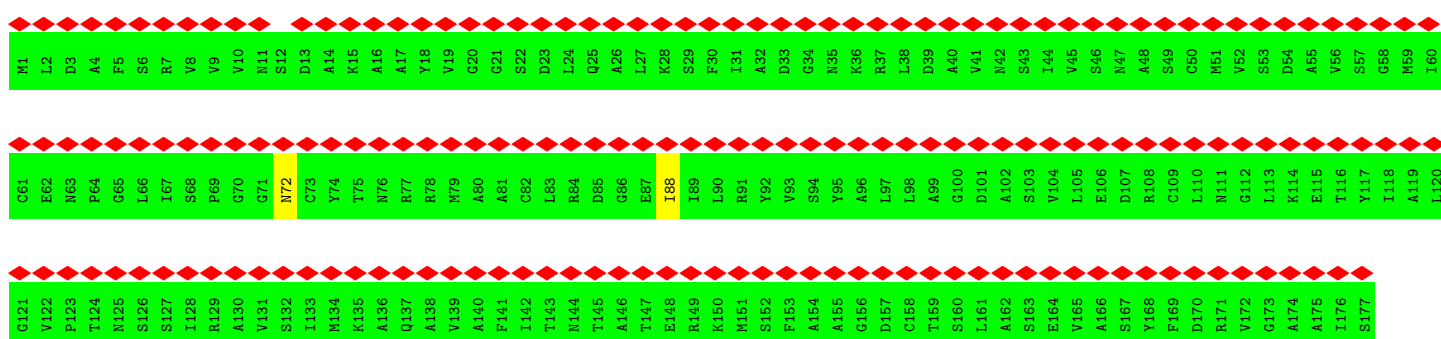
• Molecule 2: B-phycoerythrin beta chain

Chain OJ:

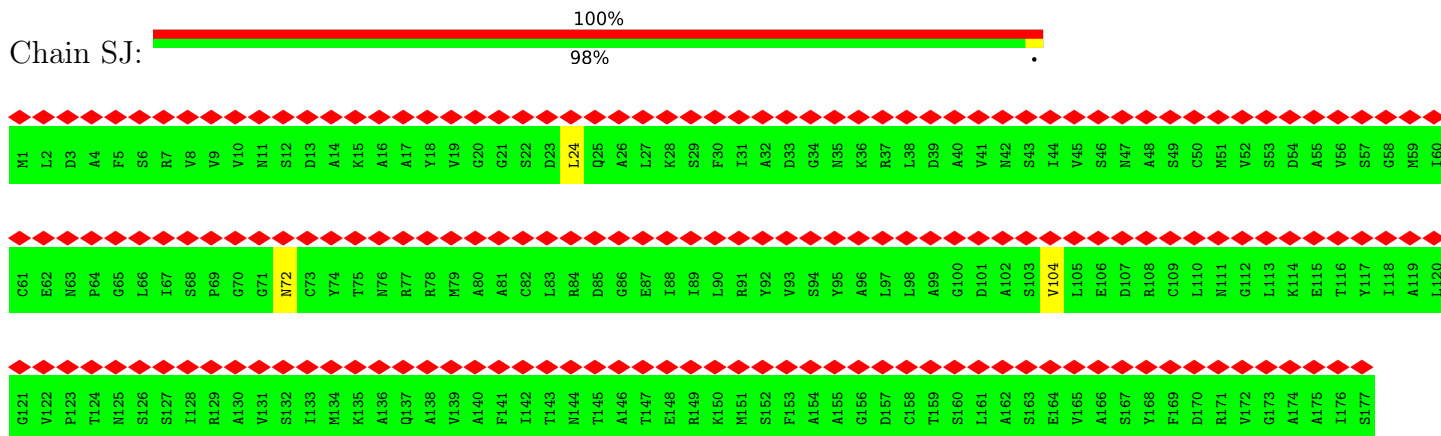


• Molecule 2: B-phycoerythrin beta chain

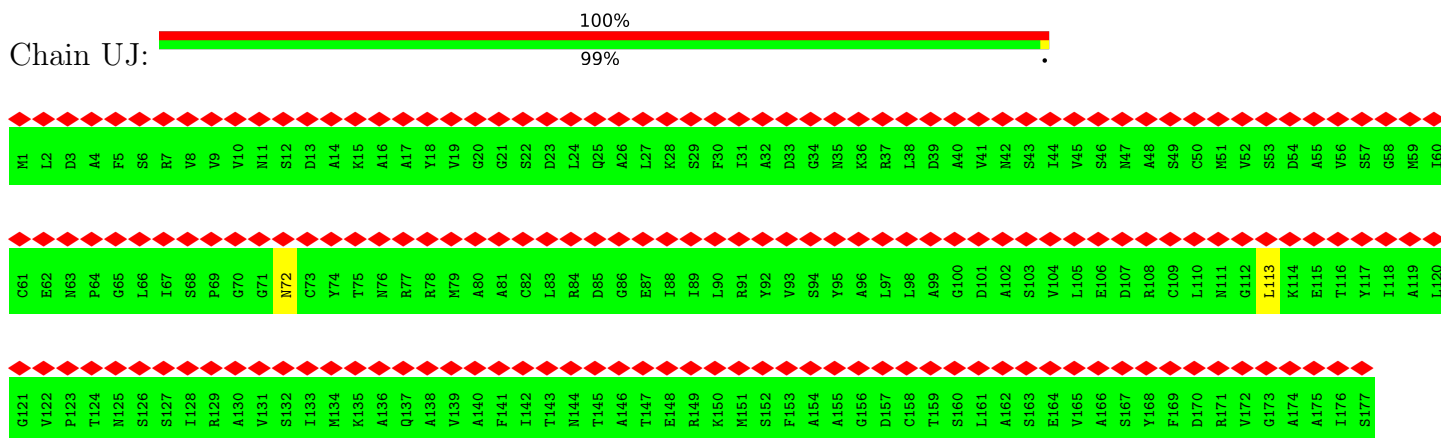
Chain QJ:



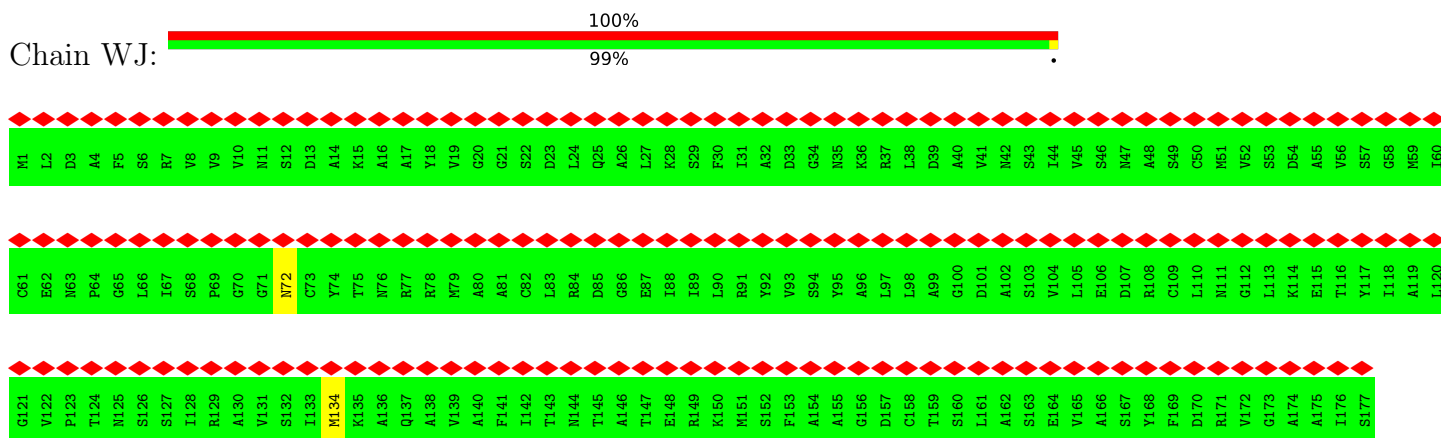
• Molecule 2: B-phycoerythrin beta chain



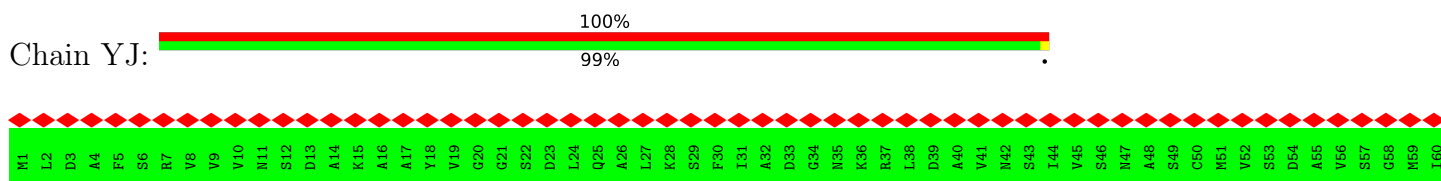
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain



C61	E62	N63	P64	G65	L66	I67	S68	P69	G70	G71	N72	C73	Y74	T76	N76	R77	R78	M79	A80	A81	C82	L83	R84	D85	G86	E87	I88	I89	L90	R91	Y92	V93	S94	Y95	A96	L97	L98	A99	G100	D101	A102	S103	V104	L105	L106	D107	R108	C109	L110	M111	G112	L113	K114	E115	T116	Y117	I118	A119	L120
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

G121	V122	P123	T124	N125	S126	I127	I128	R129	A130	V131	S132	I133	M134	K135	A136	Q137	A138	V139	A140	F141	I142	T143	M144	T145	A146	T147	E148	R149	K150	M151	S152	F153	A154	A155	G156	D157	C158	T159	S160	L161	A162	S163	E164	V165	A166	S167	Y168	F169	D170	R171	V172	G173	A174	A175	I176	S177
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 3: LR7



MET	ALA	ALA	PHE	VAL	VAL	GLY	ALA	GLN	VAL	SER	GLY	PHE	MET	GLY	CYS	ALA	ALA	PRO	ARG	THR	LYS	ARG	LYS	ALA	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LYS	LEU	LEU	ASN	THR	VAL	LYS	PRO	MET	LYS	ARG	GLN	VAL	GLN	PRO	ASN	PRO	THR	THR	ASN	GLU	GLY	THR	ALA	ARG	SER	PRO	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

D121	F122	M123	A124	R125	S126	I127	A128	M129	Q130	A131	K132	A133	S134	A135	A136	S138	G139	LEU	LEU	GLY	THR	PHE	ALA	ARG	SER	PRO	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Y181	E182	G183	R184	K185	Y186	A187	M188	K189	A190	V191	G192	H193	I194	C195	N196	Y197	S198	C199	E200	K201	F202	Q203	Q204	Y205	N206	K207	T208	A209	A210	A211	Y212	V213	M214	G215	K216	Q217	E218	T219	L220	L221	S222	C223	D224	M225	Y226	A227	Q228	P229	A230	N231	K232	A233	E234	E235	Y236	I237	Q238	K239	S240
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

V241	Q242	M243	Q244	M245	K246	K247	R248	S249	I250	P251	Y252	G253	V254	Y255	T256	T257	S258	C259	A260	D261	G262	T263	V264	K265	G266	M267	A268	E269	N270	A271	R272	V273	A274	K275	E276	S277	A278	N279	F280	R281	A282	R283	D284	M285	S286	A287	G288	A289	K290	A291	A292	A293	R294	F295	N296	Y297	R298	R299	V300
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

A301	N303	D303	V304	H305	N306	N307	G308	C309	N310	Y311	E312	E313	K314	L315	T316	S317	F318	F319	P320	I201	A322	A323	S324	S325	V326	R327	P328	T329	T330	N331	R332	Y333
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

• Molecule 3: LR7

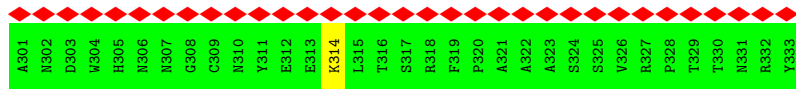
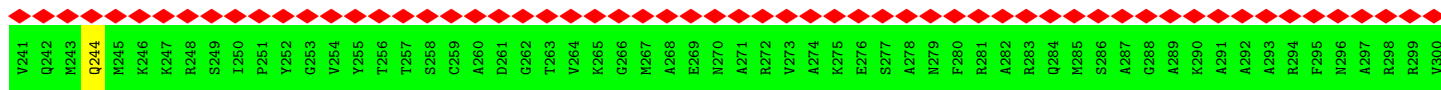


MET	ALA	ALA	PHE	VAL	VAL	GLY	ALA	GLN	VAL	SER	GLY	PHE	MET	GLY	CYS	ALA	ALA	PRO	ARG	THR	LYS	ARG	LYS	ALA	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

LYS	LEU	LEU	ASN	THR	VAL	LYS	PRO	MET	LYS	ARG	GLN	VAL	GLN	PRO	ASN	PRO	THR	THR	ASN	GLU	GLY	THR	ALA	ARG	SER	PRO	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

D121	F122	M123	A124	R125	S126	I127	A128	M129	Q130	A131	K132	A133	S134	A135	A136	S138	G139	LEU	LEU	GLY	THR	PHE	ALA	ARG	SER	PRO	ALA	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	LYS	LYS	TYR	GLN	THR	THR	ASN	THR	SER	THR	SER	THR	SER	LYS	LYS	TRP	ASP
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

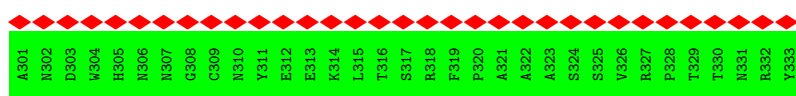
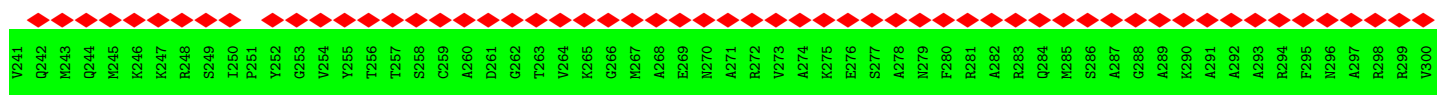
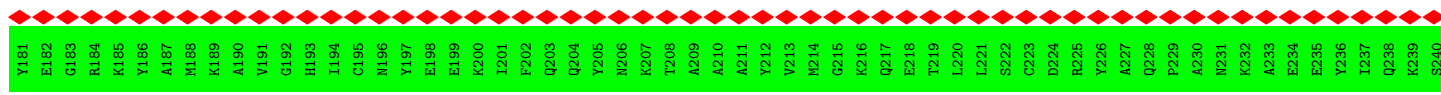
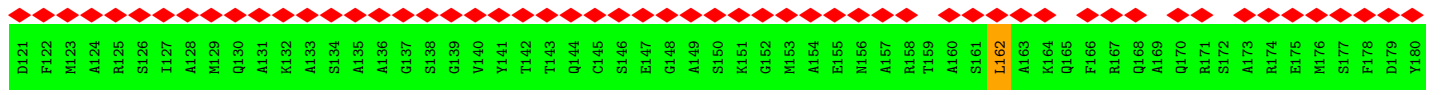
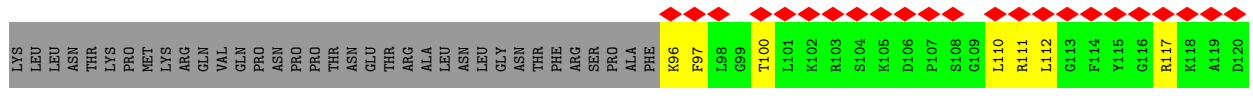
Y181	E182	G183	R184	K185	Y186	A187	M188	K189	A190	V191	G192	H193	I194	C195	N196	Y197	S198	C199	E200	K201	F202	Q203	Q204	Y205	N206	K207	T208	A209	A210	A211	Y212	V213	M214	G215	K216	Q217	E218	T219	L220	L221	S222	C223	D224	M225	Y226	A227	Q228	P229	A230	N231	K232	A233	E234	E235	Y236	I237	Q238	K239	S240
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------



• Molecule 3: LR7



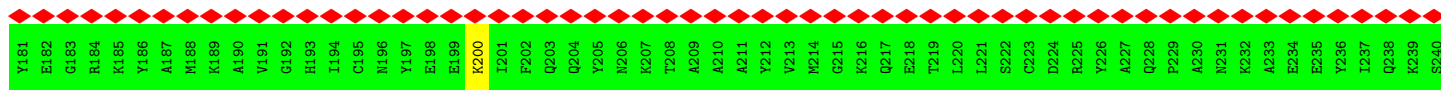
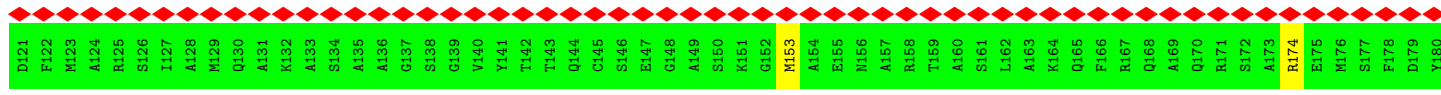
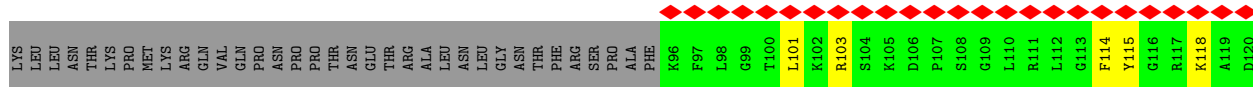
MET	ALA	VAL	VAL	ALA	VAL	GLN	SER	GLY	PHE	MET	GLY	CYS	ALA	ALA	PRO	ARG	THR	GLN	GLY	ALA	ALA	LYS	ALA	ALA	VAL	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	THR	THR	SER	SER	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

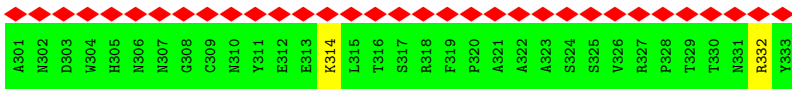
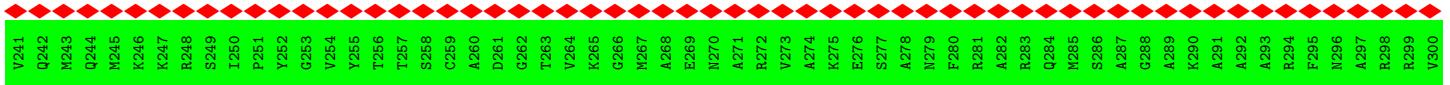


• Molecule 3: LR7

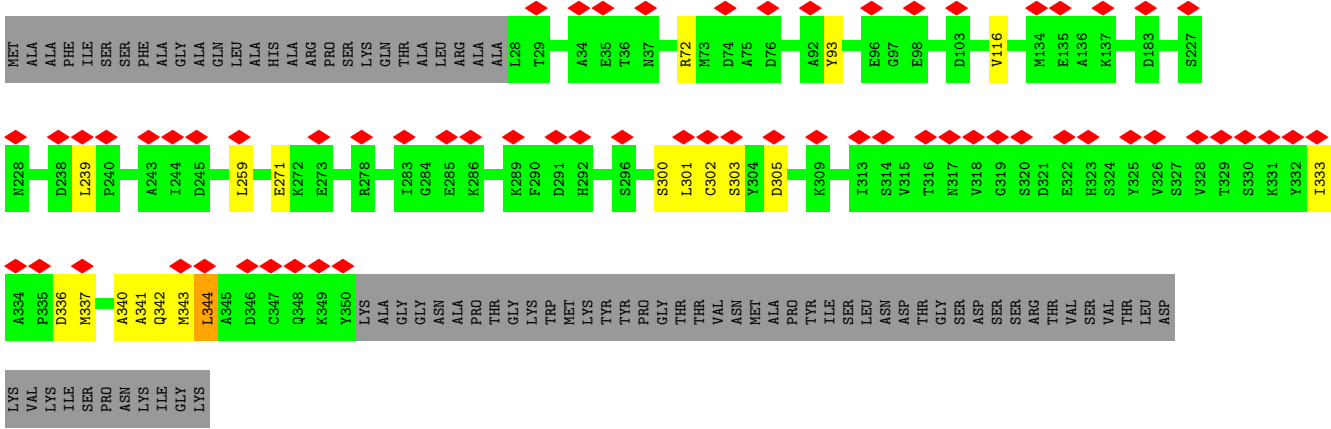
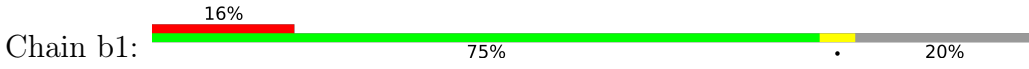


MET	ALA	ALA	VAL	VAL	ALA	VAL	SER	GLY	PHE	MET	GLY	CYS	ALA	ALA	PRO	ARG	THR	GLN	GLY	ALA	ALA	LYS	ALA	ALA	VAL	VAL	SER	MET	ARG	ILE	ILE	ILE	GLN	ASP	LYS	ASN	SER	TYR	TYR	LYS	LYS	TYR	GLN	THR	THR	THR	SER	SER	LYS	TRP	ASP
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

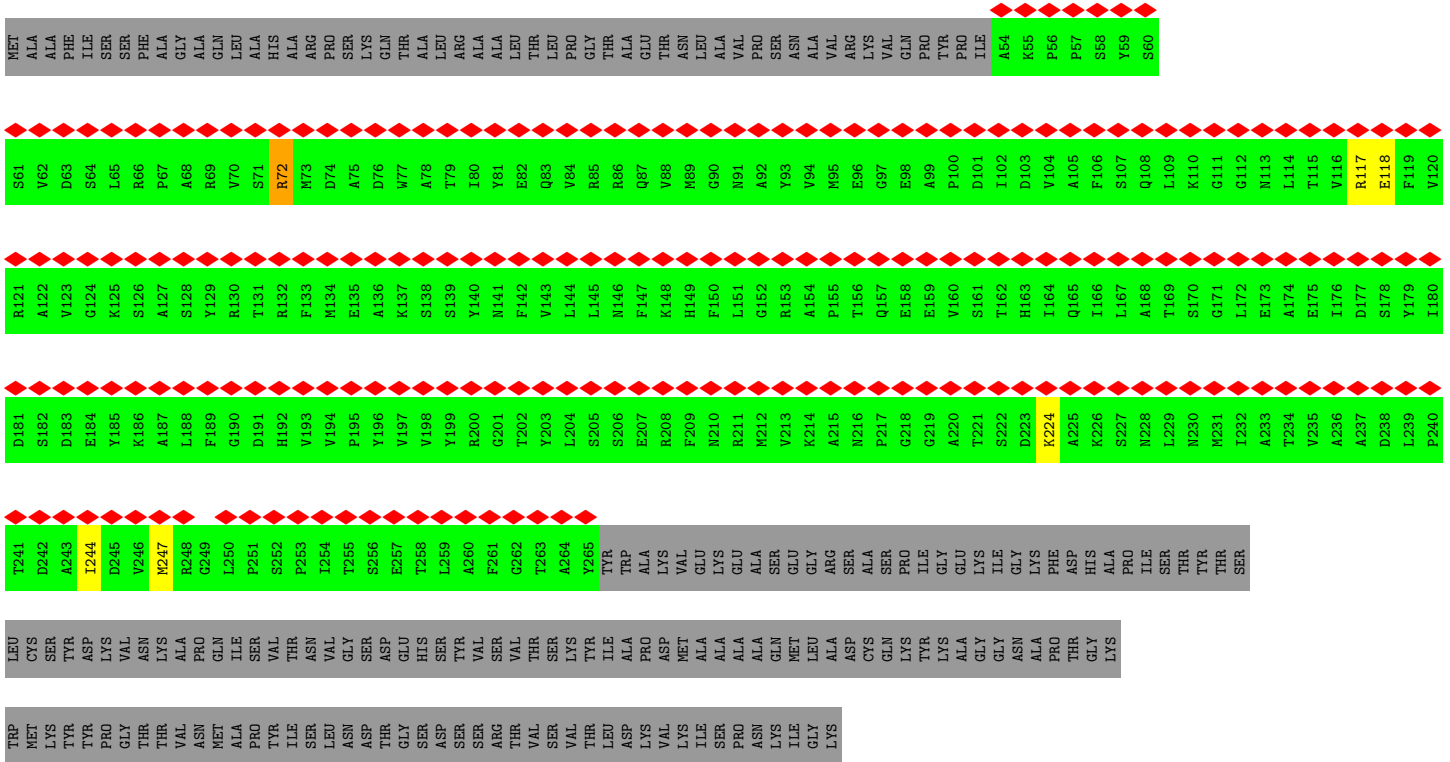




• Molecule 4: LR2_Hb

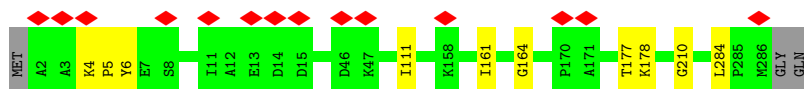


• Molecule 4: LR2_Hb

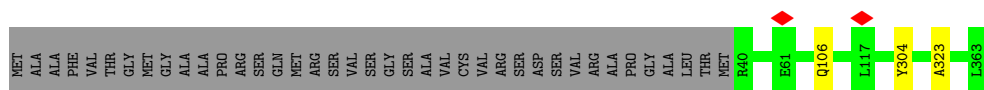
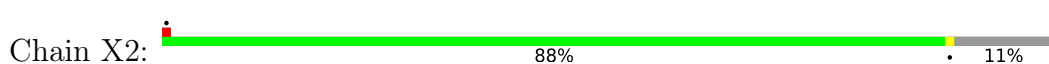




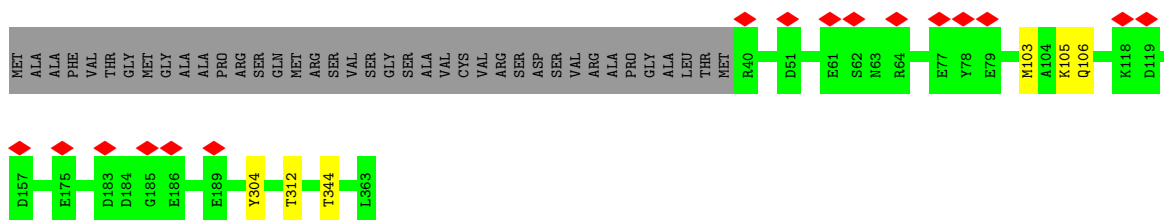
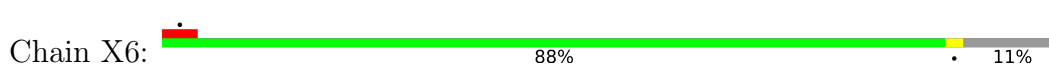
• Molecule 5: LR9



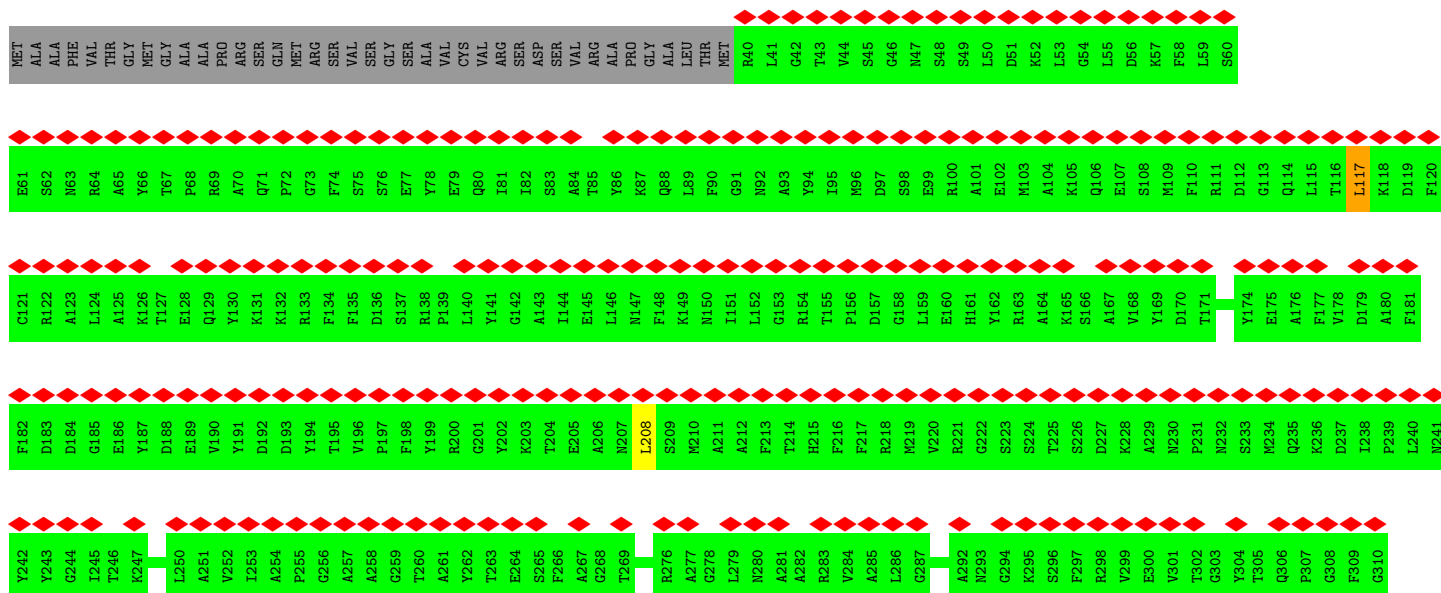
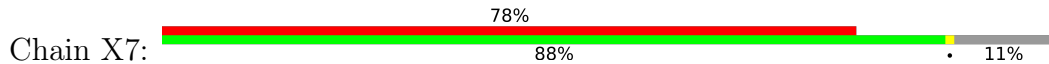
• Molecule 6: LR1

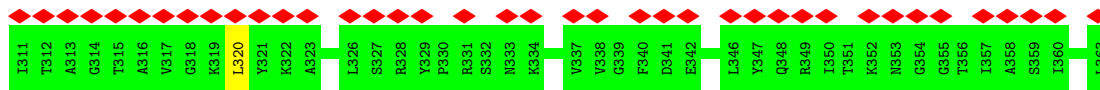


• Molecule 6: LR1

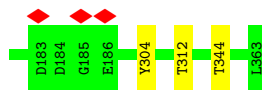
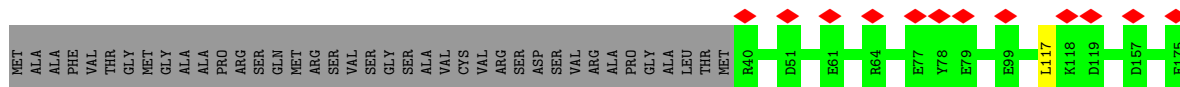
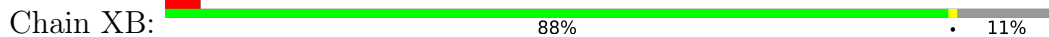


• Molecule 6: LR1

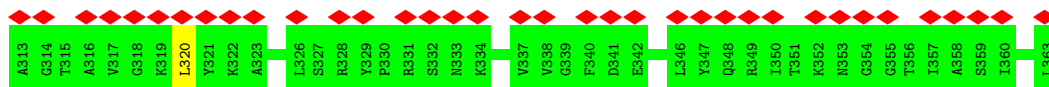
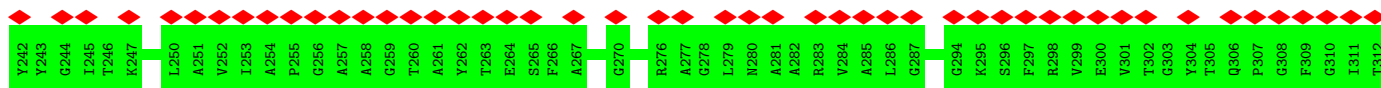
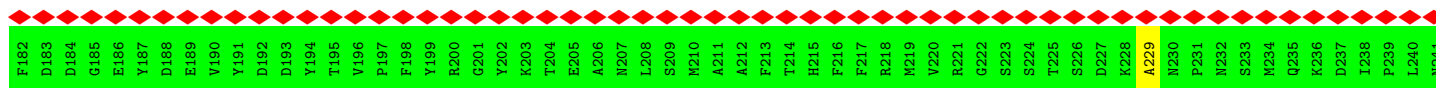
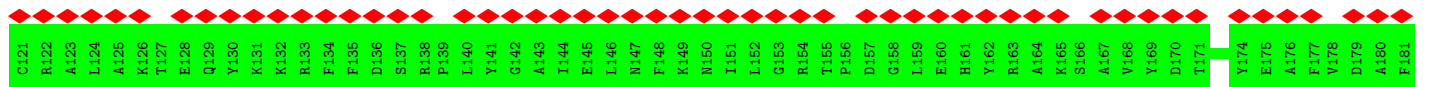
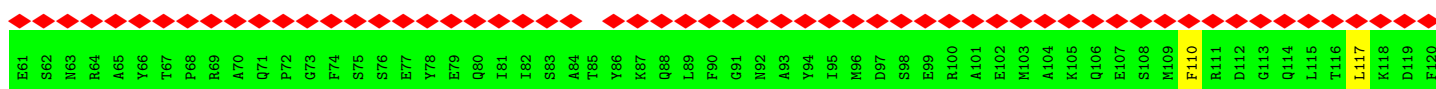
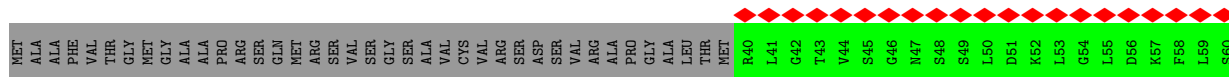
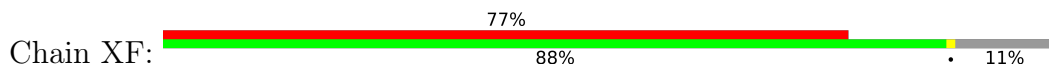




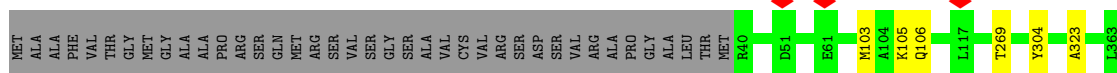
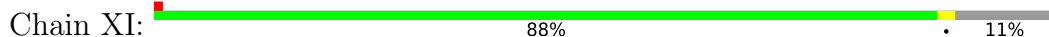
• Molecule 6: LR1



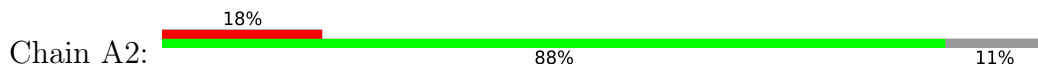
• Molecule 6: LR1

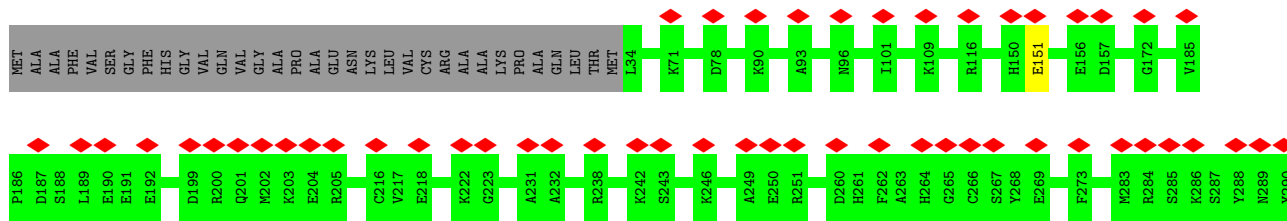


• Molecule 6: LR1

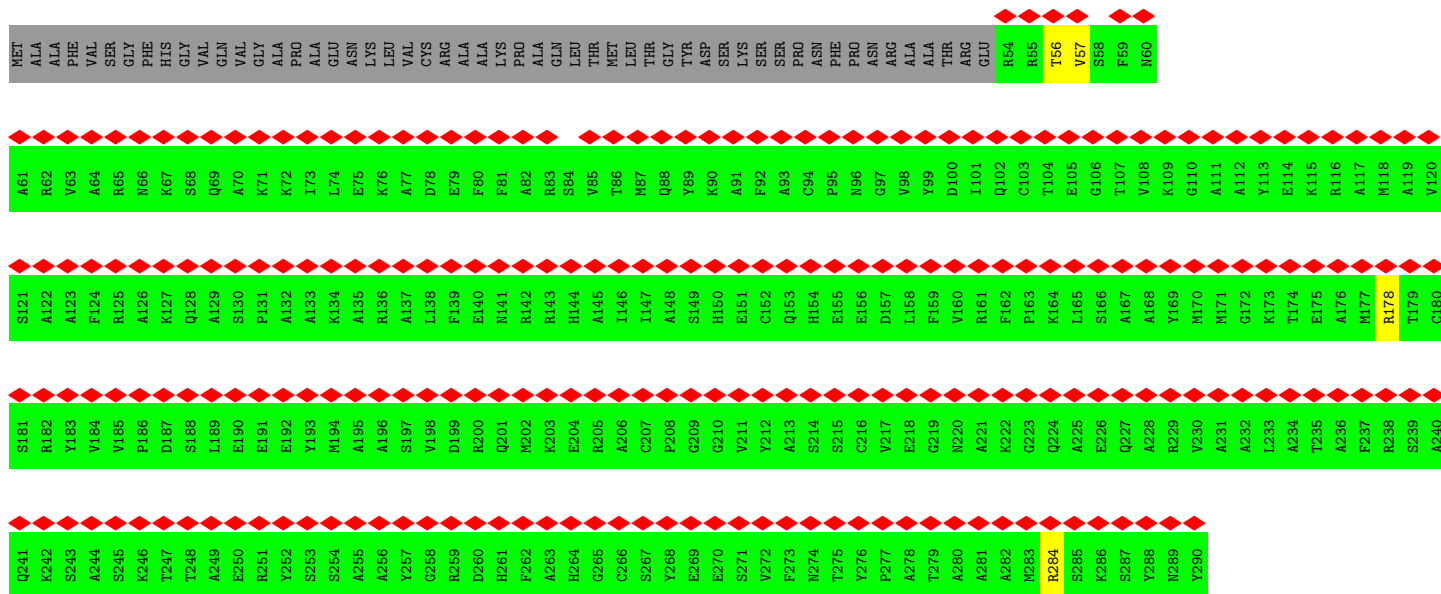
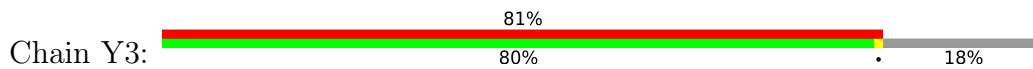


• Molecule 7: LR4

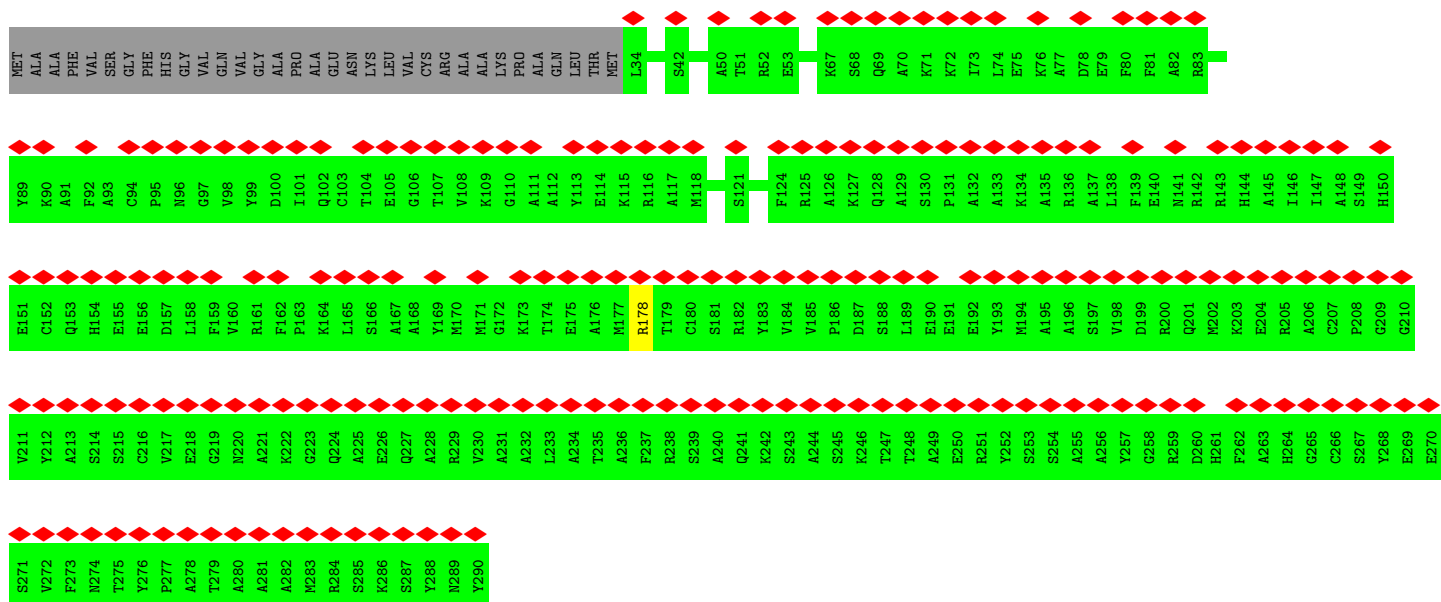
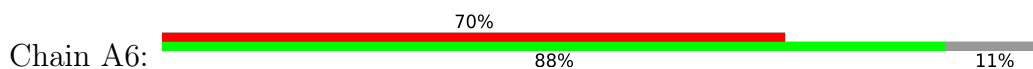




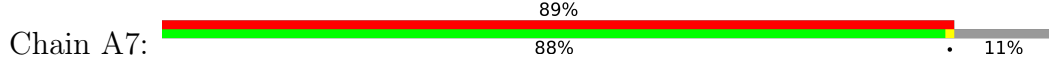
• Molecule 7: LR4



• Molecule 7: LR4

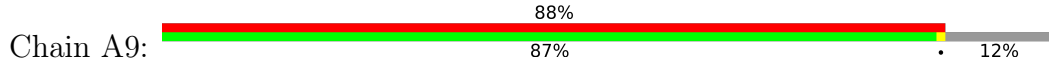


• Molecule 7: LR4



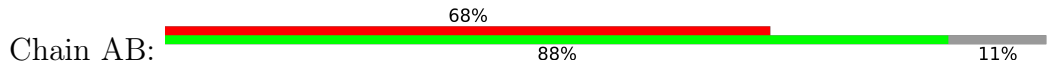
MET	ALA	ALA	PHE	VAL	SER	GLY	PHE	HIS	GLY	VAL	GLN	VAL	GLY	ALA	PRO	GLU	ASN	LYS	VAL	CYS	ARG	ALA	ALA	LYS	PRO	ALA	GLN	LEU	THR	MET	L34	T35	G36	Y37	D38	S39	K40	S41	S42	P43	N44	F45	P46	N47	R48	A49	A50	T51	R52	E53	R54	R55	T56	V57	S58	F59	N60		
A61	R62	V63	A64	R65	N66	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83	S84	W85	T86	M87	Q88	R89	K90	A91	F92	A93	C94	P95	N96	G97	D98	V99	D100	I101	Q102	C103	T104	E105	G106	T107	V108	K109	G110	A111	A112	Y113	E114	K115	R116	A117	M118	A119	V120
S121	A122	F124	F124	V125	A126	K127	Q128	L129	S130	P131	A132	K134	A135	R136	A137	L138	F139	E140	M141	R142	R143	H144	A145	I146	I147	A148	S149	H150	E151	C152	Q153	H154	E155	E156	D157	L158	F159	V160	R161	F162	P163	K164	L165	S166	A167	A168	V169	M170	M171	G172	K173	T174	E175	A236	M177	R178	T179	C180	
S181	R182	Y183	V184	V185	P186	D187	S188	L189	E190	E191	E192	M194	A195	A196	S197	V198	D199	R200	Q201	M202	K203	E204	R205	A206	C207	P208	G209	G210	V211	Y212	A213	S214	S215	C216	V217	E218	G219	N220	A221	K222	G223	Q224	A225	E226	Q227	A228	R229	V230	A231	A232	L233	A234	T235	A236	F237	R238	S239	A240	
Q241	K242	S243	A244	S245	K246	T247	T248	A249	E250	R251	Y252	S253	S254	A255	A256	Y257	G258	R259	D260	H261	F262	A263	H264	G265	S267	Y268	E269	E270	S271	V272	F273	N274	T275	Y276	P277	A278	T279	A280	A281	A282	M283	R284	S285	K286	S287	Y288	N289	Y290											

• Molecule 7: LR4

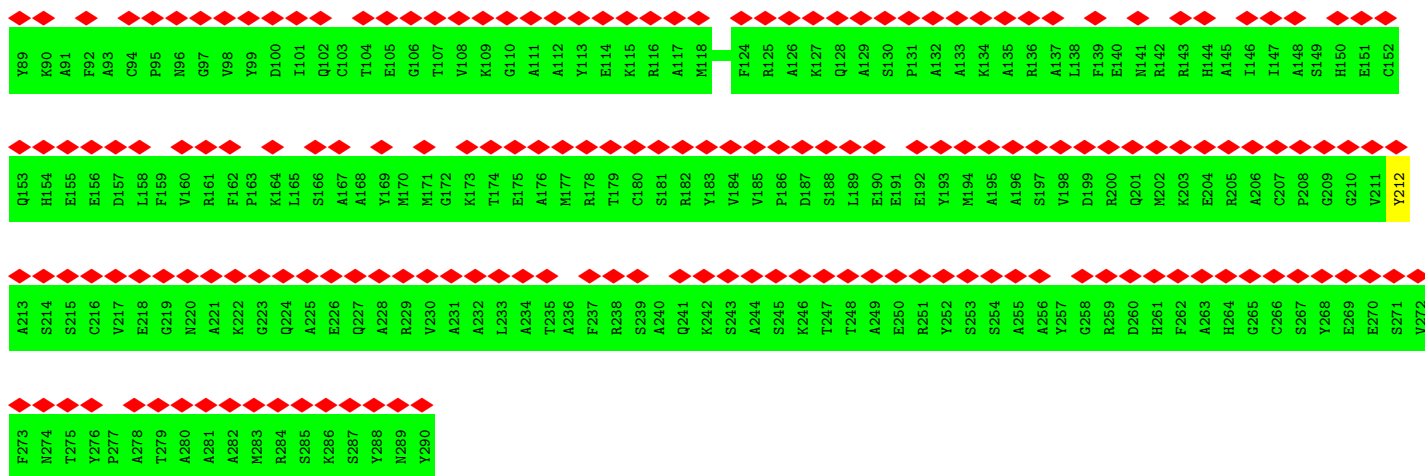


MET	ALA	ALA	PHE	VAL	SER	GLY	PHE	HIS	GLY	VAL	GLN	VAL	GLY	ALA	PRO	GLU	ASN	LYS	VAL	CYS	ARG	ALA	ALA	LYS	PRO	ALA	GLN	LEU	THR	MET	LEU	T35	G36	Y37	D38	S39	K40	S41	S42	P43	N44	F45	P46	N47	R48	A49	A50	T51	R52	E53	R54	R55	T56	V57	S58	F59	N60		
A61	R62	V63	A64	R65	N66	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83	S84	W85	T86	M87	Q88	R89	K90	A91	F92	A93	C94	P95	N96	G97	D98	V99	D100	I101	Q102	C103	T104	E105	G106	T107	V108	K109	G110	A111	A112	Y113	E114	K115	R116	A117	M118	A119	V120
S121	A122	F124	F124	V125	A126	K127	Q128	L129	S130	P131	A132	K134	A135	R136	A137	L138	F139	E140	M141	R142	R143	H144	A145	I146	I147	A148	S149	H150	E151	C152	Q153	H154	E155	E156	D157	L158	F159	V160	R161	F162	P163	K164	L165	S166	A167	A168	V169	M170	M171	G172	K173	T174	E175	A176	M177	R178	T179	C180	
S181	R182	Y183	V184	V185	P186	D187	S188	L189	E190	E191	E192	M194	A195	A196	S197	V198	D199	R200	Q201	M202	K203	E204	R205	A206	C207	P208	G209	G210	V211	Y212	A213	S214	S215	C216	V217	E218	G219	N220	A221	K222	G223	Q224	A225	E226	Q227	A228	R229	V230	A231	A232	L233	A234	T235	A236	F237	R238	S239	A240	
Q241	K242	S243	A244	S245	K246	T247	T248	A249	E250	R251	Y252	S253	S254	A255	A256	Y257	G258	R259	D260	H261	F262	A263	H264	G265	S267	Y268	E269	E270	S271	V272	F273	N274	T275	Y276	P277	A278	T279	A280	A281	A282	M283	R284	S285	K286	S287	Y288	N289	Y290											

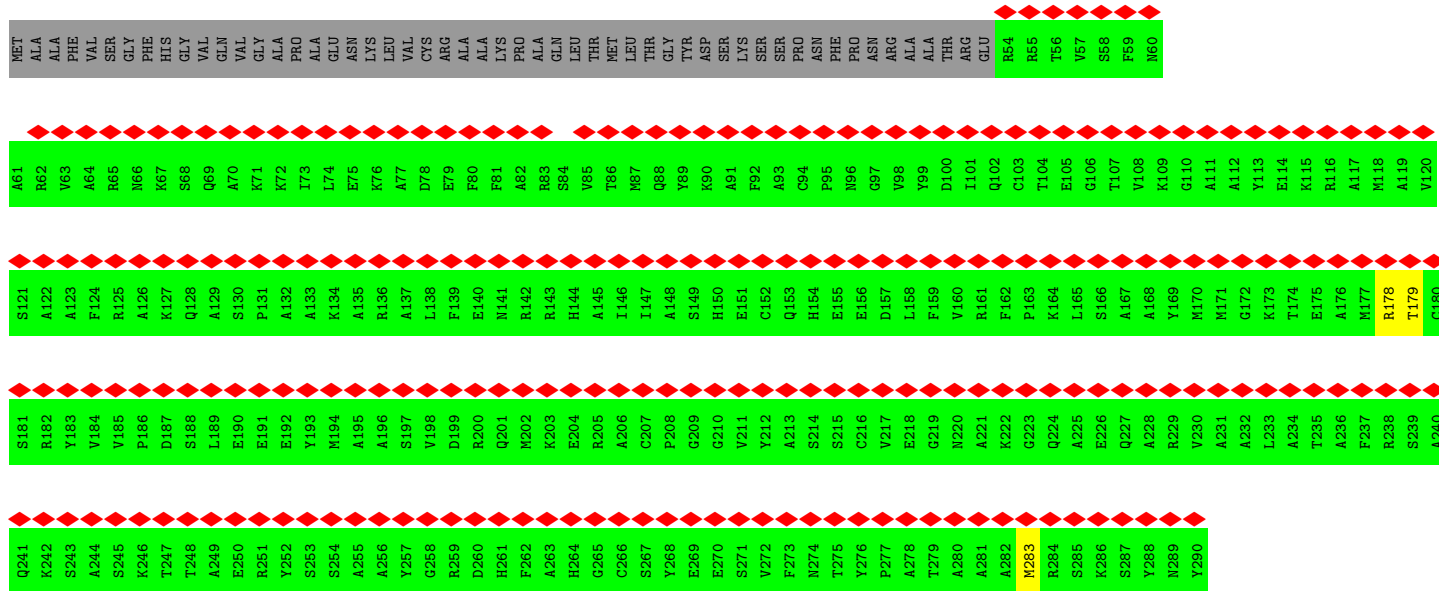
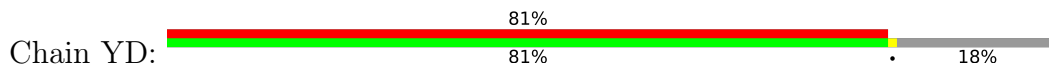
• Molecule 7: LR4



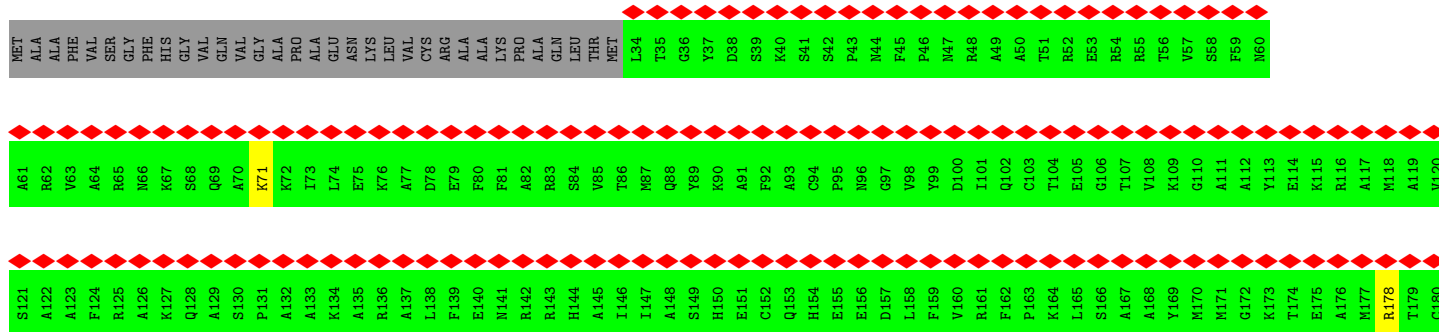
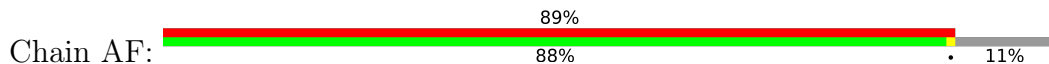
MET	ALA	ALA	PHE	VAL	SER	GLY	PHE	HIS	GLY	VAL	GLN	VAL	GLY	ALA	PRO	GLU	ASN	LYS	VAL	CYS	ARG	ALA	ALA	LYS	PRO	ALA	GLN	LEU	THR	MET	L34	D38	S42	R52	E53	K67	S68	Q69	A70	K71	K72	I73	L74	E75	K76	A77	D78	E79	F80	F81	A82	R83
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

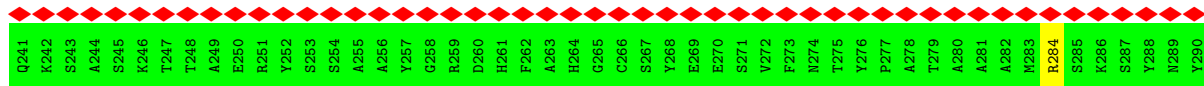
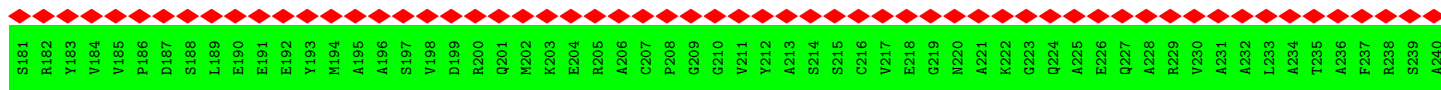


• Molecule 7: LR4

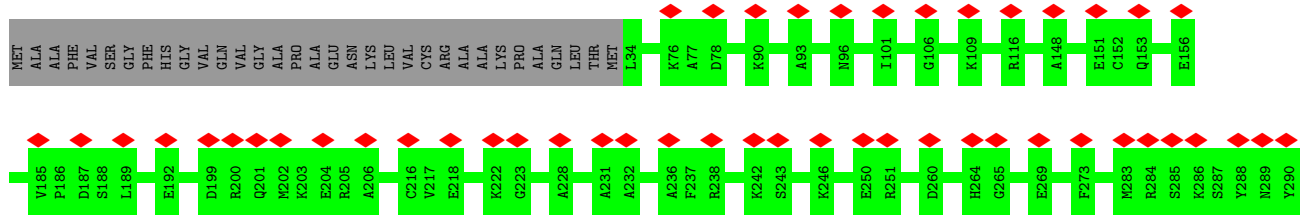
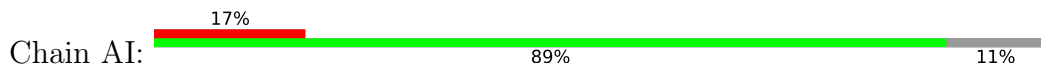


• Molecule 7: LR4

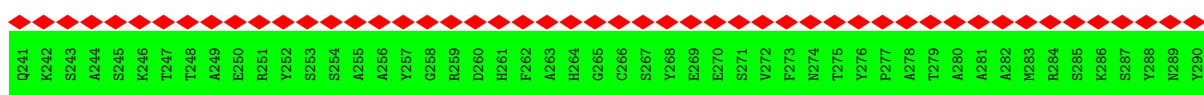
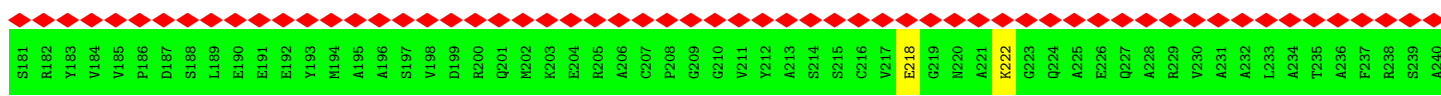
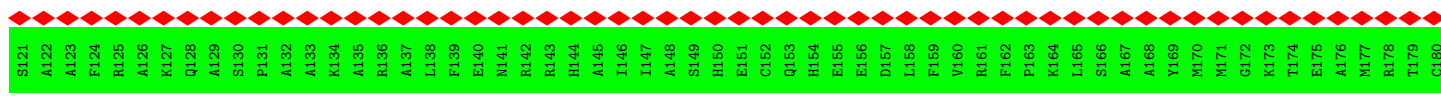
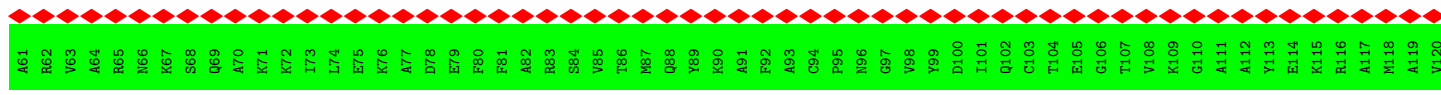
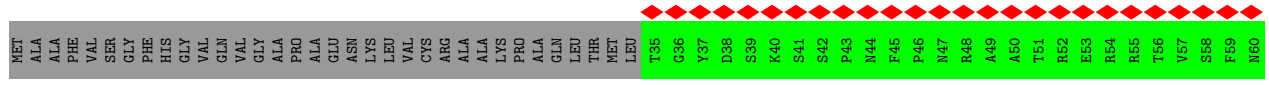
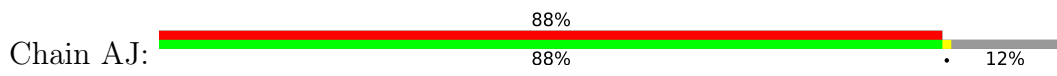




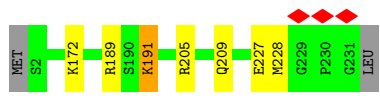
• Molecule 7: LR4



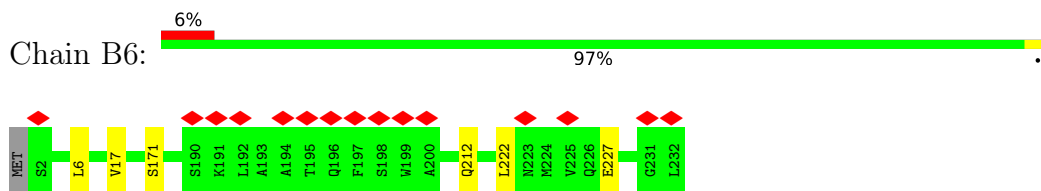
• Molecule 7: LR4



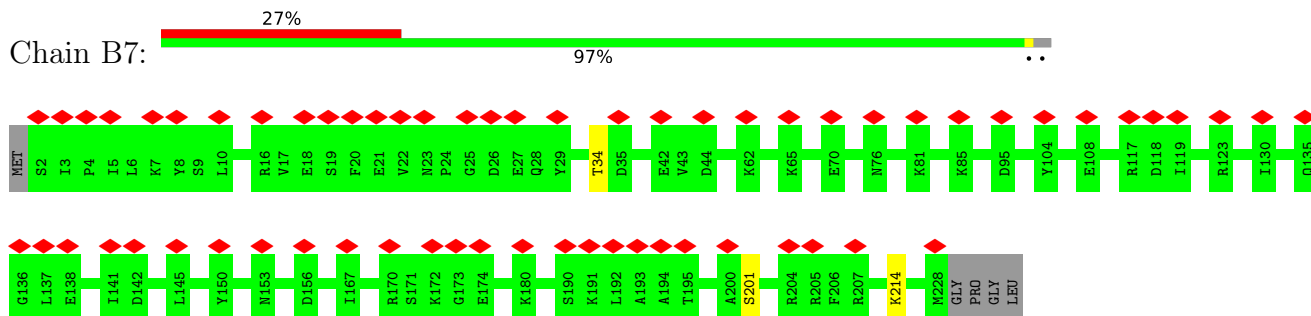
• Molecule 8: Phycobilisome rod-core linker polypeptide



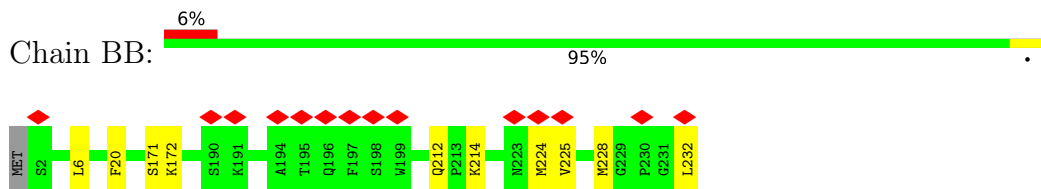
• Molecule 8: Phycobilisome rod-core linker polypeptide



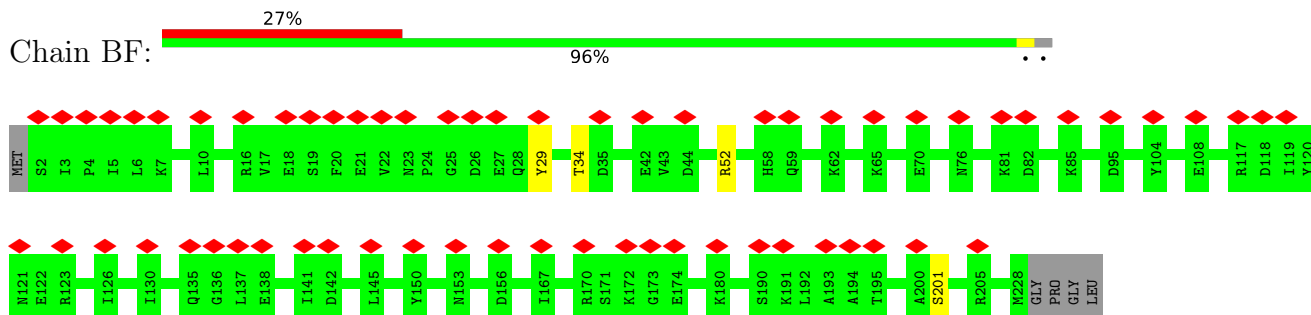
- Molecule 8: Phycobilisome rod-core linker polypeptide



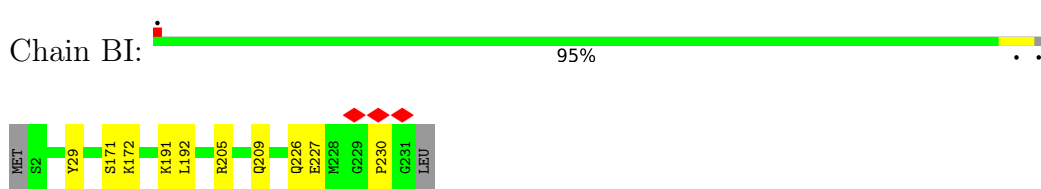
- Molecule 8: Phycobilisome rod-core linker polypeptide



- Molecule 8: Phycobilisome rod-core linker polypeptide



- Molecule 8: Phycobilisome rod-core linker polypeptide



- Molecule 9: C-phycoerythrin alpha subunit



There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain E2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain G2:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain I2:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain K2:  99%



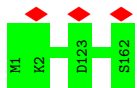
- Molecule 9: C-phyco cyanin alpha subunit

Chain M2:  99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain C6:  100%



- Molecule 9: C-phyco cyanin alpha subunit

Chain E6:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain G6:  100%

There are no outlier residues recorded for this chain.

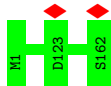
- Molecule 9: C-phyco cyanin alpha subunit

Chain I6:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain K6:  100%




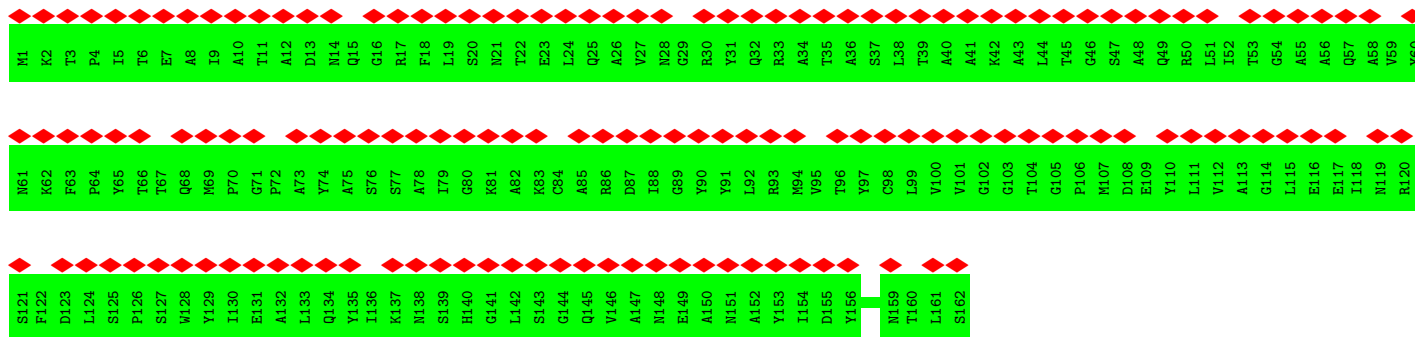
- Molecule 9: C-phycoerythrin alpha subunit

Chain M6:  100%

There are no outlier residues recorded for this chain.

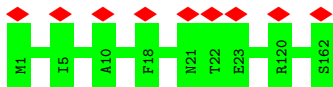
- Molecule 9: C-phycoerythrin alpha subunit

Chain C7:  91%
100%




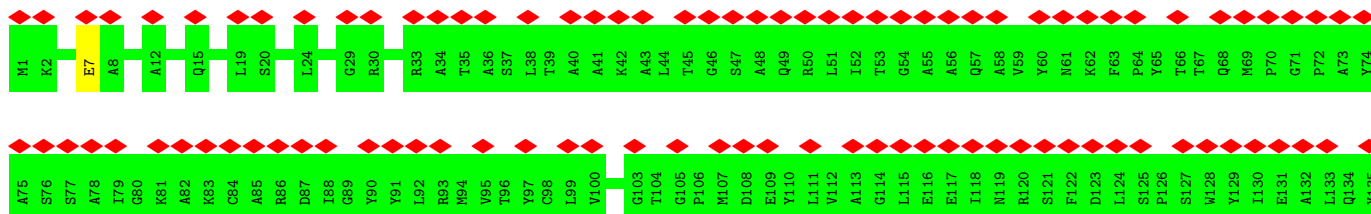
- Molecule 9: C-phycoerythrin alpha subunit

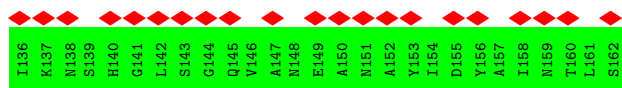
Chain E7:  6%
100%



- Molecule 9: C-phycoerythrin alpha subunit

Chain G7:  72%
99%

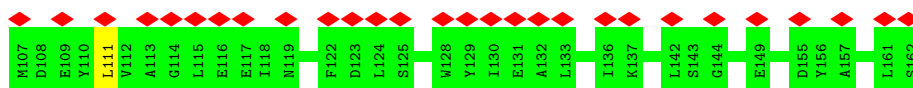
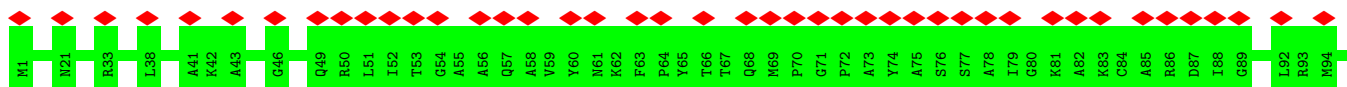




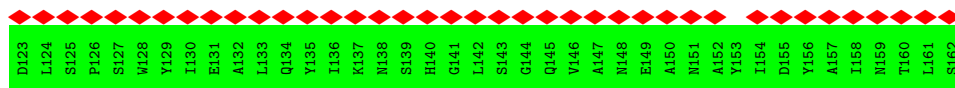
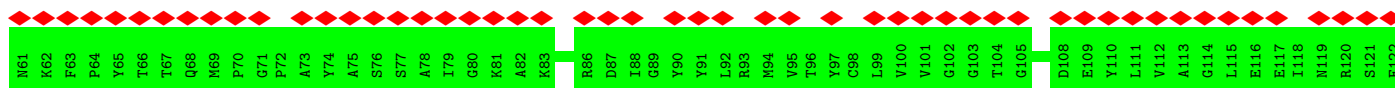
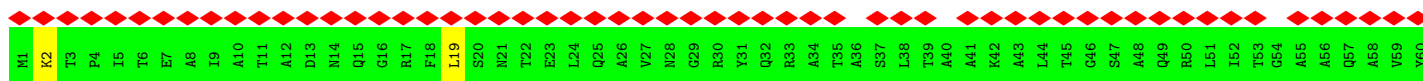
- Molecule 9: C-phycoerythrin alpha subunit



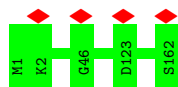
- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



- Molecule 9: C-phycoerythrin alpha subunit



There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain GB:  100%

There are no outlier residues recorded for this chain.

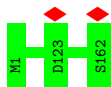
- Molecule 9: C-phycoerythrin alpha subunit

Chain IB:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phycoerythrin alpha subunit

Chain KB:  100%



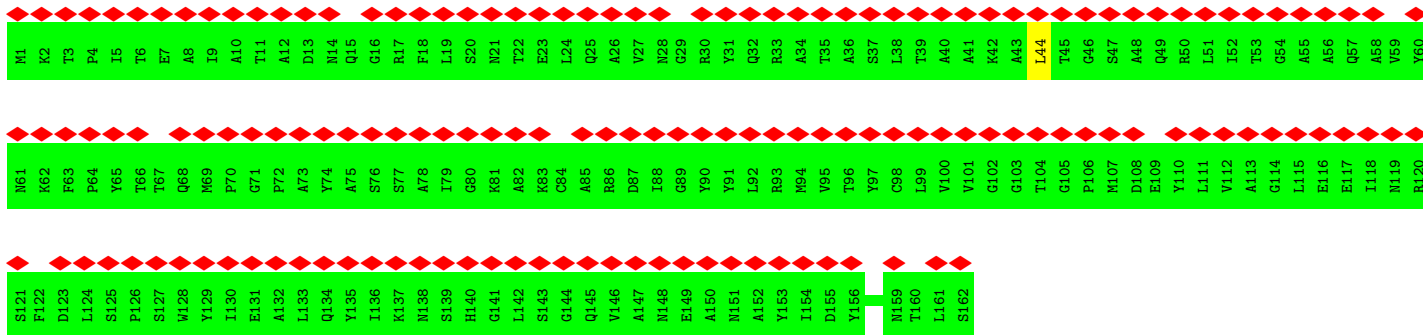
- Molecule 9: C-phycoerythrin alpha subunit

Chain MB:  100%

There are no outlier residues recorded for this chain.

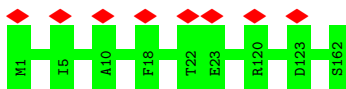
- Molecule 9: C-phycoerythrin alpha subunit

Chain CF:  94%
99%




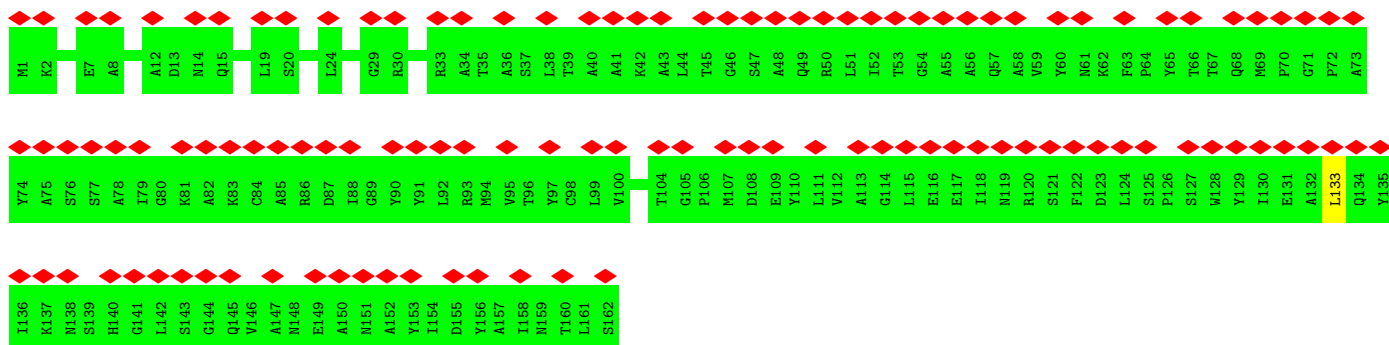
- Molecule 9: C-phycoerythrin alpha subunit

Chain EF:  5%
100%

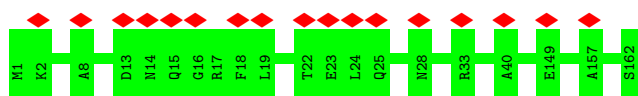


- Molecule 9: C-phycoerythrin alpha subunit

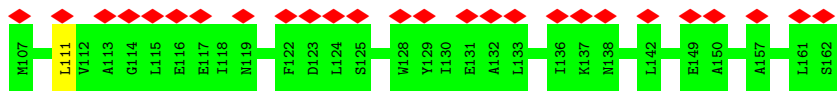
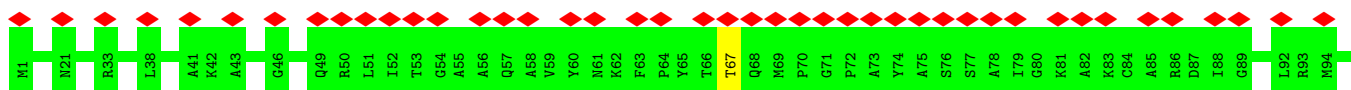
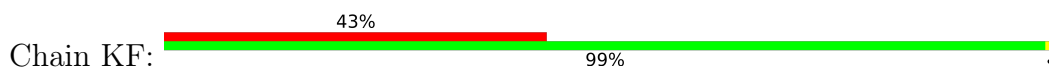
Chain GF:  71%
99%



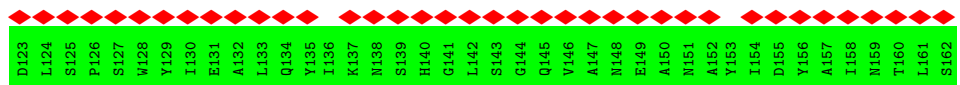
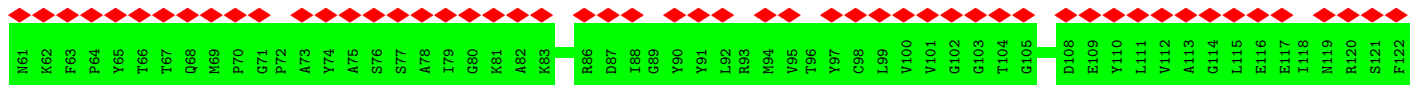
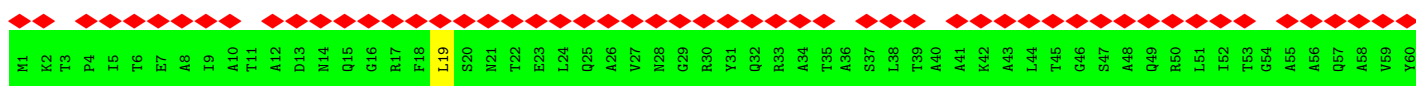
• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit



• Molecule 9: C-phycoyanin alpha subunit





- Molecule 9: C-phyco cyanin alpha subunit

Chain EI: 100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain GI: 99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain II: 100%

There are no outlier residues recorded for this chain.

- Molecule 9: C-phyco cyanin alpha subunit

Chain KI: 99%



- Molecule 9: C-phyco cyanin alpha subunit

Chain MI: 99%



- Molecule 10: C-phyco cyanin beta subunit

Chain D2: 99%



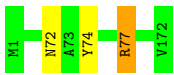
- Molecule 10: C-phyco cyanin beta subunit

Chain F2: 99%



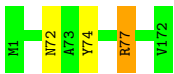
- Molecule 10: C-phyco cyanin beta subunit

Chain H2:  98% ..



● Molecule 10: C-phycocyanin beta subunit

Chain J2:  98% ..



● Molecule 10: C-phycocyanin beta subunit

Chain L2:  98% .



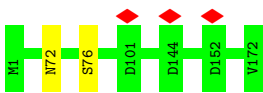
● Molecule 10: C-phycocyanin beta subunit

Chain N2:  98% .



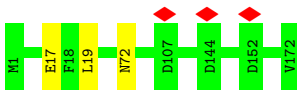
● Molecule 10: C-phycocyanin beta subunit

Chain D6:  99% .



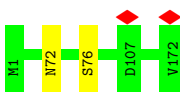
● Molecule 10: C-phycocyanin beta subunit

Chain F6:  98% .



● Molecule 10: C-phycocyanin beta subunit

Chain H6:  99% .



● Molecule 10: C-phycocyanin beta subunit

Chain J6:  97%



- Molecule 10: C-phyco cyanin beta subunit

Chain L6:  98%



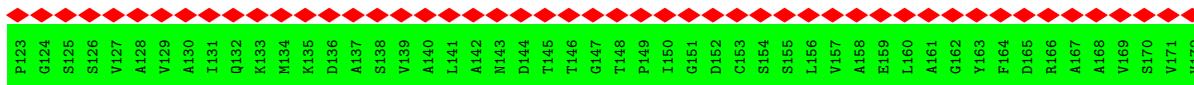
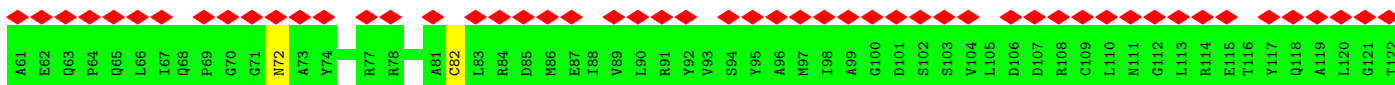
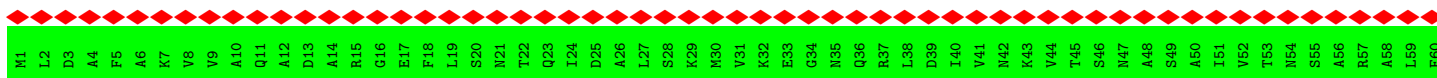
- Molecule 10: C-phyco cyanin beta subunit

Chain N6:  99%



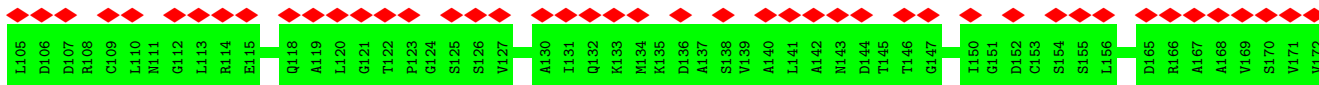
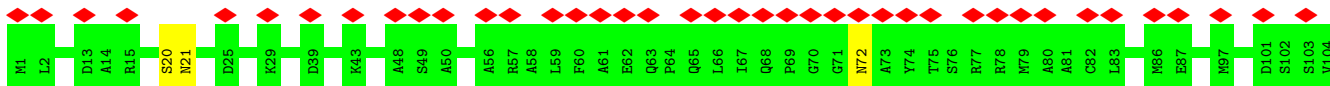
- Molecule 10: C-phyco cyanin beta subunit

Chain D7:  94%
99%



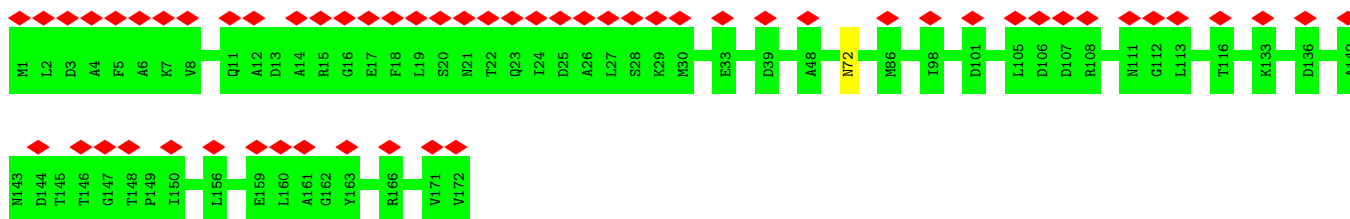
- Molecule 10: C-phyco cyanin beta subunit

Chain F7:  49%
98%

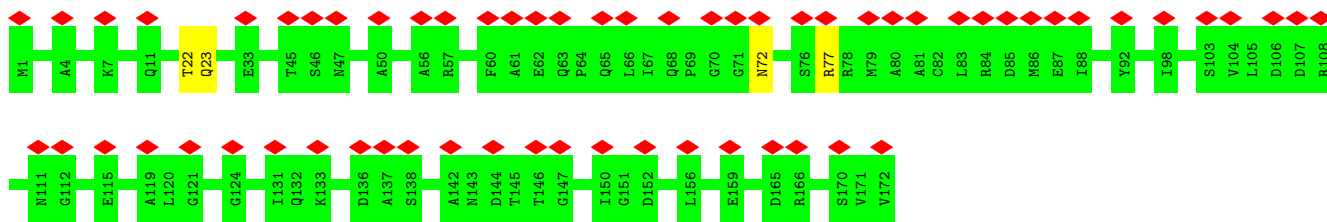


- Molecule 10: C-phyco cyanin beta subunit

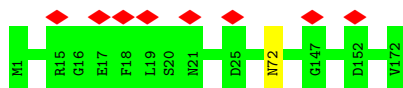
Chain H7:  33%
99%



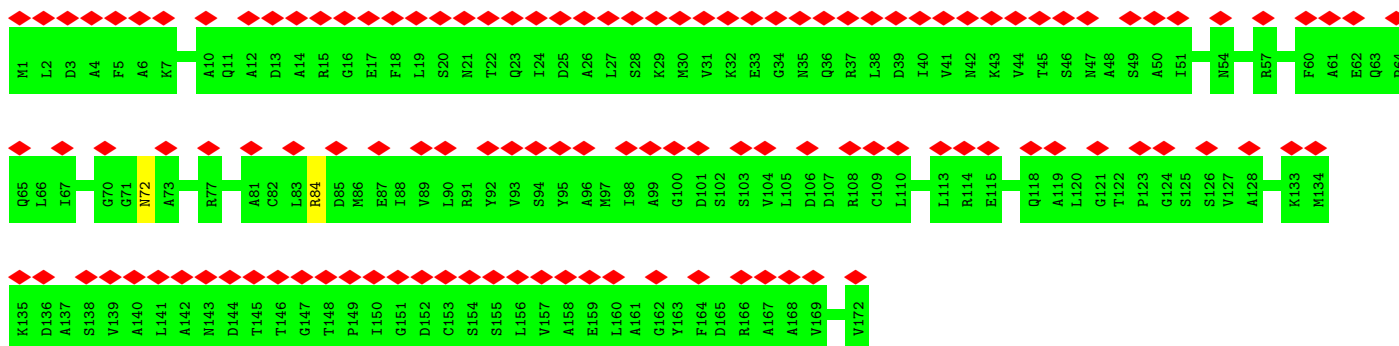
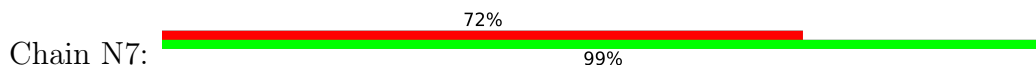
- Molecule 10: C-phycoerythrin beta subunit



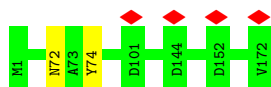
- Molecule 10: C-phycoerythrin beta subunit



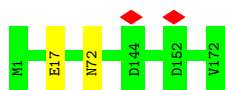
- Molecule 10: C-phycoerythrin beta subunit



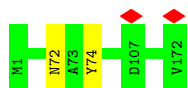
- Molecule 10: C-phycoerythrin beta subunit



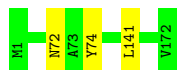
- Molecule 10: C-phycoerythrin beta subunit



• Molecule 10: C-phycoerythrin beta subunit



• Molecule 10: C-phycoerythrin beta subunit



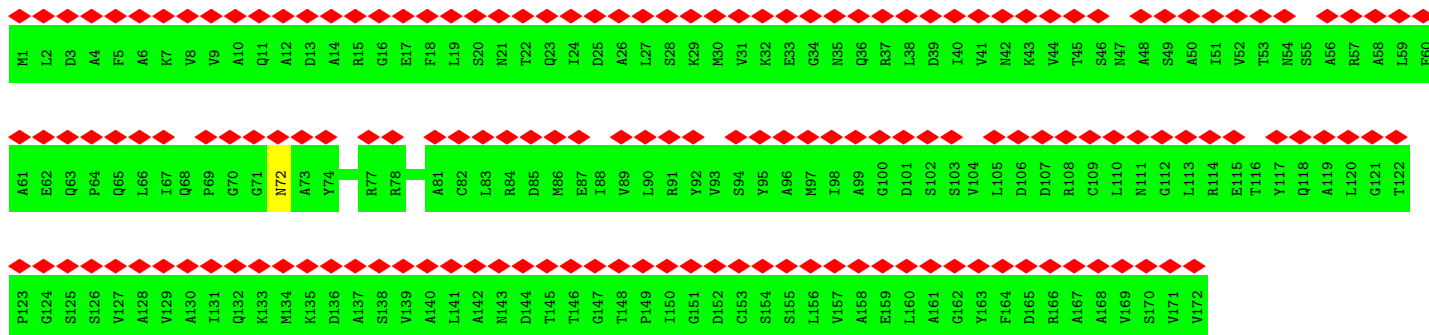
• Molecule 10: C-phycoerythrin beta subunit



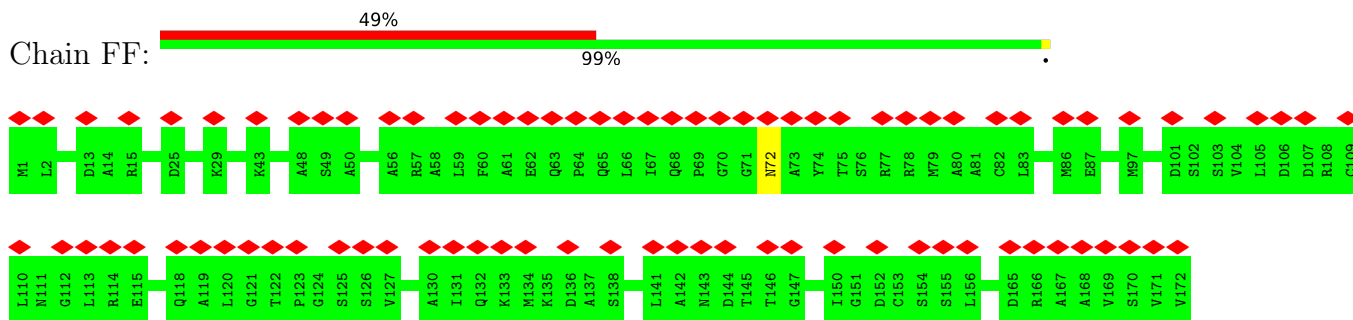
• Molecule 10: C-phycoerythrin beta subunit



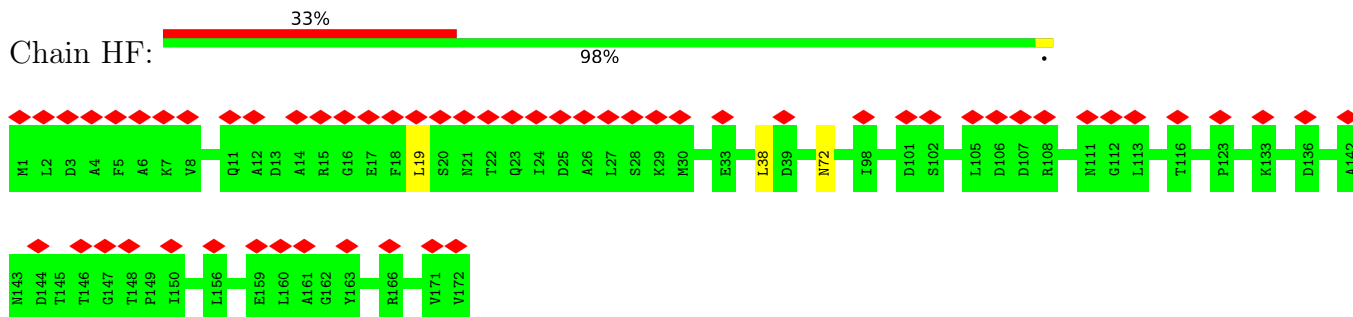
• Molecule 10: C-phycoerythrin beta subunit



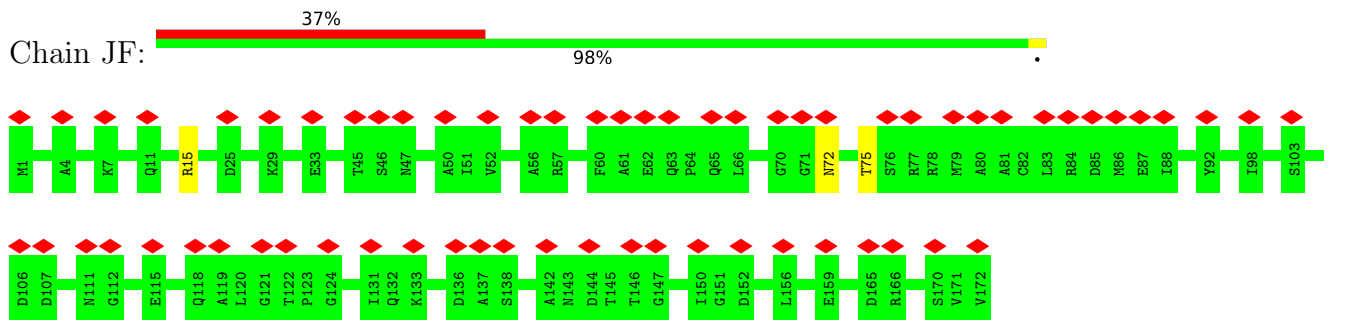
• Molecule 10: C-phycoerythrin beta subunit



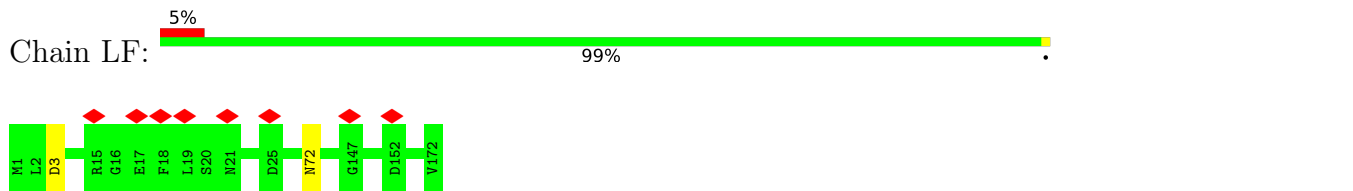
• Molecule 10: C-phycoyanin beta subunit



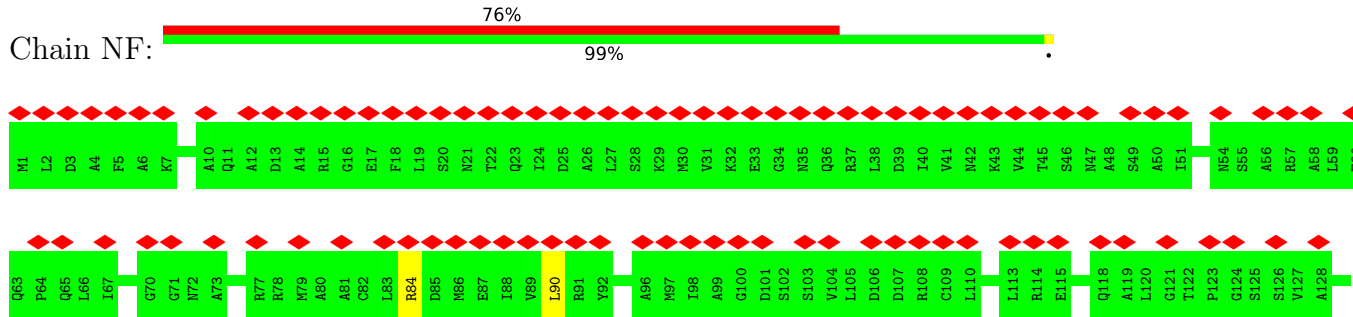
• Molecule 10: C-phycoyanin beta subunit

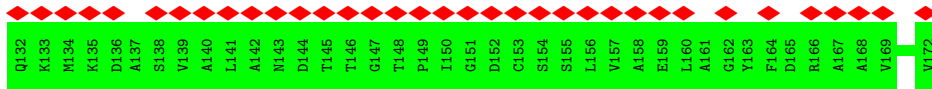


• Molecule 10: C-phycoyanin beta subunit



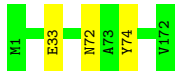
• Molecule 10: C-phycoyanin beta subunit





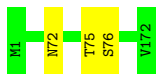
- Molecule 10: C-phycoerythrin beta subunit

Chain DI: 98%



- Molecule 10: C-phycoerythrin beta subunit

Chain FI: 98%



- Molecule 10: C-phycoerythrin beta subunit

Chain HI: 98%



- Molecule 10: C-phycoerythrin beta subunit

Chain JI: 99%



- Molecule 10: C-phycoerythrin beta subunit

Chain LI: 98%



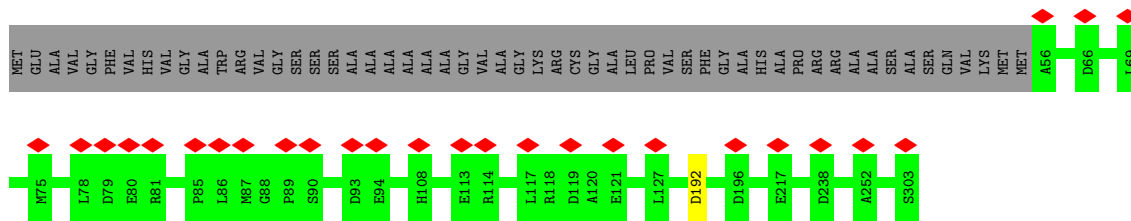
- Molecule 10: C-phycoerythrin beta subunit

Chain NI: 98%

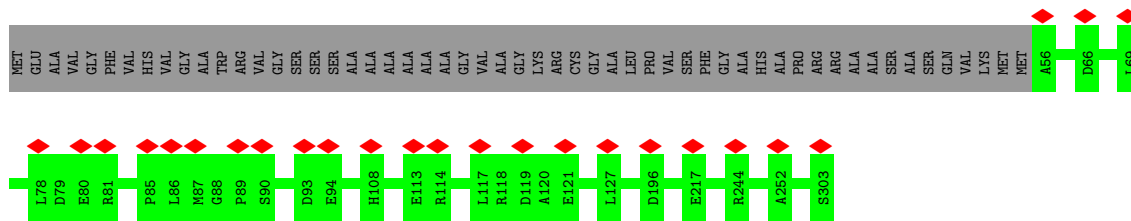
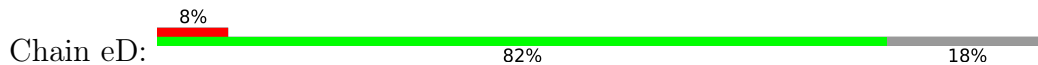


- Molecule 11: LR2

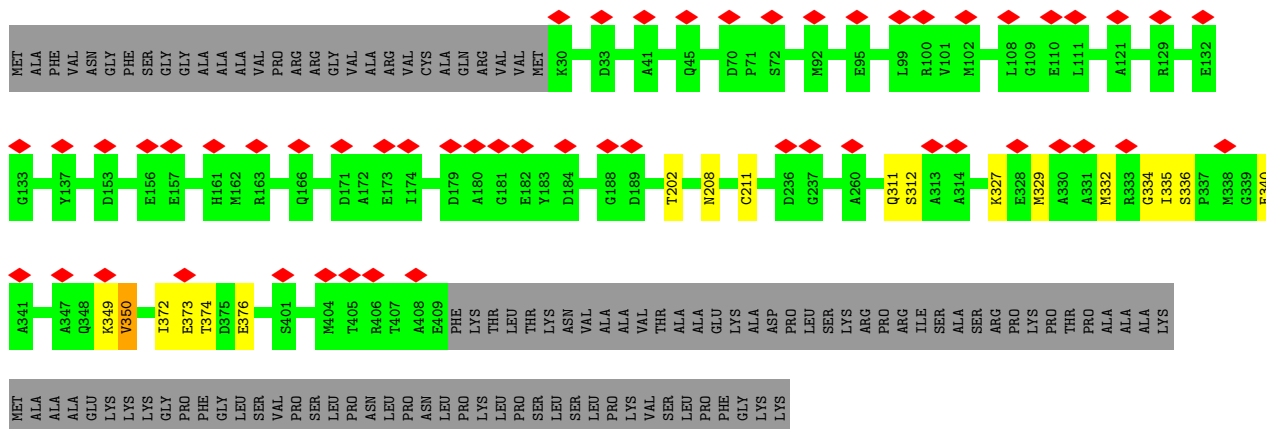
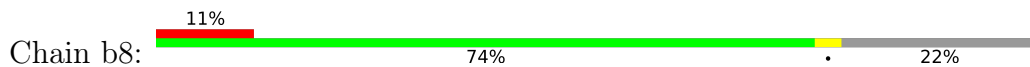
Chain e3: 9% 82% 18%



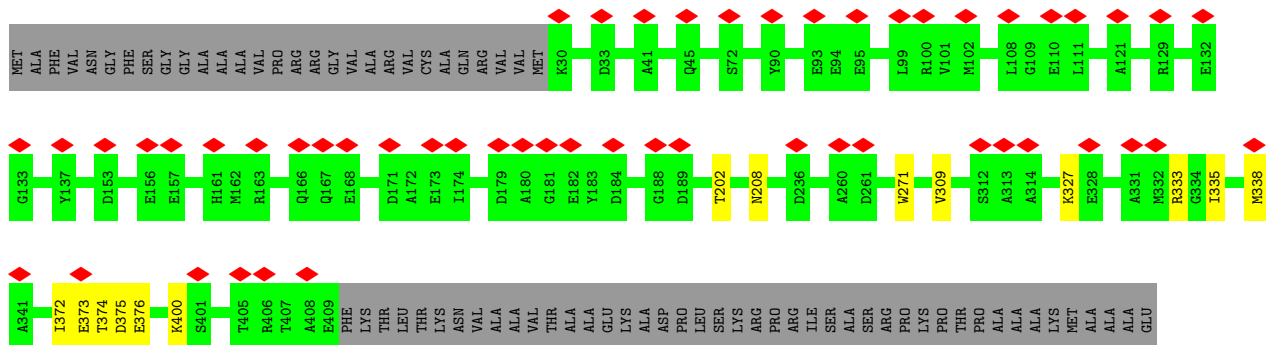
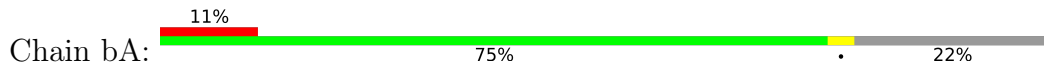
• Molecule 11: LR2

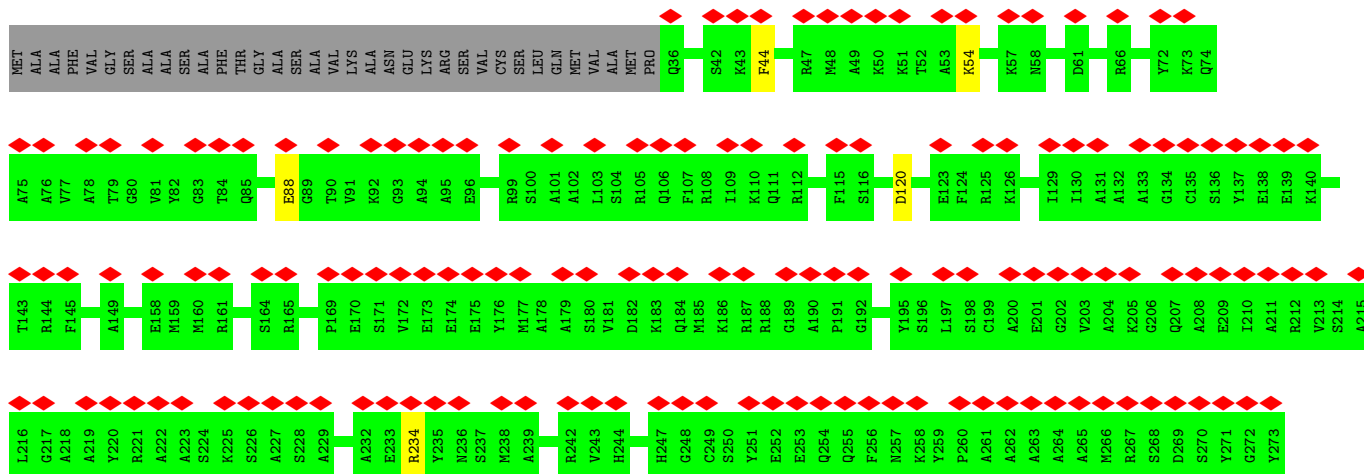


• Molecule 12: LRC2

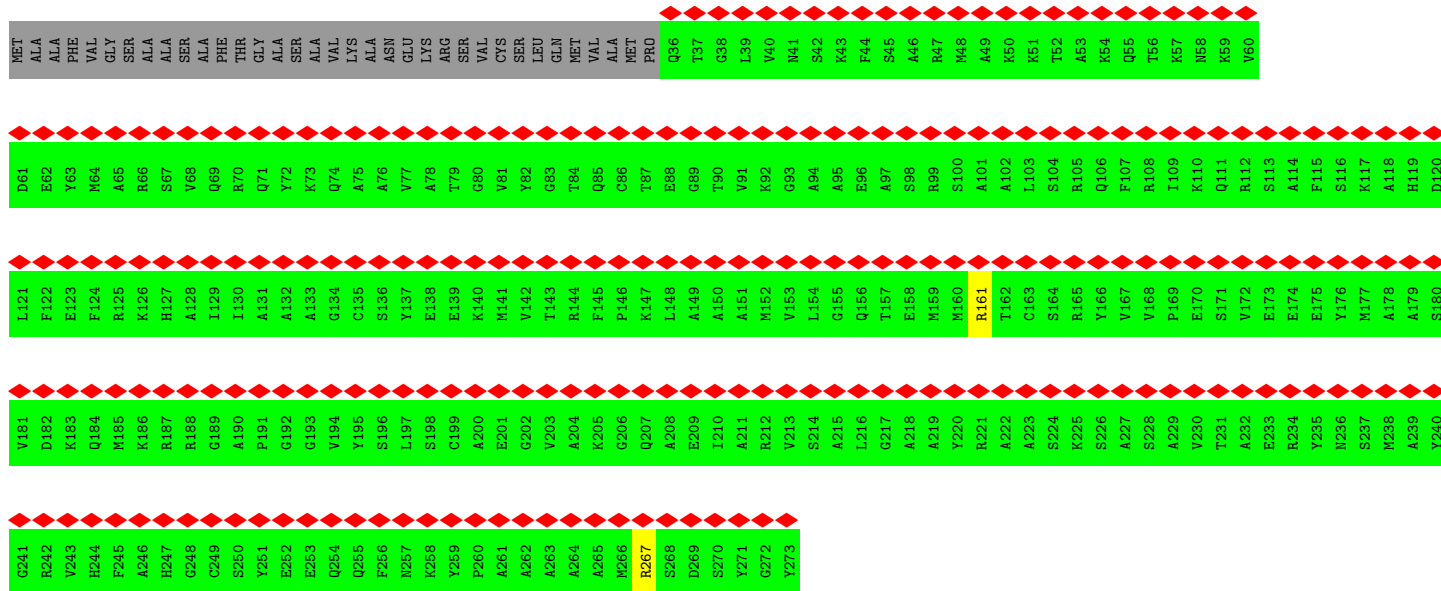
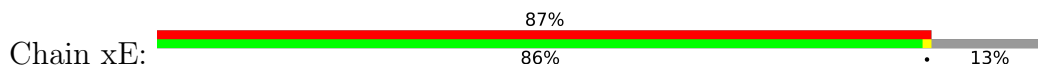


• Molecule 12: LRC2

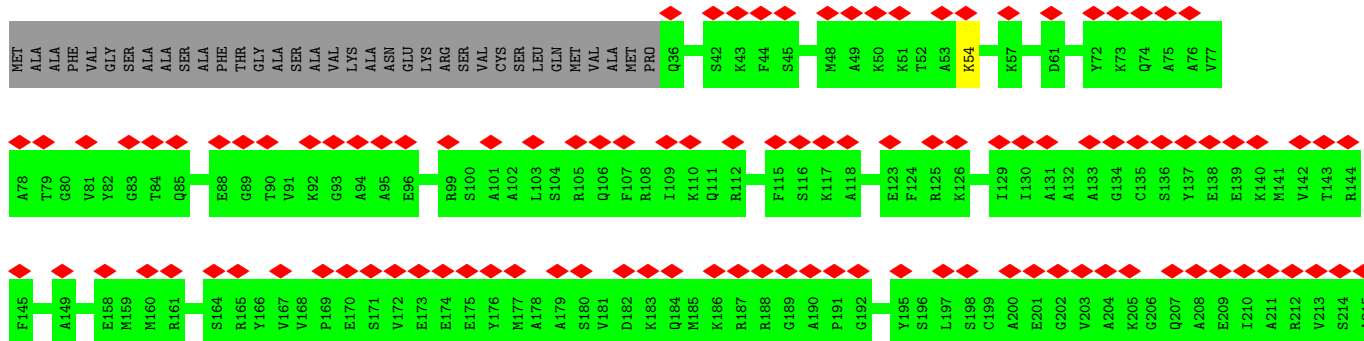


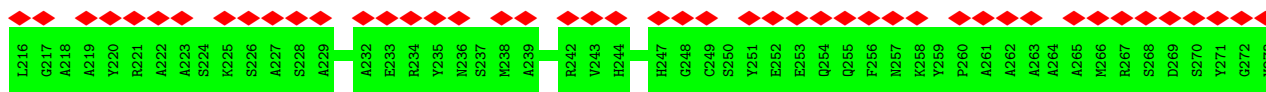


• Molecule 13: LR5

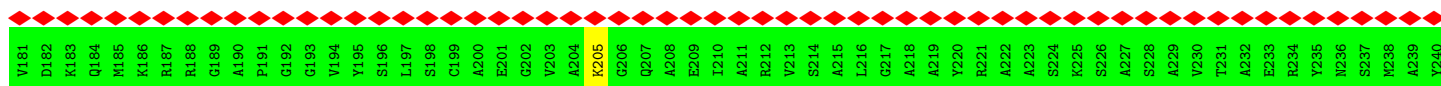
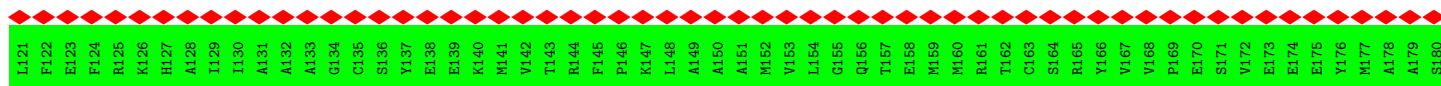
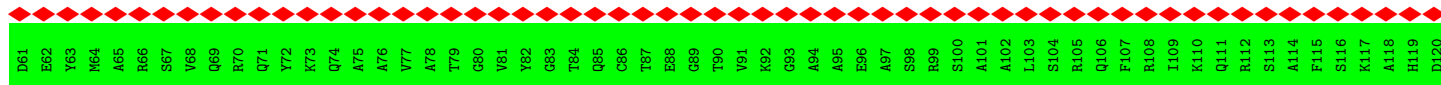
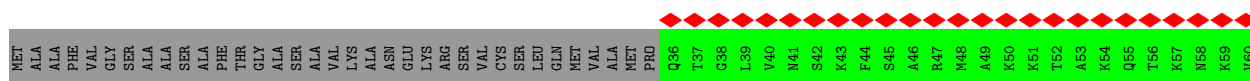
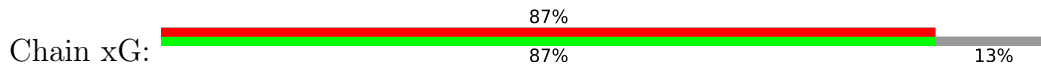


• Molecule 13: LR5

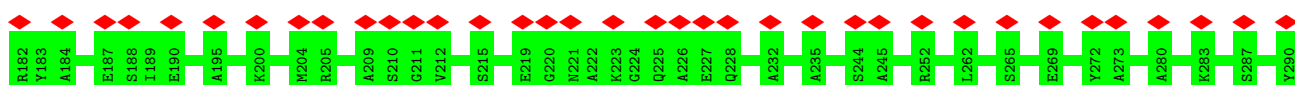
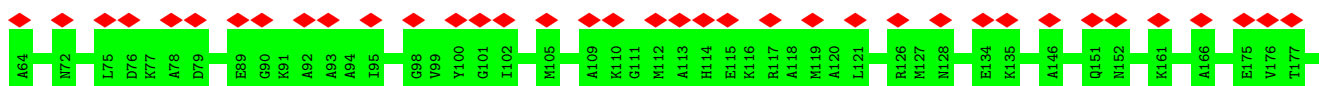
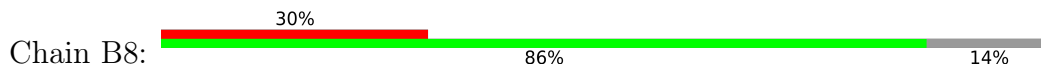




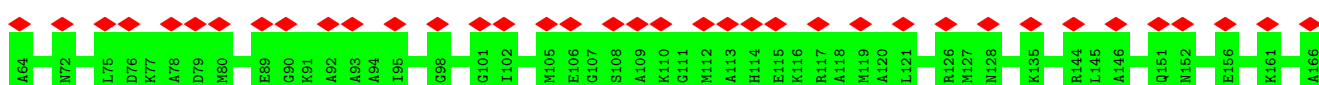
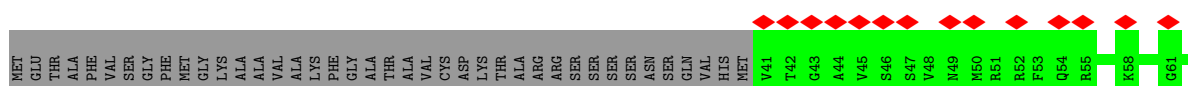
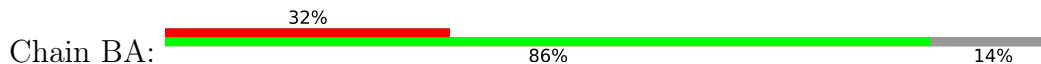
• Molecule 13: LR5

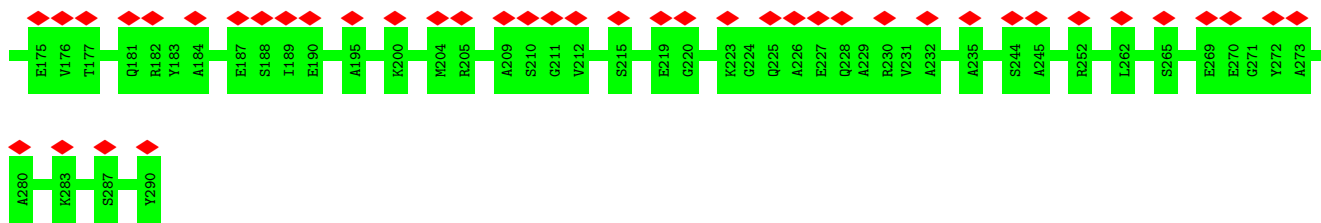


• Molecule 14: LR8

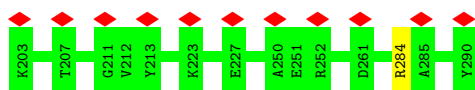
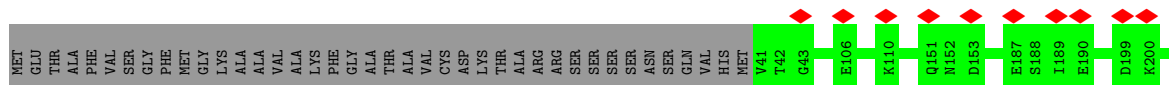
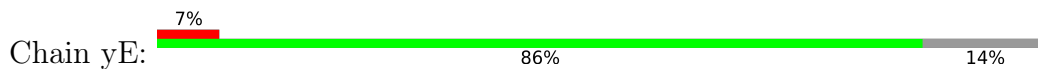


• Molecule 14: LR8

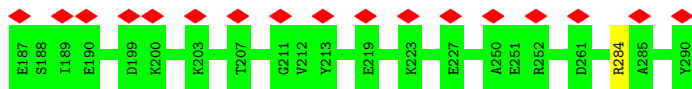
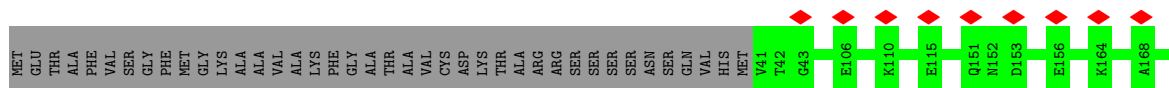
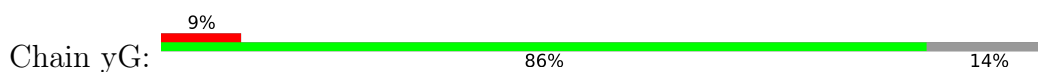




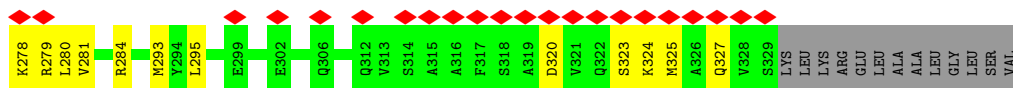
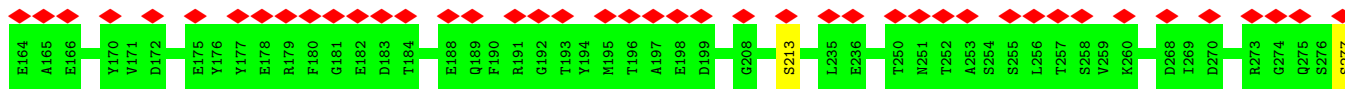
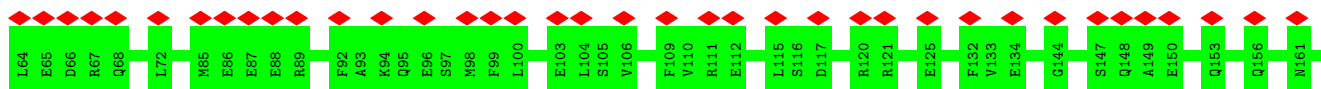
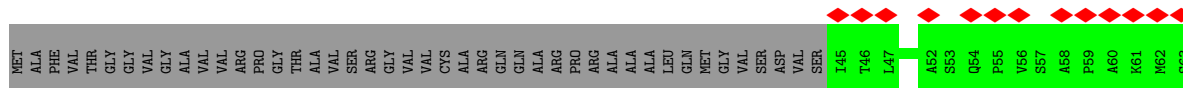
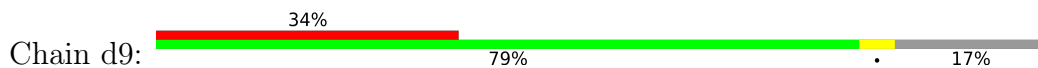
• Molecule 14: LR8



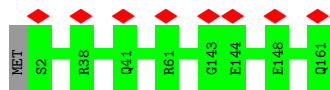
• Molecule 14: LR8



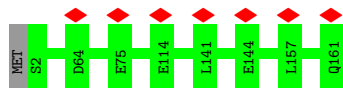
• Molecule 15: LR3



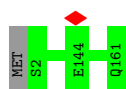
• Molecule 15: LR3



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



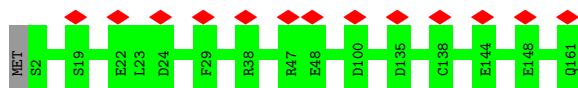
- Molecule 17: Allophycocyanin alpha subunit



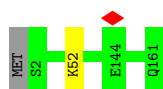
- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit



- Molecule 17: Allophycocyanin alpha subunit

Chain PH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain RH:  99%



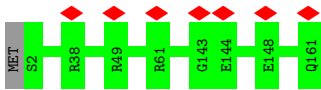
- Molecule 17: Allophycocyanin alpha subunit

Chain TH:  99%



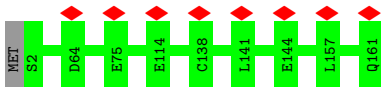
- Molecule 17: Allophycocyanin alpha subunit

Chain cH:  99%



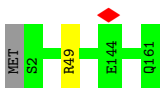
- Molecule 17: Allophycocyanin alpha subunit

Chain eH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain gH:  99%



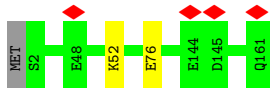
- Molecule 17: Allophycocyanin alpha subunit

Chain iH:  99%



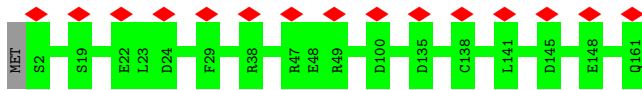
- Molecule 17: Allophycocyanin alpha subunit

Chain IH:  98%



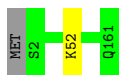
- Molecule 17: Allophycocyanin alpha subunit

Chain mH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain pH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain rH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain tH:  99%



- Molecule 17: Allophycocyanin alpha subunit

Chain vH:  99%



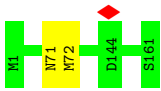
- Molecule 18: Allophycocyanin beta subunit

Chain DH:  99%



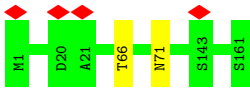
- Molecule 18: Allophycocyanin beta subunit

Chain FH:  99%



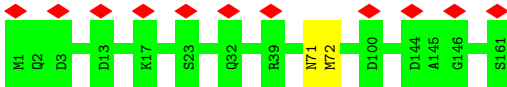
- Molecule 18: Allophycocyanin beta subunit

Chain BH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain HH:  99%



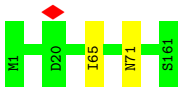
- Molecule 18: Allophycocyanin beta subunit

Chain IH:  99%



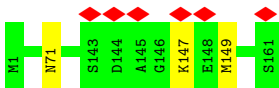
- Molecule 18: Allophycocyanin beta subunit

Chain LH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain MH:  98%



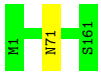
- Molecule 18: Allophycocyanin beta subunit

Chain OH:  99%



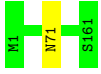
- Molecule 18: Allophycocyanin beta subunit

Chain QH:  99%



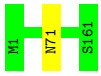
- Molecule 18: Allophycocyanin beta subunit

Chain SH:  99%



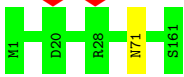
- Molecule 18: Allophycocyanin beta subunit

Chain UH:  99%



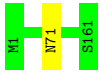
- Molecule 18: Allophycocyanin beta subunit

Chain dH:  99%



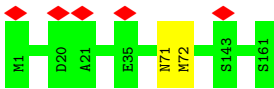
- Molecule 18: Allophycocyanin beta subunit

Chain fH:  99%



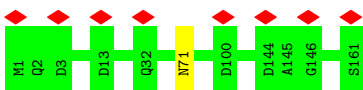
- Molecule 18: Allophycocyanin beta subunit

Chain hH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain jH:  99%



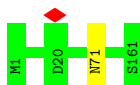
- Molecule 18: Allophycocyanin beta subunit

Chain kH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain nH:  99%



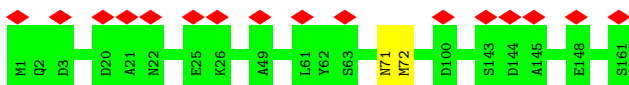
- Molecule 18: Allophycocyanin beta subunit

Chain oH:  96%



- Molecule 18: Allophycocyanin beta subunit

Chain qH:  10%  99%



- Molecule 18: Allophycocyanin beta subunit

Chain sH:  99%



- Molecule 18: Allophycocyanin beta subunit

Chain uH:  99%

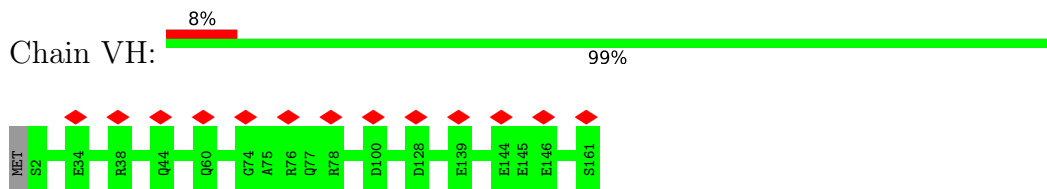


- Molecule 18: Allophycocyanin beta subunit

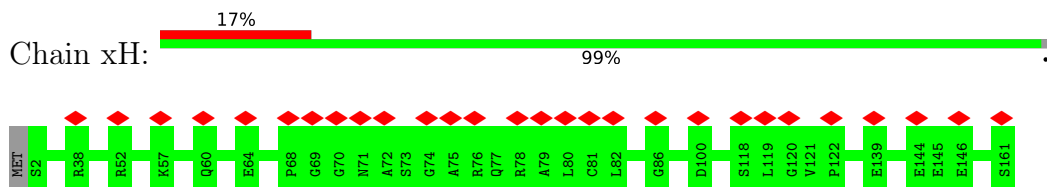
Chain wH:  99%



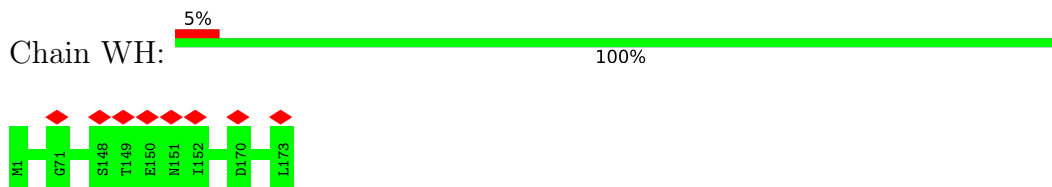
- Molecule 19: Allophycocyanin gamma subunit



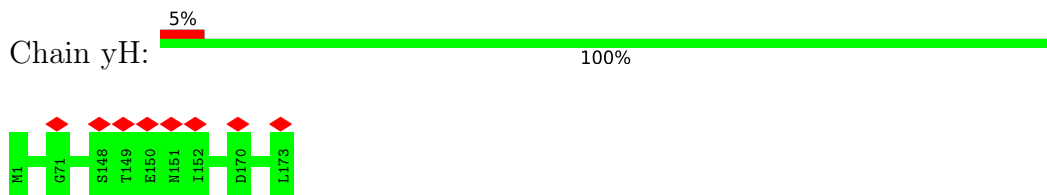
- Molecule 19: Allophycocyanin gamma subunit



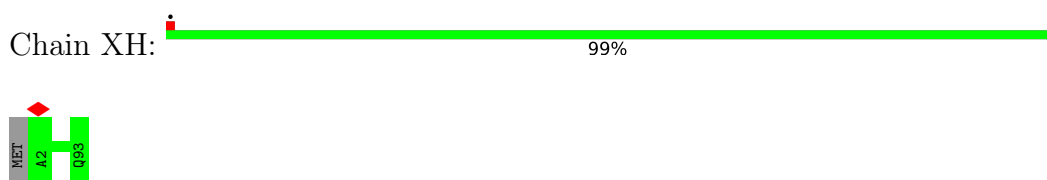
- Molecule 20: Allophycocyanin beta 18 subunit



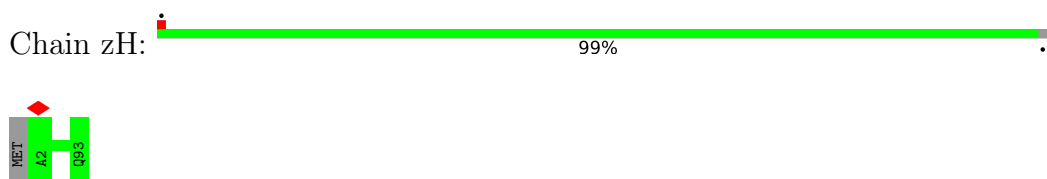
- Molecule 20: Allophycocyanin beta 18 subunit



- Molecule 21: LC

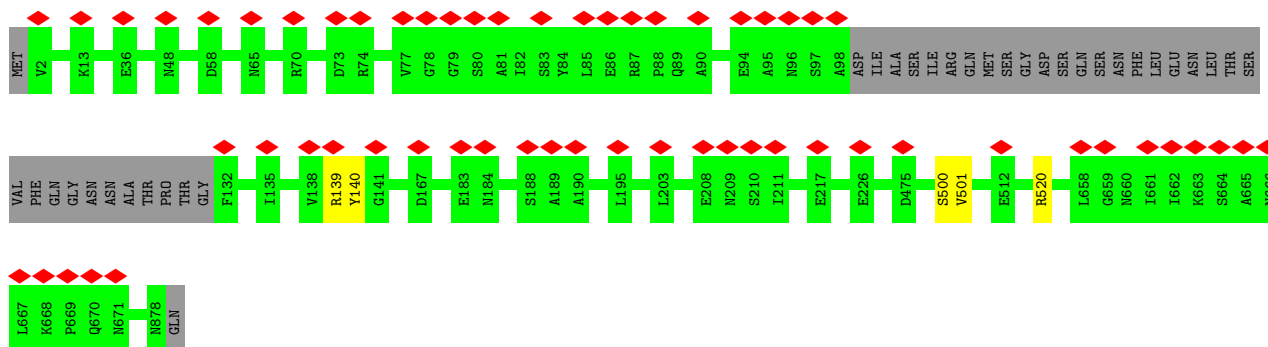


- Molecule 21: LC



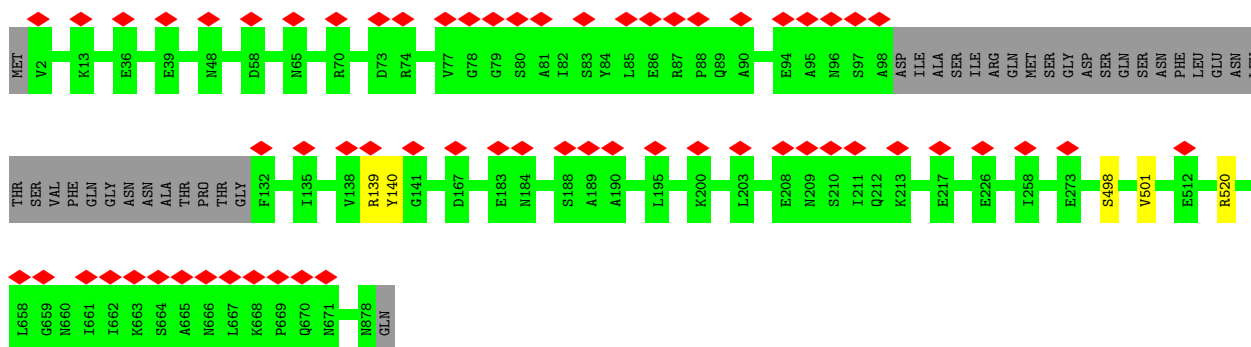
- Molecule 22: Phycobilisome linker polypeptide





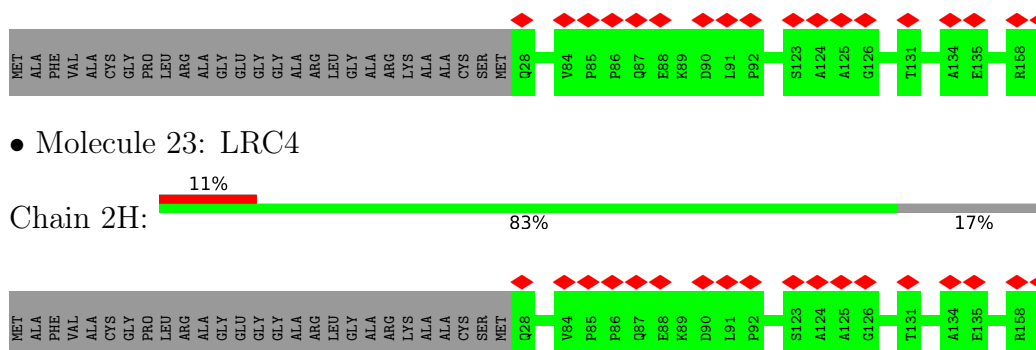
- Molecule 22: Phycobilisome linker polypeptide

Chain 1H: 7% 95%



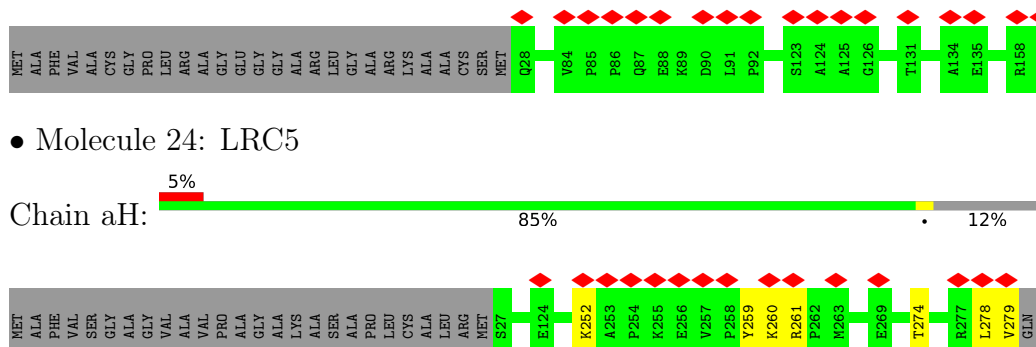
- Molecule 23: LRC4

Chain ZH: 11% 83% 17%

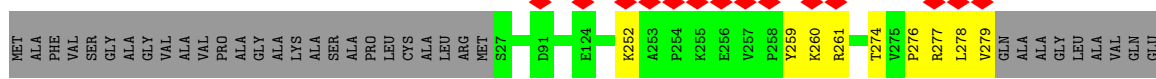
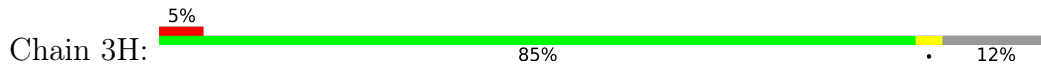


- Molecule 23: LRC4

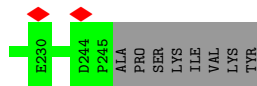
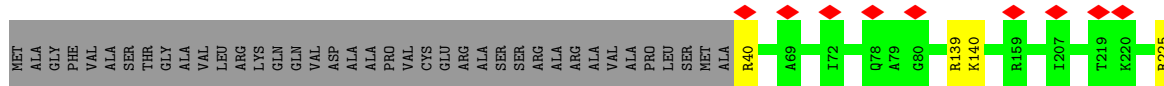
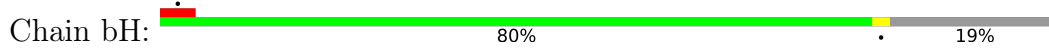
Chain 2H: 11% 83% 17%



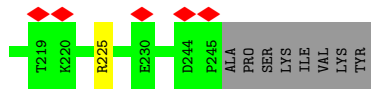
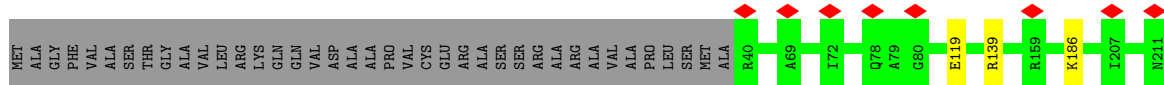
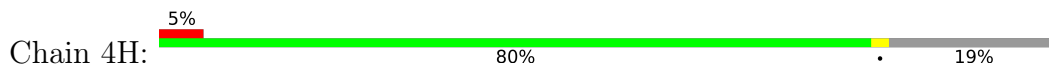
- Molecule 24: LRC5



• Molecule 25: LRC6



• Molecule 25: LRC6



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	191825	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	48	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.143	Depositor
Minimum map value	-0.087	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	610.95996, 610.95996, 610.95996	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.091, 1.091, 1.091	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: PUB, MEN, PEB, CYC

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	A1	0.33	0/1271	0.59	0/1721
1	A3	0.35	0/1271	0.63	0/1721
1	A4	0.32	0/1271	0.59	0/1721
1	AD	0.34	0/1271	0.64	0/1721
1	AE	0.33	0/1271	0.57	0/1721
1	AG	0.32	0/1271	0.59	1/1721 (0.1%)
1	B9	0.35	0/1271	0.60	0/1721
1	BJ	0.36	0/1271	0.61	0/1721
1	C1	0.32	0/1271	0.62	1/1721 (0.1%)
1	C3	0.36	0/1271	0.63	1/1721 (0.1%)
1	C4	0.32	0/1271	0.61	1/1721 (0.1%)
1	C8	0.42	0/1271	0.53	0/1721
1	CA	0.41	0/1271	0.54	0/1721
1	CD	0.33	0/1271	0.58	0/1721
1	CE	0.32	0/1271	0.63	0/1721
1	CG	0.33	0/1271	0.71	3/1721 (0.2%)
1	D9	0.38	0/1271	0.63	0/1721
1	DJ	0.43	0/1271	0.64	0/1721
1	E1	0.34	0/1271	0.62	0/1721
1	E3	0.34	0/1271	0.63	0/1721
1	E4	0.33	0/1271	0.61	0/1721
1	E8	0.38	0/1271	0.53	0/1721
1	EA	0.37	0/1271	0.55	0/1721
1	ED	0.33	0/1271	0.61	1/1721 (0.1%)
1	EE	0.36	0/1271	0.60	1/1721 (0.1%)
1	EG	0.38	0/1271	0.64	2/1721 (0.1%)
1	F9	0.38	0/1271	0.60	0/1721
1	FJ	0.39	0/1271	0.61	0/1721
1	G1	0.36	0/1271	0.62	0/1721
1	G3	0.36	0/1271	0.64	0/1721
1	G4	0.32	0/1271	0.61	0/1721
1	G8	0.35	0/1271	0.55	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	GA	0.35	0/1271	0.54	1/1721 (0.1%)
1	GD	0.34	0/1271	0.61	1/1721 (0.1%)
1	GE	0.44	0/1271	0.69	3/1721 (0.2%)
1	GG	0.49	0/1271	0.83	5/1721 (0.3%)
1	H9	0.34	0/1271	0.60	0/1721
1	HJ	0.36	0/1271	0.63	0/1721
1	I1	0.34	0/1271	0.63	1/1721 (0.1%)
1	I3	0.35	0/1271	0.67	2/1721 (0.1%)
1	I4	0.31	0/1271	0.63	1/1721 (0.1%)
1	I8	0.41	0/1271	0.51	0/1721
1	IA	0.39	0/1271	0.51	1/1721 (0.1%)
1	ID	0.32	0/1271	0.62	1/1721 (0.1%)
1	IE	0.43	0/1271	0.70	3/1721 (0.2%)
1	IG	0.49	0/1271	0.78	4/1721 (0.2%)
1	J5	0.71	0/1271	0.59	0/1721
1	J9	0.33	0/1271	0.58	0/1721
1	JC	0.49	0/1271	0.53	0/1721
1	JJ	0.34	0/1271	0.59	0/1721
1	K1	0.34	0/1271	0.63	2/1721 (0.1%)
1	K3	0.37	0/1271	0.64	1/1721 (0.1%)
1	K4	0.33	0/1271	0.58	0/1721
1	K8	0.50	0/1271	0.56	0/1721
1	KA	0.48	0/1271	0.54	0/1721
1	KD	0.35	0/1271	0.64	1/1721 (0.1%)
1	KE	0.36	0/1271	0.61	1/1721 (0.1%)
1	KG	0.38	0/1271	0.60	0/1721
1	L9	0.35	0/1271	0.59	0/1721
1	LJ	0.35	0/1271	0.61	0/1721
1	M3	0.38	0/1271	0.59	0/1721
1	M8	0.60	0/1271	0.54	0/1721
1	MA	0.58	0/1271	0.54	0/1721
1	MD	0.35	0/1271	0.57	0/1721
1	ME	0.30	0/1271	0.60	0/1721
1	MG	0.31	0/1271	0.60	0/1721
1	N1	0.47	0/1271	0.65	1/1721 (0.1%)
1	N4	0.48	0/1271	0.63	1/1721 (0.1%)
1	N9	0.32	0/1271	0.60	1/1721 (0.1%)
1	NJ	0.33	0/1271	0.63	1/1721 (0.1%)
1	O2	0.34	0/1271	0.45	0/1721
1	O3	0.52	0/1271	0.66	1/1721 (0.1%)
1	O6	0.36	0/1271	0.48	0/1721
1	O7	0.28	0/1271	0.55	1/1721 (0.1%)
1	O8	0.39	0/1271	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	OA	0.37	0/1271	0.50	0/1721
1	OB	0.38	0/1271	0.49	0/1721
1	OD	0.47	0/1271	0.63	1/1721 (0.1%)
1	OE	0.33	0/1271	0.62	0/1721
1	OF	0.33	0/1271	0.59	0/1721
1	OG	0.34	0/1271	0.60	0/1721
1	OI	0.34	0/1271	0.47	0/1721
1	P1	0.35	0/1271	0.60	0/1721
1	P4	0.34	0/1271	0.60	0/1721
1	P9	0.34	0/1271	0.63	0/1721
1	PJ	0.34	0/1271	0.64	0/1721
1	Q2	0.39	0/1271	0.50	0/1721
1	Q3	0.50	0/1271	0.63	1/1721 (0.1%)
1	Q6	0.33	0/1271	0.50	0/1721
1	Q7	0.28	0/1271	0.51	1/1721 (0.1%)
1	Q8	0.36	0/1271	0.53	0/1721
1	QA	0.38	0/1271	0.51	0/1721
1	QB	0.33	0/1271	0.49	0/1721
1	QD	0.44	0/1271	0.60	0/1721
1	QE	0.33	0/1271	0.67	2/1721 (0.1%)
1	QF	0.34	0/1271	0.60	2/1721 (0.1%)
1	QG	0.35	0/1271	0.66	1/1721 (0.1%)
1	QI	0.39	0/1271	0.48	0/1721
1	R1	0.32	0/1271	0.57	1/1721 (0.1%)
1	R4	0.33	0/1271	0.57	1/1721 (0.1%)
1	R9	0.35	0/1271	0.63	1/1721 (0.1%)
1	RJ	0.37	0/1271	0.65	1/1721 (0.1%)
1	S2	0.36	0/1271	0.48	0/1721
1	S3	0.51	0/1271	0.66	1/1721 (0.1%)
1	S6	0.34	0/1271	0.49	0/1721
1	S7	0.29	0/1271	0.50	0/1721
1	S8	0.36	0/1271	0.52	0/1721
1	SA	0.35	0/1271	0.52	0/1721
1	SB	0.34	0/1271	0.49	0/1721
1	SD	0.45	0/1271	0.63	0/1721
1	SE	0.38	0/1271	0.76	3/1721 (0.2%)
1	SF	0.35	0/1271	0.65	2/1721 (0.1%)
1	SG	0.39	0/1271	0.67	2/1721 (0.1%)
1	SI	0.35	0/1271	0.49	0/1721
1	T1	0.33	0/1271	0.57	0/1721
1	T4	0.33	0/1271	0.57	0/1721
1	T9	0.35	0/1271	0.62	0/1721
1	TJ	0.36	0/1271	0.64	2/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	U2	0.40	0/1271	0.51	0/1721
1	U3	0.42	0/1271	0.61	0/1721
1	U6	0.32	0/1271	0.50	0/1721
1	U7	0.29	0/1271	0.60	2/1721 (0.1%)
1	U8	0.46	0/1271	0.55	0/1721
1	UA	0.43	0/1271	0.53	0/1721
1	UB	0.33	0/1271	0.52	0/1721
1	UD	0.38	0/1271	0.58	0/1721
1	UE	0.39	0/1271	0.72	5/1721 (0.3%)
1	UF	0.33	0/1271	0.69	3/1721 (0.2%)
1	UG	0.40	0/1271	0.67	2/1721 (0.1%)
1	UI	0.39	0/1271	0.48	0/1721
1	V1	0.38	0/1271	0.60	0/1721
1	V4	0.36	0/1271	0.57	0/1721
1	V9	0.34	0/1271	0.62	1/1721 (0.1%)
1	VJ	0.36	0/1271	0.66	3/1721 (0.2%)
1	W2	0.36	0/1271	0.48	0/1721
1	W3	0.42	0/1271	0.58	0/1721
1	W6	0.38	0/1271	0.50	0/1721
1	W7	0.29	0/1271	0.50	0/1721
1	W8	0.58	0/1271	0.55	0/1721
1	WA	0.57	0/1271	0.56	0/1721
1	WB	0.39	0/1271	0.51	0/1721
1	WD	0.38	0/1271	0.56	0/1721
1	WE	0.34	0/1271	0.56	0/1721
1	WF	0.33	0/1271	0.64	2/1721 (0.1%)
1	WG	0.34	0/1271	0.62	3/1721 (0.2%)
1	WI	0.36	0/1271	0.48	0/1721
1	X1	0.50	0/1271	0.66	0/1721
1	X4	0.50	0/1271	0.65	1/1721 (0.1%)
1	X9	0.34	0/1271	0.65	1/1721 (0.1%)
1	XJ	0.34	0/1271	0.62	0/1721
1	Y8	0.49	0/1271	0.53	0/1721
1	YA	0.47	0/1271	0.53	0/1721
1	YE	0.31	0/1271	0.58	0/1721
1	YG	0.33	0/1271	0.57	0/1721
1	Z2	0.38	0/1271	0.48	0/1721
1	Z6	0.36	0/1271	0.50	0/1721
1	Z7	0.28	0/1271	0.51	0/1721
1	ZB	0.37	0/1271	0.51	0/1721
1	ZF	0.32	0/1271	0.59	0/1721
1	ZI	0.39	0/1271	0.48	0/1721
1	a8	0.34	0/1271	0.51	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	aA	0.33	0/1271	0.52	0/1721
1	aE	0.34	0/1271	0.61	0/1721
1	aG	0.33	0/1271	0.62	0/1721
1	b2	0.30	0/1271	0.51	0/1721
1	b6	0.31	0/1271	0.53	1/1721 (0.1%)
1	b7	0.27	0/1271	0.53	1/1721 (0.1%)
1	bB	0.32	0/1271	0.53	0/1721
1	bF	0.32	0/1271	0.71	2/1721 (0.1%)
1	bI	0.29	0/1271	0.52	0/1721
1	c1	0.32	0/1271	0.63	1/1721 (0.1%)
1	c4	0.33	0/1271	0.58	0/1721
1	cE	0.33	0/1271	0.65	2/1721 (0.1%)
1	cG	0.33	0/1271	0.62	1/1721 (0.1%)
1	d2	0.31	0/1271	0.51	0/1721
1	d6	0.29	0/1271	0.50	0/1721
1	d7	0.28	0/1271	0.62	2/1721 (0.1%)
1	d8	0.35	0/1271	0.54	0/1721
1	dA	0.34	0/1271	0.54	0/1721
1	dB	0.29	0/1271	0.55	0/1721
1	dF	0.34	0/1271	0.70	2/1721 (0.1%)
1	dI	0.30	0/1271	0.51	0/1721
1	e1	0.34	0/1271	0.60	0/1721
1	e4	0.31	0/1271	0.60	0/1721
1	eE	0.32	0/1271	0.59	0/1721
1	eG	0.33	0/1271	0.65	1/1721 (0.1%)
1	f2	0.28	0/1271	0.52	0/1721
1	f6	0.28	0/1271	0.51	0/1721
1	f7	0.27	0/1271	0.51	1/1721 (0.1%)
1	f8	0.32	0/1271	0.56	1/1721 (0.1%)
1	fA	0.31	0/1271	0.57	1/1721 (0.1%)
1	fB	0.29	0/1271	0.50	0/1721
1	fF	0.34	0/1271	0.69	2/1721 (0.1%)
1	fI	0.29	0/1271	0.53	0/1721
1	g1	0.33	0/1271	0.69	3/1721 (0.2%)
1	g4	0.33	0/1271	0.64	1/1721 (0.1%)
1	gE	0.33	0/1271	0.59	0/1721
1	gG	0.31	0/1271	0.58	0/1721
1	h2	0.32	0/1271	0.50	0/1721
1	h6	0.30	0/1271	0.51	0/1721
1	h7	0.27	0/1271	0.55	1/1721 (0.1%)
1	h8	0.33	0/1271	0.59	1/1721 (0.1%)
1	hA	0.32	0/1271	0.55	0/1721
1	hB	0.31	0/1271	0.60	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	hF	0.32	0/1271	0.69	3/1721 (0.2%)
1	hI	0.31	0/1271	0.49	0/1721
1	i1	0.31	0/1271	0.59	0/1721
1	i4	0.32	0/1271	0.60	0/1721
1	iE	0.32	0/1271	0.61	0/1721
1	iG	0.35	0/1271	0.62	2/1721 (0.1%)
1	j2	0.31	0/1271	0.50	0/1721
1	j6	0.29	0/1271	0.47	0/1721
1	j7	0.28	0/1271	0.55	1/1721 (0.1%)
1	j8	0.33	0/1271	0.57	1/1721 (0.1%)
1	jA	0.31	0/1271	0.55	0/1721
1	jB	0.29	0/1271	0.47	0/1721
1	jF	0.35	0/1271	0.72	3/1721 (0.2%)
1	jI	0.30	0/1271	0.50	0/1721
1	k1	0.32	0/1271	0.62	0/1721
1	k4	0.31	0/1271	0.60	0/1721
1	kE	0.35	0/1271	0.64	3/1721 (0.2%)
1	kG	0.33	0/1271	0.63	0/1721
1	l2	0.31	0/1271	0.47	0/1721
1	l6	0.28	0/1271	0.50	0/1721
1	l7	0.29	0/1271	0.56	0/1721
1	l8	0.39	0/1271	0.58	1/1721 (0.1%)
1	lA	0.37	0/1271	0.57	0/1721
1	lB	0.29	0/1271	0.54	0/1721
1	lF	0.37	0/1271	0.76	7/1721 (0.4%)
1	lI	0.31	0/1271	0.48	0/1721
1	m1	0.34	0/1271	0.64	0/1721
1	m4	0.32	0/1271	0.62	2/1721 (0.1%)
1	mE	0.37	0/1271	0.86	9/1721 (0.5%)
1	mG	0.34	0/1271	0.65	0/1721
1	oE	0.32	0/1271	0.65	0/1721
1	oG	0.32	0/1271	0.64	0/1721
1	p1	0.34	0/1271	0.63	1/1721 (0.1%)
1	p4	0.33	0/1271	0.61	0/1721
1	qE	0.31	0/1271	0.63	1/1721 (0.1%)
1	qG	0.32	0/1271	0.65	1/1721 (0.1%)
1	r1	0.34	0/1271	0.64	1/1721 (0.1%)
1	r4	0.35	0/1271	0.63	1/1721 (0.1%)
1	sE	0.32	0/1271	0.58	1/1721 (0.1%)
1	sG	0.36	0/1271	0.60	2/1721 (0.1%)
1	t1	0.33	0/1271	0.64	2/1721 (0.1%)
1	t4	0.34	0/1271	0.61	0/1721
1	uE	0.32	0/1271	0.60	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	uG	0.33	0/1271	0.62	1/1721 (0.1%)
1	v1	0.34	0/1271	0.69	2/1721 (0.1%)
1	v4	0.34	0/1271	0.72	1/1721 (0.1%)
1	x1	0.36	0/1271	0.73	2/1721 (0.1%)
1	x4	0.33	0/1271	0.66	1/1721 (0.1%)
1	z1	0.33	0/1271	0.65	0/1721
1	z4	0.33	0/1271	0.64	0/1721
2	11	0.32	0/1297	0.63	1/1750 (0.1%)
2	14	0.32	0/1297	0.67	2/1750 (0.1%)
2	A5	0.29	0/1065	0.50	0/1437
2	AC	0.28	0/1065	0.49	0/1437
2	B1	0.32	0/1297	0.61	0/1750
2	B3	0.35	0/1297	0.67	1/1750 (0.1%)
2	B4	0.32	0/1297	0.59	0/1750
2	B5	0.28	0/1065	0.53	0/1437
2	BC	0.32	0/1065	0.52	0/1437
2	BD	0.32	0/1297	0.66	0/1750
2	BE	0.32	0/1303	0.63	1/1758 (0.1%)
2	BG	0.32	0/1303	0.56	1/1758 (0.1%)
2	C5	0.26	0/1065	0.49	0/1437
2	C9	0.37	0/1297	0.61	0/1750
2	CC	0.27	0/1065	0.46	0/1437
2	CJ	0.38	0/1297	0.63	0/1750
2	D1	0.32	0/1297	0.61	1/1750 (0.1%)
2	D3	0.34	0/1297	0.67	3/1750 (0.2%)
2	D4	0.32	0/1297	0.62	2/1750 (0.1%)
2	D8	0.36	0/1315	0.54	1/1774 (0.1%)
2	DA	0.36	0/1315	0.52	0/1774
2	DD	0.32	0/1297	0.62	0/1750
2	DE	0.33	0/1315	0.61	1/1774 (0.1%)
2	DG	0.34	0/1315	0.58	0/1774
2	E9	0.37	0/1297	0.63	1/1750 (0.1%)
2	EJ	0.39	0/1297	0.63	1/1750 (0.1%)
2	F1	0.31	0/1297	0.55	0/1750
2	F3	0.33	0/1297	0.63	1/1750 (0.1%)
2	F4	0.30	0/1297	0.55	0/1750
2	F5	0.41	0/1065	0.56	0/1437
2	F8	0.43	0/1315	0.58	1/1774 (0.1%)
2	FA	0.41	0/1315	0.57	1/1774 (0.1%)
2	FC	0.32	0/1065	0.51	0/1437
2	FD	0.33	0/1297	0.63	1/1750 (0.1%)
2	FE	0.40	0/1315	0.69	3/1774 (0.2%)
2	FG	0.43	0/1315	0.62	0/1774

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	G5	0.34	0/1065	0.51	0/1437
2	G9	0.32	0/1297	0.61	1/1750 (0.1%)
2	GC	0.27	0/1065	0.48	0/1437
2	GJ	0.34	0/1297	0.64	1/1750 (0.1%)
2	H1	0.32	0/1303	0.72	3/1758 (0.2%)
2	H3	0.34	0/1309	0.63	1/1766 (0.1%)
2	H4	0.32	0/1309	0.64	1/1766 (0.1%)
2	H5	0.54	0/1065	0.60	0/1437
2	H8	0.38	0/1315	0.59	1/1774 (0.1%)
2	HA	0.36	0/1315	0.55	0/1774
2	HC	0.39	0/1065	0.53	0/1437
2	HD	0.34	0/1309	0.64	0/1766
2	HE	0.34	0/1315	0.55	0/1774
2	HG	0.37	0/1315	0.56	0/1774
2	I5	0.44	0/1297	0.53	0/1750
2	I9	0.41	0/1309	0.71	3/1766 (0.2%)
2	IC	0.33	0/1289	0.49	0/1740
2	IJ	0.45	0/1309	0.66	0/1766
2	J1	0.32	0/1297	0.59	0/1750
2	J3	0.33	0/1297	0.64	1/1750 (0.1%)
2	J4	0.32	0/1297	0.55	0/1750
2	J8	0.37	0/1309	0.53	0/1766
2	JA	0.34	0/1309	0.56	1/1766 (0.1%)
2	JD	0.34	0/1297	0.65	0/1750
2	JE	0.35	0/1315	0.56	0/1774
2	JG	0.39	0/1315	0.60	2/1774 (0.1%)
2	K5	0.56	0/1297	0.56	0/1750
2	K9	0.33	0/1297	0.57	0/1750
2	KC	0.41	0/1297	0.50	0/1750
2	KJ	0.35	0/1297	0.60	1/1750 (0.1%)
2	L1	0.30	0/1297	0.61	1/1750 (0.1%)
2	L3	0.34	0/1297	0.65	0/1750
2	L4	0.30	0/1297	0.56	0/1750
2	L5	0.57	0/1065	0.58	0/1437
2	L8	0.49	0/1315	0.56	2/1774 (0.1%)
2	LA	0.47	0/1315	0.55	2/1774 (0.1%)
2	LC	0.43	0/1065	0.50	0/1437
2	LD	0.34	0/1297	0.65	0/1750
2	LE	0.43	0/1315	0.62	0/1774
2	LG	0.48	0/1315	0.67	2/1774 (0.1%)
2	M9	0.33	0/1297	0.61	0/1750
2	MJ	0.36	0/1297	0.63	1/1750 (0.1%)
2	N3	0.39	0/1315	0.60	1/1774 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	N8	0.53	0/1315	0.60	0/1774
2	NA	0.51	0/1315	0.61	1/1774 (0.1%)
2	ND	0.35	0/1315	0.56	0/1774
2	NE	0.31	0/1315	0.59	0/1774
2	NG	0.33	0/1315	0.62	0/1774
2	O1	0.36	0/1297	0.64	1/1750 (0.1%)
2	O4	0.37	0/1297	0.63	2/1750 (0.1%)
2	O9	0.33	0/1297	0.62	1/1750 (0.1%)
2	OJ	0.33	0/1297	0.68	2/1750 (0.1%)
2	P2	0.30	0/1297	0.47	0/1750
2	P3	0.44	0/1315	0.61	0/1774
2	P6	0.36	0/1297	0.47	0/1750
2	P7	0.30	0/1297	0.50	0/1750
2	P8	0.31	0/1297	0.50	0/1750
2	PA	0.31	0/1297	0.50	0/1750
2	PB	0.37	0/1297	0.48	0/1750
2	PD	0.41	0/1315	0.59	0/1774
2	PE	0.31	0/1315	0.59	0/1774
2	PF	0.34	0/1297	0.62	2/1750 (0.1%)
2	PG	0.33	0/1315	0.59	0/1774
2	PI	0.30	0/1297	0.47	0/1750
2	Q1	0.39	0/1297	0.64	1/1750 (0.1%)
2	Q4	0.39	0/1297	0.62	1/1750 (0.1%)
2	Q9	0.33	0/1297	0.67	4/1750 (0.2%)
2	QJ	0.34	0/1297	0.69	1/1750 (0.1%)
2	R2	0.35	0/1297	0.49	0/1750
2	R3	0.45	0/1315	0.60	0/1774
2	R6	0.32	0/1297	0.49	0/1750
2	R7	0.28	0/1297	0.50	0/1750
2	R8	0.39	0/1303	0.55	1/1758 (0.1%)
2	RA	0.37	0/1303	0.54	1/1758 (0.1%)
2	RB	0.34	0/1297	0.51	0/1750
2	RD	0.41	0/1315	0.58	0/1774
2	RE	0.33	0/1309	0.56	0/1766
2	RF	0.34	0/1297	0.62	1/1750 (0.1%)
2	RG	0.36	0/1309	0.58	0/1766
2	RI	0.35	0/1297	0.49	0/1750
2	S1	0.34	0/1297	0.65	2/1750 (0.1%)
2	S4	0.33	0/1297	0.65	2/1750 (0.1%)
2	S9	0.34	0/1297	0.60	0/1750
2	SJ	0.36	0/1297	0.67	1/1750 (0.1%)
2	T2	0.33	0/1297	0.47	0/1750
2	T3	0.62	0/1315	0.65	0/1774

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	T6	0.36	0/1297	0.49	0/1750
2	T7	0.29	0/1297	0.50	0/1750
2	T8	0.40	0/1315	0.54	0/1774
2	TA	0.39	0/1315	0.55	0/1774
2	TB	0.37	0/1297	0.50	0/1750
2	TD	0.54	0/1315	0.62	0/1774
2	TE	0.35	0/1309	0.57	0/1766
2	TF	0.33	0/1297	0.62	0/1750
2	TG	0.37	0/1309	0.61	1/1766 (0.1%)
2	TI	0.33	0/1297	0.47	0/1750
2	U1	0.35	0/1309	0.62	0/1766
2	U4	0.33	0/1309	0.60	0/1766
2	U9	0.35	0/1309	0.66	0/1766
2	UJ	0.34	0/1309	0.65	1/1766 (0.1%)
2	V2	0.37	0/1297	0.48	0/1750
2	V3	0.37	0/1315	0.61	0/1774
2	V6	0.31	0/1309	0.53	2/1766 (0.1%)
2	V7	0.31	0/1309	0.53	0/1766
2	V8	0.38	0/1315	0.57	1/1774 (0.1%)
2	VA	0.37	0/1315	0.55	0/1774
2	VB	0.31	0/1309	0.55	2/1766 (0.1%)
2	VD	0.34	0/1315	0.57	0/1774
2	VE	0.32	0/1309	0.62	2/1766 (0.1%)
2	VF	0.33	0/1309	0.64	1/1766 (0.1%)
2	VG	0.34	0/1309	0.60	2/1766 (0.1%)
2	VI	0.38	0/1297	0.49	0/1750
2	W1	0.45	0/1297	0.69	1/1750 (0.1%)
2	W4	0.44	0/1297	0.66	2/1750 (0.1%)
2	W9	0.32	0/1297	0.70	4/1750 (0.2%)
2	WJ	0.33	0/1297	0.64	0/1750
2	X3	0.46	0/1315	0.60	0/1774
2	X8	0.43	0/1309	0.56	1/1766 (0.1%)
2	XA	0.41	0/1309	0.57	1/1766 (0.1%)
2	XD	0.41	0/1315	0.59	0/1774
2	XE	0.35	0/1315	0.64	1/1774 (0.1%)
2	XG	0.37	0/1315	0.62	0/1774
2	Y1	0.37	0/1297	0.64	1/1750 (0.1%)
2	Y2	0.32	0/1297	0.47	0/1750
2	Y4	0.38	0/1297	0.64	1/1750 (0.1%)
2	Y6	0.40	0/1297	0.49	0/1750
2	Y7	0.29	0/1297	0.52	0/1750
2	Y9	0.33	0/1297	0.62	0/1750
2	YB	0.41	0/1297	0.49	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	YF	0.32	0/1297	0.61	0/1750
2	YI	0.31	0/1297	0.47	0/1750
2	YJ	0.36	0/1297	0.66	0/1750
2	Z1	0.33	0/1065	0.55	0/1437
2	Z4	0.34	0/1065	0.59	0/1437
2	Z8	0.51	0/1315	0.55	0/1774
2	ZA	0.49	0/1315	0.55	0/1774
2	ZE	0.34	0/1315	0.69	2/1774 (0.1%)
2	ZG	0.33	0/1315	0.69	2/1774 (0.1%)
2	a1	0.30	0/1065	0.60	1/1437 (0.1%)
2	a2	0.37	0/1297	0.51	0/1750
2	a4	0.30	0/1065	0.64	1/1437 (0.1%)
2	a6	0.32	0/1297	0.48	0/1750
2	a7	0.28	0/1297	0.52	0/1750
2	aB	0.33	0/1297	0.49	0/1750
2	aF	0.32	0/1297	0.63	0/1750
2	aI	0.37	0/1297	0.52	0/1750
2	bE	0.31	0/1315	0.56	1/1774 (0.1%)
2	bG	0.33	0/1315	0.58	0/1774
2	c2	0.28	0/1297	0.50	0/1750
2	c6	0.30	0/1297	0.53	0/1750
2	c7	0.27	0/1297	0.50	0/1750
2	c8	0.30	0/1309	0.57	0/1766
2	cA	0.30	0/1309	0.56	0/1766
2	cB	0.30	0/1297	0.51	0/1750
2	cF	0.33	0/1297	0.60	1/1750 (0.1%)
2	cI	0.26	0/1297	0.46	0/1750
2	d1	0.32	0/1297	0.64	1/1750 (0.1%)
2	d4	0.32	0/1297	0.65	2/1750 (0.1%)
2	dE	0.33	0/1309	0.60	0/1766
2	dG	0.33	0/1309	0.63	2/1766 (0.1%)
2	e2	0.29	0/1297	0.48	0/1750
2	e6	0.28	0/1297	0.52	0/1750
2	e7	0.30	0/1297	0.55	0/1750
2	e8	0.38	0/1315	0.56	0/1774
2	eA	0.37	0/1315	0.56	1/1774 (0.1%)
2	eB	0.29	0/1297	0.53	0/1750
2	eF	0.34	0/1297	0.63	0/1750
2	eI	0.28	0/1297	0.48	0/1750
2	f1	0.32	0/1297	0.61	0/1750
2	f4	0.33	0/1297	0.65	1/1750 (0.1%)
2	fE	0.32	0/1309	0.64	3/1766 (0.2%)
2	fG	0.33	0/1309	0.61	0/1766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	g2	0.26	0/1297	0.54	1/1750 (0.1%)
2	g6	0.29	0/1297	0.50	0/1750
2	g7	0.29	0/1297	0.53	0/1750
2	g8	0.30	0/1315	0.58	1/1774 (0.1%)
2	gA	0.31	0/1315	0.58	1/1774 (0.1%)
2	gB	0.30	0/1297	0.51	0/1750
2	gF	0.34	0/1297	0.62	0/1750
2	gI	0.27	0/1297	0.50	0/1750
2	h1	0.32	0/1297	0.60	2/1750 (0.1%)
2	h4	0.32	0/1297	0.62	0/1750
2	hE	0.32	0/1315	0.59	1/1774 (0.1%)
2	hG	0.32	0/1315	0.61	0/1774
2	i2	0.28	0/1303	0.49	0/1758
2	i6	0.29	0/1309	0.57	0/1766
2	i7	0.28	0/1309	0.56	0/1766
2	i8	0.33	0/1315	0.58	0/1774
2	iA	0.34	0/1315	0.56	0/1774
2	iB	0.29	0/1309	0.59	1/1766 (0.1%)
2	iF	0.34	0/1309	0.68	1/1766 (0.1%)
2	iI	0.28	0/1303	0.51	0/1758
2	j1	0.33	0/1303	0.67	3/1758 (0.2%)
2	j4	0.32	0/1303	0.66	1/1758 (0.1%)
2	jE	0.30	0/1315	0.56	0/1774
2	jG	0.32	0/1315	0.58	0/1774
2	k2	0.30	0/1297	0.50	0/1750
2	k6	0.30	0/1297	0.50	0/1750
2	k7	0.27	0/1297	0.51	0/1750
2	k8	0.32	0/1315	0.56	0/1774
2	kA	0.31	0/1315	0.56	0/1774
2	kB	0.30	0/1297	0.51	0/1750
2	kF	0.32	0/1297	0.64	1/1750 (0.1%)
2	kI	0.29	0/1297	0.52	0/1750
2	l1	0.32	0/1297	0.63	2/1750 (0.1%)
2	l4	0.31	0/1297	0.61	2/1750 (0.1%)
2	lE	0.32	0/1315	0.65	1/1774 (0.1%)
2	lG	0.32	0/1315	0.64	2/1774 (0.1%)
2	m2	0.28	0/1297	0.46	0/1750
2	m6	0.28	0/1297	0.56	0/1750
2	m7	0.28	0/1297	0.49	0/1750
2	m8	0.34	0/1315	0.56	0/1774
2	mA	0.34	0/1315	0.56	0/1774
2	mB	0.28	0/1297	0.56	1/1750 (0.1%)
2	mF	0.35	0/1297	0.68	2/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	mI	0.27	0/1297	0.46	0/1750
2	n1	0.31	0/1297	0.62	0/1750
2	n4	0.31	0/1297	0.63	0/1750
2	nE	0.34	0/1315	0.68	1/1774 (0.1%)
2	nG	0.34	0/1315	0.62	2/1774 (0.1%)
2	pE	0.32	0/1315	0.63	0/1774
2	pG	0.31	0/1315	0.66	2/1774 (0.1%)
2	q1	0.33	0/1297	0.69	2/1750 (0.1%)
2	q4	0.32	0/1297	0.60	0/1750
2	rE	0.32	0/1315	0.62	1/1774 (0.1%)
2	rG	0.32	0/1315	0.66	2/1774 (0.1%)
2	s1	0.33	0/1297	0.66	3/1750 (0.2%)
2	s4	0.31	0/1297	0.67	3/1750 (0.2%)
2	tE	0.34	0/1309	0.67	2/1766 (0.1%)
2	tG	0.33	0/1309	0.65	0/1766
2	u1	0.34	0/1297	0.62	1/1750 (0.1%)
2	u4	0.33	0/1297	0.60	1/1750 (0.1%)
2	vE	0.32	0/1315	0.61	0/1774
2	vG	0.33	0/1315	0.67	2/1774 (0.1%)
2	w1	0.31	0/1309	0.64	1/1766 (0.1%)
2	w4	0.33	0/1309	0.67	3/1766 (0.2%)
2	y1	0.33	0/1297	0.68	2/1750 (0.1%)
2	y4	0.33	0/1297	0.66	0/1750
3	21	0.37	0/1877	0.63	0/2511
3	24	0.38	0/1877	0.60	1/2511 (0.0%)
3	M1	0.37	0/1877	0.66	2/2511 (0.1%)
3	M4	0.36	0/1877	0.63	3/2511 (0.1%)
4	b1	0.44	0/2539	0.71	2/3449 (0.1%)
4	b4	0.44	0/2539	0.69	1/3449 (0.0%)
4	o1	0.38	0/1679	0.75	1/2276 (0.0%)
4	o4	0.38	0/1679	0.74	2/2276 (0.1%)
5	31	0.45	0/2233	0.65	1/3024 (0.0%)
5	34	0.45	0/2233	0.62	1/3024 (0.0%)
6	X2	0.43	0/2585	0.58	1/3492 (0.0%)
6	X6	0.44	0/2585	0.59	0/3492
6	X7	0.32	0/2585	0.56	2/3492 (0.1%)
6	XB	0.45	0/2585	0.58	1/3492 (0.0%)
6	XF	0.37	0/2585	0.67	3/3492 (0.1%)
6	XI	0.43	0/2585	0.58	1/3492 (0.0%)
7	A2	0.30	0/2025	0.50	0/2722
7	A6	0.30	0/2025	0.50	0/2722
7	A7	0.29	0/2025	0.50	0/2722
7	A9	0.36	0/2017	0.59	0/2711

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	AB	0.30	0/2025	0.49	0/2722
7	AF	0.35	0/2025	0.59	0/2722
7	AI	0.30	0/2025	0.48	0/2722
7	AJ	0.36	0/2017	0.62	0/2711
7	Y3	0.36	0/1866	0.64	0/2506
7	YD	0.35	0/1866	0.58	0/2506
8	B2	0.48	0/1933	0.59	0/2614
8	B6	0.53	0/1941	0.63	2/2625 (0.1%)
8	B7	0.35	0/1917	0.53	0/2592
8	BB	0.53	0/1941	0.63	1/2625 (0.0%)
8	BF	0.40	0/1917	0.64	0/2592
8	BI	0.48	0/1933	0.59	0/2614
9	C2	0.42	0/1251	0.50	0/1699
9	C6	0.37	0/1251	0.48	0/1699
9	C7	0.27	0/1251	0.49	0/1699
9	CB	0.38	0/1251	0.47	0/1699
9	CF	0.31	0/1251	0.59	0/1699
9	CI	0.43	0/1251	0.52	1/1699 (0.1%)
9	E2	0.41	0/1251	0.49	0/1699
9	E6	0.43	0/1251	0.50	0/1699
9	E7	0.38	0/1251	0.49	0/1699
9	EB	0.45	0/1251	0.51	0/1699
9	EF	0.41	0/1251	0.59	0/1699
9	EI	0.41	0/1251	0.49	0/1699
9	G2	0.40	0/1251	0.48	0/1699
9	G6	0.51	0/1251	0.52	0/1699
9	G7	0.28	0/1251	0.47	0/1699
9	GB	0.53	0/1251	0.54	0/1699
9	GF	0.32	0/1251	0.58	1/1699 (0.1%)
9	GI	0.40	0/1251	0.48	0/1699
9	I2	0.41	0/1251	0.48	0/1699
9	I6	0.50	0/1251	0.52	0/1699
9	I7	0.40	0/1251	0.51	0/1699
9	IB	0.51	0/1251	0.52	0/1699
9	IF	0.42	0/1251	0.59	0/1699
9	II	0.41	0/1251	0.48	0/1699
9	K2	0.45	0/1251	0.48	0/1699
9	K6	0.40	0/1251	0.46	0/1699
9	K7	0.31	0/1251	0.50	1/1699 (0.1%)
9	KB	0.42	0/1251	0.46	0/1699
9	KF	0.36	0/1251	0.56	1/1699 (0.1%)
9	KI	0.45	0/1251	0.49	0/1699
9	M2	0.42	0/1251	0.49	0/1699

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	M6	0.48	0/1251	0.50	0/1699
9	M7	0.28	0/1251	0.48	1/1699 (0.1%)
9	MB	0.50	0/1251	0.51	0/1699
9	MF	0.31	0/1251	0.55	1/1699 (0.1%)
9	MI	0.41	0/1251	0.49	0/1699
10	D2	0.38	0/1274	0.51	0/1723
10	D6	0.42	0/1274	0.50	0/1723
10	D7	0.28	0/1274	0.50	0/1723
10	DB	0.43	0/1274	0.52	0/1723
10	DF	0.31	0/1274	0.61	0/1723
10	DI	0.38	0/1274	0.52	0/1723
10	F2	0.41	0/1274	0.50	0/1723
10	F6	0.38	0/1274	0.48	0/1723
10	F7	0.31	0/1274	0.46	0/1723
10	FB	0.38	0/1274	0.50	0/1723
10	FF	0.32	0/1274	0.52	0/1723
10	FI	0.41	0/1274	0.50	0/1723
10	H2	0.39	0/1274	0.54	1/1723 (0.1%)
10	H6	0.44	0/1274	0.52	0/1723
10	H7	0.31	0/1274	0.54	0/1723
10	HB	0.46	0/1274	0.52	0/1723
10	HF	0.37	0/1274	0.60	1/1723 (0.1%)
10	HI	0.39	0/1274	0.55	1/1723 (0.1%)
10	J2	0.42	0/1274	0.62	2/1723 (0.1%)
10	J6	0.58	0/1274	0.61	2/1723 (0.1%)
10	J7	0.31	0/1274	0.47	0/1723
10	JB	0.60	0/1274	0.59	1/1723 (0.1%)
10	JF	0.34	0/1274	0.56	0/1723
10	JI	0.41	0/1274	0.54	0/1723
10	L2	0.44	0/1274	0.57	0/1723
10	L6	0.47	0/1274	0.53	0/1723
10	L7	0.40	0/1274	0.53	0/1723
10	LB	0.48	0/1274	0.52	0/1723
10	LF	0.46	0/1274	0.67	1/1723 (0.1%)
10	LI	0.44	0/1274	0.57	0/1723
10	N2	0.43	0/1274	0.53	0/1723
10	N6	0.43	0/1274	0.52	0/1723
10	N7	0.29	0/1274	0.53	1/1723 (0.1%)
10	NB	0.45	0/1274	0.54	0/1723
10	NF	0.32	0/1274	0.62	3/1723 (0.2%)
10	NI	0.43	0/1274	0.52	0/1723
11	e3	0.51	0/1973	0.68	1/2657 (0.0%)
11	eD	0.47	0/1973	0.65	0/2657

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	b8	0.52	0/3022	0.59	0/4084
12	bA	0.51	0/3022	0.58	0/4084
13	A8	0.34	0/1843	0.54	1/2469 (0.0%)
13	AA	0.34	0/1843	0.54	1/2469 (0.0%)
13	wE	0.33	0/1843	0.55	0/2469
13	wG	0.33	0/1843	0.55	0/2469
13	xE	0.32	0/1843	0.57	0/2469
13	xG	0.33	0/1843	0.57	0/2469
14	B8	0.40	0/1932	0.50	0/2590
14	BA	0.38	0/1932	0.51	0/2590
14	yE	0.34	0/1932	0.58	0/2590
14	yG	0.36	0/1932	0.56	0/2590
15	d9	0.42	0/2242	0.64	0/3026
15	dJ	0.45	0/2242	0.70	1/3026 (0.0%)
16	zE	0.39	0/2964	0.59	0/4003
16	zG	0.43	0/2964	0.59	0/4003
17	AH	0.25	0/1241	0.38	0/1676
17	CH	0.26	0/1241	0.39	0/1676
17	EH	0.27	0/1241	0.38	0/1676
17	GH	0.27	0/1241	0.38	0/1676
17	JH	0.28	0/1241	0.39	0/1676
17	KH	0.25	0/1241	0.38	0/1676
17	NH	0.28	0/1241	0.40	0/1676
17	PH	0.30	0/1241	0.39	0/1676
17	RH	0.29	0/1241	0.39	0/1676
17	TH	0.30	0/1241	0.39	0/1676
17	cH	0.27	0/1241	0.38	0/1676
17	eH	0.25	0/1241	0.37	0/1676
17	gH	0.27	0/1241	0.38	0/1676
17	iH	0.27	0/1241	0.39	0/1676
17	lH	0.29	0/1241	0.39	0/1676
17	mH	0.25	0/1241	0.38	0/1676
17	pH	0.28	0/1241	0.39	0/1676
17	rH	0.30	0/1241	0.39	0/1676
17	tH	0.30	0/1241	0.40	0/1676
17	vH	0.30	0/1241	0.39	0/1676
18	BH	0.25	0/1226	0.38	0/1655
18	DH	0.28	0/1226	0.39	0/1655
18	FH	0.26	0/1226	0.38	0/1655
18	HH	0.25	0/1226	0.37	0/1655
18	IH	0.28	0/1226	0.40	0/1655
18	LH	0.29	0/1226	0.39	0/1655
18	MH	0.28	0/1226	0.40	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
18	OH	0.25	0/1226	0.37	0/1655
18	QH	0.31	0/1226	0.42	0/1655
18	SH	0.31	0/1226	0.40	0/1655
18	UH	0.31	0/1226	0.40	0/1655
18	dH	0.27	0/1226	0.40	0/1655
18	fH	0.26	0/1226	0.39	0/1655
18	hH	0.25	0/1226	0.39	0/1655
18	jH	0.26	0/1226	0.38	0/1655
18	kH	0.28	0/1226	0.40	0/1655
18	nH	0.27	0/1226	0.39	0/1655
18	oH	0.29	0/1226	0.41	0/1655
18	qH	0.25	0/1226	0.37	0/1655
18	sH	0.31	0/1226	0.41	0/1655
18	uH	0.30	0/1226	0.41	0/1655
18	wH	0.30	0/1226	0.41	0/1655
19	VH	0.25	0/1281	0.38	0/1731
19	xH	0.25	0/1281	0.41	0/1731
20	WH	0.26	0/1396	0.37	0/1886
20	yH	0.26	0/1396	0.37	0/1886
21	XH	0.26	0/732	0.41	0/981
21	zH	0.26	0/732	0.42	0/981
22	1H	0.29	0/6891	0.42	0/9305
22	YH	0.28	0/6891	0.42	0/9305
23	2H	0.27	0/1027	0.45	0/1399
23	ZH	0.27	0/1027	0.46	0/1399
24	3H	0.32	0/1940	0.46	0/2637
24	aH	0.31	0/1940	0.45	0/2637
25	4H	0.31	0/1569	0.44	0/2147
25	bH	0.30	0/1569	0.44	0/2147
All	All	0.36	0/954792	0.57	378/1290312 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C3	0	1
1	C8	0	2
1	EE	0	1
1	EG	0	1
1	G1	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
1	ID	0	1
1	J5	0	1
1	MD	0	1
1	ME	0	1
1	X9	0	1
1	a8	0	1
1	cE	0	1
1	cG	0	1
1	f7	0	1
1	fF	0	2
1	i1	0	1
1	k1	0	1
1	kE	0	1
1	mG	0	2
1	r4	0	1
1	x1	0	1
1	x4	0	1
1	z1	0	1
2	BE	0	2
2	FE	0	1
2	I9	0	1
2	JA	0	1
2	L1	0	1
2	O9	0	1
2	OJ	0	2
2	TG	0	1
2	U9	0	1
2	VF	0	1
2	XA	0	1
2	XE	0	1
2	eA	0	1
2	mF	0	1
2	nG	0	1
2	q4	0	1
2	w4	0	1
3	21	0	1
4	b1	0	1
4	o1	0	1
4	o4	0	2
5	31	0	1
5	34	0	1
7	A2	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
7	AB	0	1
7	Y3	0	1
8	BB	0	1
8	BF	0	1
10	D2	0	1
10	DB	0	1
10	DI	0	2
10	F2	0	1
10	H2	0	1
10	HB	0	1
10	HF	0	1
10	HI	0	1
10	J2	0	1
10	JB	0	1
10	JI	0	1
10	L2	0	1
10	L6	0	1
10	LI	0	1
10	N2	0	2
10	N6	0	1
10	NB	0	1
10	NI	0	1
12	b8	0	1
12	bA	0	3
13	wE	0	1
15	dJ	0	2
16	zE	0	3
16	zG	0	1
All	All	0	88

There are no bond length outliers.

The worst 5 of 378 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	GG	78	LYS	CD-CE-NZ	18.17	153.50	111.70
1	mE	84	ARG	NE-CZ-NH2	-12.59	114.00	120.30
1	SE	78	LYS	CD-CE-NZ	12.05	139.42	111.70
2	S1	39	ASP	CB-CG-OD1	10.70	127.93	118.30
1	fF	137	ARG	NE-CZ-NH2	-10.59	115.00	120.30

There are no chirality outliers.

5 of 88 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G1	159	LEU	Peptide
2	L1	13	ASP	Peptide
4	b1	340	ALA	Peptide
1	i1	138	LEU	Peptide
1	k1	140	VAL	Peptide

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	A3	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	A4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	AD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	AE	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	AG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	B9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	BJ	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	C1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	C3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	C4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	C8	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	CA	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	CD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	CE	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	D9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	DJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	E1	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	E3	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	E4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	E8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	ED	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	EG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	F9	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	FJ	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	G1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	G3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	G4	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	G8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	GA	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	GD	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	GE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	GG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	H9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	HJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	I1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	I3	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	I4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	I8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	IA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ID	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	IE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	IG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J5	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	J9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	JC	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	JJ	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	K1	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	K3	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	K4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	K8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	KA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	KD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	KE	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	KG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	L9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	LJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	M3	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	M8	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	MA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	MD	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	ME	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	MG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	N1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	N4	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	N9	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	NJ	162/164 (99%)	142 (88%)	20 (12%)	0	100	100
1	O2	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	O3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	O6	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	O7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	O8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	OA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	OB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	OD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	OE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	OF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	OG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	OI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	P1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	P4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	P9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	PJ	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Q2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	Q3	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	Q6	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	Q7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Q8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	QA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	QB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	QD	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	QE	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	QF	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	QG	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	QI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	R1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	R4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	R9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	RJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	S2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	S3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	S6	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	S7	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	S8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	SA	162/164 (99%)	147 (91%)	15 (9%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	SB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	SD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SE	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	SG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	SI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	T1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	T4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	T9	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	TJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	U2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	U3	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	U6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	U7	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	U8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	UA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	UB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	UD	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	UE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	UF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	UG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	UI	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	V1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	V4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	V9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	VJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	W2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	W3	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	W6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	W7	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	W8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	WA	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	WB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	WD	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	WE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	WF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	WG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	WI	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	X1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	X4	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
1	X9	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	XJ	162/164 (99%)	145 (90%)	17 (10%)	0	100	100
1	Y8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	YA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	YE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	YG	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	Z2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	Z6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	Z7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ZB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	ZF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	ZI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	a8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	aA	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	aE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	aG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	b2	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	b6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	b7	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	bB	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
1	bF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	bI	162/164 (99%)	158 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	c1	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	c4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	cE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	cG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	d2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	d6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	d7	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	d8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	dA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	dB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	dF	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	dI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	e1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	e4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	eE	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	eG	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	f2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
1	f6	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	f7	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	f8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	fA	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	fB	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	fF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	fI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	g1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	g4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	gE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	gG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	h2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
1	h6	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	h7	162/164 (99%)	154 (95%)	8 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	h8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	hA	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	hB	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	hF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	hI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	i1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	i4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	iE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	iG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	j2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	j6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	j7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	j8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	jA	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	jB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	jF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	jI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	k1	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	k4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	kE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	kG	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	l2	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	l6	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	l7	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	l8	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	lA	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	lB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	lF	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	lI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	m1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	m4	162/164 (99%)	150 (93%)	12 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	mE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	mG	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
1	oE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
1	oG	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
1	p1	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
1	p4	162/164 (99%)	147 (91%)	15 (9%)	0	100	100
1	qE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	qG	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	r1	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	r4	162/164 (99%)	147 (91%)	15 (9%)	0	100	100
1	sE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	sG	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
1	t1	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	t4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	uE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
1	uG	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
1	v1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	v4	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	x1	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
1	x4	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
1	z1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
1	z4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
2	11	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	14	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	A5	143/177 (81%)	133 (93%)	10 (7%)	0	100	100
2	AC	143/177 (81%)	131 (92%)	12 (8%)	0	100	100
2	B1	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	B3	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	B4	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	B5	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	BC	143/177 (81%)	131 (92%)	11 (8%)	1 (1%)	22	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	BE	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	BG	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	C5	143/177 (81%)	139 (97%)	4 (3%)	0	100	100
2	C9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	CC	143/177 (81%)	132 (92%)	10 (7%)	1 (1%)	22	53
2	CJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	D1	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	D3	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	D4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	D8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	DA	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	DD	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	DE	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	DG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	E9	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	EJ	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	F1	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	F3	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	F4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	F5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	F8	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	FA	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	FC	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	FD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	FE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	FG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	G5	143/177 (81%)	133 (93%)	10 (7%)	0	100	100
2	G9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	GC	143/177 (81%)	137 (96%)	6 (4%)	0	100	100
2	GJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H1	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	H3	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	H4	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	H5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	H8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	HA	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	HC	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	HD	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	HE	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	HG	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	I5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	I9	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	IC	173/177 (98%)	167 (96%)	6 (4%)	0	100	100
2	IJ	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	J1	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	J3	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	J4	174/177 (98%)	164 (94%)	9 (5%)	1 (1%)	25	56
2	J8	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	JA	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	JD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	JE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	JG	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	K5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	K9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	KC	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	KJ	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	L1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	L3	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	L4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	L5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	L8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LA	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	LC	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	LD	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	LE	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	LG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	M9	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	MJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	N3	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	N8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	NA	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	ND	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	NE	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	NG	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	O1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	O4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	O9	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	OJ	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	P2	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	P3	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	P6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	P7	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	P8	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	PA	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	PB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	PD	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	PE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	PF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	PG	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	PI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	Q1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	Q4	174/177 (98%)	170 (98%)	4 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Q9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	QJ	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	R2	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	R3	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	R6	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	R7	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	R8	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
2	RA	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	RB	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	RD	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	RE	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	RF	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	RG	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	RI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	S1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	S4	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	S9	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	SJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	T2	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	T3	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	T6	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	T7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	T8	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	TA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	TB	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	TD	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	TE	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TF	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	TG	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TI	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	U1	176/177 (99%)	167 (95%)	9 (5%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	U4	176/177 (99%)	166 (94%)	10 (6%)	0	100	100
2	U9	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	UJ	176/177 (99%)	166 (94%)	10 (6%)	0	100	100
2	V2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	V3	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	V6	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	V7	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	V8	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	VA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	VB	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	VD	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	VE	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	VF	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	VG	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	VI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	W1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	W4	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	W9	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	WJ	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	X3	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	X8	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	XA	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	XD	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	XE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	XG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	Y1	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	Y2	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	Y4	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	Y6	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	Y7	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	Y9	174/177 (98%)	161 (92%)	13 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	YB	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	YF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	YI	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	YJ	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	Z1	143/177 (81%)	138 (96%)	5 (4%)	0	100	100
2	Z4	143/177 (81%)	137 (96%)	6 (4%)	0	100	100
2	Z8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	ZA	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	ZE	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	ZG	177/177 (100%)	168 (95%)	8 (4%)	1 (1%)	25	56
2	a1	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	a2	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	a4	143/177 (81%)	135 (94%)	8 (6%)	0	100	100
2	a6	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	a7	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	aB	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	aF	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	aI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	bE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	bG	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	c2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	c6	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	c7	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	c8	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	cA	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	cB	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	cF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	cI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	d1	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
2	d4	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	dE	176/177 (99%)	170 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	dG	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	e2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	e6	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	e7	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	e8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	eA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	eB	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	eF	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	eI	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	f1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	f4	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	fE	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	fG	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	g2	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	g6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	g7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	g8	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	gA	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	gB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	gF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	gI	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	h1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	h4	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	hE	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	hG	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	i2	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	i6	176/177 (99%)	161 (92%)	15 (8%)	0	100	100
2	i7	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	i8	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	iA	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	iB	176/177 (99%)	163 (93%)	13 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	iF	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
2	iI	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
2	j1	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	j4	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
2	jE	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	jG	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	k2	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	k6	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	k7	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	k8	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	kA	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	kB	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	kF	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	kI	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	l1	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	l4	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	lE	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	lG	177/177 (100%)	160 (90%)	17 (10%)	0	100	100
2	m2	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	m6	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	m7	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	m8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	mA	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	mB	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	mF	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	mI	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	n1	174/177 (98%)	163 (94%)	10 (6%)	1 (1%)	25	56
2	n4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
2	nE	177/177 (100%)	168 (95%)	9 (5%)	0	100	100
2	nG	177/177 (100%)	164 (93%)	13 (7%)	0	100	100
2	pE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	pG	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	q1	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	q4	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	rE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	rG	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	s1	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
2	s4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
2	tE	176/177 (99%)	168 (96%)	8 (4%)	0	100	100
2	tG	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	u1	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	u4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
2	vE	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	vG	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	w1	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	w4	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	y1	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	y4	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
3	21	236/333 (71%)	209 (89%)	27 (11%)	0	100	100
3	24	236/333 (71%)	216 (92%)	20 (8%)	0	100	100
3	M1	236/333 (71%)	209 (89%)	25 (11%)	2 (1%)	19	49
3	M4	236/333 (71%)	211 (89%)	25 (11%)	0	100	100
4	b1	321/405 (79%)	274 (85%)	44 (14%)	3 (1%)	17	46
4	b4	321/405 (79%)	276 (86%)	43 (13%)	2 (1%)	25	56
4	o1	210/405 (52%)	177 (84%)	32 (15%)	1 (0%)	29	61
4	o4	210/405 (52%)	179 (85%)	29 (14%)	2 (1%)	15	44
5	31	283/288 (98%)	264 (93%)	17 (6%)	2 (1%)	22	53
5	34	283/288 (98%)	260 (92%)	21 (7%)	2 (1%)	22	53
6	X2	322/363 (89%)	291 (90%)	31 (10%)	0	100	100
6	X6	322/363 (89%)	282 (88%)	40 (12%)	0	100	100
6	X7	322/363 (89%)	295 (92%)	26 (8%)	1 (0%)	41	72
6	XB	322/363 (89%)	280 (87%)	42 (13%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	XF	322/363 (89%)	295 (92%)	27 (8%)	0	100	100
6	XI	322/363 (89%)	290 (90%)	32 (10%)	0	100	100
7	A2	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
7	A6	255/290 (88%)	235 (92%)	20 (8%)	0	100	100
7	A7	255/290 (88%)	233 (91%)	22 (9%)	0	100	100
7	A9	254/290 (88%)	231 (91%)	23 (9%)	0	100	100
7	AB	255/290 (88%)	225 (88%)	30 (12%)	0	100	100
7	AF	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
7	AI	255/290 (88%)	238 (93%)	17 (7%)	0	100	100
7	AJ	254/290 (88%)	229 (90%)	25 (10%)	0	100	100
7	Y3	235/290 (81%)	216 (92%)	18 (8%)	1 (0%)	34	66
7	YD	235/290 (81%)	216 (92%)	19 (8%)	0	100	100
8	B2	228/232 (98%)	204 (90%)	23 (10%)	1 (0%)	34	66
8	B6	229/232 (99%)	209 (91%)	20 (9%)	0	100	100
8	B7	225/232 (97%)	199 (88%)	25 (11%)	1 (0%)	34	66
8	BB	229/232 (99%)	209 (91%)	20 (9%)	0	100	100
8	BF	225/232 (97%)	202 (90%)	22 (10%)	1 (0%)	34	66
8	BI	228/232 (98%)	207 (91%)	20 (9%)	1 (0%)	34	66
9	C2	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	C6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	C7	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	CB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	CF	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
9	CI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	E2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	E6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	E7	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	EB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	EF	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	EI	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	G2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	G6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	G7	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	GB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	GF	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	GI	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
9	I2	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
9	I6	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	I7	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	IB	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	IF	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
9	II	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
9	K2	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	K6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	K7	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
9	KB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	KF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	KI	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
9	M2	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	M6	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	M7	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	MB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
9	MF	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
9	MI	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
10	D2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	D6	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	56
10	D7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	DB	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
10	DF	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
10	DI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	F2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	F6	169/172 (98%)	166 (98%)	3 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	F7	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	FB	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	FF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	FI	169/172 (98%)	158 (94%)	9 (5%)	2 (1%)	13	39
10	H2	169/172 (98%)	159 (94%)	10 (6%)	0	100	100
10	H6	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	56
10	H7	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	HB	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	HF	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	HI	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	J2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	J6	169/172 (98%)	164 (97%)	3 (2%)	2 (1%)	13	39
10	J7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	JB	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	JF	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	JI	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
10	L2	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	L6	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
10	L7	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	LB	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
10	LF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	LI	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
10	N2	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
10	N6	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	N7	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	NB	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	NF	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
10	NI	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
11	e3	246/303 (81%)	226 (92%)	20 (8%)	0	100	100
11	eD	246/303 (81%)	222 (90%)	24 (10%)	0	100	100
12	b8	378/490 (77%)	334 (88%)	39 (10%)	5 (1%)	12	36

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
12	bA	378/490 (77%)	334 (88%)	44 (12%)	0	100	100
13	A8	236/273 (86%)	217 (92%)	19 (8%)	0	100	100
13	AA	236/273 (86%)	218 (92%)	18 (8%)	0	100	100
13	wE	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
13	wG	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
13	xE	236/273 (86%)	221 (94%)	15 (6%)	0	100	100
13	xG	236/273 (86%)	221 (94%)	15 (6%)	0	100	100
14	B8	248/290 (86%)	234 (94%)	14 (6%)	0	100	100
14	BA	248/290 (86%)	235 (95%)	13 (5%)	0	100	100
14	yE	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
14	yG	248/290 (86%)	237 (96%)	11 (4%)	0	100	100
15	d9	283/342 (83%)	250 (88%)	32 (11%)	1 (0%)	34	66
15	dJ	283/342 (83%)	241 (85%)	40 (14%)	2 (1%)	22	53
16	zE	368/498 (74%)	335 (91%)	33 (9%)	0	100	100
16	zG	368/498 (74%)	341 (93%)	27 (7%)	0	100	100
17	AH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	CH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	EH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	GH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	JH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	KH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	NH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	PH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	RH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	TH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
17	cH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	eH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	gH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	iH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
17	lH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	mH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
17	pH	158/161 (98%)	157 (99%)	1 (1%)	0	100	100
17	rH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
17	tH	158/161 (98%)	156 (99%)	2 (1%)	0	100	100
17	vH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	BH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	DH	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	25	56
18	FH	158/161 (98%)	154 (98%)	3 (2%)	1 (1%)	25	56
18	HH	158/161 (98%)	153 (97%)	4 (2%)	1 (1%)	25	56
18	IH	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	56
18	LH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
18	MH	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
18	OH	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	56
18	QH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	SH	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
18	UH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	dH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	fH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	hH	158/161 (98%)	155 (98%)	2 (1%)	1 (1%)	25	56
18	jH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
18	kH	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
18	nH	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
18	oH	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
18	qH	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	56
18	sH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
18	uH	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
18	wH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
19	VH	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
19	xH	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
20	WH	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
20	yH	171/173 (99%)	165 (96%)	6 (4%)	0	100	100
21	XH	90/93 (97%)	86 (96%)	4 (4%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
21	zH	90/93 (97%)	86 (96%)	4 (4%)	0	100	100
22	1H	840/879 (96%)	785 (94%)	55 (6%)	0	100	100
22	YH	840/879 (96%)	787 (94%)	53 (6%)	0	100	100
23	2H	130/159 (82%)	122 (94%)	8 (6%)	0	100	100
23	ZH	130/159 (82%)	122 (94%)	8 (6%)	0	100	100
24	3H	251/288 (87%)	235 (94%)	15 (6%)	1 (0%)	34	66
24	aH	251/288 (87%)	234 (93%)	17 (7%)	0	100	100
25	4H	204/253 (81%)	187 (92%)	17 (8%)	0	100	100
25	bH	204/253 (81%)	188 (92%)	16 (8%)	0	100	100
All	All	124066/129014 (96%)	117523 (95%)	6496 (5%)	47 (0%)	100	100

5 of 47 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	31	132	SER
7	Y3	57	VAL
2	J4	16	ALA
4	b4	302	CYS
2	BC	74	TYR

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	A3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	A4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	AD	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	AE	128/128 (100%)	128 (100%)	0	100	100
1	AG	128/128 (100%)	128 (100%)	0	100	100
1	B9	128/128 (100%)	126 (98%)	2 (2%)	62	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	BJ	128/128 (100%)	128 (100%)	0	100	100
1	C1	128/128 (100%)	128 (100%)	0	100	100
1	C3	128/128 (100%)	128 (100%)	0	100	100
1	C4	128/128 (100%)	128 (100%)	0	100	100
1	C8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	CA	128/128 (100%)	128 (100%)	0	100	100
1	CD	128/128 (100%)	128 (100%)	0	100	100
1	CE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	CG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	D9	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	DJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	E1	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	E3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	E4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	E8	128/128 (100%)	128 (100%)	0	100	100
1	EA	128/128 (100%)	128 (100%)	0	100	100
1	ED	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	EE	128/128 (100%)	128 (100%)	0	100	100
1	EG	128/128 (100%)	128 (100%)	0	100	100
1	F9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	FJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G1	128/128 (100%)	122 (95%)	6 (5%)	26	59
1	G3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	G8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	GA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	GD	128/128 (100%)	128 (100%)	0	100	100
1	GE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	GG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	H9	128/128 (100%)	128 (100%)	0	100	100
1	HJ	128/128 (100%)	127 (99%)	1 (1%)	81	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	I3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	I4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	I8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	IA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ID	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	IE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	IG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	J5	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	J9	128/128 (100%)	128 (100%)	0	100	100
1	JC	128/128 (100%)	128 (100%)	0	100	100
1	JJ	128/128 (100%)	128 (100%)	0	100	100
1	K1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	K3	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	K4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	K8	128/128 (100%)	128 (100%)	0	100	100
1	KA	128/128 (100%)	128 (100%)	0	100	100
1	KD	128/128 (100%)	128 (100%)	0	100	100
1	KE	128/128 (100%)	128 (100%)	0	100	100
1	KG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	L9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	LJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	M3	128/128 (100%)	128 (100%)	0	100	100
1	M8	128/128 (100%)	128 (100%)	0	100	100
1	MA	128/128 (100%)	128 (100%)	0	100	100
1	MD	128/128 (100%)	128 (100%)	0	100	100
1	ME	128/128 (100%)	128 (100%)	0	100	100
1	MG	128/128 (100%)	128 (100%)	0	100	100
1	N1	128/128 (100%)	128 (100%)	0	100	100
1	N4	128/128 (100%)	128 (100%)	0	100	100
1	N9	128/128 (100%)	127 (99%)	1 (1%)	81	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	NJ	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	O2	128/128 (100%)	128 (100%)	0	100	100
1	O3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	O6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	O7	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	O8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	OA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	OB	128/128 (100%)	128 (100%)	0	100	100
1	OD	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	OE	128/128 (100%)	128 (100%)	0	100	100
1	OF	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	OG	128/128 (100%)	128 (100%)	0	100	100
1	OI	128/128 (100%)	128 (100%)	0	100	100
1	P1	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	P4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	P9	128/128 (100%)	128 (100%)	0	100	100
1	PJ	128/128 (100%)	128 (100%)	0	100	100
1	Q2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Q3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Q6	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	Q7	128/128 (100%)	128 (100%)	0	100	100
1	Q8	128/128 (100%)	128 (100%)	0	100	100
1	QA	128/128 (100%)	128 (100%)	0	100	100
1	QB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	QD	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	QE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	QF	128/128 (100%)	128 (100%)	0	100	100
1	QG	128/128 (100%)	128 (100%)	0	100	100
1	QI	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	R1	128/128 (100%)	128 (100%)	0	100	100
1	R4	128/128 (100%)	128 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	R9	128/128 (100%)	128 (100%)	0	100	100
1	RJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	S2	128/128 (100%)	128 (100%)	0	100	100
1	S3	128/128 (100%)	128 (100%)	0	100	100
1	S6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	S7	128/128 (100%)	128 (100%)	0	100	100
1	S8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	SA	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	SB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	SD	128/128 (100%)	128 (100%)	0	100	100
1	SE	128/128 (100%)	128 (100%)	0	100	100
1	SF	128/128 (100%)	128 (100%)	0	100	100
1	SG	128/128 (100%)	128 (100%)	0	100	100
1	SI	128/128 (100%)	128 (100%)	0	100	100
1	T1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	T4	128/128 (100%)	128 (100%)	0	100	100
1	T9	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	TJ	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	U2	128/128 (100%)	128 (100%)	0	100	100
1	U3	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	U6	128/128 (100%)	128 (100%)	0	100	100
1	U7	128/128 (100%)	128 (100%)	0	100	100
1	U8	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	UA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	UD	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	UF	128/128 (100%)	128 (100%)	0	100	100
1	UG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	UI	128/128 (100%)	128 (100%)	0	100	100
1	V1	128/128 (100%)	128 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	V4	128/128 (100%)	128 (100%)	0	100	100
1	V9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	VJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	W2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	W3	128/128 (100%)	128 (100%)	0	100	100
1	W6	128/128 (100%)	128 (100%)	0	100	100
1	W7	128/128 (100%)	128 (100%)	0	100	100
1	W8	128/128 (100%)	128 (100%)	0	100	100
1	WA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	WB	128/128 (100%)	128 (100%)	0	100	100
1	WD	128/128 (100%)	128 (100%)	0	100	100
1	WE	128/128 (100%)	128 (100%)	0	100	100
1	WF	128/128 (100%)	128 (100%)	0	100	100
1	WG	128/128 (100%)	128 (100%)	0	100	100
1	WI	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	X1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	X4	128/128 (100%)	128 (100%)	0	100	100
1	X9	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	XJ	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	Y8	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	YA	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	YE	128/128 (100%)	128 (100%)	0	100	100
1	YG	128/128 (100%)	128 (100%)	0	100	100
1	Z2	128/128 (100%)	128 (100%)	0	100	100
1	Z6	128/128 (100%)	128 (100%)	0	100	100
1	Z7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ZB	128/128 (100%)	128 (100%)	0	100	100
1	ZF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	ZI	128/128 (100%)	128 (100%)	0	100	100
1	a8	128/128 (100%)	128 (100%)	0	100	100
1	aA	128/128 (100%)	127 (99%)	1 (1%)	81	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	aE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	aG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	b2	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	b6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	b7	128/128 (100%)	128 (100%)	0	100	100
1	bB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	bF	128/128 (100%)	128 (100%)	0	100	100
1	bI	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	c1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	c4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	cE	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	cG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d6	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	d7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	d8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	dA	128/128 (100%)	128 (100%)	0	100	100
1	dB	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	dF	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	dI	128/128 (100%)	128 (100%)	0	100	100
1	e1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	e4	128/128 (100%)	128 (100%)	0	100	100
1	eE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	eG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	f2	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	f6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	f7	128/128 (100%)	128 (100%)	0	100	100
1	f8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	fA	128/128 (100%)	128 (100%)	0	100	100
1	fB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	fF	128/128 (100%)	128 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	fI	128/128 (100%)	128 (100%)	0	100	100
1	g1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	g4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	gE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	gG	128/128 (100%)	128 (100%)	0	100	100
1	h2	128/128 (100%)	128 (100%)	0	100	100
1	h6	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	h7	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	h8	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	hA	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hB	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	hI	128/128 (100%)	128 (100%)	0	100	100
1	i1	128/128 (100%)	128 (100%)	0	100	100
1	i4	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	iE	128/128 (100%)	128 (100%)	0	100	100
1	iG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	j2	128/128 (100%)	128 (100%)	0	100	100
1	j6	128/128 (100%)	128 (100%)	0	100	100
1	j7	128/128 (100%)	128 (100%)	0	100	100
1	j8	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	jA	128/128 (100%)	128 (100%)	0	100	100
1	jB	128/128 (100%)	128 (100%)	0	100	100
1	jF	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	jI	128/128 (100%)	128 (100%)	0	100	100
1	k1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	k4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	kE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	kG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	l2	128/128 (100%)	128 (100%)	0	100	100
1	l6	128/128 (100%)	126 (98%)	2 (2%)	62	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	l7	128/128 (100%)	128 (100%)	0	100	100
1	l8	128/128 (100%)	119 (93%)	9 (7%)	15	40
1	lA	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	lB	128/128 (100%)	128 (100%)	0	100	100
1	lF	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	lI	128/128 (100%)	128 (100%)	0	100	100
1	m1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	m4	128/128 (100%)	128 (100%)	0	100	100
1	mE	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	mG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	oE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	oG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	p1	128/128 (100%)	128 (100%)	0	100	100
1	p4	128/128 (100%)	128 (100%)	0	100	100
1	qE	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	qG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	r1	128/128 (100%)	124 (97%)	4 (3%)	40	74
1	r4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	sE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	sG	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	t1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	t4	128/128 (100%)	128 (100%)	0	100	100
1	uE	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	uG	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	v1	128/128 (100%)	128 (100%)	0	100	100
1	v4	128/128 (100%)	126 (98%)	2 (2%)	62	88
1	x1	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	x4	128/128 (100%)	125 (98%)	3 (2%)	50	82
1	z1	128/128 (100%)	127 (99%)	1 (1%)	81	94
1	z4	128/128 (100%)	126 (98%)	2 (2%)	62	88
2	11	137/137 (100%)	137 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	14	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	A5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	AC	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	B1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	B3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	B4	137/137 (100%)	137 (100%)	0	100	100
2	B5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	BC	113/137 (82%)	101 (89%)	12 (11%)	6	20
2	BD	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	BE	138/137 (101%)	137 (99%)	1 (1%)	84	95
2	BG	138/137 (101%)	138 (100%)	0	100	100
2	C5	113/137 (82%)	113 (100%)	0	100	100
2	C9	137/137 (100%)	137 (100%)	0	100	100
2	CC	113/137 (82%)	110 (97%)	3 (3%)	44	78
2	CJ	137/137 (100%)	137 (100%)	0	100	100
2	D1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	D3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	D4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	D8	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DD	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	DE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	DG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	E9	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	EJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F3	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	F4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	F5	113/137 (82%)	113 (100%)	0	100	100
2	F8	140/137 (102%)	140 (100%)	0	100	100
2	FA	140/137 (102%)	140 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FC	113/137 (82%)	113 (100%)	0	100	100
2	FD	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	FE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	FG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	G5	113/137 (82%)	110 (97%)	3 (3%)	44	78
2	G9	137/137 (100%)	137 (100%)	0	100	100
2	GC	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	GJ	137/137 (100%)	137 (100%)	0	100	100
2	H1	138/137 (101%)	138 (100%)	0	100	100
2	H3	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	H4	139/137 (102%)	139 (100%)	0	100	100
2	H5	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	H8	140/137 (102%)	140 (100%)	0	100	100
2	HA	140/137 (102%)	140 (100%)	0	100	100
2	HC	113/137 (82%)	113 (100%)	0	100	100
2	HD	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	HE	140/137 (102%)	140 (100%)	0	100	100
2	HG	140/137 (102%)	140 (100%)	0	100	100
2	I5	137/137 (100%)	132 (96%)	5 (4%)	35	69
2	I9	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	IC	136/137 (99%)	136 (100%)	0	100	100
2	IJ	139/137 (102%)	139 (100%)	0	100	100
2	J1	137/137 (100%)	137 (100%)	0	100	100
2	J3	137/137 (100%)	137 (100%)	0	100	100
2	J4	137/137 (100%)	137 (100%)	0	100	100
2	J8	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	JA	139/137 (102%)	139 (100%)	0	100	100
2	JD	137/137 (100%)	137 (100%)	0	100	100
2	JE	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	JG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	K5	137/137 (100%)	133 (97%)	4 (3%)	42	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K9	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	KC	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	KJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	L1	137/137 (100%)	137 (100%)	0	100	100
2	L3	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	L4	137/137 (100%)	137 (100%)	0	100	100
2	L5	113/137 (82%)	104 (92%)	9 (8%)	12	34
2	L8	140/137 (102%)	140 (100%)	0	100	100
2	LA	140/137 (102%)	140 (100%)	0	100	100
2	LC	113/137 (82%)	107 (95%)	6 (5%)	22	54
2	LD	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	LE	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	LG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	M9	137/137 (100%)	137 (100%)	0	100	100
2	MJ	137/137 (100%)	137 (100%)	0	100	100
2	N3	140/137 (102%)	140 (100%)	0	100	100
2	N8	140/137 (102%)	134 (96%)	6 (4%)	29	62
2	NA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ND	140/137 (102%)	140 (100%)	0	100	100
2	NE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	NG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	O1	137/137 (100%)	137 (100%)	0	100	100
2	O4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	O9	137/137 (100%)	137 (100%)	0	100	100
2	OJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	P2	137/137 (100%)	137 (100%)	0	100	100
2	P3	140/137 (102%)	136 (97%)	4 (3%)	42	76
2	P6	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	P7	137/137 (100%)	137 (100%)	0	100	100
2	P8	137/137 (100%)	137 (100%)	0	100	100
2	PA	137/137 (100%)	135 (98%)	2 (2%)	65	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	PB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	PD	140/137 (102%)	135 (96%)	5 (4%)	35	69
2	PE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	PF	137/137 (100%)	137 (100%)	0	100	100
2	PG	140/137 (102%)	140 (100%)	0	100	100
2	PI	137/137 (100%)	137 (100%)	0	100	100
2	Q1	137/137 (100%)	137 (100%)	0	100	100
2	Q4	137/137 (100%)	137 (100%)	0	100	100
2	Q9	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	QJ	137/137 (100%)	137 (100%)	0	100	100
2	R2	137/137 (100%)	137 (100%)	0	100	100
2	R3	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	R6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	R7	137/137 (100%)	137 (100%)	0	100	100
2	R8	138/137 (101%)	138 (100%)	0	100	100
2	RA	138/137 (101%)	137 (99%)	1 (1%)	84	95
2	RB	137/137 (100%)	137 (100%)	0	100	100
2	RD	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	RE	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	RF	137/137 (100%)	137 (100%)	0	100	100
2	RG	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	RI	137/137 (100%)	137 (100%)	0	100	100
2	S1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	S4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	S9	137/137 (100%)	137 (100%)	0	100	100
2	SJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	T2	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	T3	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	T6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	T7	137/137 (100%)	137 (100%)	0	100	100
2	T8	140/137 (102%)	140 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	TA	140/137 (102%)	140 (100%)	0	100	100
2	TB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	TD	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	TE	139/137 (102%)	139 (100%)	0	100	100
2	TF	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	TG	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	TI	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	U1	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	U4	139/137 (102%)	139 (100%)	0	100	100
2	U9	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	UJ	139/137 (102%)	139 (100%)	0	100	100
2	V2	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	V3	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	V6	139/137 (102%)	139 (100%)	0	100	100
2	V7	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	V8	140/137 (102%)	140 (100%)	0	100	100
2	VA	140/137 (102%)	140 (100%)	0	100	100
2	VB	139/137 (102%)	139 (100%)	0	100	100
2	VD	140/137 (102%)	140 (100%)	0	100	100
2	VE	139/137 (102%)	136 (98%)	3 (2%)	52	83
2	VF	139/137 (102%)	139 (100%)	0	100	100
2	VG	139/137 (102%)	138 (99%)	1 (1%)	84	95
2	VI	137/137 (100%)	132 (96%)	5 (4%)	35	69
2	W1	137/137 (100%)	137 (100%)	0	100	100
2	W4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	W9	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	WJ	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	X3	140/137 (102%)	140 (100%)	0	100	100
2	X8	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	XA	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	XD	140/137 (102%)	139 (99%)	1 (1%)	84	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	XE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	XG	140/137 (102%)	140 (100%)	0	100	100
2	Y1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	Y2	137/137 (100%)	137 (100%)	0	100	100
2	Y4	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	Y6	137/137 (100%)	137 (100%)	0	100	100
2	Y7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	Y9	137/137 (100%)	137 (100%)	0	100	100
2	YB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	YF	137/137 (100%)	137 (100%)	0	100	100
2	YI	137/137 (100%)	137 (100%)	0	100	100
2	YJ	137/137 (100%)	137 (100%)	0	100	100
2	Z1	113/137 (82%)	113 (100%)	0	100	100
2	Z4	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	Z8	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ZA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	ZE	140/137 (102%)	140 (100%)	0	100	100
2	ZG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	a1	113/137 (82%)	113 (100%)	0	100	100
2	a2	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	a4	113/137 (82%)	112 (99%)	1 (1%)	78	94
2	a6	137/137 (100%)	137 (100%)	0	100	100
2	a7	137/137 (100%)	137 (100%)	0	100	100
2	aB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	aF	137/137 (100%)	137 (100%)	0	100	100
2	aI	137/137 (100%)	133 (97%)	4 (3%)	42	76
2	bE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	bG	140/137 (102%)	140 (100%)	0	100	100
2	c2	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	c6	137/137 (100%)	137 (100%)	0	100	100
2	c7	137/137 (100%)	137 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	c8	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	cA	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	cB	137/137 (100%)	137 (100%)	0	100	100
2	cF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	cI	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	d1	137/137 (100%)	137 (100%)	0	100	100
2	d4	137/137 (100%)	137 (100%)	0	100	100
2	dE	139/137 (102%)	139 (100%)	0	100	100
2	dG	139/137 (102%)	139 (100%)	0	100	100
2	e2	137/137 (100%)	137 (100%)	0	100	100
2	e6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	e7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	e8	140/137 (102%)	140 (100%)	0	100	100
2	eA	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	eB	137/137 (100%)	137 (100%)	0	100	100
2	eF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	eI	137/137 (100%)	137 (100%)	0	100	100
2	f1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	f4	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	fE	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	fG	139/137 (102%)	139 (100%)	0	100	100
2	g2	137/137 (100%)	137 (100%)	0	100	100
2	g6	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	g7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	g8	140/137 (102%)	140 (100%)	0	100	100
2	gA	140/137 (102%)	140 (100%)	0	100	100
2	gB	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	gF	137/137 (100%)	137 (100%)	0	100	100
2	gI	137/137 (100%)	137 (100%)	0	100	100
2	h1	137/137 (100%)	137 (100%)	0	100	100
2	h4	137/137 (100%)	136 (99%)	1 (1%)	84	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	hE	140/137 (102%)	140 (100%)	0	100	100
2	hG	140/137 (102%)	140 (100%)	0	100	100
2	i2	138/137 (101%)	138 (100%)	0	100	100
2	i6	139/137 (102%)	139 (100%)	0	100	100
2	i7	139/137 (102%)	139 (100%)	0	100	100
2	i8	140/137 (102%)	140 (100%)	0	100	100
2	iA	140/137 (102%)	140 (100%)	0	100	100
2	iB	139/137 (102%)	139 (100%)	0	100	100
2	iF	139/137 (102%)	135 (97%)	4 (3%)	42	76
2	iI	138/137 (101%)	138 (100%)	0	100	100
2	j1	138/137 (101%)	136 (99%)	2 (1%)	67	90
2	j4	138/137 (101%)	138 (100%)	0	100	100
2	jE	140/137 (102%)	140 (100%)	0	100	100
2	jG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	k2	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	k6	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	k7	137/137 (100%)	137 (100%)	0	100	100
2	k8	140/137 (102%)	140 (100%)	0	100	100
2	kA	140/137 (102%)	140 (100%)	0	100	100
2	kB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	kF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	kI	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	l1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	l4	137/137 (100%)	137 (100%)	0	100	100
2	lE	140/137 (102%)	140 (100%)	0	100	100
2	lG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	m2	137/137 (100%)	137 (100%)	0	100	100
2	m6	137/137 (100%)	137 (100%)	0	100	100
2	m7	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	m8	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	mA	140/137 (102%)	137 (98%)	3 (2%)	53	84

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	mB	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	mF	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	mI	137/137 (100%)	137 (100%)	0	100	100
2	n1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	n4	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	nE	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	nG	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	pE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	pG	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	q1	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	q4	137/137 (100%)	134 (98%)	3 (2%)	52	83
2	rE	140/137 (102%)	139 (99%)	1 (1%)	84	95
2	rG	140/137 (102%)	137 (98%)	3 (2%)	53	84
2	s1	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	s4	137/137 (100%)	137 (100%)	0	100	100
2	tE	139/137 (102%)	137 (99%)	2 (1%)	67	90
2	tG	139/137 (102%)	139 (100%)	0	100	100
2	u1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	u4	137/137 (100%)	135 (98%)	2 (2%)	65	89
2	vE	140/137 (102%)	138 (99%)	2 (1%)	67	90
2	vG	140/137 (102%)	140 (100%)	0	100	100
2	w1	139/137 (102%)	139 (100%)	0	100	100
2	w4	139/137 (102%)	139 (100%)	0	100	100
2	y1	137/137 (100%)	136 (99%)	1 (1%)	84	95
2	y4	137/137 (100%)	136 (99%)	1 (1%)	84	95
3	21	183/262 (70%)	171 (93%)	12 (7%)	16	44
3	24	183/262 (70%)	174 (95%)	9 (5%)	25	57
3	M1	183/262 (70%)	177 (97%)	6 (3%)	38	72
3	M4	183/262 (70%)	177 (97%)	6 (3%)	38	72
4	b1	268/331 (81%)	254 (95%)	14 (5%)	23	55
4	b4	268/331 (81%)	254 (95%)	14 (5%)	23	55

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	o1	176/331 (53%)	172 (98%)	4 (2%)	50	82
4	o4	176/331 (53%)	169 (96%)	7 (4%)	31	65
5	31	227/229 (99%)	221 (97%)	6 (3%)	46	79
5	34	227/229 (99%)	221 (97%)	6 (3%)	46	79
6	X2	261/289 (90%)	259 (99%)	2 (1%)	81	94
6	X6	261/289 (90%)	255 (98%)	6 (2%)	50	82
6	X7	261/289 (90%)	260 (100%)	1 (0%)	91	97
6	XB	261/289 (90%)	258 (99%)	3 (1%)	73	92
6	XF	261/289 (90%)	260 (100%)	1 (0%)	91	97
6	XI	261/289 (90%)	256 (98%)	5 (2%)	57	85
7	A2	199/222 (90%)	199 (100%)	0	100	100
7	A6	199/222 (90%)	198 (100%)	1 (0%)	88	96
7	A7	199/222 (90%)	197 (99%)	2 (1%)	76	93
7	A9	198/222 (89%)	194 (98%)	4 (2%)	55	84
7	AB	199/222 (90%)	199 (100%)	0	100	100
7	AF	199/222 (90%)	196 (98%)	3 (2%)	65	89
7	AI	199/222 (90%)	199 (100%)	0	100	100
7	AJ	198/222 (89%)	196 (99%)	2 (1%)	76	93
7	Y3	182/222 (82%)	180 (99%)	2 (1%)	73	92
7	YD	182/222 (82%)	179 (98%)	3 (2%)	62	88
8	B2	209/211 (99%)	202 (97%)	7 (3%)	38	72
8	B6	210/211 (100%)	206 (98%)	4 (2%)	57	85
8	B7	208/211 (99%)	206 (99%)	2 (1%)	76	93
8	BB	210/211 (100%)	202 (96%)	8 (4%)	33	67
8	BF	208/211 (99%)	206 (99%)	2 (1%)	76	93
8	BI	209/211 (99%)	200 (96%)	9 (4%)	29	62
9	C2	125/125 (100%)	125 (100%)	0	100	100
9	C6	125/125 (100%)	125 (100%)	0	100	100
9	C7	125/125 (100%)	125 (100%)	0	100	100
9	CB	125/125 (100%)	125 (100%)	0	100	100
9	CF	125/125 (100%)	124 (99%)	1 (1%)	81	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	CI	125/125 (100%)	125 (100%)	0	100	100
9	E2	125/125 (100%)	125 (100%)	0	100	100
9	E6	125/125 (100%)	125 (100%)	0	100	100
9	E7	125/125 (100%)	125 (100%)	0	100	100
9	EB	125/125 (100%)	125 (100%)	0	100	100
9	EF	125/125 (100%)	125 (100%)	0	100	100
9	EI	125/125 (100%)	125 (100%)	0	100	100
9	G2	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	G6	125/125 (100%)	125 (100%)	0	100	100
9	G7	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	GB	125/125 (100%)	125 (100%)	0	100	100
9	GF	125/125 (100%)	125 (100%)	0	100	100
9	GI	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	I2	125/125 (100%)	125 (100%)	0	100	100
9	I6	125/125 (100%)	125 (100%)	0	100	100
9	I7	125/125 (100%)	123 (98%)	2 (2%)	62	88
9	IB	125/125 (100%)	125 (100%)	0	100	100
9	IF	125/125 (100%)	125 (100%)	0	100	100
9	II	125/125 (100%)	125 (100%)	0	100	100
9	K2	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	K6	125/125 (100%)	125 (100%)	0	100	100
9	K7	125/125 (100%)	125 (100%)	0	100	100
9	KB	125/125 (100%)	125 (100%)	0	100	100
9	KF	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	KI	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	M2	125/125 (100%)	123 (98%)	2 (2%)	62	88
9	M6	125/125 (100%)	125 (100%)	0	100	100
9	M7	125/125 (100%)	124 (99%)	1 (1%)	81	94
9	MB	125/125 (100%)	125 (100%)	0	100	100
9	MF	125/125 (100%)	125 (100%)	0	100	100
9	MI	125/125 (100%)	123 (98%)	2 (2%)	62	88

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	D2	134/134 (100%)	134 (100%)	0	100	100
10	D6	134/134 (100%)	134 (100%)	0	100	100
10	D7	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	DB	134/134 (100%)	134 (100%)	0	100	100
10	DF	134/134 (100%)	134 (100%)	0	100	100
10	DI	134/134 (100%)	134 (100%)	0	100	100
10	F2	134/134 (100%)	134 (100%)	0	100	100
10	F6	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	F7	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	FB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	FF	134/134 (100%)	134 (100%)	0	100	100
10	FI	134/134 (100%)	134 (100%)	0	100	100
10	H2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	H6	134/134 (100%)	134 (100%)	0	100	100
10	H7	134/134 (100%)	134 (100%)	0	100	100
10	HB	134/134 (100%)	134 (100%)	0	100	100
10	HF	134/134 (100%)	134 (100%)	0	100	100
10	HI	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	J2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	J6	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	J7	134/134 (100%)	131 (98%)	3 (2%)	52	83
10	JB	134/134 (100%)	134 (100%)	0	100	100
10	JF	134/134 (100%)	132 (98%)	2 (2%)	65	89
10	JI	134/134 (100%)	134 (100%)	0	100	100
10	L2	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	L6	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	L7	134/134 (100%)	134 (100%)	0	100	100
10	LB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	LF	134/134 (100%)	134 (100%)	0	100	100
10	LI	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	N2	134/134 (100%)	134 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	N6	134/134 (100%)	134 (100%)	0	100	100
10	N7	134/134 (100%)	134 (100%)	0	100	100
10	NB	134/134 (100%)	133 (99%)	1 (1%)	84	95
10	NF	134/134 (100%)	134 (100%)	0	100	100
10	NI	134/134 (100%)	133 (99%)	1 (1%)	84	95
11	e3	204/237 (86%)	204 (100%)	0	100	100
11	eD	204/237 (86%)	204 (100%)	0	100	100
12	b8	304/389 (78%)	291 (96%)	13 (4%)	29	62
12	bA	304/389 (78%)	293 (96%)	11 (4%)	35	69
13	A8	179/203 (88%)	177 (99%)	2 (1%)	73	92
13	AA	179/203 (88%)	179 (100%)	0	100	100
13	wE	179/203 (88%)	175 (98%)	4 (2%)	52	83
13	wG	179/203 (88%)	178 (99%)	1 (1%)	86	96
13	xE	179/203 (88%)	177 (99%)	2 (1%)	73	92
13	xG	179/203 (88%)	178 (99%)	1 (1%)	86	96
14	B8	188/218 (86%)	188 (100%)	0	100	100
14	BA	188/218 (86%)	188 (100%)	0	100	100
14	yE	188/218 (86%)	187 (100%)	1 (0%)	88	96
14	yG	188/218 (86%)	187 (100%)	1 (0%)	88	96
15	d9	238/278 (86%)	225 (94%)	13 (6%)	21	52
15	dJ	238/278 (86%)	229 (96%)	9 (4%)	33	67
16	zE	303/406 (75%)	301 (99%)	2 (1%)	84	95
16	zG	303/406 (75%)	302 (100%)	1 (0%)	92	98
17	AH	130/131 (99%)	130 (100%)	0	100	100
17	CH	130/131 (99%)	130 (100%)	0	100	100
17	EH	130/131 (99%)	130 (100%)	0	100	100
17	GH	130/131 (99%)	130 (100%)	0	100	100
17	JH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	KH	130/131 (99%)	130 (100%)	0	100	100
17	NH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	PH	130/131 (99%)	129 (99%)	1 (1%)	81	94

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
17	RH	130/131 (99%)	130 (100%)	0	100	100
17	TH	130/131 (99%)	130 (100%)	0	100	100
17	cH	130/131 (99%)	130 (100%)	0	100	100
17	eH	130/131 (99%)	130 (100%)	0	100	100
17	gH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	iH	130/131 (99%)	130 (100%)	0	100	100
17	lH	130/131 (99%)	128 (98%)	2 (2%)	65	89
17	mH	130/131 (99%)	130 (100%)	0	100	100
17	pH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	rH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	tH	130/131 (99%)	129 (99%)	1 (1%)	81	94
17	vH	130/131 (99%)	130 (100%)	0	100	100
18	BH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	DH	124/124 (100%)	124 (100%)	0	100	100
18	FH	124/124 (100%)	124 (100%)	0	100	100
18	HH	124/124 (100%)	124 (100%)	0	100	100
18	IH	124/124 (100%)	124 (100%)	0	100	100
18	LH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	MH	124/124 (100%)	122 (98%)	2 (2%)	62	88
18	OH	124/124 (100%)	124 (100%)	0	100	100
18	QH	124/124 (100%)	124 (100%)	0	100	100
18	SH	124/124 (100%)	124 (100%)	0	100	100
18	UH	124/124 (100%)	124 (100%)	0	100	100
18	dH	124/124 (100%)	124 (100%)	0	100	100
18	fH	124/124 (100%)	124 (100%)	0	100	100
18	hH	124/124 (100%)	124 (100%)	0	100	100
18	jH	124/124 (100%)	124 (100%)	0	100	100
18	kH	124/124 (100%)	123 (99%)	1 (1%)	81	94
18	nH	124/124 (100%)	124 (100%)	0	100	100
18	oH	124/124 (100%)	119 (96%)	5 (4%)	31	65
18	qH	124/124 (100%)	124 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	sH	124/124 (100%)	124 (100%)	0	100	100
18	uH	124/124 (100%)	124 (100%)	0	100	100
18	wH	124/124 (100%)	124 (100%)	0	100	100
19	VH	133/136 (98%)	133 (100%)	0	100	100
19	xH	133/136 (98%)	133 (100%)	0	100	100
20	WH	147/153 (96%)	147 (100%)	0	100	100
20	yH	147/153 (96%)	147 (100%)	0	100	100
21	XH	78/79 (99%)	78 (100%)	0	100	100
21	zH	78/79 (99%)	78 (100%)	0	100	100
22	1H	742/772 (96%)	737 (99%)	5 (1%)	84	95
22	YH	742/772 (96%)	737 (99%)	5 (1%)	84	95
23	2H	106/121 (88%)	106 (100%)	0	100	100
23	ZH	106/121 (88%)	106 (100%)	0	100	100
24	3H	194/214 (91%)	186 (96%)	8 (4%)	30	64
24	aH	194/214 (91%)	187 (96%)	7 (4%)	35	69
25	4H	165/199 (83%)	161 (98%)	4 (2%)	49	81
25	bH	165/199 (83%)	161 (98%)	4 (2%)	49	81
All	All	98470/100830 (98%)	97640 (99%)	830 (1%)	82	94

5 of 830 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	ZA	132[B]	SER
1	GE	78	LYS
1	bI	140	VAL
6	XB	304	TYR
2	ZA	132[A]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1083 such sidechains are listed below:

Mol	Chain	Res	Type
17	pH	53	GLN
22	1H	415	GLN
18	oH	47	ASN
1	DJ	32	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	17	88	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](#)

332 non-standard protein/DNA/RNA residues 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
18	MEN	FH	71	18	7,7,9	0.99	0	6,8,11	1.18	1 (16%)
2	MEN	s1	72	2	7,8,9	0.93	0	6,9,11	1.40	2 (33%)
2	MEN	XA	72	2	7,8,9	0.88	0	6,9,11	1.78	2 (33%)
2	MEN	RF	72	2	7,8,9	0.84	0	6,9,11	1.13	1 (16%)
2	MEN	LE	72	2,26	7,8,9	1.80	1 (14%)	6,9,11	3.66	3 (50%)
10	MEN	HI	72	10	7,8,9	0.86	0	6,9,11	1.67	2 (33%)
10	MEN	NB	72	10	7,8,9	0.84	0	6,9,11	1.64	2 (33%)
2	MEN	C9	72	2	7,8,9	0.85	0	6,9,11	1.48	2 (33%)
2	MEN	11	72	2	7,8,9	0.95	0	6,9,11	1.29	1 (16%)
18	MEN	qH	71	18	7,7,9	0.95	0	6,8,11	1.92	2 (33%)
2	MEN	XG	72	2,26	7,8,9	1.93	1 (14%)	6,9,11	3.18	2 (33%)
2	MEN	n4	72	2	7,8,9	0.88	0	6,9,11	1.05	0
2	MEN	gI	72	2	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
2	MEN	y4	72	2	7,8,9	1.01	0	6,9,11	1.22	1 (16%)
2	MEN	H5	72	2	7,8,9	0.85	0	6,9,11	1.27	1 (16%)
2	MEN	TA	72	2	7,8,9	0.84	0	6,9,11	1.74	2 (33%)
2	MEN	BD	72	2	7,8,9	0.97	0	6,9,11	1.13	1 (16%)
2	MEN	i2	72	2	7,8,9	0.88	0	6,9,11	1.53	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	jE	72	2,26	7,8,9	1.29	1 (14%)	6,9,11	1.65	1 (16%)
18	MEN	uH	71	18	7,8,9	0.88	0	6,9,11	1.43	2 (33%)
2	MEN	kI	72	2	7,8,9	0.89	0	6,9,11	1.50	1 (16%)
18	MEN	hH	71	18	7,7,9	0.97	0	6,8,11	1.99	1 (16%)
2	MEN	YI	72	2	7,8,9	0.83	0	6,9,11	1.45	1 (16%)
2	MEN	a1	72	2	7,8,9	0.79	0	6,9,11	1.66	2 (33%)
18	MEN	oH	71	18	7,7,9	0.99	0	6,8,11	1.67	1 (16%)
2	MEN	m8	72	2	7,8,9	0.90	0	6,9,11	1.58	2 (33%)
2	MEN	k2	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	C5	72	2	7,8,9	0.91	0	6,9,11	1.49	2 (33%)
2	MEN	H1	72	2	7,8,9	0.93	0	6,9,11	1.42	1 (16%)
2	MEN	gA	72	2	7,8,9	0.88	0	6,9,11	1.20	1 (16%)
2	MEN	u4	72	2	7,8,9	0.91	0	6,9,11	1.21	1 (16%)
2	MEN	ZE	72	2,26	7,8,9	1.65	1 (14%)	6,9,11	2.27	2 (33%)
18	MEN	wH	71	18	7,8,9	0.94	0	6,9,11	1.46	1 (16%)
2	MEN	vG	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	1.16	1 (16%)
10	MEN	H6	72	10	7,8,9	0.90	0	6,9,11	1.41	2 (33%)
2	MEN	L1	72	2	7,8,9	0.89	0	6,9,11	1.60	1 (16%)
2	MEN	YB	72	2	7,8,9	0.94	0	6,9,11	1.37	1 (16%)
2	MEN	Z8	72	2	7,8,9	0.85	0	6,9,11	1.60	2 (33%)
2	MEN	g7	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	VI	72	2	7,8,9	0.91	0	6,9,11	1.34	2 (33%)
2	MEN	DA	72	2	7,8,9	0.81	0	6,9,11	1.33	1 (16%)
10	MEN	J7	72	10	7,8,9	0.87	0	6,9,11	1.38	1 (16%)
2	MEN	T3	72	2	7,8,9	0.95	0	6,9,11	3.30	3 (50%)
2	MEN	L3	72	2	7,8,9	0.86	0	6,9,11	1.35	1 (16%)
2	MEN	WJ	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	d1	72	2	7,8,9	0.86	0	6,9,11	1.66	1 (16%)
18	MEN	UH	71	18	7,8,9	0.85	0	6,9,11	1.22	1 (16%)
2	MEN	G9	72	2	7,8,9	0.86	0	6,9,11	1.77	2 (33%)
2	MEN	FA	72	2	7,8,9	0.96	0	6,9,11	1.44	1 (16%)
2	MEN	TB	72	2	7,8,9	0.99	0	6,9,11	1.45	1 (16%)
2	MEN	q1	72	2	7,8,9	0.94	0	6,9,11	1.50	2 (33%)
2	MEN	e7	72	2	7,8,9	0.89	0	6,9,11	1.40	2 (33%)
2	MEN	DG	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.43	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	L5	72	2	7,8,9	1.05	0	6,9,11	1.11	1 (16%)
2	MEN	iA	72	2	7,8,9	0.91	0	6,9,11	1.40	1 (16%)
2	MEN	M9	72	2	7,8,9	0.86	0	6,9,11	1.72	2 (33%)
2	MEN	LG	72	2,26	7,8,9	1.83	1 (14%)	6,9,11	3.79	3 (50%)
10	MEN	F2	72	10	7,8,9	0.90	0	6,9,11	1.63	1 (16%)
2	MEN	w1	72	2	7,8,9	0.94	0	6,9,11	1.24	1 (16%)
2	MEN	eA	72	2	7,8,9	0.87	0	6,9,11	1.33	0
2	MEN	jG	72	2,26	7,8,9	1.31	1 (14%)	6,9,11	1.80	2 (33%)
2	MEN	a7	72	2	7,8,9	0.89	0	6,9,11	1.25	1 (16%)
2	MEN	i7	72	2	7,8,9	0.86	0	6,9,11	1.62	2 (33%)
2	MEN	GJ	72	2	7,8,9	0.91	0	6,9,11	1.87	2 (33%)
2	MEN	F4	72	2	7,8,9	0.94	0	6,9,11	1.59	1 (16%)
2	MEN	P8	72	2	7,8,9	0.94	0	6,9,11	1.34	1 (16%)
10	MEN	DB	72	10,6	7,8,9	0.89	0	6,9,11	1.72	2 (33%)
2	MEN	U1	72	2	7,8,9	0.88	0	6,9,11	1.62	2 (33%)
2	MEN	e8	72	2	7,8,9	0.90	0	6,9,11	1.38	1 (16%)
2	MEN	RG	72	2,26	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	DE	72	2,26	7,8,9	1.50	1 (14%)	6,9,11	2.02	2 (33%)
2	MEN	tG	72	2,26	7,8,9	1.18	1 (14%)	6,9,11	1.44	1 (16%)
2	MEN	TE	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	2.23	2 (33%)
2	MEN	hG	72	2,26	7,8,9	1.21	1 (14%)	6,9,11	0.86	0
2	MEN	aI	72	2	7,8,9	0.87	0	6,9,11	1.45	2 (33%)
2	MEN	eI	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	BG	72	2,26	7,8,9	1.62	1 (14%)	6,9,11	3.02	1 (16%)
2	MEN	MJ	72	2	7,8,9	0.84	0	6,9,11	1.82	2 (33%)
2	MEN	V2	72	2	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
10	MEN	LI	72	10	7,8,9	0.83	0	6,9,11	1.85	2 (33%)
2	MEN	j1	72	2	7,8,9	0.85	0	6,9,11	2.41	2 (33%)
10	MEN	DI	72	10	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
2	MEN	kB	72	2	7,8,9	0.89	0	6,9,11	1.51	1 (16%)
2	MEN	W4	72	2	7,8,9	0.87	0	6,9,11	1.61	1 (16%)
2	MEN	c6	72	2	7,8,9	0.89	0	6,9,11	1.10	1 (16%)
2	MEN	RI	72	2	7,8,9	0.88	0	6,9,11	1.46	2 (33%)
2	MEN	PD	72	2	7,8,9	0.84	0	6,9,11	1.45	1 (16%)
2	MEN	l4	72	2	7,8,9	0.88	0	6,9,11	1.25	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	q4	72	2	7,8,9	0.90	0	6,9,11	1.64	1 (16%)
2	MEN	F3	72	2	7,8,9	0.92	0	6,9,11	1.47	1 (16%)
2	MEN	JA	72	2	7,8,9	0.83	0	6,9,11	1.66	1 (16%)
2	MEN	ZG	72	2	7,8,9	0.90	0	6,9,11	1.38	1 (16%)
10	MEN	JI	72	10	7,8,9	0.84	0	6,9,11	1.86	2 (33%)
2	MEN	H3	72	2	7,8,9	0.91	0	6,9,11	1.68	1 (16%)
10	MEN	FF	72	10	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	mI	72	2	7,8,9	0.88	0	6,9,11	1.52	2 (33%)
18	MEN	SH	71	18	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	S4	72	2	7,8,9	0.91	0	6,9,11	1.32	1 (16%)
2	MEN	HD	72	2	7,8,9	0.92	0	6,9,11	1.76	1 (16%)
18	MEN	dH	71	18	7,7,9	0.98	0	6,8,11	1.81	2 (33%)
2	MEN	FC	72	2	7,8,9	0.90	0	6,9,11	1.11	0
2	MEN	eB	72	2	7,8,9	0.86	0	6,9,11	1.50	1 (16%)
10	MEN	FB	72	10	7,8,9	0.87	0	6,9,11	1.60	1 (16%)
2	MEN	iB	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	i8	72	2	7,8,9	0.95	0	6,9,11	1.39	1 (16%)
2	MEN	l1	72	2	7,8,9	0.89	0	6,9,11	1.23	1 (16%)
2	MEN	mF	72	2	7,8,9	0.84	0	6,9,11	1.29	1 (16%)
2	MEN	K5	72	2	7,8,9	0.93	0	6,9,11	1.90	2 (33%)
18	MEN	jH	71	18	7,7,9	0.94	0	6,8,11	1.66	1 (16%)
18	MEN	OH	71	18	7,7,9	0.94	0	6,8,11	1.75	2 (33%)
2	MEN	HG	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.44	2 (33%)
2	MEN	hE	72	2,26	7,8,9	1.24	1 (14%)	6,9,11	1.16	1 (16%)
2	MEN	P6	72	2	7,8,9	0.83	0	6,9,11	1.59	1 (16%)
18	MEN	BH	71	18	7,7,9	0.94	0	6,8,11	1.92	2 (33%)
2	MEN	V6	72	2	7,8,9	0.83	0	6,9,11	1.54	2 (33%)
18	MEN	IH	71	18	7,7,9	0.90	0	6,8,11	1.86	2 (33%)
2	MEN	k8	72	2	7,8,9	0.95	0	6,9,11	1.43	1 (16%)
2	MEN	Y9	72	2	7,8,9	0.90	0	6,9,11	1.64	1 (16%)
18	MEN	QH	71	18	7,8,9	0.88	0	6,9,11	1.84	2 (33%)
2	MEN	bG	72	2	7,8,9	0.92	0	6,9,11	1.30	1 (16%)
2	MEN	FD	72	2	7,8,9	0.99	0	6,9,11	1.62	2 (33%)
2	MEN	Q4	72	2	7,8,9	0.89	0	6,9,11	1.65	2 (33%)
2	MEN	h1	72	2	7,8,9	0.92	0	6,9,11	1.76	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	g2	72	2	7,8,9	0.89	0	6,9,11	1.41	1 (16%)
2	MEN	N3	72	2	7,8,9	0.93	0	6,9,11	1.47	1 (16%)
2	MEN	JD	72	2	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	P3	72	2	7,8,9	0.86	0	6,9,11	2.01	2 (33%)
2	MEN	J4	72	2	7,8,9	0.87	0	6,9,11	1.53	2 (33%)
10	MEN	D2	72	10	7,8,9	0.87	0	6,9,11	1.40	2 (33%)
2	MEN	lG	72	2,26	7,8,9	1.03	0	6,9,11	1.69	2 (33%)
2	MEN	kA	72	2	7,8,9	0.93	0	6,9,11	1.49	2 (33%)
2	MEN	LC	72	2	7,8,9	0.97	0	6,9,11	0.78	0
2	MEN	NE	72	2,26	7,8,9	1.50	1 (14%)	6,9,11	2.66	2 (33%)
2	MEN	Y2	72	2	7,8,9	0.83	0	6,9,11	1.47	1 (16%)
2	MEN	B4	72	2	7,8,9	0.85	0	6,9,11	1.68	2 (33%)
10	MEN	LF	72	10	7,8,9	0.88	0	6,9,11	2.58	2 (33%)
2	MEN	e2	72	2	7,8,9	0.88	0	6,9,11	1.64	2 (33%)
2	MEN	Y6	72	2	7,8,9	0.93	0	6,9,11	1.33	1 (16%)
2	MEN	HC	72	2	7,8,9	0.81	0	6,9,11	1.18	1 (16%)
10	MEN	FI	72	10	7,8,9	0.90	0	6,9,11	1.55	1 (16%)
2	MEN	BE	72	2,26	7,8,9	1.54	1 (14%)	6,9,11	2.69	1 (16%)
2	MEN	CC	72	2	7,8,9	0.65	0	6,9,11	0.77	0
2	MEN	V8	72	2	7,8,9	0.81	0	6,9,11	1.57	2 (33%)
2	MEN	iF	72	2	7,8,9	0.84	0	6,9,11	1.40	1 (16%)
2	MEN	bE	72	2,26	7,8,9	1.48	1 (14%)	6,9,11	2.02	2 (33%)
2	MEN	D4	72	2	7,8,9	0.90	0	6,9,11	1.59	2 (33%)
2	MEN	YF	72	2	7,8,9	0.94	0	6,9,11	1.29	1 (16%)
2	MEN	c8	72	2	7,8,9	0.89	0	6,9,11	1.54	1 (16%)
2	MEN	D8	72	2	7,8,9	0.81	0	6,9,11	1.34	1 (16%)
10	MEN	NI	72	10	7,8,9	0.91	0	6,9,11	1.40	2 (33%)
10	MEN	L7	72	10	7,8,9	0.87	0	6,9,11	2.23	1 (16%)
2	MEN	X8	72	2	7,8,9	0.87	0	6,9,11	1.81	2 (33%)
2	MEN	n1	72	2	7,8,9	0.91	0	6,9,11	1.36	1 (16%)
2	MEN	IJ	72	2	7,8,9	0.84	0	6,9,11	1.72	1 (16%)
2	MEN	SJ	72	2	7,8,9	0.96	0	6,9,11	1.37	1 (16%)
2	MEN	RA	72	2	7,8,9	0.86	0	6,9,11	1.47	1 (16%)
2	MEN	DD	72	2	7,8,9	0.90	0	6,9,11	1.10	1 (16%)
10	MEN	JB	72	10	7,8,9	0.91	0	6,9,11	1.59	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	y1	72	2	7,8,9	0.94	0	6,9,11	1.21	1 (16%)
18	MEN	fH	71	18	7,7,9	0.95	0	6,8,11	1.78	2 (33%)
2	MEN	P2	72	2	7,8,9	0.90	0	6,9,11	1.28	0
2	MEN	X3	72	2	7,8,9	0.93	0	6,9,11	1.64	2 (33%)
2	MEN	XD	72	2	7,8,9	0.92	0	6,9,11	1.59	2 (33%)
2	MEN	YJ	72	2	7,8,9	0.85	0	6,9,11	1.94	2 (33%)
10	MEN	J6	72	10	7,8,9	0.88	0	6,9,11	1.56	1 (16%)
2	MEN	cA	72	2	7,8,9	0.87	0	6,9,11	1.63	1 (16%)
2	MEN	CJ	72	2	7,8,9	0.86	0	6,9,11	1.43	2 (33%)
10	MEN	L6	72	10	7,8,9	0.96	0	6,9,11	1.60	2 (33%)
2	MEN	L8	72	2	7,8,9	0.97	0	6,9,11	1.19	1 (16%)
2	MEN	lE	72	2,26	7,8,9	1.01	0	6,9,11	1.78	1 (16%)
2	MEN	cB	72	2	7,8,9	0.90	0	6,9,11	1.07	0
18	MEN	nH	71	18	7,7,9	0.95	0	6,8,11	1.86	2 (33%)
2	MEN	i6	72	2	7,8,9	0.92	0	6,9,11	1.19	1 (16%)
2	MEN	vE	72	2,26	7,8,9	1.39	1 (14%)	6,9,11	1.40	1 (16%)
2	MEN	LD	72	2	7,8,9	0.90	0	6,9,11	1.20	0
2	MEN	kF	72	2	7,8,9	0.91	0	6,9,11	1.11	1 (16%)
2	MEN	IC	72	2	7,8,9	0.90	0	6,9,11	1.69	1 (16%)
10	MEN	D6	72	10,6	7,8,9	0.88	0	6,9,11	1.60	2 (33%)
2	MEN	TG	72	2,26	7,8,9	1.41	1 (14%)	6,9,11	2.25	2 (33%)
2	MEN	a6	72	2	7,8,9	0.88	0	6,9,11	1.69	2 (33%)
2	MEN	LA	72	2	7,8,9	0.95	0	6,9,11	1.20	1 (16%)
2	MEN	m2	72	2	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	g8	72	2	7,8,9	0.89	0	6,9,11	1.27	1 (16%)
2	MEN	u1	72	2	7,8,9	1.00	0	6,9,11	0.90	1 (16%)
2	MEN	rE	72	2,26	7,8,9	1.25	1 (14%)	6,9,11	1.09	1 (16%)
2	MEN	UJ	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
2	MEN	cI	72	2	7,8,9	0.89	0	6,9,11	1.27	1 (16%)
10	MEN	F6	72	10	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	TD	72	2,11	7,8,9	0.86	0	6,9,11	3.06	2 (33%)
2	MEN	O1	72	2	7,8,9	0.92	0	6,9,11	1.17	0
2	MEN	ND	72	2	7,8,9	0.93	0	6,9,11	1.45	1 (16%)
2	MEN	HA	72	2	7,8,9	0.87	0	6,9,11	1.62	1 (16%)
2	MEN	VB	72	2	7,8,9	0.82	0	6,9,11	1.58	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	JG	72	2,26	7,8,9	1.47	1 (14%)	6,9,11	2.19	2 (33%)
2	MEN	pG	72	2,26	7,8,9	1.11	0	6,9,11	1.34	1 (16%)
2	MEN	O9	72	2	7,8,9	0.92	0	6,9,11	1.30	2 (33%)
2	MEN	PI	72	2	7,8,9	0.90	0	6,9,11	1.24	0
2	MEN	Y7	72	2	7,8,9	0.91	0	6,9,11	1.03	0
2	MEN	14	72	2	7,8,9	0.91	0	6,9,11	1.48	2 (33%)
2	MEN	PF	72	2	7,8,9	0.88	0	6,9,11	1.67	2 (33%)
2	MEN	S9	72	2	7,8,9	0.94	0	6,9,11	1.34	1 (16%)
2	MEN	Q1	72	2	7,8,9	0.89	0	6,9,11	1.69	2 (33%)
18	MEN	MH	71	18	7,7,9	0.93	0	6,8,11	1.89	2 (33%)
10	MEN	H2	72	10	7,8,9	0.87	0	6,9,11	1.53	2 (33%)
2	MEN	S1	72	2	7,8,9	0.91	0	6,9,11	1.31	1 (16%)
2	MEN	U4	72	2	7,8,9	0.85	0	6,9,11	1.62	1 (16%)
2	MEN	XE	72	2,26	7,8,9	1.87	1 (14%)	6,9,11	3.03	2 (33%)
2	MEN	g6	72	2	7,8,9	0.86	0	6,9,11	1.54	1 (16%)
2	MEN	TI	72	2	7,8,9	0.82	0	6,9,11	1.63	2 (33%)
2	MEN	RB	72	2	7,8,9	0.92	0	6,9,11	1.50	1 (16%)
2	MEN	dE	72	2,26	7,8,9	1.44	1 (14%)	6,9,11	1.79	1 (16%)
2	MEN	Z1	72	2	7,8,9	0.82	0	6,9,11	1.75	2 (33%)
2	MEN	aF	72	2	7,8,9	0.89	0	6,9,11	1.33	1 (16%)
2	MEN	c2	72	2	7,8,9	0.90	0	6,9,11	1.22	0
2	MEN	tE	72	2,26	7,8,9	1.20	1 (14%)	6,9,11	1.66	1 (16%)
2	MEN	W1	72	2	7,8,9	0.88	0	6,9,11	1.49	1 (16%)
2	MEN	f4	72	2	7,8,9	0.97	0	6,9,11	1.08	1 (16%)
2	MEN	R8	72	2	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	mA	72	2	7,8,9	0.91	0	6,9,11	1.52	2 (33%)
2	MEN	T6	72	2	7,8,9	0.96	0	6,9,11	1.44	1 (16%)
2	MEN	h4	72	2	7,8,9	0.91	0	6,9,11	1.91	2 (33%)
2	MEN	a4	72	2	7,8,9	0.81	0	6,9,11	1.71	2 (33%)
10	MEN	HF	72	10	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
2	MEN	rG	72	2,26	7,8,9	1.28	1 (14%)	6,9,11	0.99	1 (16%)
2	MEN	O4	72	2	7,8,9	0.94	0	6,9,11	1.29	2 (33%)
2	MEN	N8	72	2	7,8,9	0.81	0	6,9,11	1.70	2 (33%)
2	MEN	eF	72	2	7,8,9	0.91	0	6,9,11	1.27	1 (16%)
2	MEN	EJ	72	2	7,8,9	0.80	0	6,9,11	1.57	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	PB	72	2	7,8,9	0.85	0	6,9,11	1.61	2 (33%)
2	MEN	R7	72	2	7,8,9	0.86	0	6,9,11	1.22	1 (16%)
2	MEN	F1	72	2	7,8,9	1.04	0	6,9,11	2.71	2 (33%)
2	MEN	nG	72	2,26	7,8,9	1.39	1 (14%)	6,9,11	1.48	1 (16%)
2	MEN	dG	72	2,26	7,8,9	1.43	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	T8	72	2	7,8,9	0.83	0	6,9,11	1.72	1 (16%)
10	MEN	JF	72	10	7,8,9	0.82	0	6,9,11	1.66	1 (16%)
2	MEN	H4	72	2	7,8,9	0.94	0	6,9,11	1.42	1 (16%)
2	MEN	I5	72	2	7,8,9	0.89	0	6,9,11	1.79	1 (16%)
2	MEN	NA	72	2	7,8,9	0.80	0	6,9,11	1.73	2 (33%)
18	MEN	kH	71	18	7,7,9	0.93	0	6,8,11	2.09	2 (33%)
2	MEN	P7	72	2	7,8,9	0.86	0	6,9,11	1.54	1 (16%)
2	MEN	Z4	72	2	7,8,9	0.85	0	6,9,11	1.71	2 (33%)
2	MEN	AC	72	2	7,8,9	1.08	0	6,9,11	1.43	1 (16%)
18	MEN	HH	71	18	7,7,9	0.93	0	6,8,11	1.53	1 (16%)
2	MEN	G5	72	2	7,8,9	0.91	0	6,9,11	1.07	0
2	MEN	s4	72	2	7,8,9	0.86	0	6,9,11	1.39	2 (33%)
2	MEN	B5	72	2	7,8,9	0.90	0	6,9,11	1.26	2 (33%)
2	MEN	Q9	72	2	7,8,9	0.81	0	6,9,11	1.70	2 (33%)
2	MEN	d4	72	2	7,8,9	0.88	0	6,9,11	1.70	1 (16%)
2	MEN	V3	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	VA	72	2	7,8,9	0.80	0	6,9,11	1.70	2 (33%)
2	MEN	VG	72	2,26	7,8,9	1.36	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	GC	72	2	7,8,9	0.91	0	6,9,11	1.07	0
2	MEN	I9	72	2	7,8,9	0.85	0	6,9,11	1.65	1 (16%)
2	MEN	K9	72	2	7,8,9	0.90	0	6,9,11	1.43	1 (16%)
18	MEN	LH	71	18	7,7,9	0.96	0	6,8,11	1.68	2 (33%)
2	MEN	J3	72	2	7,8,9	0.89	0	6,9,11	1.21	1 (16%)
2	MEN	W9	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
18	MEN	sH	71	18	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	T2	72	2	7,8,9	0.83	0	6,9,11	1.61	2 (33%)
10	MEN	F7	72	10	7,8,9	0.89	0	6,9,11	1.38	1 (16%)
2	MEN	RD	72	2	7,8,9	0.92	0	6,9,11	1.20	0
18	MEN	DH	71	18	7,7,9	0.95	0	6,8,11	1.74	2 (33%)
2	MEN	c7	72	2	7,8,9	0.84	0	6,9,11	1.64	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	R3	72	2	7,8,9	0.93	0	6,9,11	1.23	0
10	MEN	LB	72	10	7,8,9	0.96	0	6,9,11	1.56	2 (33%)
2	MEN	H8	72	2	7,8,9	0.89	0	6,9,11	1.75	1 (16%)
10	MEN	J2	72	10	7,8,9	0.85	0	6,9,11	1.87	2 (33%)
2	MEN	VE	72	2,26	7,8,9	1.40	1 (14%)	6,9,11	1.50	1 (16%)
2	MEN	RE	72	2,26	7,8,9	1.72	1 (14%)	6,9,11	3.06	2 (33%)
2	MEN	KJ	72	2	7,8,9	0.87	0	6,9,11	1.63	2 (33%)
2	MEN	PE	72	2,26	7,8,9	1.60	1 (14%)	6,9,11	2.64	3 (50%)
2	MEN	D3	72	2	7,8,9	0.90	0	6,9,11	1.34	1 (16%)
2	MEN	mB	72	2	7,8,9	0.92	0	6,9,11	1.24	1 (16%)
2	MEN	VD	72	2	7,8,9	0.86	0	6,9,11	1.40	1 (16%)
10	MEN	HB	72	10	7,8,9	0.92	0	6,9,11	1.30	2 (33%)
2	MEN	k6	72	2	7,8,9	0.88	0	6,9,11	1.49	1 (16%)
2	MEN	V7	72	2	7,8,9	0.85	0	6,9,11	1.52	1 (16%)
2	MEN	k7	72	2	7,8,9	0.89	0	6,9,11	1.50	1 (16%)
10	MEN	H7	72	10	7,8,9	0.86	0	6,9,11	1.43	1 (16%)
2	MEN	T7	72	2	7,8,9	0.88	0	6,9,11	1.57	1 (16%)
2	MEN	cF	72	2	7,8,9	0.82	0	6,9,11	1.84	1 (16%)
2	MEN	D1	72	2	7,8,9	0.87	0	6,9,11	1.59	2 (33%)
2	MEN	Y4	72	2	7,8,9	0.88	0	6,9,11	1.36	1 (16%)
2	MEN	Y1	72	2	7,8,9	0.87	0	6,9,11	1.31	1 (16%)
2	MEN	FE	72	2,26	7,8,9	1.89	1 (14%)	6,9,11	3.65	3 (50%)
10	MEN	N7	72	10	7,8,9	0.94	0	6,9,11	1.26	1 (16%)
2	MEN	nE	72	2,26	7,8,9	1.34	1 (14%)	6,9,11	1.51	1 (16%)
2	MEN	gF	72	2	7,8,9	0.90	0	6,9,11	1.62	2 (33%)
2	MEN	j4	72	2	7,8,9	0.91	0	6,9,11	2.20	2 (33%)
2	MEN	ZA	72	2	7,8,9	0.86	0	6,9,11	1.65	2 (33%)
2	MEN	fE	72	2,26	7,8,9	1.29	1 (14%)	6,9,11	2.26	2 (33%)
2	MEN	m6	72	2	7,8,9	0.91	0	6,9,11	1.40	1 (16%)
2	MEN	PA	72	2	7,8,9	0.94	0	6,9,11	1.33	1 (16%)
2	MEN	R6	72	2	7,8,9	0.91	0	6,9,11	1.47	1 (16%)
2	MEN	F8	72	2	7,8,9	1.00	0	6,9,11	1.37	1 (16%)
10	MEN	N6	72	10	7,8,9	0.85	0	6,9,11	1.51	2 (33%)
2	MEN	e6	72	2	7,8,9	0.84	0	6,9,11	1.48	1 (16%)
2	MEN	U9	72	2	7,8,9	0.97	0	6,9,11	1.66	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	R2	72	2	7,8,9	0.89	0	6,9,11	1.44	2 (33%)
2	MEN	F5	72	2	7,8,9	0.89	0	6,9,11	1.08	0
10	MEN	N2	72	10	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	gB	72	2	7,8,9	0.86	0	6,9,11	1.55	1 (16%)
2	MEN	VF	72	2	7,8,9	0.86	0	6,9,11	1.61	2 (33%)
2	MEN	pE	72	2,26	7,8,9	1.00	0	6,9,11	1.82	2 (33%)
2	MEN	FG	72	2,26	7,8,9	1.92	1 (14%)	6,9,11	3.70	3 (50%)
2	MEN	f1	72	2	7,8,9	0.96	0	6,9,11	1.09	1 (16%)
2	MEN	fG	72	2,26	7,8,9	1.30	1 (14%)	6,9,11	2.30	2 (33%)
2	MEN	QJ	72	2	7,8,9	0.82	0	6,9,11	1.77	2 (33%)
2	MEN	PG	72	2,26	7,8,9	1.56	1 (14%)	6,9,11	2.52	2 (33%)
2	MEN	m7	72	2	7,8,9	0.87	0	6,9,11	1.40	1 (16%)
2	MEN	JE	72	2,26	7,8,9	1.54	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	A5	72	2	7,8,9	1.16	0	6,9,11	1.89	2 (33%)
2	MEN	NG	72	2,26	7,8,9	1.51	1 (14%)	6,9,11	2.75	2 (33%)
2	MEN	B1	72	2	7,8,9	0.86	0	6,9,11	1.40	1 (16%)
2	MEN	J8	72	2	7,8,9	0.84	0	6,9,11	1.65	1 (16%)
2	MEN	a2	72	2	7,8,9	0.88	0	6,9,11	1.44	2 (33%)
2	MEN	iI	72	2	7,8,9	0.87	0	6,9,11	1.49	1 (16%)
2	MEN	HE	72	2,26	7,8,9	1.58	1 (14%)	6,9,11	2.51	2 (33%)
2	MEN	w4	72	2	7,8,9	0.93	0	6,9,11	0.94	0
2	MEN	E9	72	2	7,8,9	0.86	0	6,9,11	1.44	1 (16%)
2	MEN	TF	72	2	7,8,9	0.93	0	6,9,11	1.79	2 (33%)
2	MEN	B3	72	2	7,8,9	0.99	0	6,9,11	0.95	0
10	MEN	DF	72	10	7,8,9	0.85	0	6,9,11	1.59	2 (33%)
2	MEN	L4	72	2	7,8,9	0.90	0	6,9,11	1.52	1 (16%)
2	MEN	J1	72	2	7,8,9	0.93	0	6,9,11	1.55	1 (16%)
10	MEN	D7	72	10	7,8,9	0.89	0	6,9,11	1.59	2 (33%)
2	MEN	OJ	72	2	7,8,9	0.93	0	6,9,11	1.31	2 (33%)
2	MEN	KC	72	2	7,8,9	0.91	0	6,9,11	1.69	2 (33%)
10	MEN	L2	72	10	7,8,9	0.80	0	6,9,11	1.84	2 (33%)
2	MEN	BC	72	2	7,8,9	0.65	0	6,9,11	0.77	0
2	MEN	aB	72	2	7,8,9	0.86	0	6,9,11	1.71	2 (33%)
10	MEN	NF	72	10	7,8,9	0.96	0	6,9,11	1.12	0

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
18	MEN	FH	71	18	-	4/6/6/10	-
2	MEN	s1	72	2	-	4/7/8/10	-
2	MEN	XA	72	2	-	4/7/8/10	-
2	MEN	RF	72	2	-	2/7/8/10	-
2	MEN	LE	72	2,26	-	3/7/8/10	-
10	MEN	HI	72	10	-	2/7/8/10	-
10	MEN	NB	72	10	-	4/7/8/10	-
2	MEN	C9	72	2	-	4/7/8/10	-
2	MEN	11	72	2	-	4/7/8/10	-
18	MEN	qH	71	18	-	2/6/6/10	-
2	MEN	XG	72	2,26	-	2/7/8/10	-
2	MEN	n4	72	2	-	2/7/8/10	-
2	MEN	gI	72	2	-	4/7/8/10	-
2	MEN	y4	72	2	-	3/7/8/10	-
2	MEN	H5	72	2	-	2/7/8/10	-
2	MEN	TA	72	2	-	2/7/8/10	-
2	MEN	BD	72	2	-	4/7/8/10	-
2	MEN	i2	72	2	-	4/7/8/10	-
2	MEN	jE	72	2,26	-	4/7/8/10	-
18	MEN	uH	71	18	-	4/7/8/10	-
2	MEN	kI	72	2	-	5/7/8/10	-
18	MEN	hH	71	18	-	2/6/6/10	-
2	MEN	YI	72	2	-	4/7/8/10	-
2	MEN	a1	72	2	-	4/7/8/10	-
18	MEN	oH	71	18	-	2/6/6/10	-
2	MEN	m8	72	2	-	4/7/8/10	-
2	MEN	k2	72	2	-	5/7/8/10	-
2	MEN	C5	72	2	-	4/7/8/10	-
2	MEN	H1	72	2	-	4/7/8/10	-
2	MEN	gA	72	2	-	3/7/8/10	-
2	MEN	u4	72	2	-	3/7/8/10	-
2	MEN	ZE	72	2,26	-	3/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	MEN	wH	71	18	-	4/7/8/10	-
2	MEN	vG	72	2,26	-	1/7/8/10	-
10	MEN	H6	72	10	-	4/7/8/10	-
2	MEN	L1	72	2	-	4/7/8/10	-
2	MEN	YB	72	2	-	5/7/8/10	-
2	MEN	Z8	72	2	-	4/7/8/10	-
2	MEN	g7	72	2	-	3/7/8/10	-
2	MEN	VI	72	2	-	2/7/8/10	-
2	MEN	DA	72	2	-	4/7/8/10	-
10	MEN	J7	72	10	-	3/7/8/10	-
2	MEN	T3	72	2	-	2/7/8/10	-
2	MEN	L3	72	2	-	5/7/8/10	-
2	MEN	WJ	72	2	-	5/7/8/10	-
2	MEN	d1	72	2	-	4/7/8/10	-
18	MEN	UH	71	18	-	2/7/8/10	-
2	MEN	G9	72	2	-	4/7/8/10	-
2	MEN	FA	72	2	-	4/7/8/10	-
2	MEN	TB	72	2	-	3/7/8/10	-
2	MEN	q1	72	2	-	2/7/8/10	-
2	MEN	e7	72	2	-	2/7/8/10	-
2	MEN	DG	72	2,26	-	2/7/8/10	-
2	MEN	L5	72	2	-	5/7/8/10	-
2	MEN	iA	72	2	-	4/7/8/10	-
2	MEN	M9	72	2	-	2/7/8/10	-
2	MEN	LG	72	2,26	-	3/7/8/10	-
10	MEN	F2	72	10	-	2/7/8/10	-
2	MEN	w1	72	2	-	2/7/8/10	-
2	MEN	eA	72	2	-	5/7/8/10	-
2	MEN	jG	72	2,26	-	4/7/8/10	-
2	MEN	a7	72	2	-	4/7/8/10	-
2	MEN	i7	72	2	-	3/7/8/10	-
2	MEN	GJ	72	2	-	4/7/8/10	-
2	MEN	F4	72	2	-	5/7/8/10	-
2	MEN	P8	72	2	-	4/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	DB	72	10,6	-	4/7/8/10	-
2	MEN	U1	72	2	-	4/7/8/10	-
2	MEN	e8	72	2	-	5/7/8/10	-
2	MEN	RG	72	2,26	-	2/7/8/10	-
2	MEN	DE	72	2,26	-	4/7/8/10	-
2	MEN	tG	72	2,26	-	4/7/8/10	-
2	MEN	TE	72	2,26	-	3/7/8/10	-
2	MEN	hG	72	2,26	-	2/7/8/10	-
2	MEN	aI	72	2	-	3/7/8/10	-
2	MEN	eI	72	2	-	5/7/8/10	-
2	MEN	BG	72	2,26	-	2/7/8/10	-
2	MEN	MJ	72	2	-	2/7/8/10	-
2	MEN	V2	72	2	-	2/7/8/10	-
10	MEN	LI	72	10	-	4/7/8/10	-
2	MEN	j1	72	2	-	4/7/8/10	-
10	MEN	DI	72	10	-	2/7/8/10	-
2	MEN	kB	72	2	-	4/7/8/10	-
2	MEN	W4	72	2	-	4/7/8/10	-
2	MEN	c6	72	2	-	3/7/8/10	-
2	MEN	RI	72	2	-	4/7/8/10	-
2	MEN	PD	72	2	-	4/7/8/10	-
2	MEN	l4	72	2	-	4/7/8/10	-
2	MEN	q4	72	2	-	3/7/8/10	-
2	MEN	F3	72	2	-	1/7/8/10	-
2	MEN	JA	72	2	-	4/7/8/10	-
2	MEN	ZG	72	2	-	5/7/8/10	-
10	MEN	JI	72	10	-	2/7/8/10	-
2	MEN	H3	72	2	-	4/7/8/10	-
10	MEN	FF	72	10	-	2/7/8/10	-
2	MEN	mI	72	2	-	4/7/8/10	-
18	MEN	SH	71	18	-	4/7/8/10	-
2	MEN	S4	72	2	-	4/7/8/10	-
2	MEN	HD	72	2	-	4/7/8/10	-
18	MEN	dH	71	18	-	2/6/6/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	FC	72	2	-	4/7/8/10	-
2	MEN	eB	72	2	-	4/7/8/10	-
10	MEN	FB	72	10	-	3/7/8/10	-
2	MEN	iB	72	2	-	2/7/8/10	-
2	MEN	i8	72	2	-	4/7/8/10	-
2	MEN	l1	72	2	-	5/7/8/10	-
2	MEN	mF	72	2	-	4/7/8/10	-
2	MEN	K5	72	2	-	2/7/8/10	-
18	MEN	jH	71	18	-	2/6/6/10	-
18	MEN	OH	71	18	-	0/6/6/10	-
2	MEN	HG	72	2,26	-	2/7/8/10	-
2	MEN	hE	72	2,26	-	1/7/8/10	-
2	MEN	P6	72	2	-	3/7/8/10	-
18	MEN	BH	71	18	-	2/6/6/10	-
2	MEN	V6	72	2	-	4/7/8/10	-
18	MEN	IH	71	18	-	3/6/6/10	-
2	MEN	k8	72	2	-	3/7/8/10	-
2	MEN	Y9	72	2	-	4/7/8/10	-
18	MEN	QH	71	18	-	2/7/8/10	-
2	MEN	bG	72	2	-	4/7/8/10	-
2	MEN	FD	72	2	-	4/7/8/10	-
2	MEN	Q4	72	2	-	4/7/8/10	-
2	MEN	h1	72	2	-	5/7/8/10	-
2	MEN	g2	72	2	-	4/7/8/10	-
2	MEN	N3	72	2	-	4/7/8/10	-
2	MEN	JD	72	2	-	1/7/8/10	-
2	MEN	P3	72	2	-	4/7/8/10	-
2	MEN	J4	72	2	-	5/7/8/10	-
10	MEN	D2	72	10	-	2/7/8/10	-
2	MEN	lG	72	2,26	-	4/7/8/10	-
2	MEN	kA	72	2	-	4/7/8/10	-
2	MEN	LC	72	2	-	5/7/8/10	-
2	MEN	NE	72	2,26	-	2/7/8/10	-
2	MEN	Y2	72	2	-	4/7/8/10	-
2	MEN	B4	72	2	-	3/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	LF	72	10	-	2/7/8/10	-
2	MEN	e2	72	2	-	4/7/8/10	-
2	MEN	Y6	72	2	-	5/7/8/10	-
2	MEN	HC	72	2	-	2/7/8/10	-
10	MEN	FI	72	10	-	3/7/8/10	-
2	MEN	BE	72	2,26	-	2/7/8/10	-
2	MEN	CC	72	2	-	3/7/8/10	-
2	MEN	V8	72	2	-	4/7/8/10	-
2	MEN	iF	72	2	-	4/7/8/10	-
2	MEN	bE	72	2,26	-	4/7/8/10	-
2	MEN	D4	72	2	-	4/7/8/10	-
2	MEN	YF	72	2	-	4/7/8/10	-
2	MEN	c8	72	2	-	4/7/8/10	-
2	MEN	D8	72	2	-	4/7/8/10	-
10	MEN	NI	72	10	-	3/7/8/10	-
10	MEN	L7	72	10	-	2/7/8/10	-
2	MEN	X8	72	2	-	4/7/8/10	-
2	MEN	n1	72	2	-	4/7/8/10	-
2	MEN	IJ	72	2	-	4/7/8/10	-
2	MEN	SJ	72	2	-	4/7/8/10	-
2	MEN	RA	72	2	-	3/7/8/10	-
2	MEN	DD	72	2	-	3/7/8/10	-
10	MEN	JB	72	10	-	2/7/8/10	-
2	MEN	y1	72	2	-	2/7/8/10	-
18	MEN	fH	71	18	-	4/6/6/10	-
2	MEN	P2	72	2	-	4/7/8/10	-
2	MEN	X3	72	2	-	4/7/8/10	-
2	MEN	XD	72	2	-	4/7/8/10	-
2	MEN	YJ	72	2	-	0/7/8/10	-
10	MEN	J6	72	10	-	2/7/8/10	-
2	MEN	cA	72	2	-	4/7/8/10	-
2	MEN	CJ	72	2	-	4/7/8/10	-
10	MEN	L6	72	10	-	4/7/8/10	-
2	MEN	L8	72	2	-	4/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	lE	72	2,26	-	5/7/8/10	-
2	MEN	cB	72	2	-	3/7/8/10	-
18	MEN	nH	71	18	-	3/6/6/10	-
2	MEN	i6	72	2	-	3/7/8/10	-
2	MEN	vE	72	2,26	-	2/7/8/10	-
2	MEN	LD	72	2	-	5/7/8/10	-
2	MEN	kF	72	2	-	4/7/8/10	-
2	MEN	IC	72	2	-	2/7/8/10	-
10	MEN	D6	72	10,6	-	4/7/8/10	-
2	MEN	TG	72	2,26	-	2/7/8/10	-
2	MEN	a6	72	2	-	4/7/8/10	-
2	MEN	LA	72	2	-	4/7/8/10	-
2	MEN	m2	72	2	-	4/7/8/10	-
2	MEN	g8	72	2	-	2/7/8/10	-
2	MEN	u1	72	2	-	3/7/8/10	-
2	MEN	rE	72	2,26	-	4/7/8/10	-
2	MEN	UJ	72	2	-	4/7/8/10	-
2	MEN	cI	72	2	-	2/7/8/10	-
10	MEN	F6	72	10	-	3/7/8/10	-
2	MEN	TD	72	2,11	-	6/7/8/10	-
2	MEN	O1	72	2	-	4/7/8/10	-
2	MEN	ND	72	2	-	4/7/8/10	-
2	MEN	HA	72	2	-	4/7/8/10	-
2	MEN	VB	72	2	-	4/7/8/10	-
2	MEN	JG	72	2,26	-	2/7/8/10	-
2	MEN	pG	72	2,26	-	3/7/8/10	-
2	MEN	O9	72	2	-	2/7/8/10	-
2	MEN	PI	72	2	-	4/7/8/10	-
2	MEN	Y7	72	2	-	4/7/8/10	-
2	MEN	14	72	2	-	4/7/8/10	-
2	MEN	PF	72	2	-	4/7/8/10	-
2	MEN	S9	72	2	-	4/7/8/10	-
2	MEN	Q1	72	2	-	4/7/8/10	-
18	MEN	MH	71	18	-	2/6/6/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MEN	H2	72	10	-	2/7/8/10	-
2	MEN	S1	72	2	-	4/7/8/10	-
2	MEN	U4	72	2	-	4/7/8/10	-
2	MEN	XE	72	2,26	-	2/7/8/10	-
2	MEN	g6	72	2	-	4/7/8/10	-
2	MEN	TI	72	2	-	3/7/8/10	-
2	MEN	RB	72	2	-	3/7/8/10	-
2	MEN	dE	72	2,26	-	2/7/8/10	-
2	MEN	Z1	72	2	-	4/7/8/10	-
2	MEN	aF	72	2	-	3/7/8/10	-
2	MEN	c2	72	2	-	2/7/8/10	-
2	MEN	tE	72	2,26	-	4/7/8/10	-
2	MEN	W1	72	2	-	4/7/8/10	-
2	MEN	f4	72	2	-	3/7/8/10	-
2	MEN	R8	72	2	-	3/7/8/10	-
2	MEN	mA	72	2	-	4/7/8/10	-
2	MEN	T6	72	2	-	3/7/8/10	-
2	MEN	h4	72	2	-	4/7/8/10	-
2	MEN	a4	72	2	-	4/7/8/10	-
10	MEN	HF	72	10	-	4/7/8/10	-
2	MEN	rG	72	2,26	-	3/7/8/10	-
2	MEN	O4	72	2	-	4/7/8/10	-
2	MEN	N8	72	2	-	2/7/8/10	-
2	MEN	eF	72	2	-	3/7/8/10	-
2	MEN	EJ	72	2	-	4/7/8/10	-
2	MEN	PB	72	2	-	3/7/8/10	-
2	MEN	R7	72	2	-	2/7/8/10	-
2	MEN	F1	72	2	-	6/7/8/10	-
2	MEN	nG	72	2,26	-	3/7/8/10	-
2	MEN	dG	72	2,26	-	3/7/8/10	-
2	MEN	T8	72	2	-	2/7/8/10	-
10	MEN	JF	72	10	-	1/7/8/10	-
2	MEN	H4	72	2	-	4/7/8/10	-
2	MEN	I5	72	2	-	2/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	NA	72	2	-	4/7/8/10	-
18	MEN	kH	71	18	-	1/6/6/10	-
2	MEN	P7	72	2	-	4/7/8/10	-
2	MEN	Z4	72	2	-	4/7/8/10	-
2	MEN	AC	72	2	-	2/7/8/10	-
18	MEN	HH	71	18	-	1/6/6/10	-
2	MEN	G5	72	2	-	4/7/8/10	-
2	MEN	s4	72	2	-	2/7/8/10	-
2	MEN	B5	72	2	-	4/7/8/10	-
2	MEN	Q9	72	2	-	4/7/8/10	-
2	MEN	d4	72	2	-	4/7/8/10	-
2	MEN	V3	72	2	-	4/7/8/10	-
2	MEN	VA	72	2	-	4/7/8/10	-
2	MEN	VG	72	2,26	-	4/7/8/10	-
2	MEN	GC	72	2	-	4/7/8/10	-
2	MEN	I9	72	2	-	4/7/8/10	-
2	MEN	K9	72	2	-	4/7/8/10	-
18	MEN	LH	71	18	-	4/6/6/10	-
2	MEN	J3	72	2	-	2/7/8/10	-
2	MEN	W9	72	2	-	4/7/8/10	-
18	MEN	sH	71	18	-	4/7/8/10	-
2	MEN	T2	72	2	-	3/7/8/10	-
10	MEN	F7	72	10	-	2/7/8/10	-
2	MEN	RD	72	2	-	4/7/8/10	-
18	MEN	DH	71	18	-	2/6/6/10	-
2	MEN	c7	72	2	-	4/7/8/10	-
2	MEN	R3	72	2	-	4/7/8/10	-
10	MEN	LB	72	10	-	4/7/8/10	-
2	MEN	H8	72	2	-	4/7/8/10	-
10	MEN	J2	72	10	-	2/7/8/10	-
2	MEN	VE	72	2,26	-	2/7/8/10	-
2	MEN	RE	72	2,26	-	2/7/8/10	-
2	MEN	KJ	72	2	-	5/7/8/10	-
2	MEN	PE	72	2,26	-	2/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	D3	72	2	-	2/7/8/10	-
2	MEN	mB	72	2	-	2/7/8/10	-
2	MEN	VD	72	2	-	4/7/8/10	-
10	MEN	HB	72	10	-	4/7/8/10	-
2	MEN	k6	72	2	-	4/7/8/10	-
2	MEN	V7	72	2	-	4/7/8/10	-
2	MEN	k7	72	2	-	3/7/8/10	-
10	MEN	H7	72	10	-	4/7/8/10	-
2	MEN	T7	72	2	-	4/7/8/10	-
2	MEN	cF	72	2	-	4/7/8/10	-
2	MEN	D1	72	2	-	4/7/8/10	-
2	MEN	Y4	72	2	-	4/7/8/10	-
2	MEN	Y1	72	2	-	4/7/8/10	-
2	MEN	FE	72	2,26	-	2/7/8/10	-
10	MEN	N7	72	10	-	2/7/8/10	-
2	MEN	nE	72	2,26	-	3/7/8/10	-
2	MEN	gF	72	2	-	3/7/8/10	-
2	MEN	j4	72	2	-	5/7/8/10	-
2	MEN	ZA	72	2	-	4/7/8/10	-
2	MEN	fE	72	2,26	-	2/7/8/10	-
2	MEN	m6	72	2	-	3/7/8/10	-
2	MEN	PA	72	2	-	4/7/8/10	-
2	MEN	R6	72	2	-	3/7/8/10	-
2	MEN	F8	72	2	-	4/7/8/10	-
10	MEN	N6	72	10	-	4/7/8/10	-
2	MEN	e6	72	2	-	2/7/8/10	-
2	MEN	U9	72	2	-	3/7/8/10	-
2	MEN	R2	72	2	-	4/7/8/10	-
2	MEN	F5	72	2	-	4/7/8/10	-
10	MEN	N2	72	10	-	2/7/8/10	-
2	MEN	gB	72	2	-	4/7/8/10	-
2	MEN	VF	72	2	-	4/7/8/10	-
2	MEN	pE	72	2,26	-	3/7/8/10	-
2	MEN	FG	72	2,26	-	2/7/8/10	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	f1	72	2	-	3/7/8/10	-
2	MEN	fG	72	2,26	-	2/7/8/10	-
2	MEN	QJ	72	2	-	4/7/8/10	-
2	MEN	PG	72	2,26	-	3/7/8/10	-
2	MEN	m7	72	2	-	4/7/8/10	-
2	MEN	JE	72	2,26	-	2/7/8/10	-
2	MEN	A5	72	2	-	2/7/8/10	-
2	MEN	NG	72	2,26	-	2/7/8/10	-
2	MEN	B1	72	2	-	2/7/8/10	-
2	MEN	J8	72	2	-	4/7/8/10	-
2	MEN	a2	72	2	-	3/7/8/10	-
2	MEN	iI	72	2	-	4/7/8/10	-
2	MEN	HE	72	2,26	-	2/7/8/10	-
2	MEN	w4	72	2	-	2/7/8/10	-
2	MEN	E9	72	2	-	3/7/8/10	-
2	MEN	TF	72	2	-	5/7/8/10	-
2	MEN	B3	72	2	-	4/7/8/10	-
10	MEN	DF	72	10	-	4/7/8/10	-
2	MEN	L4	72	2	-	4/7/8/10	-
2	MEN	J1	72	2	-	5/7/8/10	-
10	MEN	D7	72	10	-	2/7/8/10	-
2	MEN	OJ	72	2	-	4/7/8/10	-
2	MEN	KC	72	2	-	3/7/8/10	-
10	MEN	L2	72	10	-	4/7/8/10	-
2	MEN	BC	72	2	-	3/7/8/10	-
2	MEN	aB	72	2	-	4/7/8/10	-
10	MEN	NF	72	10	-	2/7/8/10	-

The worst 5 of 42 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	XG	72	MEN	OD1-CG	4.45	1.32	1.23
2	FG	72	MEN	OD1-CG	4.39	1.32	1.23
2	FE	72	MEN	OD1-CG	4.31	1.32	1.23
2	XE	72	MEN	OD1-CG	4.27	1.32	1.23
2	LG	72	MEN	OD1-CG	4.18	1.31	1.23

The worst 5 of 459 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	LG	72	MEN	CB-CG-ND2	-8.39	104.21	115.48
2	LE	72	MEN	CB-CG-ND2	-8.05	104.66	115.48
2	FG	72	MEN	CB-CG-ND2	-7.90	104.86	115.48
2	FE	72	MEN	CB-CG-ND2	-7.76	105.05	115.48
2	T3	72	MEN	CB-CG-ND2	6.91	124.78	115.48

There are no chirality outliers.

5 of 1102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B1	72	MEN	C-CA-CB-CG
2	D1	72	MEN	C-CA-CB-CG
2	F1	72	MEN	CB-CG-ND2-CE2
2	F1	72	MEN	OD1-CG-ND2-CE2
2	H1	72	MEN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1598 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
26	PEB	V2	203	2	43,46,46	3.42	12 (27%)	45,67,67	2.04	15 (33%)
26	PEB	LJ	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.31	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	WB	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.32	17 (37%)
26	PEB	L3	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.81	18 (40%)
26	PEB	K3	201	1	43,46,46	3.29	11 (25%)	45,67,67	2.26	16 (35%)
26	PEB	SE	202	1	43,46,46	2.83	11 (25%)	45,67,67	2.58	18 (40%)
26	PEB	I4	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.96	12 (26%)
26	PEB	W7	201	1	43,46,46	3.37	10 (23%)	45,67,67	2.01	13 (28%)
26	PEB	VE	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.79	16 (35%)
26	PEB	O3	201	1	43,46,46	3.06	10 (23%)	45,67,67	2.86	21 (46%)
26	PEB	e4	201	1	43,46,46	3.39	8 (18%)	45,67,67	1.90	13 (28%)
28	CYC	N2	1001	10	42,46,46	3.30	15 (35%)	50,67,67	2.78	21 (42%)
26	PEB	KG	203	1	43,46,46	3.33	9 (20%)	45,67,67	2.06	17 (37%)
26	PEB	g2	203	2	43,46,46	3.46	11 (25%)	45,67,67	2.18	15 (33%)
26	PEB	l6	202	1	43,46,46	3.34	11 (25%)	45,67,67	2.01	14 (31%)
26	PEB	NI	1002	10	43,46,46	3.31	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	d8	203	1	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	24	405	3	43,46,46	3.52	12 (27%)	45,67,67	2.52	15 (33%)
26	PEB	c4	203	2,1	43,46,46	3.35	12 (27%)	45,67,67	2.40	14 (31%)
26	PEB	b2	202	1	43,46,46	3.43	12 (27%)	45,67,67	1.97	13 (28%)
26	PEB	mB	201	2	43,46,46	3.46	12 (27%)	45,67,67	1.94	15 (33%)
26	PEB	OA	201	1	43,46,46	3.37	10 (23%)	45,67,67	1.99	15 (33%)
26	PEB	21	405	3	43,46,46	3.42	13 (30%)	45,67,67	2.61	16 (35%)
28	CYC	YH	1001	22	42,46,46	3.39	15 (35%)	50,67,67	3.17	19 (38%)
26	PEB	e6	201	2	43,46,46	3.39	11 (25%)	45,67,67	1.95	14 (31%)
28	CYC	dH	1001	-	42,46,46	3.39	15 (35%)	50,67,67	5.15	19 (38%)
26	PEB	iG	203	1	43,46,46	3.47	12 (27%)	45,67,67	2.04	14 (31%)
26	PEB	iA	201	2,13	43,46,46	3.46	11 (25%)	45,67,67	2.46	14 (31%)
26	PEB	sG	203	2,1	43,46,46	3.49	13 (30%)	45,67,67	2.76	16 (35%)
26	PEB	EE	201	1	43,46,46	3.10	8 (18%)	45,67,67	2.02	13 (28%)
26	PEB	DG	203	2	43,46,46	3.44	10 (23%)	45,67,67	2.02	14 (31%)
26	PEB	kG	202	1	43,46,46	3.59	11 (25%)	45,67,67	1.91	12 (26%)
26	PEB	WG	203	1	43,46,46	3.41	11 (25%)	45,67,67	2.15	12 (26%)
26	PEB	SB	203	2,1	43,46,46	3.23	10 (23%)	45,67,67	2.47	14 (31%)
26	PEB	w4	204	2,1	43,46,46	3.42	10 (23%)	45,67,67	1.93	11 (24%)
26	PEB	QJ	201	2,7	43,46,46	3.47	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	D1	202	2	43,46,46	3.34	12 (27%)	45,67,67	2.55	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	J4	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.39	15 (33%)
26	PEB	Y4	202	2	43,46,46	3.40	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	Z6	201	2,1	43,46,46	3.14	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	TJ	203	1	43,46,46	3.35	8 (18%)	45,67,67	2.28	12 (26%)
26	PEB	m6	201	2	43,46,46	3.48	13 (30%)	45,67,67	1.94	13 (28%)
26	PEB	q4	201	2	43,46,46	3.53	12 (27%)	45,67,67	2.11	14 (31%)
26	PEB	UA	201	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.41	15 (33%)
26	PEB	pG	201	2	43,46,46	3.33	9 (20%)	45,67,67	2.72	17 (37%)
26	PEB	j2	202	1	43,46,46	3.36	10 (23%)	45,67,67	1.93	12 (26%)
26	PEB	f6	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.96	13 (28%)
26	PEB	IA	203	1	43,46,46	3.52	12 (27%)	45,67,67	2.16	15 (33%)
26	PEB	oE	202	1	43,46,46	3.49	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	II	201	1	43,46,46	3.32	11 (25%)	45,67,67	2.26	17 (37%)
27	PUB	24	402	3	42,46,46	3.54	8 (19%)	37,67,67	3.35	15 (40%)
27	PUB	yG	303	14	42,46,46	3.30	7 (16%)	37,67,67	3.12	13 (35%)
26	PEB	SE	201	2,1	43,46,46	3.25	11 (25%)	45,67,67	2.56	18 (40%)
26	PEB	U4	201	2,4	43,46,46	3.61	12 (27%)	45,67,67	2.17	17 (37%)
26	PEB	S6	203	2,1	43,46,46	3.22	9 (20%)	45,67,67	2.46	14 (31%)
26	PEB	pG	202	2	43,46,46	3.60	11 (25%)	45,67,67	2.73	18 (40%)
26	PEB	E8	203	1	43,46,46	3.45	10 (23%)	45,67,67	1.97	14 (31%)
26	PEB	OF	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.47	15 (33%)
26	PEB	R6	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.18	17 (37%)
26	PEB	RI	201	2,6	43,46,46	3.32	10 (23%)	45,67,67	2.38	14 (31%)
26	PEB	Z7	202	1	43,46,46	3.20	9 (20%)	45,67,67	2.09	17 (37%)
26	PEB	SA	203	2,1	43,46,46	3.31	12 (27%)	45,67,67	2.41	14 (31%)
26	PEB	CE	203	1	43,46,46	3.39	11 (25%)	45,67,67	2.06	16 (35%)
26	PEB	g2	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.33	15 (33%)
26	PEB	RD	202	2	43,46,46	3.09	10 (23%)	45,67,67	2.93	15 (33%)
26	PEB	jE	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.14	13 (28%)
26	PEB	U6	201	2,1	43,46,46	3.28	10 (23%)	45,67,67	2.38	16 (35%)
26	PEB	pE	201	2	43,46,46	3.43	9 (20%)	45,67,67	2.70	16 (35%)
26	PEB	U3	201	1	43,46,46	3.14	10 (23%)	45,67,67	2.69	15 (33%)
26	PEB	N1	202	1	43,46,46	3.31	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	D8	202	2	43,46,46	3.27	12 (27%)	45,67,67	2.67	17 (37%)
26	PEB	IG	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.57	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	PUB	A7	304	7	42,46,46	3.53	8 (19%)	37,67,67	3.70	18 (48%)
26	PEB	u4	201	3,2	43,46,46	3.53	14 (32%)	45,67,67	2.26	18 (40%)
28	CYC	JH	1001	18,17	42,46,46	3.51	14 (33%)	50,67,67	2.91	22 (44%)
26	PEB	f8	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.03	14 (31%)
26	PEB	FC	201	2	43,46,46	3.35	10 (23%)	45,67,67	1.95	14 (31%)
26	PEB	CG	203	1	43,46,46	3.44	12 (27%)	45,67,67	1.99	16 (35%)
26	PEB	NG	201	2	43,46,46	3.34	10 (23%)	45,67,67	3.07	17 (37%)
26	PEB	T3	202	2	43,46,46	2.67	9 (20%)	45,67,67	3.13	20 (44%)
26	PEB	hG	202	2	43,46,46	3.44	9 (20%)	45,67,67	1.99	15 (33%)
26	PEB	hB	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.05	16 (35%)
26	PEB	M9	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	IE	203	2,1	43,46,46	3.01	10 (23%)	45,67,67	2.66	17 (37%)
26	PEB	M4	402	3,26	43,46,46	3.43	10 (23%)	45,67,67	2.18	14 (31%)
26	PEB	i6	201	2	43,46,46	3.45	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	JI	1002	10	43,46,46	3.31	11 (25%)	45,67,67	2.11	14 (31%)
26	PEB	L9	201	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.42	16 (35%)
26	PEB	KB	201	9,10	43,46,46	3.32	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	P2	202	2	43,46,46	3.26	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	W8	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.20	15 (33%)
26	PEB	LB	1002	9,10	43,46,46	3.32	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	JE	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.19	18 (40%)
26	PEB	c2	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.40	16 (35%)
26	PEB	aG	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	VF	201	2	43,46,46	3.40	12 (27%)	45,67,67	2.41	18 (40%)
26	PEB	EJ	201	2,15	43,46,46	3.27	11 (25%)	45,67,67	2.20	17 (37%)
26	PEB	tE	202	2	43,46,46	3.65	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	m4	201	2,1	43,46,46	3.22	12 (27%)	45,67,67	2.62	16 (35%)
26	PEB	d6	204	1	43,46,46	3.42	13 (30%)	45,67,67	2.12	13 (28%)
26	PEB	S4	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.14	15 (33%)
26	PEB	I5	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.29	16 (35%)
26	PEB	fG	201	2,13	43,46,46	3.41	10 (23%)	45,67,67	3.07	16 (35%)
28	CYC	qH	1002	-	42,46,46	3.48	14 (33%)	50,67,67	3.10	24 (48%)
26	PEB	A8	302	13	43,46,46	3.32	10 (23%)	45,67,67	2.77	18 (40%)
26	PEB	x4	202	1	43,46,46	3.41	10 (23%)	45,67,67	2.61	19 (42%)
28	CYC	D7	1001	10	42,46,46	3.34	13 (30%)	50,67,67	2.82	18 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	IC	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.18	15 (33%)
26	PEB	c1	203	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.57	15 (33%)
28	CYC	J7	1003	9,10	42,46,46	3.24	12 (28%)	50,67,67	2.70	18 (36%)
26	PEB	BC	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.93	13 (28%)
26	PEB	ZE	201	2	43,46,46	3.44	10 (23%)	45,67,67	3.41	16 (35%)
28	CYC	FH	1001	18	42,46,46	1.10	1 (2%)	50,67,67	0.95	2 (4%)
26	PEB	X9	202	1	43,46,46	3.55	11 (25%)	45,67,67	1.92	14 (31%)
26	PEB	H9	202	1	43,46,46	3.40	12 (27%)	45,67,67	2.44	16 (35%)
26	PEB	Z4	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	KC	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	VD	203	2	43,46,46	3.55	12 (27%)	45,67,67	1.97	16 (35%)
26	PEB	S6	202	1	43,46,46	1.08	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	y1	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.43	14 (31%)
26	PEB	ZG	202	2	43,46,46	3.58	12 (27%)	45,67,67	2.05	15 (33%)
27	PUB	xG	305	13	42,46,46	3.39	7 (16%)	37,67,67	3.26	15 (40%)
26	PEB	SA	202	1	43,46,46	3.28	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	S7	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.62	13 (28%)
26	PEB	fA	203	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.29	15 (33%)
26	PEB	Y7	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.14	15 (33%)
26	PEB	CG	202	1	43,46,46	3.08	9 (20%)	45,67,67	2.08	15 (33%)
26	PEB	N4	201	1	43,46,46	3.18	10 (23%)	45,67,67	2.74	21 (46%)
26	PEB	HC	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.14	14 (31%)
26	PEB	n4	201	2,4	43,46,46	3.31	10 (23%)	45,67,67	2.35	19 (42%)
26	PEB	Y6	201	2	43,46,46	3.10	10 (23%)	45,67,67	2.60	19 (42%)
26	PEB	c8	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.59	16 (35%)
26	PEB	N9	203	1	43,46,46	3.36	8 (18%)	45,67,67	2.03	13 (28%)
26	PEB	X4	201	2,1	43,46,46	3.35	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	oG	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.26	15 (33%)
26	PEB	L1	201	3,2	43,46,46	3.51	12 (27%)	45,67,67	2.10	17 (37%)
26	PEB	C8	201	1	43,46,46	3.39	11 (25%)	45,67,67	2.24	19 (42%)
26	PEB	a2	203	2	43,46,46	3.43	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	PJ	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.12	12 (26%)
26	PEB	v1	202	1	43,46,46	3.58	12 (27%)	45,67,67	2.87	20 (44%)
26	PEB	f2	201	1	43,46,46	3.30	11 (25%)	45,67,67	2.41	16 (35%)
26	PEB	kG	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.05	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	aI	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.57	15 (33%)
26	PEB	I8	201	2,1	43,46,46	3.33	11 (25%)	45,67,67	2.36	15 (33%)
26	PEB	l4	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	i4	201	1	43,46,46	3.52	12 (27%)	45,67,67	2.07	16 (35%)
26	PEB	YJ	201	2,26	43,46,46	3.48	10 (23%)	45,67,67	2.04	18 (40%)
26	PEB	TI	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.16	17 (37%)
26	PEB	gG	201	1	43,46,46	3.11	11 (25%)	45,67,67	2.38	15 (33%)
26	PEB	k2	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.30	14 (31%)
28	CYC	J2	1001	10	42,46,46	3.03	16 (38%)	50,67,67	3.13	24 (48%)
26	PEB	Z2	201	1	43,46,46	3.33	12 (27%)	45,67,67	2.76	18 (40%)
26	PEB	vG	201	2	43,46,46	3.50	10 (23%)	45,67,67	2.87	18 (40%)
26	PEB	J1	203	2	43,46,46	3.53	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	OB	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	JD	201	2,7	43,46,46	3.30	9 (20%)	45,67,67	2.44	13 (28%)
26	PEB	K5	203	2	43,46,46	3.38	10 (23%)	45,67,67	1.96	14 (31%)
26	PEB	NJ	203	1	43,46,46	3.36	8 (18%)	45,67,67	2.12	13 (28%)
26	PEB	OI	202	1	43,46,46	3.37	11 (25%)	45,67,67	1.85	11 (24%)
26	PEB	LI	1002	10	43,46,46	3.35	10 (23%)	45,67,67	2.67	18 (40%)
26	PEB	M3	202	1	43,46,46	3.33	10 (23%)	45,67,67	1.96	14 (31%)
27	PUB	B8	302	14	42,46,46	3.25	8 (19%)	37,67,67	3.22	16 (43%)
26	PEB	V7	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.08	15 (33%)
28	CYC	NI	1001	10	42,46,46	3.36	15 (35%)	50,67,67	2.83	21 (42%)
26	PEB	gE	203	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.61	16 (35%)
26	PEB	S8	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.34	17 (37%)
26	PEB	rG	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	g4	201	1	43,46,46	3.37	9 (20%)	45,67,67	2.21	16 (35%)
26	PEB	UJ	202	2	43,46,46	3.53	10 (23%)	45,67,67	1.91	13 (28%)
26	PEB	HB	1002	9,10	43,46,46	3.29	12 (27%)	45,67,67	2.13	13 (28%)
26	PEB	TG	201	2	43,46,46	3.28	9 (20%)	45,67,67	2.94	15 (33%)
26	PEB	WI	201	1	43,46,46	3.29	11 (25%)	45,67,67	2.59	16 (35%)
26	PEB	FF	1002	10	43,46,46	3.32	10 (23%)	45,67,67	2.15	12 (26%)
26	PEB	mG	201	1	43,46,46	3.41	14 (32%)	45,67,67	2.54	16 (35%)
26	PEB	mB	202	2	43,46,46	3.41	11 (25%)	45,67,67	2.41	14 (31%)
26	PEB	a8	204	2,1	43,46,46	3.08	10 (23%)	45,67,67	2.35	17 (37%)
26	PEB	aA	204	2,1	43,46,46	3.07	11 (25%)	45,67,67	2.80	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	CH	1001	18,17	42,46,46	3.49	15 (35%)	50,67,67	2.88	21 (42%)
26	PEB	WJ	201	2,7	43,46,46	3.62	9 (20%)	45,67,67	2.09	15 (33%)
26	PEB	UI	201	1	43,46,46	3.20	10 (23%)	45,67,67	2.80	19 (42%)
26	PEB	L5	202	2	43,46,46	3.20	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	eI	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.24	16 (35%)
26	PEB	mE	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.01	13 (28%)
26	PEB	J3	202	2	43,46,46	3.16	9 (20%)	45,67,67	3.13	18 (40%)
26	PEB	A2	305	7	43,46,46	3.35	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	FD	203	2	43,46,46	3.58	12 (27%)	45,67,67	1.98	17 (37%)
27	PUB	A2	302	7	42,46,46	3.48	8 (19%)	37,67,67	3.19	16 (43%)
26	PEB	CJ	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.01	15 (33%)
28	CYC	wH	1001	-	42,46,46	3.38	13 (30%)	50,67,67	2.90	22 (44%)
26	PEB	DJ	201	2,1	43,46,46	3.11	11 (25%)	45,67,67	2.83	14 (31%)
26	PEB	dF	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.12	15 (33%)
26	PEB	mI	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.38	15 (33%)
26	PEB	zG	501	2,16	43,46,46	3.39	10 (23%)	45,67,67	3.33	17 (37%)
26	PEB	MG	201	1	43,46,46	3.28	10 (23%)	45,67,67	1.88	13 (28%)
26	PEB	B5	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	I1	201	1	43,46,46	3.43	9 (20%)	45,67,67	2.13	16 (35%)
28	CYC	I2	1001	9	42,46,46	3.18	13 (30%)	50,67,67	2.82	20 (40%)
26	PEB	aI	201	2	43,46,46	3.33	11 (25%)	45,67,67	2.30	17 (37%)
26	PEB	D1	201	3,2	43,46,46	3.37	10 (23%)	45,67,67	2.05	14 (31%)
28	CYC	kH	1001	-	42,46,46	3.41	13 (30%)	50,67,67	2.88	18 (36%)
26	PEB	lB	202	1	43,46,46	3.34	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	J7	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	Z4	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.28	14 (31%)
26	PEB	C1	202	1	43,46,46	3.43	9 (20%)	45,67,67	1.86	12 (26%)
28	CYC	J7	1001	10	42,46,46	3.24	15 (35%)	50,67,67	2.89	23 (46%)
26	PEB	p1	202	1	43,46,46	3.75	11 (25%)	45,67,67	2.73	18 (40%)
26	PEB	U8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.47	19 (42%)
26	PEB	VF	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	H6	1002	9,10	43,46,46	3.30	12 (27%)	45,67,67	2.12	12 (26%)
26	PEB	nG	202	2	43,46,46	3.60	13 (30%)	45,67,67	1.93	13 (28%)
26	PEB	N8	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.52	18 (40%)
26	PEB	aF	201	2	43,46,46	3.40	9 (20%)	45,67,67	2.13	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	j2	201	1	43,46,46	3.36	11 (25%)	45,67,67	2.28	19 (42%)
26	PEB	VI	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.00	15 (33%)
26	PEB	K5	202	2	43,46,46	3.22	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	FJ	202	1	43,46,46	3.38	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	NJ	202	1	43,46,46	3.47	11 (25%)	45,67,67	1.94	14 (31%)
26	PEB	PG	202	2	43,46,46	3.58	11 (25%)	45,67,67	2.07	14 (31%)
26	PEB	mF	201	2	43,46,46	3.48	11 (25%)	45,67,67	1.90	15 (33%)
28	CYC	hH	1001	22,18	42,46,46	3.47	14 (33%)	50,67,67	3.04	21 (42%)
26	PEB	C3	201	1	43,46,46	3.25	12 (27%)	45,67,67	2.58	17 (37%)
26	PEB	jB	201	1	43,46,46	3.43	13 (30%)	45,67,67	2.00	15 (33%)
26	PEB	P8	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.41	17 (37%)
26	PEB	Q8	203	1	43,46,46	3.26	10 (23%)	45,67,67	2.39	15 (33%)
26	PEB	J2	1002	10	43,46,46	3.35	11 (25%)	45,67,67	2.06	14 (31%)
27	PUB	yG	302	14	42,46,46	3.36	7 (16%)	37,67,67	3.16	19 (51%)
26	PEB	EG	201	1	43,46,46	3.08	9 (20%)	45,67,67	2.32	14 (31%)
26	PEB	JA	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.32	17 (37%)
28	CYC	JI	1001	10	42,46,46	3.13	16 (38%)	50,67,67	2.96	21 (42%)
26	PEB	c4	202	1	43,46,46	3.58	11 (25%)	45,67,67	2.26	16 (35%)
28	CYC	E7	1001	9,10	42,46,46	3.07	15 (35%)	50,67,67	3.04	18 (36%)
26	PEB	Y9	202	2	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
26	PEB	VE	202	2	43,46,46	3.43	11 (25%)	45,67,67	2.71	18 (40%)
26	PEB	S8	203	2,1	43,46,46	3.28	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	24	401	3	43,46,46	3.43	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	P8	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.53	18 (40%)
26	PEB	Y1	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	Z1	202	2	43,46,46	3.24	10 (23%)	45,67,67	2.25	13 (28%)
26	PEB	rE	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	HA	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.25	17 (37%)
26	PEB	J5	202	1	43,46,46	3.16	10 (23%)	45,67,67	2.38	16 (35%)
26	PEB	K4	202	1	43,46,46	3.35	10 (23%)	45,67,67	1.93	13 (28%)
26	PEB	V4	202	1	43,46,46	3.30	12 (27%)	45,67,67	2.03	13 (28%)
26	PEB	OA	203	2,1	43,46,46	3.20	10 (23%)	45,67,67	2.68	17 (37%)
28	CYC	FI	1001	10	42,46,46	3.26	14 (33%)	50,67,67	2.99	20 (40%)
26	PEB	SB	201	1	43,46,46	3.29	10 (23%)	45,67,67	2.10	16 (35%)
26	PEB	A9	304	7,26	43,46,46	3.48	10 (23%)	45,67,67	2.65	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	nE	201	2	43,46,46	3.47	9 (20%)	45,67,67	2.99	18 (40%)
26	PEB	H4	201	3,2	43,46,46	3.49	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	d2	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	gA	202	2	43,46,46	3.40	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	RG	202	2	43,46,46	3.38	11 (25%)	45,67,67	2.31	15 (33%)
27	PUB	24	403	3,1	42,46,46	3.37	8 (19%)	37,67,67	3.47	13 (35%)
26	PEB	RJ	203	2,1	43,46,46	3.40	12 (27%)	45,67,67	2.35	15 (33%)
26	PEB	ME	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	A6	304	7	43,46,46	3.30	10 (23%)	45,67,67	2.15	16 (35%)
28	CYC	F2	1001	10	42,46,46	3.37	15 (35%)	50,67,67	3.37	23 (46%)
26	PEB	L1	203	2	43,46,46	3.41	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	CA	203	2,1	43,46,46	3.24	10 (23%)	45,67,67	2.48	16 (35%)
26	PEB	S9	202	2	43,46,46	3.36	9 (20%)	45,67,67	1.98	16 (35%)
26	PEB	ME	202	1	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	X9	201	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	i2	203	2	43,46,46	3.50	12 (27%)	45,67,67	1.89	12 (26%)
26	PEB	CC	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.12	16 (35%)
26	PEB	DD	201	2,7	43,46,46	3.40	13 (30%)	45,67,67	2.41	14 (31%)
26	PEB	eF	202	2	43,46,46	3.44	12 (27%)	45,67,67	1.96	14 (31%)
26	PEB	mG	202	1	43,46,46	3.38	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	OG	202	1	43,46,46	3.10	9 (20%)	45,67,67	2.20	15 (33%)
26	PEB	E8	201	2,1	43,46,46	3.28	11 (25%)	45,67,67	2.28	14 (31%)
26	PEB	u1	203	2	43,46,46	3.43	10 (23%)	45,67,67	2.07	14 (31%)
26	PEB	bE	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.88	16 (35%)
26	PEB	cG	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	B4	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.38	14 (31%)
26	PEB	NJ	204	2,1	43,46,46	3.47	10 (23%)	45,67,67	2.29	18 (40%)
26	PEB	uG	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.03	14 (31%)
26	PEB	e1	201	1	43,46,46	3.50	12 (27%)	45,67,67	1.89	13 (28%)
26	PEB	SI	202	1	43,46,46	3.33	11 (25%)	45,67,67	1.96	13 (28%)
26	PEB	gB	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	16 (35%)
26	PEB	VJ	203	2,1	43,46,46	3.22	12 (27%)	45,67,67	2.28	14 (31%)
28	CYC	fH	1001	18	42,46,46	3.44	15 (35%)	50,67,67	2.94	21 (42%)
26	PEB	RD	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
26	PEB	M1	403	3	43,46,46	3.34	10 (23%)	45,67,67	2.29	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	M2	1001	9	42,46,46	3.23	14 (33%)	50,67,67	2.89	20 (40%)
26	PEB	X8	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.66	19 (42%)
26	PEB	S3	202	1	43,46,46	3.23	10 (23%)	45,67,67	2.02	12 (26%)
26	PEB	K9	202	2	43,46,46	3.35	9 (20%)	45,67,67	2.15	15 (33%)
26	PEB	c8	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.34	16 (35%)
26	PEB	IG	202	1	43,46,46	3.19	10 (23%)	45,67,67	2.11	13 (28%)
26	PEB	oG	202	1	43,46,46	3.51	9 (20%)	45,67,67	1.95	12 (26%)
26	PEB	CG	201	1	43,46,46	3.39	9 (20%)	45,67,67	2.28	14 (31%)
26	PEB	YF	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.03	12 (26%)
26	PEB	TF	201	2,6	43,46,46	3.35	12 (27%)	45,67,67	2.21	19 (42%)
26	PEB	BJ	203	2,1	43,46,46	2.91	9 (20%)	45,67,67	2.47	16 (35%)
26	PEB	sG	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	OA	202	1	43,46,46	3.40	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	YG	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.69	17 (37%)
26	PEB	i4	202	1	43,46,46	3.38	9 (20%)	45,67,67	2.09	13 (28%)
26	PEB	e4	202	1	43,46,46	3.60	11 (25%)	45,67,67	2.17	15 (33%)
26	PEB	c2	201	2	43,46,46	3.36	11 (25%)	45,67,67	1.94	12 (26%)
26	PEB	VF	202	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.53	16 (35%)
26	PEB	v4	202	1	43,46,46	3.53	11 (25%)	45,67,67	2.54	17 (37%)
26	PEB	qG	203	1	43,46,46	3.50	12 (27%)	45,67,67	2.31	16 (35%)
26	PEB	hI	202	1	43,46,46	3.41	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	lF	202	1	43,46,46	3.45	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	Q6	201	2,1	43,46,46	3.16	11 (25%)	45,67,67	2.64	17 (37%)
26	PEB	WG	201	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.63	21 (46%)
26	PEB	e7	202	2	43,46,46	3.55	12 (27%)	45,67,67	1.96	14 (31%)
26	PEB	s1	202	2	43,46,46	3.43	11 (25%)	45,67,67	2.22	17 (37%)
26	PEB	T2	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.16	17 (37%)
26	PEB	XA	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.98	20 (44%)
26	PEB	aI	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.00	14 (31%)
26	PEB	hF	201	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.45	16 (35%)
26	PEB	W2	201	1	43,46,46	3.33	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	R4	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	GC	201	2	43,46,46	3.47	11 (25%)	45,67,67	2.04	16 (35%)
26	PEB	w1	202	2	43,46,46	3.55	12 (27%)	45,67,67	2.53	16 (35%)
26	PEB	u1	202	2	43,46,46	3.51	12 (27%)	45,67,67	2.42	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	uG	201	2,1	43,46,46	3.49	12 (27%)	45,67,67	2.19	12 (26%)
26	PEB	P9	203	1	43,46,46	3.39	9 (20%)	45,67,67	2.11	12 (26%)
26	PEB	c1	202	1	43,46,46	3.57	10 (23%)	45,67,67	2.37	17 (37%)
26	PEB	k1	202	1	43,46,46	3.28	9 (20%)	45,67,67	2.07	15 (33%)
26	PEB	hA	202	1	43,46,46	3.30	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	q4	203	2	43,46,46	3.46	10 (23%)	45,67,67	2.09	14 (31%)
26	PEB	O9	201	2,7,26	43,46,46	3.39	9 (20%)	45,67,67	1.99	15 (33%)
26	PEB	fl	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.23	16 (35%)
28	CYC	HF	1001	10	42,46,46	3.31	13 (30%)	50,67,67	2.89	22 (44%)
26	PEB	lE	202	2	43,46,46	3.53	11 (25%)	45,67,67	2.18	14 (31%)
26	PEB	AB	301	7	43,46,46	3.32	10 (23%)	45,67,67	2.45	17 (37%)
26	PEB	fE	202	2	43,46,46	3.58	13 (30%)	45,67,67	1.98	17 (37%)
27	PUB	A8	304	13	42,46,46	3.45	8 (19%)	37,67,67	3.08	13 (35%)
26	PEB	R9	202	1	43,46,46	3.37	12 (27%)	45,67,67	1.98	13 (28%)
26	PEB	VB	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.11	16 (35%)
26	PEB	C5	202	2	43,46,46	3.48	12 (27%)	45,67,67	2.07	13 (28%)
28	CYC	N7	1001	8,10	42,46,46	3.35	15 (35%)	50,67,67	2.77	19 (38%)
26	PEB	j6	201	1	43,46,46	3.43	12 (27%)	45,67,67	2.09	15 (33%)
26	PEB	TE	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.19	16 (35%)
26	PEB	DJ	202	1	43,46,46	3.13	11 (25%)	45,67,67	2.83	19 (42%)
26	PEB	z4	201	1	43,46,46	3.62	10 (23%)	45,67,67	2.30	19 (42%)
26	PEB	GA	202	1	43,46,46	3.39	11 (25%)	45,67,67	2.14	13 (28%)
26	PEB	lI	202	1	43,46,46	3.47	12 (27%)	45,67,67	1.91	15 (33%)
28	CYC	EF	1001	9,10	42,46,46	3.04	14 (33%)	50,67,67	3.19	20 (40%)
26	PEB	U9	202	2	43,46,46	3.51	9 (20%)	45,67,67	1.89	15 (33%)
26	PEB	XE	202	2	43,46,46	3.48	11 (25%)	45,67,67	2.27	18 (40%)
26	PEB	f1	202	2	43,46,46	3.56	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	PJ	201	2,1	43,46,46	3.38	13 (30%)	45,67,67	2.44	13 (28%)
26	PEB	lF	201	2,1	43,46,46	3.36	10 (23%)	45,67,67	2.26	15 (33%)
26	PEB	KE	201	2,1	43,46,46	3.08	11 (25%)	45,67,67	2.82	20 (44%)
27	PUB	AB	302	7	42,46,46	3.50	8 (19%)	37,67,67	3.24	14 (37%)
28	CYC	SH	1001	18	42,46,46	3.33	13 (30%)	50,67,67	2.95	22 (44%)
26	PEB	l1	202	2	43,46,46	3.71	12 (27%)	45,67,67	1.80	12 (26%)
26	PEB	g7	201	2	43,46,46	3.52	10 (23%)	45,67,67	1.88	15 (33%)
26	PEB	H3	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.55	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	XA	201	2	43,46,46	3.29	11 (25%)	45,67,67	2.33	14 (31%)
26	PEB	XD	202	2	43,46,46	3.02	9 (20%)	45,67,67	2.62	19 (42%)
26	PEB	I5	201	2	43,46,46	3.23	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	F3	203	2	43,46,46	3.69	13 (30%)	45,67,67	2.12	15 (33%)
26	PEB	j8	203	2,1	43,46,46	3.22	11 (25%)	45,67,67	2.27	17 (37%)
26	PEB	P7	201	2,6	43,46,46	3.37	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	D3	203	2	43,46,46	3.39	11 (25%)	45,67,67	1.88	16 (35%)
26	PEB	d6	203	1	43,46,46	3.49	12 (27%)	45,67,67	2.07	15 (33%)
26	PEB	J1	201	2	43,46,46	3.25	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	m1	203	1	43,46,46	3.50	12 (27%)	45,67,67	2.07	16 (35%)
26	PEB	I4	201	1	43,46,46	3.43	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	O7	202	1	43,46,46	3.42	12 (27%)	45,67,67	2.45	15 (33%)
26	PEB	gF	202	2	43,46,46	3.52	11 (25%)	45,67,67	2.21	14 (31%)
26	PEB	R9	201	1	43,46,46	3.51	12 (27%)	45,67,67	2.09	13 (28%)
26	PEB	eF	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	YD	301	7	43,46,46	3.41	10 (23%)	45,67,67	2.73	18 (40%)
26	PEB	OG	201	2,1	43,46,46	3.30	12 (27%)	45,67,67	2.57	18 (40%)
26	PEB	X9	203	1	43,46,46	3.41	10 (23%)	45,67,67	1.97	13 (28%)
26	PEB	J1	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.51	15 (33%)
26	PEB	rG	201	2,13	43,46,46	3.46	11 (25%)	45,67,67	2.23	13 (28%)
26	PEB	B4	201	3,2,26	43,46,46	3.36	8 (18%)	45,67,67	1.94	12 (26%)
26	PEB	F5	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.00	16 (35%)
28	CYC	BB	1001	8,10	42,46,46	3.34	14 (33%)	50,67,67	2.82	22 (44%)
26	PEB	WB	203	2,1	43,46,46	3.11	10 (23%)	45,67,67	2.31	17 (37%)
28	CYC	MH	1001	18	42,46,46	3.42	15 (35%)	50,67,67	2.86	19 (38%)
27	PUB	A7	303	7	42,46,46	3.52	8 (19%)	37,67,67	3.12	15 (40%)
26	PEB	GA	201	1	43,46,46	3.27	11 (25%)	45,67,67	2.40	17 (37%)
26	PEB	iG	202	1	43,46,46	3.26	10 (23%)	45,67,67	2.31	18 (40%)
28	CYC	EI	1001	9	42,46,46	3.19	15 (35%)	50,67,67	2.95	19 (38%)
26	PEB	qE	203	1	43,46,46	3.46	12 (27%)	45,67,67	2.05	14 (31%)
26	PEB	XE	201	2	43,46,46	3.38	10 (23%)	45,67,67	3.69	17 (37%)
26	PEB	GJ	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.38	15 (33%)
26	PEB	K8	203	2,1	43,46,46	2.98	10 (23%)	45,67,67	2.46	16 (35%)
26	PEB	B3	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.99	18 (40%)
26	PEB	N7	1002	10	43,46,46	3.40	11 (25%)	45,67,67	2.20	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	PB	201	2,6	43,46,46	3.34	10 (23%)	45,67,67	2.22	18 (40%)
28	CYC	eH	1001	18,17	42,46,46	3.45	15 (35%)	50,67,67	2.93	23 (46%)
26	PEB	ZI	201	1	43,46,46	3.33	12 (27%)	45,67,67	2.77	18 (40%)
26	PEB	D9	201	2,1	43,46,46	3.17	11 (25%)	45,67,67	2.39	14 (31%)
26	PEB	S2	202	1	43,46,46	3.37	11 (25%)	45,67,67	1.95	13 (28%)
27	PUB	A4	203	3,1	42,46,46	3.48	7 (16%)	37,67,67	3.21	16 (43%)
26	PEB	YD	303	7,26	43,46,46	3.33	11 (25%)	45,67,67	3.20	18 (40%)
26	PEB	YE	202	1	43,46,46	3.43	12 (27%)	45,67,67	1.85	13 (28%)
26	PEB	UE	203	2,1	43,46,46	3.06	13 (30%)	45,67,67	3.16	17 (37%)
26	PEB	GD	201	1	43,46,46	3.11	10 (23%)	45,67,67	2.23	13 (28%)
26	PEB	RA	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.39	15 (33%)
26	PEB	Y6	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.28	17 (37%)
27	PUB	wG	304	13	42,46,46	3.41	8 (19%)	37,67,67	3.12	17 (45%)
26	PEB	V2	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.22	16 (35%)
26	PEB	J9	201	1	43,46,46	3.41	12 (27%)	45,67,67	2.19	15 (33%)
26	PEB	YD	304	7,26	43,46,46	3.30	11 (25%)	45,67,67	2.58	13 (28%)
26	PEB	iF	202	2	43,46,46	3.53	10 (23%)	45,67,67	1.85	12 (26%)
26	PEB	G3	202	1	43,46,46	3.33	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	S9	201	2,7	43,46,46	3.39	10 (23%)	45,67,67	2.09	13 (28%)
26	PEB	QE	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	P2	203	2	43,46,46	3.32	9 (20%)	45,67,67	1.90	12 (26%)
26	PEB	d4	203	2	43,46,46	3.49	10 (23%)	45,67,67	1.95	15 (33%)
28	CYC	YH	1004	22	42,46,46	3.44	13 (30%)	50,67,67	2.92	18 (36%)
26	PEB	F2	1002	10	43,46,46	3.27	10 (23%)	45,67,67	2.26	17 (37%)
26	PEB	k8	202	2	43,46,46	3.38	12 (27%)	45,67,67	2.54	17 (37%)
26	PEB	XJ	203	1	43,46,46	3.45	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	eB	203	2	43,46,46	3.56	11 (25%)	45,67,67	2.01	16 (35%)
26	PEB	VI	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.21	16 (35%)
26	PEB	GE	202	1	43,46,46	2.78	9 (20%)	45,67,67	2.92	21 (46%)
26	PEB	m1	202	1	43,46,46	3.53	12 (27%)	45,67,67	2.11	15 (33%)
26	PEB	UA	202	1	43,46,46	3.26	10 (23%)	45,67,67	2.46	18 (40%)
28	CYC	H2	1001	10	42,46,46	3.27	15 (35%)	50,67,67	3.07	23 (46%)
26	PEB	NA	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	V3	201	2,11	43,46,46	3.31	10 (23%)	45,67,67	2.22	16 (35%)
26	PEB	DA	201	14,2	43,46,46	3.41	11 (25%)	45,67,67	2.45	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	b7	201	1	43,46,46	3.37	11 (25%)	45,67,67	1.99	16 (35%)
26	PEB	Q1	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.11	15 (33%)
26	PEB	T9	201	2,1	43,46,46	3.35	13 (30%)	45,67,67	2.30	13 (28%)
26	PEB	O8	203	2,1	43,46,46	3.23	10 (23%)	45,67,67	2.66	17 (37%)
26	PEB	n1	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	U7	202	1	43,46,46	3.33	12 (27%)	45,67,67	2.07	13 (28%)
27	PUB	A8	303	13	42,46,46	3.41	9 (21%)	37,67,67	3.36	18 (48%)
26	PEB	cG	203	2,1	43,46,46	3.30	13 (30%)	45,67,67	2.77	17 (37%)
26	PEB	h4	203	2	43,46,46	3.44	9 (20%)	45,67,67	1.88	15 (33%)
26	PEB	Z8	202	2	43,46,46	3.07	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	O3	202	1	43,46,46	3.23	10 (23%)	45,67,67	2.05	16 (35%)
26	PEB	TI	202	2	43,46,46	3.36	11 (25%)	45,67,67	2.24	14 (31%)
28	CYC	PH	1001	17	42,46,46	3.35	15 (35%)	50,67,67	3.00	22 (44%)
26	PEB	B9	203	2,1	43,46,46	2.94	9 (20%)	45,67,67	2.38	14 (31%)
26	PEB	ED	201	1	43,46,46	3.57	12 (27%)	45,67,67	2.31	14 (31%)
26	PEB	fB	203	2,1	43,46,46	3.48	10 (23%)	45,67,67	2.29	12 (26%)
26	PEB	mI	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	T3	201	2	43,46,46	3.58	11 (25%)	45,67,67	2.40	17 (37%)
26	PEB	AI	305	7	43,46,46	3.38	10 (23%)	45,67,67	2.00	13 (28%)
28	CYC	JF	1001	10	42,46,46	3.22	15 (35%)	50,67,67	2.85	23 (46%)
26	PEB	hE	201	2	43,46,46	3.49	12 (27%)	45,67,67	2.60	18 (40%)
26	PEB	A7	302	7	43,46,46	3.41	10 (23%)	45,67,67	1.95	13 (28%)
26	PEB	T6	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.29	19 (42%)
26	PEB	h1	202	2	43,46,46	3.47	9 (20%)	45,67,67	2.00	15 (33%)
26	PEB	H1	201	3,2	43,46,46	3.53	12 (27%)	45,67,67	1.92	12 (26%)
26	PEB	Q4	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	m2	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	P1	203	1	43,46,46	3.58	11 (25%)	45,67,67	1.80	12 (26%)
26	PEB	f8	203	2,1	43,46,46	3.32	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	FG	201	2	43,46,46	3.51	10 (23%)	45,67,67	3.86	16 (35%)
26	PEB	UE	202	1	43,46,46	3.27	9 (20%)	45,67,67	2.13	12 (26%)
26	PEB	KA	203	2,1	43,46,46	3.00	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	B1	201	3,2,26	43,46,46	3.37	9 (20%)	45,67,67	2.00	13 (28%)
26	PEB	RJ	201	1	43,46,46	3.53	12 (27%)	45,67,67	2.07	14 (31%)
26	PEB	xG	303	13	43,46,46	3.44	9 (20%)	45,67,67	1.98	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	L4	203	2	43,46,46	3.43	10 (23%)	45,67,67	1.94	14 (31%)
26	PEB	hF	202	1	43,46,46	3.38	12 (27%)	45,67,67	2.16	14 (31%)
26	PEB	C9	201	2,7	43,46,46	3.13	11 (25%)	45,67,67	2.24	18 (40%)
26	PEB	WJ	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.86	15 (33%)
28	CYC	cH	1001	17	42,46,46	3.49	14 (33%)	50,67,67	4.76	20 (40%)
26	PEB	U1	201	2,4	43,46,46	3.61	12 (27%)	45,67,67	2.17	18 (40%)
26	PEB	AC	201	2	43,46,46	3.49	9 (20%)	45,67,67	1.96	13 (28%)
26	PEB	AF	305	7	43,46,46	3.43	10 (23%)	45,67,67	2.42	15 (33%)
26	PEB	b1	501	2,4	43,46,46	3.48	9 (20%)	45,67,67	2.24	14 (31%)
26	PEB	yE	301	14	43,46,46	3.35	10 (23%)	45,67,67	2.11	16 (35%)
28	CYC	NB	1001	8,10	42,46,46	3.18	15 (35%)	50,67,67	2.93	27 (54%)
26	PEB	ZB	202	1	43,46,46	3.39	11 (25%)	45,67,67	2.16	16 (35%)
26	PEB	BE	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.30	14 (31%)
26	PEB	ND	202	2	43,46,46	3.02	9 (20%)	45,67,67	3.13	17 (37%)
26	PEB	I8	203	1	43,46,46	3.52	12 (27%)	45,67,67	2.20	16 (35%)
26	PEB	xE	303	13	43,46,46	3.38	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	bI	201	1	43,46,46	3.39	10 (23%)	45,67,67	2.38	17 (37%)
26	PEB	fF	202	1	43,46,46	3.47	9 (20%)	45,67,67	2.59	15 (33%)
26	PEB	NB	1002	9,10	43,46,46	3.37	11 (25%)	45,67,67	2.21	15 (33%)
26	PEB	aB	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.17	19 (42%)
28	CYC	rH	1001	17	42,46,46	3.36	15 (35%)	50,67,67	3.04	21 (42%)
26	PEB	l7	201	2,1	43,46,46	3.34	9 (20%)	45,67,67	2.31	15 (33%)
26	PEB	e6	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.31	13 (28%)
26	PEB	WA	203	2,1	43,46,46	2.99	11 (25%)	45,67,67	2.52	16 (35%)
26	PEB	J8	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.42	17 (37%)
26	PEB	OI	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	iI	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.00	15 (33%)
26	PEB	LF	1002	10	43,46,46	3.11	10 (23%)	45,67,67	2.37	15 (33%)
26	PEB	j6	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.95	14 (31%)
26	PEB	UD	202	1	43,46,46	3.34	10 (23%)	45,67,67	1.95	13 (28%)
26	PEB	dB	202	2,1	43,46,46	3.34	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	MD	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	wG	303	13	43,46,46	3.47	11 (25%)	45,67,67	2.08	15 (33%)
26	PEB	xG	302	13	43,46,46	3.37	11 (25%)	45,67,67	2.91	13 (28%)
26	PEB	ZG	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.41	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	EA	203	1	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
26	PEB	i8	201	2,13	43,46,46	3.43	12 (27%)	45,67,67	2.62	16 (35%)
26	PEB	cA	203	2	43,46,46	3.32	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	Z6	203	1	43,46,46	3.34	11 (25%)	45,67,67	2.15	16 (35%)
28	CYC	K2	1001	9	42,46,46	3.26	15 (35%)	50,67,67	2.88	19 (38%)
27	PUB	AB	303	7	42,46,46	3.42	7 (16%)	37,67,67	3.00	14 (37%)
26	PEB	a2	202	2	43,46,46	3.28	13 (30%)	45,67,67	2.57	16 (35%)
26	PEB	BJ	201	1	43,46,46	3.18	11 (25%)	45,67,67	2.40	18 (40%)
26	PEB	NG	202	2	43,46,46	3.48	10 (23%)	45,67,67	1.92	13 (28%)
26	PEB	L5	203	2	43,46,46	3.16	11 (25%)	45,67,67	2.08	15 (33%)
26	PEB	J3	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.32	14 (31%)
26	PEB	l6	203	1	43,46,46	3.46	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	mA	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.56	18 (40%)
26	PEB	G4	202	1	43,46,46	3.45	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	mF	202	2	43,46,46	3.71	10 (23%)	45,67,67	1.85	11 (24%)
26	PEB	GJ	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.22	17 (37%)
26	PEB	B5	203	2	43,46,46	3.55	12 (27%)	45,67,67	1.97	14 (31%)
26	PEB	RF	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.17	18 (40%)
26	PEB	E9	201	2,15	43,46,46	3.29	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	SB	202	1	43,46,46	3.43	10 (23%)	45,67,67	1.83	13 (28%)
26	PEB	m7	202	2	43,46,46	3.61	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	m8	201	2,13	43,46,46	3.42	11 (25%)	45,67,67	2.49	19 (42%)
27	PUB	AJ	302	1,7	42,46,46	3.54	8 (19%)	37,67,67	3.03	15 (40%)
26	PEB	e2	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.14	15 (33%)
26	PEB	gE	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.99	14 (31%)
28	CYC	C6	1001	9,10	42,46,46	3.25	15 (35%)	50,67,67	2.71	18 (36%)
26	PEB	B1	203	2	43,46,46	3.44	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	D4	201	3,2	43,46,46	3.32	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	X1	202	1	43,46,46	3.35	10 (23%)	45,67,67	2.58	16 (35%)
26	PEB	AJ	303	7,26	43,46,46	3.39	11 (25%)	45,67,67	2.54	15 (33%)
28	CYC	yH	1001	-	42,46,46	3.56	14 (33%)	50,67,67	2.88	19 (38%)
26	PEB	O7	203	2,1	43,46,46	3.23	9 (20%)	45,67,67	2.21	14 (31%)
26	PEB	AC	203	2	43,46,46	3.54	12 (27%)	45,67,67	1.84	13 (28%)
26	PEB	VD	201	2,11	43,46,46	3.34	10 (23%)	45,67,67	2.11	13 (28%)
26	PEB	V7	201	2	43,46,46	3.42	13 (30%)	45,67,67	2.17	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	M6	1001	9,10	42,46,46	3.17	14 (33%)	50,67,67	2.89	19 (38%)
26	PEB	W3	201	1	43,46,46	3.18	10 (23%)	45,67,67	2.35	18 (40%)
26	PEB	FD	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.72	18 (40%)
26	PEB	Q2	201	1	43,46,46	3.32	11 (25%)	45,67,67	2.69	20 (44%)
26	PEB	cB	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	P9	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.21	16 (35%)
26	PEB	HD	203	2	43,46,46	3.56	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	f6	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.18	13 (28%)
26	PEB	LD	202	2	43,46,46	3.18	10 (23%)	45,67,67	2.76	17 (37%)
26	PEB	bE	202	2	43,46,46	3.64	10 (23%)	45,67,67	2.35	13 (28%)
26	PEB	RI	202	2	43,46,46	3.21	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	Q9	202	2	43,46,46	3.48	13 (30%)	45,67,67	1.83	13 (28%)
26	PEB	D4	202	2	43,46,46	3.47	13 (30%)	45,67,67	2.42	15 (33%)
28	CYC	C7	1001	9,10	42,46,46	3.32	13 (30%)	50,67,67	2.81	19 (38%)
26	PEB	tG	201	2	43,46,46	3.51	10 (23%)	45,67,67	2.85	16 (35%)
26	PEB	F4	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.43	15 (33%)
26	PEB	R2	201	2,6	43,46,46	3.32	10 (23%)	45,67,67	2.38	15 (33%)
28	CYC	IB	1001	9,10	42,46,46	3.17	13 (30%)	50,67,67	2.81	18 (36%)
28	CYC	KB	202	9,10	42,46,46	3.19	14 (33%)	50,67,67	2.74	20 (40%)
26	PEB	SJ	202	2	43,46,46	3.36	9 (20%)	45,67,67	1.97	15 (33%)
26	PEB	H5	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.27	14 (31%)
26	PEB	d7	201	2,1	43,46,46	3.34	10 (23%)	45,67,67	2.23	14 (31%)
26	PEB	z4	202	1	43,46,46	3.53	9 (20%)	45,67,67	2.50	17 (37%)
26	PEB	kI	201	2	43,46,46	3.41	12 (27%)	45,67,67	1.96	12 (26%)
28	CYC	DI	1001	10	42,46,46	3.11	13 (30%)	50,67,67	2.80	20 (40%)
26	PEB	h8	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.17	16 (35%)
26	PEB	h7	203	2,1	43,46,46	3.48	13 (30%)	45,67,67	2.63	16 (35%)
26	PEB	a7	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	IG	203	2,1	43,46,46	3.05	10 (23%)	45,67,67	2.73	18 (40%)
26	PEB	gB	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.59	13 (28%)
26	PEB	HI	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	g7	202	2	43,46,46	3.49	11 (25%)	45,67,67	2.30	16 (35%)
26	PEB	f4	202	2	43,46,46	3.56	11 (25%)	45,67,67	2.18	14 (31%)
26	PEB	qG	201	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.69	17 (37%)
26	PEB	hB	203	1	43,46,46	3.31	11 (25%)	45,67,67	2.09	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	V4	203	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.14	13 (28%)
28	CYC	iH	1001	18,17	42,46,46	3.44	15 (35%)	50,67,67	2.96	22 (44%)
26	PEB	OE	203	1	43,46,46	3.39	10 (23%)	45,67,67	2.09	17 (37%)
28	CYC	JF	1003	9,10	42,46,46	3.20	11 (26%)	50,67,67	2.65	19 (38%)
26	PEB	XD	201	2,11	43,46,46	3.64	11 (25%)	45,67,67	2.35	19 (42%)
26	PEB	MG	203	2,1	43,46,46	3.33	13 (30%)	45,67,67	2.57	16 (35%)
26	PEB	T6	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.31	19 (42%)
26	PEB	k6	201	2,7	43,46,46	3.45	12 (27%)	45,67,67	2.24	17 (37%)
26	PEB	eE	203	1	43,46,46	3.40	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	K1	201	1	43,46,46	3.41	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	e7	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.08	17 (37%)
26	PEB	lA	203	1	43,46,46	3.24	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	W8	203	2,1	43,46,46	3.00	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	QE	203	2,1	43,46,46	3.26	12 (27%)	45,67,67	2.72	17 (37%)
26	PEB	c2	203	2	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	O8	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.03	15 (33%)
28	CYC	pH	1001	17	42,46,46	3.46	14 (33%)	50,67,67	2.89	21 (42%)
26	PEB	j8	202	1	43,46,46	3.43	11 (25%)	45,67,67	2.61	17 (37%)
26	PEB	NF	1002	10	43,46,46	3.27	12 (27%)	45,67,67	2.09	12 (26%)
26	PEB	H2	1002	10	43,46,46	3.24	10 (23%)	45,67,67	2.09	16 (35%)
28	CYC	H7	1001	10	42,46,46	3.36	14 (33%)	50,67,67	2.92	20 (40%)
26	PEB	c7	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.20	14 (31%)
26	PEB	CE	202	1	43,46,46	3.03	9 (20%)	45,67,67	2.14	13 (28%)
26	PEB	Q8	202	2,1	43,46,46	3.29	11 (25%)	45,67,67	2.28	15 (33%)
26	PEB	wE	303	13	43,46,46	3.46	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	E3	202	1	43,46,46	3.40	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	bF	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.03	15 (33%)
26	PEB	11	203	2	43,46,46	3.43	9 (20%)	45,67,67	1.91	13 (28%)
26	PEB	iB	202	2	43,46,46	3.50	11 (25%)	45,67,67	2.00	13 (28%)
26	PEB	P9	201	2,1	43,46,46	3.47	12 (27%)	45,67,67	2.13	13 (28%)
26	PEB	T7	202	2	43,46,46	3.33	10 (23%)	45,67,67	1.78	12 (26%)
26	PEB	DE	203	2	43,46,46	3.46	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	i7	201	2	43,46,46	3.46	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	OB	202	1	43,46,46	3.39	10 (23%)	45,67,67	2.04	13 (28%)
26	PEB	N3	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.43	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	Y9	201	2,26	43,46,46	3.51	11 (25%)	45,67,67	1.99	12 (26%)
26	PEB	LJ	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.47	16 (35%)
26	PEB	O9	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.98	15 (33%)
26	PEB	AJ	305	2,7,26	43,46,46	3.45	11 (25%)	45,67,67	1.95	12 (26%)
26	PEB	f7	202	1	43,46,46	3.39	9 (20%)	45,67,67	2.66	14 (31%)
26	PEB	N1	201	1	43,46,46	3.23	10 (23%)	45,67,67	2.74	21 (46%)
26	PEB	sE	201	1	43,46,46	3.32	9 (20%)	45,67,67	2.04	13 (28%)
26	PEB	TI	203	2	43,46,46	3.41	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	Y3	301	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	16 (35%)
26	PEB	M9	202	2	43,46,46	3.31	9 (20%)	45,67,67	1.99	13 (28%)
26	PEB	wG	301	13	43,46,46	3.22	9 (20%)	45,67,67	2.29	15 (33%)
26	PEB	OJ	201	2	43,46,46	3.38	11 (25%)	45,67,67	2.53	16 (35%)
26	PEB	u4	203	2	43,46,46	3.59	11 (25%)	45,67,67	2.09	16 (35%)
26	PEB	fl	202	1	43,46,46	3.41	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	HE	201	2	43,46,46	3.13	13 (30%)	45,67,67	3.10	19 (42%)
26	PEB	YE	201	1	43,46,46	3.47	9 (20%)	45,67,67	1.88	15 (33%)
26	PEB	ZF	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.50	16 (35%)
26	PEB	YA	201	2,1	43,46,46	3.08	10 (23%)	45,67,67	2.55	17 (37%)
26	PEB	JJ	202	1	43,46,46	3.17	9 (20%)	45,67,67	2.07	13 (28%)
26	PEB	cE	203	2,1	43,46,46	3.37	16 (37%)	45,67,67	3.00	17 (37%)
26	PEB	AG	201	1	43,46,46	3.25	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	G3	201	1	43,46,46	3.21	9 (20%)	45,67,67	2.15	13 (28%)
26	PEB	FI	1002	10	43,46,46	3.26	10 (23%)	45,67,67	2.23	17 (37%)
26	PEB	S4	201	2,4	43,46,46	3.47	12 (27%)	45,67,67	2.31	18 (40%)
26	PEB	eE	202	1	43,46,46	3.19	11 (25%)	45,67,67	2.33	19 (42%)
26	PEB	j8	201	1	43,46,46	3.31	11 (25%)	45,67,67	2.09	14 (31%)
26	PEB	lF	203	1	43,46,46	3.48	11 (25%)	45,67,67	2.75	15 (33%)
26	PEB	W9	201	2,7	43,46,46	3.43	11 (25%)	45,67,67	2.10	15 (33%)
26	PEB	UB	203	1	43,46,46	3.37	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	21	401	3	43,46,46	3.42	10 (23%)	45,67,67	2.28	17 (37%)
26	PEB	c7	201	2	43,46,46	3.36	10 (23%)	45,67,67	1.89	14 (31%)
26	PEB	E4	201	1	43,46,46	3.42	9 (20%)	45,67,67	1.91	12 (26%)
26	PEB	j1	201	2,4	43,46,46	3.54	11 (25%)	45,67,67	2.16	16 (35%)
26	PEB	M8	201	2,1	43,46,46	3.06	11 (25%)	45,67,67	2.68	15 (33%)
26	PEB	P3	201	2,11	43,46,46	3.43	10 (23%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	VJ	202	1	43,46,46	3.46	11 (25%)	45,67,67	1.94	14 (31%)
26	PEB	J4	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.08	16 (35%)
26	PEB	A7	305	7	43,46,46	3.42	10 (23%)	45,67,67	2.38	14 (31%)
26	PEB	SF	202	1	43,46,46	3.31	10 (23%)	45,67,67	2.40	13 (28%)
26	PEB	W1	201	2	43,46,46	3.50	12 (27%)	45,67,67	2.40	23 (51%)
26	PEB	T4	201	2,1	43,46,46	3.47	12 (27%)	45,67,67	2.29	17 (37%)
26	PEB	Y3	304	7,26	43,46,46	3.31	11 (25%)	45,67,67	2.42	13 (28%)
26	PEB	n4	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.05	14 (31%)
28	CYC	VH	1001	-	42,46,46	3.47	14 (33%)	50,67,67	3.12	19 (38%)
26	PEB	H8	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	KC	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	d1	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.01	14 (31%)
26	PEB	gI	203	2	43,46,46	3.46	11 (25%)	45,67,67	2.19	13 (28%)
26	PEB	oE	201	1	43,46,46	3.46	12 (27%)	45,67,67	2.53	17 (37%)
28	CYC	E2	1001	9	42,46,46	3.21	15 (35%)	50,67,67	2.92	20 (40%)
26	PEB	HG	201	2	43,46,46	3.14	12 (27%)	45,67,67	2.94	21 (46%)
26	PEB	N3	202	2	43,46,46	2.92	10 (23%)	45,67,67	3.31	18 (40%)
26	PEB	b7	203	2,1	43,46,46	3.45	11 (25%)	45,67,67	2.26	14 (31%)
26	PEB	i1	203	1	43,46,46	3.41	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	MA	201	2,1	43,46,46	3.05	11 (25%)	45,67,67	2.65	15 (33%)
26	PEB	k7	201	2	43,46,46	3.39	11 (25%)	45,67,67	1.92	13 (28%)
28	CYC	G7	1001	9,10	42,46,46	3.23	11 (26%)	50,67,67	2.88	19 (38%)
26	PEB	BJ	202	1	43,46,46	3.33	10 (23%)	45,67,67	1.97	15 (33%)
26	PEB	TA	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.34	14 (31%)
26	PEB	K8	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	C5	203	2	43,46,46	3.45	9 (20%)	45,67,67	2.22	14 (31%)
26	PEB	HF	1002	10	43,46,46	3.44	11 (25%)	45,67,67	2.30	14 (31%)
26	PEB	F1	201	3,2	43,46,46	3.56	12 (27%)	45,67,67	2.11	16 (35%)
26	PEB	vE	201	2	43,46,46	3.47	9 (20%)	45,67,67	3.06	17 (37%)
26	PEB	Q4	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.32	20 (44%)
26	PEB	Q3	202	1	43,46,46	3.11	9 (20%)	45,67,67	1.98	14 (31%)
26	PEB	KA	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.30	15 (33%)
26	PEB	F1	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	F8	202	2	43,46,46	3.31	11 (25%)	45,67,67	2.50	18 (40%)
26	PEB	aE	201	2,1	43,46,46	3.42	12 (27%)	45,67,67	2.60	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	X8	201	2	43,46,46	3.28	11 (25%)	45,67,67	2.37	15 (33%)
26	PEB	JJ	201	1	43,46,46	3.38	13 (30%)	45,67,67	2.20	13 (28%)
27	PUB	xG	306	13	42,46,46	3.61	7 (16%)	37,67,67	2.91	15 (40%)
26	PEB	a4	203	2	43,46,46	3.29	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	V9	201	1	43,46,46	3.20	10 (23%)	45,67,67	2.30	12 (26%)
26	PEB	ZF	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.18	17 (37%)
26	PEB	VA	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.56	18 (40%)
26	PEB	NE	201	2	43,46,46	3.35	10 (23%)	45,67,67	3.08	16 (35%)
26	PEB	H5	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
26	PEB	i2	202	2	43,46,46	3.29	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	L6	1002	9,10	43,46,46	3.33	10 (23%)	45,67,67	1.89	13 (28%)
26	PEB	g8	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.50	16 (35%)
26	PEB	l8	203	1	43,46,46	3.23	11 (25%)	45,67,67	2.06	13 (28%)
26	PEB	UB	202	1	43,46,46	3.46	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	T8	202	2	43,46,46	3.17	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	Q6	203	1	43,46,46	3.39	9 (20%)	45,67,67	2.00	15 (33%)
26	PEB	Y3	303	7,26	43,46,46	3.30	12 (27%)	45,67,67	2.79	14 (31%)
26	PEB	VJ	201	1	43,46,46	3.48	11 (25%)	45,67,67	1.86	13 (28%)
26	PEB	z1	201	1	43,46,46	3.56	11 (25%)	45,67,67	2.45	17 (37%)
26	PEB	i1	202	1	43,46,46	3.47	12 (27%)	45,67,67	2.12	18 (40%)
26	PEB	qE	201	2,1	43,46,46	3.39	11 (25%)	45,67,67	2.62	16 (35%)
26	PEB	F9	203	2,1	43,46,46	3.41	13 (30%)	45,67,67	3.08	13 (28%)
26	PEB	VD	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.57	18 (40%)
28	CYC	H6	1001	10	42,46,46	3.13	14 (33%)	50,67,67	3.07	21 (42%)
26	PEB	j7	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.45	17 (37%)
26	PEB	IC	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	J8	202	2	43,46,46	3.35	12 (27%)	45,67,67	2.28	15 (33%)
26	PEB	Q7	202	1	43,46,46	3.38	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	b6	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	V3	202	2	43,46,46	3.18	9 (20%)	45,67,67	2.62	16 (35%)
26	PEB	R1	203	2,1	43,46,46	3.47	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	KJ	201	2	43,46,46	3.48	12 (27%)	45,67,67	2.02	15 (33%)
28	CYC	FF	1001	10	42,46,46	3.32	15 (35%)	50,67,67	2.89	18 (36%)
26	PEB	J3	201	2,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	14 (31%)
26	PEB	D2	1002	10	43,46,46	3.30	10 (23%)	45,67,67	2.08	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	F4	203	2	43,46,46	3.40	11 (25%)	45,67,67	1.91	15 (33%)
26	PEB	q1	202	2	43,46,46	3.37	12 (27%)	45,67,67	2.56	15 (33%)
28	CYC	HI	1001	10	42,46,46	3.24	14 (33%)	50,67,67	3.08	23 (46%)
27	PUB	A9	302	1,7	42,46,46	3.48	8 (19%)	37,67,67	3.18	15 (40%)
28	CYC	D2	1001	10	42,46,46	3.14	14 (33%)	50,67,67	2.83	21 (42%)
26	PEB	B3	203	2	43,46,46	3.48	13 (30%)	45,67,67	2.13	14 (31%)
26	PEB	Y7	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.11	16 (35%)
28	CYC	jH	1001	22,18	42,46,46	3.50	15 (35%)	50,67,67	2.88	19 (38%)
26	PEB	dI	202	1	43,46,46	3.35	11 (25%)	45,67,67	1.89	12 (26%)
26	PEB	IJ	201	2,15	43,46,46	3.61	12 (27%)	45,67,67	2.28	15 (33%)
26	PEB	R6	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.24	17 (37%)
26	PEB	XG	203	2	43,46,46	3.48	11 (25%)	45,67,67	2.28	17 (37%)
26	PEB	iA	202	2	43,46,46	3.38	11 (25%)	45,67,67	2.21	16 (35%)
28	CYC	sH	1001	22,18	42,46,46	3.42	13 (30%)	50,67,67	2.85	17 (34%)
26	PEB	d6	202	2,1	43,46,46	3.36	10 (23%)	45,67,67	2.43	16 (35%)
26	PEB	BD	203	2	43,46,46	3.33	9 (20%)	45,67,67	1.99	14 (31%)
26	PEB	gF	201	2	43,46,46	3.57	10 (23%)	45,67,67	1.92	15 (33%)
26	PEB	lB	201	2,1	43,46,46	3.32	11 (25%)	45,67,67	2.37	14 (31%)
26	PEB	WF	201	1	43,46,46	3.21	11 (25%)	45,67,67	2.22	15 (33%)
26	PEB	w4	202	2	43,46,46	3.56	10 (23%)	45,67,67	2.61	14 (31%)
26	PEB	PD	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.19	16 (35%)
26	PEB	O2	201	1	43,46,46	3.38	11 (25%)	45,67,67	2.51	17 (37%)
26	PEB	O7	201	1	43,46,46	3.34	13 (30%)	45,67,67	2.27	18 (40%)
26	PEB	QD	201	1	43,46,46	3.23	11 (25%)	45,67,67	2.65	17 (37%)
26	PEB	j7	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	ID	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.87	12 (26%)
26	PEB	kG	203	2,1	43,46,46	3.44	12 (27%)	45,67,67	2.31	11 (24%)
26	PEB	T9	203	1	43,46,46	3.39	8 (18%)	45,67,67	2.14	12 (26%)
26	PEB	FJ	201	1	43,46,46	3.23	11 (25%)	45,67,67	2.53	17 (37%)
26	PEB	z1	202	1	43,46,46	3.70	10 (23%)	45,67,67	2.58	19 (42%)
27	PUB	AA	304	13	42,46,46	3.47	9 (21%)	37,67,67	3.01	14 (37%)
26	PEB	C5	204	2	43,46,46	3.54	12 (27%)	45,67,67	1.88	15 (33%)
28	CYC	D6	1001	10	42,46,46	3.17	14 (33%)	50,67,67	3.01	21 (42%)
26	PEB	m2	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	ME	203	2,1	43,46,46	3.35	13 (30%)	45,67,67	2.46	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	UA	203	3,1	43,46,46	3.33	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	QD	202	1	43,46,46	3.19	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	Q2	202	10,1	43,46,46	3.38	9 (20%)	45,67,67	1.87	12 (26%)
26	PEB	L2	1002	10	43,46,46	3.38	11 (25%)	45,67,67	2.75	16 (35%)
26	PEB	y4	202	2	43,46,46	3.37	9 (20%)	45,67,67	2.17	14 (31%)
26	PEB	A5	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	OG	203	1	43,46,46	3.28	9 (20%)	45,67,67	2.00	16 (35%)
26	PEB	H9	203	1	43,46,46	3.42	11 (25%)	45,67,67	2.12	12 (26%)
26	PEB	J5	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.84	17 (37%)
26	PEB	M3	201	1	43,46,46	3.25	10 (23%)	45,67,67	2.48	16 (35%)
26	PEB	OB	203	2,1	43,46,46	3.19	11 (25%)	45,67,67	2.32	16 (35%)
26	PEB	SE	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.16	15 (33%)
26	PEB	iG	201	2,1	43,46,46	3.41	11 (25%)	45,67,67	2.38	14 (31%)
26	PEB	jI	202	1	43,46,46	3.34	11 (25%)	45,67,67	1.95	12 (26%)
26	PEB	wE	302	13	43,46,46	3.34	9 (20%)	45,67,67	2.19	15 (33%)
26	PEB	T4	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.06	16 (35%)
28	CYC	E6	1001	9,10	42,46,46	3.21	15 (35%)	50,67,67	2.76	21 (42%)
26	PEB	B4	203	2	43,46,46	3.42	10 (23%)	45,67,67	1.93	16 (35%)
26	PEB	SD	202	1	43,46,46	3.20	10 (23%)	45,67,67	1.96	12 (26%)
26	PEB	JG	201	2	43,46,46	3.41	10 (23%)	45,67,67	3.06	17 (37%)
26	PEB	p4	202	1	43,46,46	3.77	10 (23%)	45,67,67	2.77	17 (37%)
26	PEB	JG	202	2	43,46,46	3.47	11 (25%)	45,67,67	2.33	16 (35%)
26	PEB	P4	201	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.23	14 (31%)
26	PEB	HC	203	2	43,46,46	3.27	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	R8	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	U6	203	1	43,46,46	3.41	11 (25%)	45,67,67	2.05	15 (33%)
26	PEB	WD	202	1	43,46,46	3.42	11 (25%)	45,67,67	2.05	13 (28%)
26	PEB	K4	201	1	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
26	PEB	IE	202	1	43,46,46	3.19	10 (23%)	45,67,67	2.10	15 (33%)
26	PEB	jF	203	2,1	43,46,46	3.48	13 (30%)	45,67,67	2.49	15 (33%)
26	PEB	Q3	201	1	43,46,46	3.26	11 (25%)	45,67,67	2.72	17 (37%)
26	PEB	hB	201	2,1	43,46,46	3.48	12 (27%)	45,67,67	2.23	14 (31%)
26	PEB	XJ	202	1	43,46,46	3.57	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	M4	401	3	43,46,46	3.43	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	eB	202	2	43,46,46	3.26	9 (20%)	45,67,67	2.27	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	TJ	201	2,1	43,46,46	3.45	13 (30%)	45,67,67	2.35	13 (28%)
28	CYC	AH	1001	17	42,46,46	3.50	13 (30%)	50,67,67	4.72	20 (40%)
26	PEB	SG	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.13	14 (31%)
26	PEB	cI	203	2	43,46,46	3.46	12 (27%)	45,67,67	1.99	11 (24%)
26	PEB	h7	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.03	15 (33%)
28	CYC	F7	1001	10	42,46,46	3.23	13 (30%)	50,67,67	2.97	18 (36%)
26	PEB	x4	201	1	43,46,46	3.51	10 (23%)	45,67,67	1.86	14 (31%)
28	CYC	NF	1001	8,10	42,46,46	3.36	16 (38%)	50,67,67	2.86	23 (46%)
26	PEB	TB	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	A2	301	7	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	x1	201	1	43,46,46	3.52	13 (30%)	45,67,67	1.87	15 (33%)
26	PEB	g1	203	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.33	13 (28%)
26	PEB	dG	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.44	16 (35%)
26	PEB	V6	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.19	15 (33%)
28	CYC	GH	1001	17	42,46,46	3.44	15 (35%)	50,67,67	3.03	24 (48%)
28	CYC	CI	1001	9	42,46,46	3.25	14 (33%)	50,67,67	2.93	21 (42%)
26	PEB	B9	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	iB	201	2	43,46,46	3.43	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	ND	203	2	43,46,46	3.33	10 (23%)	45,67,67	2.35	17 (37%)
27	PUB	KD	203	1,7	42,46,46	3.37	7 (16%)	37,67,67	3.59	17 (45%)
28	CYC	K7	1001	9,10	42,46,46	3.24	12 (28%)	50,67,67	2.86	19 (38%)
26	PEB	dB	201	1,7	43,46,46	3.36	8 (18%)	45,67,67	2.18	14 (31%)
26	PEB	e6	203	2	43,46,46	3.56	12 (27%)	45,67,67	2.70	18 (40%)
26	PEB	bB	201	1	43,46,46	3.34	10 (23%)	45,67,67	2.21	14 (31%)
28	CYC	IF	1001	9,10	42,46,46	3.17	12 (28%)	50,67,67	2.96	22 (44%)
26	PEB	lG	202	2	43,46,46	3.44	9 (20%)	45,67,67	2.10	15 (33%)
26	PEB	DE	202	2,1	43,46,46	3.16	13 (30%)	45,67,67	3.17	16 (35%)
26	PEB	a4	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	f8	202	1	43,46,46	3.39	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	PI	202	2	43,46,46	3.29	11 (25%)	45,67,67	2.47	16 (35%)
26	PEB	AI	304	7	43,46,46	3.36	10 (23%)	45,67,67	2.06	13 (28%)
26	PEB	Y2	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.33	15 (33%)
26	PEB	I9	201	2,15	43,46,46	3.67	13 (30%)	45,67,67	2.35	18 (40%)
26	PEB	K9	201	2	43,46,46	3.35	11 (25%)	45,67,67	1.97	14 (31%)
26	PEB	O6	202	1	43,46,46	3.36	10 (23%)	45,67,67	2.06	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	L7	1002	10	43,46,46	3.25	10 (23%)	45,67,67	2.23	14 (31%)
26	PEB	L4	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.34	15 (33%)
26	PEB	BG	201	2,16	43,46,46	3.38	12 (27%)	45,67,67	3.49	16 (35%)
26	PEB	c6	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	16 (35%)
26	PEB	R9	203	2,1	43,46,46	3.39	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	D6	1002	9,10	43,46,46	3.31	12 (27%)	45,67,67	2.25	15 (33%)
26	PEB	k4	202	1	43,46,46	3.38	9 (20%)	45,67,67	1.95	14 (31%)
26	PEB	R3	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	N4	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	WE	202	1	43,46,46	2.99	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	EJ	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	B8	301	14	43,46,46	3.42	10 (23%)	45,67,67	2.43	14 (31%)
26	PEB	QG	202	1	43,46,46	3.40	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	Y1	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.22	18 (40%)
26	PEB	SG	202	1	43,46,46	3.26	12 (27%)	45,67,67	2.40	16 (35%)
26	PEB	UB	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.30	16 (35%)
26	PEB	V4	201	1	43,46,46	3.44	10 (23%)	45,67,67	2.04	17 (37%)
26	PEB	GG	201	2,1	43,46,46	3.18	12 (27%)	45,67,67	3.06	20 (44%)
26	PEB	WA	202	1	43,46,46	3.47	10 (23%)	45,67,67	2.26	13 (28%)
26	PEB	L3	201	2,26	43,46,46	3.39	10 (23%)	45,67,67	2.32	18 (40%)
26	PEB	g1	202	1	43,46,46	3.44	11 (25%)	45,67,67	2.12	14 (31%)
26	PEB	V6	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.05	16 (35%)
27	PUB	BA	302	14	42,46,46	3.29	7 (16%)	37,67,67	3.20	16 (43%)
26	PEB	QB	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.01	15 (33%)
26	PEB	C8	203	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.45	16 (35%)
26	PEB	AB	304	7	43,46,46	3.29	9 (20%)	45,67,67	2.10	17 (37%)
26	PEB	B9	201	1	43,46,46	3.22	11 (25%)	45,67,67	2.32	16 (35%)
26	PEB	T7	201	2,6	43,46,46	3.40	12 (27%)	45,67,67	2.02	16 (35%)
26	PEB	L9	203	1	43,46,46	3.37	9 (20%)	45,67,67	2.04	14 (31%)
26	PEB	XD	203	2	43,46,46	3.49	11 (25%)	45,67,67	2.30	18 (40%)
26	PEB	LG	202	2	43,46,46	3.67	11 (25%)	45,67,67	2.71	15 (33%)
26	PEB	VI	202	2	43,46,46	3.13	10 (23%)	45,67,67	2.43	17 (37%)
26	PEB	aG	203	1	43,46,46	3.35	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	O8	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.98	13 (28%)
26	PEB	a8	201	1,13	43,46,46	3.10	10 (23%)	45,67,67	2.30	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	cA	202	2,1	43,46,46	3.55	12 (27%)	45,67,67	2.28	13 (28%)
28	CYC	FB	1001	10	42,46,46	3.25	13 (30%)	50,67,67	2.90	18 (36%)
26	PEB	G9	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.09	17 (37%)
26	PEB	m4	203	1	43,46,46	3.54	11 (25%)	45,67,67	2.16	17 (37%)
26	PEB	U7	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.24	14 (31%)
26	PEB	X1	203	1	43,46,46	3.22	11 (25%)	45,67,67	2.18	14 (31%)
26	PEB	MD	201	1	43,46,46	3.28	11 (25%)	45,67,67	2.42	14 (31%)
26	PEB	m6	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.55	14 (31%)
26	PEB	DE	201	2	43,46,46	3.30	8 (18%)	45,67,67	2.95	17 (37%)
26	PEB	T1	202	1	43,46,46	3.31	10 (23%)	45,67,67	2.13	16 (35%)
26	PEB	K6	201	9,10	43,46,46	3.31	11 (25%)	45,67,67	2.10	15 (33%)
28	CYC	MI	1001	9	42,46,46	3.16	12 (28%)	50,67,67	2.89	17 (34%)
26	PEB	KC	203	2	43,46,46	3.40	10 (23%)	45,67,67	1.91	13 (28%)
26	PEB	gI	202	2	43,46,46	3.32	11 (25%)	45,67,67	2.31	14 (31%)
26	PEB	eI	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.16	15 (33%)
26	PEB	Y2	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.17	15 (33%)
26	PEB	k7	202	2	43,46,46	3.45	9 (20%)	45,67,67	2.09	16 (35%)
26	PEB	UJ	201	2,7	43,46,46	3.49	11 (25%)	45,67,67	2.10	17 (37%)
26	PEB	G5	203	2	43,46,46	3.43	9 (20%)	45,67,67	2.28	14 (31%)
26	PEB	r1	202	1	43,46,46	3.63	11 (25%)	45,67,67	2.49	14 (31%)
26	PEB	h1	201	2,4	43,46,46	3.64	11 (25%)	45,67,67	2.05	13 (28%)
26	PEB	O1	201	2,4	43,46,46	3.40	11 (25%)	45,67,67	2.36	20 (44%)
26	PEB	X3	202	2	43,46,46	2.97	9 (20%)	45,67,67	2.61	17 (37%)
26	PEB	g4	203	2,1	43,46,46	3.37	12 (27%)	45,67,67	2.44	13 (28%)
26	PEB	U4	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	e8	201	2,13	43,46,46	3.31	11 (25%)	45,67,67	2.39	16 (35%)
26	PEB	U3	202	1	43,46,46	3.36	9 (20%)	45,67,67	1.91	14 (31%)
28	CYC	EB	1001	9,10	42,46,46	3.24	16 (38%)	50,67,67	2.85	19 (38%)
26	PEB	M1	402	3,26	43,46,46	3.47	10 (23%)	45,67,67	2.08	14 (31%)
26	PEB	kA	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.63	14 (31%)
26	PEB	t4	202	1	43,46,46	3.62	12 (27%)	45,67,67	2.47	16 (35%)
26	PEB	h8	203	1	43,46,46	3.47	11 (25%)	45,67,67	1.97	13 (28%)
26	PEB	H3	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	VA	202	2	43,46,46	3.46	14 (32%)	45,67,67	2.80	16 (35%)
26	PEB	U2	201	1	43,46,46	3.22	10 (23%)	45,67,67	2.77	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	V8	202	2	43,46,46	3.45	13 (30%)	45,67,67	3.22	19 (42%)
26	PEB	g8	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.54	16 (35%)
26	PEB	uE	201	2,1	43,46,46	3.37	13 (30%)	45,67,67	2.34	14 (31%)
26	PEB	AC	202	2	43,46,46	3.44	9 (20%)	45,67,67	2.19	14 (31%)
26	PEB	yG	301	14	43,46,46	3.36	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	HJ	202	1	43,46,46	3.39	12 (27%)	45,67,67	2.49	16 (35%)
26	PEB	QF	201	2,1	43,46,46	3.32	11 (25%)	45,67,67	2.51	17 (37%)
26	PEB	F5	202	2	43,46,46	3.17	10 (23%)	45,67,67	1.94	12 (26%)
26	PEB	HD	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.58	17 (37%)
26	PEB	PF	201	2,6	43,46,46	3.38	10 (23%)	45,67,67	2.25	17 (37%)
26	PEB	C1	201	1	43,46,46	3.42	10 (23%)	45,67,67	1.98	12 (26%)
26	PEB	H7	1002	10	43,46,46	3.47	12 (27%)	45,67,67	2.24	15 (33%)
26	PEB	DD	203	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	16 (35%)
26	PEB	KG	201	2,1	43,46,46	3.11	10 (23%)	45,67,67	2.52	14 (31%)
28	CYC	L2	1001	10	42,46,46	3.18	16 (38%)	50,67,67	2.97	22 (44%)
26	PEB	l4	202	2	43,46,46	3.63	11 (25%)	45,67,67	2.06	13 (28%)
27	PUB	A6	302	7	42,46,46	3.39	9 (21%)	37,67,67	3.30	16 (43%)
26	PEB	YA	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.31	16 (35%)
26	PEB	AD	201	1	43,46,46	3.47	12 (27%)	45,67,67	2.30	17 (37%)
26	PEB	gI	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	fG	202	2	43,46,46	3.60	12 (27%)	45,67,67	2.01	18 (40%)
27	PUB	21	402	3	42,46,46	3.49	8 (19%)	37,67,67	3.50	17 (45%)
26	PEB	LD	201	2,26	43,46,46	3.44	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	A3	202	1	43,46,46	3.49	11 (25%)	45,67,67	2.19	13 (28%)
26	PEB	KG	202	1	43,46,46	3.33	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	24	404	3	43,46,46	3.42	11 (25%)	45,67,67	2.73	16 (35%)
26	PEB	vG	202	2	43,46,46	3.49	10 (23%)	45,67,67	1.96	16 (35%)
26	PEB	d8	202	1	43,46,46	3.21	10 (23%)	45,67,67	2.22	15 (33%)
26	PEB	K3	202	1	43,46,46	3.43	9 (20%)	45,67,67	1.88	14 (31%)
26	PEB	AD	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.98	12 (26%)
26	PEB	X3	201	2,11	43,46,46	3.64	11 (25%)	45,67,67	2.37	18 (40%)
26	PEB	C5	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.15	14 (31%)
26	PEB	21	404	3	43,46,46	3.40	11 (25%)	45,67,67	2.36	15 (33%)
26	PEB	U7	203	1	43,46,46	3.34	10 (23%)	45,67,67	2.25	15 (33%)
26	PEB	C4	202	1	43,46,46	3.46	10 (23%)	45,67,67	1.87	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	LB	1001	10	42,46,46	3.22	15 (35%)	50,67,67	3.12	22 (44%)
26	PEB	TA	202	2	43,46,46	3.17	10 (23%)	45,67,67	2.36	16 (35%)
26	PEB	OE	202	1	43,46,46	3.07	10 (23%)	45,67,67	2.19	17 (37%)
26	PEB	LA	202	2	43,46,46	3.34	11 (25%)	45,67,67	2.64	18 (40%)
26	PEB	S2	201	1	43,46,46	3.42	11 (25%)	45,67,67	2.60	20 (44%)
26	PEB	HJ	201	2,1	43,46,46	3.14	10 (23%)	45,67,67	2.49	18 (40%)
26	PEB	lA	202	1	43,46,46	3.27	10 (23%)	45,67,67	2.32	15 (33%)
26	PEB	UG	202	1	43,46,46	3.23	9 (20%)	45,67,67	2.16	13 (28%)
26	PEB	V8	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.52	18 (40%)
26	PEB	eA	201	2,13	43,46,46	3.32	10 (23%)	45,67,67	2.37	16 (35%)
26	PEB	x1	202	1	43,46,46	3.28	10 (23%)	45,67,67	2.88	17 (37%)
26	PEB	MJ	202	2	43,46,46	3.27	9 (20%)	45,67,67	2.03	14 (31%)
26	PEB	11	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.42	15 (33%)
27	PUB	A1	203	3,1	42,46,46	3.63	7 (16%)	37,67,67	3.36	17 (45%)
26	PEB	BC	201	2	43,46,46	3.50	10 (23%)	45,67,67	1.90	14 (31%)
26	PEB	jA	203	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	lB	203	1	43,46,46	3.44	10 (23%)	45,67,67	1.97	16 (35%)
26	PEB	GE	201	2,1	43,46,46	3.03	13 (30%)	45,67,67	3.31	19 (42%)
26	PEB	YB	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.38	17 (37%)
26	PEB	X4	203	1	43,46,46	3.20	11 (25%)	45,67,67	2.14	14 (31%)
26	PEB	hF	203	2,1	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
26	PEB	H4	203	2	43,46,46	3.54	11 (25%)	45,67,67	2.11	14 (31%)
26	PEB	s4	202	2	43,46,46	3.55	11 (25%)	45,67,67	2.38	15 (33%)
28	CYC	I7	1001	9,10	42,46,46	3.21	13 (30%)	50,67,67	2.85	18 (36%)
26	PEB	CE	201	2,1	43,46,46	3.16	13 (30%)	45,67,67	3.51	17 (37%)
27	PUB	A6	303	7	42,46,46	3.44	7 (16%)	37,67,67	3.00	14 (37%)
26	PEB	jG	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	zE	501	2,16	43,46,46	3.37	10 (23%)	45,67,67	3.37	15 (33%)
26	PEB	bB	202	1	43,46,46	3.48	10 (23%)	45,67,67	2.36	15 (33%)
26	PEB	ED	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.99	13 (28%)
26	PEB	Y4	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	Q1	201	2	43,46,46	3.40	12 (27%)	45,67,67	2.34	21 (46%)
26	PEB	VG	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.64	18 (40%)
26	PEB	T9	202	1	43,46,46	3.44	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	jE	201	2	43,46,46	3.29	9 (20%)	45,67,67	2.72	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	QF	203	1	43,46,46	3.29	10 (23%)	45,67,67	2.07	14 (31%)
28	CYC	DF	1001	10	42,46,46	3.36	15 (35%)	50,67,67	2.85	18 (36%)
26	PEB	fF	203	2,1	43,46,46	3.46	11 (25%)	45,67,67	2.21	15 (33%)
26	PEB	D8	201	14,2	43,46,46	3.41	11 (25%)	45,67,67	2.47	13 (28%)
26	PEB	u4	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.44	13 (28%)
28	CYC	LI	1001	10	42,46,46	3.13	16 (38%)	50,67,67	2.97	22 (44%)
26	PEB	dB	203	1	43,46,46	3.51	12 (27%)	45,67,67	2.04	15 (33%)
26	PEB	PA	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.51	16 (35%)
26	PEB	AI	301	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
26	PEB	hI	201	1	43,46,46	3.41	11 (25%)	45,67,67	2.34	18 (40%)
27	PUB	AI	302	7	42,46,46	3.45	7 (16%)	37,67,67	3.14	16 (43%)
26	PEB	sE	203	2,1	43,46,46	3.40	13 (30%)	45,67,67	2.37	14 (31%)
26	PEB	R8	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.18	17 (37%)
26	PEB	W8	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.40	19 (42%)
26	PEB	UG	201	1	43,46,46	2.76	10 (23%)	45,67,67	2.99	16 (35%)
28	CYC	YH	1003	22	42,46,46	3.48	15 (35%)	50,67,67	2.89	20 (40%)
26	PEB	B3	201	2,26	43,46,46	3.37	9 (20%)	45,67,67	2.23	16 (35%)
26	PEB	DG	201	2	43,46,46	3.26	8 (18%)	45,67,67	3.08	17 (37%)
26	PEB	cI	201	2	43,46,46	3.38	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	JA	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.20	16 (35%)
28	CYC	GI	1001	9	42,46,46	3.31	14 (33%)	50,67,67	2.92	19 (38%)
26	PEB	MJ	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	P4	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.08	17 (37%)
26	PEB	GG	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.65	22 (48%)
28	CYC	G2	1001	9	42,46,46	3.26	14 (33%)	50,67,67	2.91	16 (32%)
26	PEB	HA	202	2	43,46,46	3.42	13 (30%)	45,67,67	2.45	15 (33%)
26	PEB	w4	203	2	43,46,46	3.51	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	cI	202	2	43,46,46	3.48	12 (27%)	45,67,67	2.37	14 (31%)
26	PEB	eG	203	1	43,46,46	3.36	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	CC	202	-	43,46,46	3.45	10 (23%)	45,67,67	2.21	14 (31%)
26	PEB	a6	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.16	20 (44%)
28	CYC	K6	202	9,10	42,46,46	3.19	14 (33%)	50,67,67	2.74	19 (38%)
26	PEB	u1	201	3,2	43,46,46	3.27	10 (23%)	45,67,67	2.49	21 (46%)
26	PEB	H5	203	2	43,46,46	3.14	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	ND	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.31	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	eB	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.01	16 (35%)
27	PUB	yE	303	14	42,46,46	3.37	7 (16%)	37,67,67	3.09	13 (35%)
26	PEB	H4	202	2	43,46,46	3.31	11 (25%)	45,67,67	2.42	17 (37%)
26	PEB	k8	201	2	43,46,46	3.40	9 (20%)	45,67,67	2.48	14 (31%)
26	PEB	R7	201	2	43,46,46	3.44	11 (25%)	45,67,67	2.04	16 (35%)
26	PEB	L8	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.73	17 (37%)
28	CYC	KF	1001	9,10	42,46,46	3.17	11 (26%)	50,67,67	2.93	22 (44%)
26	PEB	RG	201	2	43,46,46	3.28	10 (23%)	45,67,67	3.69	21 (46%)
26	PEB	y1	201	2	43,46,46	3.54	11 (25%)	45,67,67	2.04	17 (37%)
26	PEB	JC	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.10	14 (31%)
26	PEB	fA	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.11	17 (37%)
26	PEB	V1	203	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.16	13 (28%)
26	PEB	UD	201	1	43,46,46	3.22	10 (23%)	45,67,67	2.61	13 (28%)
26	PEB	fB	201	1	43,46,46	3.32	10 (23%)	45,67,67	2.11	17 (37%)
26	PEB	FA	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.48	18 (40%)
26	PEB	R4	203	2,1	43,46,46	3.49	13 (30%)	45,67,67	1.96	13 (28%)
26	PEB	V2	202	2	43,46,46	3.15	10 (23%)	45,67,67	2.33	14 (31%)
26	PEB	GC	203	2	43,46,46	3.47	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	W4	201	2	43,46,46	3.52	12 (27%)	45,67,67	2.34	21 (46%)
28	CYC	L7	1001	10	42,46,46	3.36	14 (33%)	50,67,67	2.77	20 (40%)
26	PEB	iI	203	2	43,46,46	3.53	12 (27%)	45,67,67	1.90	14 (31%)
26	PEB	uG	203	1	43,46,46	3.45	11 (25%)	45,67,67	1.98	15 (33%)
26	PEB	Z7	203	1	43,46,46	3.43	11 (25%)	45,67,67	2.31	15 (33%)
26	PEB	fA	202	1	43,46,46	3.63	13 (30%)	45,67,67	1.99	13 (28%)
26	PEB	A6	301	7	43,46,46	3.34	11 (25%)	45,67,67	2.35	16 (35%)
26	PEB	f1	201	2	43,46,46	3.55	13 (30%)	45,67,67	2.13	17 (37%)
28	CYC	C2	1001	9	42,46,46	3.25	15 (35%)	50,67,67	2.93	21 (42%)
26	PEB	A5	202	2	43,46,46	3.56	12 (27%)	45,67,67	1.84	12 (26%)
26	PEB	IE	201	1	43,46,46	2.80	13 (30%)	45,67,67	2.85	18 (40%)
26	PEB	KD	202	1	43,46,46	3.44	10 (23%)	45,67,67	1.81	11 (24%)
26	PEB	c6	202	2	43,46,46	3.47	11 (25%)	45,67,67	1.99	13 (28%)
26	PEB	dE	201	2	43,46,46	3.48	10 (23%)	45,67,67	2.35	16 (35%)
26	PEB	WE	201	2,1	43,46,46	3.14	13 (30%)	45,67,67	2.85	20 (44%)
26	PEB	aE	202	1	43,46,46	3.10	9 (20%)	45,67,67	2.66	12 (26%)
26	PEB	G4	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.26	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	l8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.36	15 (33%)
26	PEB	U2	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.87	11 (24%)
27	PUB	AF	304	7	42,46,46	3.73	8 (19%)	37,67,67	3.97	17 (45%)
26	PEB	Q6	202	1	43,46,46	3.44	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	EG	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.01	16 (35%)
26	PEB	R3	202	2	43,46,46	3.02	11 (25%)	45,67,67	3.00	15 (33%)
26	PEB	QI	201	1	43,46,46	3.31	11 (25%)	45,67,67	2.70	20 (44%)
26	PEB	RB	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	cF	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	t1	202	1	43,46,46	3.68	10 (23%)	45,67,67	2.56	16 (35%)
26	PEB	F9	202	1	43,46,46	3.42	12 (27%)	45,67,67	2.00	15 (33%)
26	PEB	QA	204	1	43,46,46	3.21	10 (23%)	45,67,67	2.13	15 (33%)
28	CYC	MB	1001	9,10	42,46,46	3.16	14 (33%)	50,67,67	2.90	19 (38%)
26	PEB	QB	201	2,1	43,46,46	3.15	11 (25%)	45,67,67	2.73	17 (37%)
26	PEB	cE	201	1	43,46,46	2.91	10 (23%)	45,67,67	2.56	14 (31%)
26	PEB	E9	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.07	14 (31%)
26	PEB	PE	202	2	43,46,46	3.59	11 (25%)	45,67,67	2.06	15 (33%)
26	PEB	h7	201	2,1	43,46,46	3.30	10 (23%)	45,67,67	2.38	15 (33%)
26	PEB	TF	202	2	43,46,46	3.32	9 (20%)	45,67,67	1.81	13 (28%)
26	PEB	TD	202	2	43,46,46	2.76	9 (20%)	45,67,67	2.99	19 (42%)
26	PEB	Q7	201	2,1	43,46,46	3.24	11 (25%)	45,67,67	2.36	16 (35%)
26	PEB	kE	201	1	43,46,46	3.36	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	g1	201	1	43,46,46	3.36	10 (23%)	45,67,67	2.28	15 (33%)
26	PEB	P6	201	2,6	43,46,46	3.36	10 (23%)	45,67,67	2.23	18 (40%)
26	PEB	14	202	2	43,46,46	3.52	12 (27%)	45,67,67	2.32	14 (31%)
26	PEB	LE	201	2	43,46,46	3.34	8 (18%)	45,67,67	3.85	16 (35%)
28	CYC	nH	1001	-	42,46,46	3.48	14 (33%)	50,67,67	3.02	20 (40%)
26	PEB	BE	201	2,16	43,46,46	3.35	10 (23%)	45,67,67	3.49	16 (35%)
26	PEB	T2	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.38	15 (33%)
26	PEB	cA	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.59	15 (33%)
26	PEB	k2	201	2	43,46,46	3.33	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	eG	201	2,1	43,46,46	3.42	13 (30%)	45,67,67	2.23	17 (37%)
26	PEB	FD	201	2,7	43,46,46	3.43	10 (23%)	45,67,67	2.07	15 (33%)
26	PEB	b6	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.13	13 (28%)
26	PEB	d8	201	2,1	43,46,46	3.53	12 (27%)	45,67,67	2.37	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	cB	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	19 (42%)
26	PEB	W7	202	1	43,46,46	3.43	10 (23%)	45,67,67	2.56	17 (37%)
26	PEB	OD	202	1	43,46,46	3.25	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	R4	202	1	43,46,46	3.32	8 (18%)	45,67,67	1.96	12 (26%)
26	PEB	iE	202	1	43,46,46	3.27	10 (23%)	45,67,67	2.32	14 (31%)
27	PUB	K3	203	1,7	42,46,46	3.41	7 (16%)	37,67,67	3.21	15 (40%)
28	CYC	WH	1001	-	42,46,46	3.56	14 (33%)	50,67,67	2.88	19 (38%)
27	PUB	xE	305	13	42,46,46	3.40	8 (19%)	37,67,67	3.08	14 (37%)
26	PEB	S1	201	2,4	43,46,46	3.45	12 (27%)	45,67,67	2.27	18 (40%)
27	PUB	K4	203	3,1	42,46,46	3.49	7 (16%)	37,67,67	3.32	19 (51%)
26	PEB	XG	202	2	43,46,46	3.25	12 (27%)	45,67,67	2.63	16 (35%)
26	PEB	y4	203	2	43,46,46	3.51	11 (25%)	45,67,67	2.28	11 (24%)
26	PEB	SJ	201	2,7	43,46,46	3.39	9 (20%)	45,67,67	2.10	10 (22%)
26	PEB	h6	203	1	43,46,46	3.32	10 (23%)	45,67,67	2.00	13 (28%)
26	PEB	wG	302	13	43,46,46	3.30	9 (20%)	45,67,67	2.22	15 (33%)
26	PEB	BD	202	2	43,46,46	3.49	11 (25%)	45,67,67	3.06	18 (40%)
26	PEB	dF	201	2,1	43,46,46	3.26	9 (20%)	45,67,67	2.35	14 (31%)
26	PEB	RA	201	2	43,46,46	3.47	10 (23%)	45,67,67	2.26	16 (35%)
26	PEB	a8	203	1	43,46,46	3.13	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	PJ	202	1	43,46,46	3.50	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	M8	203	1	43,46,46	3.26	10 (23%)	45,67,67	2.27	15 (33%)
26	PEB	B5	201	2	43,46,46	3.48	11 (25%)	45,67,67	1.93	12 (26%)
26	PEB	O6	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	R3	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.22	17 (37%)
28	CYC	DF	1003	9,10	42,46,46	3.14	12 (28%)	50,67,67	2.94	20 (40%)
26	PEB	GA	203	2,1	43,46,46	3.30	12 (27%)	45,67,67	2.55	14 (31%)
26	PEB	DI	1002	10	43,46,46	3.33	10 (23%)	45,67,67	2.19	17 (37%)
26	PEB	d1	203	2	43,46,46	3.45	10 (23%)	45,67,67	2.04	15 (33%)
26	PEB	CJ	201	2,7	43,46,46	3.09	11 (25%)	45,67,67	2.51	21 (46%)
26	PEB	ZB	203	1	43,46,46	3.33	10 (23%)	45,67,67	2.12	15 (33%)
28	CYC	oH	1001	18	42,46,46	3.43	15 (35%)	50,67,67	2.87	21 (42%)
26	PEB	D9	203	1	43,46,46	3.27	10 (23%)	45,67,67	2.25	15 (33%)
26	PEB	U8	201	2,1	43,46,46	3.21	10 (23%)	45,67,67	2.44	15 (33%)
26	PEB	H3	203	2	43,46,46	3.55	12 (27%)	45,67,67	2.41	16 (35%)
27	PUB	Y3	302	7	42,46,46	3.56	8 (19%)	37,67,67	3.05	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	PG	201	2	43,46,46	3.34	9 (20%)	45,67,67	3.22	18 (40%)
26	PEB	bG	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.08	15 (33%)
26	PEB	AF	302	7	43,46,46	3.39	10 (23%)	45,67,67	1.95	12 (26%)
27	PUB	21	403	3,1	42,46,46	3.47	7 (16%)	37,67,67	3.31	16 (43%)
26	PEB	IJ	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	OD	201	1	43,46,46	3.10	10 (23%)	45,67,67	2.81	20 (44%)
26	PEB	RE	201	2	43,46,46	3.32	10 (23%)	45,67,67	3.60	19 (42%)
26	PEB	l7	203	1	43,46,46	3.35	12 (27%)	45,67,67	2.73	15 (33%)
26	PEB	DA	202	2	43,46,46	3.24	12 (27%)	45,67,67	2.74	19 (42%)
27	PUB	xE	301	13	42,46,46	3.39	7 (16%)	37,67,67	3.19	19 (51%)
28	CYC	LH	1001	-	42,46,46	3.45	14 (33%)	50,67,67	3.04	22 (44%)
26	PEB	X1	201	2,1	43,46,46	3.35	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	S3	201	1	43,46,46	3.11	10 (23%)	45,67,67	2.78	17 (37%)
26	PEB	W6	203	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	A9	303	7,26	43,46,46	3.45	11 (25%)	45,67,67	2.28	17 (37%)
26	PEB	HC	202	2	43,46,46	3.31	10 (23%)	45,67,67	1.99	13 (28%)
26	PEB	DF	1002	10	43,46,46	3.33	11 (25%)	45,67,67	2.14	15 (33%)
26	PEB	kF	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.10	16 (35%)
26	PEB	y1	203	2	43,46,46	3.45	11 (25%)	45,67,67	2.45	15 (33%)
26	PEB	c4	201	1	43,46,46	3.47	9 (20%)	45,67,67	2.22	15 (33%)
26	PEB	jF	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.63	16 (35%)
26	PEB	rE	201	2,13	43,46,46	3.47	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	S8	202	1	43,46,46	3.27	11 (25%)	45,67,67	1.90	14 (31%)
26	PEB	PI	203	2	43,46,46	3.34	8 (18%)	45,67,67	1.85	13 (28%)
26	PEB	a8	202	1	43,46,46	3.21	10 (23%)	45,67,67	2.09	16 (35%)
26	PEB	AA	302	13	43,46,46	3.36	10 (23%)	45,67,67	2.82	18 (40%)
26	PEB	f2	202	1	43,46,46	3.49	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	h2	201	1	43,46,46	3.39	12 (27%)	45,67,67	2.31	20 (44%)
26	PEB	f7	201	1	43,46,46	3.50	13 (30%)	45,67,67	1.96	15 (33%)
26	PEB	14	203	2	43,46,46	3.46	9 (20%)	45,67,67	1.83	12 (26%)
26	PEB	l1	202	1	43,46,46	3.40	10 (23%)	45,67,67	1.88	12 (26%)
26	PEB	h8	201	2,1	43,46,46	3.34	12 (27%)	45,67,67	2.56	15 (33%)
26	PEB	H1	203	2	43,46,46	3.51	10 (23%)	45,67,67	2.15	14 (31%)
26	PEB	YE	203	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.15	14 (31%)
26	PEB	G1	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.94	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	m8	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.49	17 (37%)
26	PEB	V1	201	1	43,46,46	3.49	11 (25%)	45,67,67	1.96	15 (33%)
26	PEB	f4	201	2	43,46,46	3.50	13 (30%)	45,67,67	2.23	15 (33%)
26	PEB	P4	203	1	43,46,46	3.60	12 (27%)	45,67,67	1.71	10 (22%)
28	CYC	NH	1001	17	42,46,46	3.46	15 (35%)	50,67,67	2.93	23 (46%)
26	PEB	A4	201	1	43,46,46	3.37	10 (23%)	45,67,67	2.41	20 (44%)
27	PUB	A2	303	7	42,46,46	3.40	7 (16%)	37,67,67	2.99	14 (37%)
26	PEB	QJ	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.11	17 (37%)
26	PEB	k1	201	1	43,46,46	3.48	10 (23%)	45,67,67	2.06	17 (37%)
26	PEB	IA	201	2,1	43,46,46	3.41	12 (27%)	45,67,67	2.31	14 (31%)
26	PEB	JD	203	2	43,46,46	3.39	10 (23%)	45,67,67	2.30	14 (31%)
26	PEB	hA	201	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.47	15 (33%)
26	PEB	iF	201	2	43,46,46	3.34	12 (27%)	45,67,67	2.05	16 (35%)
26	PEB	gA	201	2	43,46,46	3.46	11 (25%)	45,67,67	2.26	16 (35%)
26	PEB	GE	203	1	43,46,46	3.31	10 (23%)	45,67,67	2.16	17 (37%)
26	PEB	a1	203	2	43,46,46	3.34	11 (25%)	45,67,67	2.04	13 (28%)
26	PEB	jG	201	2	43,46,46	3.33	11 (25%)	45,67,67	2.84	18 (40%)
26	PEB	dB	204	1	43,46,46	3.42	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	h4	201	2,4	43,46,46	3.55	11 (25%)	45,67,67	1.98	14 (31%)
26	PEB	PF	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.00	17 (37%)
26	PEB	J9	203	2,1	43,46,46	3.21	12 (27%)	45,67,67	2.23	12 (26%)
26	PEB	m7	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	A1	202	1	43,46,46	3.51	12 (27%)	45,67,67	1.88	14 (31%)
28	CYC	I6	1001	9,10	42,46,46	3.18	13 (30%)	50,67,67	2.82	18 (36%)
26	PEB	gE	201	1	43,46,46	3.10	11 (25%)	45,67,67	2.73	19 (42%)
26	PEB	iE	201	2,1	43,46,46	3.37	11 (25%)	45,67,67	2.42	16 (35%)
26	PEB	QF	202	1	43,46,46	3.39	12 (27%)	45,67,67	2.50	17 (37%)
26	PEB	AJ	301	7	43,46,46	3.30	9 (20%)	45,67,67	2.05	17 (37%)
26	PEB	pE	202	2	43,46,46	3.66	12 (27%)	45,67,67	2.48	11 (24%)
26	PEB	U6	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	V3	203	2	43,46,46	3.57	12 (27%)	45,67,67	2.00	15 (33%)
28	CYC	G6	1001	9,10	42,46,46	3.18	13 (30%)	50,67,67	2.89	19 (38%)
26	PEB	FC	202	2	43,46,46	3.25	10 (23%)	45,67,67	1.95	12 (26%)
26	PEB	DG	202	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.68	16 (35%)
26	PEB	v4	201	1	43,46,46	3.53	12 (27%)	45,67,67	2.11	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	RJ	202	1	43,46,46	3.30	10 (23%)	45,67,67	1.99	14 (31%)
26	PEB	g6	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.02	16 (35%)
26	PEB	QB	202	1	43,46,46	3.40	10 (23%)	45,67,67	2.13	14 (31%)
26	PEB	L1	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.56	16 (35%)
26	PEB	i6	202	2	43,46,46	3.47	10 (23%)	45,67,67	2.02	15 (33%)
26	PEB	m2	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.15	14 (31%)
26	PEB	i7	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.16	13 (28%)
26	PEB	a1	202	2	43,46,46	3.50	12 (27%)	45,67,67	1.99	12 (26%)
26	PEB	s1	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.15	15 (33%)
26	PEB	e3	401	1,11	43,46,46	3.38	10 (23%)	45,67,67	1.95	15 (33%)
26	PEB	L9	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.26	14 (31%)
26	PEB	dE	202	2	43,46,46	3.64	11 (25%)	45,67,67	2.00	14 (31%)
28	CYC	QH	1001	22,18	42,46,46	3.43	14 (33%)	50,67,67	2.90	18 (36%)
26	PEB	ZI	202	1	43,46,46	3.30	10 (23%)	45,67,67	1.94	12 (26%)
26	PEB	LG	201	2	43,46,46	3.36	11 (25%)	45,67,67	3.50	19 (42%)
26	PEB	aG	202	1	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	eA	202	2	43,46,46	3.26	11 (25%)	45,67,67	2.61	19 (42%)
26	PEB	xE	302	13	43,46,46	3.37	11 (25%)	45,67,67	2.95	15 (33%)
26	PEB	m4	202	1	43,46,46	3.46	12 (27%)	45,67,67	2.16	16 (35%)
26	PEB	YJ	202	2	43,46,46	3.47	9 (20%)	45,67,67	2.00	14 (31%)
27	PUB	N9	201	1,7	42,46,46	3.76	9 (21%)	37,67,67	3.15	12 (32%)
26	PEB	A8	301	13	43,46,46	3.20	11 (25%)	45,67,67	2.28	15 (33%)
26	PEB	JD	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.75	16 (35%)
26	PEB	c1	201	1	43,46,46	3.42	9 (20%)	45,67,67	2.10	14 (31%)
26	PEB	C9	202	2	43,46,46	3.45	10 (23%)	45,67,67	1.99	15 (33%)
26	PEB	R1	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.86	13 (28%)
26	PEB	U1	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.09	16 (35%)
28	CYC	gH	1001	17	42,46,46	3.48	14 (33%)	50,67,67	2.95	21 (42%)
26	PEB	b4	501	2,4	43,46,46	3.47	10 (23%)	45,67,67	2.24	14 (31%)
26	PEB	UF	202	1	43,46,46	3.29	12 (27%)	45,67,67	2.13	16 (35%)
26	PEB	fE	201	2,13	43,46,46	3.43	10 (23%)	45,67,67	3.05	16 (35%)
26	PEB	DB	1002	9,10	43,46,46	3.34	12 (27%)	45,67,67	2.13	15 (33%)
26	PEB	G5	202	2	43,46,46	3.37	9 (20%)	45,67,67	1.94	13 (28%)
26	PEB	IA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.36	17 (37%)
26	PEB	SF	201	1	43,46,46	3.31	12 (27%)	45,67,67	2.37	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	qH	1001	-	42,46,46	3.47	15 (35%)	50,67,67	2.92	21 (42%)
26	PEB	TG	202	2	43,46,46	3.43	12 (27%)	45,67,67	2.22	17 (37%)
26	PEB	TE	201	2	43,46,46	3.32	8 (18%)	45,67,67	2.97	15 (33%)
26	PEB	QA	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.23	15 (33%)
26	PEB	w1	201	3,2	43,46,46	3.58	11 (25%)	45,67,67	2.25	14 (31%)
26	PEB	aB	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.39	14 (31%)
27	PUB	AF	303	7	42,46,46	3.60	8 (19%)	37,67,67	3.20	15 (40%)
26	PEB	U9	201	2,7	43,46,46	3.51	11 (25%)	45,67,67	2.13	17 (37%)
26	PEB	HG	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.37	16 (35%)
26	PEB	iI	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.31	14 (31%)
26	PEB	I3	202	1	43,46,46	3.45	11 (25%)	45,67,67	1.87	13 (28%)
26	PEB	A7	301	7	43,46,46	3.43	12 (27%)	45,67,67	2.80	14 (31%)
26	PEB	YG	202	1	43,46,46	3.41	10 (23%)	45,67,67	1.89	13 (28%)
26	PEB	wE	301	13	43,46,46	3.27	10 (23%)	45,67,67	2.21	15 (33%)
28	CYC	TH	1001	17	42,46,46	3.43	15 (35%)	50,67,67	2.90	19 (38%)
26	PEB	KD	201	1	43,46,46	3.26	11 (25%)	45,67,67	2.48	17 (37%)
27	PUB	xG	301	13	42,46,46	3.25	8 (19%)	37,67,67	3.35	19 (51%)
26	PEB	FE	201	2	43,46,46	3.48	10 (23%)	45,67,67	3.83	16 (35%)
26	PEB	T4	203	1	43,46,46	3.37	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	xE	304	13	43,46,46	3.44	11 (25%)	45,67,67	2.44	17 (37%)
26	PEB	D3	201	2,7	43,46,46	3.33	13 (30%)	45,67,67	2.12	13 (28%)
26	PEB	d6	201	1,7	43,46,46	3.35	8 (18%)	45,67,67	2.16	14 (31%)
26	PEB	kI	203	2	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
28	CYC	LF	1001	10	42,46,46	3.51	16 (38%)	50,67,67	3.08	24 (48%)
26	PEB	cE	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.07	14 (31%)
26	PEB	F3	202	2	43,46,46	3.28	10 (23%)	45,67,67	2.64	15 (33%)
26	PEB	C8	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.35	15 (33%)
26	PEB	w4	201	3,2	43,46,46	3.54	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	PA	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.32	17 (37%)
26	PEB	bG	202	2	43,46,46	3.62	9 (20%)	45,67,67	2.36	15 (33%)
26	PEB	RE	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.29	15 (33%)
26	PEB	aA	203	1	43,46,46	3.22	10 (23%)	45,67,67	2.19	14 (31%)
26	PEB	gG	202	1	43,46,46	3.34	10 (23%)	45,67,67	2.05	15 (33%)
26	PEB	D7	1002	10	43,46,46	3.37	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	UF	201	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.54	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	j4	201	2,4	43,46,46	3.50	10 (23%)	45,67,67	1.88	14 (31%)
26	PEB	ZA	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.57	18 (40%)
26	PEB	P3	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.09	14 (31%)
26	PEB	Y8	203	1	43,46,46	3.21	10 (23%)	45,67,67	2.20	16 (35%)
26	PEB	D1	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.09	15 (33%)
26	PEB	s4	203	2	43,46,46	3.56	10 (23%)	45,67,67	1.96	14 (31%)
28	CYC	RH	1001	17	42,46,46	3.35	14 (33%)	50,67,67	3.04	22 (44%)
26	PEB	P6	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.30	18 (40%)
26	PEB	C3	202	1	43,46,46	3.28	11 (25%)	45,67,67	2.02	12 (26%)
26	PEB	WB	202	1	43,46,46	3.29	9 (20%)	45,67,67	1.98	13 (28%)
26	PEB	jB	202	1	43,46,46	3.42	12 (27%)	45,67,67	1.98	14 (31%)
26	PEB	e2	203	2	43,46,46	3.32	9 (20%)	45,67,67	1.95	12 (26%)
26	PEB	k2	203	2	43,46,46	3.49	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	bF	203	2,1	43,46,46	3.32	12 (27%)	45,67,67	2.58	16 (35%)
26	PEB	qE	202	1	43,46,46	3.50	12 (27%)	45,67,67	3.55	15 (33%)
26	PEB	LC	203	2	43,46,46	3.26	11 (25%)	45,67,67	2.11	15 (33%)
26	PEB	g4	202	1	43,46,46	3.47	11 (25%)	45,67,67	1.93	12 (26%)
26	PEB	LD	203	2	43,46,46	3.47	10 (23%)	45,67,67	1.81	13 (28%)
26	PEB	RI	203	2	43,46,46	3.44	10 (23%)	45,67,67	1.98	11 (24%)
26	PEB	lE	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.65	17 (37%)
26	PEB	UE	201	1	43,46,46	2.80	10 (23%)	45,67,67	2.98	19 (42%)
26	PEB	D4	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.05	14 (31%)
26	PEB	W3	202	1	43,46,46	3.41	12 (27%)	45,67,67	2.08	15 (33%)
26	PEB	C4	201	1	43,46,46	3.44	10 (23%)	45,67,67	1.97	14 (31%)
28	CYC	UH	1001	-	42,46,46	3.37	15 (35%)	50,67,67	3.11	24 (48%)
26	PEB	LJ	203	1	43,46,46	3.37	9 (20%)	45,67,67	2.01	15 (33%)
26	PEB	N9	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.83	12 (26%)
26	PEB	h6	202	1	43,46,46	3.37	11 (25%)	45,67,67	2.00	14 (31%)
26	PEB	d4	201	2	43,46,46	3.52	11 (25%)	45,67,67	1.94	15 (33%)
26	PEB	kB	201	2,7	43,46,46	3.40	12 (27%)	45,67,67	2.25	18 (40%)
26	PEB	WD	201	1	43,46,46	3.16	10 (23%)	45,67,67	2.30	15 (33%)
27	PUB	Q8	201	14,1	42,46,46	3.30	7 (16%)	37,67,67	3.36	18 (48%)
26	PEB	S1	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.07	16 (35%)
26	PEB	ZB	201	2,1	43,46,46	3.15	10 (23%)	45,67,67	2.45	17 (37%)
26	PEB	jA	202	1	43,46,46	3.52	10 (23%)	45,67,67	2.54	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	JE	201	2	43,46,46	3.39	10 (23%)	45,67,67	3.30	17 (37%)
26	PEB	kI	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.37	14 (31%)
26	PEB	TJ	202	1	43,46,46	3.32	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	XG	201	2	43,46,46	3.38	10 (23%)	45,67,67	3.73	17 (37%)
26	PEB	dI	201	1	43,46,46	3.27	10 (23%)	45,67,67	2.20	16 (35%)
26	PEB	F3	201	2,7	43,46,46	3.46	11 (25%)	45,67,67	2.03	15 (33%)
26	PEB	k4	203	2,1	43,46,46	3.27	10 (23%)	45,67,67	2.50	17 (37%)
26	PEB	YI	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	d4	202	2,1	43,46,46	3.27	12 (27%)	45,67,67	2.41	13 (28%)
26	PEB	m1	201	2,1	43,46,46	3.18	11 (25%)	45,67,67	2.70	17 (37%)
26	PEB	O1	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.04	14 (31%)
26	PEB	fF	201	1	43,46,46	3.48	12 (27%)	45,67,67	1.99	14 (31%)
26	PEB	DD	202	2	43,46,46	3.22	11 (25%)	45,67,67	2.50	16 (35%)
28	CYC	vH	1001	17	42,46,46	3.45	15 (35%)	50,67,67	2.89	20 (40%)
26	PEB	YA	203	1	43,46,46	3.23	11 (25%)	45,67,67	2.16	14 (31%)
26	PEB	CC	203	2	43,46,46	3.50	11 (25%)	45,67,67	1.89	14 (31%)
26	PEB	aF	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.09	16 (35%)
26	PEB	ZE	202	2	43,46,46	3.59	10 (23%)	45,67,67	1.93	14 (31%)
26	PEB	H9	201	2,1	43,46,46	3.20	11 (25%)	45,67,67	2.43	16 (35%)
26	PEB	W1	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.29	16 (35%)
26	PEB	N3	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.36	17 (37%)
26	PEB	e1	202	1	43,46,46	3.65	11 (25%)	45,67,67	2.21	15 (33%)
28	CYC	CB	1001	9,10	42,46,46	3.26	15 (35%)	50,67,67	2.74	17 (34%)
26	PEB	l2	202	1	43,46,46	3.38	12 (27%)	45,67,67	1.98	13 (28%)
26	PEB	J4	203	2	43,46,46	3.51	9 (20%)	45,67,67	1.95	13 (28%)
26	PEB	BC	203	2	43,46,46	3.51	12 (27%)	45,67,67	1.94	13 (28%)
26	PEB	sE	202	1	43,46,46	3.48	11 (25%)	45,67,67	2.02	14 (31%)
26	PEB	P1	201	2,1	43,46,46	3.31	12 (27%)	45,67,67	2.27	14 (31%)
26	PEB	E3	201	1	43,46,46	3.49	12 (27%)	45,67,67	2.29	15 (33%)
26	PEB	bF	202	1	43,46,46	3.53	11 (25%)	45,67,67	2.60	17 (37%)
26	PEB	mA	201	2,13	43,46,46	3.43	11 (25%)	45,67,67	2.50	19 (42%)
28	CYC	IH	1001	18,17	42,46,46	3.51	15 (35%)	50,67,67	2.98	23 (46%)
26	PEB	SA	201	1	43,46,46	3.26	10 (23%)	45,67,67	2.17	17 (37%)
26	PEB	jF	201	1	43,46,46	3.16	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	y4	201	2	43,46,46	3.46	11 (25%)	45,67,67	2.13	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	oE	203	2,1	43,46,46	3.37	12 (27%)	45,67,67	2.57	16 (35%)
26	PEB	m6	203	2	43,46,46	3.48	11 (25%)	45,67,67	1.96	15 (33%)
26	PEB	h6	201	2,1	43,46,46	3.61	13 (30%)	45,67,67	2.56	10 (22%)
26	PEB	L4	201	3,2	43,46,46	3.49	12 (27%)	45,67,67	2.05	16 (35%)
26	PEB	PB	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.27	17 (37%)
27	PUB	QA	201	14,1	42,46,46	3.35	8 (19%)	37,67,67	3.56	16 (43%)
26	PEB	Z8	201	2	43,46,46	3.19	10 (23%)	45,67,67	2.50	17 (37%)
26	PEB	HE	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.36	16 (35%)
26	PEB	GG	202	1	43,46,46	2.62	11 (25%)	45,67,67	3.01	20 (44%)
26	PEB	k4	201	1	43,46,46	3.48	11 (25%)	45,67,67	2.05	15 (33%)
26	PEB	G6	1002	9,10	43,46,46	3.23	10 (23%)	45,67,67	2.30	17 (37%)
26	PEB	RF	202	2	43,46,46	3.51	11 (25%)	45,67,67	1.72	10 (22%)
26	PEB	OF	203	2,1	43,46,46	3.25	10 (23%)	45,67,67	2.41	14 (31%)
26	PEB	eG	202	1	43,46,46	3.13	10 (23%)	45,67,67	2.25	20 (44%)
26	PEB	cF	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.32	16 (35%)
28	CYC	B6	1002	8,10	42,46,46	3.22	15 (35%)	50,67,67	2.91	23 (46%)
26	PEB	P7	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.06	15 (33%)
26	PEB	RD	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.24	19 (42%)
26	PEB	SG	201	2,1	43,46,46	3.22	11 (25%)	45,67,67	2.57	15 (33%)
26	PEB	aA	202	1	43,46,46	3.24	10 (23%)	45,67,67	2.04	15 (33%)
27	PUB	YD	302	7	42,46,46	3.53	8 (19%)	37,67,67	3.04	16 (43%)
26	PEB	F1	203	2	43,46,46	3.36	10 (23%)	45,67,67	1.89	14 (31%)
26	PEB	mI	203	2	43,46,46	3.47	13 (30%)	45,67,67	2.18	14 (31%)
26	PEB	N1	203	2,1	43,46,46	3.45	11 (25%)	45,67,67	2.06	13 (28%)
26	PEB	WG	202	1	43,46,46	3.31	11 (25%)	45,67,67	2.28	18 (40%)
26	PEB	YI	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.34	15 (33%)
26	PEB	aE	203	1	43,46,46	3.40	11 (25%)	45,67,67	2.07	15 (33%)
26	PEB	G1	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.11	19 (42%)
27	PUB	AI	303	7	42,46,46	3.40	7 (16%)	37,67,67	3.00	14 (37%)
26	PEB	JJ	203	2,1	43,46,46	3.20	13 (30%)	45,67,67	2.26	13 (28%)
26	PEB	q1	201	2	43,46,46	3.50	11 (25%)	45,67,67	2.27	19 (42%)
26	PEB	X4	202	1	43,46,46	3.37	10 (23%)	45,67,67	2.59	16 (35%)
26	PEB	WA	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.40	18 (40%)
26	PEB	V1	202	1	43,46,46	3.25	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	V9	203	2,1	43,46,46	3.28	13 (30%)	45,67,67	2.38	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	CA	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.22	18 (40%)
26	PEB	bI	202	1	43,46,46	3.43	11 (25%)	45,67,67	1.99	13 (28%)
26	PEB	d2	202	1	43,46,46	3.39	10 (23%)	45,67,67	1.88	12 (26%)
28	CYC	DB	1001	10	42,46,46	3.19	14 (33%)	50,67,67	3.00	21 (42%)
26	PEB	TD	203	2	43,46,46	3.31	10 (23%)	45,67,67	2.26	17 (37%)
26	PEB	GC	202	2	43,46,46	3.40	9 (20%)	45,67,67	1.93	13 (28%)
26	PEB	i1	201	2,1	43,46,46	3.37	13 (30%)	45,67,67	2.28	14 (31%)
28	CYC	II	1001	9	42,46,46	3.20	13 (30%)	50,67,67	2.82	20 (40%)
26	PEB	A9	301	7	43,46,46	3.30	9 (20%)	45,67,67	1.99	16 (35%)
26	PEB	JC	201	1	43,46,46	3.39	11 (25%)	45,67,67	2.78	16 (35%)
26	PEB	G9	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	W9	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.97	16 (35%)
26	PEB	HJ	203	1	43,46,46	3.41	10 (23%)	45,67,67	2.25	14 (31%)
26	PEB	E8	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.27	12 (26%)
26	PEB	AJ	304	7,26	43,46,46	3.51	11 (25%)	45,67,67	2.61	14 (31%)
26	PEB	E4	202	1	43,46,46	3.45	12 (27%)	45,67,67	1.77	12 (26%)
26	PEB	F5	203	2	43,46,46	3.37	11 (25%)	45,67,67	1.87	13 (28%)
26	PEB	eD	401	1,11	43,46,46	3.36	10 (23%)	45,67,67	1.96	13 (28%)
26	PEB	G8	201	1	43,46,46	3.30	11 (25%)	45,67,67	2.37	17 (37%)
26	PEB	VB	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.19	15 (33%)
26	PEB	A1	201	1	43,46,46	3.42	14 (32%)	45,67,67	2.17	17 (37%)
26	PEB	W7	203	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.22	15 (33%)
26	PEB	H8	202	2	43,46,46	3.39	12 (27%)	45,67,67	2.59	17 (37%)
26	PEB	IC	203	2	43,46,46	3.37	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	Z6	202	1	43,46,46	3.35	11 (25%)	45,67,67	2.17	16 (35%)
26	PEB	PI	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.22	17 (37%)
26	PEB	K8	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.26	18 (40%)
26	PEB	Y8	201	2,1	43,46,46	3.07	10 (23%)	45,67,67	2.56	17 (37%)
26	PEB	YF	201	2	43,46,46	3.51	11 (25%)	45,67,67	2.31	18 (40%)
26	PEB	g6	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.50	13 (28%)
28	CYC	uH	1001	18	42,46,46	3.27	13 (30%)	50,67,67	3.25	26 (52%)
26	PEB	mE	203	1	43,46,46	3.48	12 (27%)	45,67,67	1.93	14 (31%)
26	PEB	14	201	2	43,46,46	3.63	11 (25%)	45,67,67	2.02	15 (33%)
26	PEB	a2	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.31	16 (35%)
26	PEB	t1	201	1	43,46,46	3.65	12 (27%)	45,67,67	1.83	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	S7	203	2,1	43,46,46	3.40	11 (25%)	45,67,67	2.39	15 (33%)
26	PEB	t4	201	1	43,46,46	3.68	11 (25%)	45,67,67	1.79	14 (31%)
26	PEB	h2	202	1	43,46,46	3.33	9 (20%)	45,67,67	2.01	16 (35%)
26	PEB	FE	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.48	17 (37%)
26	PEB	vE	202	2	43,46,46	3.52	10 (23%)	45,67,67	2.06	16 (35%)
26	PEB	PD	202	2	43,46,46	3.14	10 (23%)	45,67,67	2.64	16 (35%)
26	PEB	I5	202	2	43,46,46	3.19	10 (23%)	45,67,67	2.34	18 (40%)
26	PEB	E1	201	1	43,46,46	3.43	11 (25%)	45,67,67	1.94	13 (28%)
26	PEB	V9	202	1	43,46,46	3.52	11 (25%)	45,67,67	2.07	12 (26%)
26	PEB	ID	201	1	43,46,46	3.35	12 (27%)	45,67,67	2.19	13 (28%)
26	PEB	A2	304	7	43,46,46	3.32	9 (20%)	45,67,67	2.12	14 (31%)
26	PEB	HD	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.13	14 (31%)
26	PEB	B1	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.33	15 (33%)
26	PEB	Z7	201	2,1	43,46,46	3.42	9 (20%)	45,67,67	3.11	14 (31%)
28	CYC	HB	1001	10	42,46,46	3.15	14 (33%)	50,67,67	3.09	21 (42%)
28	CYC	KI	1001	9	42,46,46	3.25	14 (33%)	50,67,67	2.87	19 (38%)
26	PEB	a6	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.35	15 (33%)
26	PEB	kE	203	2,1	43,46,46	3.42	11 (25%)	45,67,67	2.28	14 (31%)
26	PEB	WF	203	2,1	43,46,46	3.40	12 (27%)	45,67,67	2.33	16 (35%)
26	PEB	A4	202	1	43,46,46	3.49	10 (23%)	45,67,67	1.83	15 (33%)
26	PEB	EA	201	2,1	43,46,46	3.25	11 (25%)	45,67,67	2.29	14 (31%)
26	PEB	Z2	202	1	43,46,46	3.29	10 (23%)	45,67,67	1.93	12 (26%)
26	PEB	Q9	201	2,7	43,46,46	3.47	10 (23%)	45,67,67	2.26	18 (40%)
26	PEB	AG	202	1	43,46,46	3.51	12 (27%)	45,67,67	1.90	12 (26%)
26	PEB	AF	301	7	43,46,46	3.41	8 (18%)	45,67,67	2.12	14 (31%)
28	CYC	EH	1001	17	42,46,46	3.47	14 (33%)	50,67,67	3.00	20 (40%)
26	PEB	F4	201	3,2	43,46,46	3.51	12 (27%)	45,67,67	2.02	16 (35%)
26	PEB	j7	203	2,1	43,46,46	3.49	11 (25%)	45,67,67	2.27	16 (35%)
26	PEB	SD	201	1	43,46,46	3.17	10 (23%)	45,67,67	2.76	16 (35%)
26	PEB	Q7	203	1	43,46,46	3.33	10 (23%)	45,67,67	2.09	14 (31%)
26	PEB	j1	202	2	43,46,46	3.59	10 (23%)	45,67,67	2.68	16 (35%)
26	PEB	fB	202	1	43,46,46	3.44	11 (25%)	45,67,67	1.95	15 (33%)
26	PEB	R2	203	2	43,46,46	3.42	10 (23%)	45,67,67	1.98	12 (26%)
26	PEB	d1	202	2,1	43,46,46	3.38	11 (25%)	45,67,67	2.48	16 (35%)
26	PEB	W4	202	2	43,46,46	3.49	12 (27%)	45,67,67	2.25	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	l6	201	2,1	43,46,46	3.36	12 (27%)	45,67,67	2.24	13 (28%)
26	PEB	d7	203	1	43,46,46	3.38	10 (23%)	45,67,67	2.79	15 (33%)
26	PEB	hG	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.44	17 (37%)
26	PEB	jI	201	1	43,46,46	3.40	11 (25%)	45,67,67	2.31	17 (37%)
27	PUB	yE	302	14	42,46,46	3.33	7 (16%)	37,67,67	3.16	18 (48%)
26	PEB	D9	202	1	43,46,46	3.16	12 (27%)	45,67,67	2.77	19 (42%)
26	PEB	p4	201	1	43,46,46	3.48	9 (20%)	45,67,67	1.94	14 (31%)
26	PEB	KJ	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.15	15 (33%)
26	PEB	qG	202	1	43,46,46	3.38	11 (25%)	45,67,67	3.43	18 (40%)
26	PEB	GD	202	1	43,46,46	3.37	10 (23%)	45,67,67	1.98	15 (33%)
26	PEB	q1	203	2	43,46,46	3.43	9 (20%)	45,67,67	2.11	15 (33%)
26	PEB	P2	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.23	17 (37%)
26	PEB	k6	202	2	43,46,46	3.34	9 (20%)	45,67,67	2.15	16 (35%)
26	PEB	mB	203	2	43,46,46	3.56	12 (27%)	45,67,67	1.99	15 (33%)
26	PEB	XJ	201	2,1	43,46,46	3.44	11 (25%)	45,67,67	2.24	14 (31%)
26	PEB	MG	202	1	43,46,46	3.46	12 (27%)	45,67,67	1.95	15 (33%)
26	PEB	EE	202	1	43,46,46	3.38	11 (25%)	45,67,67	2.00	16 (35%)
26	PEB	eI	203	2	43,46,46	3.31	9 (20%)	45,67,67	1.98	12 (26%)
26	PEB	f7	203	2,1	43,46,46	3.46	11 (25%)	45,67,67	2.36	14 (31%)
26	PEB	IJ	202	2	43,46,46	3.14	11 (25%)	45,67,67	2.53	15 (33%)
26	PEB	RB	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.22	17 (37%)
26	PEB	S6	201	1	43,46,46	3.29	10 (23%)	45,67,67	2.09	17 (37%)
26	PEB	O2	202	1	43,46,46	3.36	10 (23%)	45,67,67	1.86	12 (26%)
26	PEB	11	201	2	43,46,46	3.60	13 (30%)	45,67,67	1.78	12 (26%)
26	PEB	xG	304	13	43,46,46	3.48	11 (25%)	45,67,67	2.27	16 (35%)
26	PEB	l7	202	1	43,46,46	3.39	13 (30%)	45,67,67	2.09	16 (35%)
27	PUB	AA	303	13	42,46,46	3.40	9 (21%)	37,67,67	3.35	17 (45%)
26	PEB	I8	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.37	17 (37%)
26	PEB	W6	202	1	43,46,46	3.33	10 (23%)	45,67,67	2.02	13 (28%)
26	PEB	CD	201	1	43,46,46	3.28	12 (27%)	45,67,67	2.55	17 (37%)
26	PEB	CD	202	1	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
26	PEB	ZA	202	2	43,46,46	3.07	11 (25%)	45,67,67	2.46	15 (33%)
26	PEB	kE	202	1	43,46,46	3.52	12 (27%)	45,67,67	2.27	13 (28%)
26	PEB	WF	202	1	43,46,46	3.36	9 (20%)	45,67,67	2.53	16 (35%)
28	CYC	L6	1001	10	42,46,46	3.24	15 (35%)	50,67,67	3.05	20 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	cG	201	1	43,46,46	3.21	10 (23%)	45,67,67	2.31	15 (33%)
26	PEB	f6	201	1	43,46,46	3.35	10 (23%)	45,67,67	2.12	17 (37%)
28	CYC	tH	1001	17	42,46,46	3.34	14 (33%)	50,67,67	3.03	20 (40%)
26	PEB	I3	201	1	43,46,46	3.45	13 (30%)	45,67,67	2.37	16 (35%)
26	PEB	LC	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.22	16 (35%)
28	CYC	B6	1001	8,10	42,46,46	3.34	14 (33%)	50,67,67	2.82	22 (44%)
26	PEB	YG	201	1	43,46,46	3.26	9 (20%)	45,67,67	2.02	15 (33%)
26	PEB	U8	203	3,1	43,46,46	3.33	10 (23%)	45,67,67	2.07	13 (28%)
26	PEB	SI	201	1	43,46,46	3.42	11 (25%)	45,67,67	2.66	18 (40%)
26	PEB	tG	202	2	43,46,46	3.66	11 (25%)	45,67,67	2.63	16 (35%)
26	PEB	R2	202	2	43,46,46	3.19	11 (25%)	45,67,67	2.49	16 (35%)
26	PEB	A3	201	1	43,46,46	3.41	9 (20%)	45,67,67	2.02	15 (33%)
26	PEB	G8	203	2,1	43,46,46	3.35	12 (27%)	45,67,67	2.19	13 (28%)
26	PEB	BA	301	14	43,46,46	3.43	10 (23%)	45,67,67	2.42	14 (31%)
26	PEB	o1	501	2,4	43,46,46	3.24	10 (23%)	45,67,67	2.24	18 (40%)
26	PEB	d7	202	1	43,46,46	3.40	12 (27%)	45,67,67	2.02	15 (33%)
26	PEB	v1	201	1	43,46,46	3.54	12 (27%)	45,67,67	2.19	16 (35%)
28	CYC	F6	1001	10	42,46,46	3.26	13 (30%)	50,67,67	2.90	18 (36%)
26	PEB	LC	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
26	PEB	T3	203	2	43,46,46	3.20	10 (23%)	45,67,67	2.28	16 (35%)
26	PEB	g2	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.98	14 (31%)
26	PEB	H1	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.49	16 (35%)
26	PEB	PD	203	2	43,46,46	3.39	10 (23%)	45,67,67	2.05	13 (28%)
26	PEB	IG	201	1	43,46,46	2.71	11 (25%)	45,67,67	2.79	15 (33%)
26	PEB	FG	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.52	17 (37%)
26	PEB	N2	1002	10	43,46,46	3.32	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	N9	204	2,1	43,46,46	3.49	9 (20%)	45,67,67	2.23	15 (33%)
26	PEB	dA	201	1	43,46,46	3.28	10 (23%)	45,67,67	2.15	16 (35%)
26	PEB	b2	201	1	43,46,46	3.38	10 (23%)	45,67,67	2.57	18 (40%)
26	PEB	i2	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.03	15 (33%)
26	PEB	FC	203	2	43,46,46	3.43	10 (23%)	45,67,67	1.88	12 (26%)
26	PEB	TB	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.34	21 (46%)
28	CYC	mH	1001	17	42,46,46	3.45	15 (35%)	50,67,67	3.02	22 (44%)
26	PEB	eE	201	2,1	43,46,46	3.46	14 (32%)	45,67,67	2.45	15 (33%)
26	PEB	LA	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.56	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	1A	201	2,1	43,46,46	3.34	9 (20%)	45,67,67	2.62	18 (40%)
26	PEB	D3	202	2	43,46,46	3.24	11 (25%)	45,67,67	2.55	15 (33%)
26	PEB	QG	201	1	43,46,46	3.14	9 (20%)	45,67,67	2.27	14 (31%)
26	PEB	YI	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.15	16 (35%)
28	CYC	CF	1001	9,10	42,46,46	3.26	13 (30%)	50,67,67	2.72	20 (40%)
26	PEB	W6	201	1	43,46,46	3.33	10 (23%)	45,67,67	2.33	18 (40%)
26	PEB	AE	201	1	43,46,46	3.06	9 (20%)	45,67,67	2.40	14 (31%)
26	PEB	dG	202	2	43,46,46	3.70	11 (25%)	45,67,67	1.85	15 (33%)
26	PEB	O4	201	2,4	43,46,46	3.42	10 (23%)	45,67,67	2.38	19 (42%)
26	PEB	J9	202	1	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)
26	PEB	K1	202	1	43,46,46	3.30	12 (27%)	45,67,67	2.36	14 (31%)
26	PEB	nE	202	2	43,46,46	3.82	13 (30%)	45,67,67	2.28	15 (33%)
26	PEB	jA	201	1	43,46,46	3.35	10 (23%)	45,67,67	1.96	13 (28%)
28	CYC	YH	1002	22	42,46,46	3.46	14 (33%)	50,67,67	2.96	21 (42%)
26	PEB	T1	201	2,1	43,46,46	3.46	12 (27%)	45,67,67	2.23	17 (37%)
26	PEB	Q8	204	1	43,46,46	3.23	10 (23%)	45,67,67	2.18	16 (35%)
26	PEB	E1	202	1	43,46,46	3.43	10 (23%)	45,67,67	1.76	12 (26%)
26	PEB	L8	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.60	16 (35%)
26	PEB	s4	201	2	43,46,46	3.46	12 (27%)	45,67,67	2.34	15 (33%)
28	CYC	OH	1001	-	42,46,46	3.45	14 (33%)	50,67,67	2.90	20 (40%)
26	PEB	j4	202	2	43,46,46	3.47	9 (20%)	45,67,67	1.95	14 (31%)
26	PEB	G5	201	2	43,46,46	3.49	11 (25%)	45,67,67	2.05	17 (37%)
26	PEB	UF	203	1	43,46,46	3.32	10 (23%)	45,67,67	2.34	15 (33%)
26	PEB	FA	201	2,12	43,46,46	3.48	9 (20%)	45,67,67	2.43	16 (35%)
26	PEB	b7	202	1	43,46,46	3.46	10 (23%)	45,67,67	2.59	16 (35%)
26	PEB	MA	203	1	43,46,46	3.23	10 (23%)	45,67,67	2.24	15 (33%)
26	PEB	kF	202	2	43,46,46	3.46	11 (25%)	45,67,67	2.05	14 (31%)
26	PEB	T2	203	2	43,46,46	3.40	10 (23%)	45,67,67	1.99	12 (26%)
26	PEB	mE	201	2,1	43,46,46	3.62	12 (27%)	45,67,67	2.51	14 (31%)
26	PEB	G8	202	1	43,46,46	3.35	12 (27%)	45,67,67	2.24	12 (26%)
26	PEB	mG	203	1	43,46,46	3.42	10 (23%)	45,67,67	2.19	14 (31%)
26	PEB	UI	202	1	43,46,46	3.31	10 (23%)	45,67,67	1.90	12 (26%)
26	PEB	F8	201	2,12	43,46,46	3.48	9 (20%)	45,67,67	2.43	16 (35%)
26	PEB	r4	201	1	43,46,46	3.32	12 (27%)	45,67,67	2.12	16 (35%)
26	PEB	iE	203	1	43,46,46	3.54	12 (27%)	45,67,67	1.79	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	PEB	JF	1002	10	43,46,46	3.19	10 (23%)	45,67,67	2.14	14 (31%)
26	PEB	ZF	201	2,1	43,46,46	3.26	9 (20%)	45,67,67	3.16	17 (37%)
26	PEB	Y2	203	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	12 (26%)
26	PEB	O6	203	2,1	43,46,46	3.23	11 (25%)	45,67,67	2.24	16 (35%)
26	PEB	a4	202	2	43,46,46	3.47	12 (27%)	45,67,67	1.98	12 (26%)
26	PEB	hE	202	2	43,46,46	3.53	9 (20%)	45,67,67	1.92	15 (33%)
26	PEB	NA	201	2	43,46,46	3.24	10 (23%)	45,67,67	2.52	17 (37%)
26	PEB	l8	201	2,1	43,46,46	3.28	10 (23%)	45,67,67	2.53	19 (42%)
26	PEB	I9	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	r4	202	1	43,46,46	3.63	12 (27%)	45,67,67	2.49	15 (33%)
26	PEB	N4	203	2,1	43,46,46	3.41	11 (25%)	45,67,67	2.02	13 (28%)
26	PEB	a1	201	2	43,46,46	3.48	11 (25%)	45,67,67	2.32	15 (33%)
26	PEB	WE	203	1	43,46,46	3.47	12 (27%)	45,67,67	1.97	12 (26%)
26	PEB	BG	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.35	14 (31%)
26	PEB	M1	401	3	43,46,46	3.48	10 (23%)	45,67,67	2.12	15 (33%)
26	PEB	sG	202	1	43,46,46	3.45	11 (25%)	45,67,67	2.04	15 (33%)
26	PEB	l1	201	2	43,46,46	3.53	13 (30%)	45,67,67	2.08	13 (28%)
26	PEB	QG	203	2,1	43,46,46	3.44	13 (30%)	45,67,67	3.26	16 (35%)
26	PEB	PE	201	2	43,46,46	3.35	9 (20%)	45,67,67	3.44	18 (40%)
26	PEB	TD	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.32	17 (37%)
26	PEB	OE	201	2,1	43,46,46	3.27	12 (27%)	45,67,67	2.85	19 (42%)
26	PEB	oG	203	1	43,46,46	3.37	12 (27%)	45,67,67	2.28	13 (28%)
28	CYC	1H	1000	22	42,46,46	3.43	13 (30%)	50,67,67	2.95	19 (38%)
26	PEB	CA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.50	15 (33%)
26	PEB	p1	201	1	43,46,46	3.52	12 (27%)	45,67,67	1.84	12 (26%)
27	PUB	wE	304	13	42,46,46	3.56	9 (21%)	37,67,67	3.09	13 (35%)
26	PEB	N8	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.61	18 (40%)
26	PEB	LE	202	2	43,46,46	3.64	11 (25%)	45,67,67	2.68	18 (40%)
26	PEB	R1	201	1	43,46,46	3.38	11 (25%)	45,67,67	2.10	16 (35%)
26	PEB	QA	202	2,1	43,46,46	3.31	11 (25%)	45,67,67	2.25	15 (33%)
26	PEB	kB	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.11	16 (35%)
26	PEB	GB	1002	9,10	43,46,46	3.24	10 (23%)	45,67,67	2.24	16 (35%)
26	PEB	tE	201	2	43,46,46	3.46	10 (23%)	45,67,67	2.48	14 (31%)
26	PEB	K5	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.14	17 (37%)
26	PEB	l2	201	1	43,46,46	3.35	11 (25%)	45,67,67	2.24	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	GB	1001	9,10	42,46,46	3.15	13 (30%)	50,67,67	2.93	18 (36%)
26	PEB	uE	203	1	43,46,46	3.55	12 (27%)	45,67,67	1.99	15 (33%)
26	PEB	T8	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.32	14 (31%)
26	PEB	KE	203	1	43,46,46	3.30	9 (20%)	45,67,67	1.99	16 (35%)
26	PEB	h4	202	2,1	43,46,46	3.29	11 (25%)	45,67,67	2.58	16 (35%)
26	PEB	gG	203	2,1	43,46,46	3.27	10 (23%)	45,67,67	2.57	16 (35%)
26	PEB	s1	203	2	43,46,46	3.58	11 (25%)	45,67,67	1.96	14 (31%)
26	PEB	L3	203	2	43,46,46	3.49	9 (20%)	45,67,67	1.82	14 (31%)
26	PEB	M8	202	1	43,46,46	3.30	9 (20%)	45,67,67	2.33	19 (42%)
26	PEB	M4	403	3	43,46,46	3.35	10 (23%)	45,67,67	2.08	15 (33%)
26	PEB	T1	203	1	43,46,46	3.36	10 (23%)	45,67,67	1.98	13 (28%)
26	PEB	w1	203	2	43,46,46	3.49	11 (25%)	45,67,67	1.99	14 (31%)
26	PEB	P1	202	1	43,46,46	3.36	11 (25%)	45,67,67	2.10	15 (33%)
26	PEB	BD	201	2,26	43,46,46	3.34	11 (25%)	45,67,67	2.17	17 (37%)
26	PEB	i8	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.41	19 (42%)
26	PEB	k1	203	2,1	43,46,46	3.30	11 (25%)	45,67,67	2.42	15 (33%)
26	PEB	VG	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.57	15 (33%)
26	PEB	hA	203	1	43,46,46	3.42	9 (20%)	45,67,67	1.99	13 (28%)
26	PEB	L5	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.32	16 (35%)
26	PEB	R7	202	2	43,46,46	3.51	11 (25%)	45,67,67	2.17	14 (31%)
26	PEB	Z1	201	2	43,46,46	3.49	10 (23%)	45,67,67	2.38	15 (33%)
26	PEB	aA	201	1,13	43,46,46	3.09	10 (23%)	45,67,67	2.40	15 (33%)
26	PEB	KA	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.33	19 (42%)
26	PEB	S7	201	1	43,46,46	3.45	12 (27%)	45,67,67	2.20	15 (33%)
26	PEB	OF	201	1	43,46,46	3.35	13 (30%)	45,67,67	2.33	17 (37%)
27	PUB	NJ	201	1,7	42,46,46	3.65	7 (16%)	37,67,67	3.54	15 (40%)
26	PEB	dF	203	1	43,46,46	3.39	11 (25%)	45,67,67	2.81	15 (33%)
26	PEB	X3	203	2	43,46,46	3.50	11 (25%)	45,67,67	2.39	18 (40%)
26	PEB	O4	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.09	15 (33%)
26	PEB	F7	1002	10	43,46,46	3.30	10 (23%)	45,67,67	2.04	13 (28%)
27	PUB	K1	203	3,1	42,46,46	3.39	7 (16%)	37,67,67	3.23	17 (45%)
26	PEB	a7	202	2	43,46,46	3.41	11 (25%)	45,67,67	2.05	15 (33%)
27	PUB	xE	306	13	42,46,46	3.69	8 (19%)	37,67,67	2.94	14 (37%)
26	PEB	r1	201	1	43,46,46	3.38	12 (27%)	45,67,67	2.22	17 (37%)
26	PEB	AA	301	13	43,46,46	3.18	11 (25%)	45,67,67	2.30	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	CYC	KH	1001	17	42,46,46	3.58	16 (38%)	50,67,67	5.42	21 (42%)
26	PEB	QE	201	1	43,46,46	3.12	8 (18%)	45,67,67	2.31	14 (31%)
26	PEB	P3	202	2	43,46,46	3.05	10 (23%)	45,67,67	2.70	15 (33%)
26	PEB	DJ	203	1	43,46,46	3.22	10 (23%)	45,67,67	2.28	15 (33%)
26	PEB	KE	202	1	43,46,46	2.97	9 (20%)	45,67,67	2.13	15 (33%)
26	PEB	e8	202	2	43,46,46	3.28	10 (23%)	45,67,67	2.63	17 (37%)
26	PEB	Y8	202	1	43,46,46	3.32	10 (23%)	45,67,67	2.32	16 (35%)
26	PEB	F9	201	1	43,46,46	3.26	12 (27%)	45,67,67	2.63	17 (37%)
26	PEB	kA	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.42	16 (35%)
26	PEB	N6	201	9,10	43,46,46	3.37	11 (25%)	45,67,67	2.22	15 (33%)
28	CYC	IH	1001	-	42,46,46	3.40	14 (33%)	50,67,67	2.97	20 (40%)
26	PEB	e2	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.20	14 (31%)
26	PEB	YB	201	2	43,46,46	3.11	11 (25%)	45,67,67	2.67	20 (44%)
26	PEB	nG	201	2	43,46,46	3.47	10 (23%)	45,67,67	3.20	17 (37%)
26	PEB	MA	202	1	43,46,46	3.29	10 (23%)	45,67,67	2.31	17 (37%)
26	PEB	NE	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.00	14 (31%)
26	PEB	uE	202	1	43,46,46	3.54	12 (27%)	45,67,67	1.93	13 (28%)
26	PEB	EA	202	1	43,46,46	3.41	11 (25%)	45,67,67	2.31	14 (31%)
26	PEB	q4	202	2	43,46,46	3.38	12 (27%)	45,67,67	2.49	16 (35%)
26	PEB	QI	202	1	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
26	PEB	AE	202	1	43,46,46	3.42	11 (25%)	45,67,67	1.91	12 (26%)

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
26	PEB	V2	203	2	-	11/24/74/74	0/4/4/4
26	PEB	LJ	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WB	201	1	-	7/24/74/74	0/4/4/4
26	PEB	L3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	K3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	SE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	I4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	W7	201	1	-	6/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	VE	201	2	-	8/24/74/74	0/4/4/4
26	PEB	O3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	e4	201	1	-	10/24/74/74	0/4/4/4
28	CYC	N2	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	KG	203	1	-	8/24/74/74	0/4/4/4
26	PEB	g2	203	2	-	10/24/74/74	0/4/4/4
26	PEB	l6	202	1	-	14/24/74/74	0/4/4/4
26	PEB	NI	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	d8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	24	405	3	-	10/24/74/74	0/4/4/4
26	PEB	c4	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	b2	202	1	-	9/24/74/74	0/4/4/4
26	PEB	mB	201	2	-	10/24/74/74	0/4/4/4
26	PEB	OA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	21	405	3	-	11/24/74/74	0/4/4/4
28	CYC	YH	1001	22	-	9/25/74/74	0/4/4/4
26	PEB	e6	201	2	-	9/24/74/74	0/4/4/4
28	CYC	dH	1001	-	-	11/25/74/74	0/4/4/4
26	PEB	iG	203	1	-	12/24/74/74	0/4/4/4
26	PEB	iA	201	2,13	-	8/24/74/74	0/4/4/4
26	PEB	sG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	EE	201	1	-	7/24/74/74	0/4/4/4
26	PEB	DG	203	2	-	12/24/74/74	0/4/4/4
26	PEB	kG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	WG	203	1	-	13/24/74/74	0/4/4/4
26	PEB	SB	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	w4	204	2,1	-	8/24/74/74	0/4/4/4
26	PEB	QJ	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	D1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	J4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y4	202	2	-	4/24/74/74	0/4/4/4
26	PEB	Z6	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	TJ	203	1	-	11/24/74/74	0/4/4/4
26	PEB	m6	201	2	-	6/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	q4	201	2	-	6/24/74/74	0/4/4/4
26	PEB	UA	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	pG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	j2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	f6	202	1	-	8/24/74/74	0/4/4/4
26	PEB	IA	203	1	-	11/24/74/74	0/4/4/4
26	PEB	oE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	II	201	1	-	8/24/74/74	0/4/4/4
27	PUB	24	402	3	-	5/24/74/74	0/4/4/4
27	PUB	yG	303	14	-	5/24/74/74	0/4/4/4
26	PEB	SE	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	U4	201	2,4	-	7/24/74/74	0/4/4/4
26	PEB	S6	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	pG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	E8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	OF	202	1	-	7/24/74/74	0/4/4/4
26	PEB	R6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	RI	201	2,6	-	2/24/74/74	0/4/4/4
26	PEB	Z7	202	1	-	9/24/74/74	0/4/4/4
26	PEB	SA	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	CE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	g2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	RD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	jE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	U6	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	pE	201	2	-	12/24/74/74	0/4/4/4
26	PEB	U3	201	1	-	6/24/74/74	0/4/4/4
26	PEB	N1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	D8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	lG	201	2	-	11/24/74/74	0/4/4/4
27	PUB	A7	304	7	-	13/24/74/74	0/4/4/4
26	PEB	u4	201	3,2	-	12/24/74/74	0/4/4/4
28	CYC	JH	1001	18,17	-	6/25/74/74	0/4/4/4
26	PEB	f8	201	1	-	9/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	FC	201	2	-	6/24/74/74	0/4/4/4
26	PEB	CG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	NG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	T3	202	2	-	9/24/74/74	0/4/4/4
26	PEB	hG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	hB	202	1	-	10/24/74/74	0/4/4/4
26	PEB	M9	201	2	-	7/24/74/74	0/4/4/4
26	PEB	IE	203	2,1	-	5/24/74/74	0/4/4/4
26	PEB	M4	402	3,26	-	12/24/74/74	0/4/4/4
26	PEB	i6	201	2	-	10/24/74/74	0/4/4/4
26	PEB	JI	1002	10	-	12/24/74/74	0/4/4/4
26	PEB	L9	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	KB	201	9,10	-	6/24/74/74	0/4/4/4
26	PEB	P2	202	2	-	8/24/74/74	0/4/4/4
26	PEB	W8	202	1	-	13/24/74/74	0/4/4/4
26	PEB	LB	1002	9,10	-	11/24/74/74	0/4/4/4
26	PEB	JE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	c2	202	2	-	11/24/74/74	0/4/4/4
26	PEB	aG	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	VF	201	2	-	2/24/74/74	0/4/4/4
26	PEB	EJ	201	2,15	-	12/24/74/74	0/4/4/4
26	PEB	tE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	m4	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	d6	204	1	-	13/24/74/74	0/4/4/4
26	PEB	S4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	fG	201	2,13	-	11/24/74/74	0/4/4/4
28	CYC	qH	1002	-	-	16/25/74/74	0/4/4/4
26	PEB	A8	302	13	-	10/24/74/74	0/4/4/4
26	PEB	x4	202	1	-	15/24/74/74	0/4/4/4
28	CYC	D7	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	IC	202	2	-	3/24/74/74	0/4/4/4
26	PEB	c1	203	2,1	-	9/24/74/74	0/4/4/4
28	CYC	J7	1003	9,10	-	6/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	BC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	ZE	201	2	-	9/24/74/74	0/4/4/4
28	CYC	FH	1001	18	-	6/25/74/74	0/4/4/4
26	PEB	X9	202	1	-	11/24/74/74	0/4/4/4
26	PEB	H9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	Z4	201	2	-	5/24/74/74	0/4/4/4
26	PEB	KC	202	2	-	6/24/74/74	0/4/4/4
26	PEB	VD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	S6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	y1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	ZG	202	2	-	10/24/74/74	0/4/4/4
27	PUB	xG	305	13	-	8/24/74/74	0/4/4/4
26	PEB	SA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	S7	202	1	-	8/24/74/74	0/4/4/4
26	PEB	fA	203	2,1	-	5/24/74/74	0/4/4/4
26	PEB	Y7	202	2	-	8/24/74/74	0/4/4/4
26	PEB	CG	202	1	-	6/24/74/74	0/4/4/4
26	PEB	N4	201	1	-	6/24/74/74	0/4/4/4
26	PEB	HC	201	2	-	8/24/74/74	0/4/4/4
26	PEB	n4	201	2,4	-	12/24/74/74	0/4/4/4
26	PEB	Y6	201	2	-	10/24/74/74	0/4/4/4
26	PEB	c8	201	2	-	10/24/74/74	0/4/4/4
26	PEB	N9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	X4	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	oG	201	1	-	13/24/74/74	0/4/4/4
26	PEB	L1	201	3,2	-	12/24/74/74	0/4/4/4
26	PEB	C8	201	1	-	4/24/74/74	0/4/4/4
26	PEB	a2	203	2	-	10/24/74/74	0/4/4/4
26	PEB	PJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	v1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	f2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	kG	201	1	-	12/24/74/74	0/4/4/4
26	PEB	aI	202	2	-	7/24/74/74	0/4/4/4
26	PEB	I8	201	2,1	-	9/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	l4	201	2	-	9/24/74/74	0/4/4/4
26	PEB	i4	201	1	-	7/24/74/74	0/4/4/4
26	PEB	YJ	201	2,26	-	5/24/74/74	0/4/4/4
26	PEB	TI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	gG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	k2	202	2	-	16/24/74/74	0/4/4/4
28	CYC	J2	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	Z2	201	1	-	7/24/74/74	0/4/4/4
26	PEB	vG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	J1	203	2	-	10/24/74/74	0/4/4/4
26	PEB	OB	201	1	-	9/24/74/74	0/4/4/4
26	PEB	JD	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	K5	203	2	-	9/24/74/74	0/4/4/4
26	PEB	NJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	OI	202	1	-	6/24/74/74	0/4/4/4
26	PEB	LI	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	M3	202	1	-	13/24/74/74	0/4/4/4
27	PUB	B8	302	14	-	4/24/74/74	0/4/4/4
26	PEB	V7	202	2	-	9/24/74/74	0/4/4/4
28	CYC	NI	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	gE	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	S8	201	1	-	10/24/74/74	0/4/4/4
26	PEB	rG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	g4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	UJ	202	2	-	9/24/74/74	0/4/4/4
26	PEB	HB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	TG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	WI	201	1	-	7/24/74/74	0/4/4/4
26	PEB	FF	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	mG	201	1	-	10/24/74/74	0/4/4/4
26	PEB	mB	202	2	-	6/24/74/74	0/4/4/4
26	PEB	a8	204	2,1	-	7/24/74/74	0/4/4/4
26	PEB	aA	204	2,1	-	6/24/74/74	0/4/4/4
28	CYC	CH	1001	18,17	-	8/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	WJ	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	UI	201	1	-	9/24/74/74	0/4/4/4
26	PEB	L5	202	2	-	10/24/74/74	0/4/4/4
26	PEB	eI	202	2	-	10/24/74/74	0/4/4/4
26	PEB	mE	202	1	-	12/24/74/74	0/4/4/4
26	PEB	J3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	A2	305	7	-	11/24/74/74	0/4/4/4
26	PEB	FD	203	2	-	11/24/74/74	0/4/4/4
27	PUB	A2	302	7	-	3/24/74/74	0/4/4/4
26	PEB	CJ	202	2	-	8/24/74/74	0/4/4/4
28	CYC	wH	1001	-	-	7/25/74/74	0/4/4/4
26	PEB	DJ	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	dF	202	1	-	10/24/74/74	0/4/4/4
26	PEB	mI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	zG	501	2,16	-	6/24/74/74	0/4/4/4
26	PEB	MG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	B5	202	2	-	9/24/74/74	0/4/4/4
26	PEB	I1	201	1	-	6/24/74/74	0/4/4/4
28	CYC	I2	1001	9	-	9/25/74/74	0/4/4/4
26	PEB	aI	201	2	-	2/24/74/74	0/4/4/4
26	PEB	D1	201	3,2	-	11/24/74/74	0/4/4/4
28	CYC	kH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	lB	202	1	-	14/24/74/74	0/4/4/4
26	PEB	J7	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	Z4	202	2	-	13/24/74/74	0/4/4/4
26	PEB	C1	202	1	-	15/24/74/74	0/4/4/4
28	CYC	J7	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	p1	202	1	-	17/24/74/74	0/4/4/4
26	PEB	U8	202	1	-	7/24/74/74	0/4/4/4
26	PEB	VF	203	2	-	9/24/74/74	0/4/4/4
26	PEB	H6	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	nG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N8	202	2	-	8/24/74/74	0/4/4/4
26	PEB	aF	201	2	-	7/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	j2	201	1	-	10/24/74/74	0/4/4/4
26	PEB	VI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	K5	202	2	-	6/24/74/74	0/4/4/4
26	PEB	FJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	NJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	PG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	mF	201	2	-	8/24/74/74	0/4/4/4
28	CYC	hH	1001	22,18	-	4/25/74/74	0/4/4/4
26	PEB	C3	201	1	-	11/24/74/74	0/4/4/4
26	PEB	jB	201	1	-	10/24/74/74	0/4/4/4
26	PEB	P8	201	2	-	10/24/74/74	0/4/4/4
26	PEB	Q8	203	1	-	4/24/74/74	0/4/4/4
26	PEB	J2	1002	10	-	11/24/74/74	0/4/4/4
27	PUB	yG	302	14	-	3/24/74/74	0/4/4/4
26	PEB	EG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	JA	201	2	-	9/24/74/74	0/4/4/4
28	CYC	JI	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	c4	202	1	-	11/24/74/74	0/4/4/4
28	CYC	E7	1001	9,10	-	5/25/74/74	0/4/4/4
26	PEB	Y9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	VE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	S8	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	24	401	3	-	15/24/74/74	0/4/4/4
26	PEB	P8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y1	202	2	-	4/24/74/74	0/4/4/4
26	PEB	Z1	202	2	-	12/24/74/74	0/4/4/4
26	PEB	rE	202	2	-	10/24/74/74	0/4/4/4
26	PEB	HA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	J5	202	1	-	7/24/74/74	0/4/4/4
26	PEB	K4	202	1	-	14/24/74/74	0/4/4/4
26	PEB	V4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	OA	203	2,1	-	6/24/74/74	0/4/4/4
28	CYC	FI	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	SB	201	1	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	A9	304	7,26	-	9/24/74/74	0/4/4/4
26	PEB	nE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	H4	201	3,2	-	9/24/74/74	0/4/4/4
26	PEB	d2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	gA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RG	202	2	-	13/24/74/74	0/4/4/4
27	PUB	24	403	3,1	-	9/24/74/74	0/4/4/4
26	PEB	RJ	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	ME	201	1	-	6/24/74/74	0/4/4/4
26	PEB	A6	304	7	-	4/24/74/74	0/4/4/4
28	CYC	F2	1001	10	-	9/25/74/74	0/4/4/4
26	PEB	L1	203	2	-	15/24/74/74	0/4/4/4
26	PEB	CA	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	S9	202	2	-	9/24/74/74	0/4/4/4
26	PEB	ME	202	1	-	10/24/74/74	0/4/4/4
26	PEB	X9	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	i2	203	2	-	14/24/74/74	0/4/4/4
26	PEB	CC	201	2	-	10/24/74/74	0/4/4/4
26	PEB	DD	201	2,7	-	11/24/74/74	0/4/4/4
26	PEB	eF	202	2	-	11/24/74/74	0/4/4/4
26	PEB	mG	202	1	-	6/24/74/74	0/4/4/4
26	PEB	OG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	E8	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	u1	203	2	-	5/24/74/74	0/4/4/4
26	PEB	bE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	cG	202	1	-	13/24/74/74	0/4/4/4
26	PEB	B4	202	2	-	7/24/74/74	0/4/4/4
26	PEB	NJ	204	2,1	-	12/24/74/74	0/4/4/4
26	PEB	uG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	e1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	SI	202	1	-	10/24/74/74	0/4/4/4
26	PEB	gB	201	2	-	7/24/74/74	0/4/4/4
26	PEB	VJ	203	2,1	-	14/24/74/74	0/4/4/4
28	CYC	fH	1001	18	-	5/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	RD	201	2	-	5/24/74/74	0/4/4/4
26	PEB	M1	403	3	-	7/24/74/74	0/4/4/4
28	CYC	M2	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	X8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	S3	202	1	-	8/24/74/74	0/4/4/4
26	PEB	K9	202	2	-	13/24/74/74	0/4/4/4
26	PEB	c8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	IG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	oG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	CG	201	1	-	6/24/74/74	0/4/4/4
26	PEB	YF	202	2	-	8/24/74/74	0/4/4/4
26	PEB	TF	201	2,6	-	9/24/74/74	0/4/4/4
26	PEB	BJ	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	sG	201	1	-	12/24/74/74	0/4/4/4
26	PEB	OA	202	1	-	7/24/74/74	0/4/4/4
26	PEB	YG	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	i4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	e4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	c2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	VF	202	2,1	-	7/24/74/74	0/4/4/4
26	PEB	v4	202	1	-	13/24/74/74	0/4/4/4
26	PEB	qG	203	1	-	10/24/74/74	0/4/4/4
26	PEB	hI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	lF	202	1	-	10/24/74/74	0/4/4/4
26	PEB	Q6	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	WG	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	e7	202	2	-	10/24/74/74	0/4/4/4
26	PEB	s1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	T2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	XA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	aI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	hF	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	W2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	R4	201	1	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	GC	201	2	-	11/24/74/74	0/4/4/4
26	PEB	w1	202	2	-	13/24/74/74	0/4/4/4
26	PEB	u1	202	2	-	7/24/74/74	0/4/4/4
26	PEB	uG	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	P9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	c1	202	1	-	9/24/74/74	0/4/4/4
26	PEB	k1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	hA	202	1	-	6/24/74/74	0/4/4/4
26	PEB	q4	203	2	-	6/24/74/74	0/4/4/4
26	PEB	O9	201	2,7,26	-	8/24/74/74	0/4/4/4
26	PEB	fl	201	1	-	11/24/74/74	0/4/4/4
28	CYC	HF	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	lE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	AB	301	7	-	10/24/74/74	0/4/4/4
26	PEB	fE	202	2	-	11/24/74/74	0/4/4/4
27	PUB	A8	304	13	-	10/24/74/74	0/4/4/4
26	PEB	R9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	VB	201	2	-	9/24/74/74	0/4/4/4
26	PEB	C5	202	2	-	8/24/74/74	0/4/4/4
28	CYC	N7	1001	8,10	-	7/25/74/74	0/4/4/4
26	PEB	j6	201	1	-	9/24/74/74	0/4/4/4
26	PEB	TE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	DJ	202	1	-	13/24/74/74	0/4/4/4
26	PEB	z4	201	1	-	11/24/74/74	0/4/4/4
26	PEB	GA	202	1	-	5/24/74/74	0/4/4/4
26	PEB	lI	202	1	-	10/24/74/74	0/4/4/4
28	CYC	EF	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	U9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	XE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	f1	202	2	-	5/24/74/74	0/4/4/4
26	PEB	PJ	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	lF	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	KE	201	2,1	-	6/24/74/74	0/4/4/4
27	PUB	AB	302	7	-	7/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	SH	1001	18	-	7/25/74/74	0/4/4/4
26	PEB	l1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	g7	201	2	-	7/24/74/74	0/4/4/4
26	PEB	H3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	XA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	XD	202	2	-	9/24/74/74	0/4/4/4
26	PEB	I5	201	2	-	4/24/74/74	0/4/4/4
26	PEB	F3	203	2	-	11/24/74/74	0/4/4/4
26	PEB	j8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	P7	201	2,6	-	6/24/74/74	0/4/4/4
26	PEB	D3	203	2	-	11/24/74/74	0/4/4/4
26	PEB	d6	203	1	-	8/24/74/74	0/4/4/4
26	PEB	J1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	m1	203	1	-	9/24/74/74	0/4/4/4
26	PEB	I4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	O7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	gF	202	2	-	6/24/74/74	0/4/4/4
26	PEB	R9	201	1	-	12/24/74/74	0/4/4/4
26	PEB	eF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	YD	301	7	-	16/24/74/74	0/4/4/4
26	PEB	OG	201	2,1	-	6/24/74/74	0/4/4/4
26	PEB	X9	203	1	-	10/24/74/74	0/4/4/4
26	PEB	J1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	rG	201	2,13	-	11/24/74/74	0/4/4/4
26	PEB	B4	201	3,2,26	-	12/24/74/74	0/4/4/4
26	PEB	F5	201	2	-	6/24/74/74	0/4/4/4
28	CYC	BB	1001	8,10	-	12/25/74/74	0/4/4/4
26	PEB	WB	203	2,1	-	7/24/74/74	0/4/4/4
28	CYC	MH	1001	18	-	10/25/74/74	0/4/4/4
27	PUB	A7	303	7	-	5/24/74/74	0/4/4/4
26	PEB	GA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	iG	202	1	-	13/24/74/74	0/4/4/4
28	CYC	EI	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	qE	203	1	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	XE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	GJ	201	2	-	5/24/74/74	0/4/4/4
26	PEB	K8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	B3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	N7	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	PB	201	2,6	-	6/24/74/74	0/4/4/4
28	CYC	eH	1001	18,17	-	8/25/74/74	0/4/4/4
26	PEB	ZI	201	1	-	7/24/74/74	0/4/4/4
26	PEB	D9	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	S2	202	1	-	10/24/74/74	0/4/4/4
27	PUB	A4	203	3,1	-	7/24/74/74	0/4/4/4
26	PEB	YD	303	7,26	-	13/24/74/74	0/4/4/4
26	PEB	YE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	UE	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	GD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	RA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Y6	202	2	-	12/24/74/74	0/4/4/4
27	PUB	wG	304	13	-	7/24/74/74	0/4/4/4
26	PEB	V2	201	2	-	4/24/74/74	0/4/4/4
26	PEB	J9	201	1	-	14/24/74/74	0/4/4/4
26	PEB	YD	304	7,26	-	13/24/74/74	0/4/4/4
26	PEB	iF	202	2	-	9/24/74/74	0/4/4/4
26	PEB	G3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	S9	201	2,7	-	6/24/74/74	0/4/4/4
26	PEB	QE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	P2	203	2	-	7/24/74/74	0/4/4/4
26	PEB	d4	203	2	-	9/24/74/74	0/4/4/4
28	CYC	YH	1004	22	-	8/25/74/74	0/4/4/4
26	PEB	F2	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	k8	202	2	-	12/24/74/74	0/4/4/4
26	PEB	XJ	203	1	-	13/24/74/74	0/4/4/4
26	PEB	eB	203	2	-	13/24/74/74	0/4/4/4
26	PEB	VI	201	2	-	4/24/74/74	0/4/4/4
26	PEB	GE	202	1	-	7/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	m1	202	1	-	9/24/74/74	0/4/4/4
26	PEB	UA	202	1	-	7/24/74/74	0/4/4/4
28	CYC	H2	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	NA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	V3	201	2,11	-	11/24/74/74	0/4/4/4
26	PEB	DA	201	14,2	-	10/24/74/74	0/4/4/4
26	PEB	b7	201	1	-	12/24/74/74	0/4/4/4
26	PEB	Q1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	T9	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	O8	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	n1	201	2	-	9/24/74/74	0/4/4/4
26	PEB	U7	202	1	-	6/24/74/74	0/4/4/4
27	PUB	A8	303	13	-	7/24/74/74	0/4/4/4
26	PEB	cG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	h4	203	2	-	7/24/74/74	0/4/4/4
26	PEB	Z8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	O3	202	1	-	10/24/74/74	0/4/4/4
26	PEB	TI	202	2	-	5/24/74/74	0/4/4/4
28	CYC	PH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	B9	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	ED	201	1	-	7/24/74/74	0/4/4/4
26	PEB	fB	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	mI	201	2	-	9/24/74/74	0/4/4/4
26	PEB	T3	201	2	-	5/24/74/74	0/4/4/4
26	PEB	AI	305	7	-	10/24/74/74	0/4/4/4
28	CYC	JF	1001	10	-	4/25/74/74	0/4/4/4
26	PEB	hE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	A7	302	7	-	10/24/74/74	0/4/4/4
26	PEB	T6	201	2	-	3/24/74/74	0/4/4/4
26	PEB	h1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	H1	201	3,2	-	9/24/74/74	0/4/4/4
26	PEB	Q4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	m2	202	2	-	9/24/74/74	0/4/4/4
26	PEB	P1	203	1	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	f8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	FG	201	2	-	5/24/74/74	0/4/4/4
26	PEB	UE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	KA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	B1	201	3,2,26	-	10/24/74/74	0/4/4/4
26	PEB	RJ	201	1	-	11/24/74/74	0/4/4/4
26	PEB	xG	303	13	-	12/24/74/74	0/4/4/4
26	PEB	L4	203	2	-	13/24/74/74	0/4/4/4
26	PEB	hF	202	1	-	11/24/74/74	0/4/4/4
26	PEB	C9	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	WJ	202	2	-	7/24/74/74	0/4/4/4
28	CYC	cH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	U1	201	2,4	-	7/24/74/74	0/4/4/4
26	PEB	AC	201	2	-	9/24/74/74	0/4/4/4
26	PEB	AF	305	7	-	12/24/74/74	0/4/4/4
26	PEB	b1	501	2,4	-	7/24/74/74	0/4/4/4
26	PEB	yE	301	14	-	8/24/74/74	0/4/4/4
28	CYC	NB	1001	8,10	-	6/25/74/74	0/4/4/4
26	PEB	ZB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	BE	202	2	-	13/24/74/74	0/4/4/4
26	PEB	ND	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I8	203	1	-	12/24/74/74	0/4/4/4
26	PEB	xE	303	13	-	11/24/74/74	0/4/4/4
26	PEB	bI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	fF	202	1	-	9/24/74/74	0/4/4/4
26	PEB	NB	1002	9,10	-	10/24/74/74	0/4/4/4
26	PEB	aB	201	2	-	7/24/74/74	0/4/4/4
28	CYC	rH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	l7	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	e6	202	2	-	6/24/74/74	0/4/4/4
26	PEB	WA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	J8	201	2	-	9/24/74/74	0/4/4/4
26	PEB	OI	201	1	-	9/24/74/74	0/4/4/4
26	PEB	iI	201	2	-	6/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	LF	1002	10	-	7/24/74/74	0/4/4/4
26	PEB	j6	202	1	-	6/24/74/74	0/4/4/4
26	PEB	UD	202	1	-	11/24/74/74	0/4/4/4
26	PEB	dB	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	MD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	wG	303	13	-	7/24/74/74	0/4/4/4
26	PEB	xG	302	13	-	12/24/74/74	0/4/4/4
26	PEB	ZG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	EA	203	1	-	10/24/74/74	0/4/4/4
26	PEB	i8	201	2,13	-	5/24/74/74	0/4/4/4
26	PEB	cA	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Z6	203	1	-	9/24/74/74	0/4/4/4
28	CYC	K2	1001	9	-	7/25/74/74	0/4/4/4
27	PUB	AB	303	7	-	9/24/74/74	0/4/4/4
26	PEB	a2	202	2	-	8/24/74/74	0/4/4/4
26	PEB	BJ	201	1	-	11/24/74/74	0/4/4/4
26	PEB	NG	202	2	-	10/24/74/74	0/4/4/4
26	PEB	L5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	J3	203	2	-	14/24/74/74	0/4/4/4
26	PEB	l6	203	1	-	7/24/74/74	0/4/4/4
26	PEB	mA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	G4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	mF	202	2	-	10/24/74/74	0/4/4/4
26	PEB	GJ	202	2	-	12/24/74/74	0/4/4/4
26	PEB	B5	203	2	-	11/24/74/74	0/4/4/4
26	PEB	RF	201	2	-	7/24/74/74	0/4/4/4
26	PEB	E9	201	2,15	-	12/24/74/74	0/4/4/4
26	PEB	SB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	m7	202	2	-	9/24/74/74	0/4/4/4
26	PEB	m8	201	2,13	-	9/24/74/74	0/4/4/4
27	PUB	AJ	302	1,7	-	7/24/74/74	0/4/4/4
26	PEB	e2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	gE	202	1	-	11/24/74/74	0/4/4/4
28	CYC	C6	1001	9,10	-	8/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	B1	203	2	-	10/24/74/74	0/4/4/4
26	PEB	D4	201	3,2	-	10/24/74/74	0/4/4/4
26	PEB	X1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	AJ	303	7,26	-	10/24/74/74	0/4/4/4
28	CYC	yH	1001	-	-	9/25/74/74	0/4/4/4
26	PEB	O7	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	AC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	VD	201	2,11	-	11/24/74/74	0/4/4/4
26	PEB	V7	201	2	-	5/24/74/74	0/4/4/4
28	CYC	M6	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	W3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	FD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Q2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	cB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	P9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	HD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	f6	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	LD	202	2	-	9/24/74/74	0/4/4/4
26	PEB	bE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RI	202	2	-	10/24/74/74	0/4/4/4
26	PEB	Q9	202	2	-	12/24/74/74	0/4/4/4
26	PEB	D4	202	2	-	8/24/74/74	0/4/4/4
28	CYC	C7	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	tG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	F4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	R2	201	2,6	-	2/24/74/74	0/4/4/4
28	CYC	IB	1001	9,10	-	8/25/74/74	0/4/4/4
28	CYC	KB	202	9,10	-	9/25/74/74	0/4/4/4
26	PEB	SJ	202	2	-	8/24/74/74	0/4/4/4
26	PEB	H5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	d7	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	z4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	kI	201	2	-	8/24/74/74	0/4/4/4
28	CYC	DI	1001	10	-	9/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	h8	202	1	-	6/24/74/74	0/4/4/4
26	PEB	h7	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	a7	201	2	-	6/24/74/74	0/4/4/4
26	PEB	IG	203	2,1	-	4/24/74/74	0/4/4/4
26	PEB	gB	202	2	-	11/24/74/74	0/4/4/4
26	PEB	HI	1002	10	-	7/24/74/74	0/4/4/4
26	PEB	g7	202	2	-	4/24/74/74	0/4/4/4
26	PEB	f4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	qG	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	hB	203	1	-	9/24/74/74	0/4/4/4
26	PEB	V4	203	2,1	-	11/24/74/74	0/4/4/4
28	CYC	iH	1001	18,17	-	8/25/74/74	0/4/4/4
26	PEB	OE	203	1	-	12/24/74/74	0/4/4/4
28	CYC	JF	1003	9,10	-	9/25/74/74	0/4/4/4
26	PEB	XD	201	2,11	-	5/24/74/74	0/4/4/4
26	PEB	MG	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	T6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	k6	201	2,7	-	8/24/74/74	0/4/4/4
26	PEB	eE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	K1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	e7	201	2	-	6/24/74/74	0/4/4/4
26	PEB	lA	203	1	-	9/24/74/74	0/4/4/4
26	PEB	W8	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	QE	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	c2	203	2	-	13/24/74/74	0/4/4/4
26	PEB	O8	201	1	-	7/24/74/74	0/4/4/4
28	CYC	pH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	j8	202	1	-	11/24/74/74	0/4/4/4
26	PEB	NF	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	H2	1002	10	-	7/24/74/74	0/4/4/4
28	CYC	H7	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	c7	202	2	-	9/24/74/74	0/4/4/4
26	PEB	CE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	Q8	202	2,1	-	6/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	wE	303	13	-	8/24/74/74	0/4/4/4
26	PEB	E3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	bF	201	1	-	10/24/74/74	0/4/4/4
26	PEB	11	203	2	-	7/24/74/74	0/4/4/4
26	PEB	iB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	P9	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	T7	202	2	-	12/24/74/74	0/4/4/4
26	PEB	DE	203	2	-	12/24/74/74	0/4/4/4
26	PEB	i7	201	2	-	4/24/74/74	0/4/4/4
26	PEB	OB	202	1	-	10/24/74/74	0/4/4/4
26	PEB	N3	203	2	-	8/24/74/74	0/4/4/4
26	PEB	Y9	201	2,26	-	7/24/74/74	0/4/4/4
26	PEB	LJ	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	O9	202	2	-	14/24/74/74	0/4/4/4
26	PEB	AJ	305	2,7,26	-	8/24/74/74	0/4/4/4
26	PEB	f7	202	1	-	10/24/74/74	0/4/4/4
26	PEB	N1	201	1	-	6/24/74/74	0/4/4/4
26	PEB	sE	201	1	-	14/24/74/74	0/4/4/4
26	PEB	TI	203	2	-	11/24/74/74	0/4/4/4
26	PEB	Y3	301	7	-	14/24/74/74	0/4/4/4
26	PEB	M9	202	2	-	10/24/74/74	0/4/4/4
26	PEB	wG	301	13	-	11/24/74/74	0/4/4/4
26	PEB	OJ	201	2	-	14/24/74/74	0/4/4/4
26	PEB	u4	203	2	-	2/24/74/74	0/4/4/4
26	PEB	fl	202	1	-	10/24/74/74	0/4/4/4
26	PEB	HE	201	2	-	11/24/74/74	0/4/4/4
26	PEB	YE	201	1	-	10/24/74/74	0/4/4/4
26	PEB	ZF	203	1	-	7/24/74/74	0/4/4/4
26	PEB	YA	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	JJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	cE	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	AG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	G3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	FI	1002	10	-	9/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	S4	201	2,4	-	10/24/74/74	0/4/4/4
26	PEB	eE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	j8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	lF	203	1	-	13/24/74/74	0/4/4/4
26	PEB	W9	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	UB	203	1	-	12/24/74/74	0/4/4/4
26	PEB	21	401	3	-	15/24/74/74	0/4/4/4
26	PEB	c7	201	2	-	7/24/74/74	0/4/4/4
26	PEB	E4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	j1	201	2,4	-	12/24/74/74	0/4/4/4
26	PEB	M8	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	P3	201	2,11	-	9/24/74/74	0/4/4/4
26	PEB	VJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	J4	201	2	-	11/24/74/74	0/4/4/4
26	PEB	A7	305	7	-	12/24/74/74	0/4/4/4
26	PEB	SF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	W1	201	2	-	8/24/74/74	0/4/4/4
26	PEB	T4	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	Y3	304	7,26	-	13/24/74/74	0/4/4/4
26	PEB	n4	202	2	-	7/24/74/74	0/4/4/4
28	CYC	VH	1001	-	-	11/25/74/74	0/4/4/4
26	PEB	H8	201	2	-	6/24/74/74	0/4/4/4
26	PEB	KC	201	2	-	5/24/74/74	0/4/4/4
26	PEB	d1	201	2	-	8/24/74/74	0/4/4/4
26	PEB	gI	203	2	-	10/24/74/74	0/4/4/4
26	PEB	oE	201	1	-	9/24/74/74	0/4/4/4
28	CYC	E2	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	HG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	N3	202	2	-	8/24/74/74	0/4/4/4
26	PEB	b7	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	i1	203	1	-	10/24/74/74	0/4/4/4
26	PEB	MA	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	k7	201	2	-	10/24/74/74	0/4/4/4
28	CYC	G7	1001	9,10	-	10/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	BJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	TA	201	2	-	7/24/74/74	0/4/4/4
26	PEB	K8	201	1	-	6/24/74/74	0/4/4/4
26	PEB	C5	203	2	-	8/24/74/74	0/4/4/4
26	PEB	HF	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	F1	201	3,2	-	8/24/74/74	0/4/4/4
26	PEB	vE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	Q4	201	2	-	4/24/74/74	0/4/4/4
26	PEB	Q3	202	1	-	9/24/74/74	0/4/4/4
26	PEB	KA	201	1	-	6/24/74/74	0/4/4/4
26	PEB	F1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	F8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	aE	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	X8	201	2	-	6/24/74/74	0/4/4/4
26	PEB	JJ	201	1	-	14/24/74/74	0/4/4/4
27	PUB	xG	306	13	-	6/24/74/74	0/4/4/4
26	PEB	a4	203	2	-	10/24/74/74	0/4/4/4
26	PEB	V9	201	1	-	12/24/74/74	0/4/4/4
26	PEB	ZF	202	1	-	9/24/74/74	0/4/4/4
26	PEB	VA	201	2	-	7/24/74/74	0/4/4/4
26	PEB	NE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	H5	202	2	-	8/24/74/74	0/4/4/4
26	PEB	i2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	L6	1002	9,10	-	10/24/74/74	0/4/4/4
26	PEB	g8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	l8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	UB	202	1	-	9/24/74/74	0/4/4/4
26	PEB	T8	202	2	-	7/24/74/74	0/4/4/4
26	PEB	Q6	203	1	-	10/24/74/74	0/4/4/4
26	PEB	Y3	303	7,26	-	16/24/74/74	0/4/4/4
26	PEB	VJ	201	1	-	7/24/74/74	0/4/4/4
26	PEB	z1	201	1	-	11/24/74/74	0/4/4/4
26	PEB	i1	202	1	-	5/24/74/74	0/4/4/4
26	PEB	qE	201	2,1	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	F9	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	VD	202	2	-	10/24/74/74	0/4/4/4
28	CYC	H6	1001	10	-	8/25/74/74	0/4/4/4
26	PEB	j7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	IC	201	2	-	3/24/74/74	0/4/4/4
26	PEB	J8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Q7	202	1	-	8/24/74/74	0/4/4/4
26	PEB	b6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	V3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	R1	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	KJ	201	2	-	9/24/74/74	0/4/4/4
28	CYC	FF	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	J3	201	2,7	-	7/24/74/74	0/4/4/4
26	PEB	D2	1002	10	-	6/24/74/74	0/4/4/4
26	PEB	F4	203	2	-	9/24/74/74	0/4/4/4
26	PEB	q1	202	2	-	9/24/74/74	0/4/4/4
28	CYC	HI	1001	10	-	7/25/74/74	0/4/4/4
27	PUB	A9	302	1,7	-	8/24/74/74	0/4/4/4
28	CYC	D2	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	B3	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Y7	201	2	-	10/24/74/74	0/4/4/4
28	CYC	jH	1001	22,18	-	8/25/74/74	0/4/4/4
26	PEB	dI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	201	2,15	-	9/24/74/74	0/4/4/4
26	PEB	R6	201	2	-	8/24/74/74	0/4/4/4
26	PEB	XG	203	2	-	11/24/74/74	0/4/4/4
26	PEB	iA	202	2	-	9/24/74/74	0/4/4/4
28	CYC	sH	1001	22,18	-	8/25/74/74	0/4/4/4
26	PEB	d6	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	BD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	gF	201	2	-	10/24/74/74	0/4/4/4
26	PEB	lB	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WF	201	1	-	8/24/74/74	0/4/4/4
26	PEB	w4	202	2	-	5/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	PD	201	2	-	4/24/74/74	0/4/4/4
26	PEB	O2	201	1	-	8/24/74/74	0/4/4/4
26	PEB	O7	201	1	-	10/24/74/74	0/4/4/4
26	PEB	QD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	j7	201	1	-	11/24/74/74	0/4/4/4
26	PEB	ID	202	1	-	12/24/74/74	0/4/4/4
26	PEB	kG	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	T9	203	1	-	13/24/74/74	0/4/4/4
26	PEB	FJ	201	1	-	12/24/74/74	0/4/4/4
26	PEB	z1	202	1	-	16/24/74/74	0/4/4/4
27	PUB	AA	304	13	-	10/24/74/74	0/4/4/4
26	PEB	C5	204	2	-	10/24/74/74	0/4/4/4
28	CYC	D6	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	m2	201	2	-	9/24/74/74	0/4/4/4
26	PEB	ME	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	UA	203	3,1	-	8/24/74/74	0/4/4/4
26	PEB	QD	202	1	-	9/24/74/74	0/4/4/4
26	PEB	Q2	202	10,1	-	11/24/74/74	0/4/4/4
26	PEB	L2	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	y4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	A5	201	2	-	11/24/74/74	0/4/4/4
26	PEB	OG	203	1	-	10/24/74/74	0/4/4/4
26	PEB	H9	203	1	-	12/24/74/74	0/4/4/4
26	PEB	J5	201	1	-	9/24/74/74	0/4/4/4
26	PEB	M3	201	1	-	10/24/74/74	0/4/4/4
26	PEB	OB	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	SE	203	1	-	10/24/74/74	0/4/4/4
26	PEB	iG	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	jI	202	1	-	8/24/74/74	0/4/4/4
26	PEB	wE	302	13	-	11/24/74/74	0/4/4/4
26	PEB	T4	202	1	-	9/24/74/74	0/4/4/4
28	CYC	E6	1001	9,10	-	6/25/74/74	0/4/4/4
26	PEB	B4	203	2	-	12/24/74/74	0/4/4/4
26	PEB	SD	202	1	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	JG	201	2	-	8/24/74/74	0/4/4/4
26	PEB	p4	202	1	-	16/24/74/74	0/4/4/4
26	PEB	JG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	P4	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	HC	203	2	-	12/24/74/74	0/4/4/4
26	PEB	R8	201	2	-	5/24/74/74	0/4/4/4
26	PEB	U6	203	1	-	13/24/74/74	0/4/4/4
26	PEB	WD	202	1	-	12/24/74/74	0/4/4/4
26	PEB	K4	201	1	-	6/24/74/74	0/4/4/4
26	PEB	IE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	jF	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	Q3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	hB	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	XJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	M4	401	3	-	12/24/74/74	0/4/4/4
26	PEB	eB	202	2	-	6/24/74/74	0/4/4/4
26	PEB	TJ	201	2,1	-	14/24/74/74	0/4/4/4
28	CYC	AH	1001	17	-	7/25/74/74	0/4/4/4
26	PEB	SG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	cI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	h7	202	1	-	14/24/74/74	0/4/4/4
28	CYC	F7	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	x4	201	1	-	11/24/74/74	0/4/4/4
28	CYC	NF	1001	8,10	-	8/25/74/74	0/4/4/4
26	PEB	TB	201	2	-	3/24/74/74	0/4/4/4
26	PEB	A2	301	7	-	8/24/74/74	0/4/4/4
26	PEB	x1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	g1	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	dG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	V6	202	2	-	10/24/74/74	0/4/4/4
28	CYC	GH	1001	17	-	9/25/74/74	0/4/4/4
28	CYC	CI	1001	9	-	9/25/74/74	0/4/4/4
26	PEB	B9	202	1	-	10/24/74/74	0/4/4/4
26	PEB	iB	201	2	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	ND	203	2	-	8/24/74/74	0/4/4/4
27	PUB	KD	203	1,7	-	6/24/74/74	0/4/4/4
28	CYC	K7	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	dB	201	1,7	-	9/24/74/74	0/4/4/4
26	PEB	e6	203	2	-	13/24/74/74	0/4/4/4
26	PEB	bB	201	1	-	5/24/74/74	0/4/4/4
28	CYC	IF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	lG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	DE	202	2,1	-	11/24/74/74	0/4/4/4
26	PEB	a4	201	2	-	4/24/74/74	0/4/4/4
26	PEB	f8	202	1	-	8/24/74/74	0/4/4/4
26	PEB	PI	202	2	-	6/24/74/74	0/4/4/4
26	PEB	AI	304	7	-	9/24/74/74	0/4/4/4
26	PEB	Y2	202	2	-	6/24/74/74	0/4/4/4
26	PEB	I9	201	2,15	-	7/24/74/74	0/4/4/4
26	PEB	K9	201	2	-	9/24/74/74	0/4/4/4
26	PEB	O6	202	1	-	10/24/74/74	0/4/4/4
26	PEB	L7	1002	10	-	10/24/74/74	0/4/4/4
26	PEB	L4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	BG	201	2,16	-	11/24/74/74	0/4/4/4
26	PEB	c6	201	2	-	5/24/74/74	0/4/4/4
26	PEB	R9	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	D6	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	k4	202	1	-	5/24/74/74	0/4/4/4
26	PEB	R3	203	2	-	12/24/74/74	0/4/4/4
26	PEB	N4	202	1	-	11/24/74/74	0/4/4/4
26	PEB	WE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	EJ	202	2	-	7/24/74/74	0/4/4/4
26	PEB	B8	301	14	-	12/24/74/74	0/4/4/4
26	PEB	QG	202	1	-	7/24/74/74	0/4/4/4
26	PEB	Y1	201	2	-	7/24/74/74	0/4/4/4
26	PEB	SG	202	1	-	7/24/74/74	0/4/4/4
26	PEB	UB	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	V4	201	1	-	7/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	GG	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WA	202	1	-	12/24/74/74	0/4/4/4
26	PEB	L3	201	2,26	-	5/24/74/74	0/4/4/4
26	PEB	g1	202	1	-	7/24/74/74	0/4/4/4
26	PEB	V6	201	2	-	8/24/74/74	0/4/4/4
27	PUB	BA	302	14	-	5/24/74/74	0/4/4/4
26	PEB	QB	203	1	-	10/24/74/74	0/4/4/4
26	PEB	C8	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	AB	304	7	-	4/24/74/74	0/4/4/4
26	PEB	B9	201	1	-	11/24/74/74	0/4/4/4
26	PEB	T7	201	2,6	-	8/24/74/74	0/4/4/4
26	PEB	L9	203	1	-	11/24/74/74	0/4/4/4
26	PEB	XD	203	2	-	12/24/74/74	0/4/4/4
26	PEB	LG	202	2	-	14/24/74/74	0/4/4/4
26	PEB	VI	202	2	-	12/24/74/74	0/4/4/4
26	PEB	aG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	O8	202	1	-	10/24/74/74	0/4/4/4
26	PEB	a8	201	1,13	-	10/24/74/74	0/4/4/4
26	PEB	cA	202	2,1	-	9/24/74/74	0/4/4/4
28	CYC	FB	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	G9	202	2	-	13/24/74/74	0/4/4/4
26	PEB	m4	203	1	-	11/24/74/74	0/4/4/4
26	PEB	U7	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	X1	203	1	-	8/24/74/74	0/4/4/4
26	PEB	MD	201	1	-	10/24/74/74	0/4/4/4
26	PEB	m6	202	2	-	7/24/74/74	0/4/4/4
26	PEB	DE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	T1	202	1	-	8/24/74/74	0/4/4/4
26	PEB	K6	201	9,10	-	6/24/74/74	0/4/4/4
28	CYC	MI	1001	9	-	8/25/74/74	0/4/4/4
26	PEB	KC	203	2	-	8/24/74/74	0/4/4/4
26	PEB	gI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	eI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	Y2	201	2	-	3/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	k7	202	2	-	11/24/74/74	0/4/4/4
26	PEB	UJ	201	2,7	-	11/24/74/74	0/4/4/4
26	PEB	G5	203	2	-	12/24/74/74	0/4/4/4
26	PEB	r1	202	1	-	16/24/74/74	0/4/4/4
26	PEB	h1	201	2,4	-	9/24/74/74	0/4/4/4
26	PEB	O1	201	2,4	-	10/24/74/74	0/4/4/4
26	PEB	X3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	g4	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	U4	202	2	-	10/24/74/74	0/4/4/4
26	PEB	e8	201	2,13	-	6/24/74/74	0/4/4/4
26	PEB	U3	202	1	-	11/24/74/74	0/4/4/4
28	CYC	EB	1001	9,10	-	6/25/74/74	0/4/4/4
26	PEB	M1	402	3,26	-	13/24/74/74	0/4/4/4
26	PEB	kA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	t4	202	1	-	18/24/74/74	0/4/4/4
26	PEB	h8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	H3	201	2	-	4/24/74/74	0/4/4/4
26	PEB	VA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	U2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	V8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	g8	201	2	-	9/24/74/74	0/4/4/4
26	PEB	uE	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	AC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	yG	301	14	-	8/24/74/74	0/4/4/4
26	PEB	HJ	202	1	-	12/24/74/74	0/4/4/4
26	PEB	QF	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	F5	202	2	-	11/24/74/74	0/4/4/4
26	PEB	HD	202	2	-	8/24/74/74	0/4/4/4
26	PEB	PF	201	2,6	-	5/24/74/74	0/4/4/4
26	PEB	C1	201	1	-	7/24/74/74	0/4/4/4
26	PEB	H7	1002	10	-	6/24/74/74	0/4/4/4
26	PEB	DD	203	2	-	11/24/74/74	0/4/4/4
26	PEB	KG	201	2,1	-	6/24/74/74	0/4/4/4
28	CYC	L2	1001	10	-	7/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	l4	202	2	-	7/24/74/74	0/4/4/4
27	PUB	A6	302	7	-	9/24/74/74	0/4/4/4
26	PEB	YA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	AD	201	1	-	11/24/74/74	0/4/4/4
26	PEB	gI	201	2	-	4/24/74/74	0/4/4/4
26	PEB	fG	202	2	-	11/24/74/74	0/4/4/4
27	PUB	21	402	3	-	9/24/74/74	0/4/4/4
26	PEB	LD	201	2,26	-	6/24/74/74	0/4/4/4
26	PEB	A3	202	1	-	13/24/74/74	0/4/4/4
26	PEB	KG	202	1	-	4/24/74/74	0/4/4/4
26	PEB	24	404	3	-	12/24/74/74	0/4/4/4
26	PEB	vG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	d8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	K3	202	1	-	7/24/74/74	0/4/4/4
26	PEB	AD	202	1	-	12/24/74/74	0/4/4/4
26	PEB	X3	201	2,11	-	6/24/74/74	0/4/4/4
26	PEB	C5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	21	404	3	-	7/24/74/74	0/4/4/4
26	PEB	U7	203	1	-	8/24/74/74	0/4/4/4
26	PEB	C4	202	1	-	13/24/74/74	0/4/4/4
28	CYC	LB	1001	10	-	7/25/74/74	0/4/4/4
26	PEB	TA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	OE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	LA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	S2	201	1	-	7/24/74/74	0/4/4/4
26	PEB	HJ	201	2,1	-	14/24/74/74	0/4/4/4
26	PEB	lA	202	1	-	5/24/74/74	0/4/4/4
26	PEB	UG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	V8	201	2	-	7/24/74/74	0/4/4/4
26	PEB	eA	201	2,13	-	6/24/74/74	0/4/4/4
26	PEB	x1	202	1	-	13/24/74/74	0/4/4/4
26	PEB	MJ	202	2	-	10/24/74/74	0/4/4/4
26	PEB	11	202	2	-	10/24/74/74	0/4/4/4
27	PUB	A1	203	3,1	-	6/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	BC	201	2	-	8/24/74/74	0/4/4/4
26	PEB	jA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	lB	203	1	-	7/24/74/74	0/4/4/4
26	PEB	GE	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YB	202	2	-	12/24/74/74	0/4/4/4
26	PEB	X4	203	1	-	7/24/74/74	0/4/4/4
26	PEB	hF	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	H4	203	2	-	10/24/74/74	0/4/4/4
26	PEB	s4	202	2	-	8/24/74/74	0/4/4/4
28	CYC	I7	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	CE	201	2,1	-	7/24/74/74	0/4/4/4
27	PUB	A6	303	7	-	8/24/74/74	0/4/4/4
26	PEB	jG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	zE	501	2,16	-	6/24/74/74	0/4/4/4
26	PEB	bB	202	1	-	7/24/74/74	0/4/4/4
26	PEB	ED	202	1	-	11/24/74/74	0/4/4/4
26	PEB	Y4	201	2	-	7/24/74/74	0/4/4/4
26	PEB	Q1	201	2	-	4/24/74/74	0/4/4/4
26	PEB	VG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	T9	202	1	-	9/24/74/74	0/4/4/4
26	PEB	jE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	QF	203	1	-	9/24/74/74	0/4/4/4
28	CYC	DF	1001	10	-	6/25/74/74	0/4/4/4
26	PEB	fF	203	2,1	-	12/24/74/74	0/4/4/4
26	PEB	D8	201	14,2	-	10/24/74/74	0/4/4/4
26	PEB	u4	202	2	-	7/24/74/74	0/4/4/4
28	CYC	LI	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	dB	203	1	-	7/24/74/74	0/4/4/4
26	PEB	PA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	AI	301	7	-	7/24/74/74	0/4/4/4
26	PEB	hI	201	1	-	10/24/74/74	0/4/4/4
27	PUB	AI	302	7	-	2/24/74/74	0/4/4/4
26	PEB	sE	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	R8	202	2	-	11/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	W8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	UG	201	1	-	8/24/74/74	0/4/4/4
28	CYC	YH	1003	22	-	8/25/74/74	0/4/4/4
26	PEB	B3	201	2,26	-	6/24/74/74	0/4/4/4
26	PEB	DG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	cI	201	2	-	7/24/74/74	0/4/4/4
26	PEB	JA	202	2	-	9/24/74/74	0/4/4/4
28	CYC	GI	1001	9	-	6/25/74/74	0/4/4/4
26	PEB	MJ	201	2	-	7/24/74/74	0/4/4/4
26	PEB	P4	202	1	-	7/24/74/74	0/4/4/4
26	PEB	GG	203	1	-	9/24/74/74	0/4/4/4
28	CYC	G2	1001	9	-	6/25/74/74	0/4/4/4
26	PEB	HA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	w4	203	2	-	5/24/74/74	0/4/4/4
26	PEB	cI	202	2	-	11/24/74/74	0/4/4/4
26	PEB	eG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	CC	202	-	-	7/24/74/74	0/4/4/4
26	PEB	a6	201	2	-	5/24/74/74	0/4/4/4
28	CYC	K6	202	9,10	-	9/25/74/74	0/4/4/4
26	PEB	u1	201	3,2	-	14/24/74/74	0/4/4/4
26	PEB	H5	203	2	-	12/24/74/74	0/4/4/4
26	PEB	ND	201	2	-	3/24/74/74	0/4/4/4
26	PEB	eB	201	2	-	9/24/74/74	0/4/4/4
27	PUB	yE	303	14	-	6/24/74/74	0/4/4/4
26	PEB	H4	202	2	-	8/24/74/74	0/4/4/4
26	PEB	k8	201	2	-	11/24/74/74	0/4/4/4
26	PEB	R7	201	2	-	5/24/74/74	0/4/4/4
26	PEB	L8	202	2	-	9/24/74/74	0/4/4/4
28	CYC	KF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	RG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	y1	201	2	-	11/24/74/74	0/4/4/4
26	PEB	JC	202	1	-	7/24/74/74	0/4/4/4
26	PEB	fA	201	1	-	9/24/74/74	0/4/4/4
26	PEB	V1	203	2,1	-	11/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	UD	201	1	-	5/24/74/74	0/4/4/4
26	PEB	fB	201	1	-	11/24/74/74	0/4/4/4
26	PEB	FA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	R4	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	V2	202	2	-	12/24/74/74	0/4/4/4
26	PEB	GC	203	2	-	14/24/74/74	0/4/4/4
26	PEB	W4	201	2	-	8/24/74/74	0/4/4/4
28	CYC	L7	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	iI	203	2	-	12/24/74/74	0/4/4/4
26	PEB	uG	203	1	-	9/24/74/74	0/4/4/4
26	PEB	Z7	203	1	-	7/24/74/74	0/4/4/4
26	PEB	fA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	A6	301	7	-	10/24/74/74	0/4/4/4
26	PEB	fI	201	2	-	9/24/74/74	0/4/4/4
28	CYC	C2	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	A5	202	2	-	10/24/74/74	0/4/4/4
26	PEB	IE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	KD	202	1	-	10/24/74/74	0/4/4/4
26	PEB	c6	202	2	-	10/24/74/74	0/4/4/4
26	PEB	dE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	WE	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	aE	202	1	-	8/24/74/74	0/4/4/4
26	PEB	G4	201	1	-	7/24/74/74	0/4/4/4
26	PEB	l8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	U2	202	1	-	10/24/74/74	0/4/4/4
27	PUB	AF	304	7	-	15/24/74/74	0/4/4/4
26	PEB	Q6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	EG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	R3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	QI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	RB	201	2	-	9/24/74/74	0/4/4/4
26	PEB	cF	201	2	-	6/24/74/74	0/4/4/4
26	PEB	t1	202	1	-	17/24/74/74	0/4/4/4
26	PEB	F9	202	1	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	QA	204	1	-	12/24/74/74	0/4/4/4
28	CYC	MB	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	QB	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	cE	201	1	-	12/24/74/74	0/4/4/4
26	PEB	E9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	PE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	h7	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	TF	202	2	-	15/24/74/74	0/4/4/4
26	PEB	TD	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Q7	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	kE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	g1	201	1	-	6/24/74/74	0/4/4/4
26	PEB	P6	201	2,6	-	4/24/74/74	0/4/4/4
26	PEB	14	202	2	-	6/24/74/74	0/4/4/4
26	PEB	LE	201	2	-	7/24/74/74	0/4/4/4
28	CYC	nH	1001	-	-	4/25/74/74	0/4/4/4
26	PEB	BE	201	2,16	-	9/24/74/74	0/4/4/4
26	PEB	T2	202	2	-	5/24/74/74	0/4/4/4
26	PEB	cA	201	2	-	10/24/74/74	0/4/4/4
26	PEB	k2	201	2	-	7/24/74/74	0/4/4/4
26	PEB	eG	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	FD	201	2,7	-	3/24/74/74	0/4/4/4
26	PEB	b6	201	1	-	6/24/74/74	0/4/4/4
26	PEB	d8	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	cB	201	2	-	6/24/74/74	0/4/4/4
26	PEB	W7	202	1	-	11/24/74/74	0/4/4/4
26	PEB	OD	202	1	-	11/24/74/74	0/4/4/4
26	PEB	R4	202	1	-	9/24/74/74	0/4/4/4
26	PEB	iE	202	1	-	11/24/74/74	0/4/4/4
27	PUB	K3	203	1,7	-	9/24/74/74	0/4/4/4
28	CYC	WH	1001	-	-	9/25/74/74	0/4/4/4
27	PUB	xE	305	13	-	6/24/74/74	0/4/4/4
26	PEB	S1	201	2,4	-	9/24/74/74	0/4/4/4
27	PUB	K4	203	3,1	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	XG	202	2	-	5/24/74/74	0/4/4/4
26	PEB	y4	203	2	-	11/24/74/74	0/4/4/4
26	PEB	SJ	201	2,7	-	5/24/74/74	0/4/4/4
26	PEB	h6	203	1	-	7/24/74/74	0/4/4/4
26	PEB	wG	302	13	-	9/24/74/74	0/4/4/4
26	PEB	BD	202	2	-	8/24/74/74	0/4/4/4
26	PEB	dF	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	RA	201	2	-	5/24/74/74	0/4/4/4
26	PEB	a8	203	1	-	11/24/74/74	0/4/4/4
26	PEB	PJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	M8	203	1	-	9/24/74/74	0/4/4/4
26	PEB	B5	201	2	-	8/24/74/74	0/4/4/4
26	PEB	O6	201	1	-	9/24/74/74	0/4/4/4
26	PEB	R3	201	2	-	5/24/74/74	0/4/4/4
28	CYC	DF	1003	9,10	-	10/25/74/74	0/4/4/4
26	PEB	GA	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	DI	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	d1	203	2	-	8/24/74/74	0/4/4/4
26	PEB	CJ	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	ZB	203	1	-	9/24/74/74	0/4/4/4
28	CYC	oH	1001	18	-	9/25/74/74	0/4/4/4
26	PEB	D9	203	1	-	10/24/74/74	0/4/4/4
26	PEB	U8	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	H3	203	2	-	14/24/74/74	0/4/4/4
27	PUB	Y3	302	7	-	3/24/74/74	0/4/4/4
26	PEB	PG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	bG	201	2	-	4/24/74/74	0/4/4/4
26	PEB	AF	302	7	-	11/24/74/74	0/4/4/4
27	PUB	21	403	3,1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	203	2	-	9/24/74/74	0/4/4/4
26	PEB	OD	201	1	-	9/24/74/74	0/4/4/4
26	PEB	RE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	17	203	1	-	8/24/74/74	0/4/4/4
26	PEB	DA	202	2	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PUB	xE	301	13	-	7/24/74/74	0/4/4/4
28	CYC	LH	1001	-	-	4/25/74/74	0/4/4/4
26	PEB	X1	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	S3	201	1	-	6/24/74/74	0/4/4/4
26	PEB	W6	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	A9	303	7,26	-	11/24/74/74	0/4/4/4
26	PEB	HC	202	2	-	8/24/74/74	0/4/4/4
26	PEB	DF	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	kF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	y1	203	2	-	8/24/74/74	0/4/4/4
26	PEB	c4	201	1	-	11/24/74/74	0/4/4/4
26	PEB	jF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	rE	201	2,13	-	9/24/74/74	0/4/4/4
26	PEB	S8	202	1	-	10/24/74/74	0/4/4/4
26	PEB	PI	203	2	-	6/24/74/74	0/4/4/4
26	PEB	a8	202	1	-	6/24/74/74	0/4/4/4
26	PEB	AA	302	13	-	10/24/74/74	0/4/4/4
26	PEB	f2	202	1	-	10/24/74/74	0/4/4/4
26	PEB	h2	201	1	-	10/24/74/74	0/4/4/4
26	PEB	f7	201	1	-	10/24/74/74	0/4/4/4
26	PEB	14	203	2	-	8/24/74/74	0/4/4/4
26	PEB	I1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	h8	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	H1	203	2	-	11/24/74/74	0/4/4/4
26	PEB	YE	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	G1	202	1	-	11/24/74/74	0/4/4/4
26	PEB	m8	202	2	-	10/24/74/74	0/4/4/4
26	PEB	V1	201	1	-	7/24/74/74	0/4/4/4
26	PEB	f4	201	2	-	9/24/74/74	0/4/4/4
26	PEB	P4	203	1	-	12/24/74/74	0/4/4/4
28	CYC	NH	1001	17	-	7/25/74/74	0/4/4/4
26	PEB	A4	201	1	-	12/24/74/74	0/4/4/4
27	PUB	A2	303	7	-	7/24/74/74	0/4/4/4
26	PEB	QJ	202	2	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	k1	201	1	-	8/24/74/74	0/4/4/4
26	PEB	IA	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	JD	203	2	-	16/24/74/74	0/4/4/4
26	PEB	hA	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	iF	201	2	-	8/24/74/74	0/4/4/4
26	PEB	gA	201	2	-	11/24/74/74	0/4/4/4
26	PEB	GE	203	1	-	10/24/74/74	0/4/4/4
26	PEB	a1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	jG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	dB	204	1	-	11/24/74/74	0/4/4/4
26	PEB	h4	201	2,4	-	8/24/74/74	0/4/4/4
26	PEB	PF	202	2	-	8/24/74/74	0/4/4/4
26	PEB	J9	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	m7	201	2	-	9/24/74/74	0/4/4/4
26	PEB	A1	202	1	-	11/24/74/74	0/4/4/4
28	CYC	I6	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	gE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	iE	201	2,1	-	7/24/74/74	0/4/4/4
26	PEB	QF	202	1	-	13/24/74/74	0/4/4/4
26	PEB	AJ	301	7	-	11/24/74/74	0/4/4/4
26	PEB	pE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	U6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	V3	203	2	-	8/24/74/74	0/4/4/4
28	CYC	G6	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	FC	202	2	-	10/24/74/74	0/4/4/4
26	PEB	DG	202	2,1	-	12/24/74/74	0/4/4/4
26	PEB	v4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	RJ	202	1	-	11/24/74/74	0/4/4/4
26	PEB	g6	201	2	-	6/24/74/74	0/4/4/4
26	PEB	QB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	L1	202	2	-	10/24/74/74	0/4/4/4
26	PEB	i6	202	2	-	10/24/74/74	0/4/4/4
26	PEB	m2	203	2	-	9/24/74/74	0/4/4/4
26	PEB	i7	202	2	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	a1	202	2	-	6/24/74/74	0/4/4/4
26	PEB	s1	201	2	-	10/24/74/74	0/4/4/4
26	PEB	e3	401	1,11	-	9/24/74/74	0/4/4/4
26	PEB	L9	202	1	-	9/24/74/74	0/4/4/4
26	PEB	dE	202	2	-	12/24/74/74	0/4/4/4
28	CYC	QH	1001	22,18	-	8/25/74/74	0/4/4/4
26	PEB	ZI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	LG	201	2	-	9/24/74/74	0/4/4/4
26	PEB	aG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	eA	202	2	-	9/24/74/74	0/4/4/4
26	PEB	xE	302	13	-	11/24/74/74	0/4/4/4
26	PEB	m4	202	1	-	10/24/74/74	0/4/4/4
26	PEB	YJ	202	2	-	8/24/74/74	0/4/4/4
27	PUB	N9	201	1,7	-	3/24/74/74	0/4/4/4
26	PEB	A8	301	13	-	13/24/74/74	0/4/4/4
26	PEB	JD	202	2	-	10/24/74/74	0/4/4/4
26	PEB	c1	201	1	-	11/24/74/74	0/4/4/4
26	PEB	C9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	R1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	U1	202	2	-	8/24/74/74	0/4/4/4
28	CYC	gH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	b4	501	2,4	-	9/24/74/74	0/4/4/4
26	PEB	UF	202	1	-	6/24/74/74	0/4/4/4
26	PEB	fE	201	2,13	-	10/24/74/74	0/4/4/4
26	PEB	DB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	G5	202	2	-	7/24/74/74	0/4/4/4
26	PEB	IA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	SF	201	1	-	5/24/74/74	0/4/4/4
28	CYC	qH	1001	-	-	5/25/74/74	0/4/4/4
26	PEB	TG	202	2	-	15/24/74/74	0/4/4/4
26	PEB	TE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	QA	203	1	-	5/24/74/74	0/4/4/4
26	PEB	w1	201	3,2	-	13/24/74/74	0/4/4/4
26	PEB	aB	202	2	-	13/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PUB	AF	303	7	-	5/24/74/74	0/4/4/4
26	PEB	U9	201	2,7	-	9/24/74/74	0/4/4/4
26	PEB	HG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	iI	202	2	-	8/24/74/74	0/4/4/4
26	PEB	I3	202	1	-	12/24/74/74	0/4/4/4
26	PEB	A7	301	7	-	9/24/74/74	0/4/4/4
26	PEB	YG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	wE	301	13	-	10/24/74/74	0/4/4/4
28	CYC	TH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	KD	201	1	-	7/24/74/74	0/4/4/4
27	PUB	xG	301	13	-	7/24/74/74	0/4/4/4
26	PEB	FE	201	2	-	5/24/74/74	0/4/4/4
26	PEB	T4	203	1	-	9/24/74/74	0/4/4/4
26	PEB	xE	304	13	-	9/24/74/74	0/4/4/4
26	PEB	D3	201	2,7	-	6/24/74/74	0/4/4/4
26	PEB	d6	201	1,7	-	11/24/74/74	0/4/4/4
26	PEB	kI	203	2	-	12/24/74/74	0/4/4/4
28	CYC	LF	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	cE	202	1	-	13/24/74/74	0/4/4/4
26	PEB	F3	202	2	-	10/24/74/74	0/4/4/4
26	PEB	C8	202	1	-	9/24/74/74	0/4/4/4
26	PEB	w4	201	3,2	-	12/24/74/74	0/4/4/4
26	PEB	PA	202	2	-	10/24/74/74	0/4/4/4
26	PEB	bG	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RE	202	2	-	15/24/74/74	0/4/4/4
26	PEB	aA	203	1	-	11/24/74/74	0/4/4/4
26	PEB	gG	202	1	-	11/24/74/74	0/4/4/4
26	PEB	D7	1002	10	-	11/24/74/74	0/4/4/4
26	PEB	UF	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	j4	201	2,4	-	10/24/74/74	0/4/4/4
26	PEB	ZA	201	2	-	4/24/74/74	0/4/4/4
26	PEB	P3	203	2	-	7/24/74/74	0/4/4/4
26	PEB	Y8	203	1	-	10/24/74/74	0/4/4/4
26	PEB	D1	203	2	-	11/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	s4	203	2	-	7/24/74/74	0/4/4/4
28	CYC	RH	1001	17	-	8/25/74/74	0/4/4/4
26	PEB	P6	202	2	-	14/24/74/74	0/4/4/4
26	PEB	C3	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	jB	202	1	-	6/24/74/74	0/4/4/4
26	PEB	e2	203	2	-	8/24/74/74	0/4/4/4
26	PEB	k2	203	2	-	12/24/74/74	0/4/4/4
26	PEB	bF	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	qE	202	1	-	11/24/74/74	0/4/4/4
26	PEB	LC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	g4	202	1	-	7/24/74/74	0/4/4/4
26	PEB	LD	203	2	-	9/24/74/74	0/4/4/4
26	PEB	RI	203	2	-	9/24/74/74	0/4/4/4
26	PEB	lE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	UE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	D4	203	2	-	11/24/74/74	0/4/4/4
26	PEB	W3	202	1	-	12/24/74/74	0/4/4/4
26	PEB	C4	201	1	-	7/24/74/74	0/4/4/4
28	CYC	UH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	LJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	N9	202	1	-	11/24/74/74	0/4/4/4
26	PEB	h6	202	1	-	11/24/74/74	0/4/4/4
26	PEB	d4	201	2	-	10/24/74/74	0/4/4/4
26	PEB	kB	201	2,7	-	7/24/74/74	0/4/4/4
26	PEB	WD	201	1	-	7/24/74/74	0/4/4/4
27	PUB	Q8	201	14,1	-	7/24/74/74	0/4/4/4
26	PEB	S1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	ZB	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	jA	202	1	-	9/24/74/74	0/4/4/4
26	PEB	JE	201	2	-	8/24/74/74	0/4/4/4
26	PEB	kI	202	2	-	13/24/74/74	0/4/4/4
26	PEB	TJ	202	1	-	10/24/74/74	0/4/4/4
26	PEB	XG	201	2	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	dI	201	1	-	8/24/74/74	0/4/4/4
26	PEB	F3	201	2,7	-	4/24/74/74	0/4/4/4
26	PEB	k4	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YI	203	2	-	11/24/74/74	0/4/4/4
26	PEB	d4	202	2,1	-	8/24/74/74	0/4/4/4
26	PEB	m1	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	O1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	fF	201	1	-	9/24/74/74	0/4/4/4
26	PEB	DD	202	2	-	14/24/74/74	0/4/4/4
28	CYC	vH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	YA	203	1	-	11/24/74/74	0/4/4/4
26	PEB	CC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	aF	202	2	-	10/24/74/74	0/4/4/4
26	PEB	ZE	202	2	-	10/24/74/74	0/4/4/4
26	PEB	H9	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	W1	202	2	-	5/24/74/74	0/4/4/4
26	PEB	N3	201	2	-	3/24/74/74	0/4/4/4
26	PEB	e1	202	1	-	12/24/74/74	0/4/4/4
28	CYC	CB	1001	9,10	-	8/25/74/74	0/4/4/4
26	PEB	l2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	J4	203	2	-	9/24/74/74	0/4/4/4
26	PEB	BC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	sE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	P1	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	E3	201	1	-	9/24/74/74	0/4/4/4
26	PEB	bF	202	1	-	8/24/74/74	0/4/4/4
26	PEB	mA	201	2,13	-	9/24/74/74	0/4/4/4
28	CYC	lH	1001	18,17	-	7/25/74/74	0/4/4/4
26	PEB	SA	201	1	-	10/24/74/74	0/4/4/4
26	PEB	jF	201	1	-	9/24/74/74	0/4/4/4
26	PEB	y4	201	2	-	12/24/74/74	0/4/4/4
26	PEB	oE	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	m6	203	2	-	8/24/74/74	0/4/4/4
26	PEB	h6	201	2,1	-	9/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	L4	201	3,2	-	13/24/74/74	0/4/4/4
26	PEB	PB	202	2	-	12/24/74/74	0/4/4/4
27	PUB	QA	201	14,1	-	8/24/74/74	0/4/4/4
26	PEB	Z8	201	2	-	4/24/74/74	0/4/4/4
26	PEB	HE	202	2	-	12/24/74/74	0/4/4/4
26	PEB	GG	202	1	-	7/24/74/74	0/4/4/4
26	PEB	k4	201	1	-	8/24/74/74	0/4/4/4
26	PEB	G6	1002	9,10	-	9/24/74/74	0/4/4/4
26	PEB	RF	202	2	-	12/24/74/74	0/4/4/4
26	PEB	OF	203	2,1	-	10/24/74/74	0/4/4/4
26	PEB	eG	202	1	-	8/24/74/74	0/4/4/4
26	PEB	cF	202	2	-	11/24/74/74	0/4/4/4
28	CYC	B6	1002	8,10	-	5/25/74/74	0/4/4/4
26	PEB	P7	202	2	-	10/24/74/74	0/4/4/4
26	PEB	RD	203	2	-	11/24/74/74	0/4/4/4
26	PEB	SG	201	2,1	-	4/24/74/74	0/4/4/4
26	PEB	aA	202	1	-	6/24/74/74	0/4/4/4
27	PUB	YD	302	7	-	3/24/74/74	0/4/4/4
26	PEB	F1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	mI	203	2	-	9/24/74/74	0/4/4/4
26	PEB	N1	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	WG	202	1	-	8/24/74/74	0/4/4/4
26	PEB	YI	202	2	-	6/24/74/74	0/4/4/4
26	PEB	aE	203	1	-	11/24/74/74	0/4/4/4
26	PEB	G1	201	1	-	9/24/74/74	0/4/4/4
27	PUB	AI	303	7	-	7/24/74/74	0/4/4/4
26	PEB	JJ	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	q1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	X4	202	1	-	8/24/74/74	0/4/4/4
26	PEB	WA	201	1	-	7/24/74/74	0/4/4/4
26	PEB	V1	202	1	-	10/24/74/74	0/4/4/4
26	PEB	V9	203	2,1	-	14/24/74/74	0/4/4/4
26	PEB	CA	201	1	-	4/24/74/74	0/4/4/4
26	PEB	bI	202	1	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	d2	202	1	-	8/24/74/74	0/4/4/4
28	CYC	DB	1001	10	-	11/25/74/74	0/4/4/4
26	PEB	TD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	GC	202	2	-	7/24/74/74	0/4/4/4
26	PEB	i1	201	2,1	-	12/24/74/74	0/4/4/4
28	CYC	II	1001	9	-	9/25/74/74	0/4/4/4
26	PEB	A9	301	7	-	10/24/74/74	0/4/4/4
26	PEB	JC	201	1	-	10/24/74/74	0/4/4/4
26	PEB	G9	201	2	-	4/24/74/74	0/4/4/4
26	PEB	W9	202	2	-	8/24/74/74	0/4/4/4
26	PEB	HJ	203	1	-	12/24/74/74	0/4/4/4
26	PEB	E8	202	1	-	9/24/74/74	0/4/4/4
26	PEB	AJ	304	7,26	-	9/24/74/74	0/4/4/4
26	PEB	E4	202	1	-	9/24/74/74	0/4/4/4
26	PEB	F5	203	2	-	10/24/74/74	0/4/4/4
26	PEB	eD	401	1,11	-	9/24/74/74	0/4/4/4
26	PEB	G8	201	1	-	7/24/74/74	0/4/4/4
26	PEB	VB	202	2	-	10/24/74/74	0/4/4/4
26	PEB	A1	201	1	-	5/24/74/74	0/4/4/4
26	PEB	W7	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	H8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	IC	203	2	-	10/24/74/74	0/4/4/4
26	PEB	Z6	202	1	-	9/24/74/74	0/4/4/4
26	PEB	PI	201	2	-	5/24/74/74	0/4/4/4
26	PEB	K8	202	1	-	8/24/74/74	0/4/4/4
26	PEB	Y8	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	YF	201	2	-	7/24/74/74	0/4/4/4
26	PEB	g6	202	2	-	11/24/74/74	0/4/4/4
28	CYC	uH	1001	18	-	8/25/74/74	0/4/4/4
26	PEB	mE	203	1	-	12/24/74/74	0/4/4/4
26	PEB	14	201	2	-	12/24/74/74	0/4/4/4
26	PEB	a2	201	2	-	2/24/74/74	0/4/4/4
26	PEB	t1	201	1	-	13/24/74/74	0/4/4/4
26	PEB	S7	203	2,1	-	7/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	t4	201	1	-	9/24/74/74	0/4/4/4
26	PEB	h2	202	1	-	11/24/74/74	0/4/4/4
26	PEB	FE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	vE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	PD	202	2	-	7/24/74/74	0/4/4/4
26	PEB	I5	202	2	-	3/24/74/74	0/4/4/4
26	PEB	E1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	V9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	ID	201	1	-	13/24/74/74	0/4/4/4
26	PEB	A2	304	7	-	10/24/74/74	0/4/4/4
26	PEB	HD	201	2	-	4/24/74/74	0/4/4/4
26	PEB	B1	202	2	-	11/24/74/74	0/4/4/4
26	PEB	Z7	201	2,1	-	12/24/74/74	0/4/4/4
28	CYC	HB	1001	10	-	7/25/74/74	0/4/4/4
28	CYC	KI	1001	9	-	7/25/74/74	0/4/4/4
26	PEB	a6	202	2	-	13/24/74/74	0/4/4/4
26	PEB	kE	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	WF	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	A4	202	1	-	15/24/74/74	0/4/4/4
26	PEB	EA	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	Z2	202	1	-	9/24/74/74	0/4/4/4
26	PEB	Q9	201	2,7	-	2/24/74/74	0/4/4/4
26	PEB	AG	202	1	-	11/24/74/74	0/4/4/4
26	PEB	AF	301	7	-	7/24/74/74	0/4/4/4
28	CYC	EH	1001	17	-	9/25/74/74	0/4/4/4
26	PEB	F4	201	3,2	-	10/24/74/74	0/4/4/4
26	PEB	j7	203	2,1	-	8/24/74/74	0/4/4/4
26	PEB	SD	201	1	-	6/24/74/74	0/4/4/4
26	PEB	Q7	203	1	-	9/24/74/74	0/4/4/4
26	PEB	j1	202	2	-	9/24/74/74	0/4/4/4
26	PEB	fB	202	1	-	8/24/74/74	0/4/4/4
26	PEB	R2	203	2	-	9/24/74/74	0/4/4/4
26	PEB	d1	202	2,1	-	4/24/74/74	0/4/4/4
26	PEB	W4	202	2	-	5/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	l6	201	2,1	-	9/24/74/74	0/4/4/4
26	PEB	d7	203	1	-	11/24/74/74	0/4/4/4
26	PEB	hG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	jI	201	1	-	11/24/74/74	0/4/4/4
27	PUB	yE	302	14	-	3/24/74/74	0/4/4/4
26	PEB	D9	202	1	-	9/24/74/74	0/4/4/4
26	PEB	p4	201	1	-	13/24/74/74	0/4/4/4
26	PEB	KJ	202	2	-	10/24/74/74	0/4/4/4
26	PEB	qG	202	1	-	15/24/74/74	0/4/4/4
26	PEB	GD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	q1	203	2	-	9/24/74/74	0/4/4/4
26	PEB	P2	201	2	-	5/24/74/74	0/4/4/4
26	PEB	k6	202	2	-	11/24/74/74	0/4/4/4
26	PEB	mB	203	2	-	9/24/74/74	0/4/4/4
26	PEB	XJ	201	2,1	-	13/24/74/74	0/4/4/4
26	PEB	MG	202	1	-	10/24/74/74	0/4/4/4
26	PEB	EE	202	1	-	10/24/74/74	0/4/4/4
26	PEB	eI	203	2	-	8/24/74/74	0/4/4/4
26	PEB	f7	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	IJ	202	2	-	9/24/74/74	0/4/4/4
26	PEB	RB	202	2	-	11/24/74/74	0/4/4/4
26	PEB	S6	201	1	-	10/24/74/74	0/4/4/4
26	PEB	O2	202	1	-	8/24/74/74	0/4/4/4
26	PEB	11	201	2	-	10/24/74/74	0/4/4/4
26	PEB	xG	304	13	-	9/24/74/74	0/4/4/4
26	PEB	l7	202	1	-	11/24/74/74	0/4/4/4
27	PUB	AA	303	13	-	9/24/74/74	0/4/4/4
26	PEB	I8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	W6	202	1	-	8/24/74/74	0/4/4/4
26	PEB	CD	201	1	-	9/24/74/74	0/4/4/4
26	PEB	CD	202	1	-	13/24/74/74	0/4/4/4
26	PEB	ZA	202	2	-	8/24/74/74	0/4/4/4
26	PEB	kE	202	1	-	9/24/74/74	0/4/4/4
26	PEB	WF	202	1	-	9/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	CYC	L6	1001	10	-	10/25/74/74	0/4/4/4
26	PEB	cG	201	1	-	11/24/74/74	0/4/4/4
26	PEB	f6	201	1	-	10/24/74/74	0/4/4/4
28	CYC	tH	1001	17	-	10/25/74/74	0/4/4/4
26	PEB	I3	201	1	-	14/24/74/74	0/4/4/4
26	PEB	LC	201	2	-	6/24/74/74	0/4/4/4
28	CYC	B6	1001	8,10	-	12/25/74/74	0/4/4/4
26	PEB	YG	201	1	-	7/24/74/74	0/4/4/4
26	PEB	U8	203	3,1	-	7/24/74/74	0/4/4/4
26	PEB	SI	201	1	-	10/24/74/74	0/4/4/4
26	PEB	tG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	R2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	A3	201	1	-	7/24/74/74	0/4/4/4
26	PEB	G8	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	BA	301	14	-	13/24/74/74	0/4/4/4
26	PEB	o1	501	2,4	-	8/24/74/74	0/4/4/4
26	PEB	d7	202	1	-	10/24/74/74	0/4/4/4
26	PEB	v1	201	1	-	11/24/74/74	0/4/4/4
28	CYC	F6	1001	10	-	5/25/74/74	0/4/4/4
26	PEB	LC	202	2	-	10/24/74/74	0/4/4/4
26	PEB	T3	203	2	-	8/24/74/74	0/4/4/4
26	PEB	g2	201	2	-	4/24/74/74	0/4/4/4
26	PEB	H1	202	2	-	8/24/74/74	0/4/4/4
26	PEB	PD	203	2	-	7/24/74/74	0/4/4/4
26	PEB	IG	201	1	-	9/24/74/74	0/4/4/4
26	PEB	FG	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N2	1002	10	-	8/24/74/74	0/4/4/4
26	PEB	N9	204	2,1	-	12/24/74/74	0/4/4/4
26	PEB	dA	201	1	-	4/24/74/74	0/4/4/4
26	PEB	b2	201	1	-	9/24/74/74	0/4/4/4
26	PEB	i2	201	2	-	6/24/74/74	0/4/4/4
26	PEB	FC	203	2	-	11/24/74/74	0/4/4/4
26	PEB	TB	202	2	-	11/24/74/74	0/4/4/4
28	CYC	mH	1001	17	-	7/25/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	eE	201	2,1	-	12/24/74/74	0/4/4/4
26	PEB	LA	201	2	-	4/24/74/74	0/4/4/4
26	PEB	lA	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	D3	202	2	-	11/24/74/74	0/4/4/4
26	PEB	QG	201	1	-	8/24/74/74	0/4/4/4
26	PEB	YI	201	2	-	2/24/74/74	0/4/4/4
28	CYC	CF	1001	9,10	-	9/25/74/74	0/4/4/4
26	PEB	W6	201	1	-	7/24/74/74	0/4/4/4
26	PEB	AE	201	1	-	9/24/74/74	0/4/4/4
26	PEB	dG	202	2	-	12/24/74/74	0/4/4/4
26	PEB	O4	201	2,4	-	8/24/74/74	0/4/4/4
26	PEB	J9	202	1	-	12/24/74/74	0/4/4/4
26	PEB	K1	202	1	-	12/24/74/74	0/4/4/4
26	PEB	nE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	jA	201	1	-	7/24/74/74	0/4/4/4
28	CYC	YH	1002	22	-	4/25/74/74	0/4/4/4
26	PEB	T1	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	Q8	204	1	-	10/24/74/74	0/4/4/4
26	PEB	E1	202	1	-	13/24/74/74	0/4/4/4
26	PEB	L8	201	2	-	4/24/74/74	0/4/4/4
26	PEB	s4	201	2	-	7/24/74/74	0/4/4/4
28	CYC	OH	1001	-	-	5/25/74/74	0/4/4/4
26	PEB	j4	202	2	-	7/24/74/74	0/4/4/4
26	PEB	G5	201	2	-	11/24/74/74	0/4/4/4
26	PEB	UF	203	1	-	9/24/74/74	0/4/4/4
26	PEB	FA	201	2,12	-	6/24/74/74	0/4/4/4
26	PEB	b7	202	1	-	7/24/74/74	0/4/4/4
26	PEB	MA	203	1	-	9/24/74/74	0/4/4/4
26	PEB	kF	202	2	-	9/24/74/74	0/4/4/4
26	PEB	T2	203	2	-	10/24/74/74	0/4/4/4
26	PEB	mE	201	2,1	-	8/24/74/74	0/4/4/4
26	PEB	G8	202	1	-	5/24/74/74	0/4/4/4
26	PEB	mG	203	1	-	11/24/74/74	0/4/4/4
26	PEB	UI	202	1	-	10/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	F8	201	2,12	-	6/24/74/74	0/4/4/4
26	PEB	r4	201	1	-	10/24/74/74	0/4/4/4
26	PEB	iE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	JF	1002	10	-	9/24/74/74	0/4/4/4
26	PEB	ZF	201	2,1	-	11/24/74/74	0/4/4/4
26	PEB	Y2	203	2	-	11/24/74/74	0/4/4/4
26	PEB	O6	203	2,1	-	6/24/74/74	0/4/4/4
26	PEB	a4	202	2	-	6/24/74/74	0/4/4/4
26	PEB	hE	202	2	-	9/24/74/74	0/4/4/4
26	PEB	NA	201	2	-	6/24/74/74	0/4/4/4
26	PEB	l8	201	2,1	-	10/24/74/74	0/4/4/4
26	PEB	I9	202	2	-	7/24/74/74	0/4/4/4
26	PEB	r4	202	1	-	16/24/74/74	0/4/4/4
26	PEB	N4	203	2,1	-	11/24/74/74	0/4/4/4
26	PEB	a1	201	2	-	4/24/74/74	0/4/4/4
26	PEB	WE	203	1	-	9/24/74/74	0/4/4/4
26	PEB	BG	202	2	-	13/24/74/74	0/4/4/4
26	PEB	M1	401	3	-	13/24/74/74	0/4/4/4
26	PEB	sG	202	1	-	9/24/74/74	0/4/4/4
26	PEB	l1	201	2	-	12/24/74/74	0/4/4/4
26	PEB	QG	203	2,1	-	7/24/74/74	0/4/4/4
26	PEB	PE	201	2	-	7/24/74/74	0/4/4/4
26	PEB	TD	201	2	-	5/24/74/74	0/4/4/4
26	PEB	OE	201	2,1	-	5/24/74/74	0/4/4/4
26	PEB	oG	203	1	-	17/24/74/74	0/4/4/4
28	CYC	1H	1000	22	-	6/25/74/74	0/4/4/4
26	PEB	CA	202	1	-	10/24/74/74	0/4/4/4
26	PEB	p1	201	1	-	13/24/74/74	0/4/4/4
27	PUB	wE	304	13	-	9/24/74/74	0/4/4/4
26	PEB	N8	201	2	-	8/24/74/74	0/4/4/4
26	PEB	LE	202	2	-	14/24/74/74	0/4/4/4
26	PEB	R1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	QA	202	2,1	-	6/24/74/74	0/4/4/4
26	PEB	kB	202	2	-	11/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	PEB	GB	1002	9,10	-	8/24/74/74	0/4/4/4
26	PEB	tE	201	2	-	9/24/74/74	0/4/4/4
26	PEB	K5	201	2	-	3/24/74/74	0/4/4/4
26	PEB	l2	201	1	-	8/24/74/74	0/4/4/4
28	CYC	GB	1001	9,10	-	7/25/74/74	0/4/4/4
26	PEB	uE	203	1	-	10/24/74/74	0/4/4/4
26	PEB	T8	201	2	-	7/24/74/74	0/4/4/4
26	PEB	KE	203	1	-	8/24/74/74	0/4/4/4
26	PEB	h4	202	2,1	-	13/24/74/74	0/4/4/4
26	PEB	gG	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	s1	203	2	-	7/24/74/74	0/4/4/4
26	PEB	L3	203	2	-	9/24/74/74	0/4/4/4
26	PEB	M8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	M4	403	3	-	6/24/74/74	0/4/4/4
26	PEB	T1	203	1	-	10/24/74/74	0/4/4/4
26	PEB	w1	203	2	-	7/24/74/74	0/4/4/4
26	PEB	P1	202	1	-	5/24/74/74	0/4/4/4
26	PEB	BD	201	2,26	-	8/24/74/74	0/4/4/4
26	PEB	i8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	k1	203	2,1	-	9/24/74/74	0/4/4/4
26	PEB	VG	201	2	-	10/24/74/74	0/4/4/4
26	PEB	hA	203	1	-	8/24/74/74	0/4/4/4
26	PEB	L5	201	2	-	7/24/74/74	0/4/4/4
26	PEB	R7	202	2	-	11/24/74/74	0/4/4/4
26	PEB	Z1	201	2	-	5/24/74/74	0/4/4/4
26	PEB	aA	201	1,13	-	8/24/74/74	0/4/4/4
26	PEB	KA	202	1	-	8/24/74/74	0/4/4/4
26	PEB	S7	201	1	-	8/24/74/74	0/4/4/4
26	PEB	OF	201	1	-	11/24/74/74	0/4/4/4
27	PUB	NJ	201	1,7	-	3/24/74/74	0/4/4/4
26	PEB	dF	203	1	-	10/24/74/74	0/4/4/4
26	PEB	X3	203	2	-	14/24/74/74	0/4/4/4
26	PEB	O4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	F7	1002	10	-	8/24/74/74	0/4/4/4

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	PUB	K1	203	3,1	-	9/24/74/74	0/4/4/4
26	PEB	a7	202	2	-	10/24/74/74	0/4/4/4
27	PUB	xE	306	13	-	4/24/74/74	0/4/4/4
26	PEB	r1	201	1	-	10/24/74/74	0/4/4/4
26	PEB	AA	301	13	-	13/24/74/74	0/4/4/4
28	CYC	KH	1001	17	-	15/25/74/74	0/4/4/4
26	PEB	QE	201	1	-	8/24/74/74	0/4/4/4
26	PEB	P3	202	2	-	7/24/74/74	0/4/4/4
26	PEB	DJ	203	1	-	10/24/74/74	0/4/4/4
26	PEB	KE	202	1	-	7/24/74/74	0/4/4/4
26	PEB	e8	202	2	-	9/24/74/74	0/4/4/4
26	PEB	Y8	202	1	-	4/24/74/74	0/4/4/4
26	PEB	F9	201	1	-	13/24/74/74	0/4/4/4
26	PEB	kA	202	2	-	11/24/74/74	0/4/4/4
26	PEB	N6	201	9,10	-	10/24/74/74	0/4/4/4
28	CYC	IH	1001	-	-	8/25/74/74	0/4/4/4
26	PEB	e2	202	2	-	10/24/74/74	0/4/4/4
26	PEB	YB	201	2	-	10/24/74/74	0/4/4/4
26	PEB	nG	201	2	-	7/24/74/74	0/4/4/4
26	PEB	MA	202	1	-	4/24/74/74	0/4/4/4
26	PEB	NE	202	2	-	11/24/74/74	0/4/4/4
26	PEB	uE	202	1	-	10/24/74/74	0/4/4/4
26	PEB	EA	202	1	-	9/24/74/74	0/4/4/4
26	PEB	q4	202	2	-	9/24/74/74	0/4/4/4
26	PEB	QI	202	1	-	9/24/74/74	0/4/4/4
26	PEB	AE	202	1	-	11/24/74/74	0/4/4/4

The worst 5 of 17214 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	p4	202	PEB	CHB-C4B	18.98	1.51	1.35
26	I9	201	PEB	CHB-C4B	18.86	1.50	1.35
26	LG	202	PEB	CHB-C4B	18.61	1.50	1.35
26	p1	202	PEB	CHB-C4B	18.61	1.50	1.35
27	N9	201	PUB	CHB-C1C	18.57	1.50	1.35

The worst 5 of 24889 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	dH	1001	CYC	C4D-CHA-C1A	26.78	160.79	128.81
28	cH	1001	CYC	C4D-CHA-C1A	23.60	157.00	128.81
28	AH	1001	CYC	C4D-CHA-C1A	23.35	156.70	128.81
28	KH	1001	CYC	CHA-C1A-NA	-22.36	97.82	128.83
26	FG	201	PEB	OA-C1A-C2A	-17.62	112.17	126.17

There are no chirality outliers.

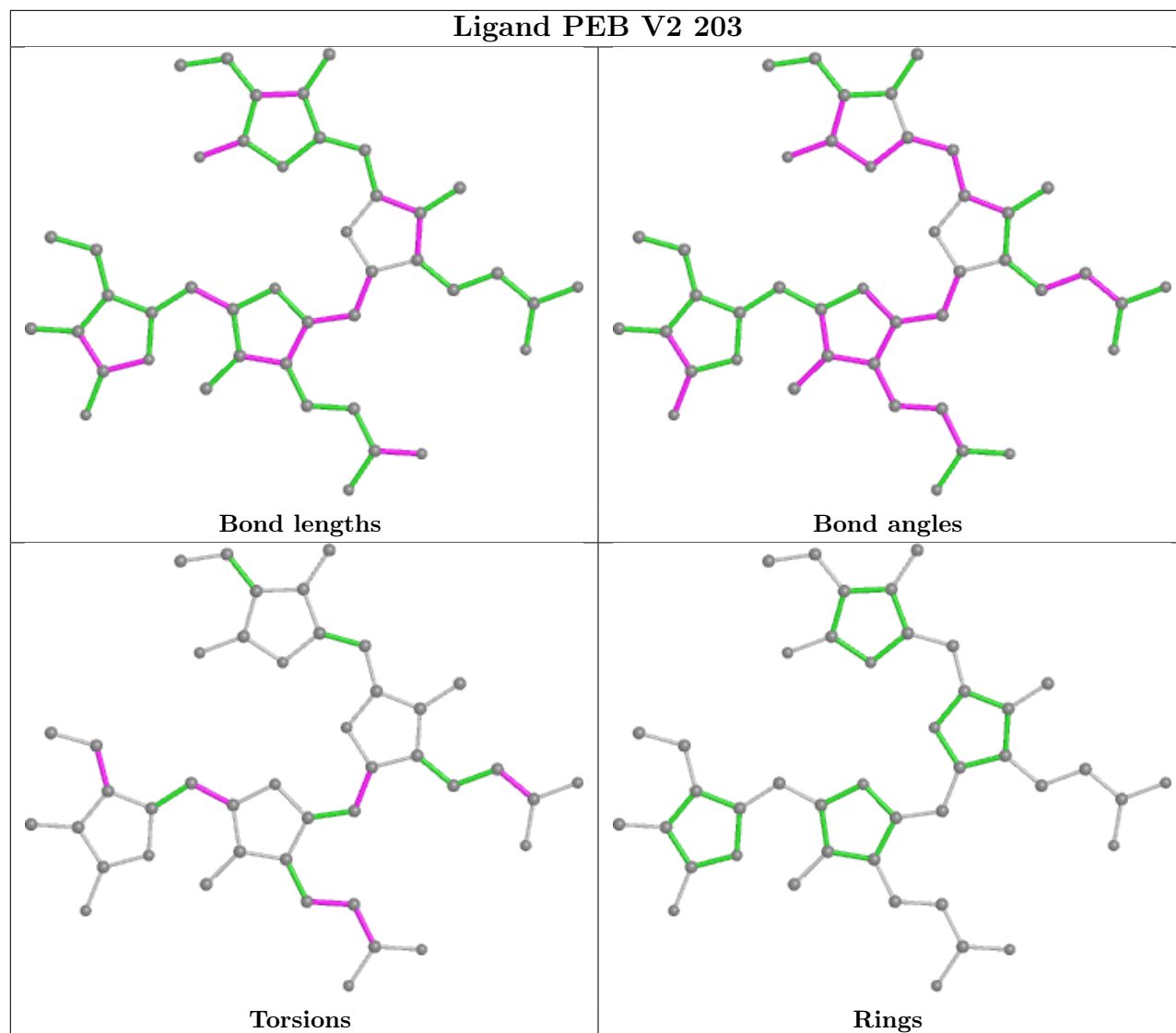
5 of 14179 torsion outliers are listed below:

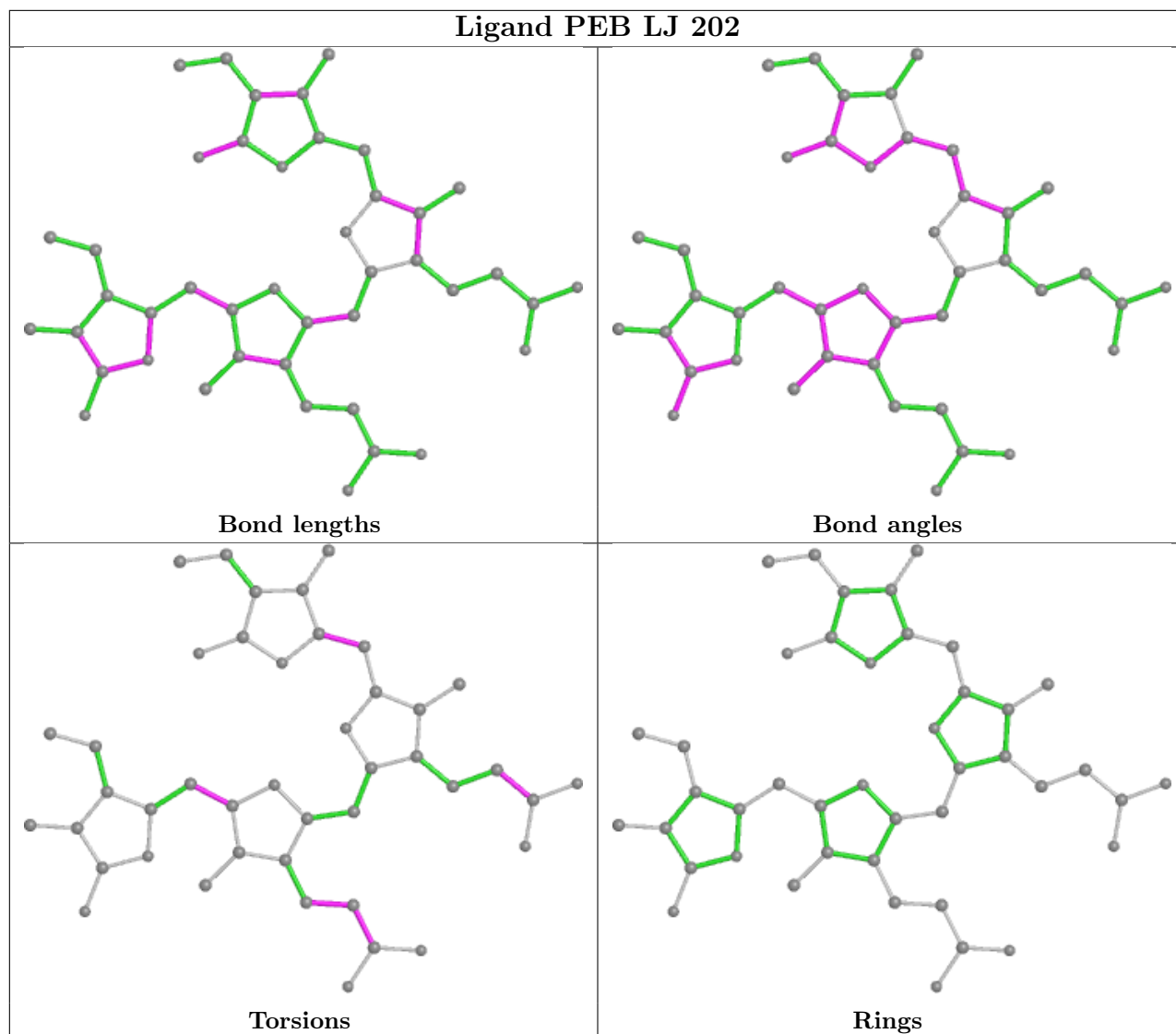
Mol	Chain	Res	Type	Atoms
26	A1	201	PEB	ND-C1D-CHC-C4C
26	A1	201	PEB	C2D-C1D-CHC-C4C
26	A1	201	PEB	NB-C1B-CHA-C4A
26	A1	201	PEB	C2B-C1B-CHA-C4A
26	A1	202	PEB	NC-C1C-CHB-C4B

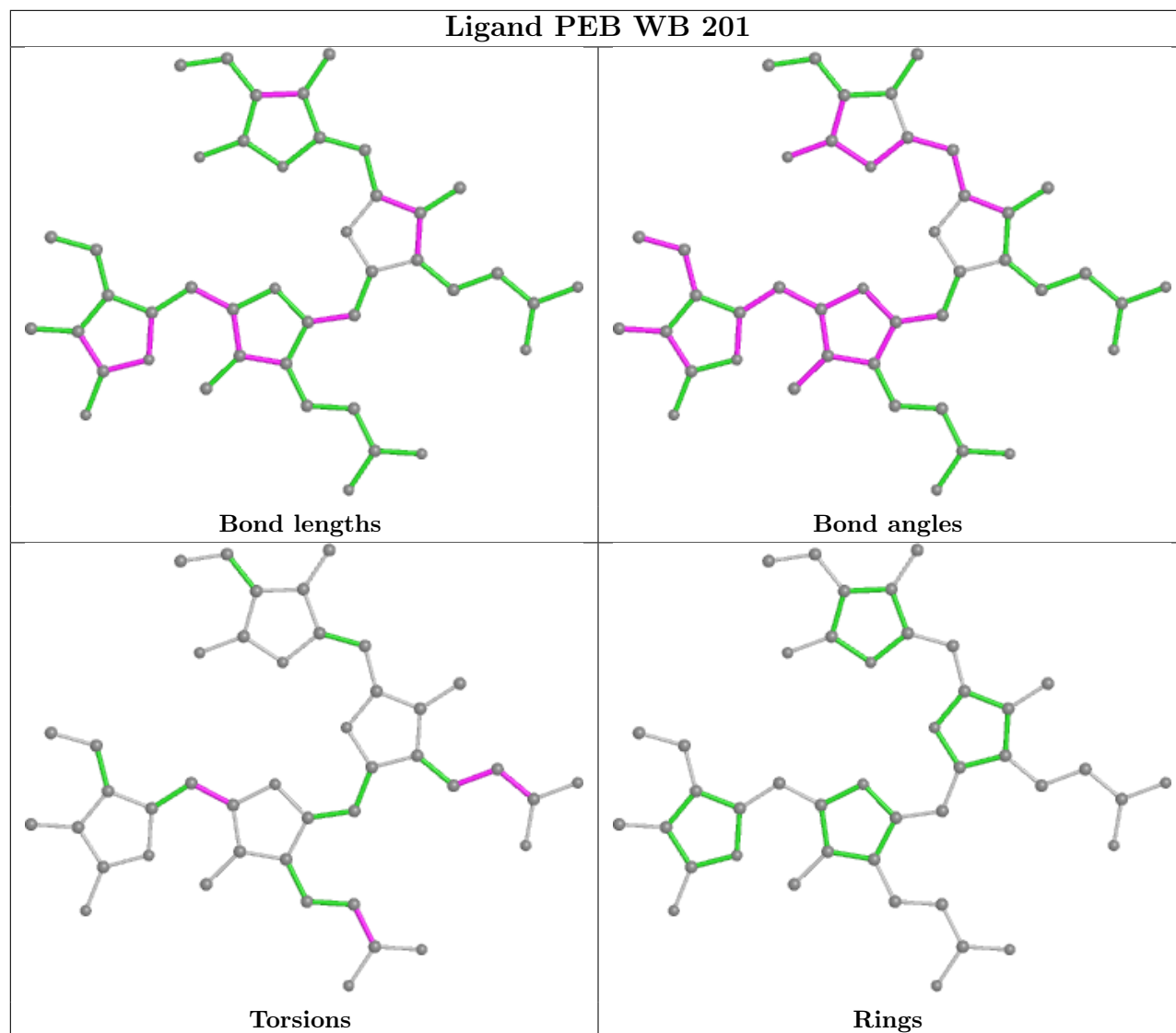
There are no ring outliers.

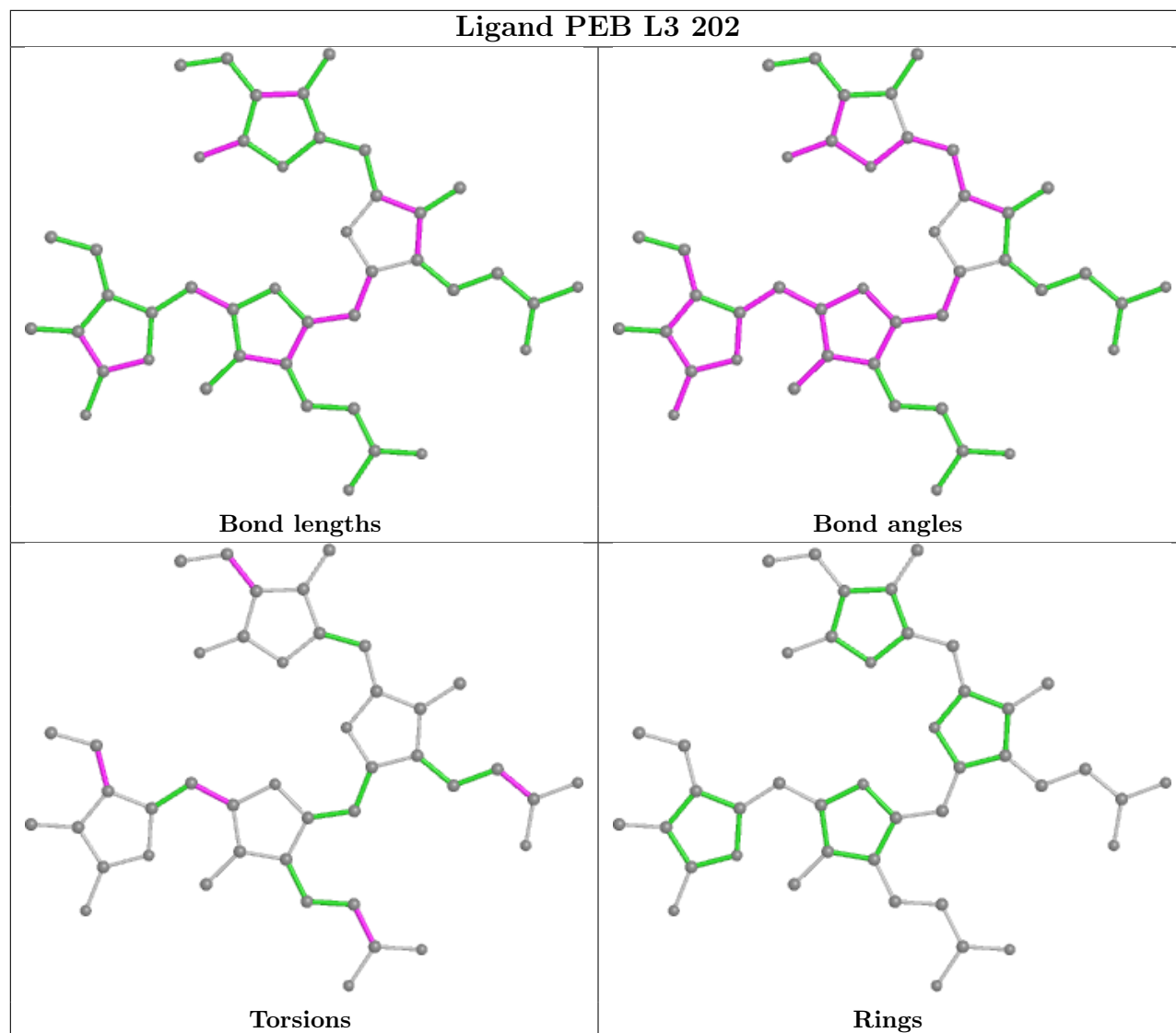
No monomer is involved in short contacts.

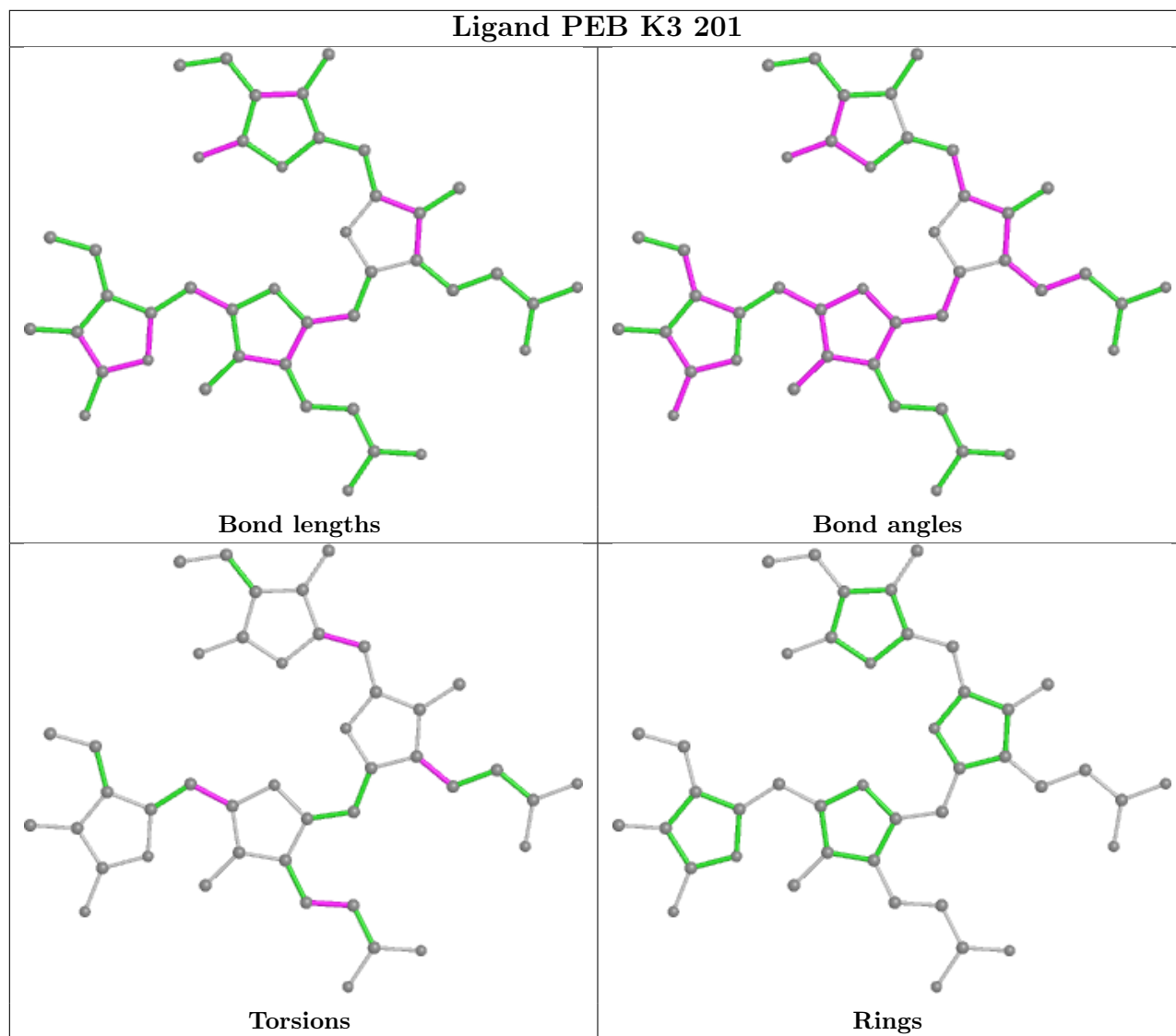
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

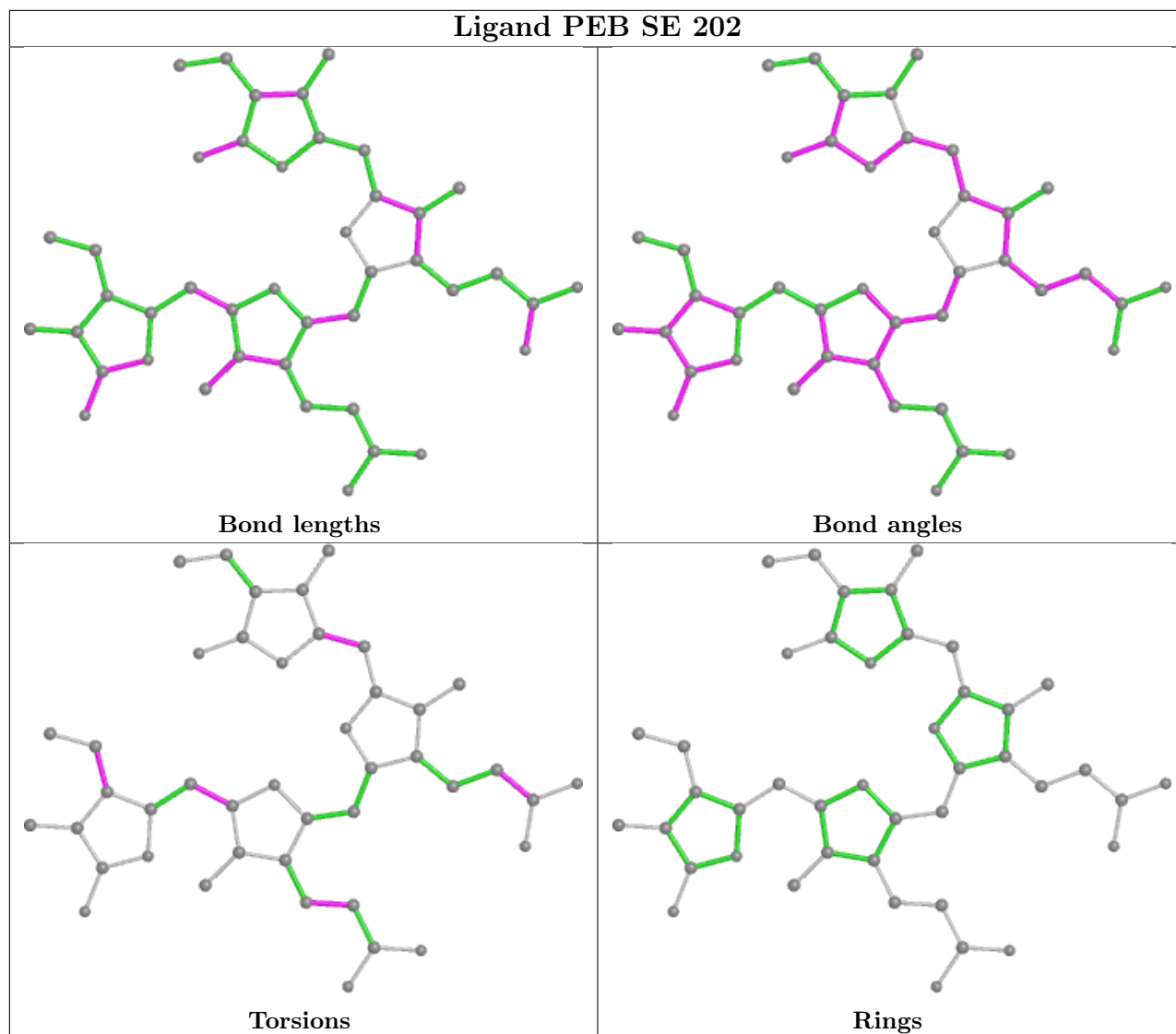


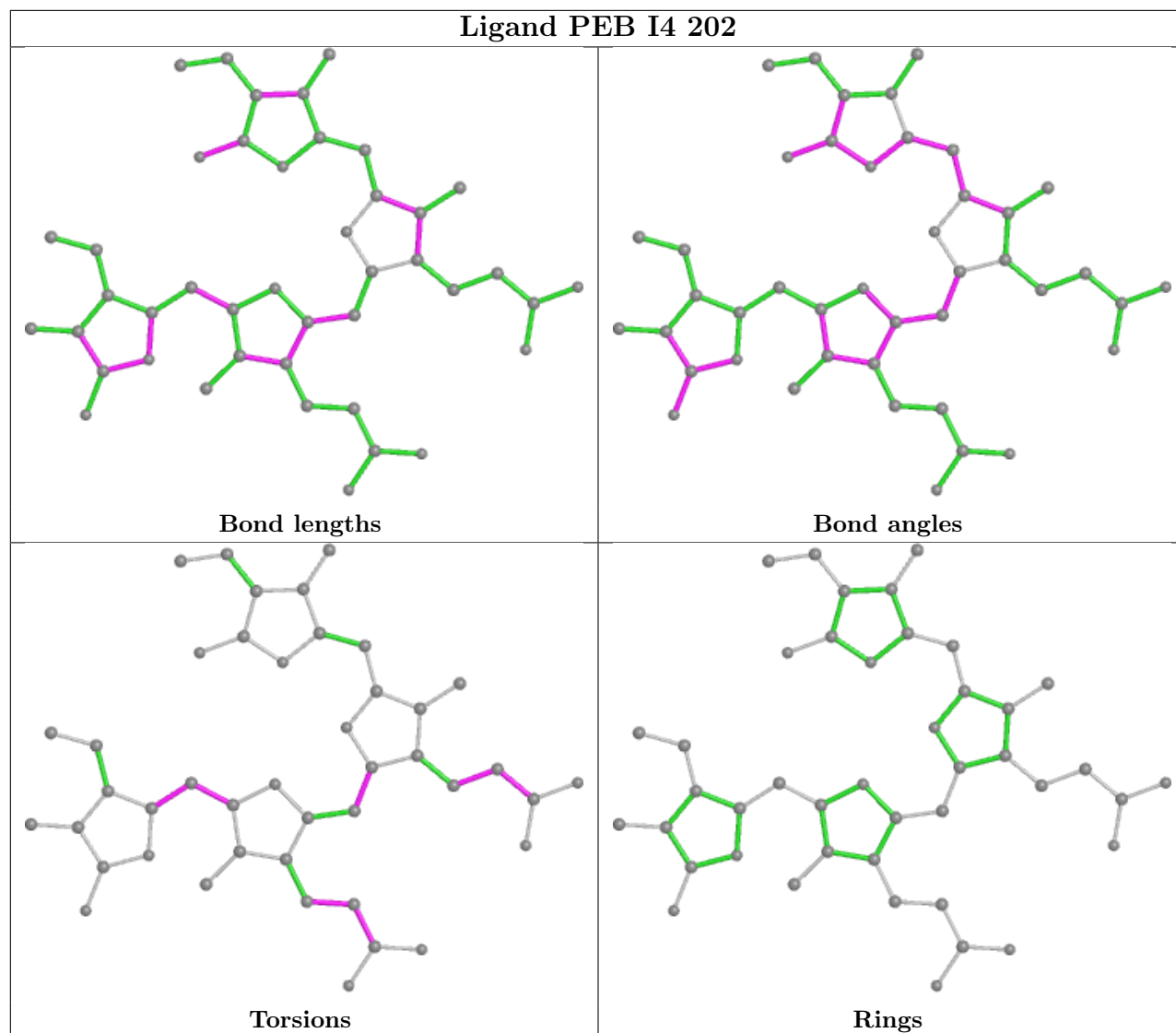


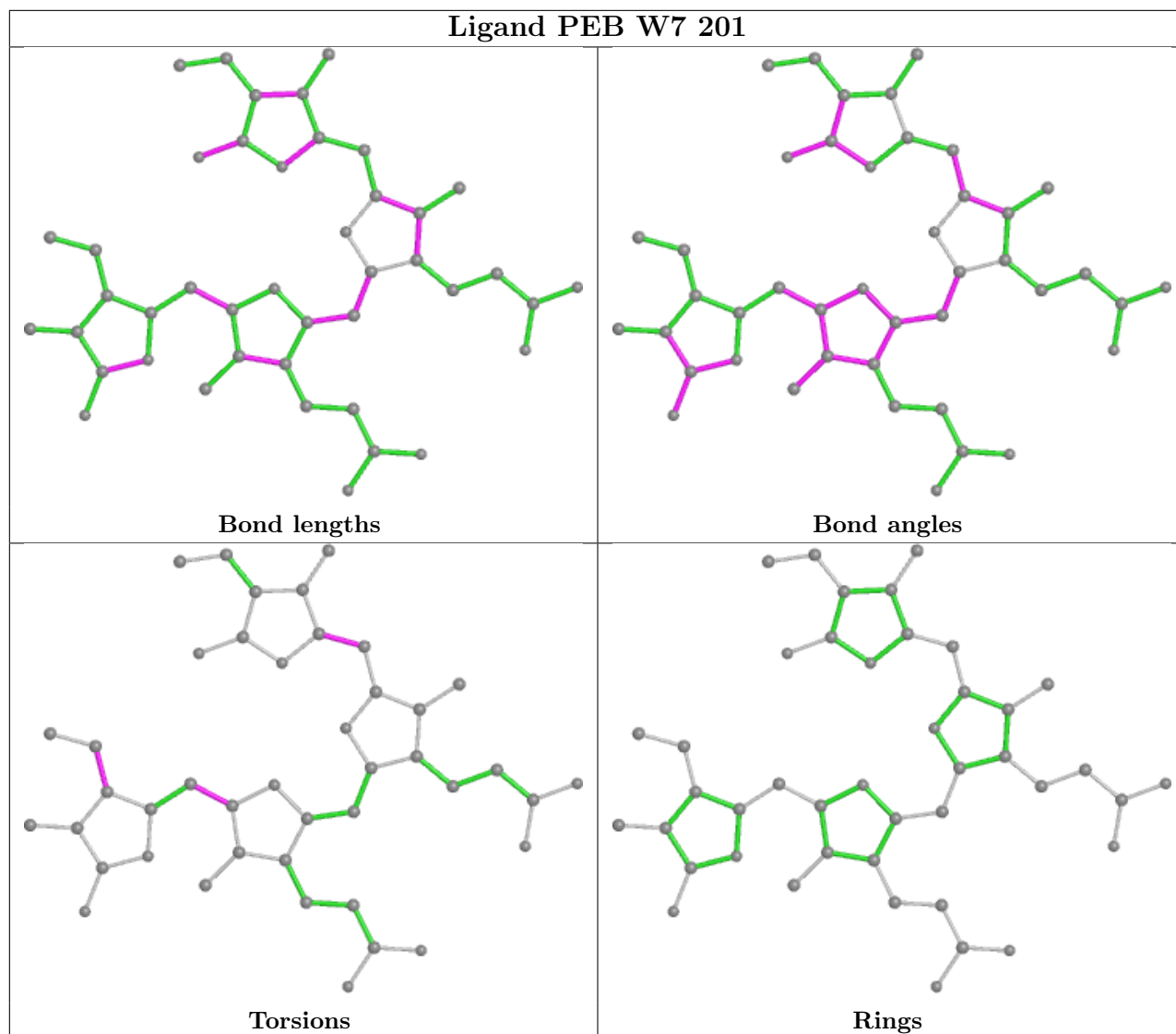


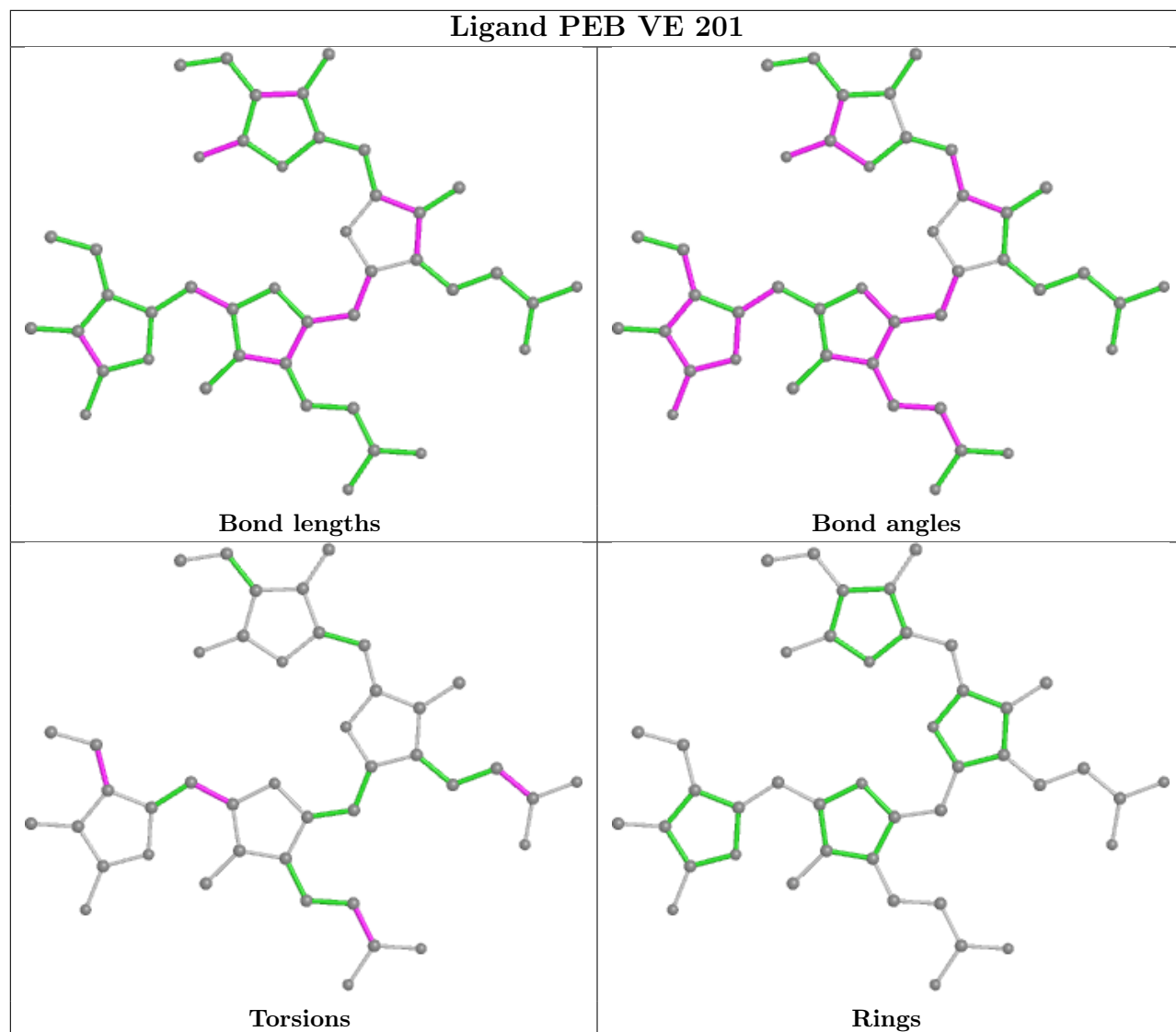


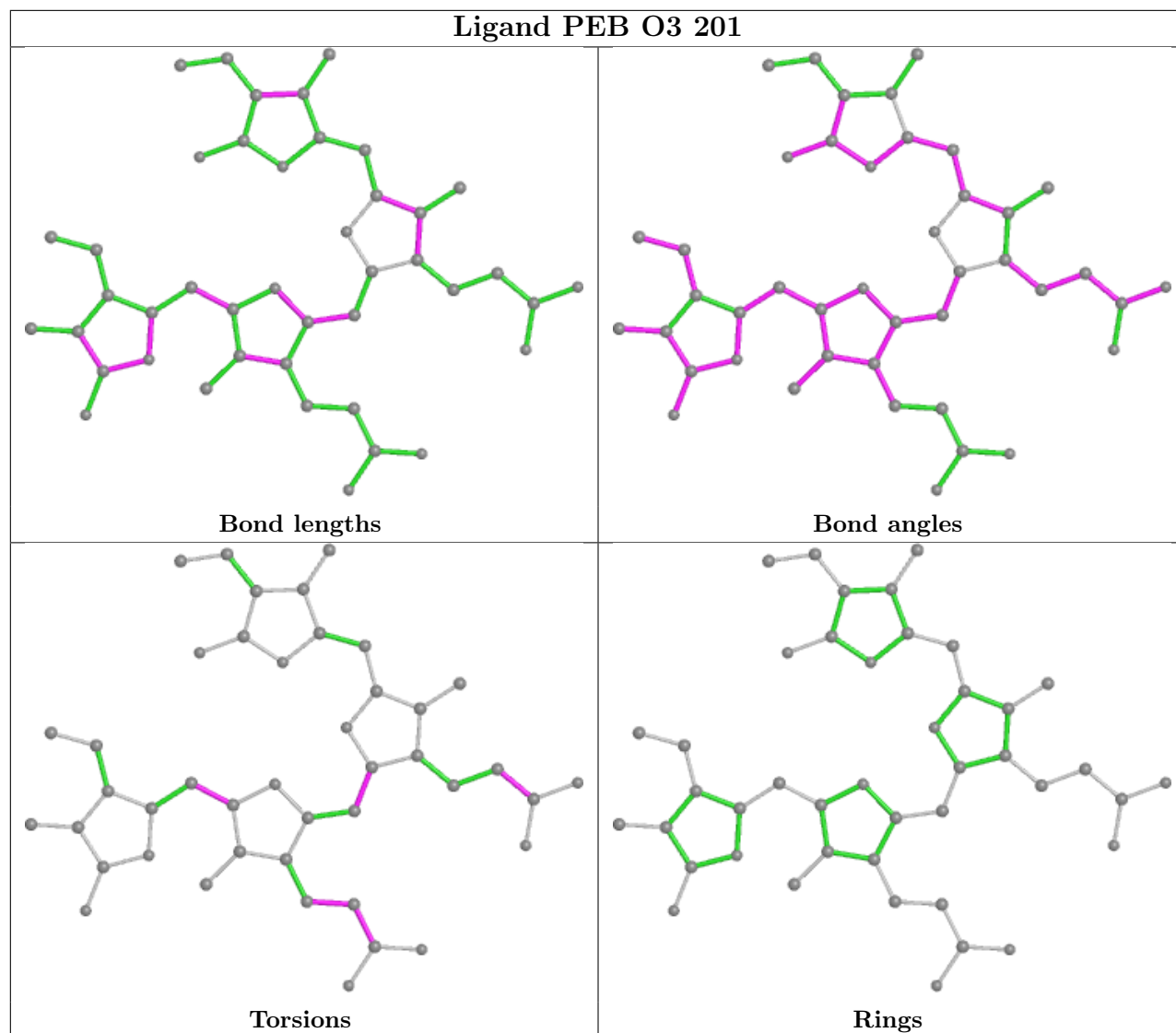


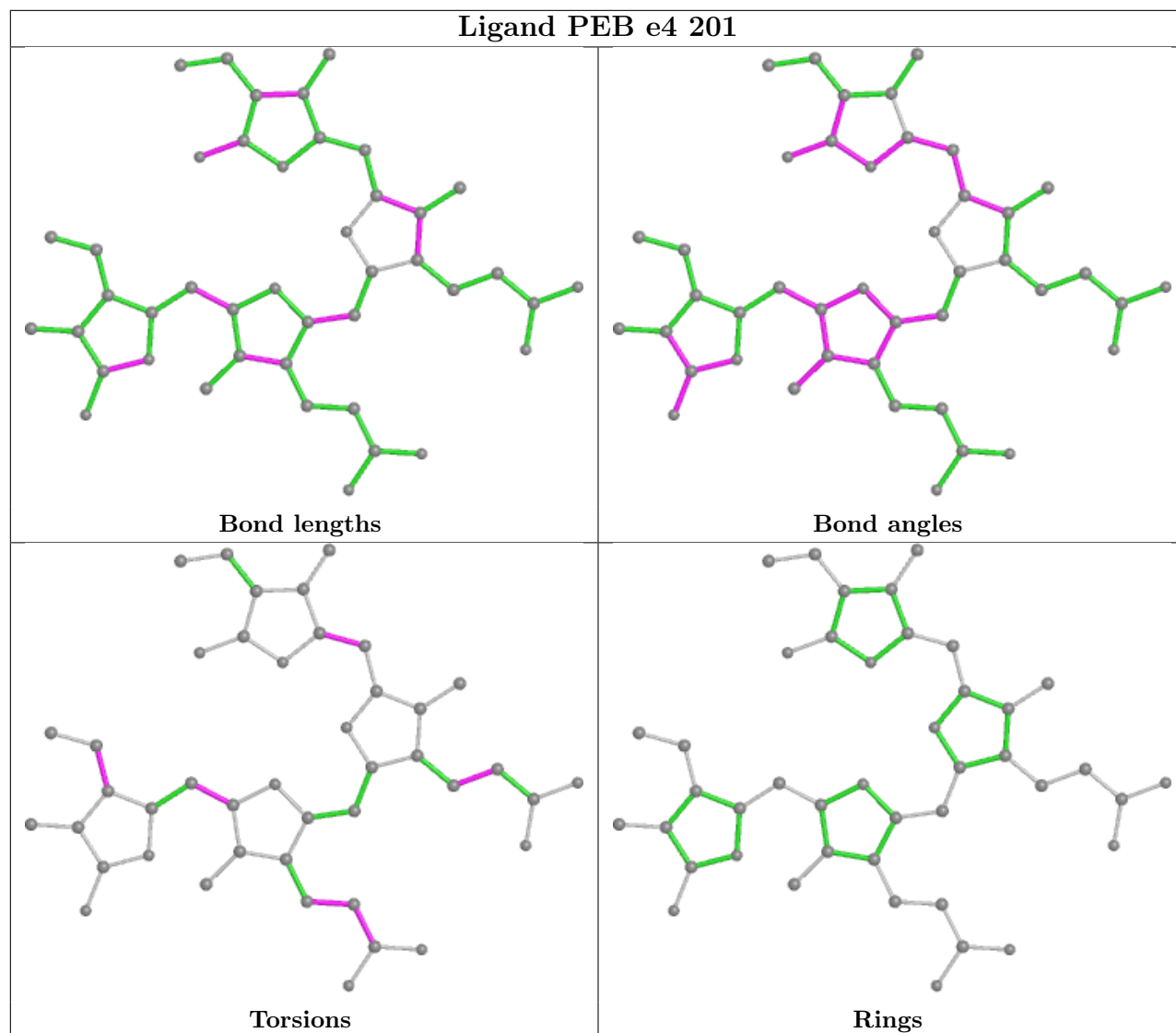


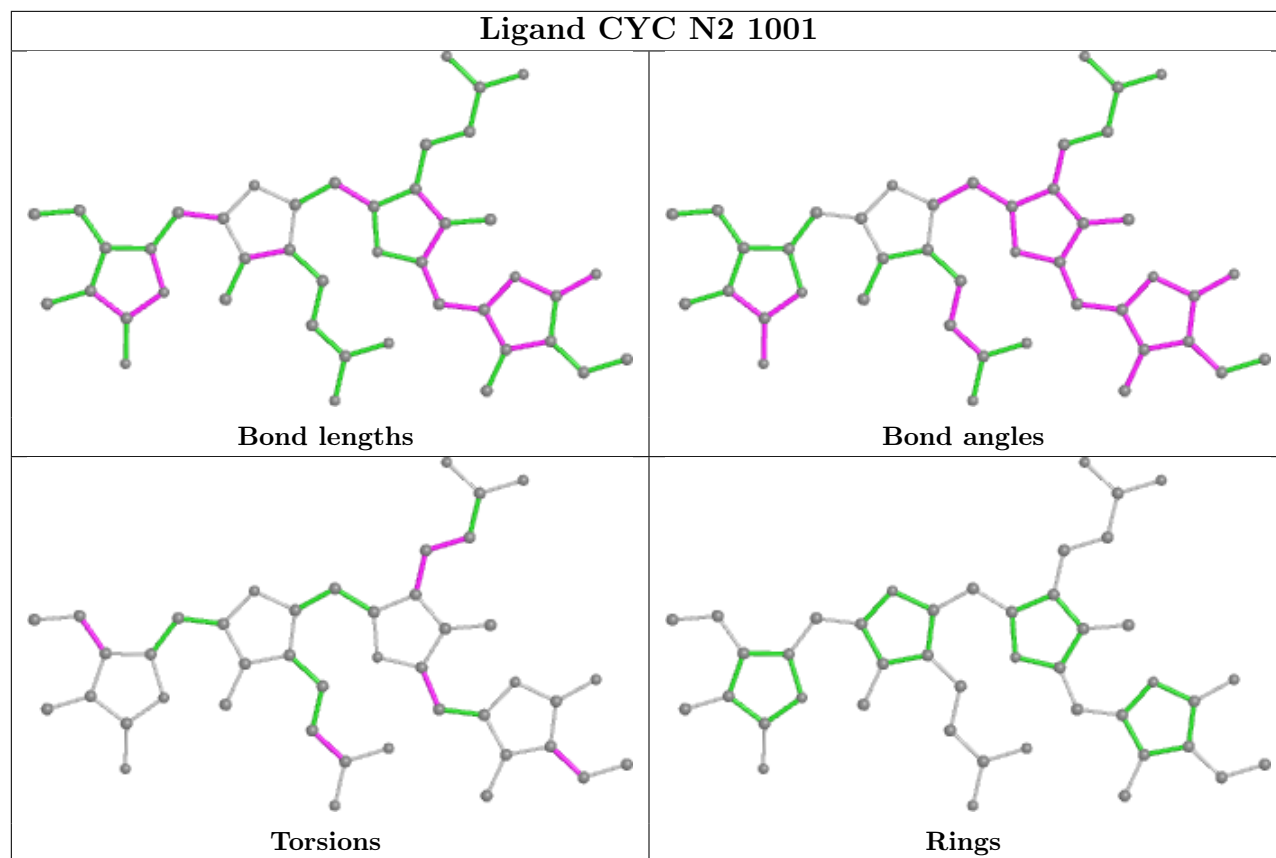


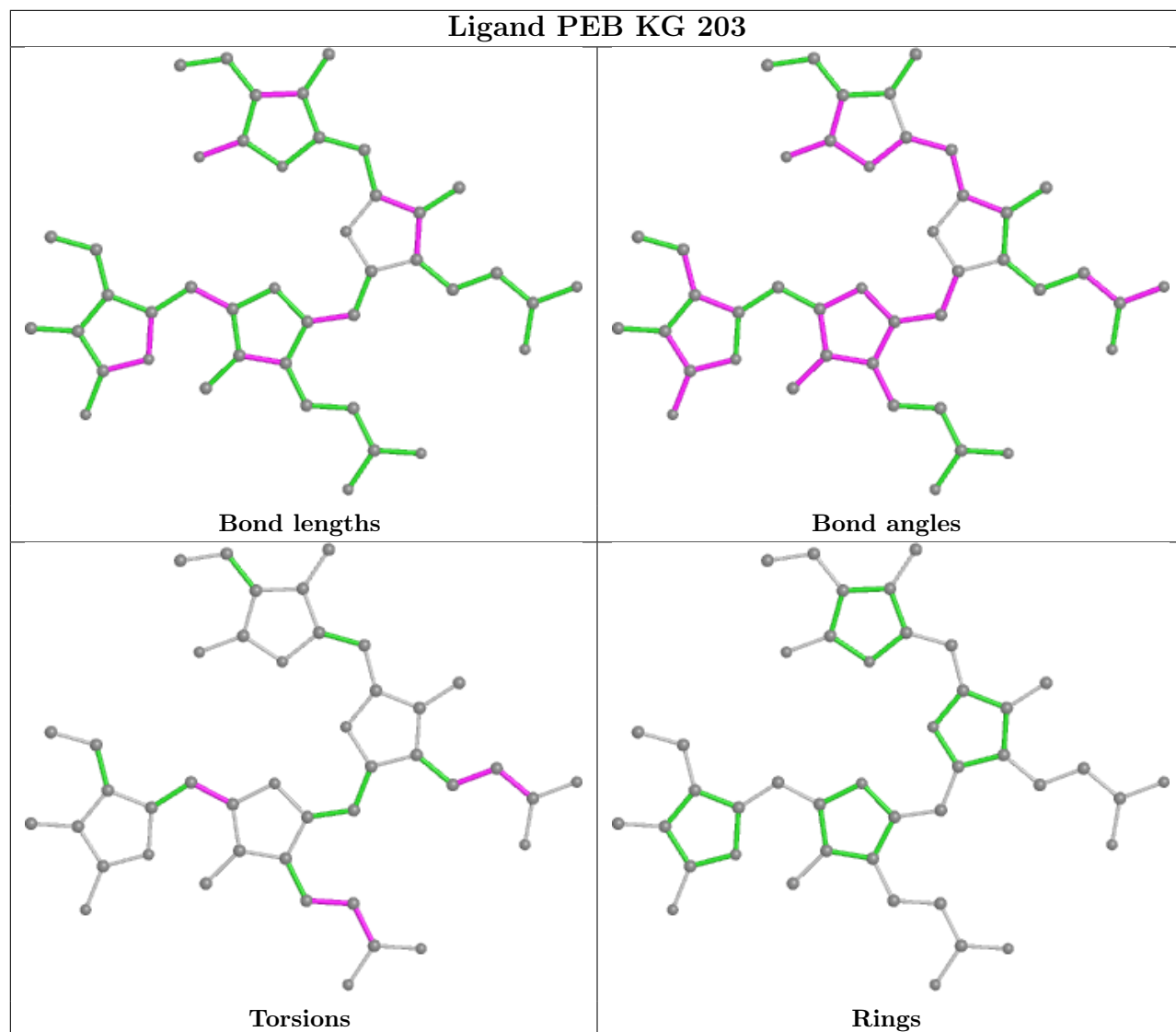


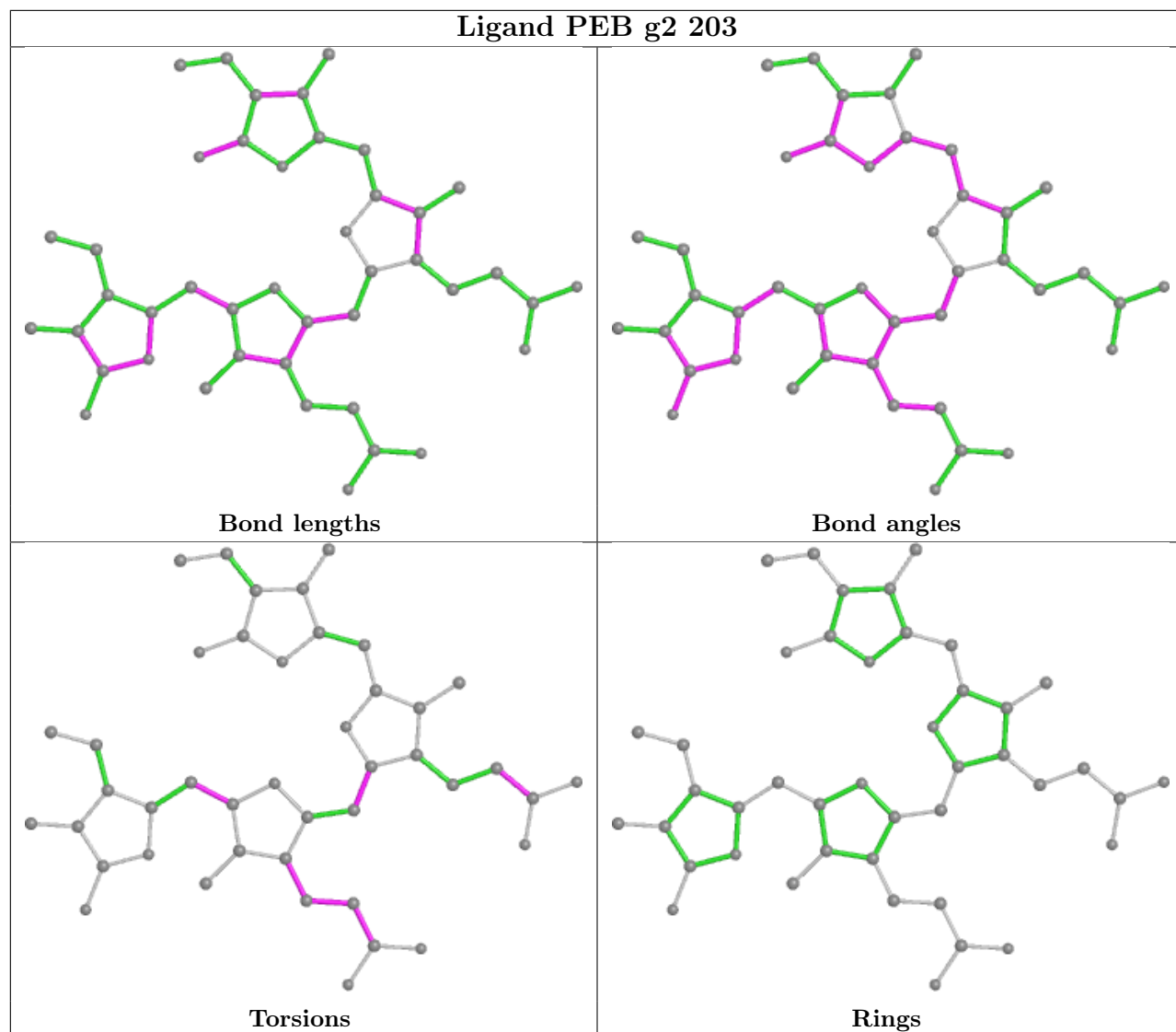


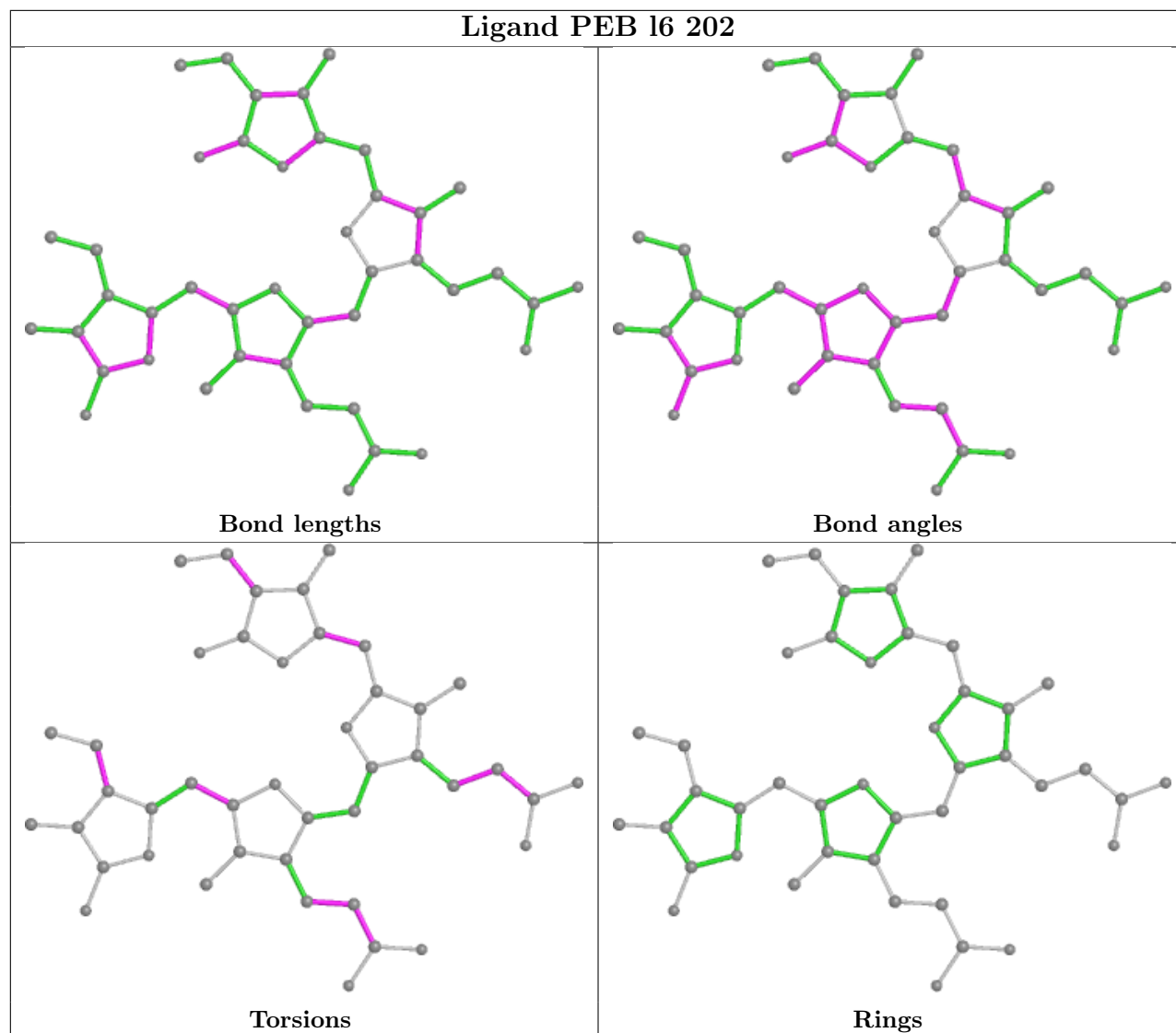


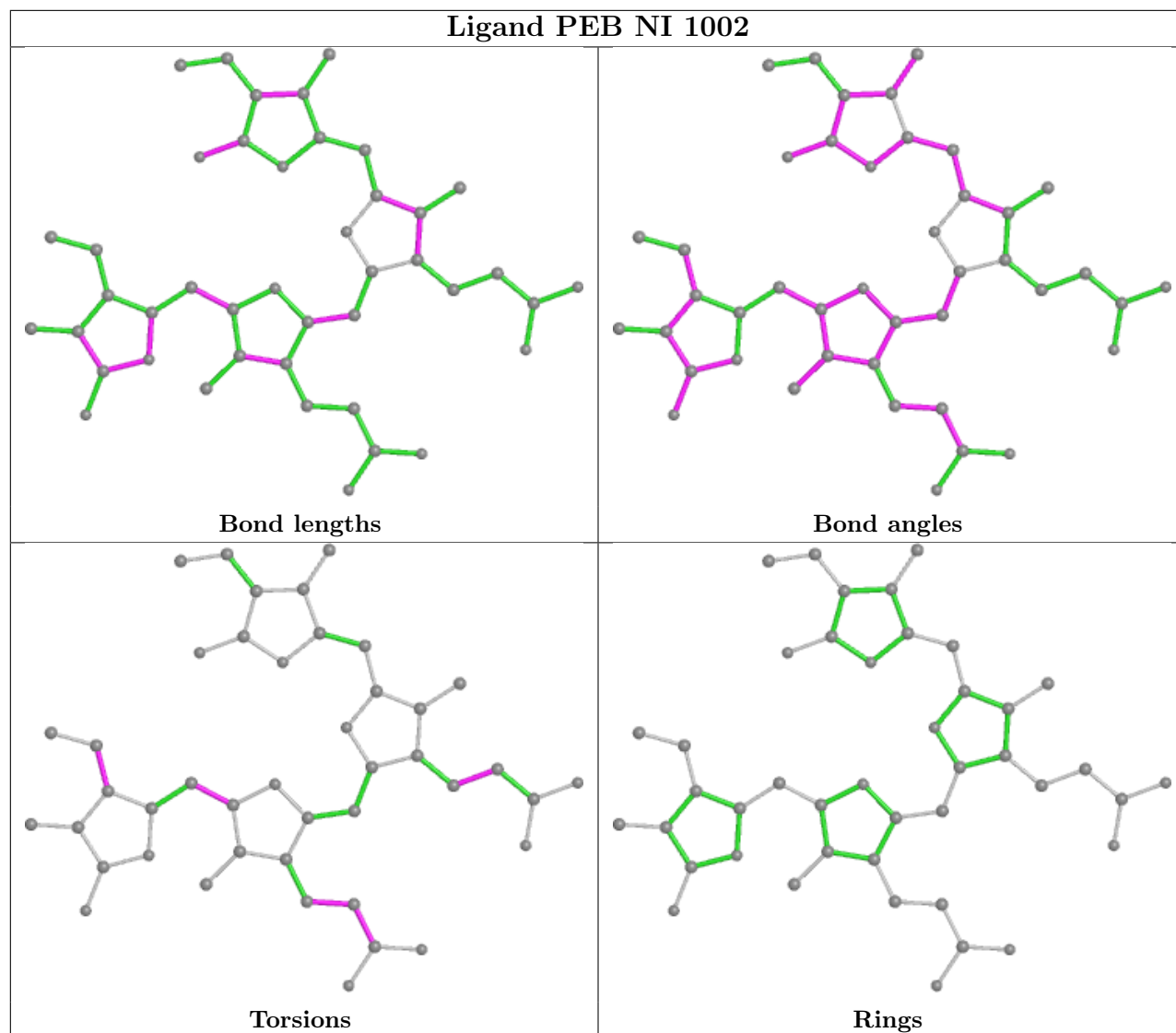


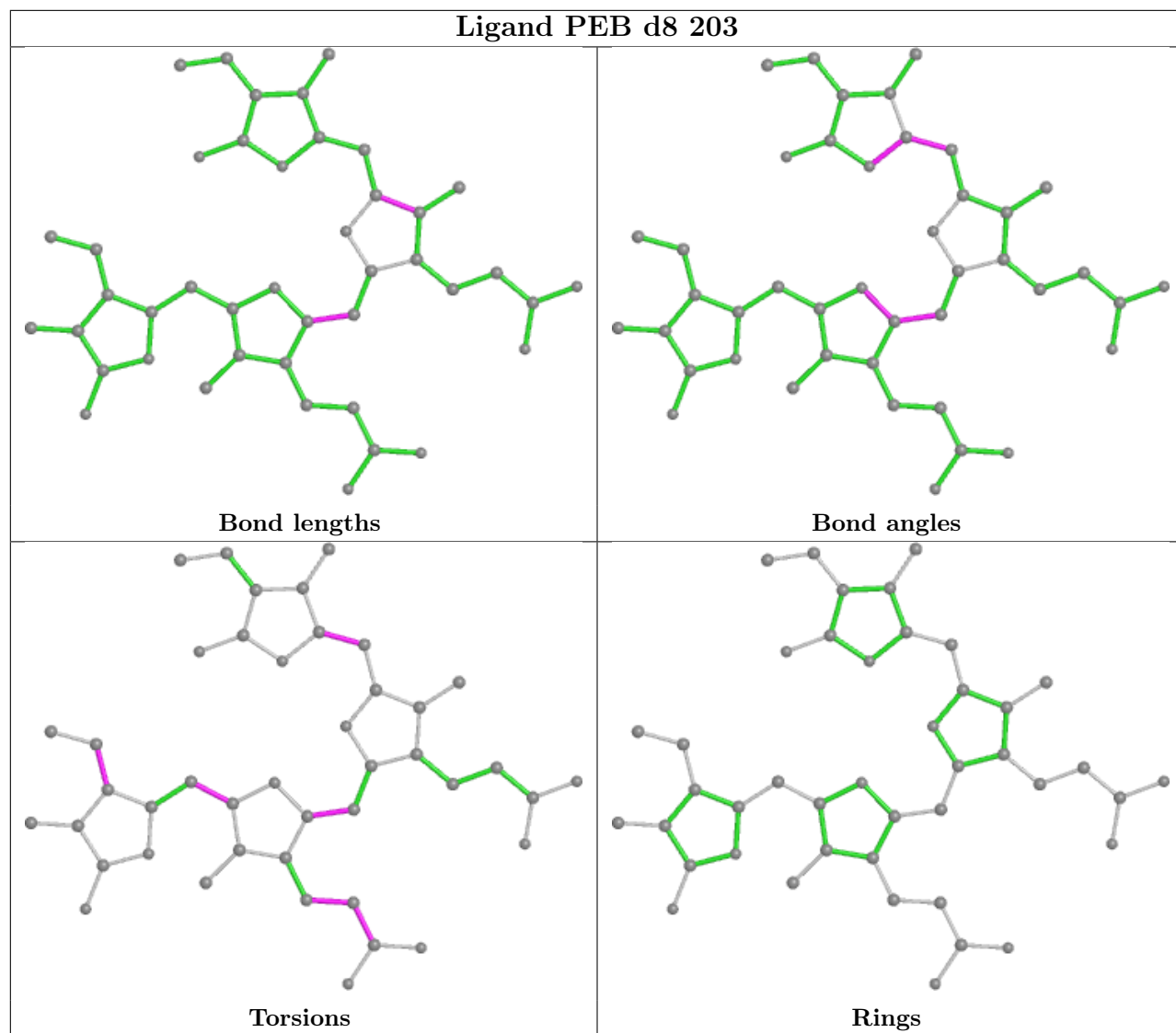


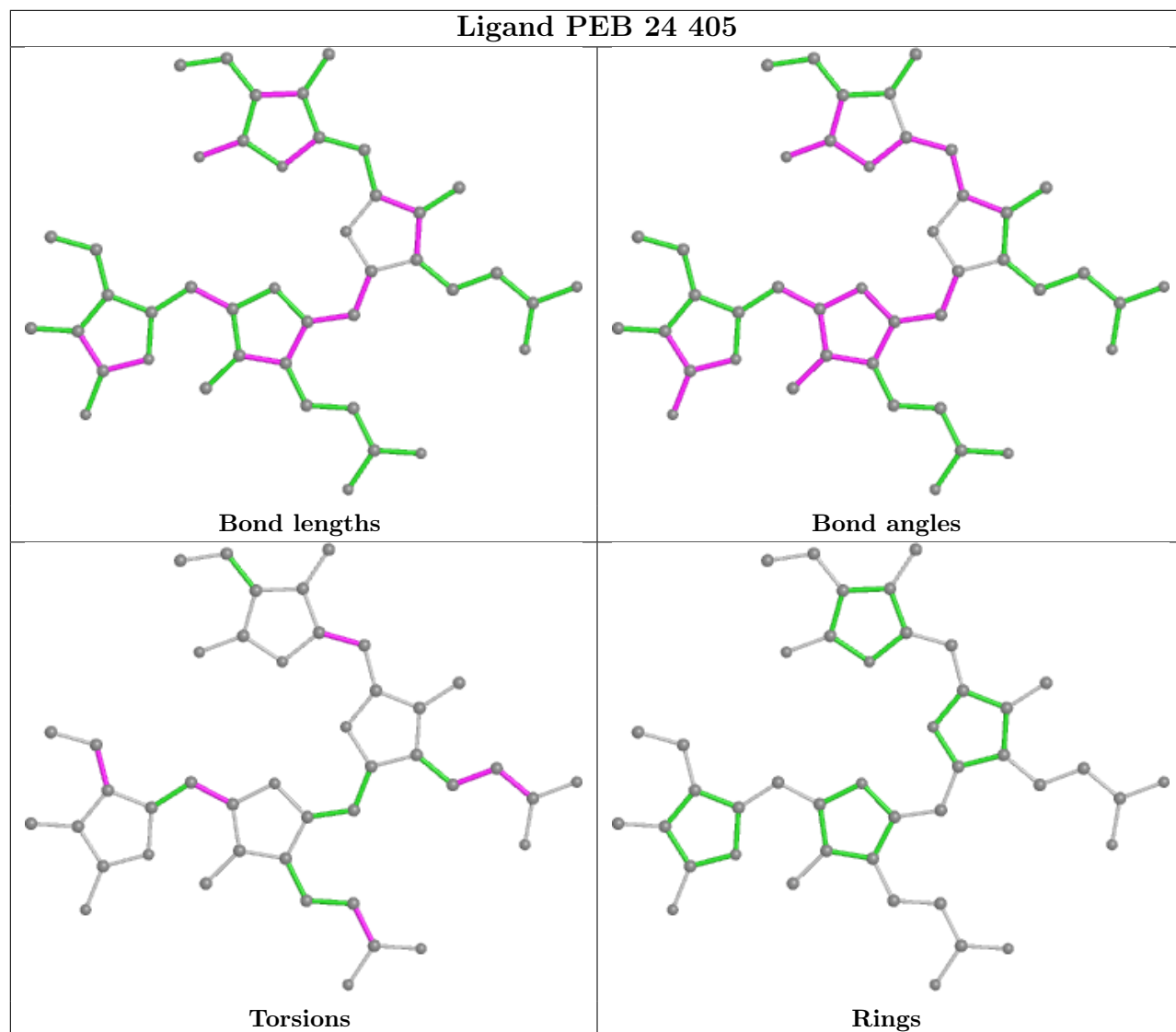


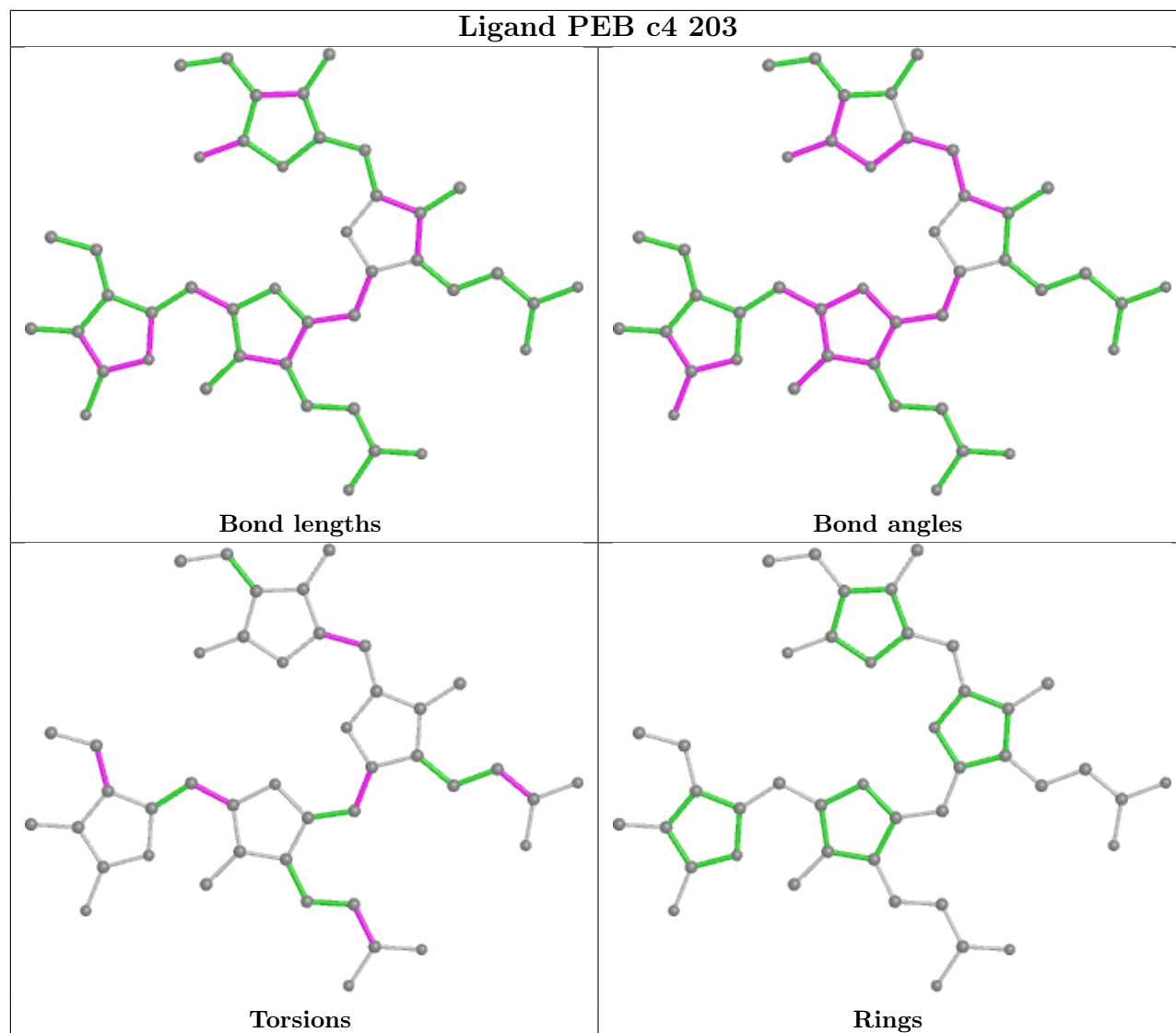


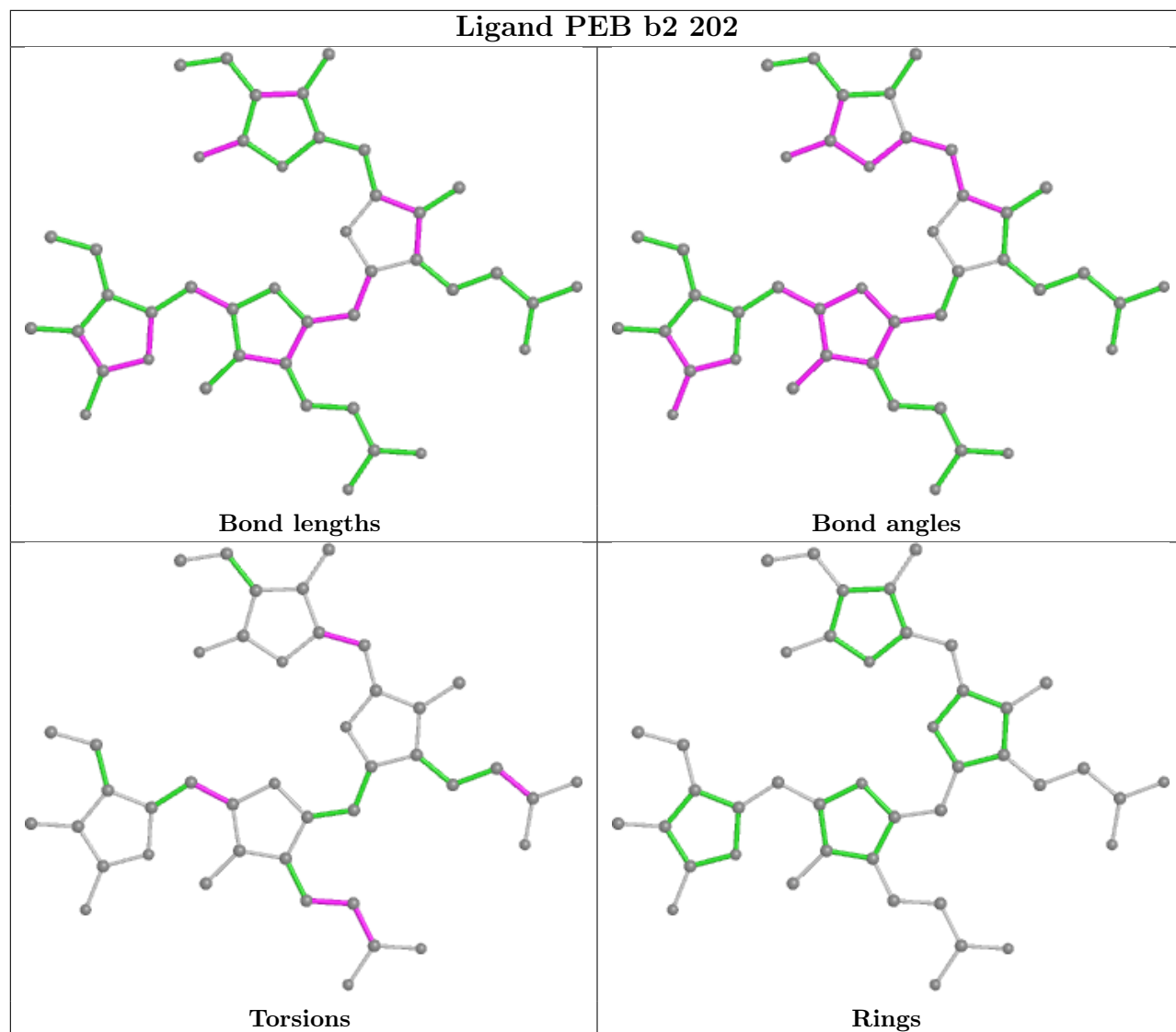


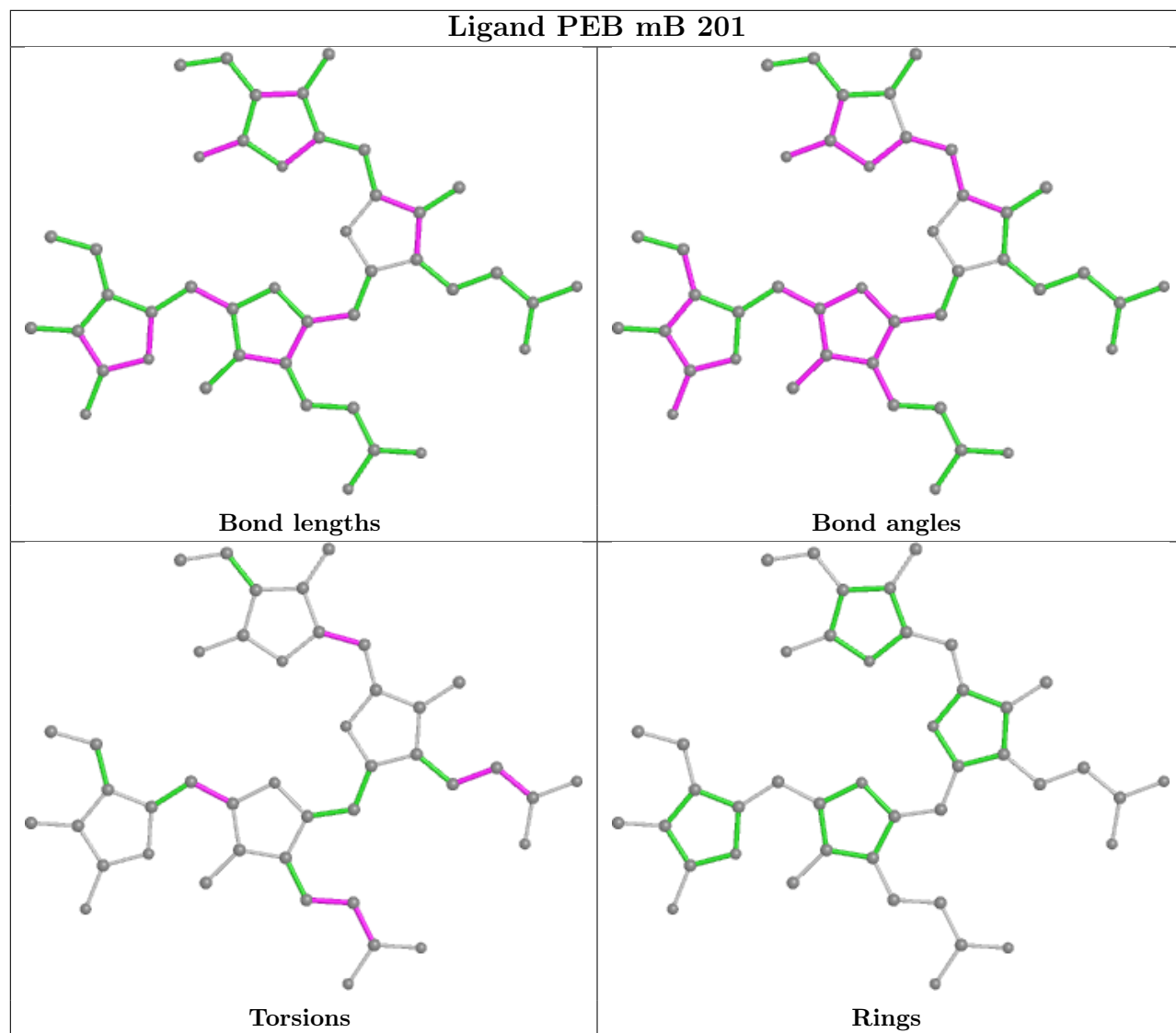


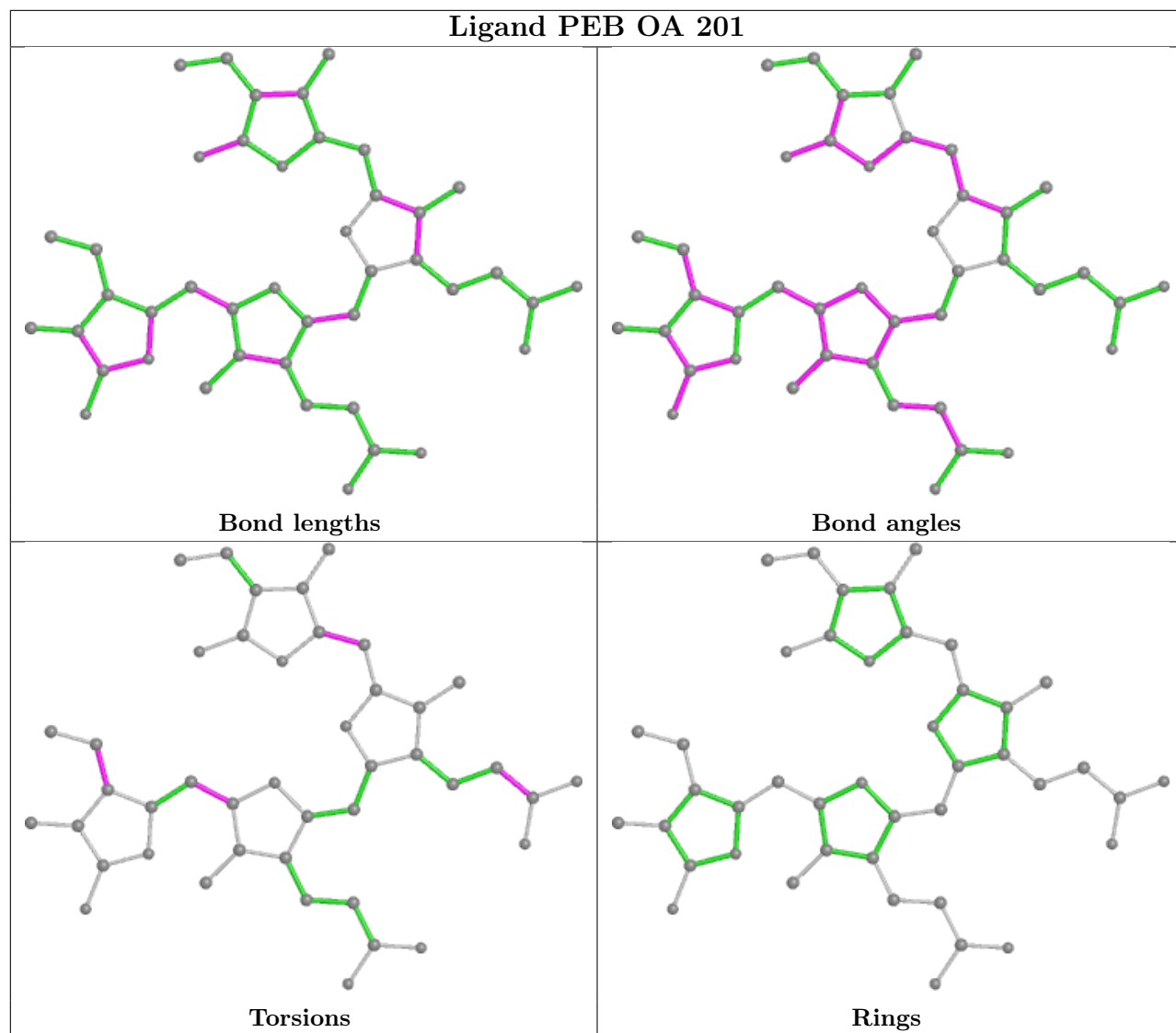


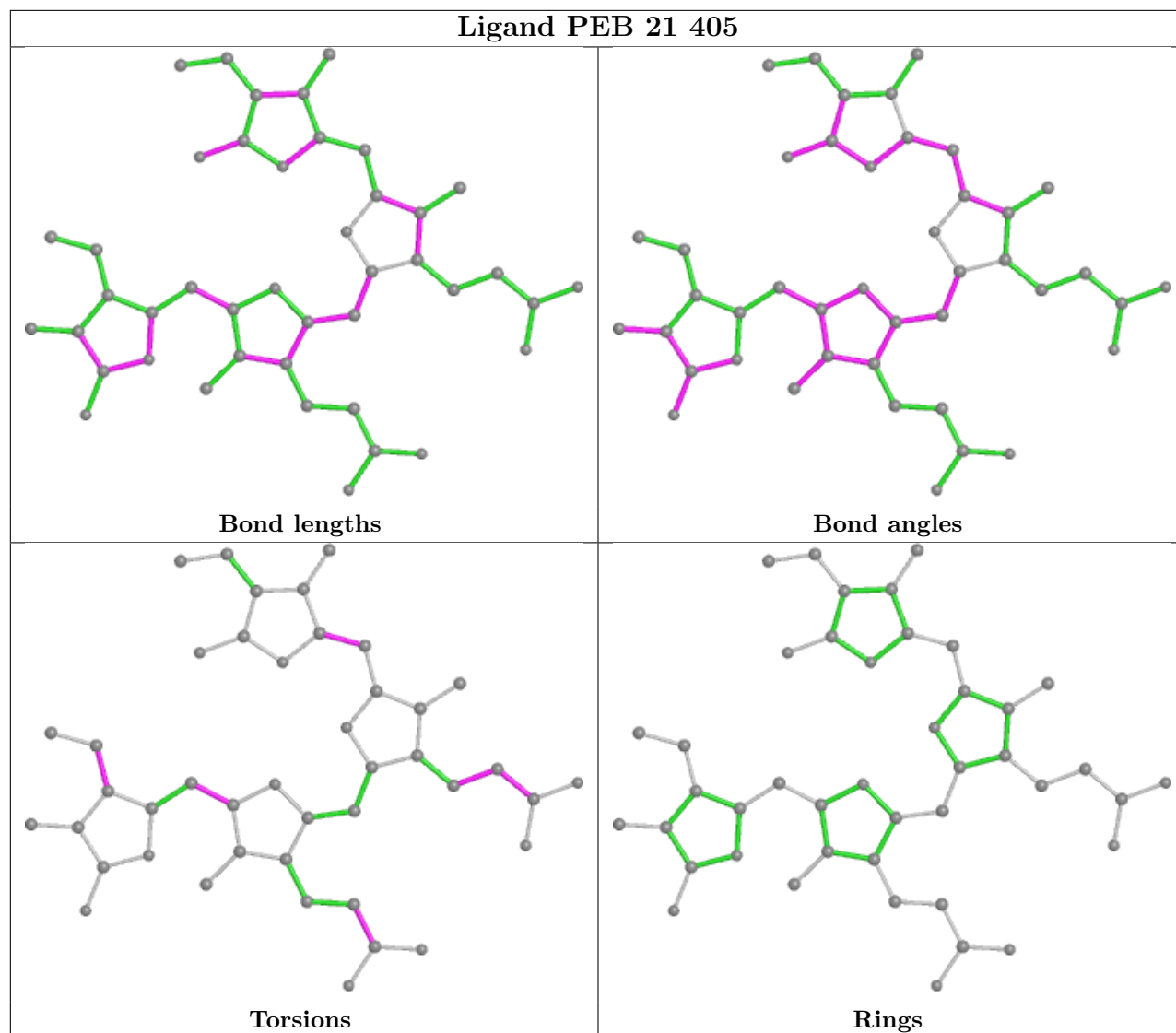


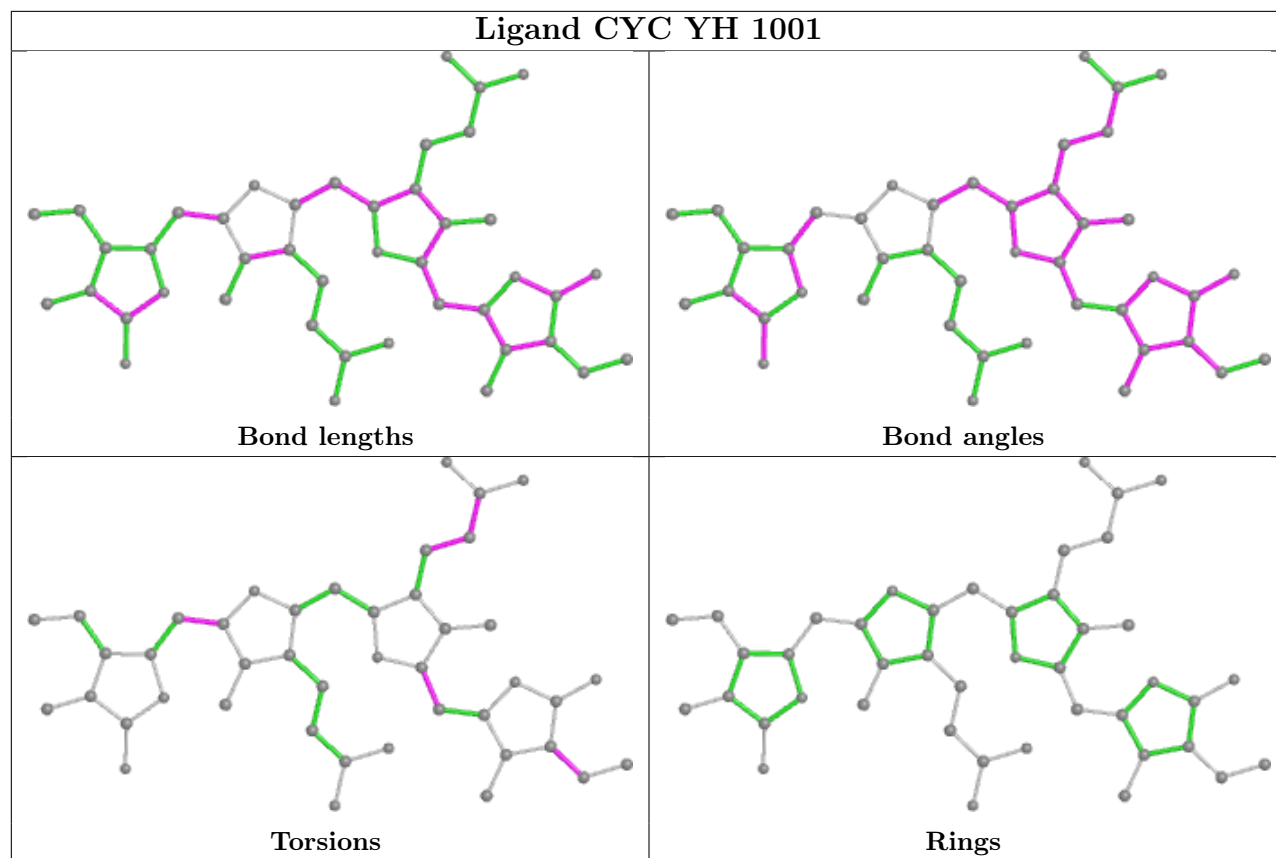


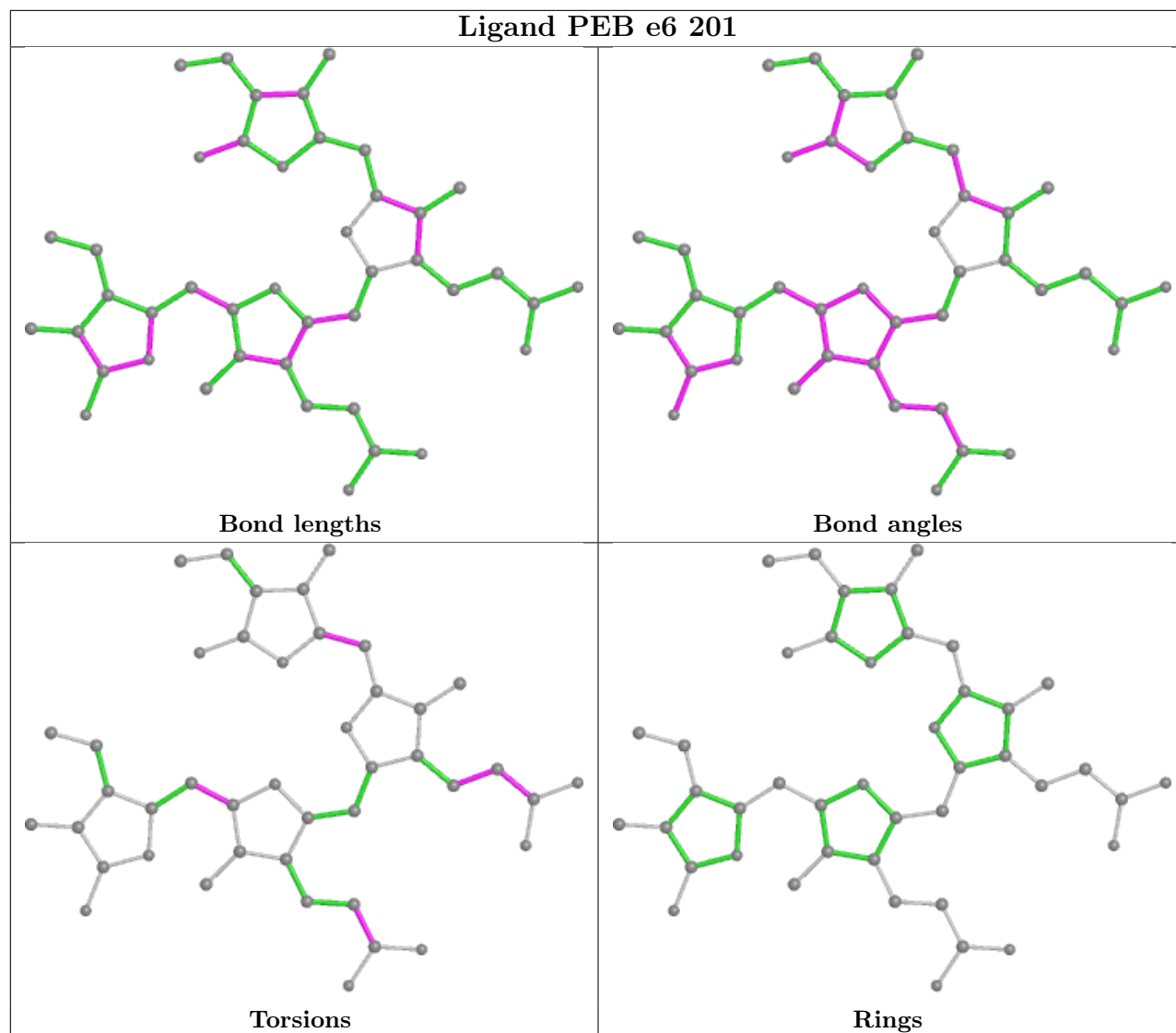


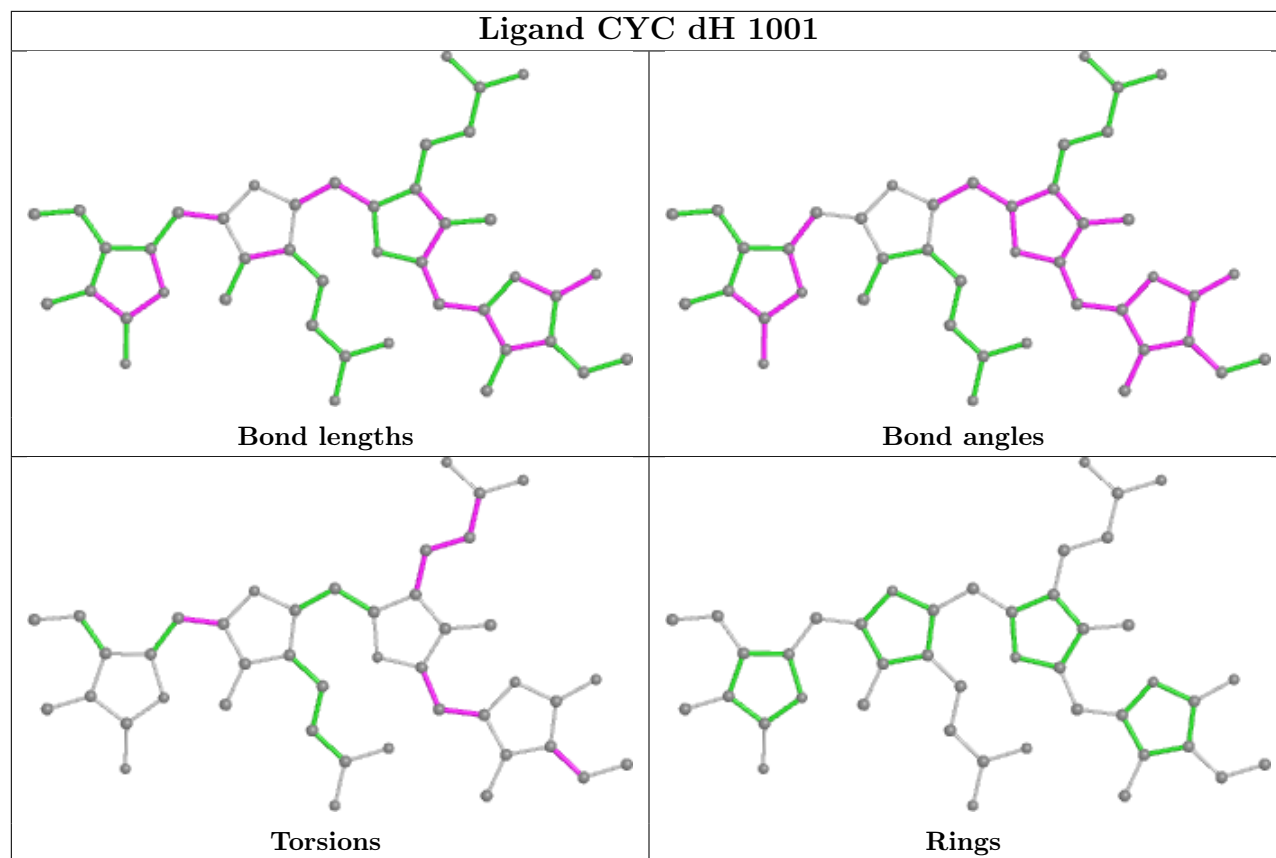


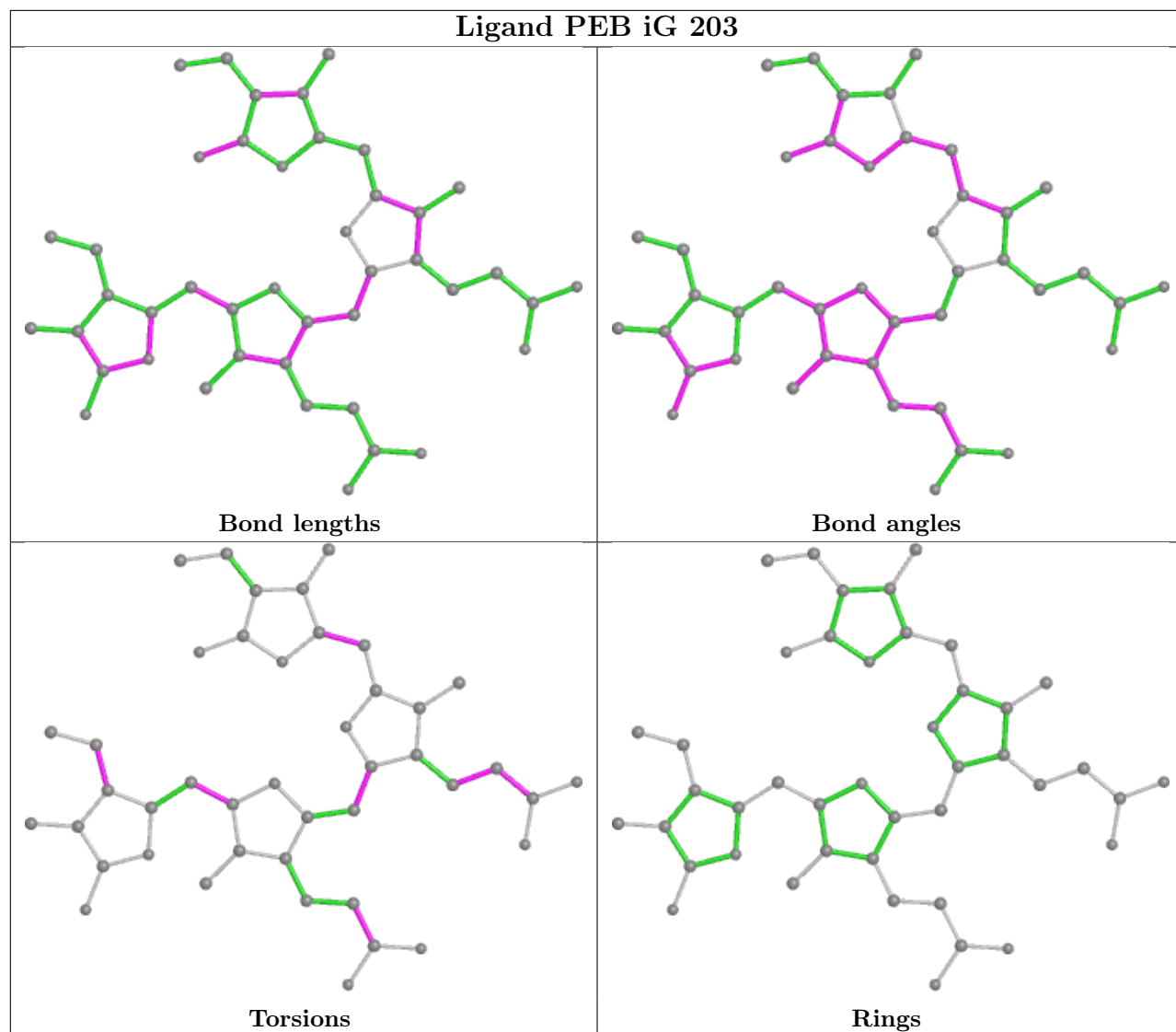


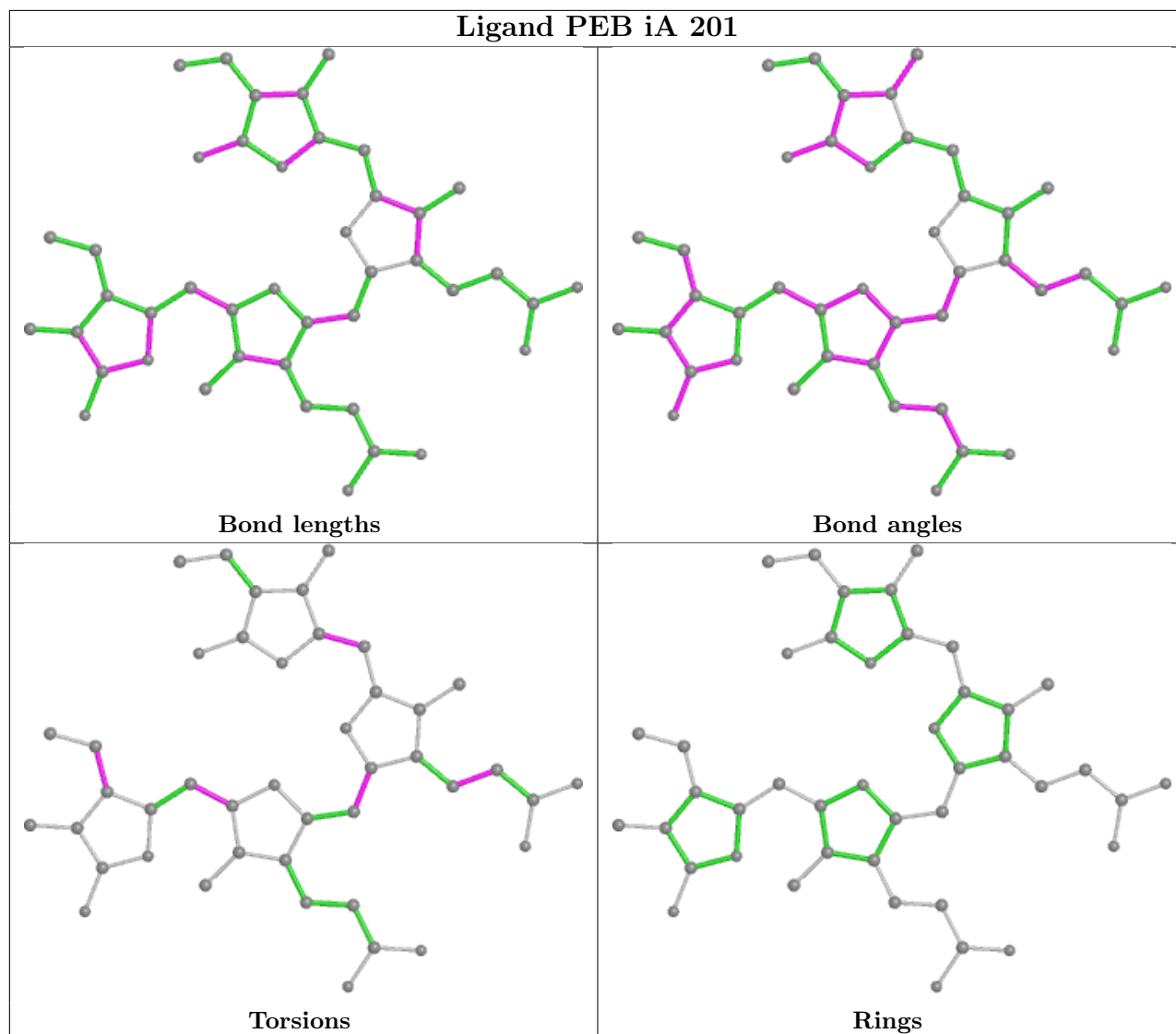


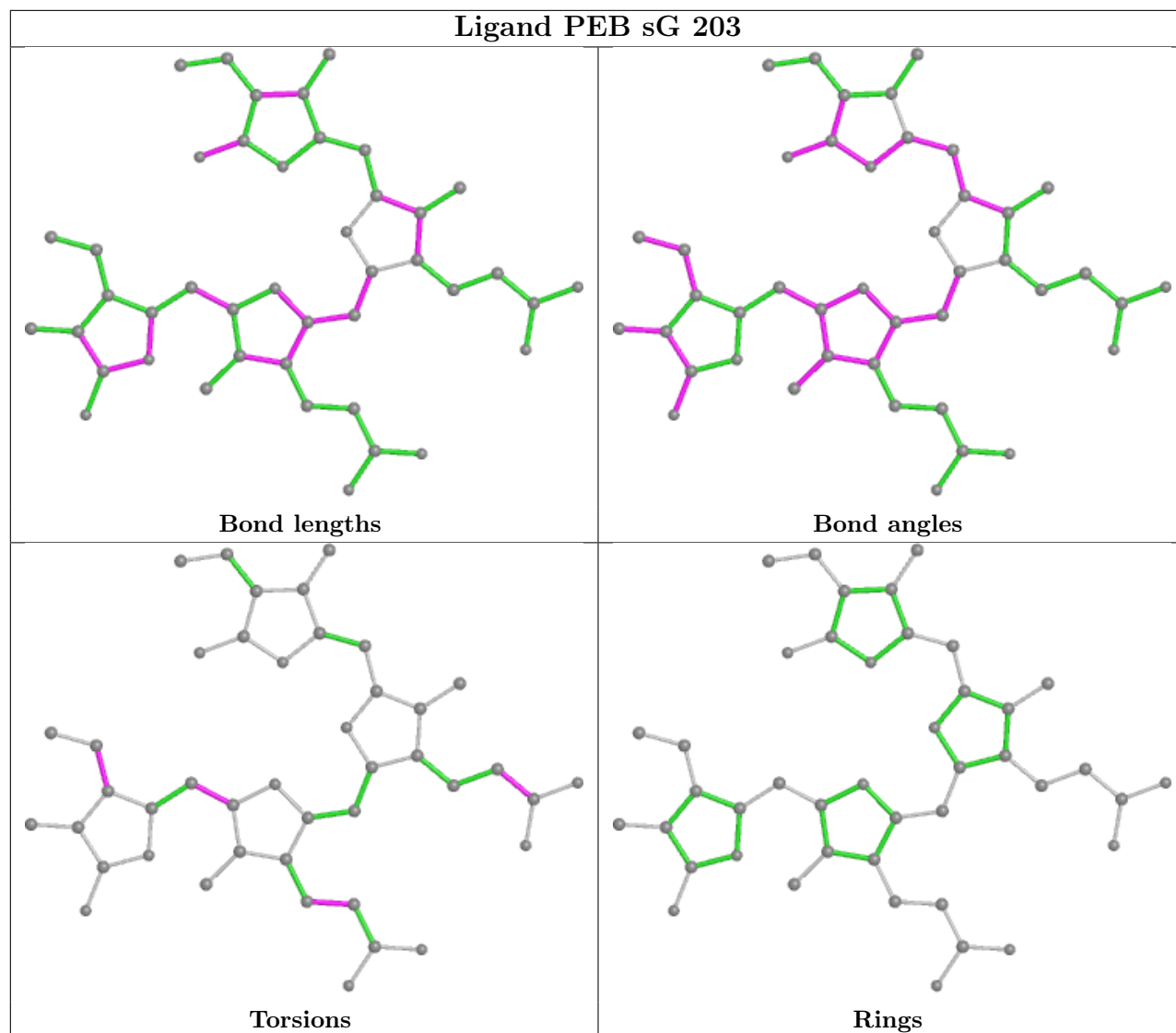


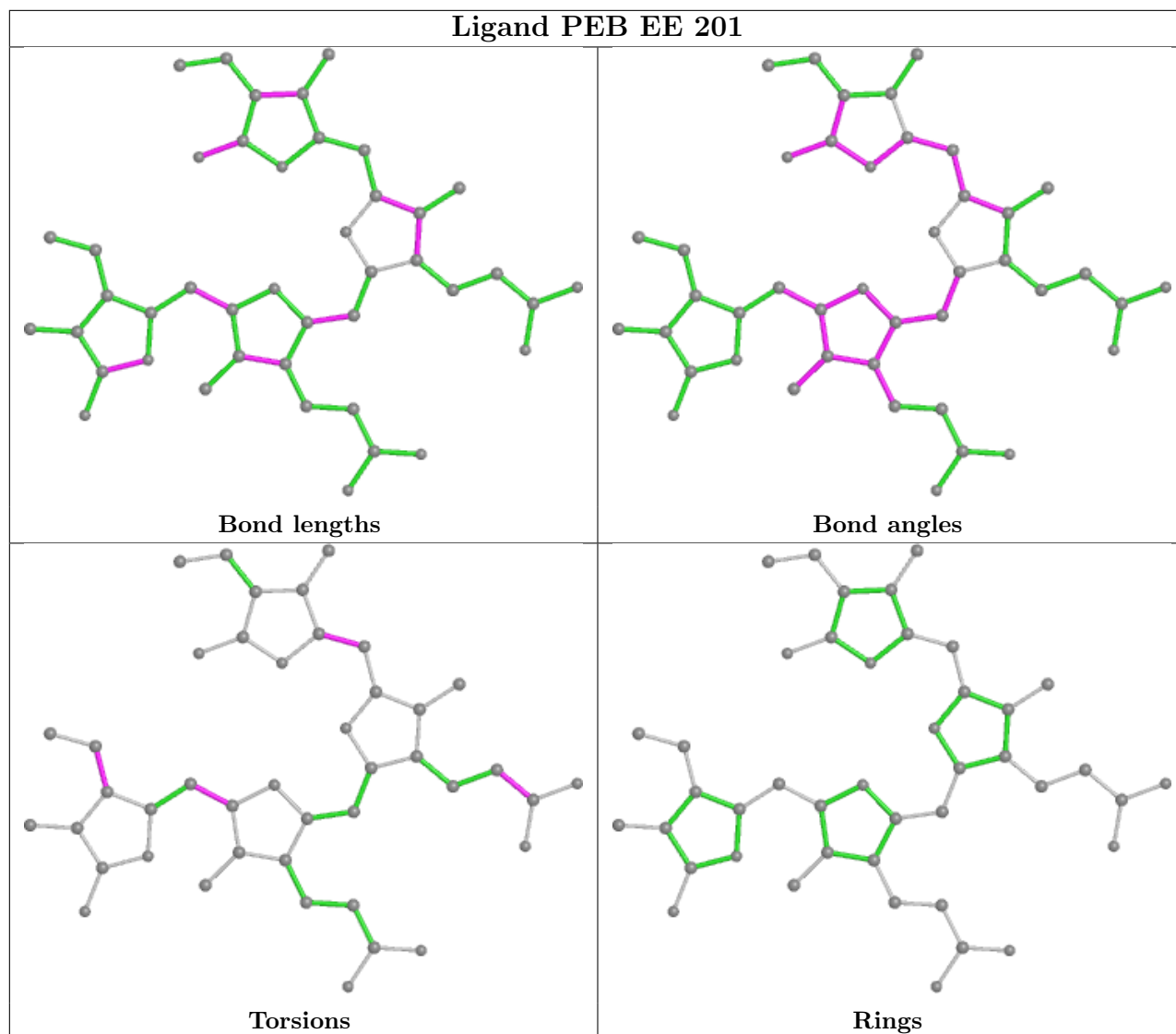


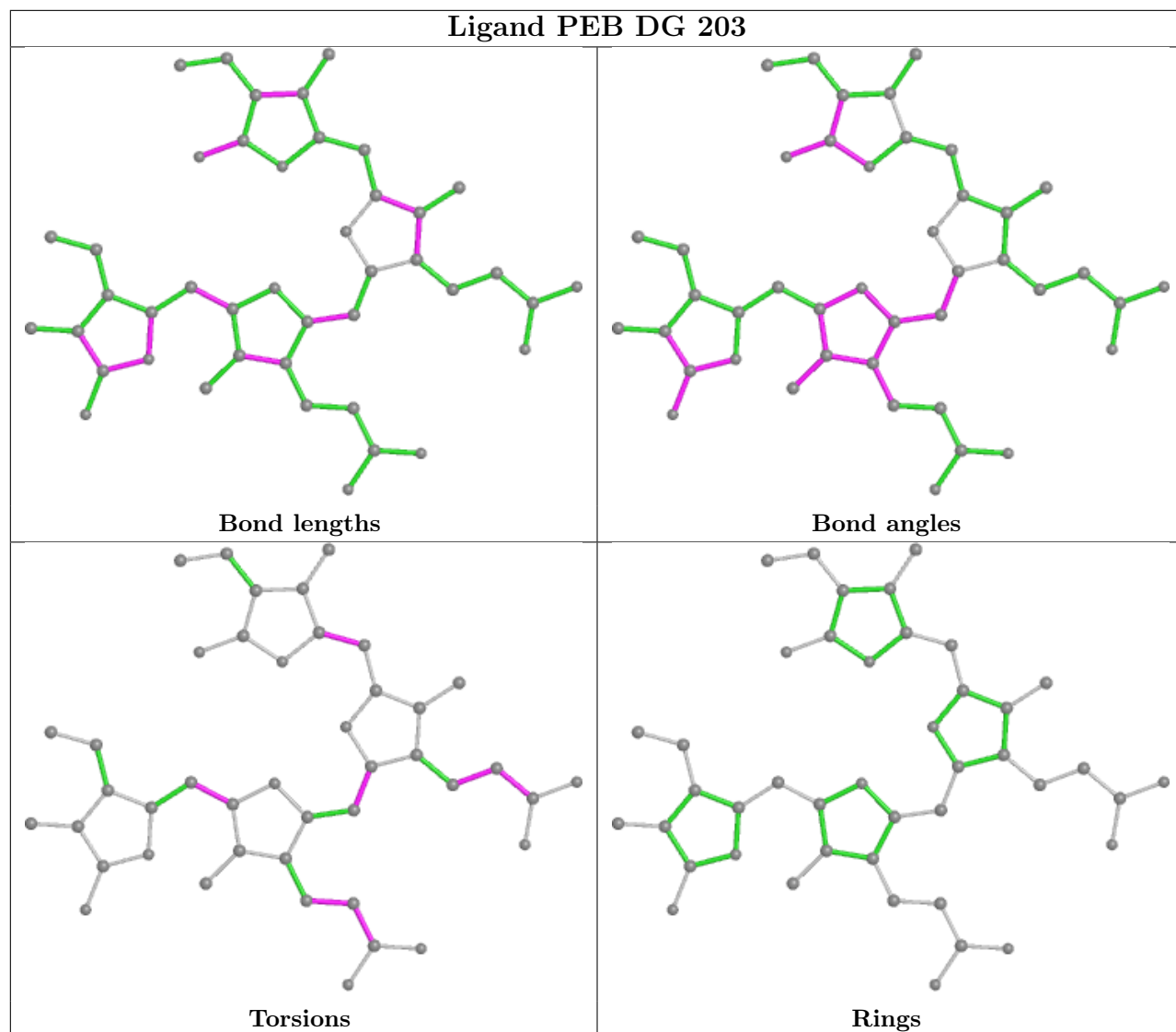


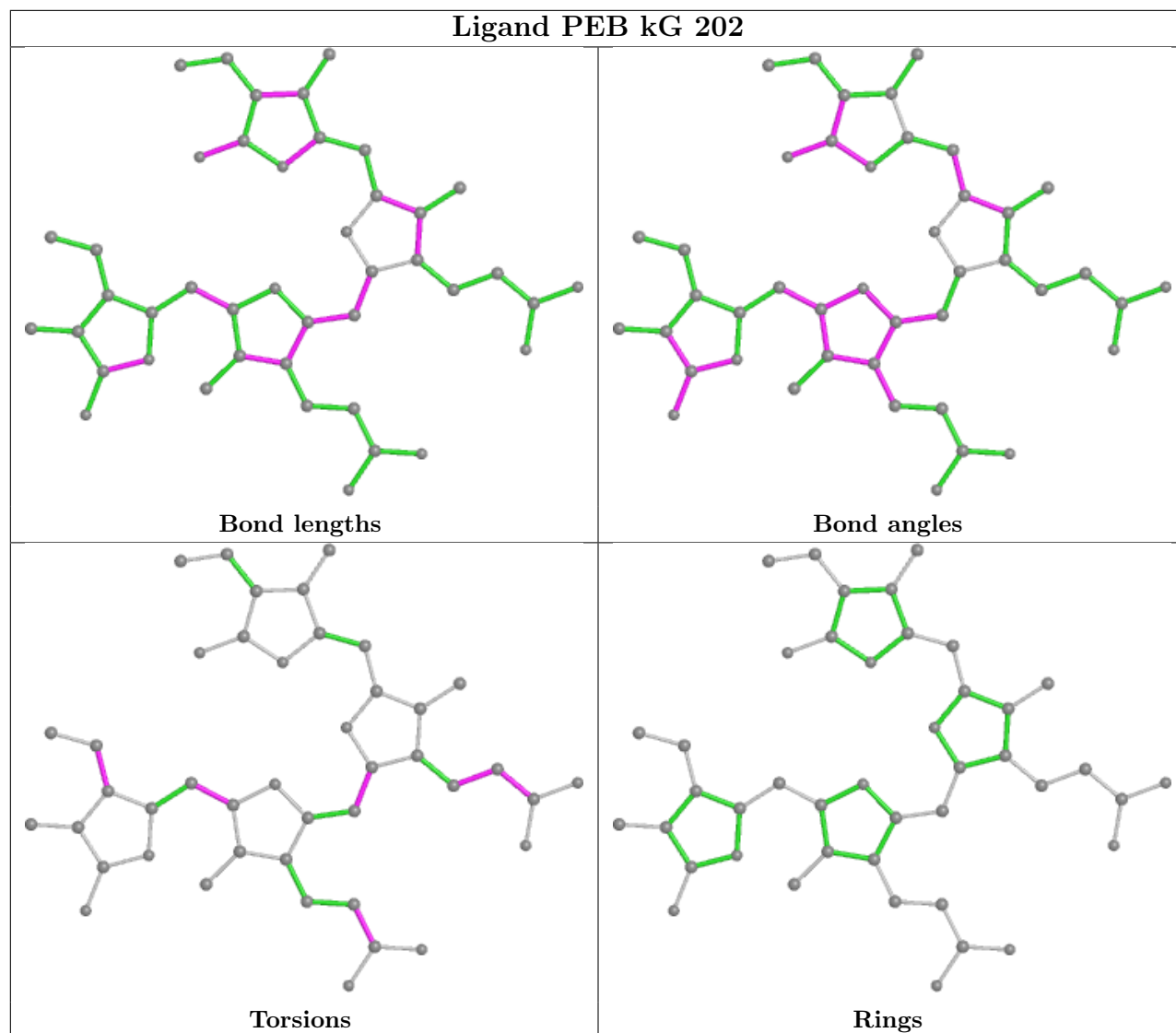


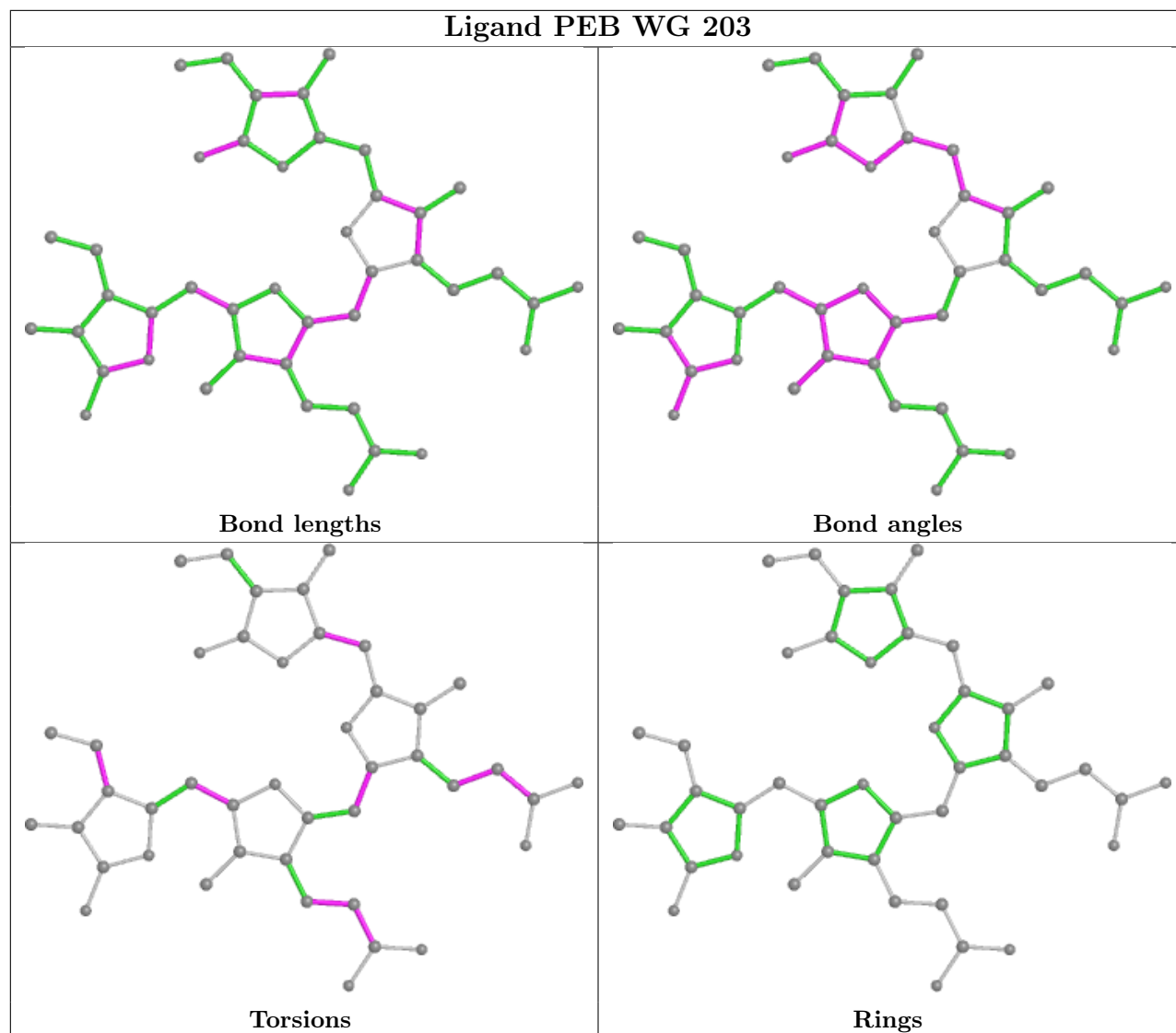


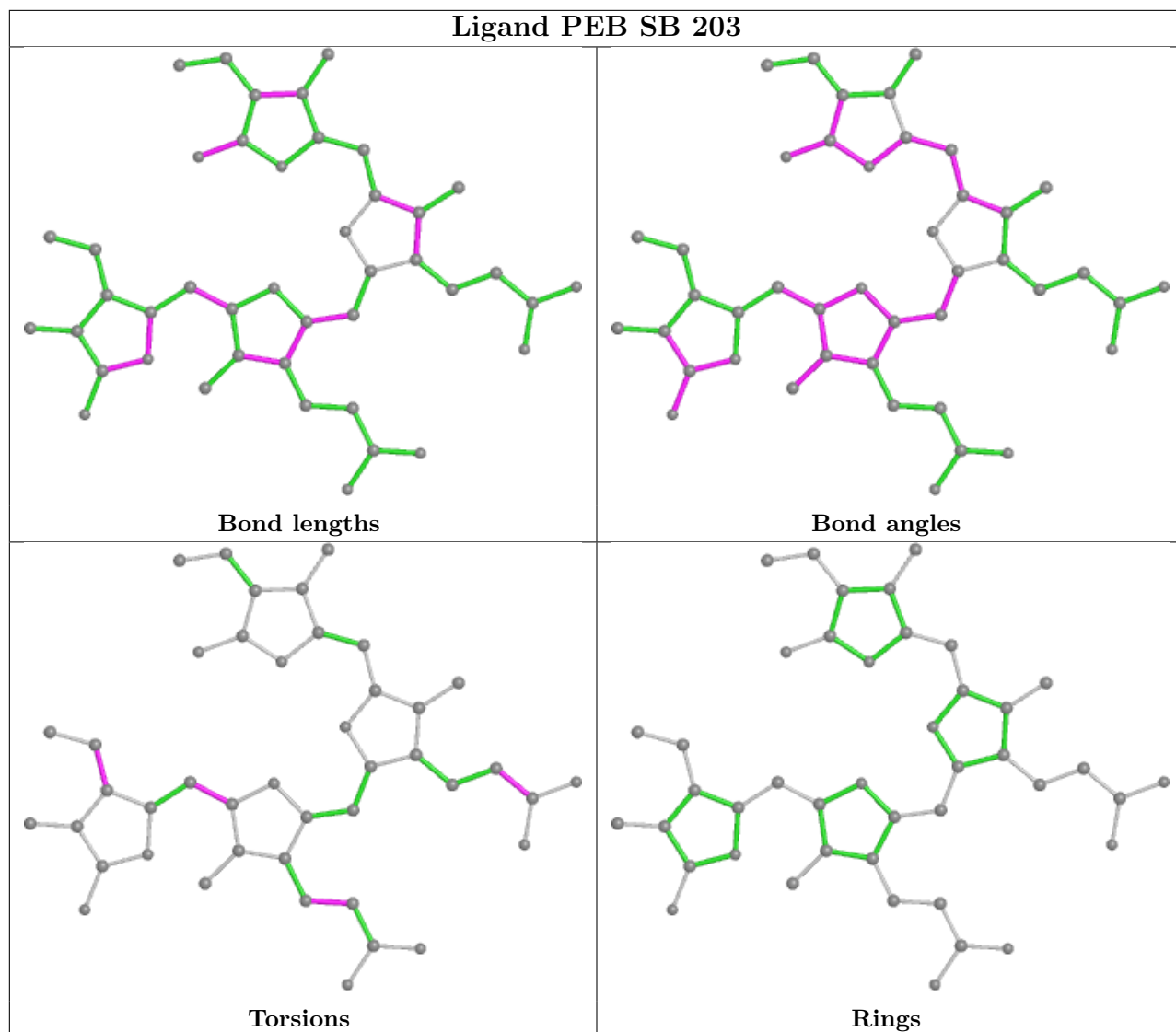


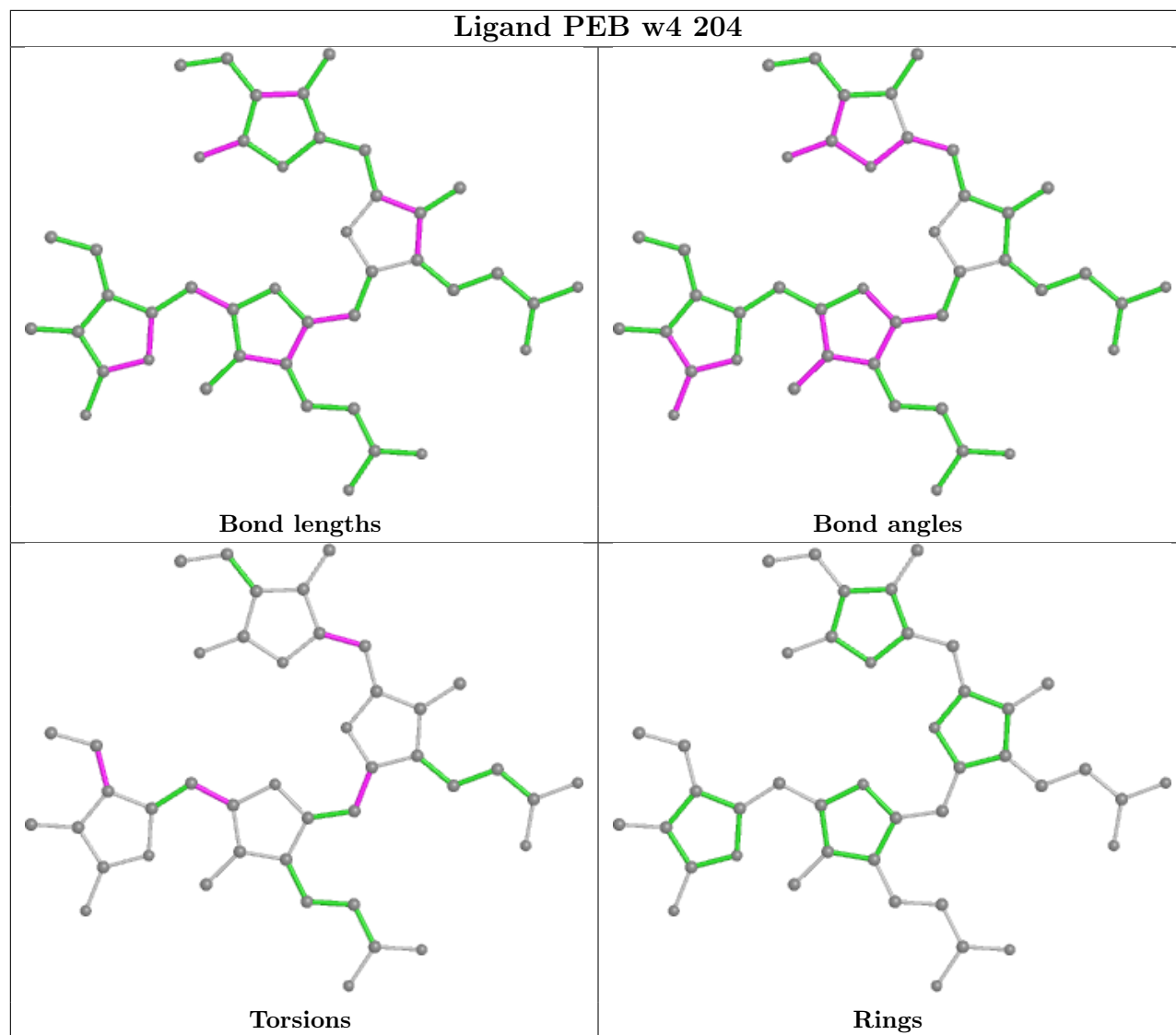


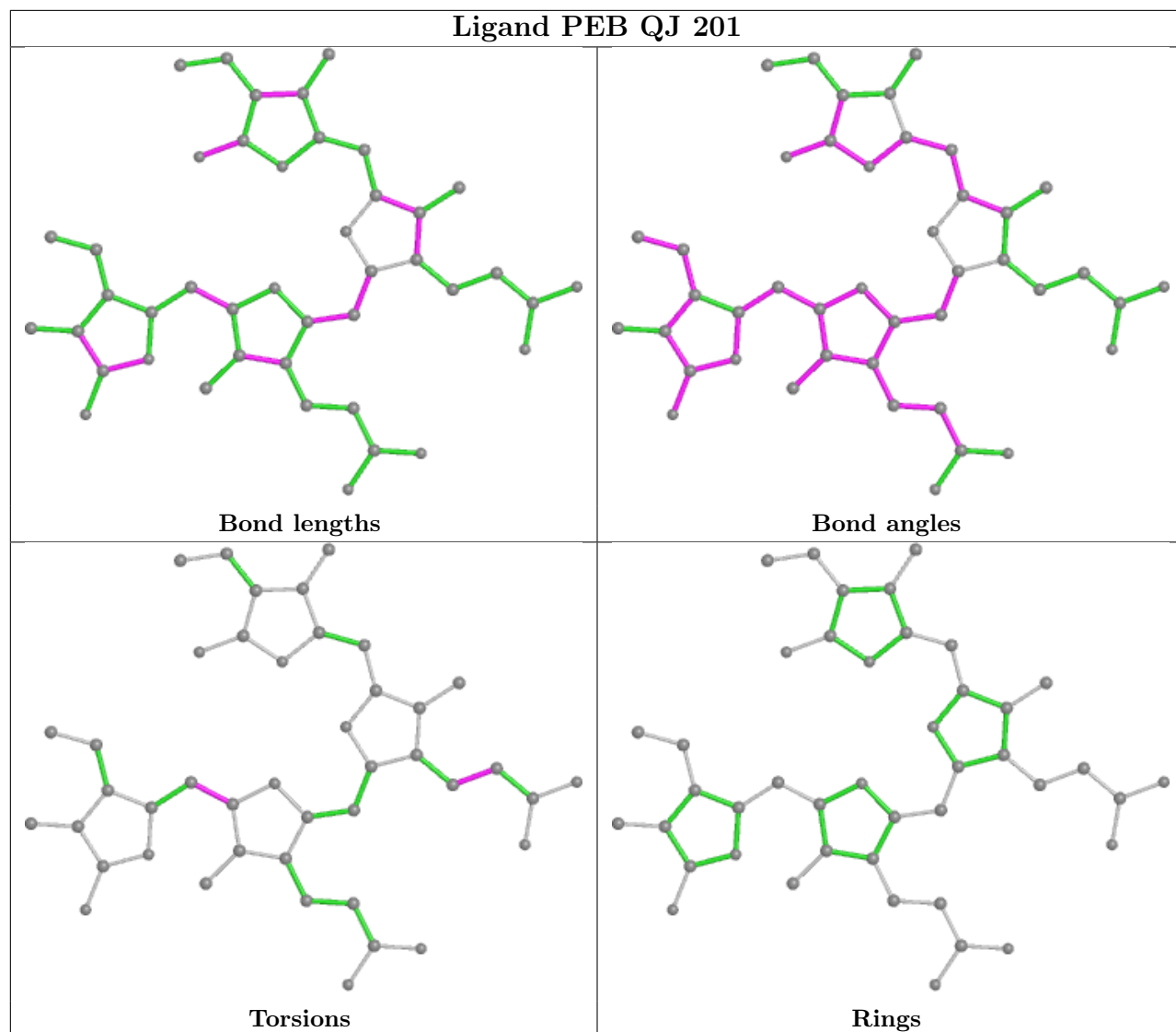


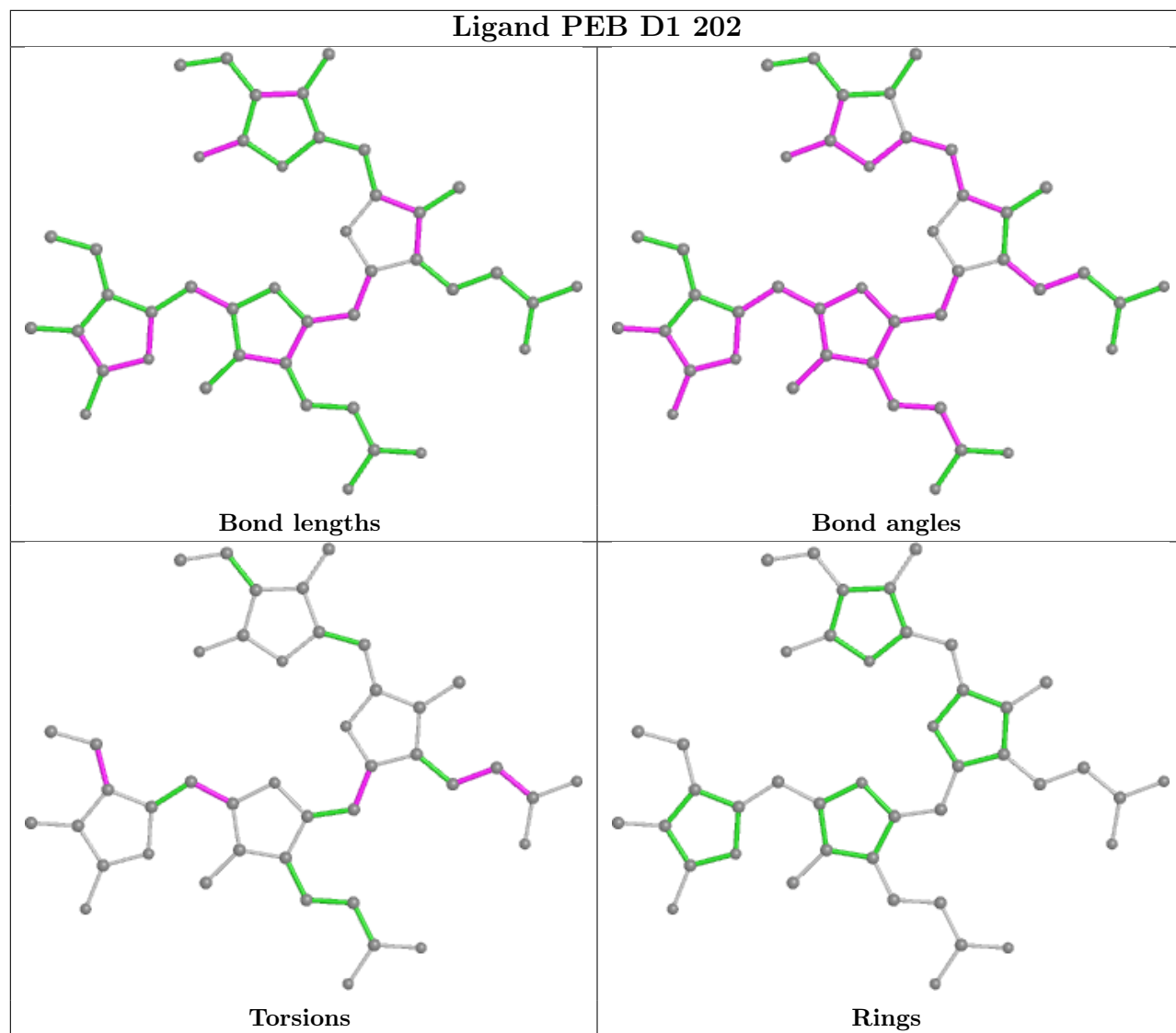


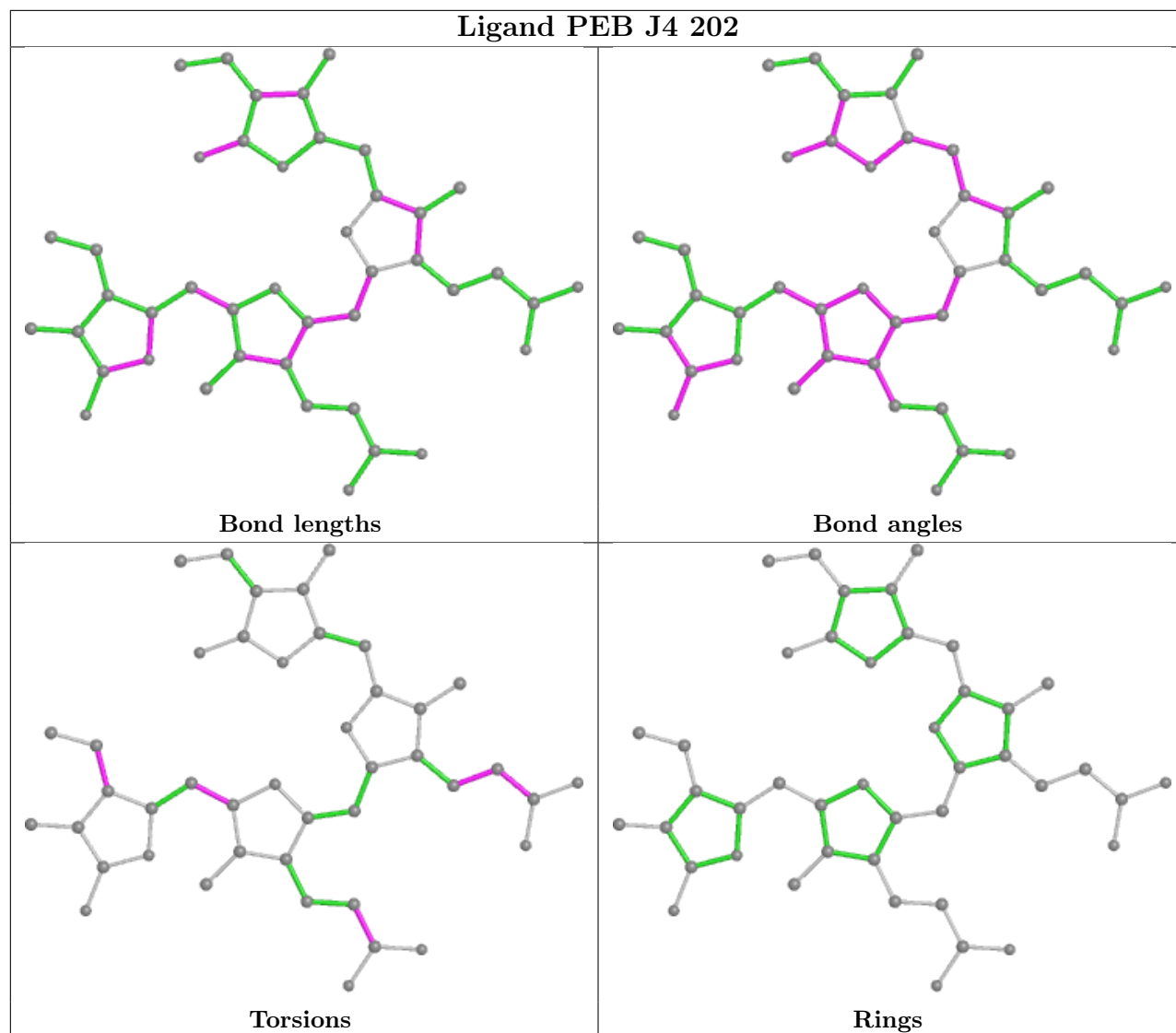


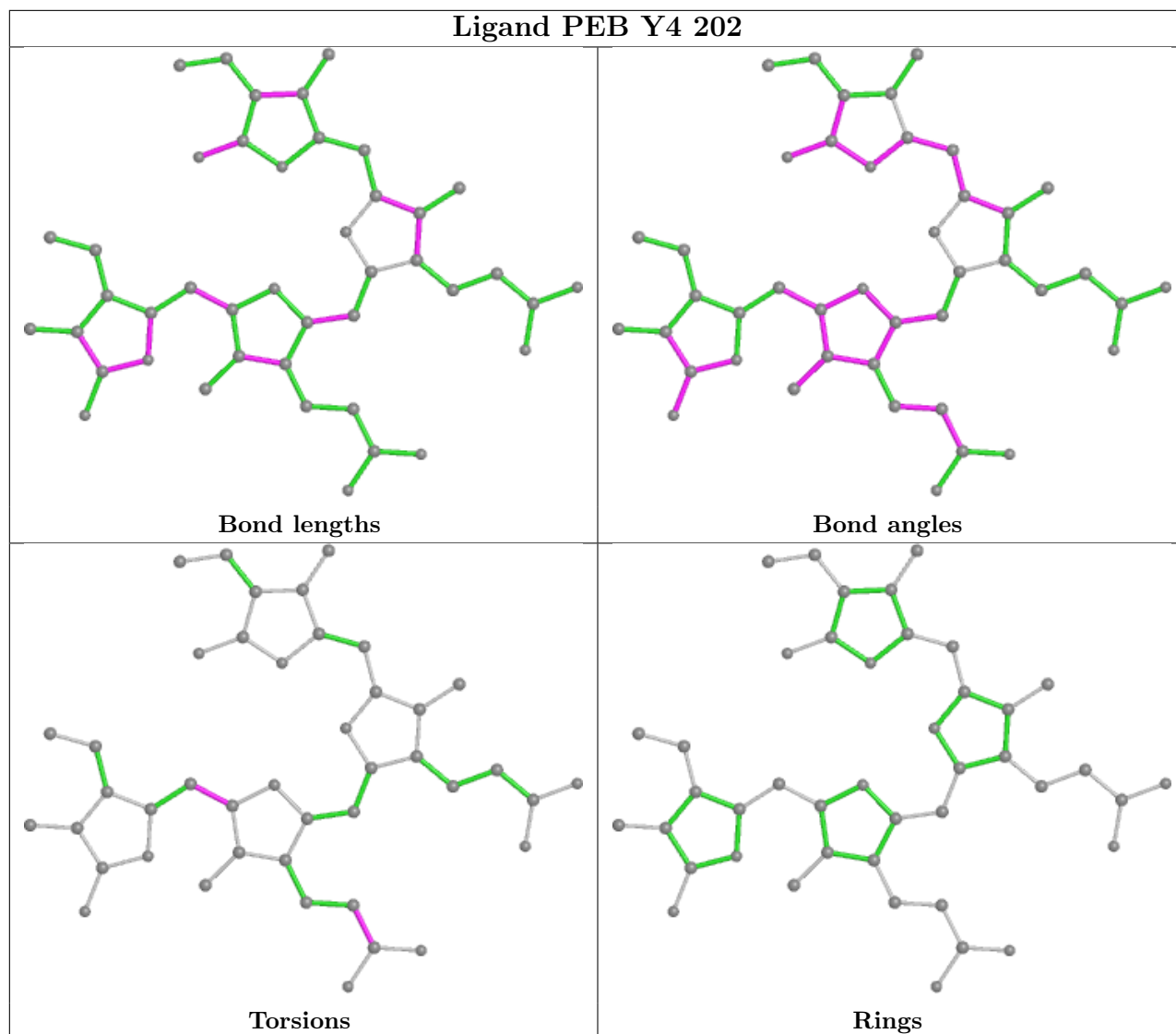


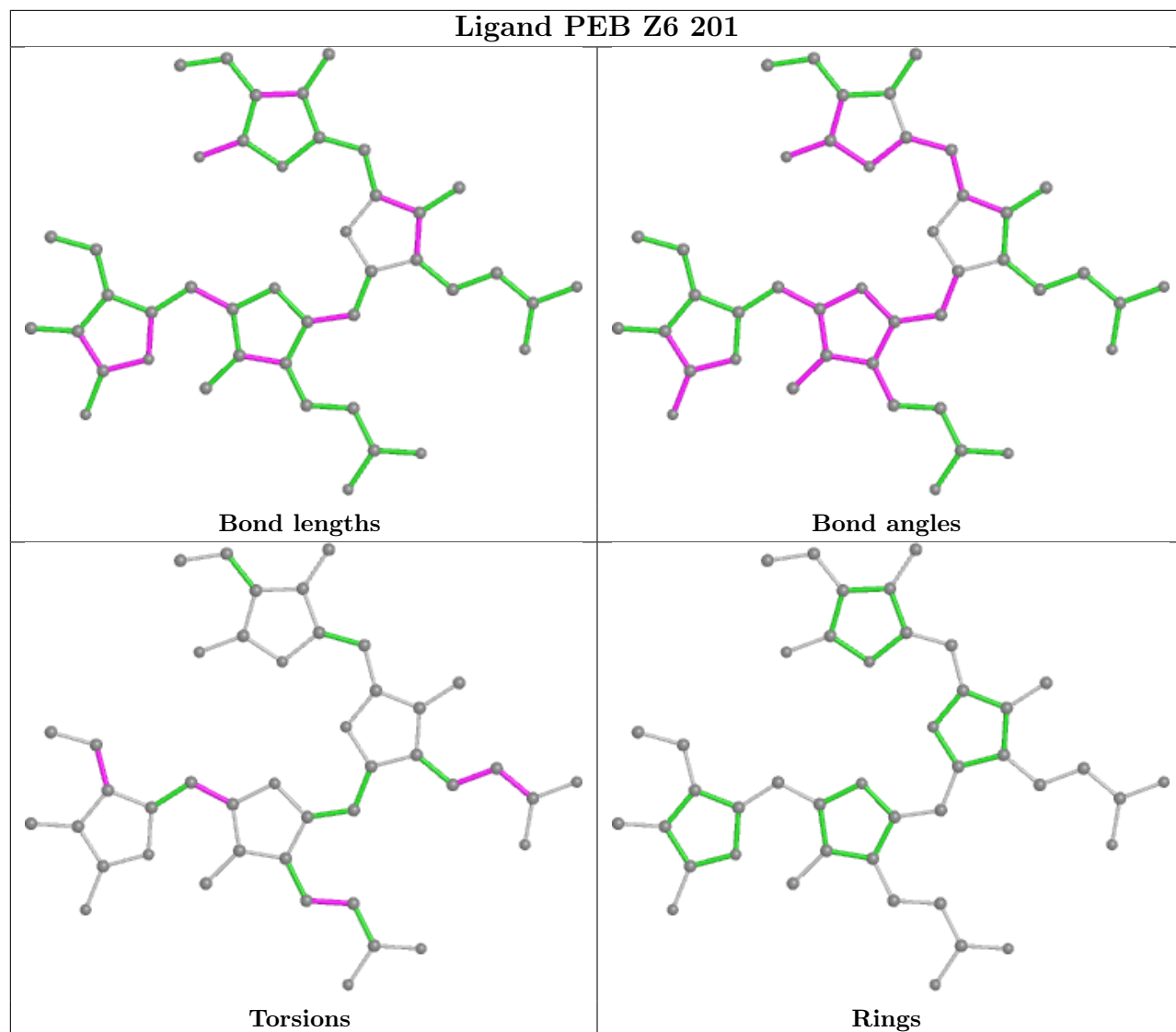


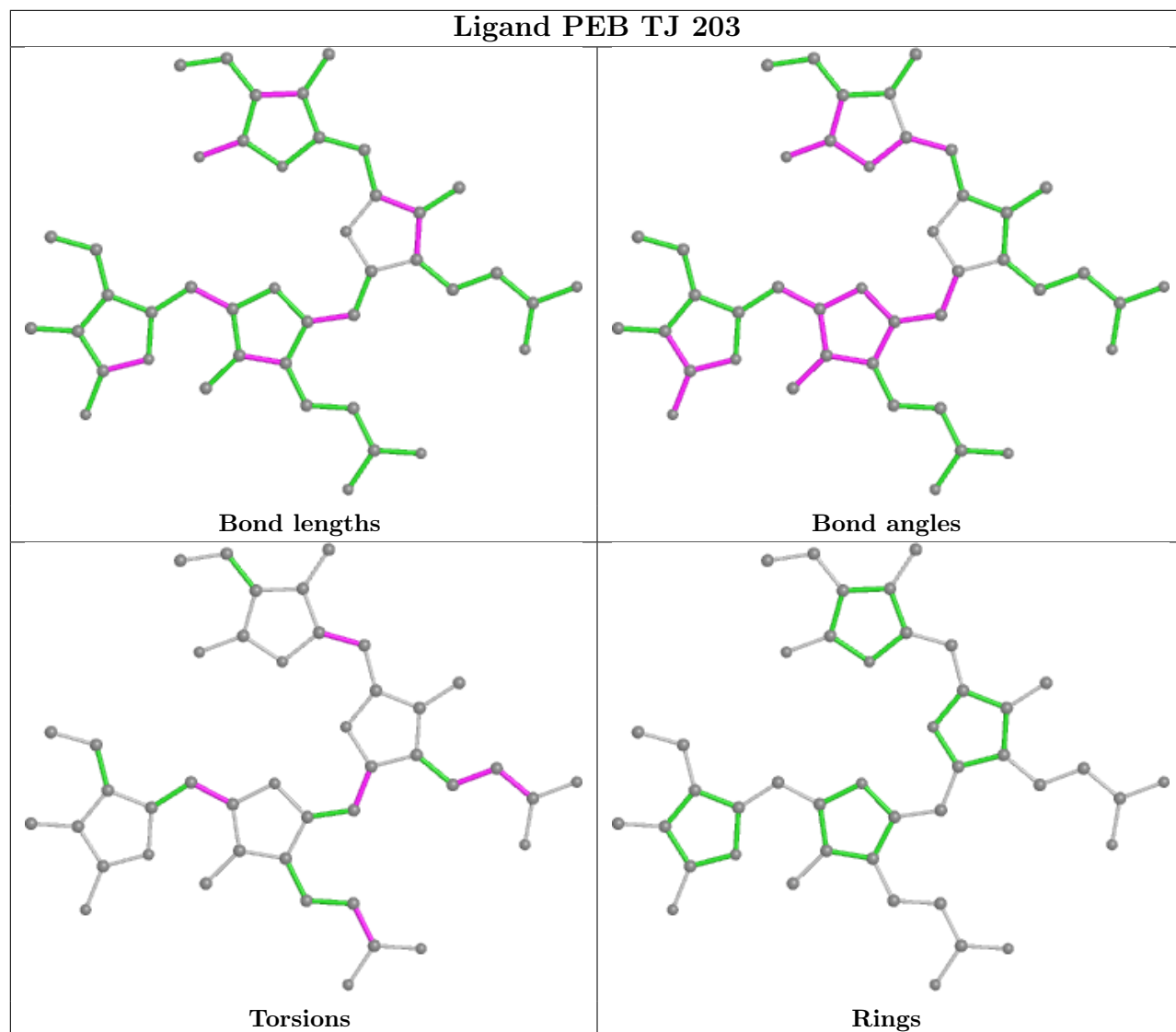


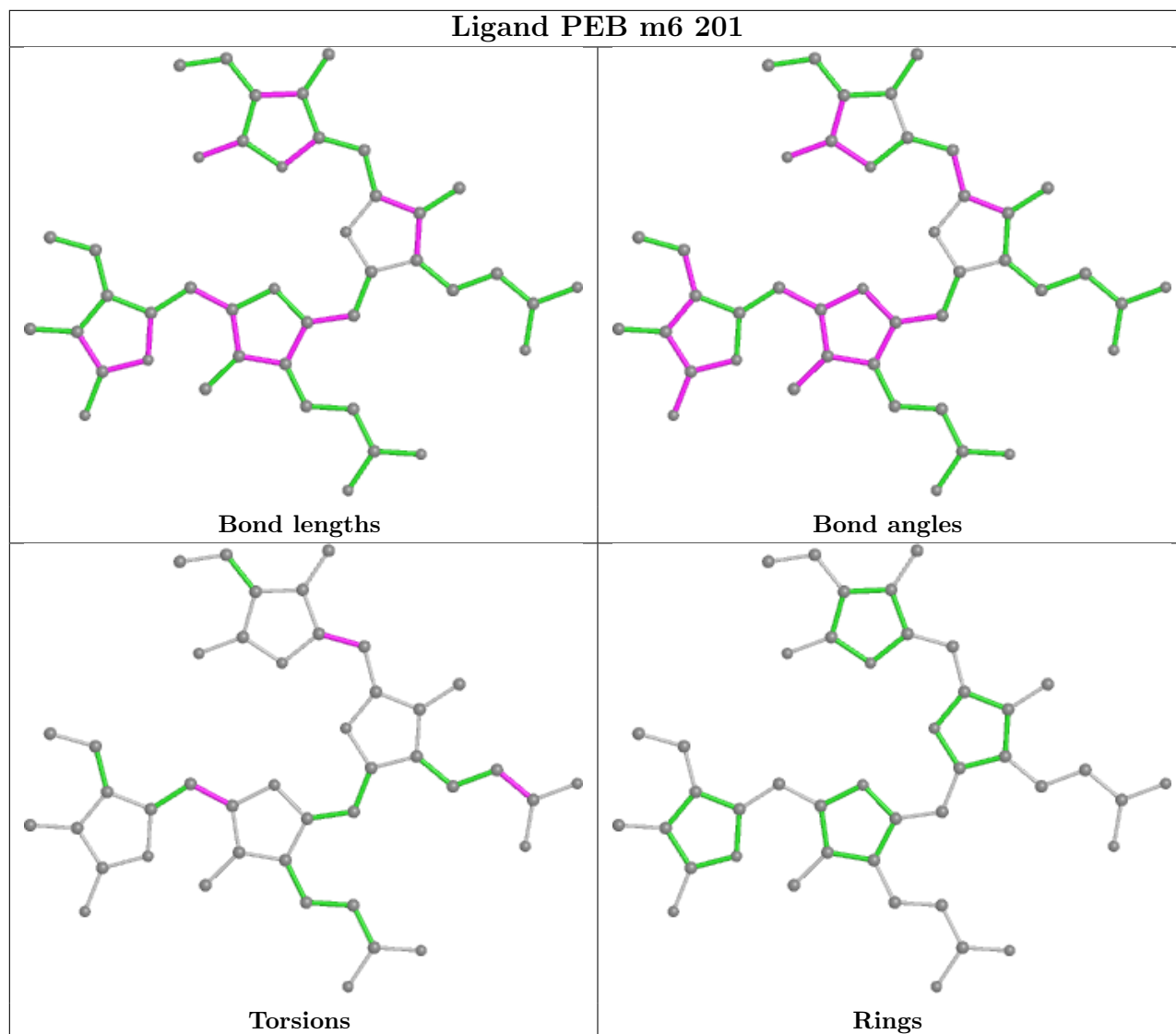


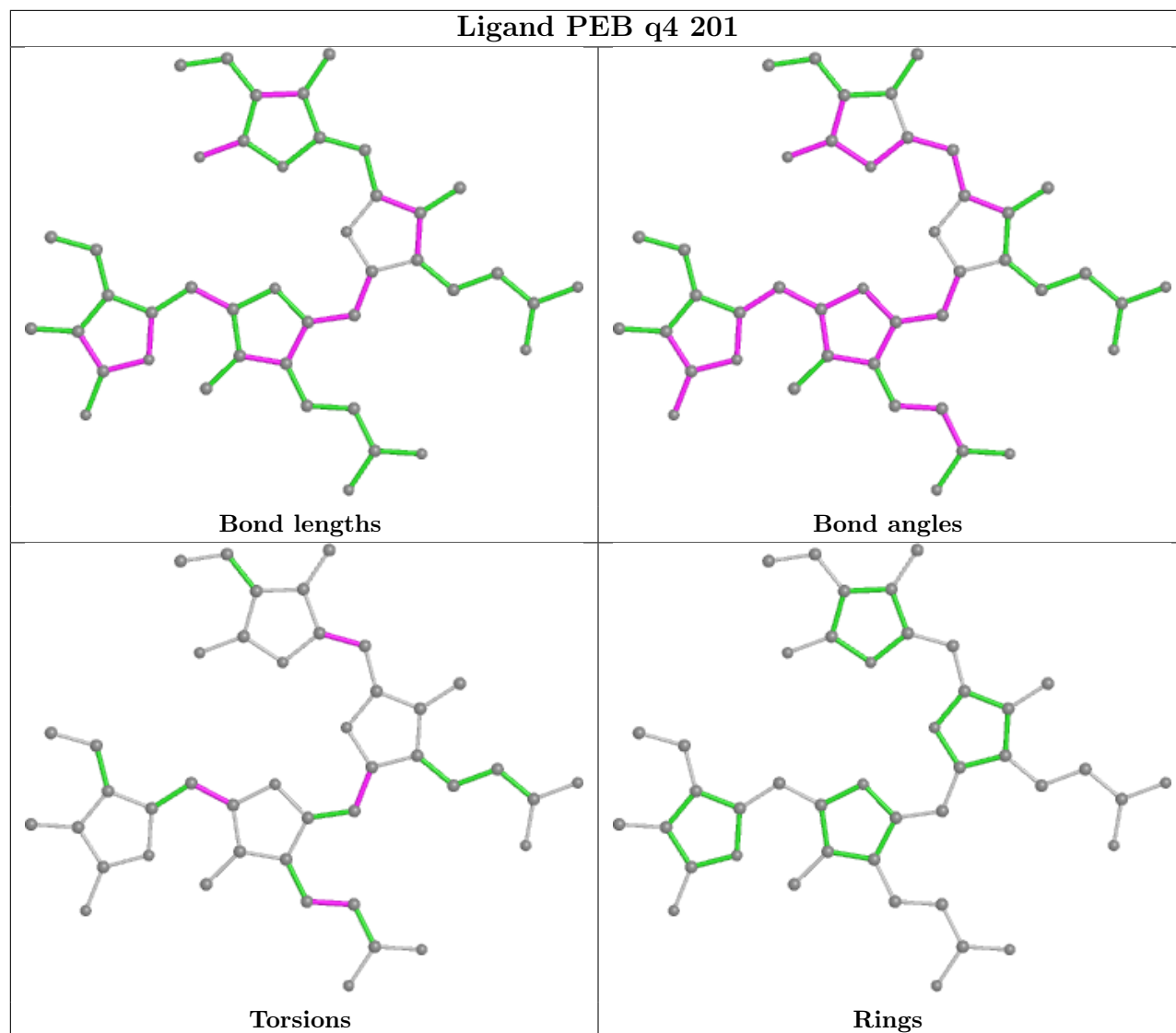


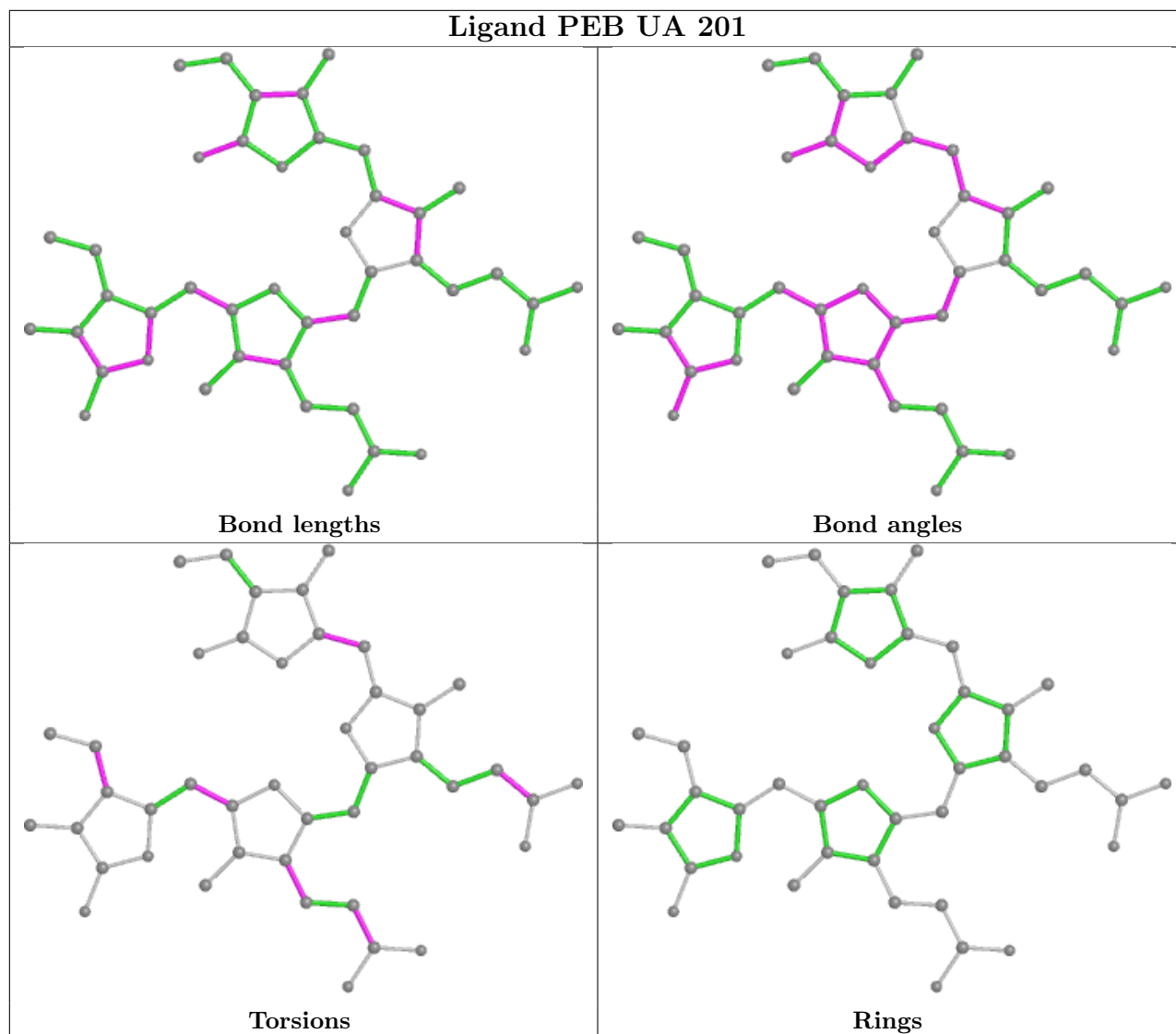


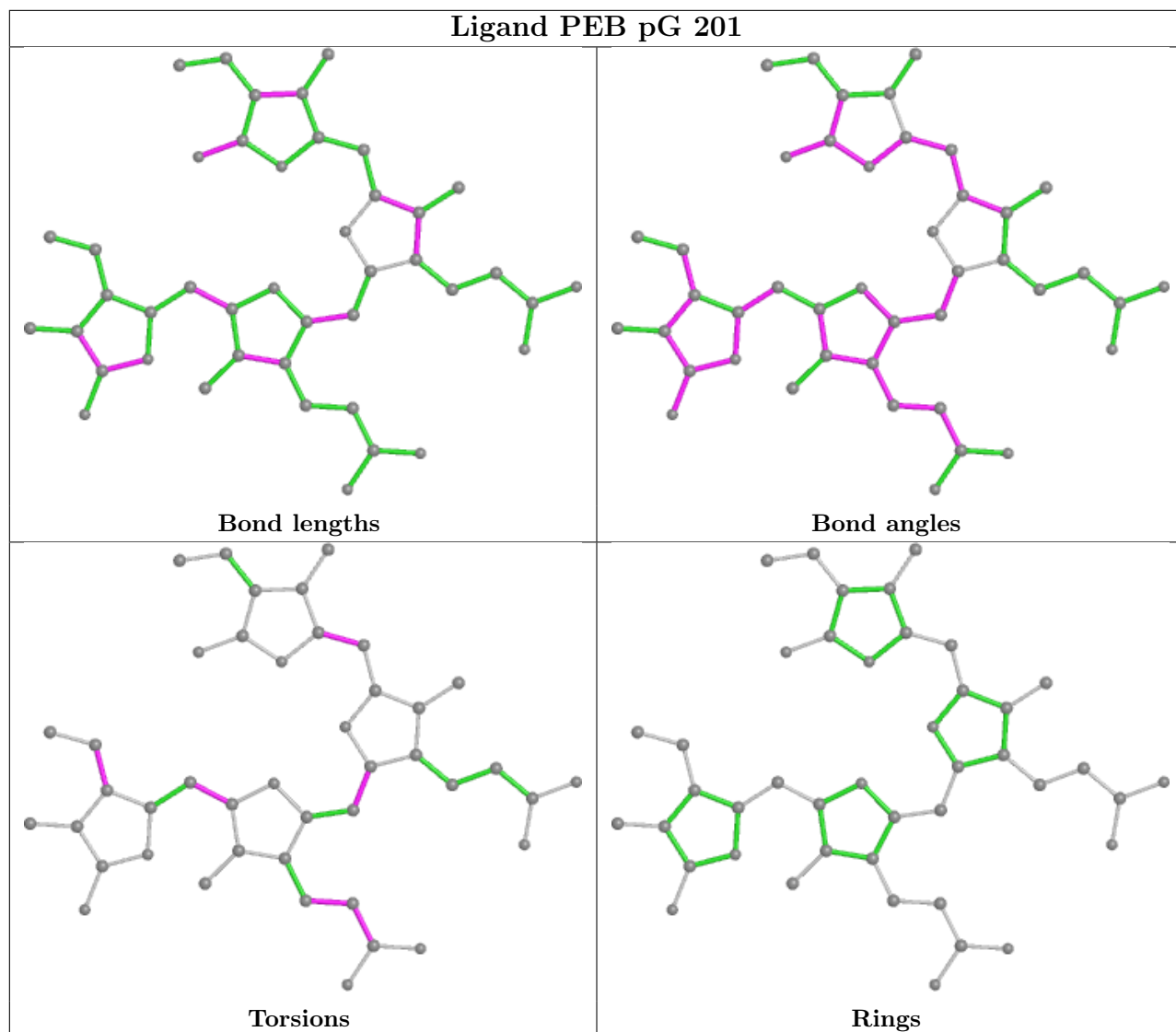


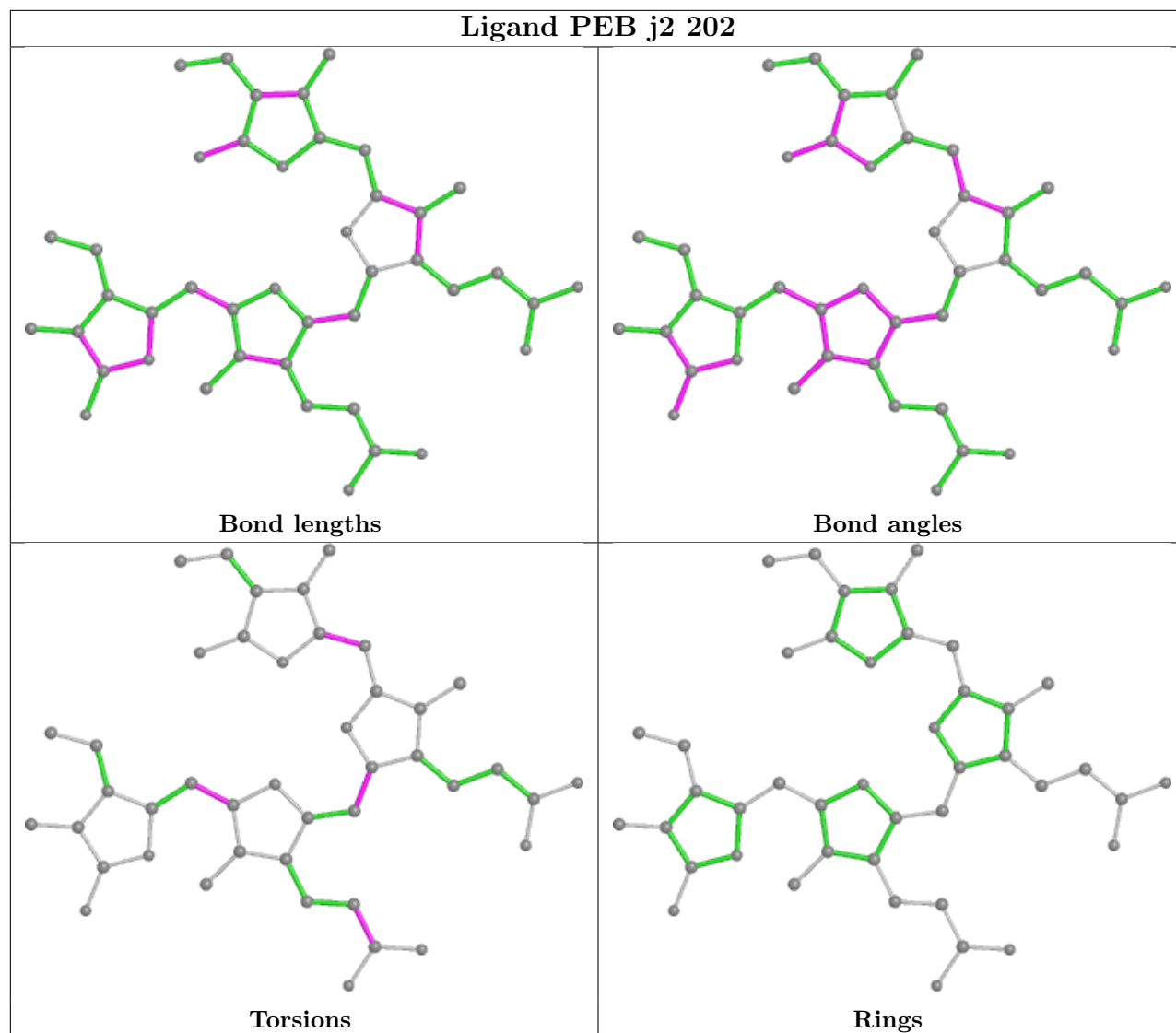


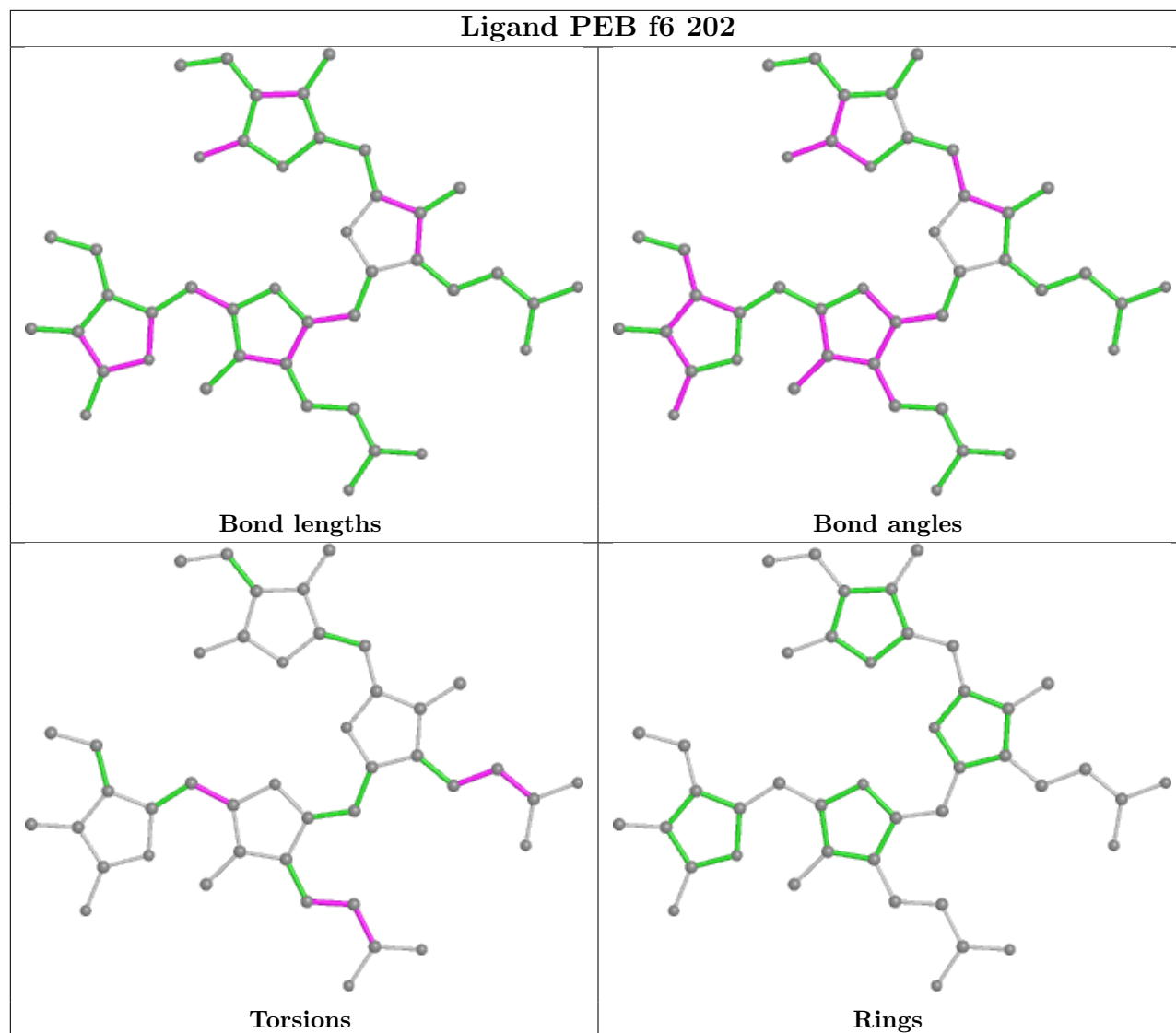


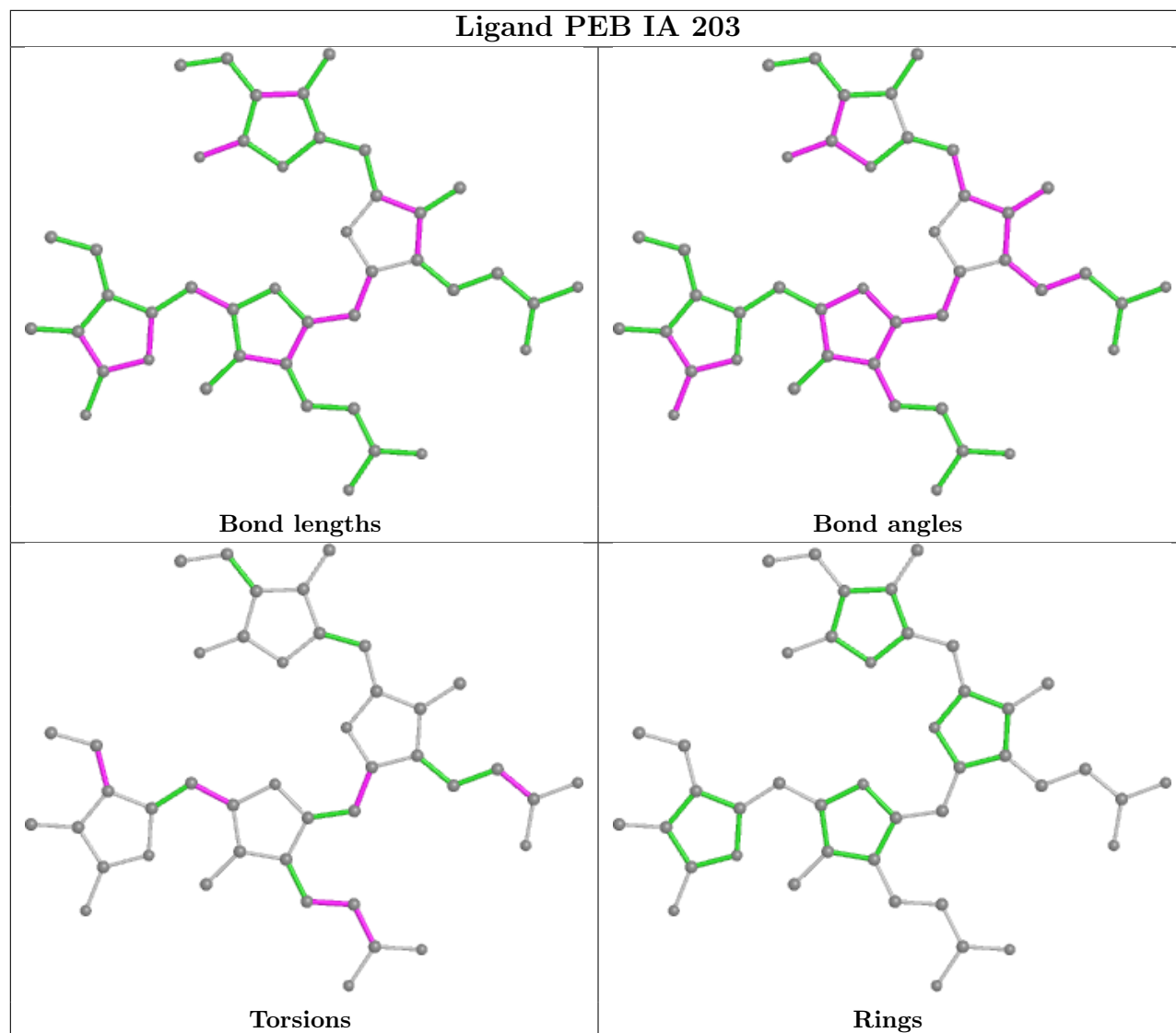


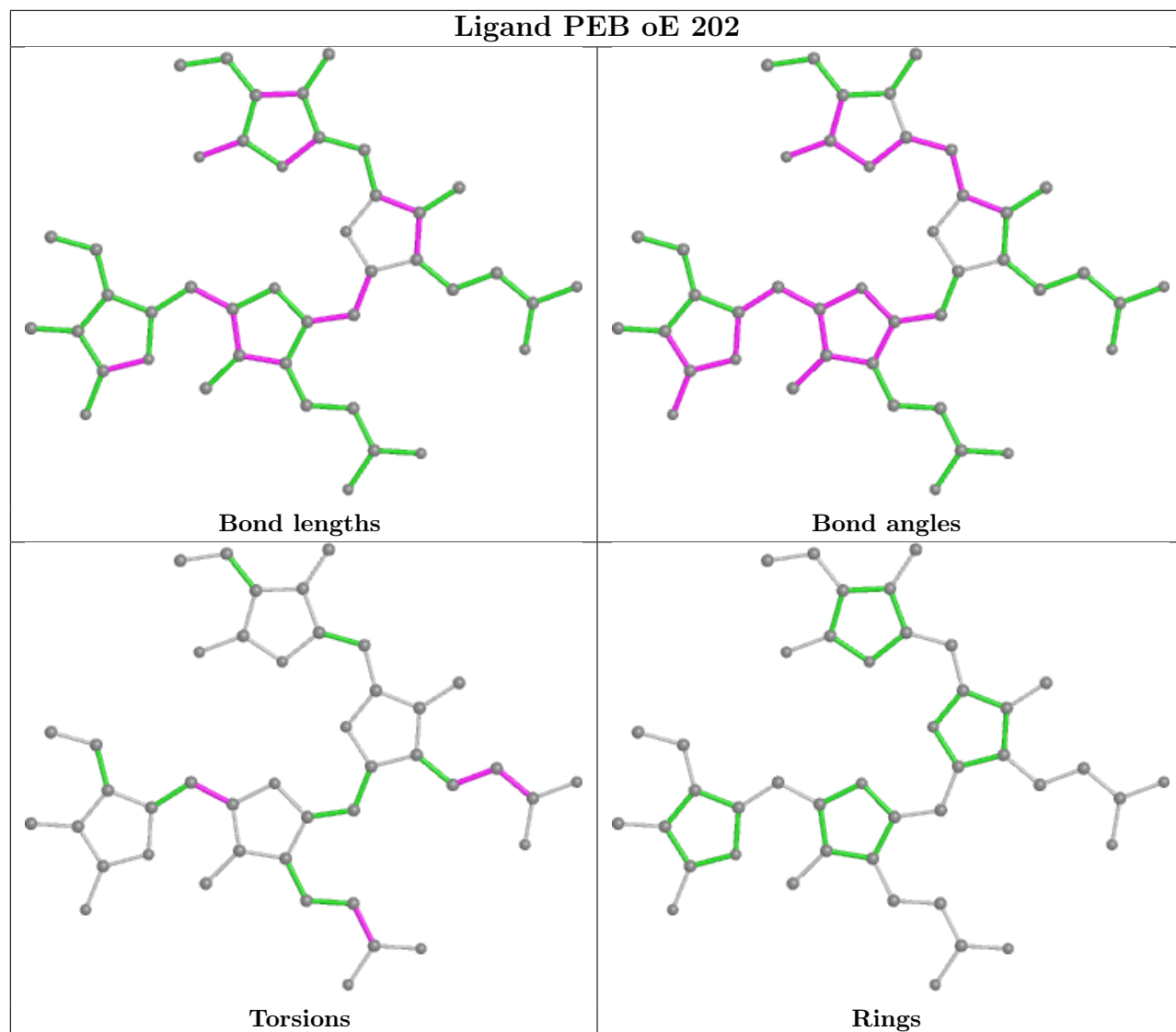


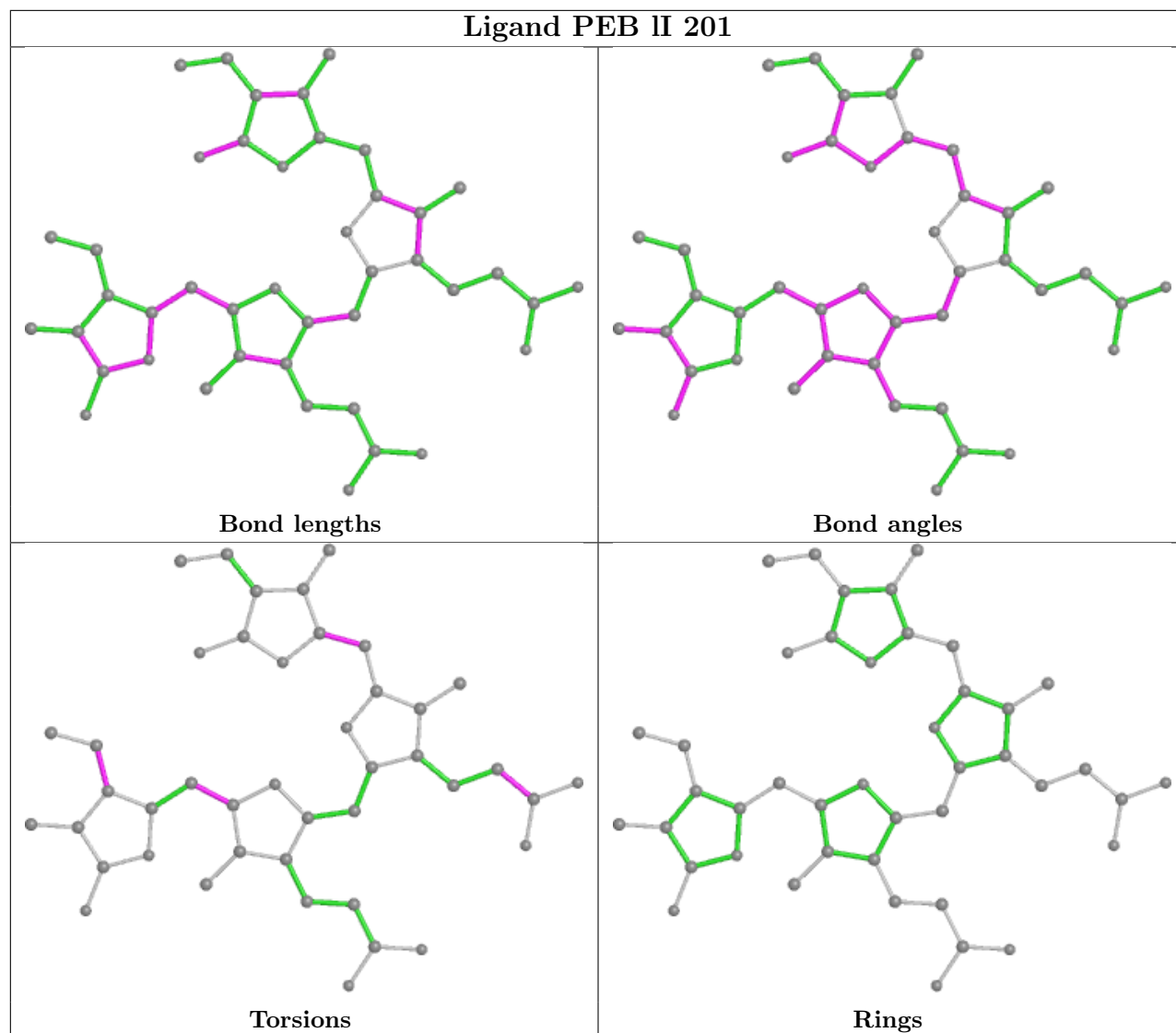


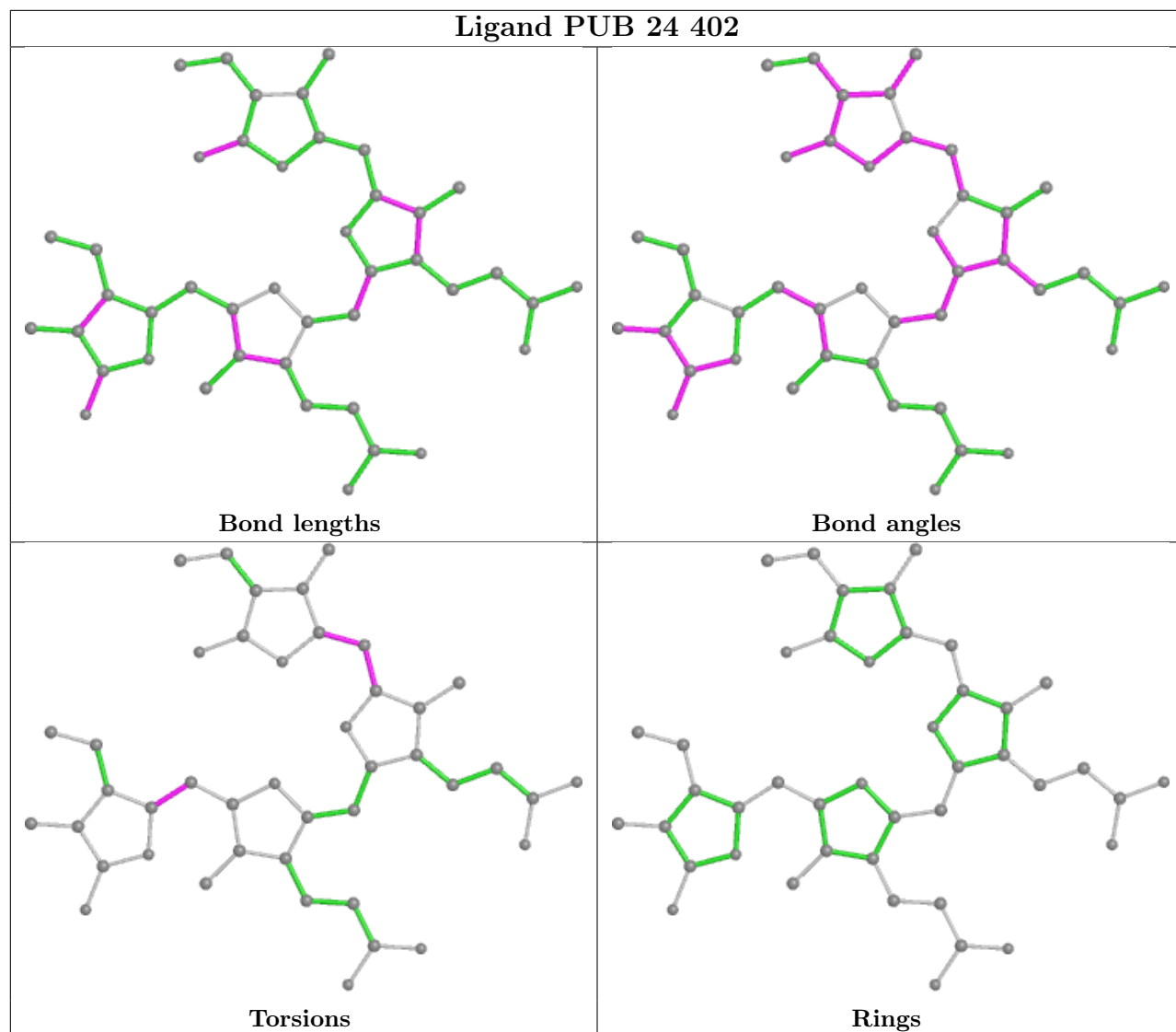


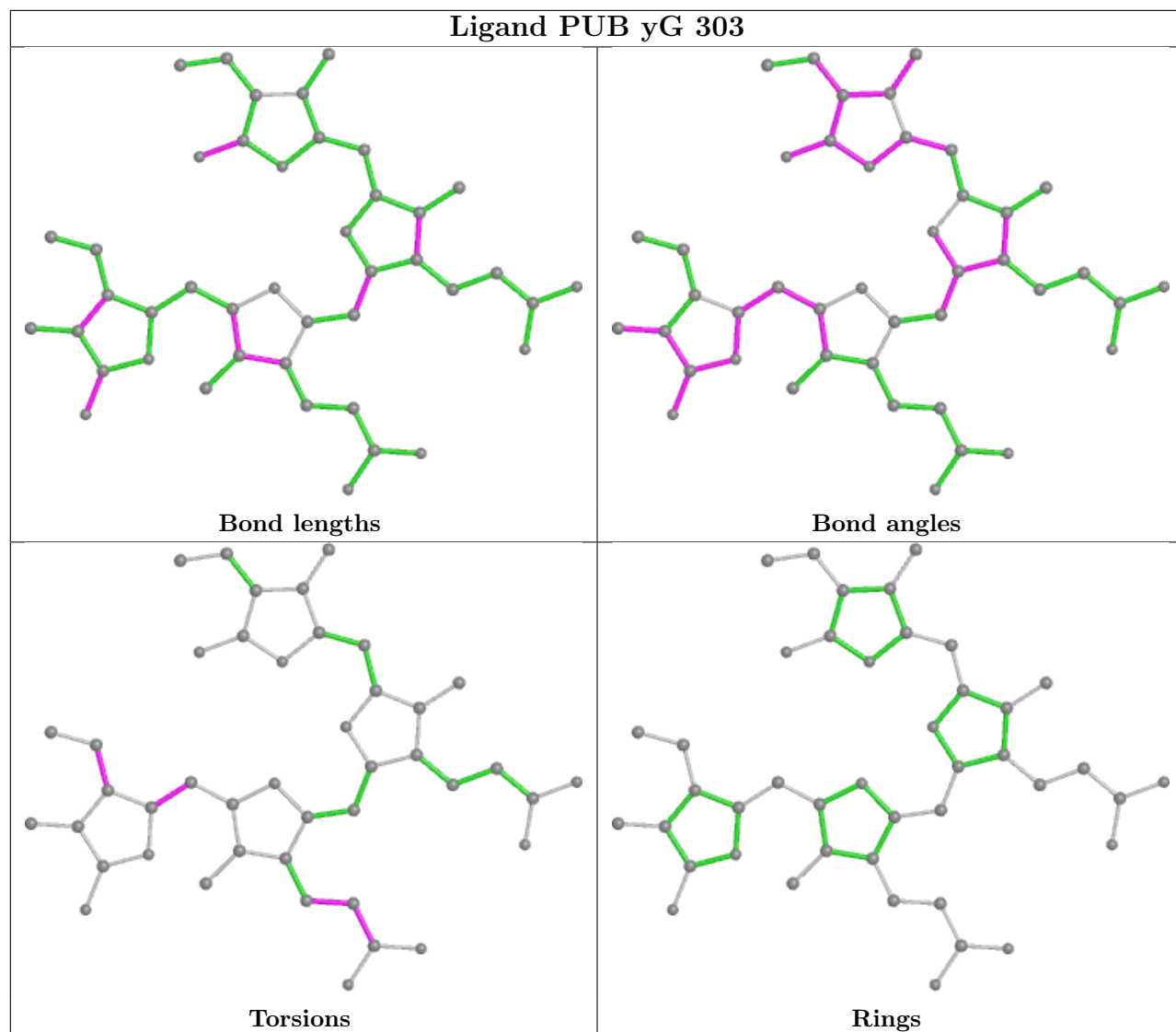


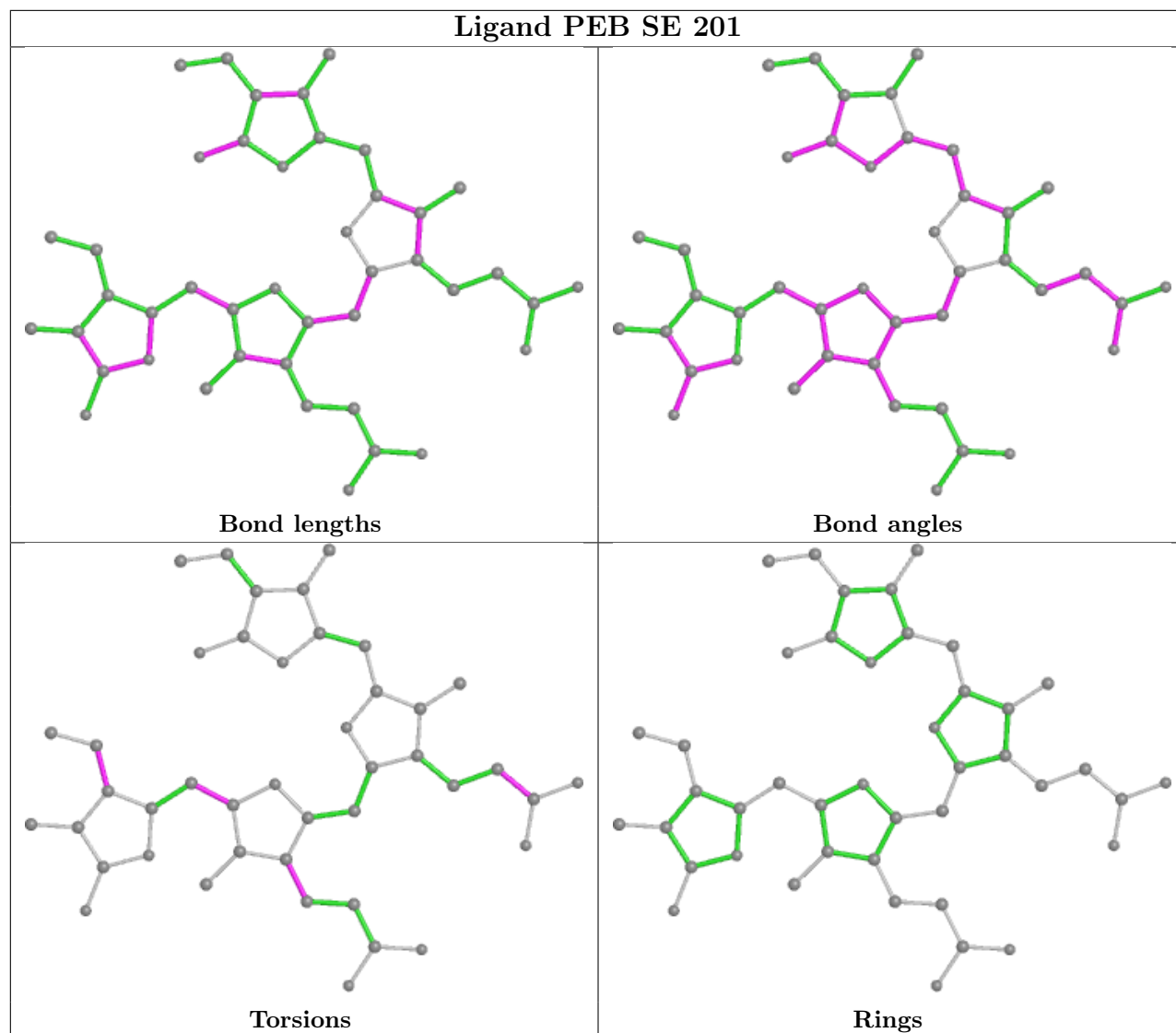


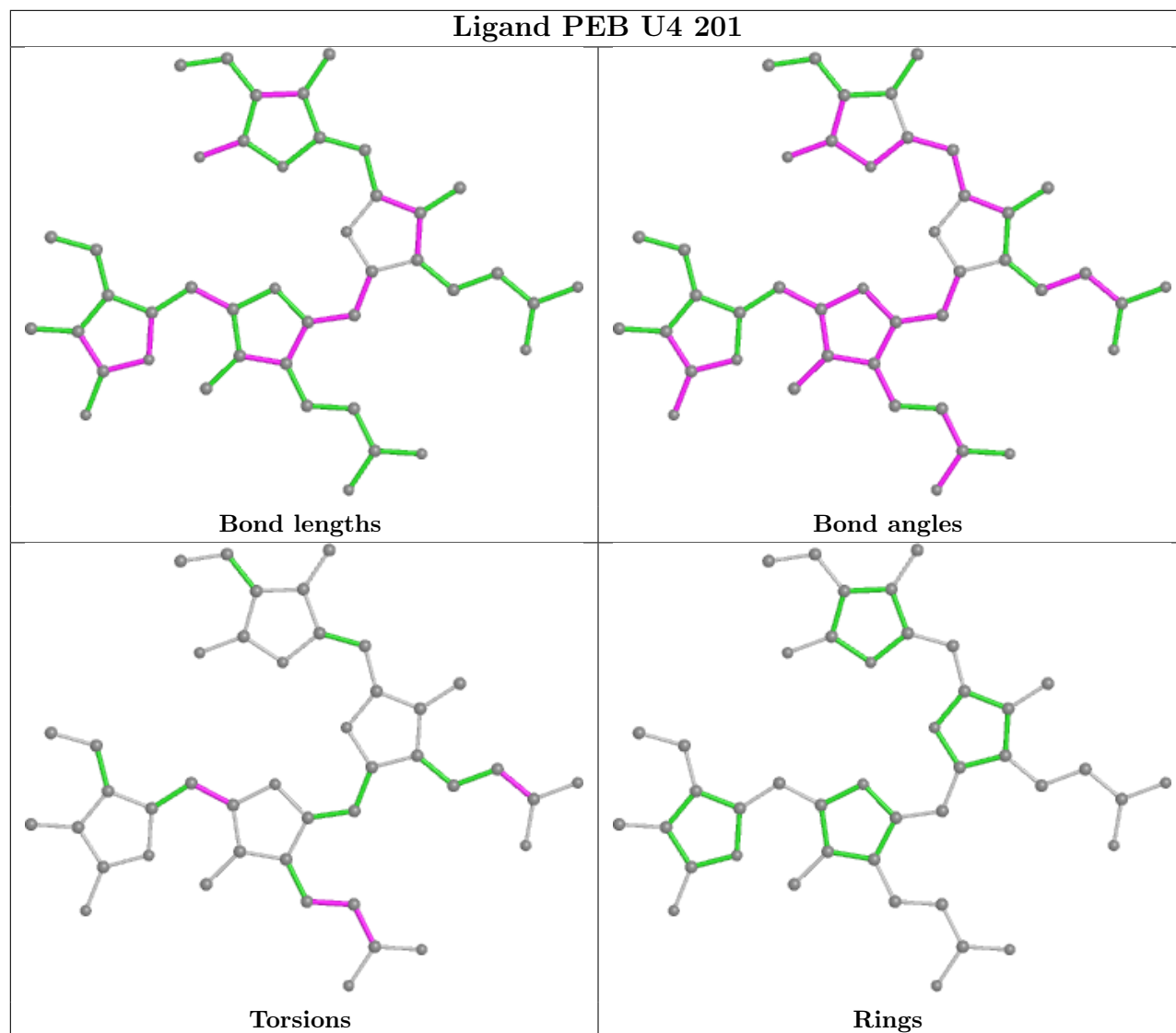


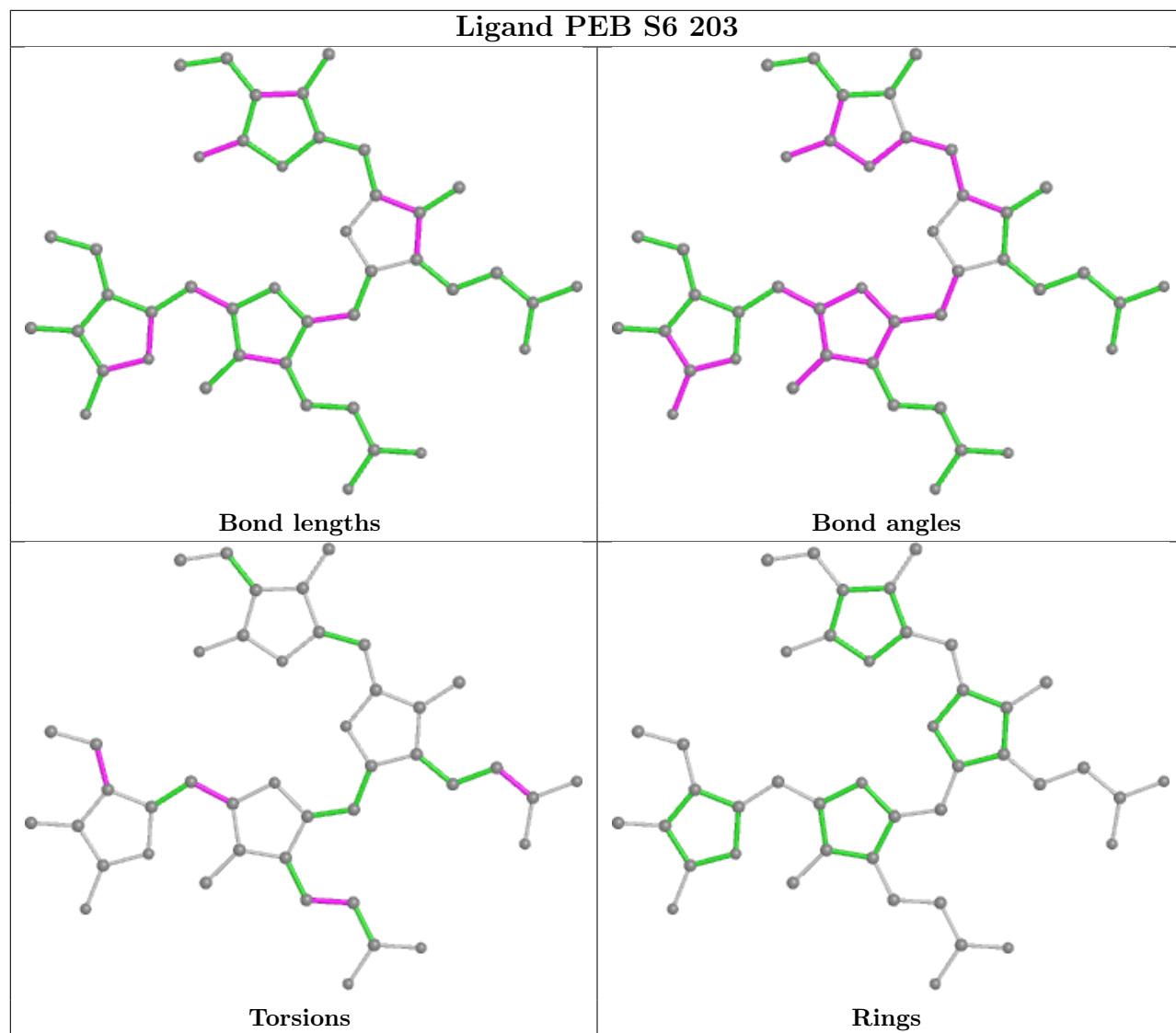


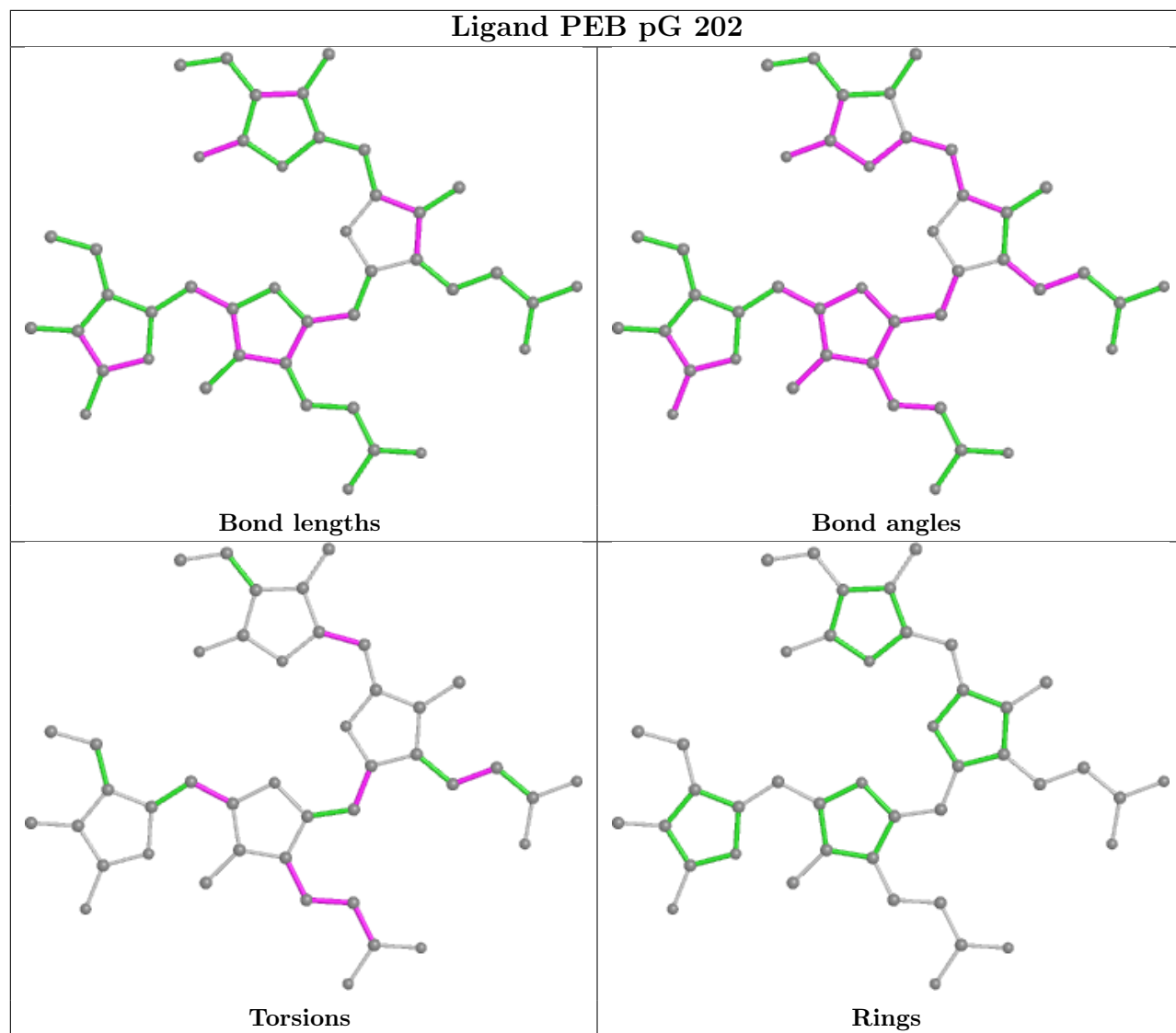


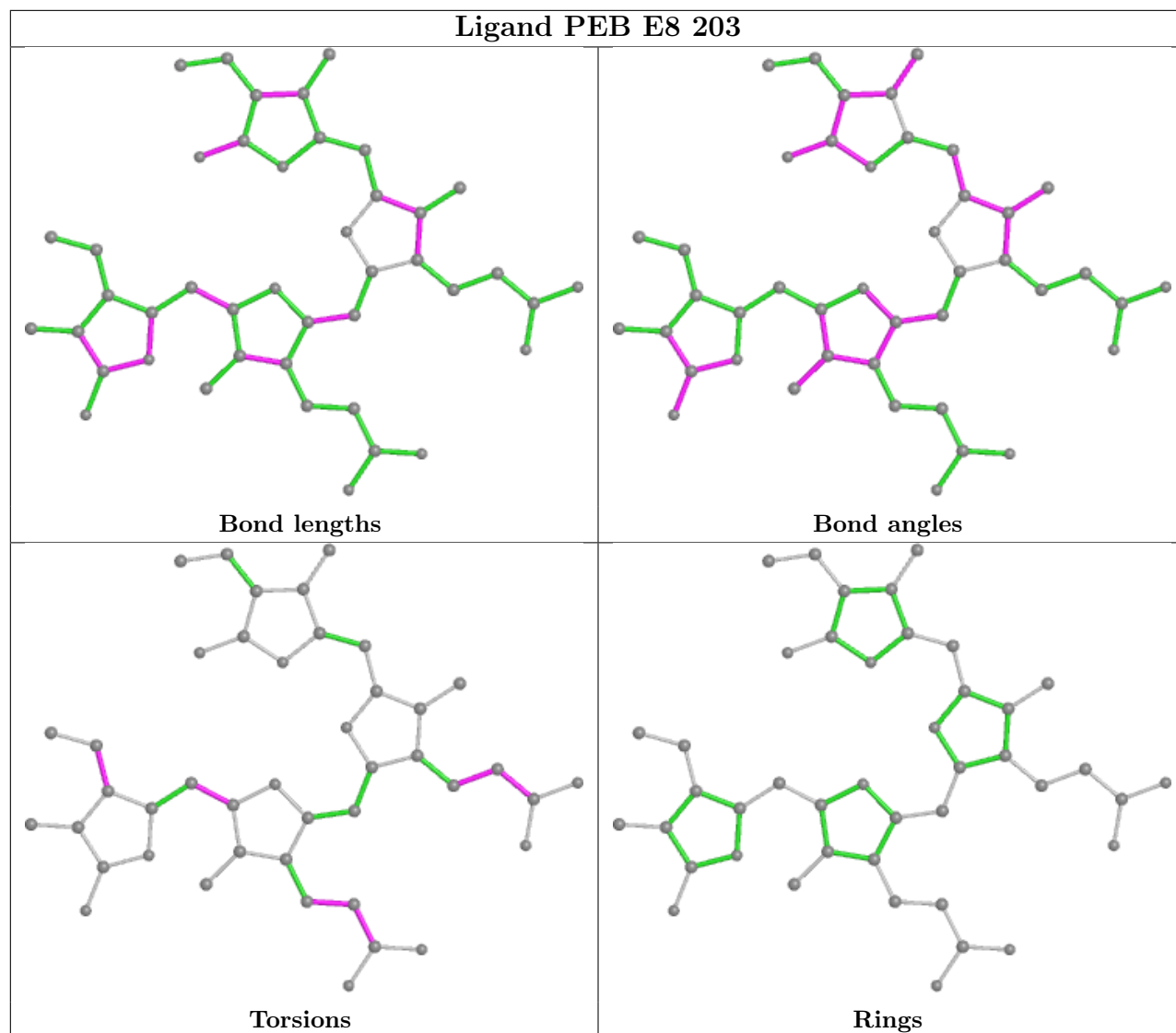


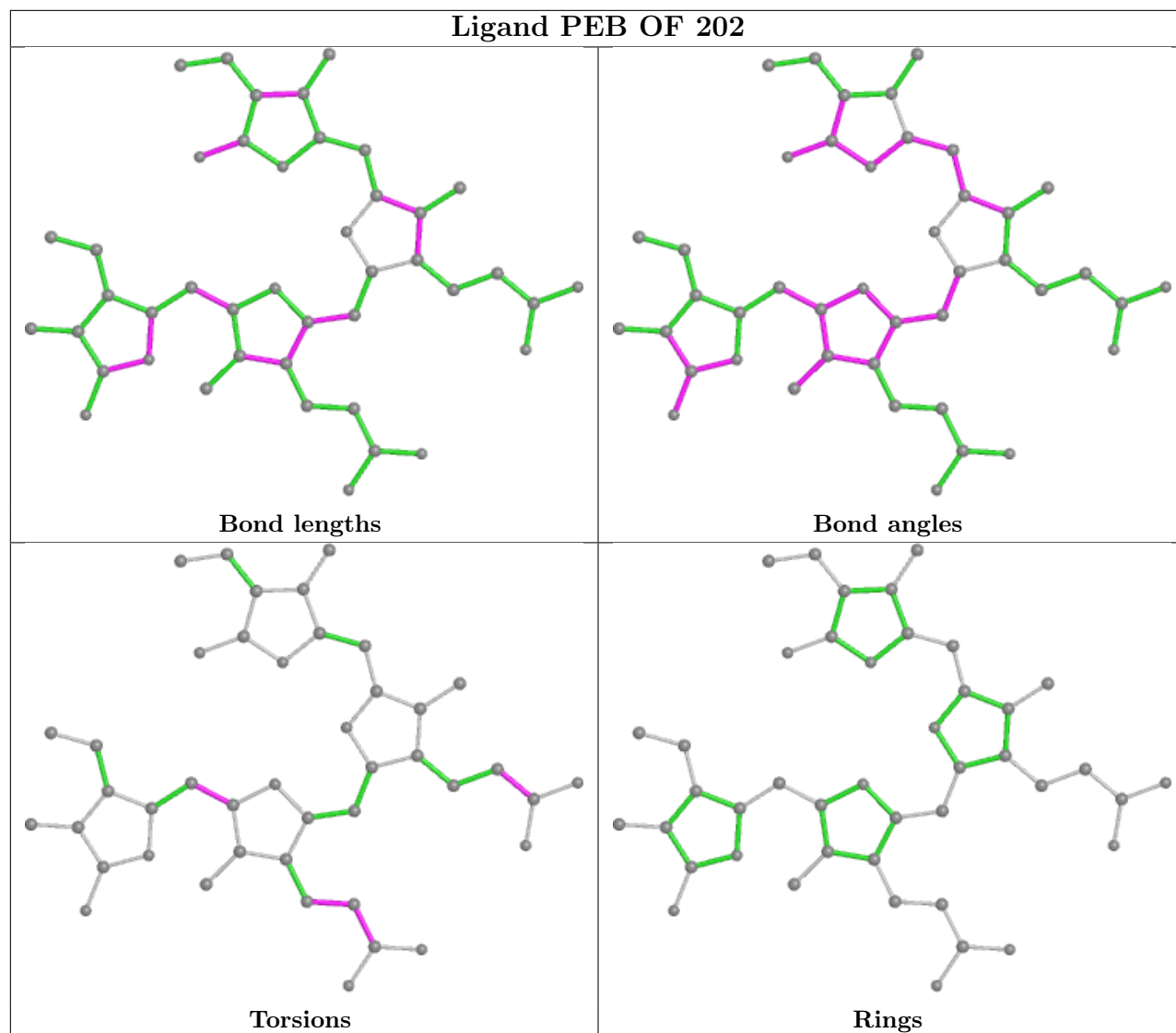


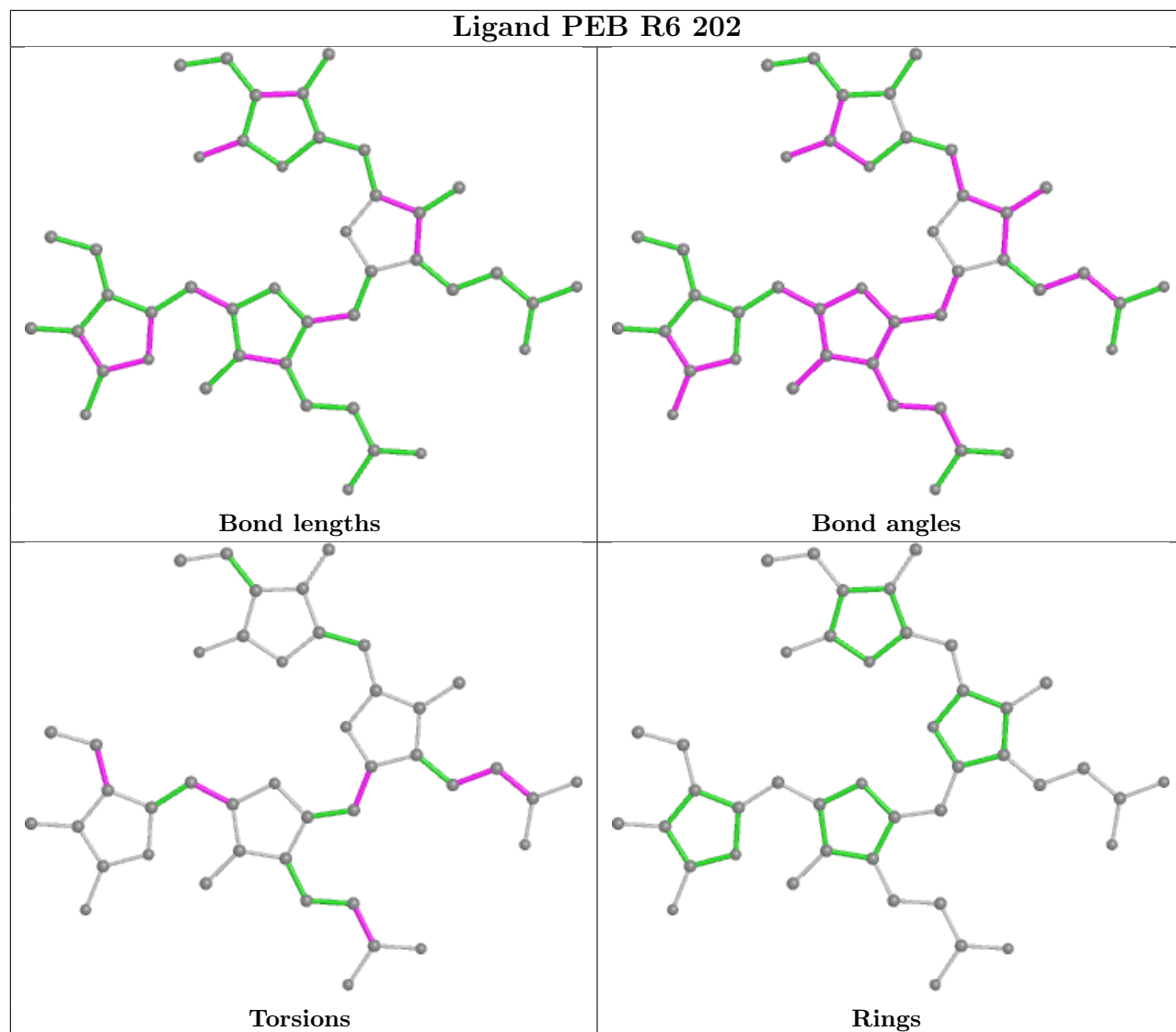


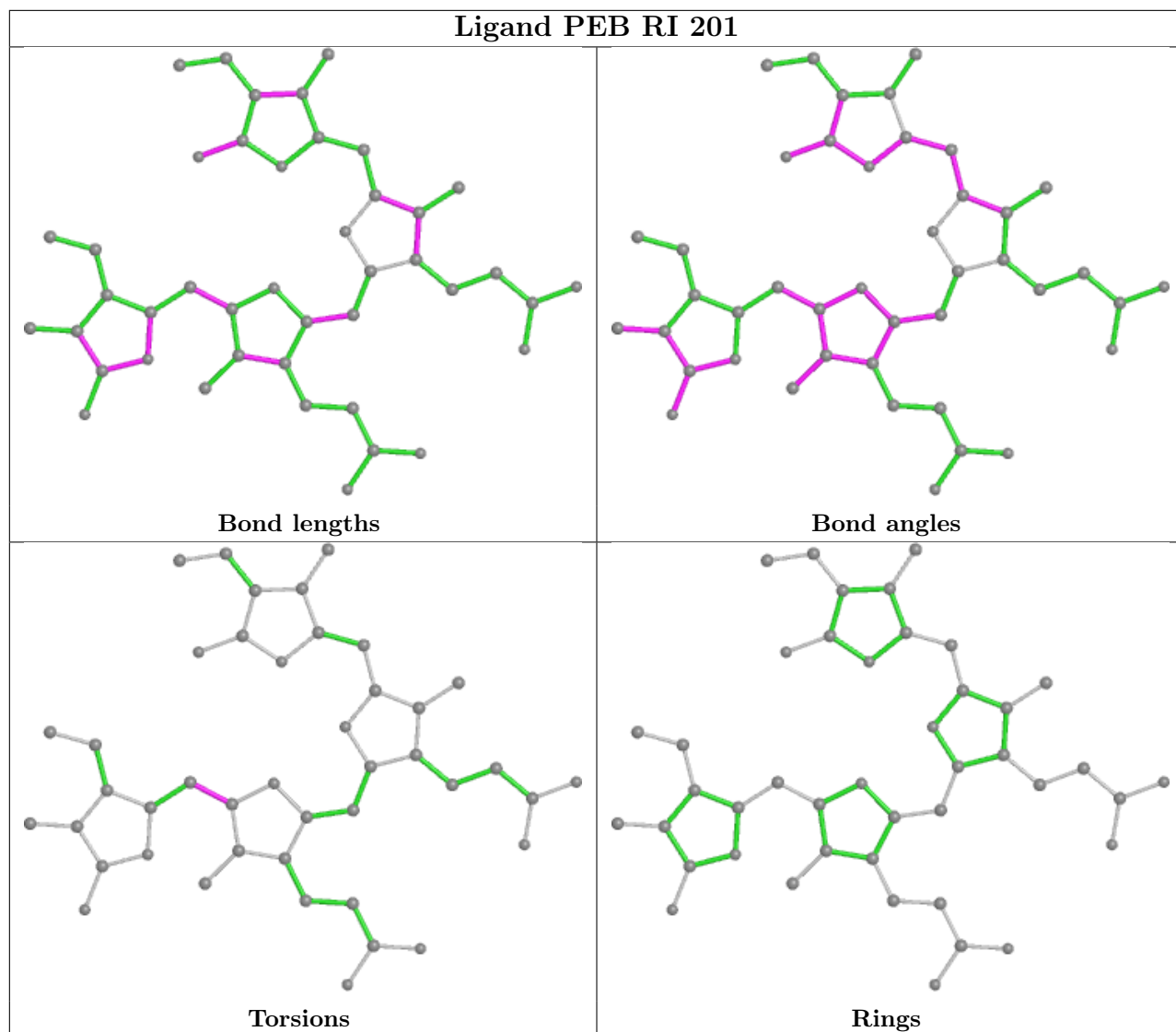


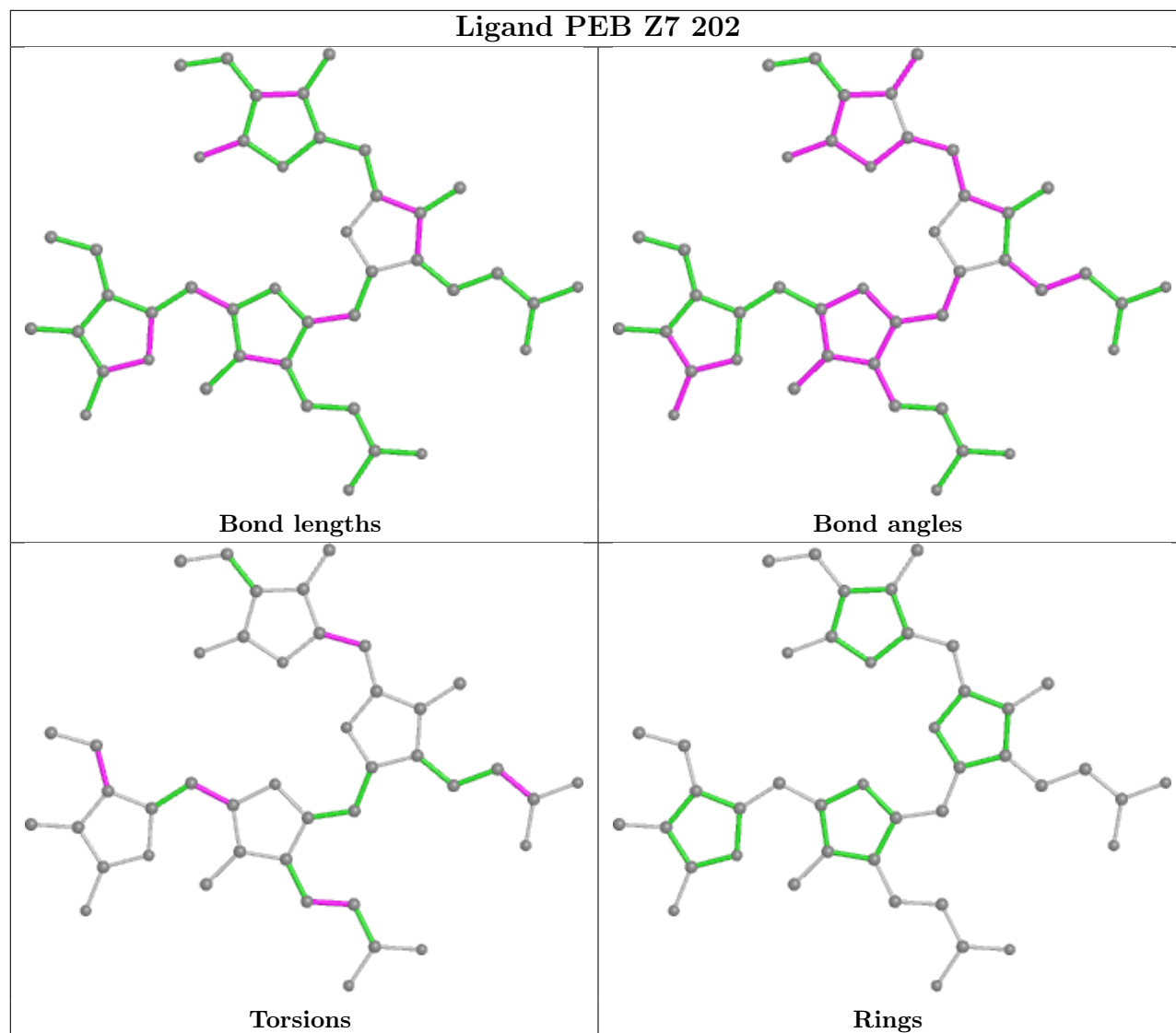


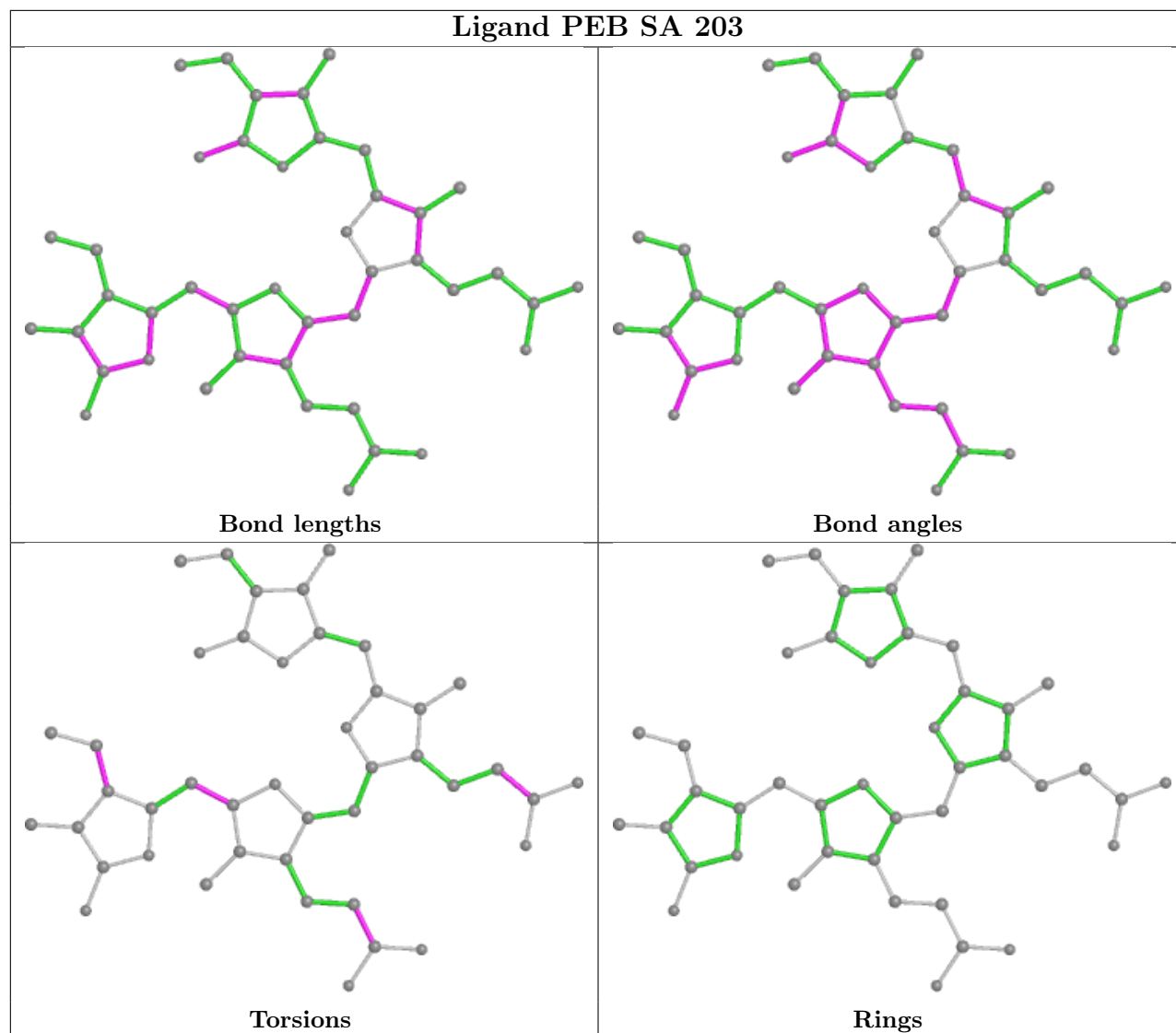


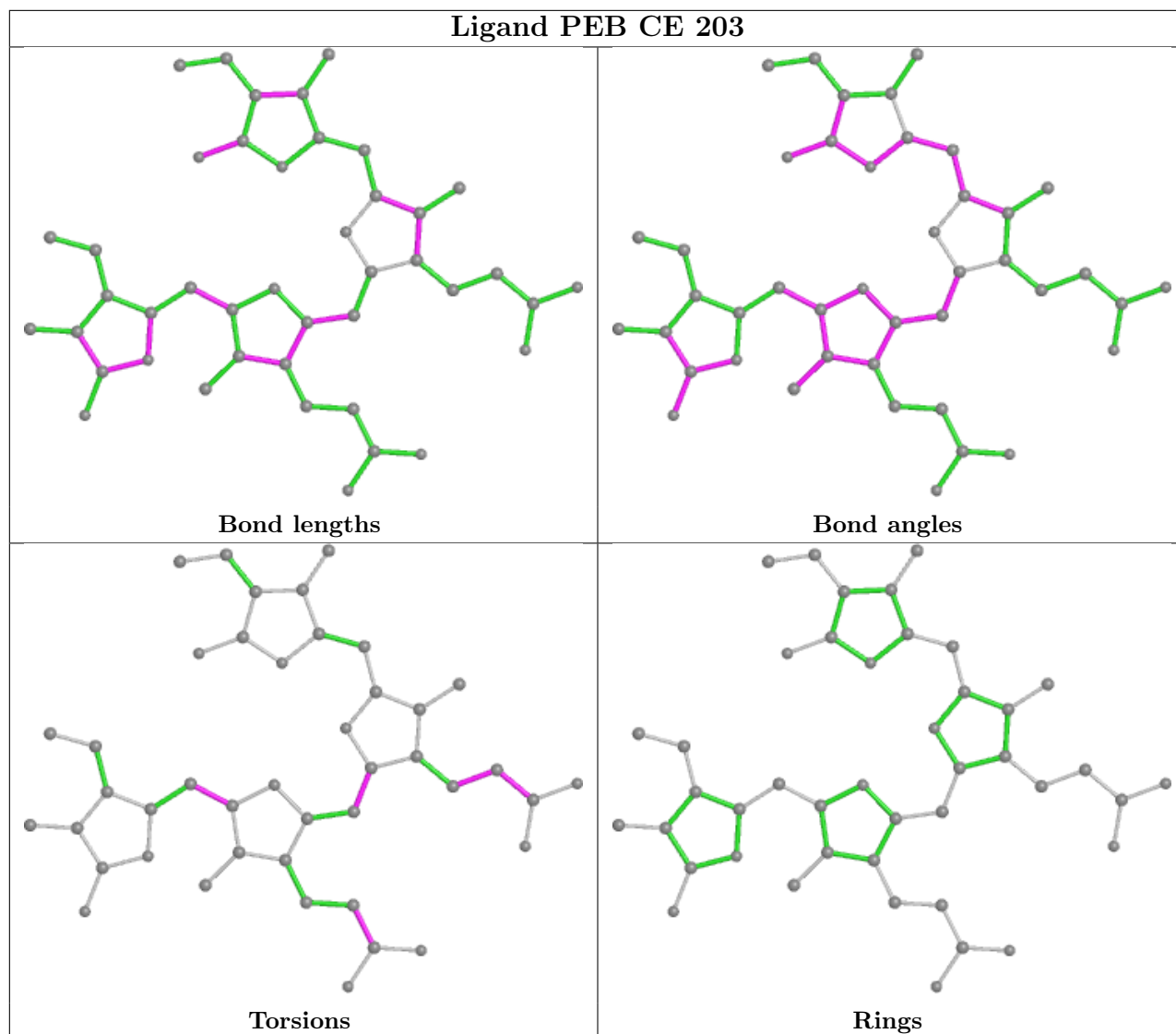


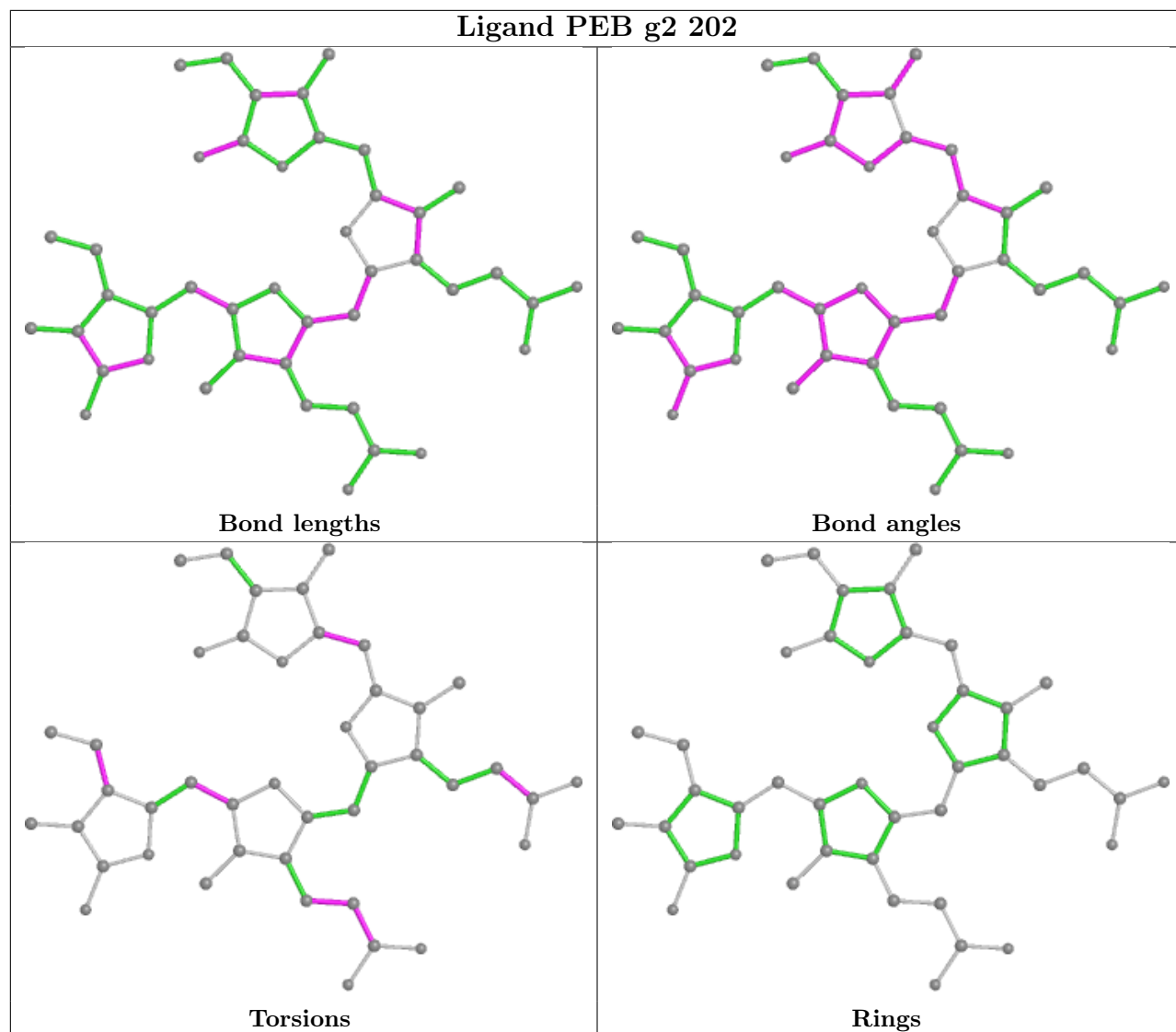


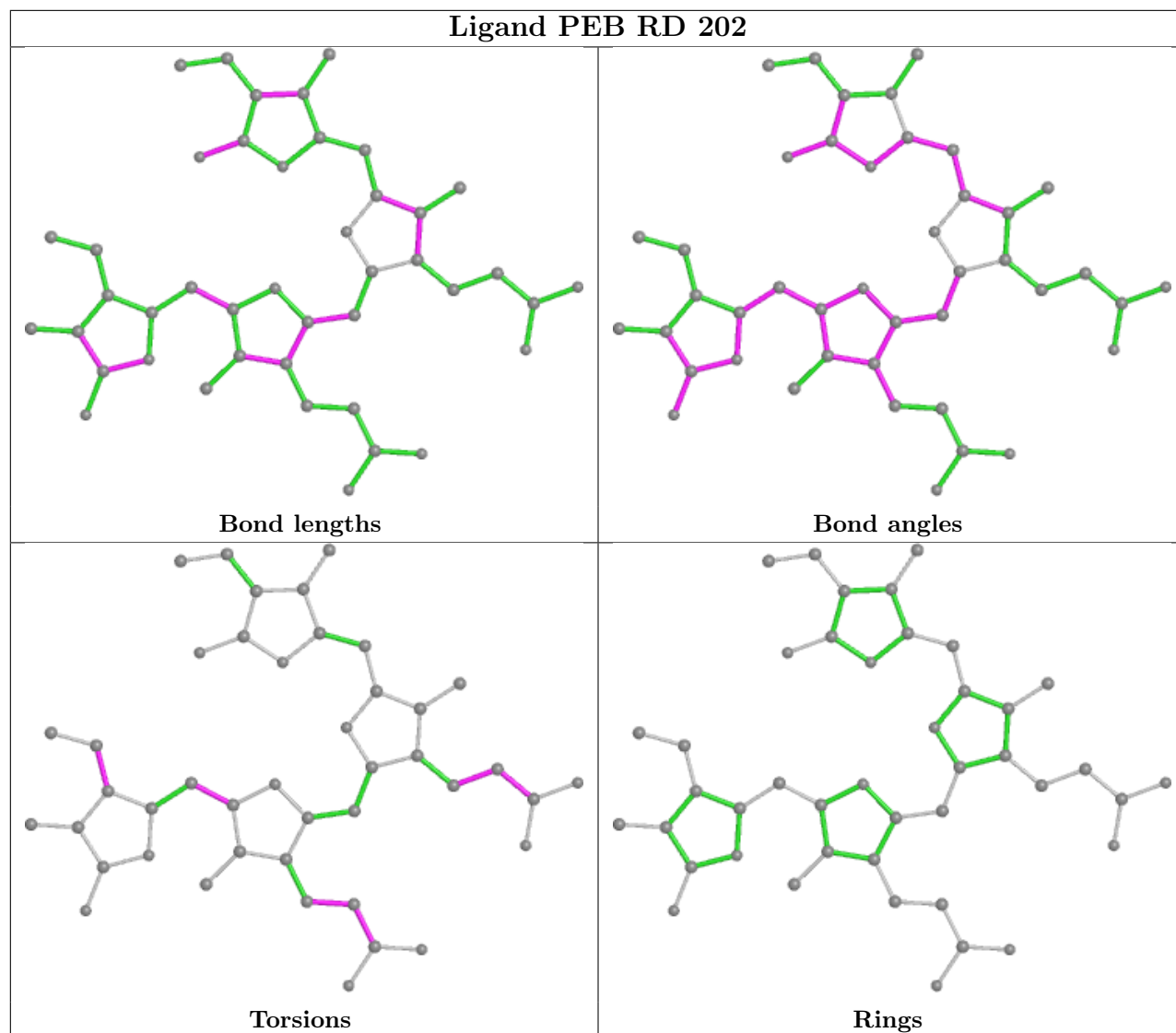


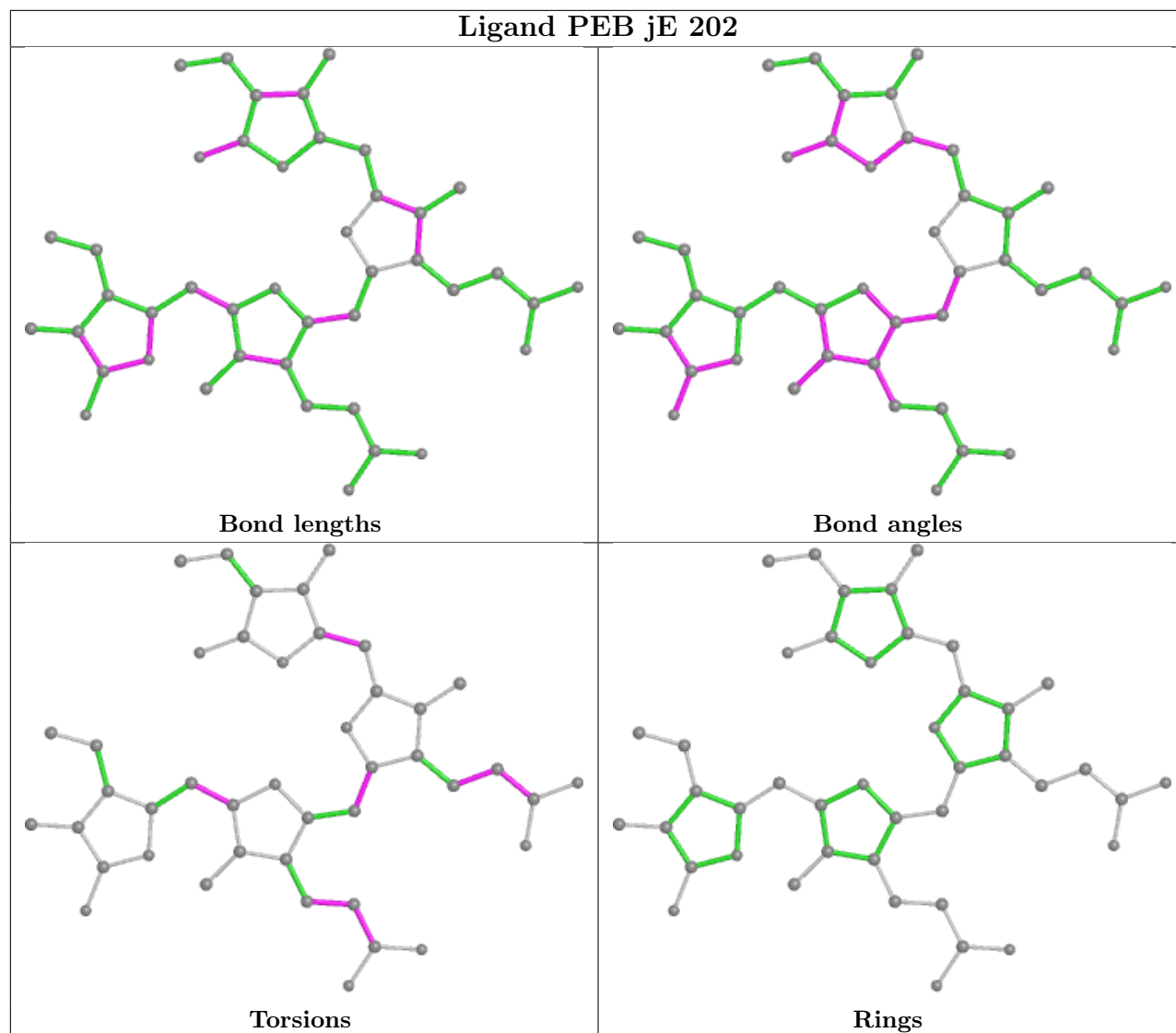


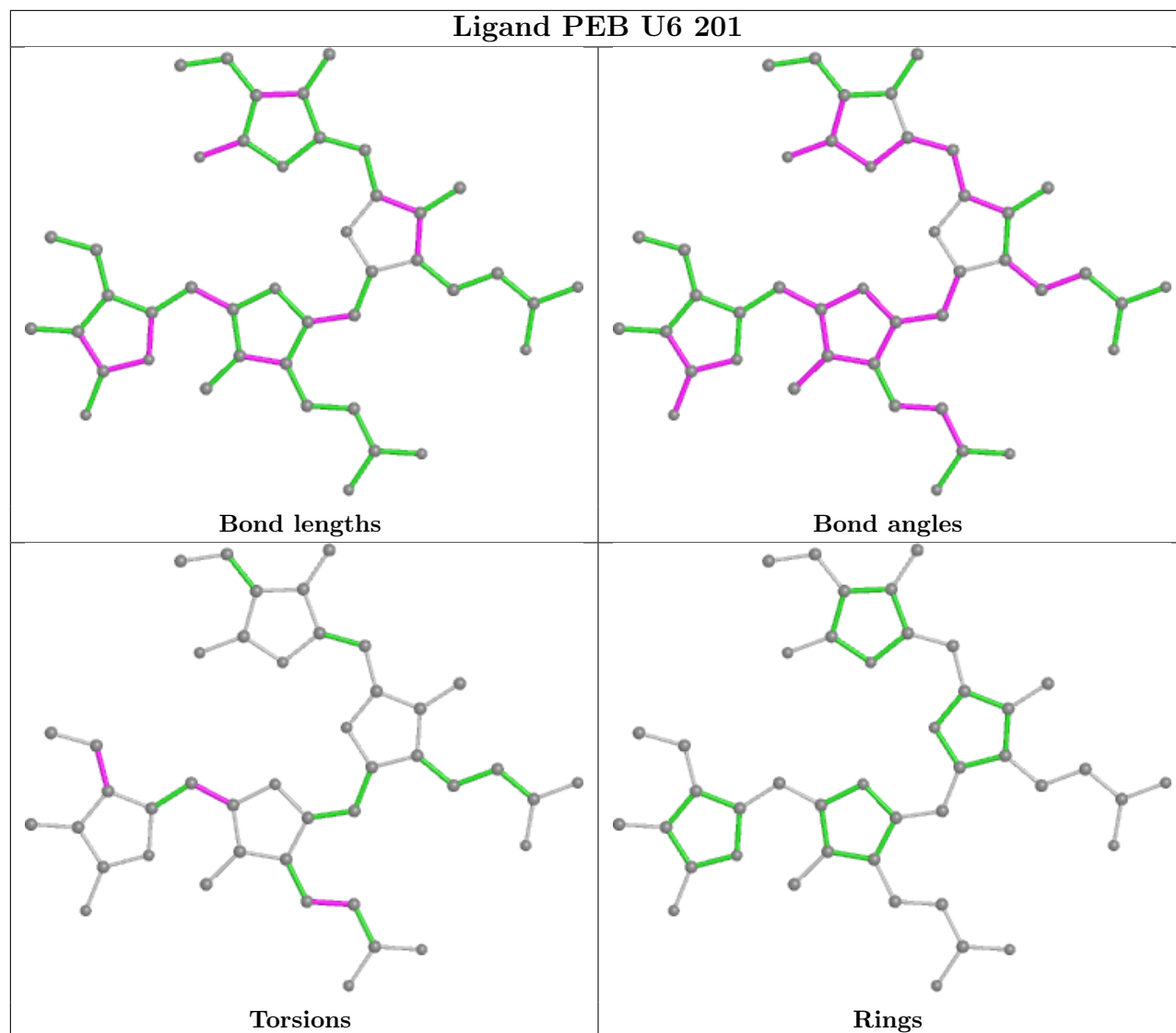


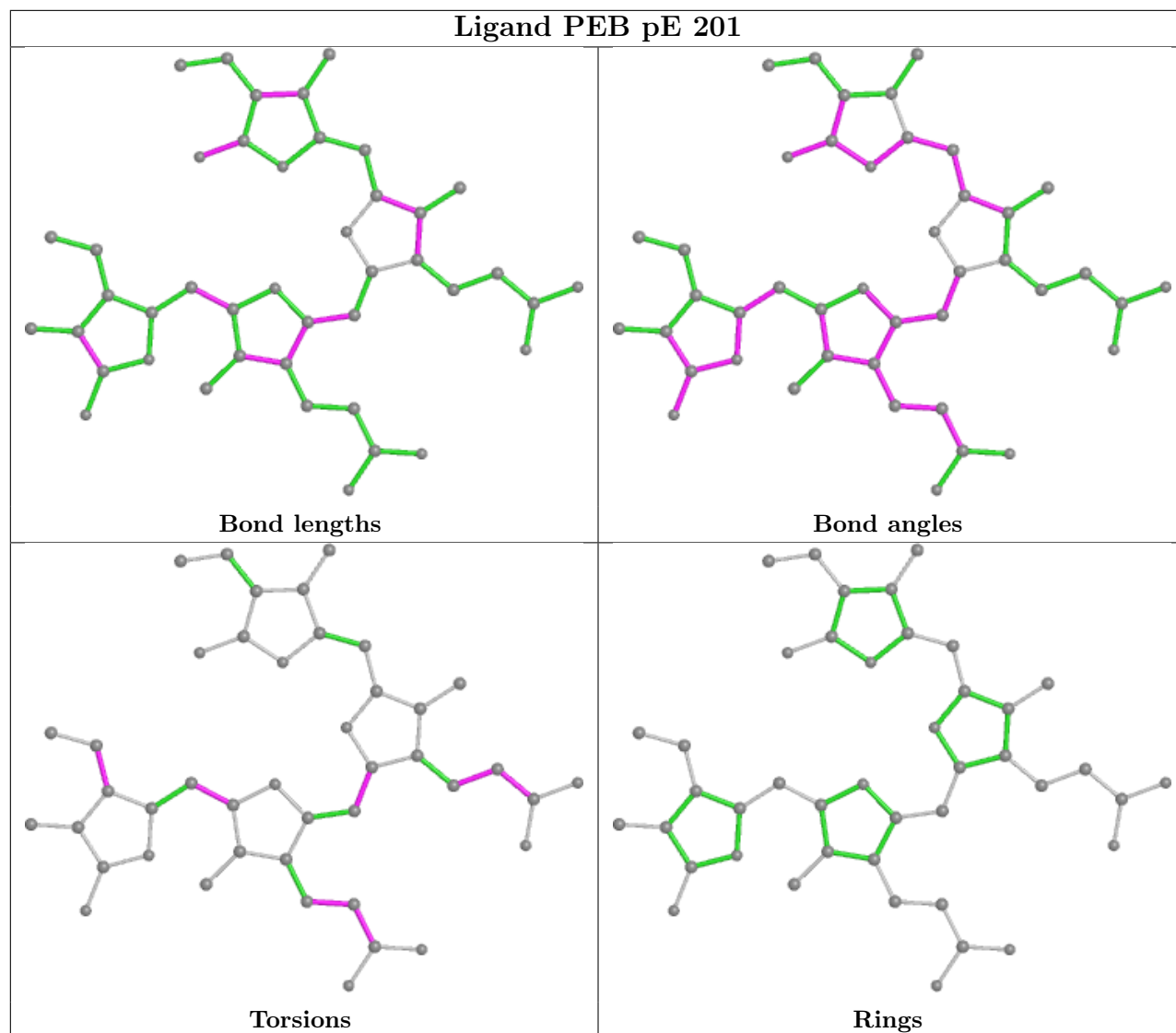


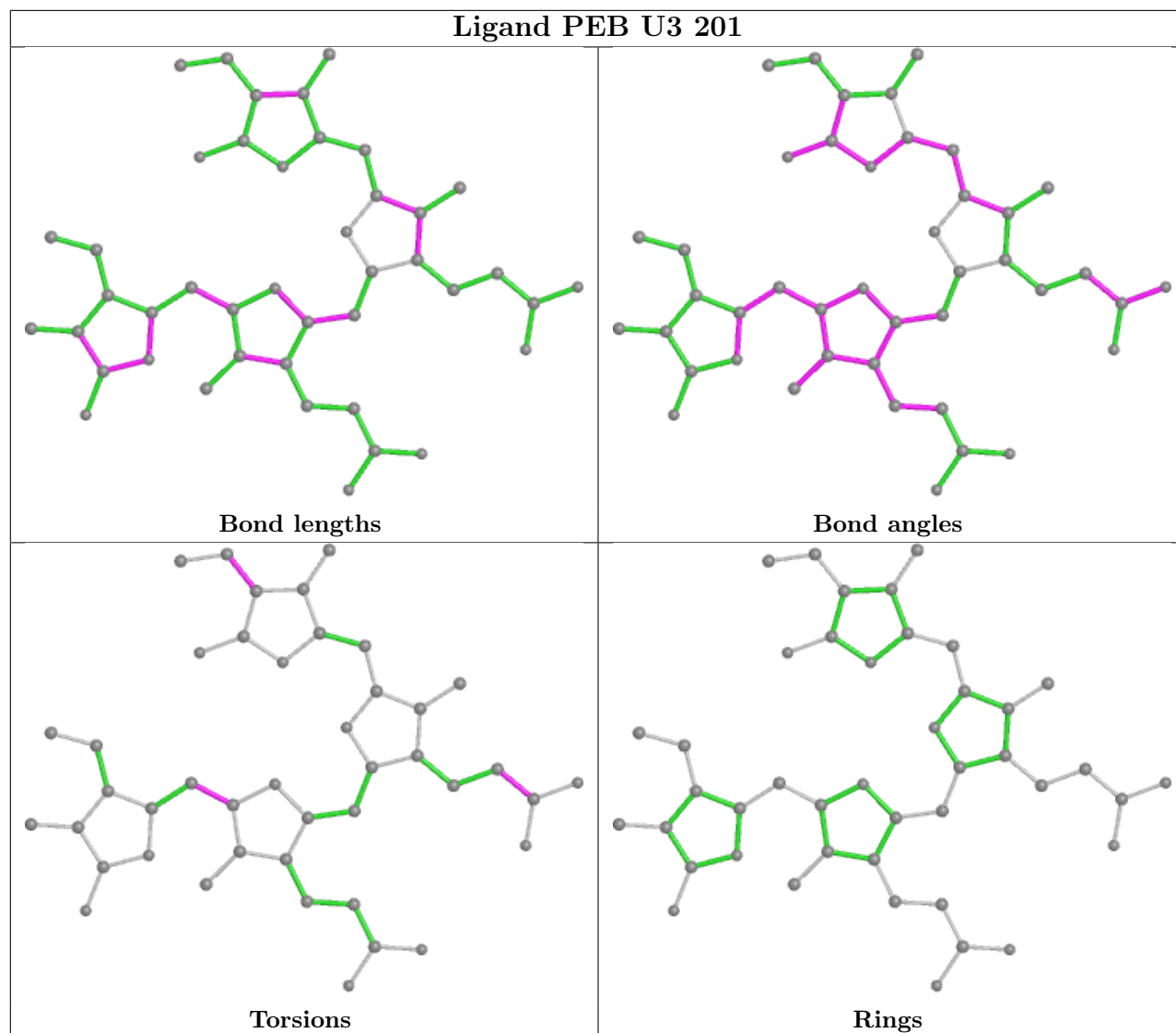


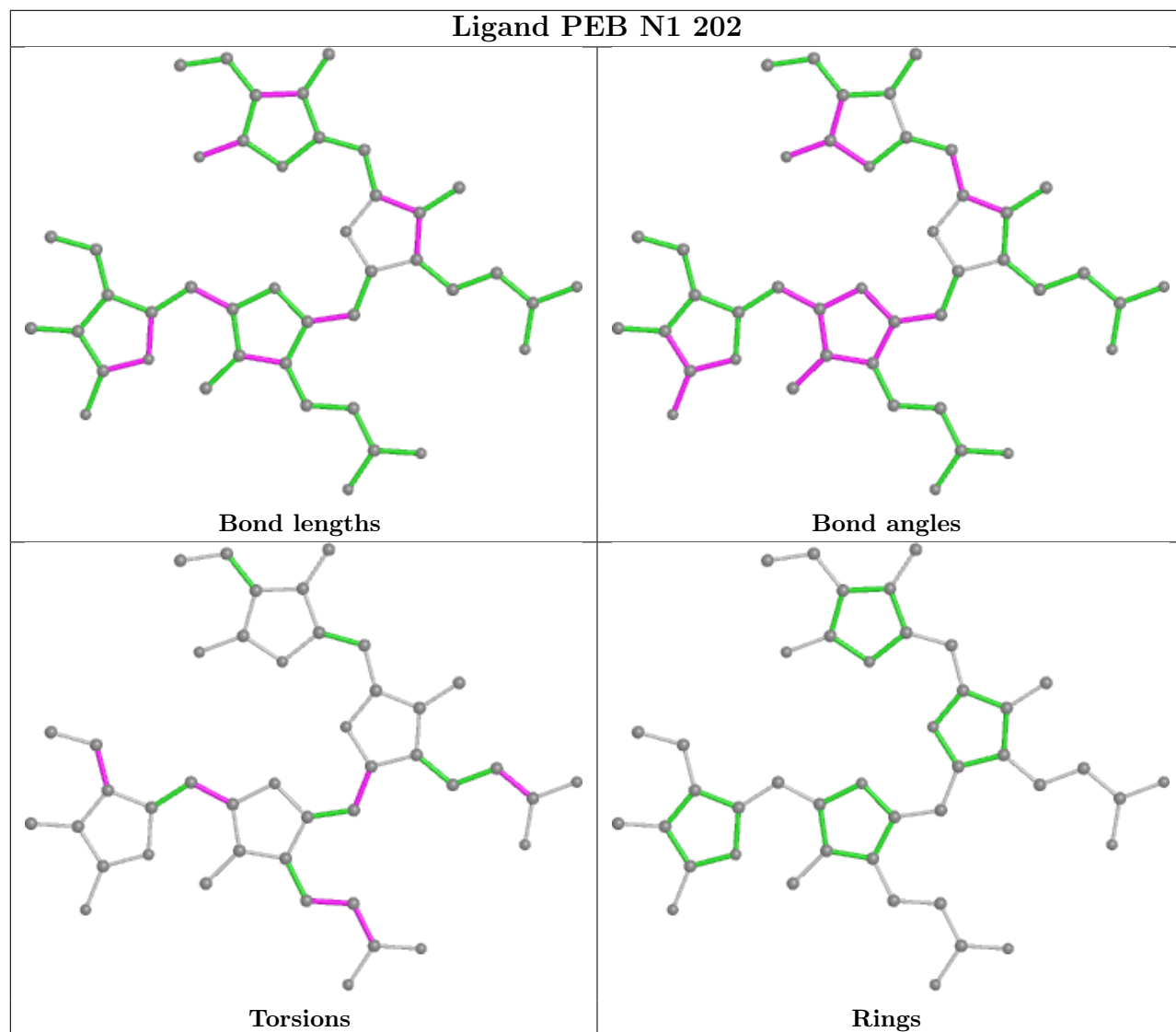


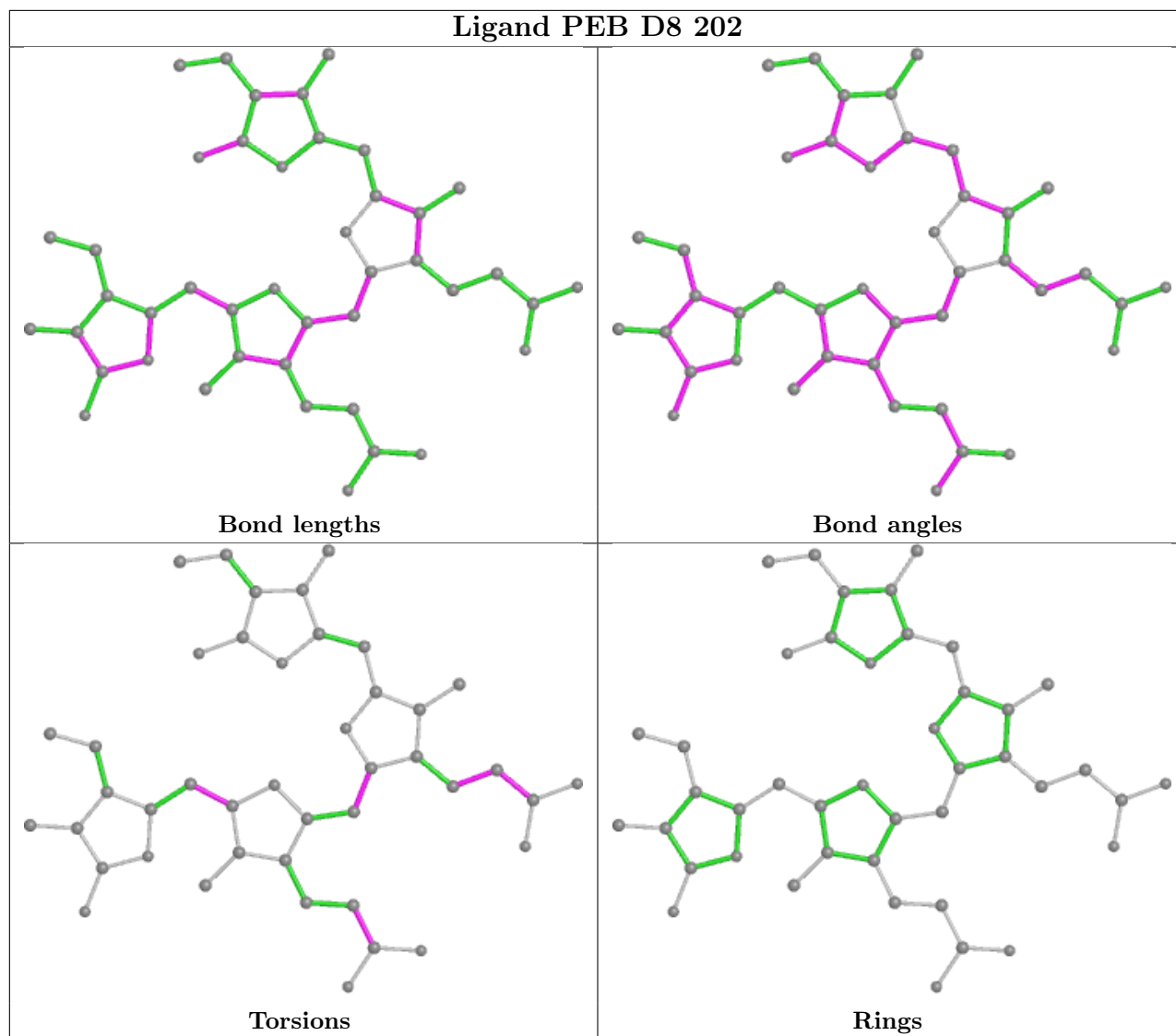


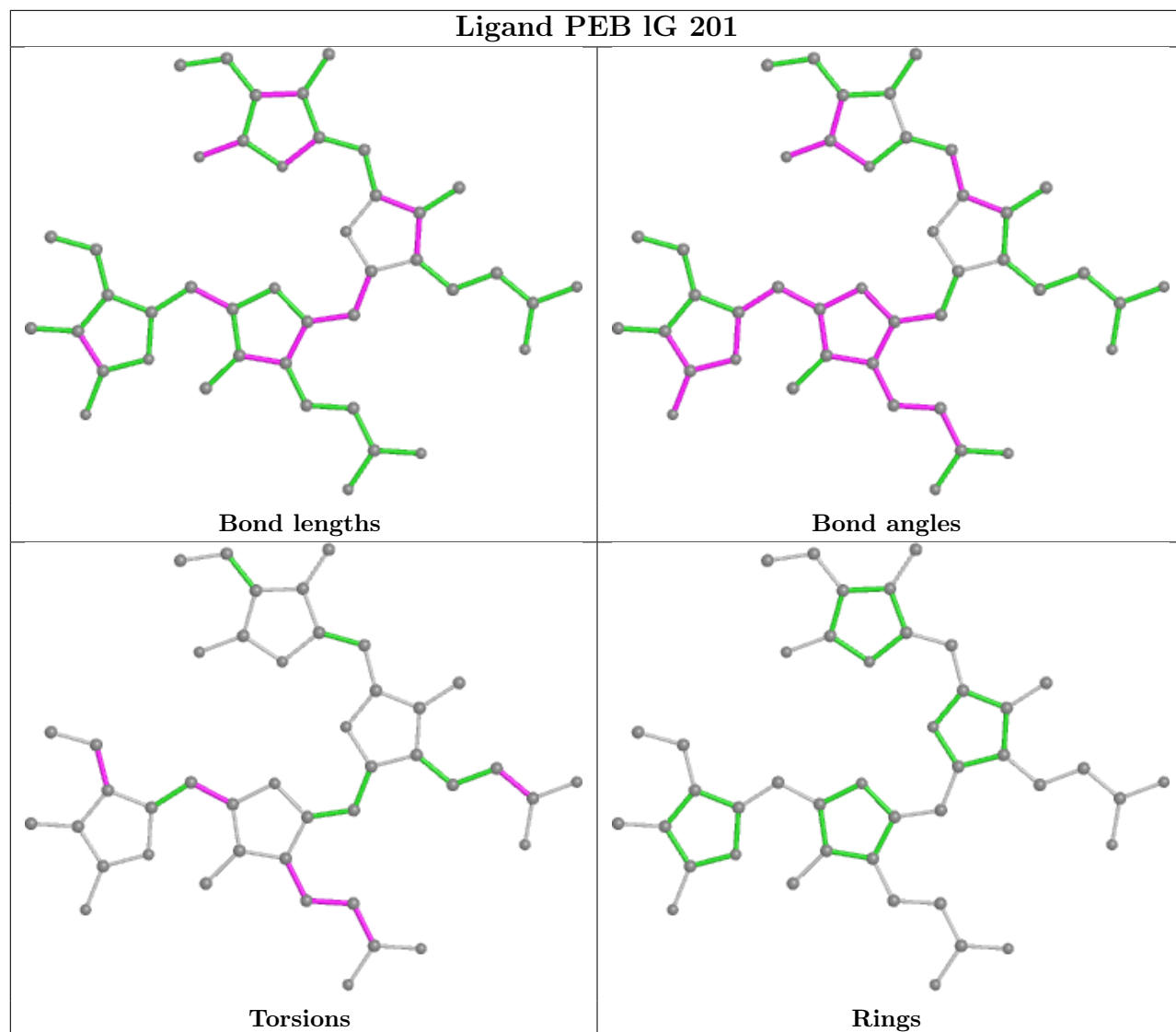


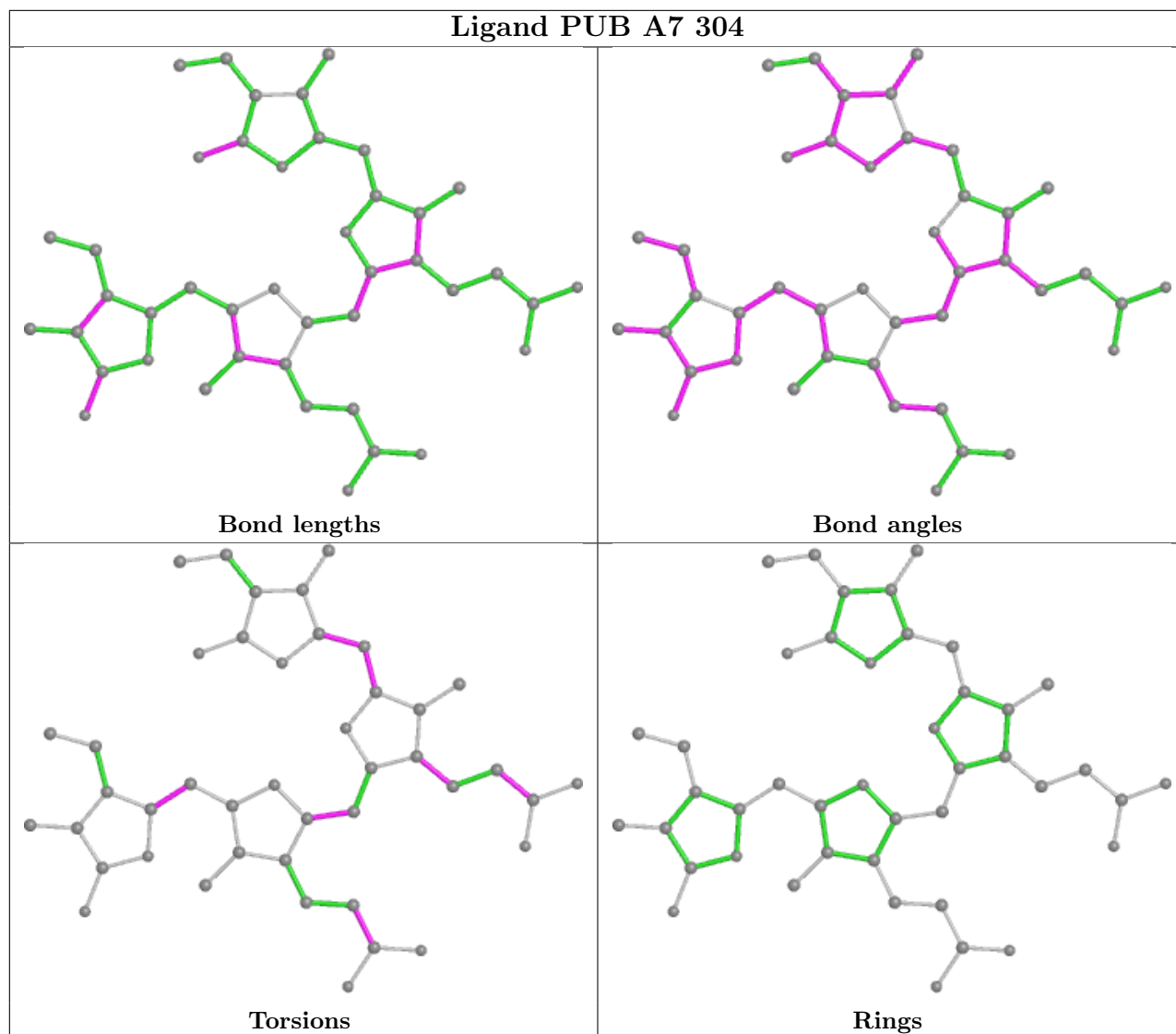


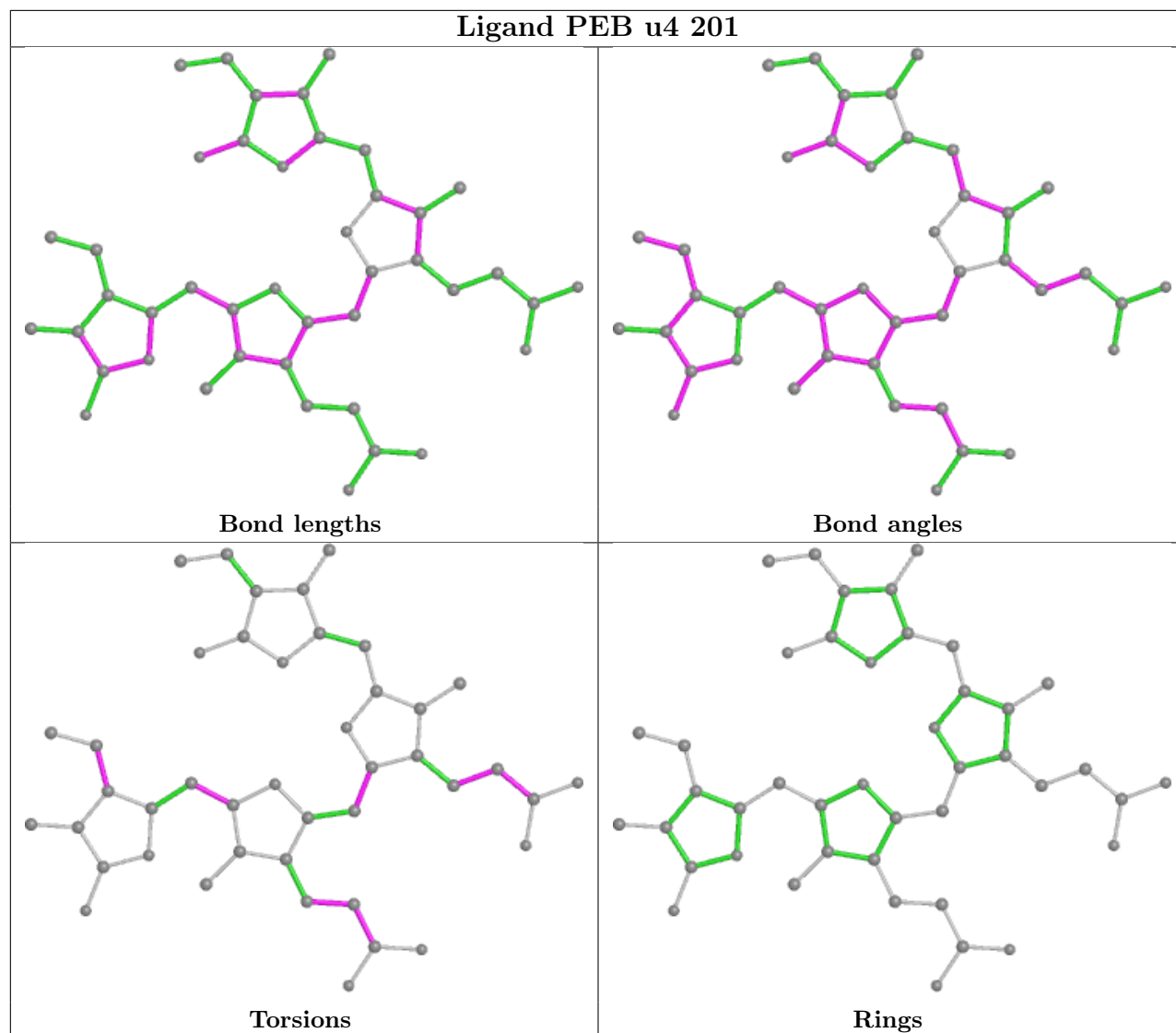


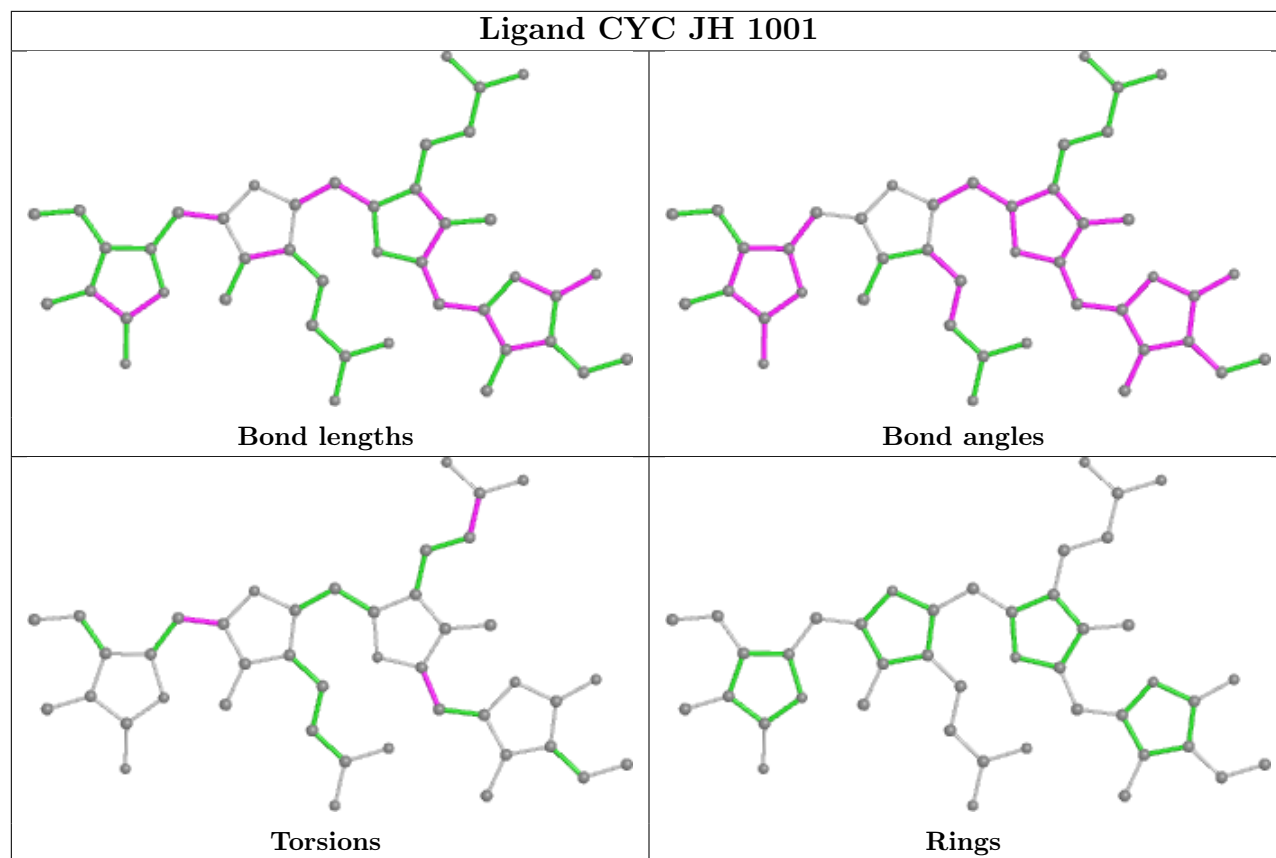


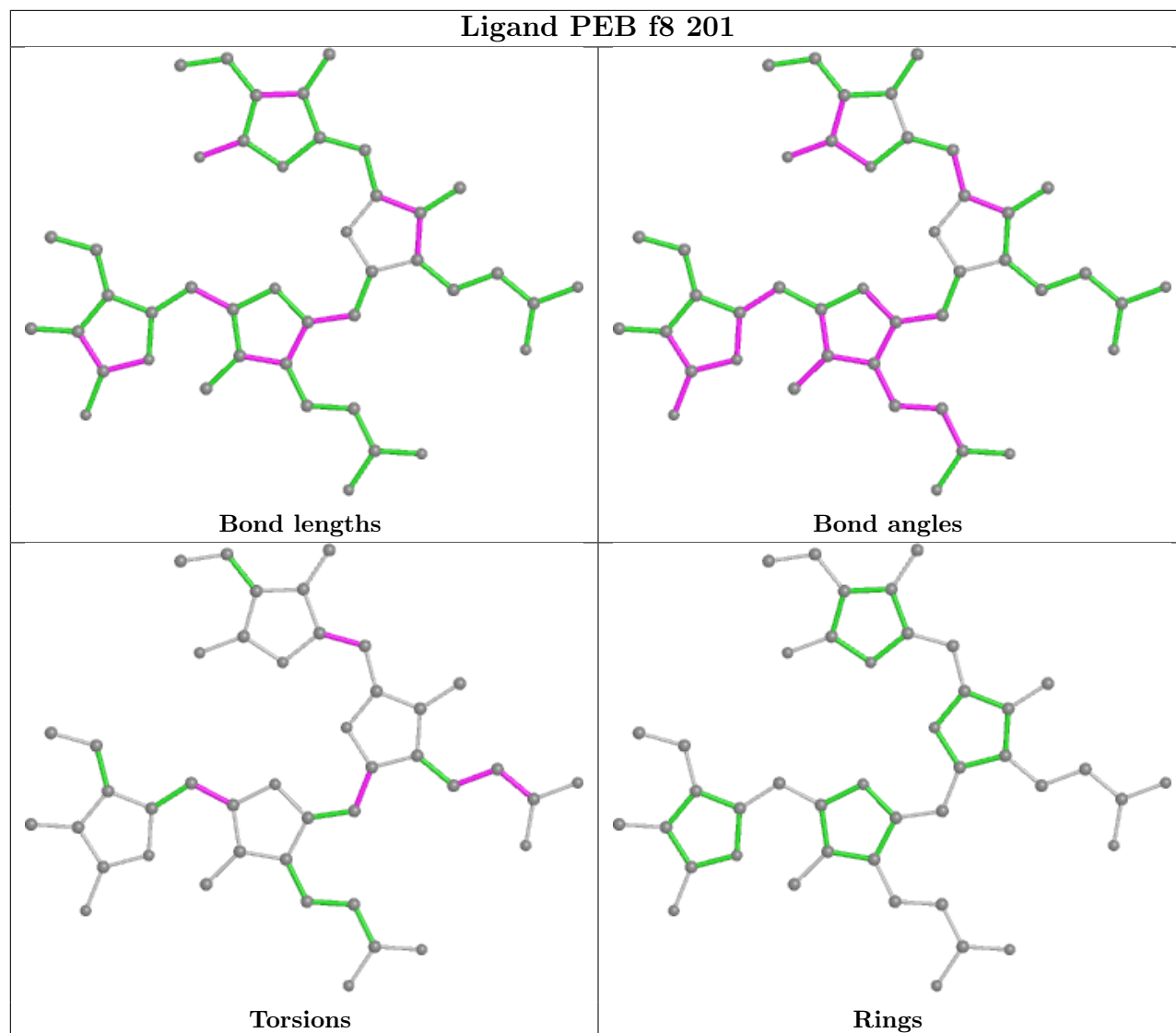


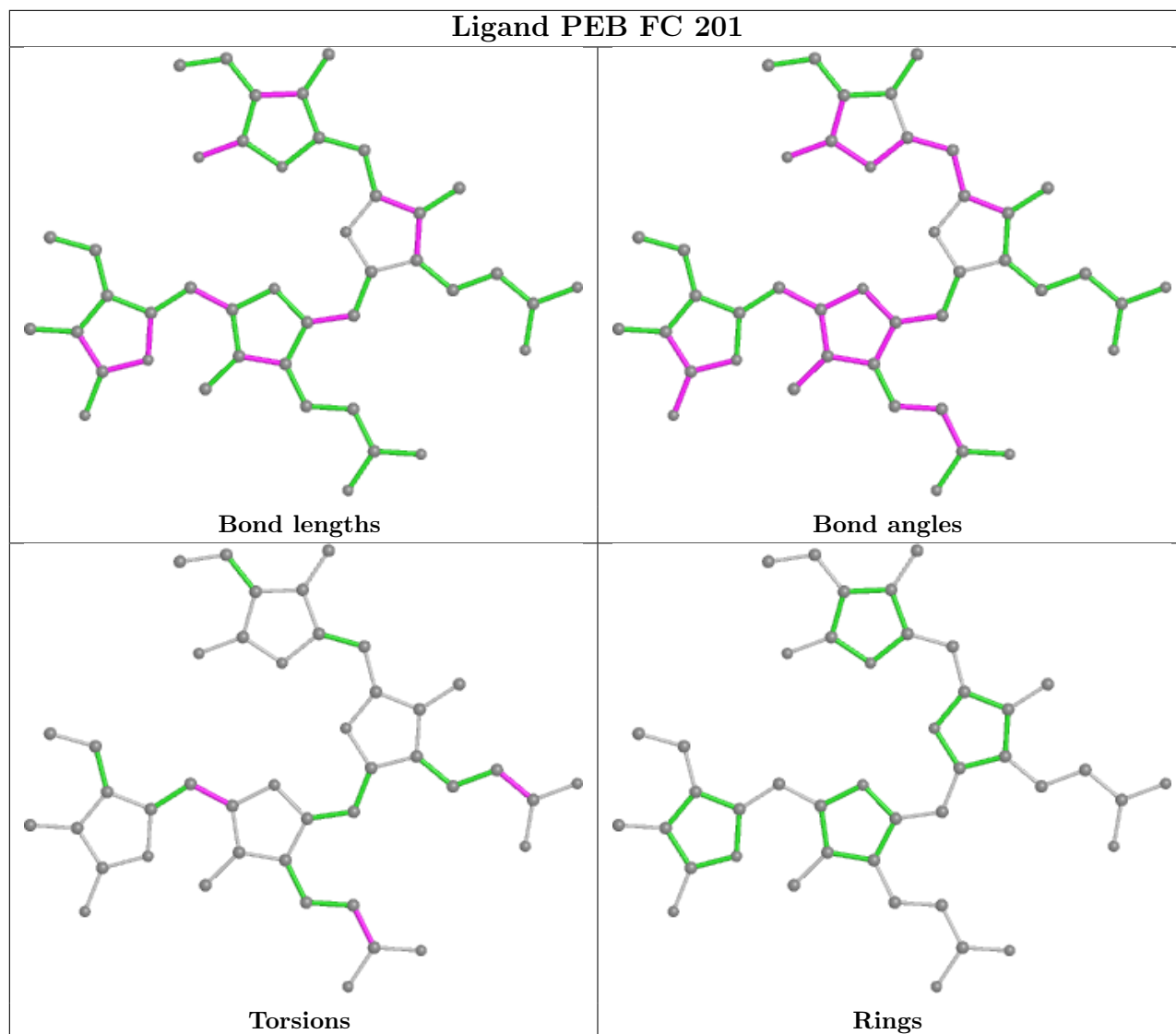


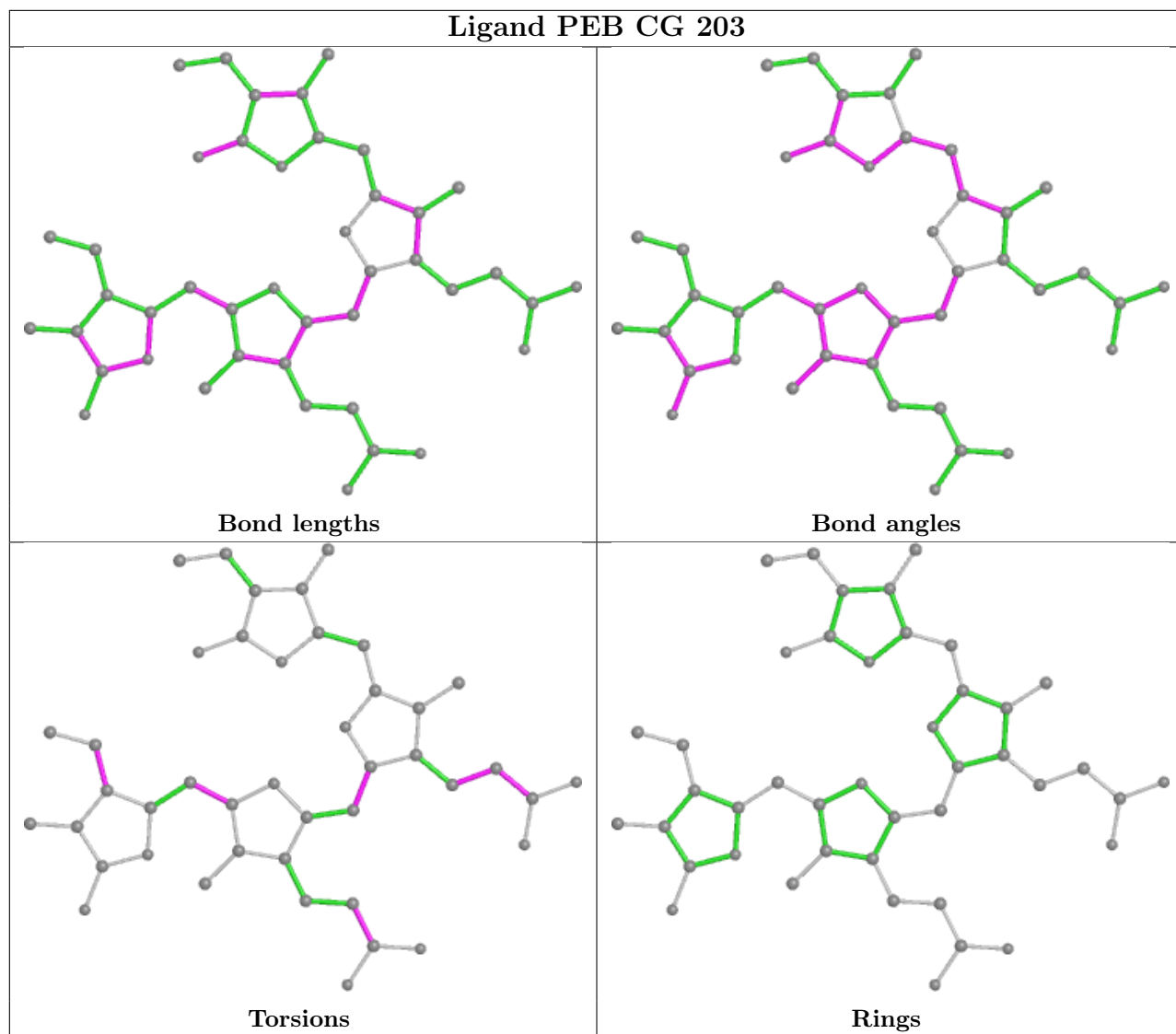


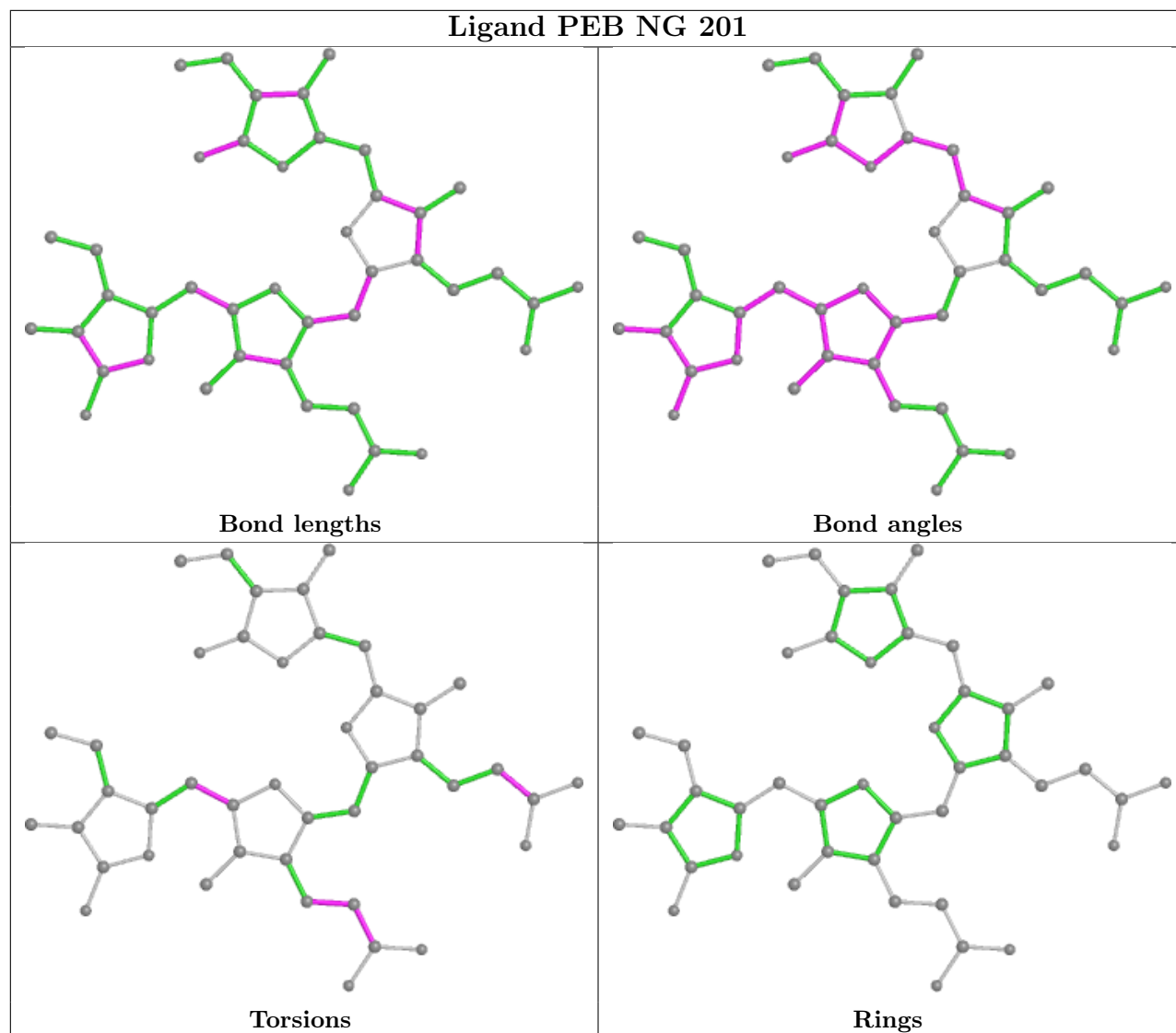


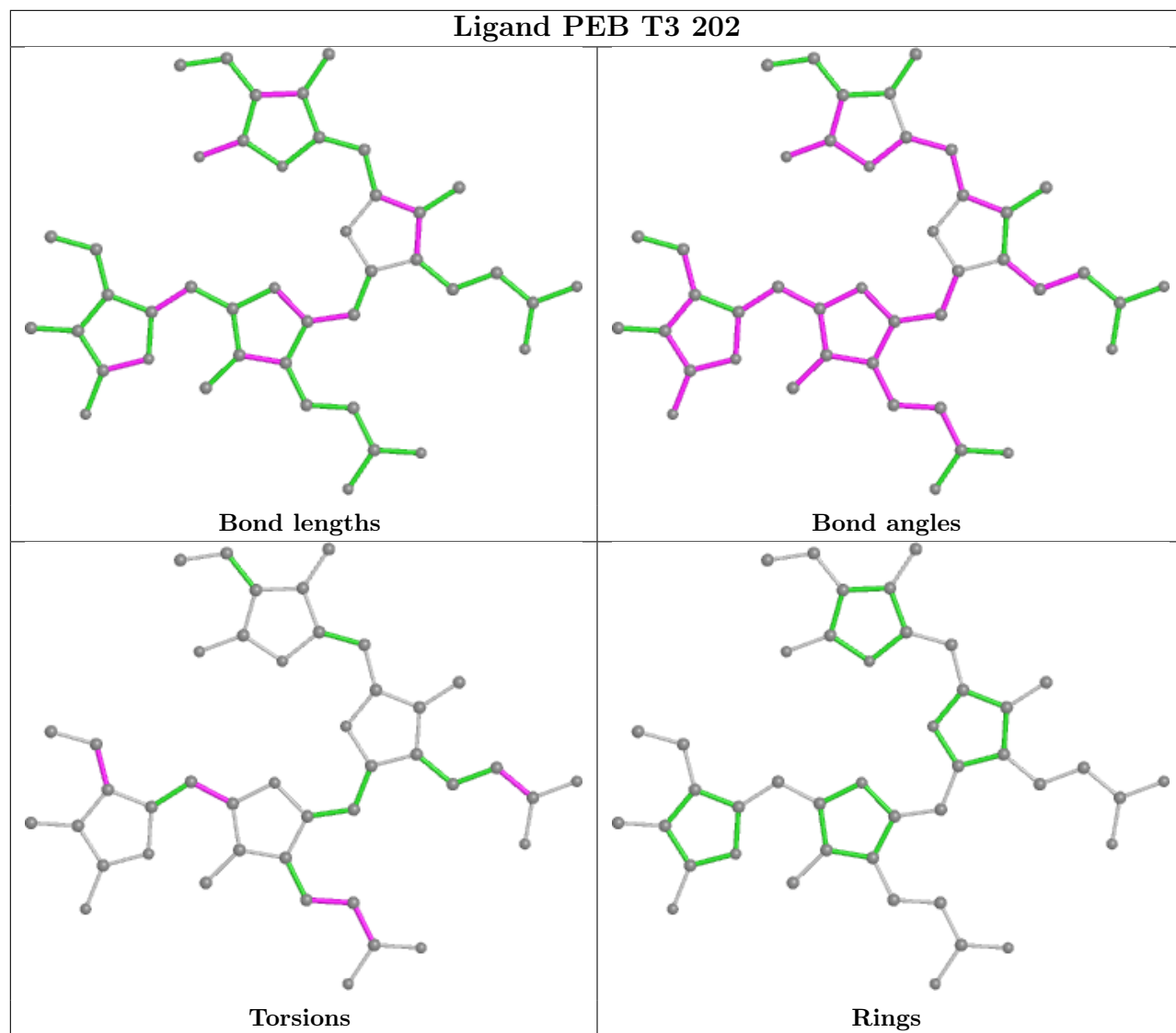


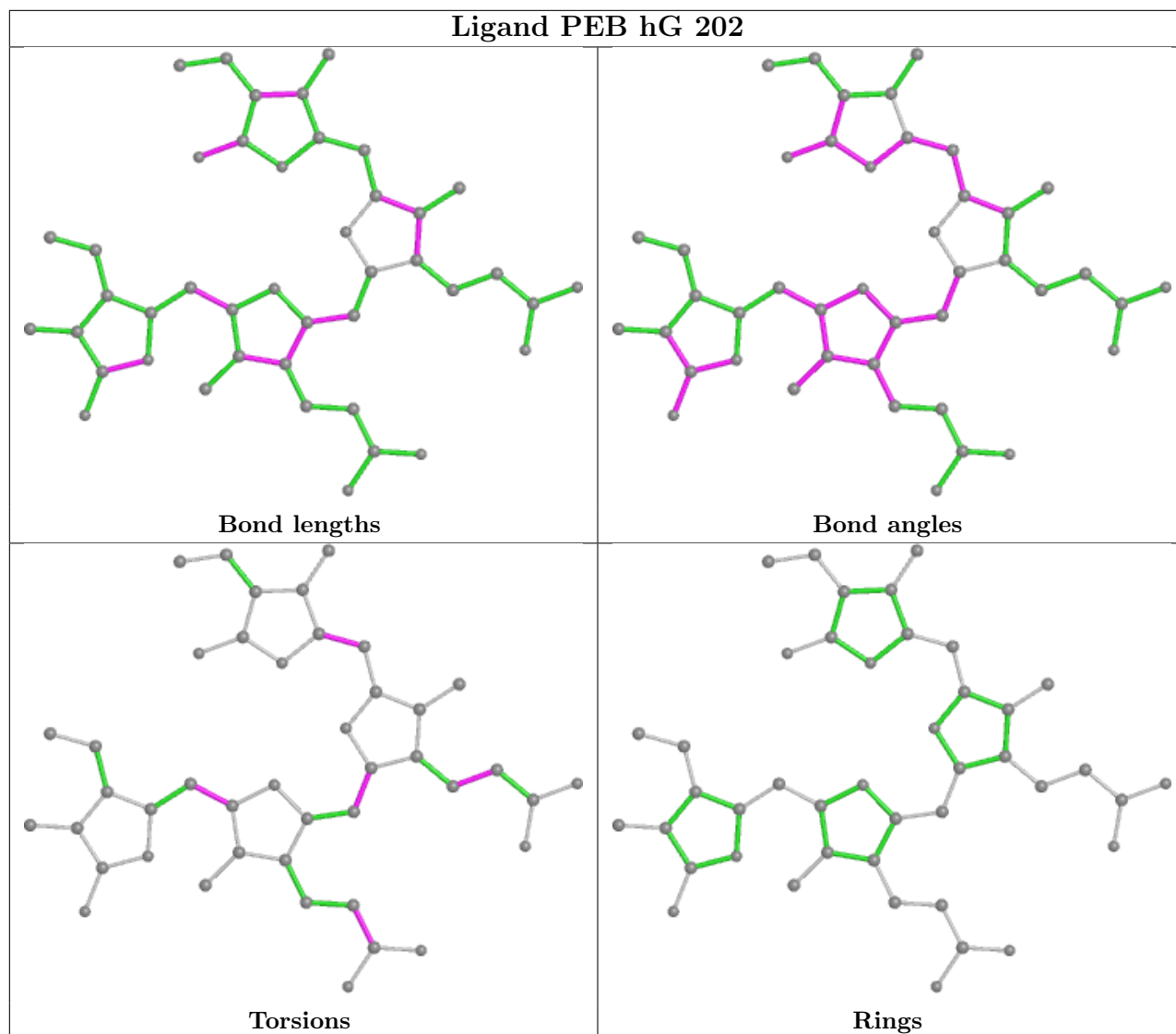


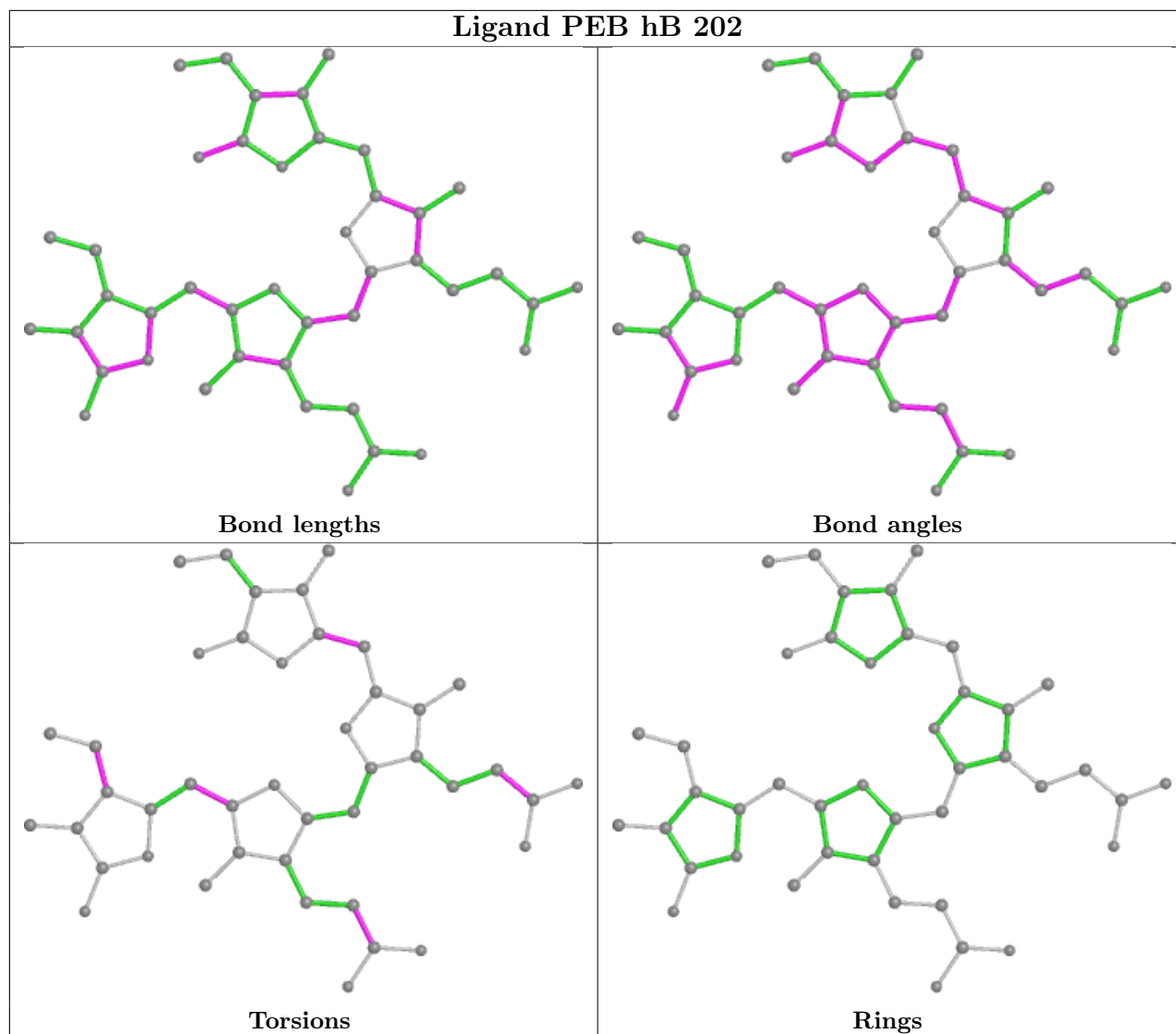


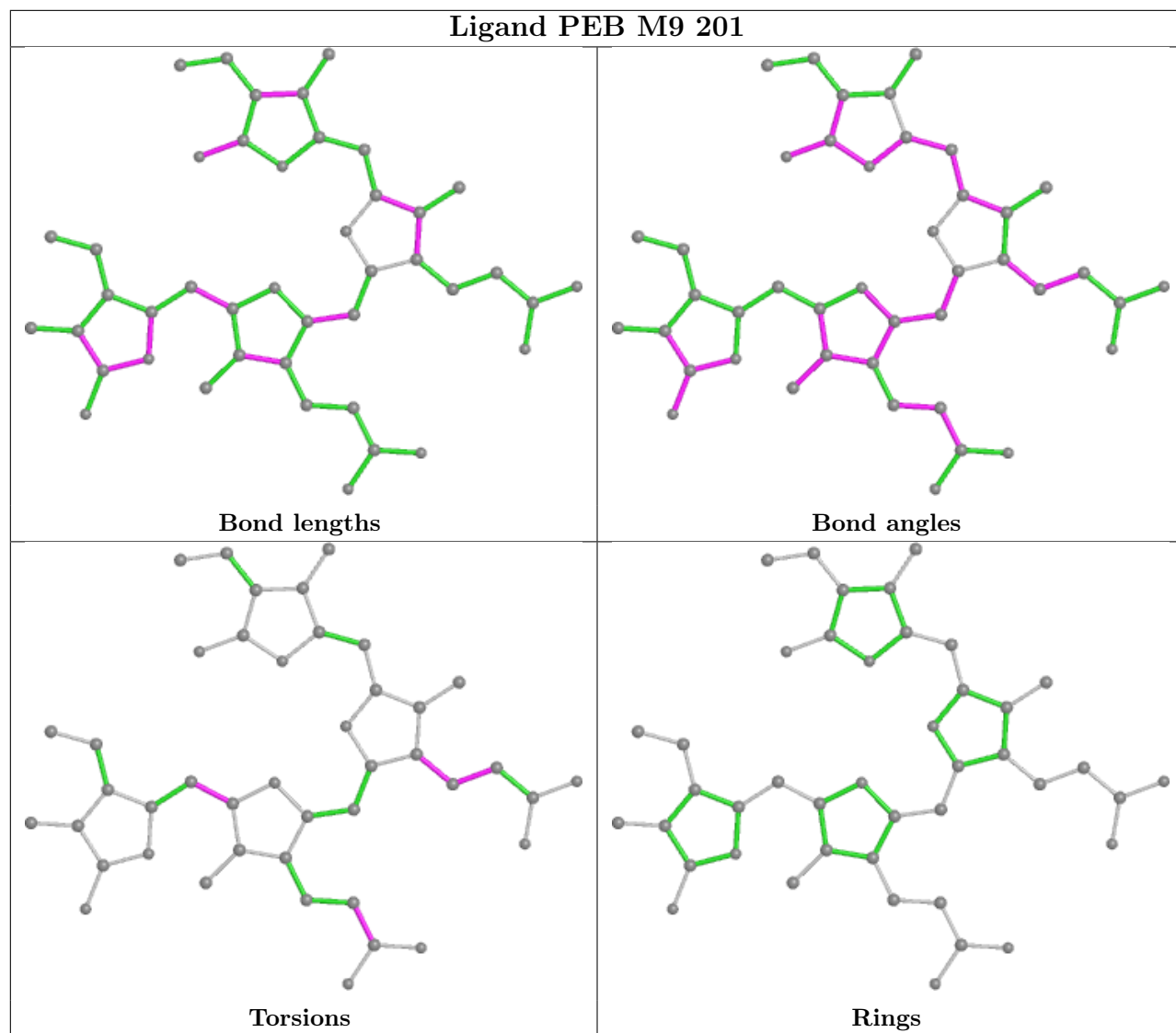


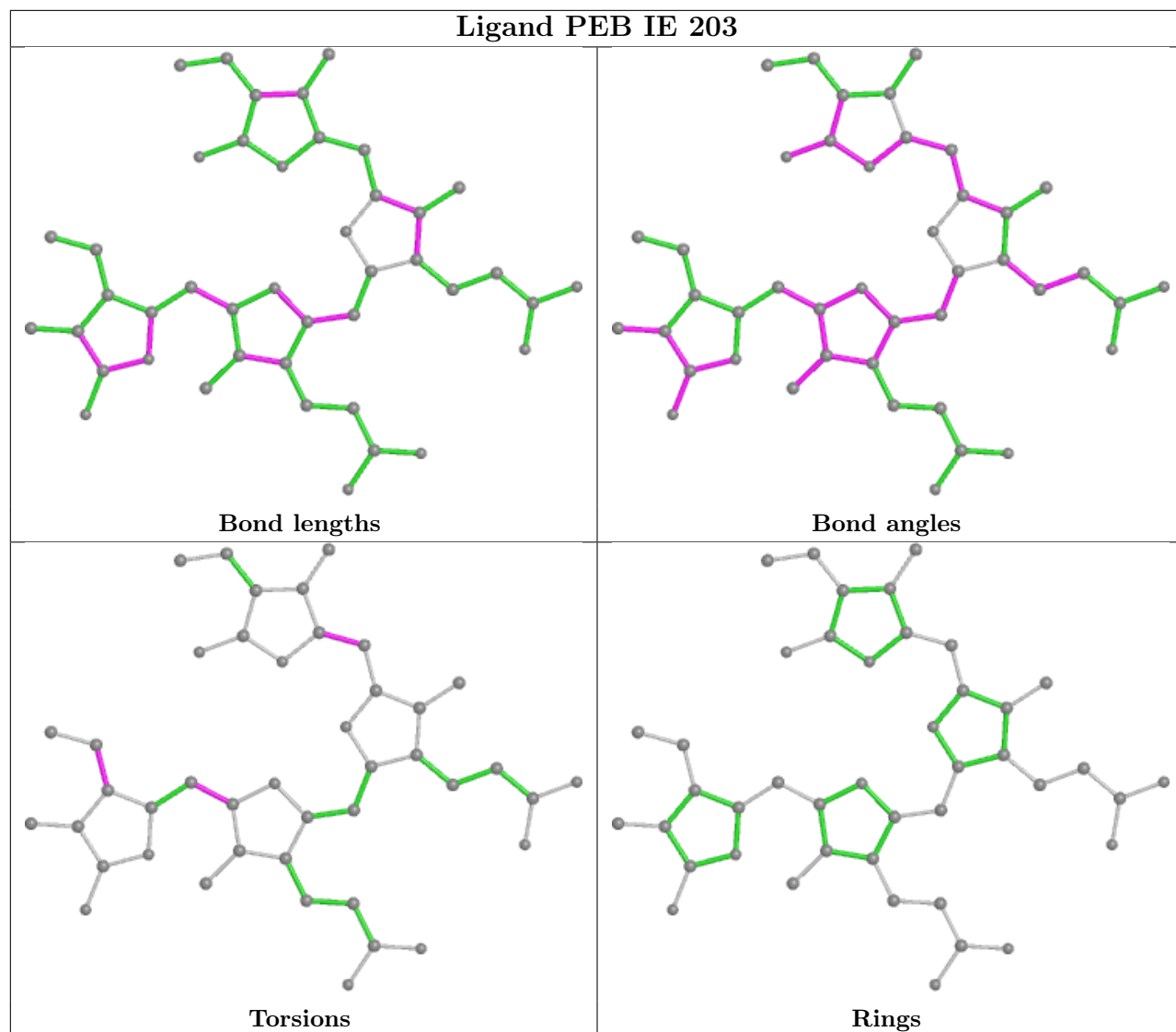


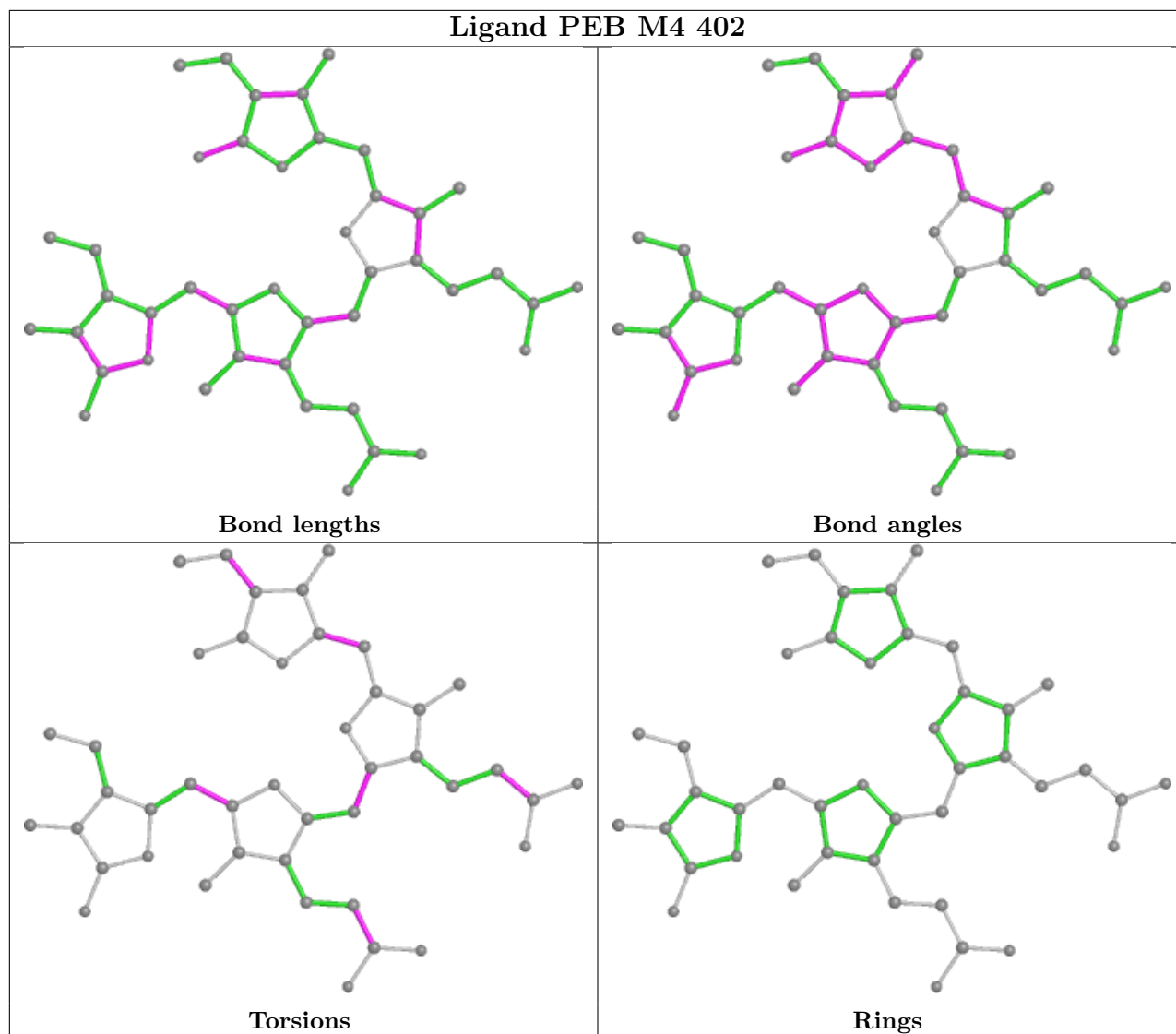


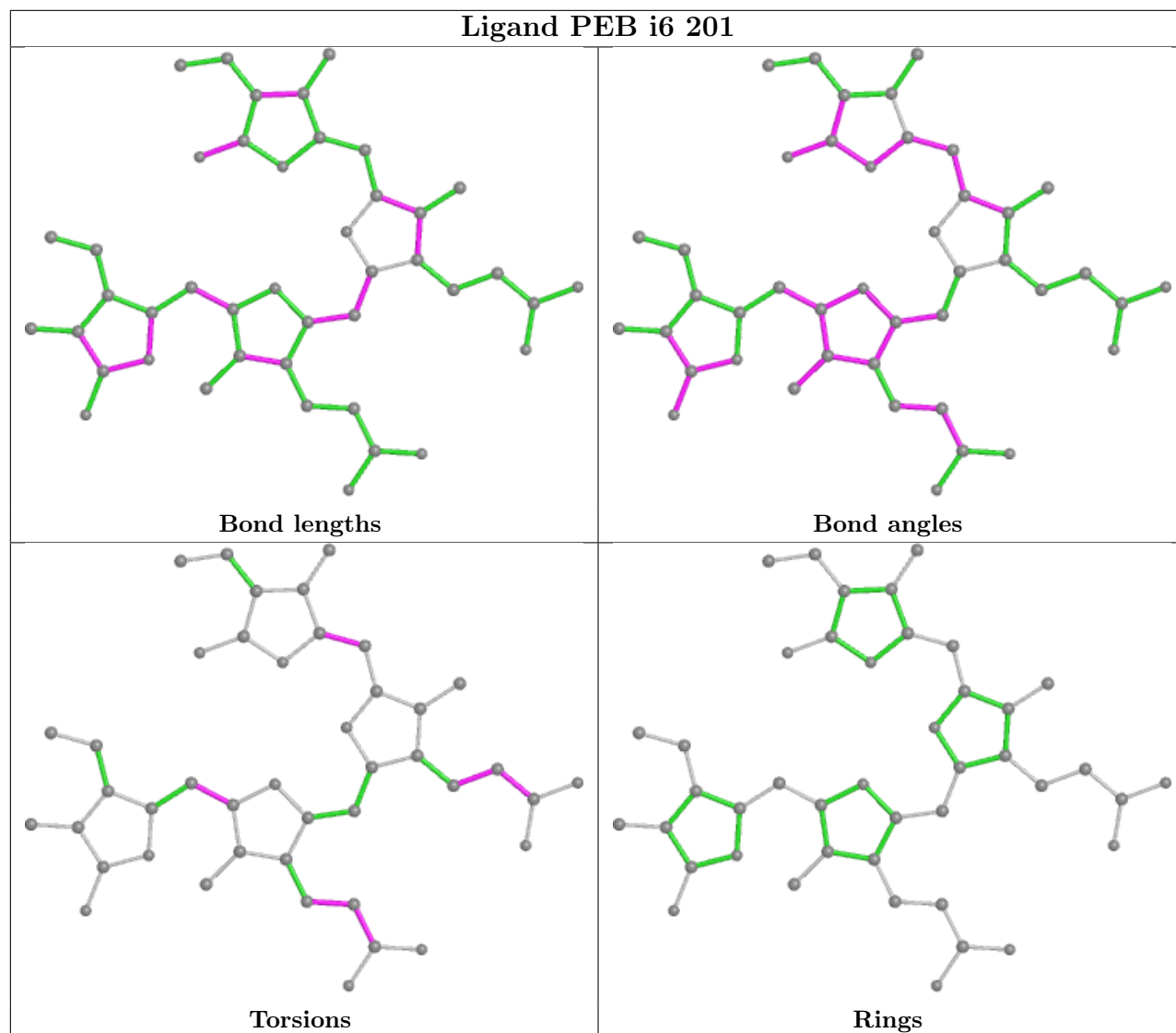


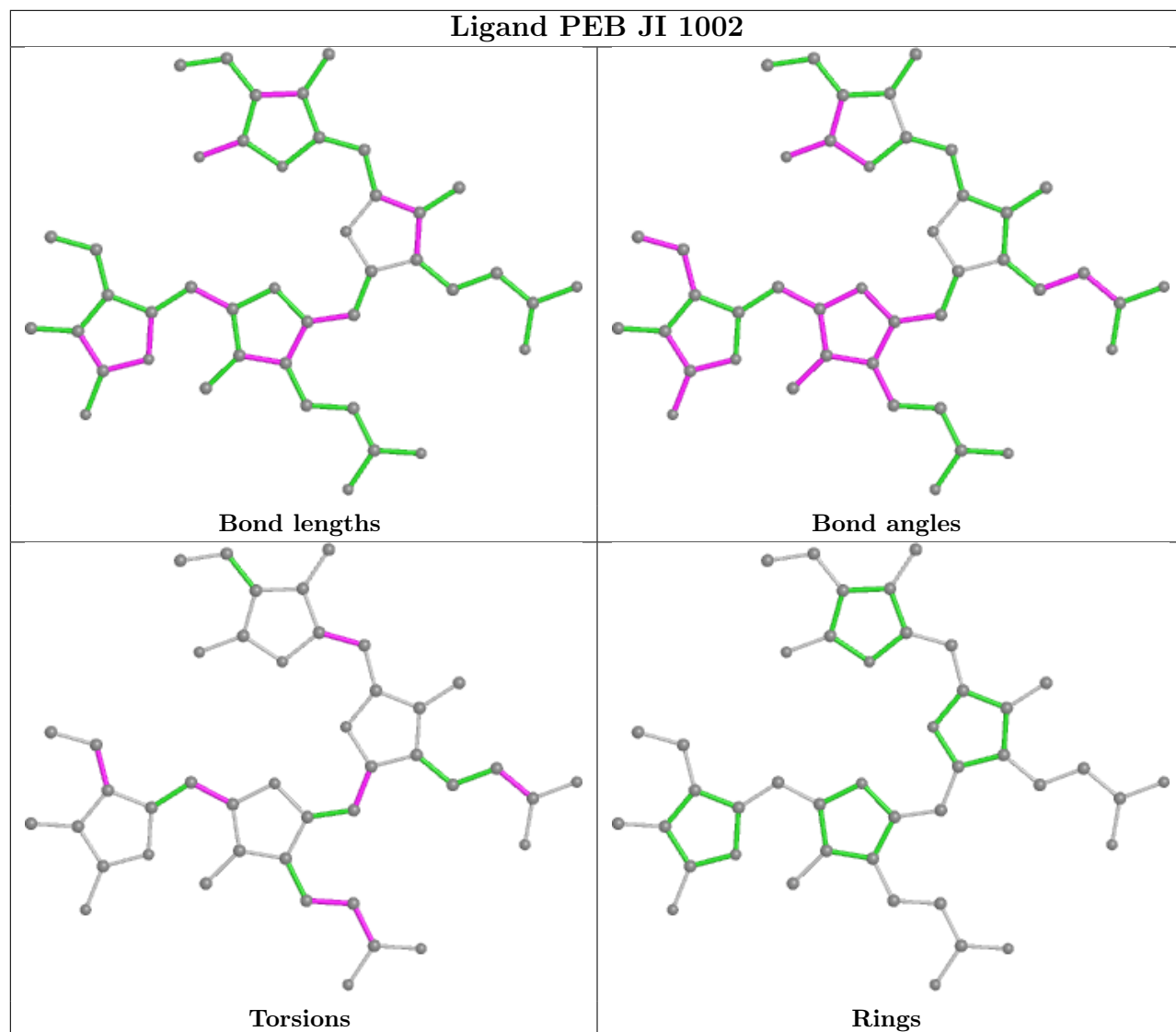


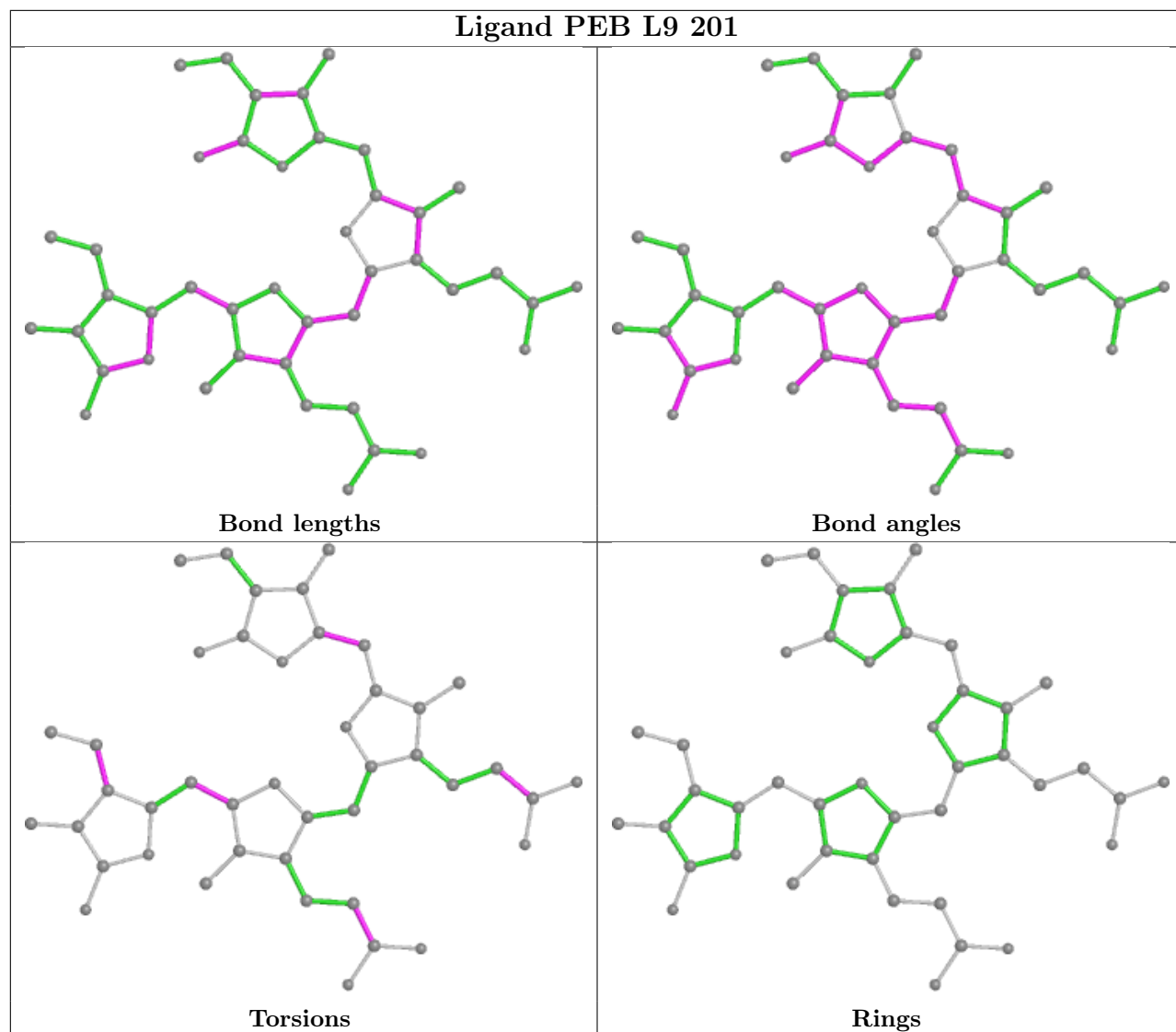


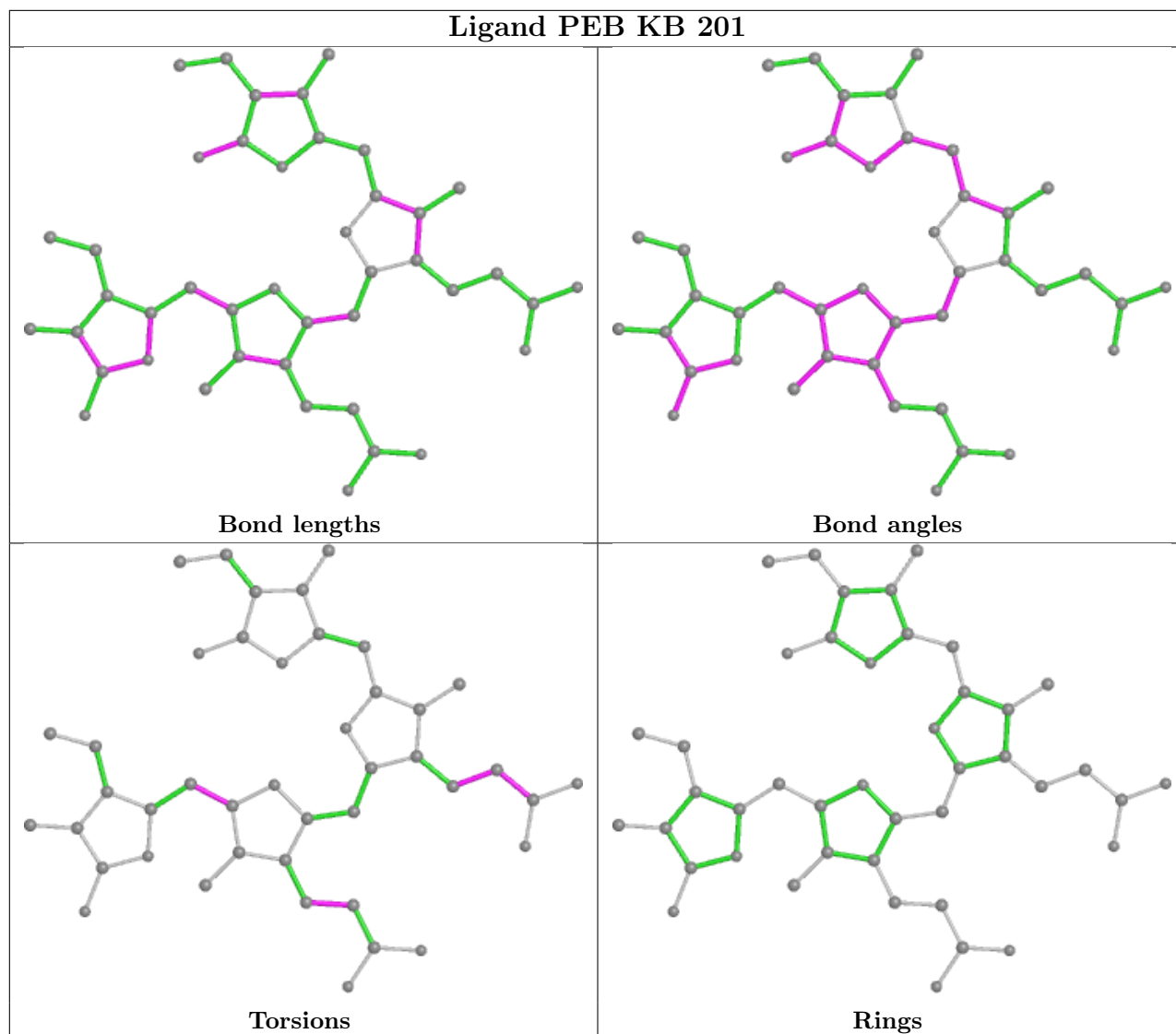


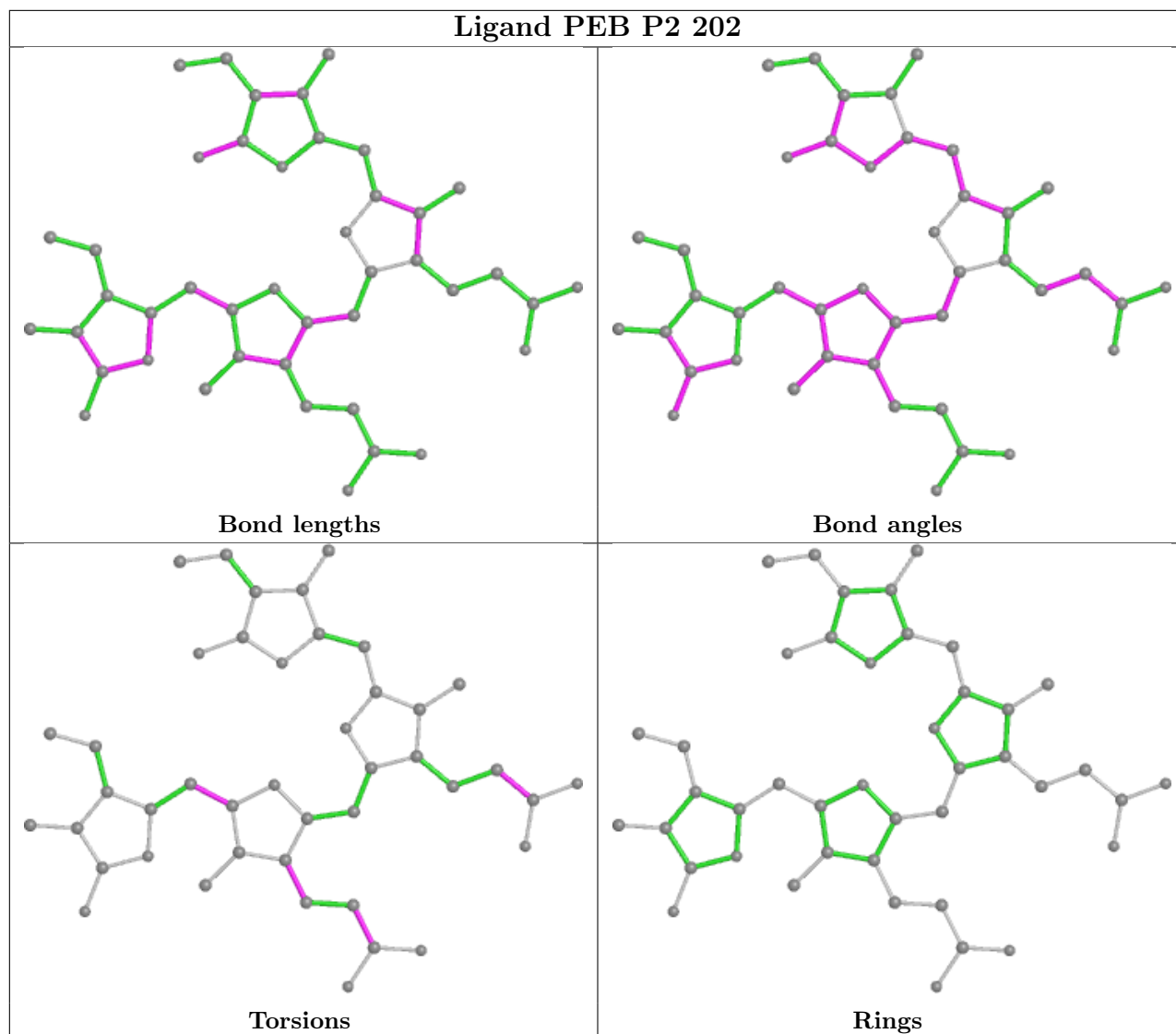


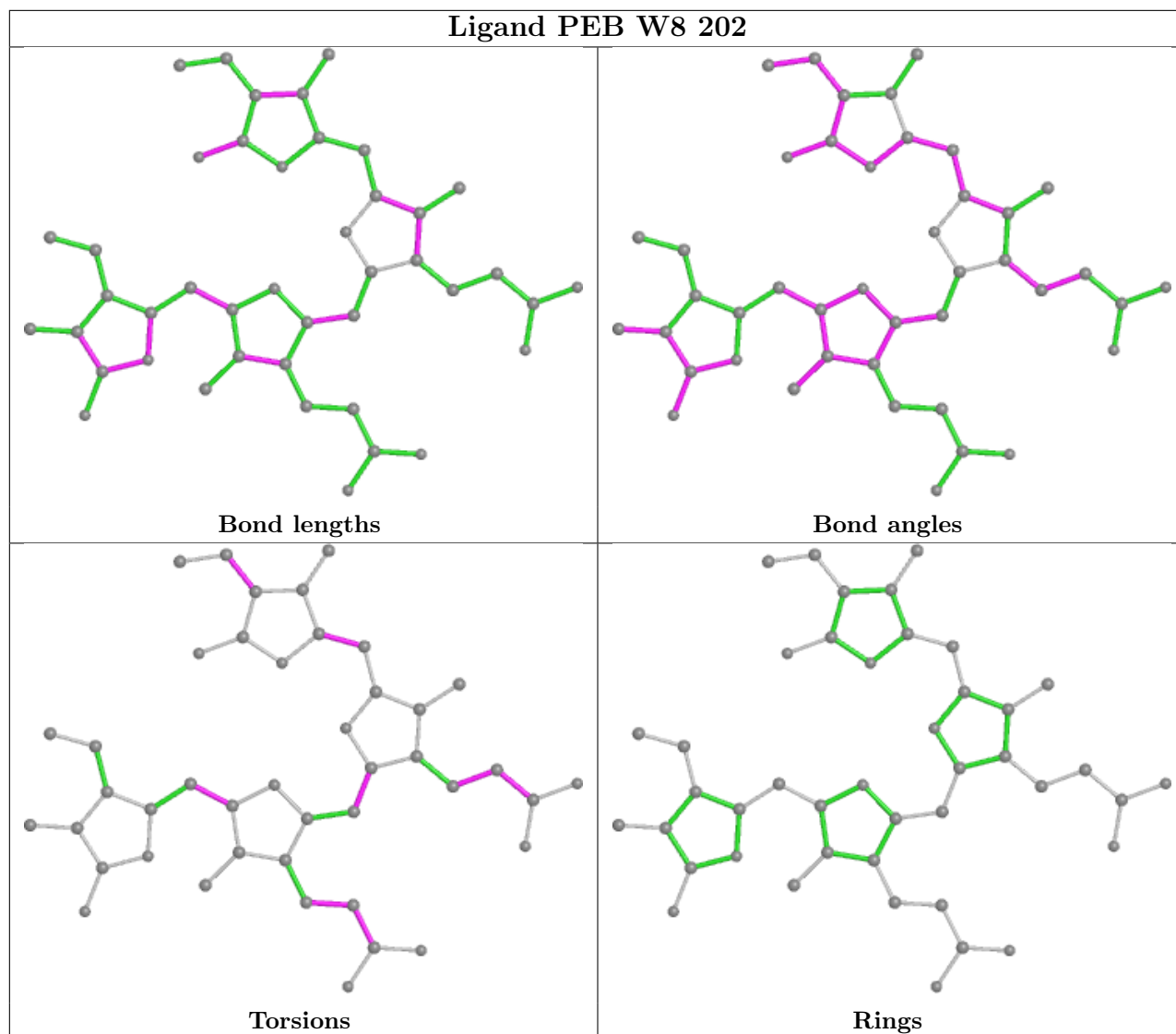


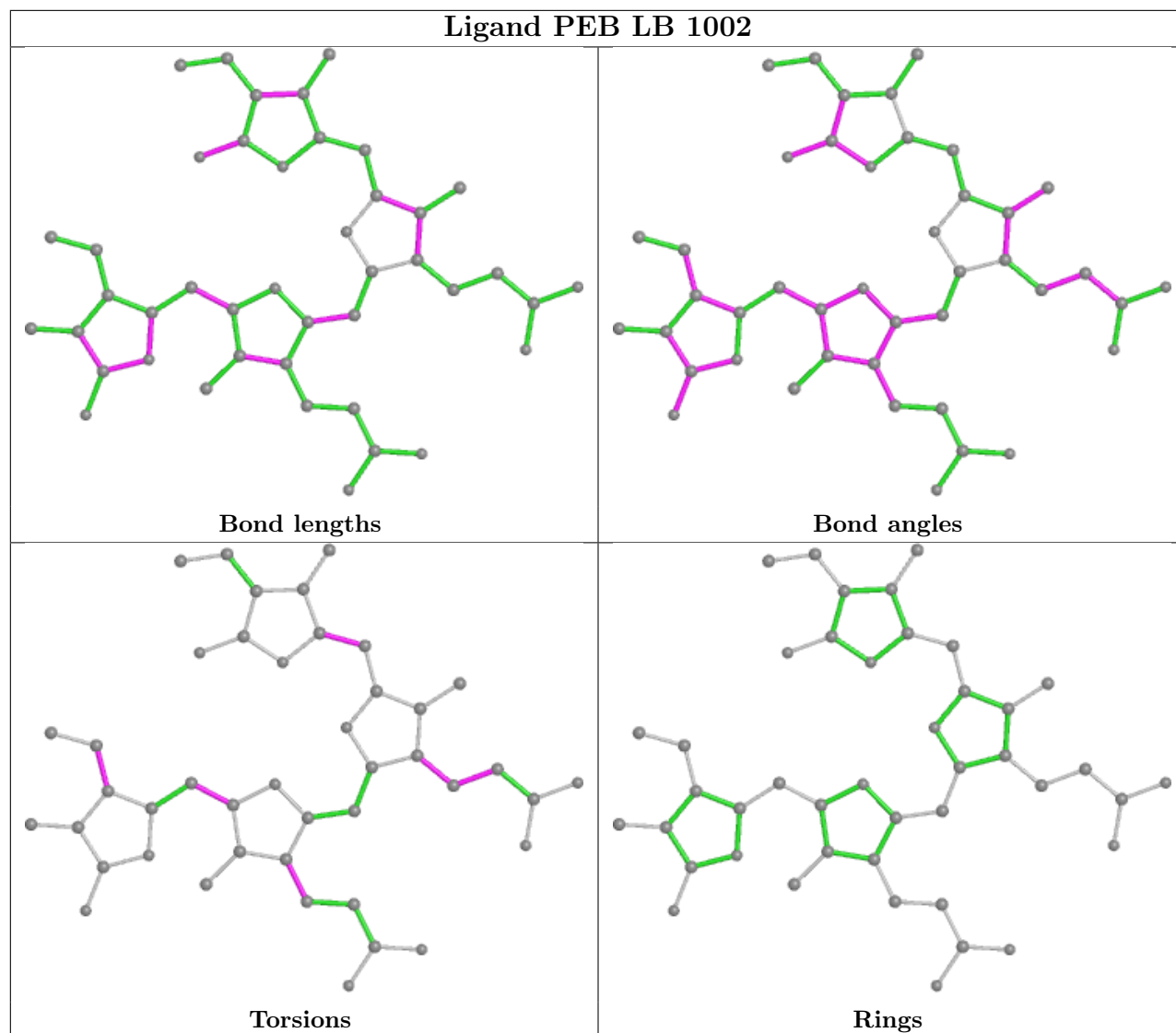


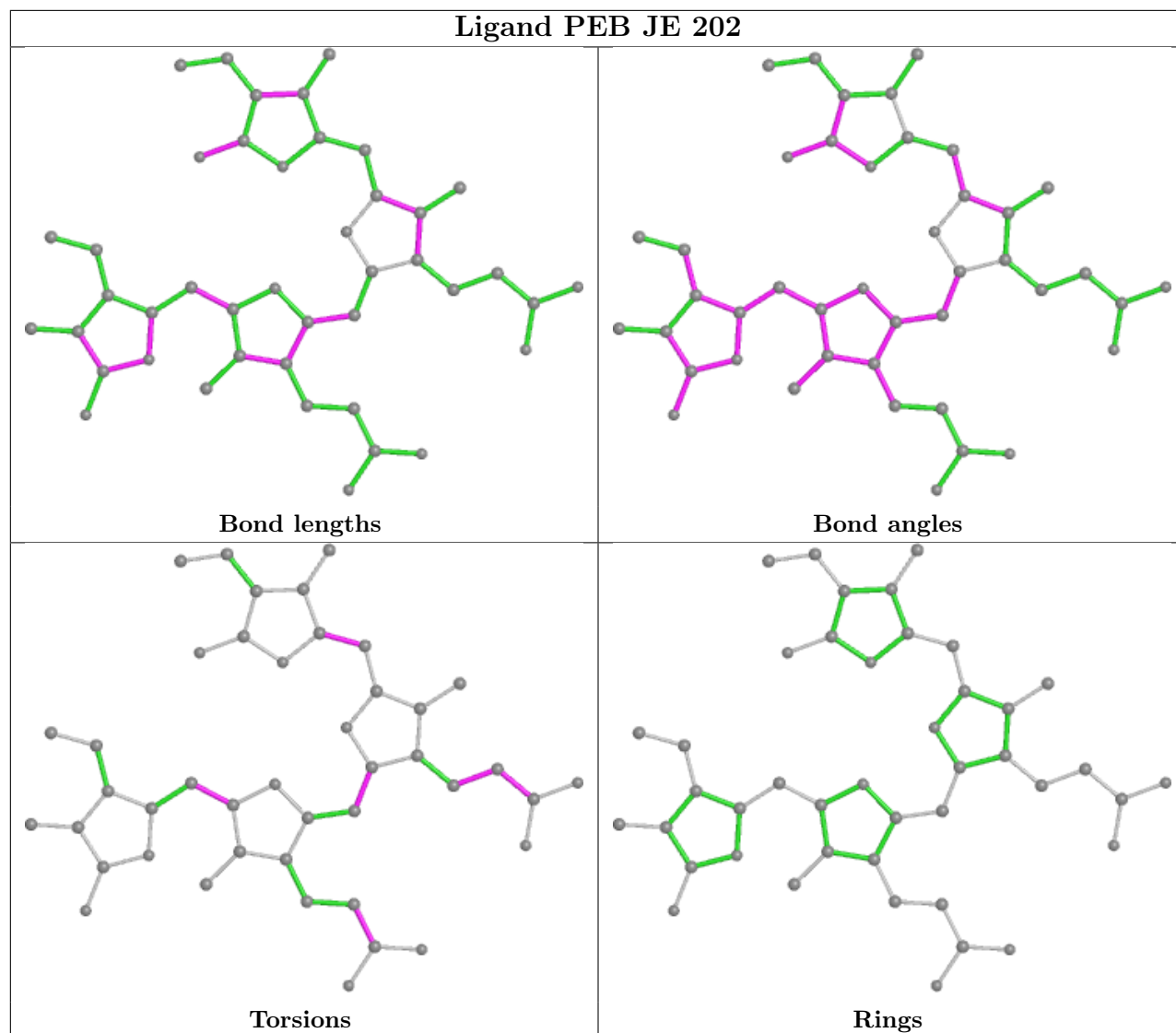


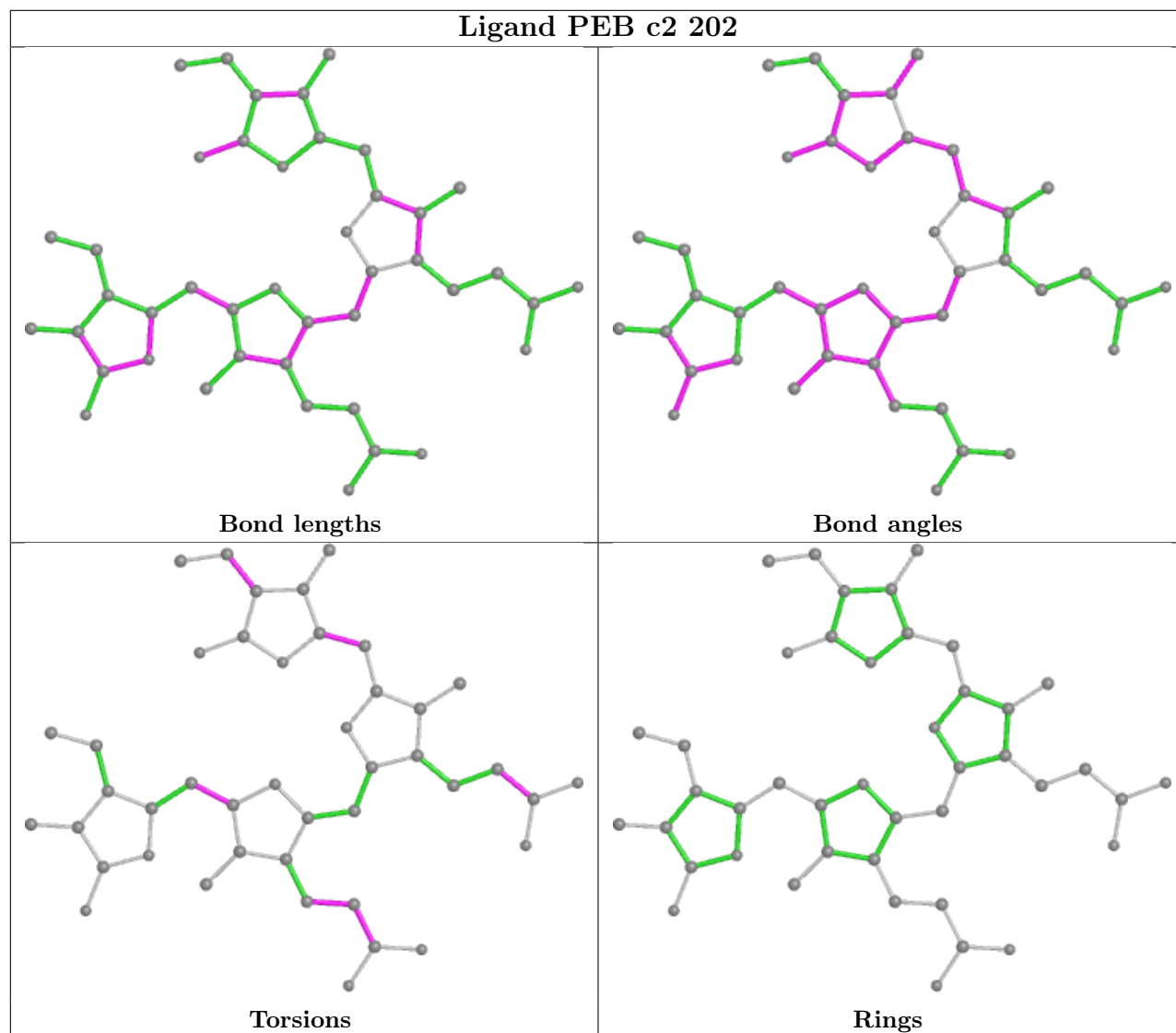


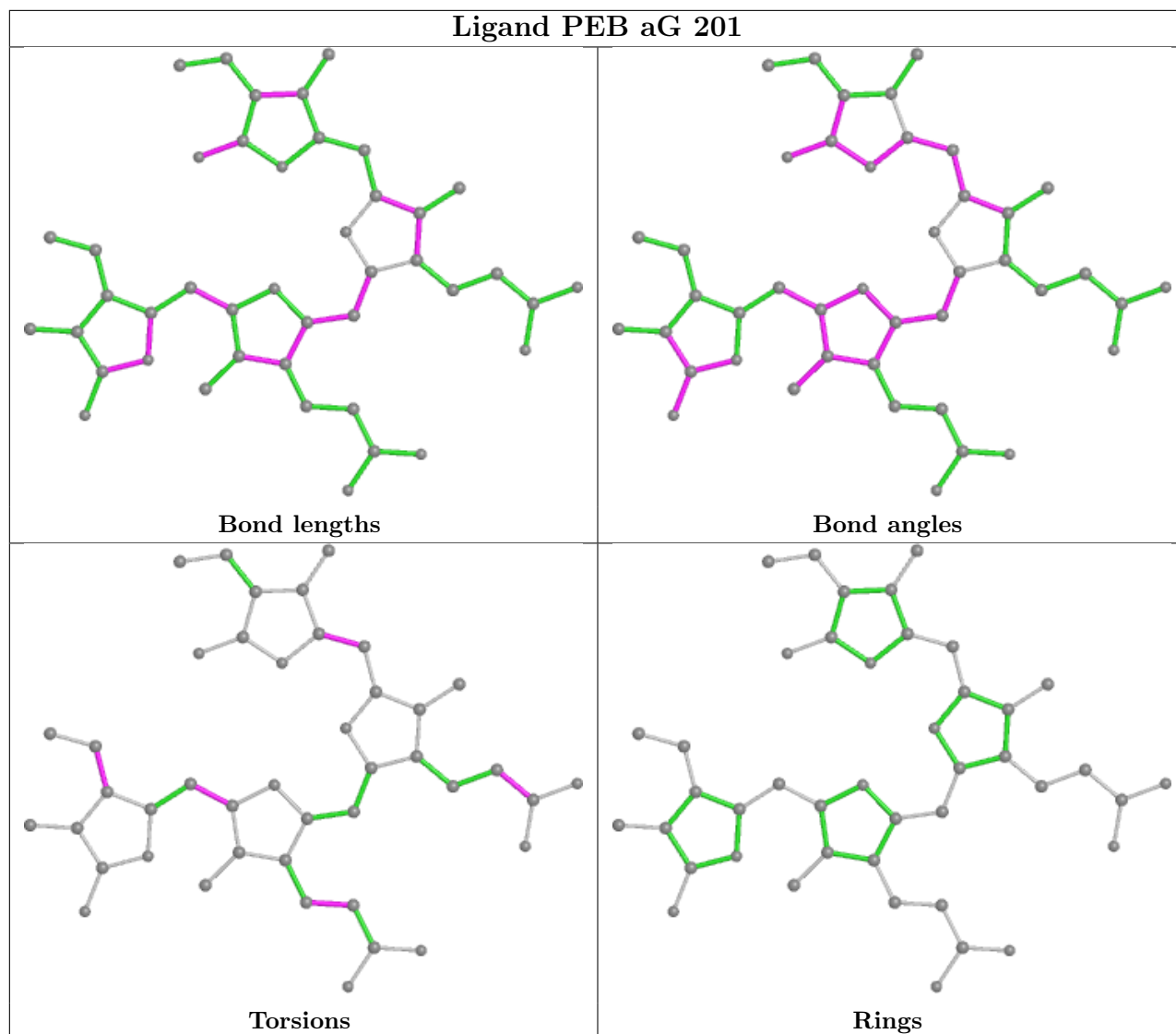


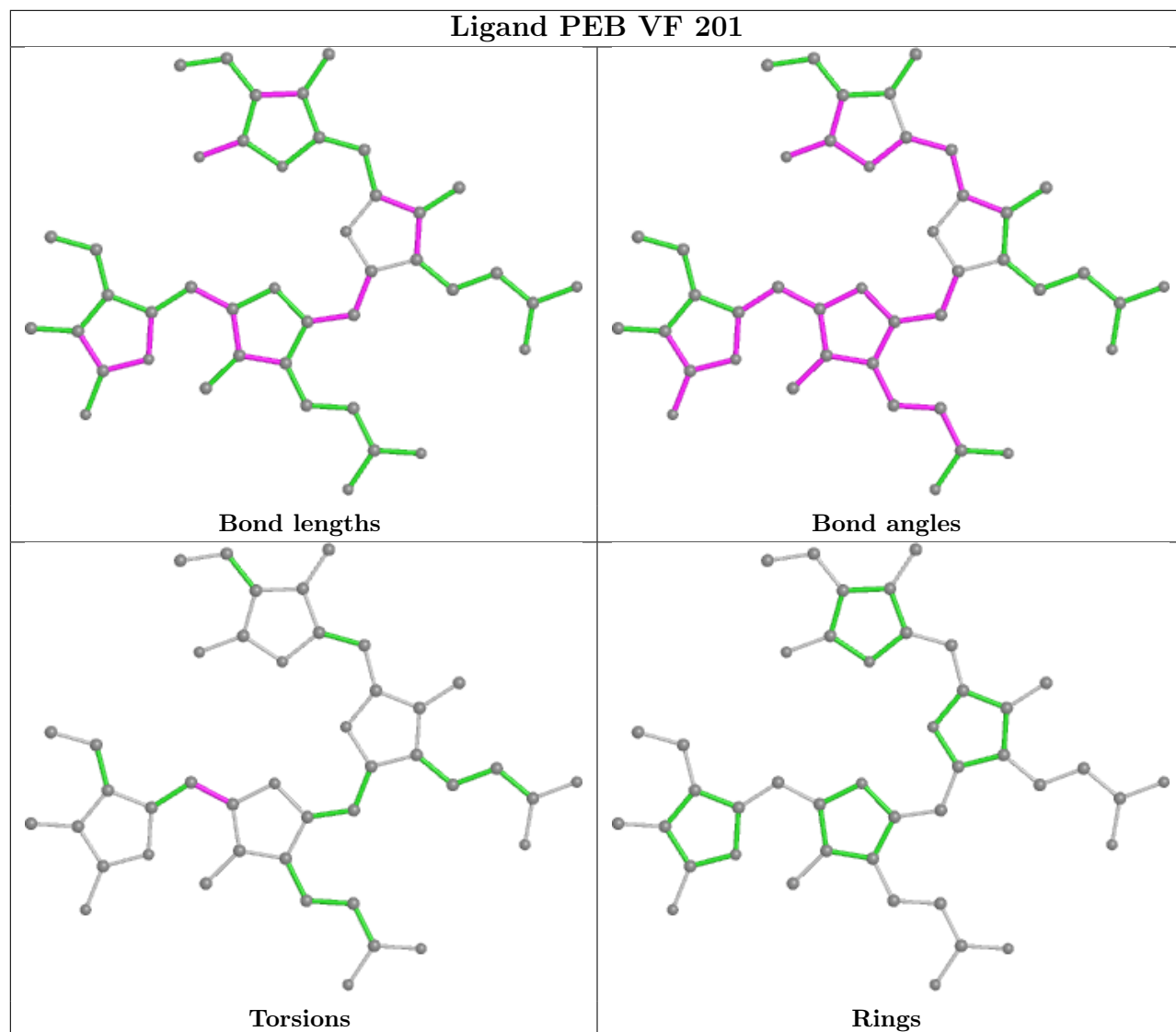


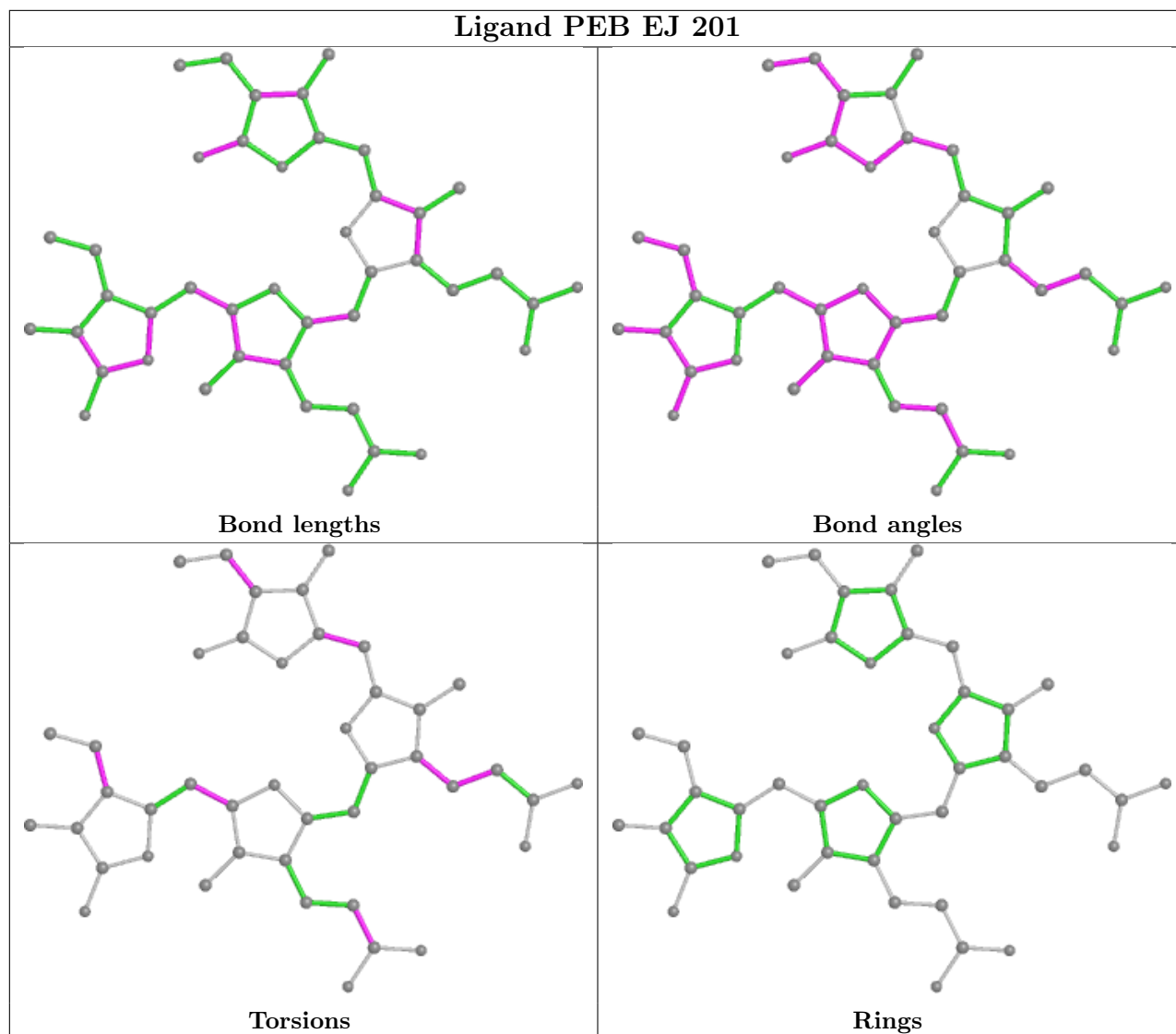


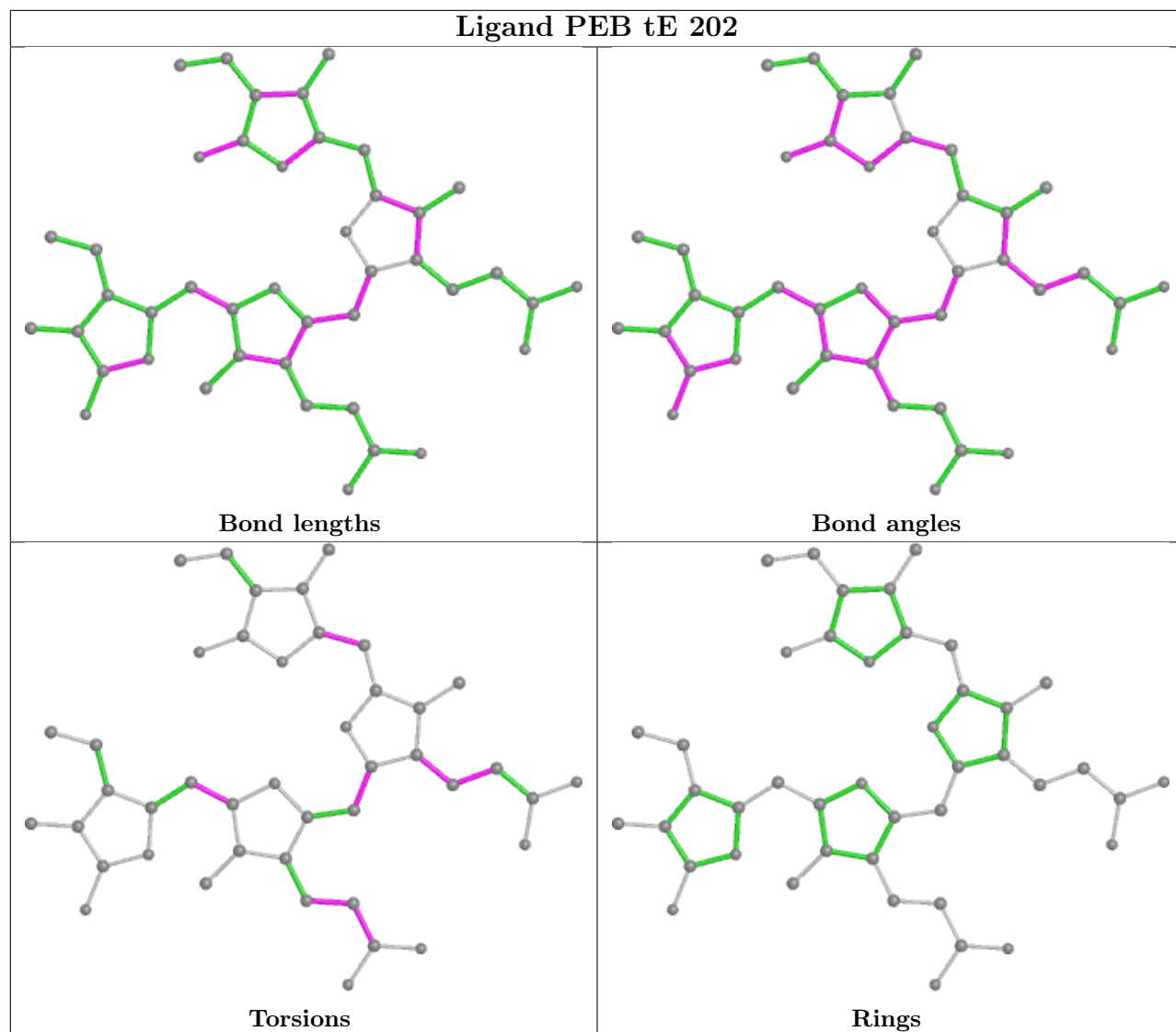


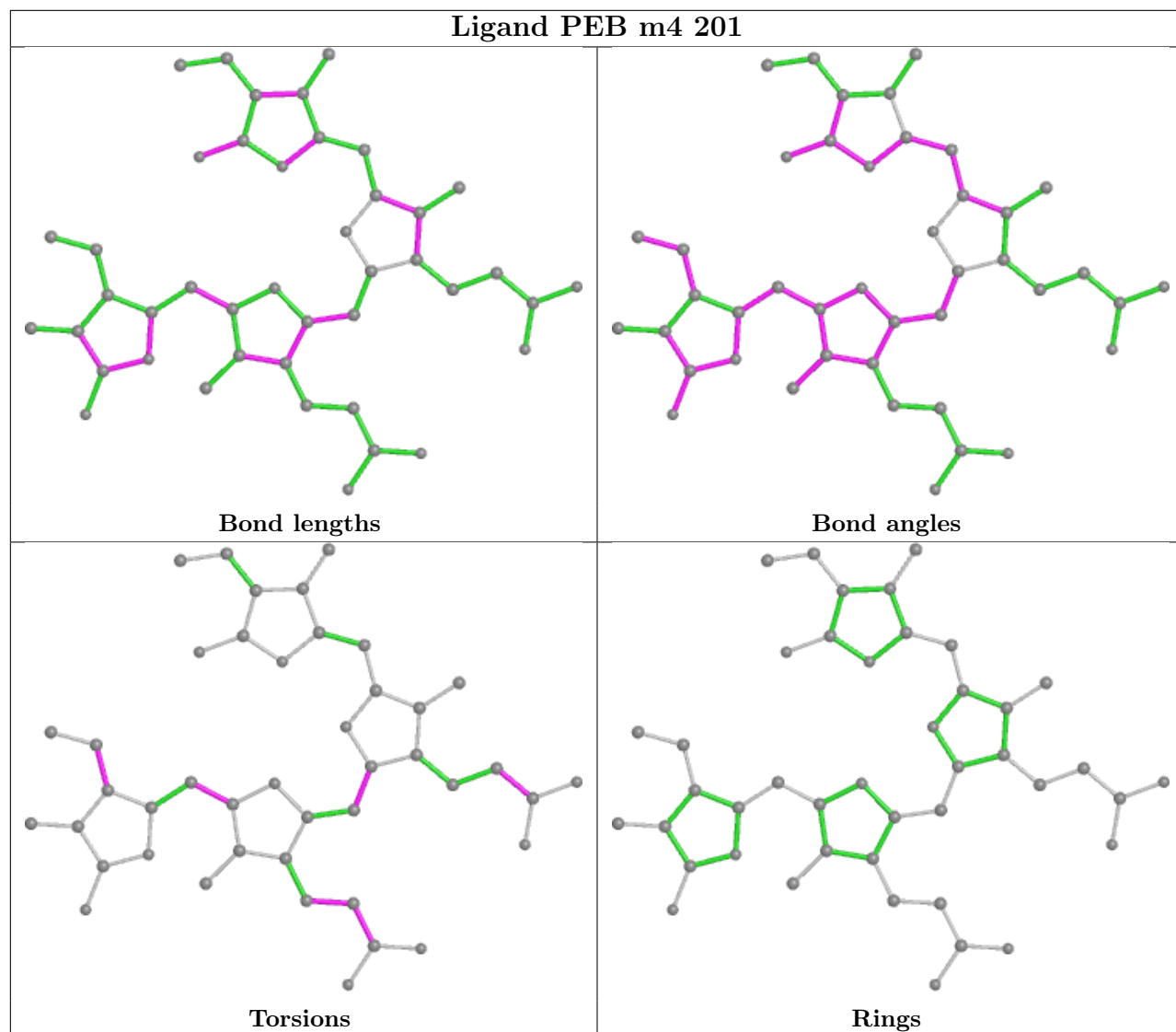


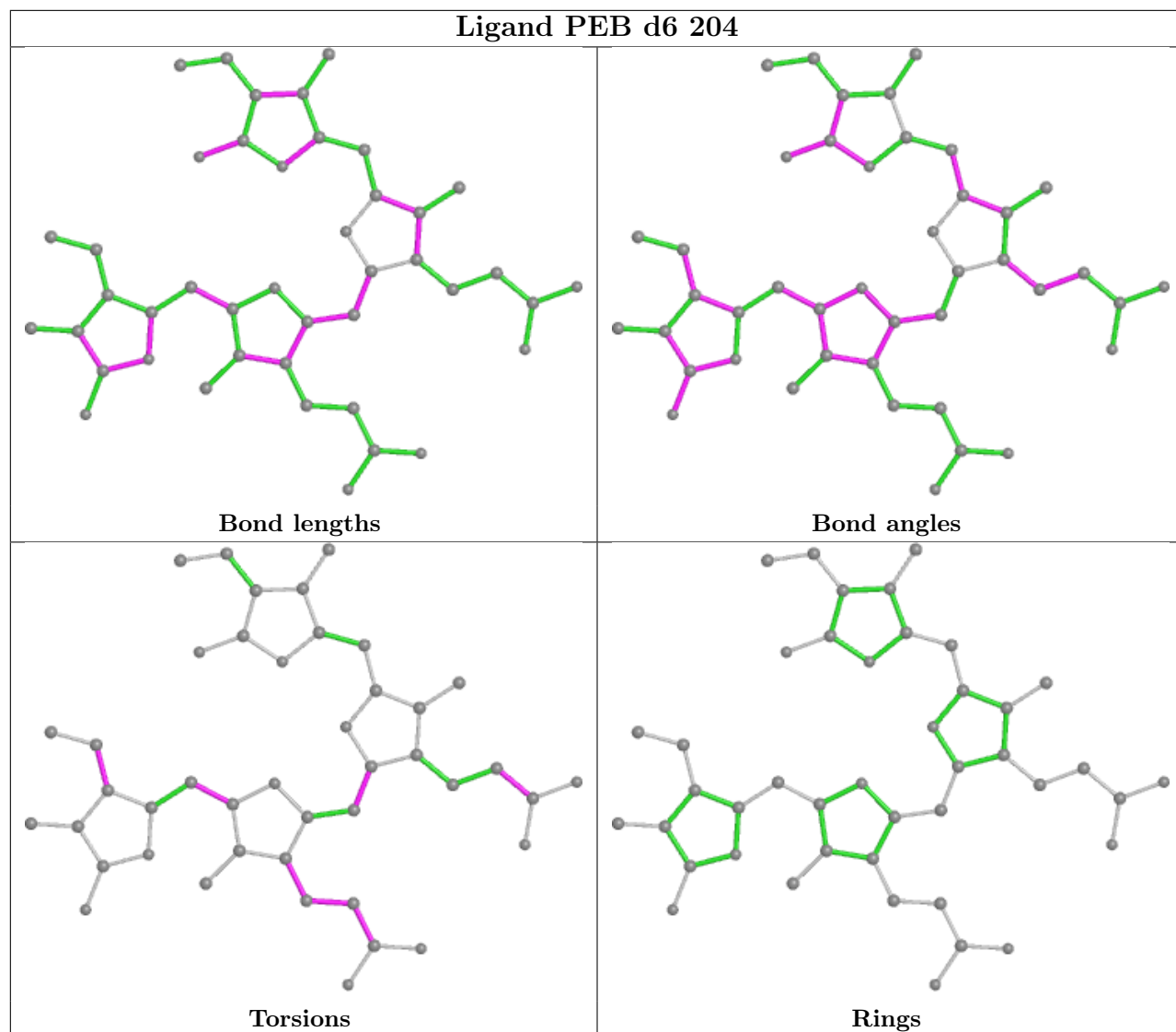


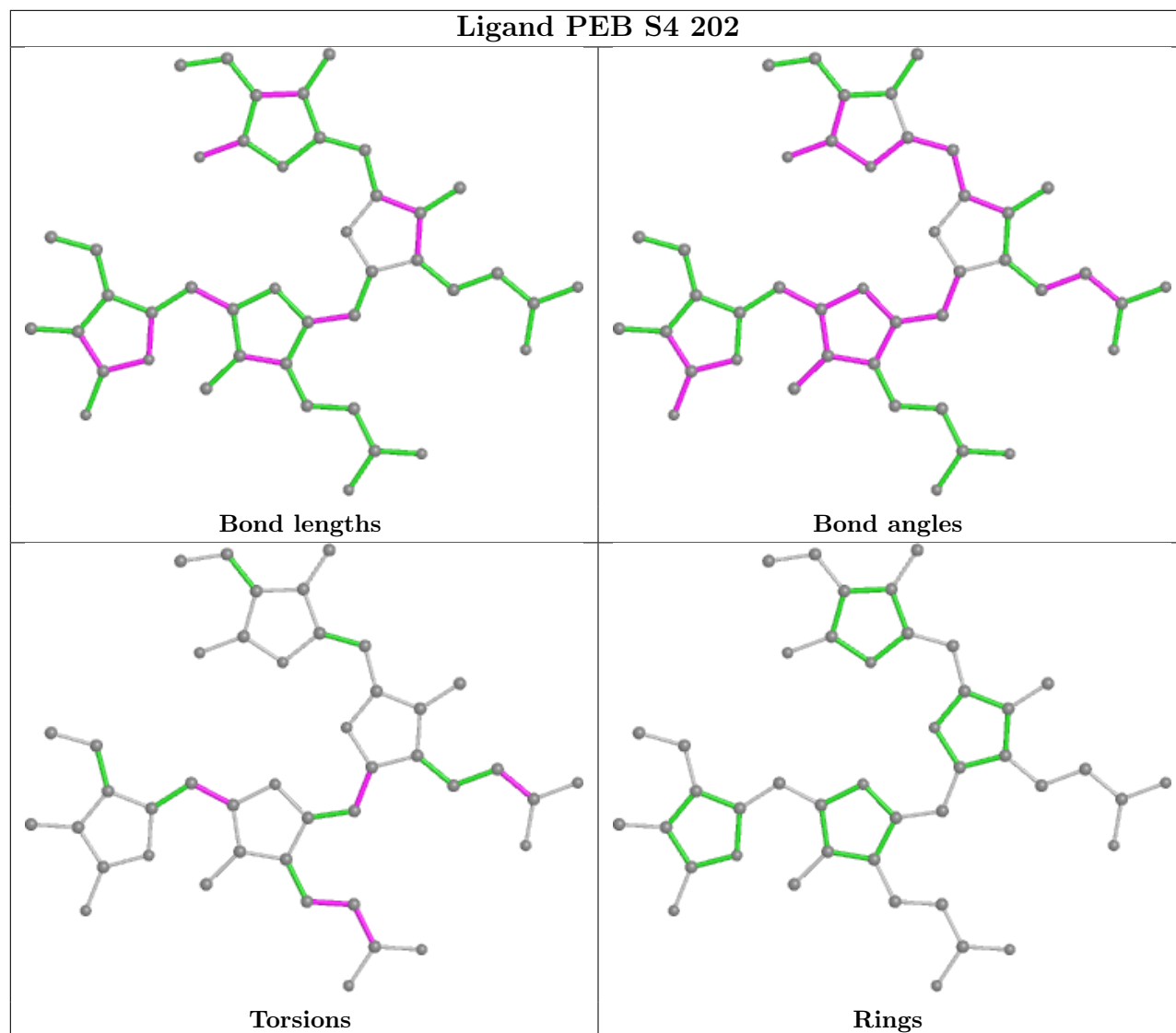


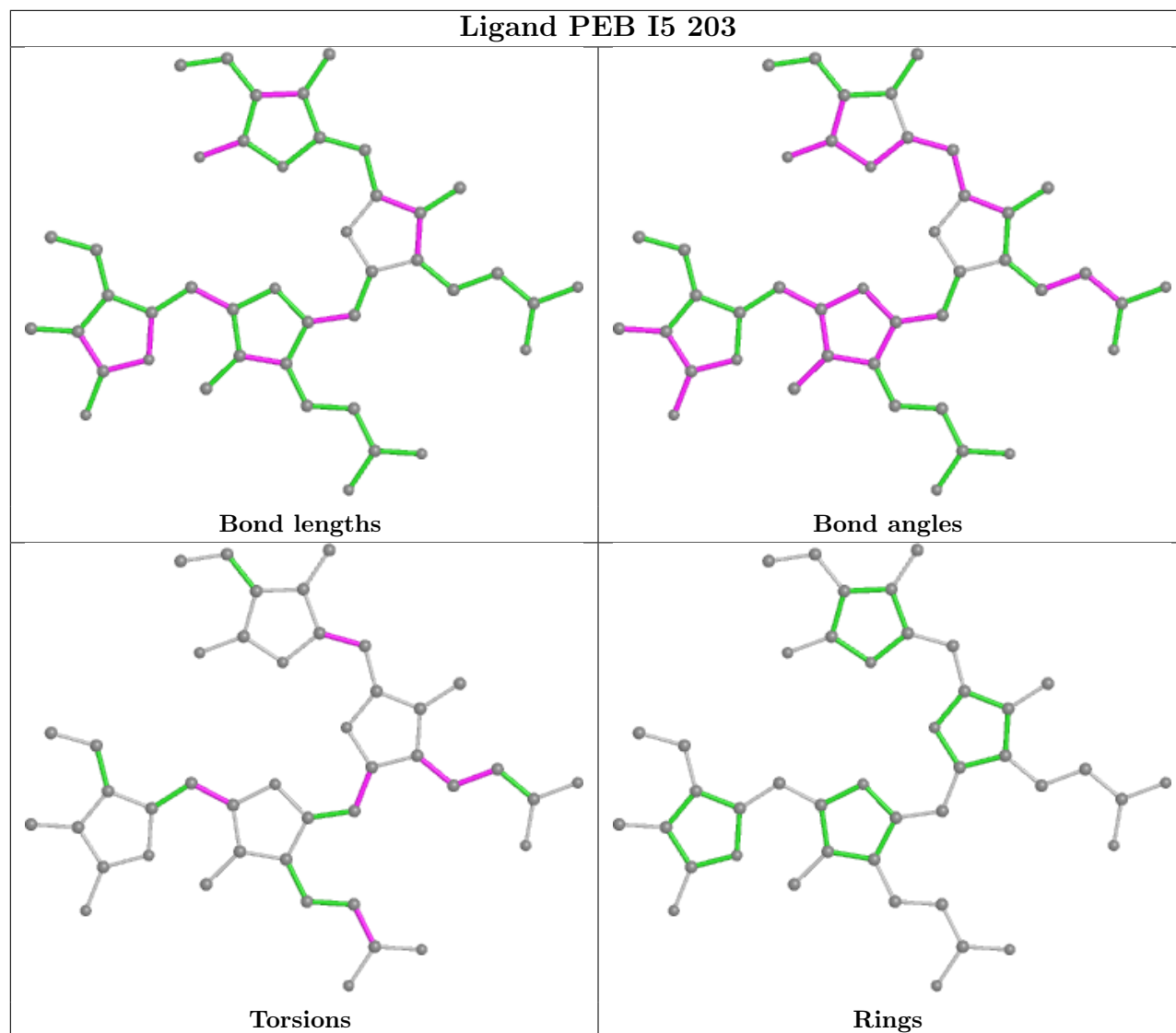


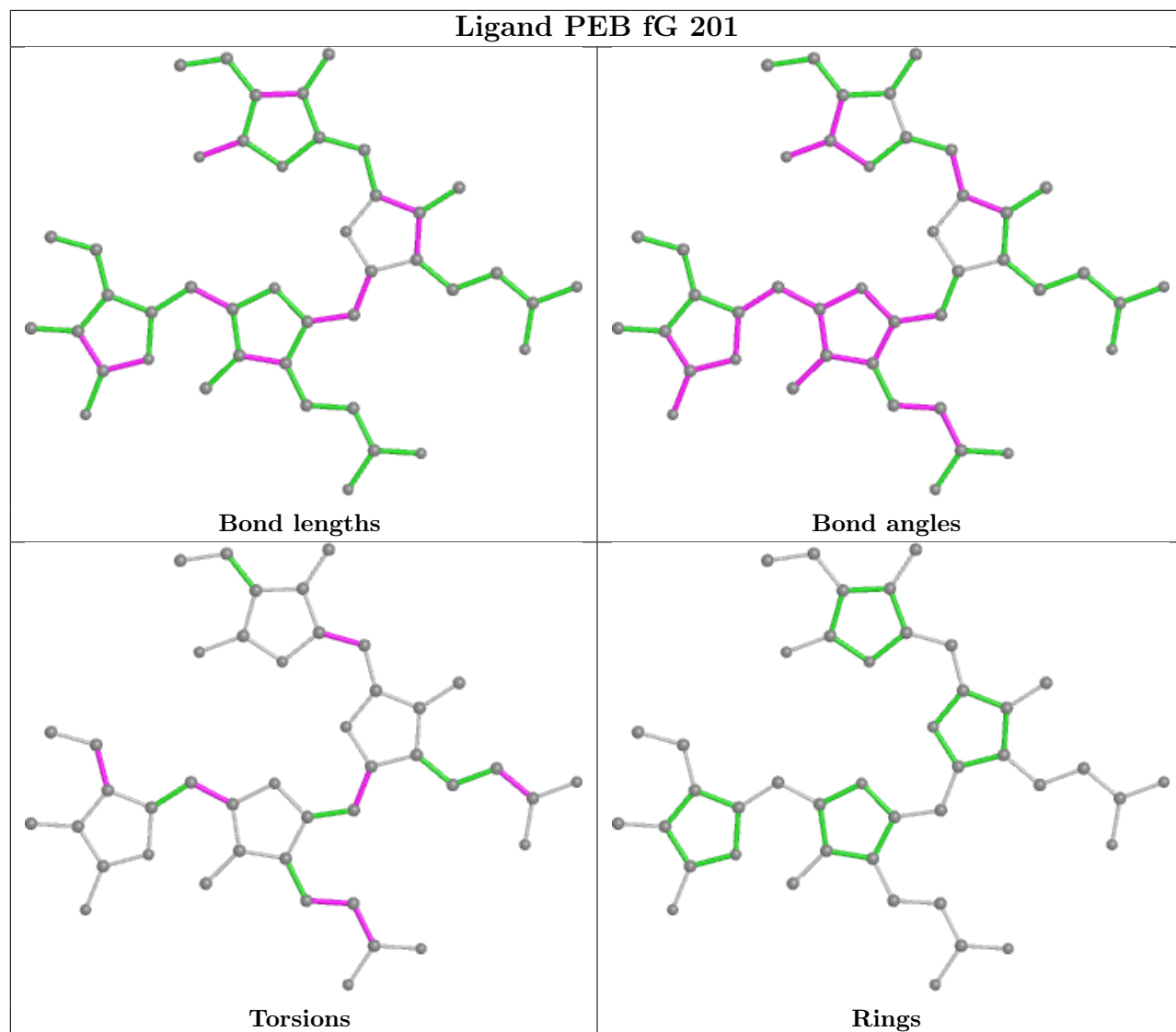


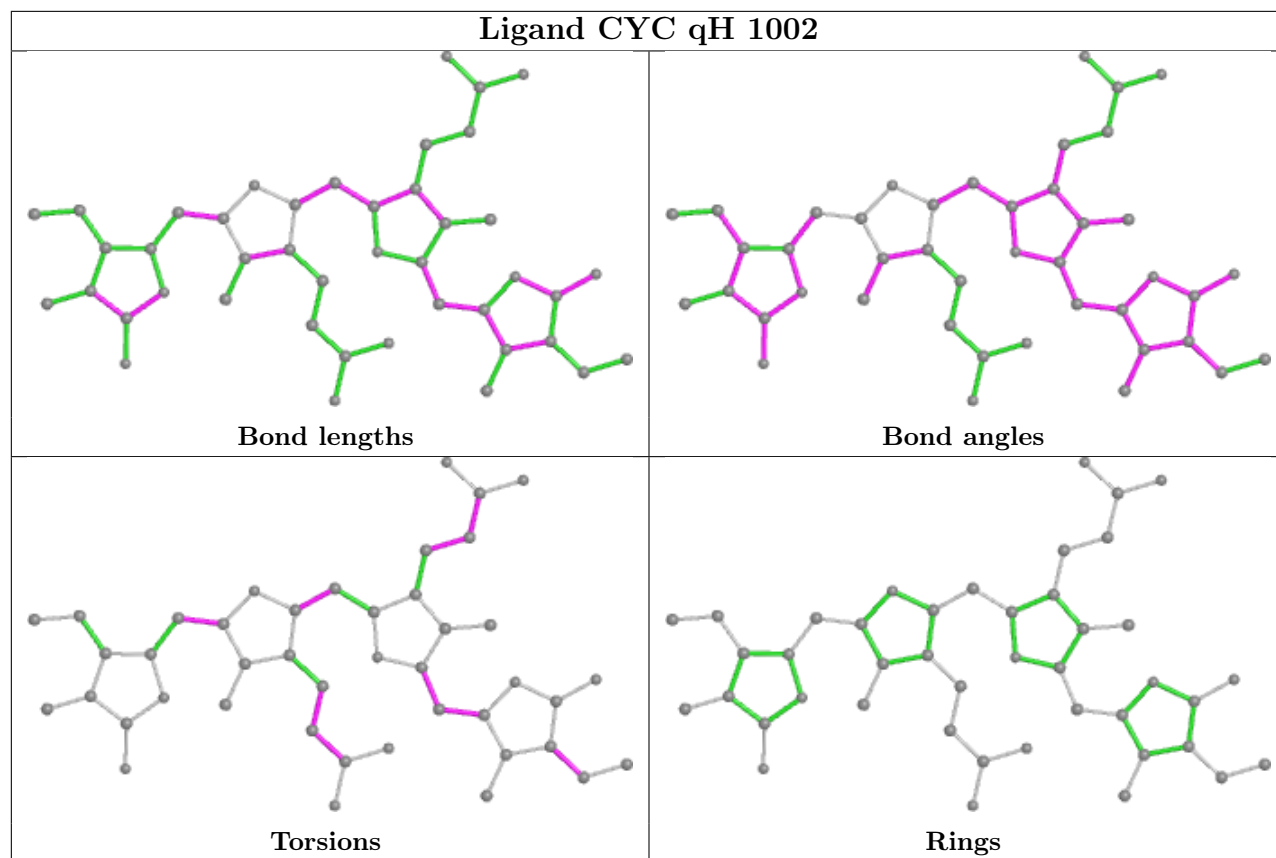


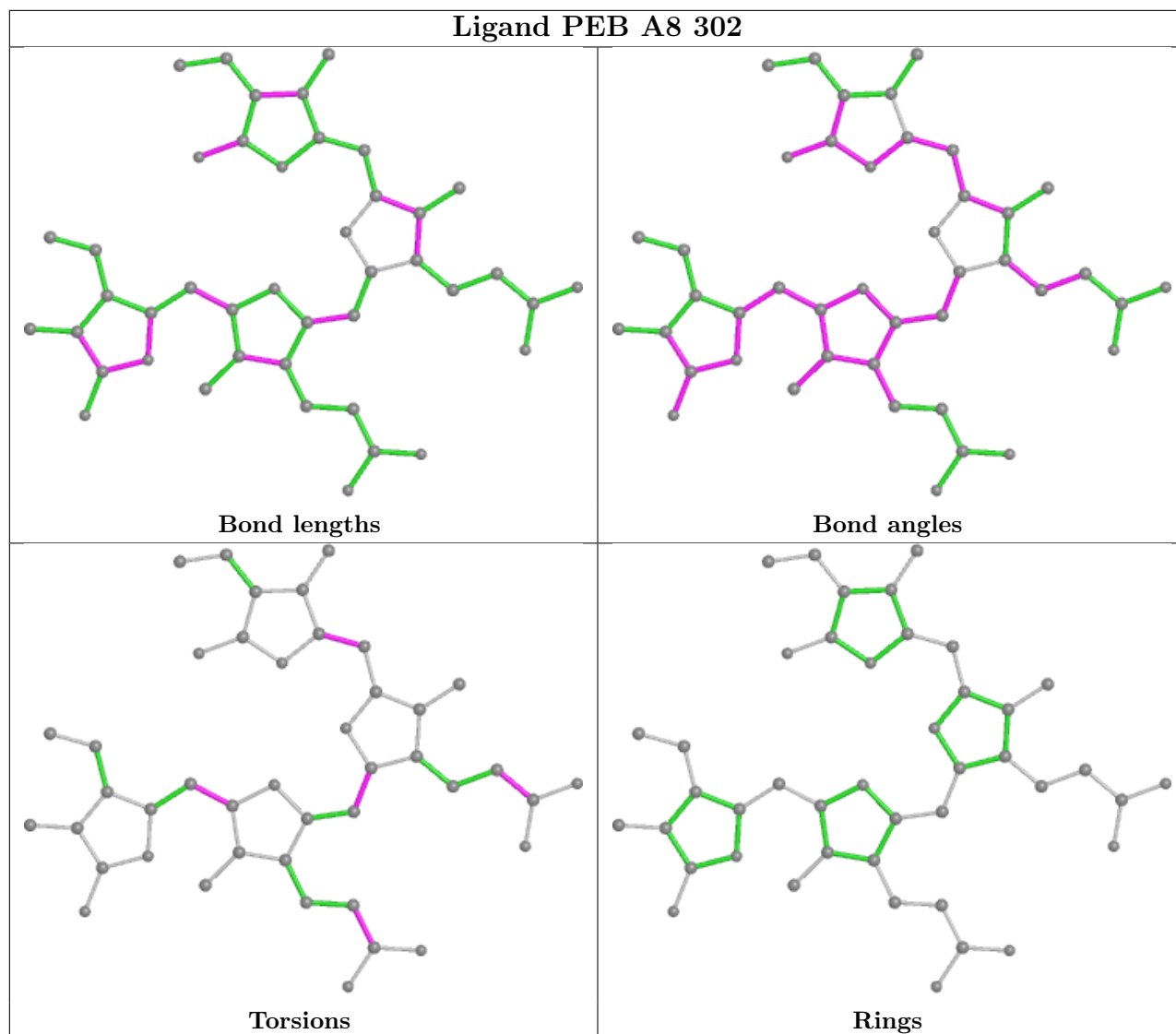


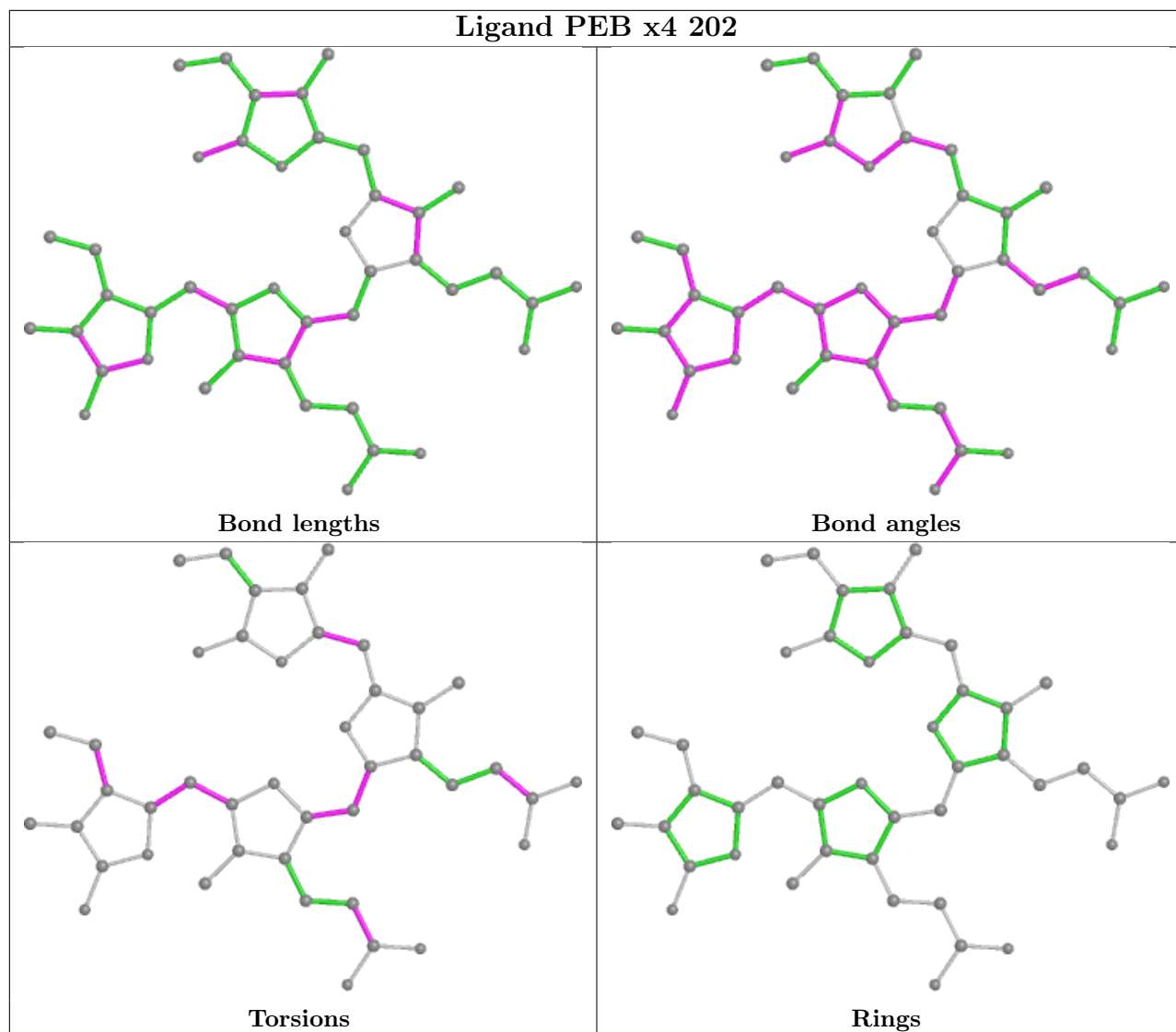


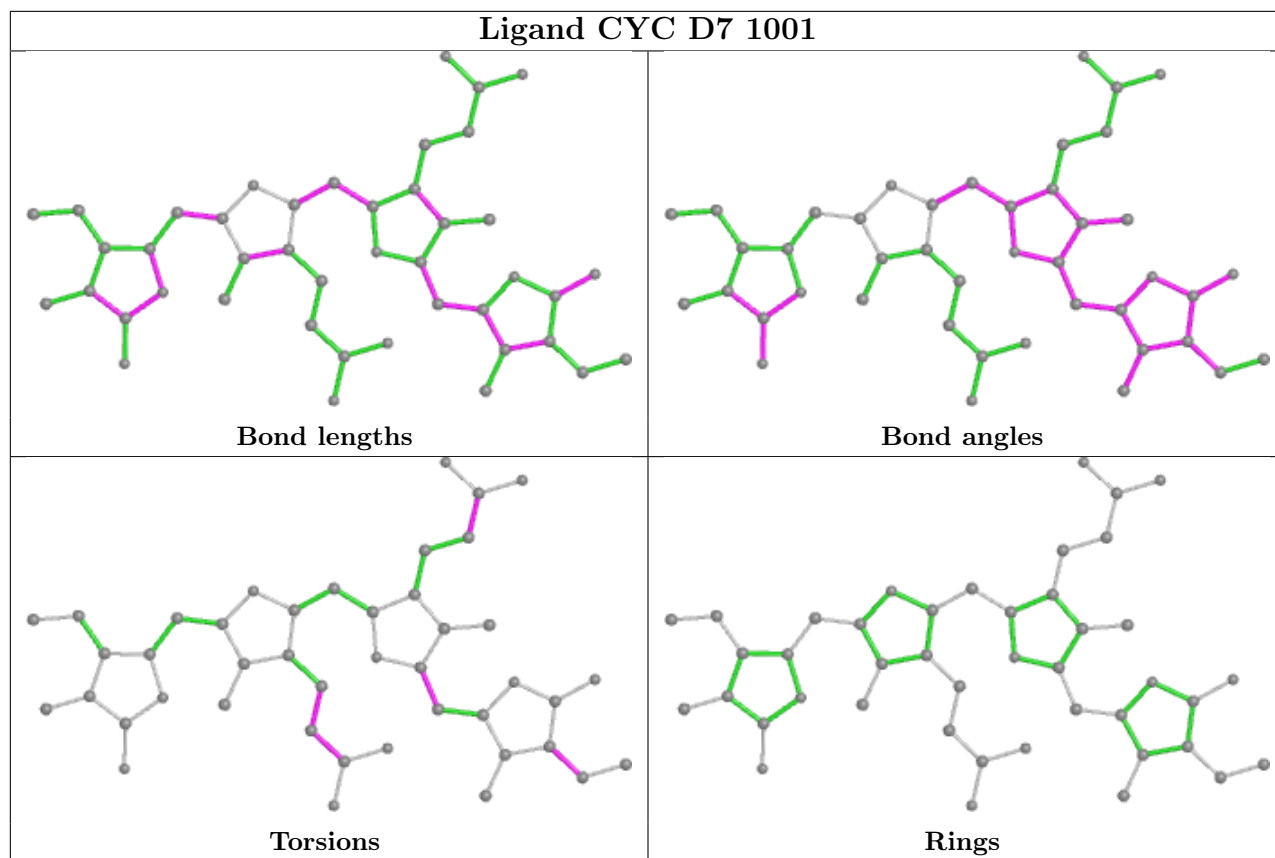


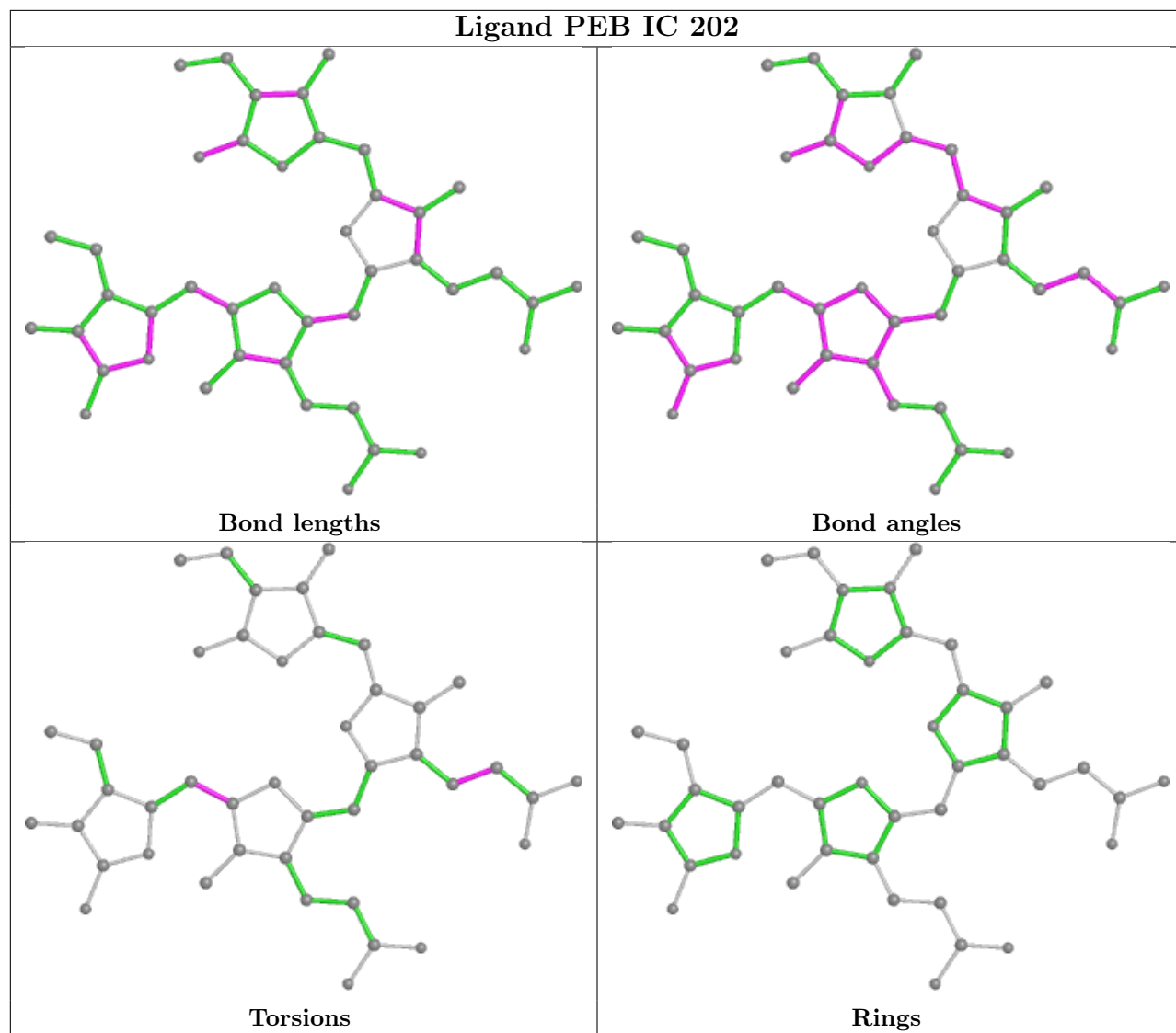


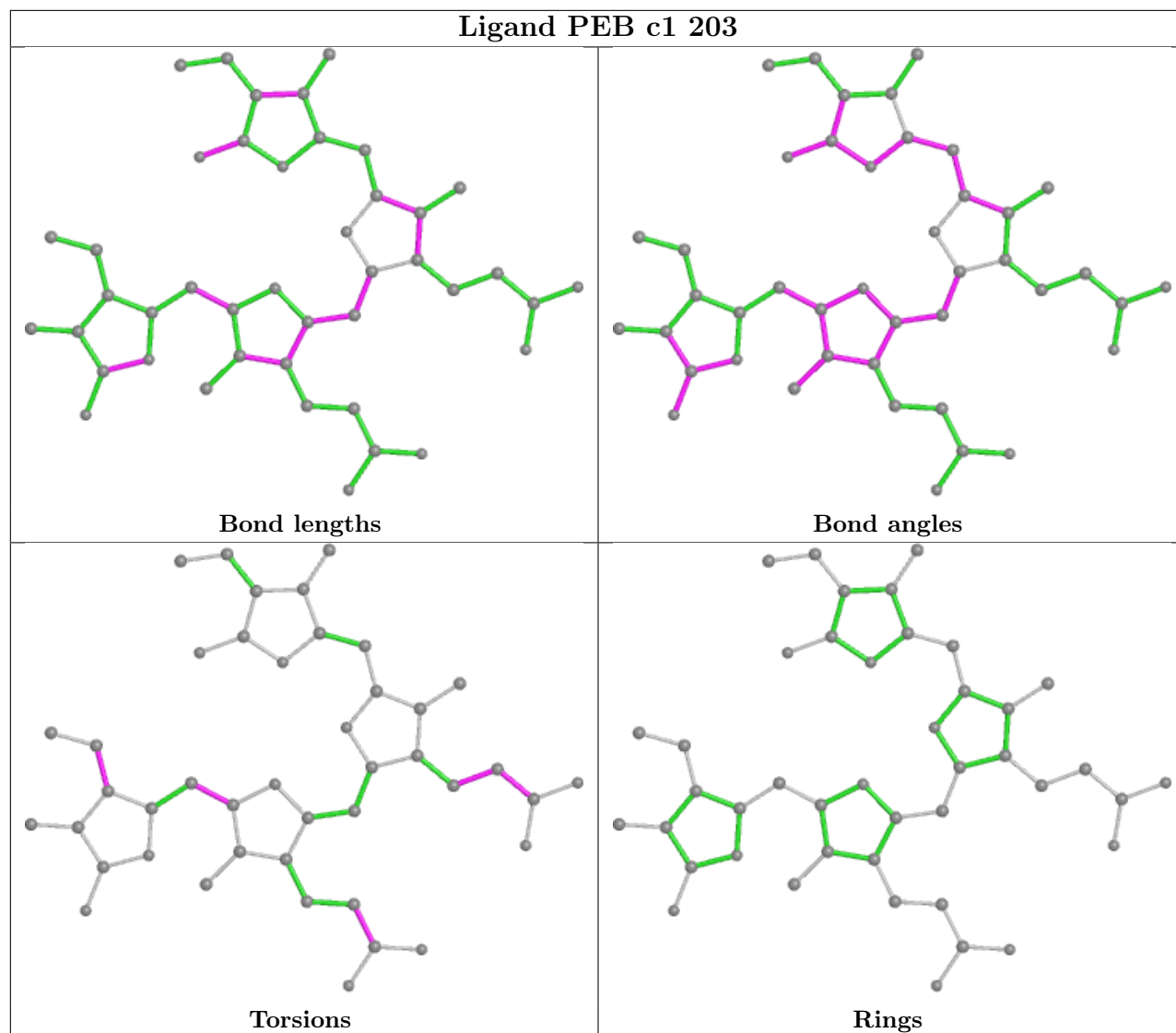


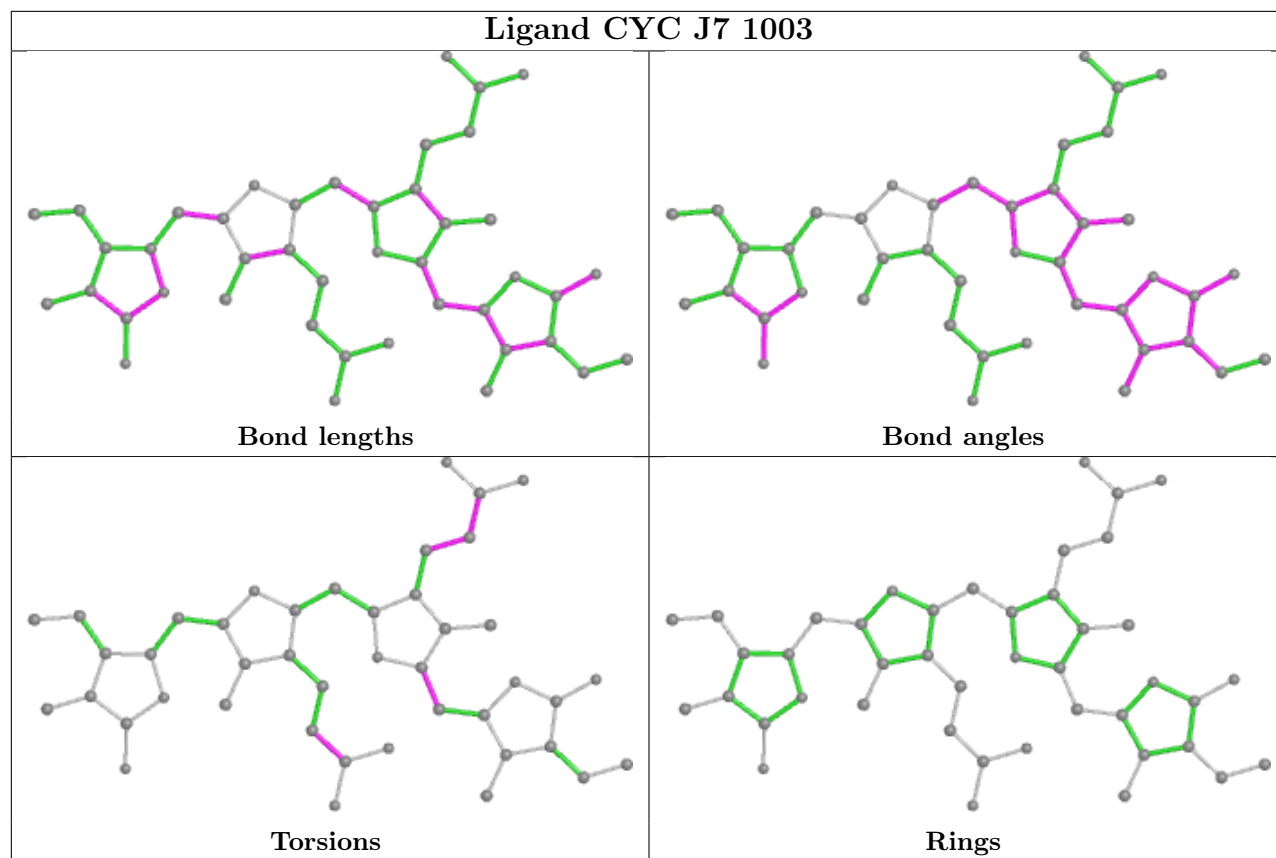


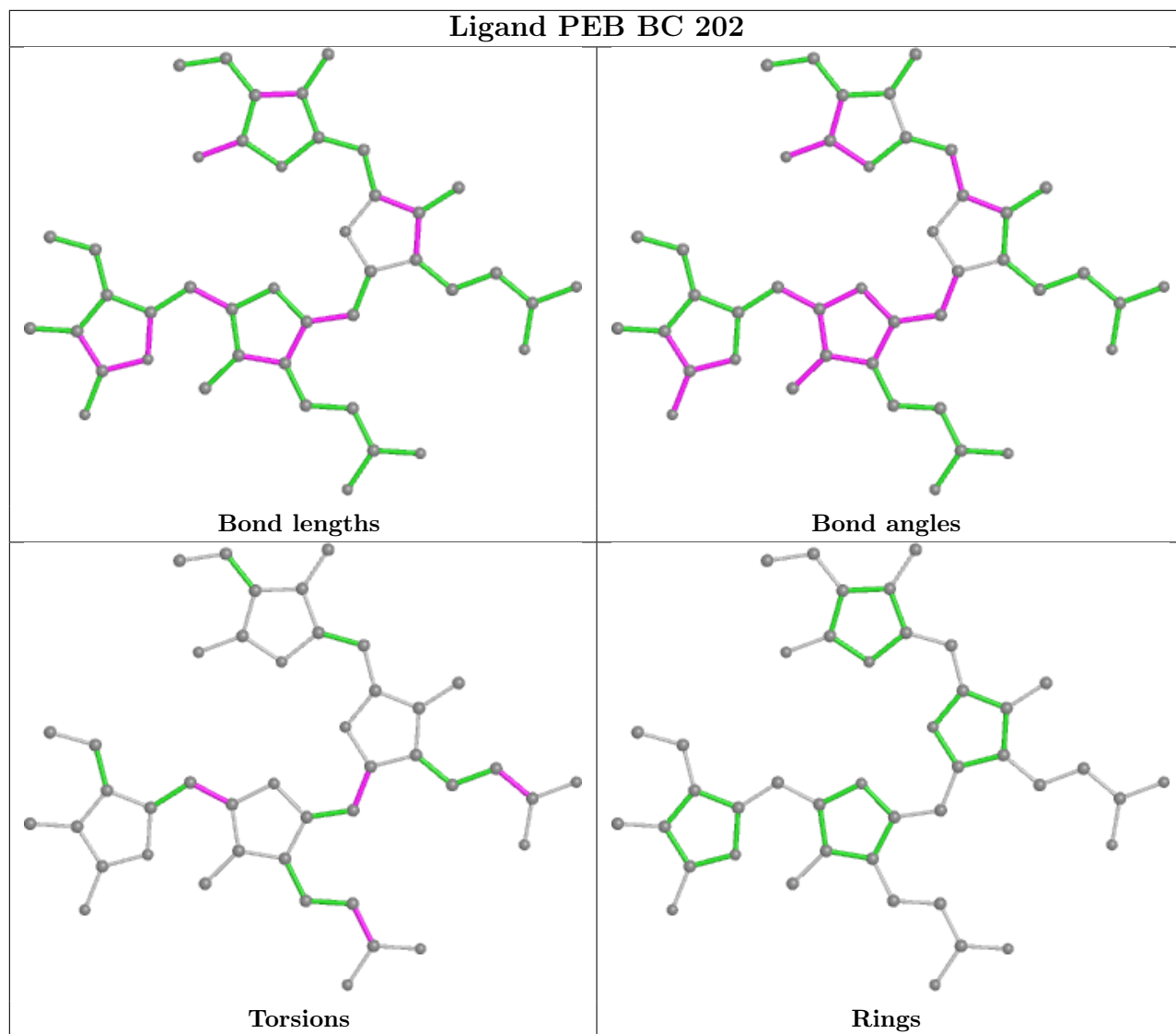


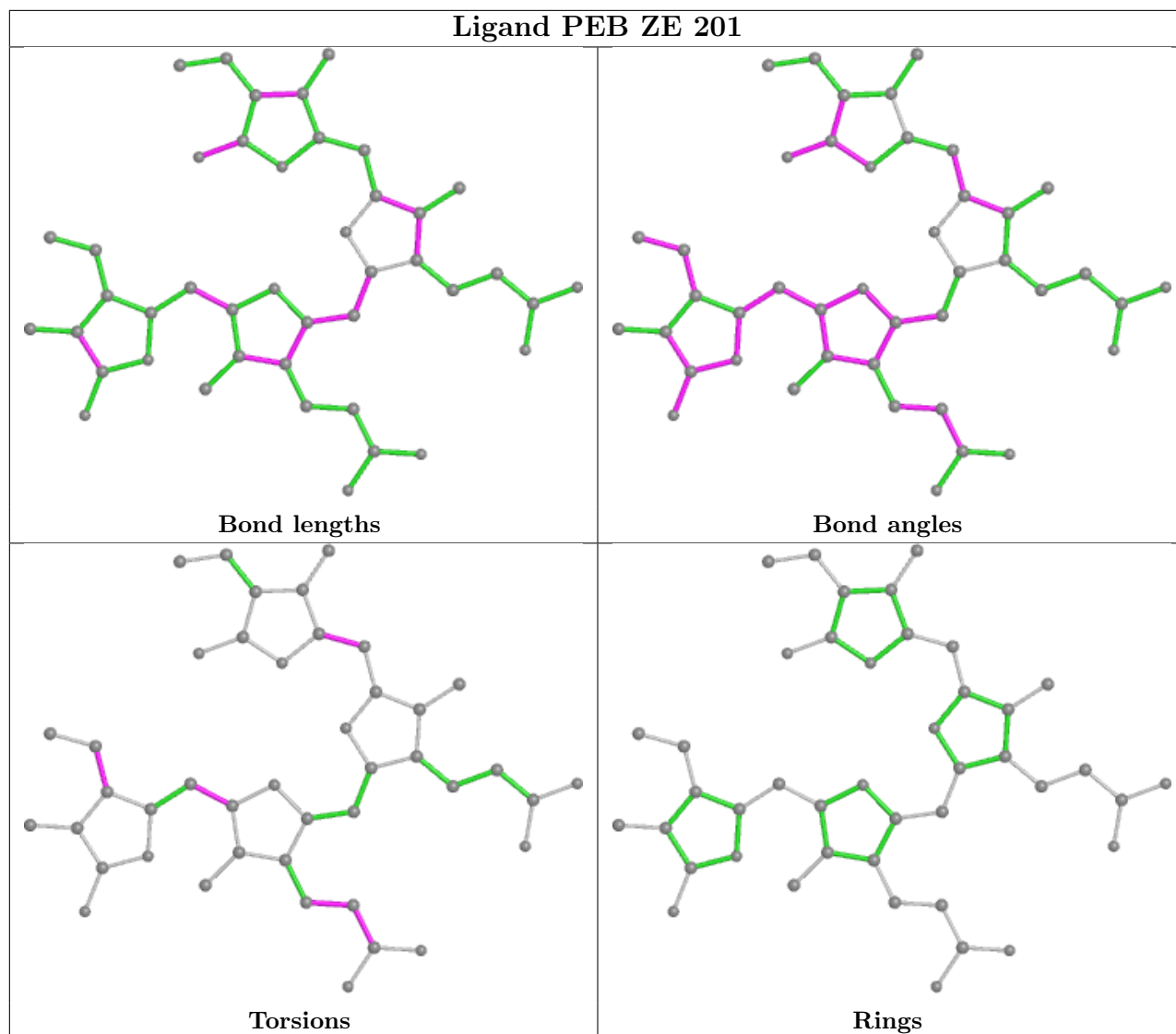


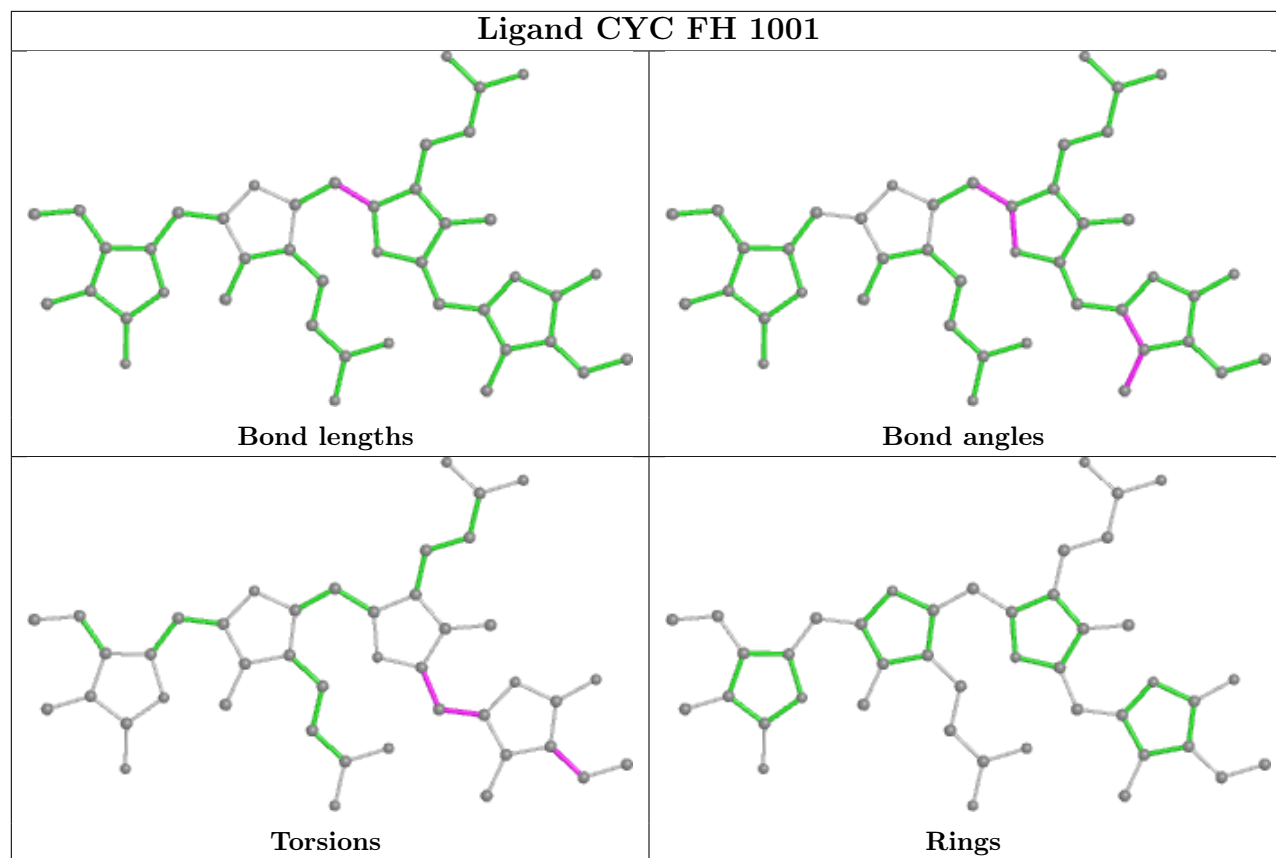


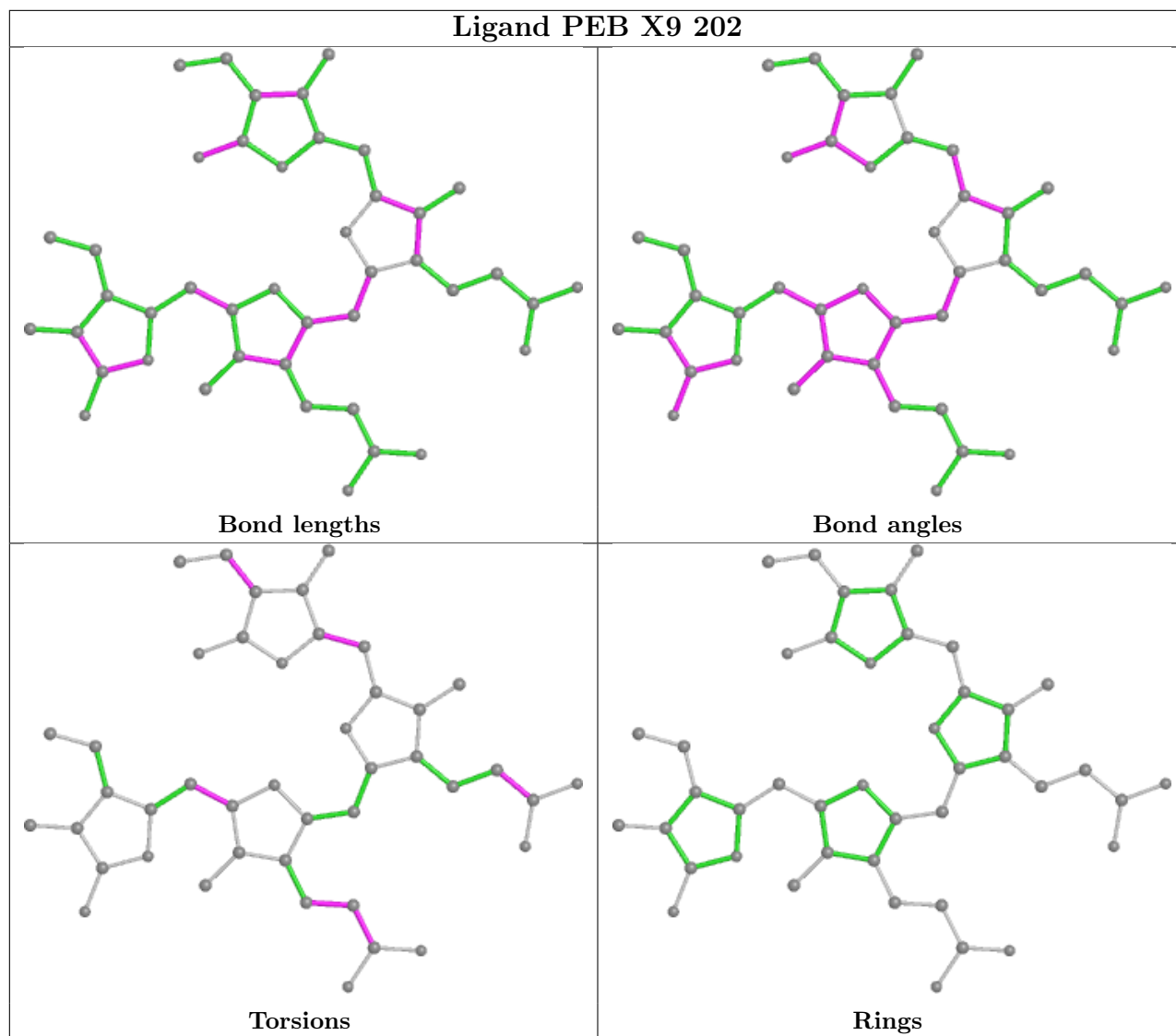


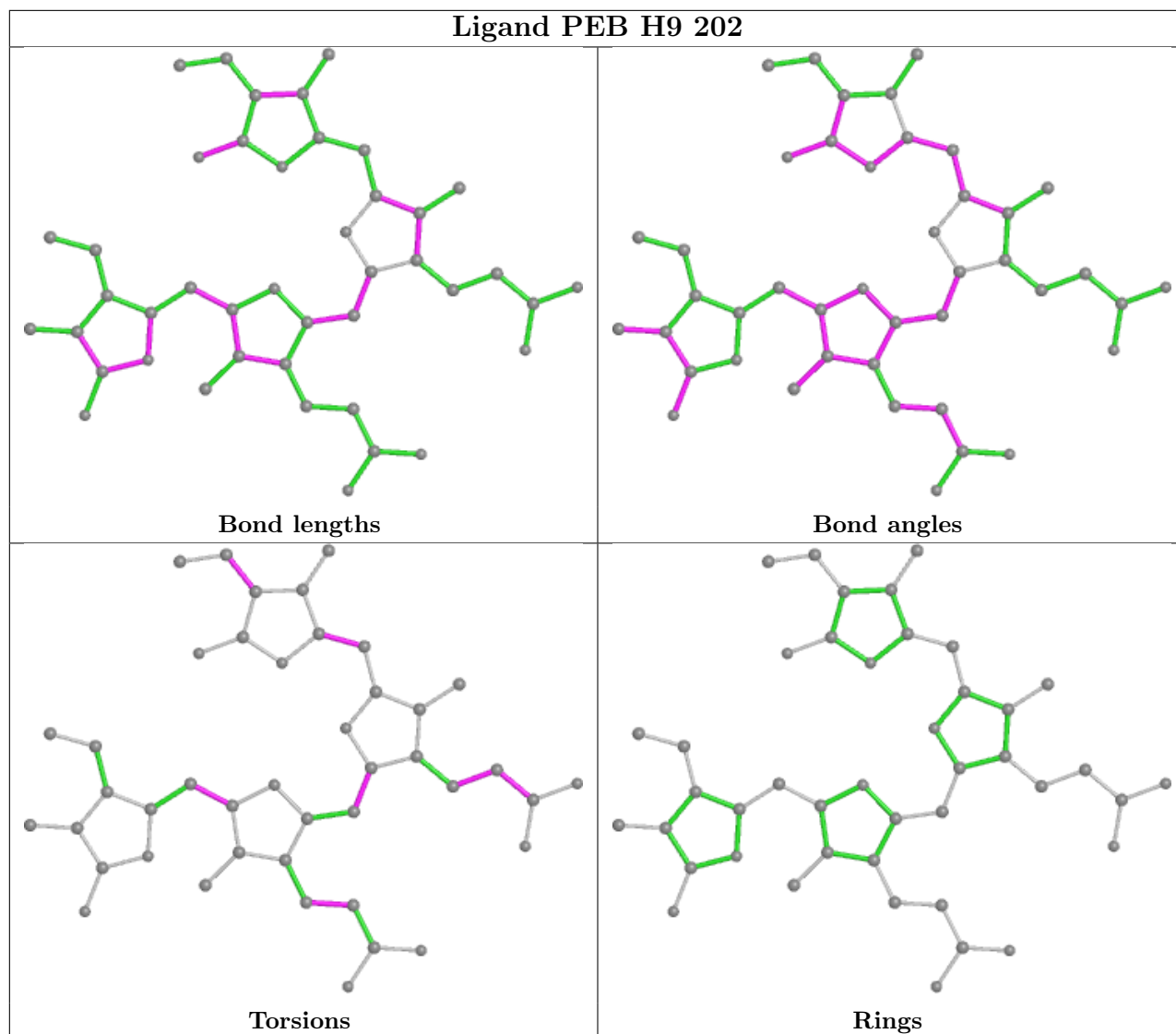


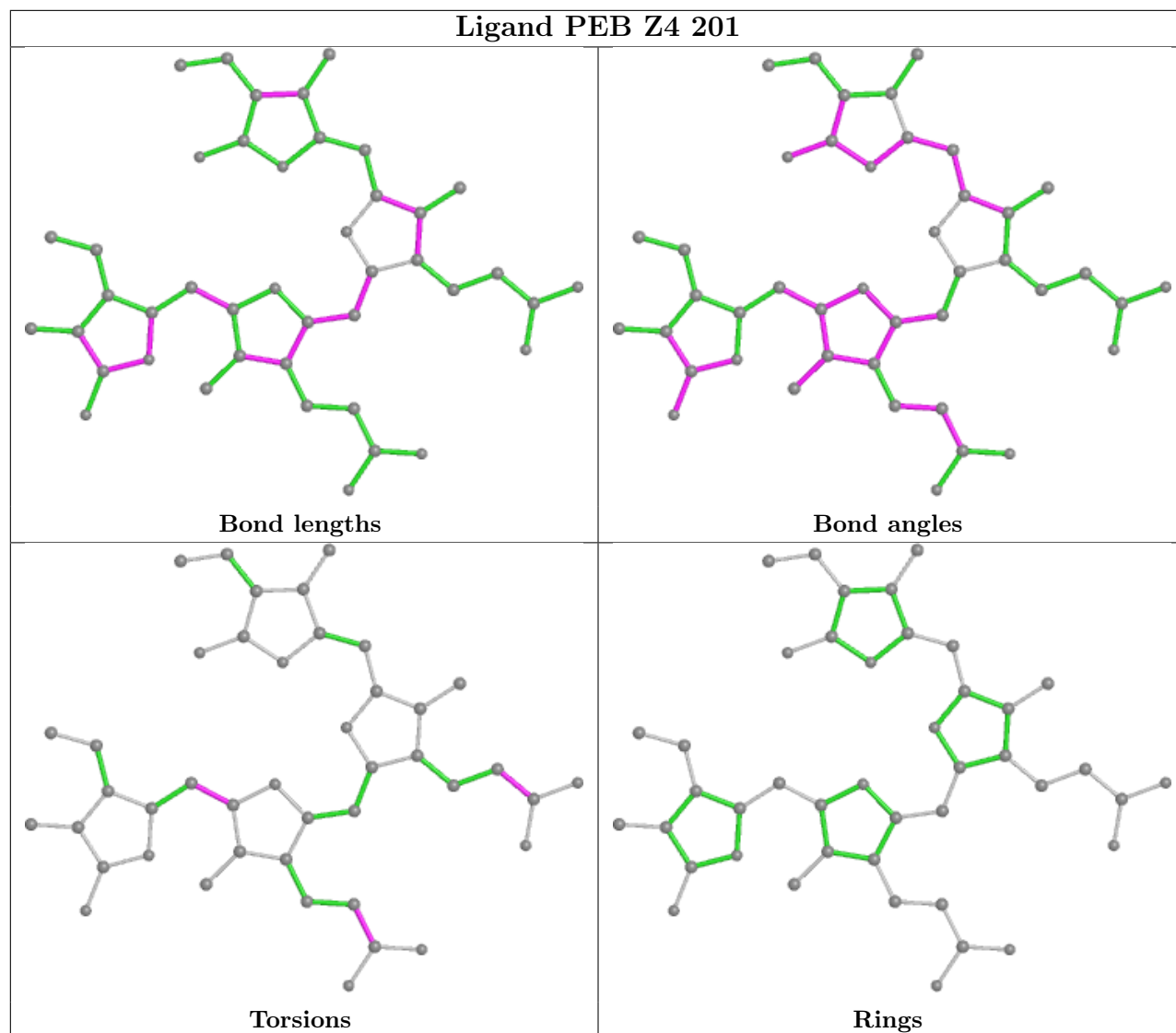


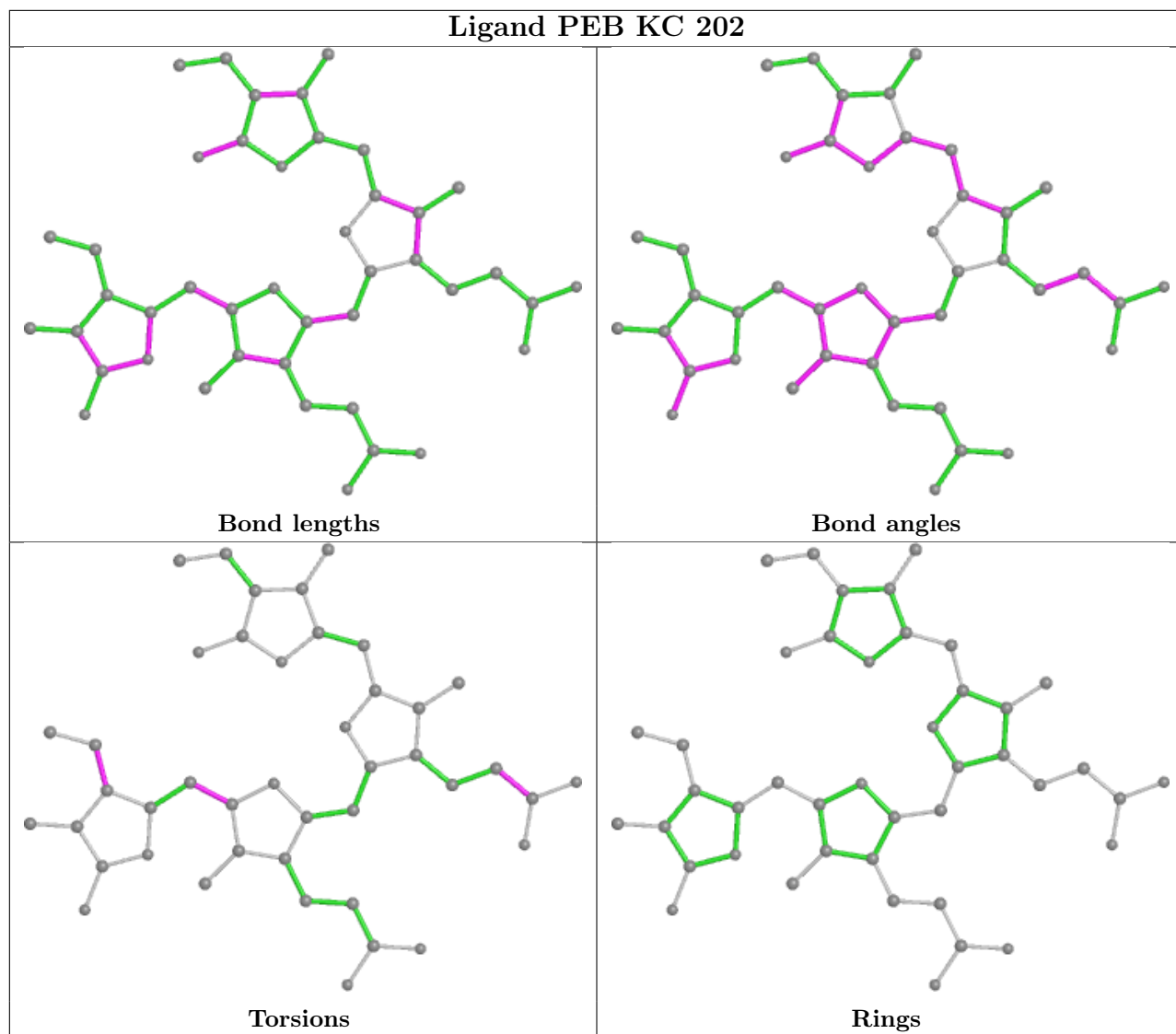


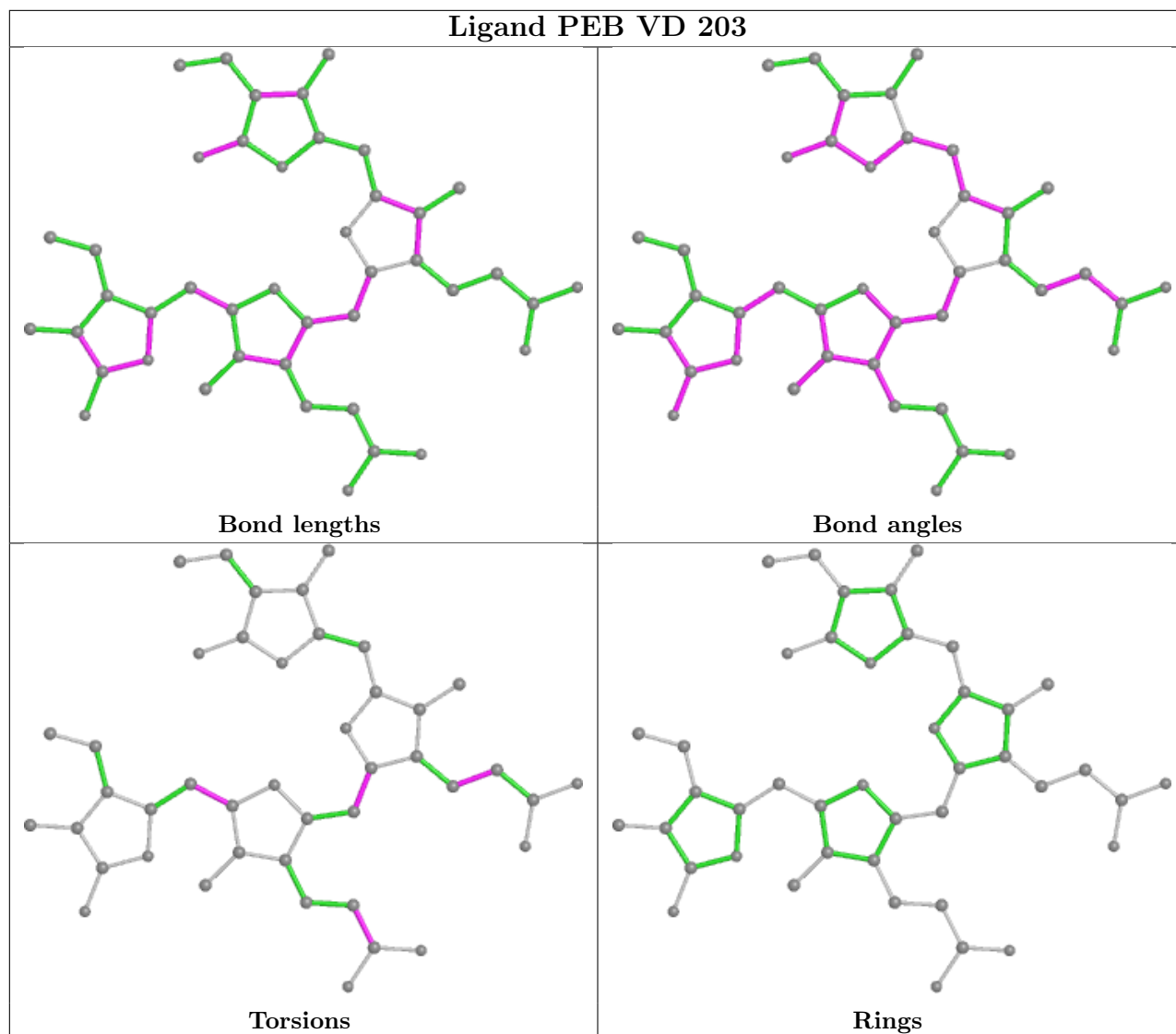


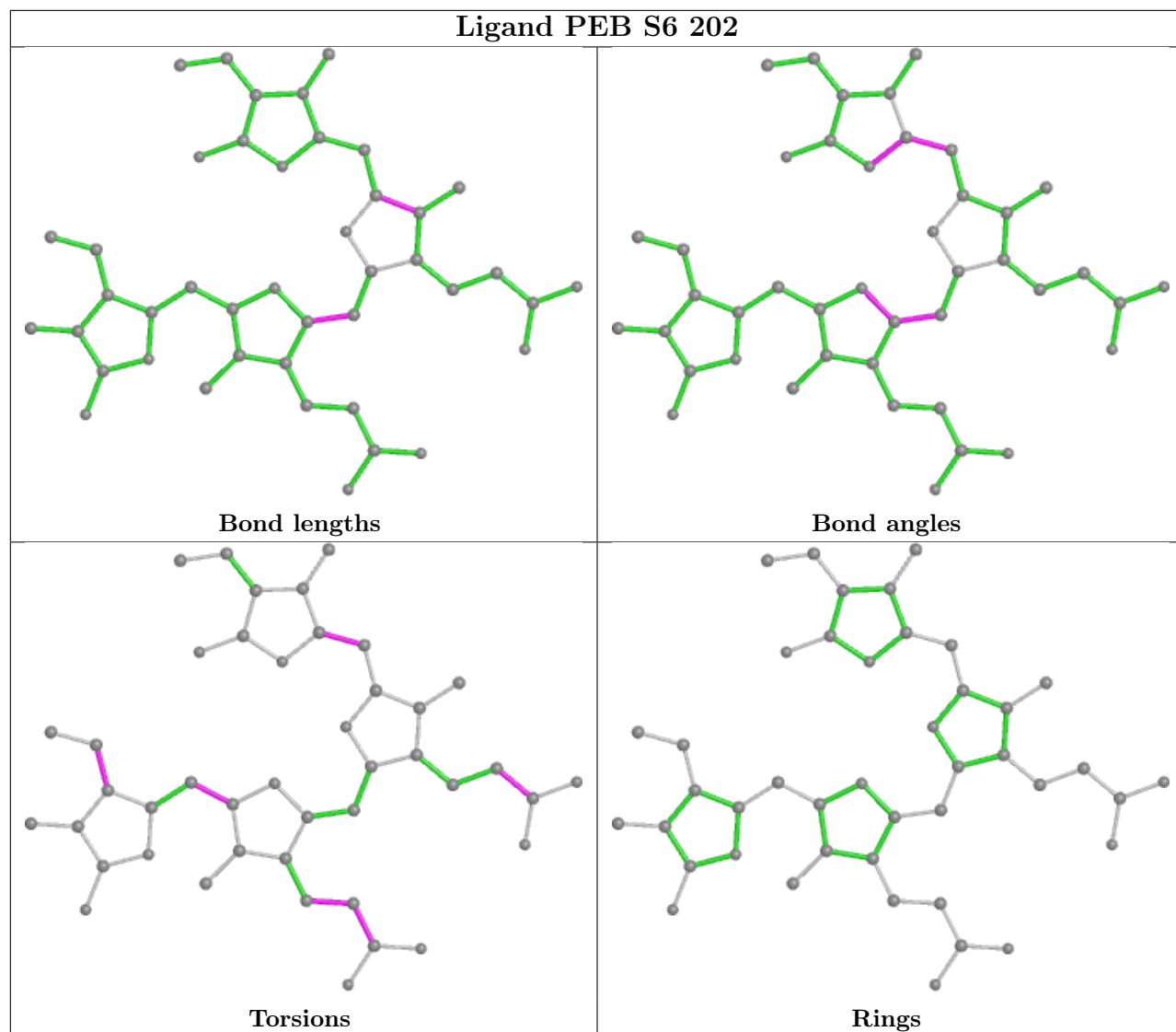


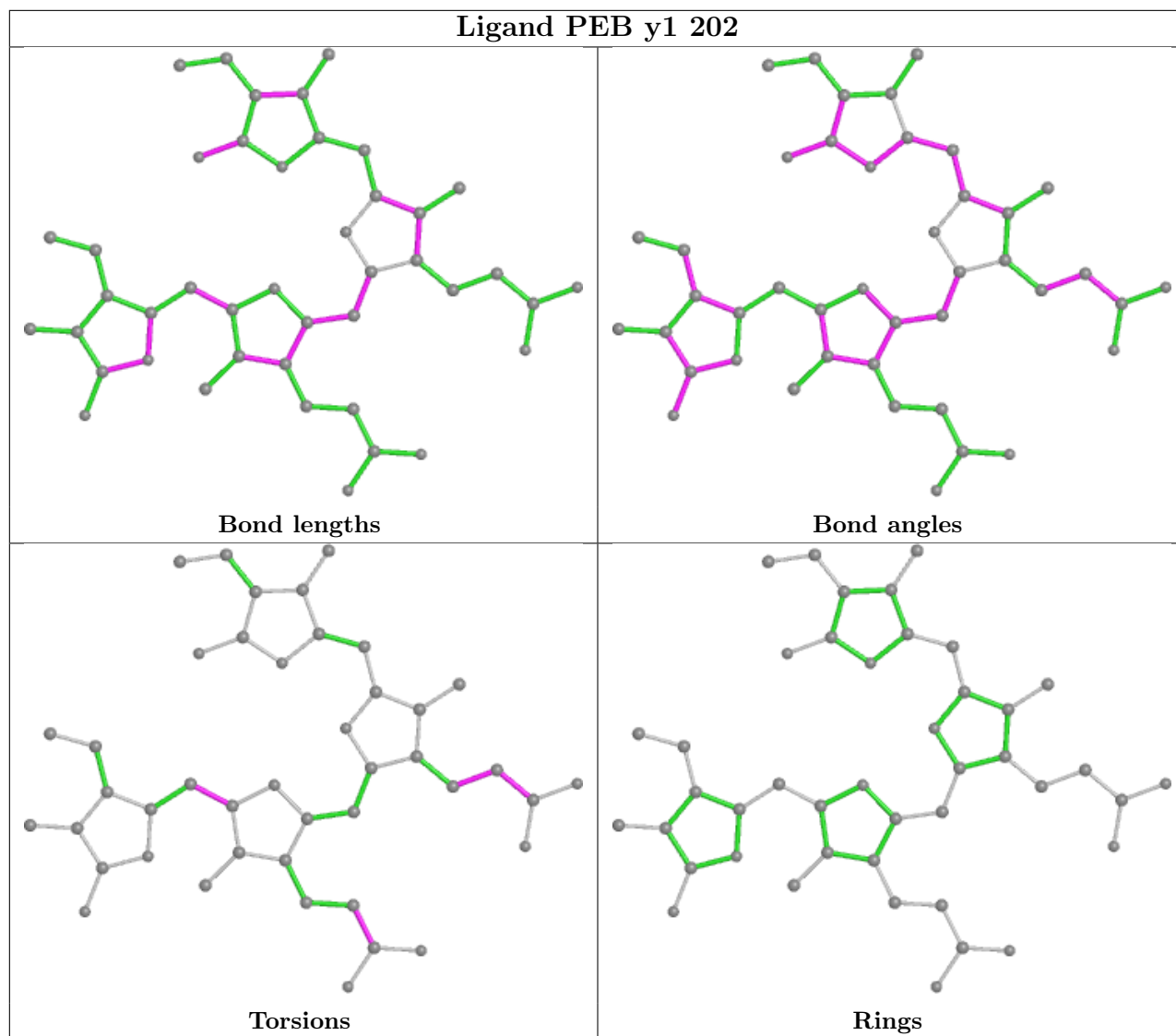


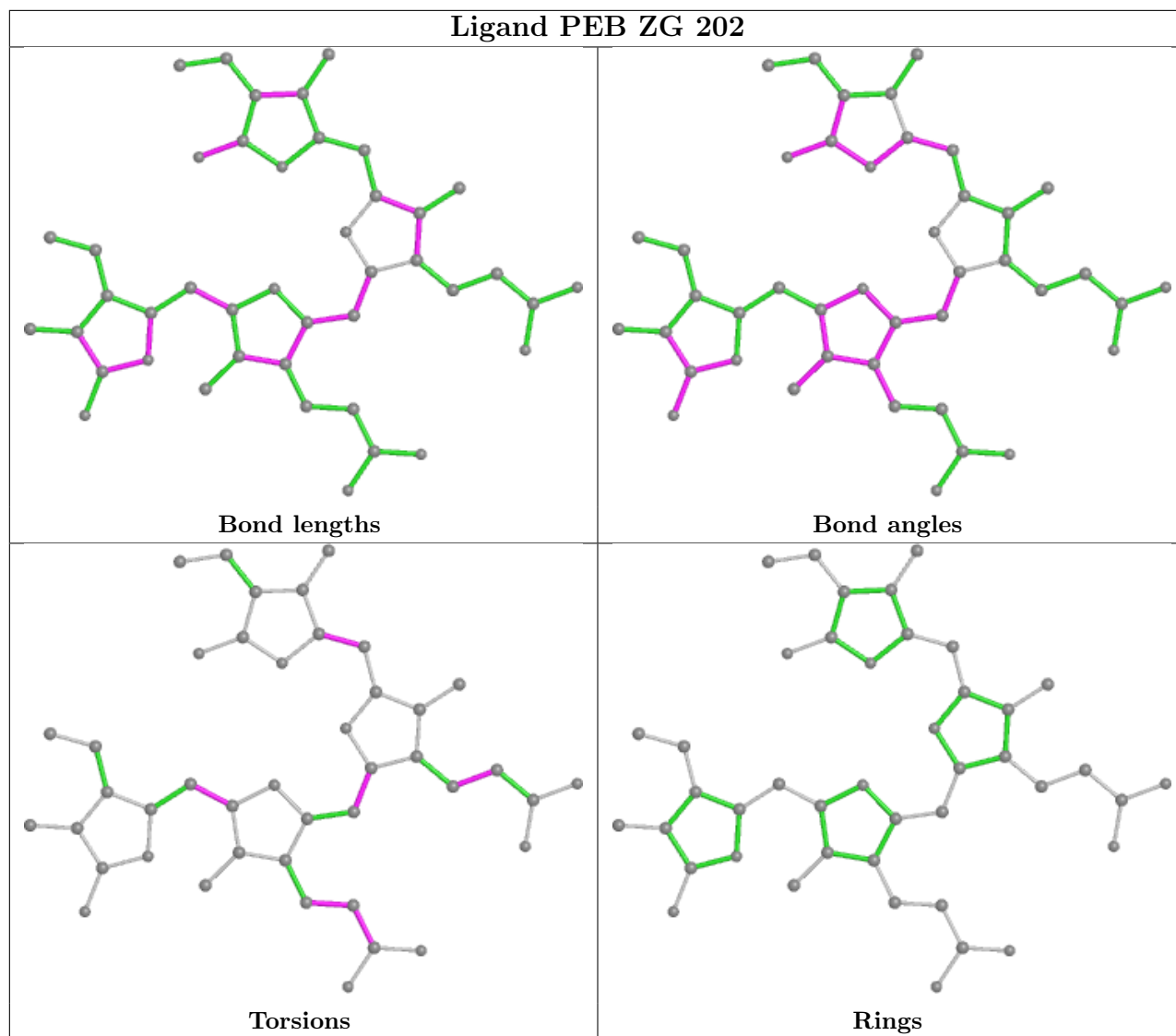


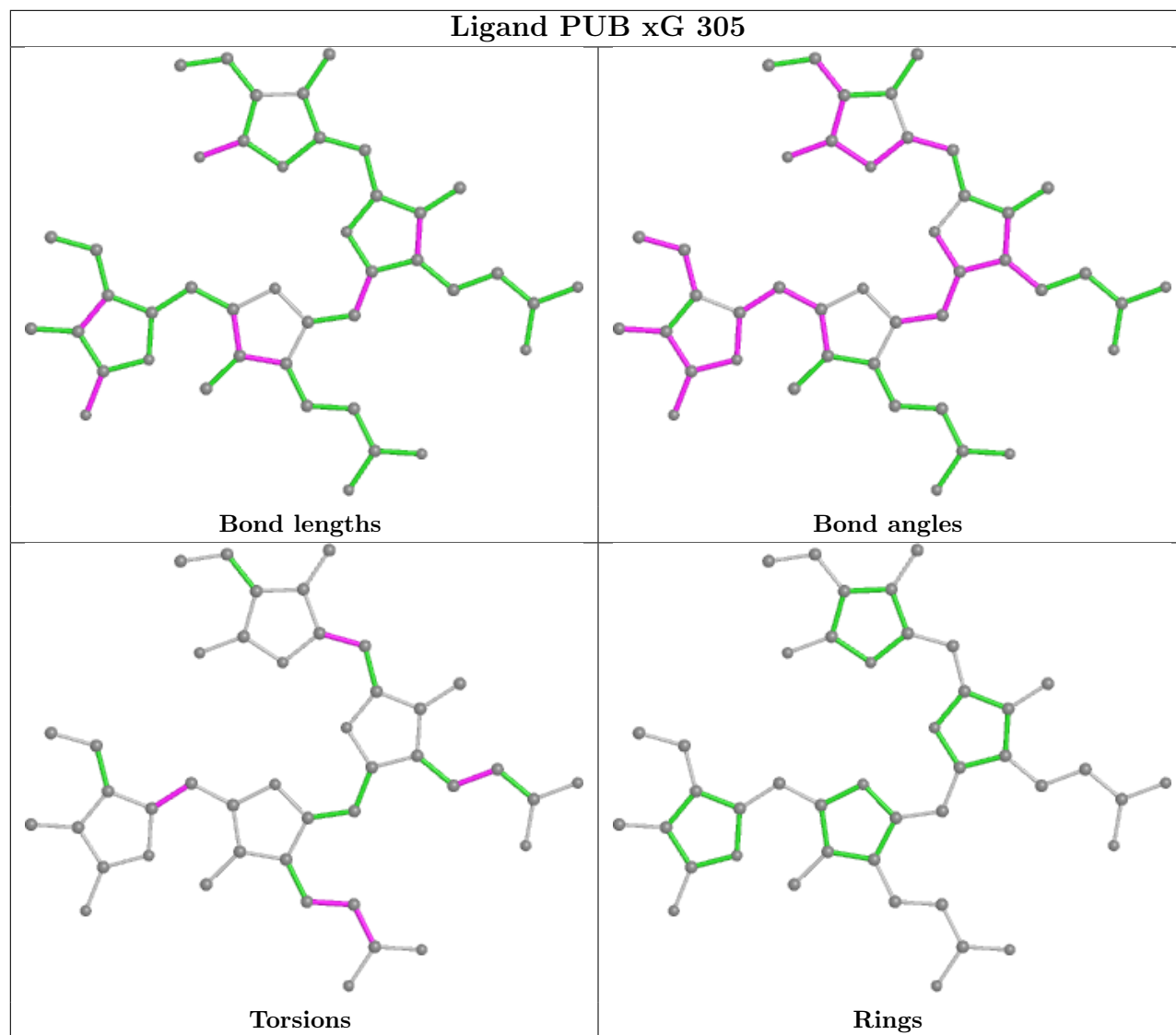


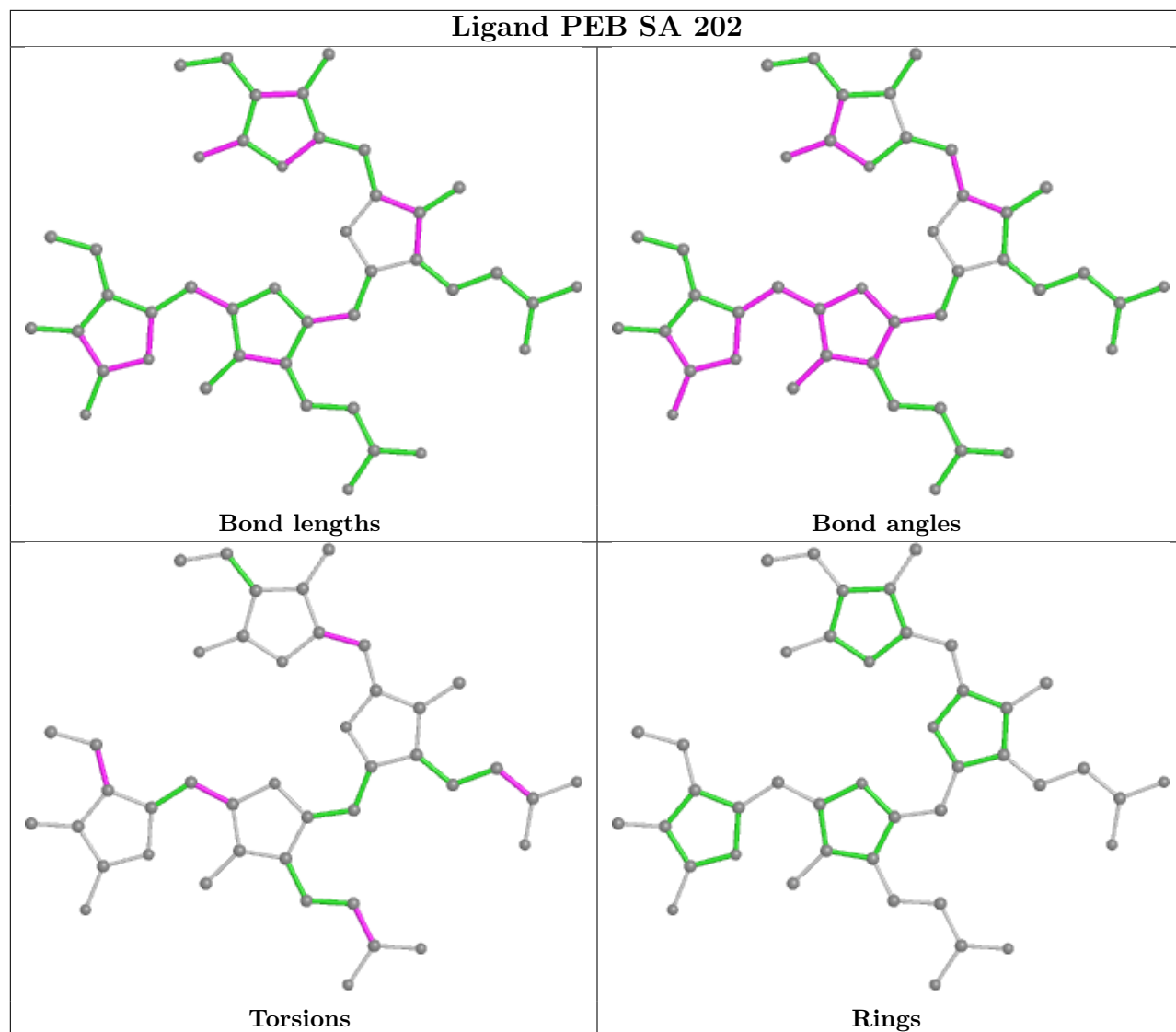


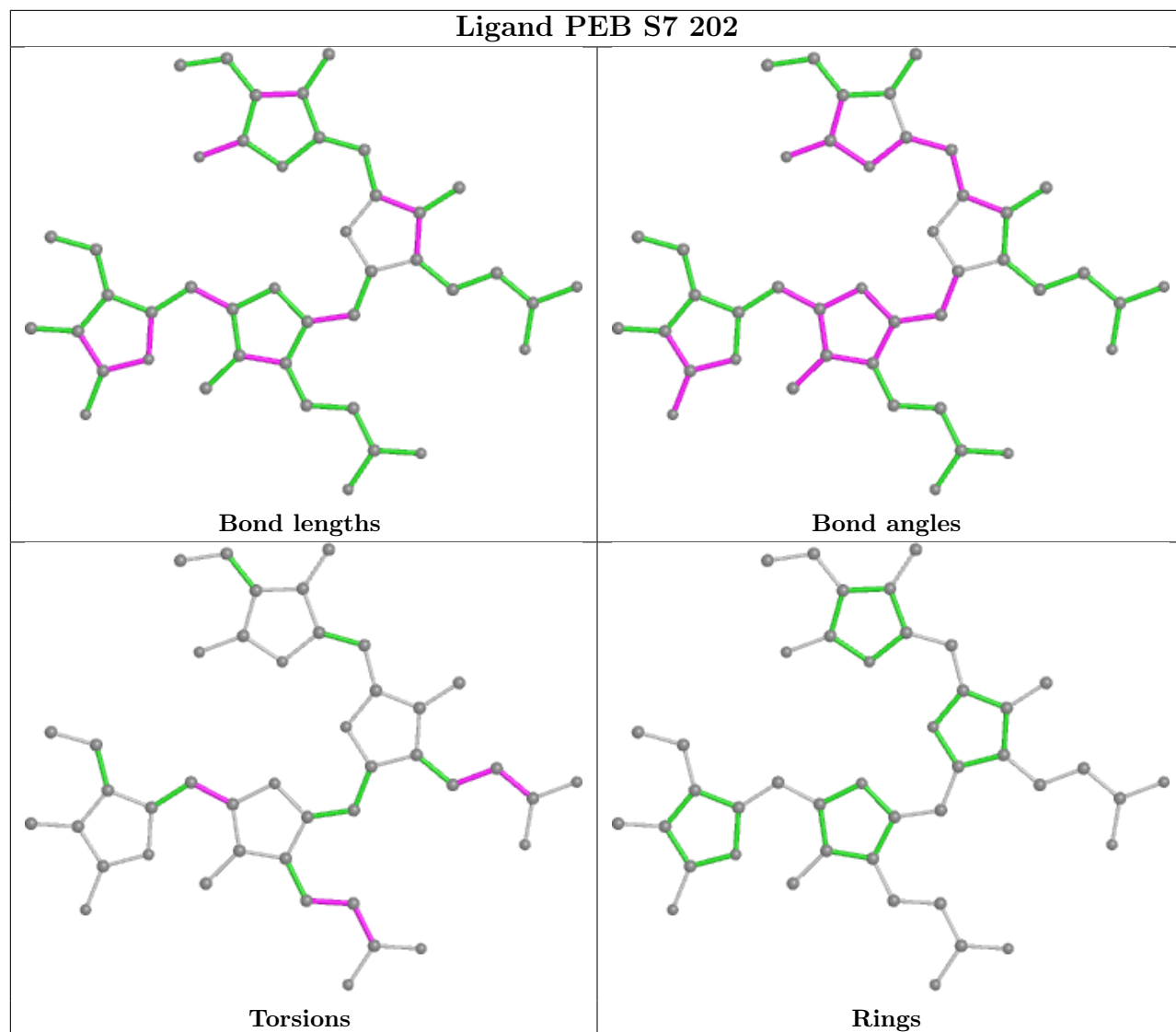


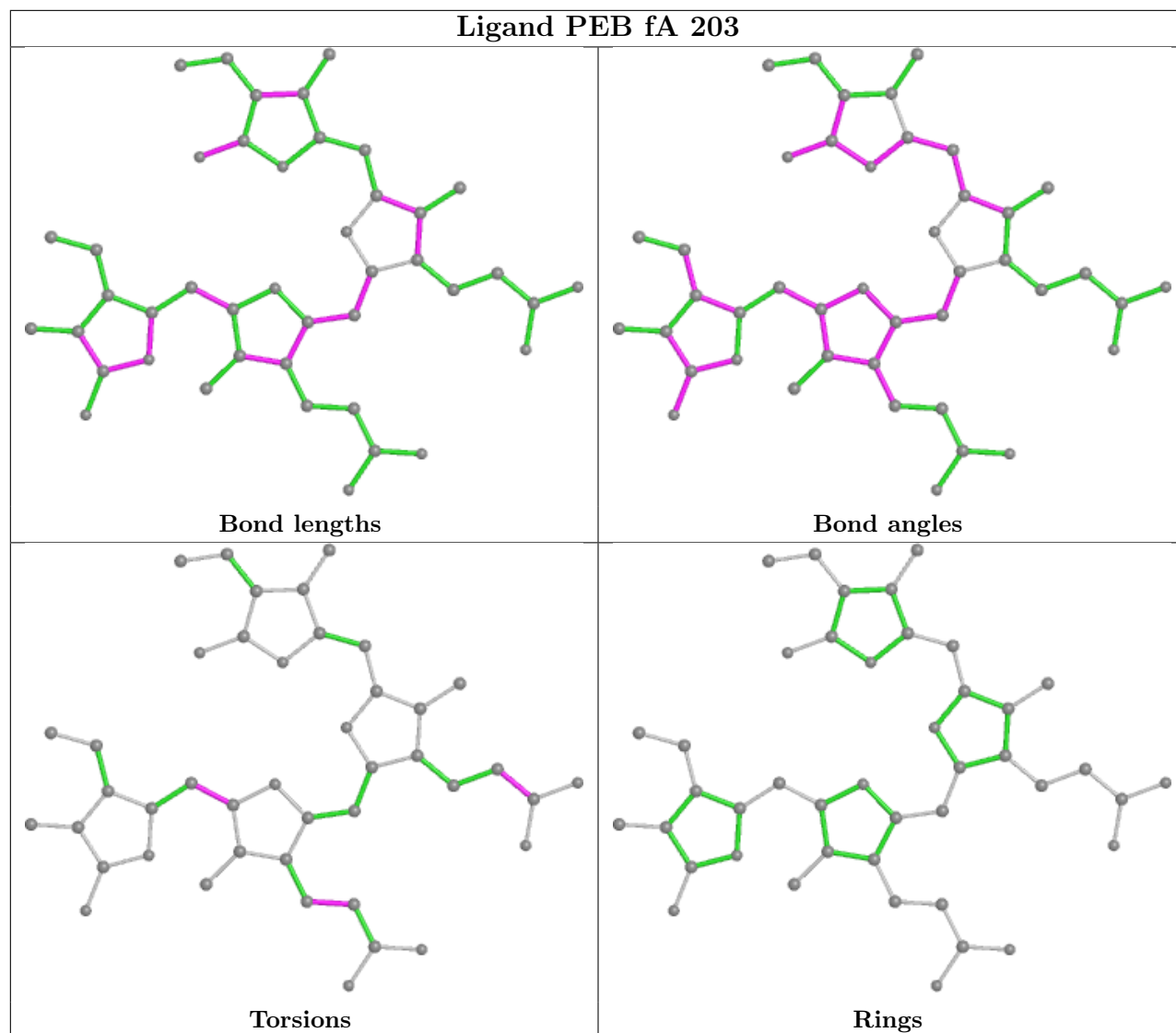


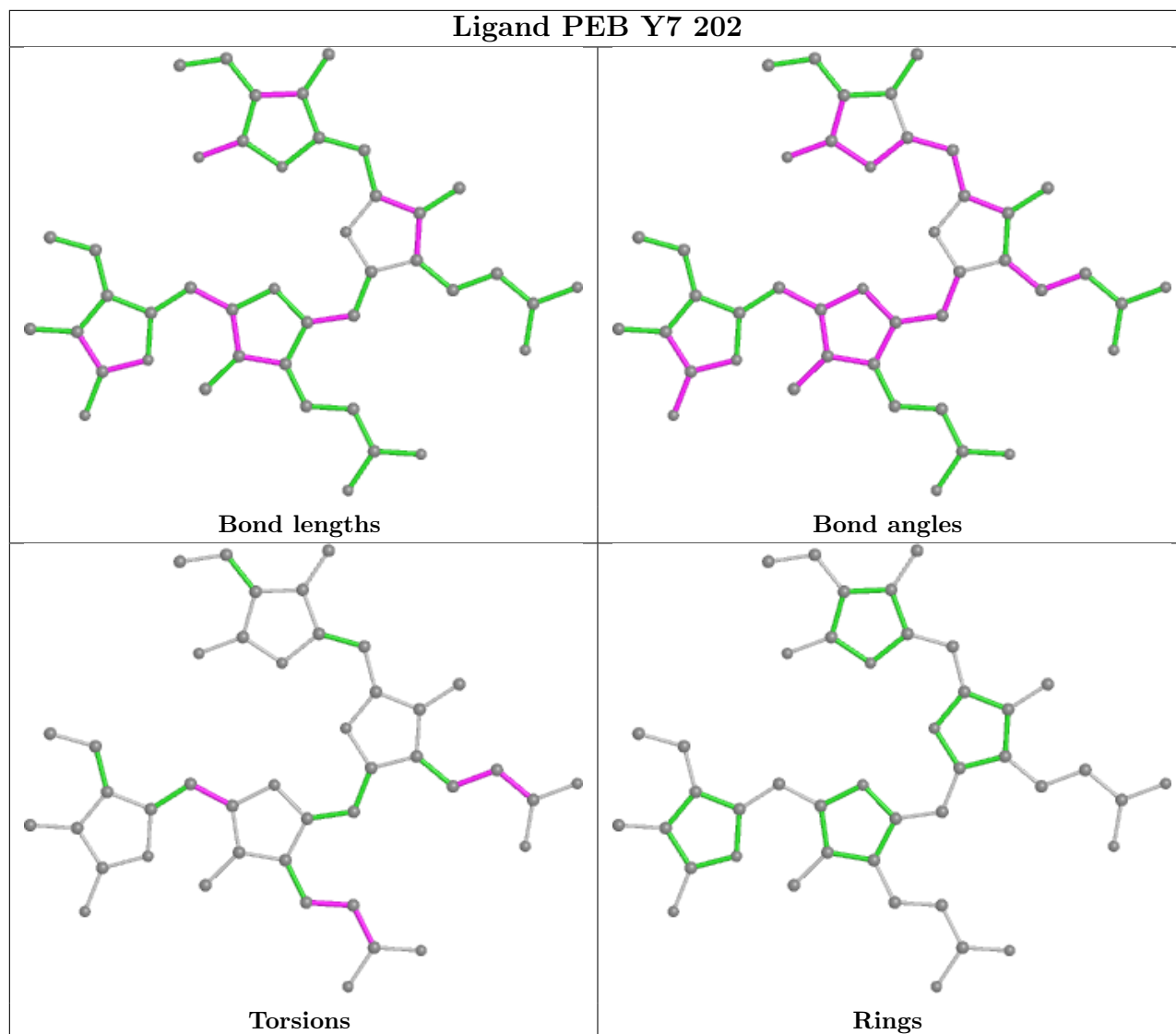


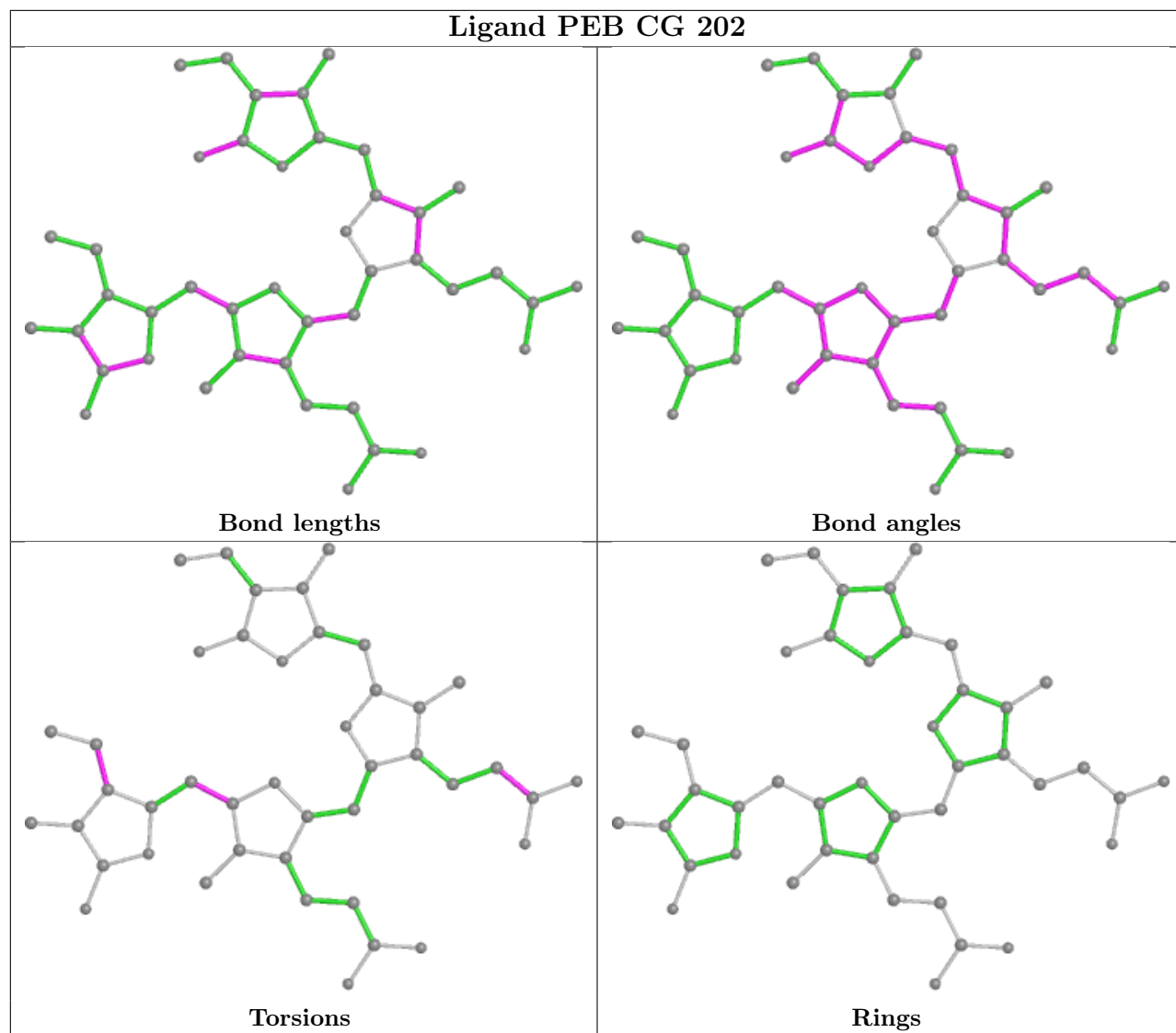


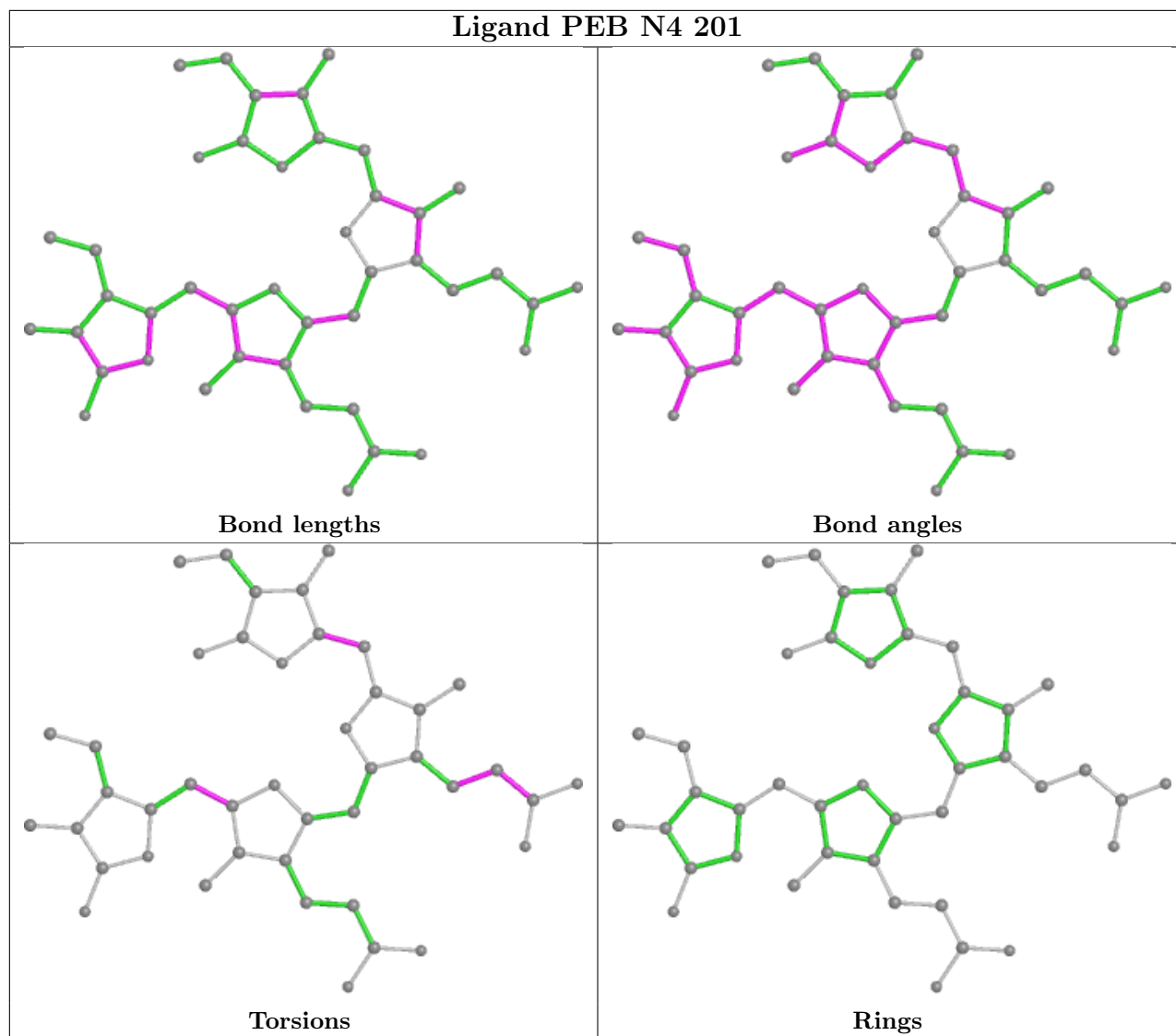


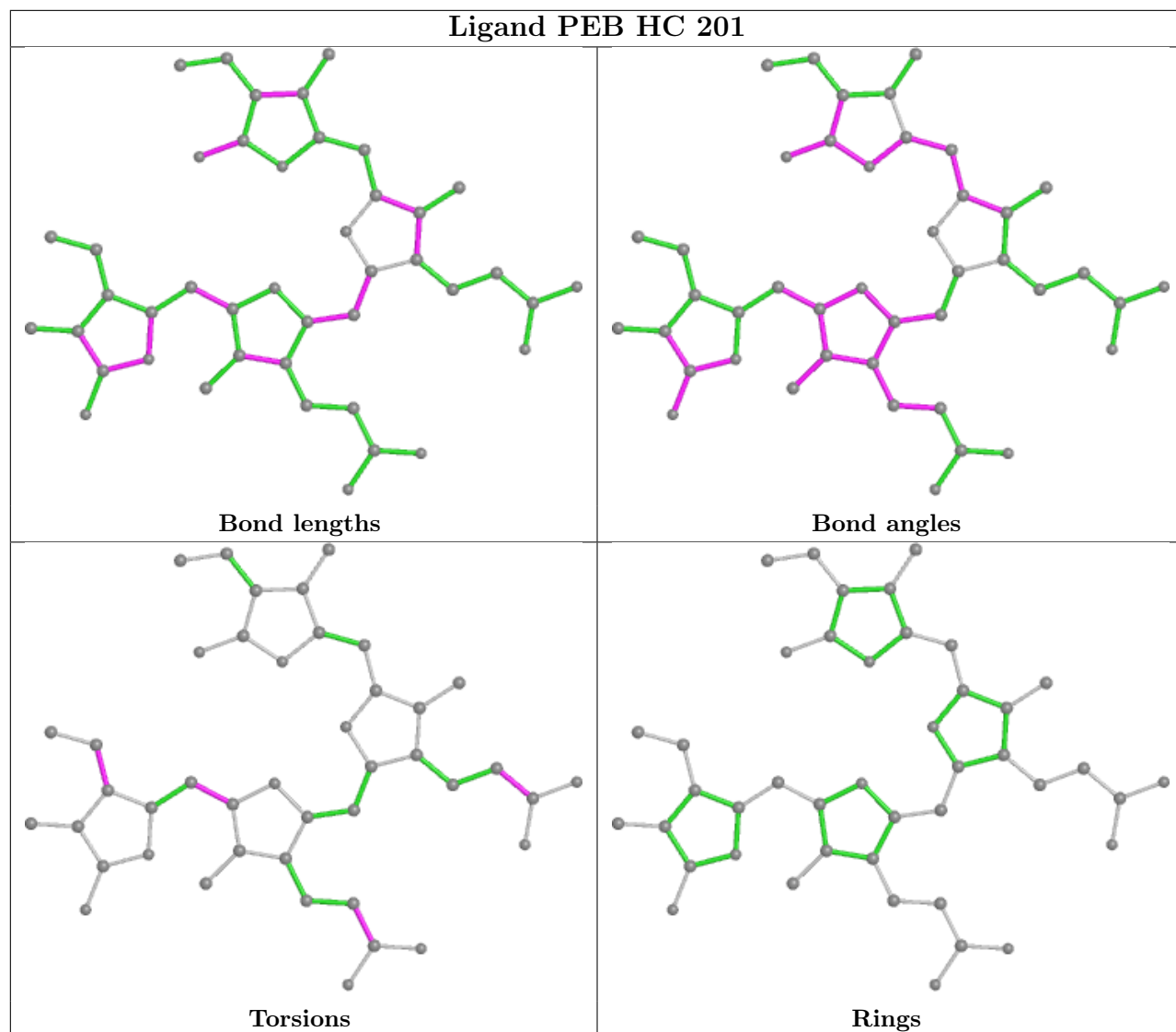


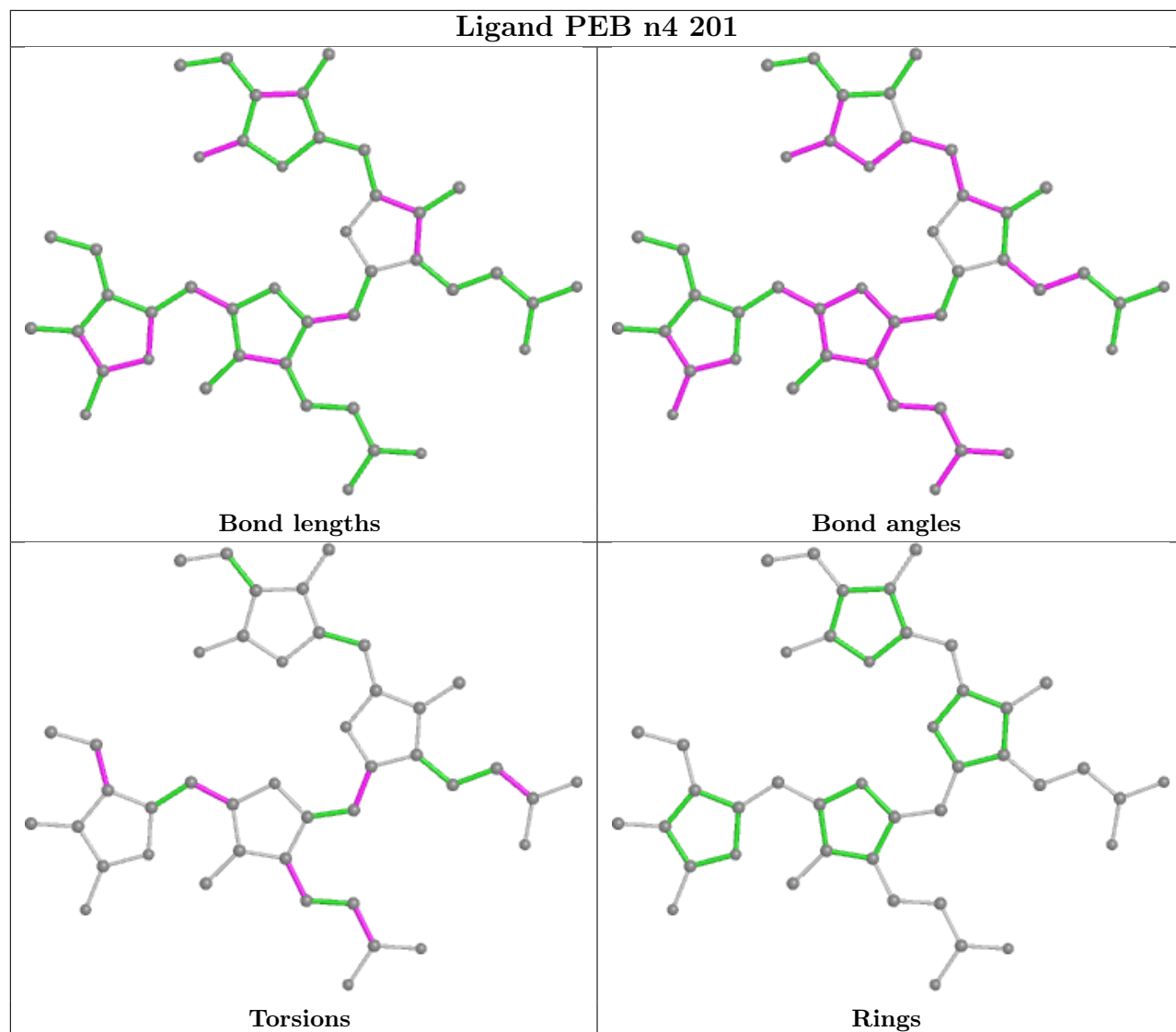


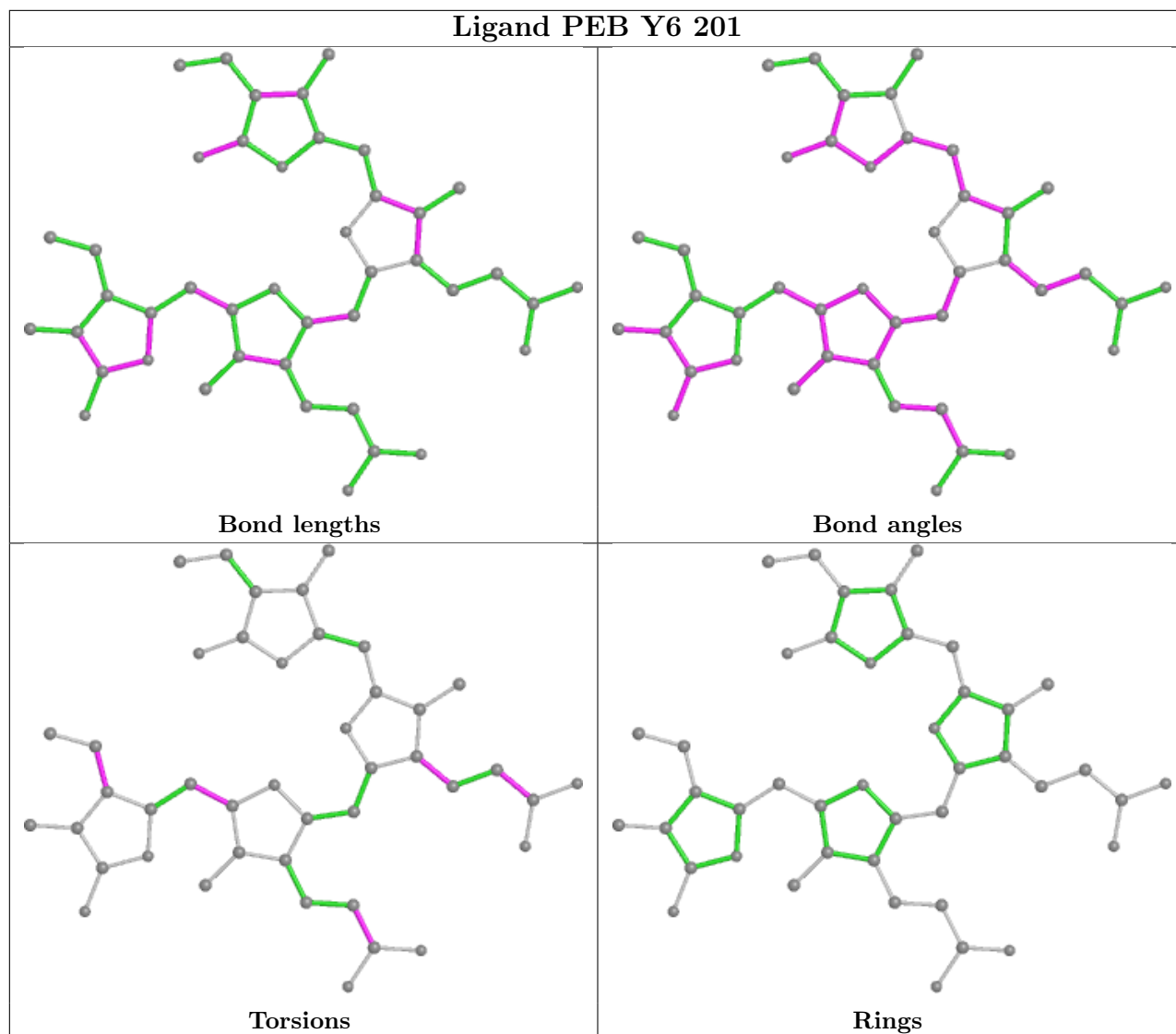


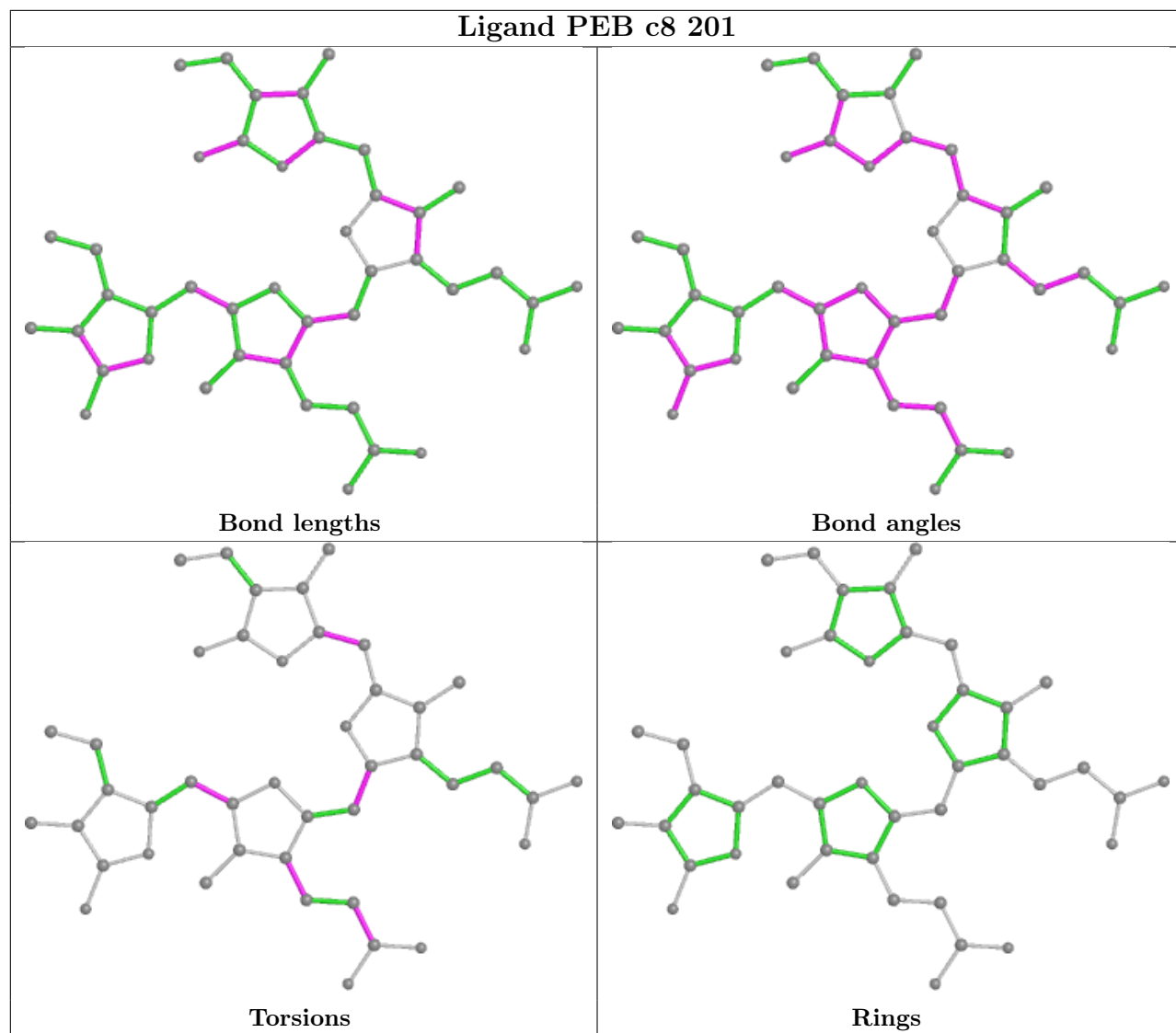


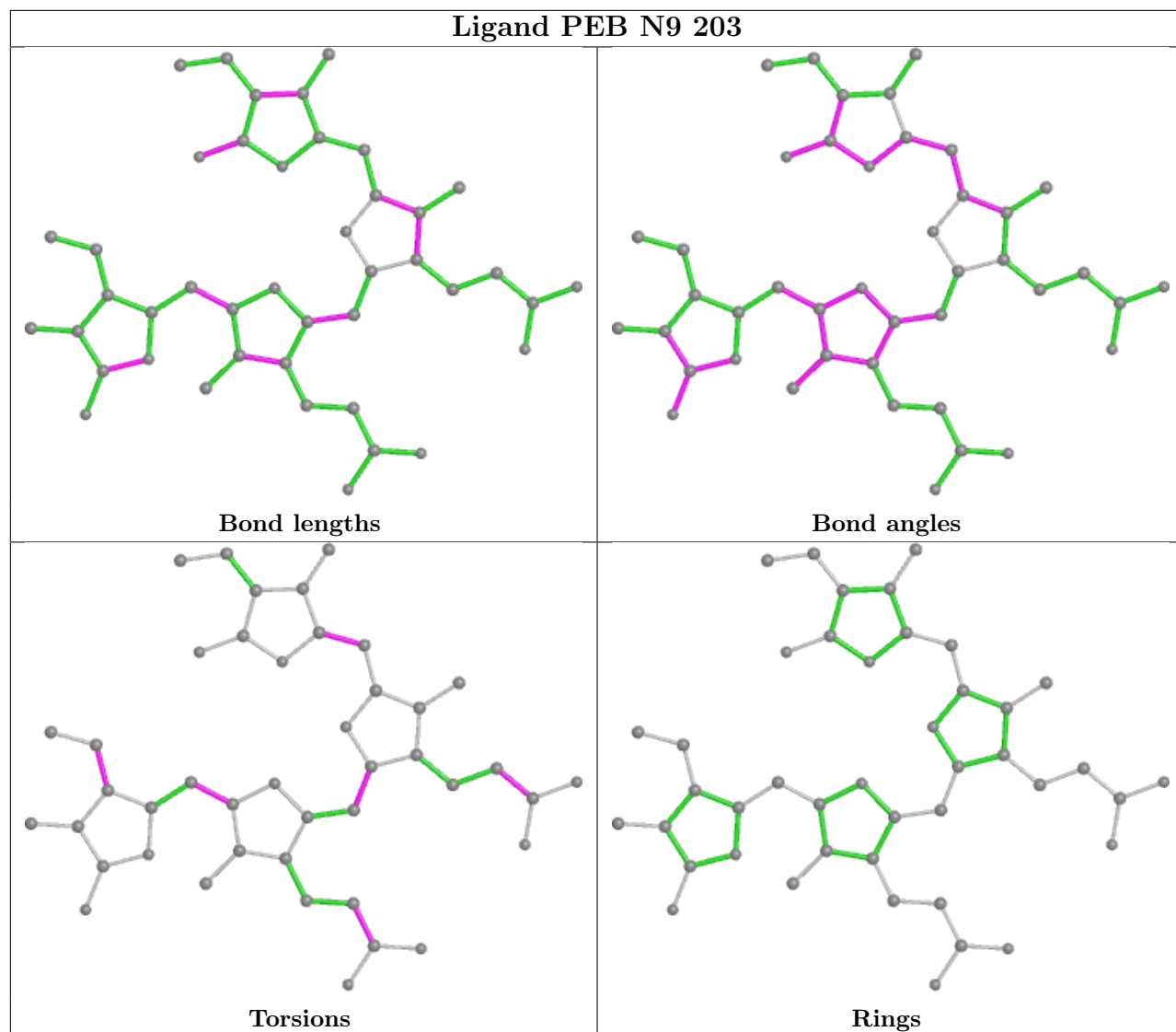


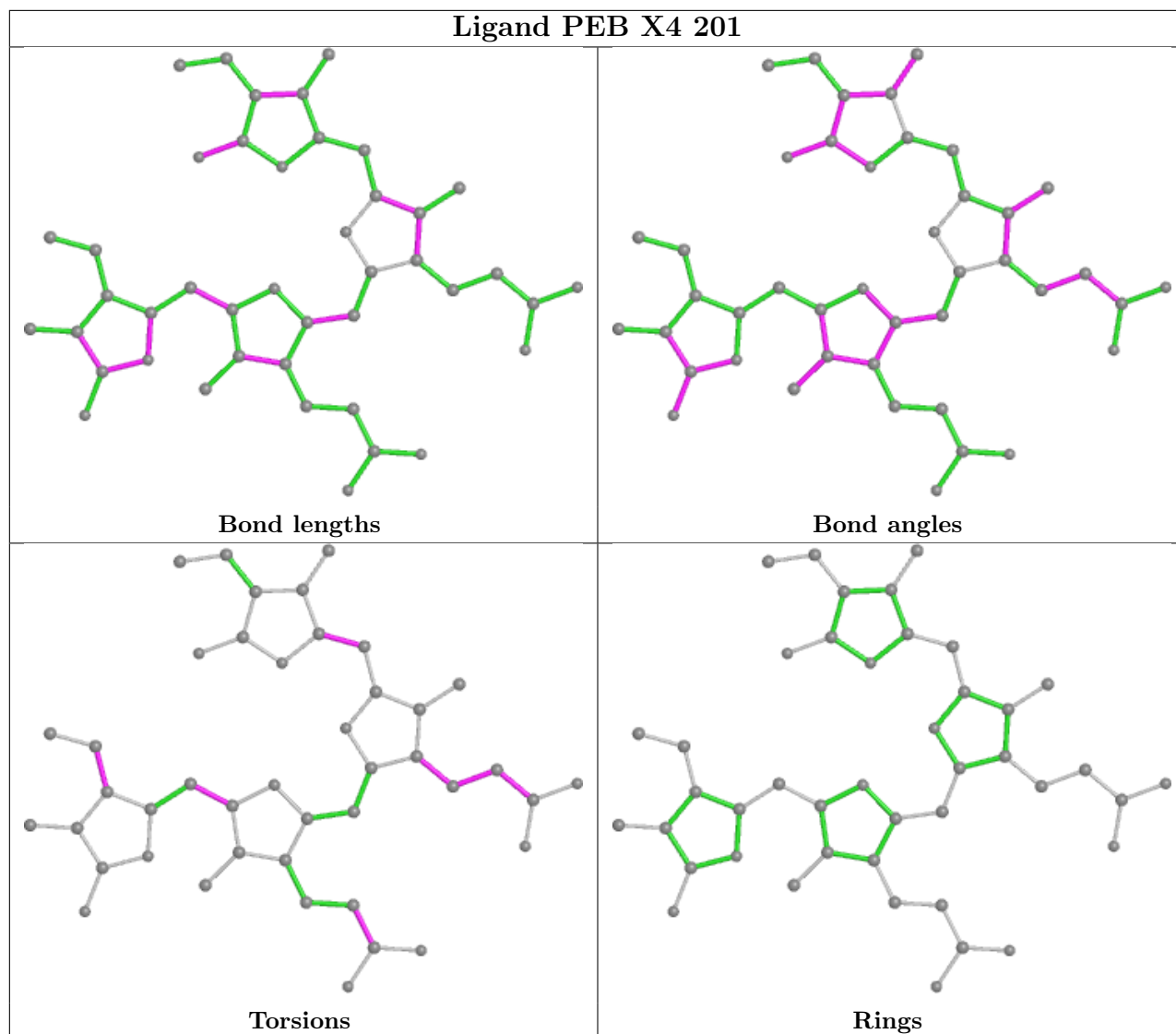


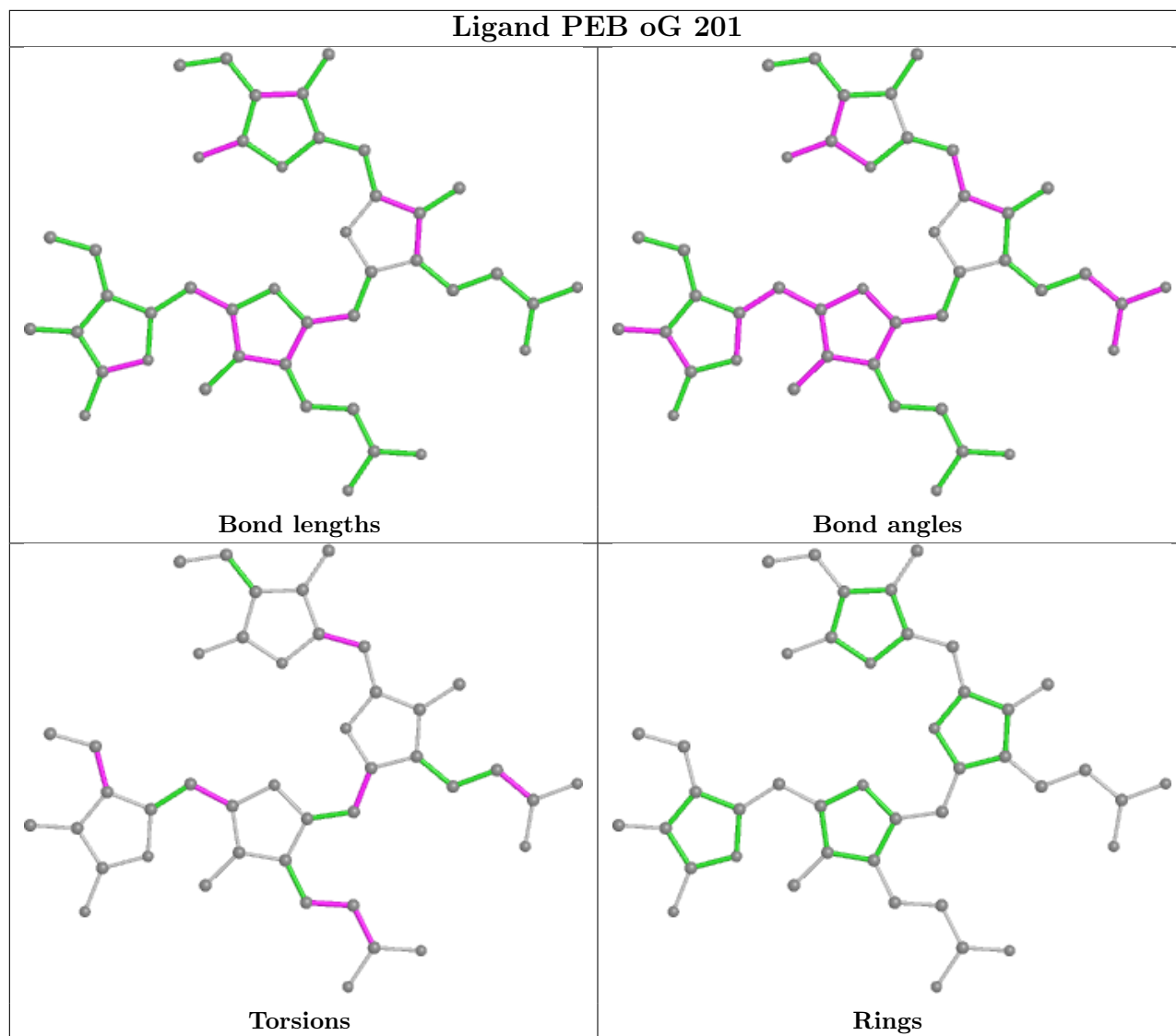


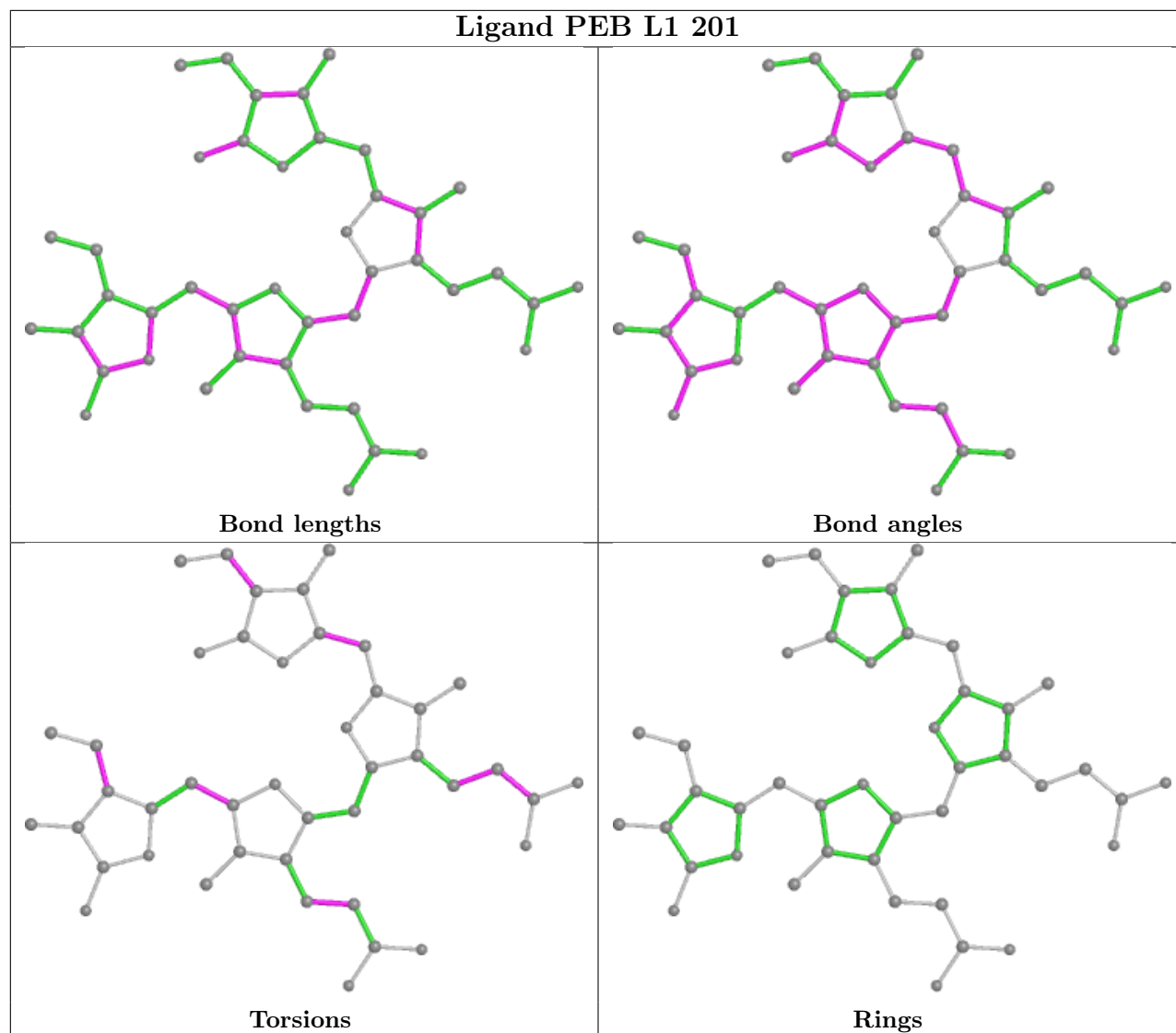


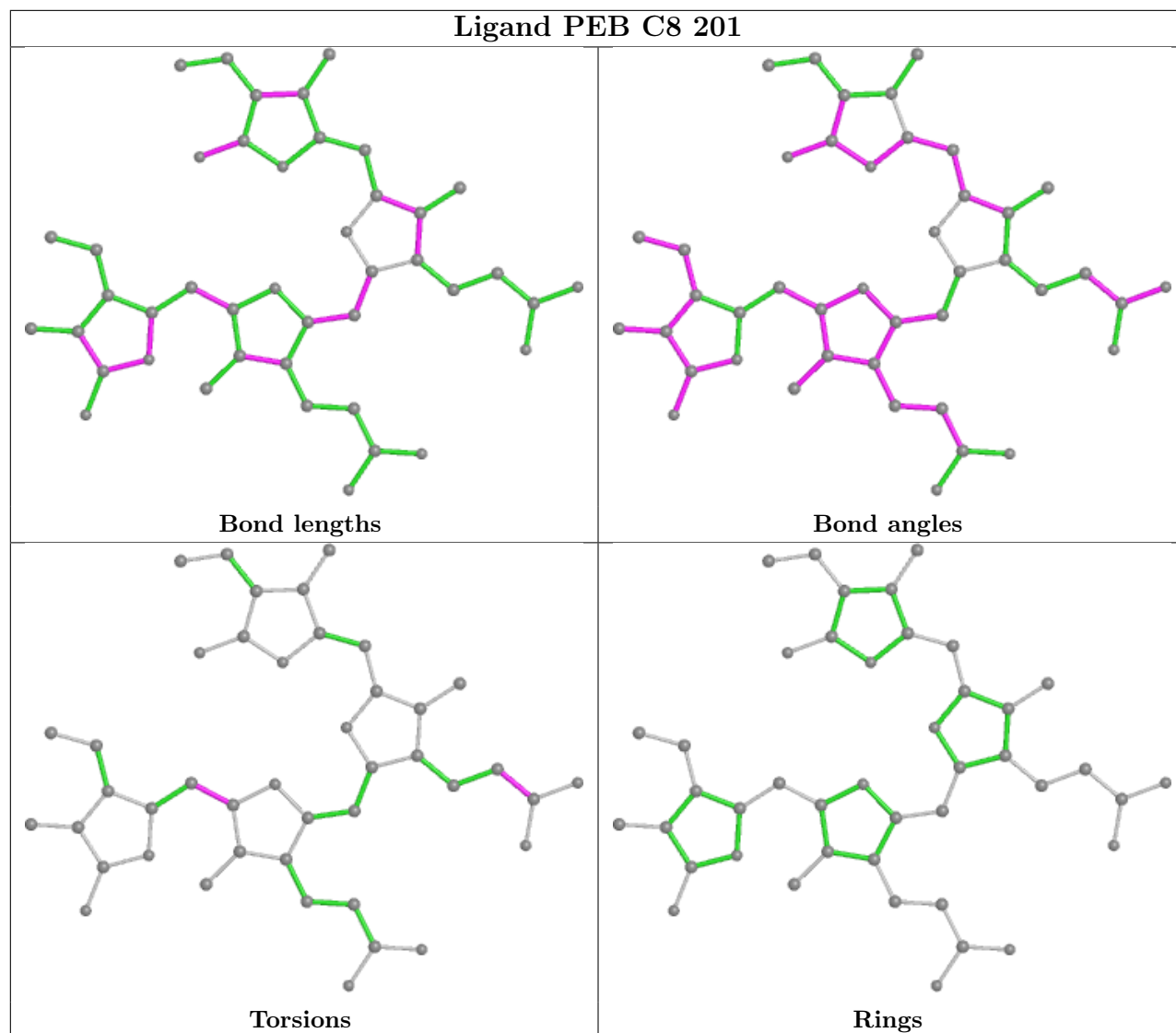


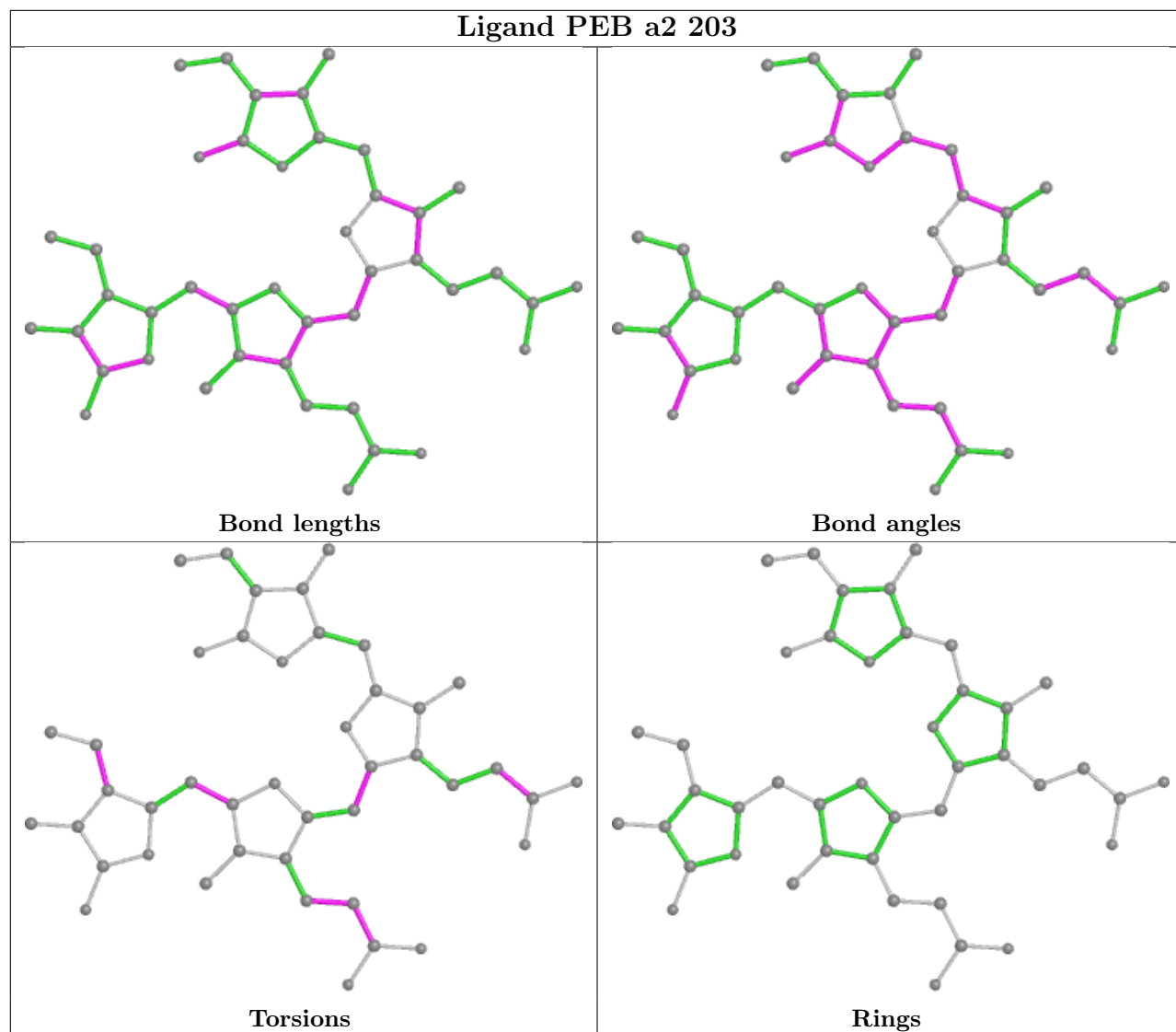


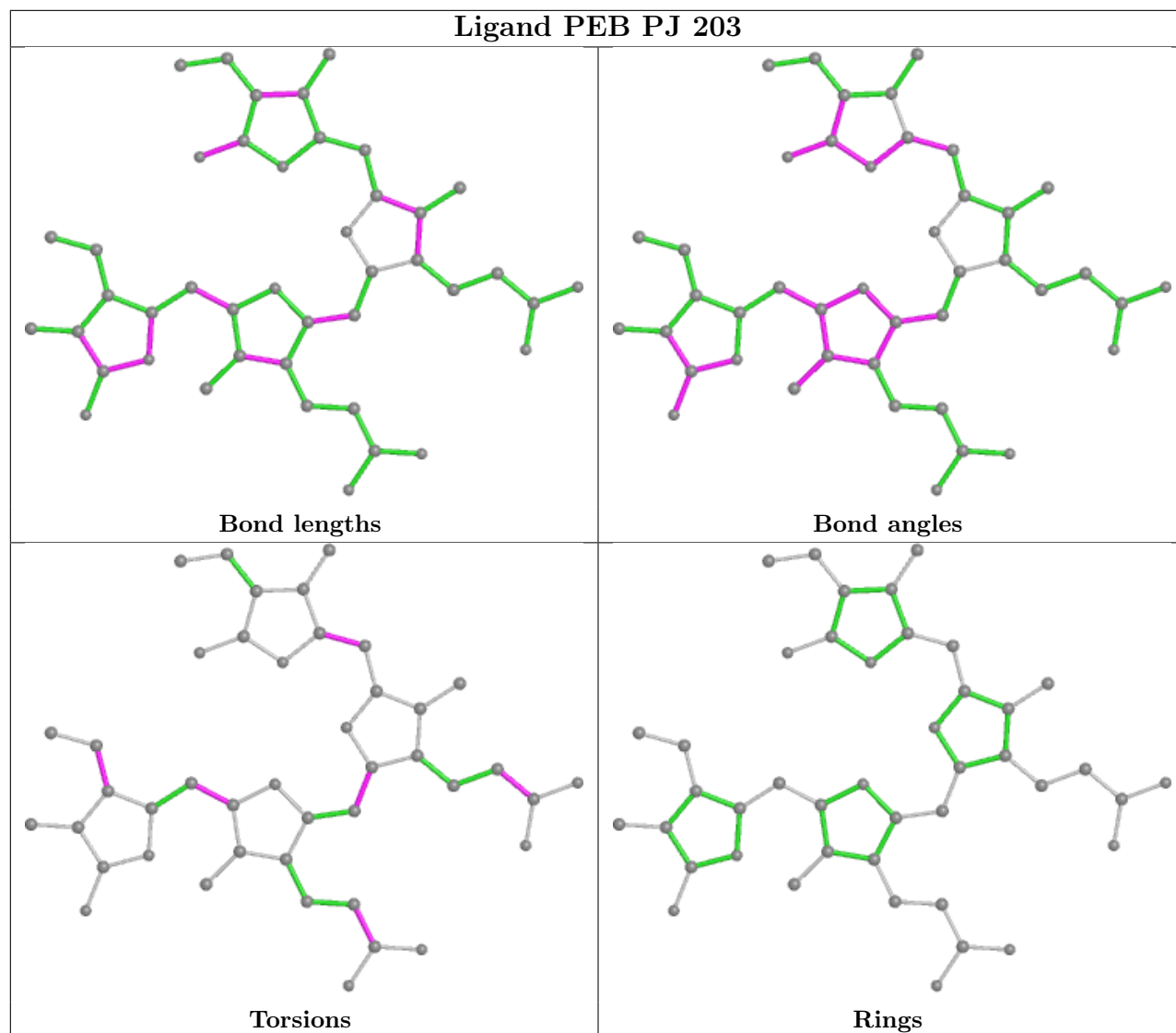


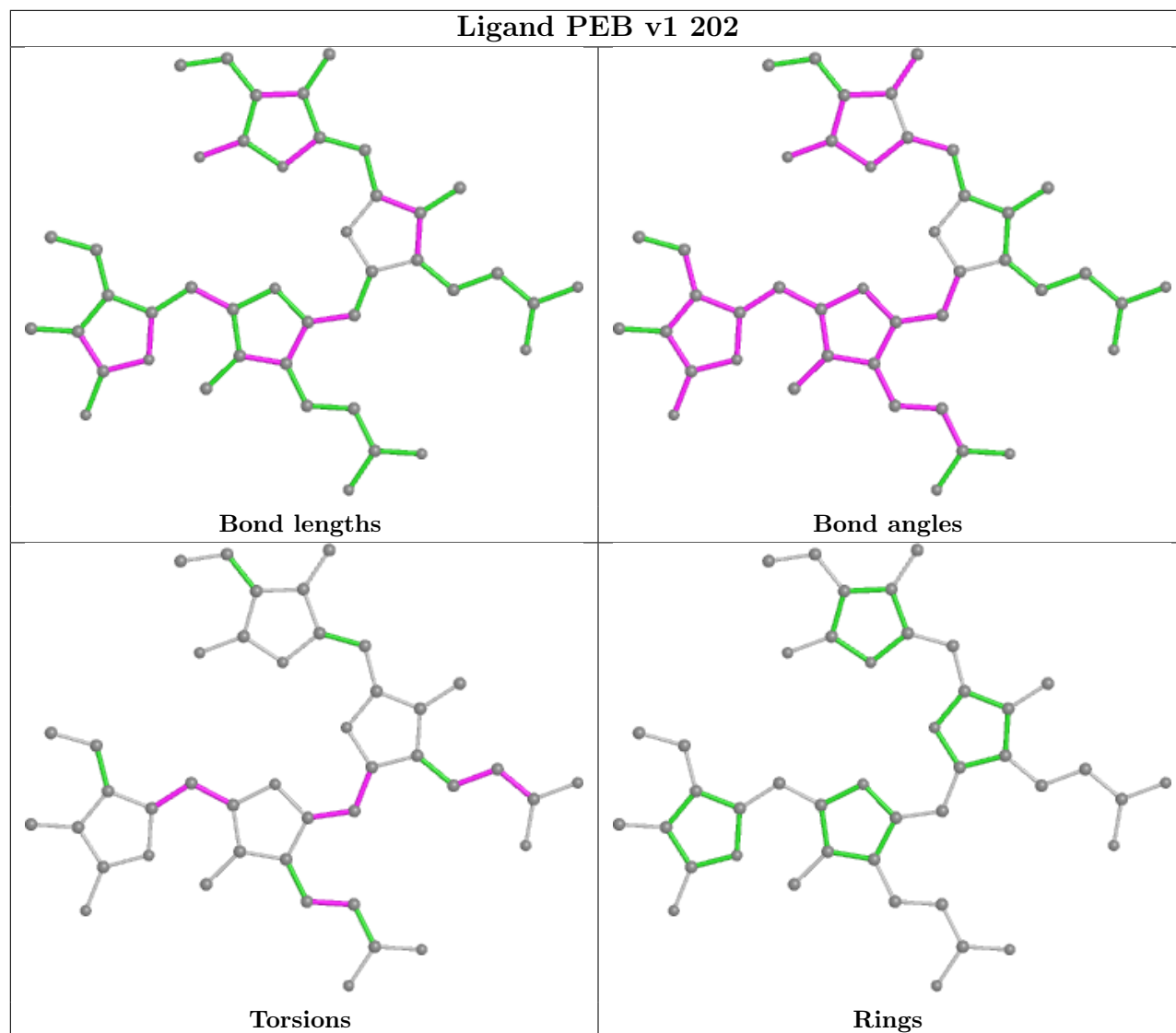


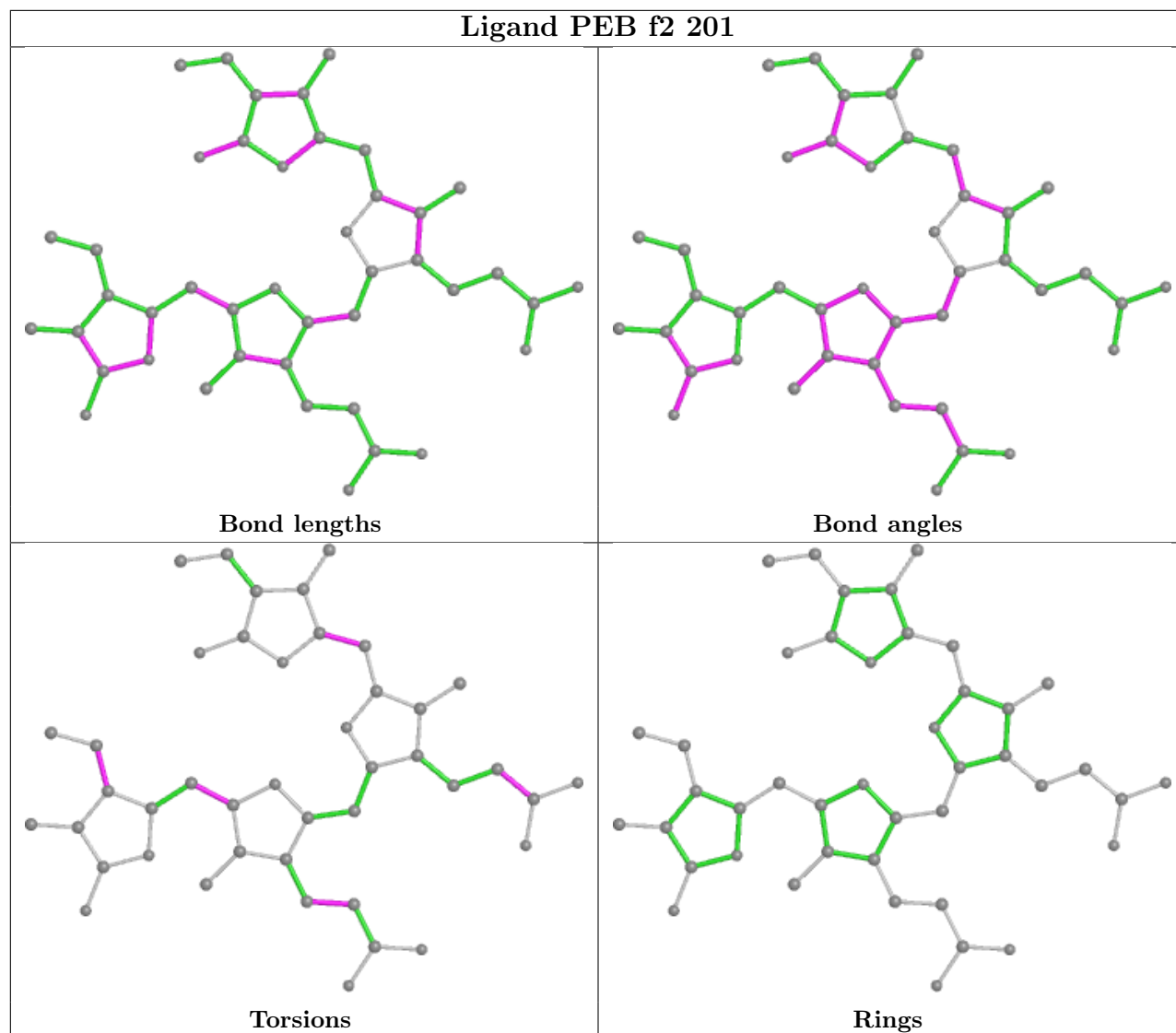


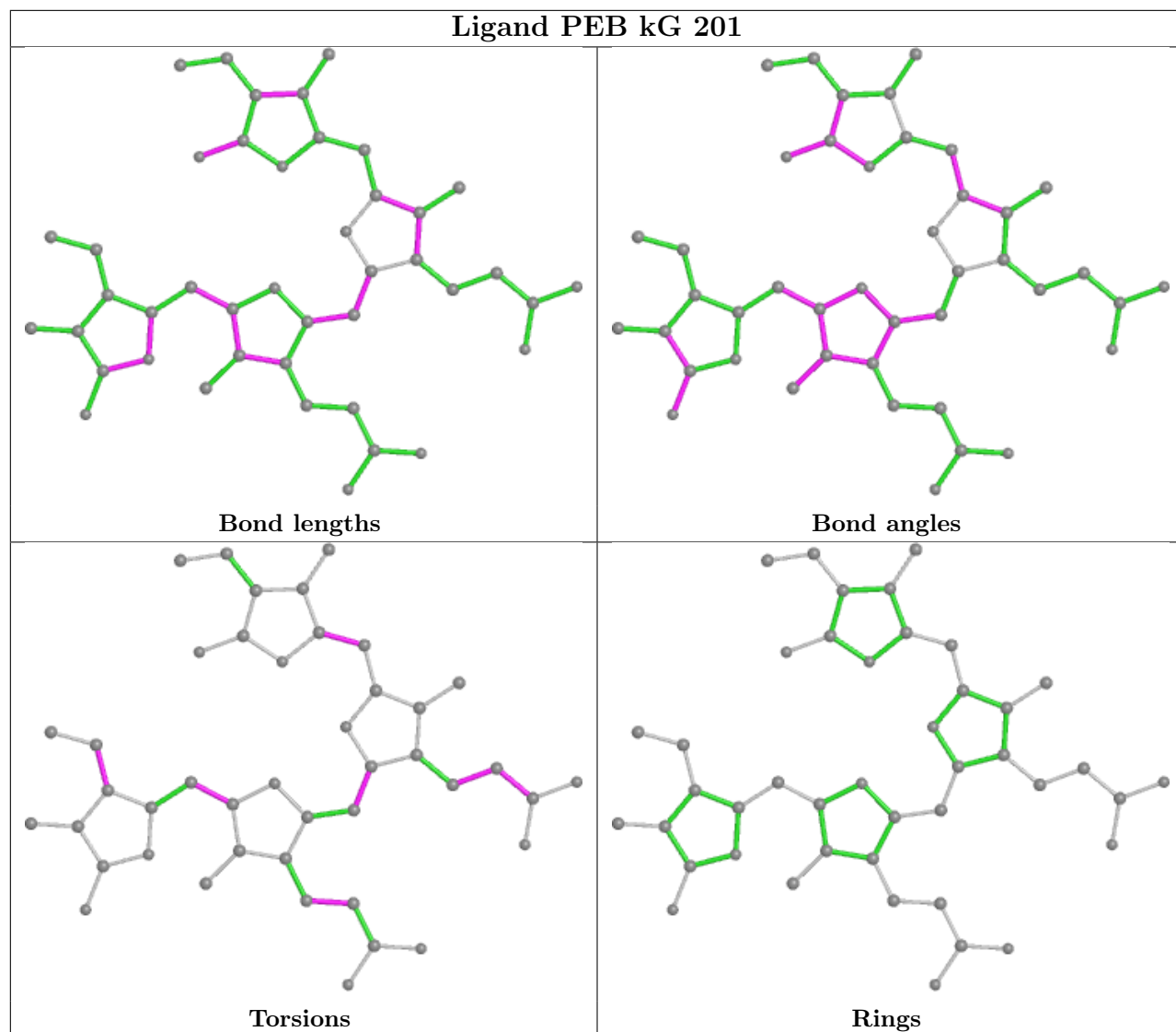


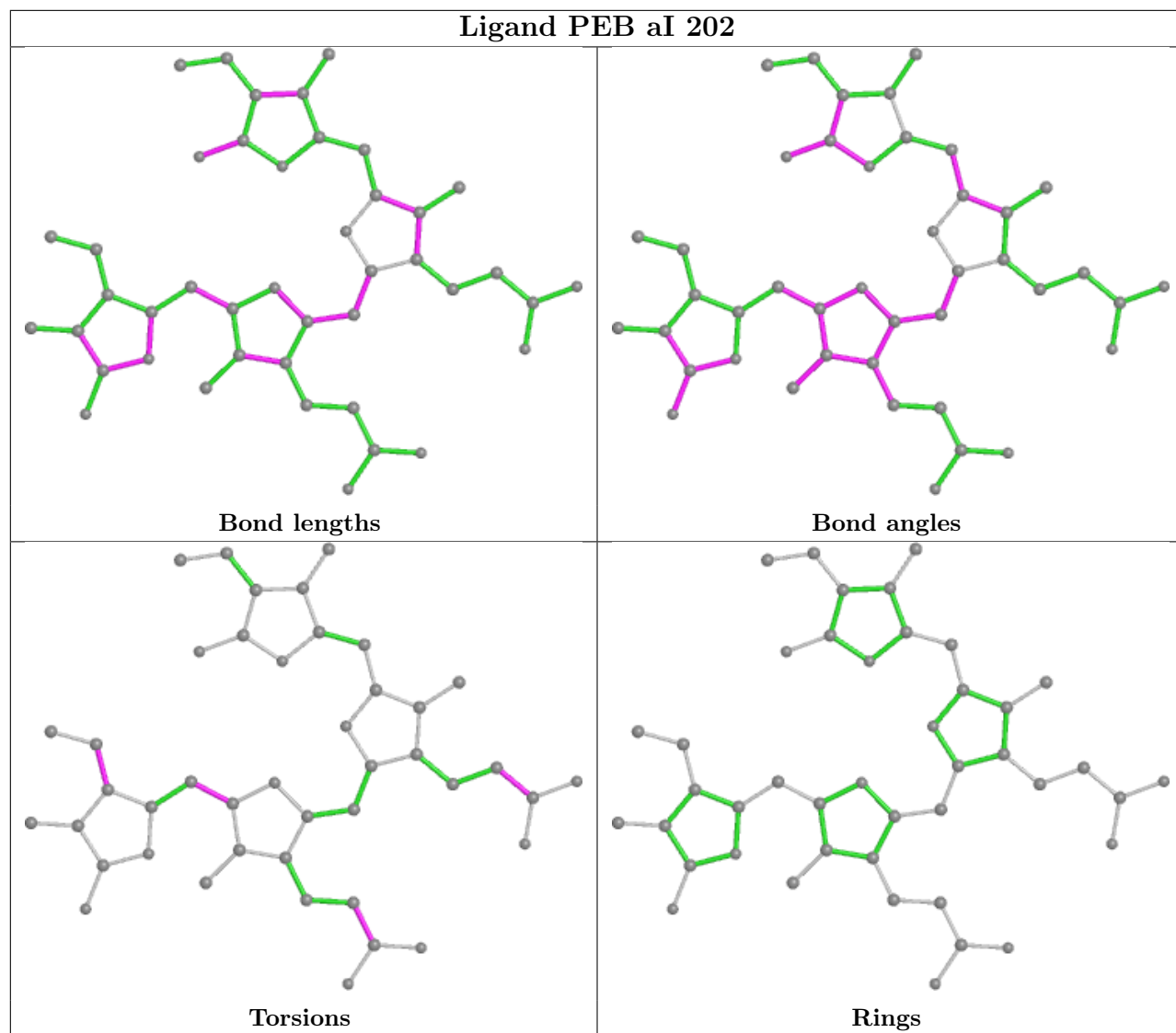


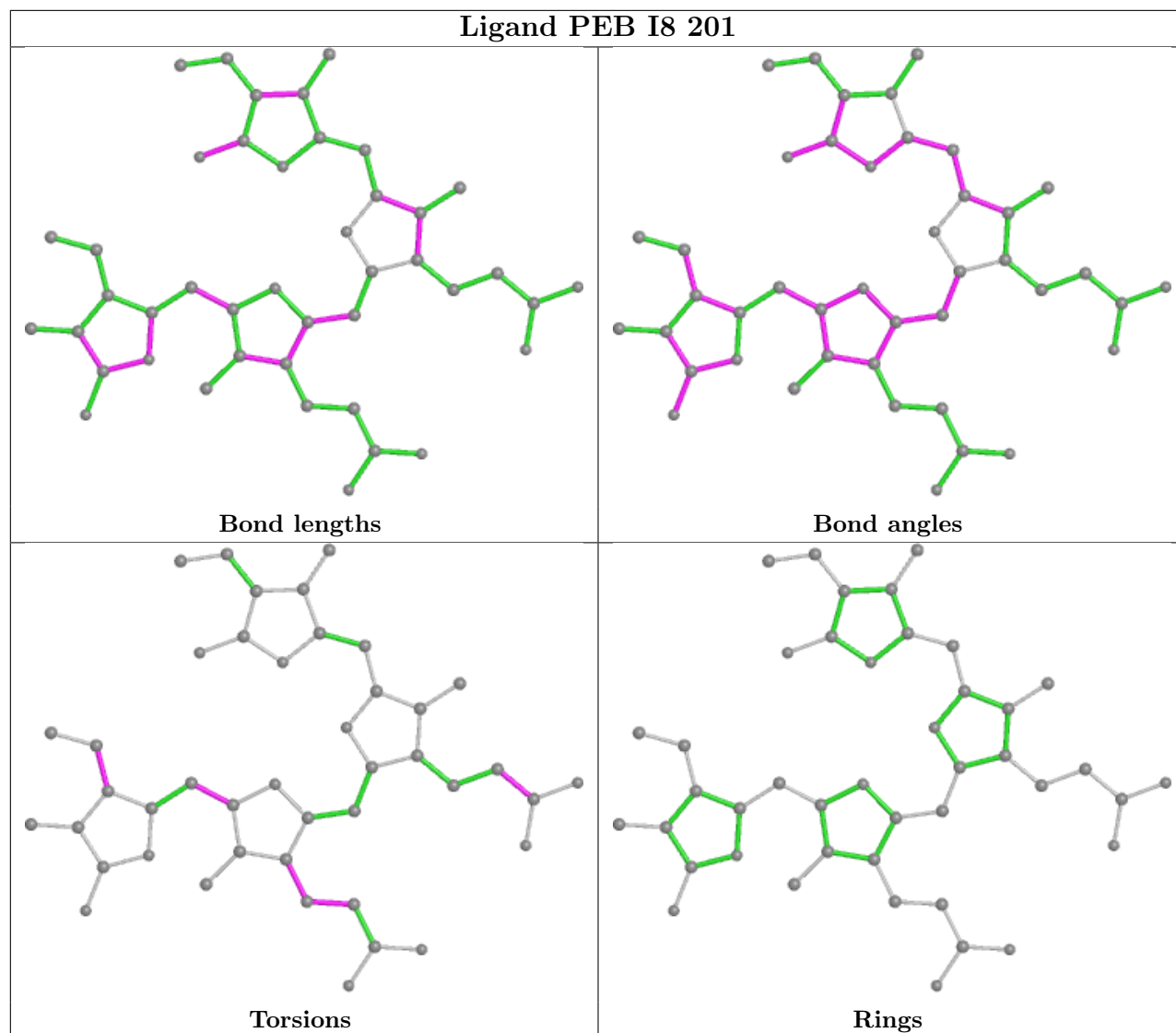


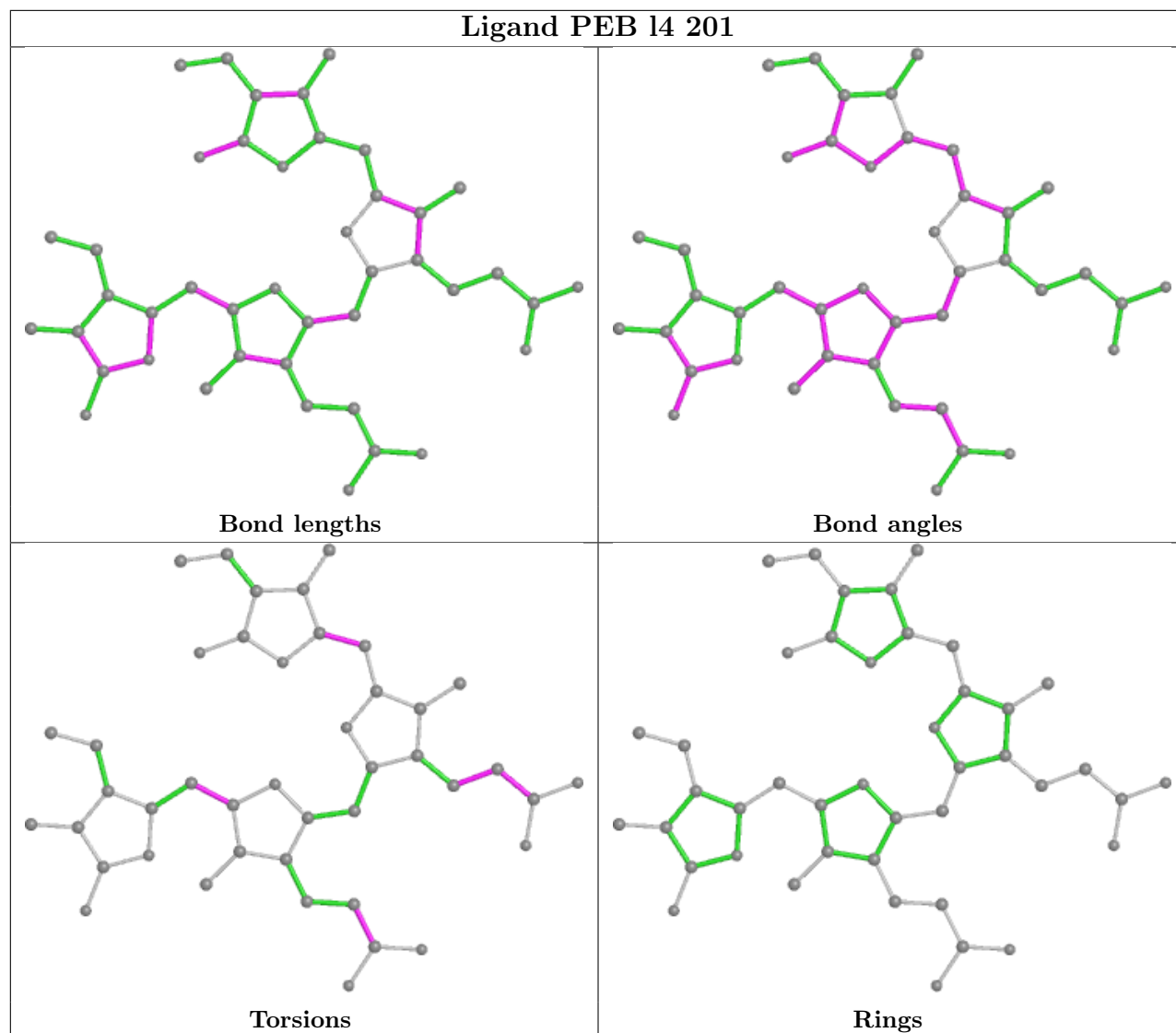


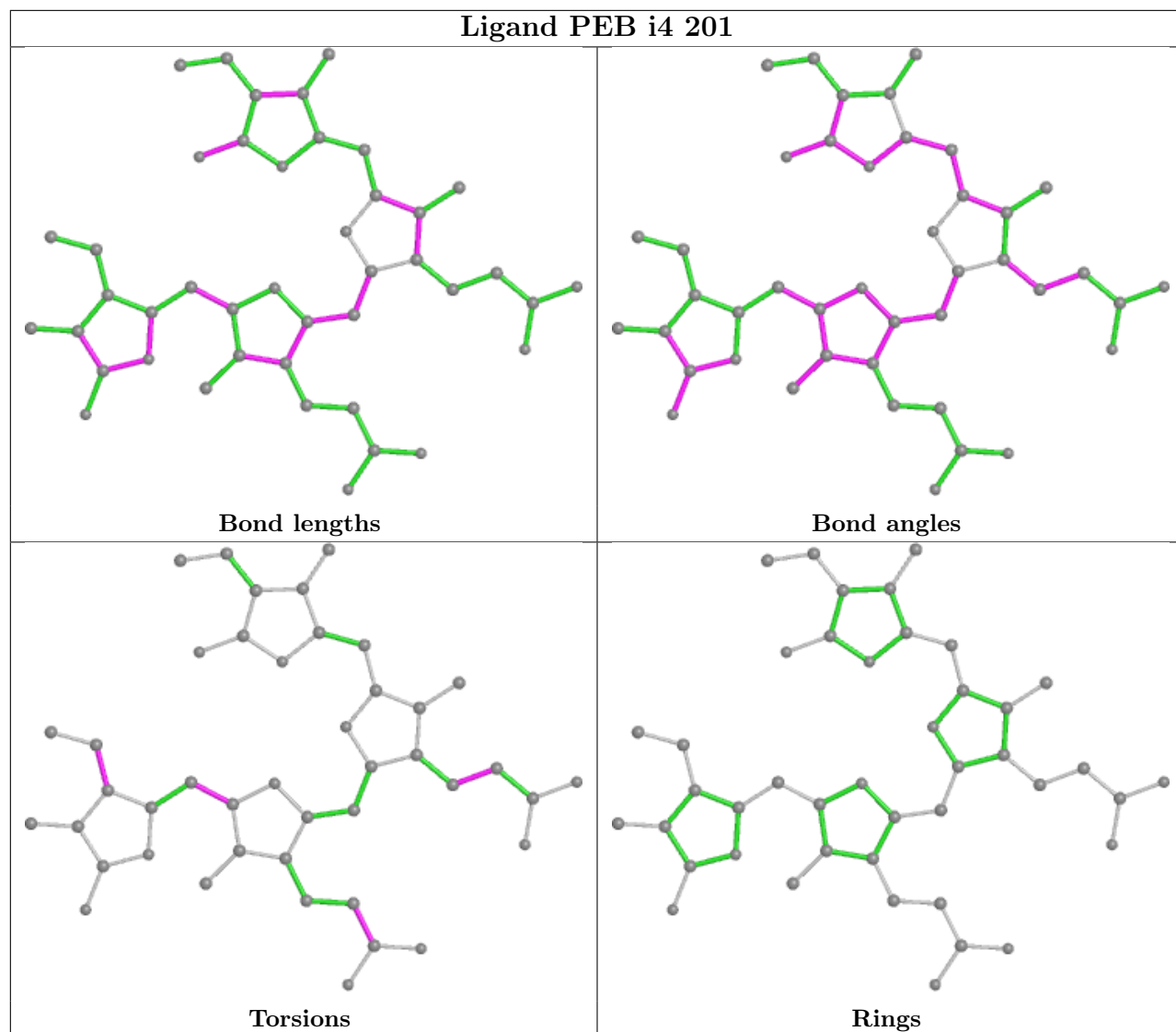


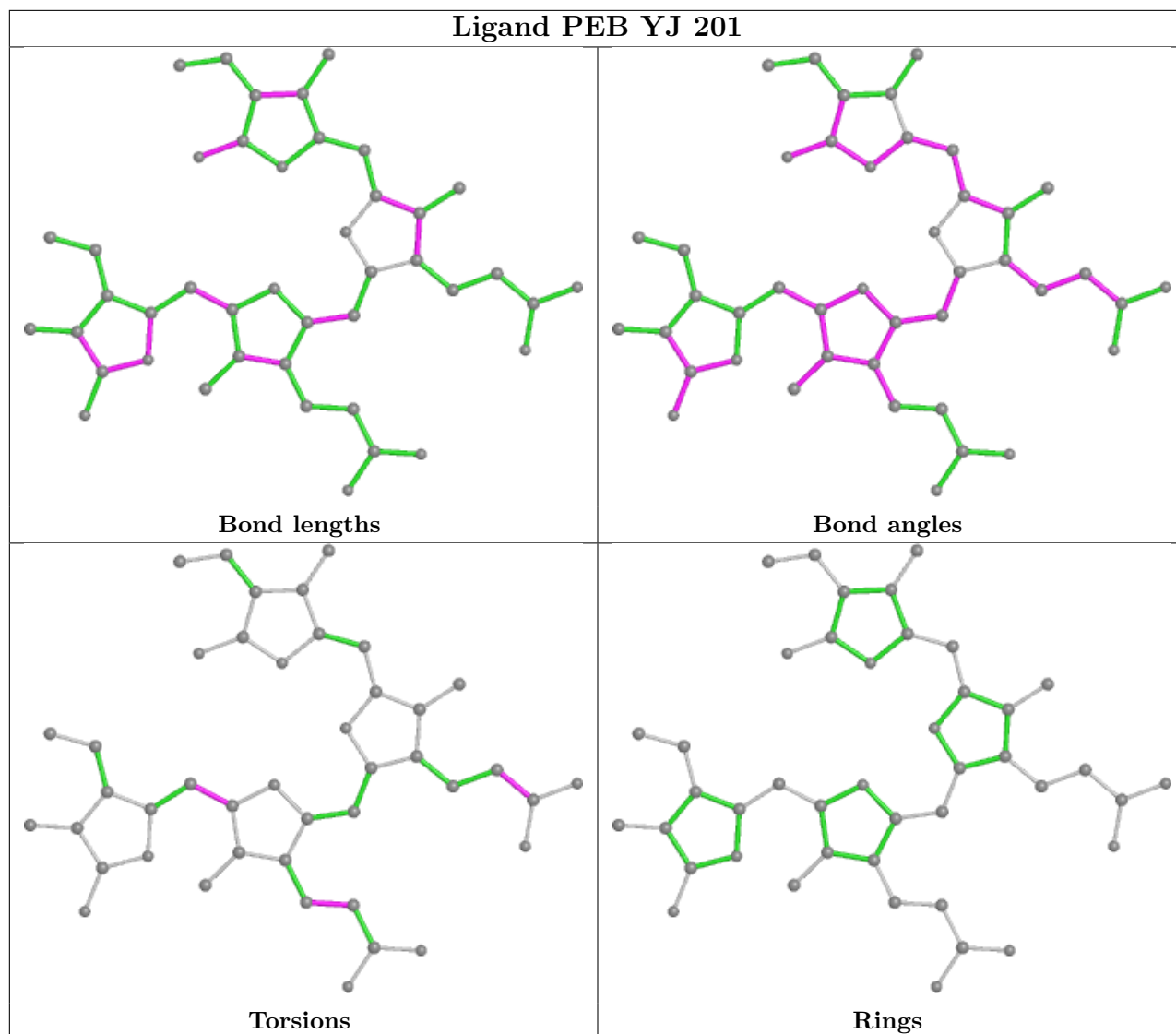


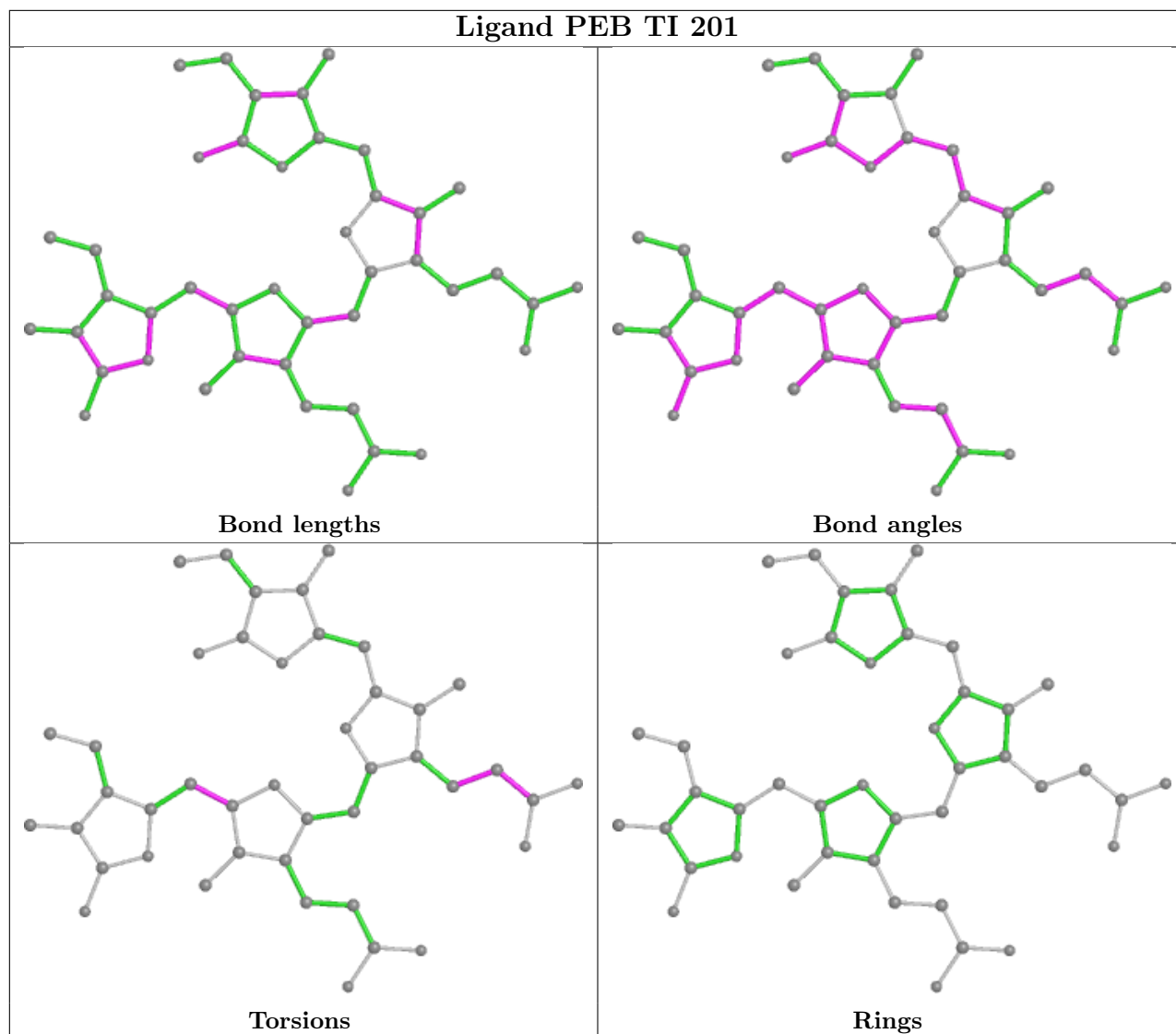


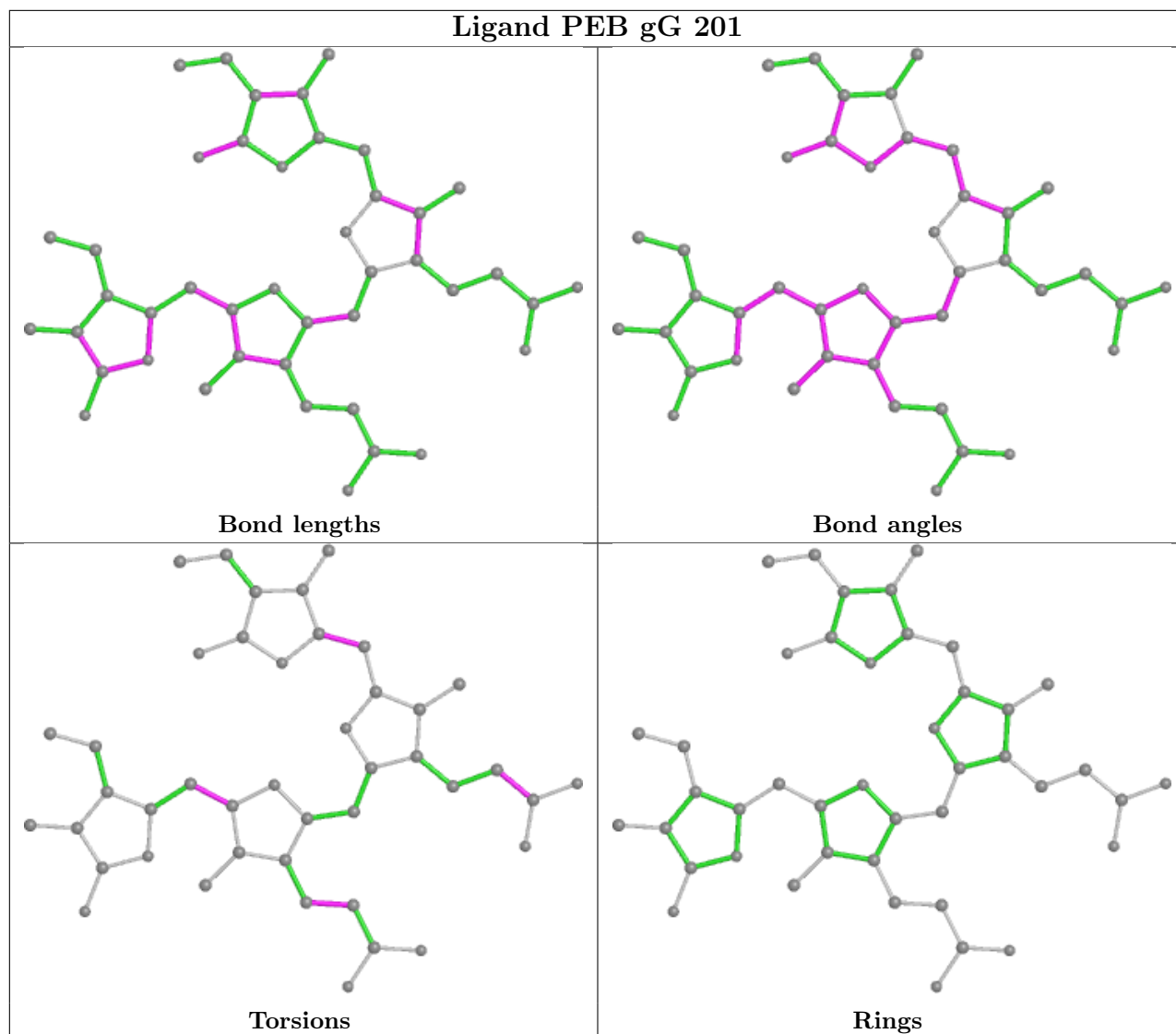


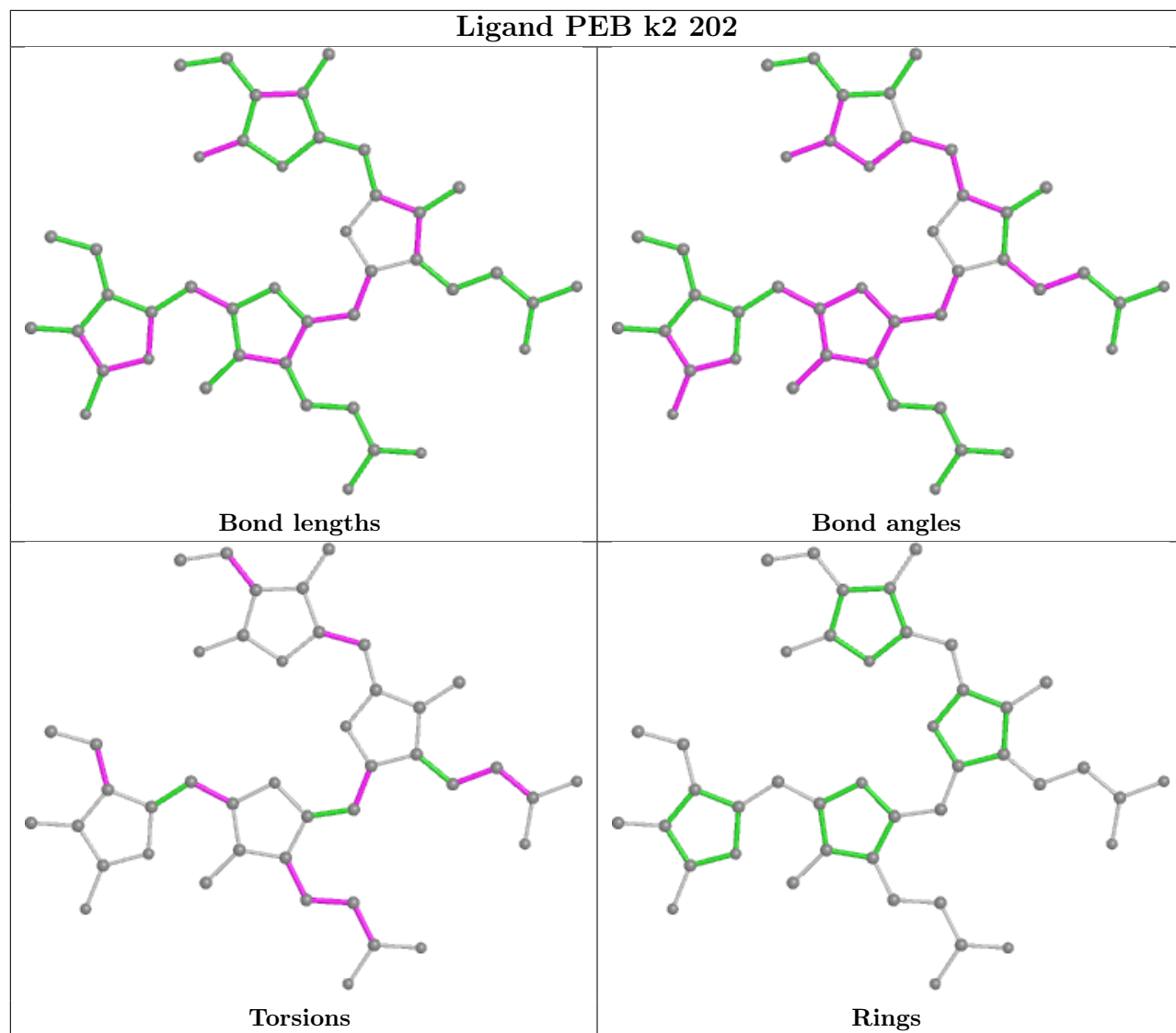


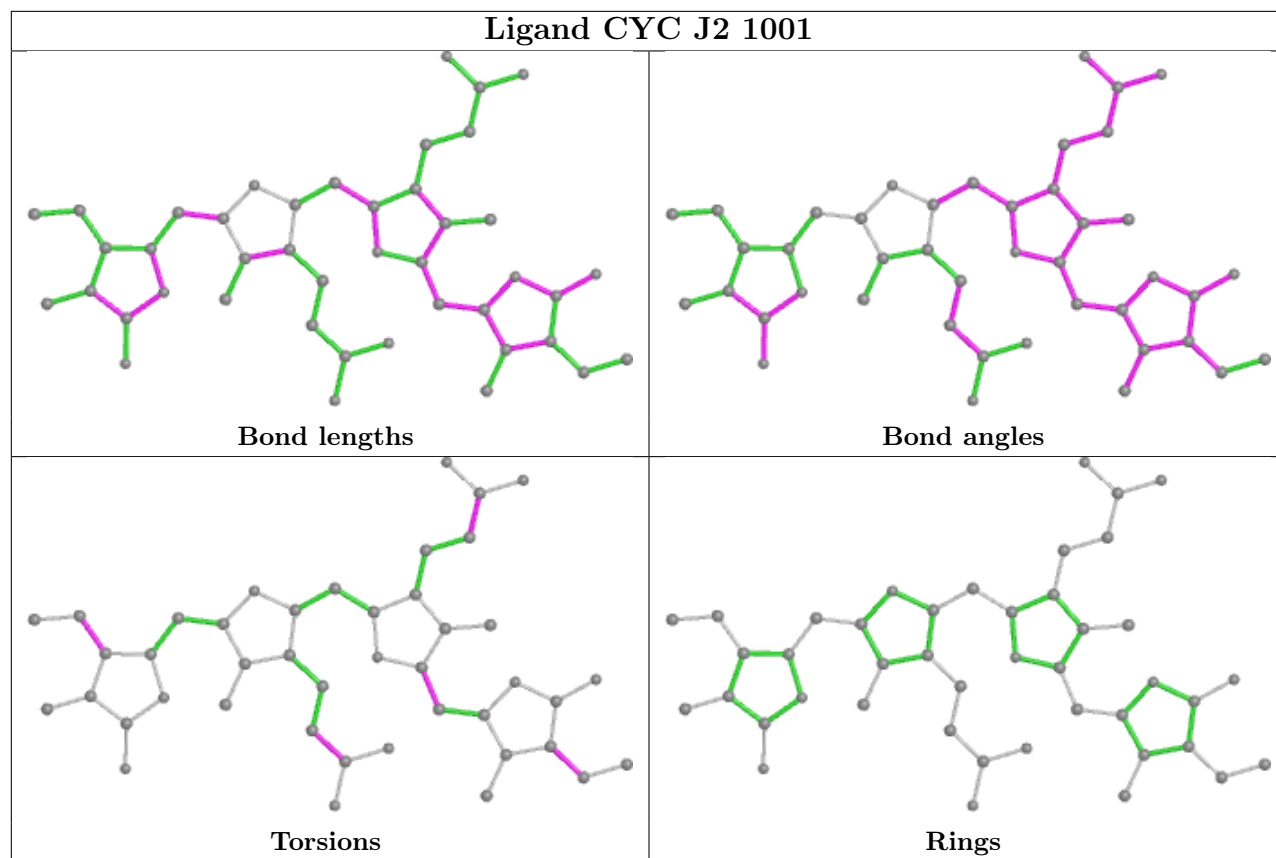


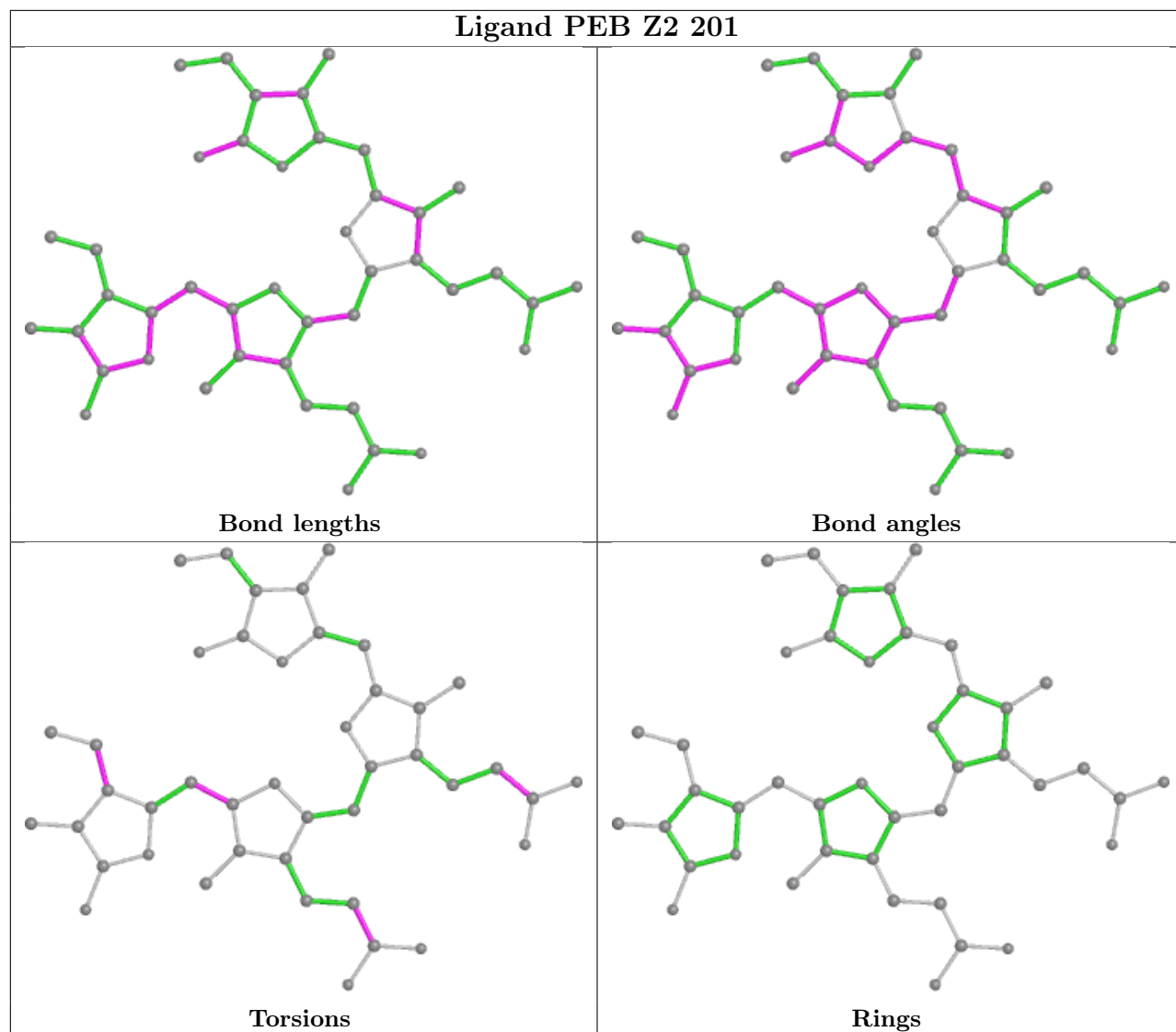


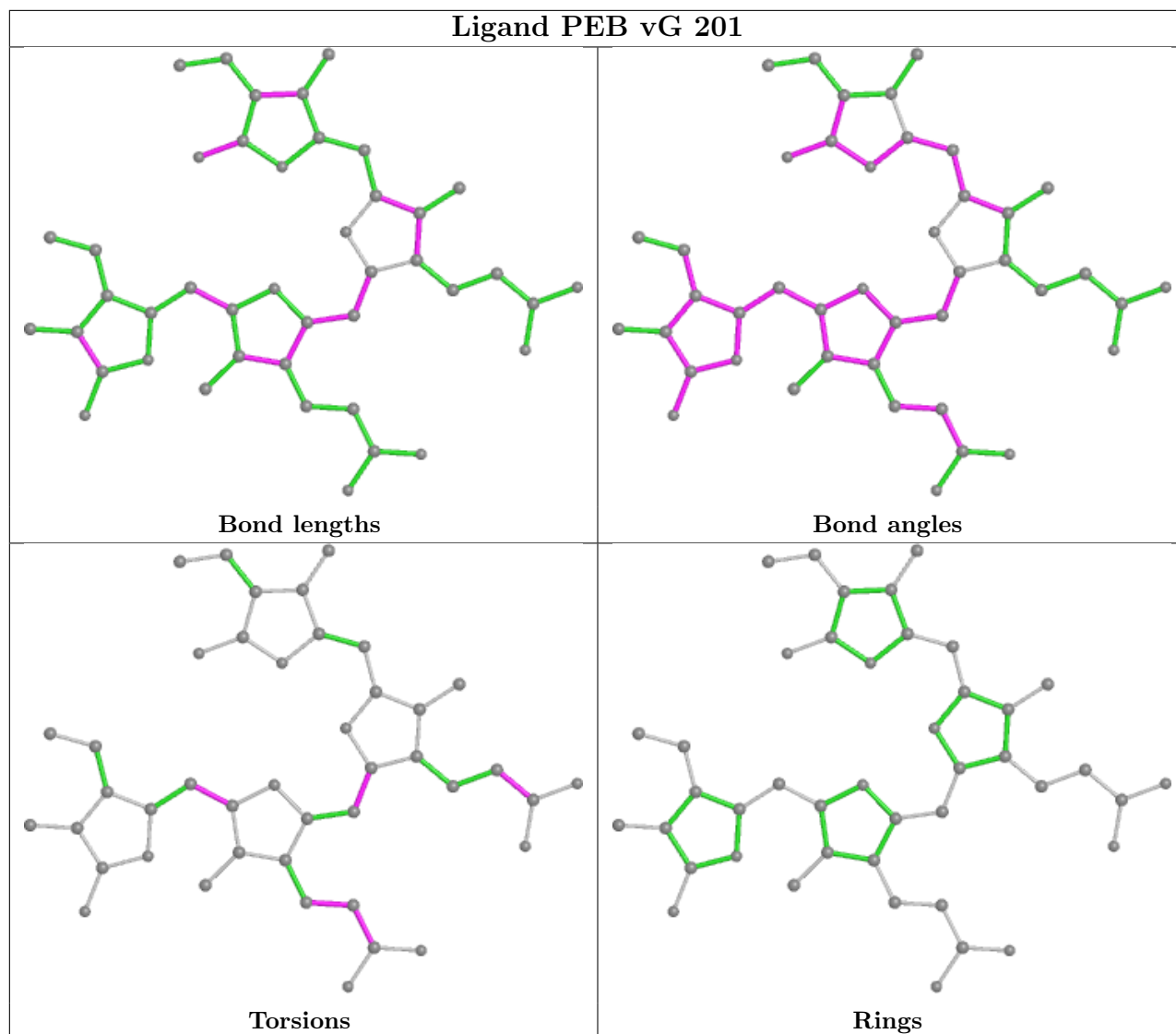


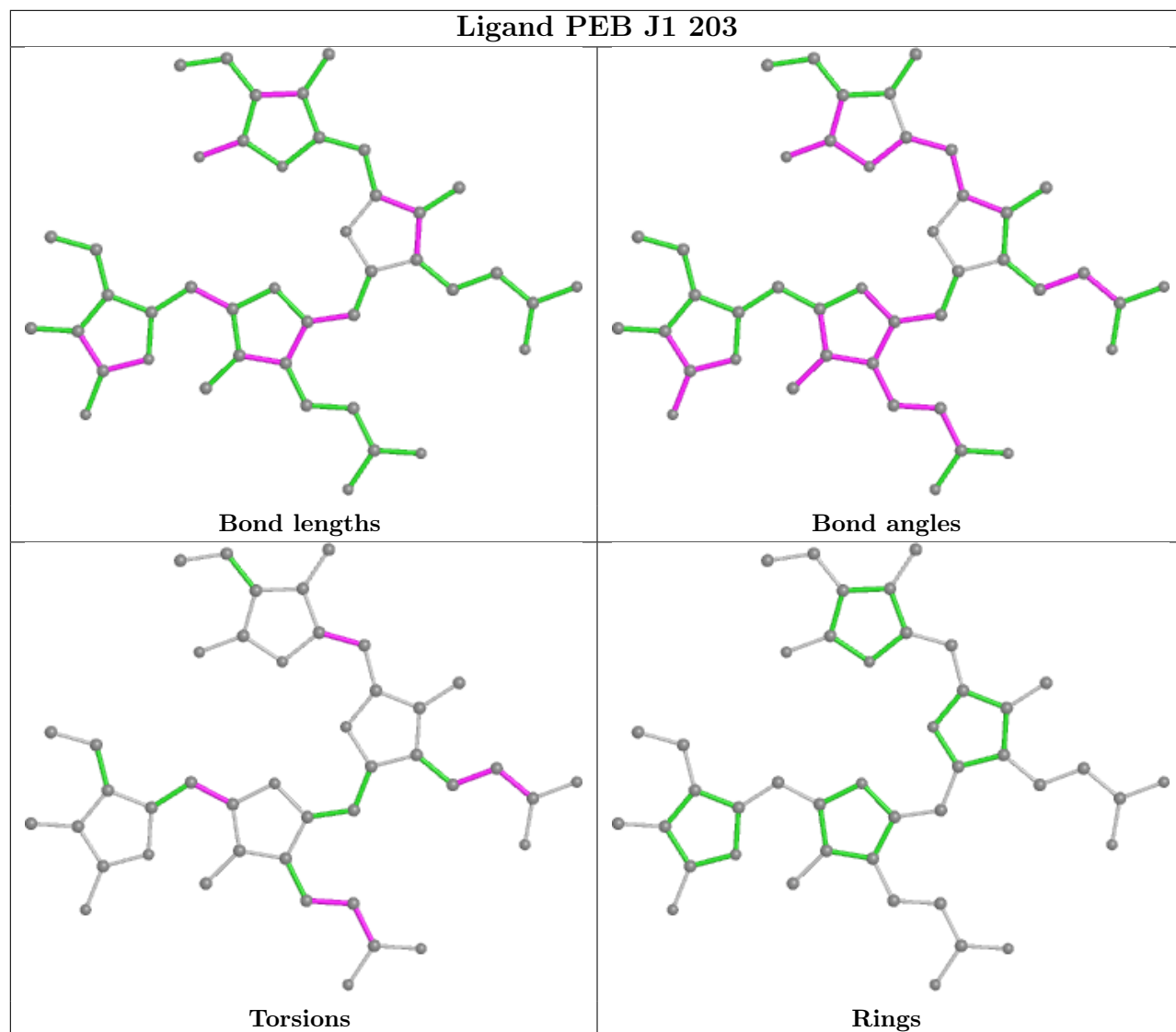


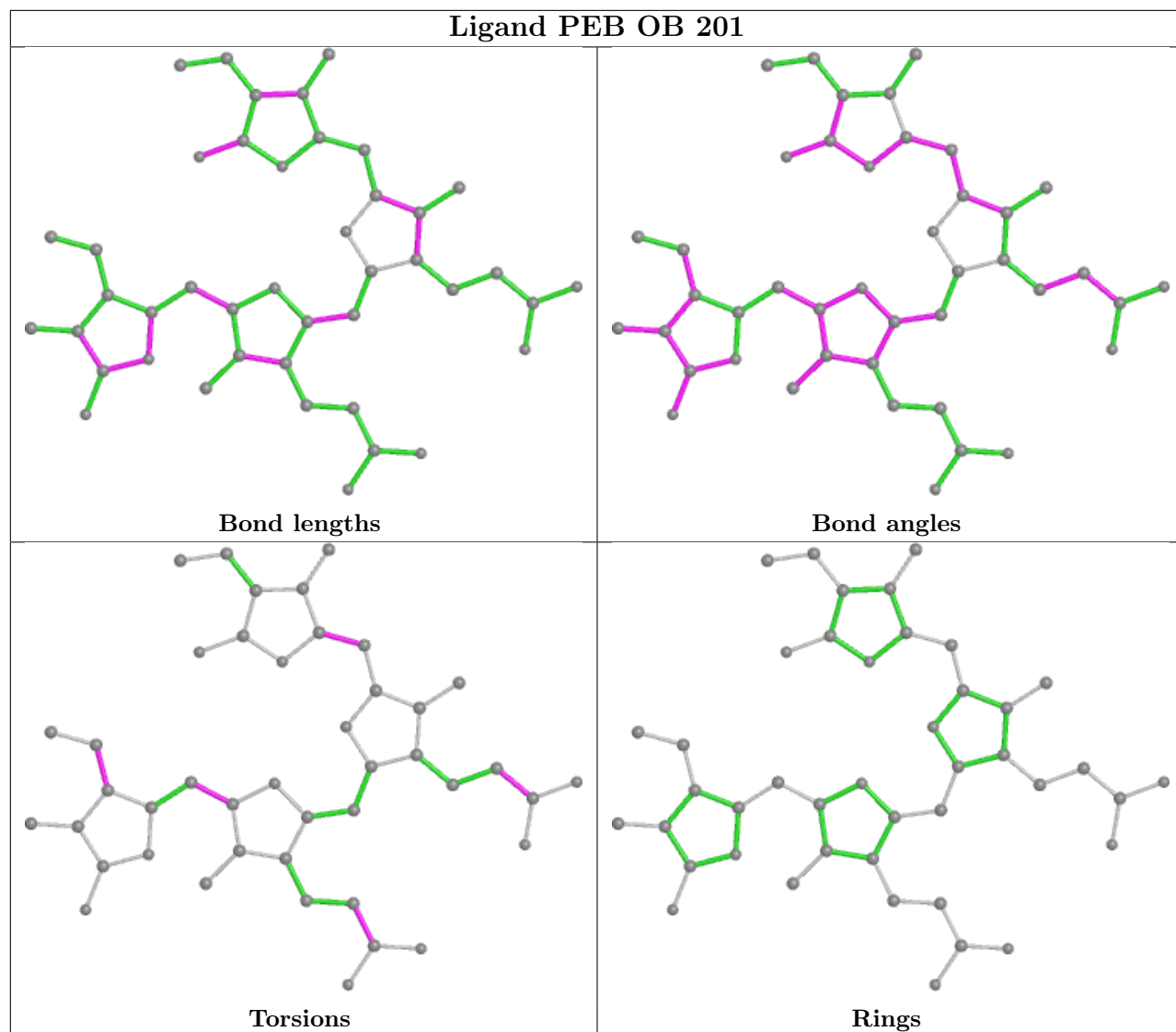


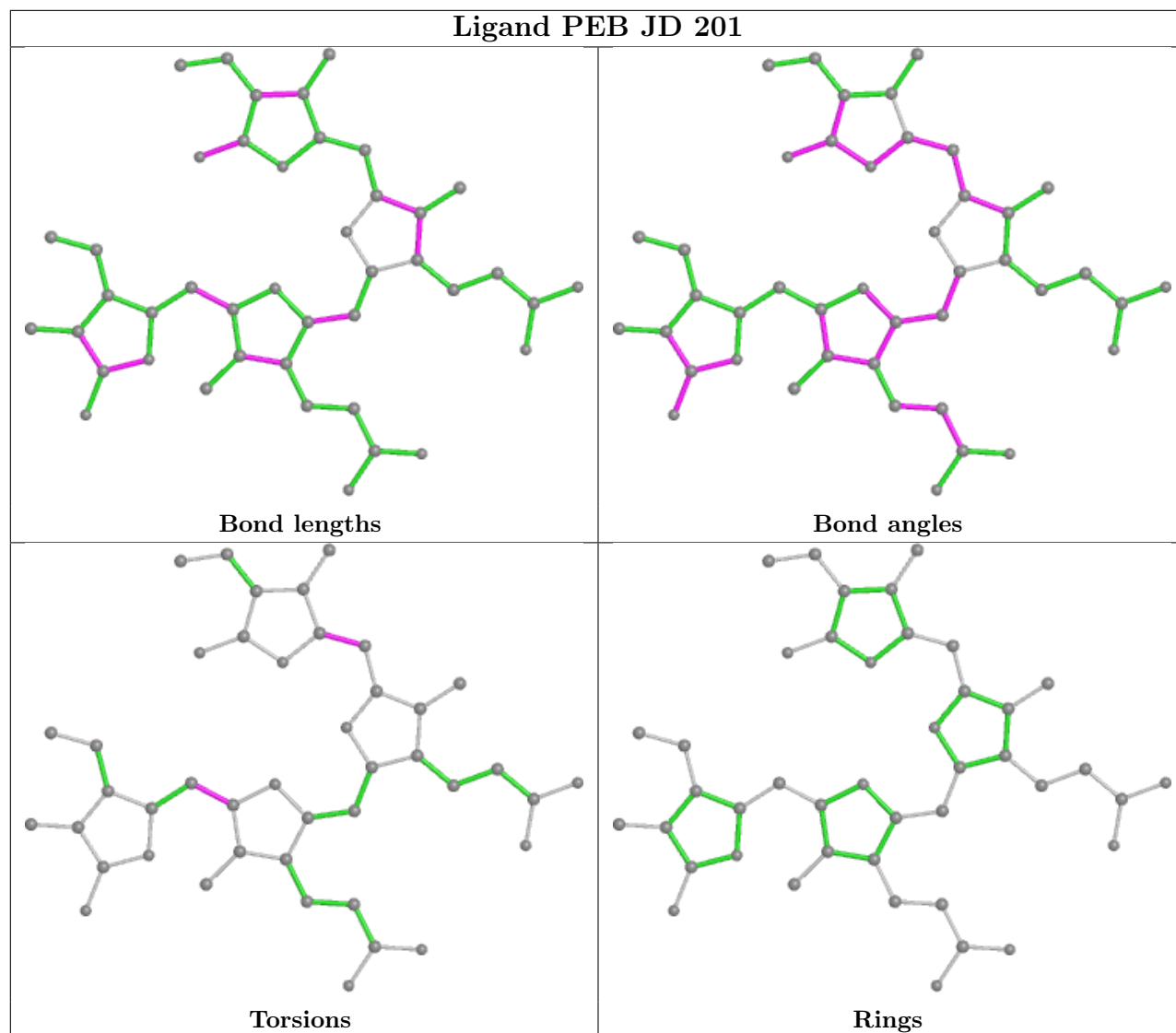


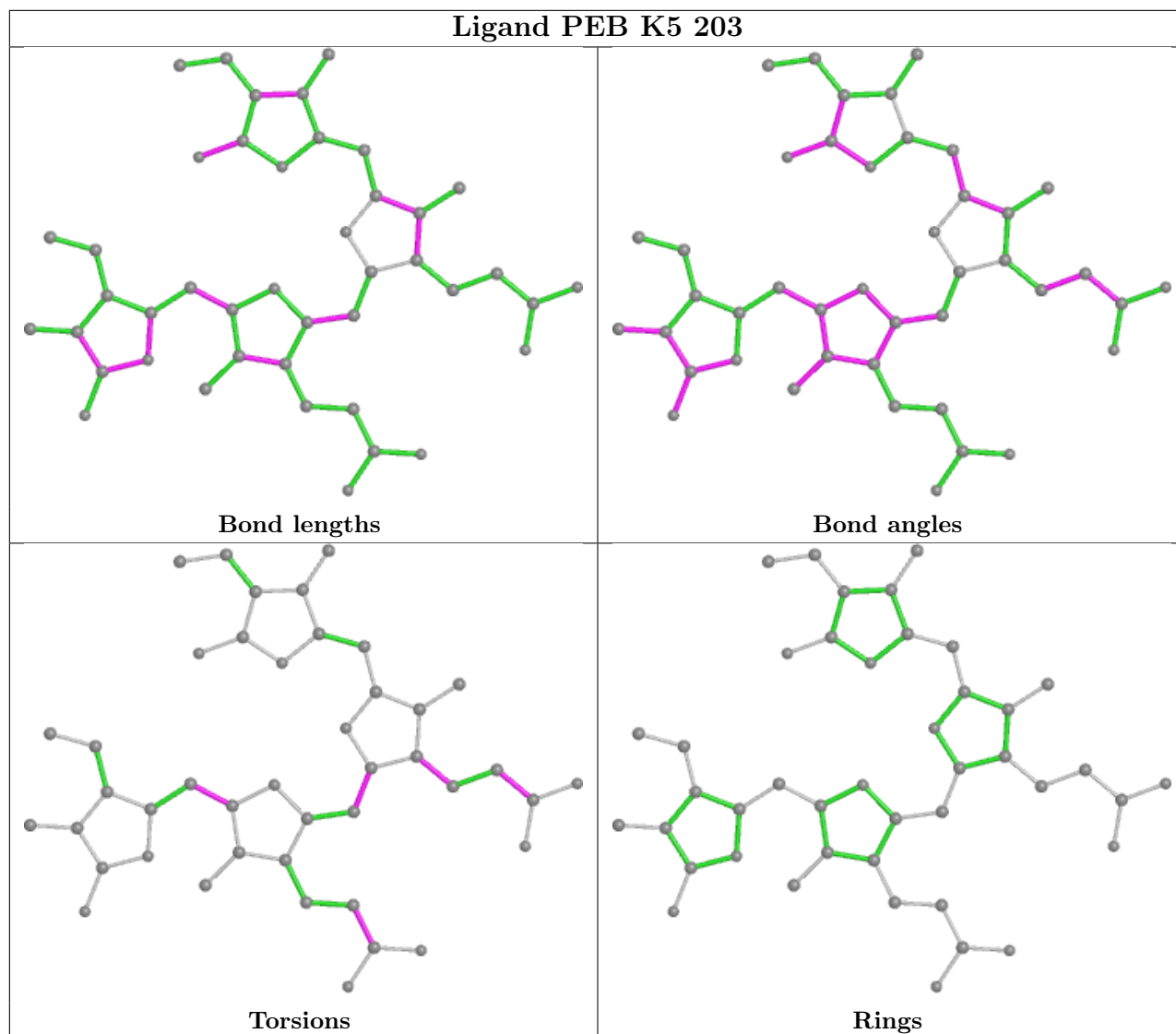


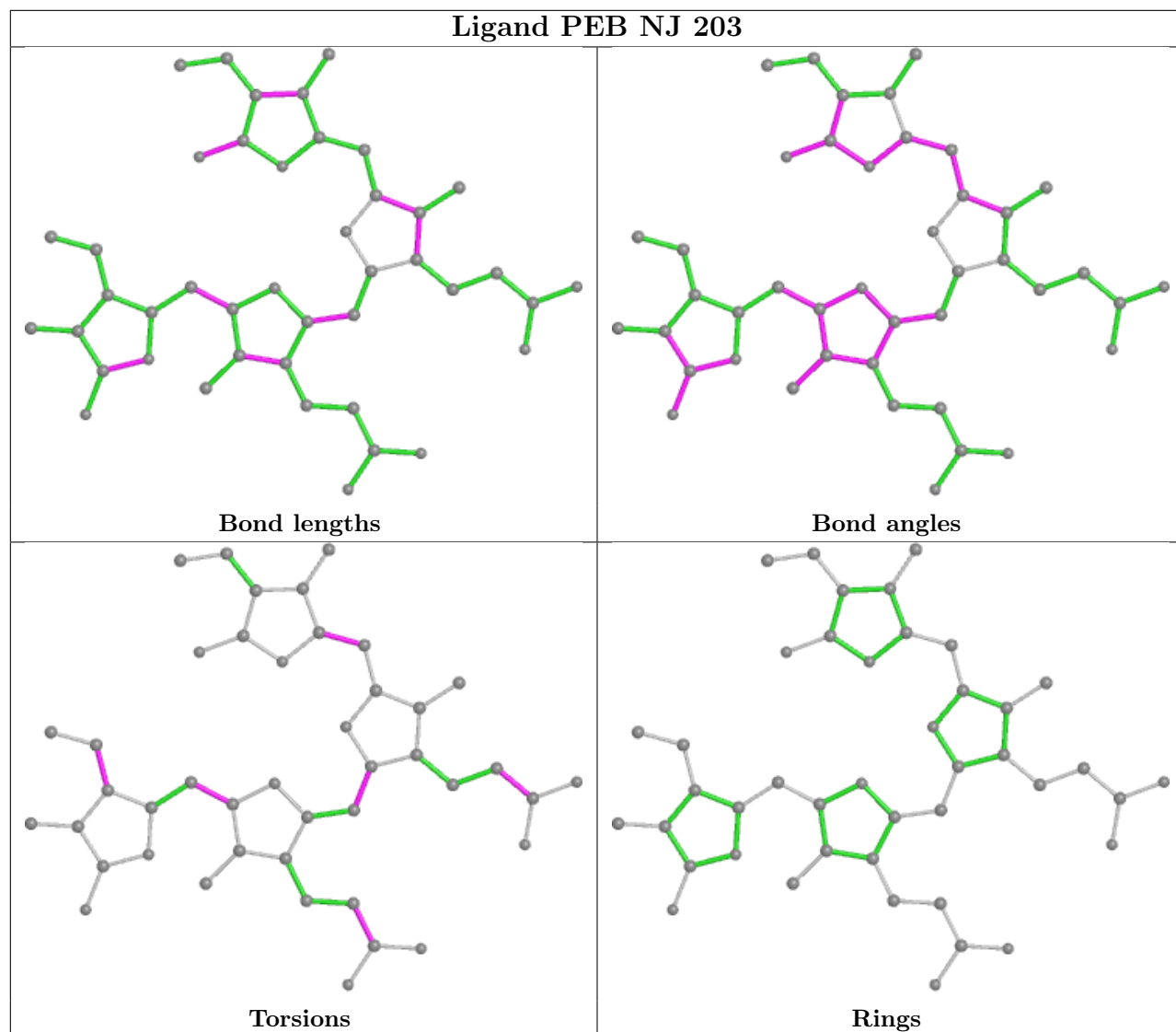


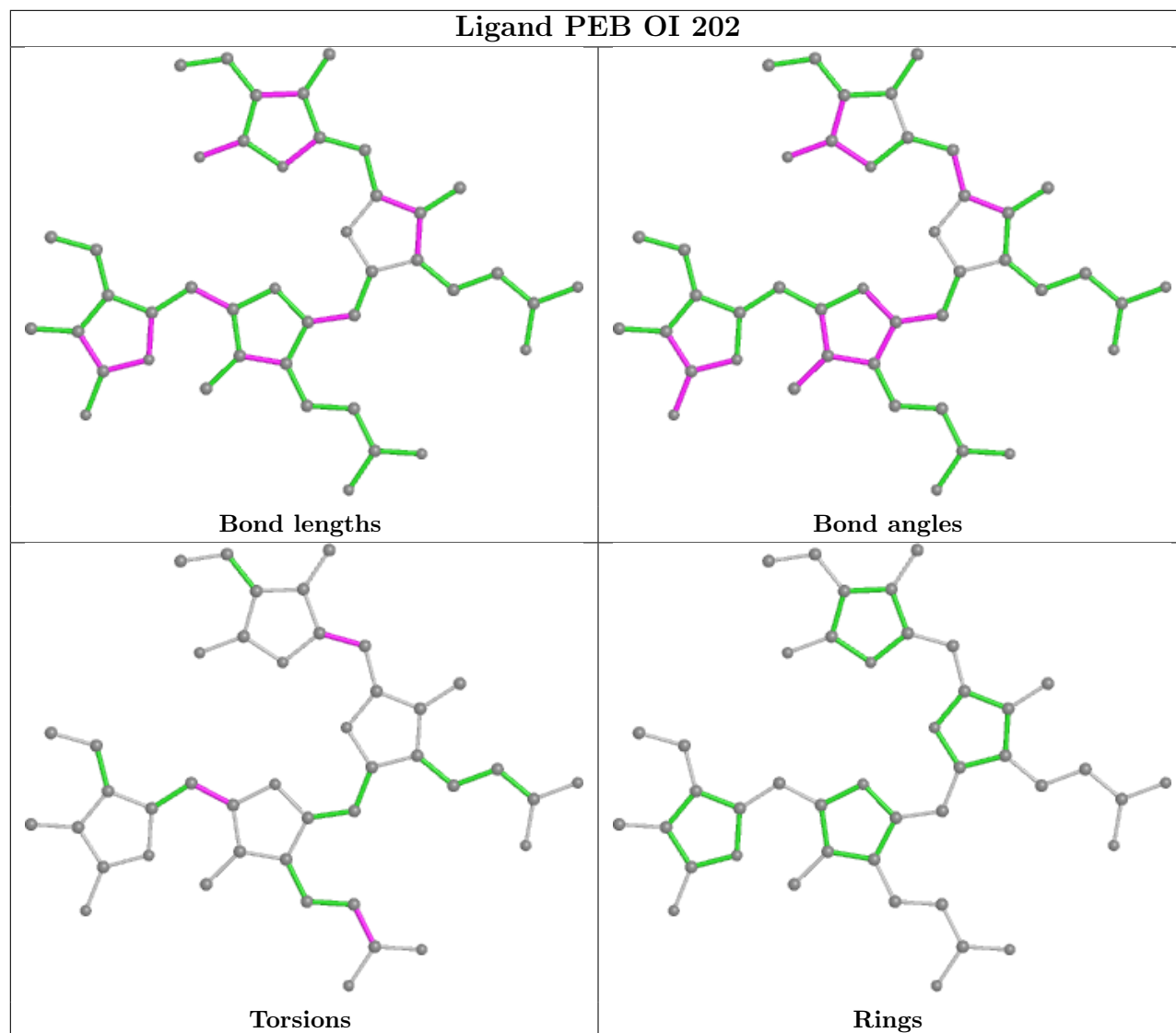


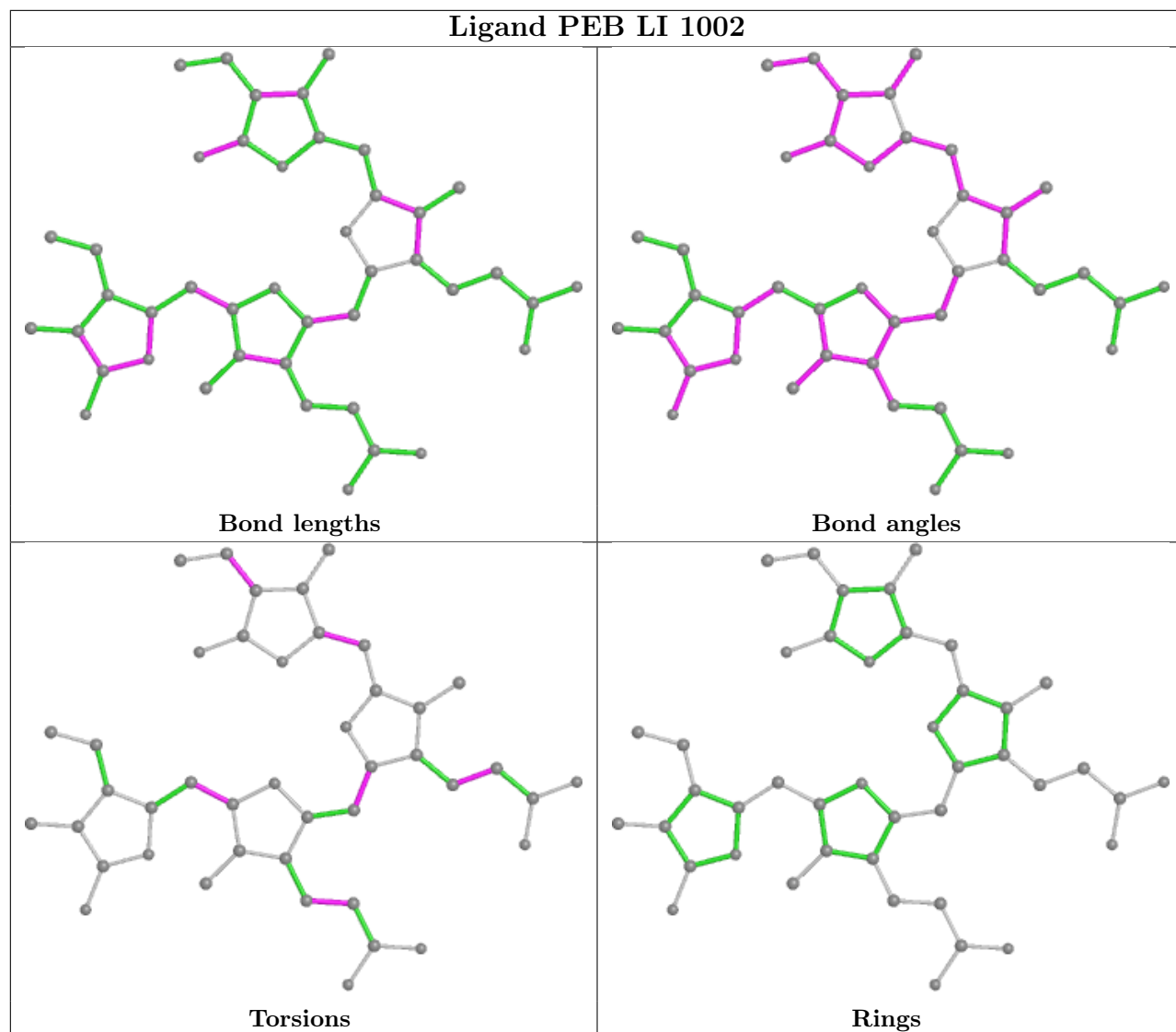


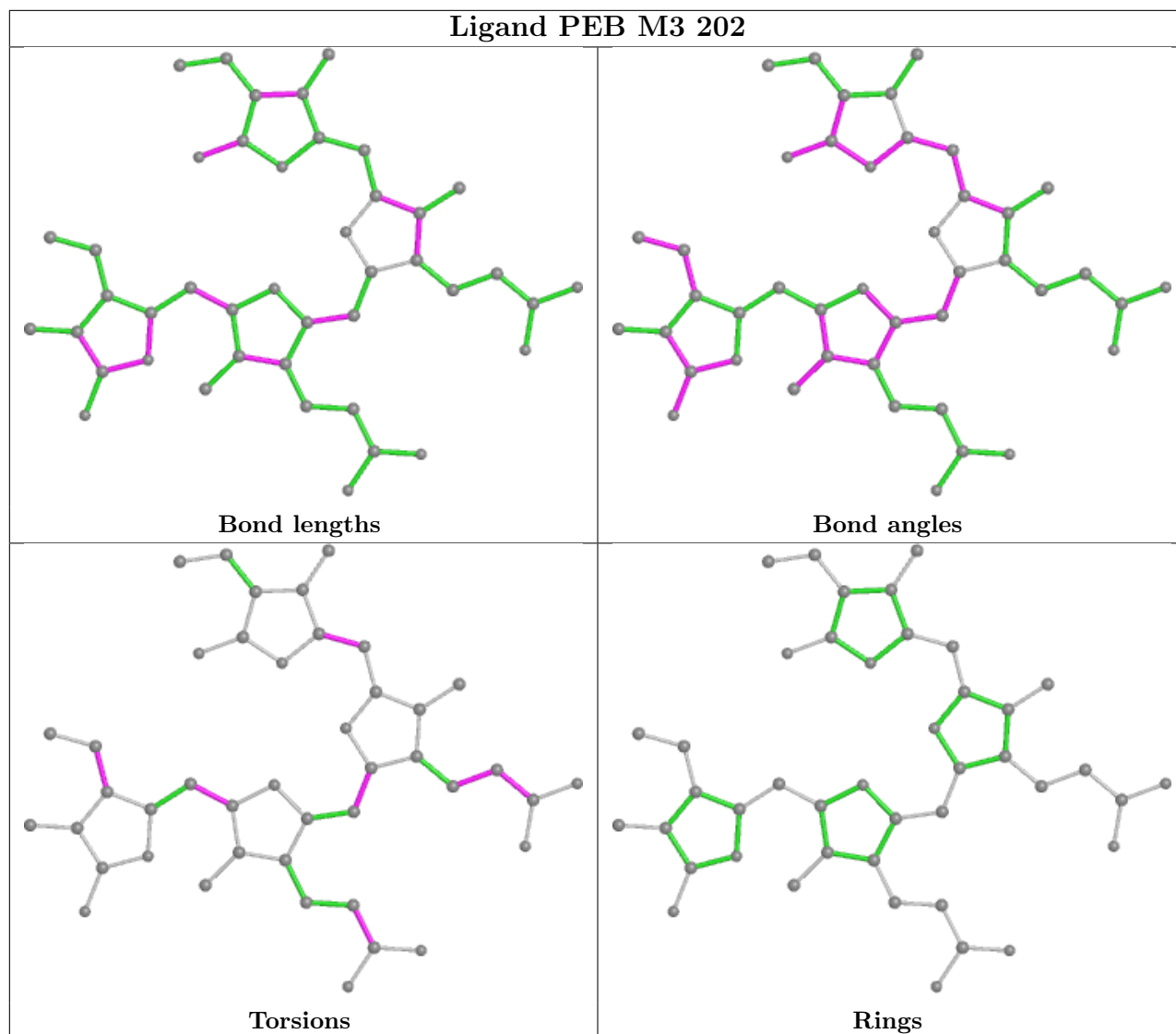


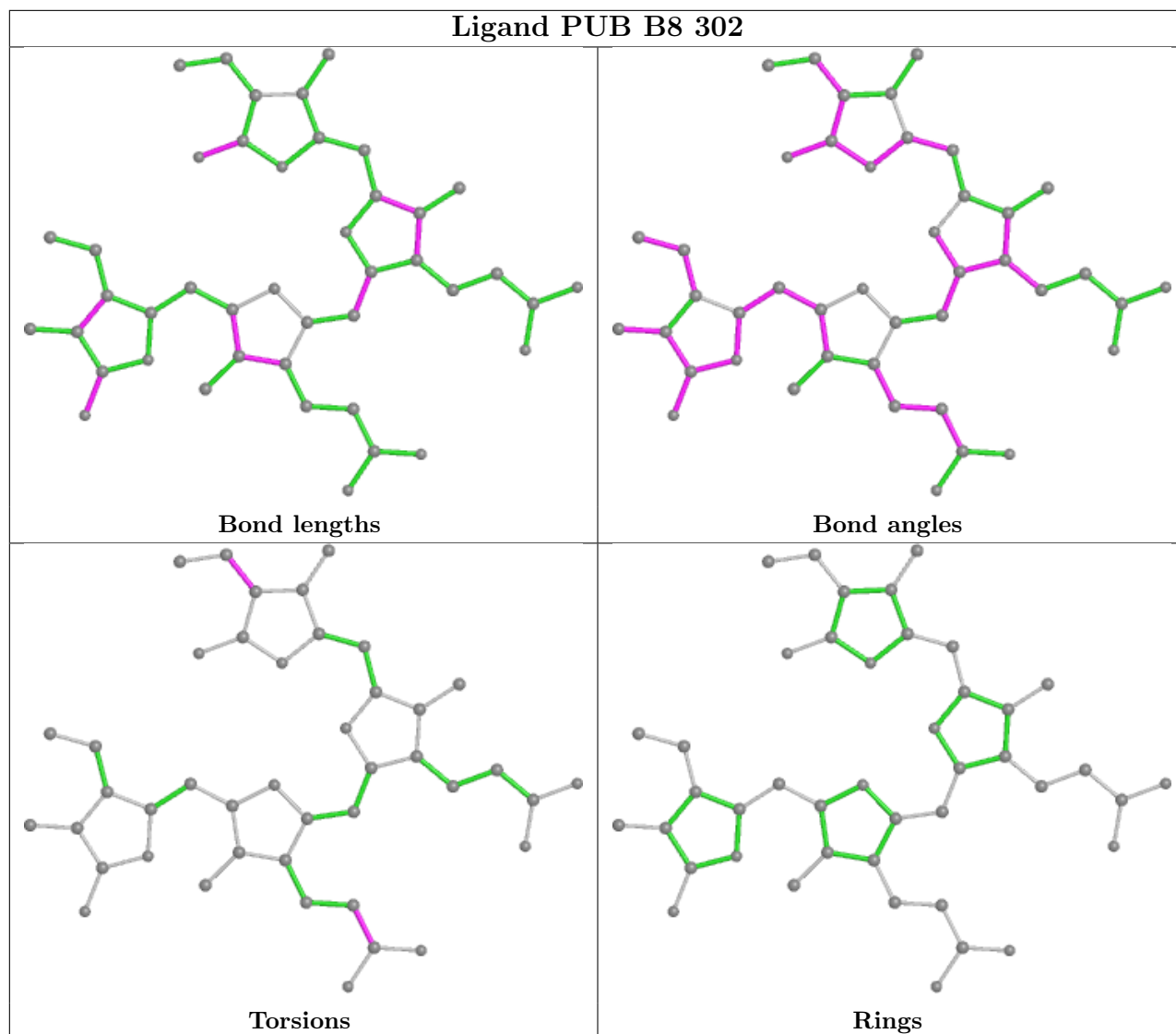


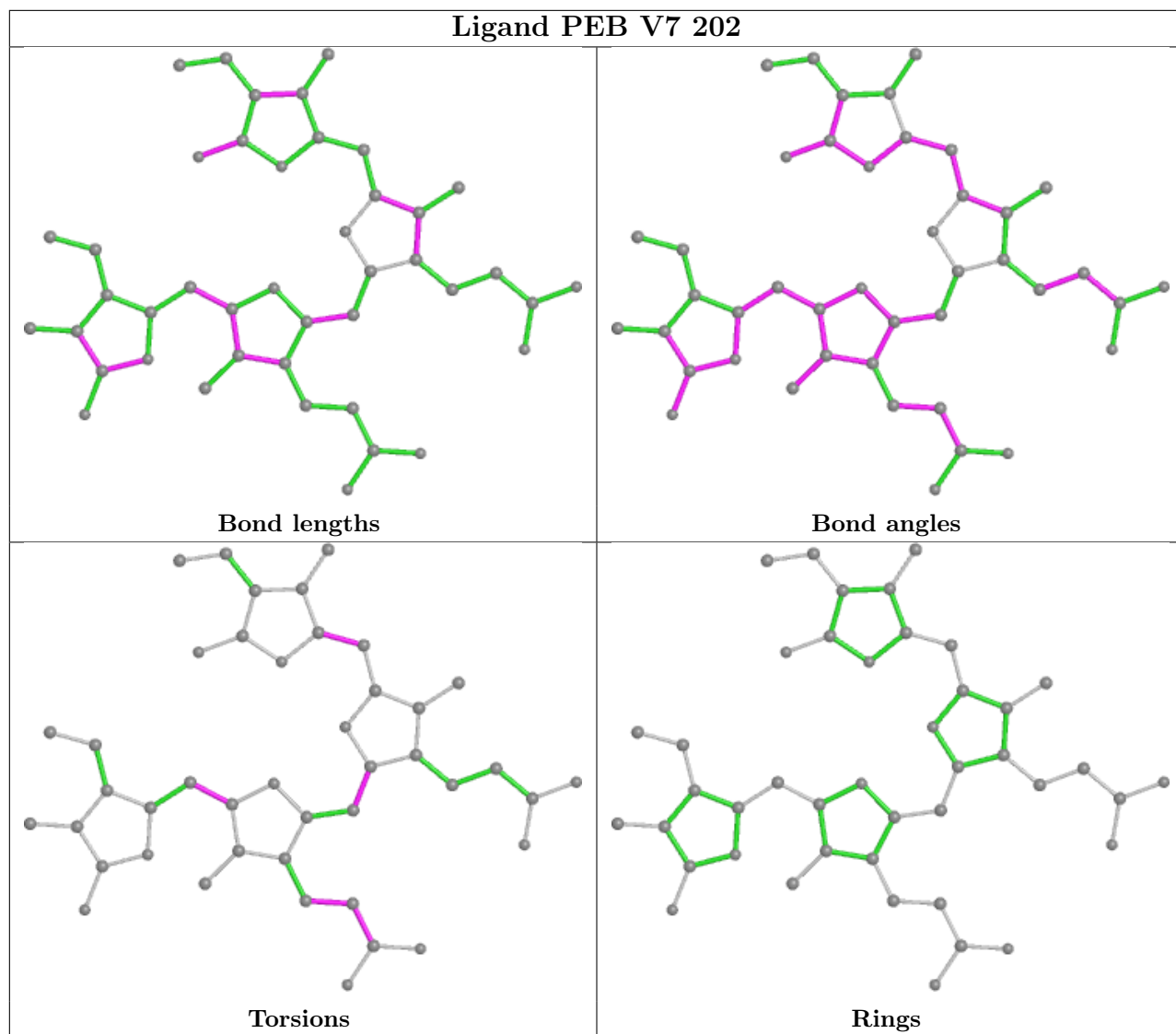


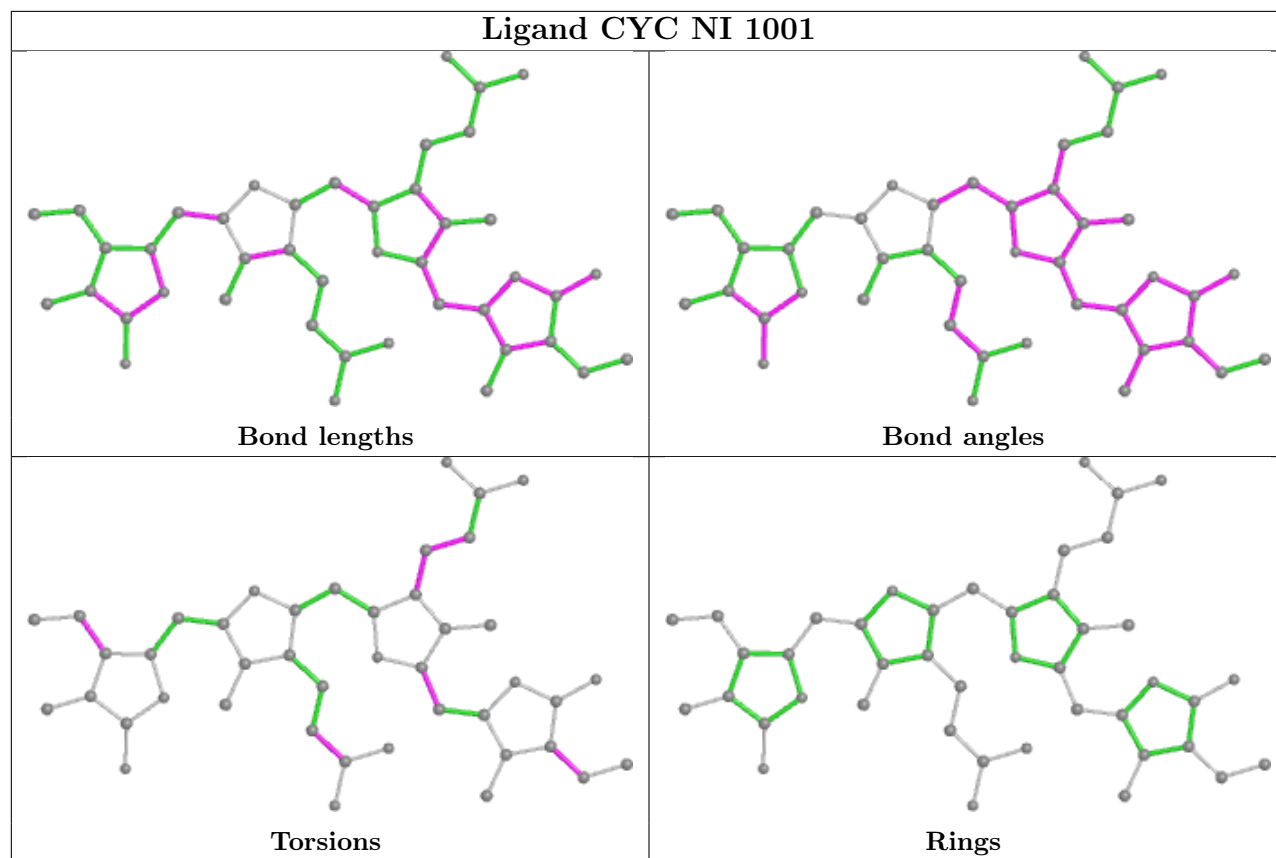


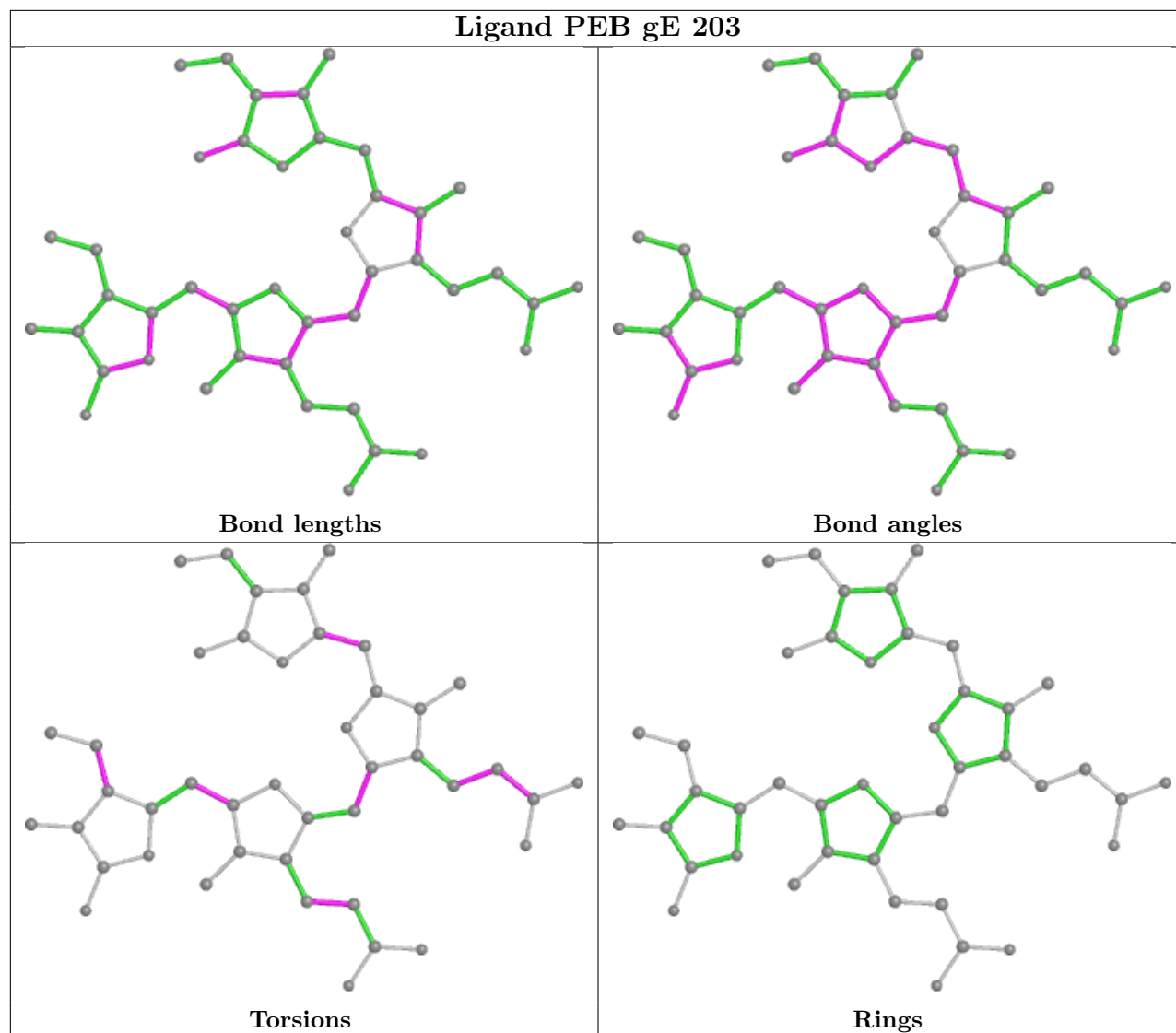


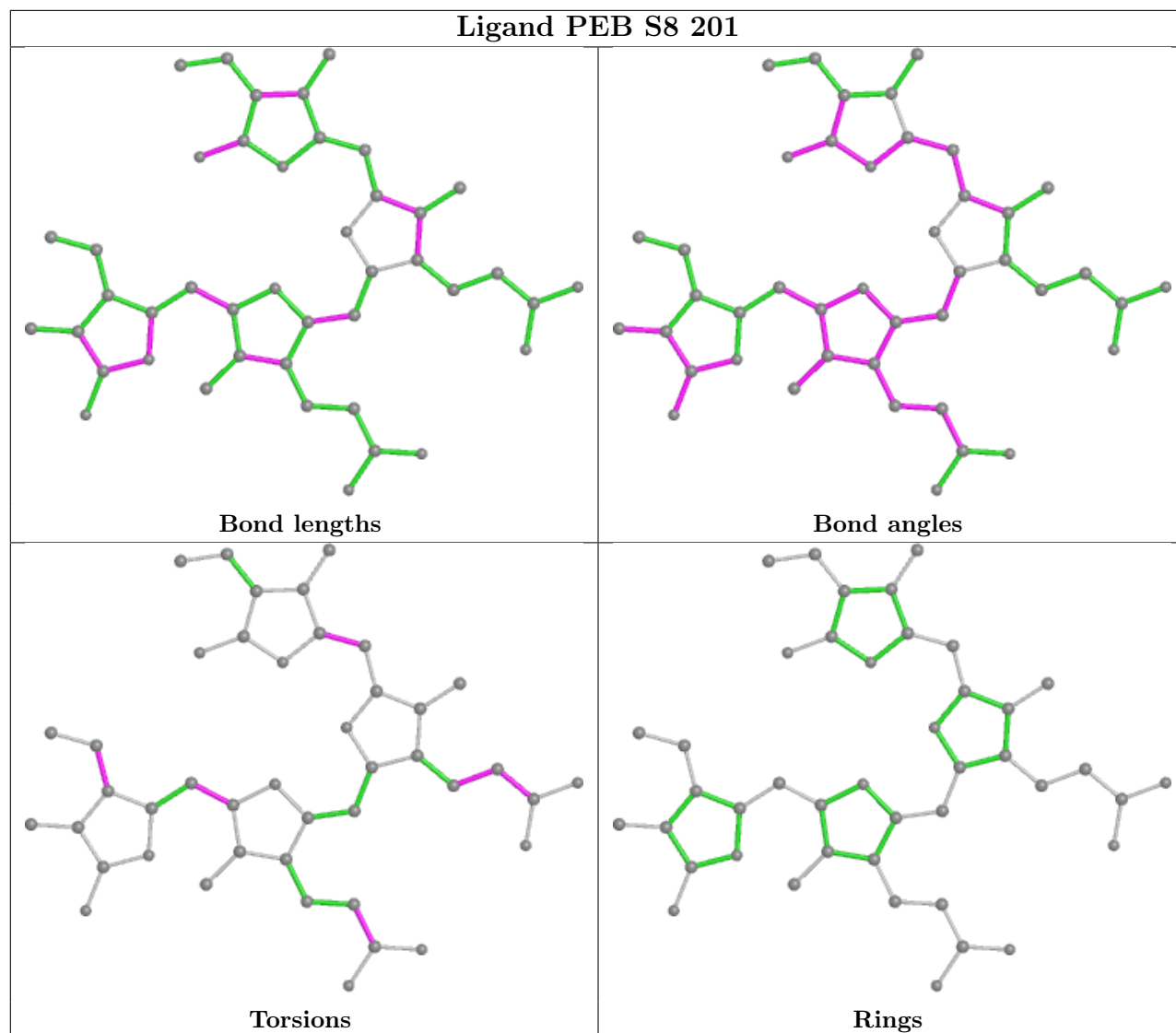


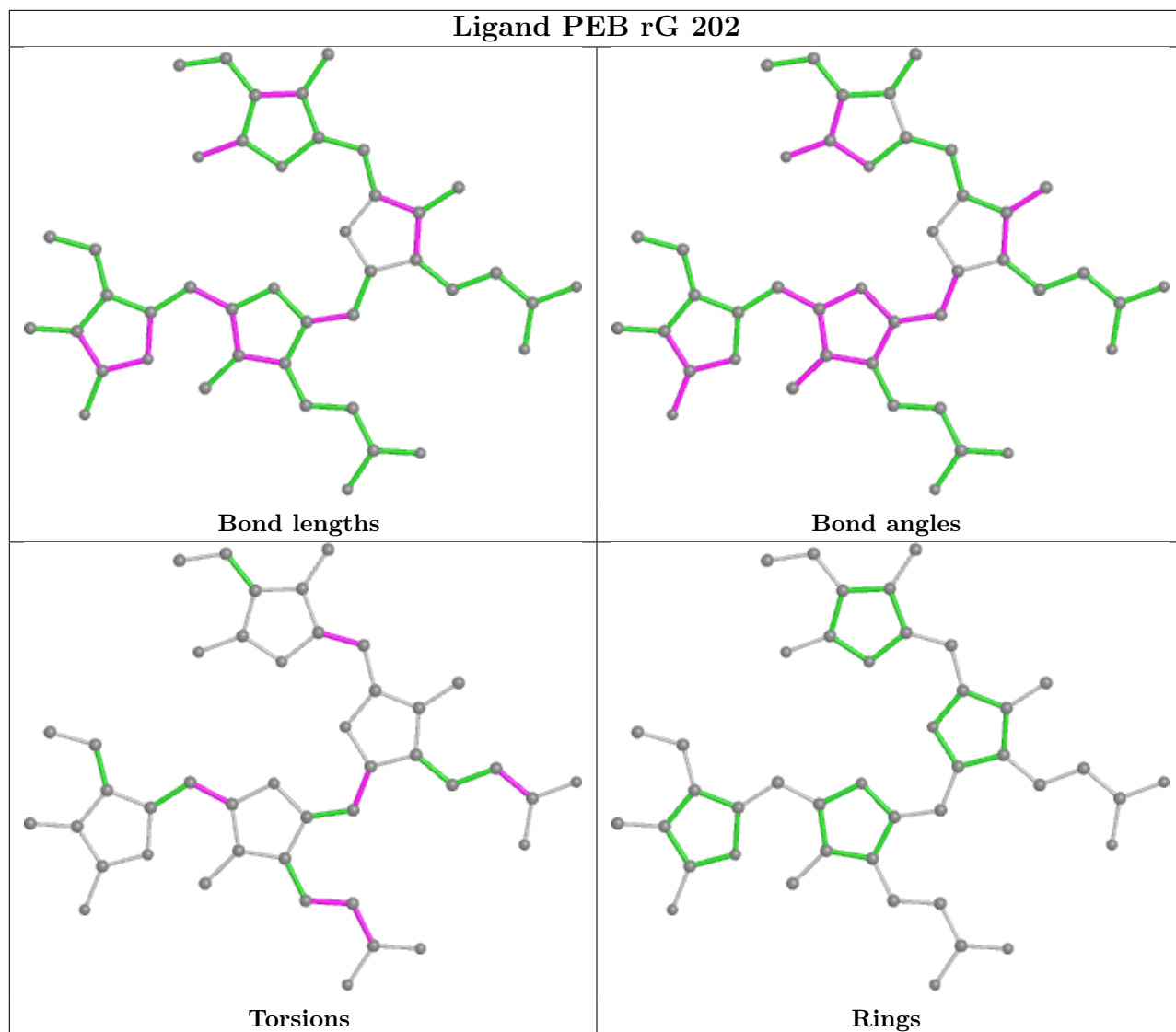


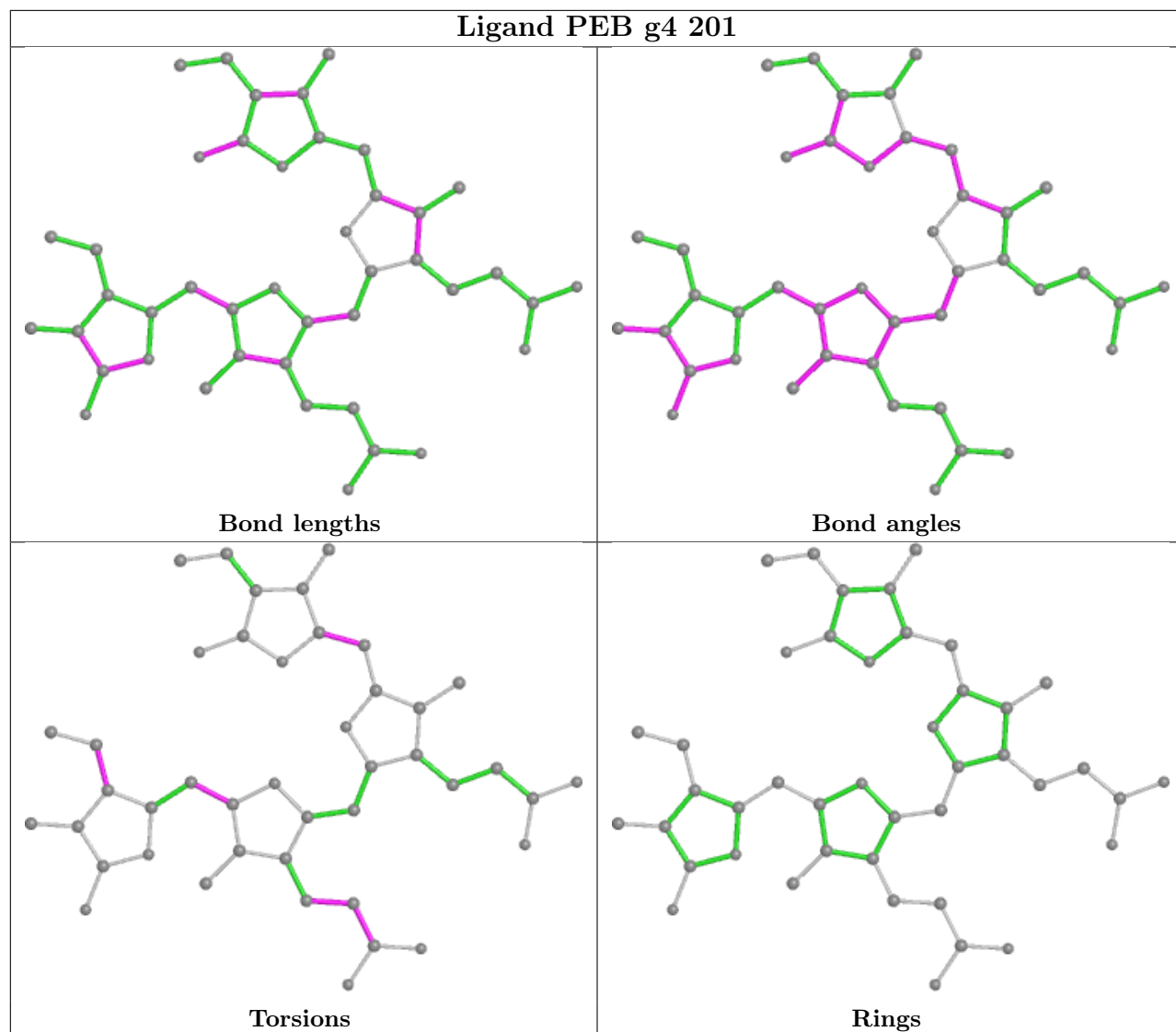


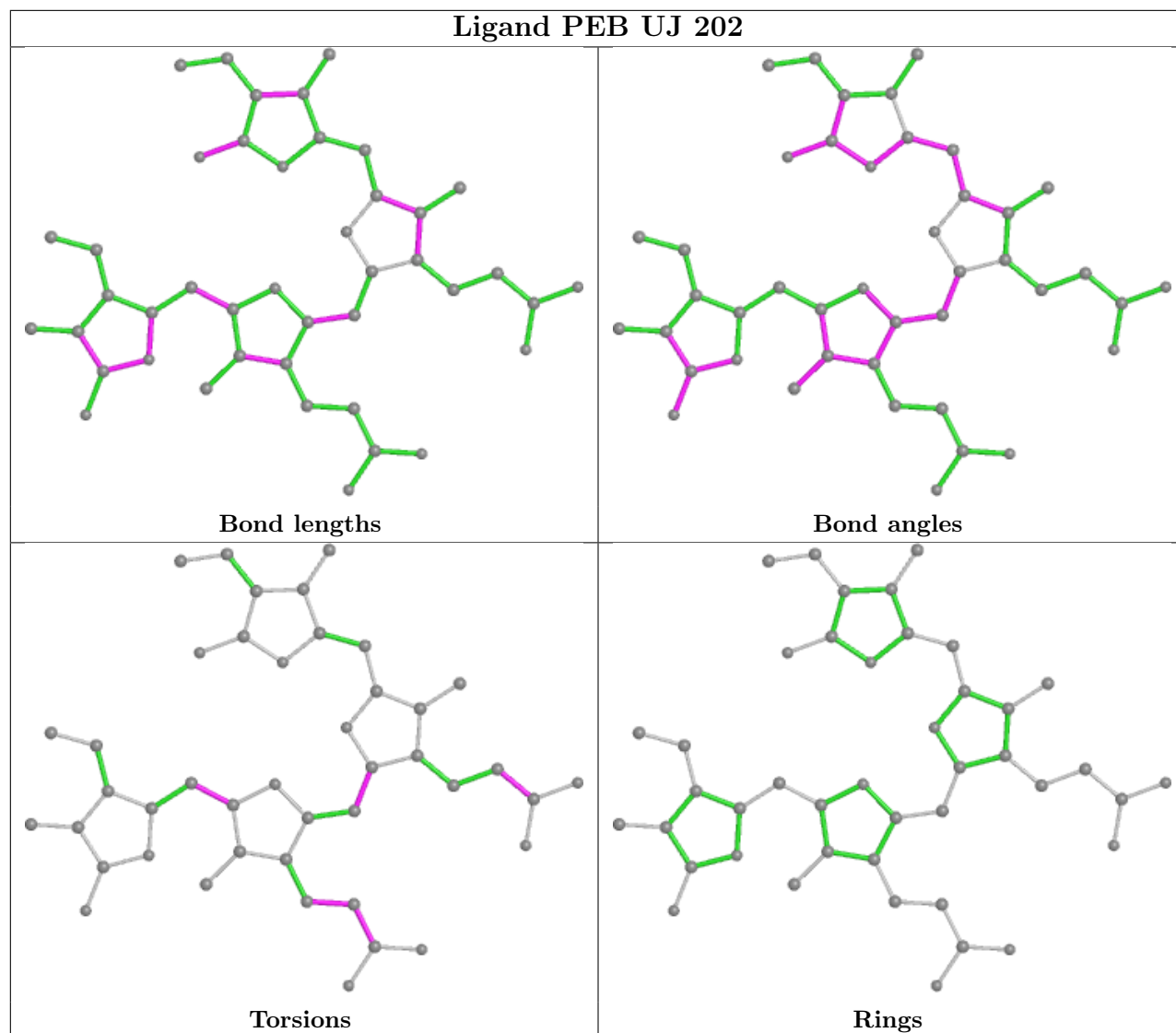


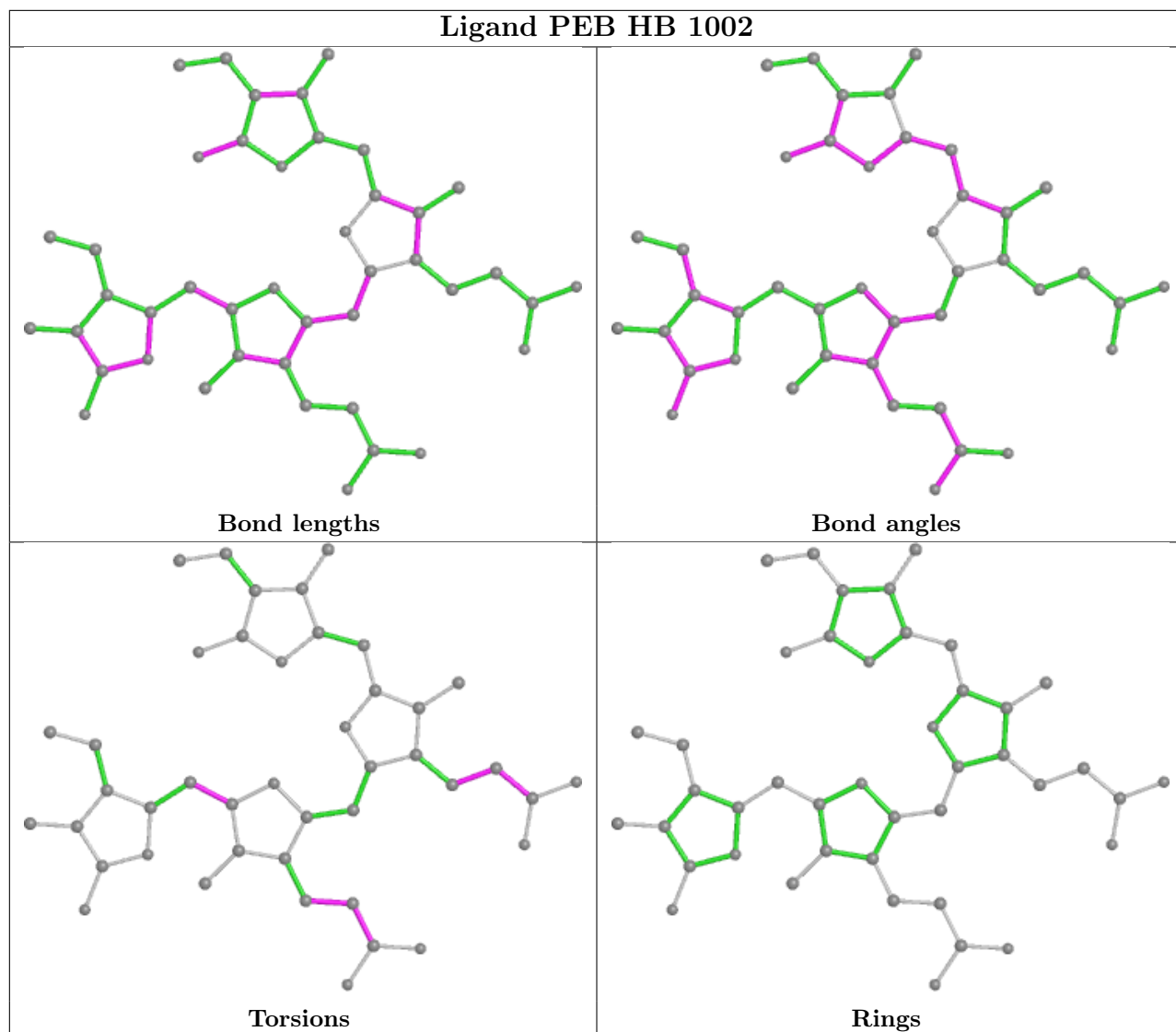


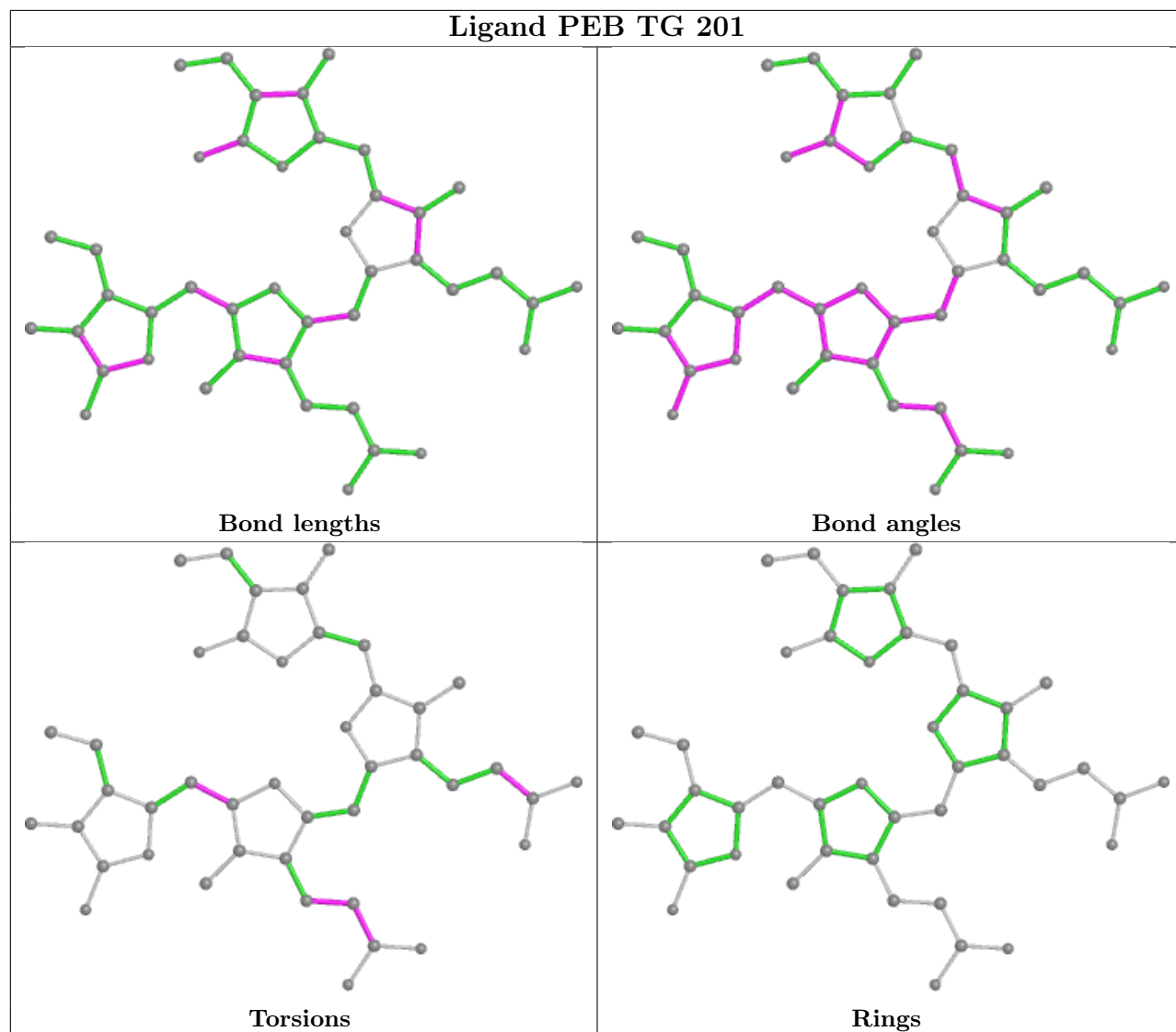


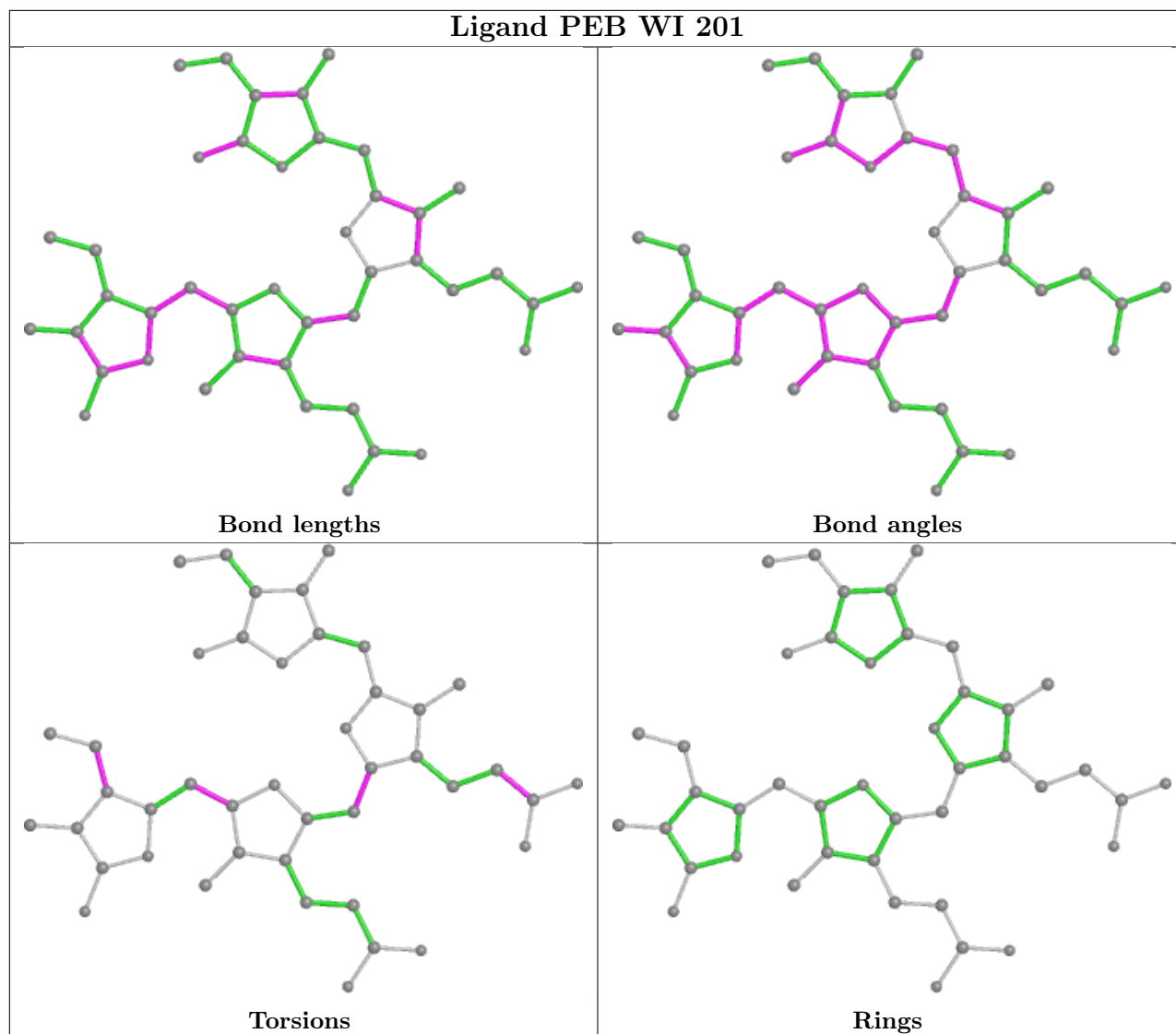


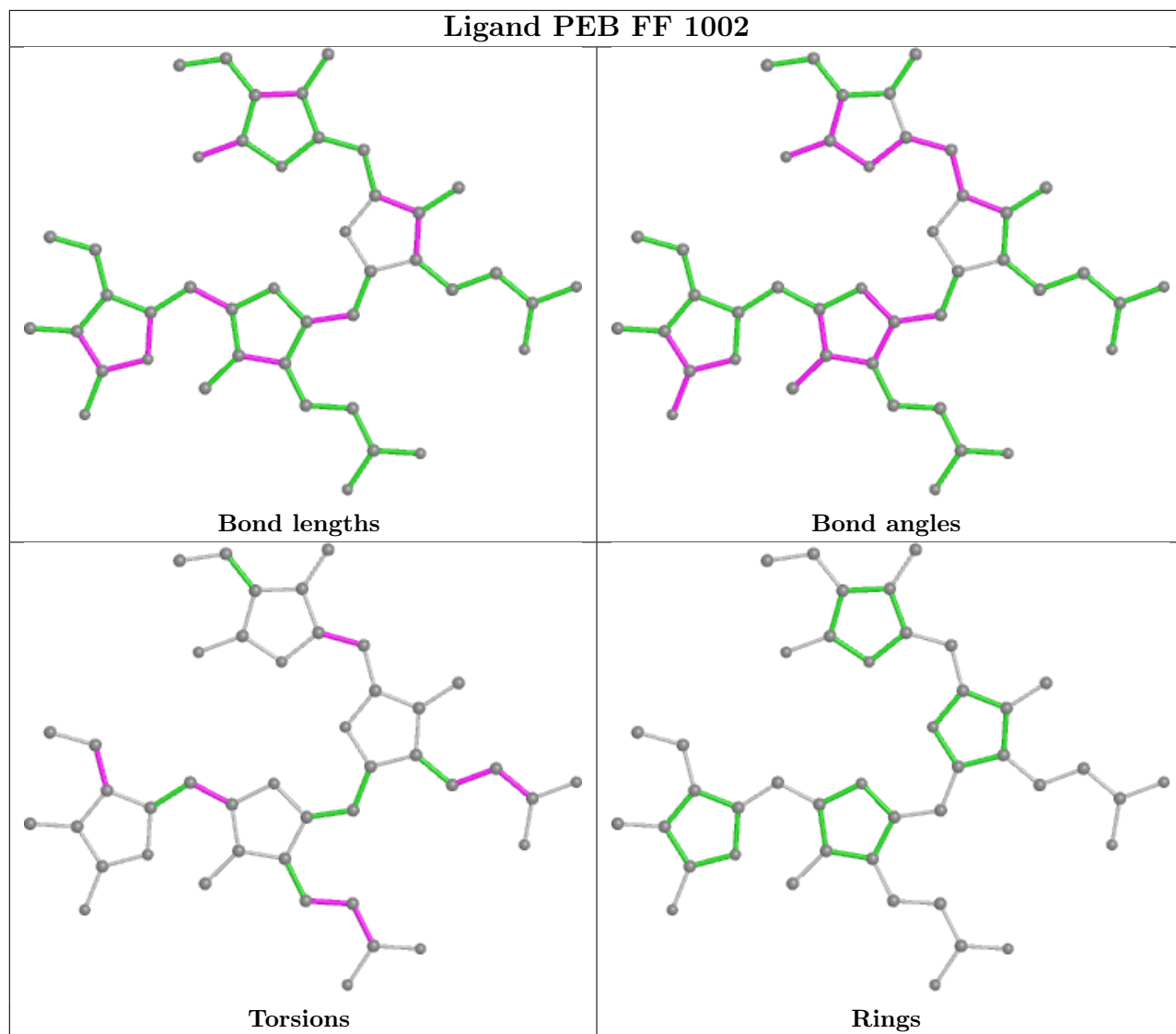


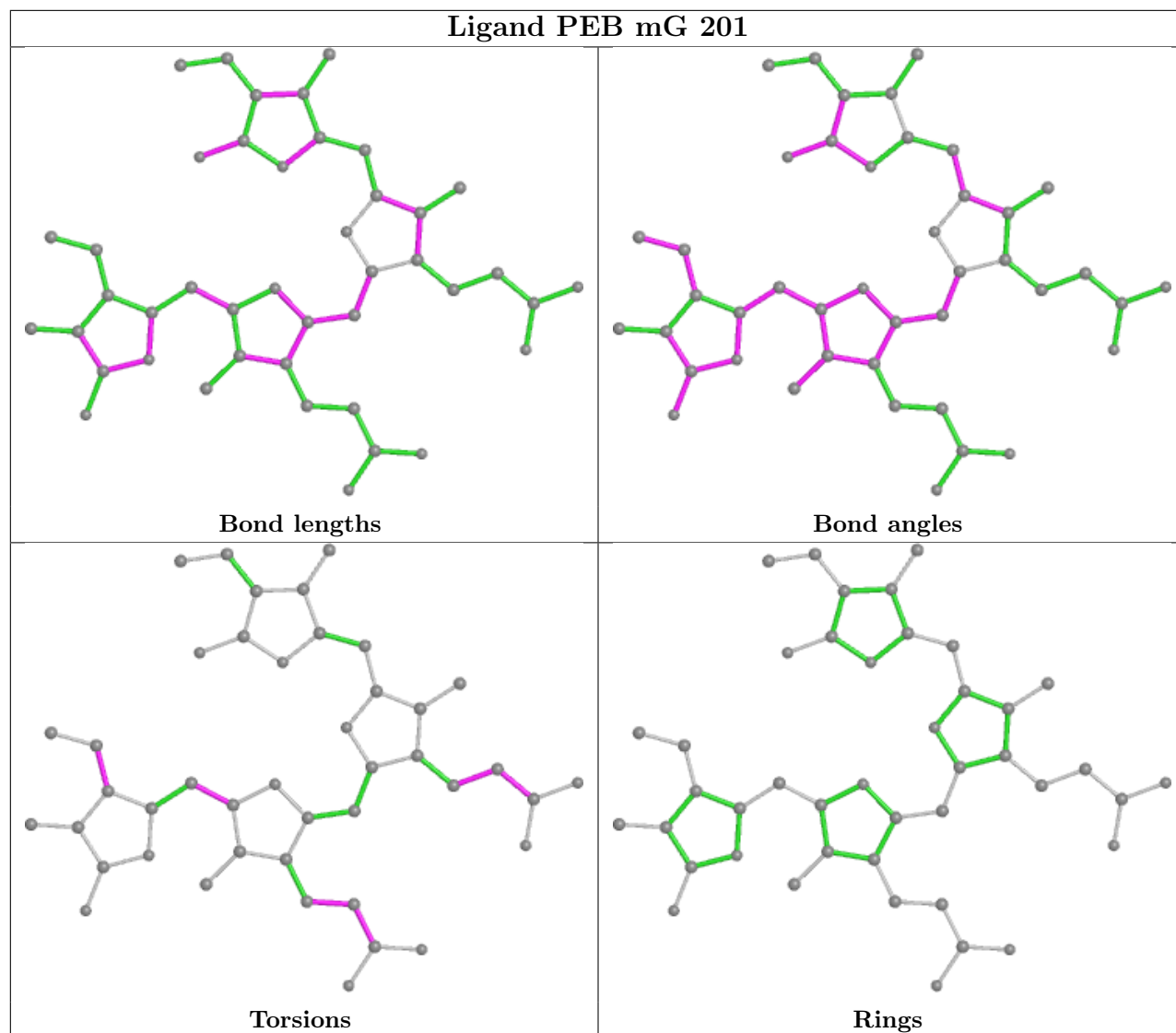


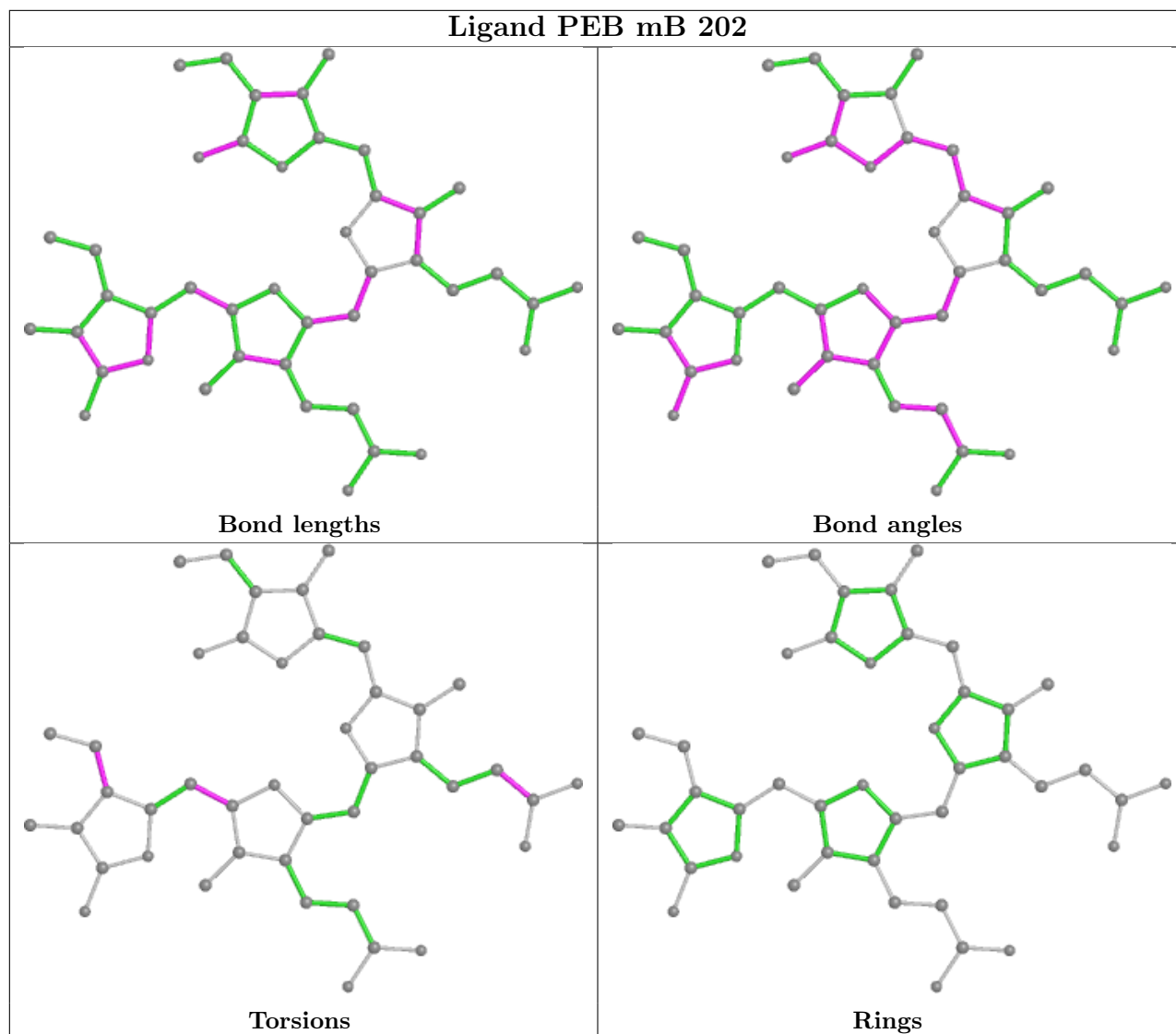


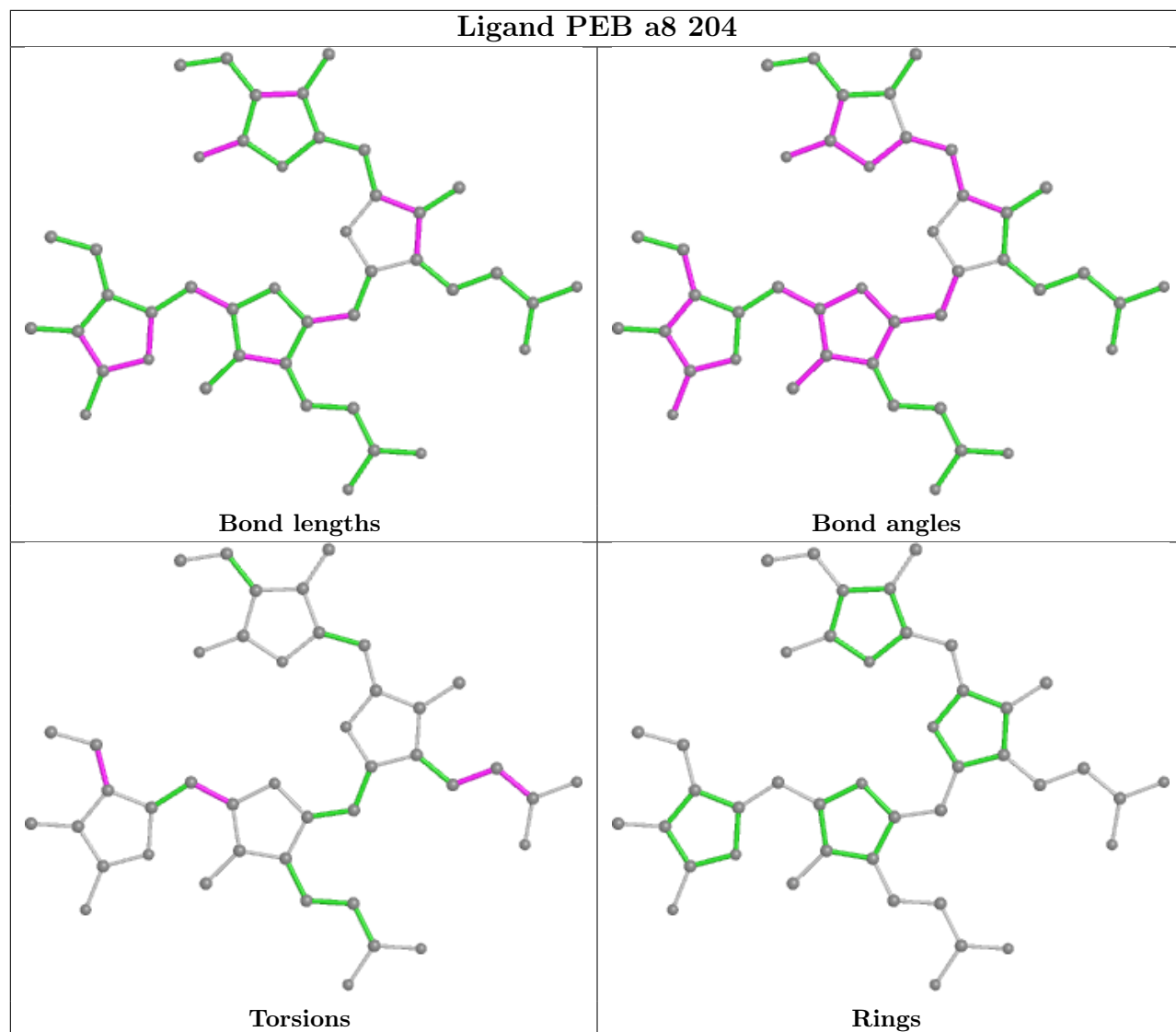


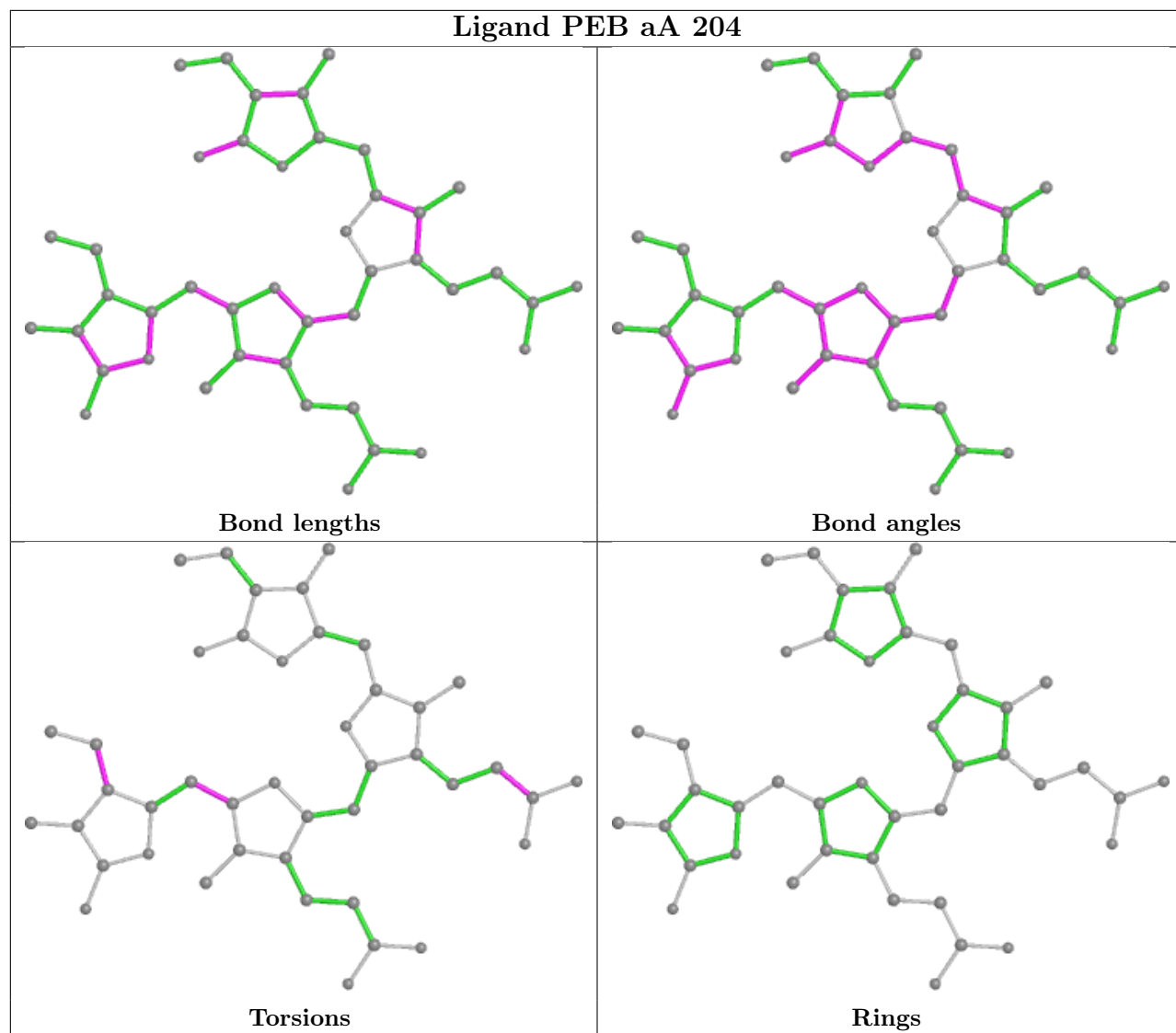


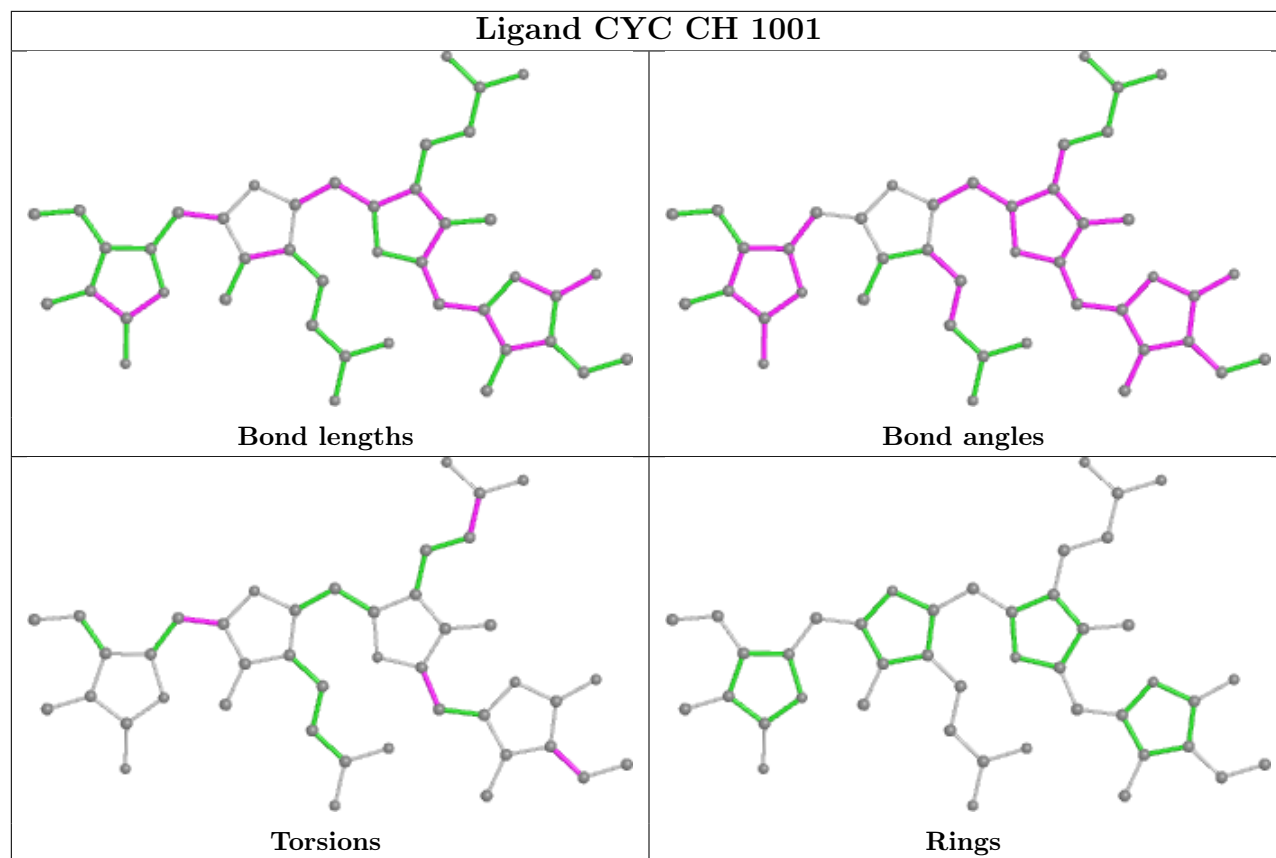


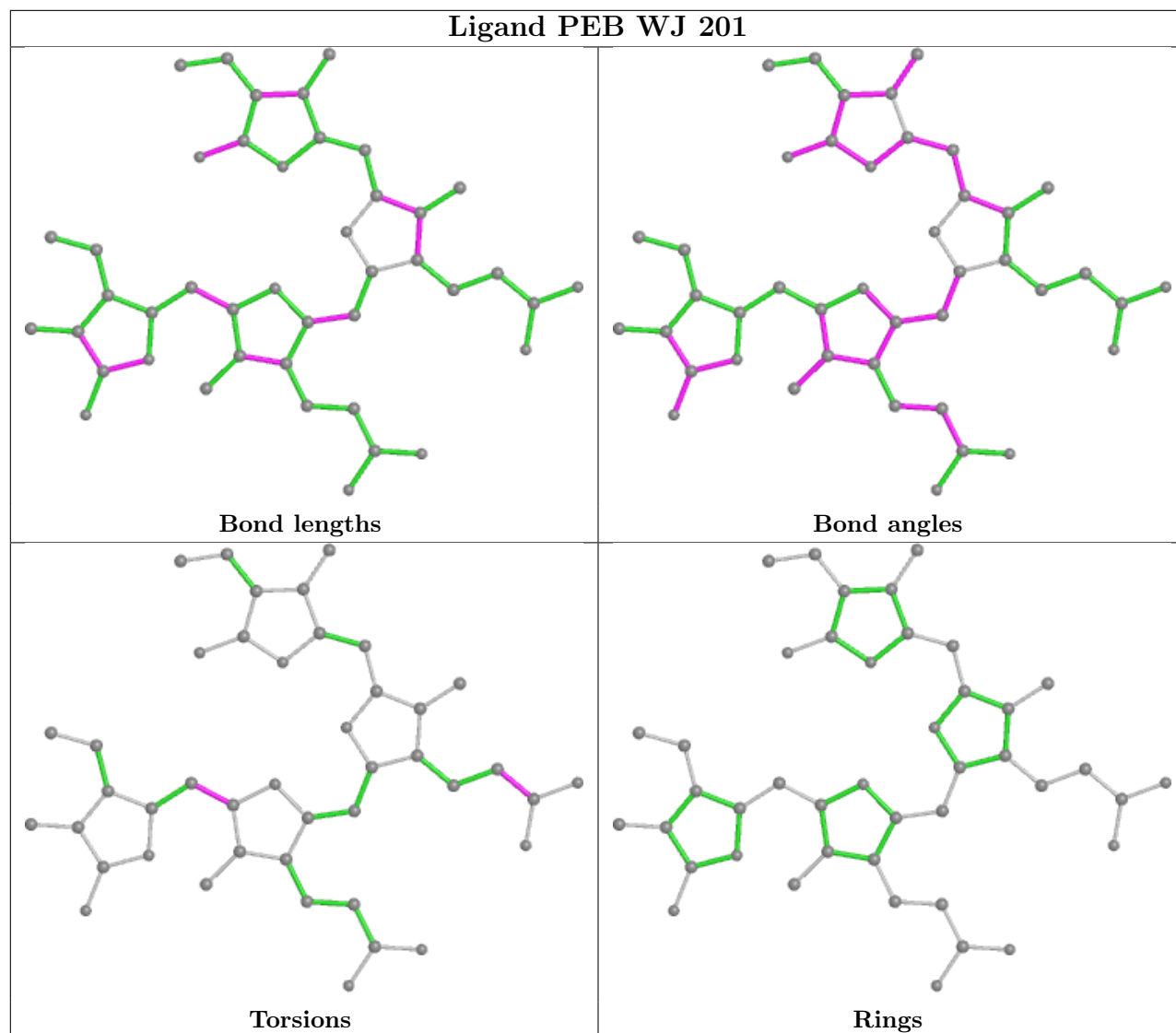


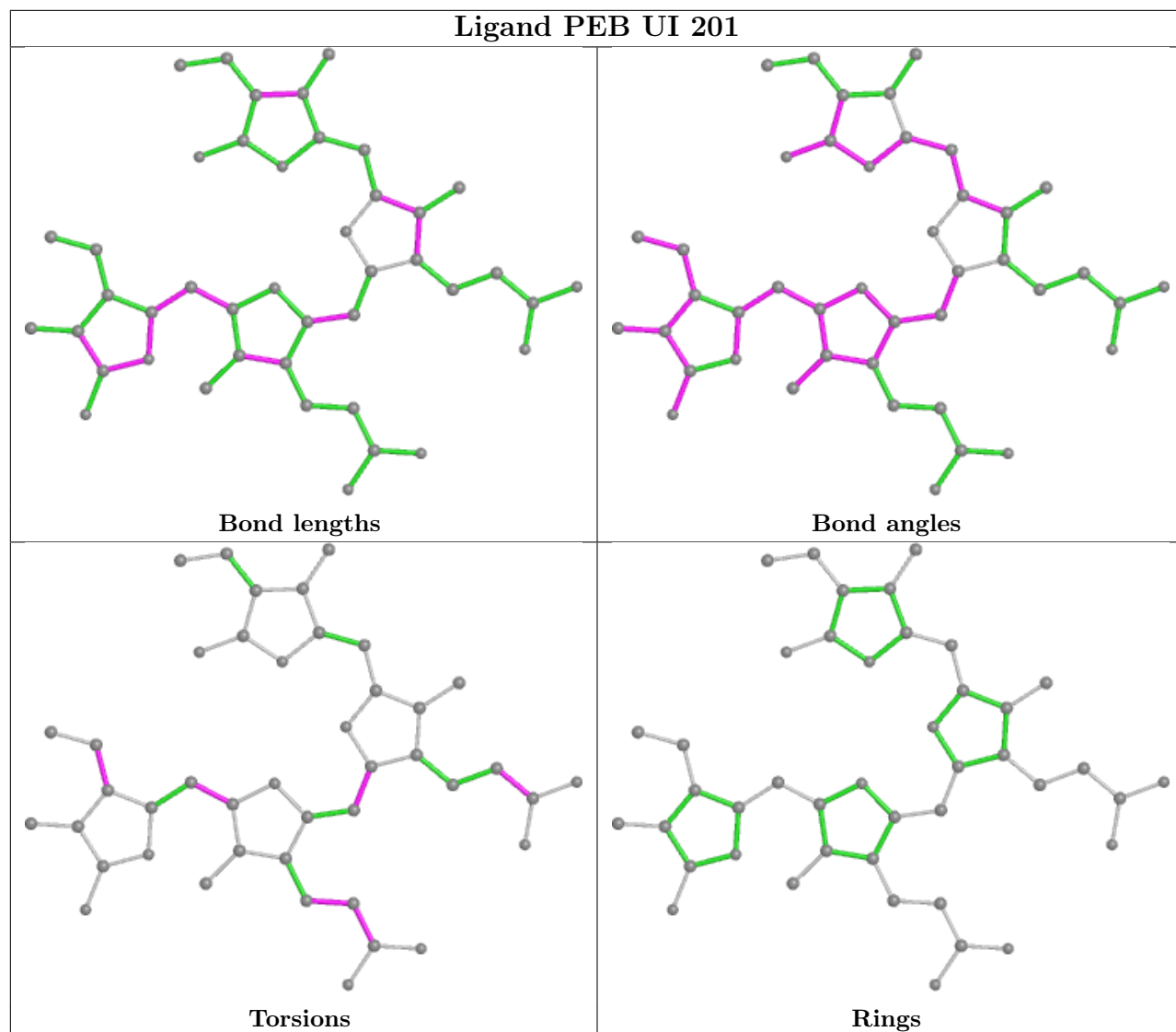


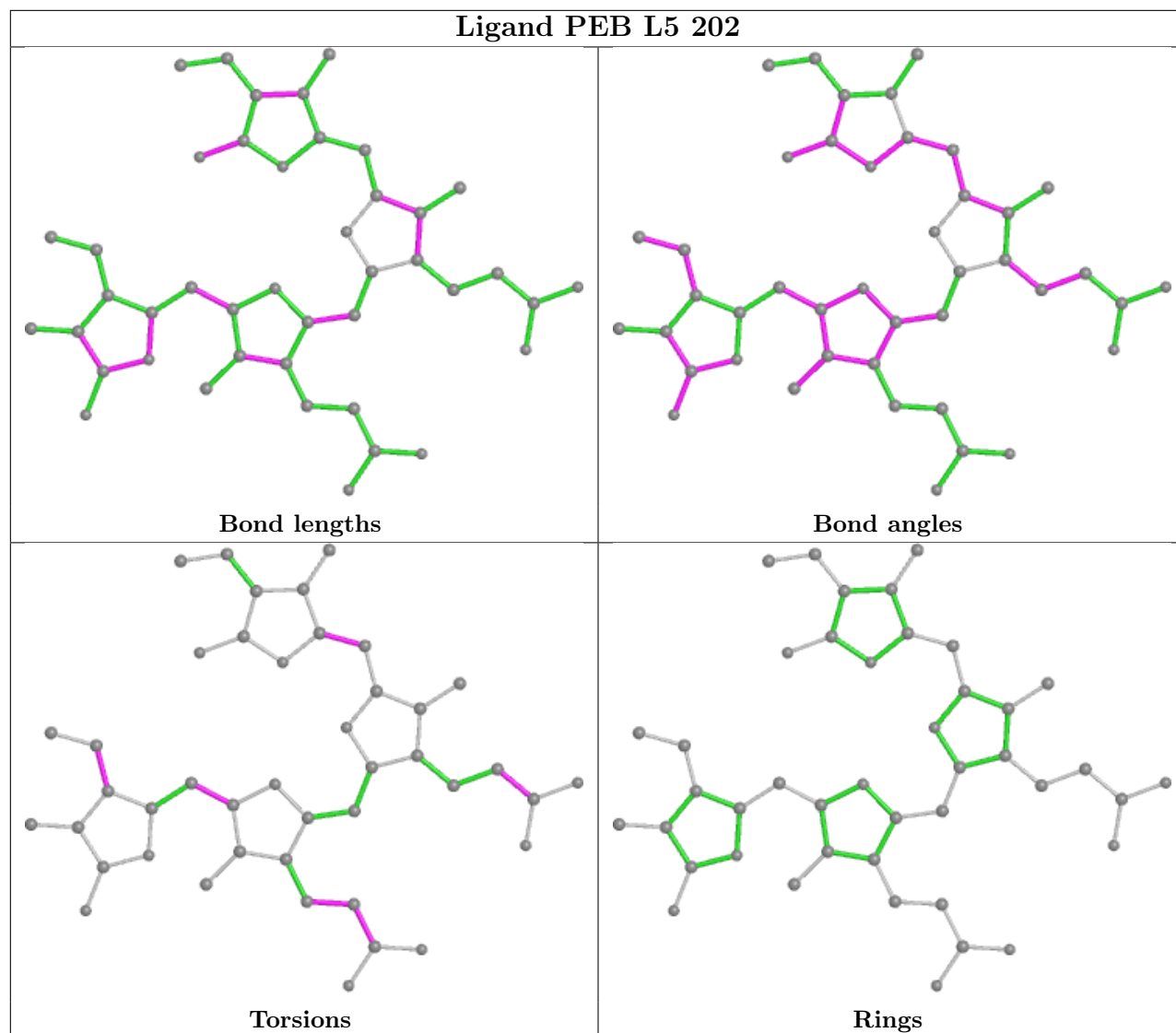


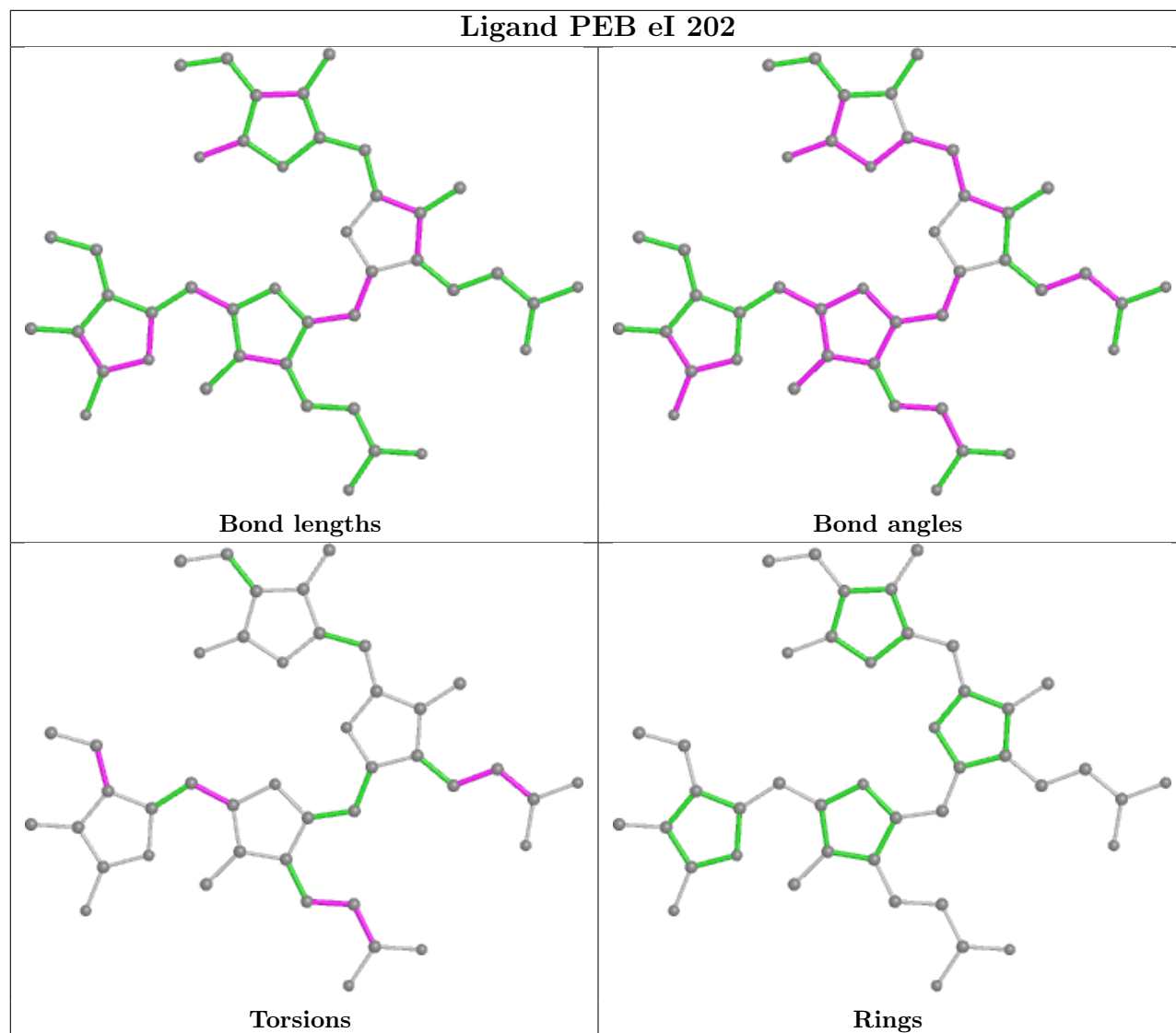


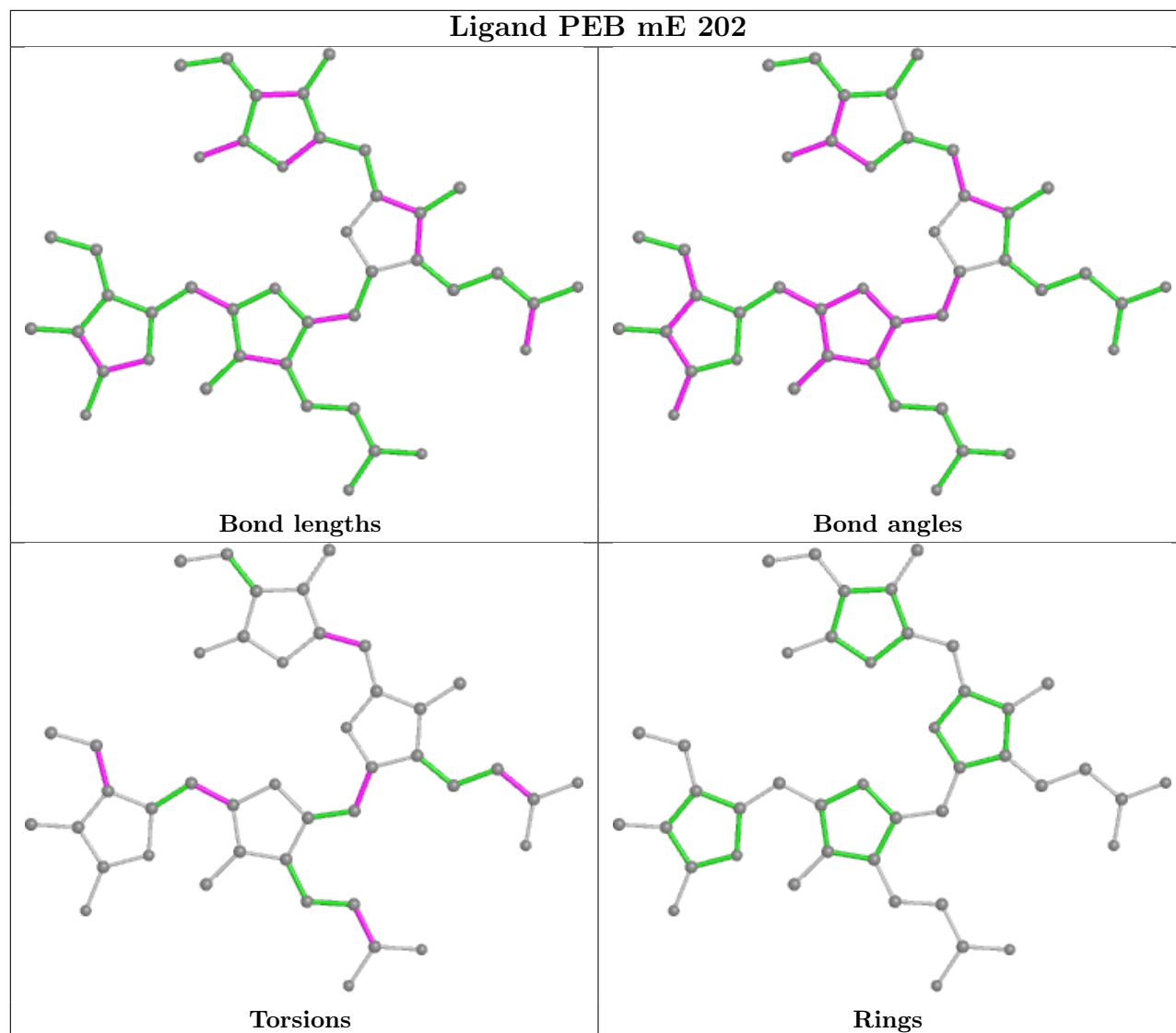


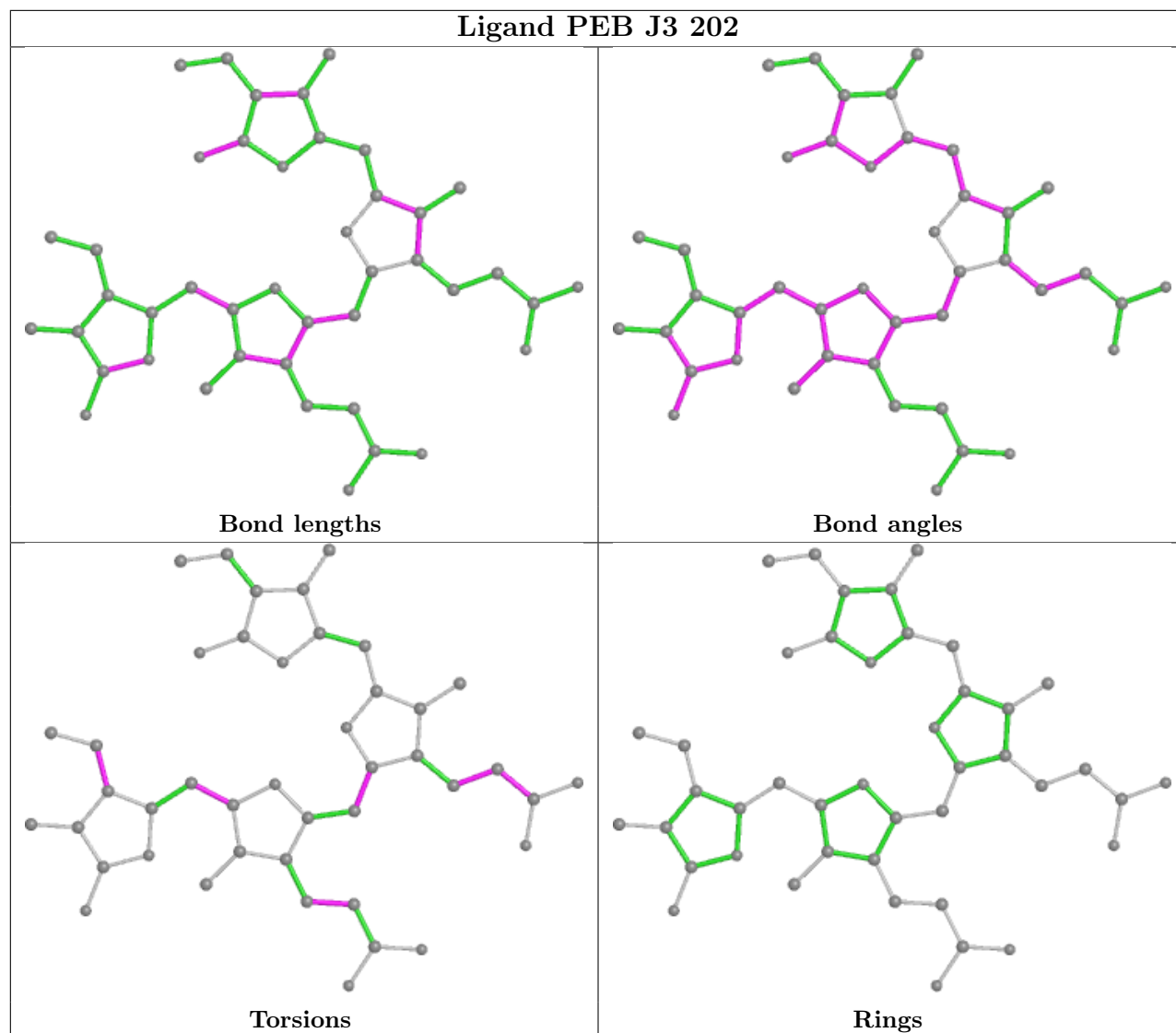


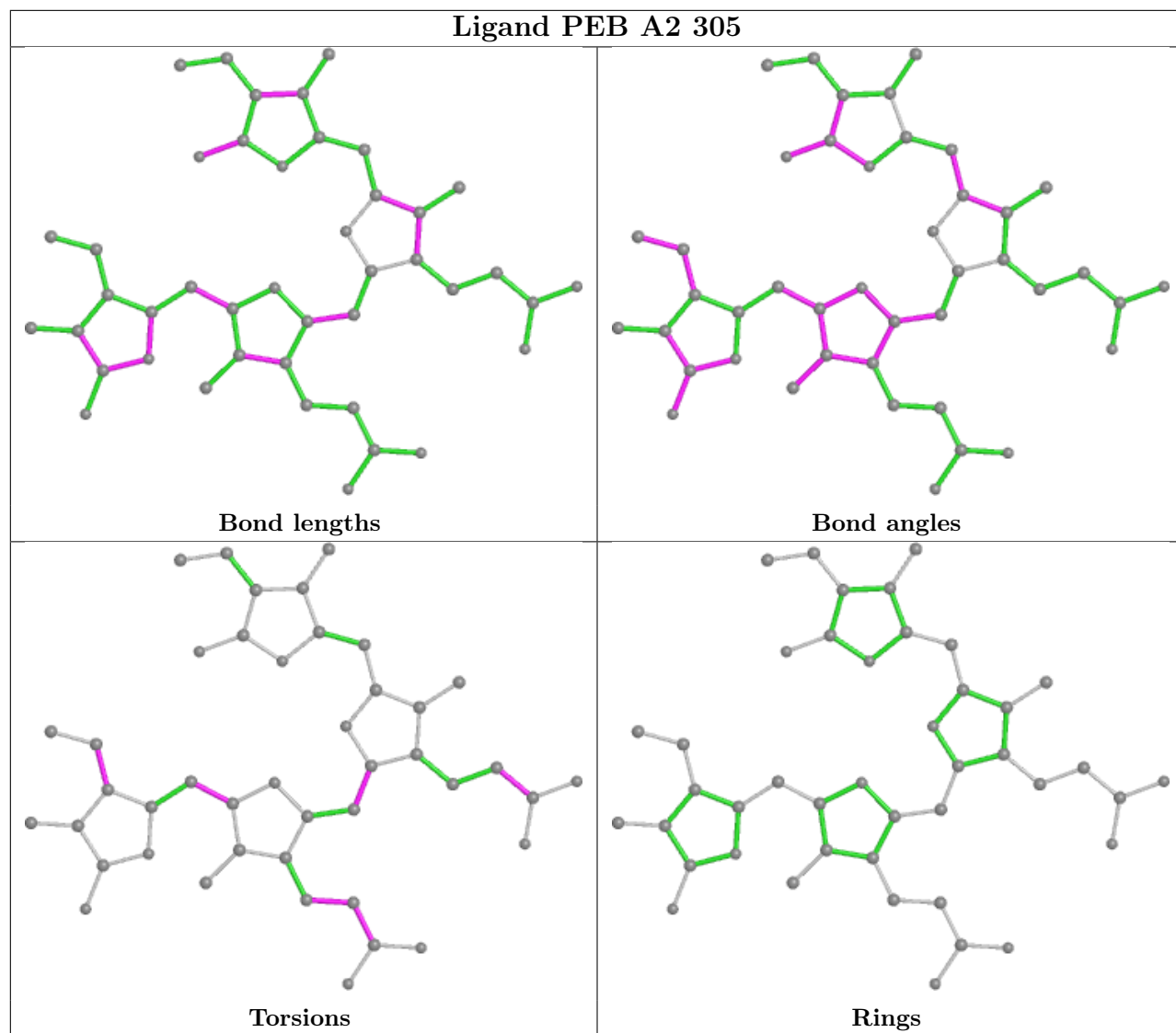


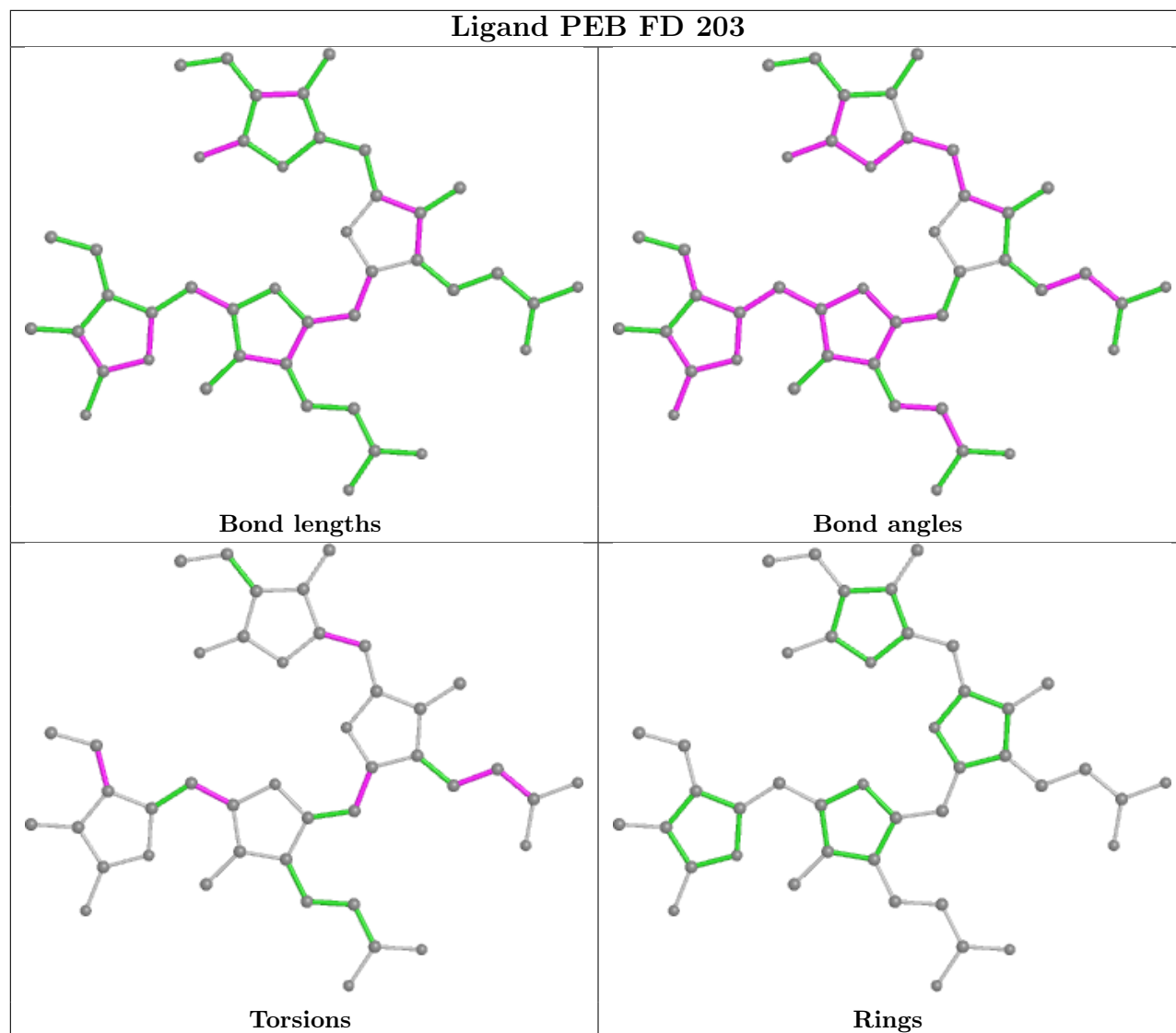


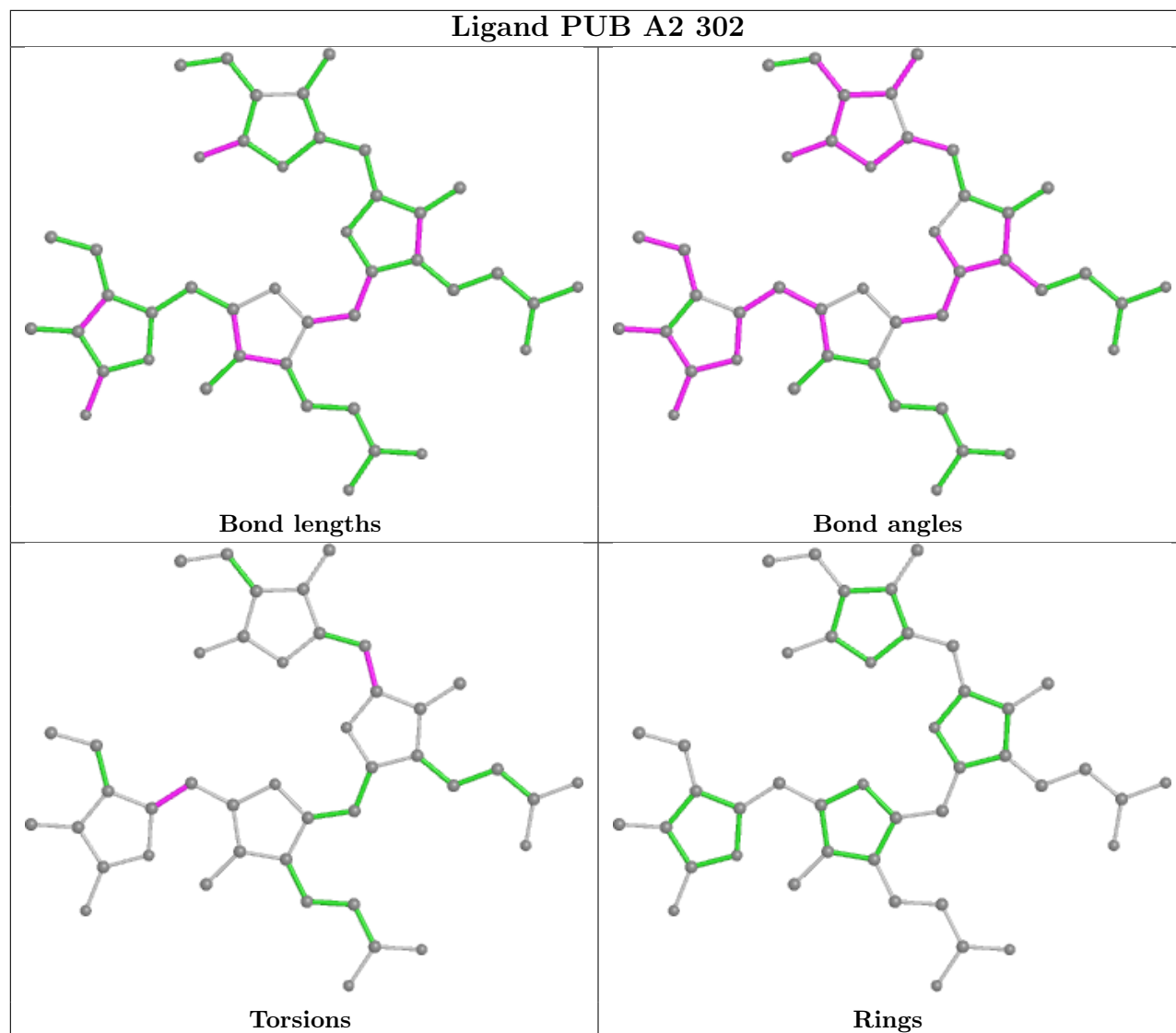


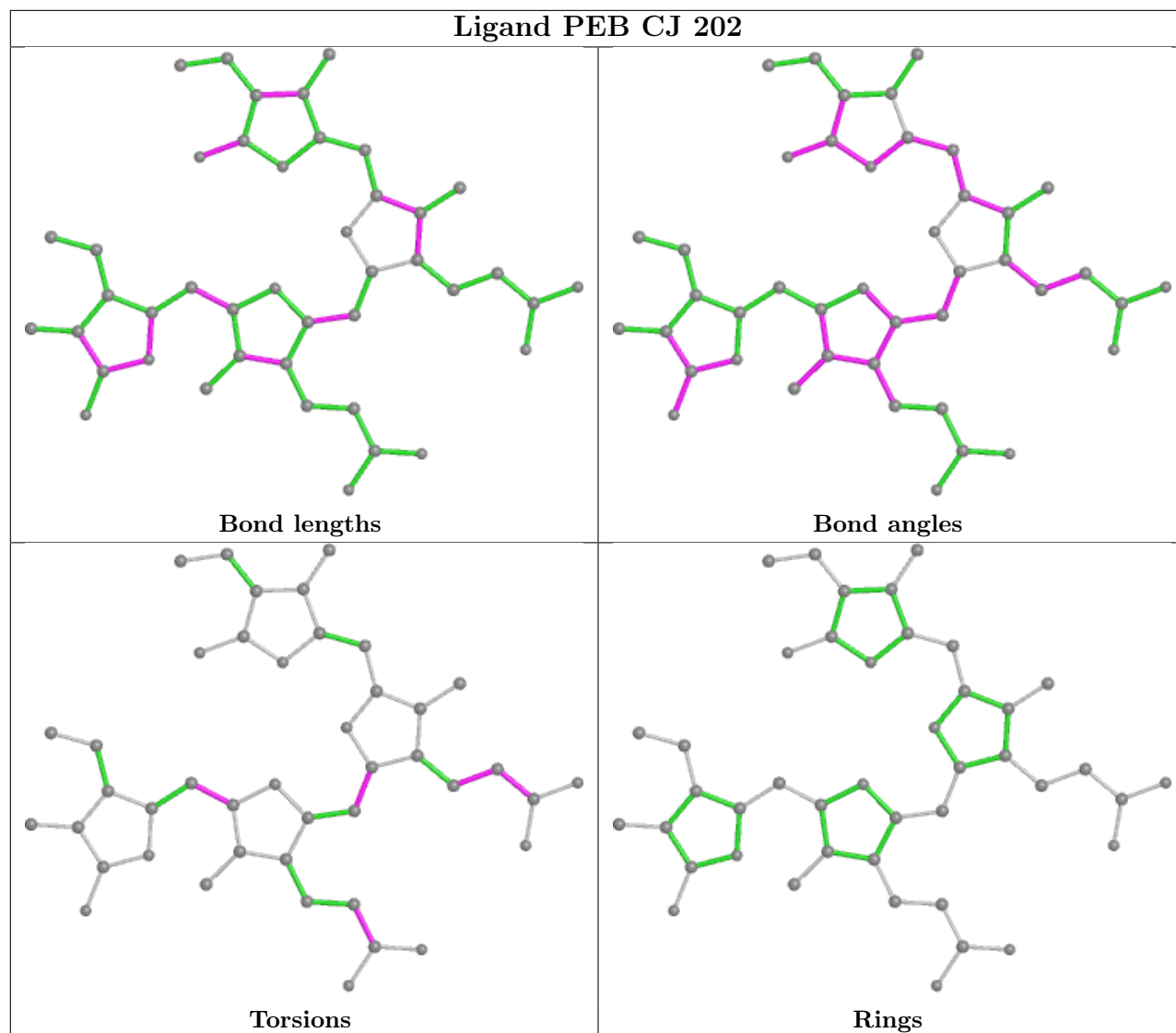


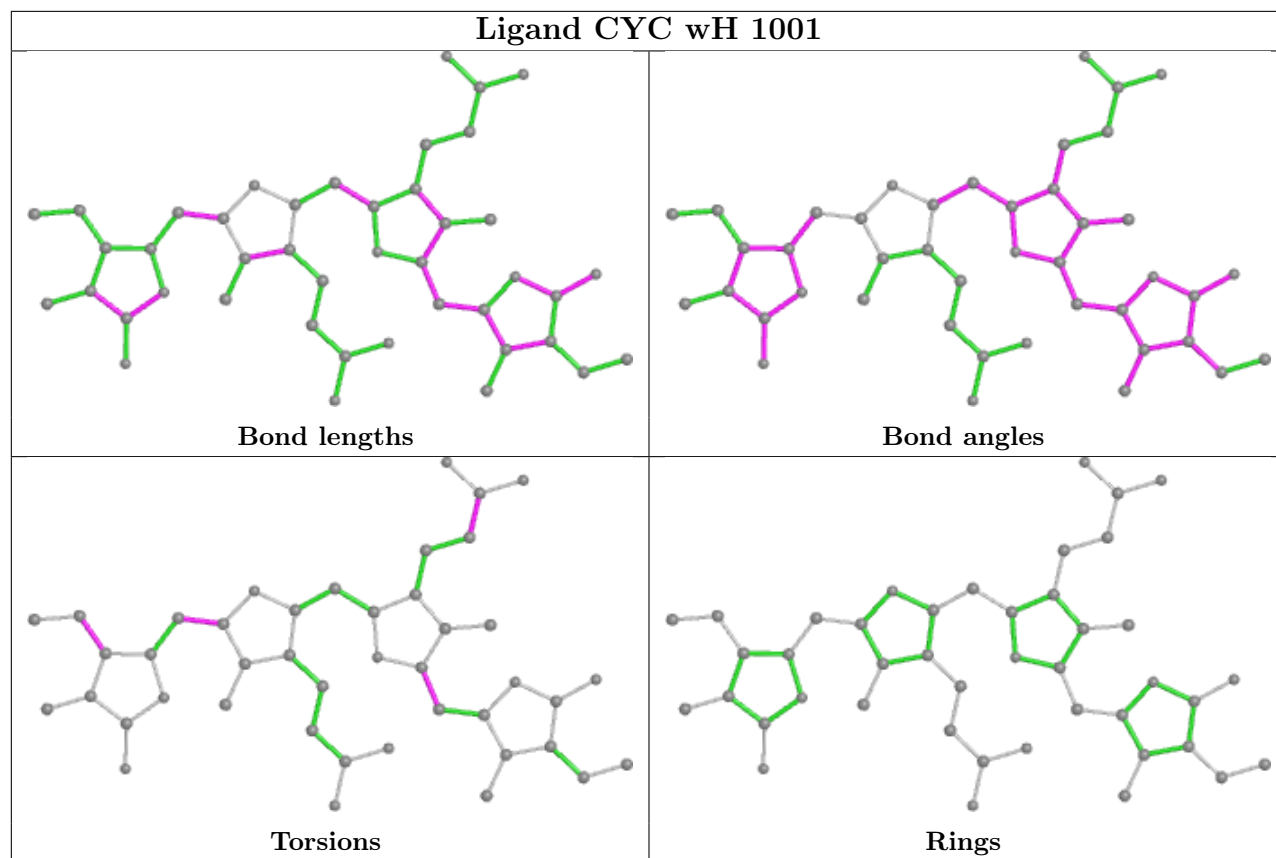


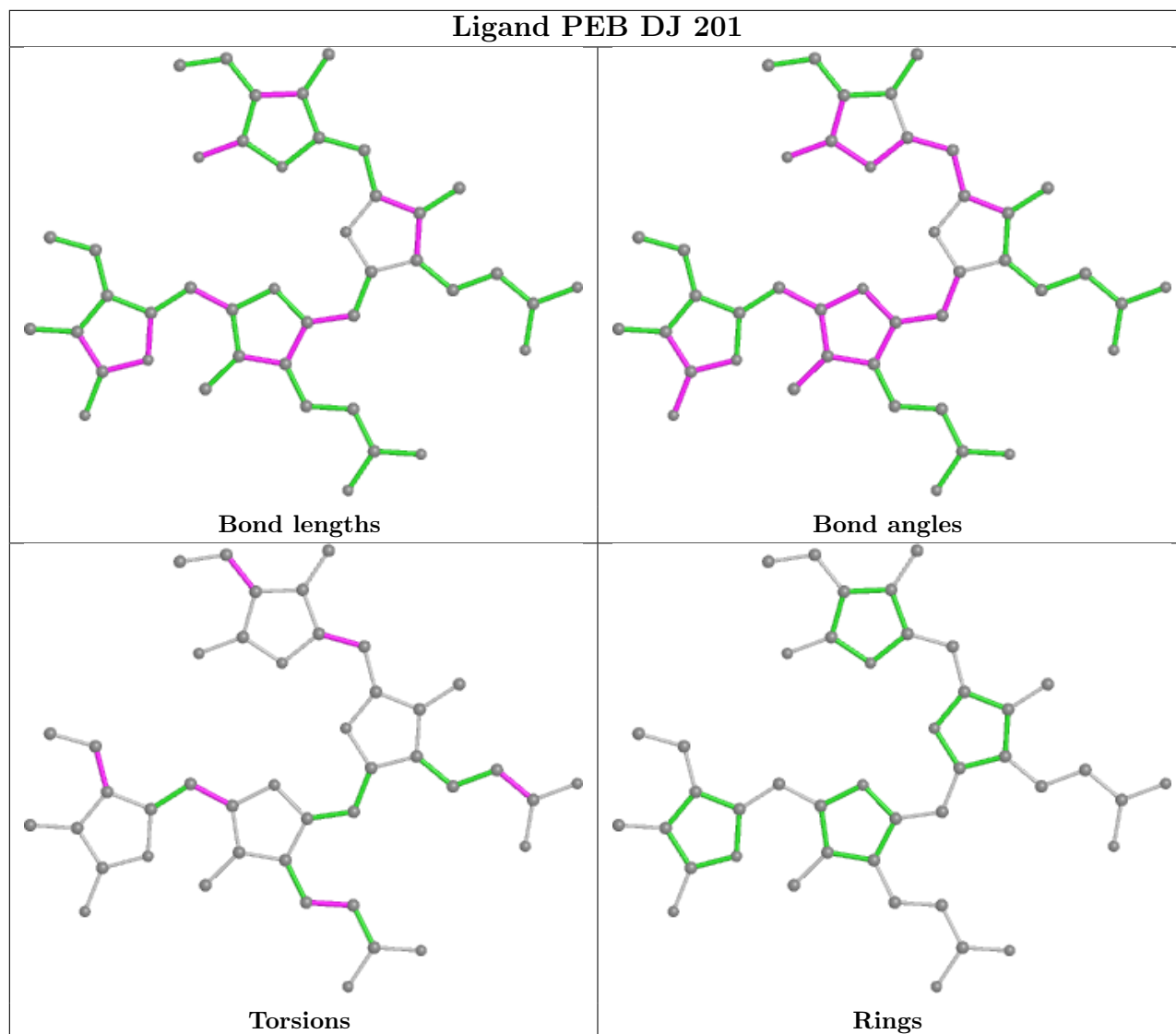


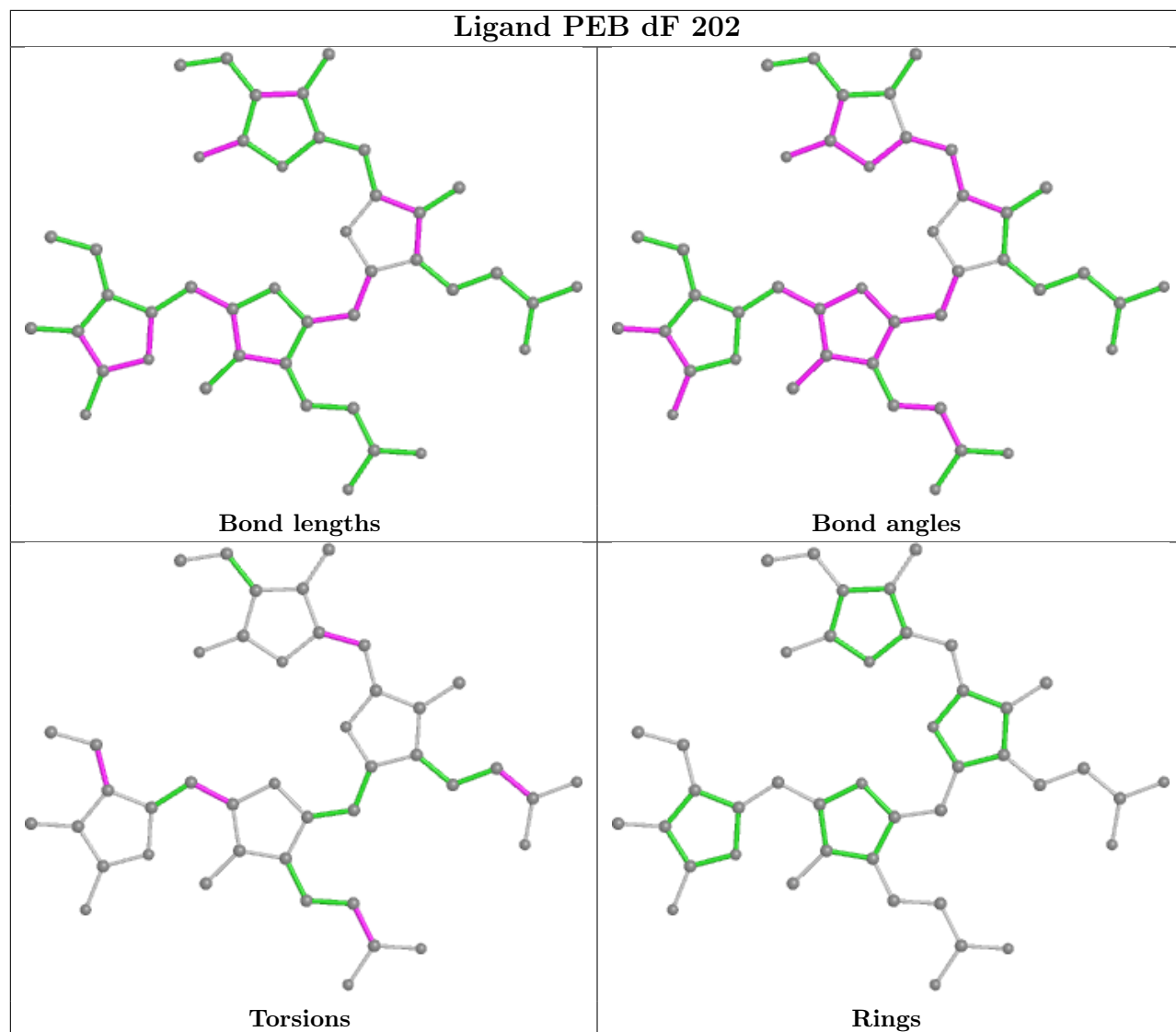


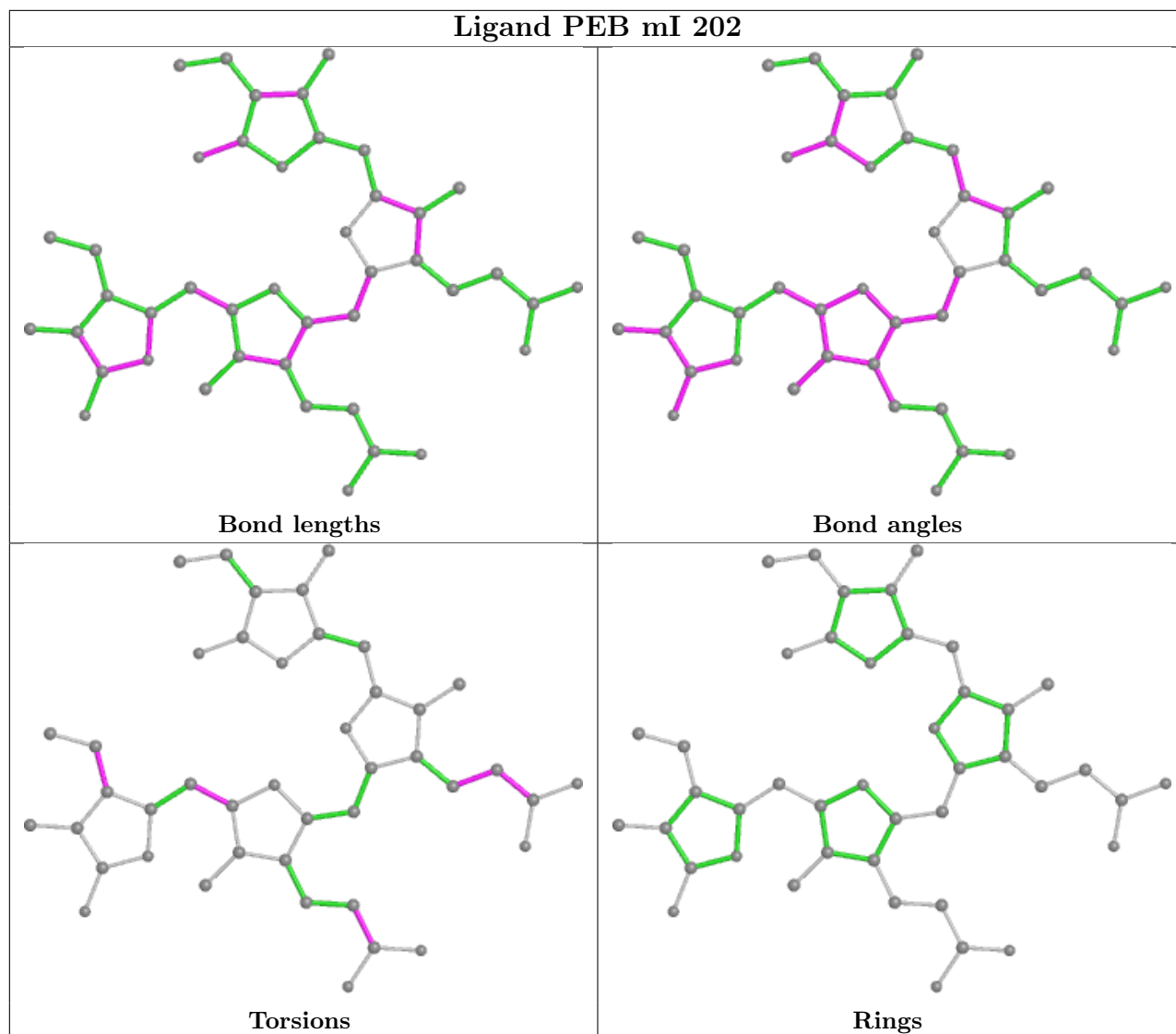


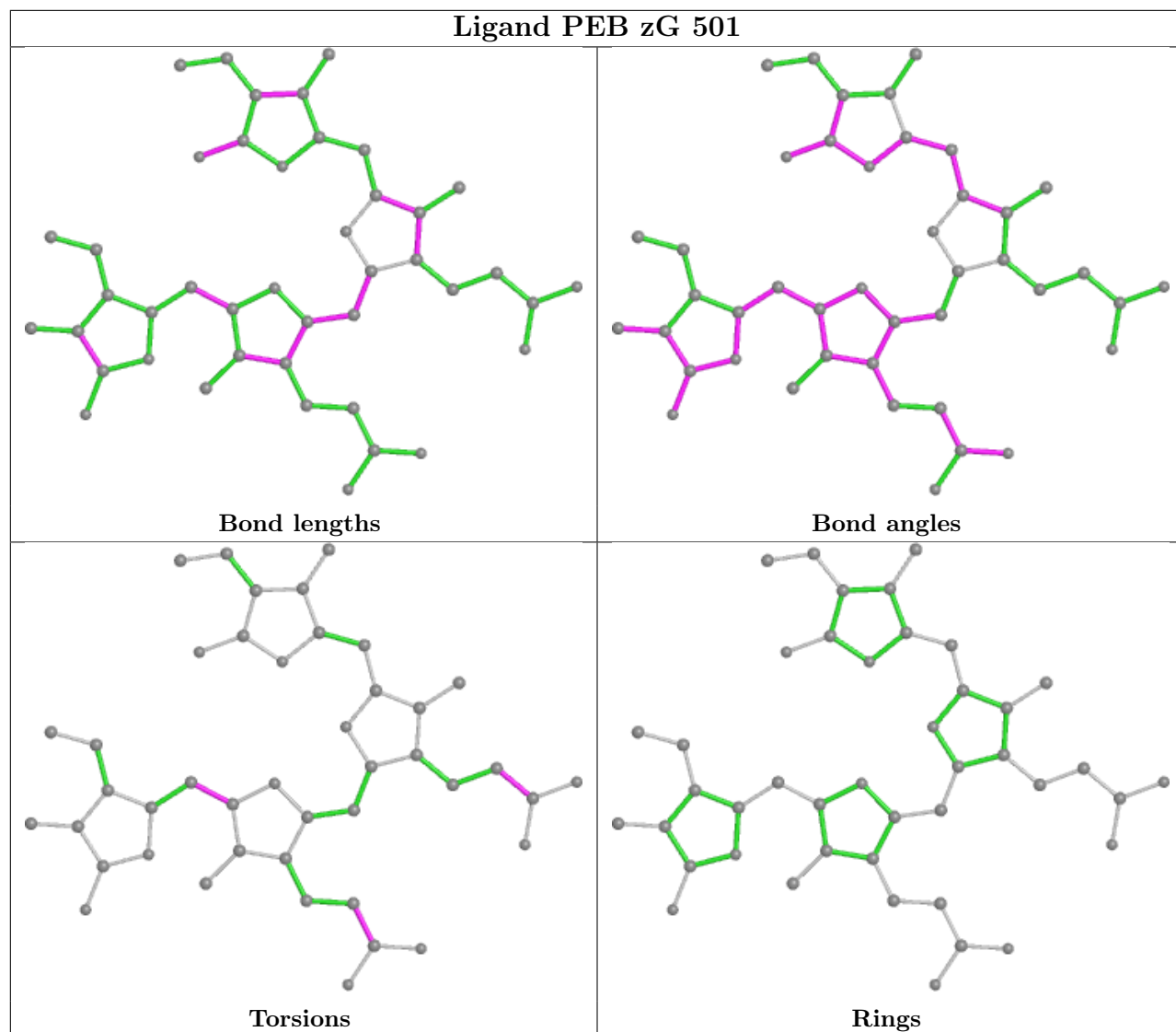


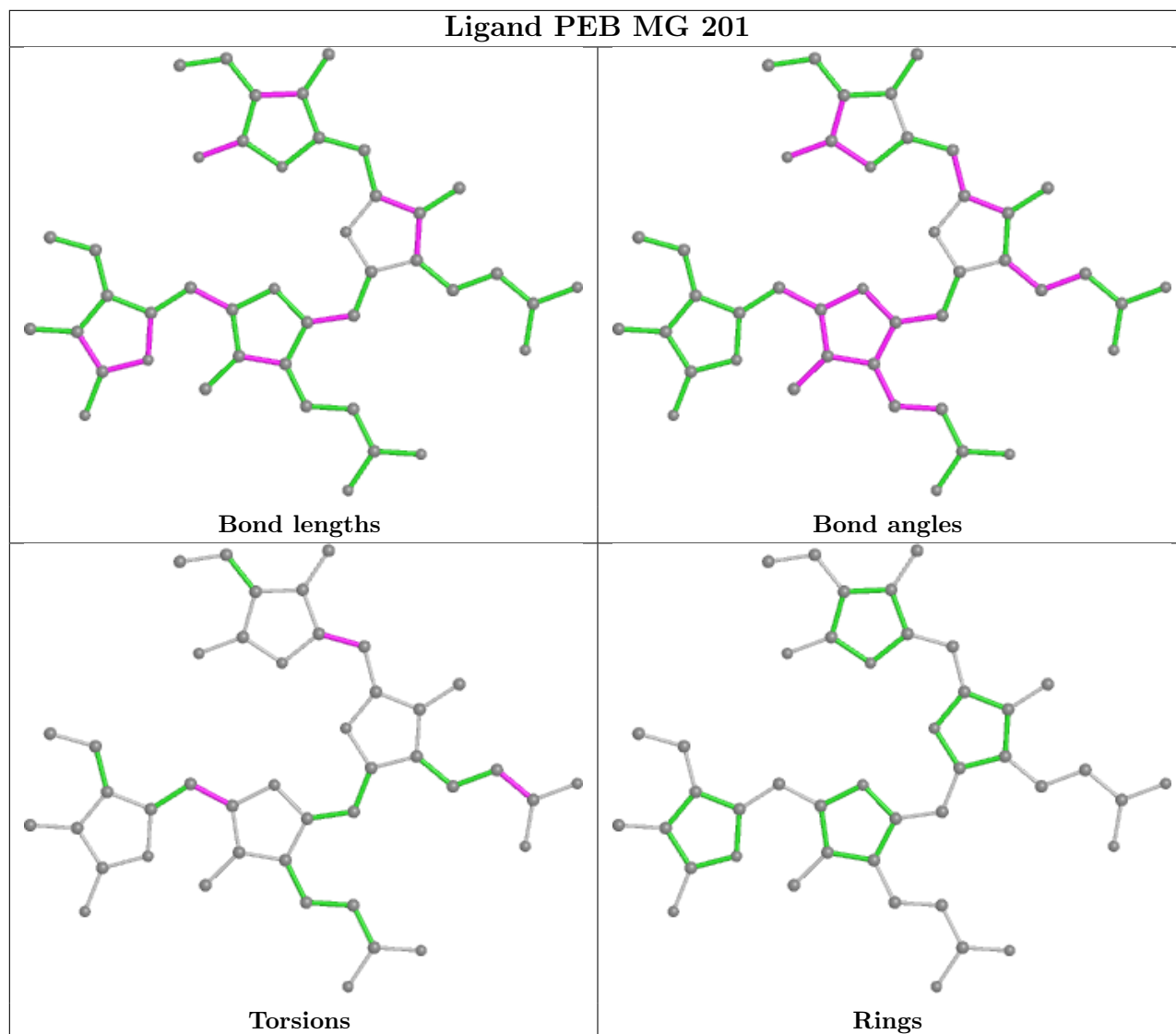


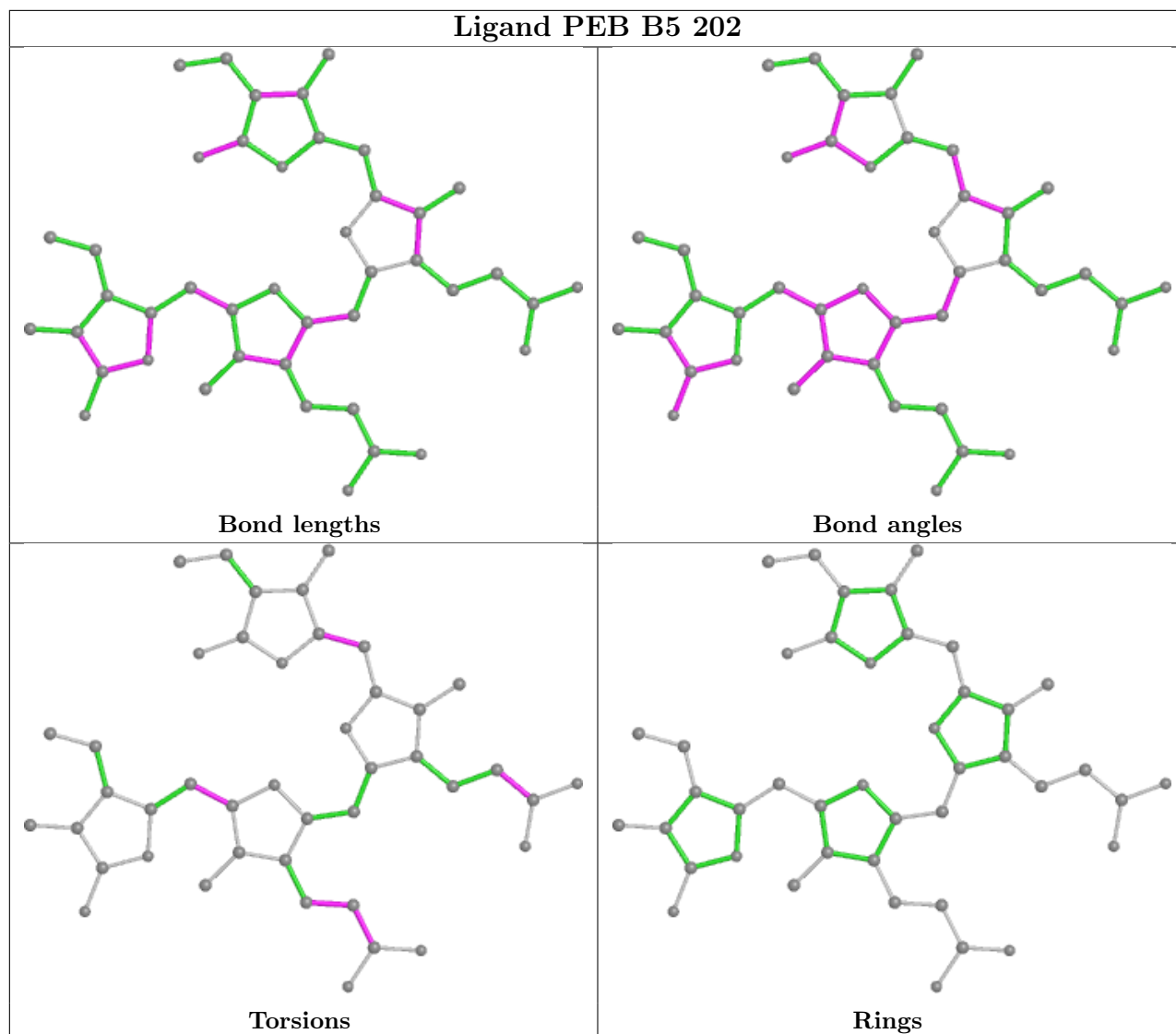


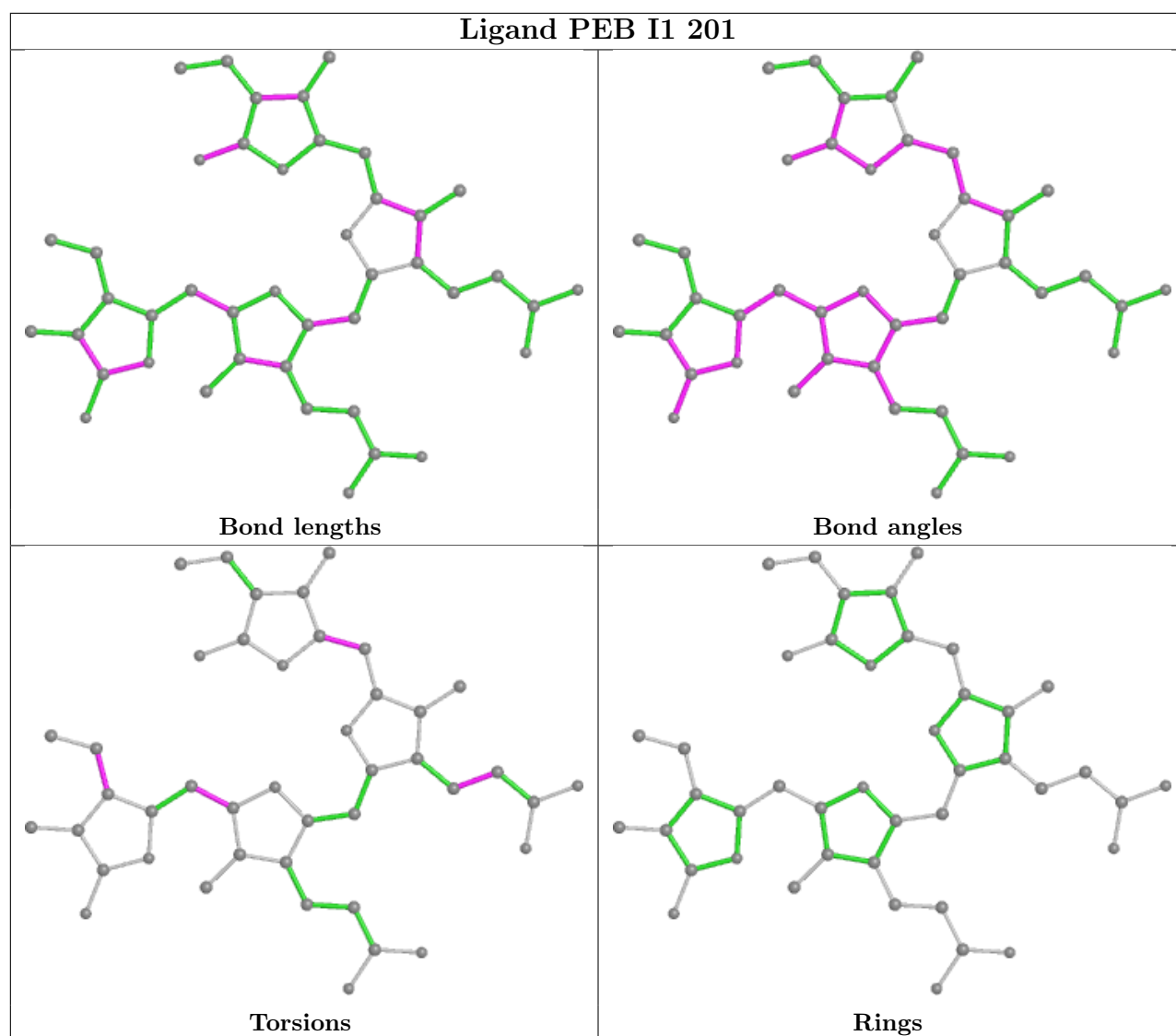


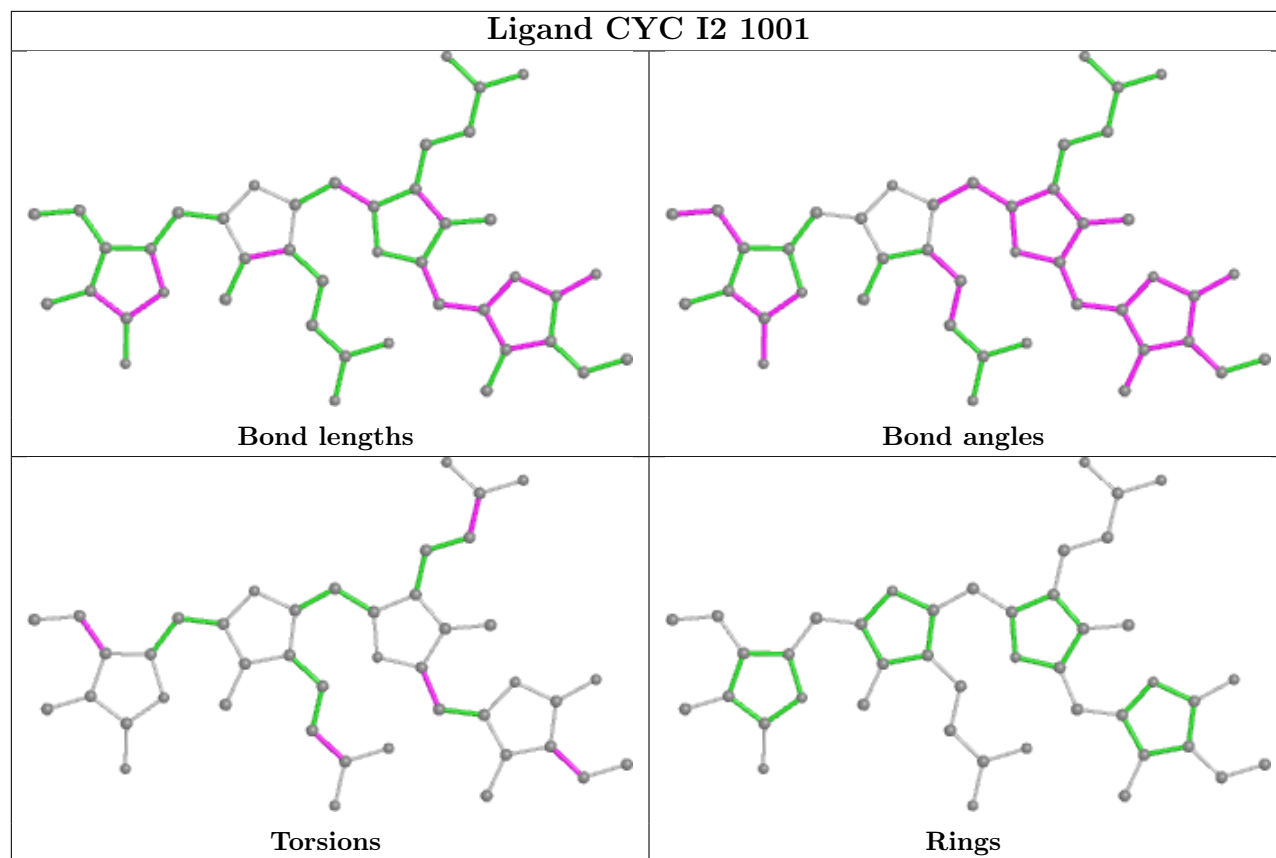


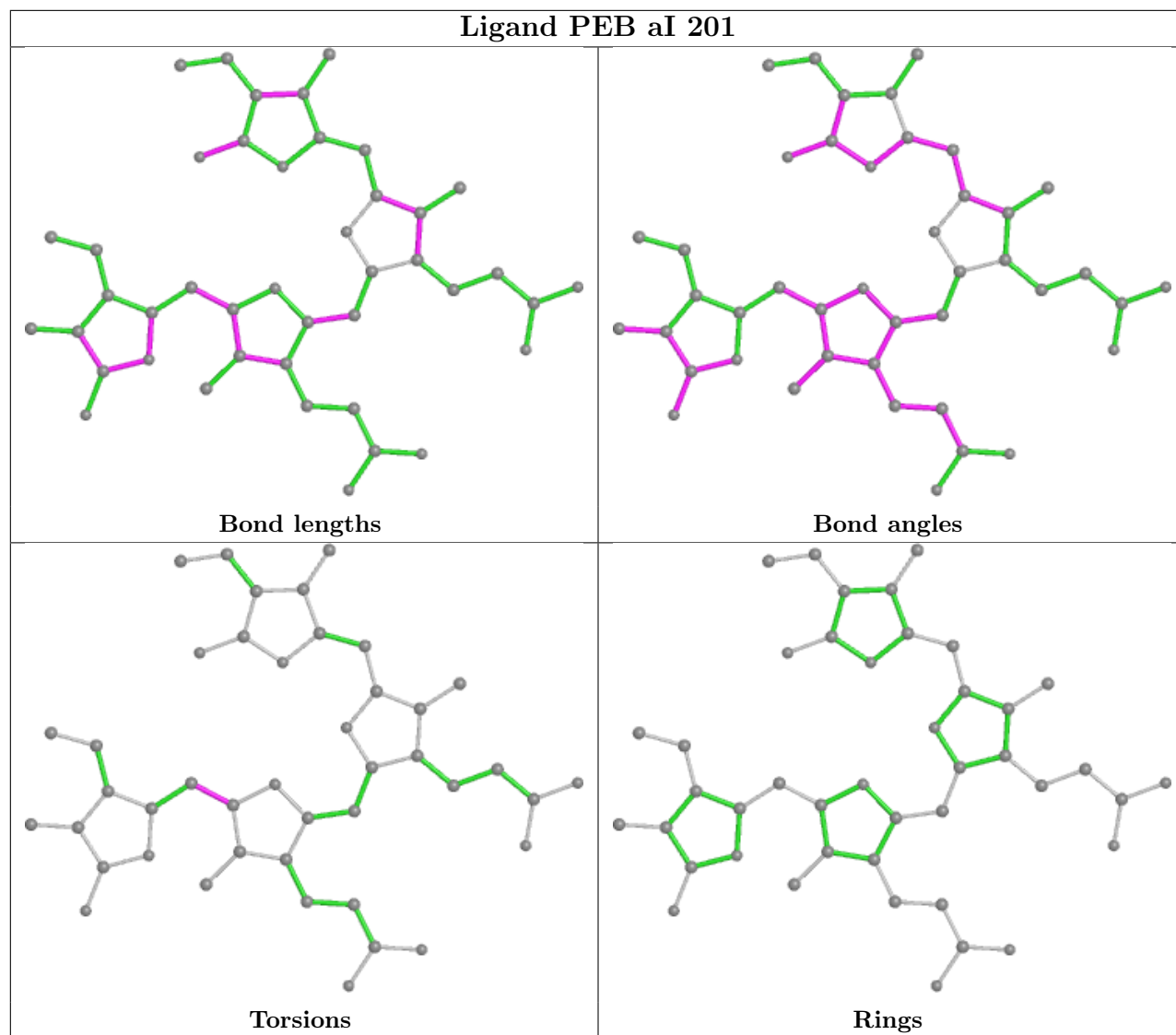


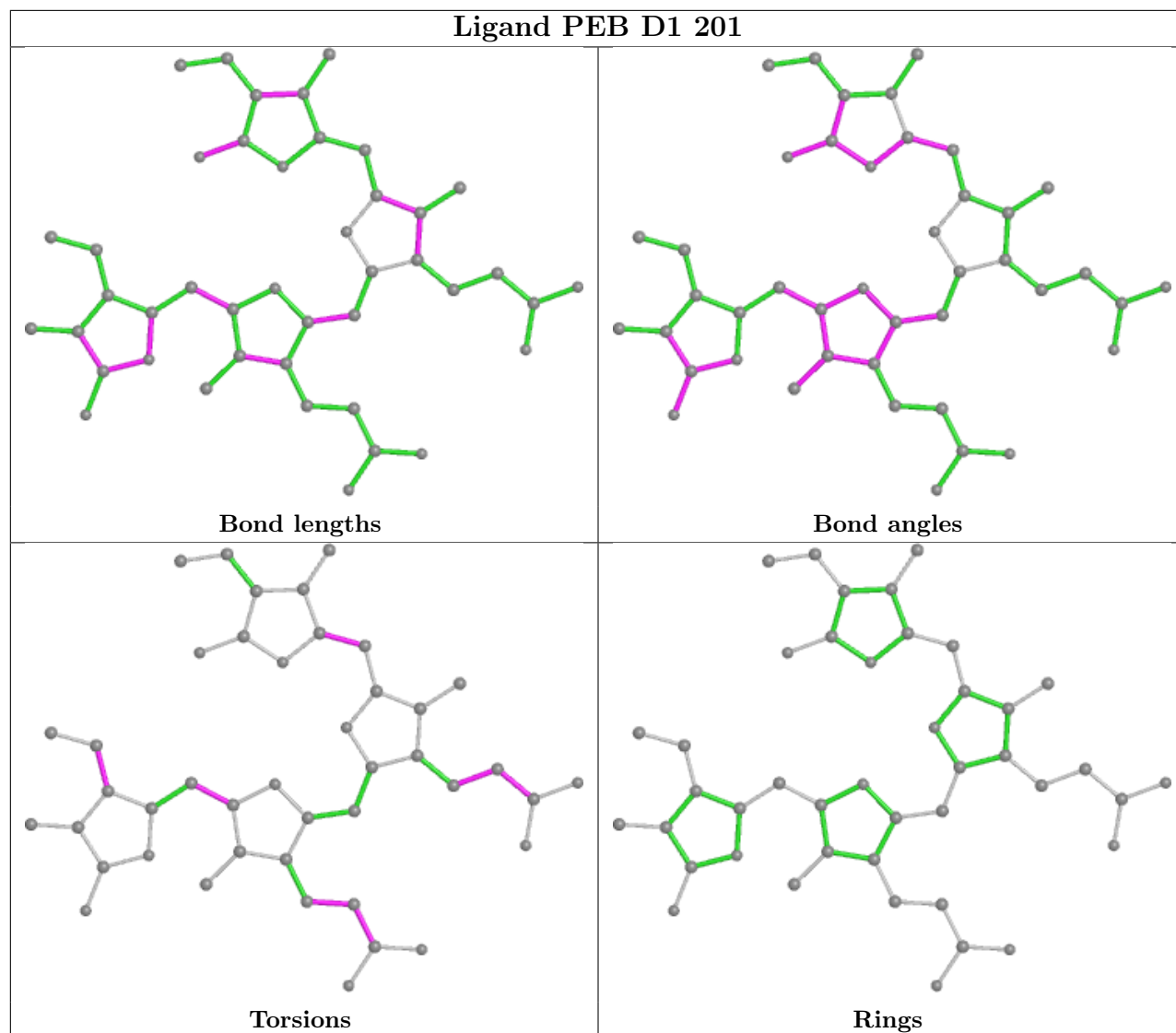


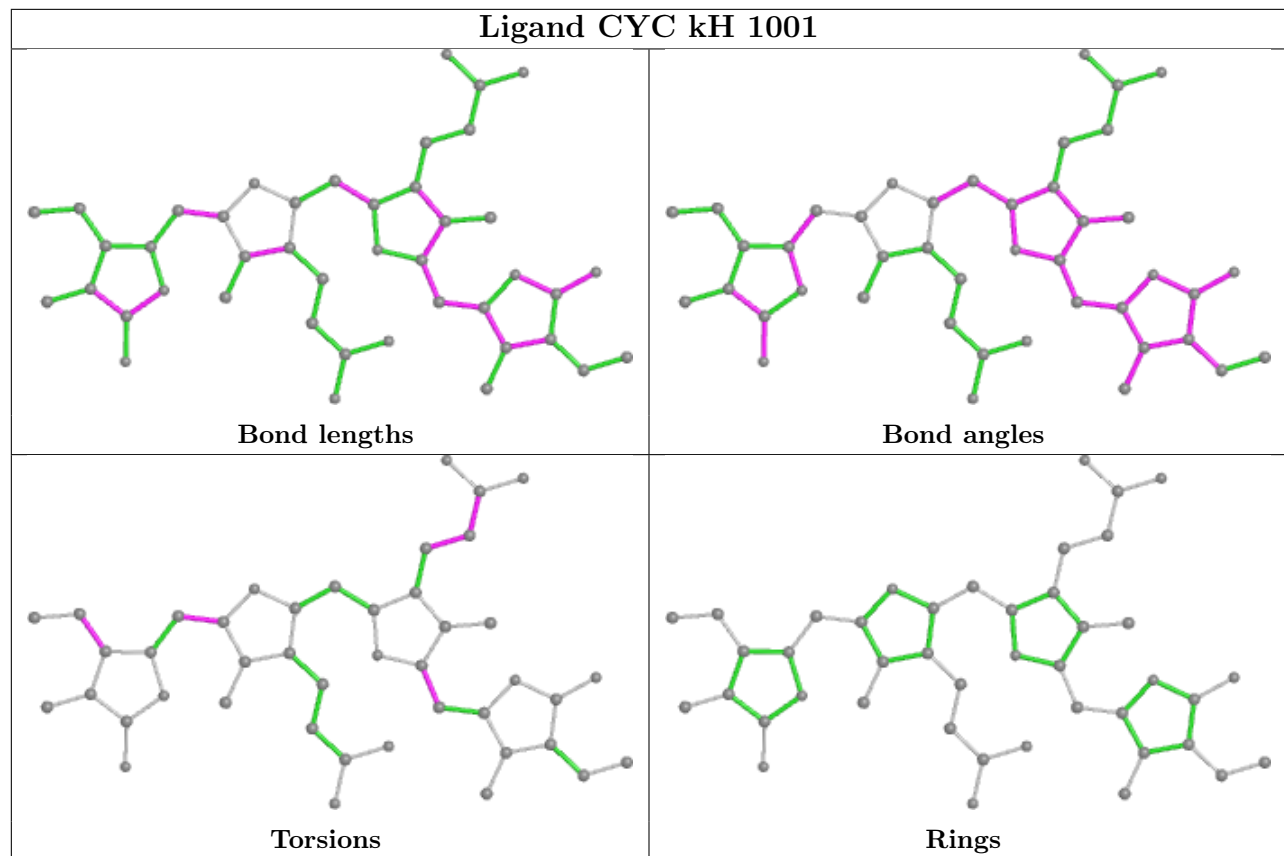


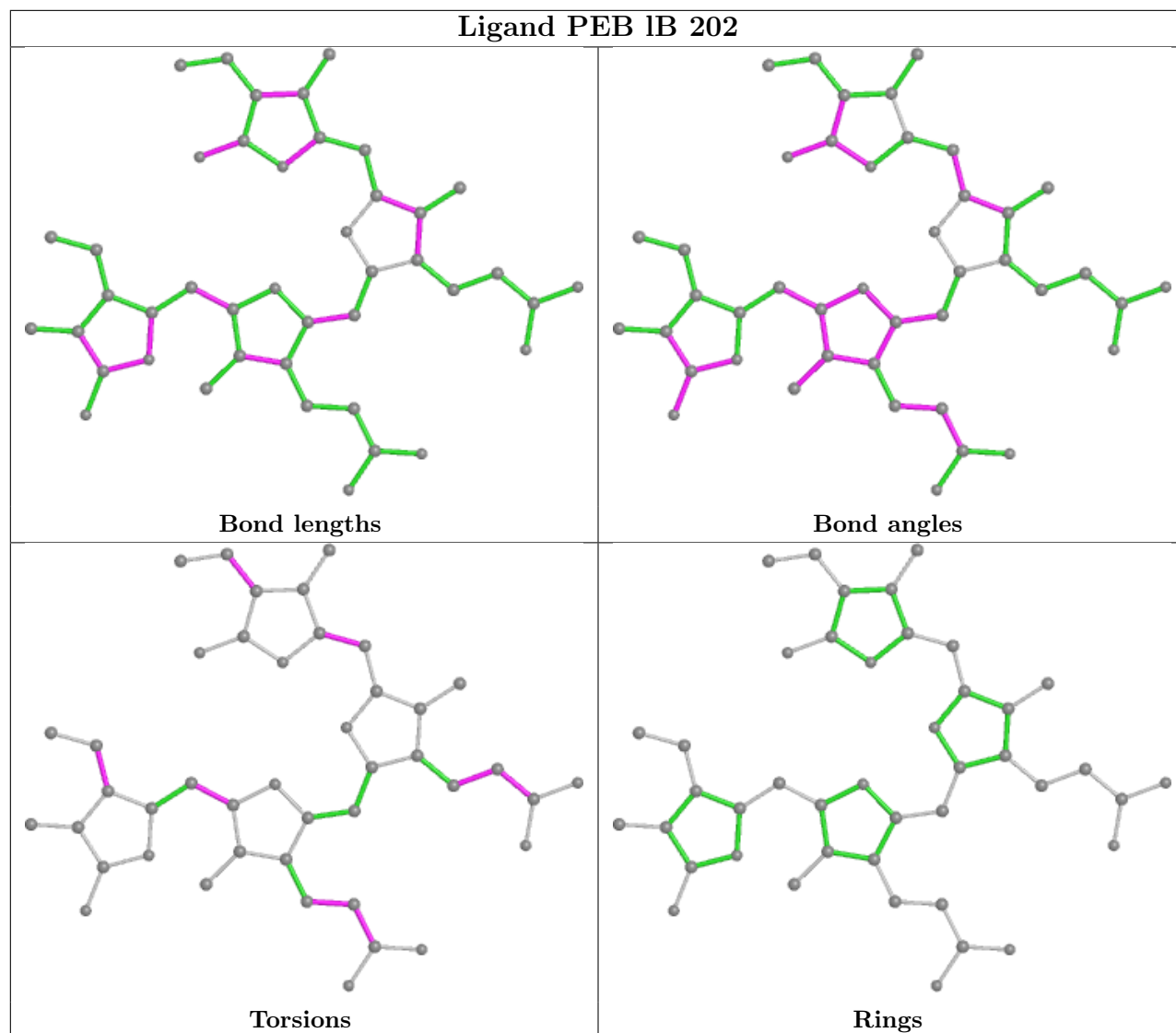


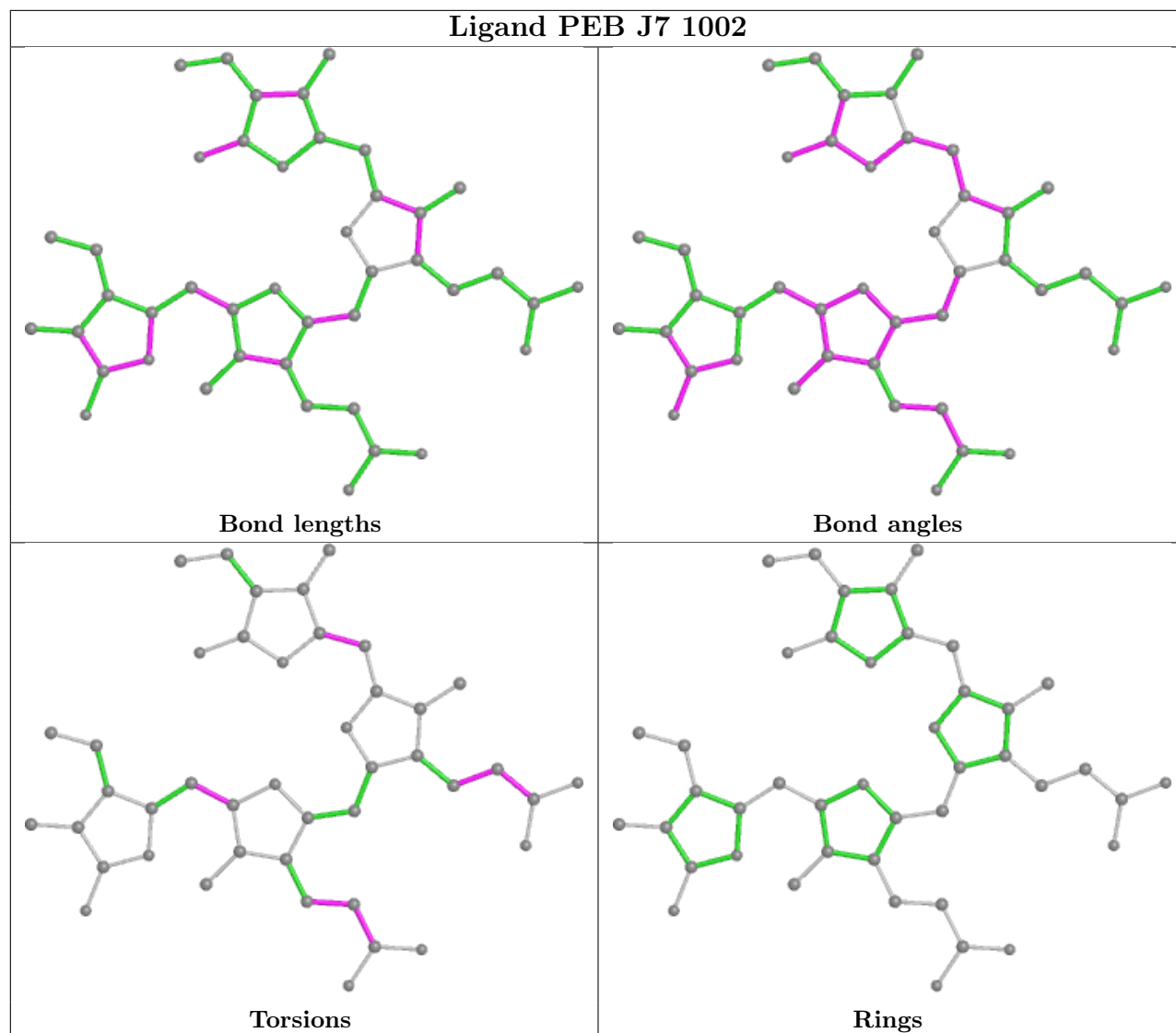


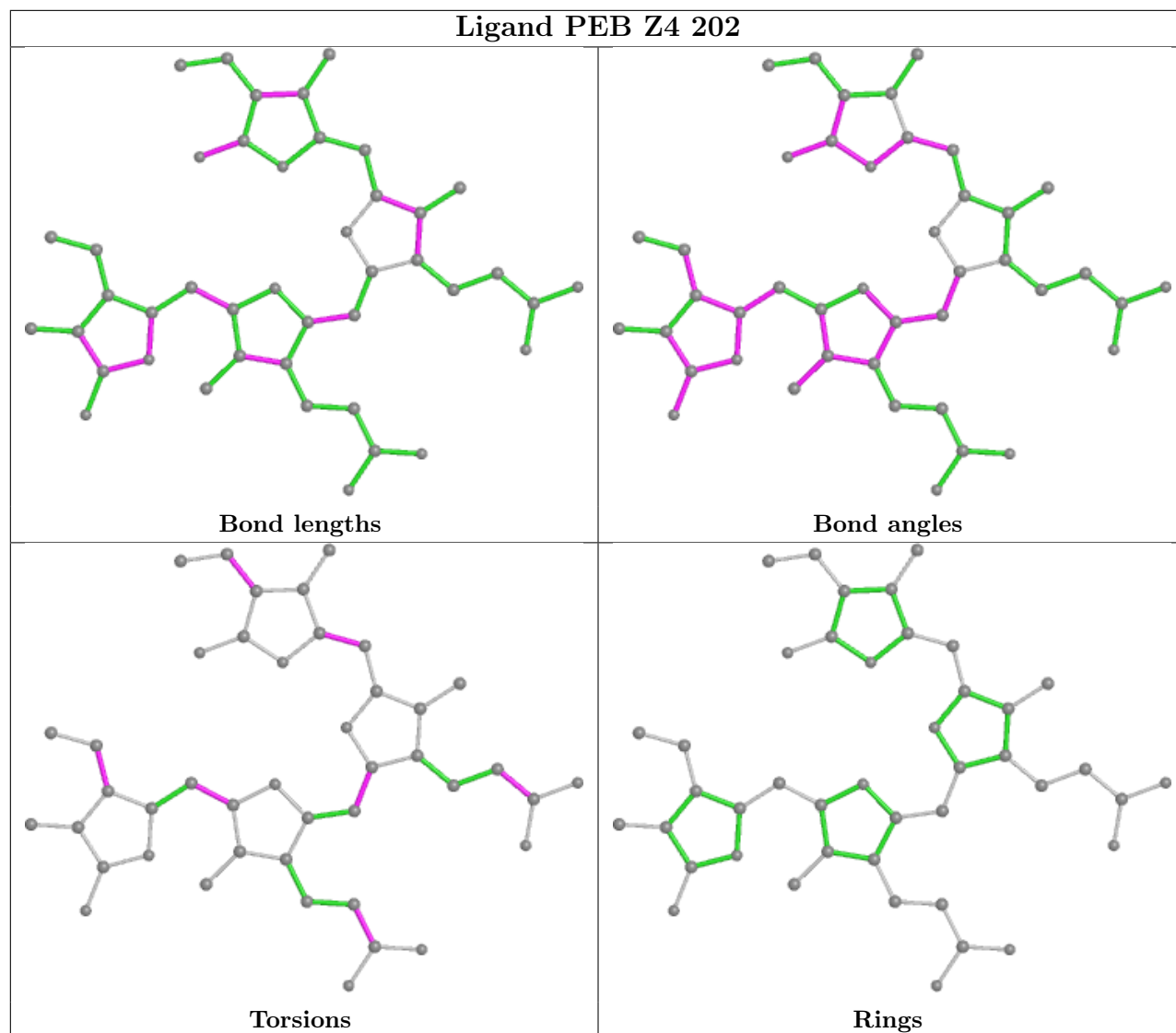


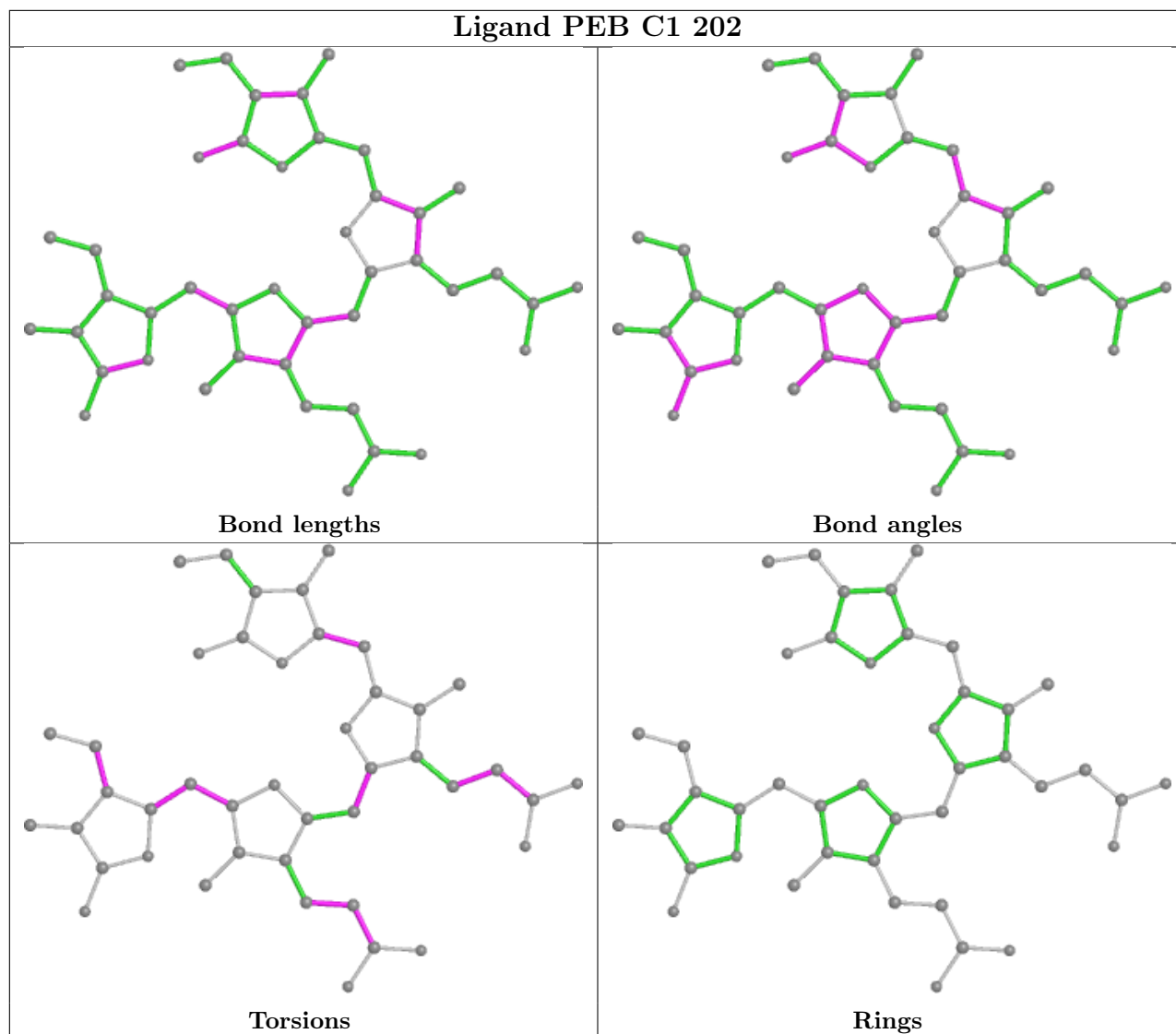


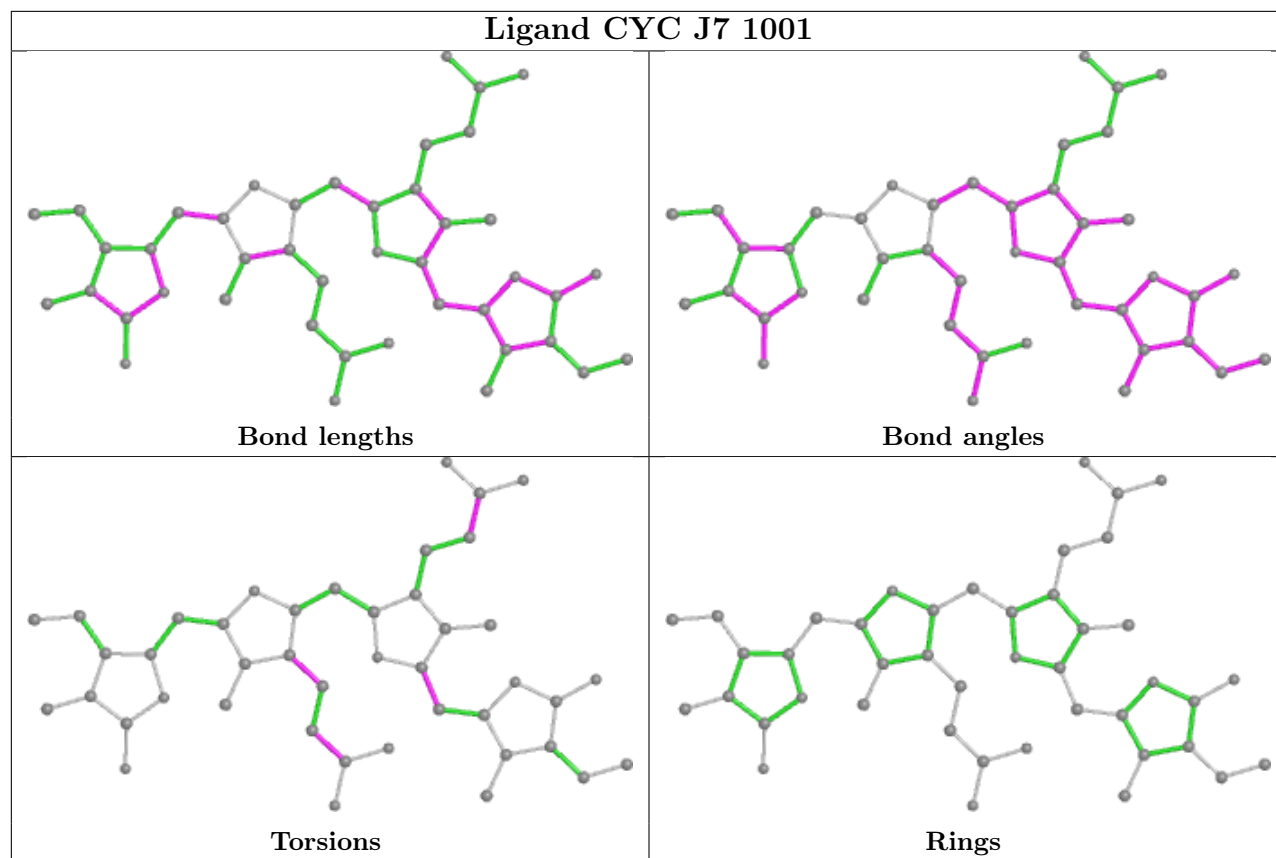


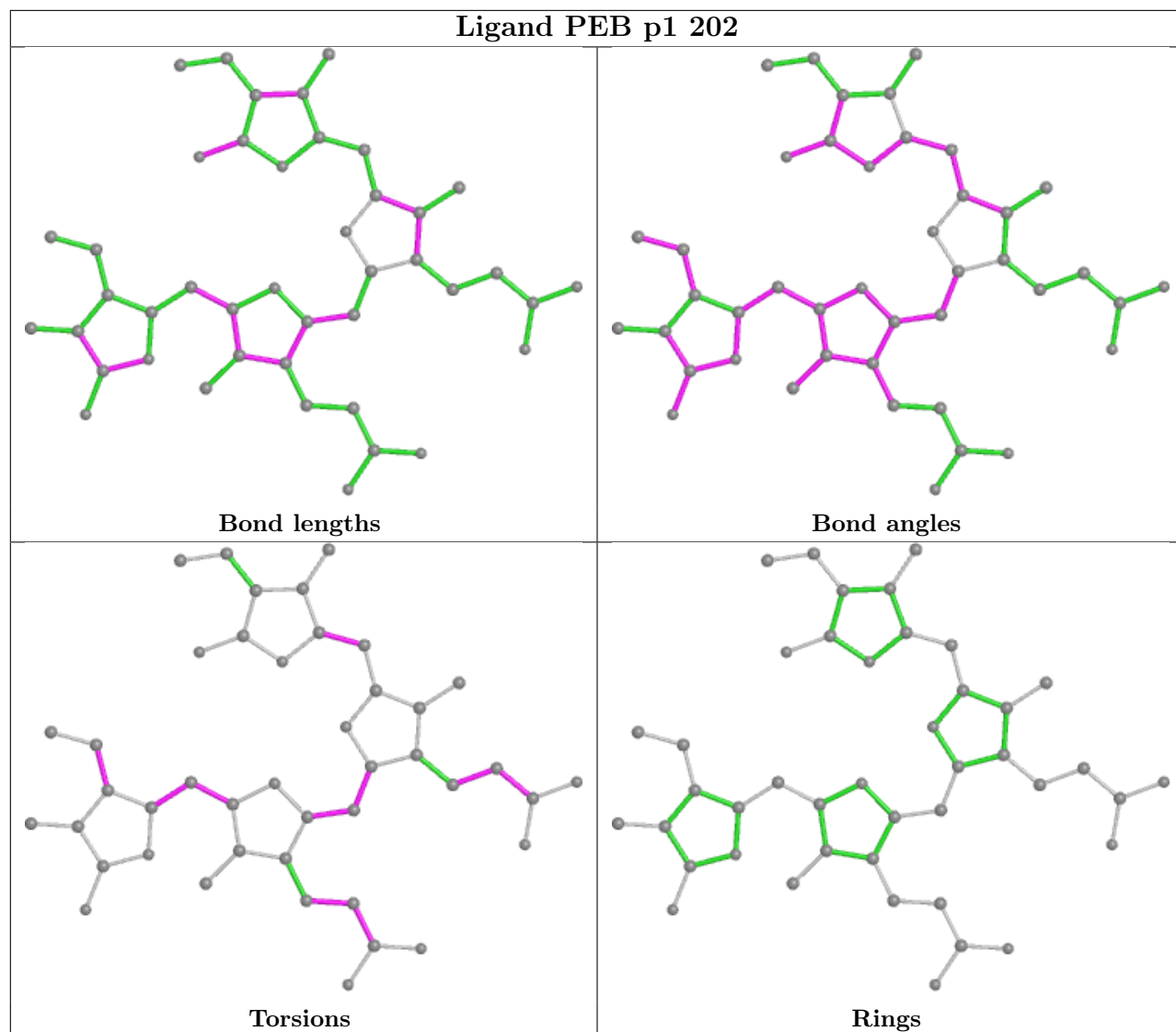


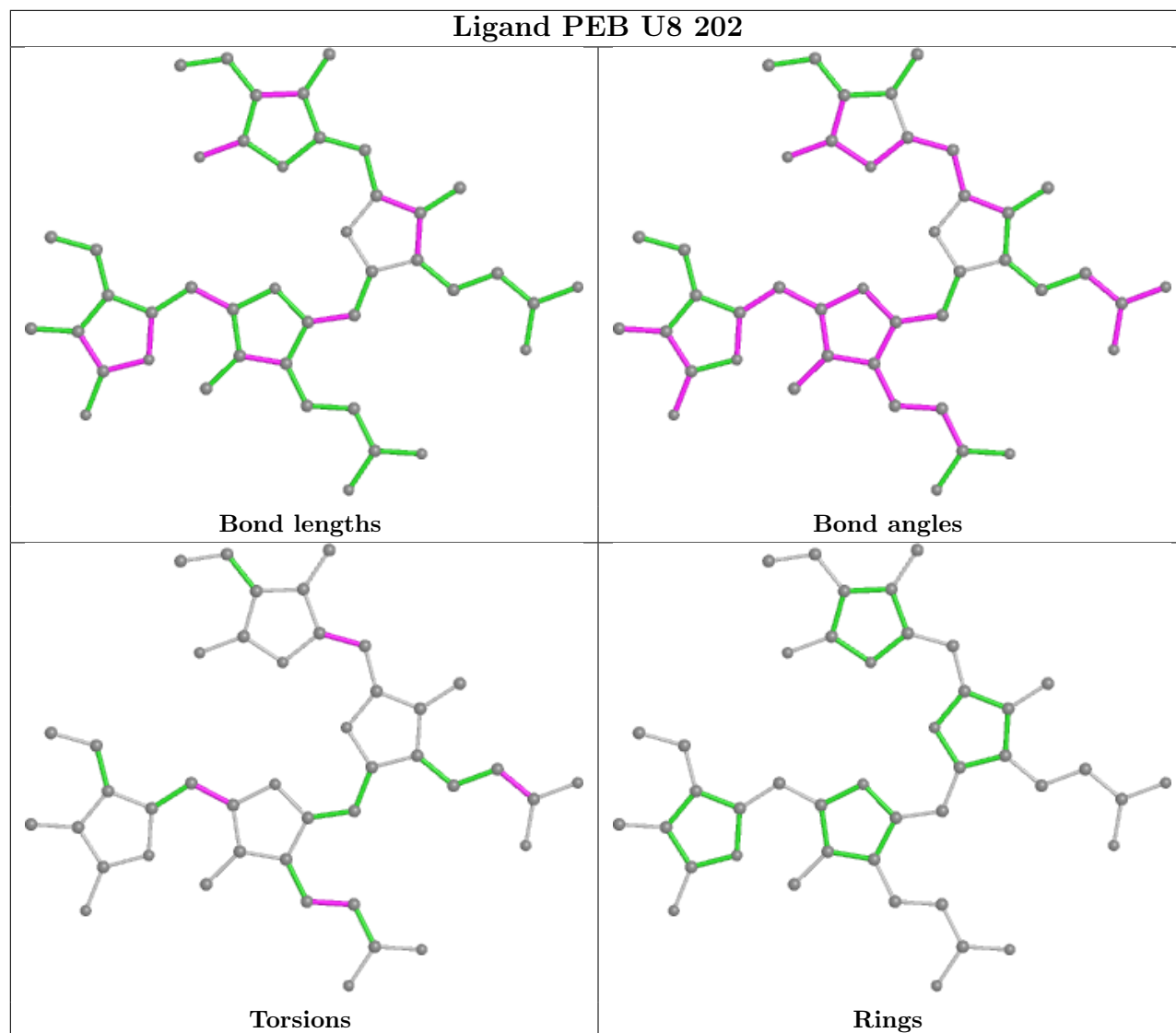


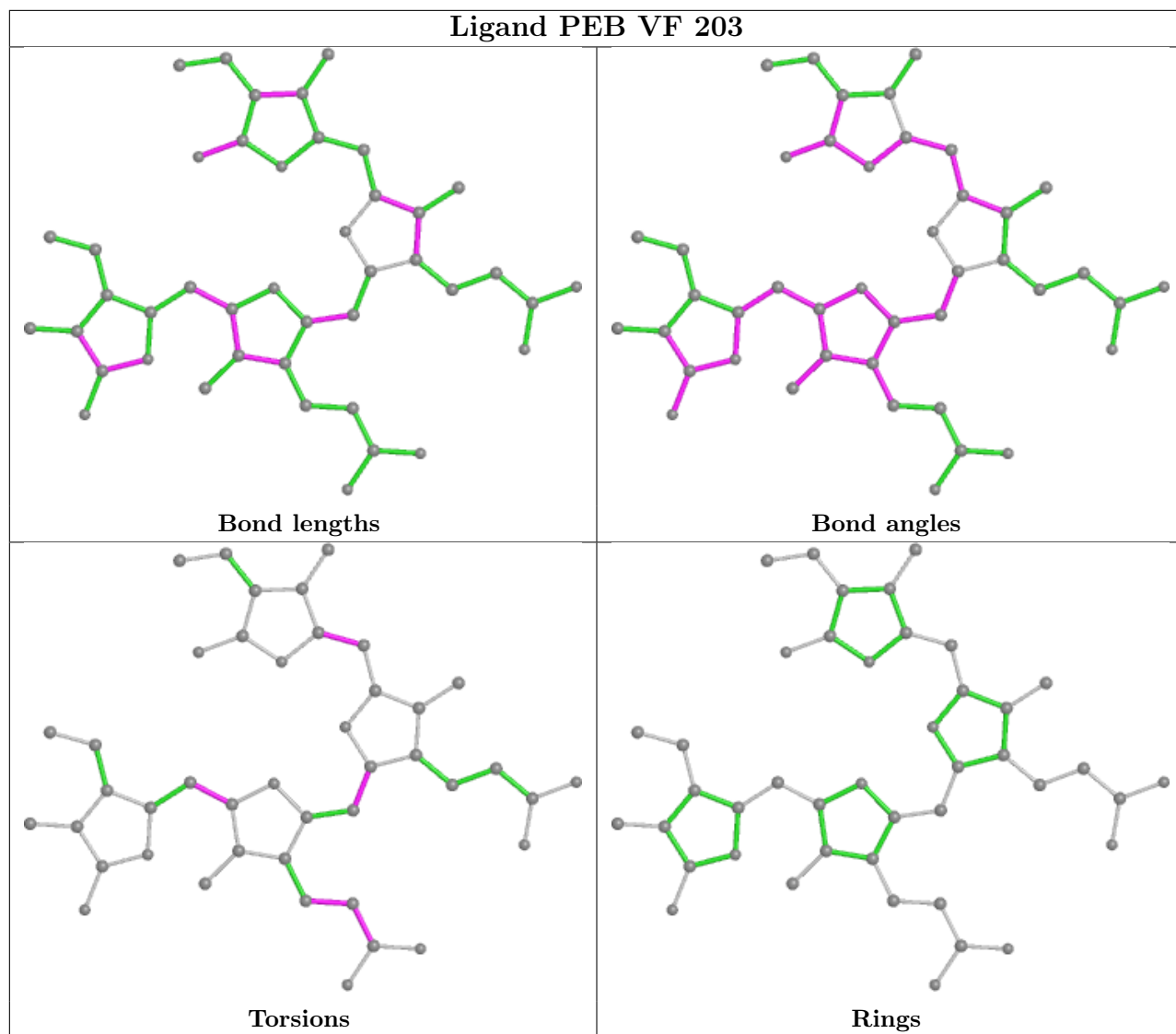


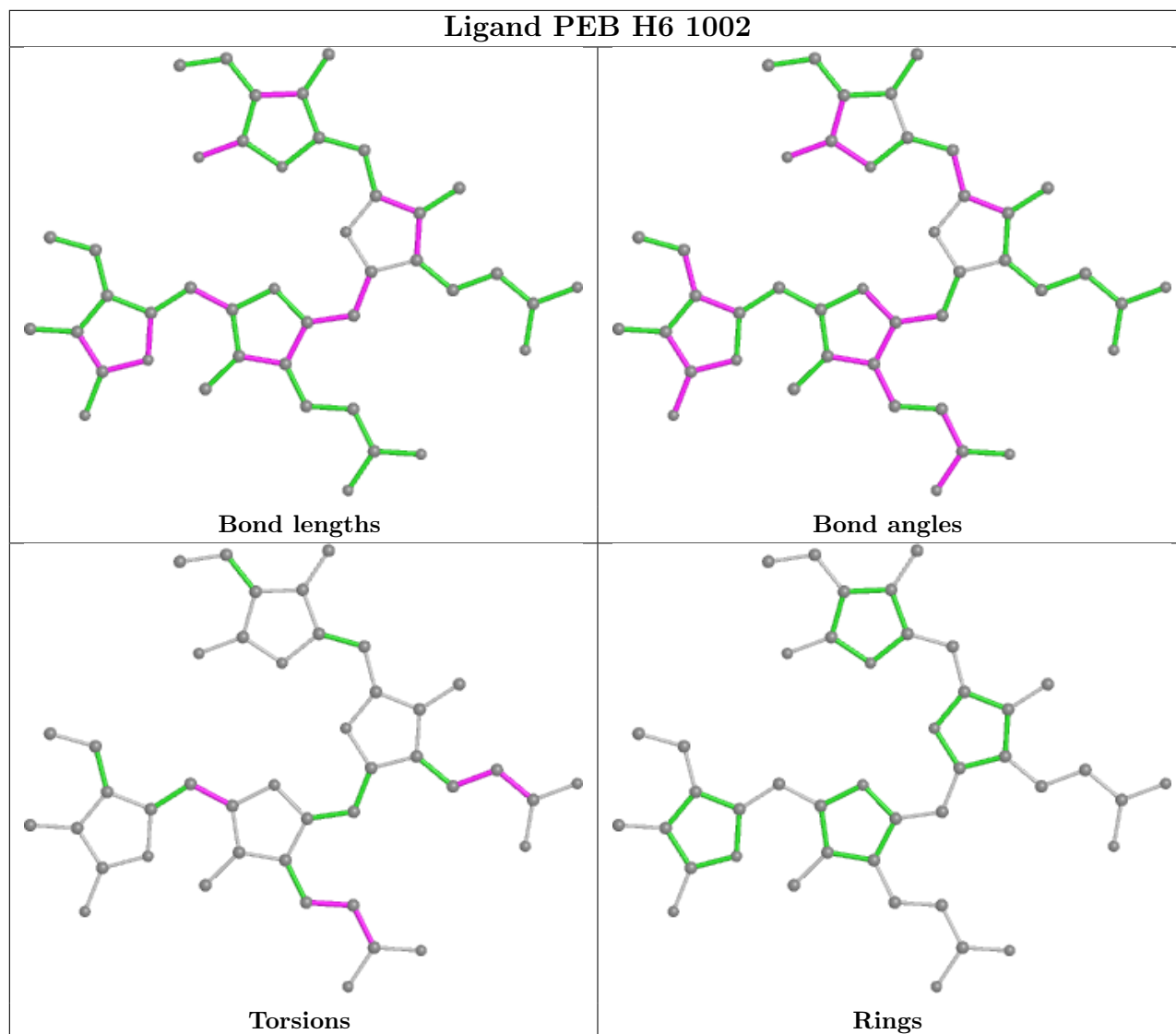


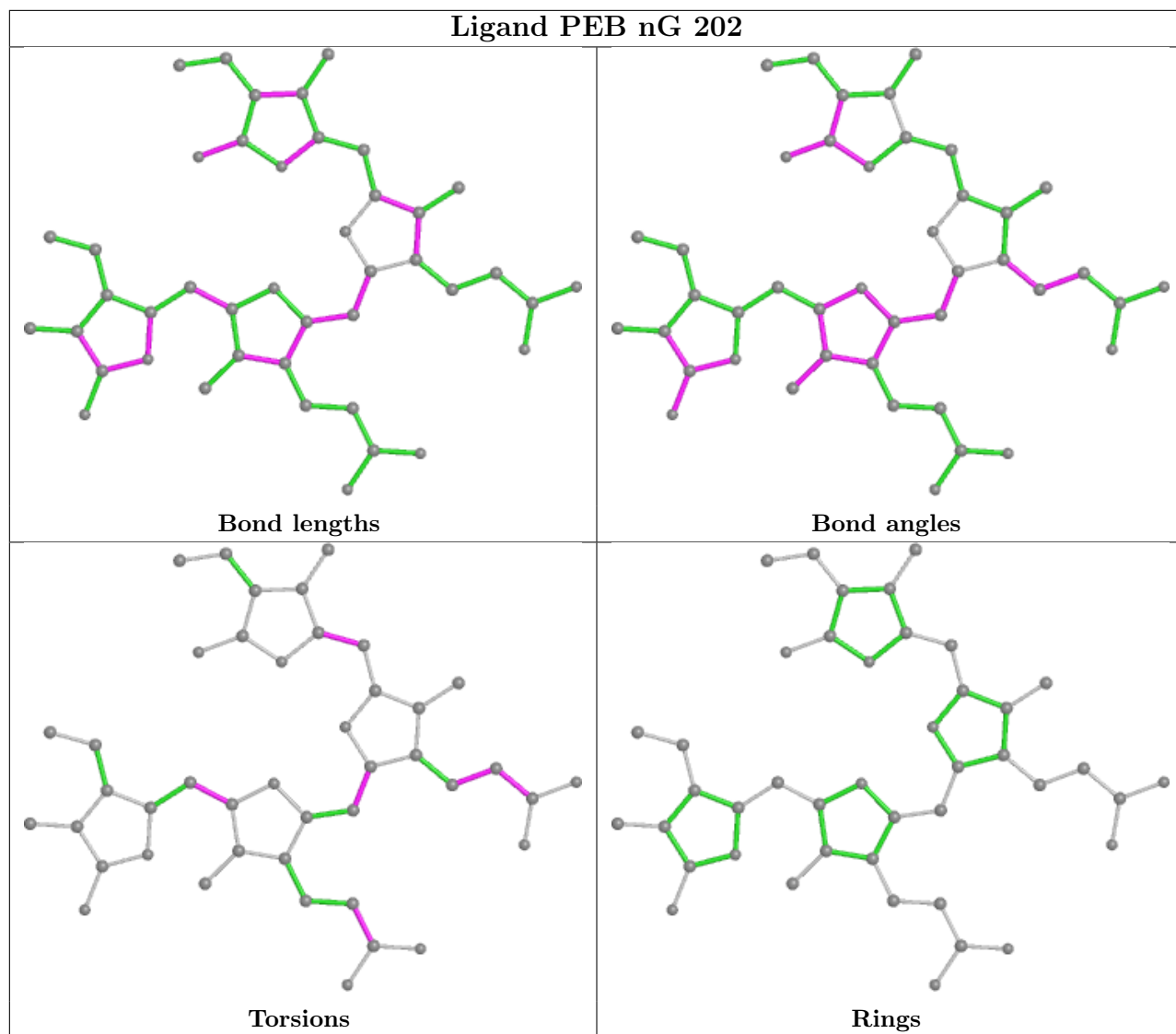


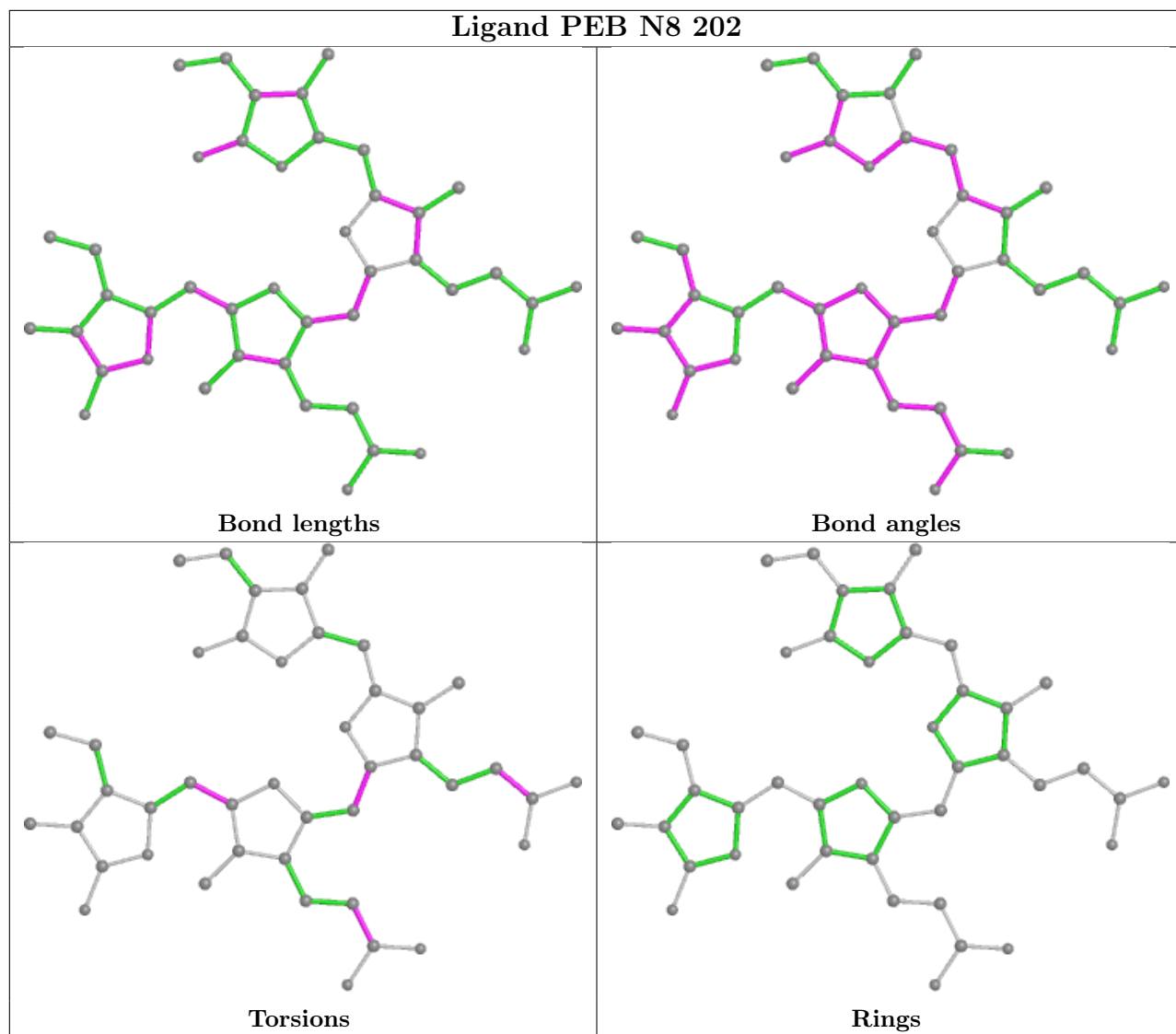


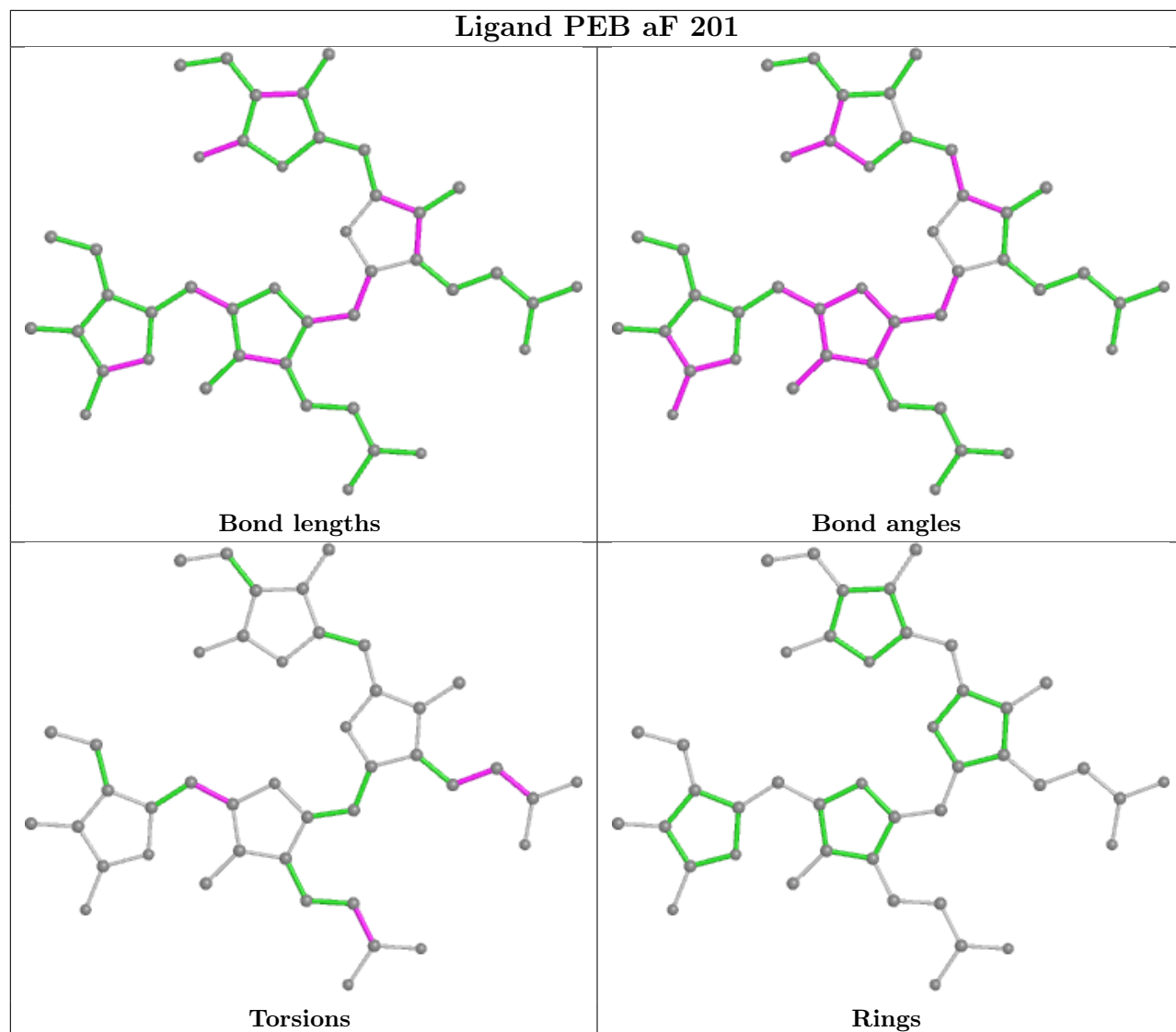


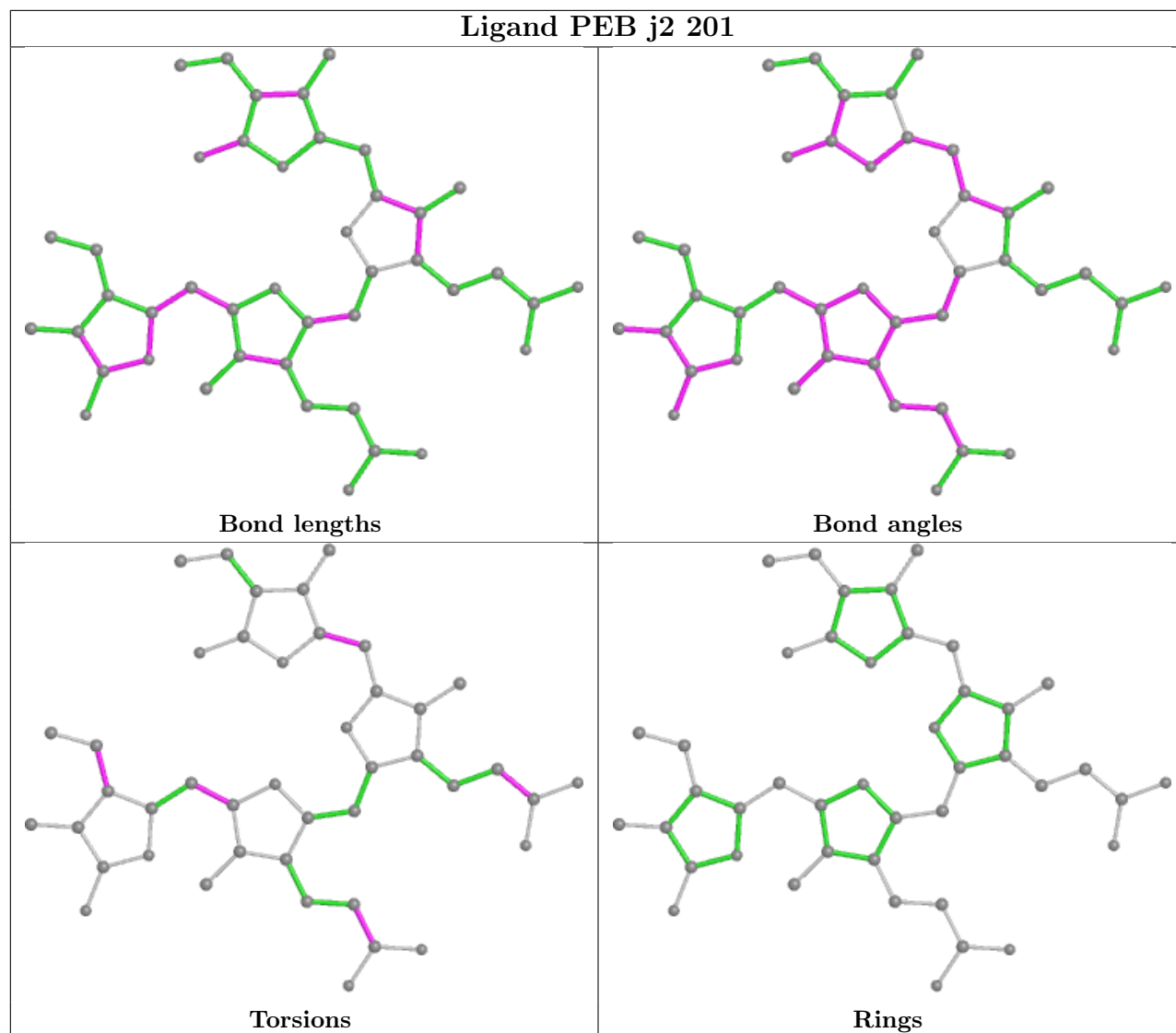


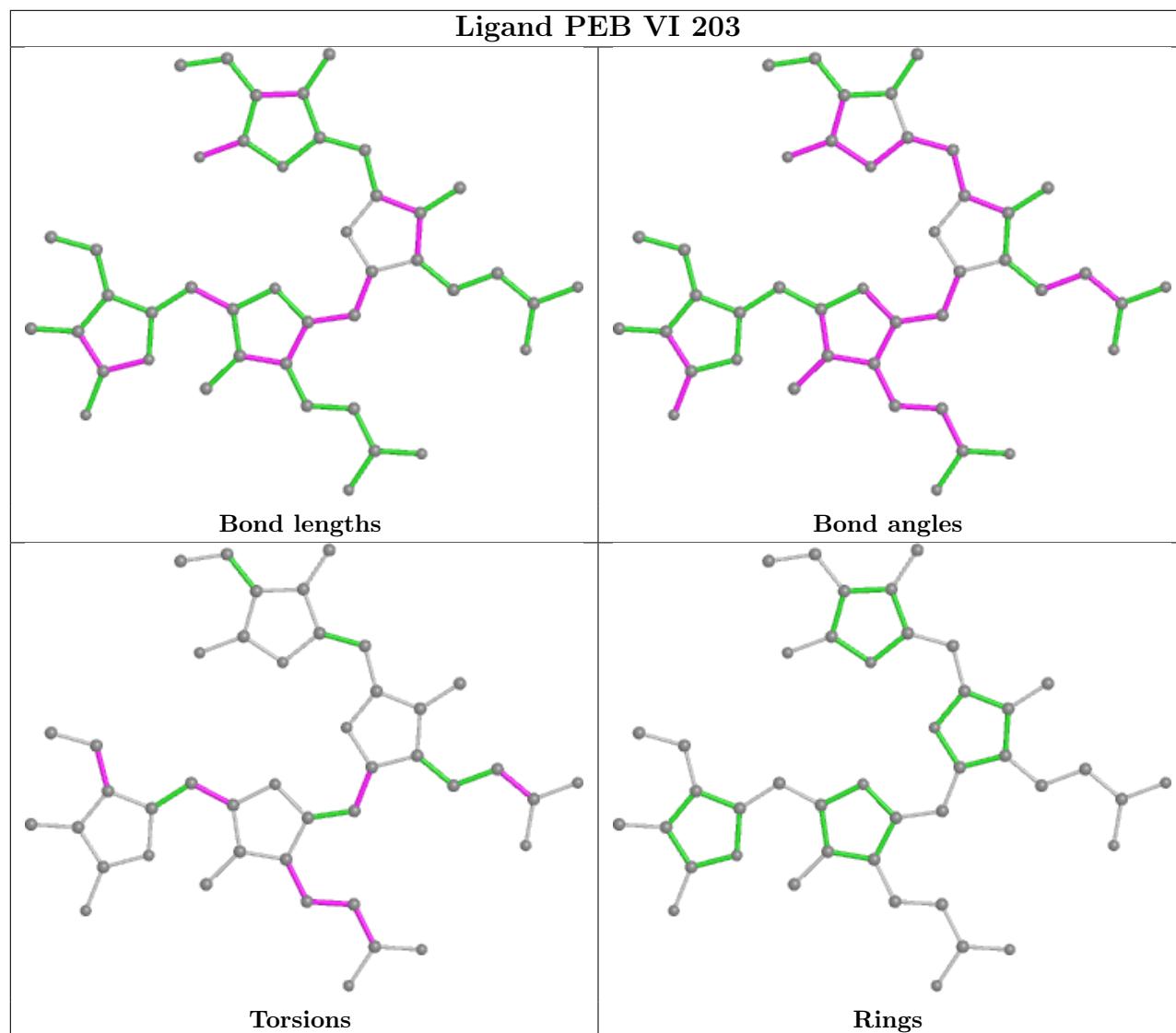


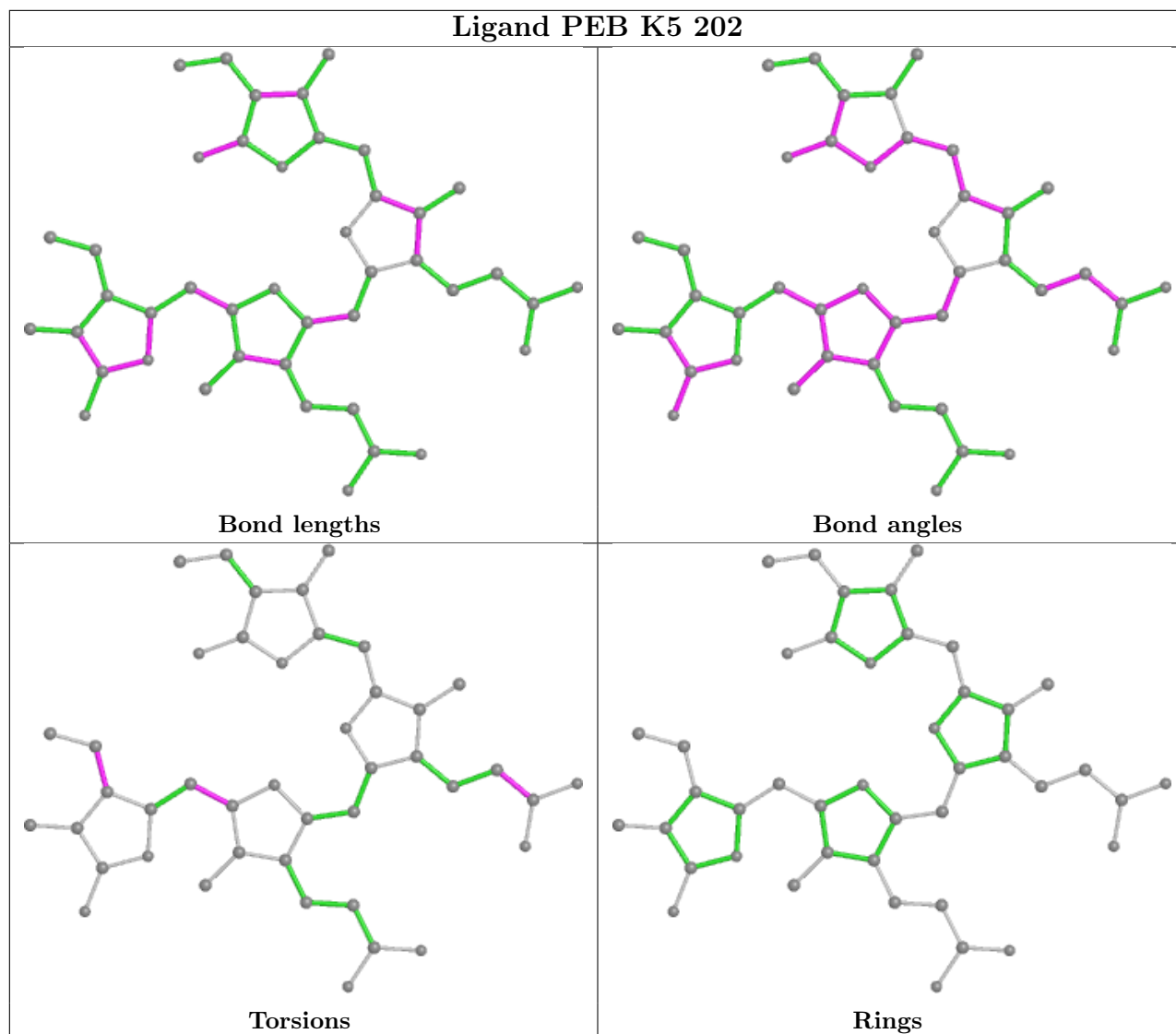


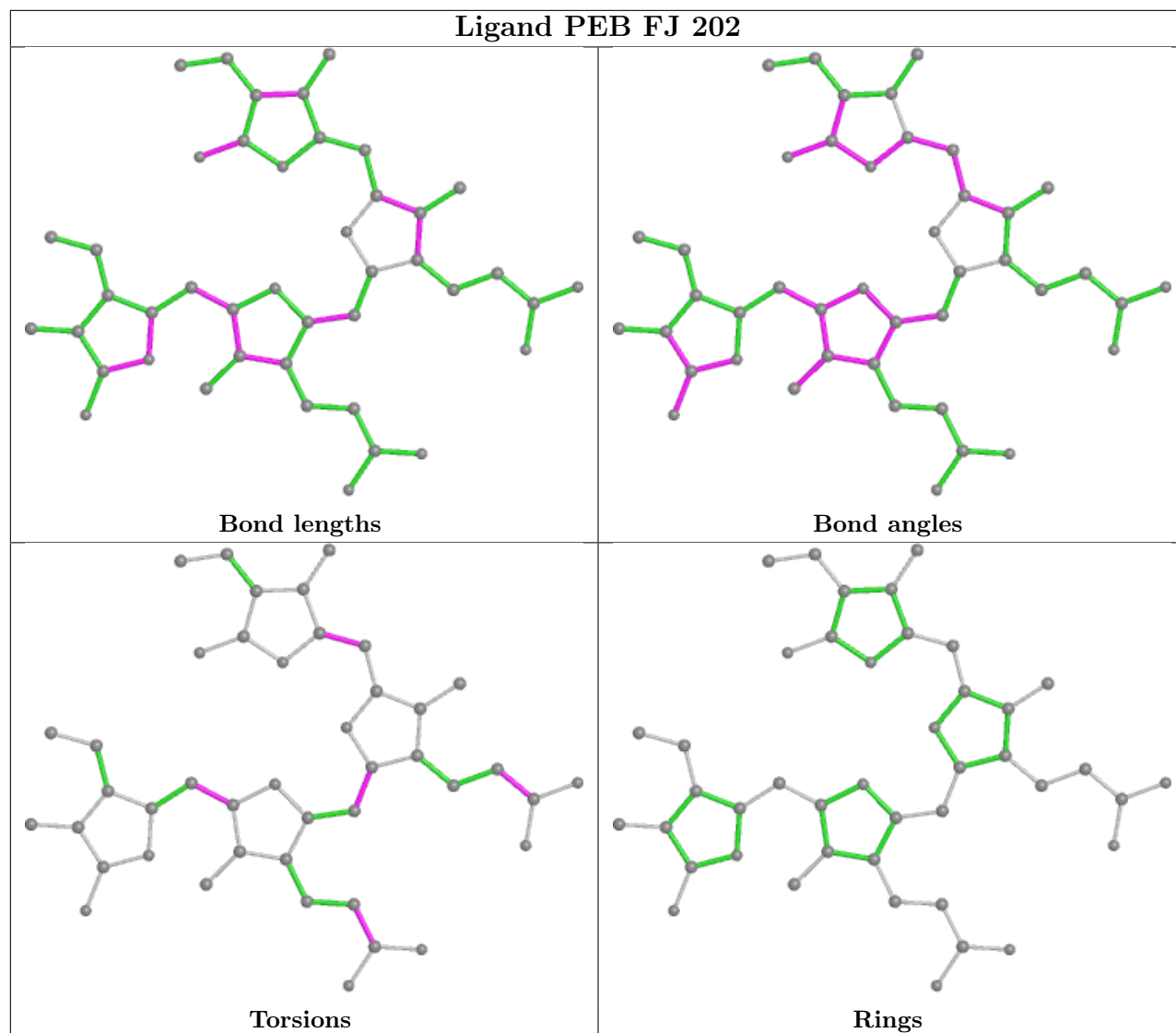


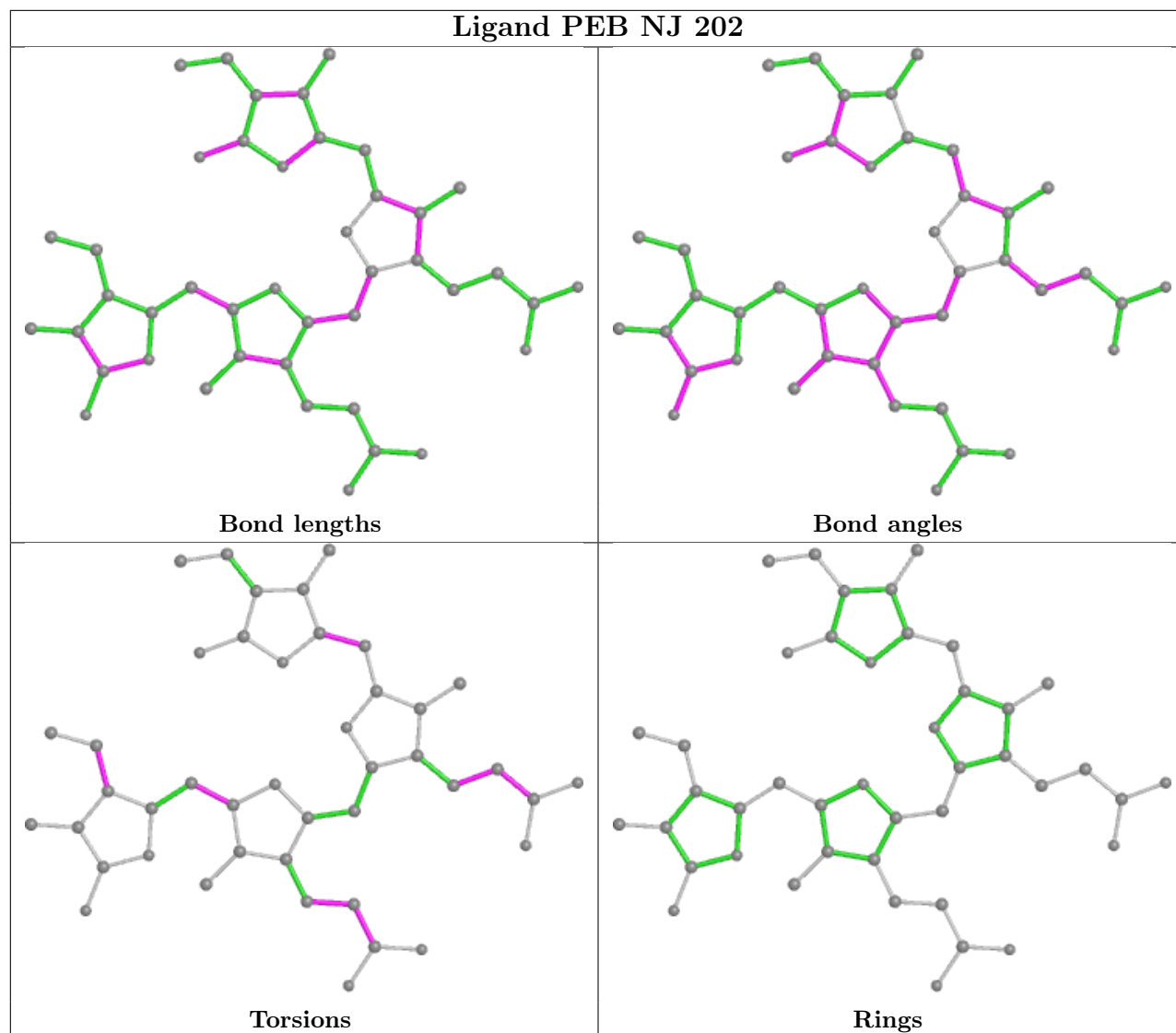


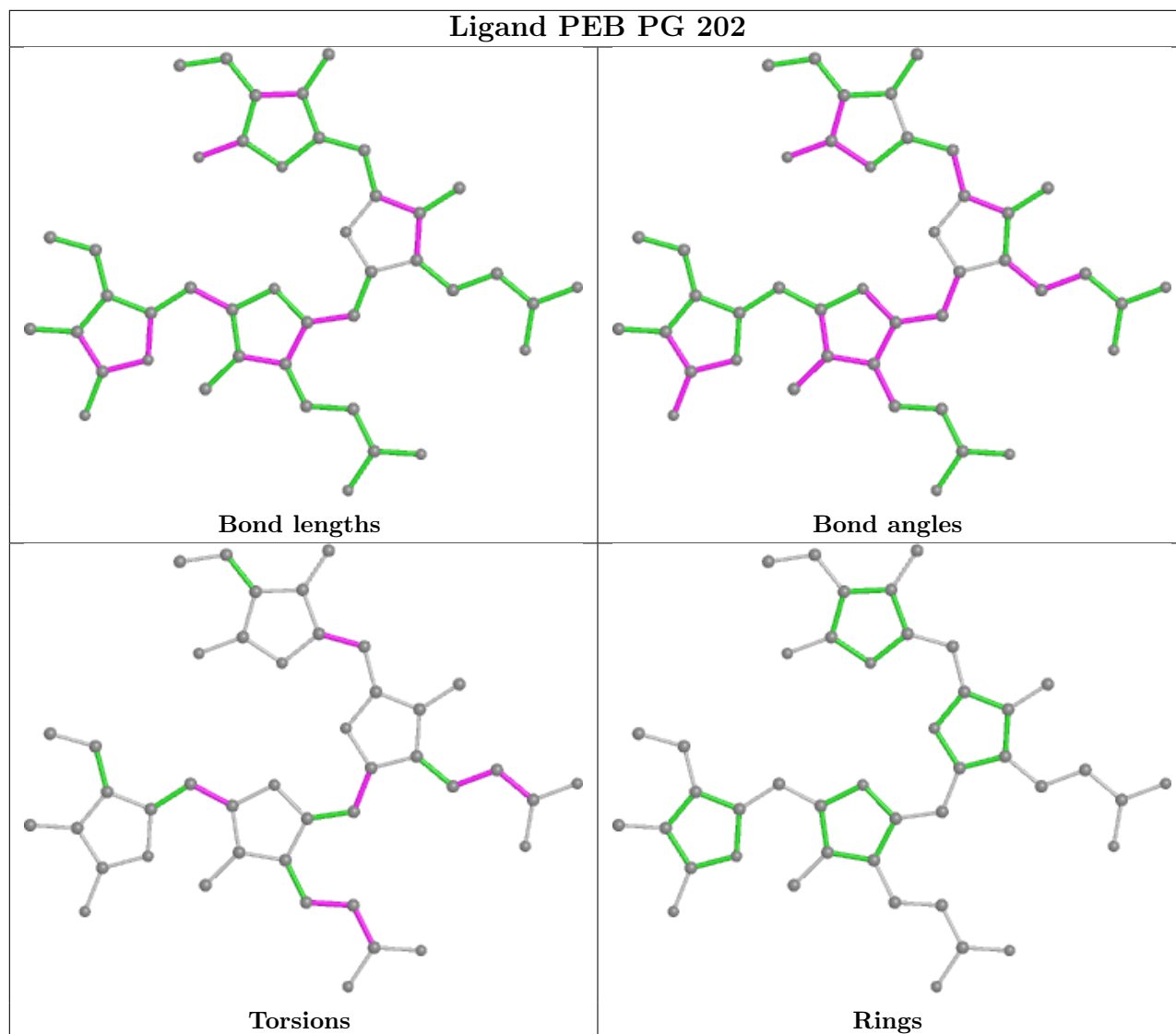


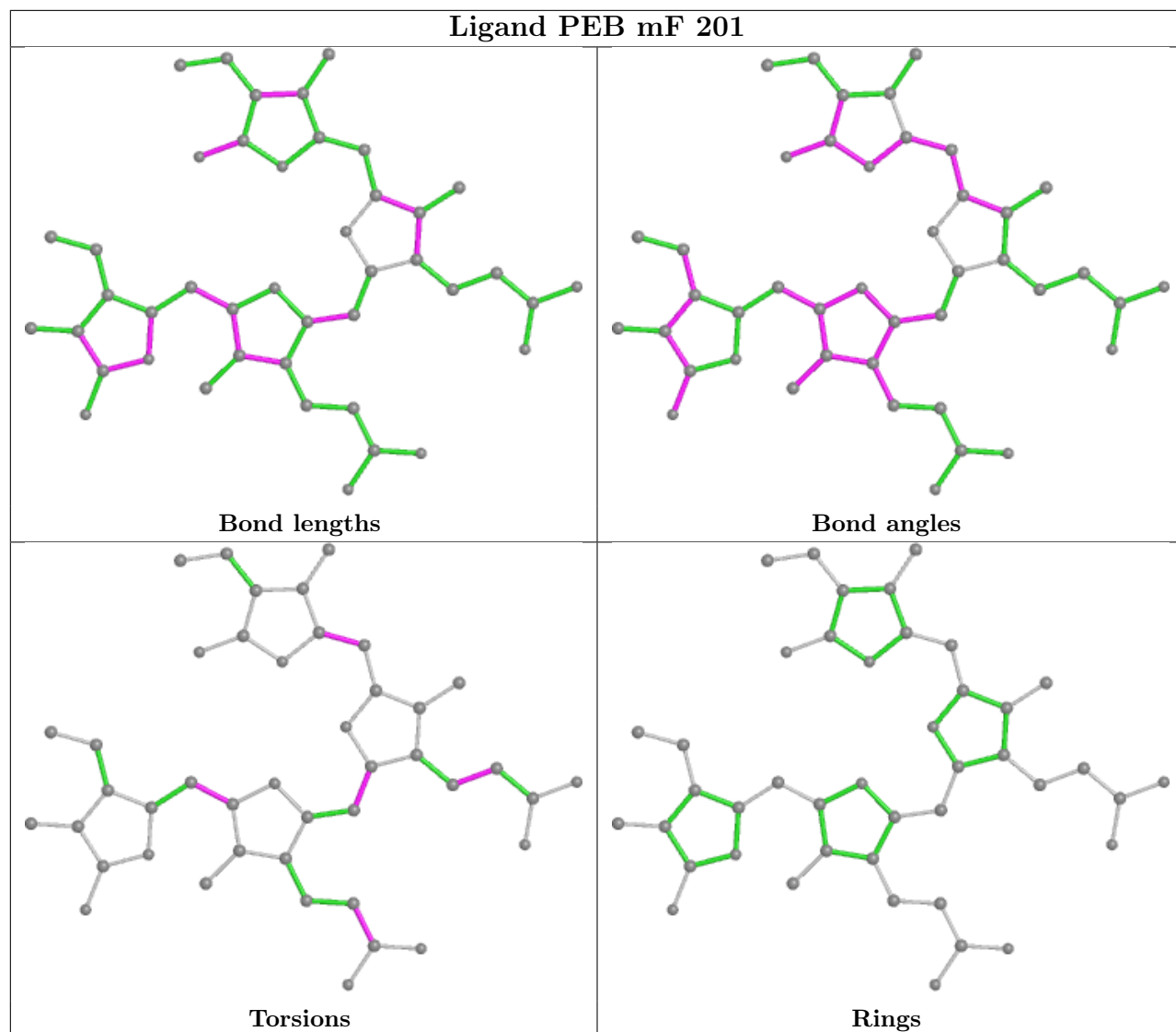


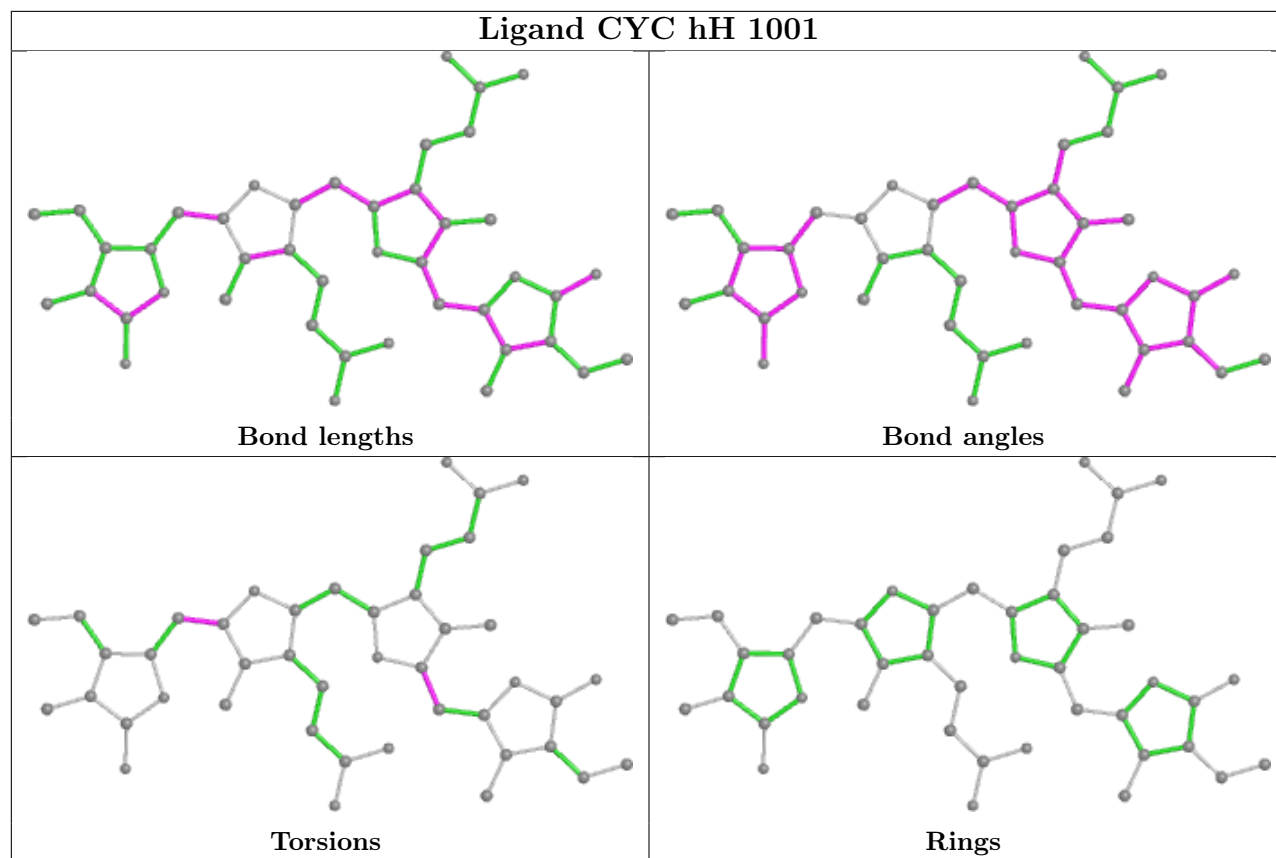


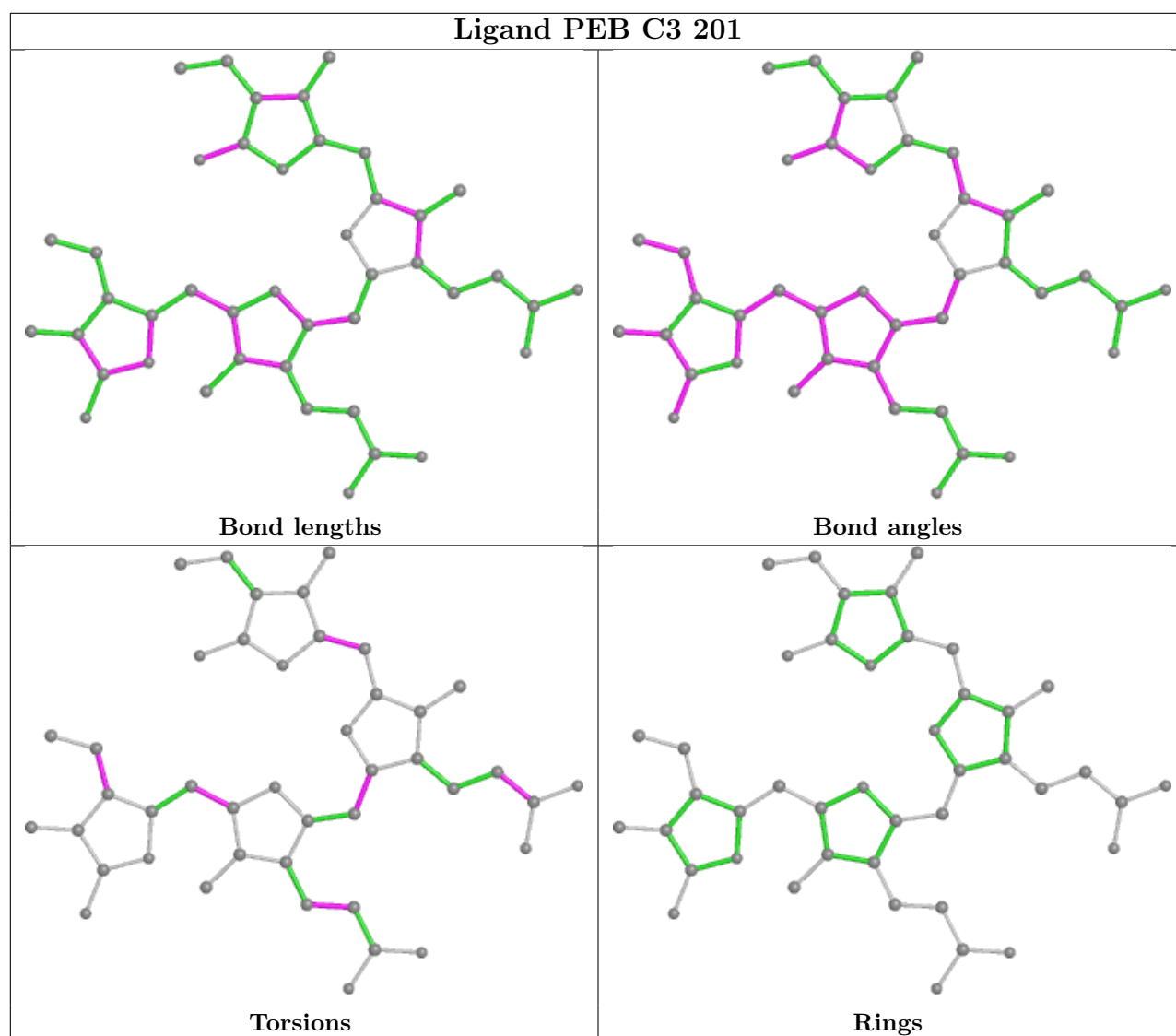


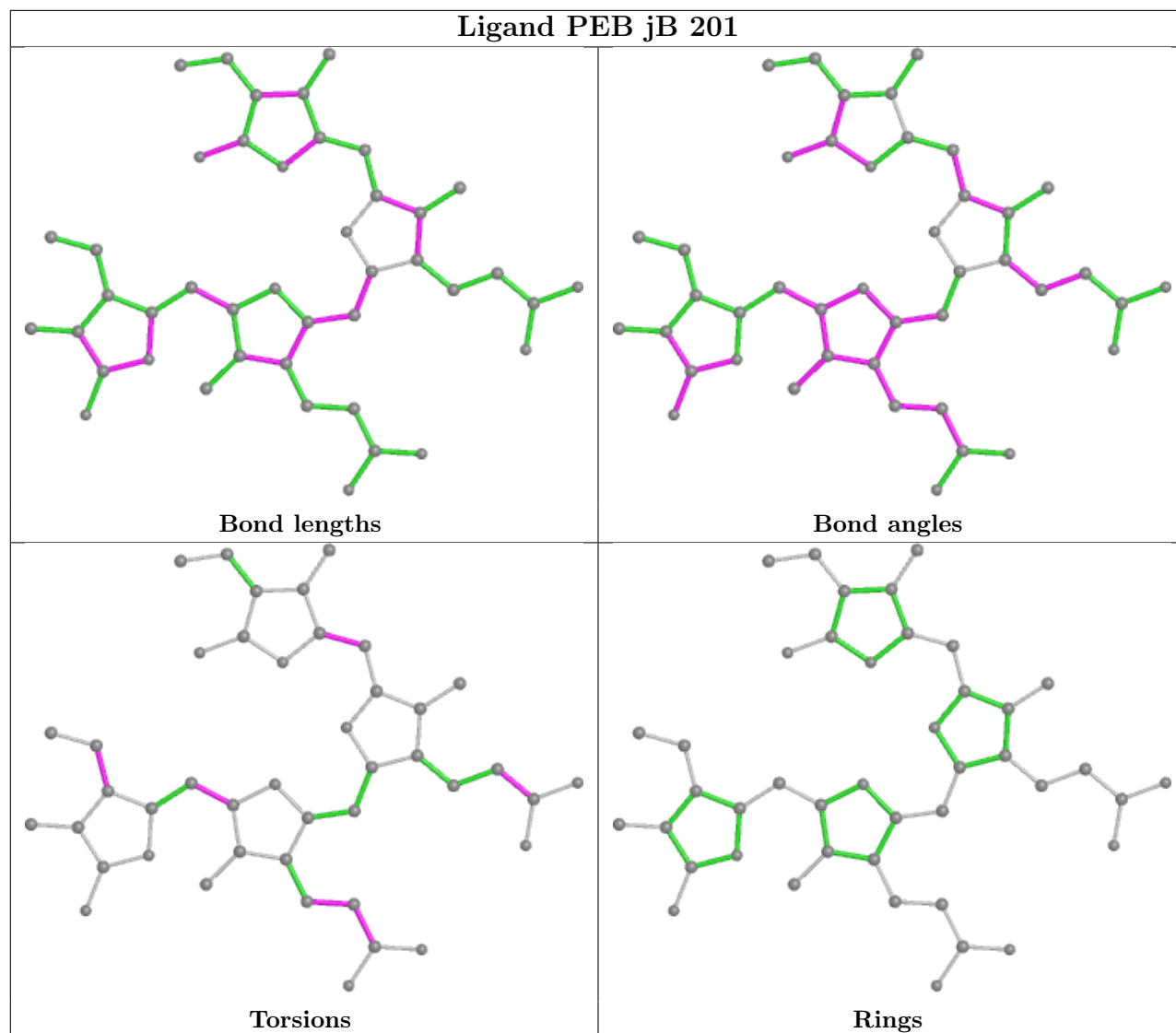


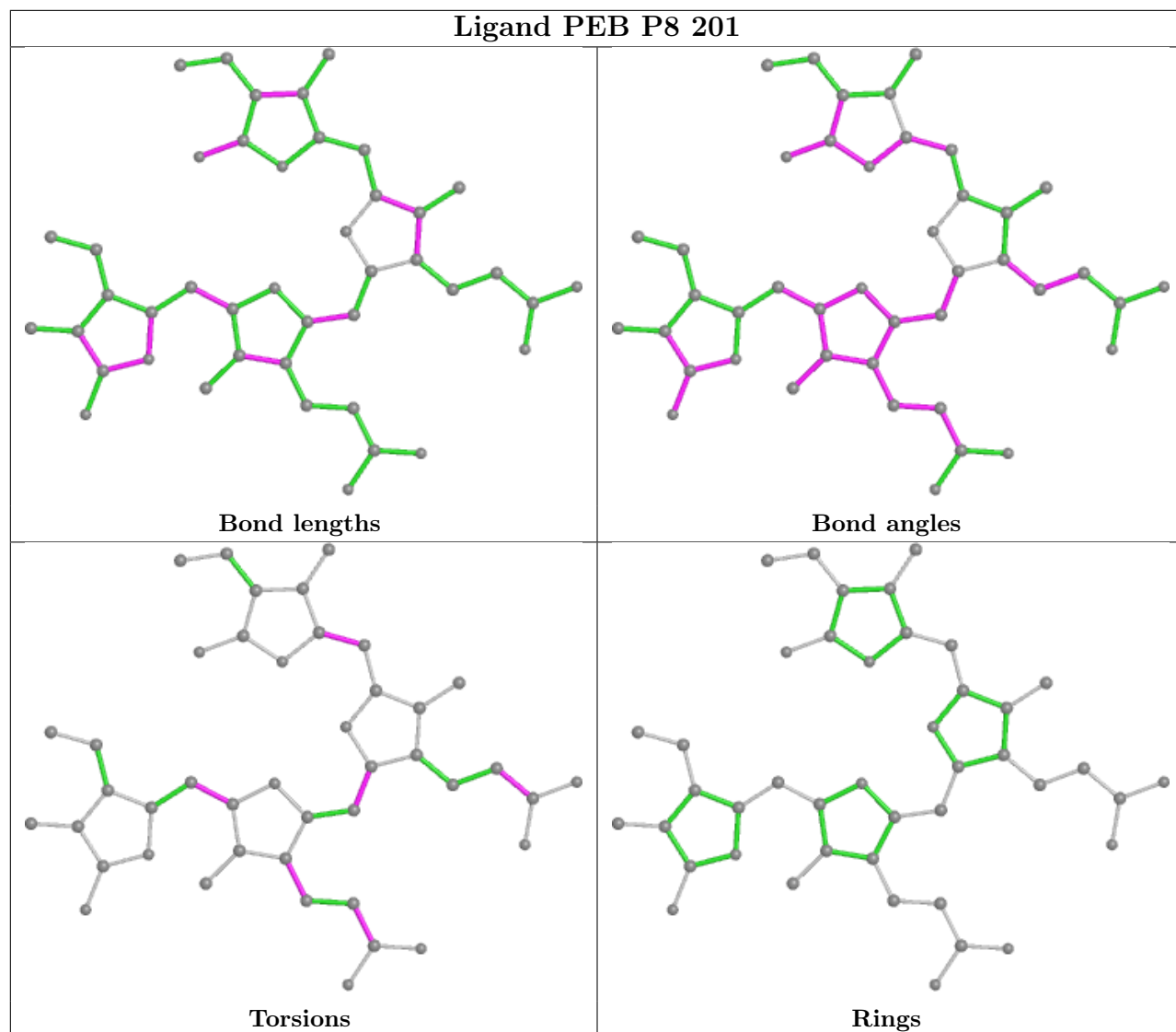


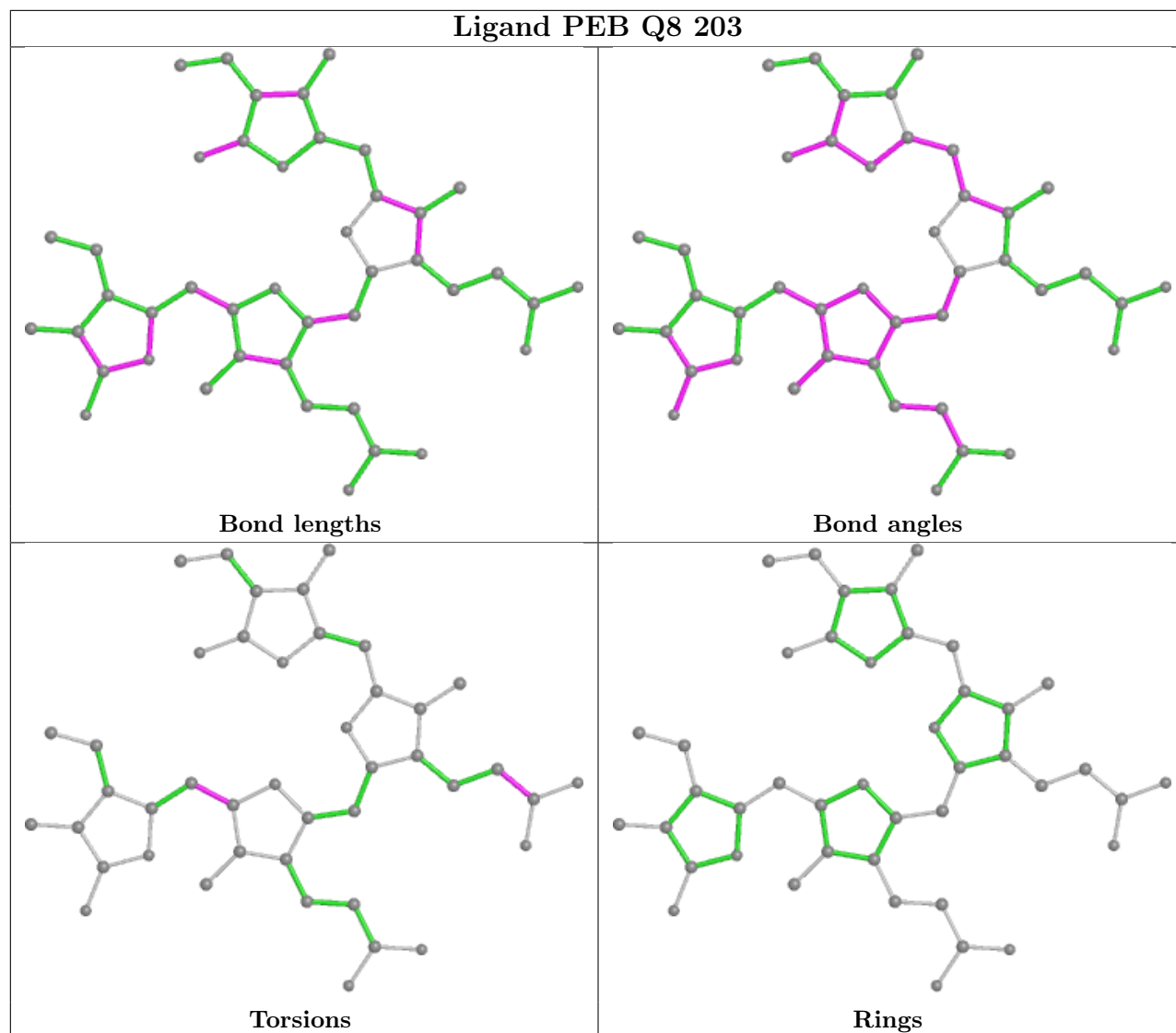


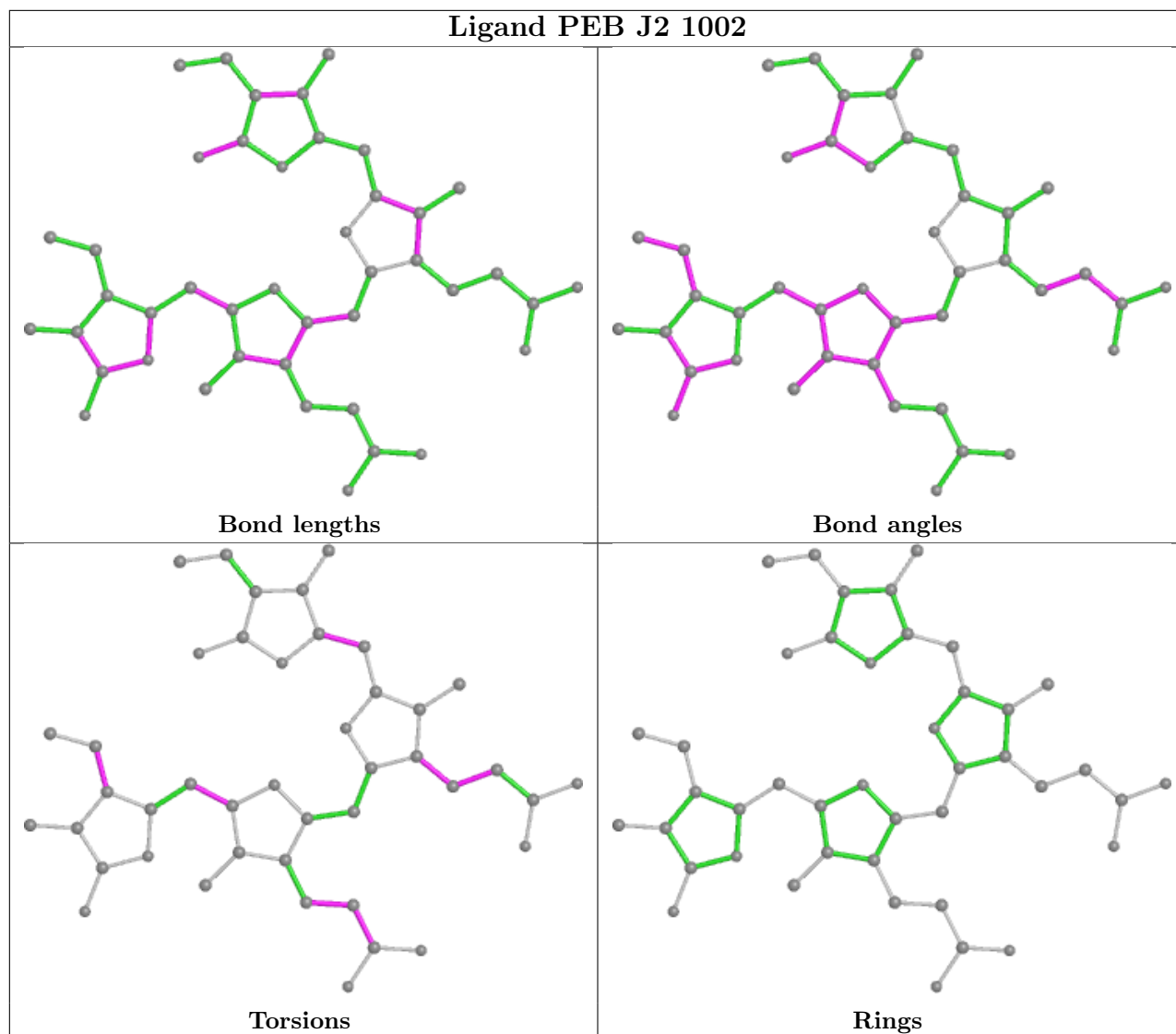


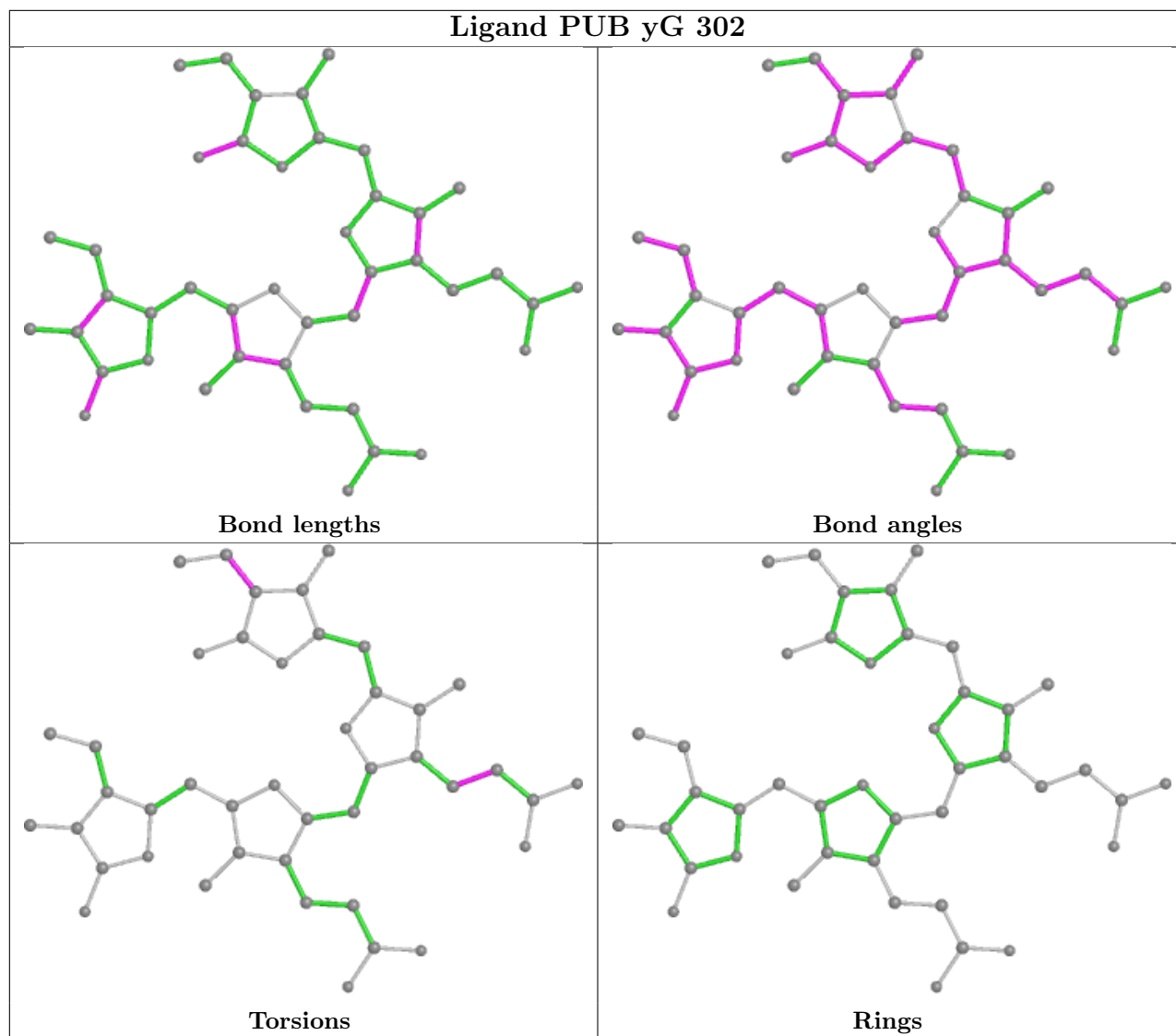


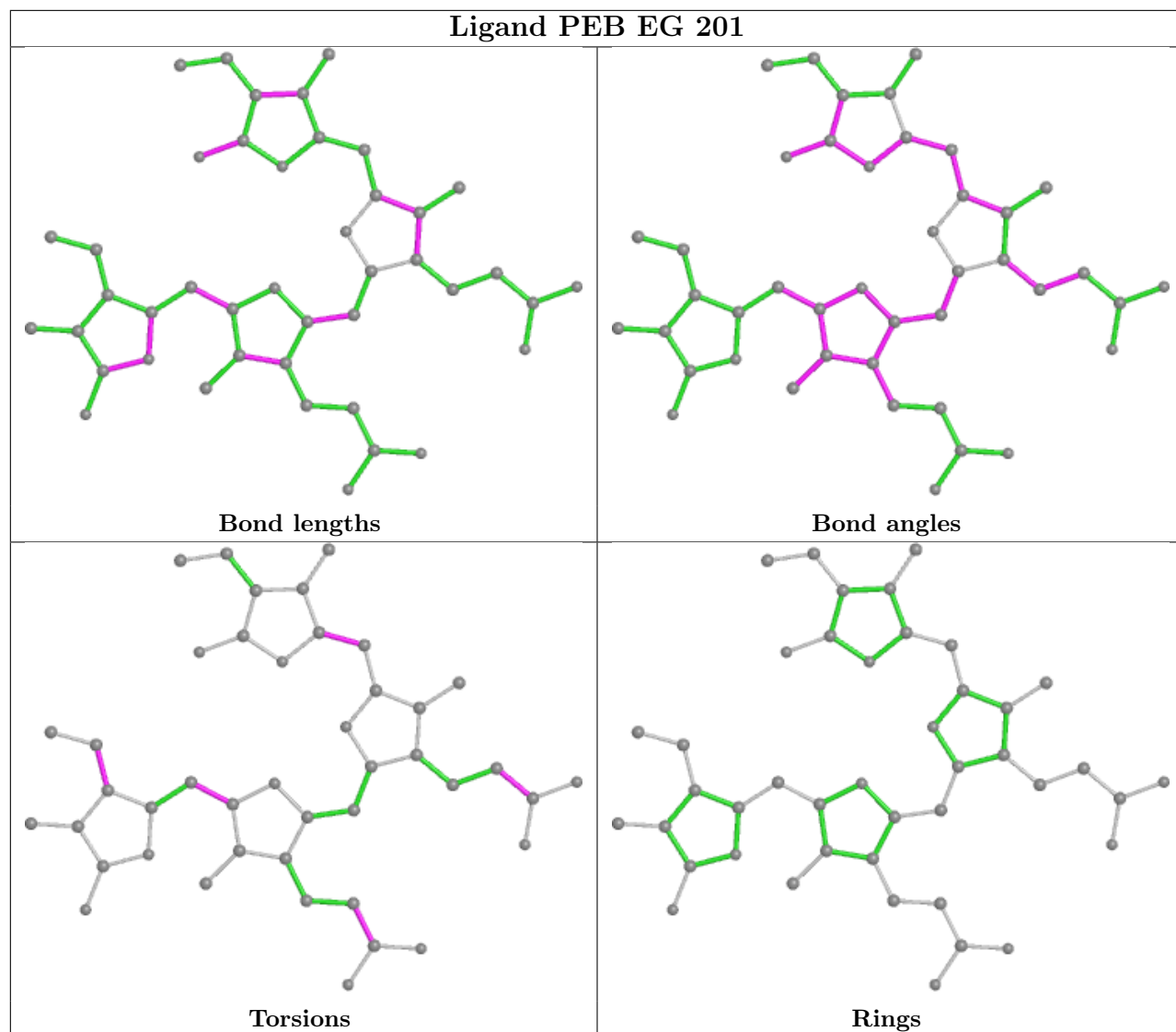


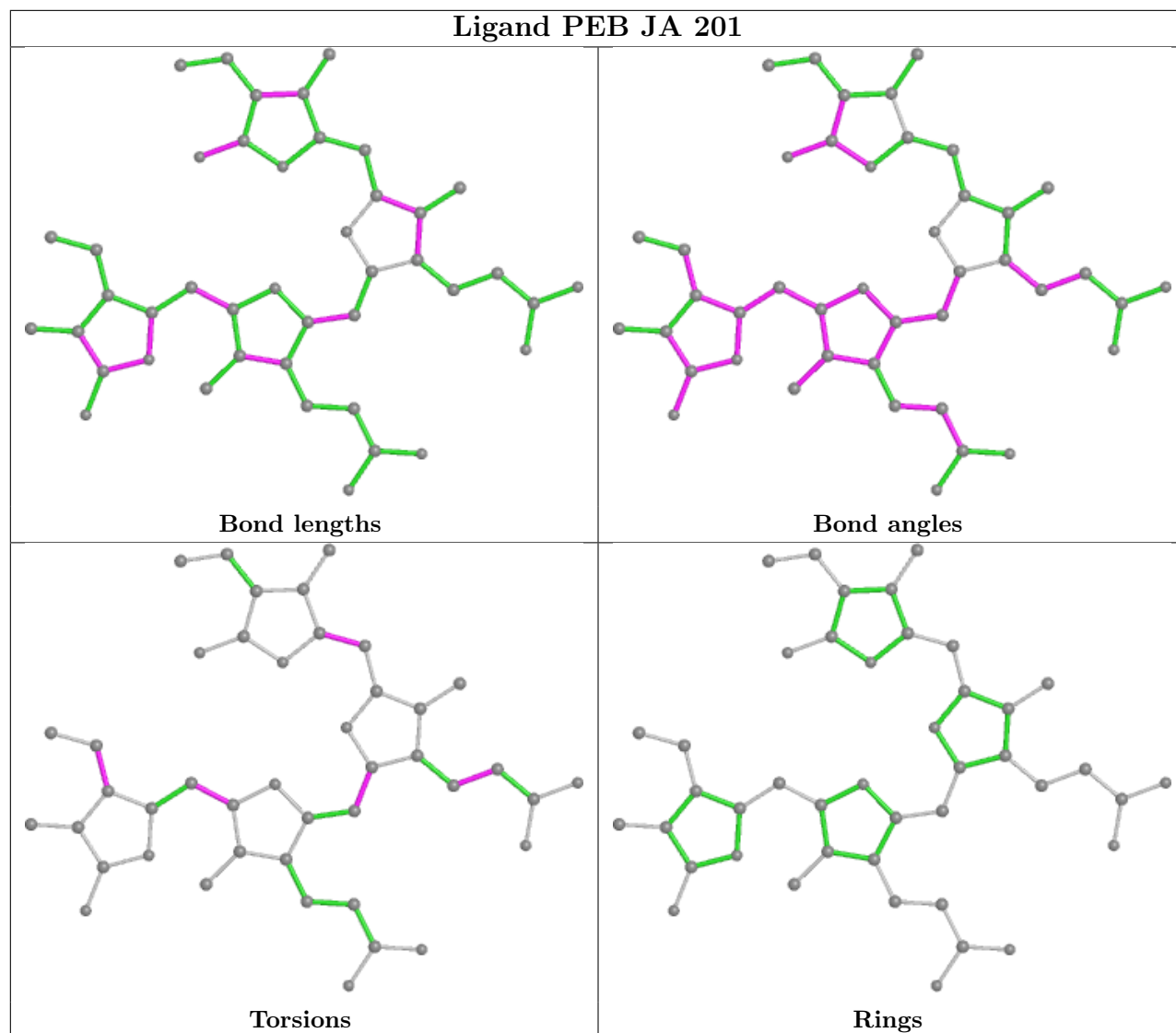


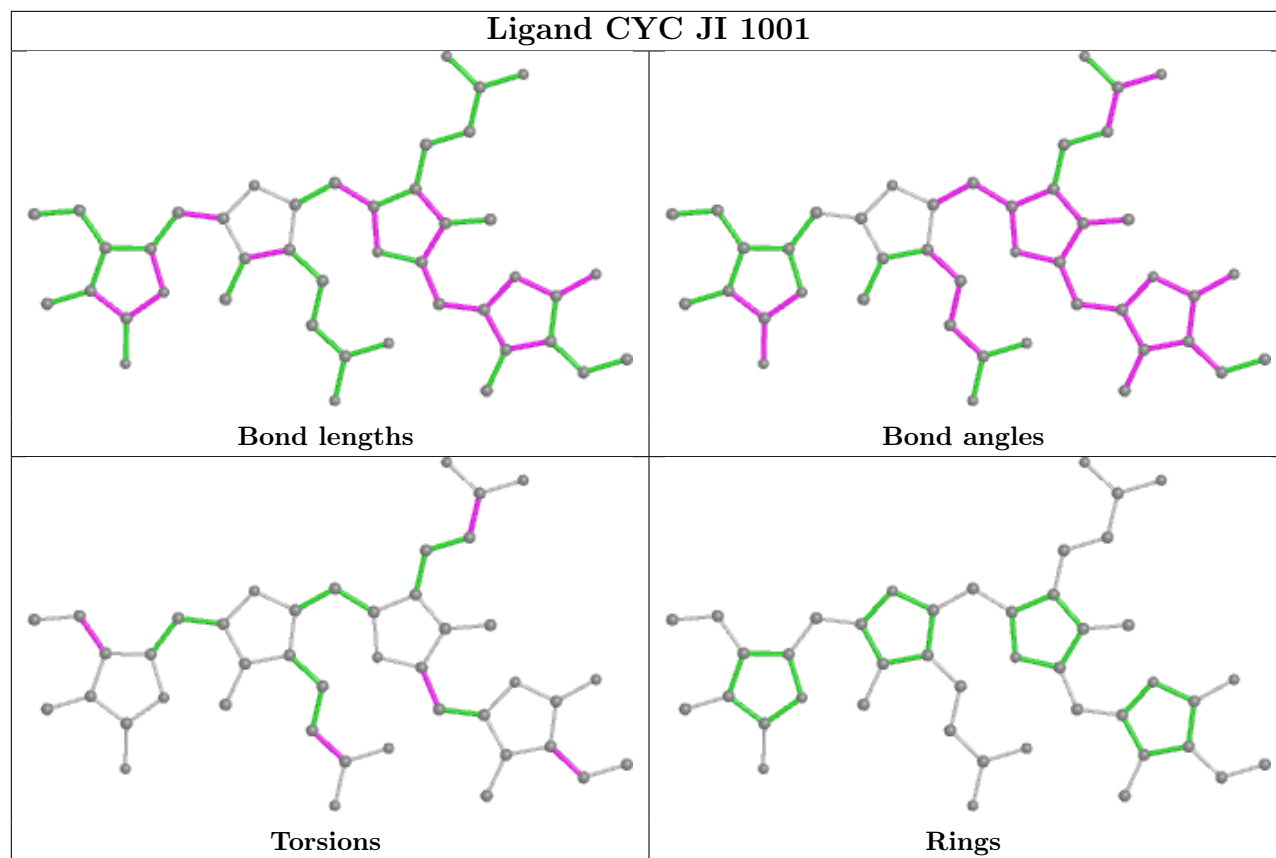


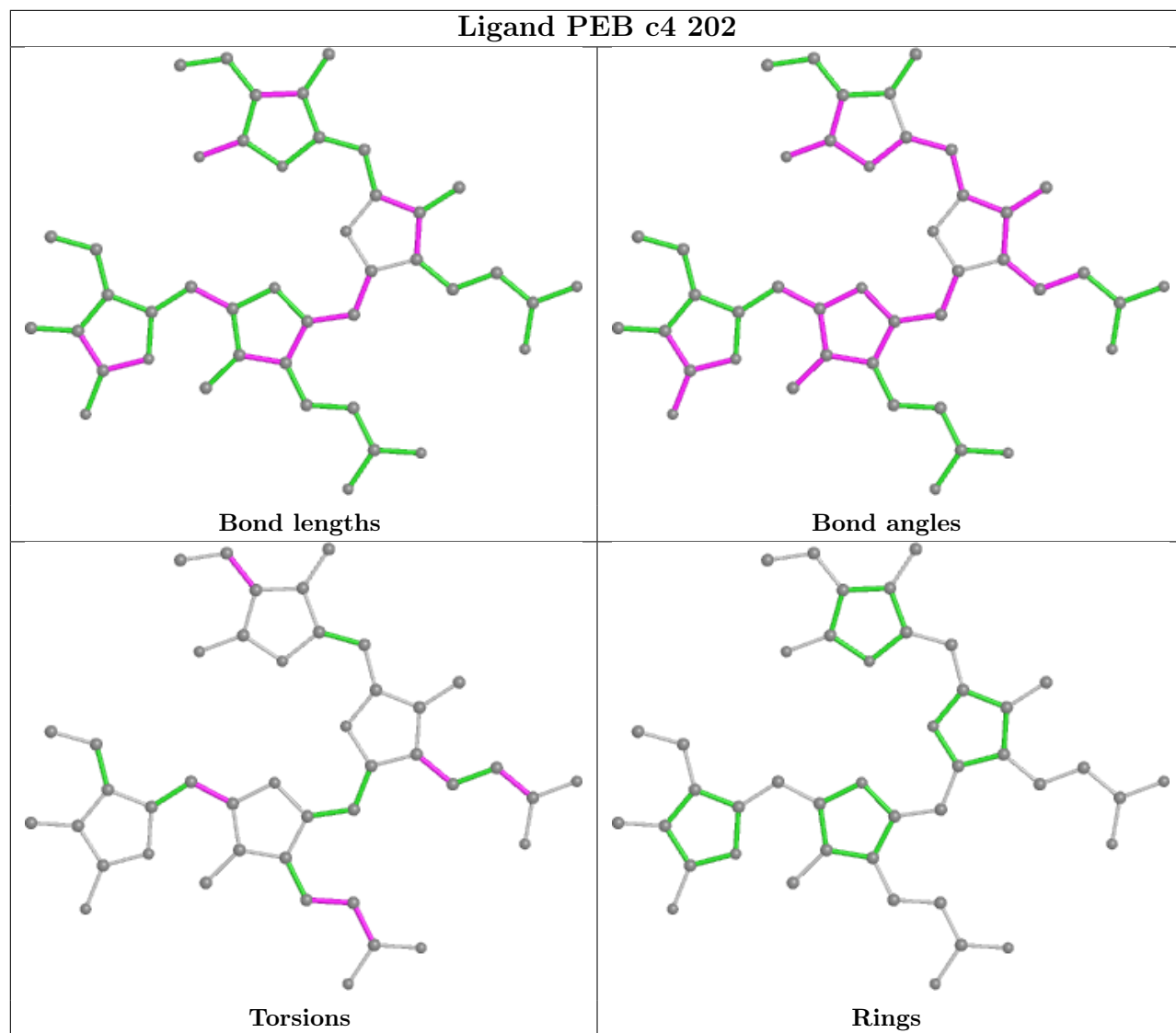


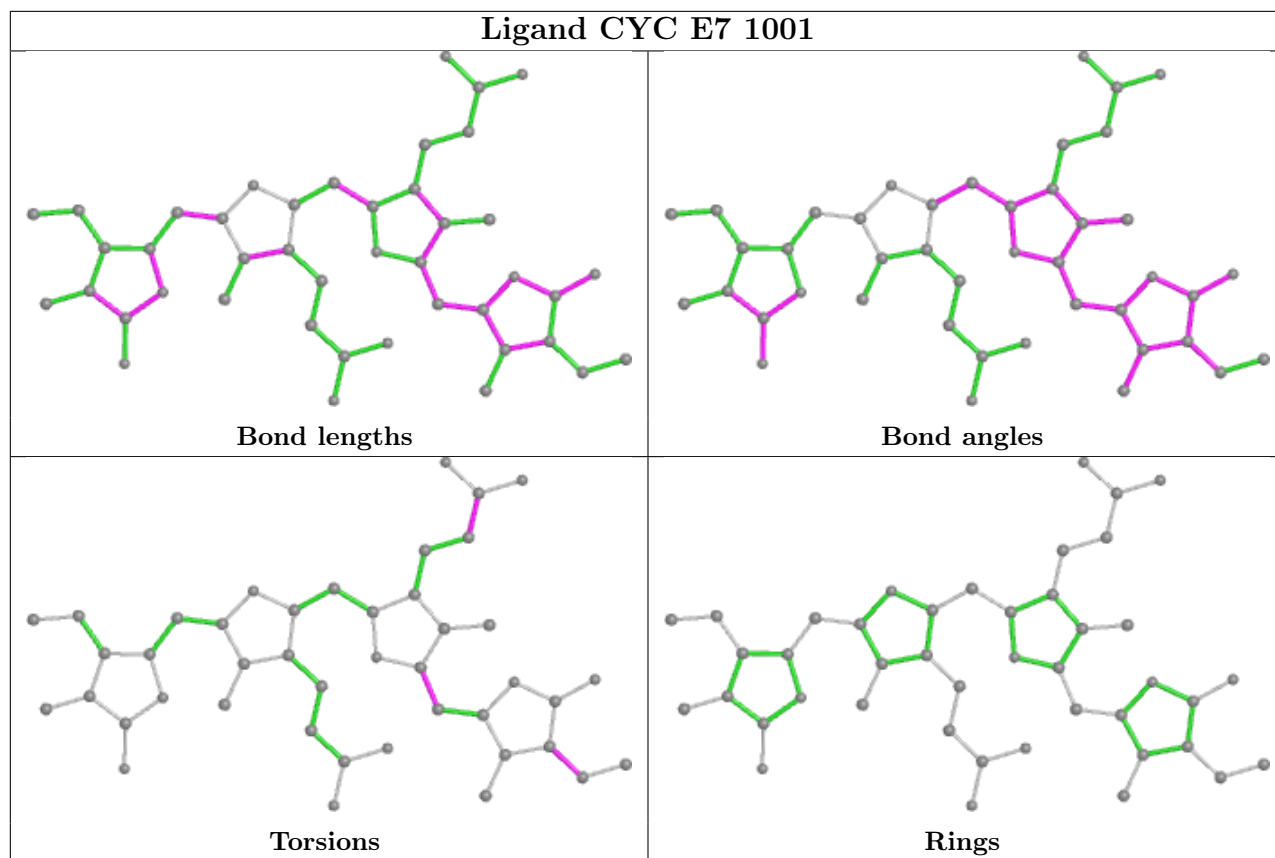


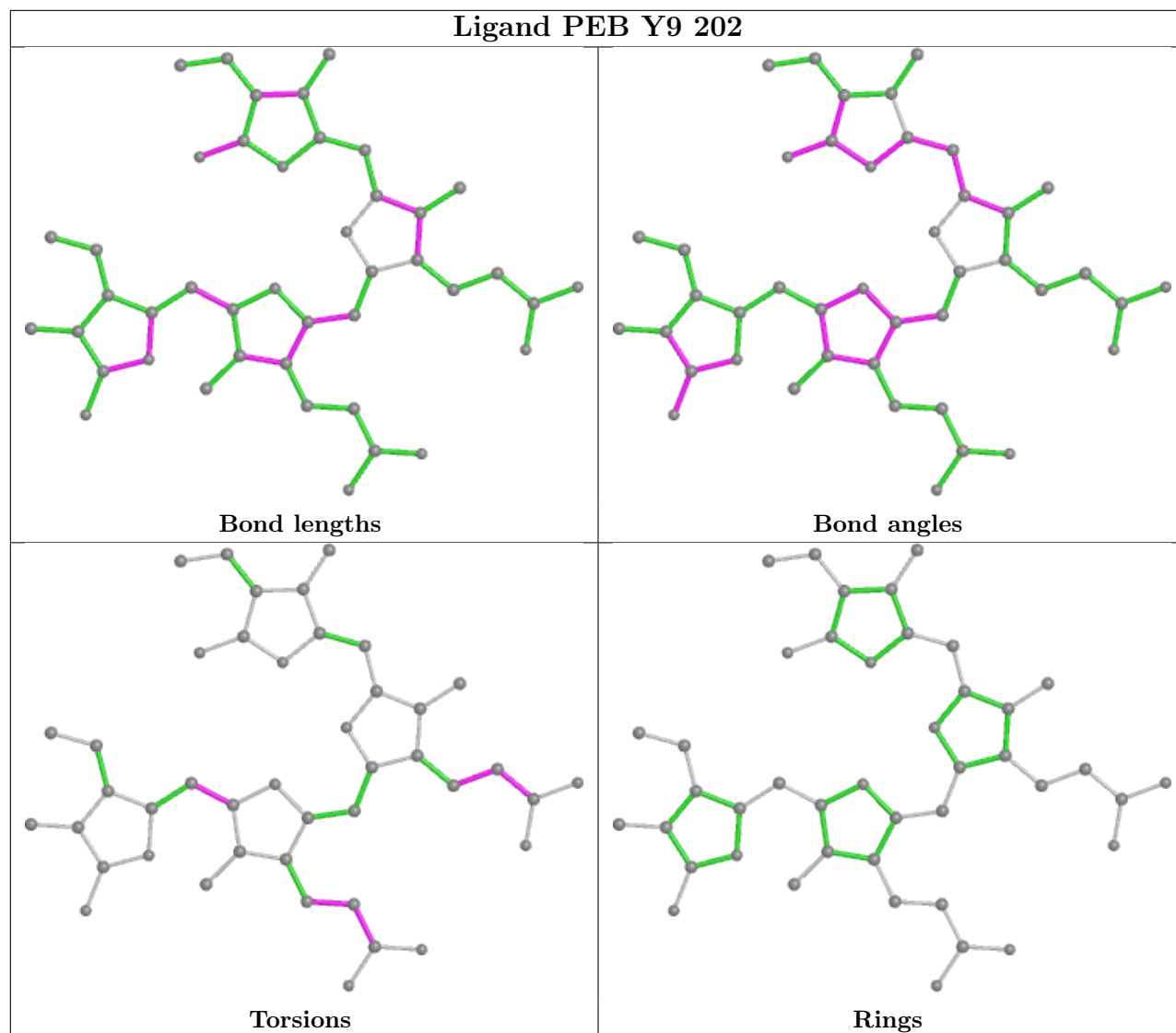


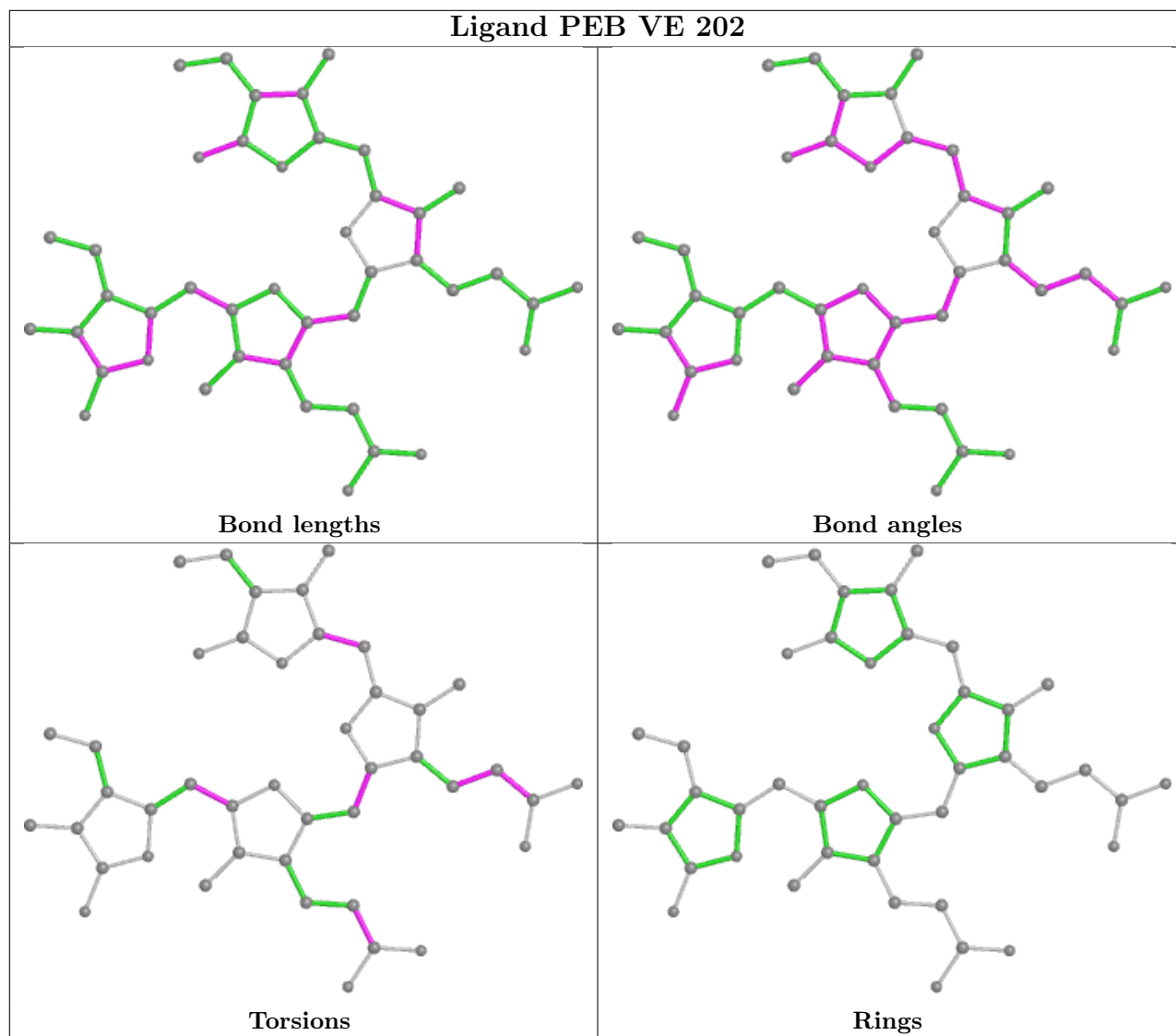


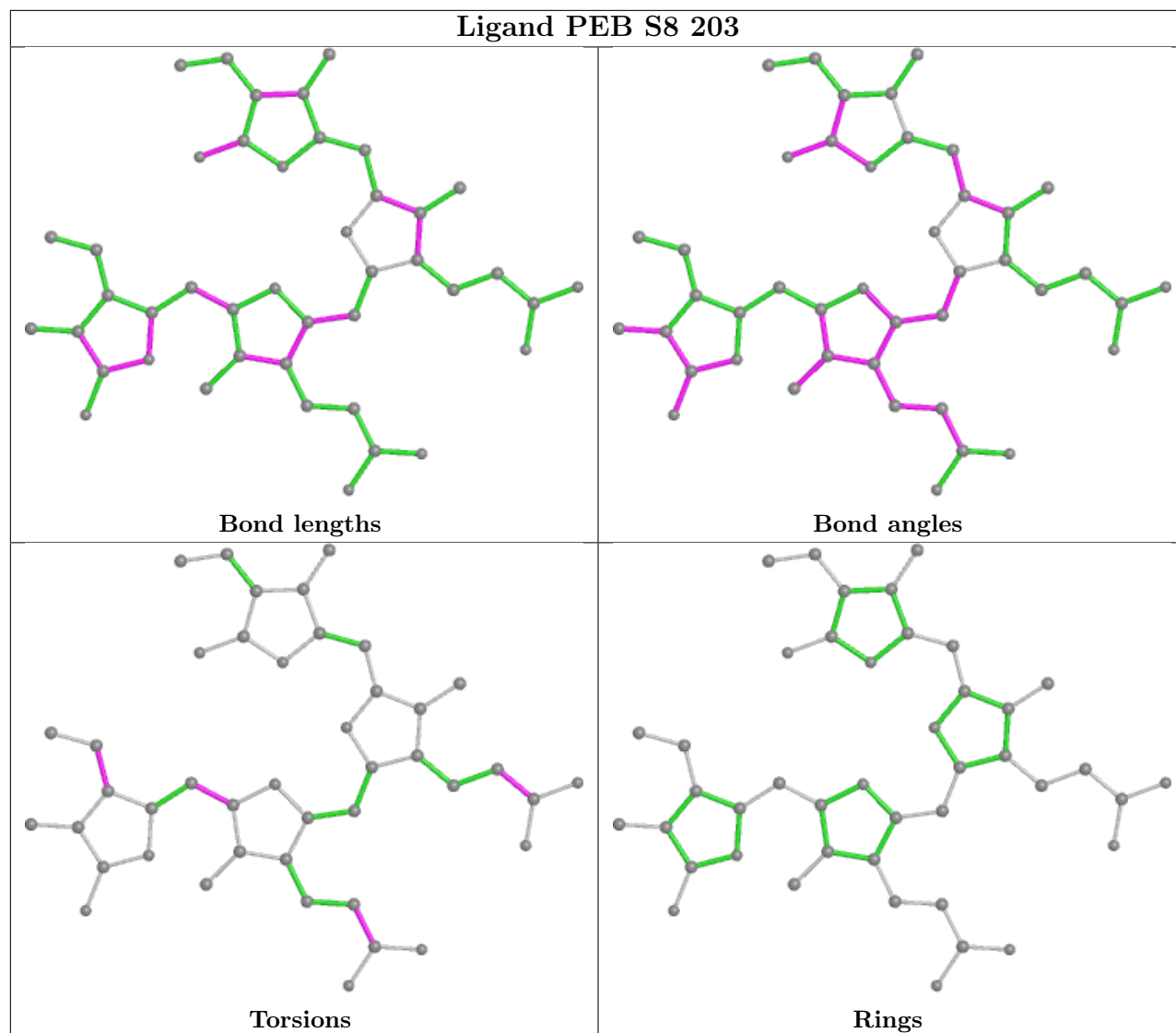


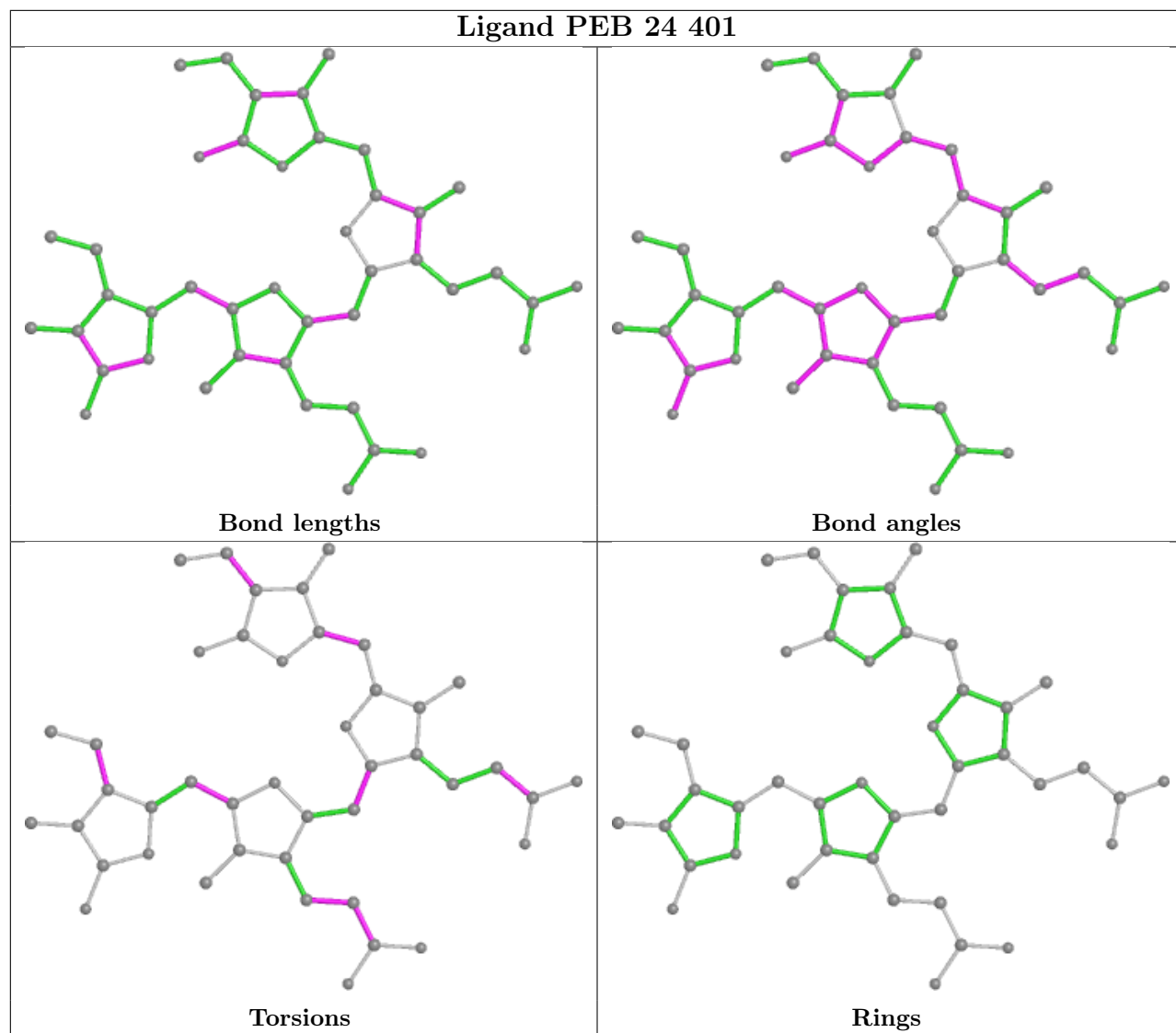


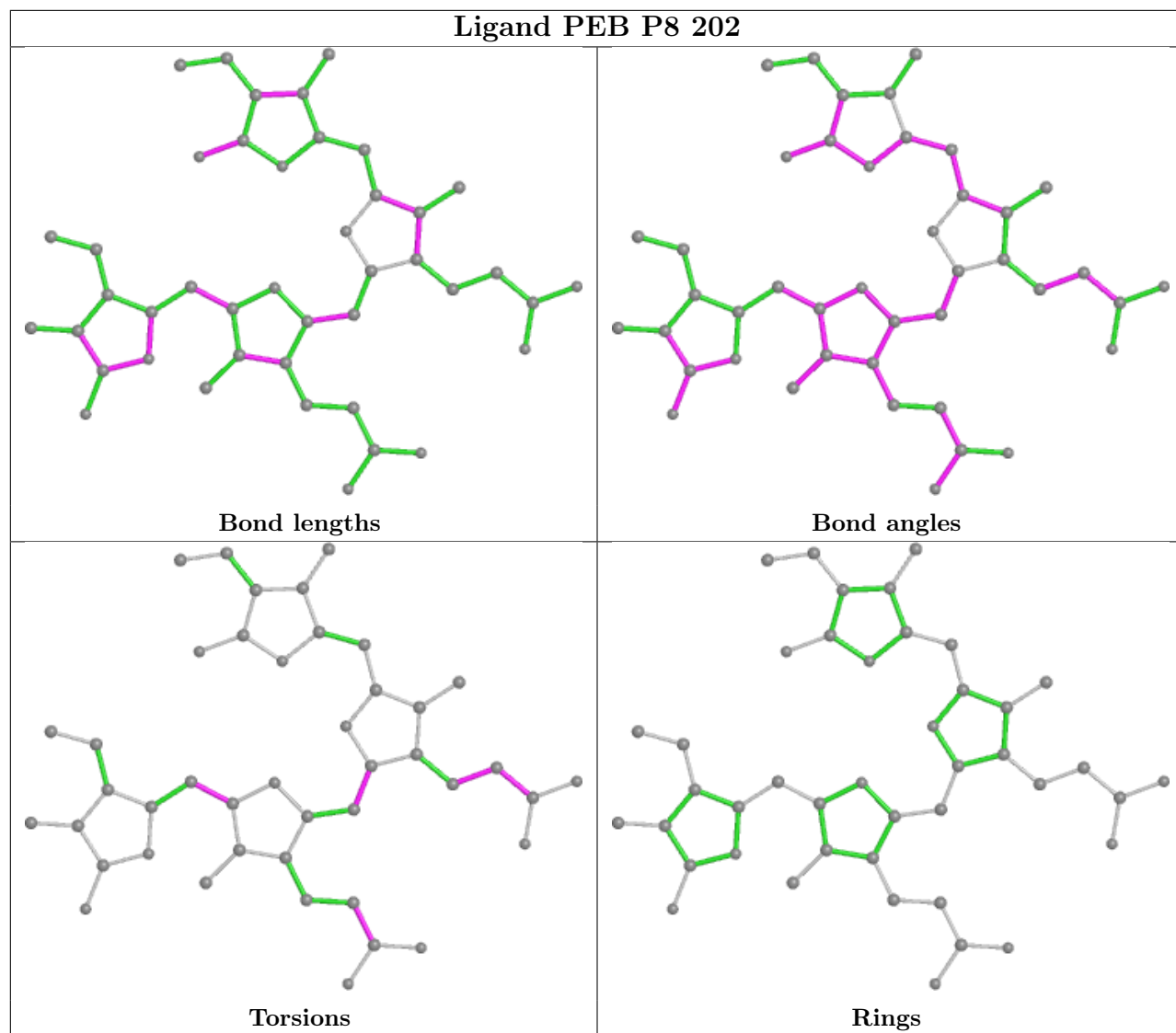


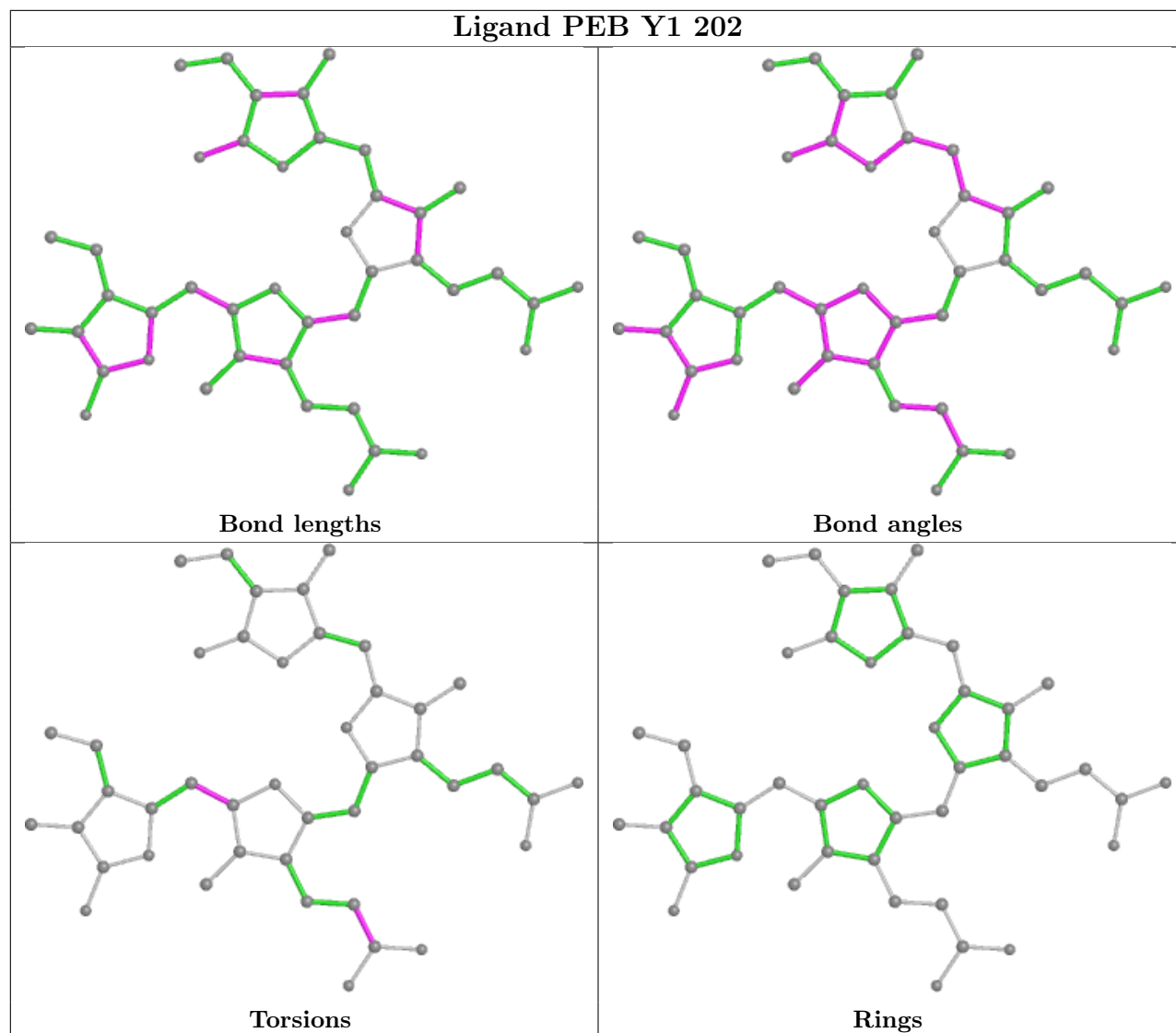


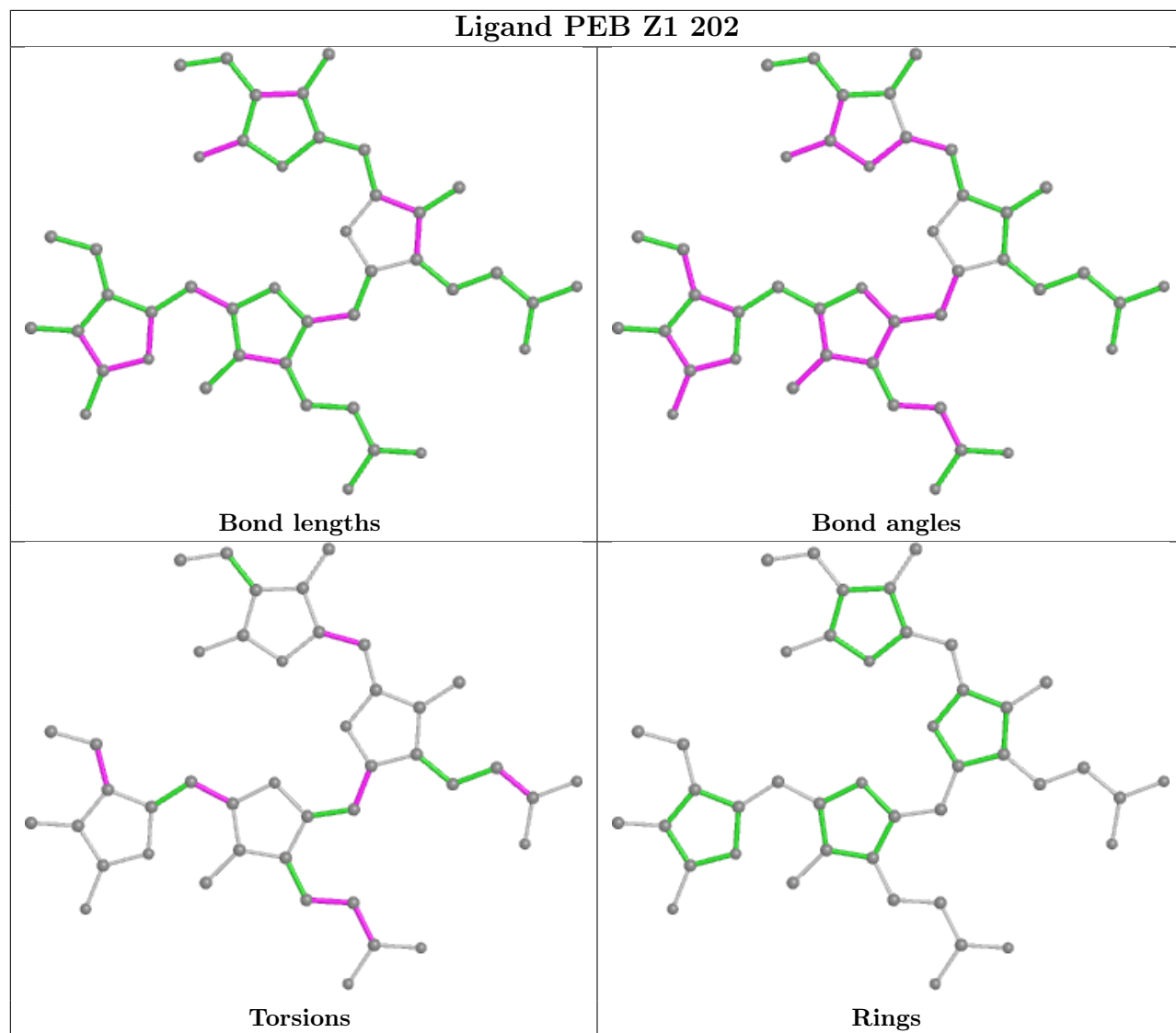


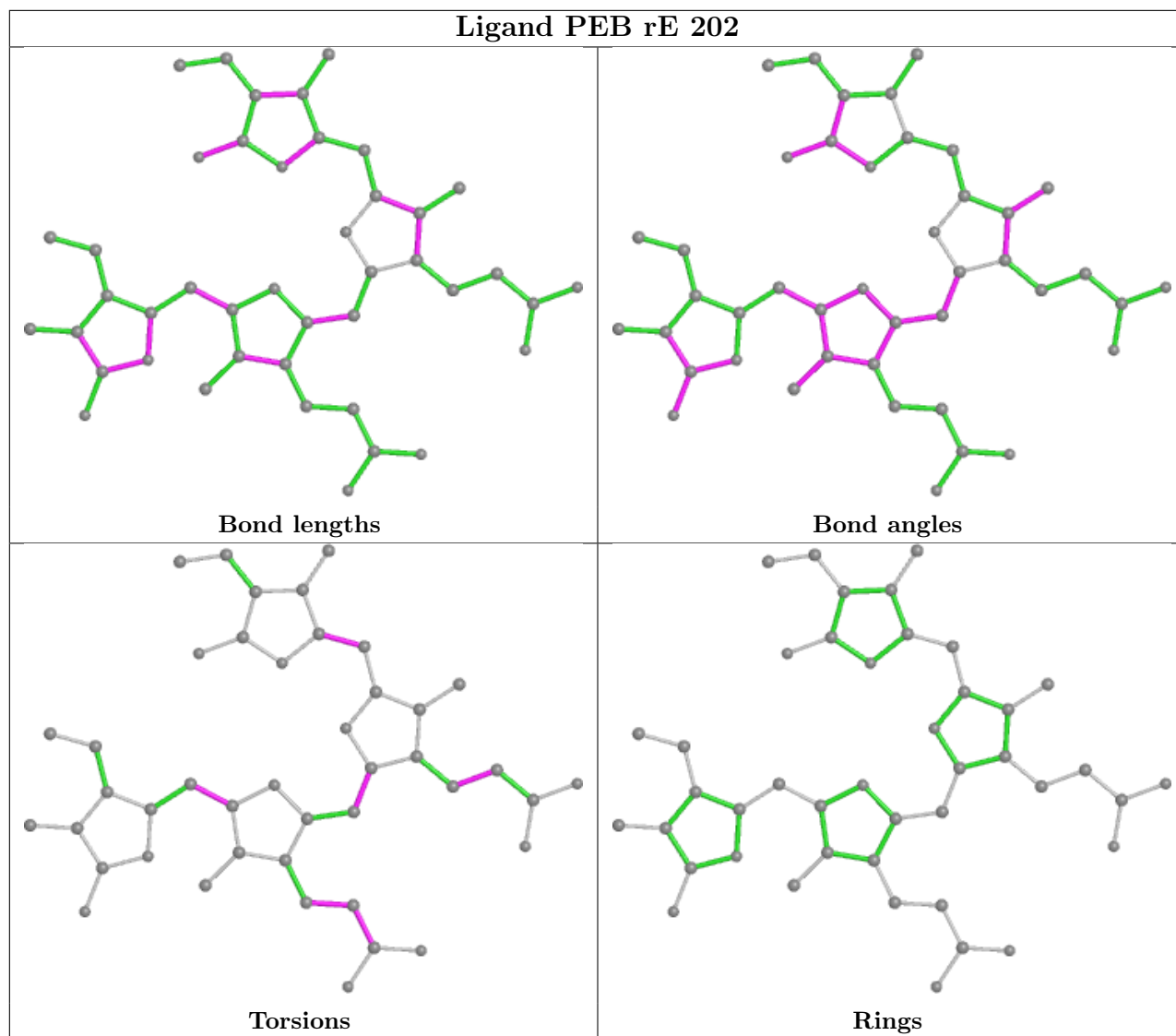


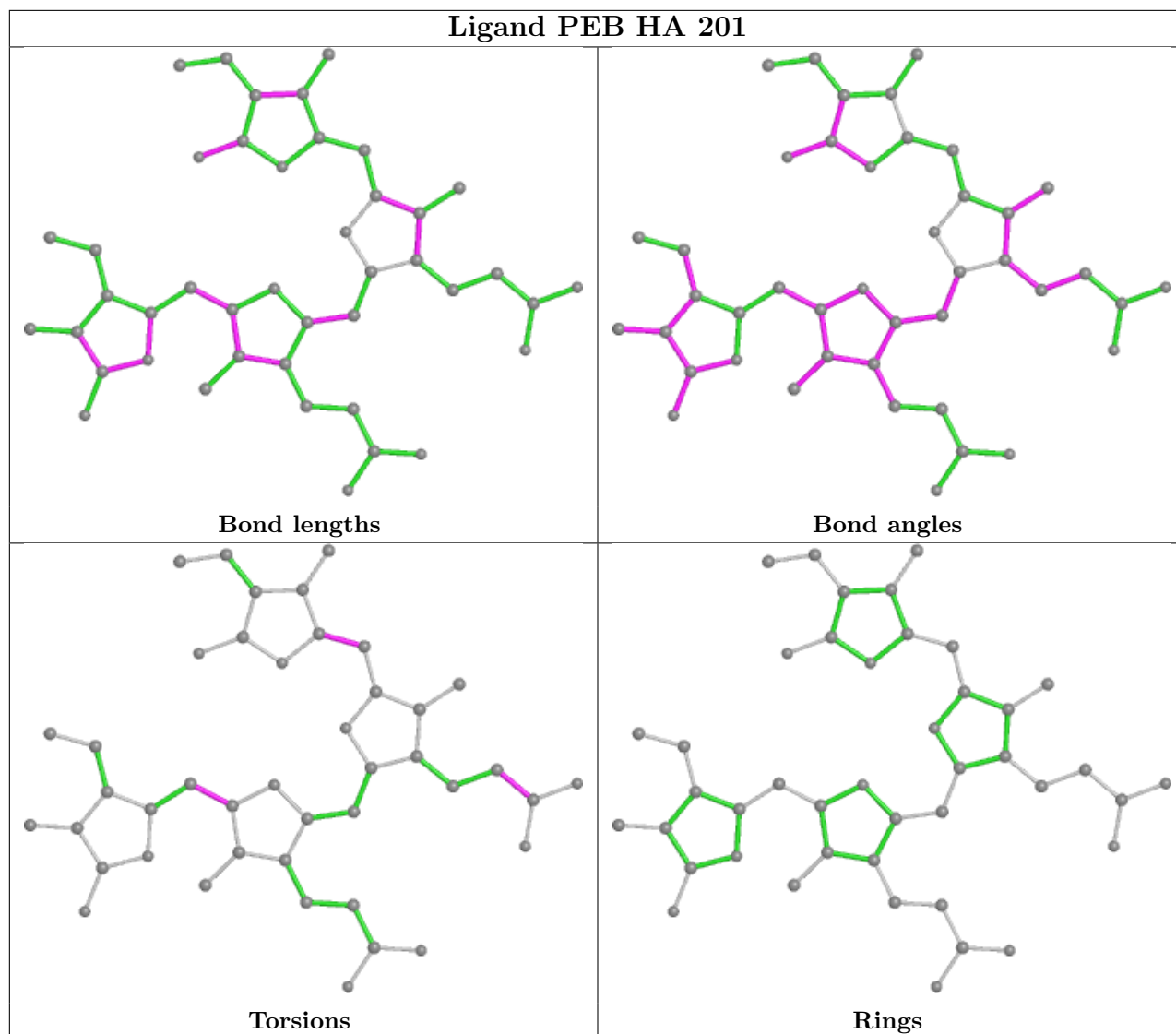


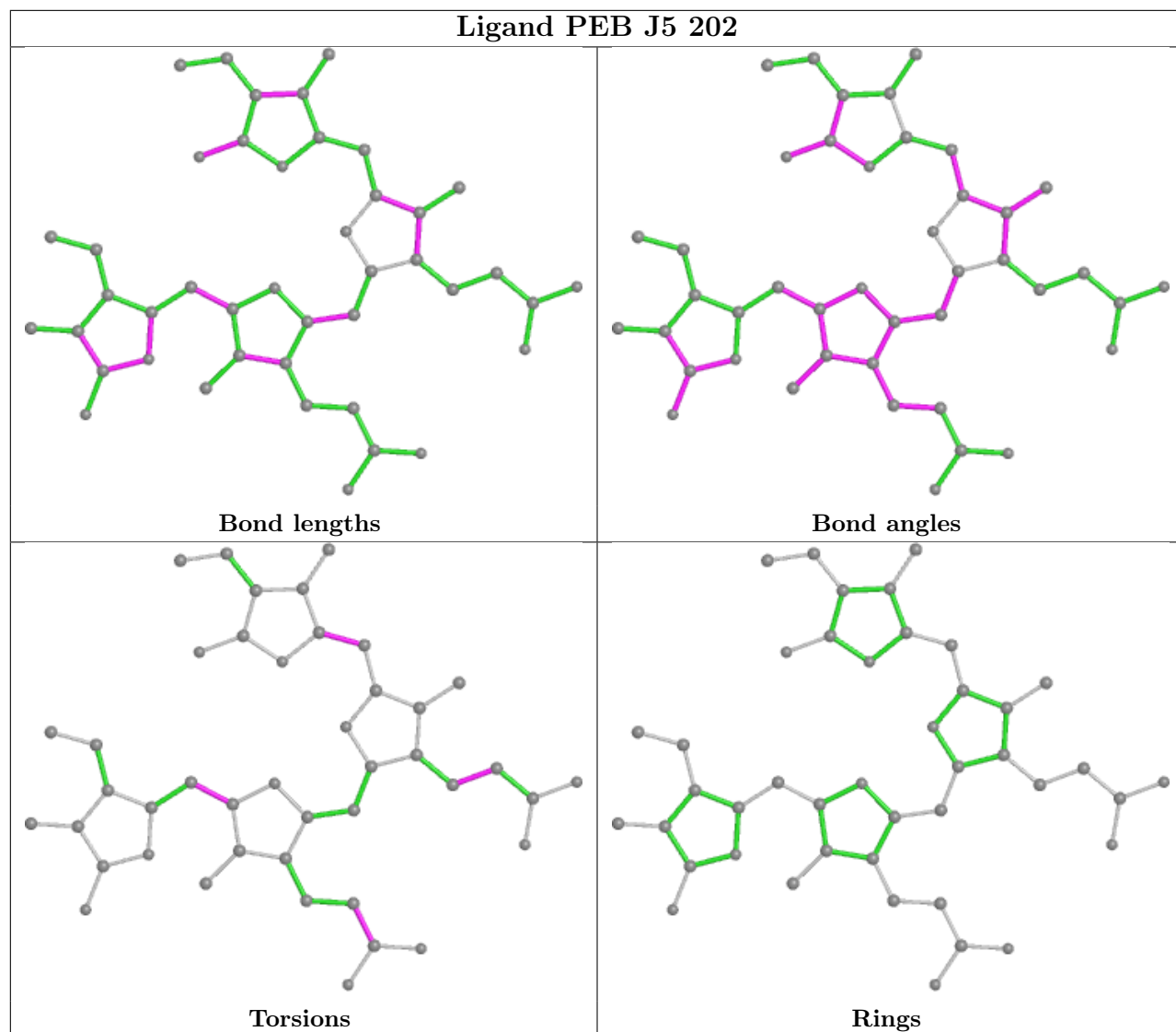


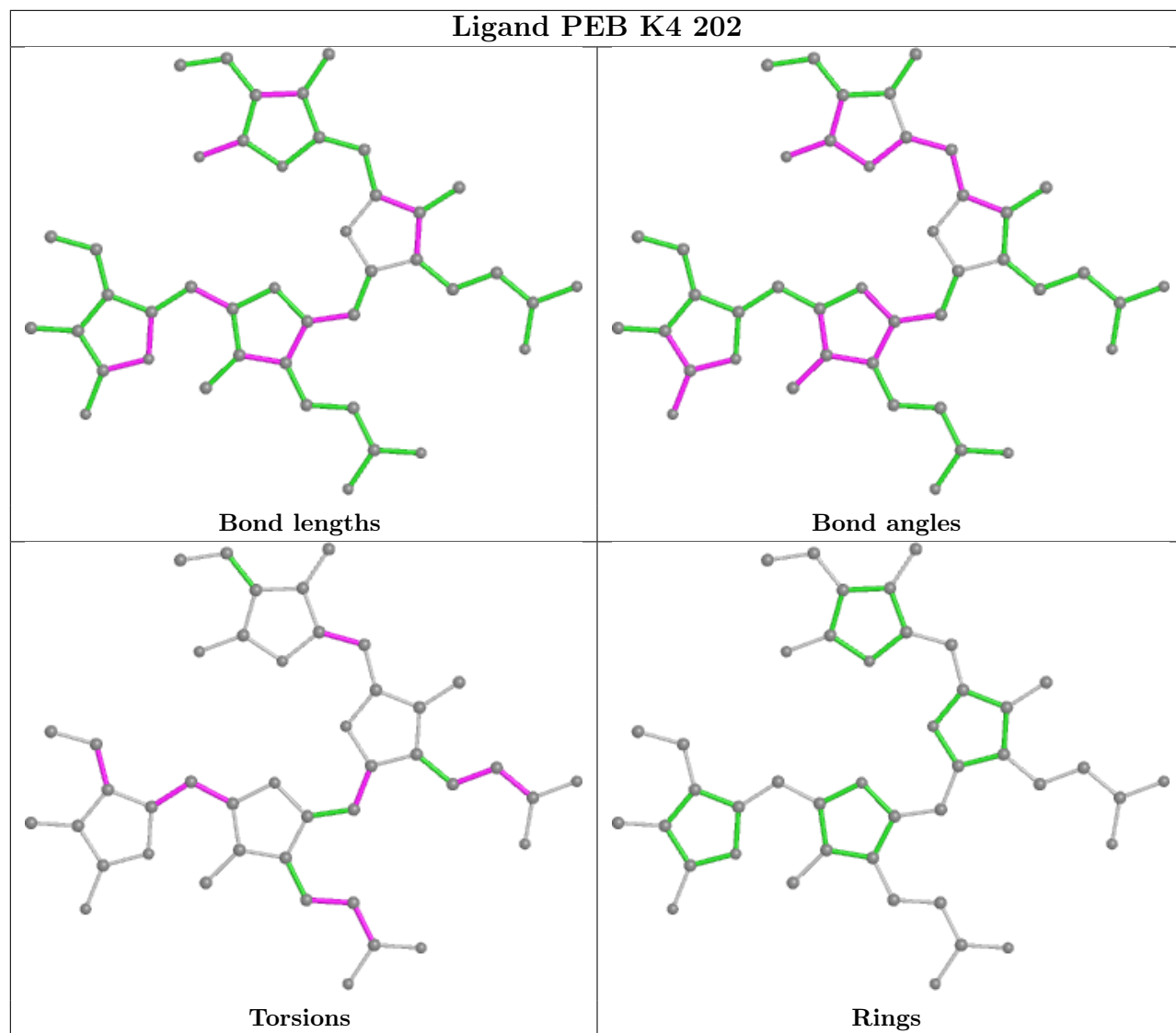


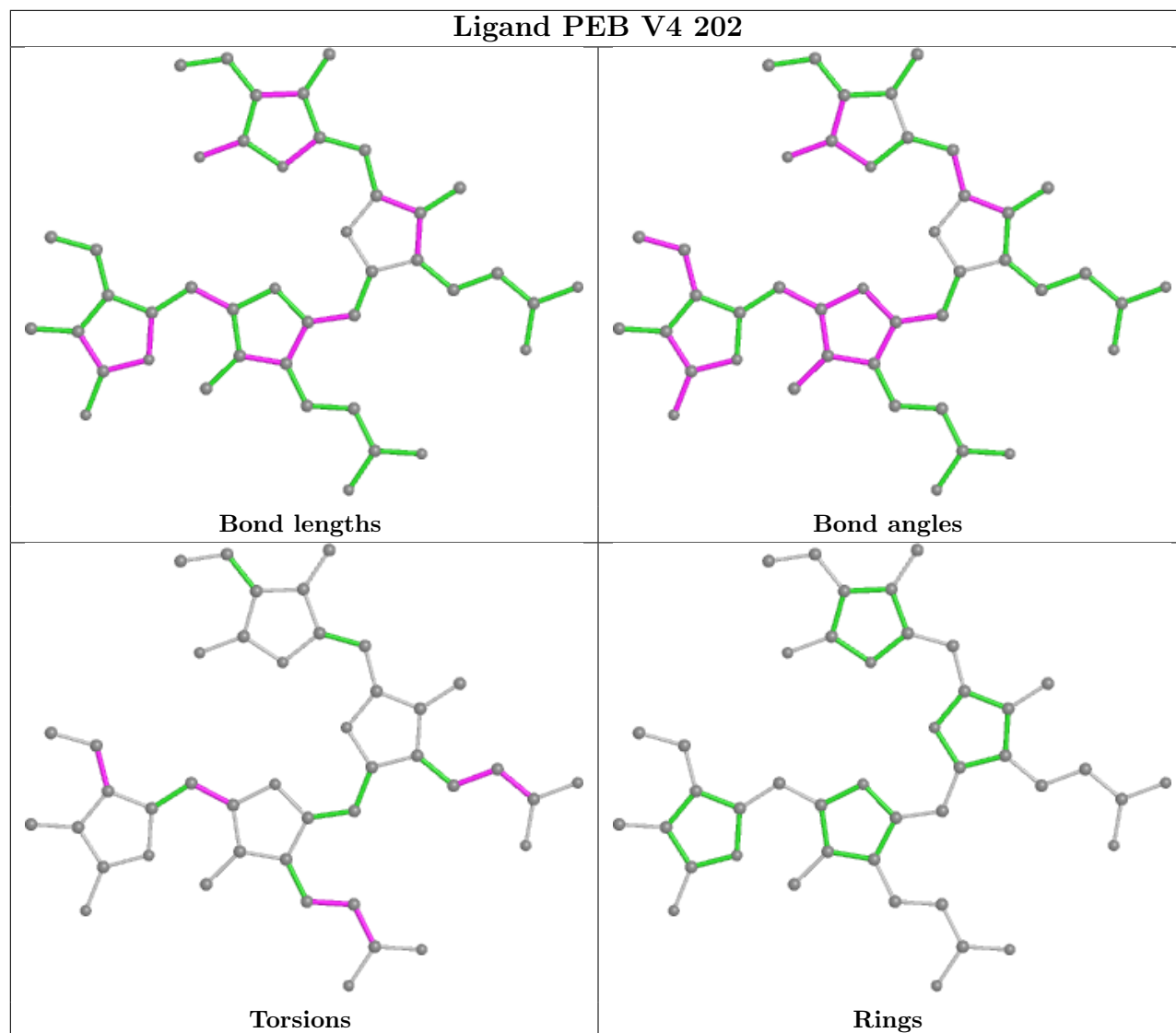


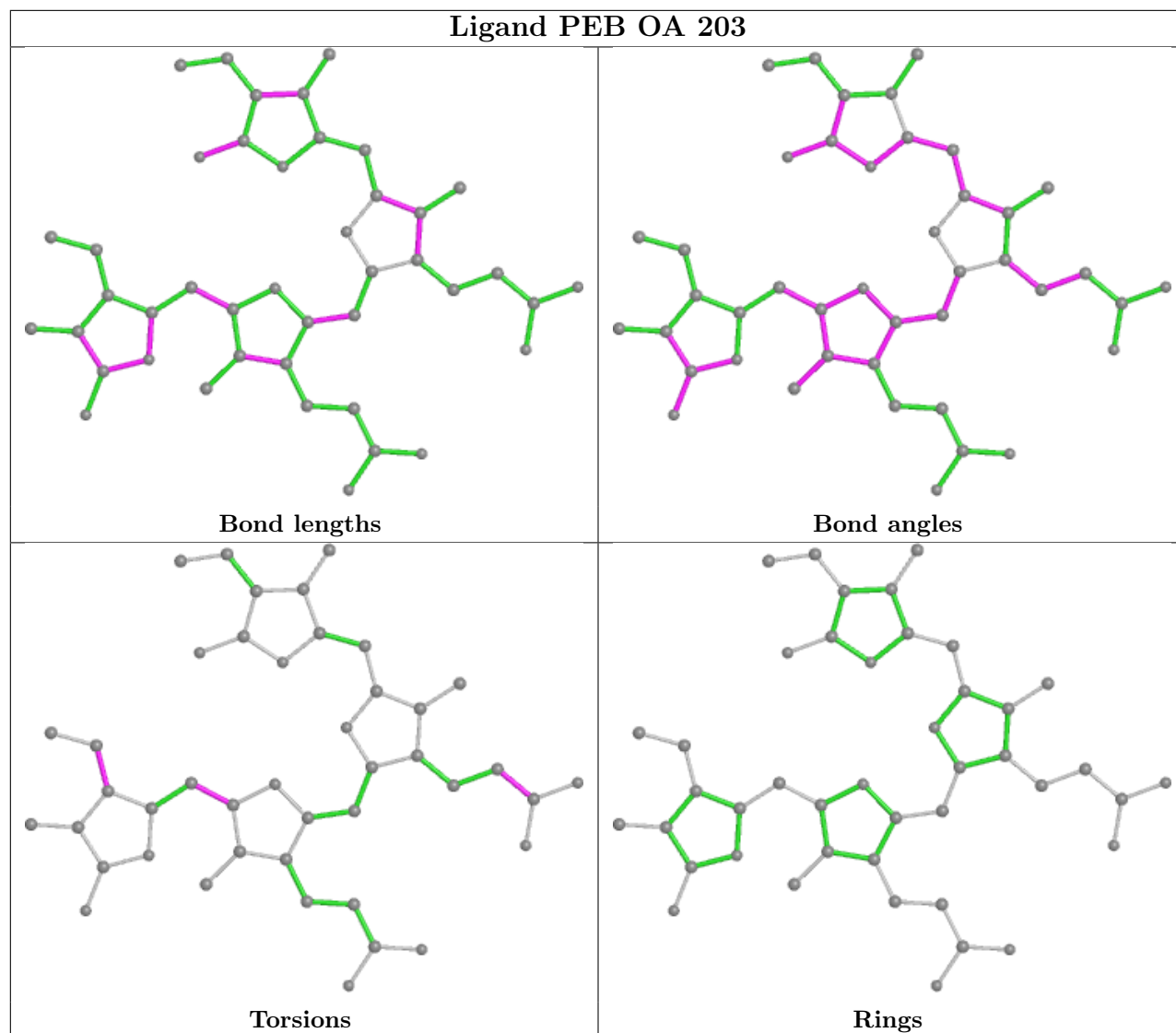


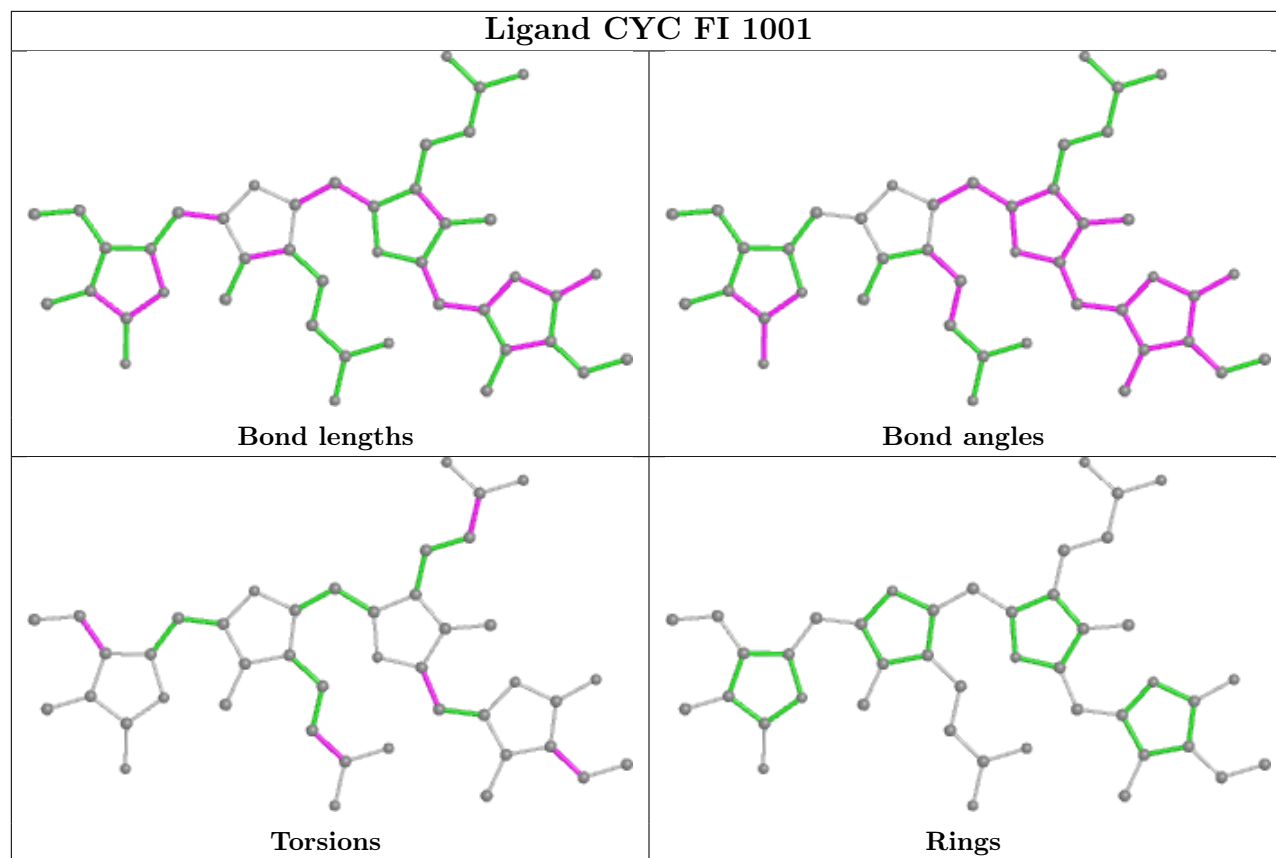


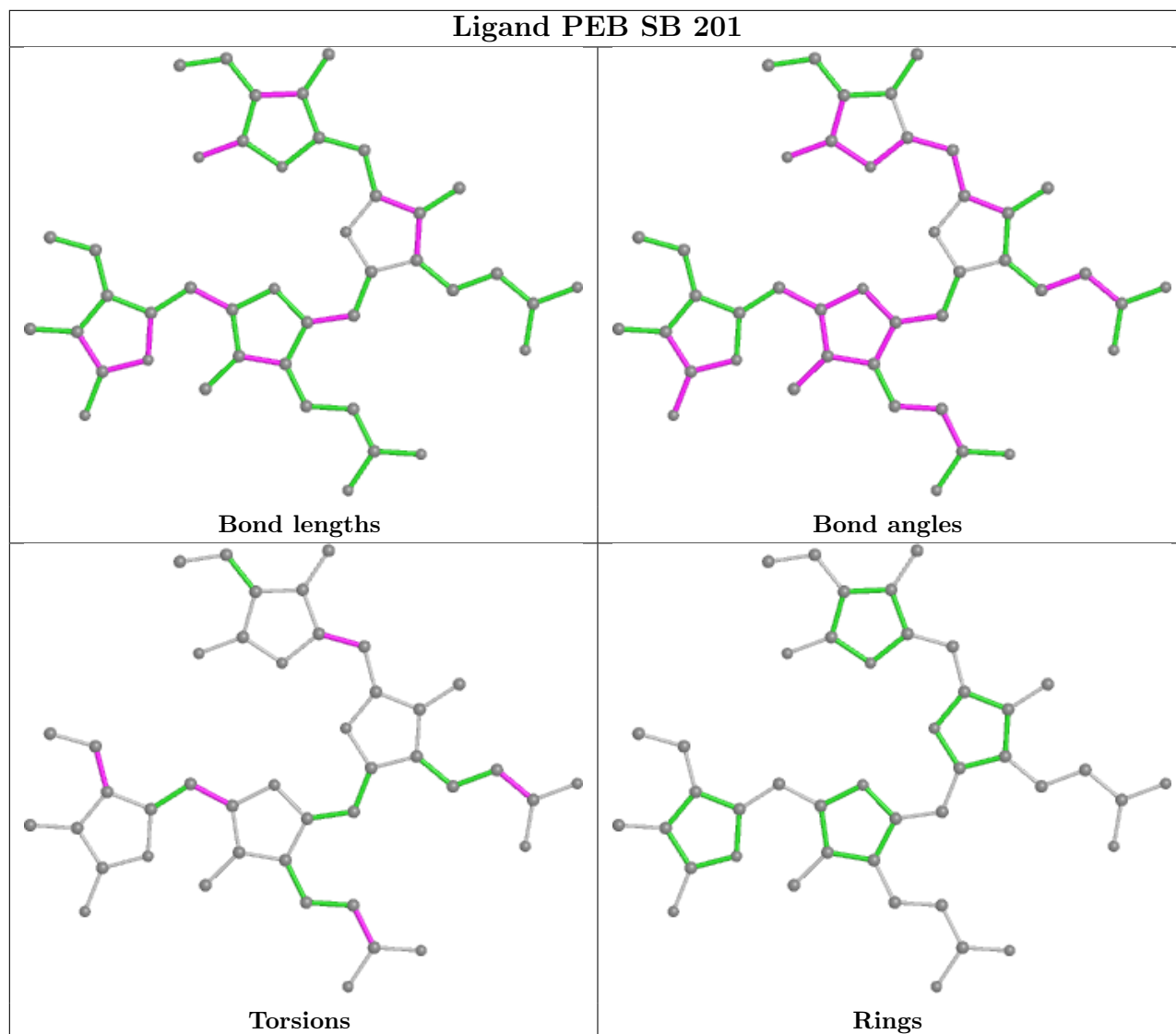


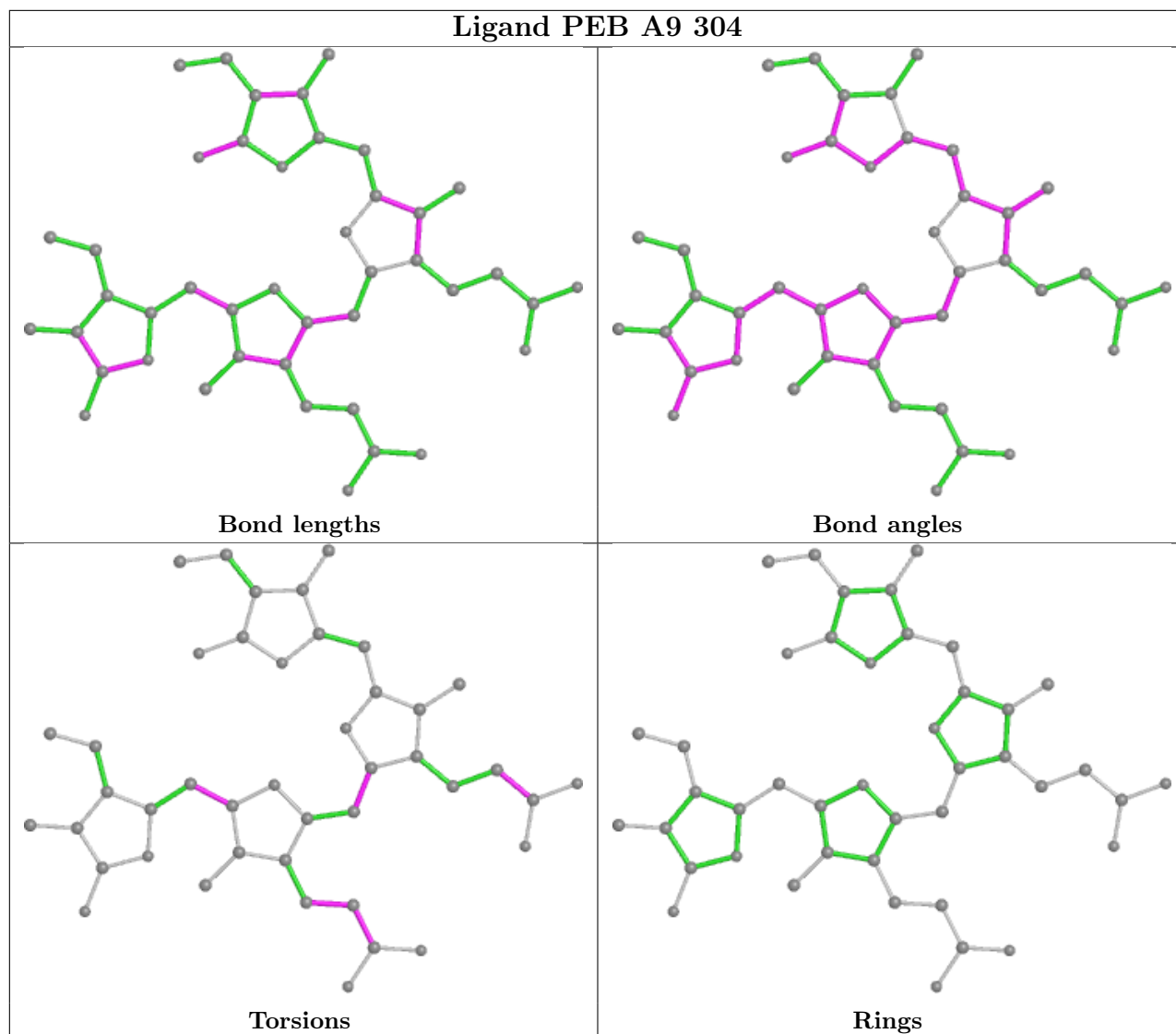


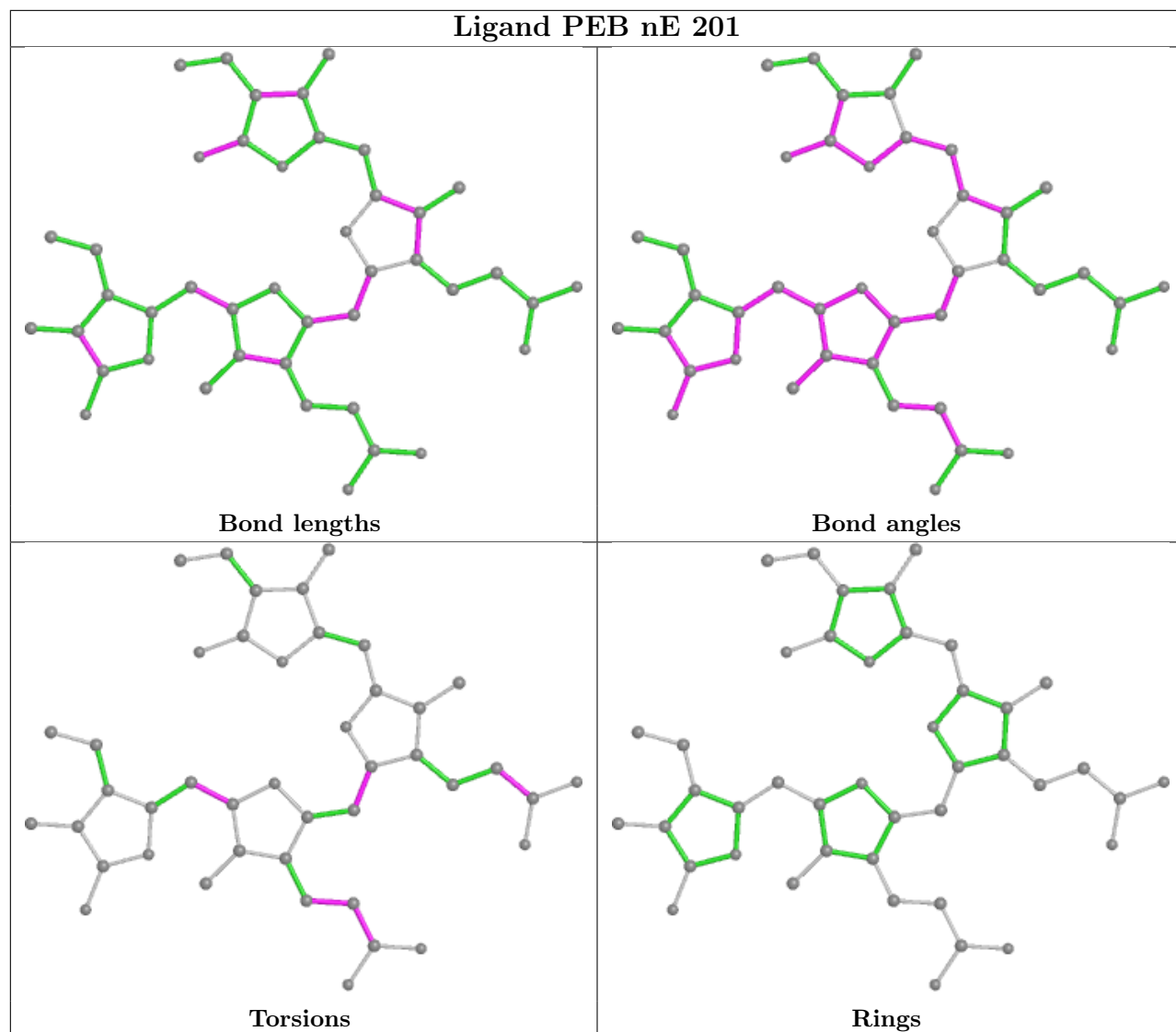


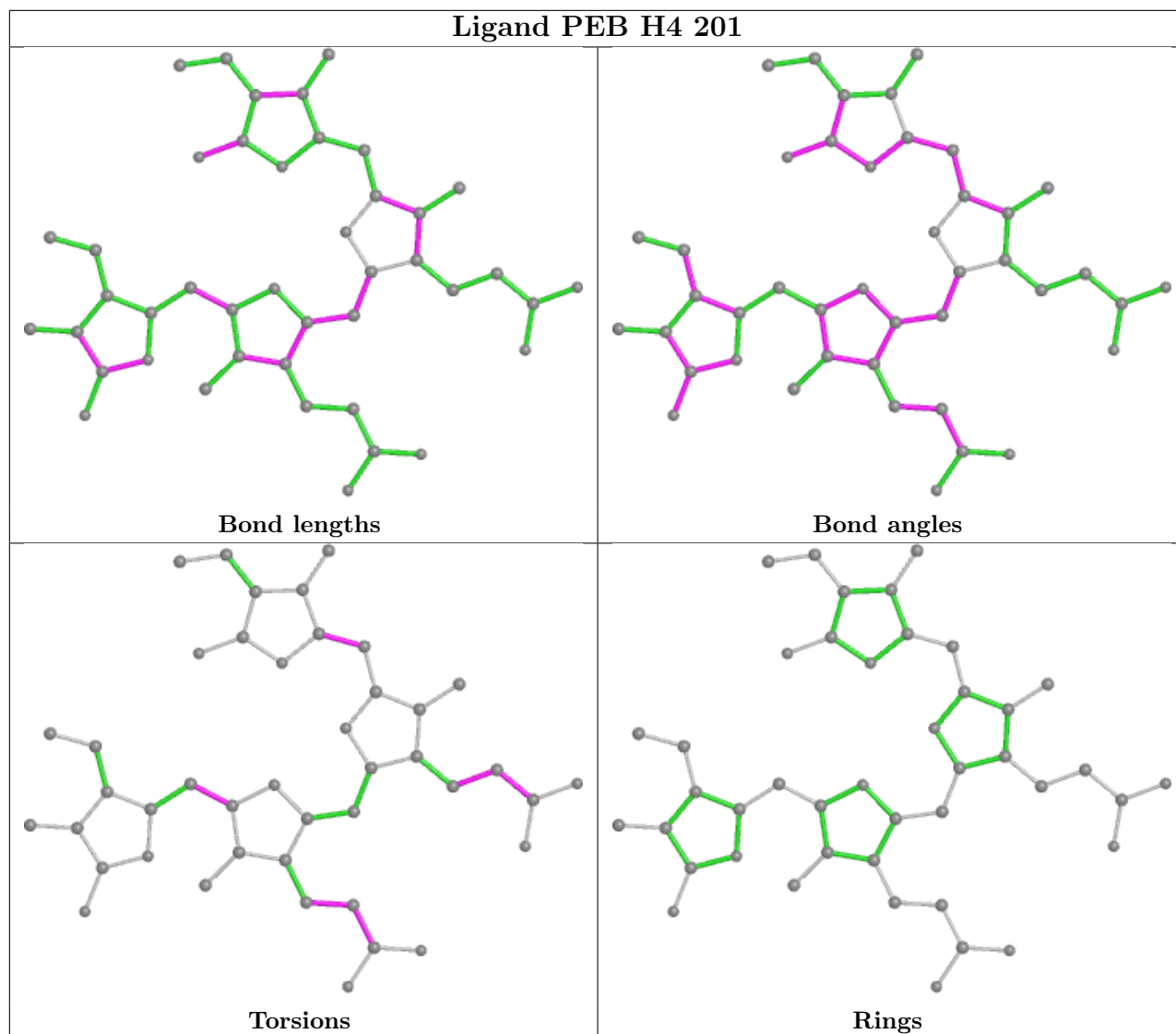


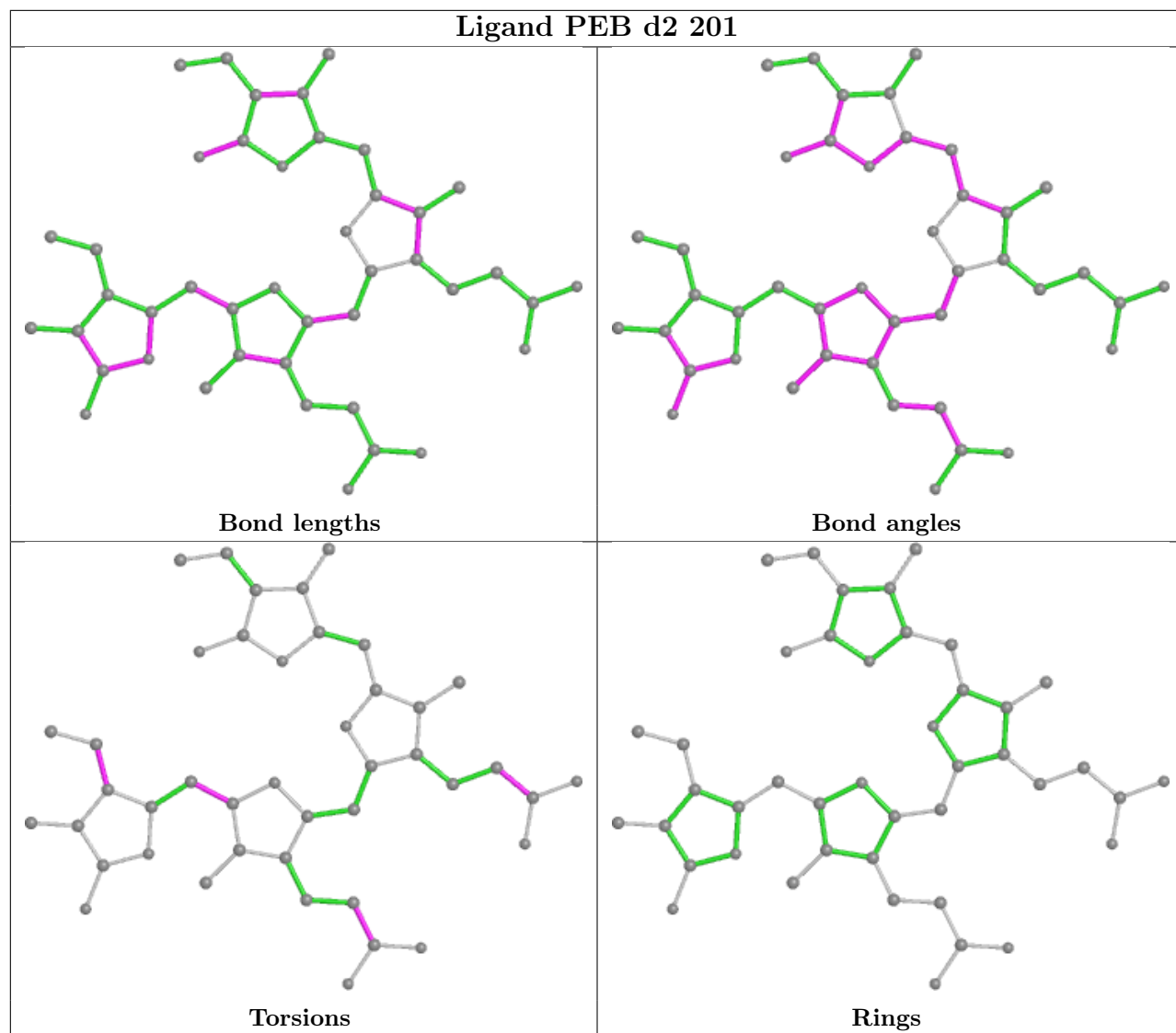


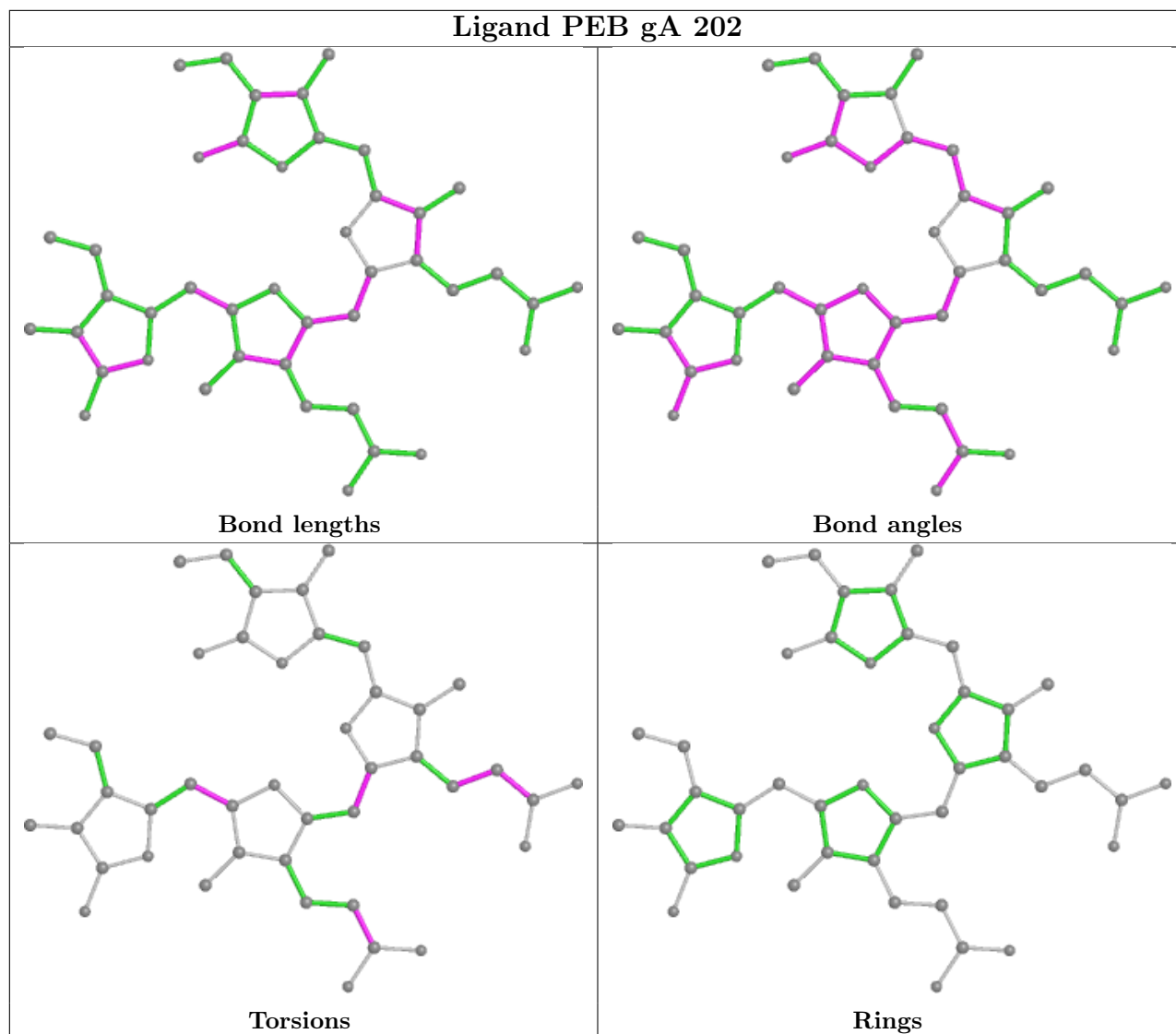


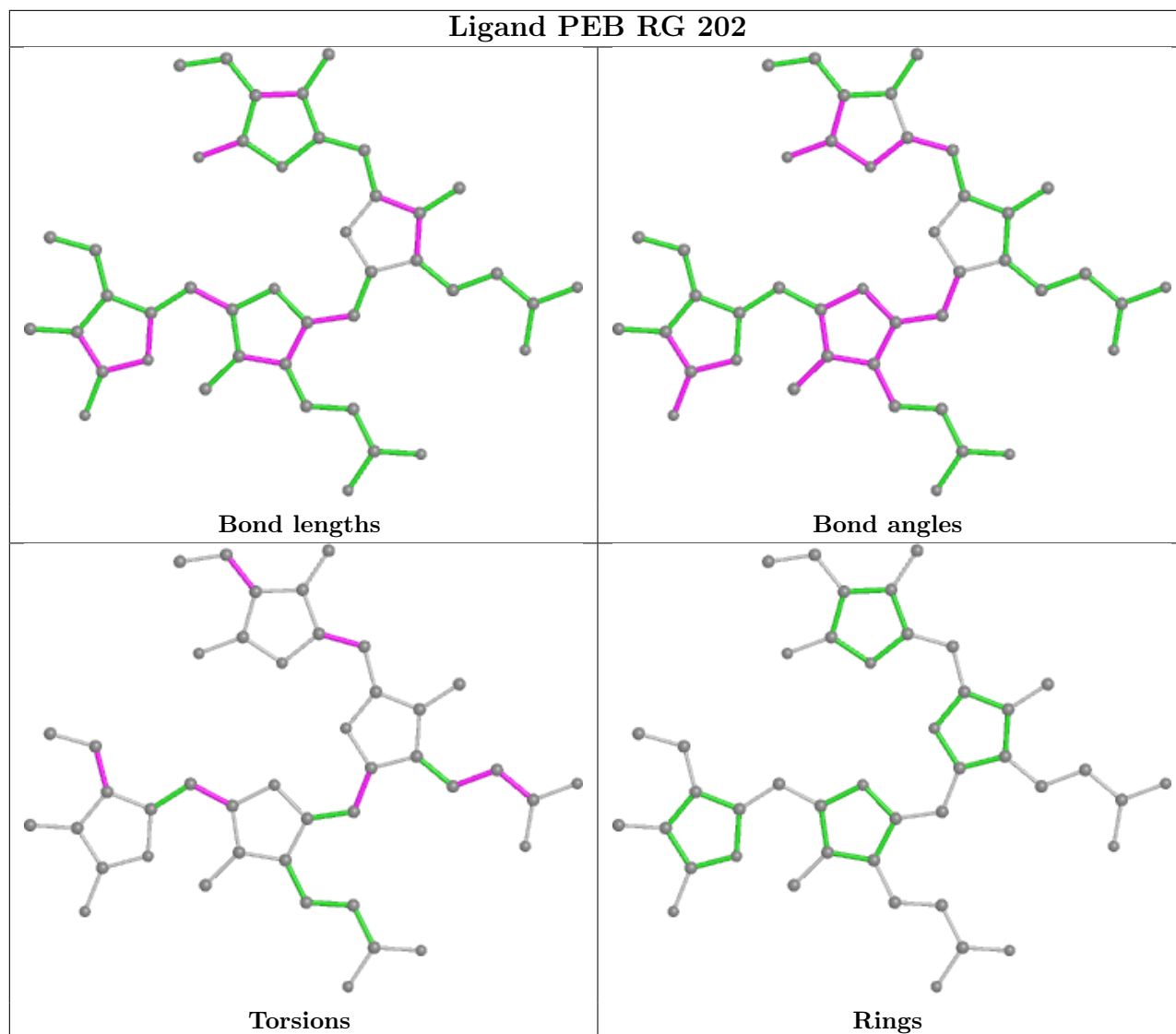


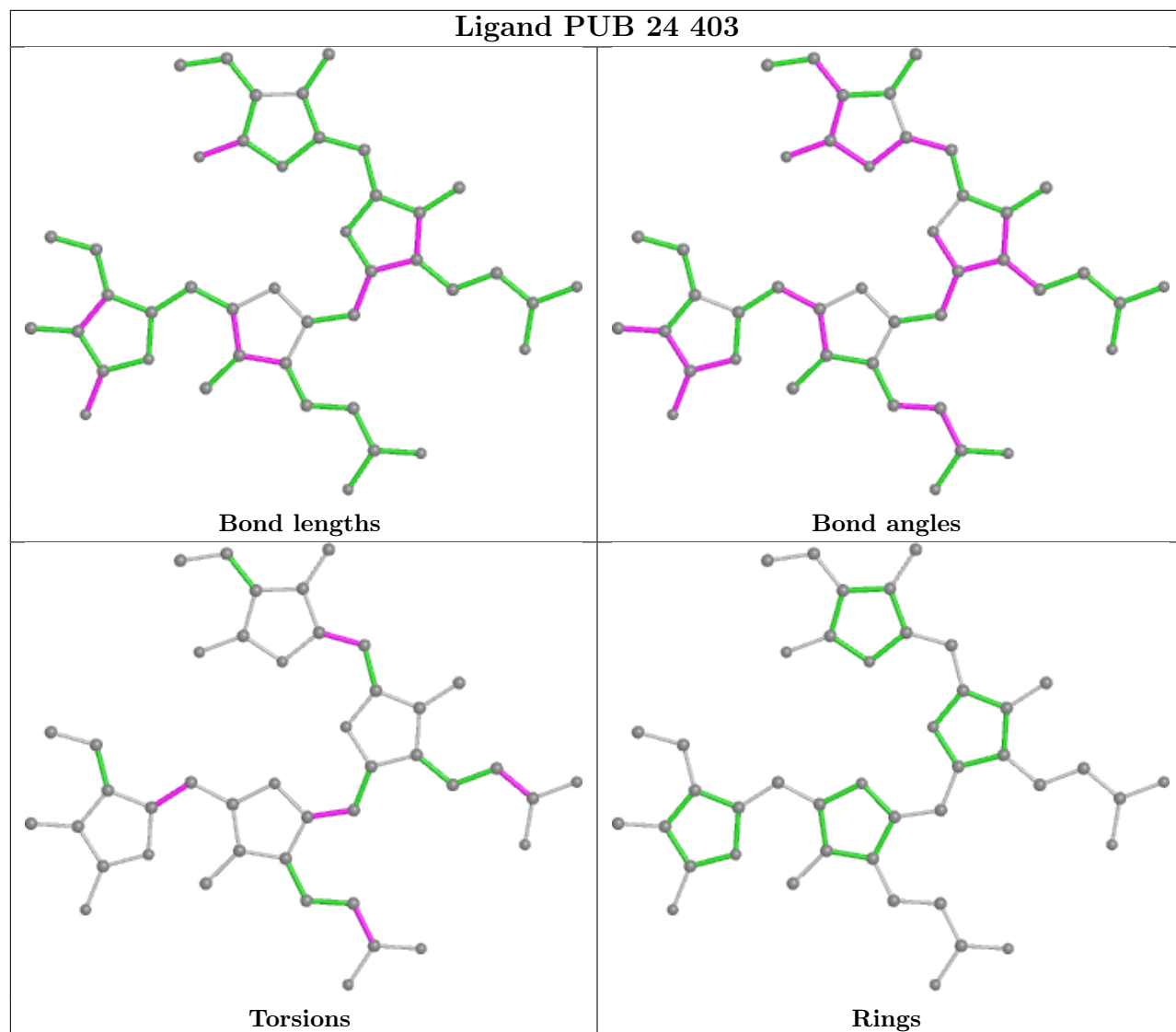


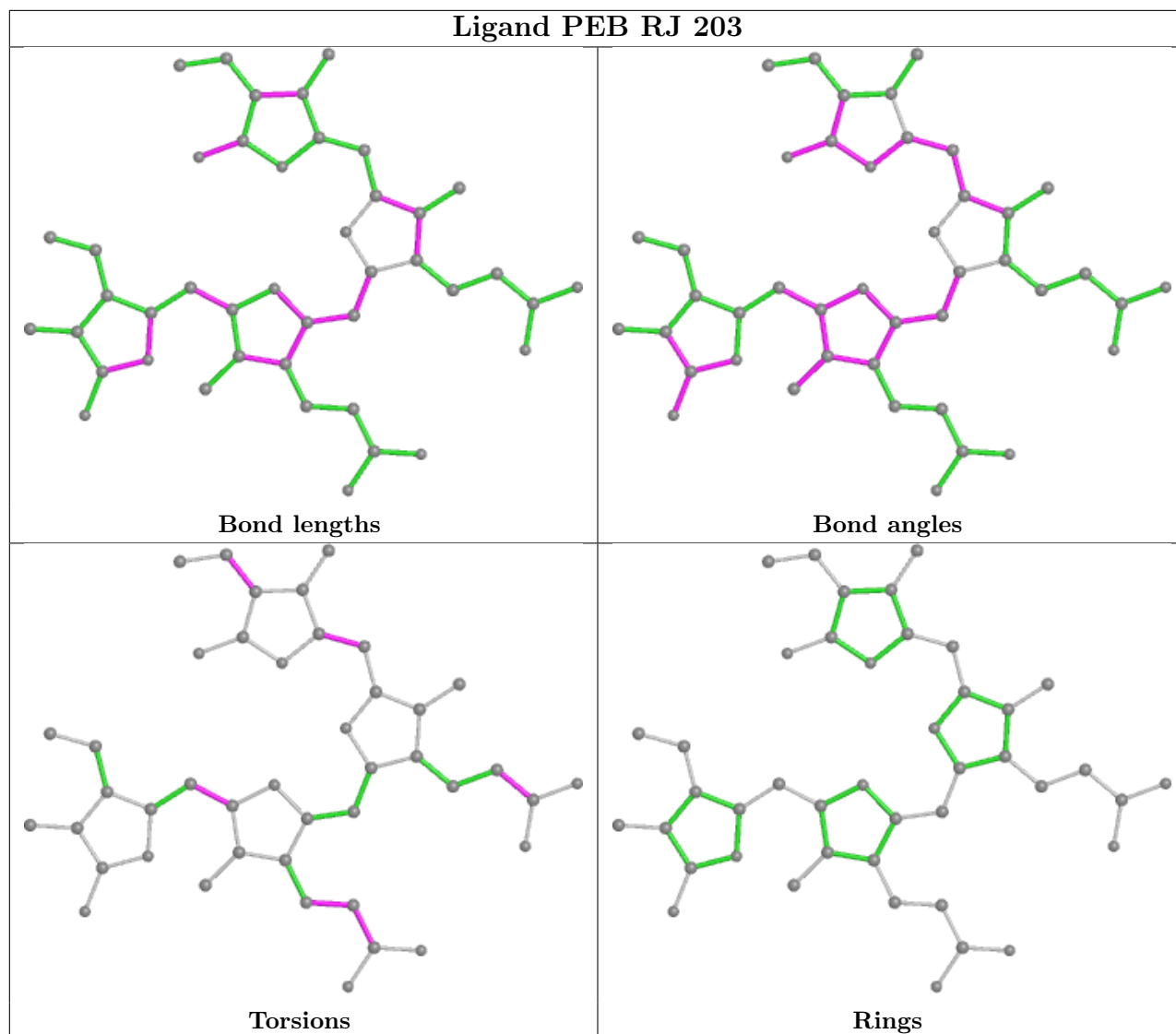


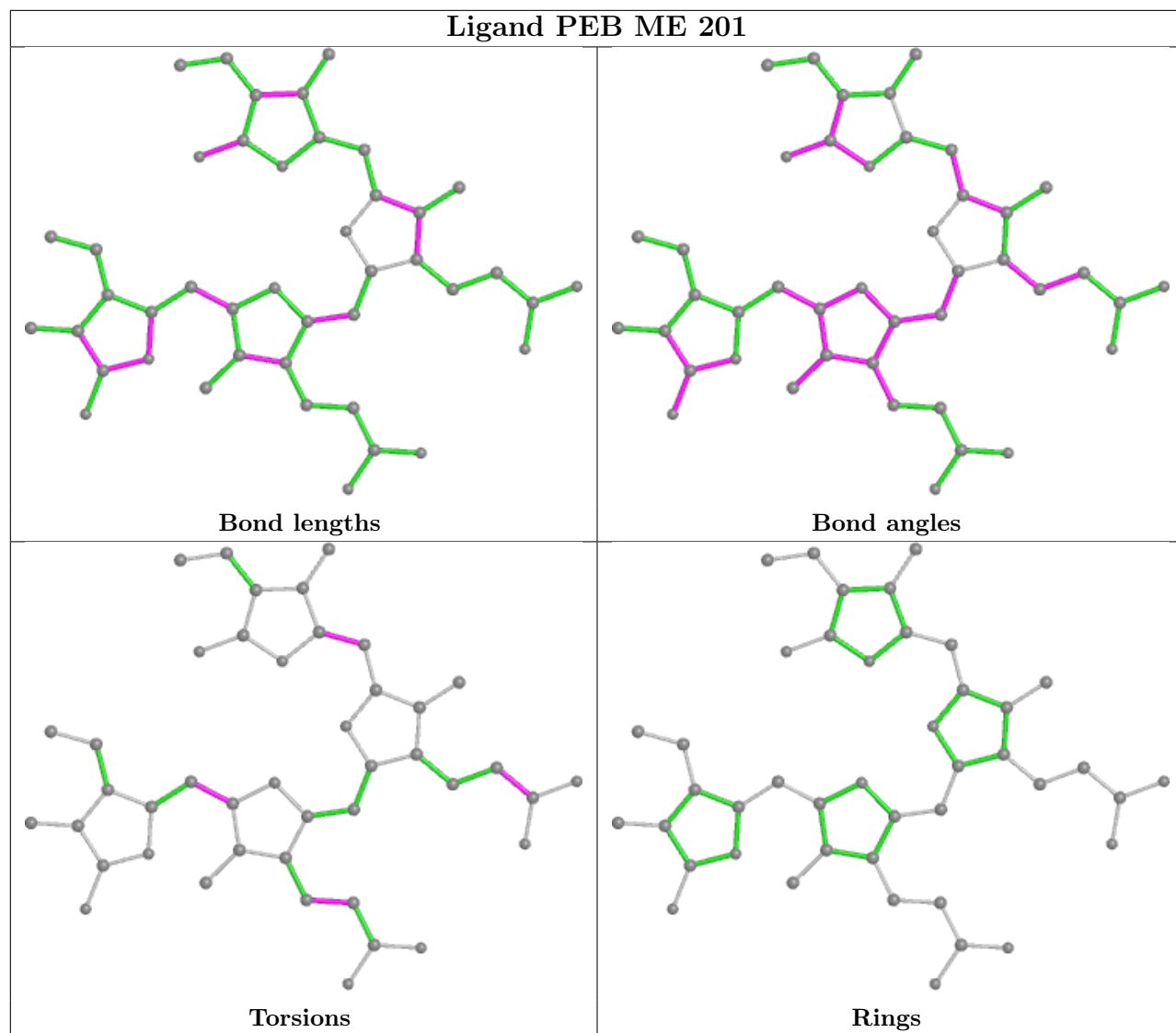


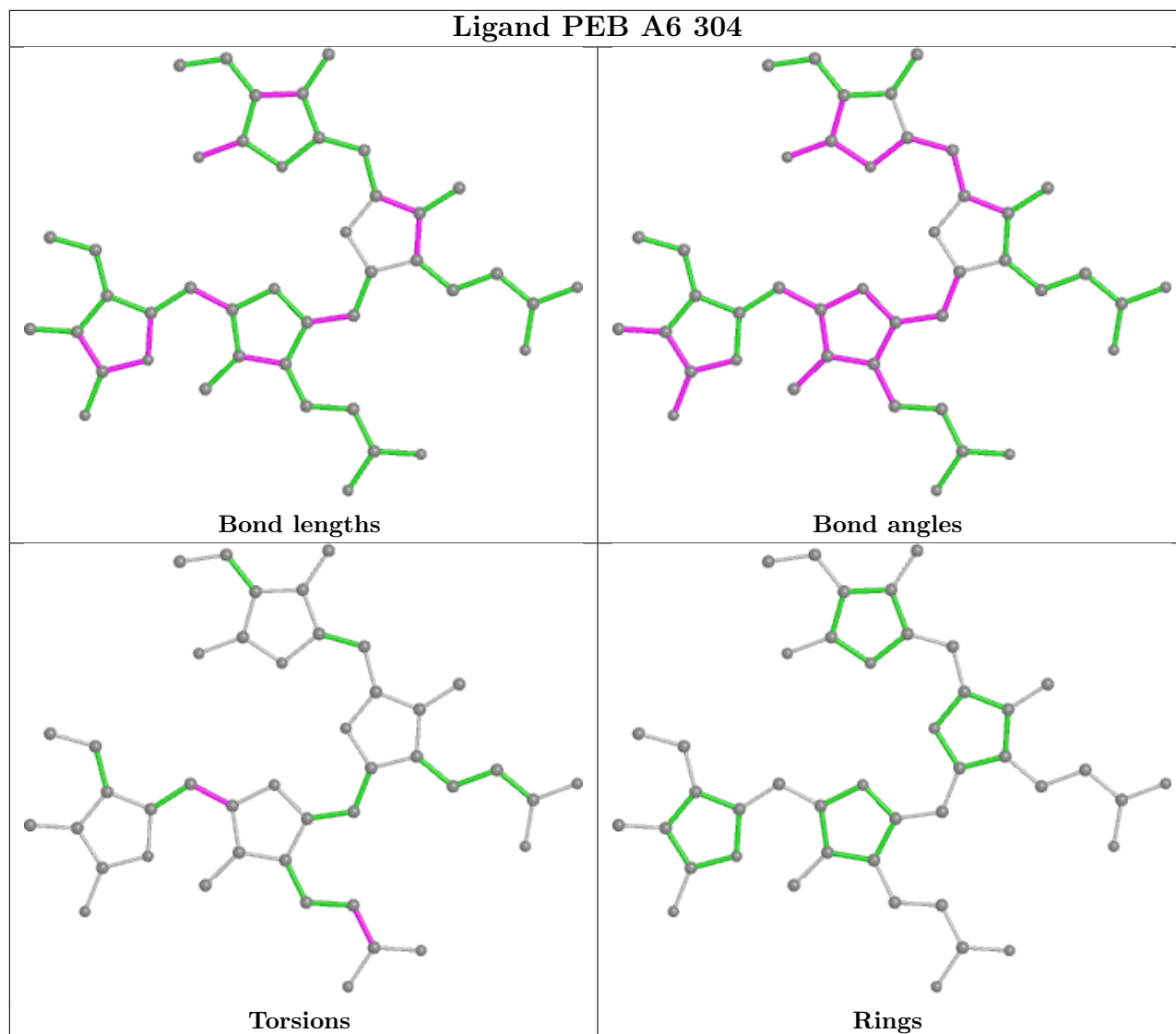


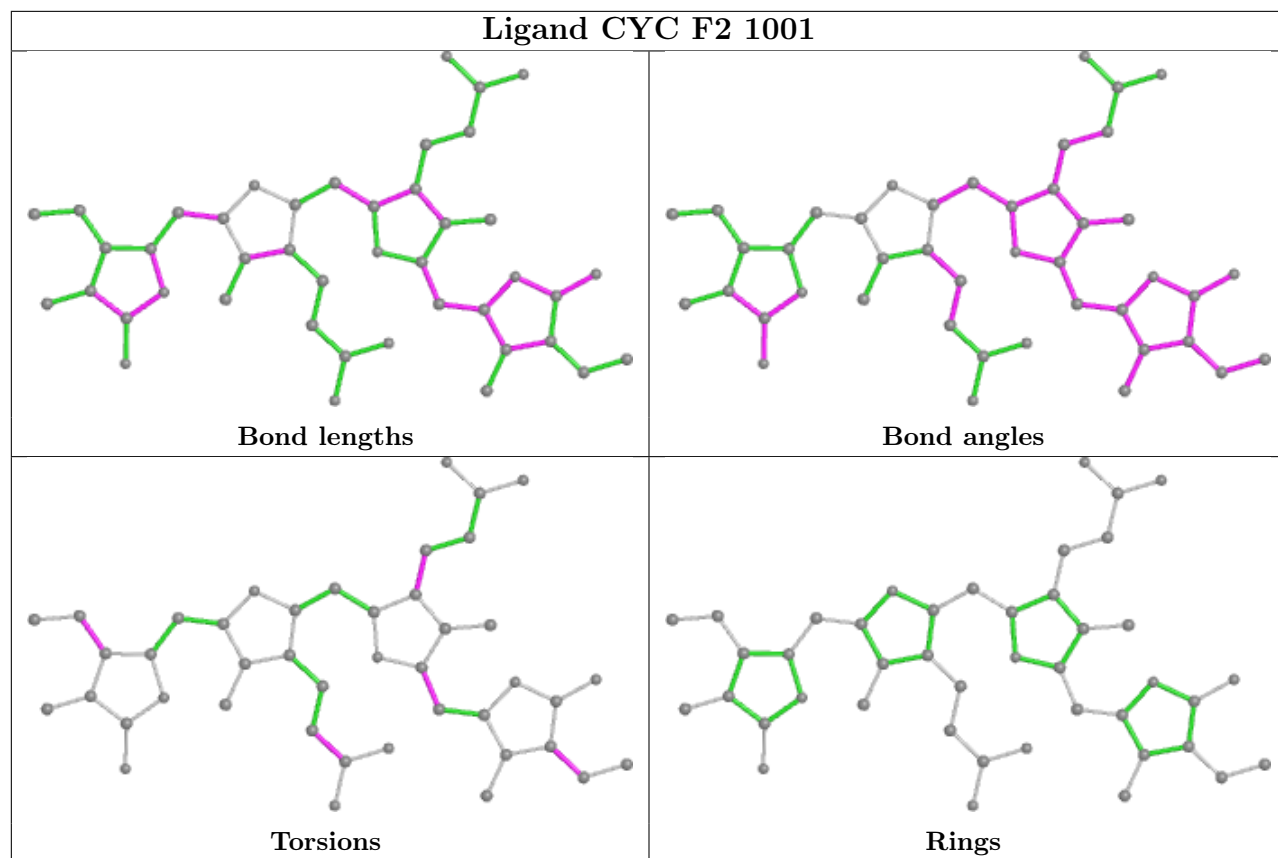


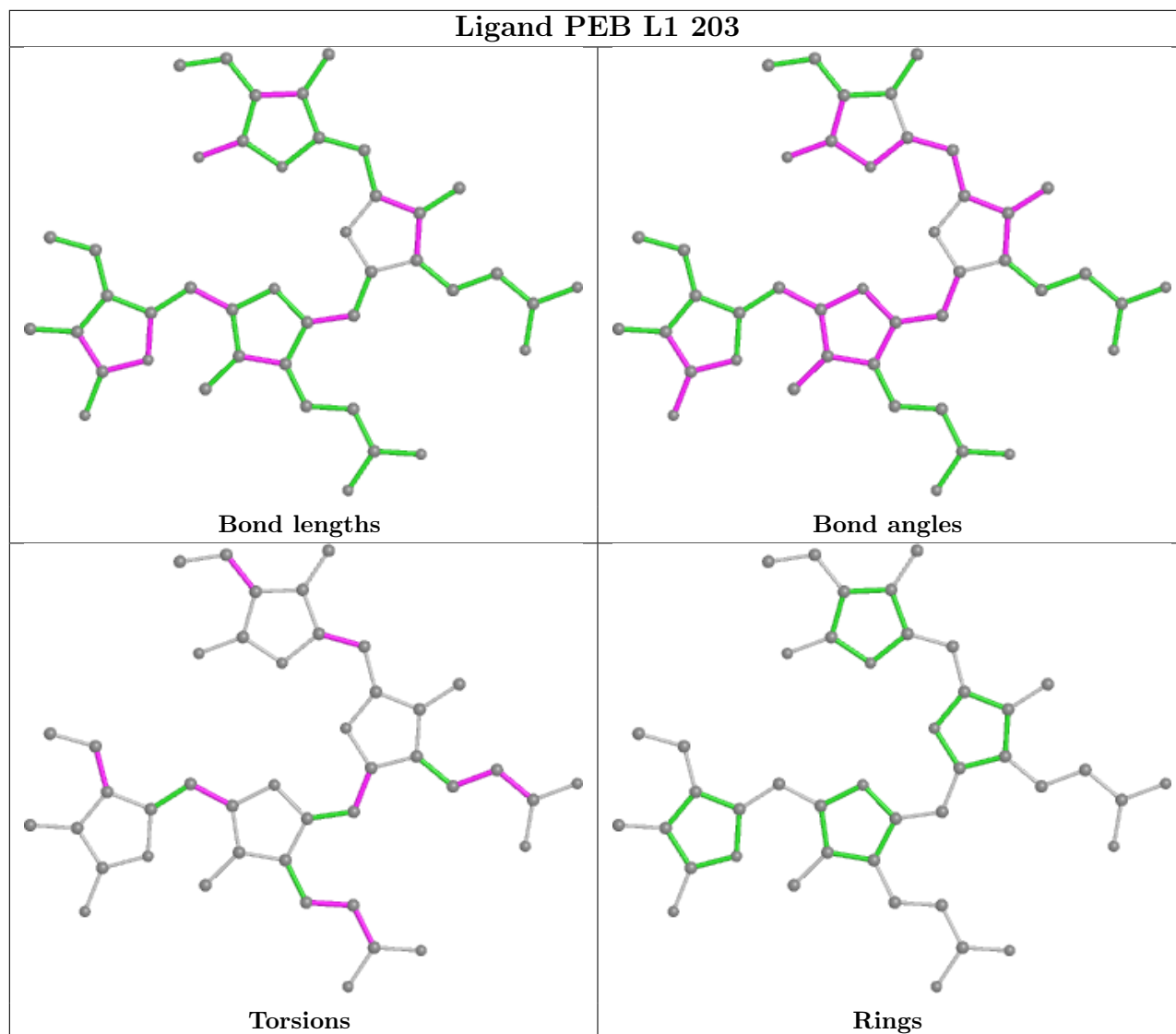


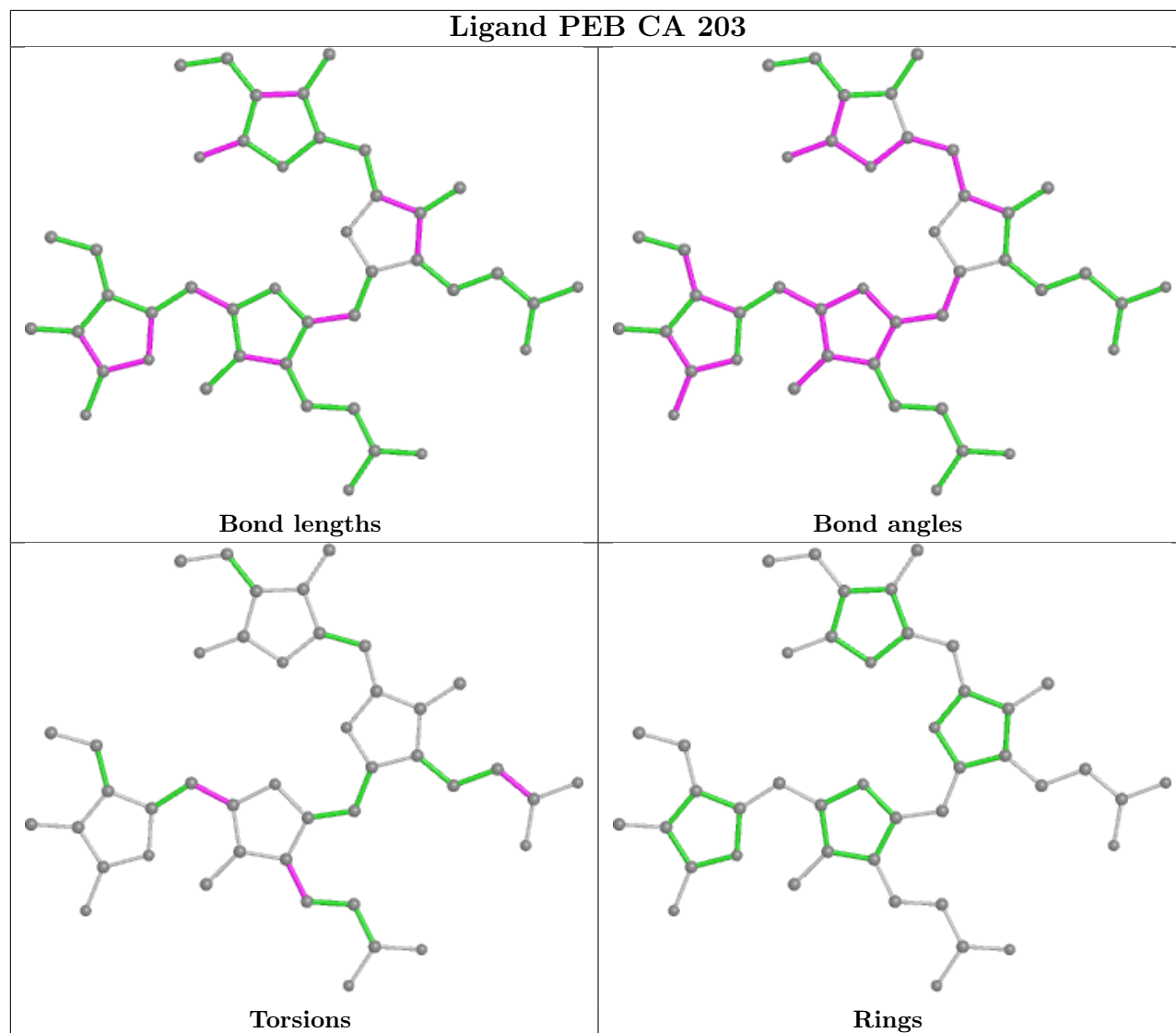


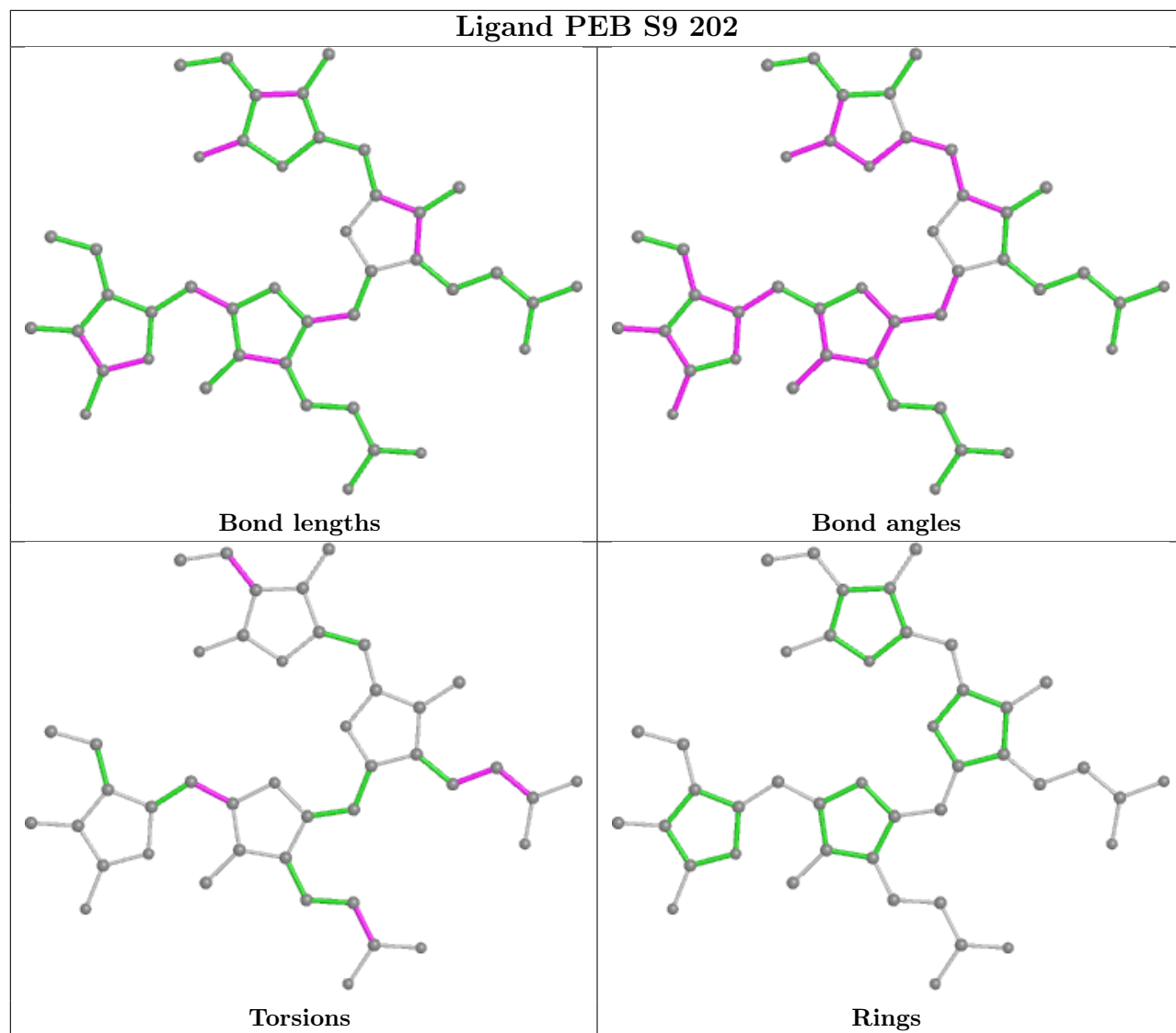


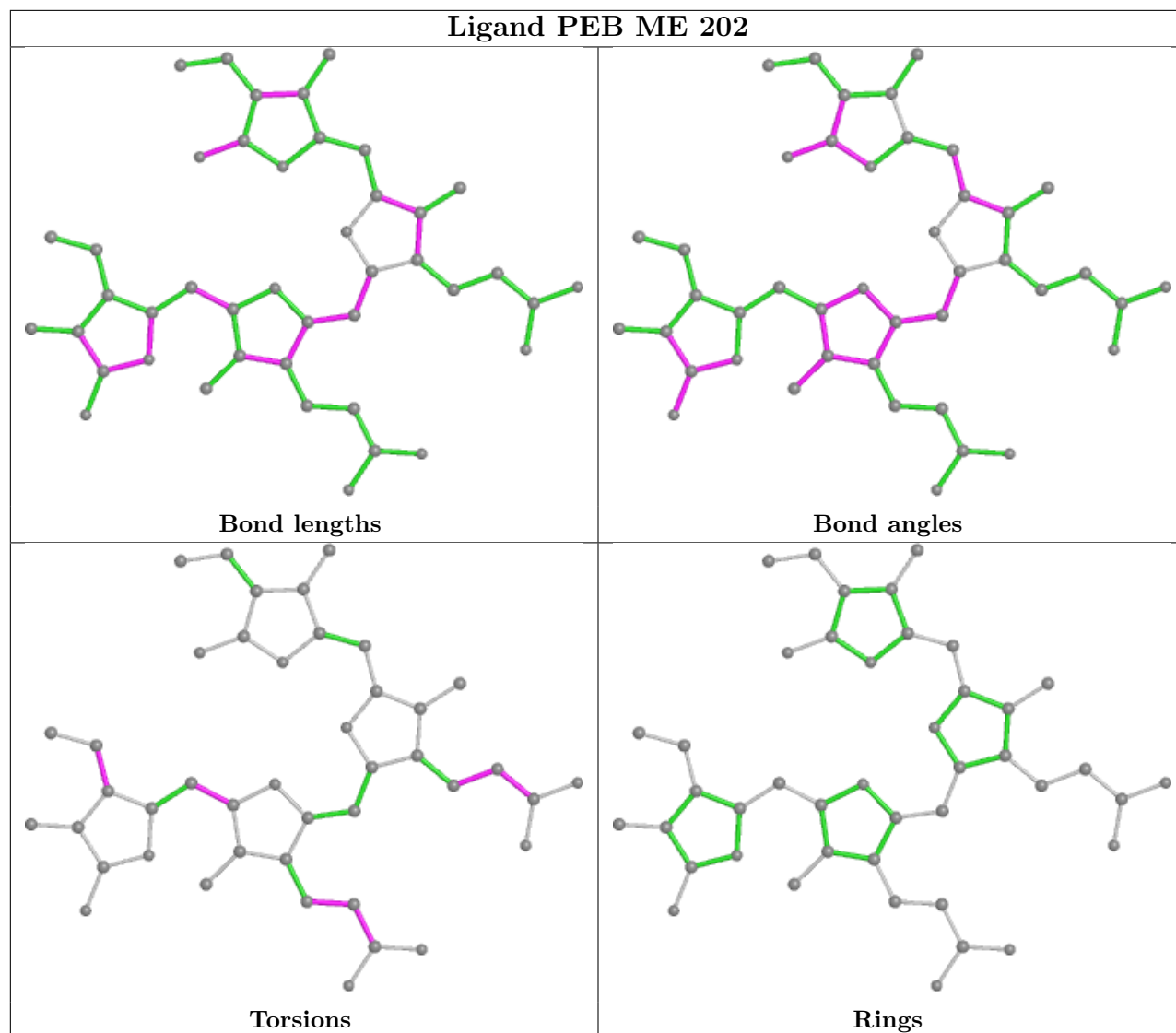


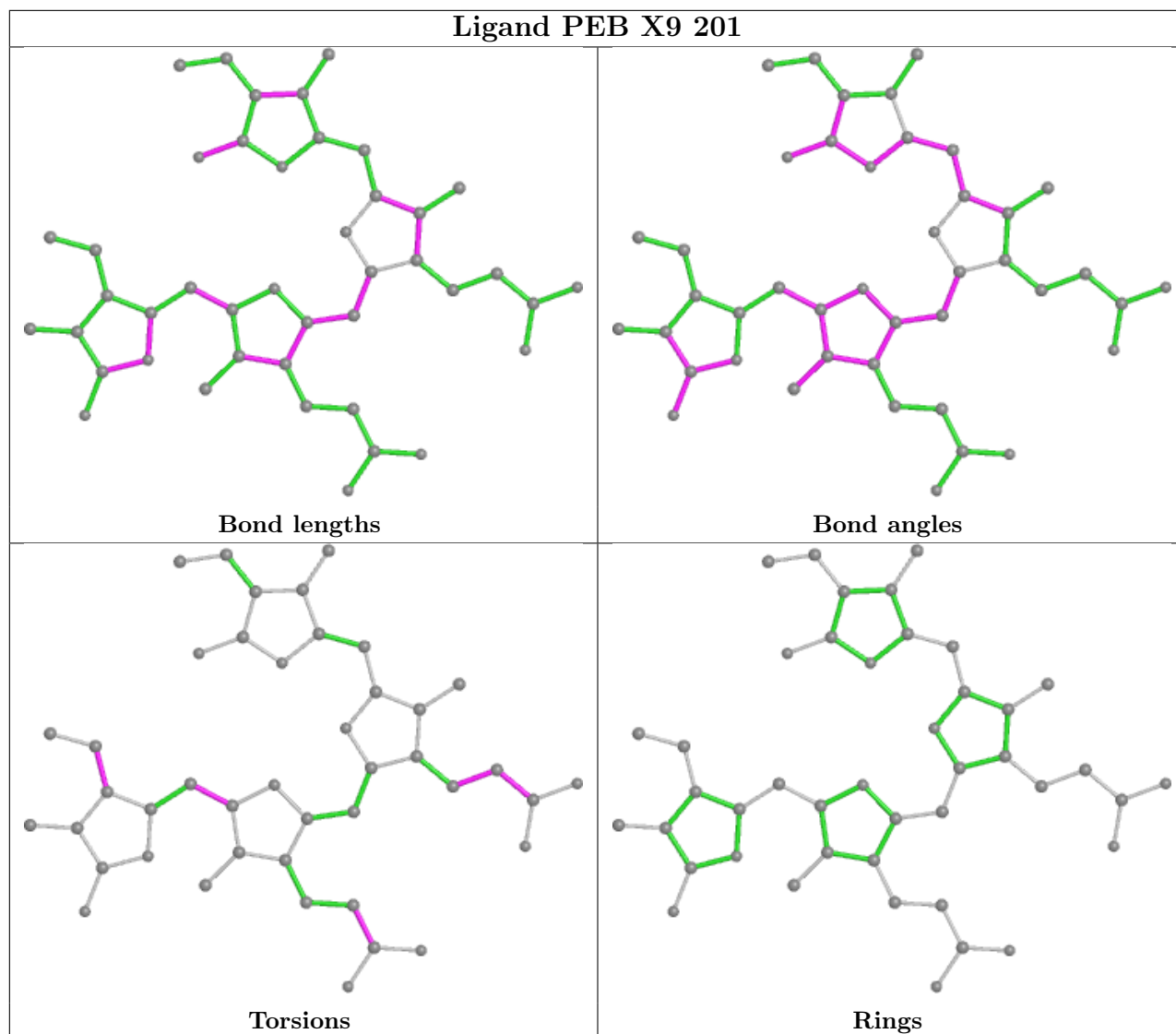


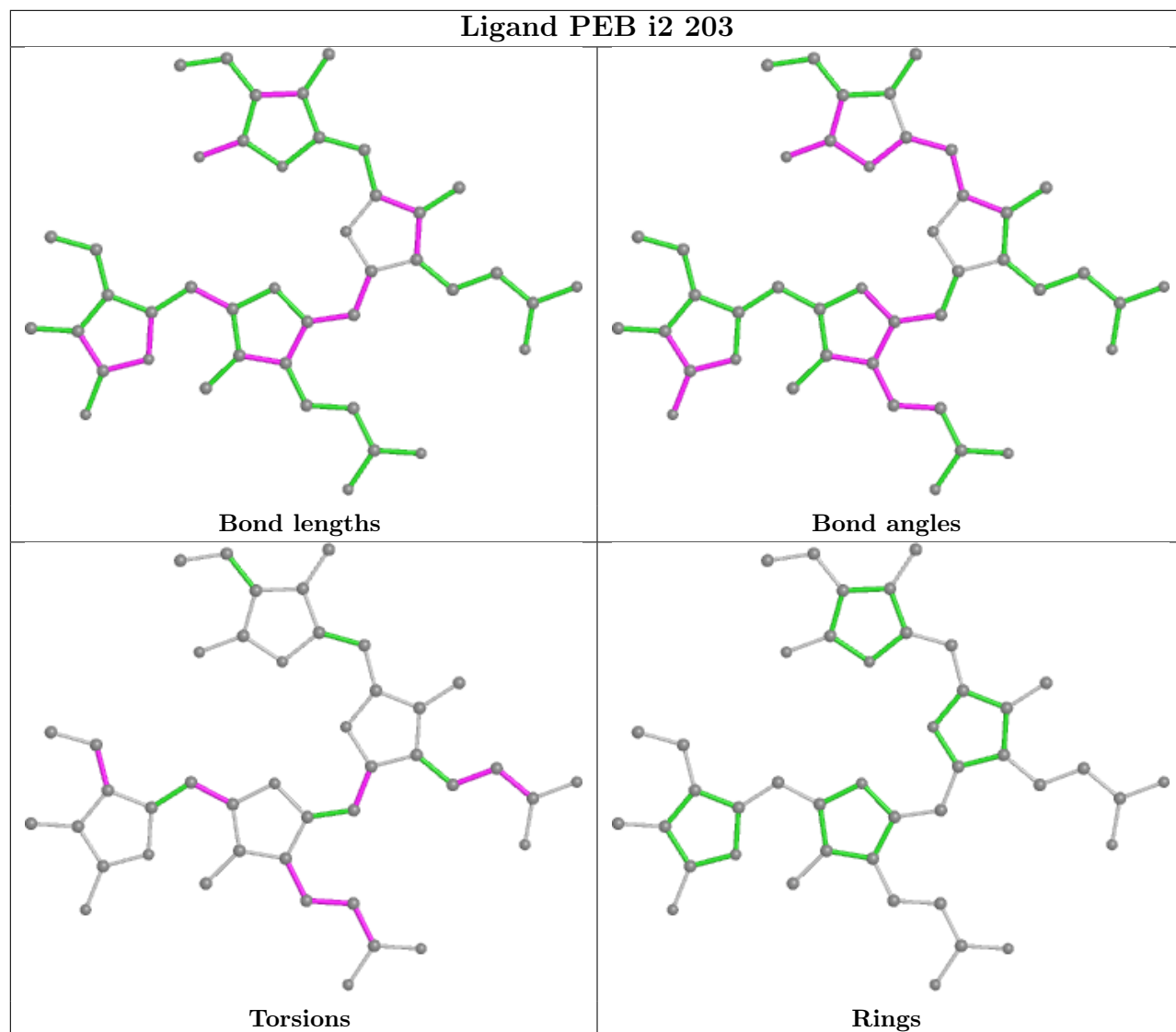


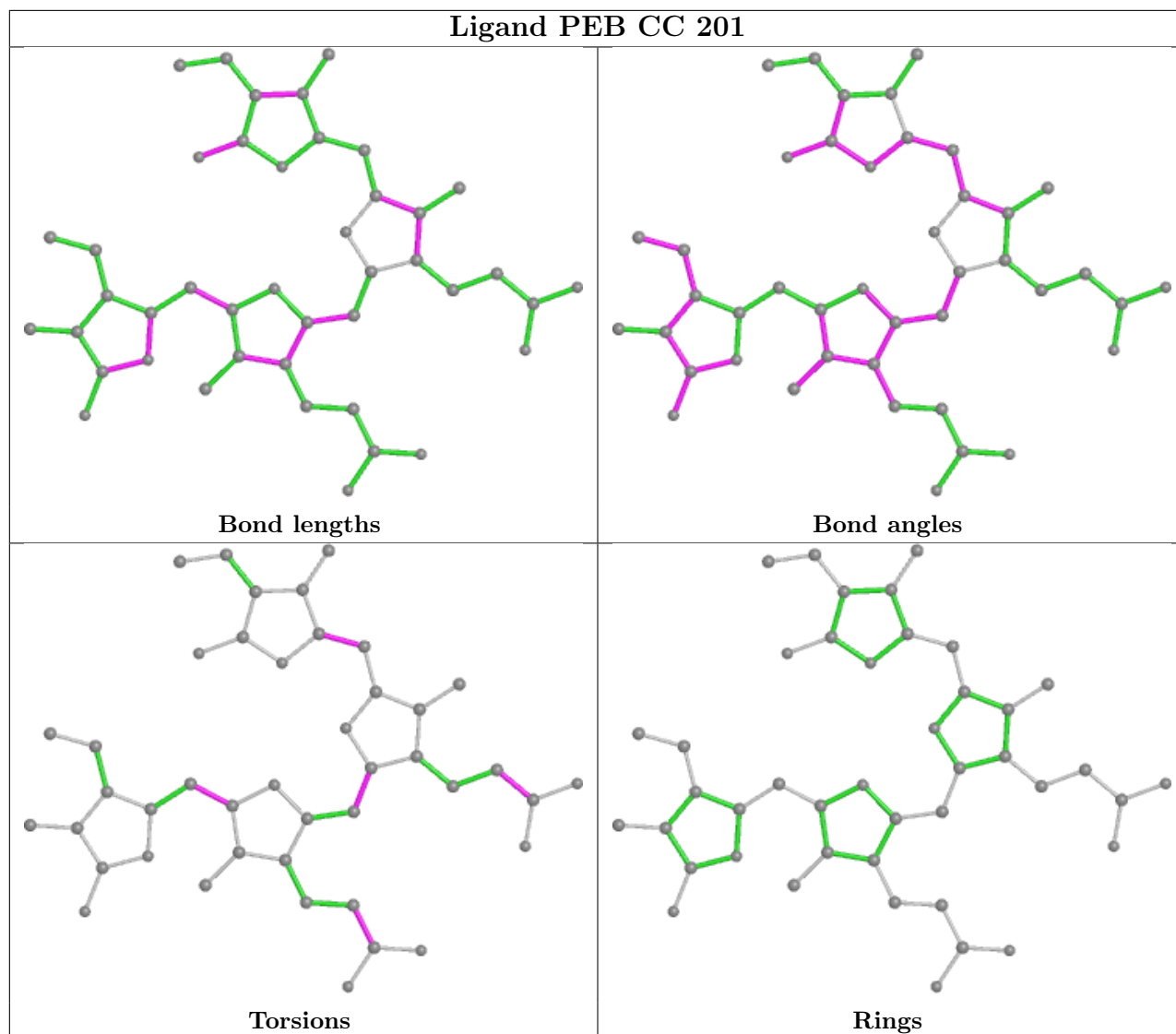


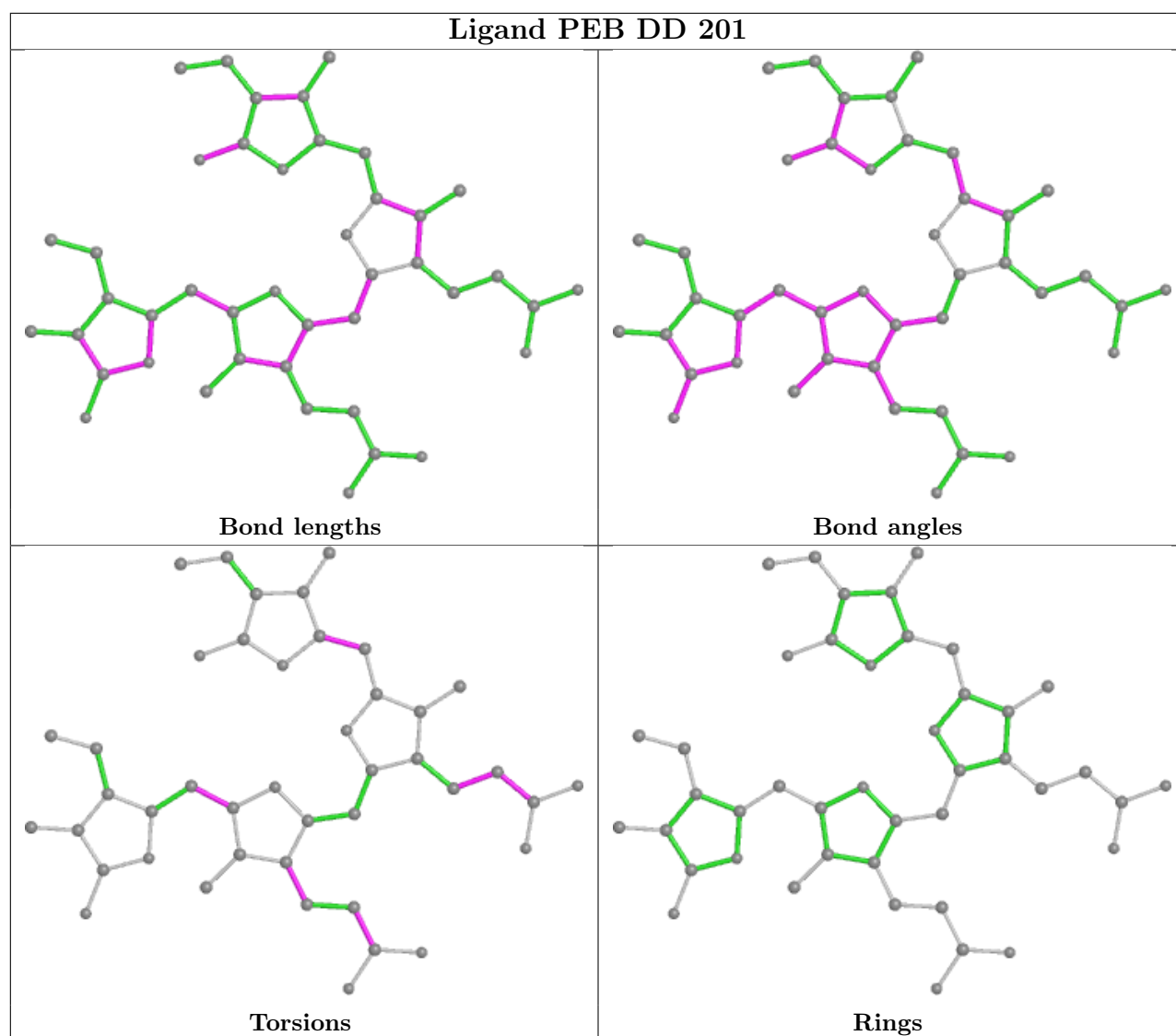


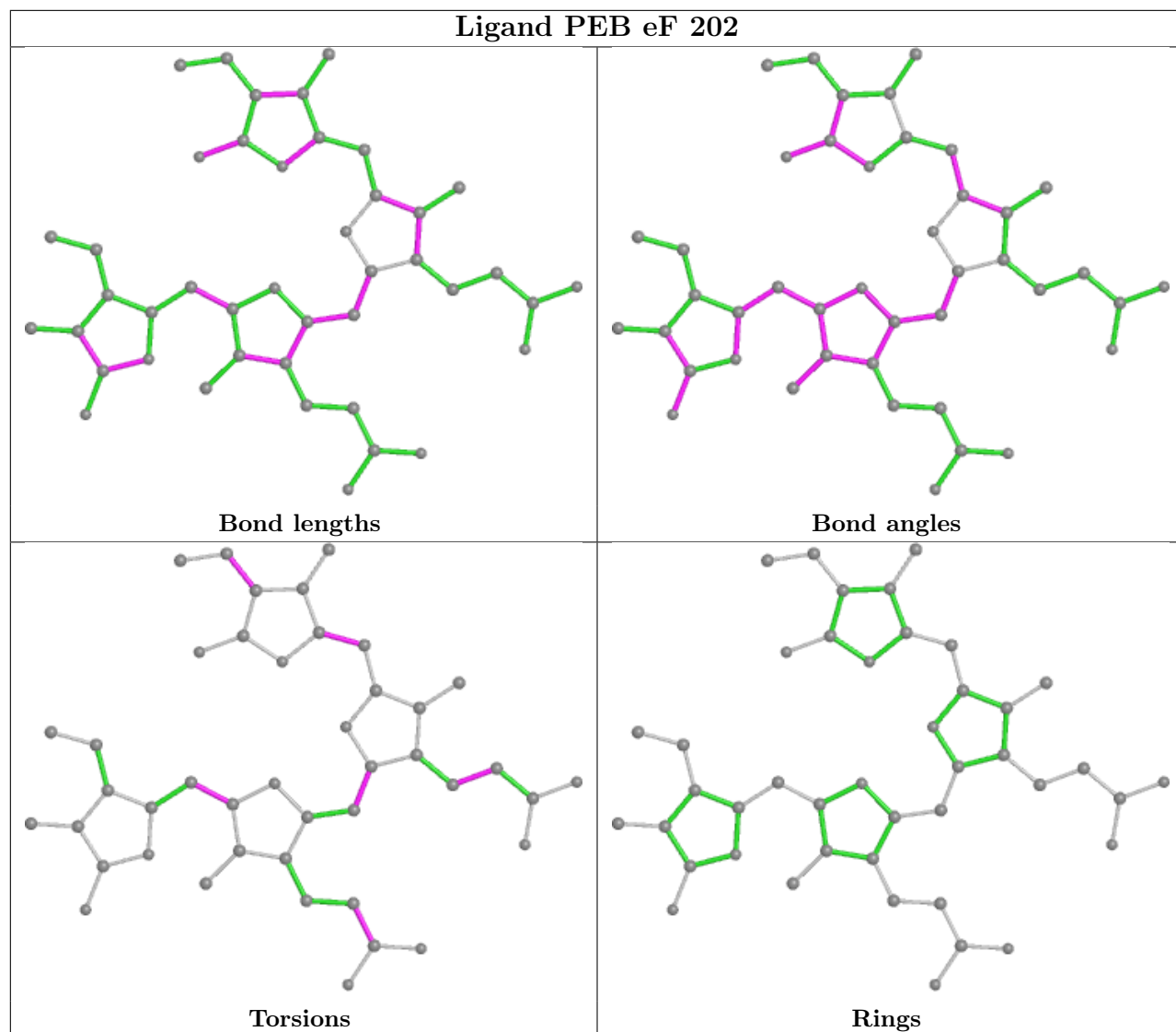


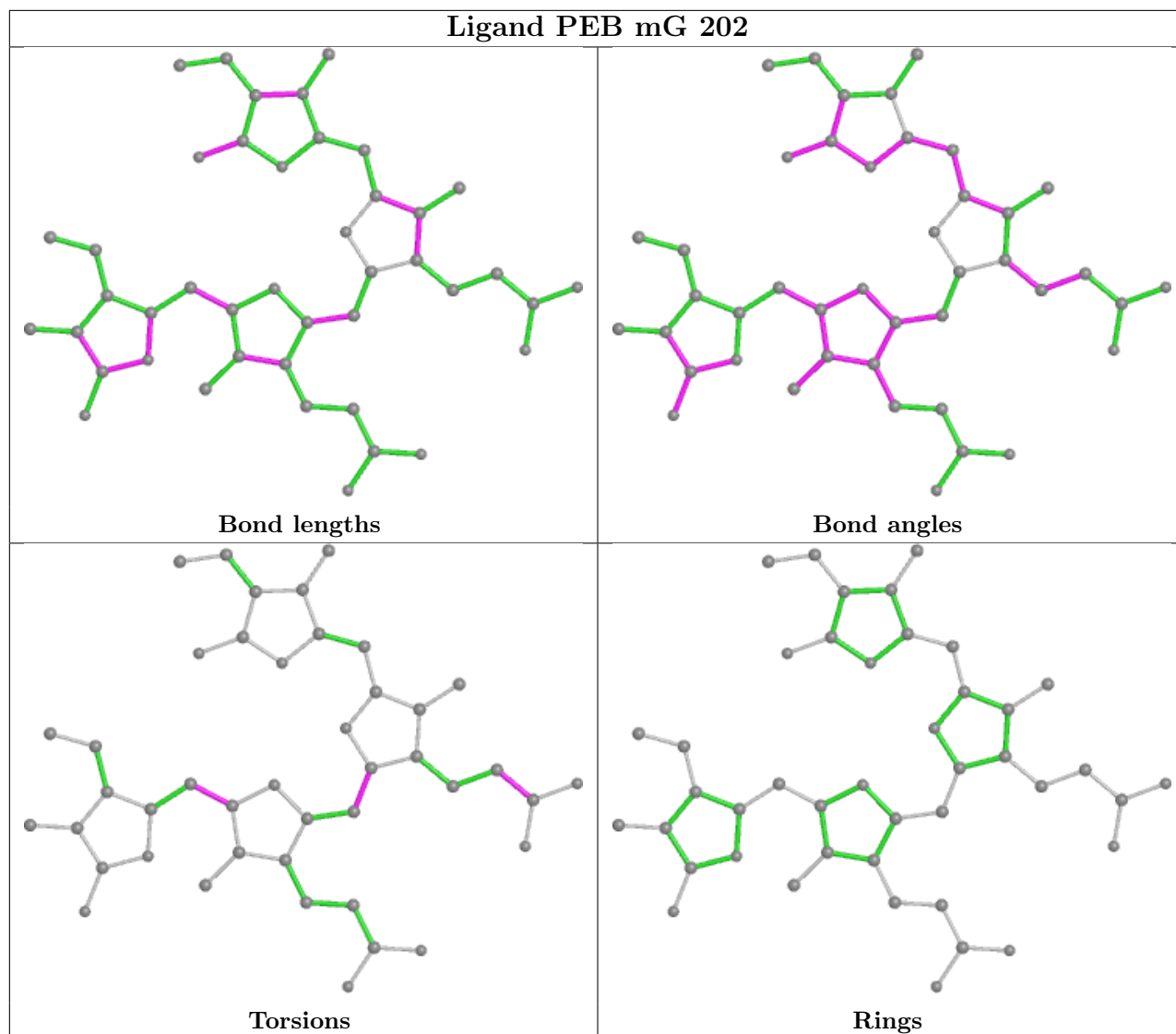


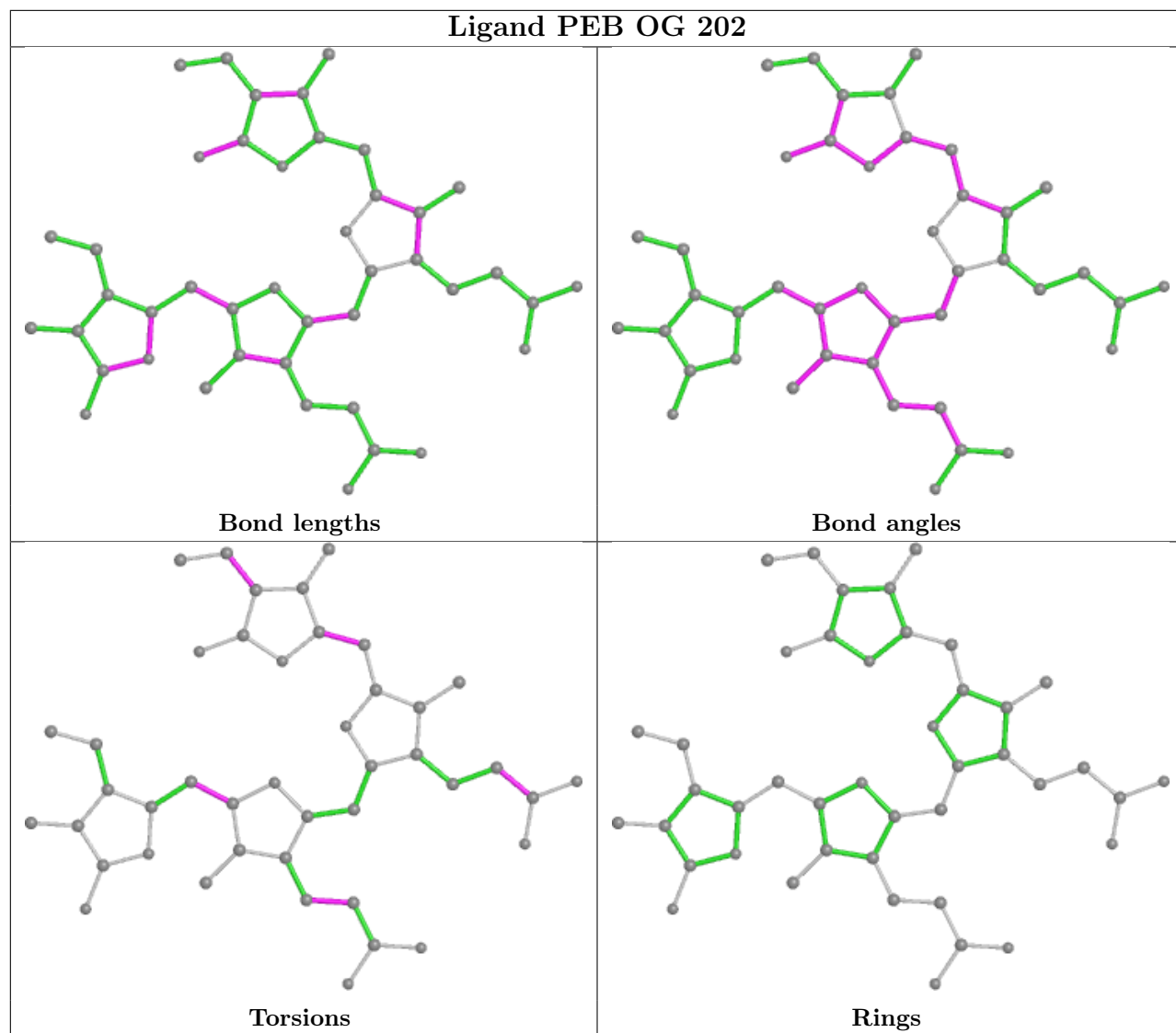


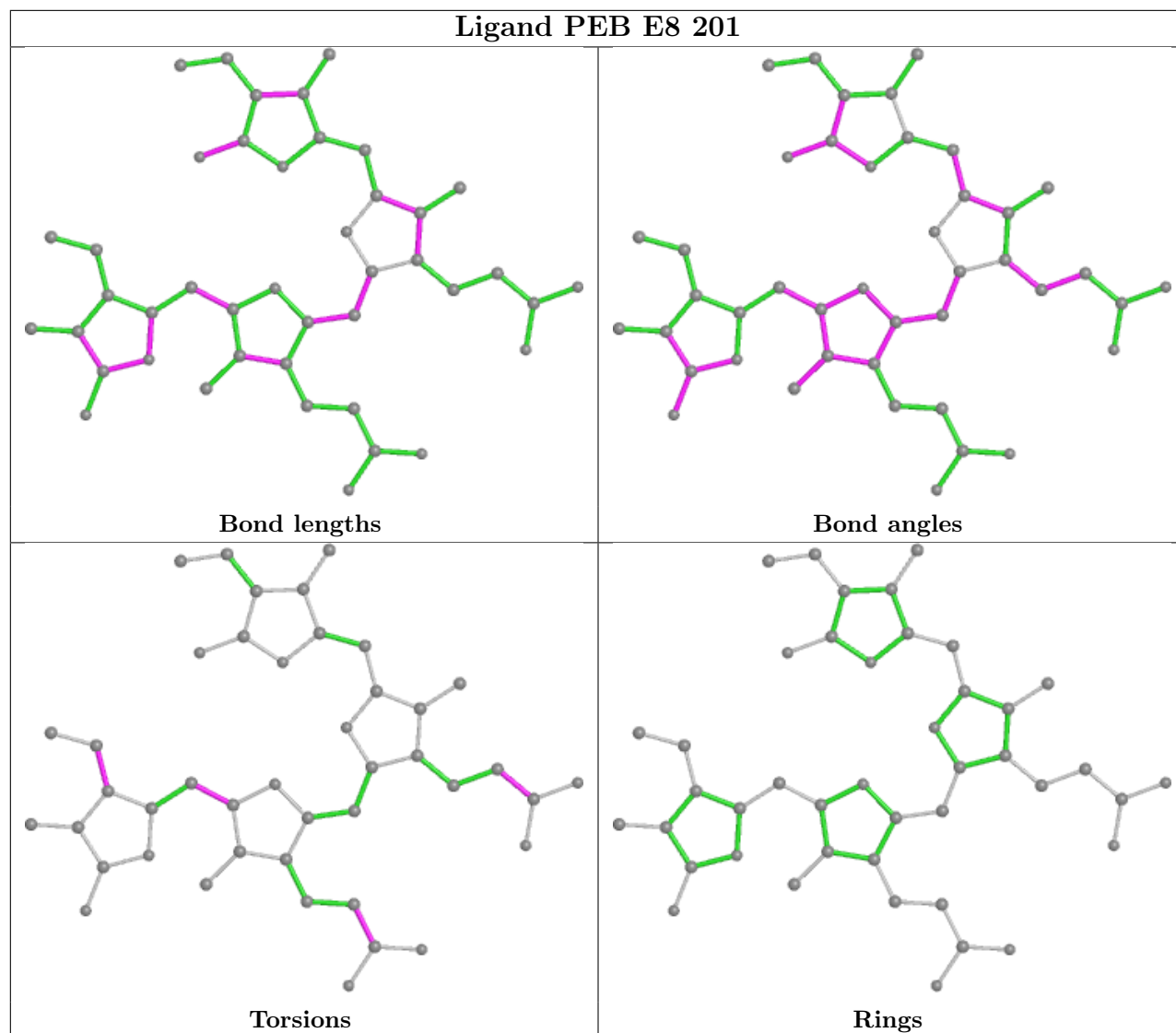


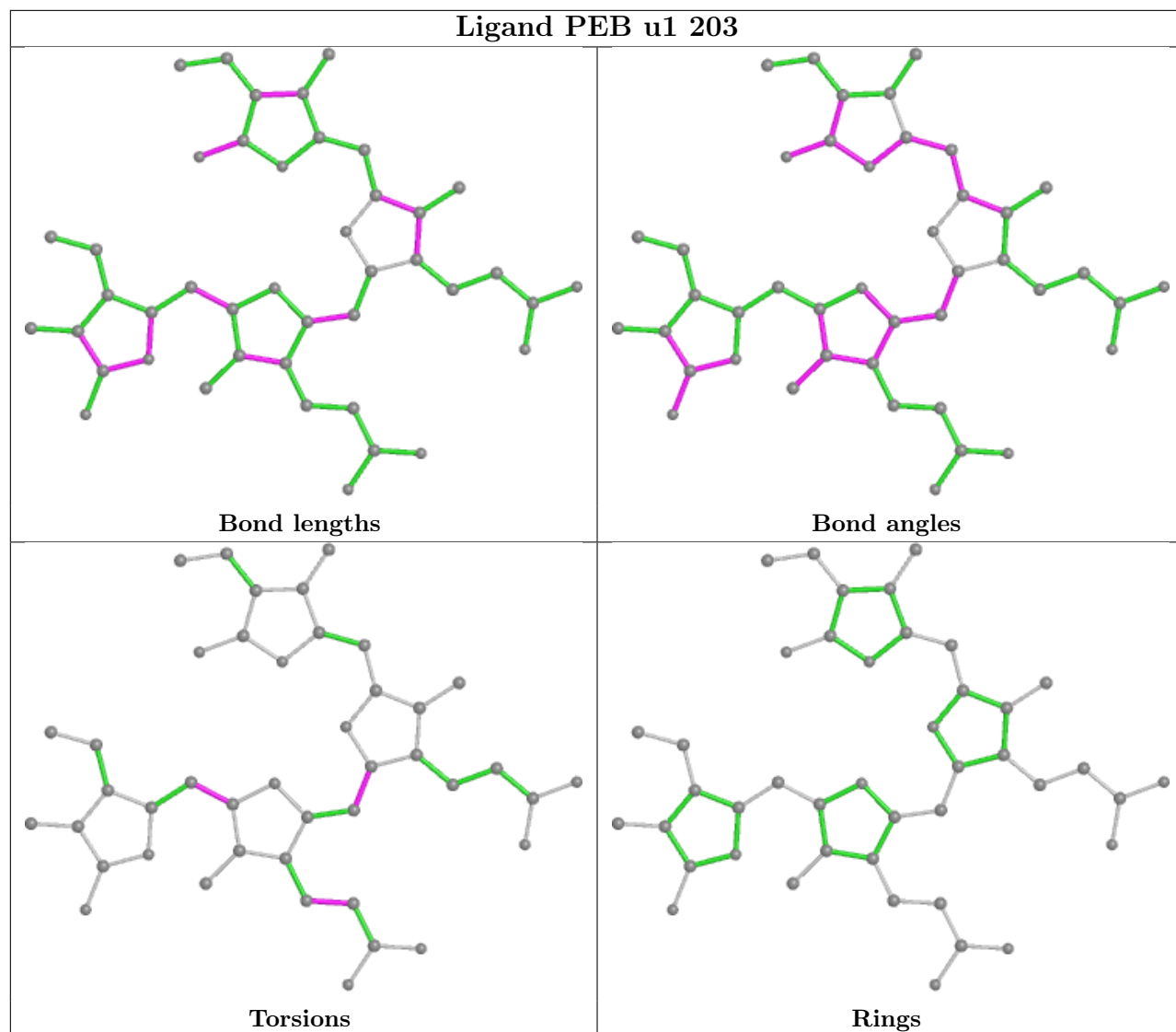


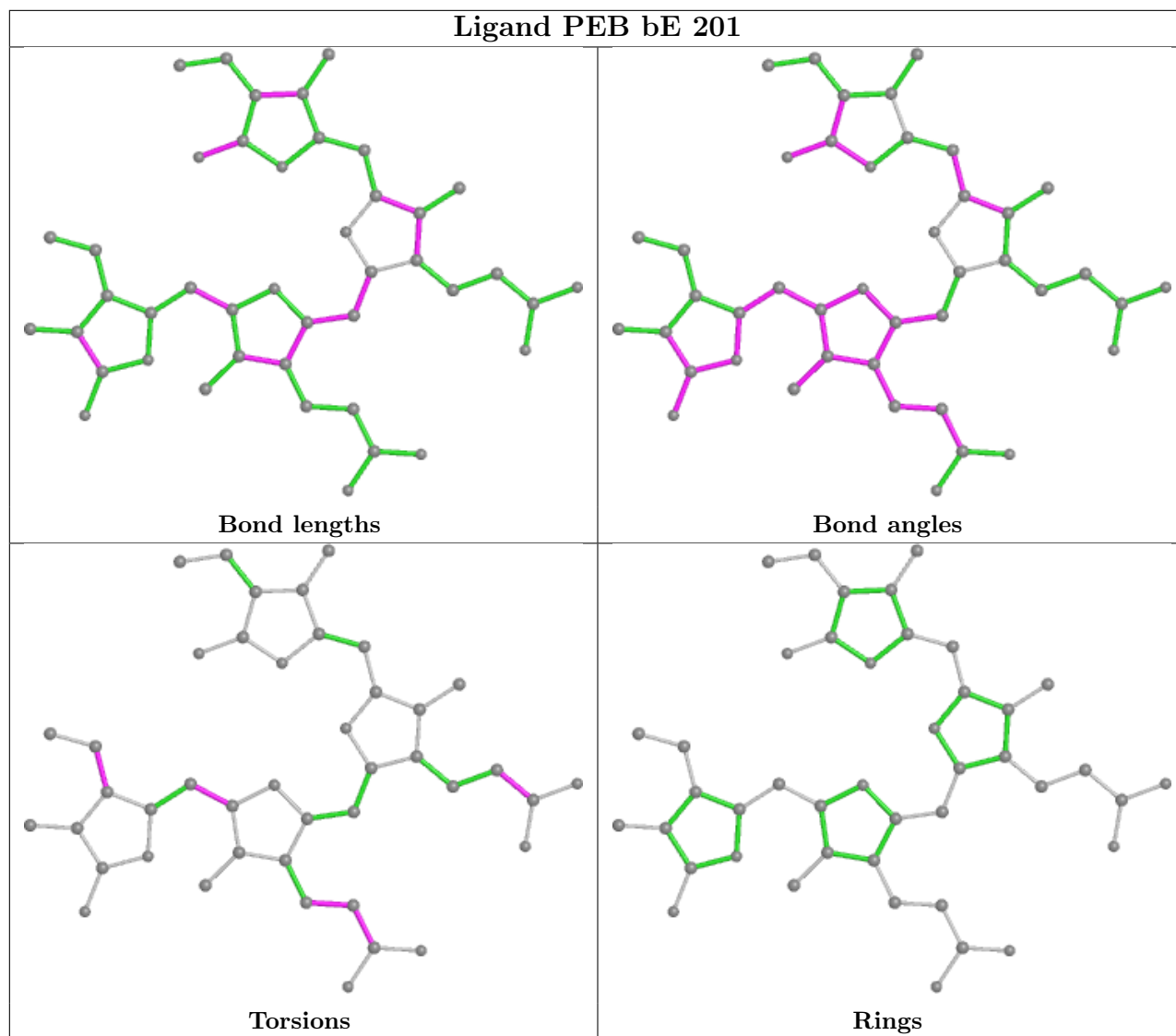


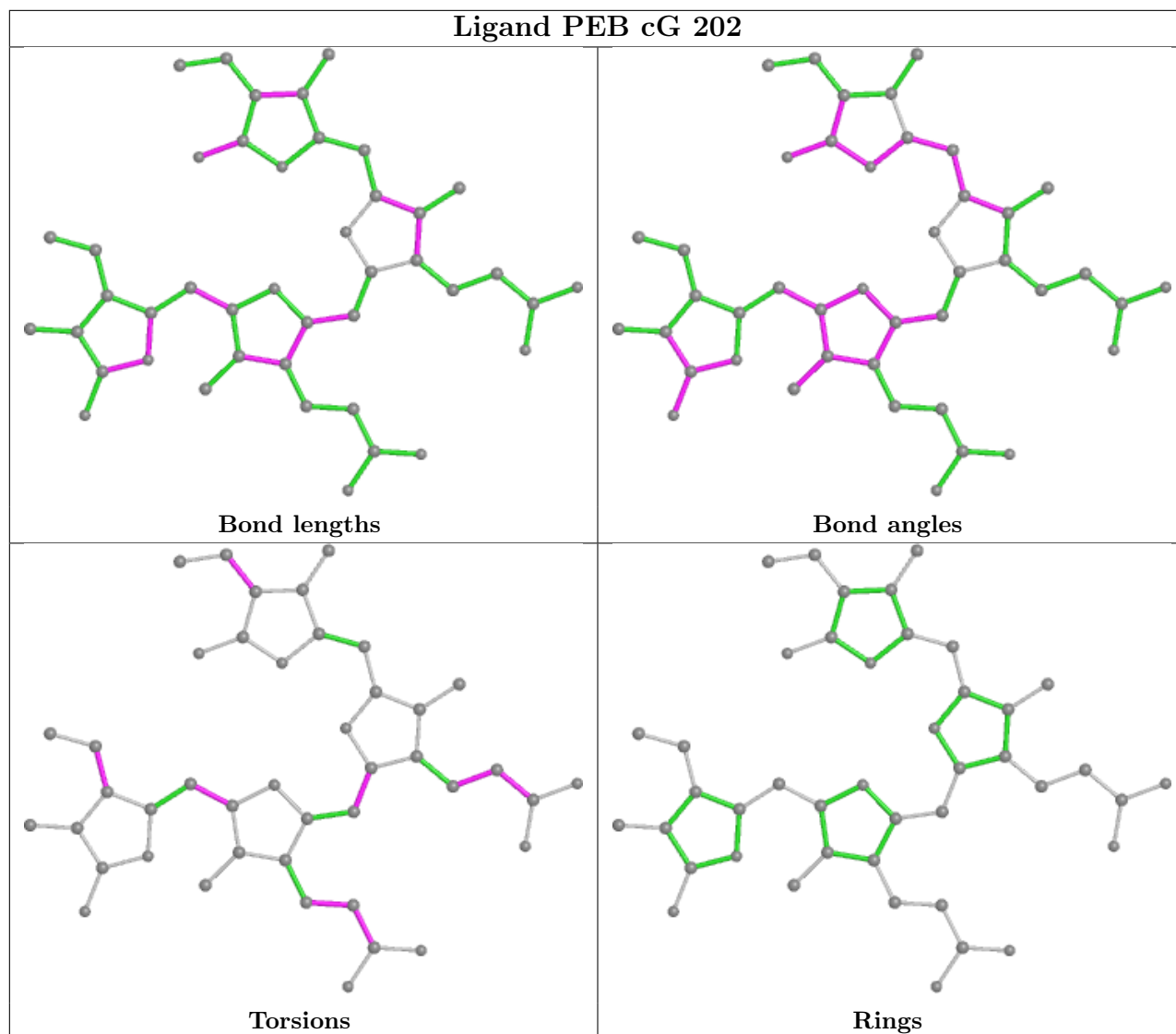


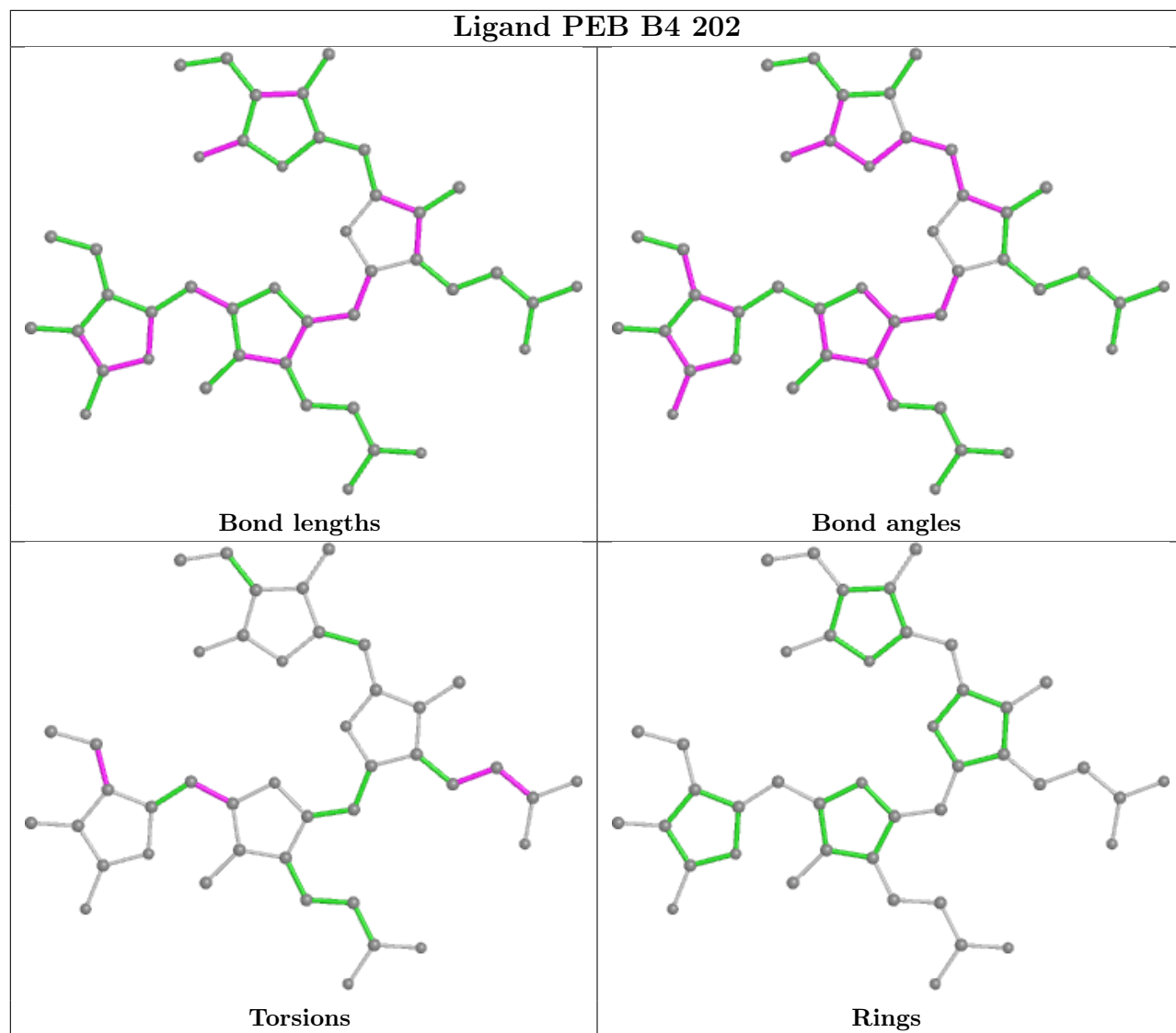


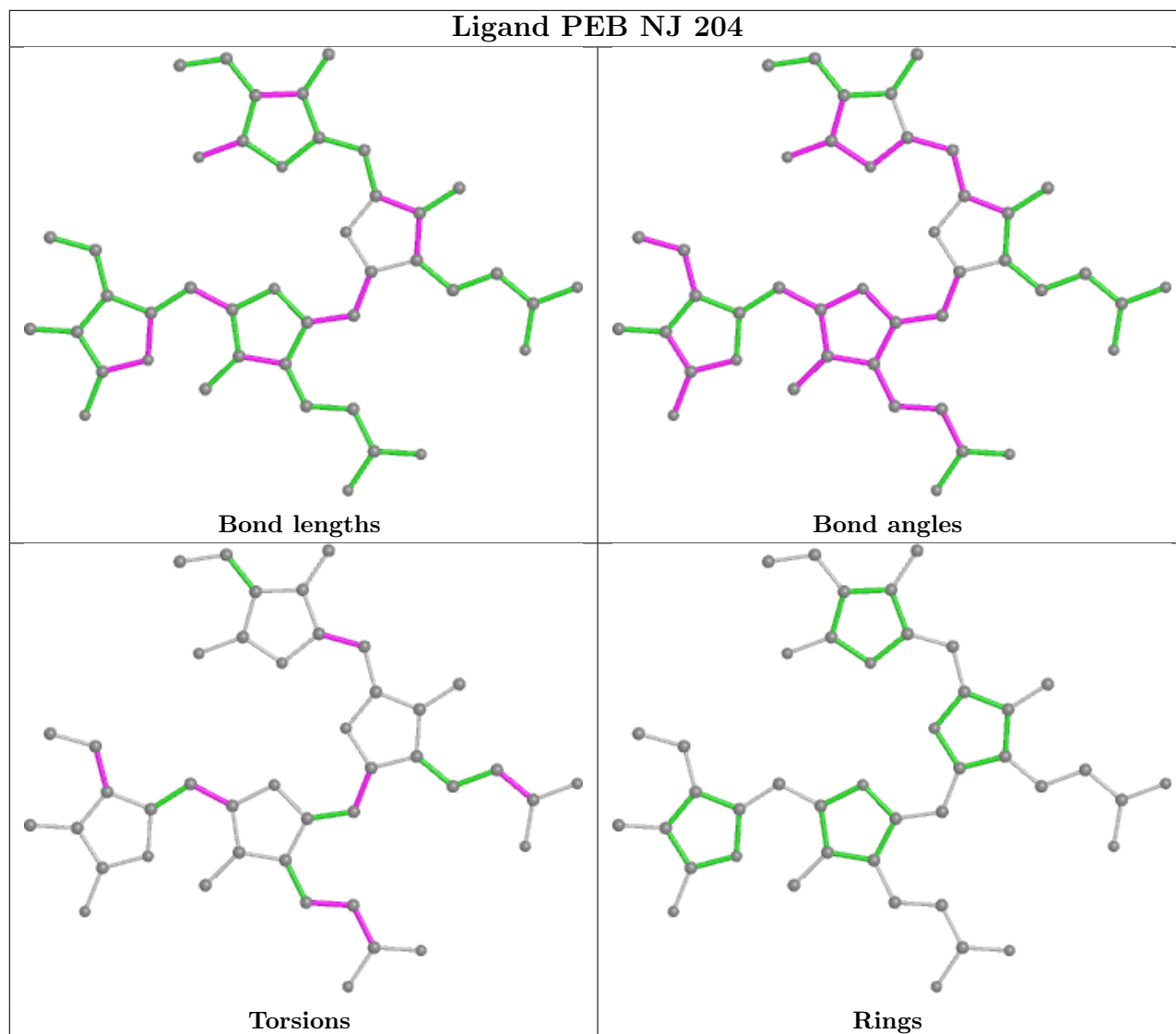


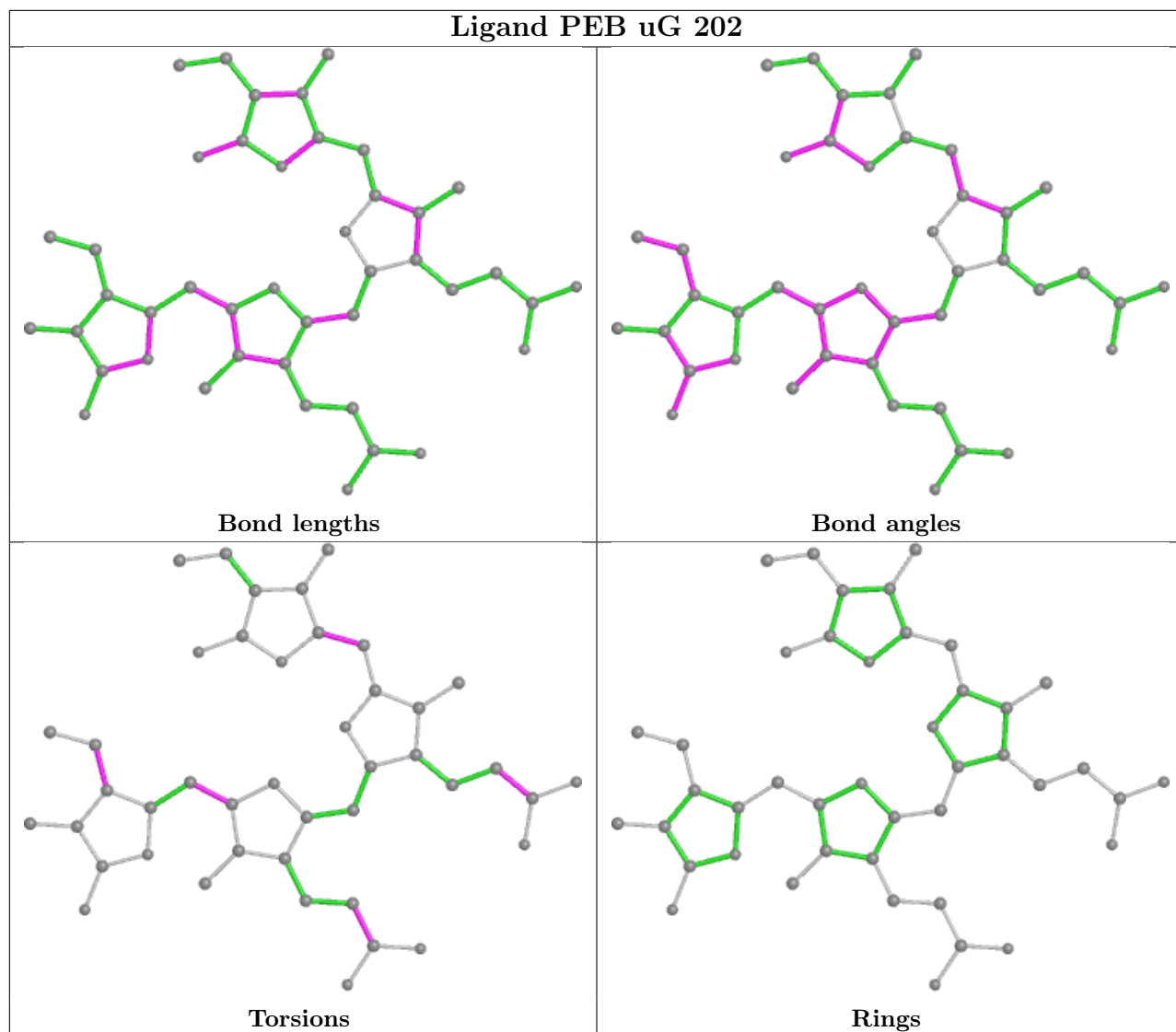


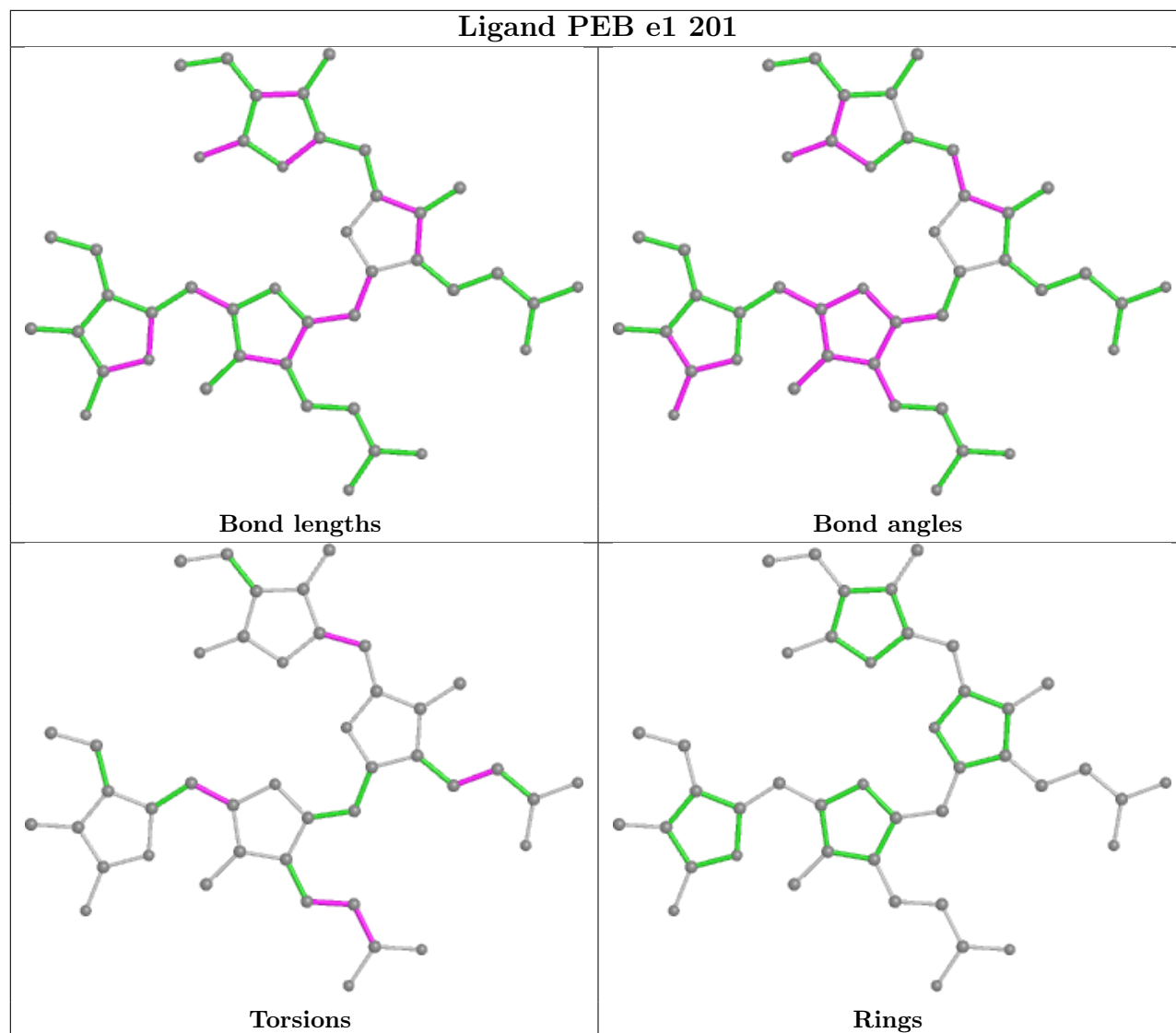


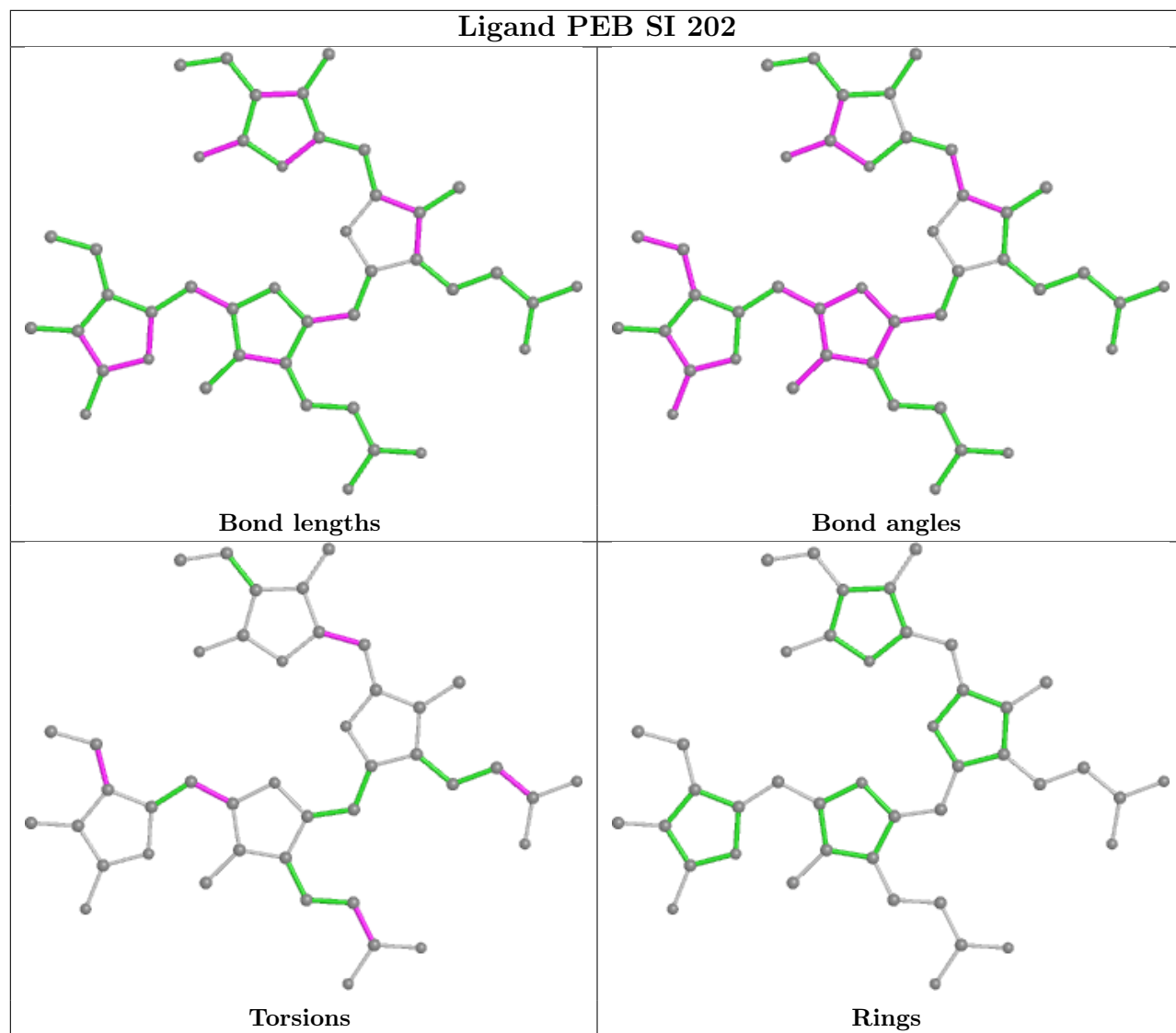


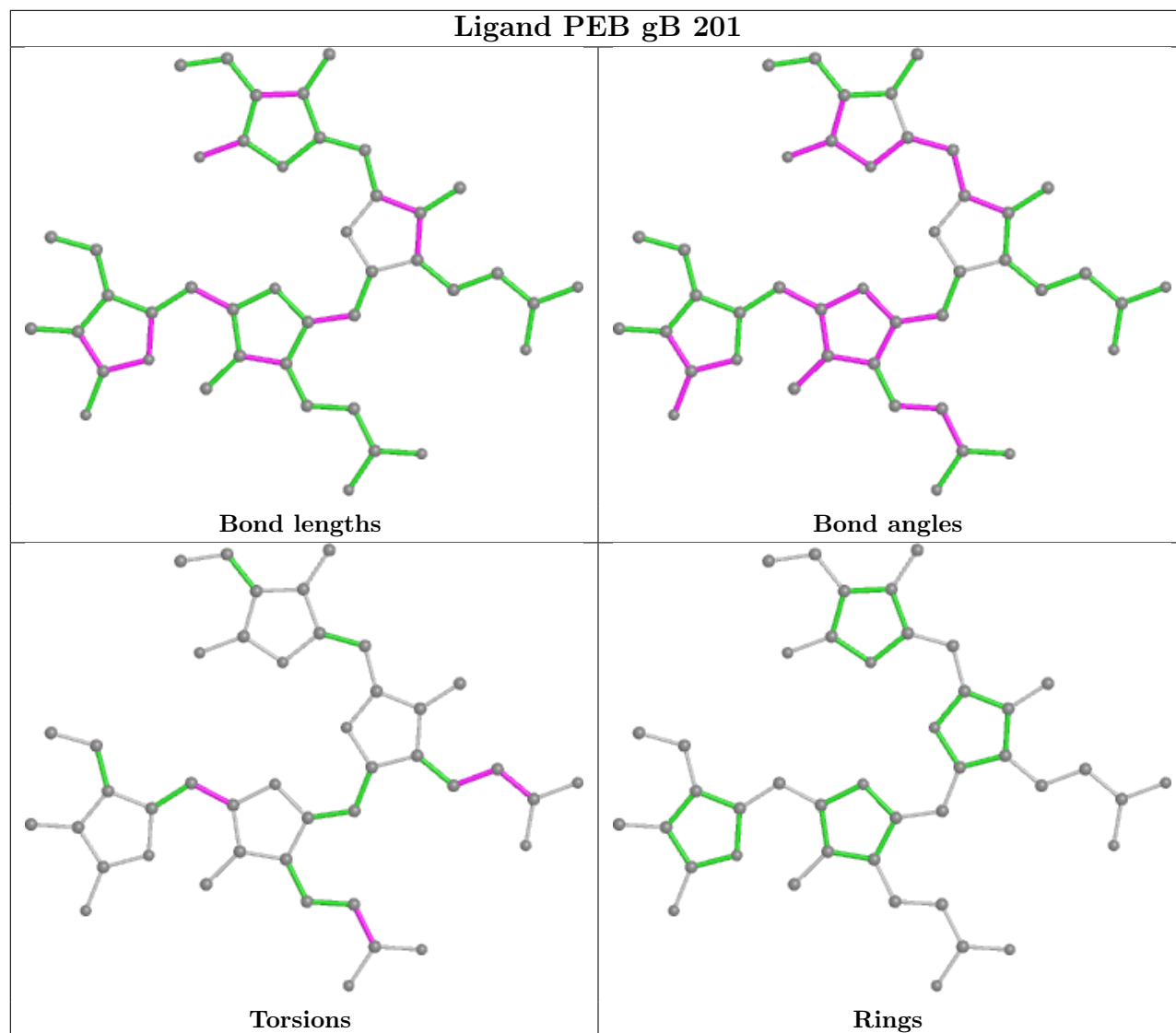


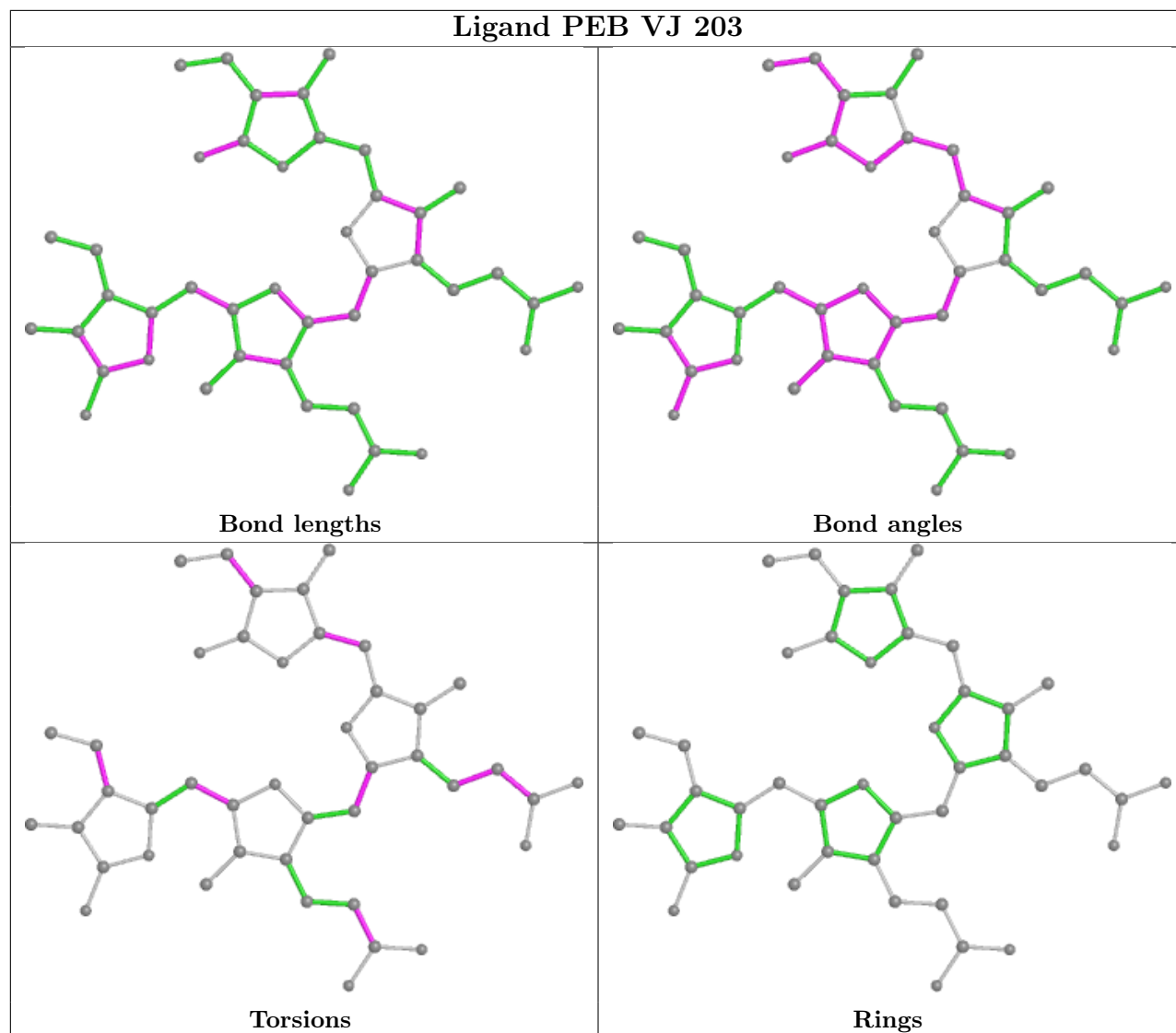


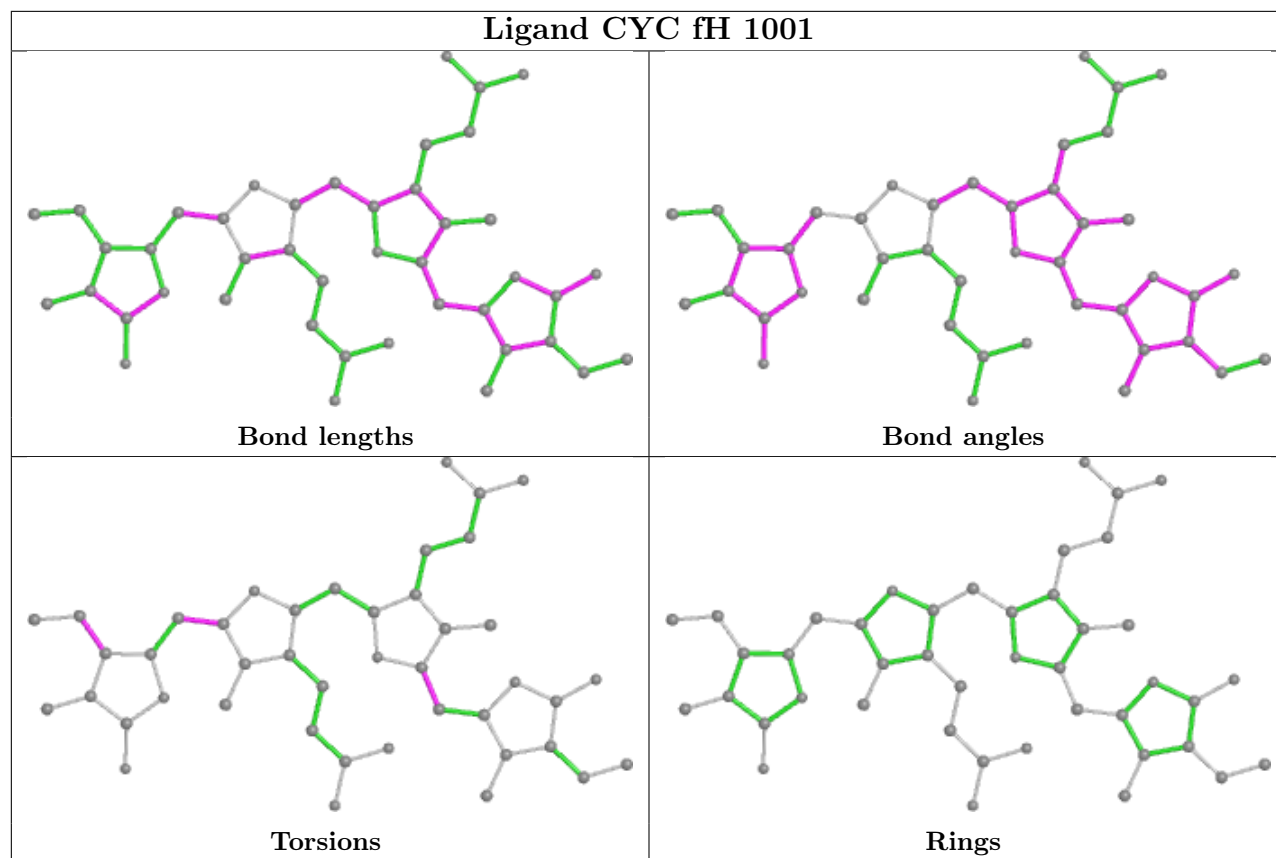


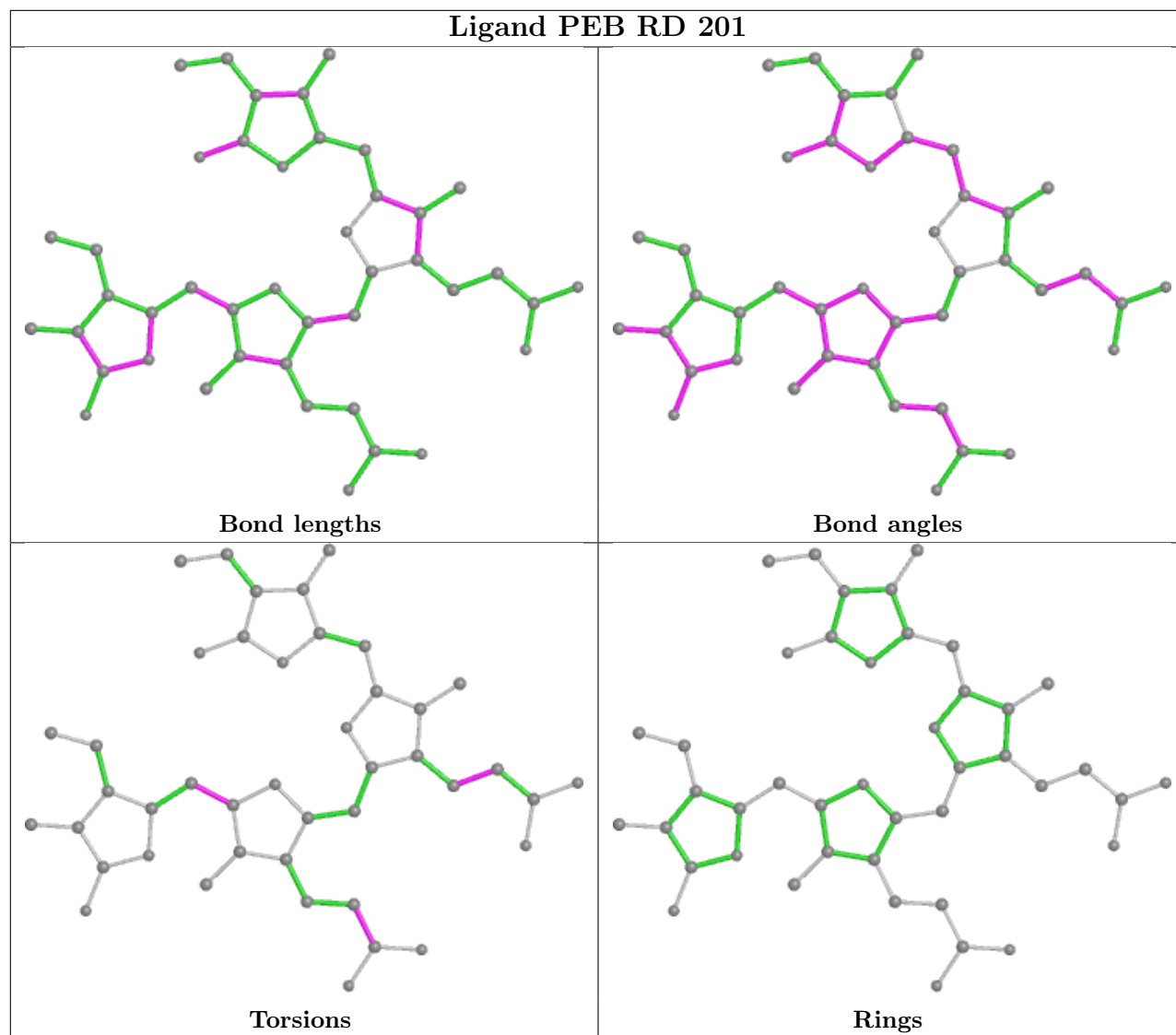


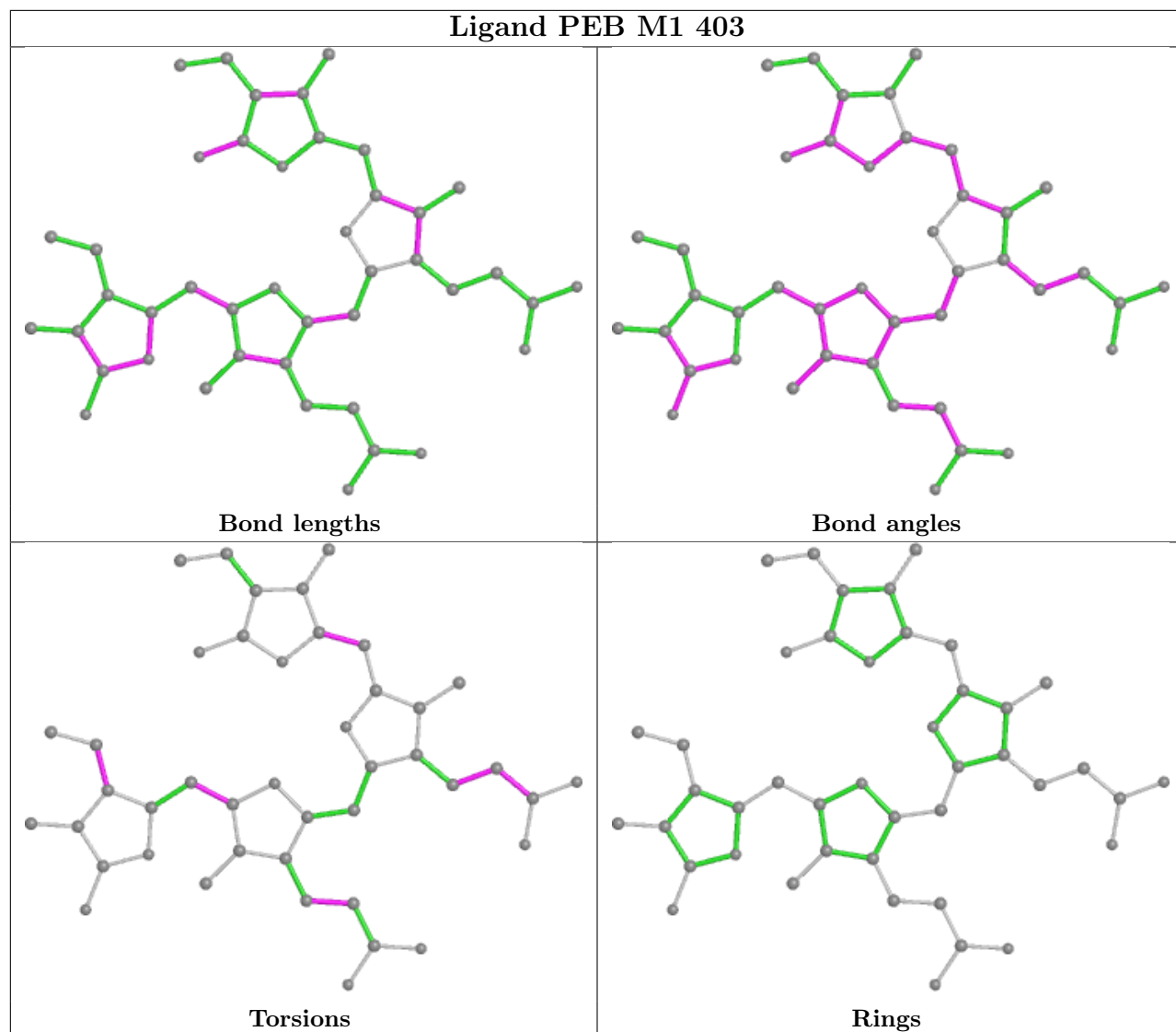


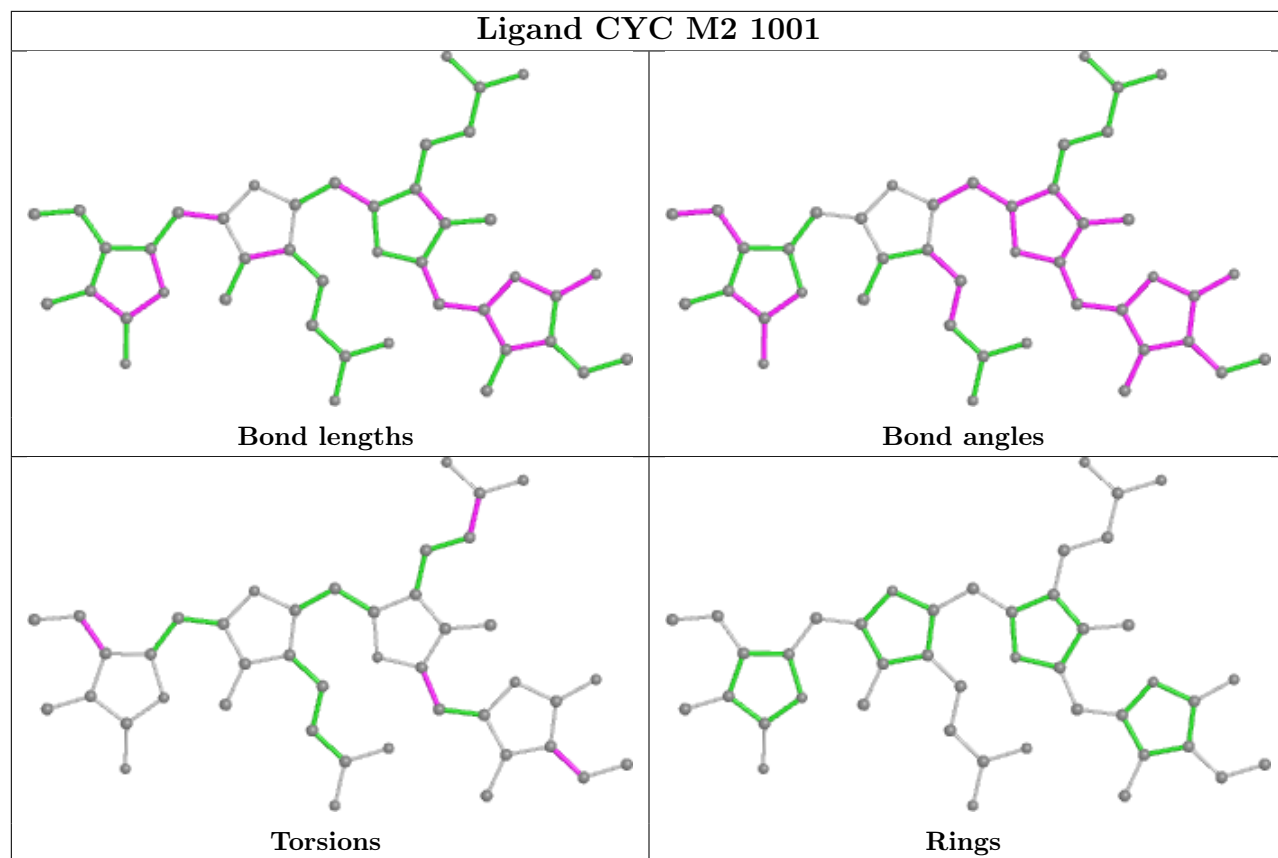


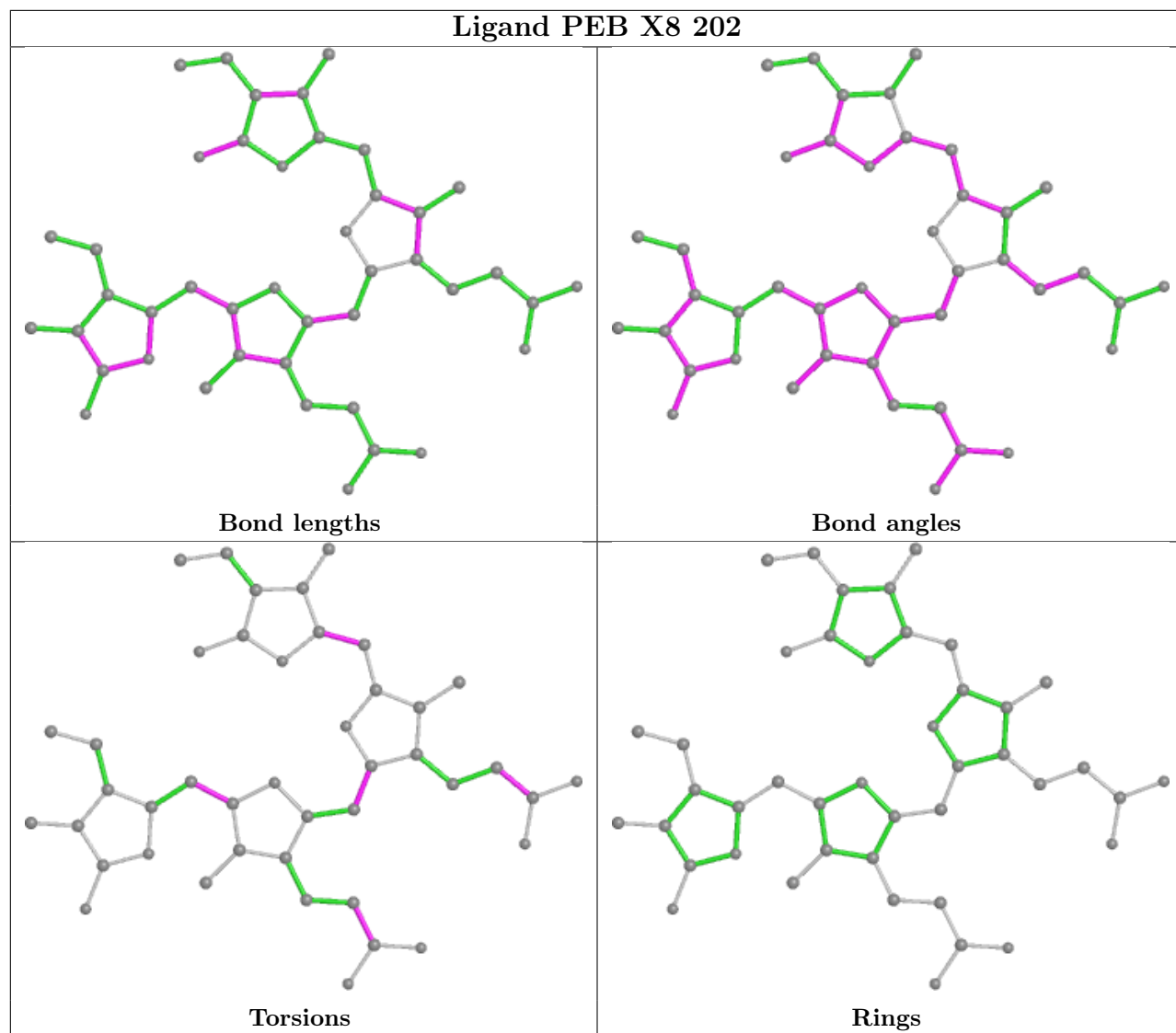


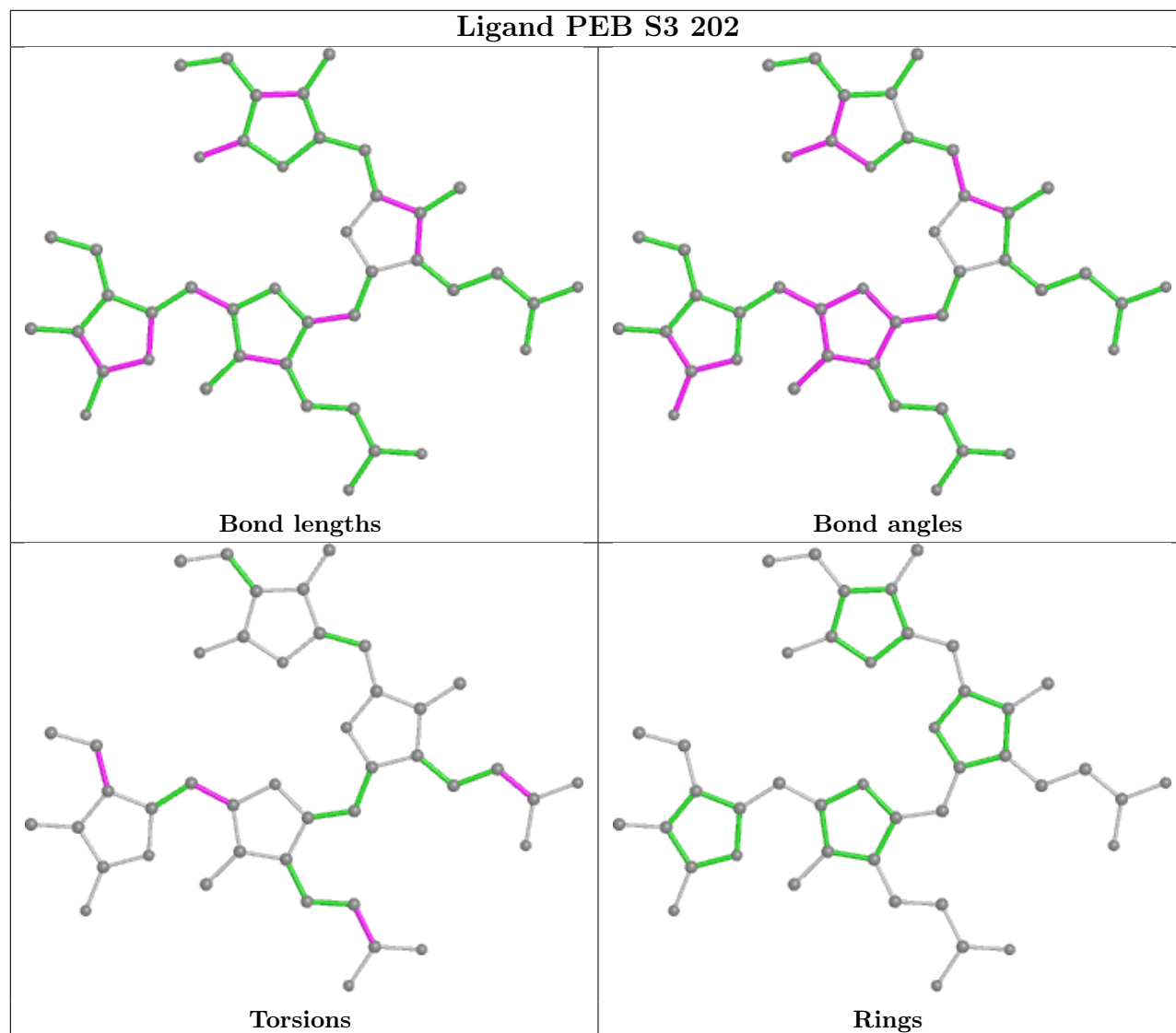


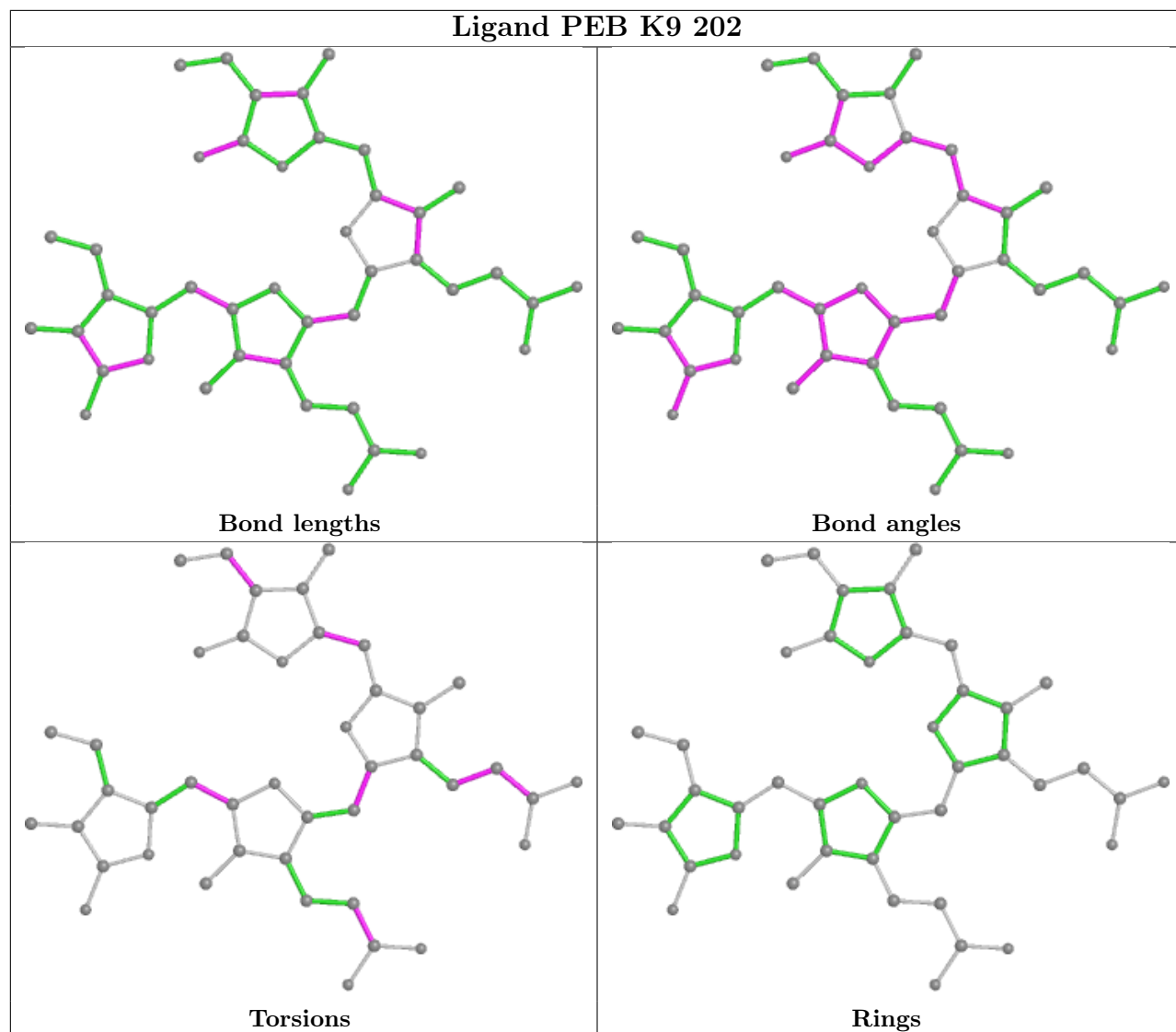


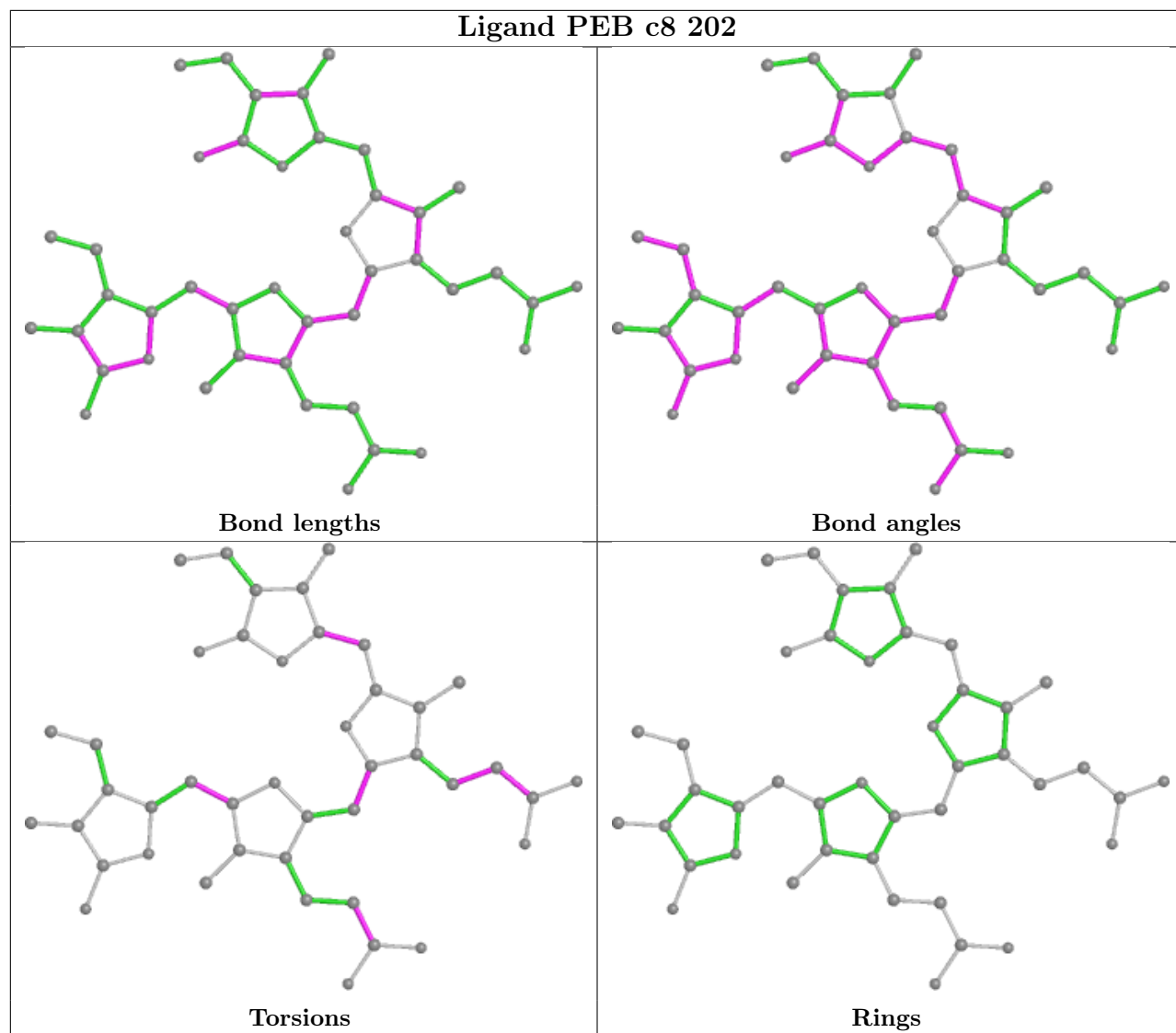


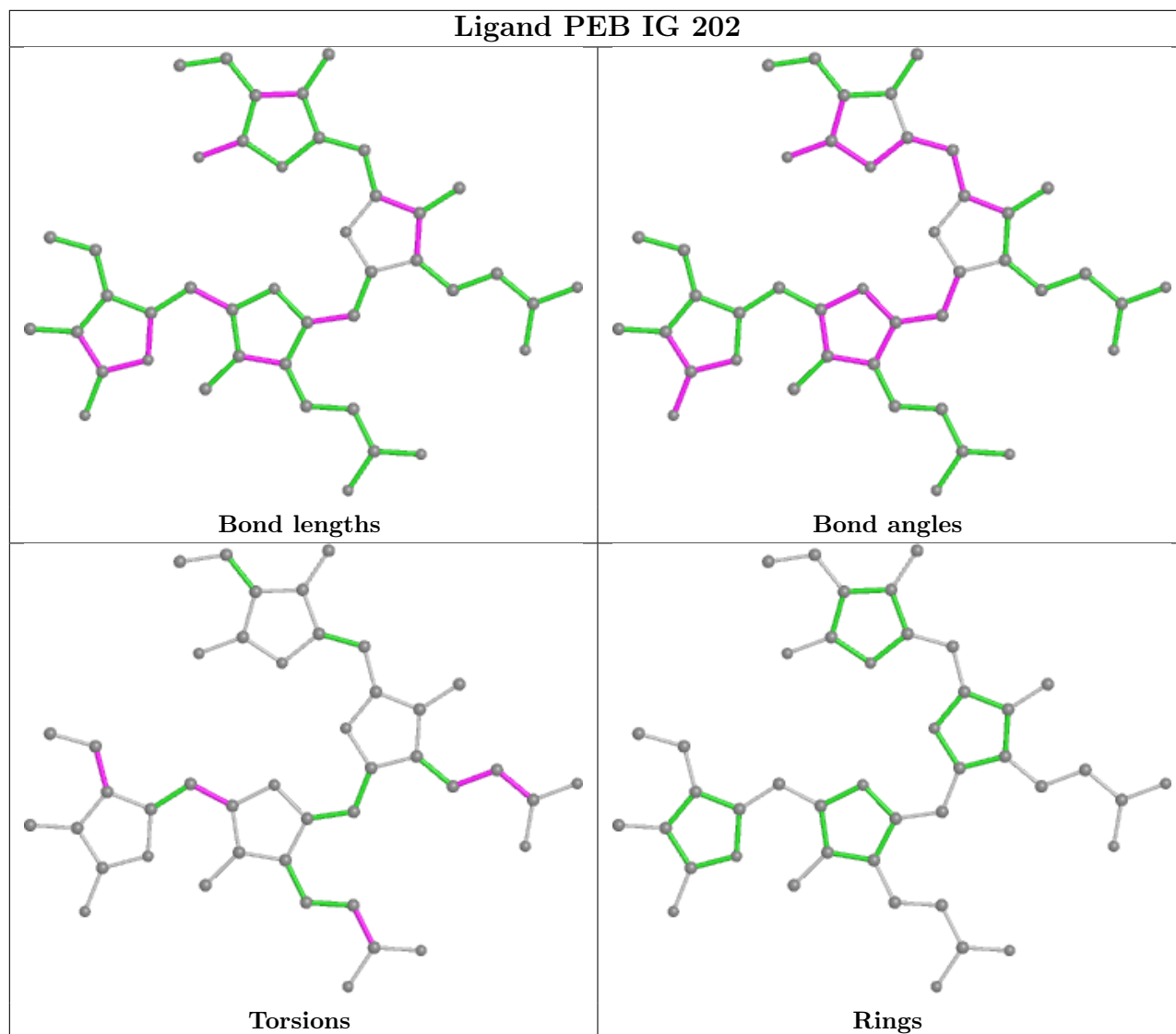


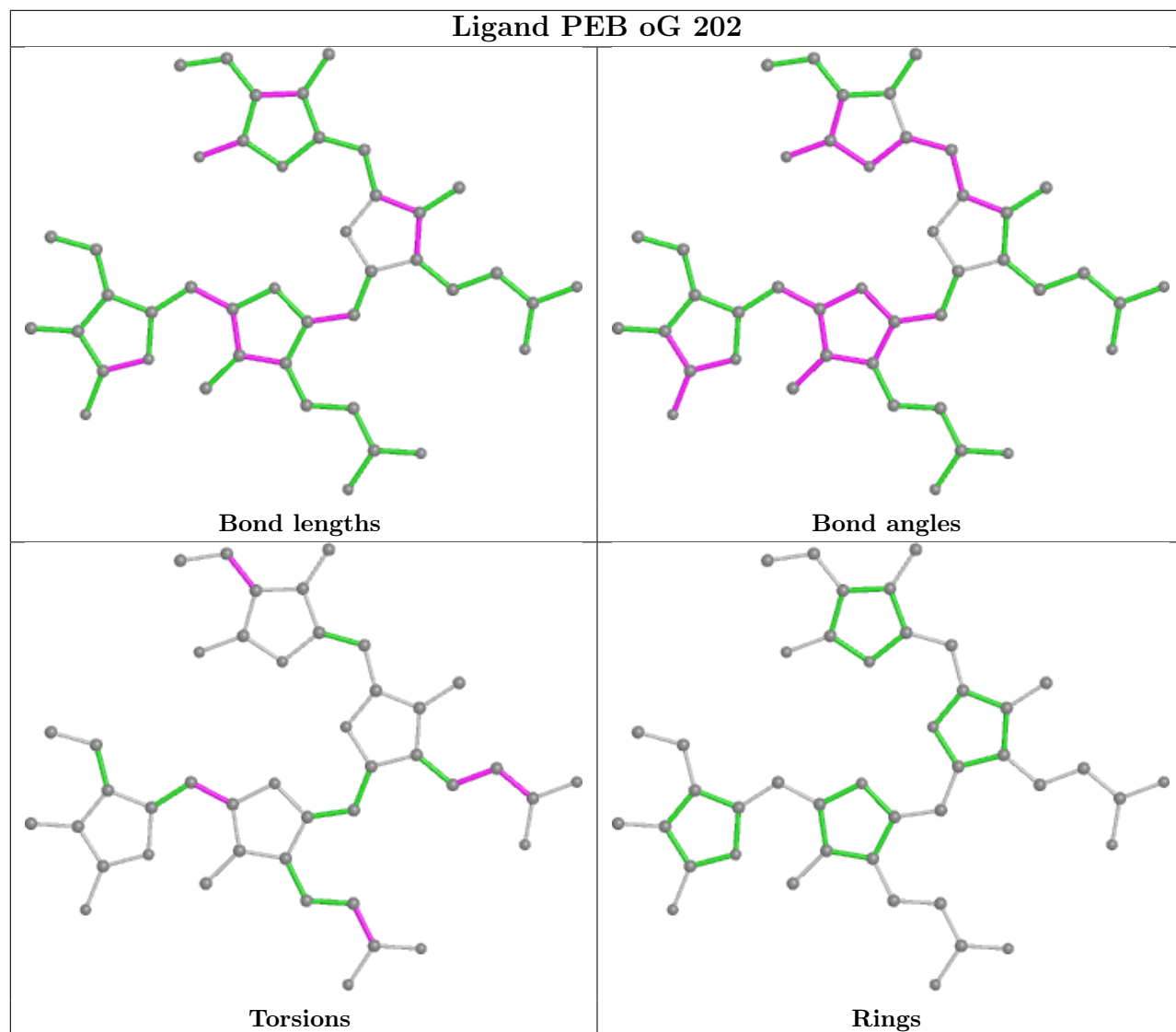


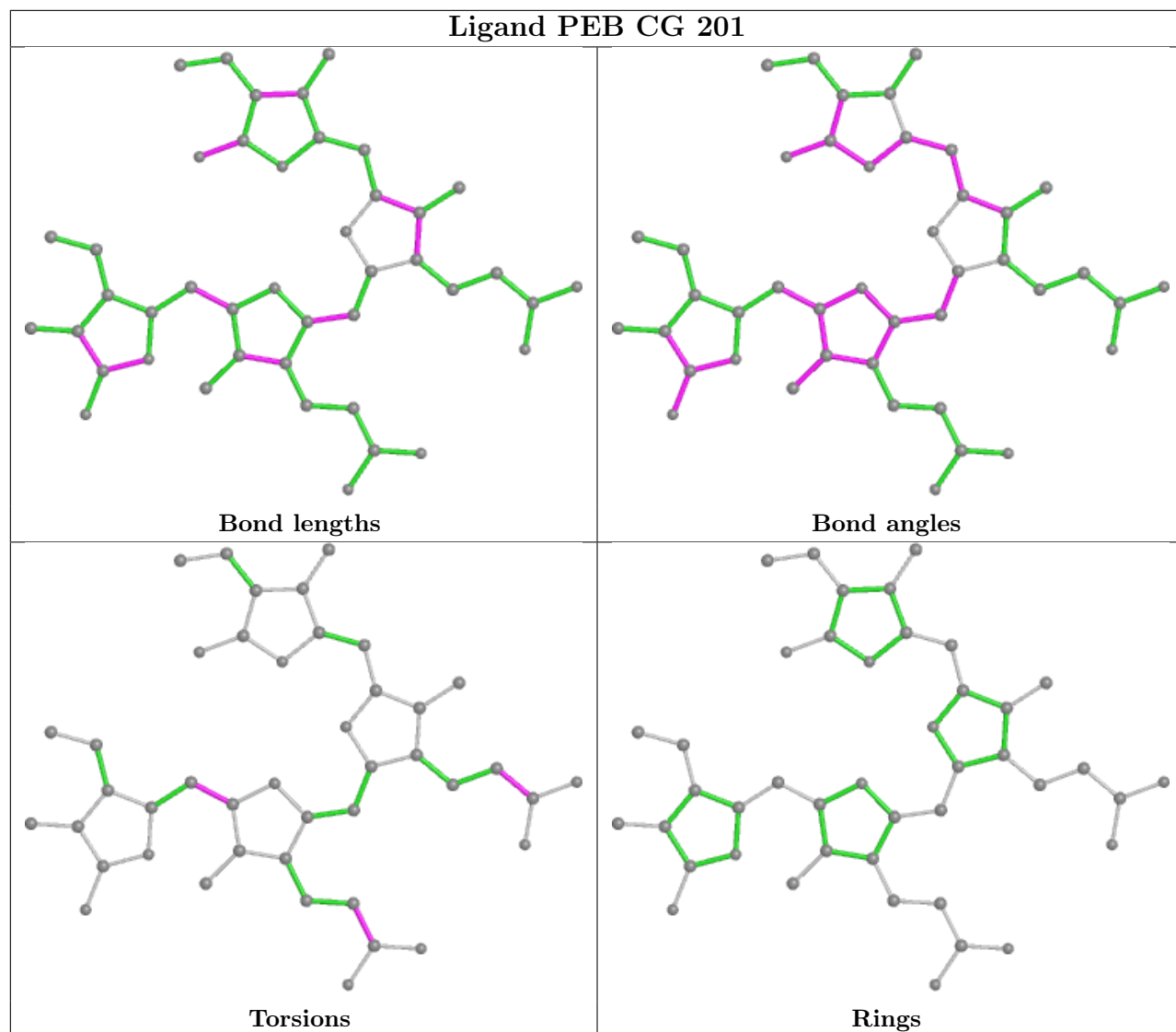


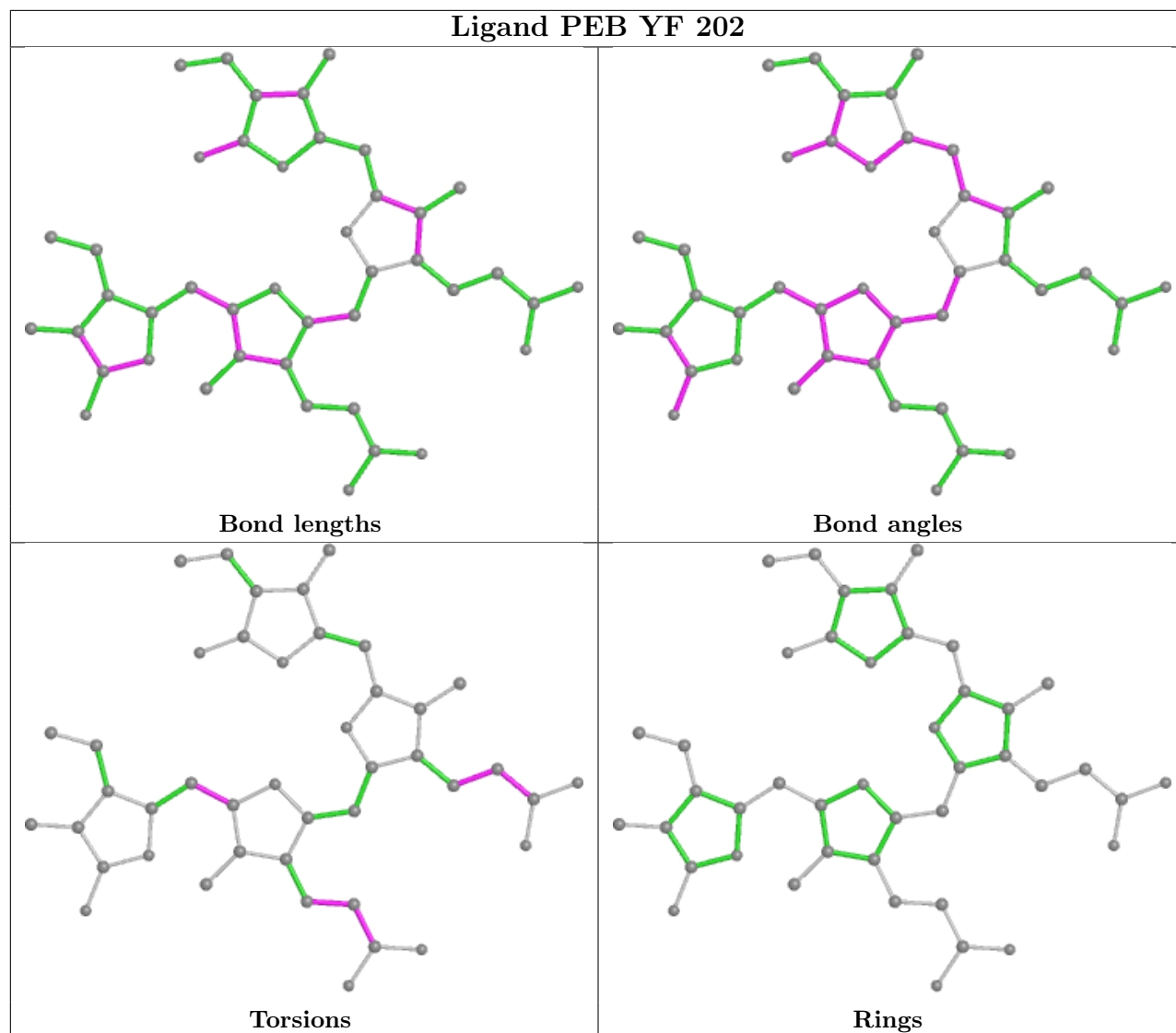


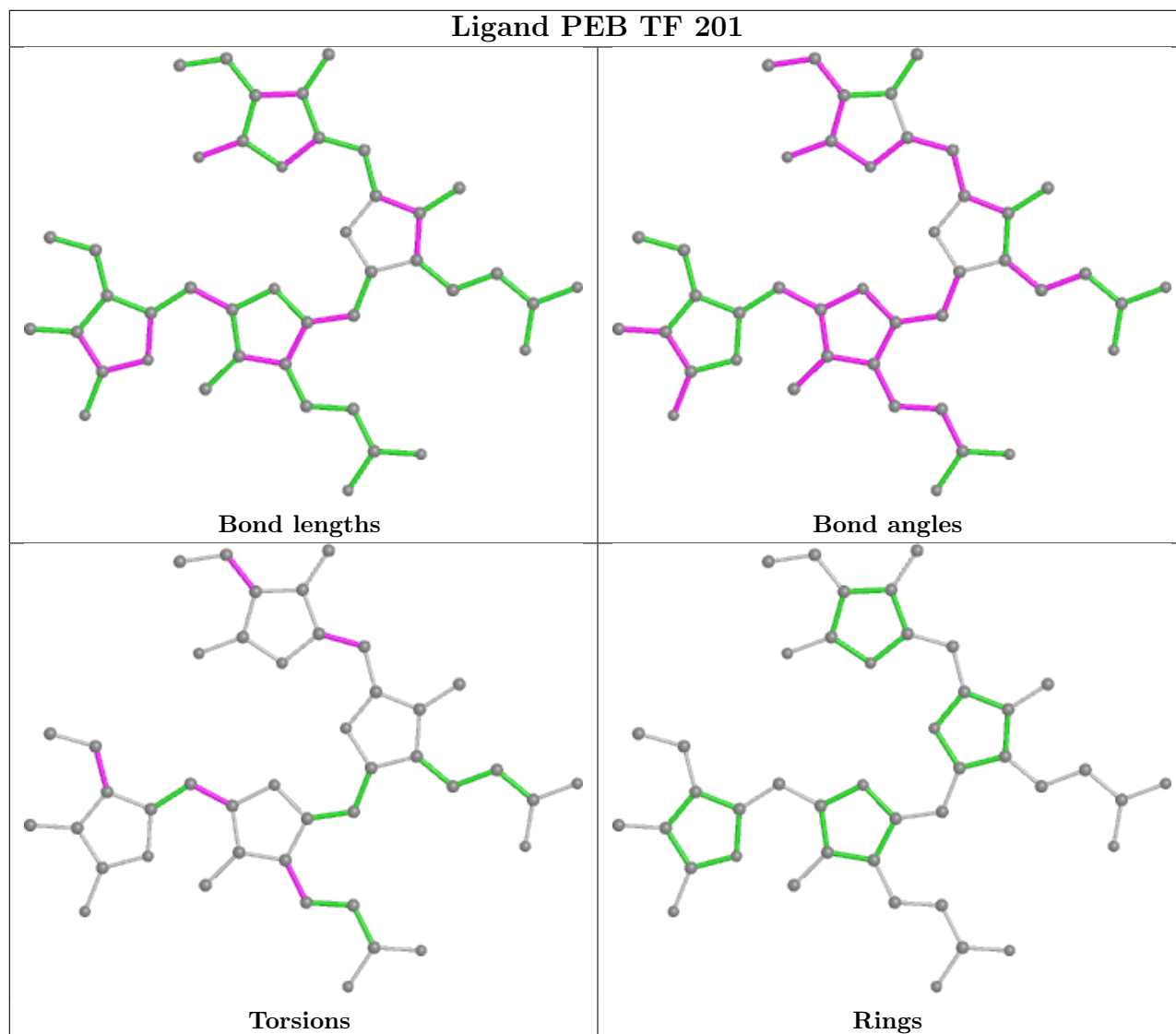


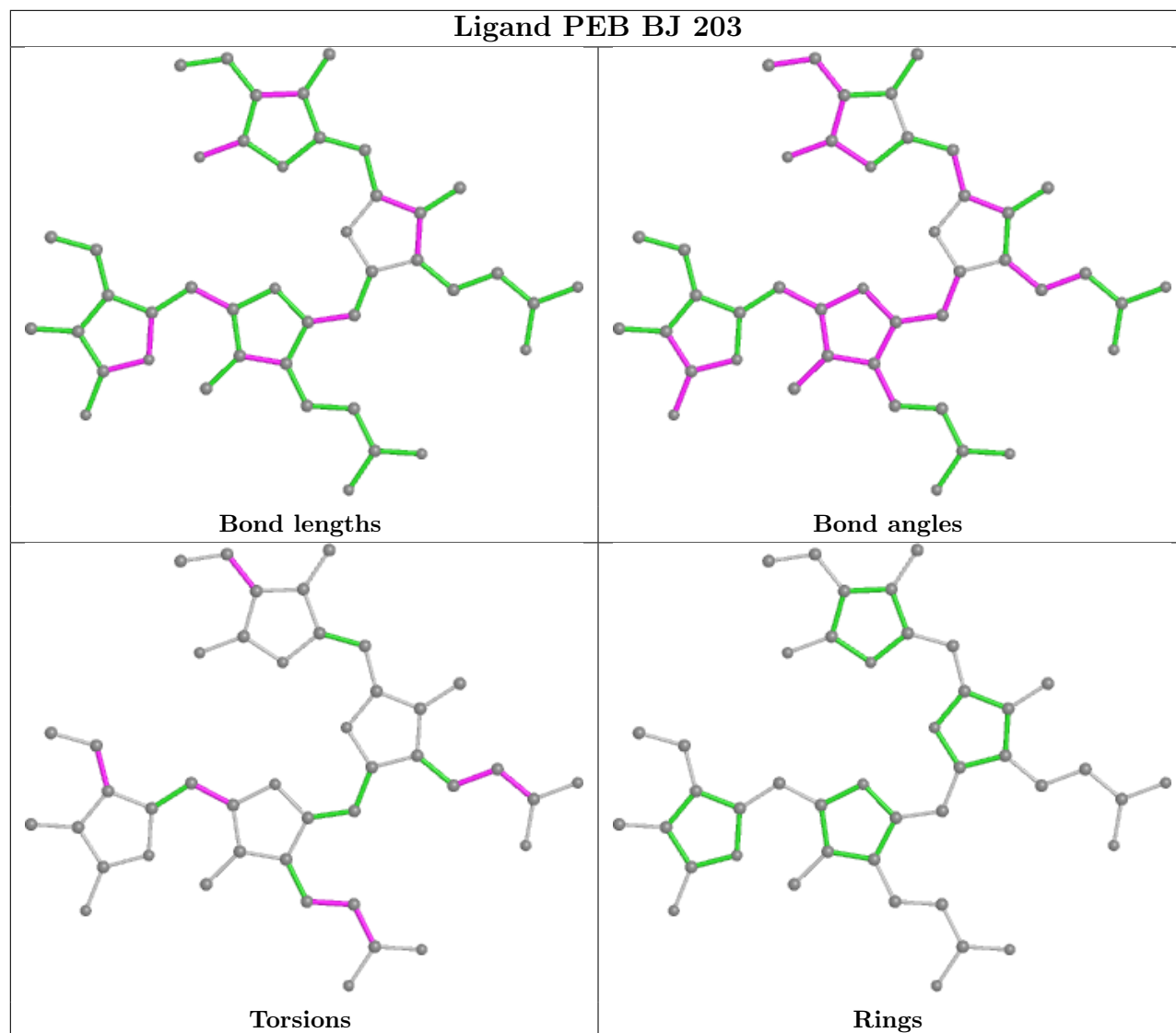


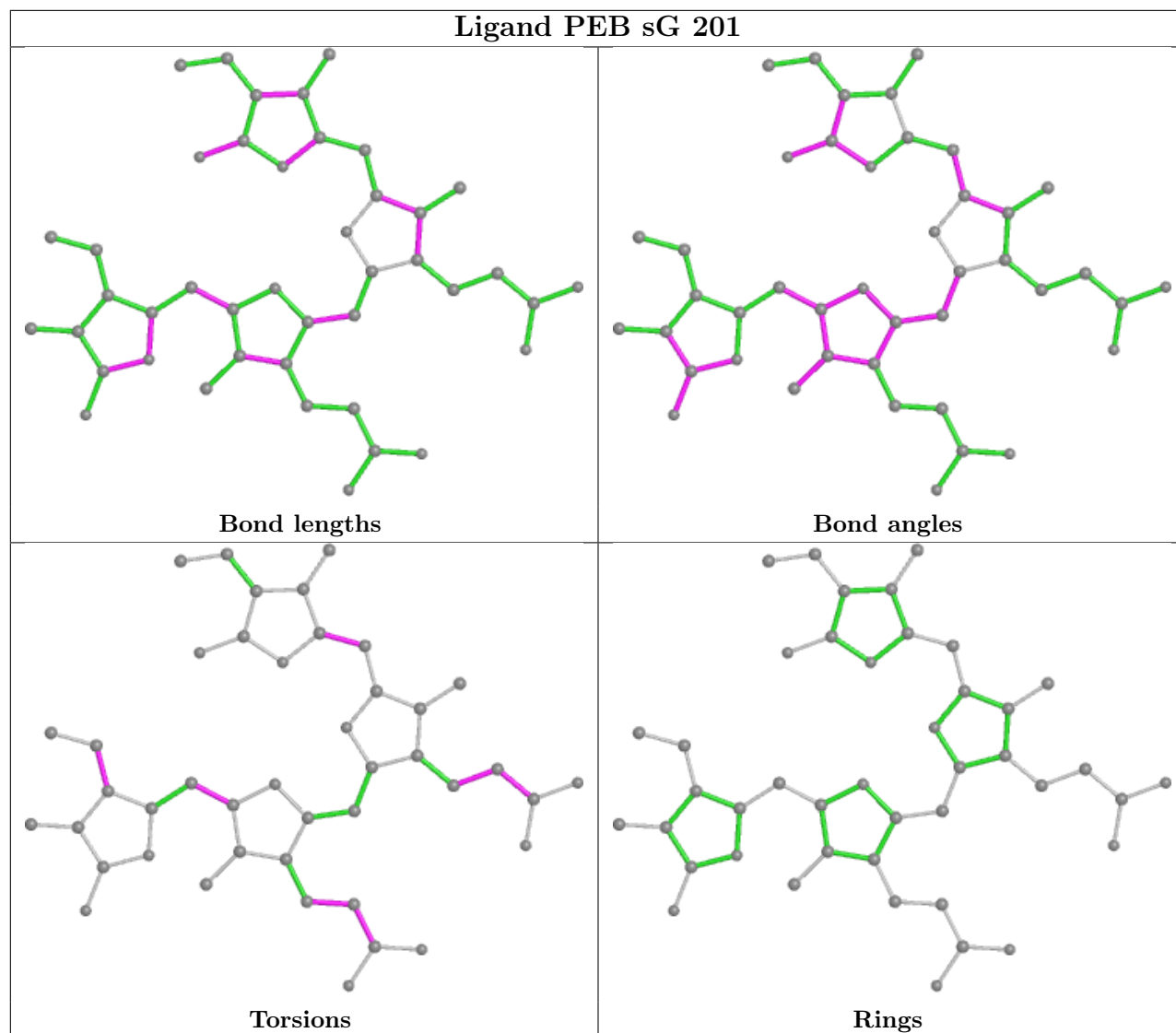


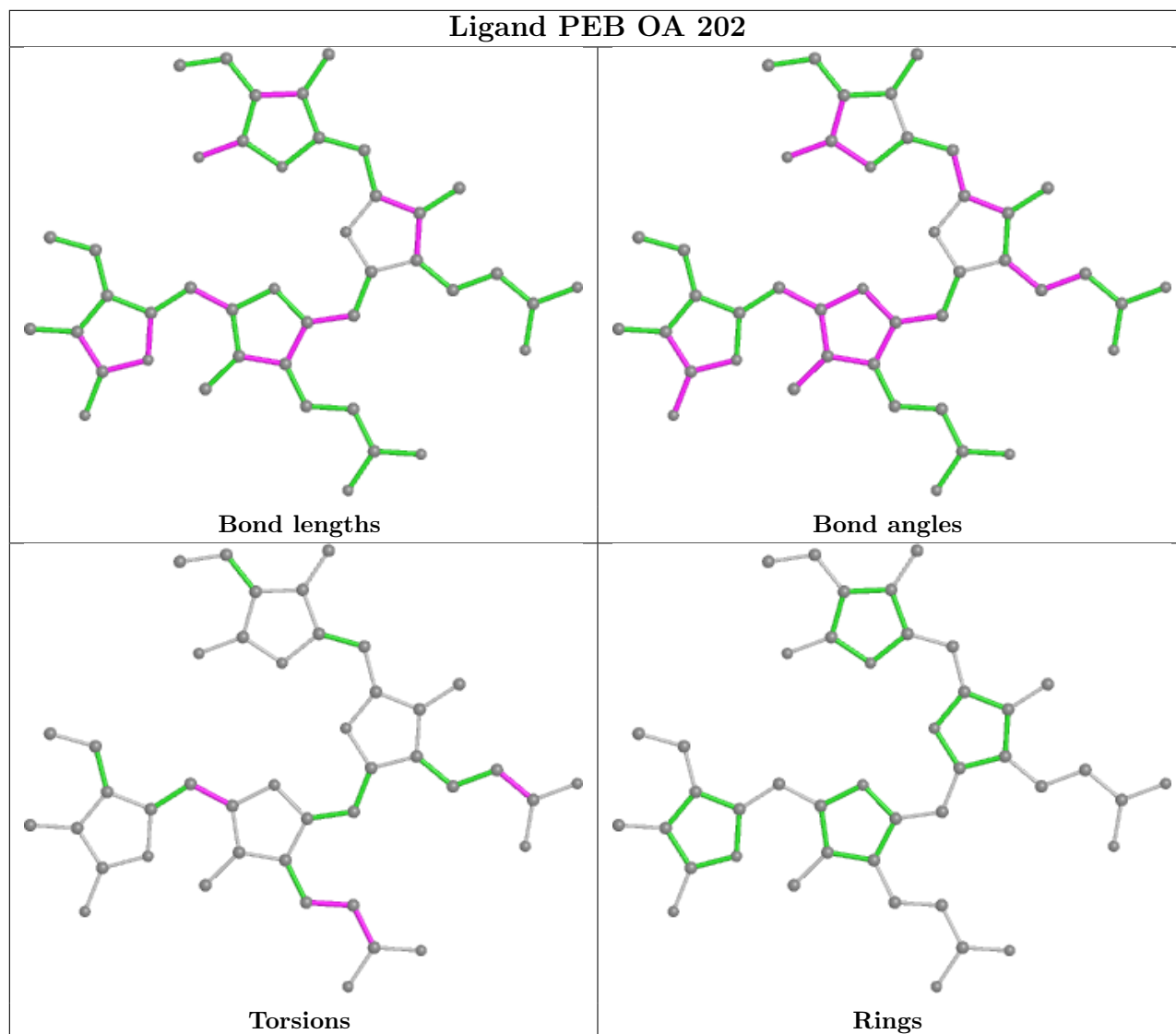


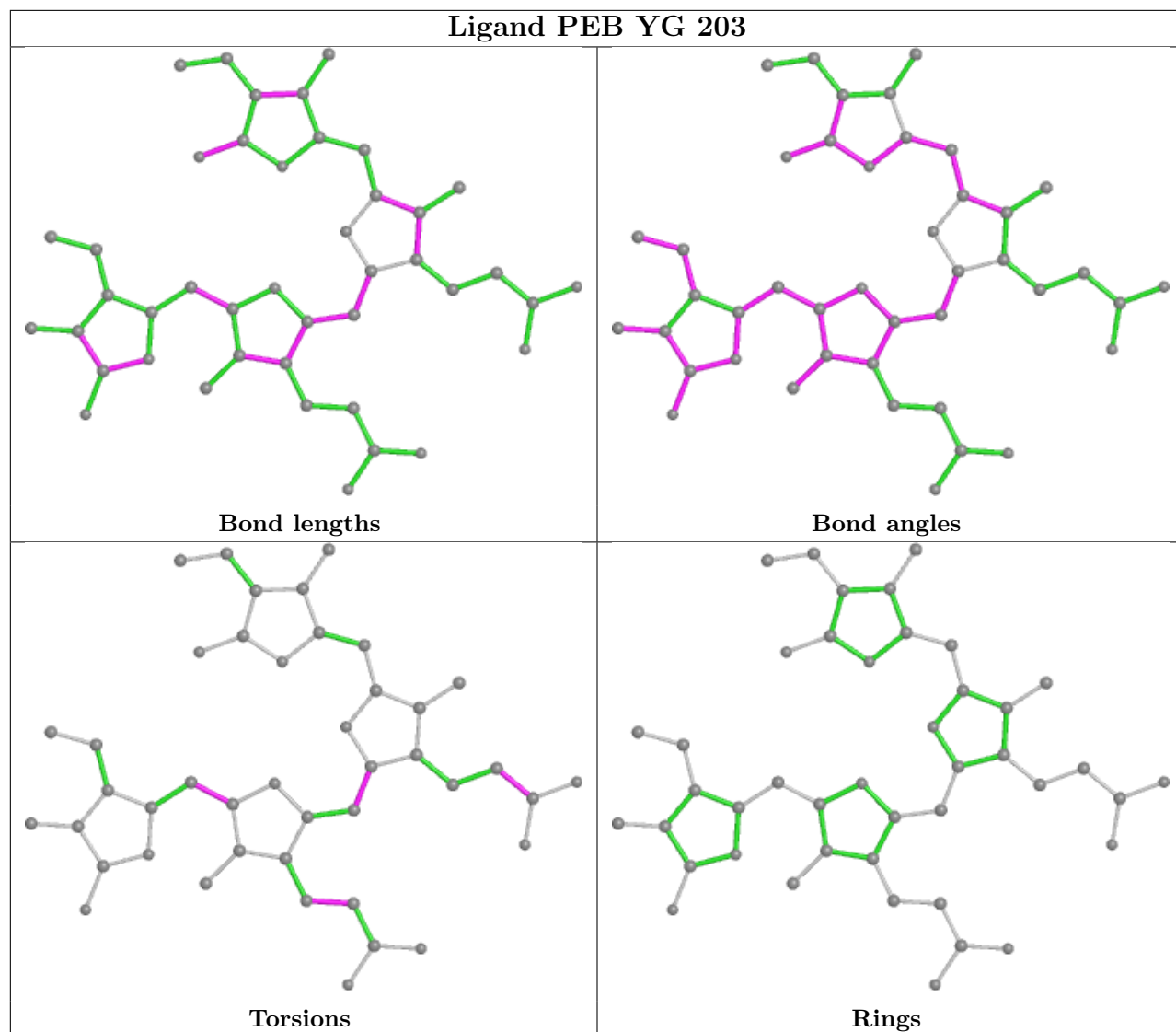


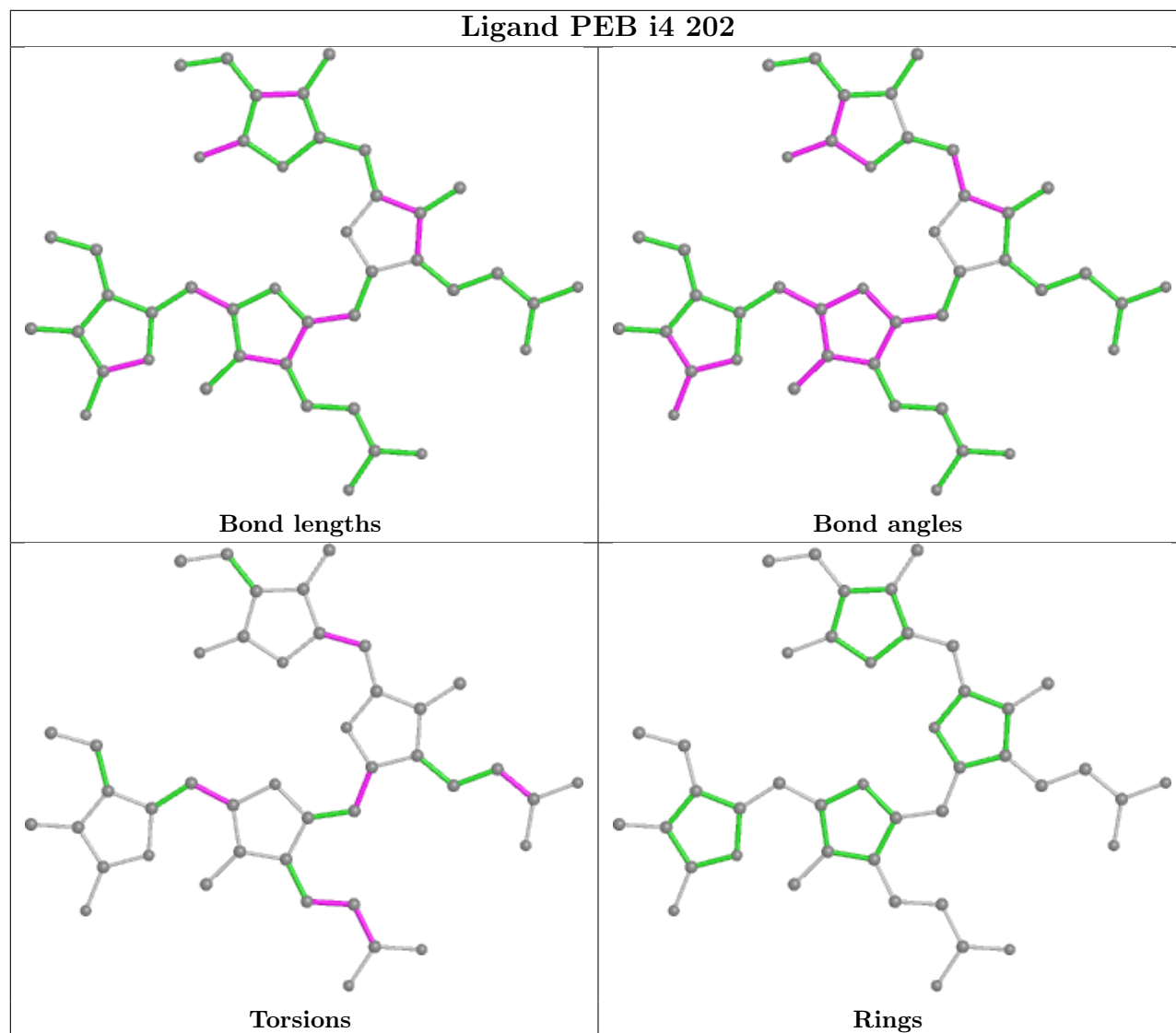


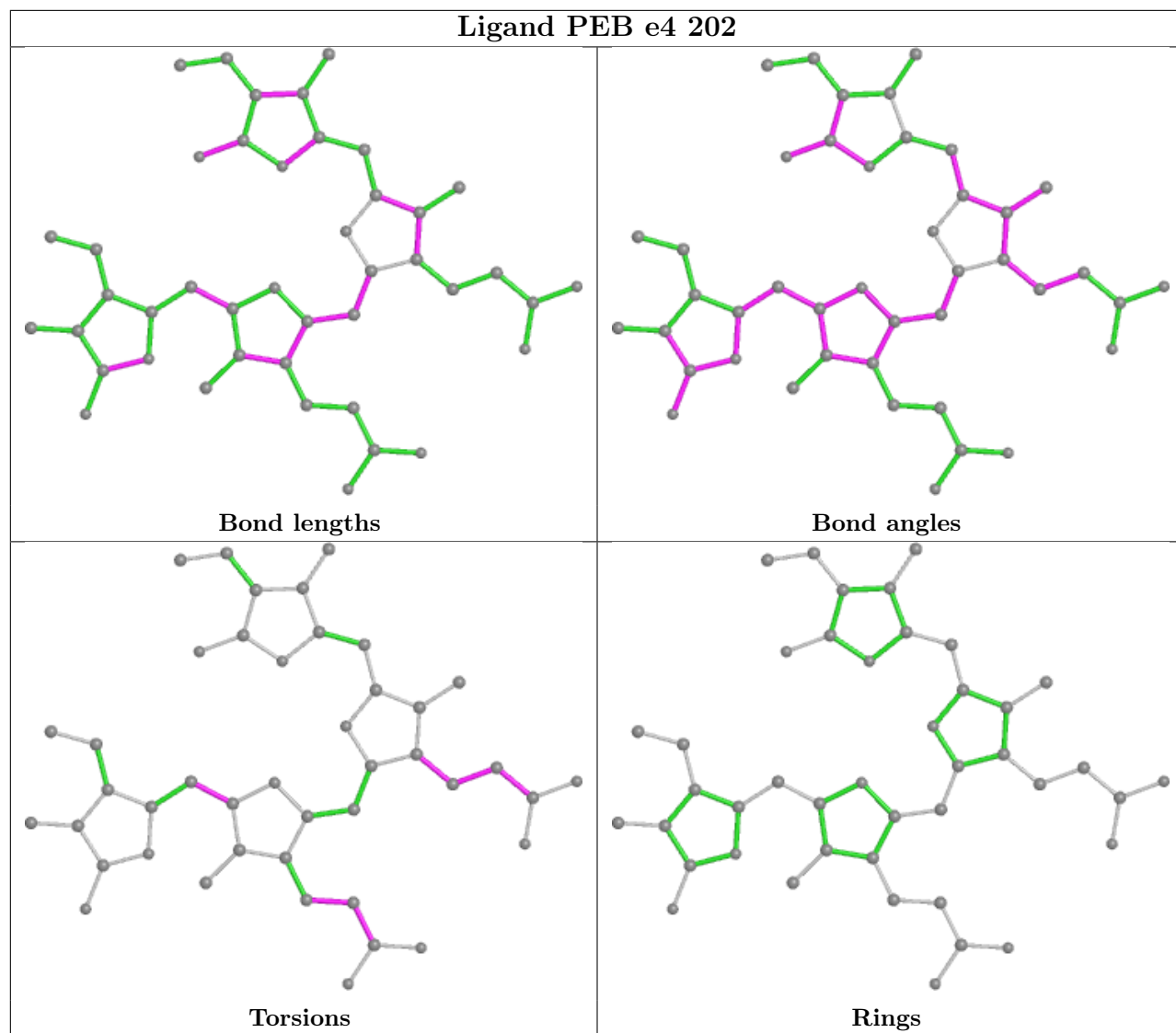


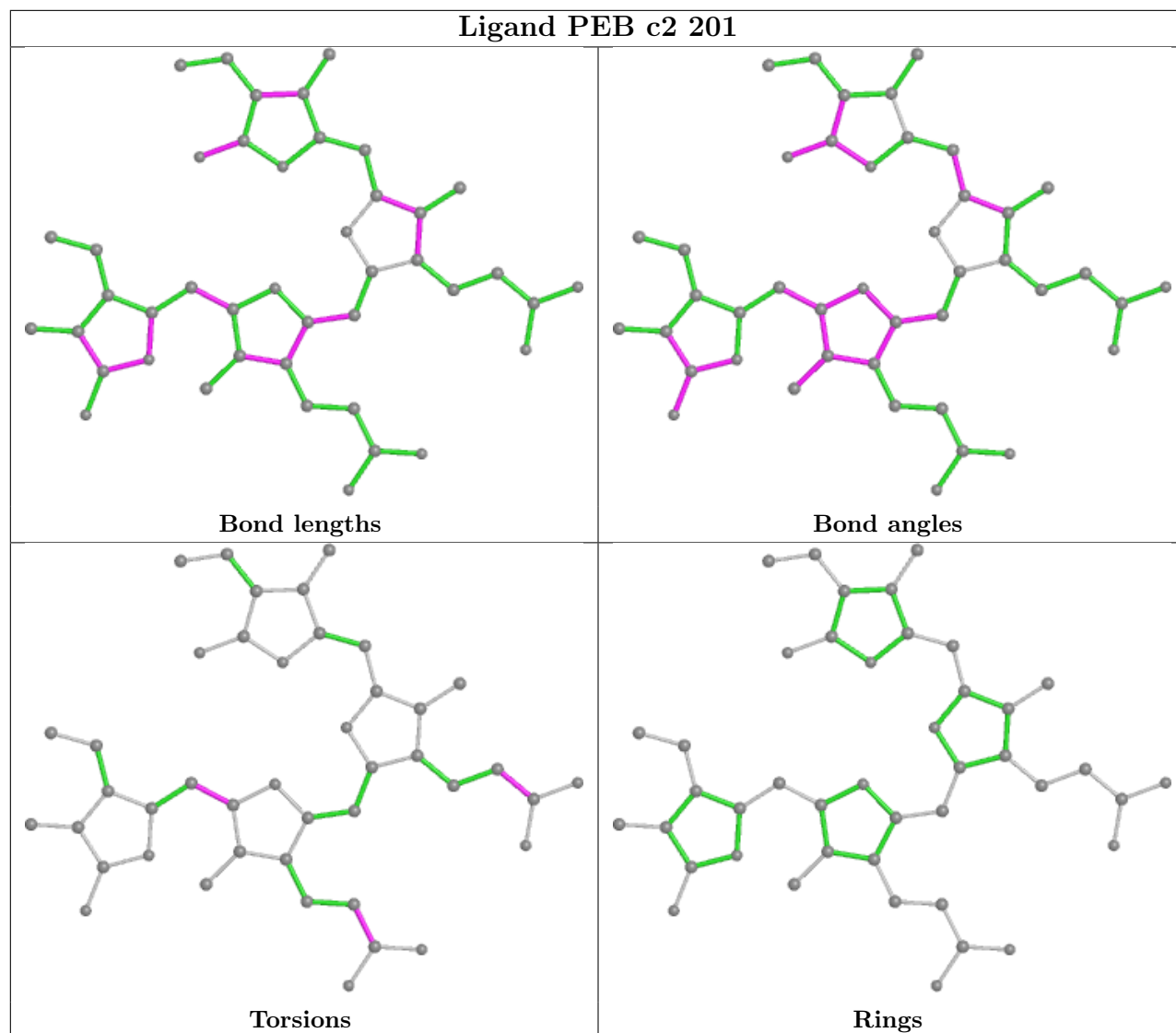


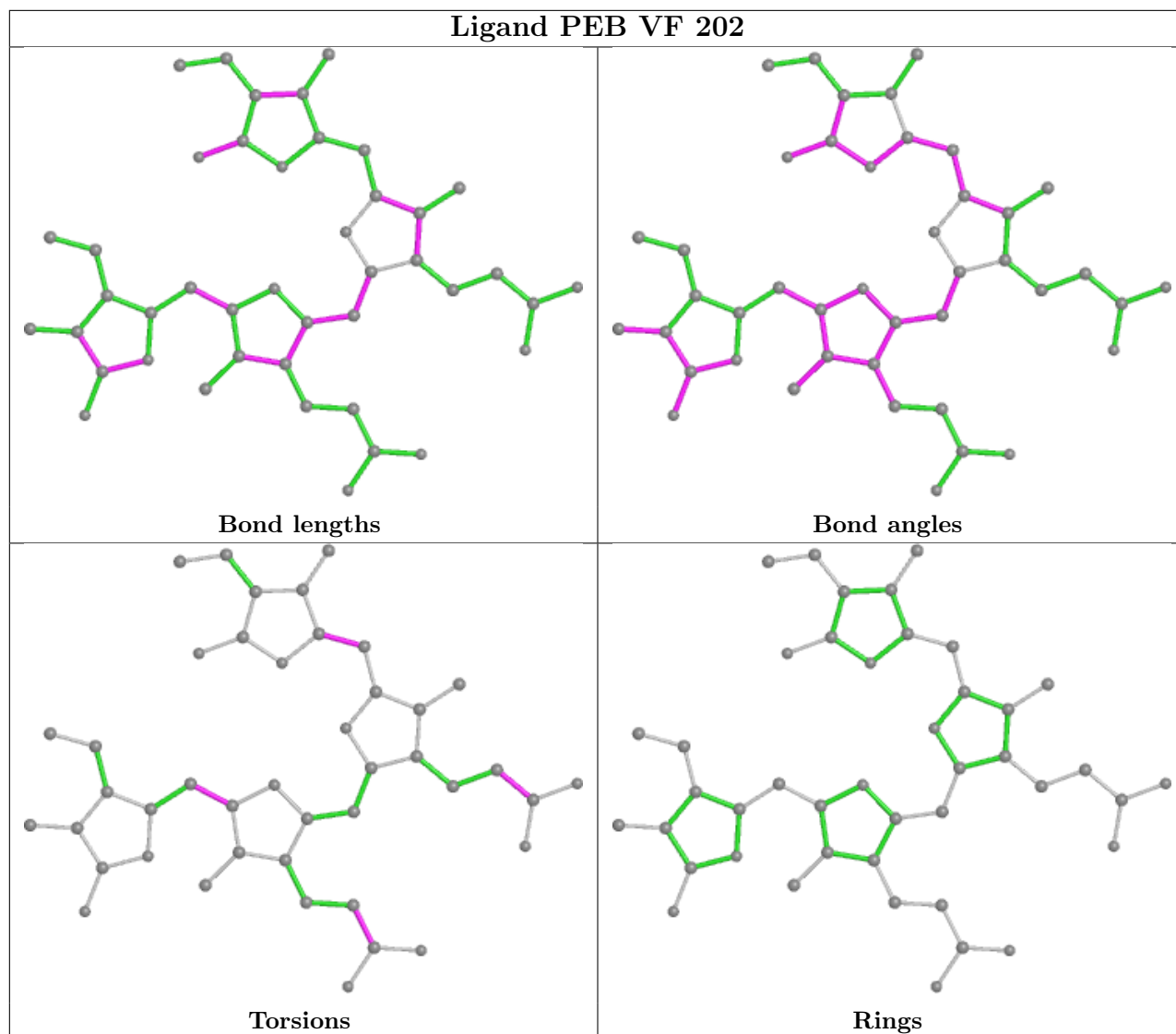


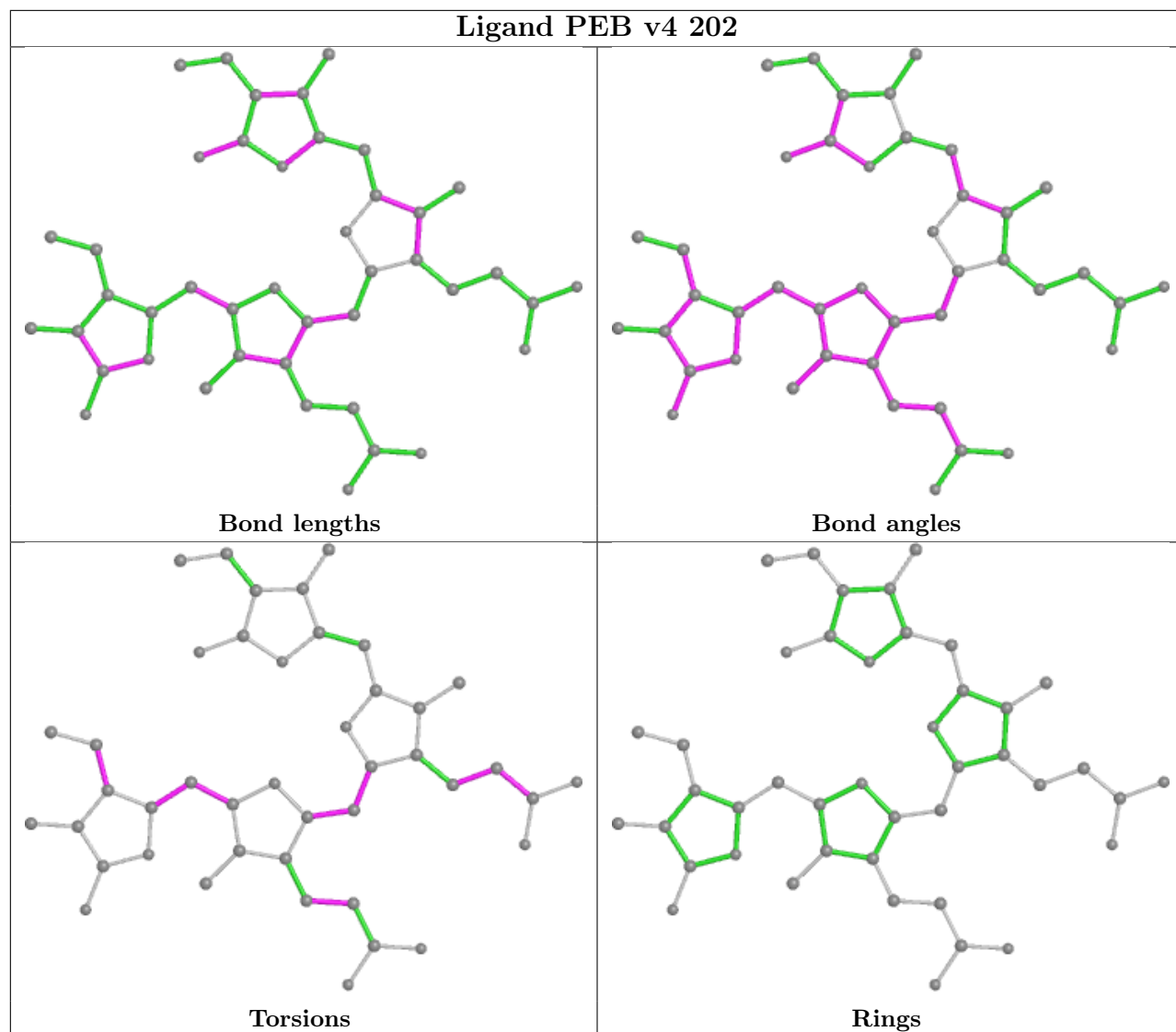


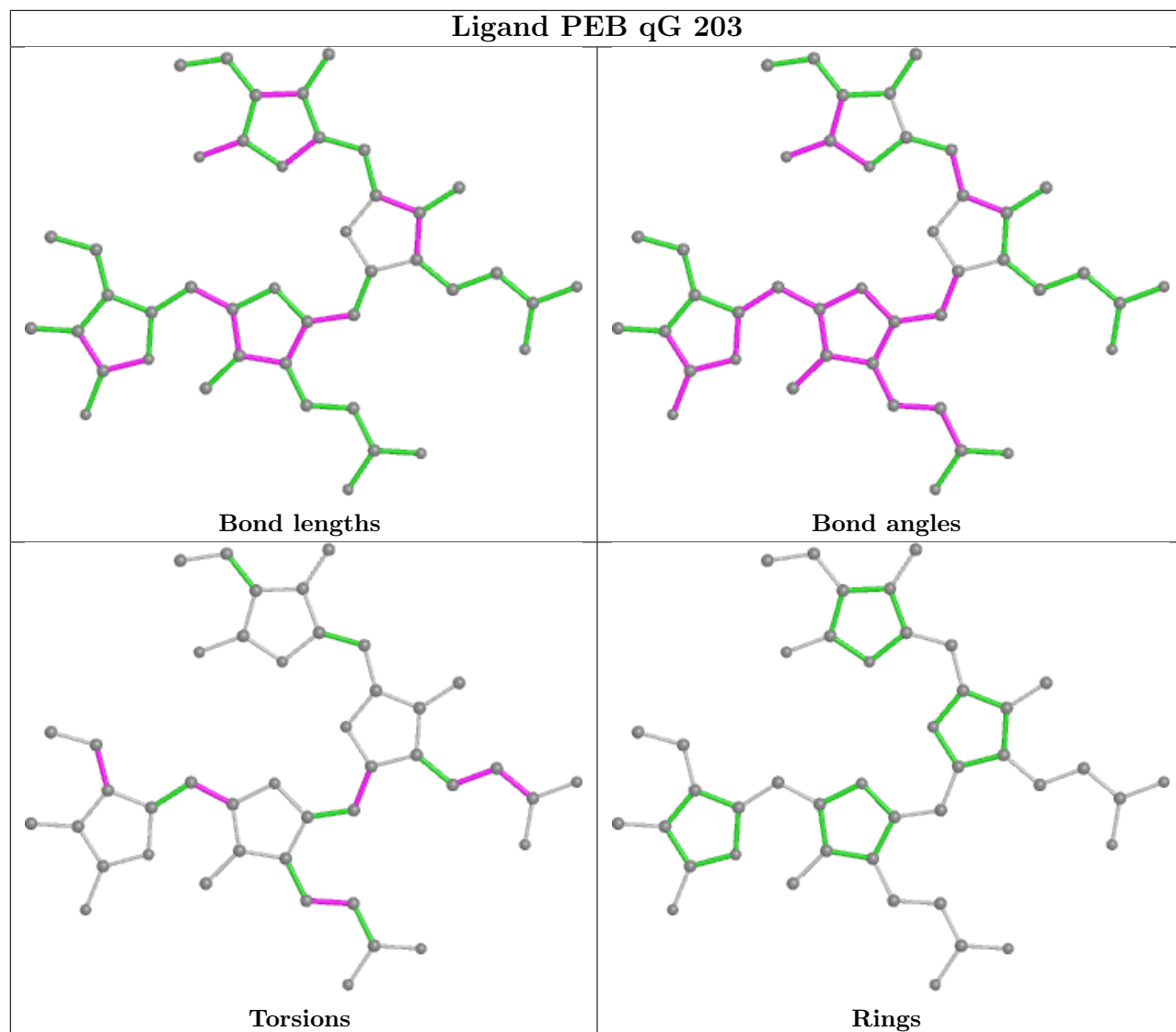


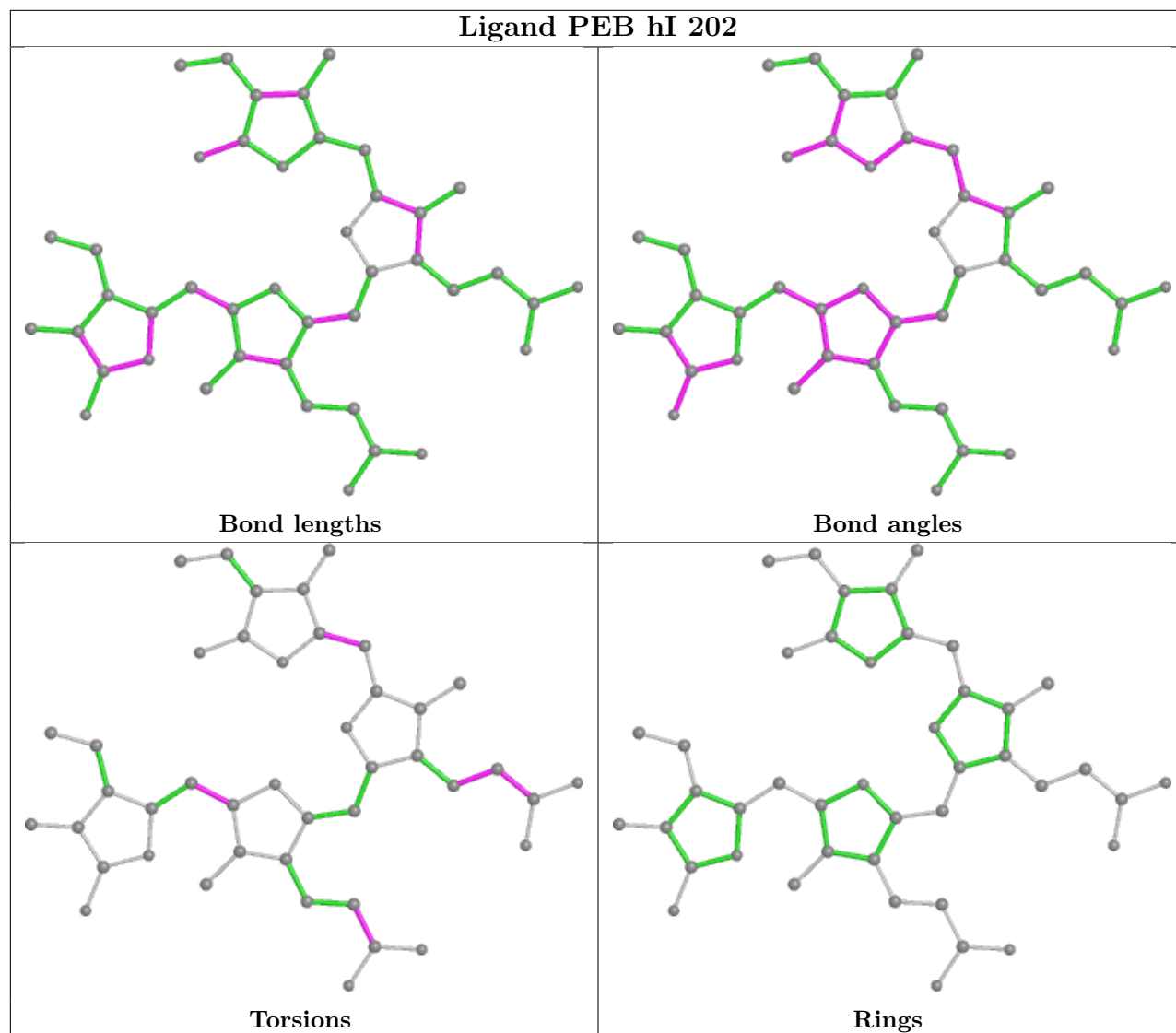


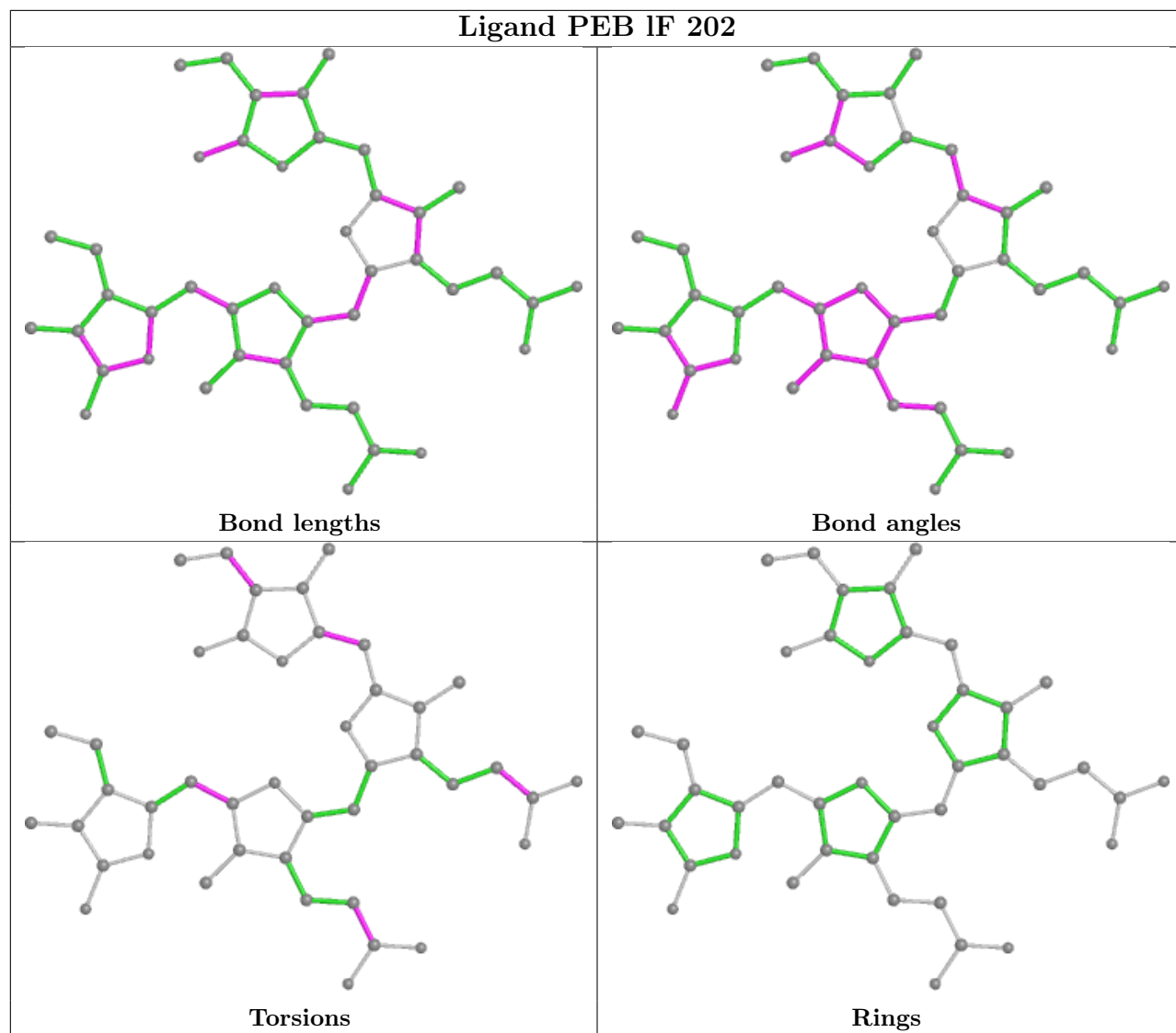


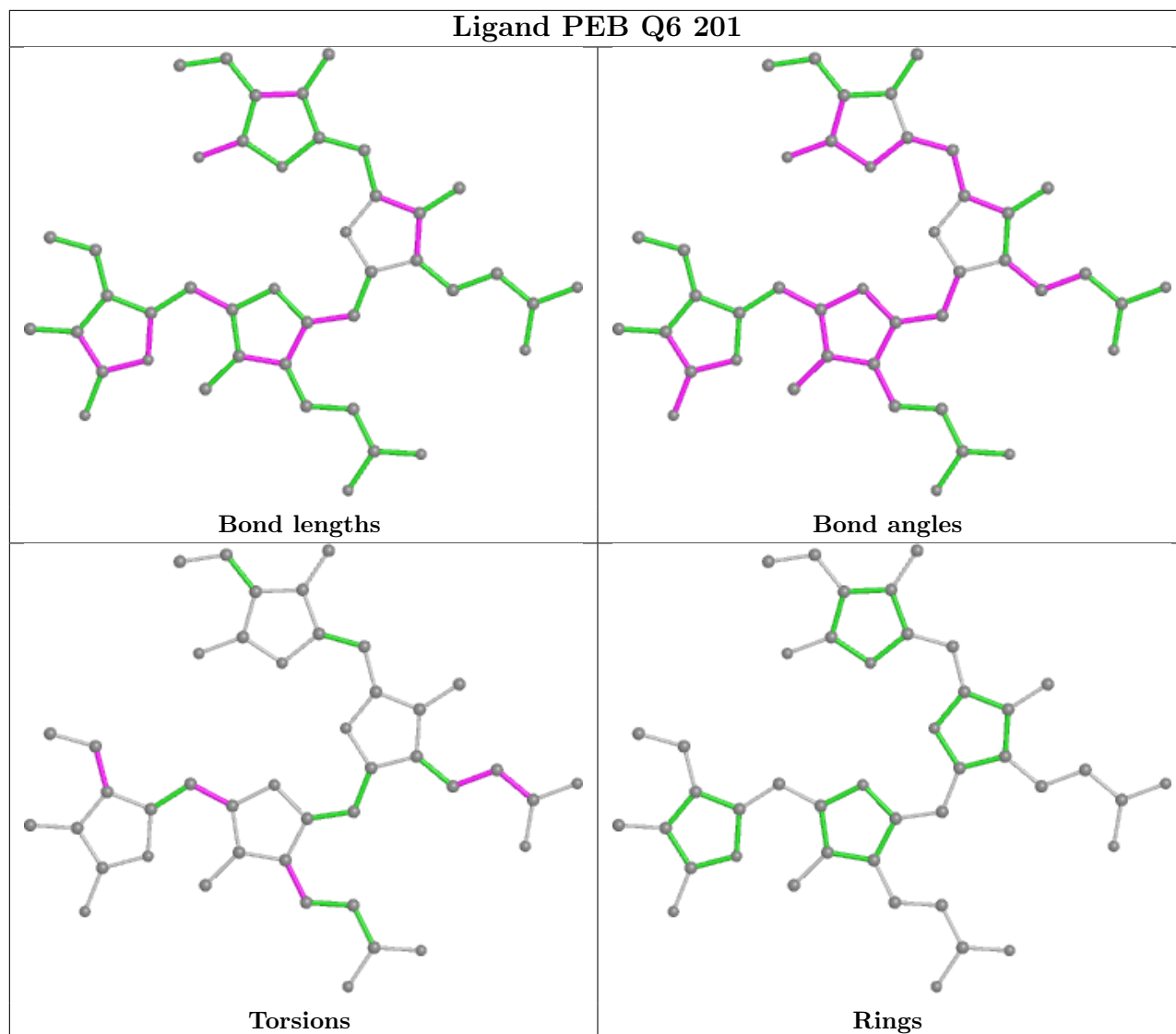


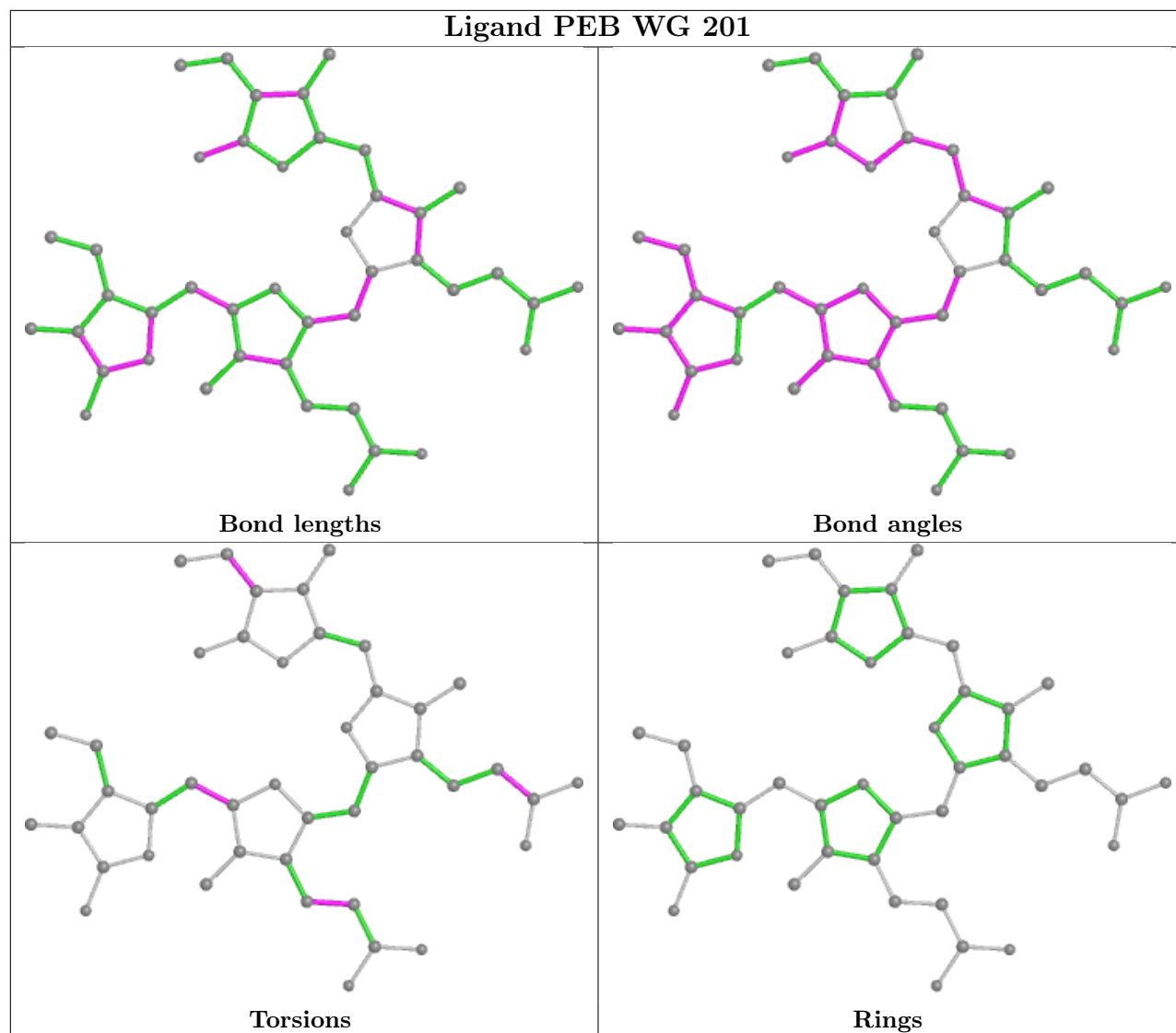


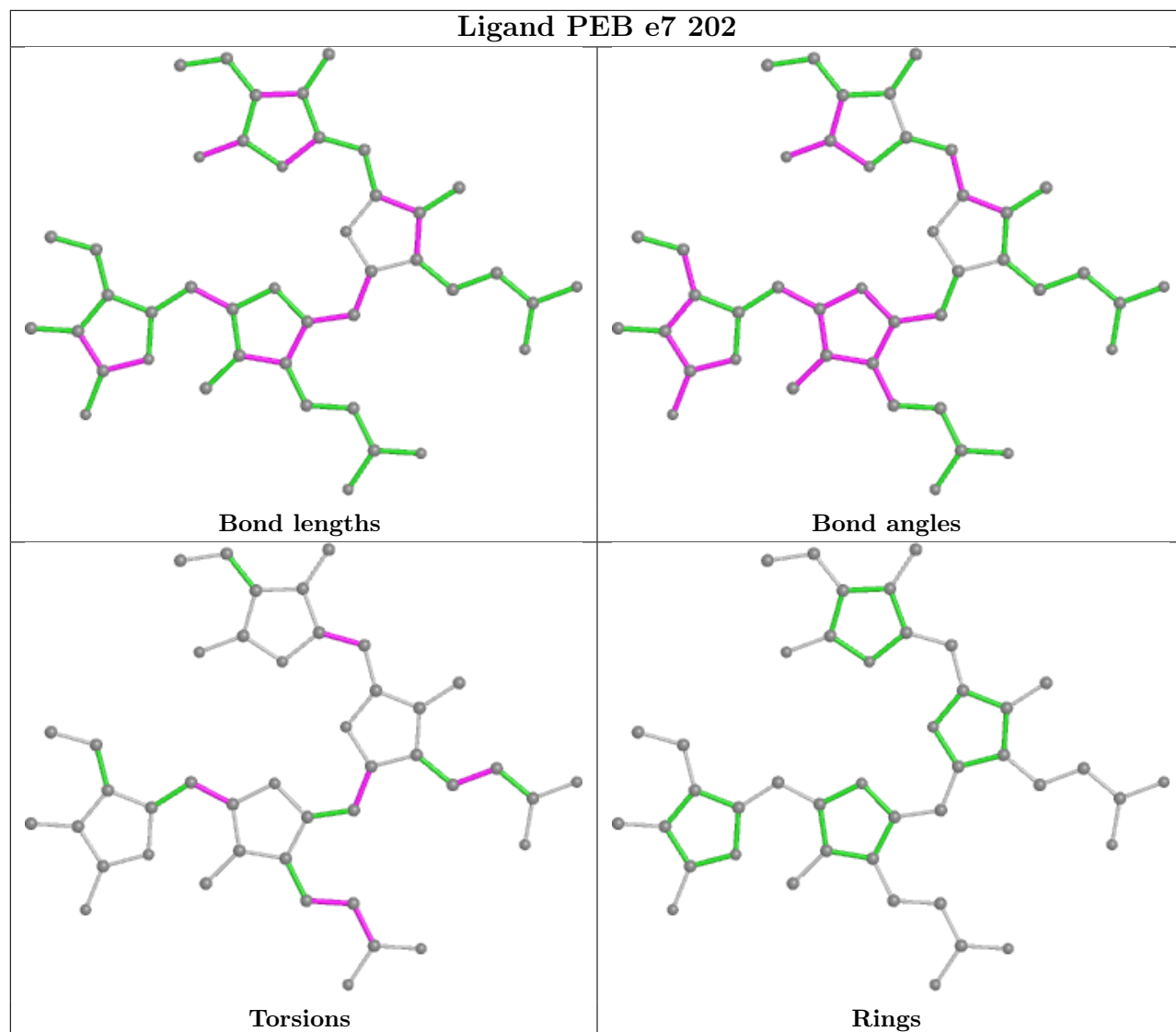


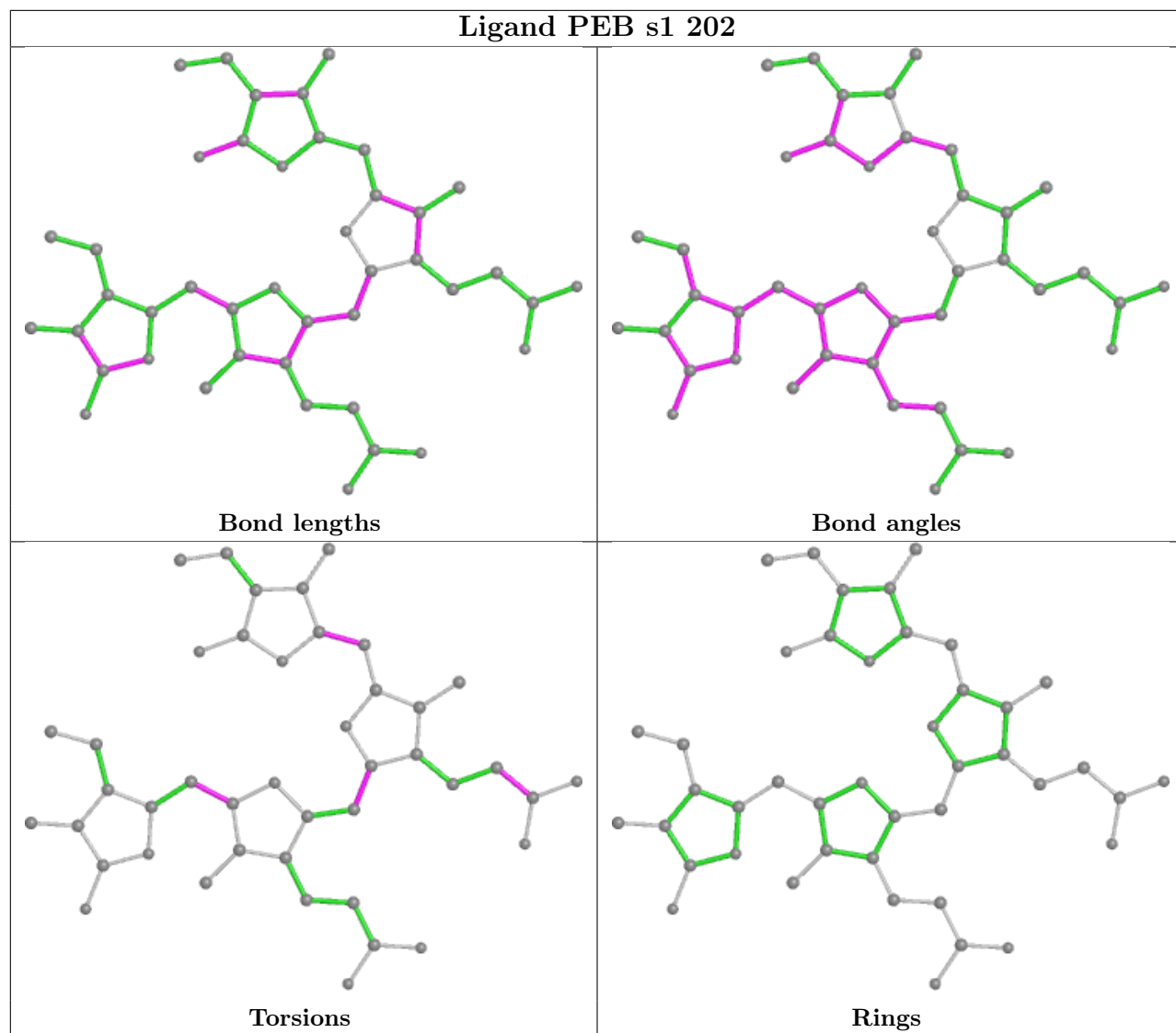


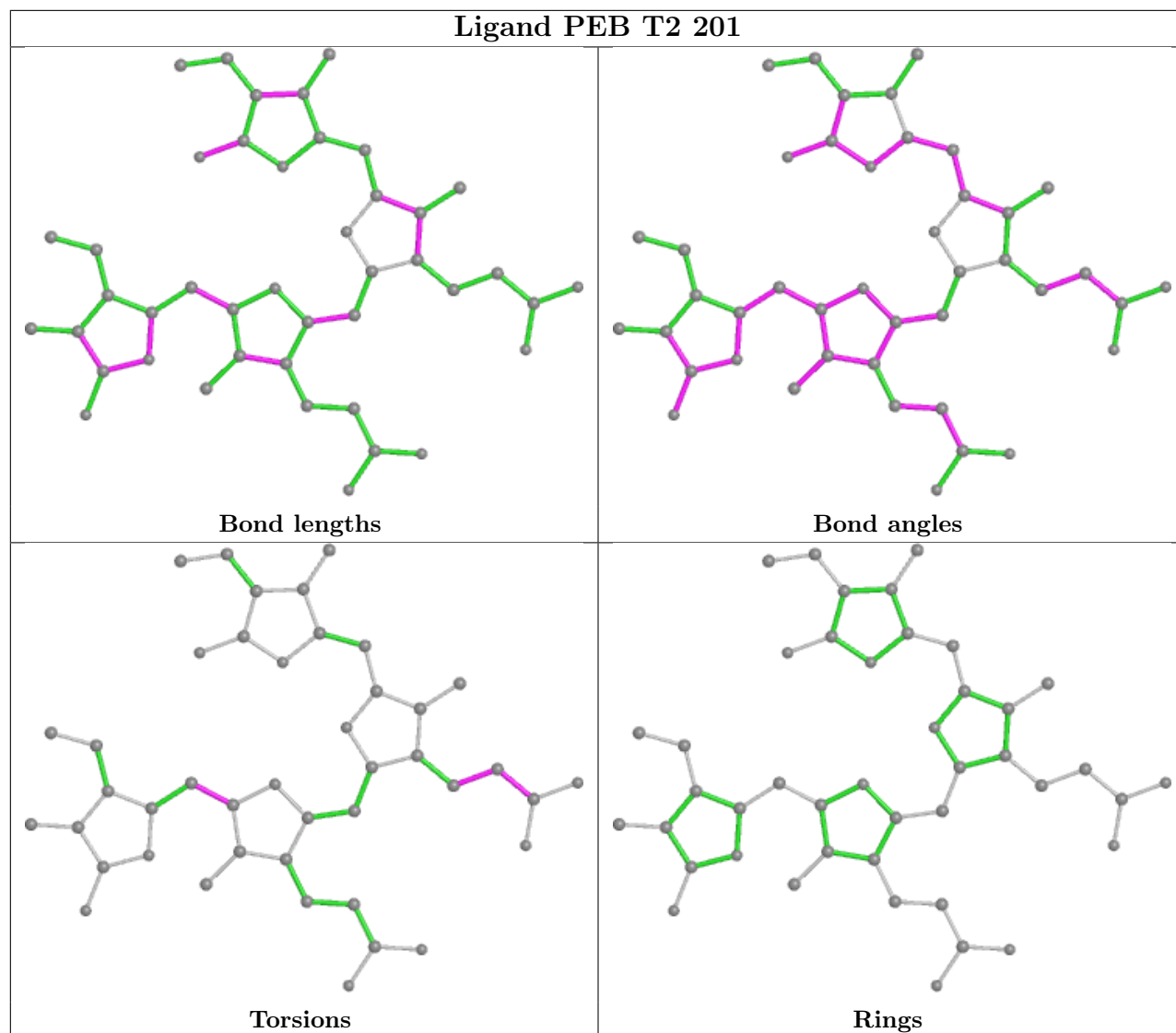


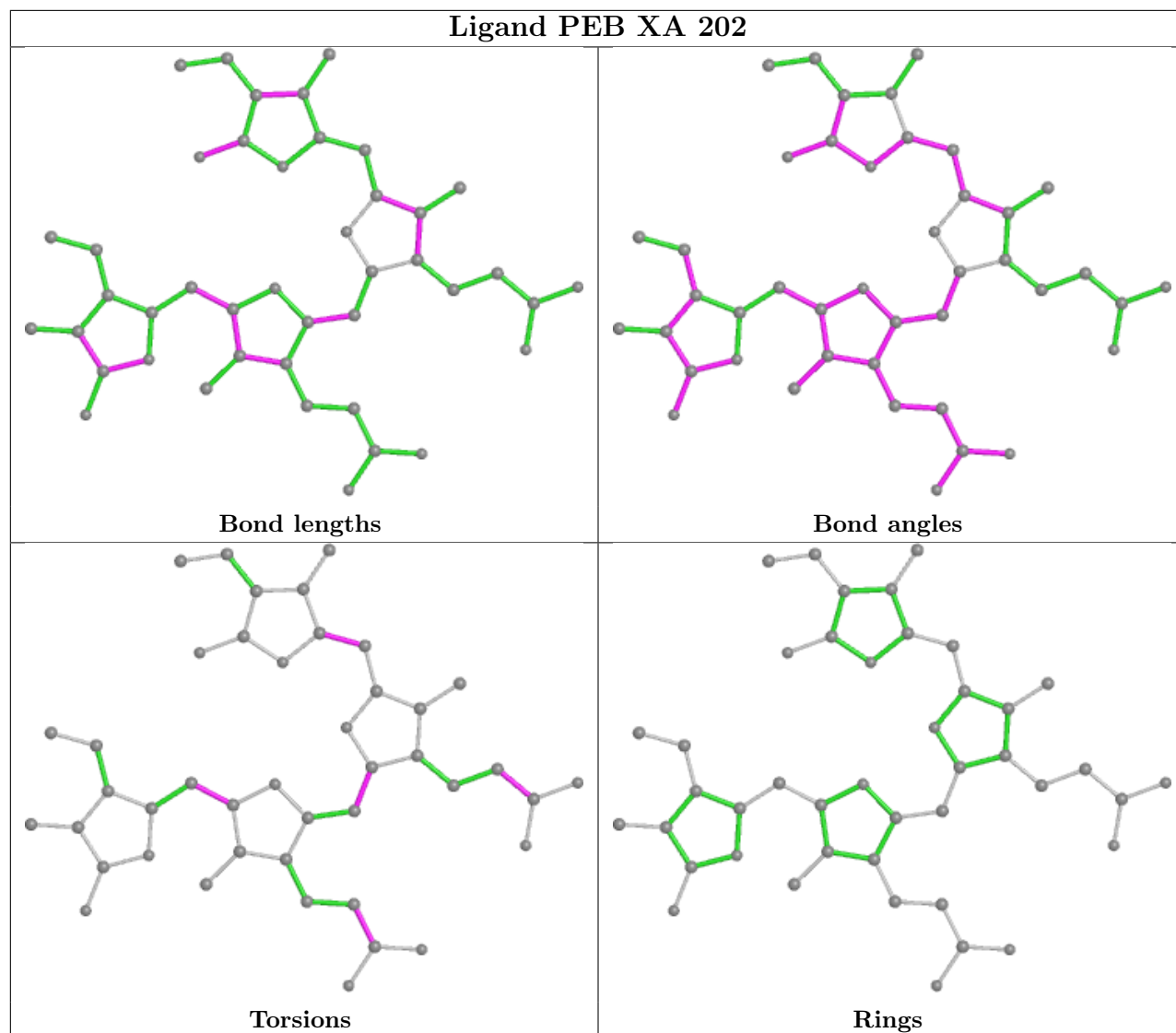


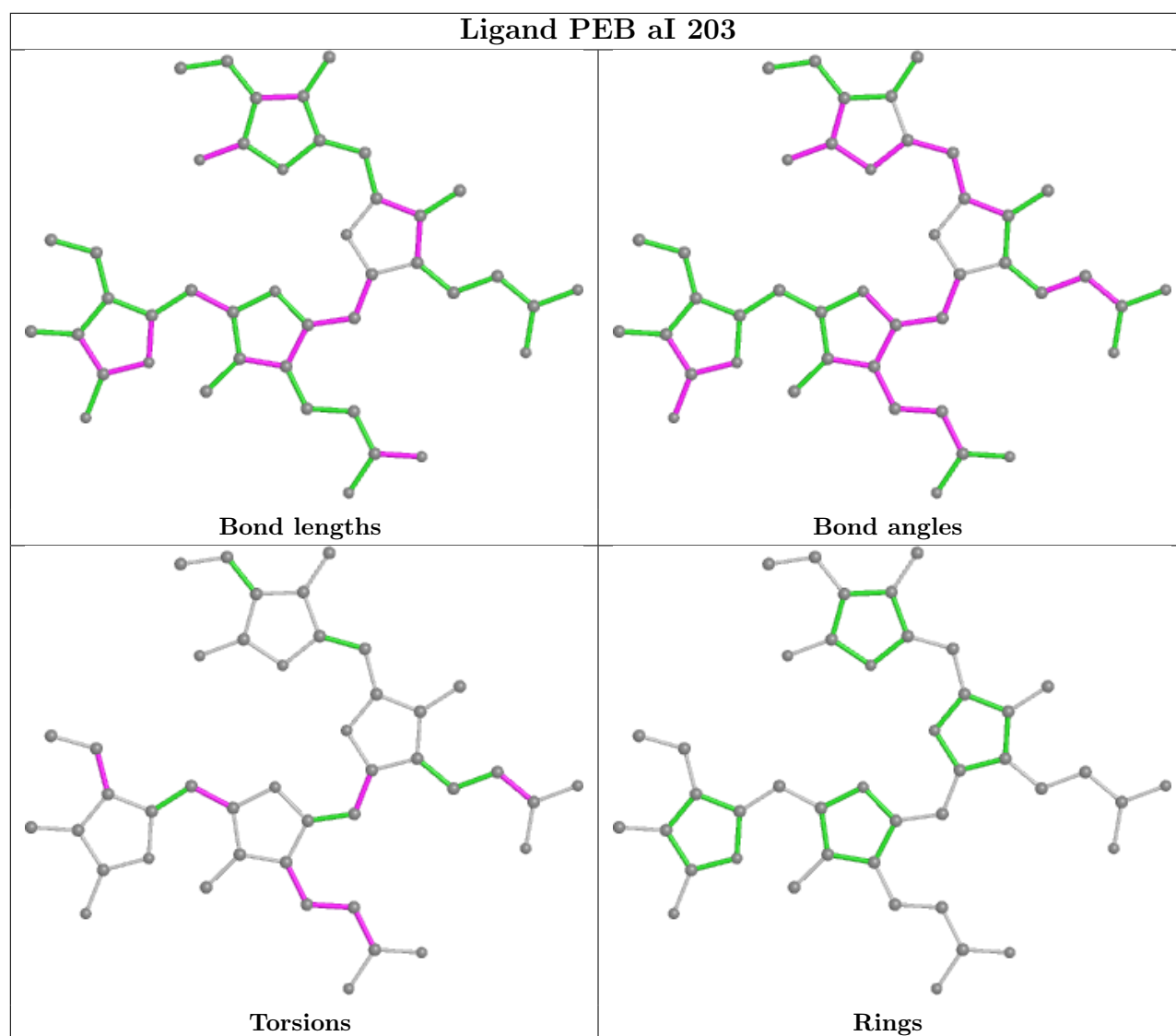


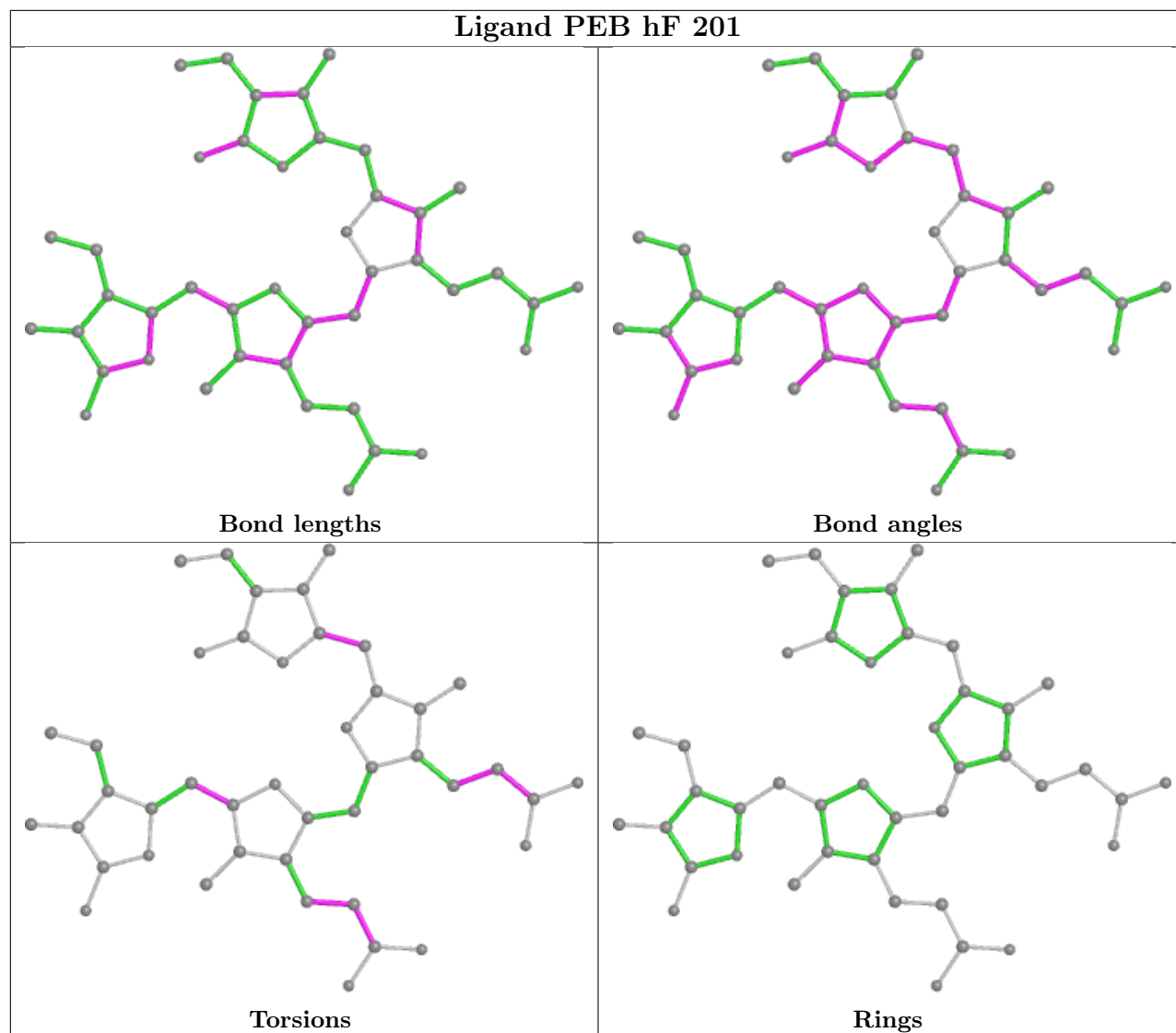


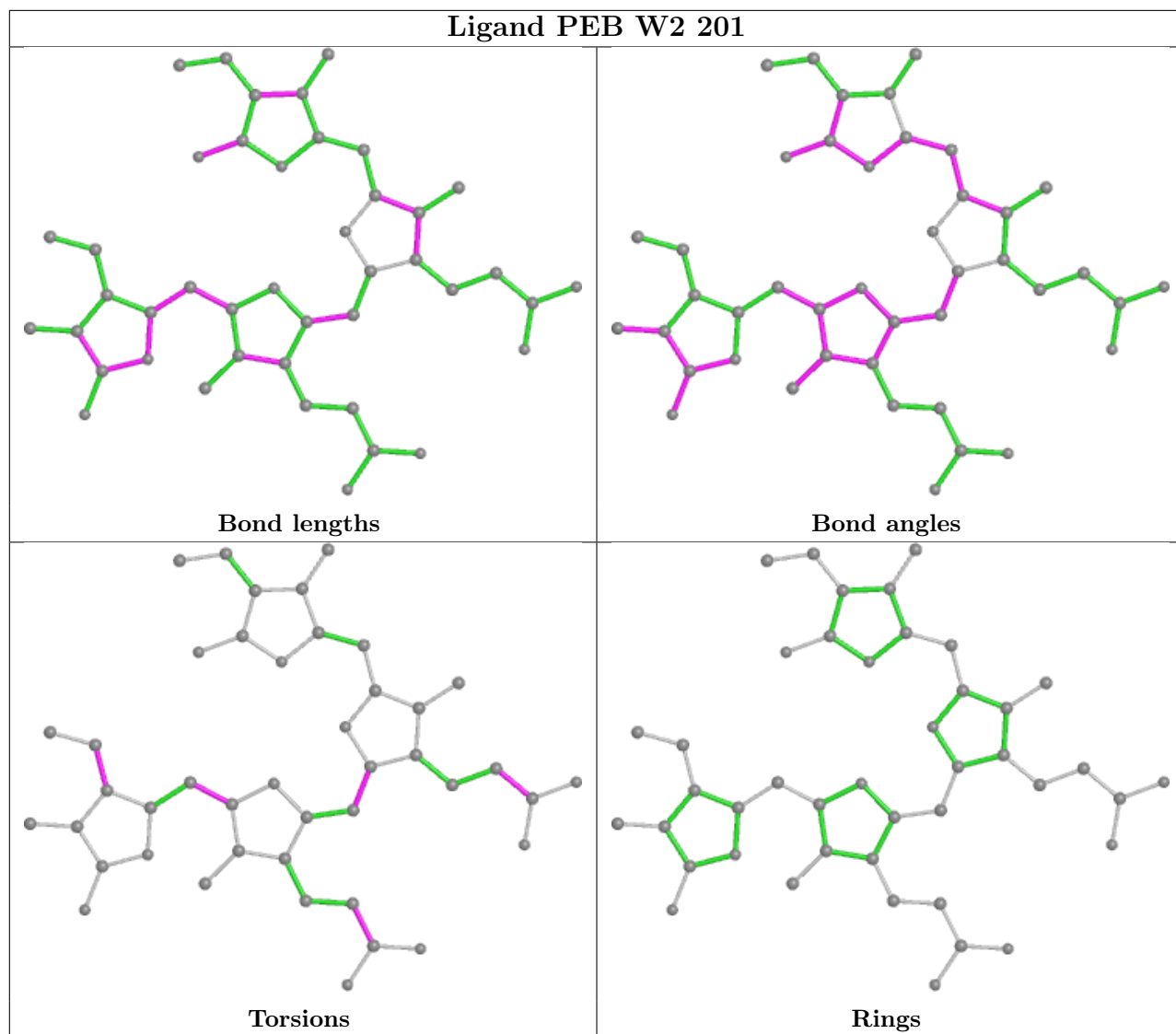


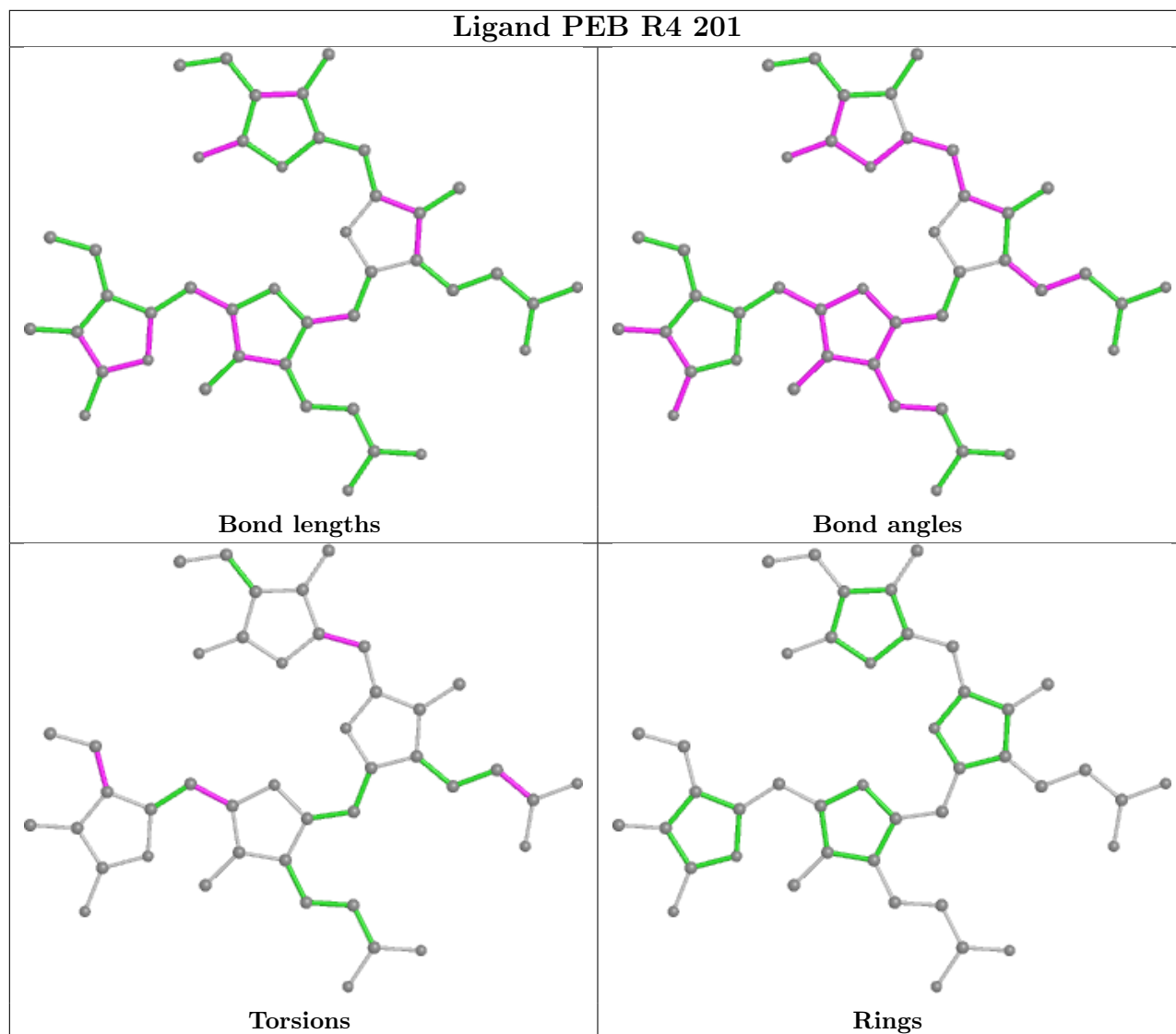


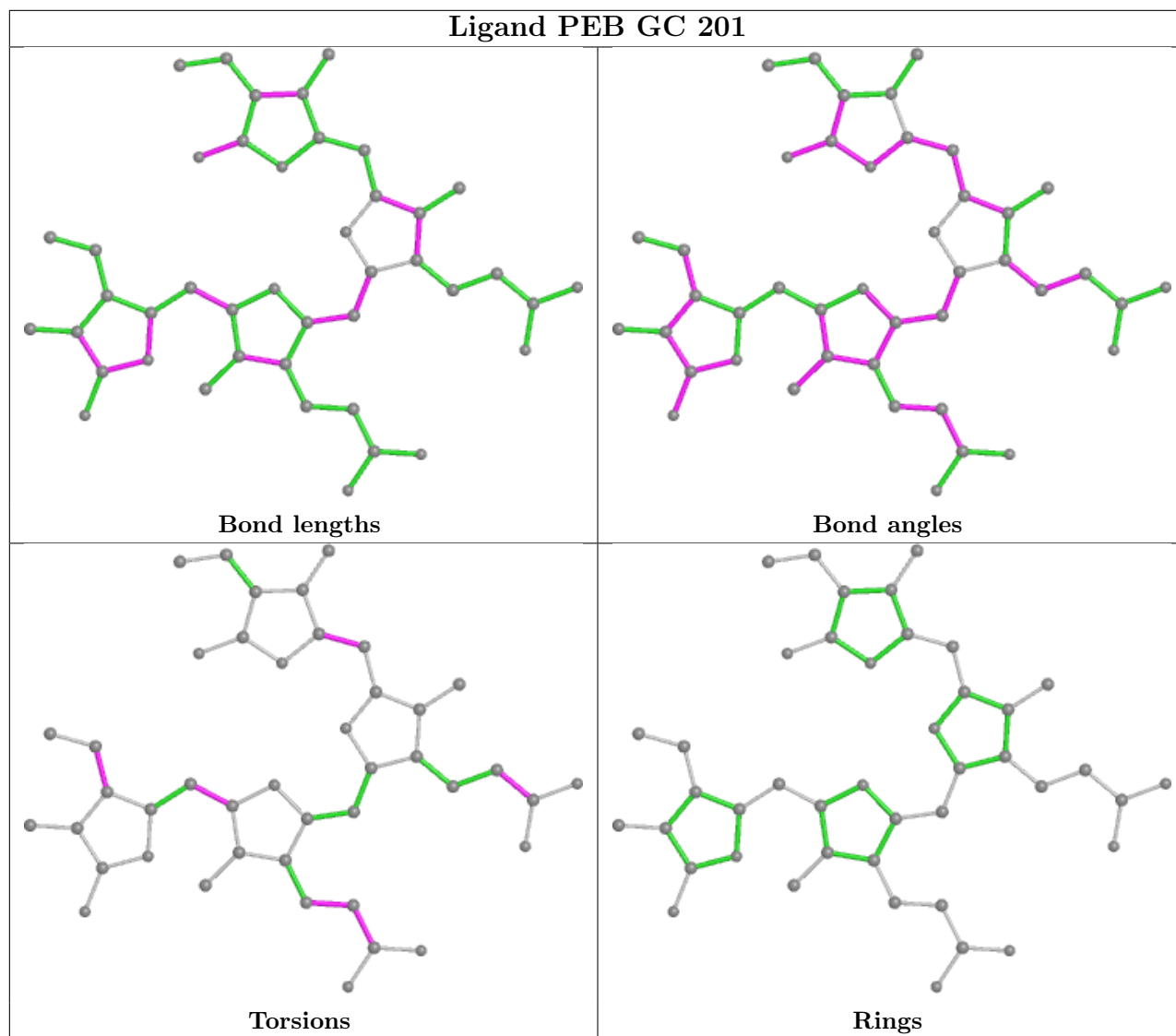


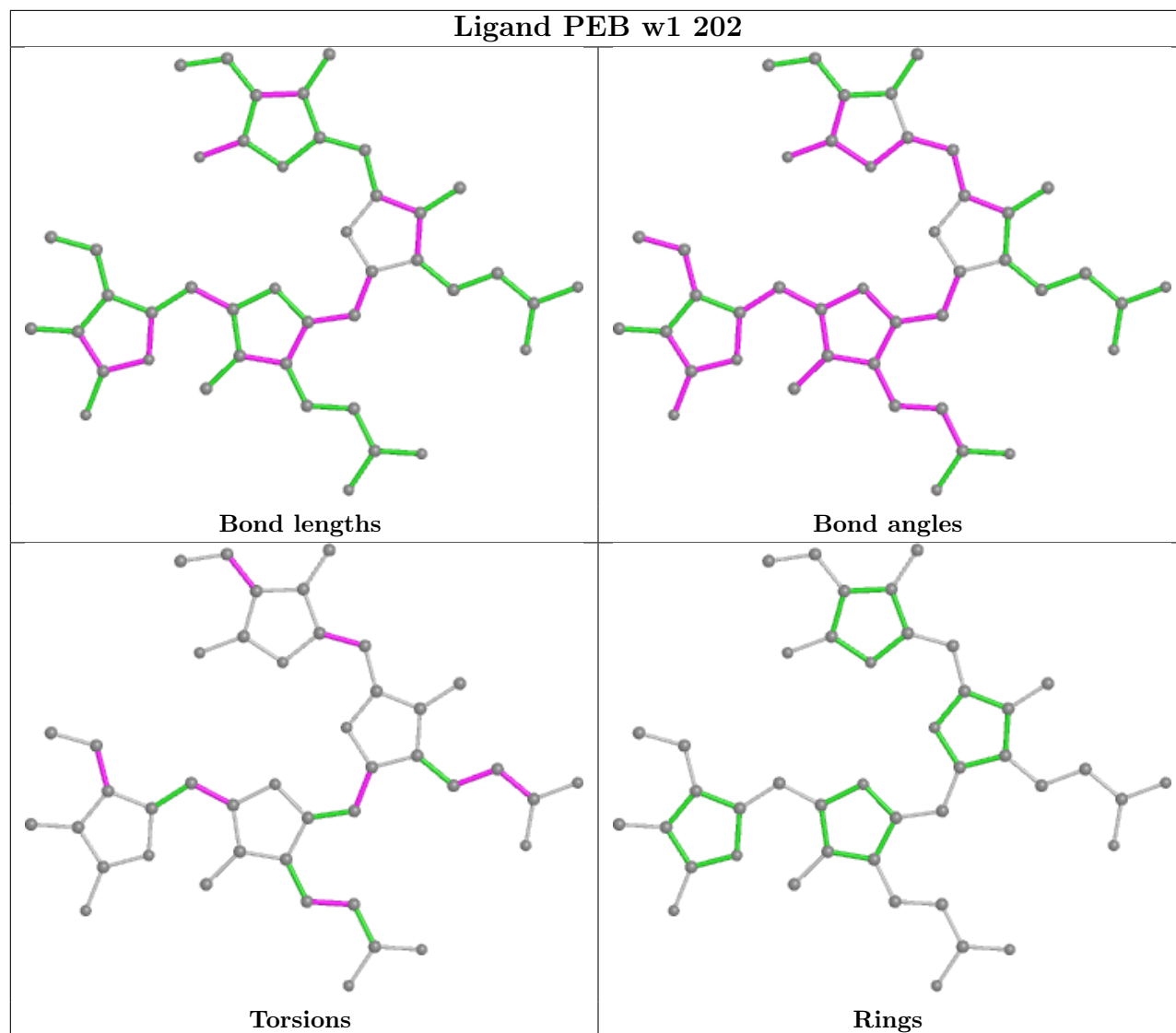


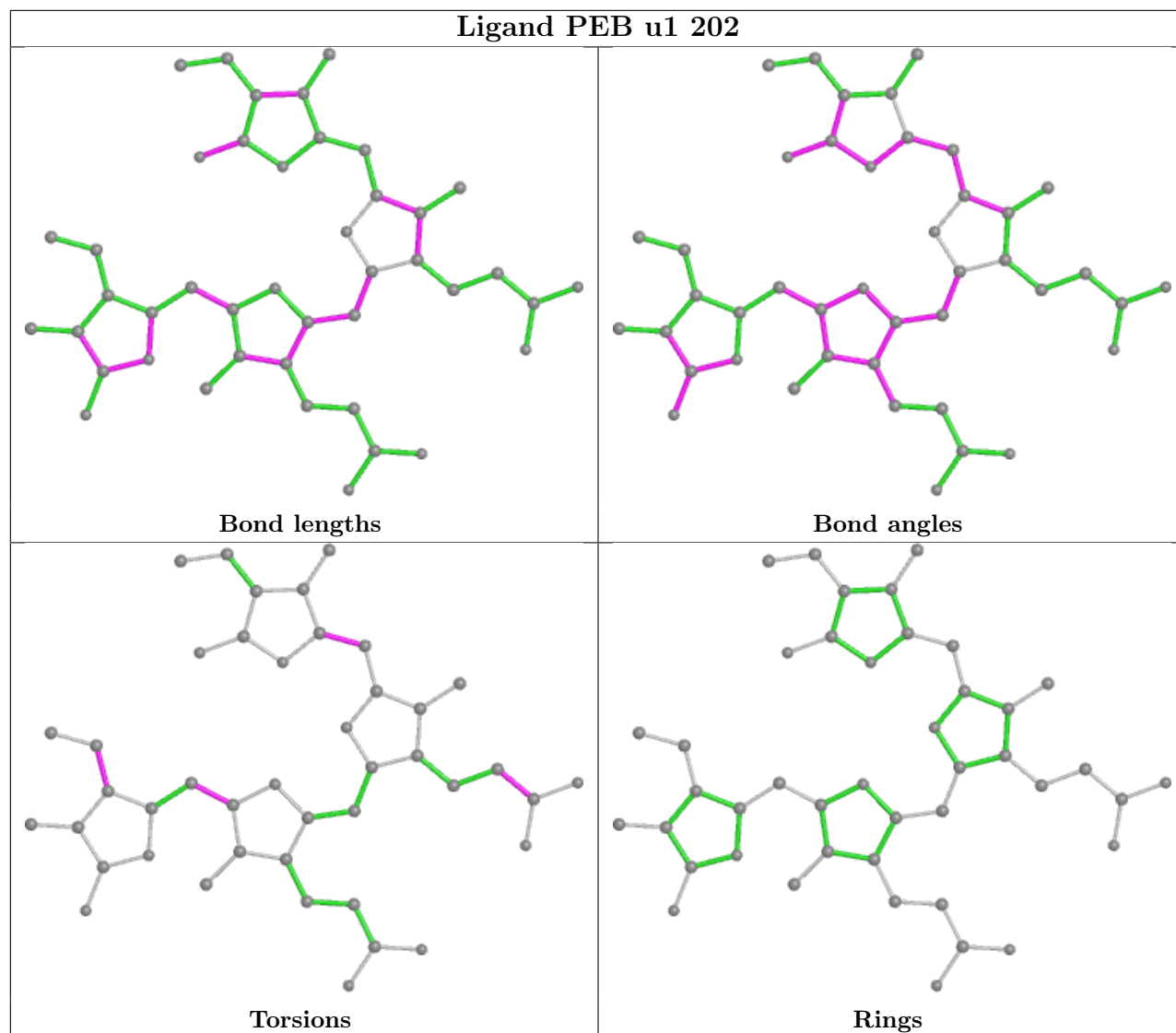


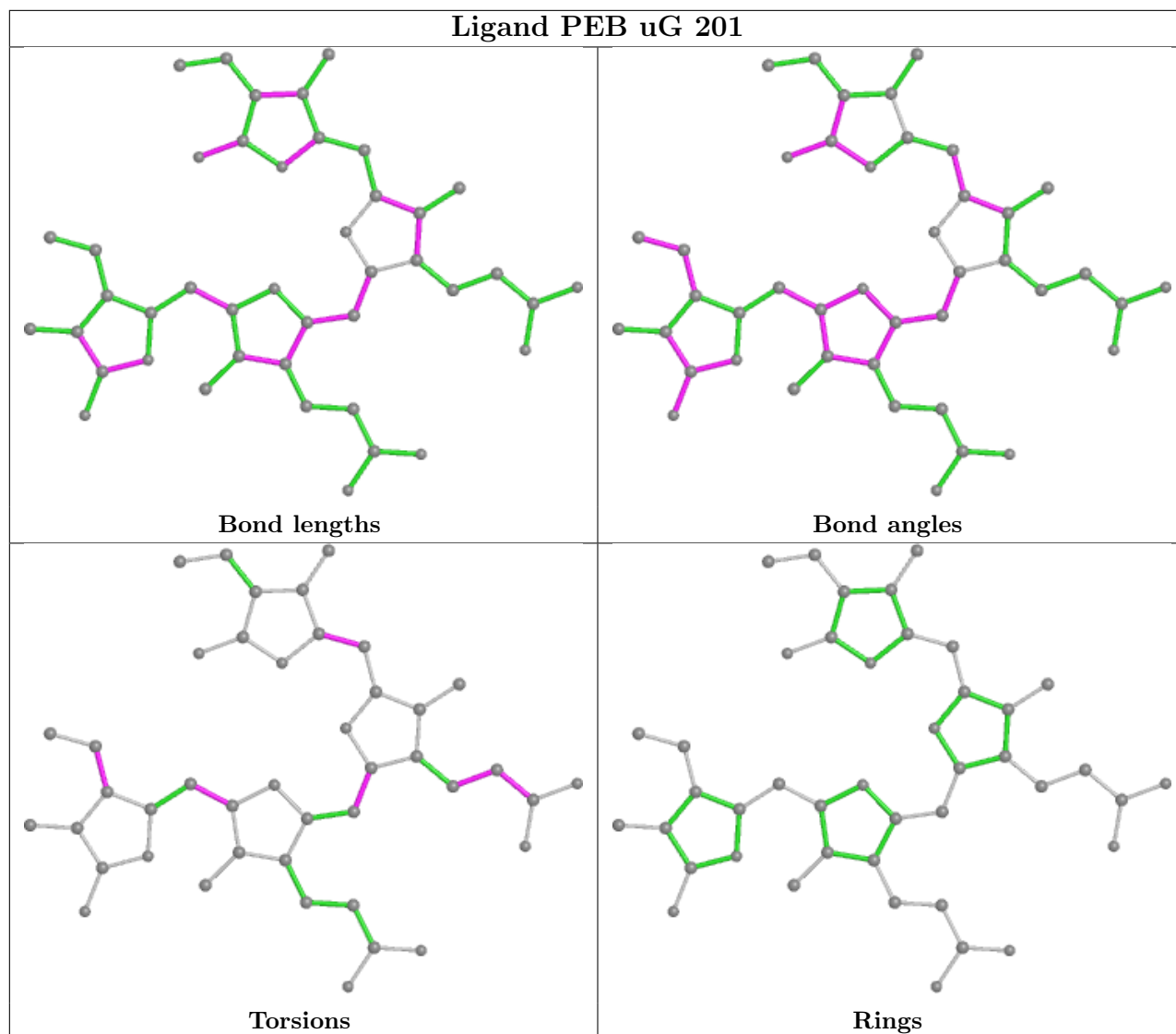


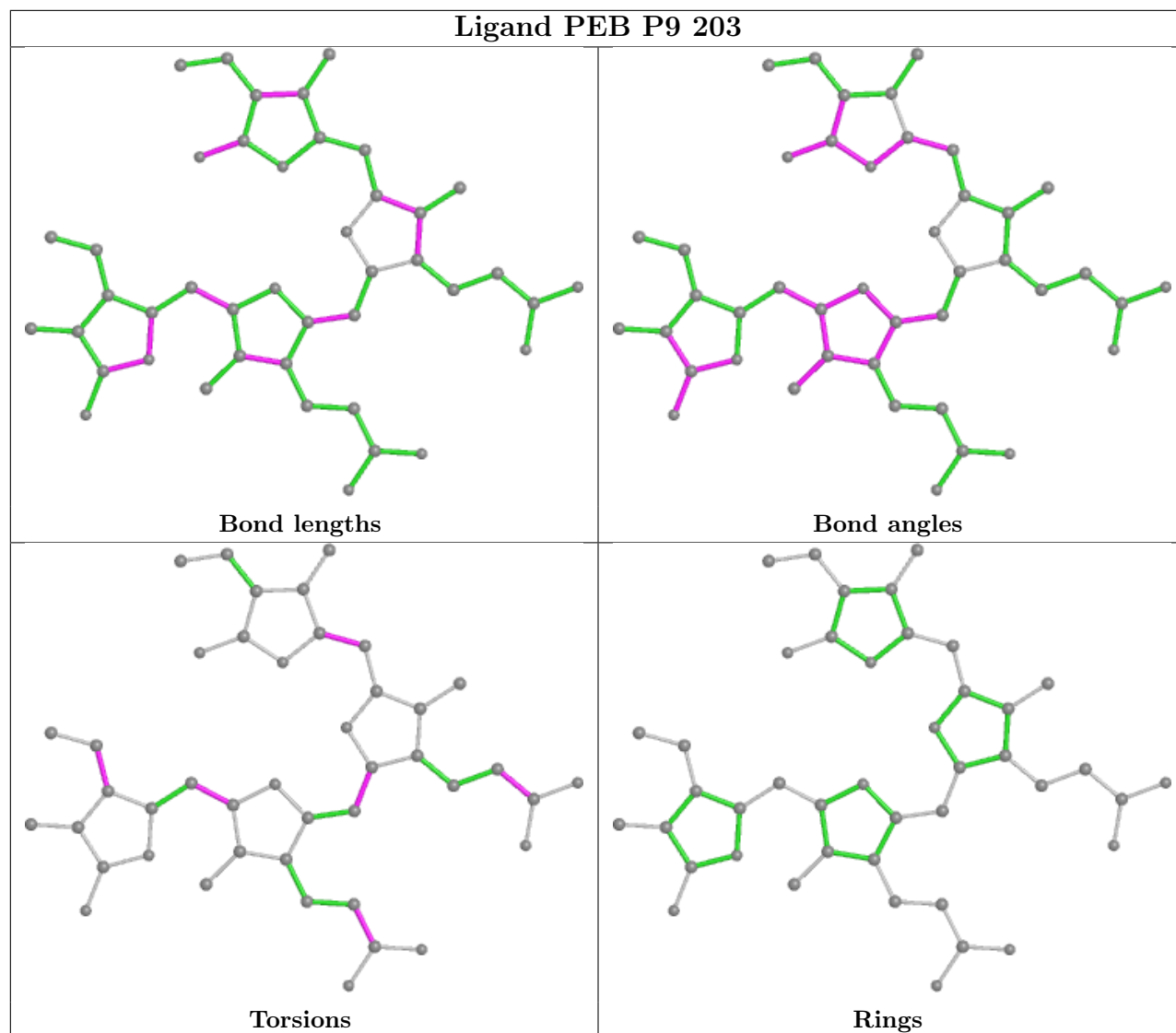


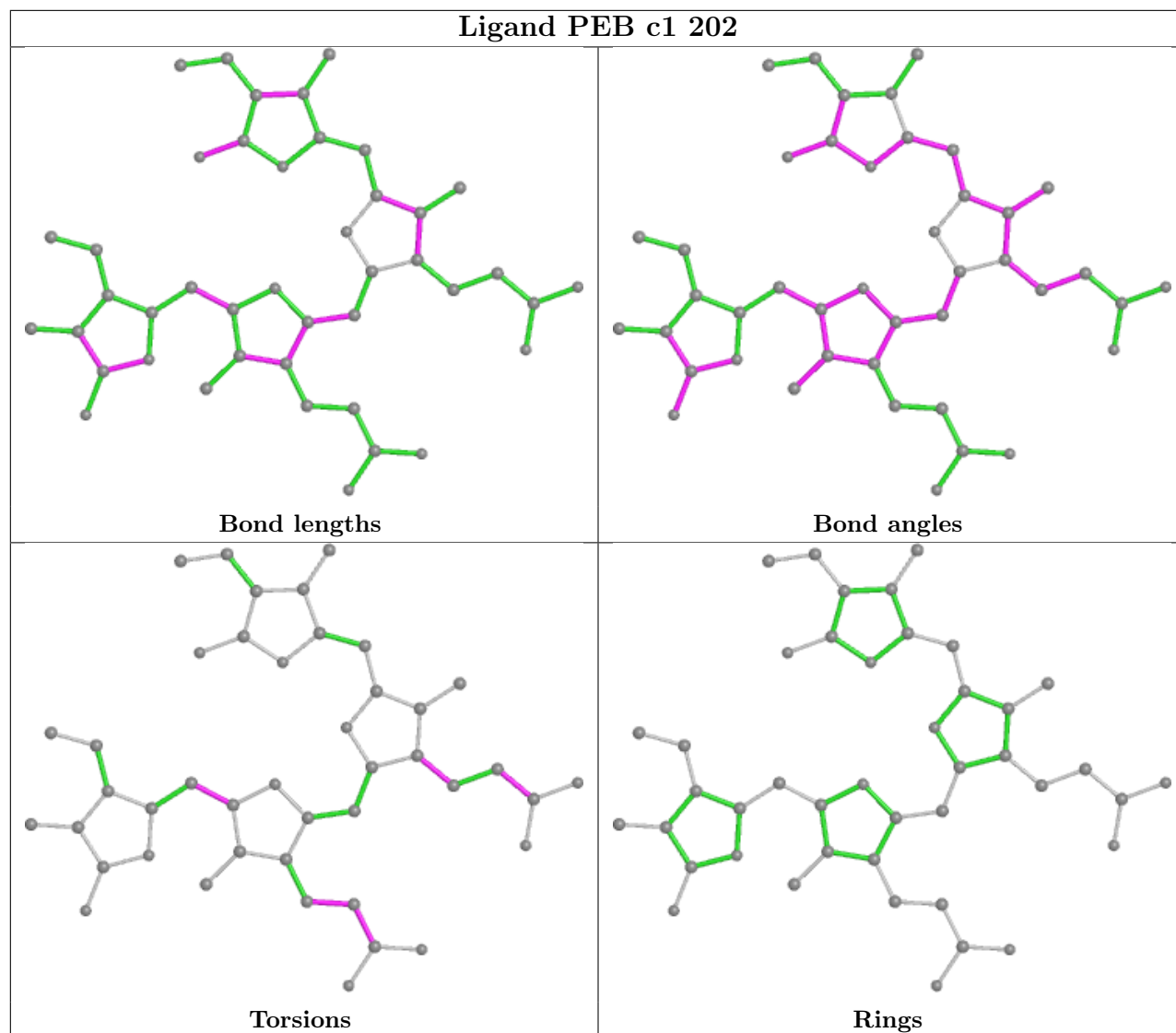


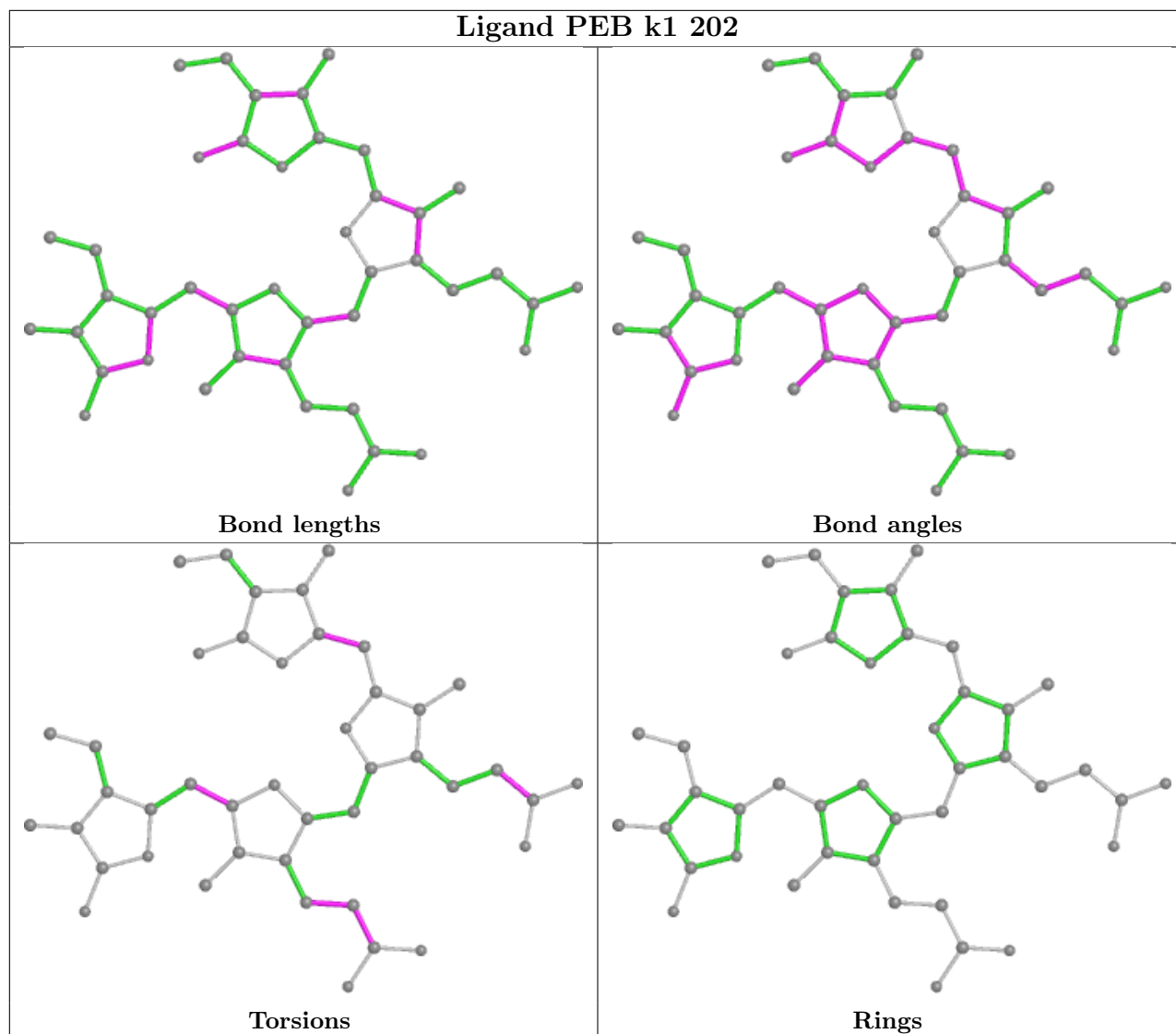


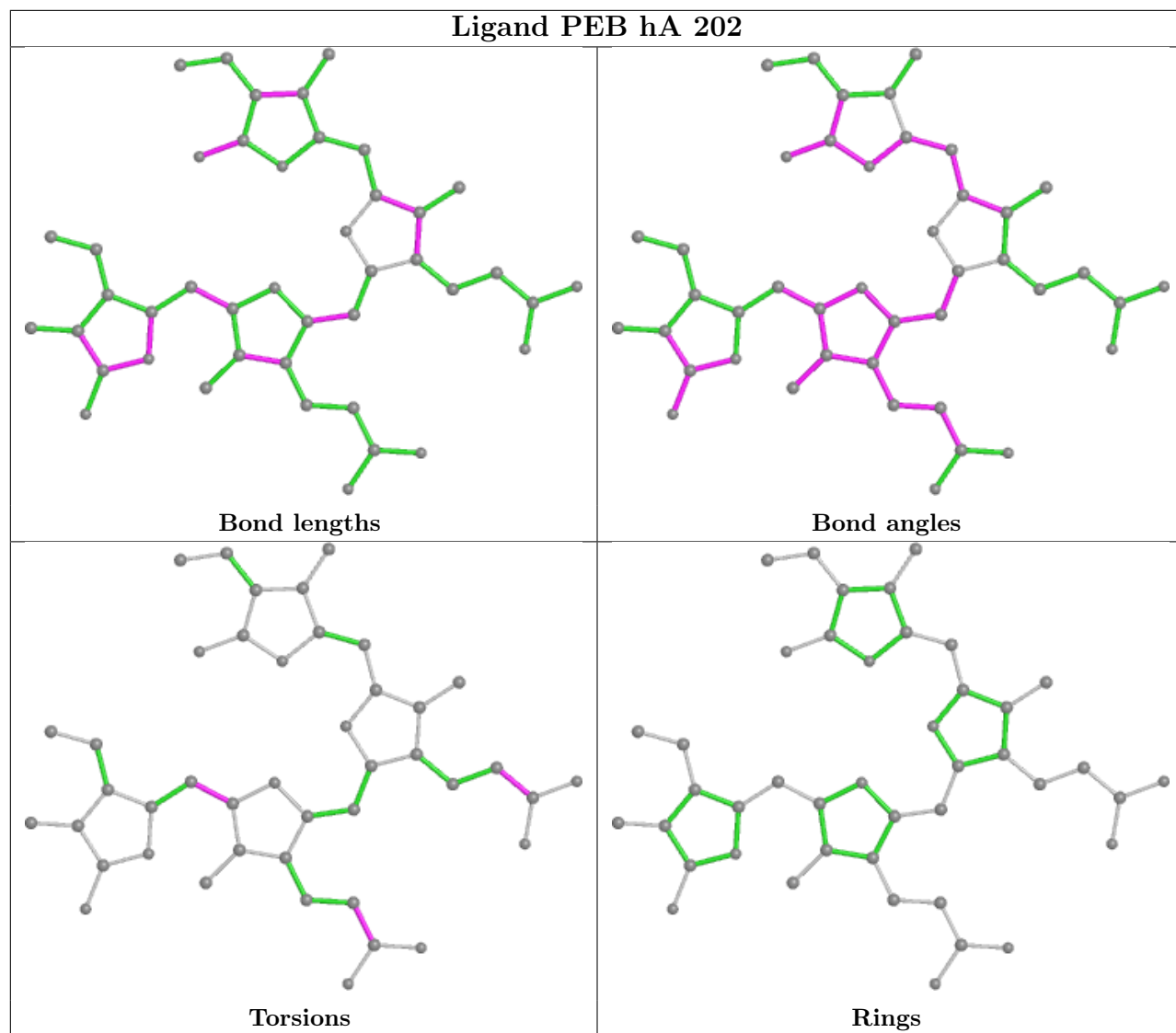


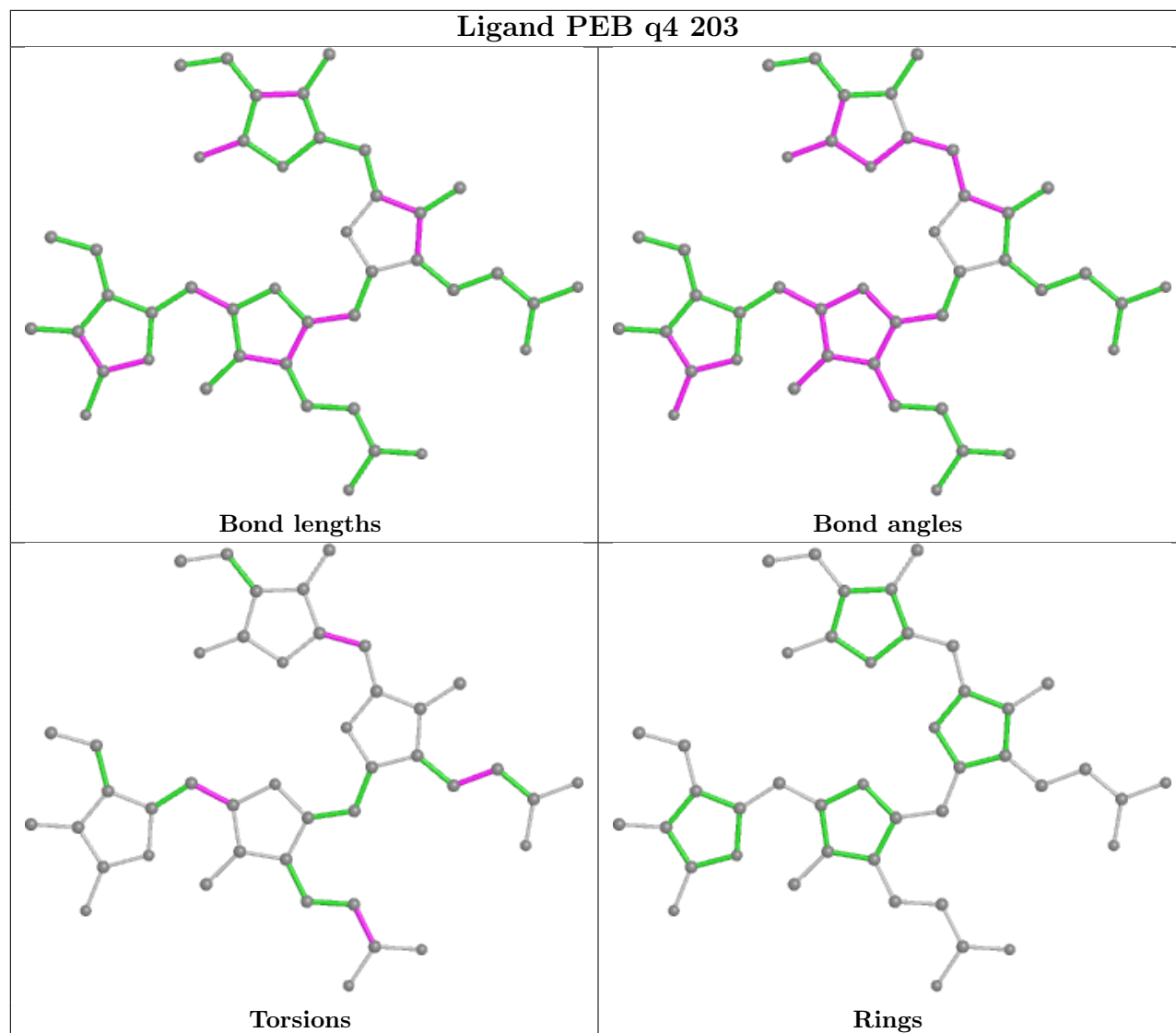


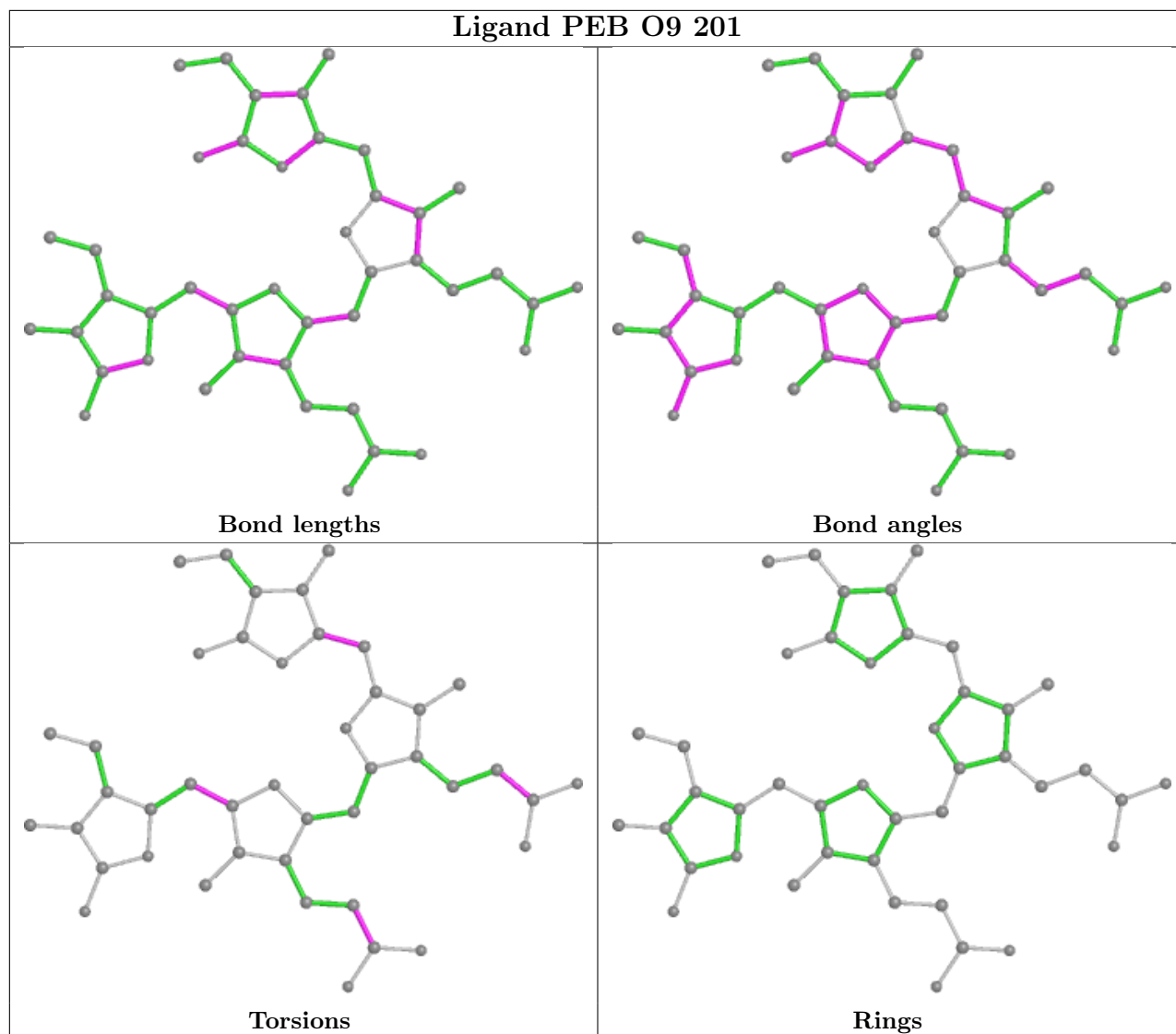


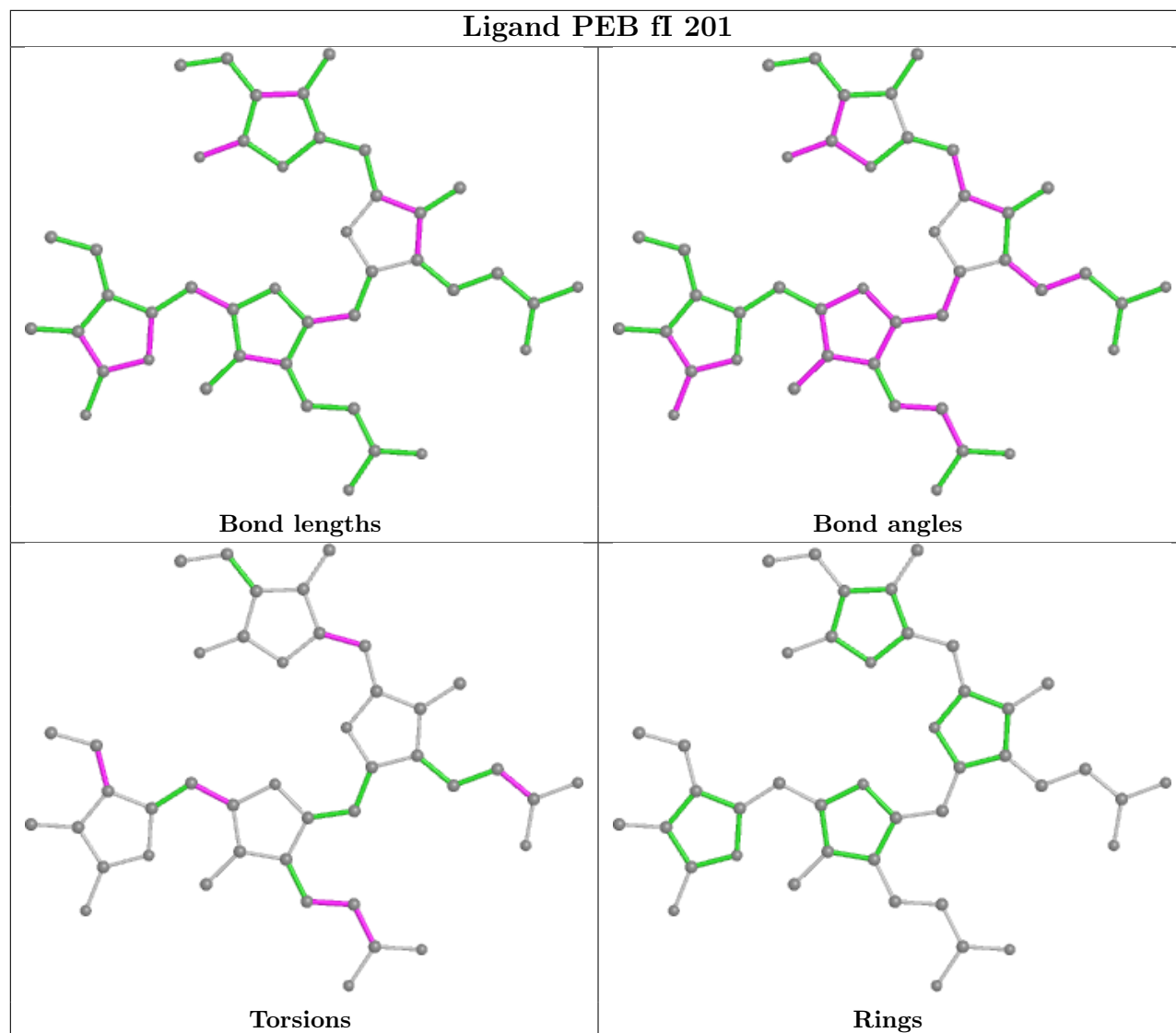


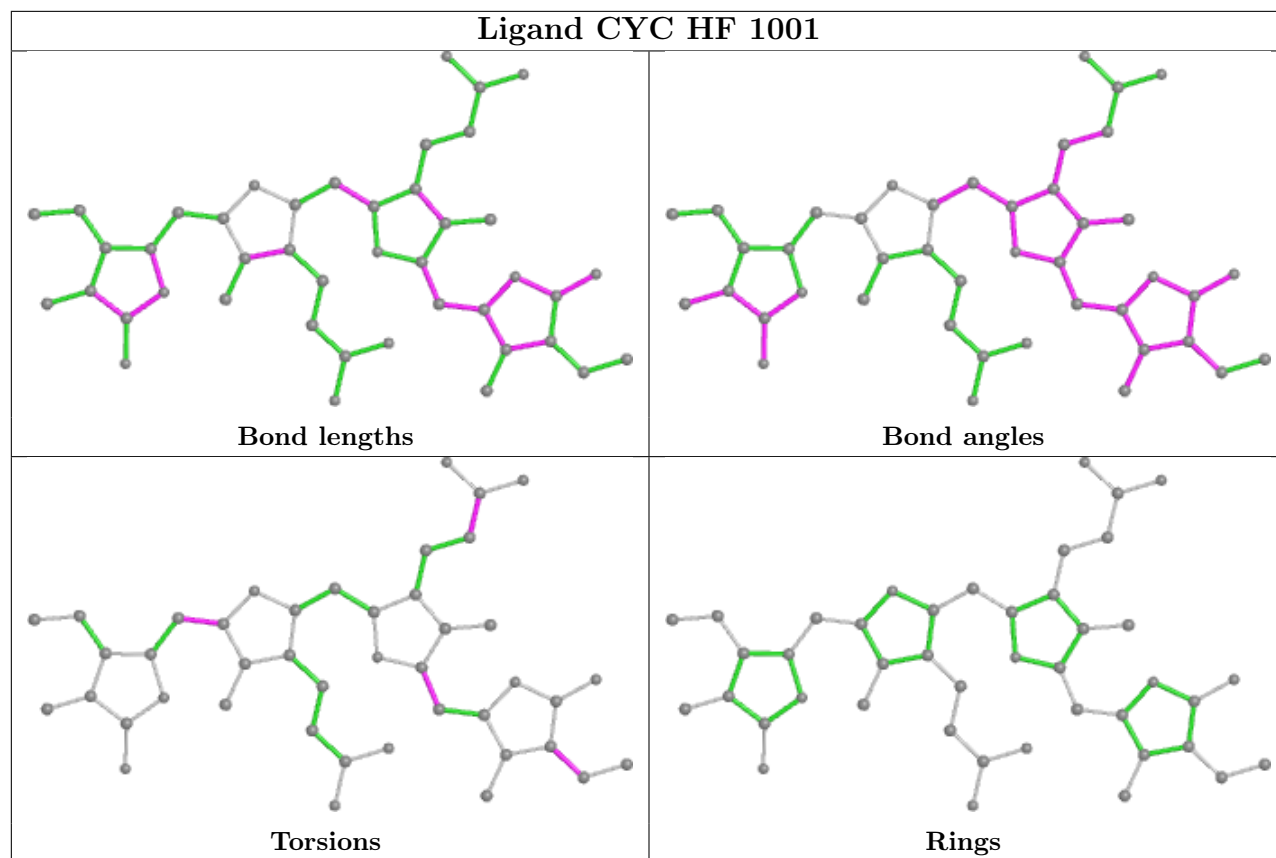


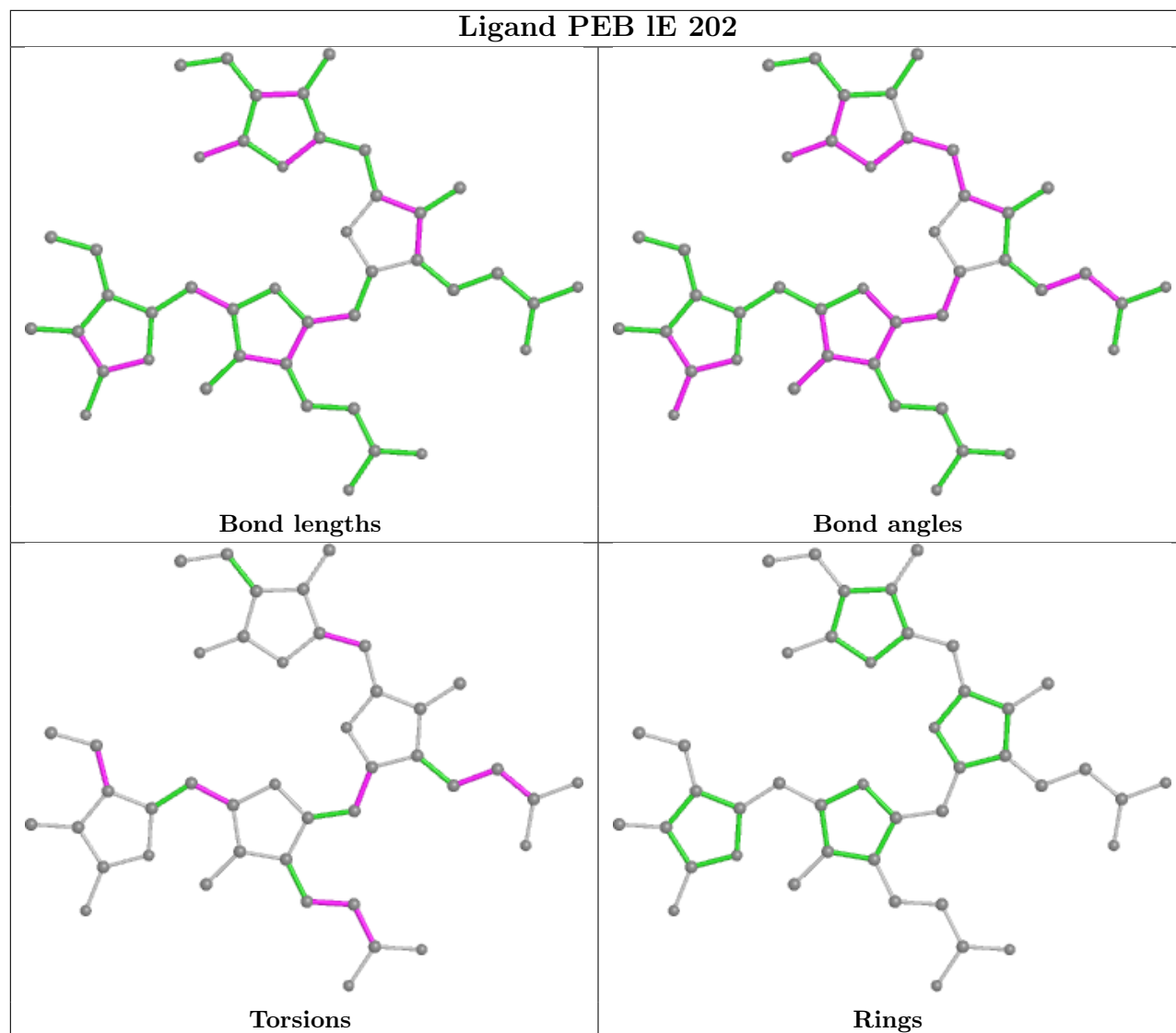


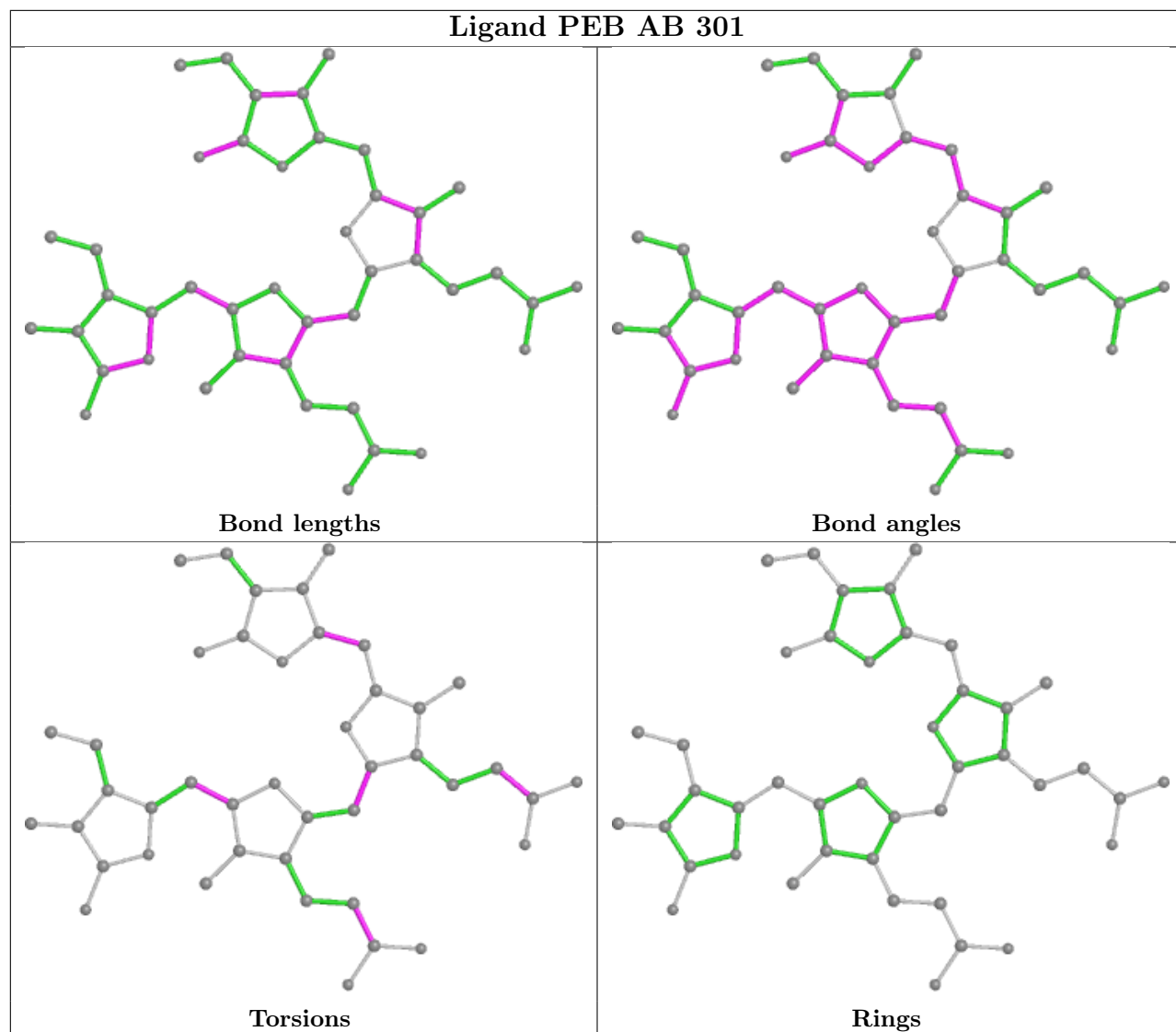


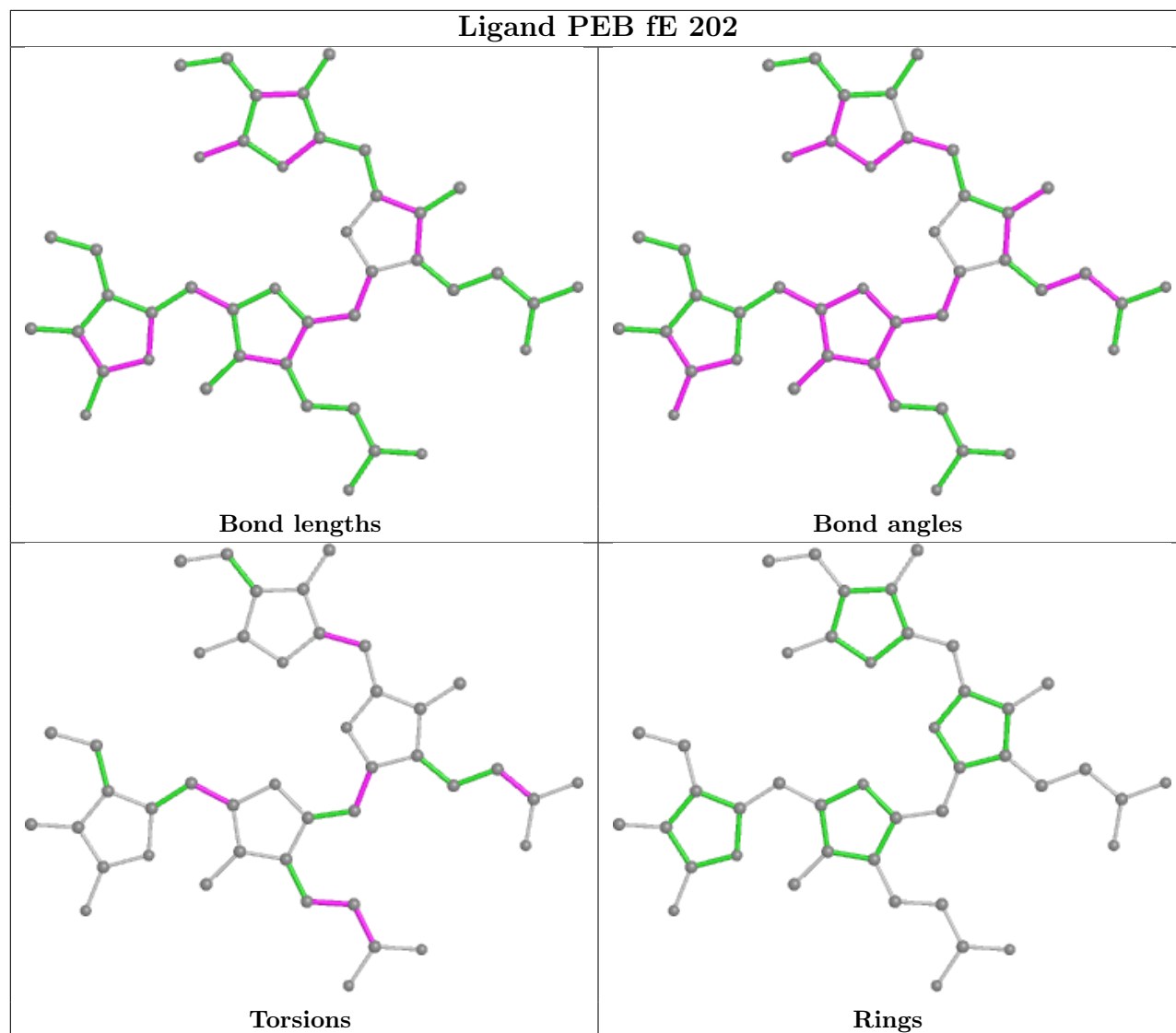


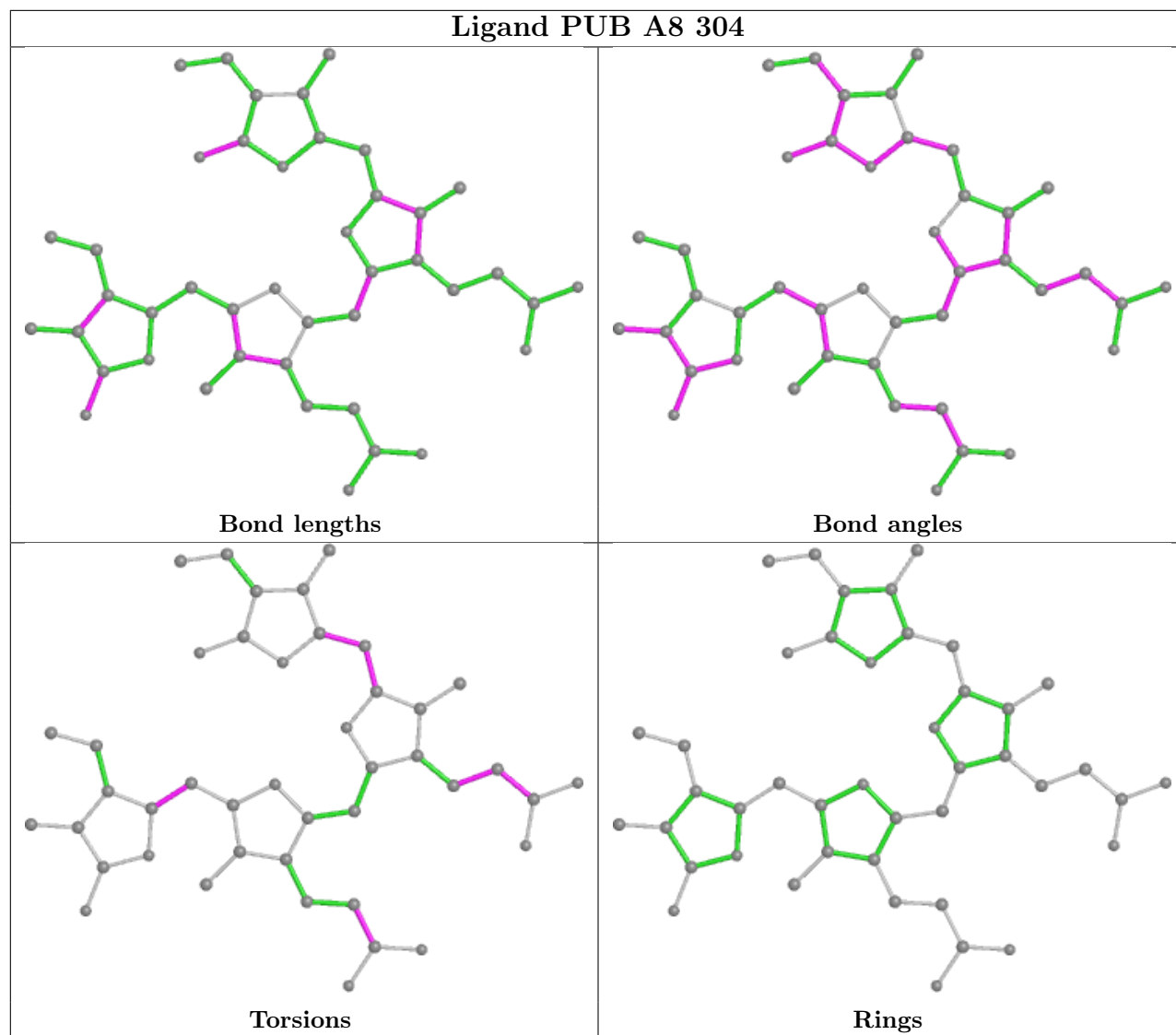


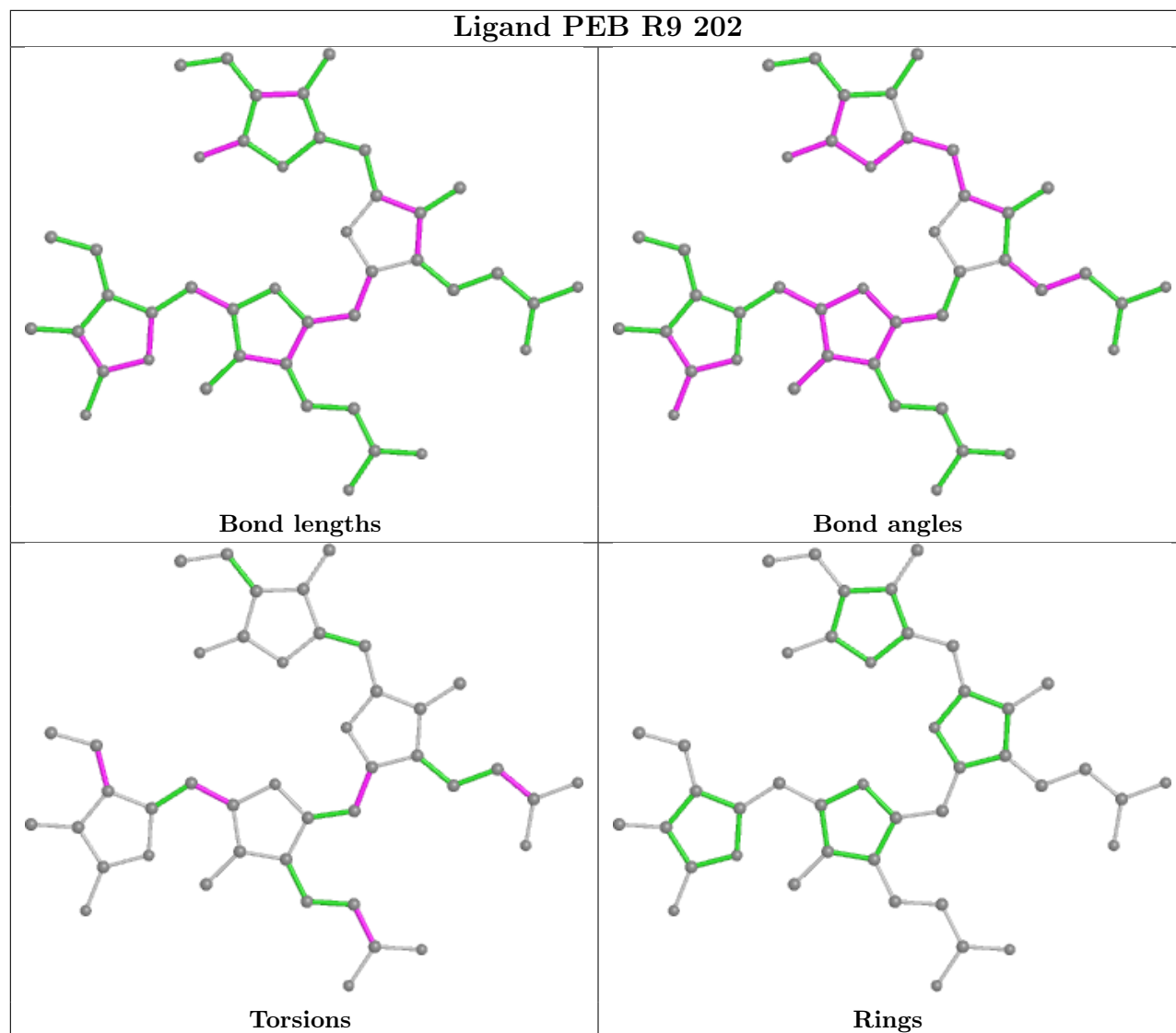


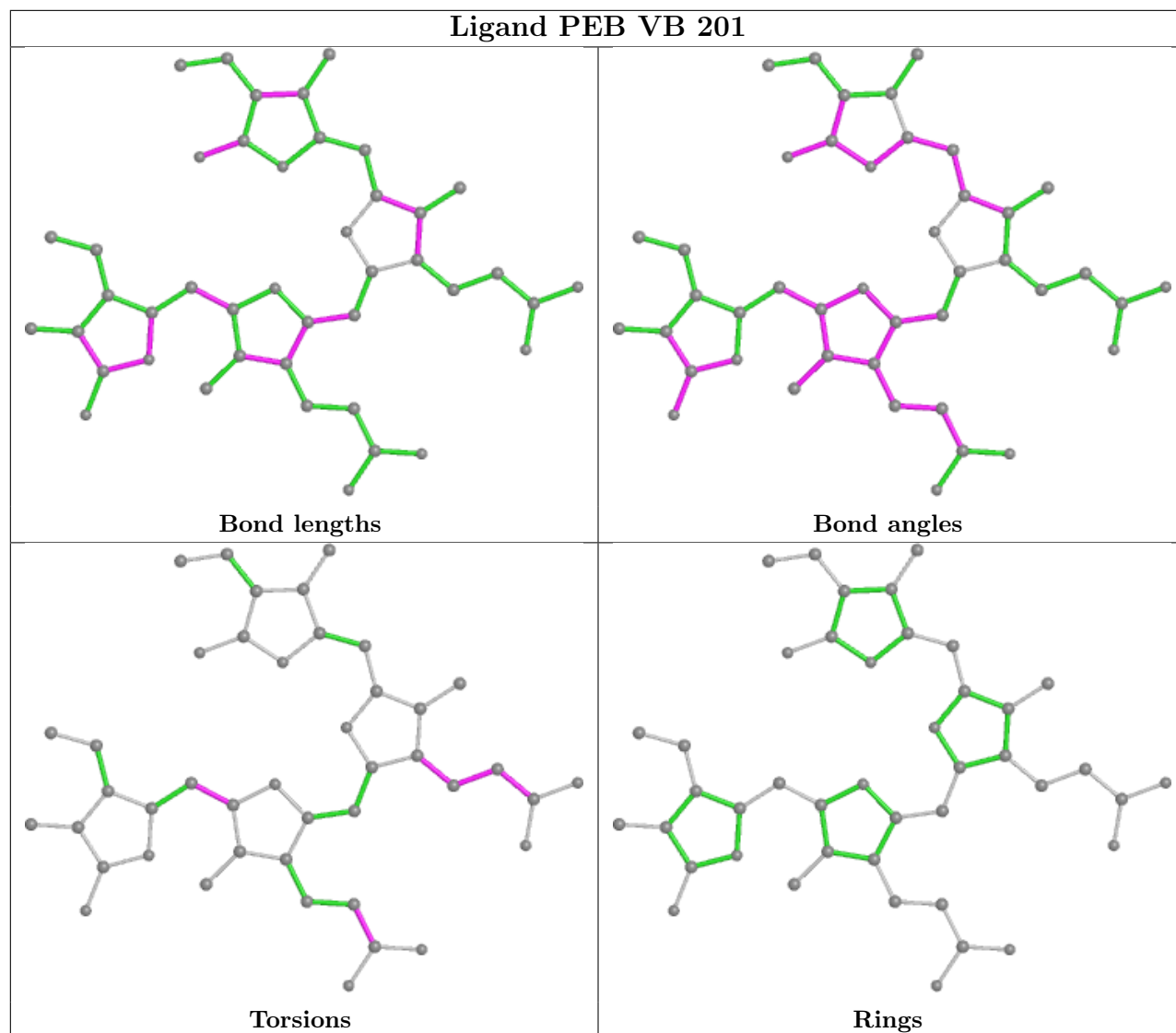


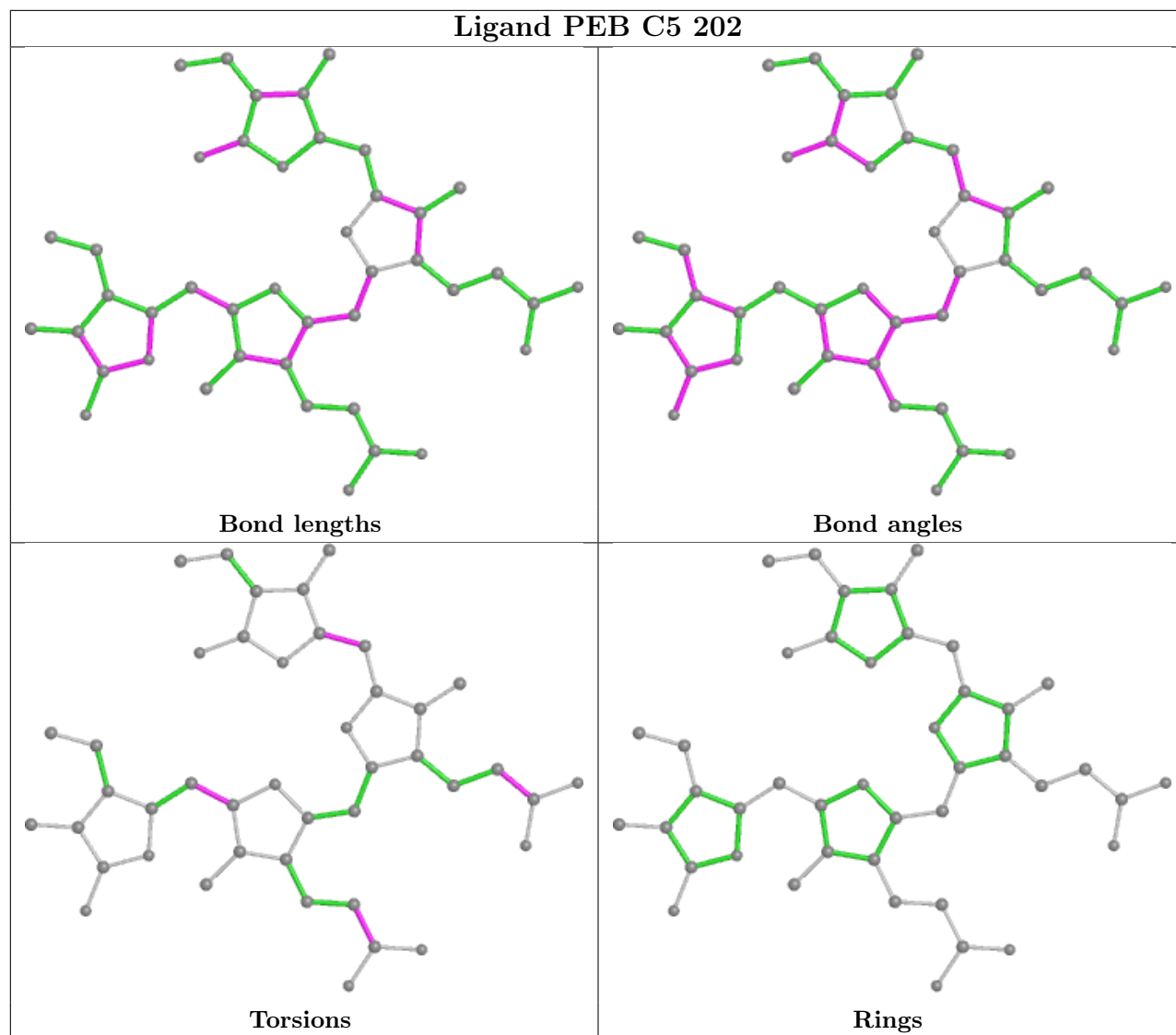


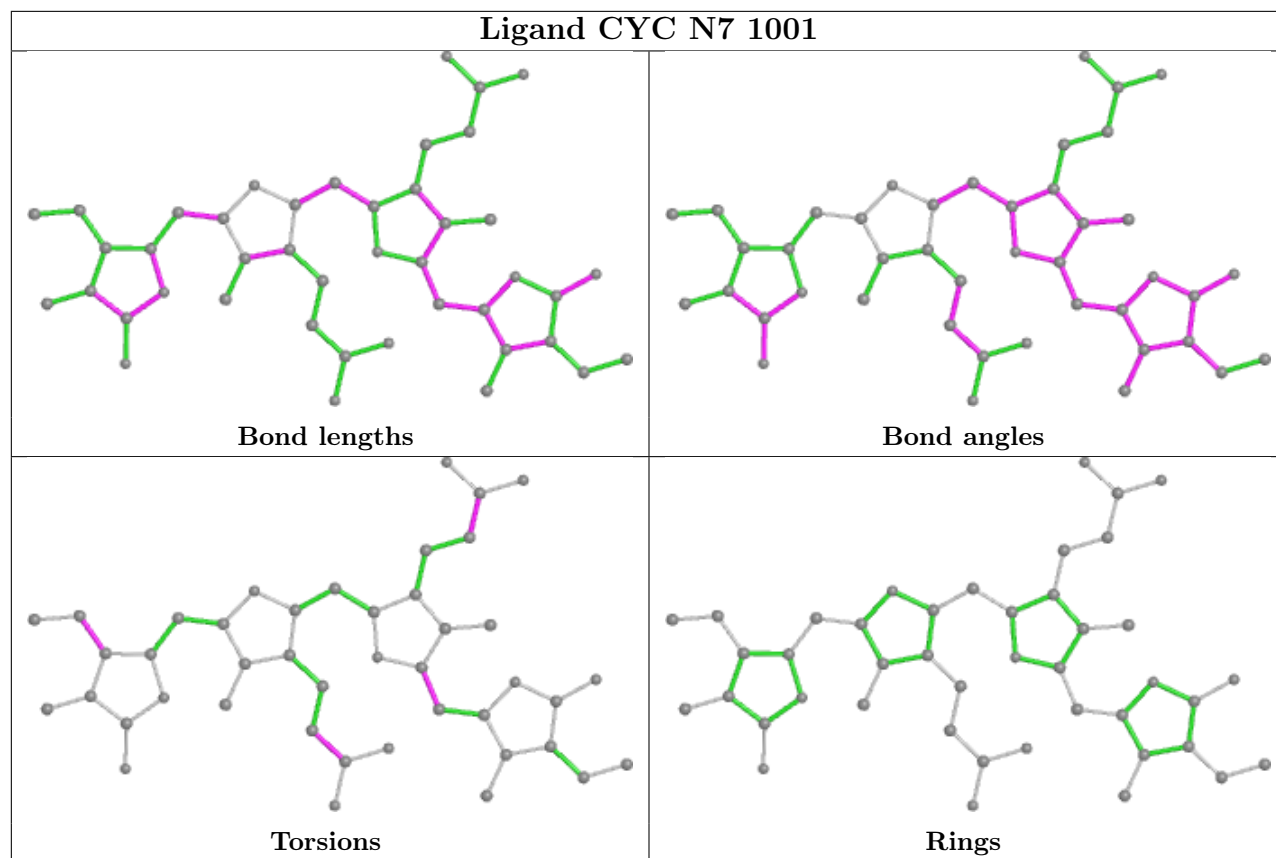


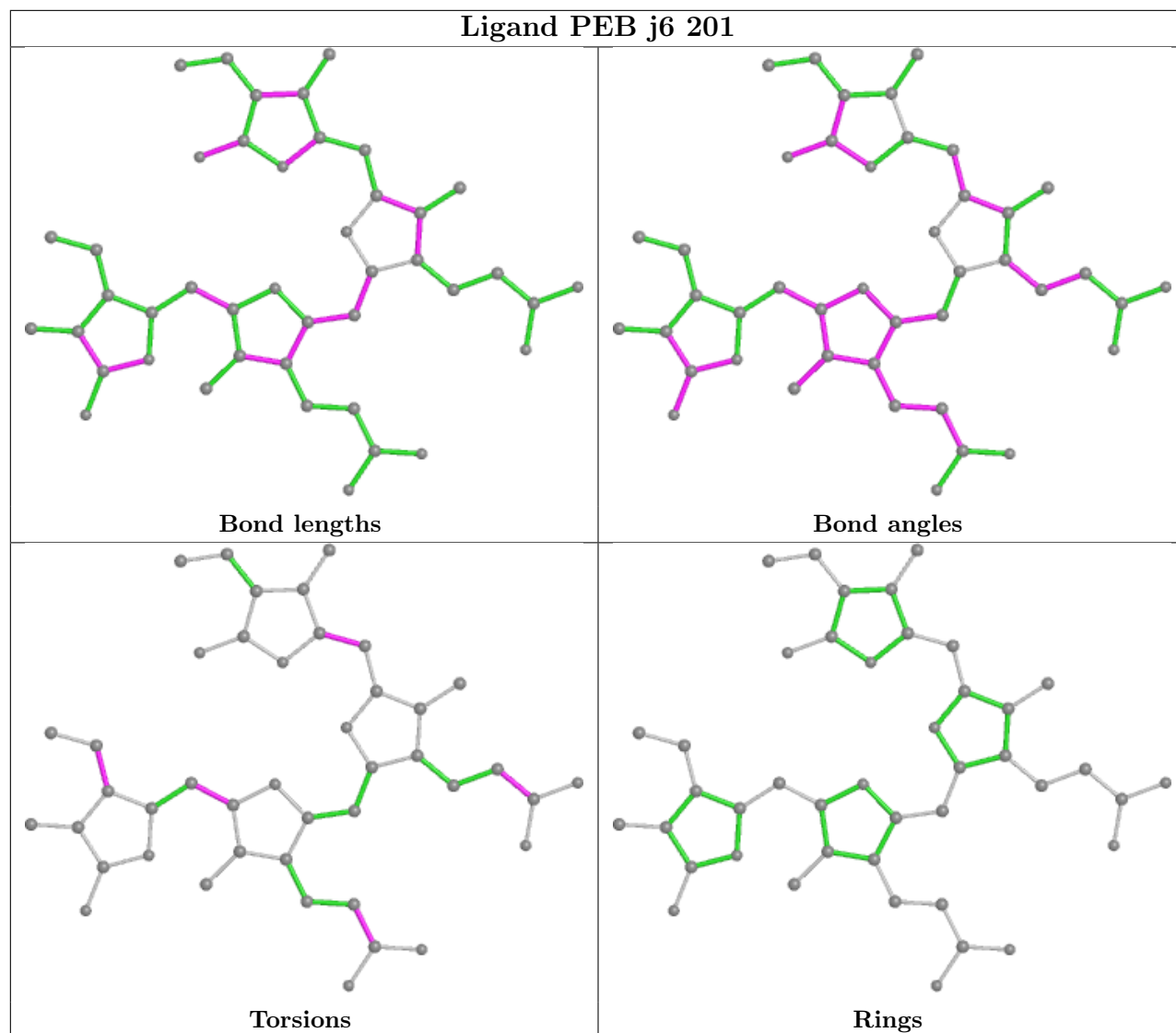


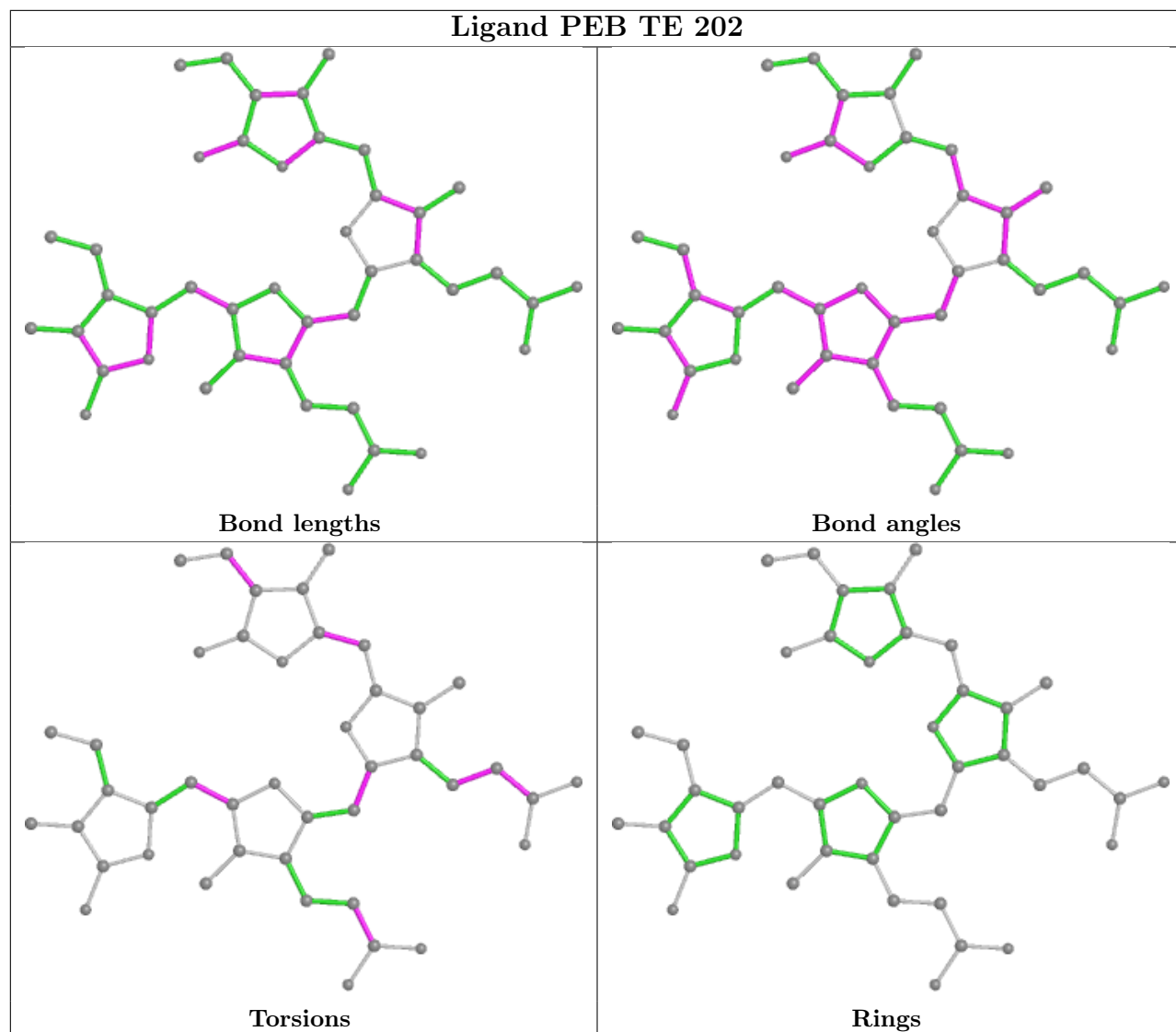


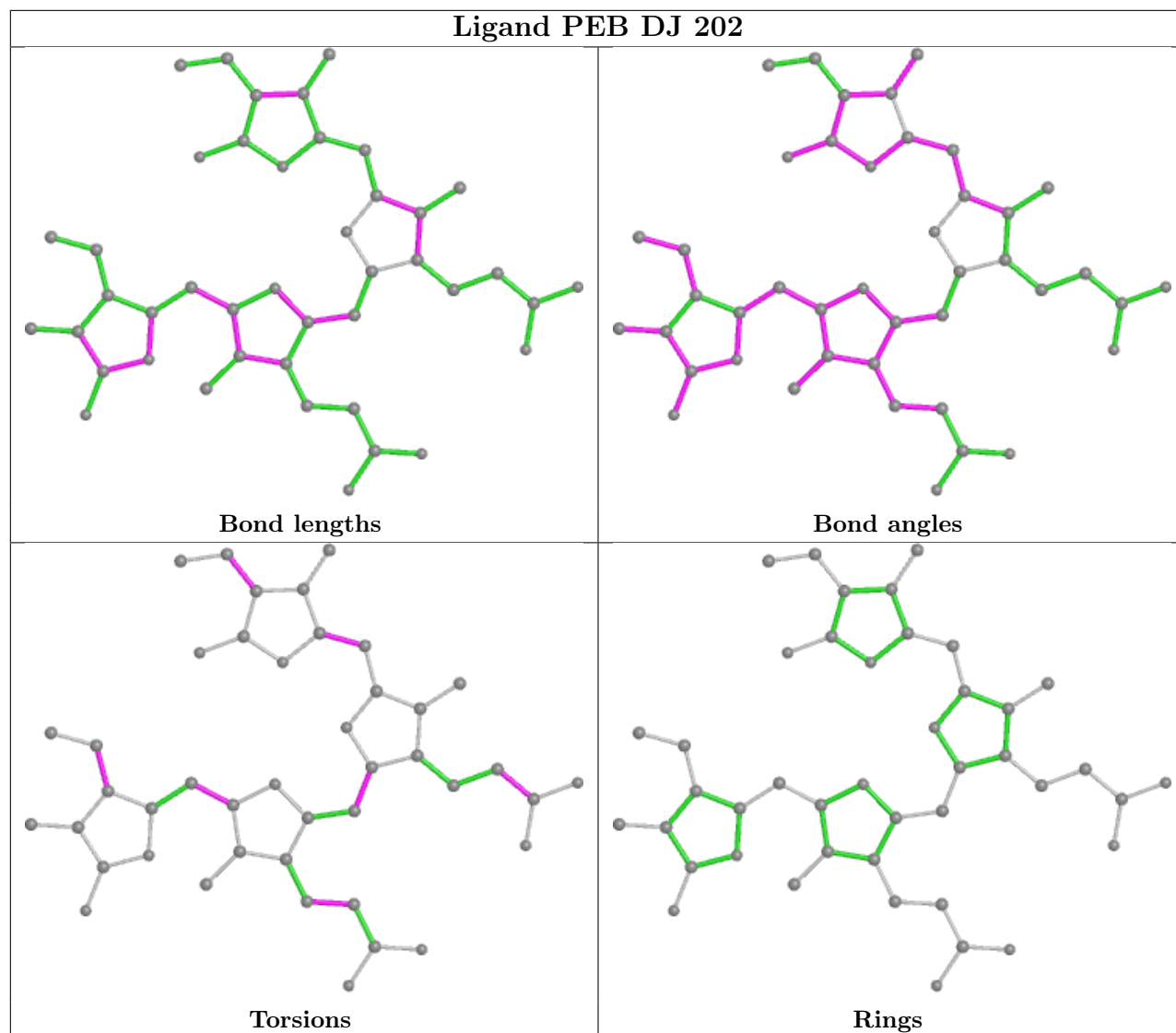


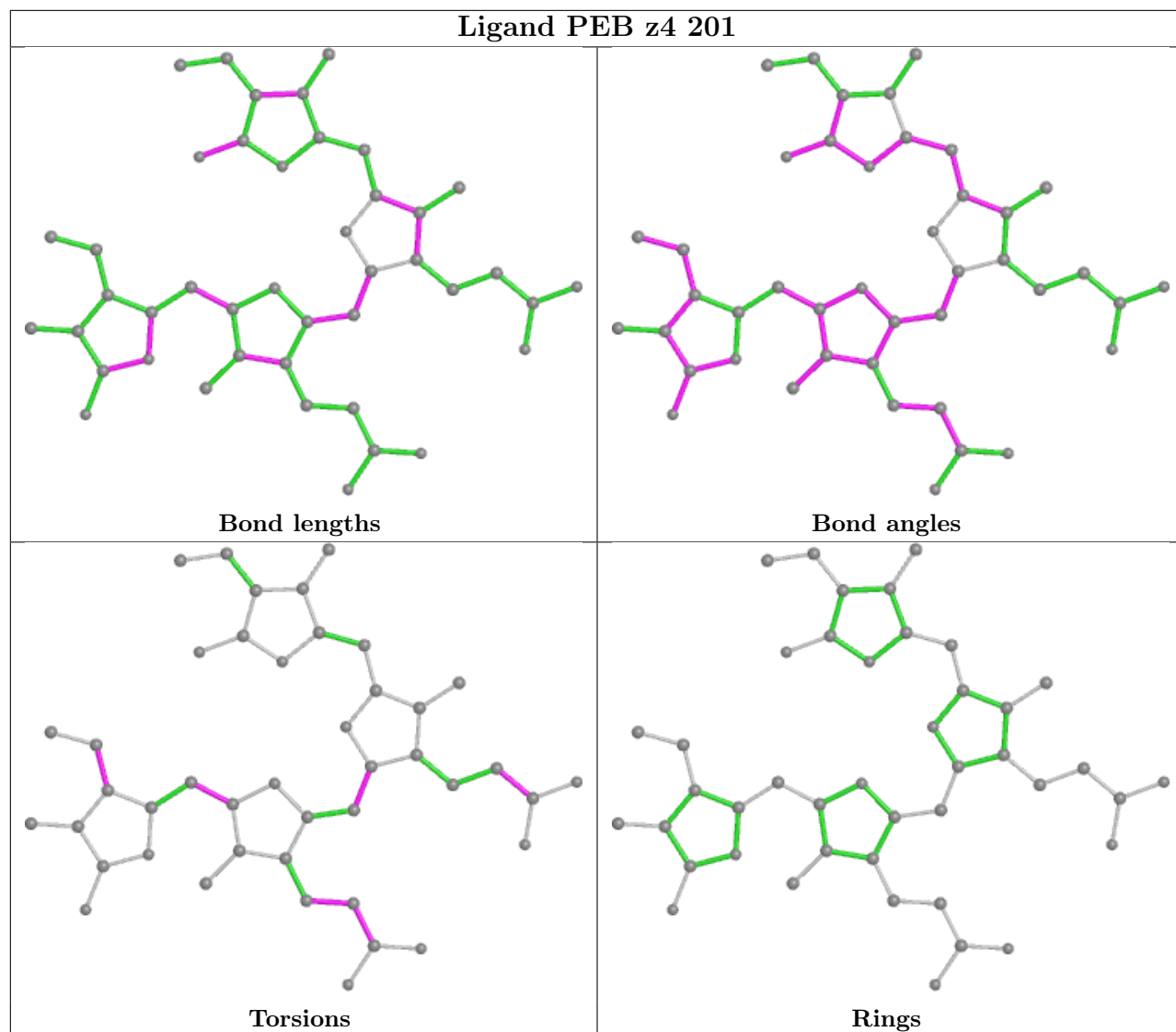


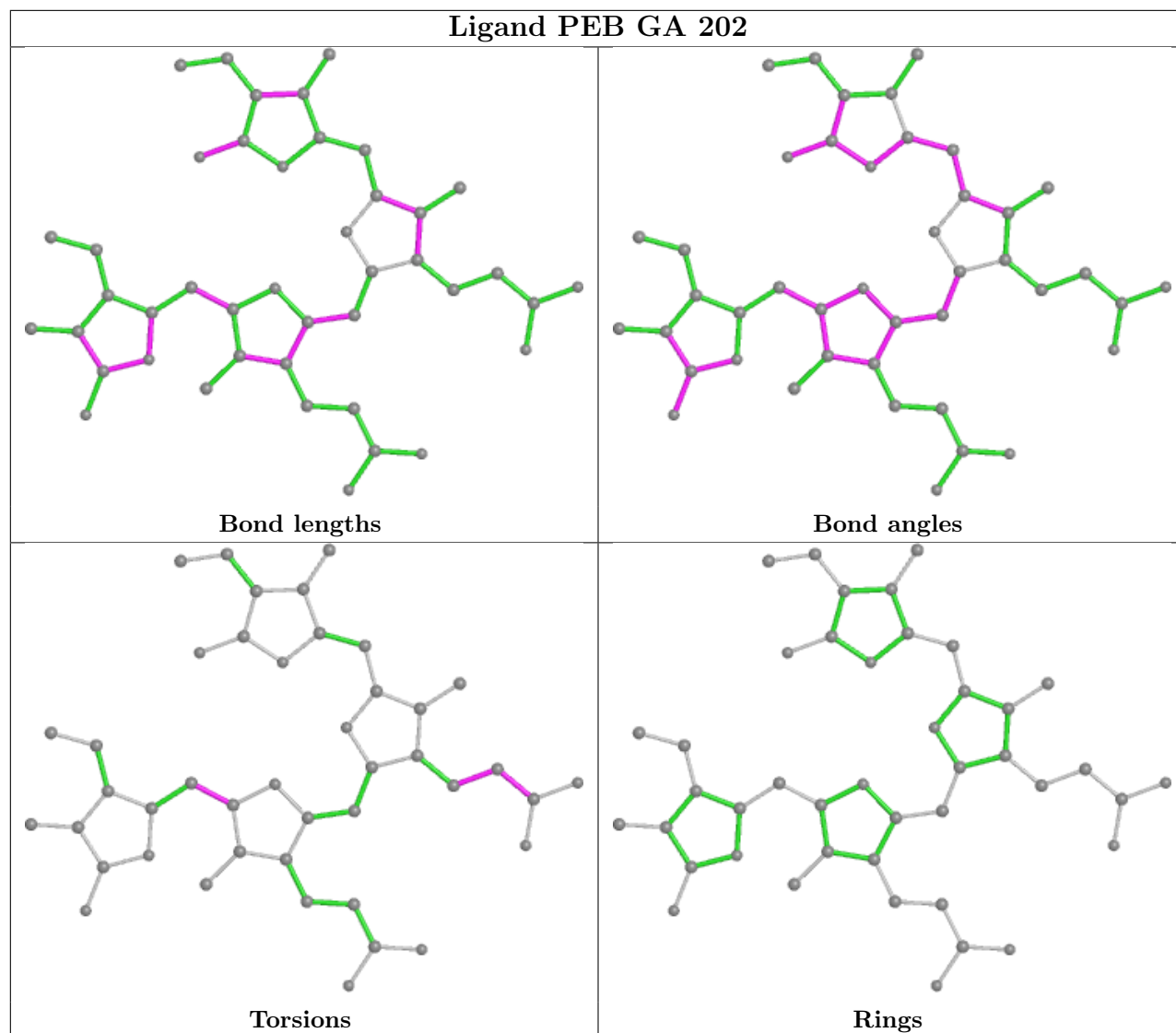


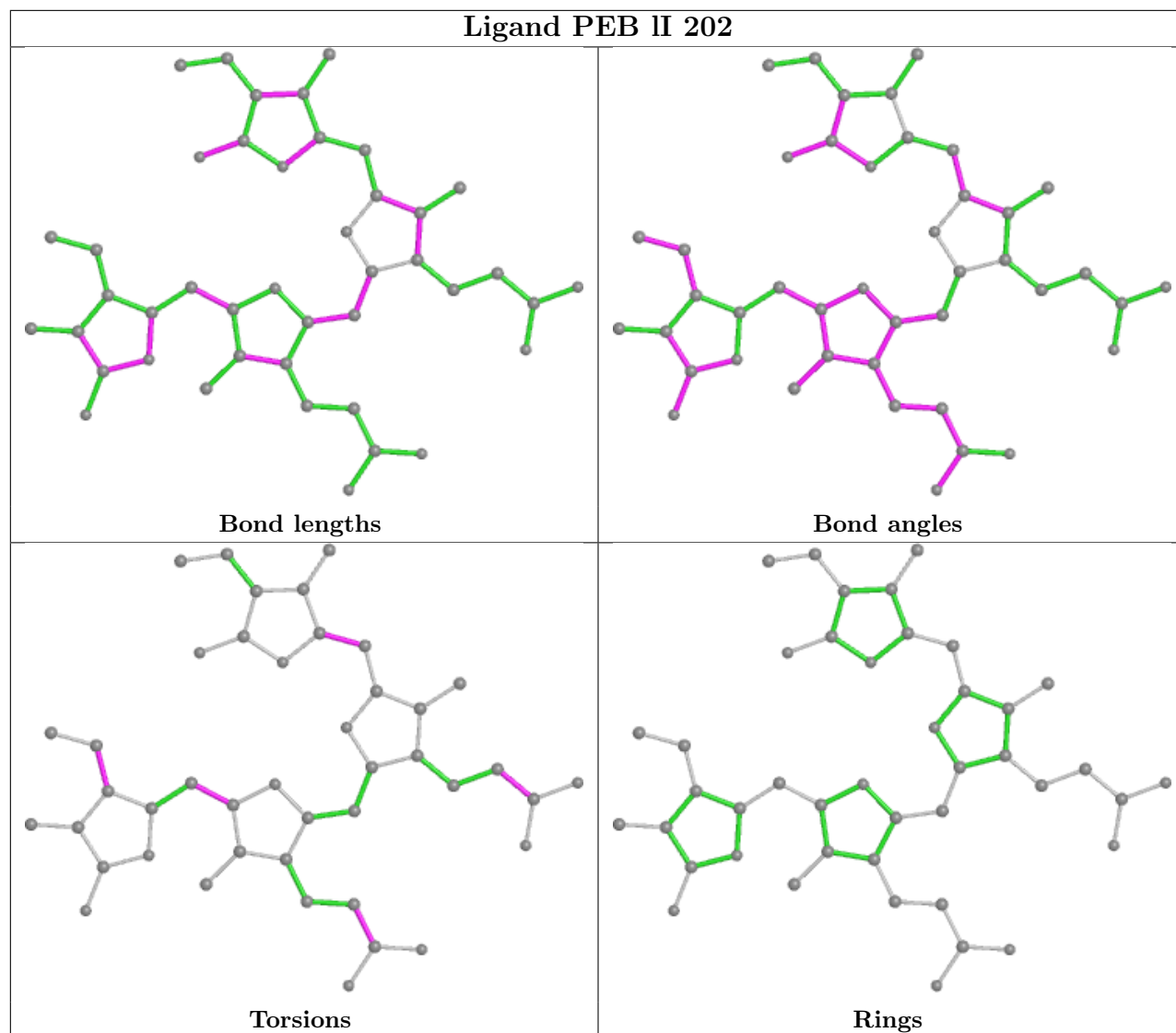


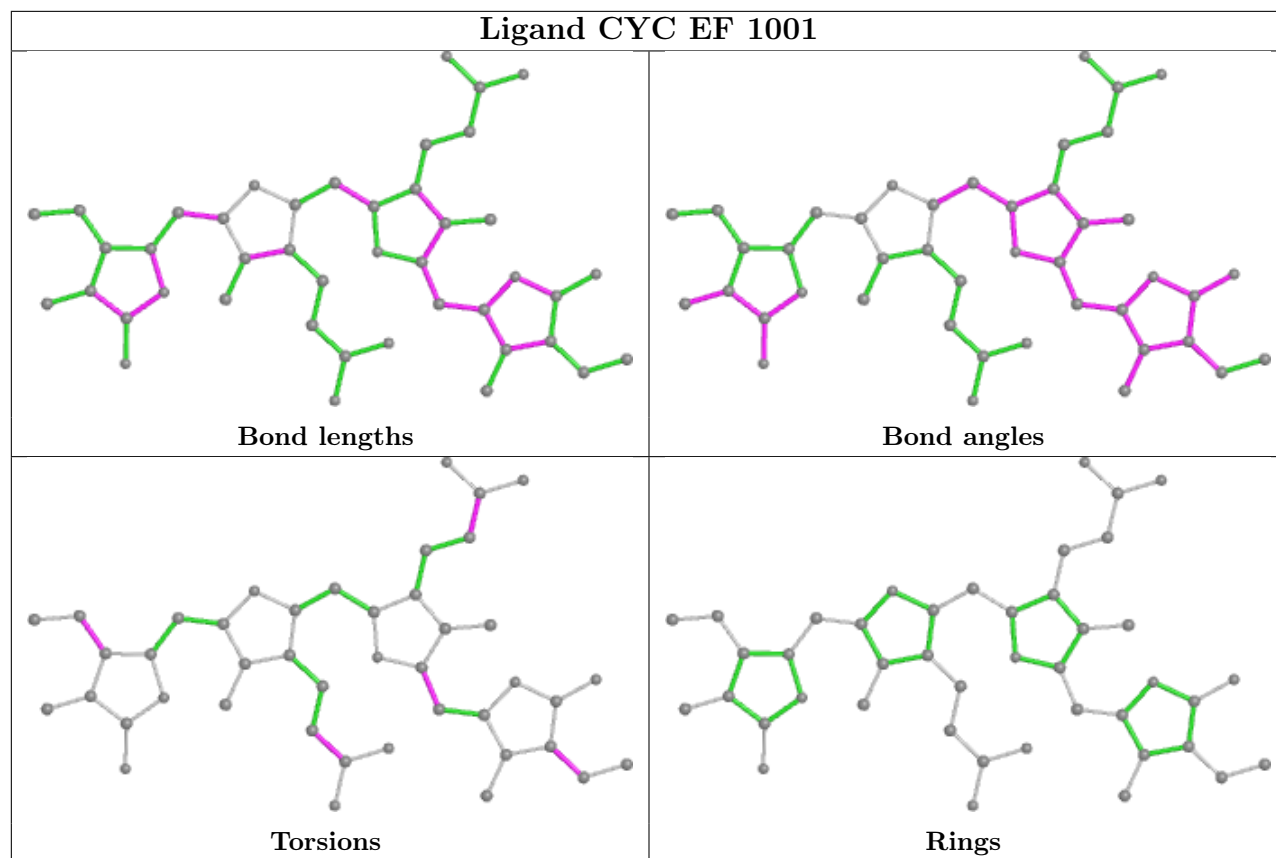


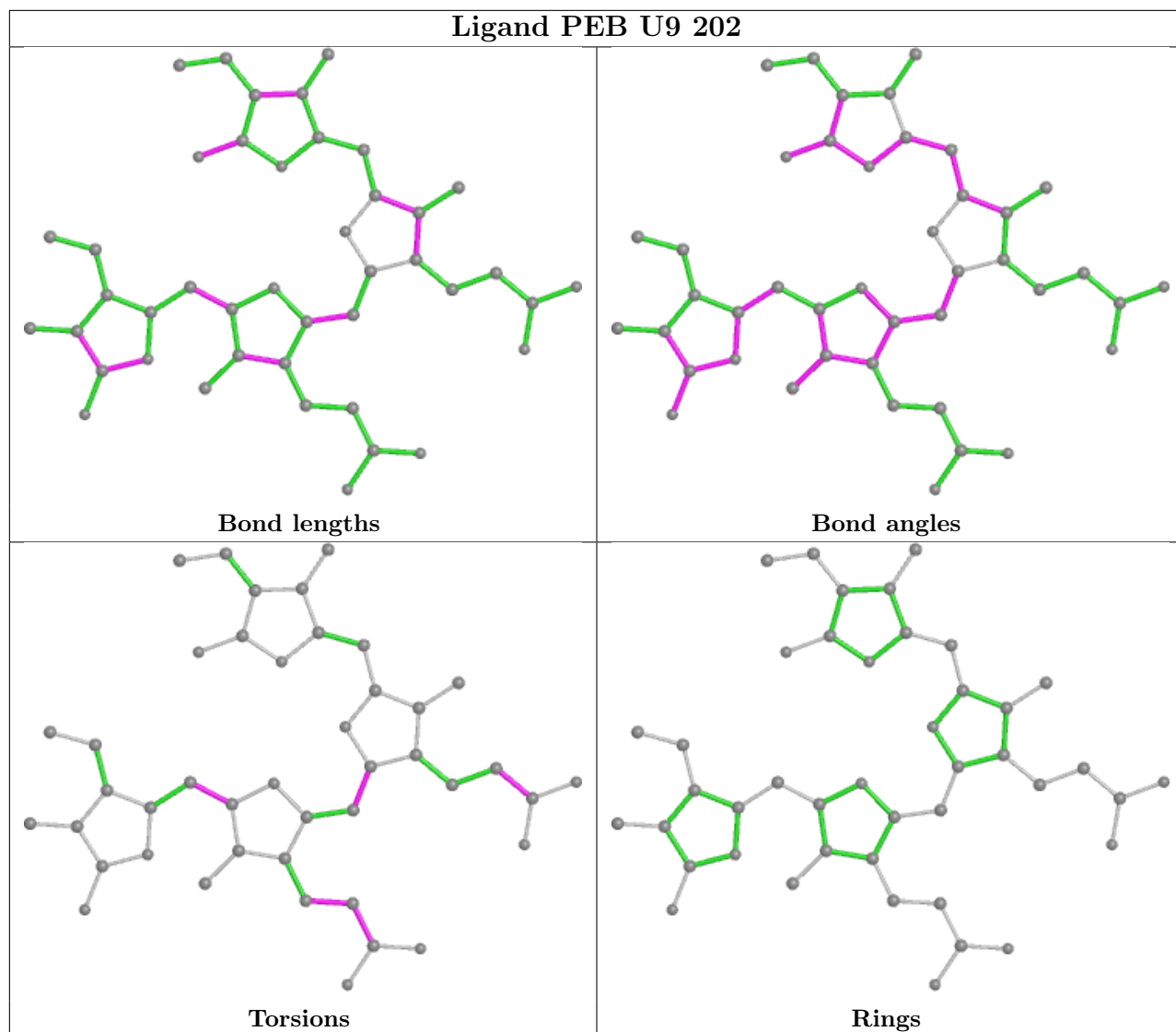


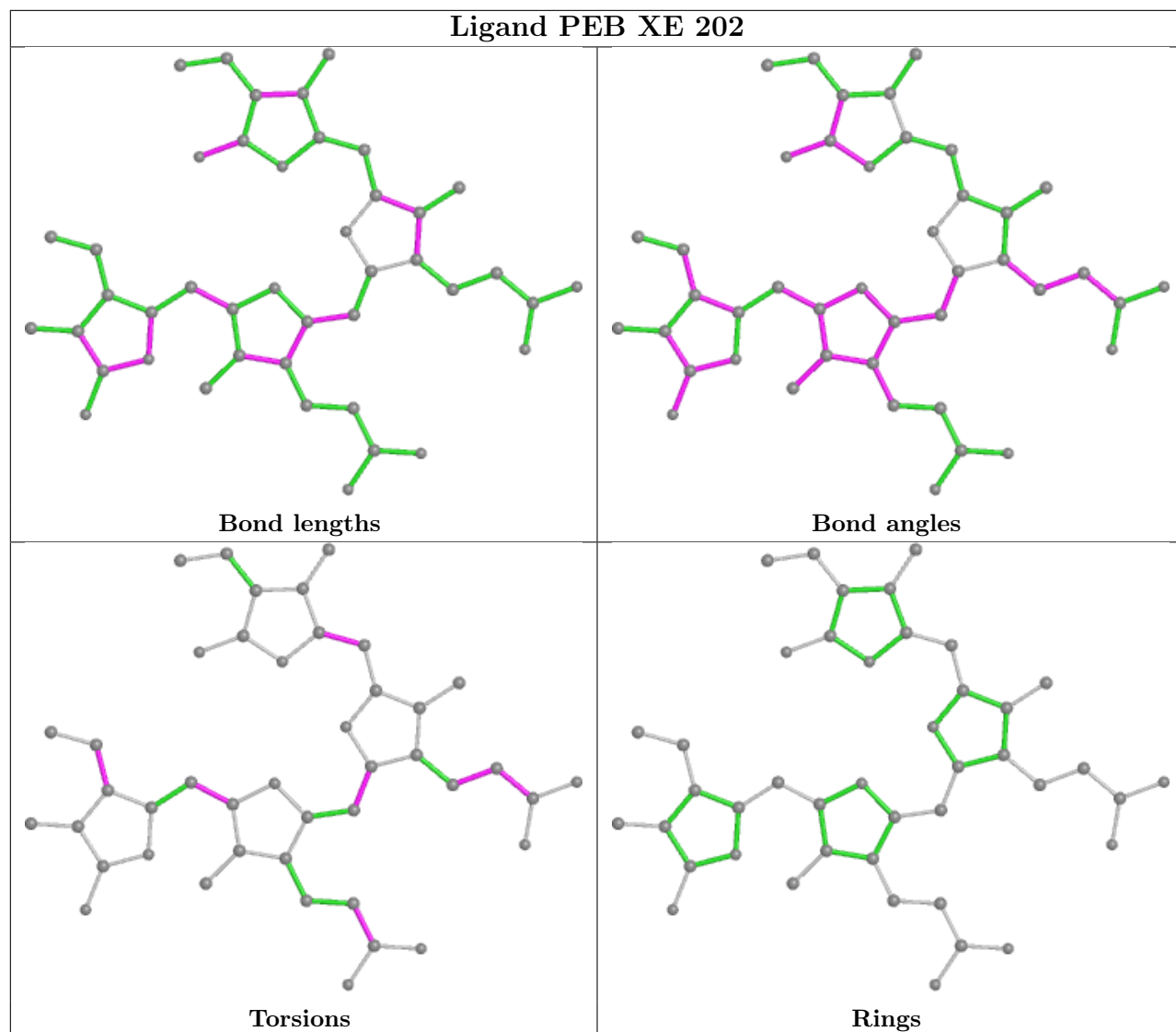


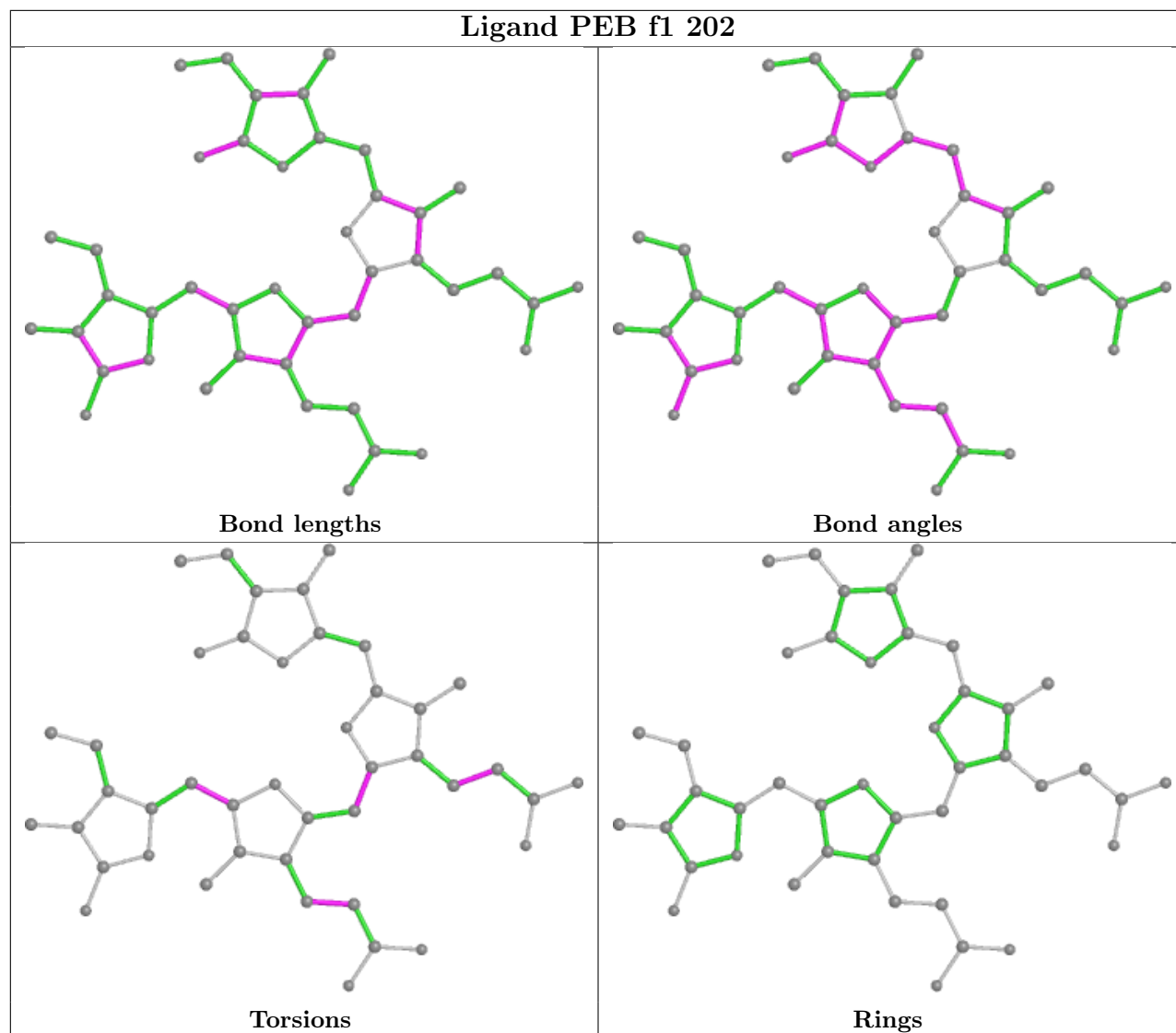


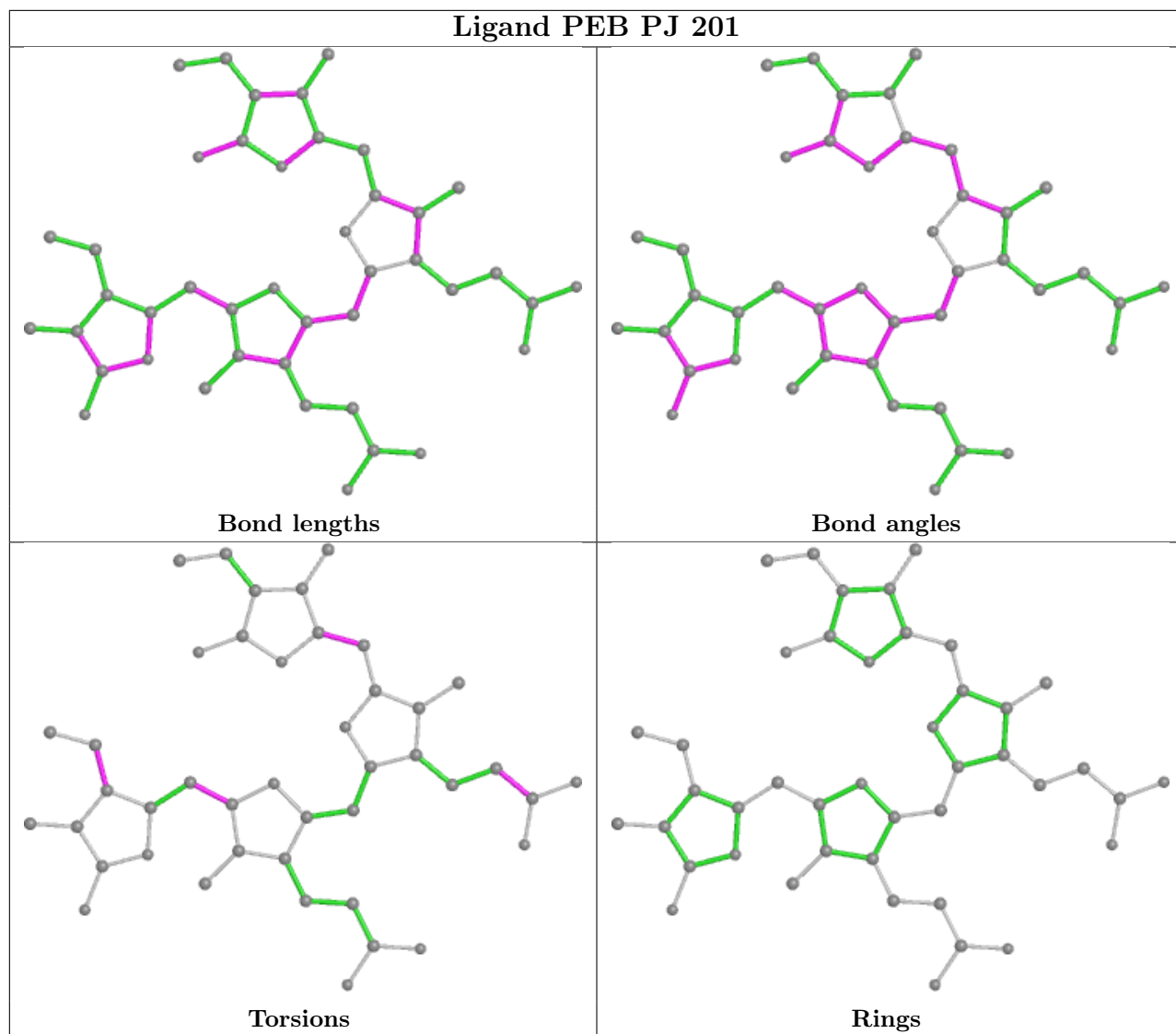


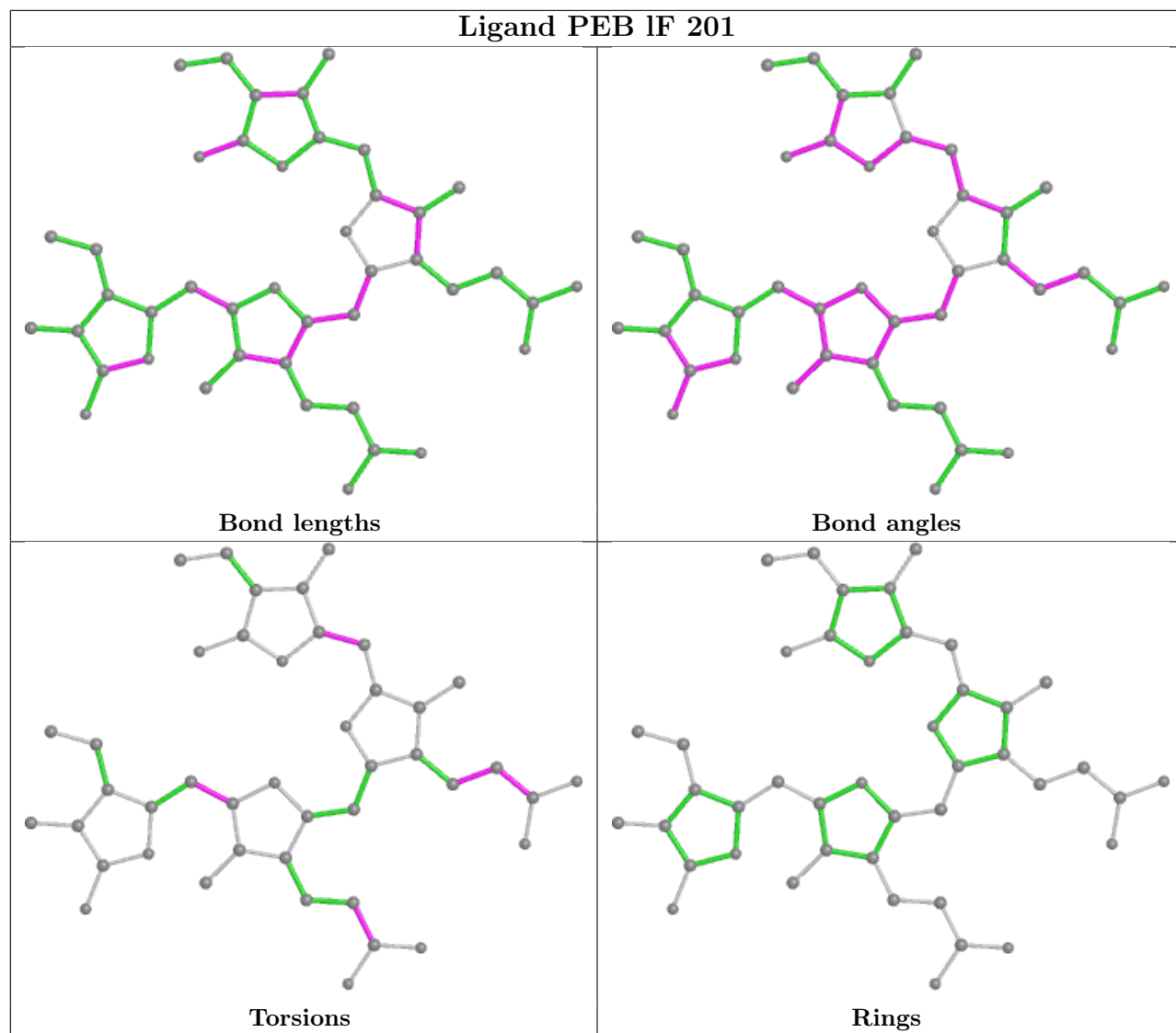


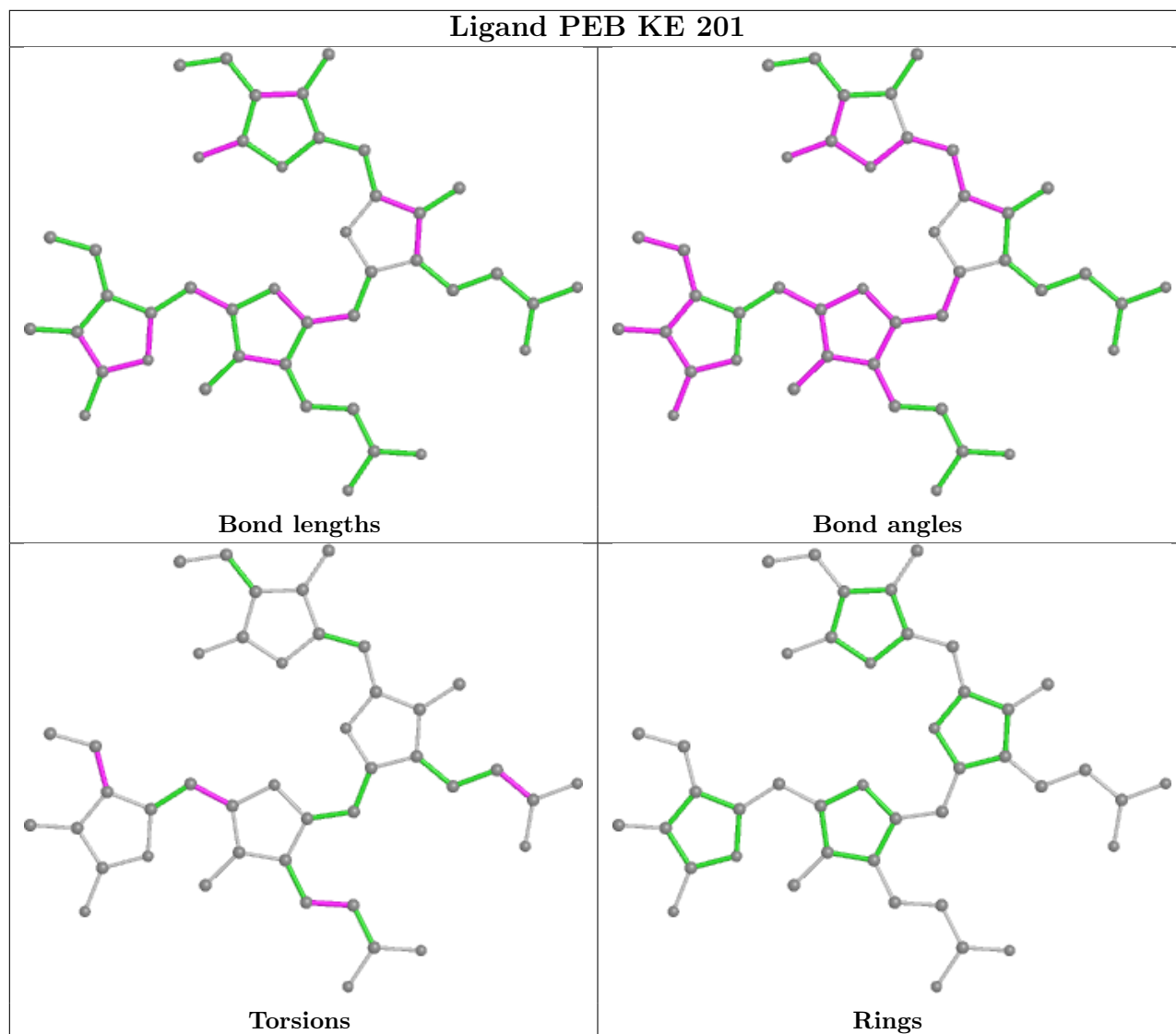


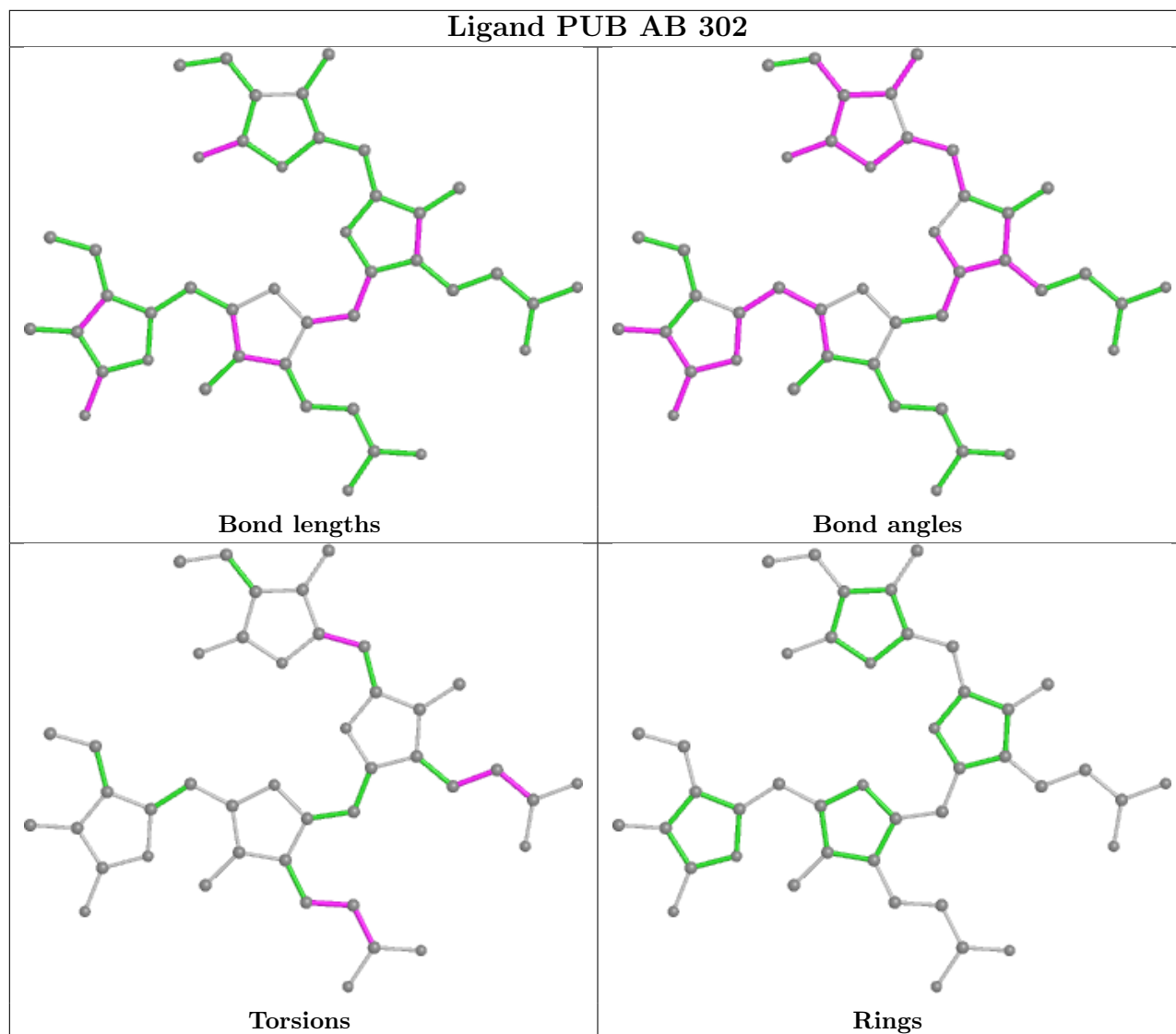


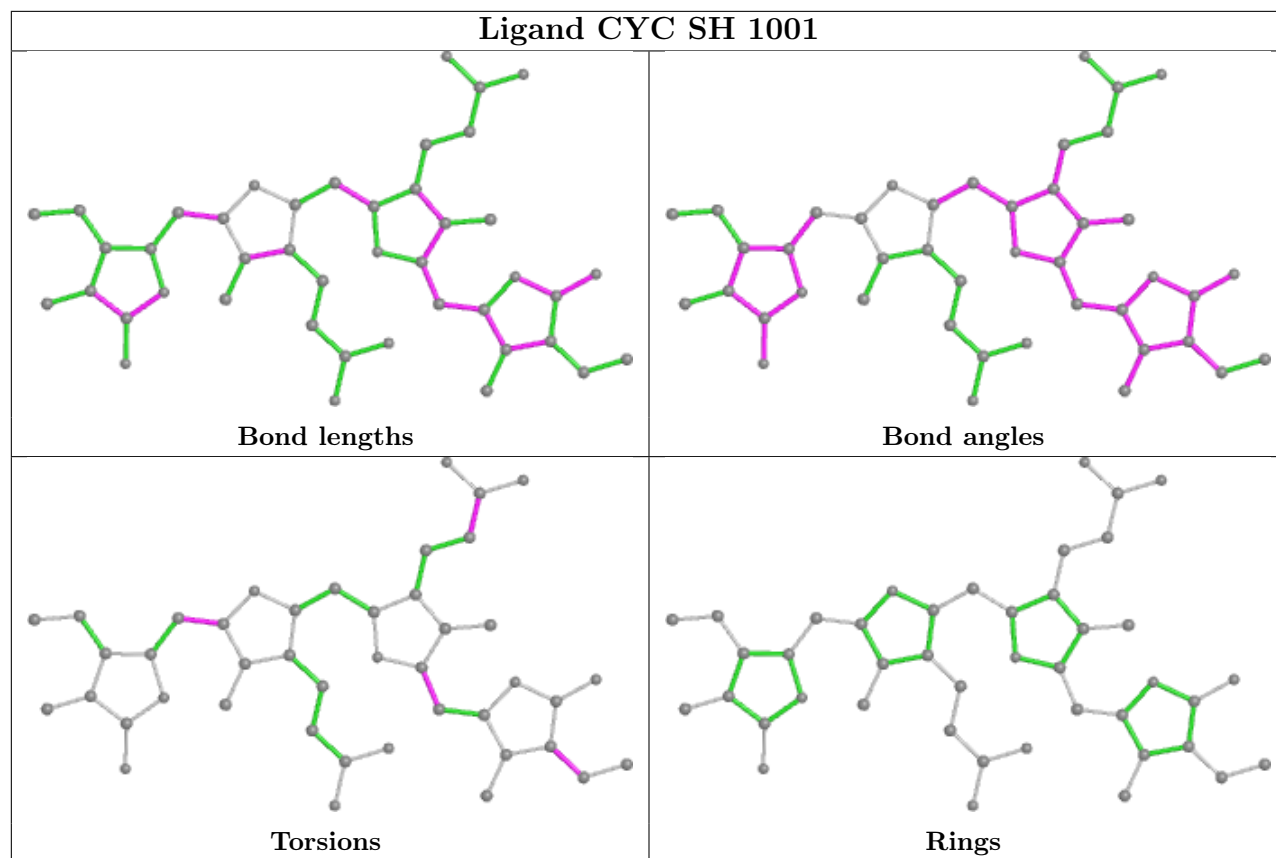


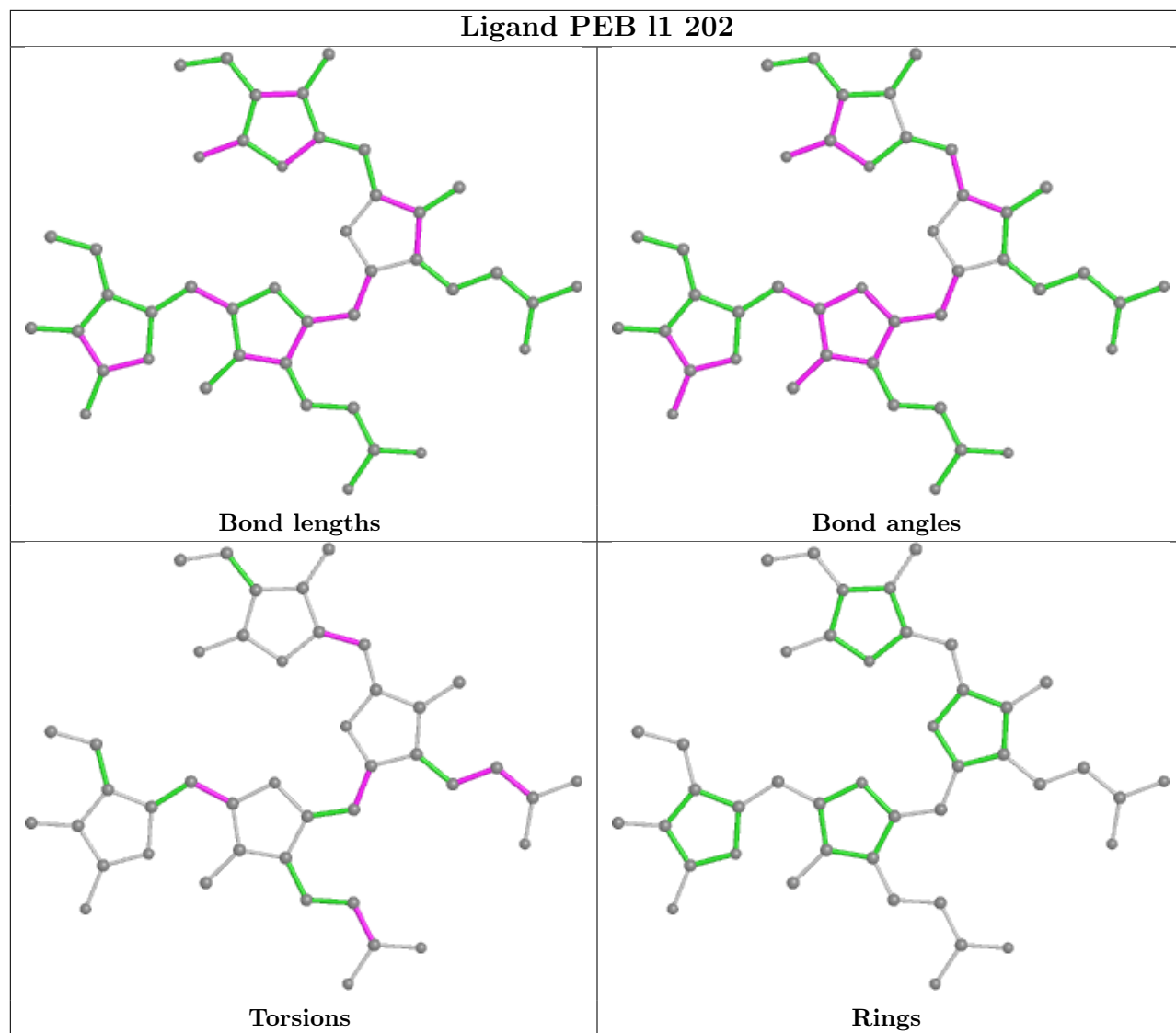


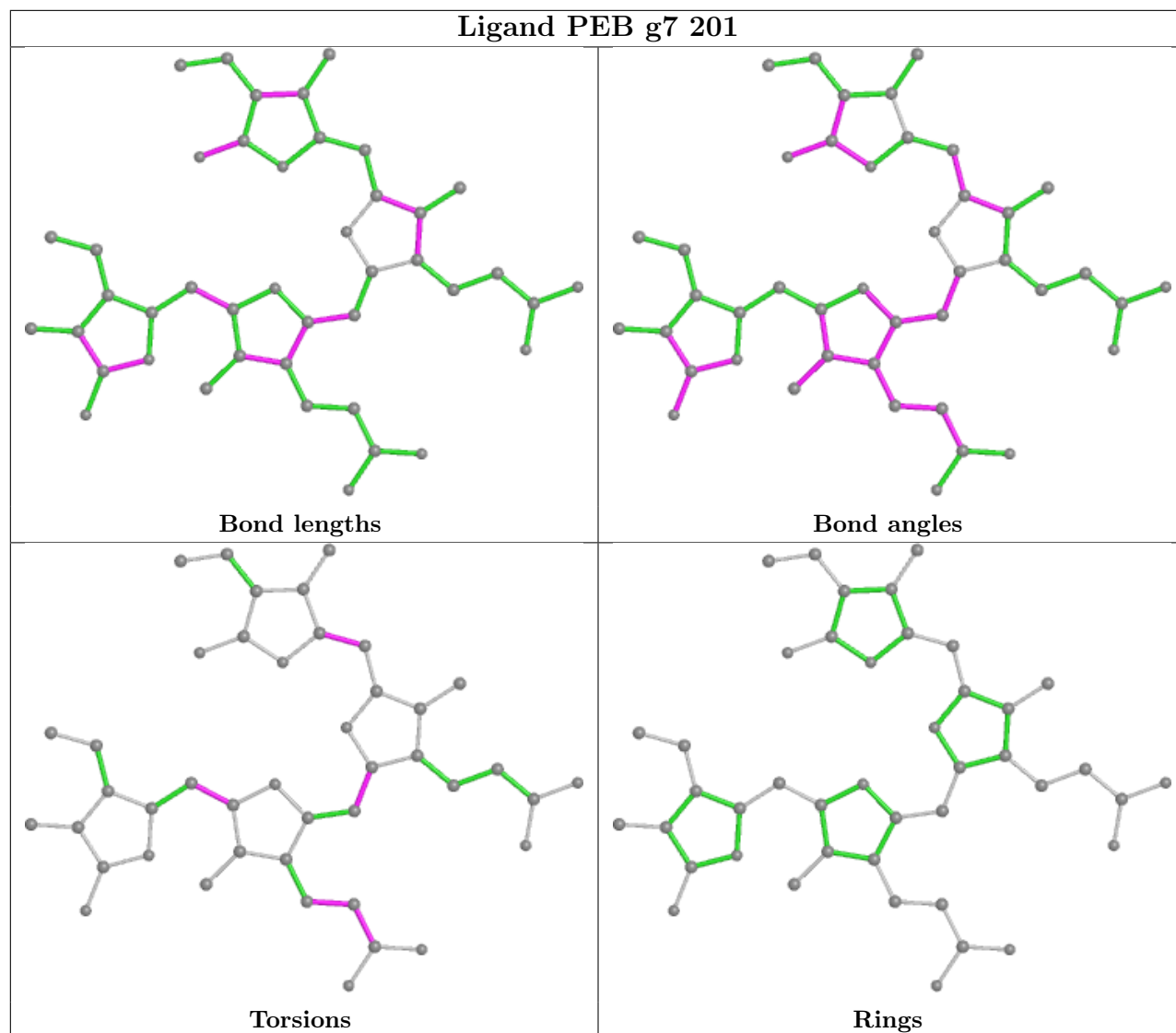


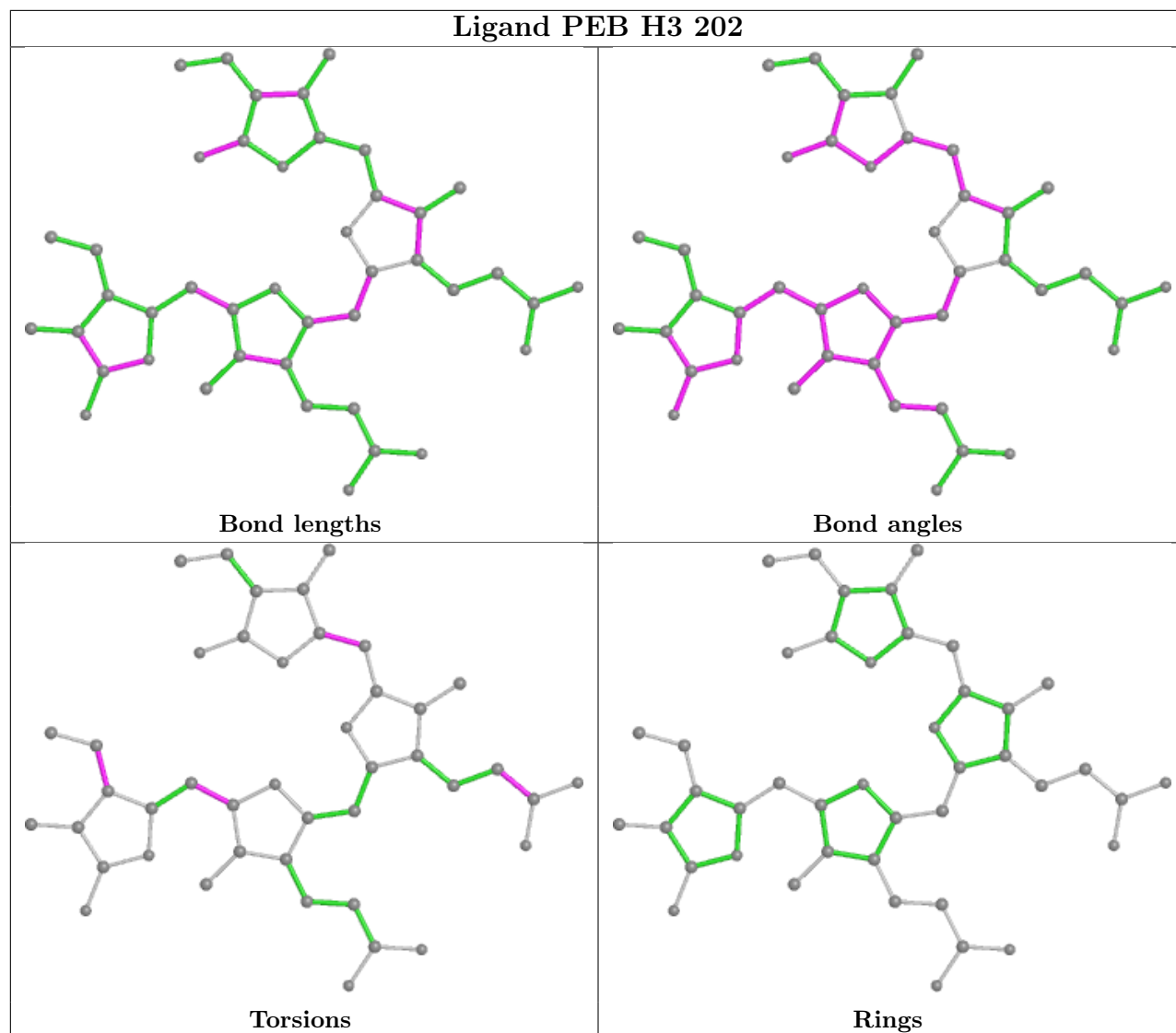


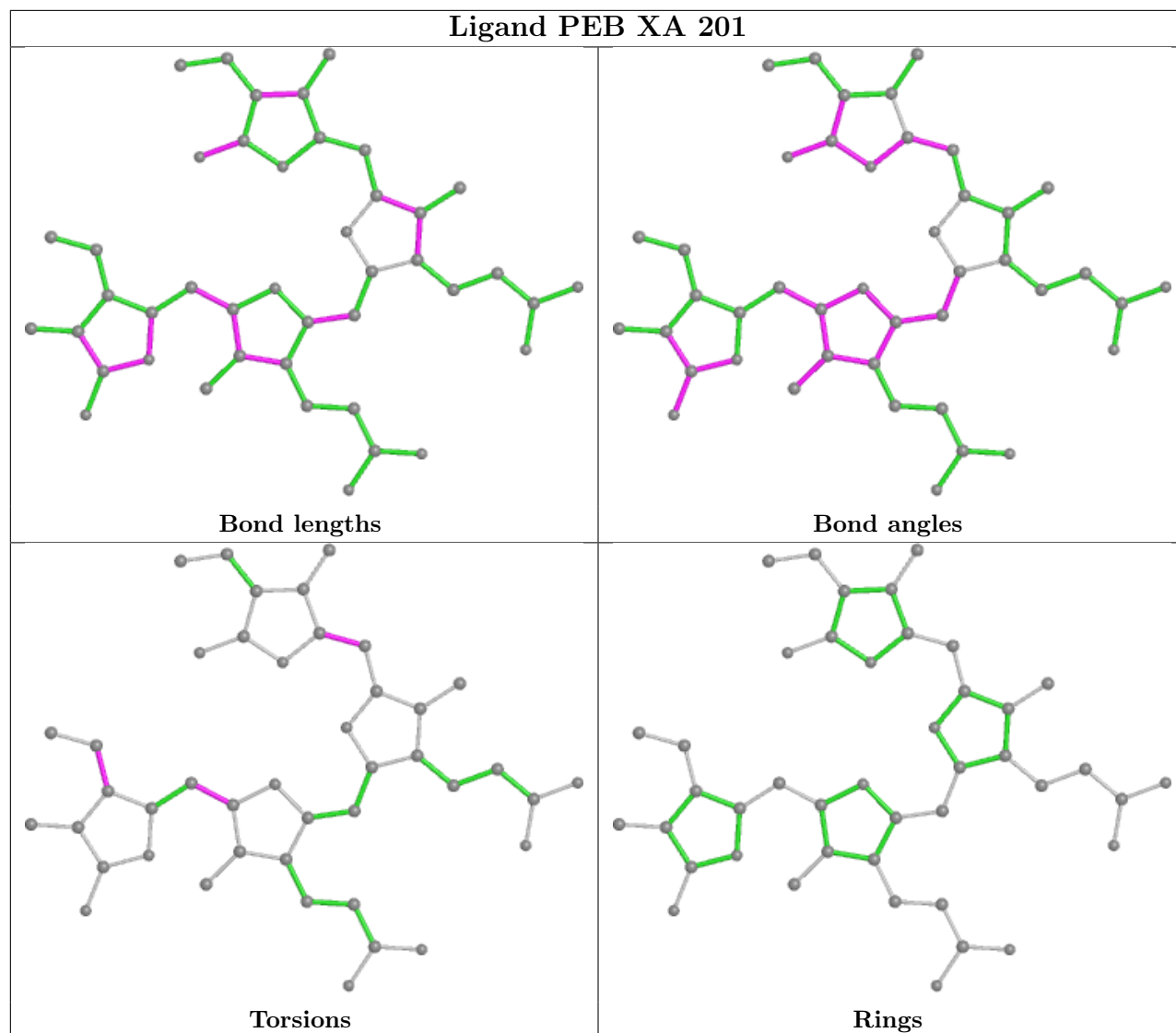


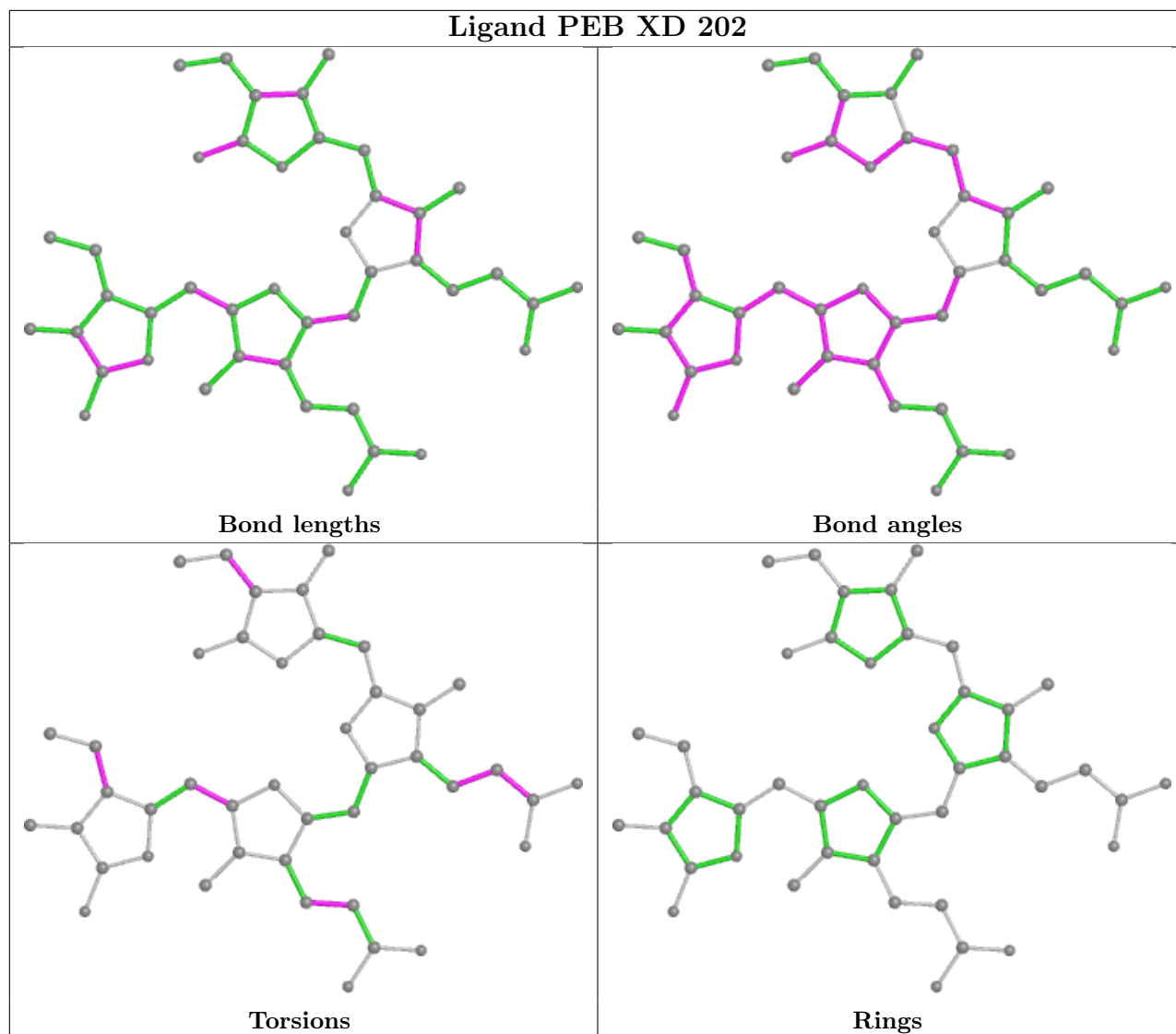


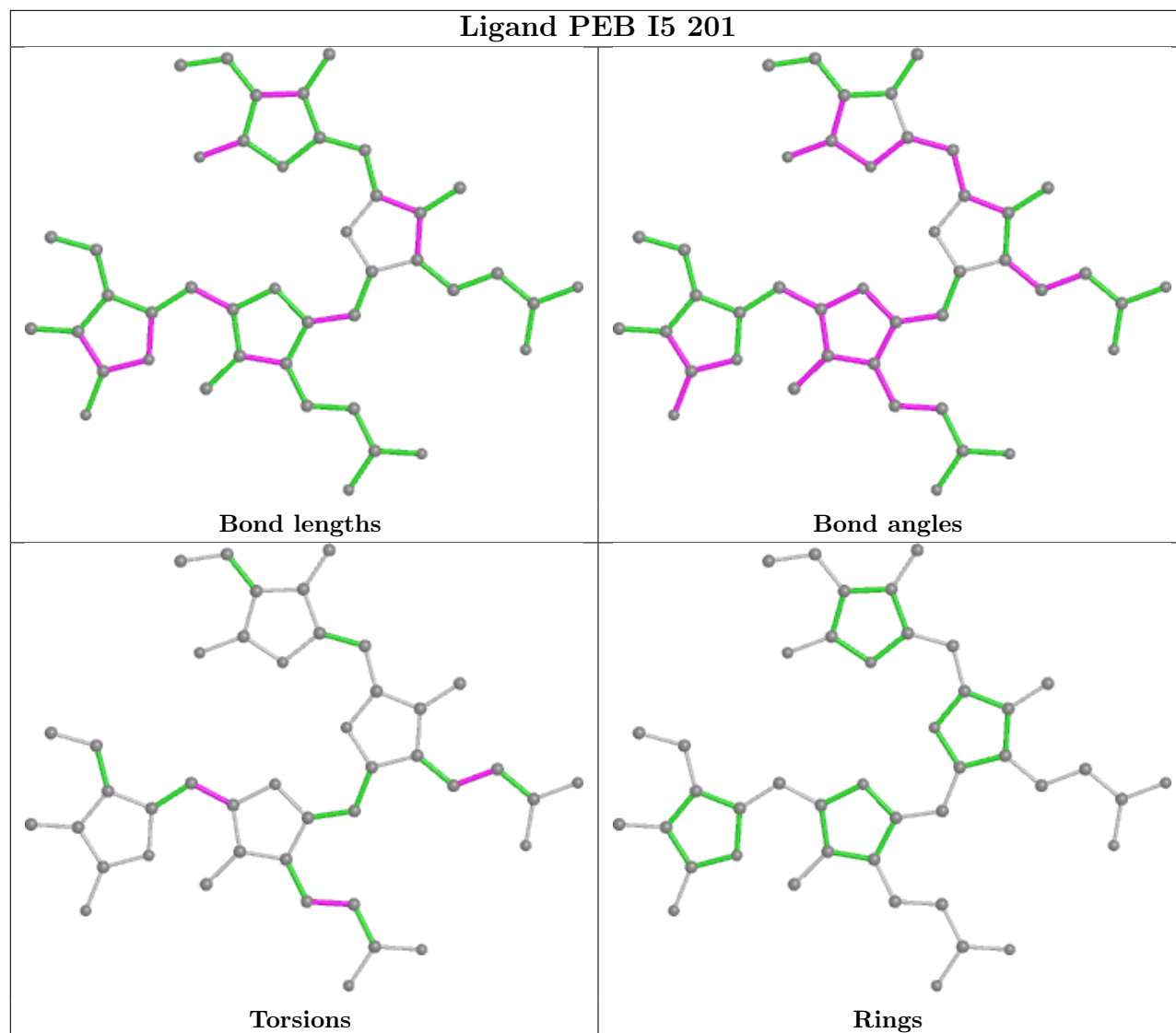


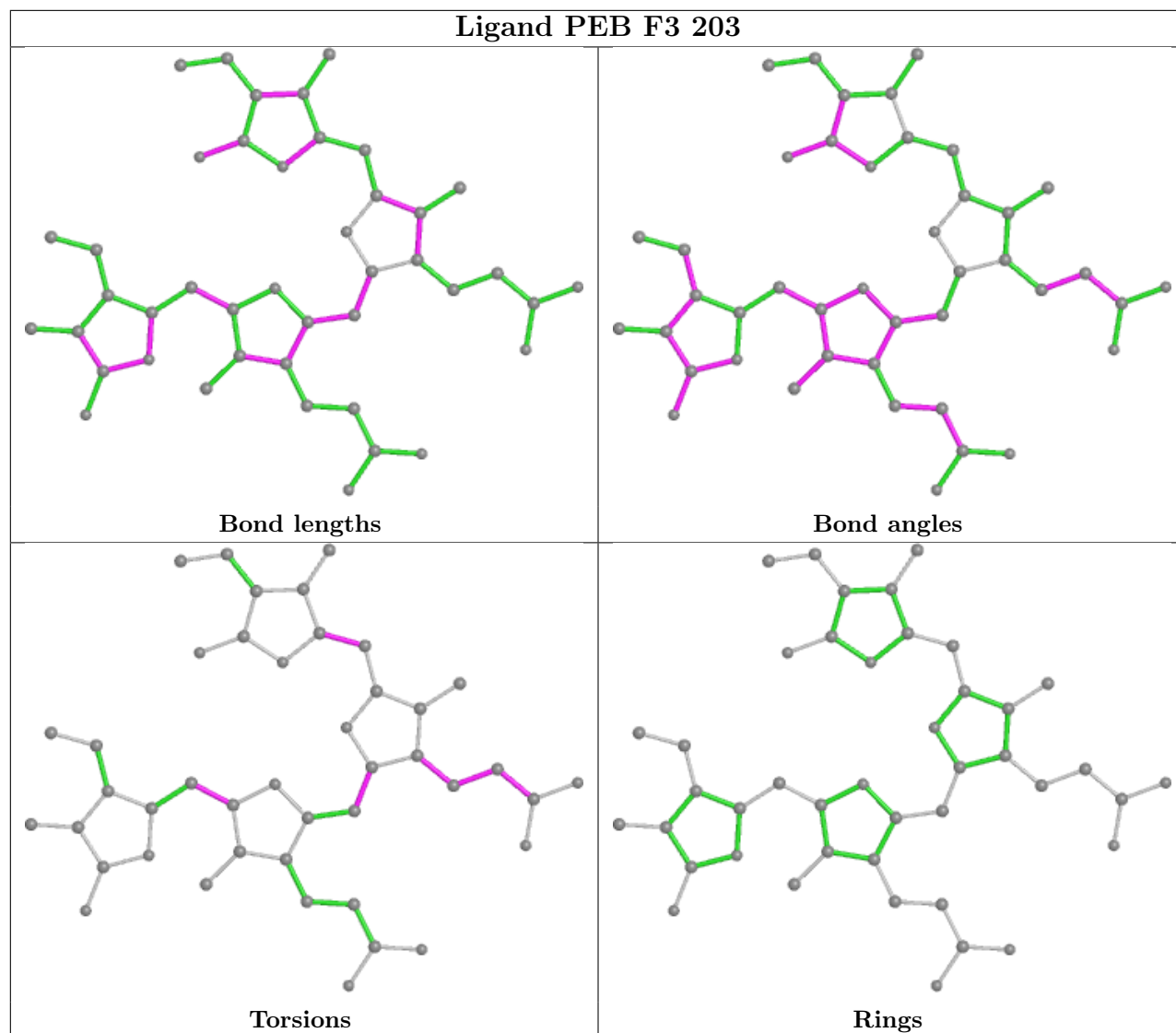


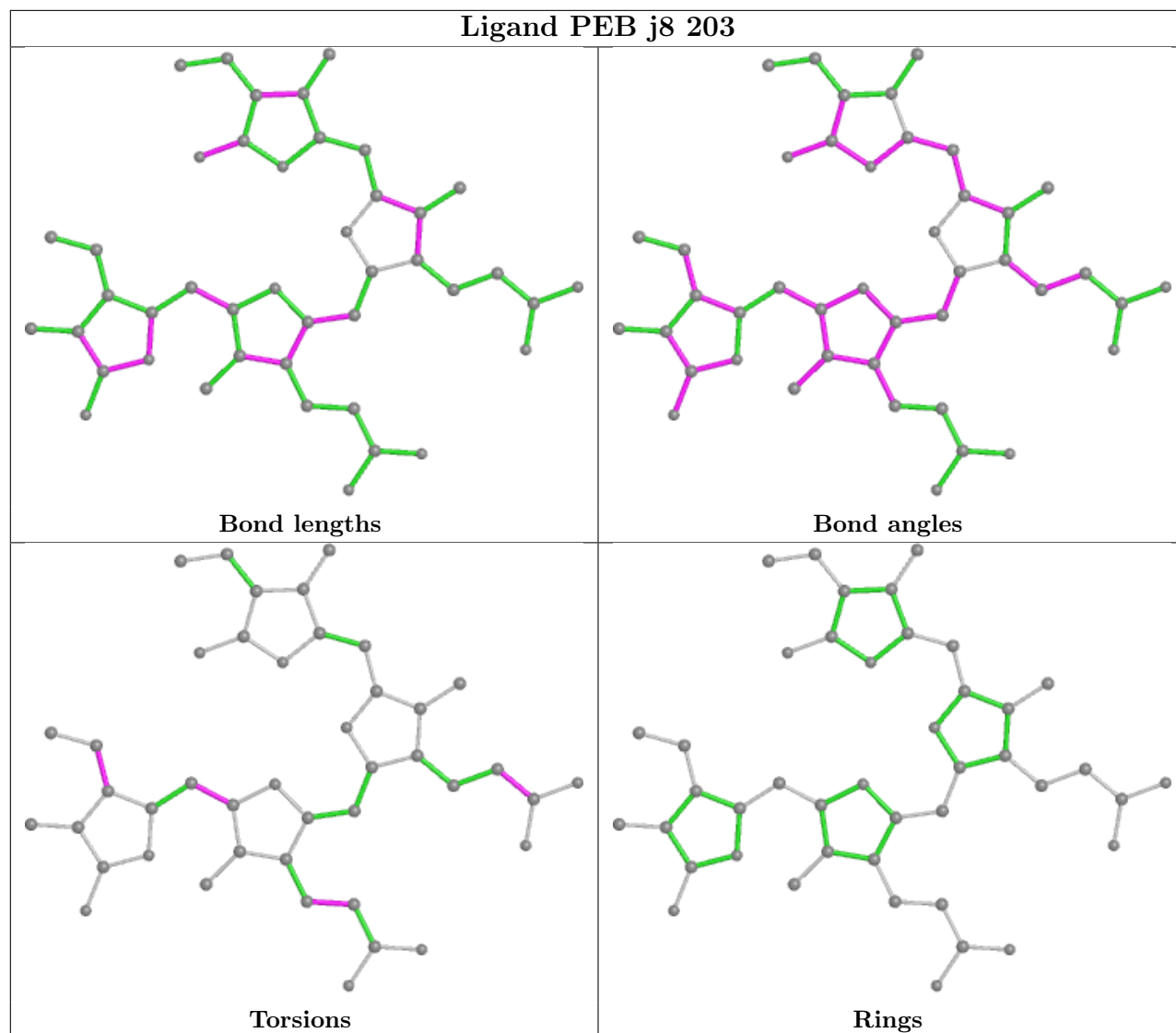


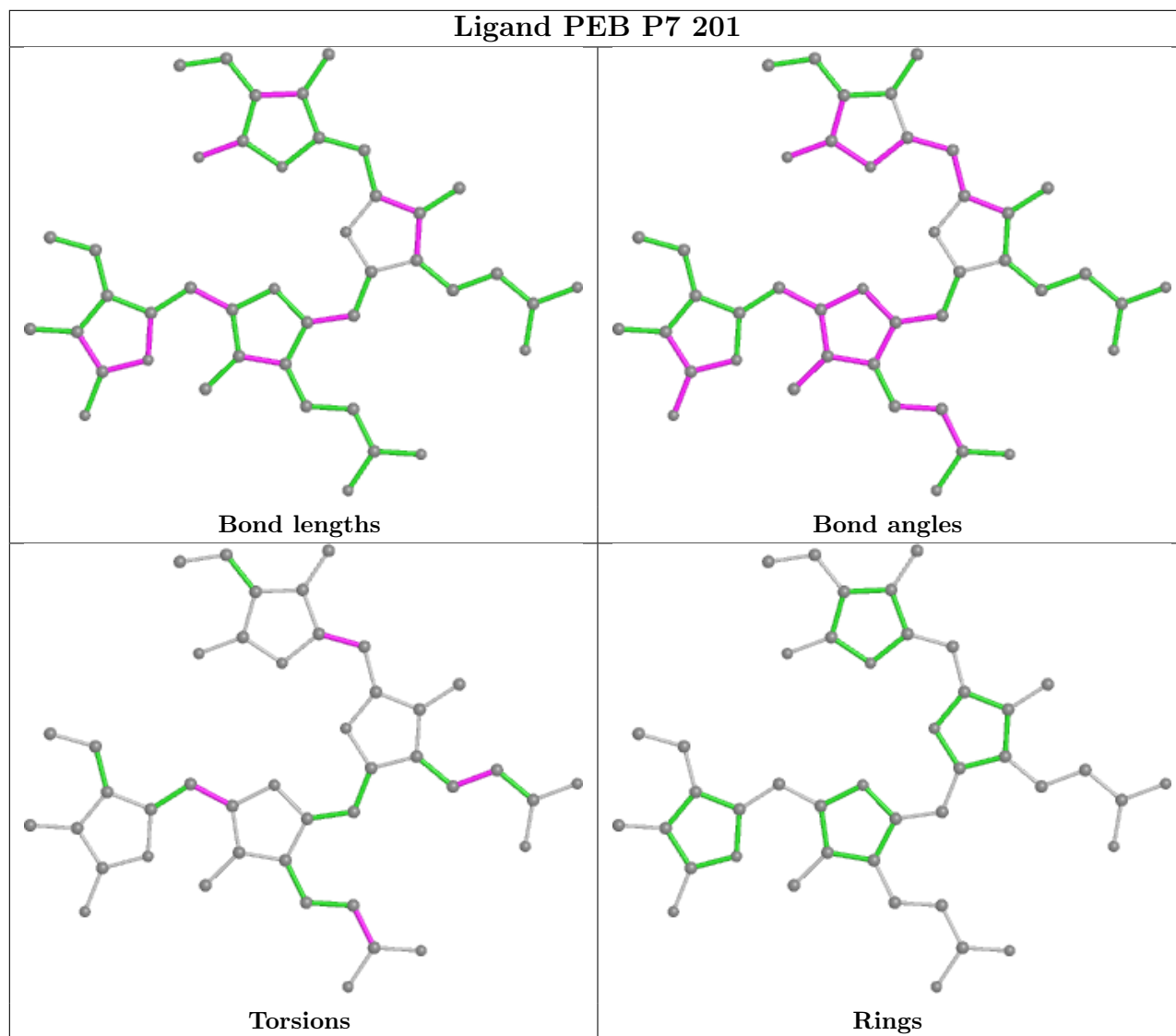


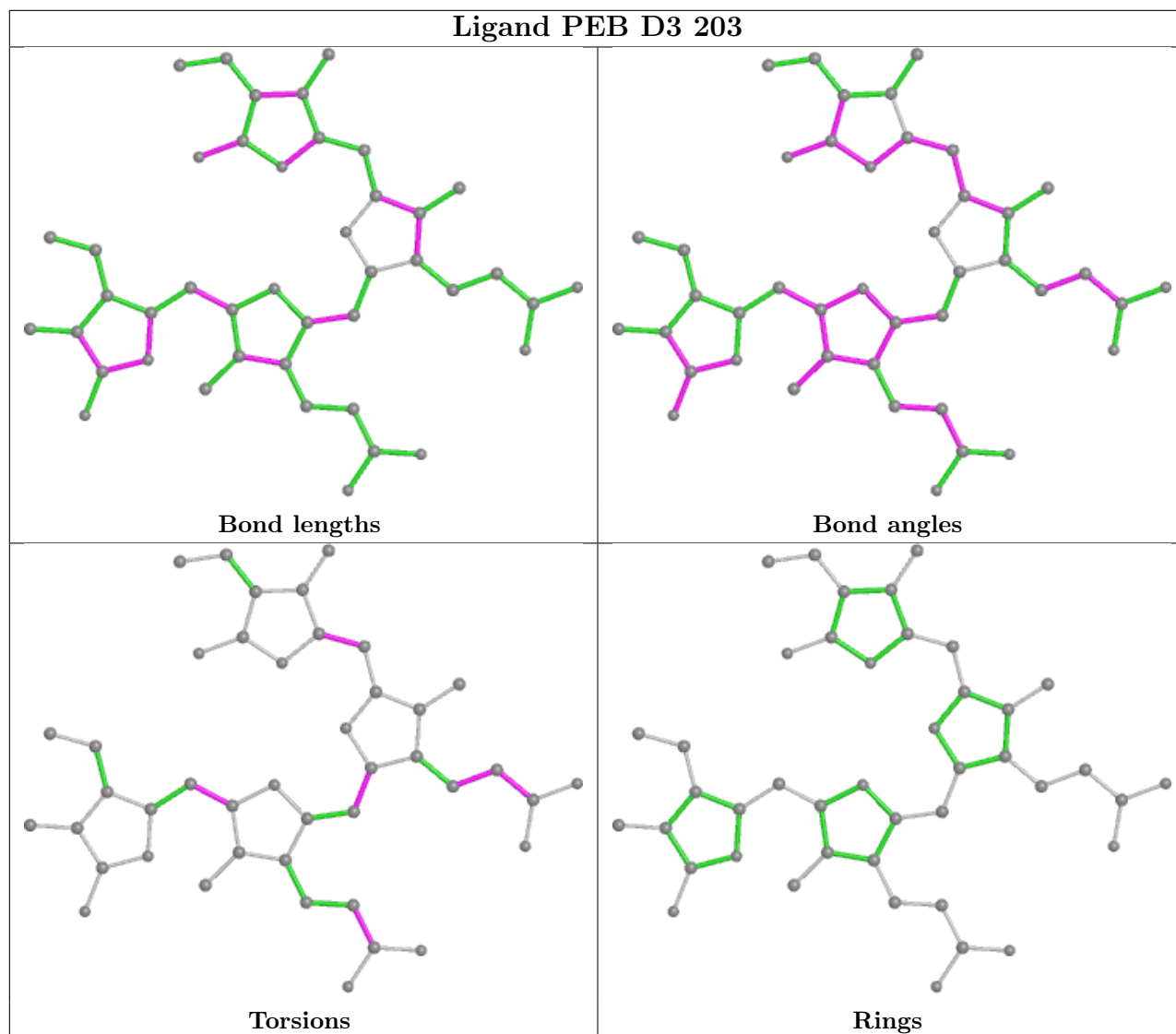


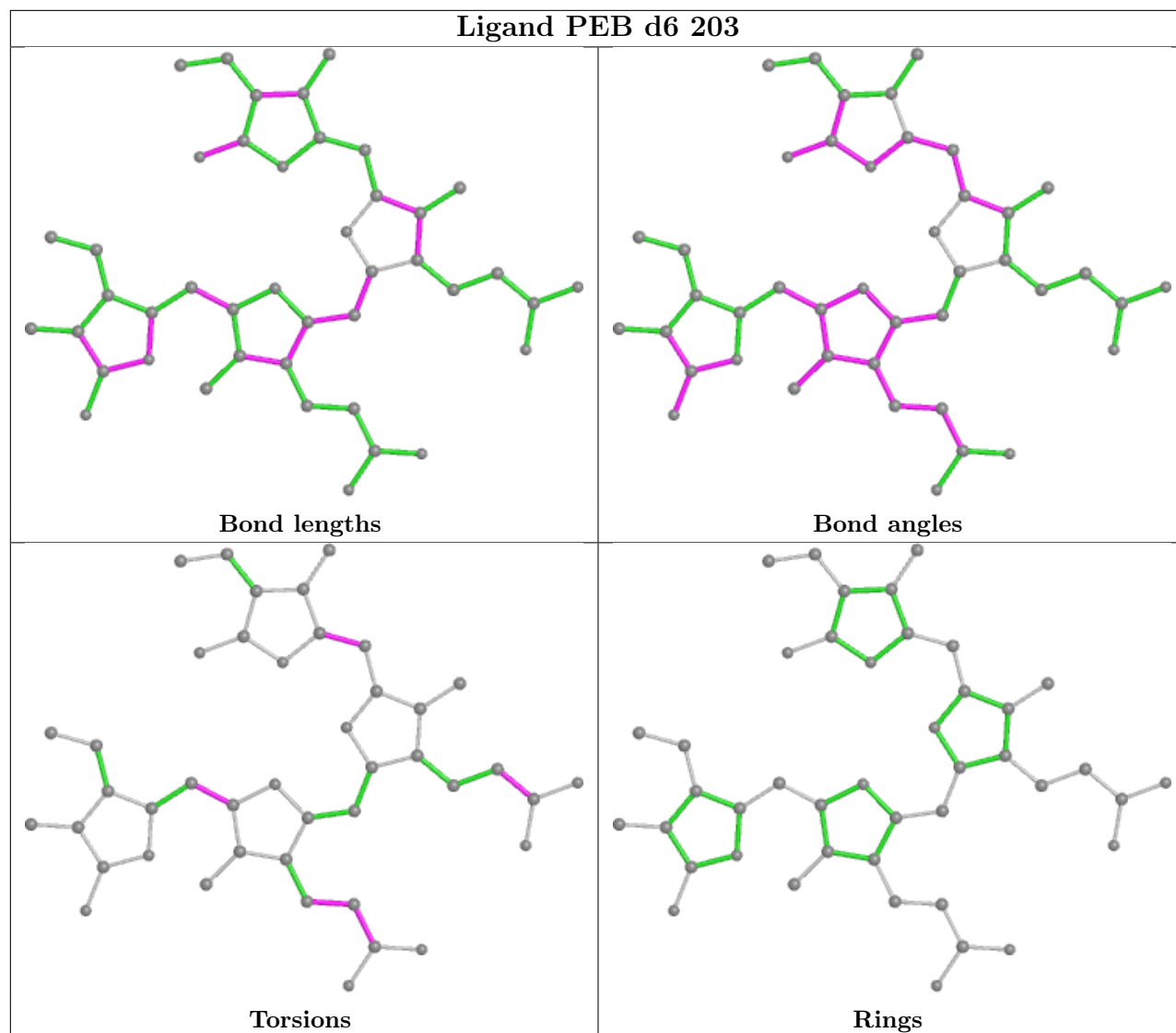


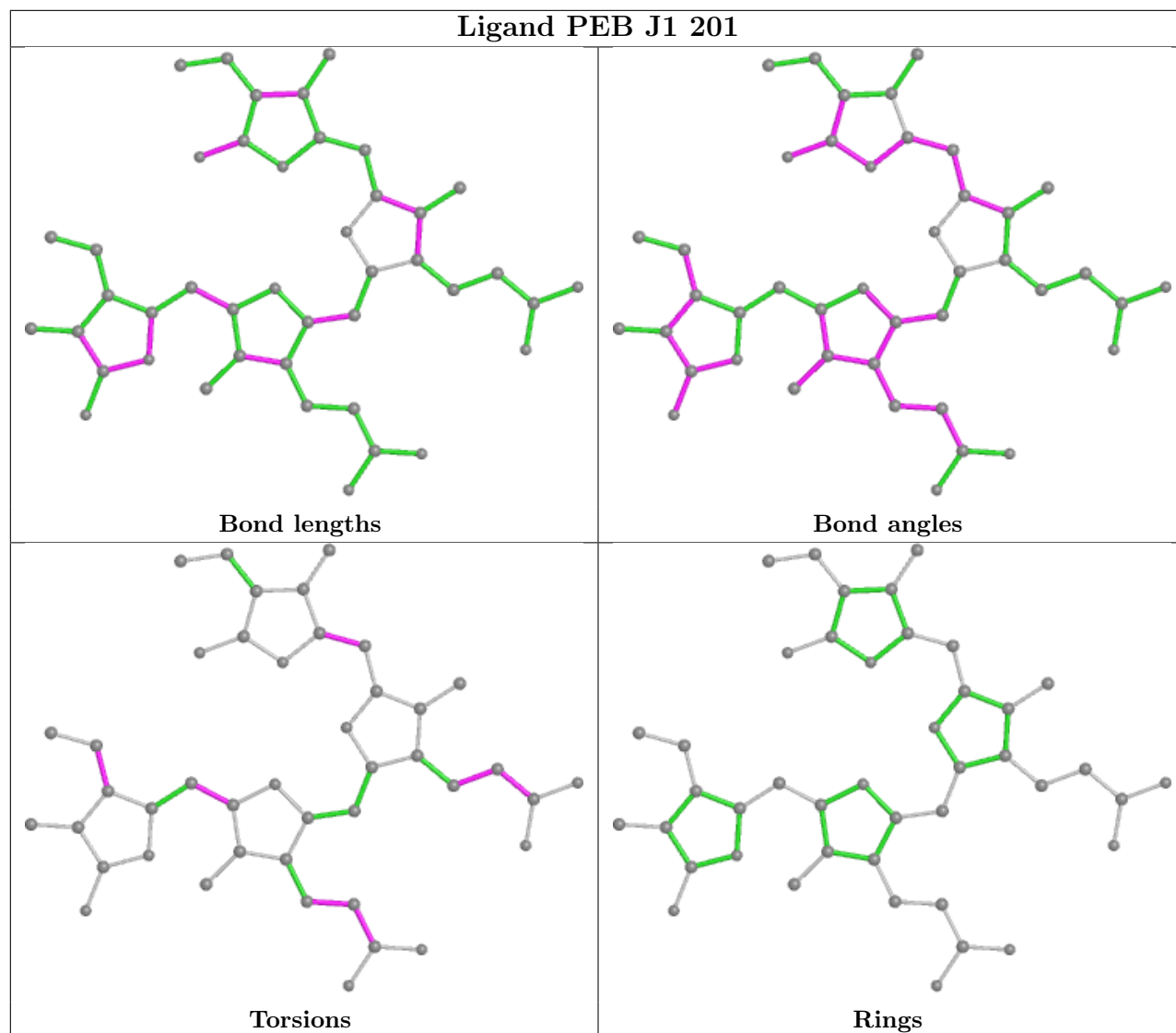


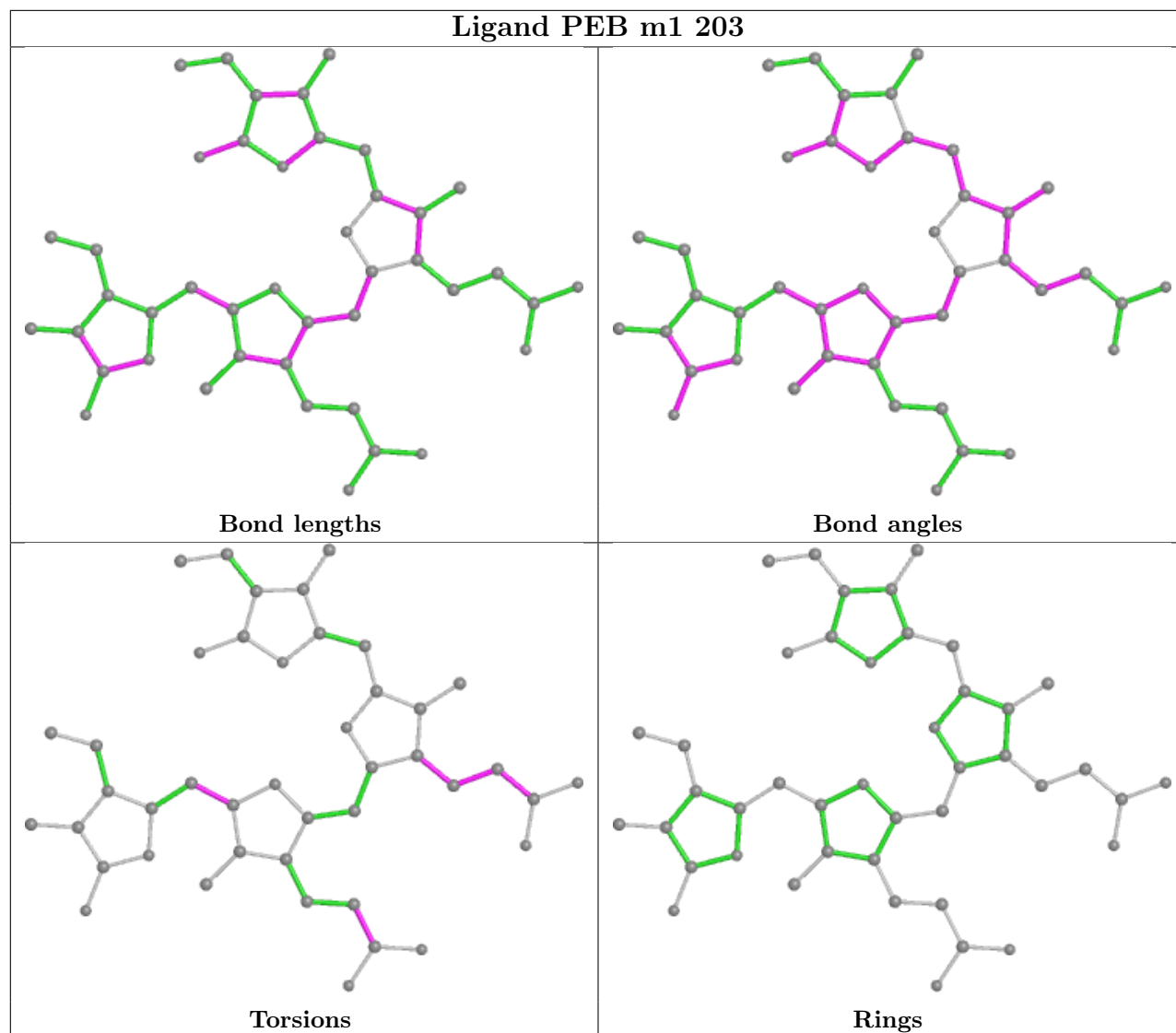


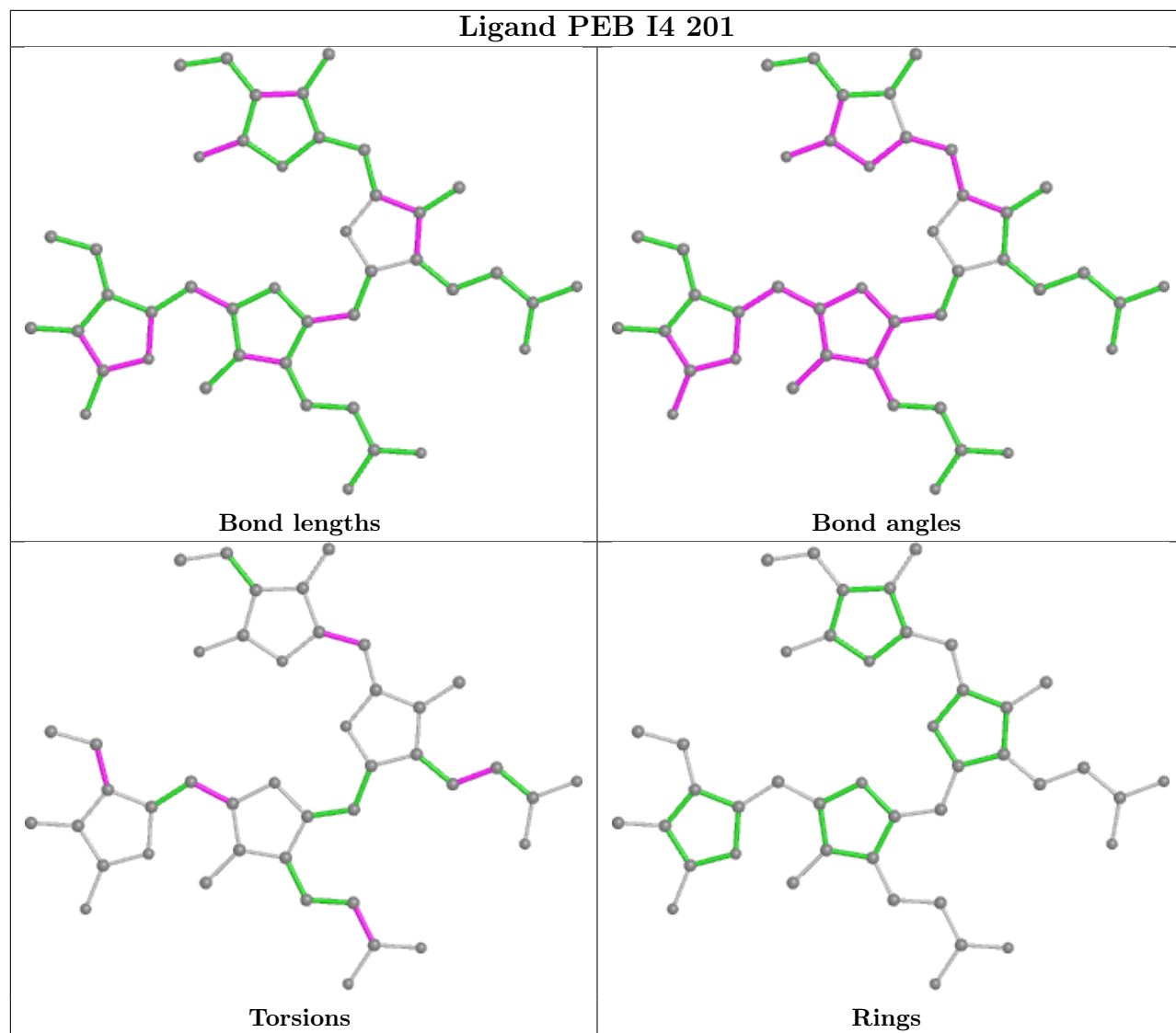


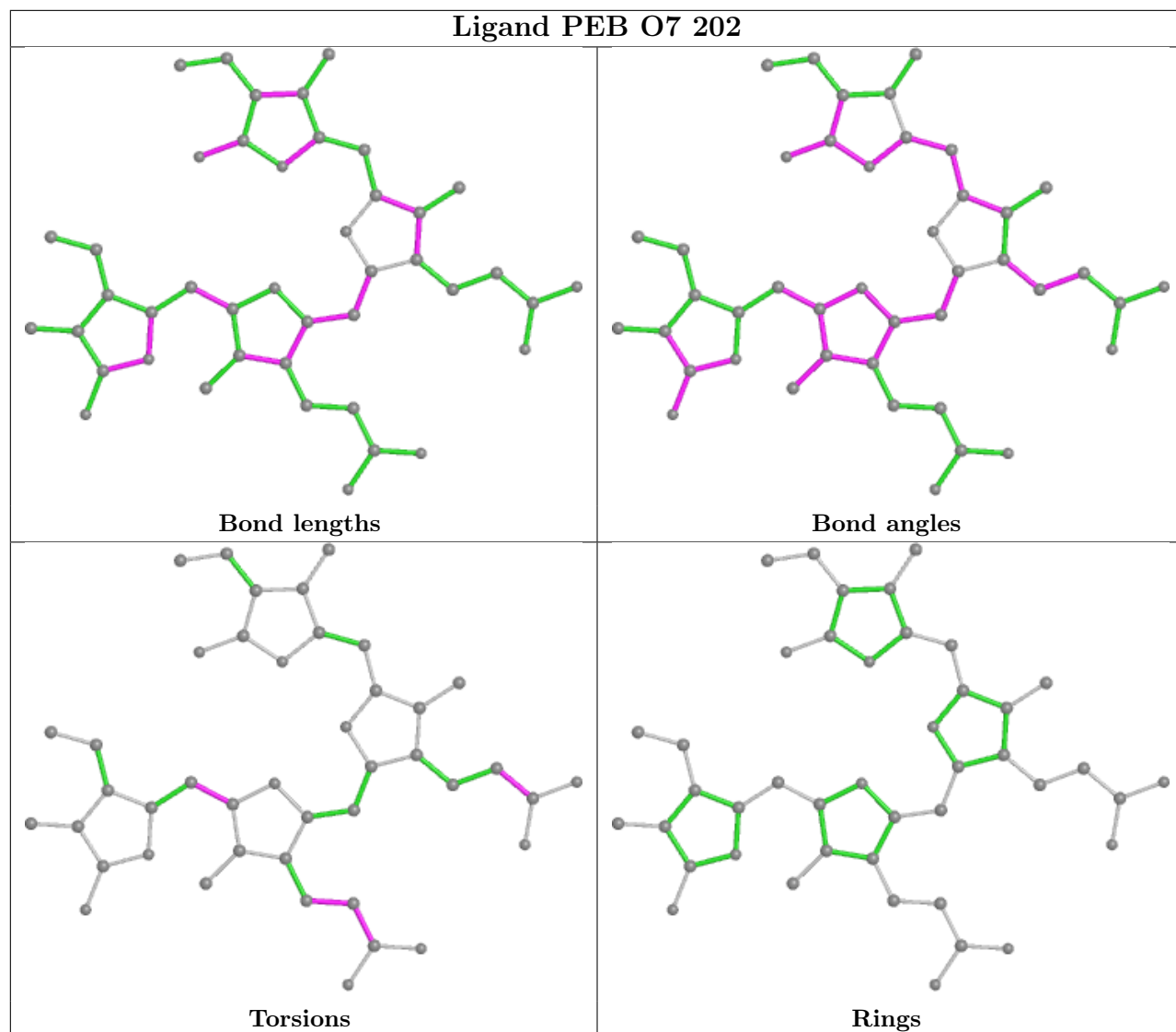


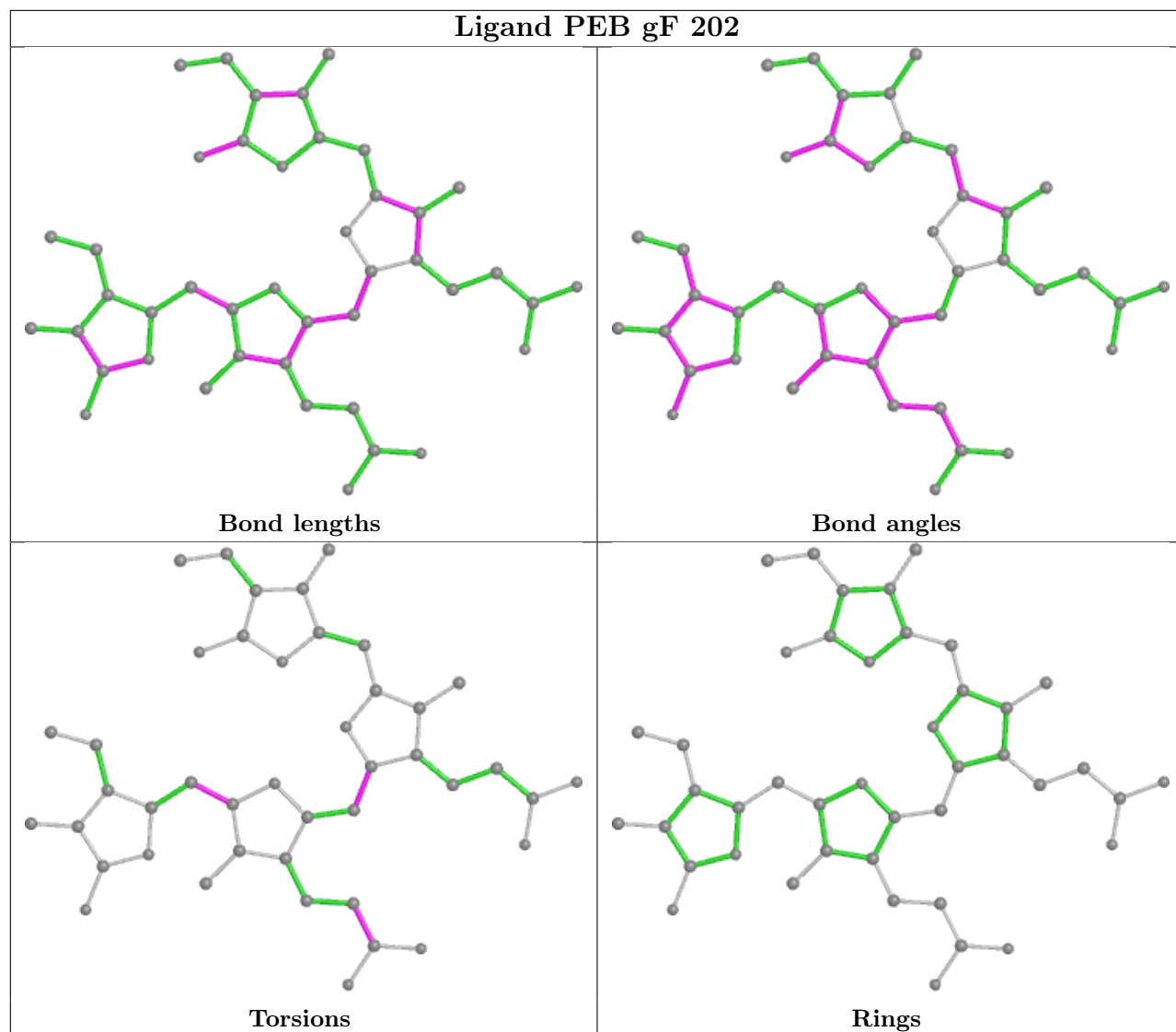


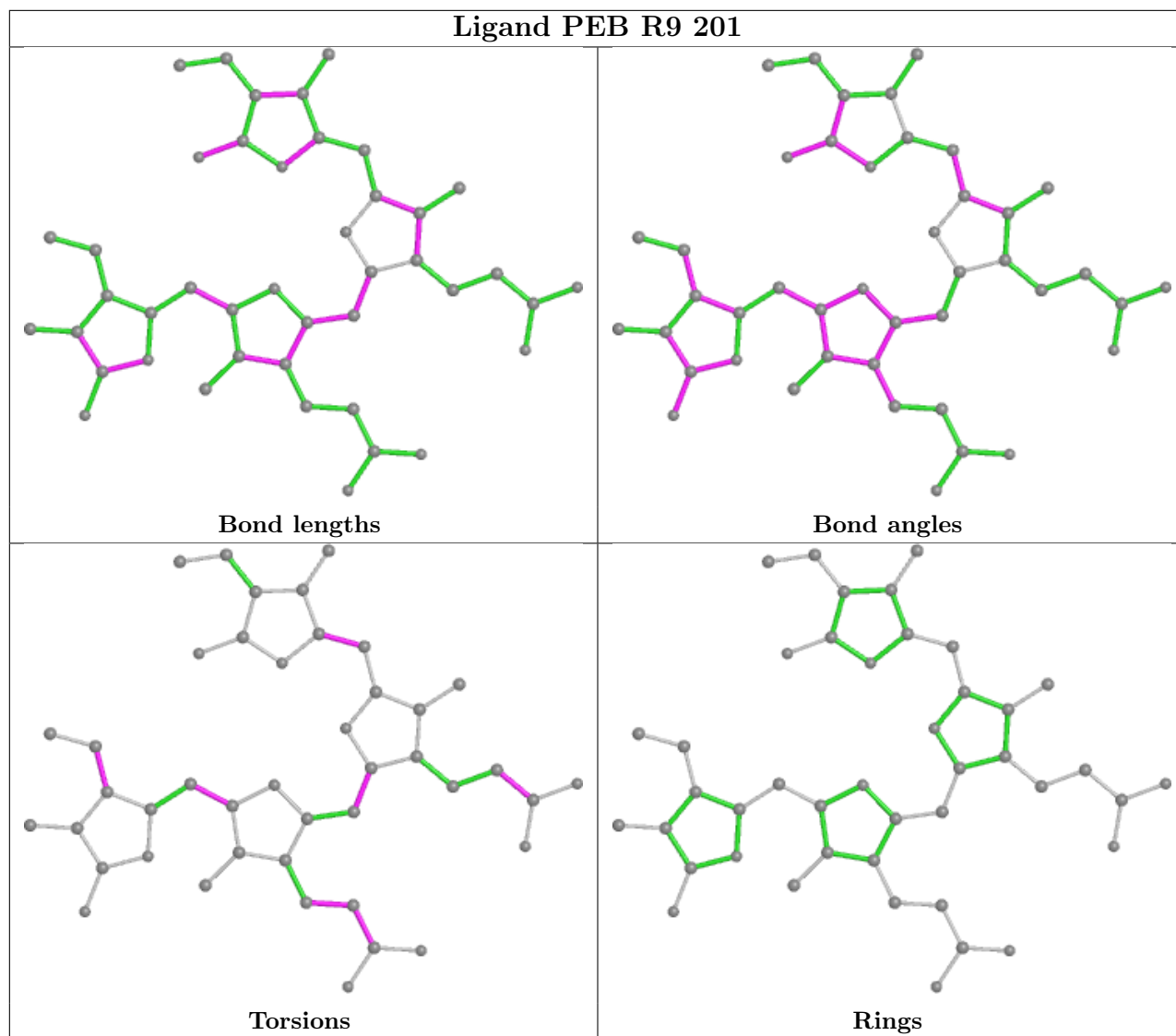


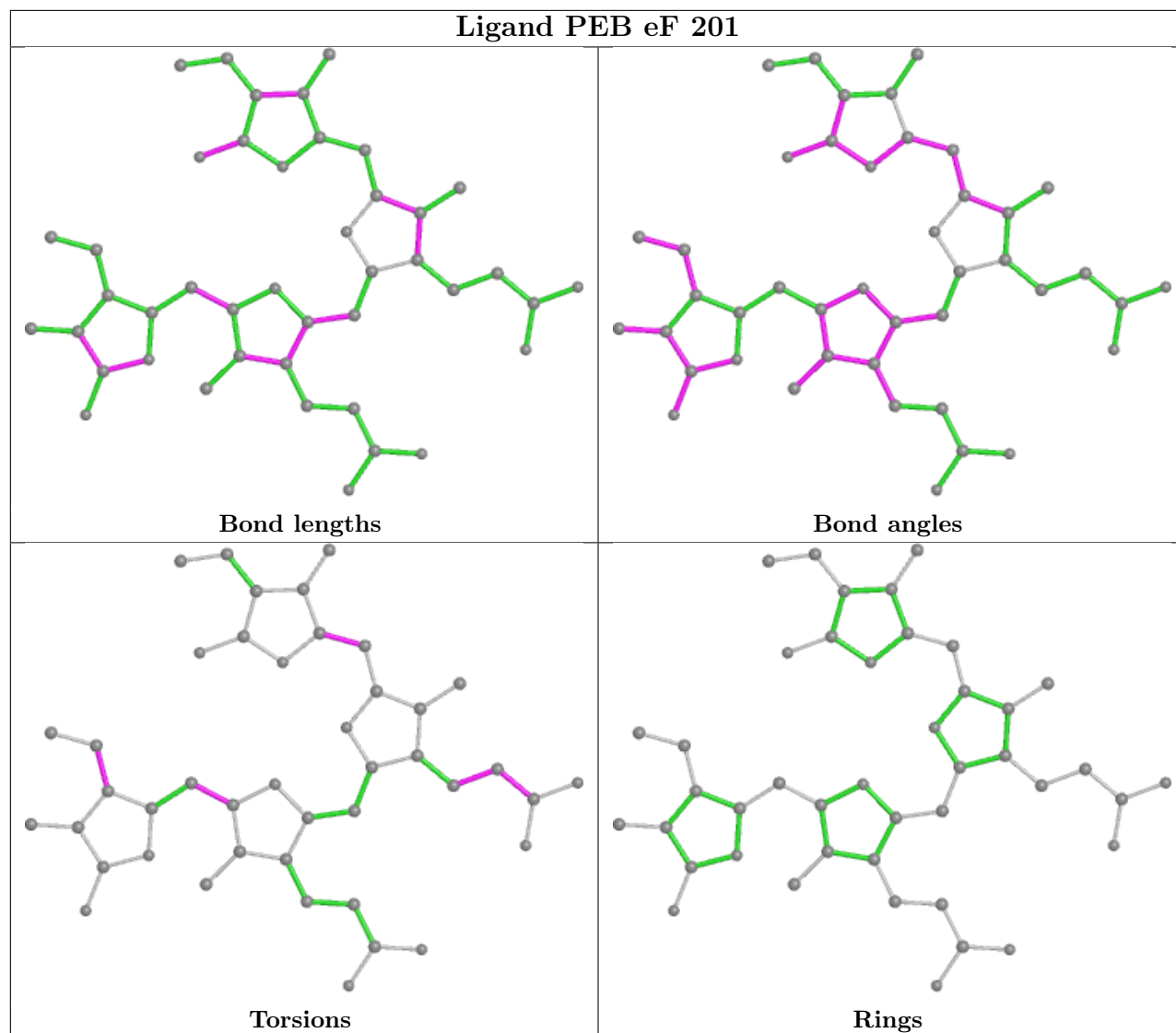


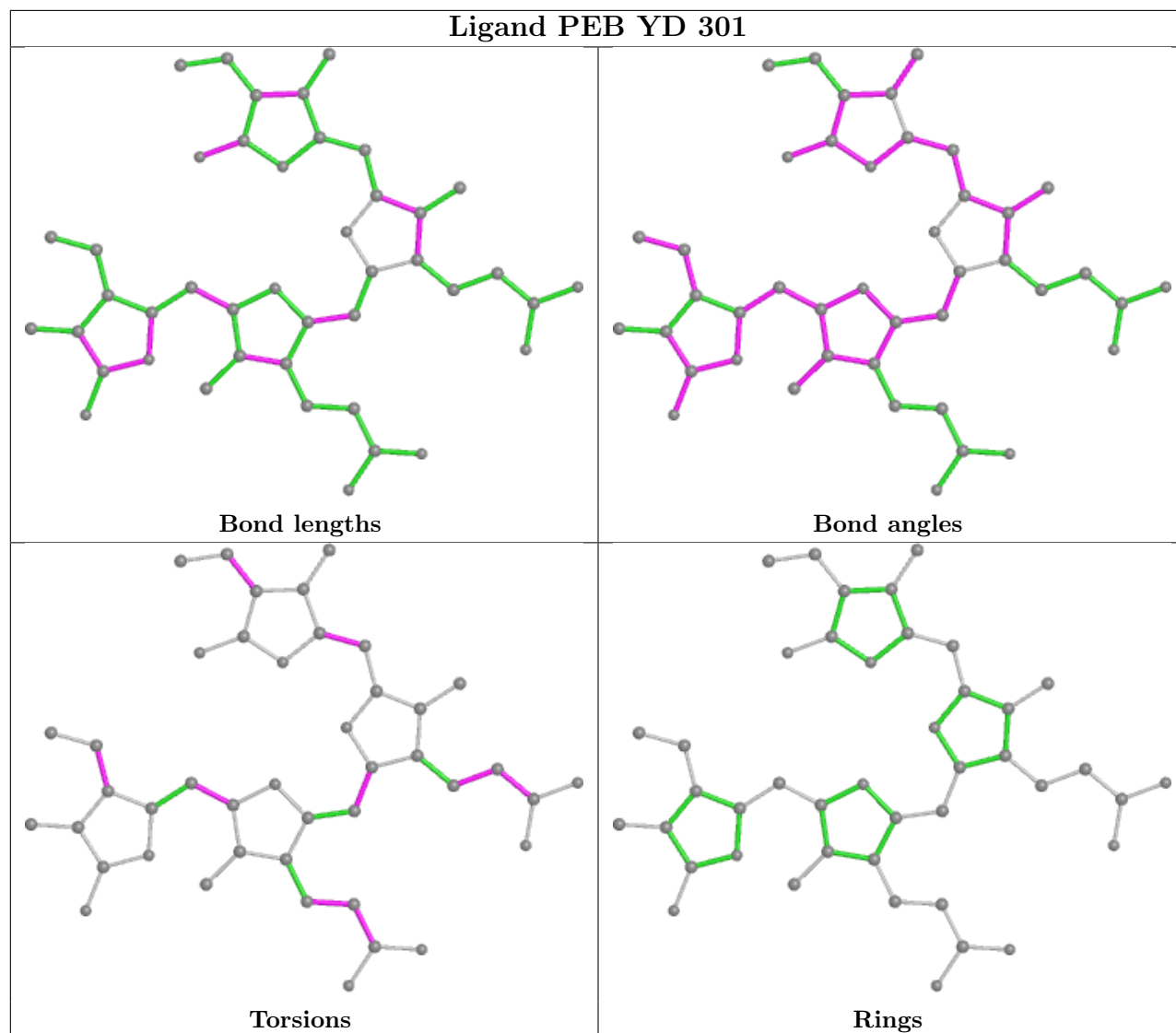


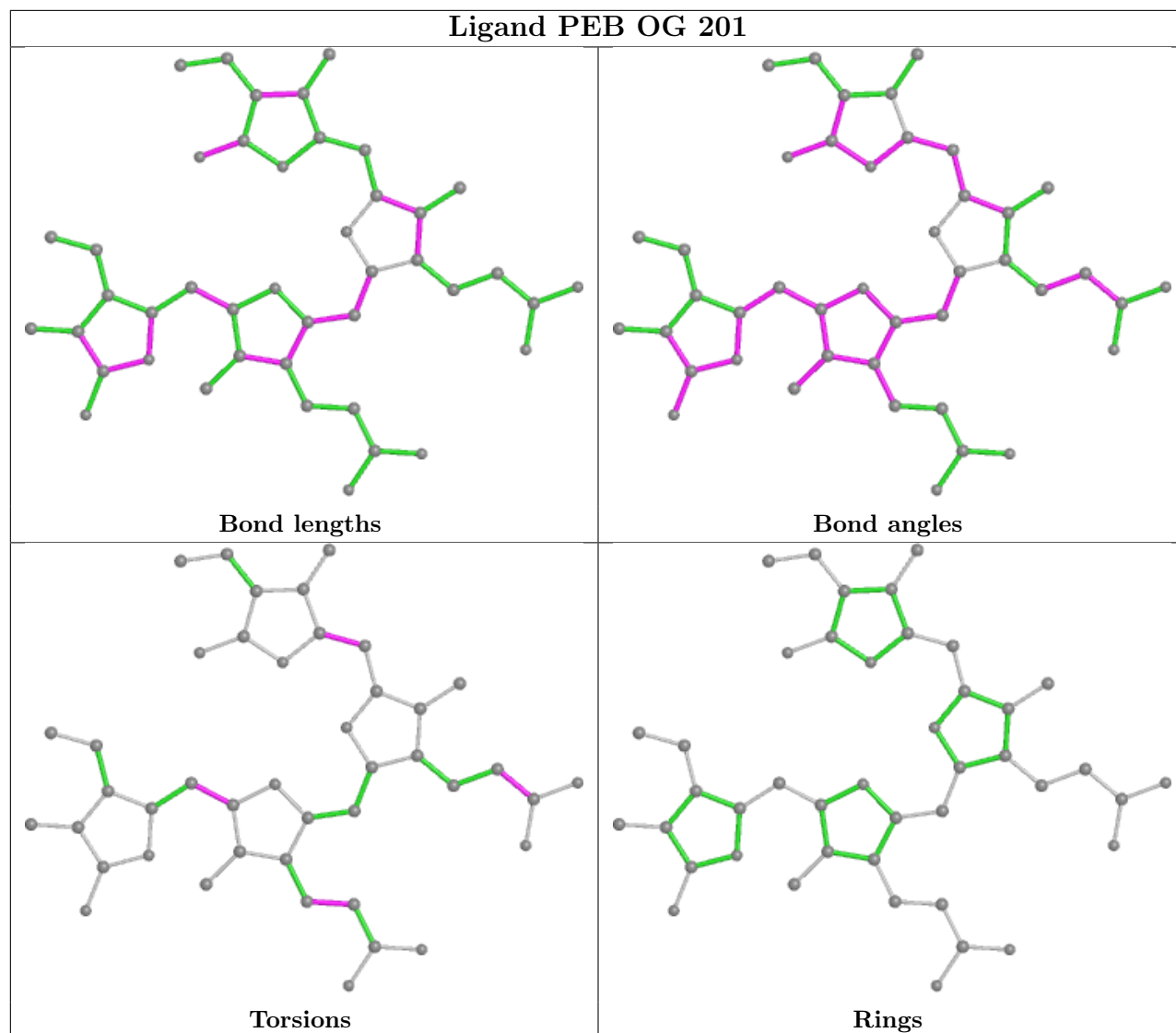


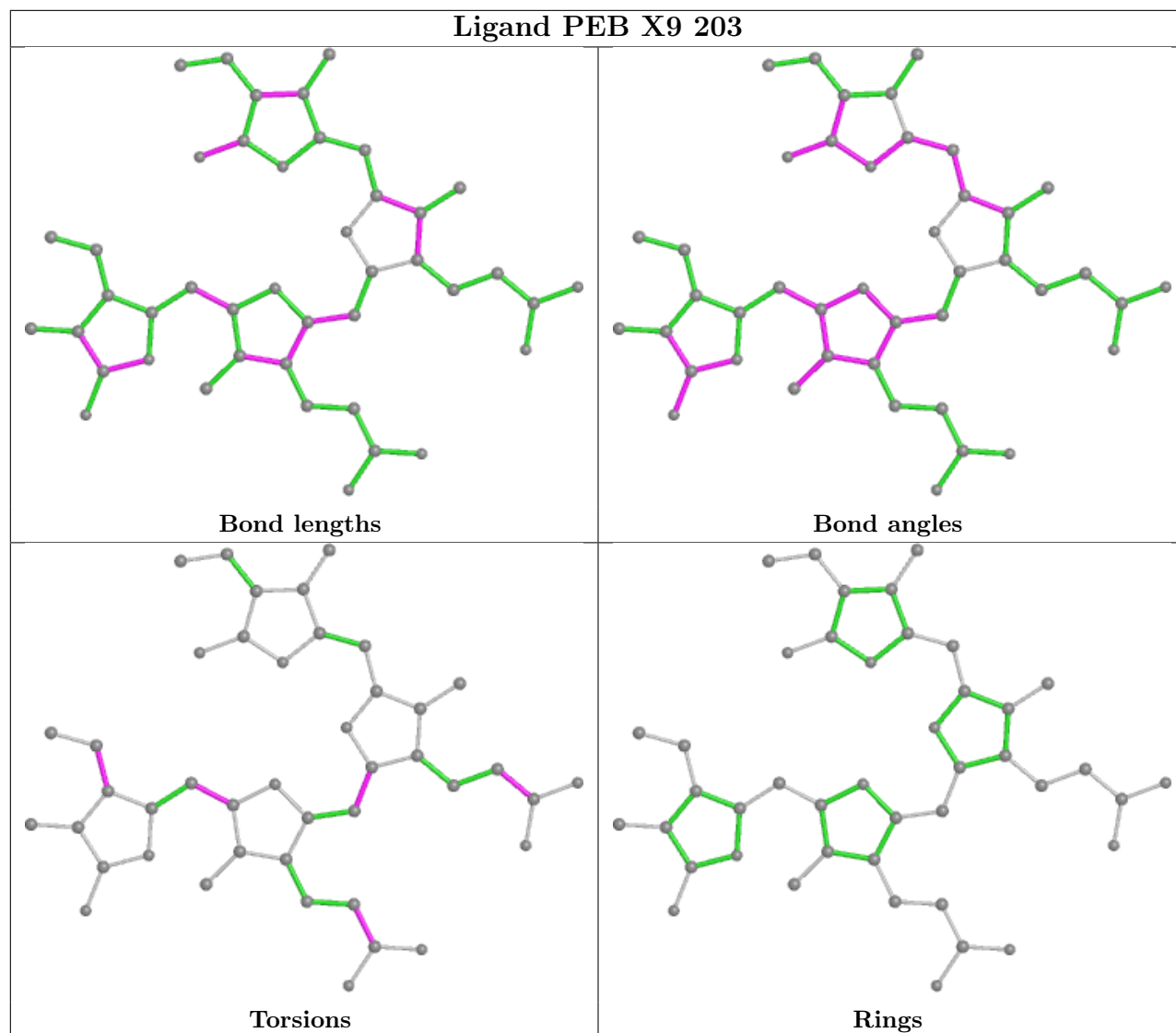


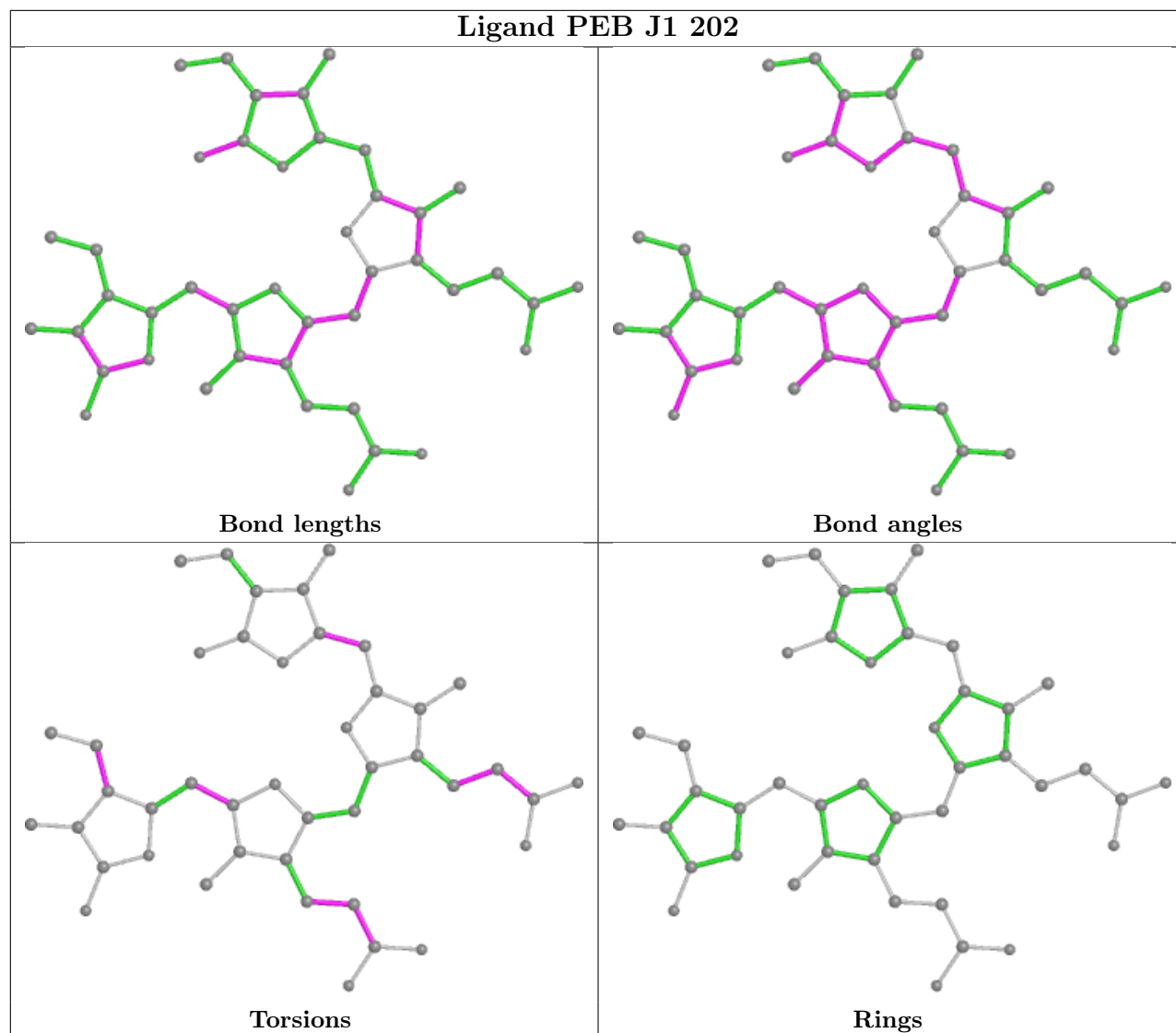


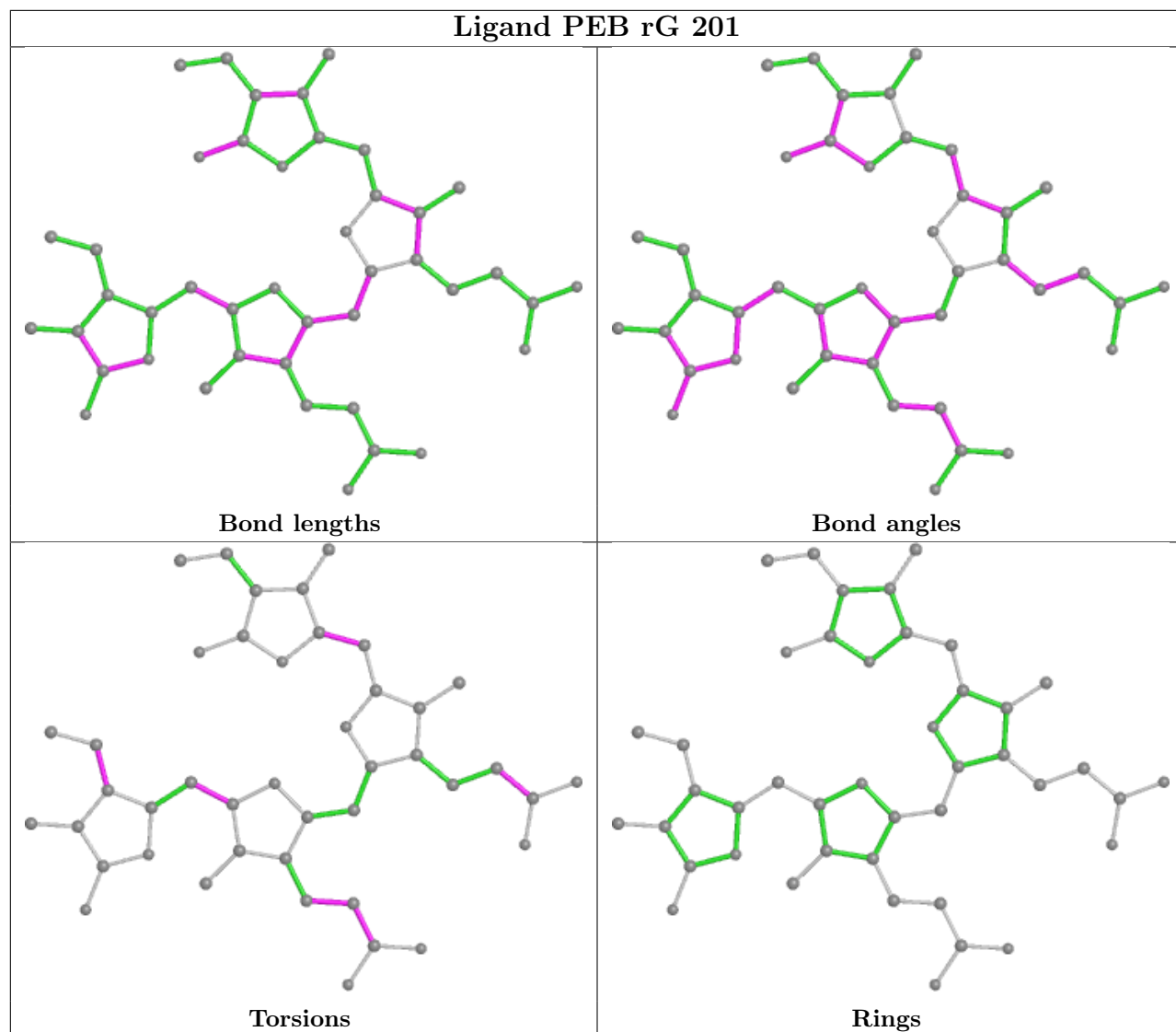


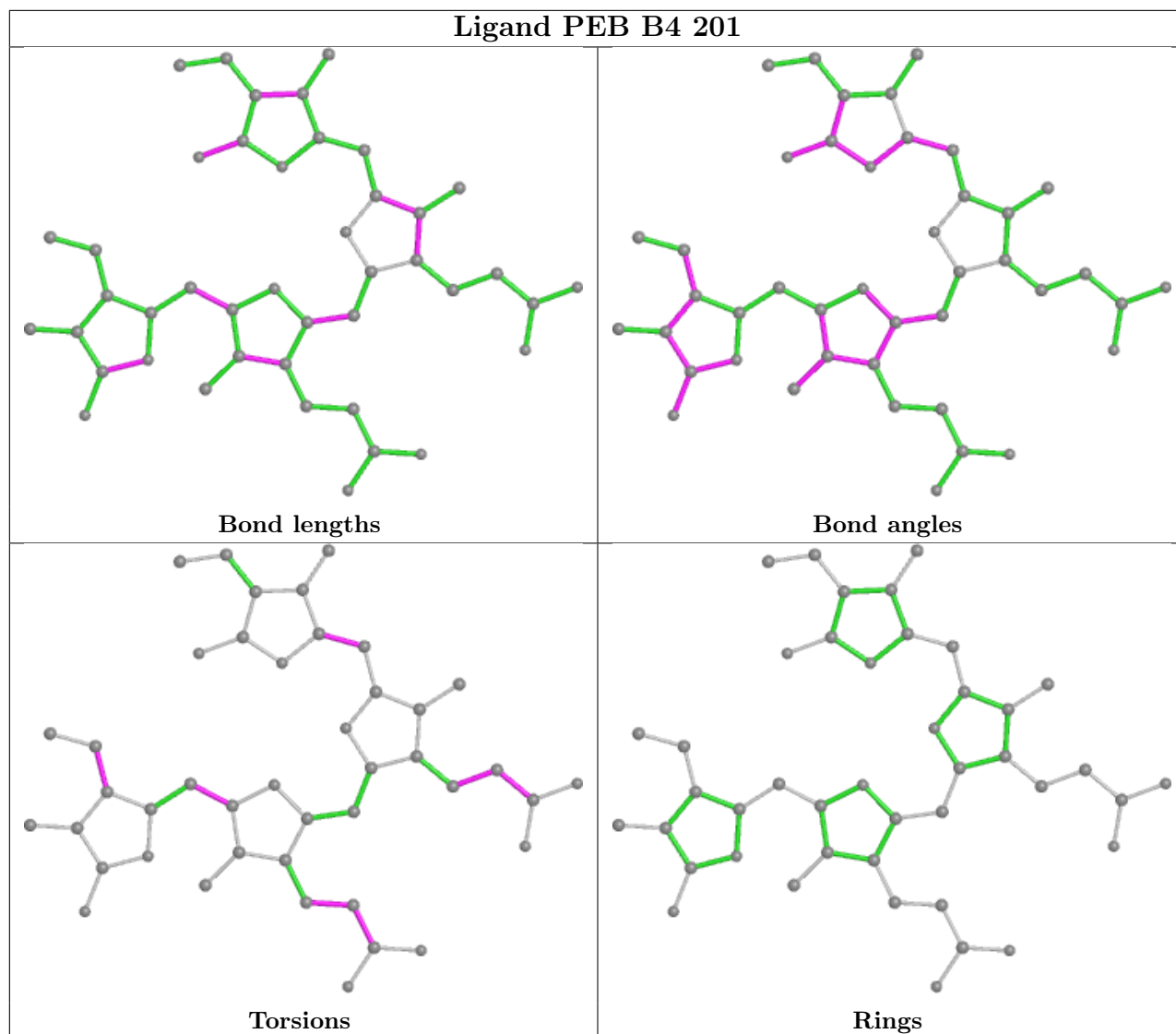


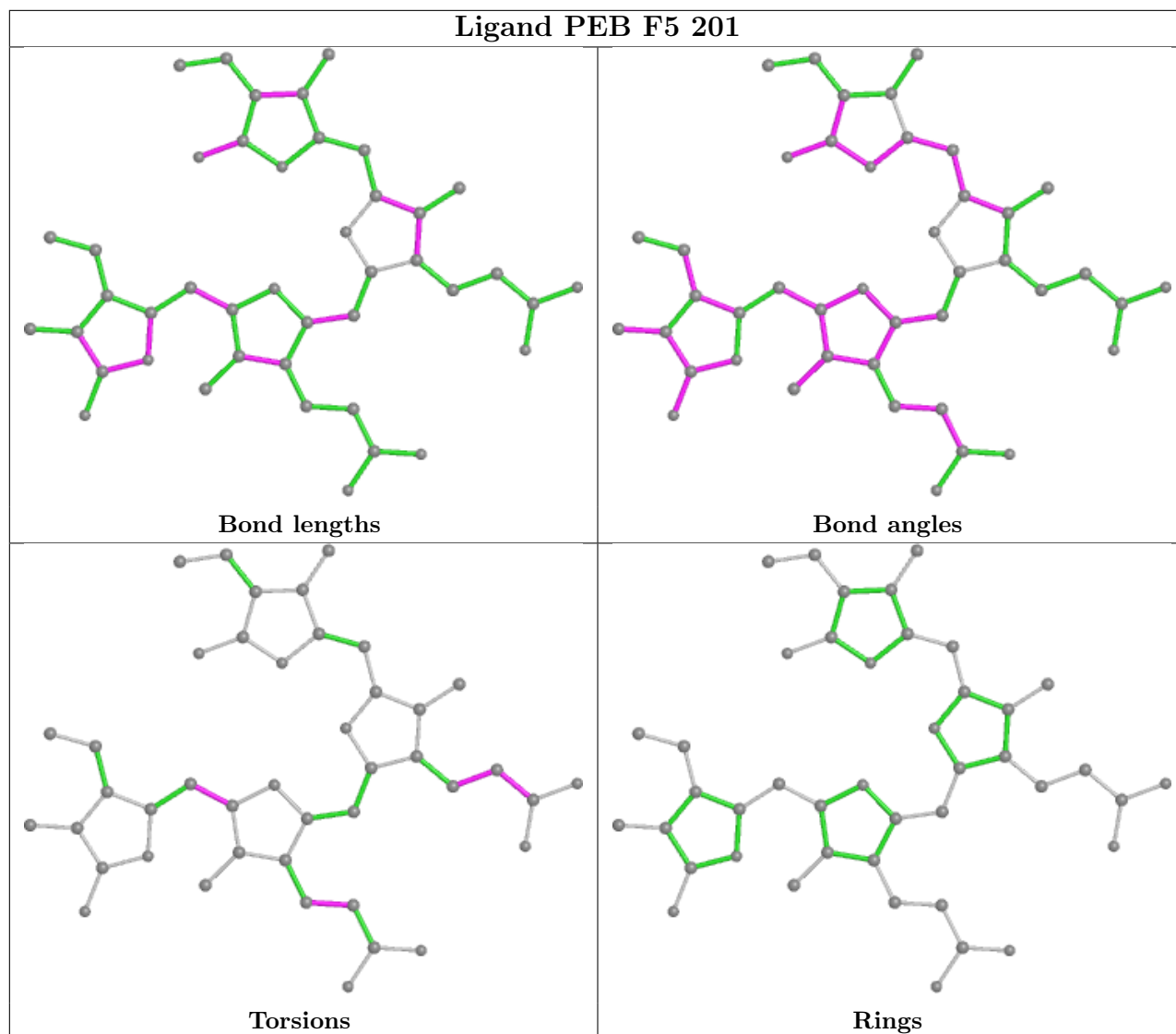


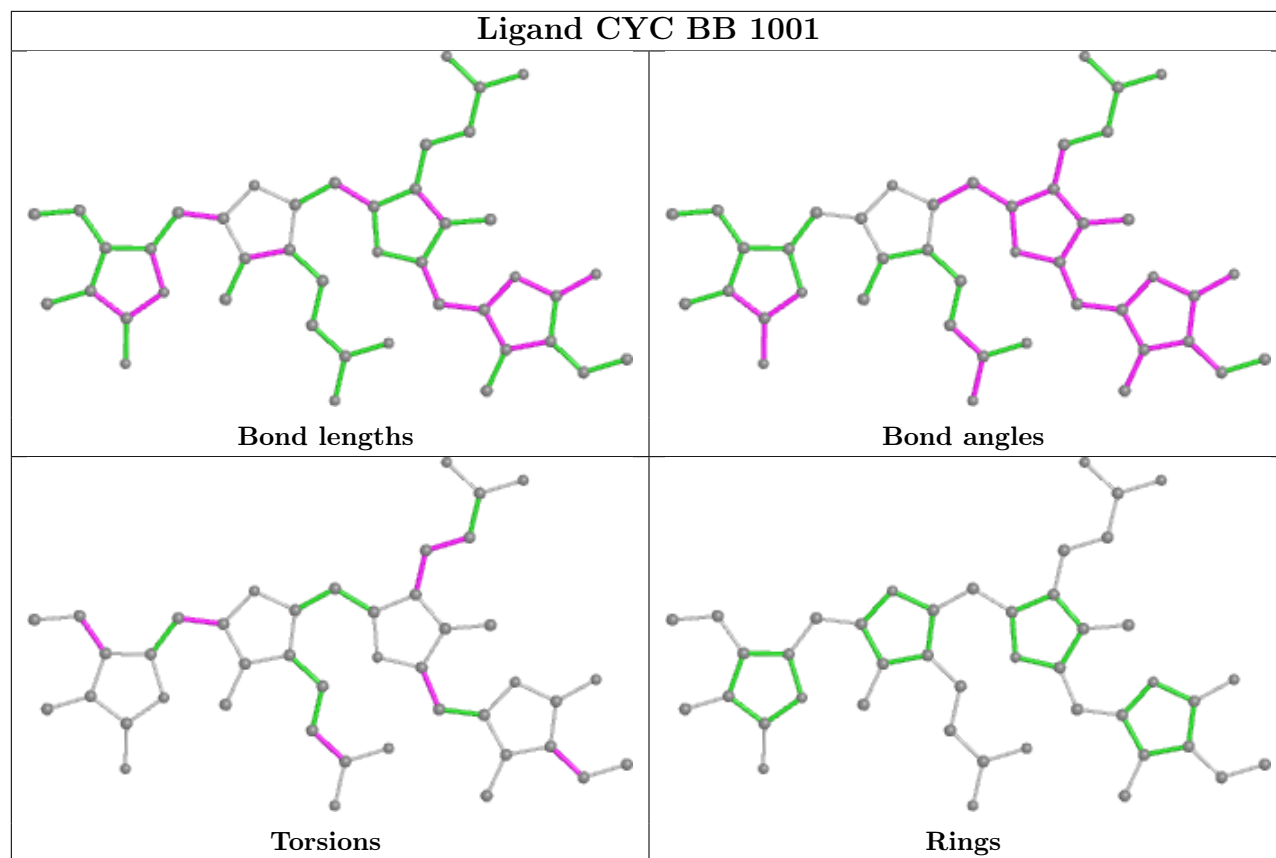


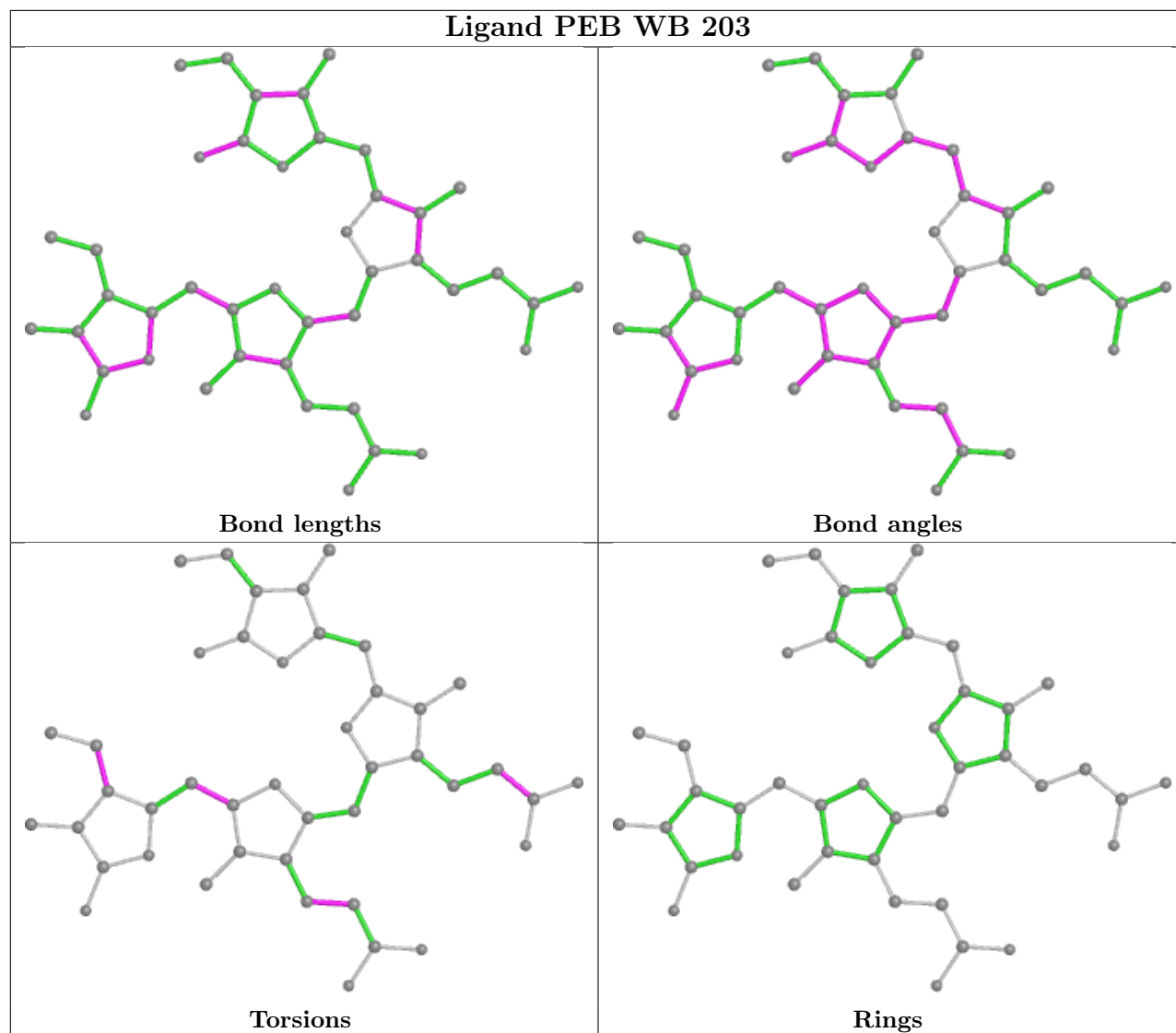


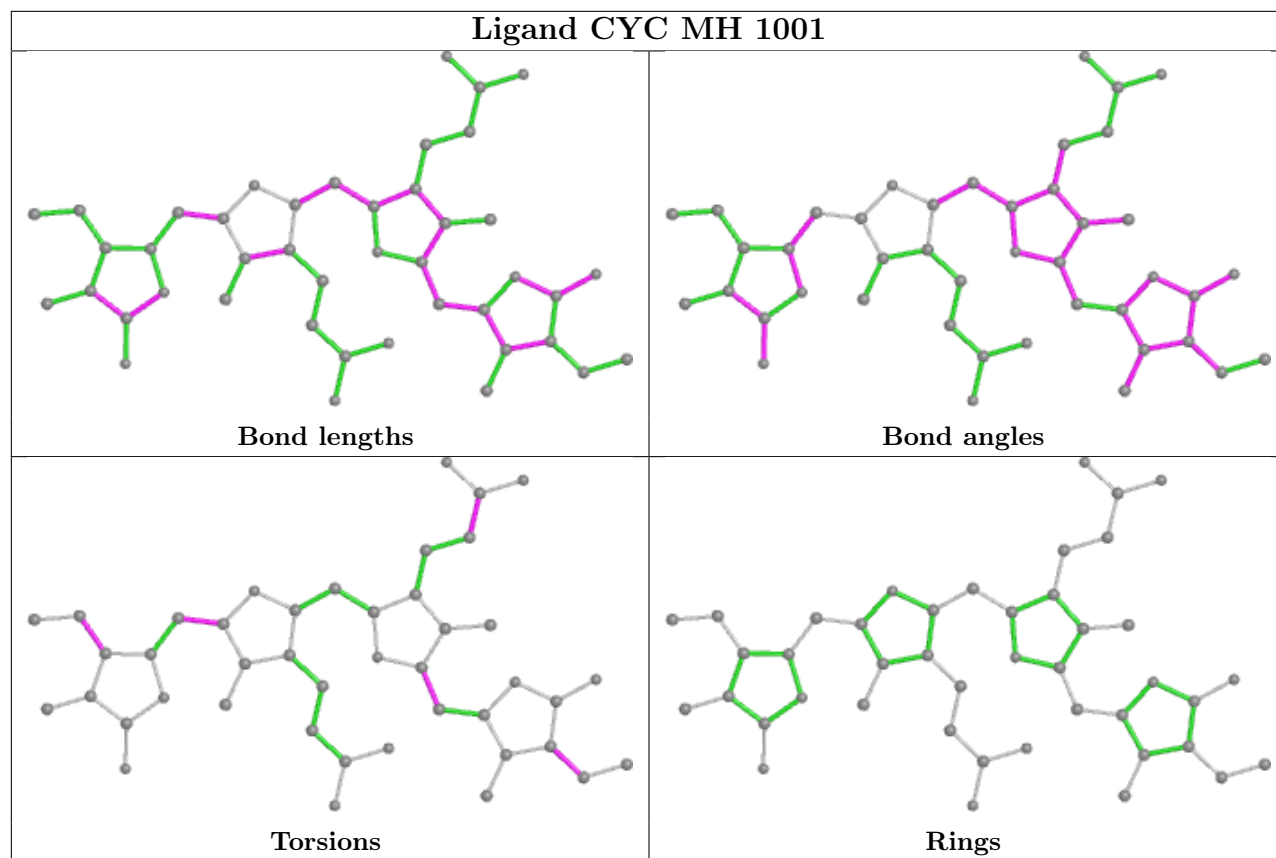


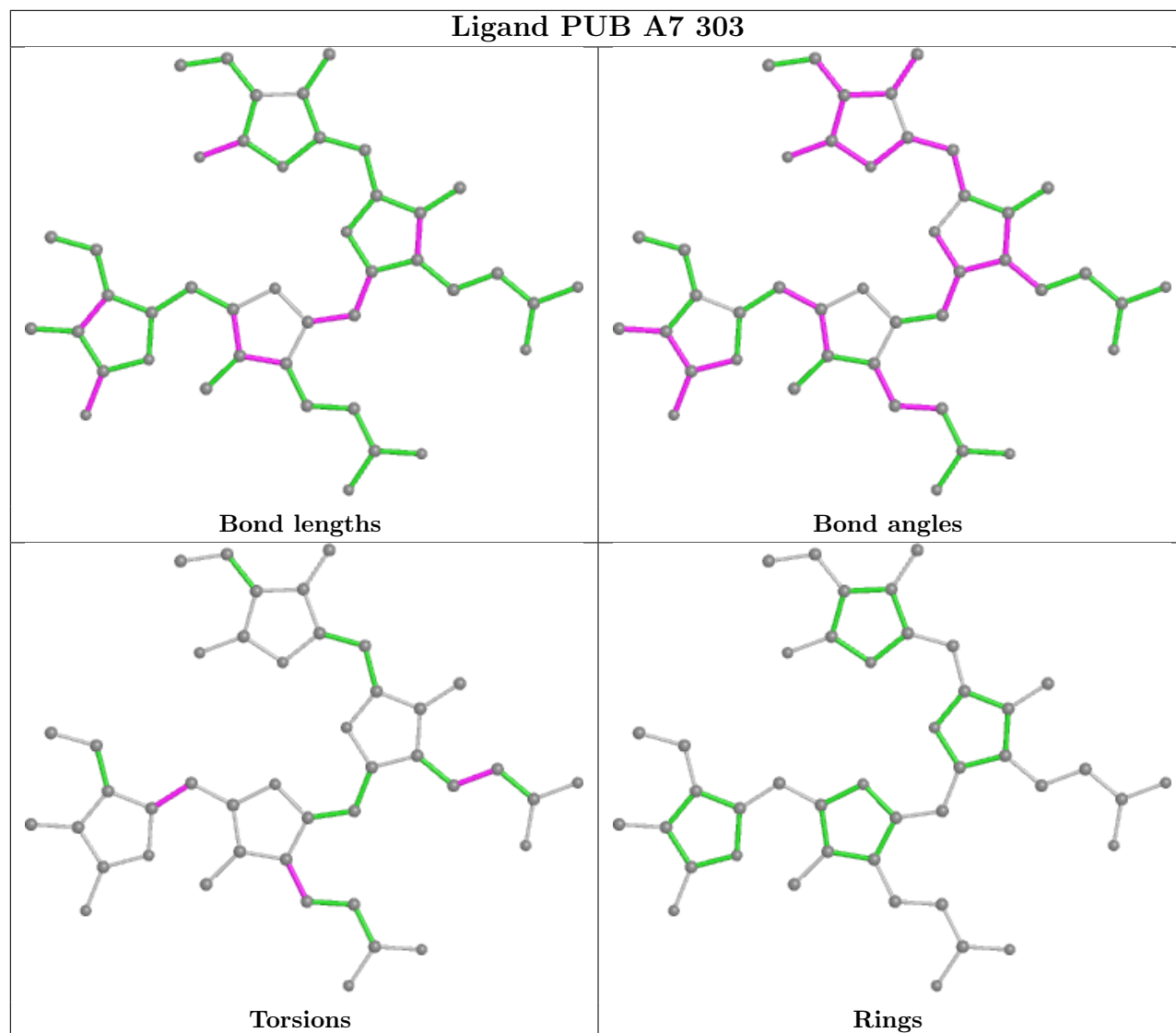


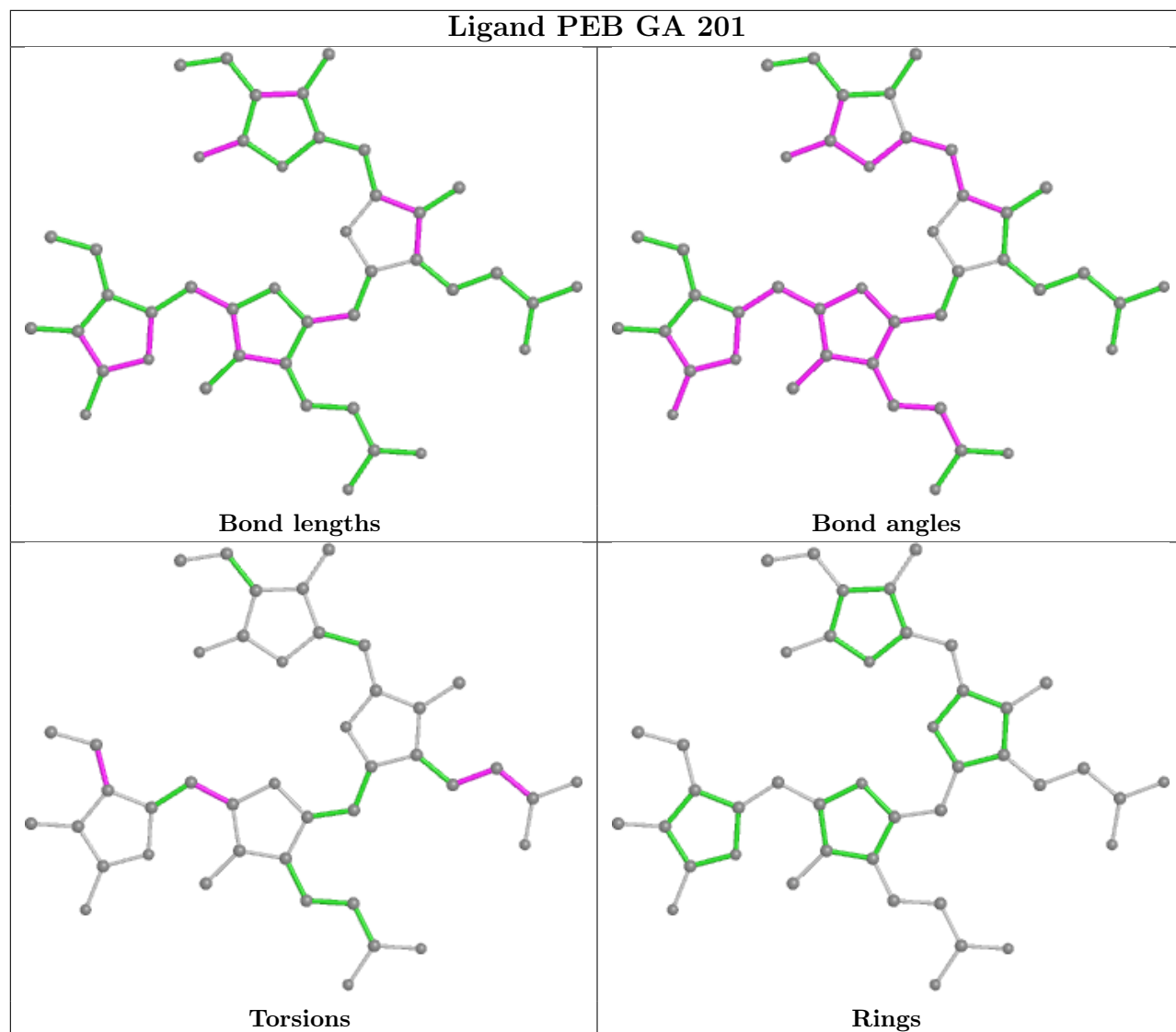


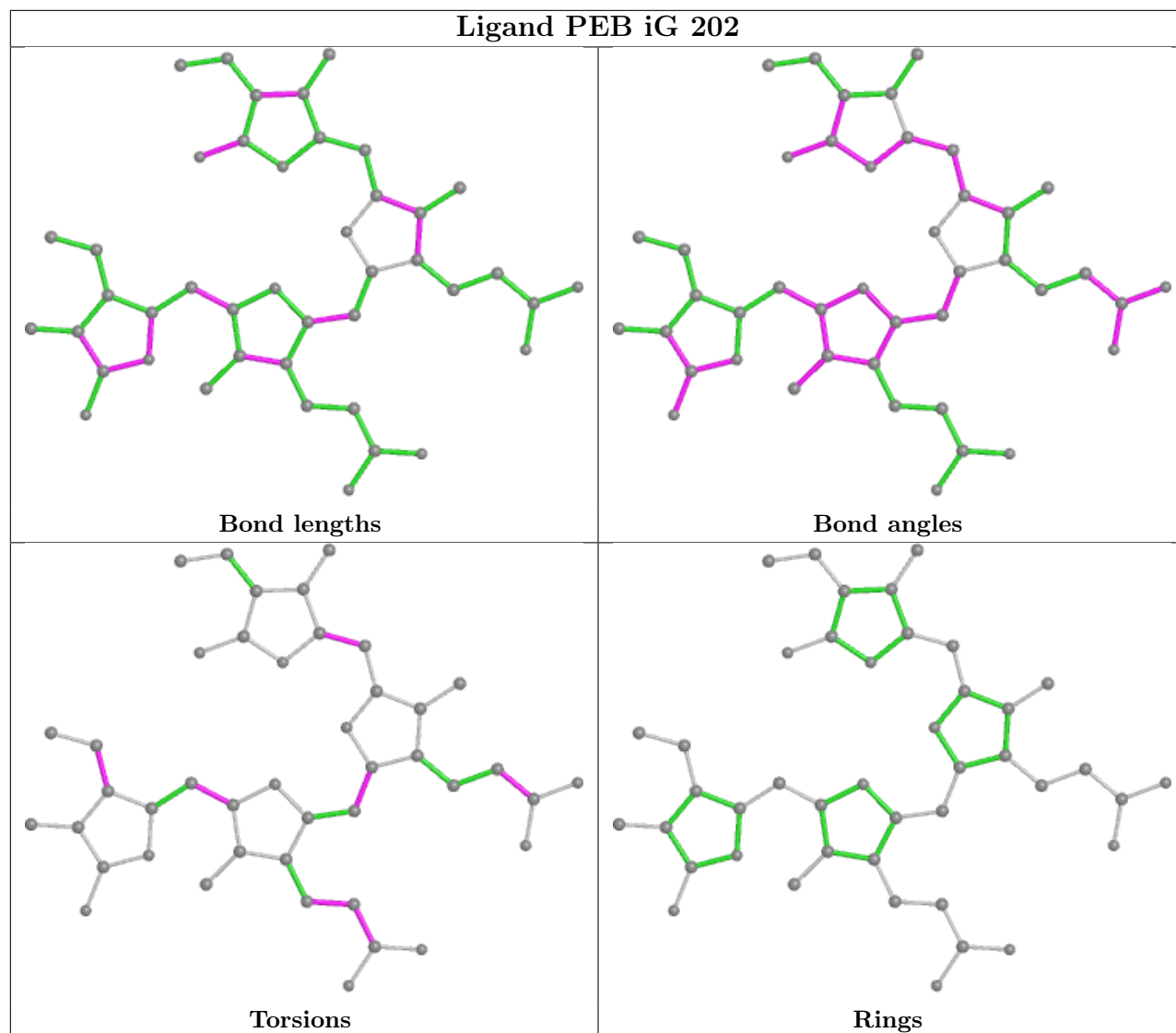


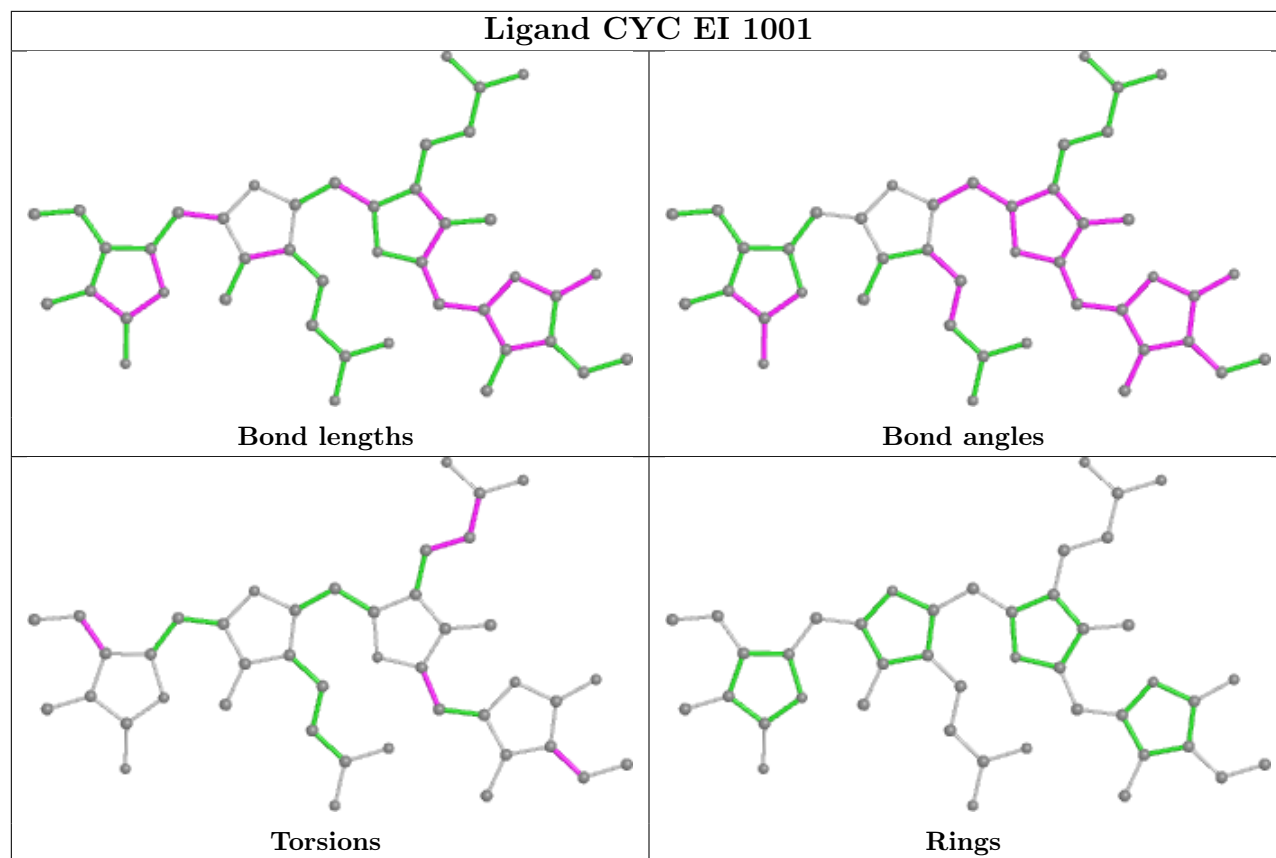


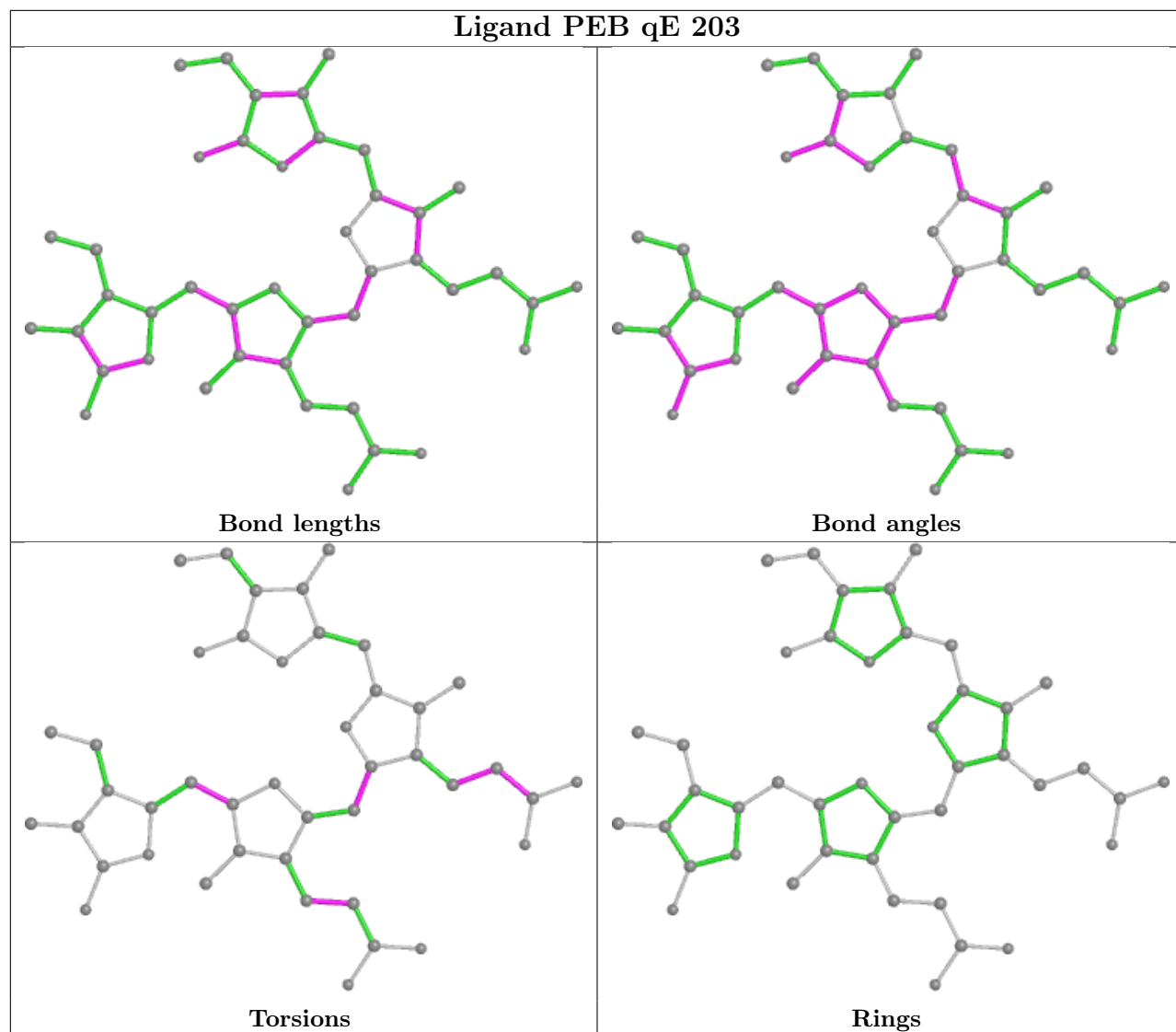


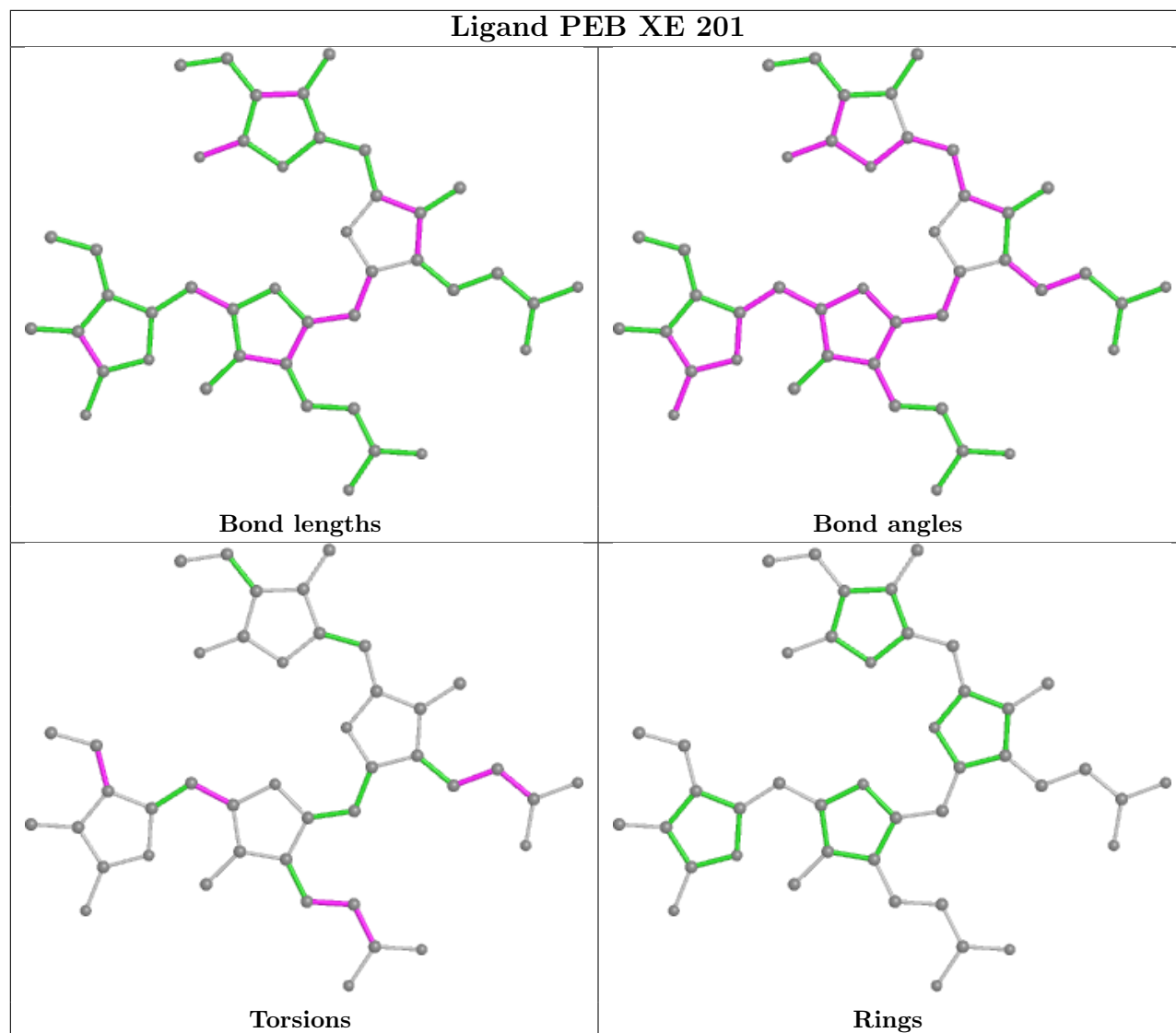


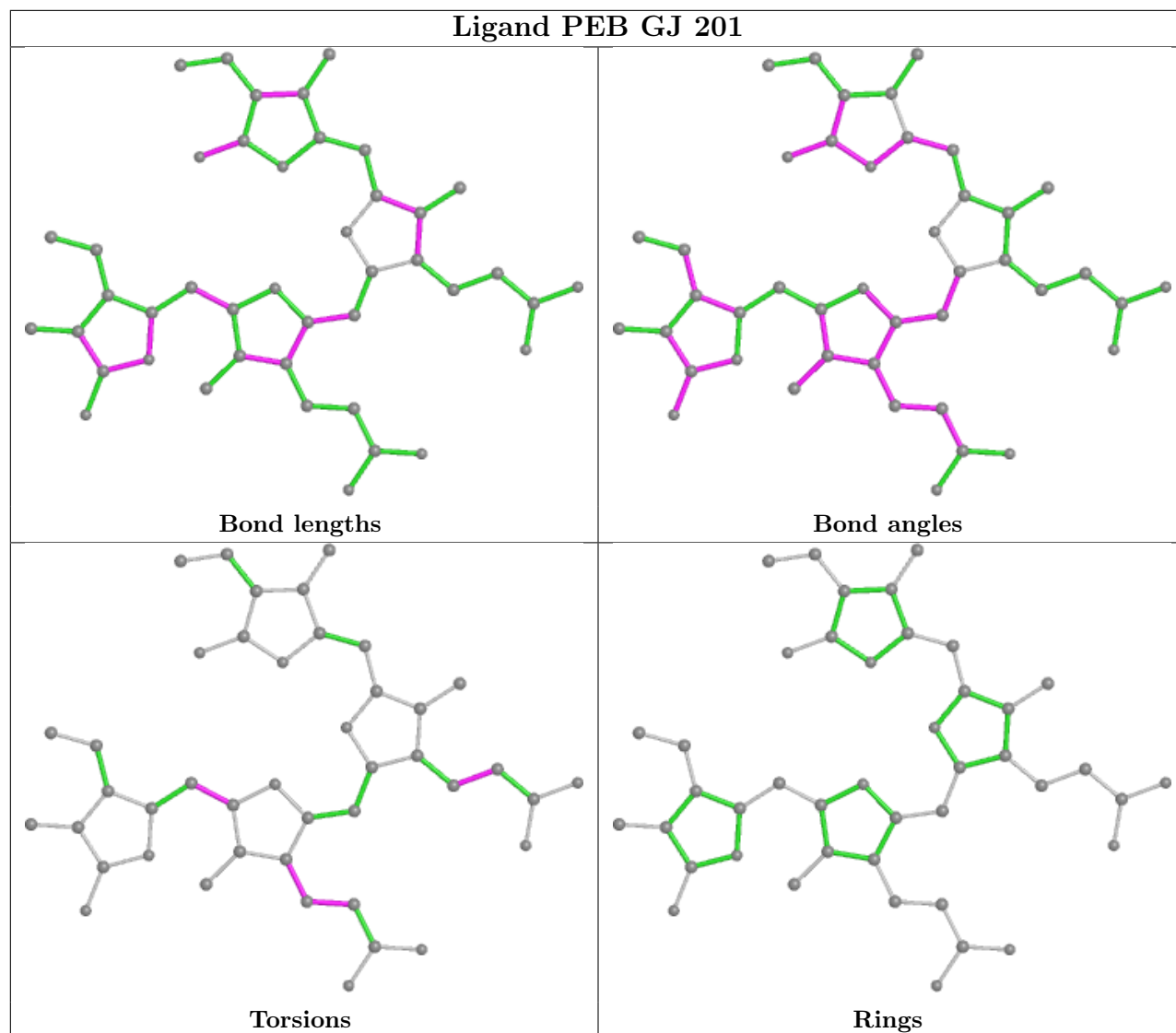


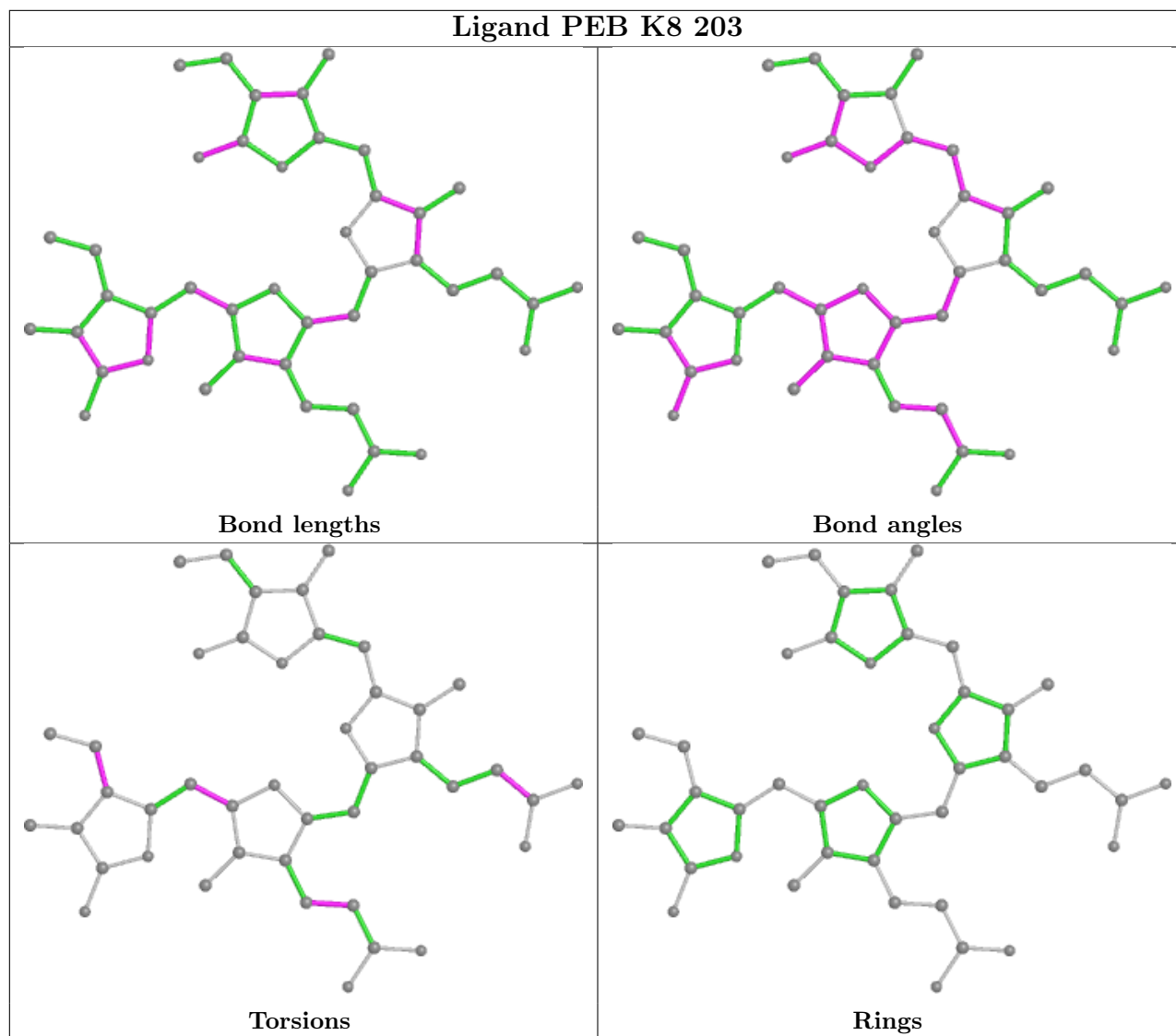


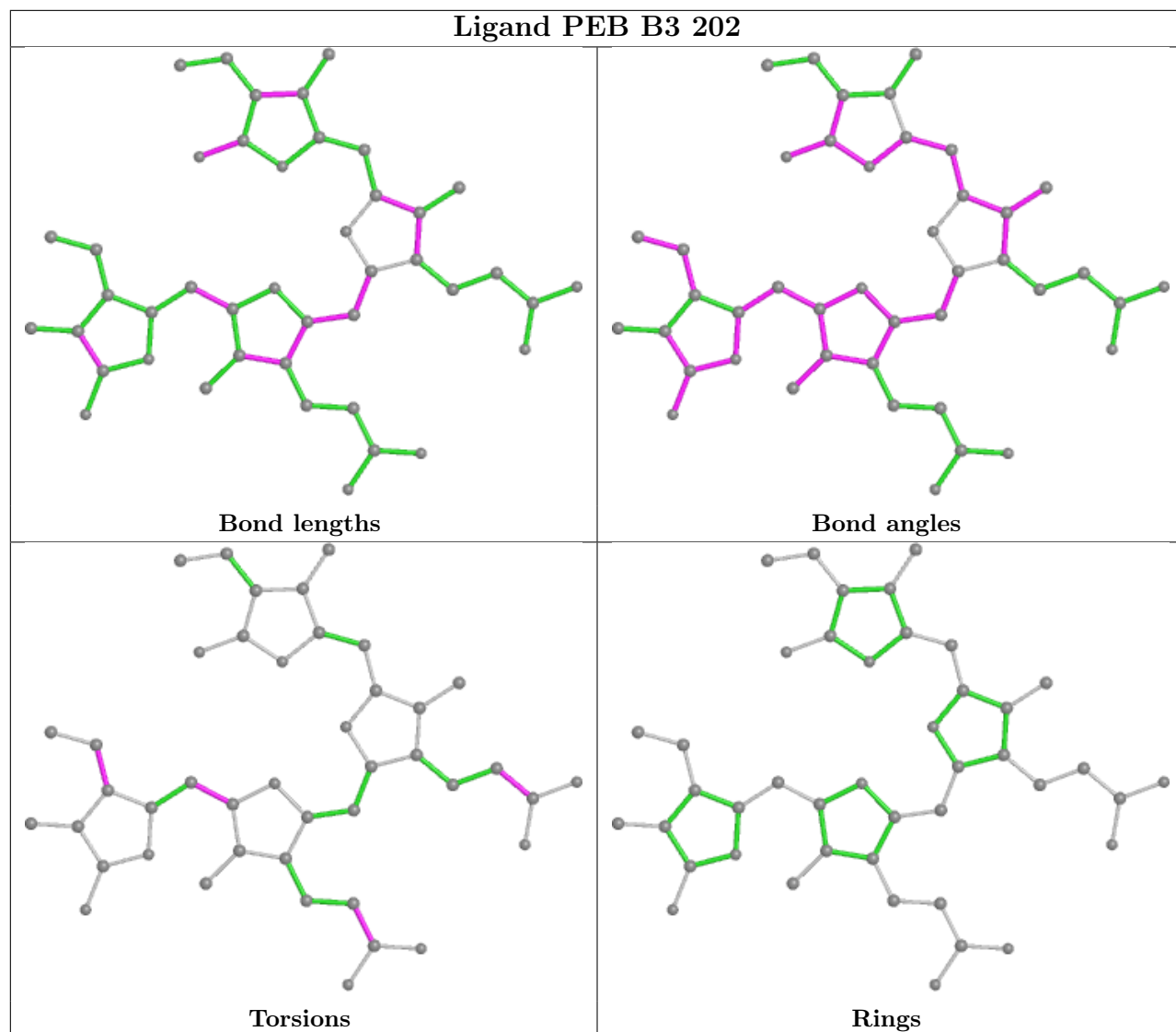


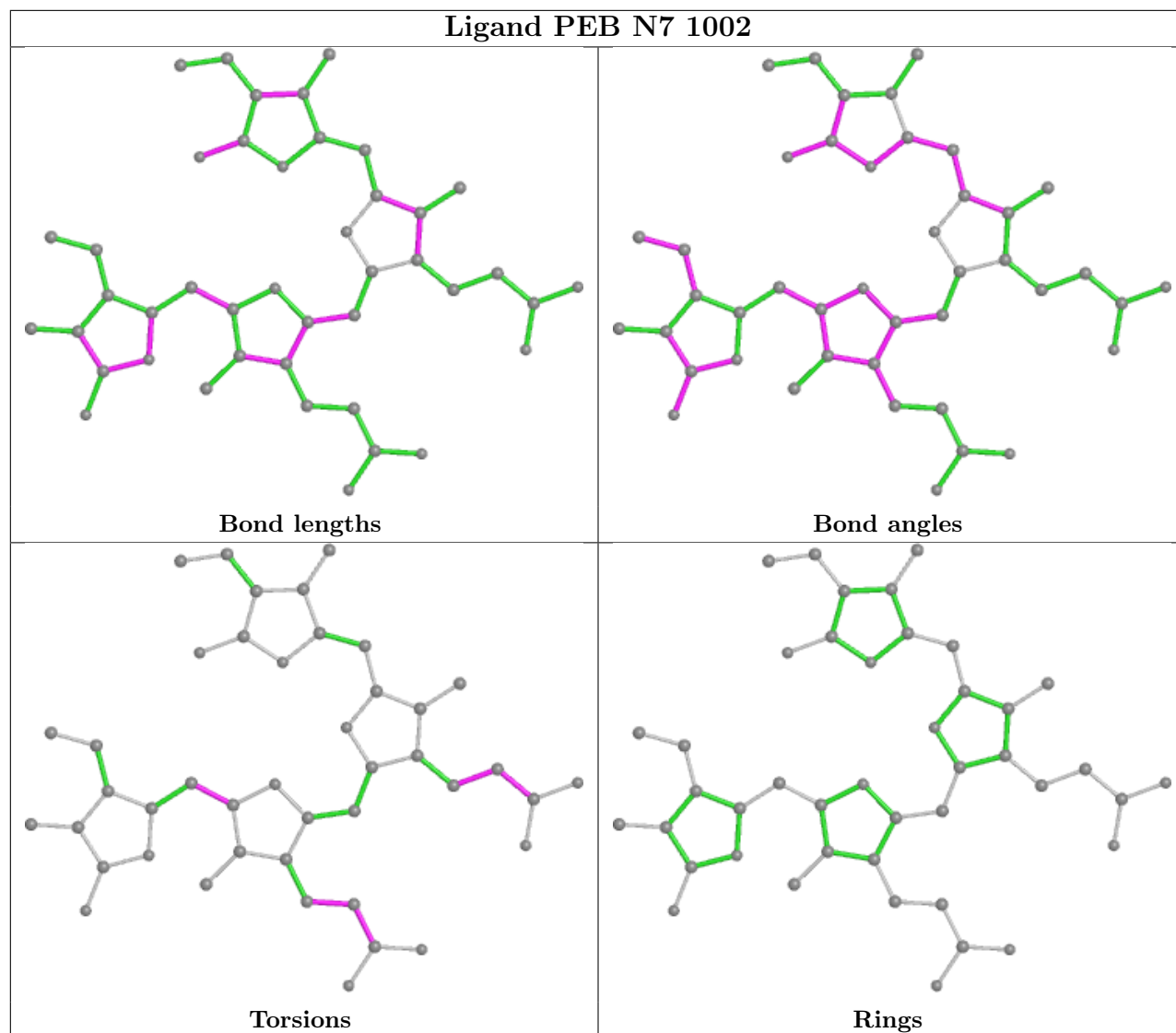


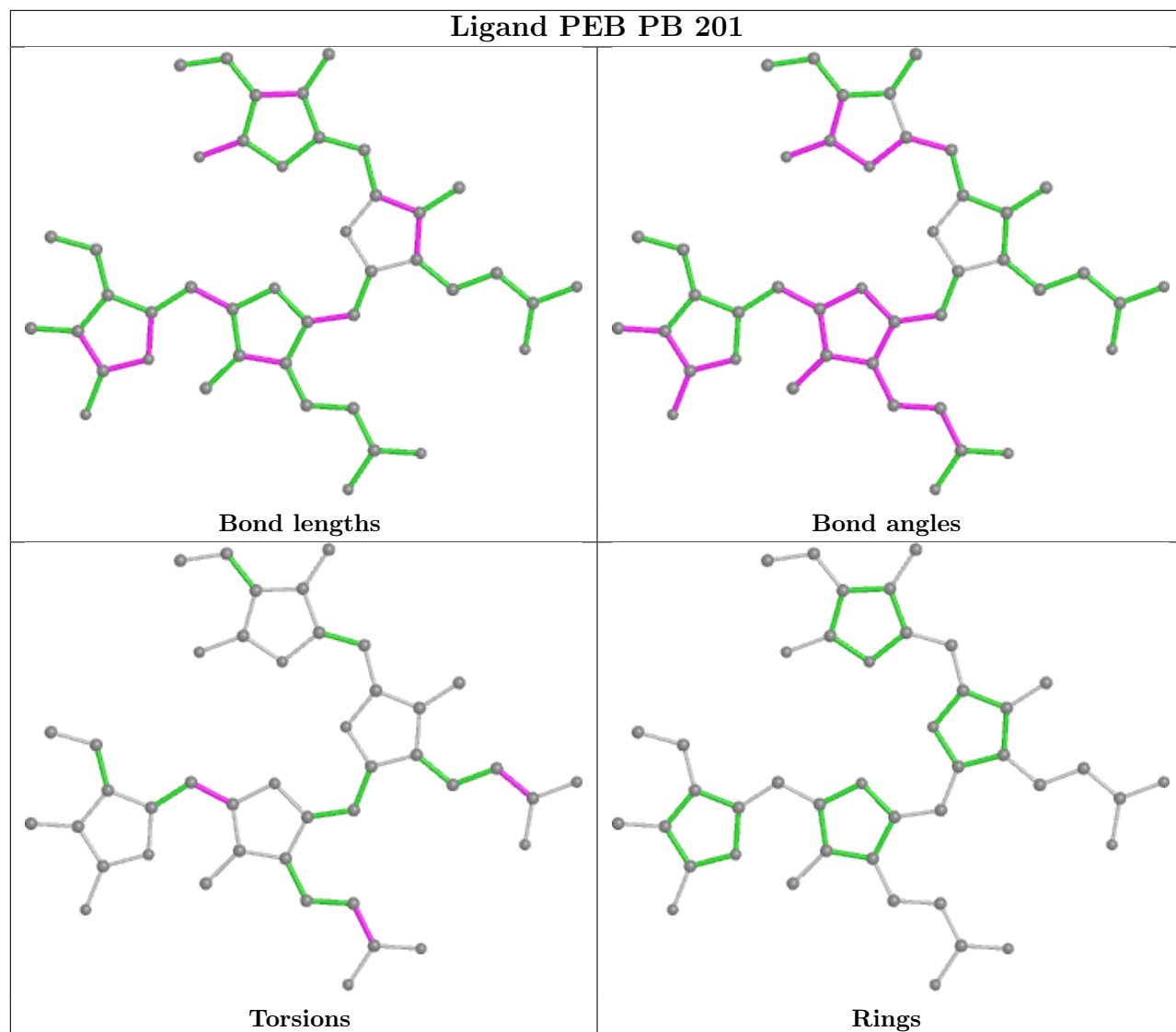


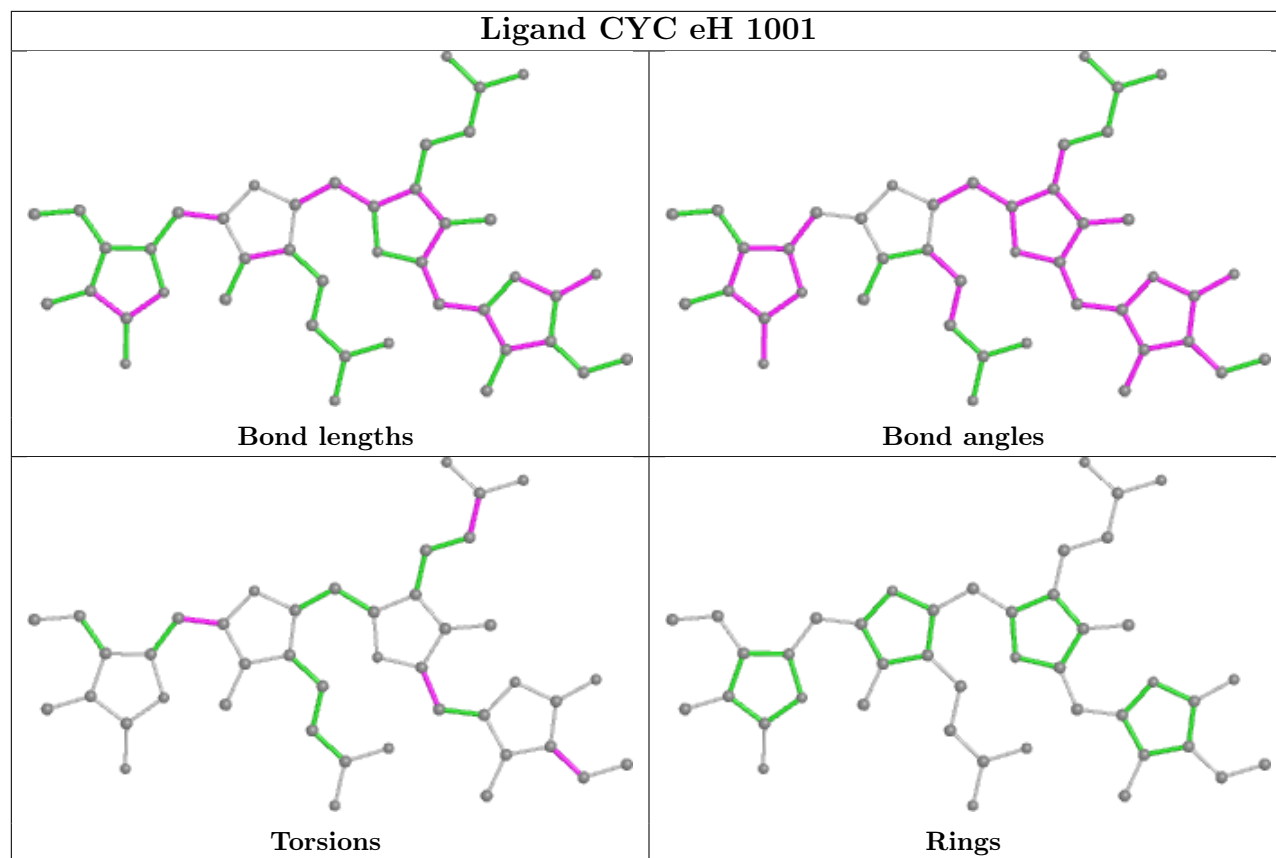


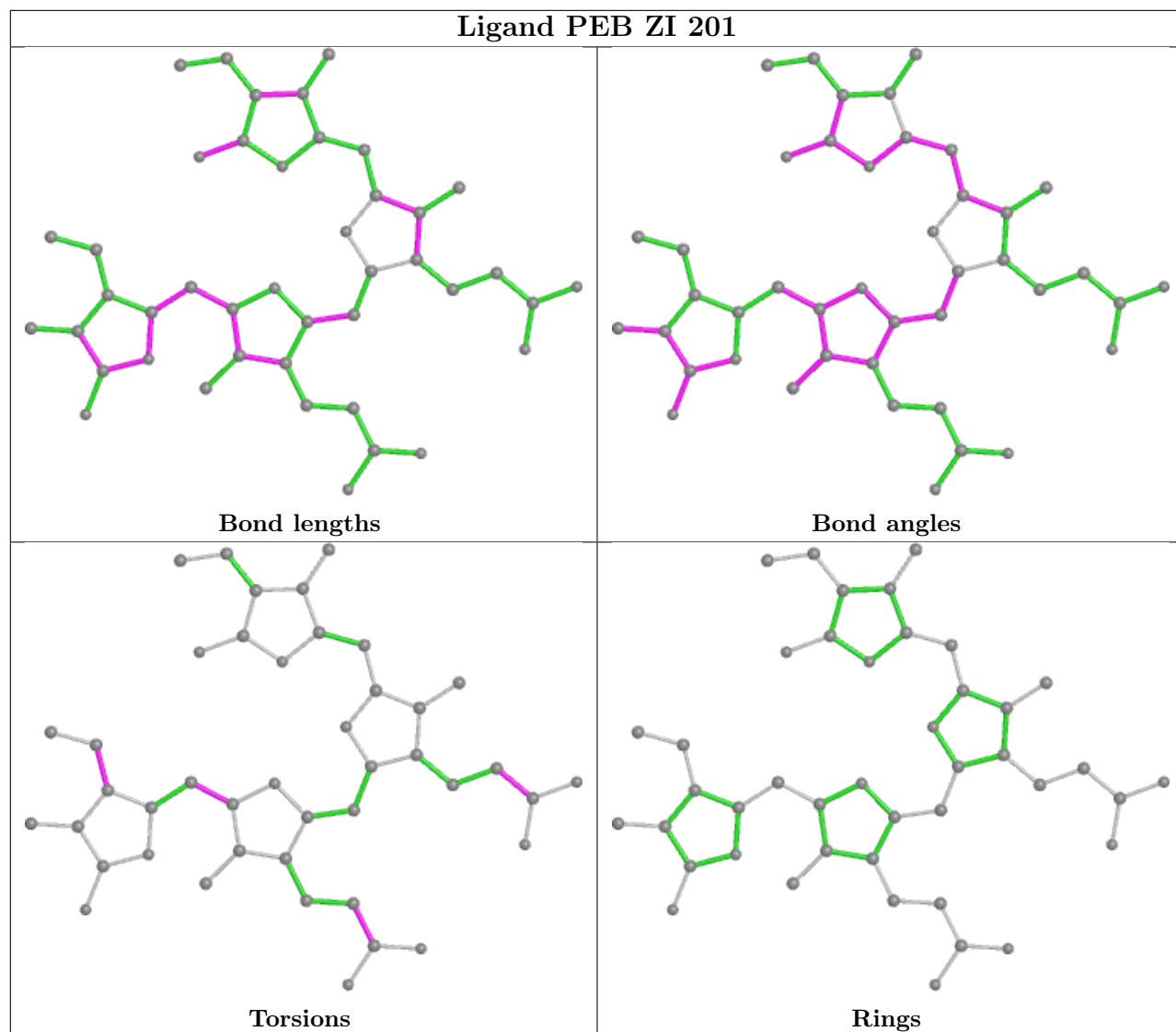


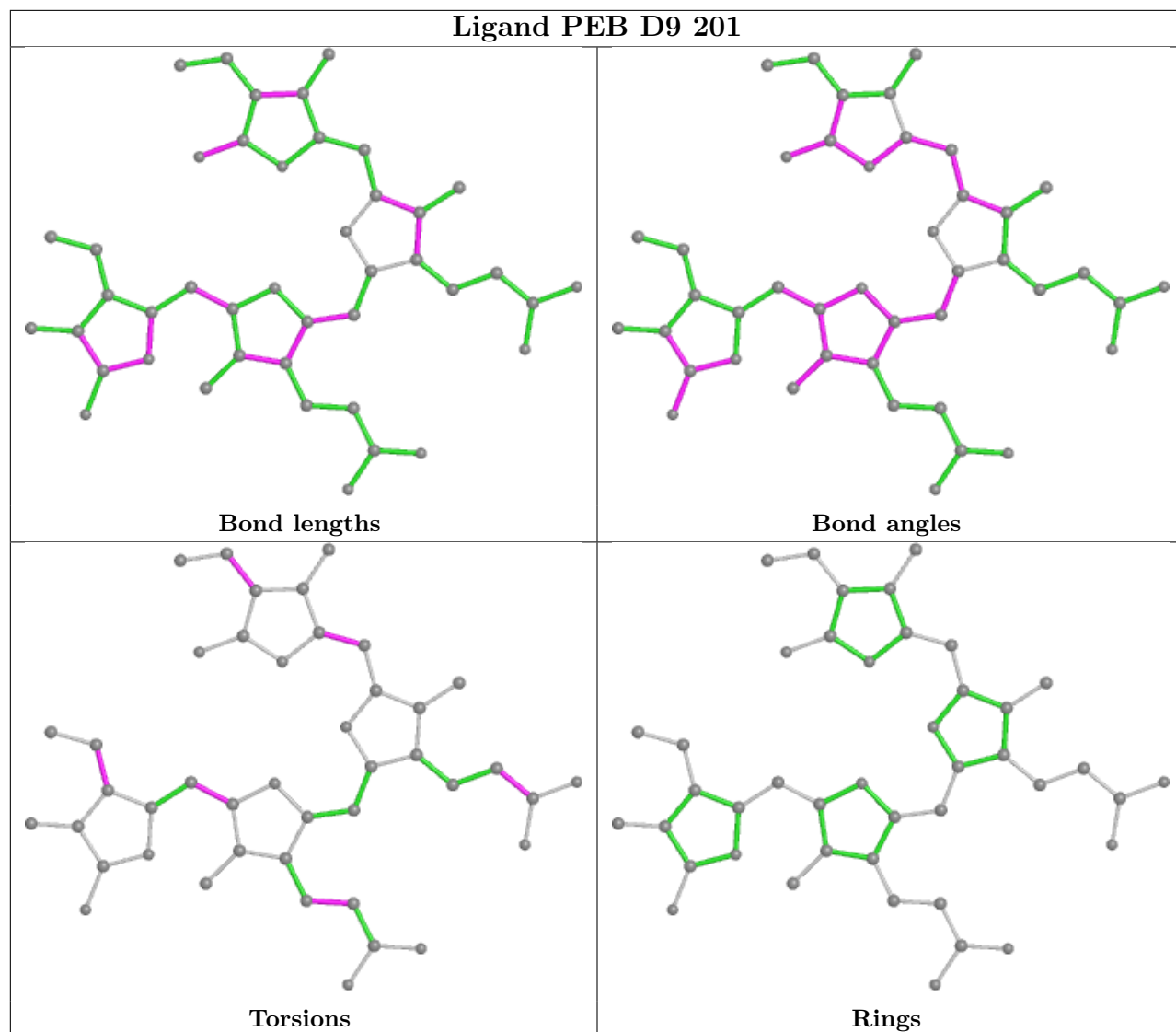


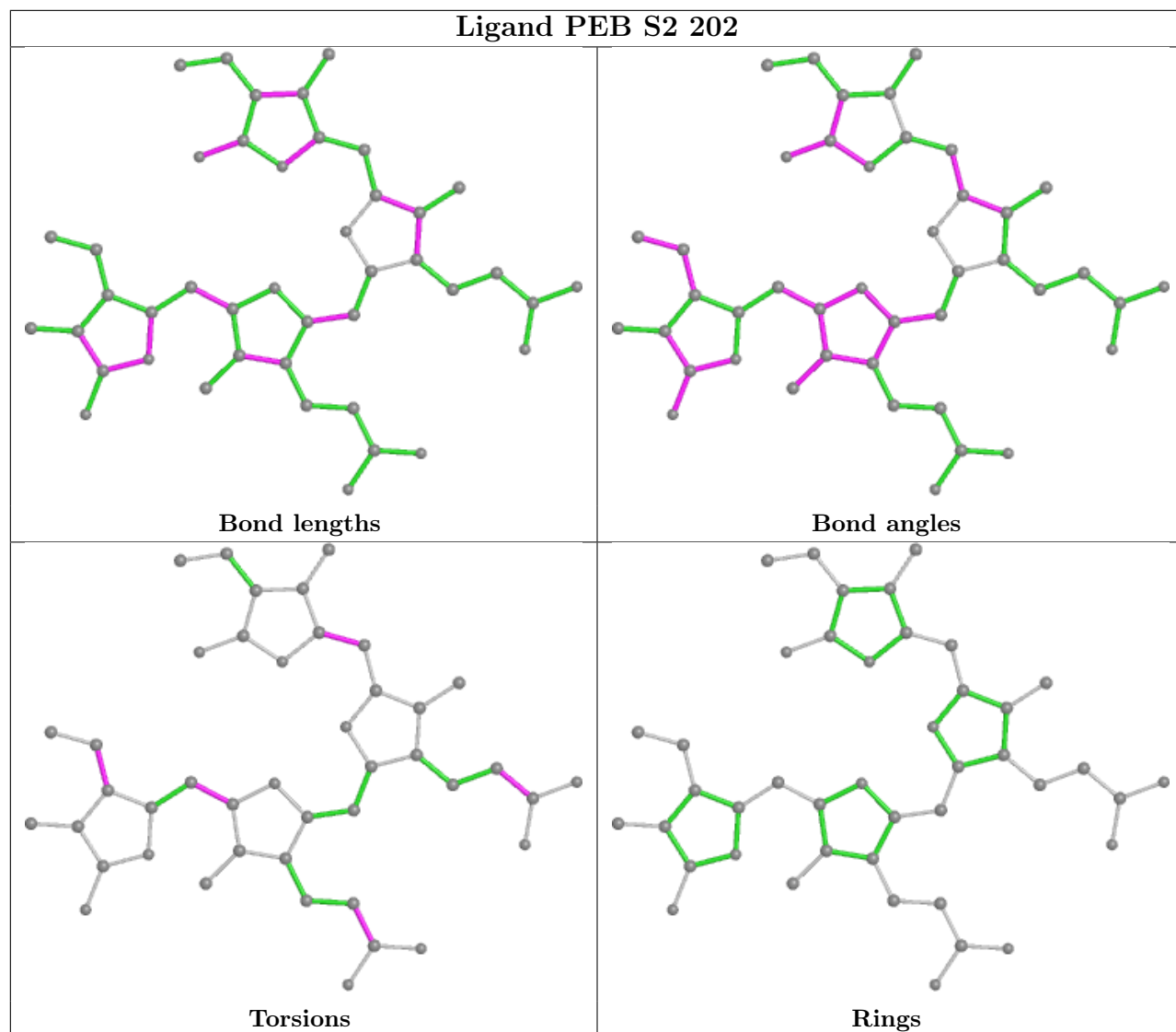


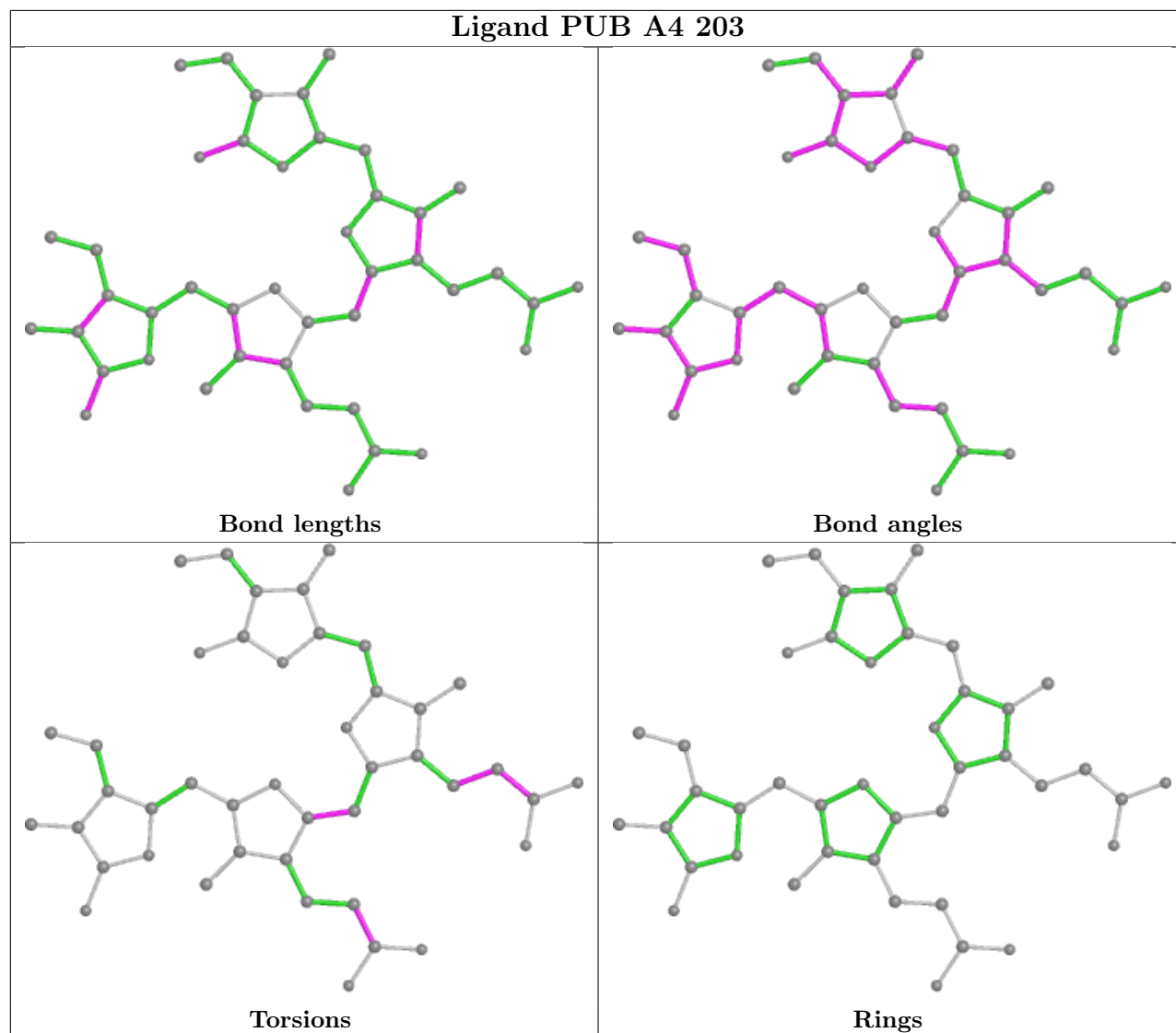


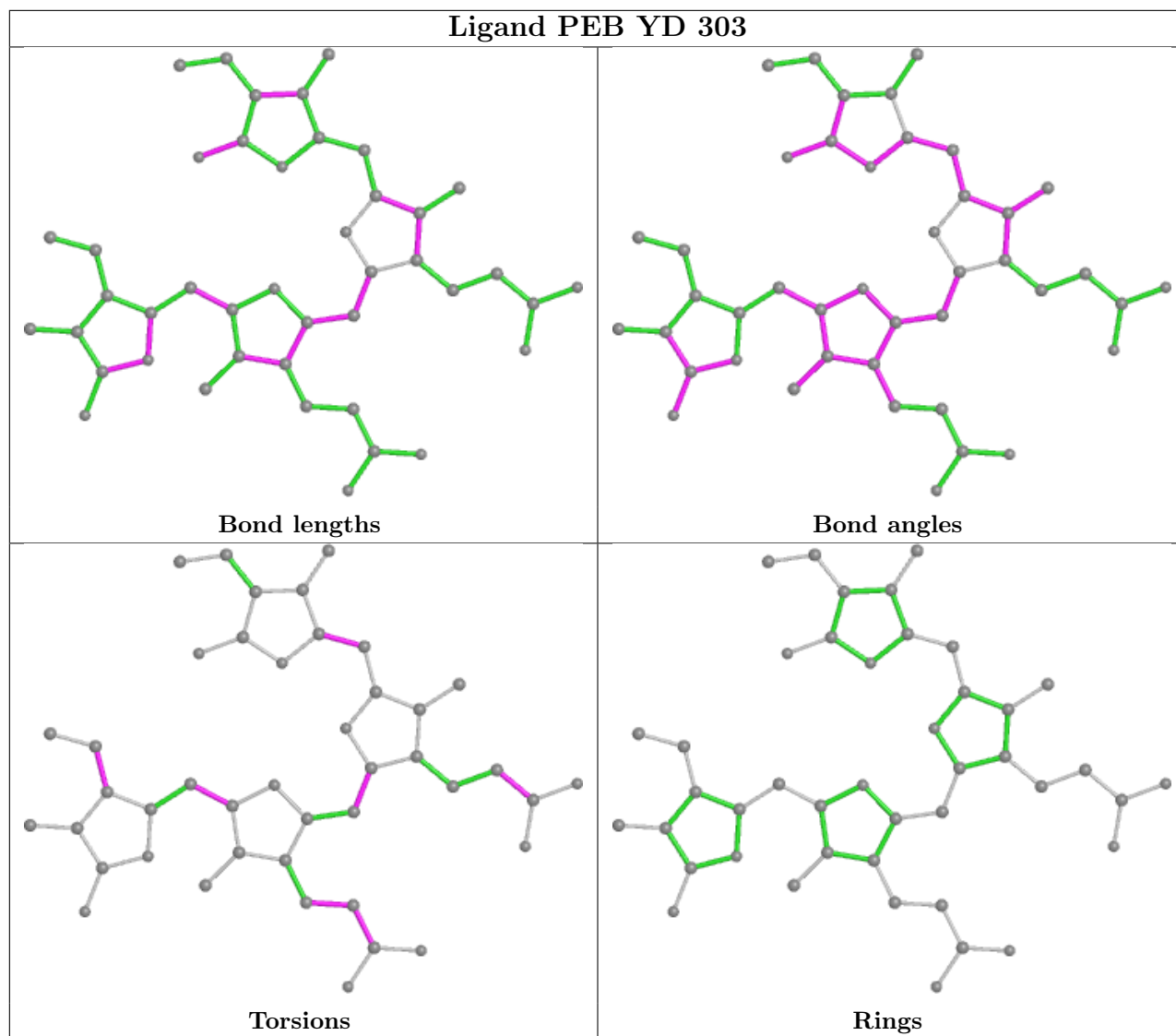


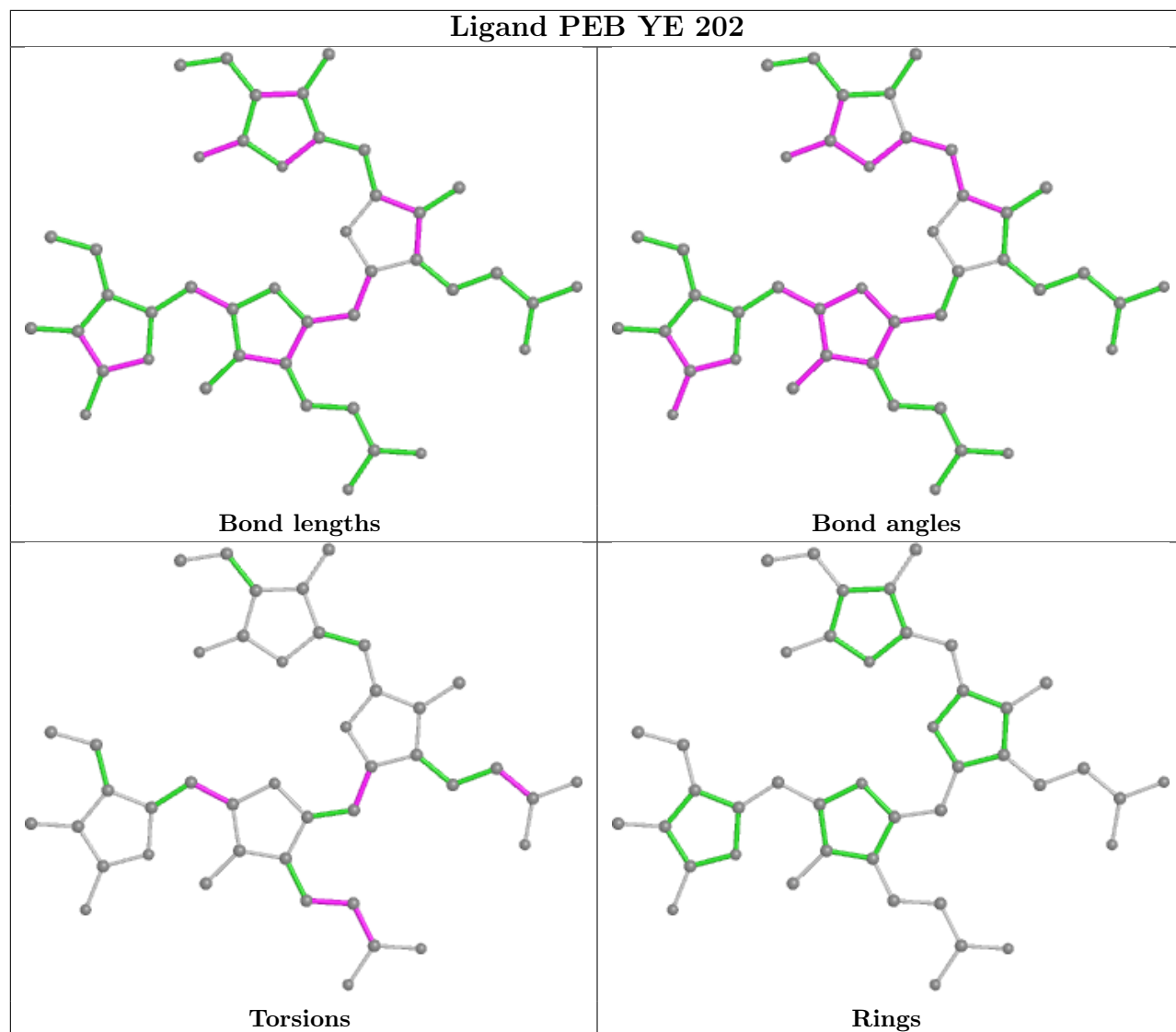


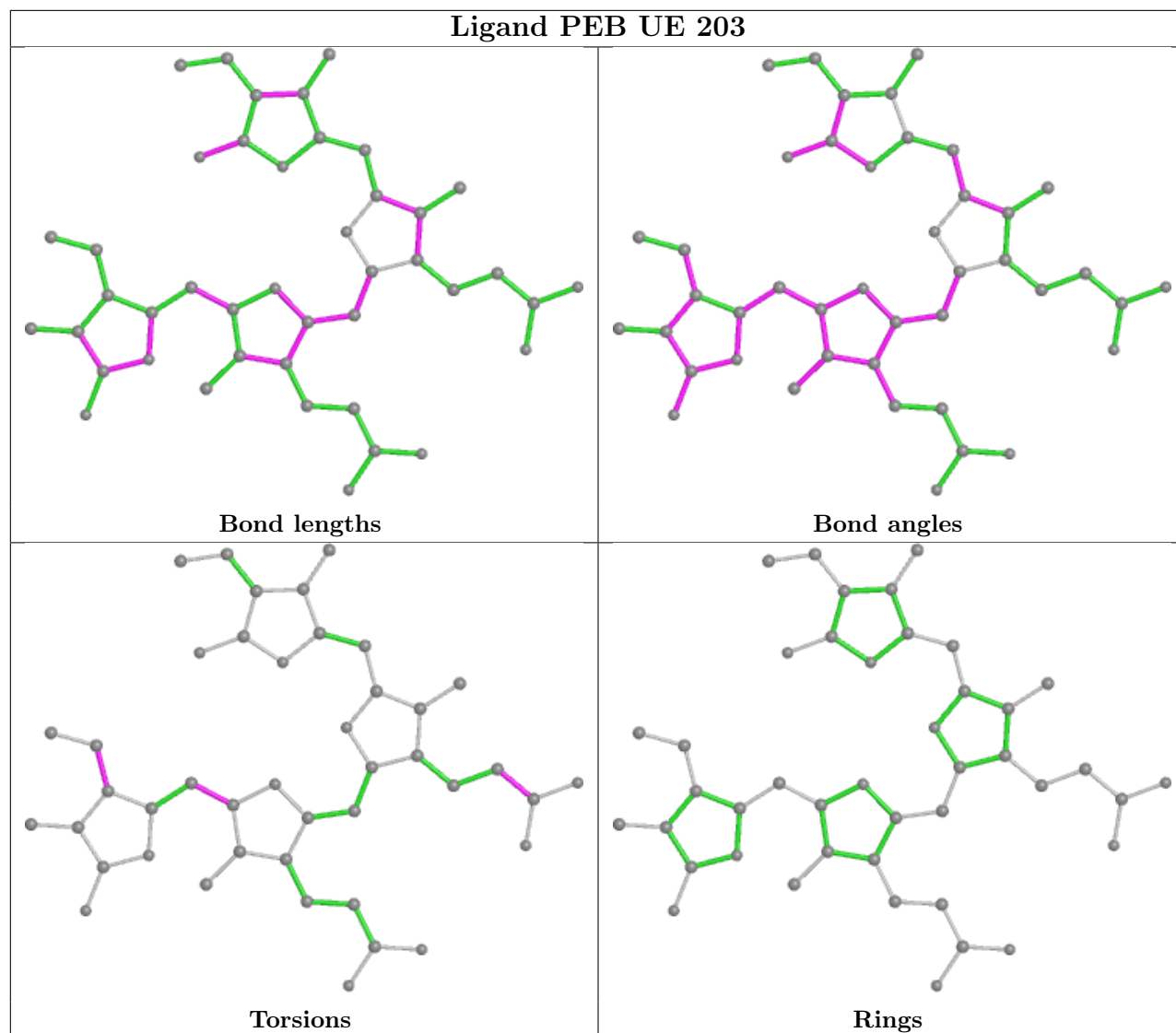


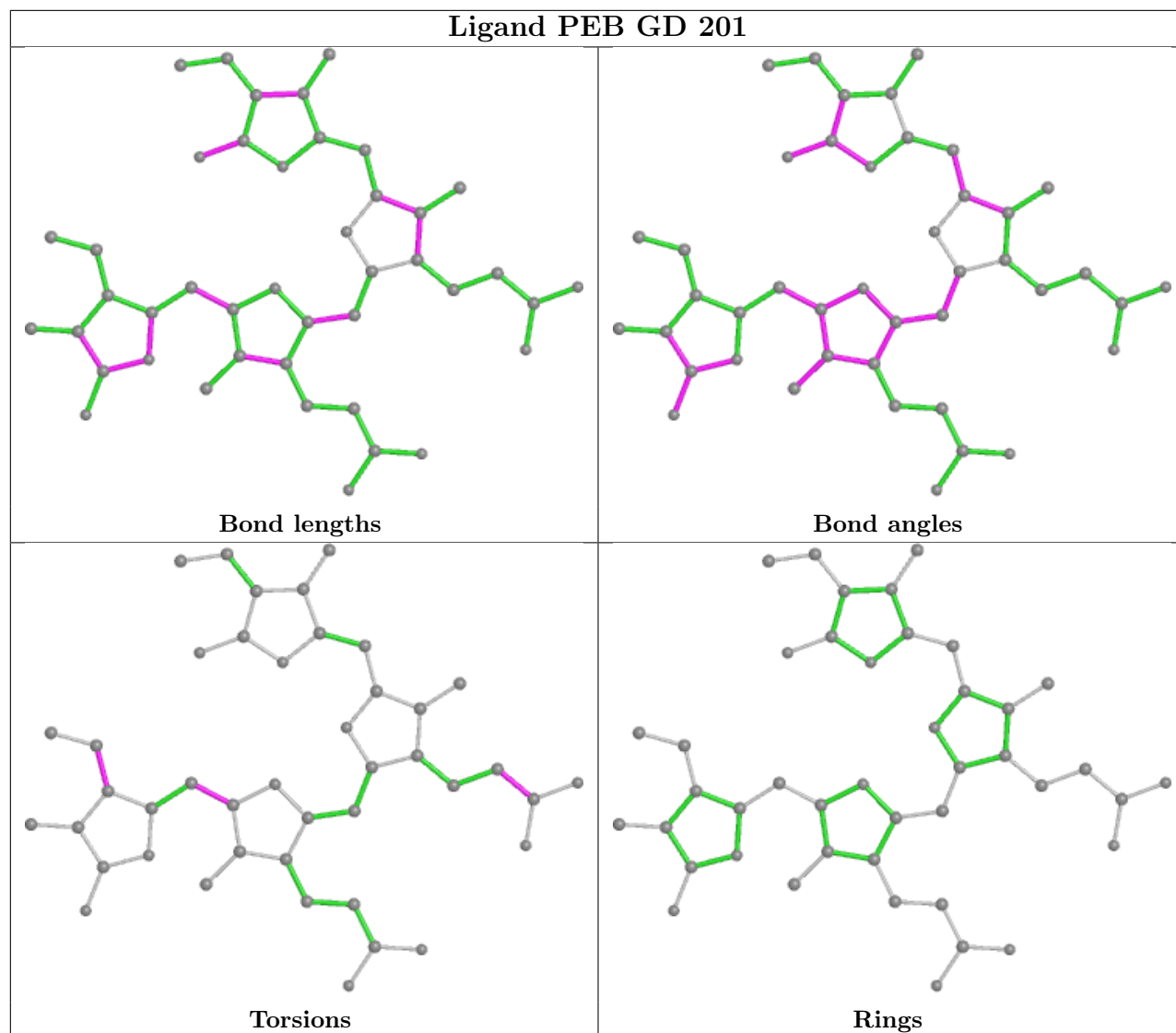


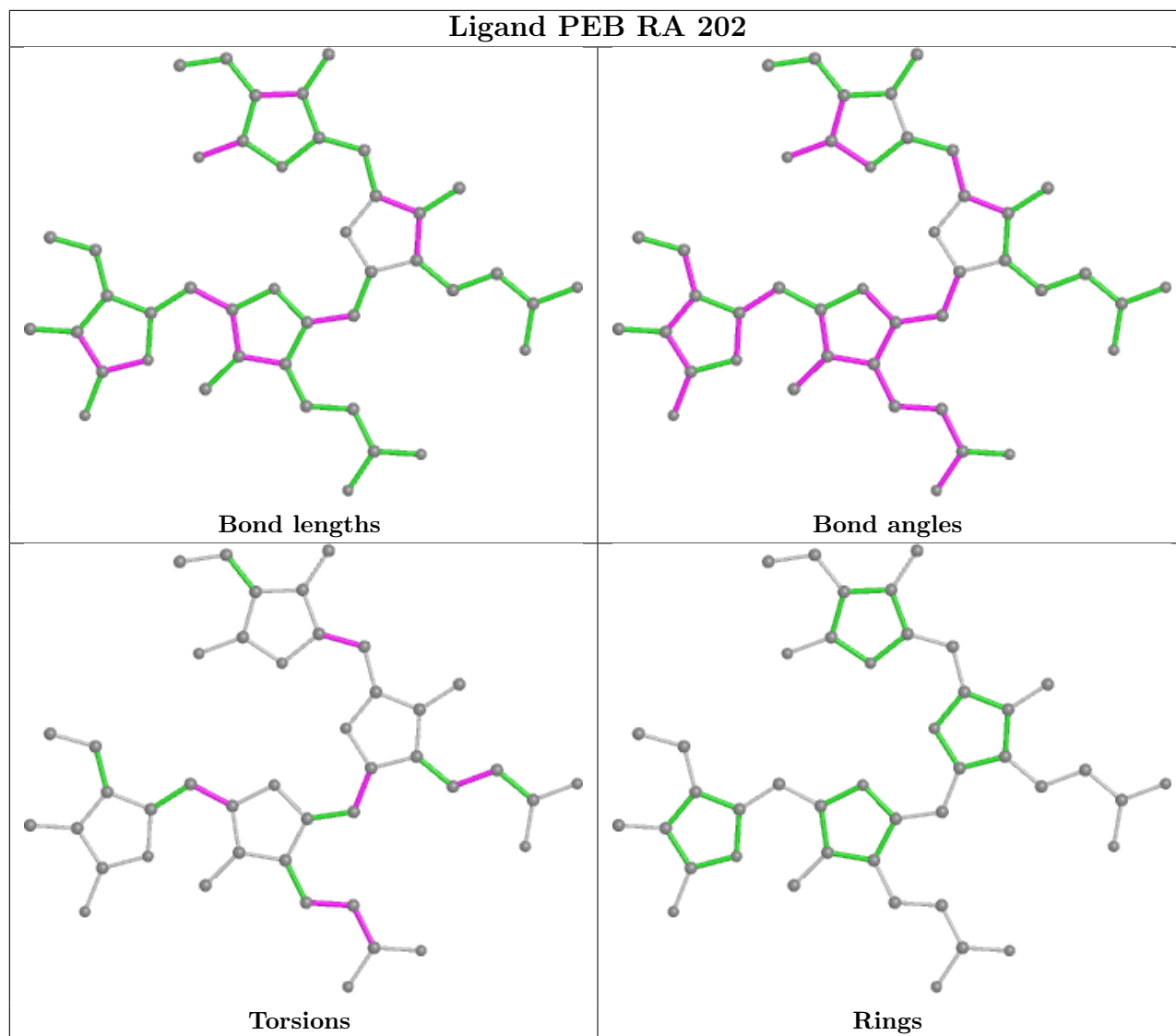


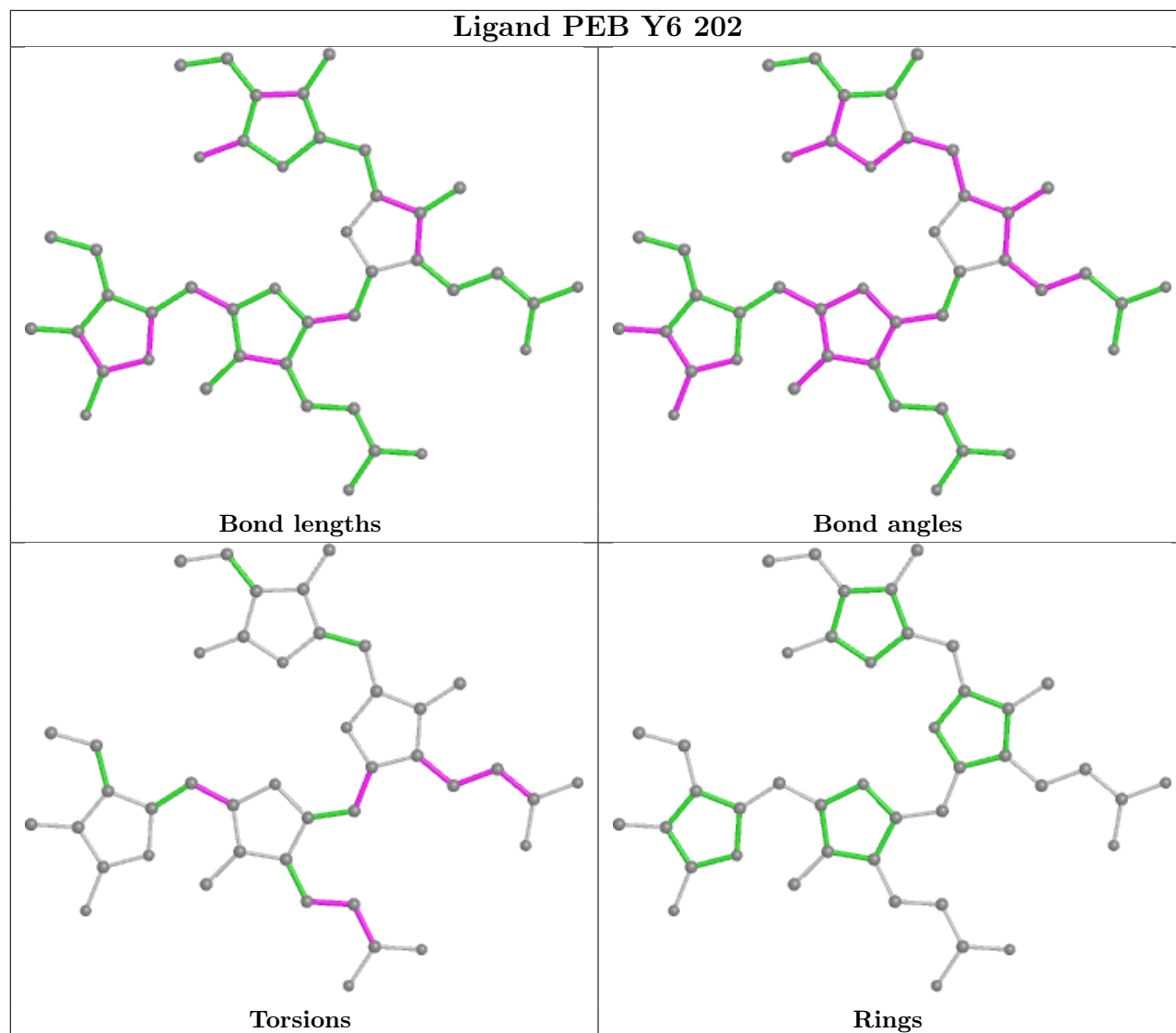


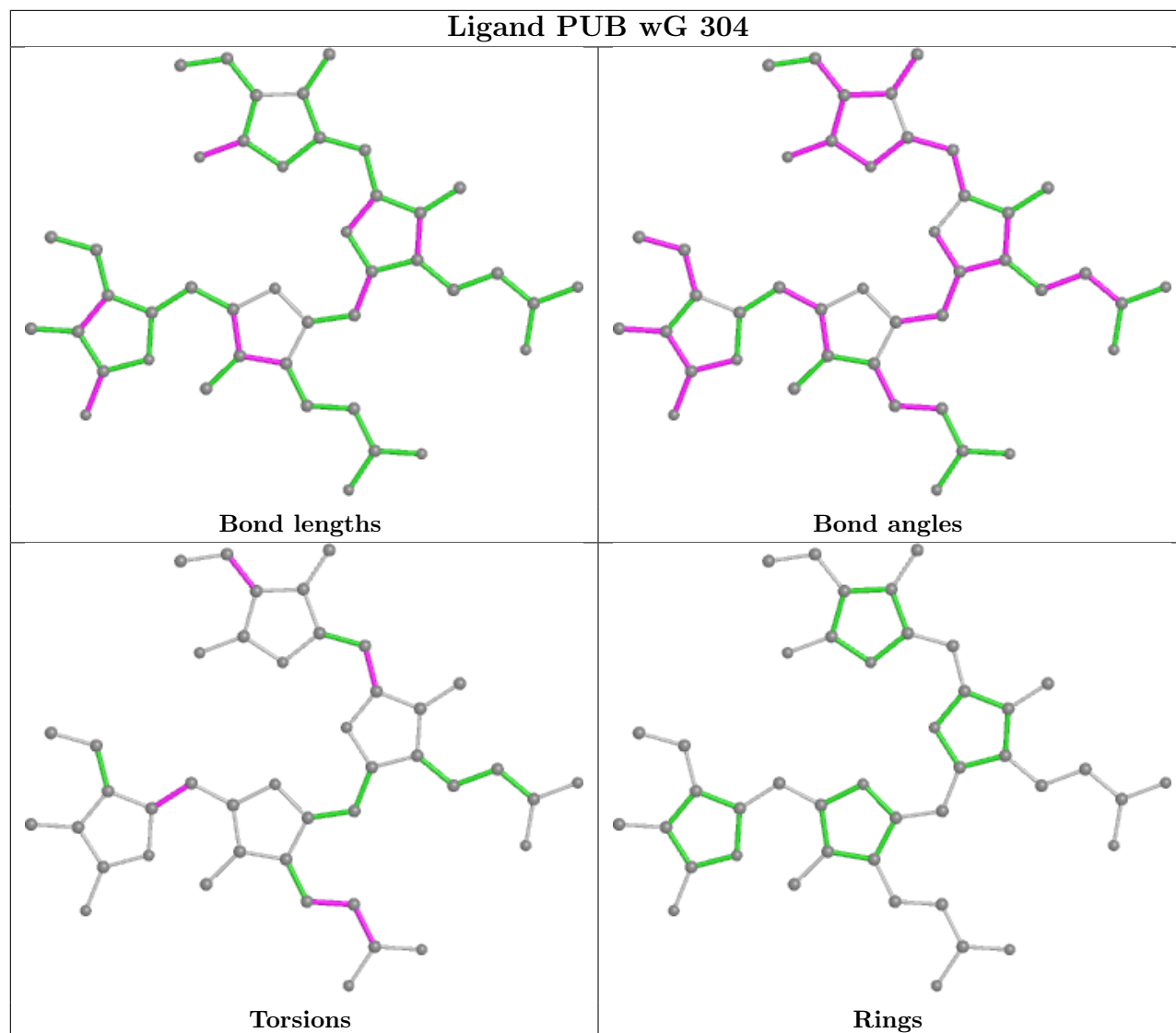


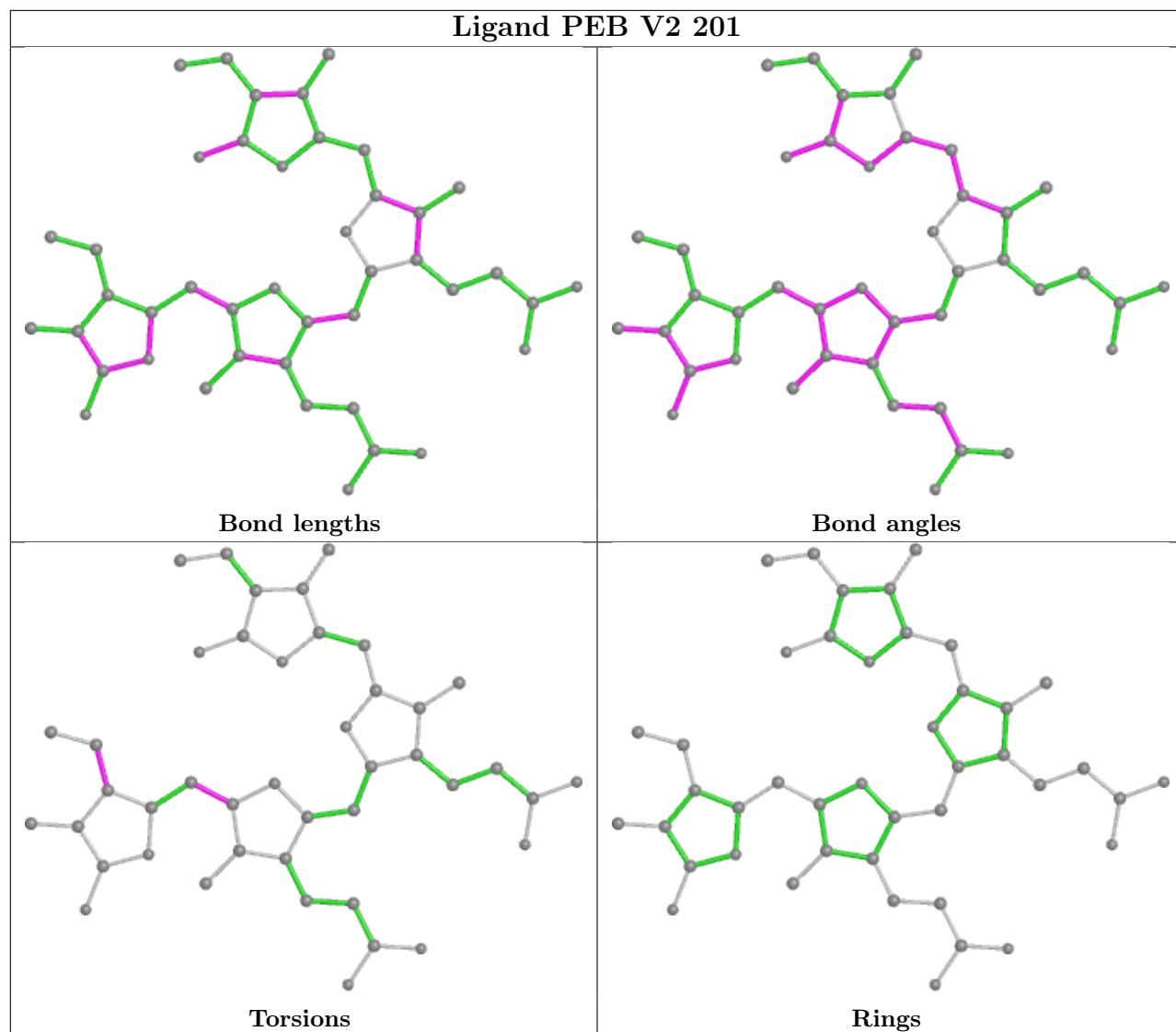


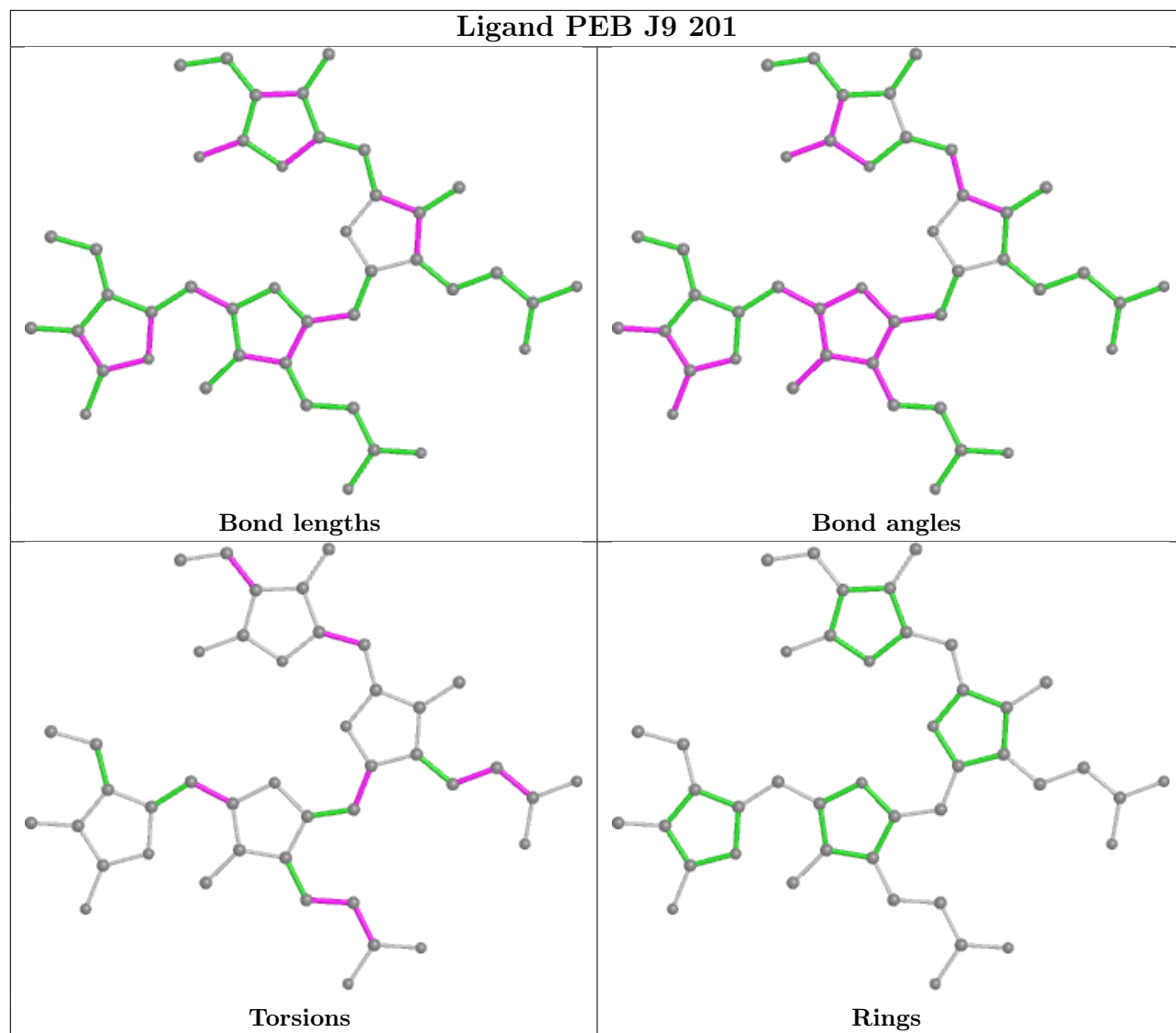


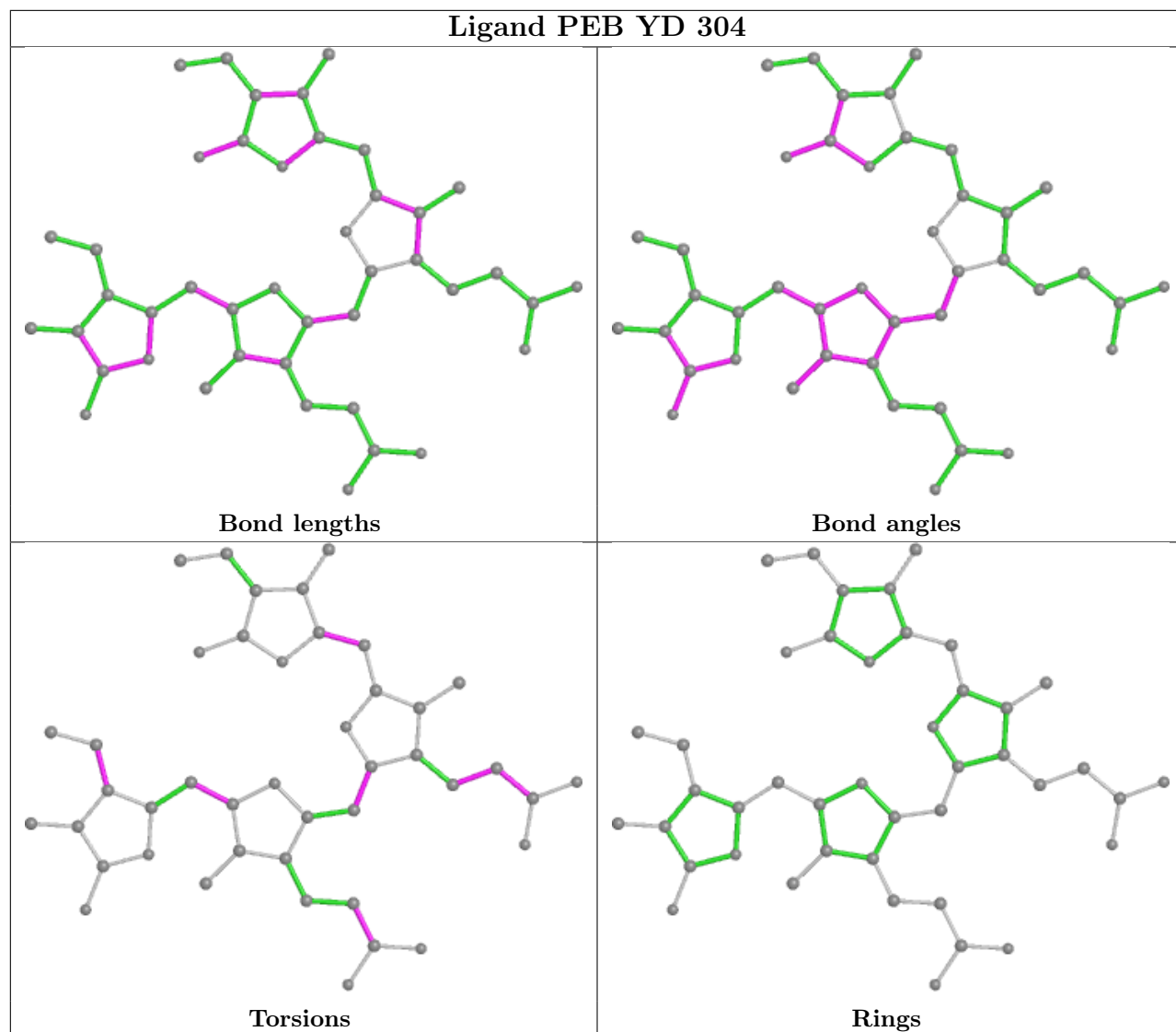


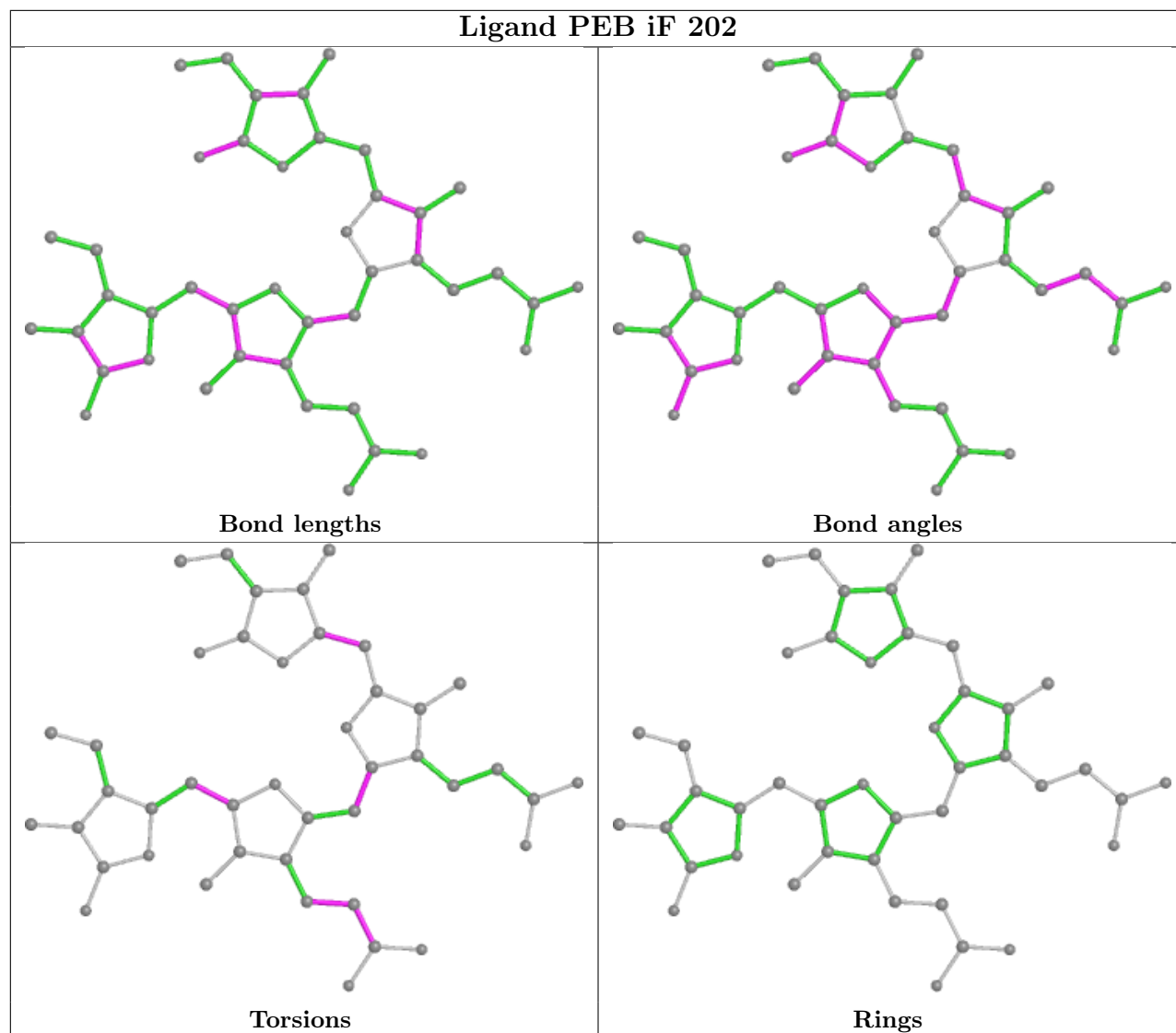


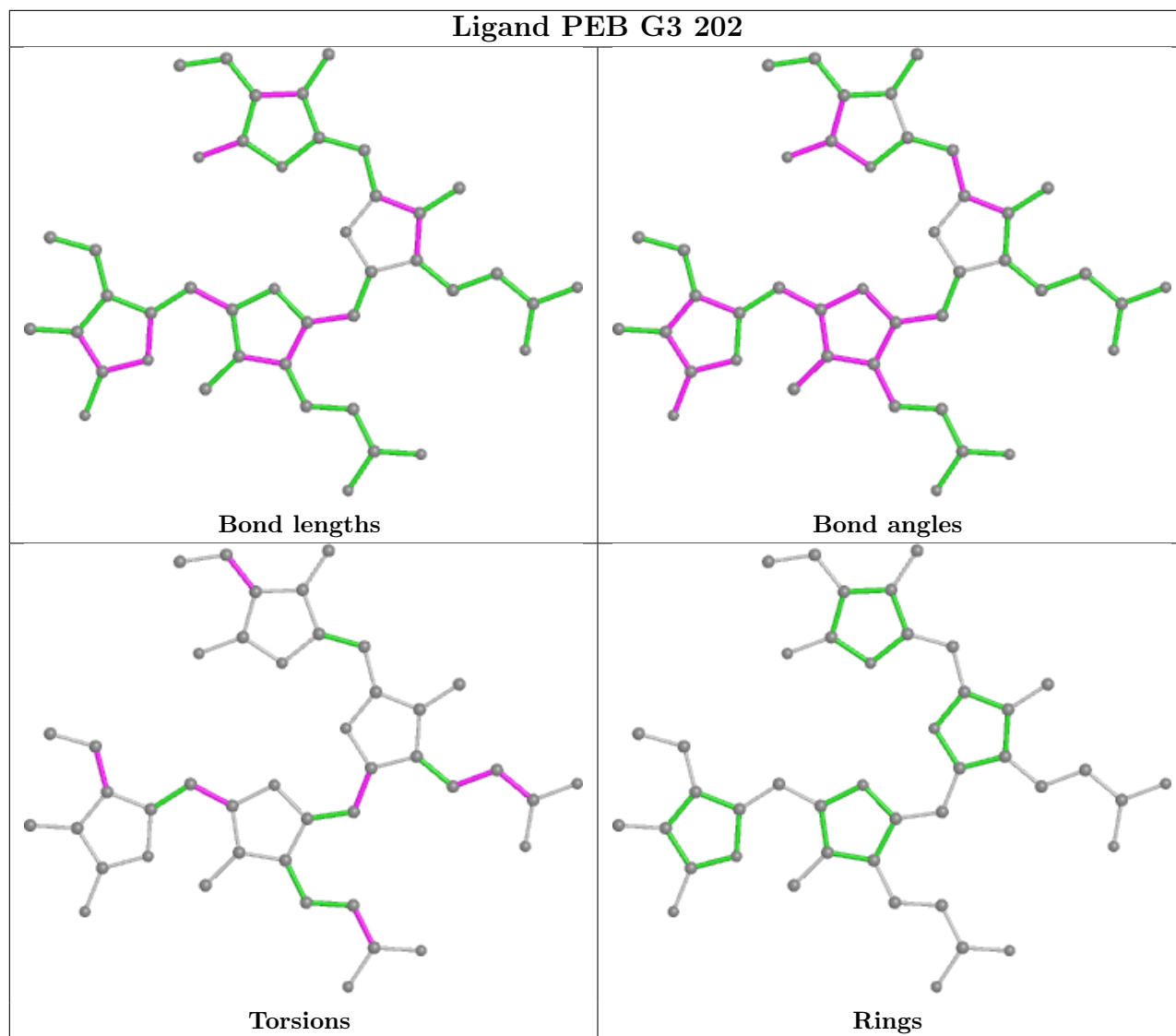


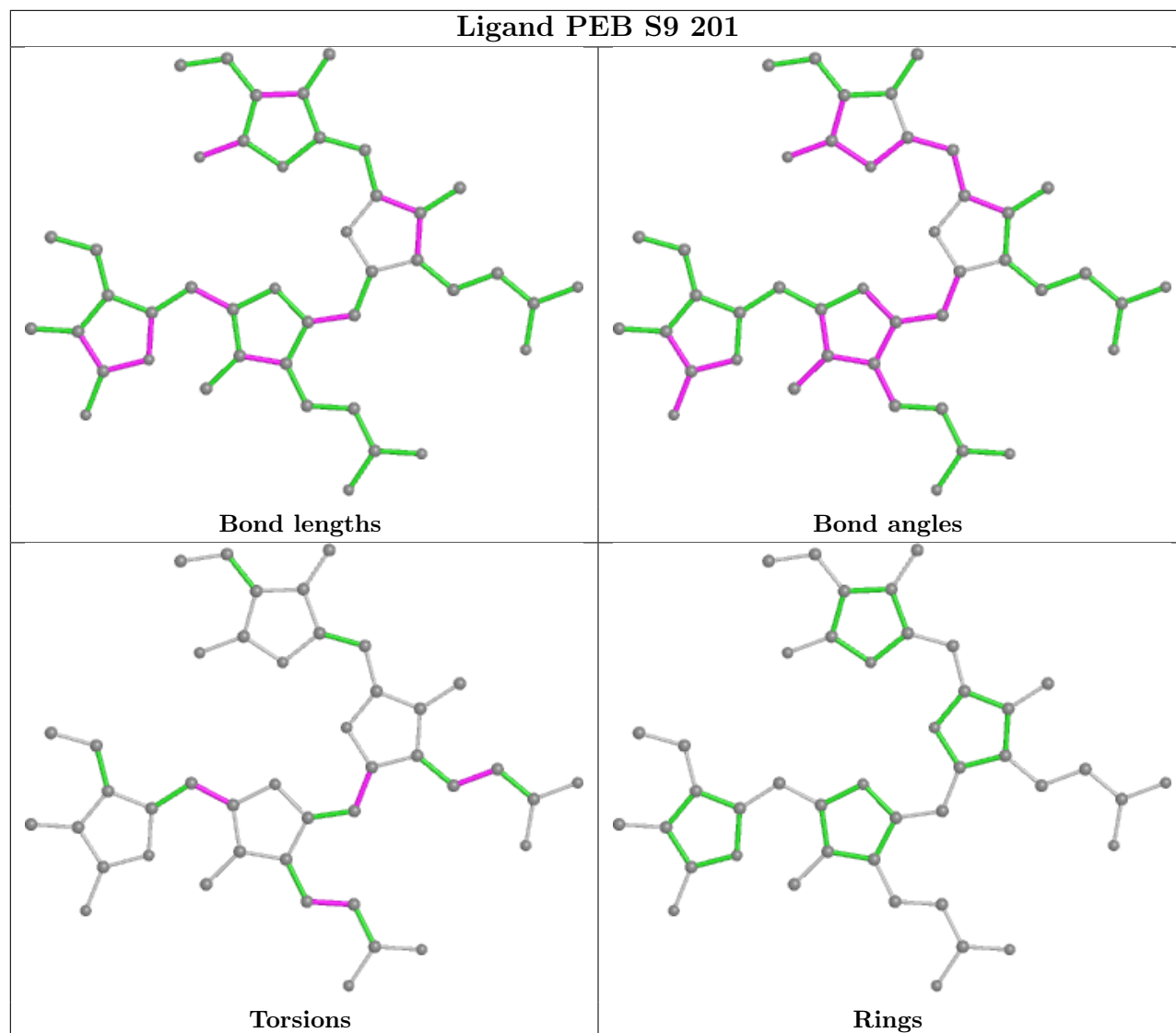


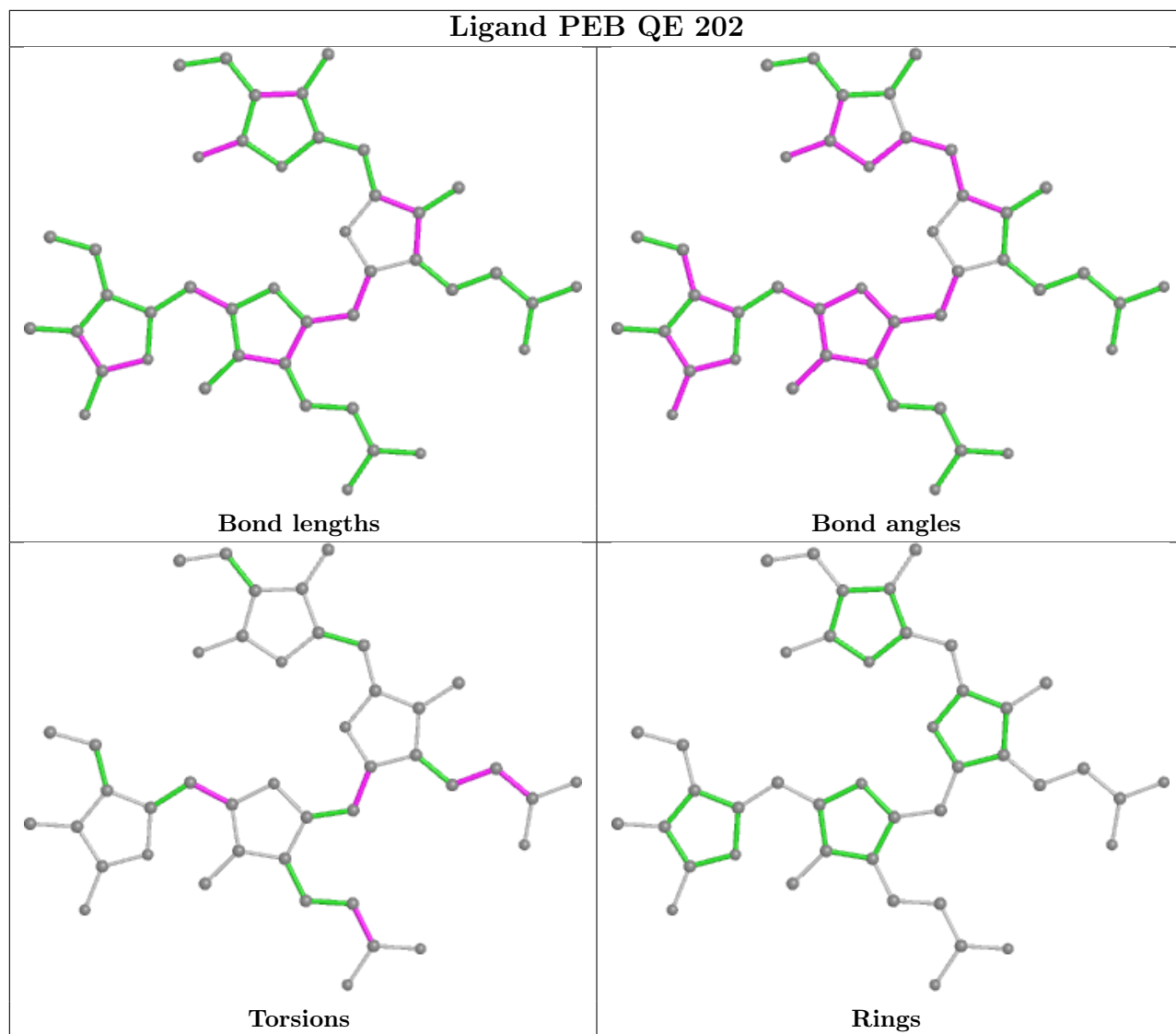


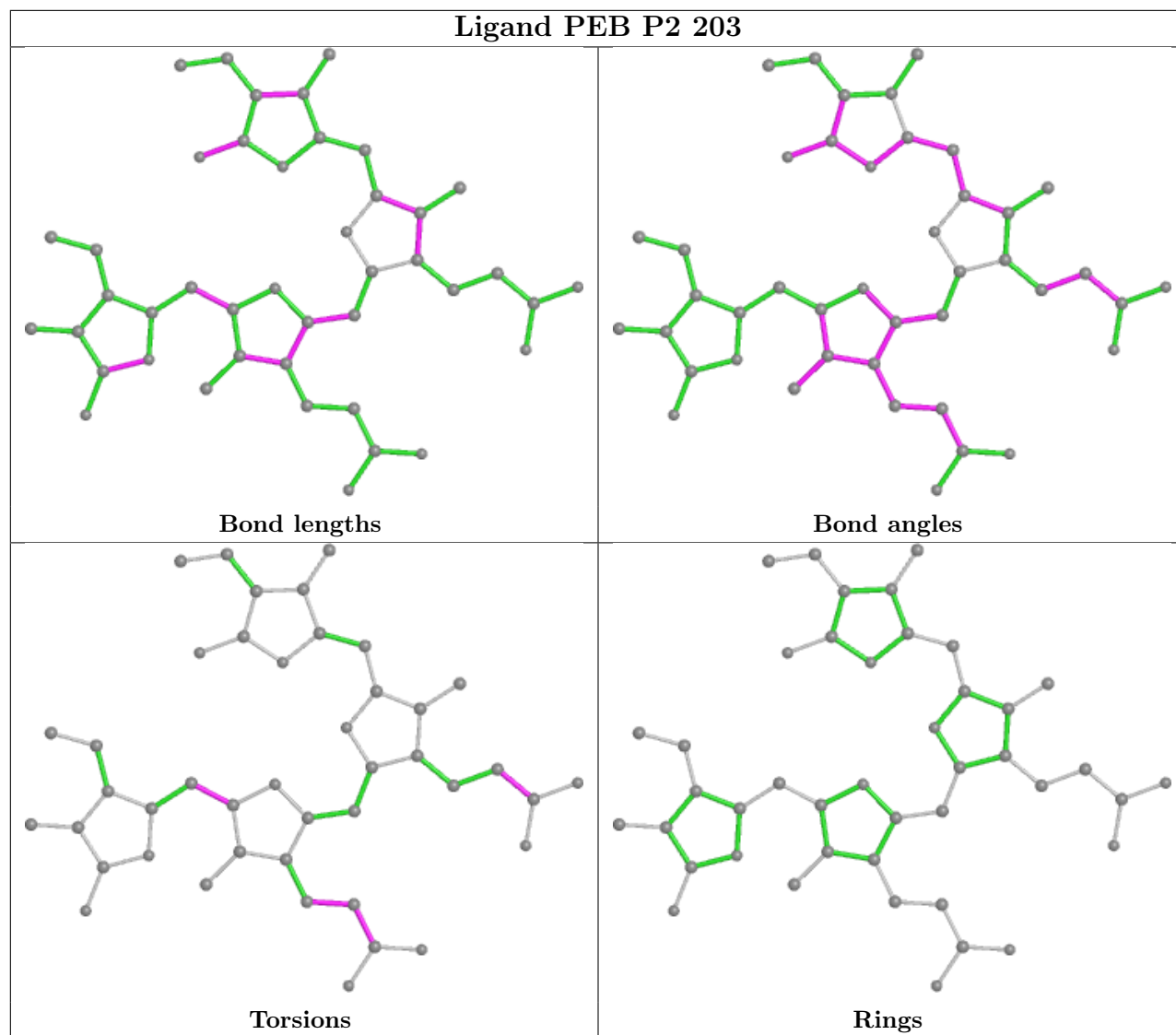


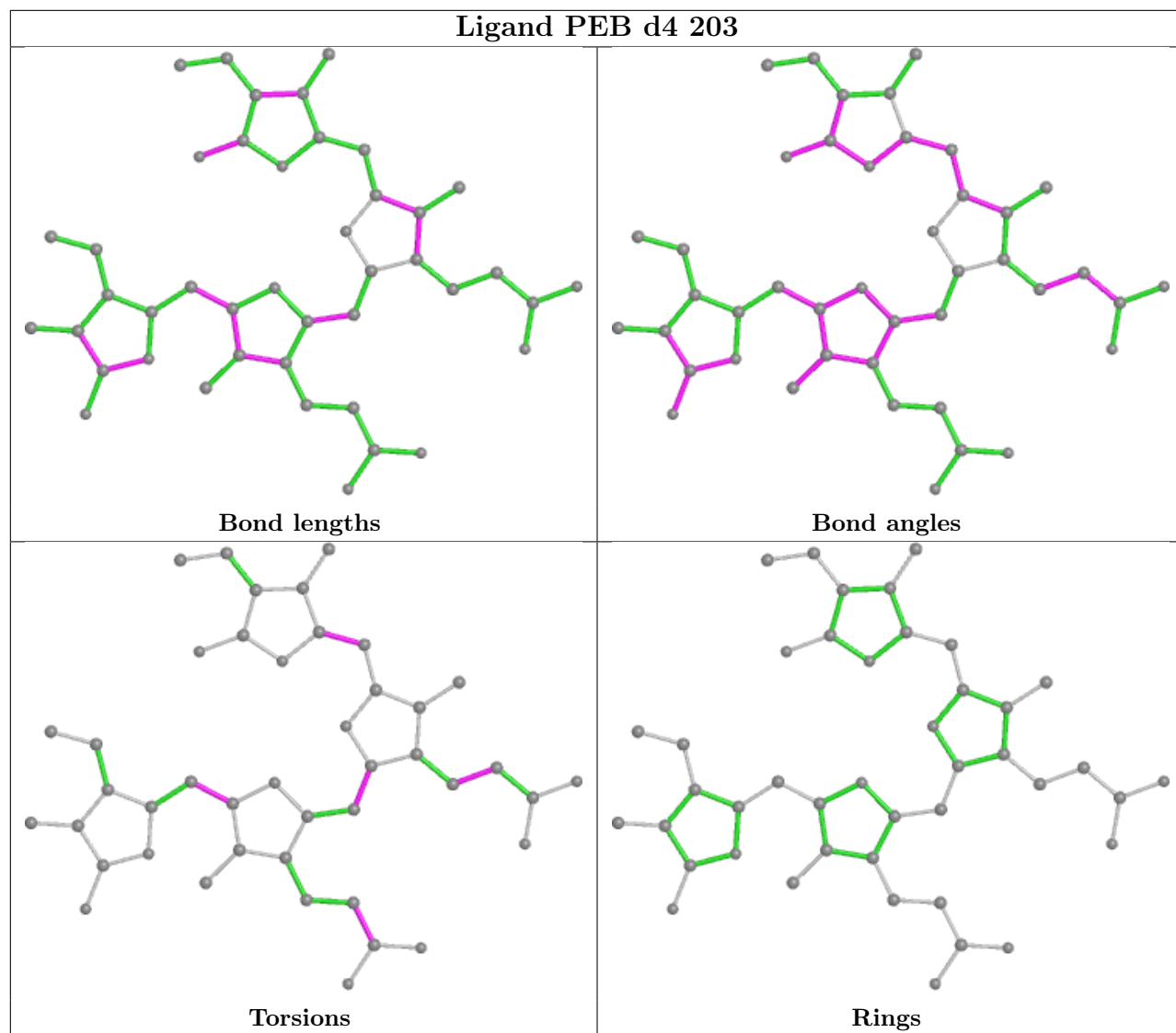


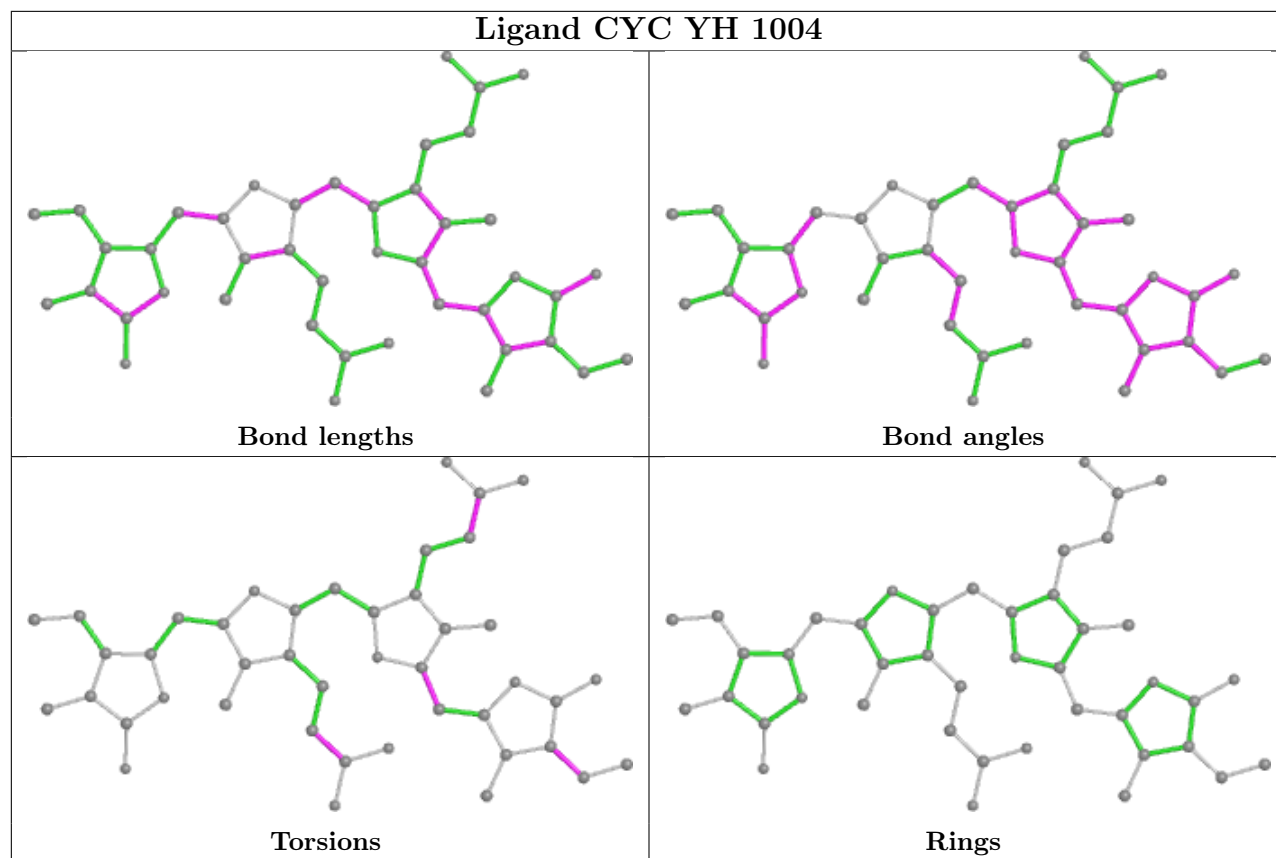


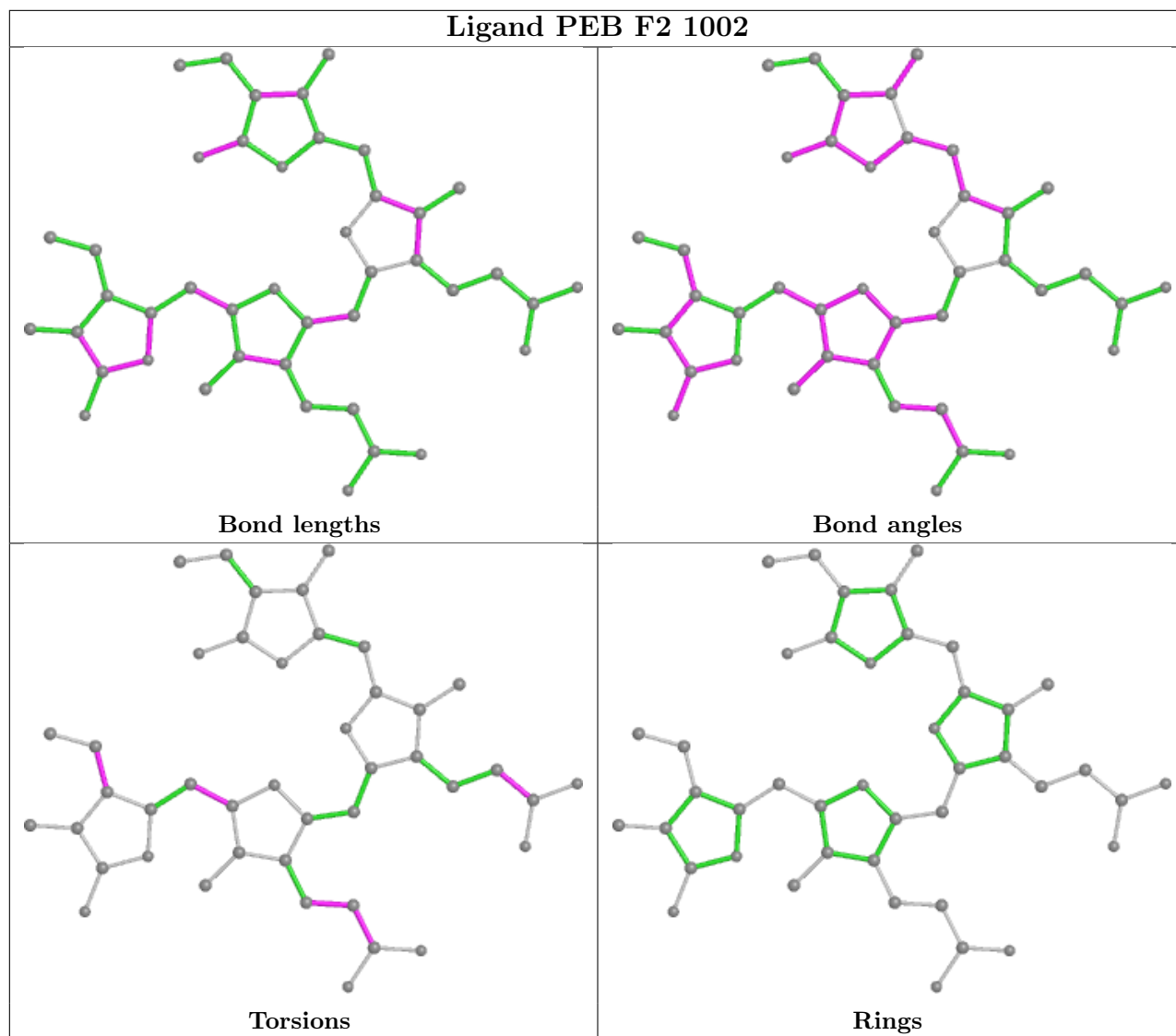


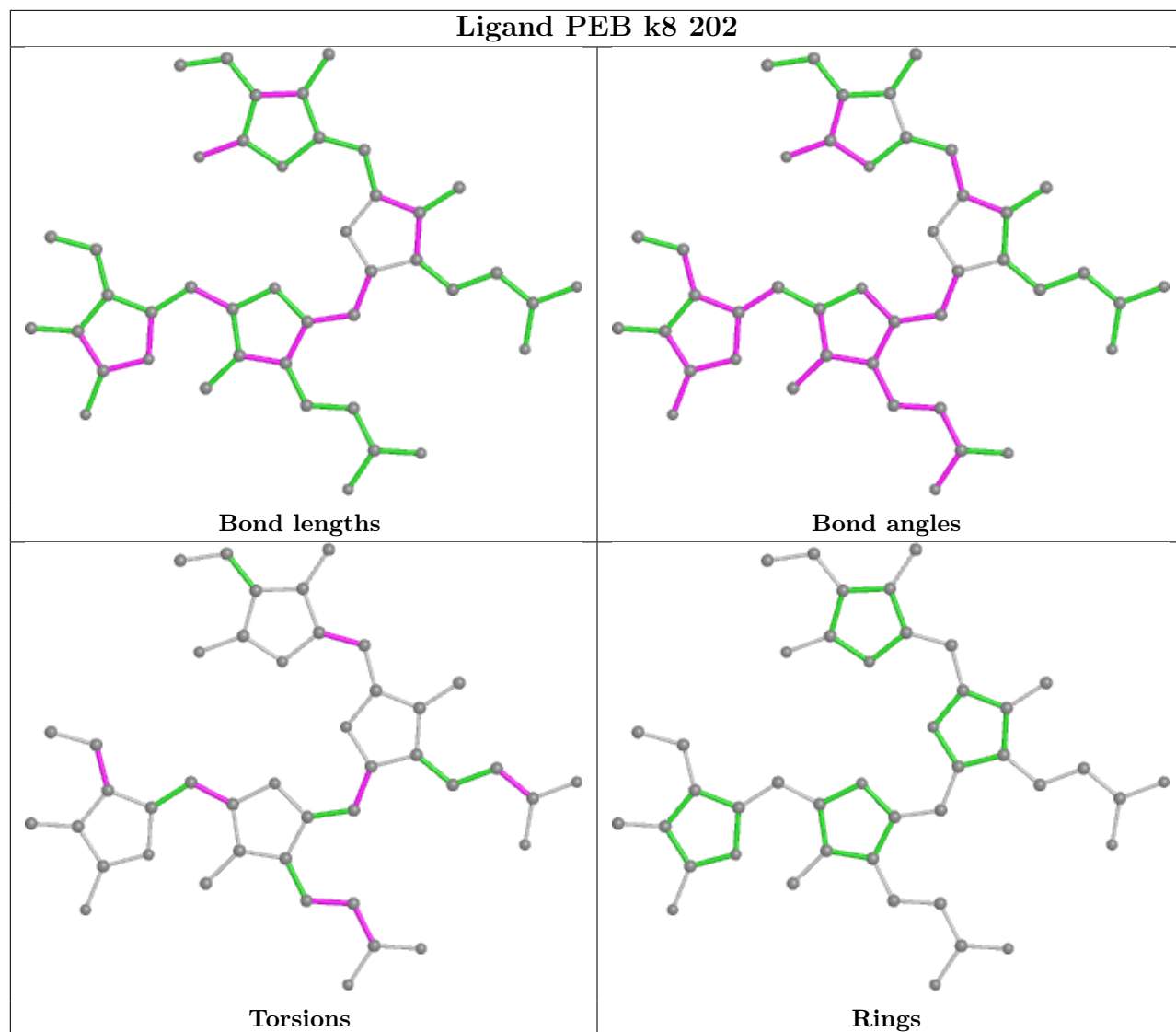


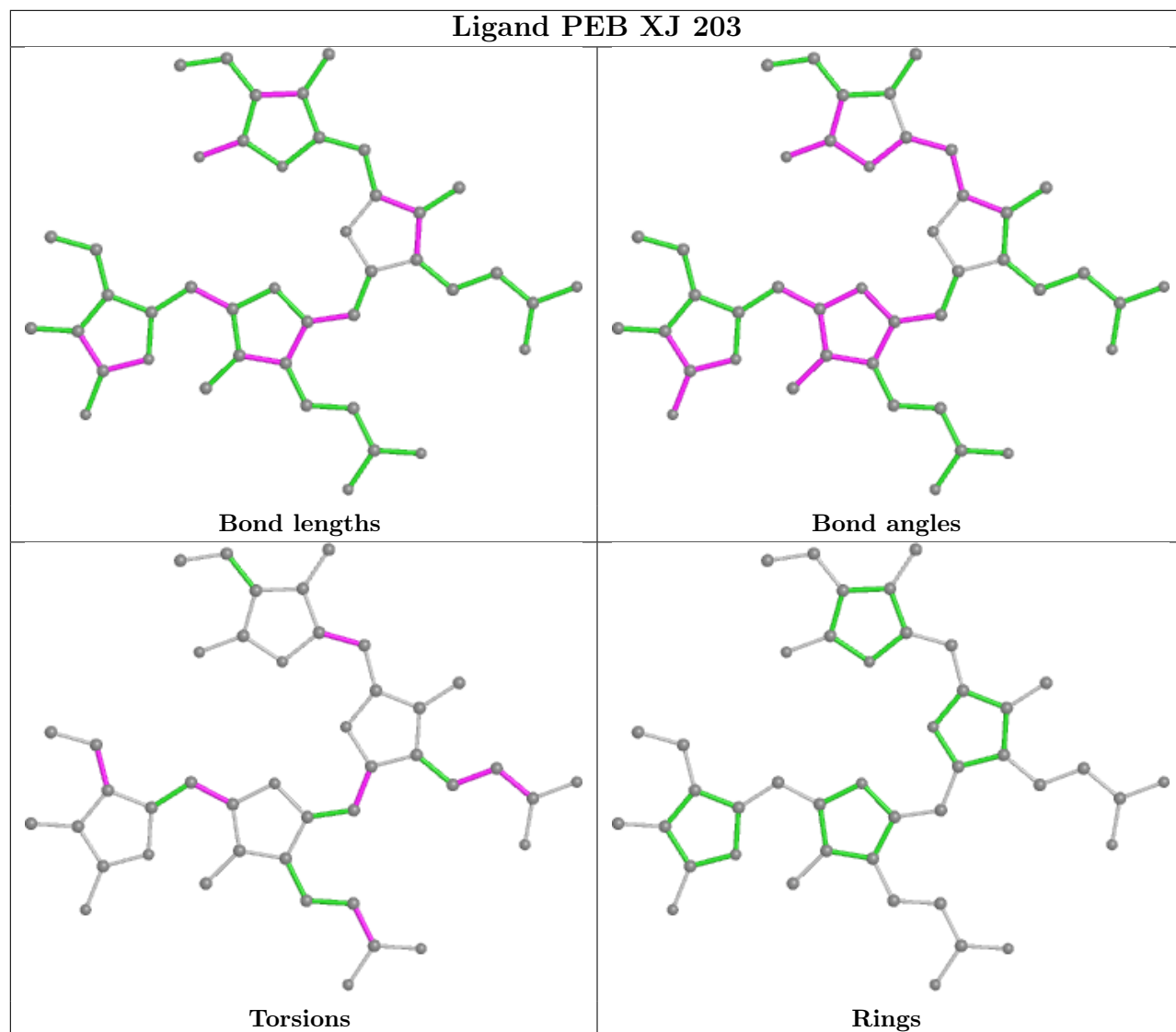


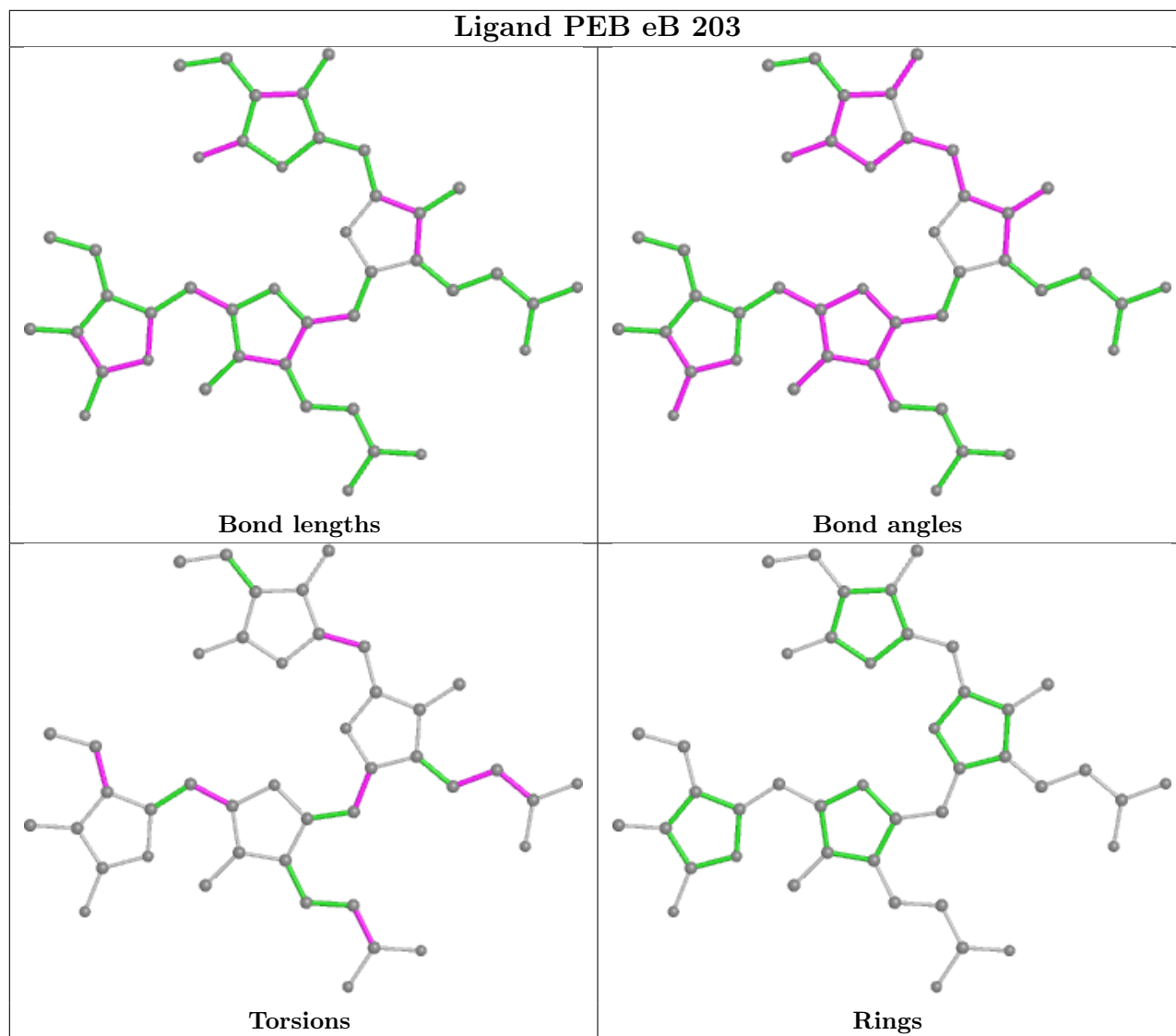


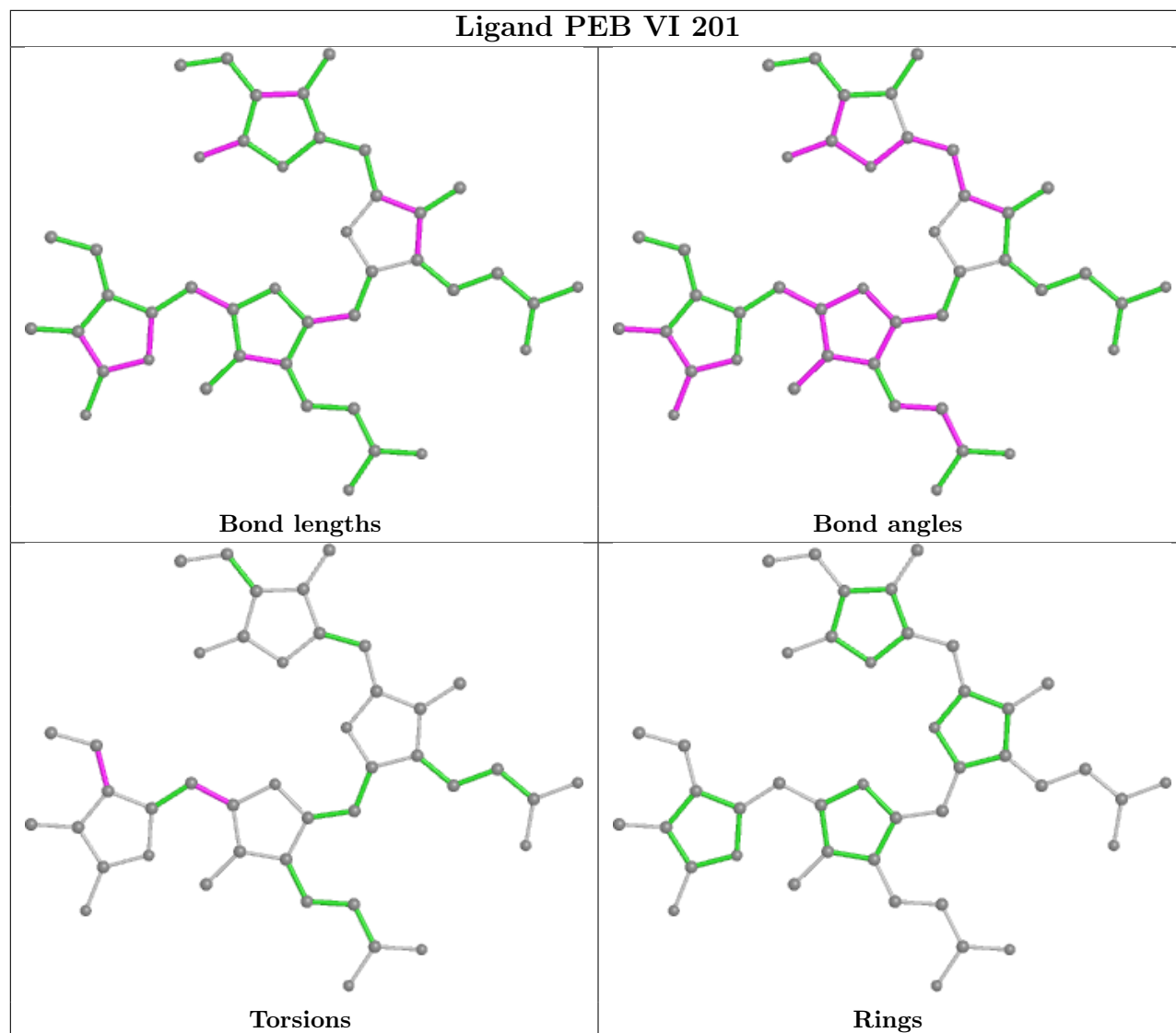


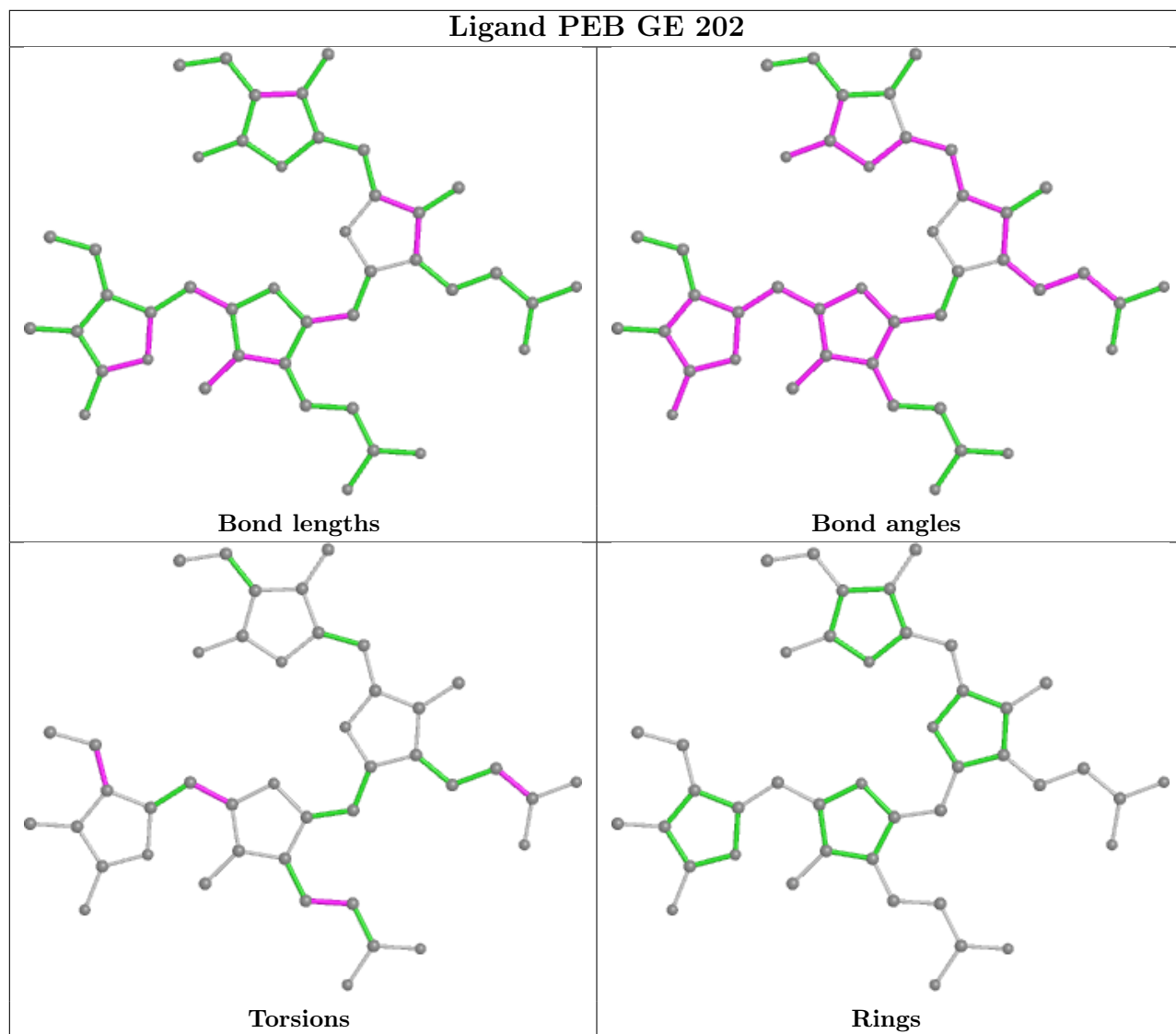


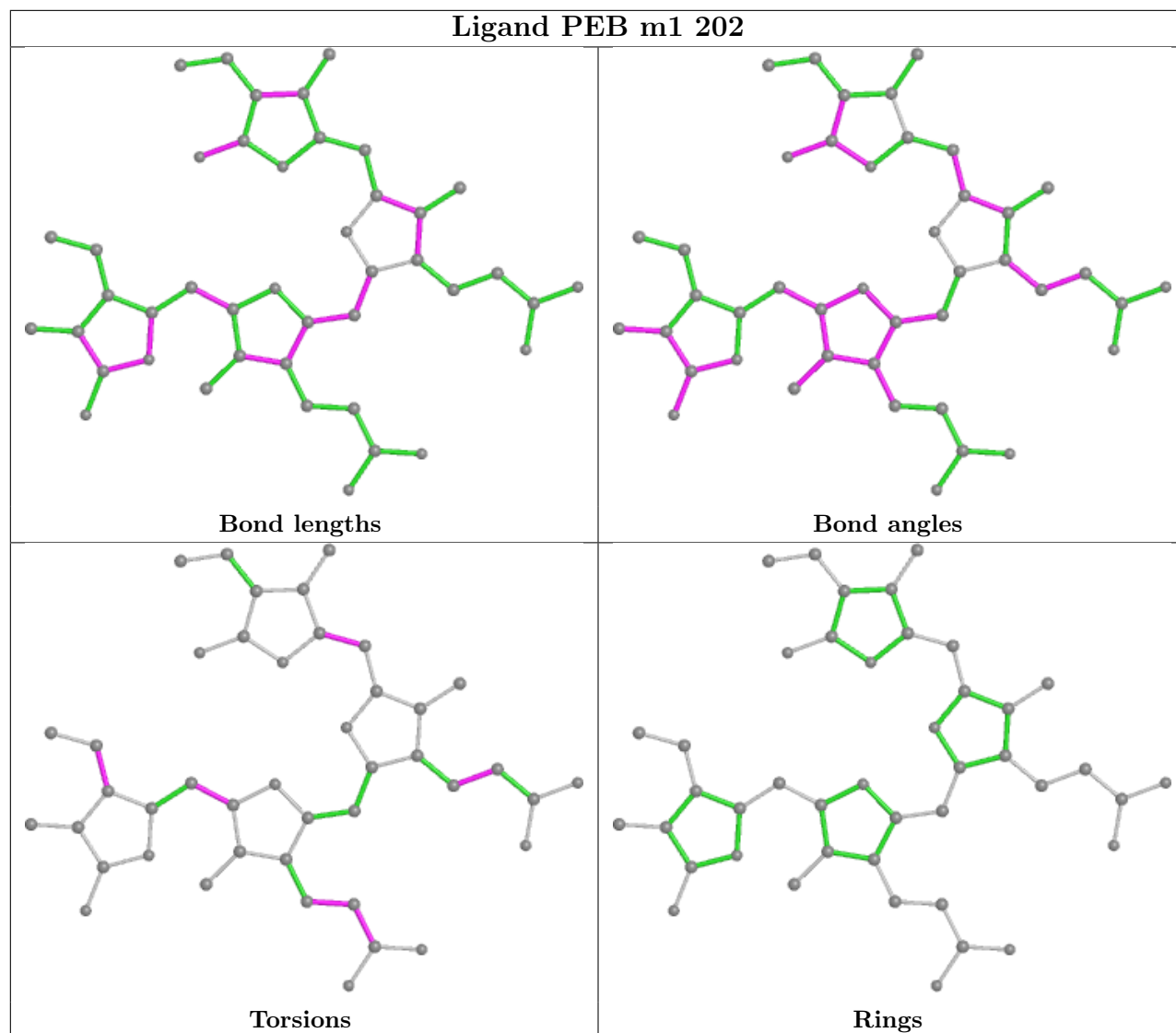


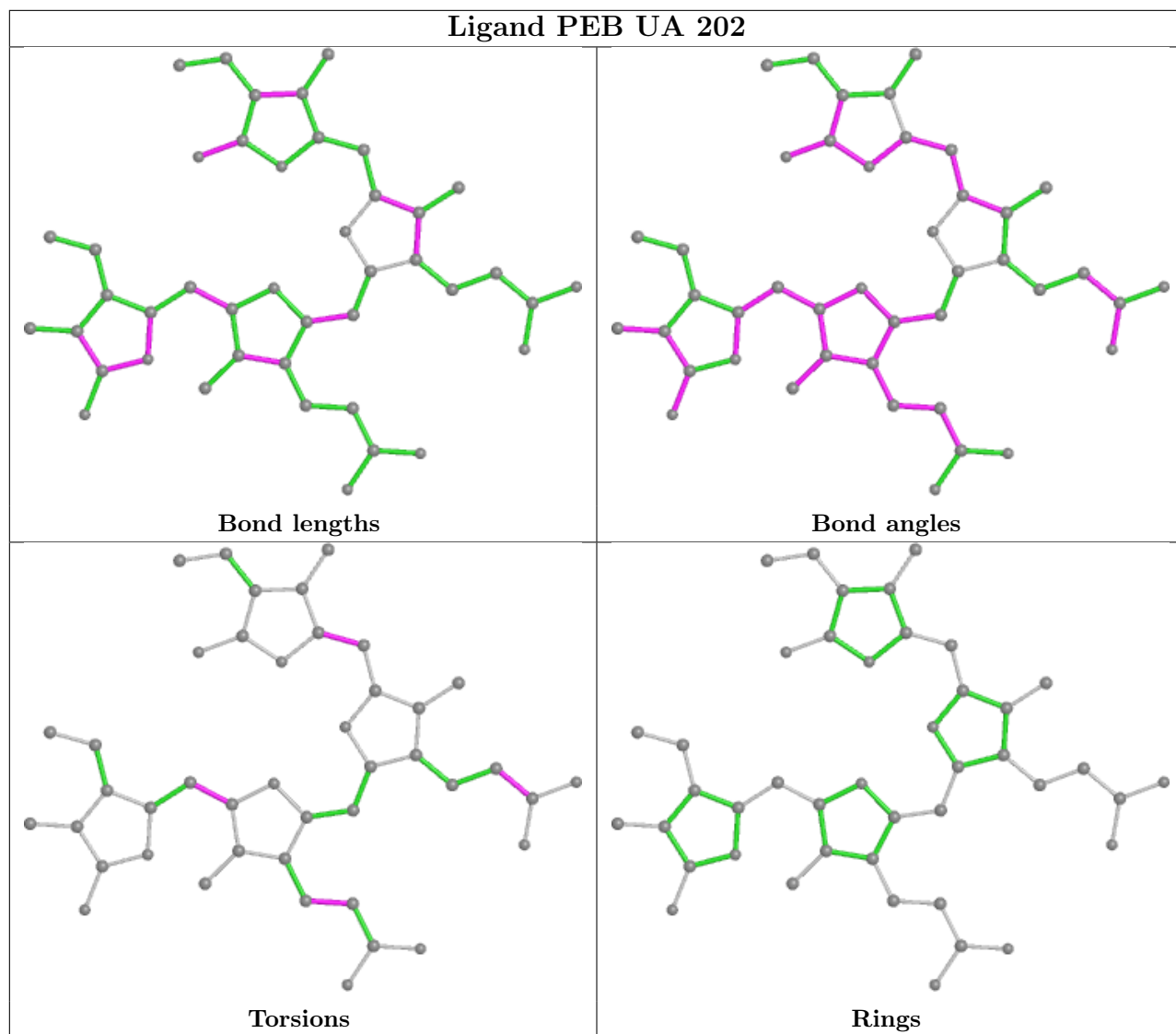


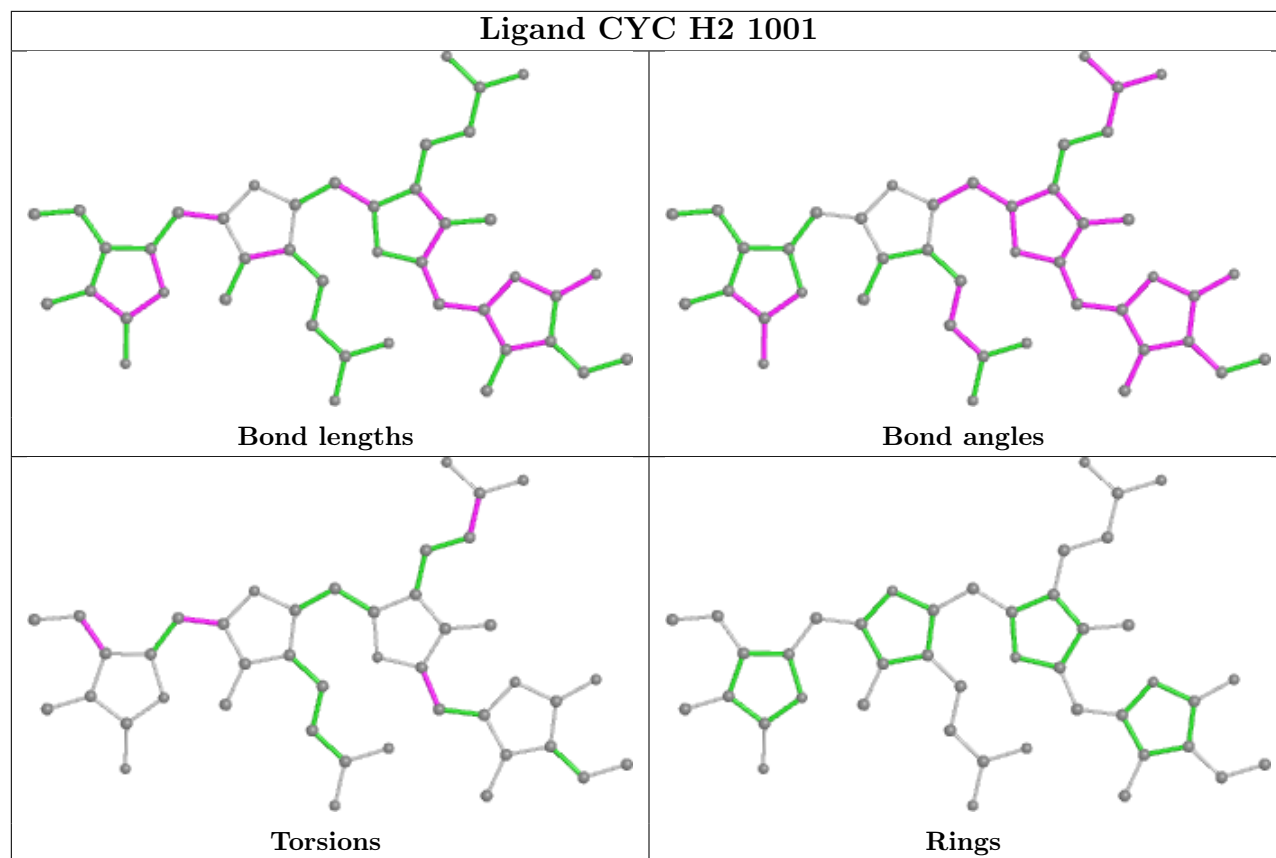


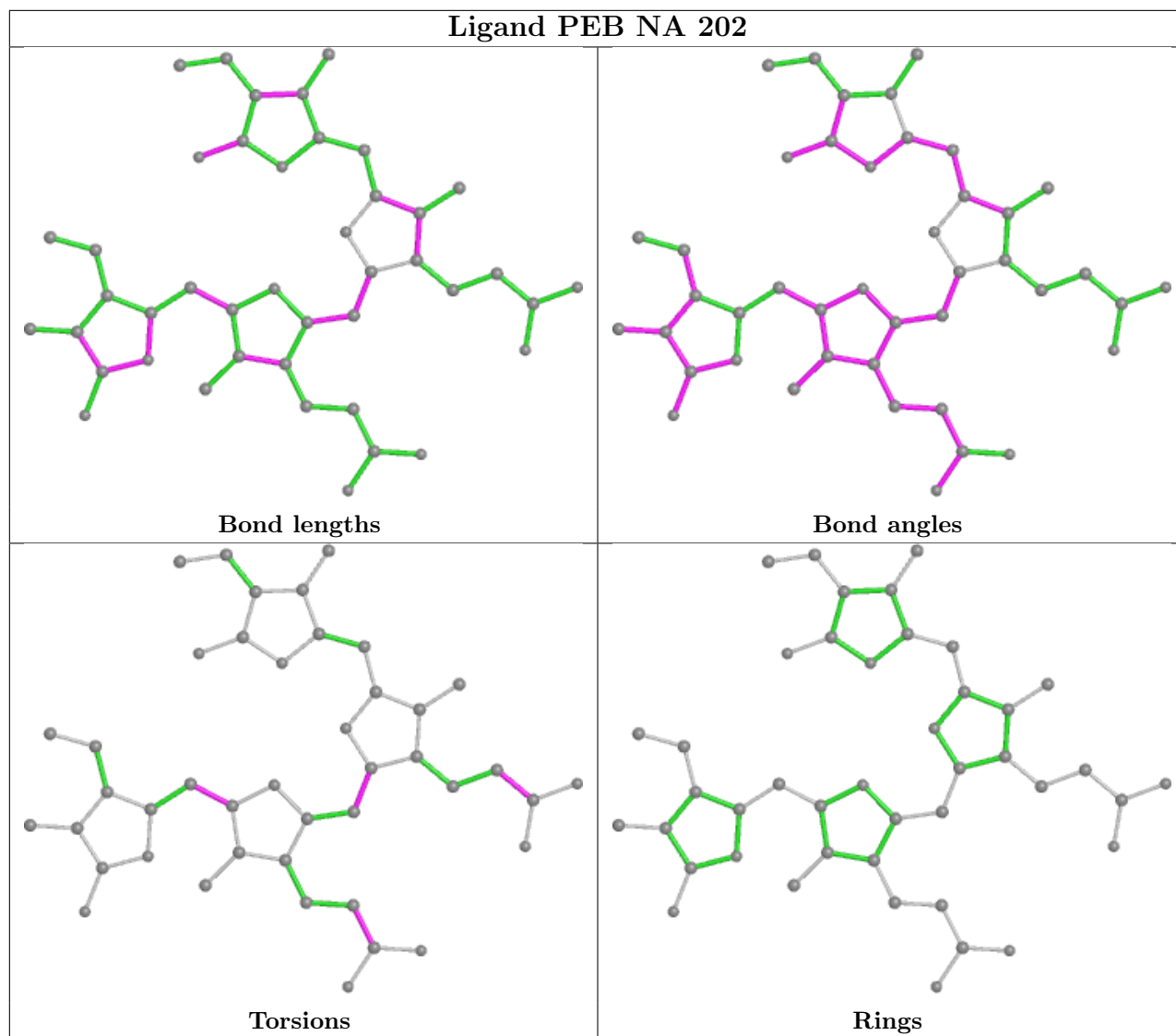


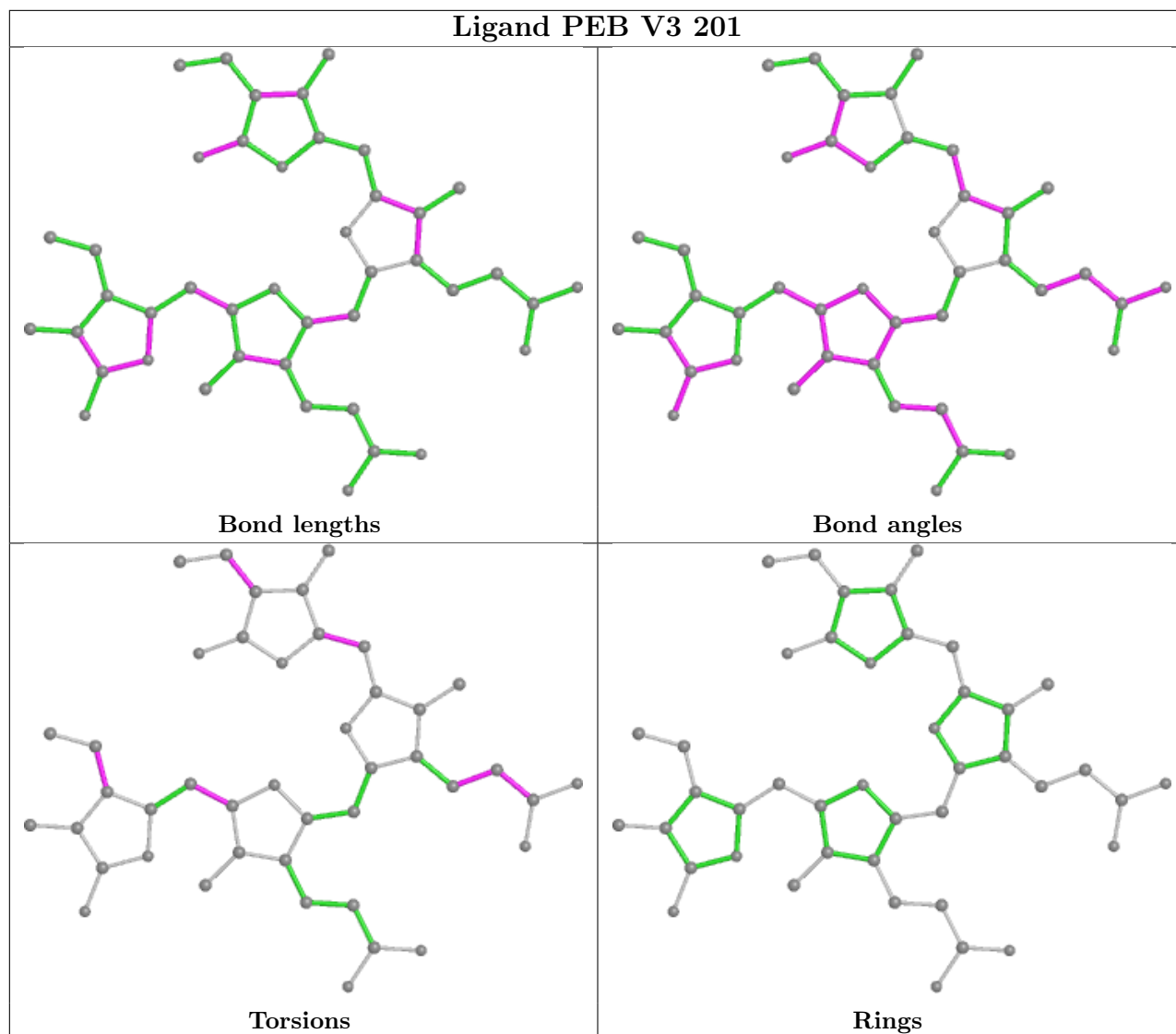


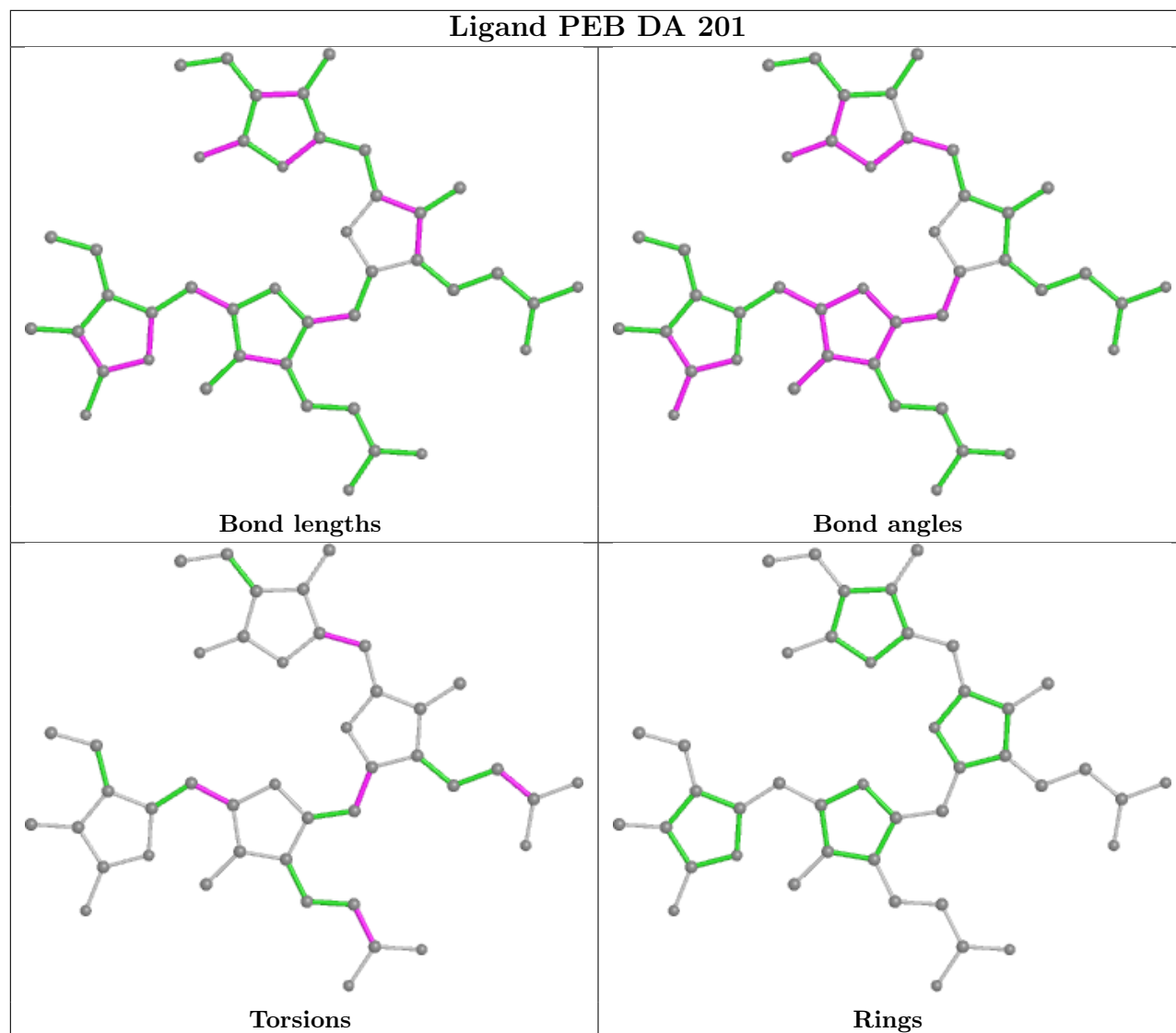


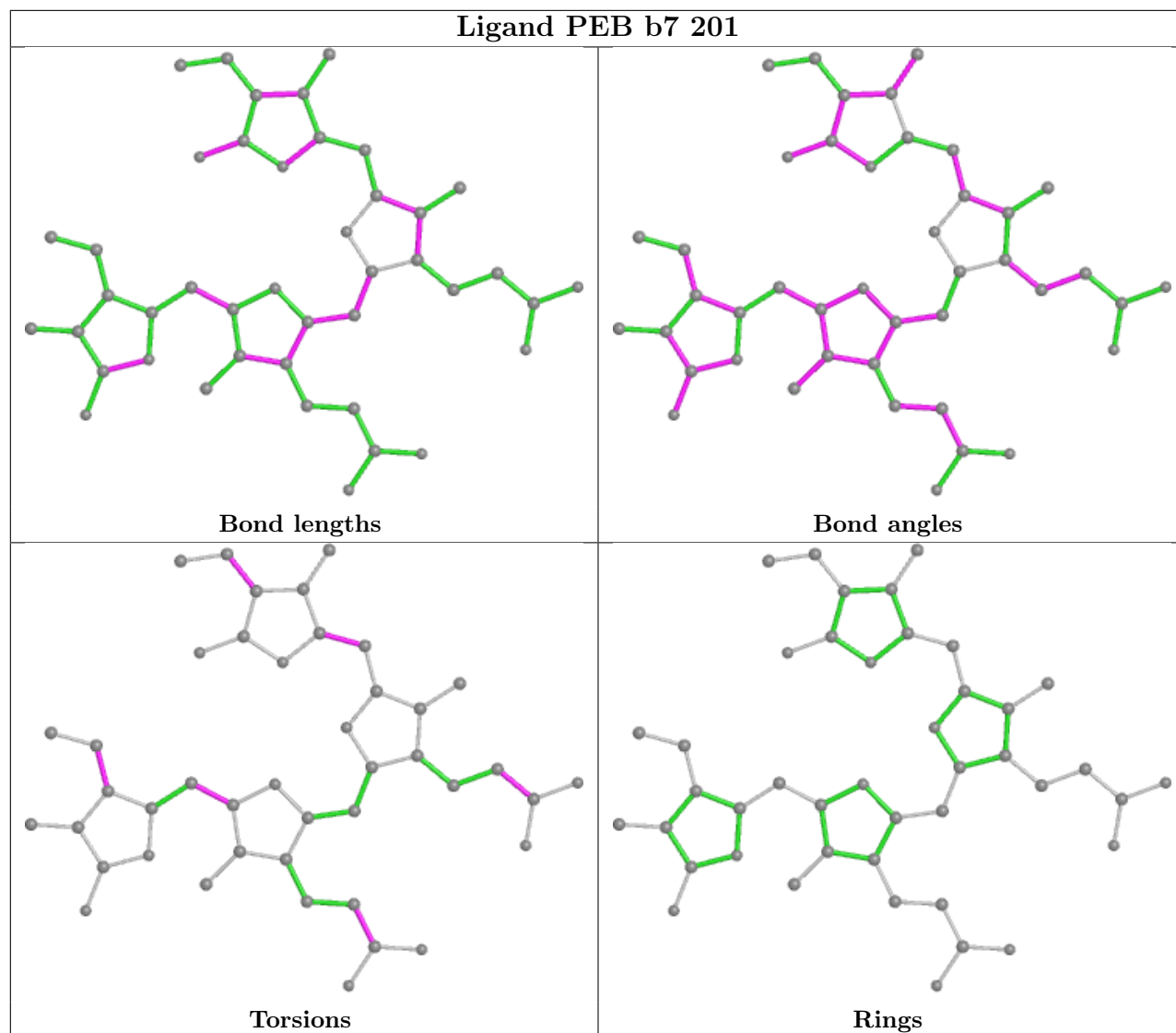


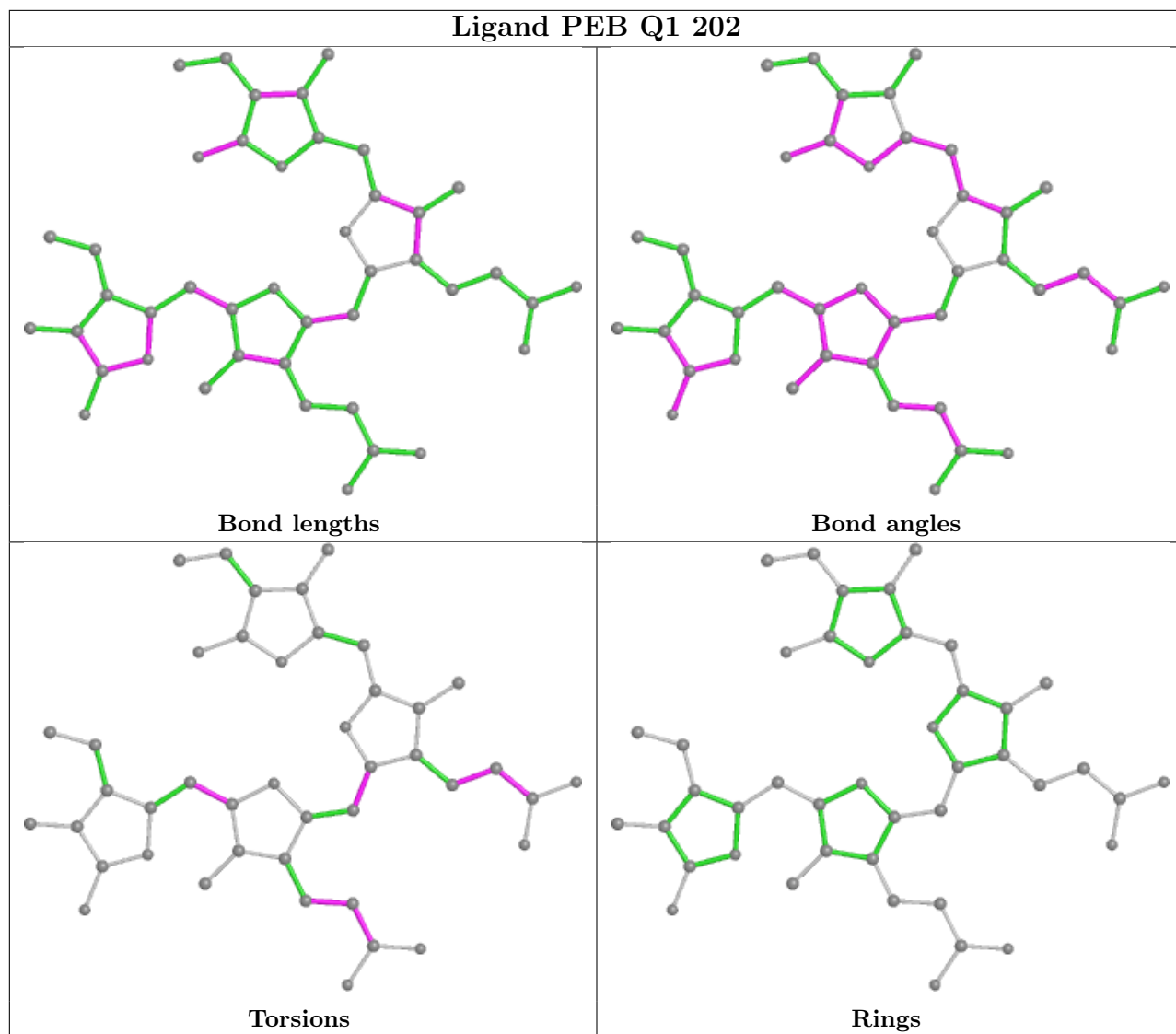


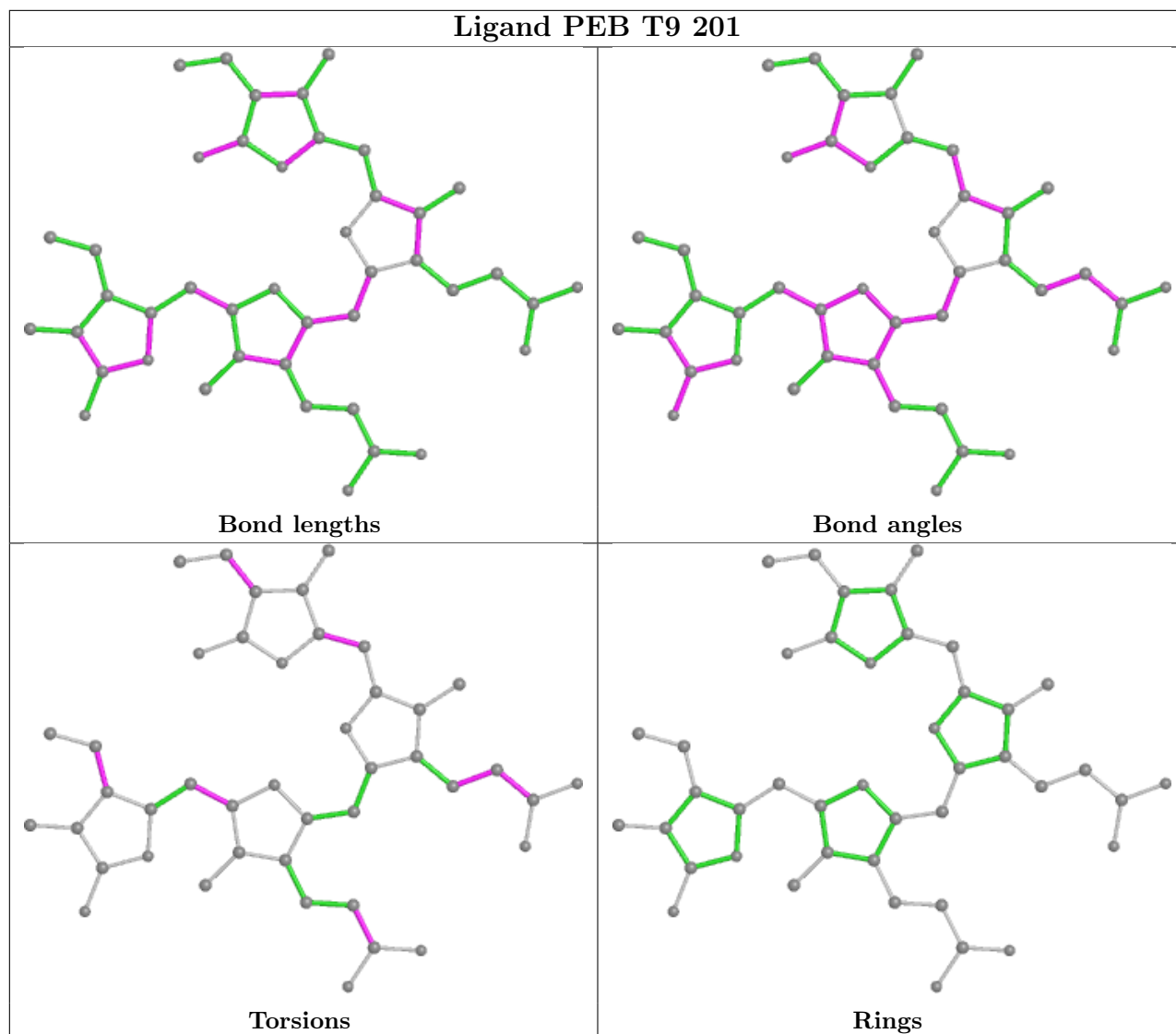


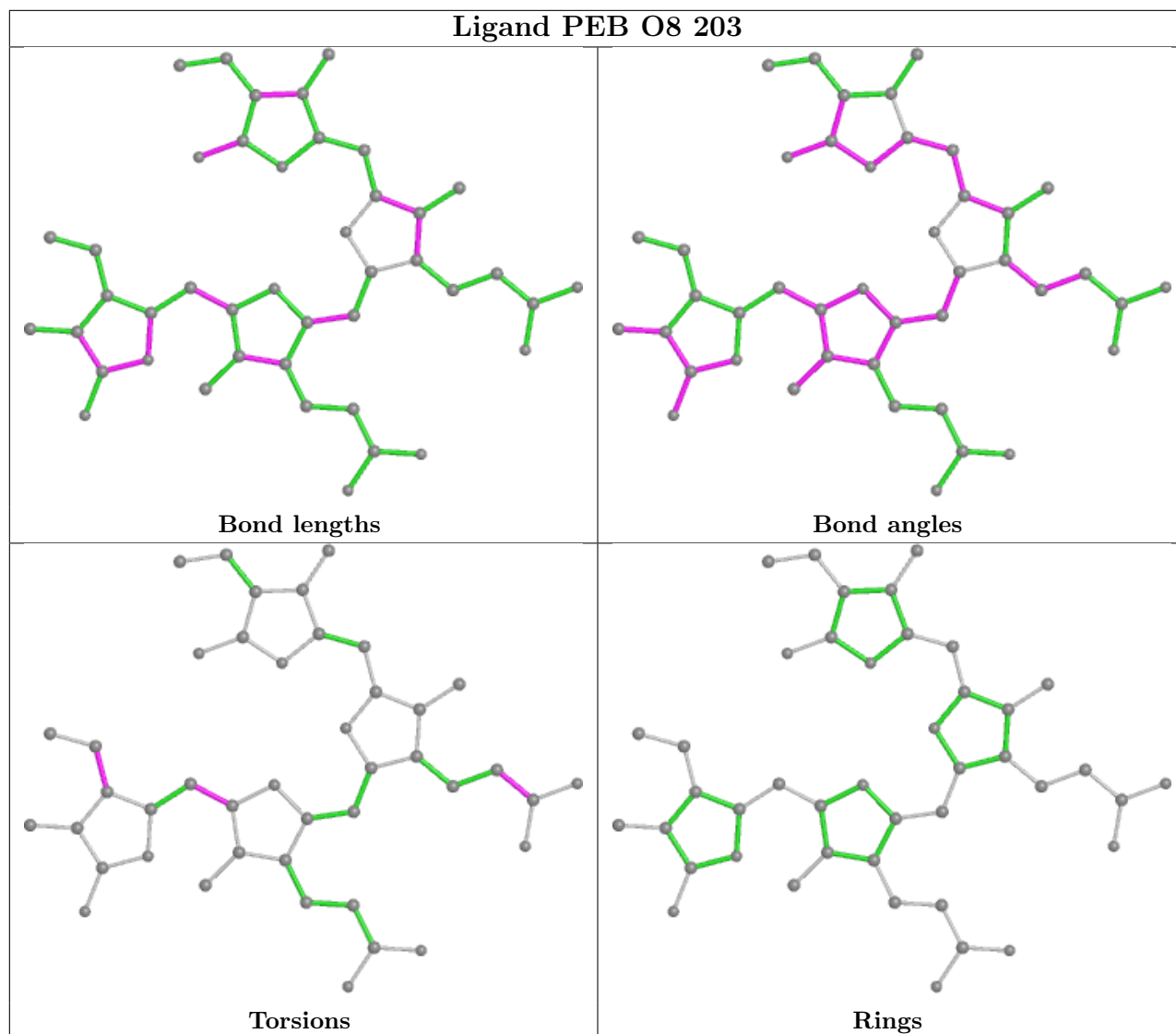


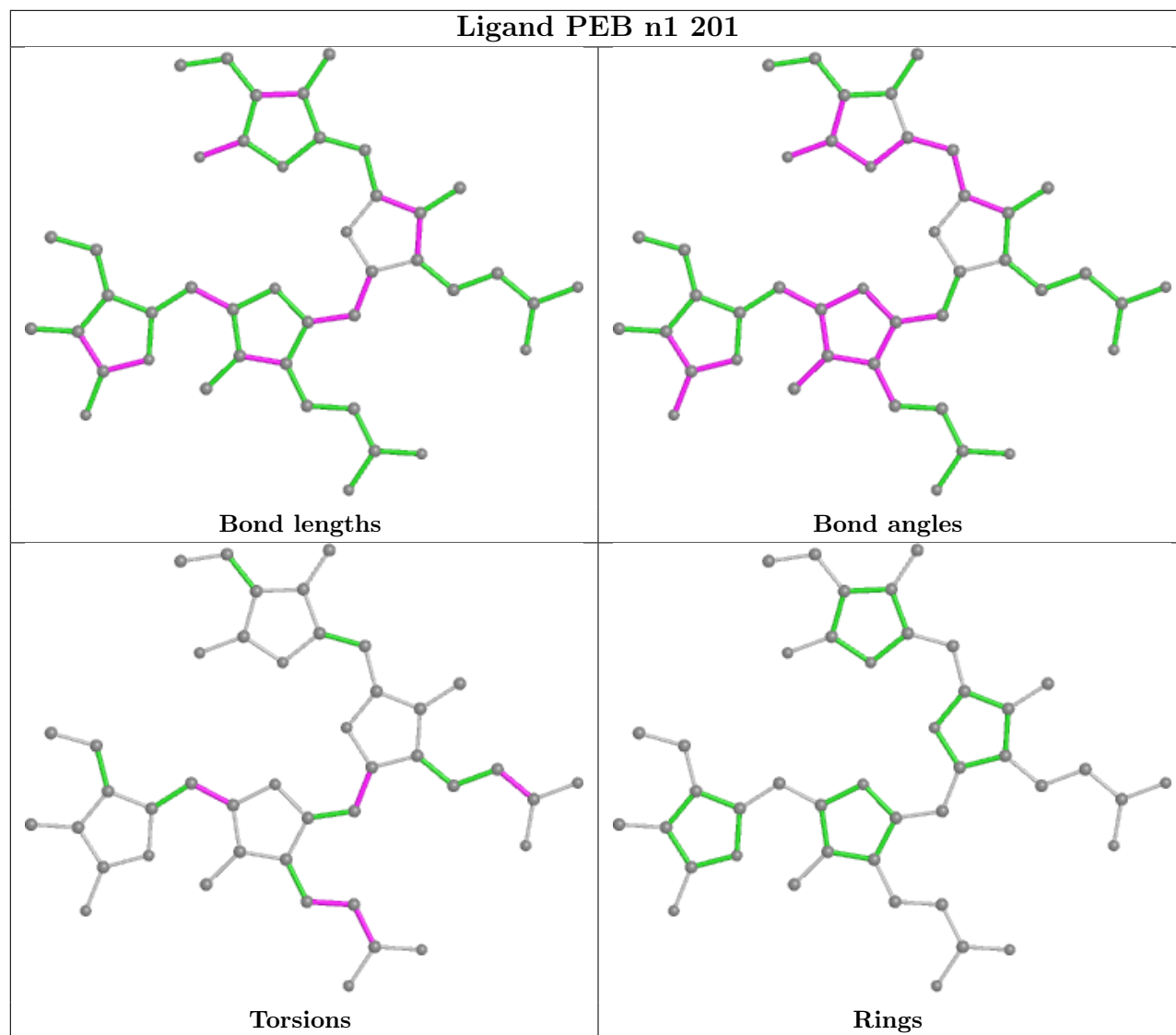


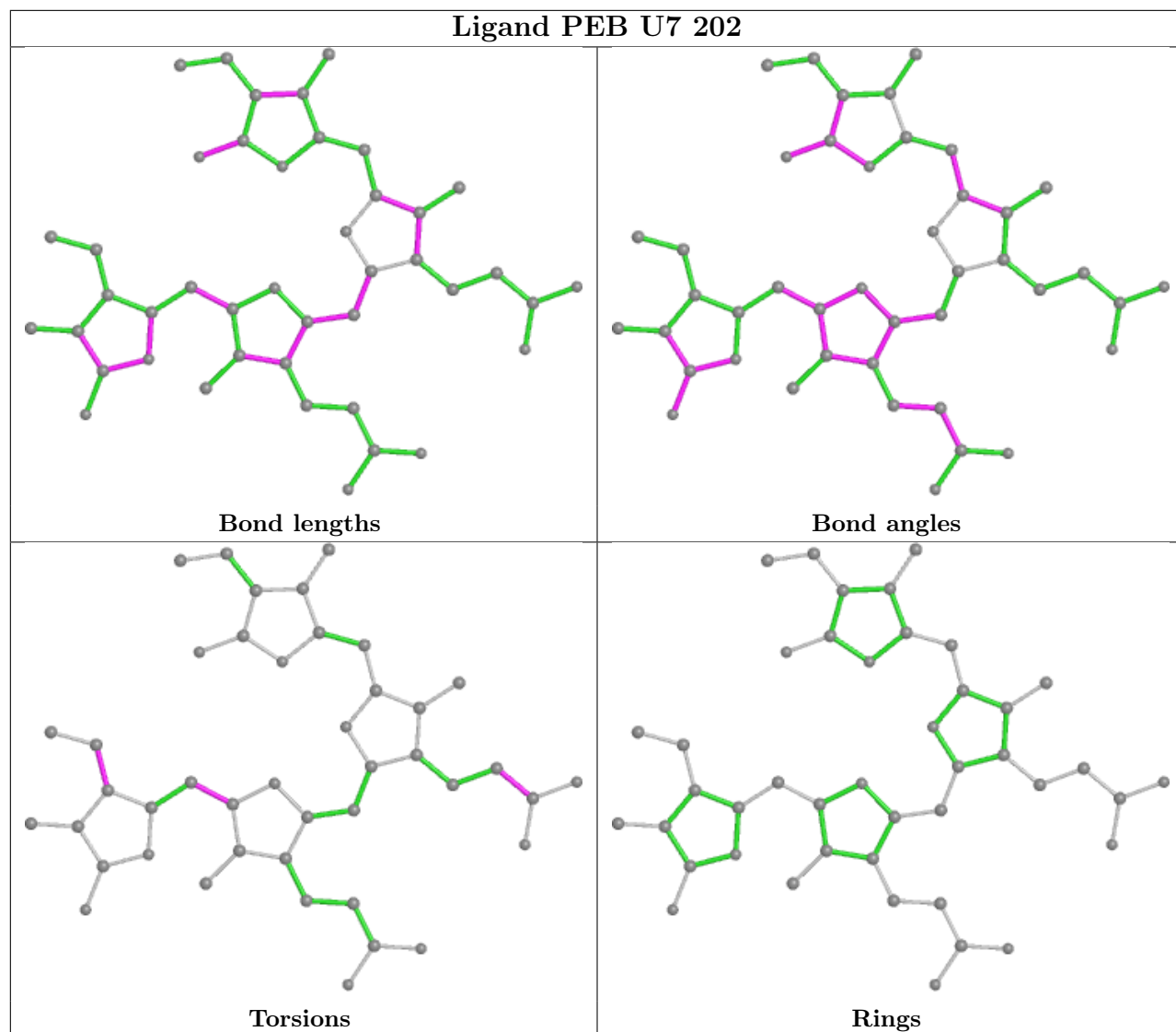


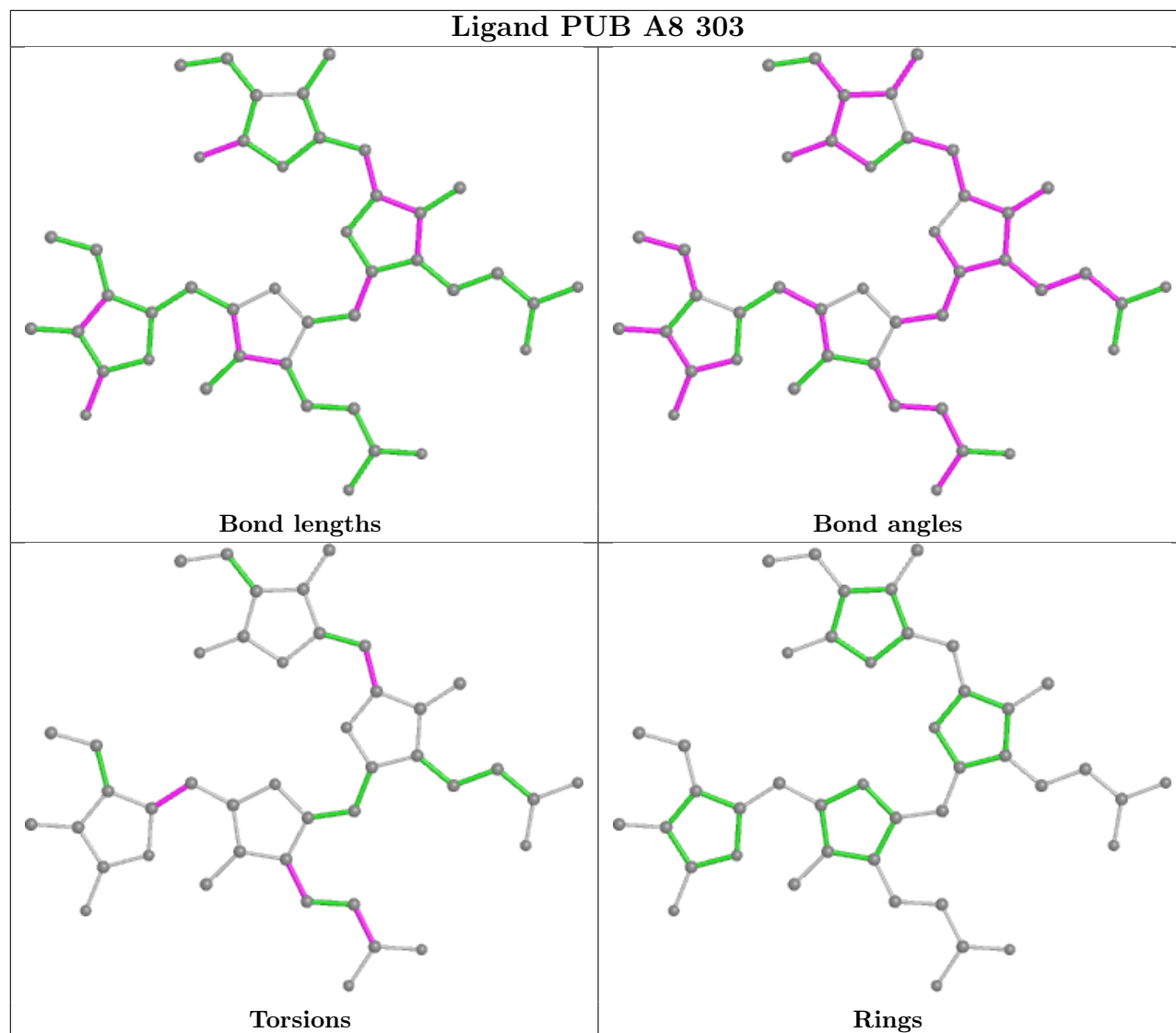


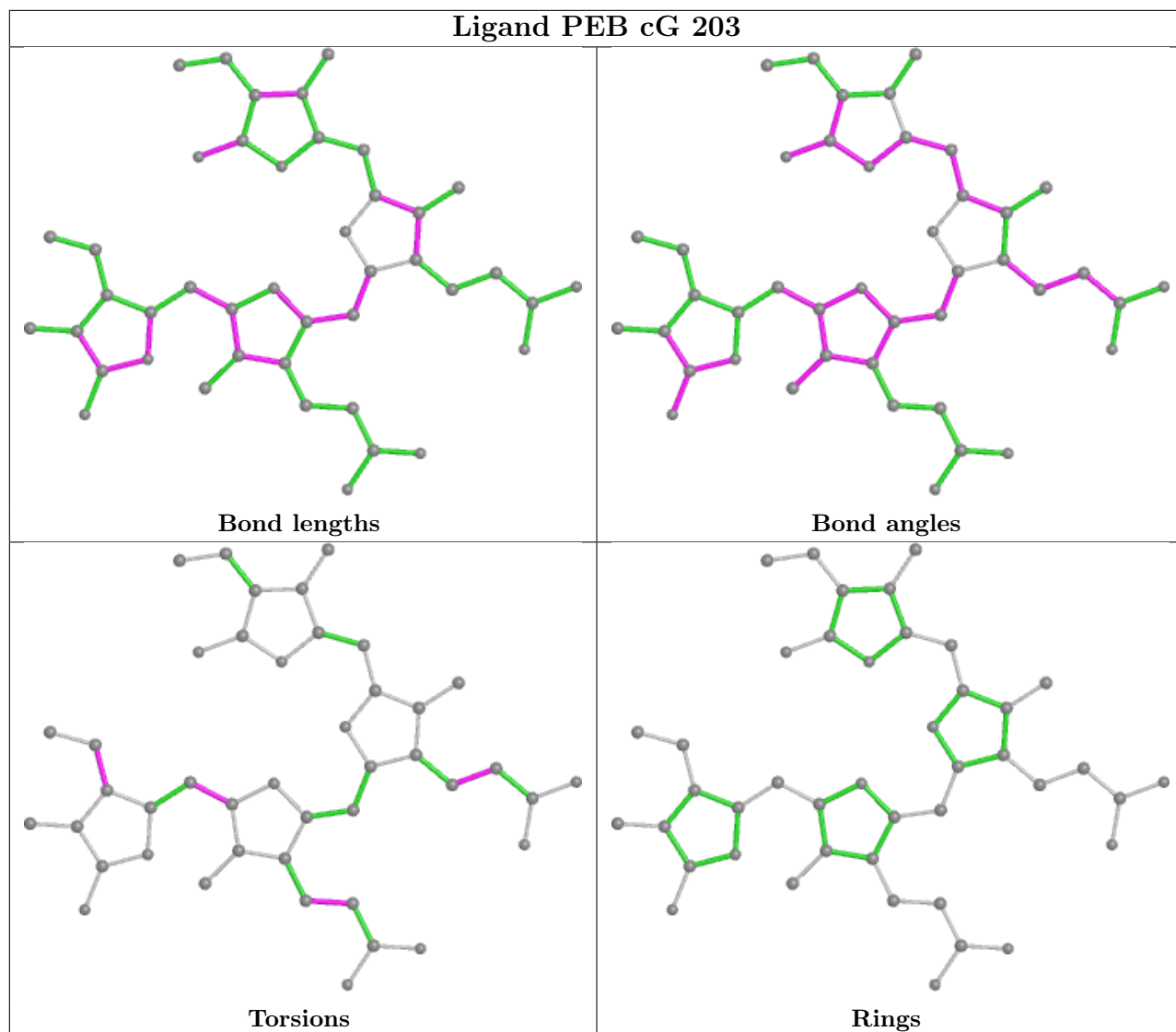


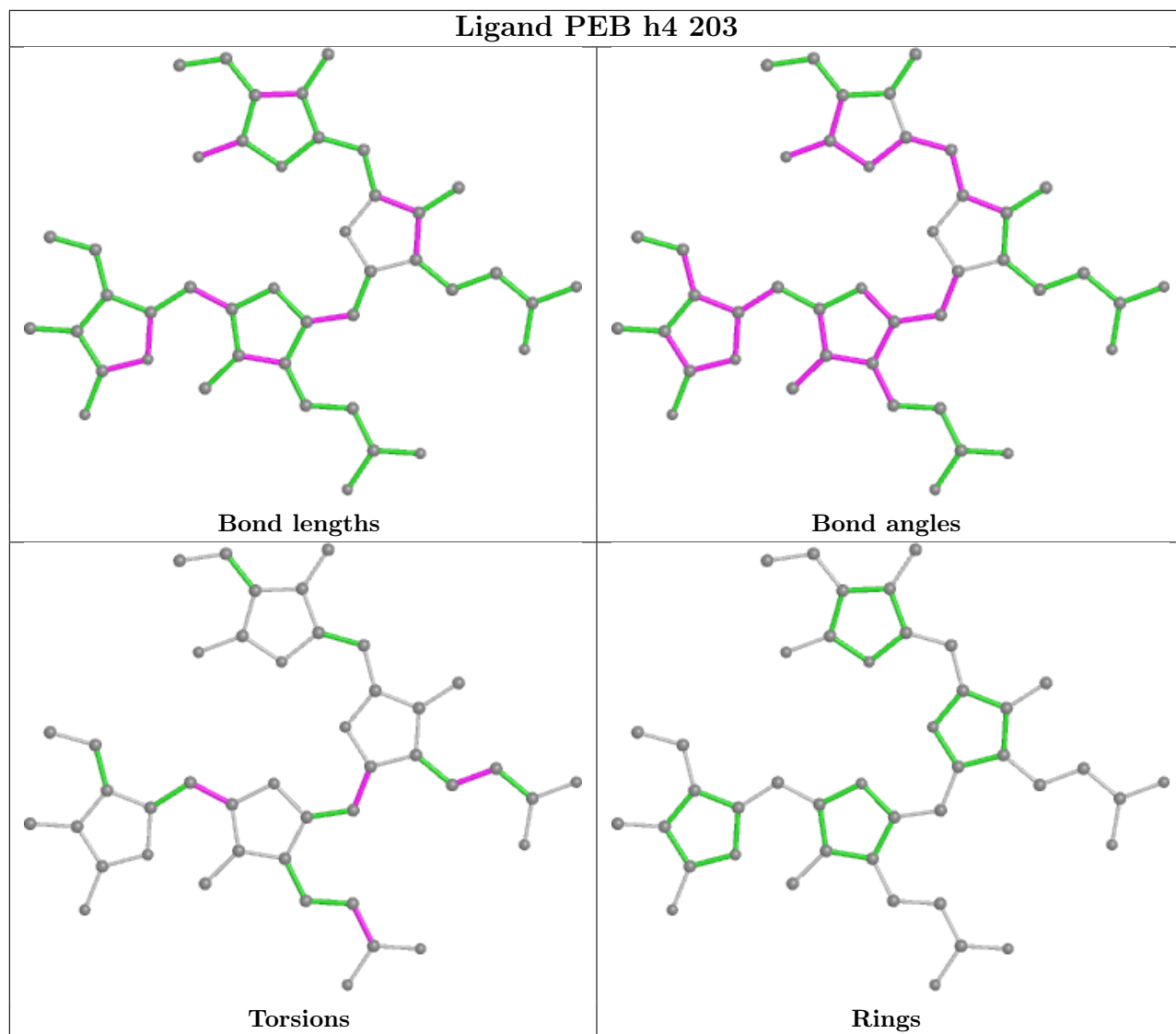


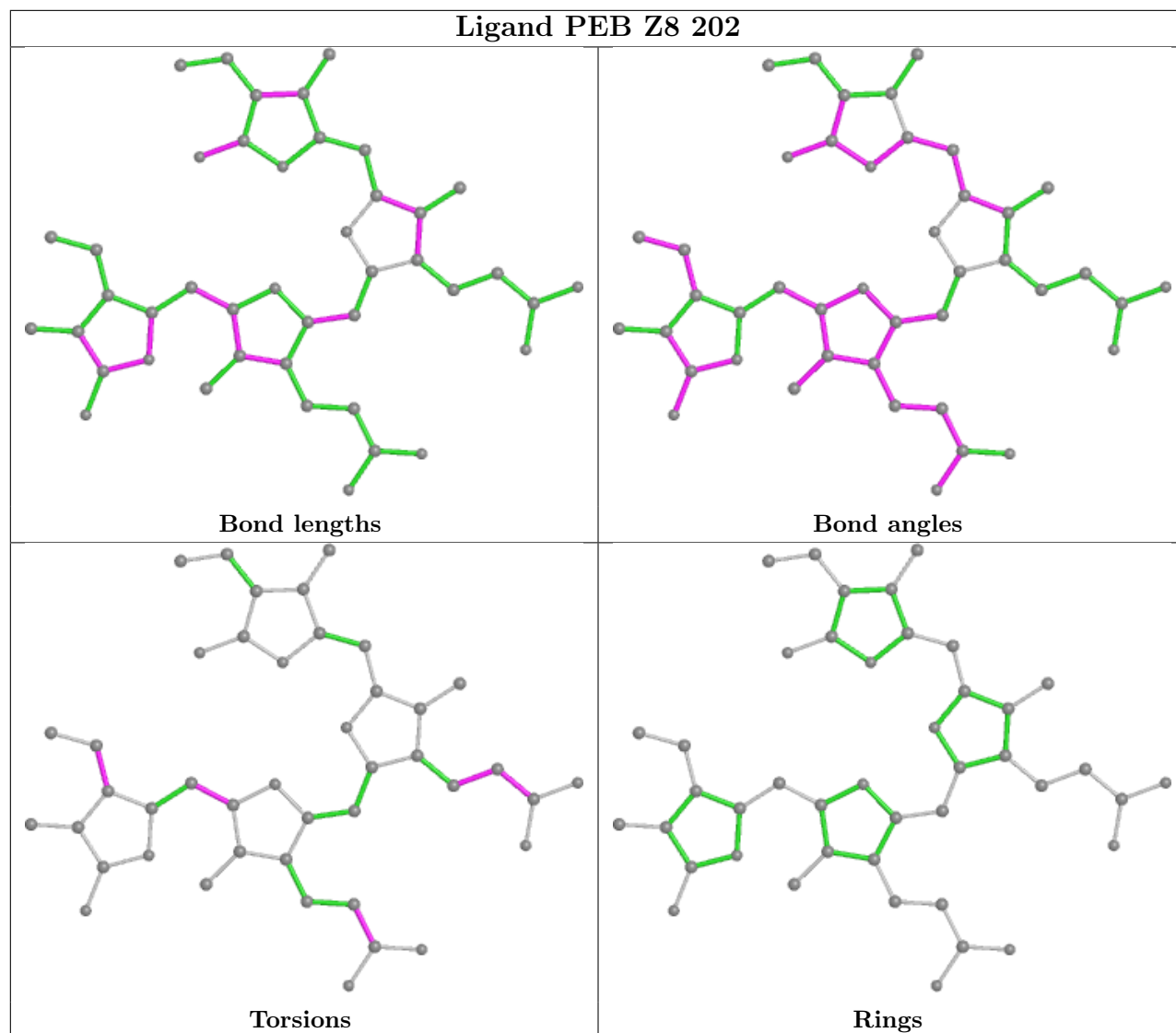


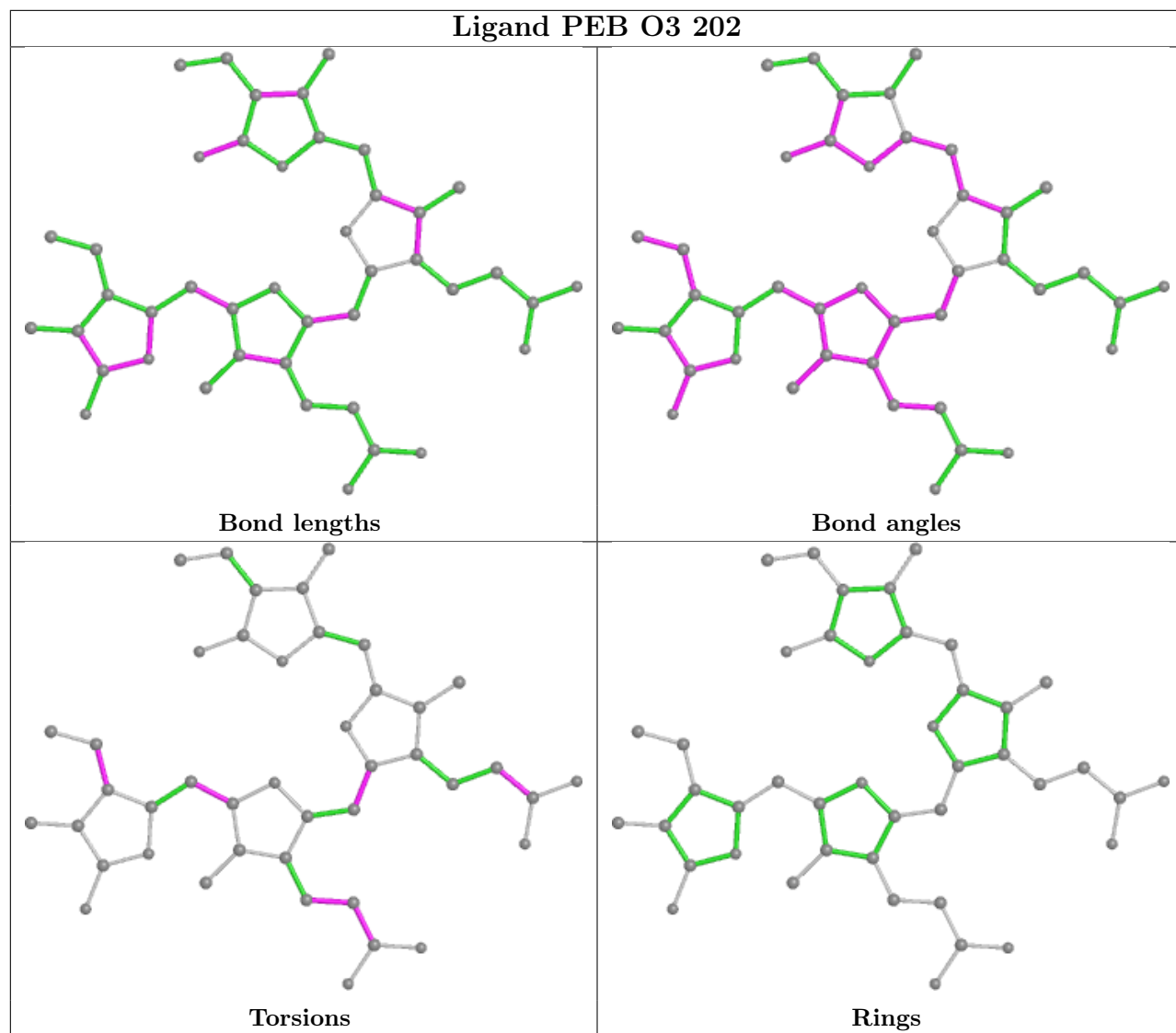


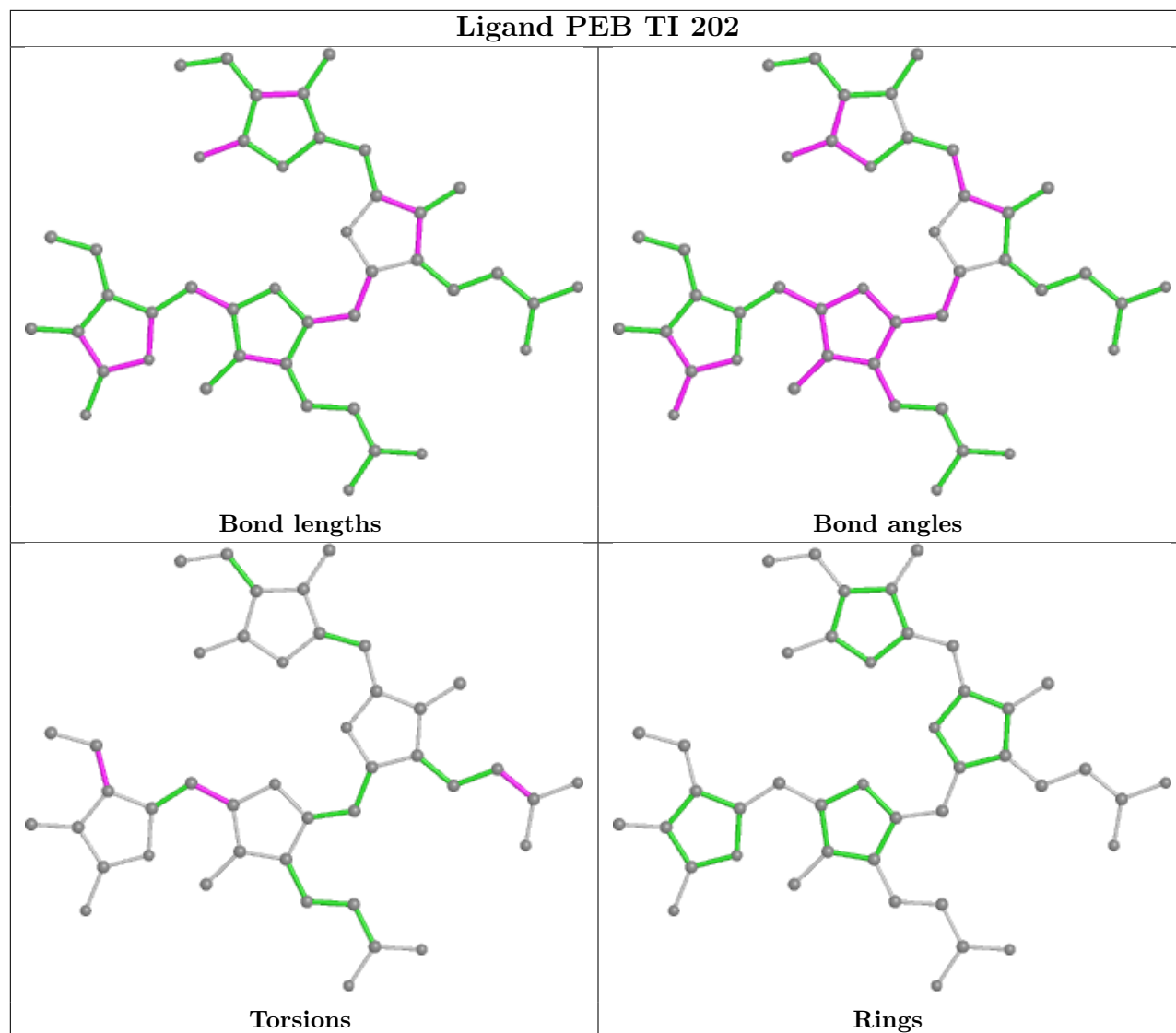


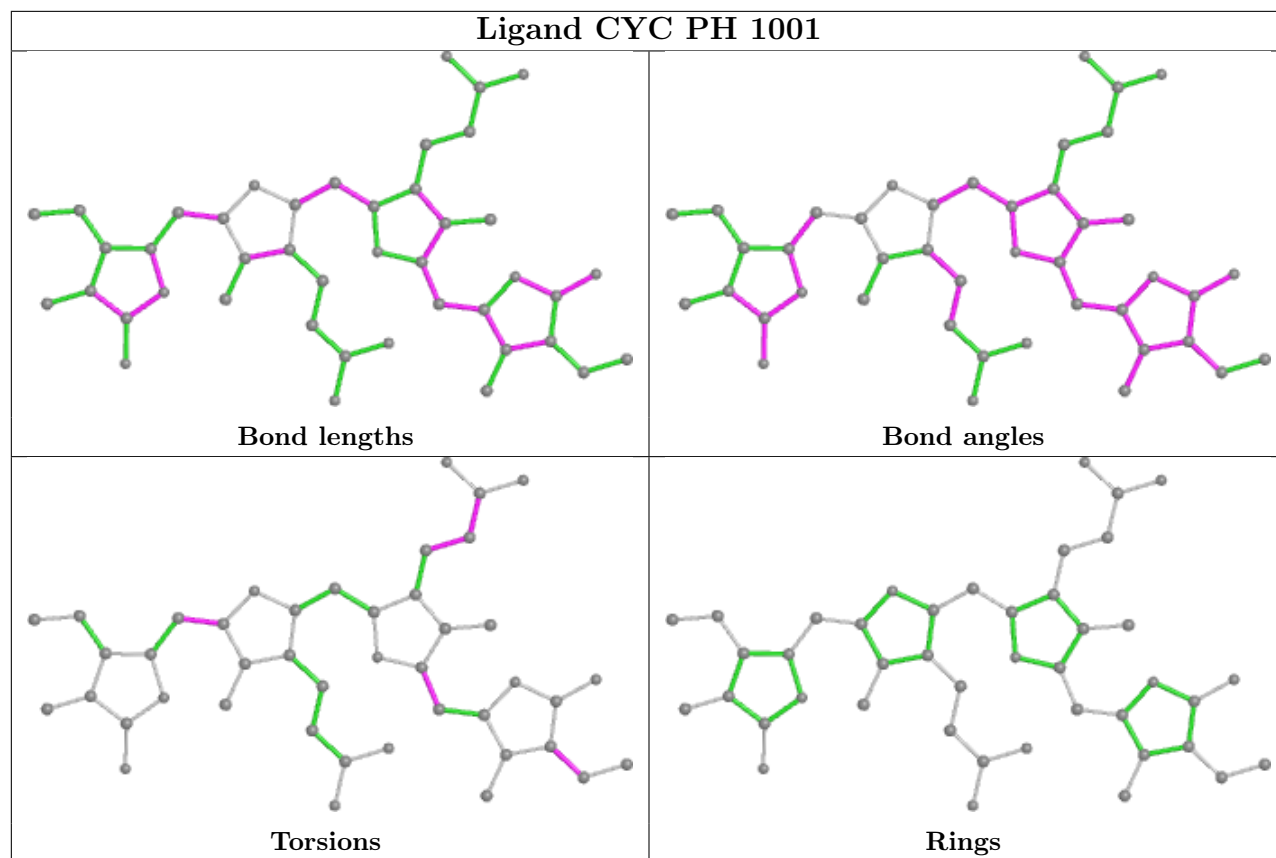


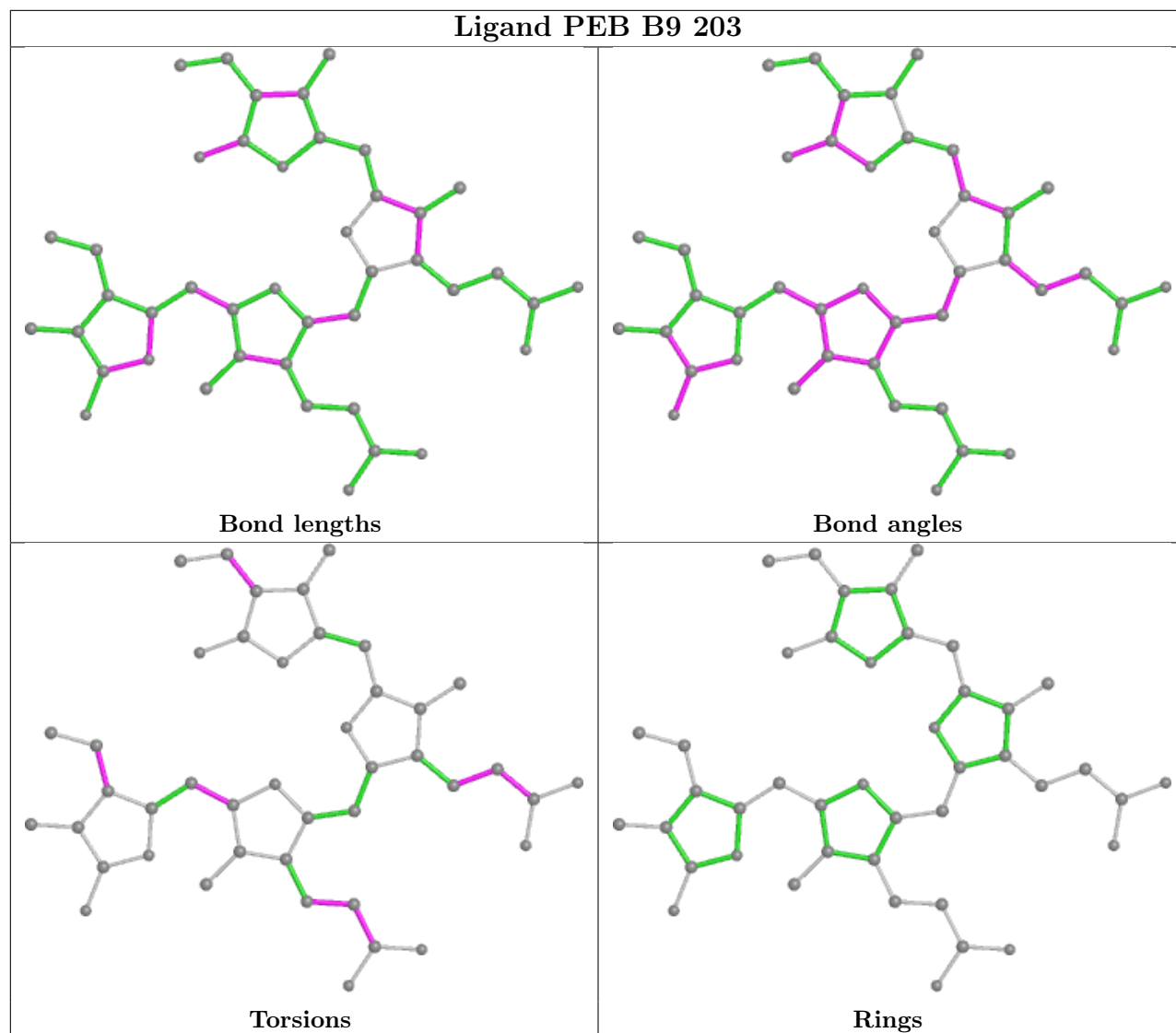


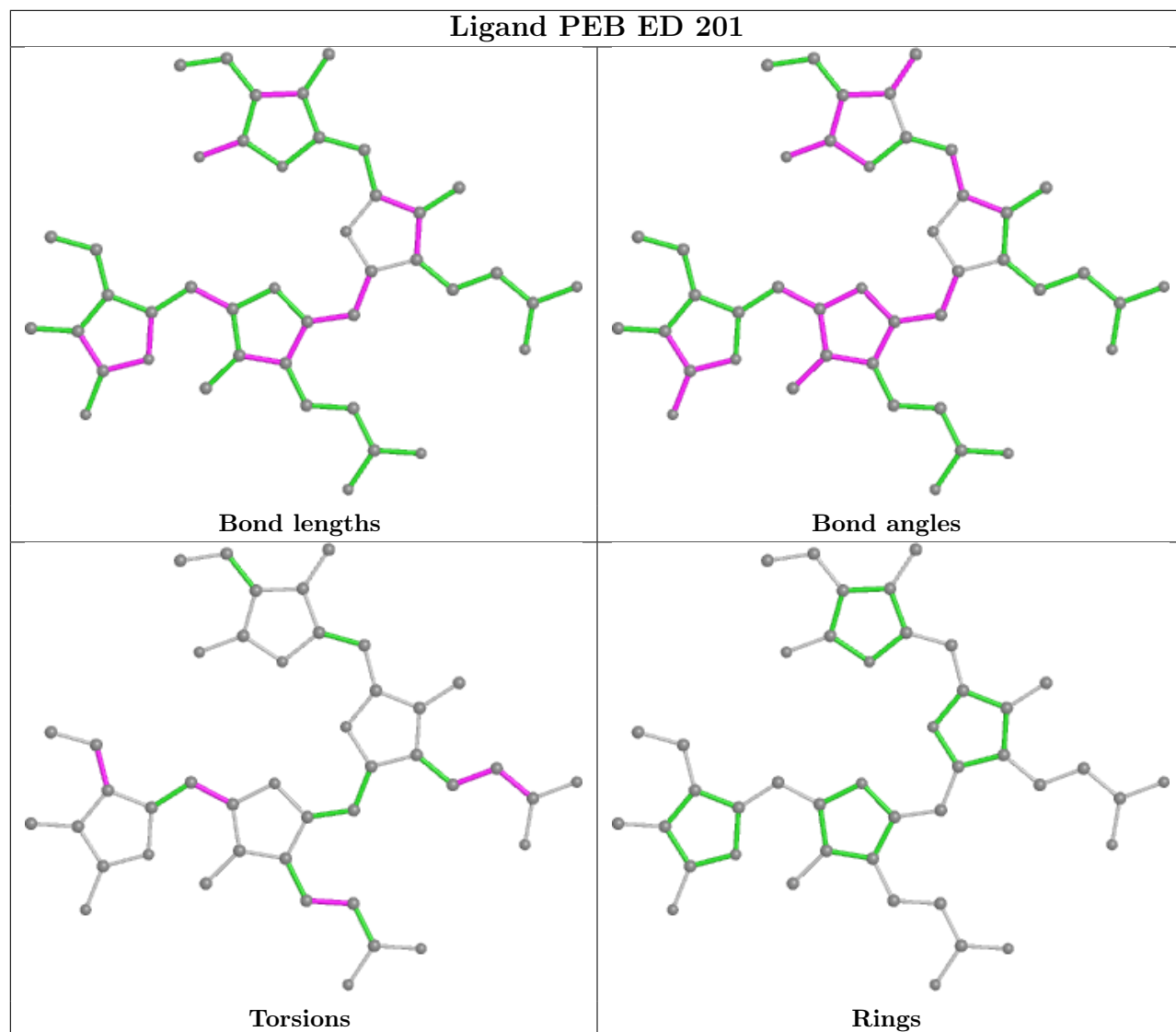


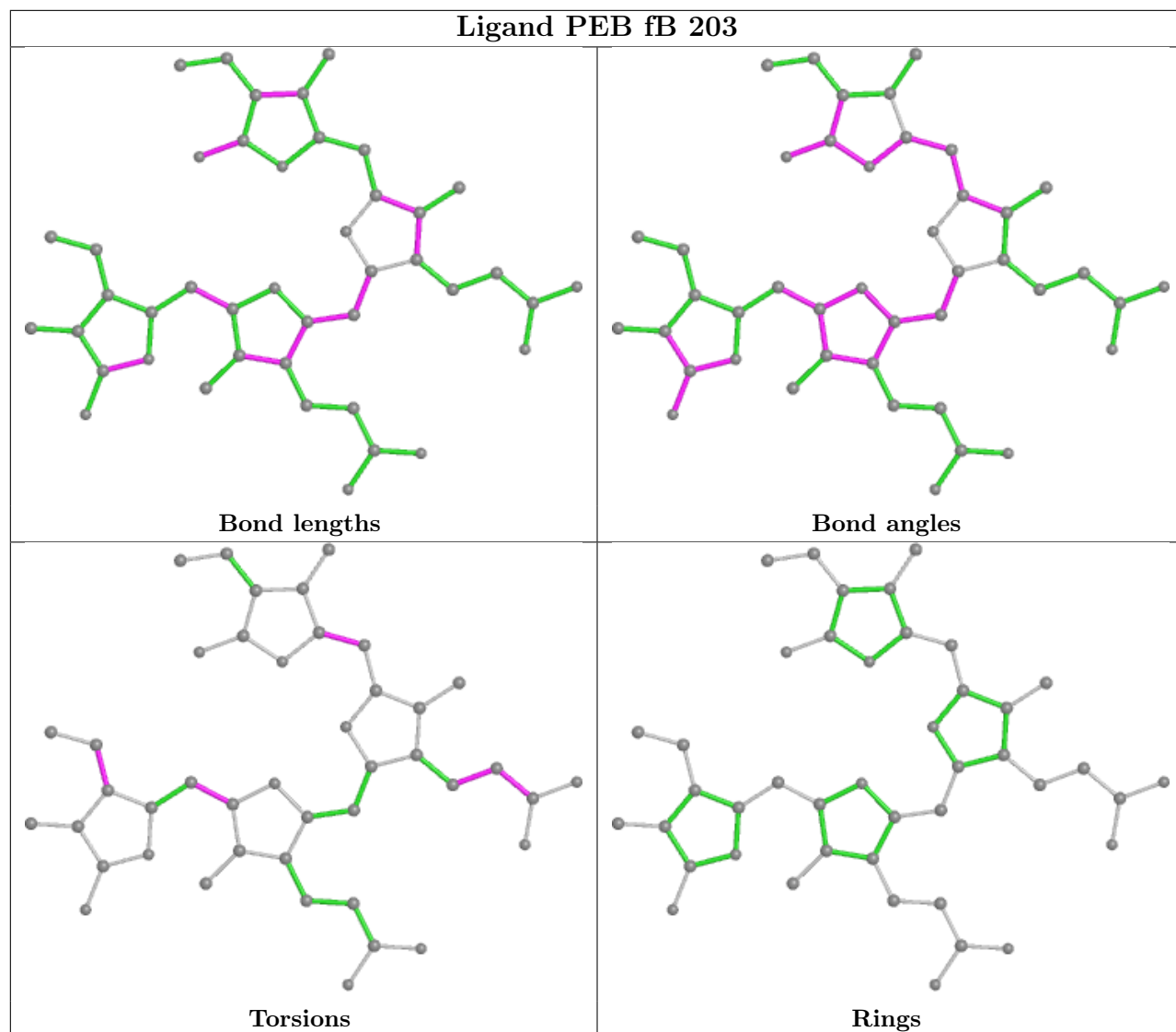


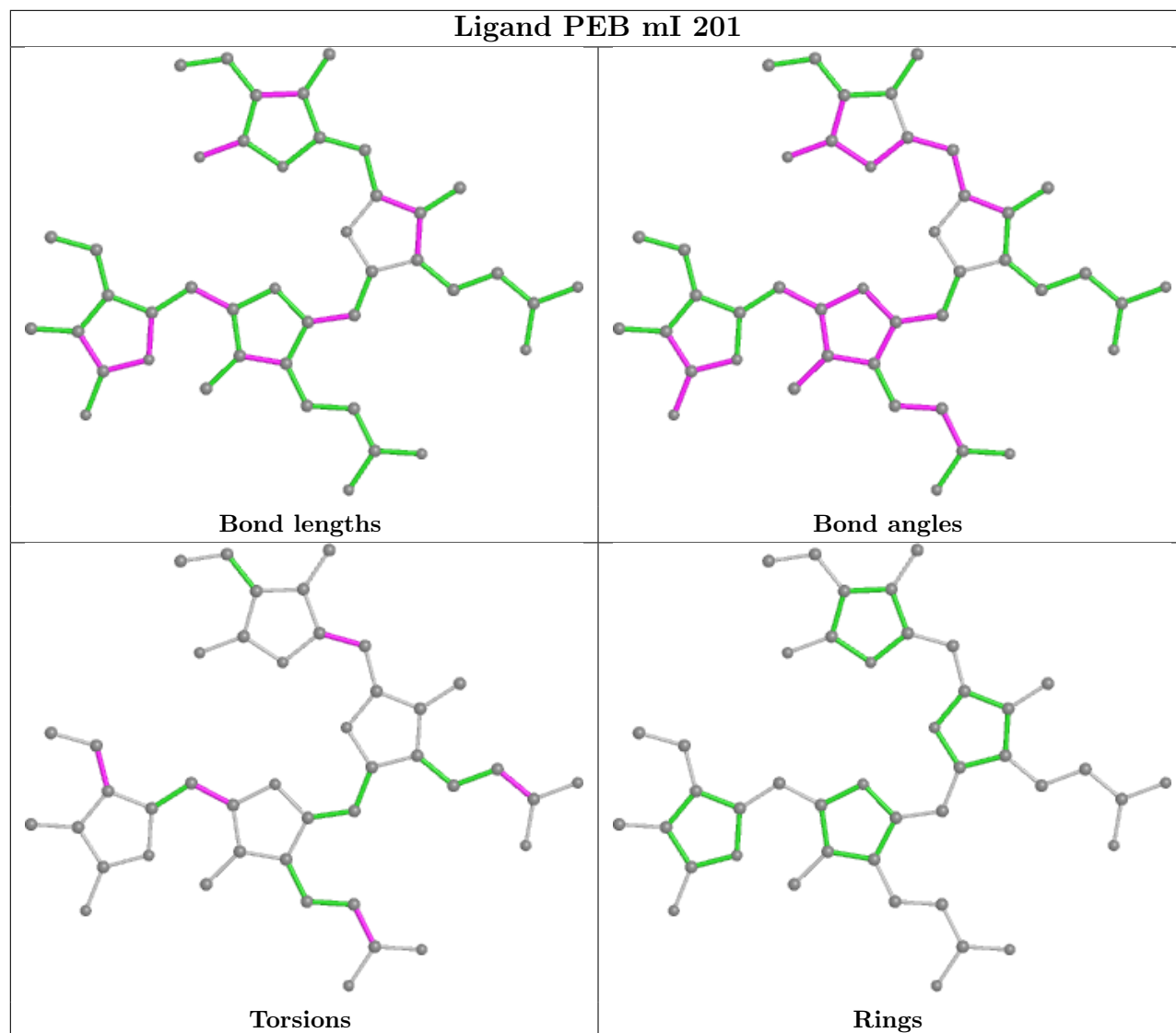


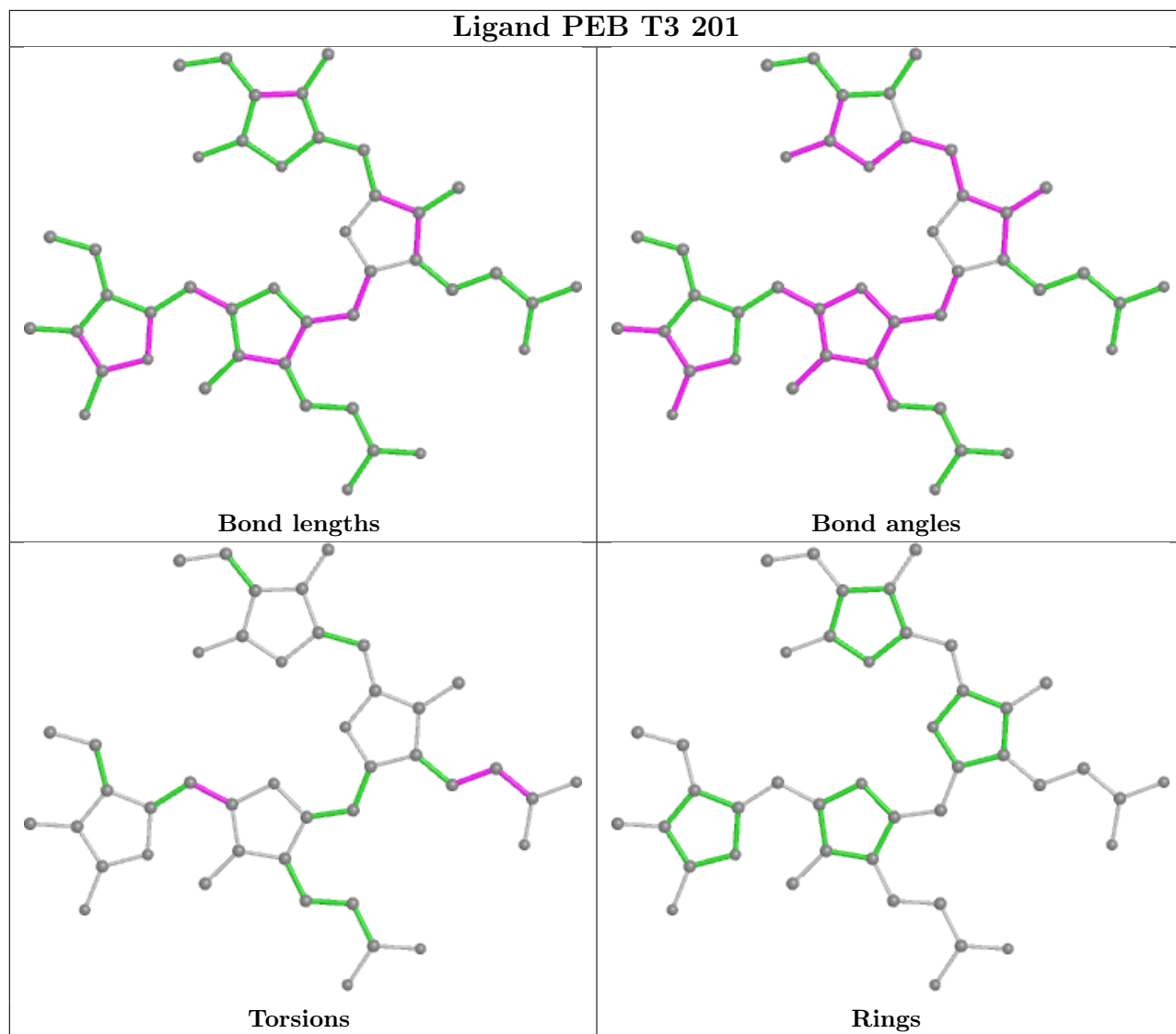


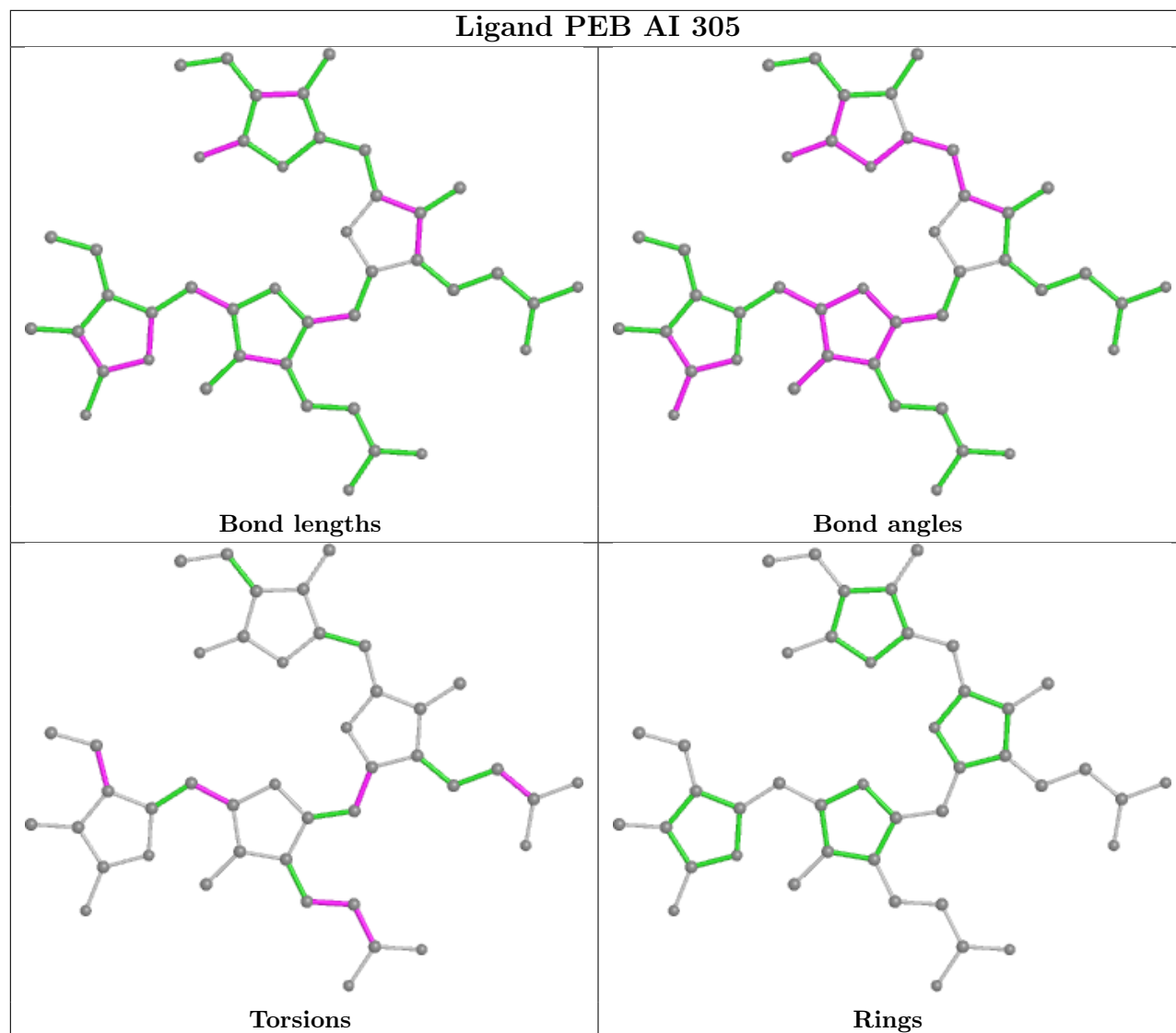


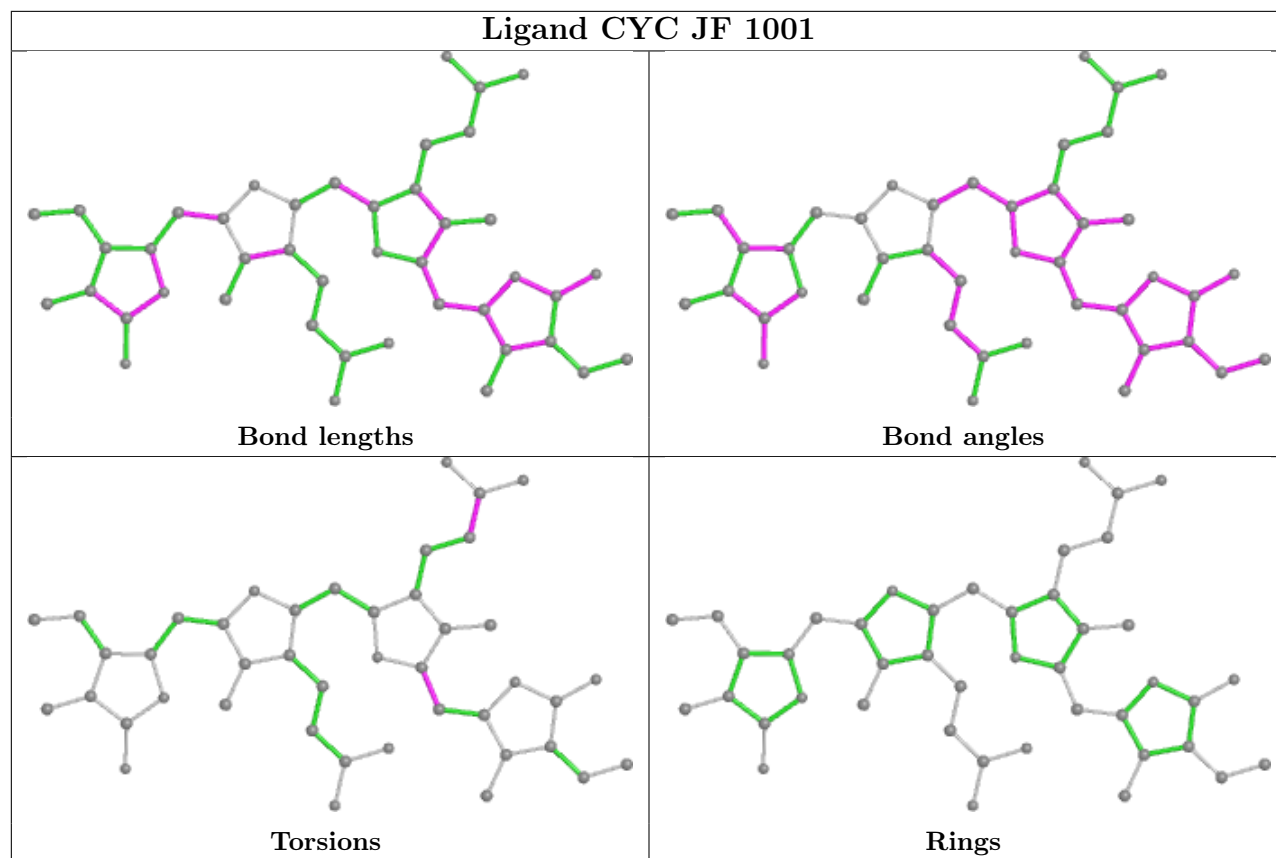


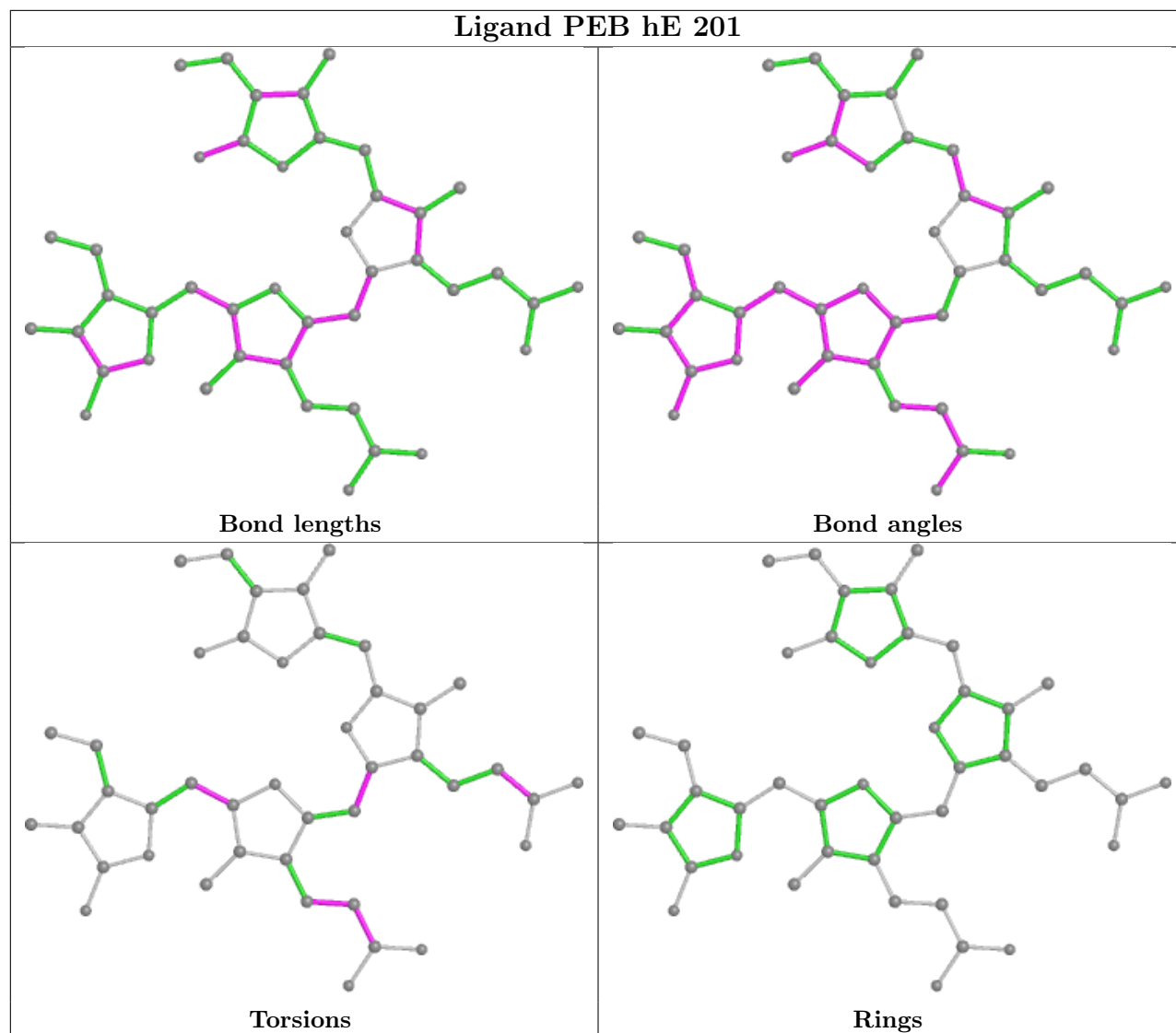


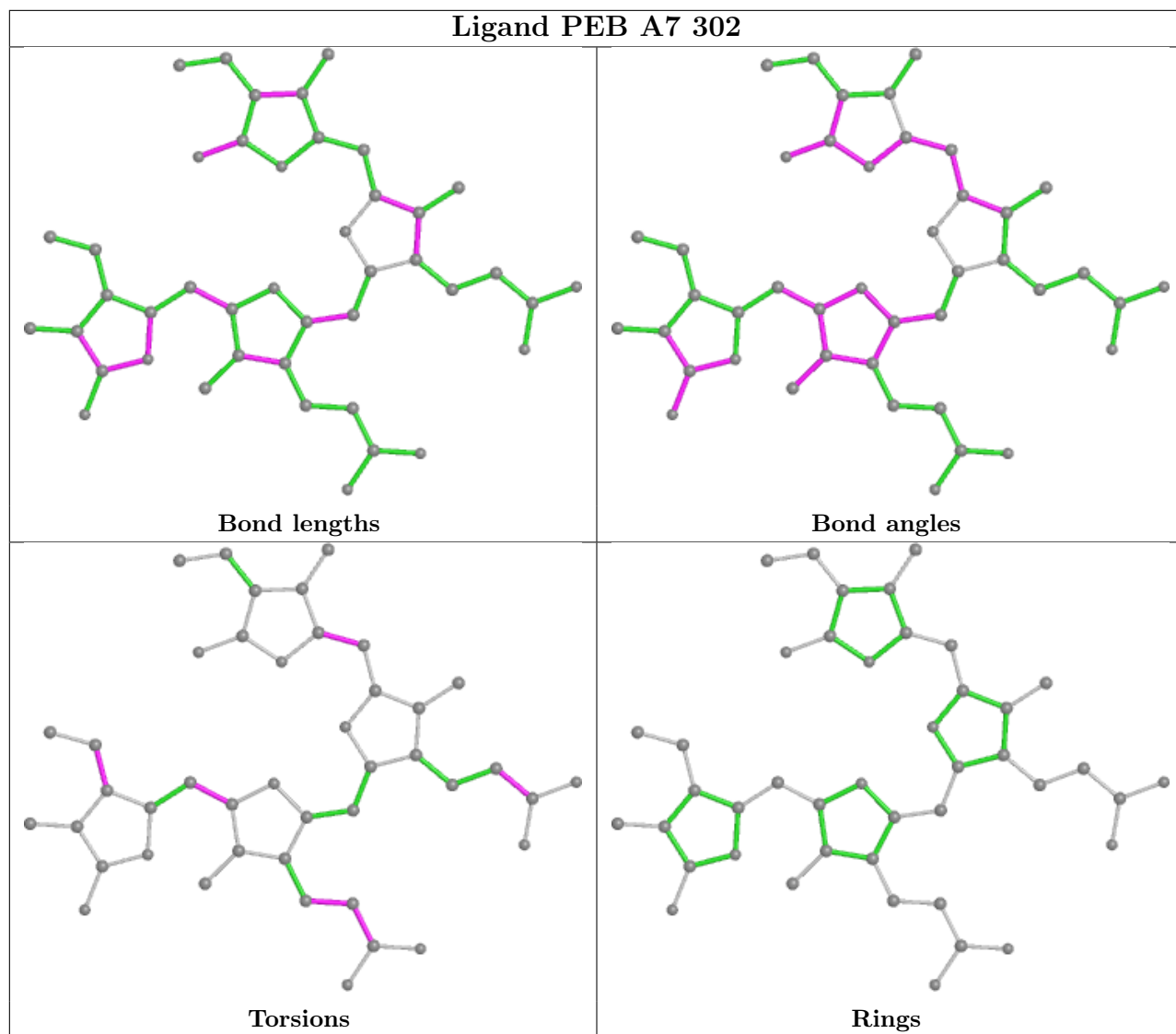


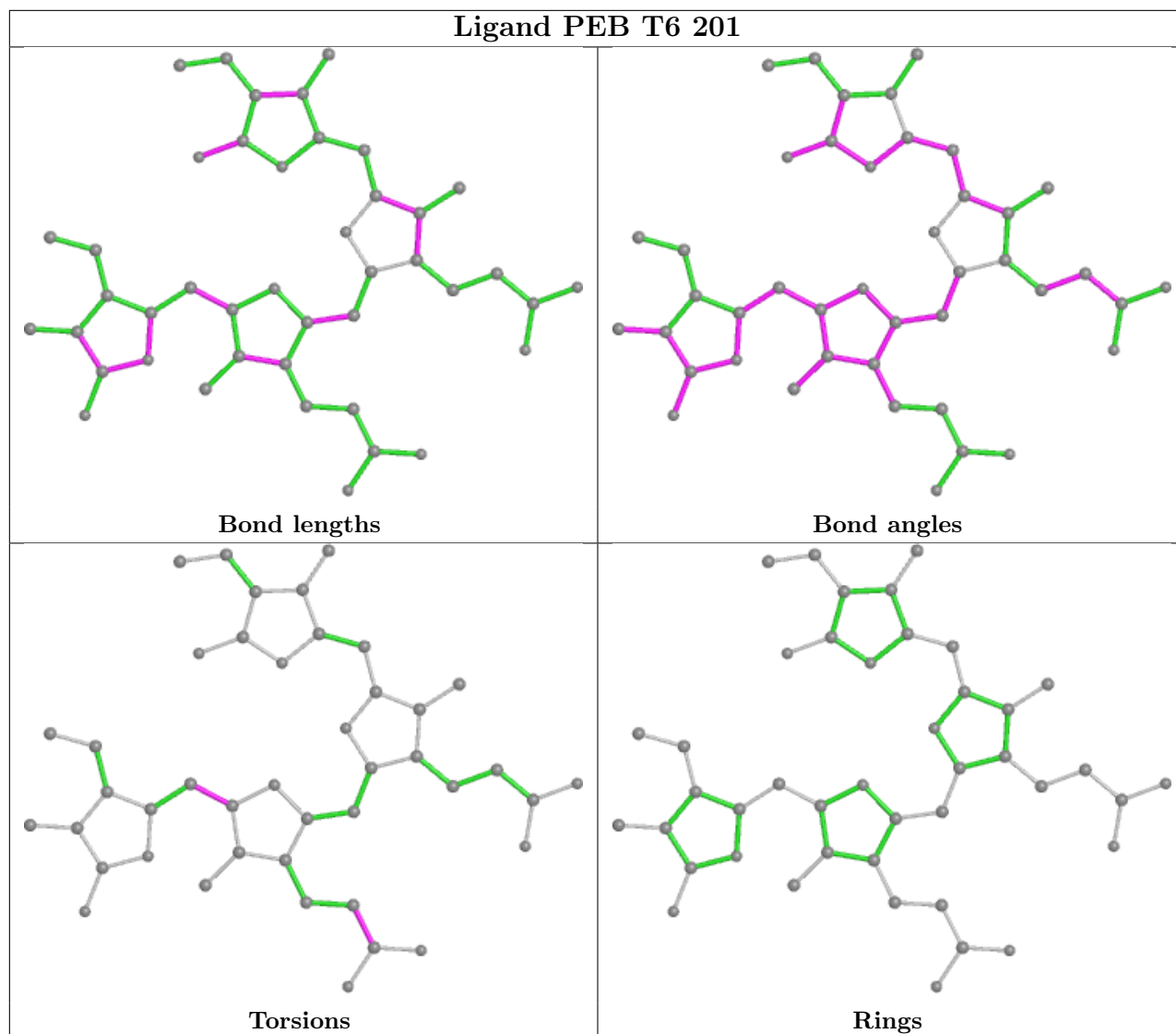


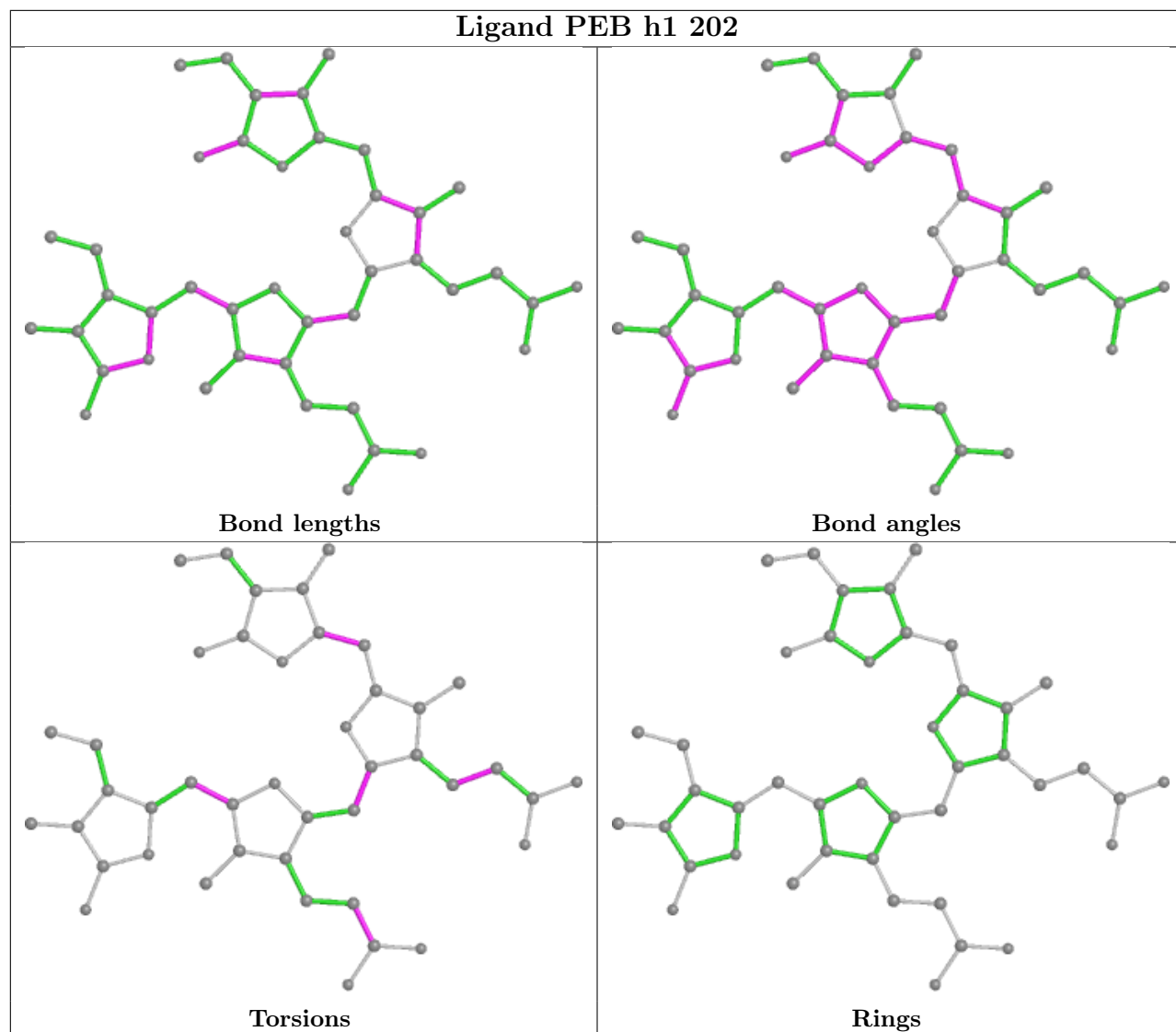


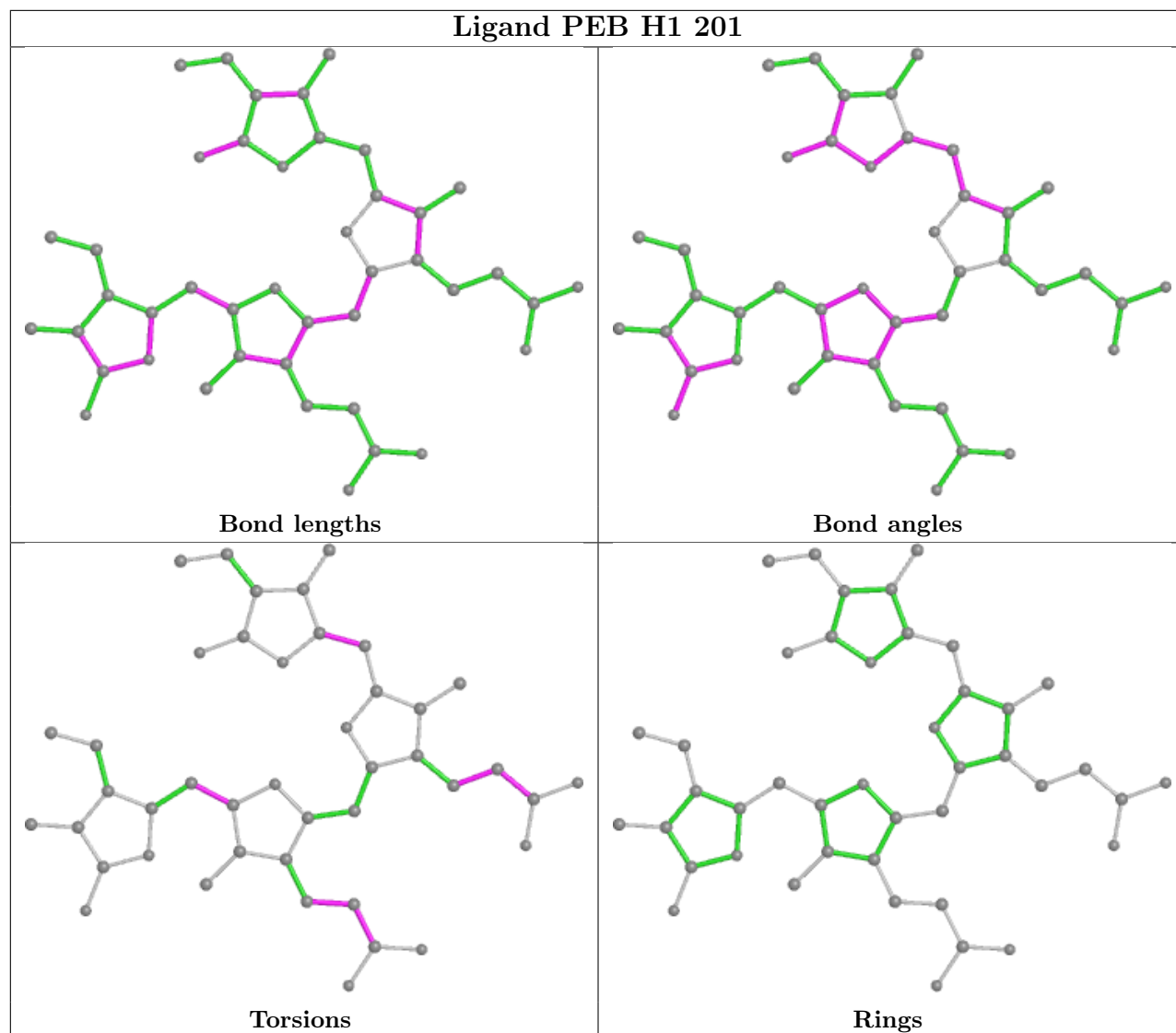


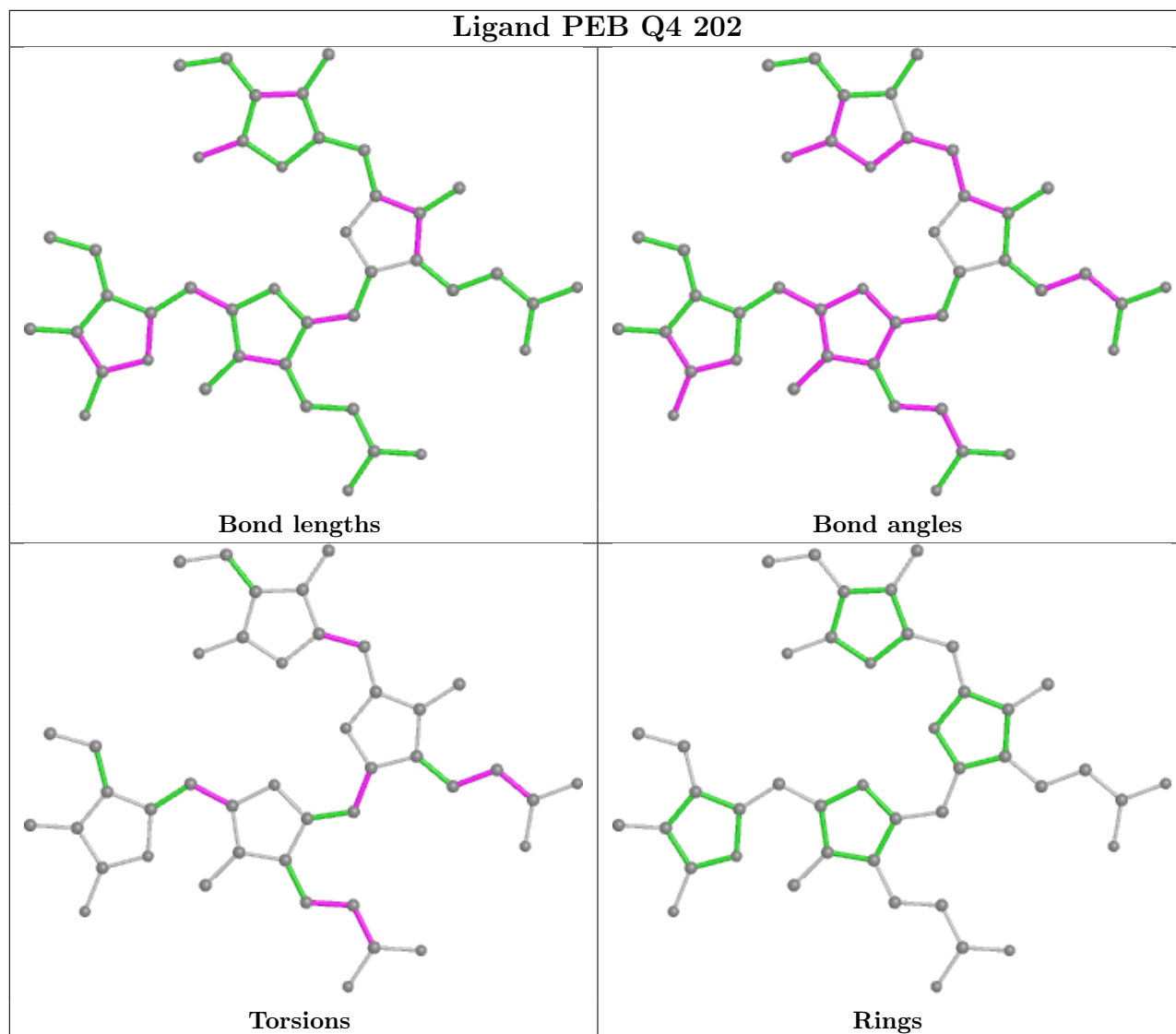


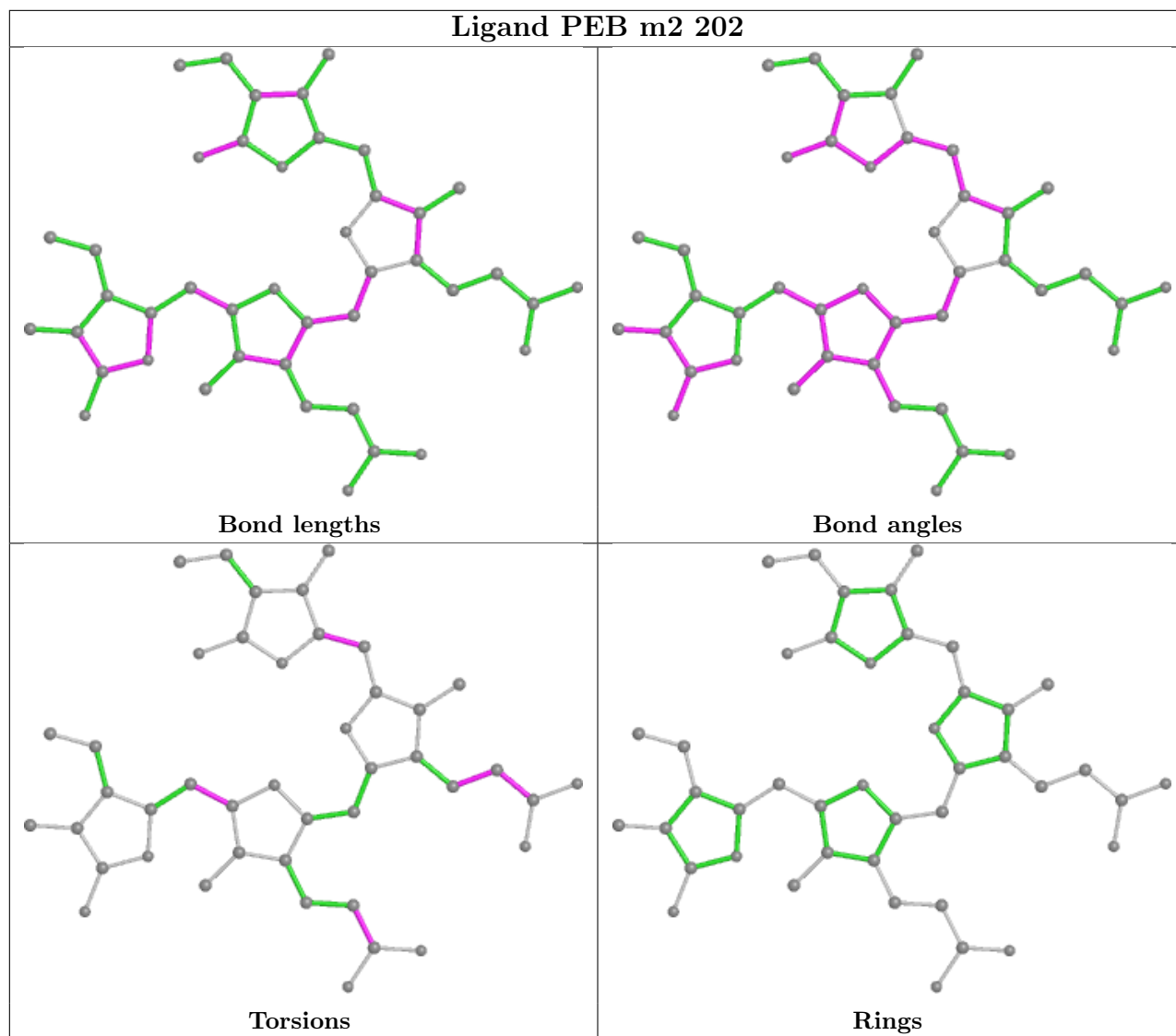


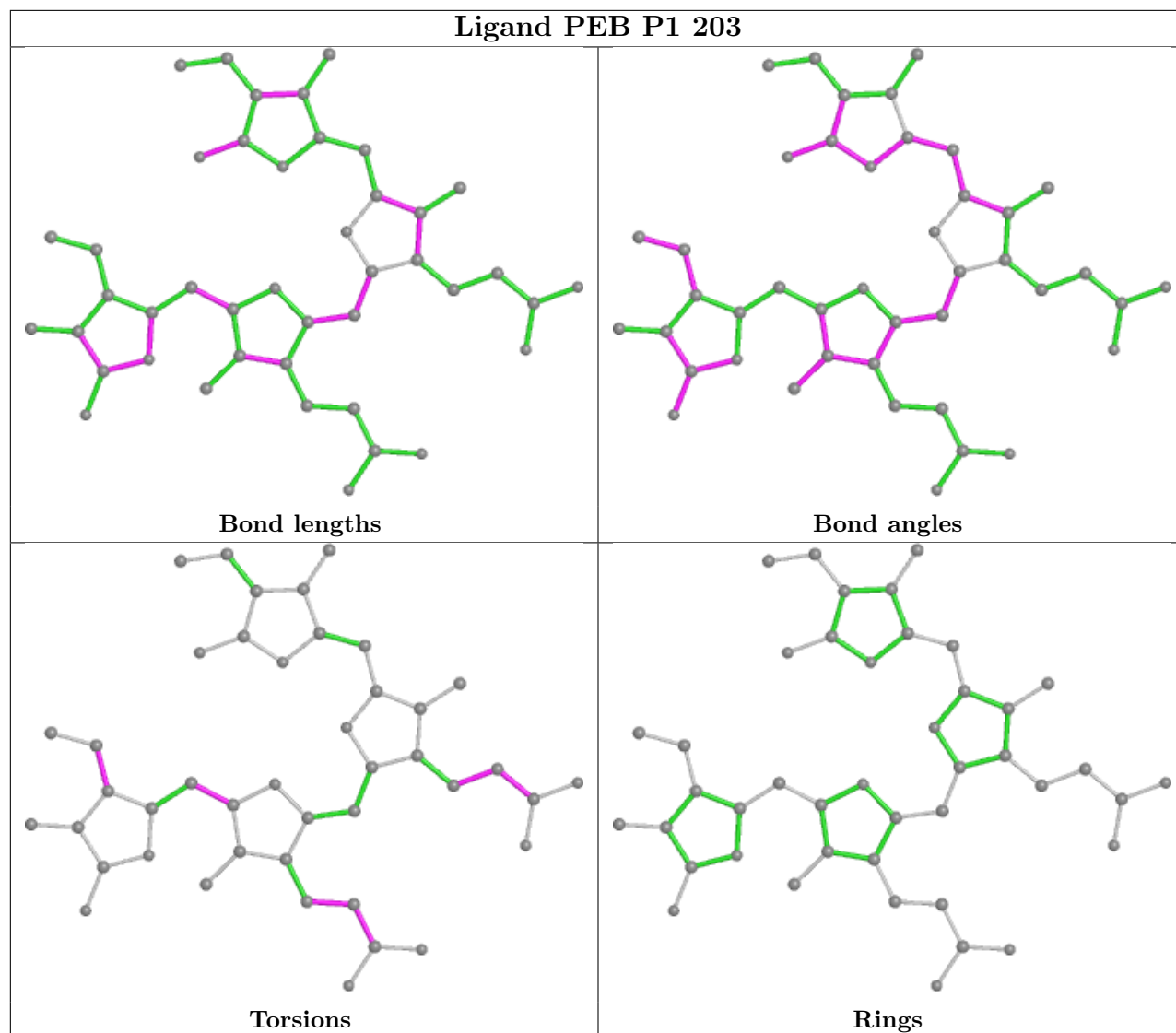


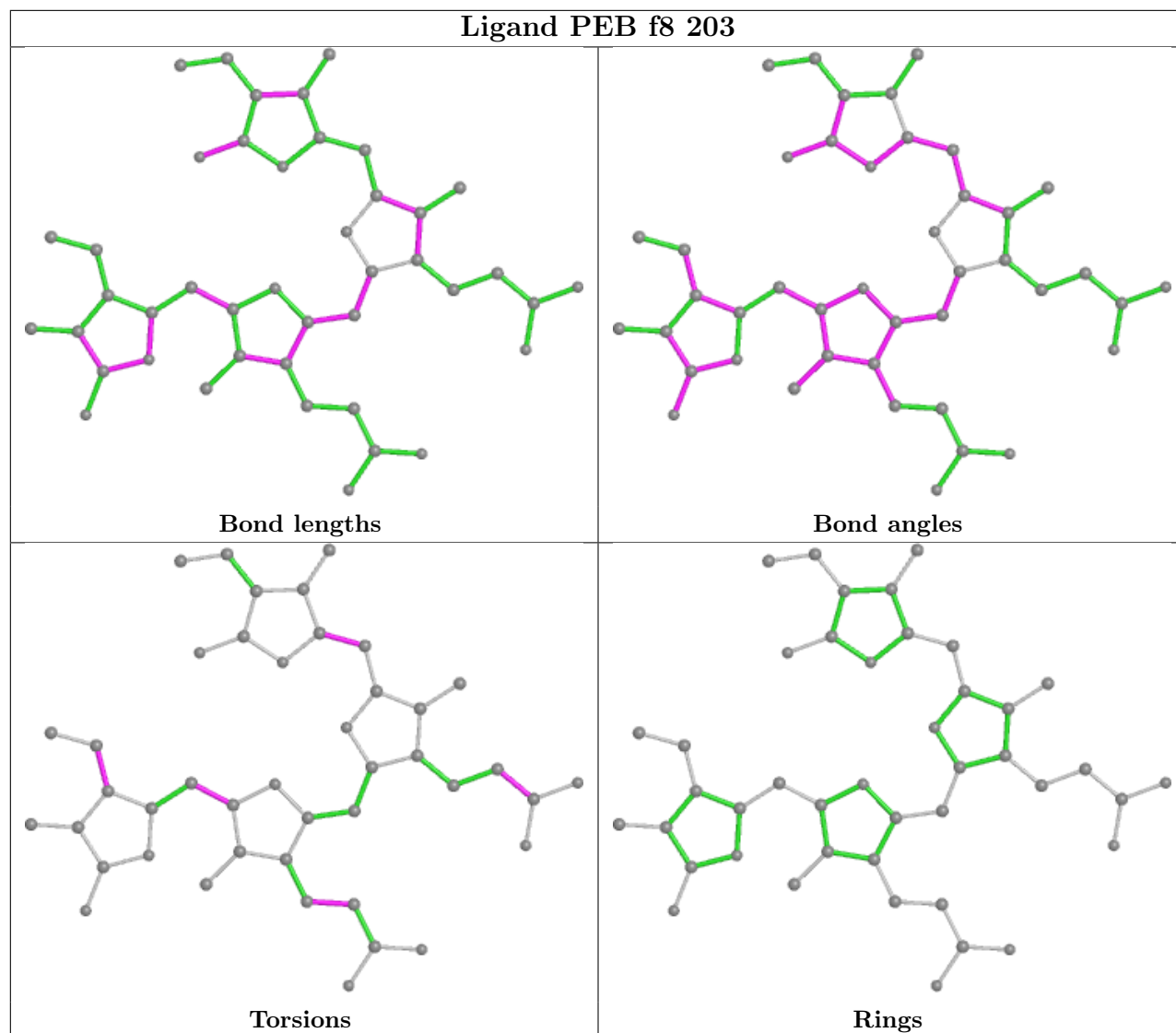


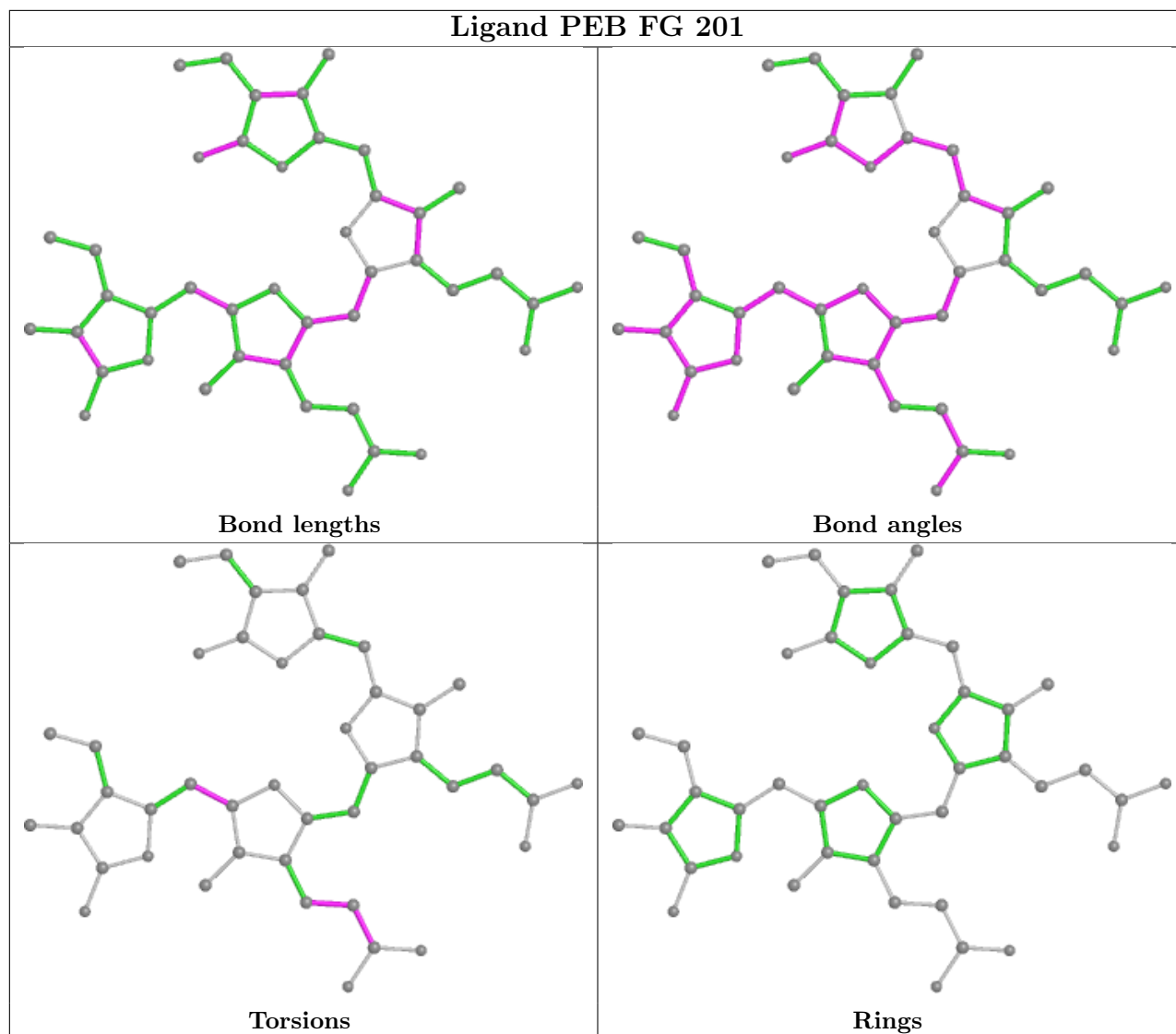


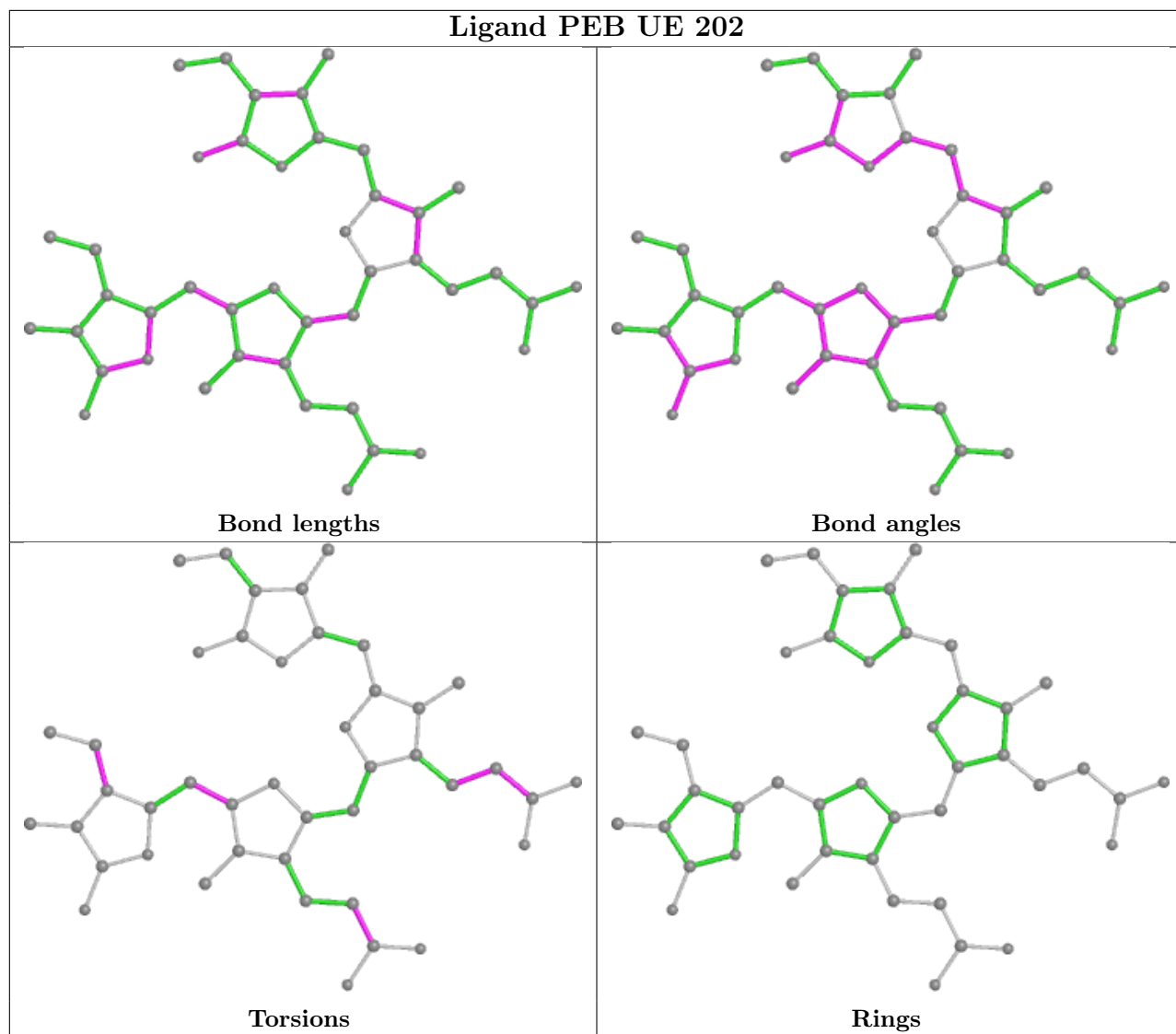


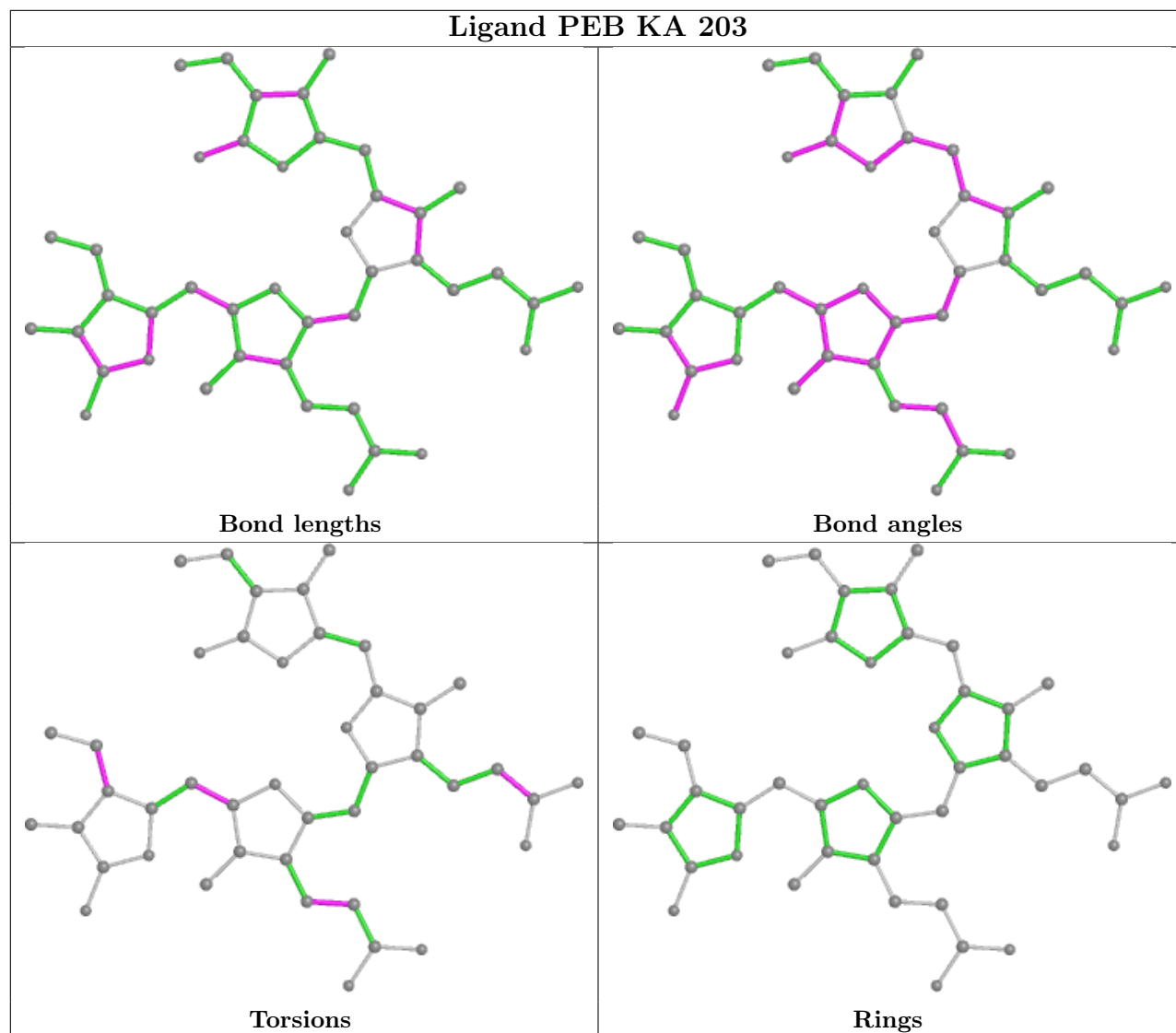


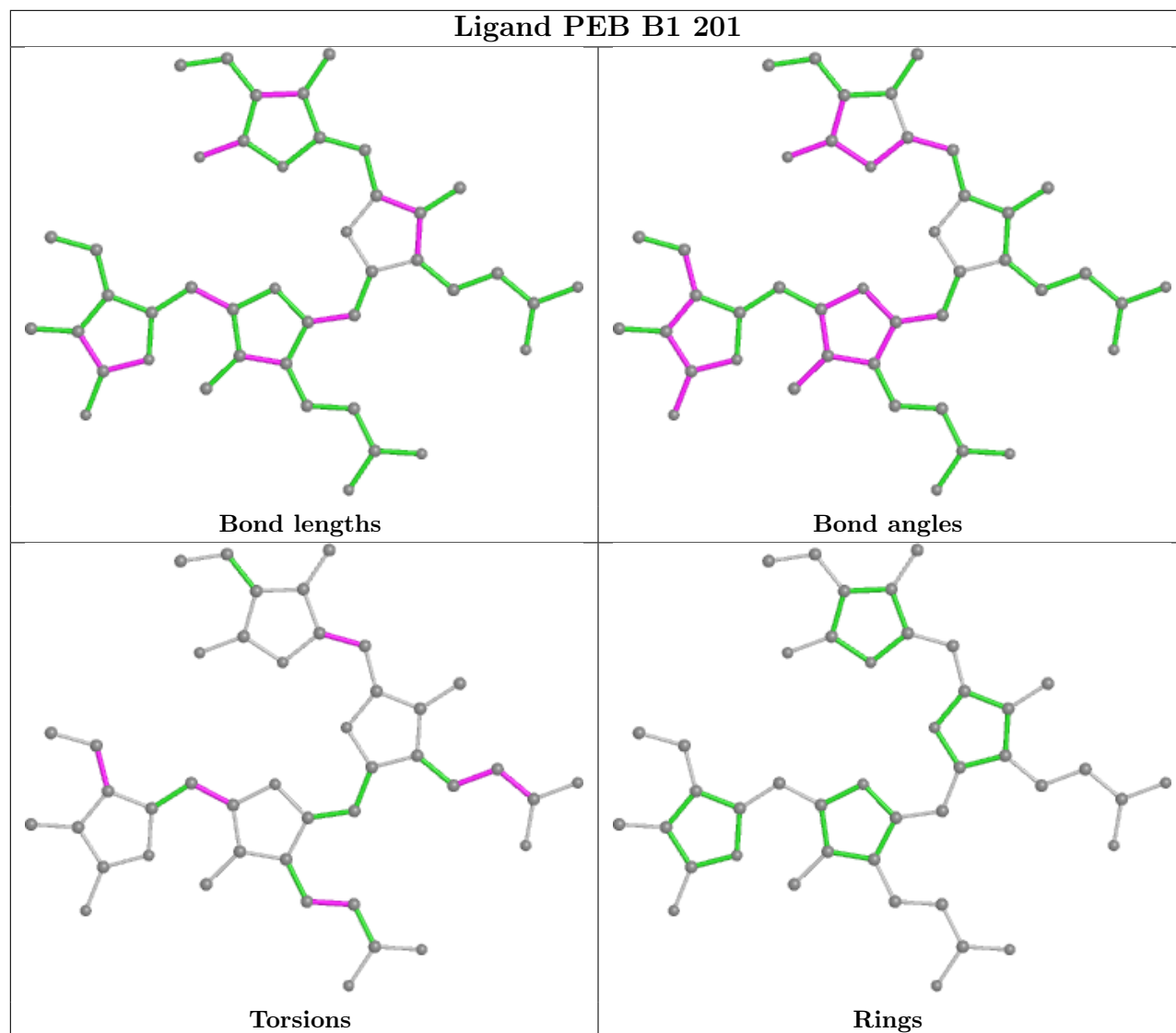


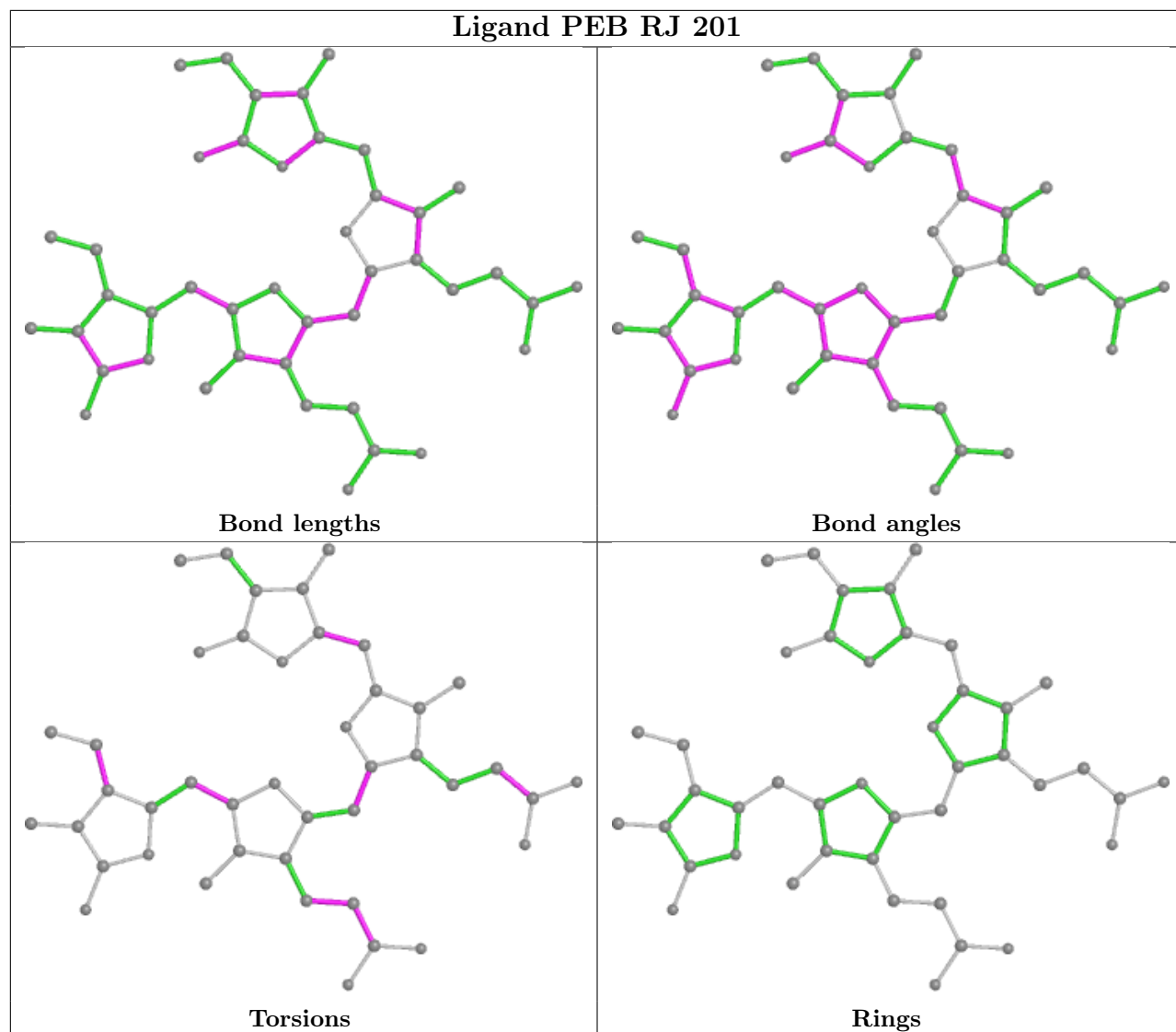


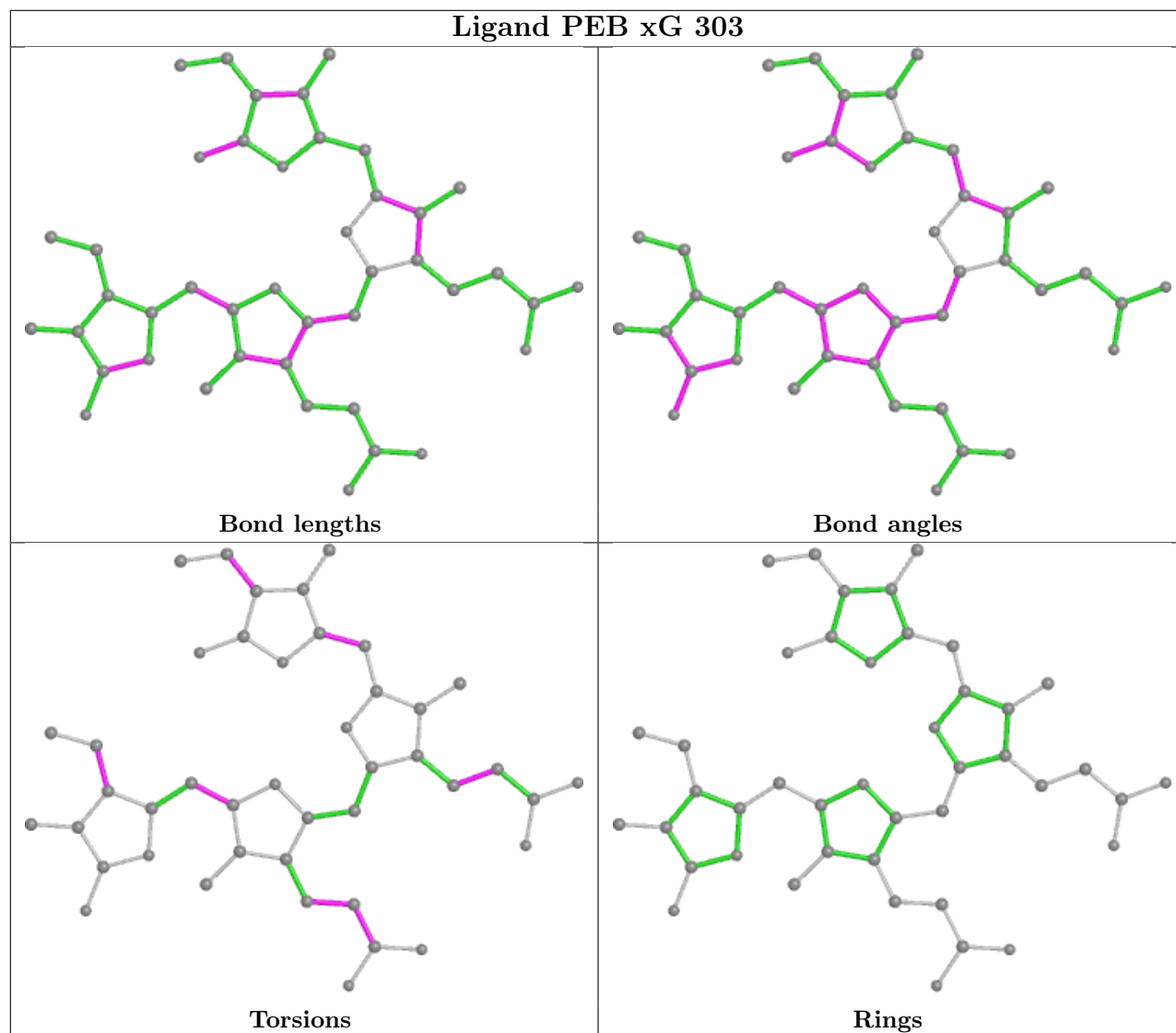


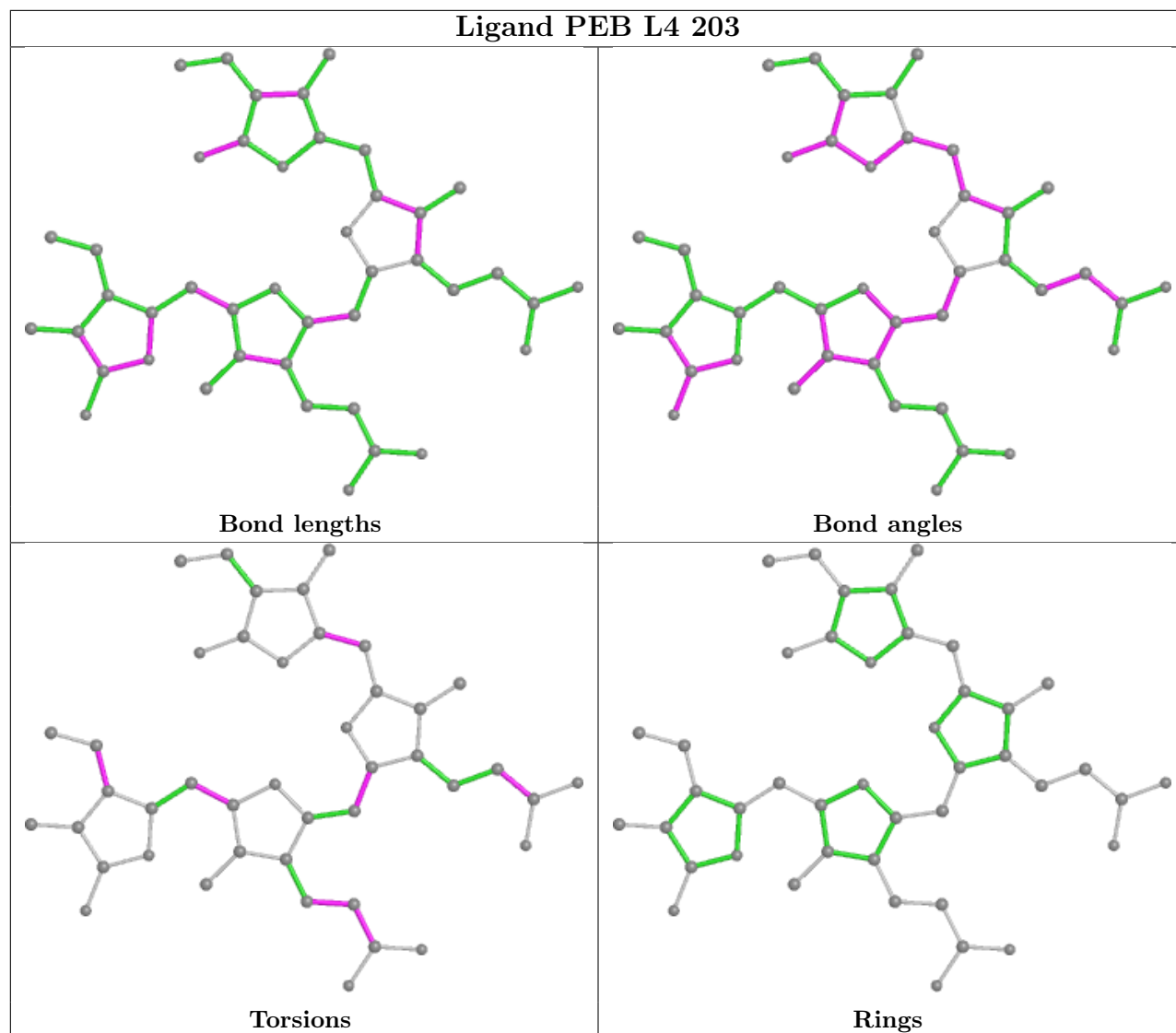


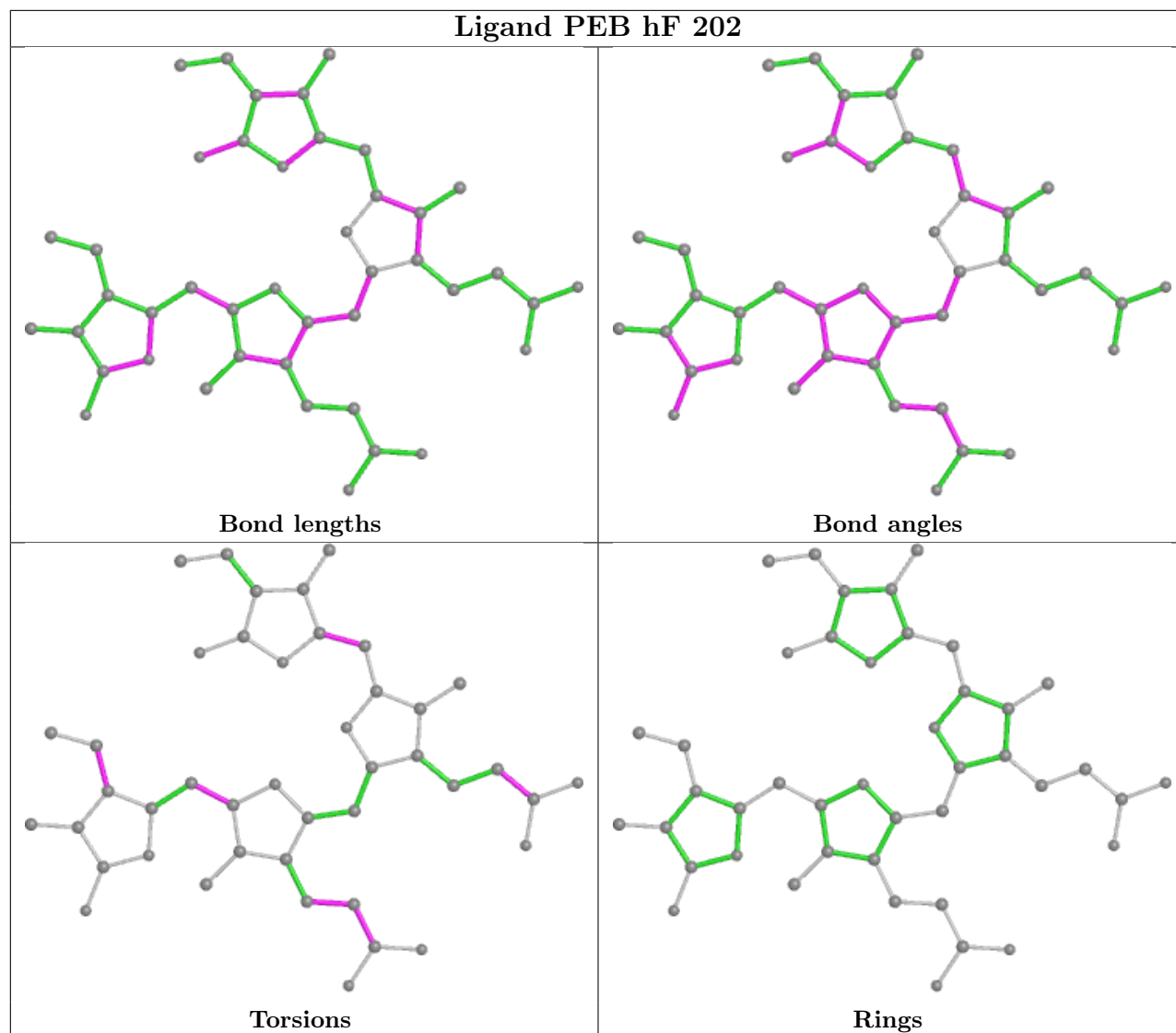


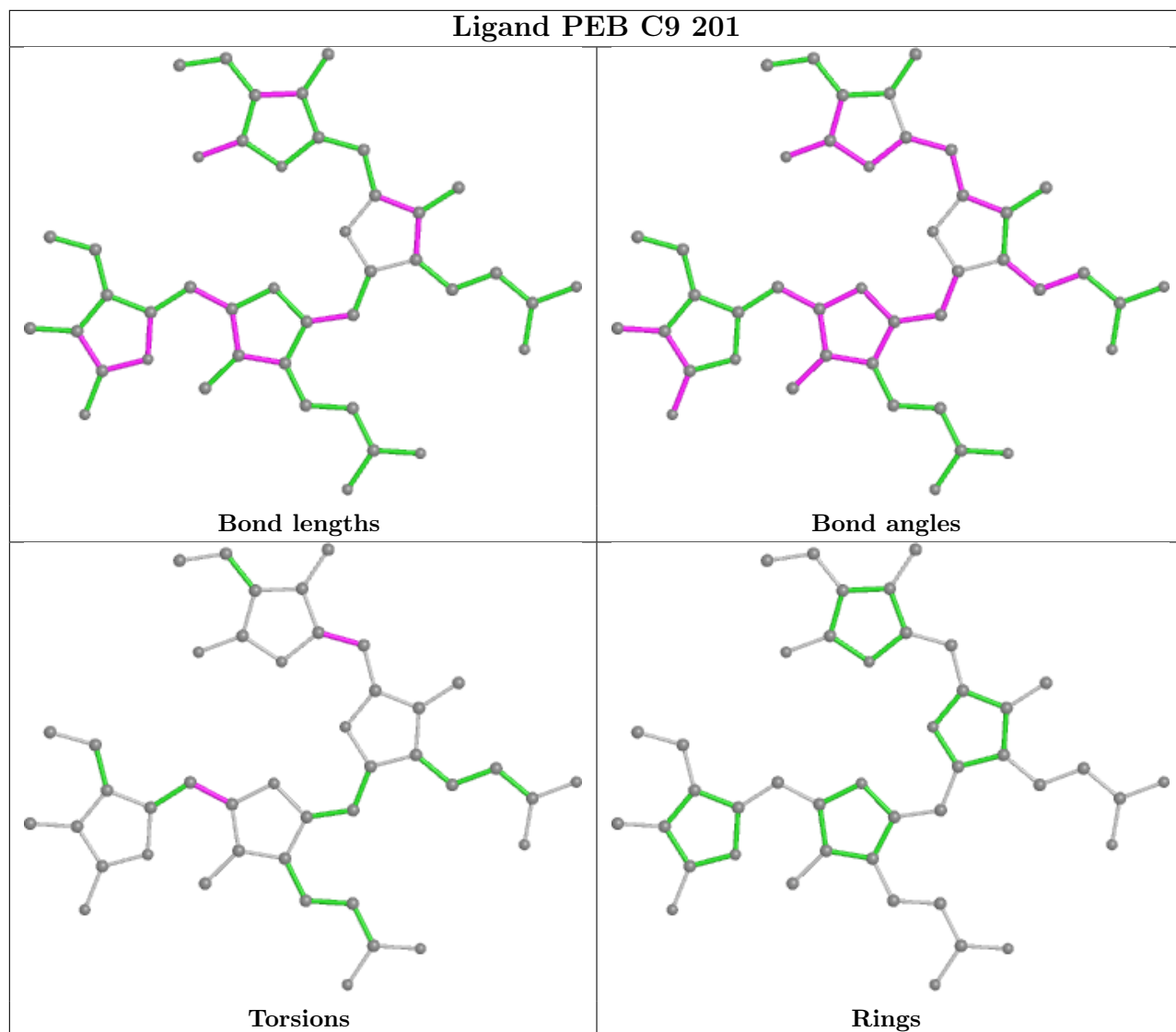


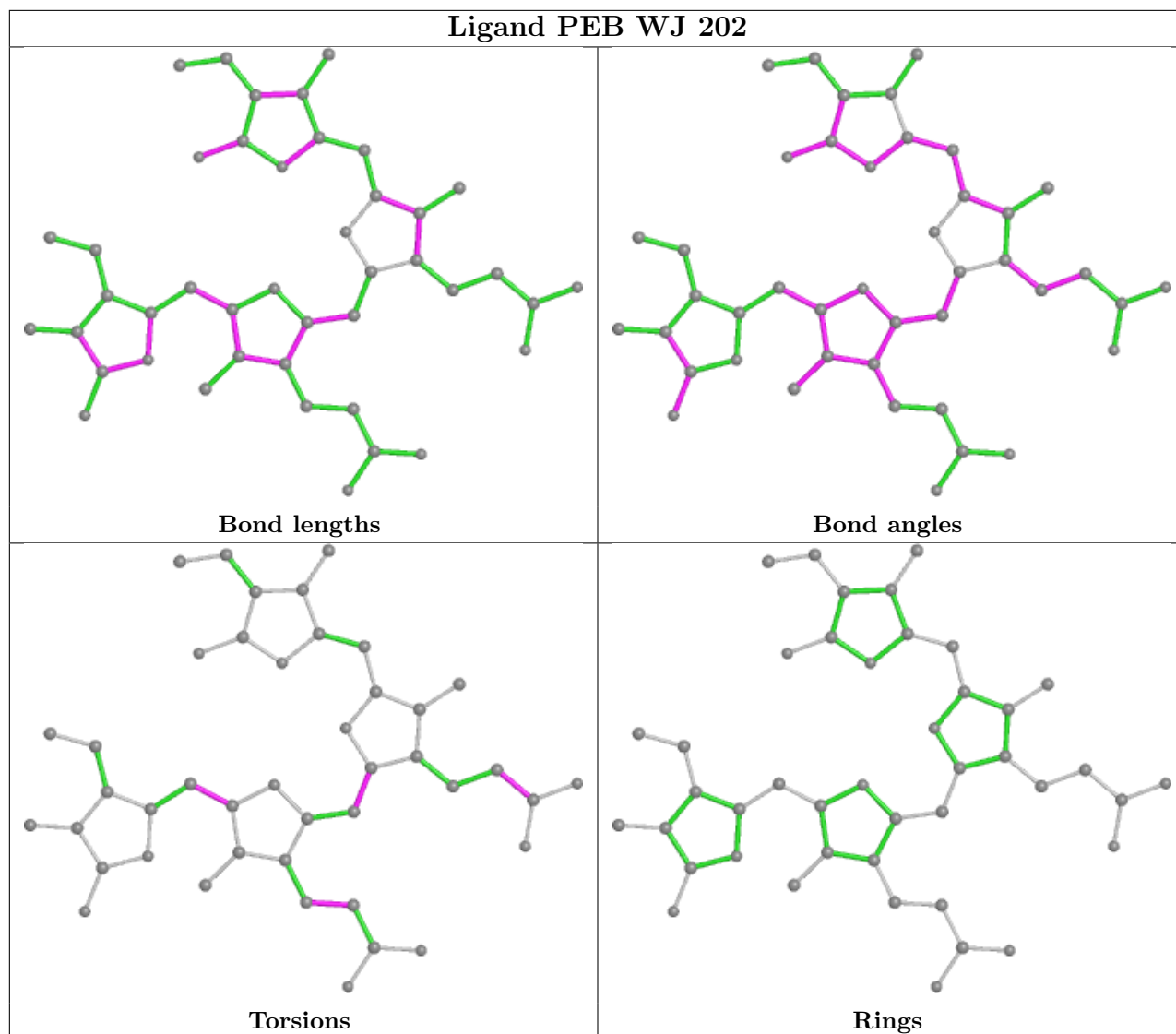


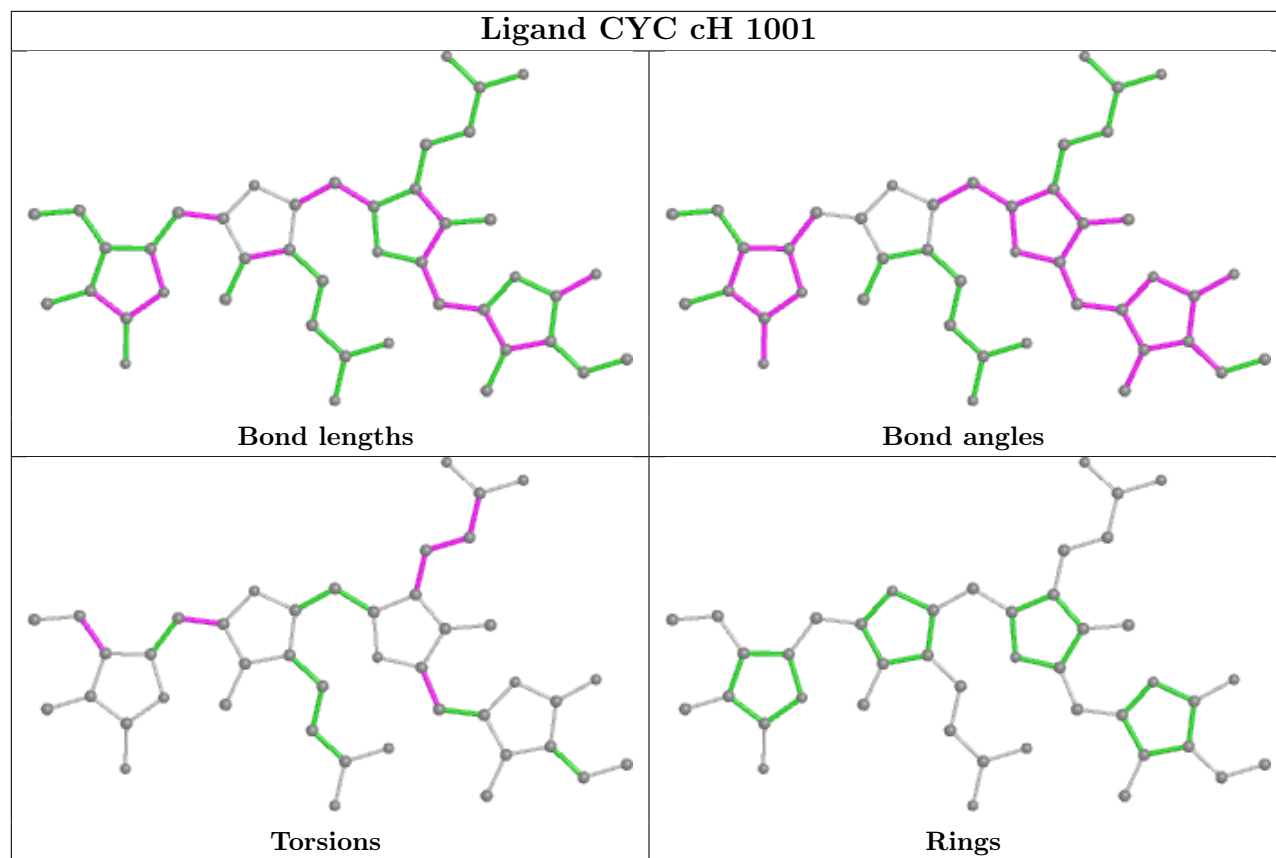


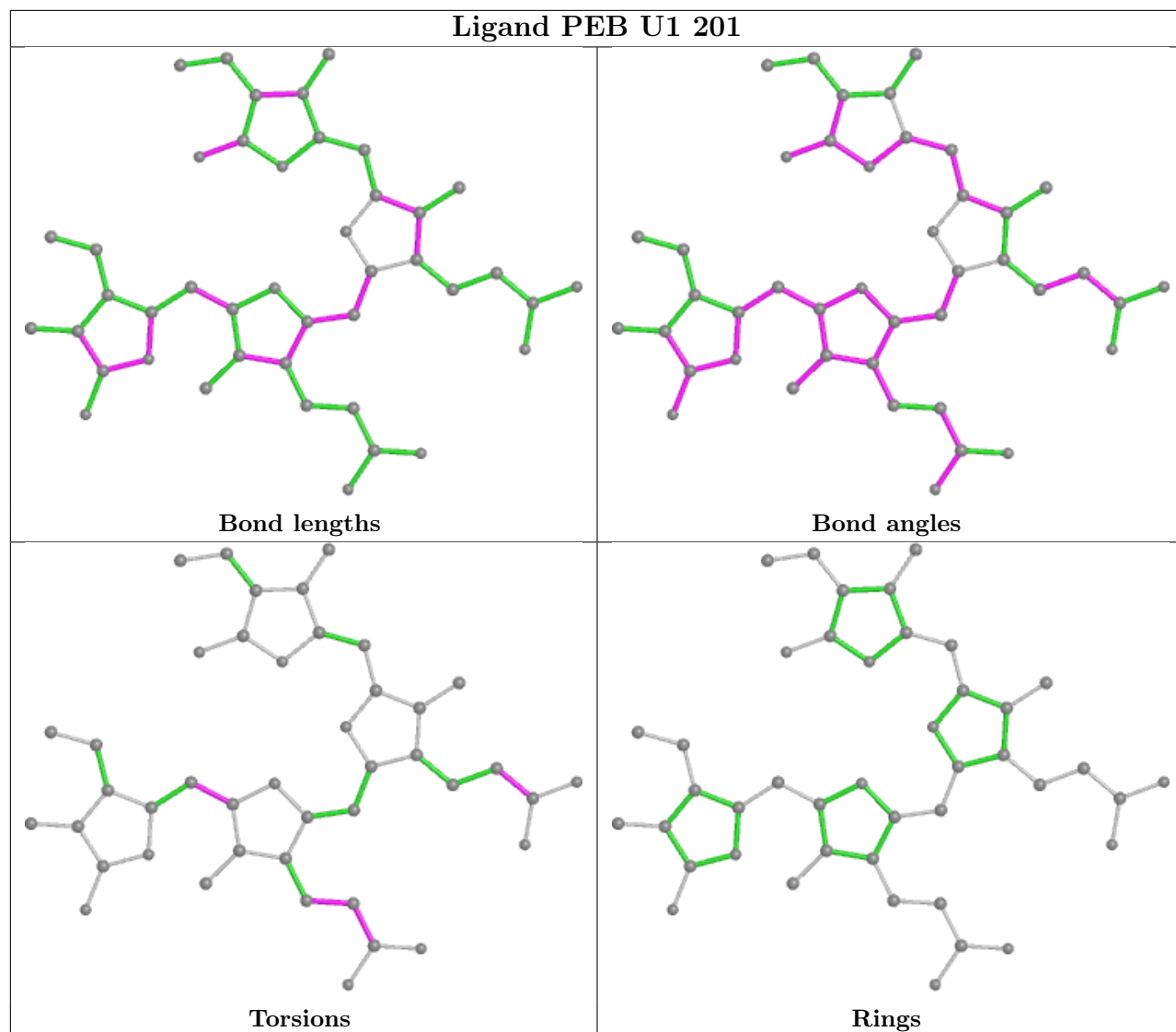


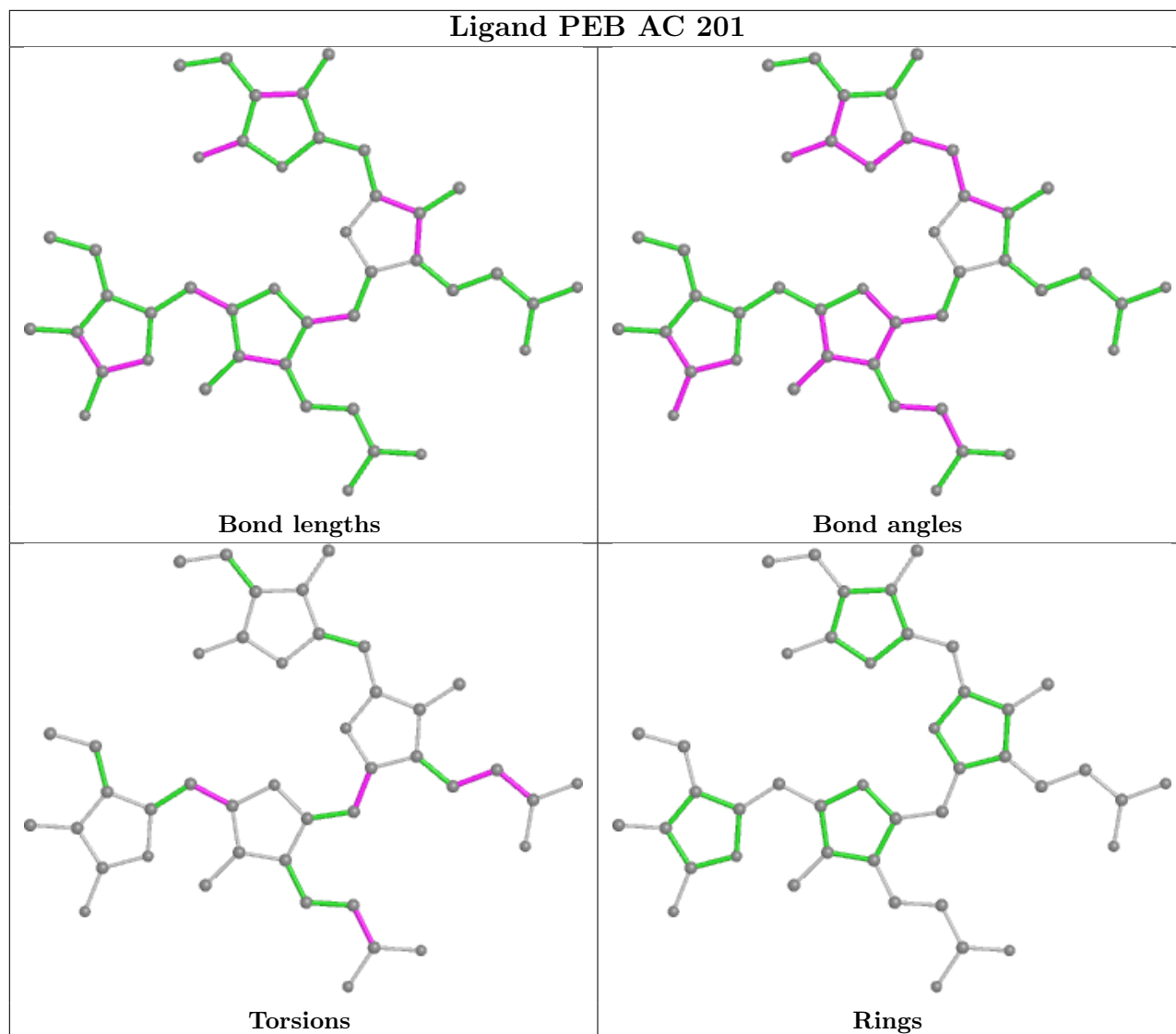


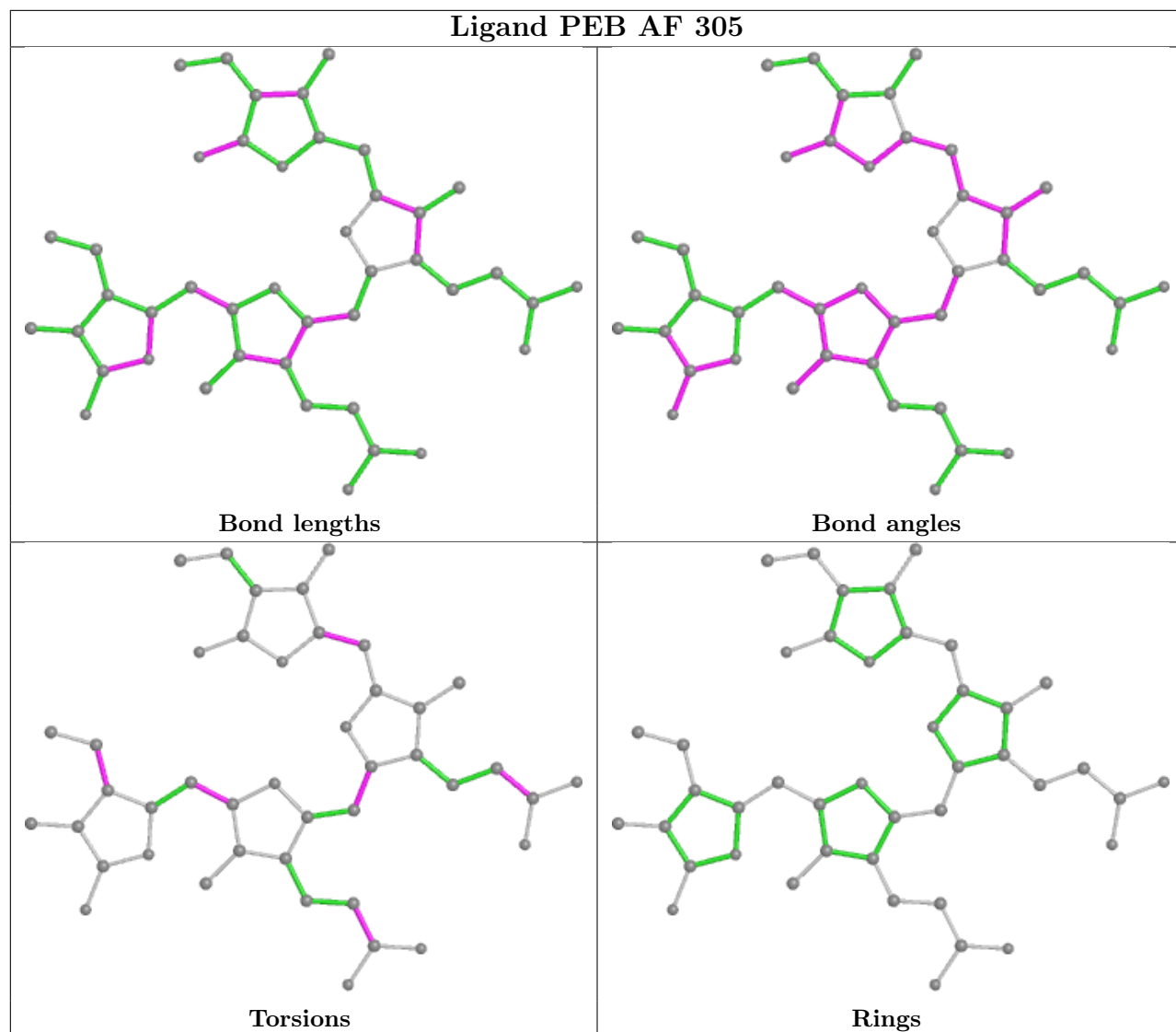


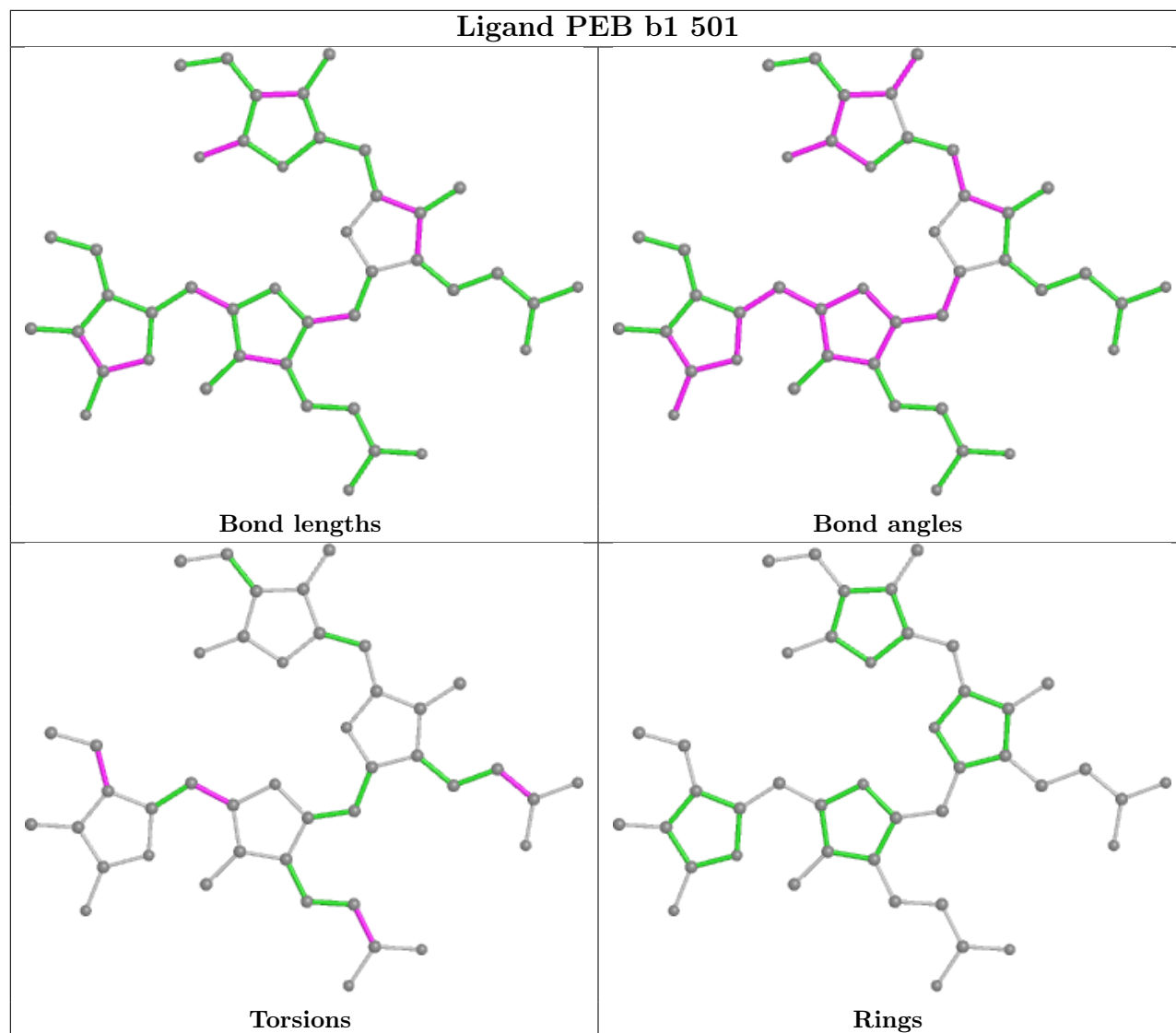


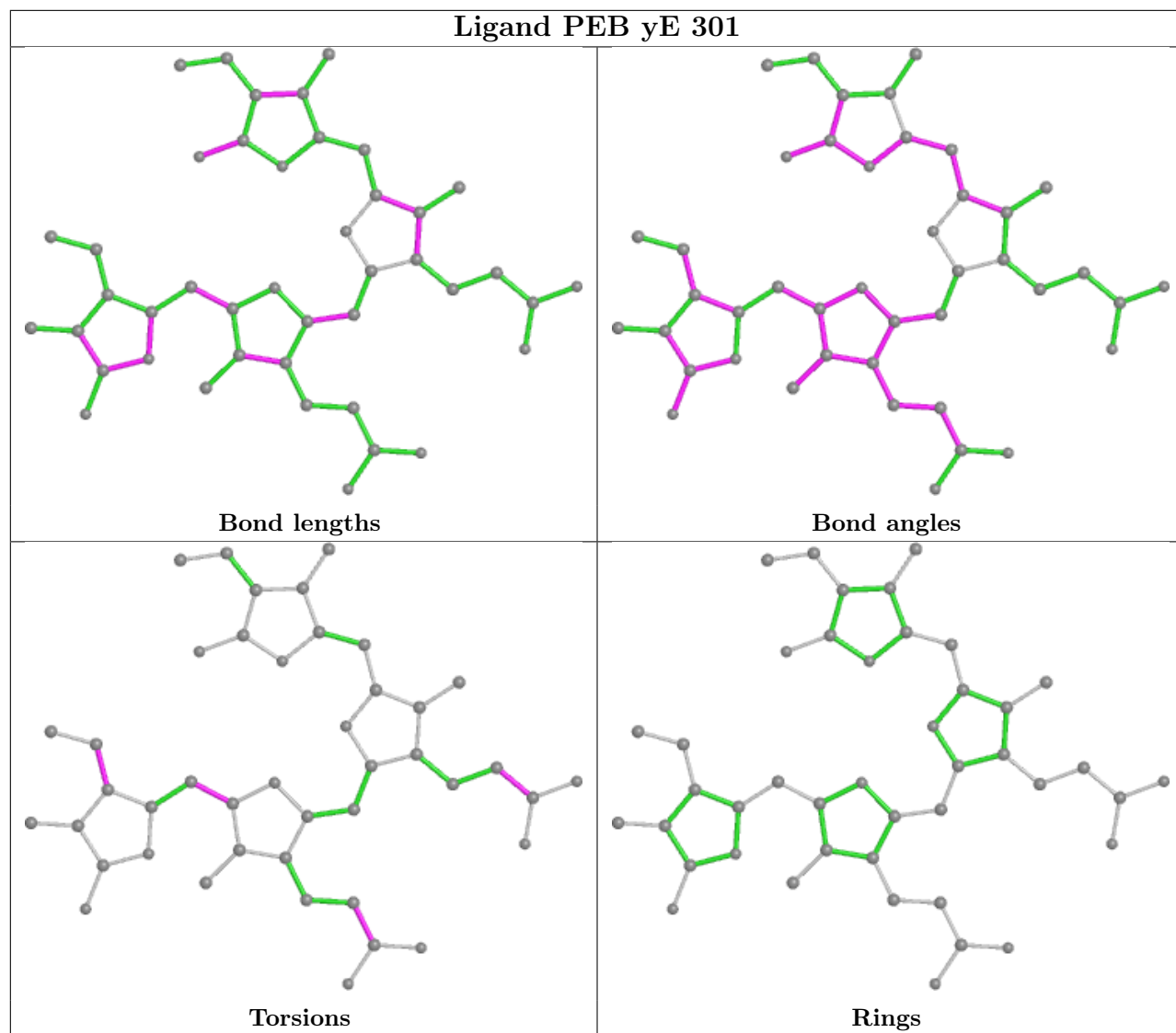


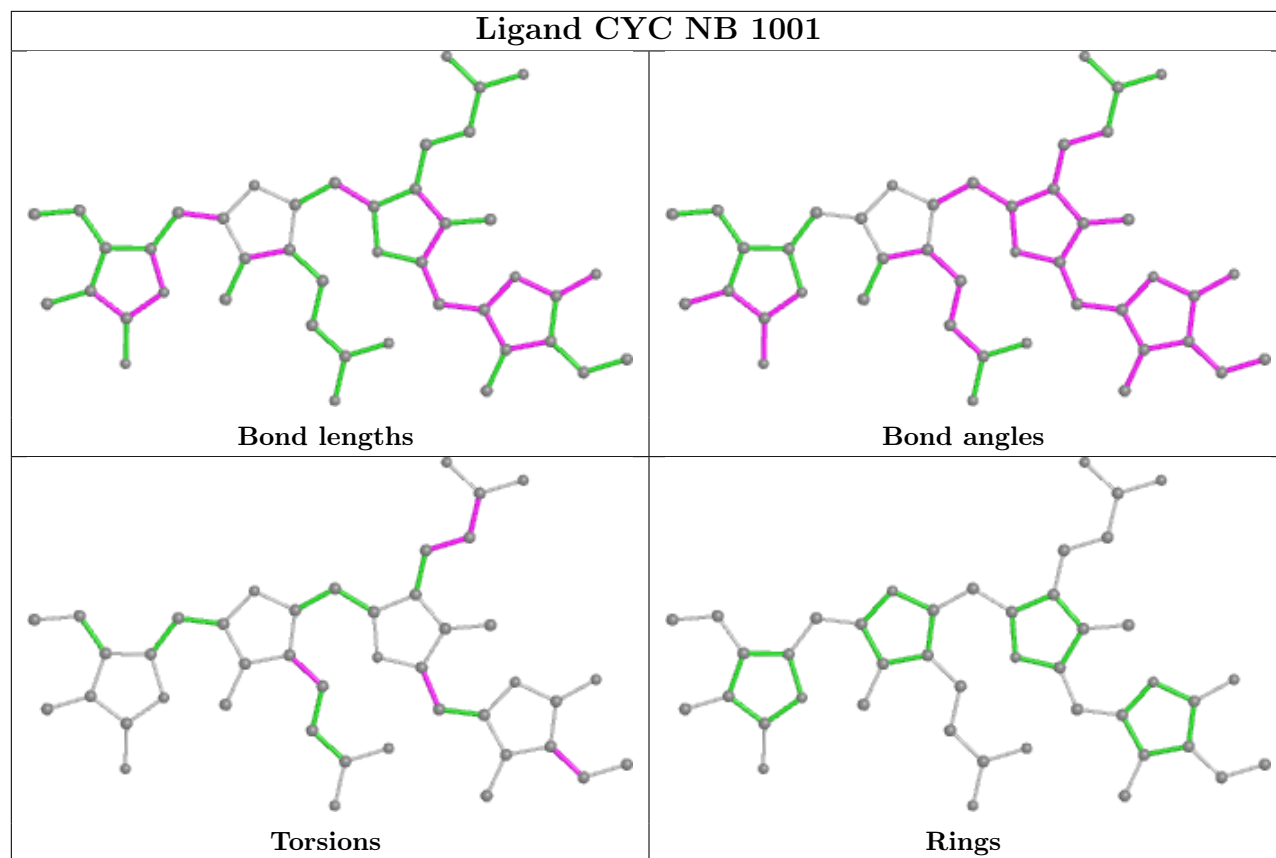


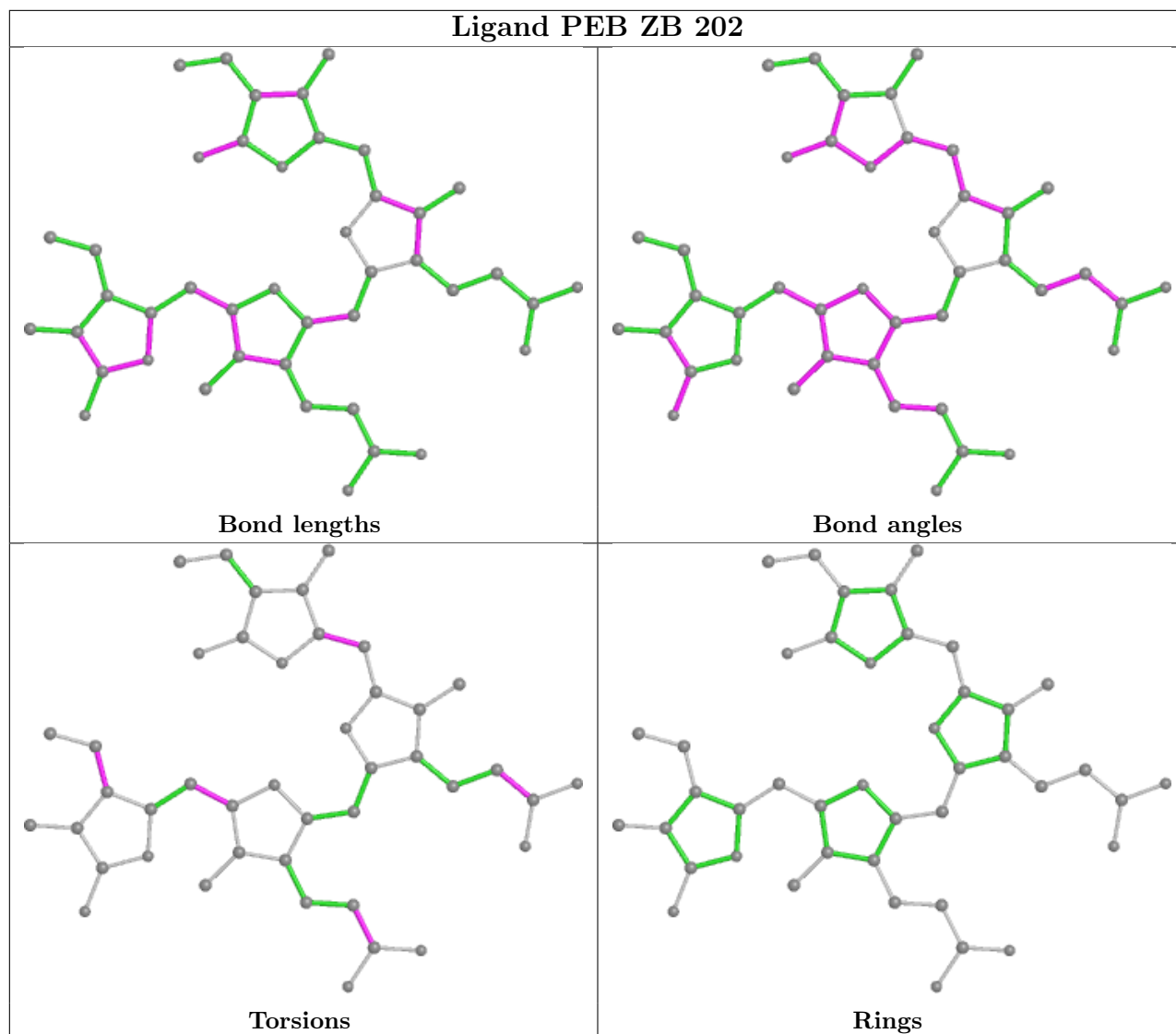


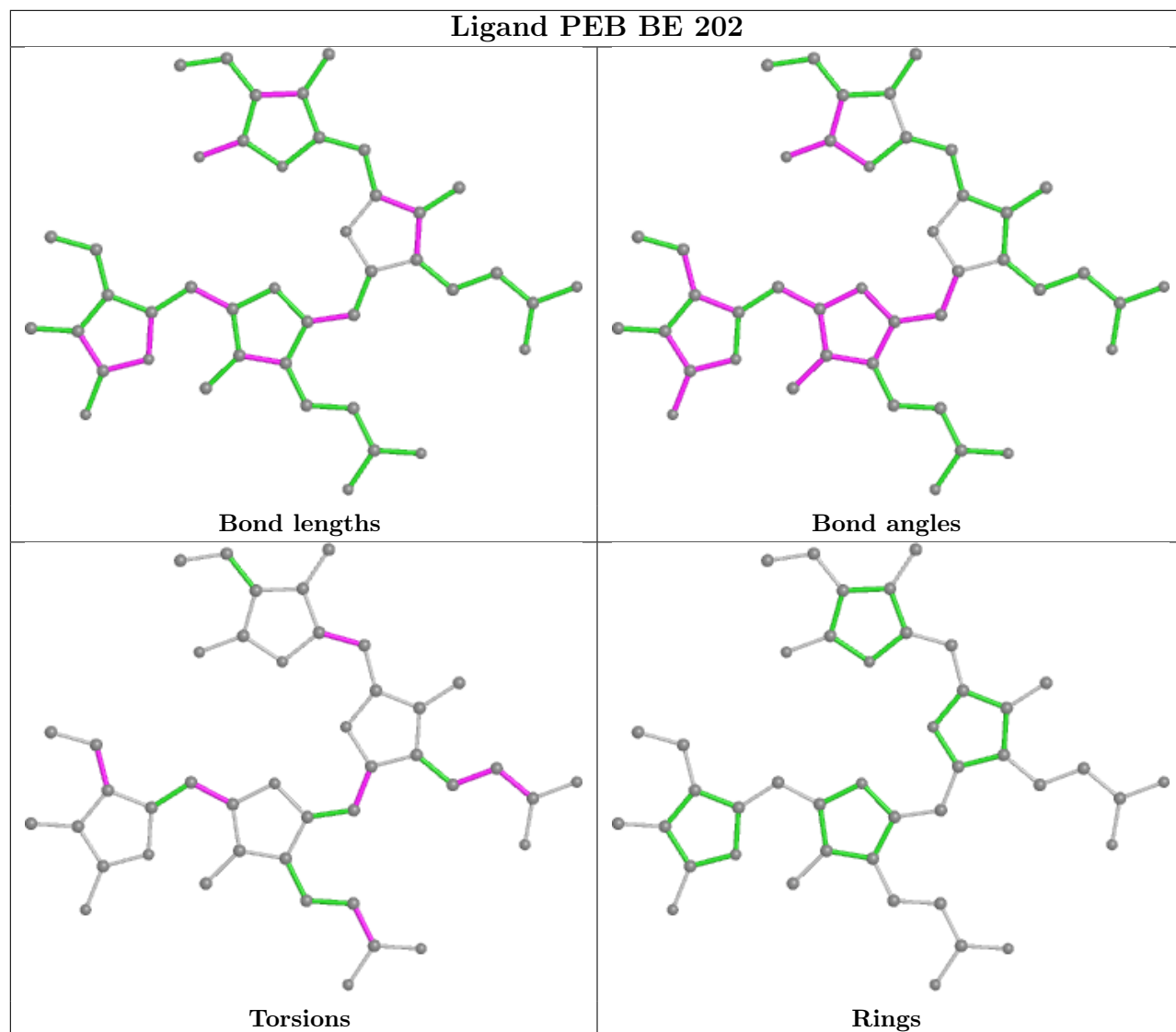


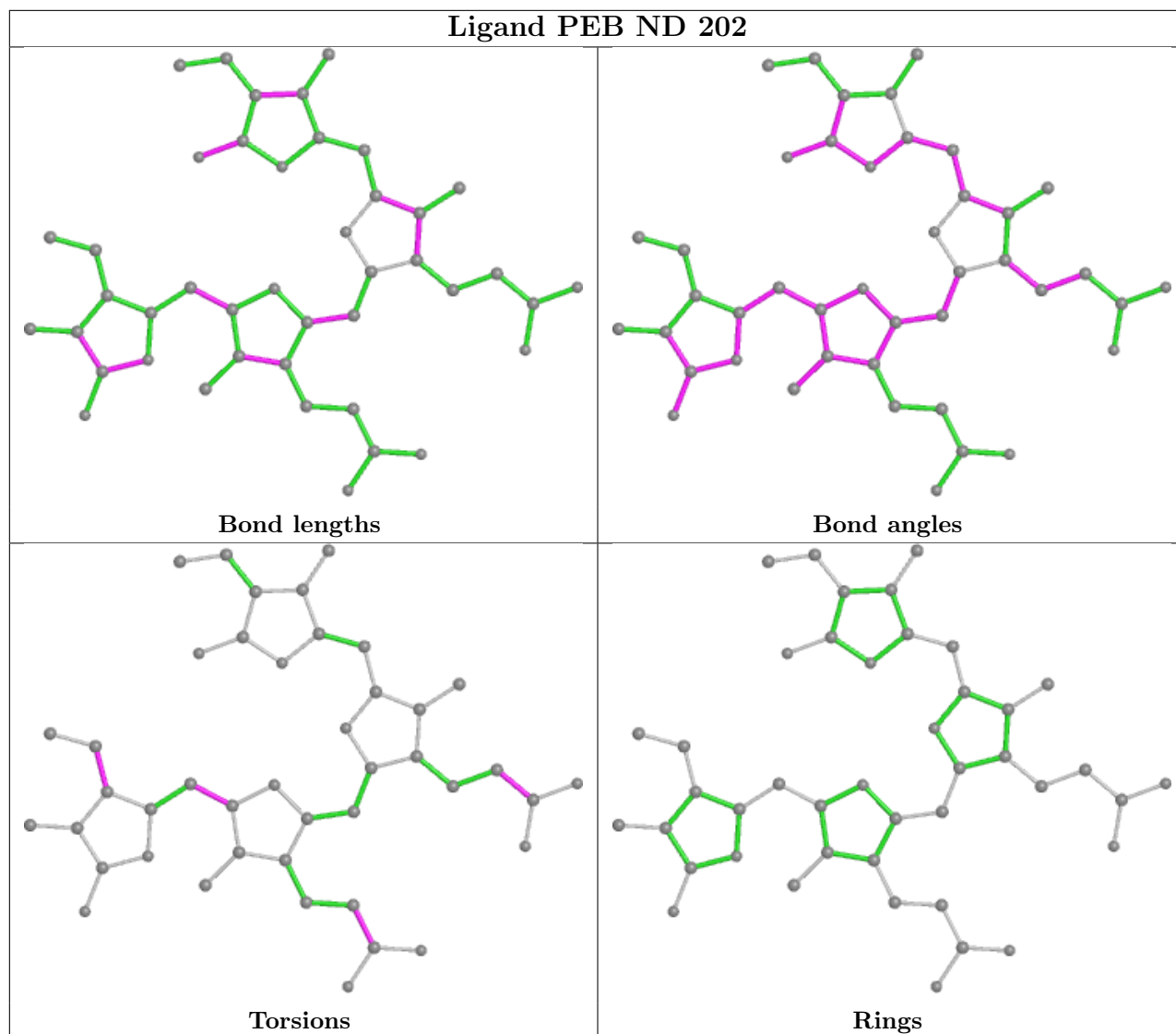


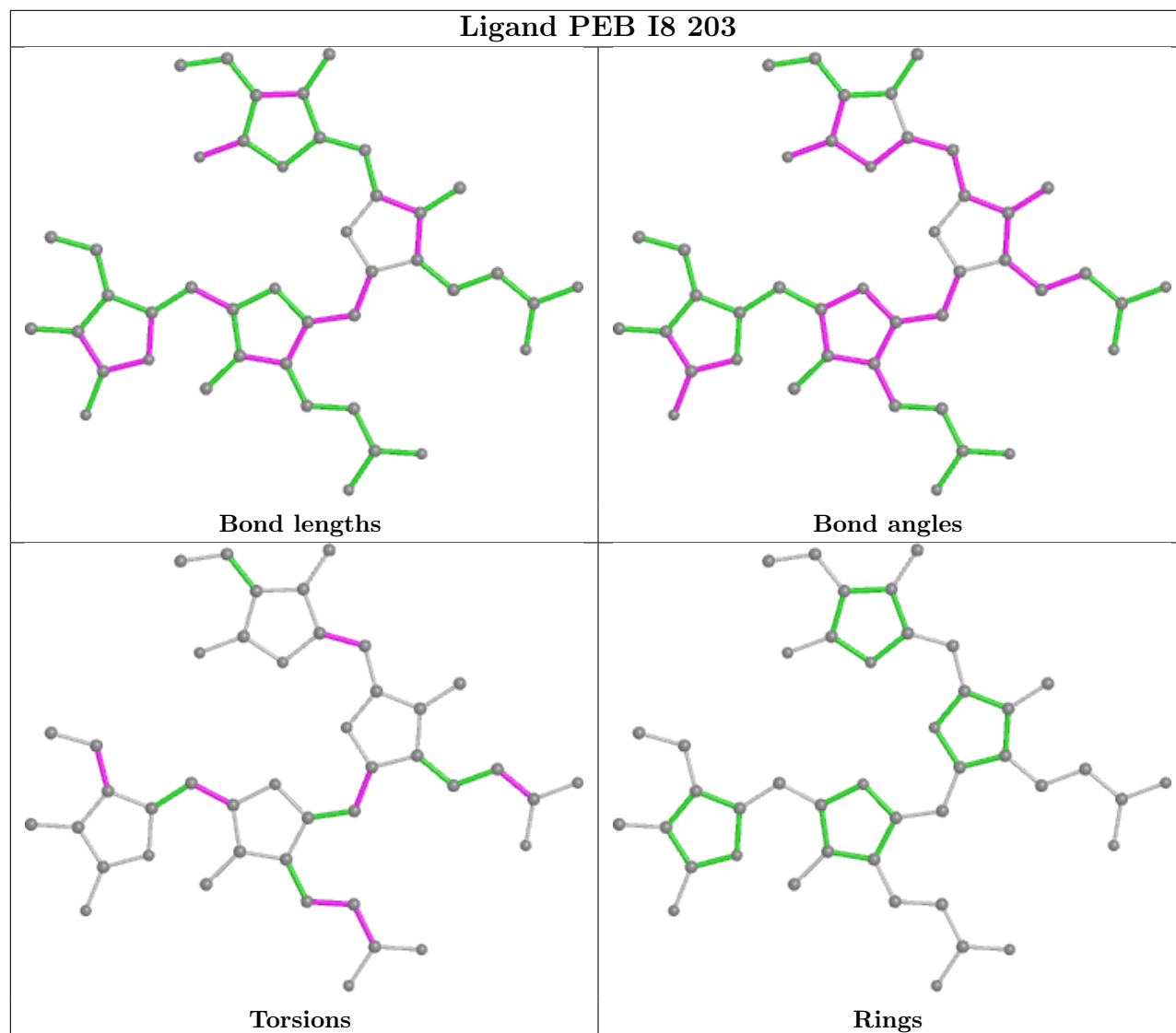


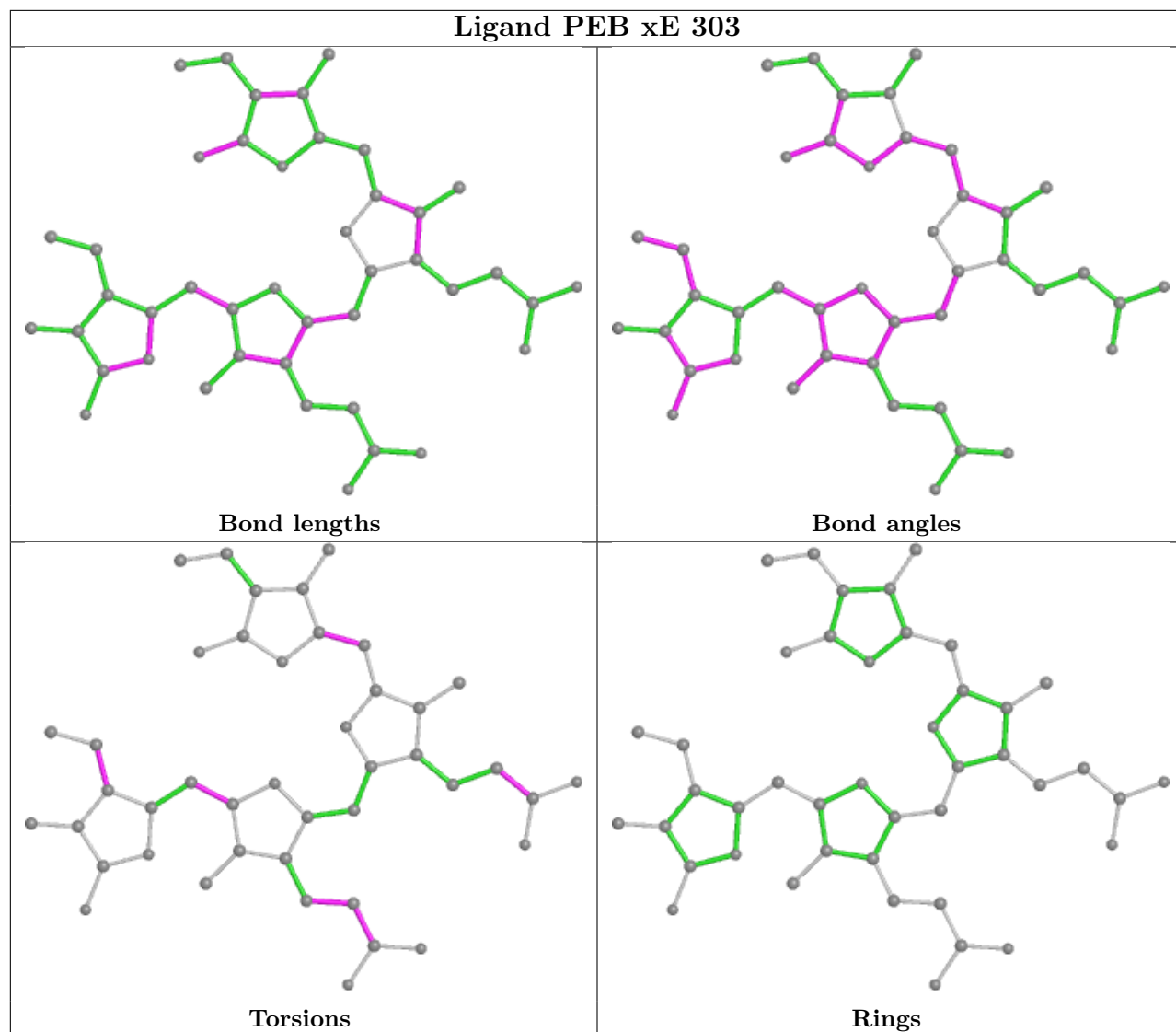


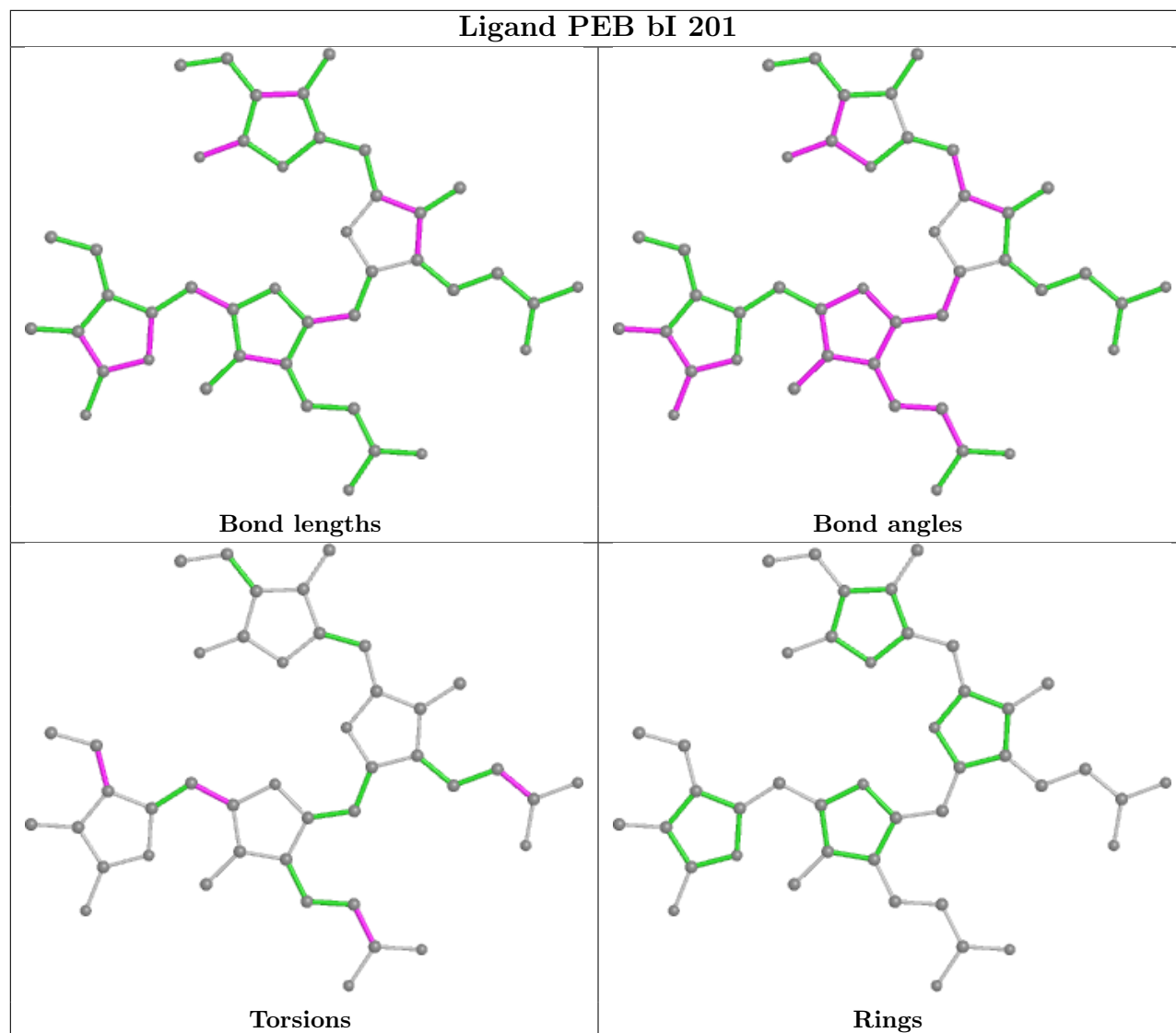


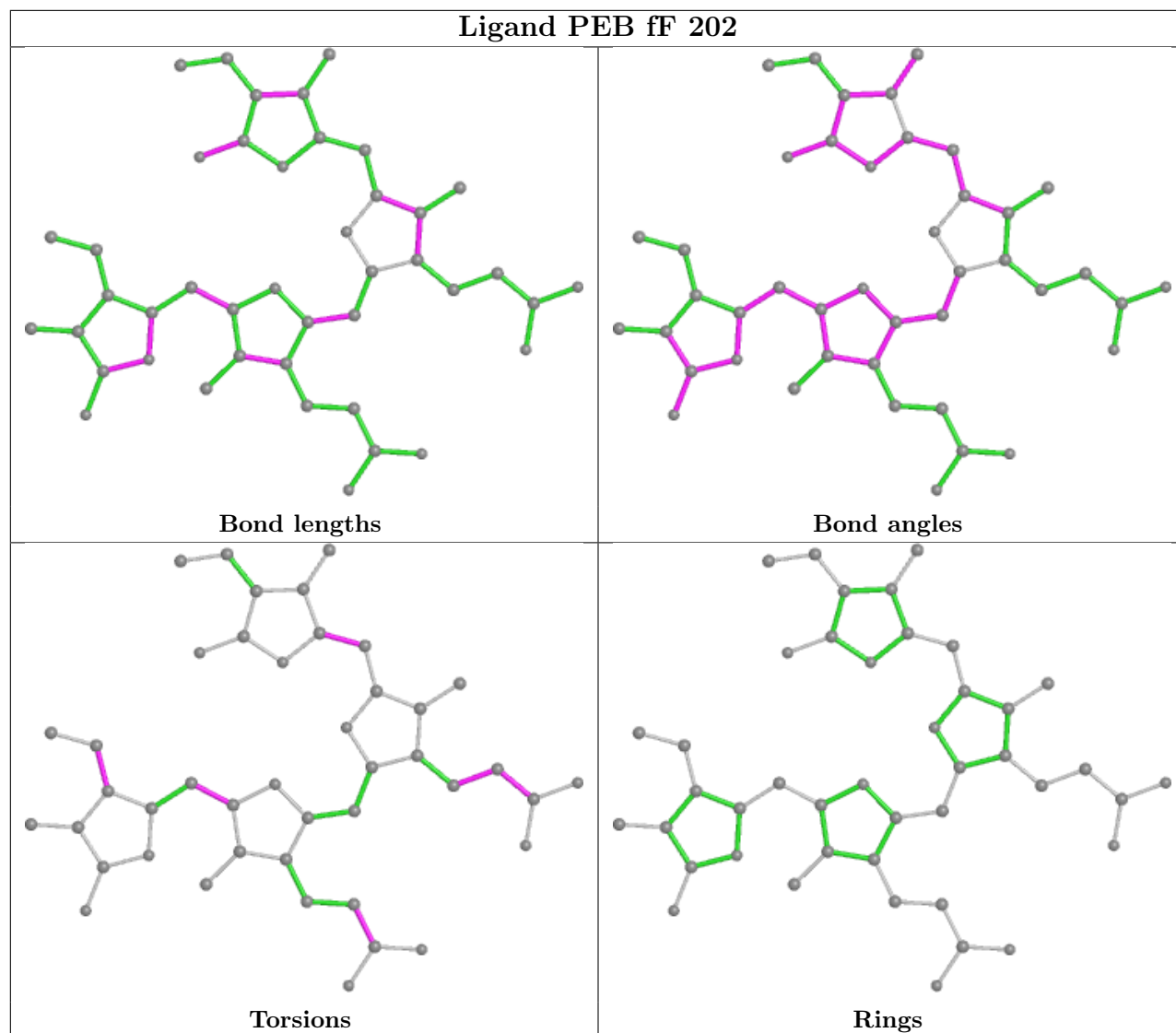


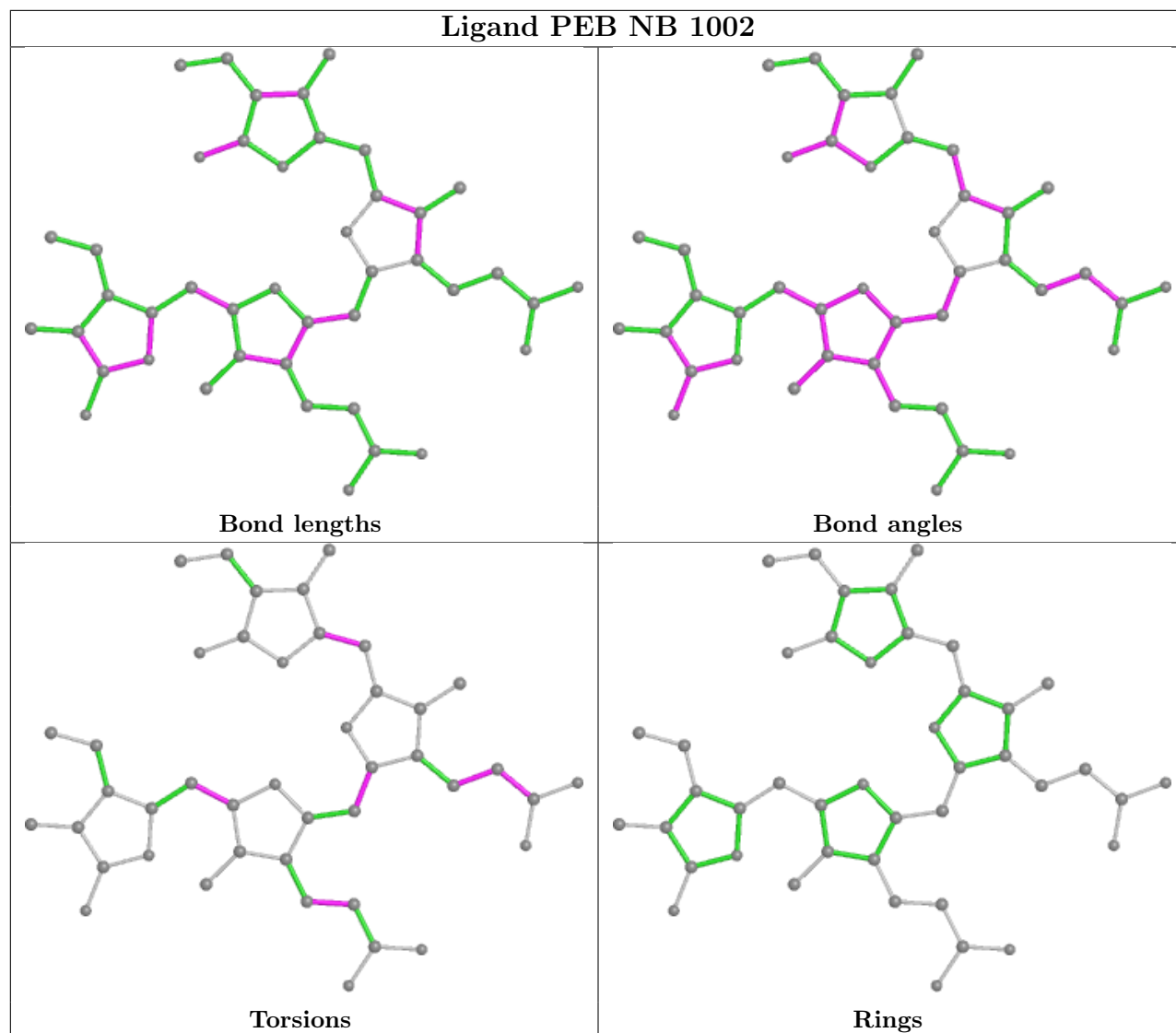


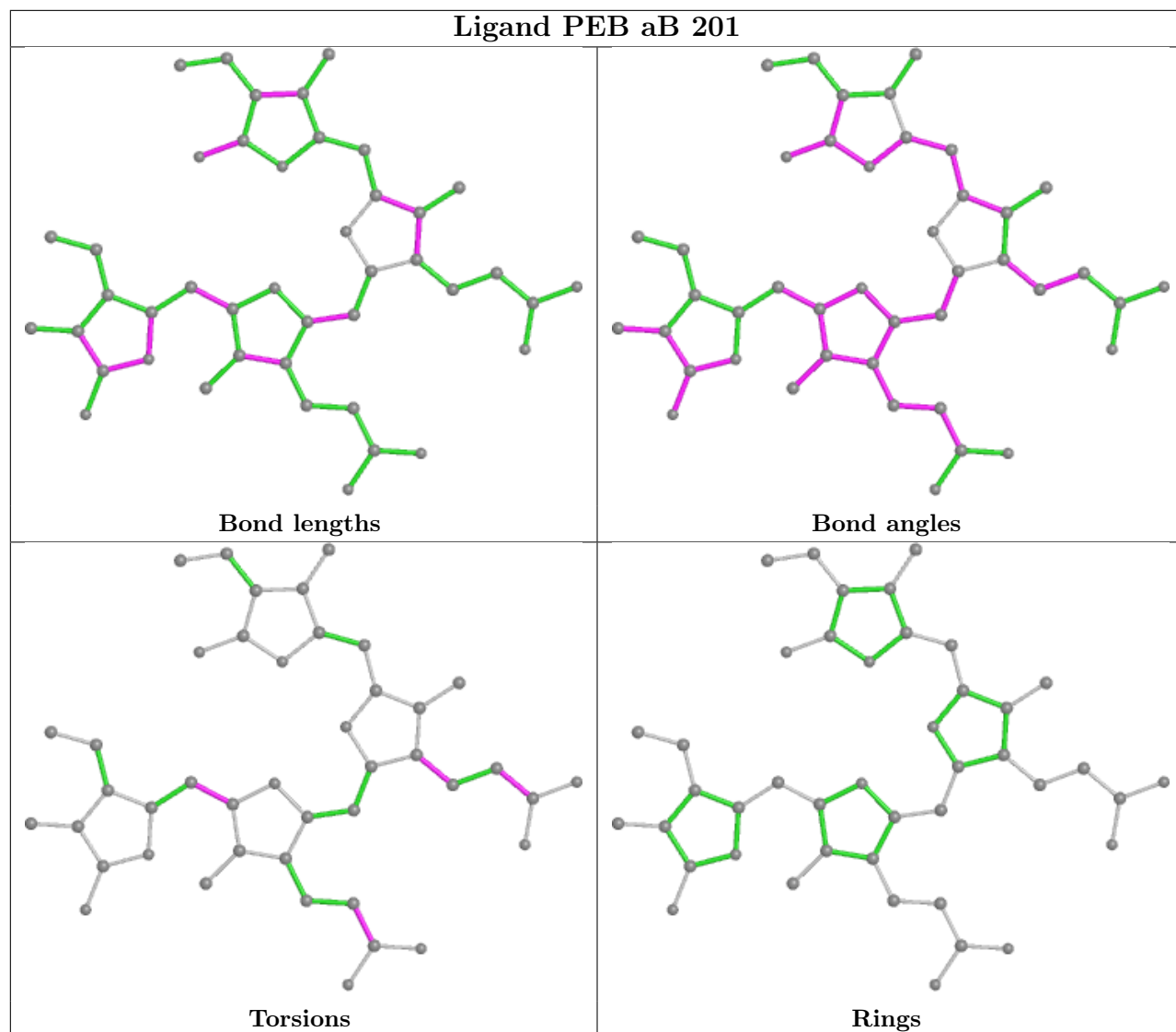


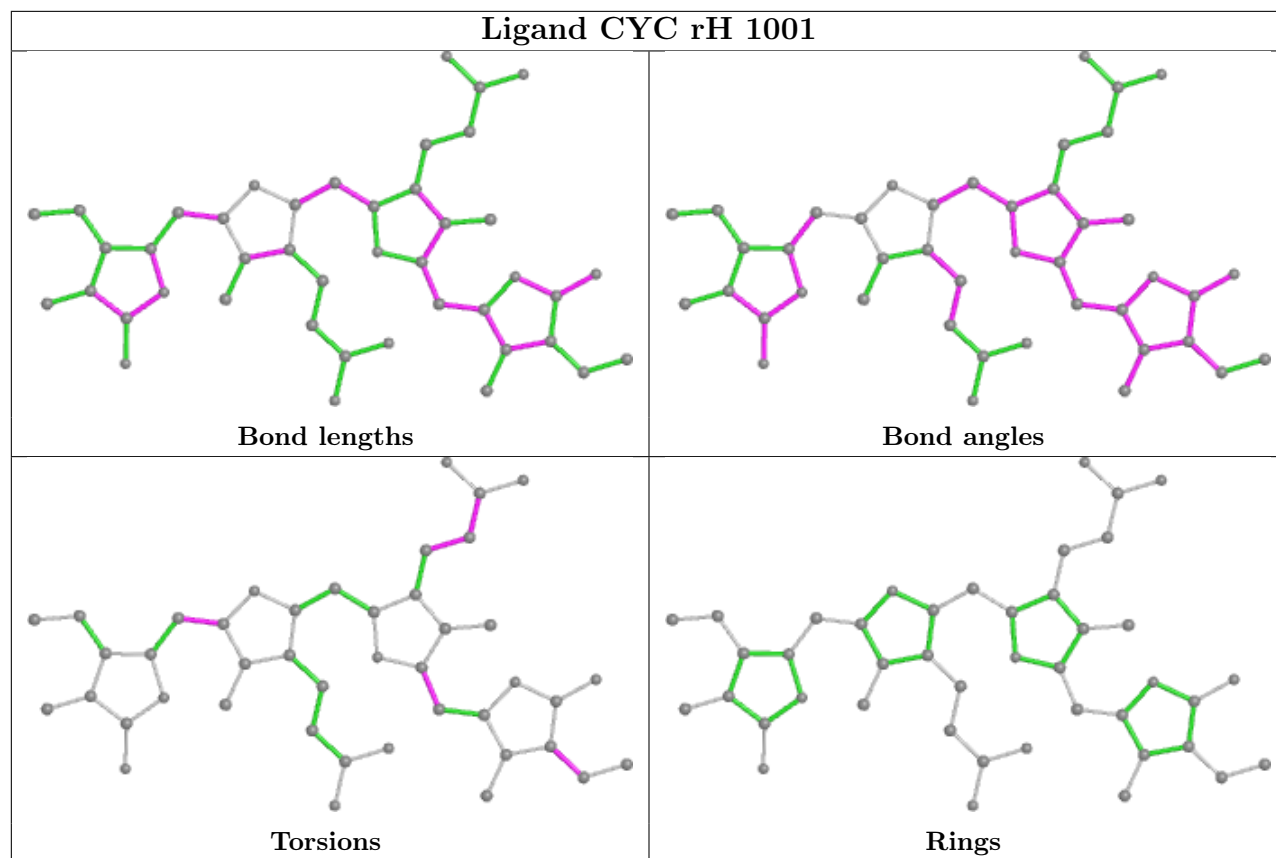


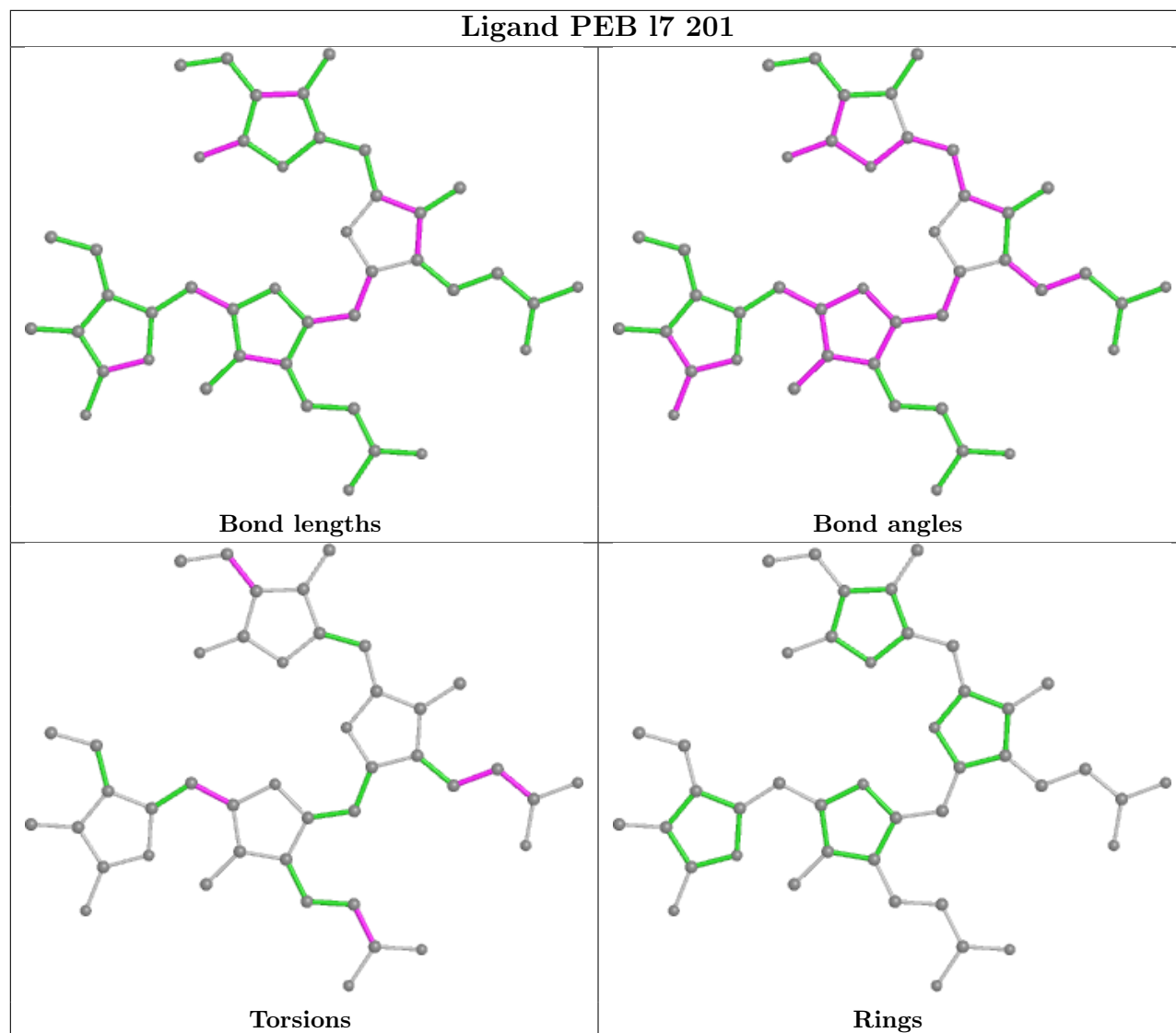


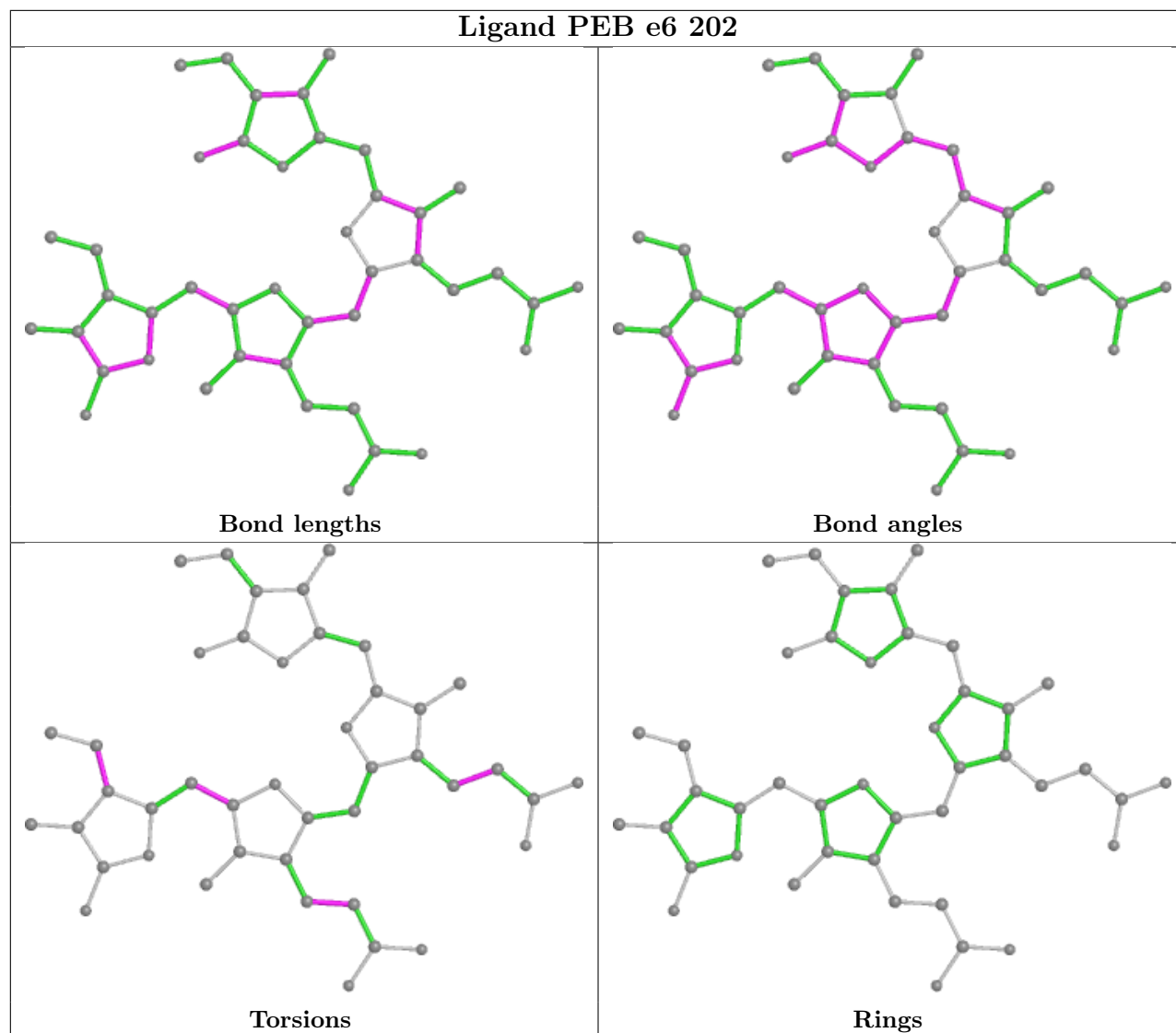


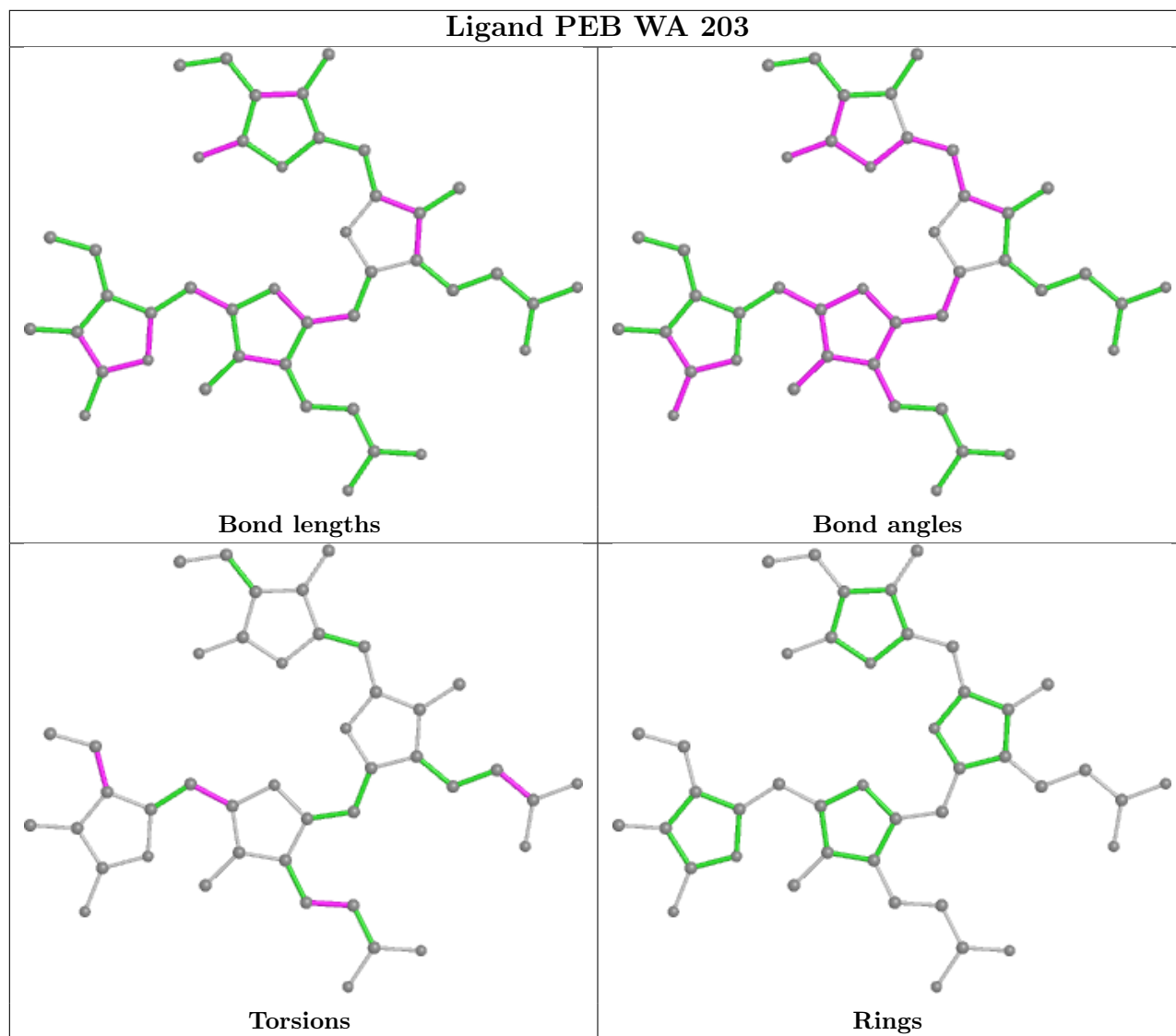


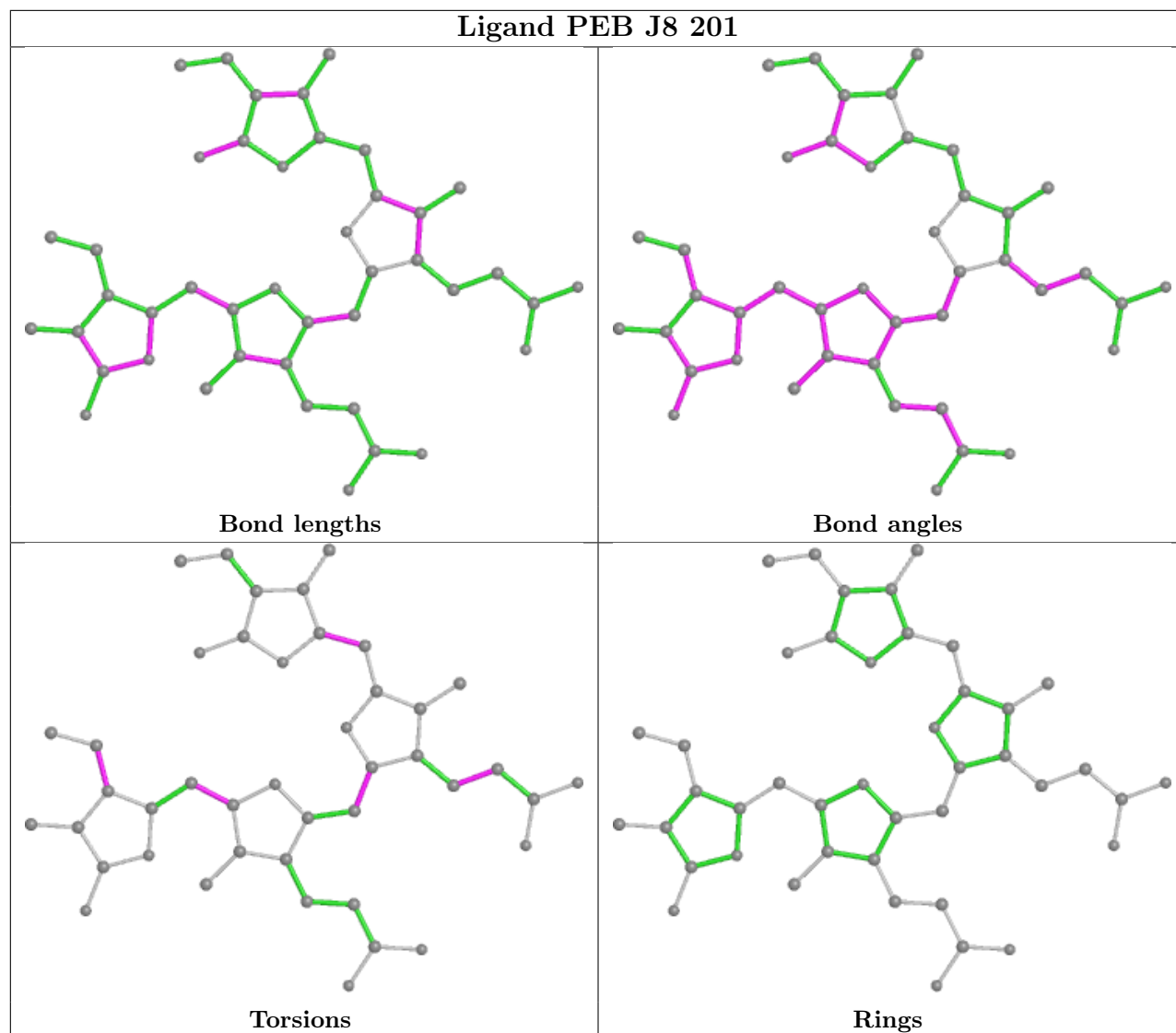


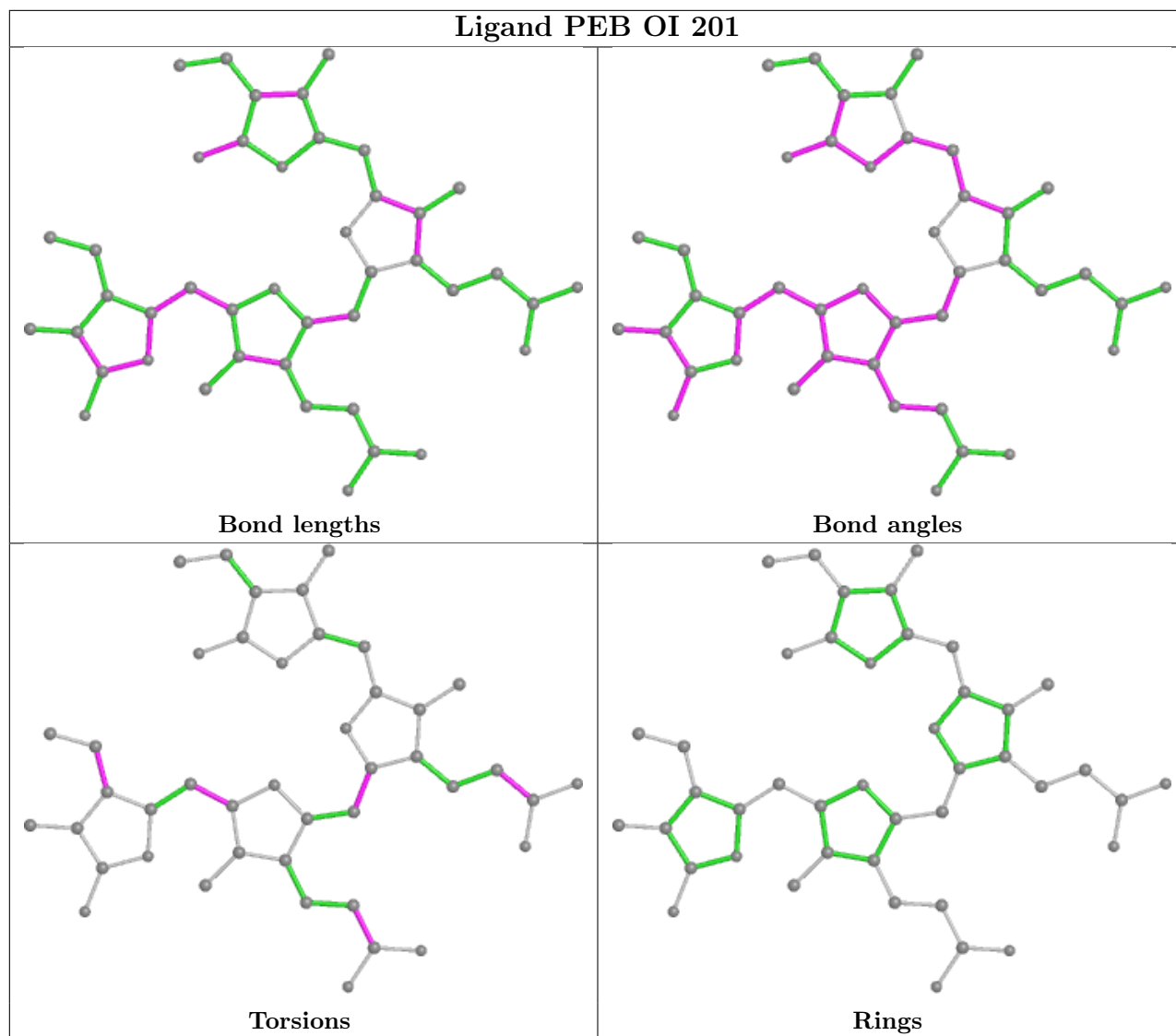


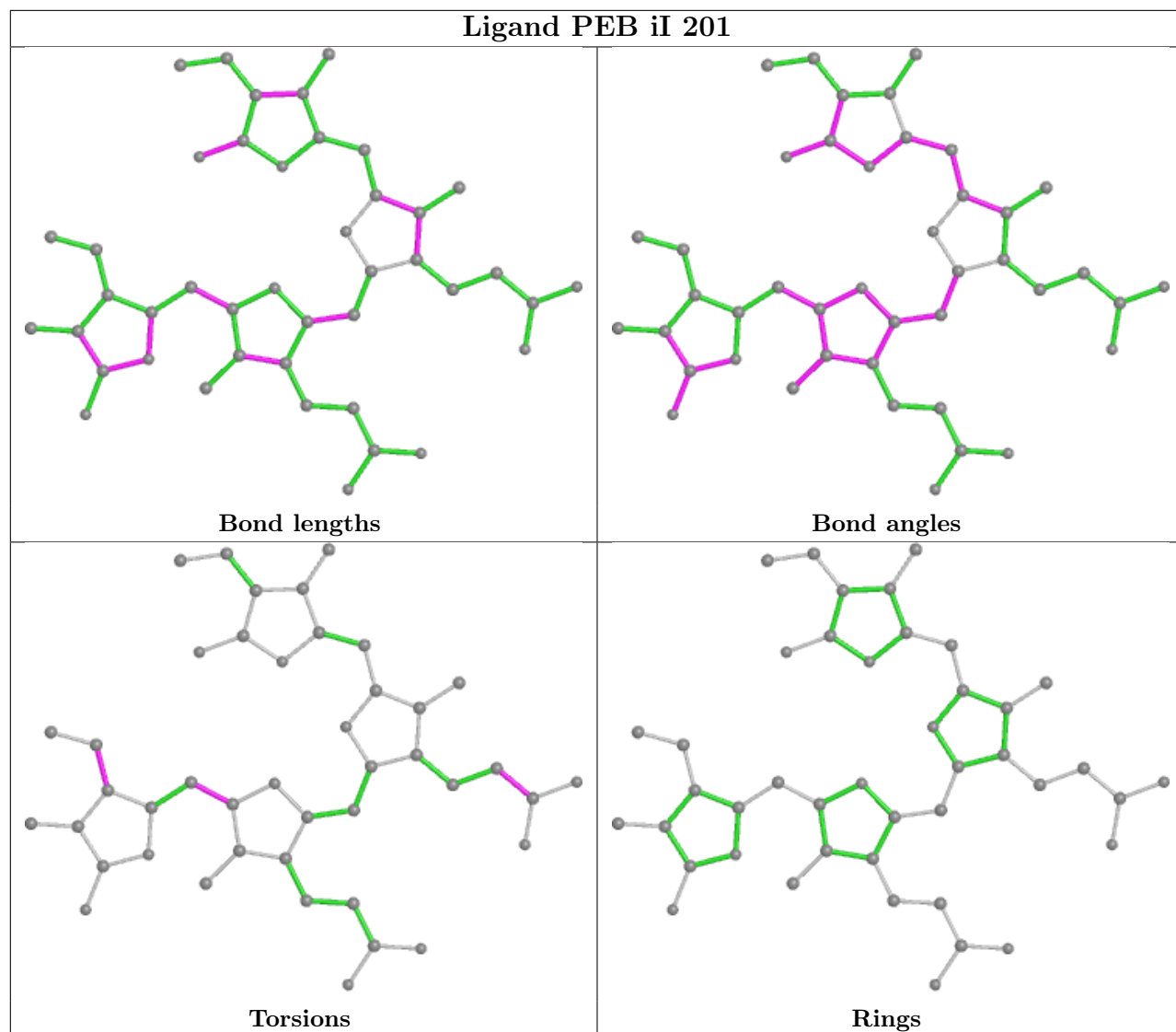


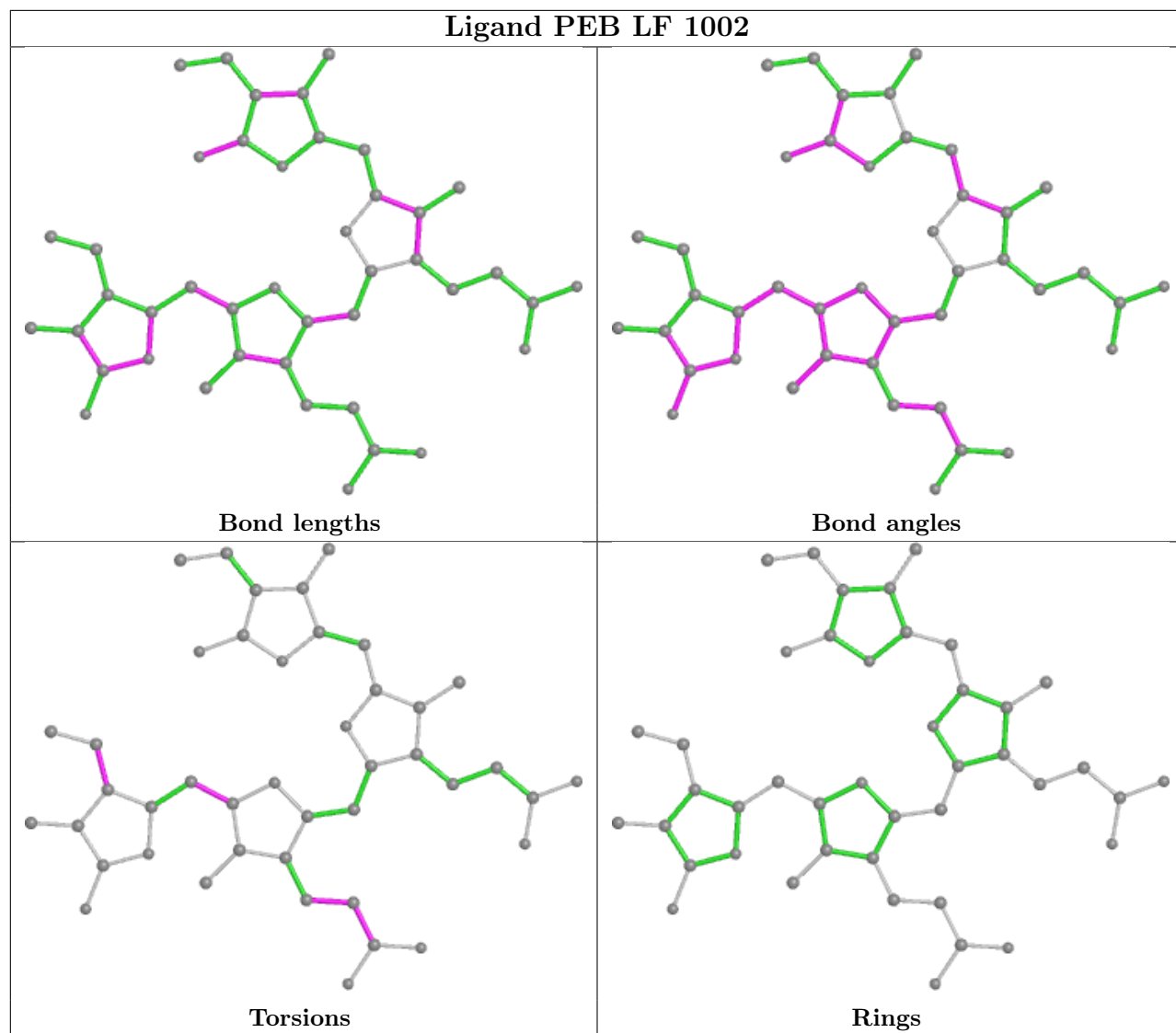


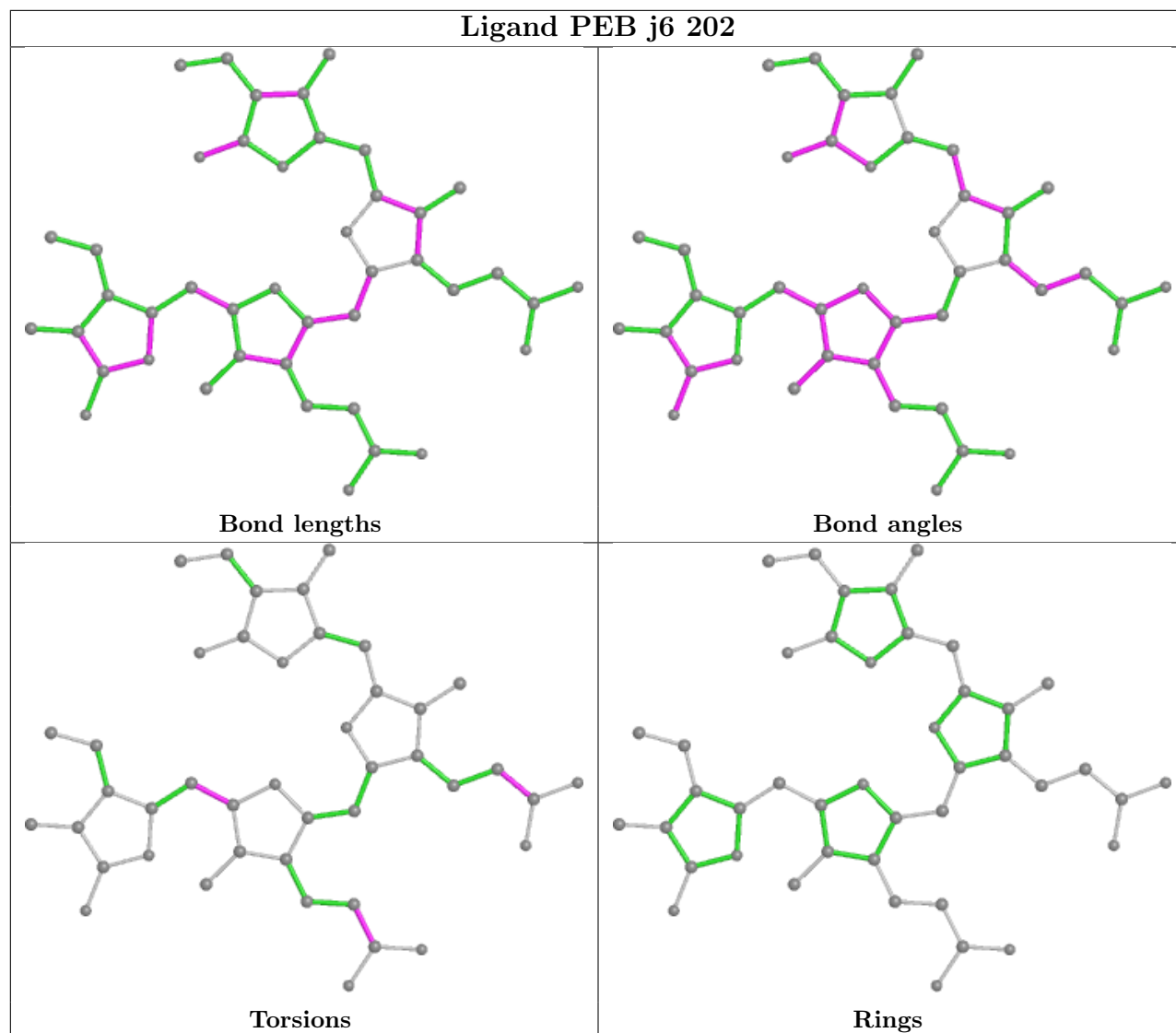


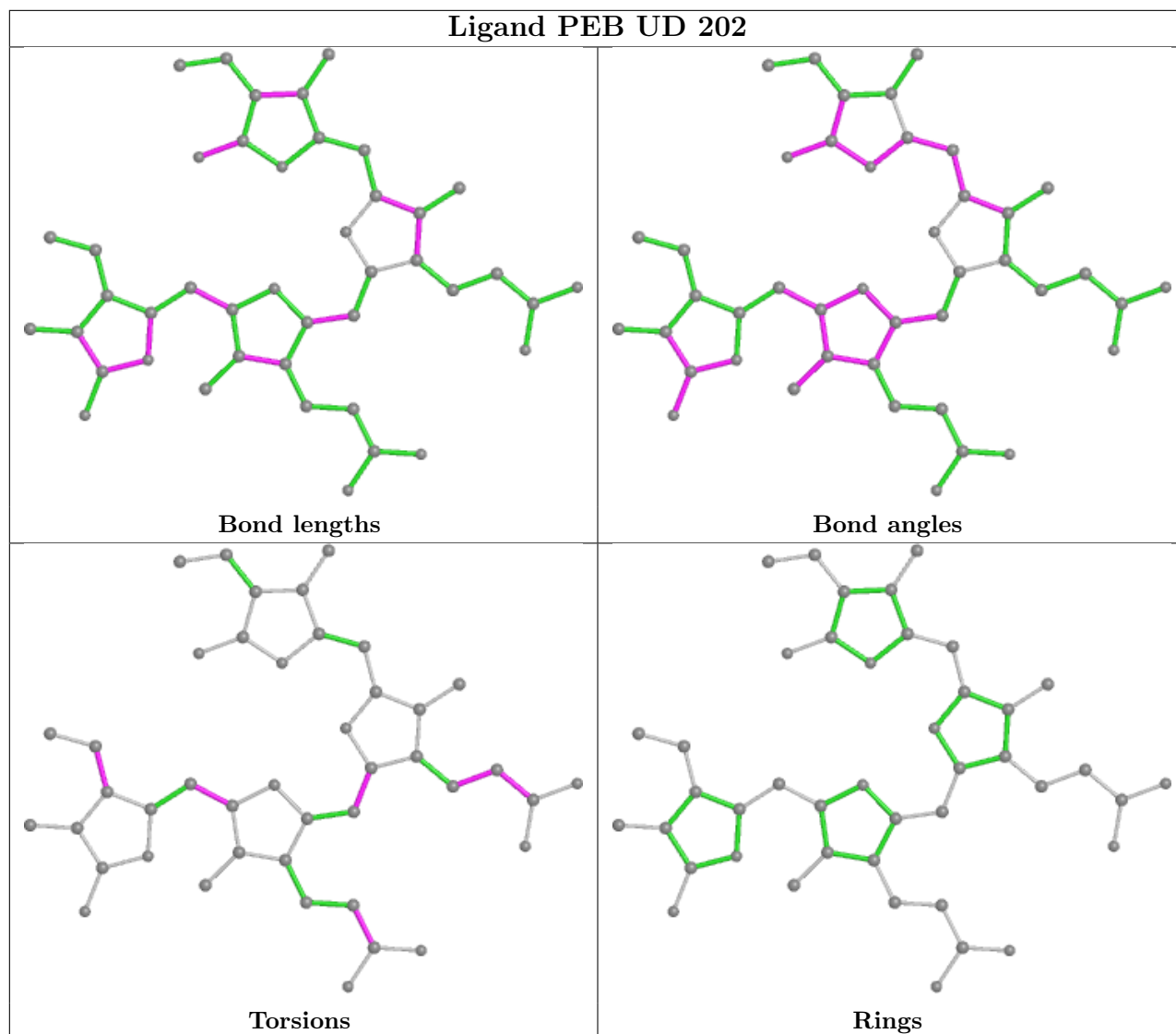


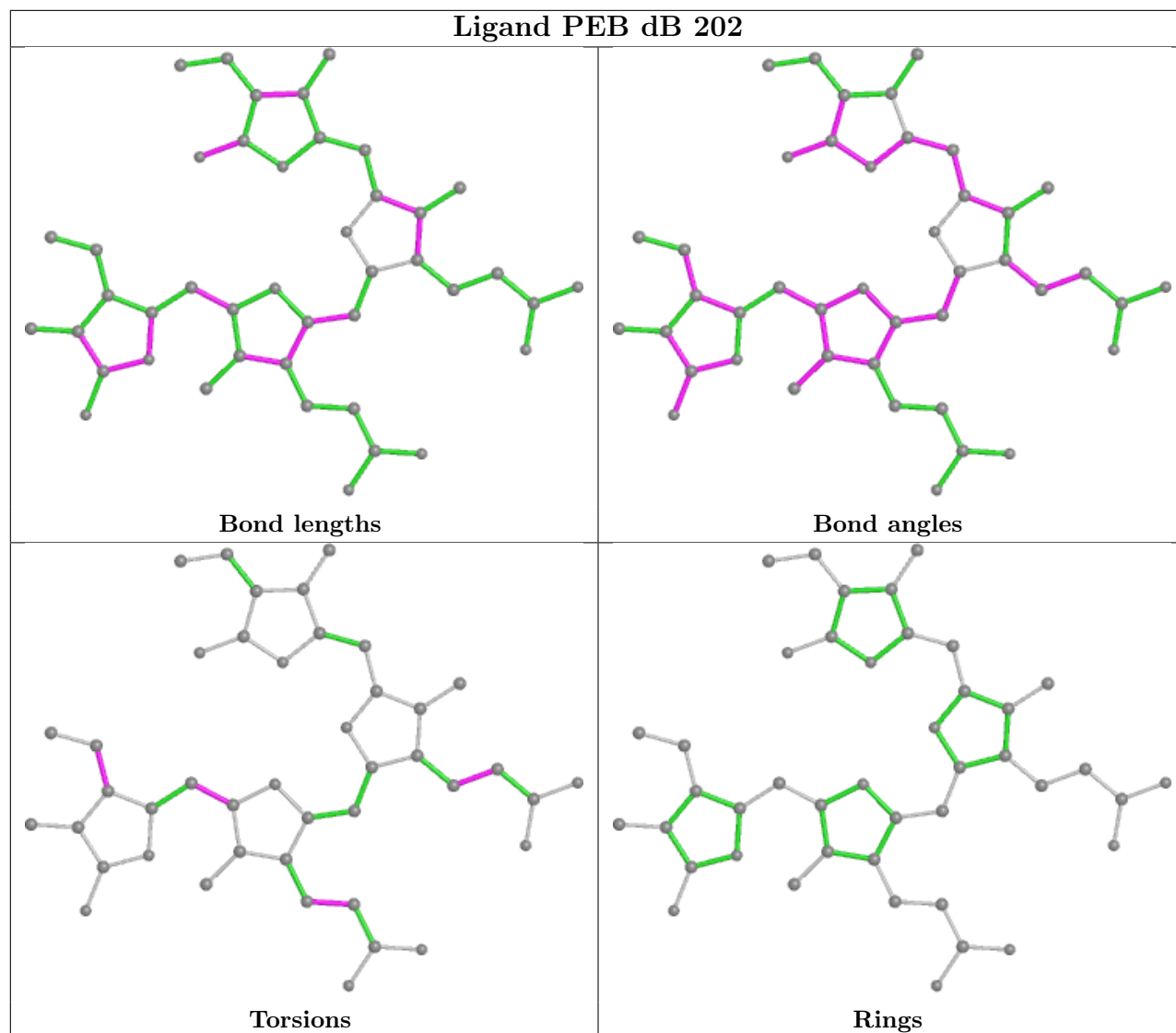


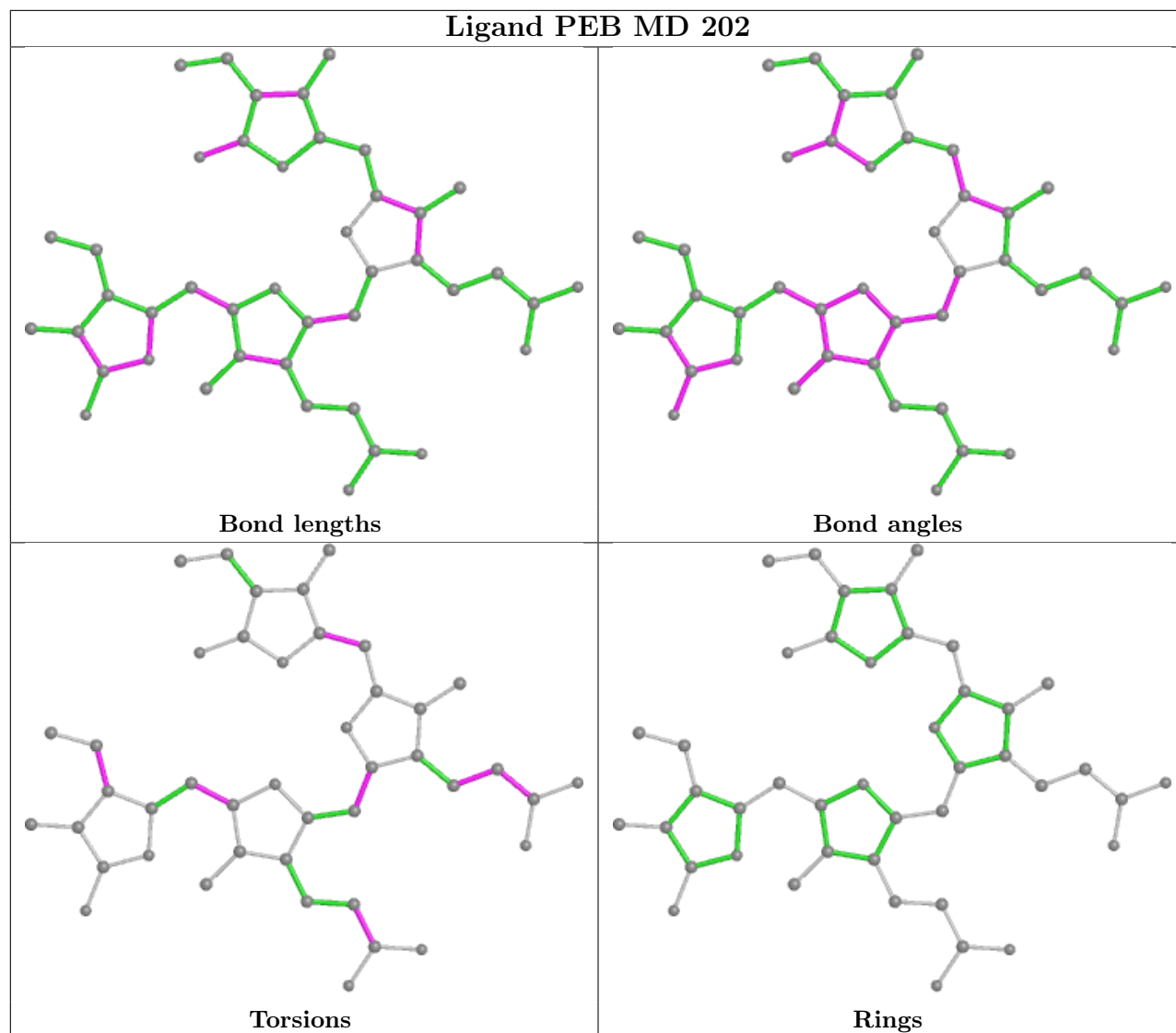


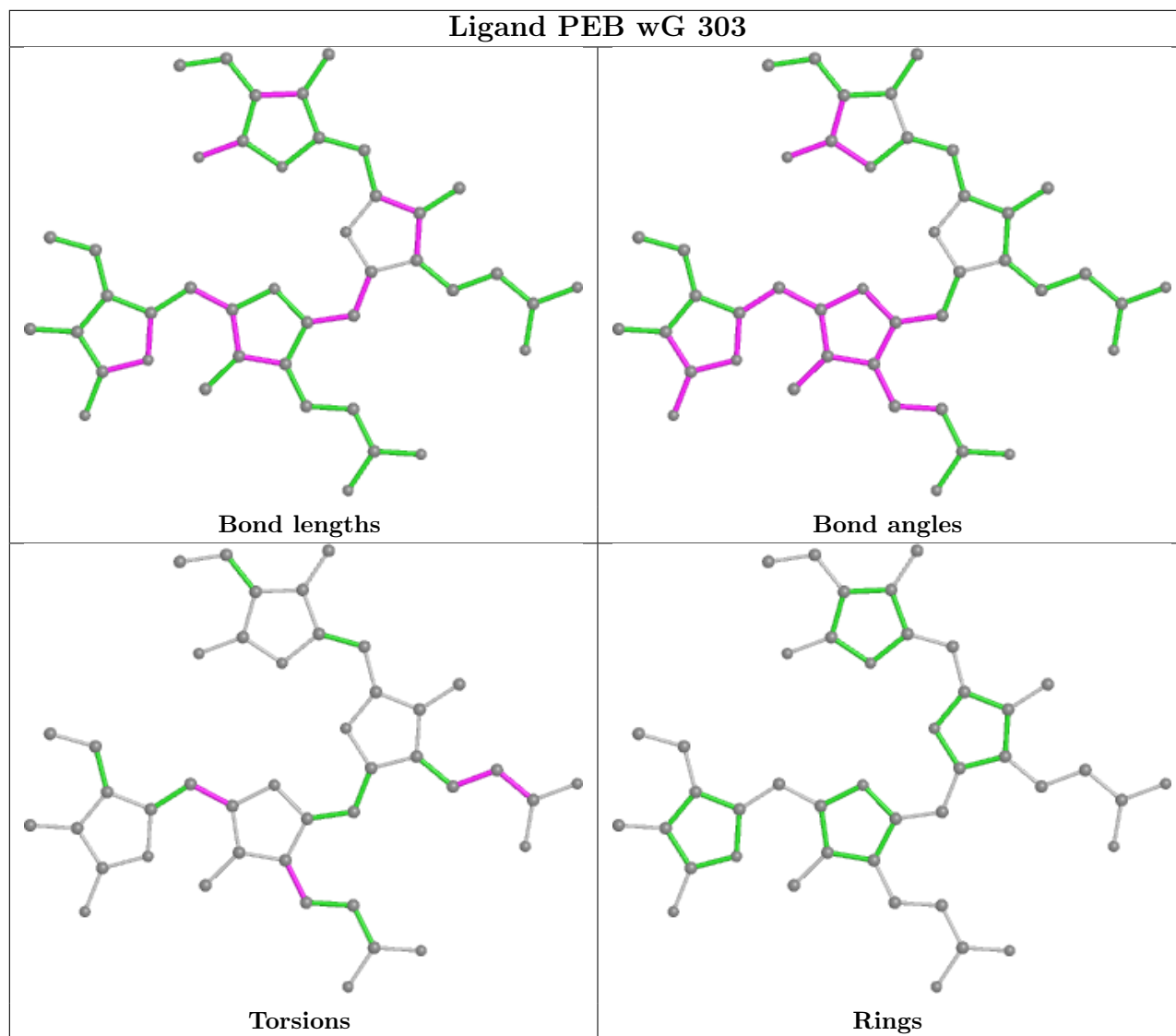


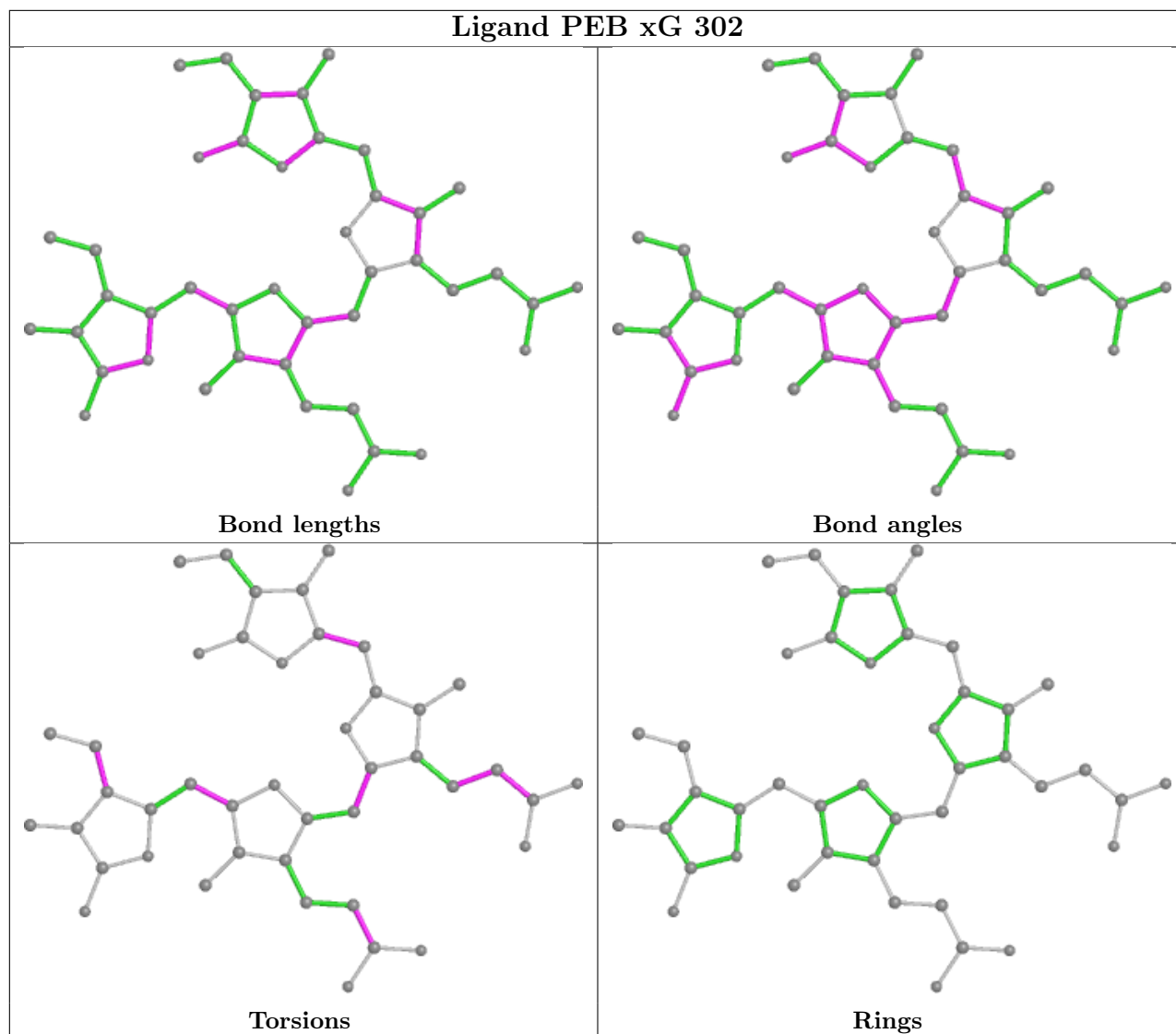


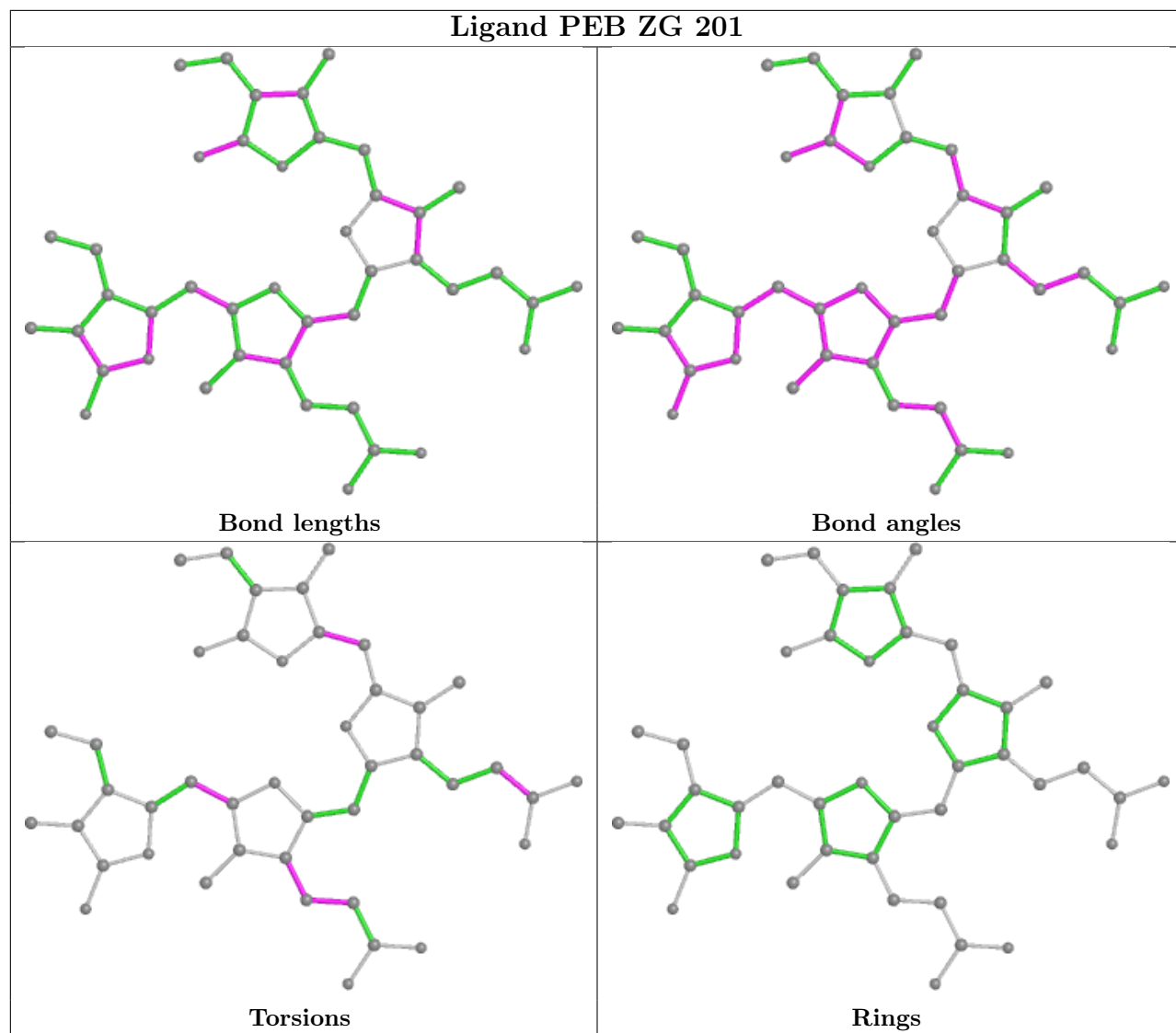


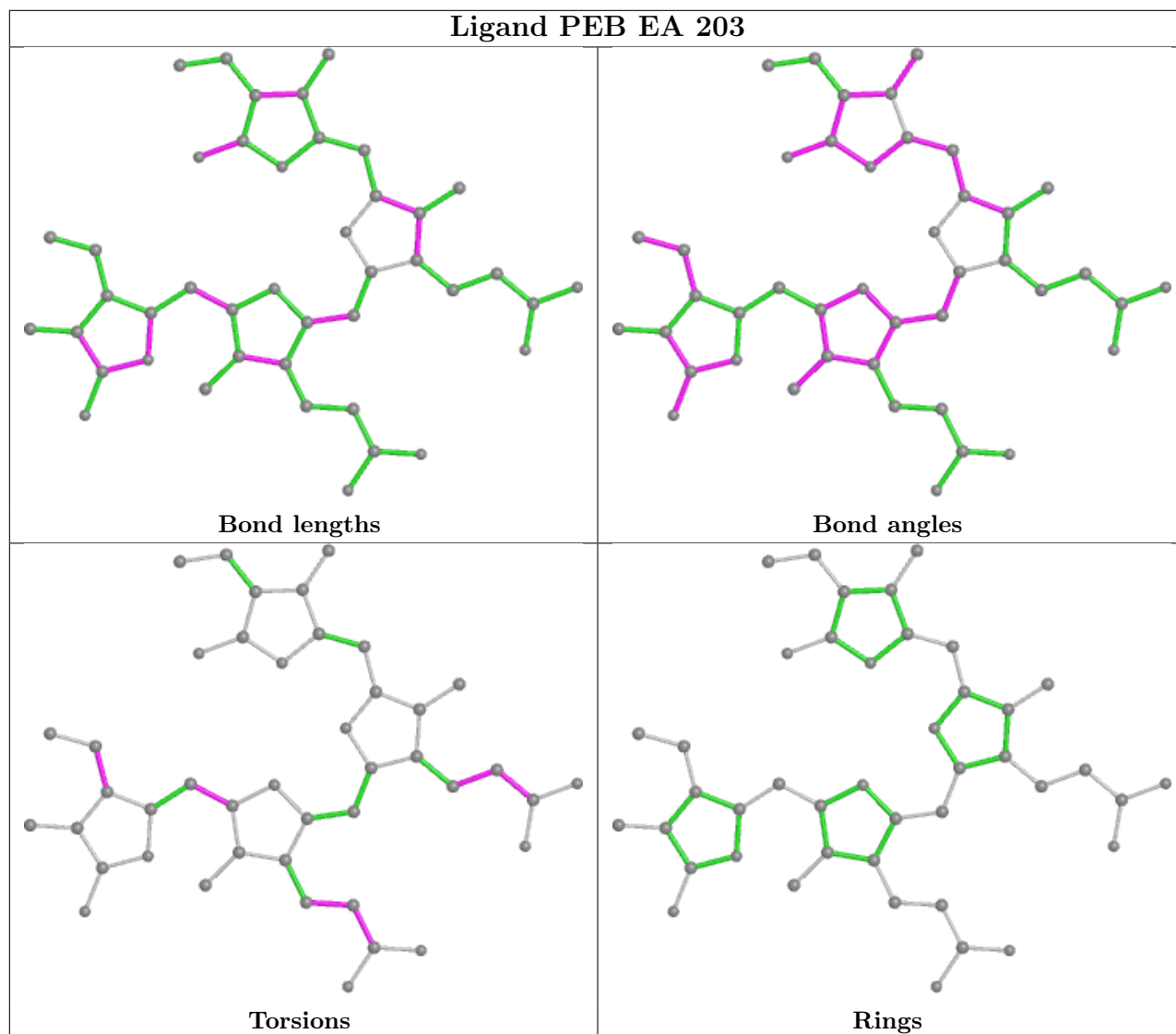


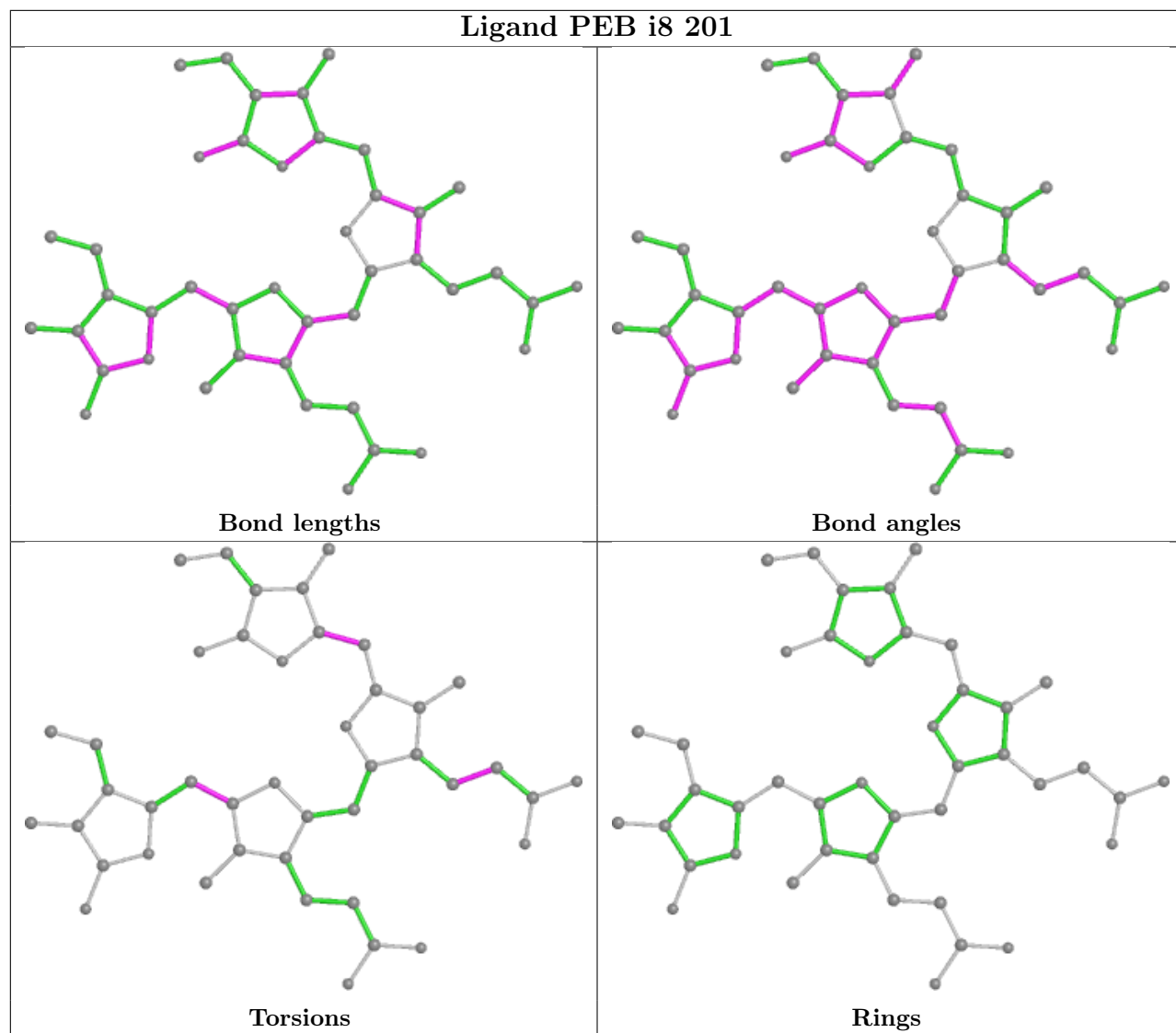


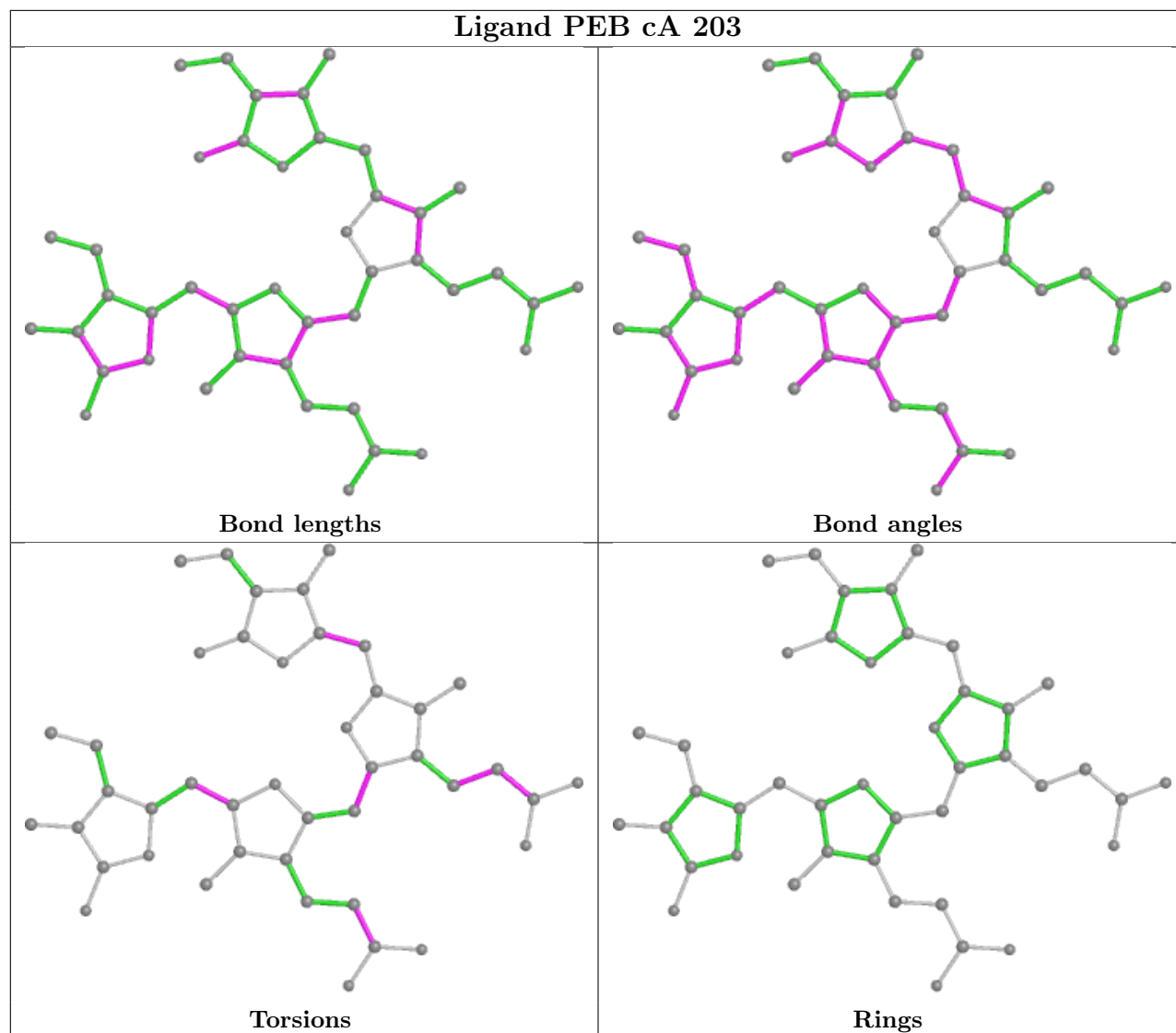


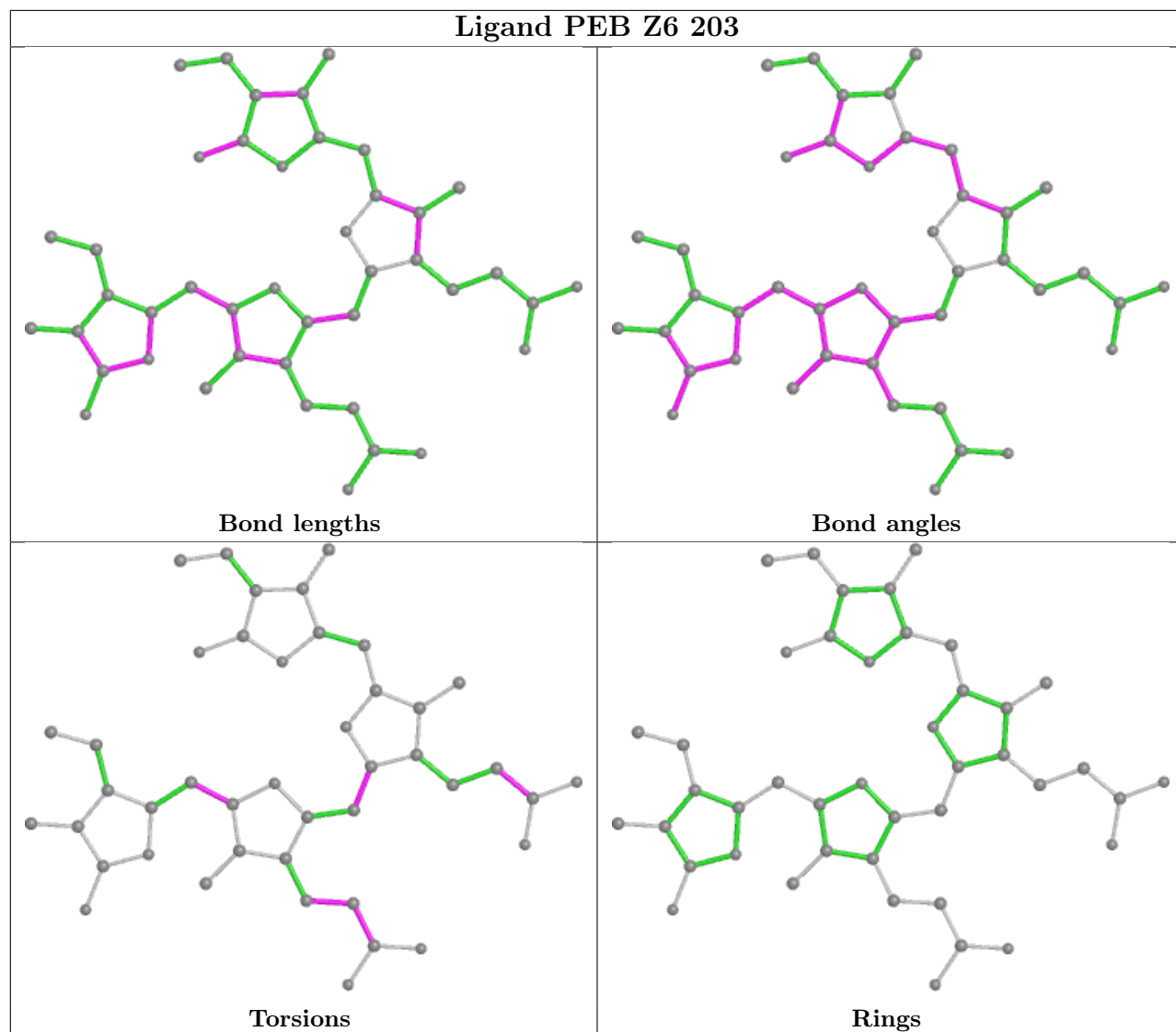


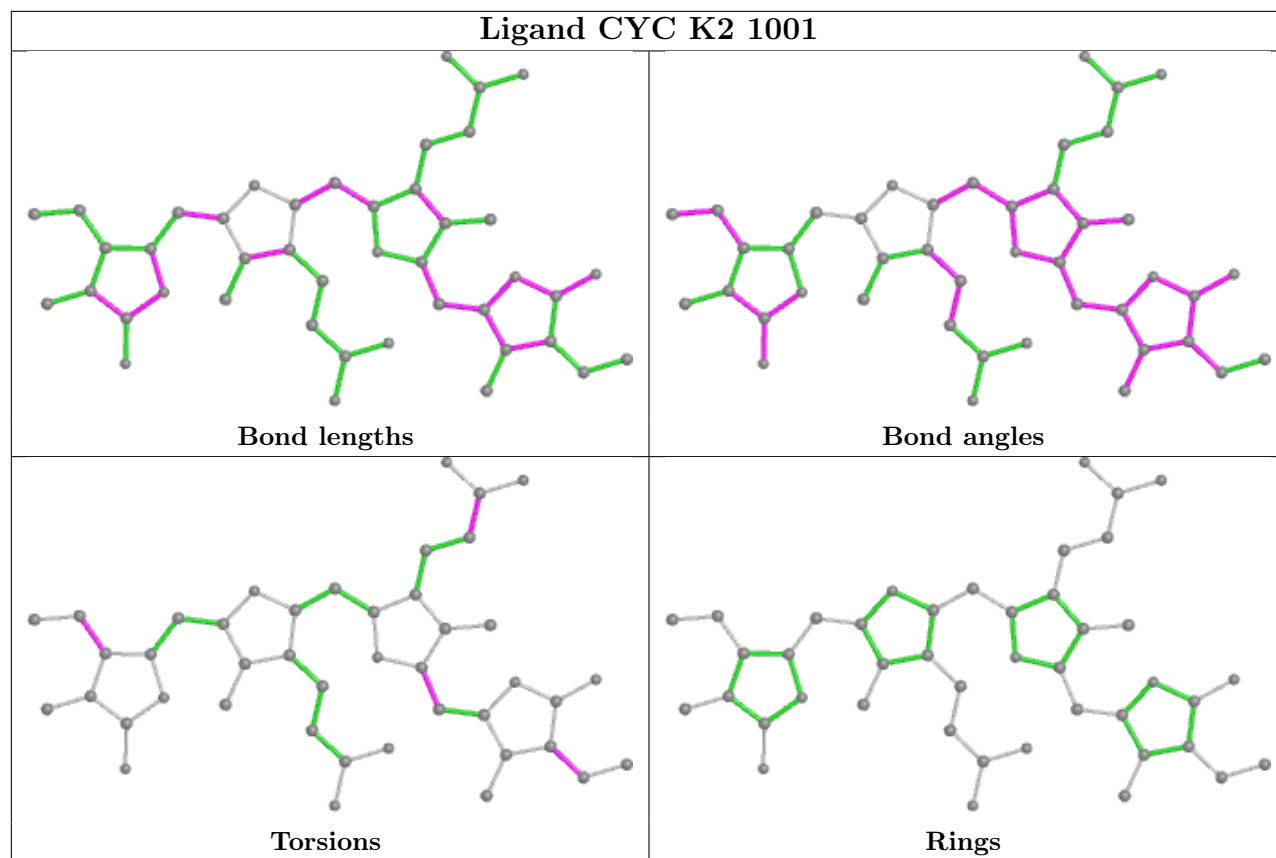


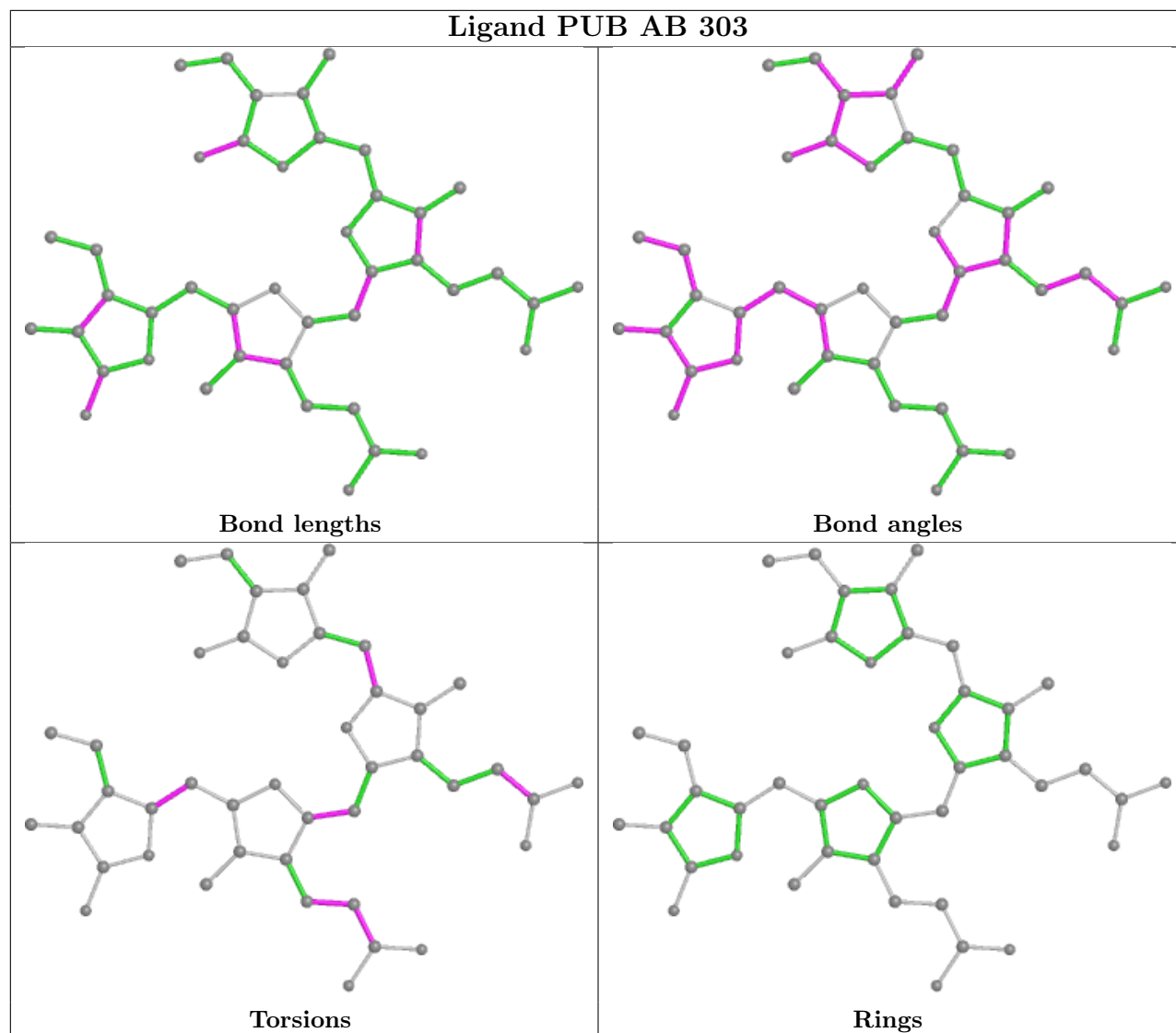


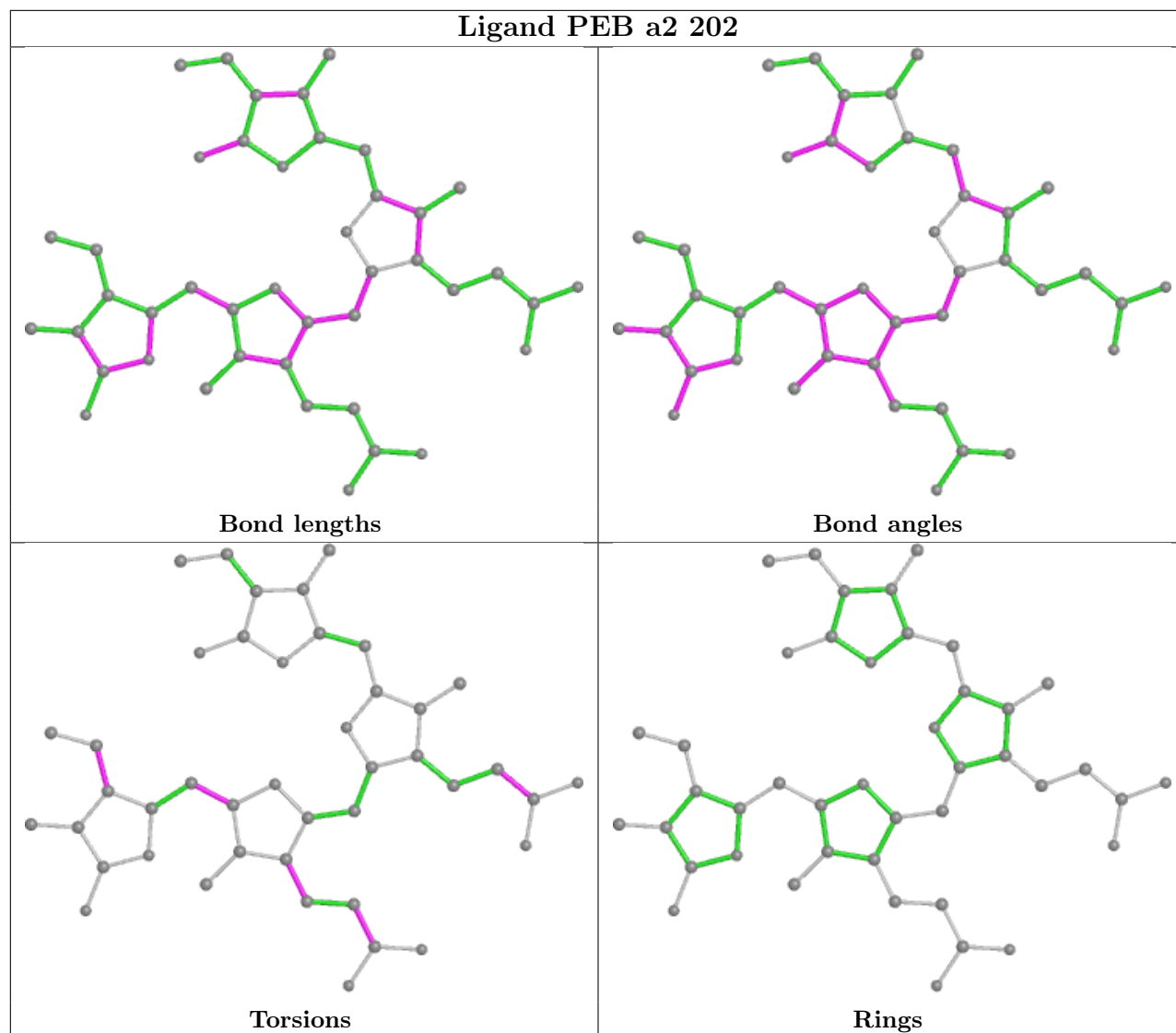


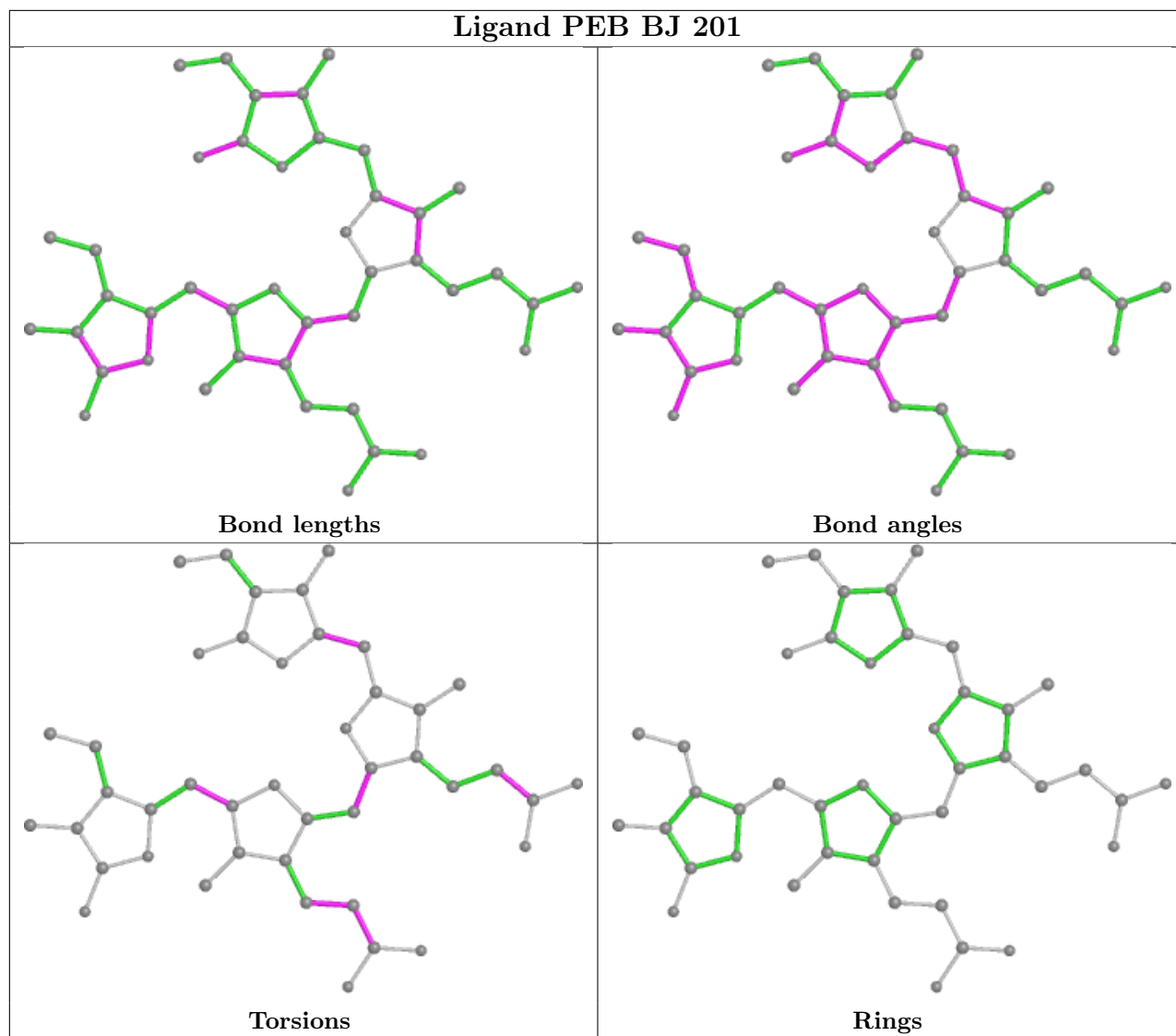


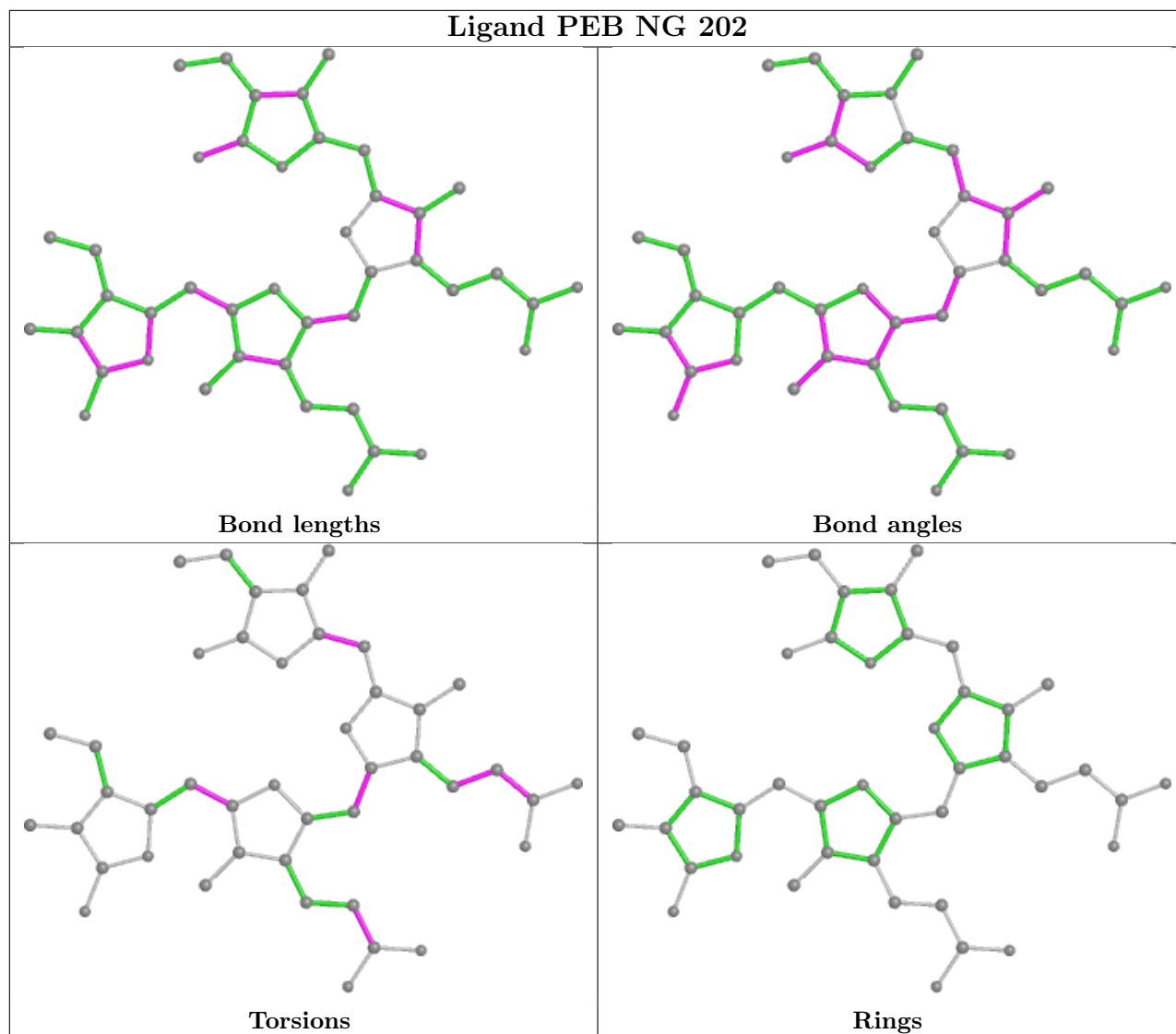


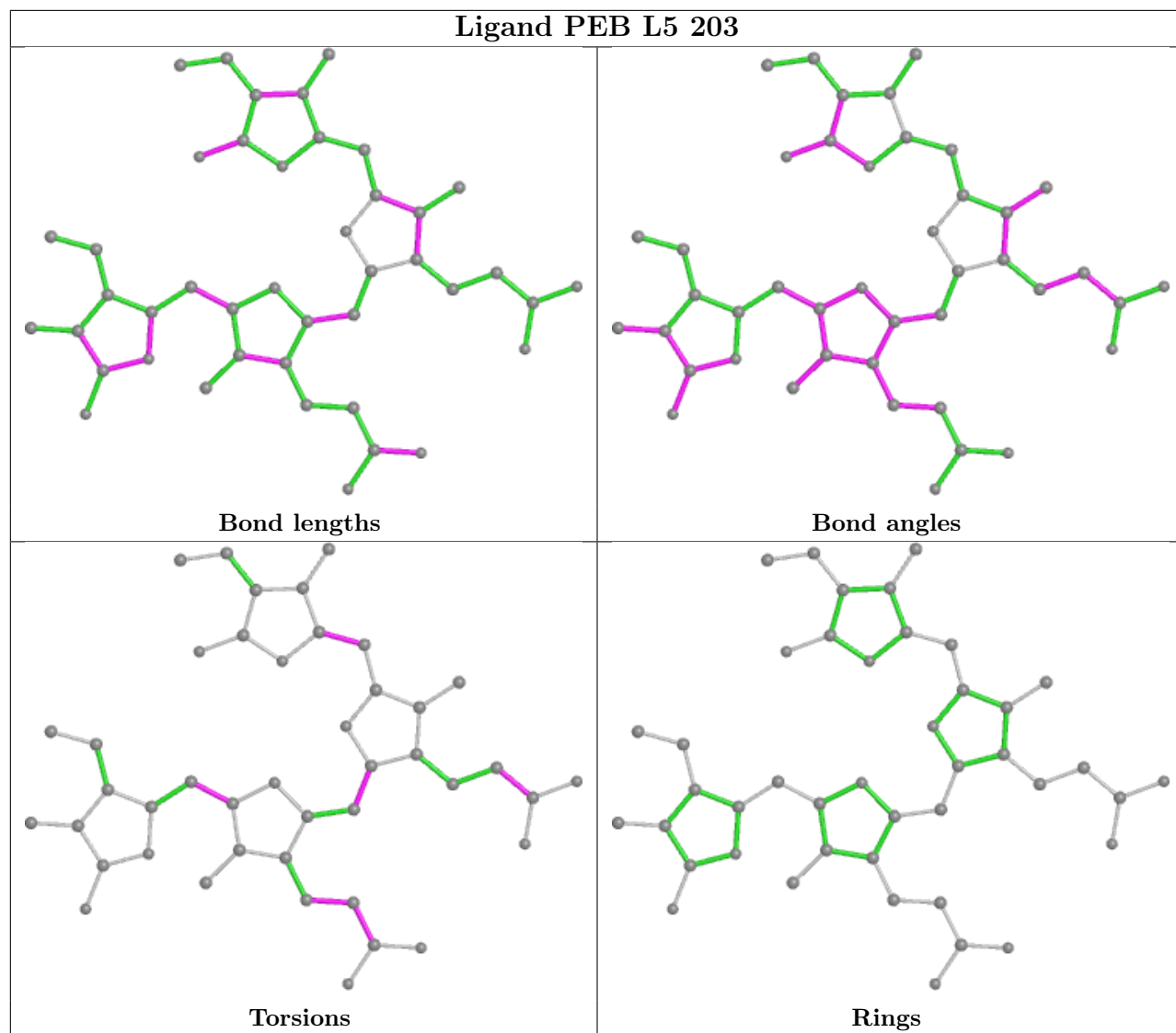


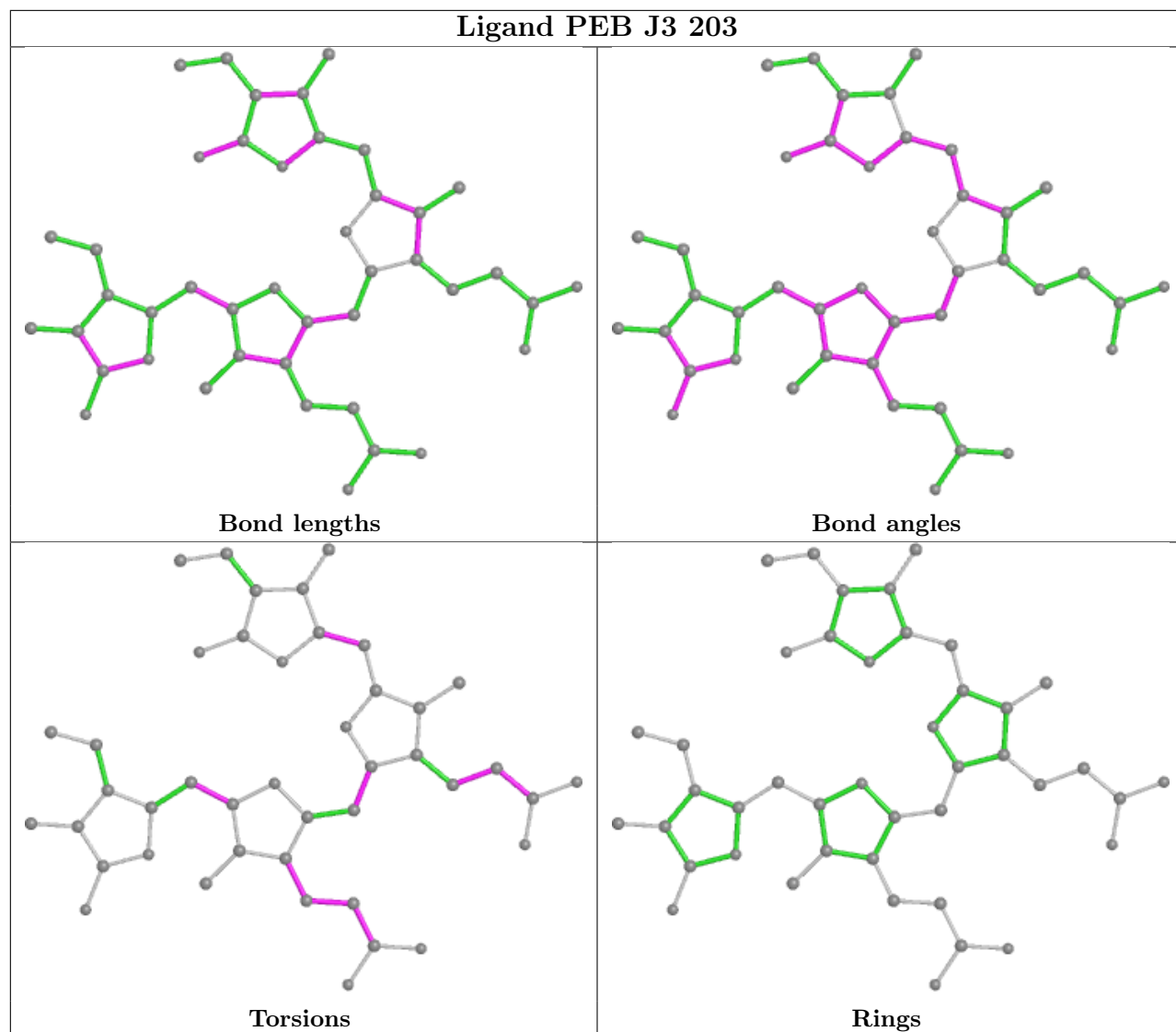


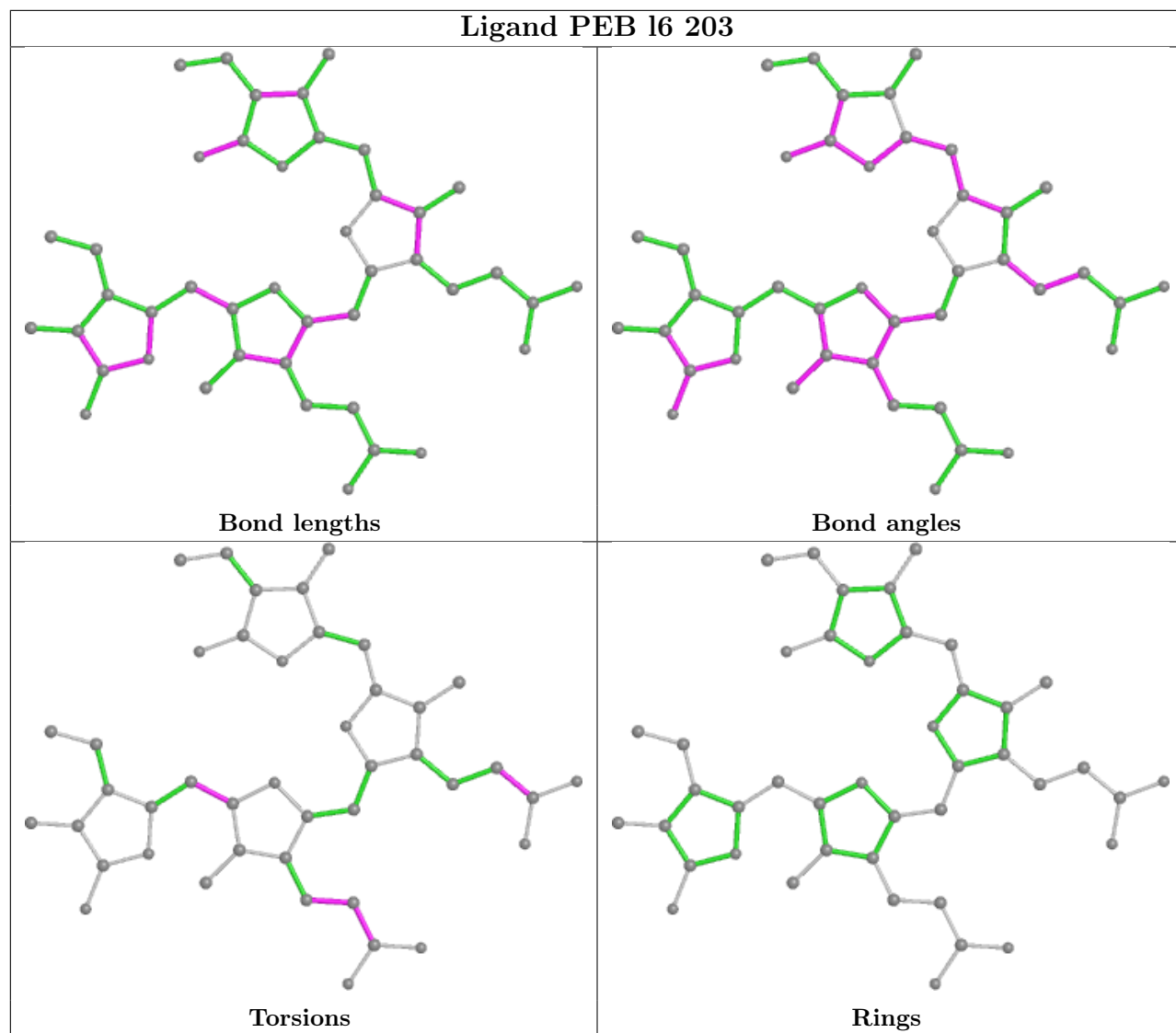


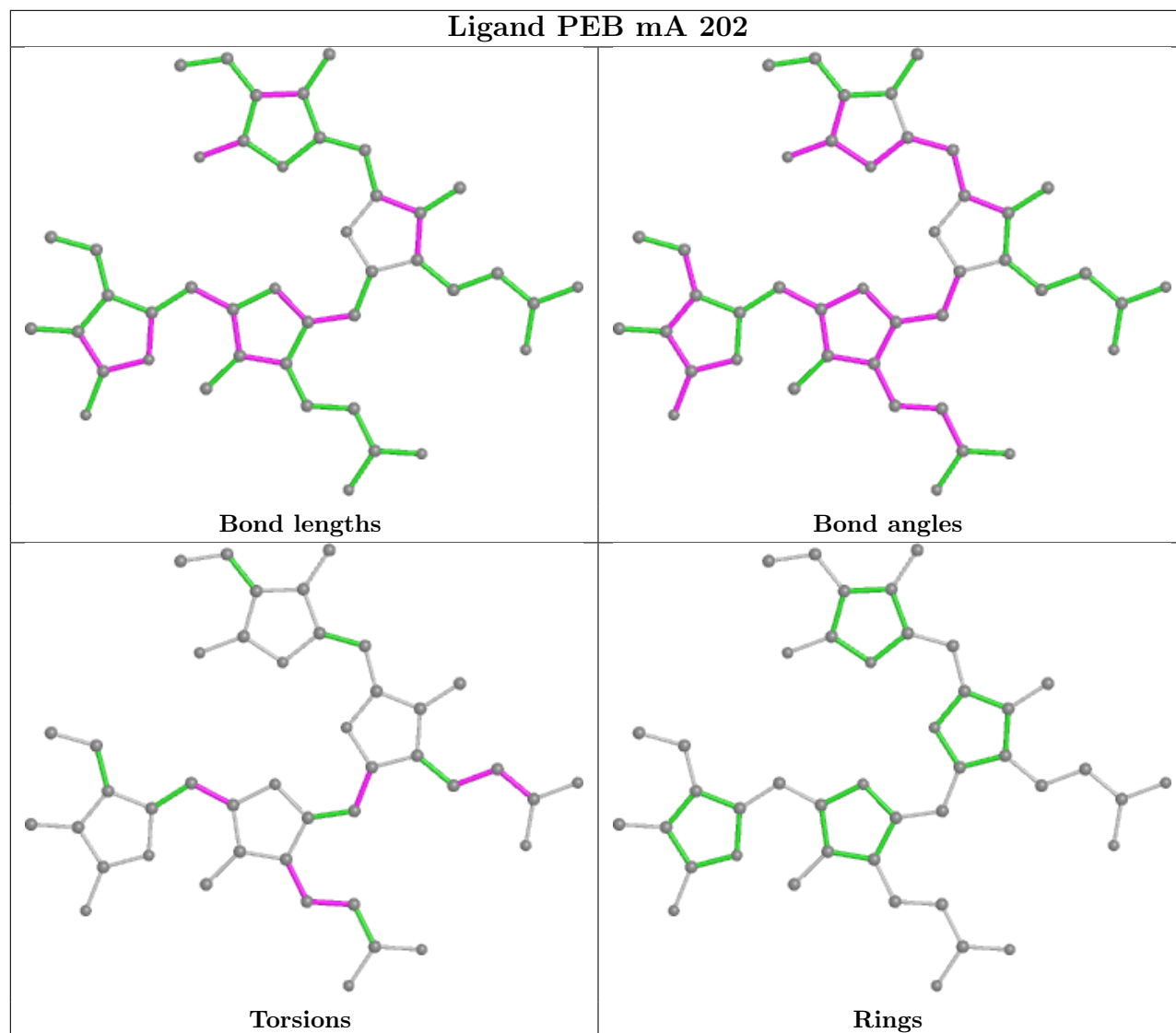


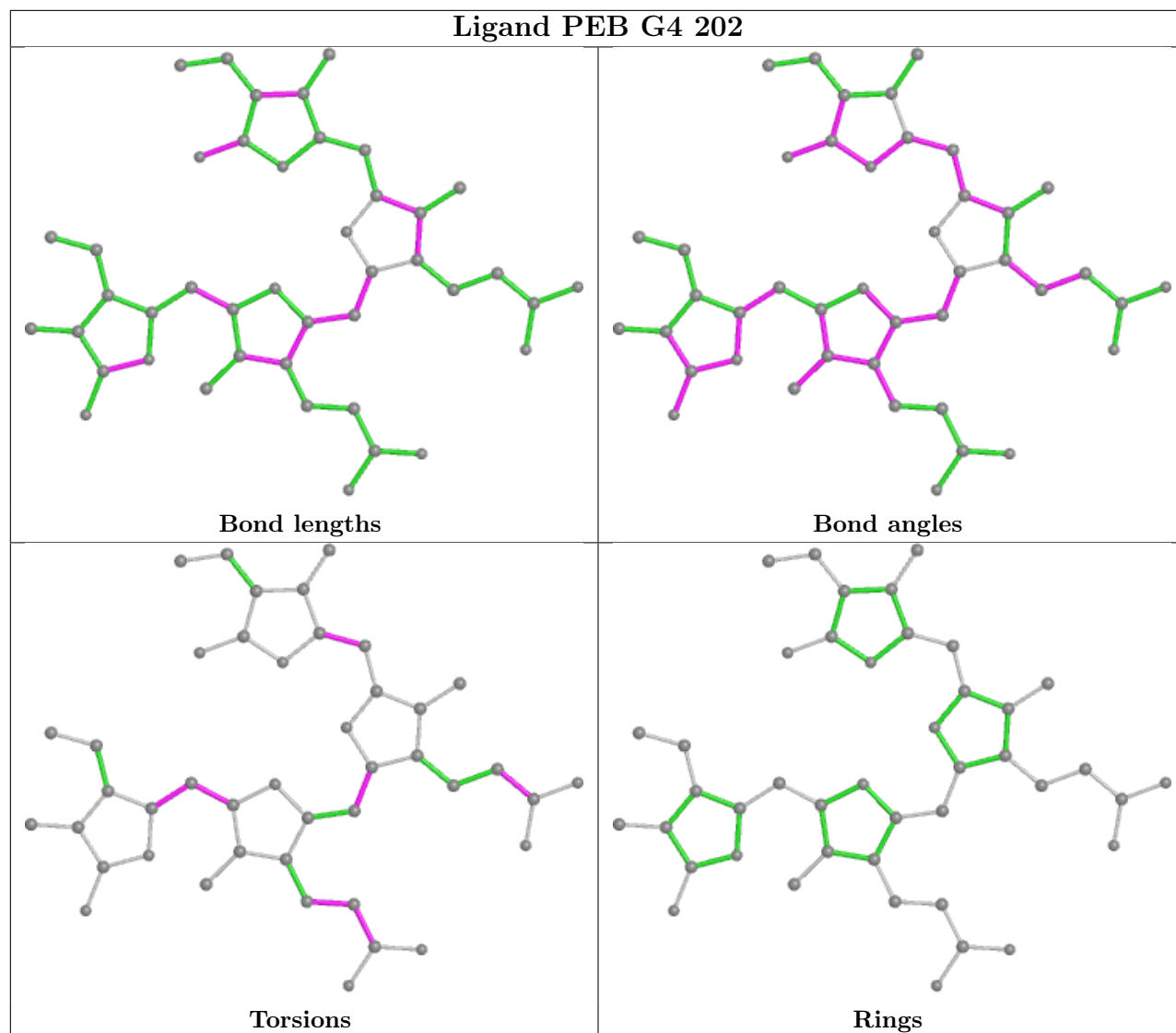


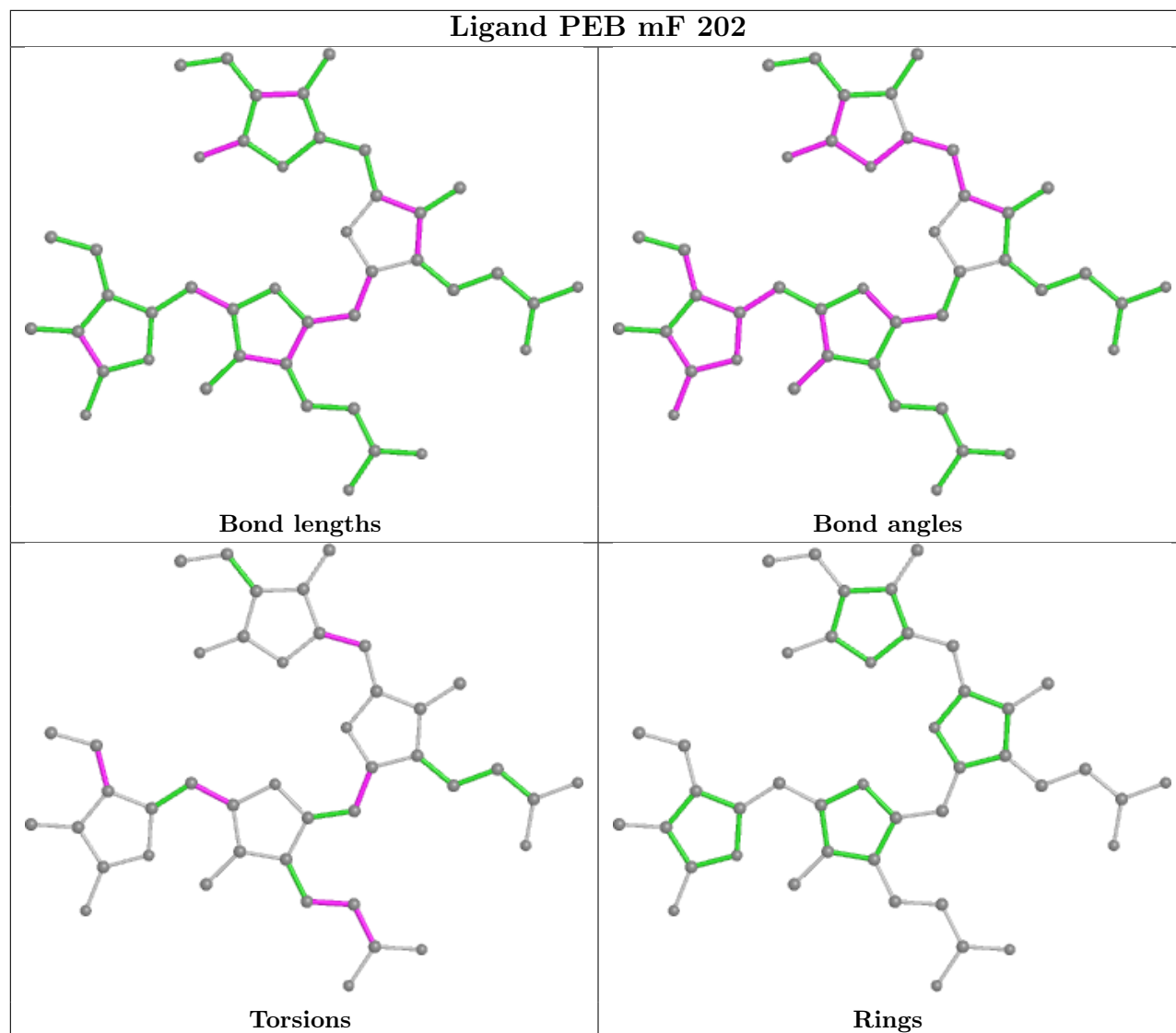


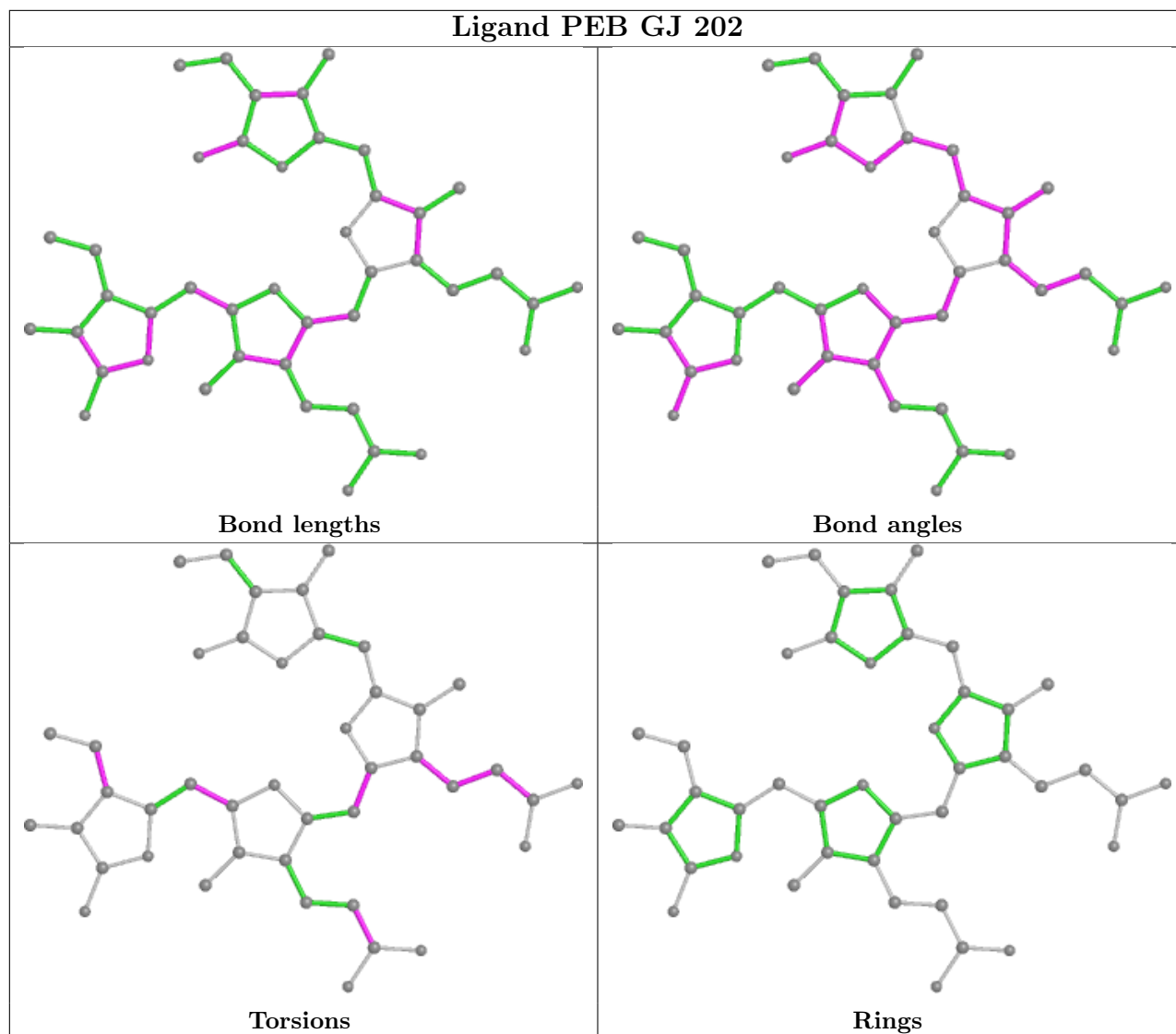


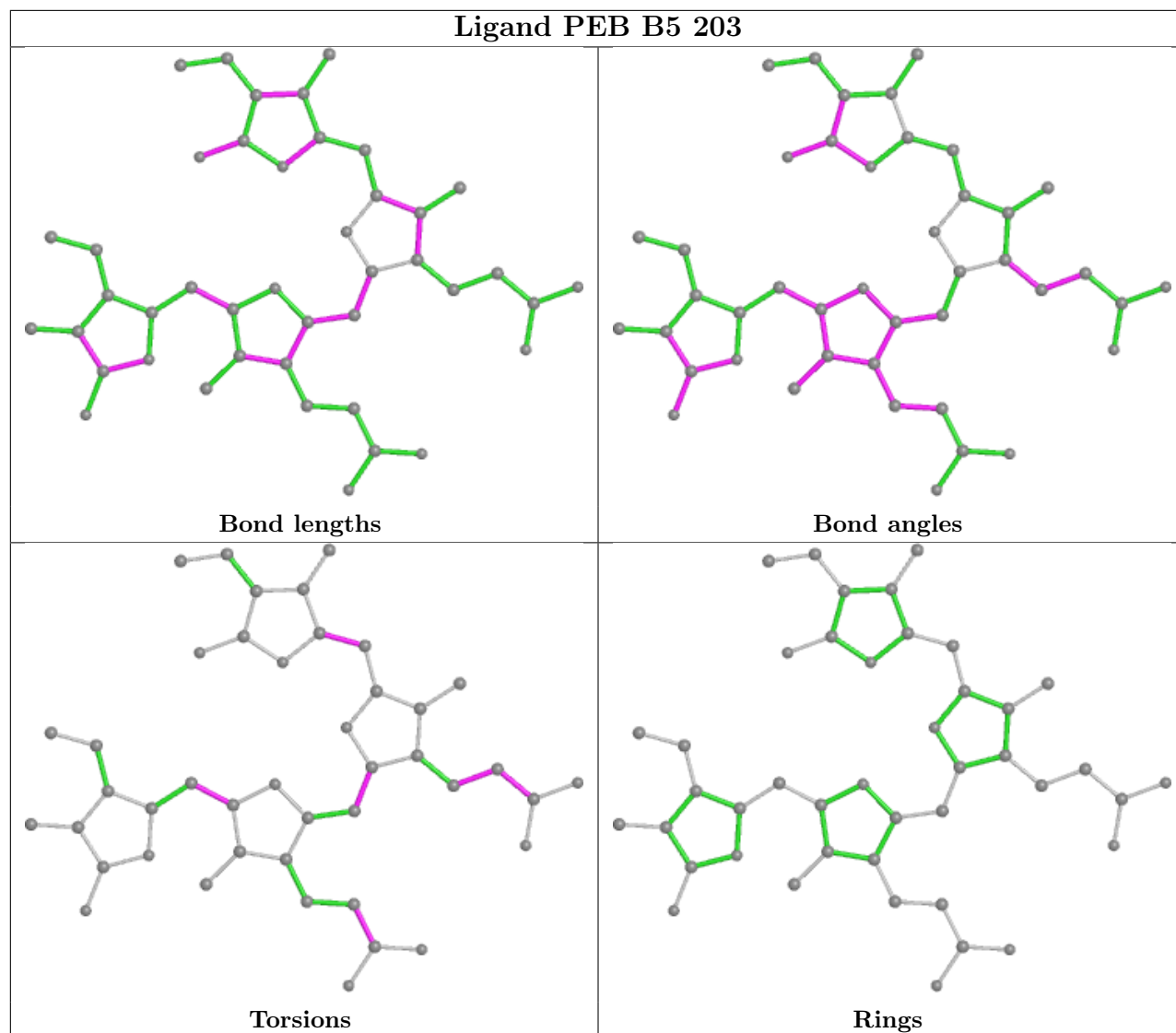


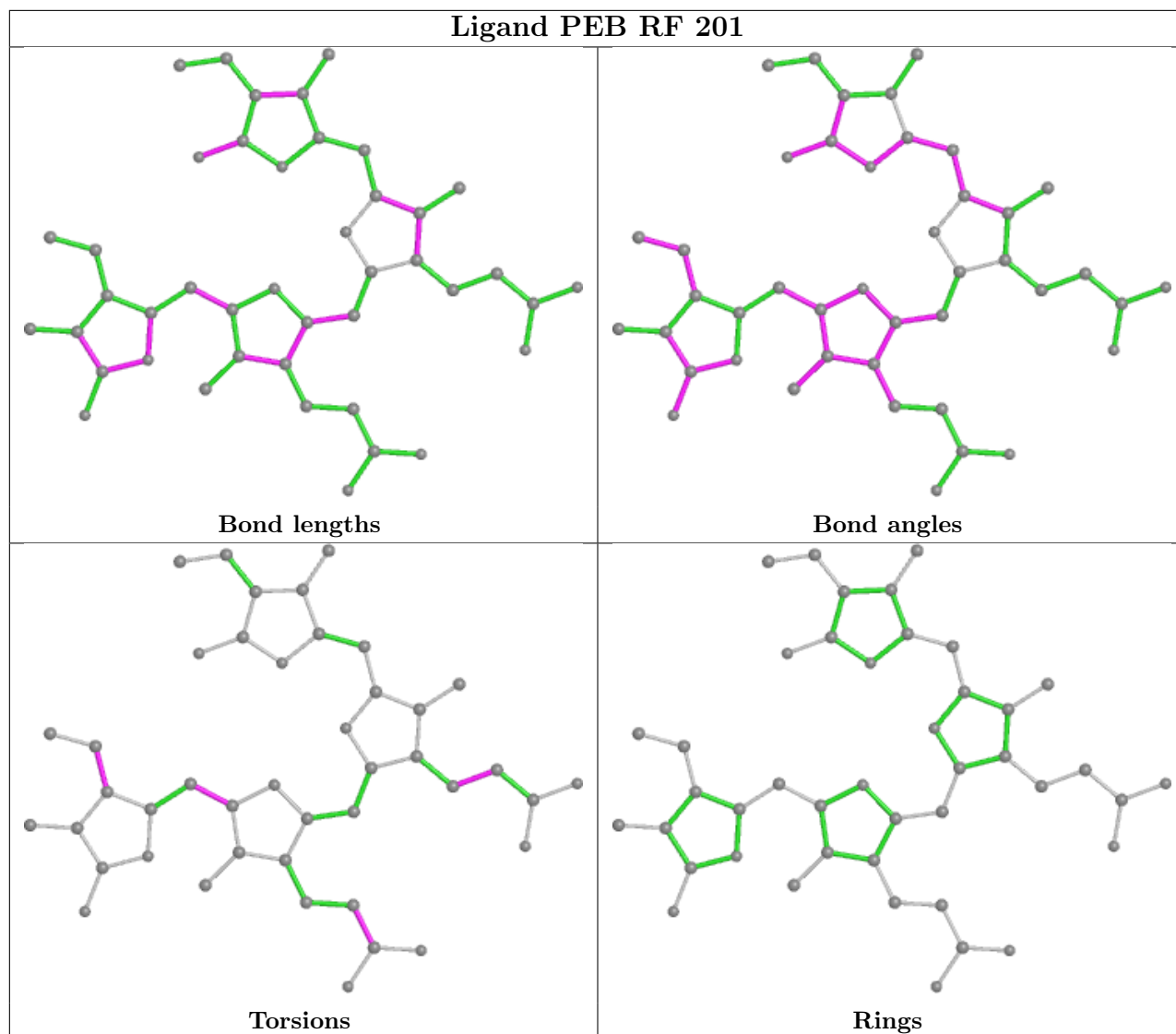


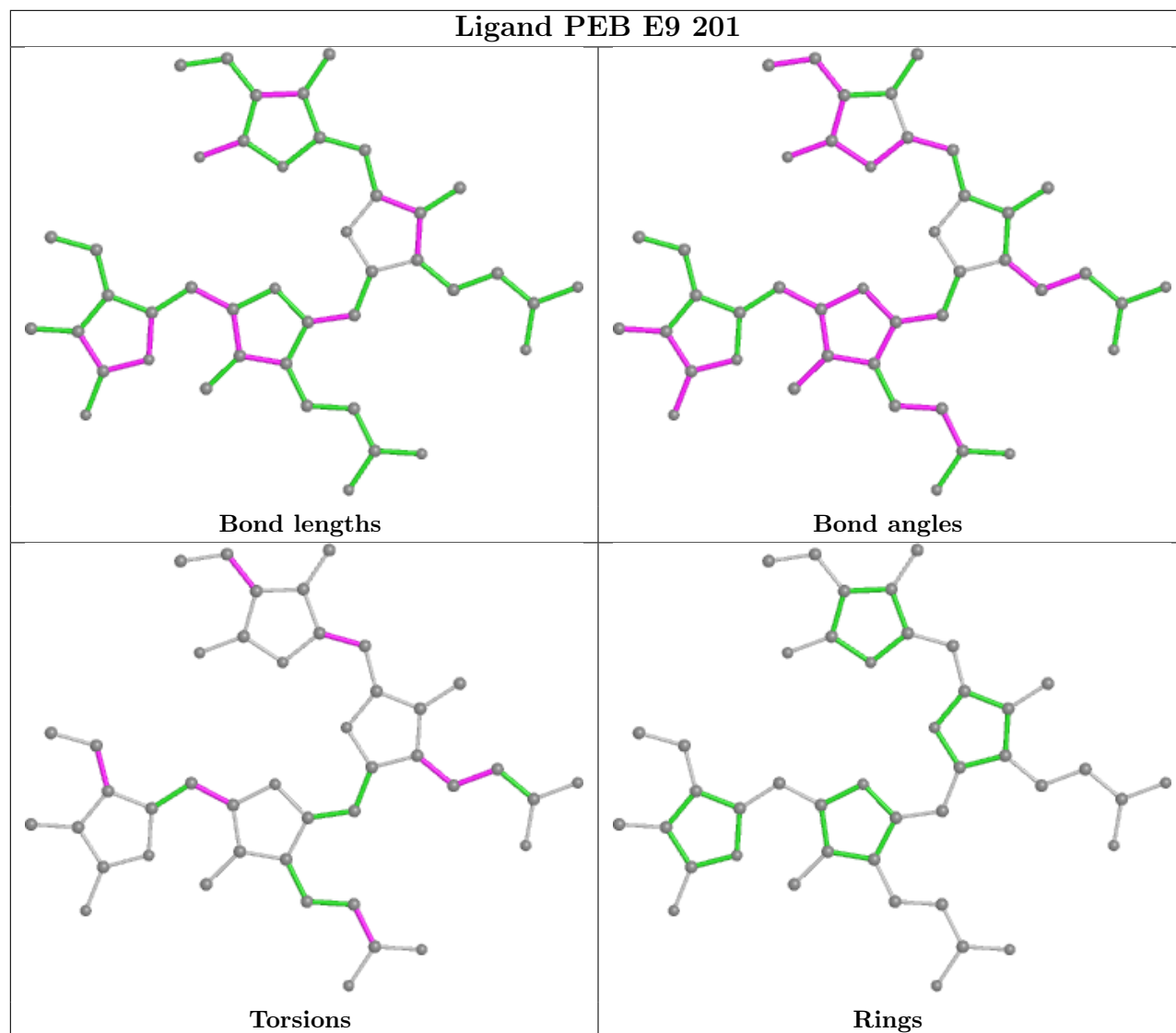


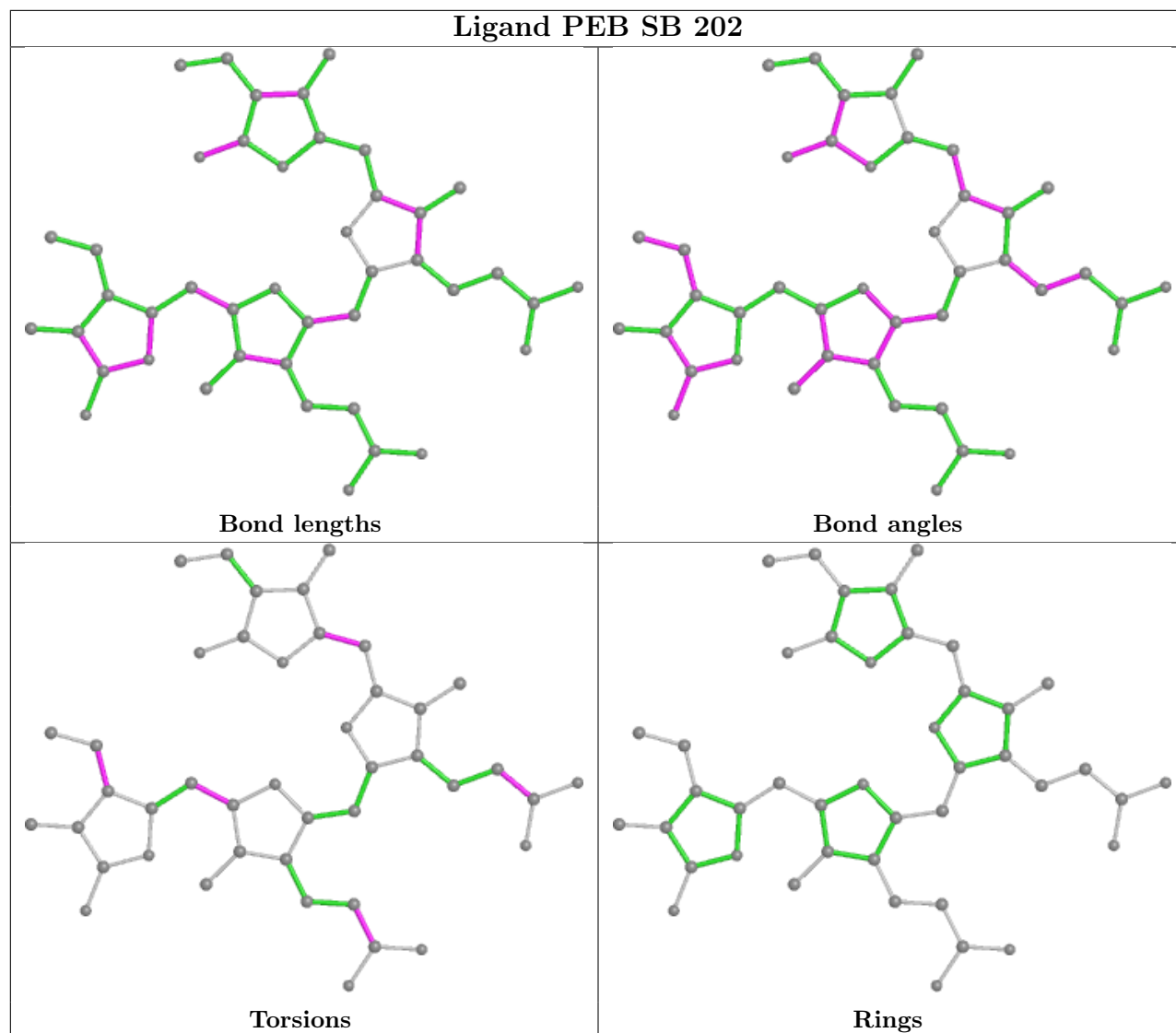


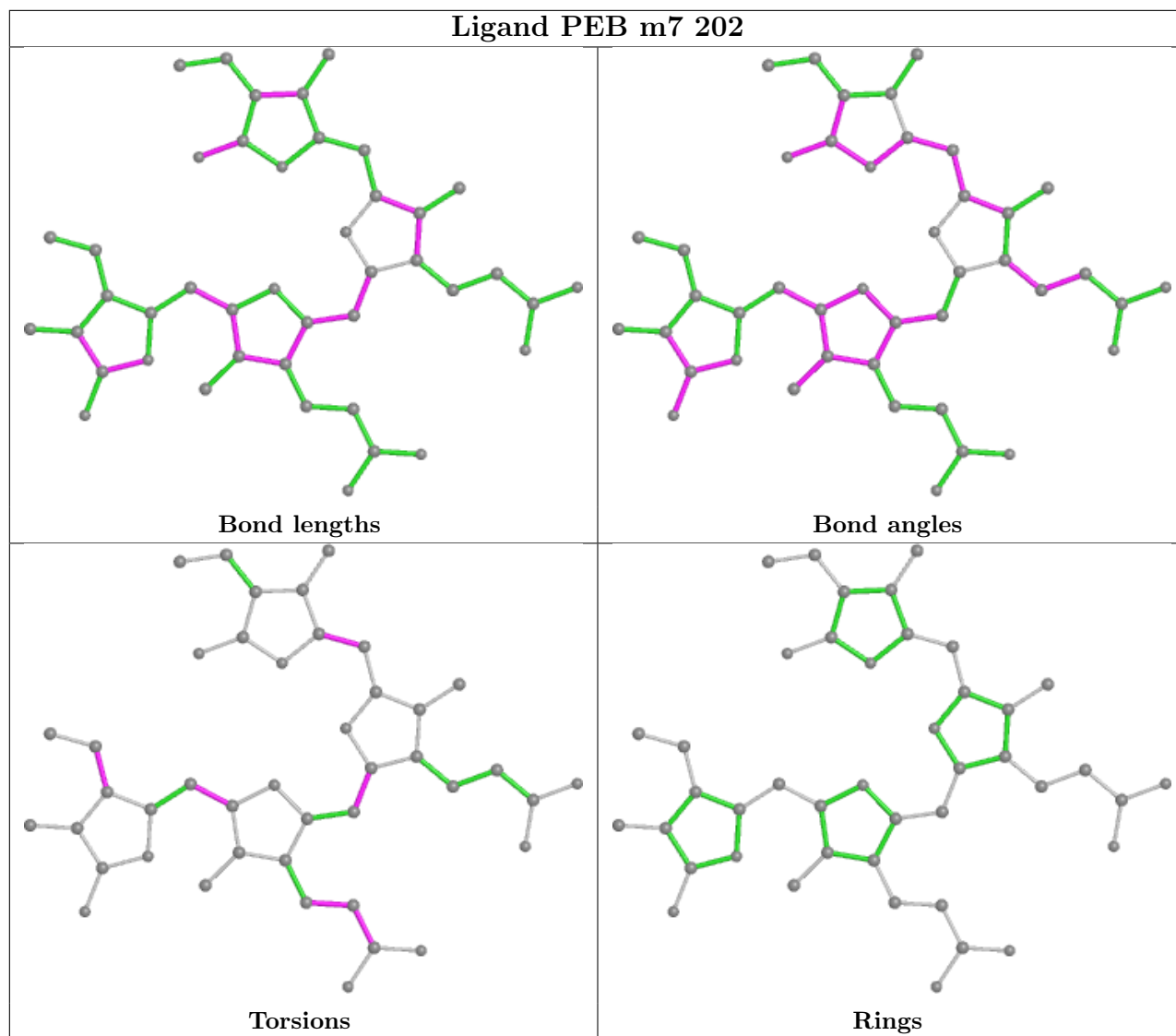


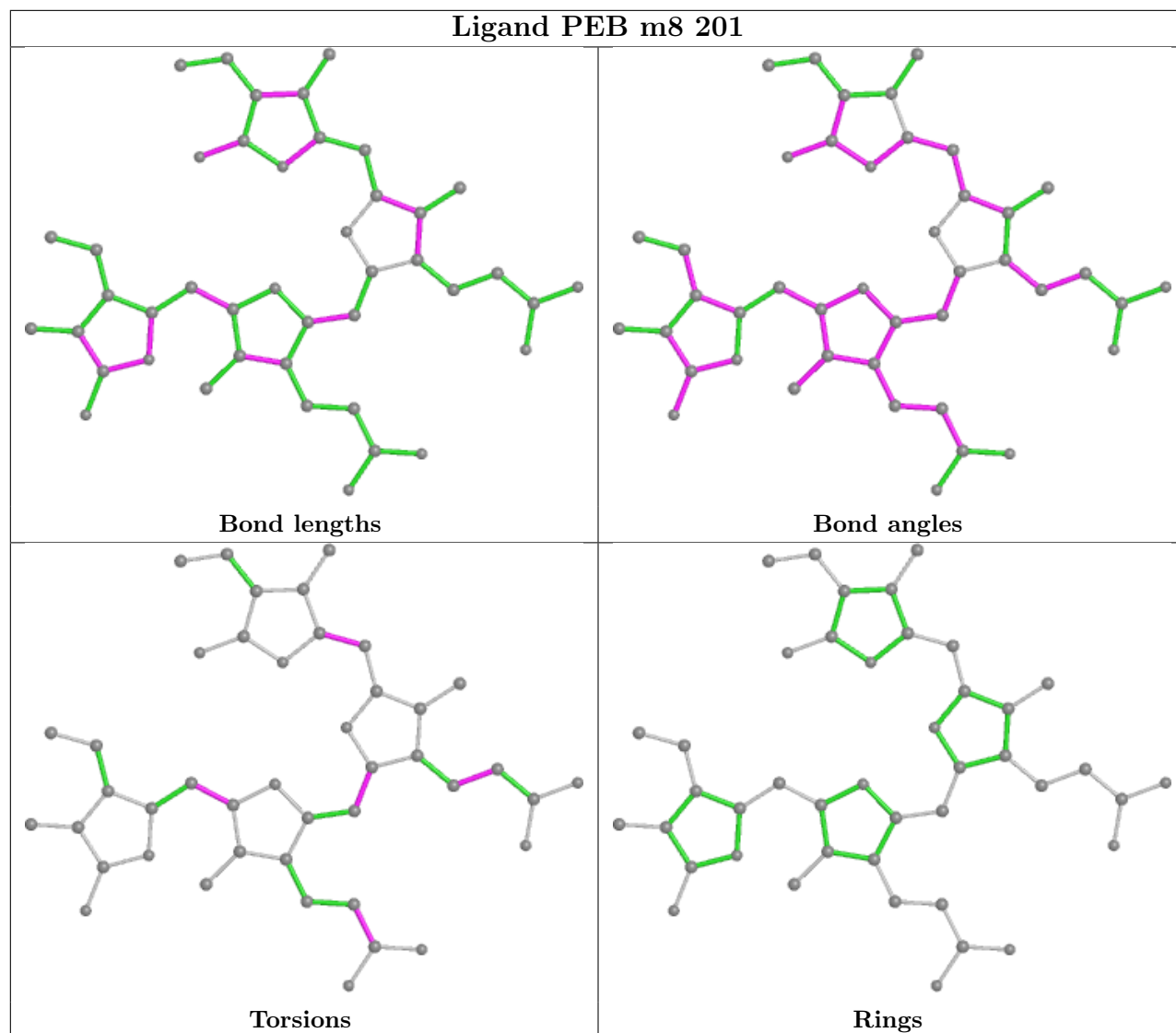


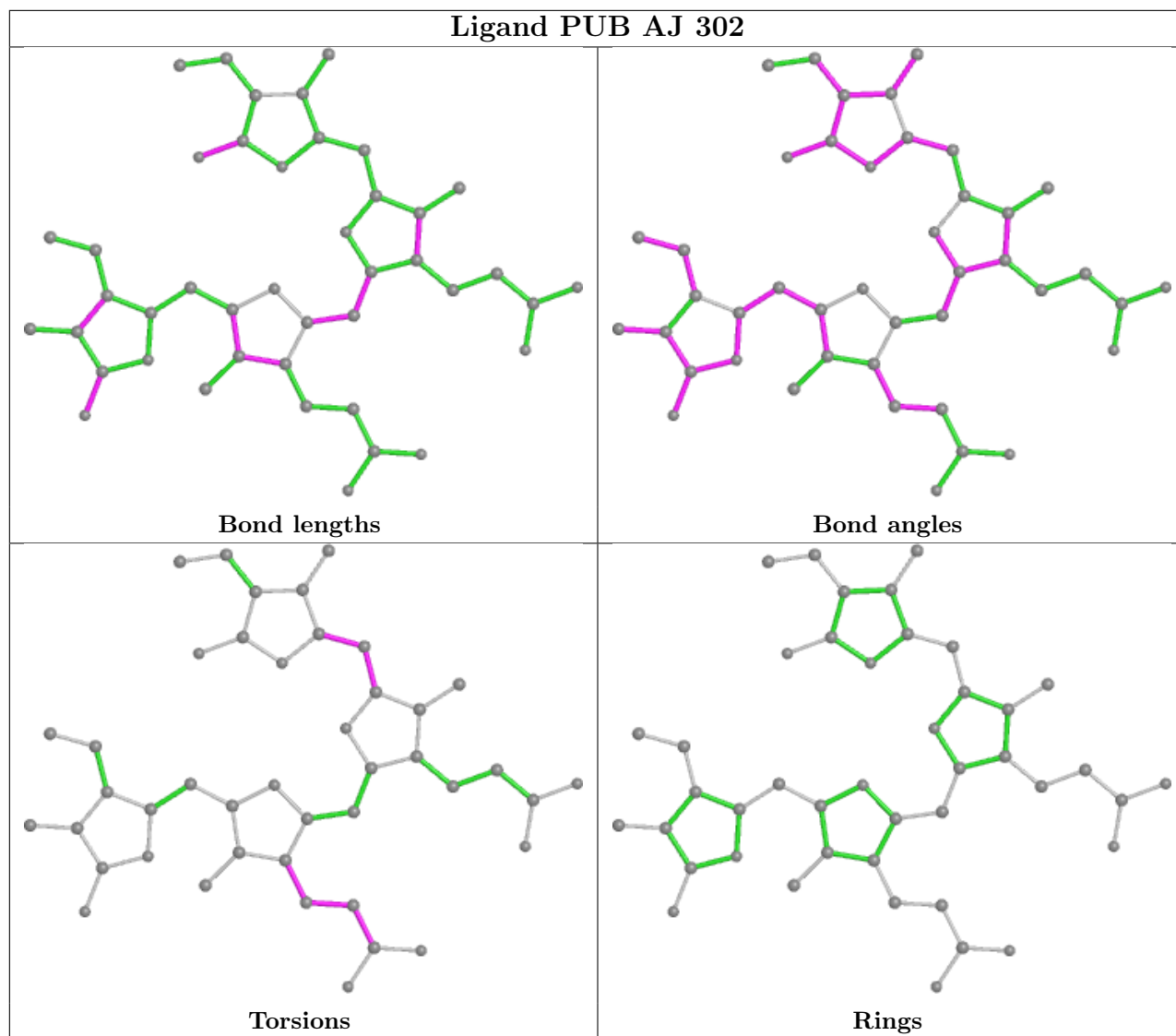


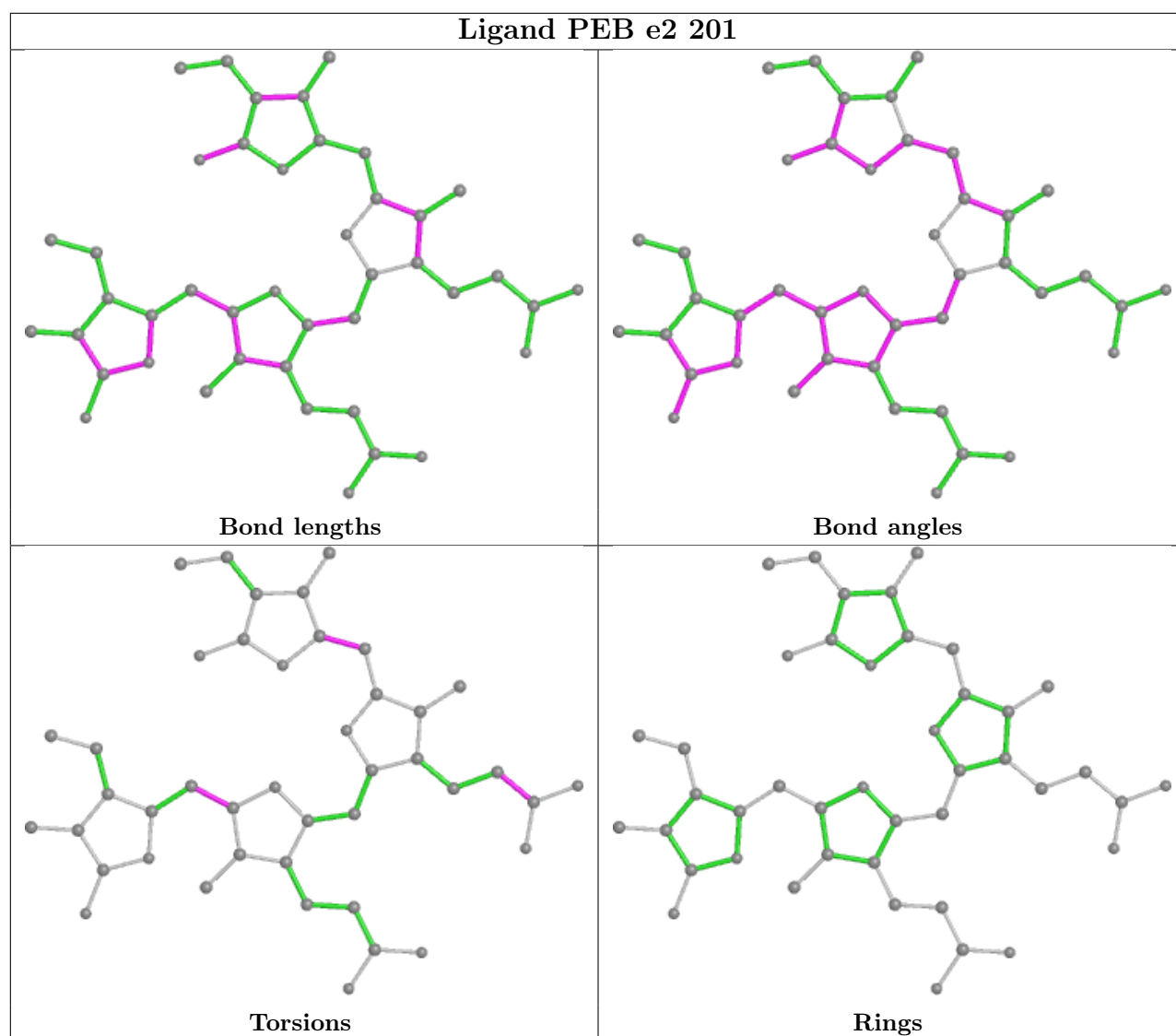


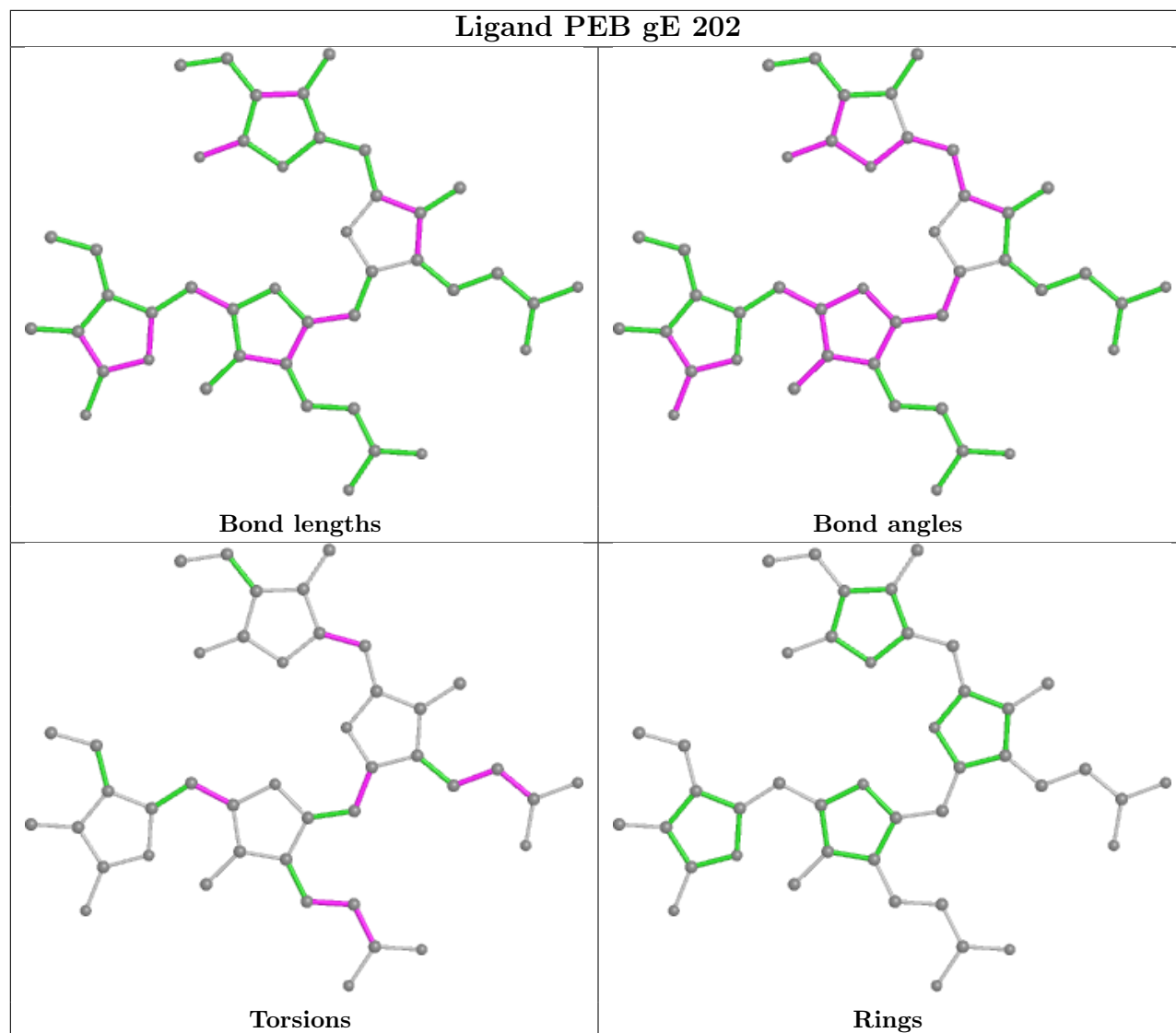


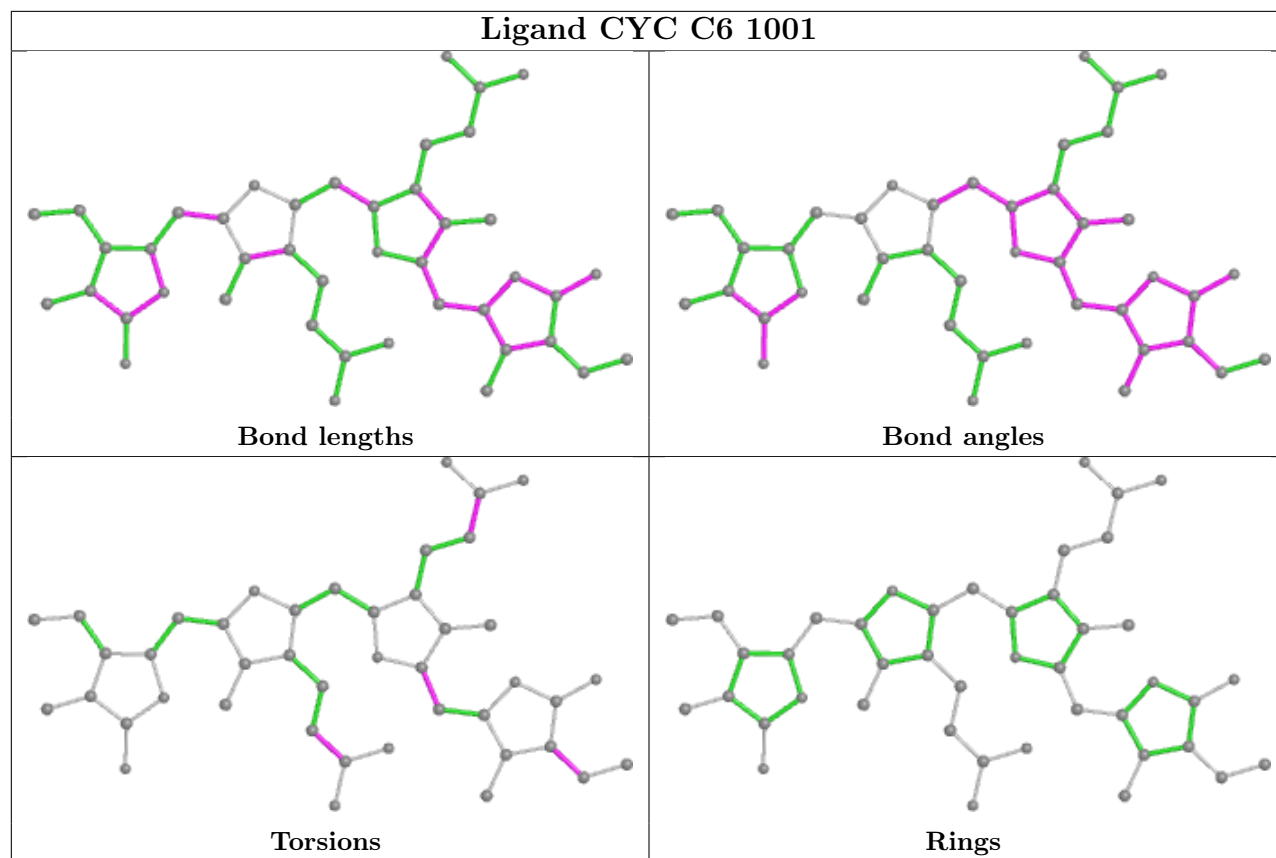


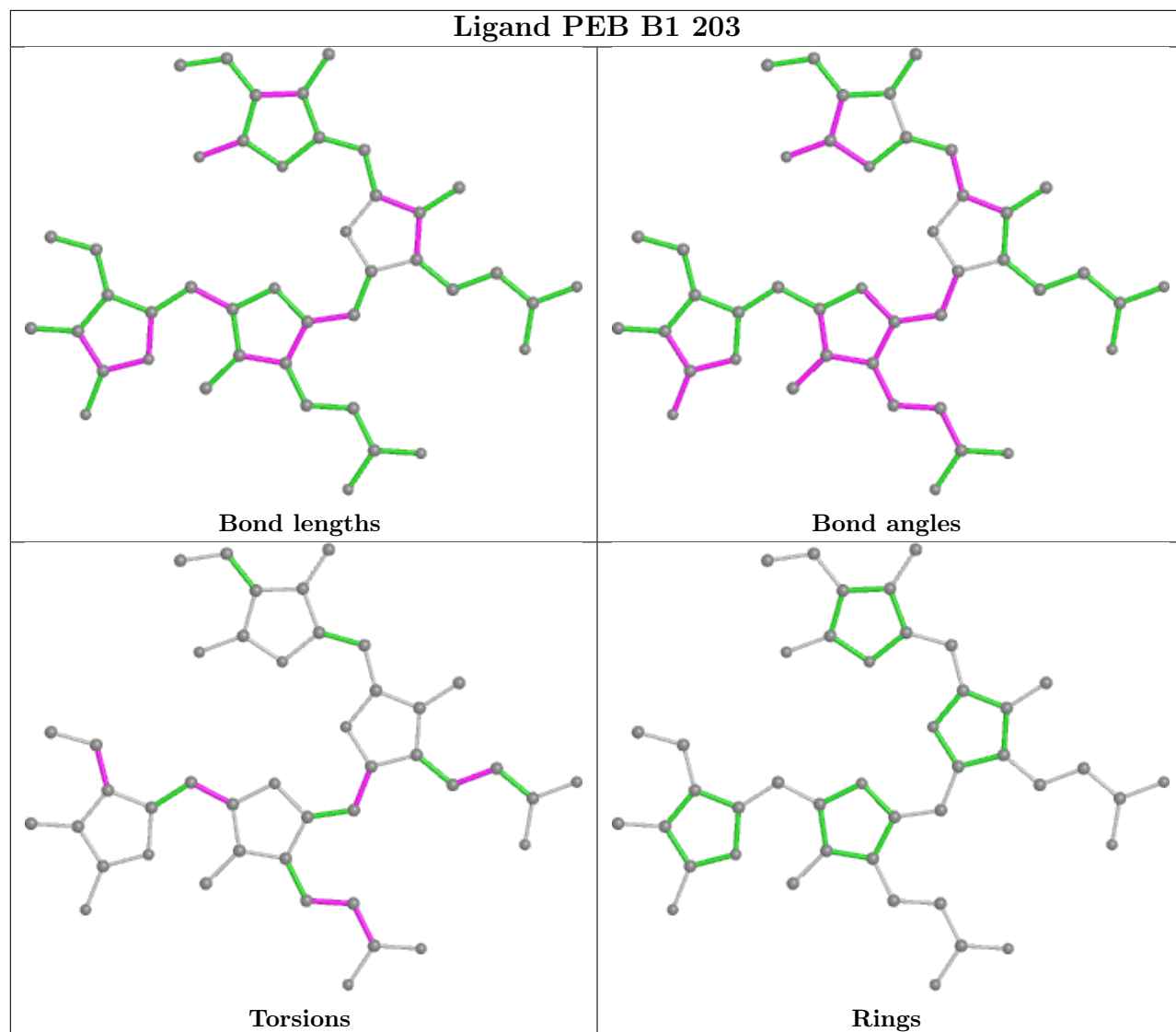


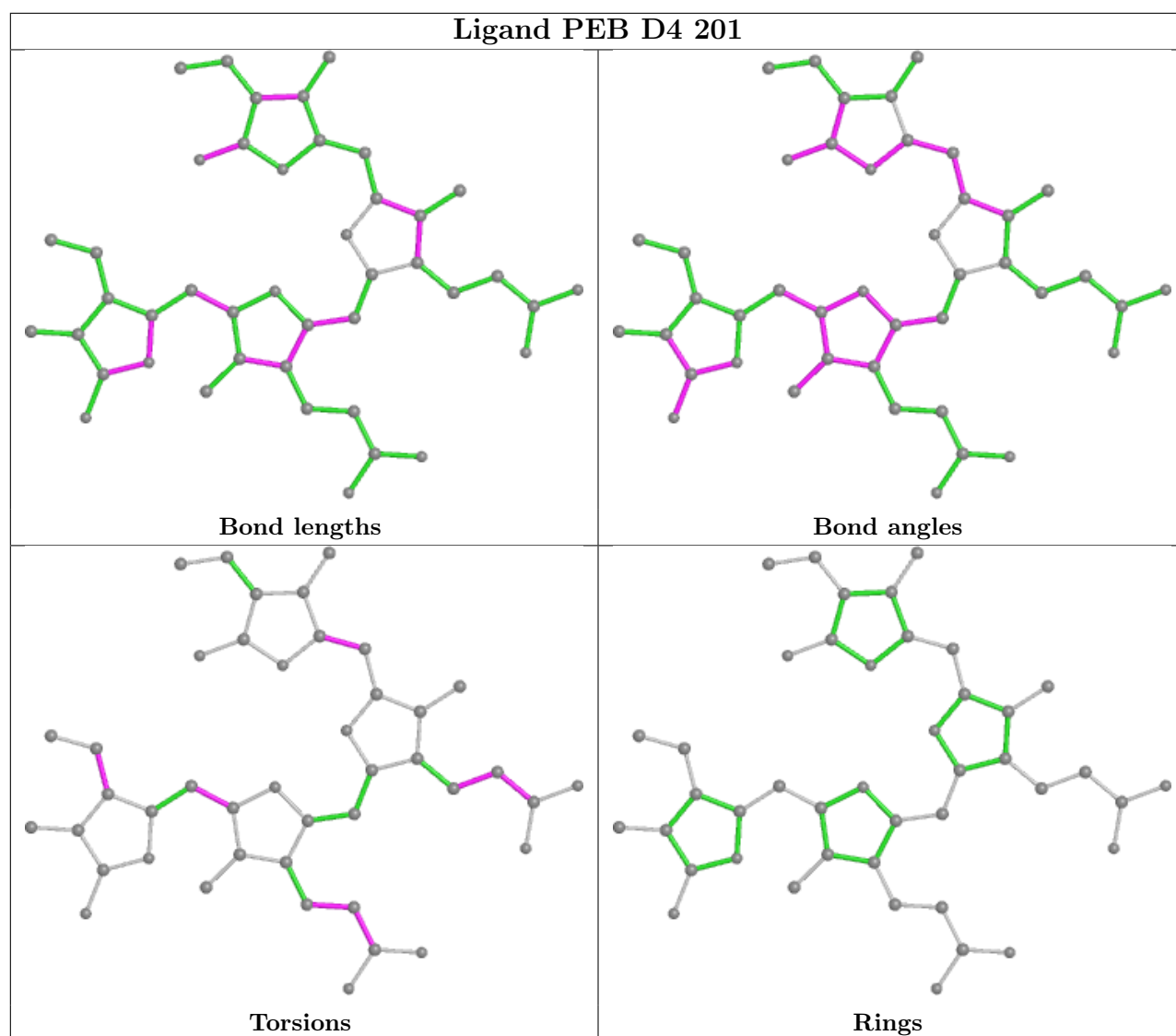


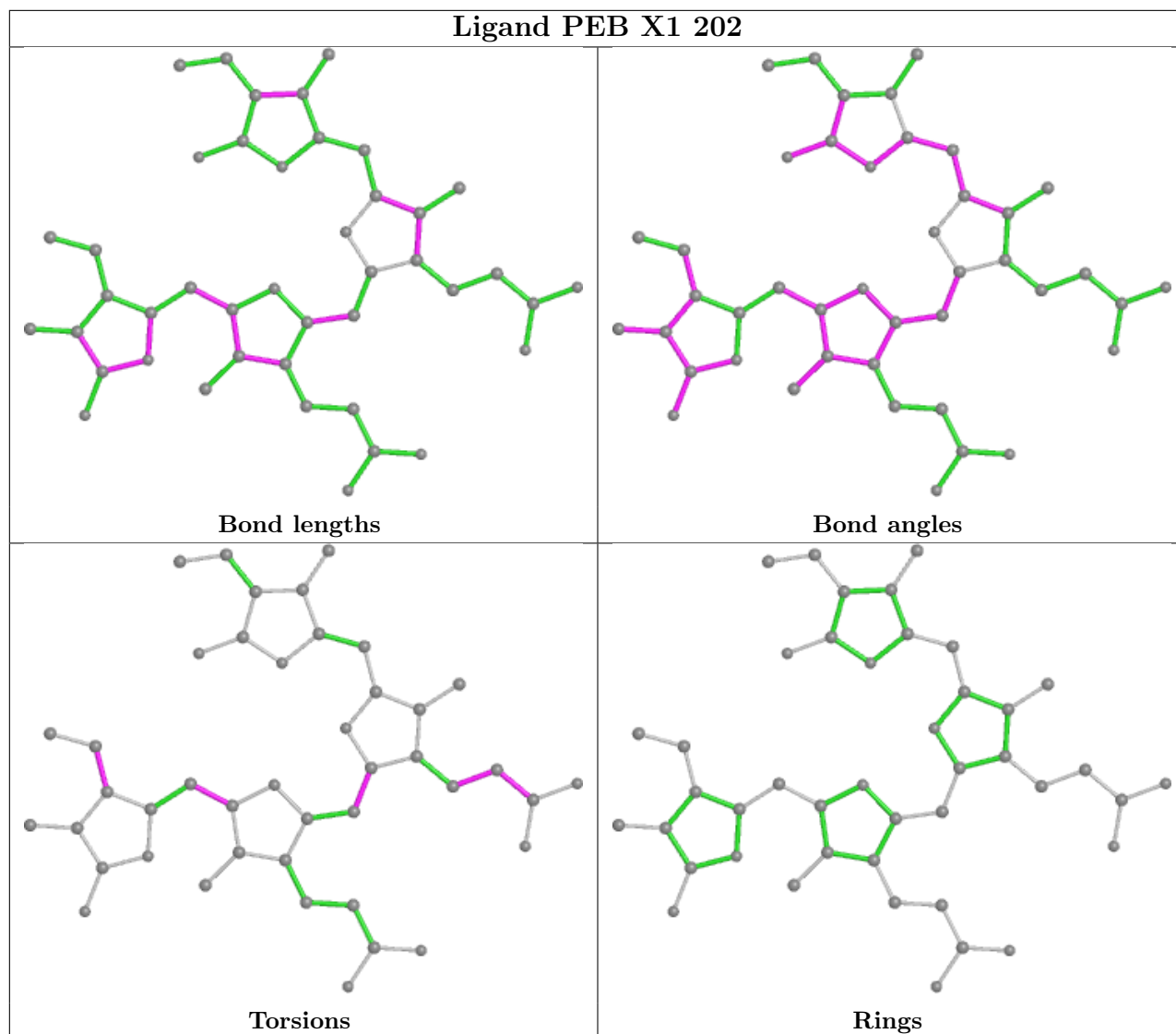


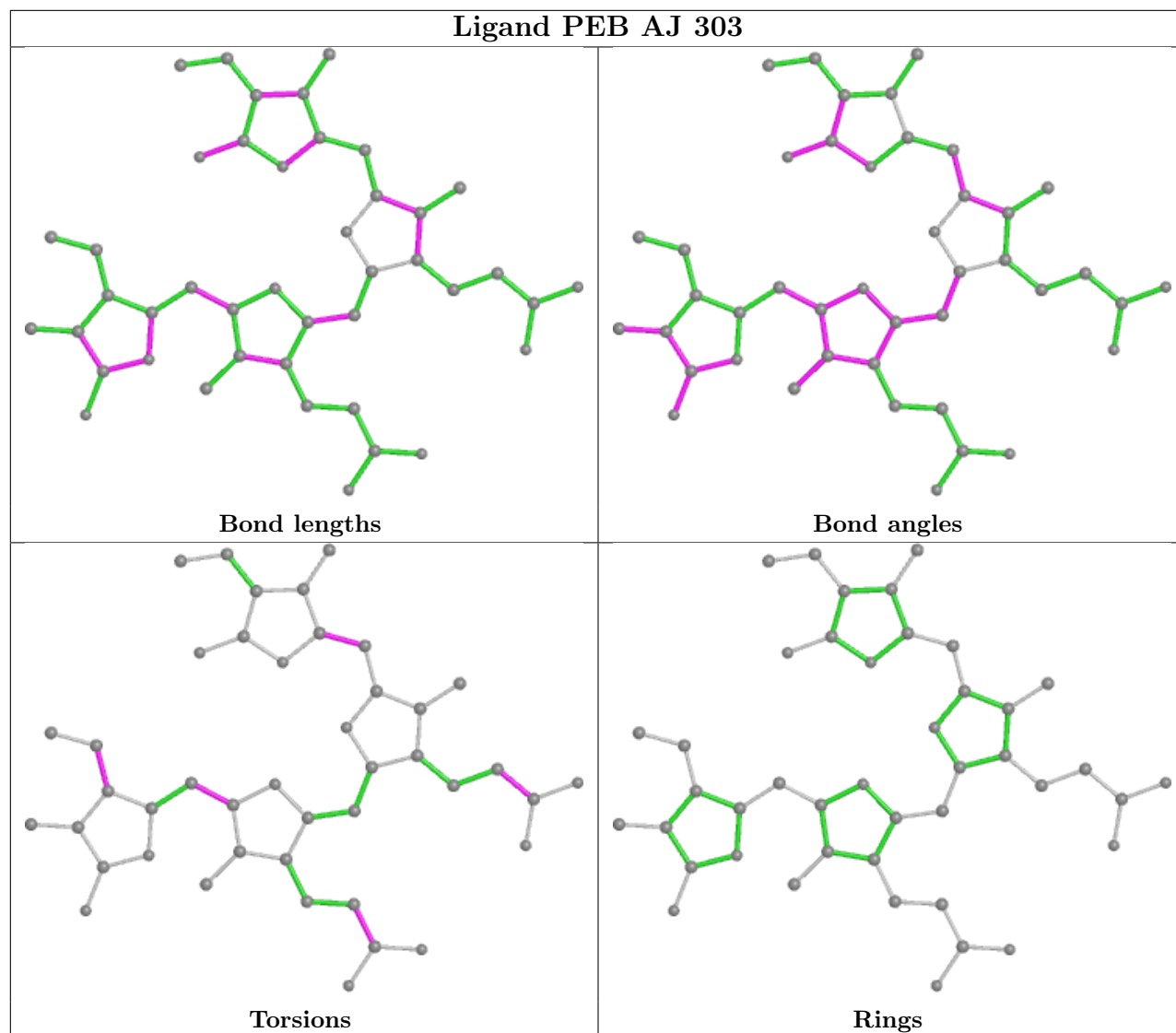


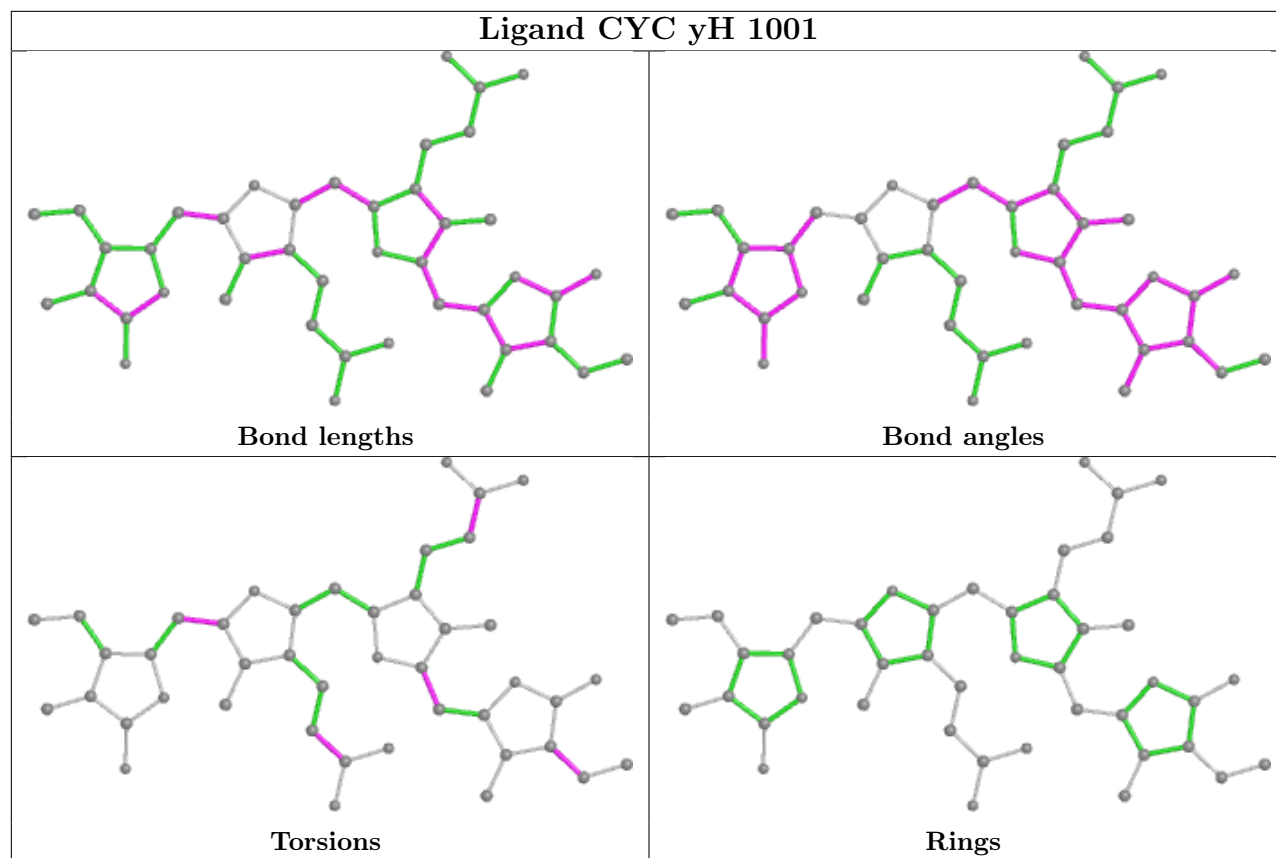


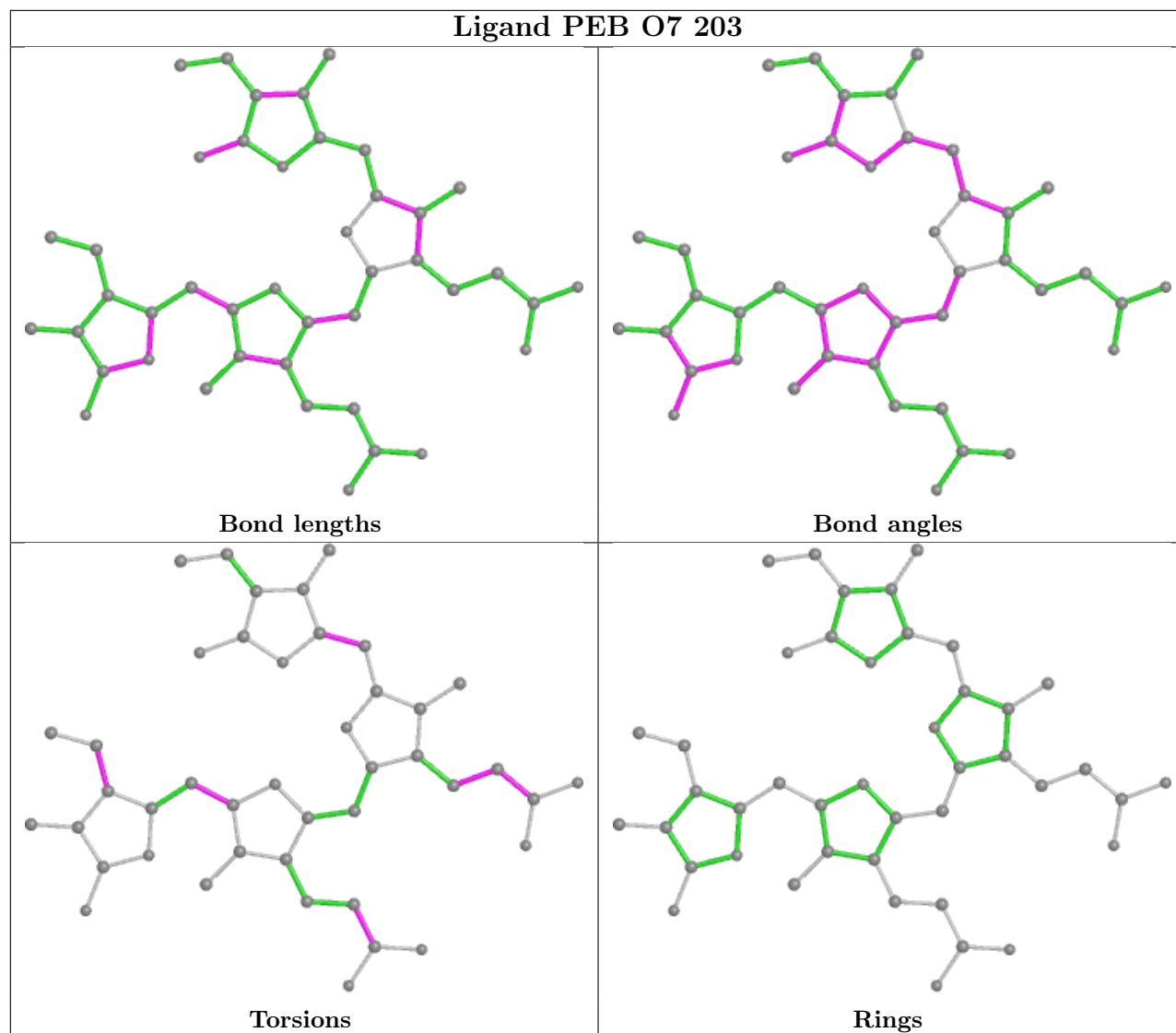


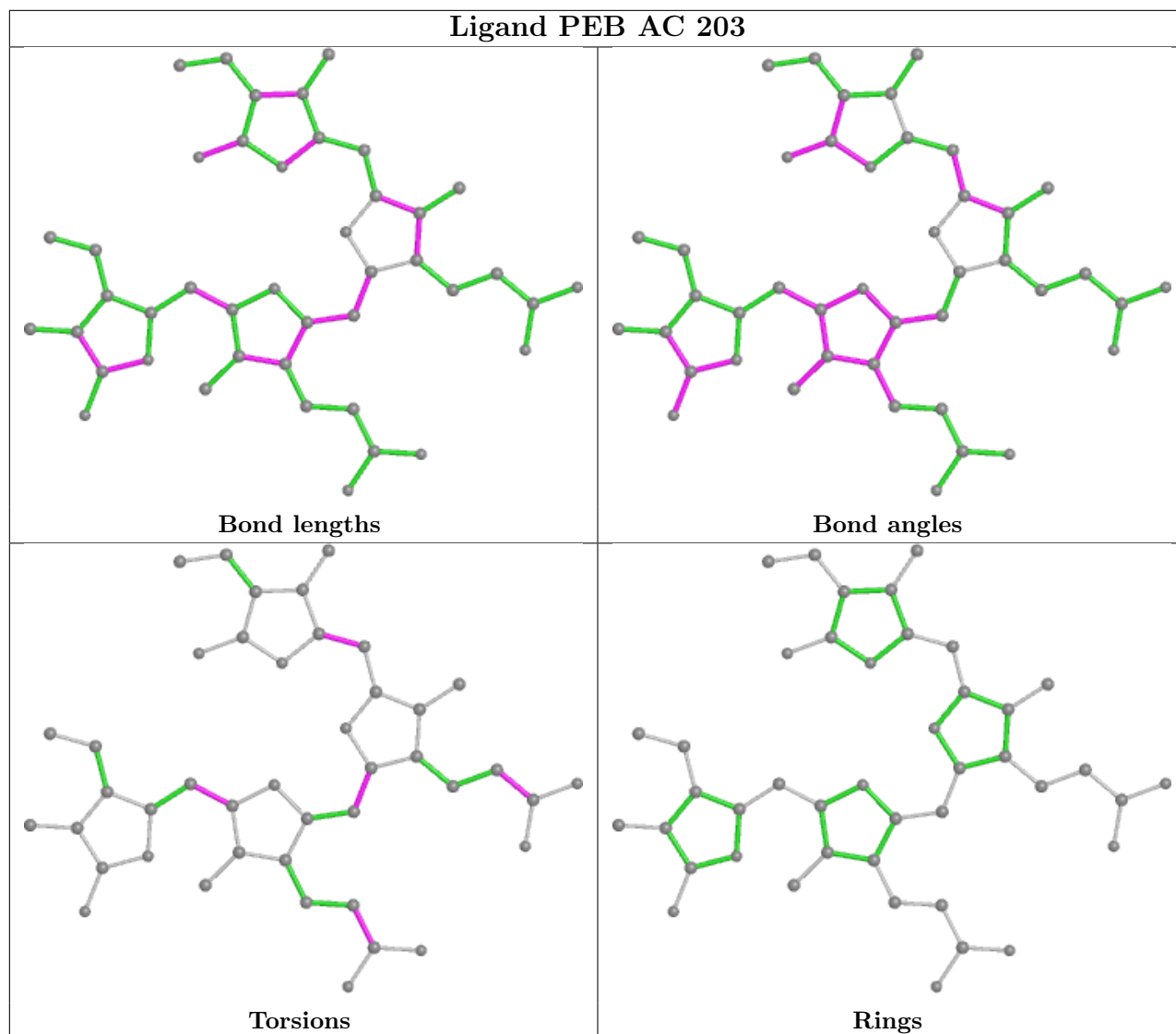


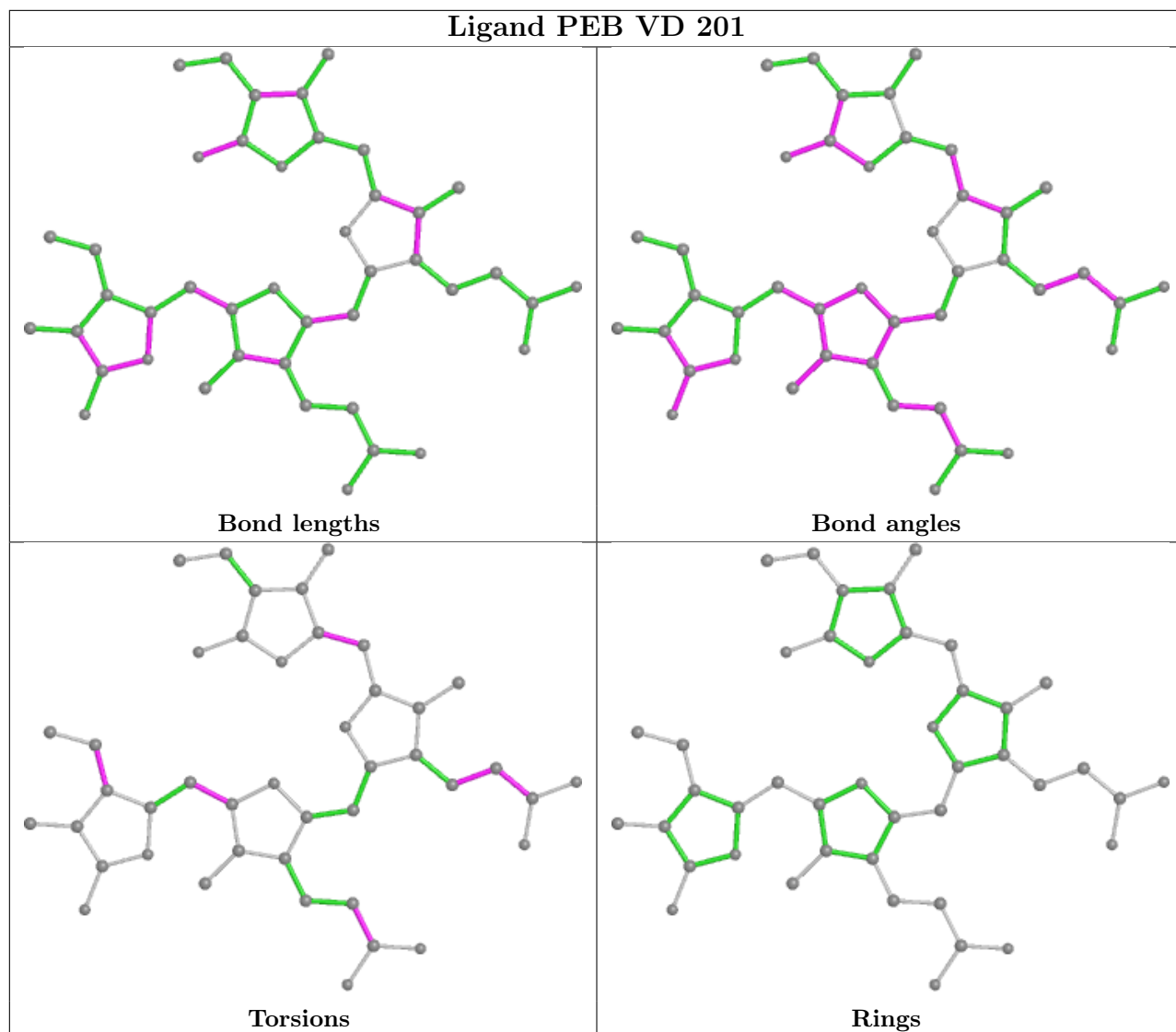


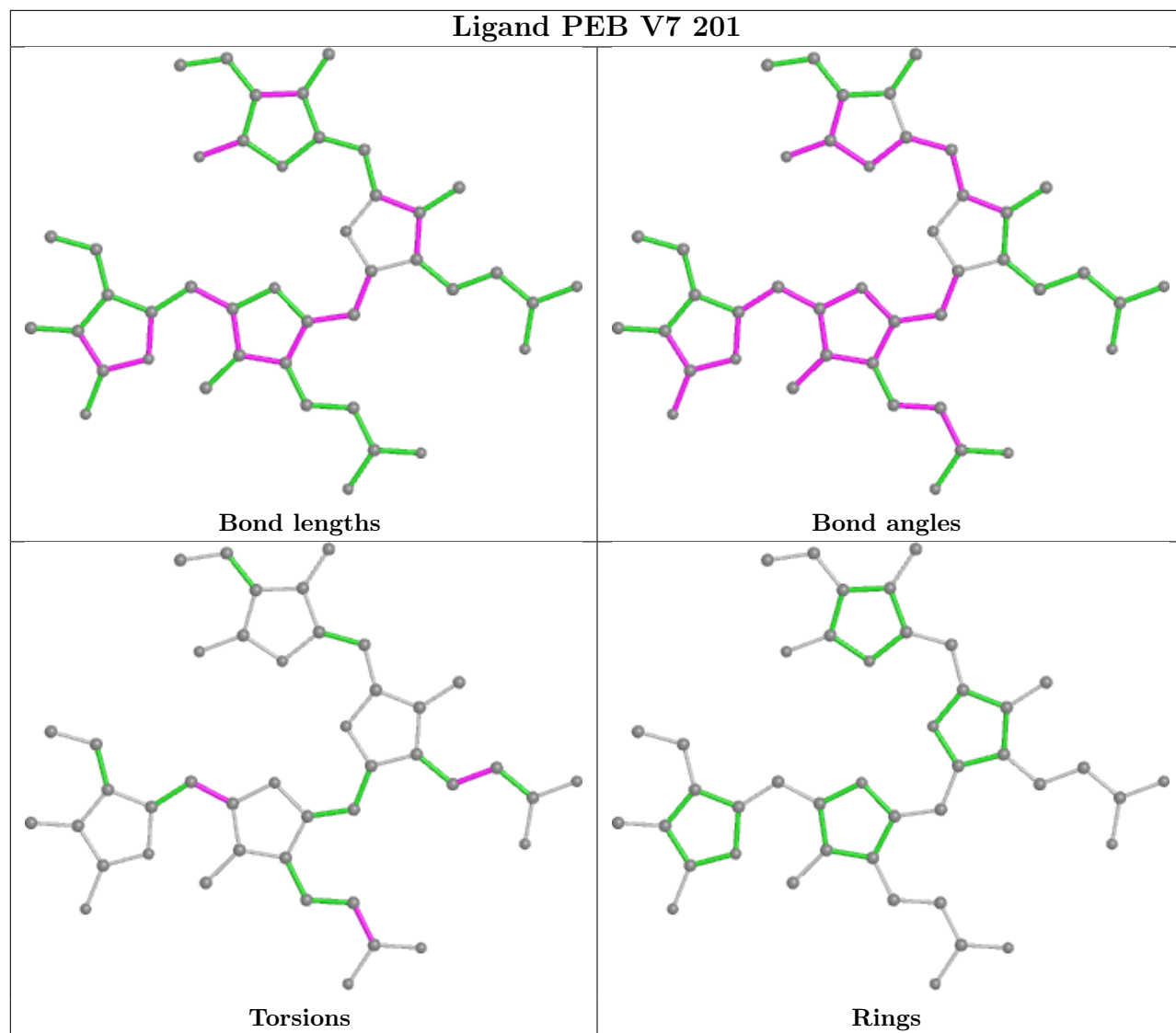


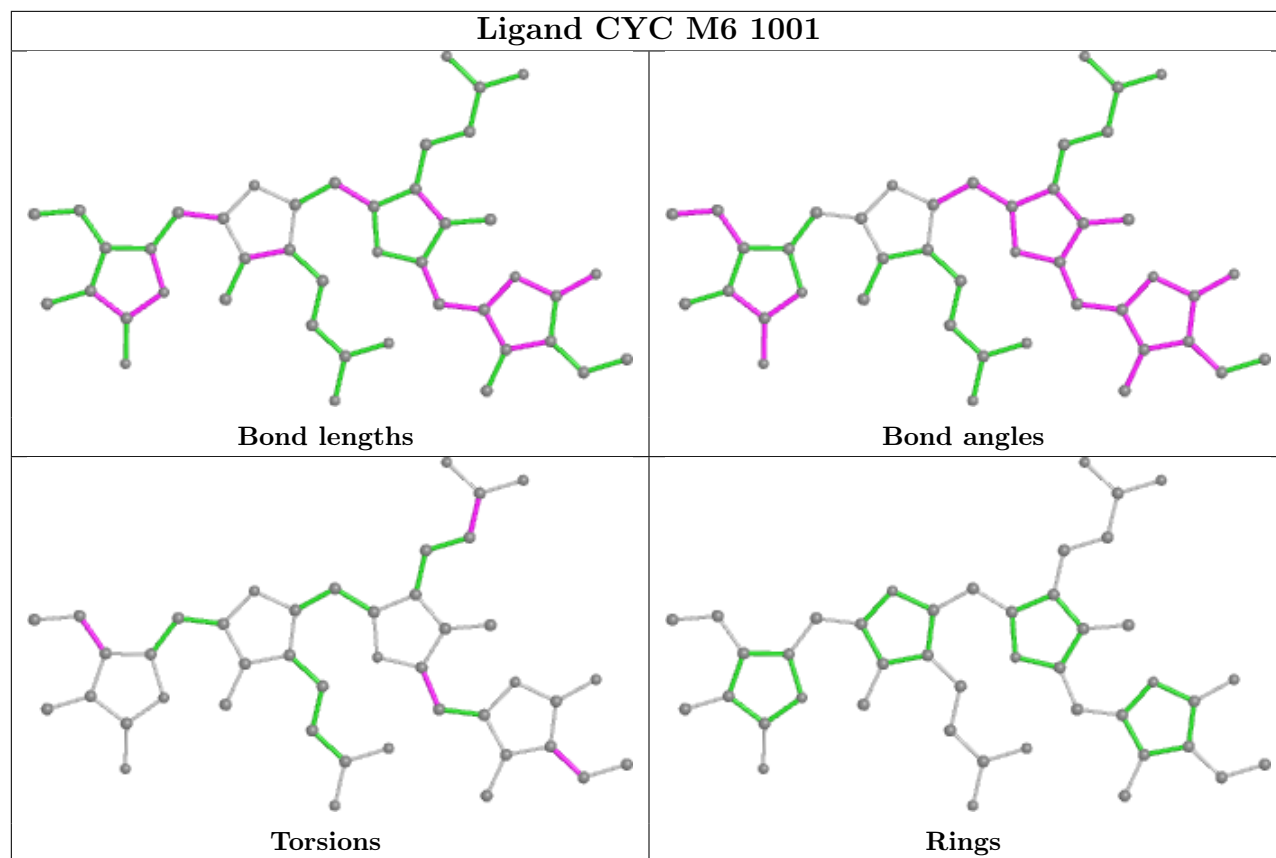


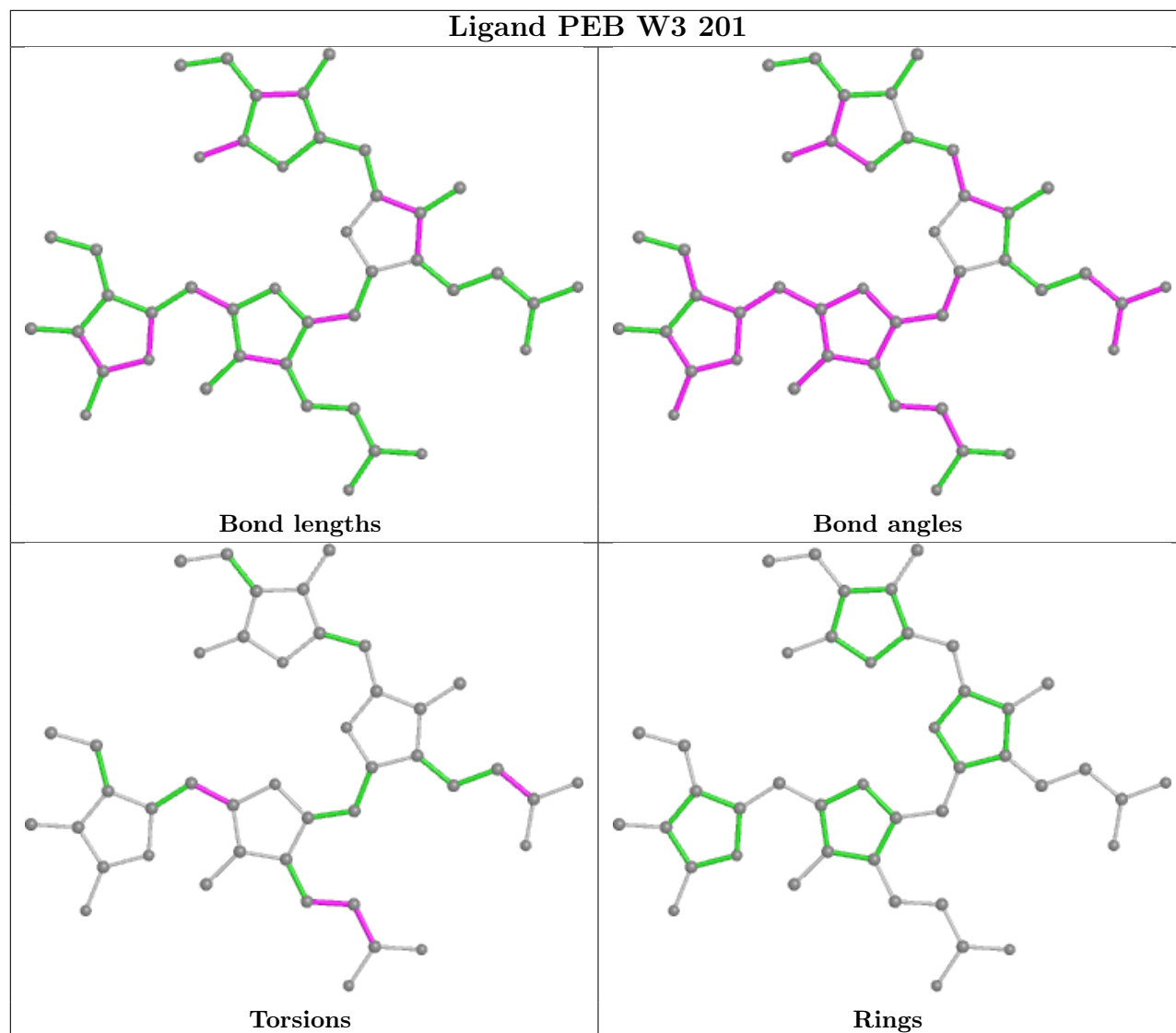


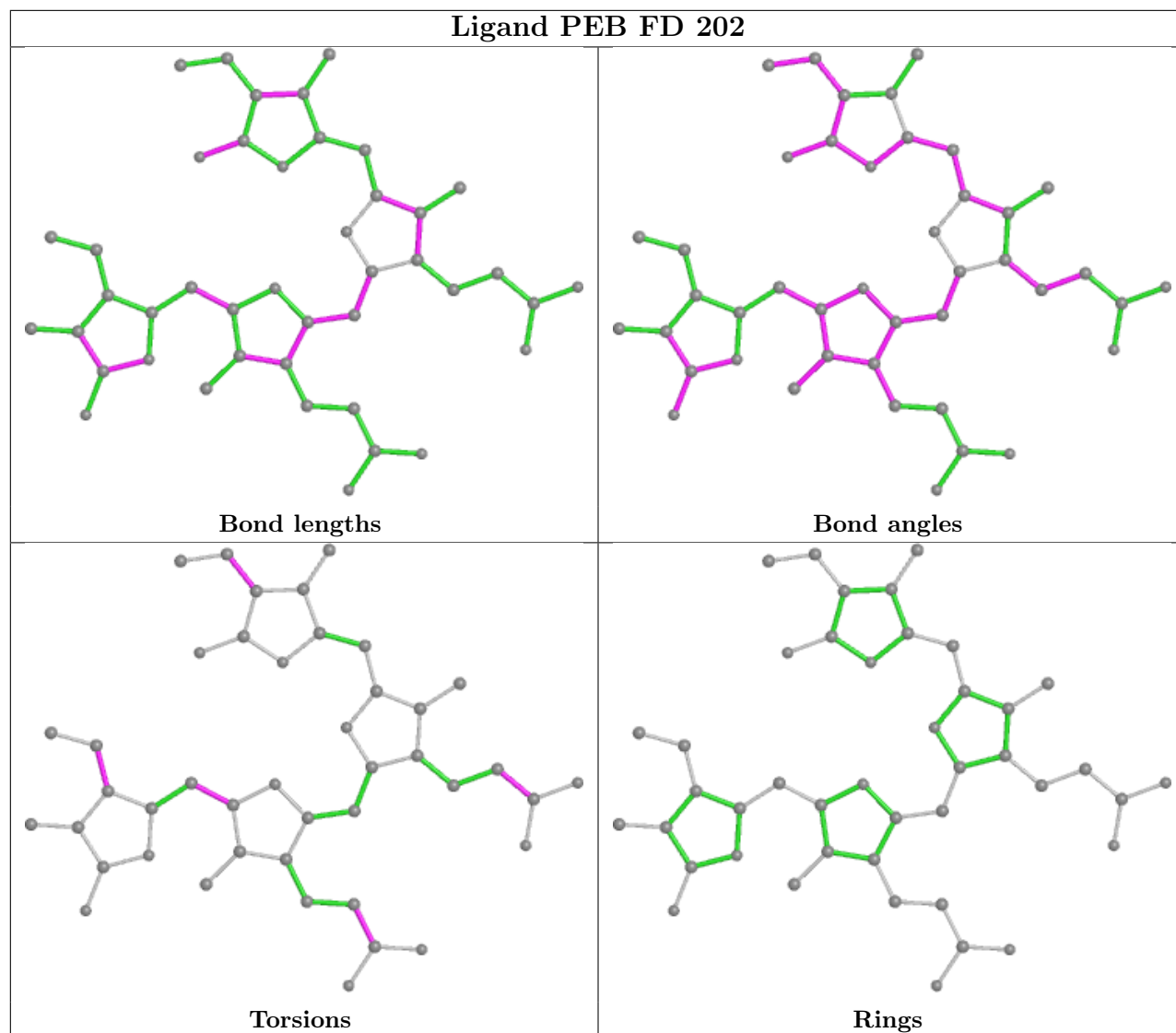


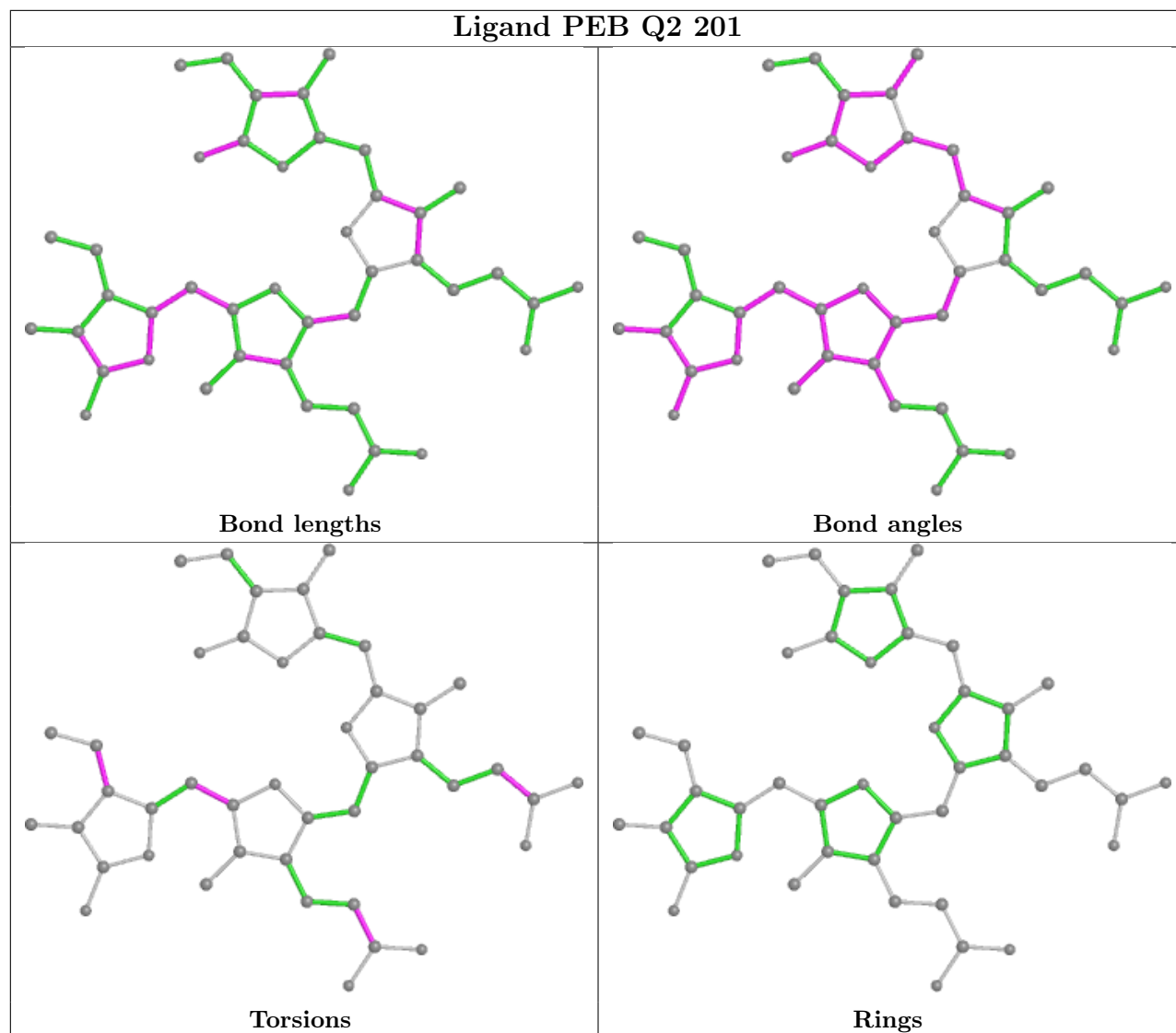


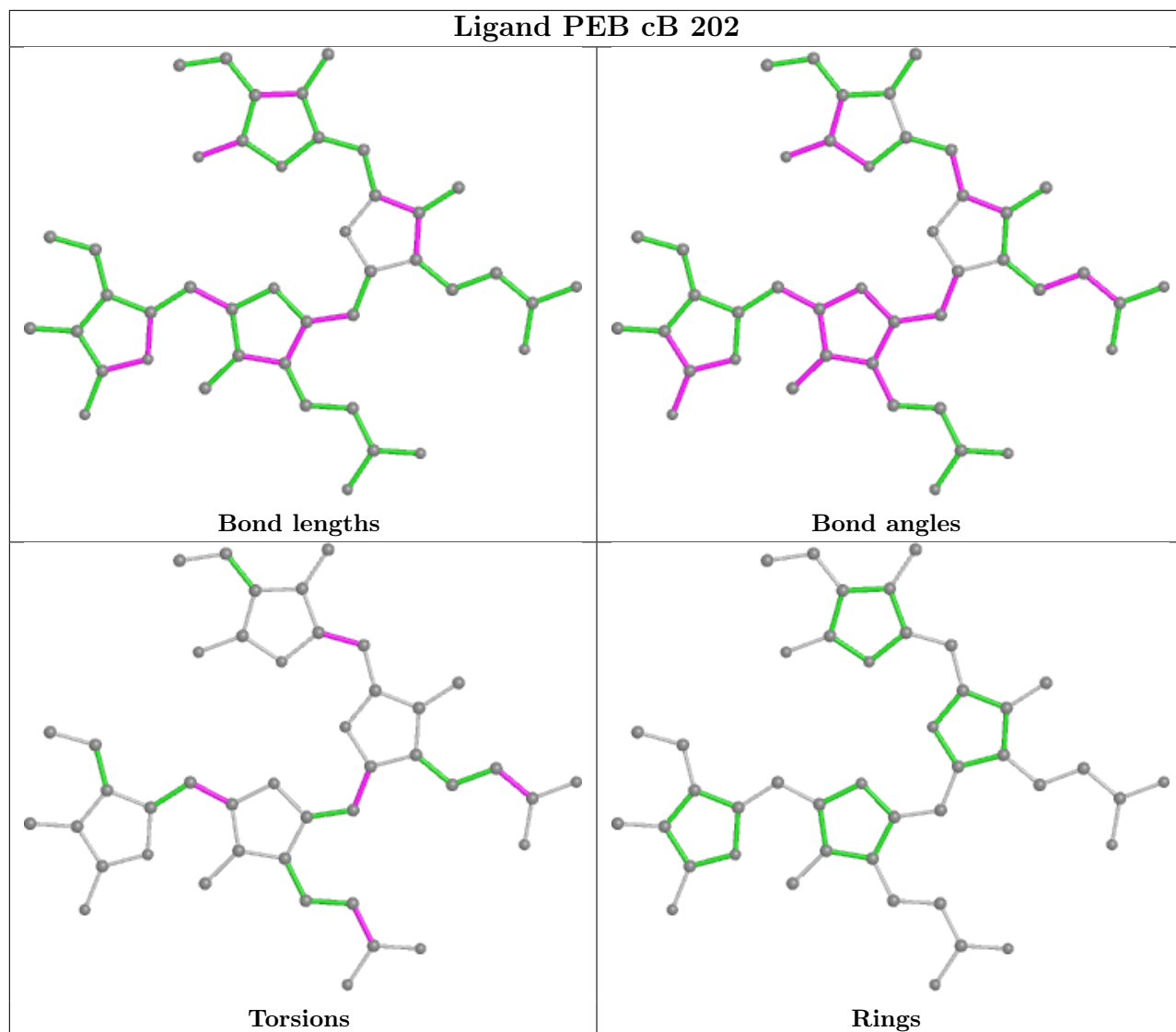


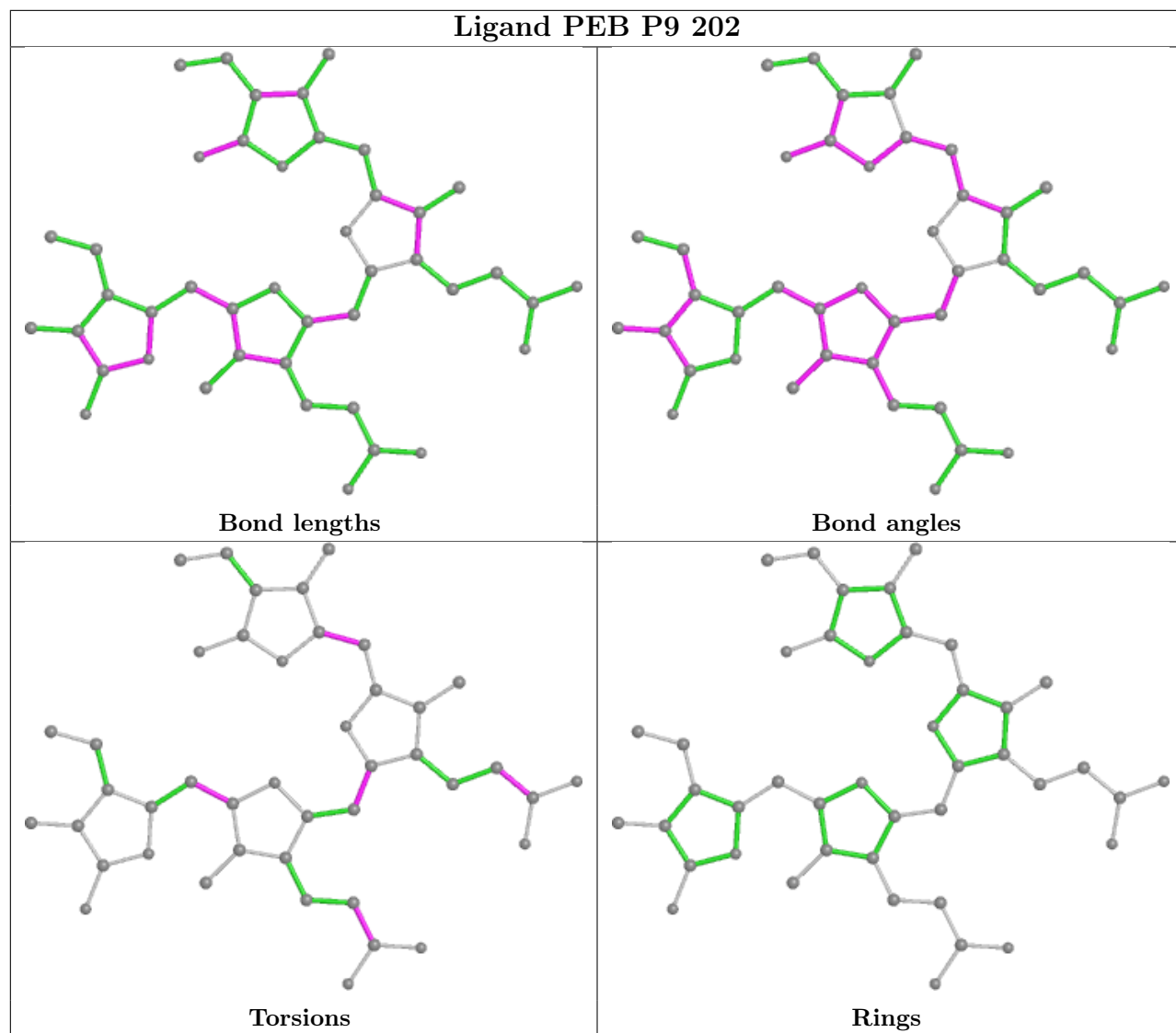


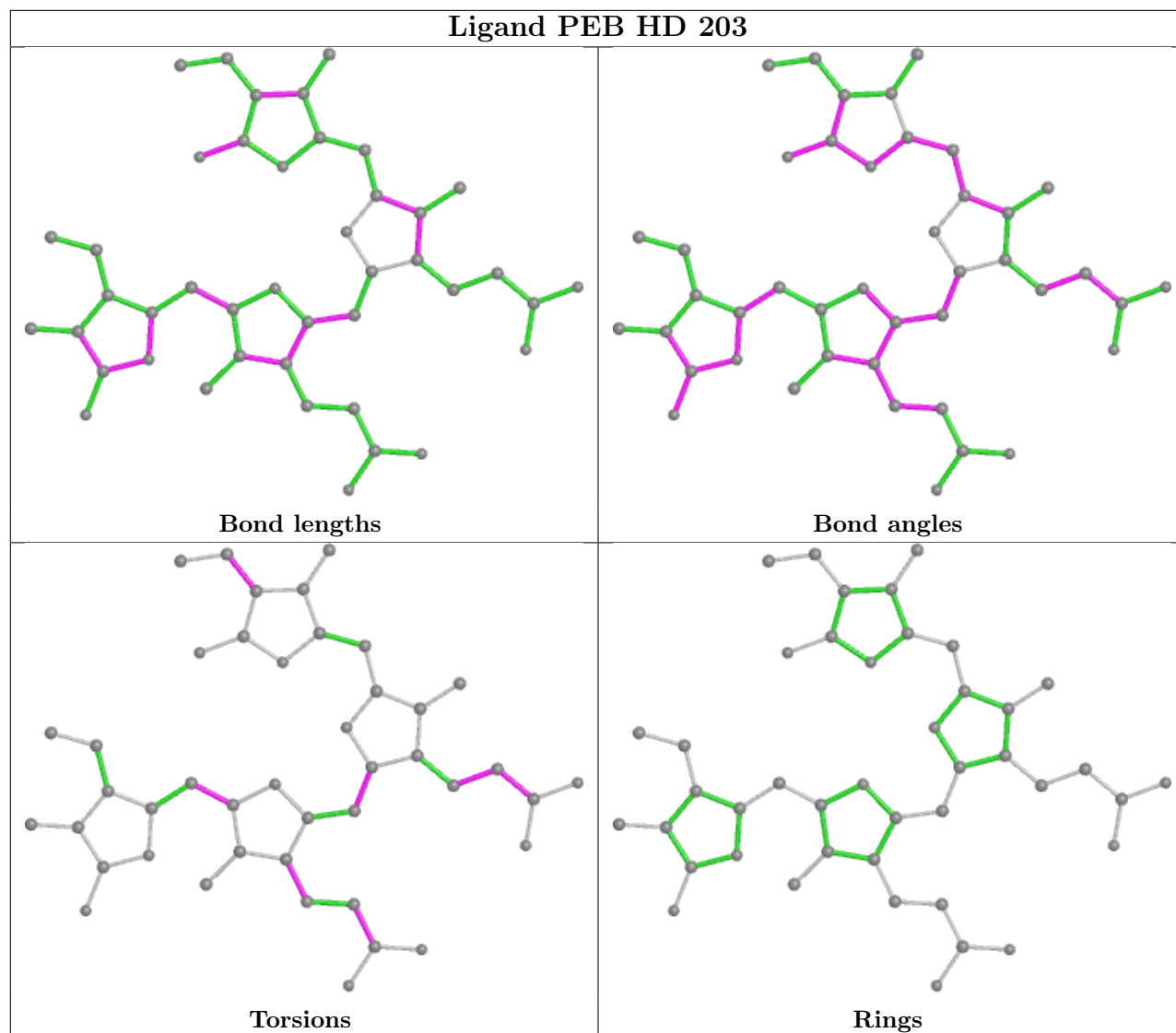


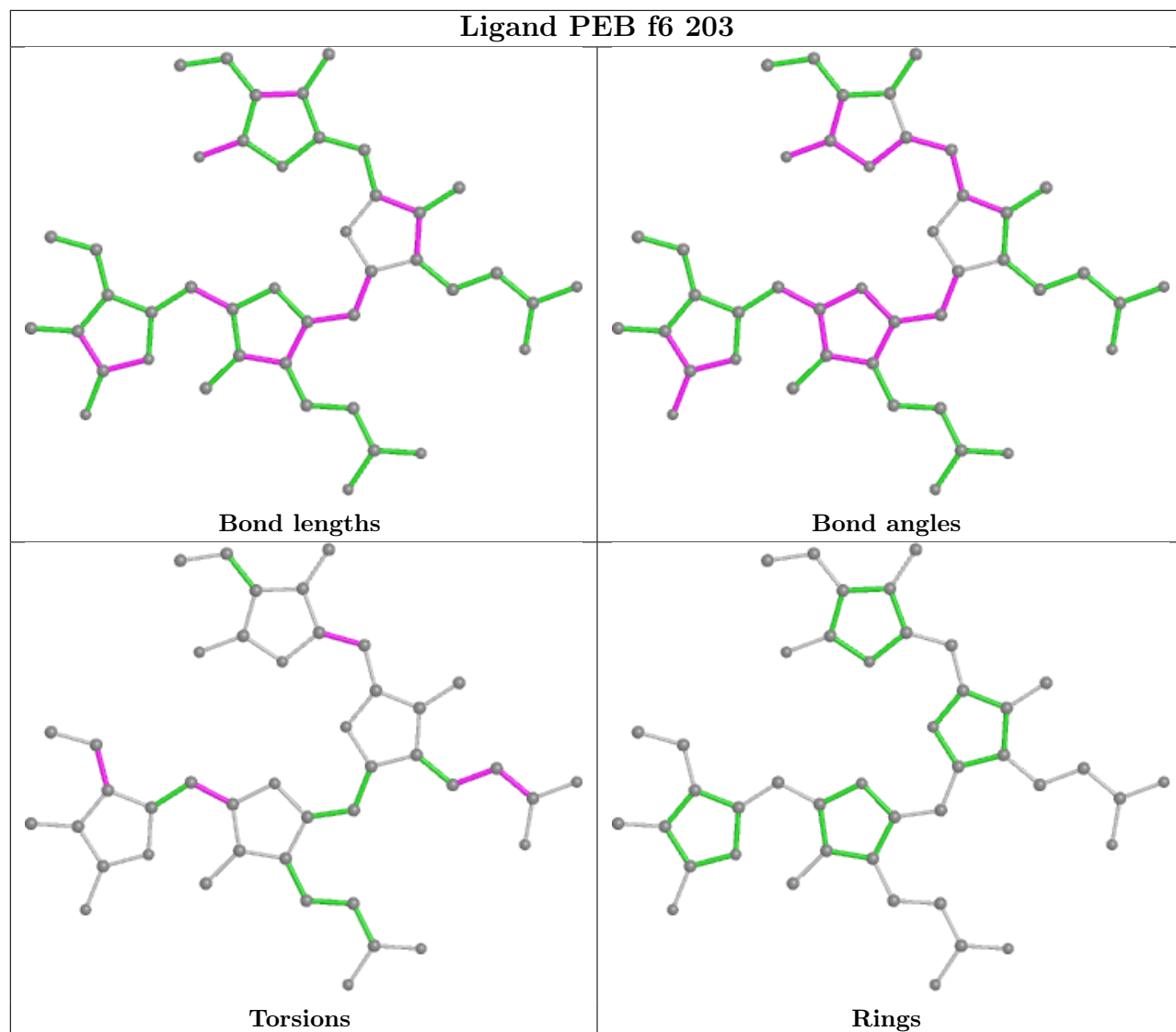


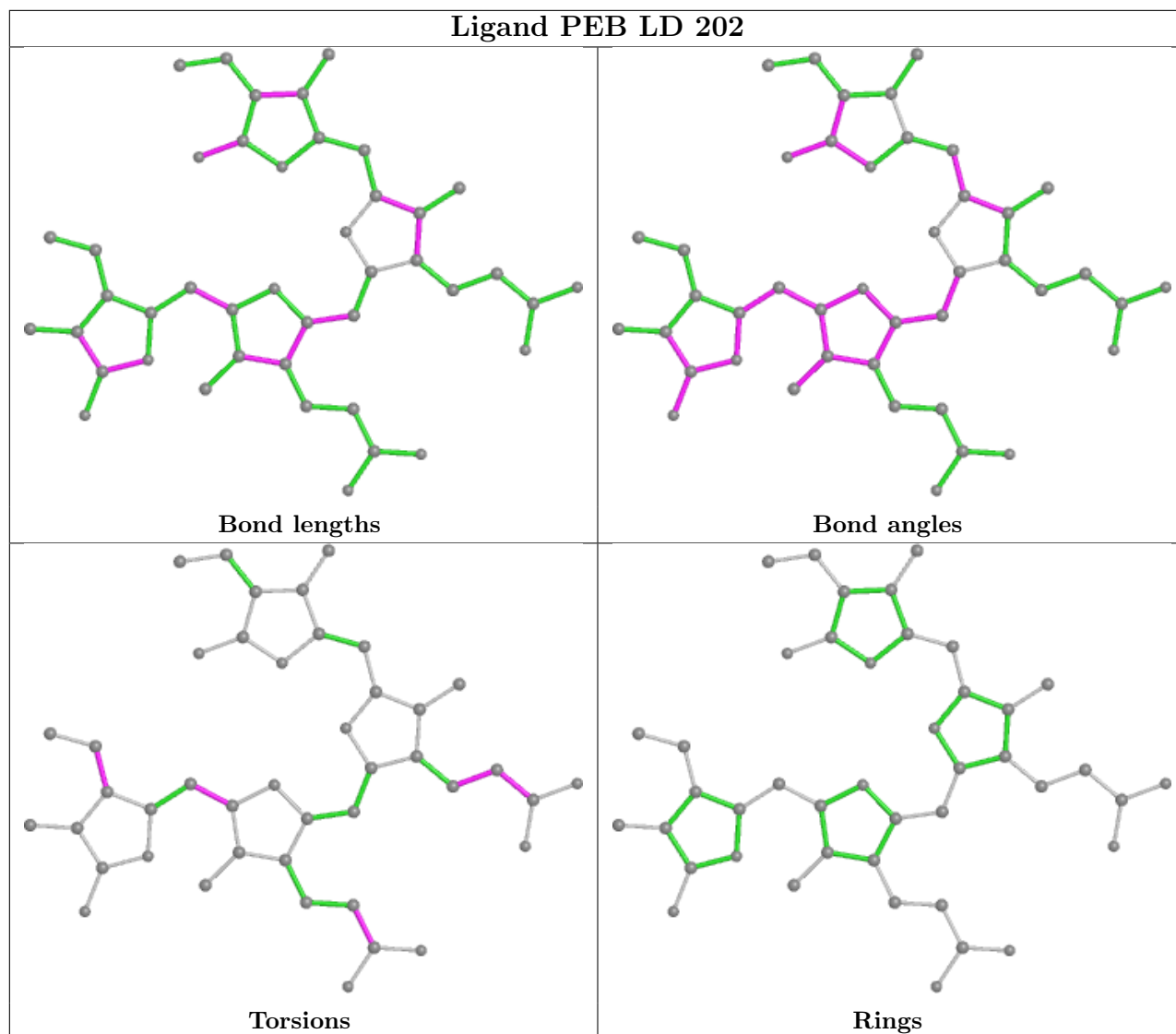


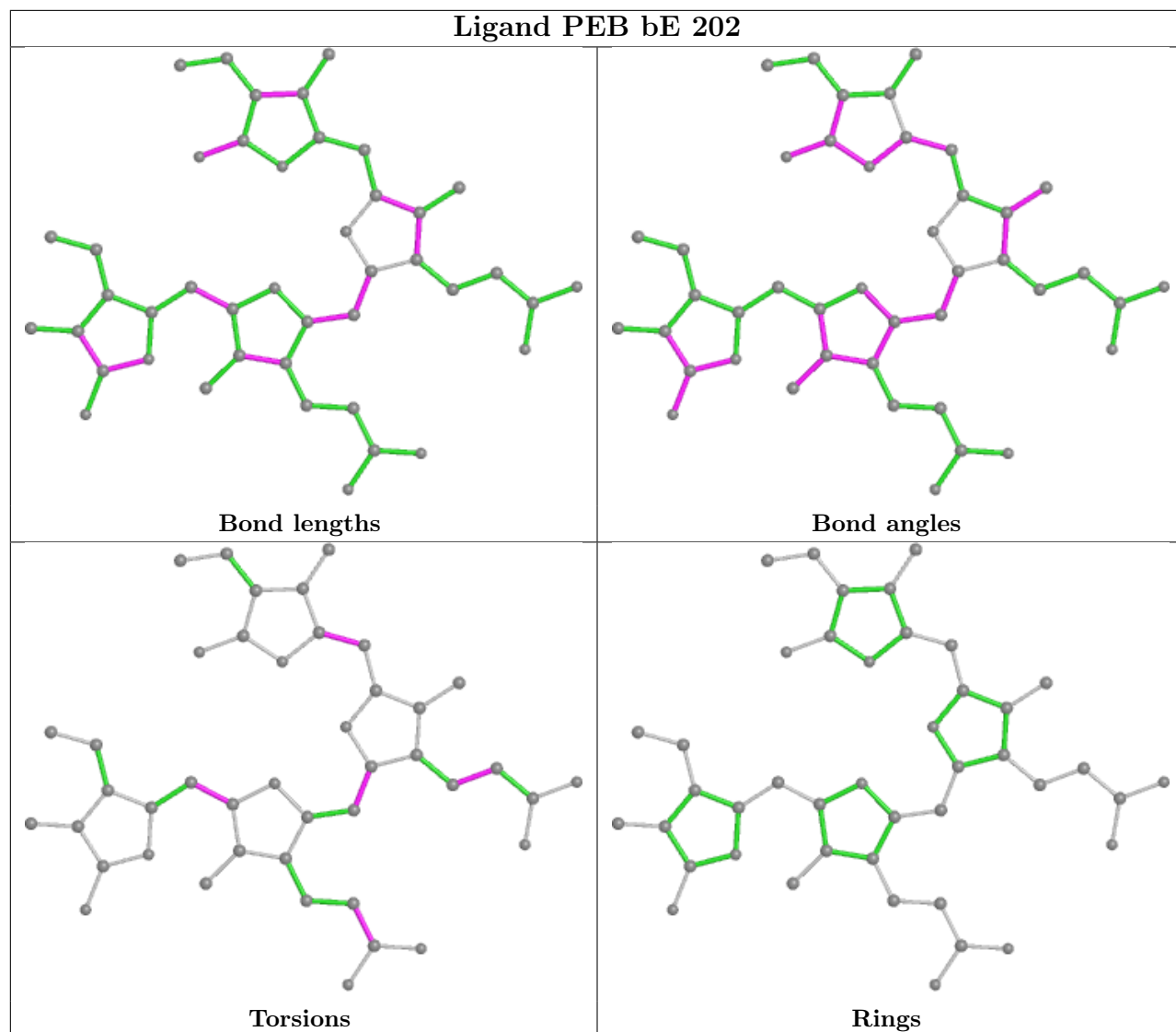


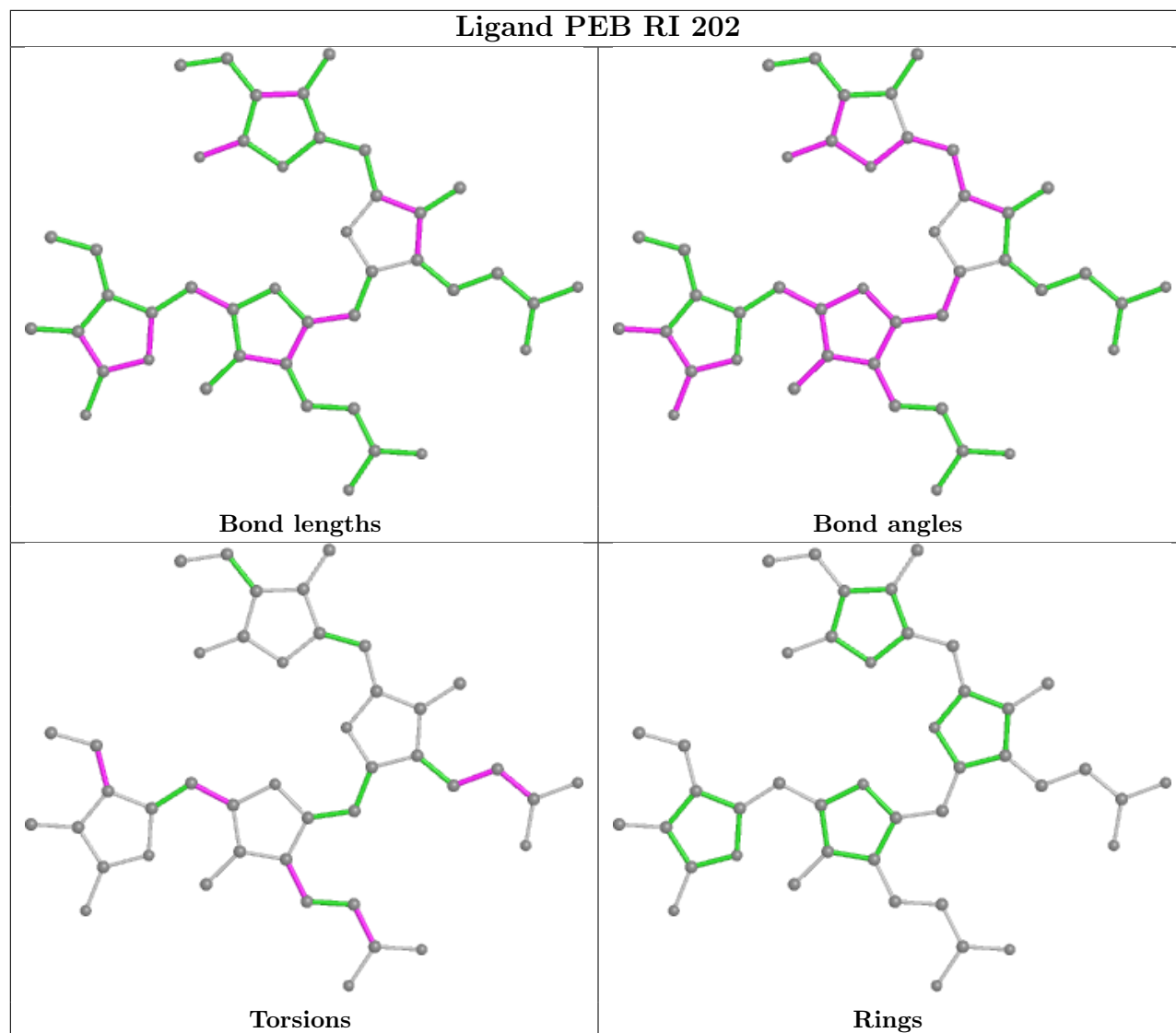


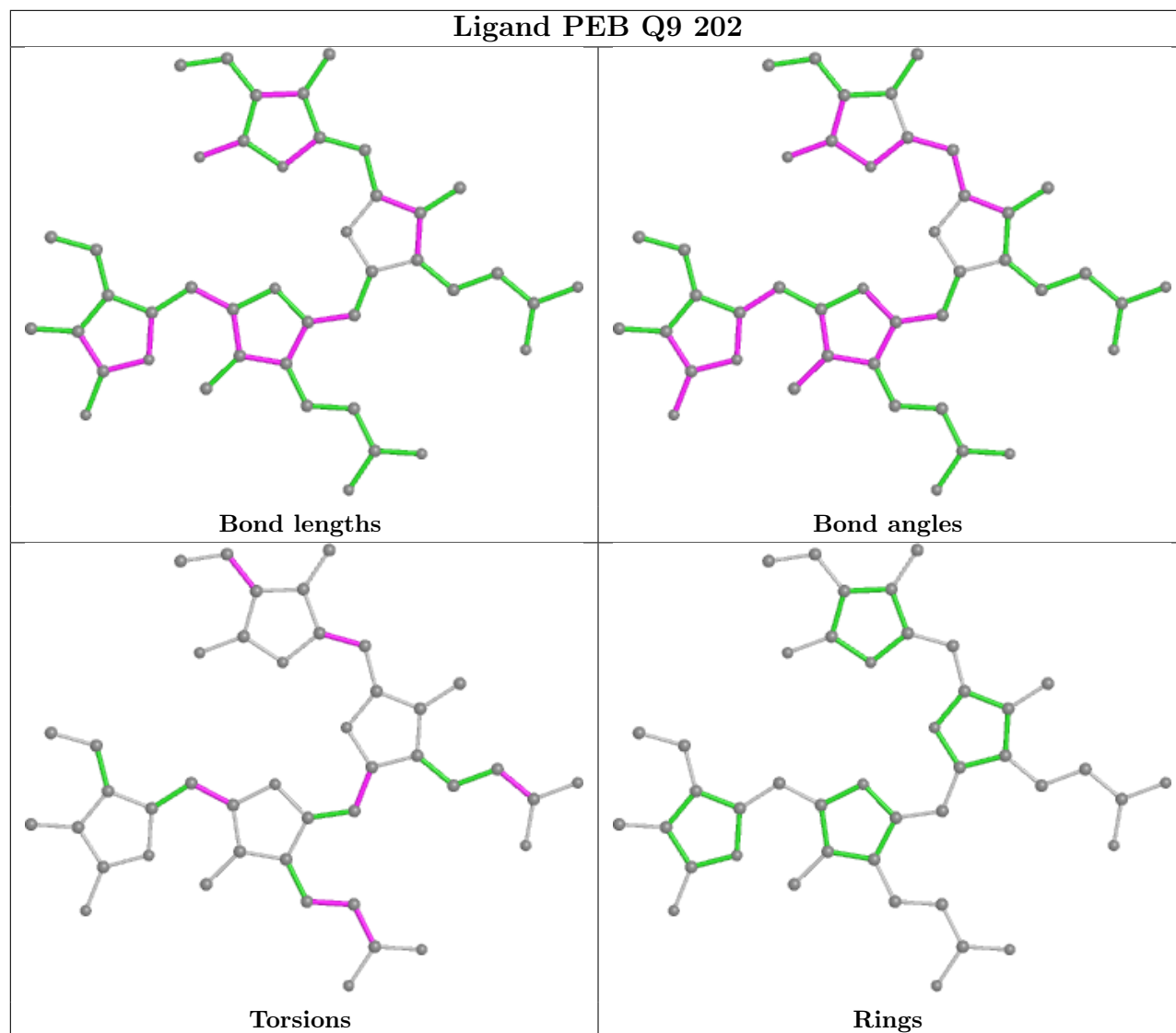


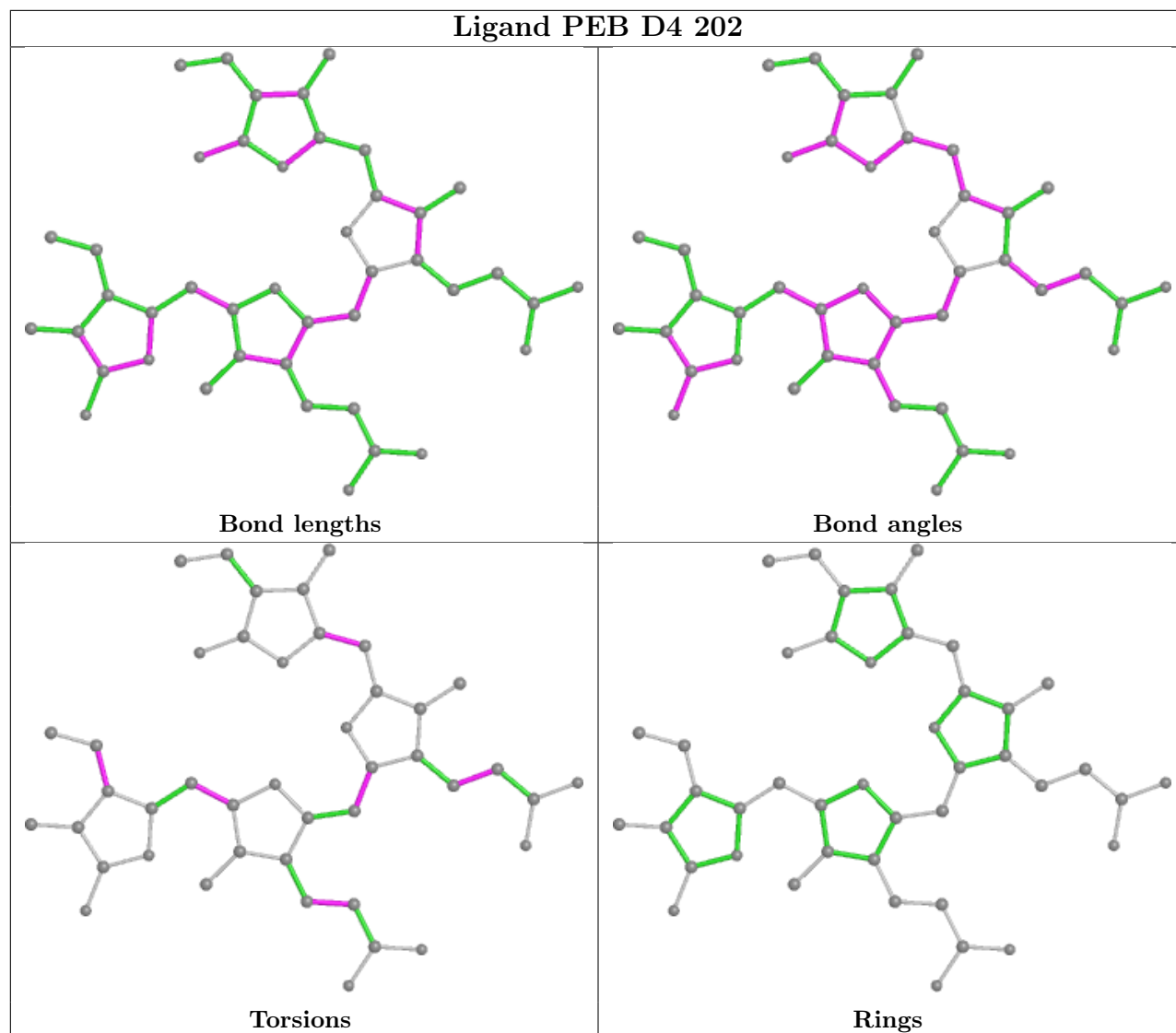


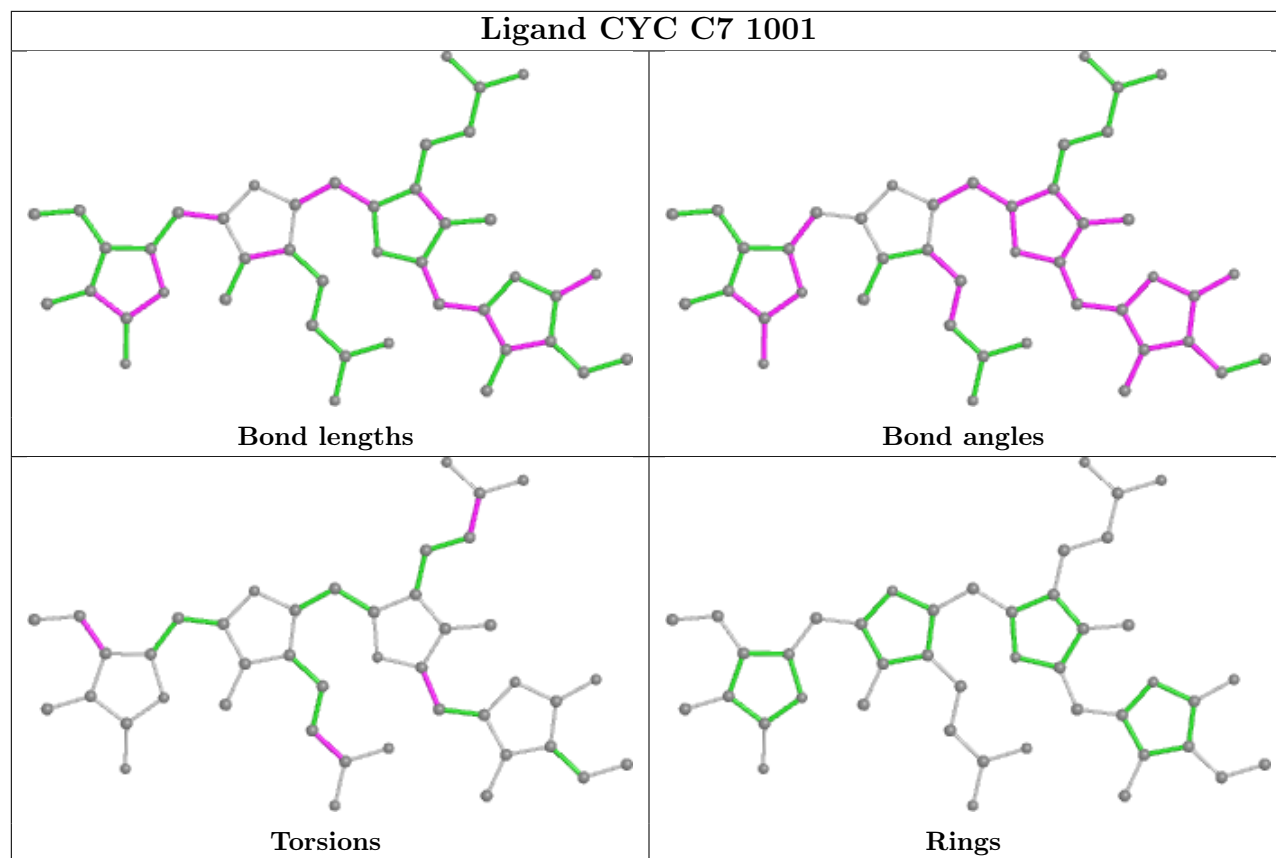


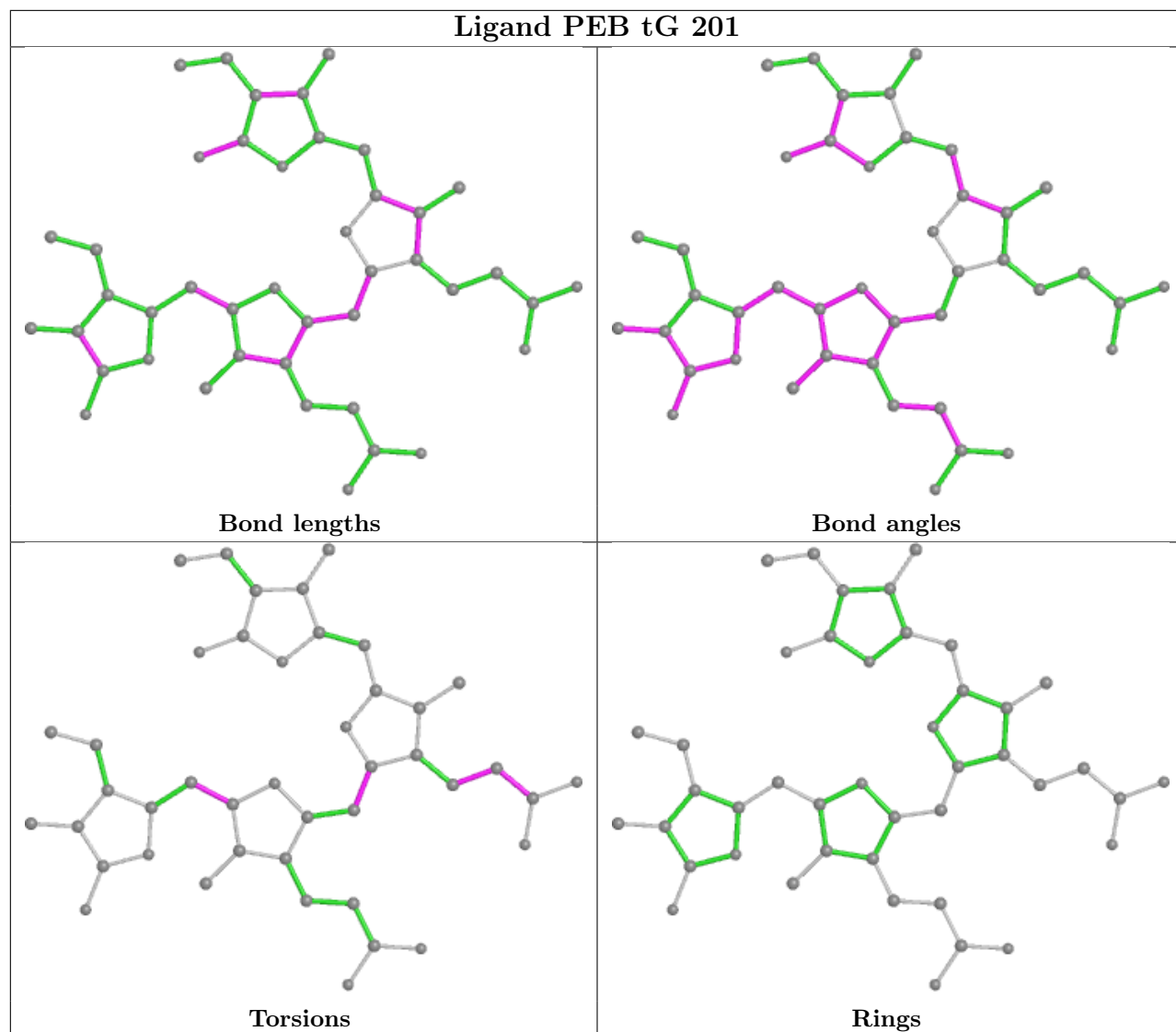


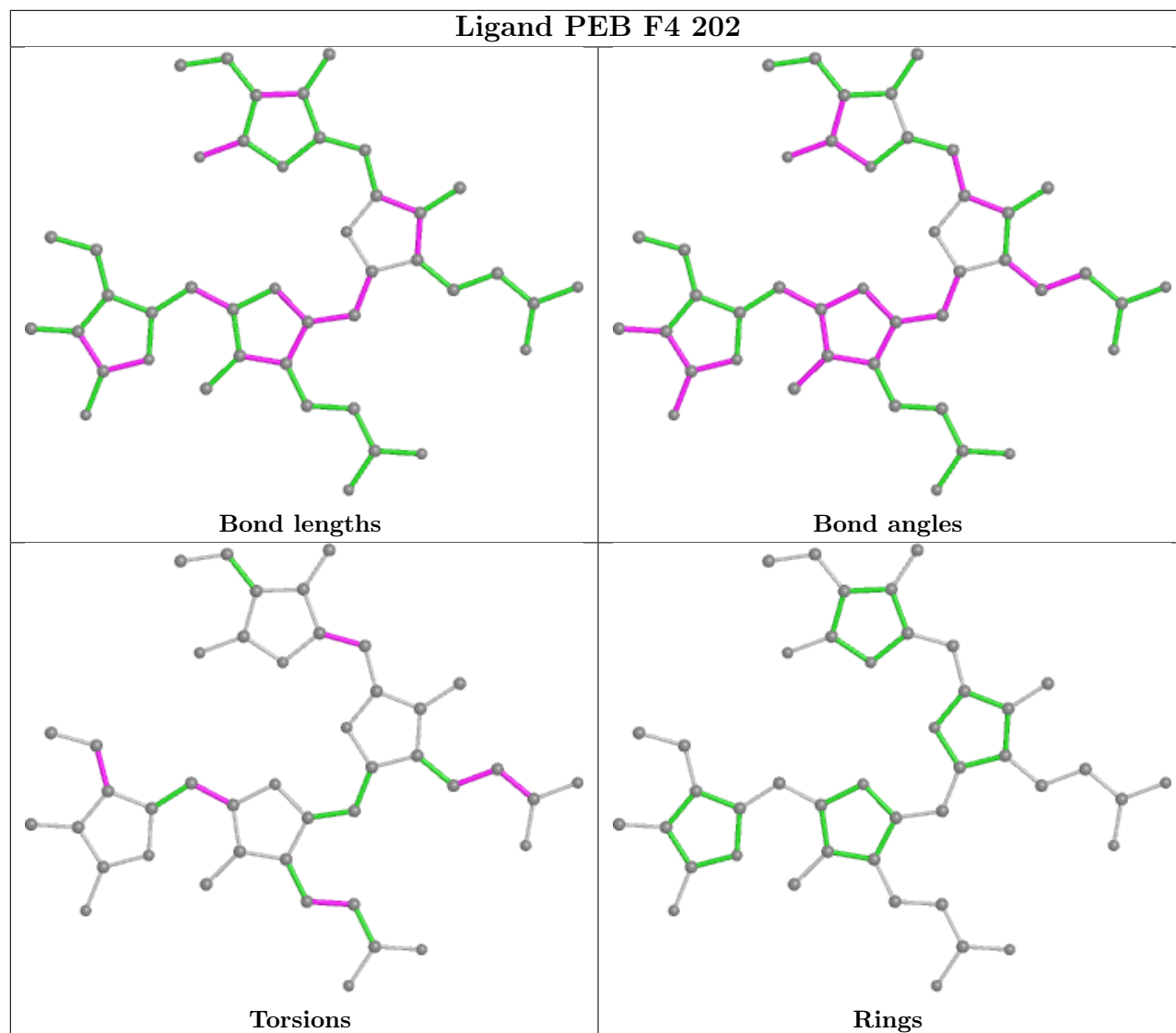


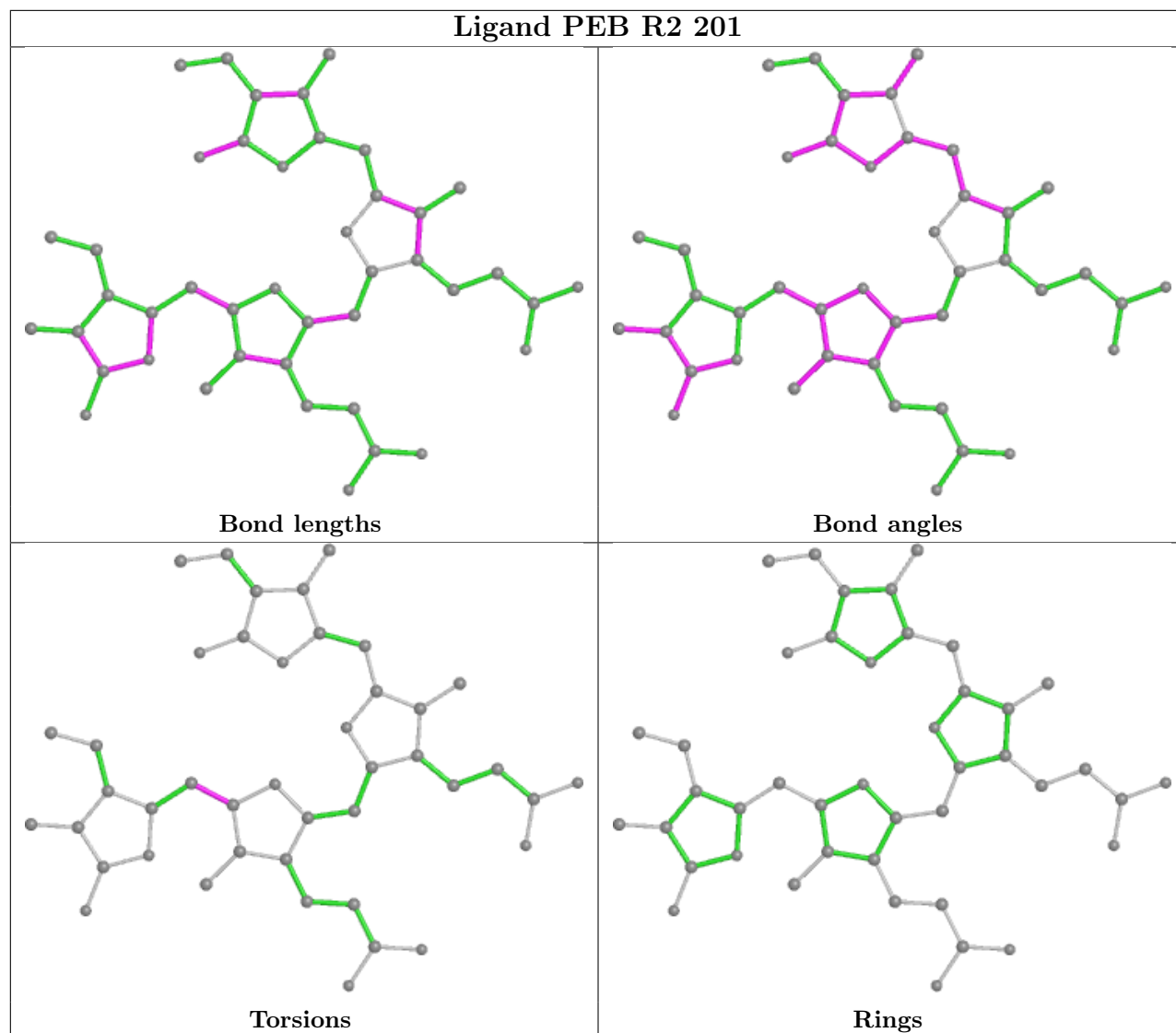


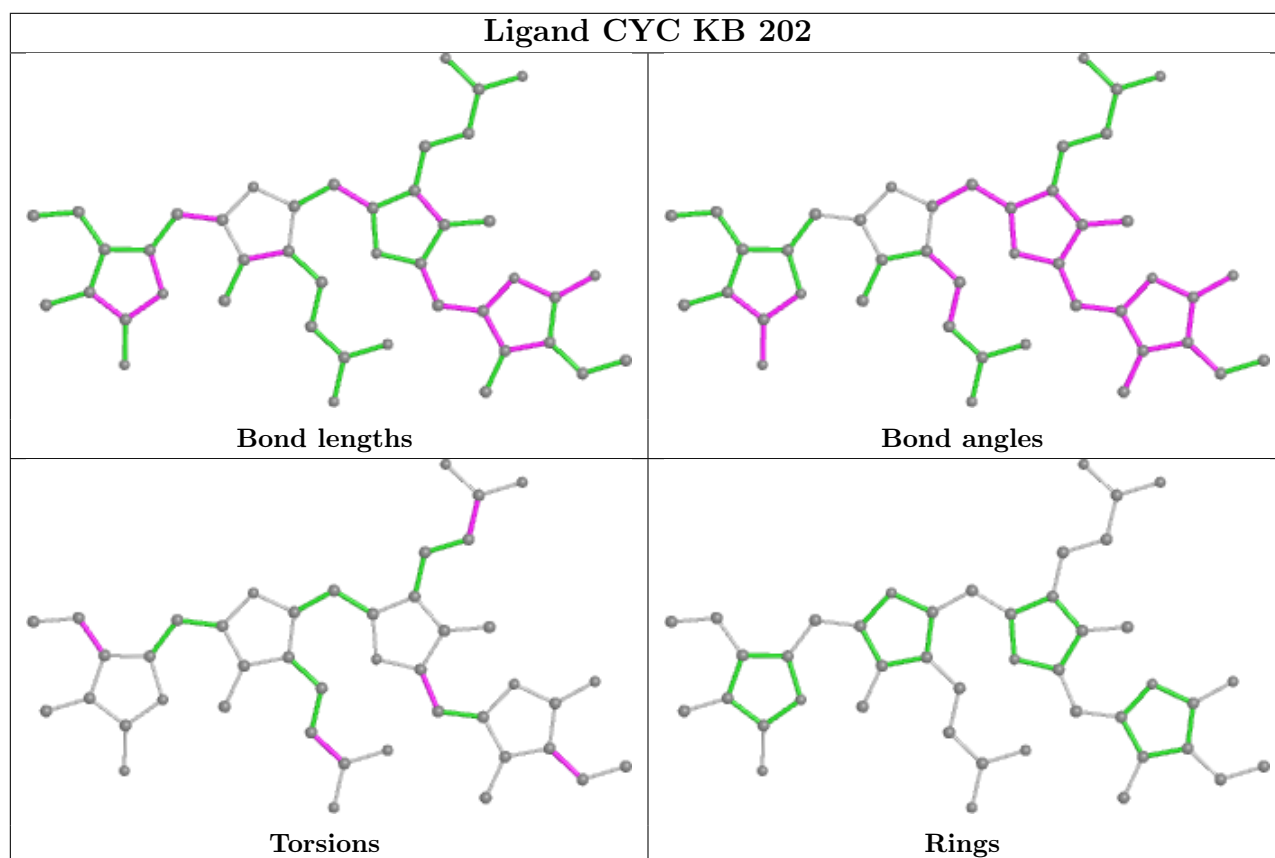
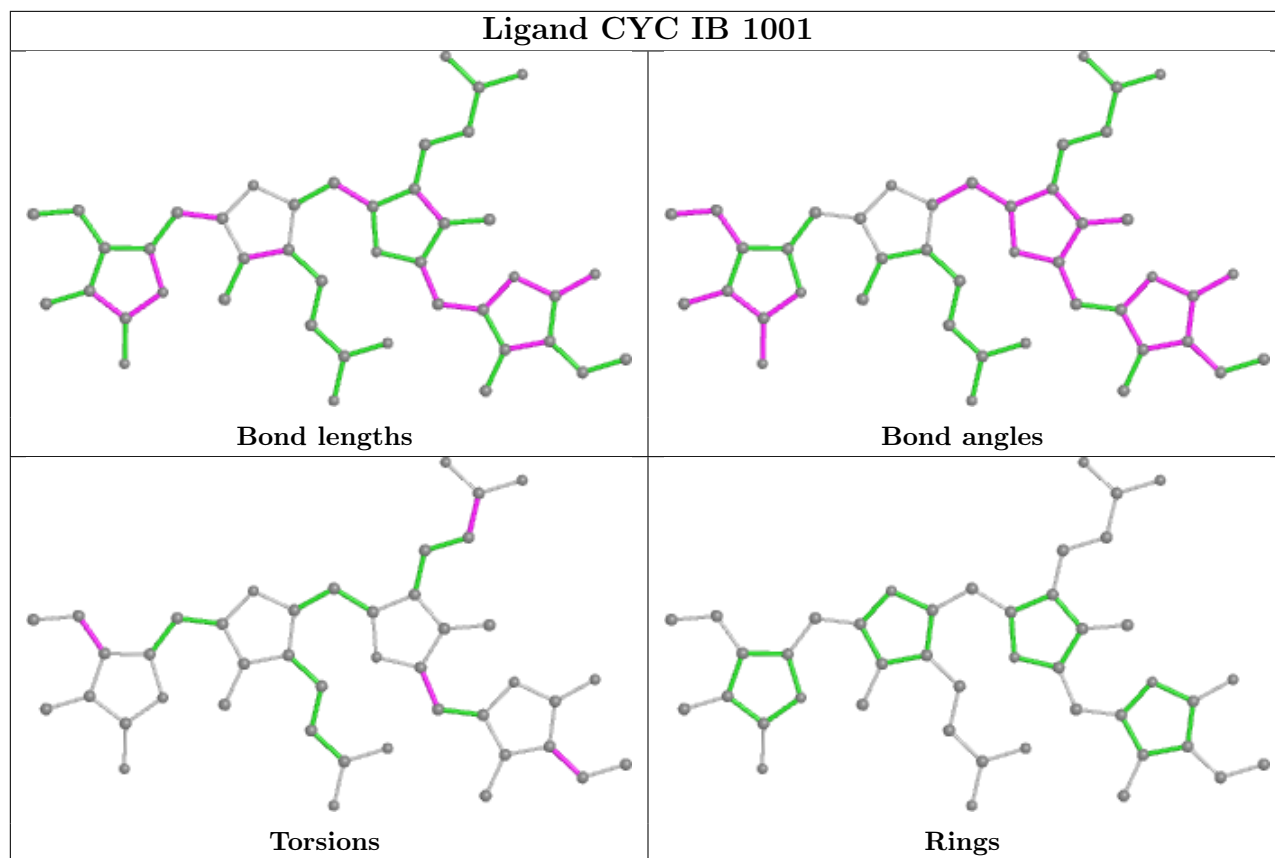


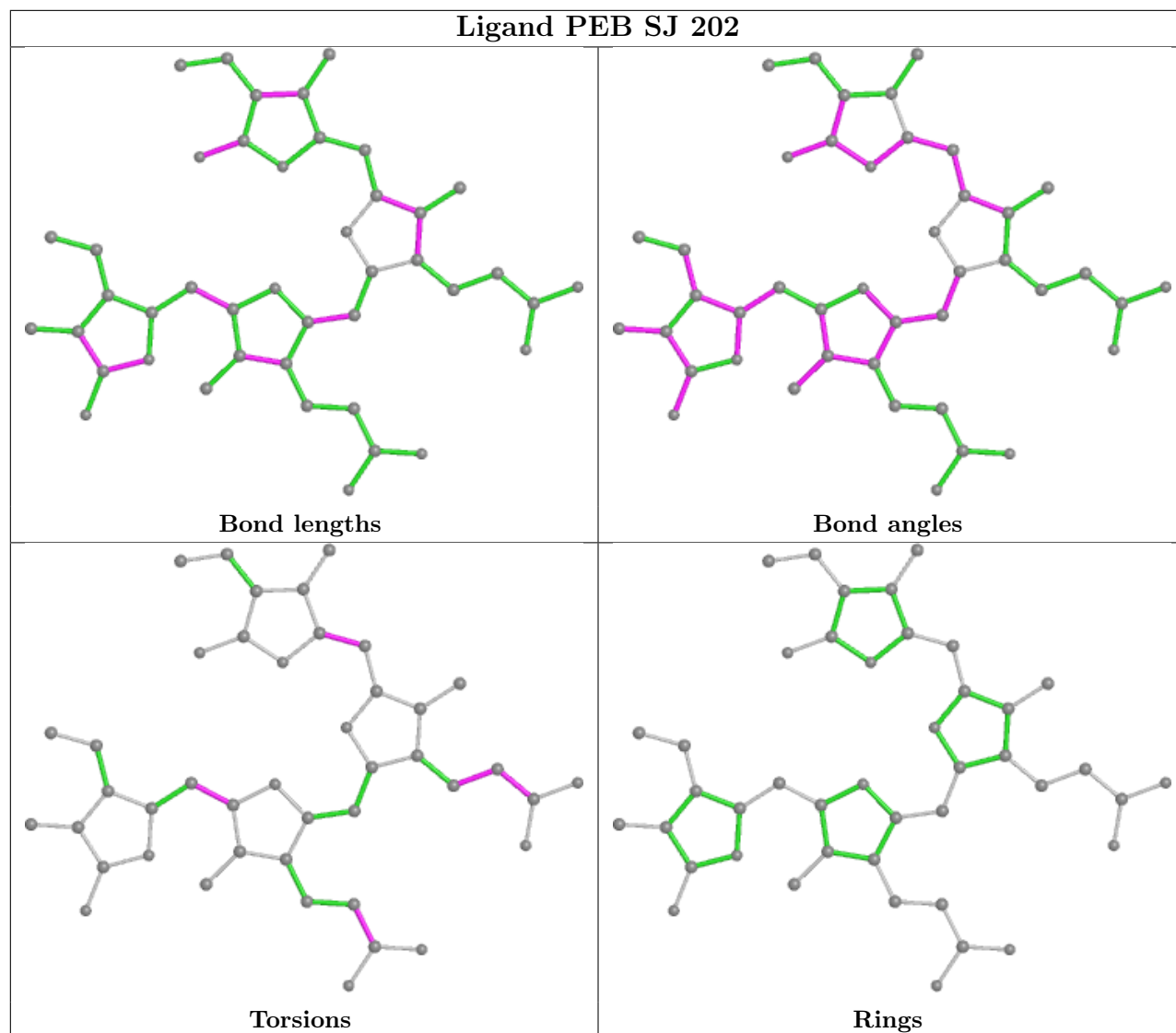


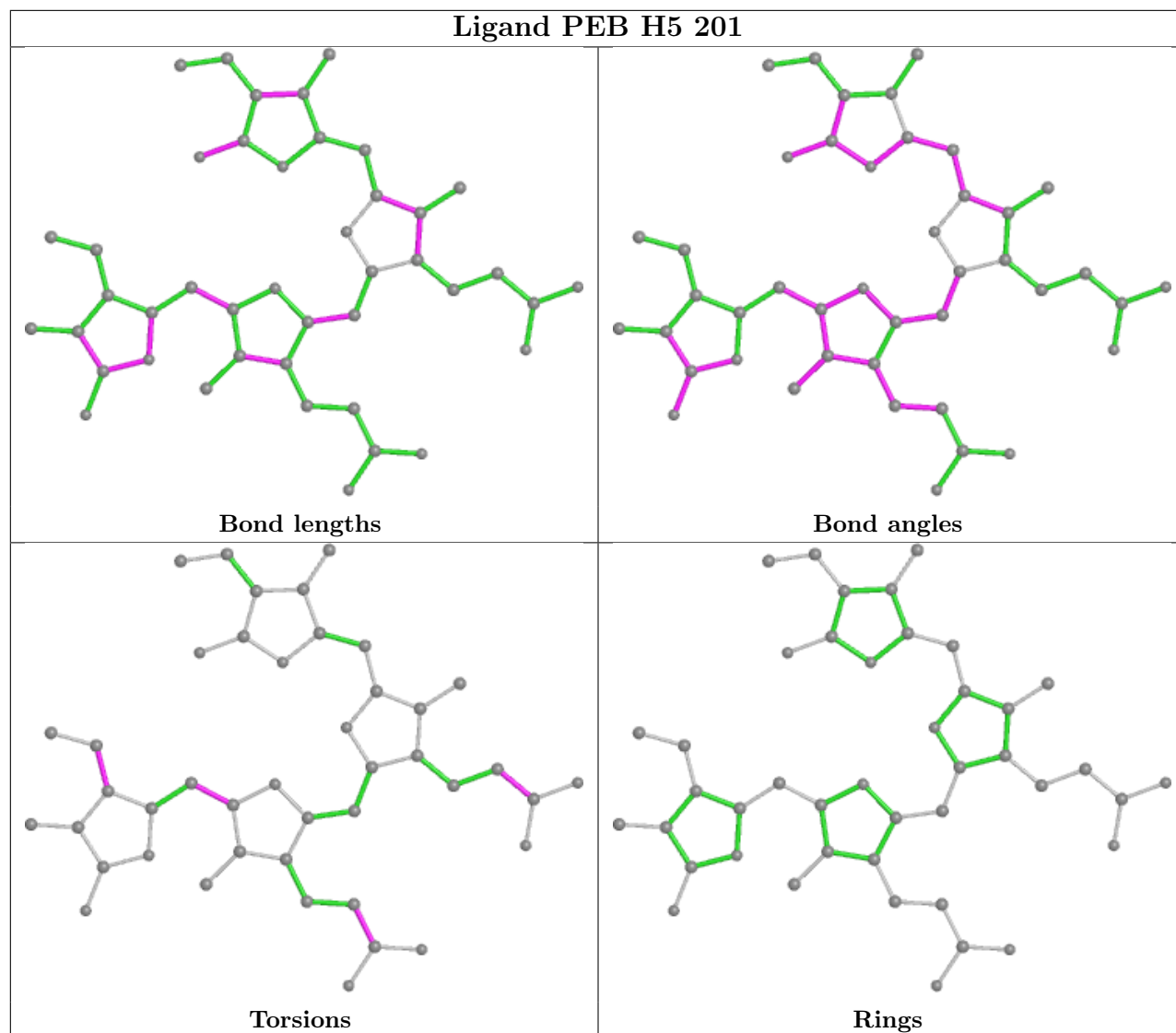


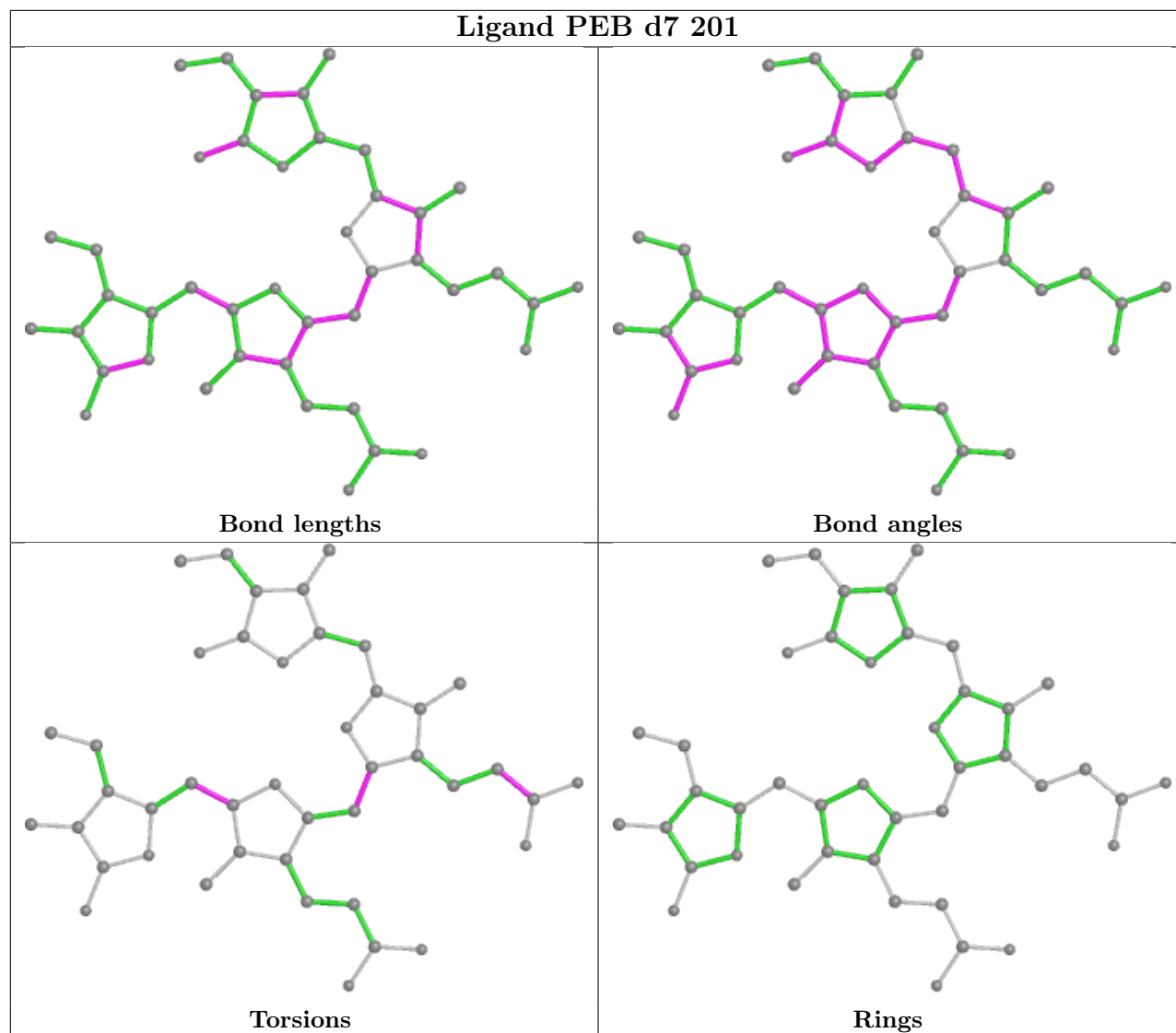


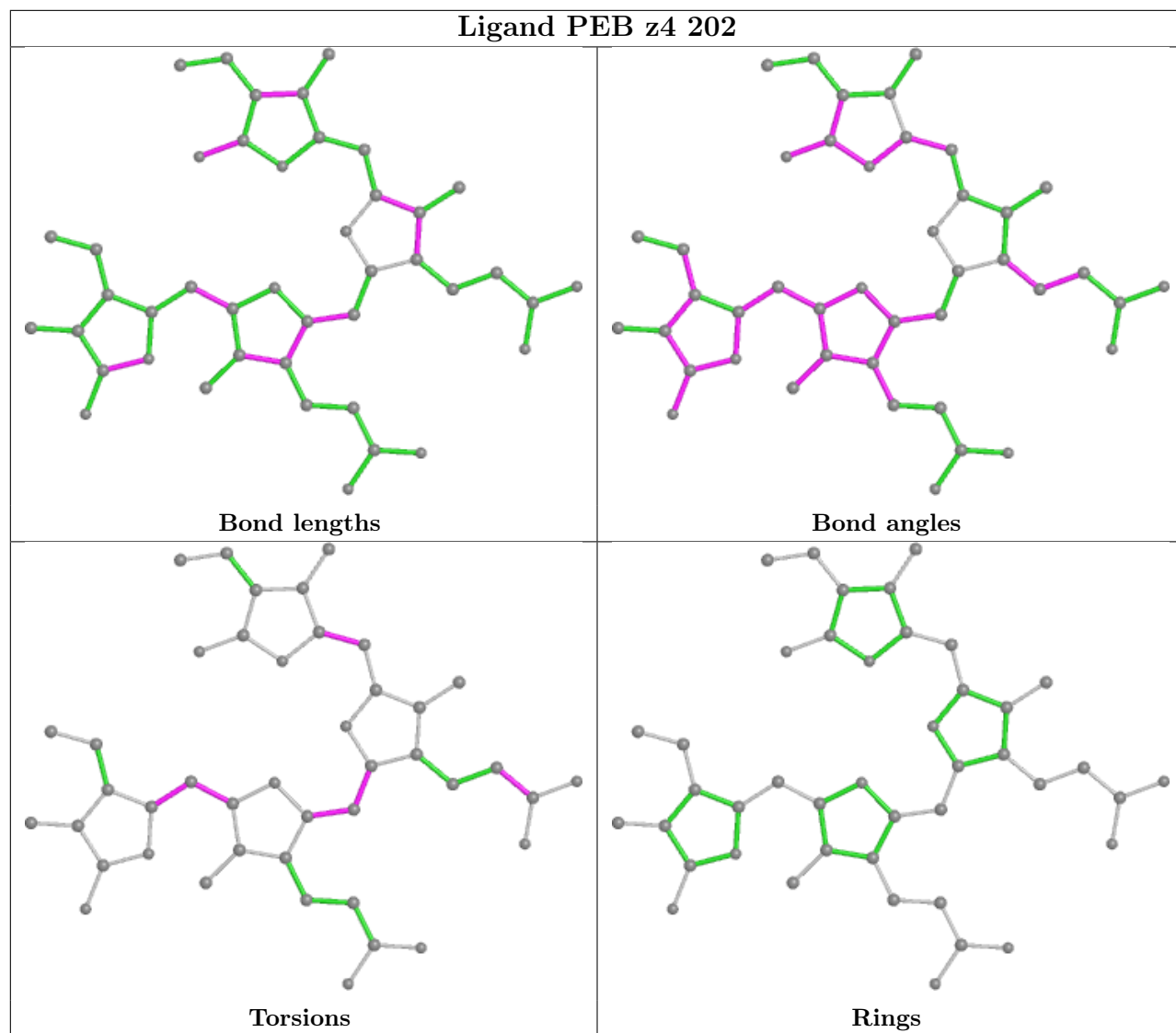


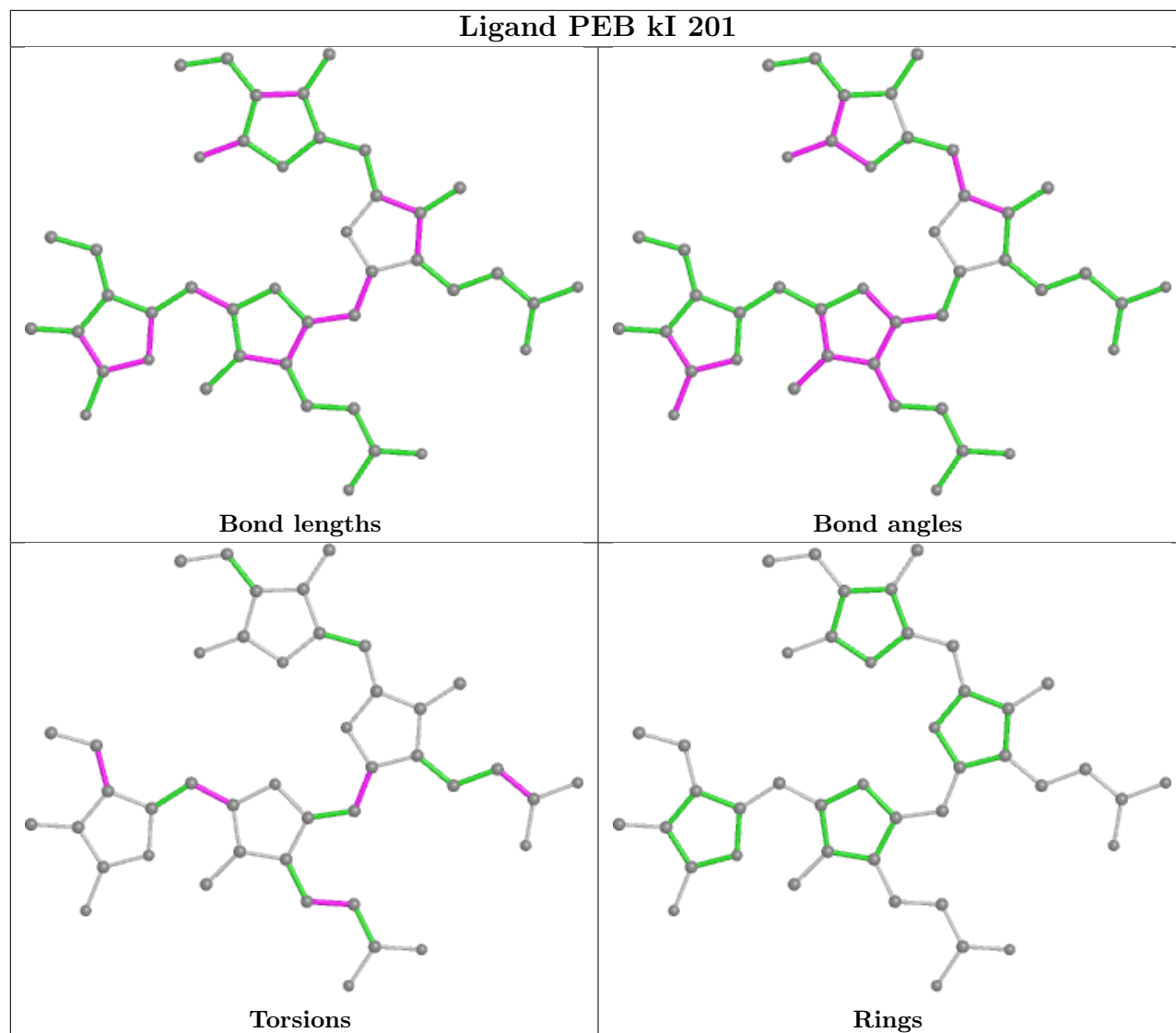


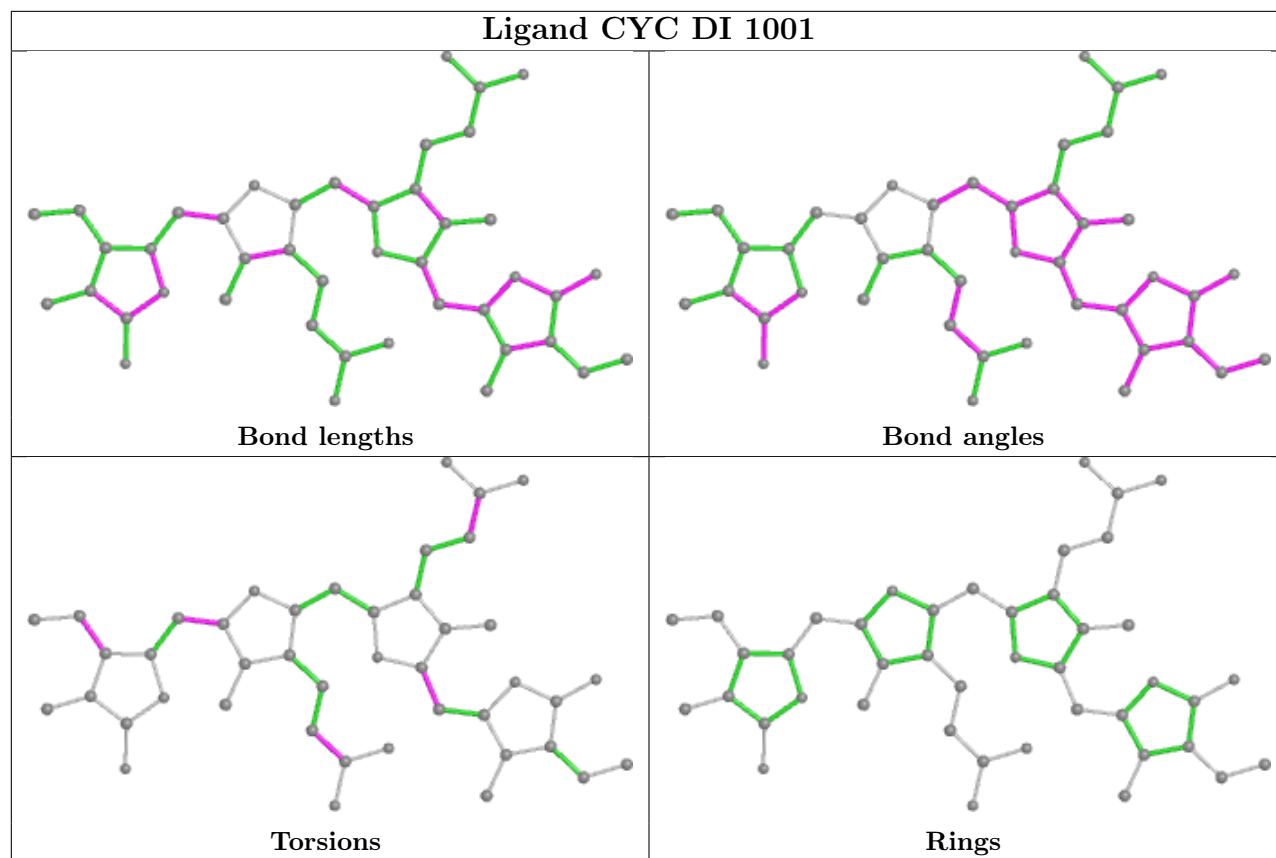


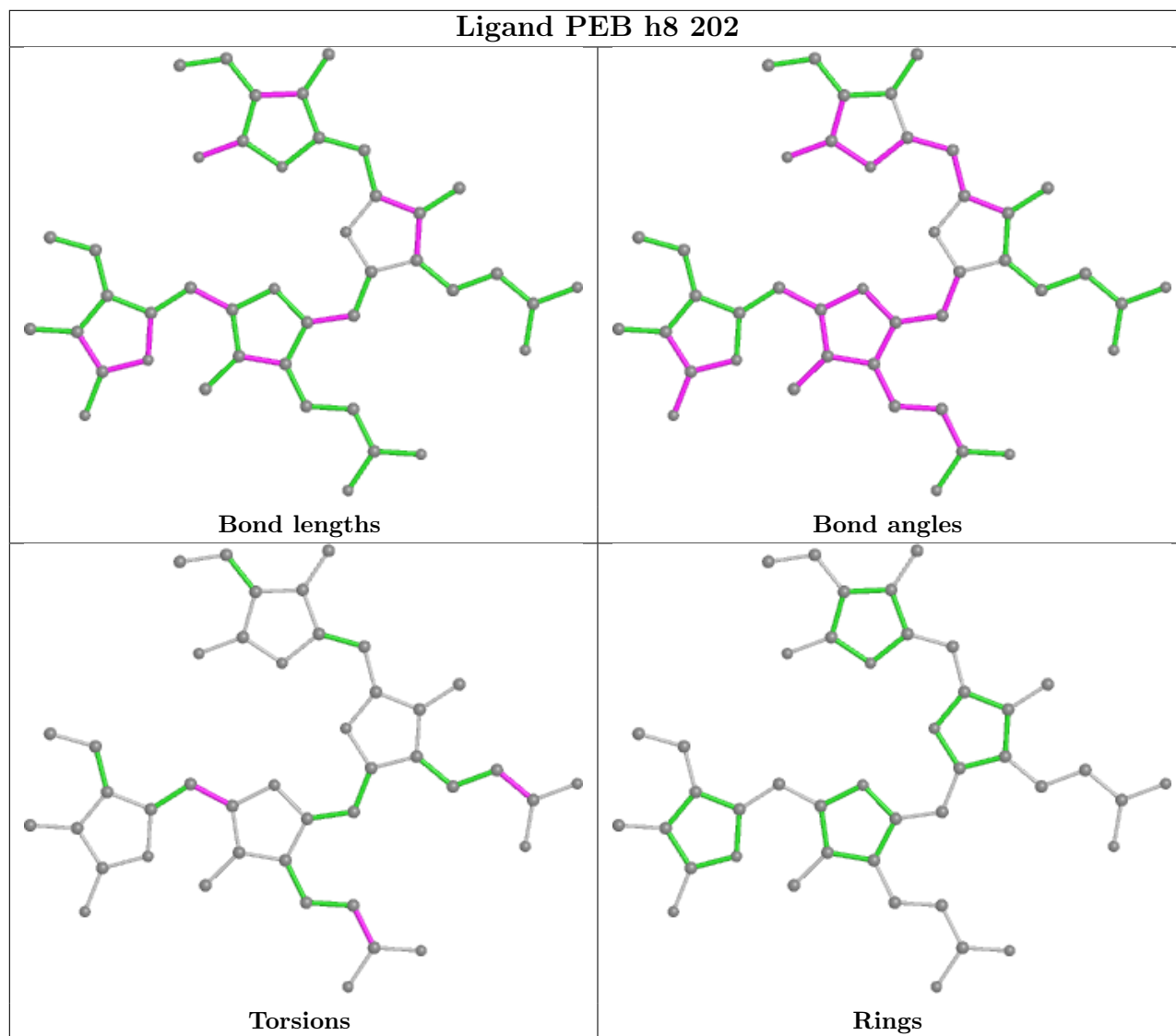


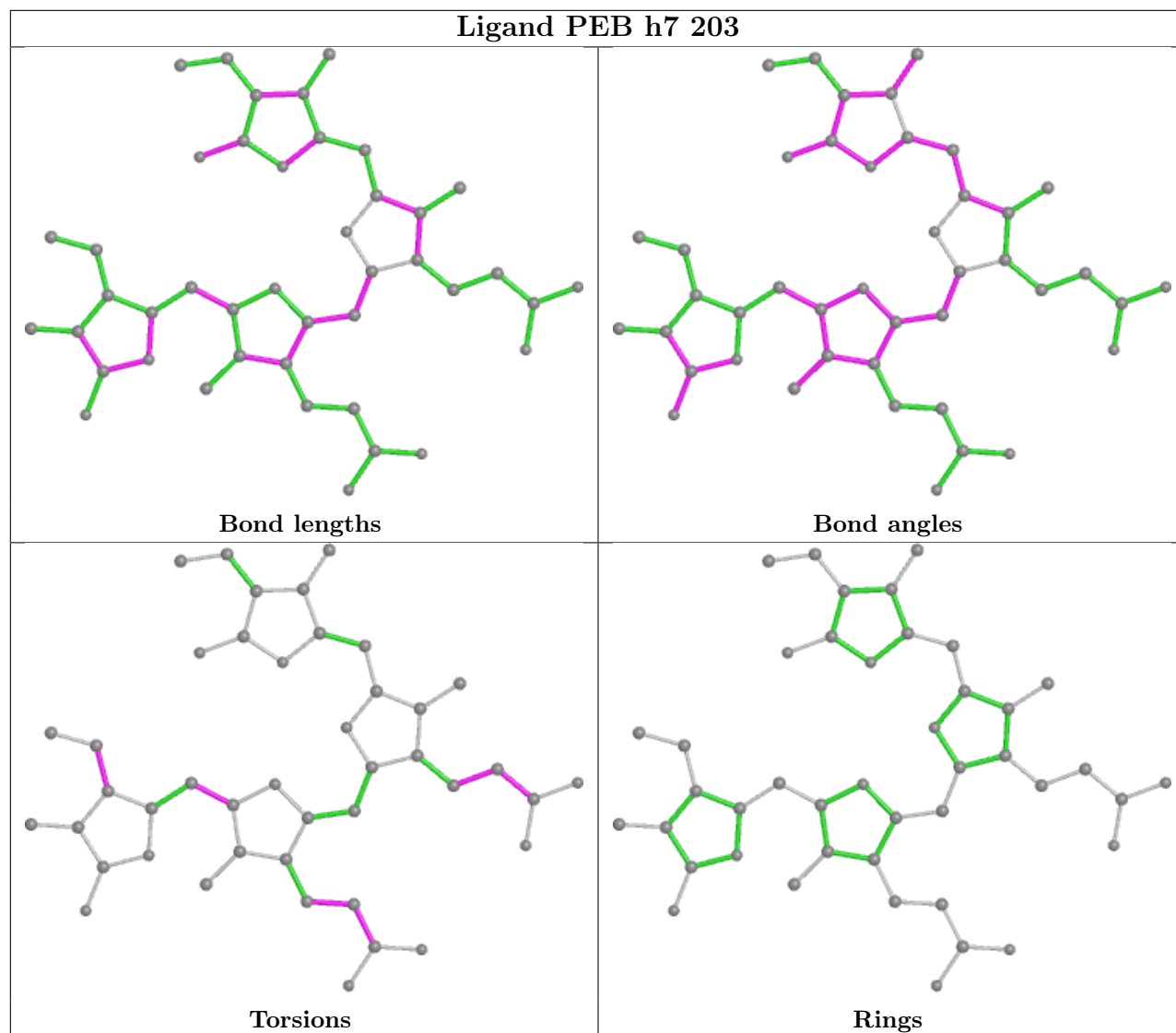


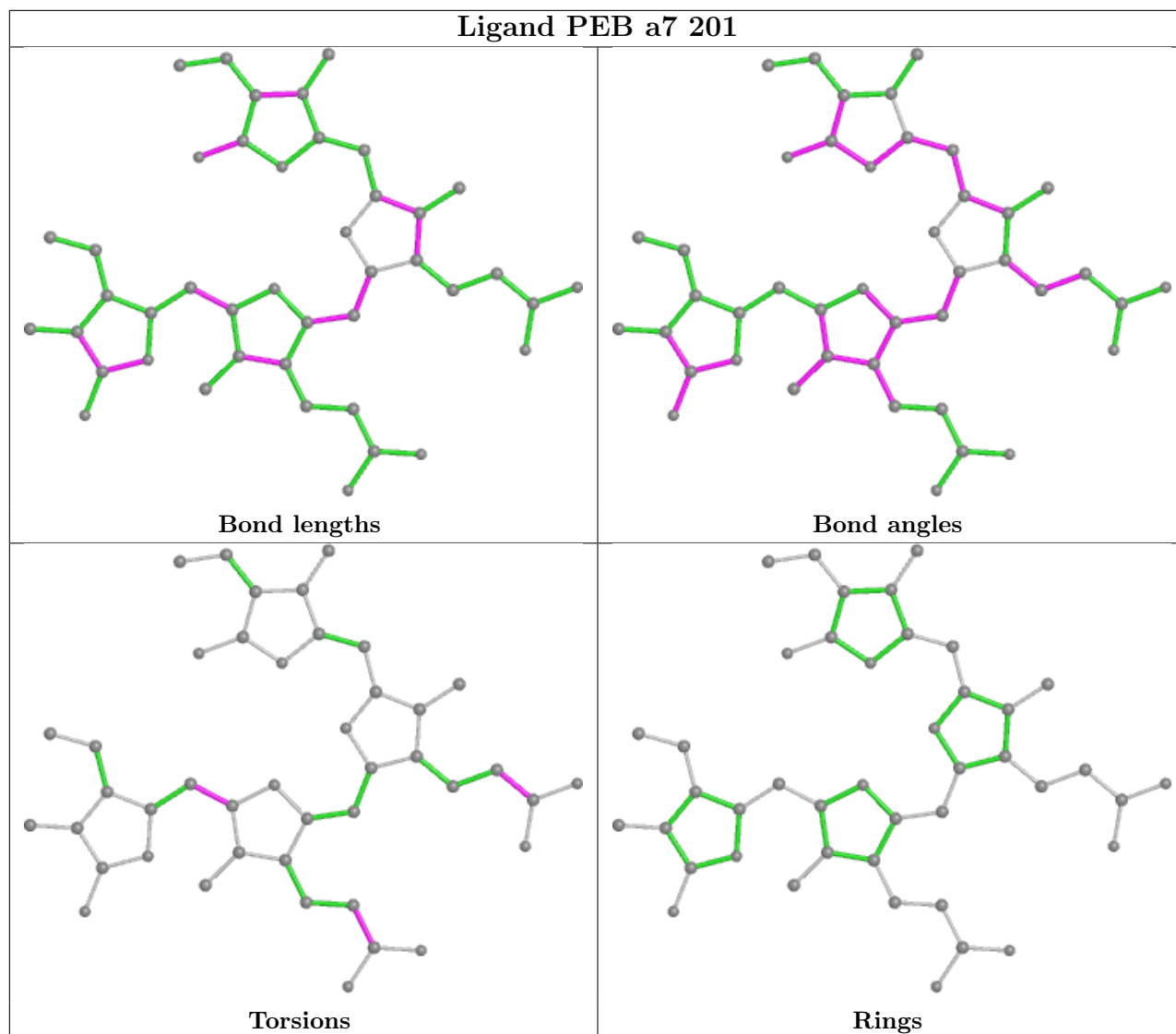


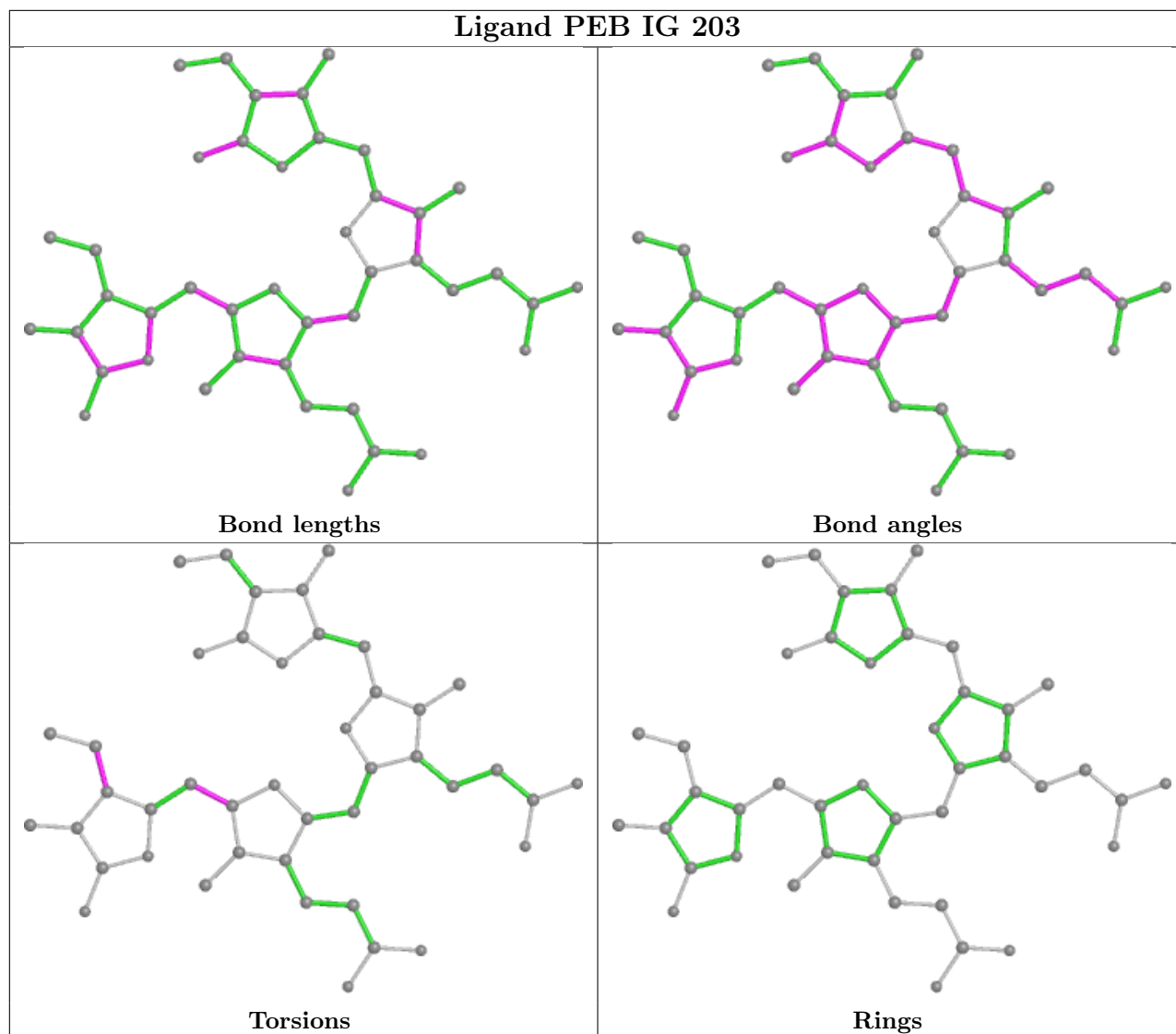


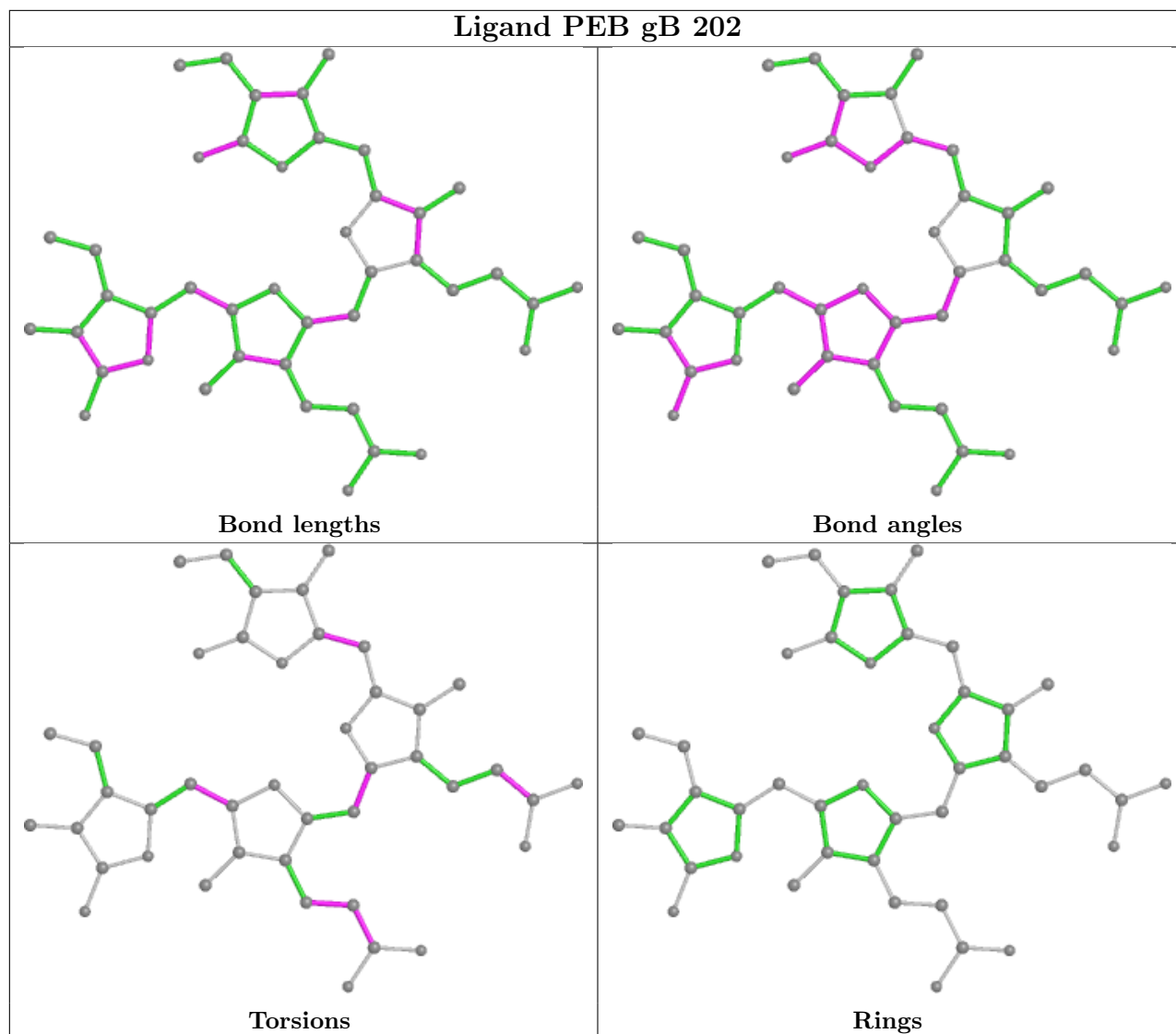


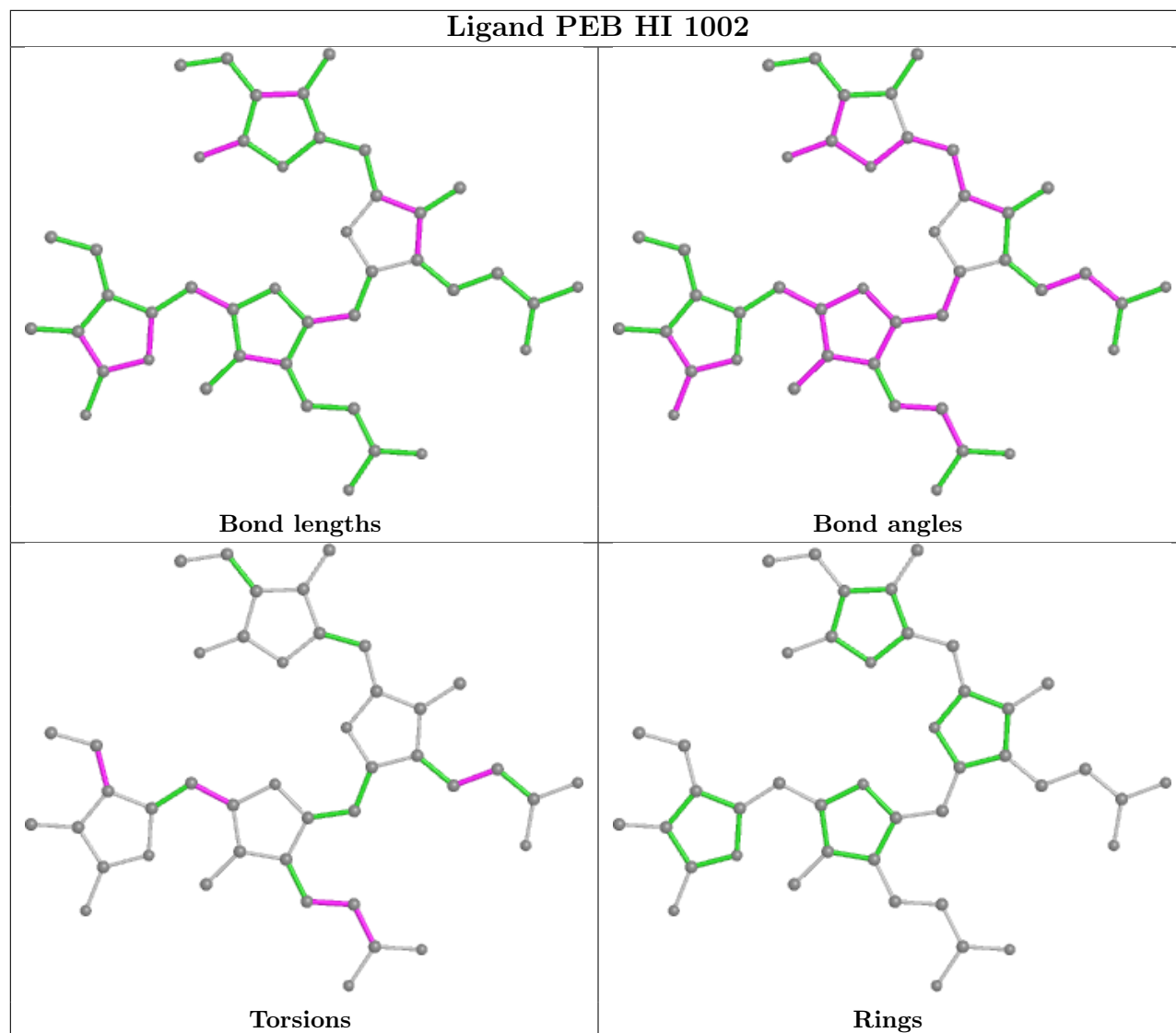


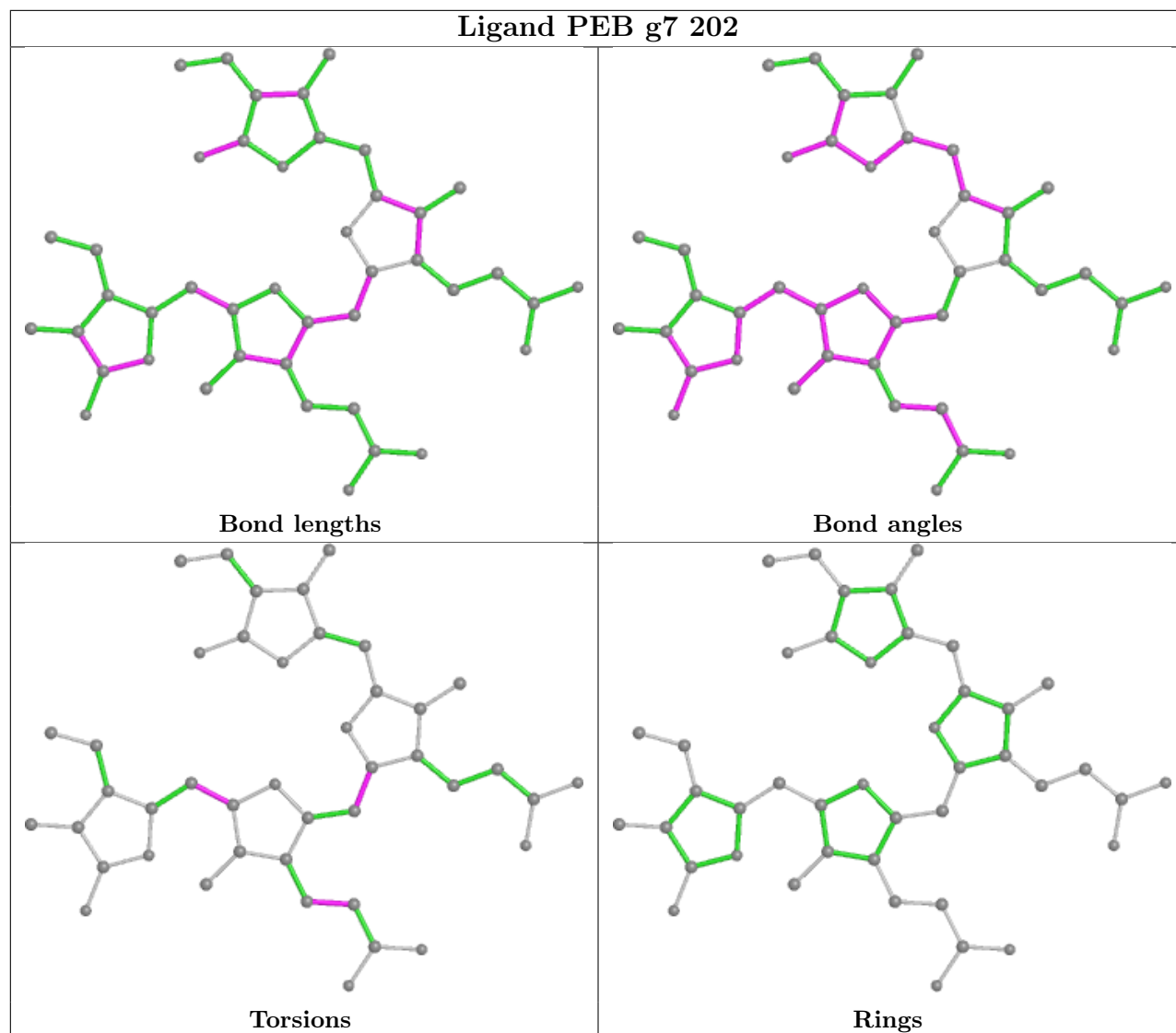


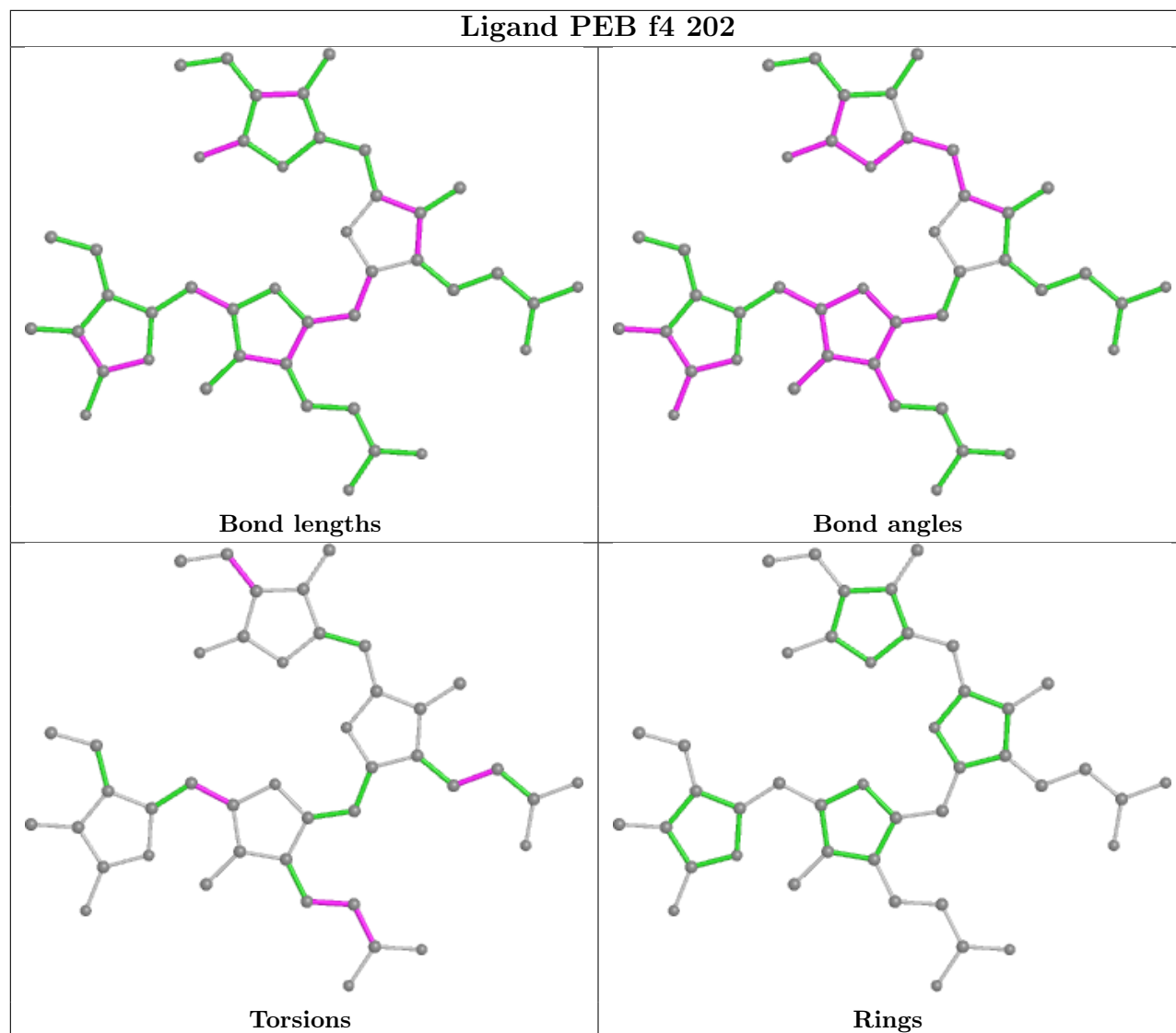


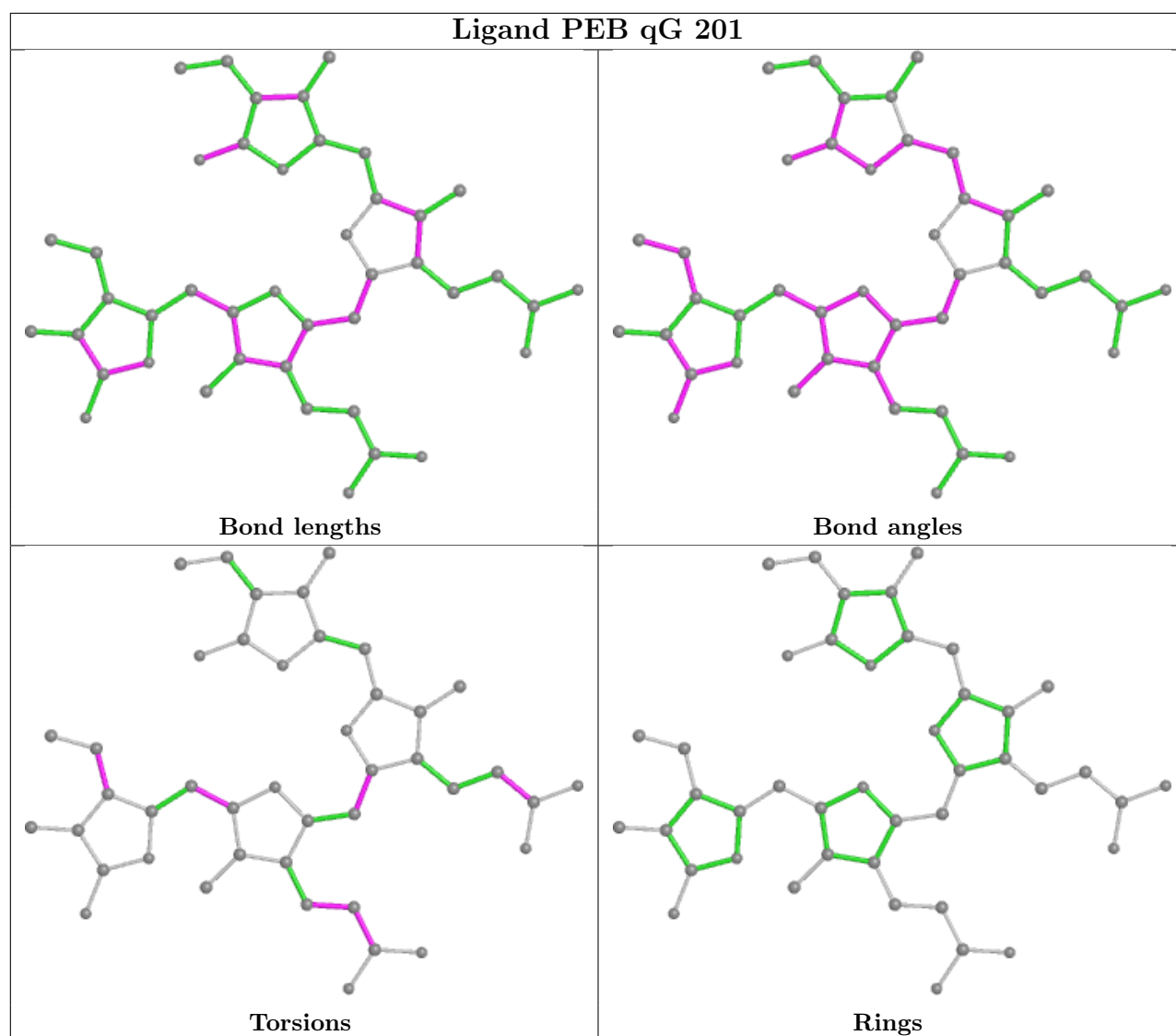


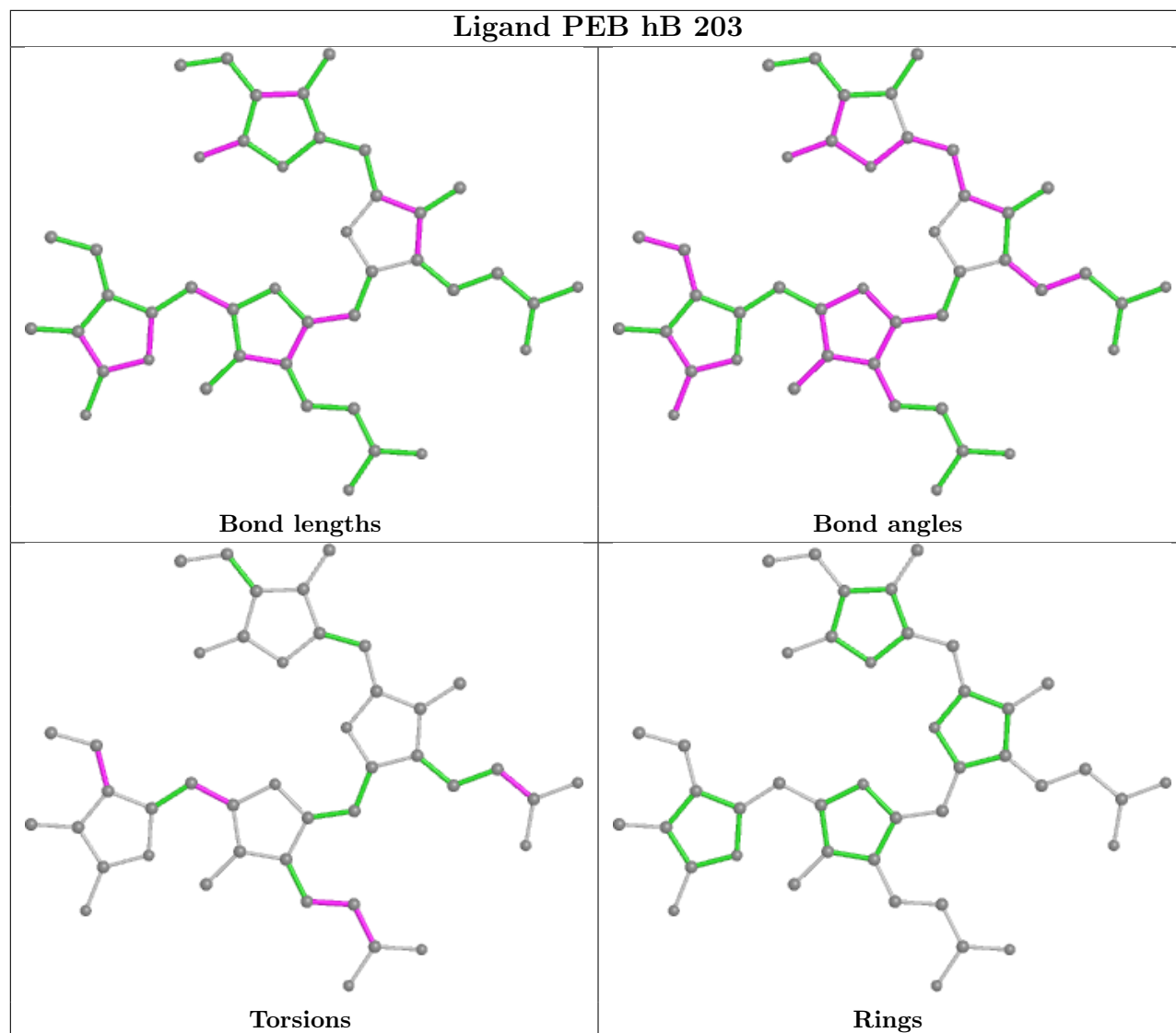


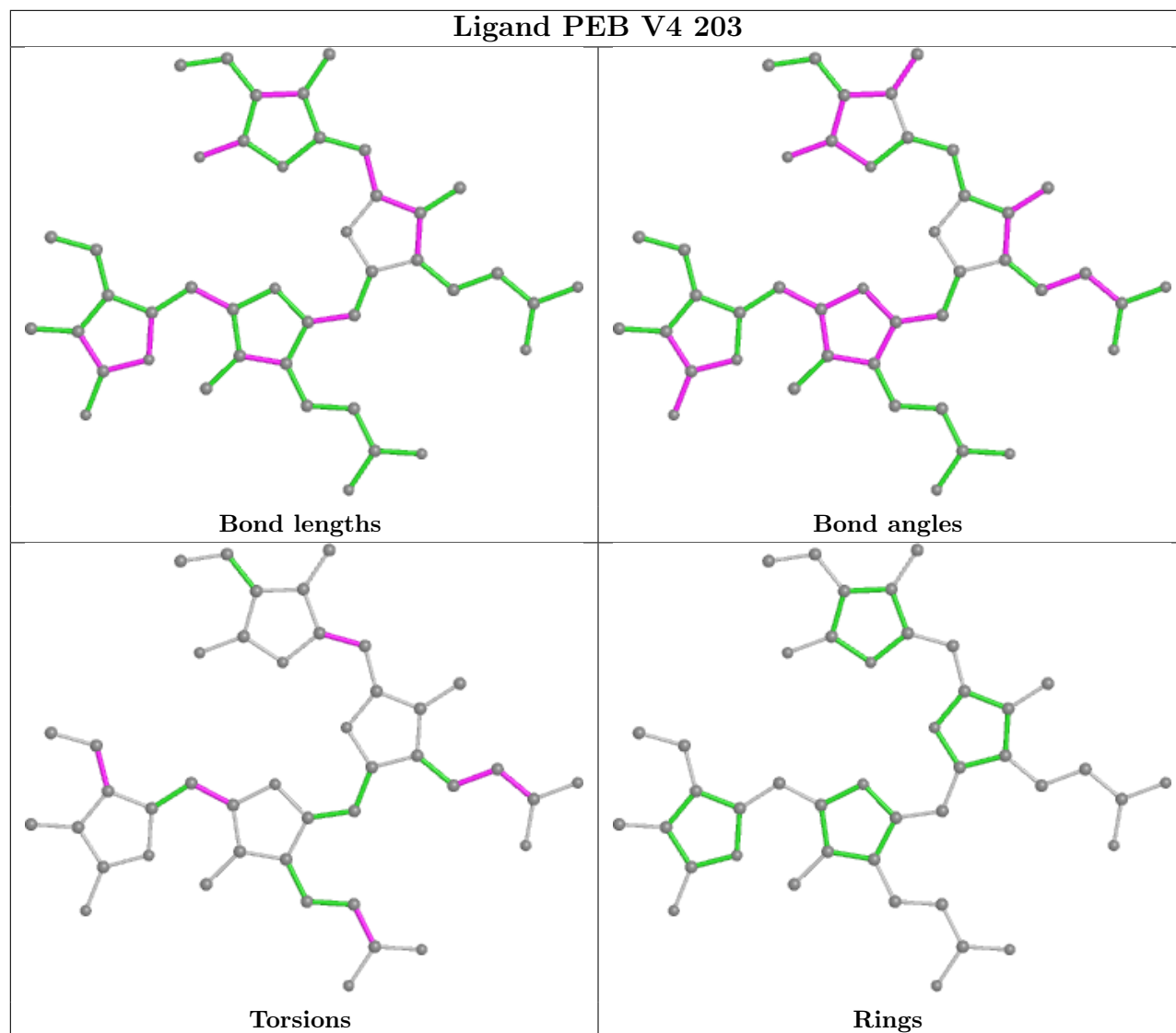


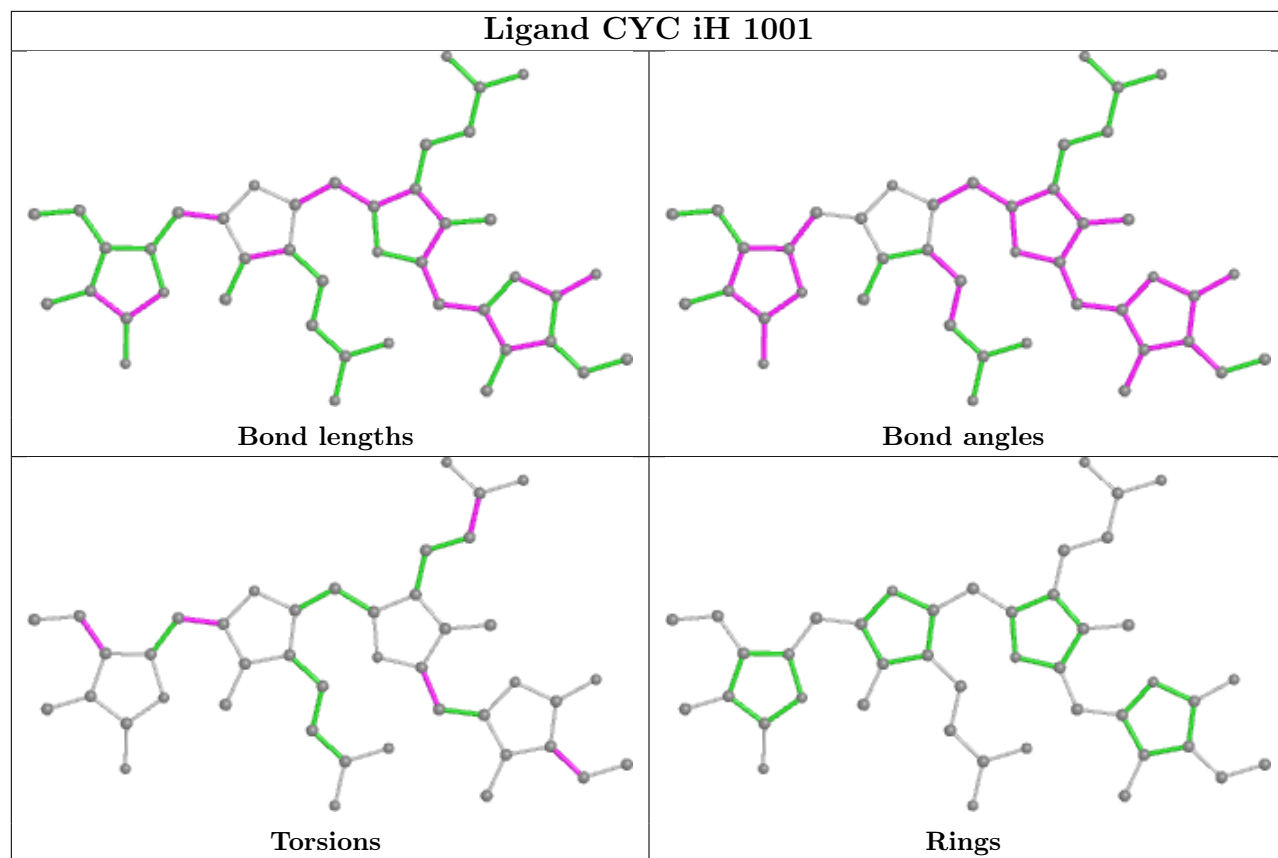


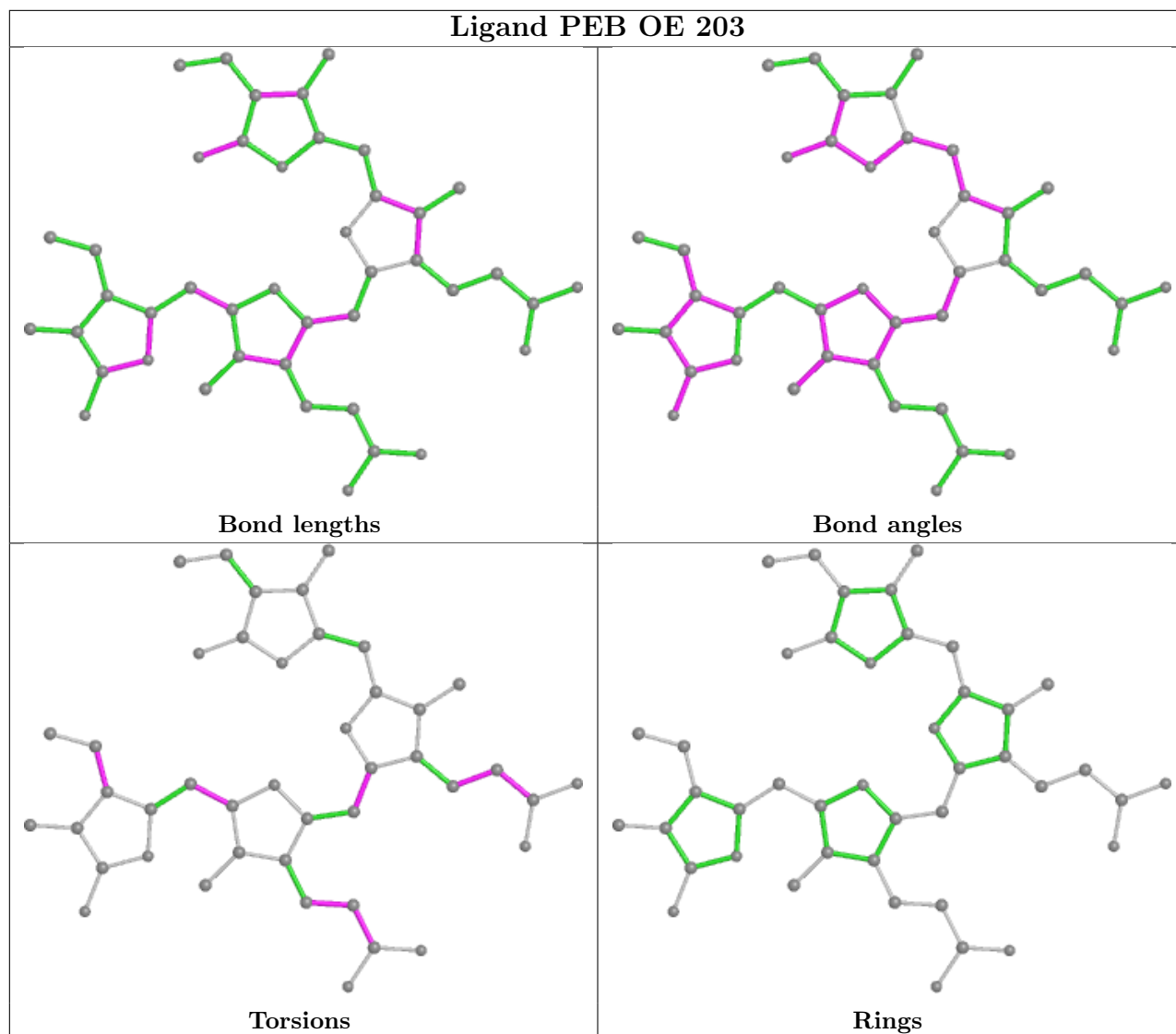


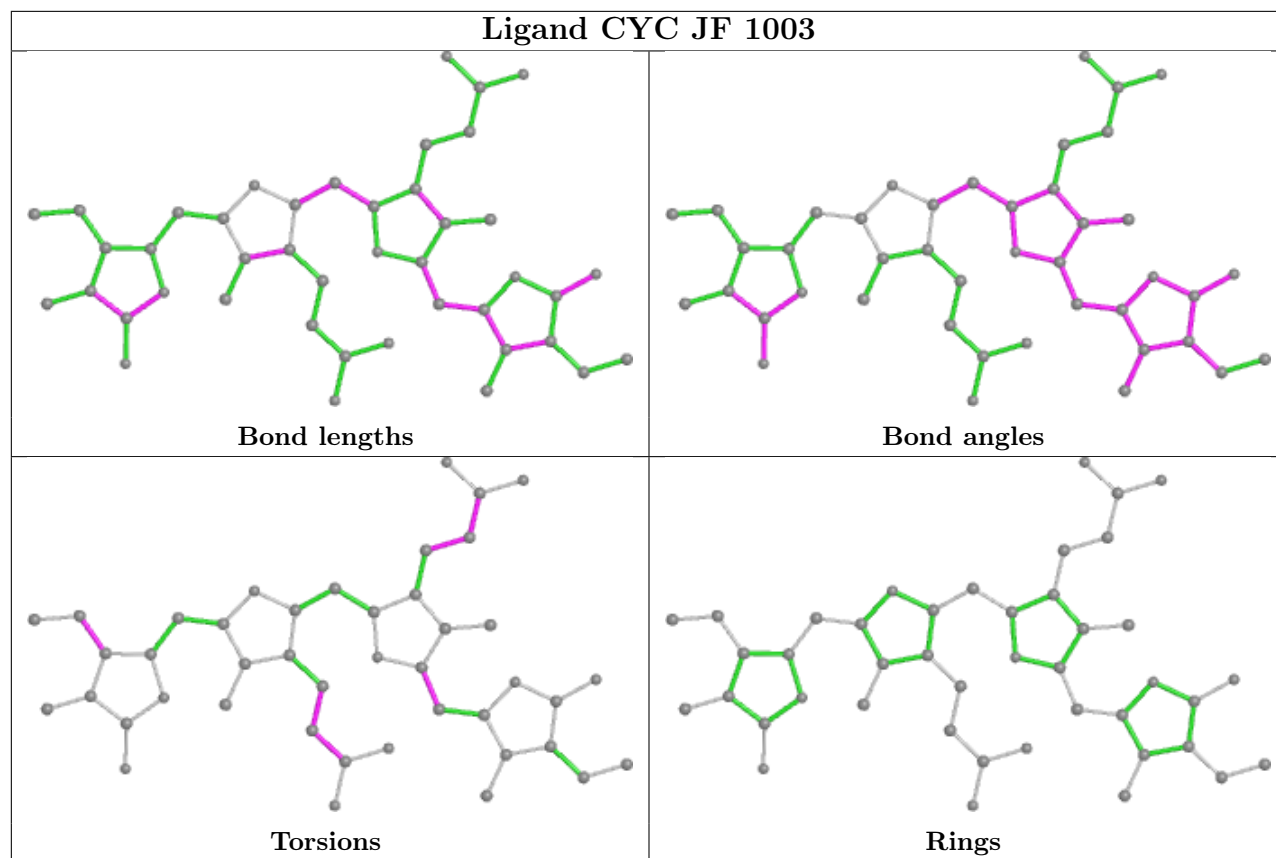


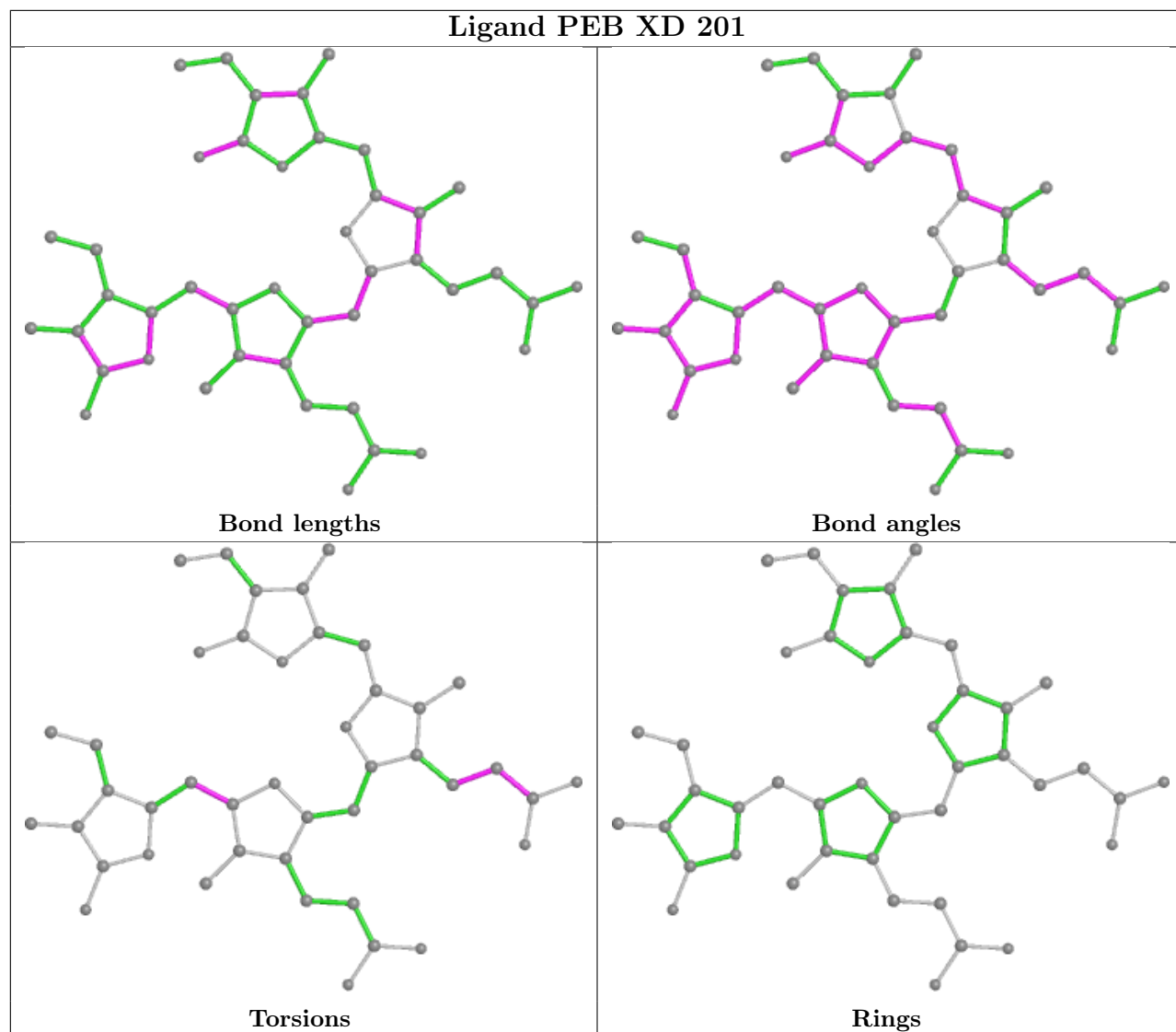


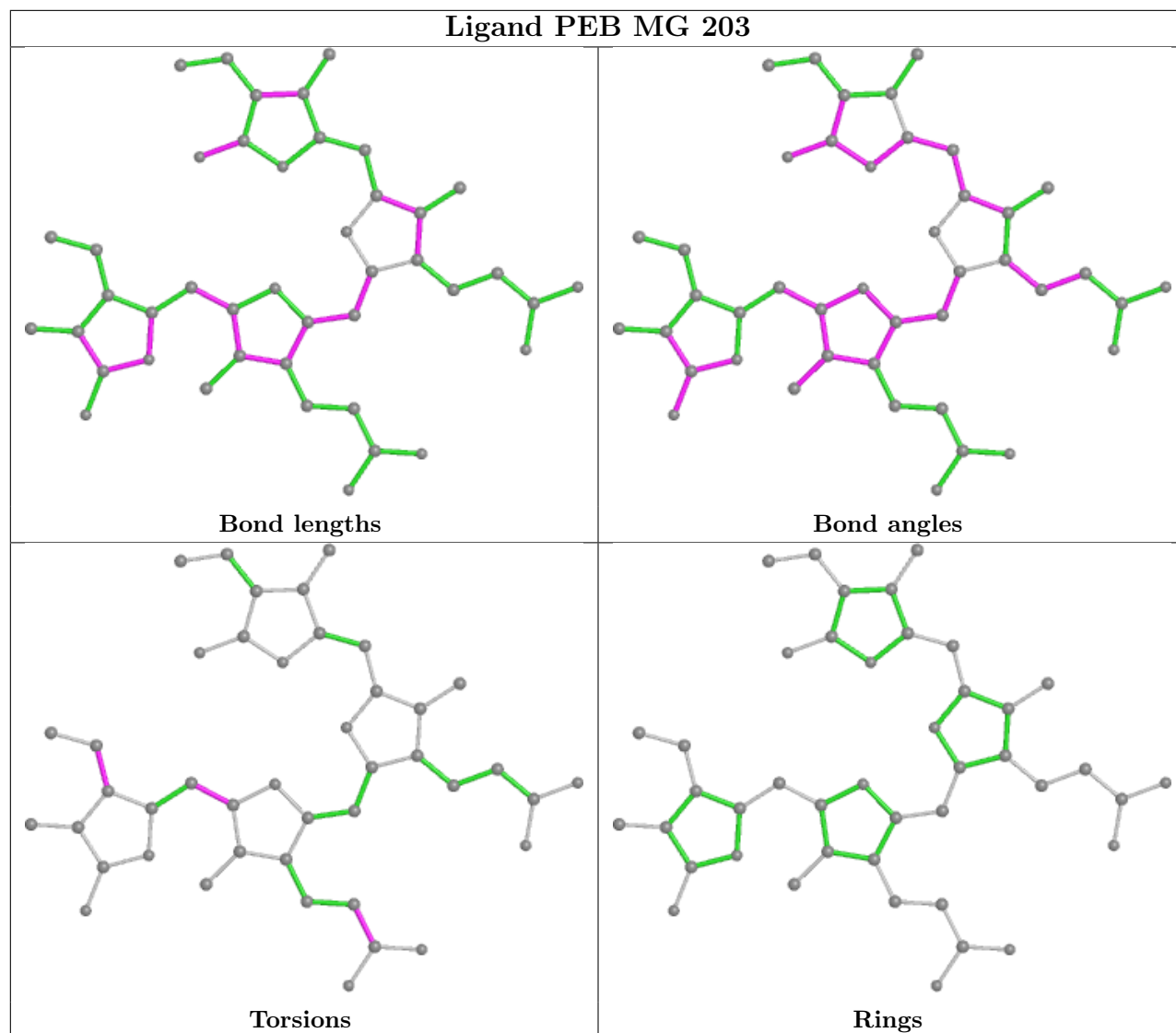


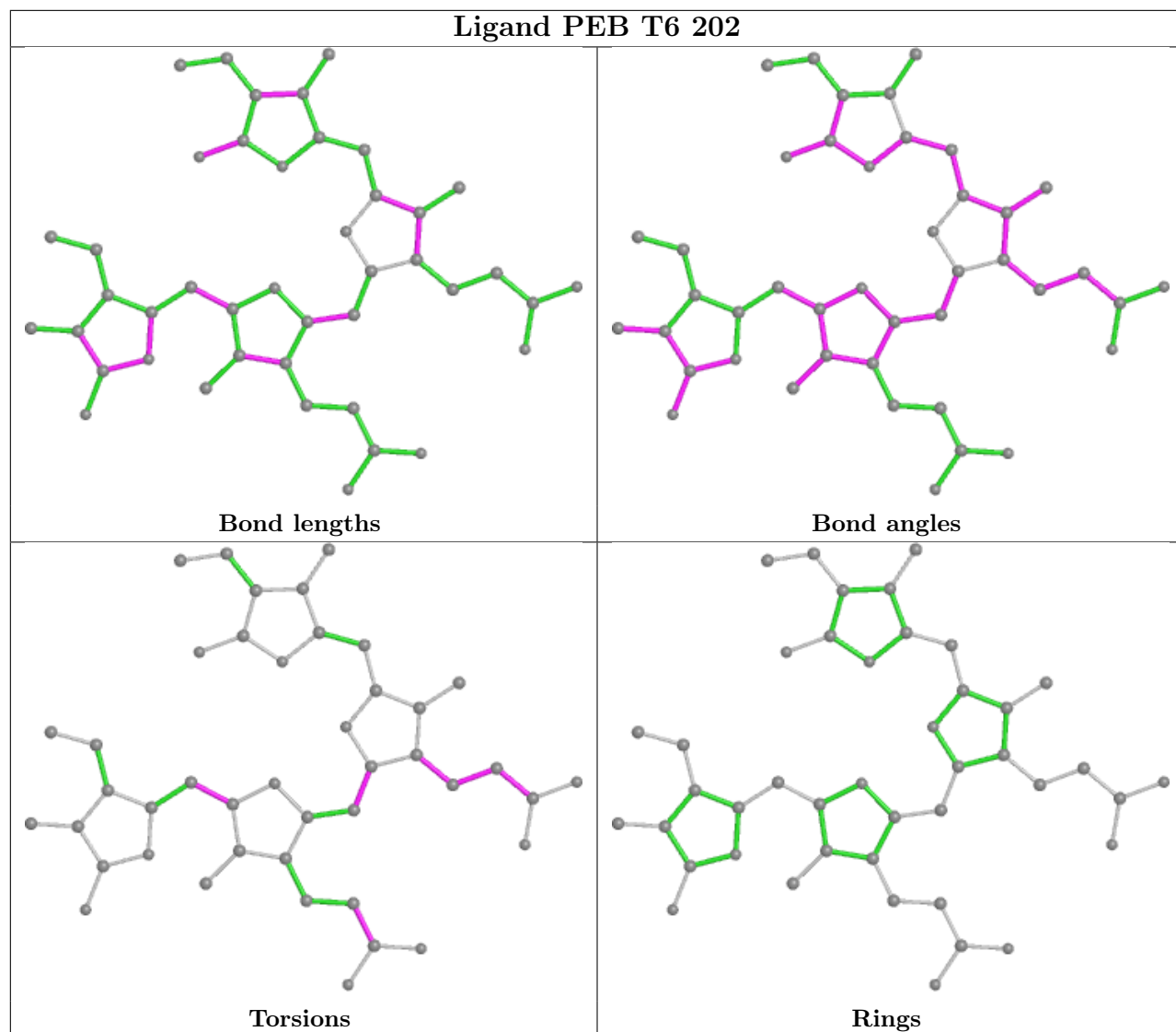


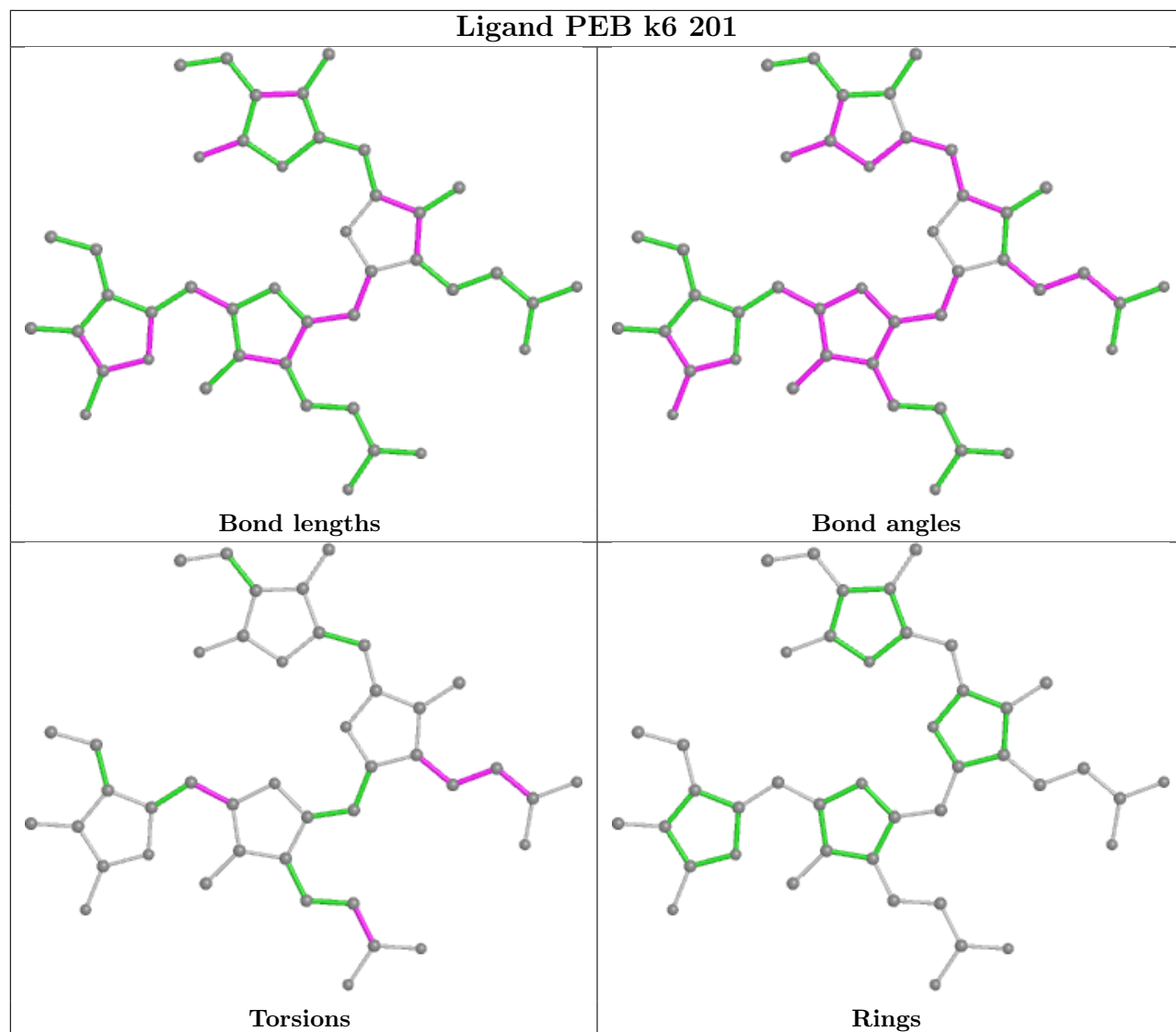


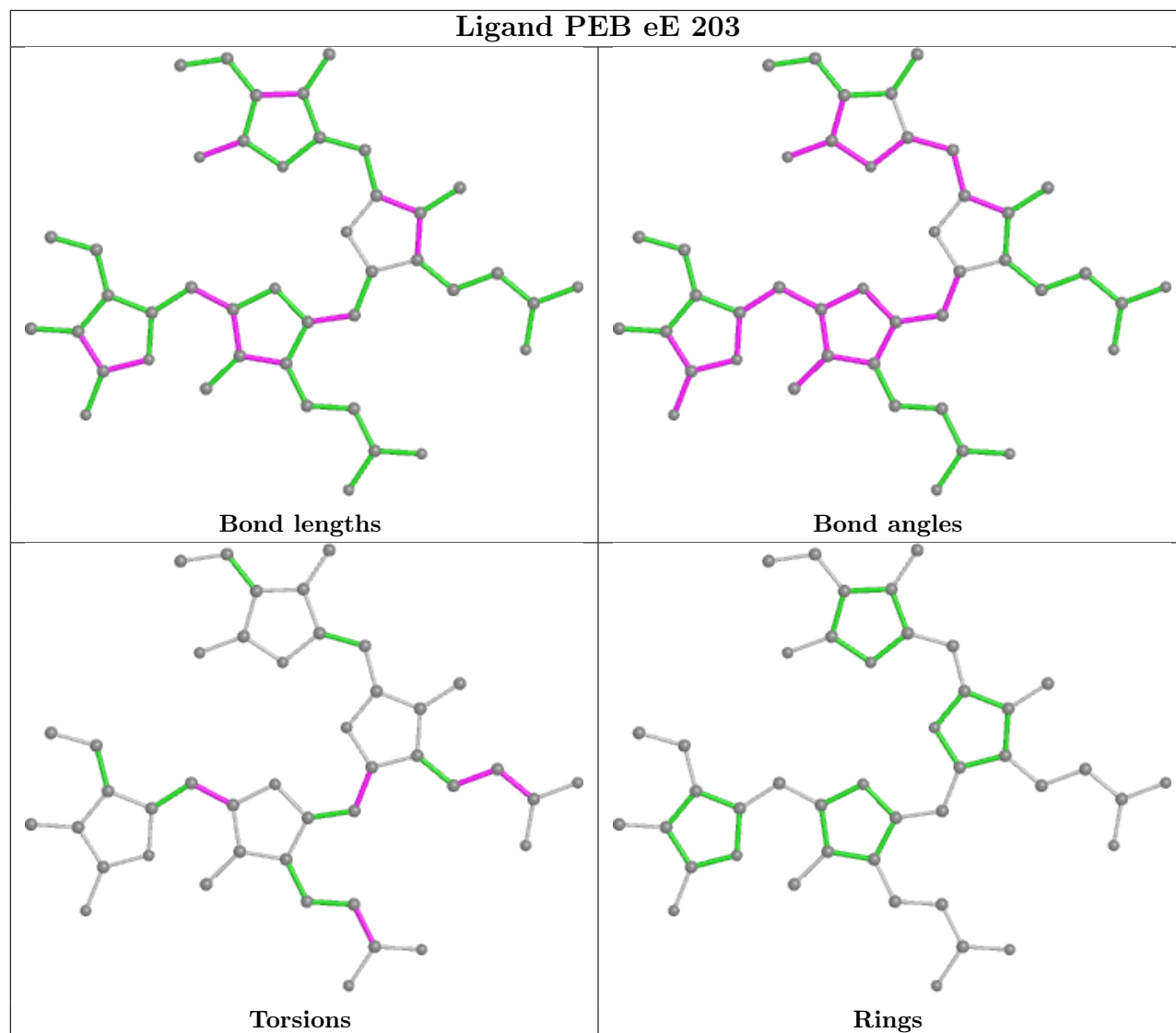


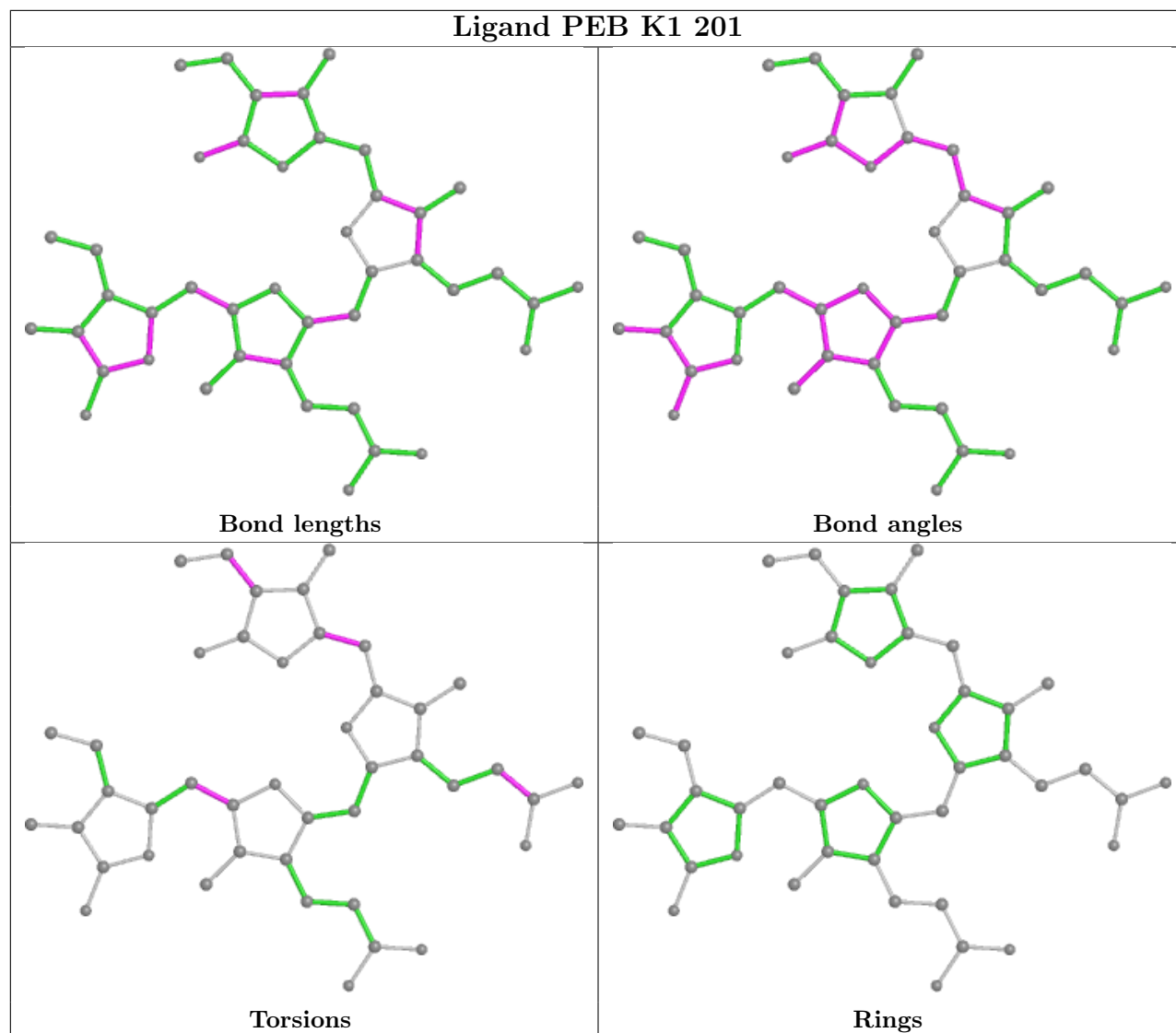


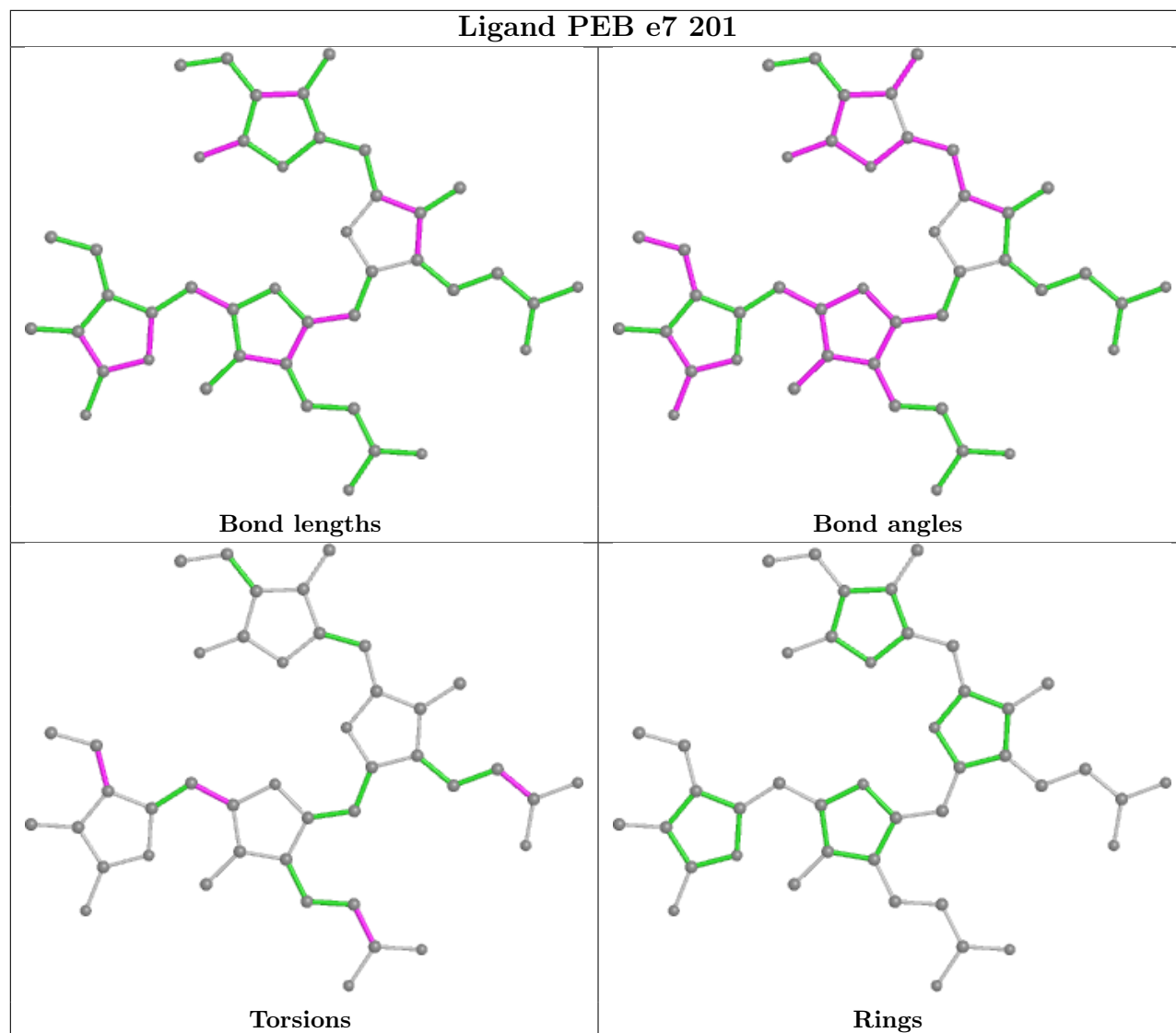


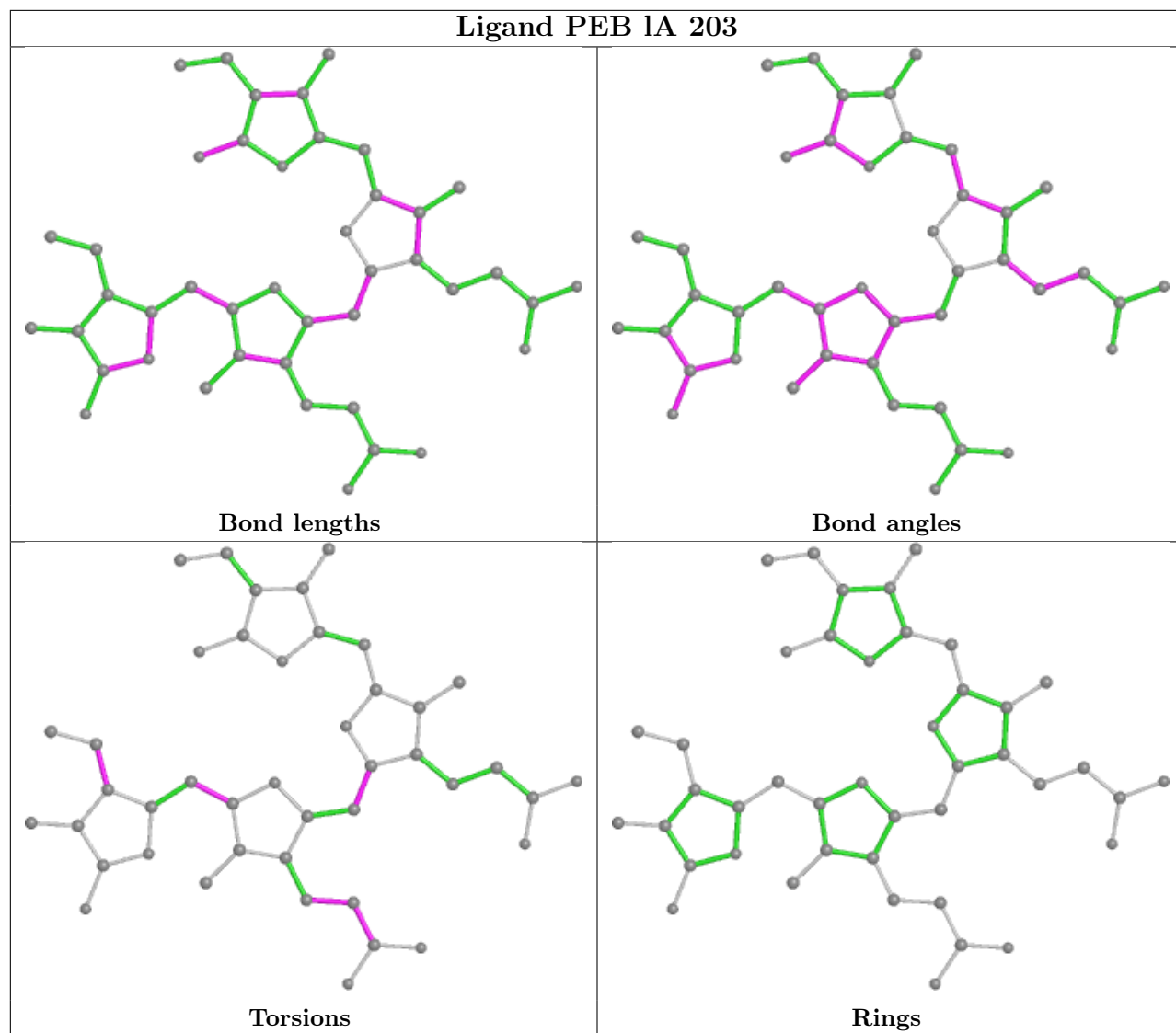


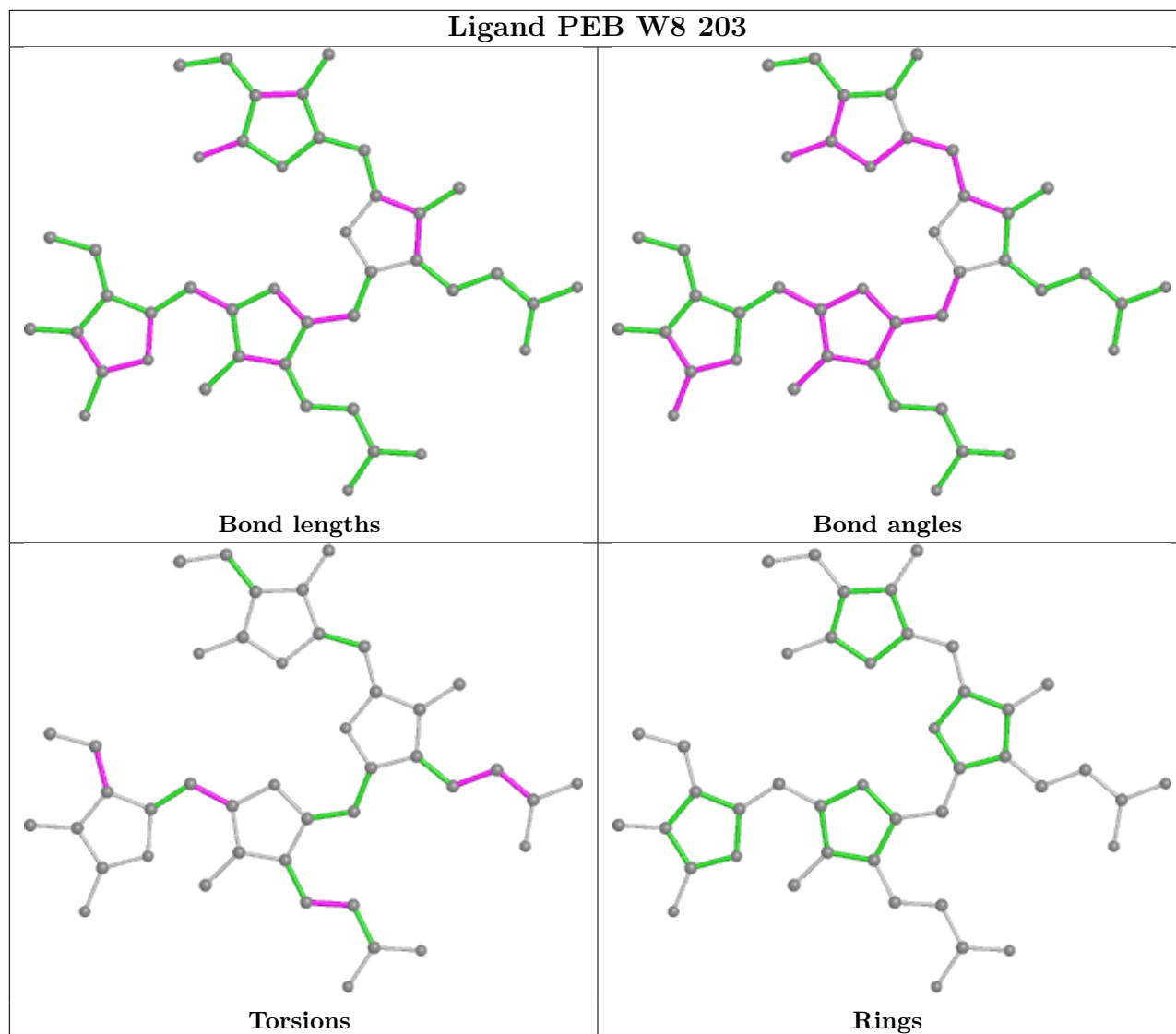


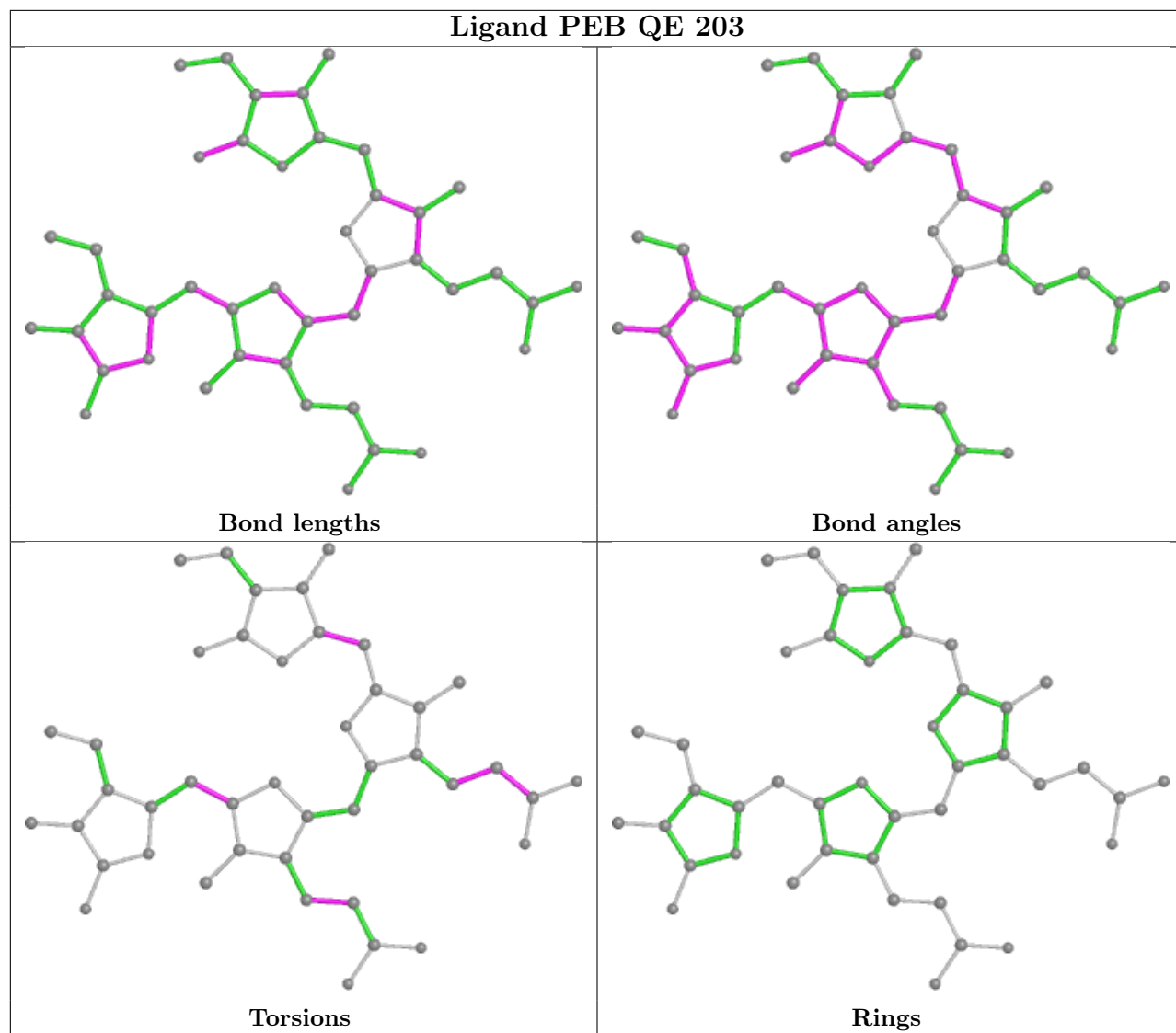


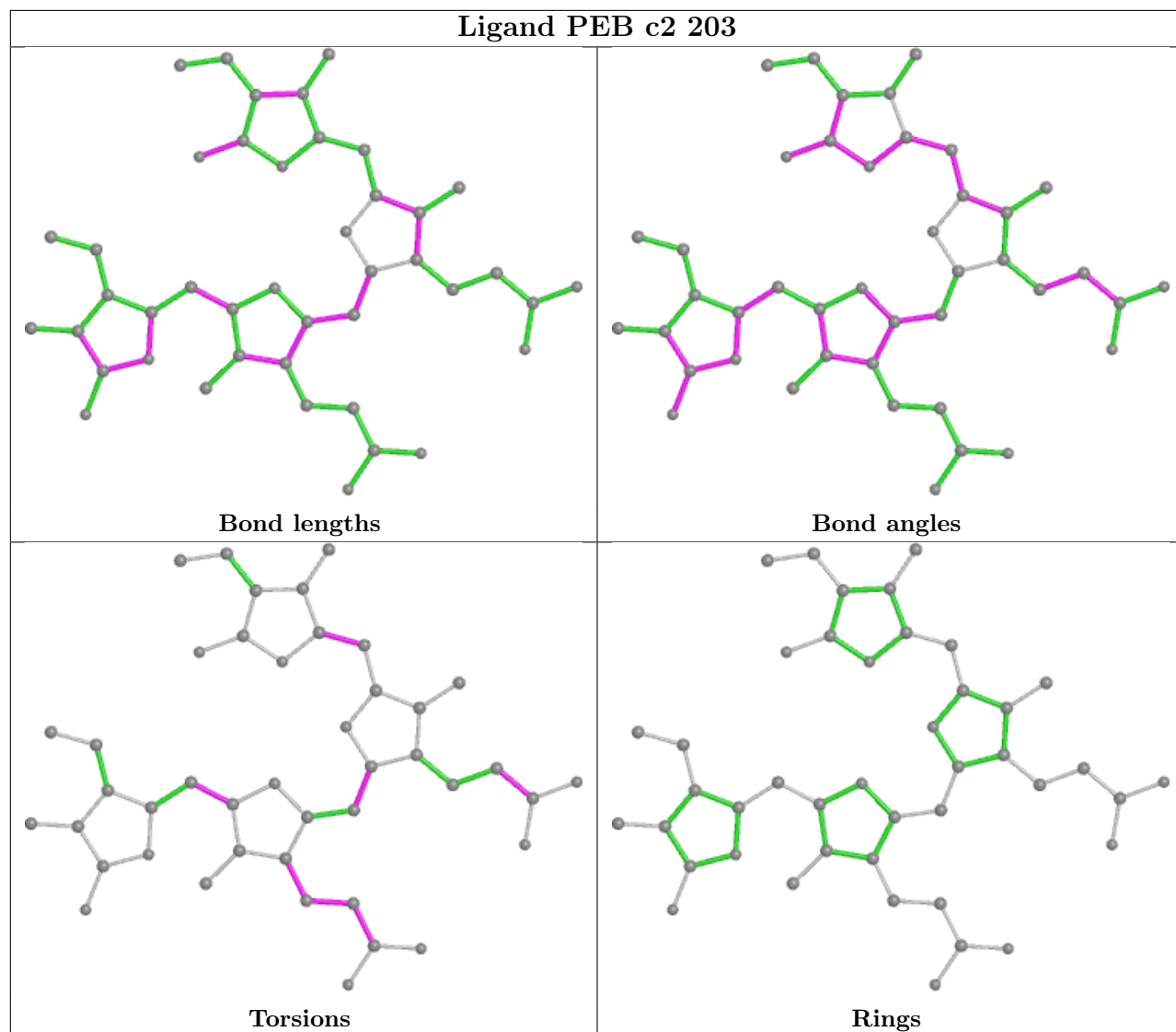


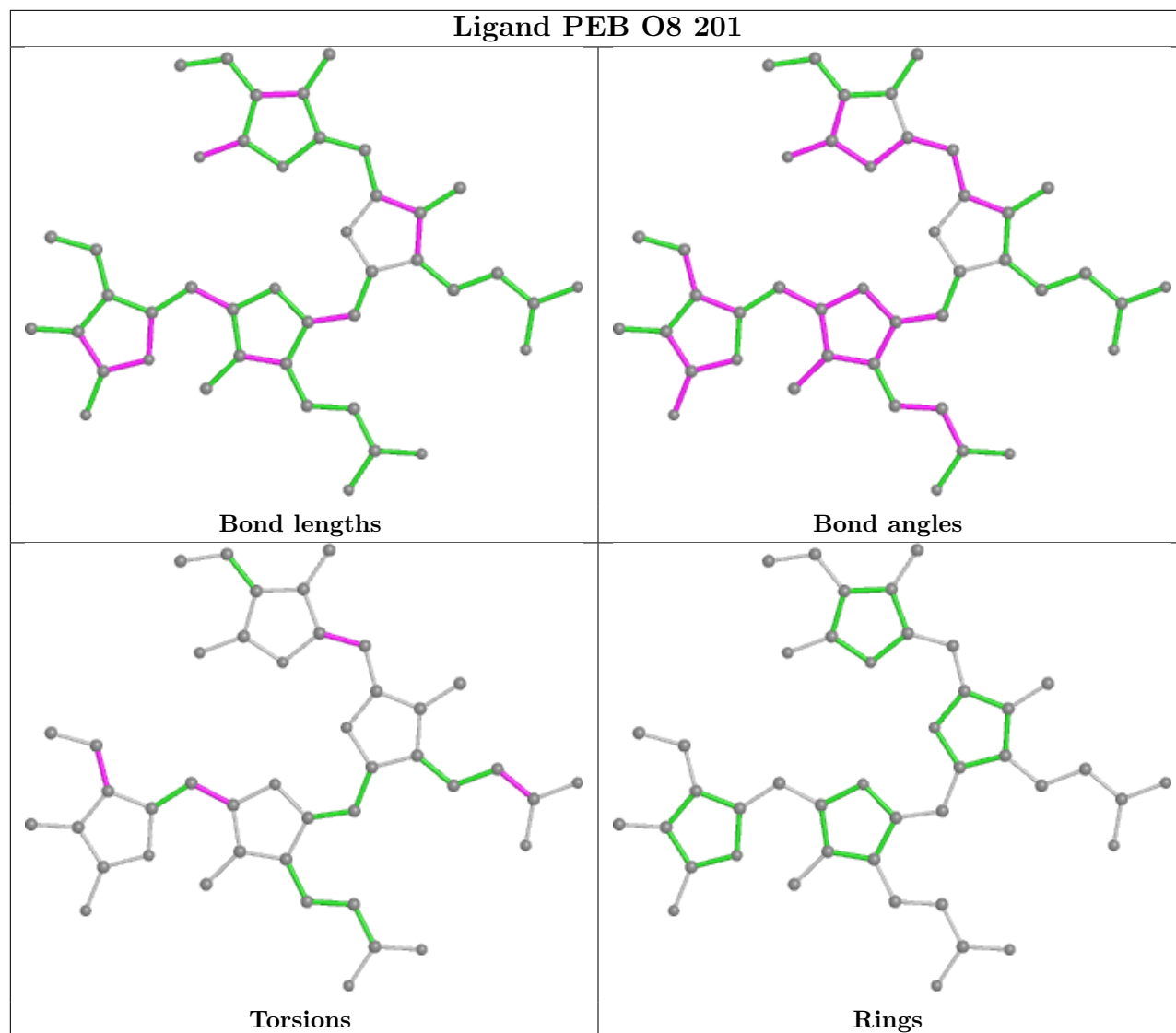


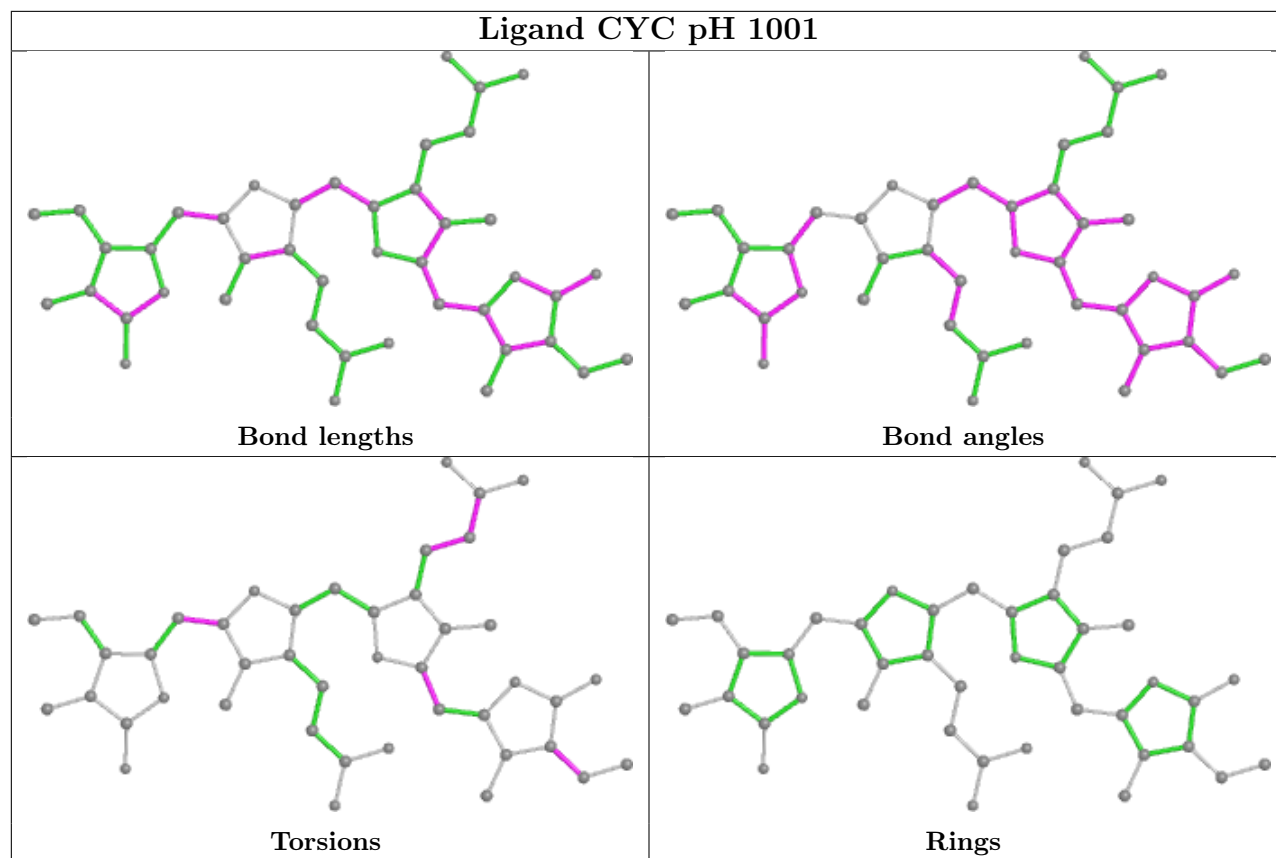


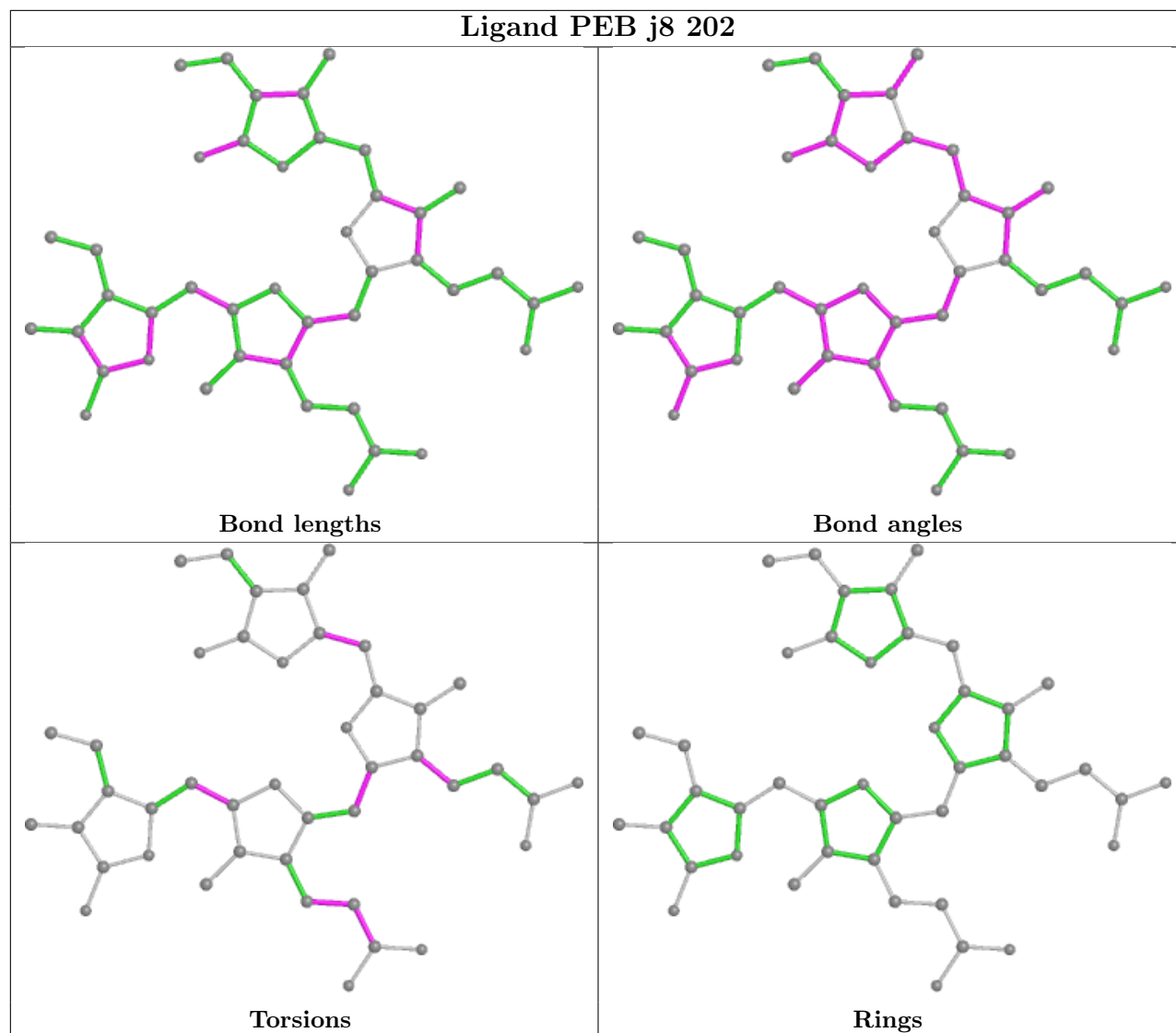


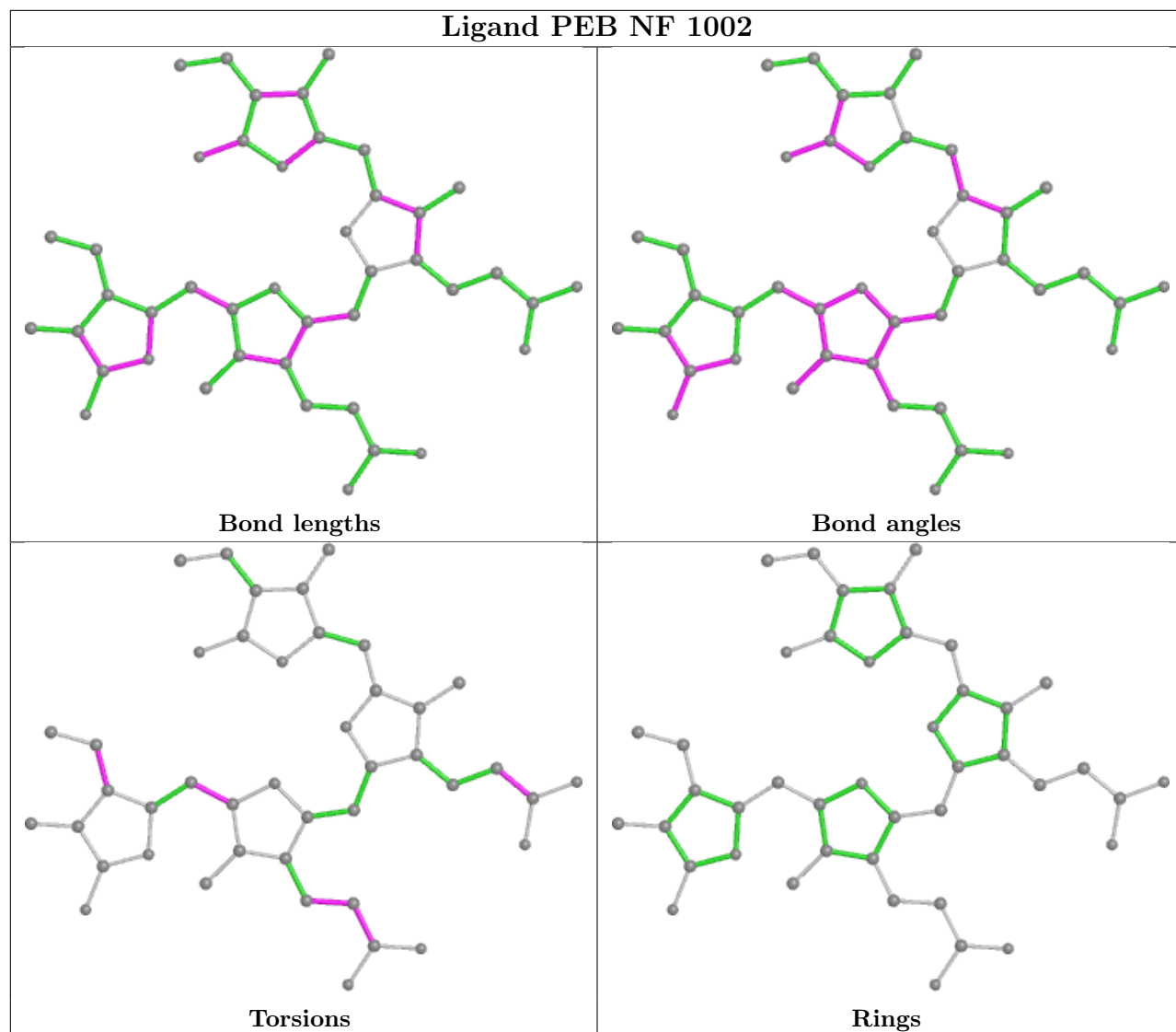


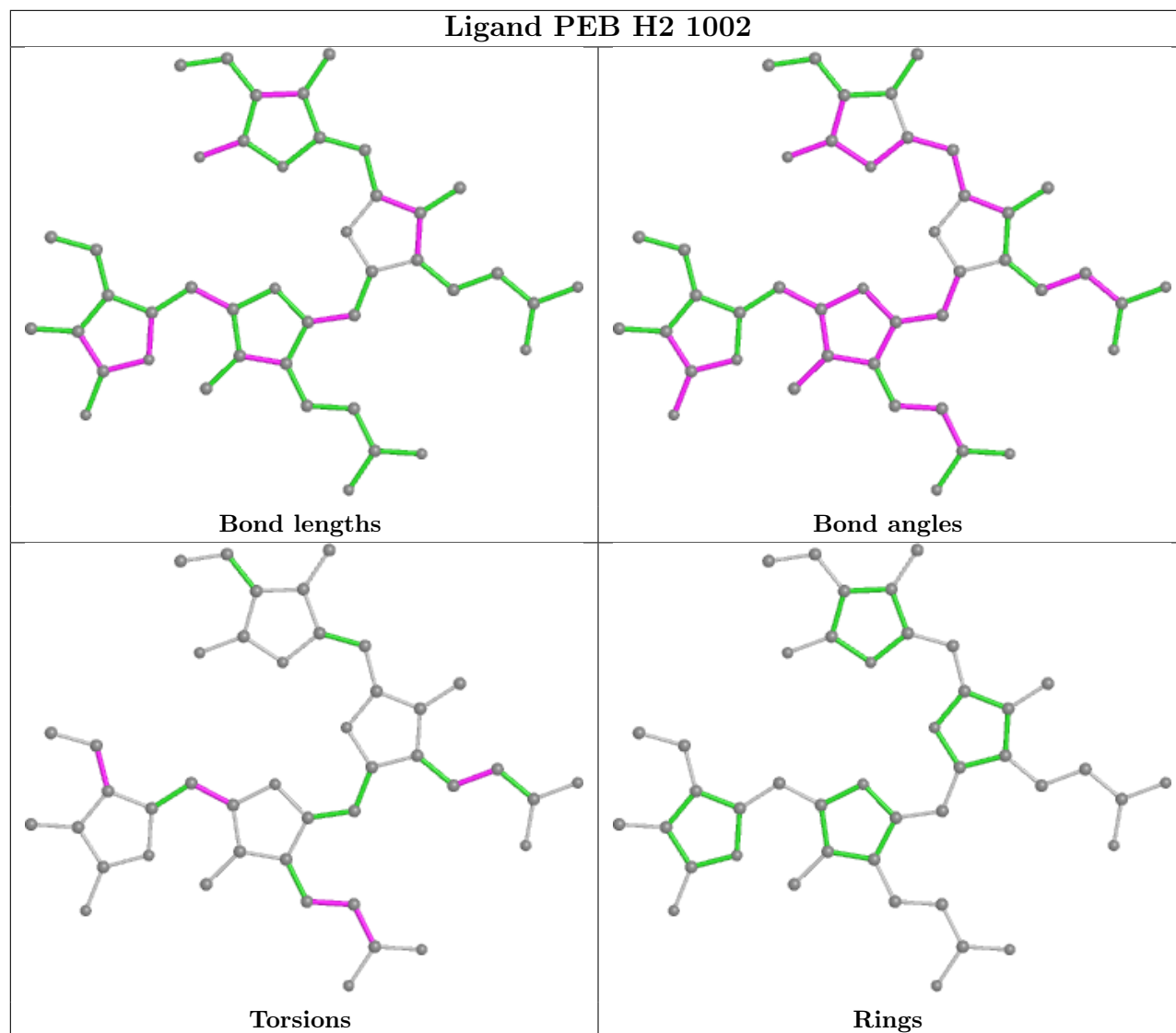


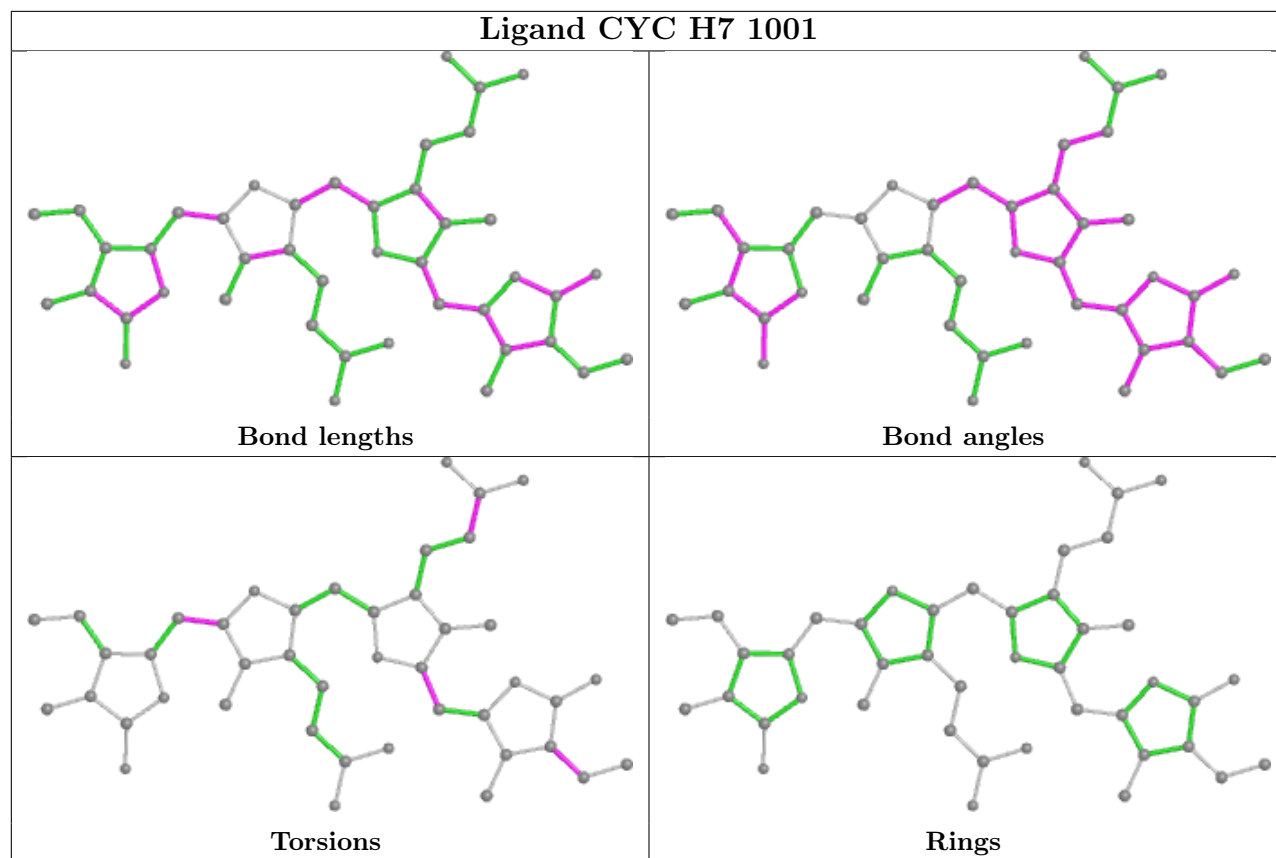


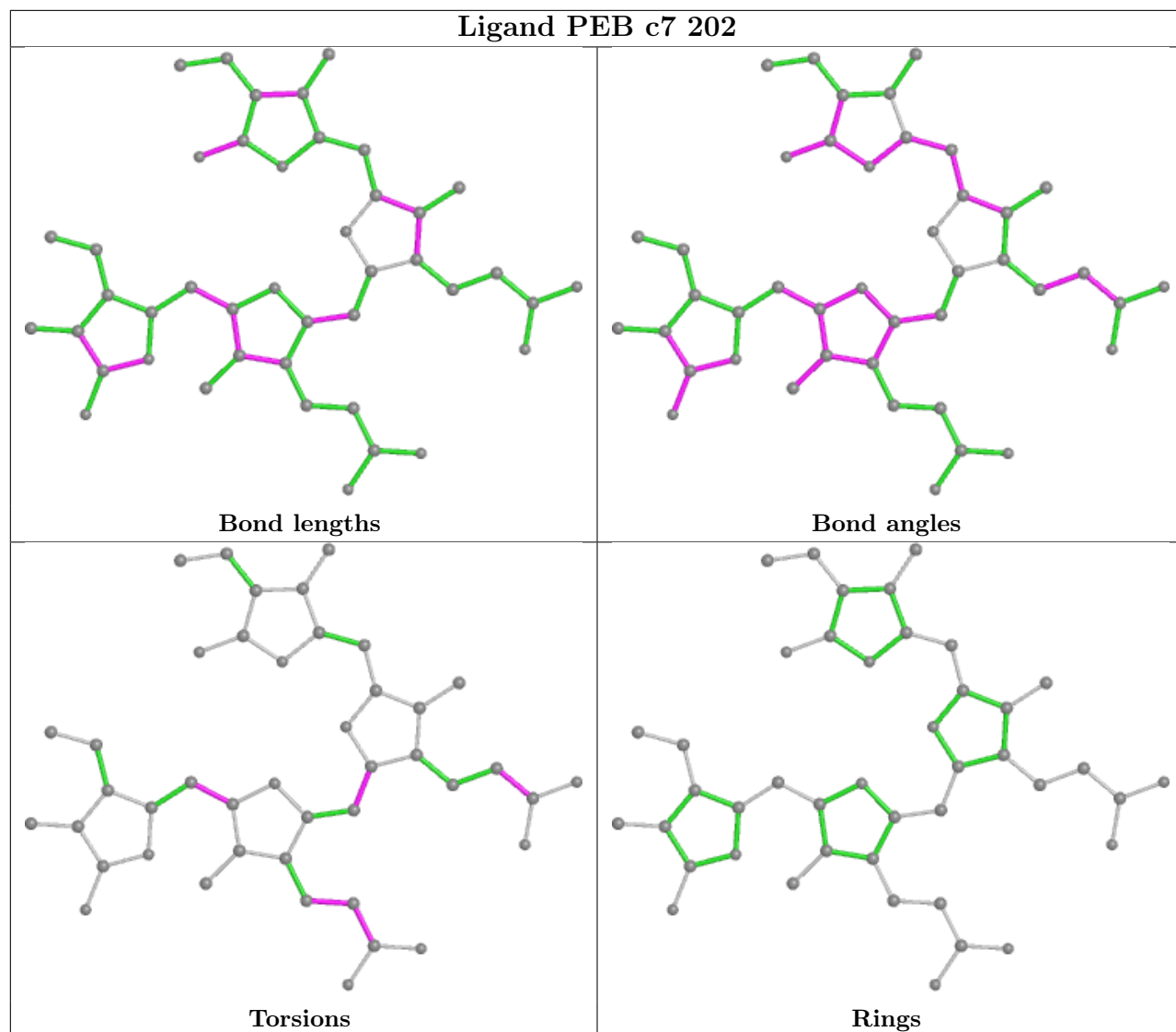


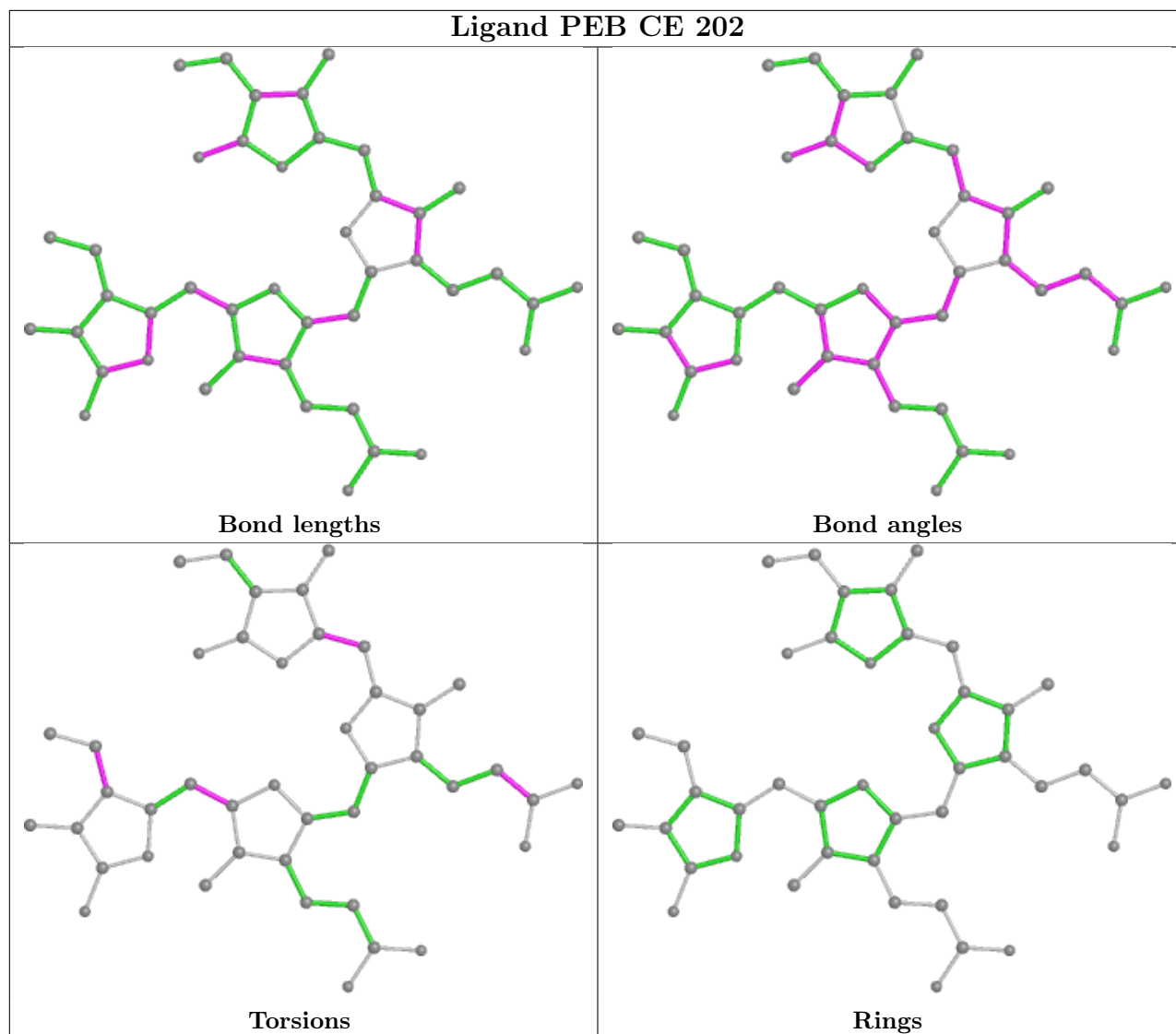


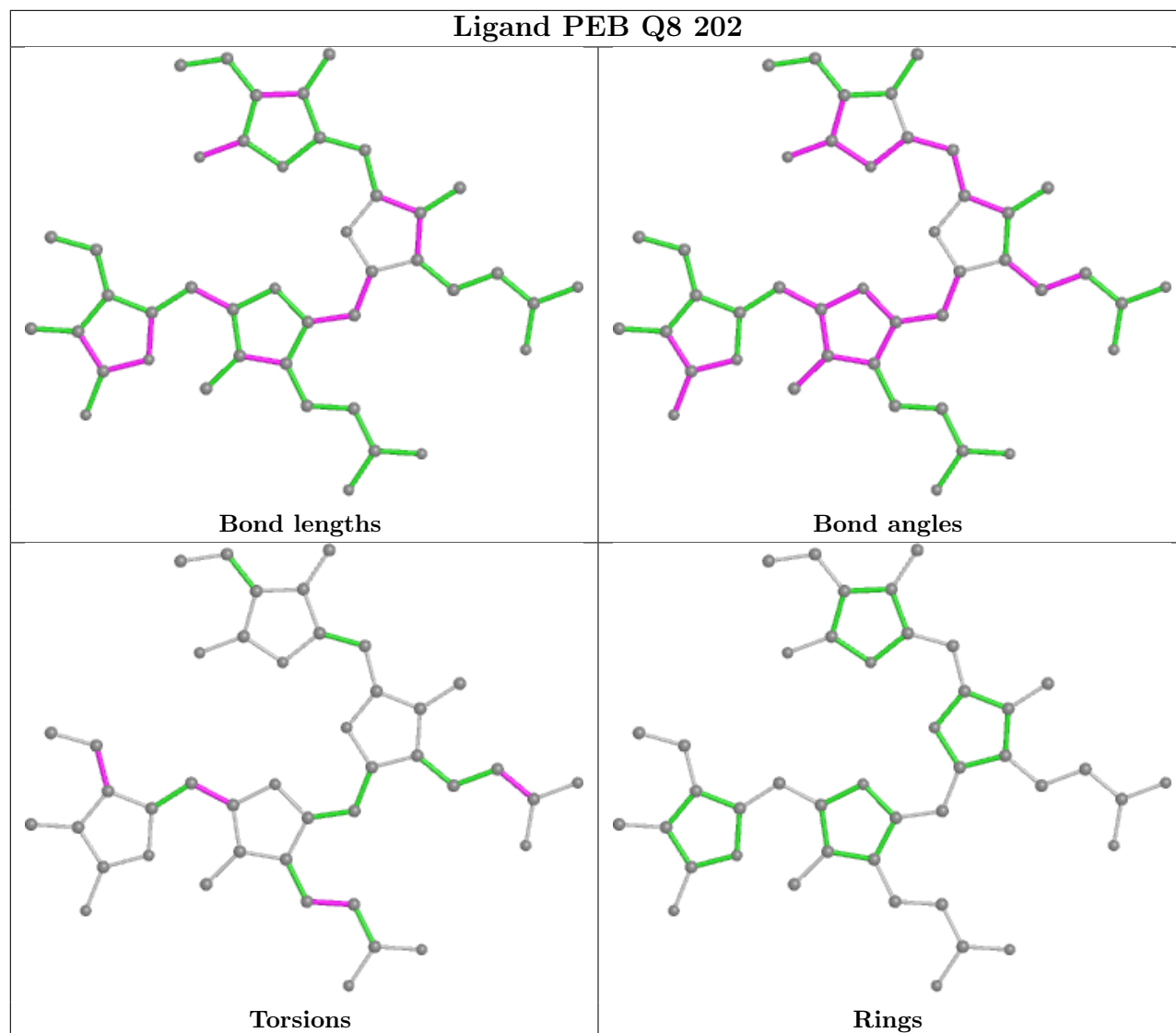


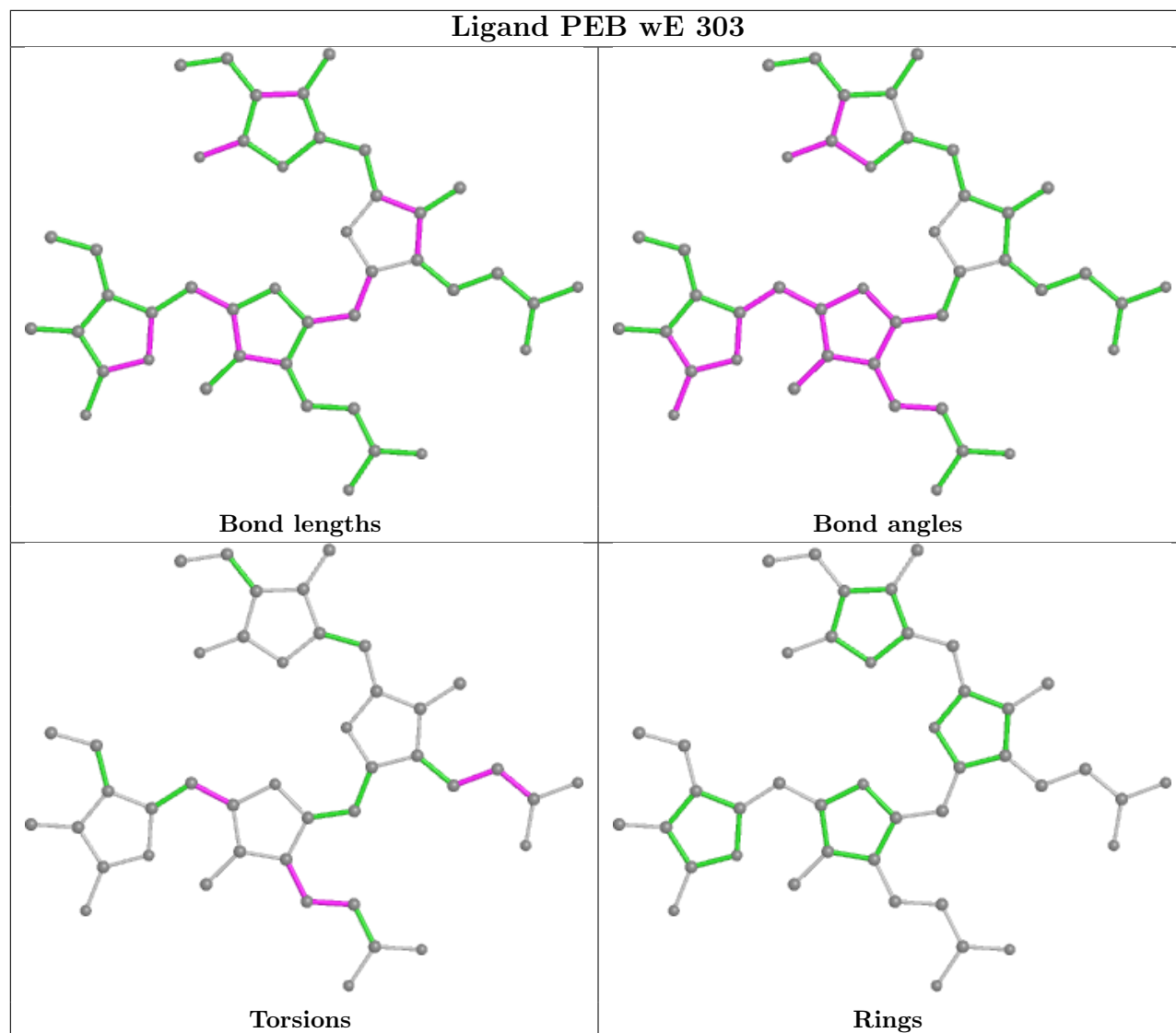


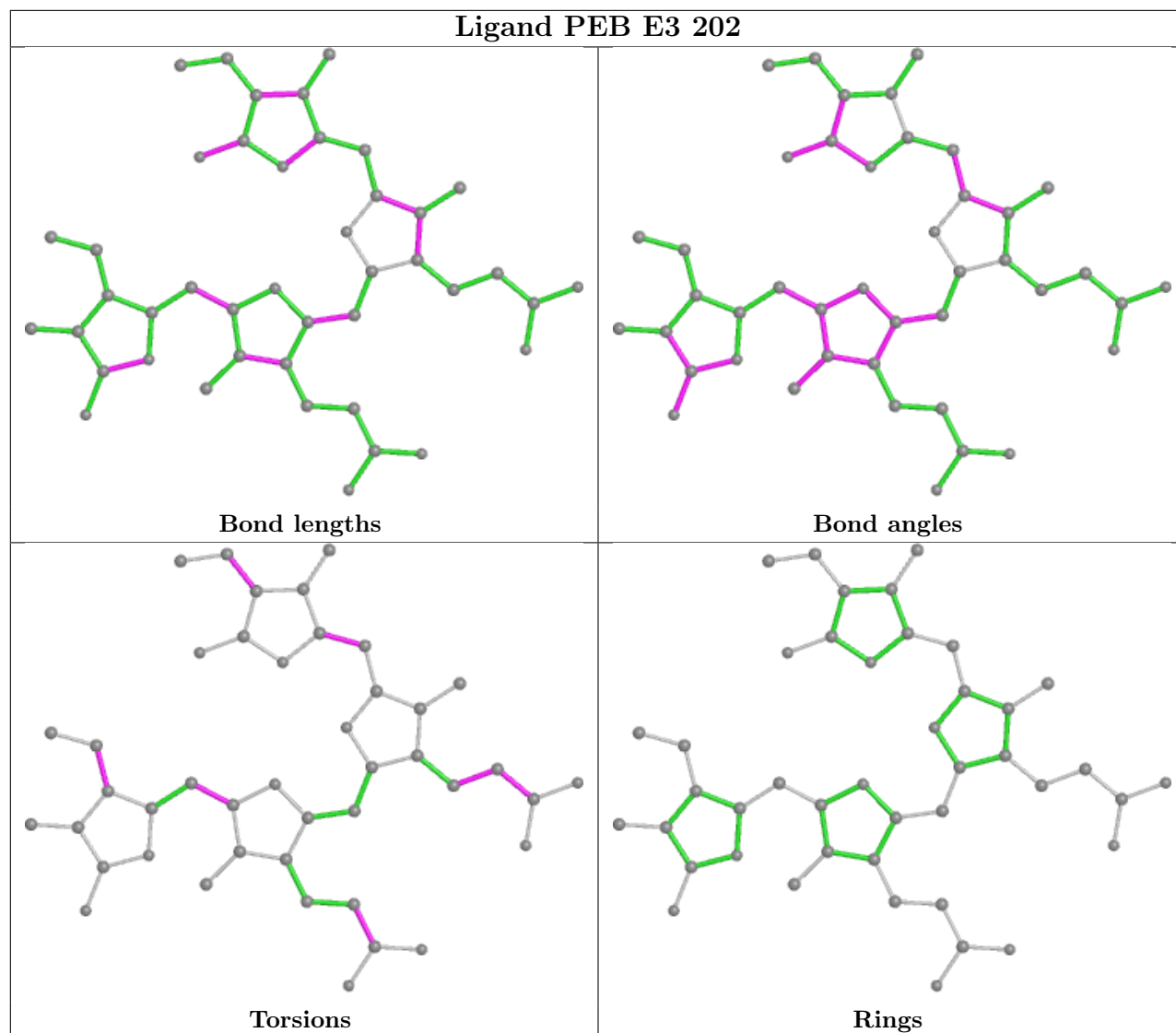


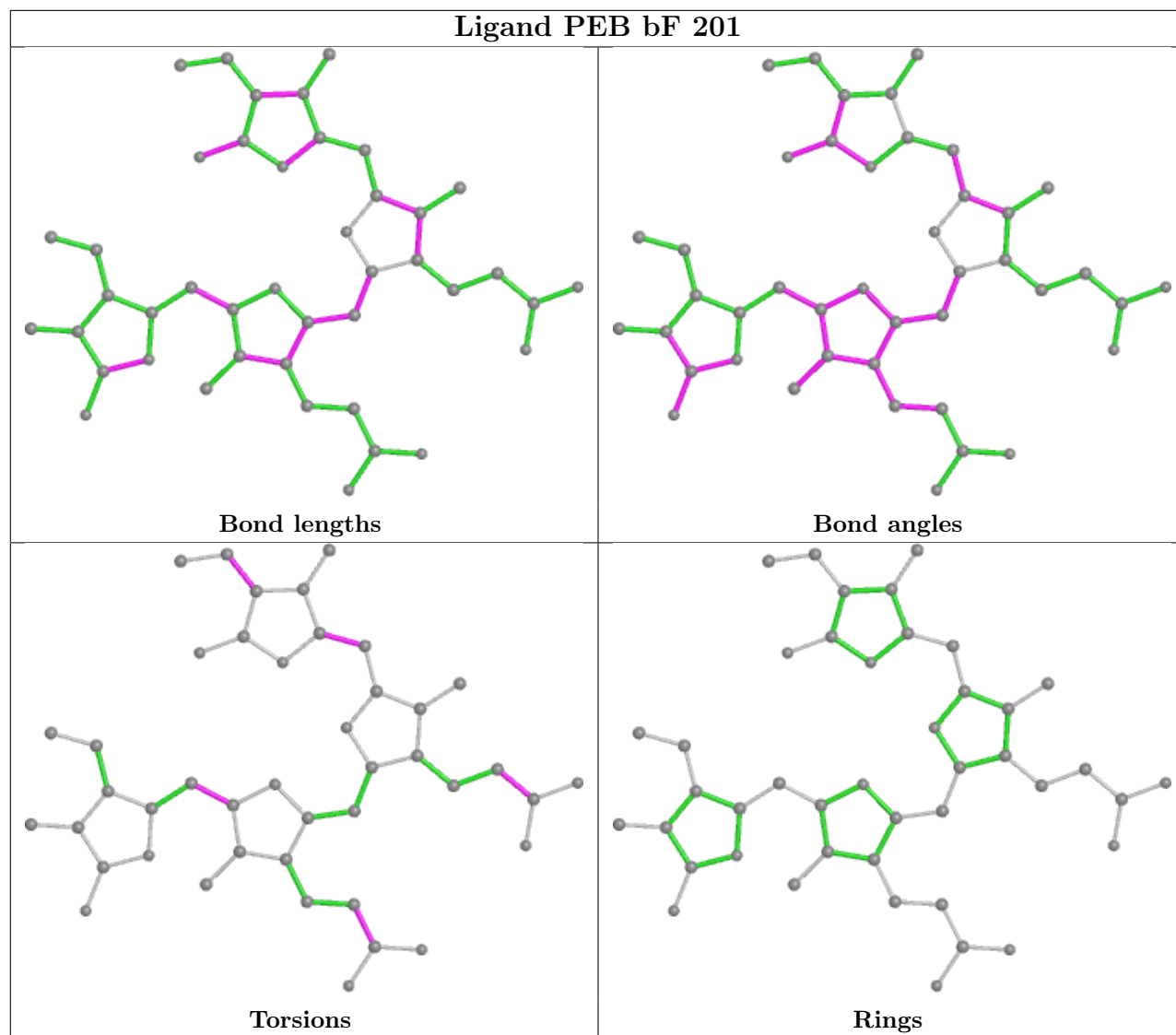


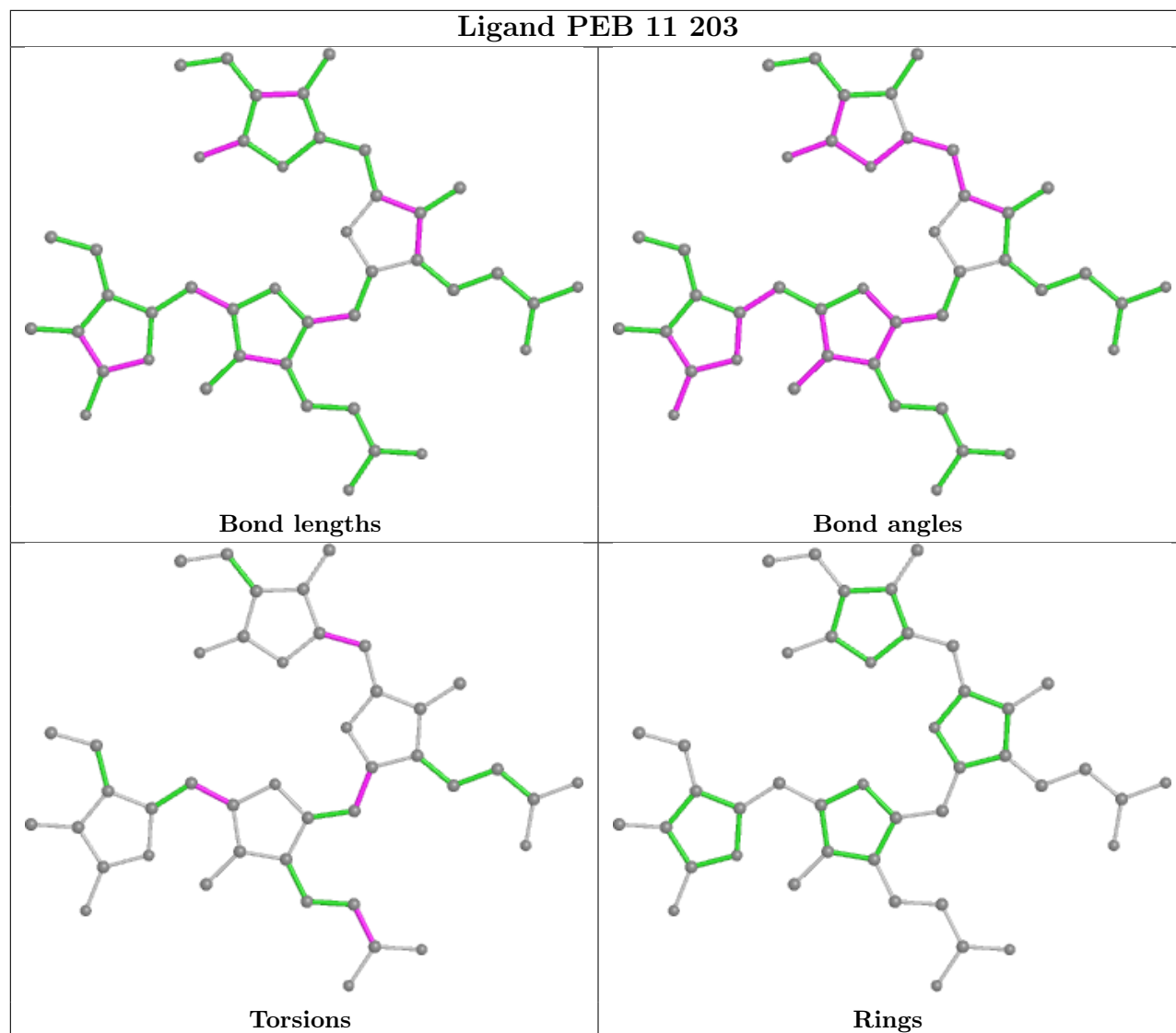


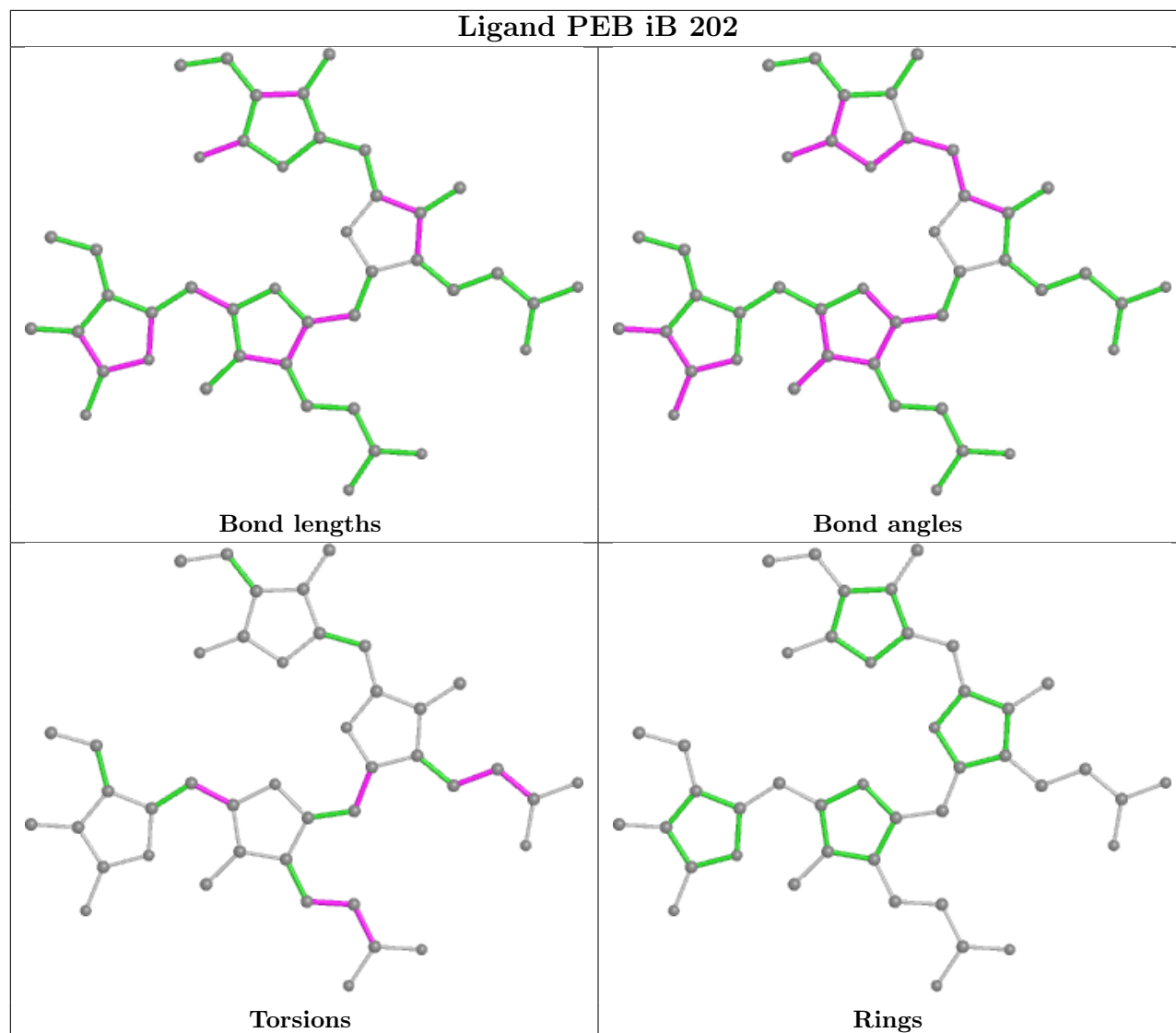


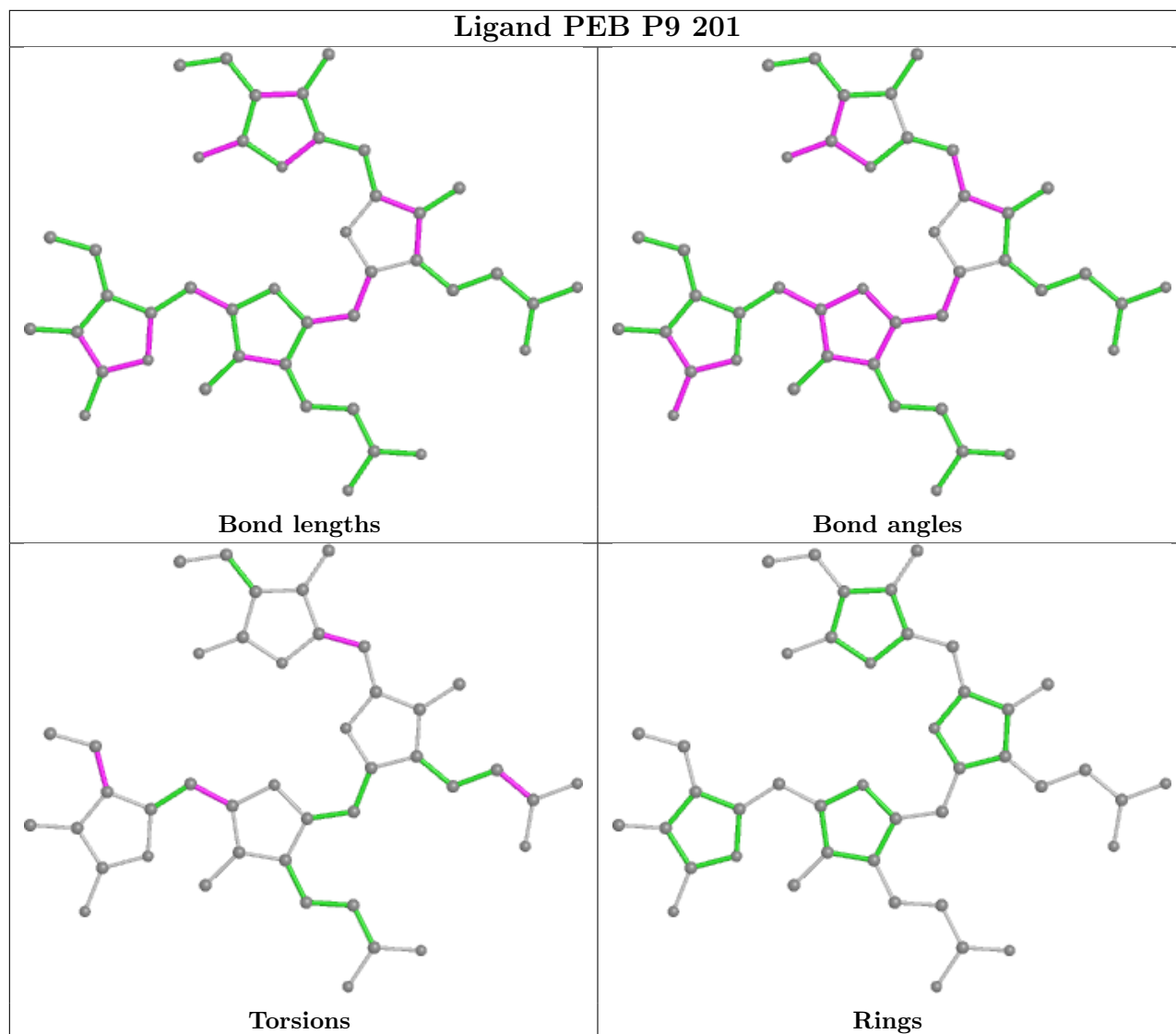


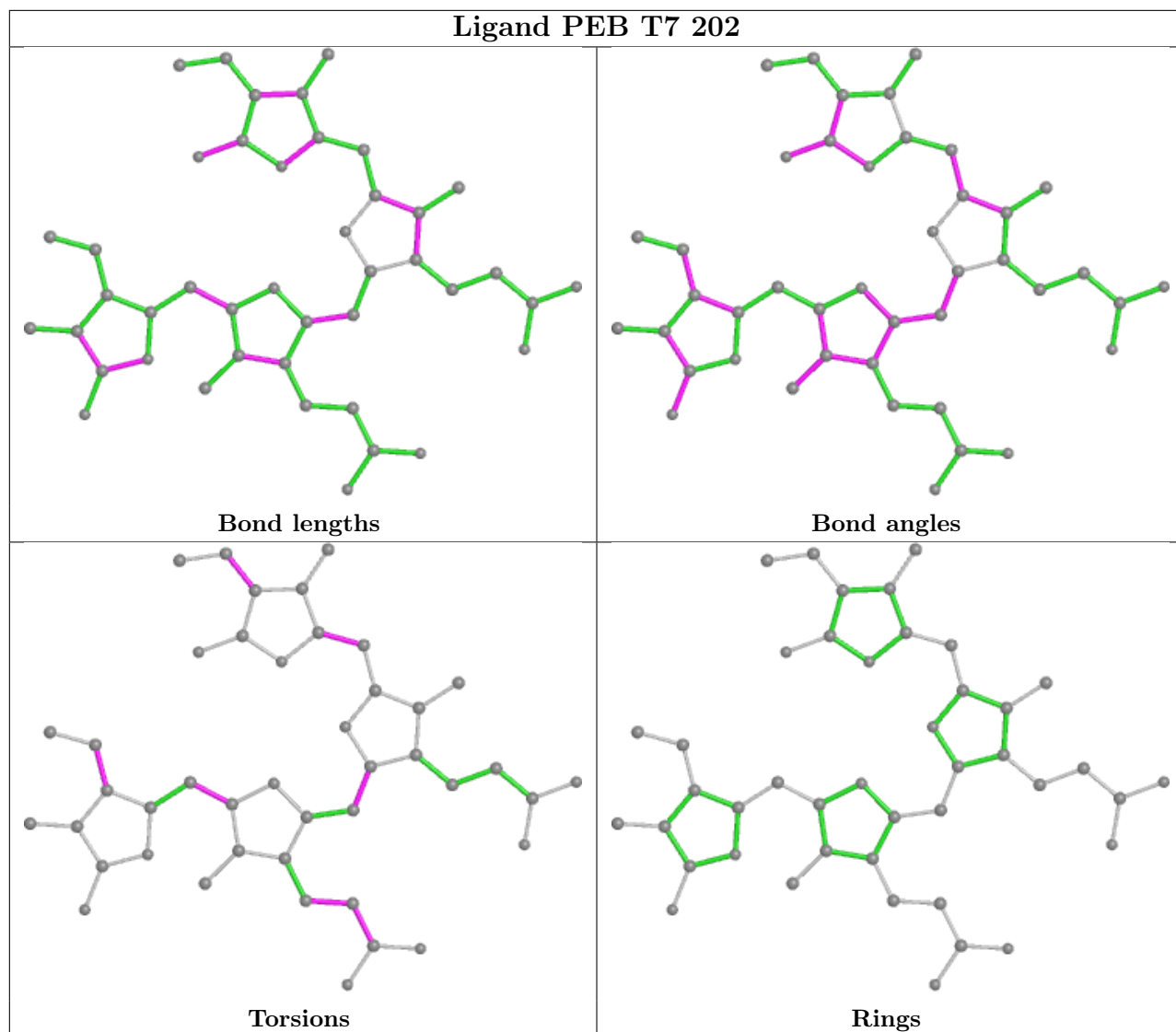


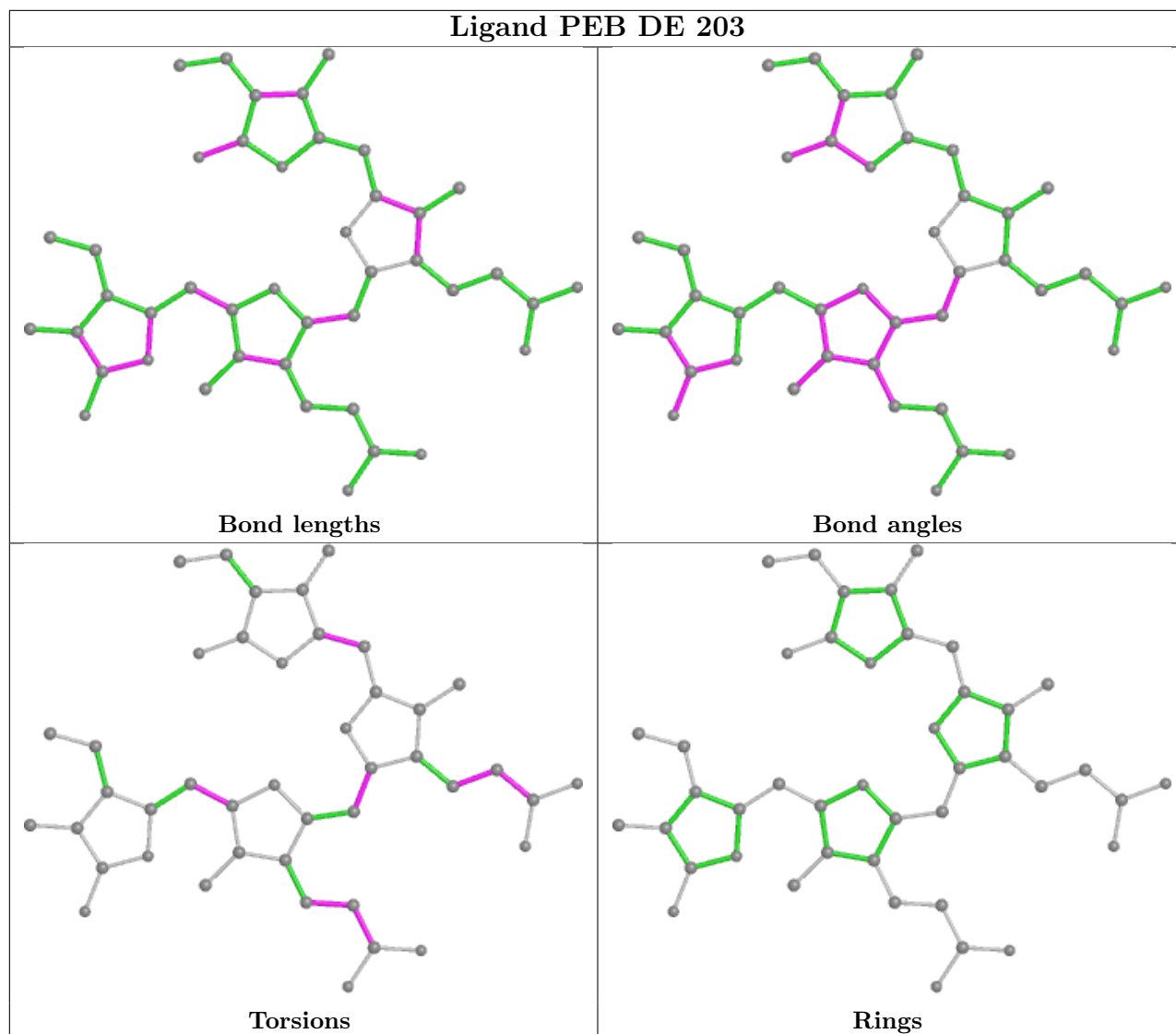


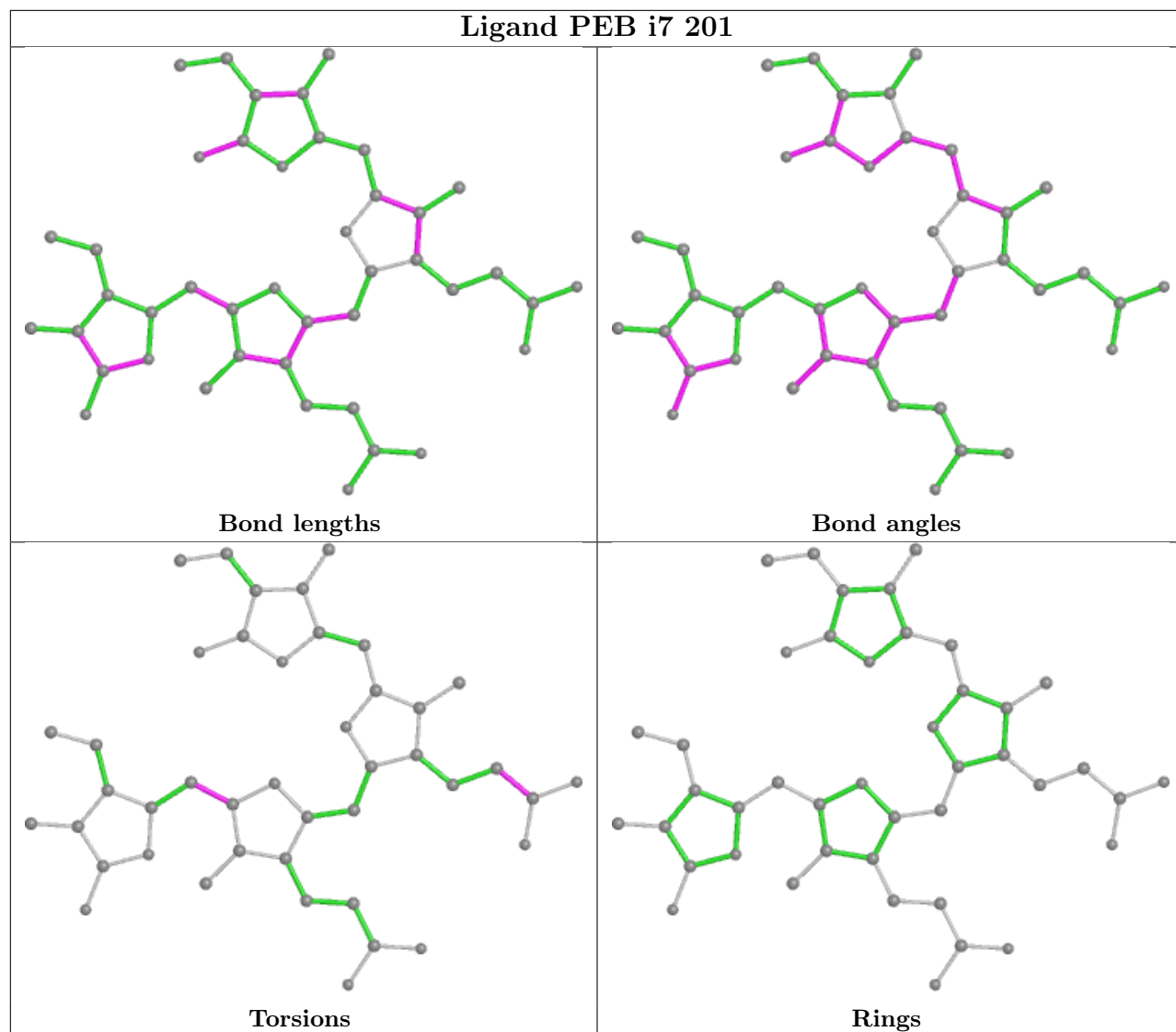


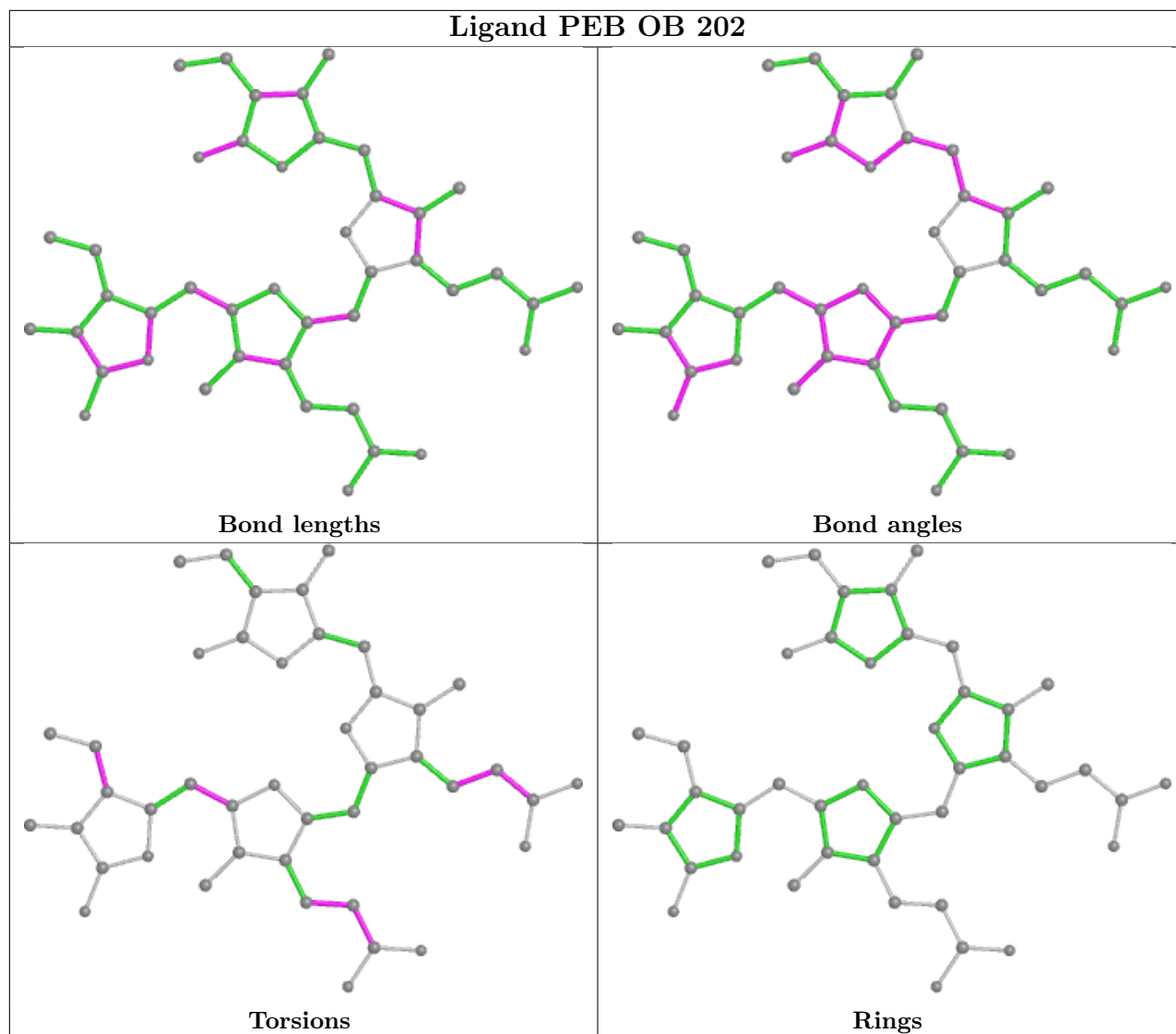


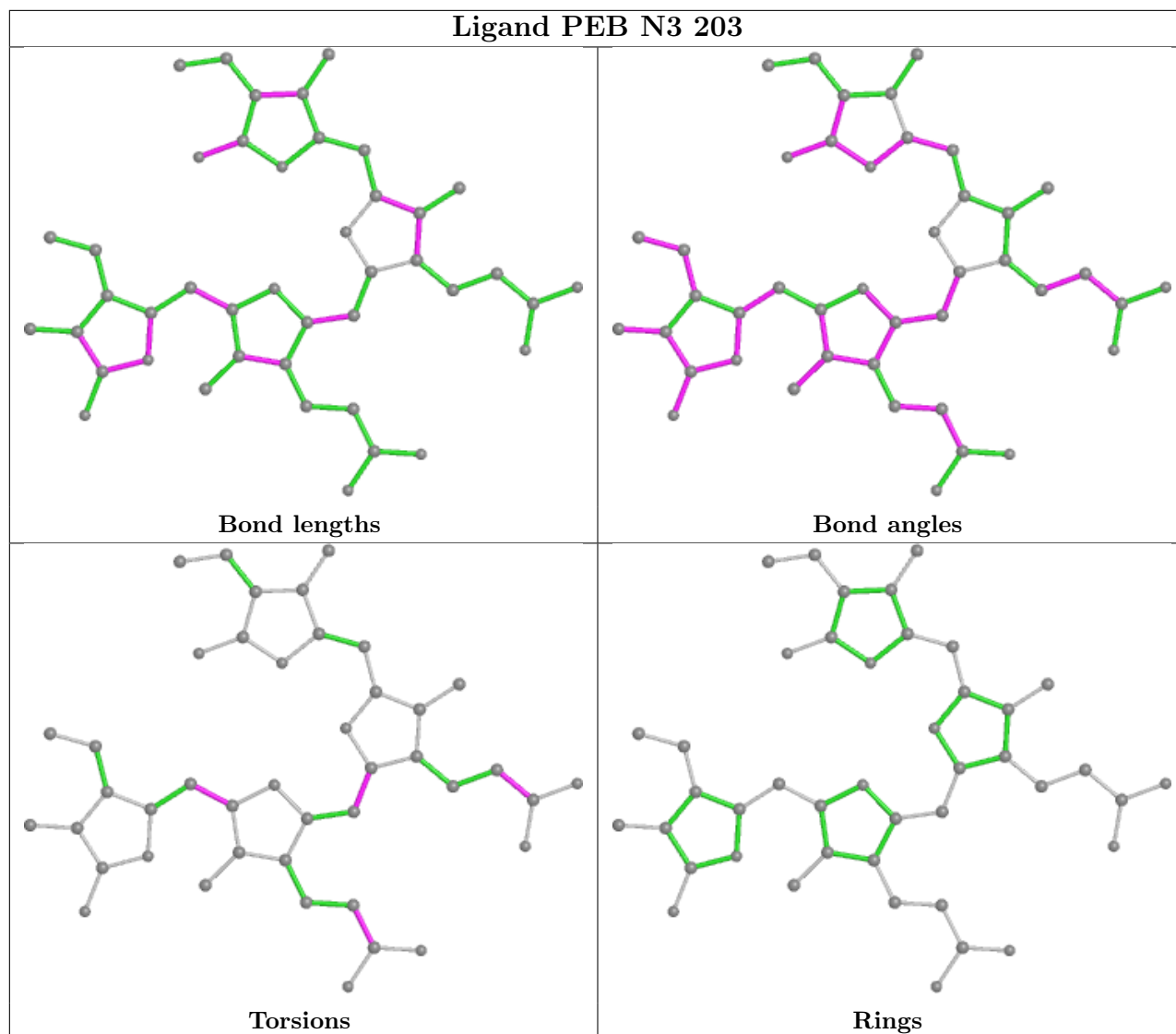


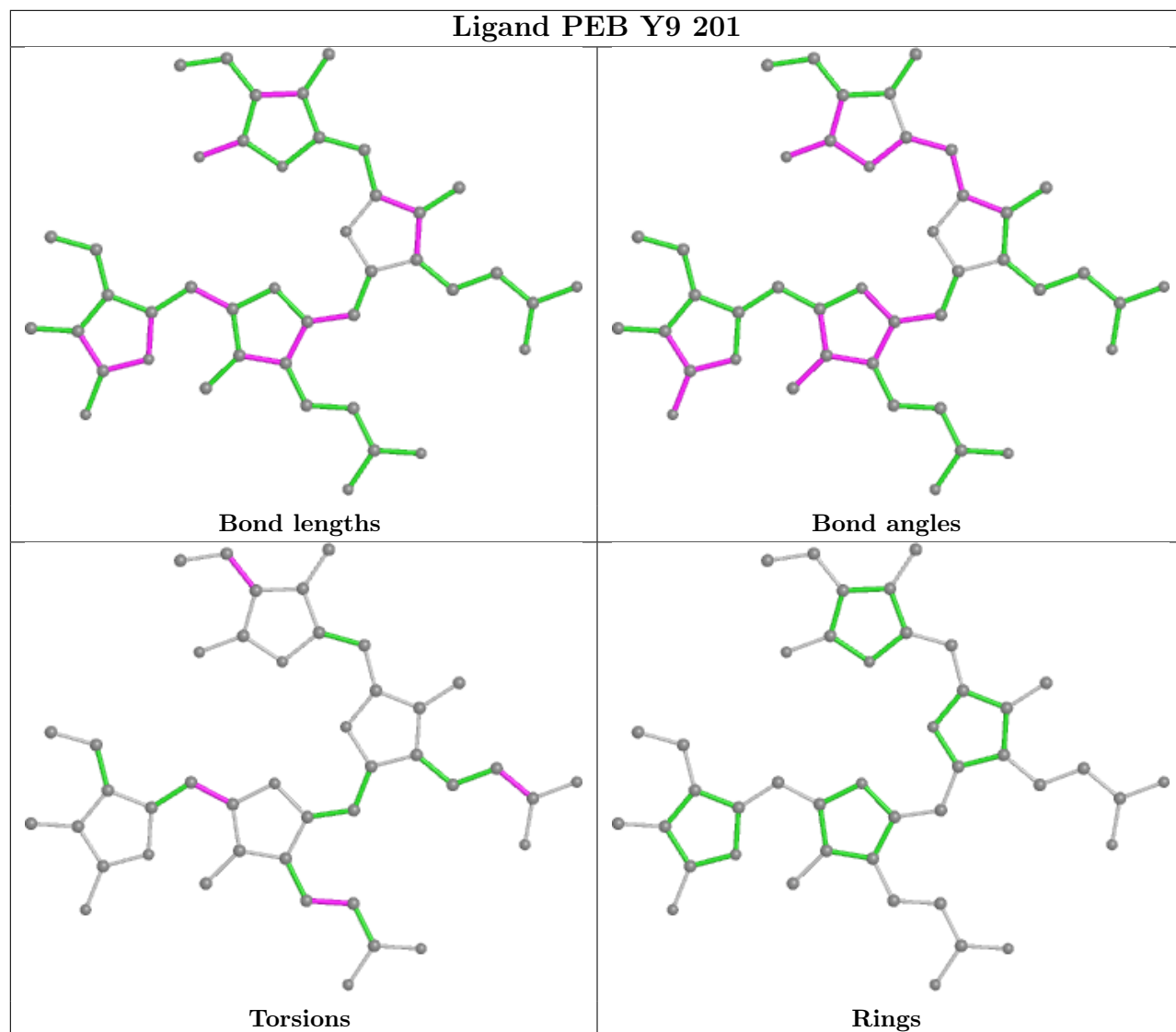


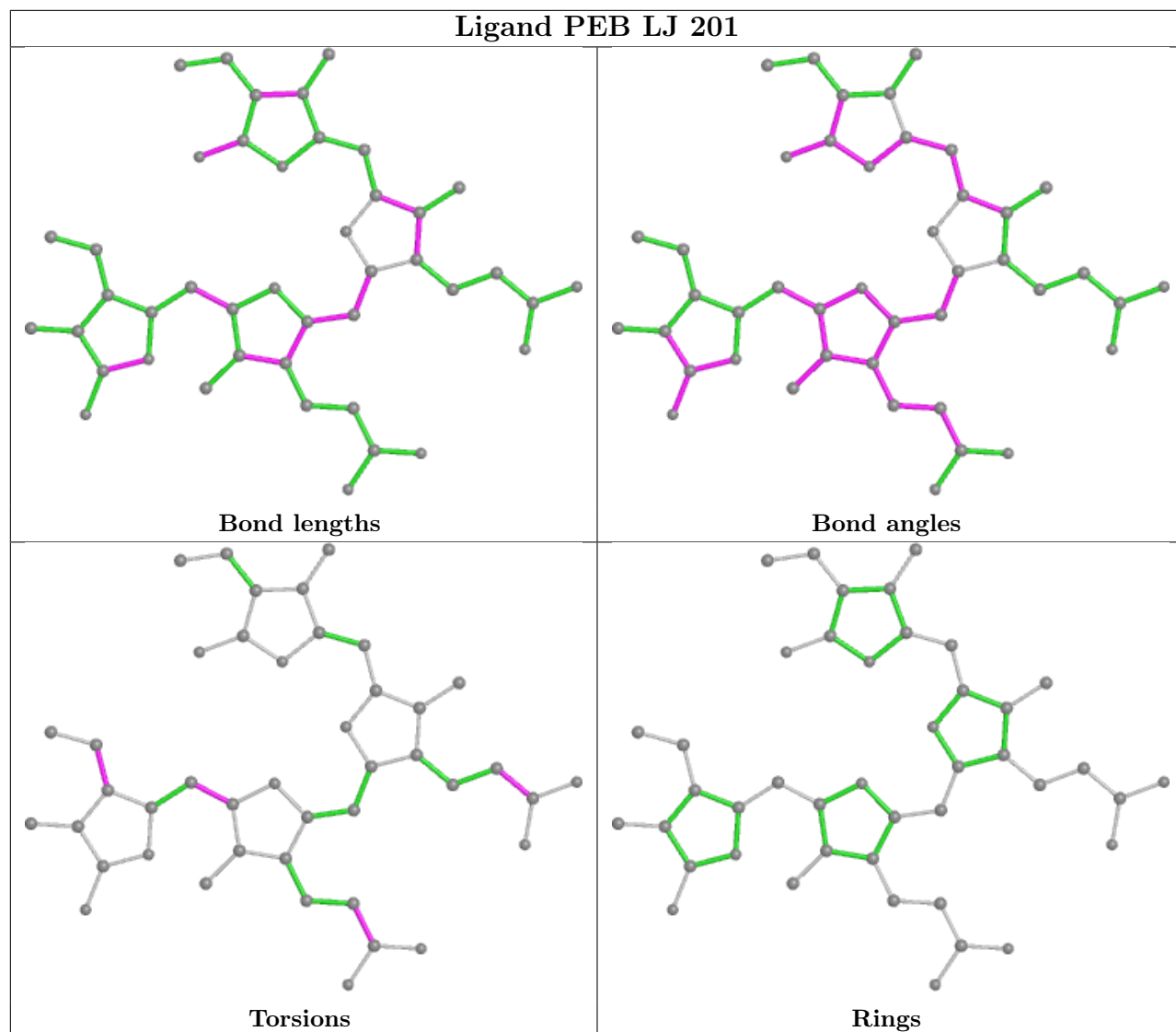


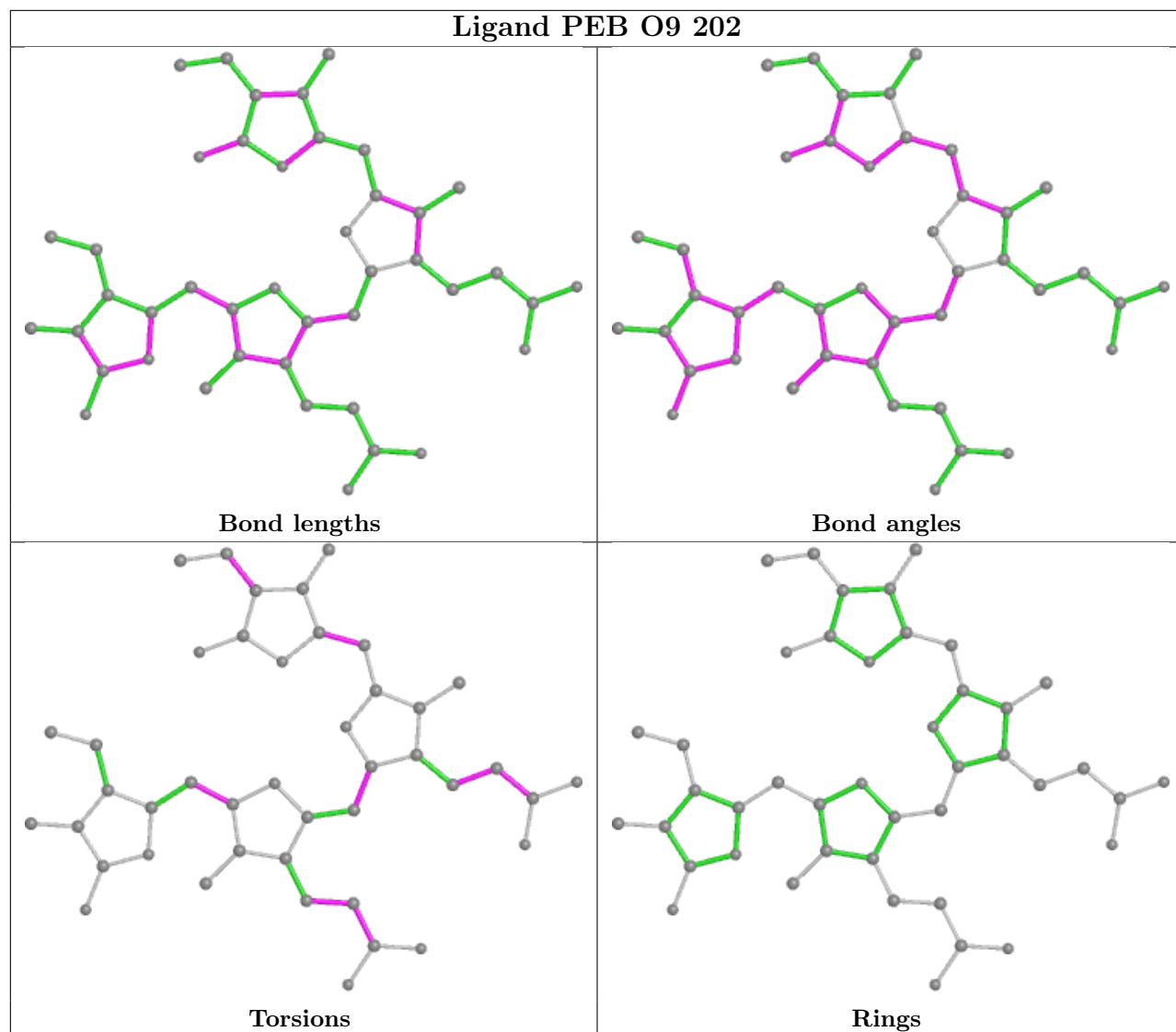


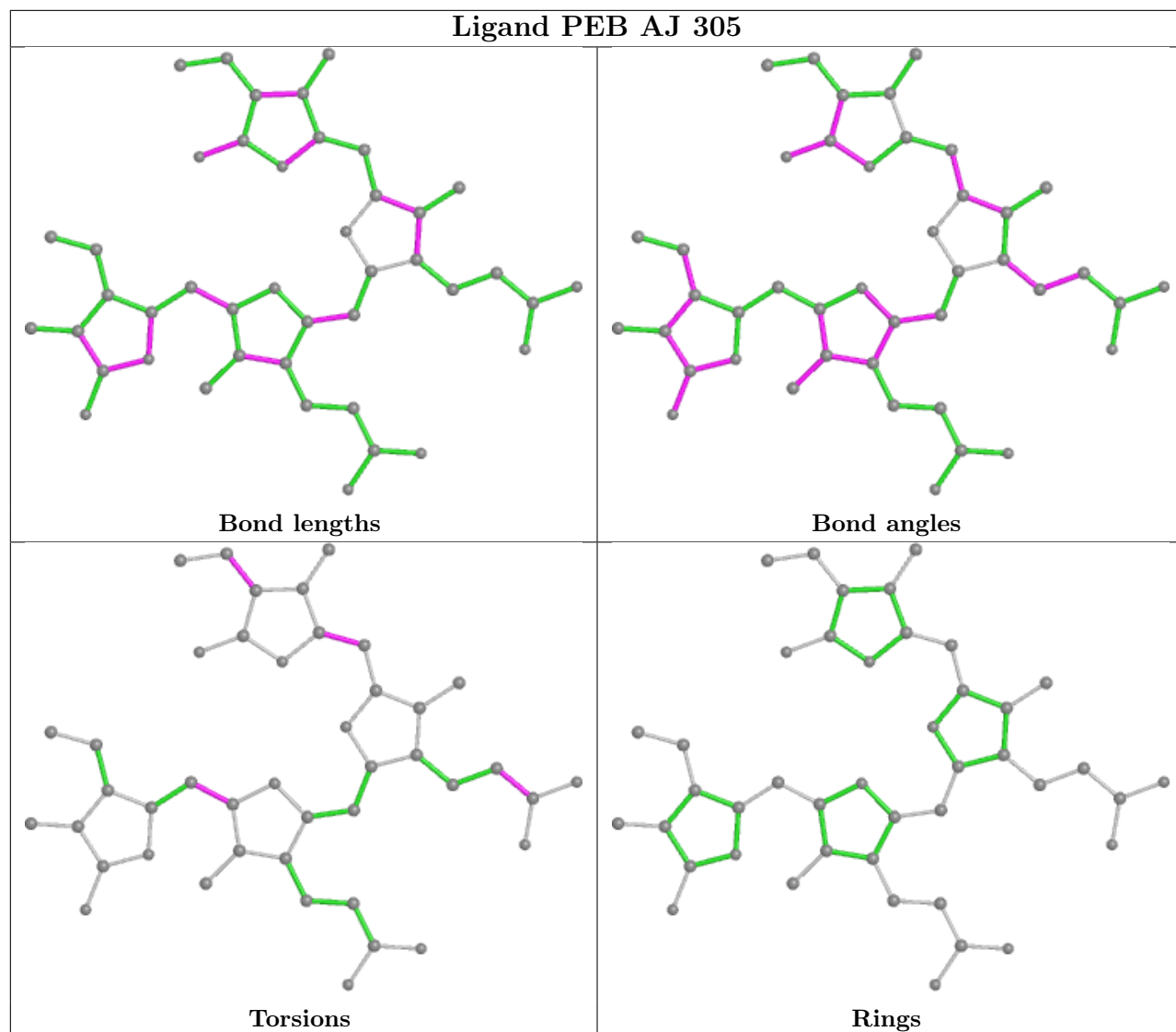


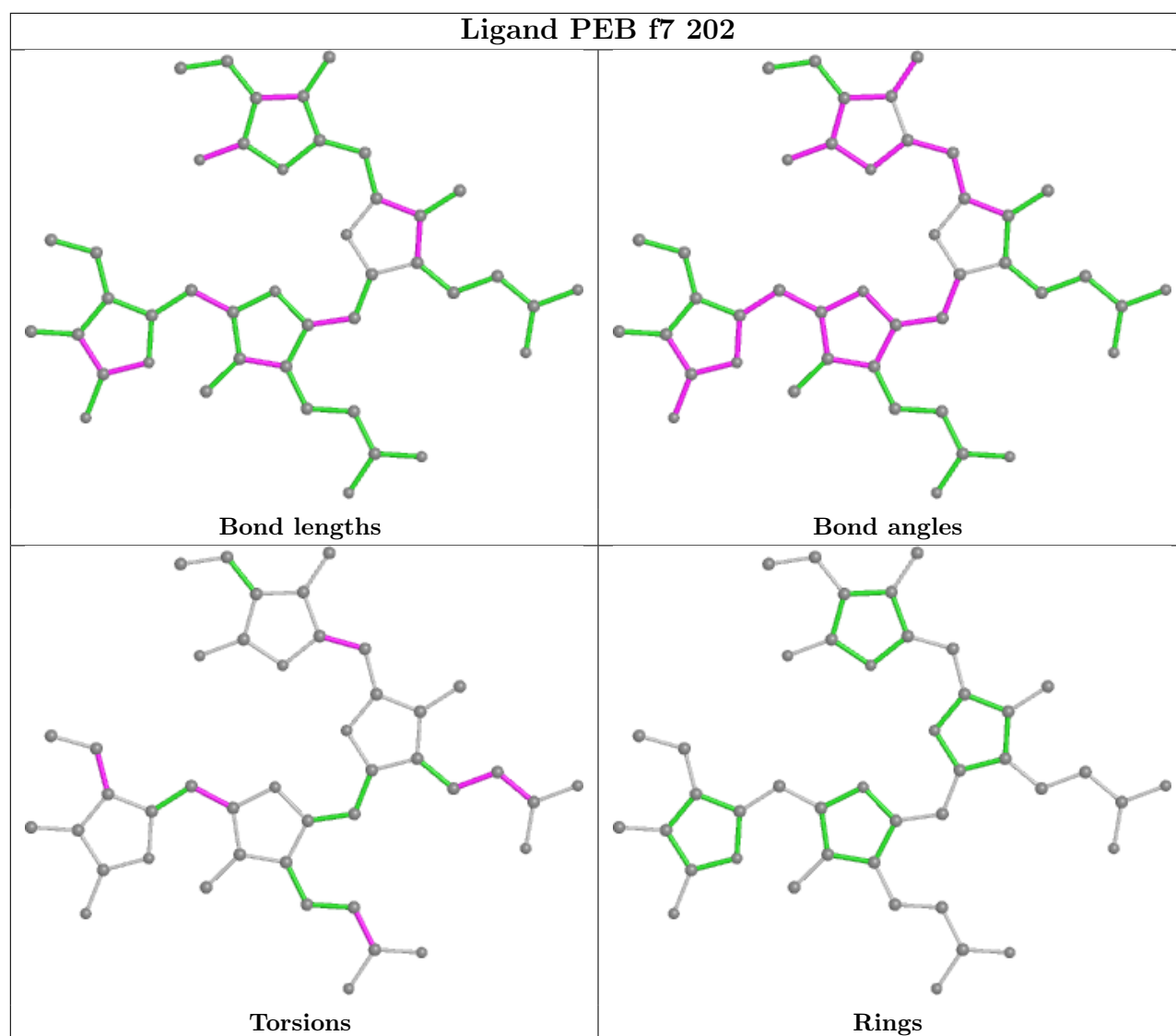


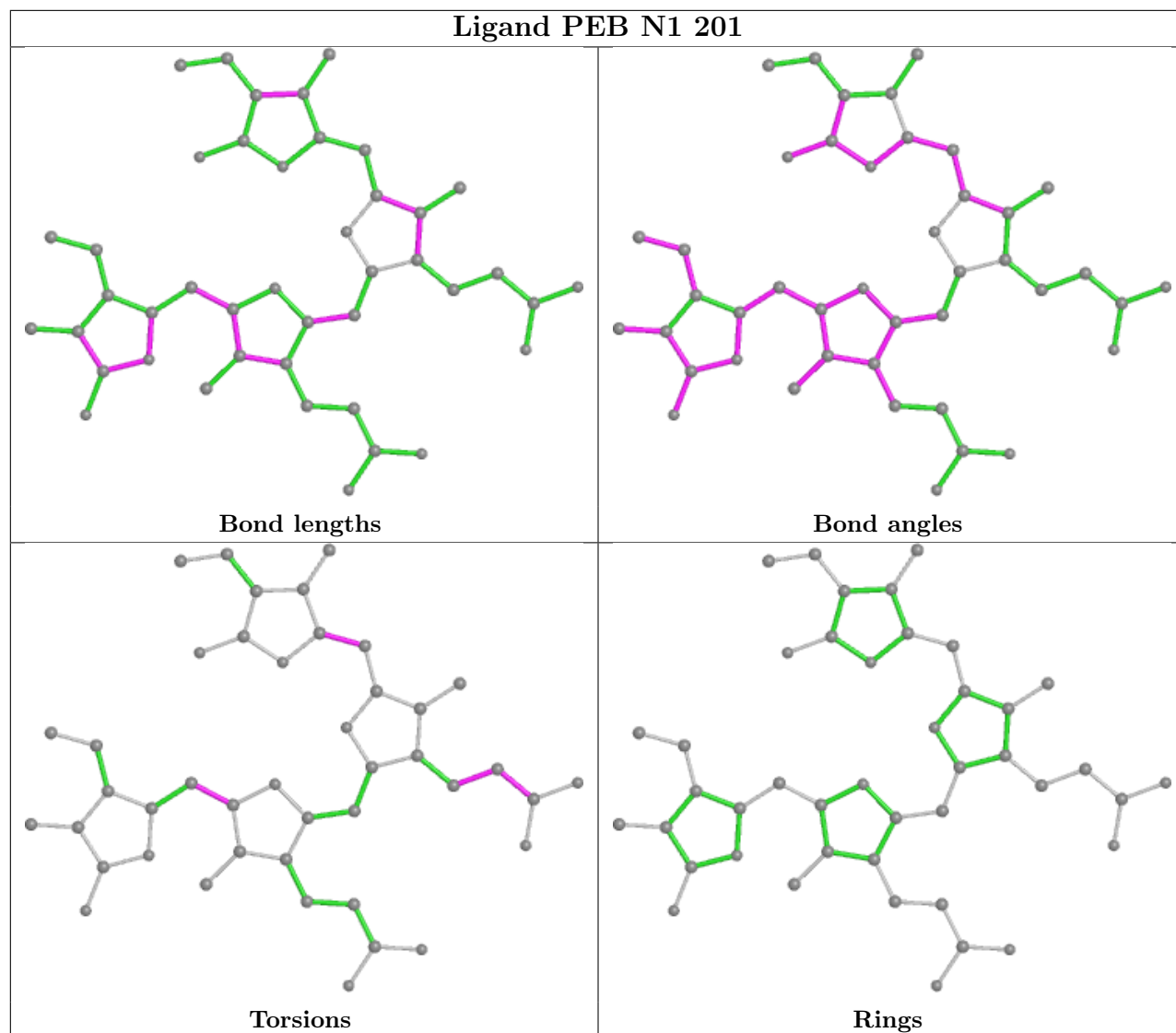


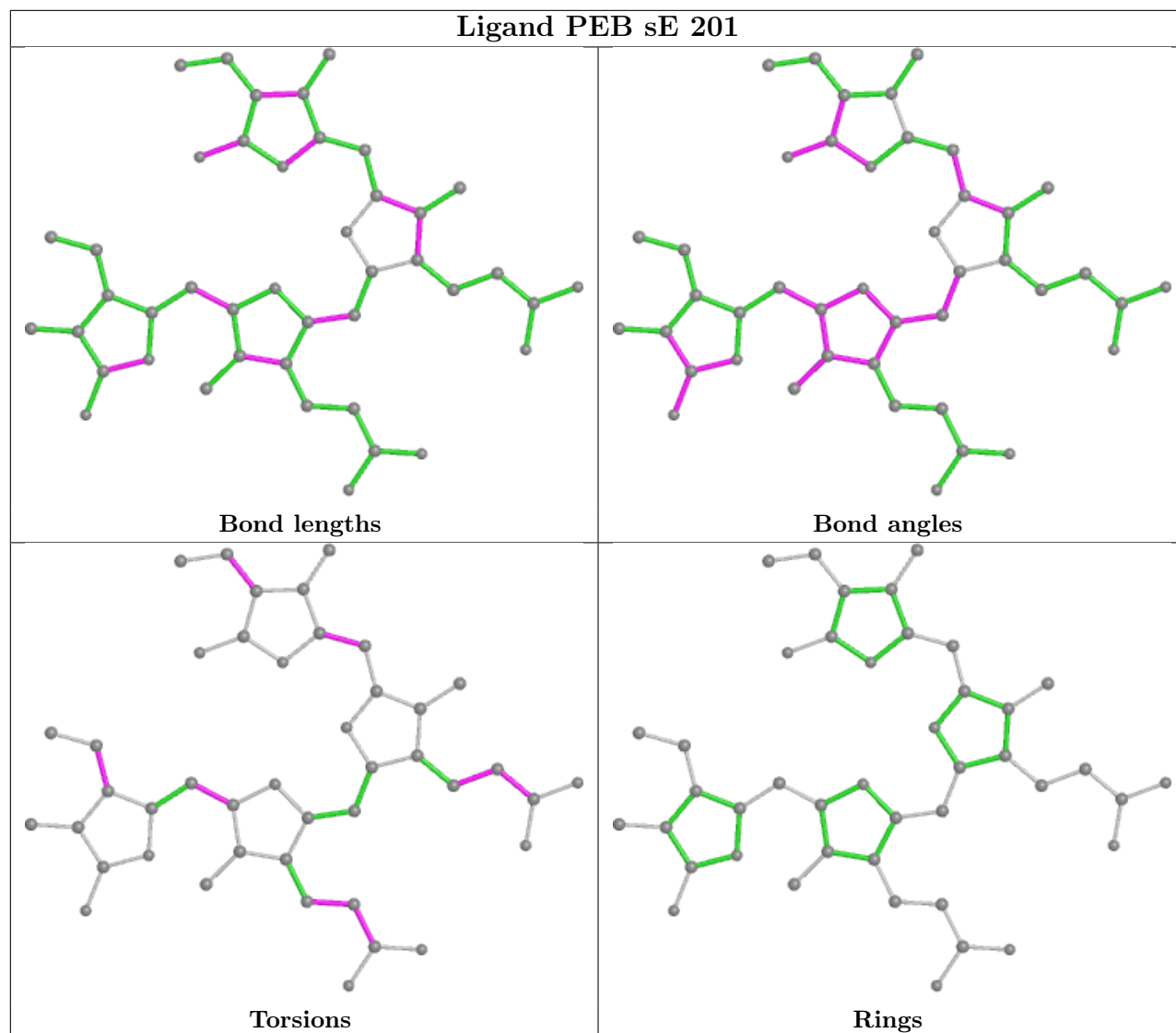


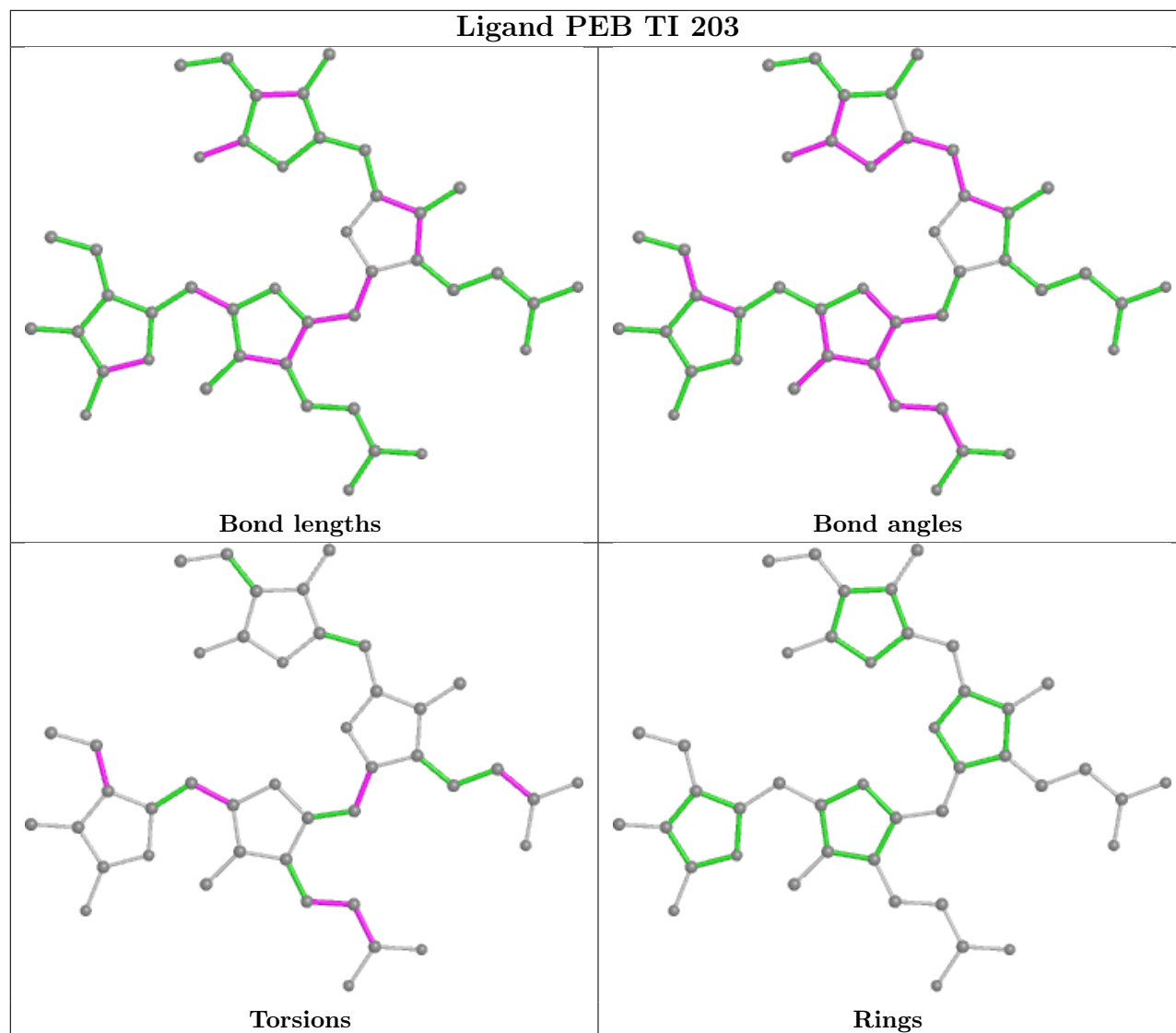


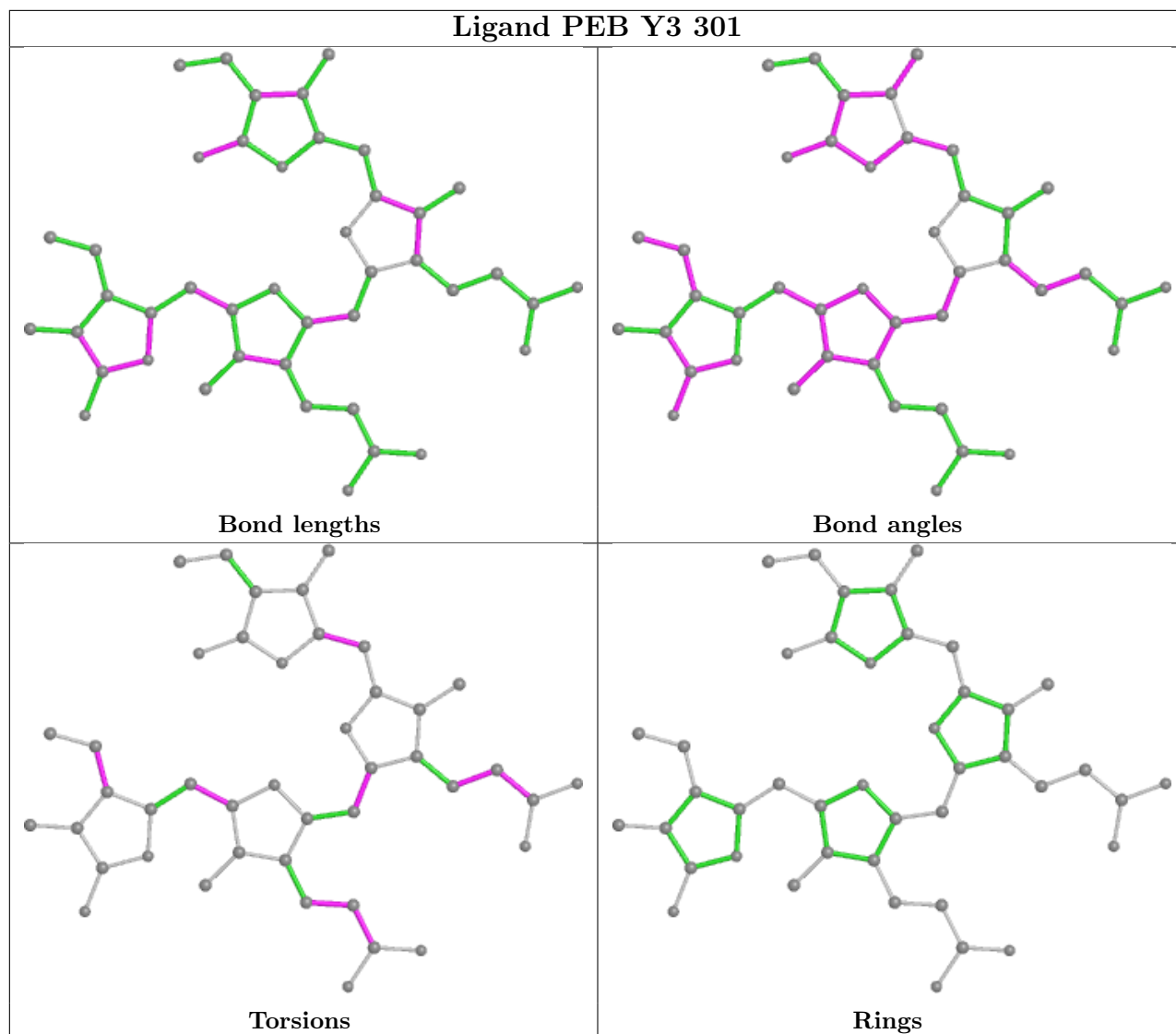


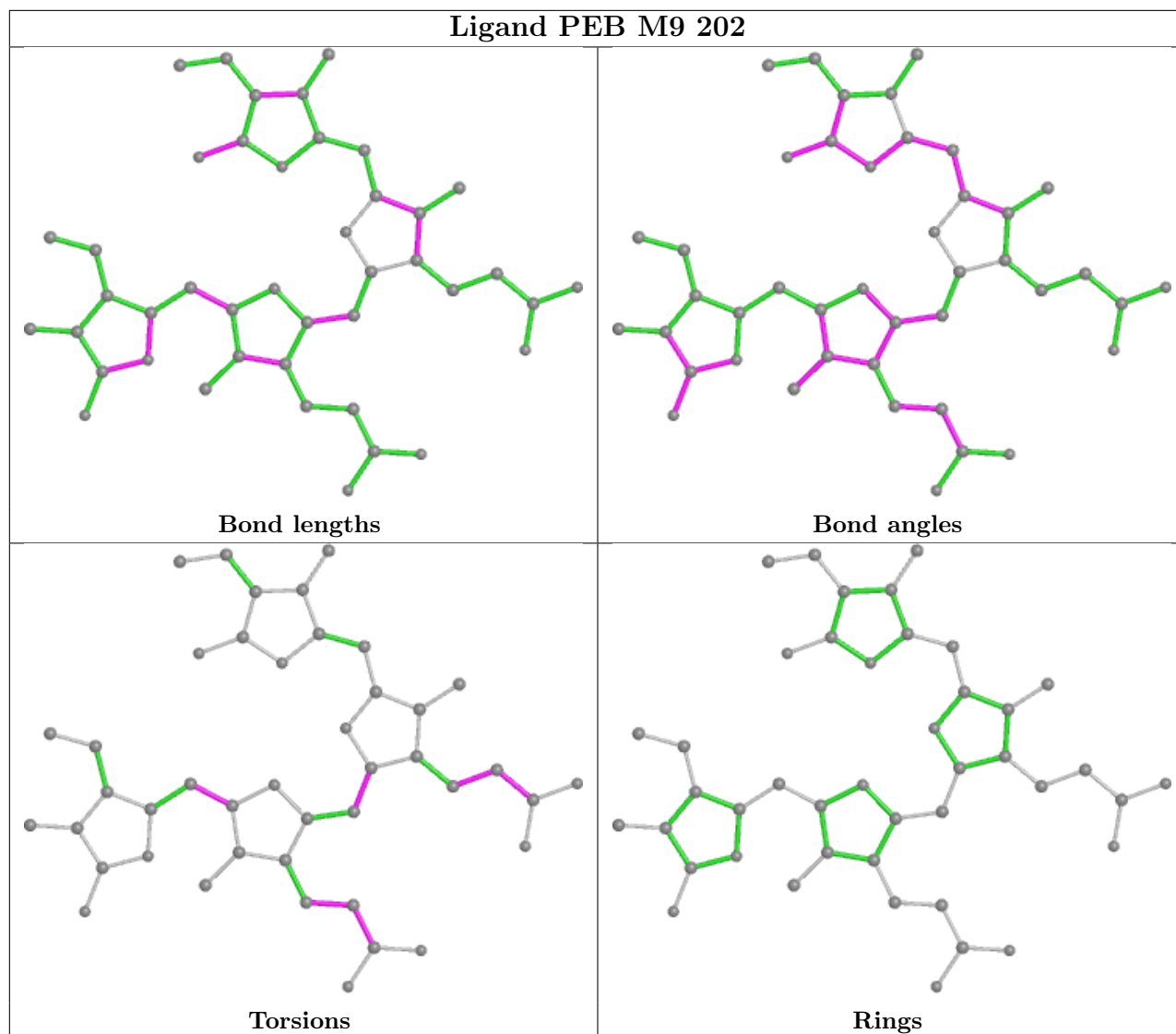


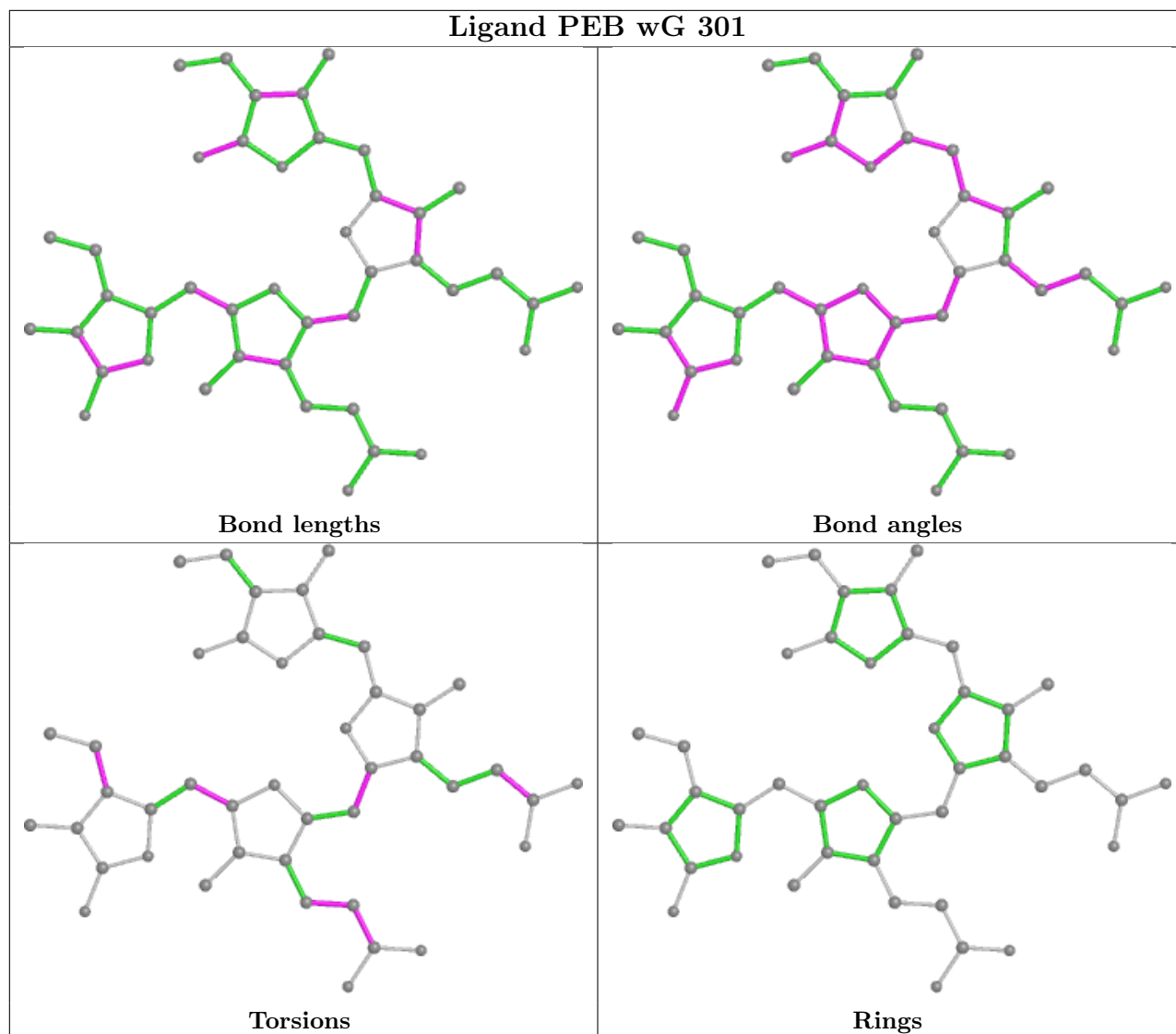


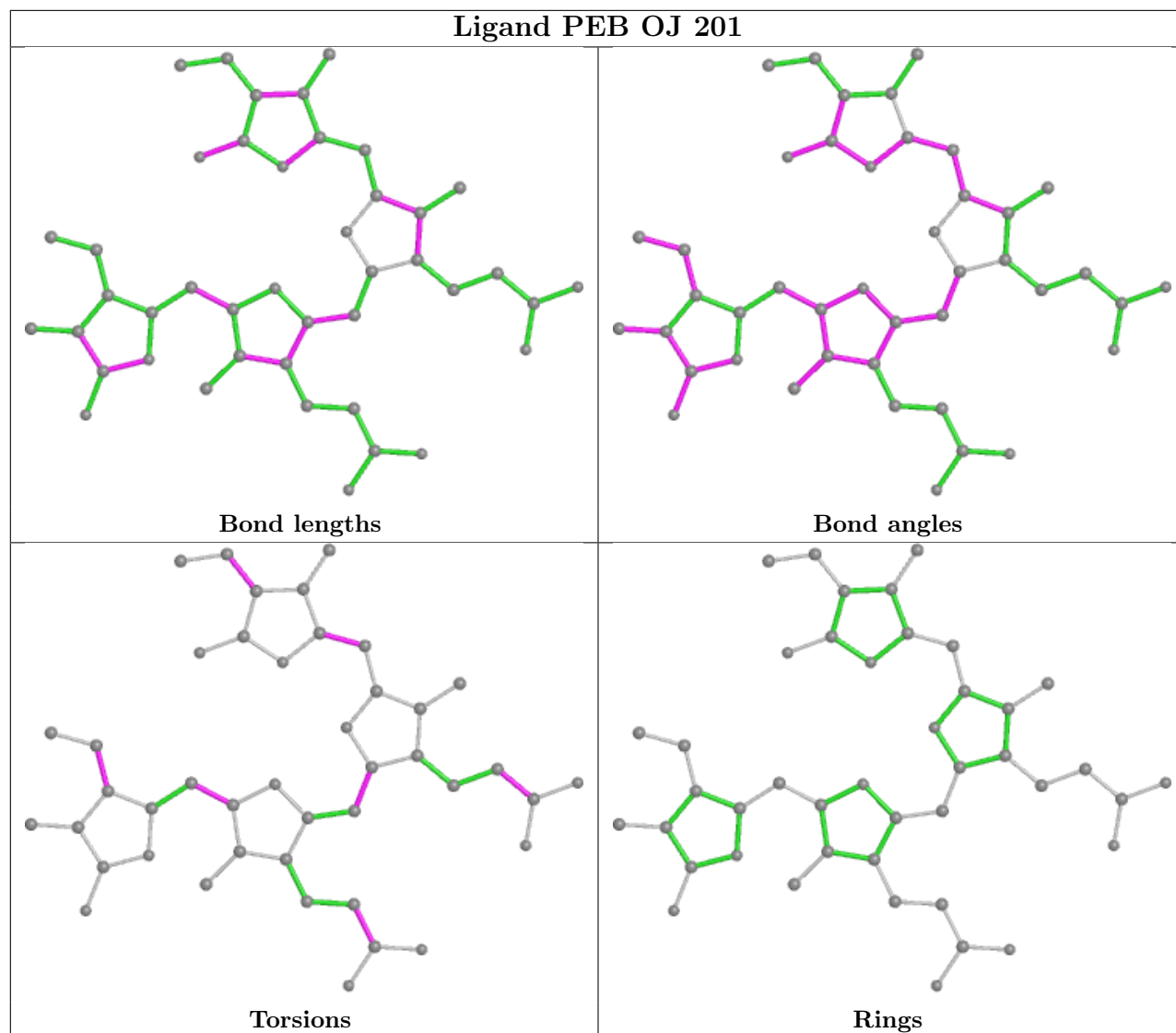


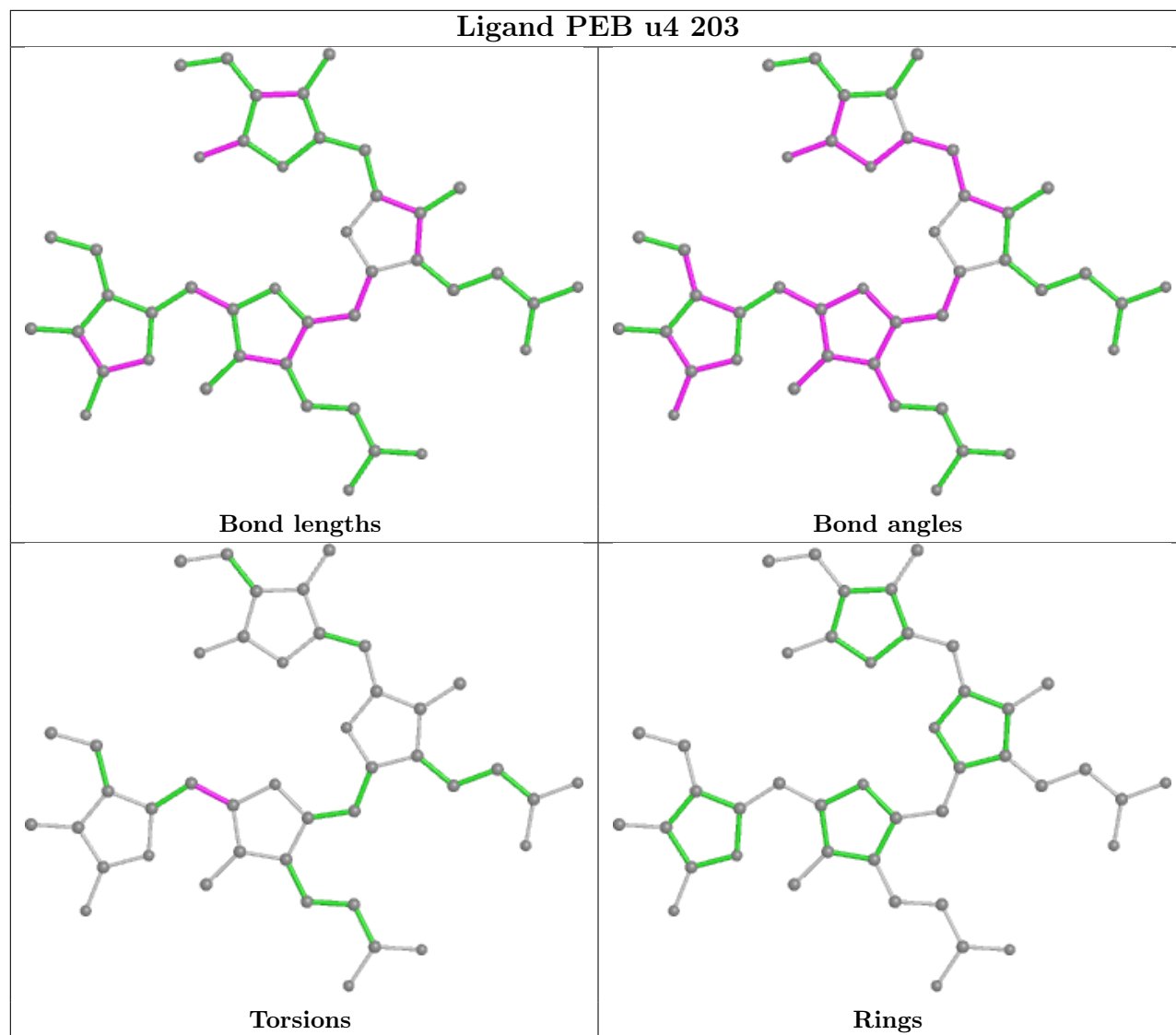


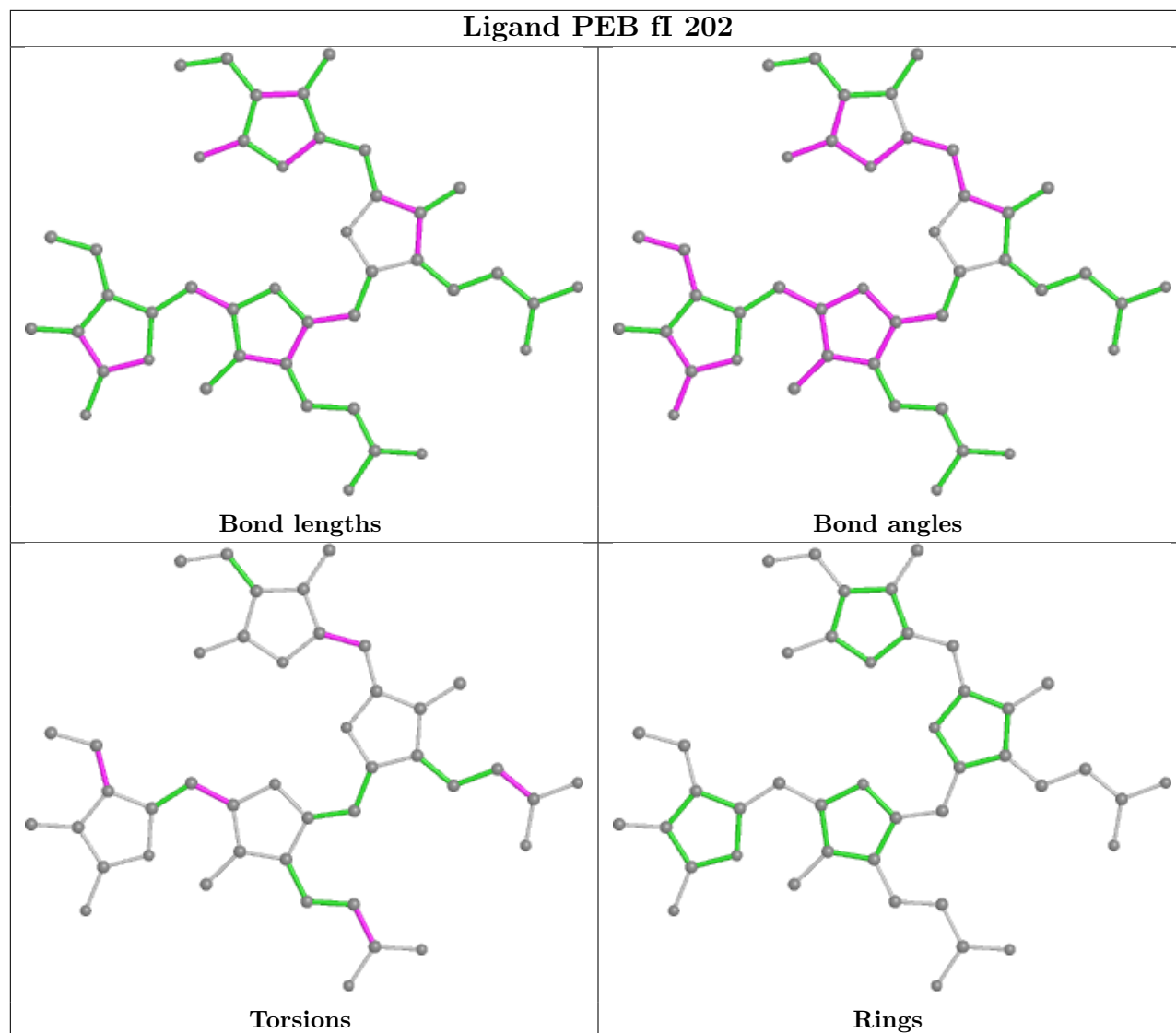


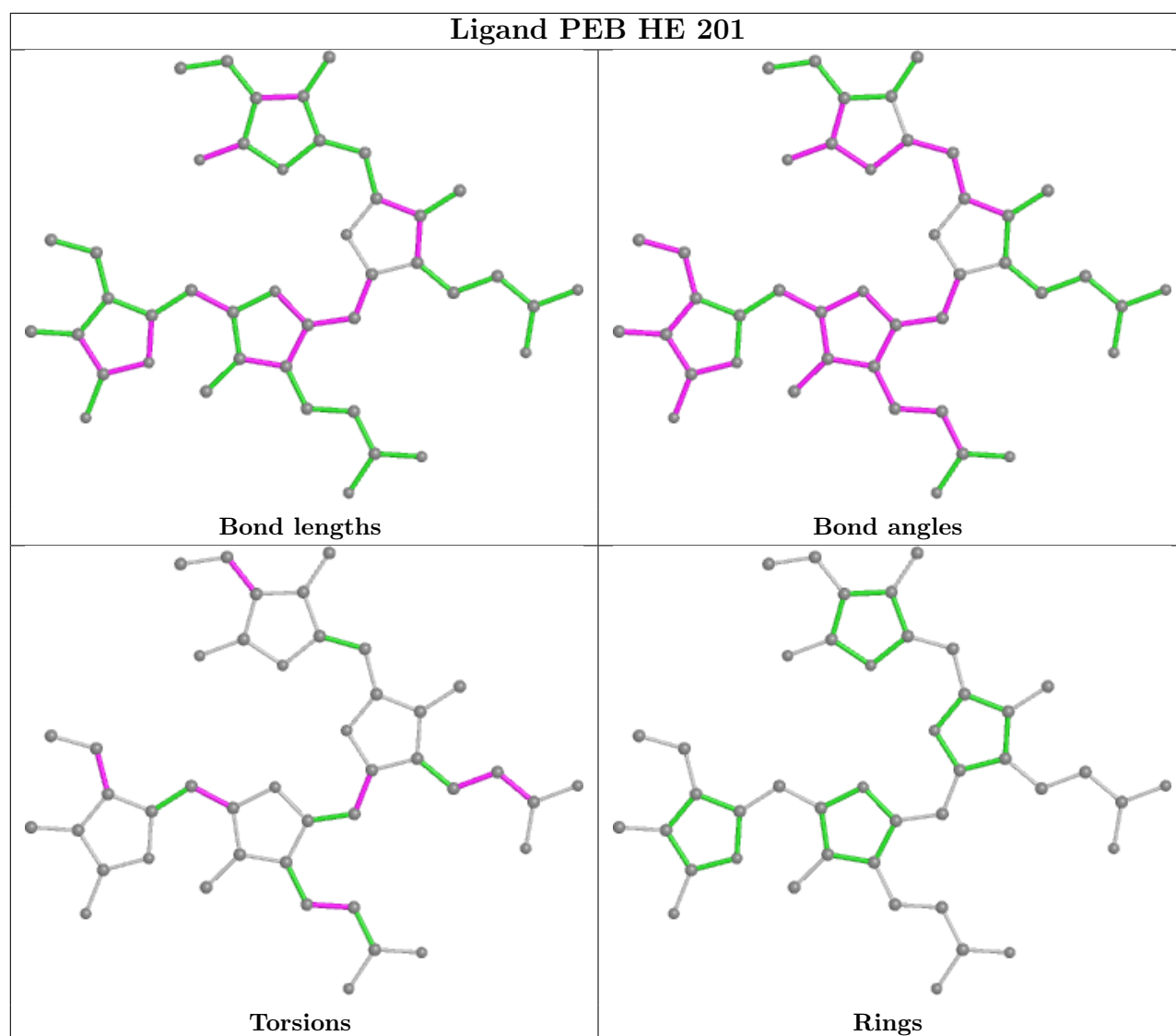


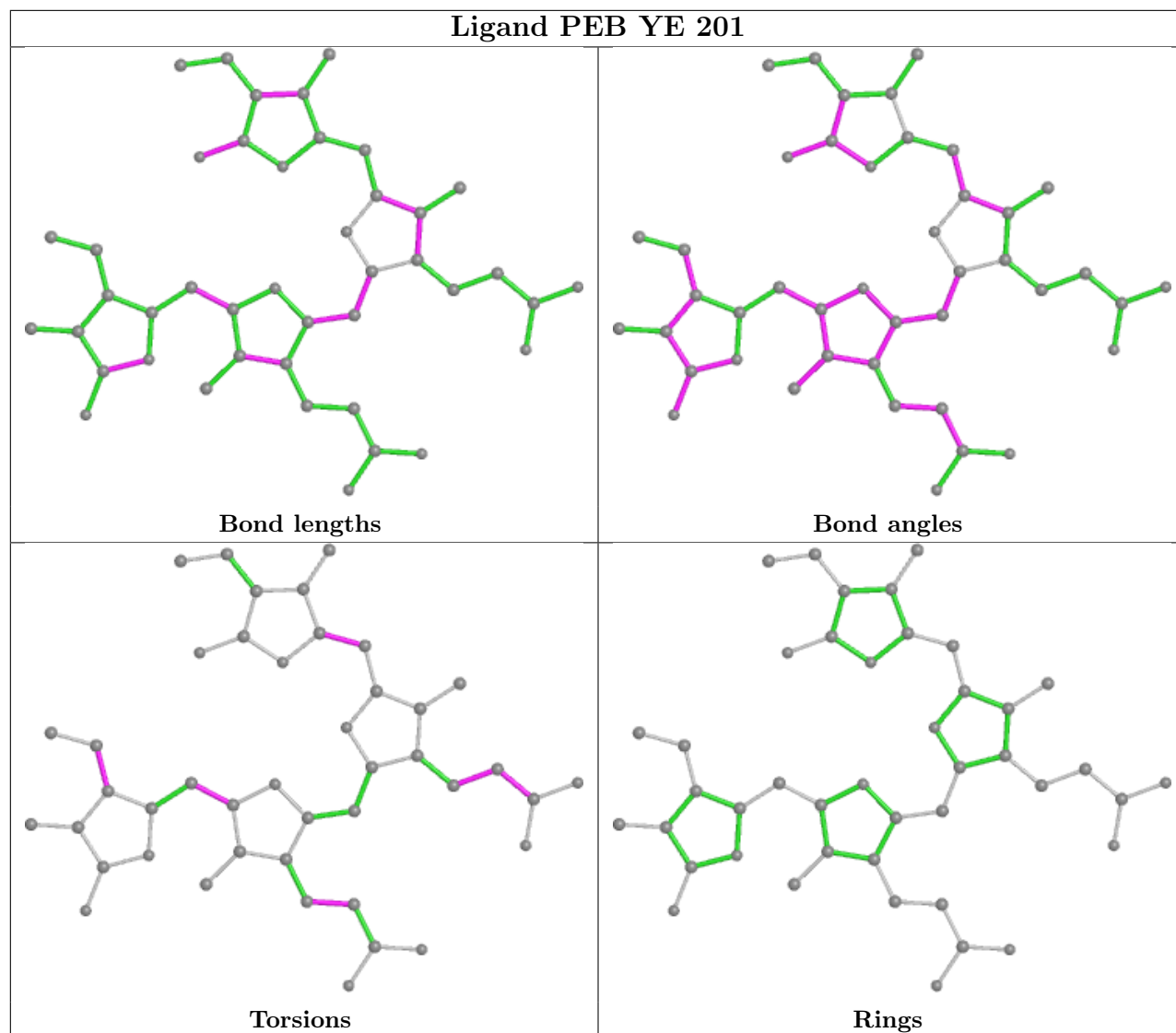


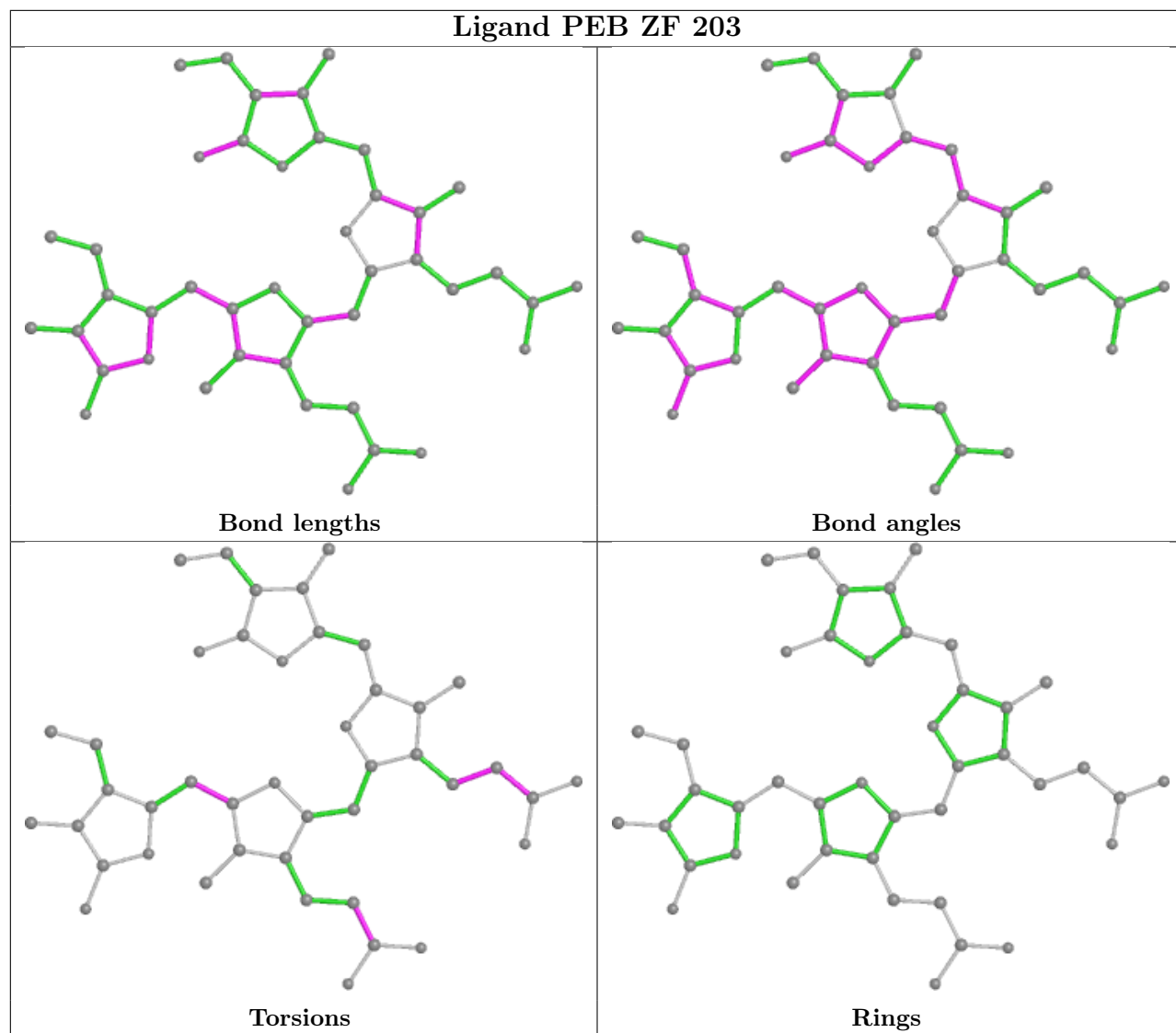


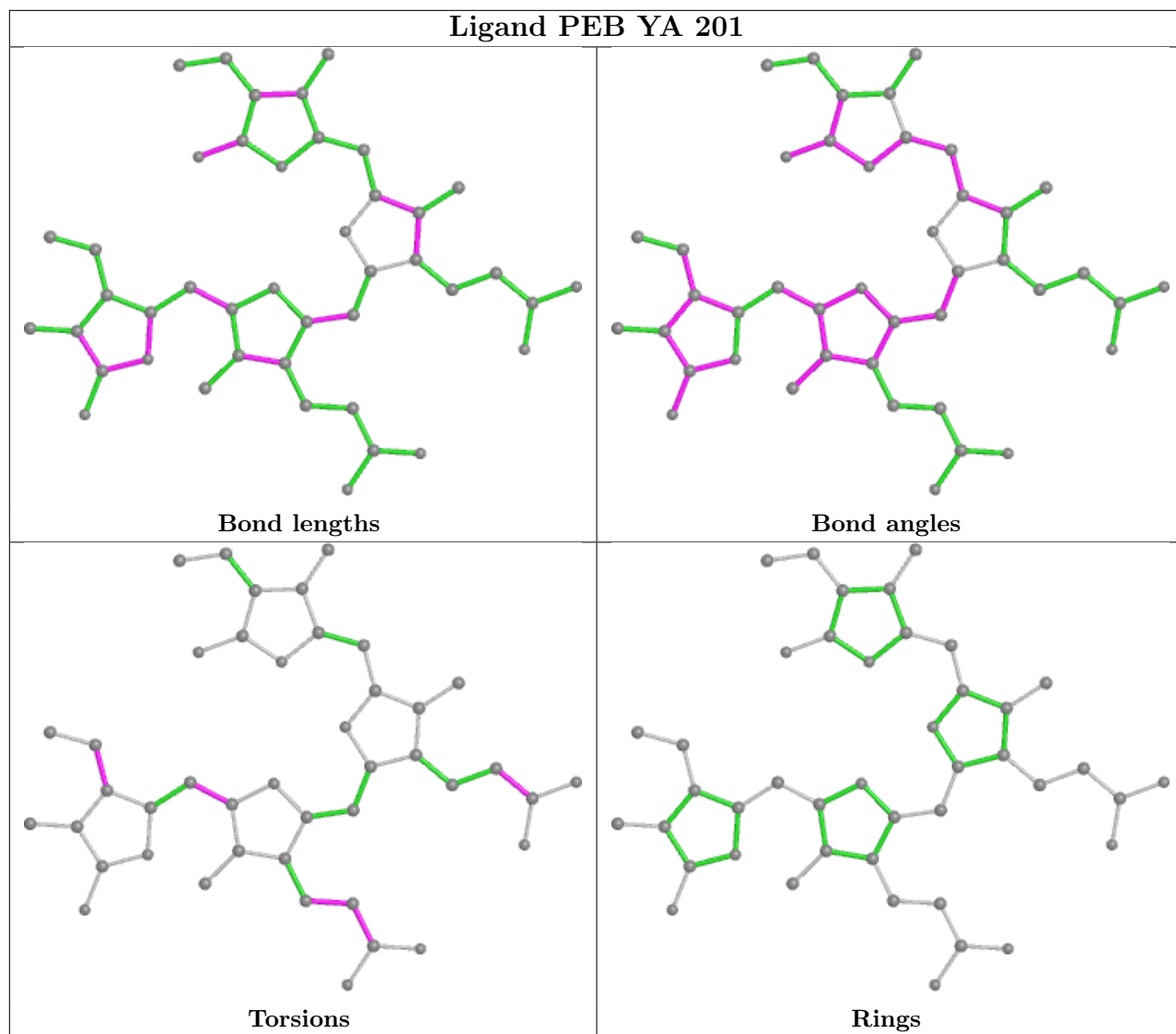


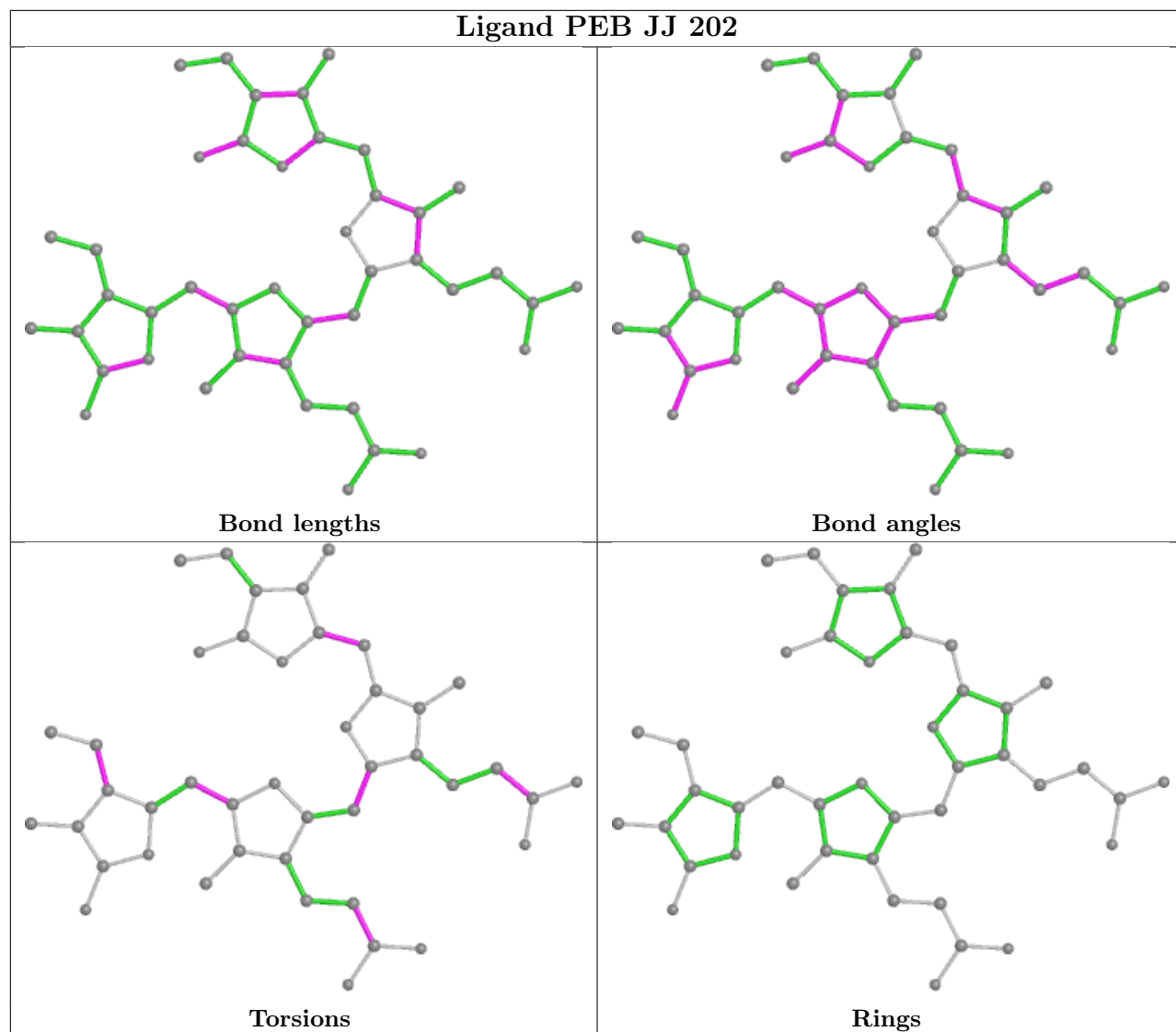


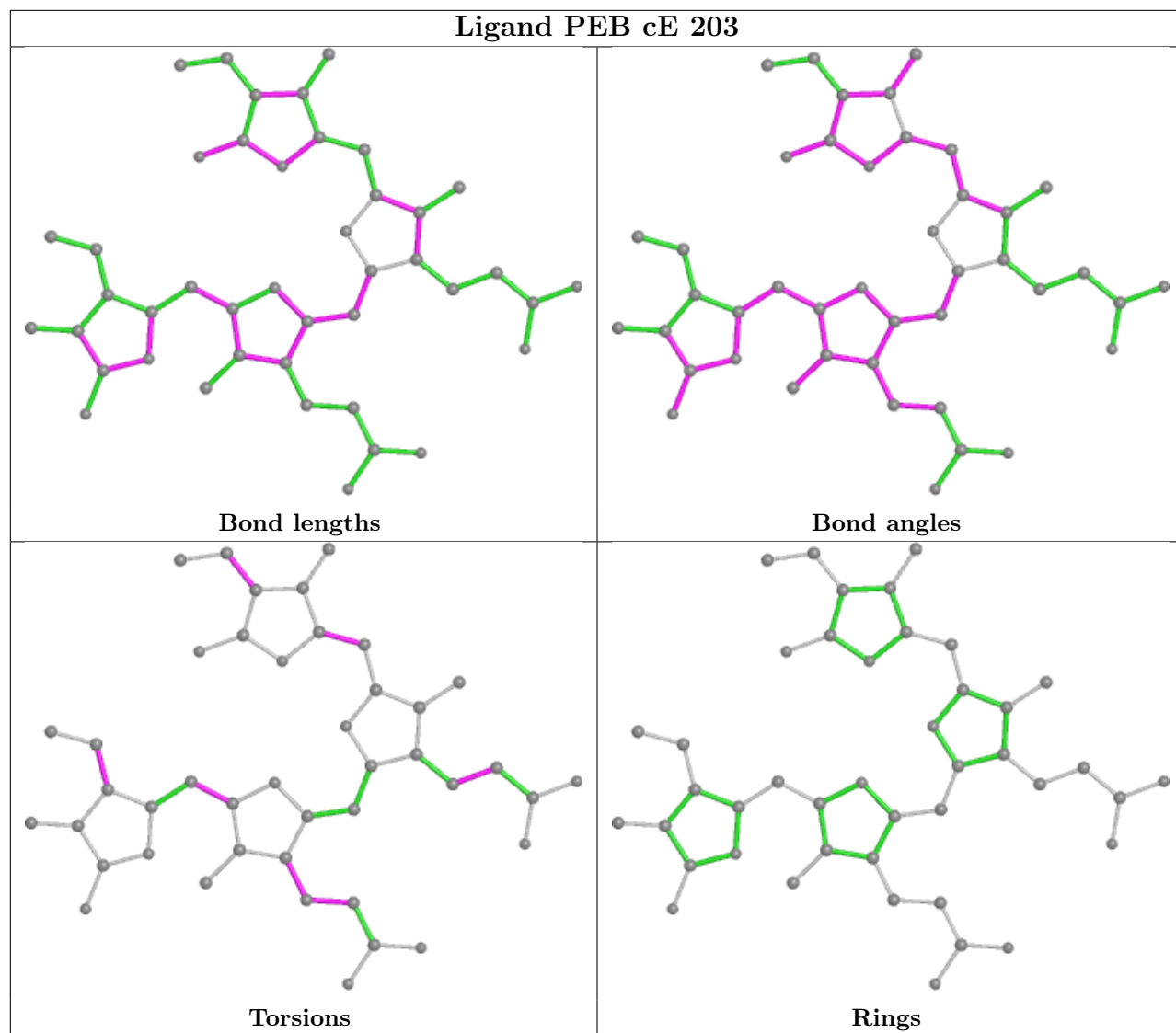


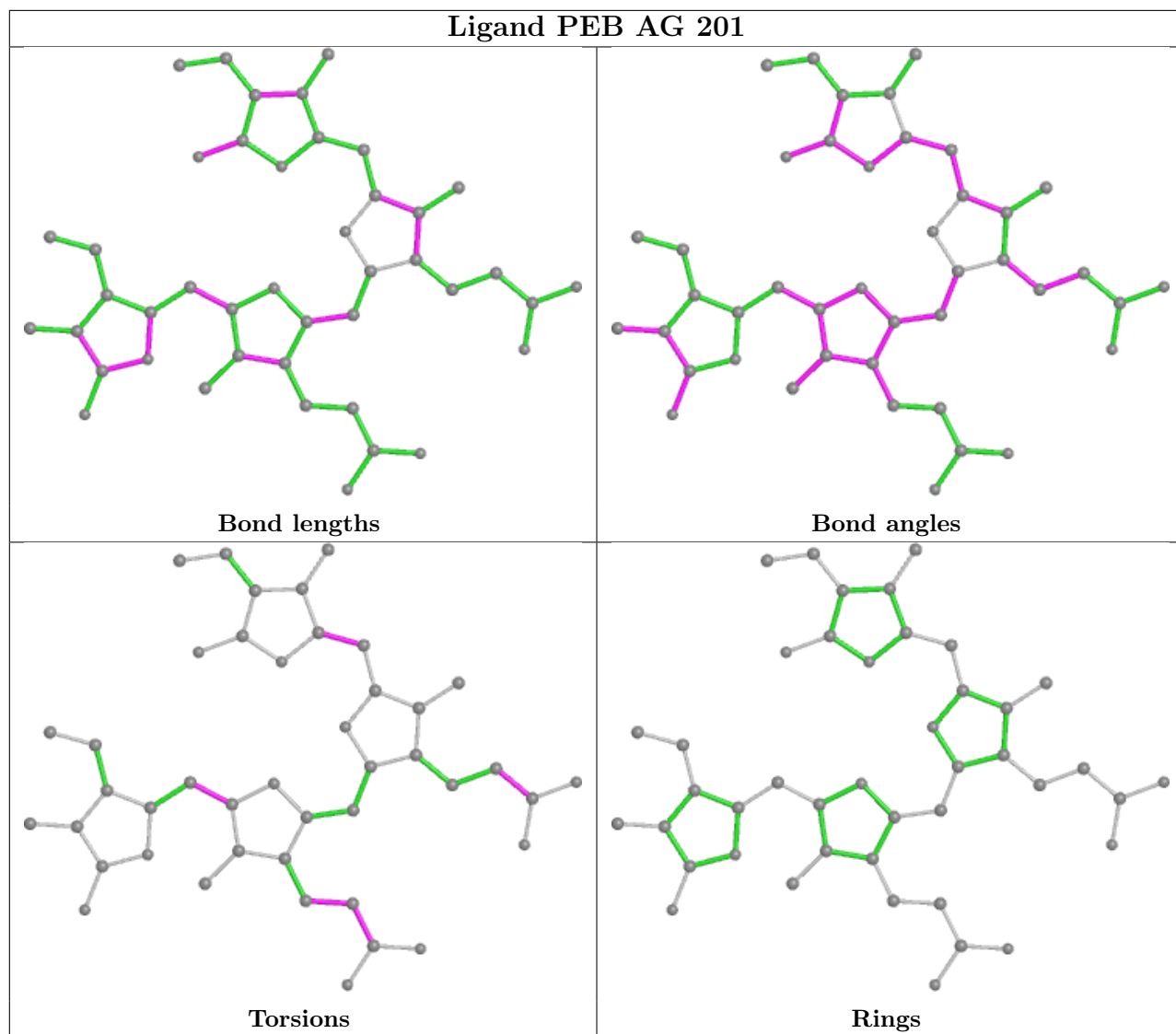


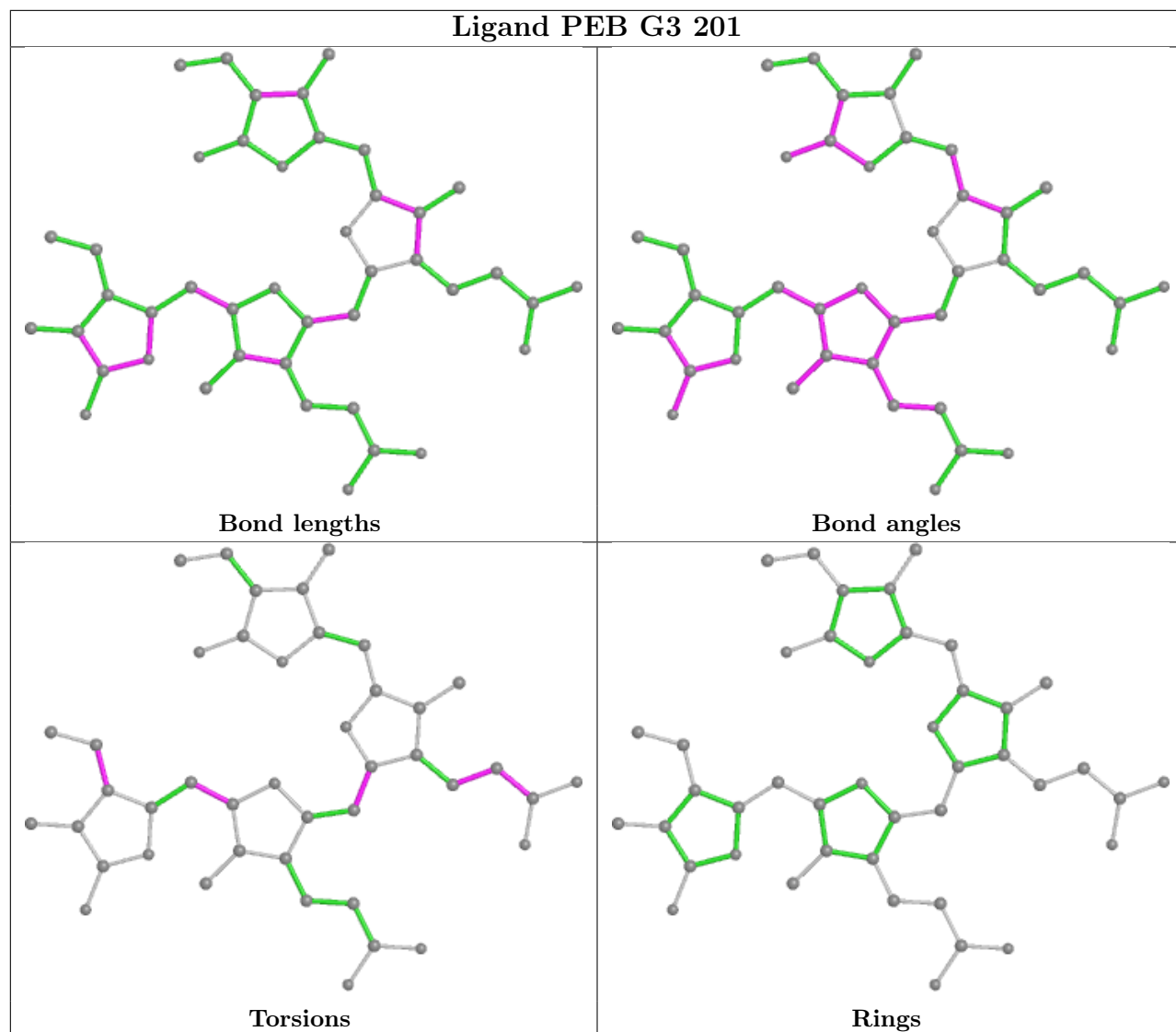


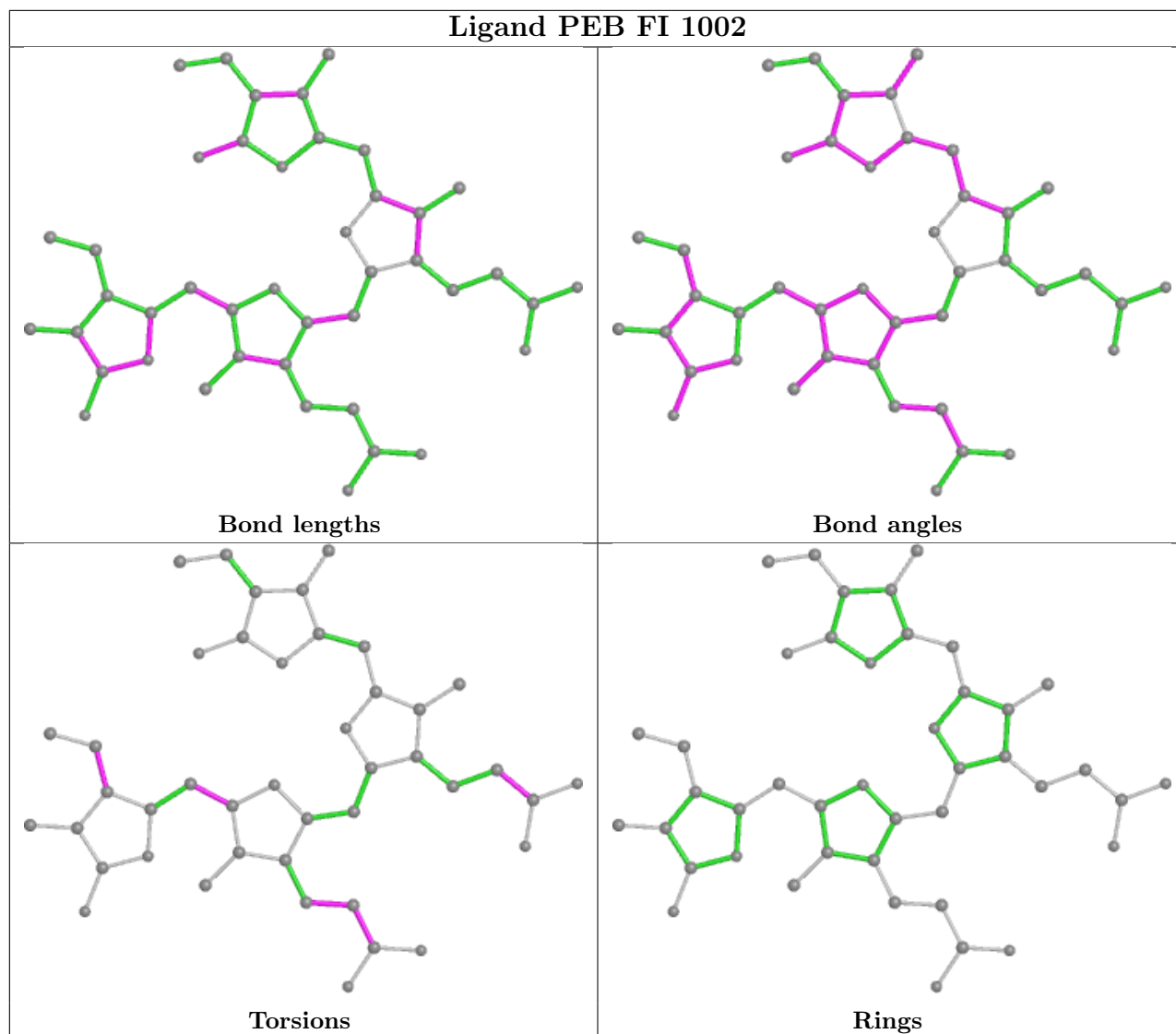


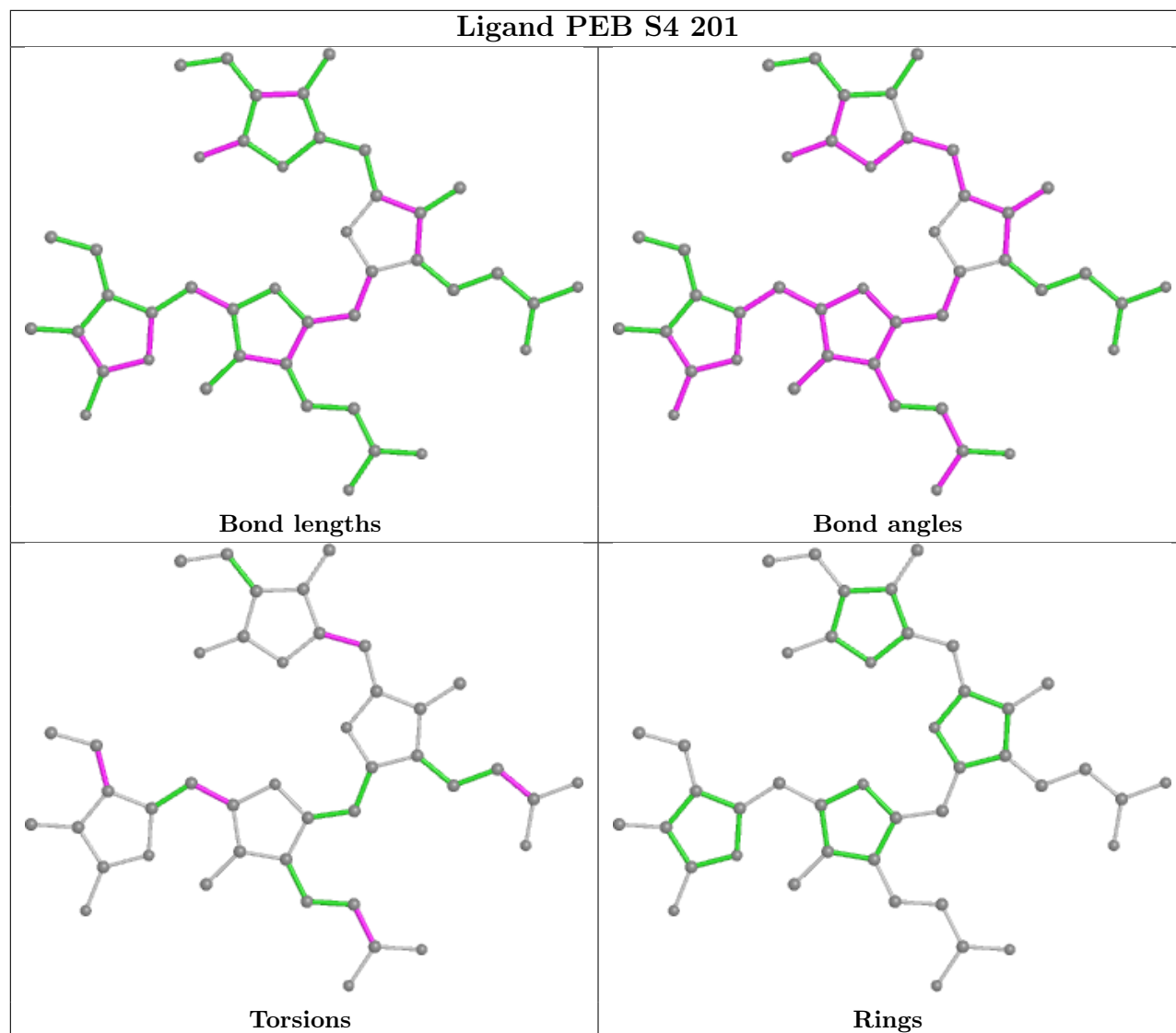


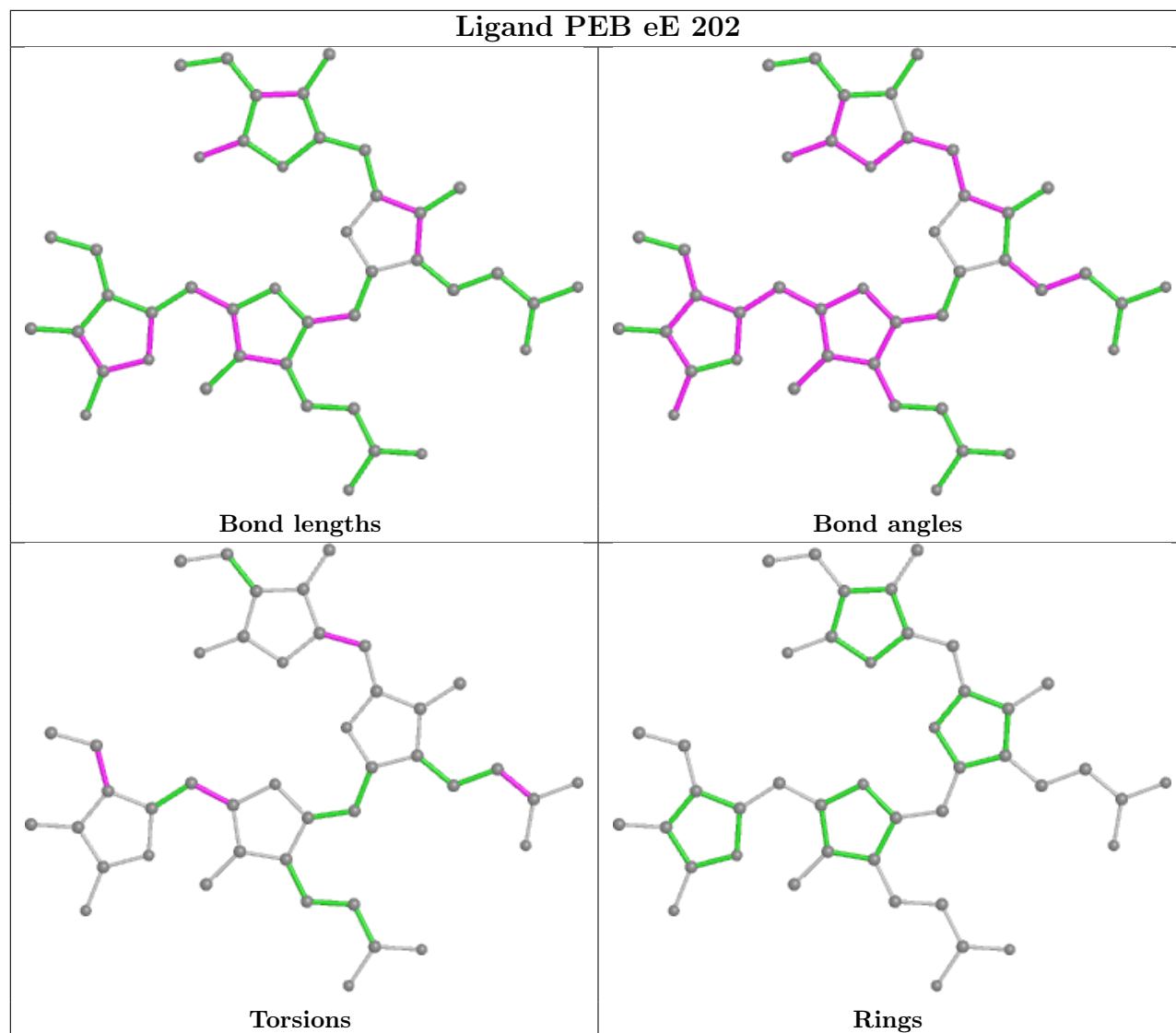


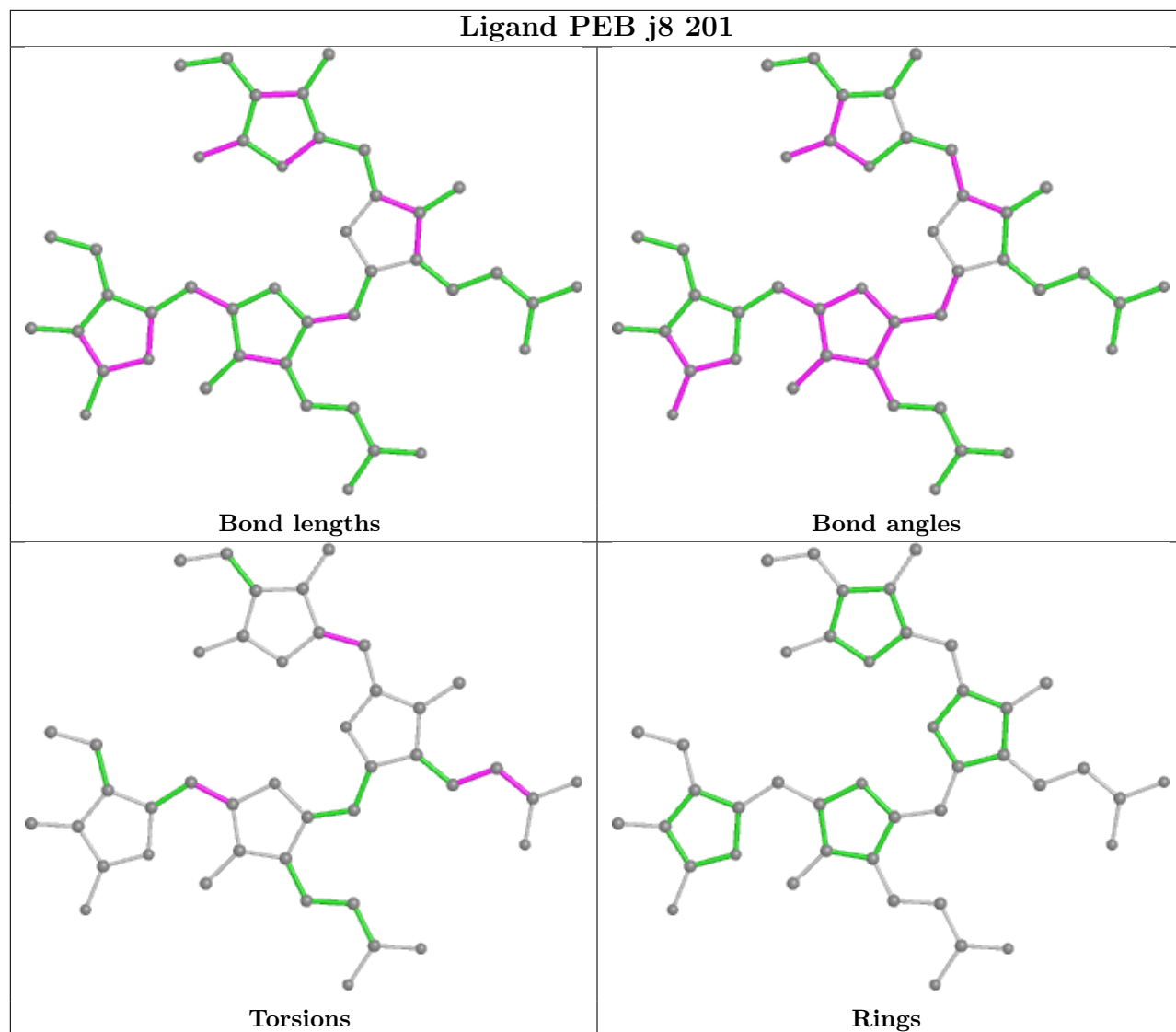


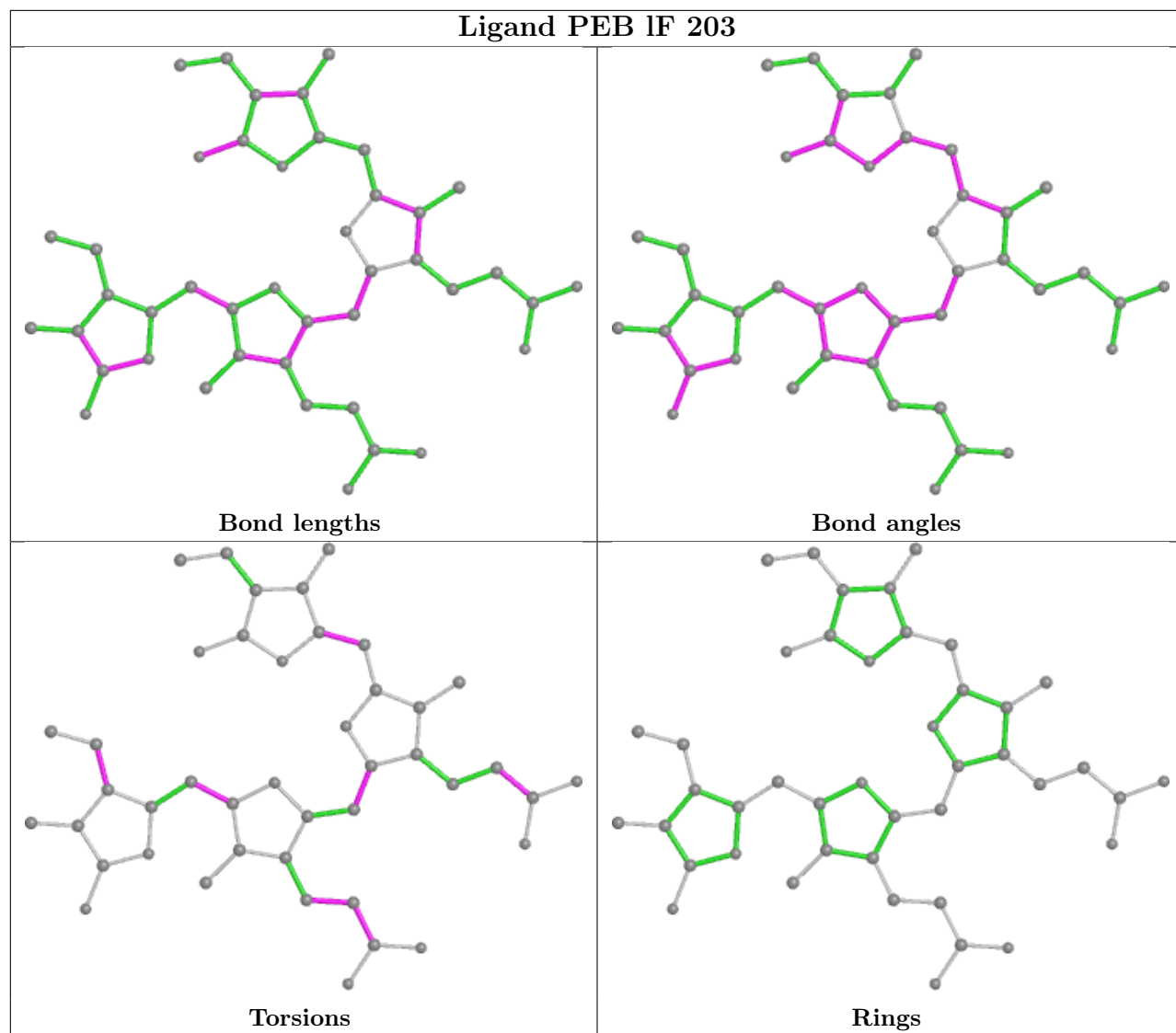


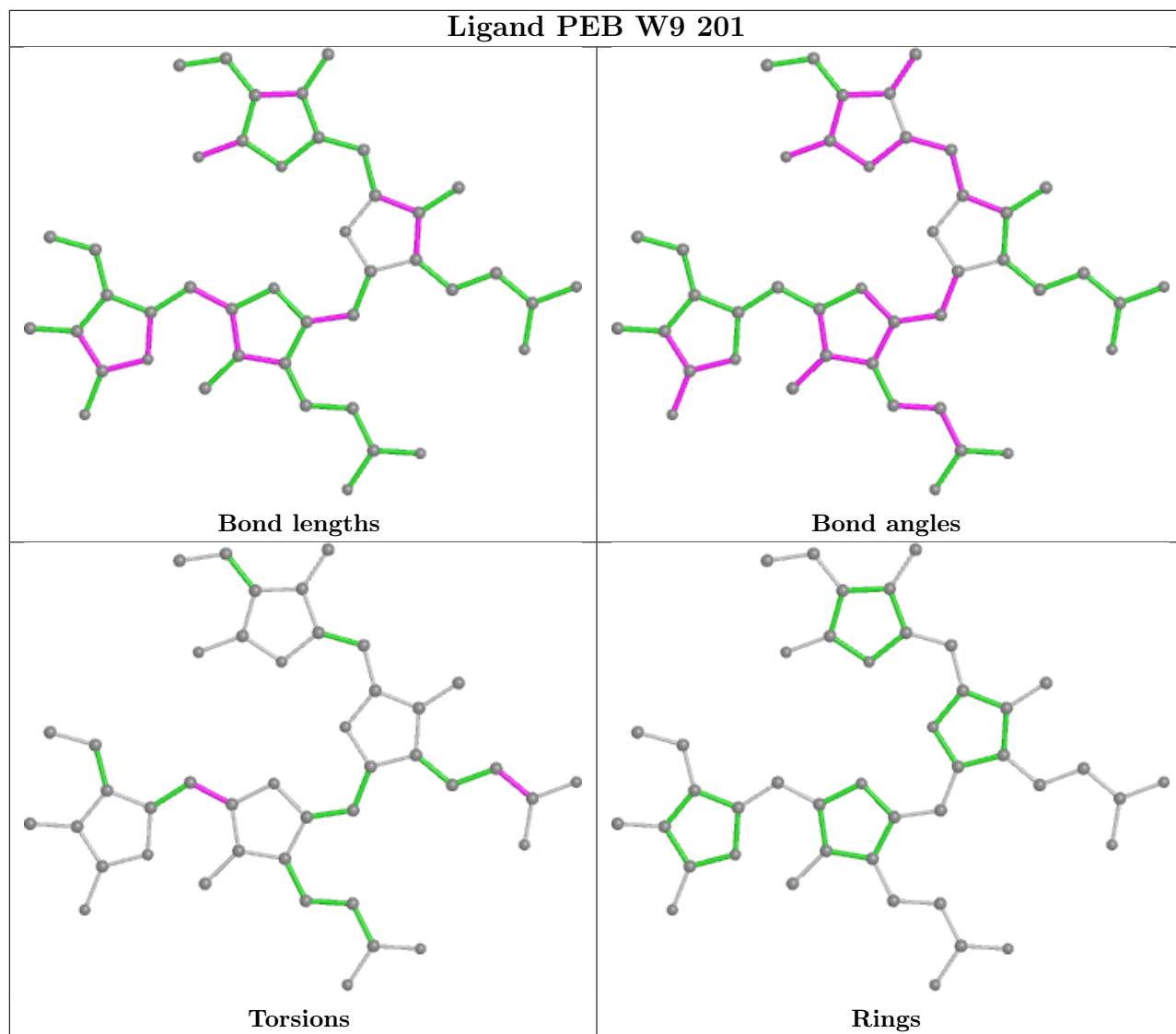


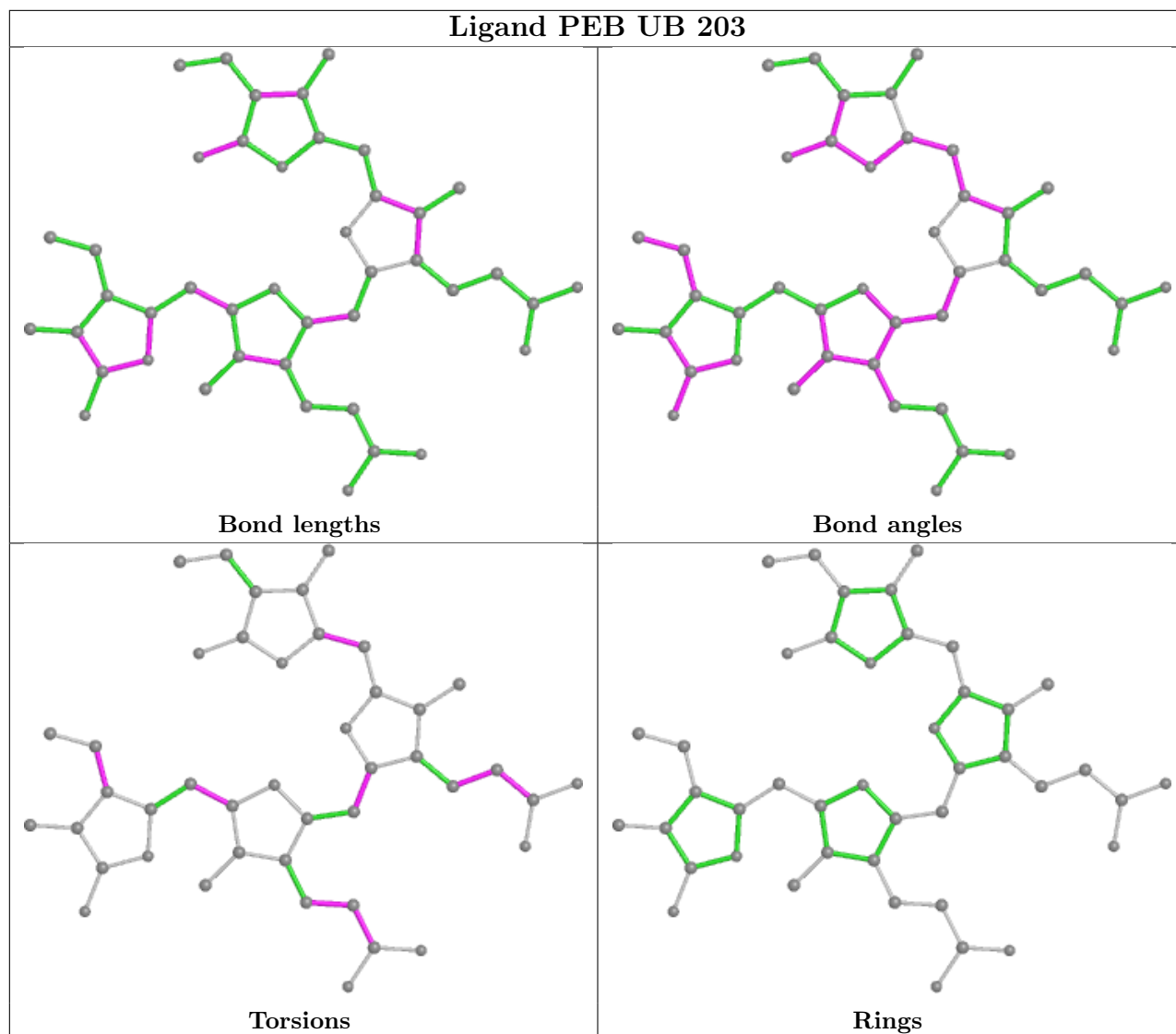


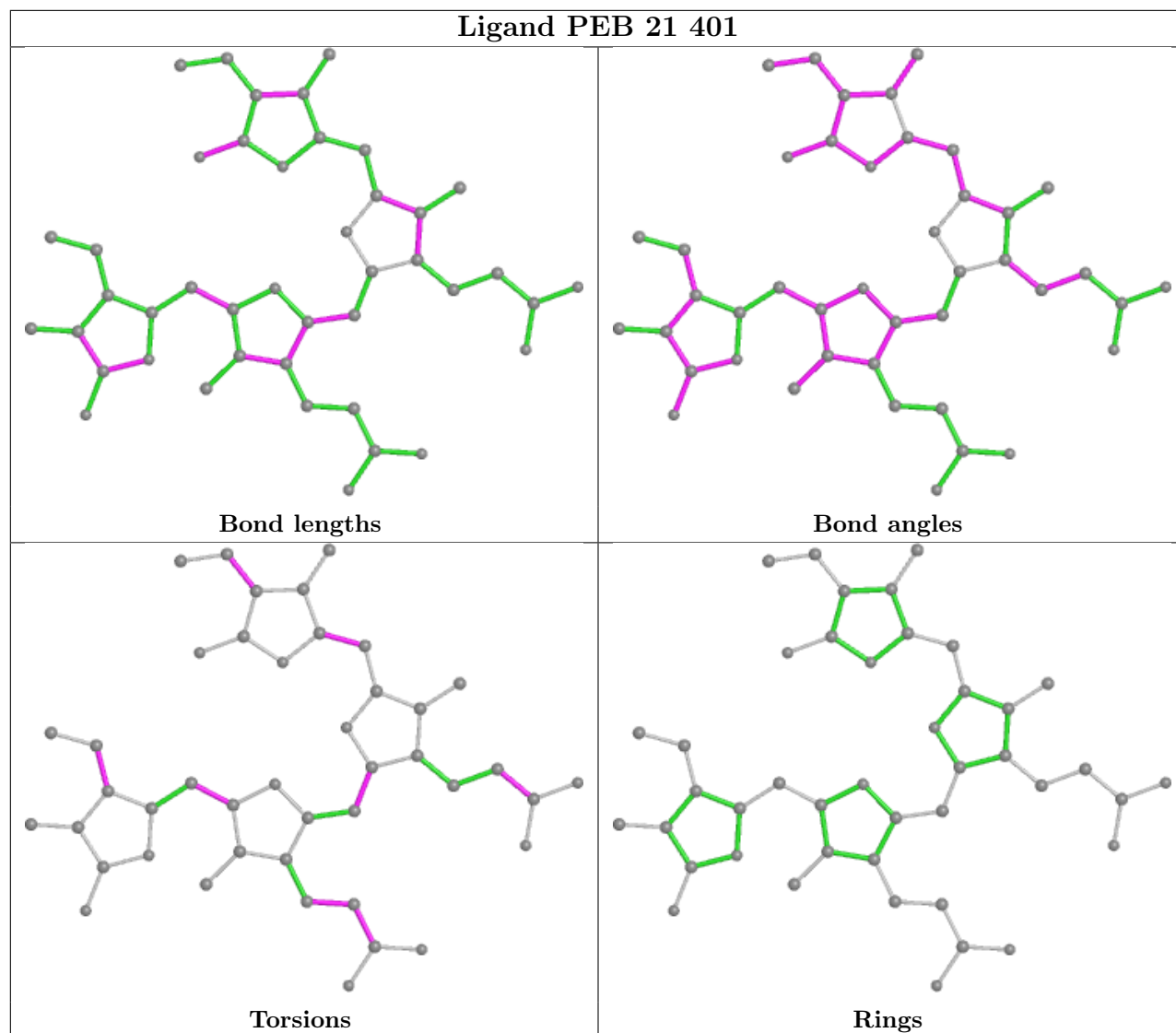


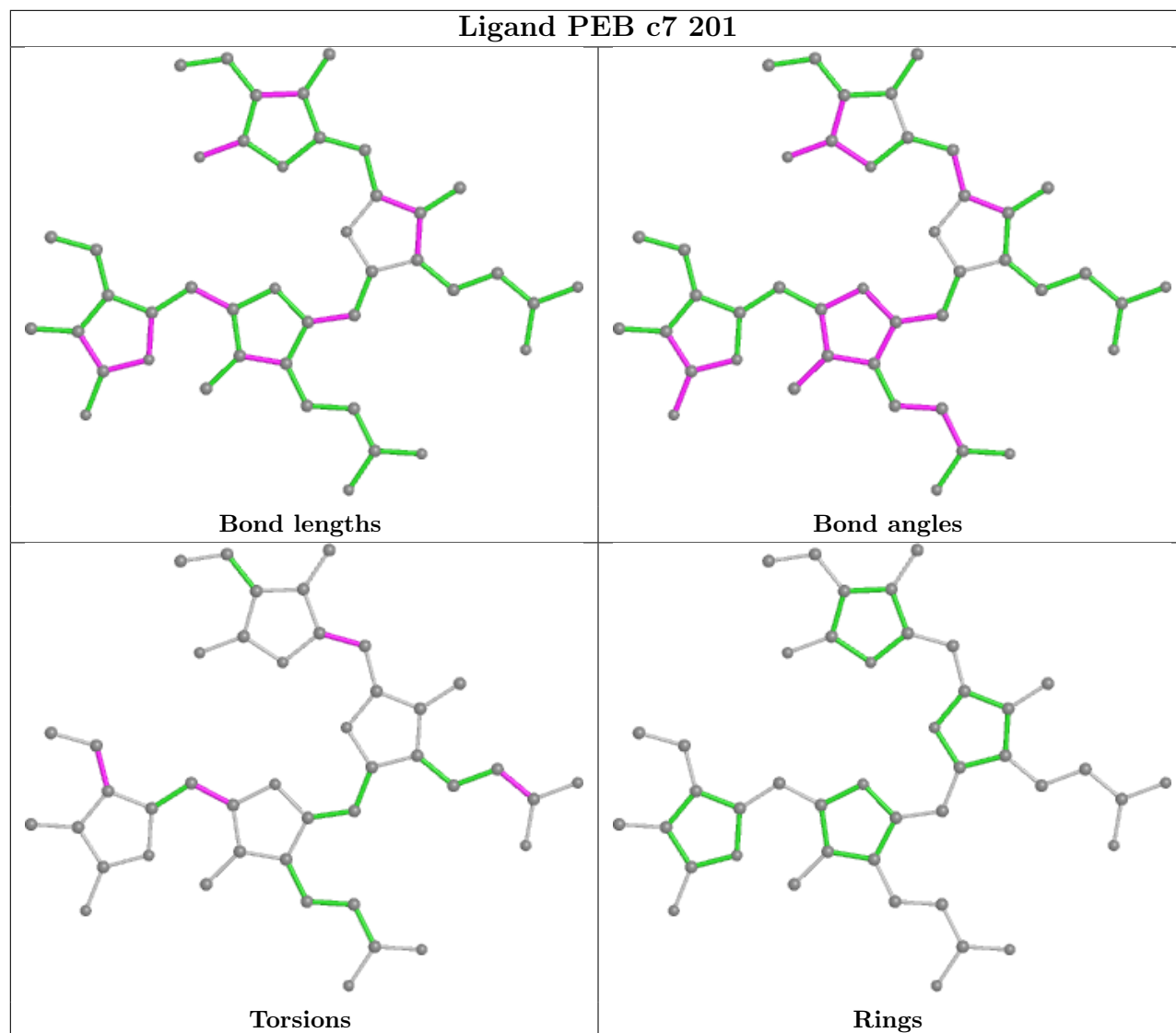


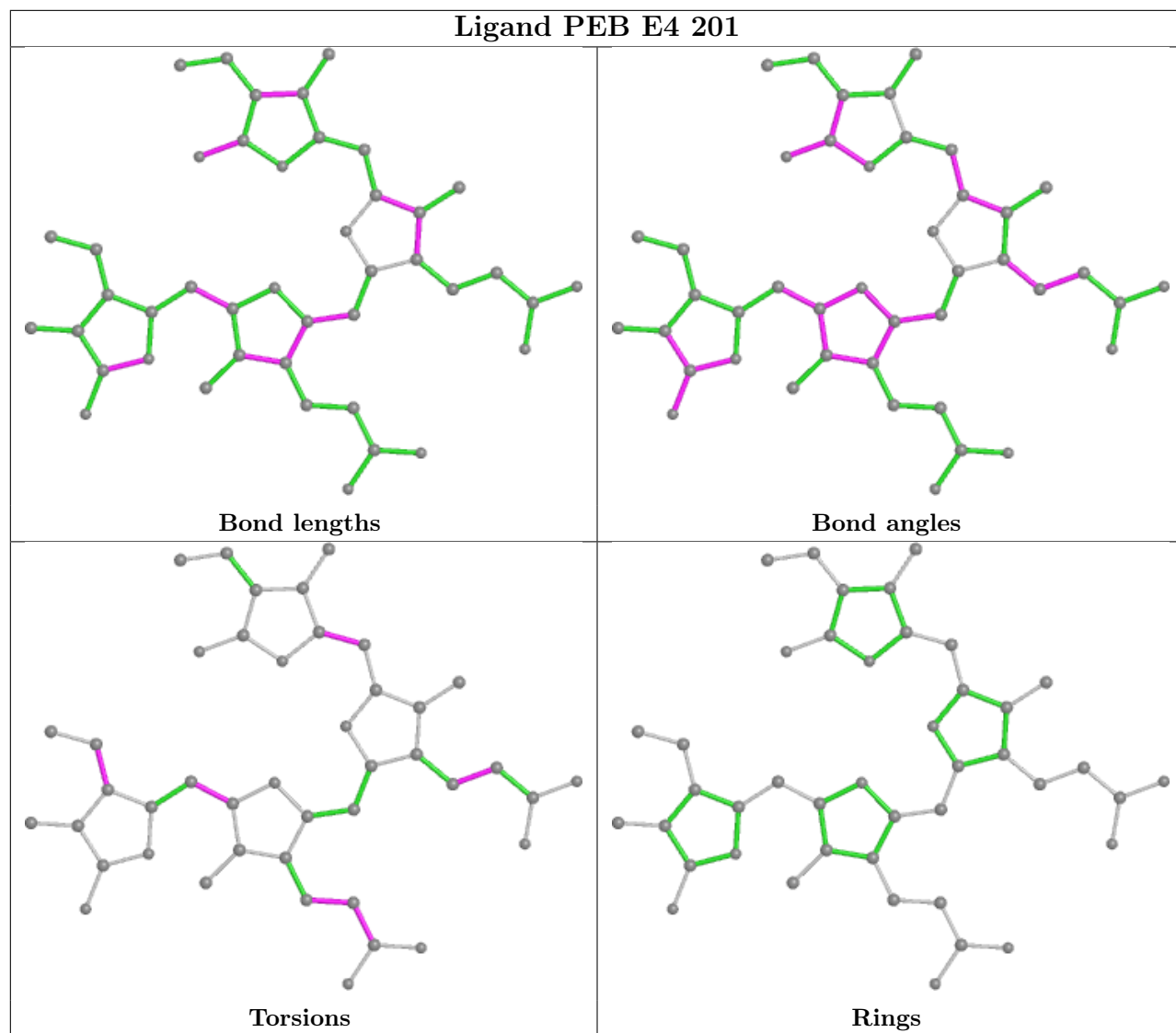


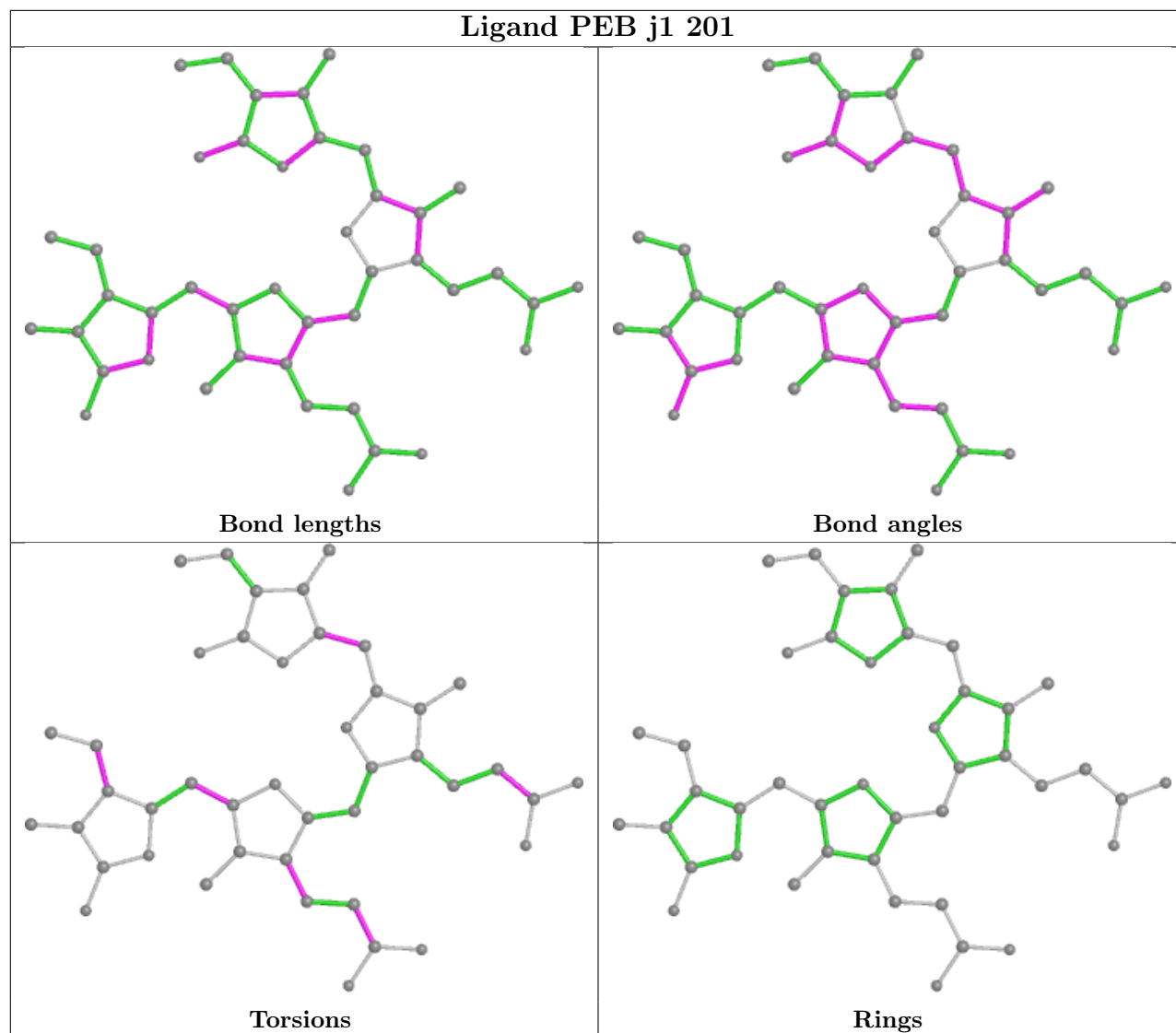


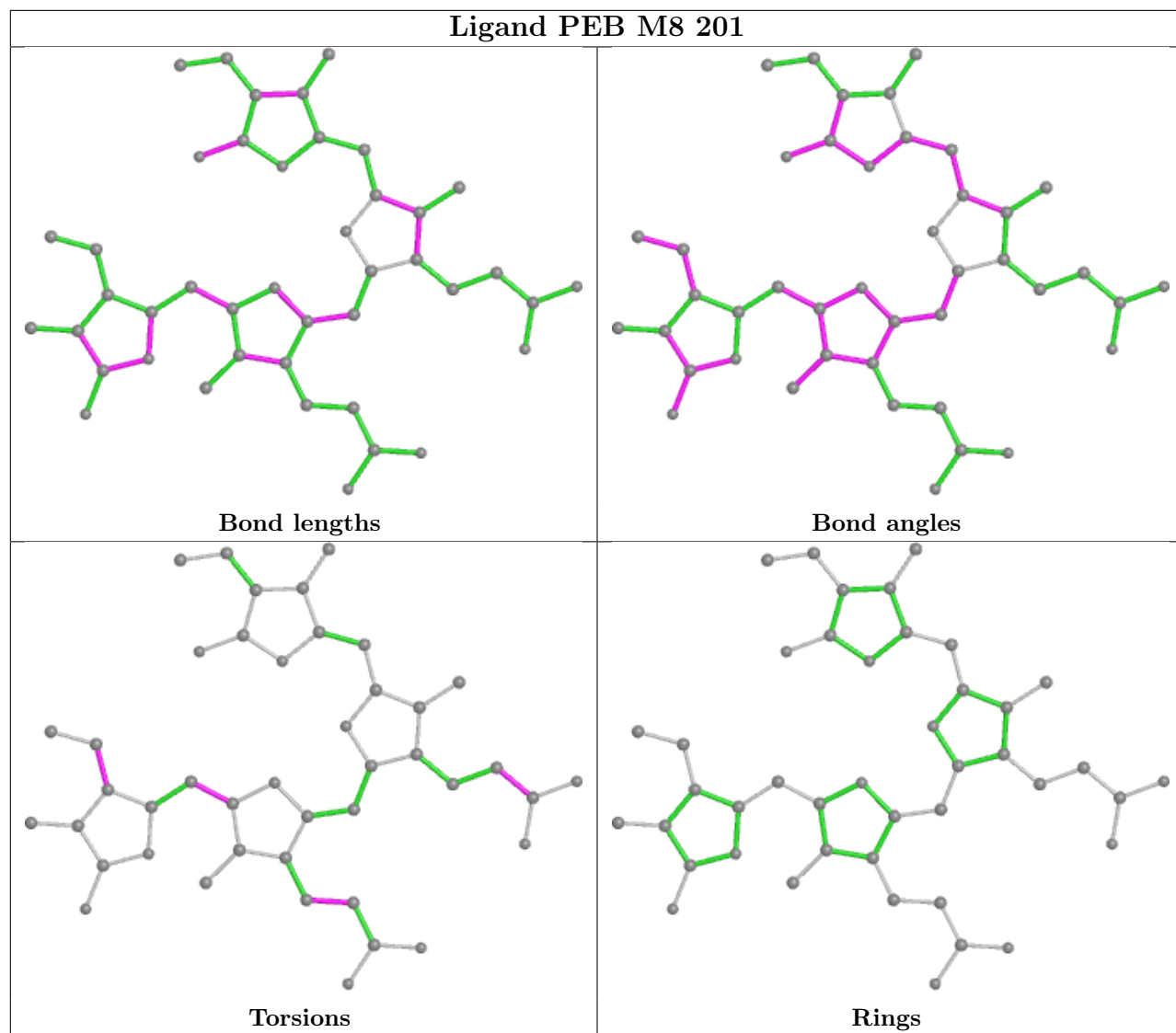


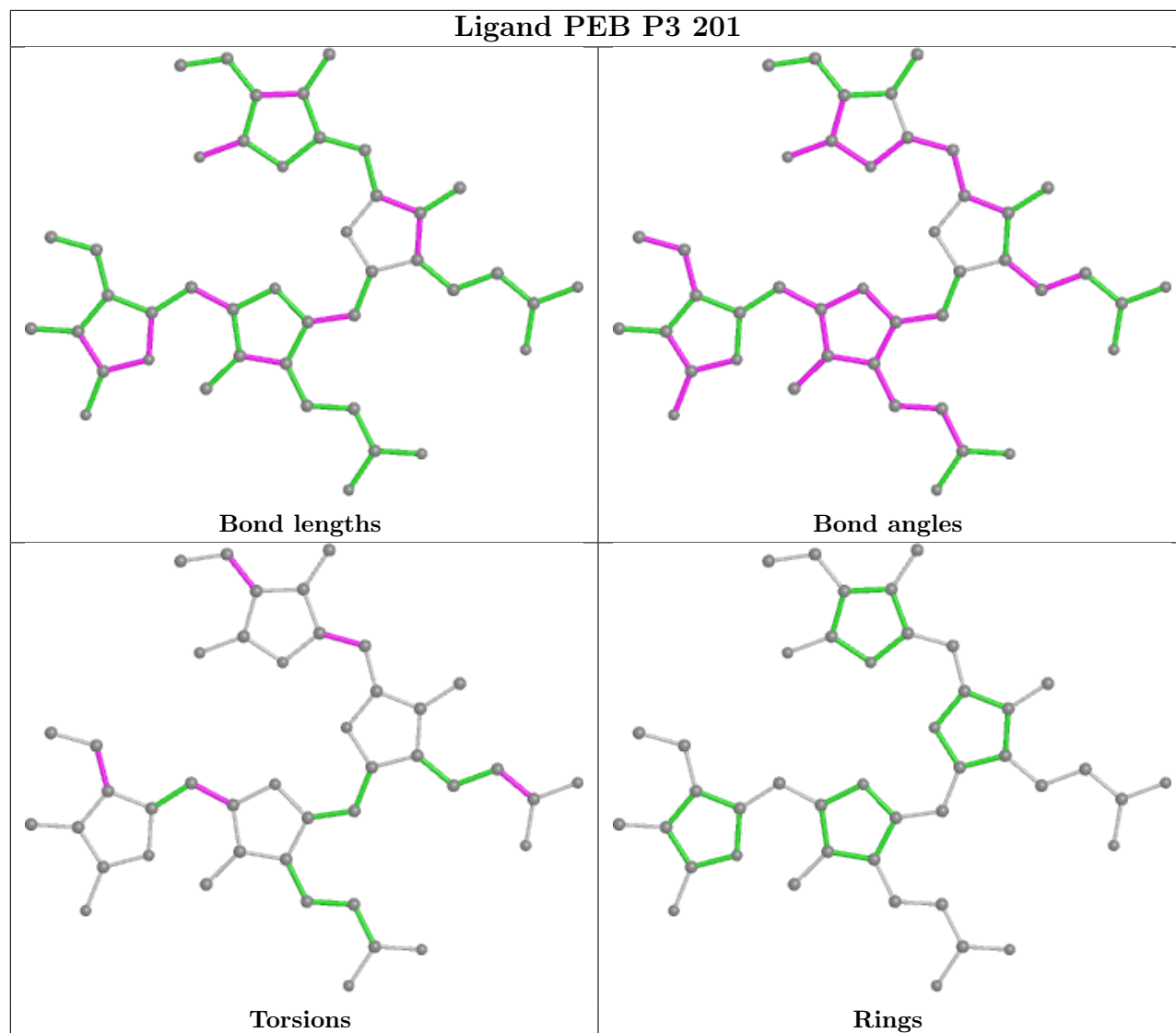


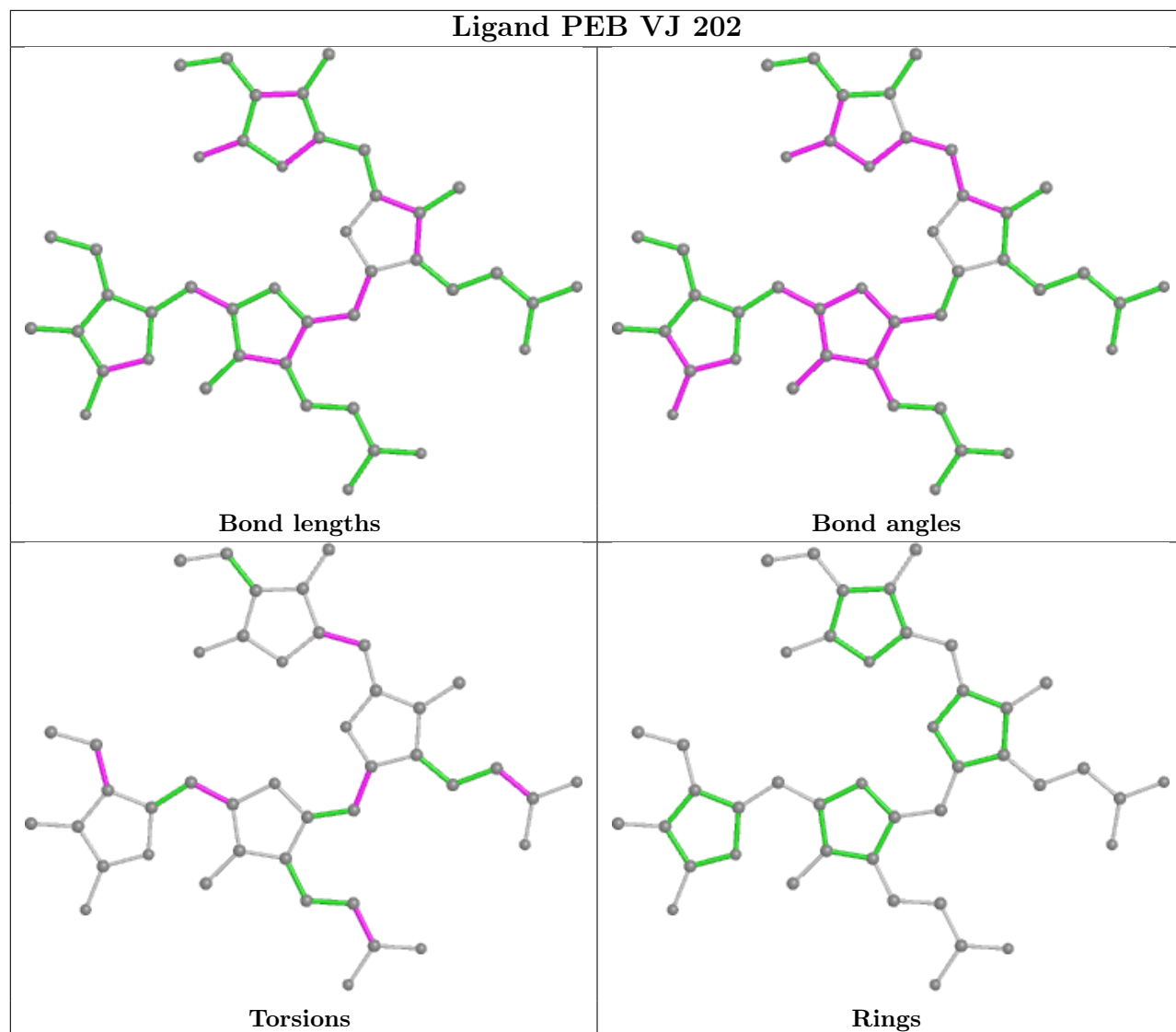


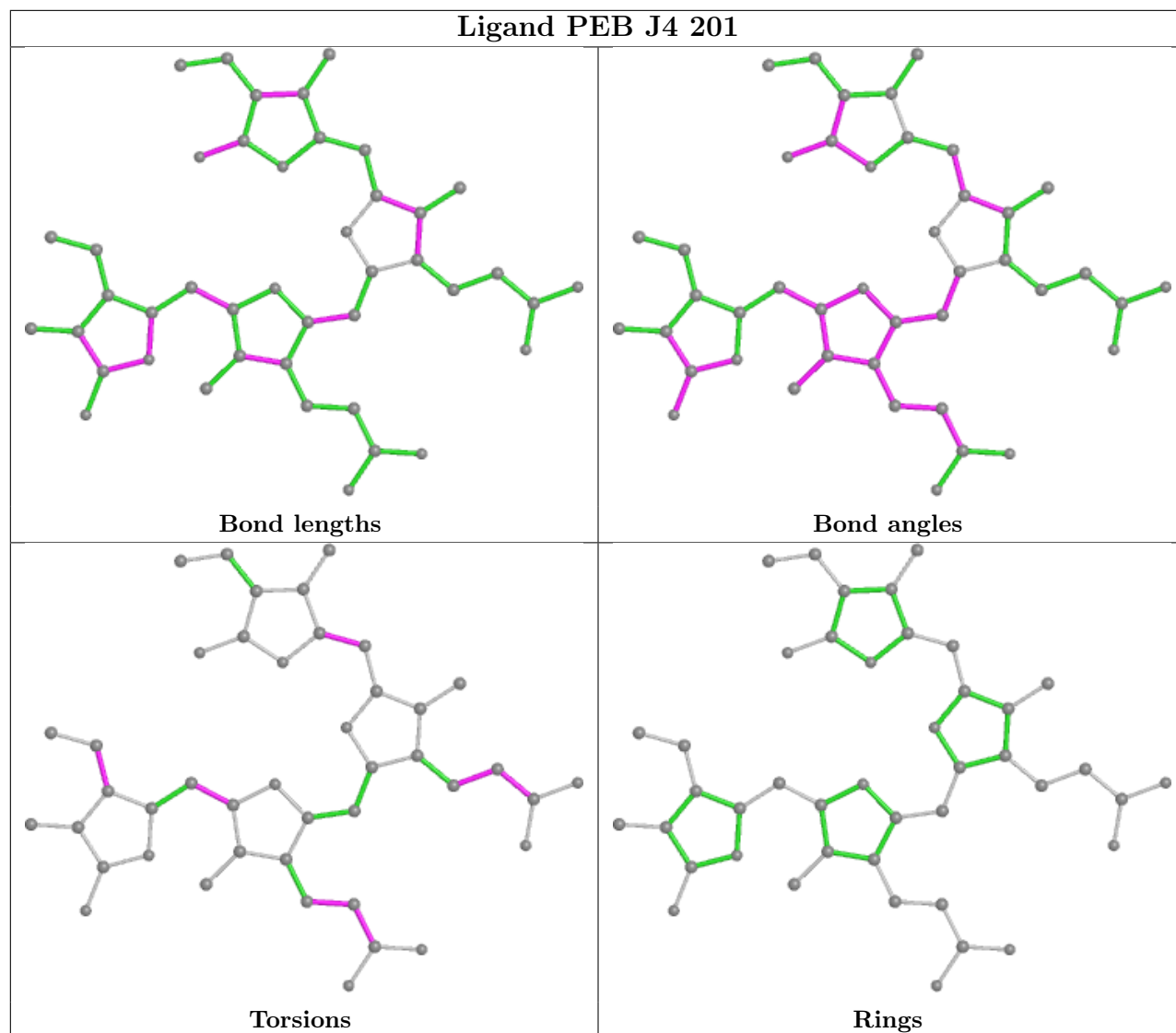


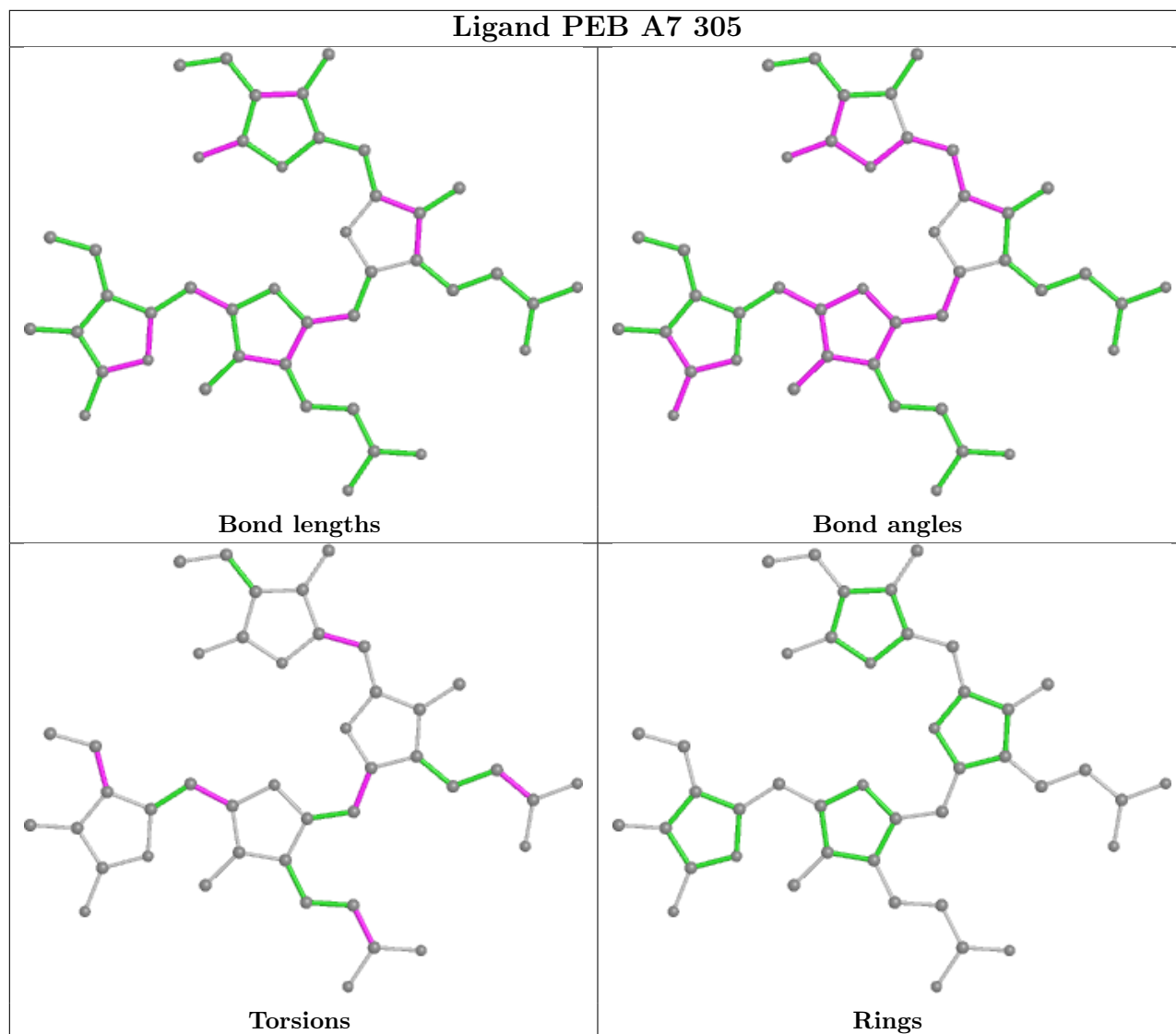


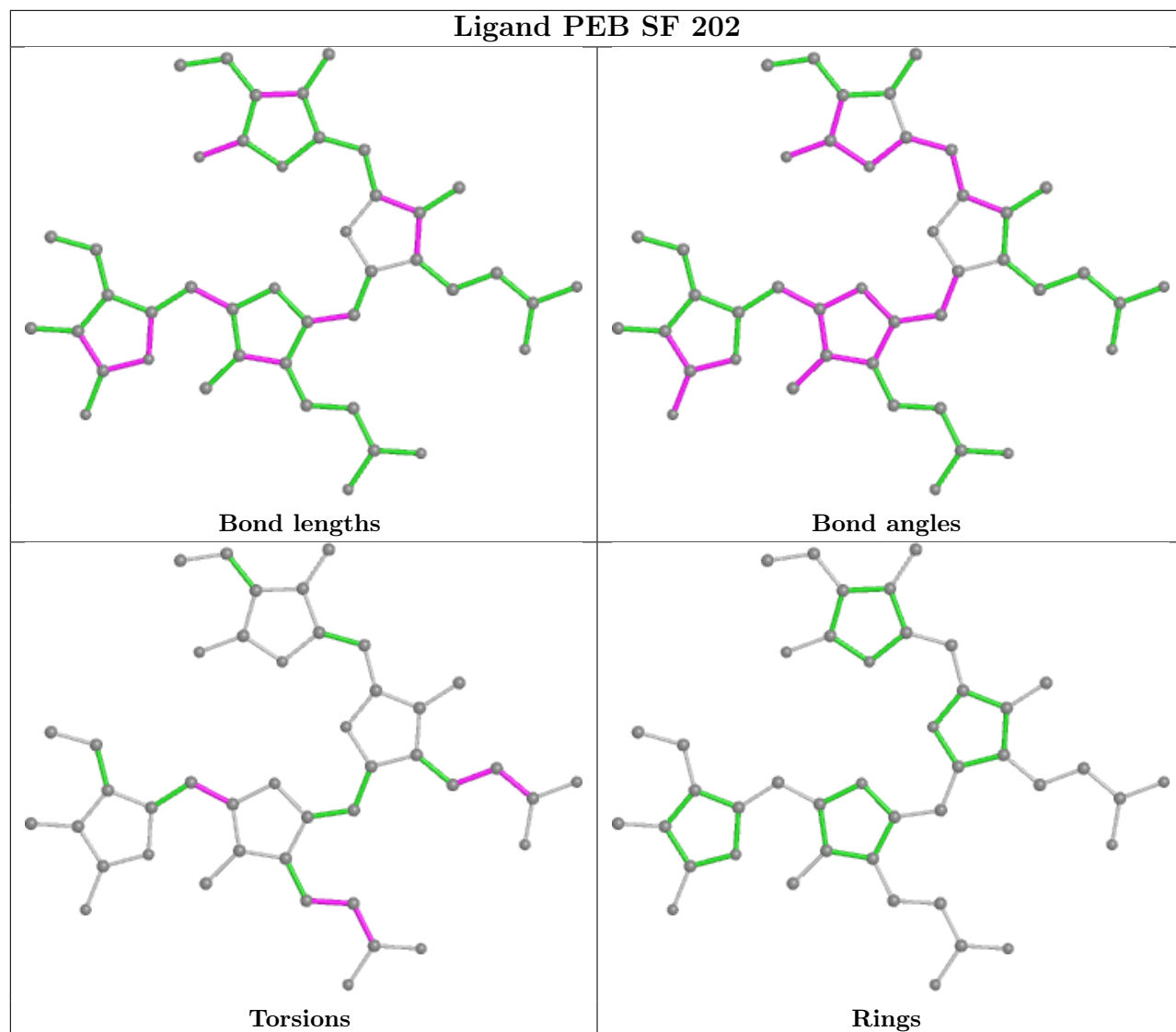


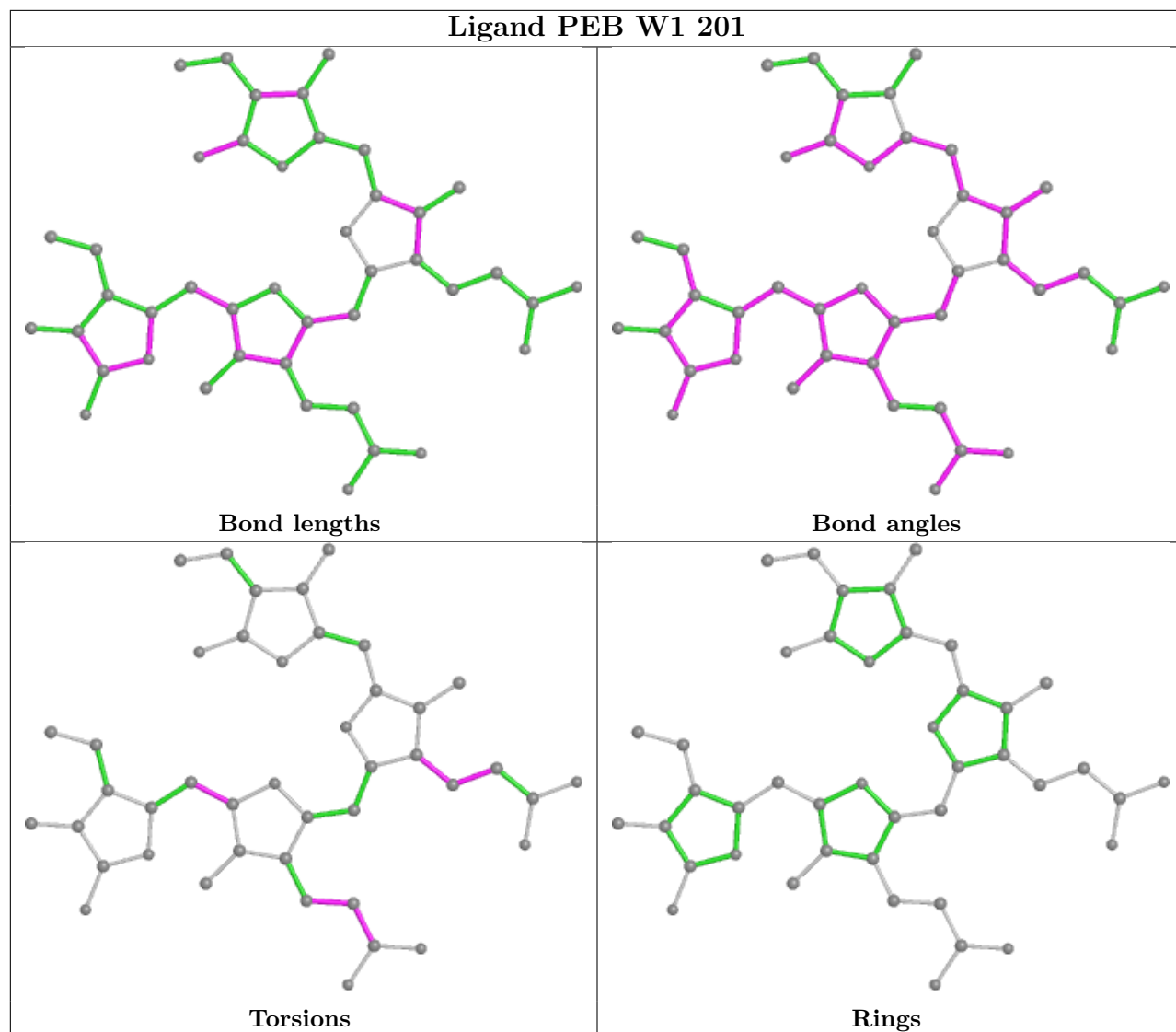


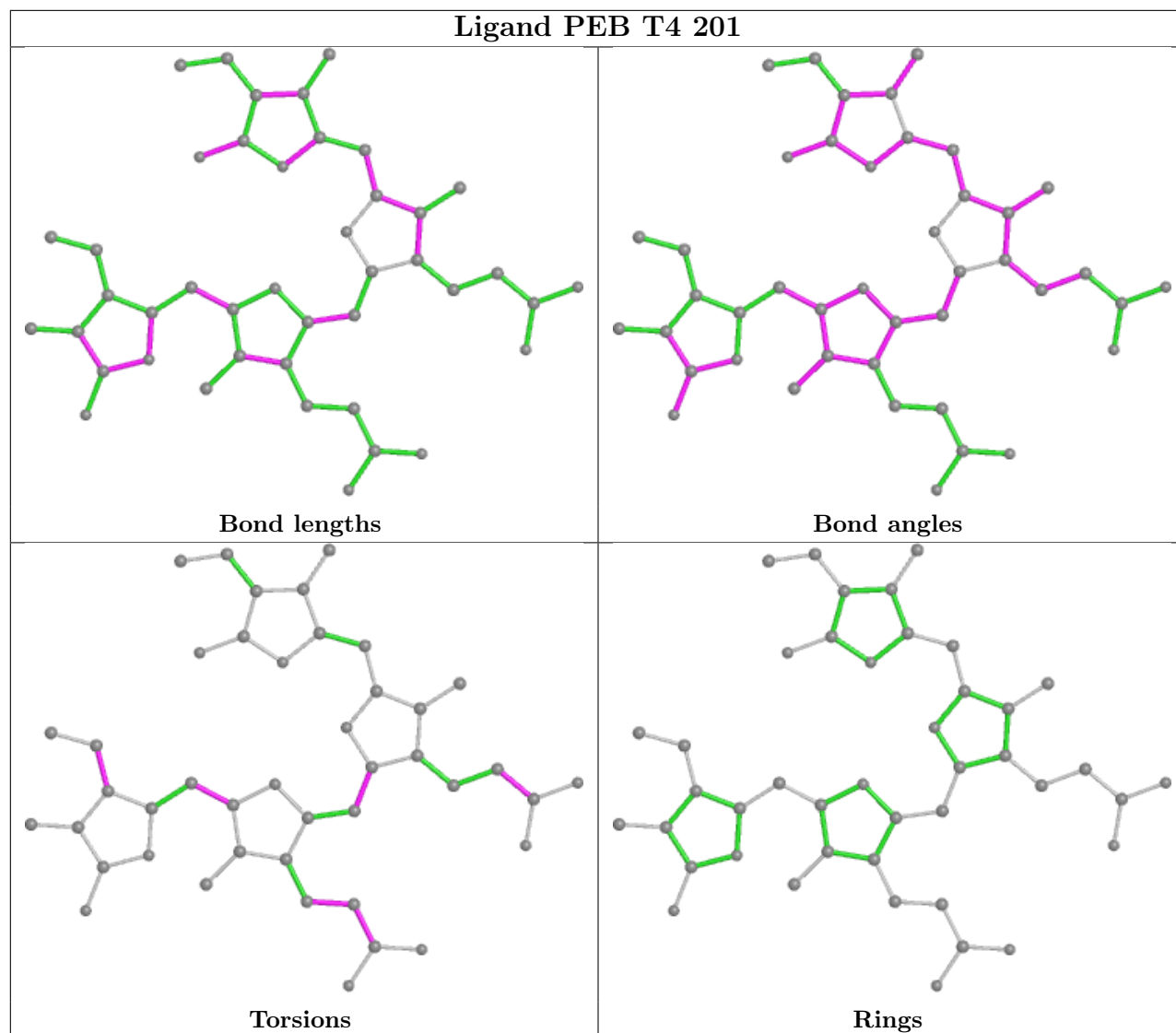


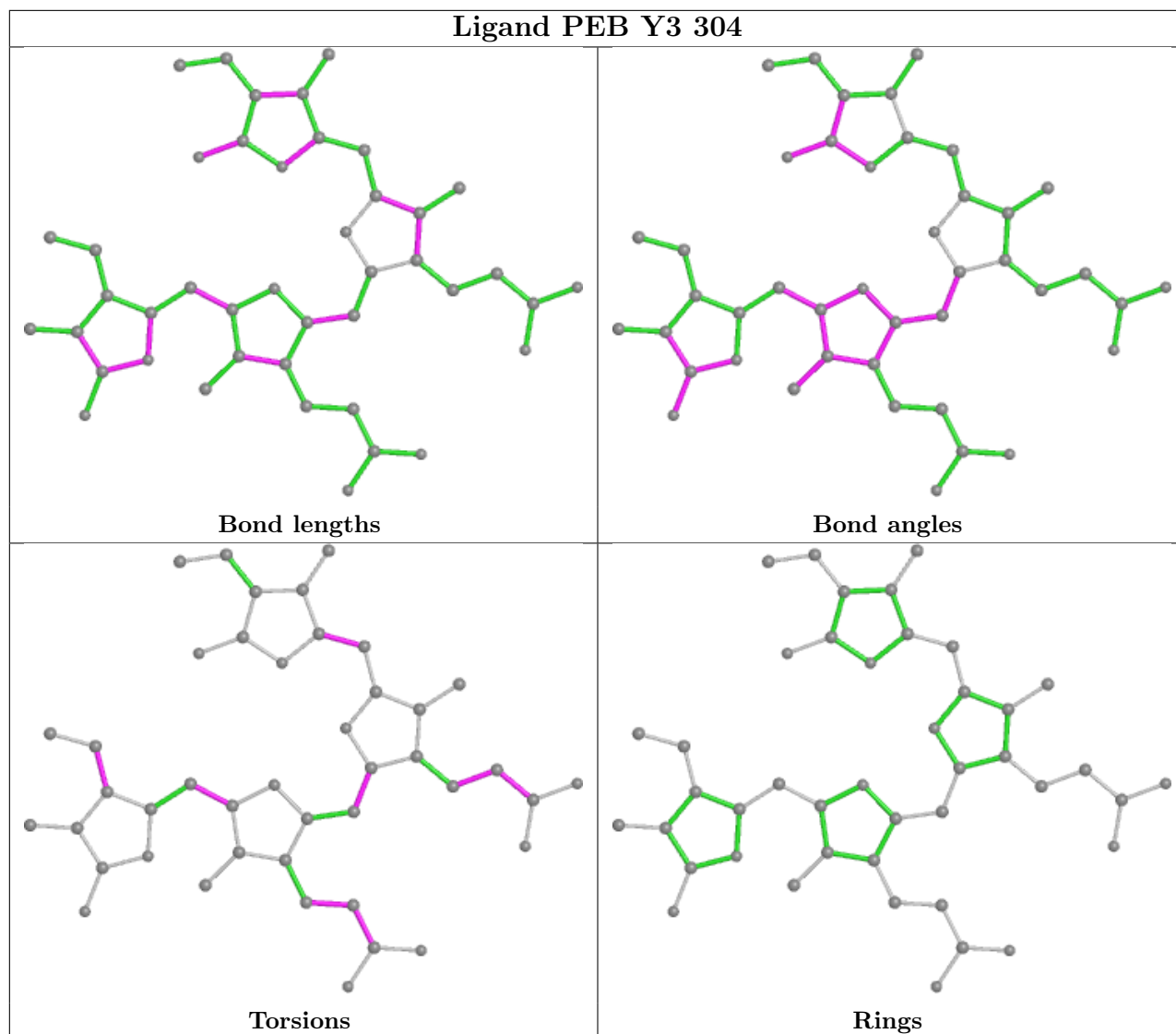


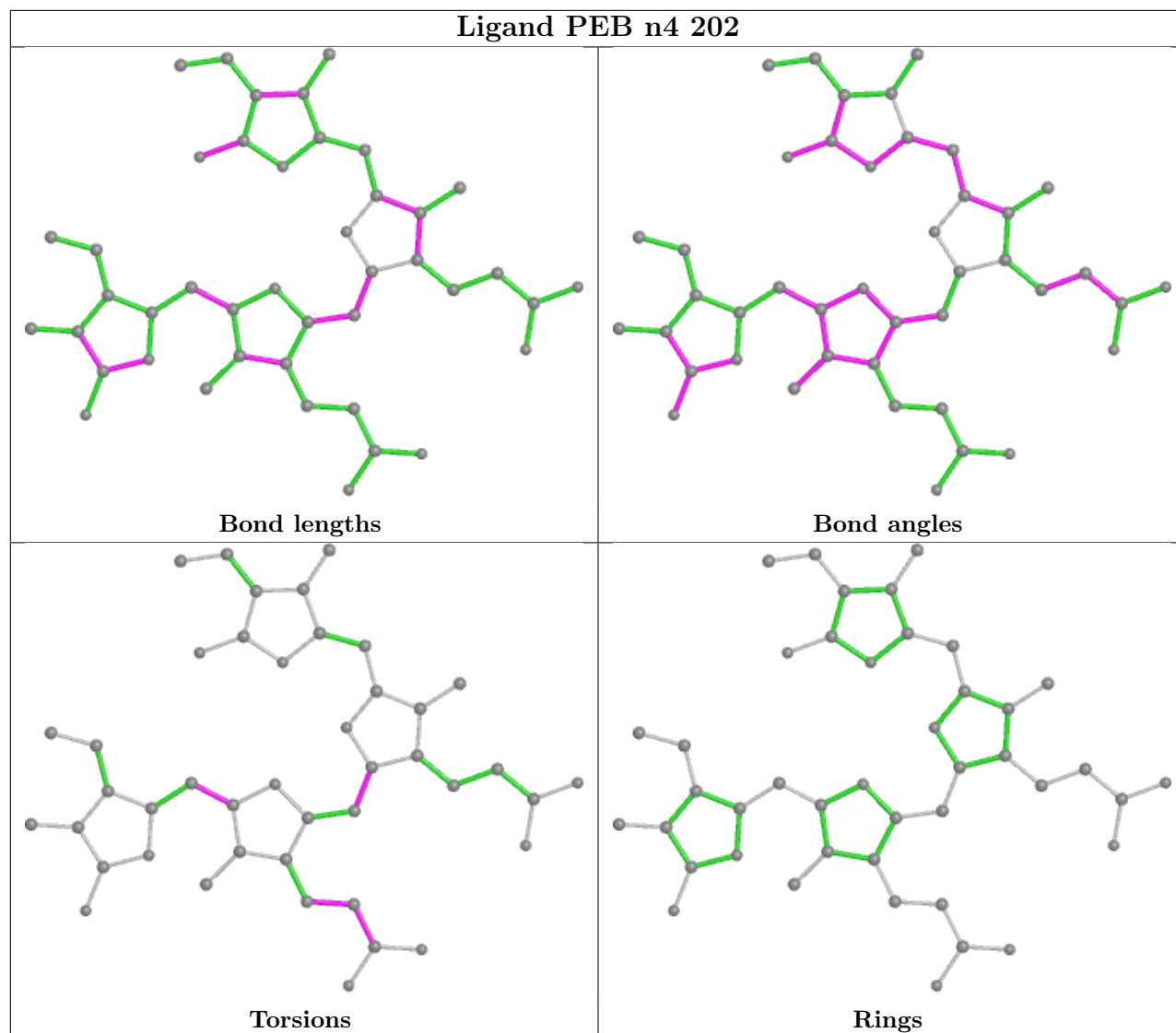


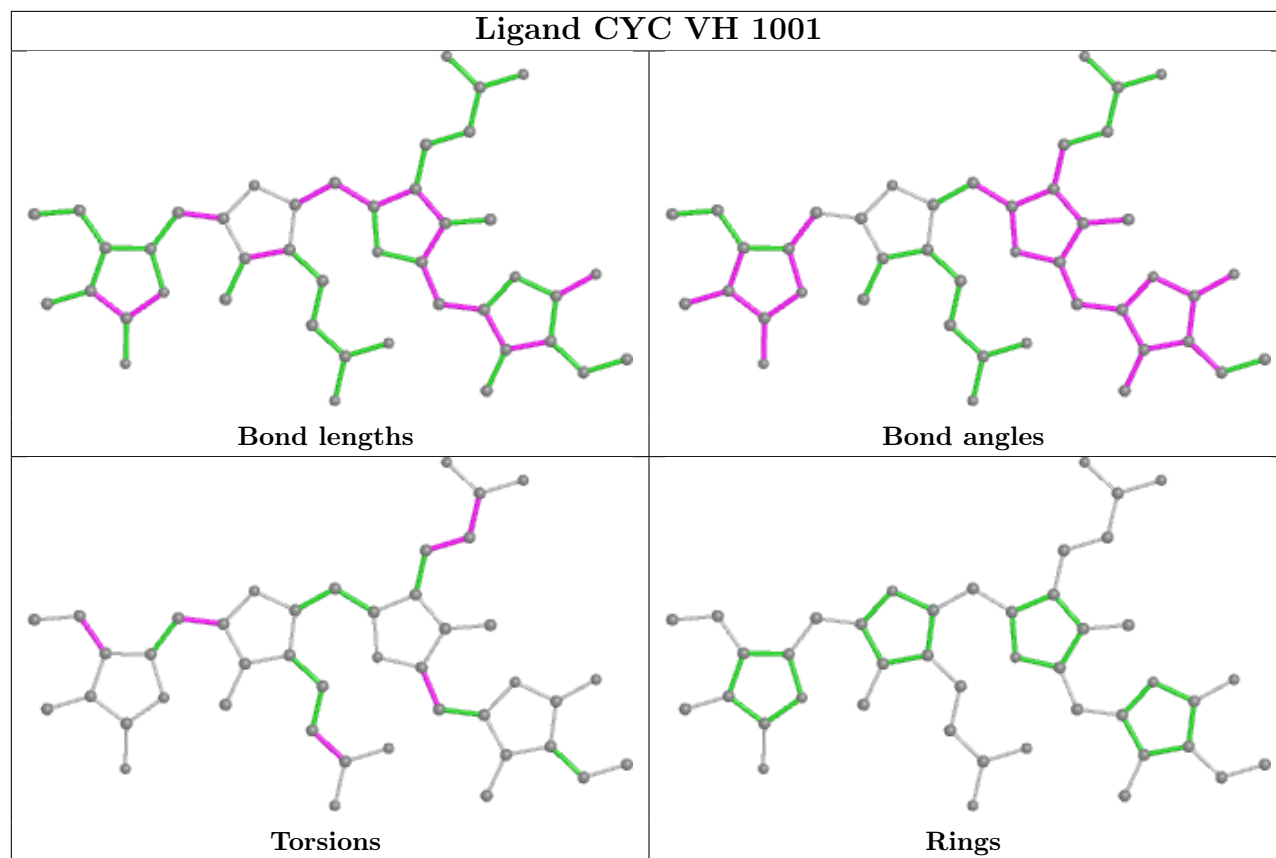


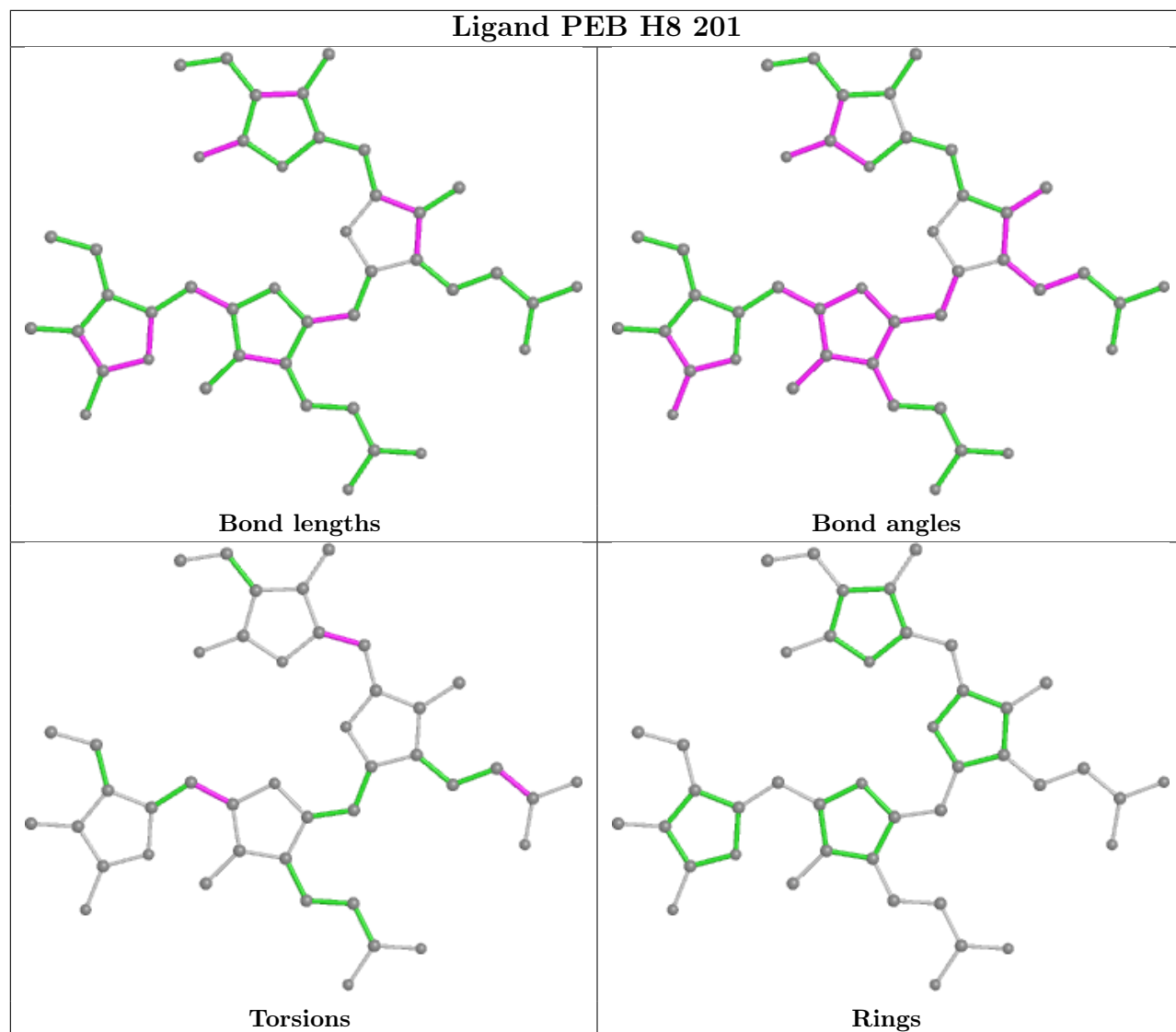


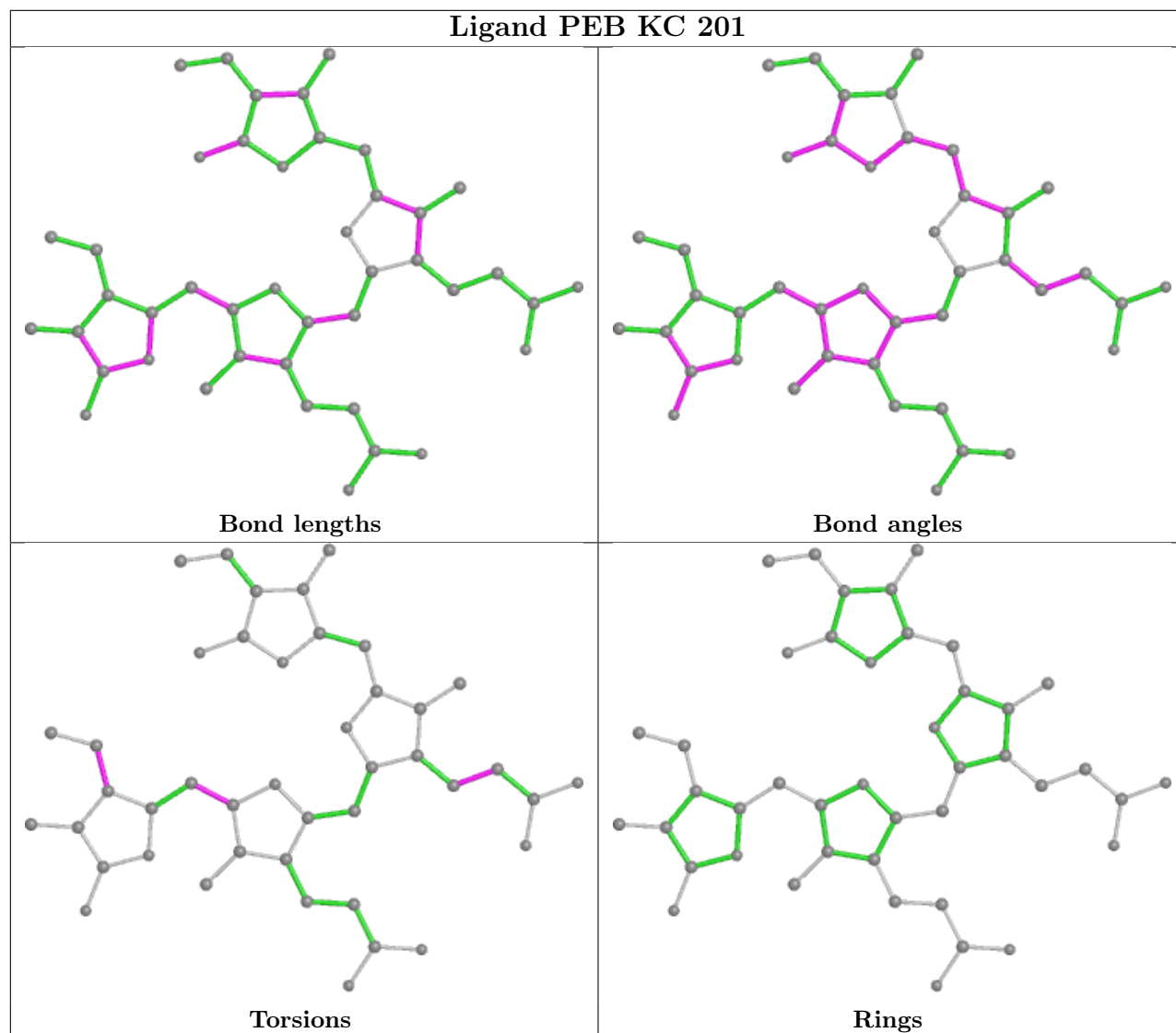


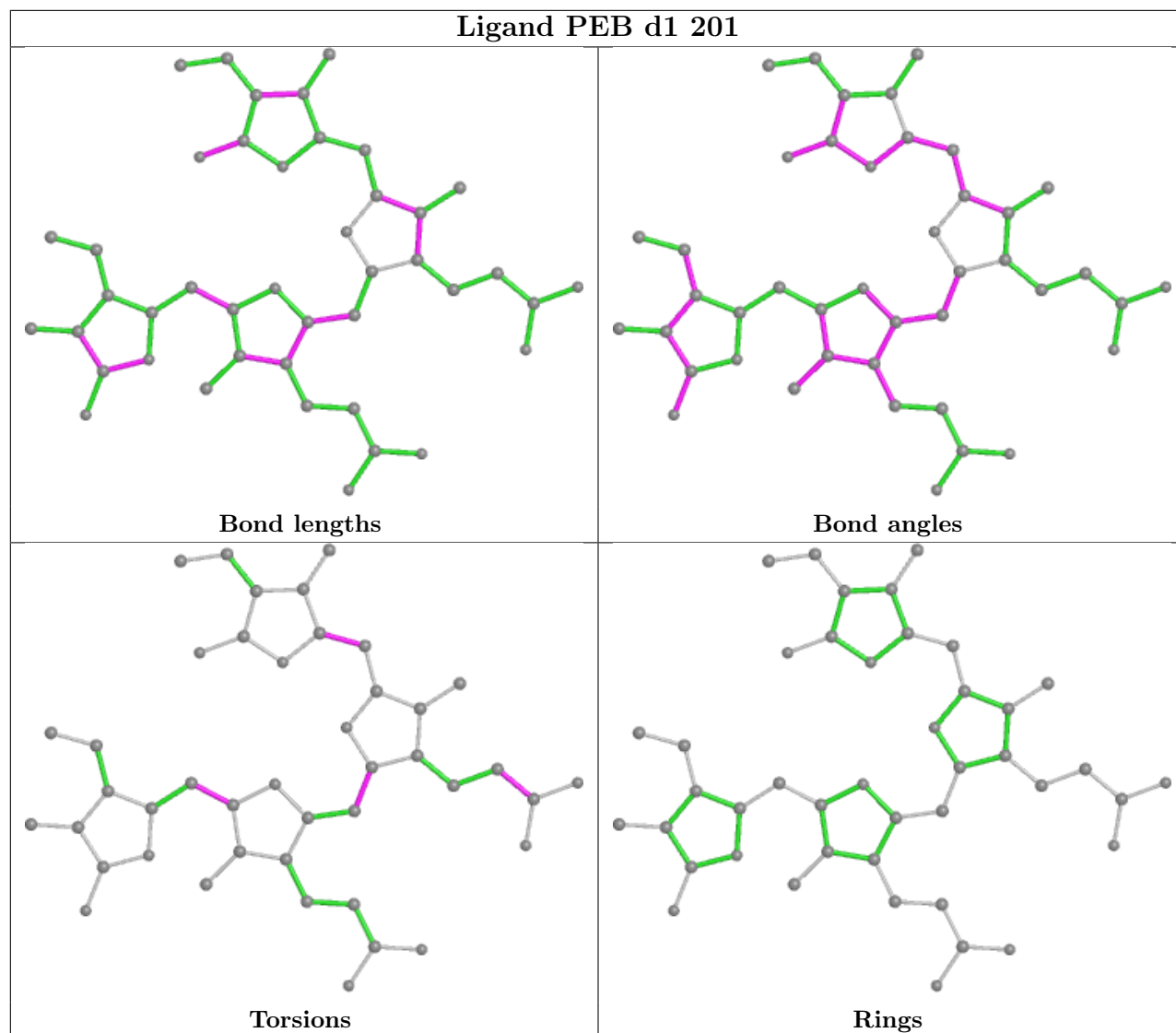


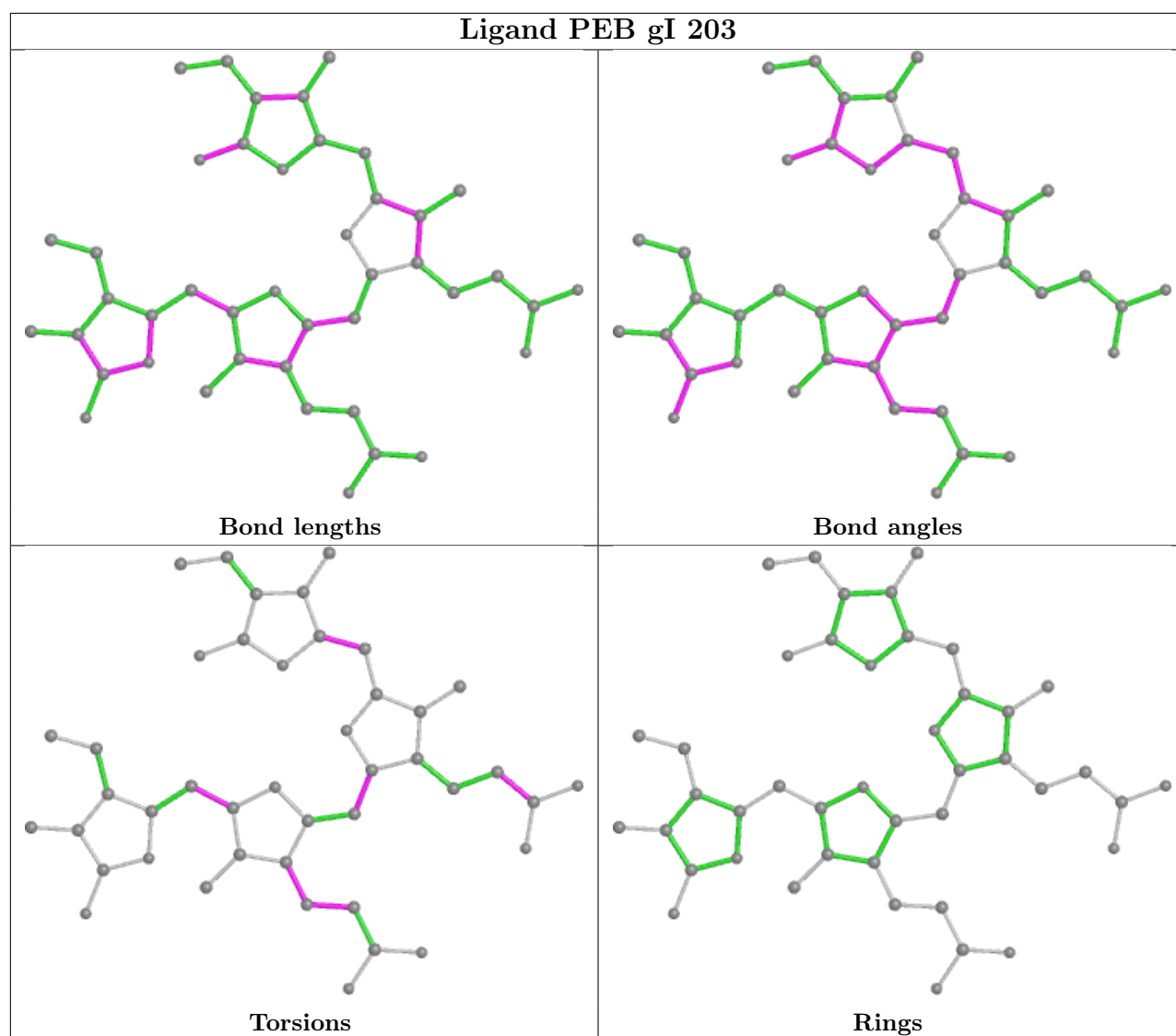


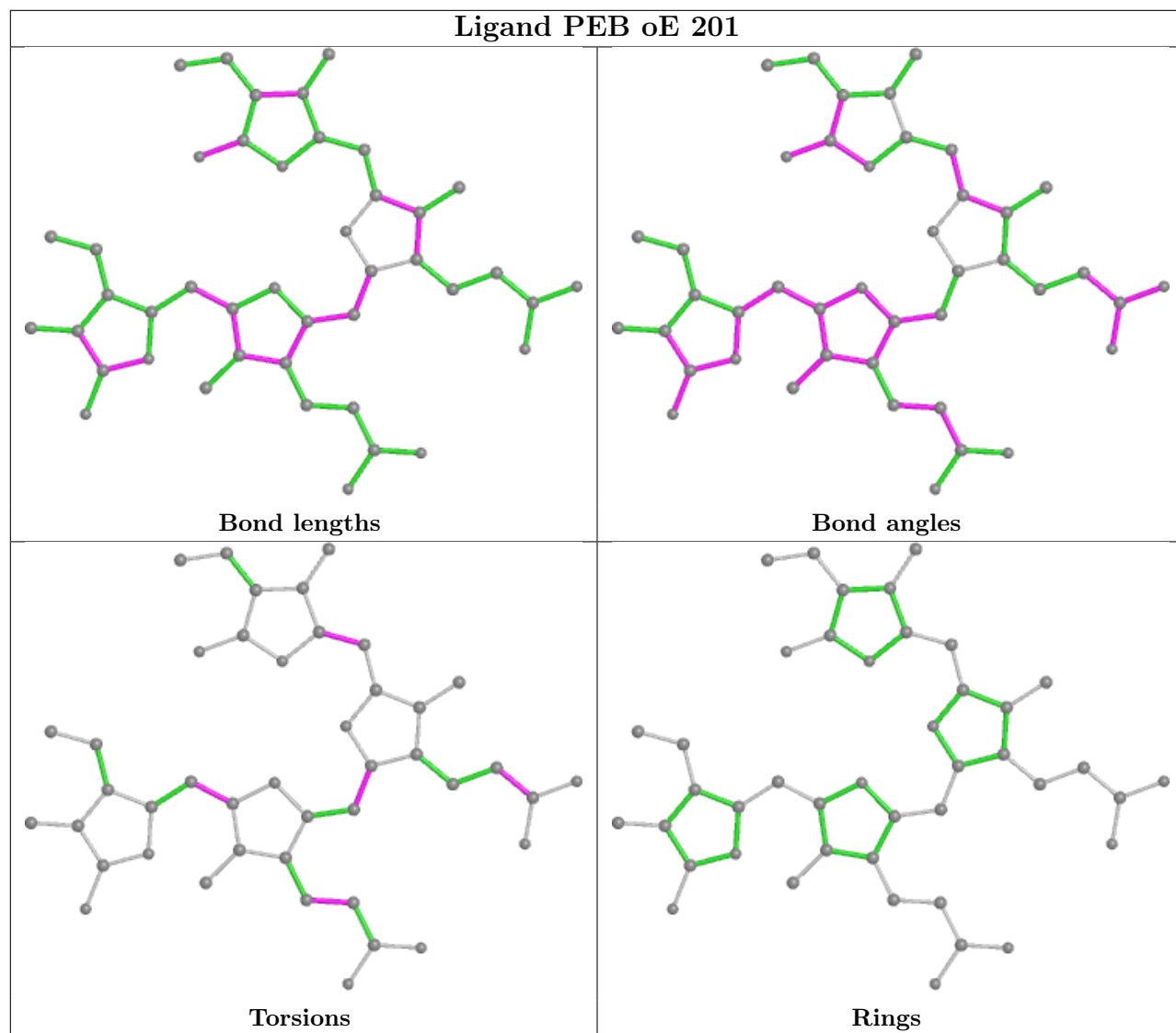


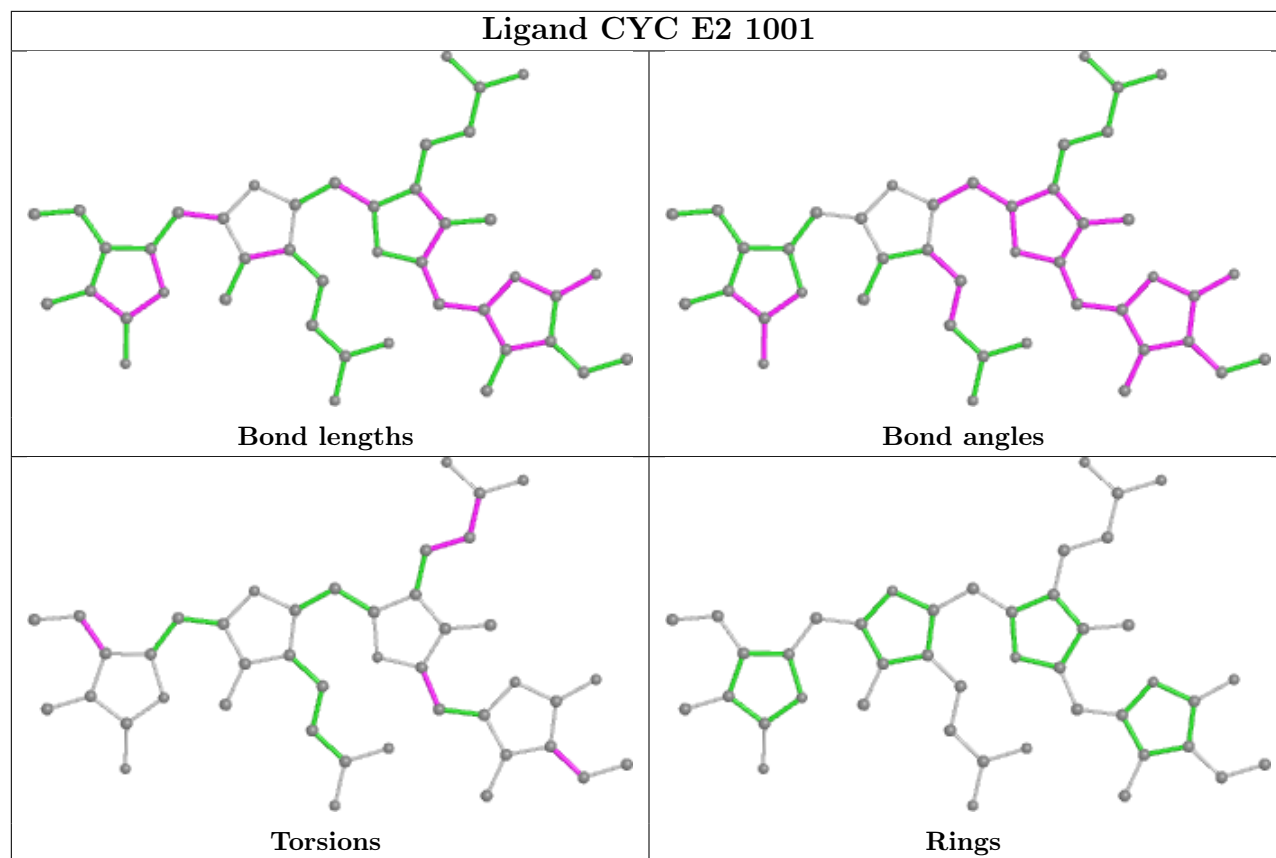


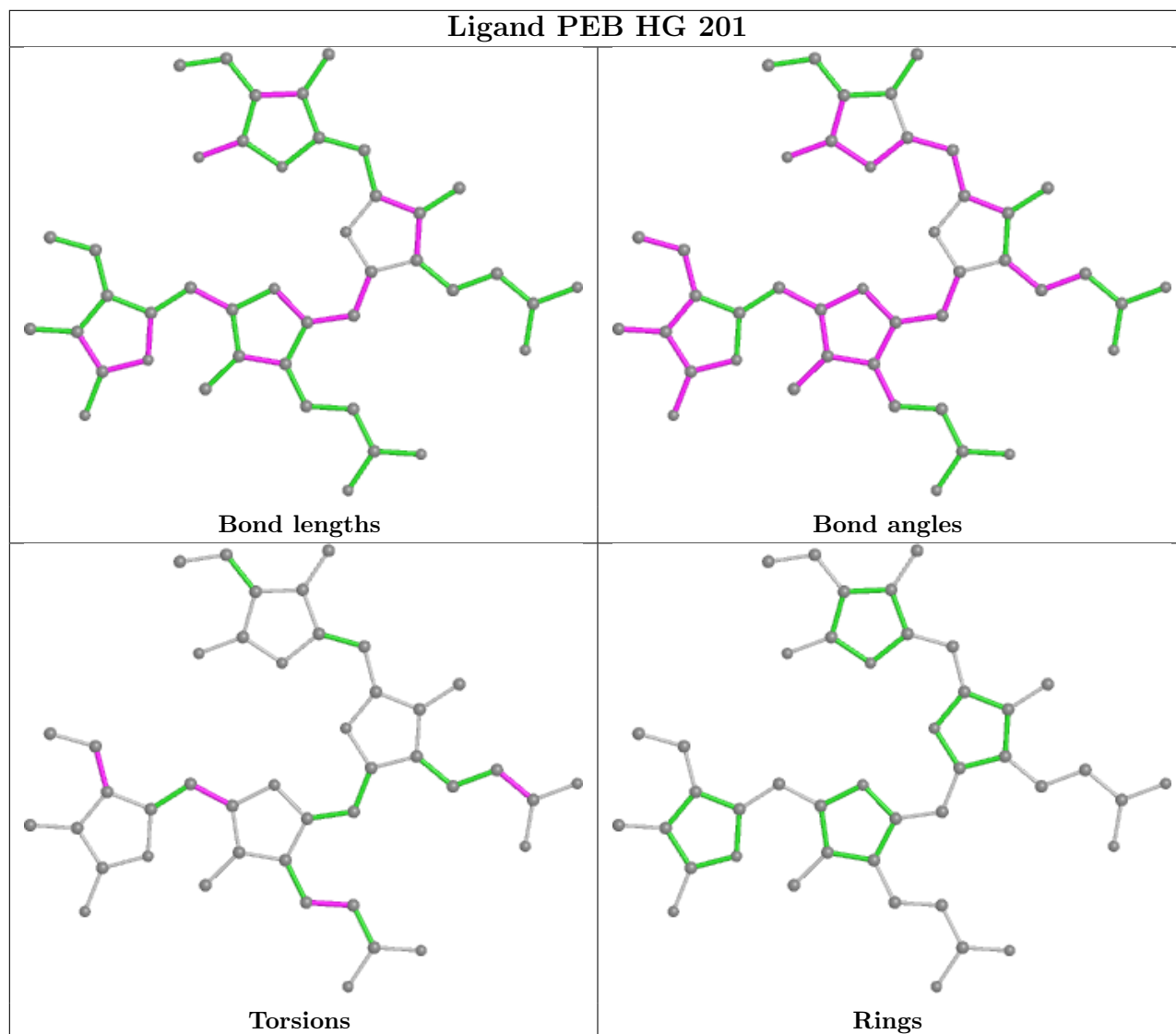


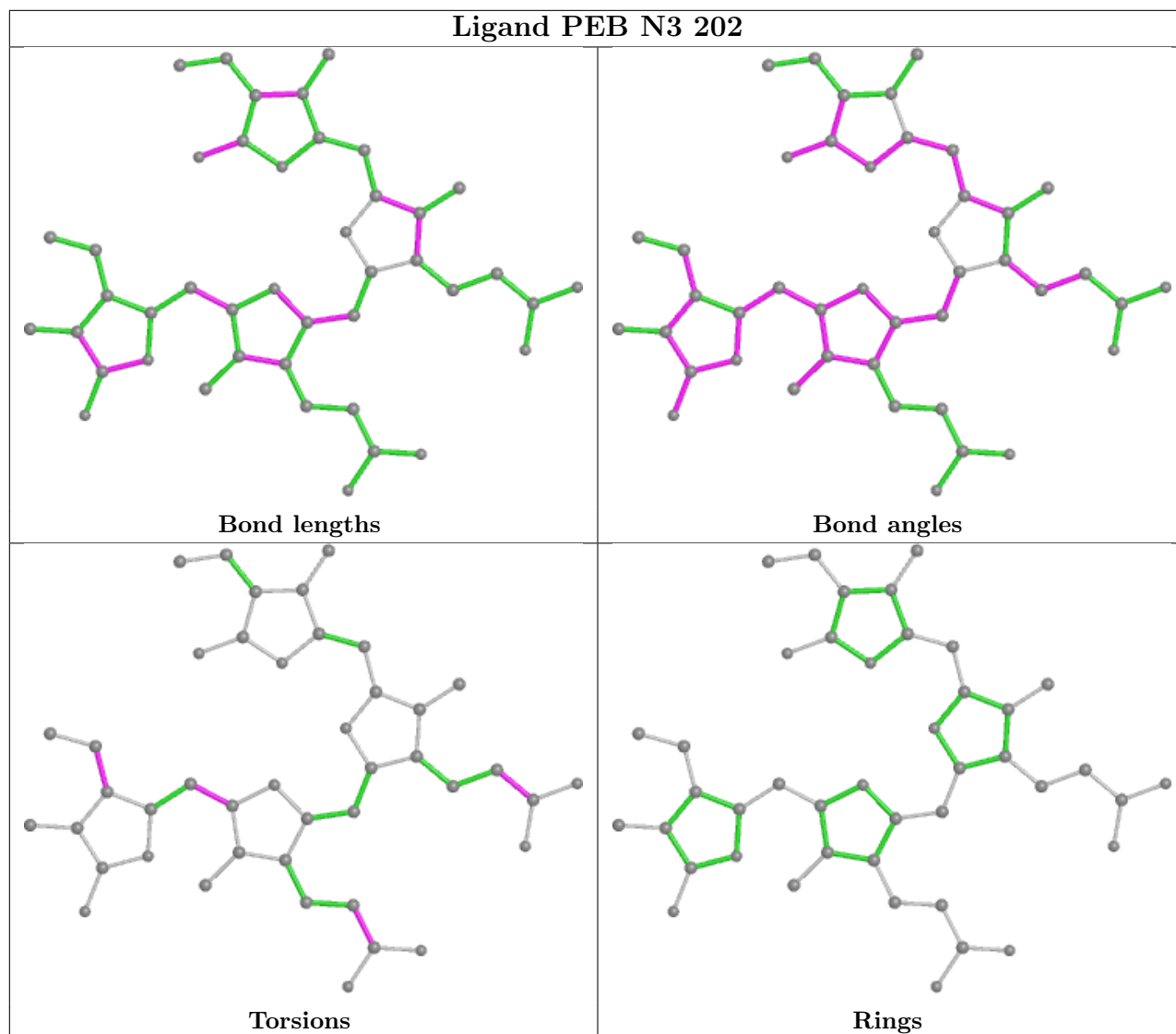


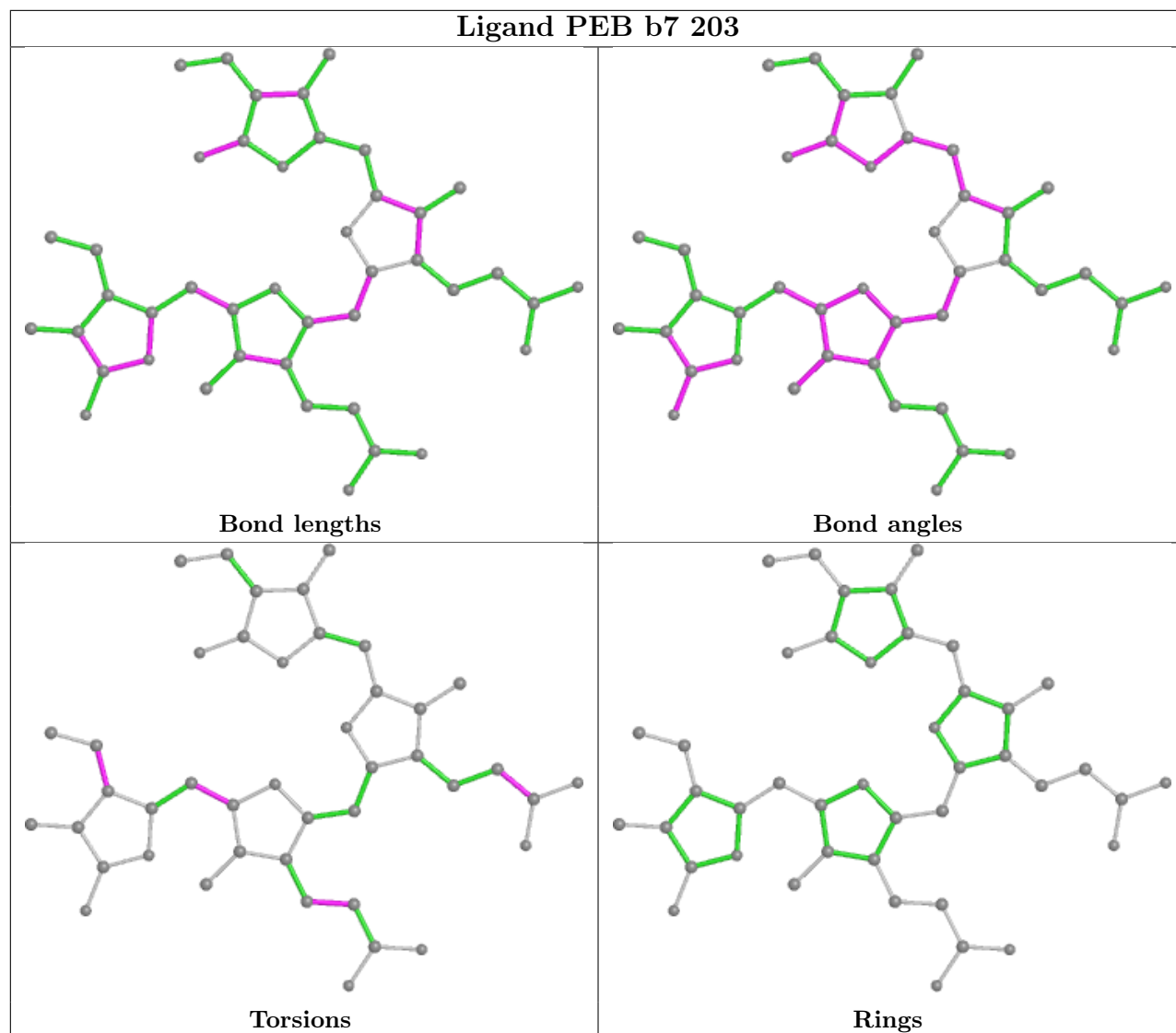


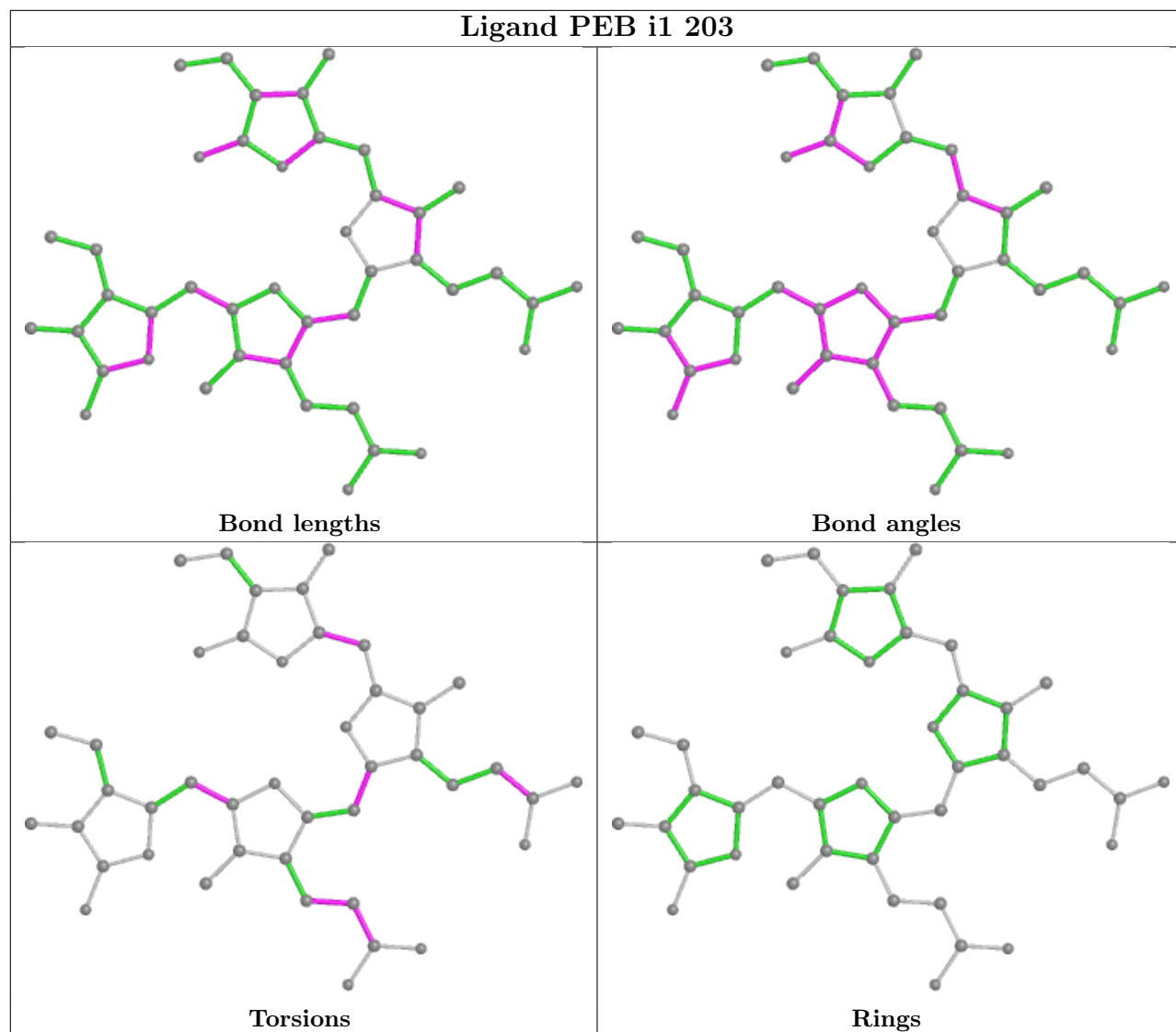


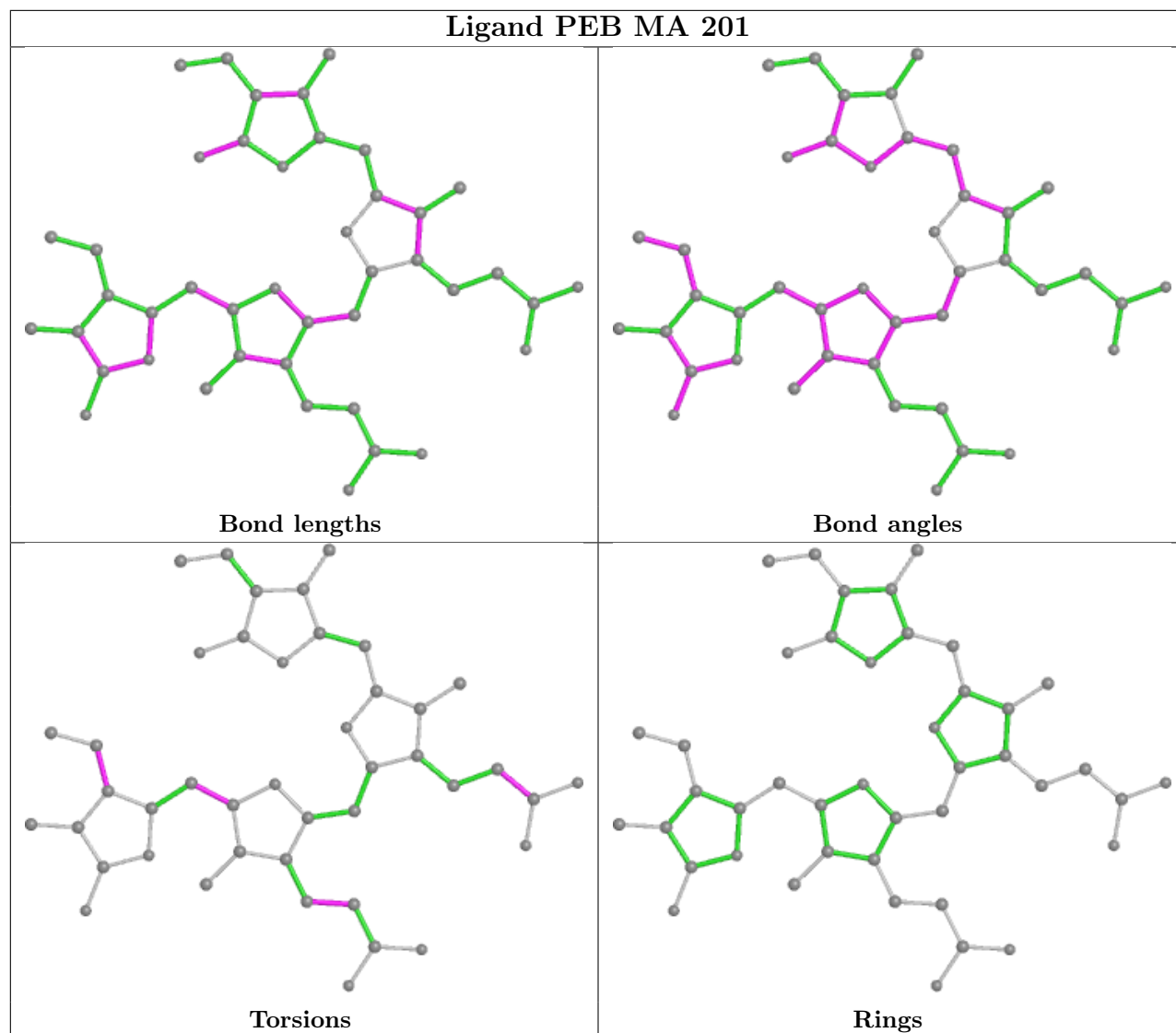


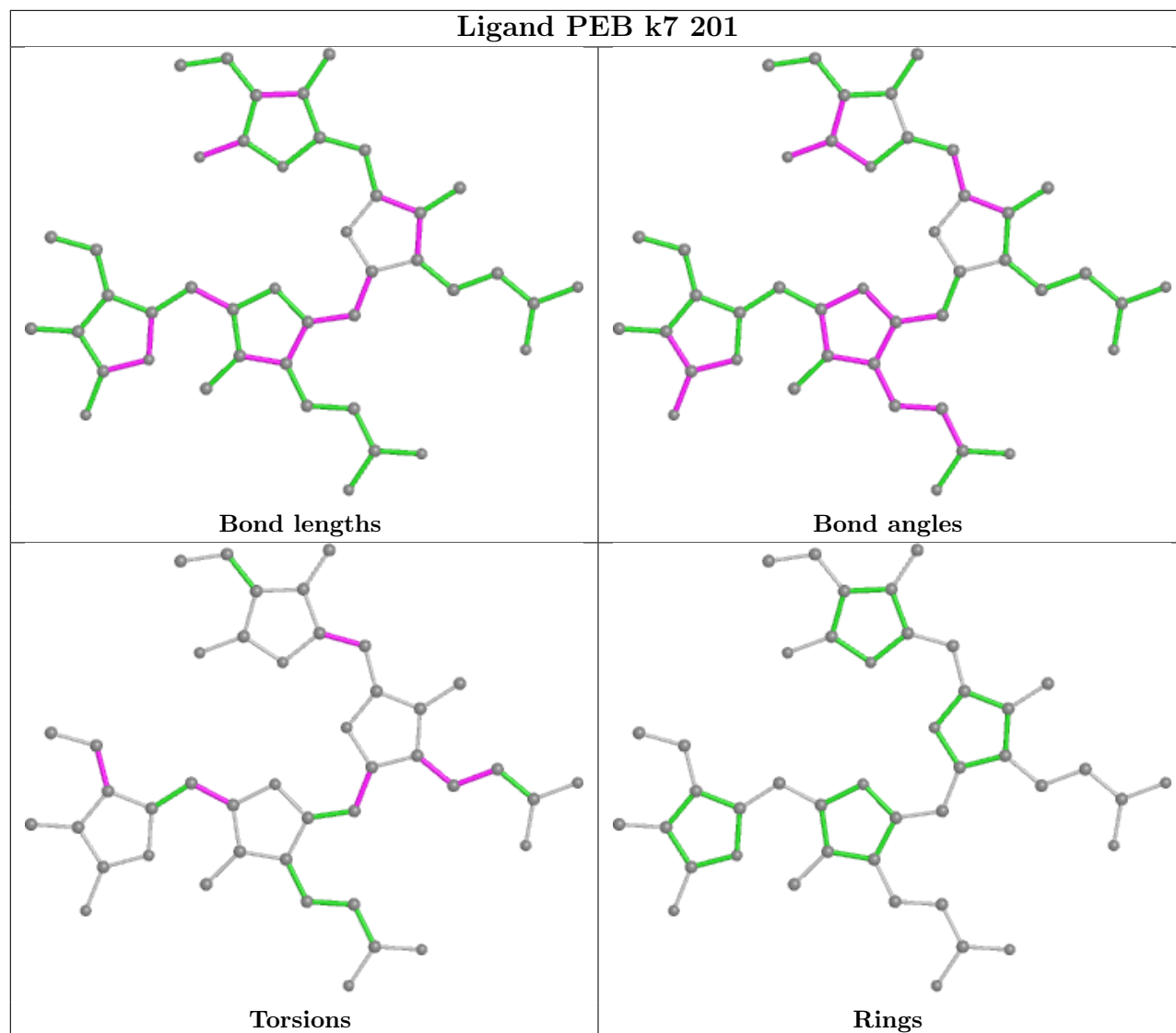


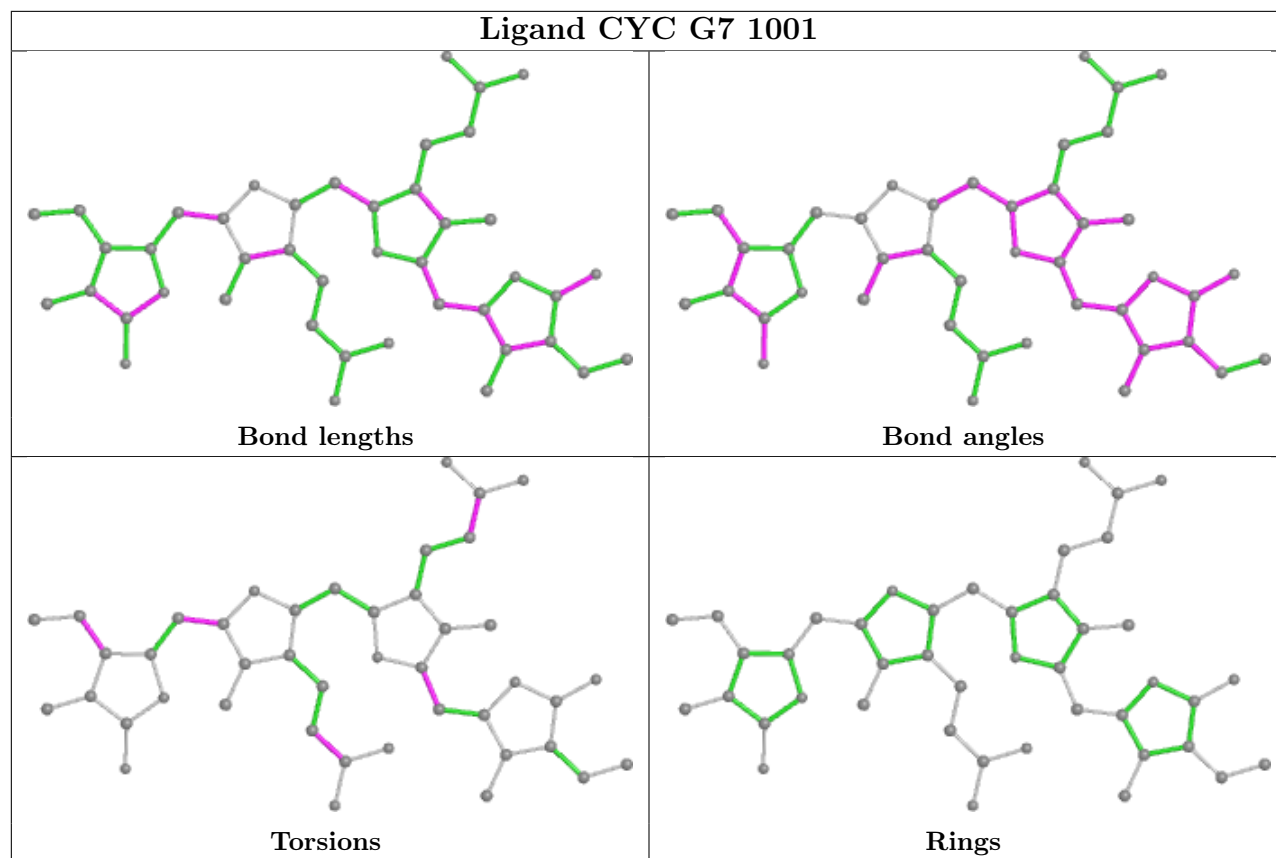


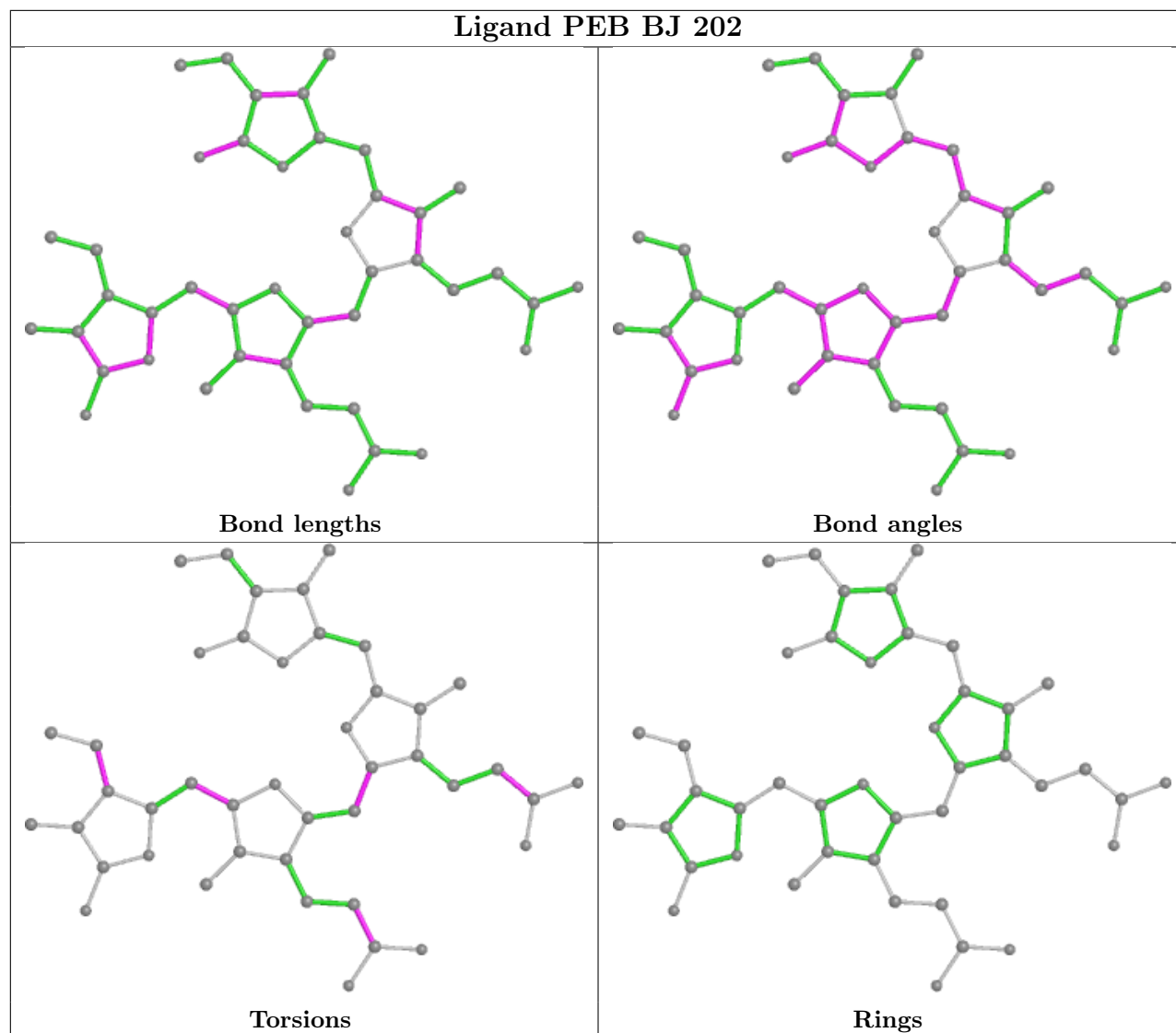


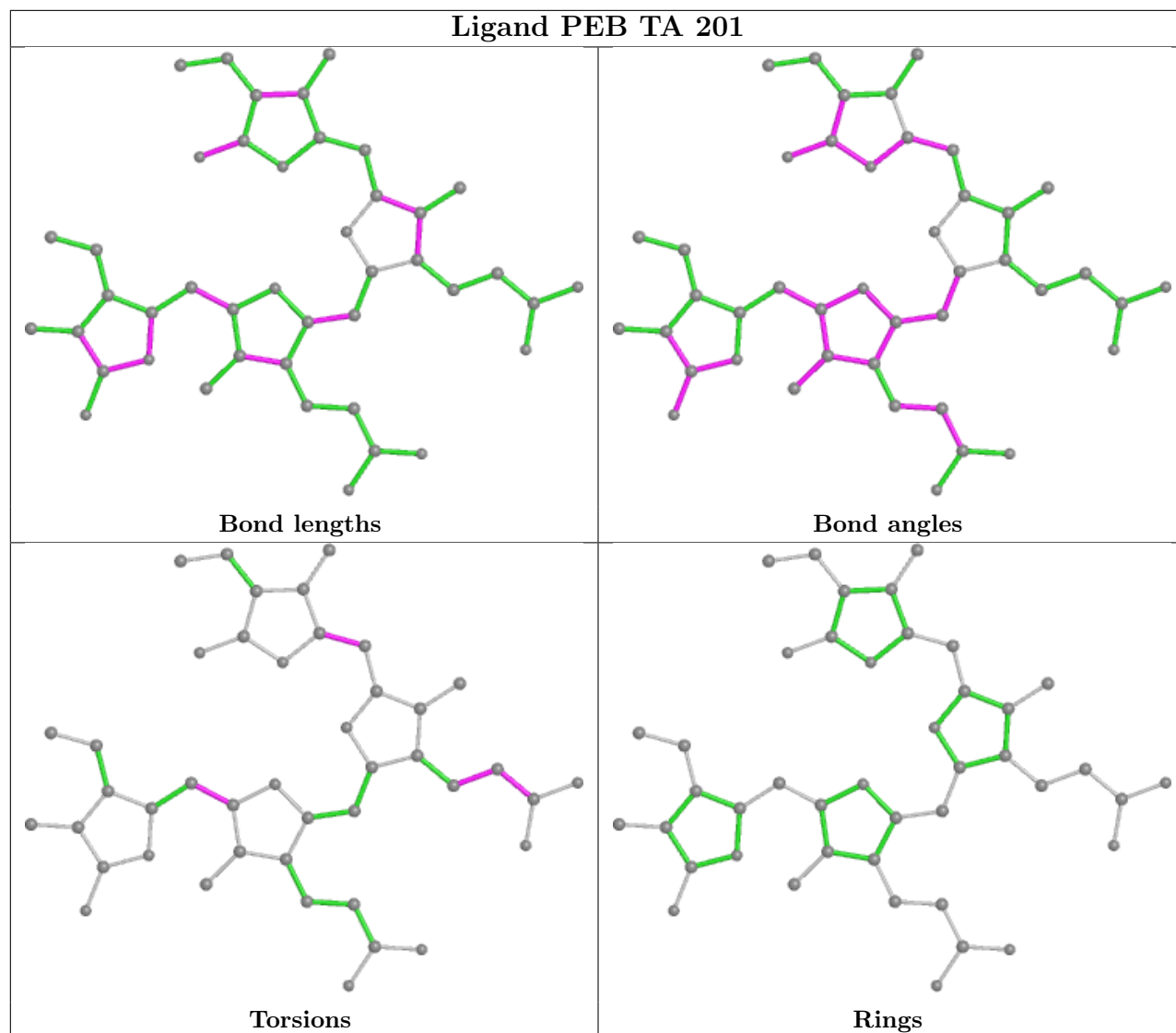


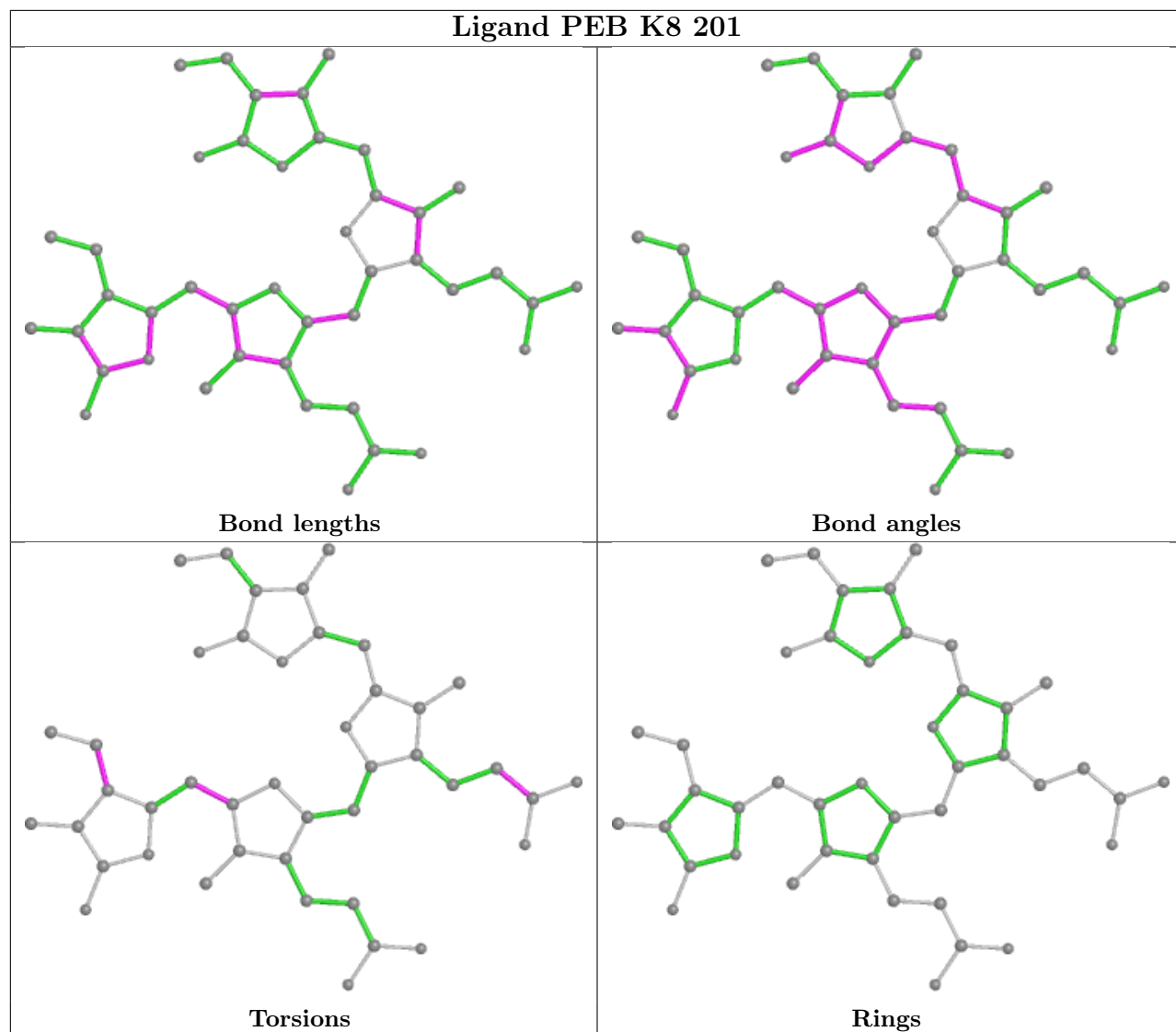


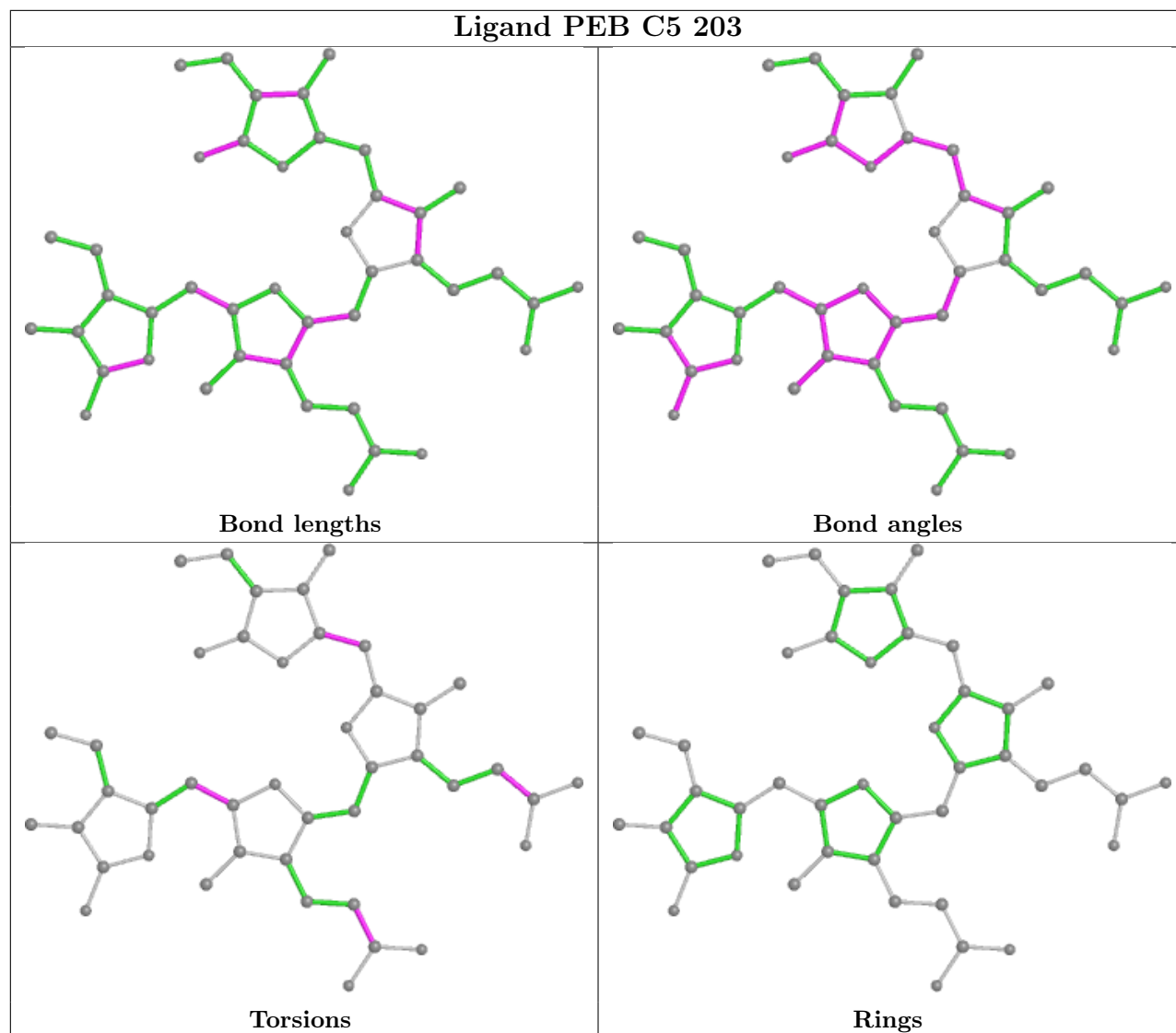


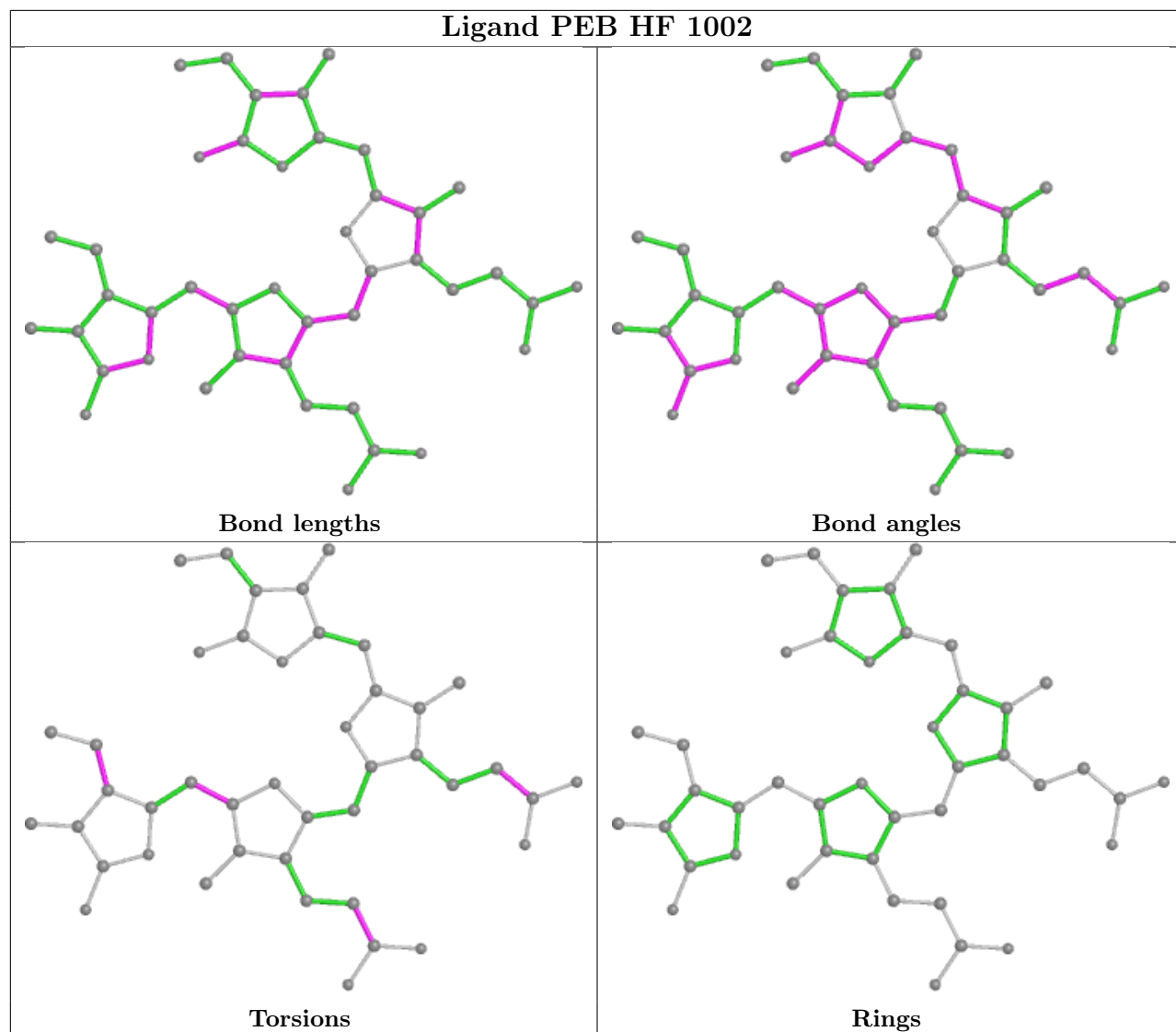


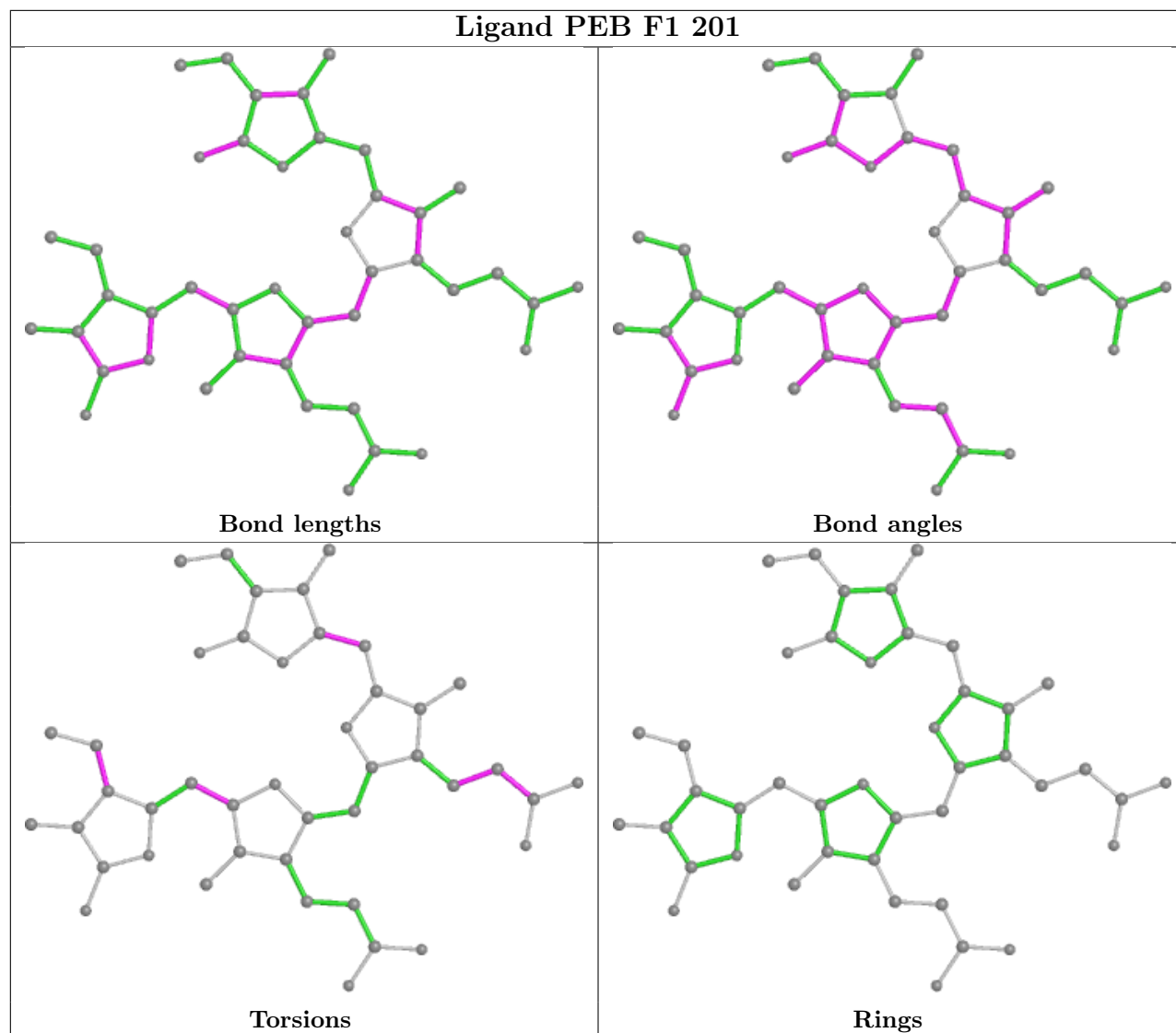


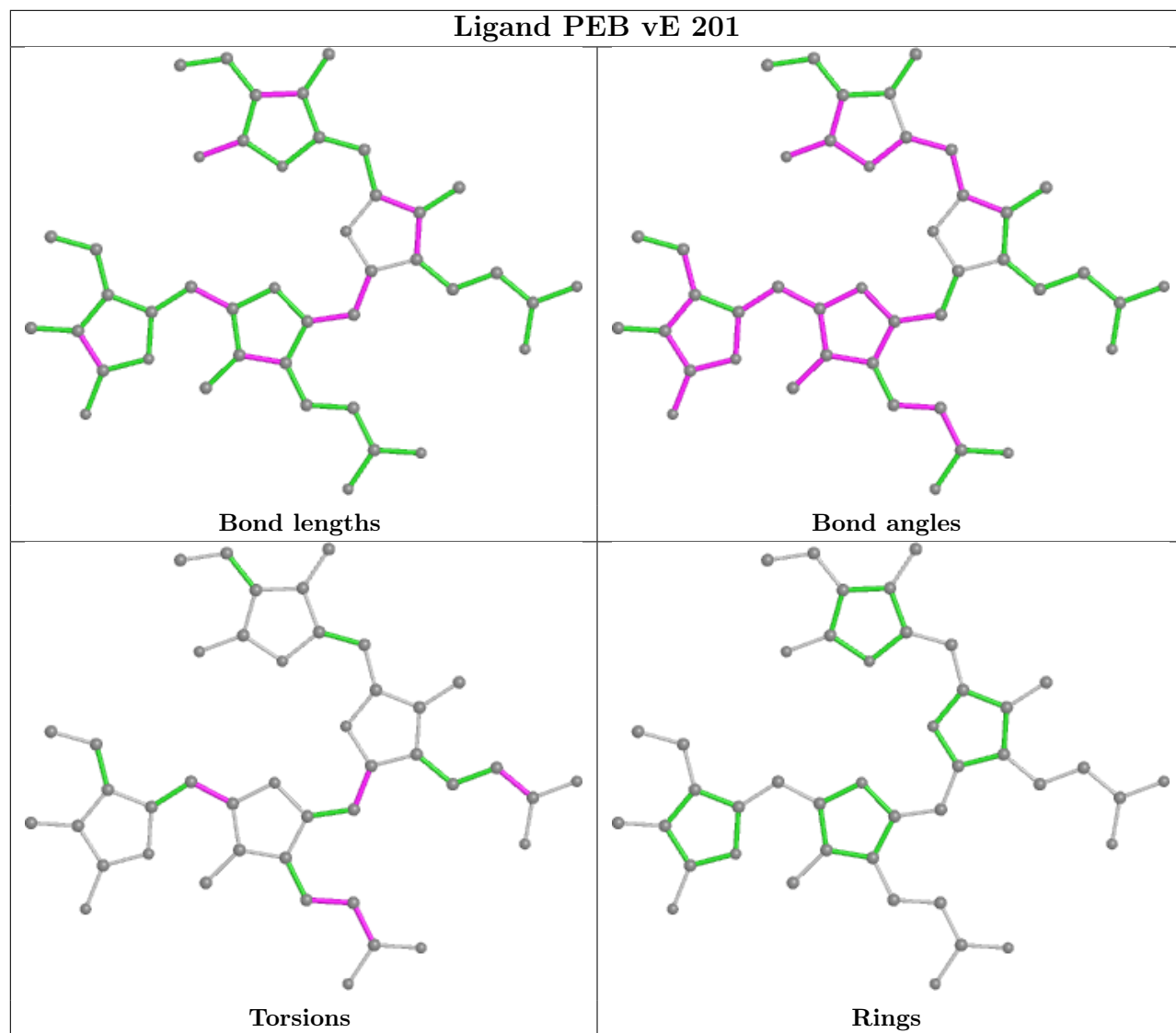


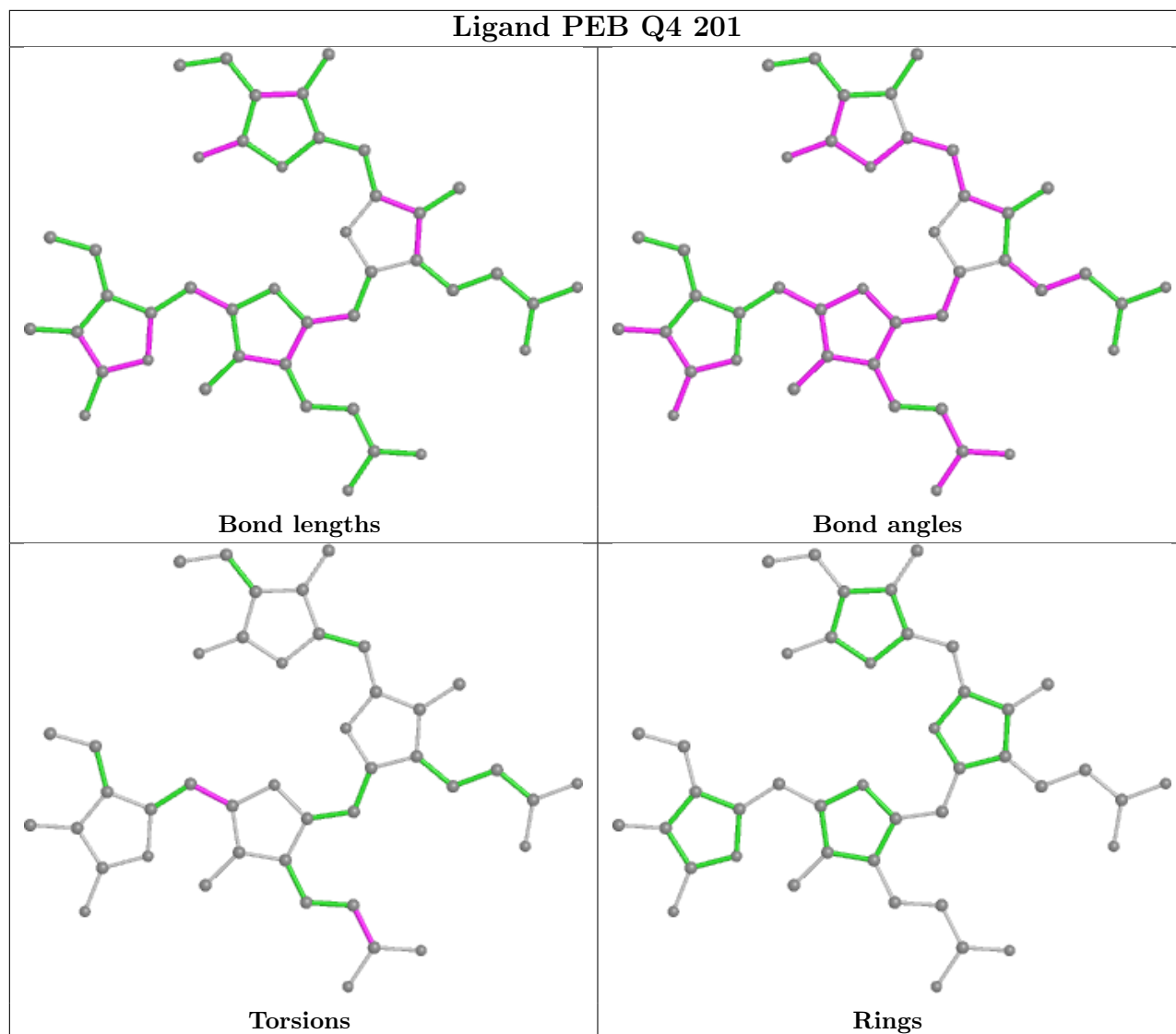


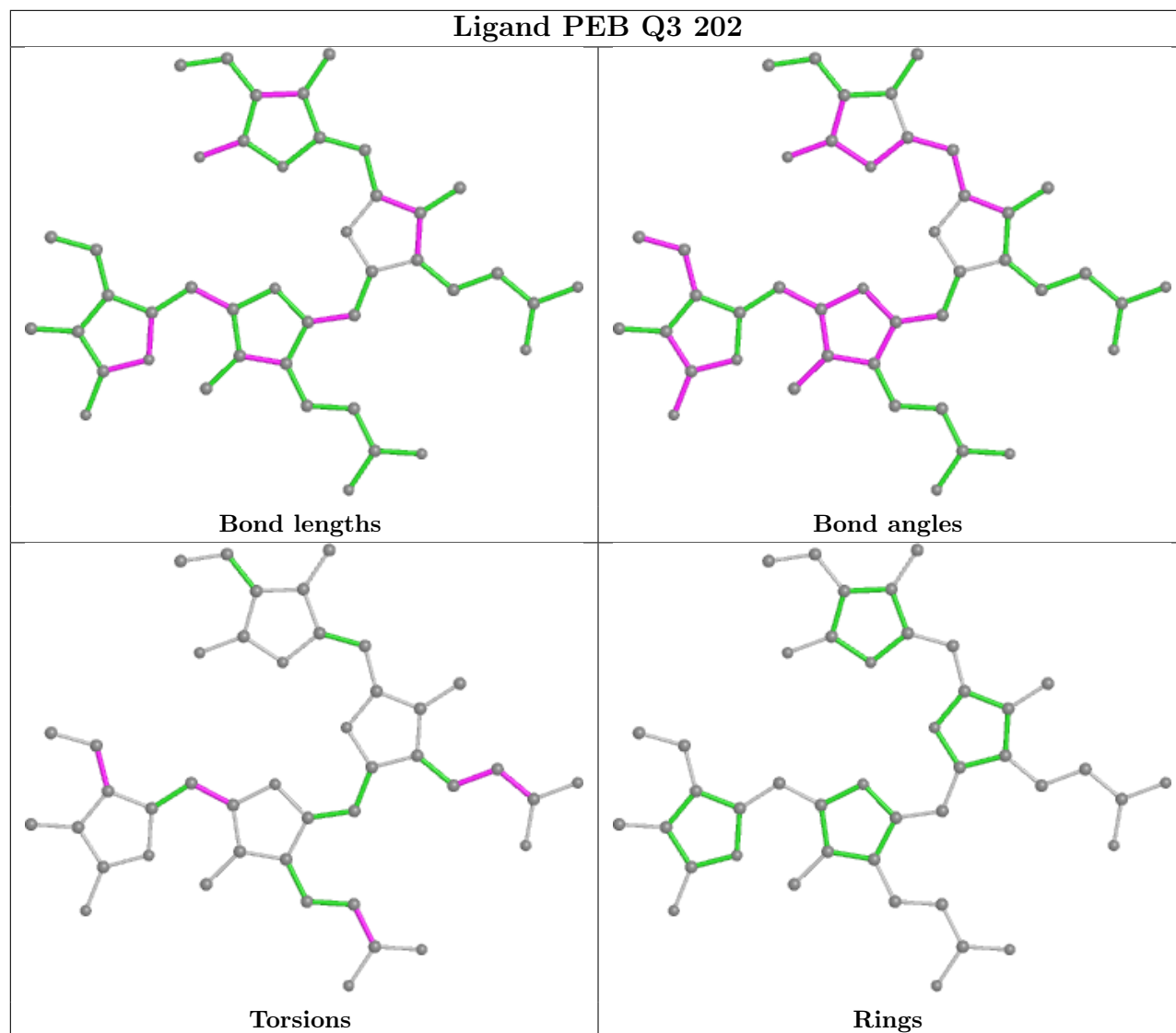


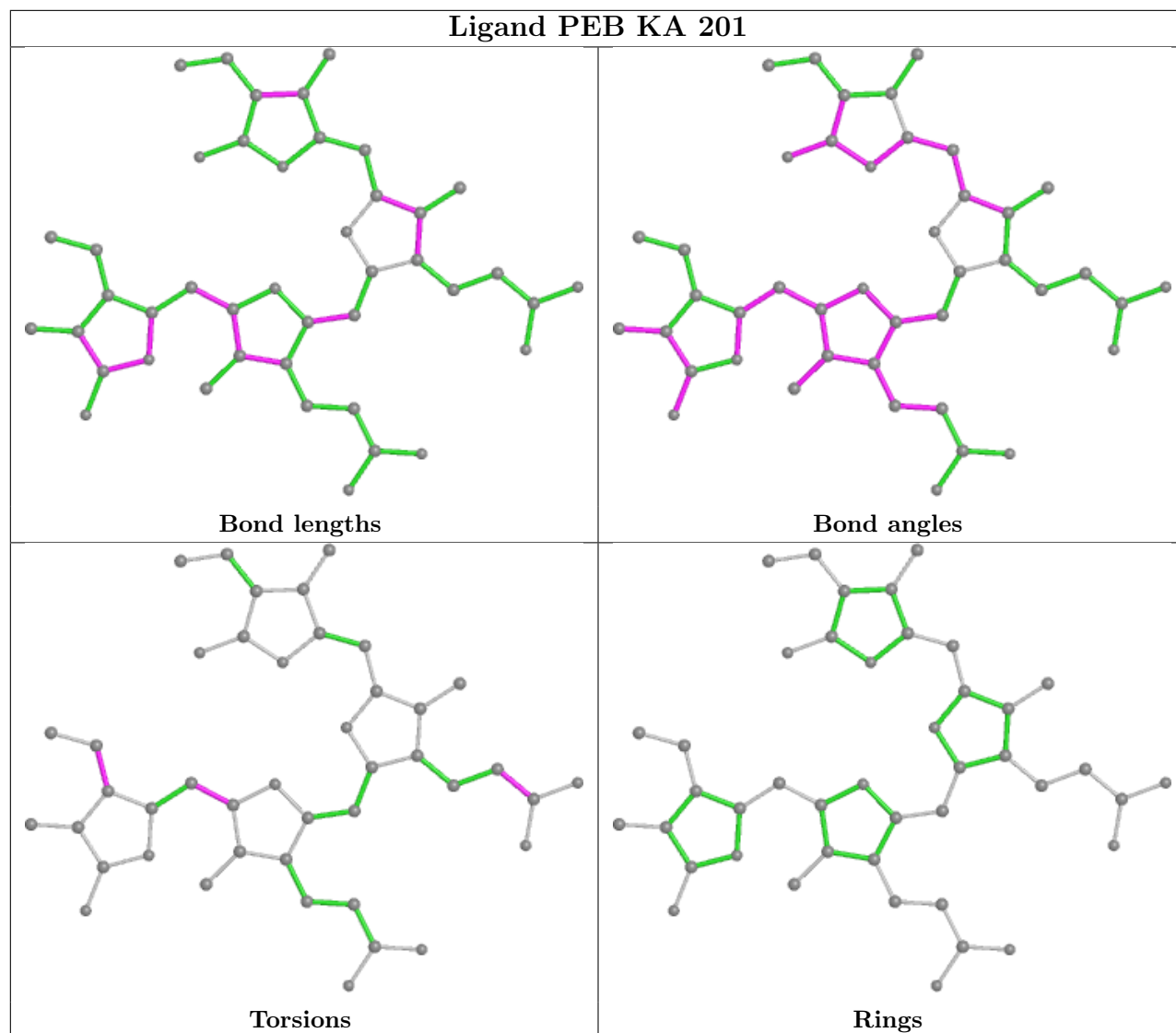


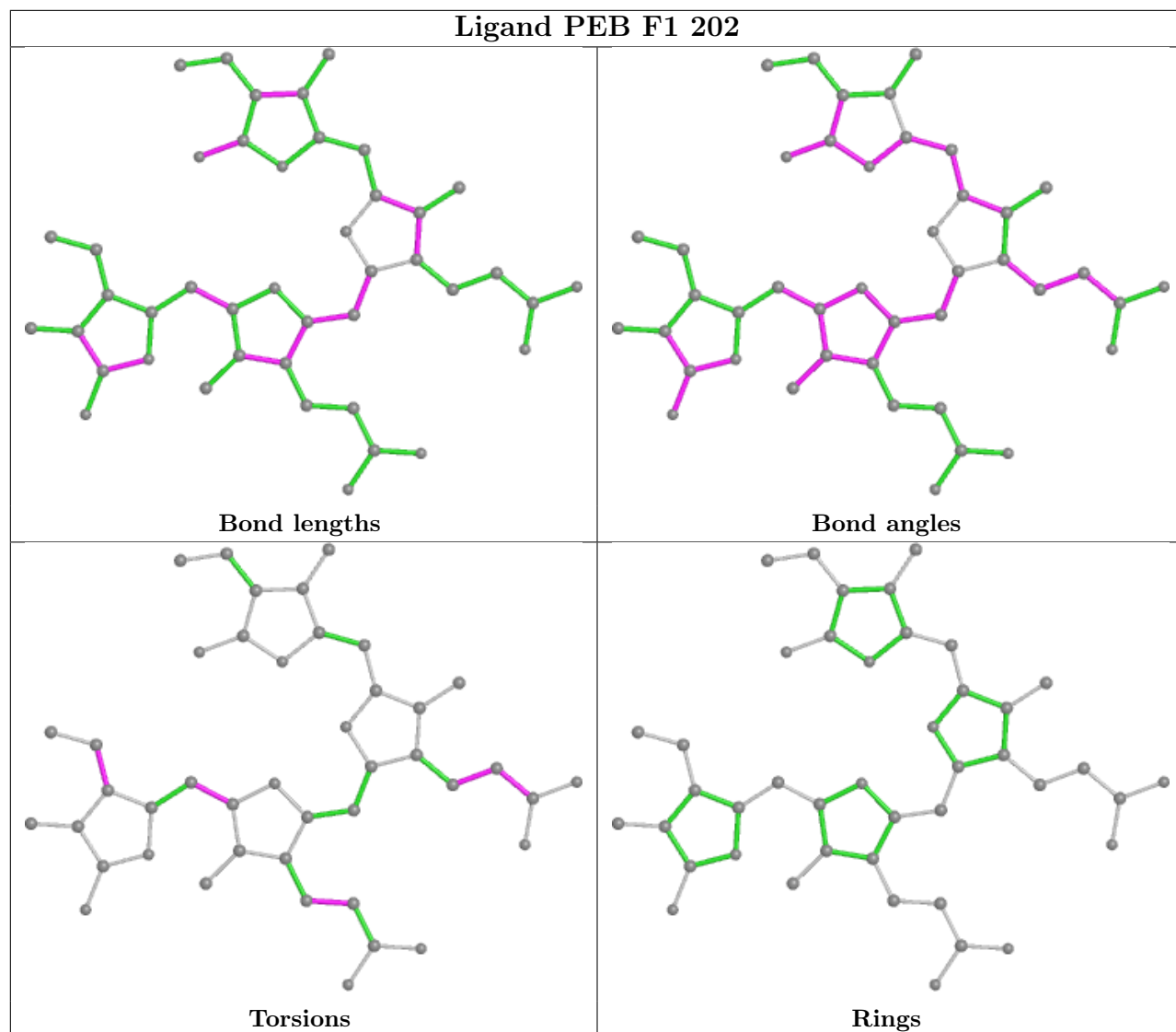


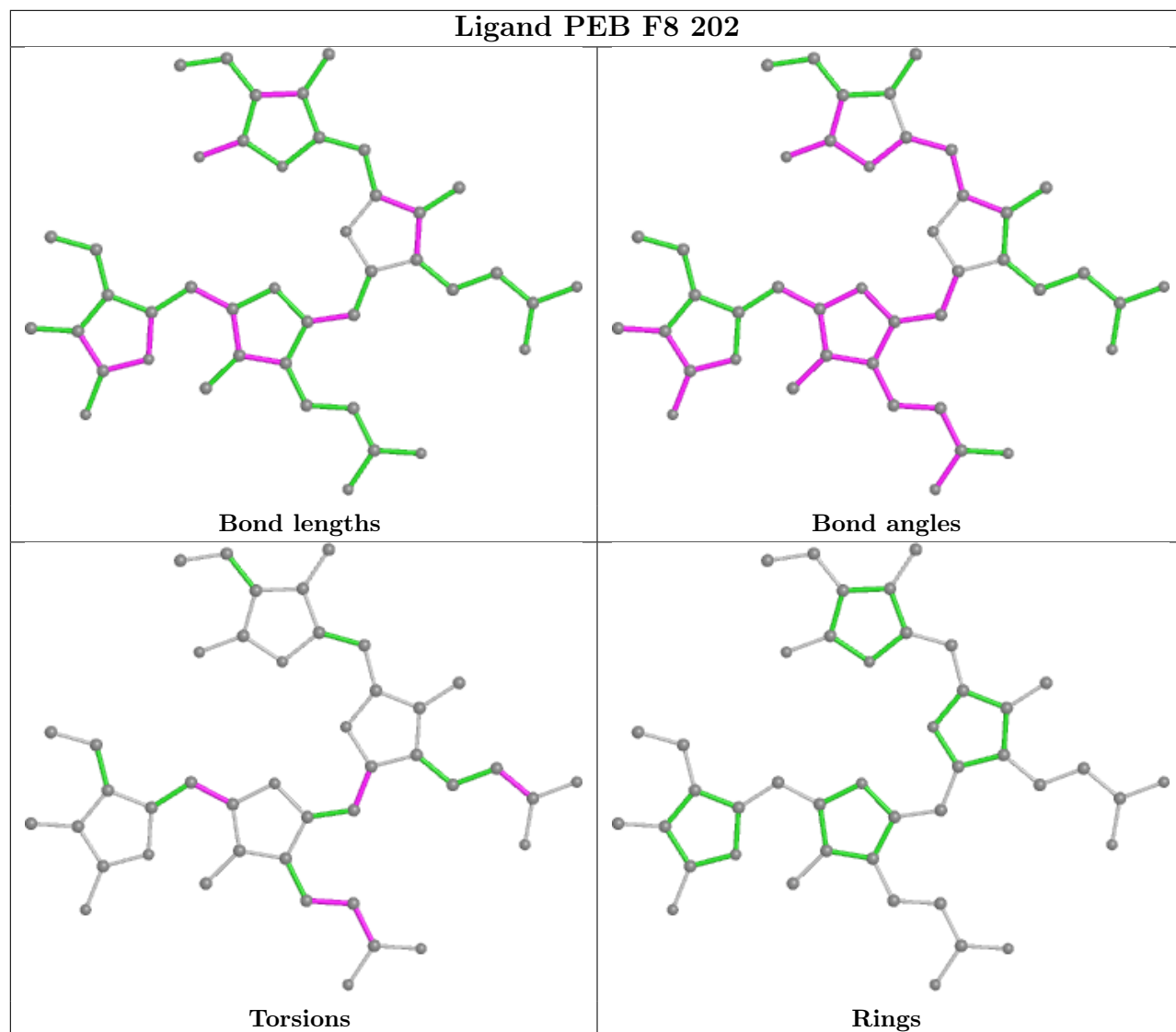


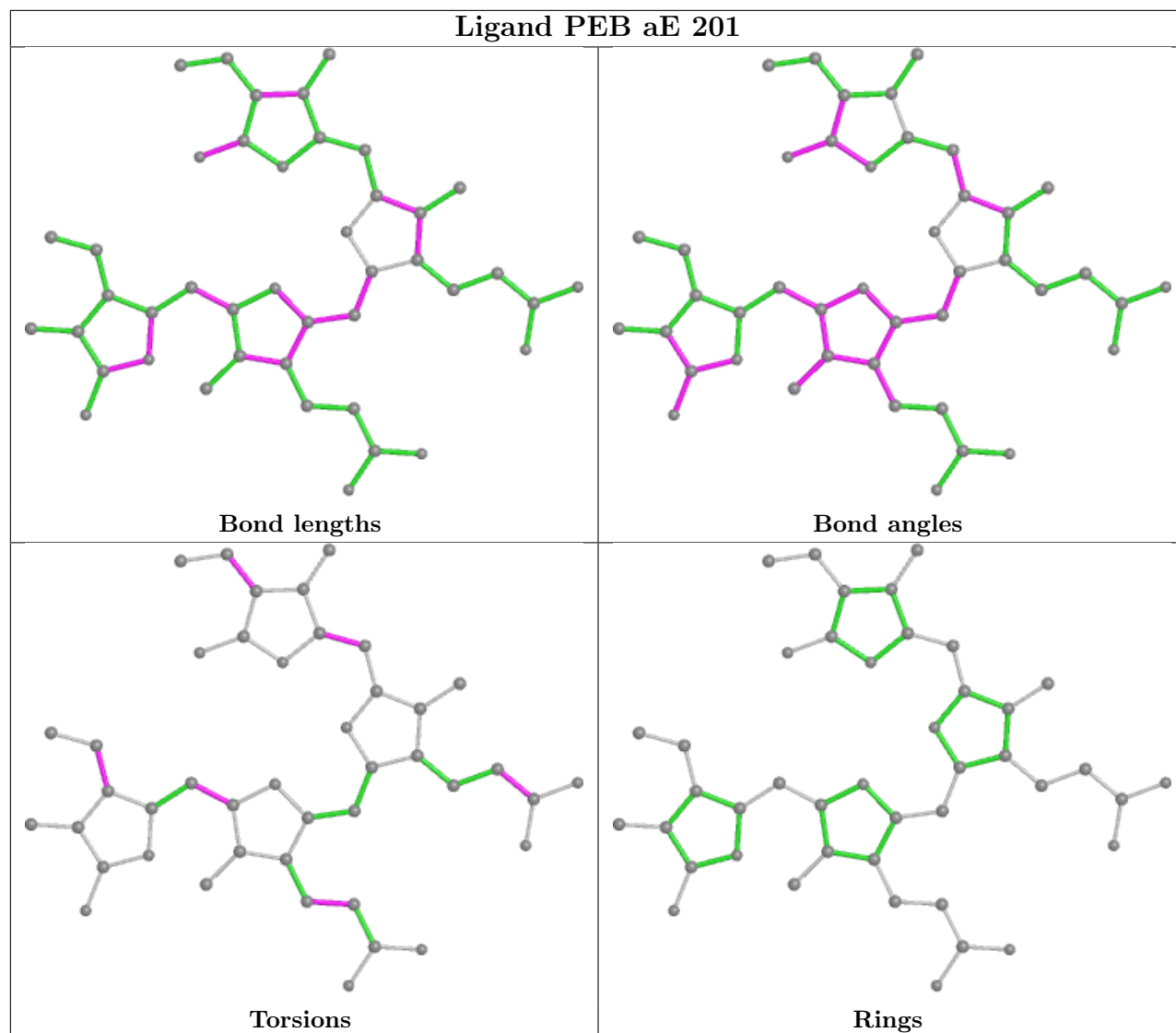


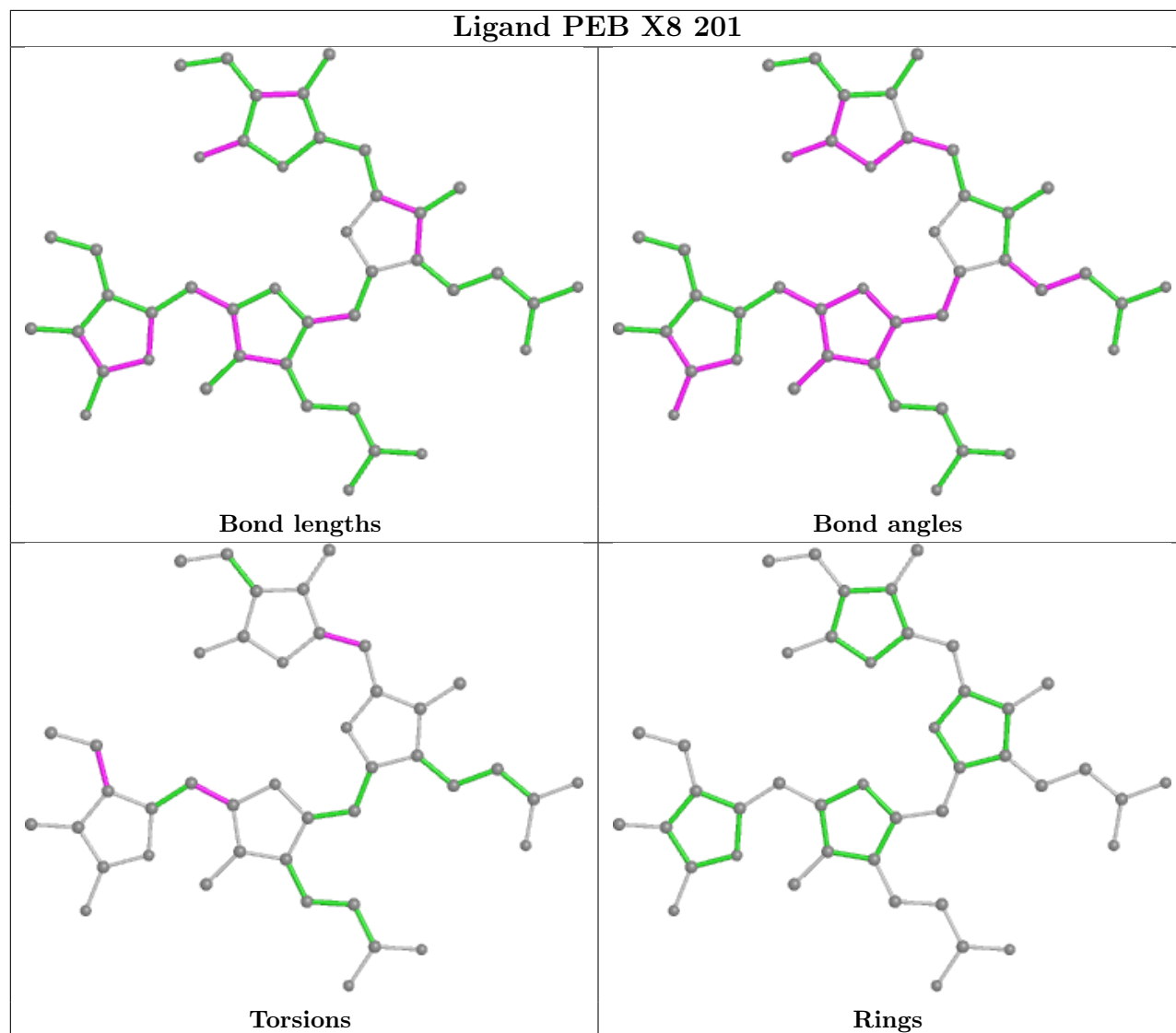


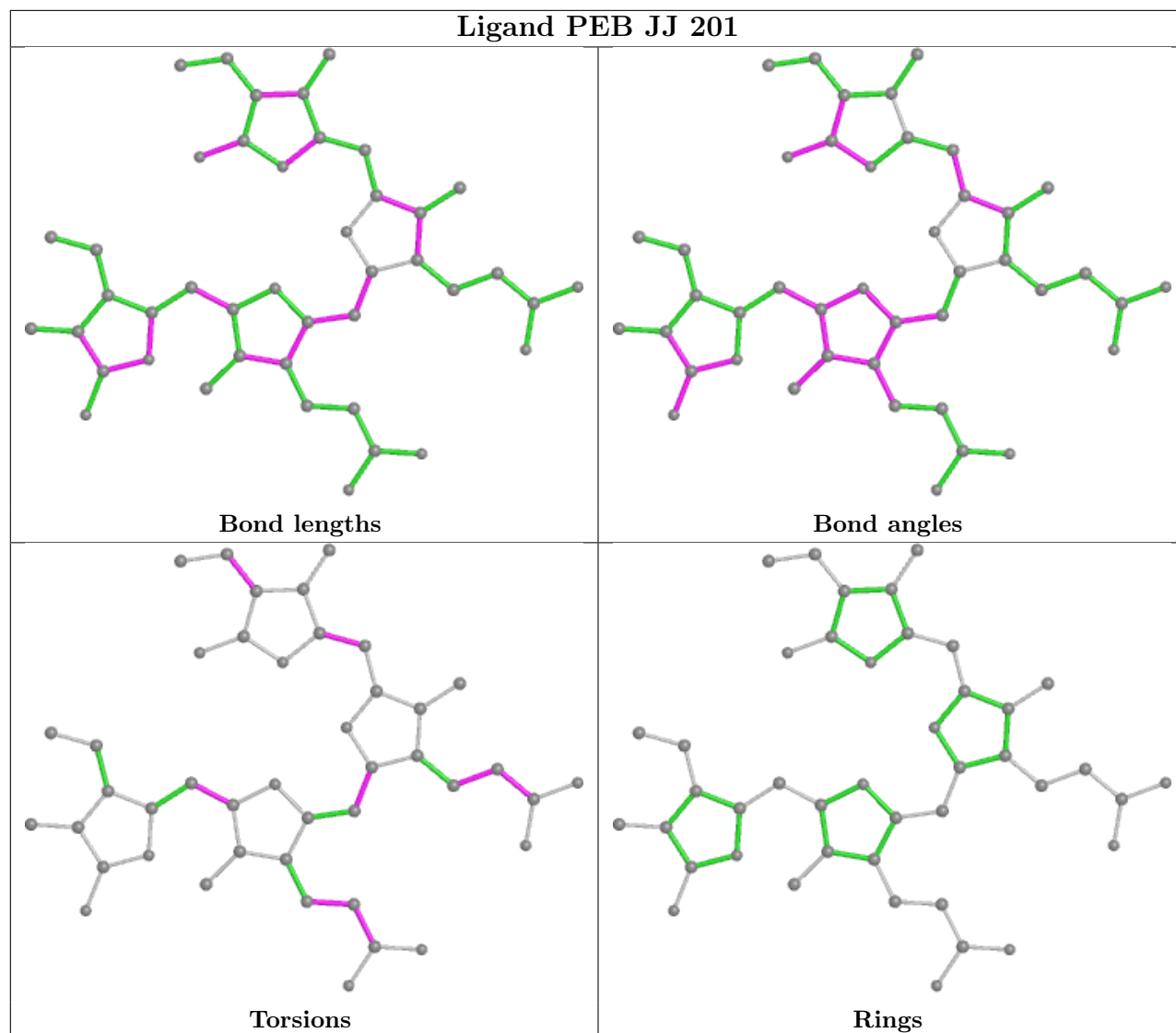


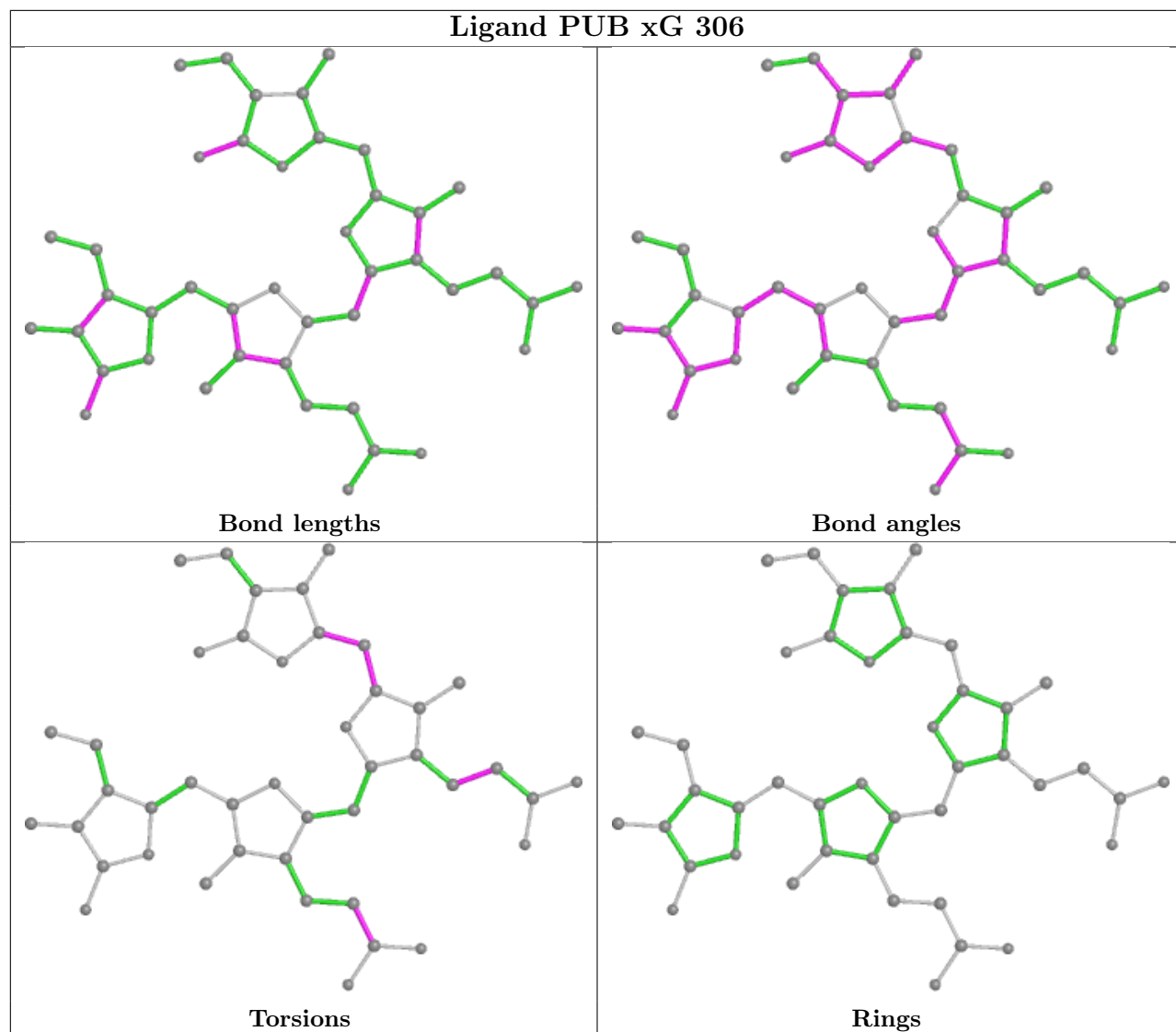


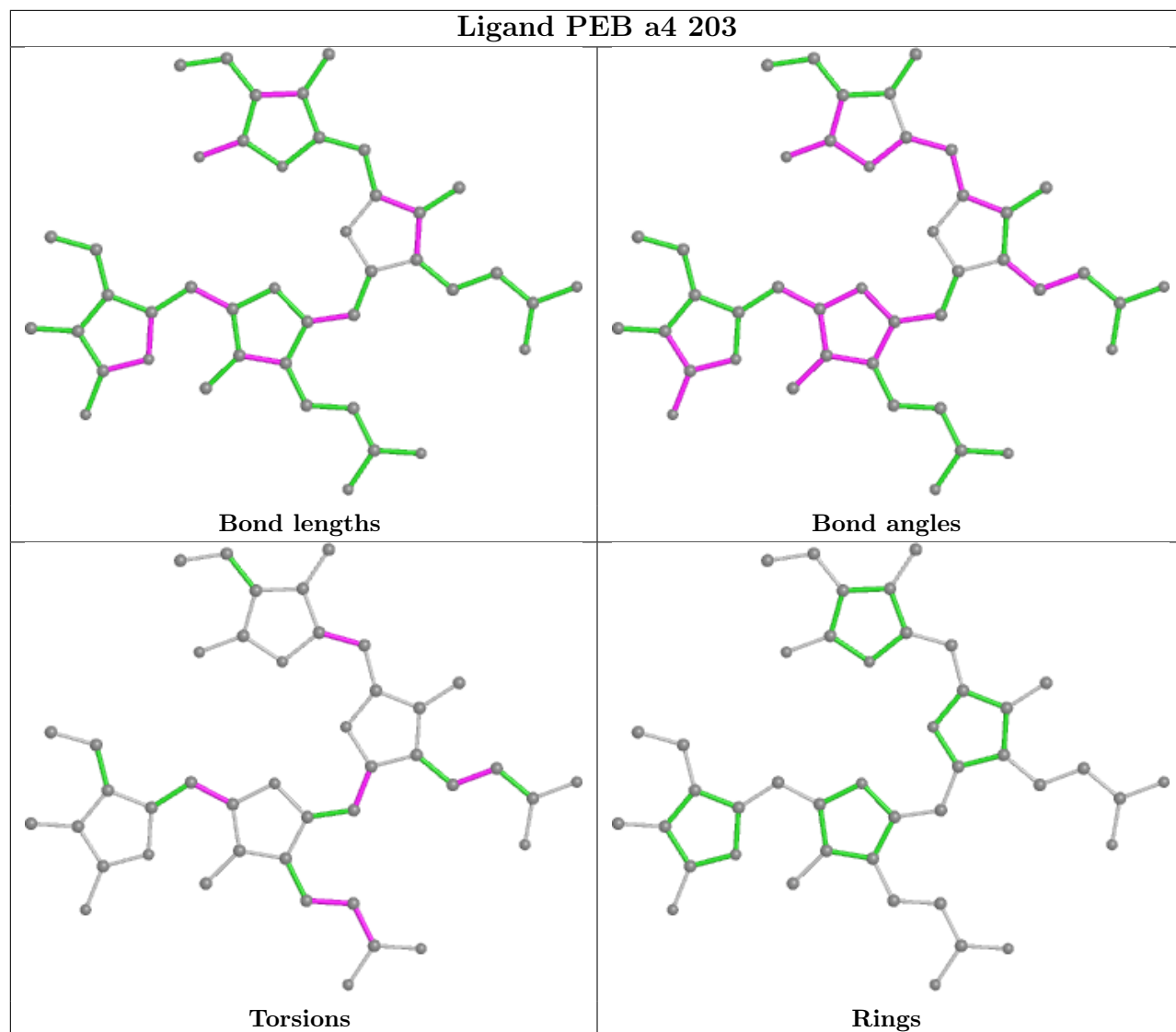


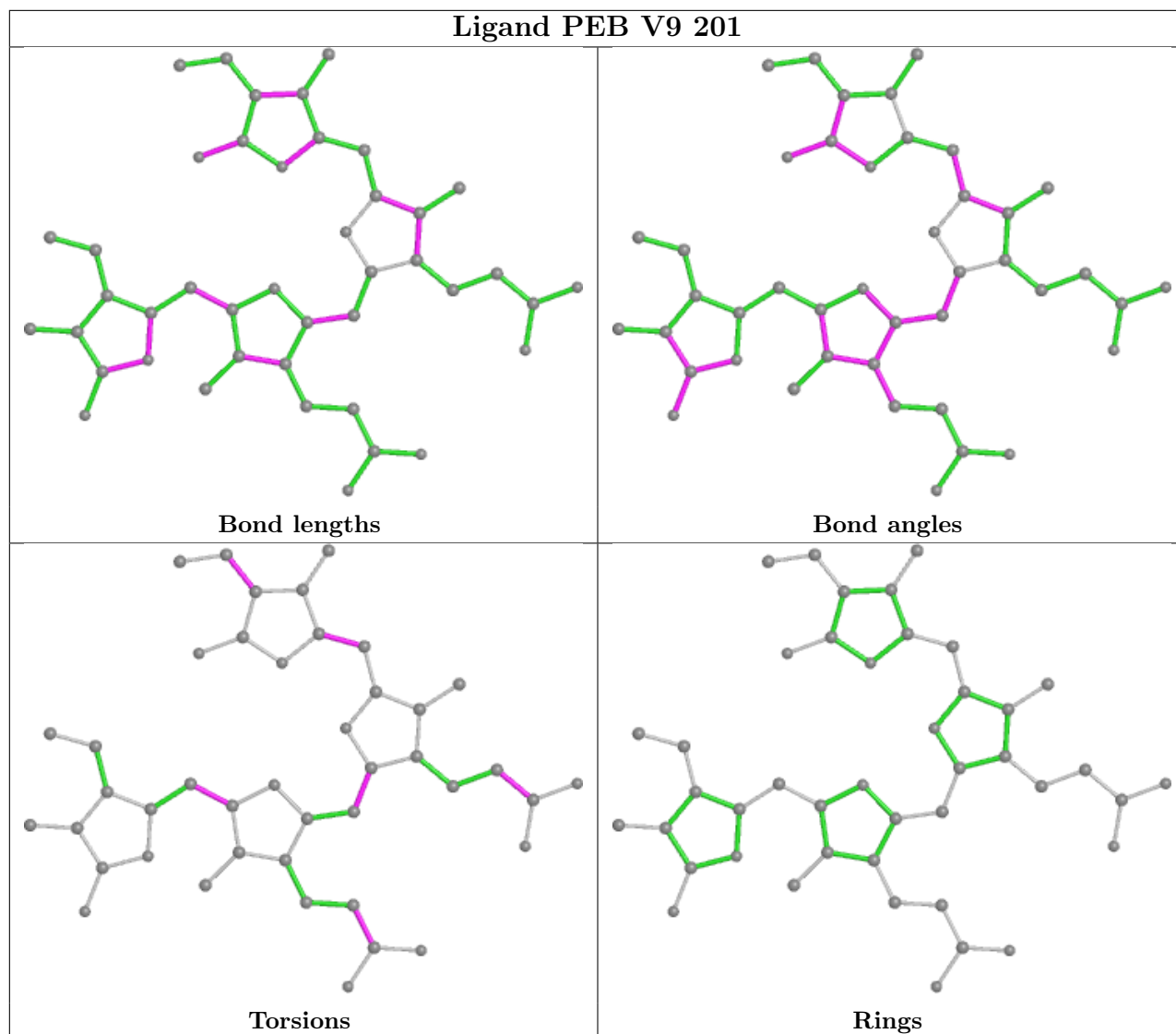


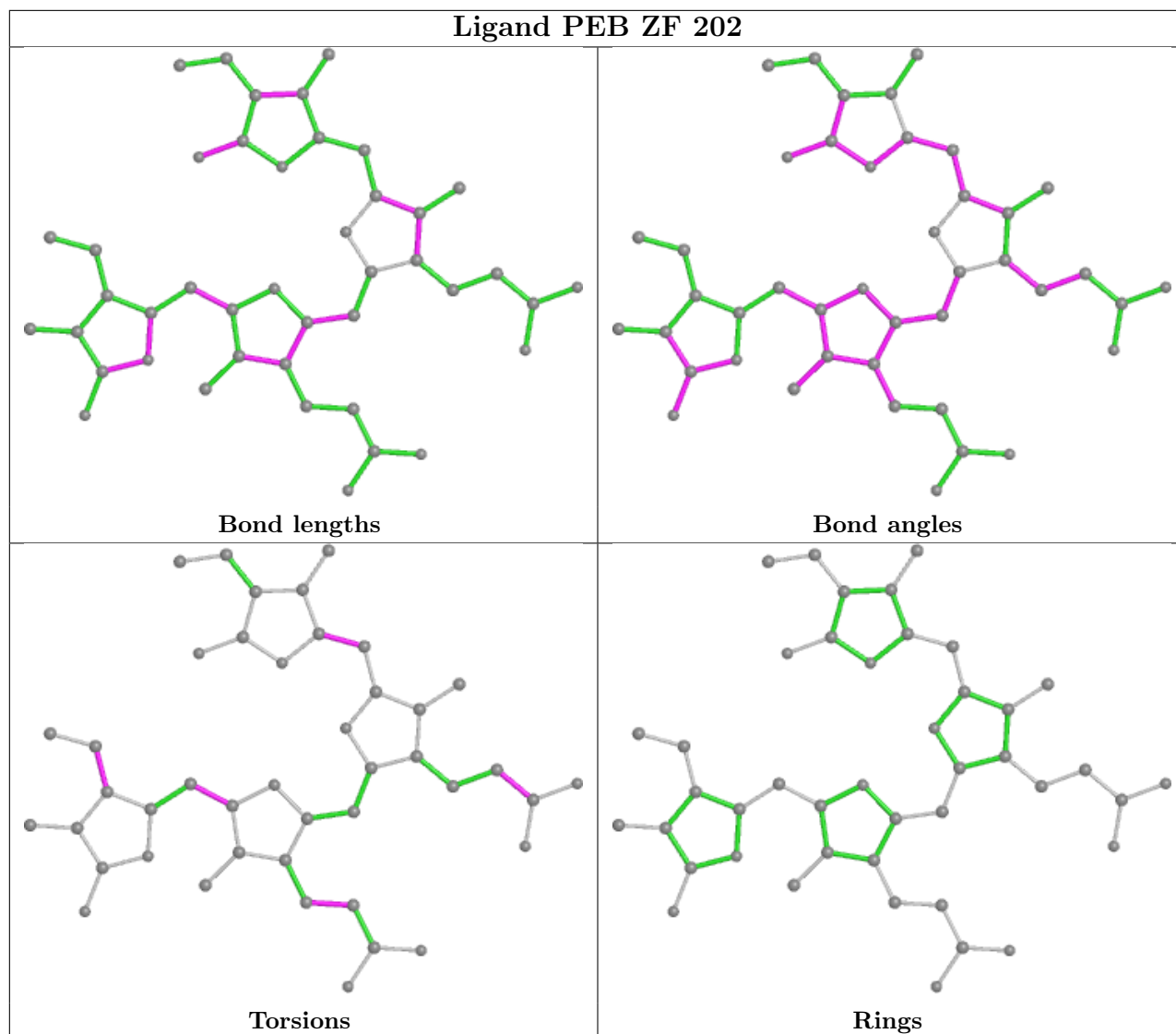


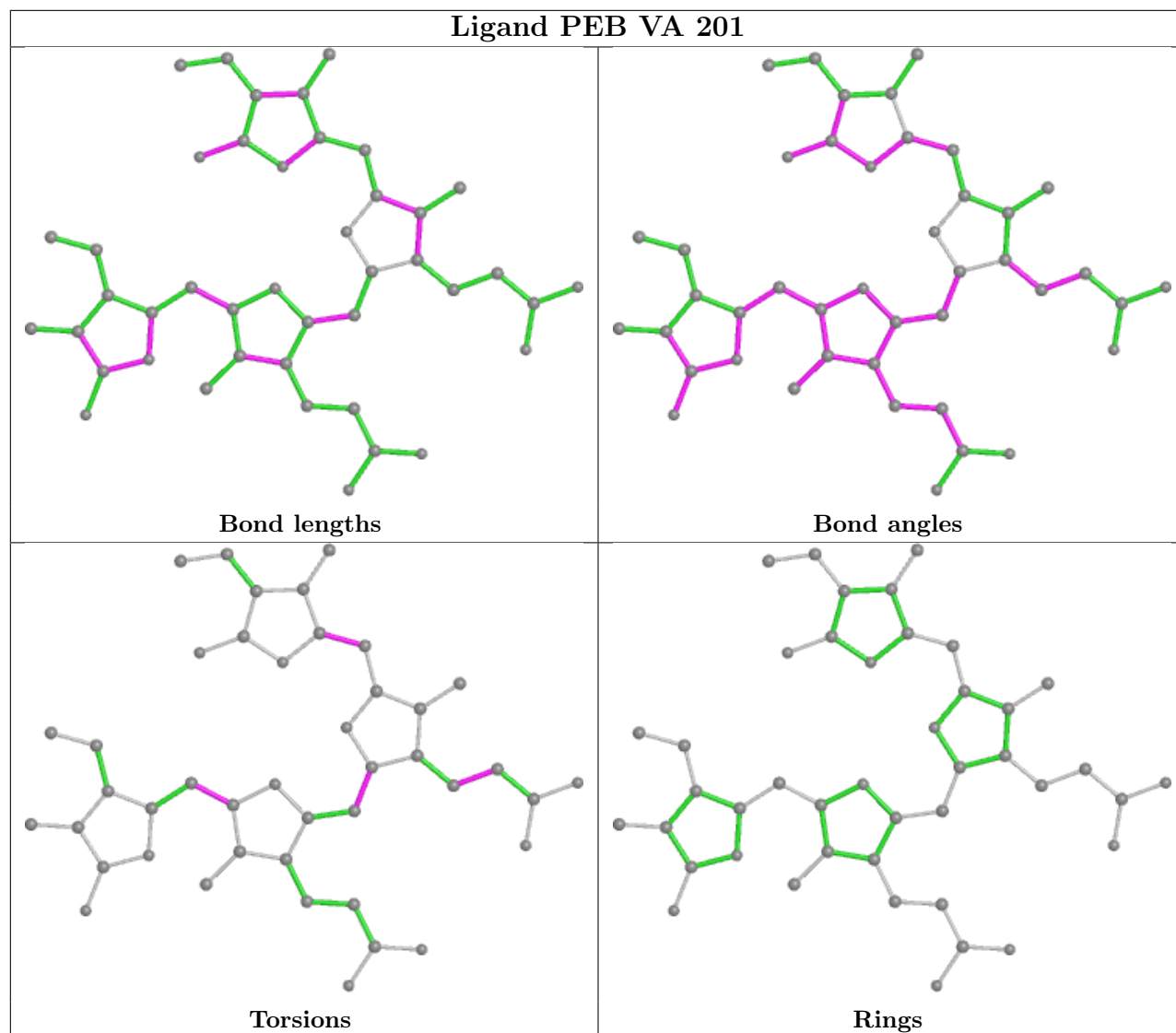


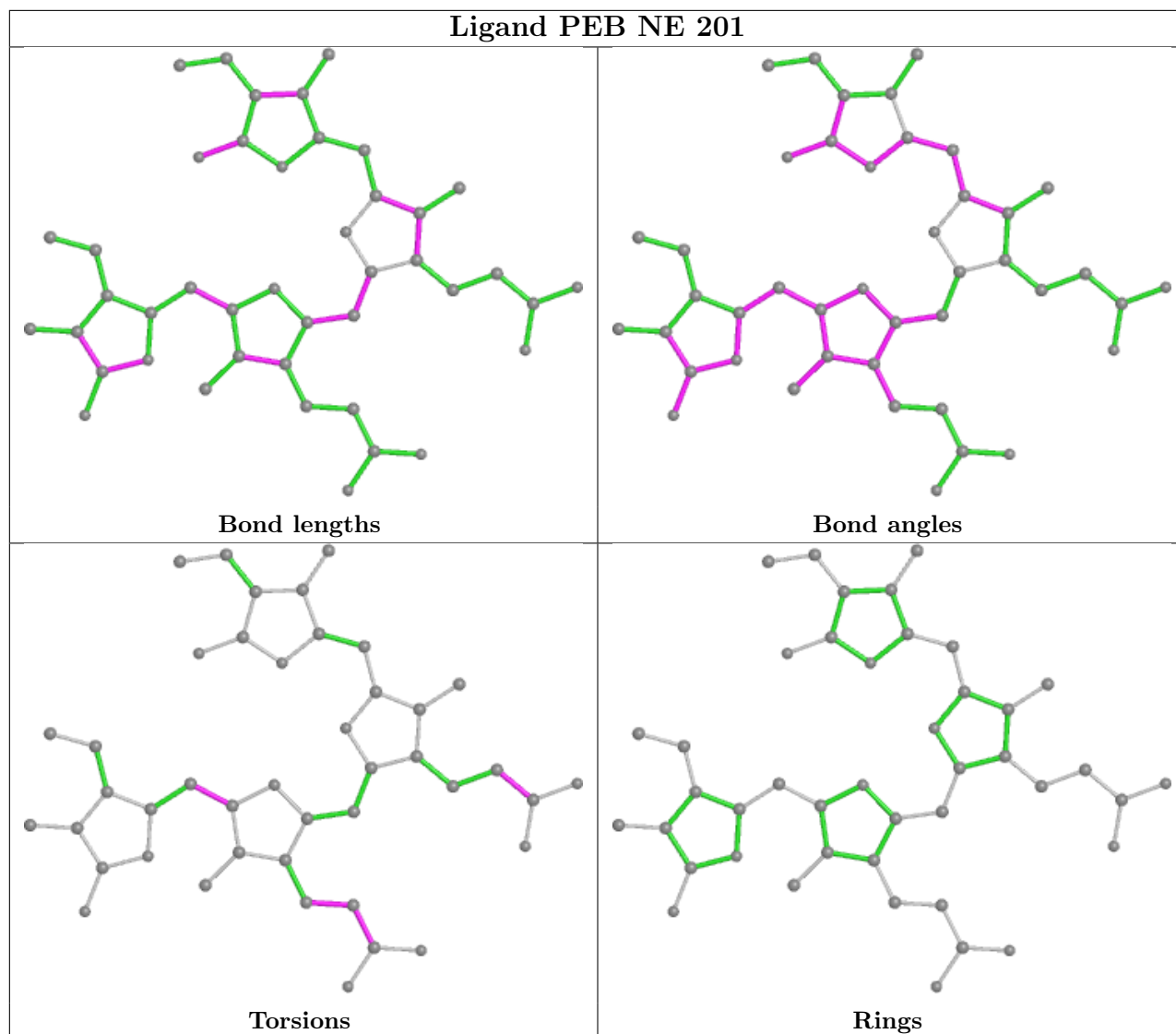


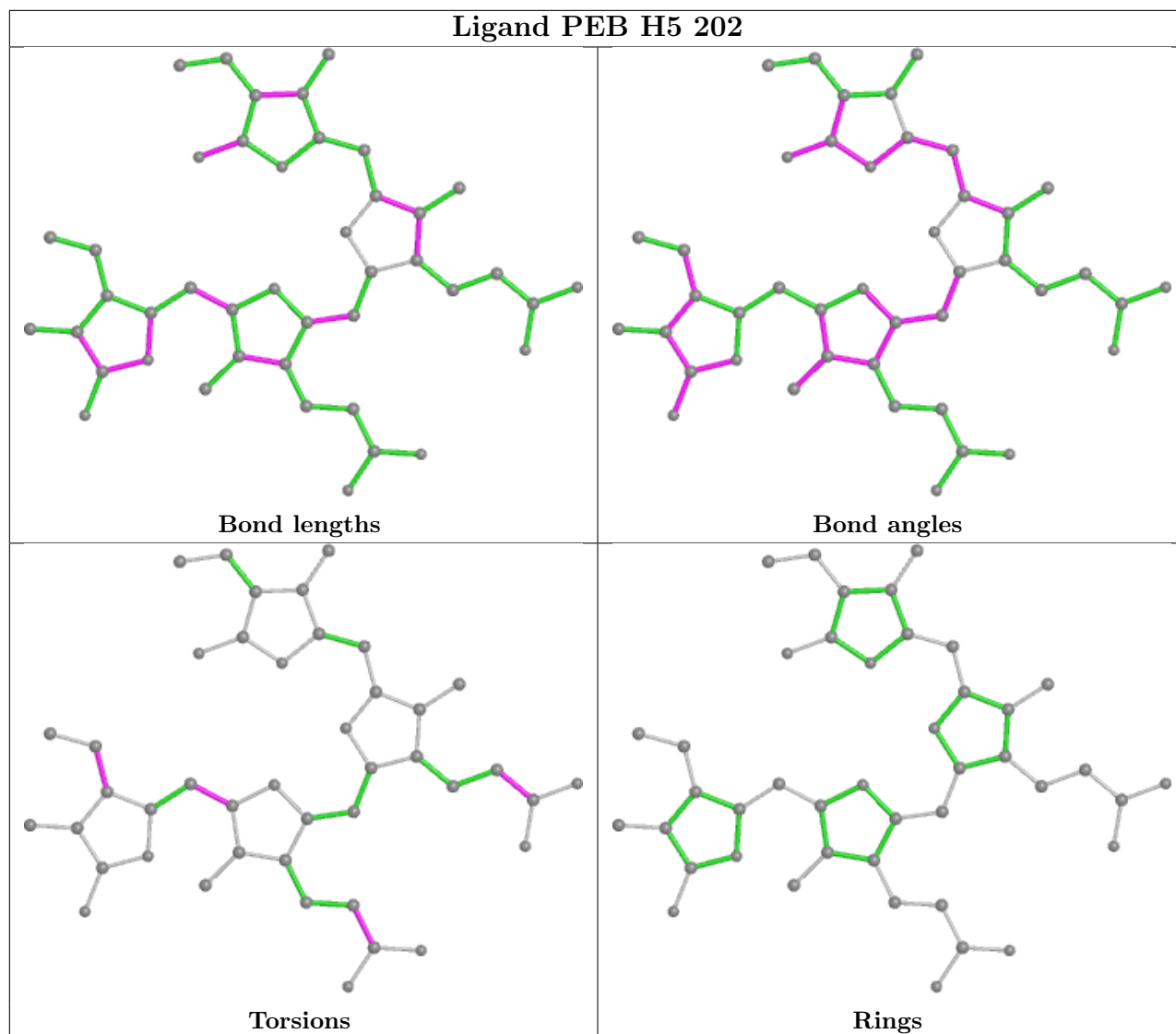


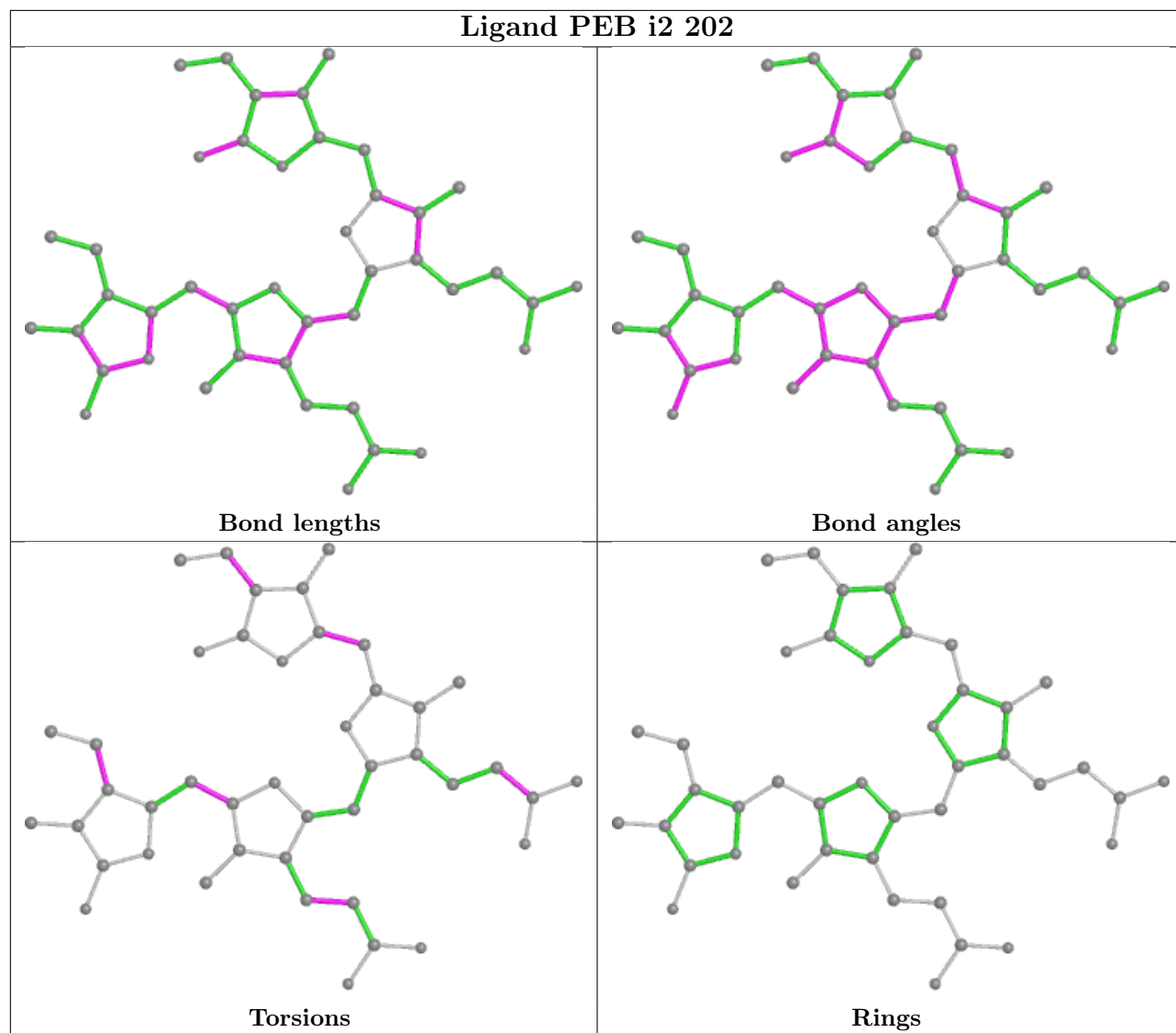


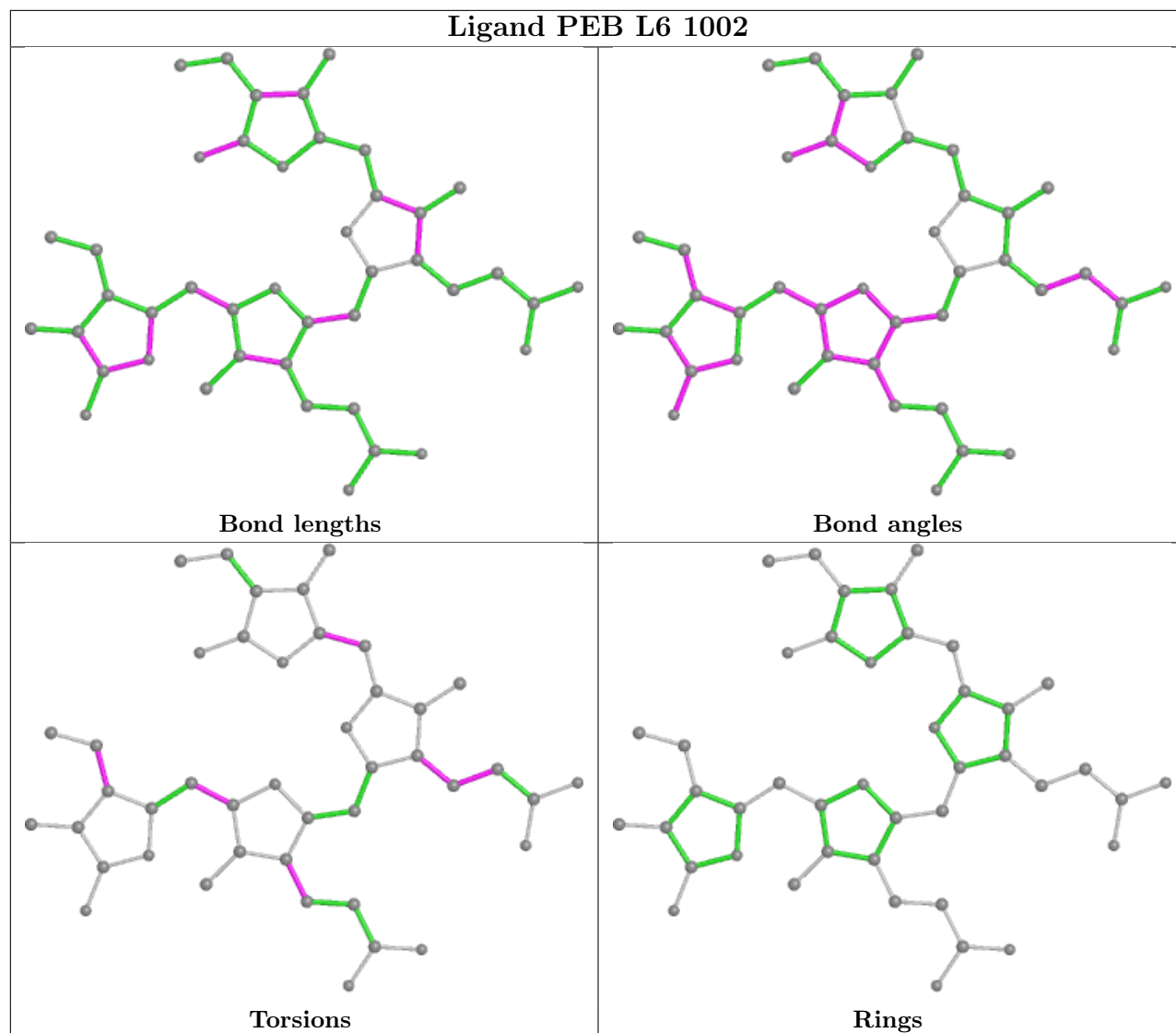


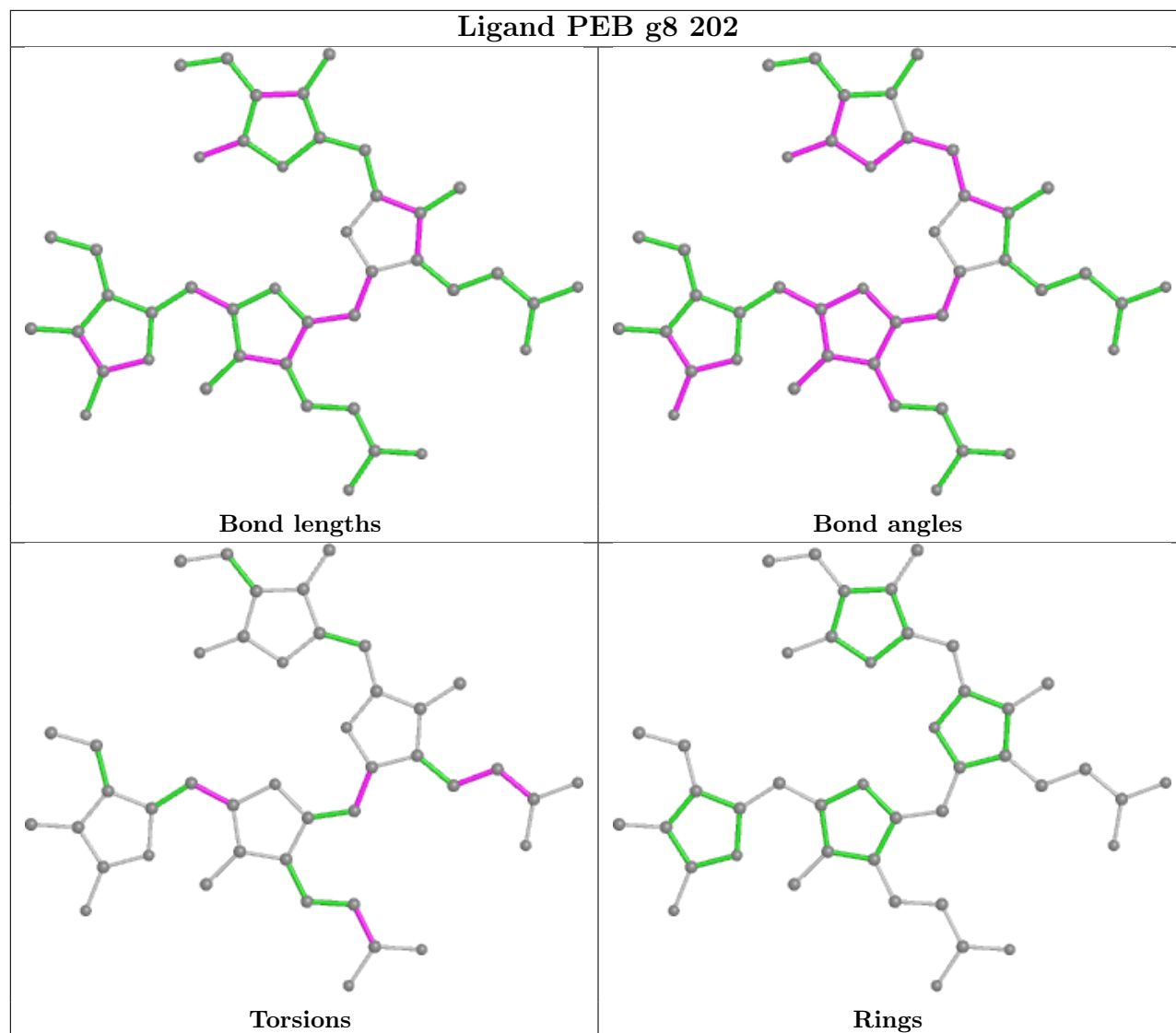


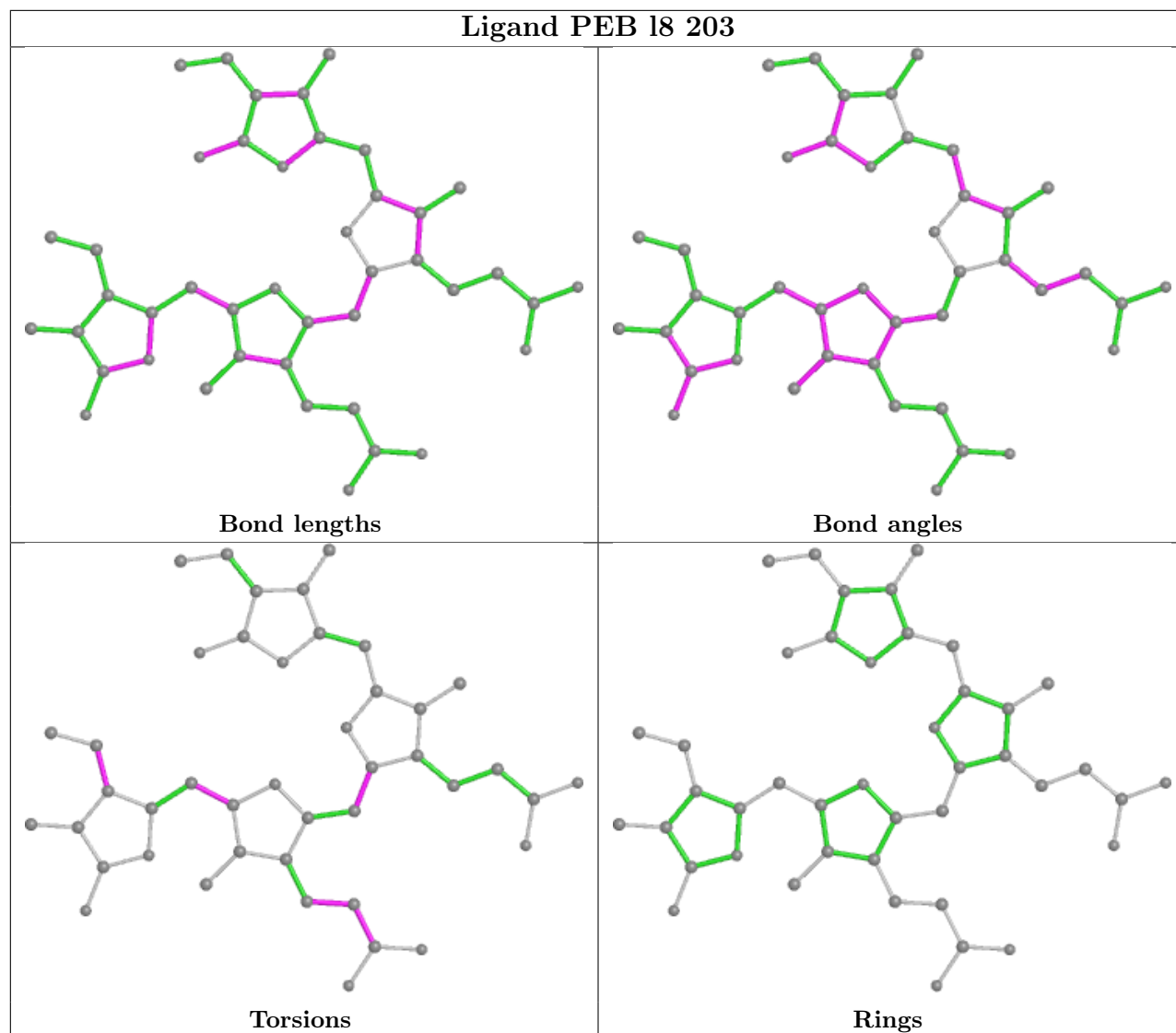


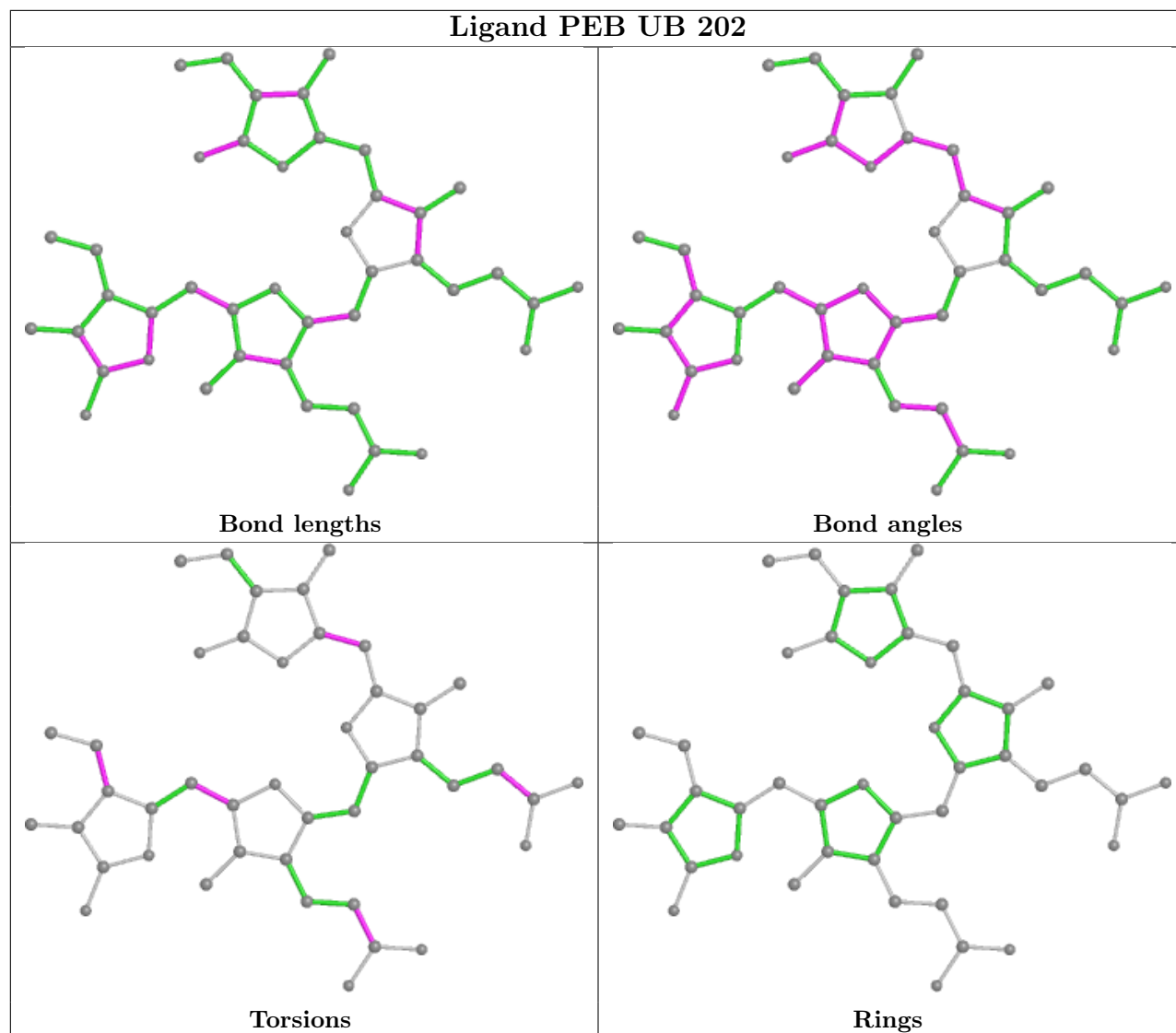


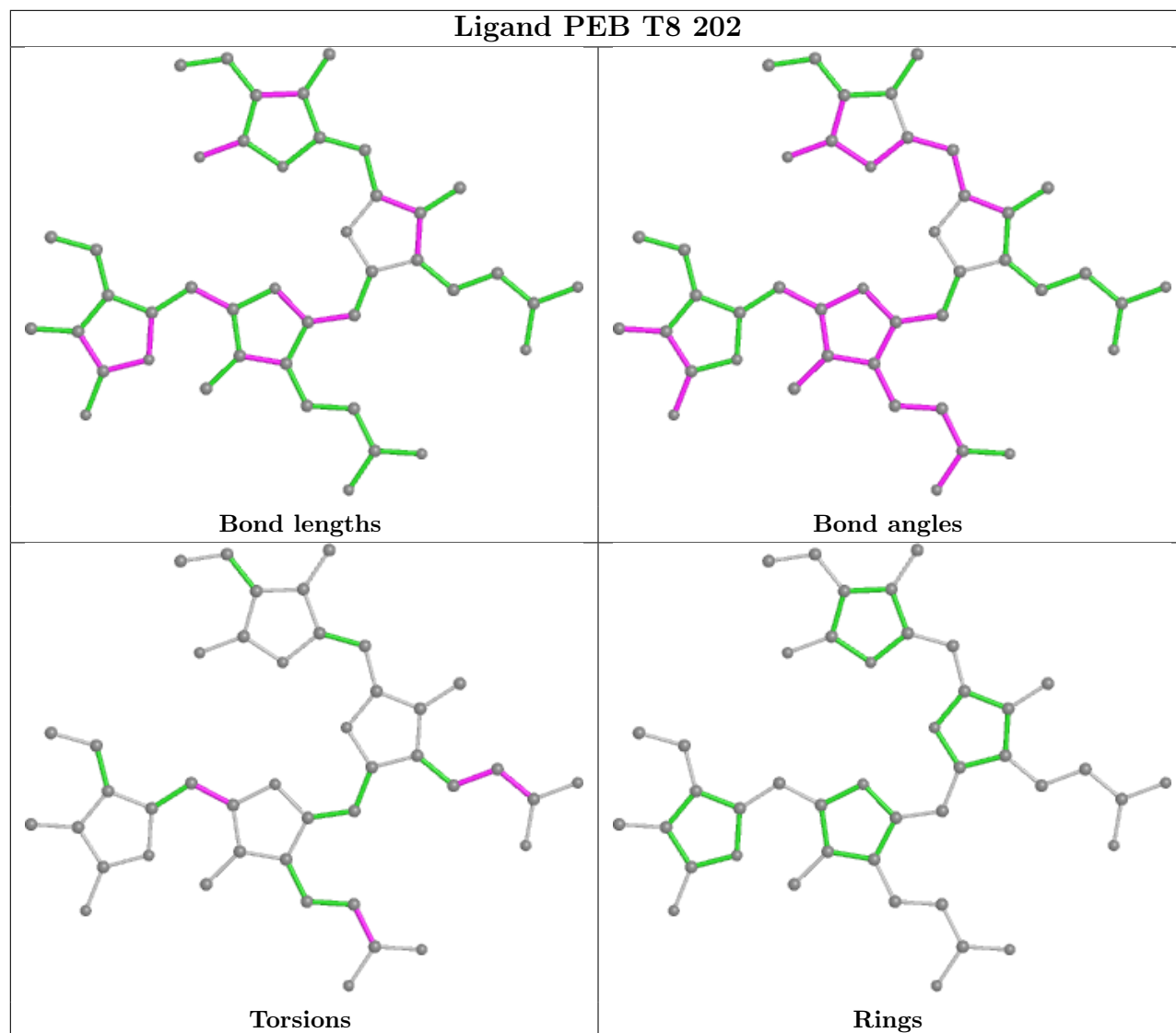


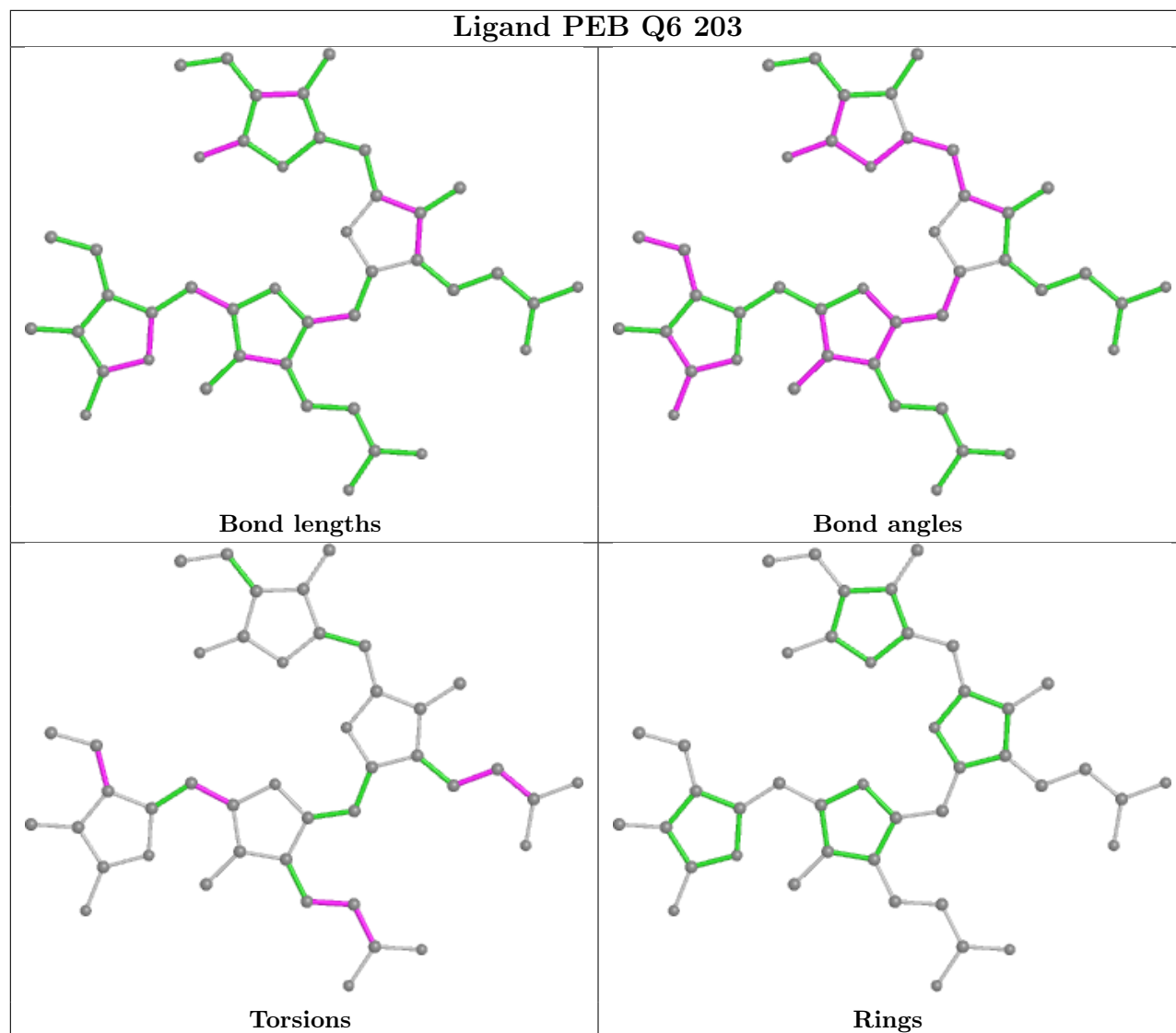


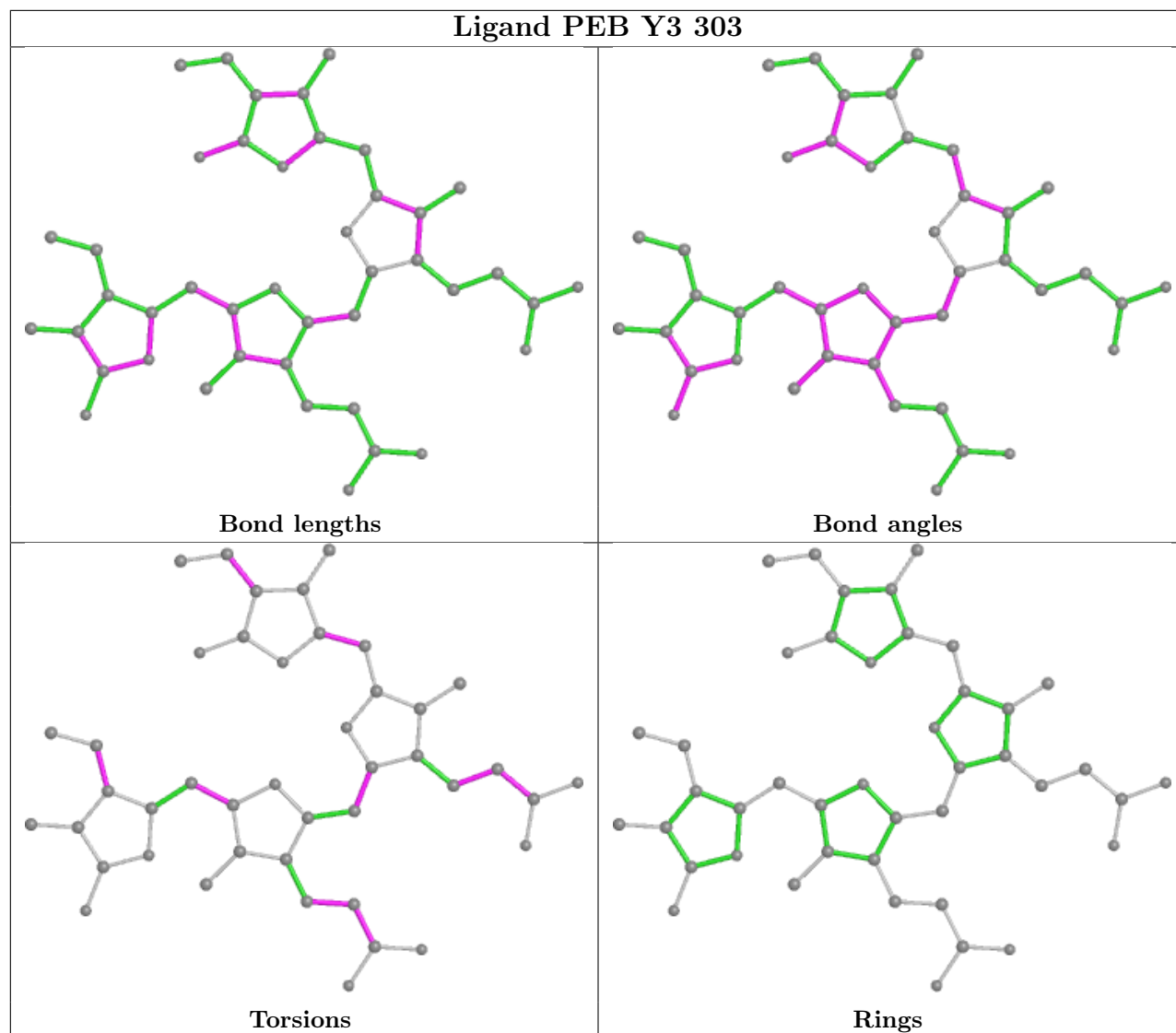


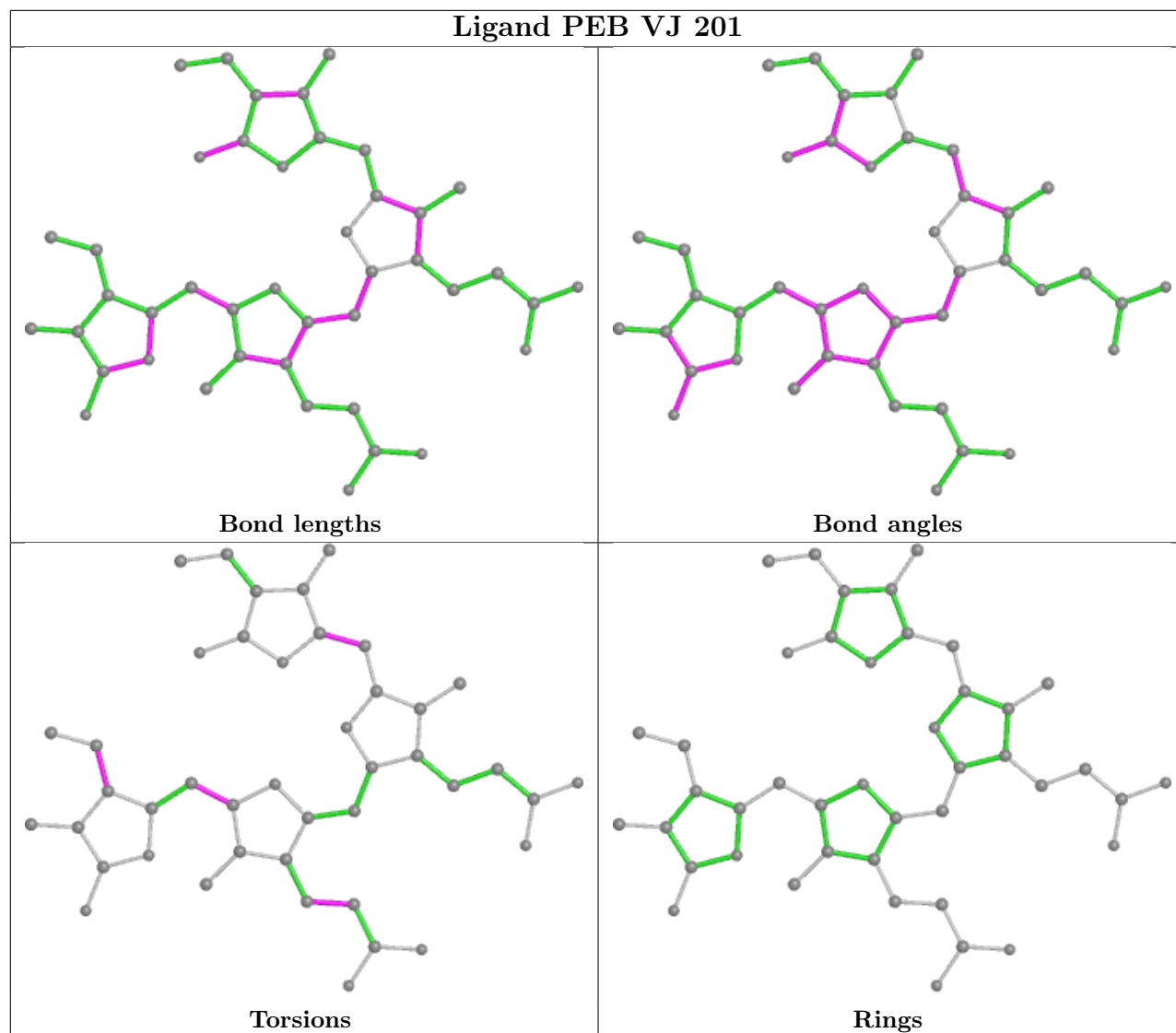


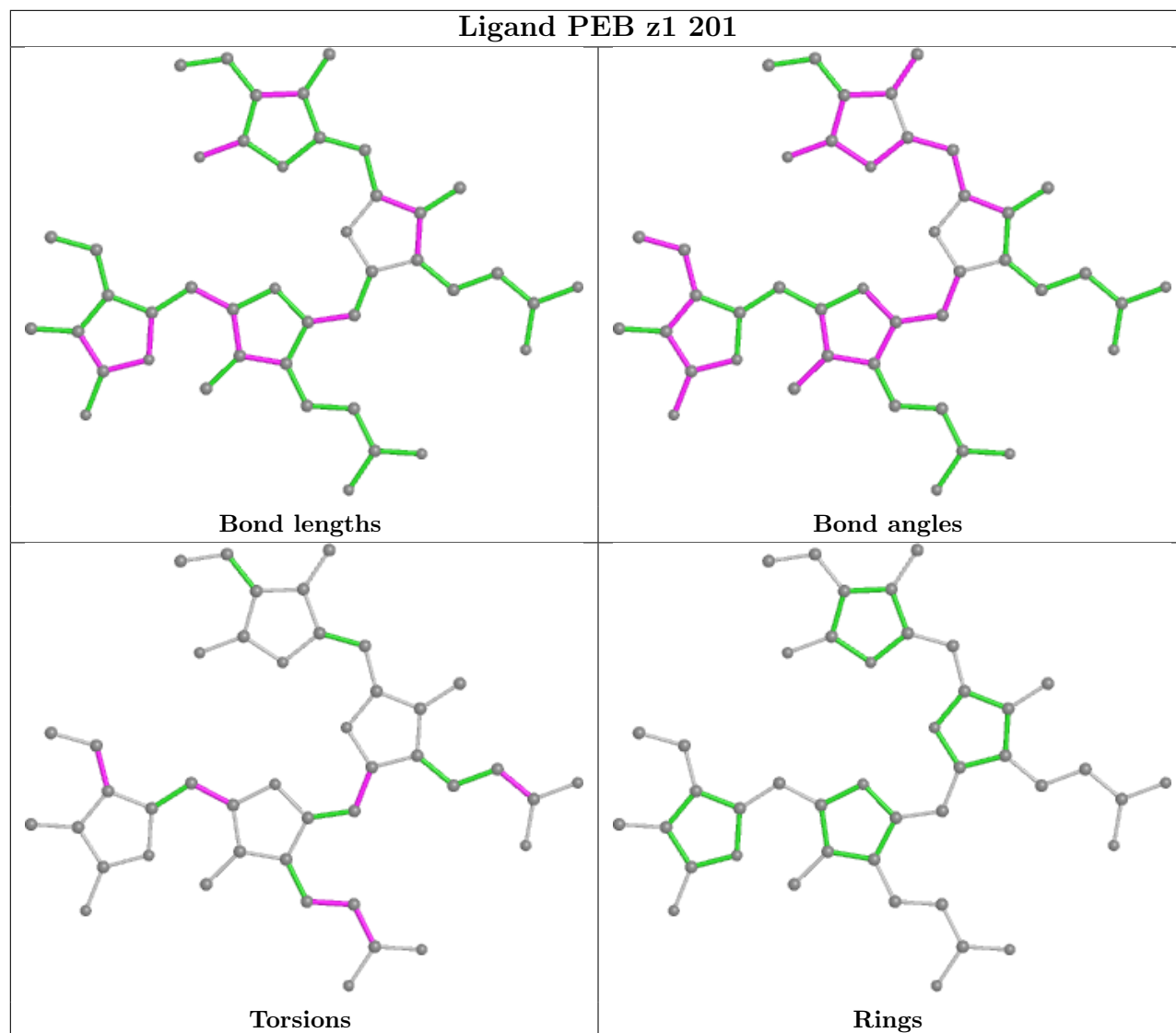


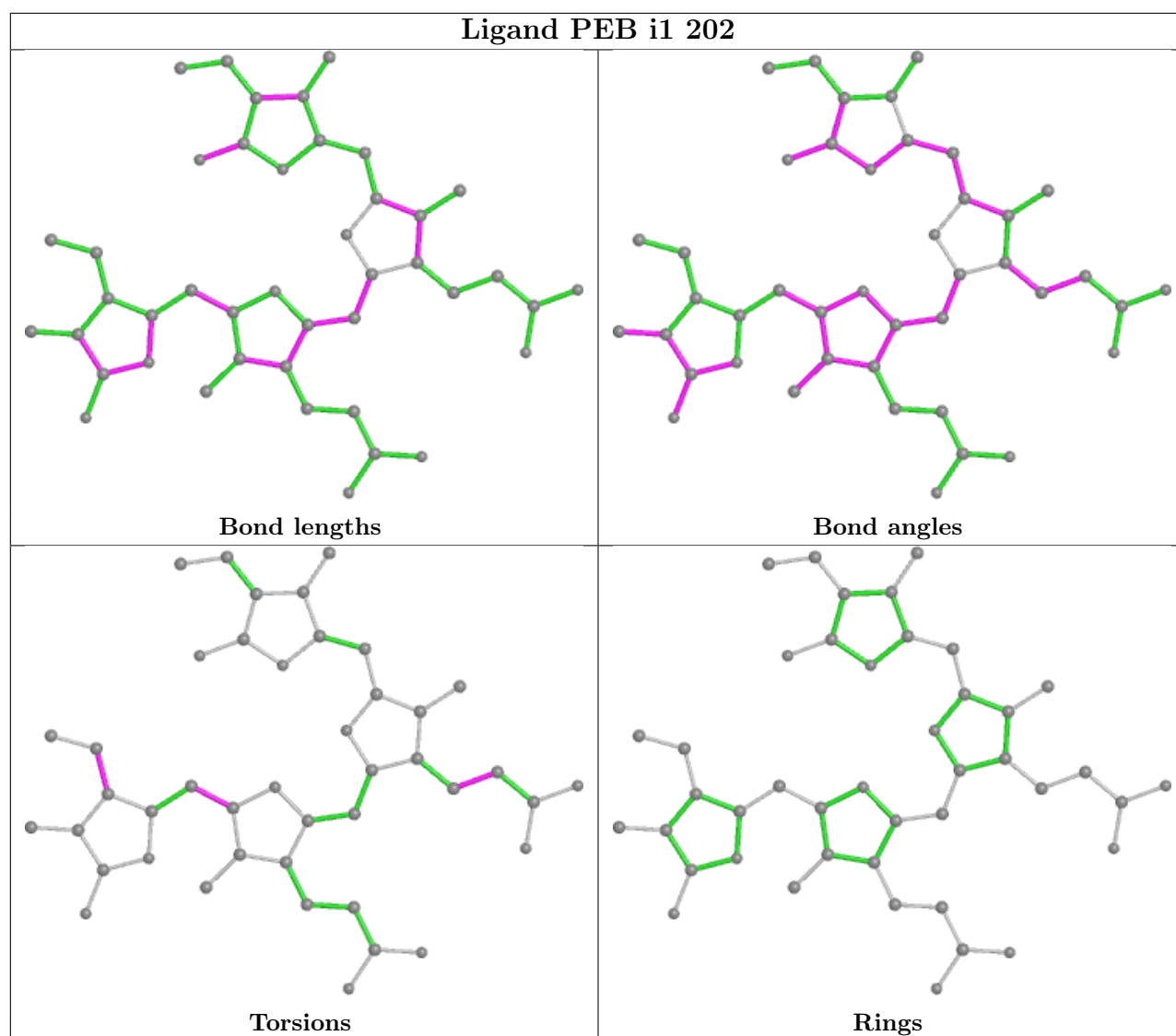


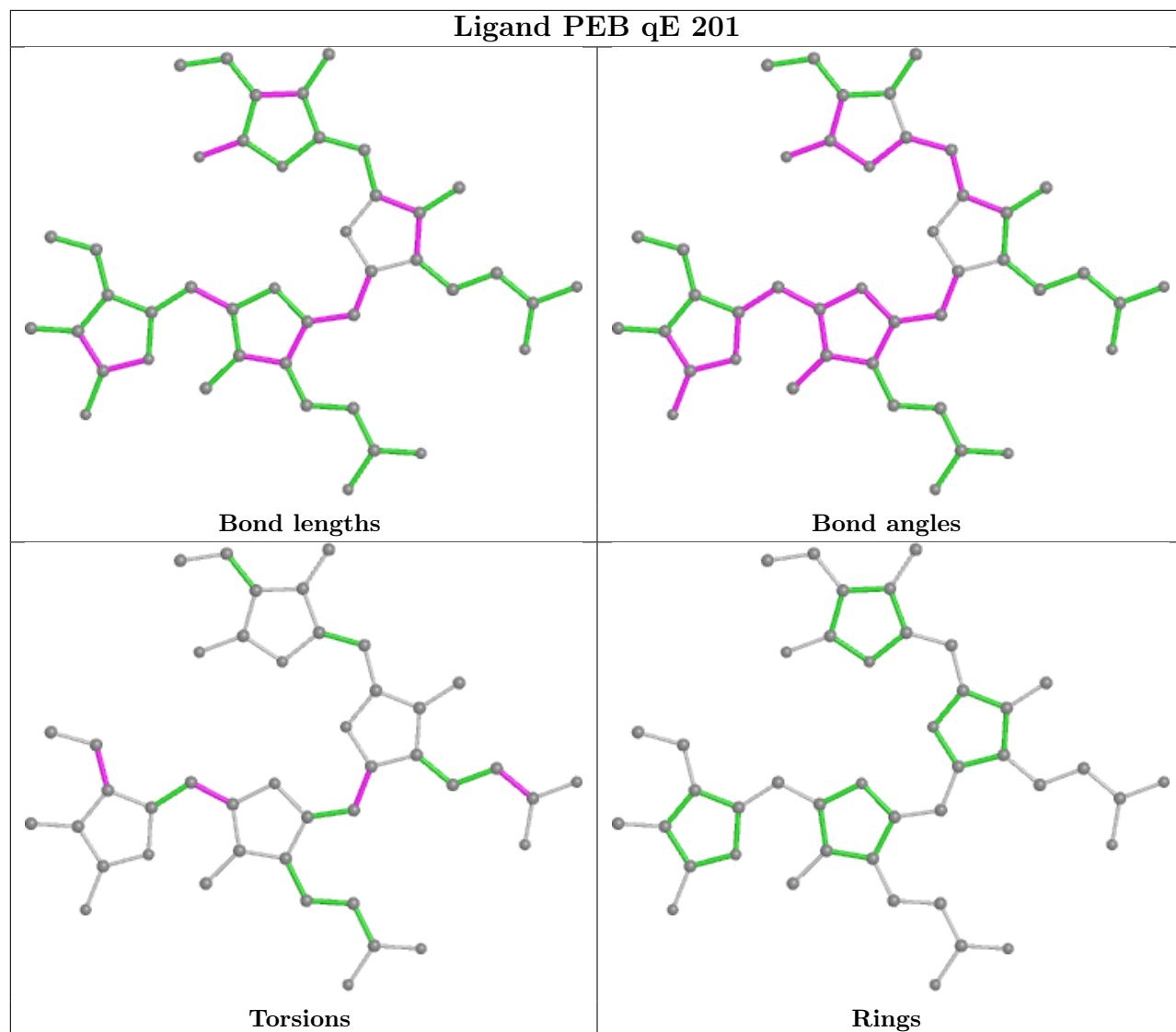


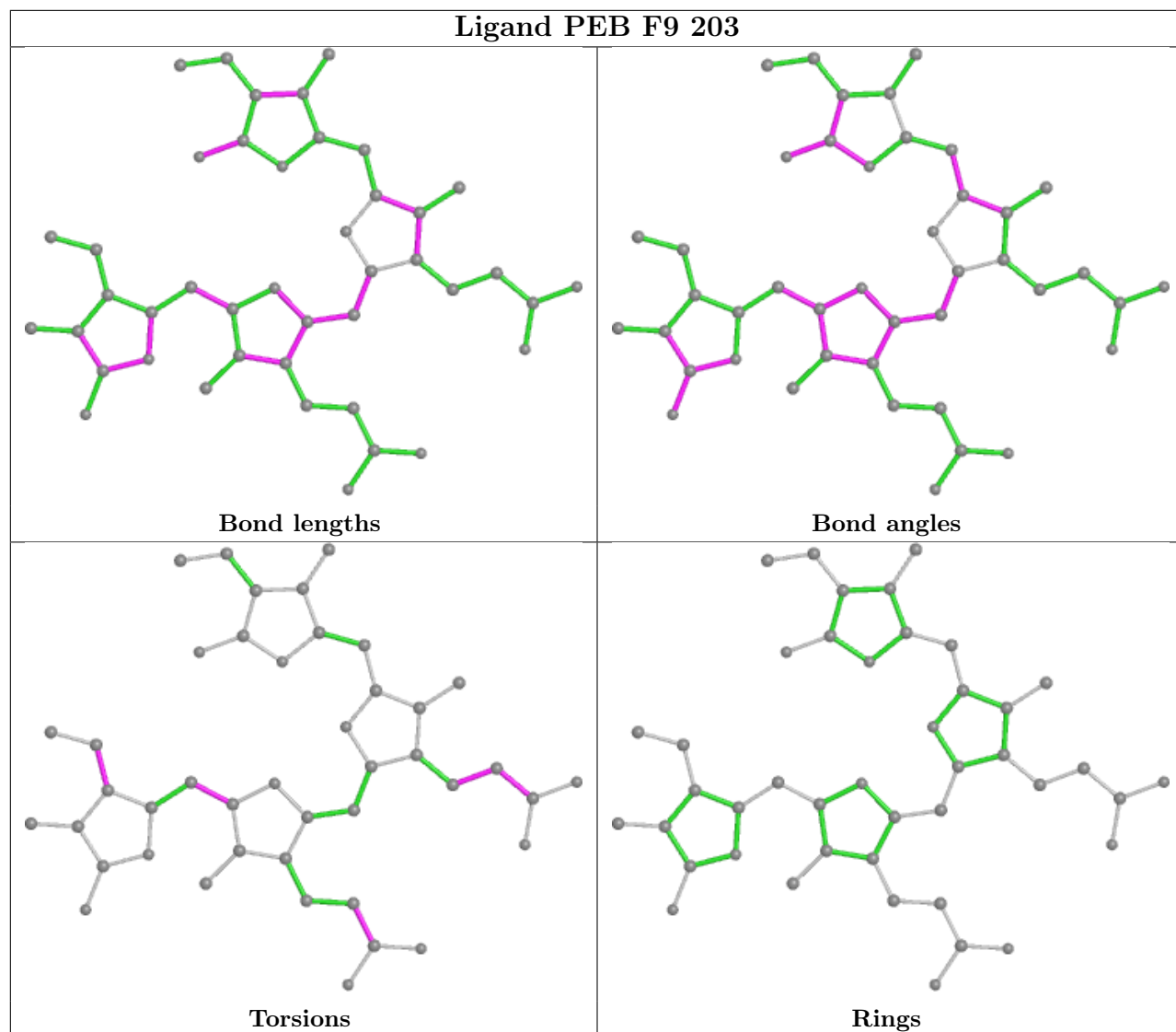


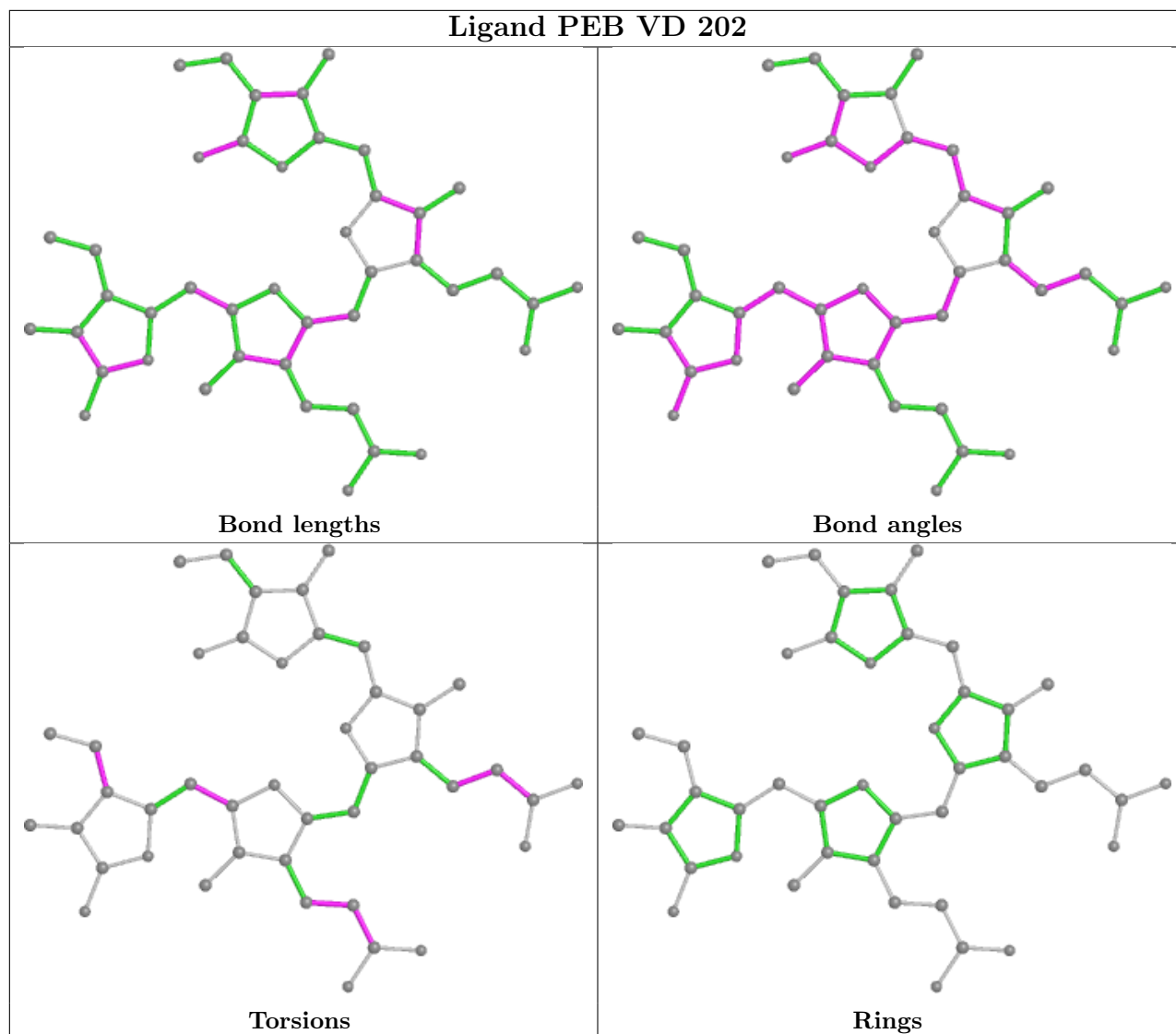


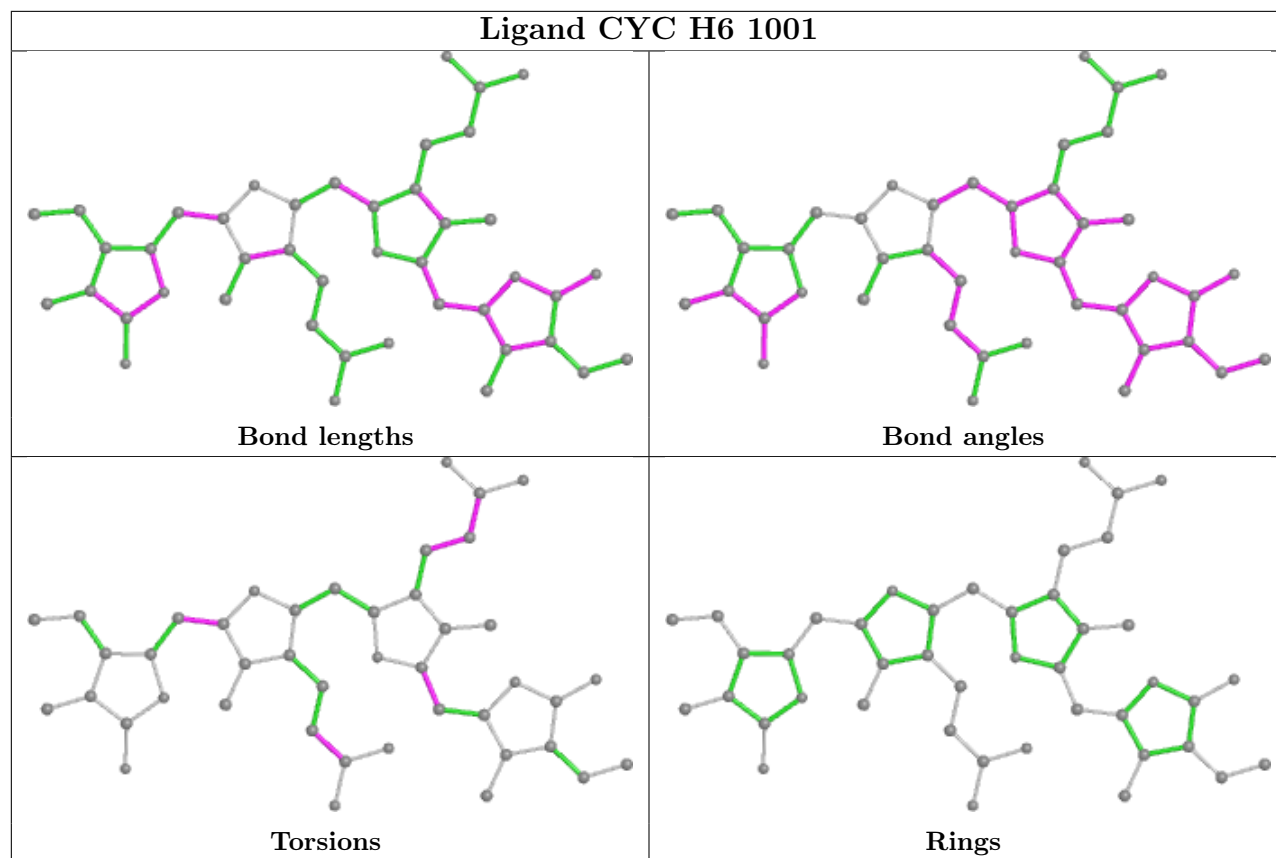


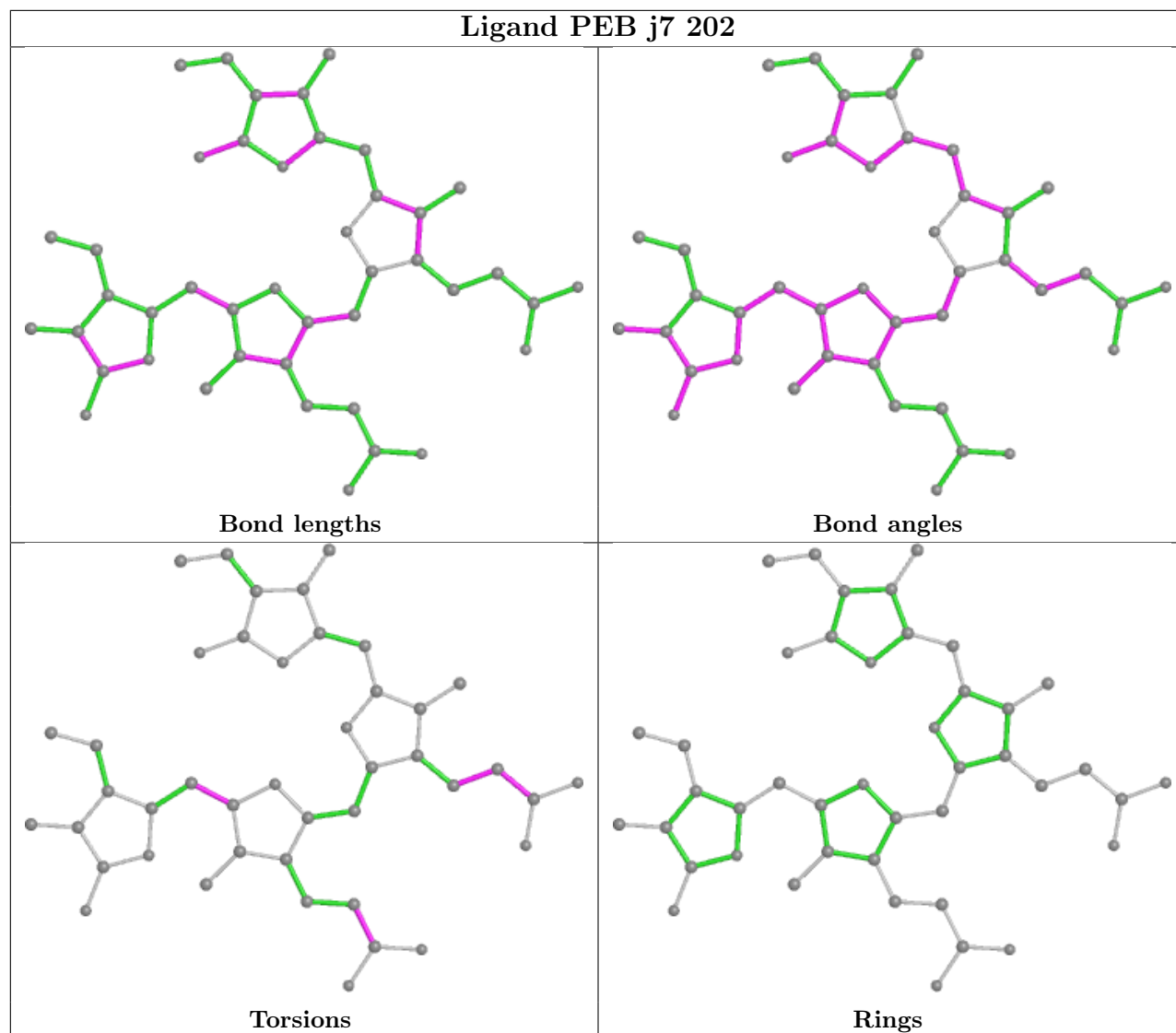


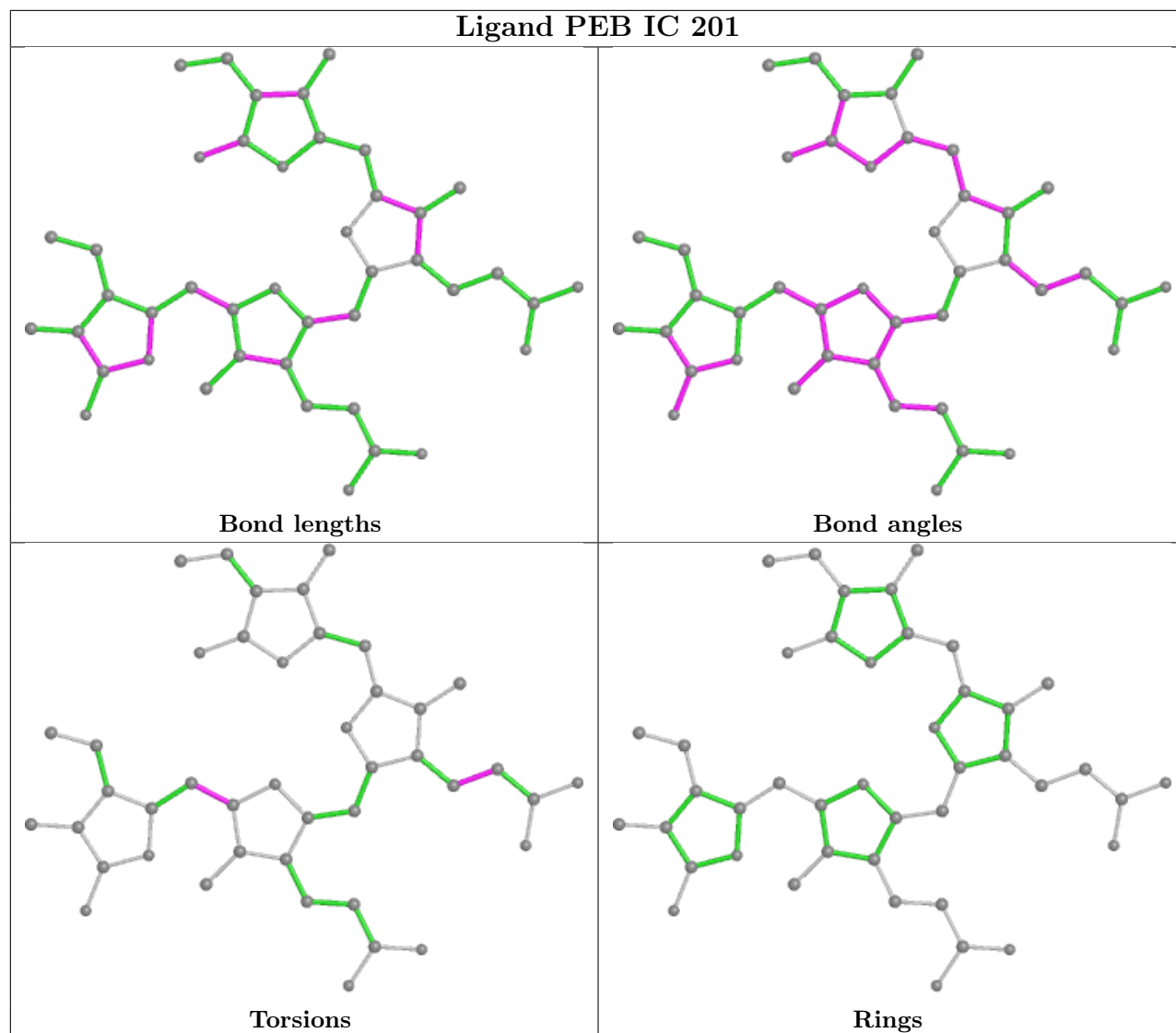


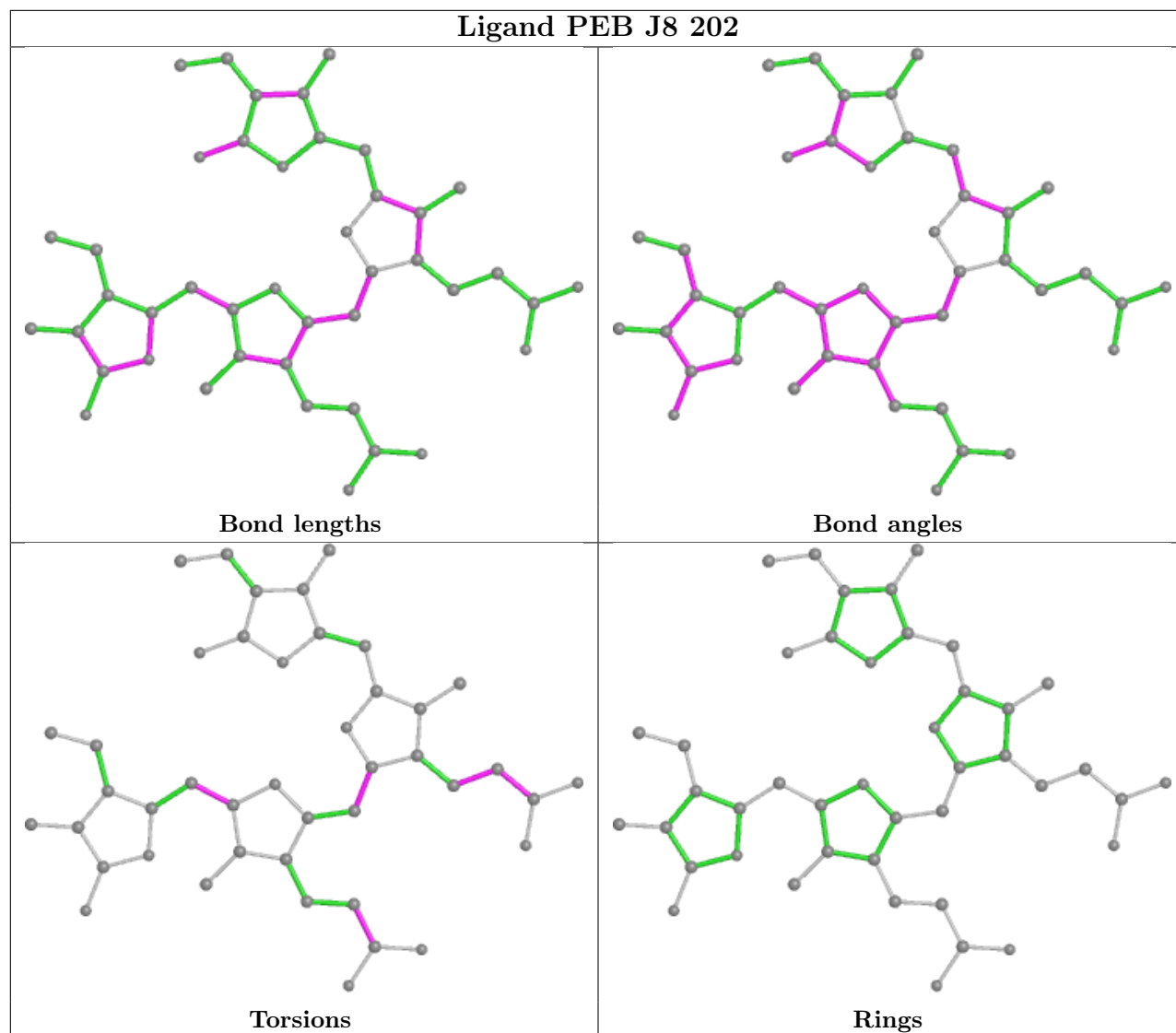


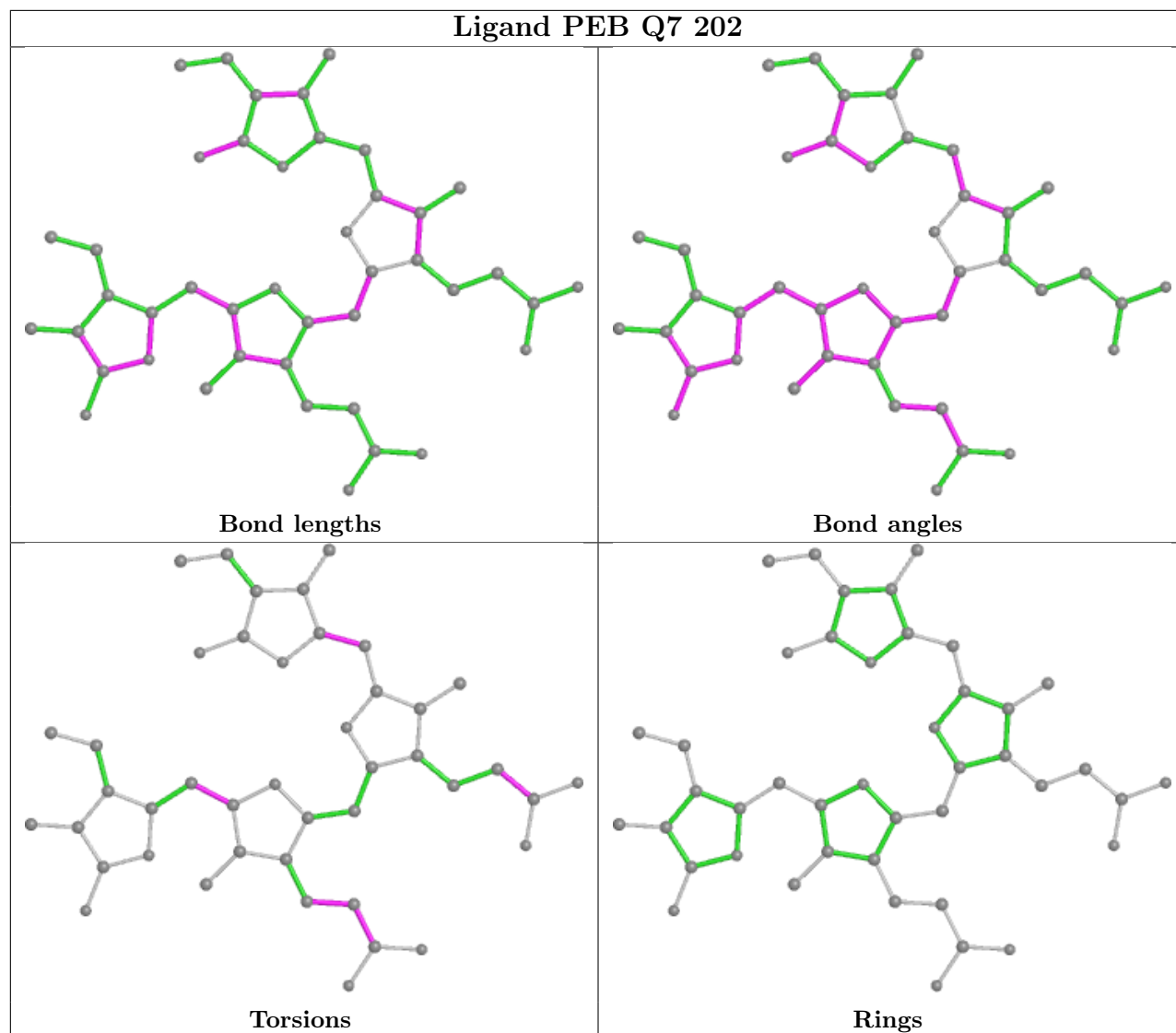


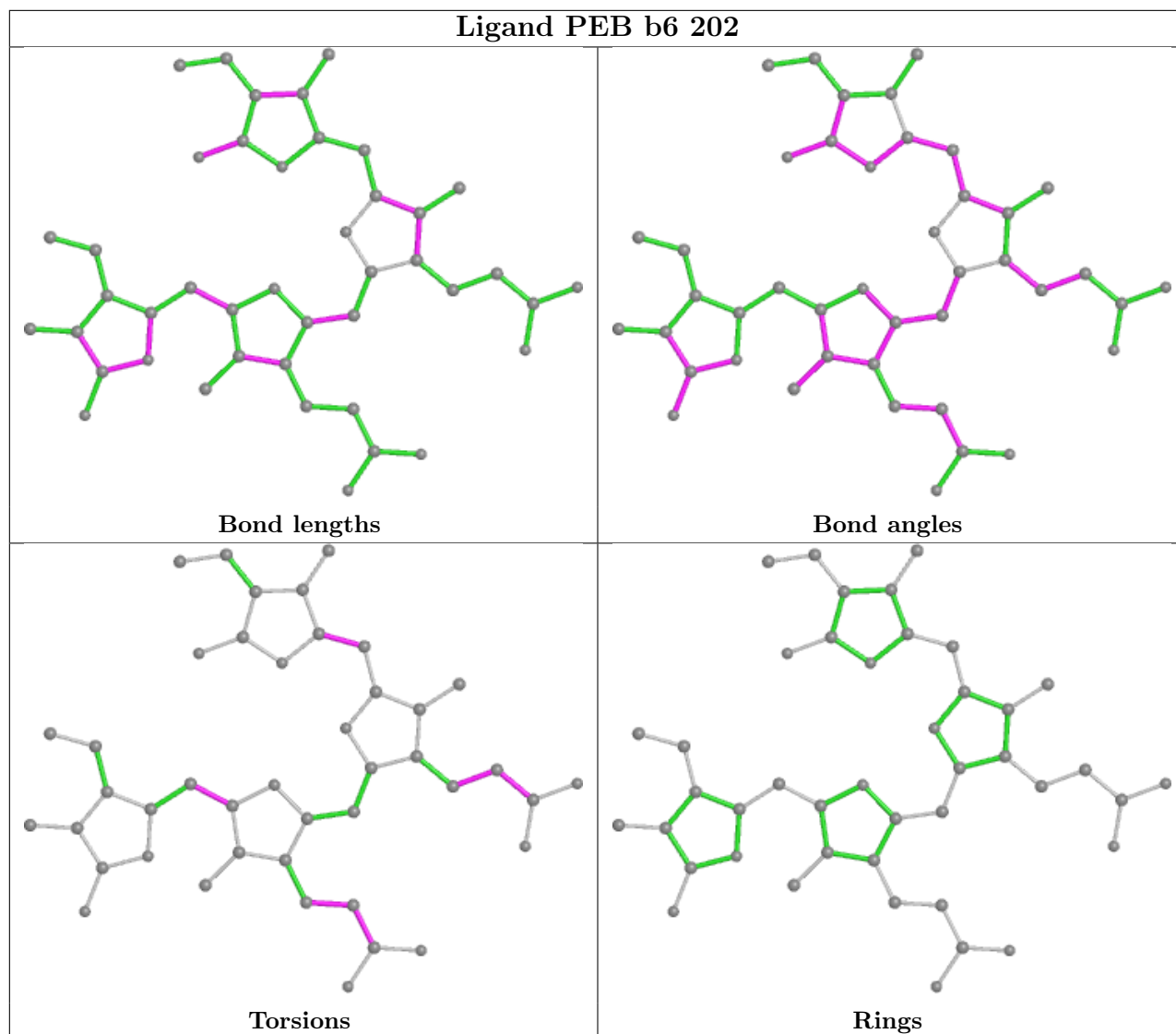


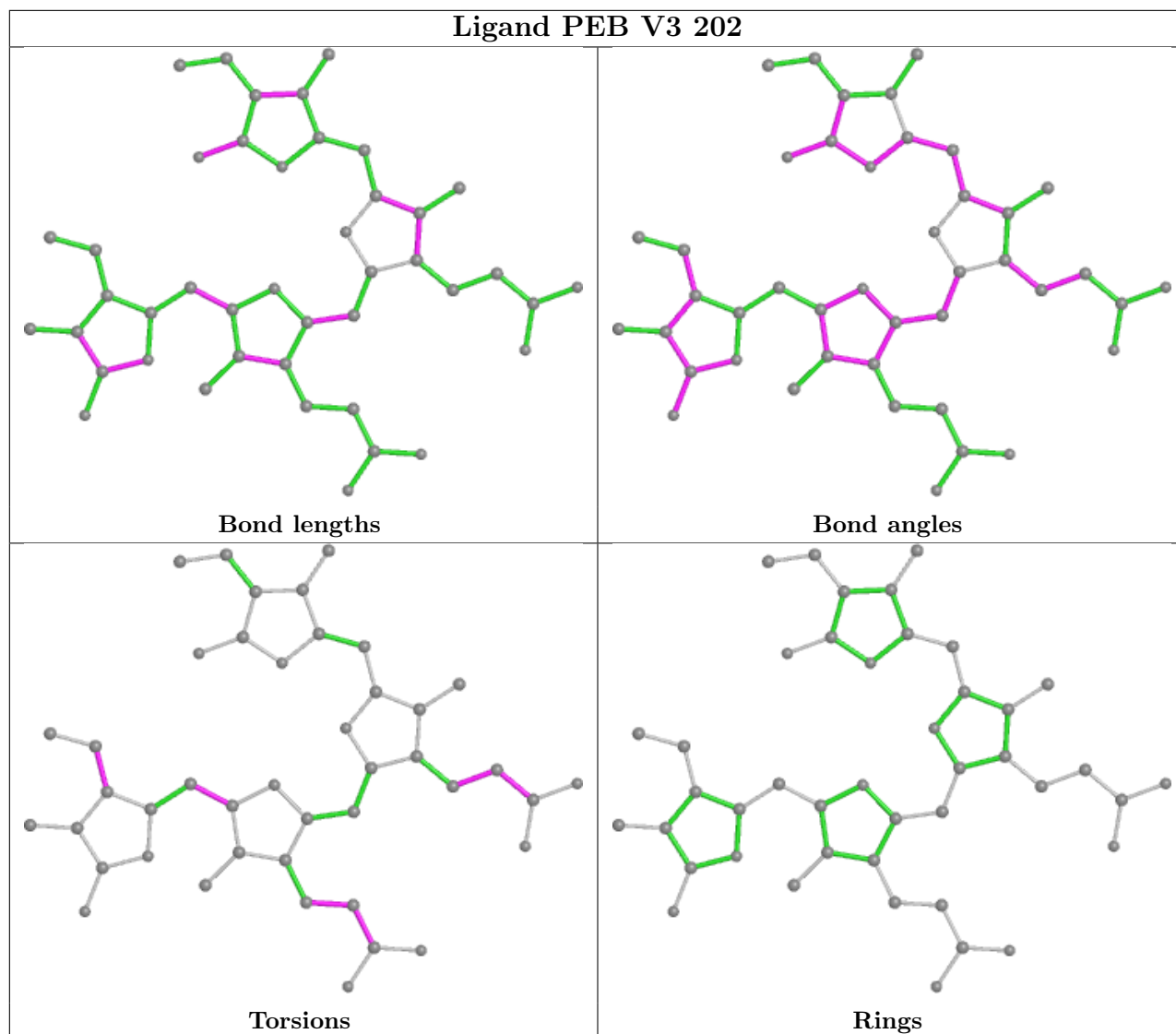


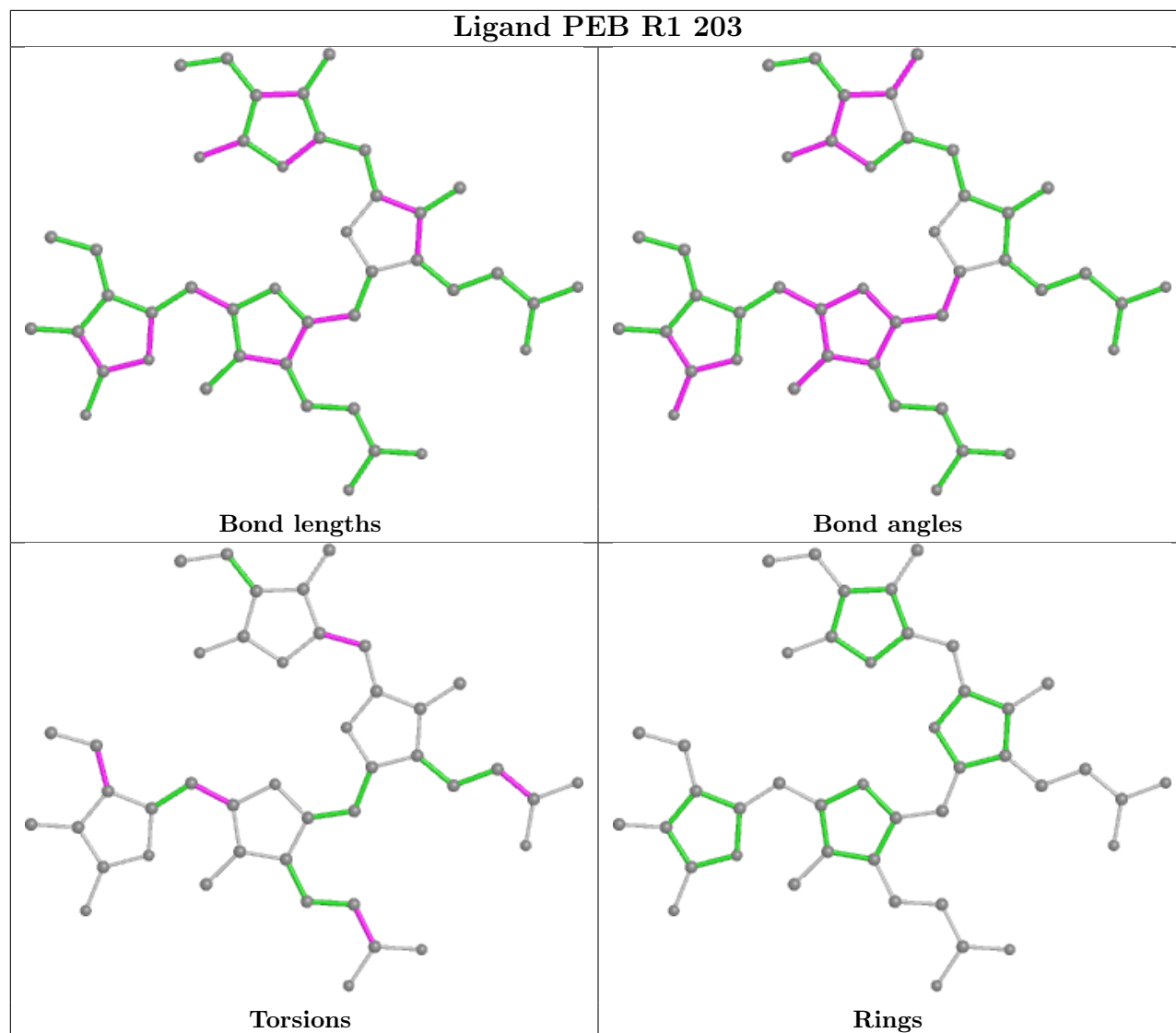


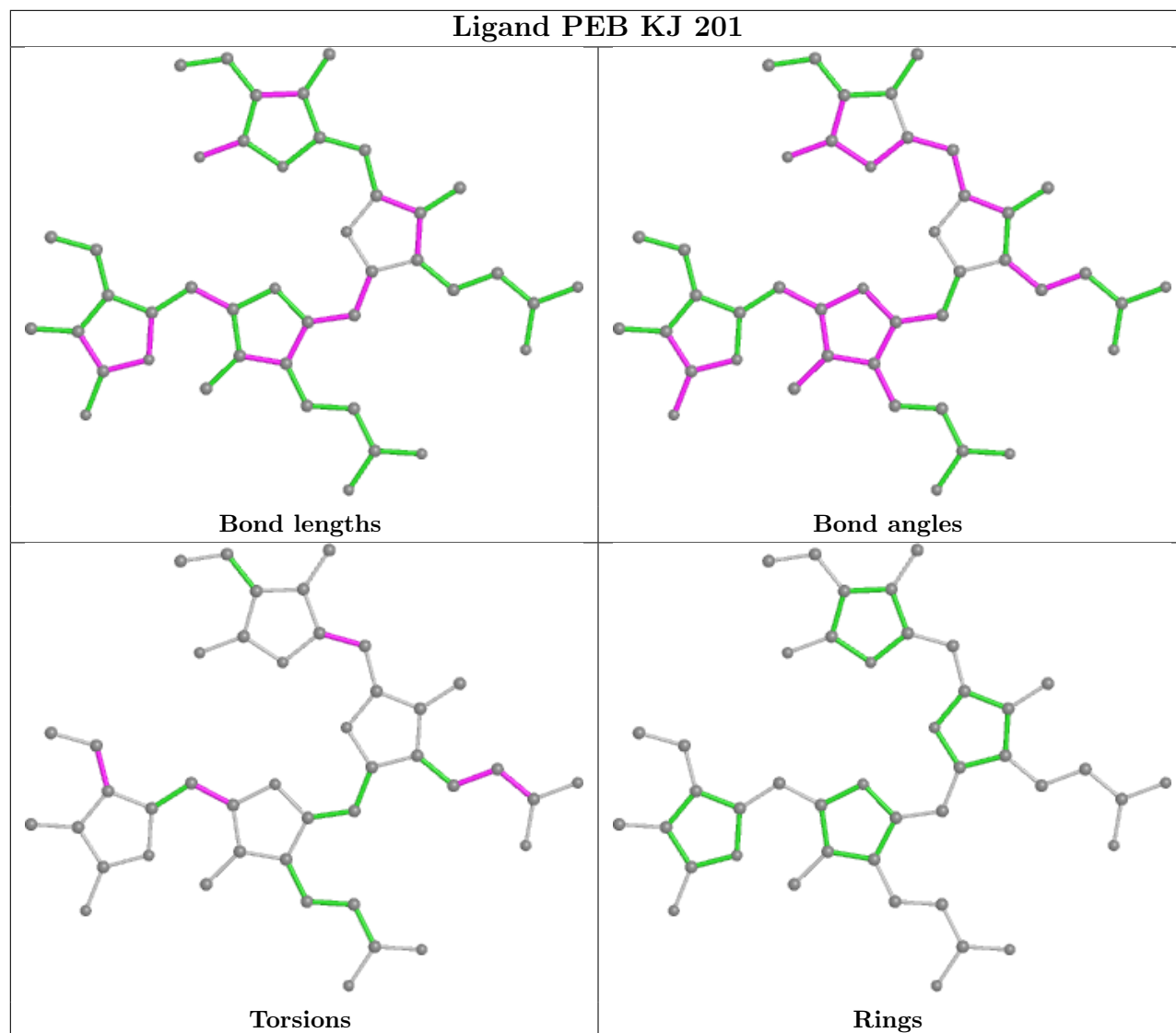


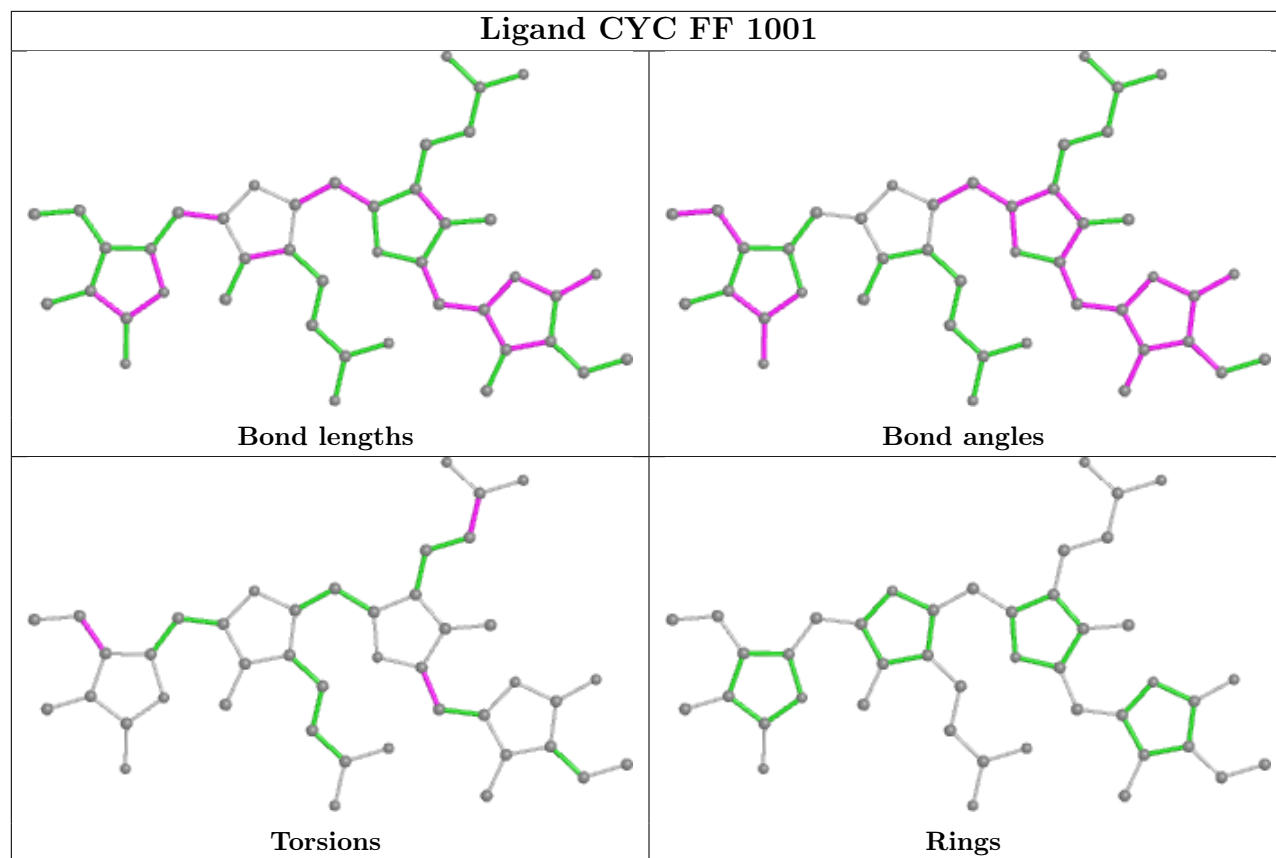


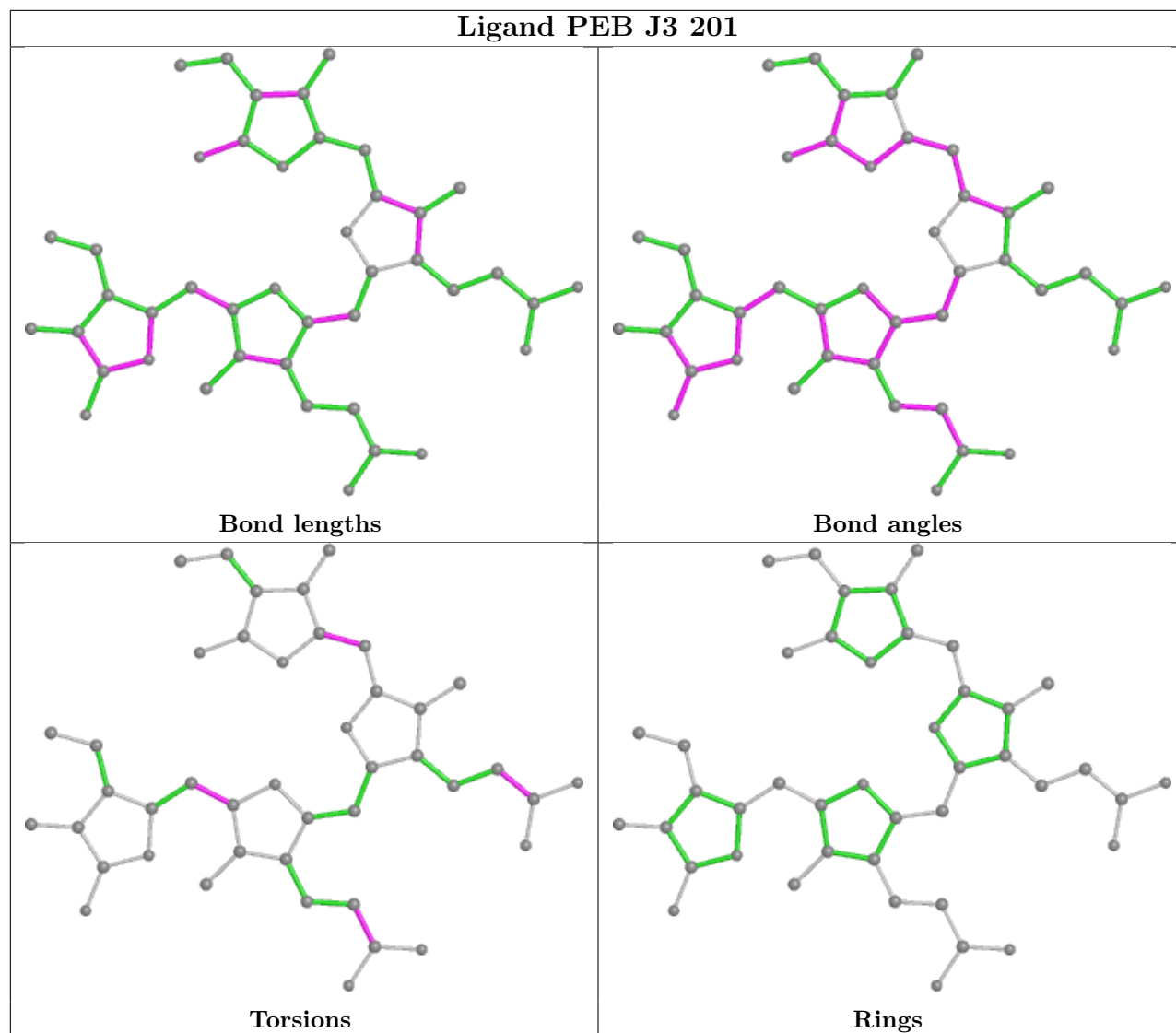


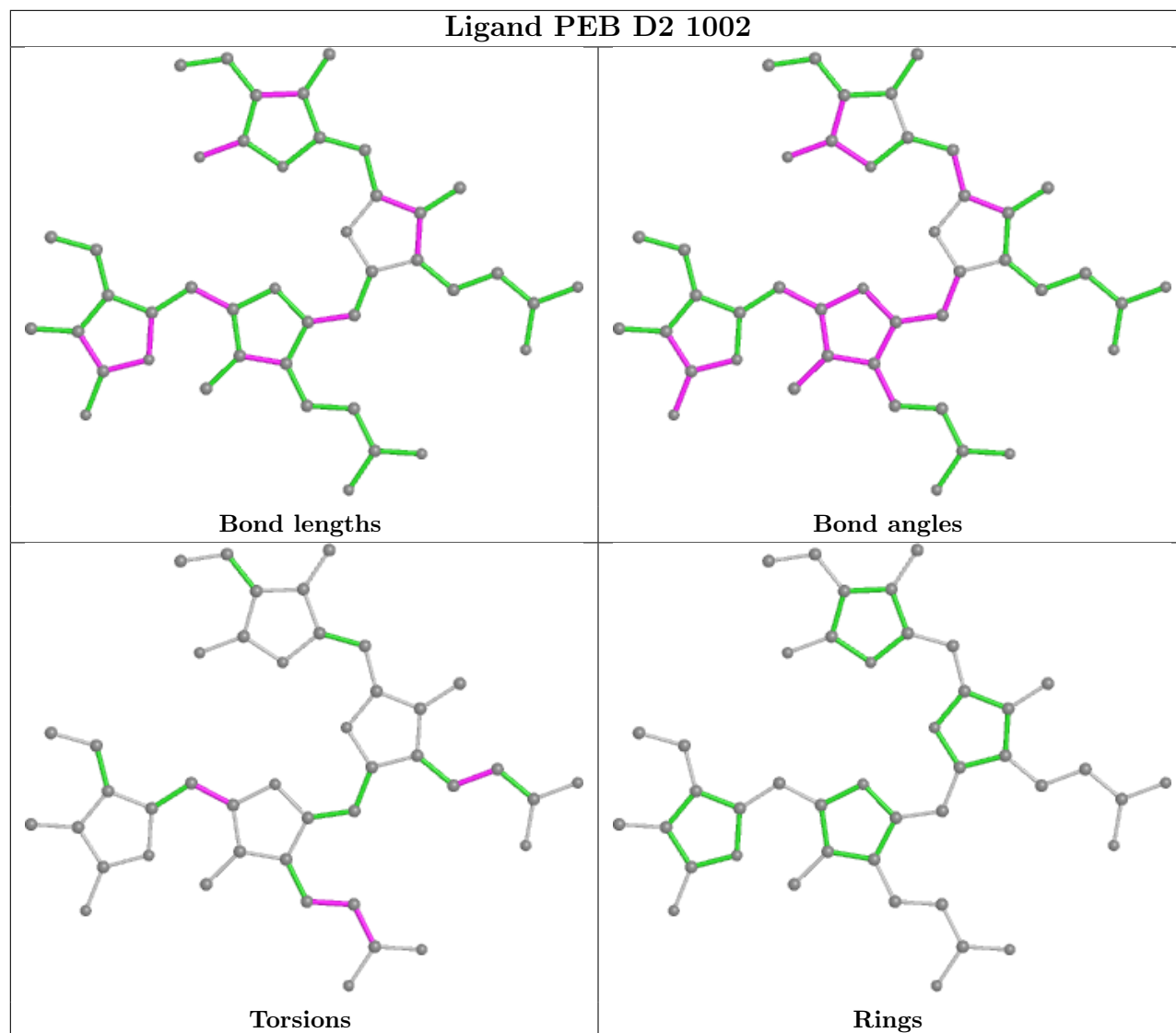


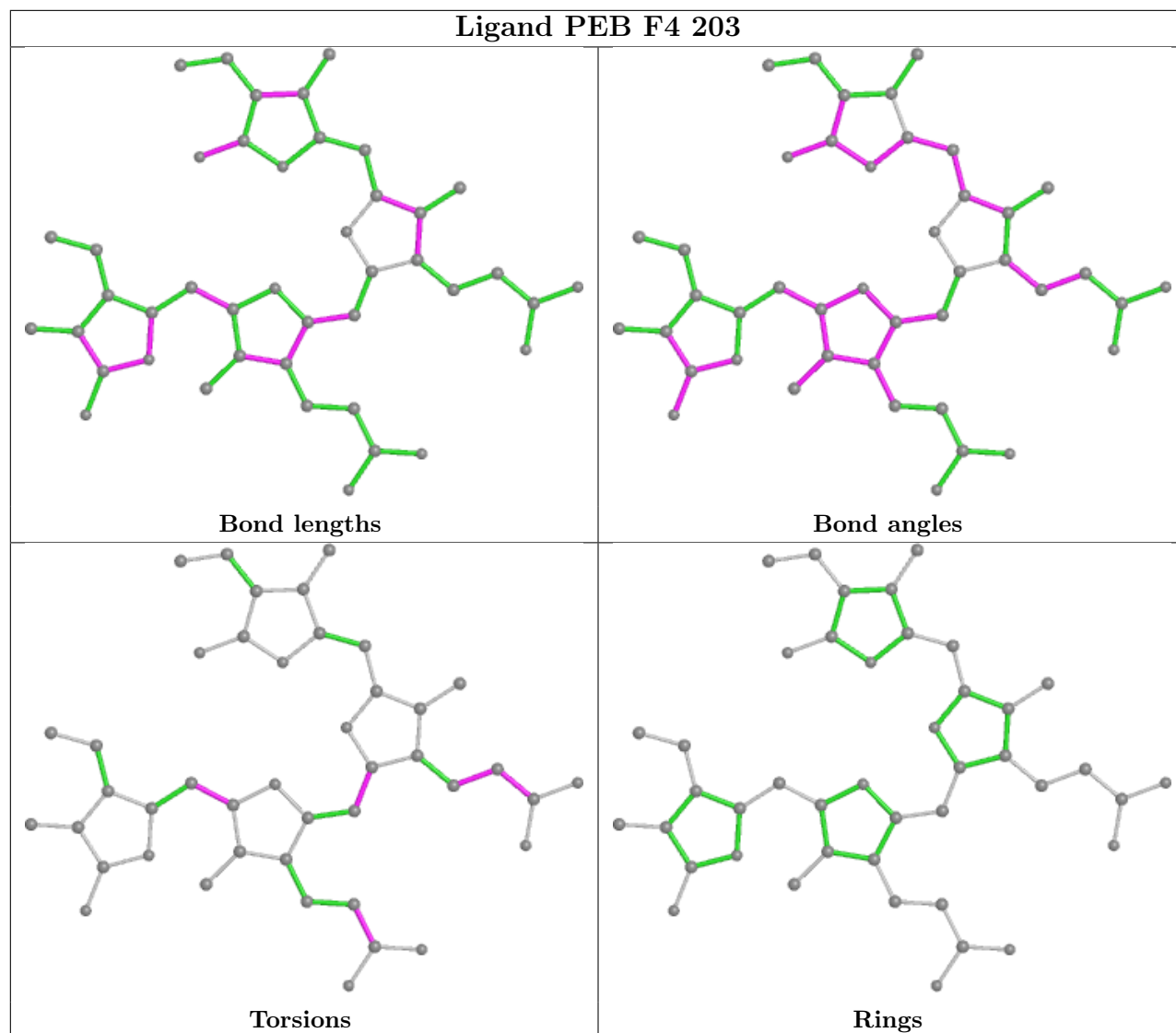


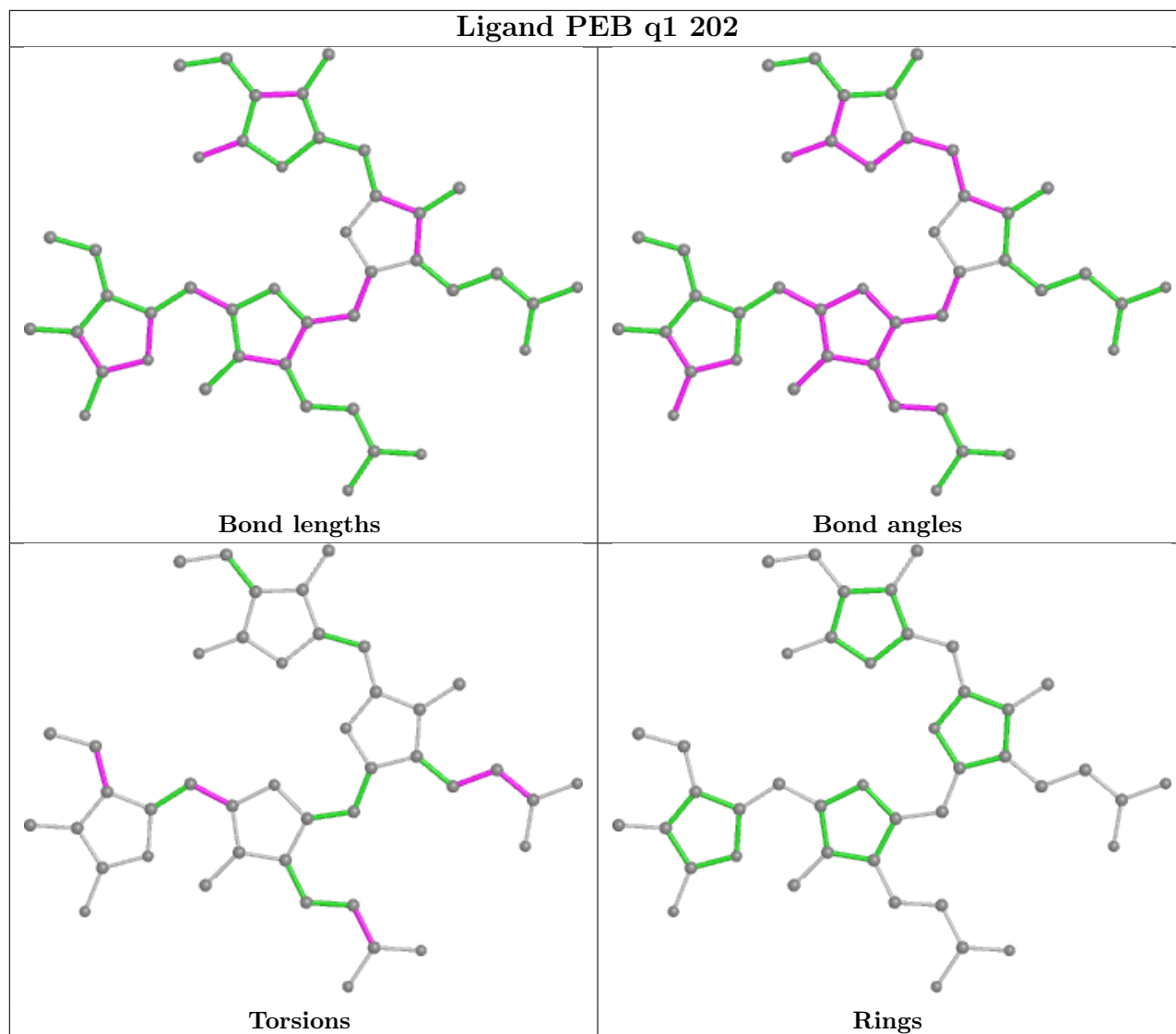


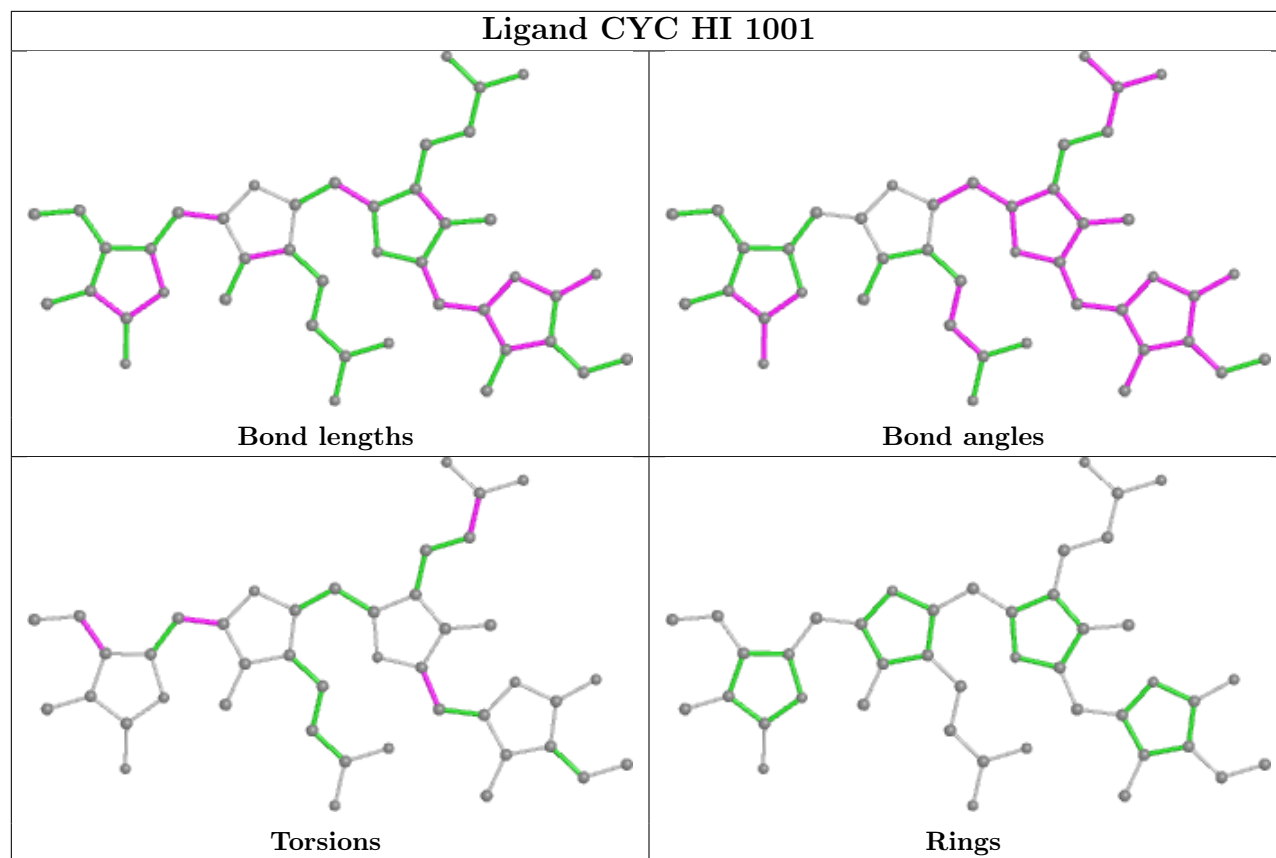


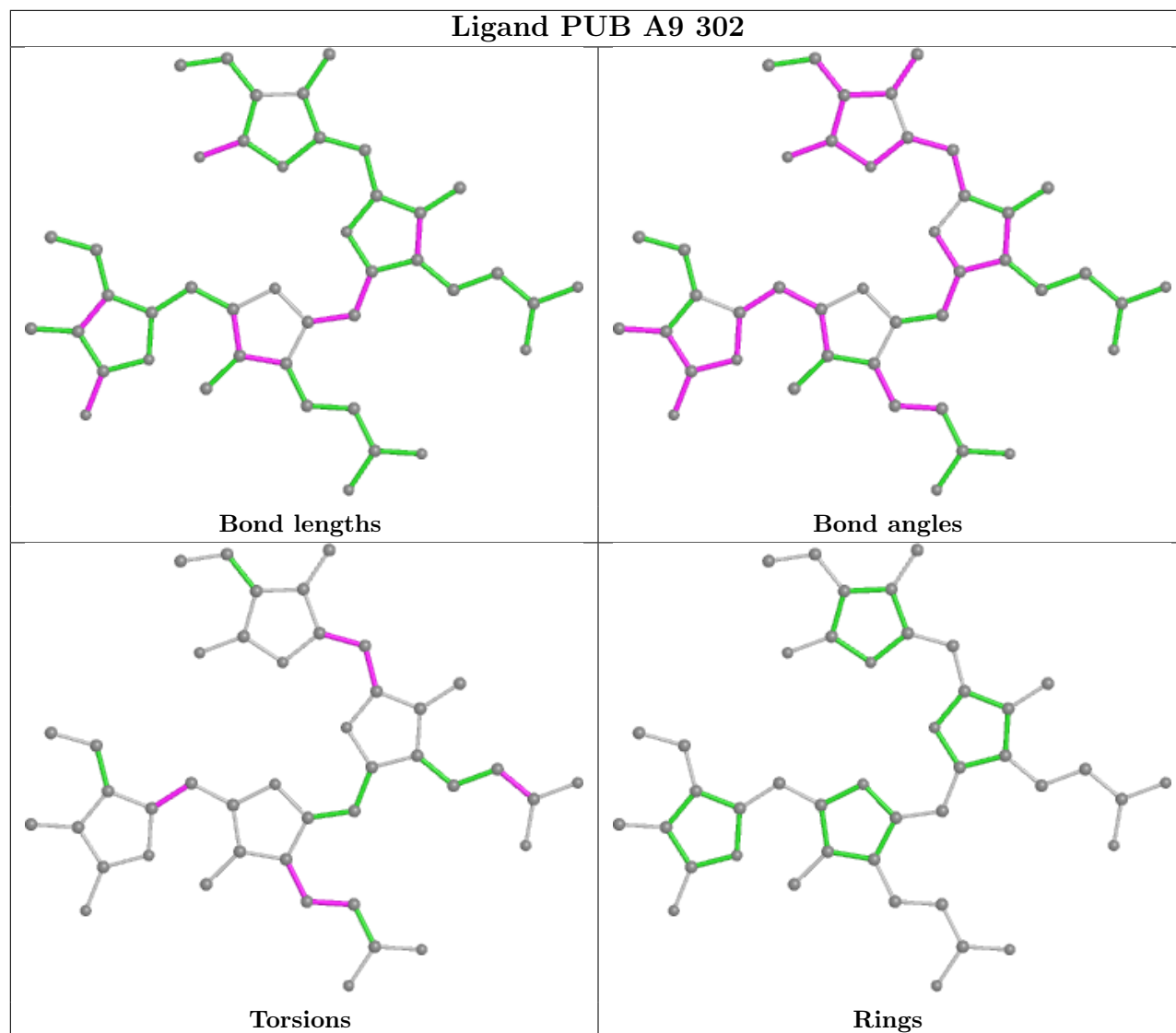


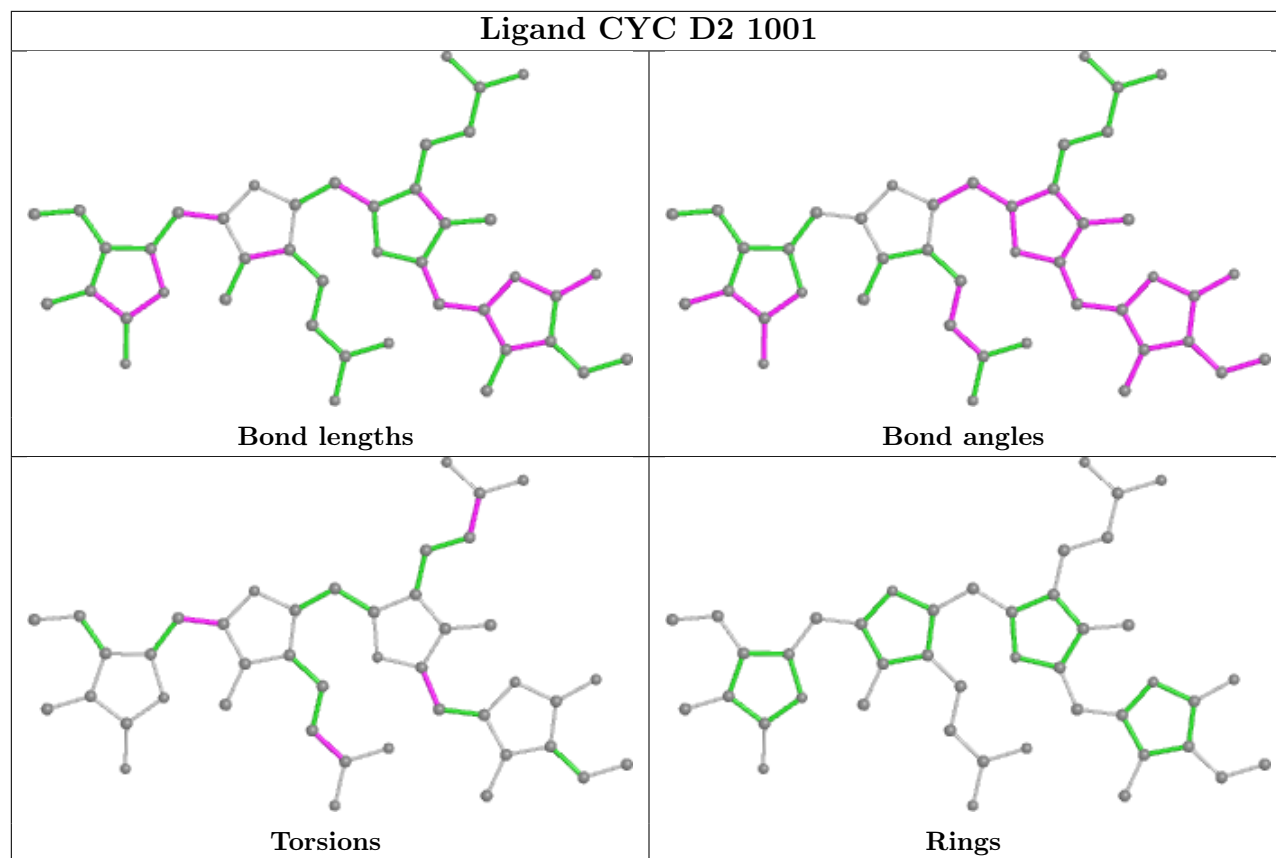


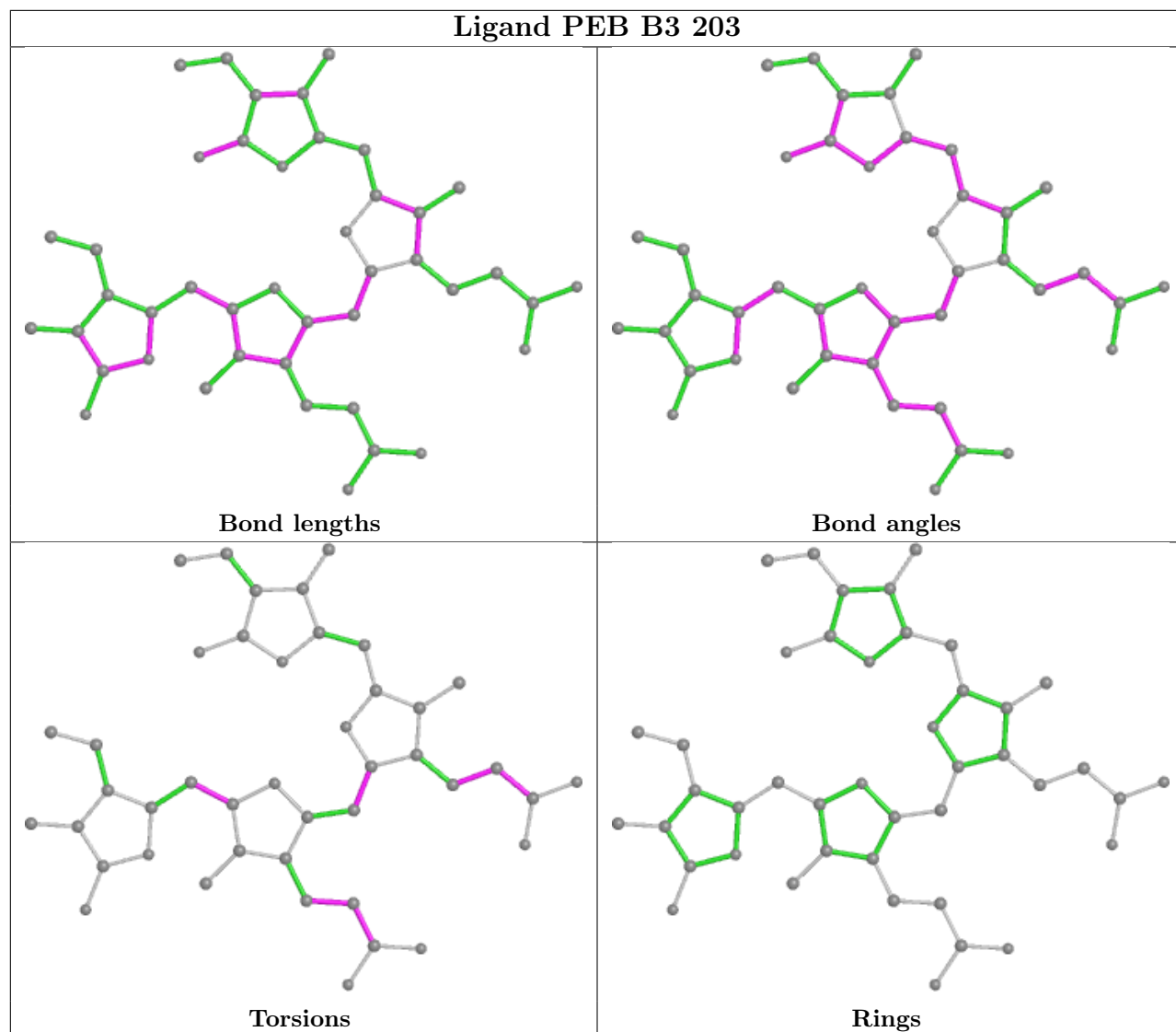


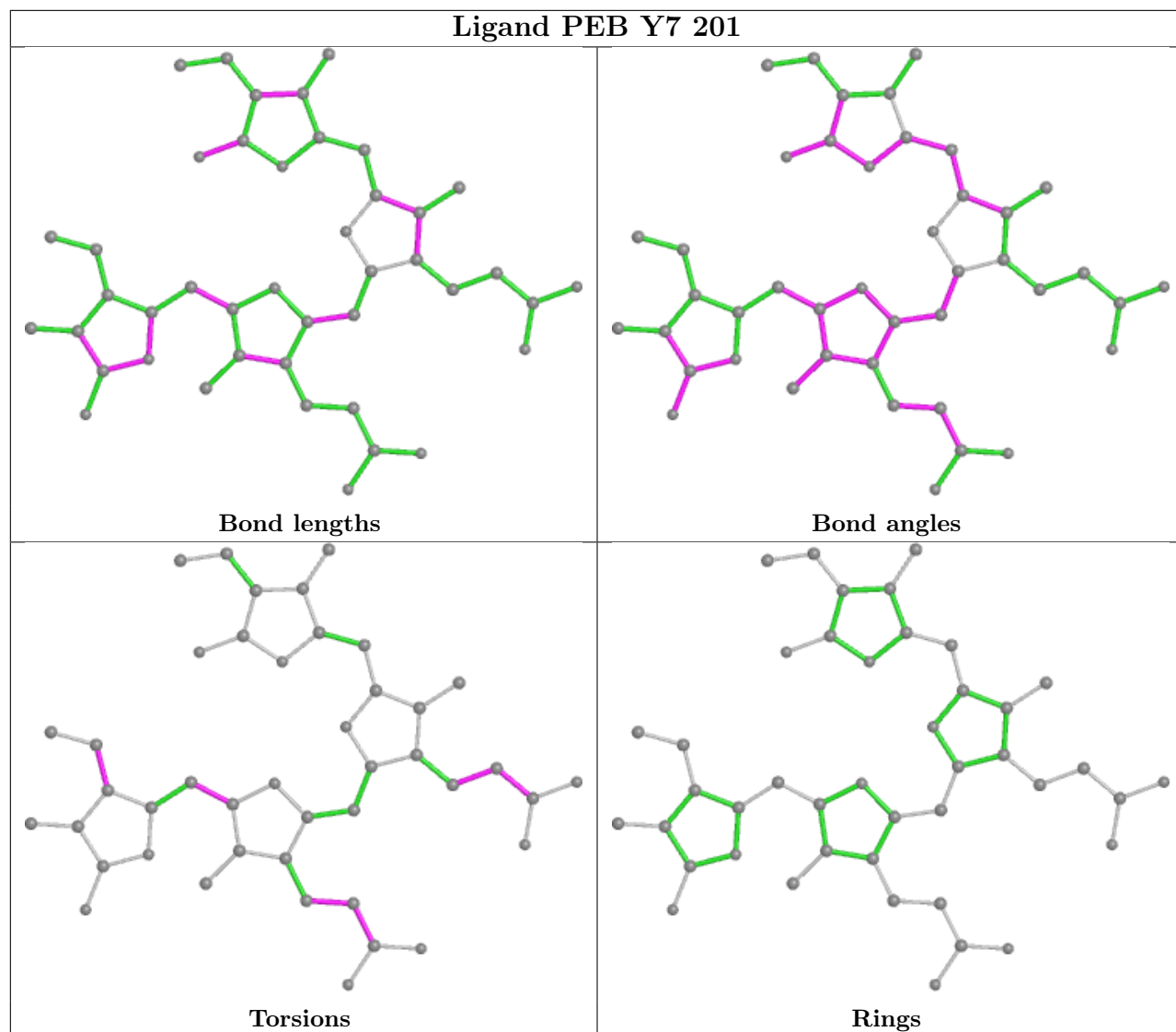


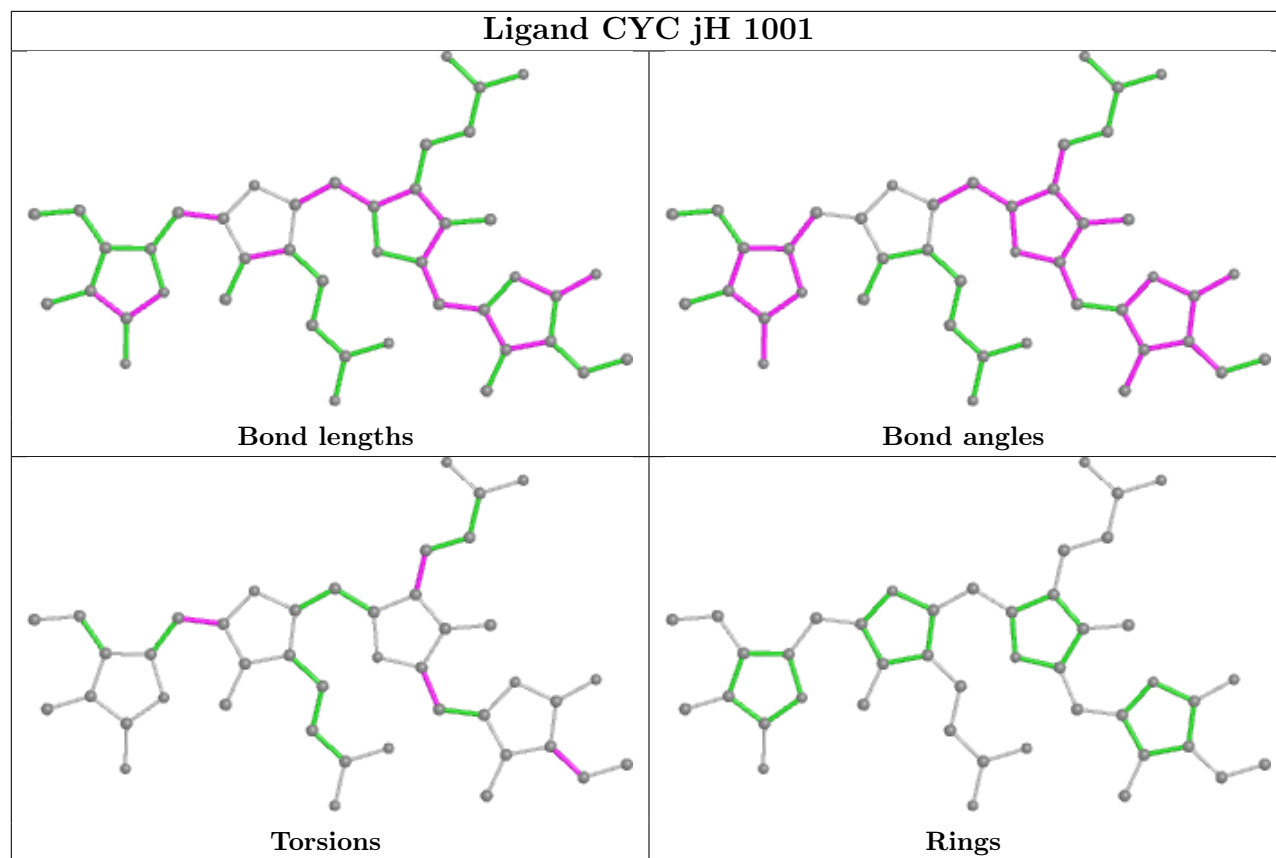


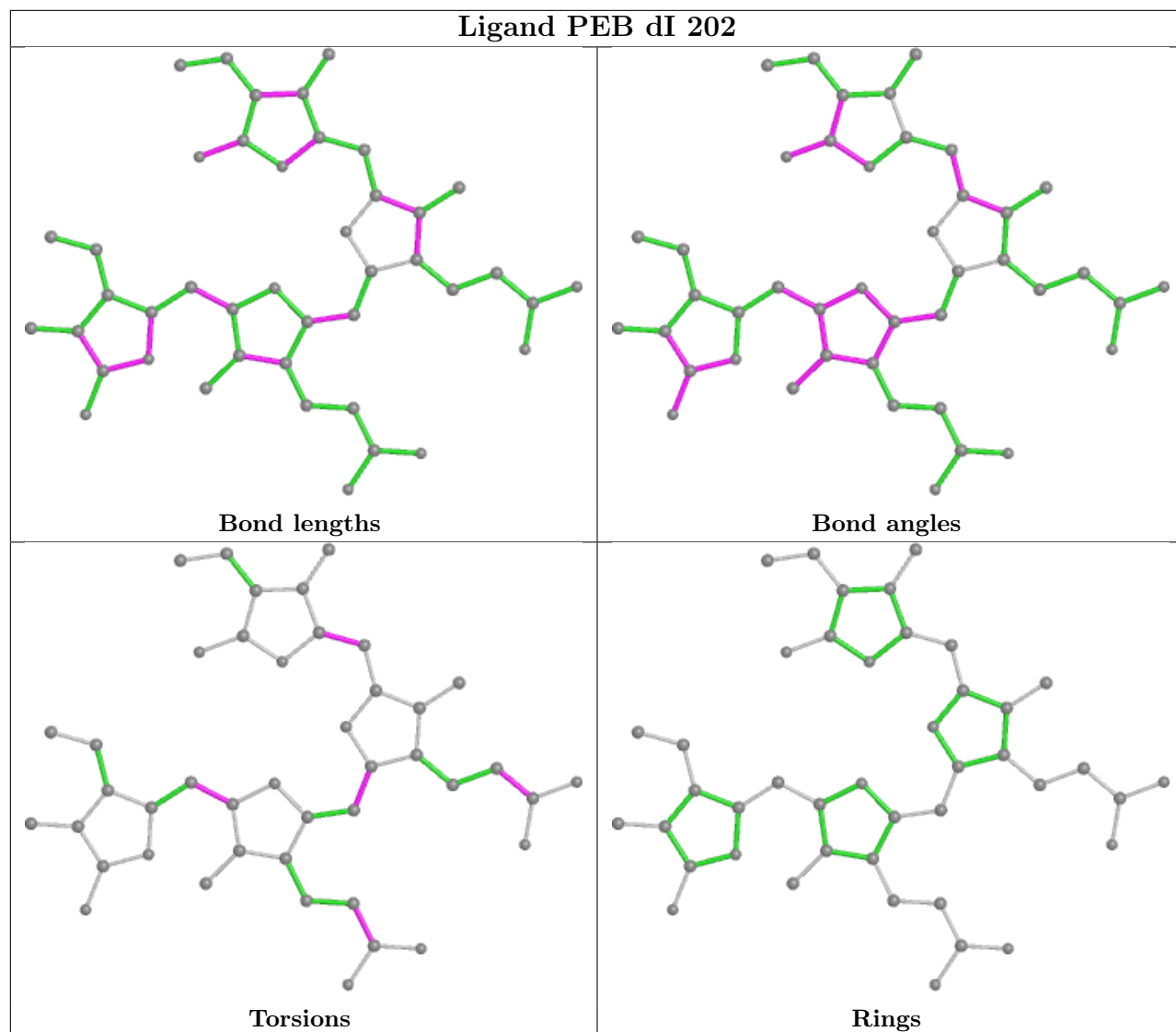


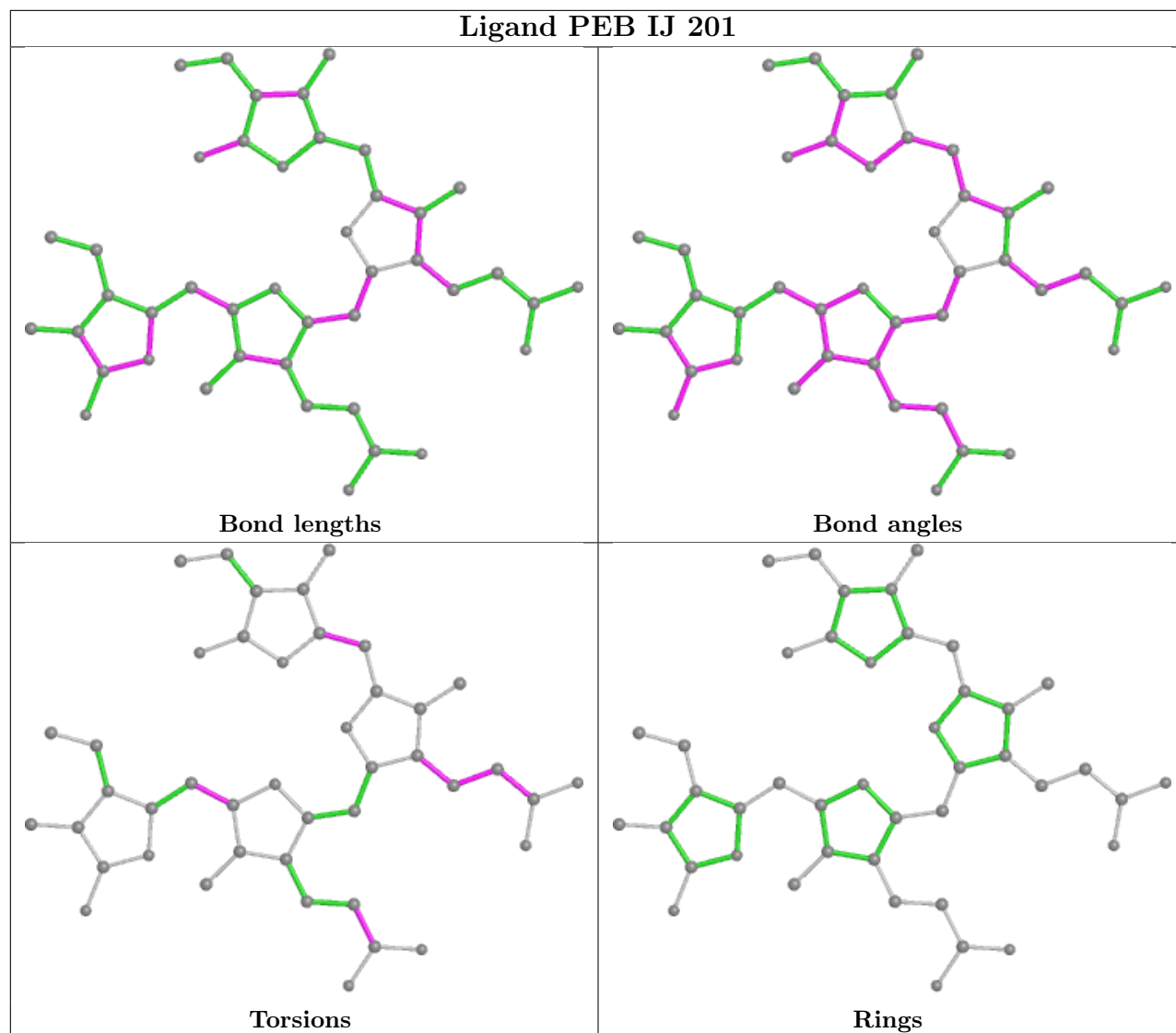


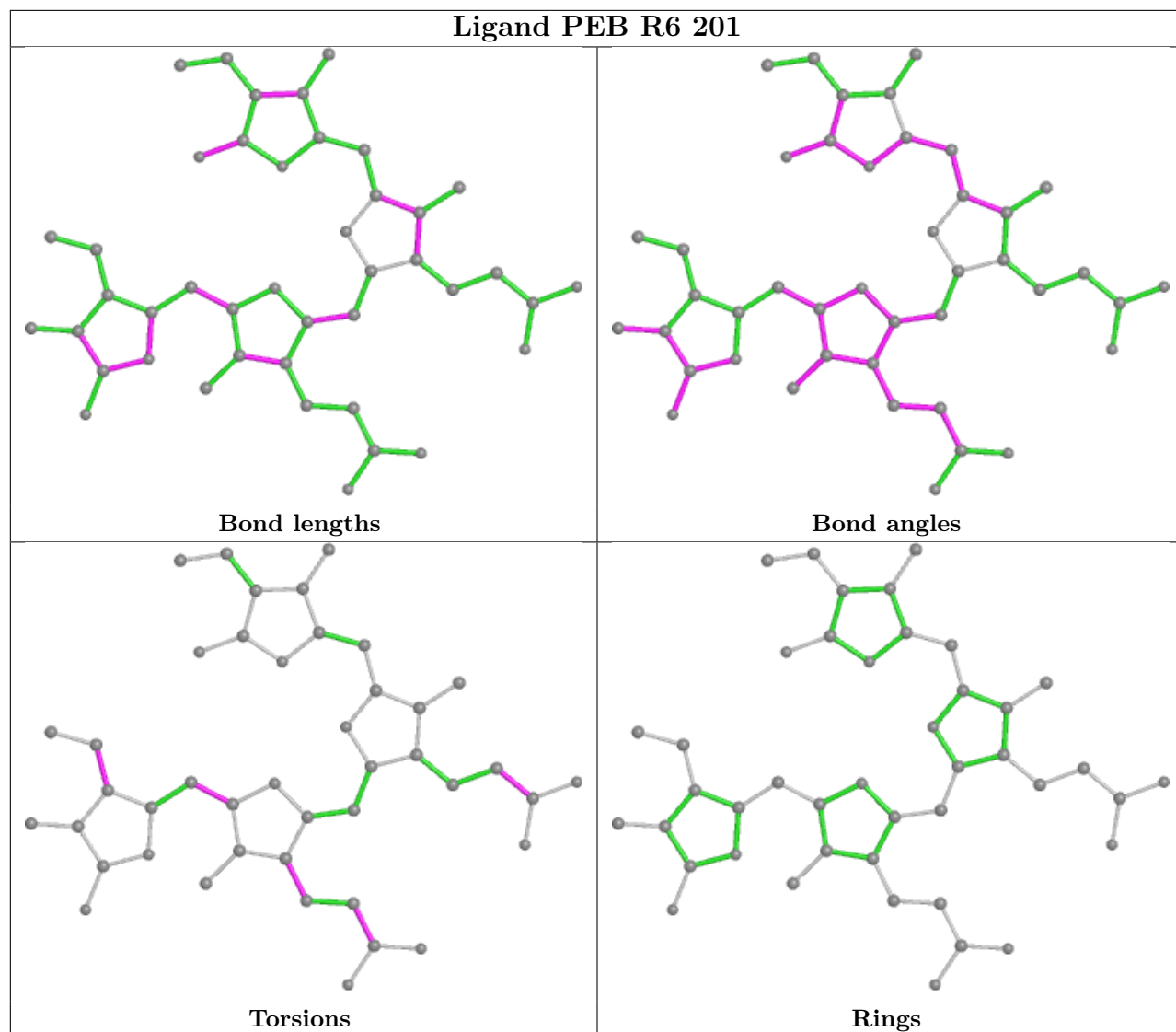


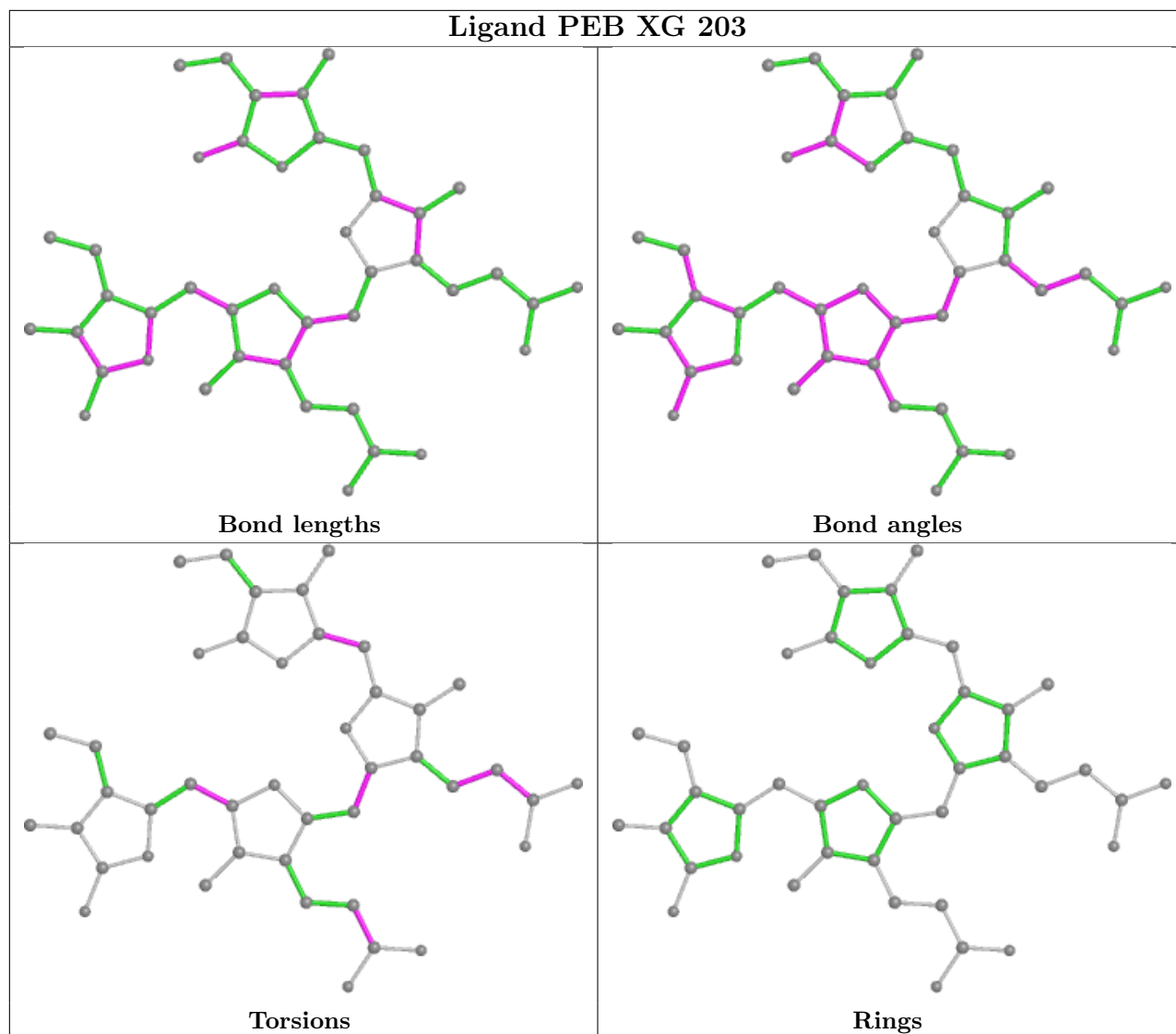


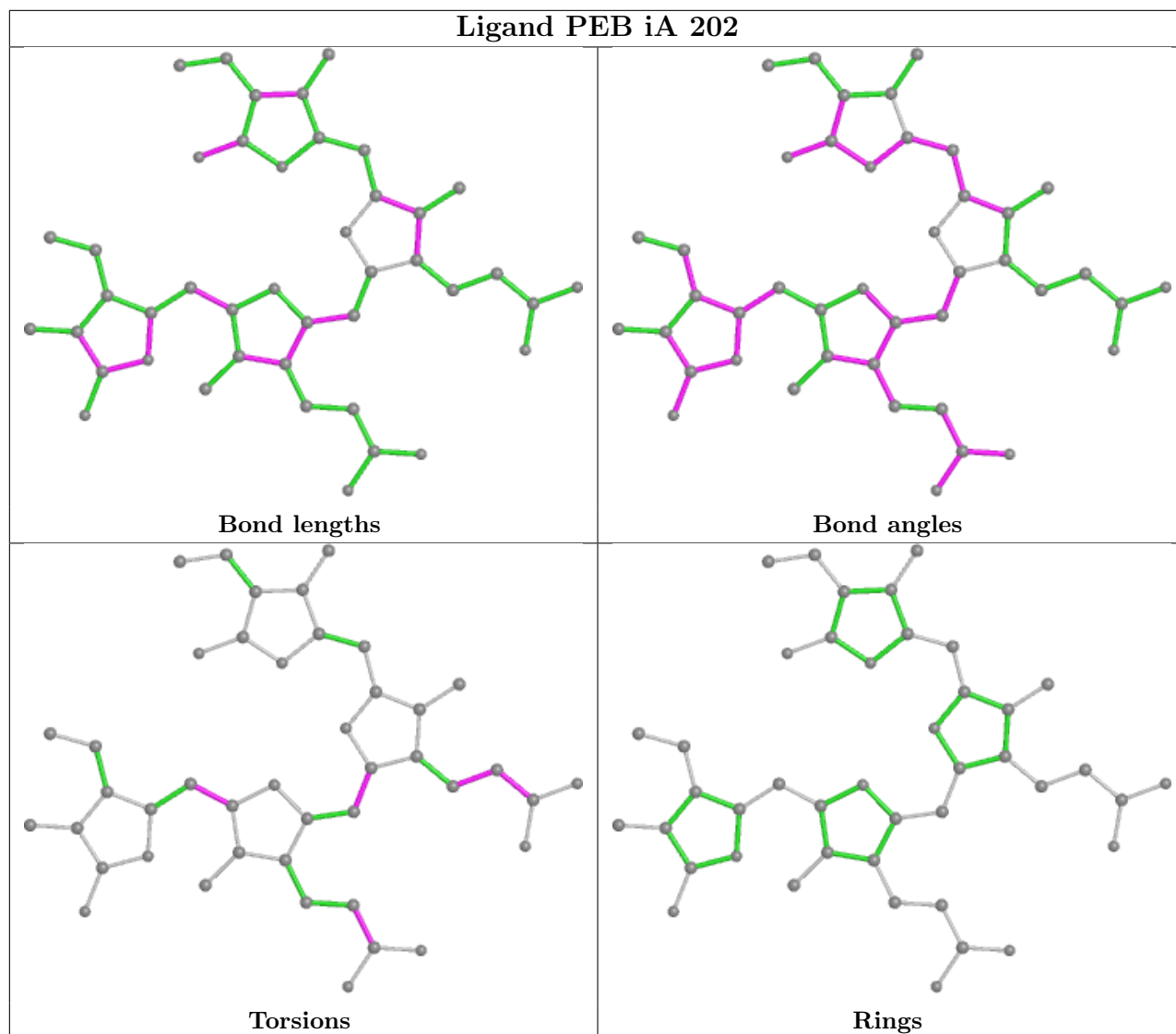


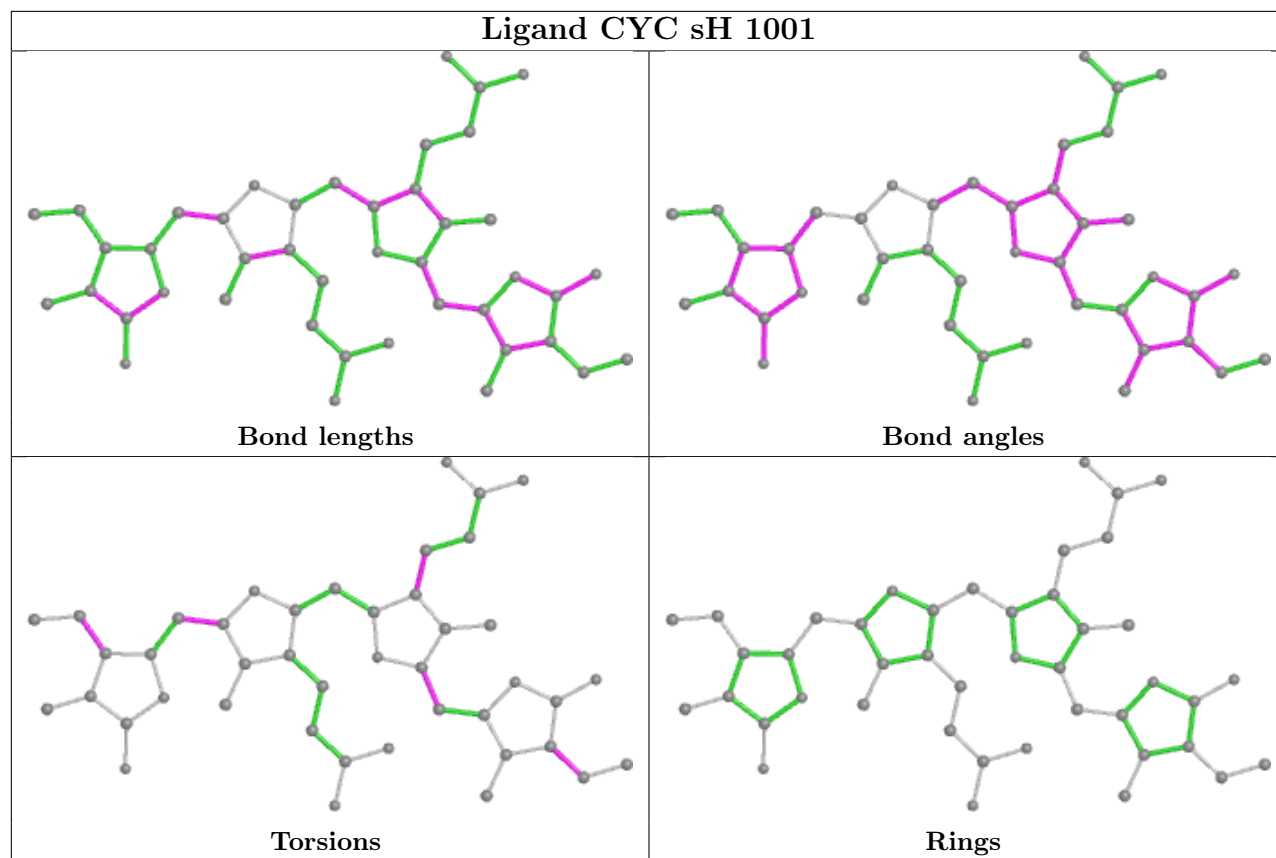


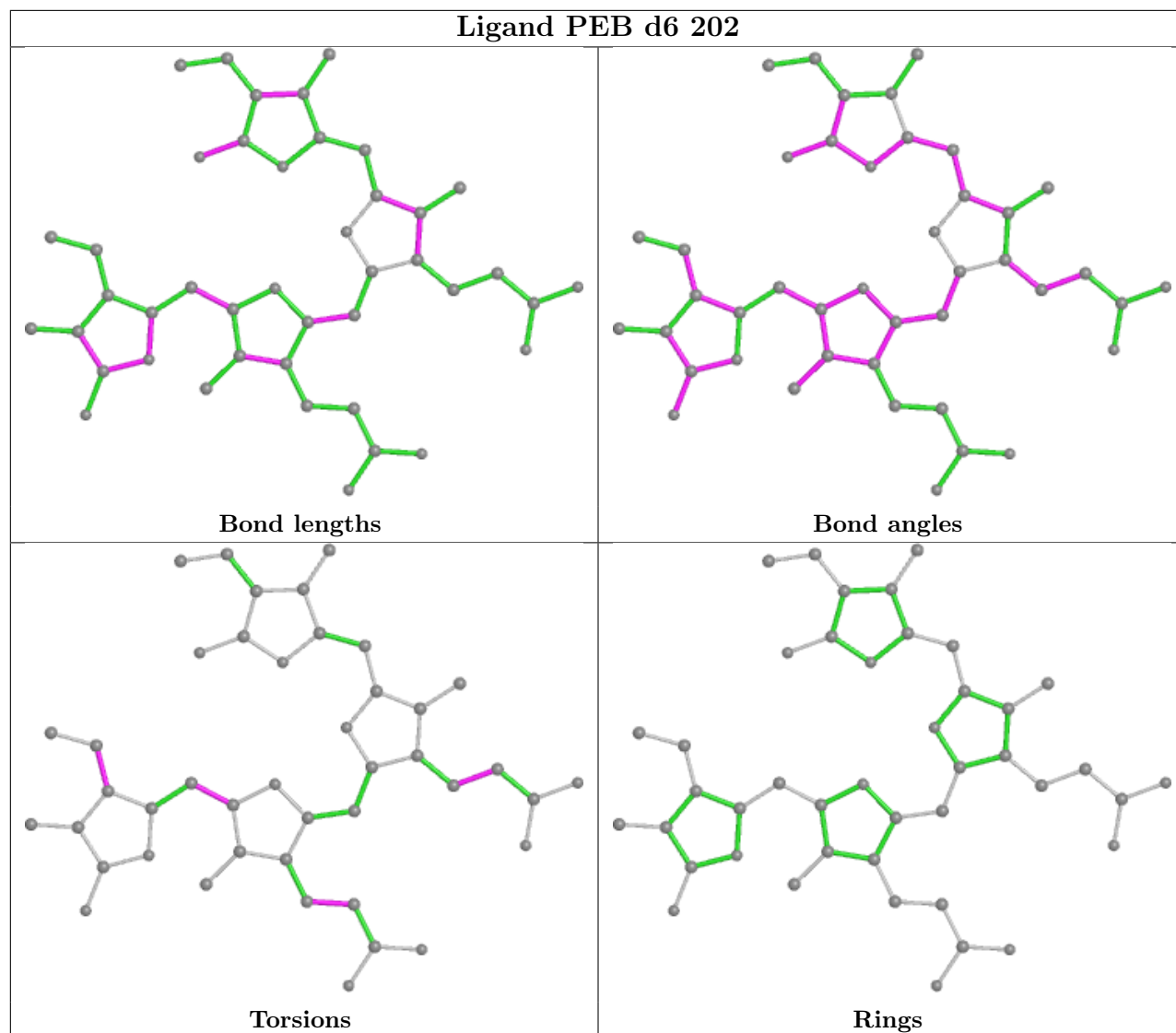


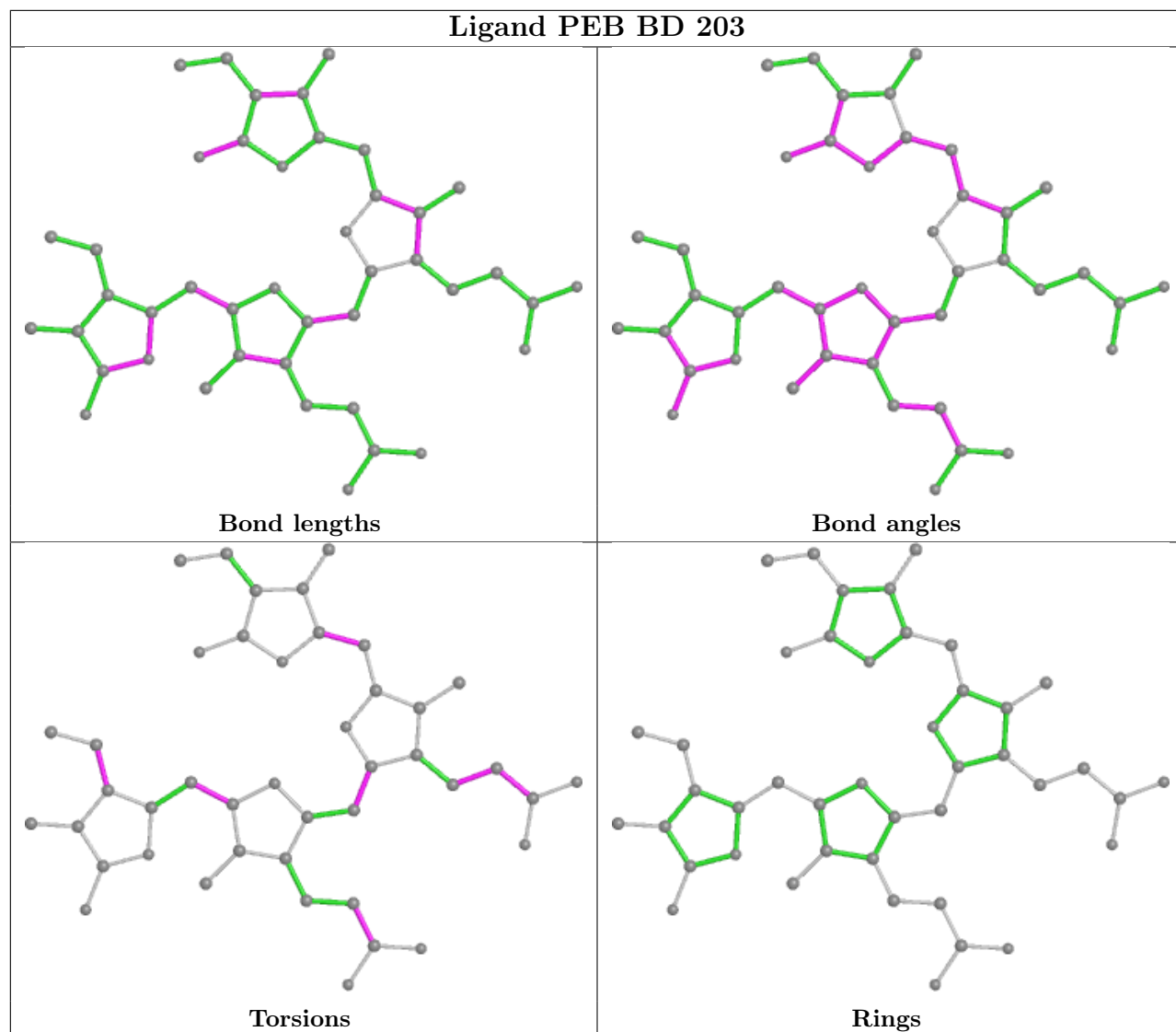


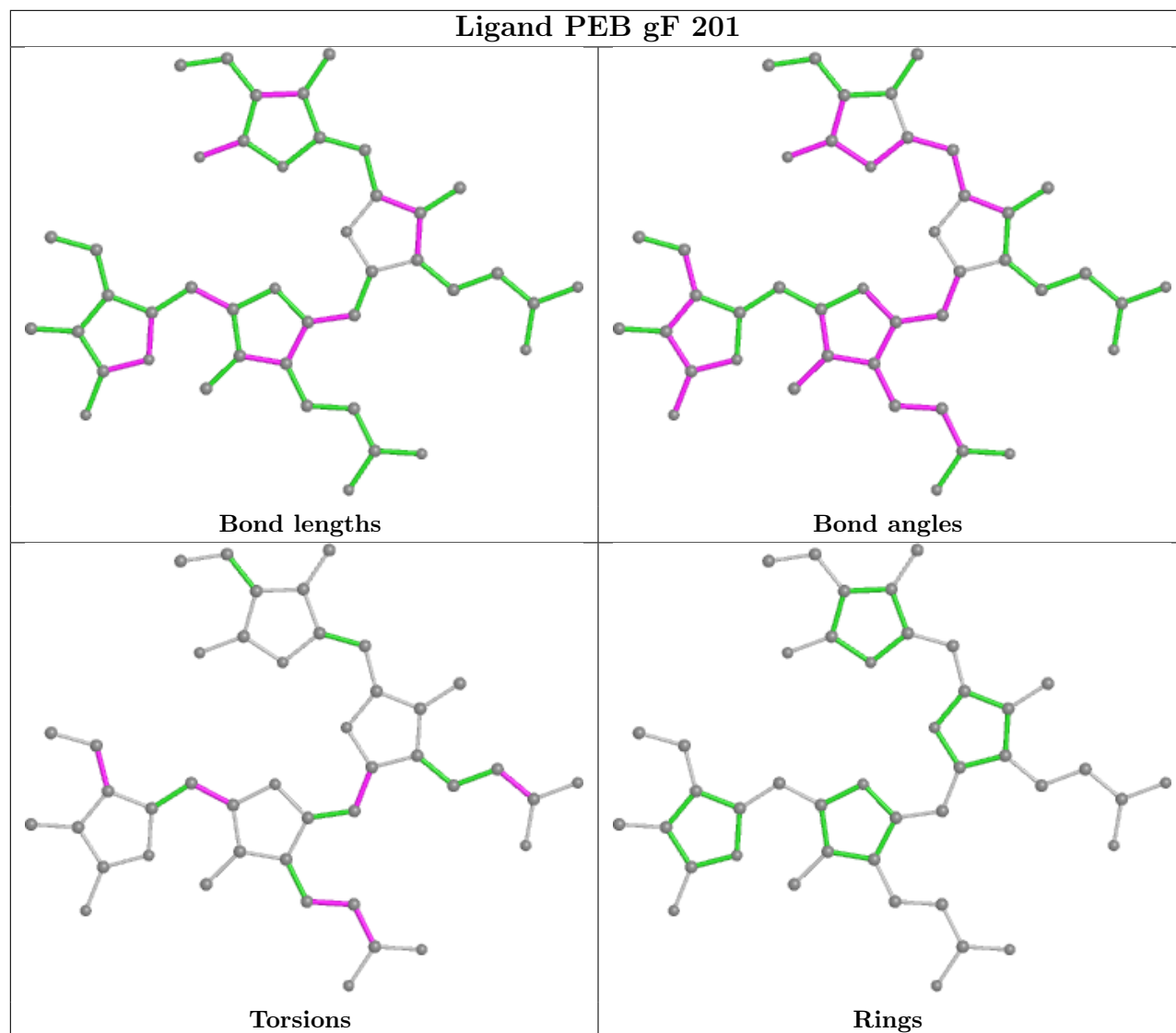


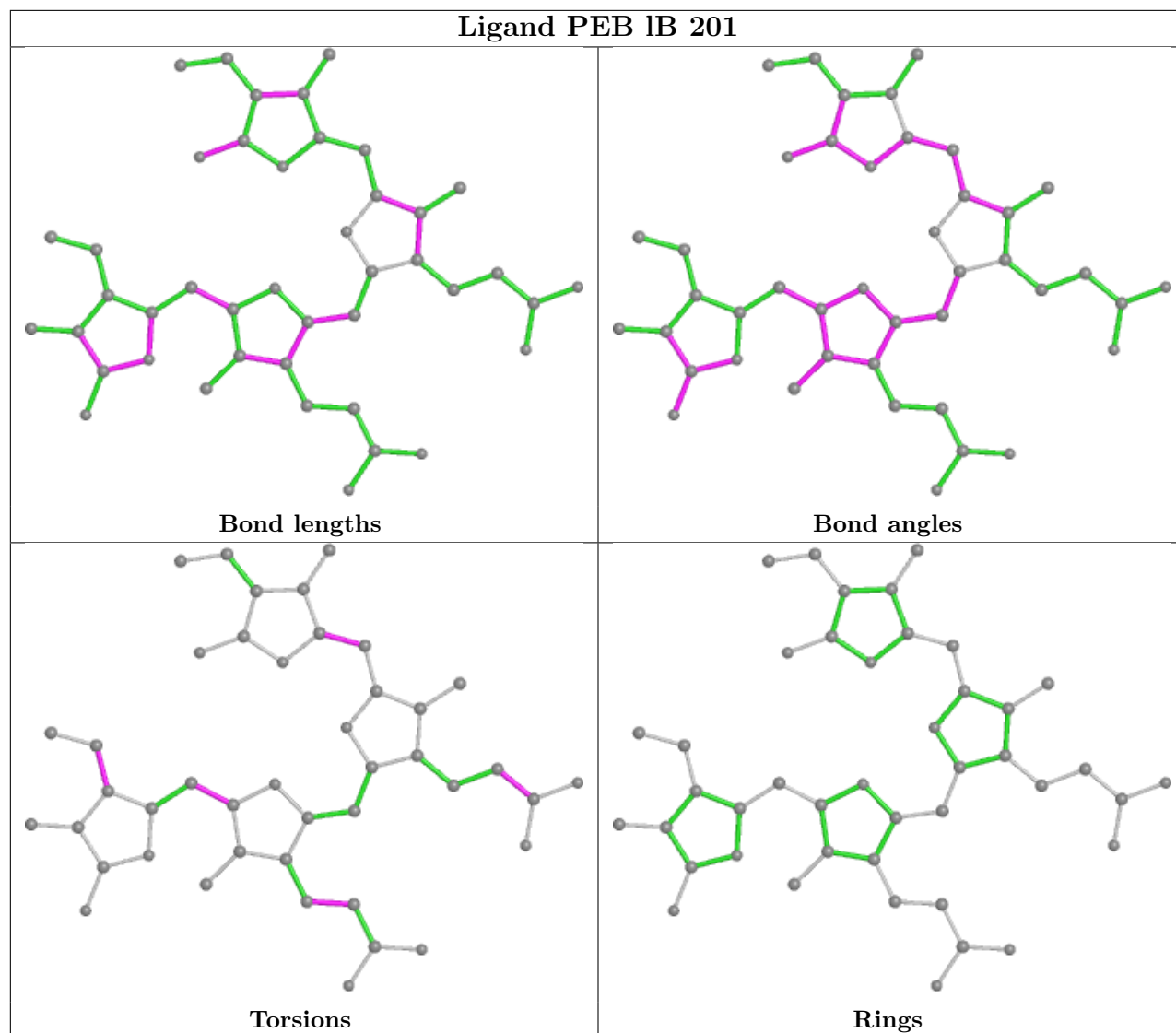


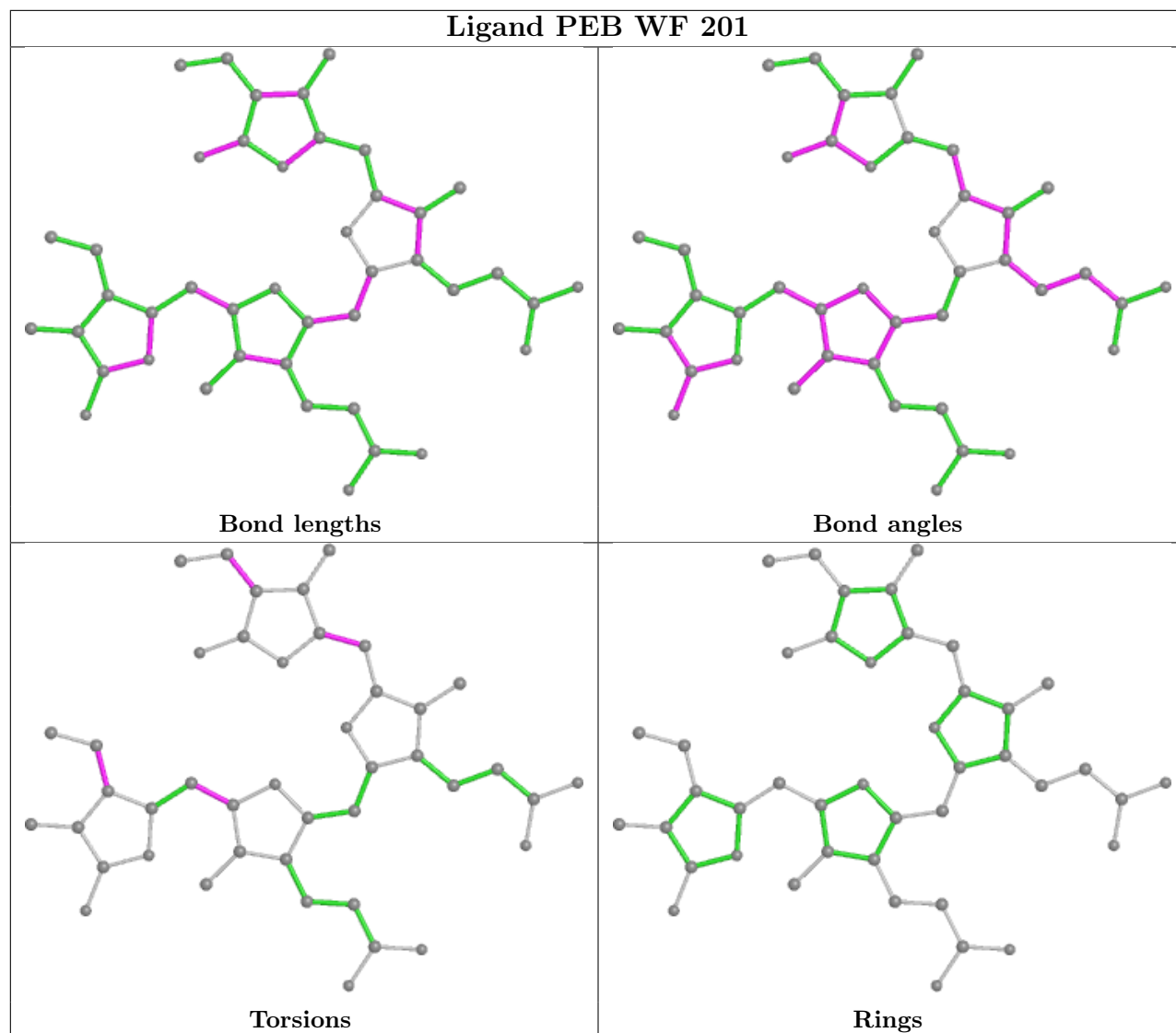


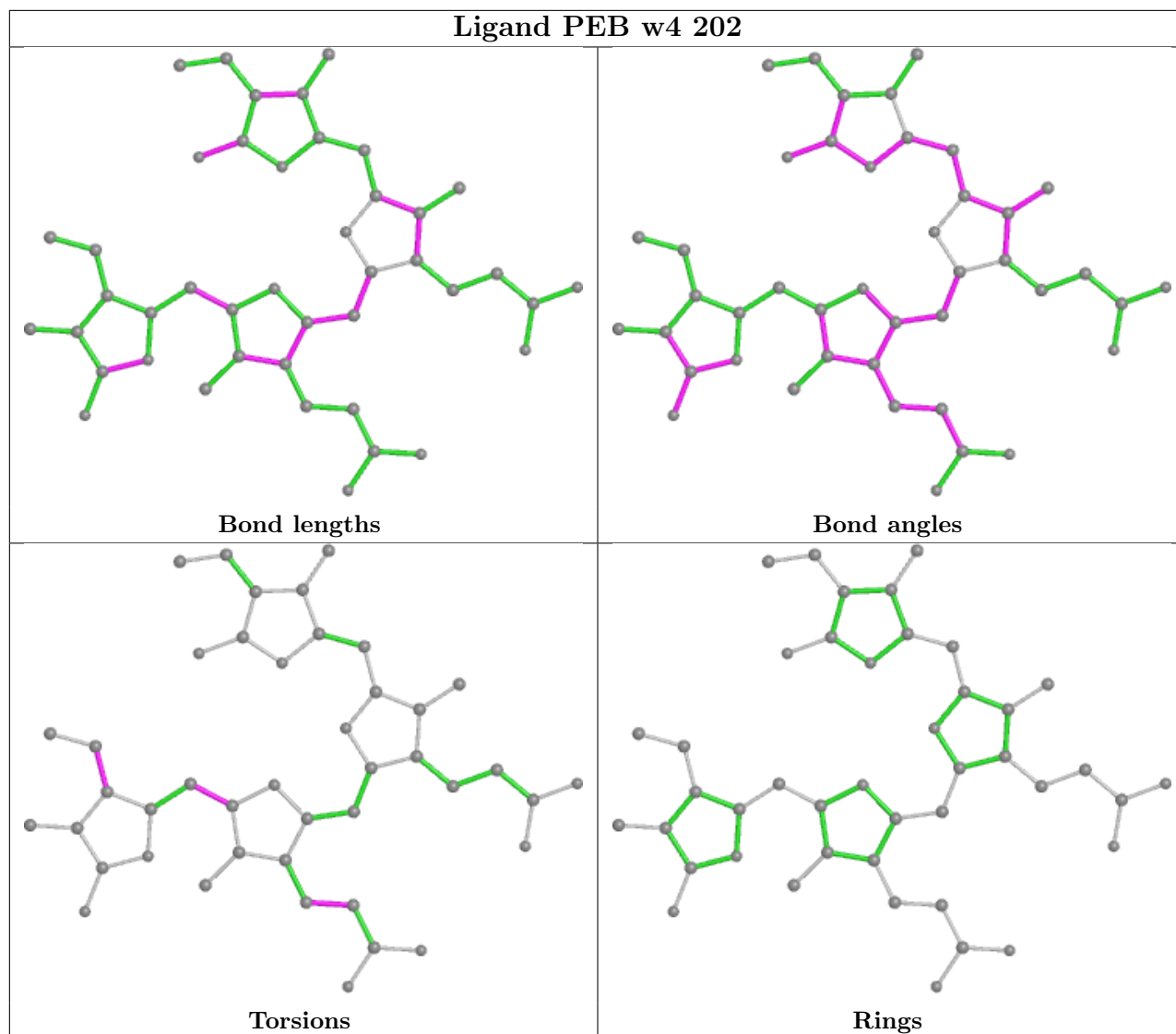


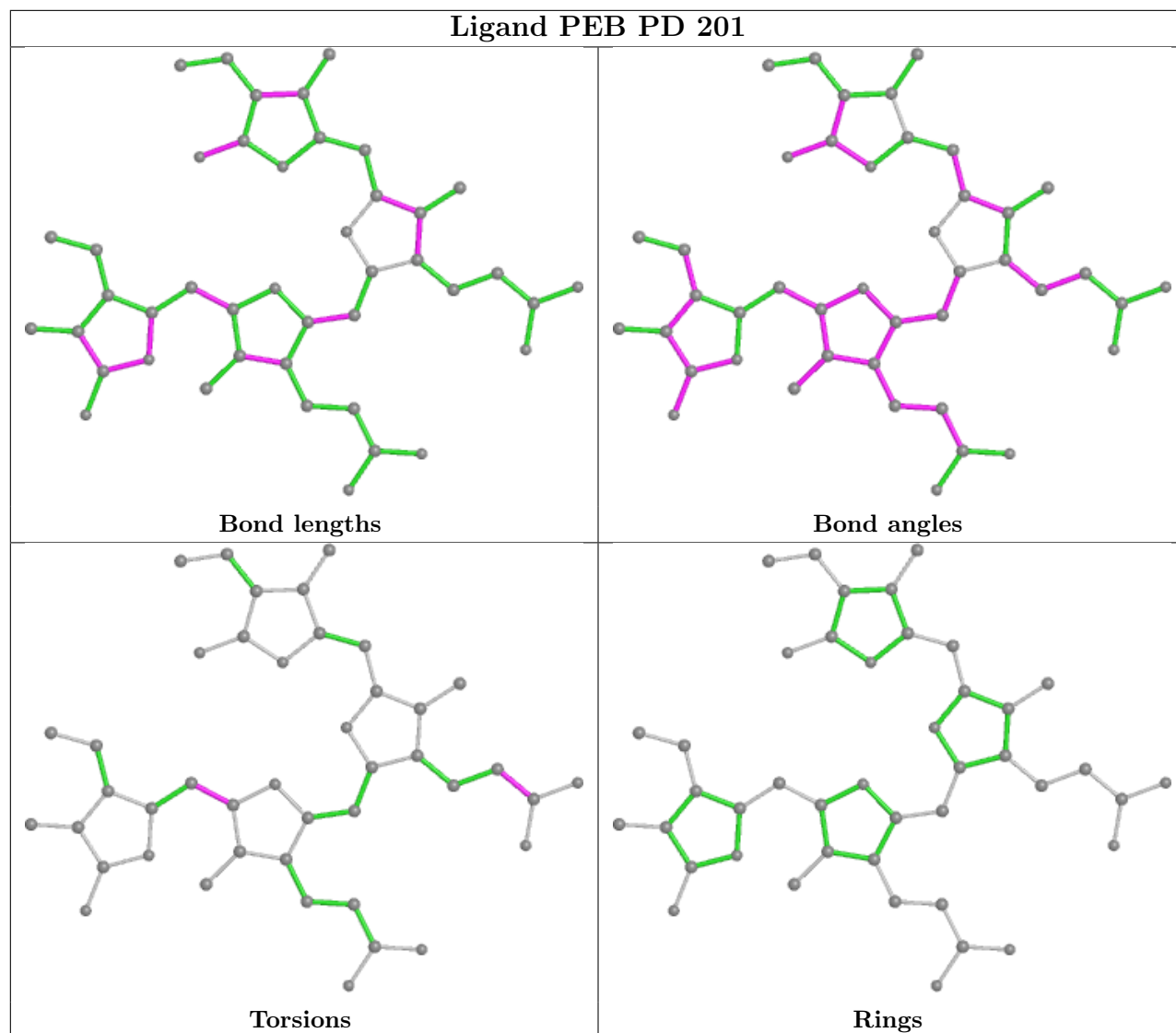


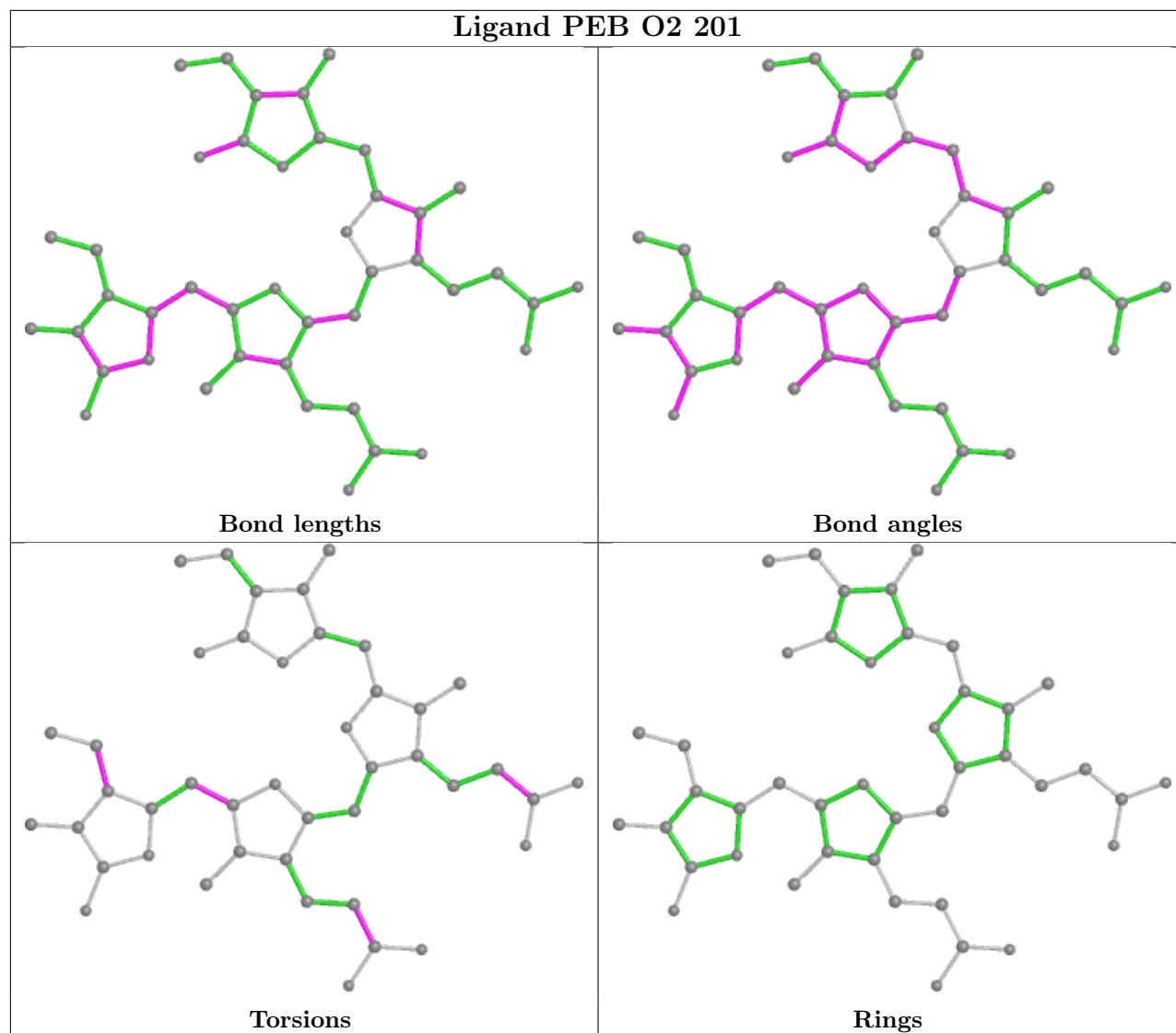


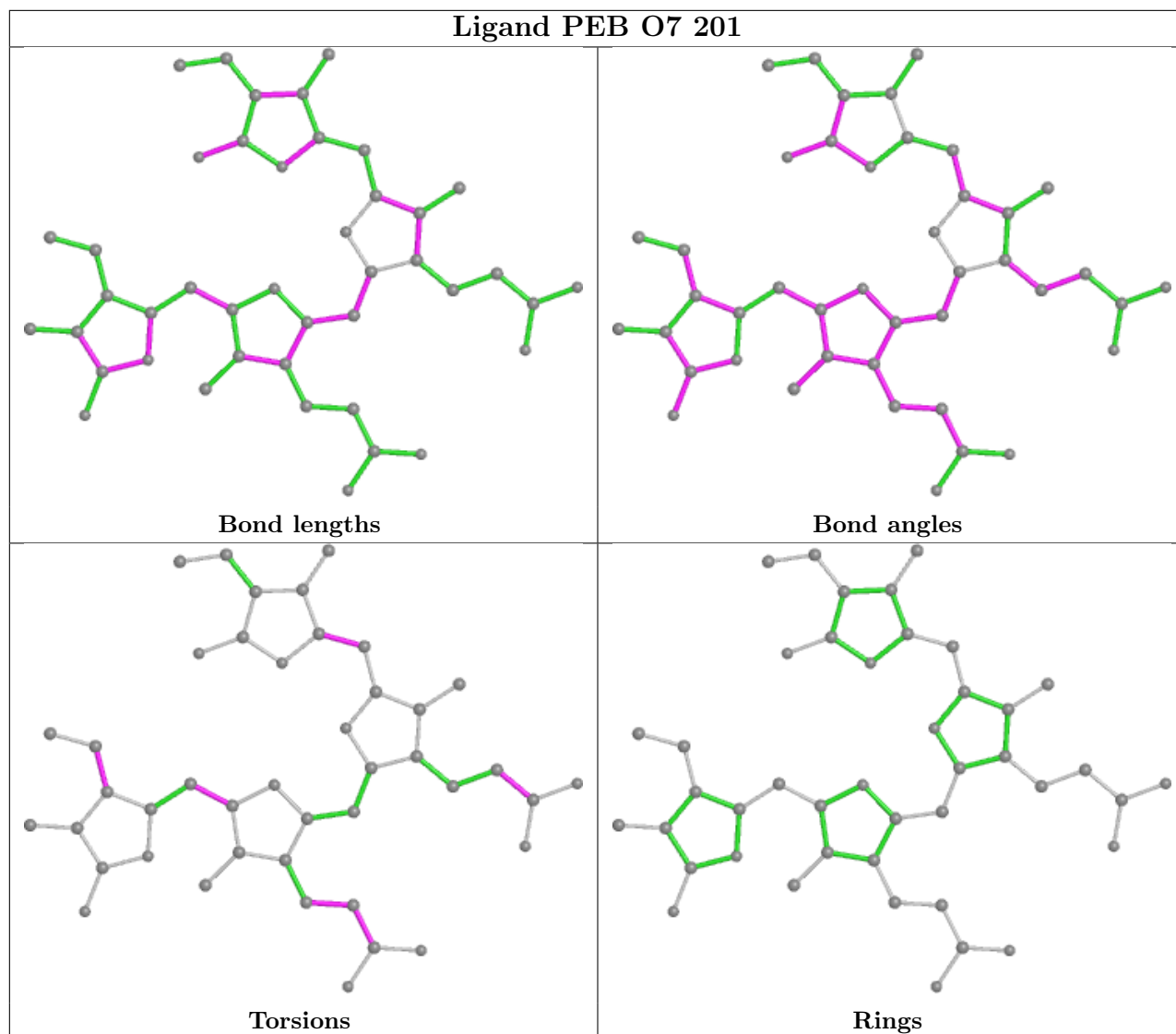


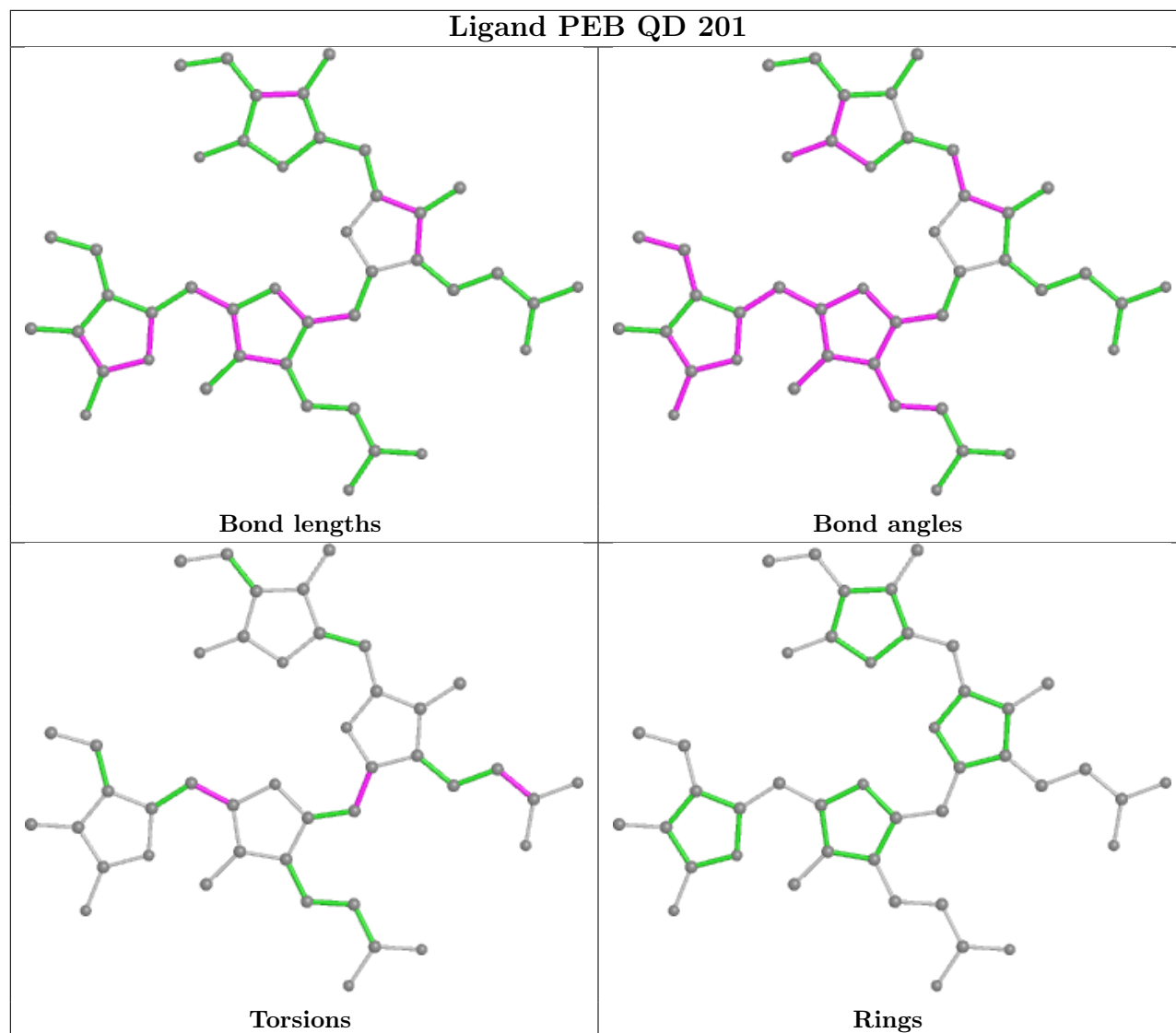


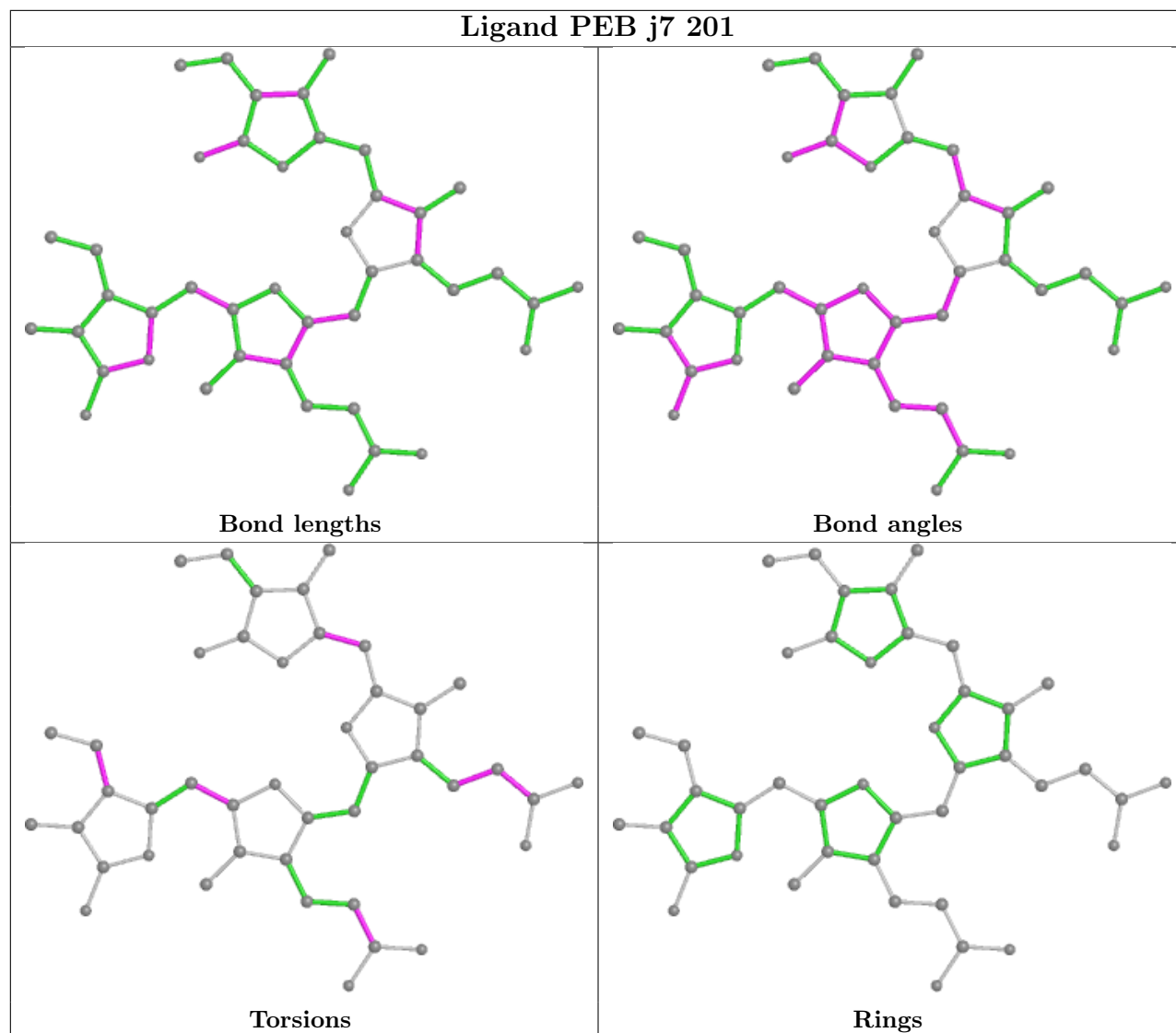


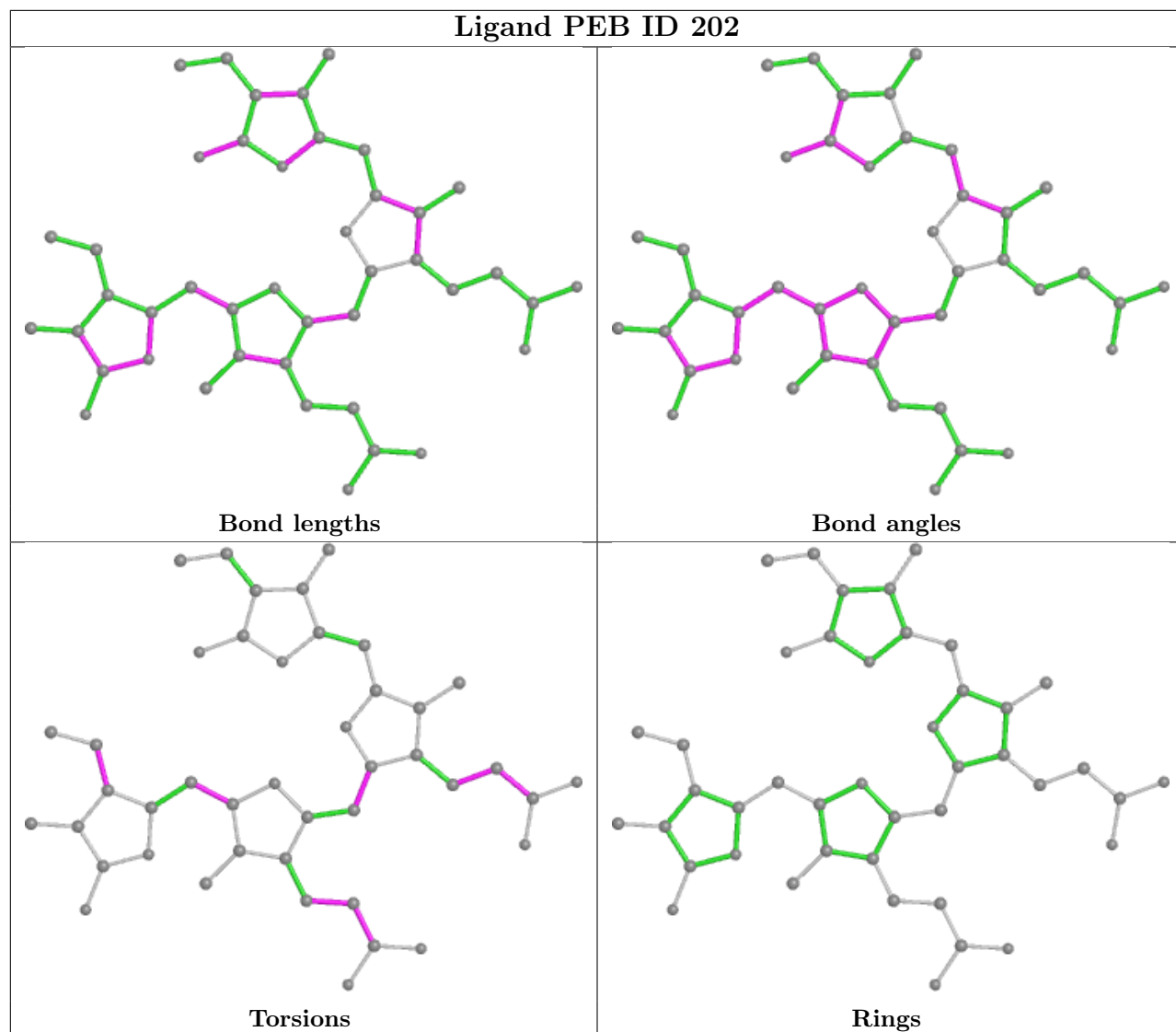


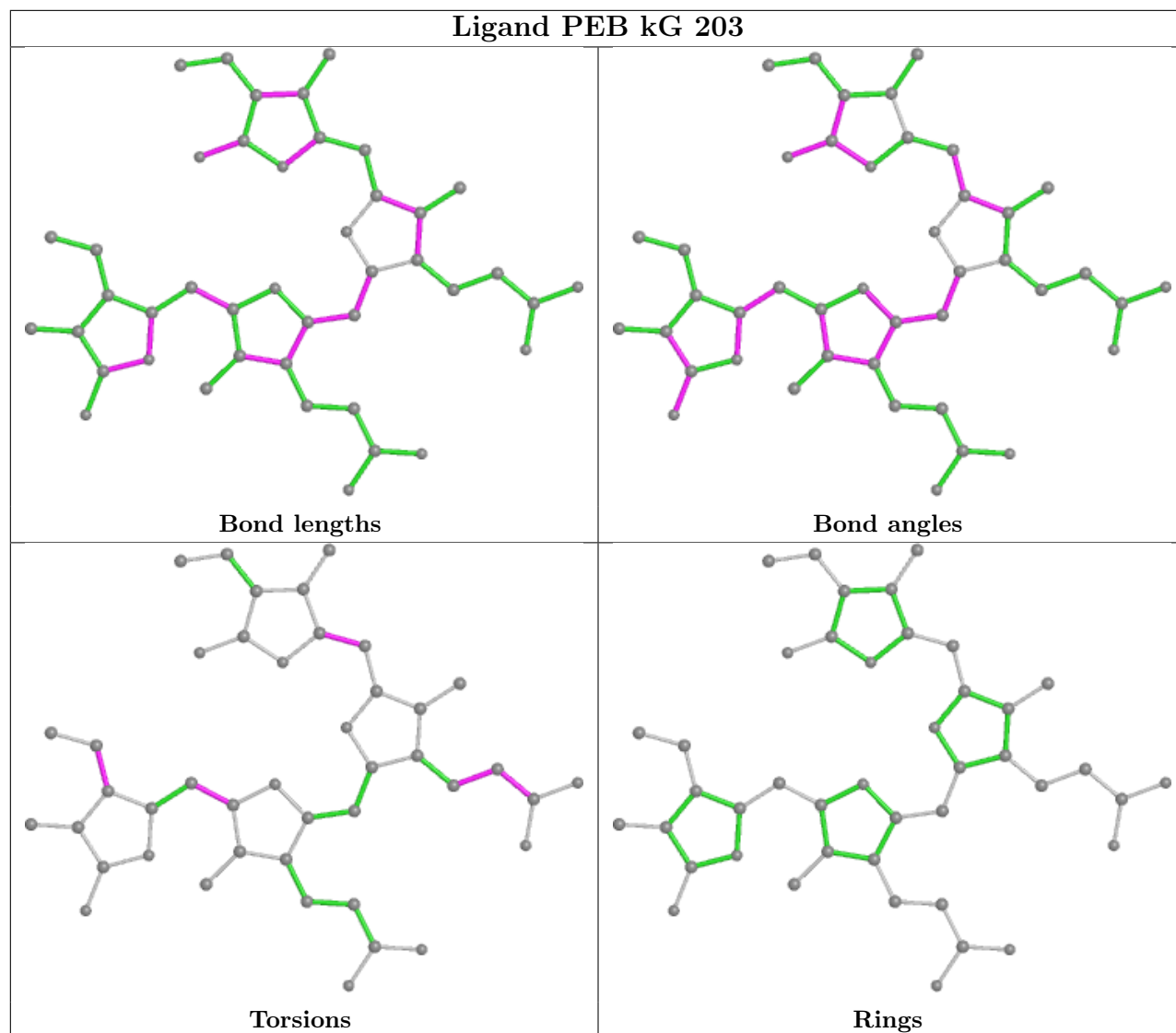


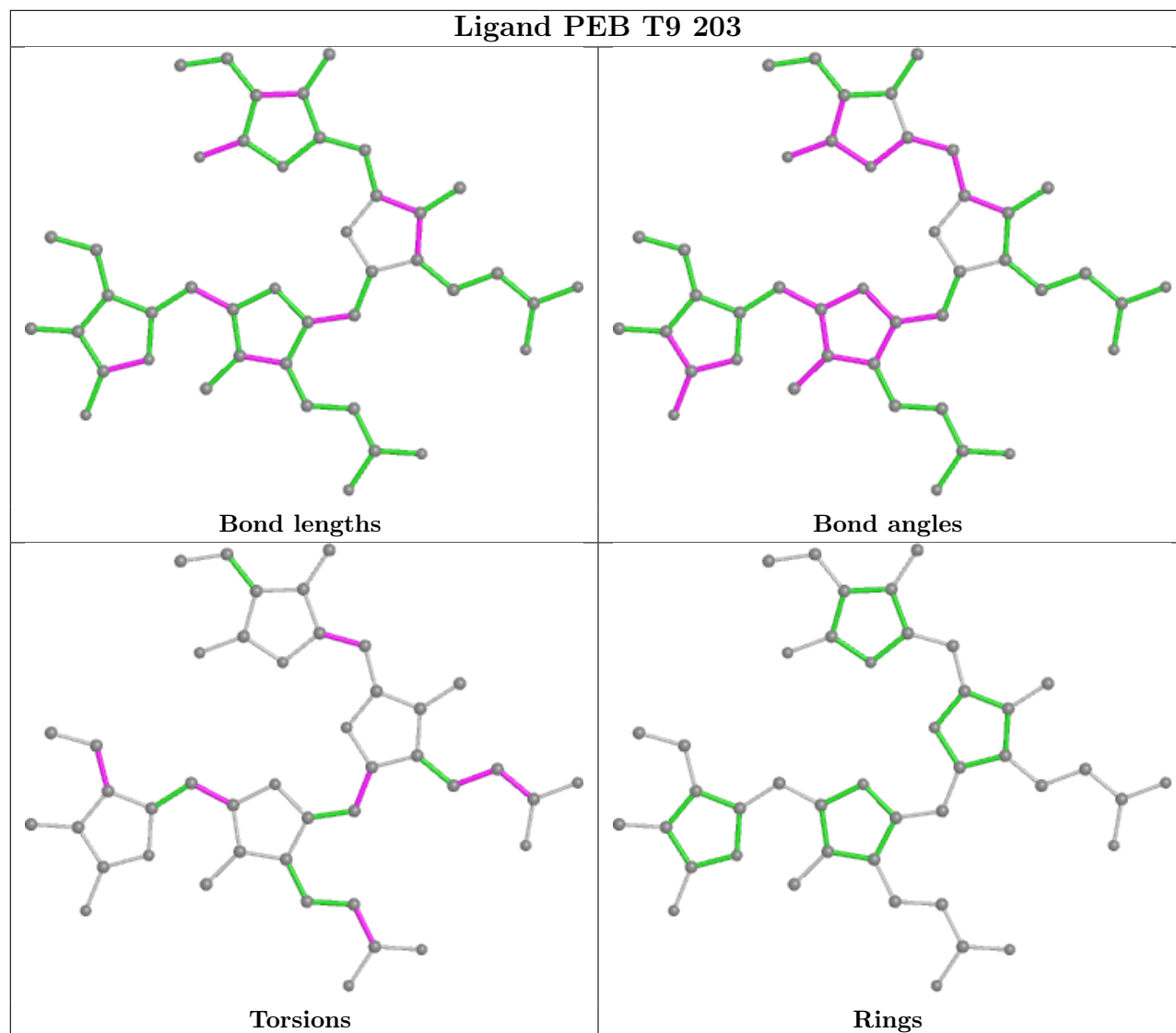


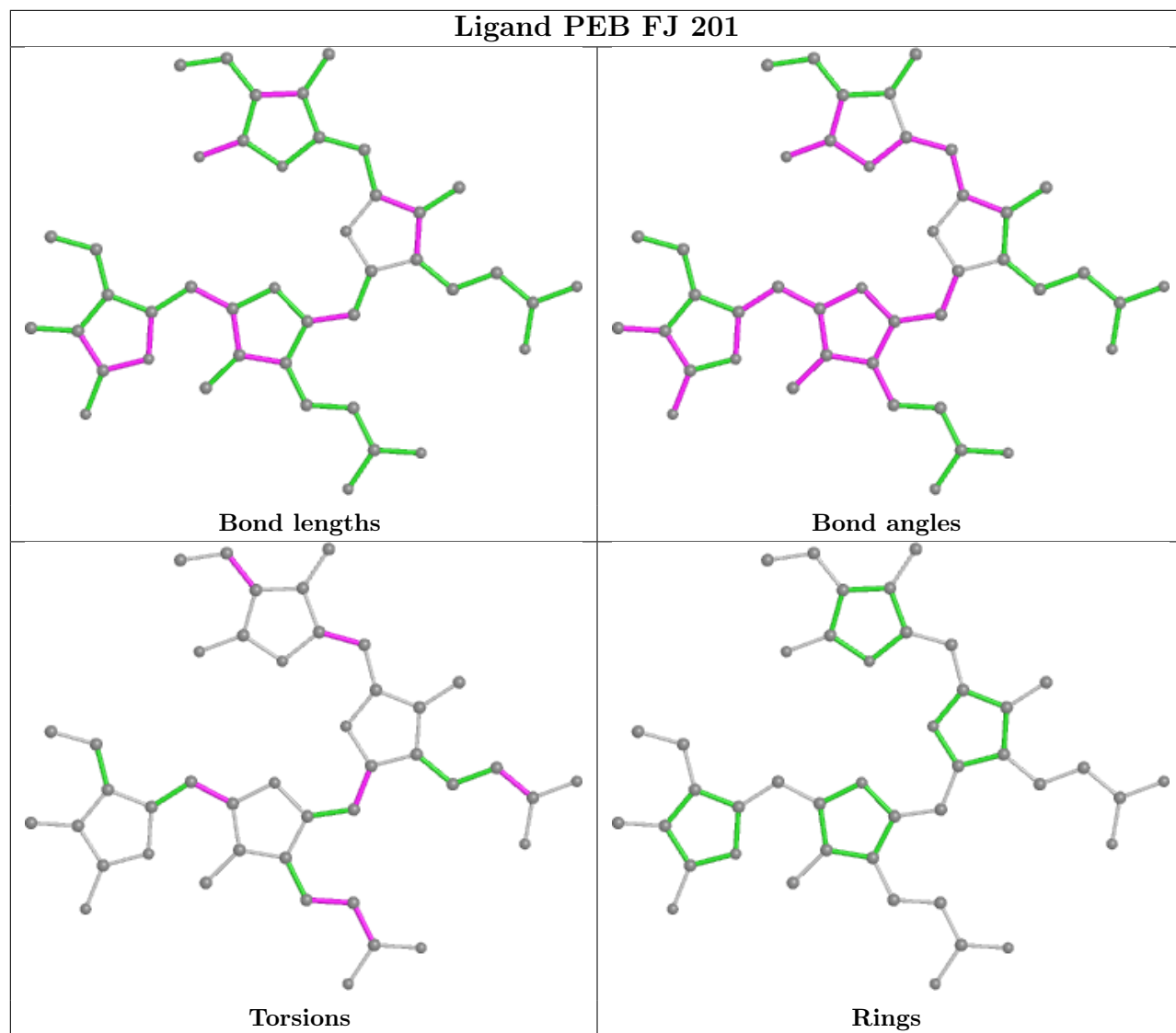


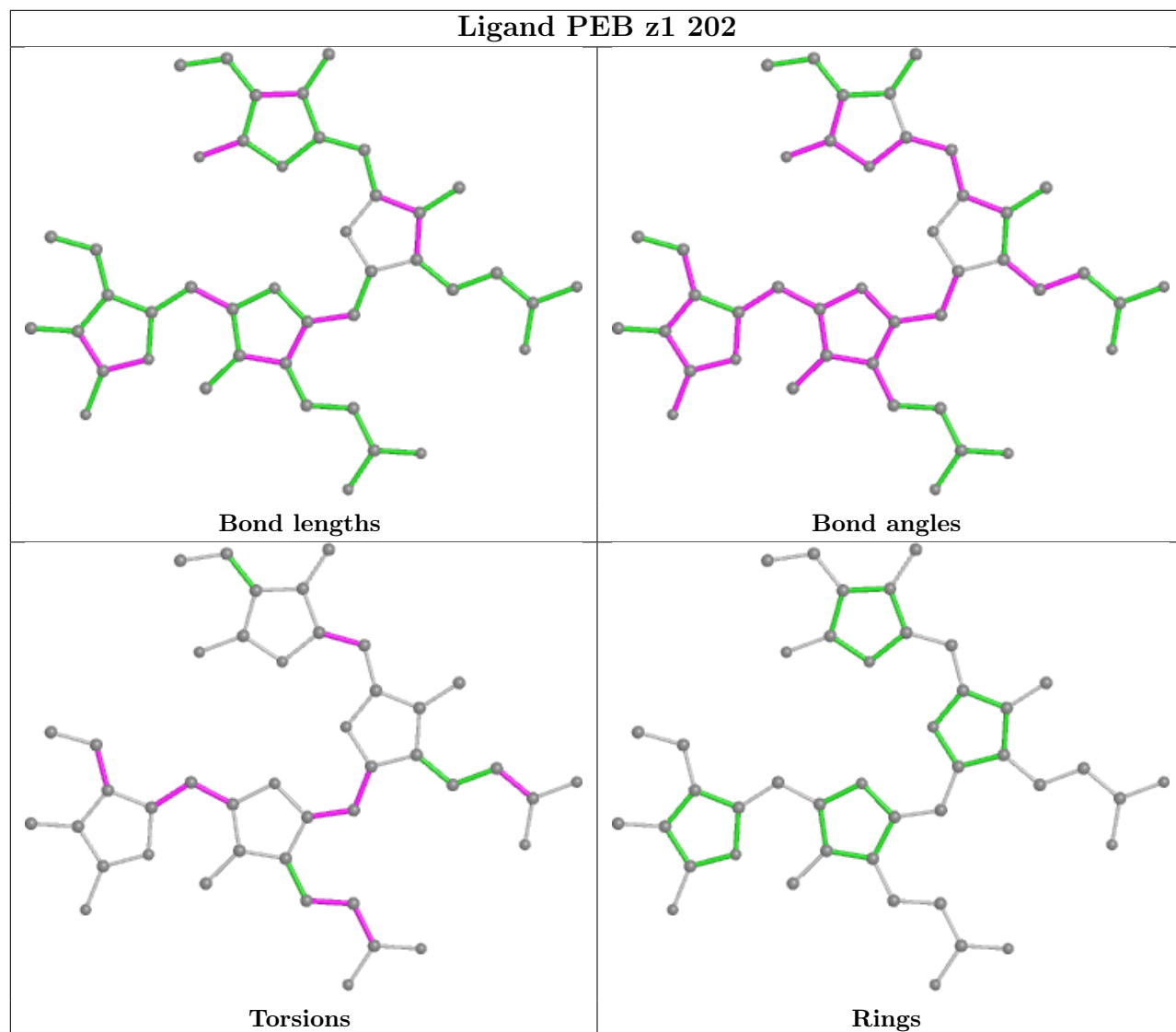


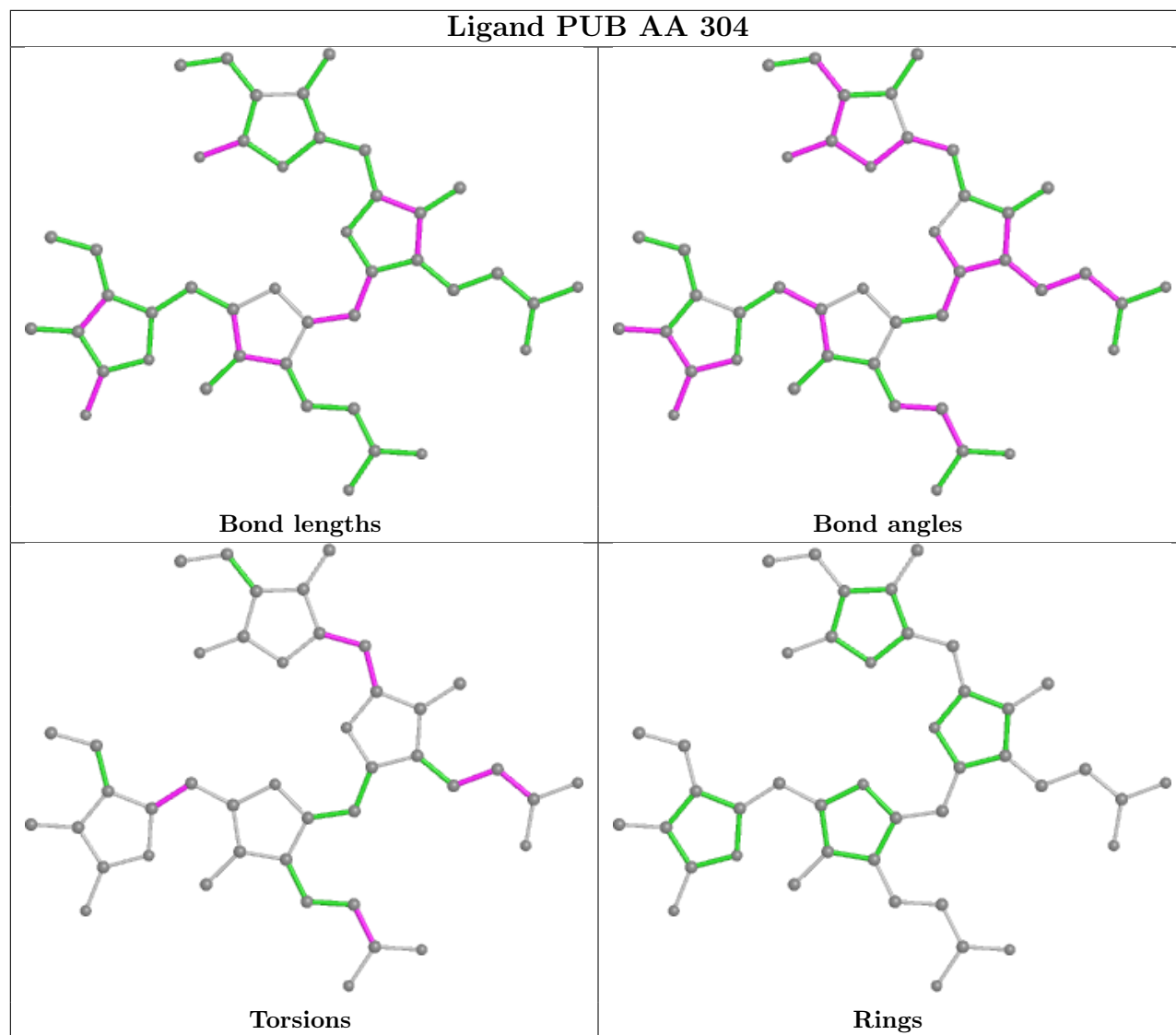


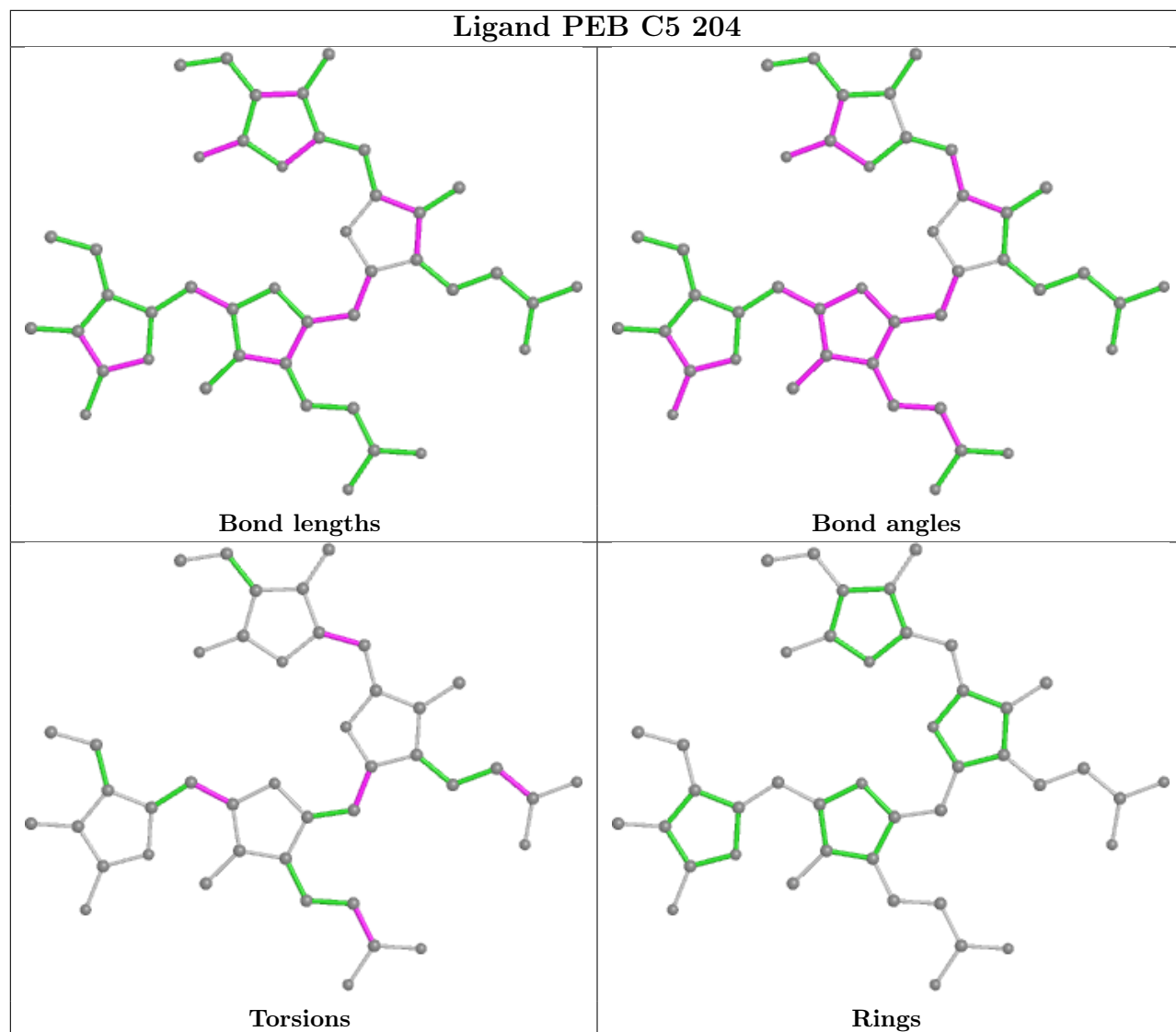


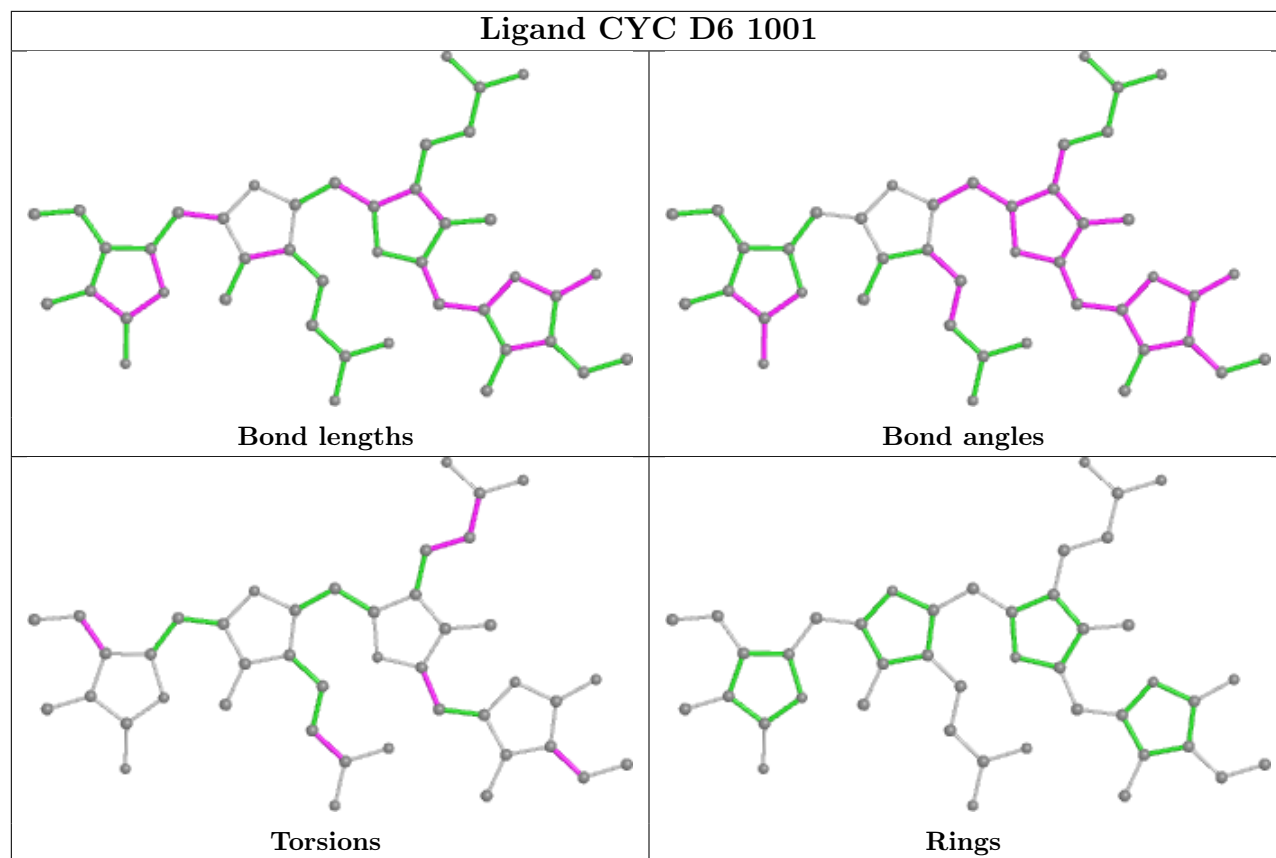


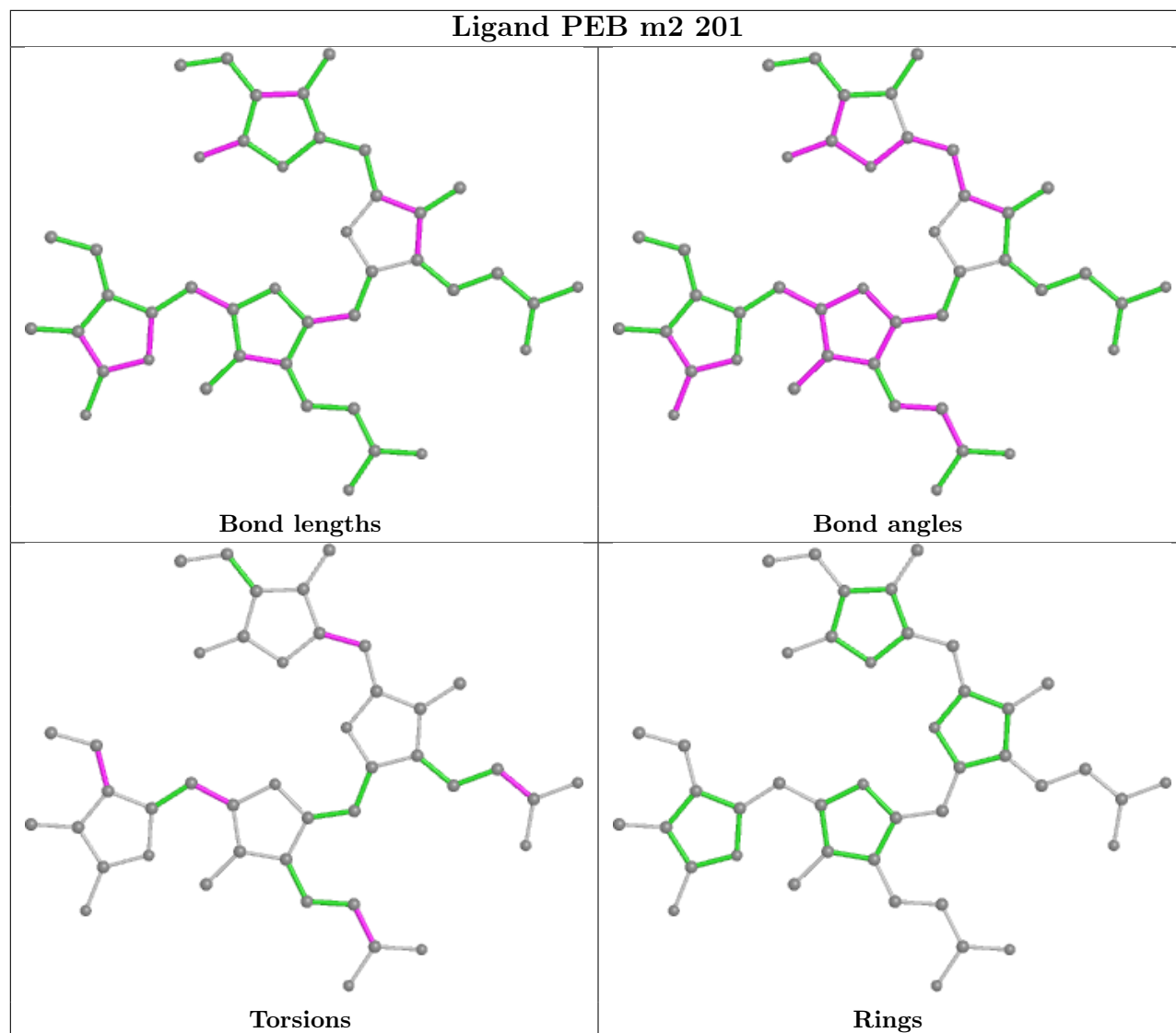


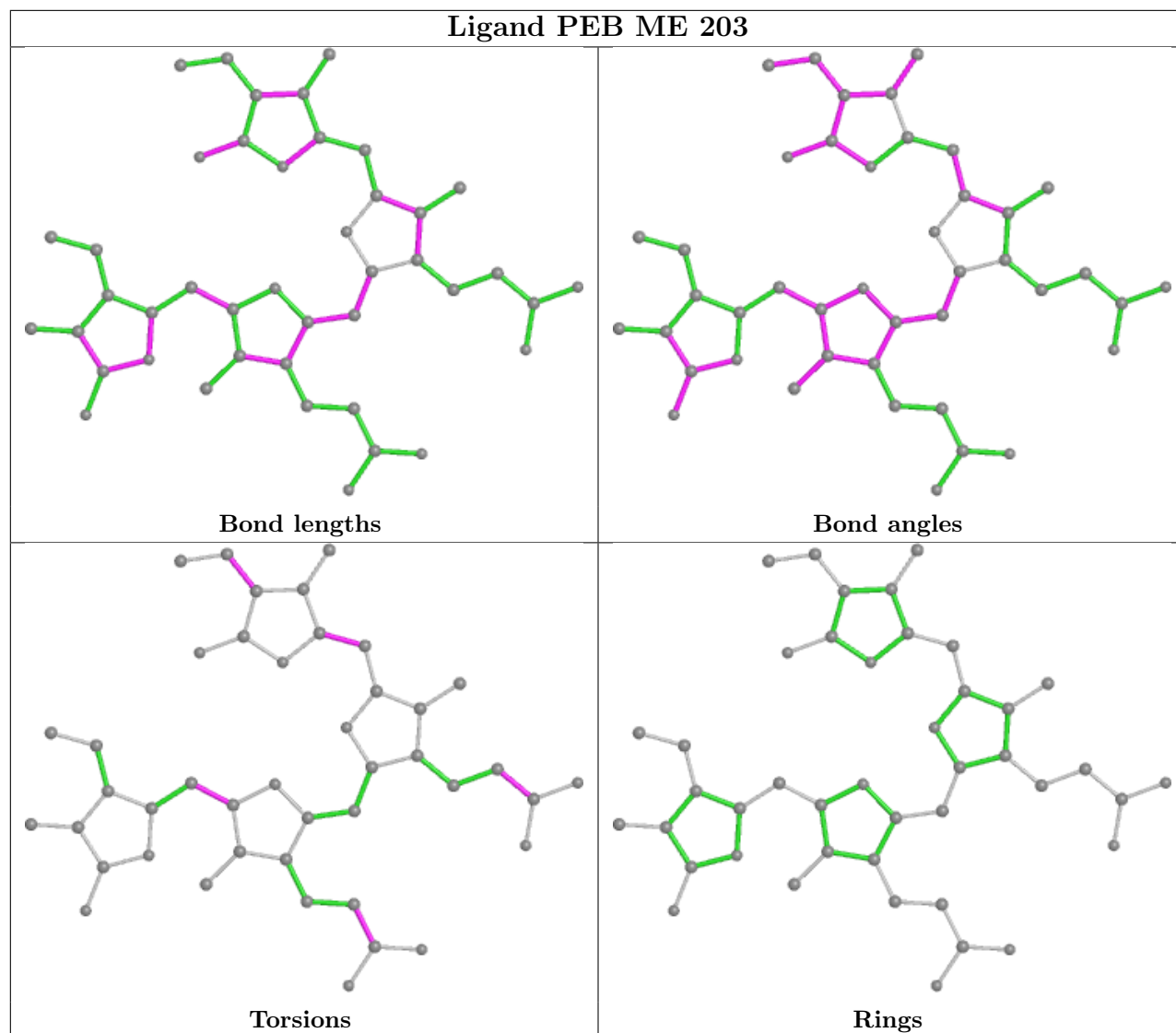


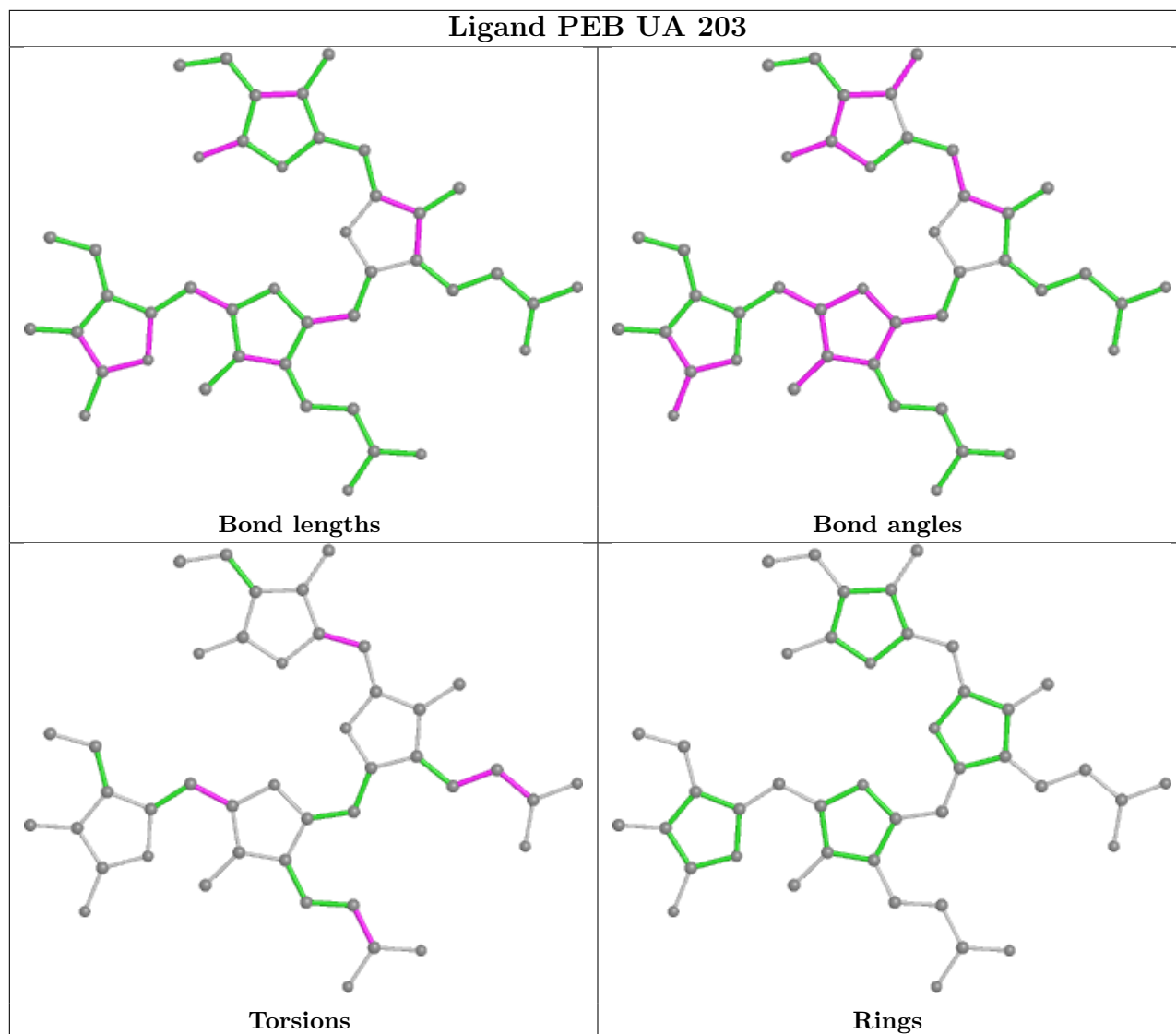


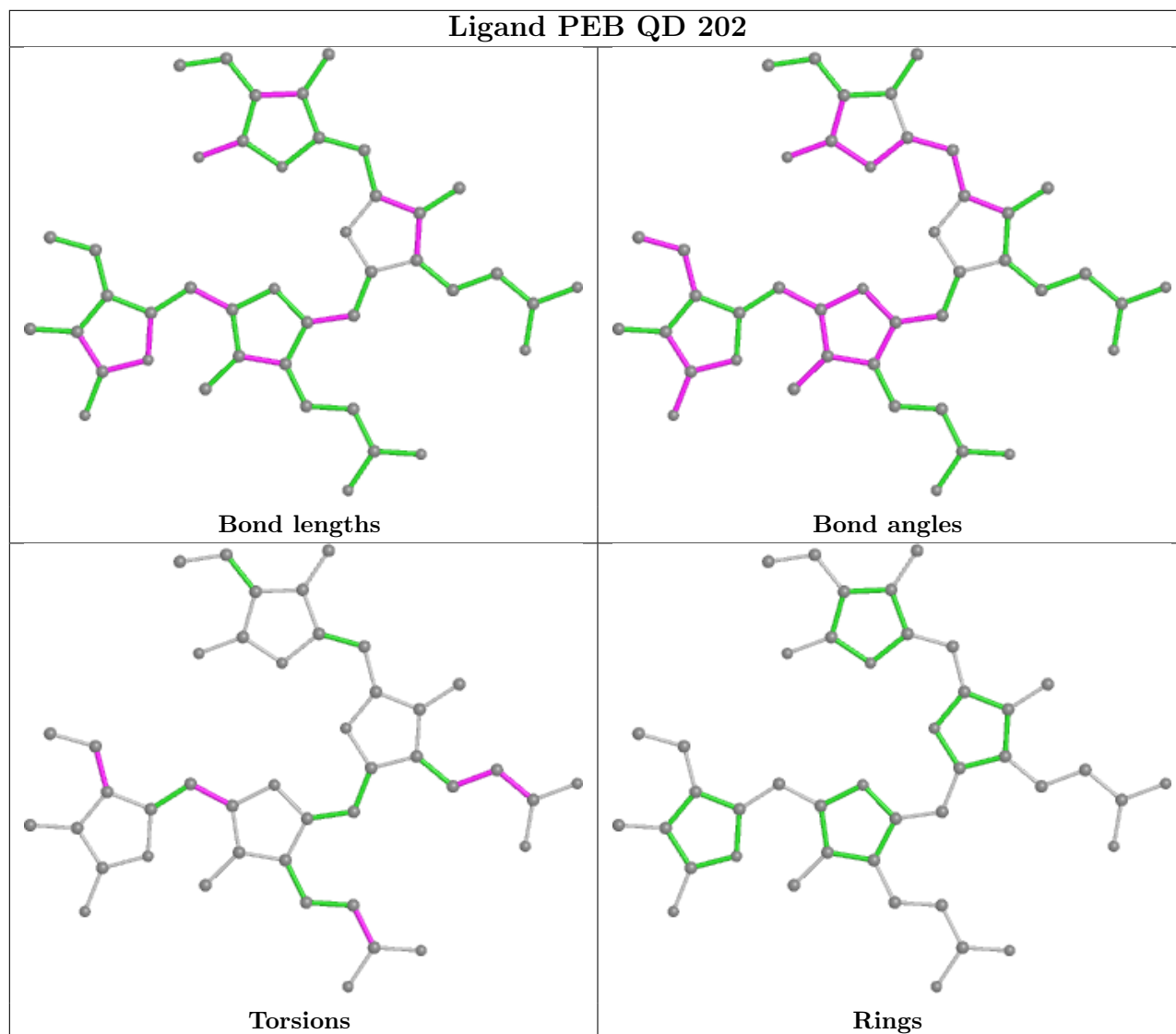


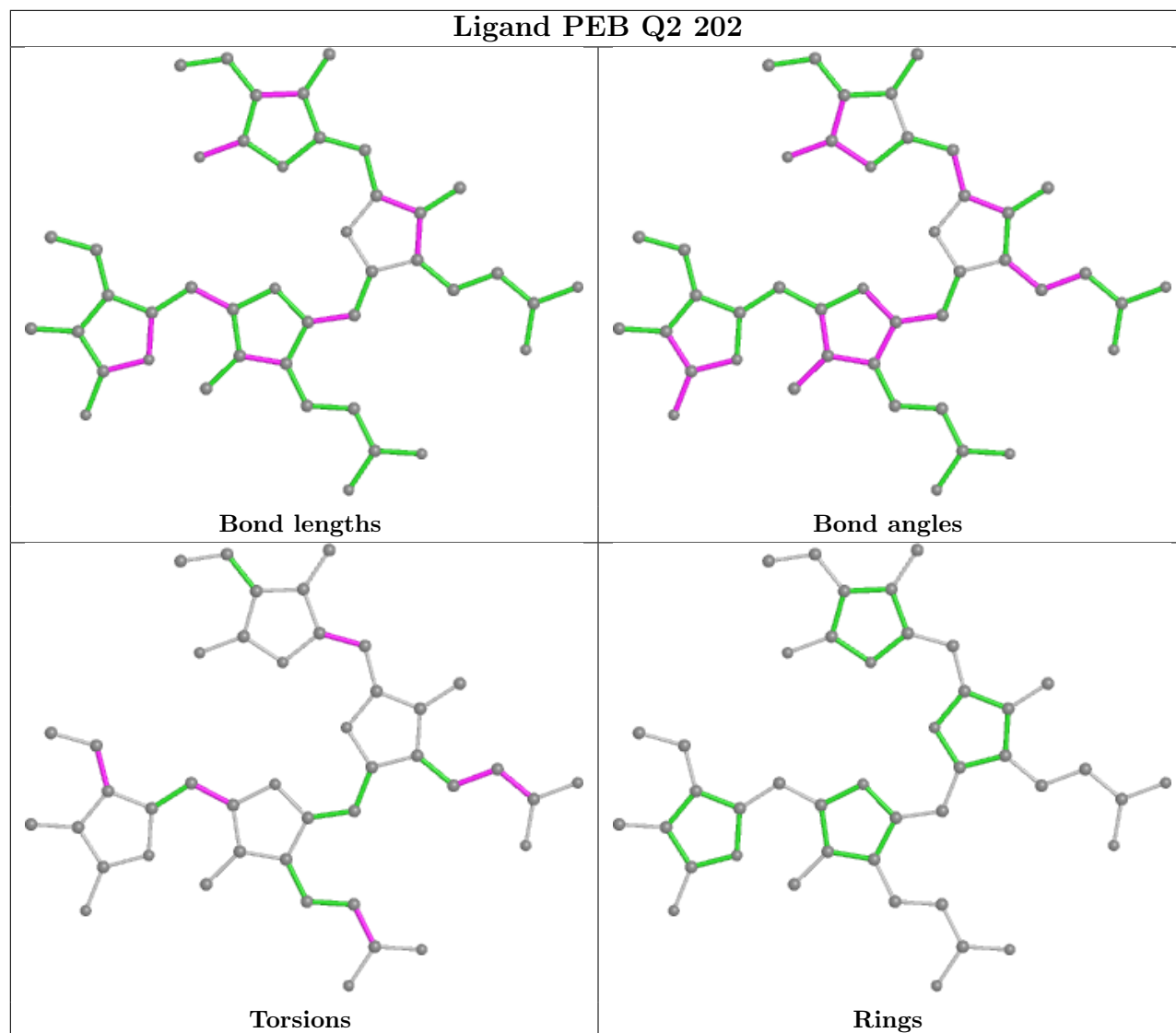


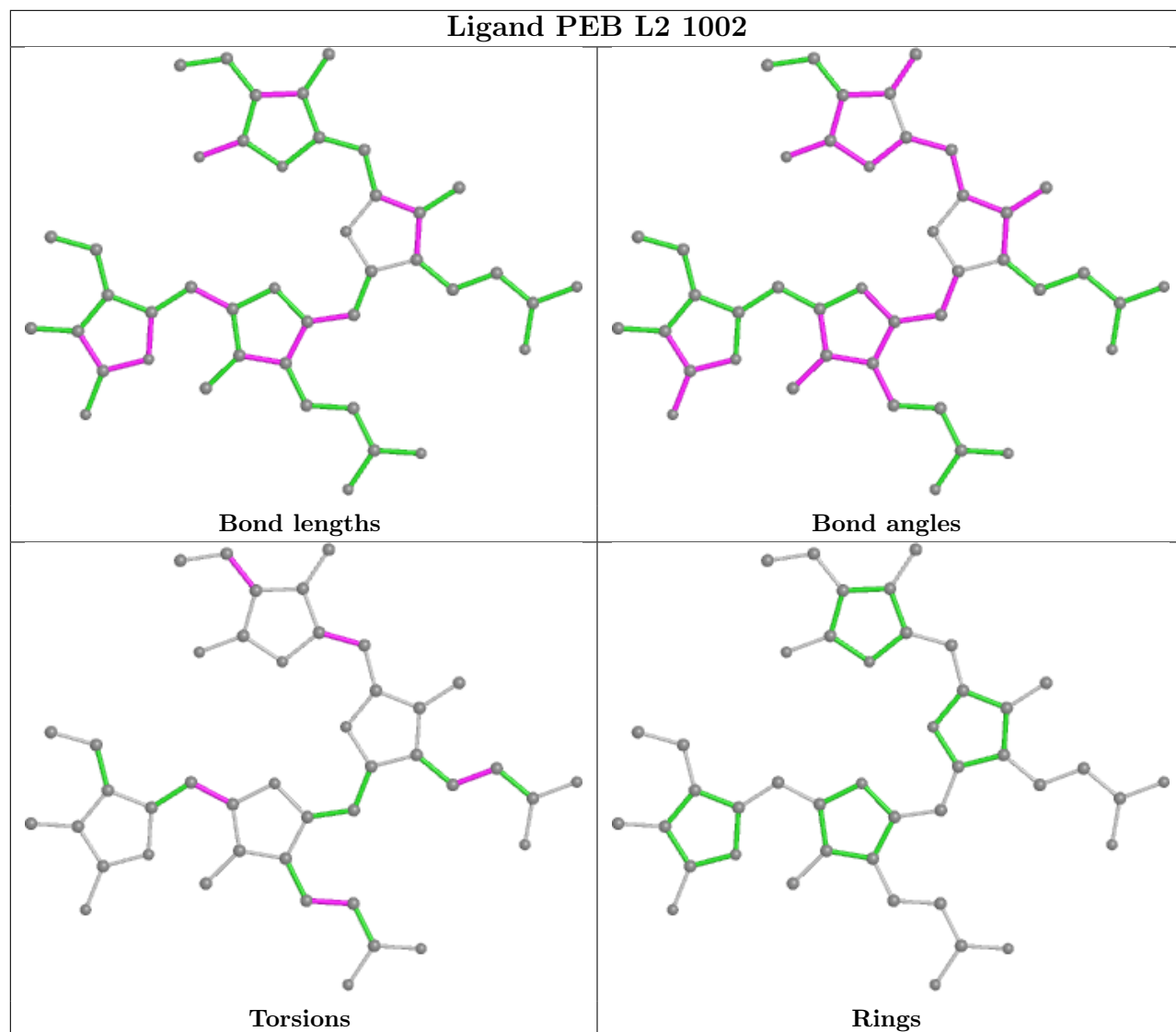


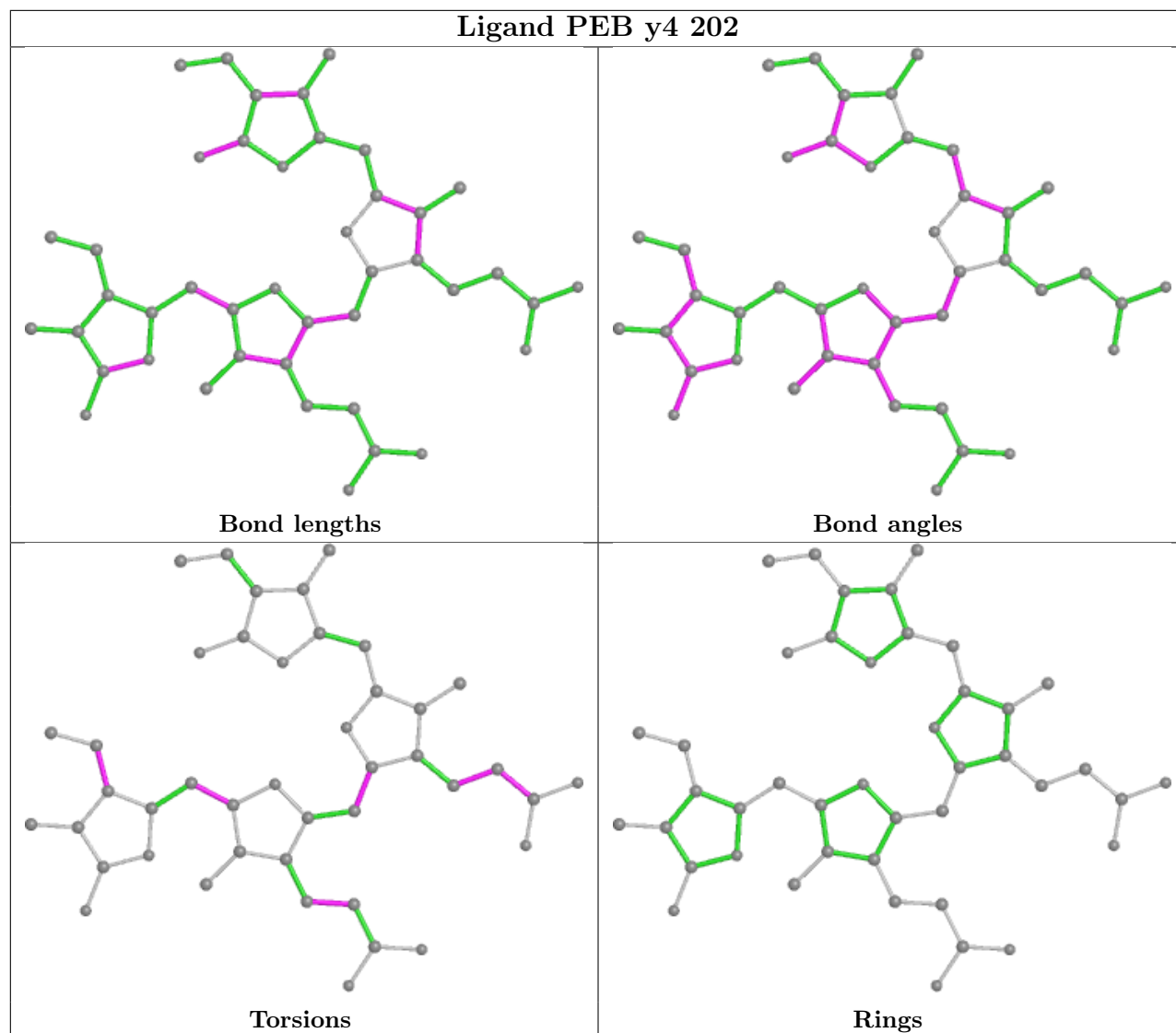


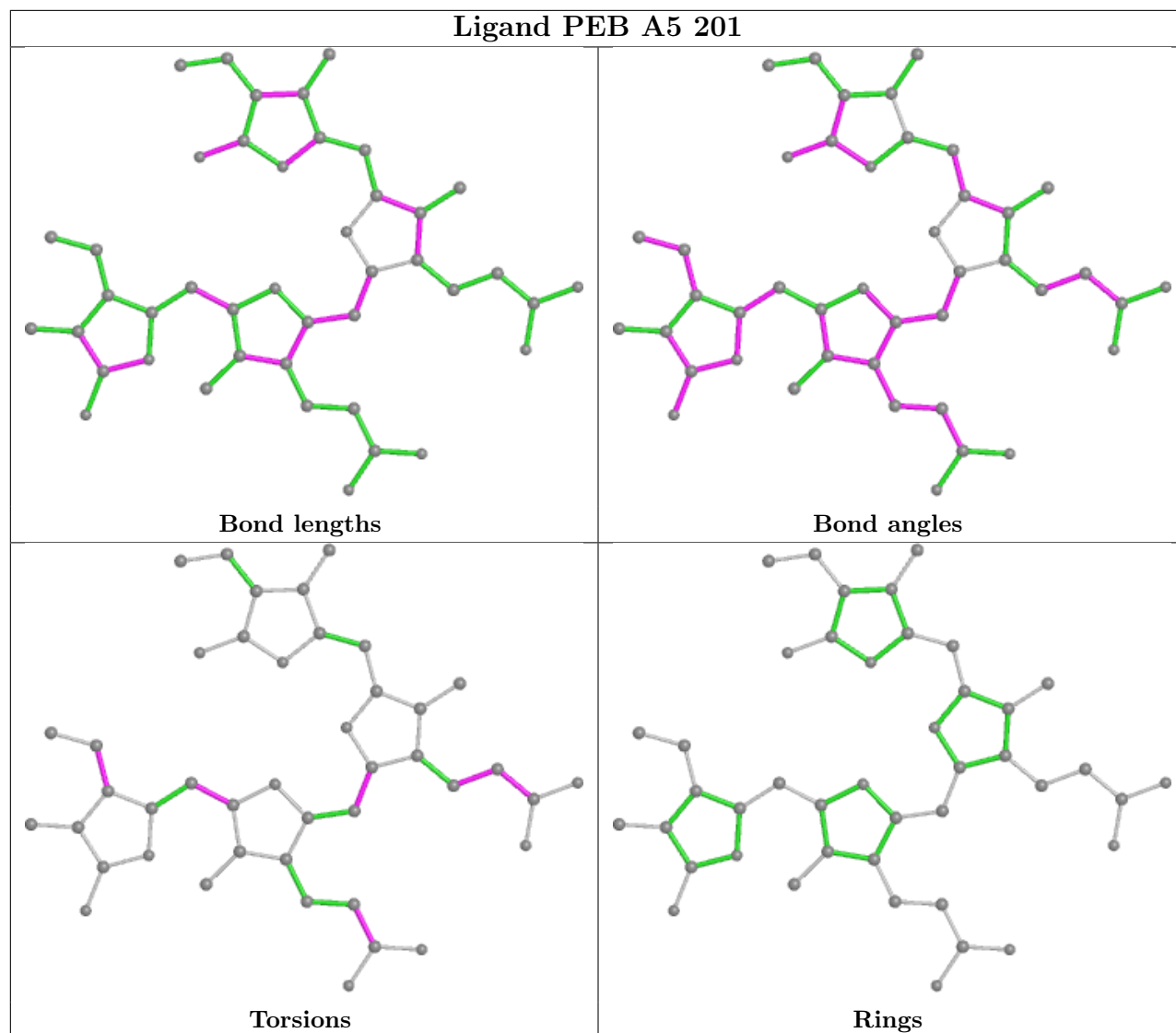


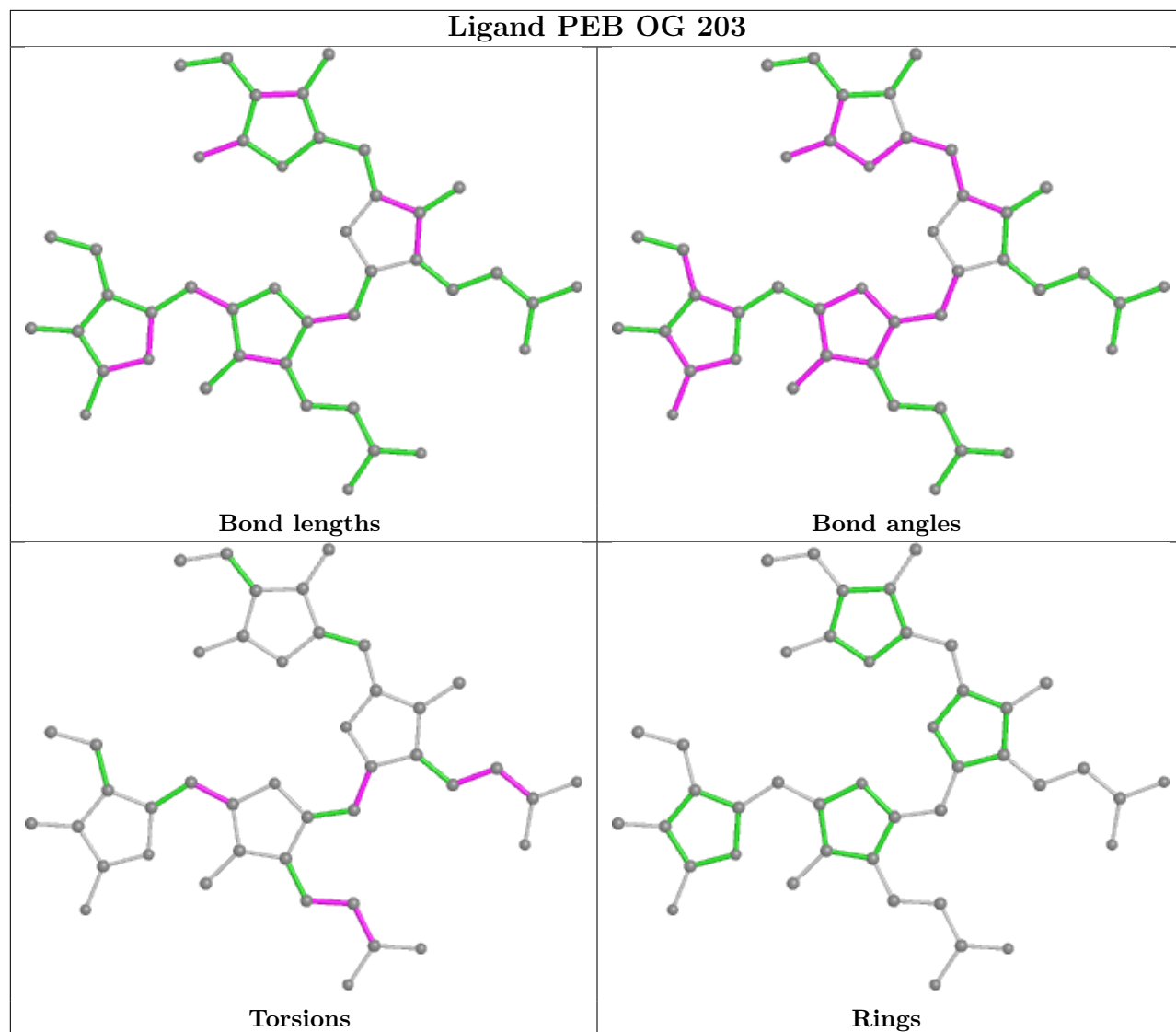


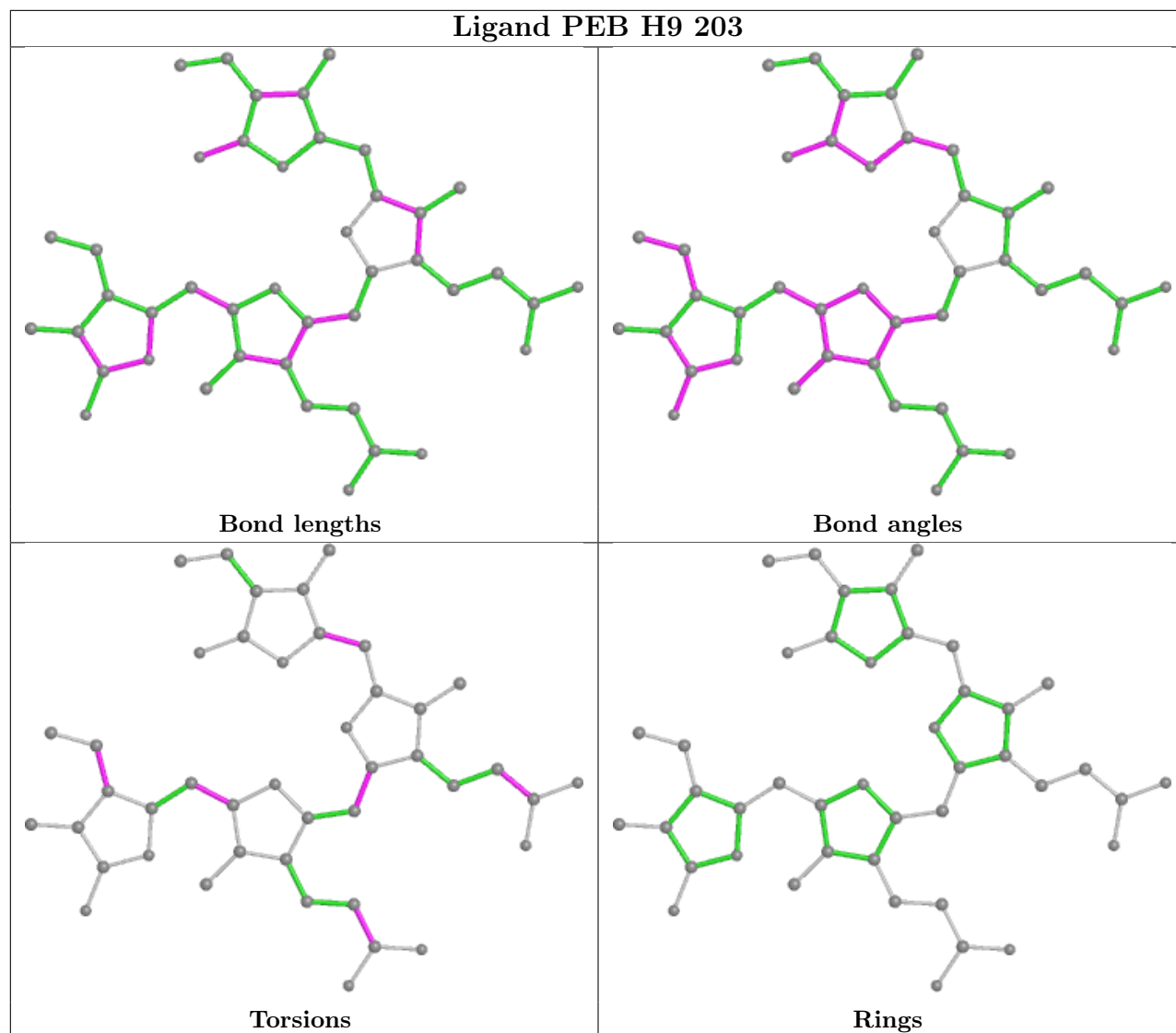


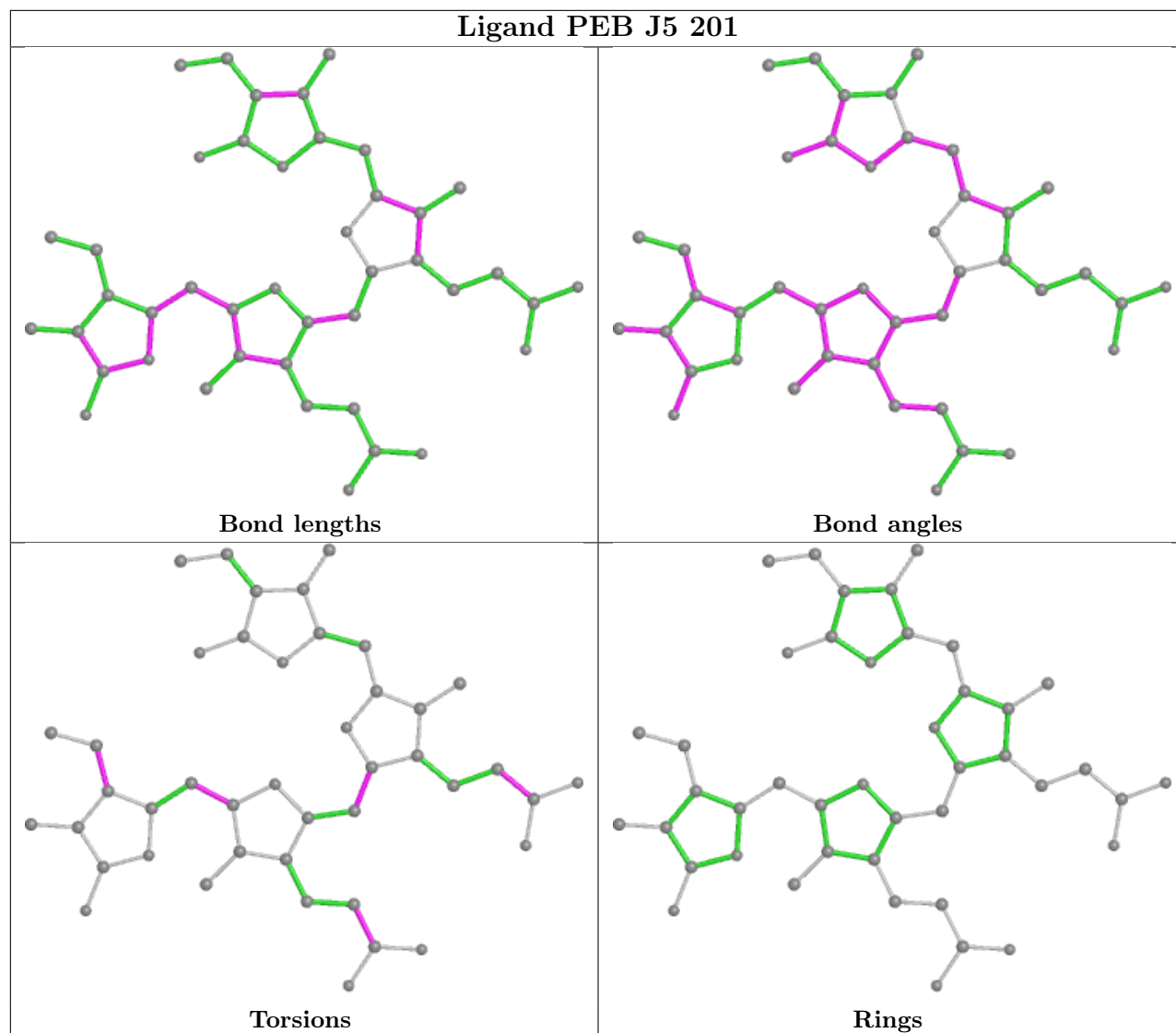


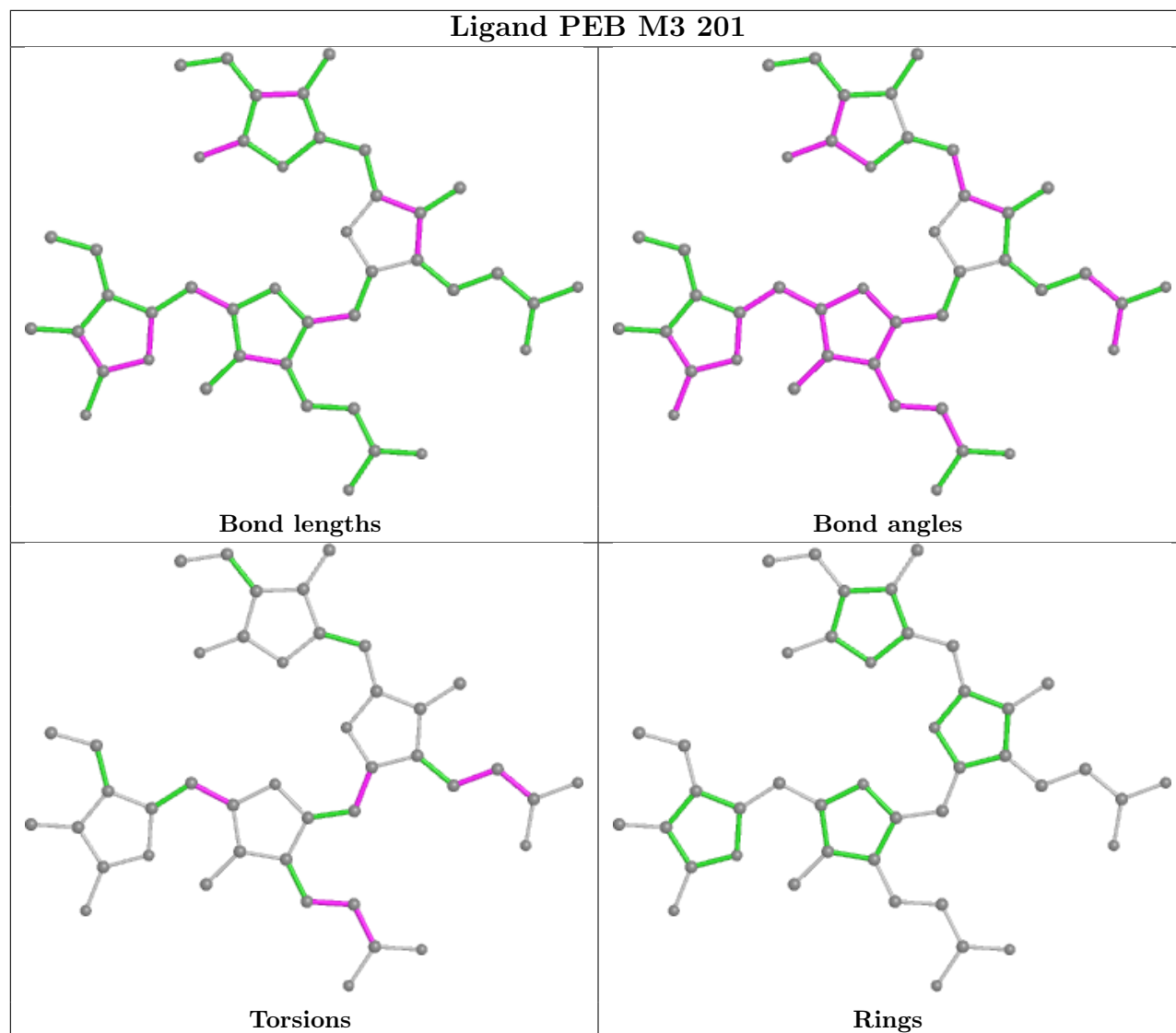


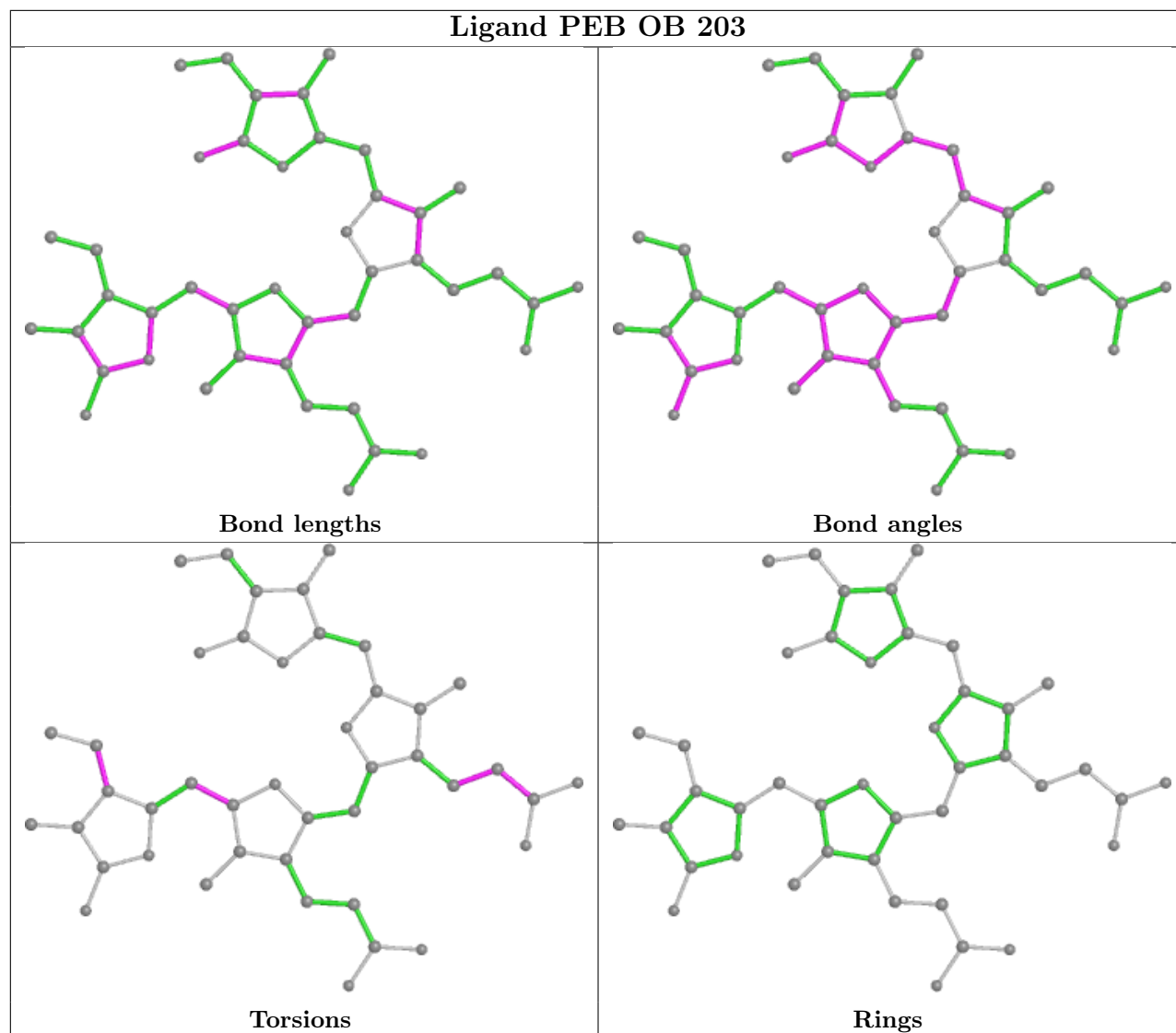


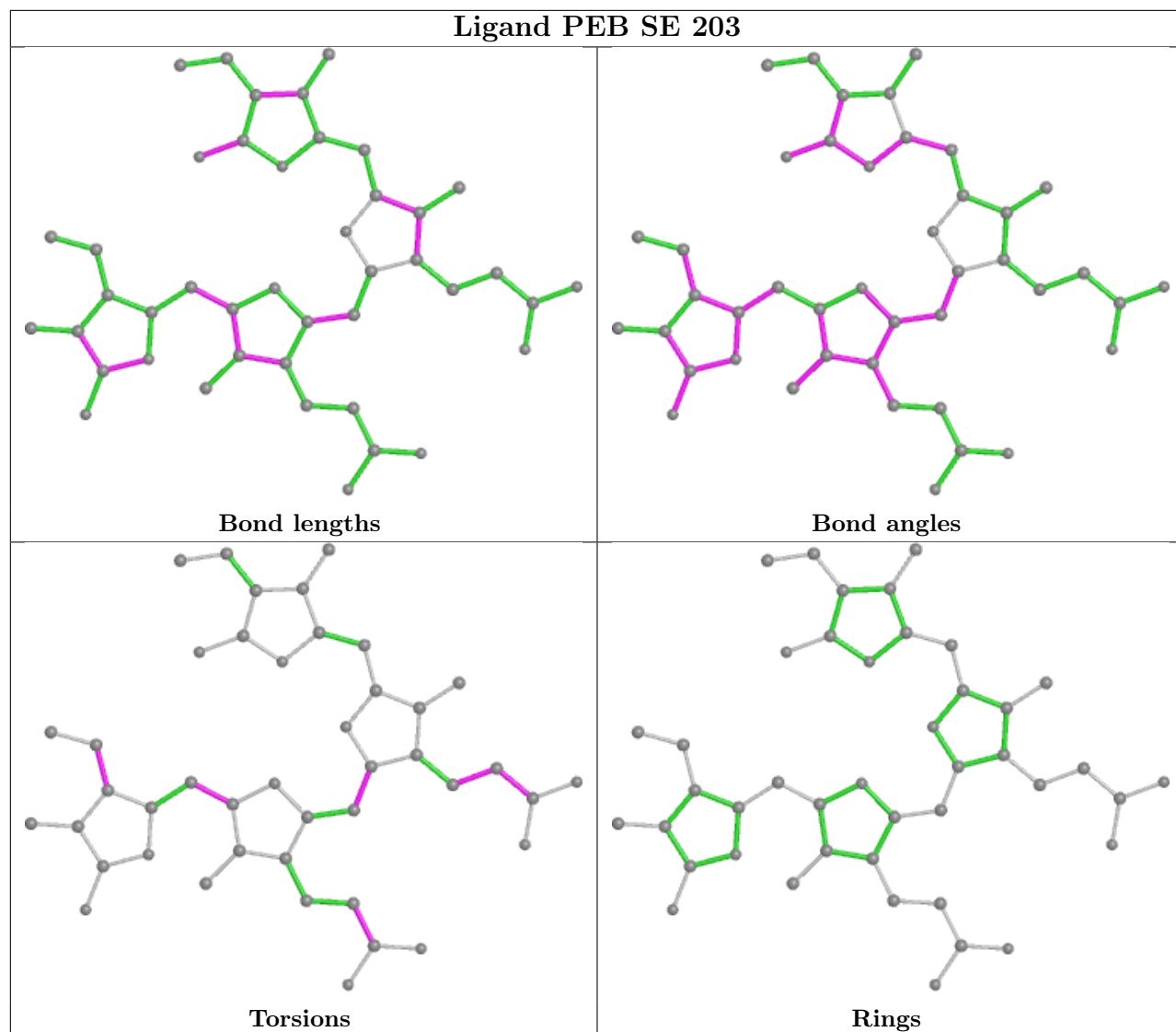


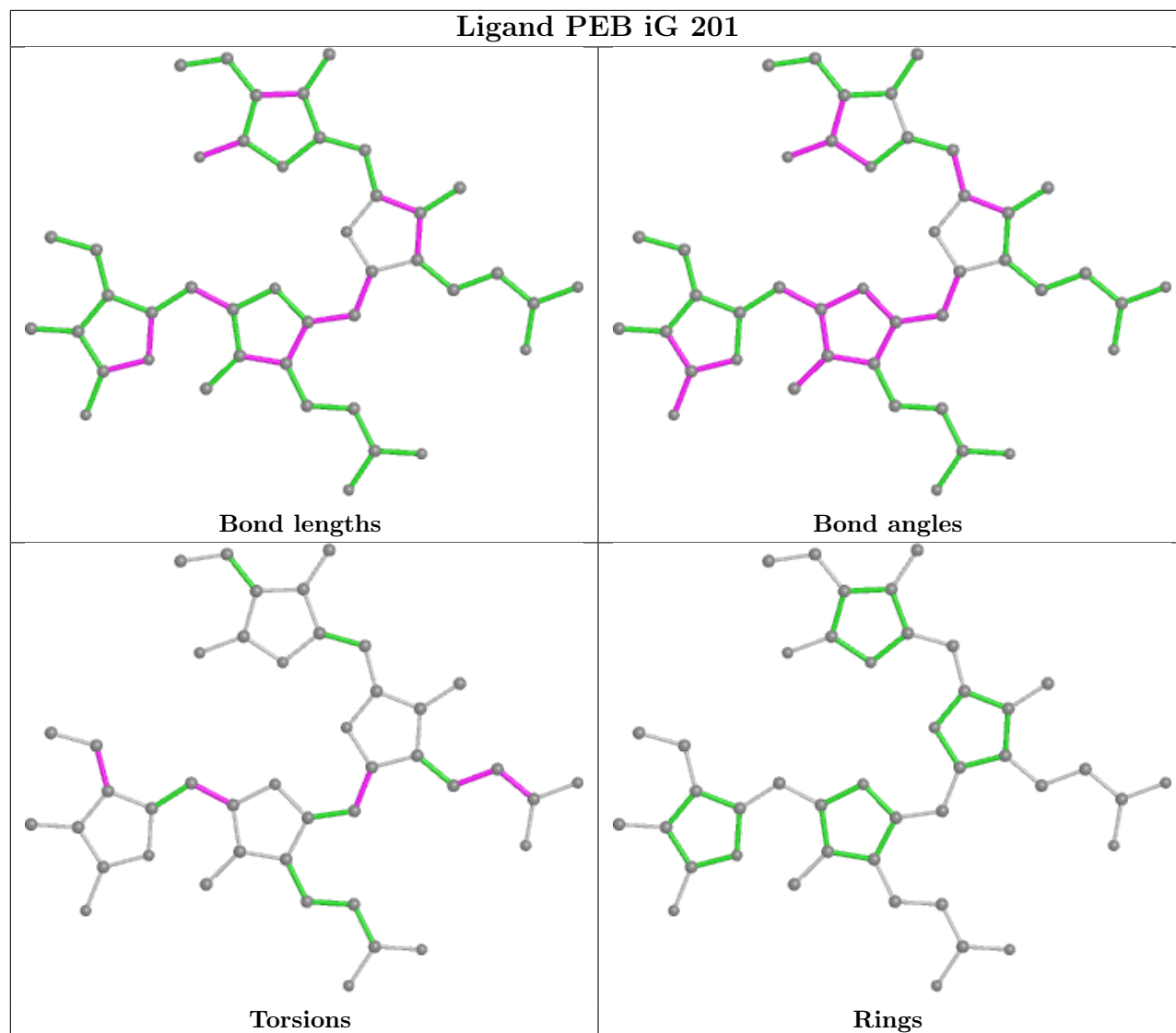


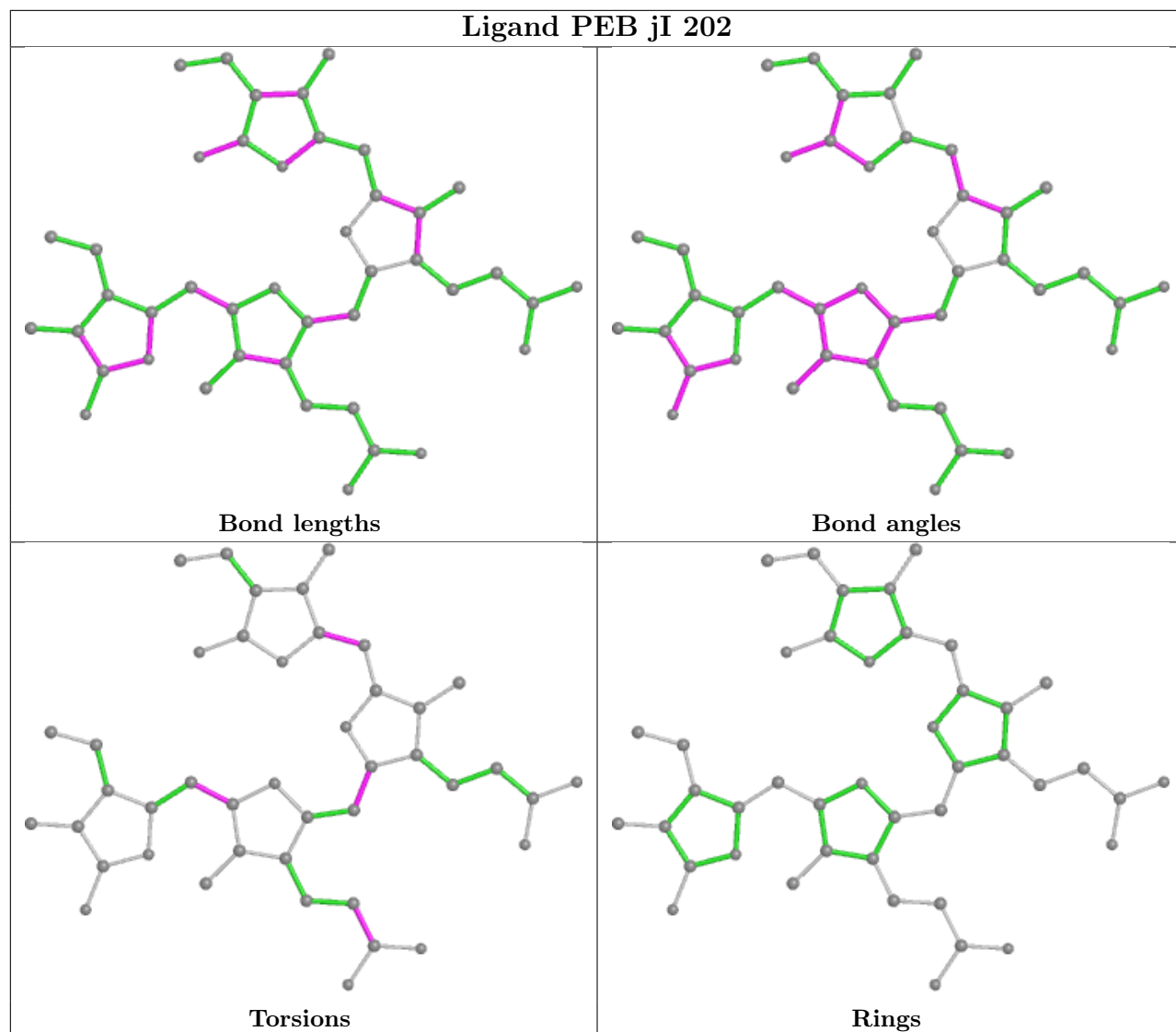


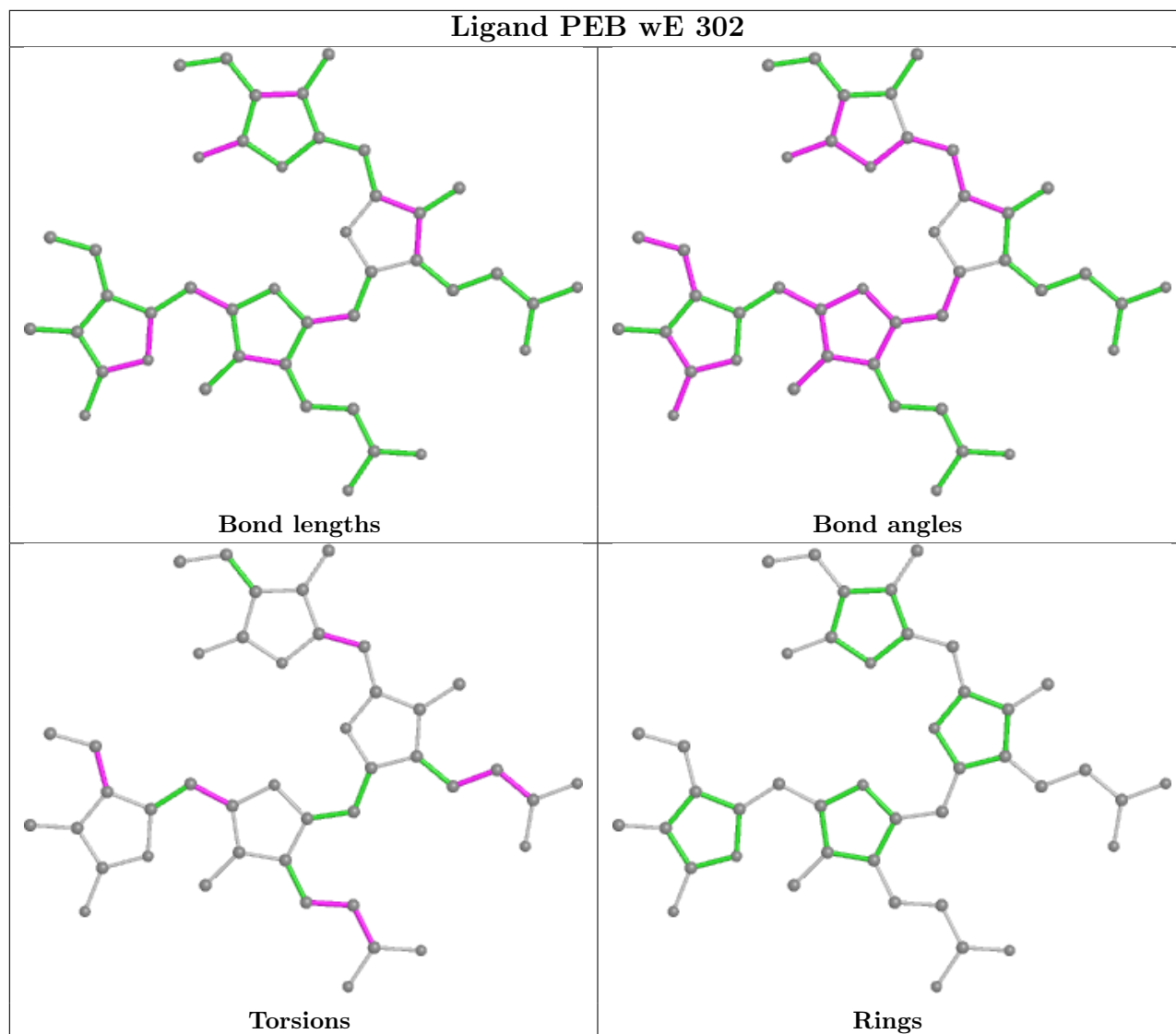


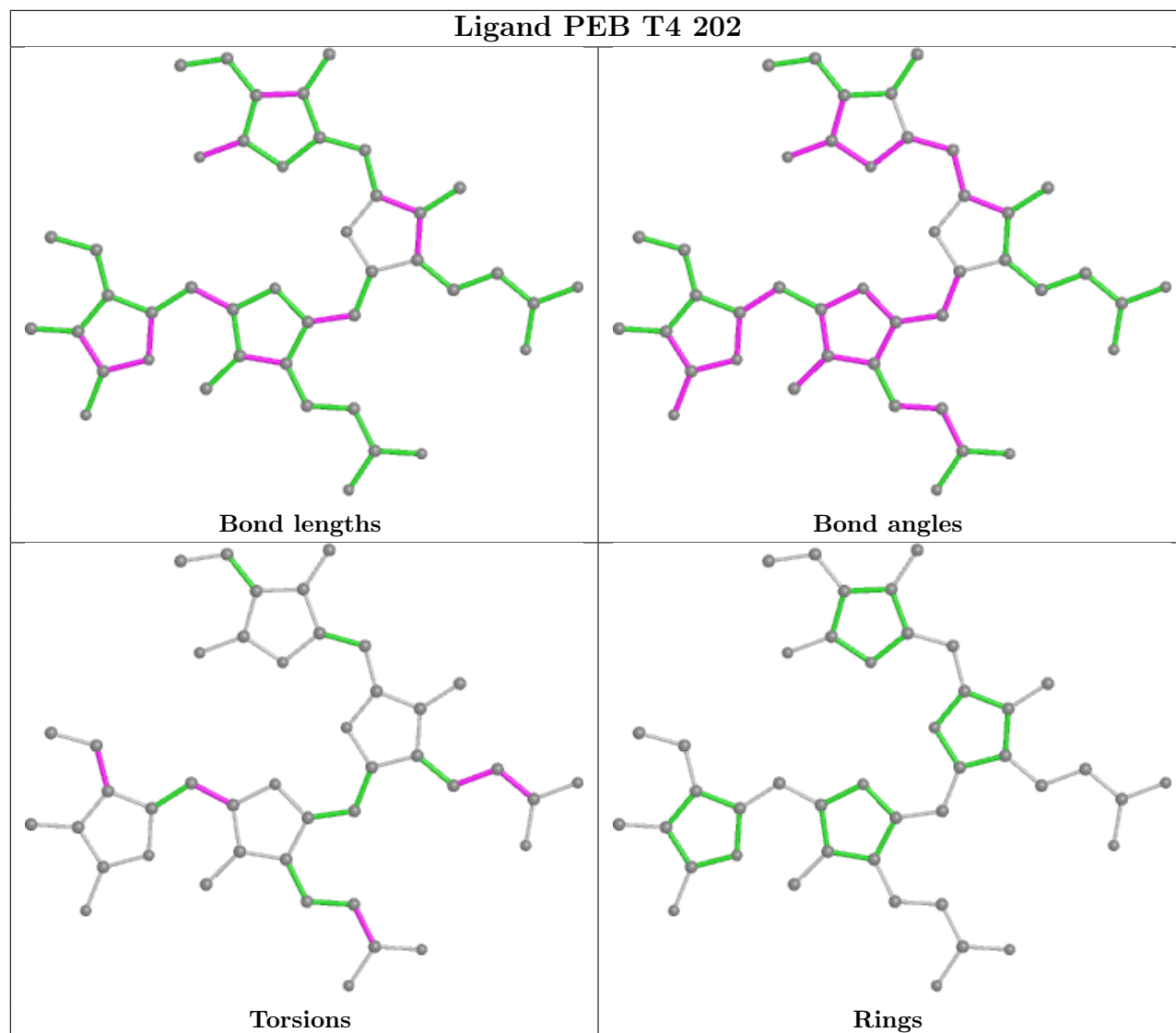


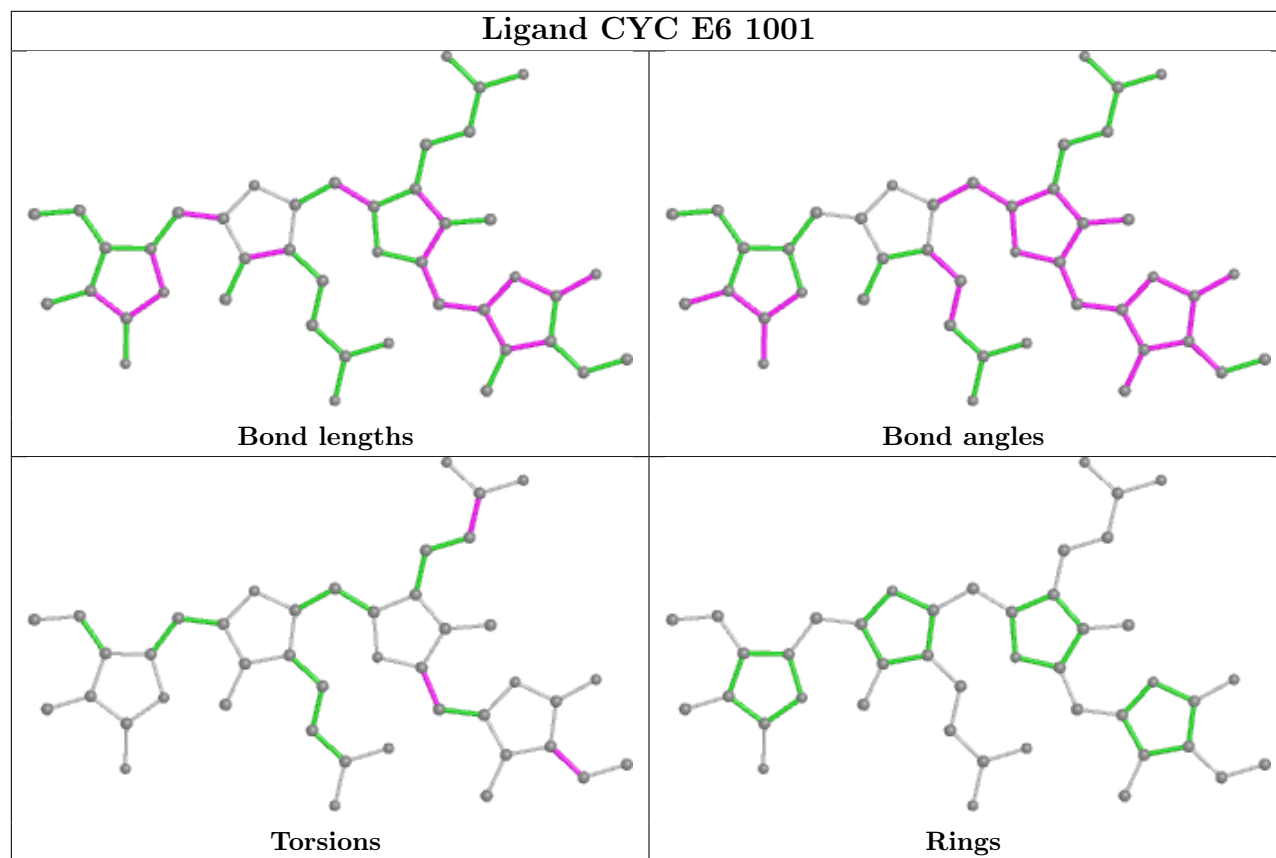


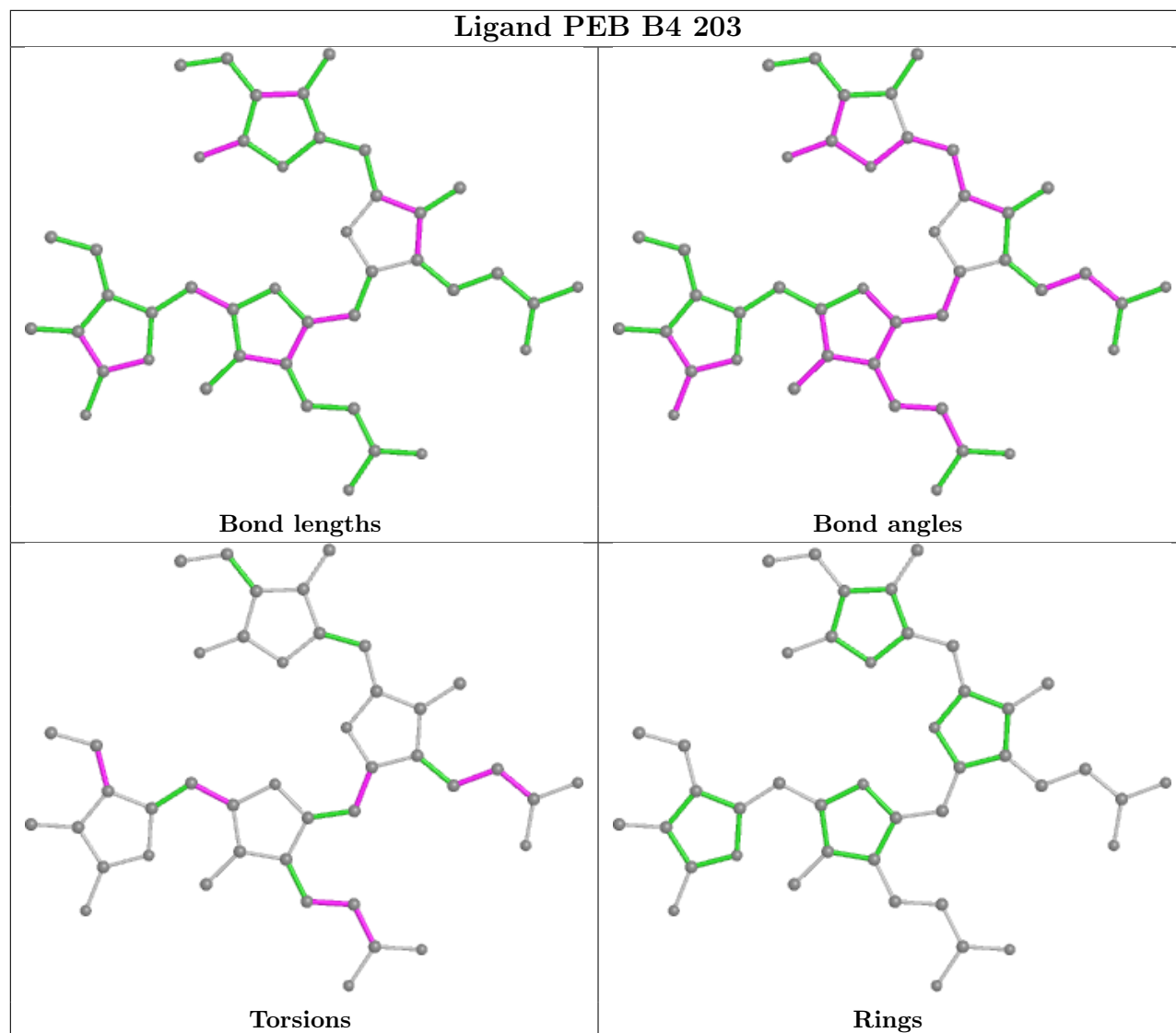


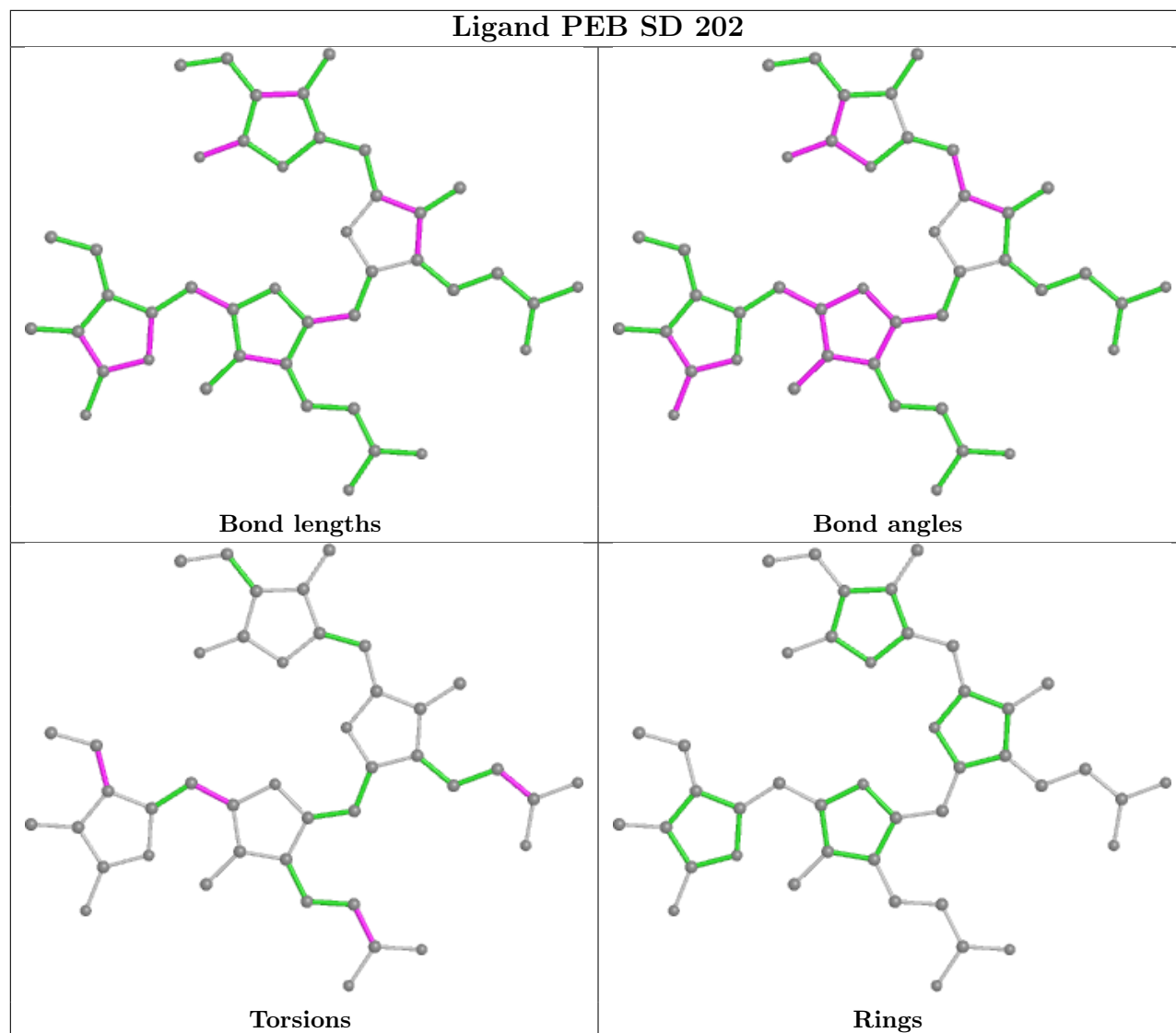


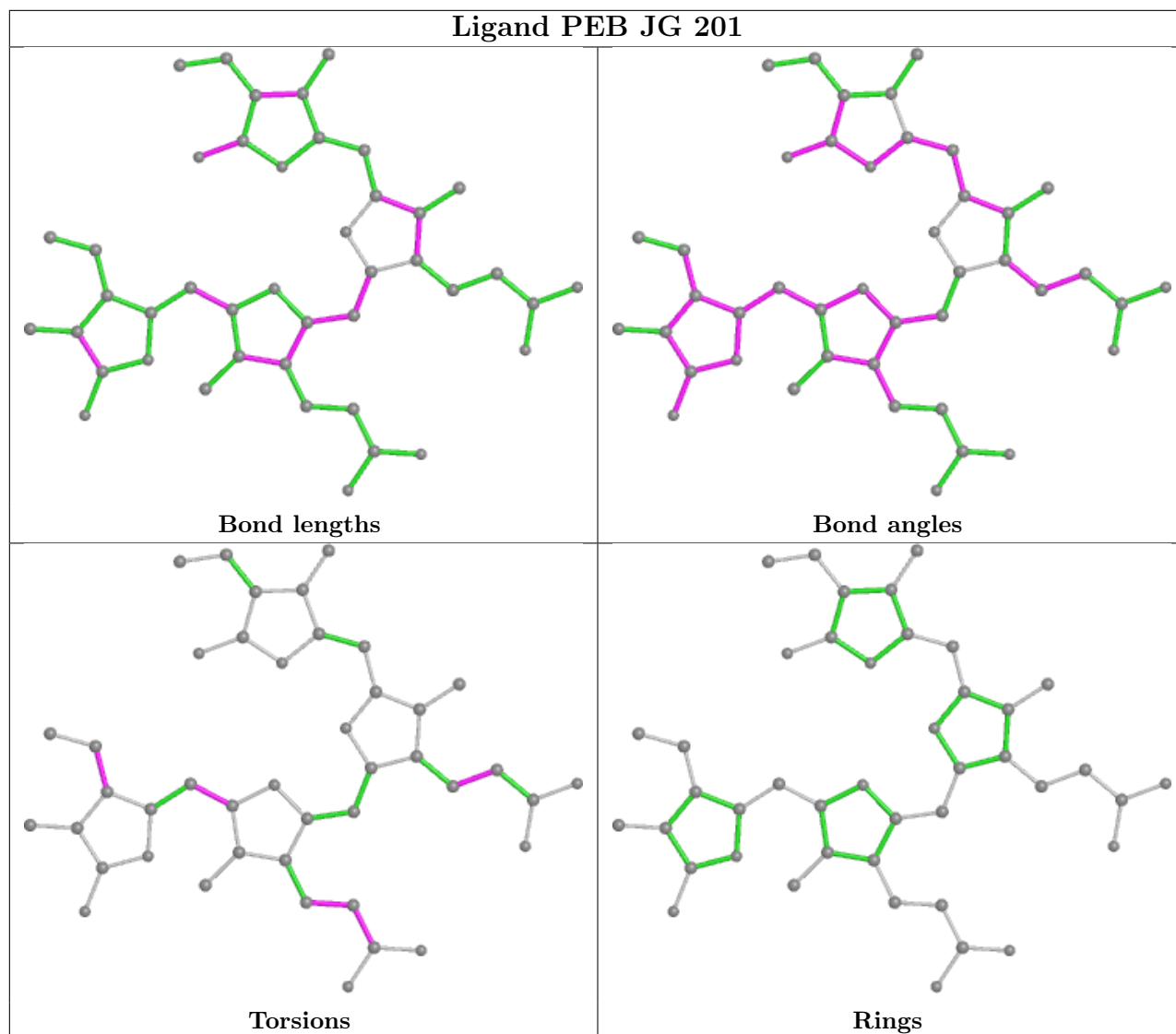


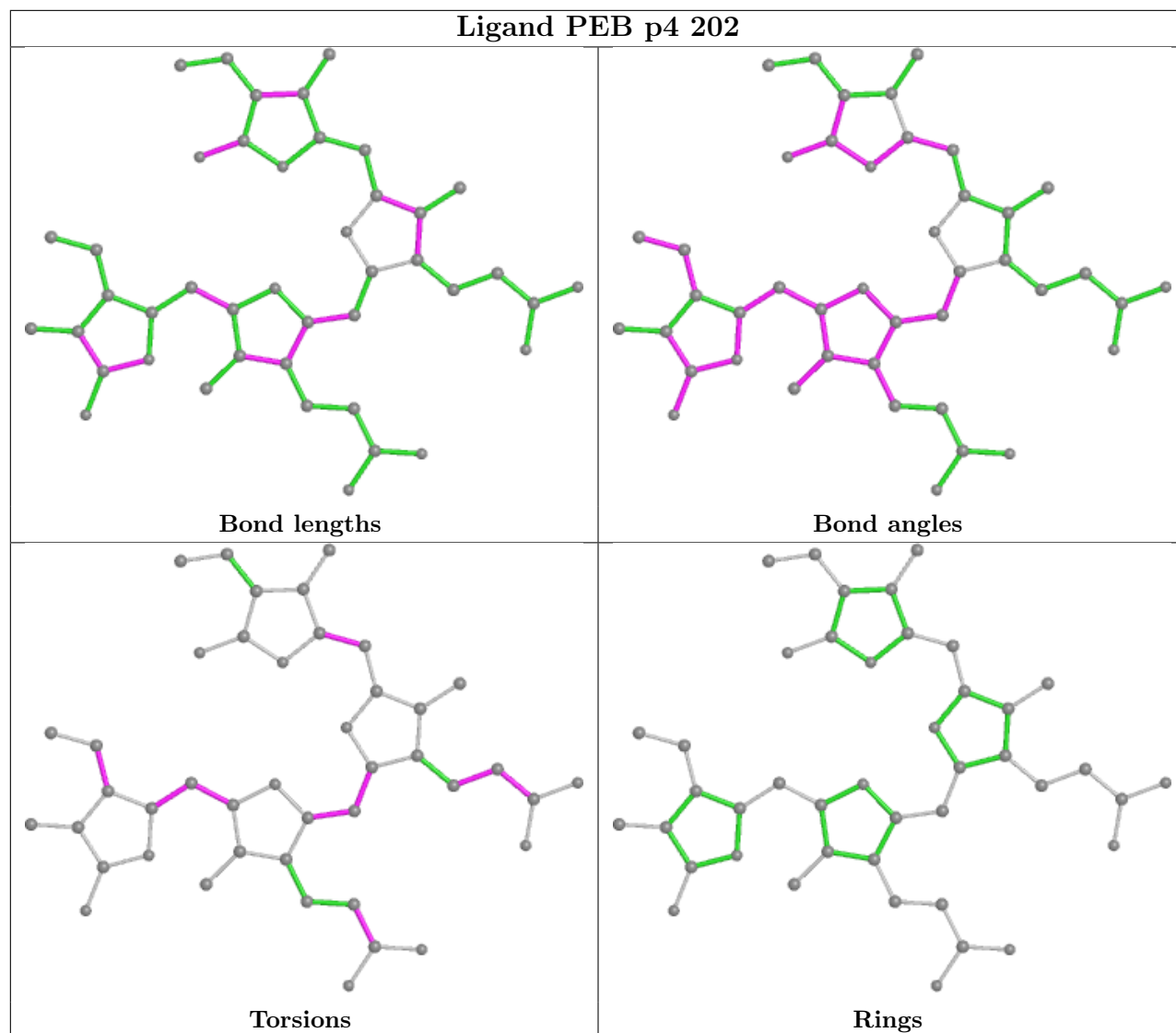


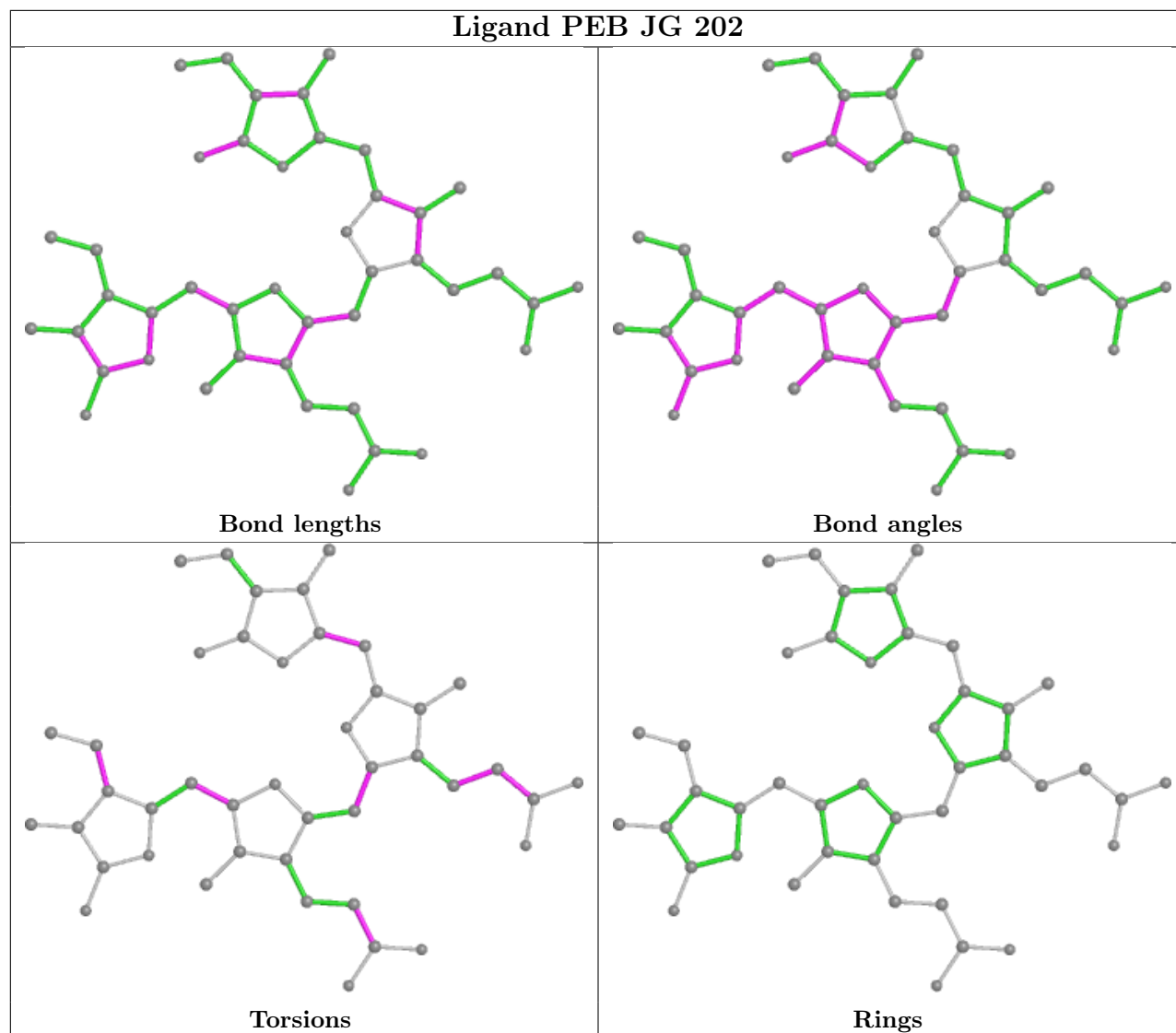


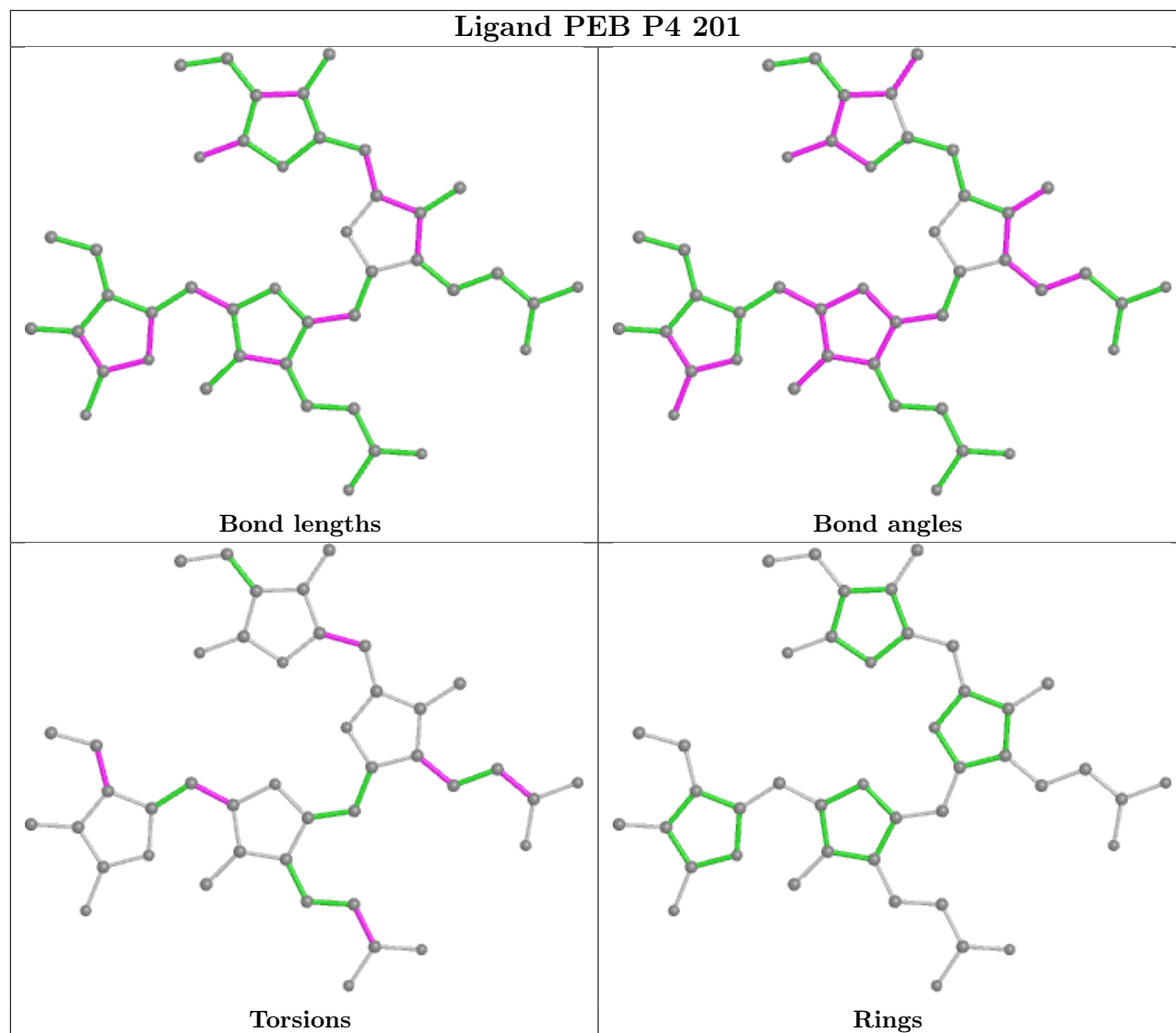


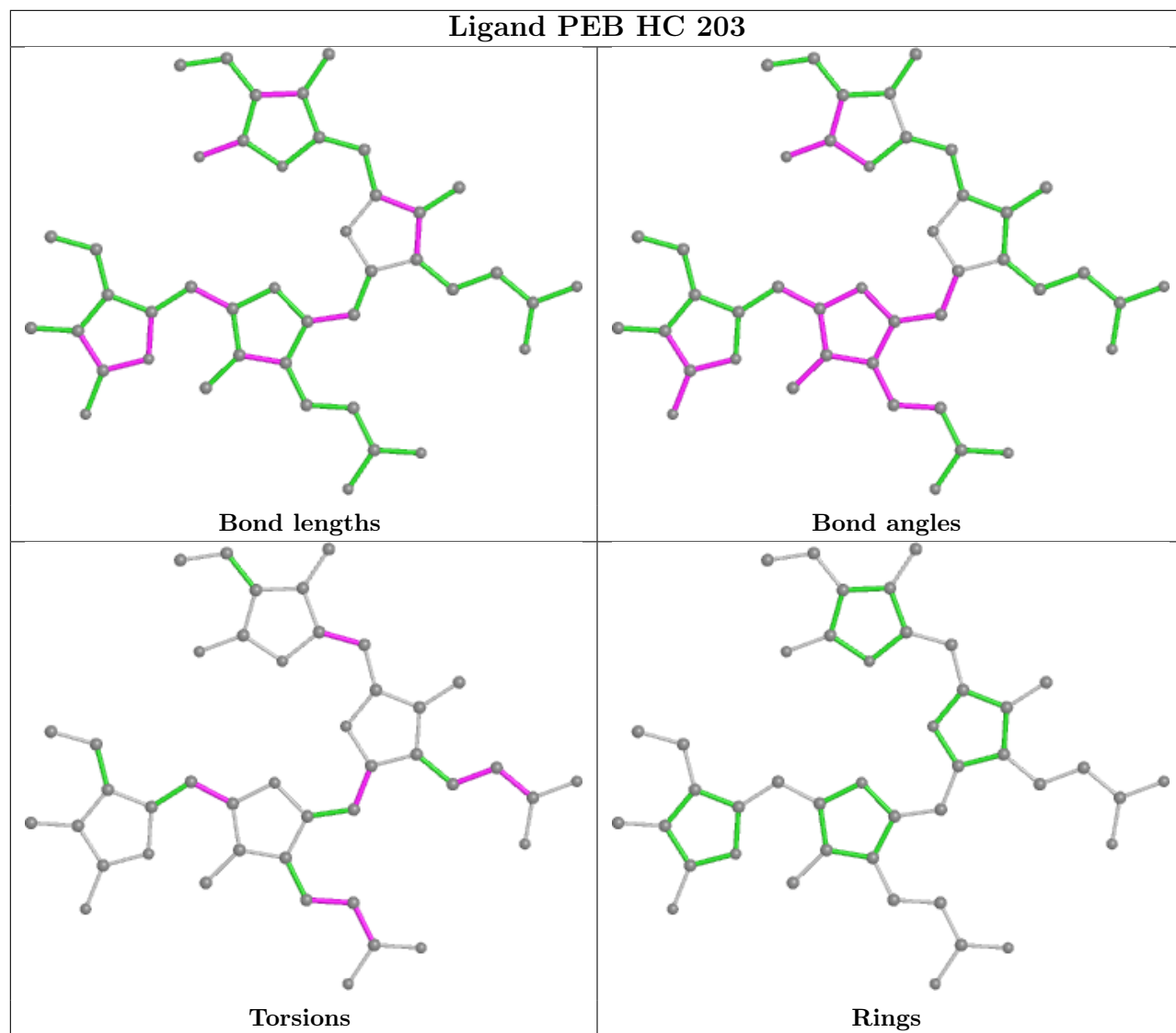


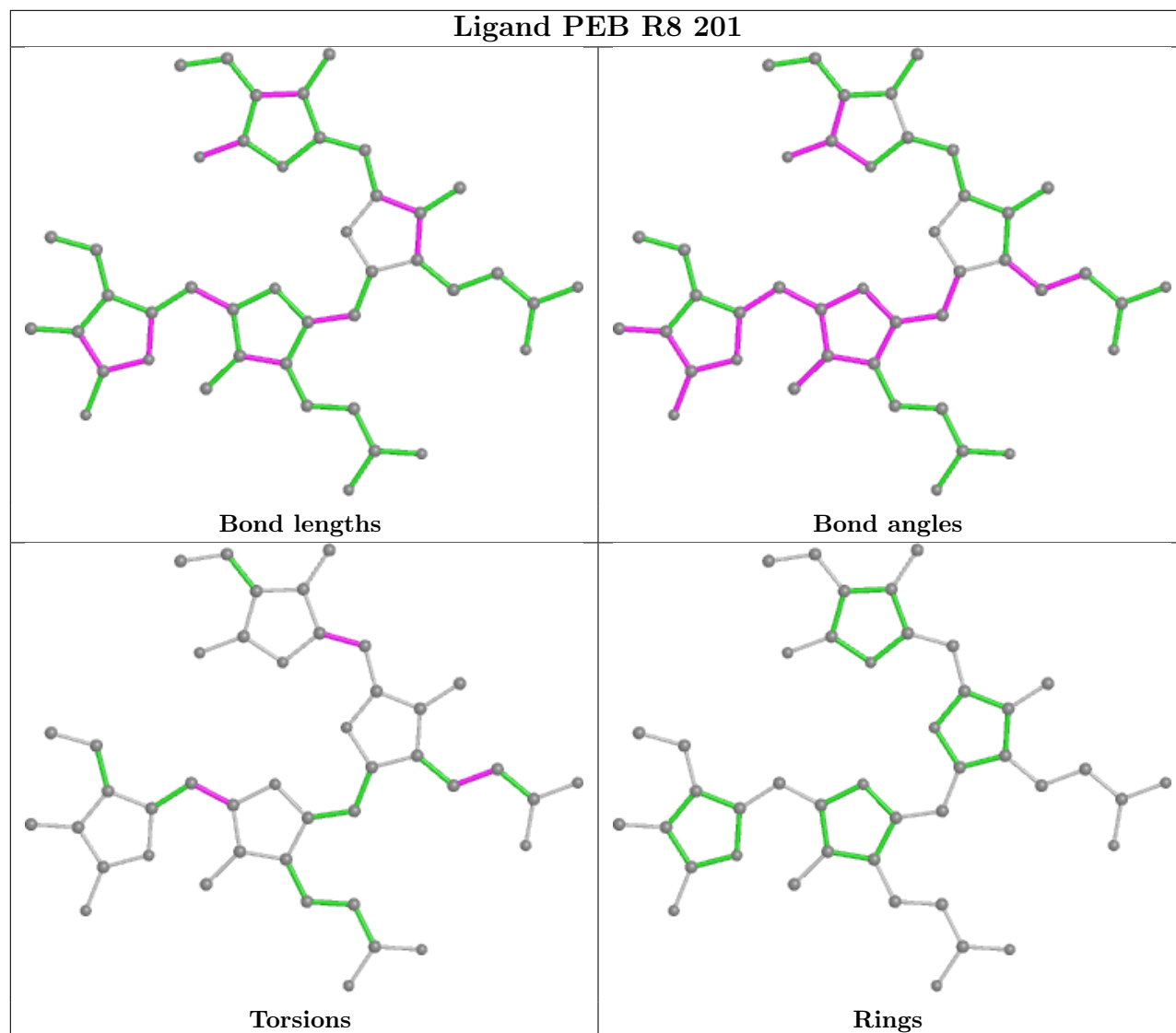


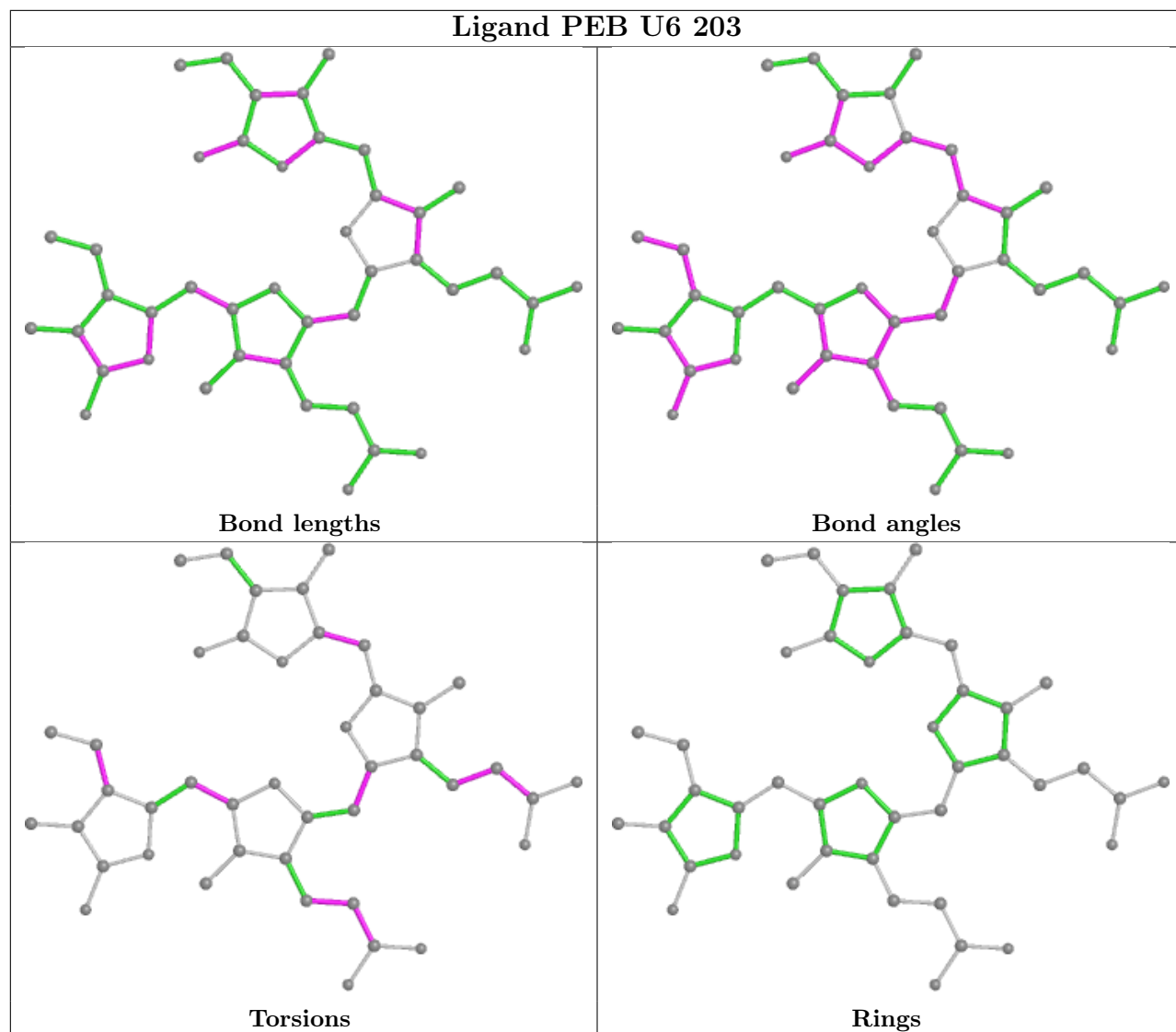


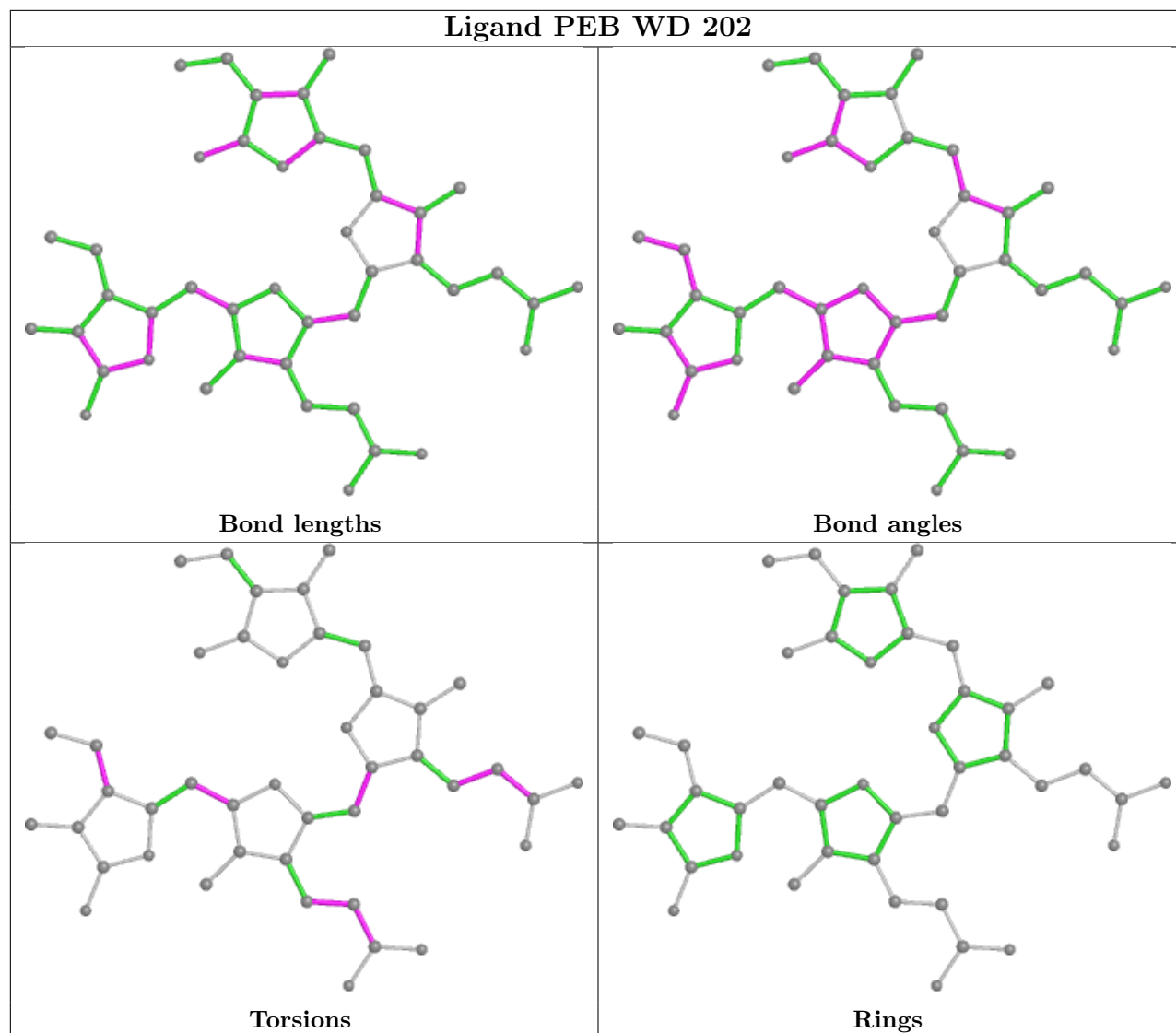


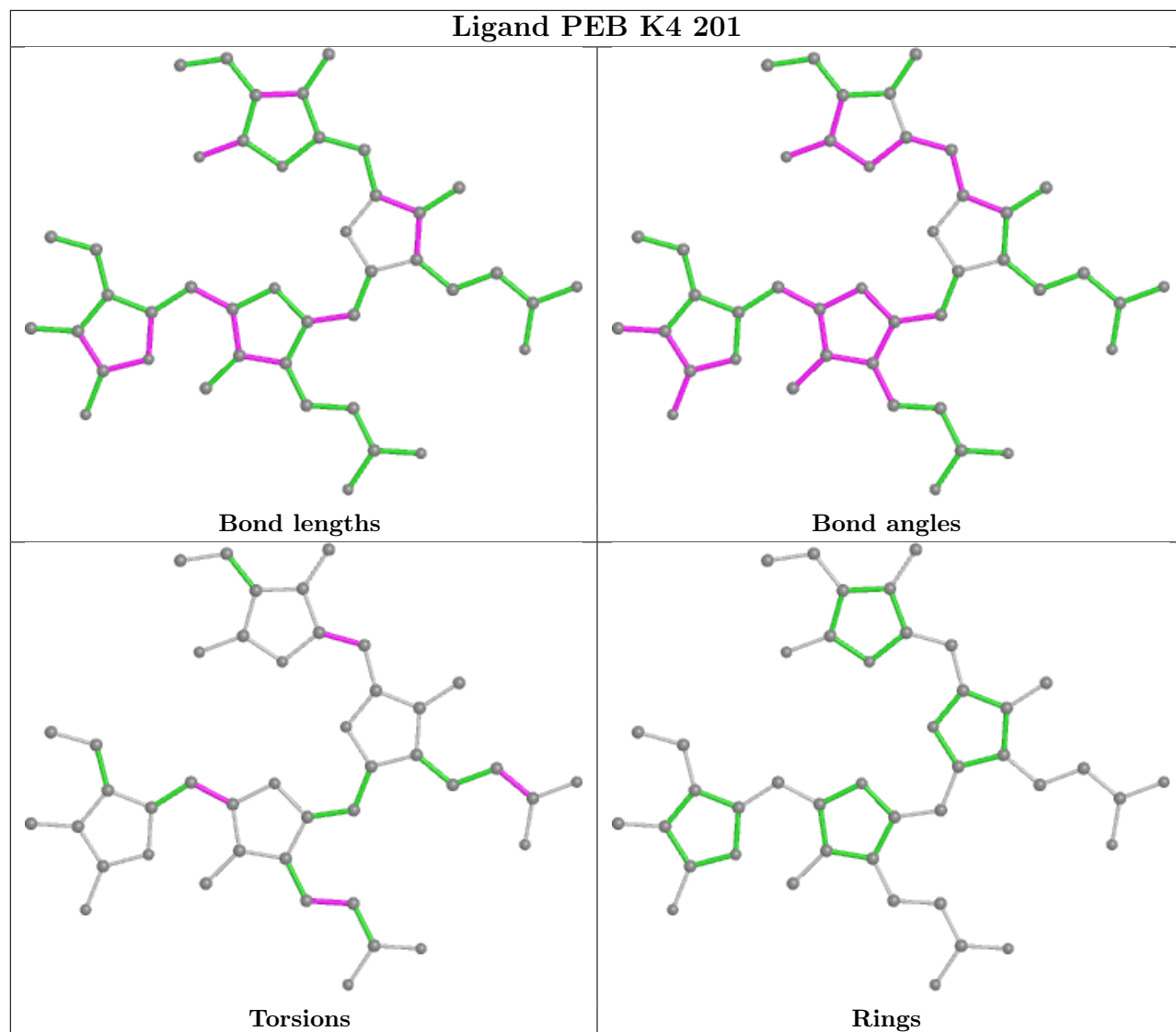


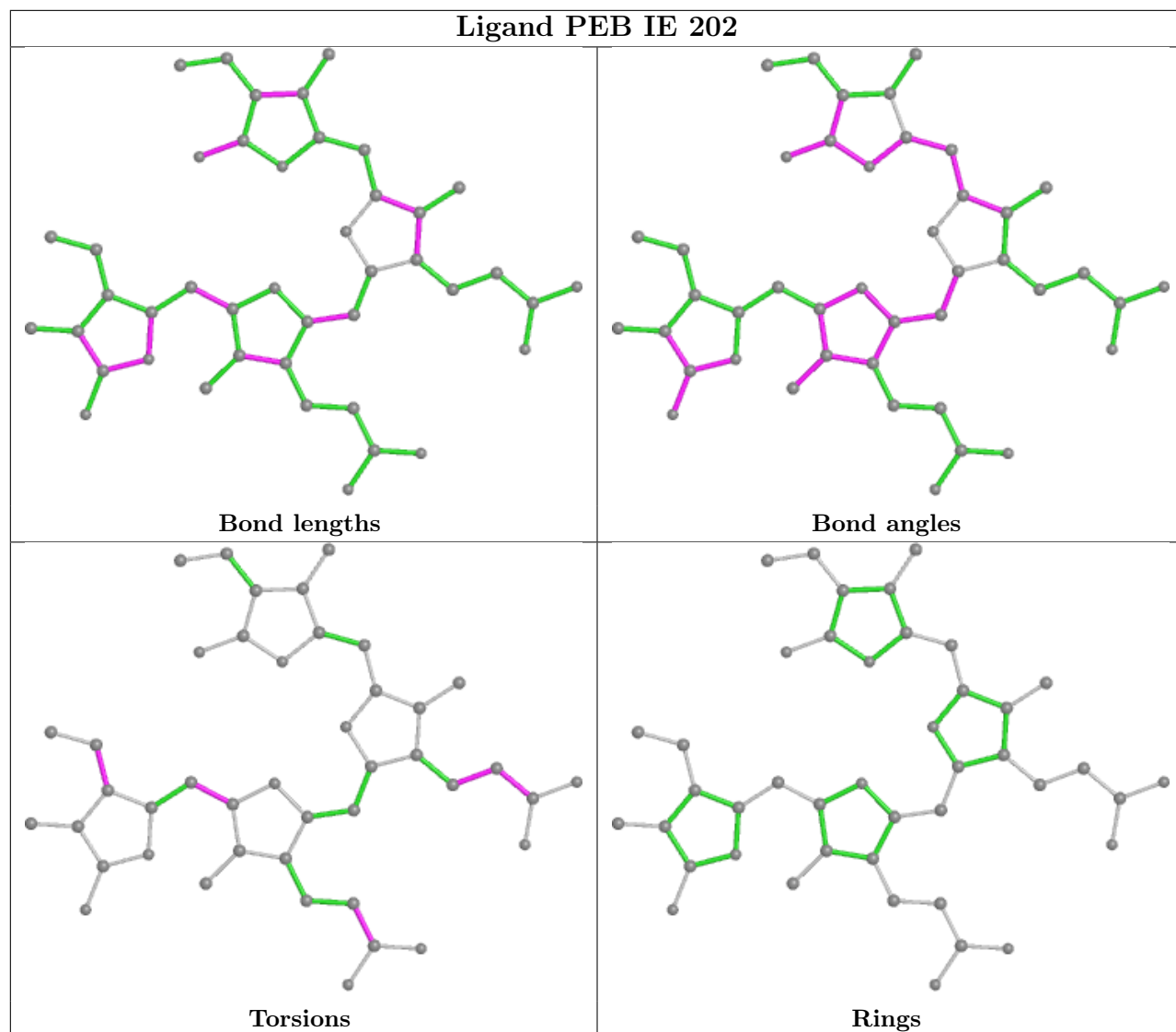


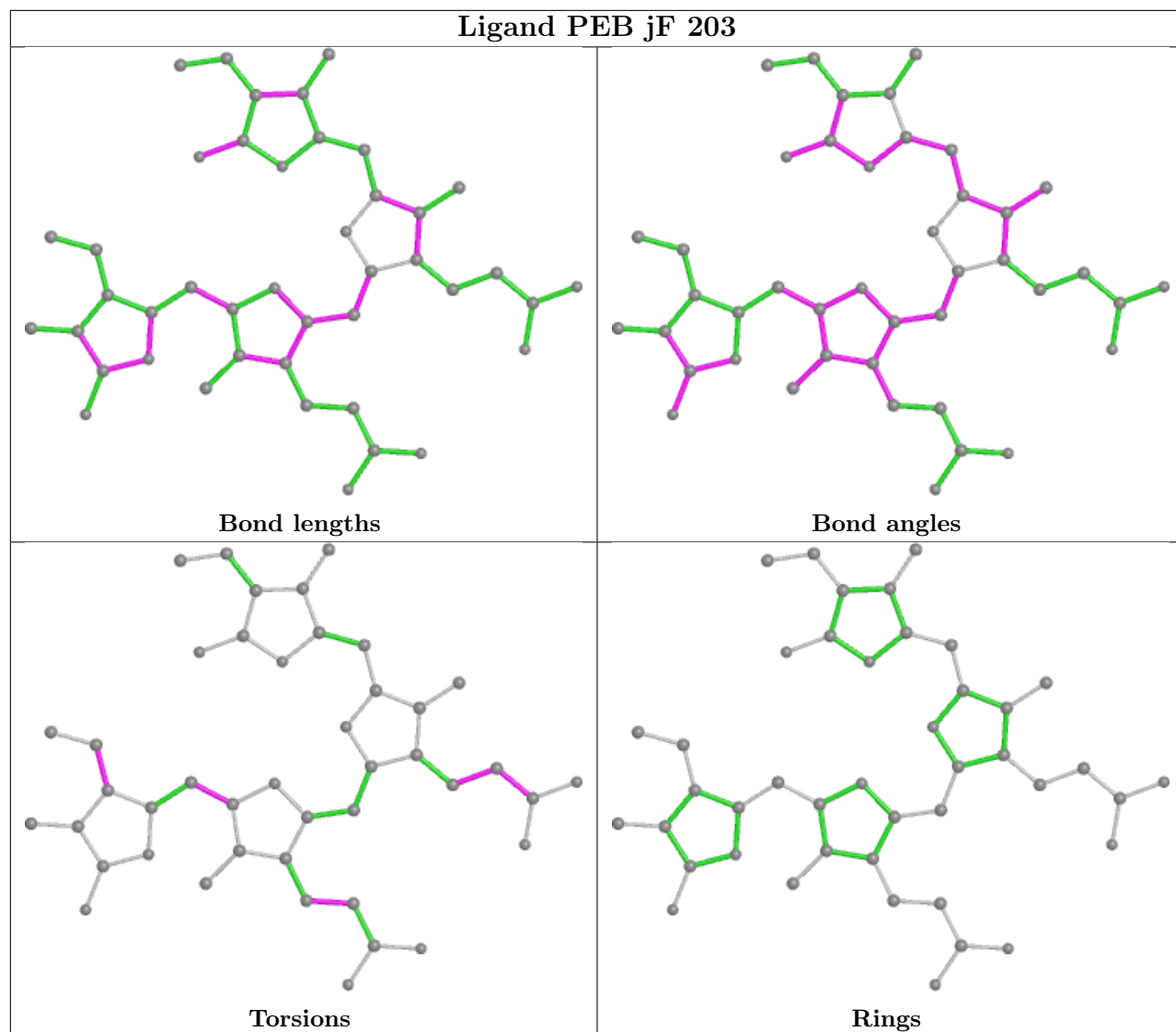


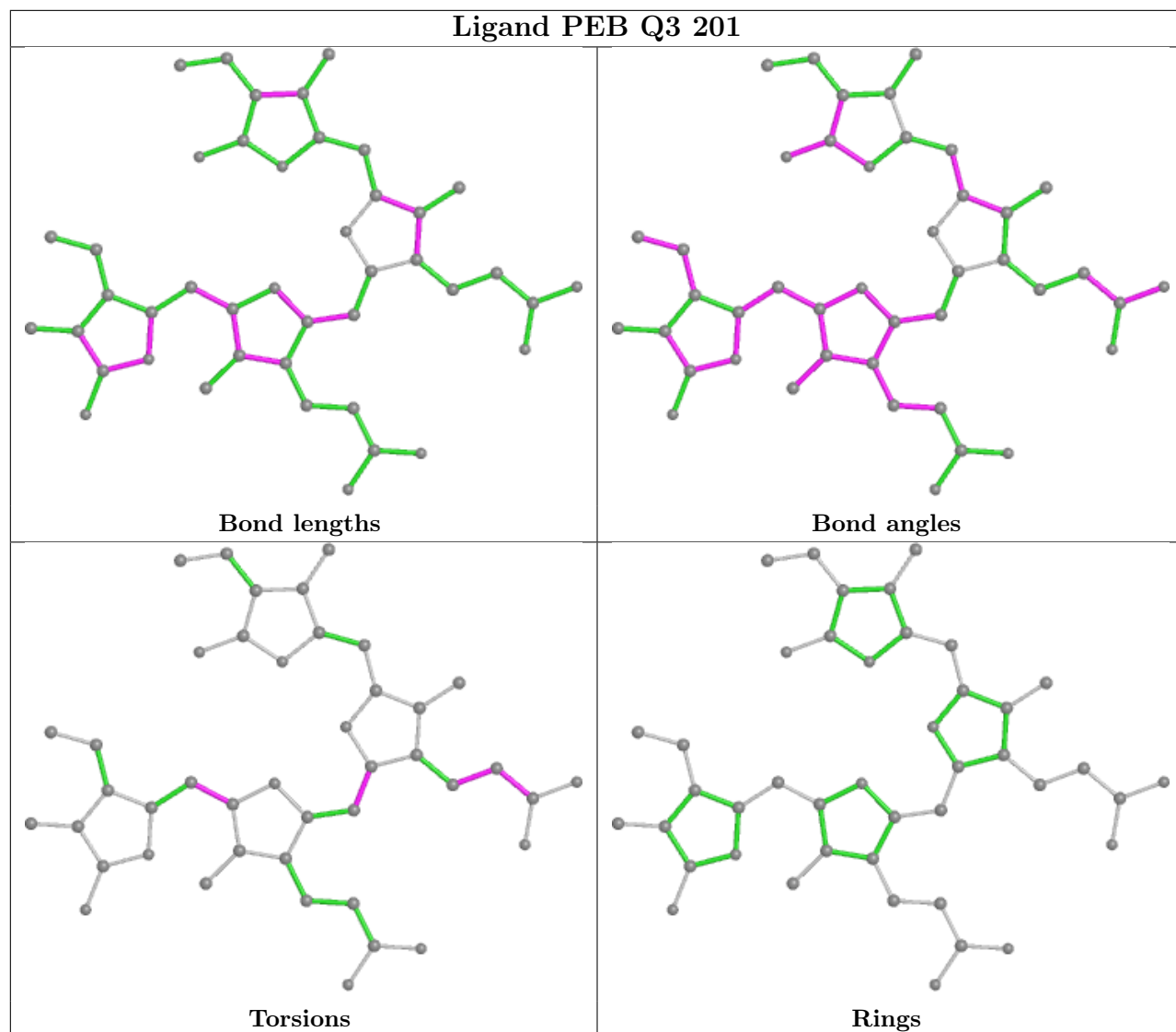


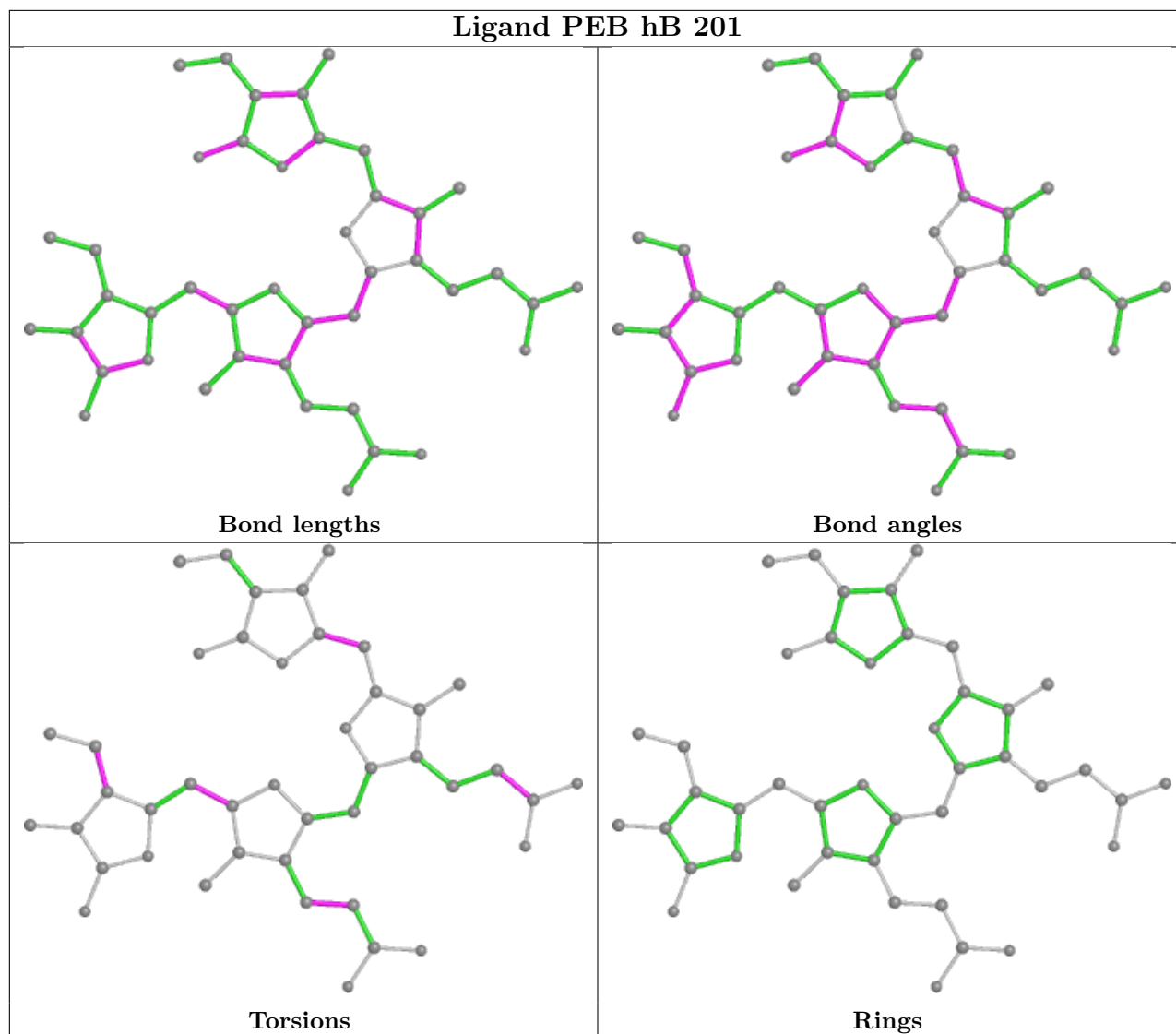


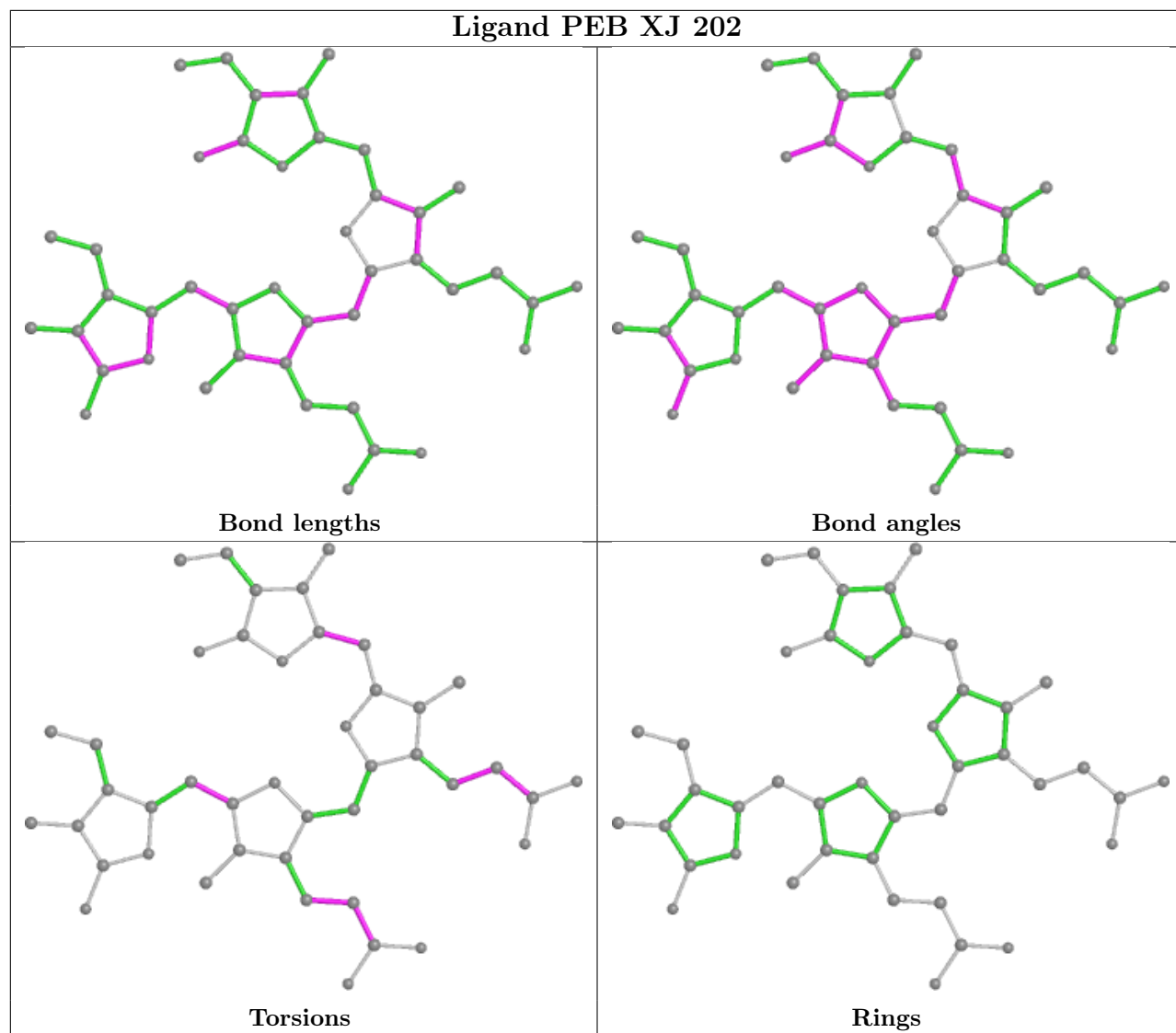


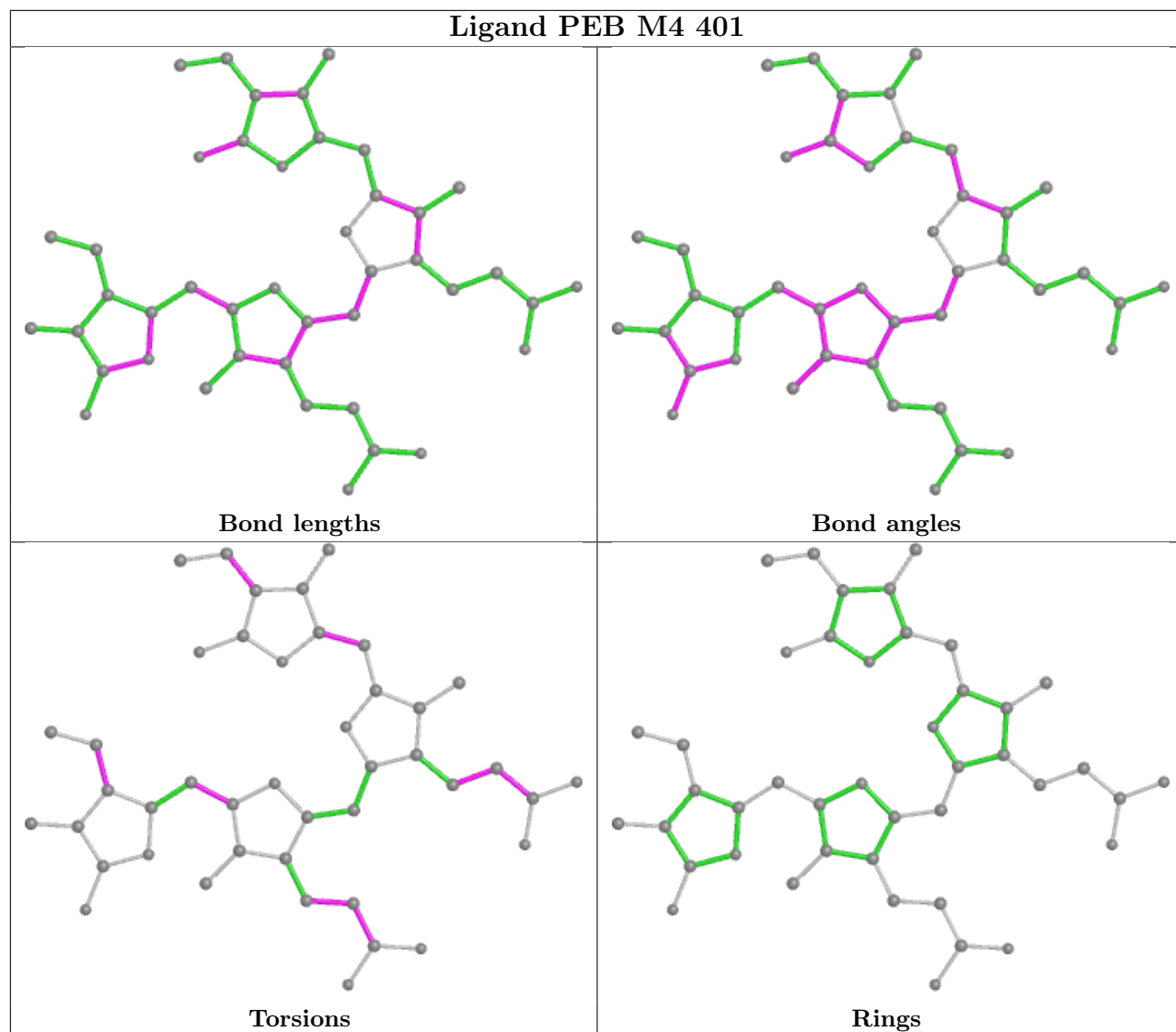


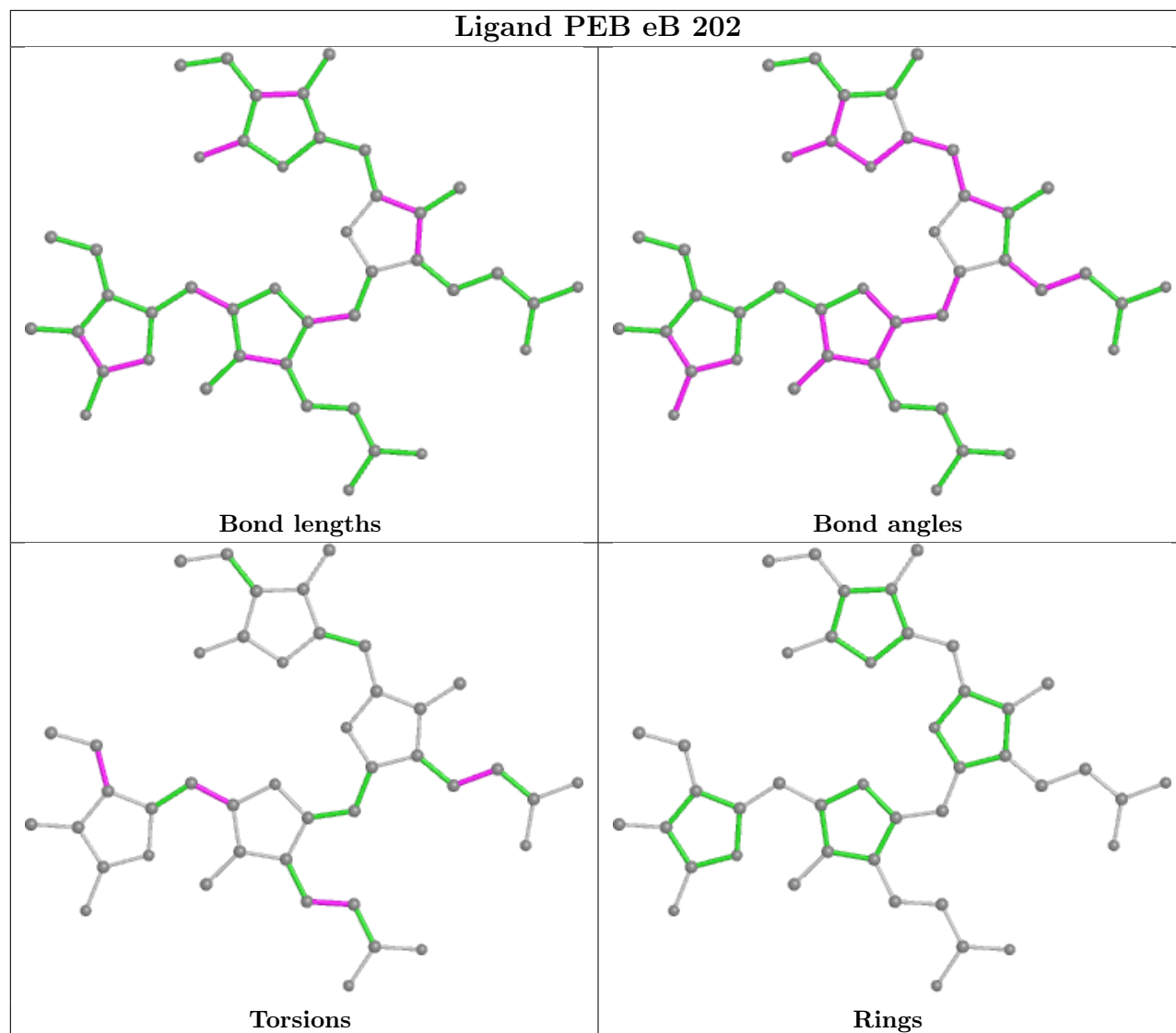


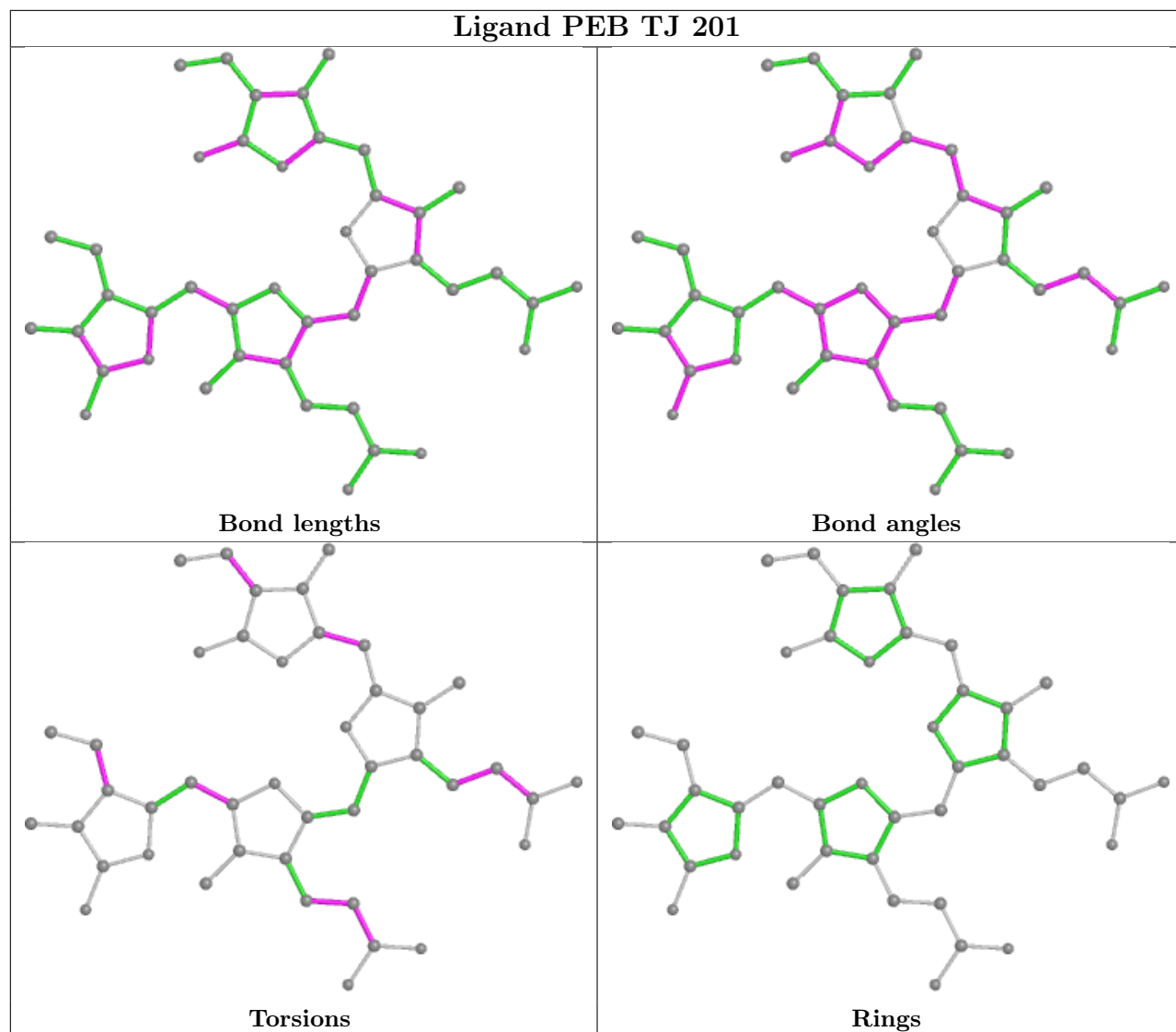


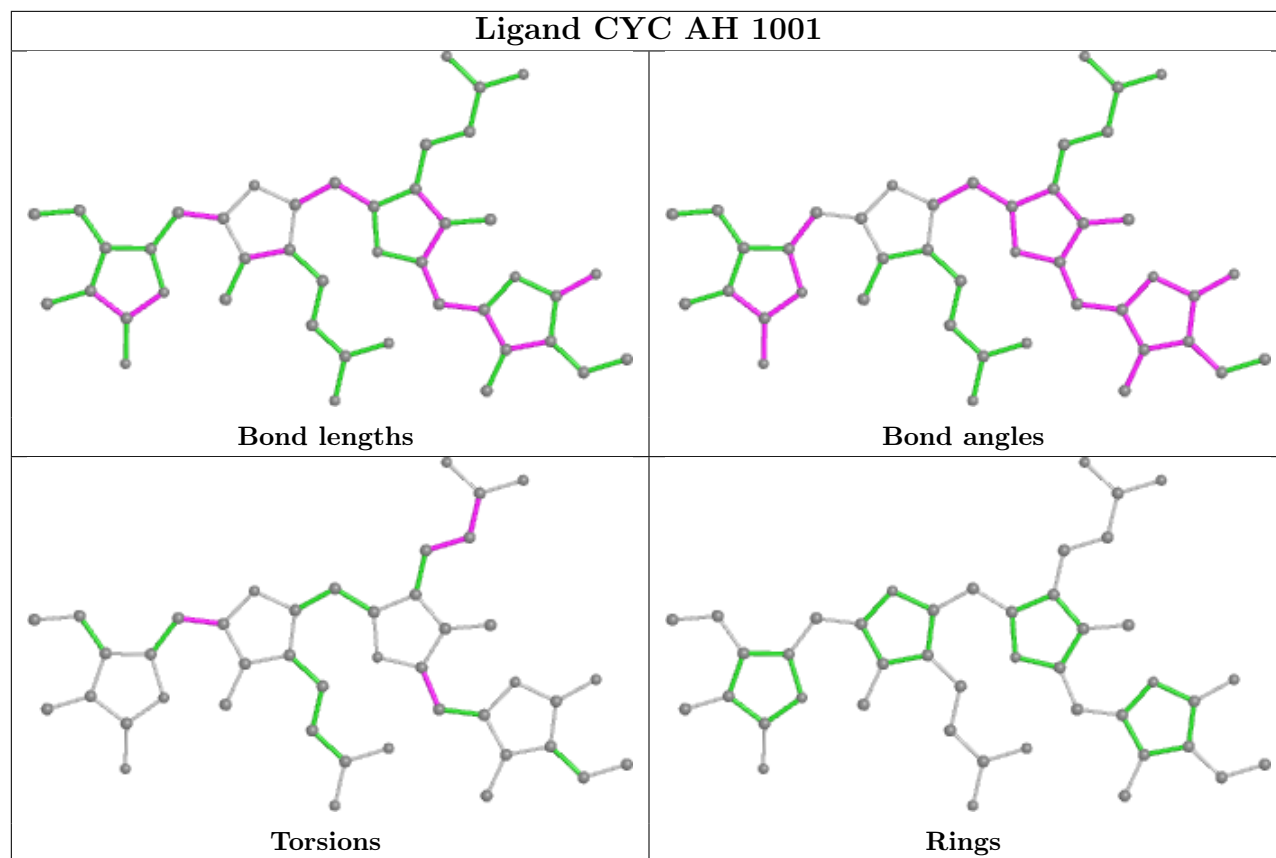


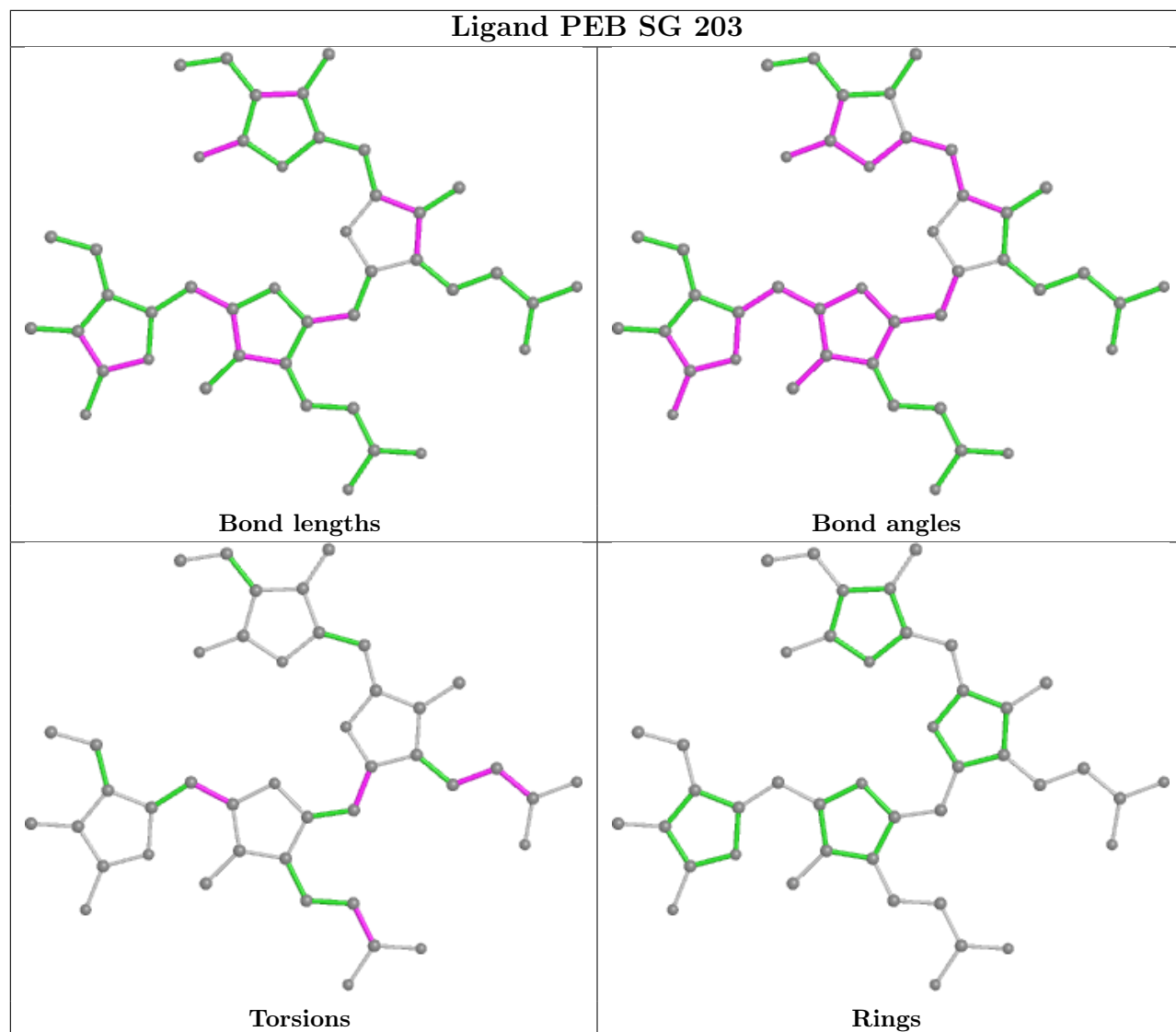


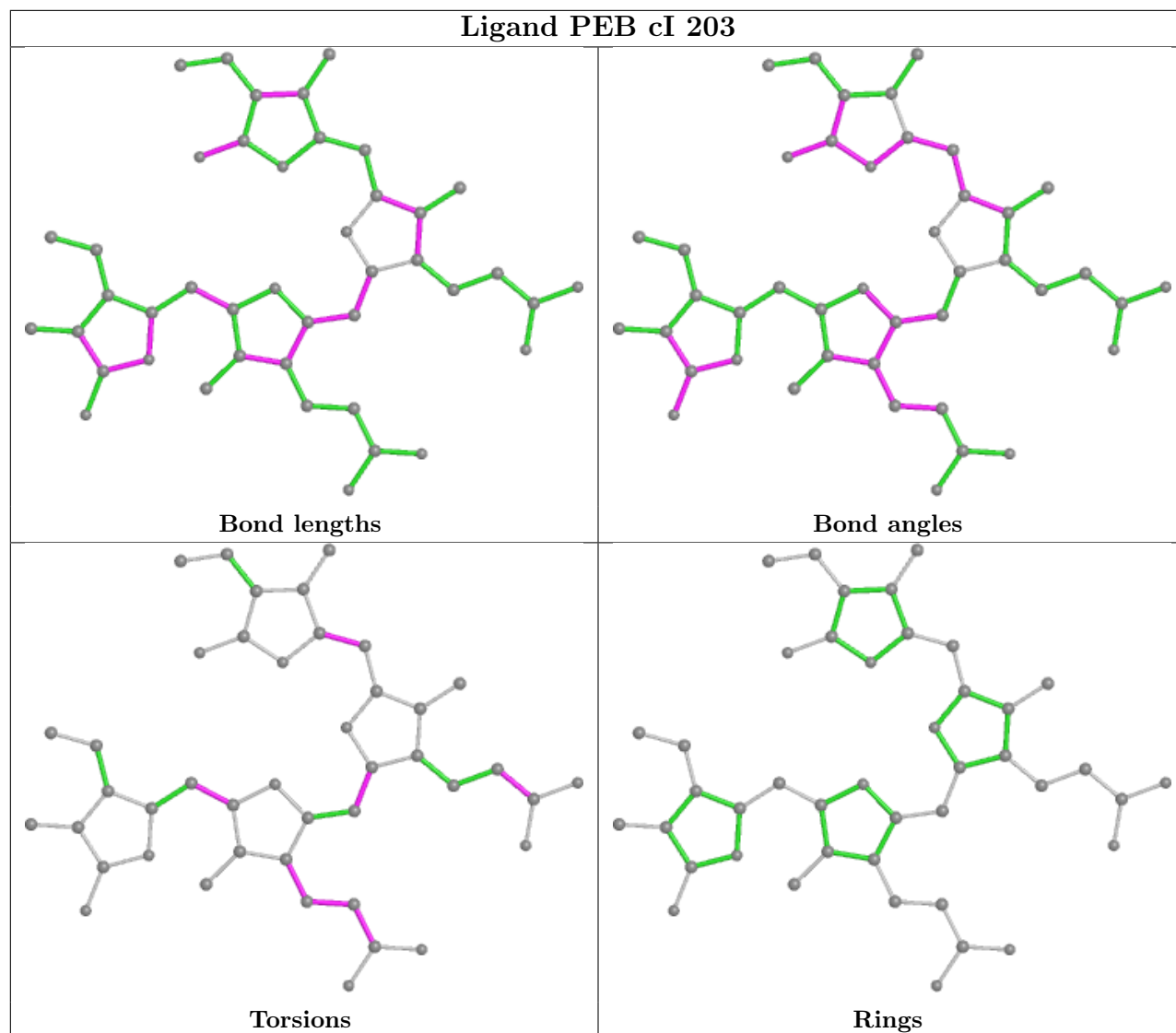


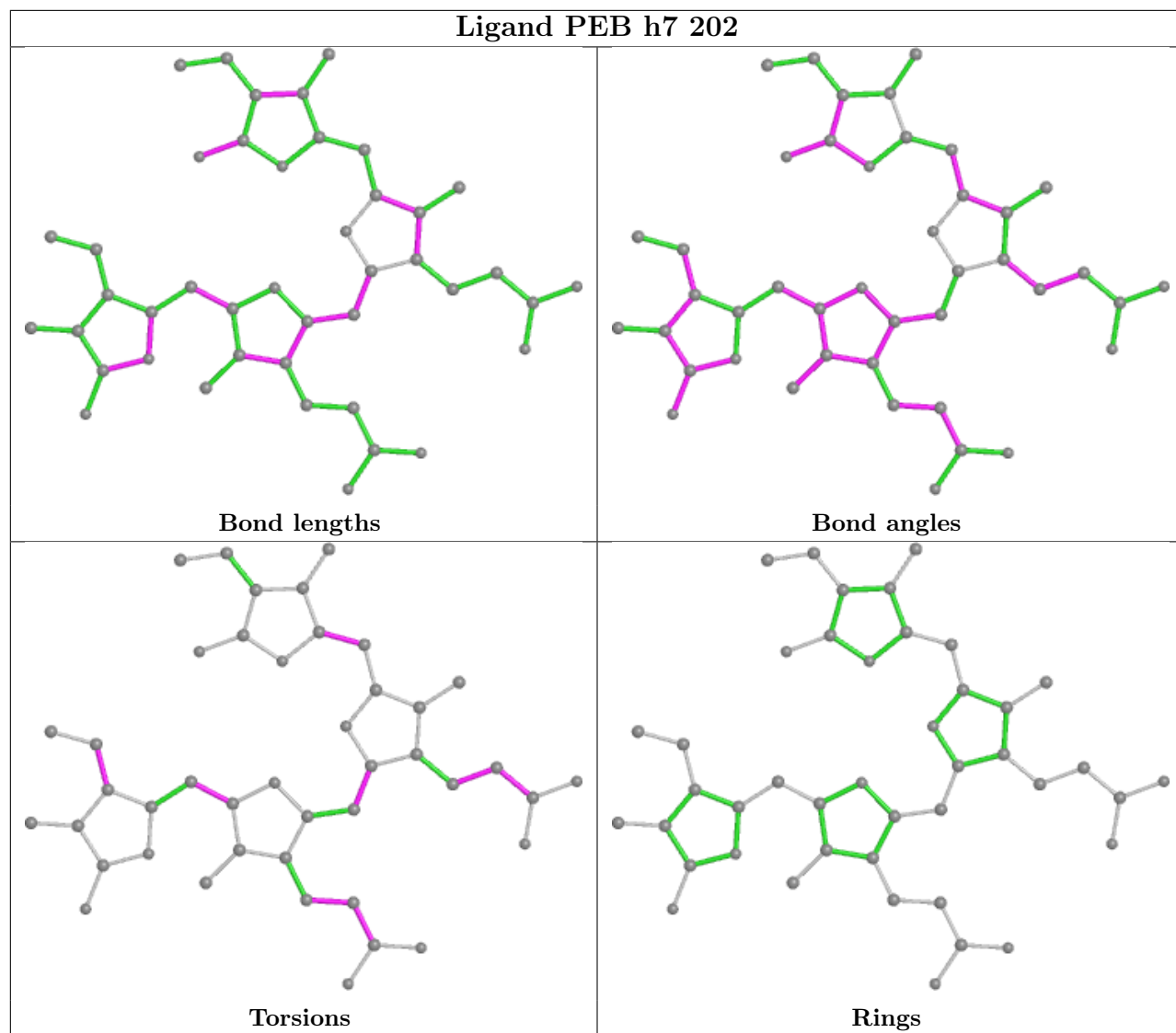


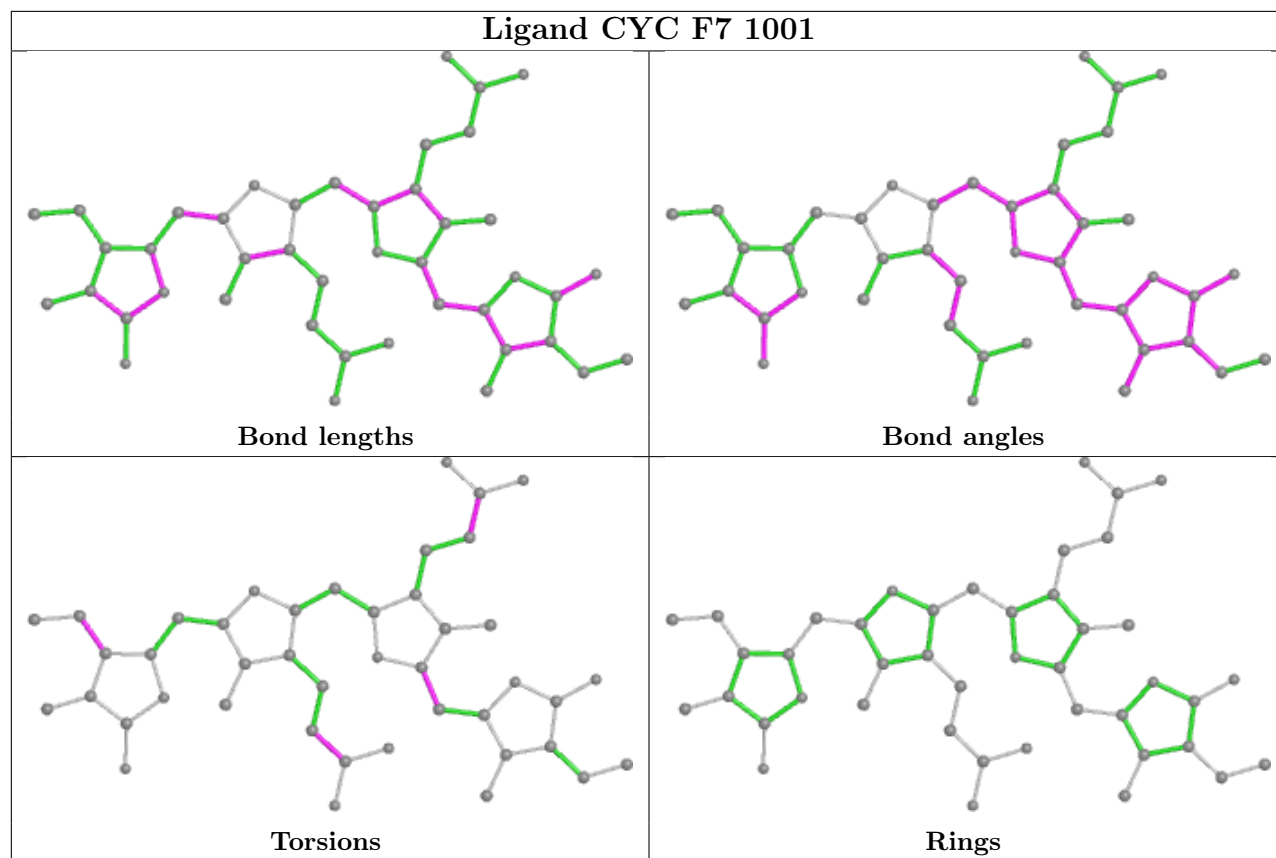


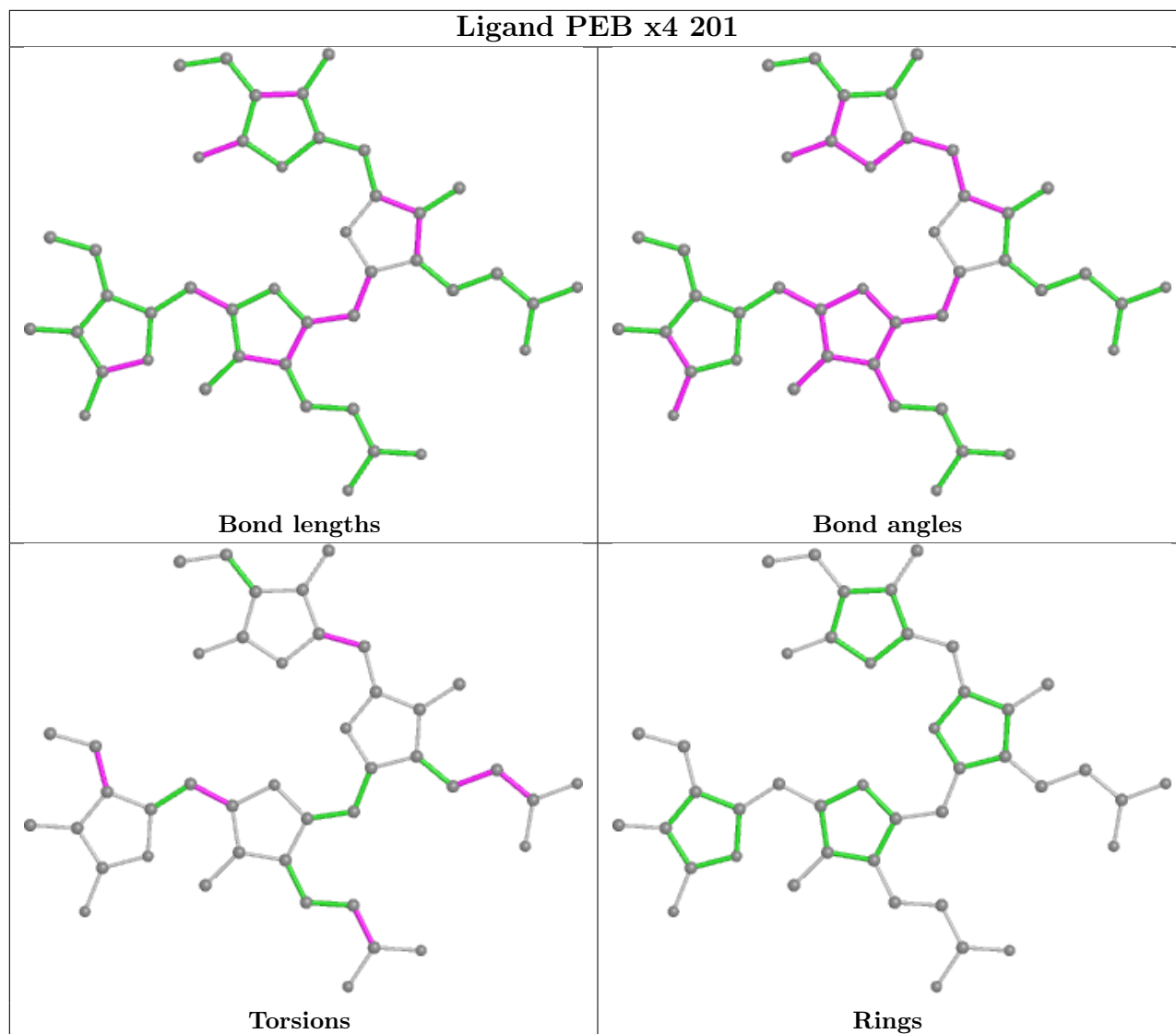


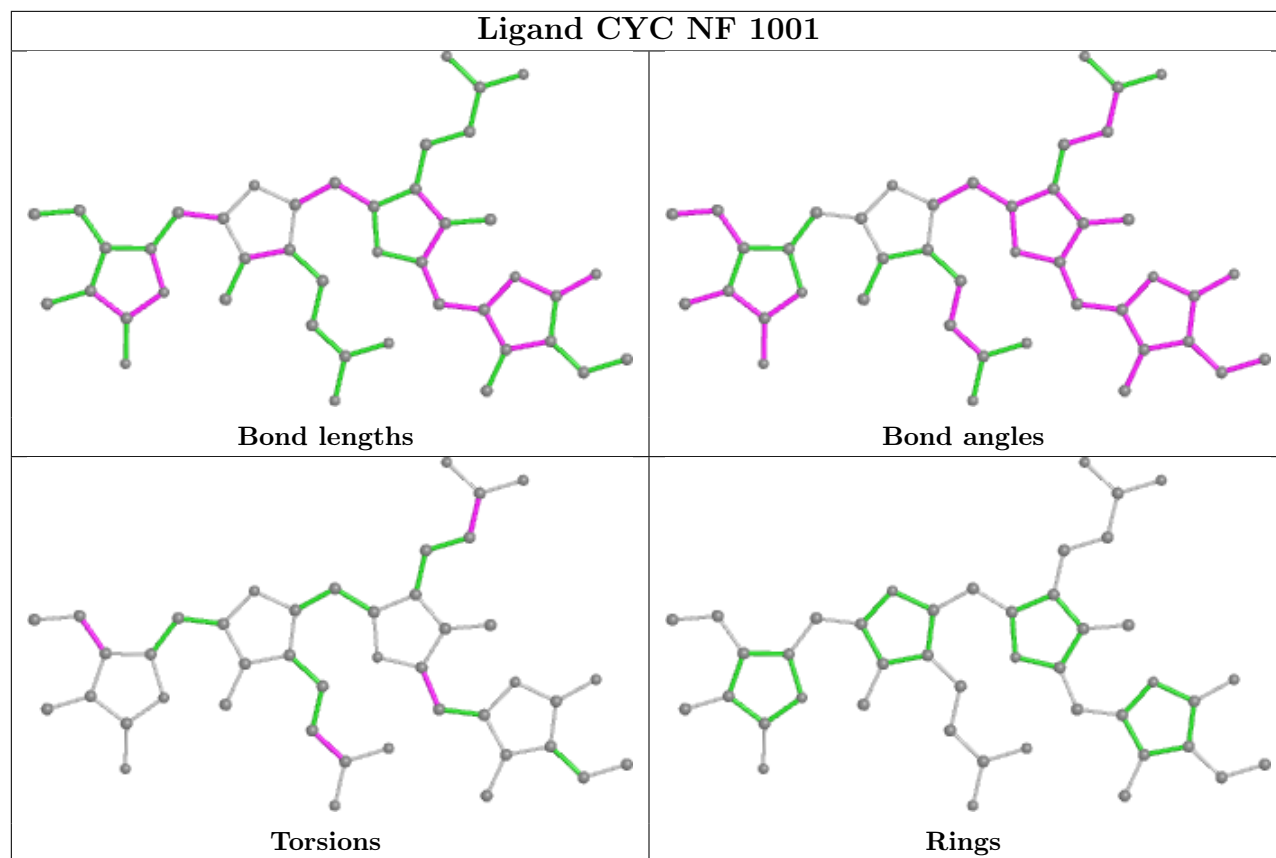


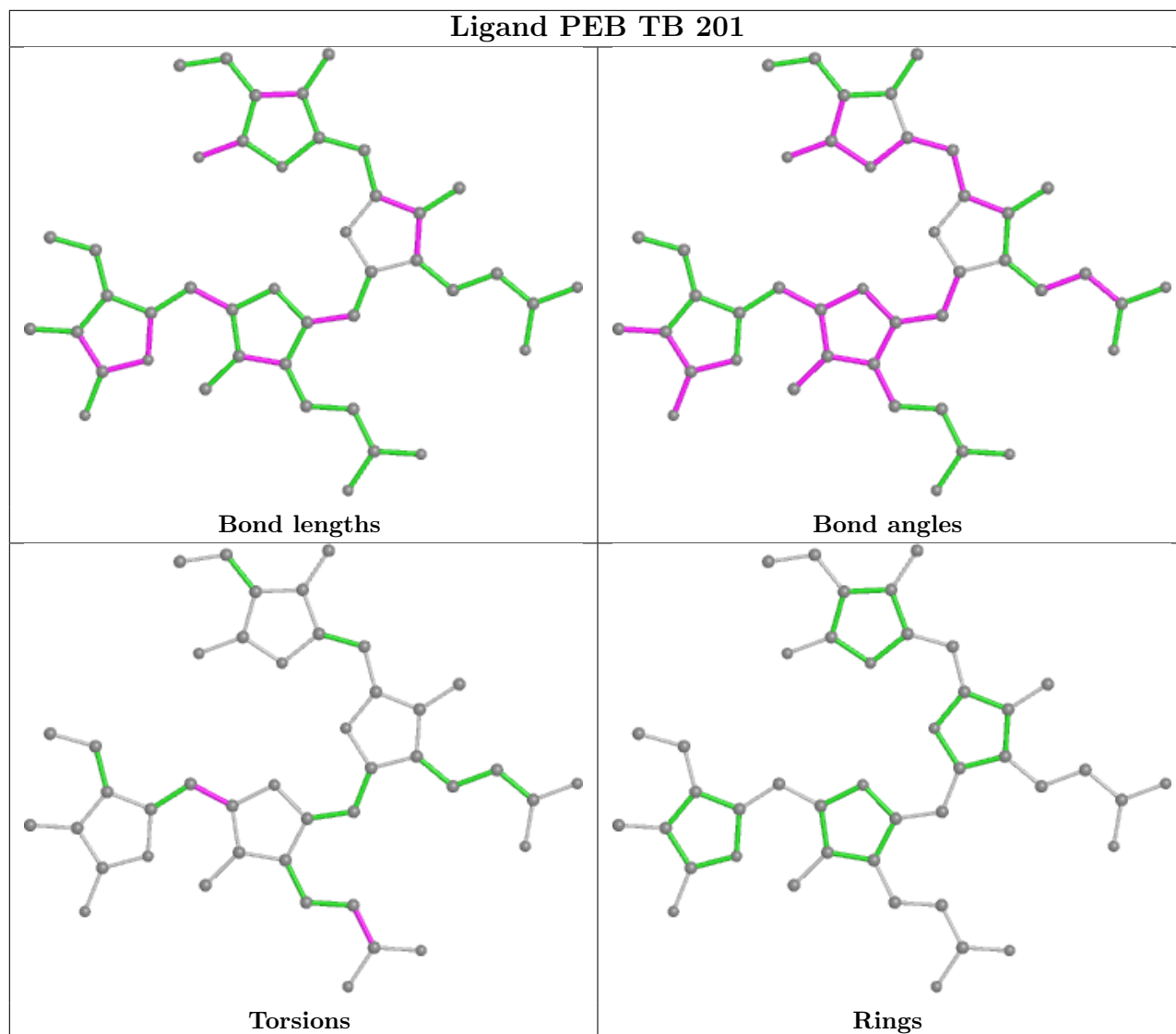


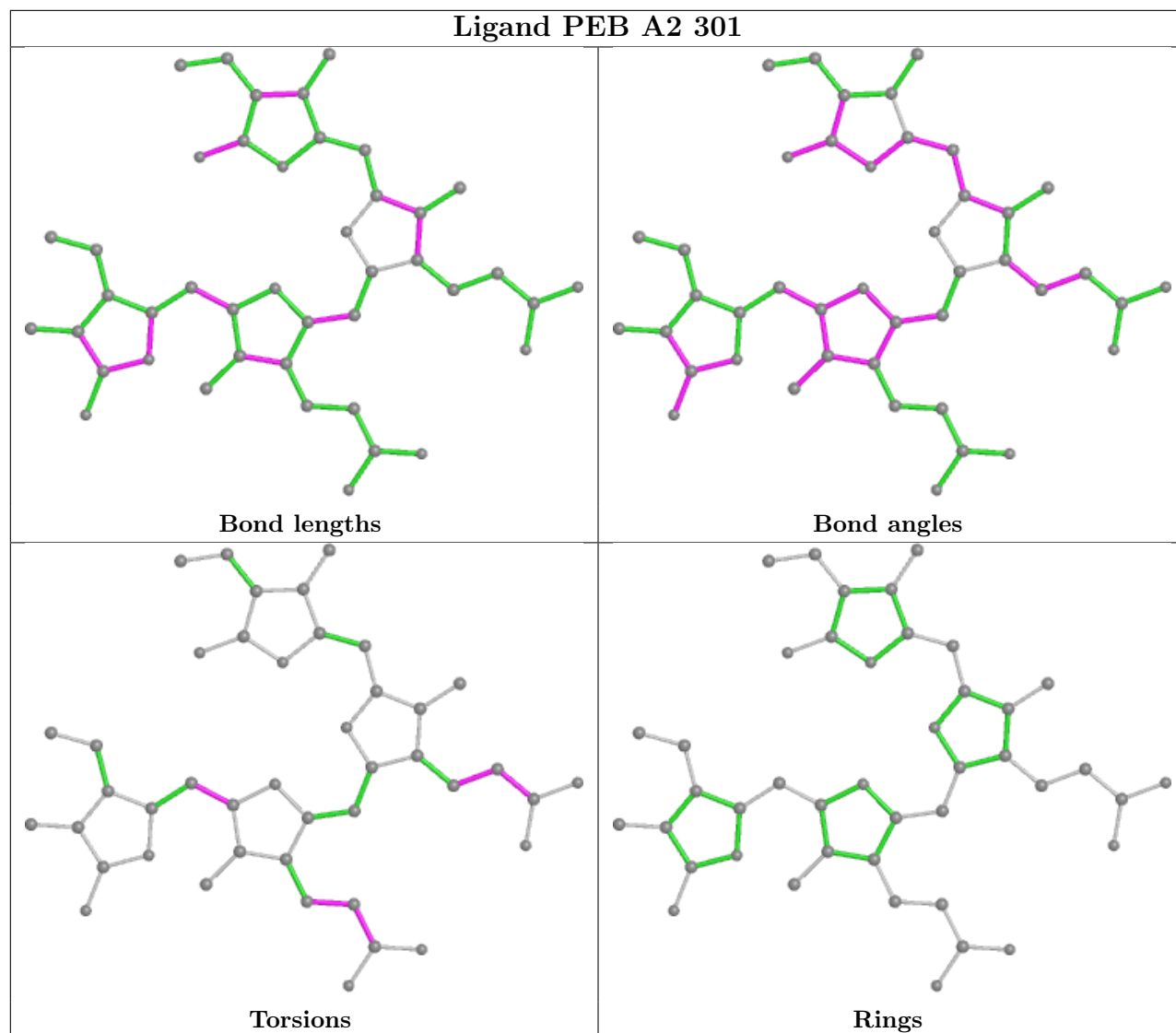


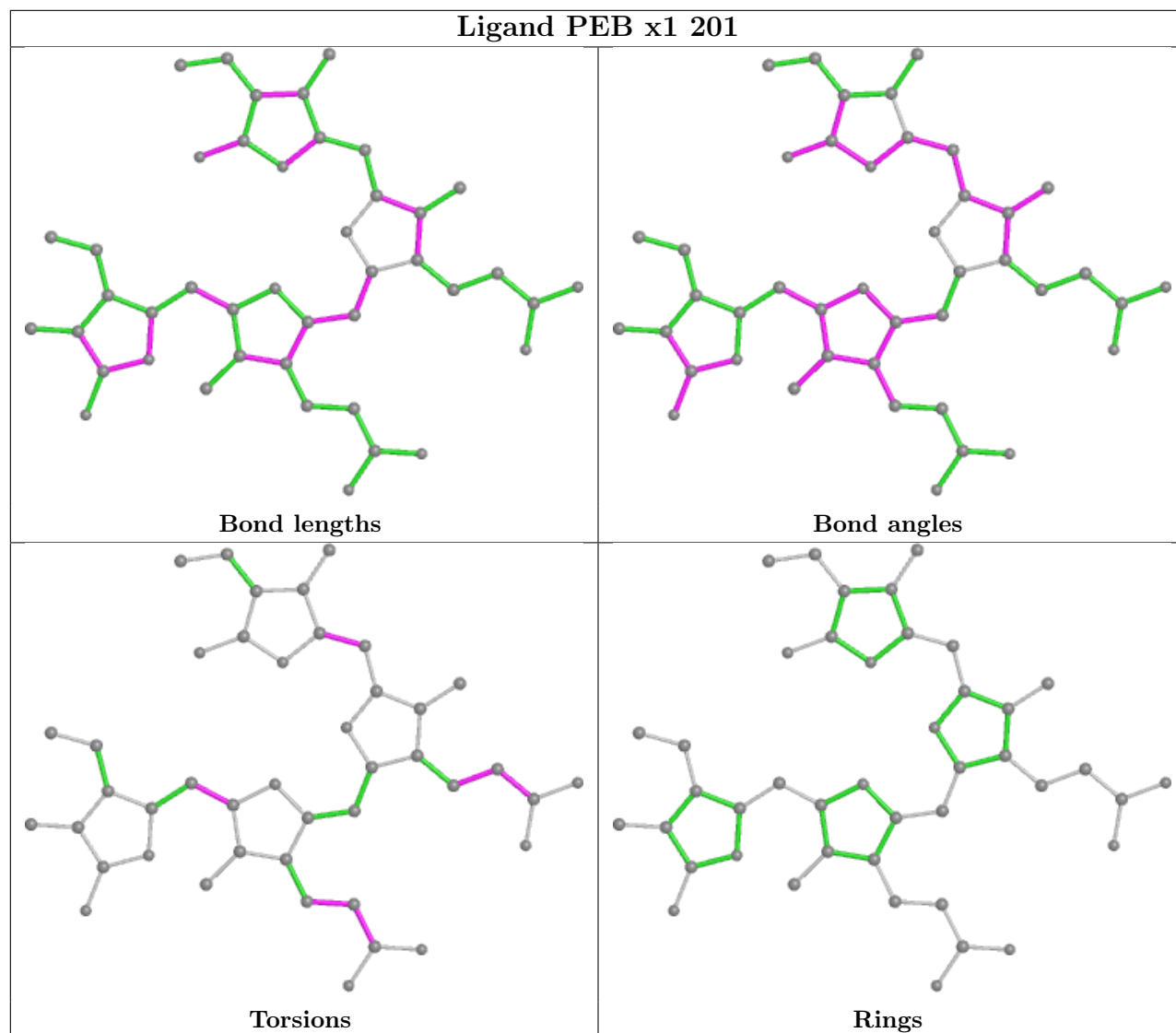


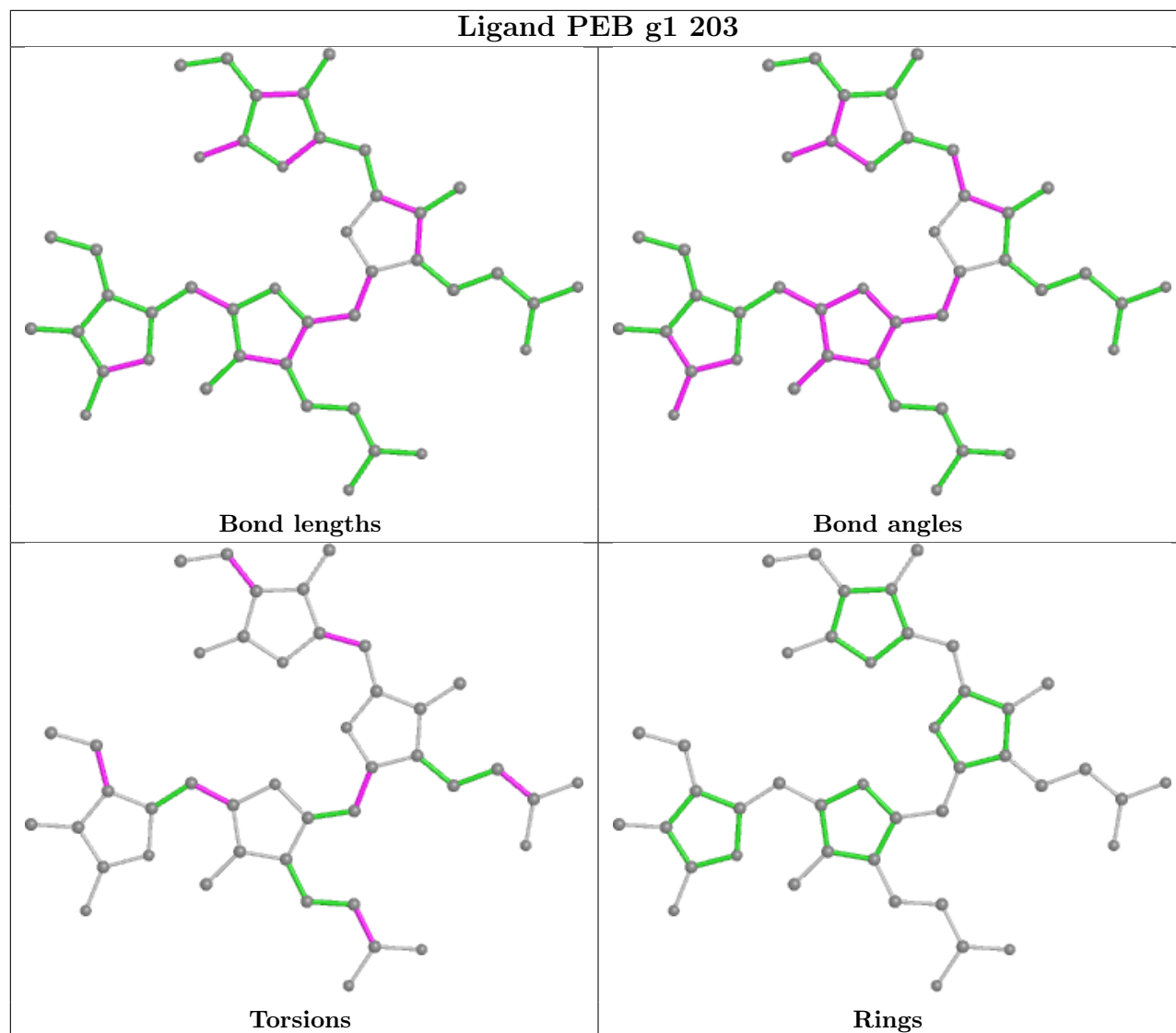


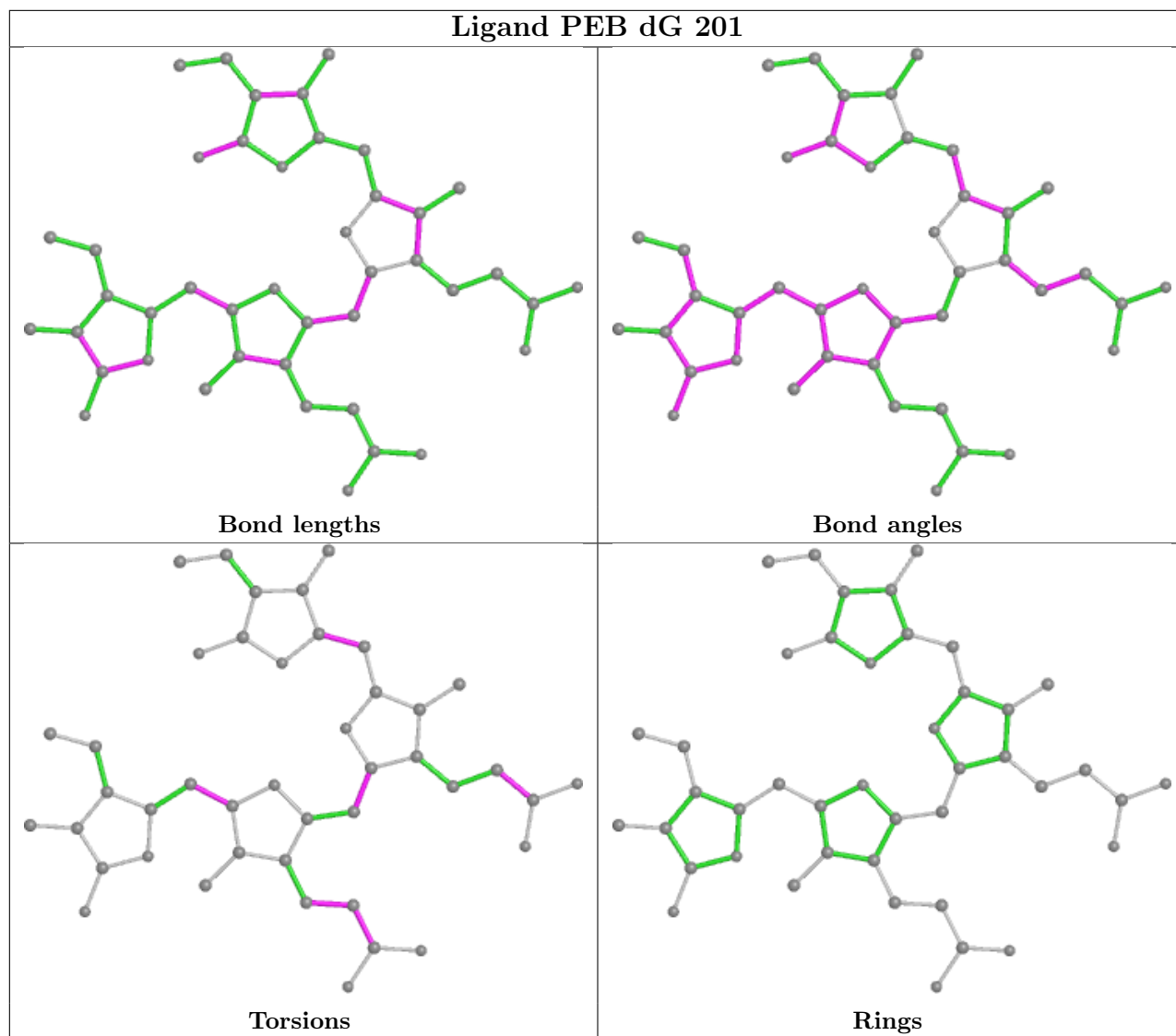


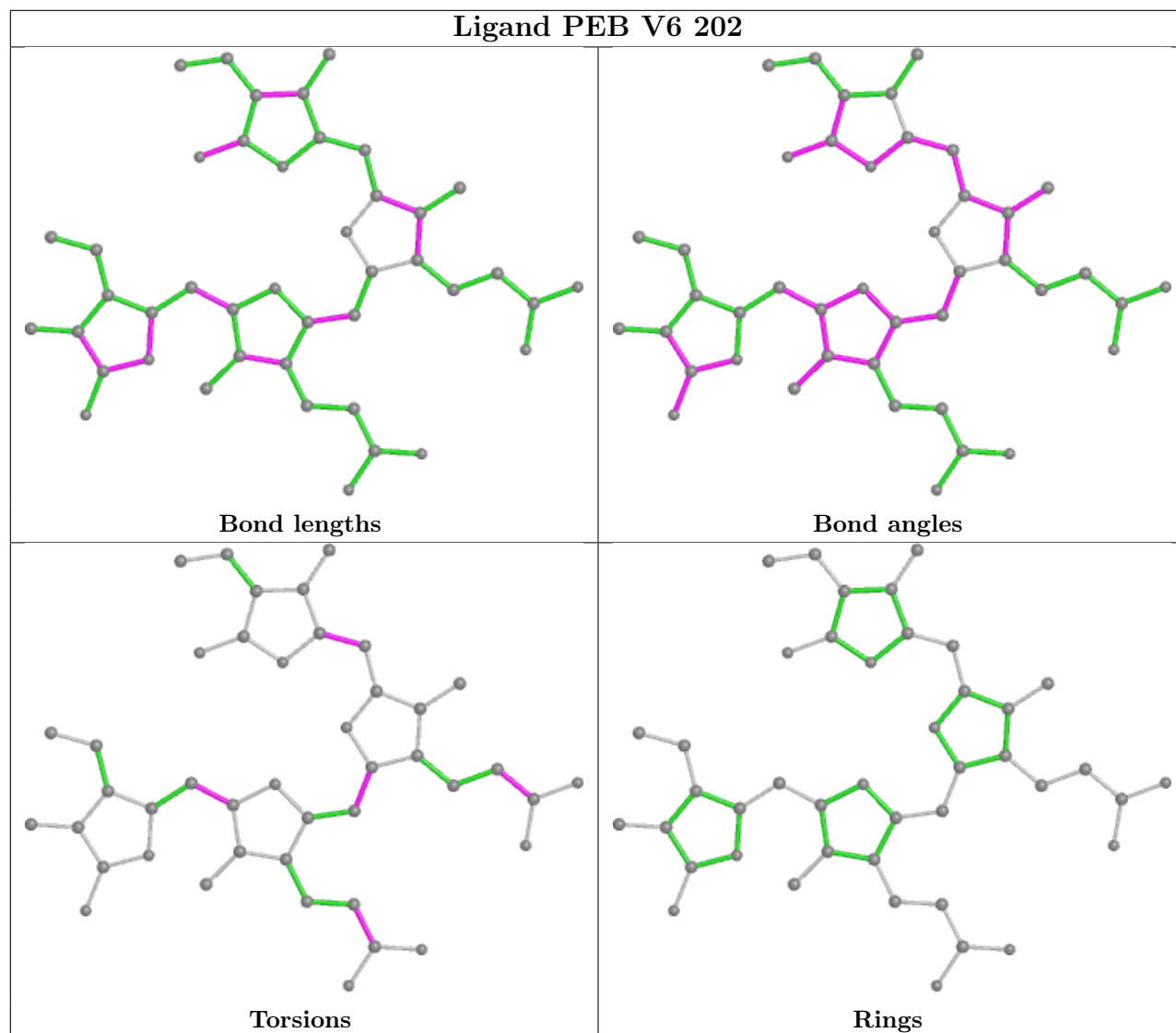


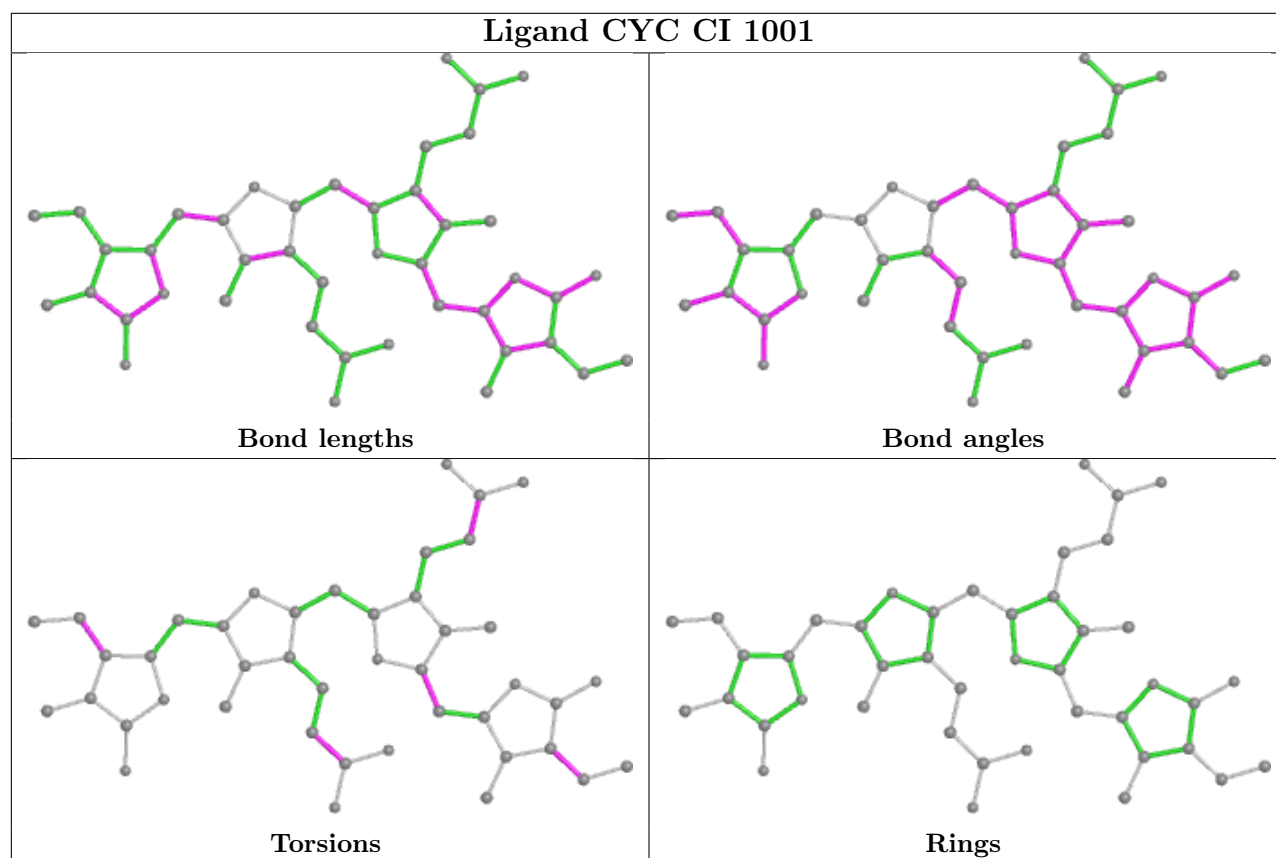
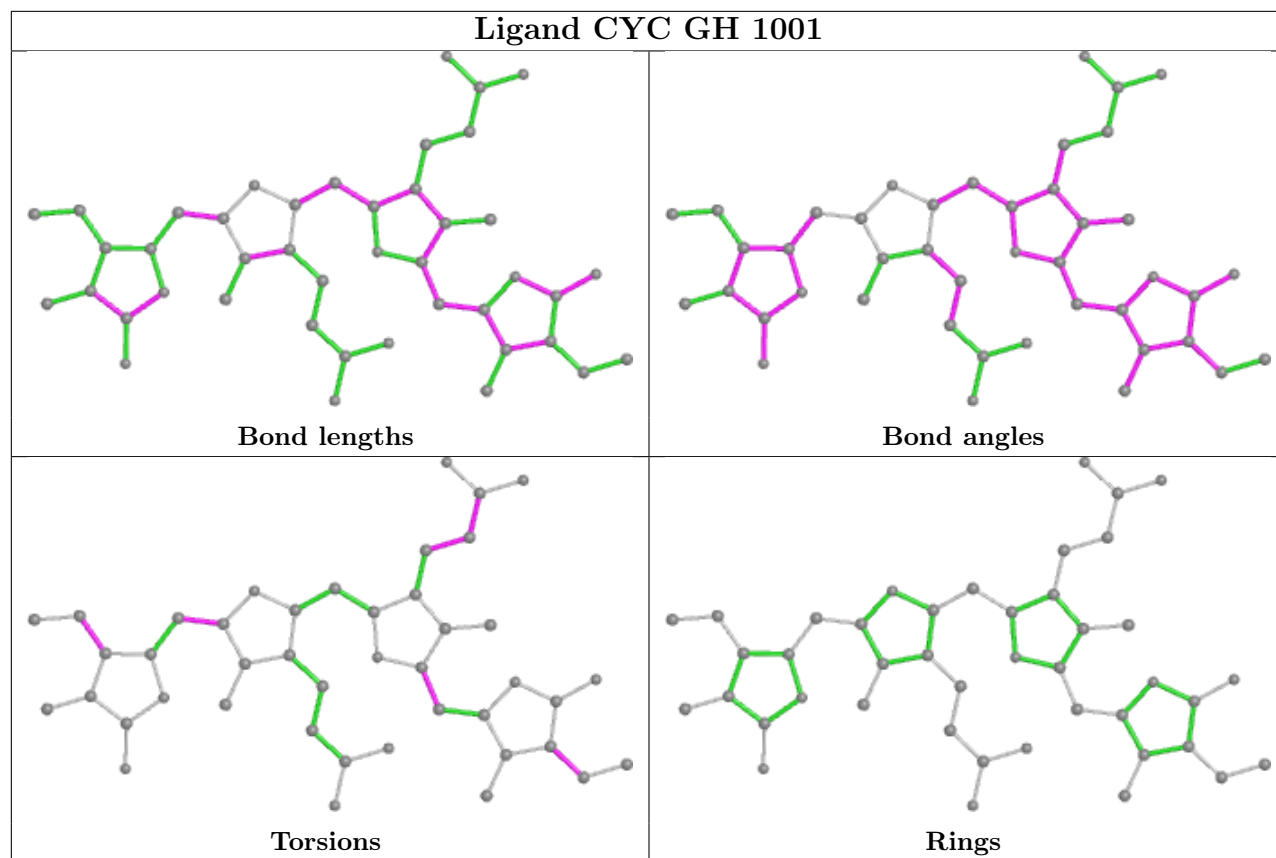


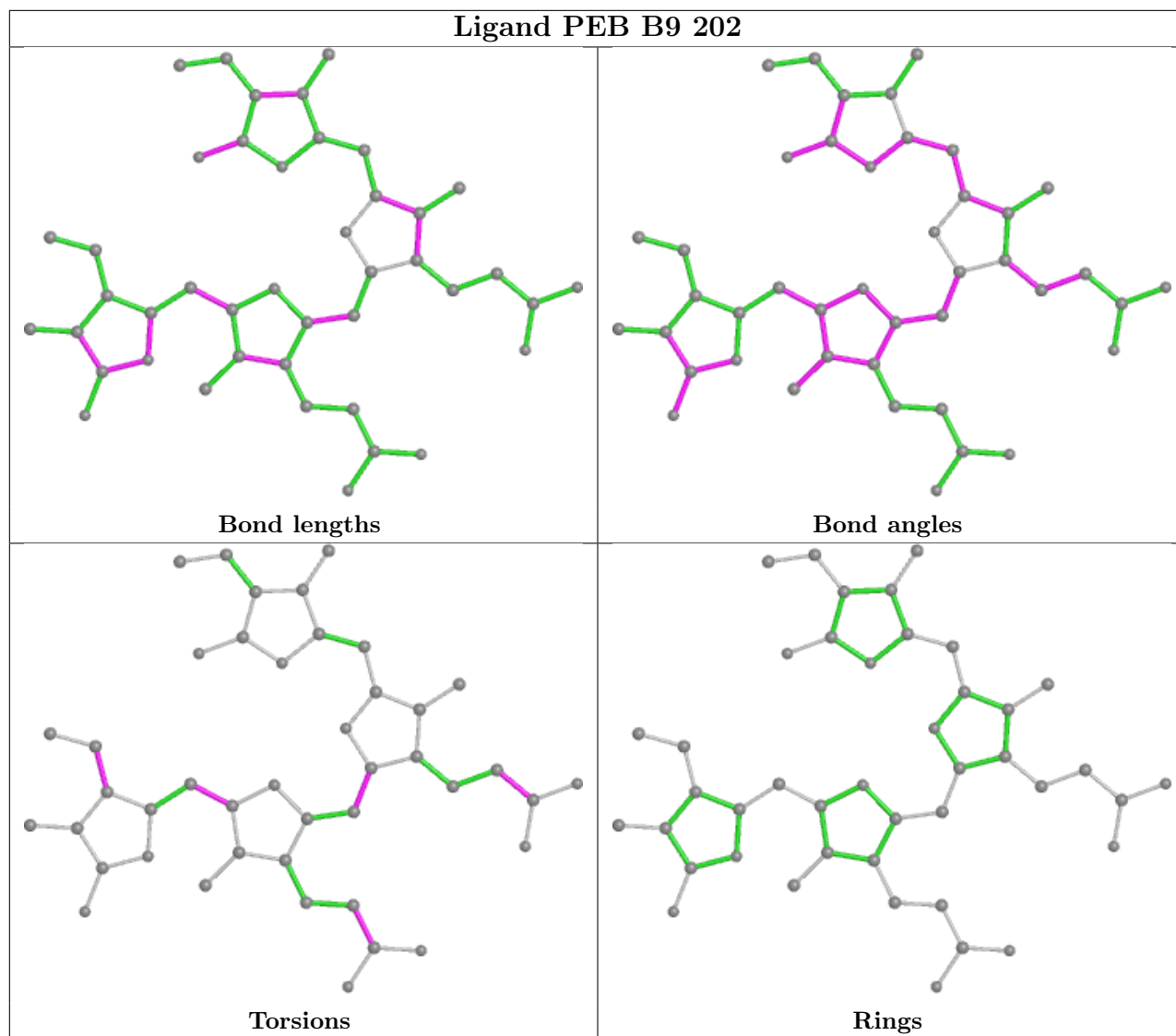


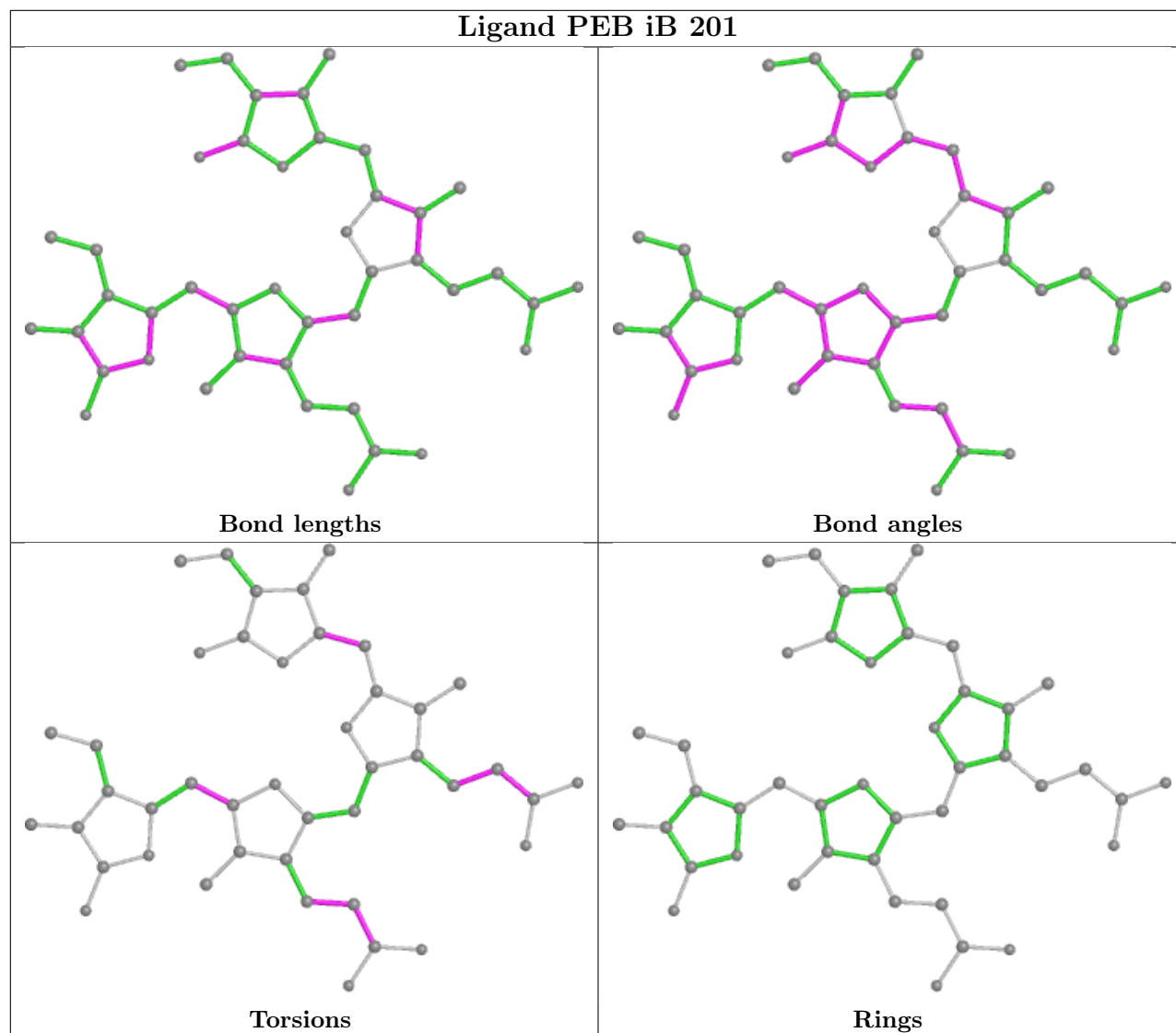


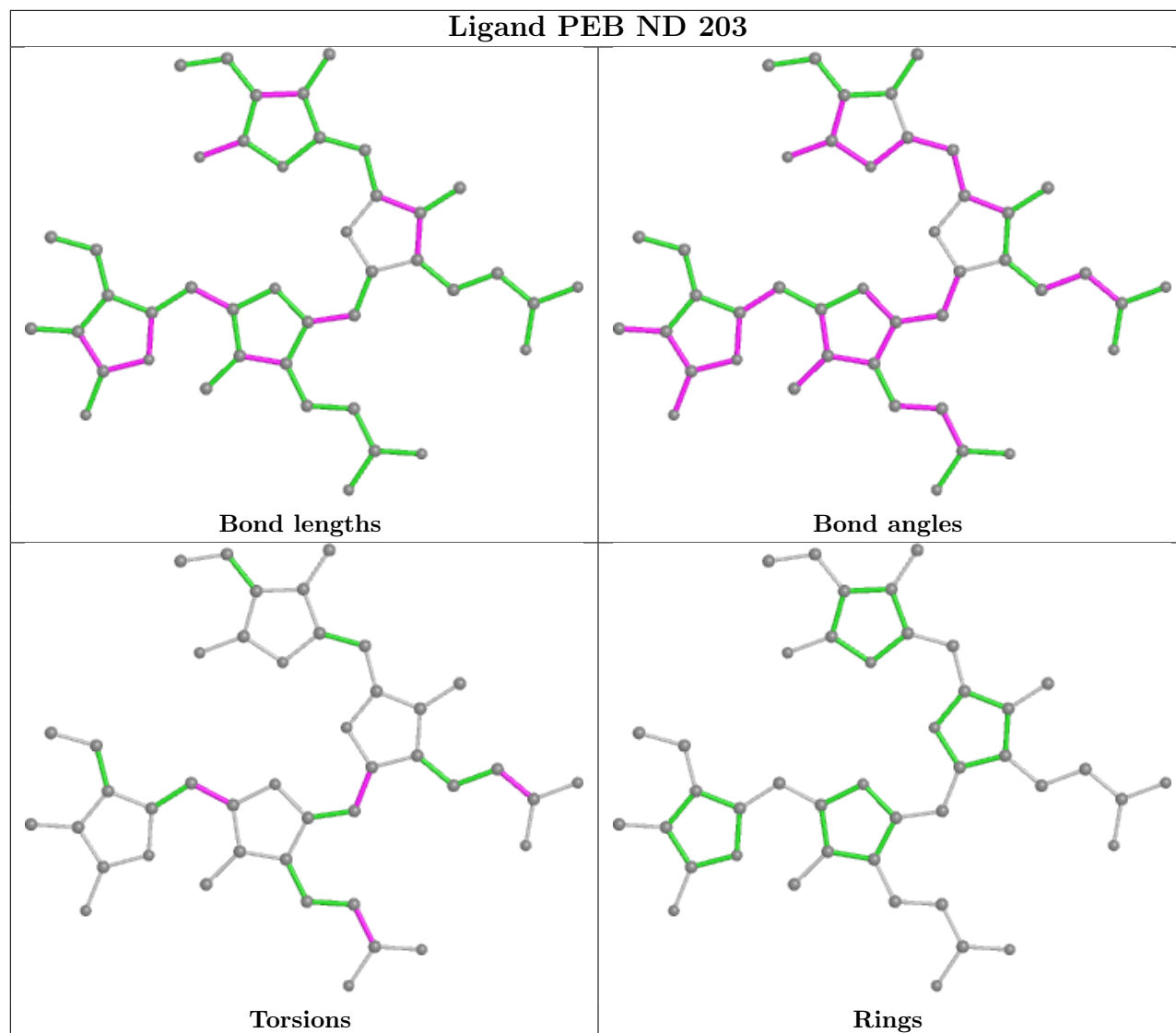


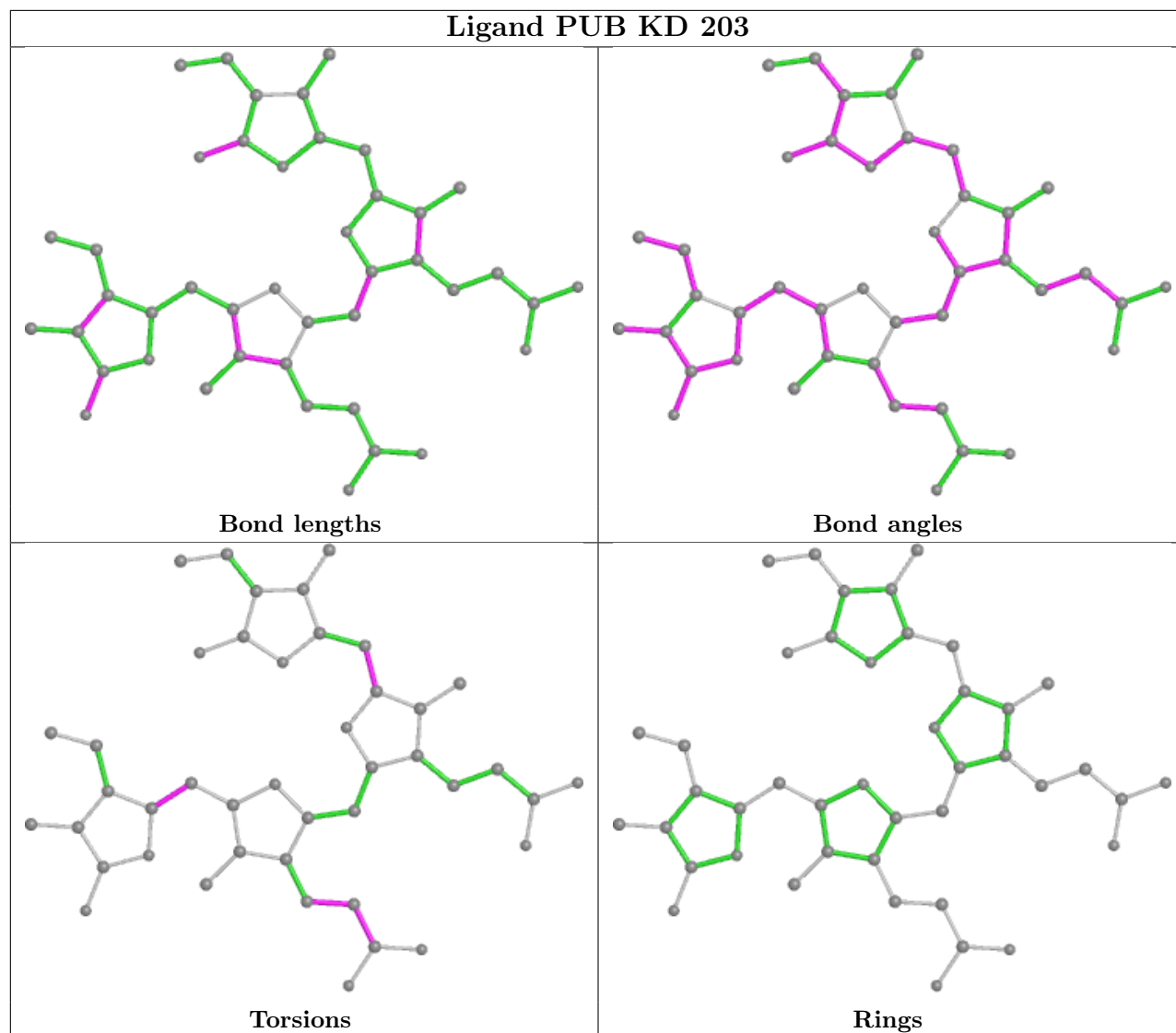


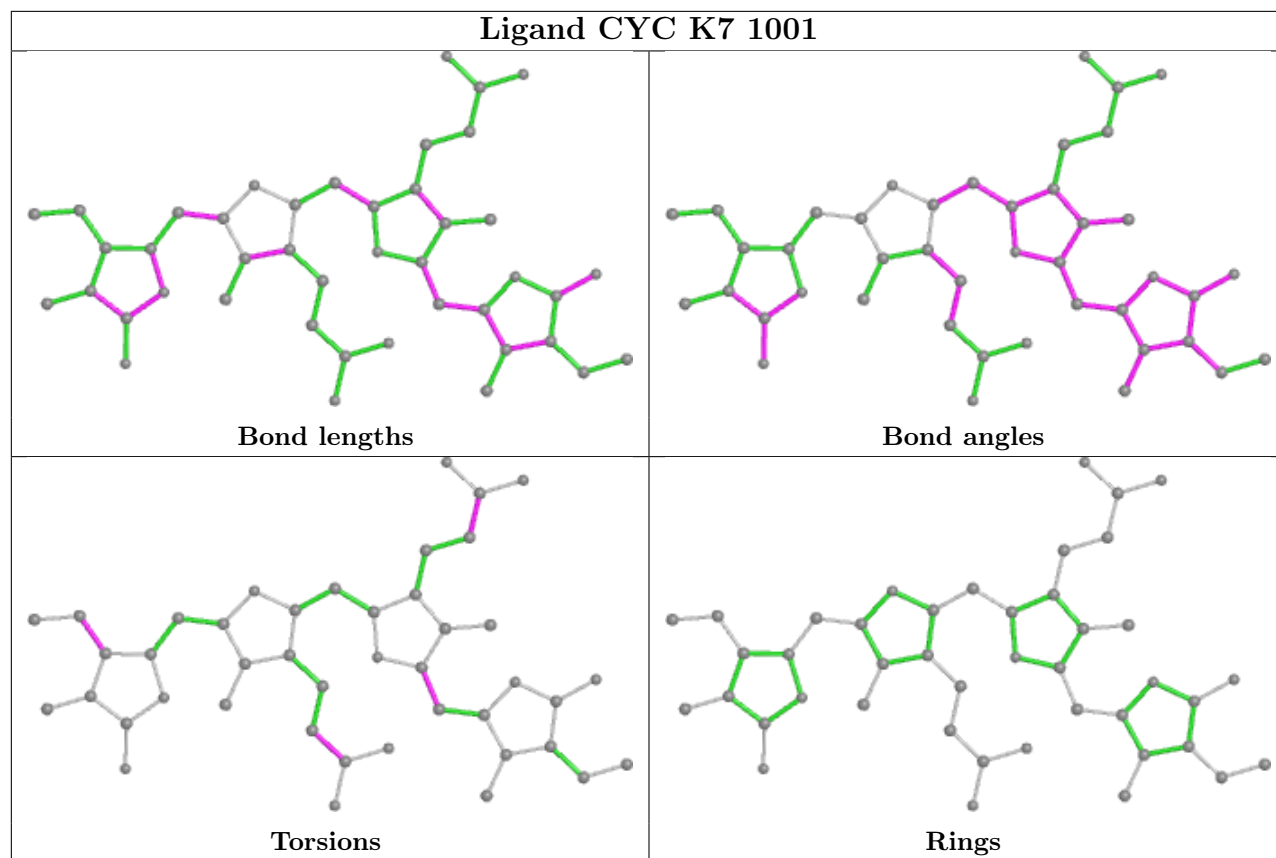


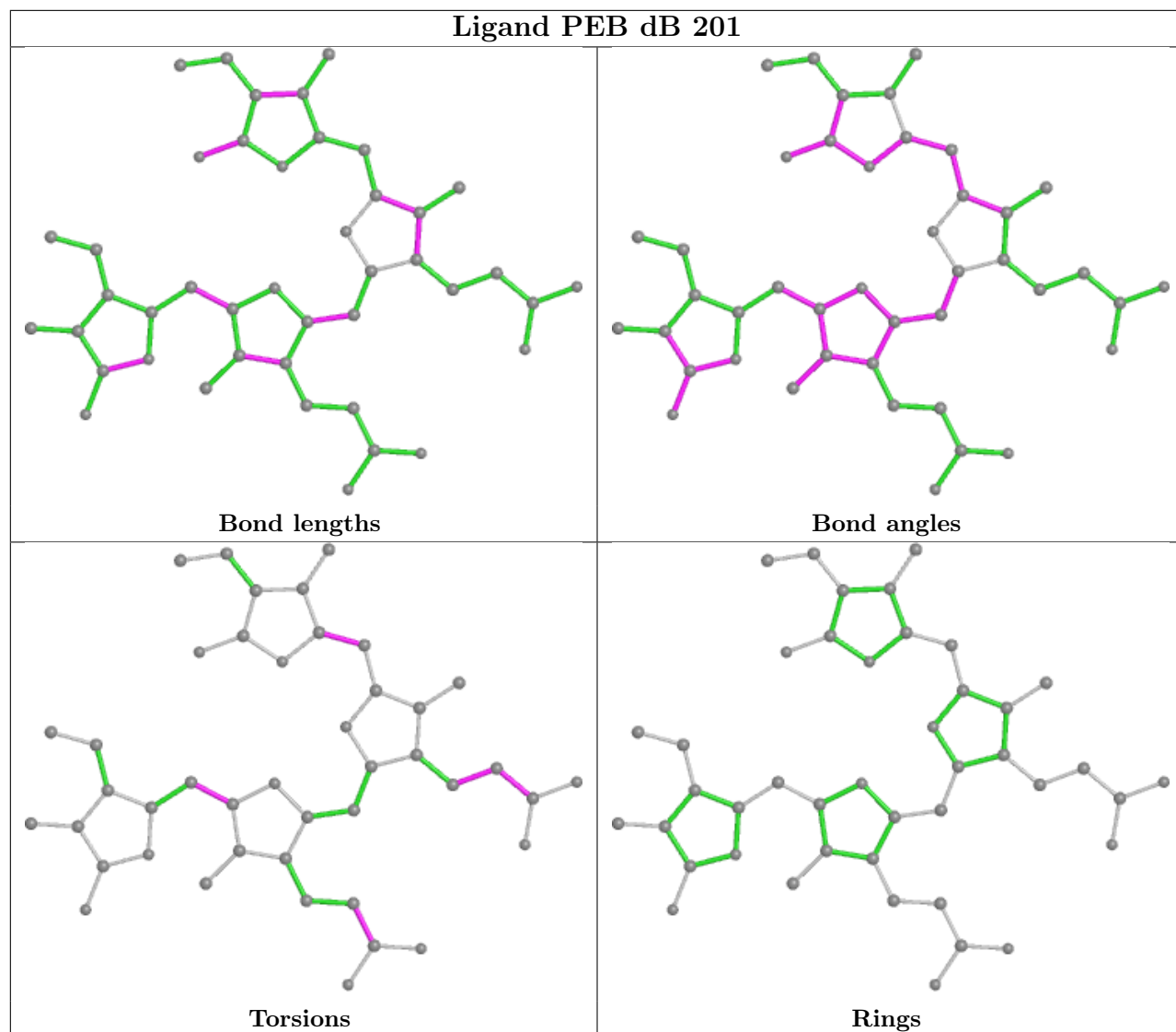


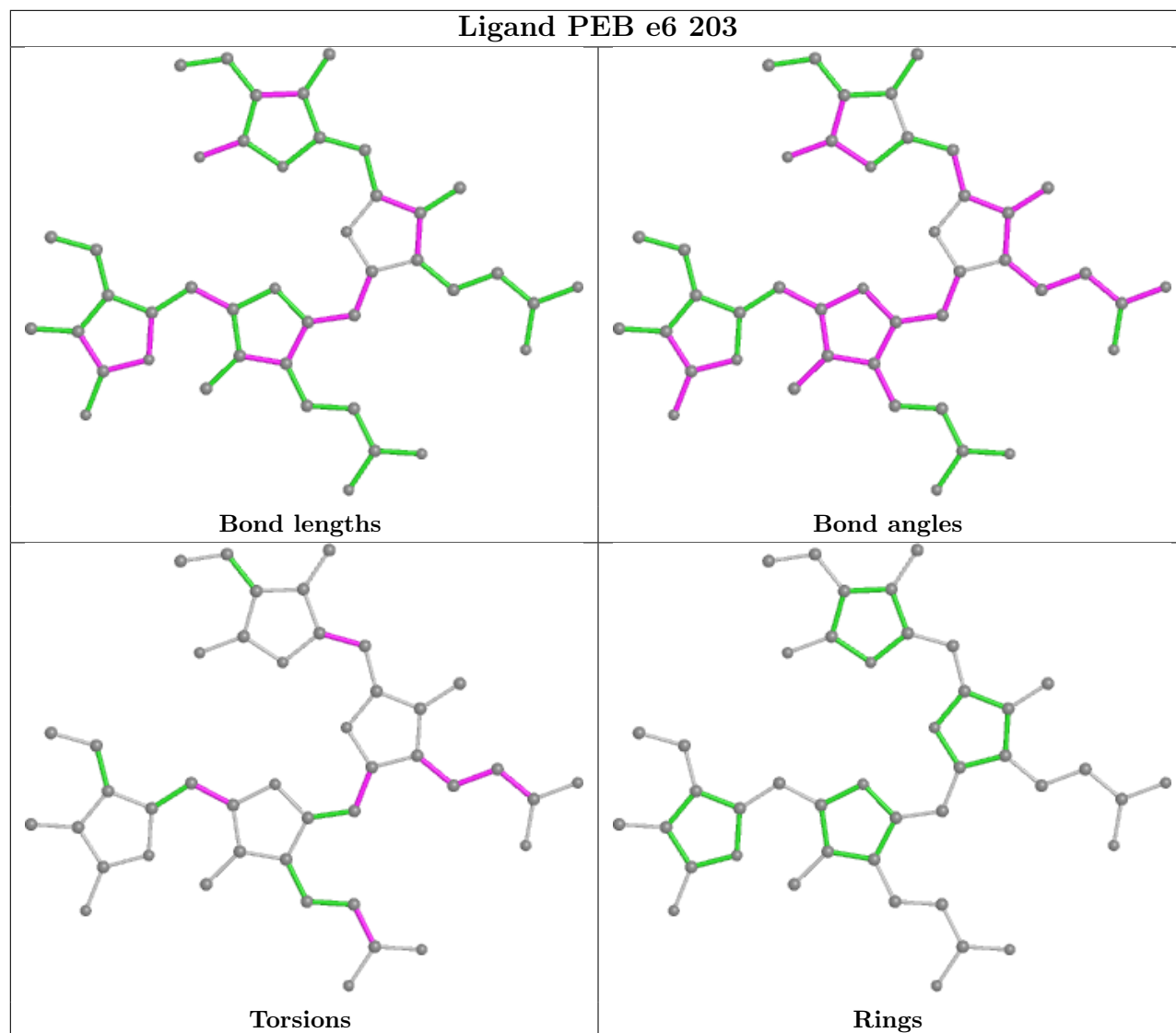


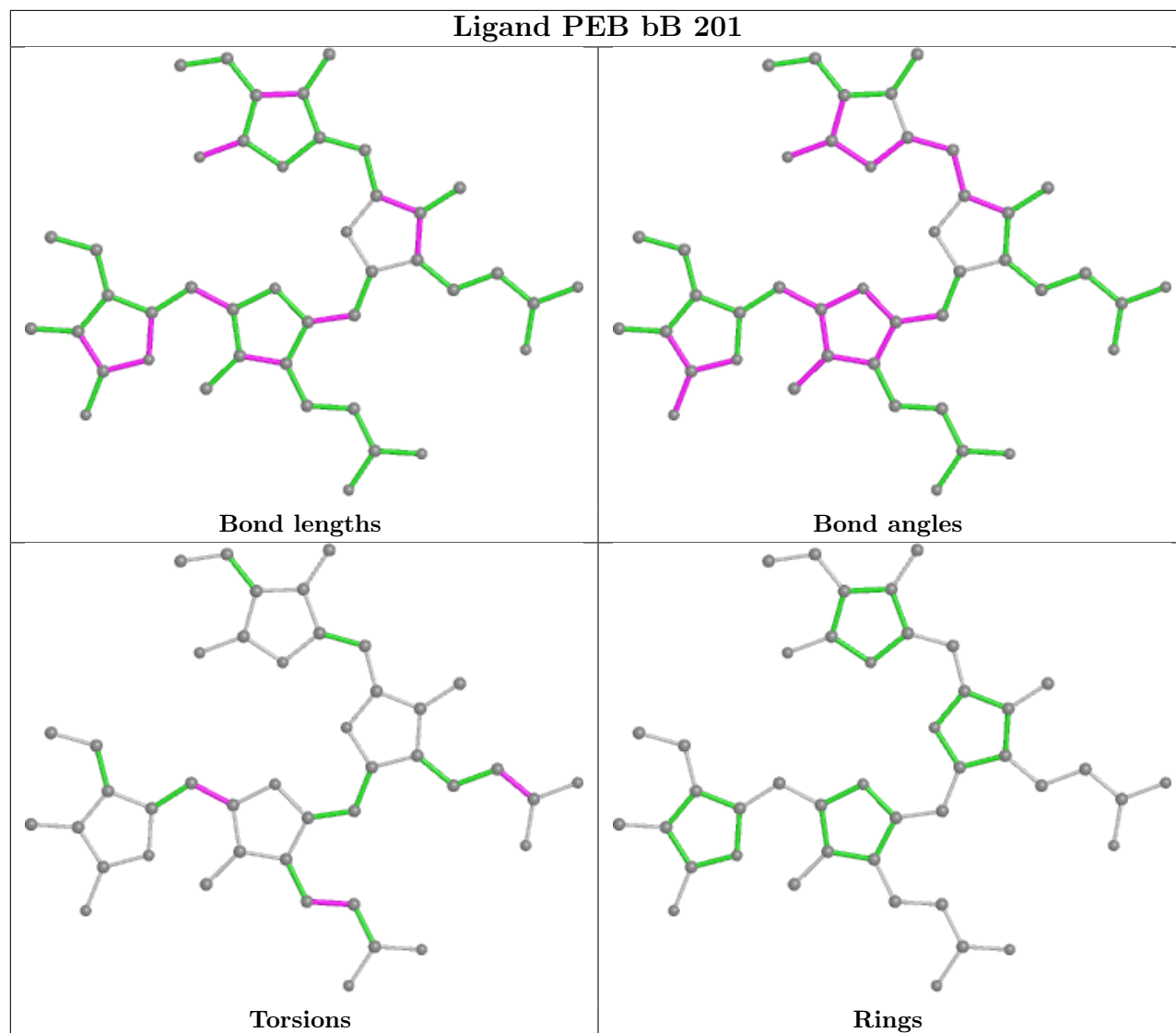


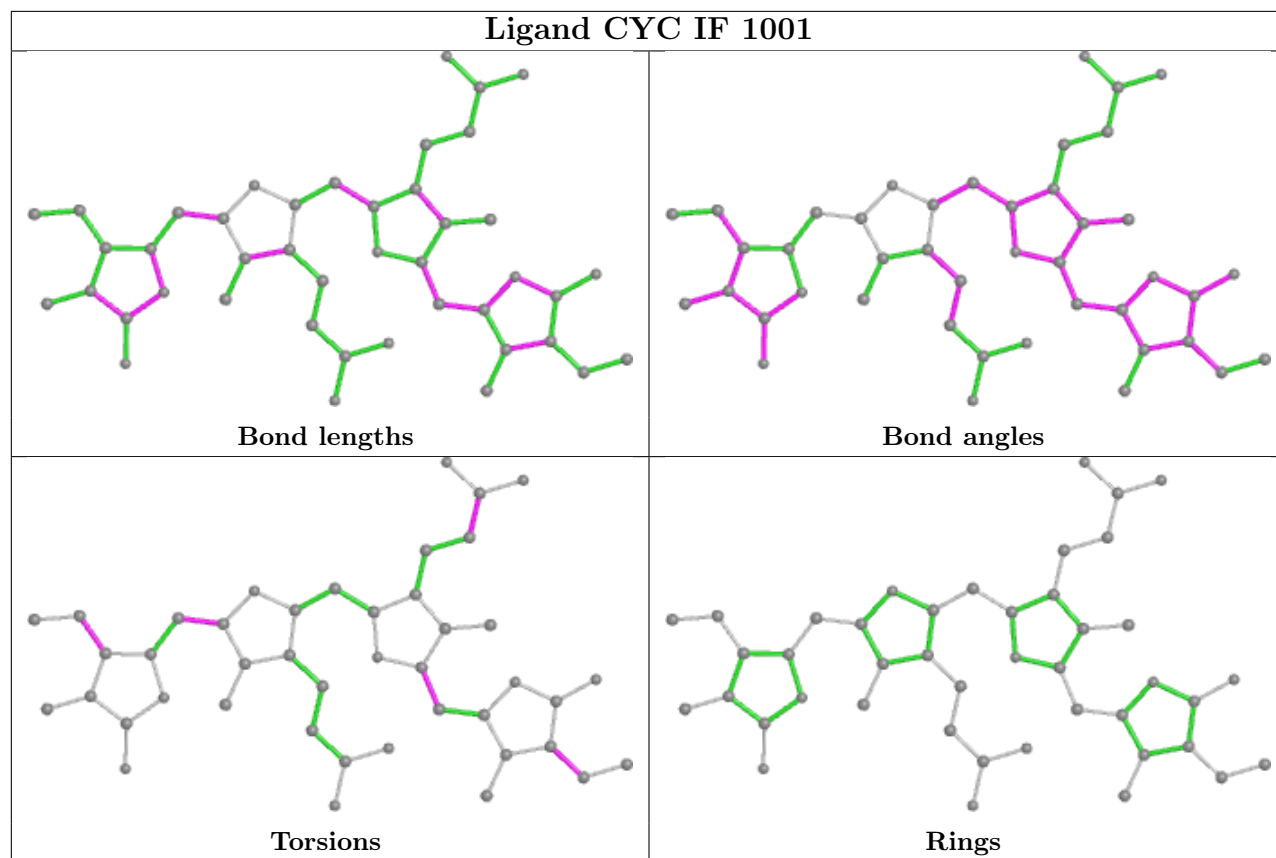


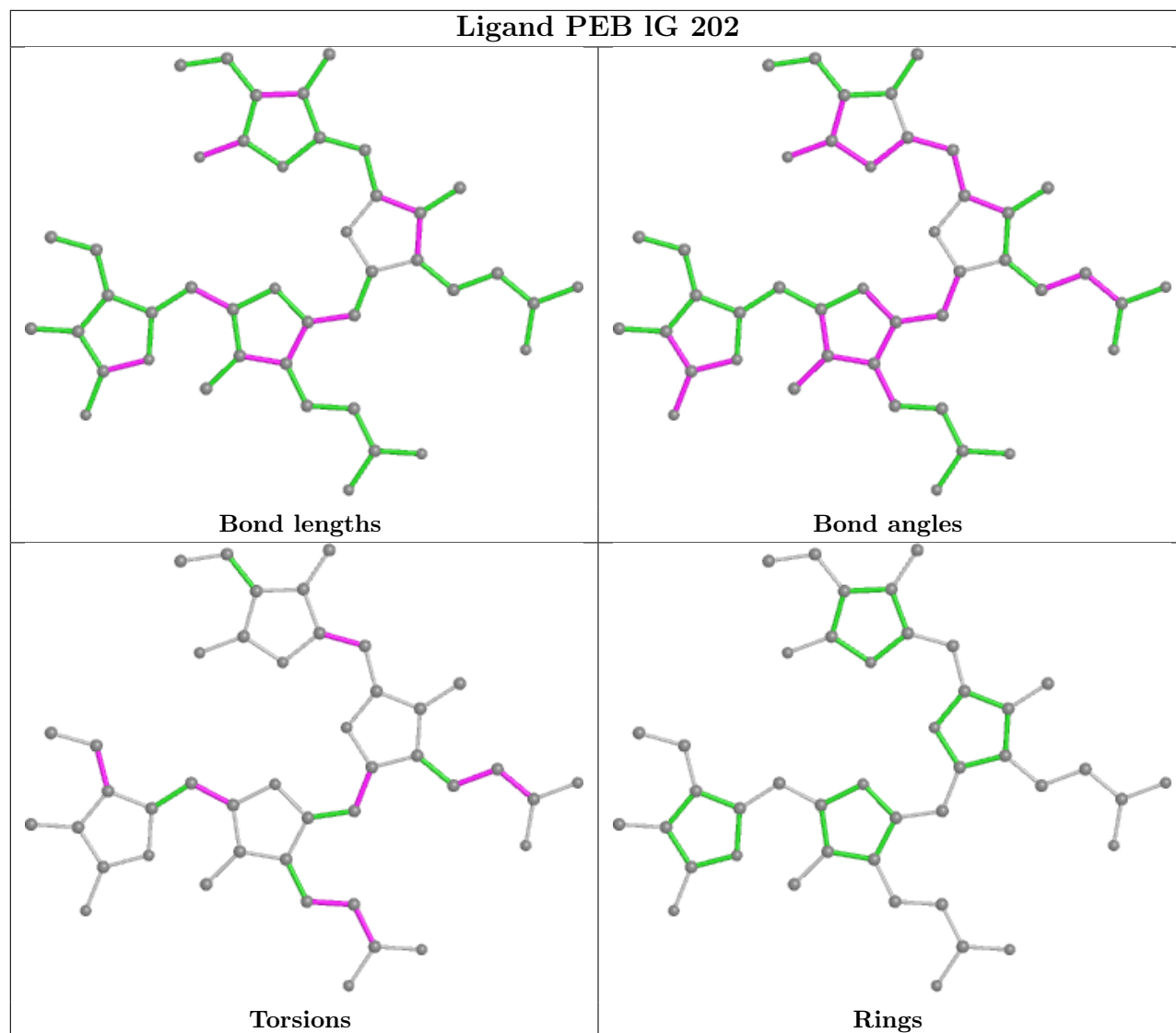


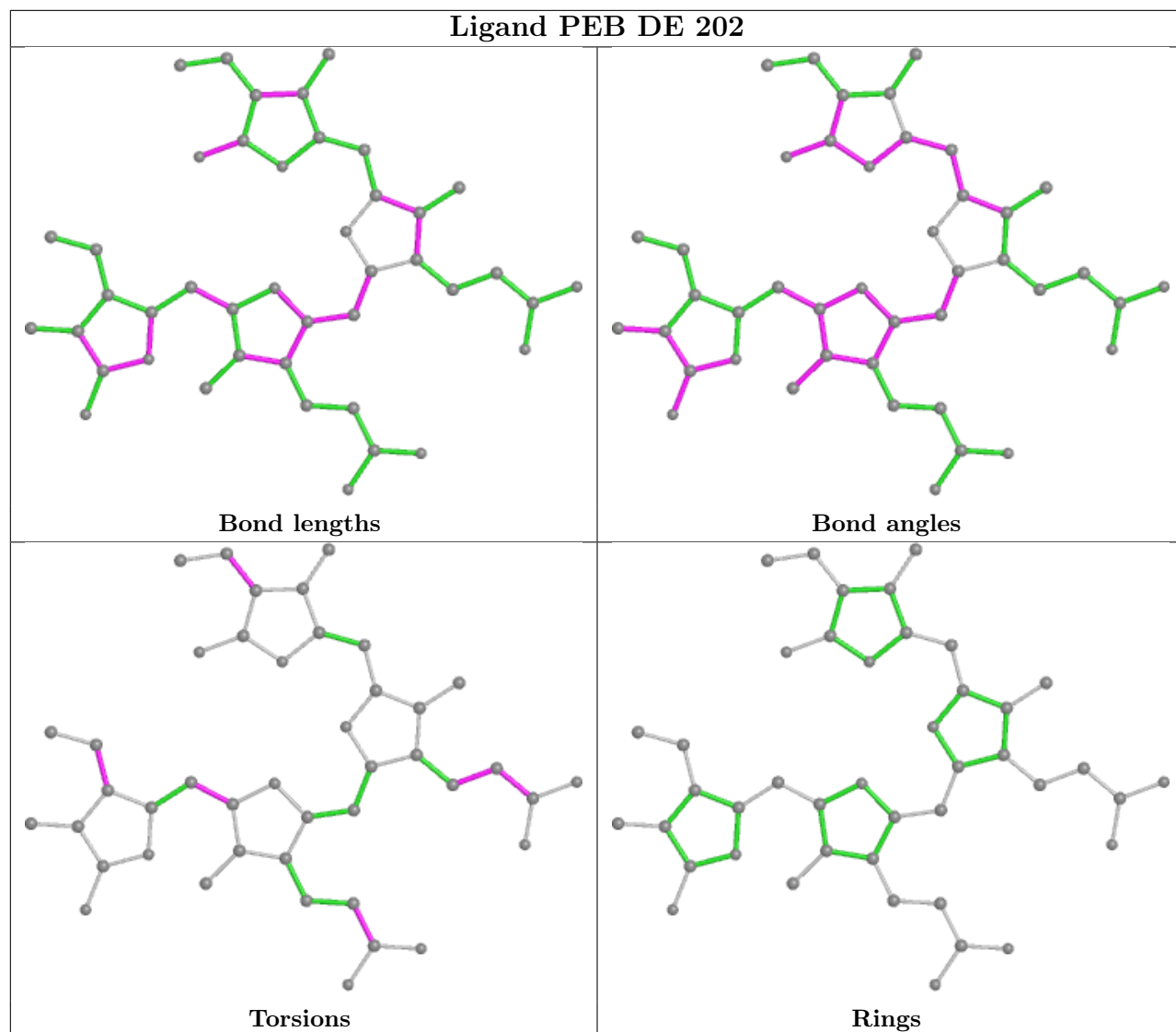


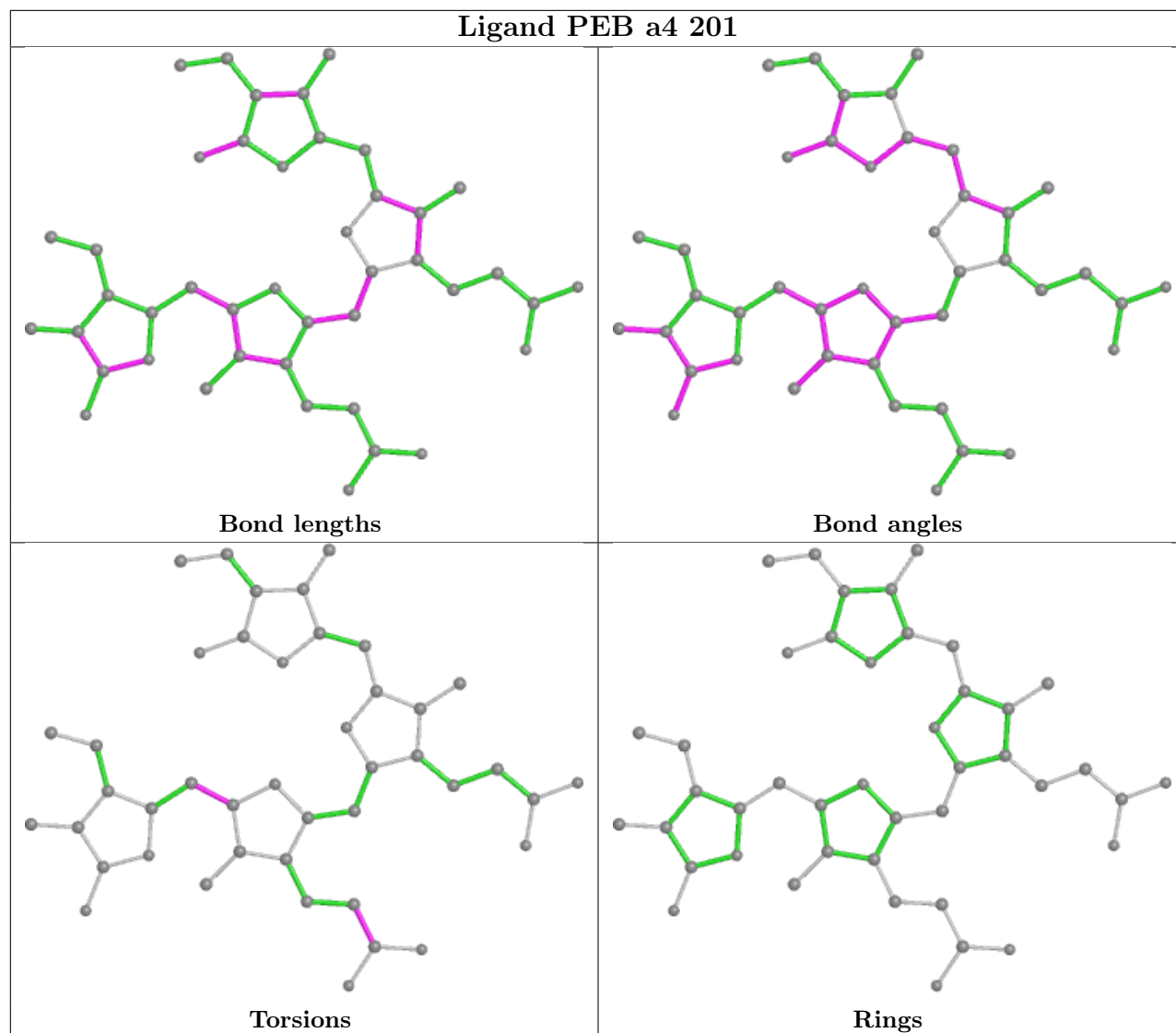


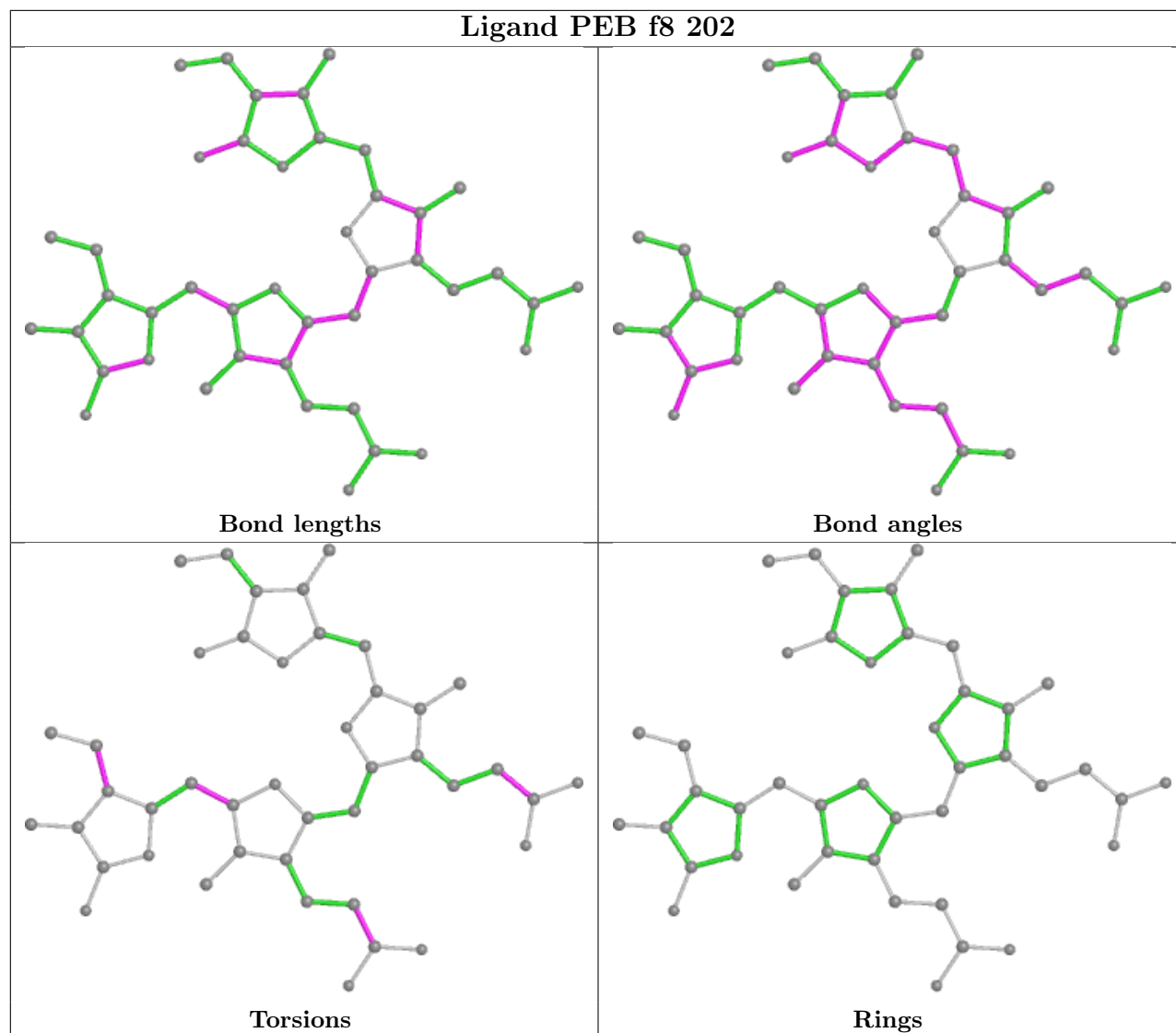


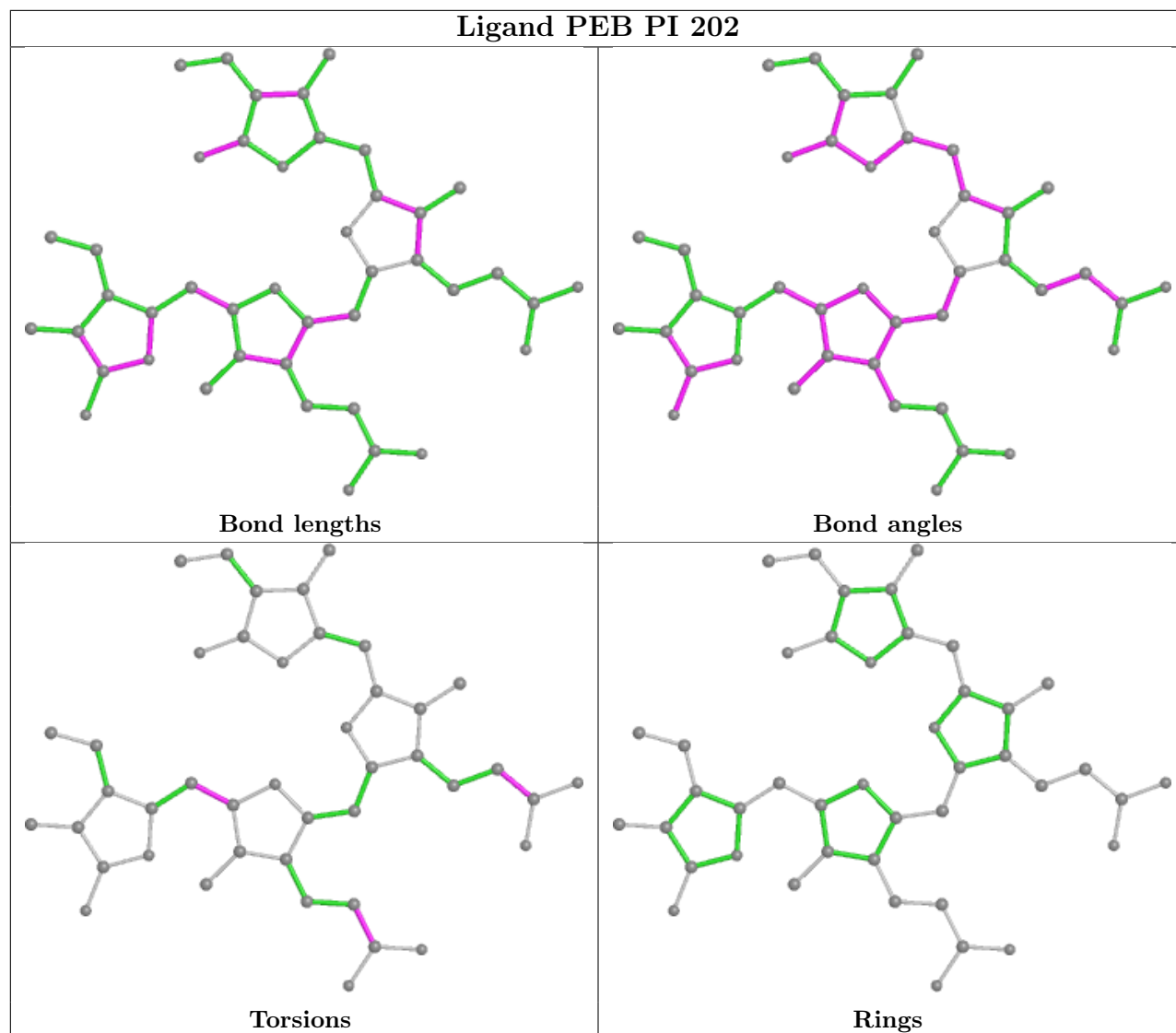


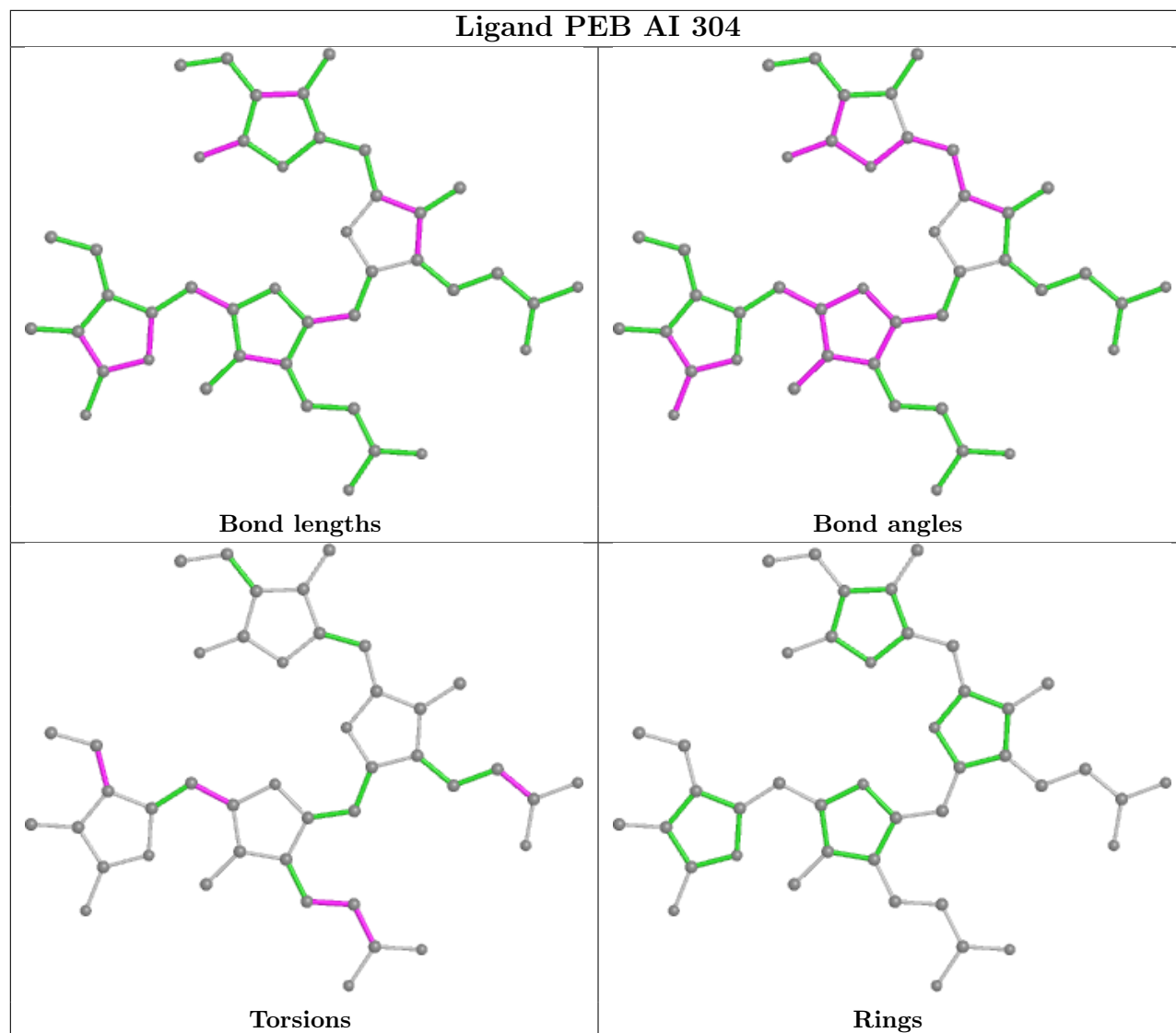


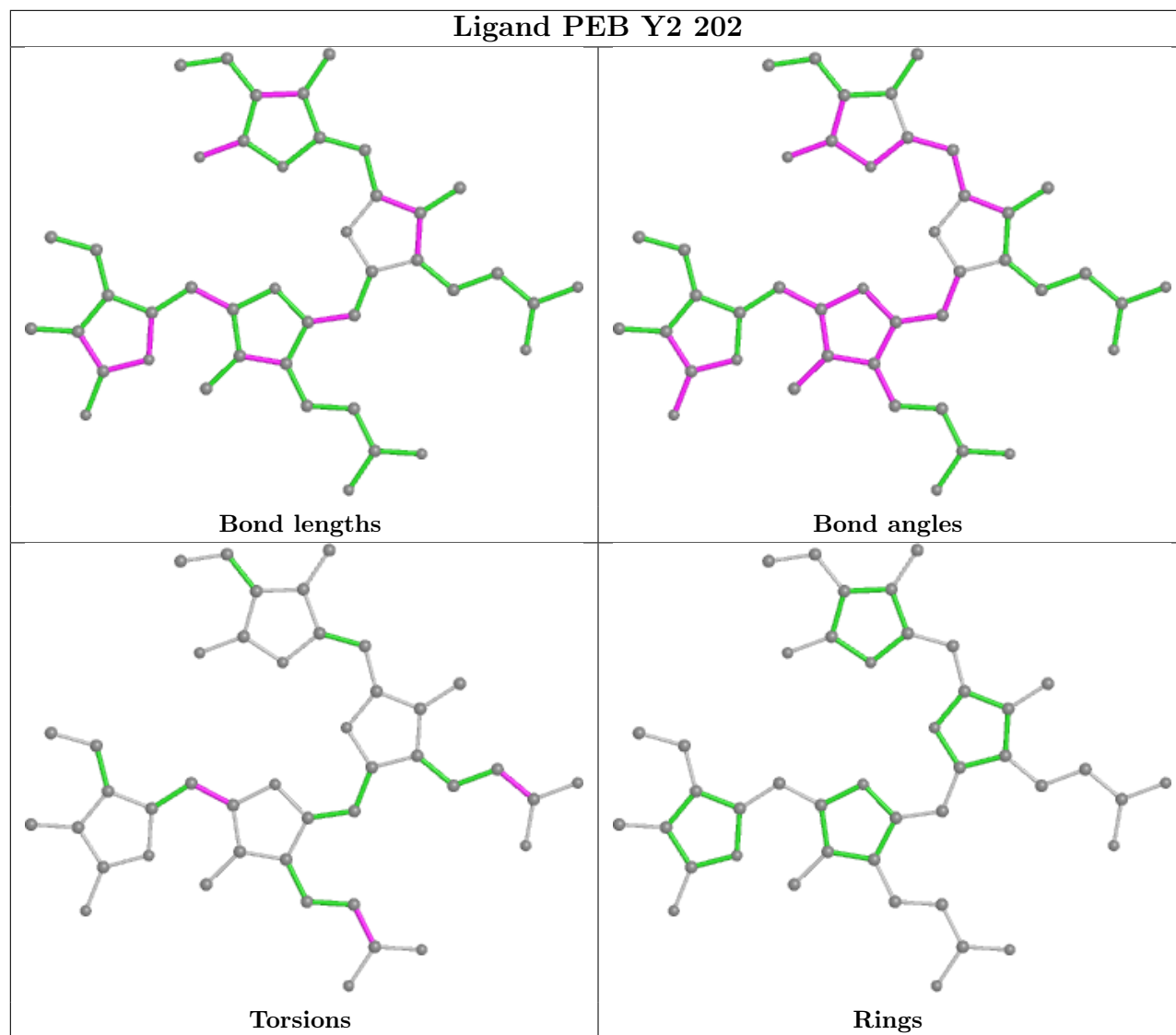


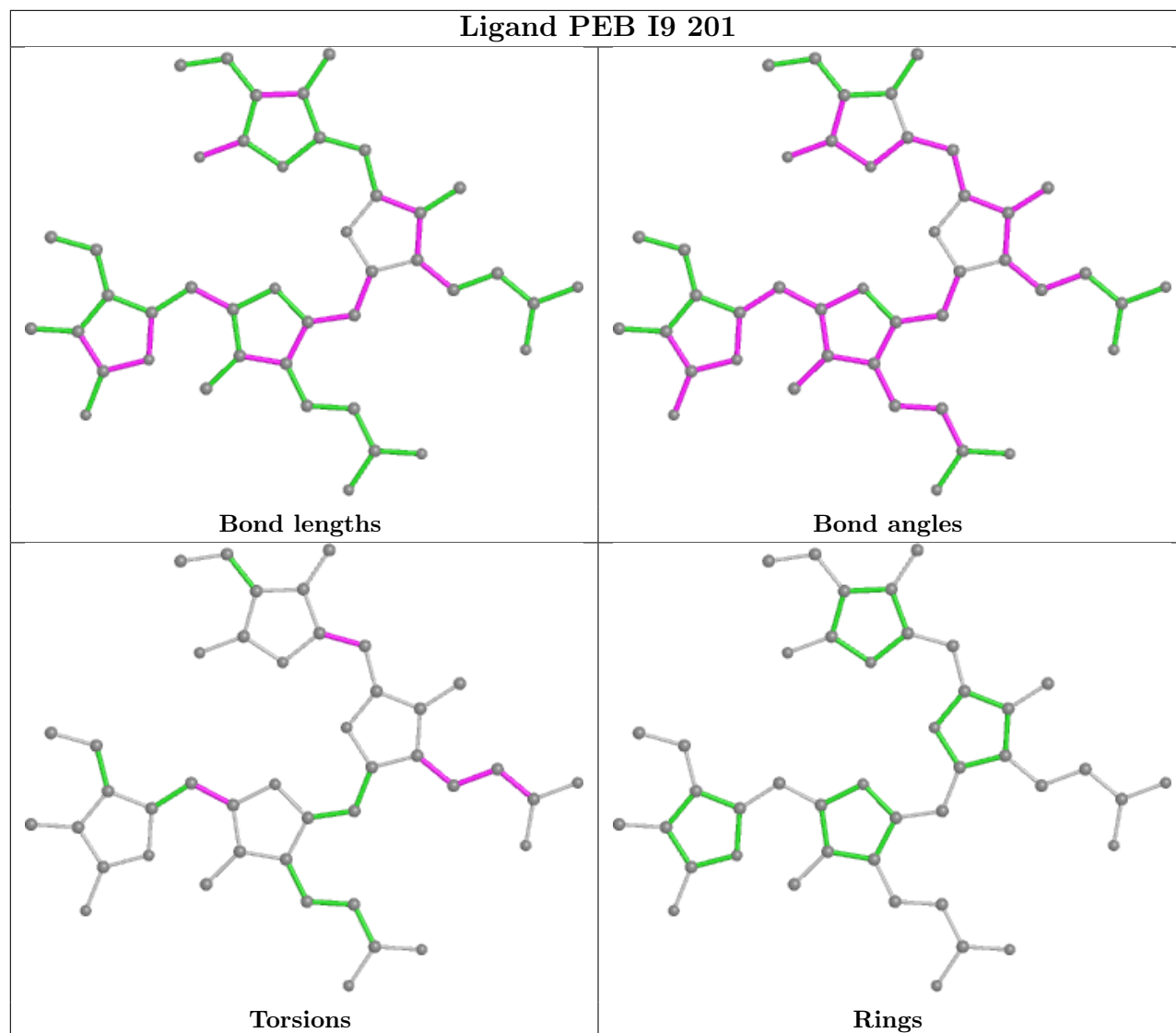


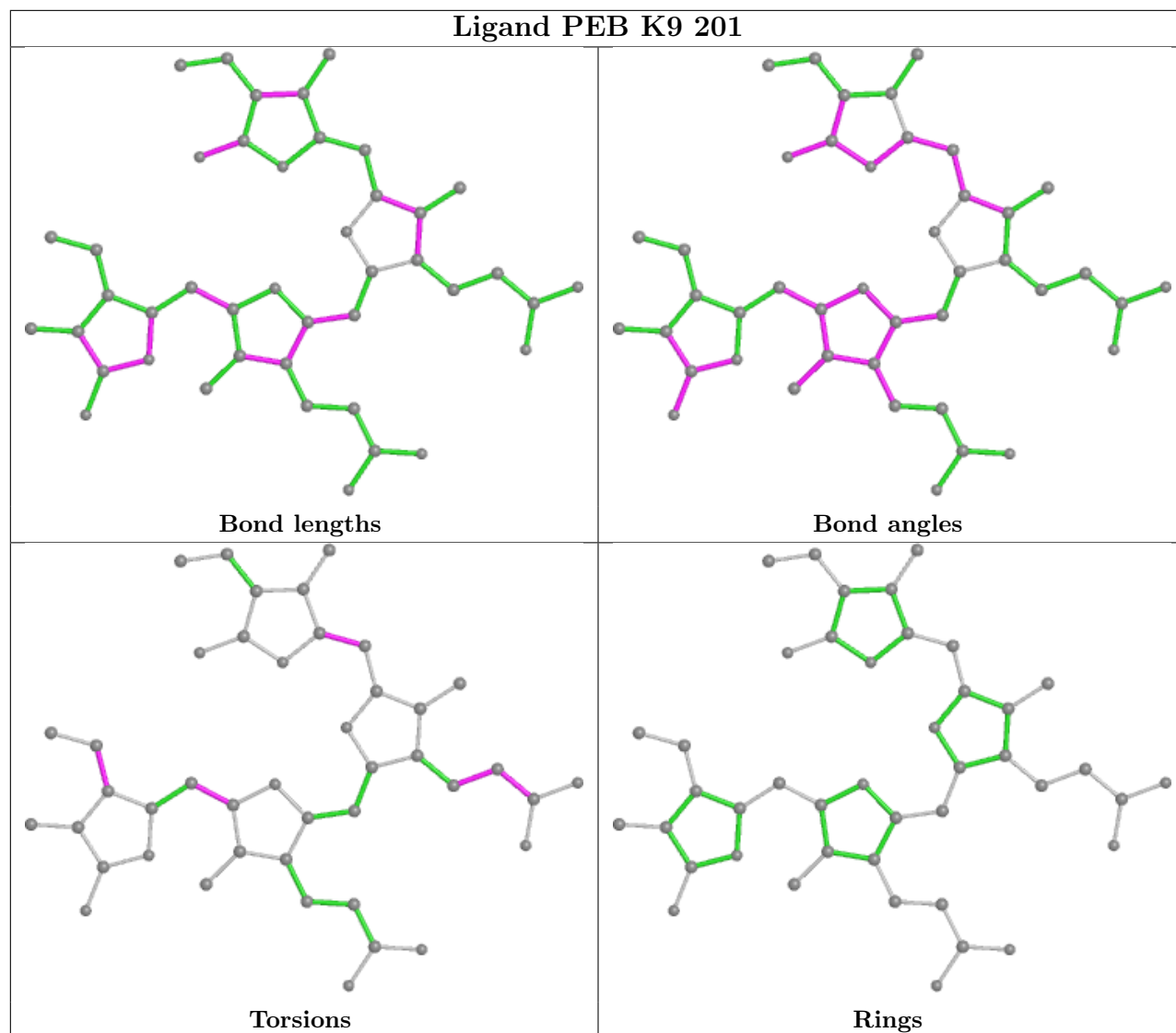


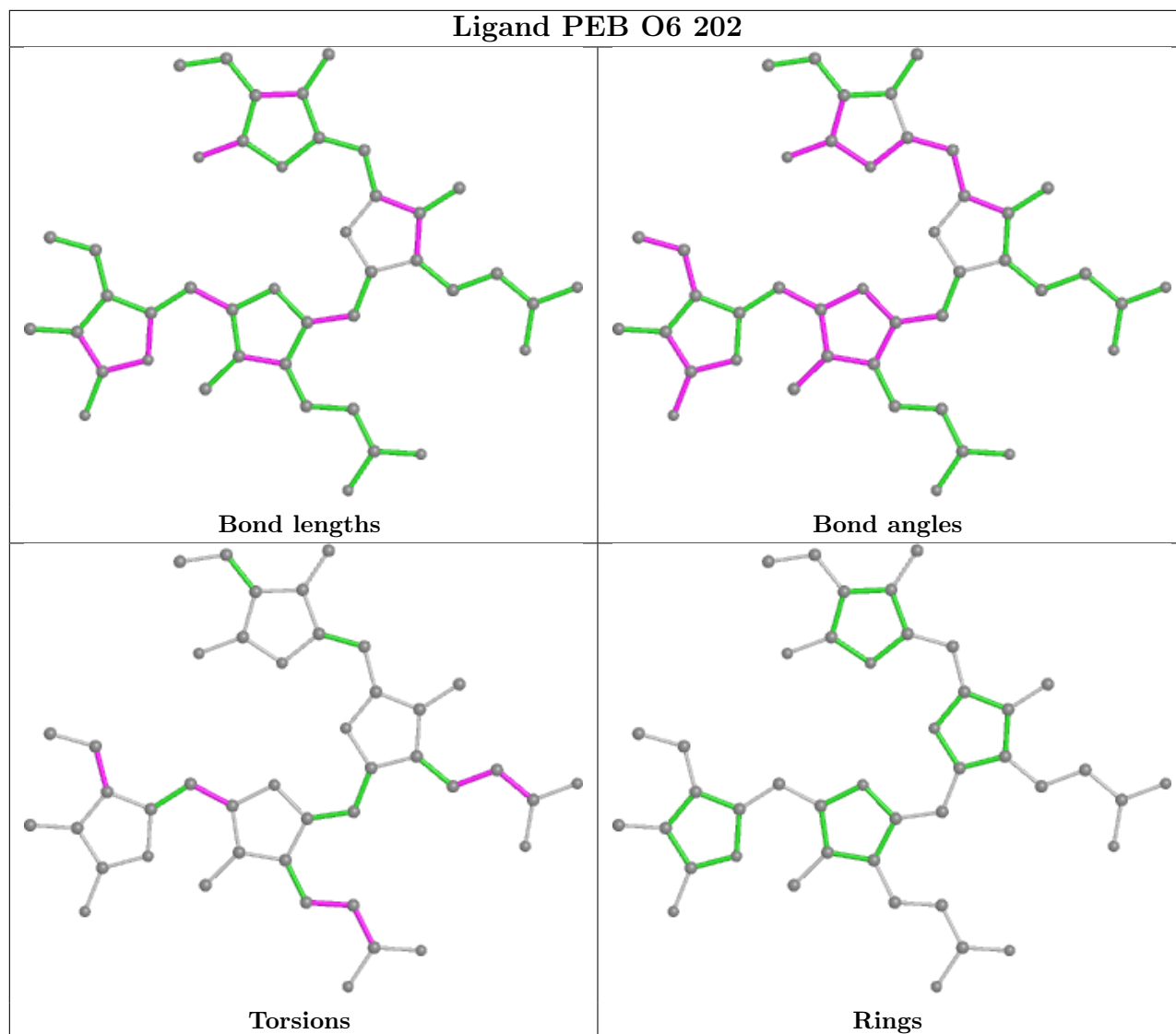


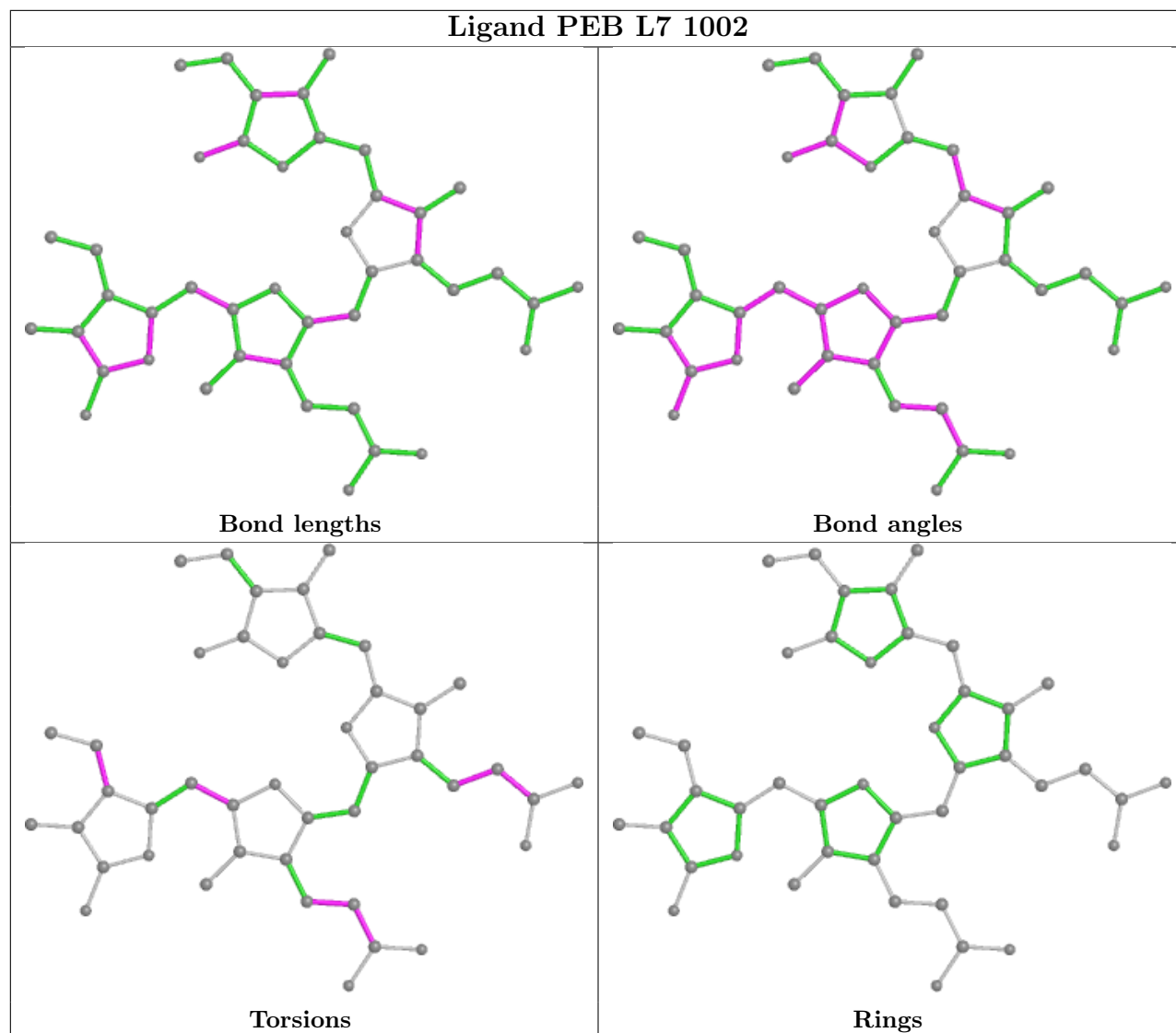


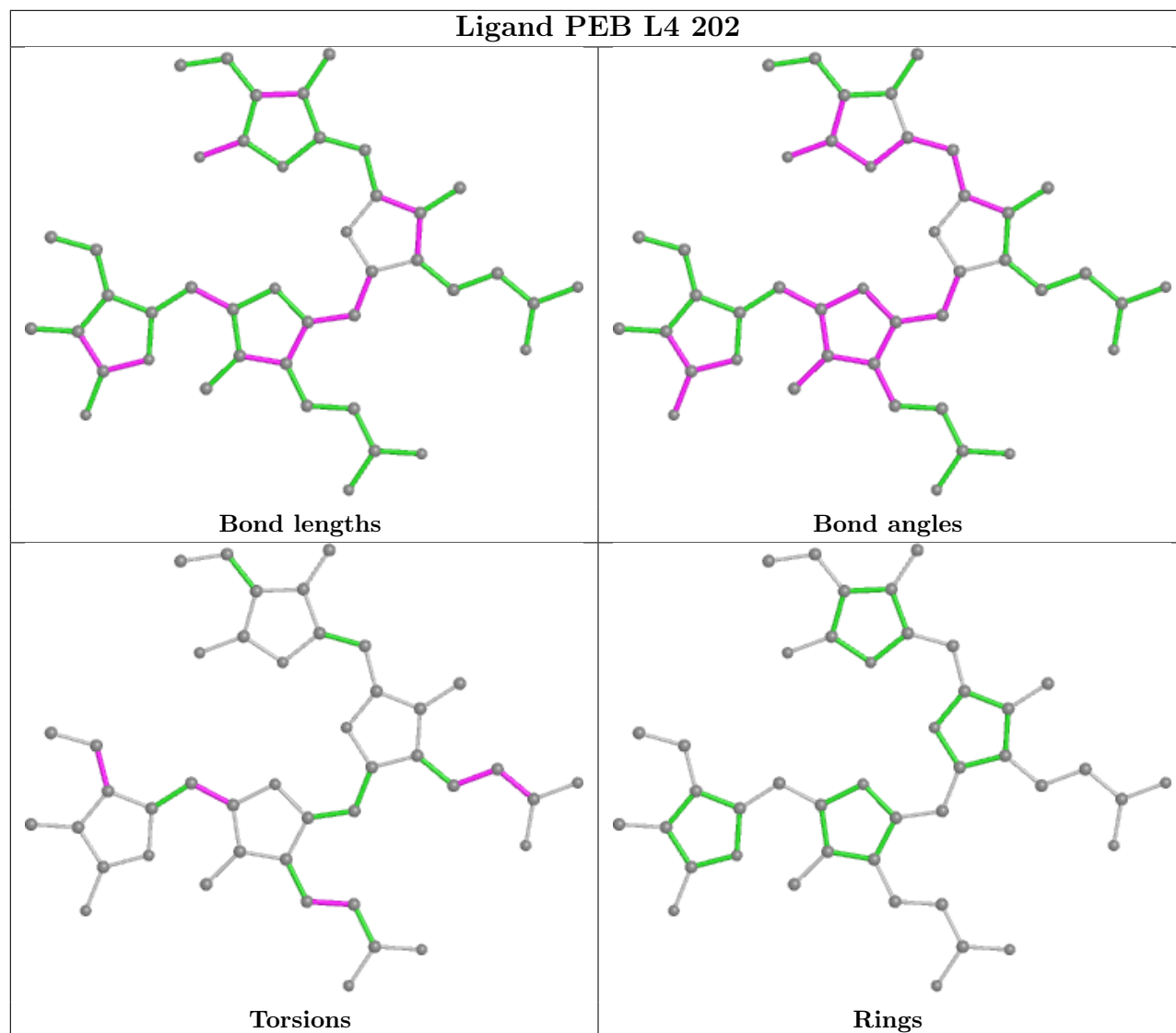


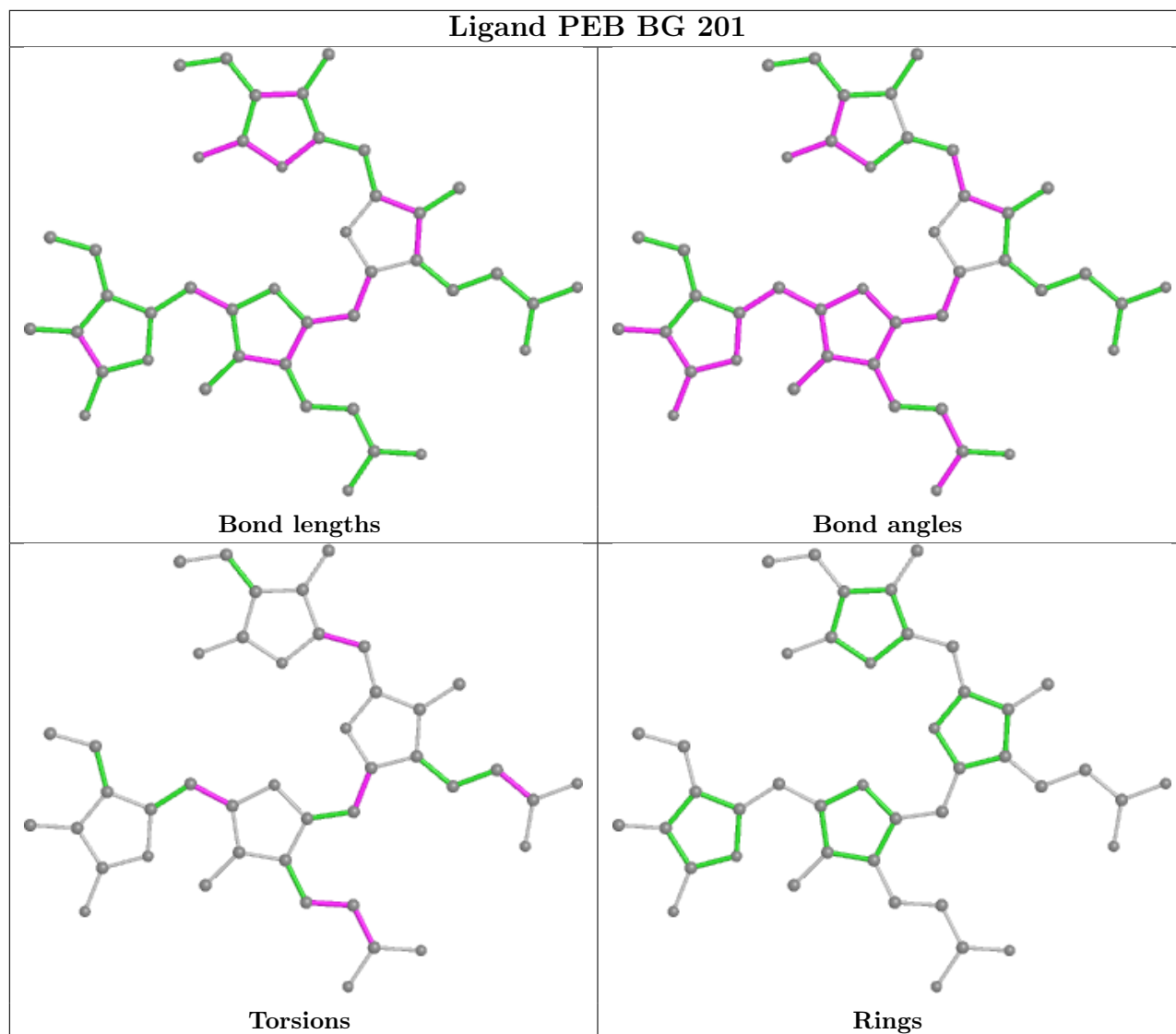


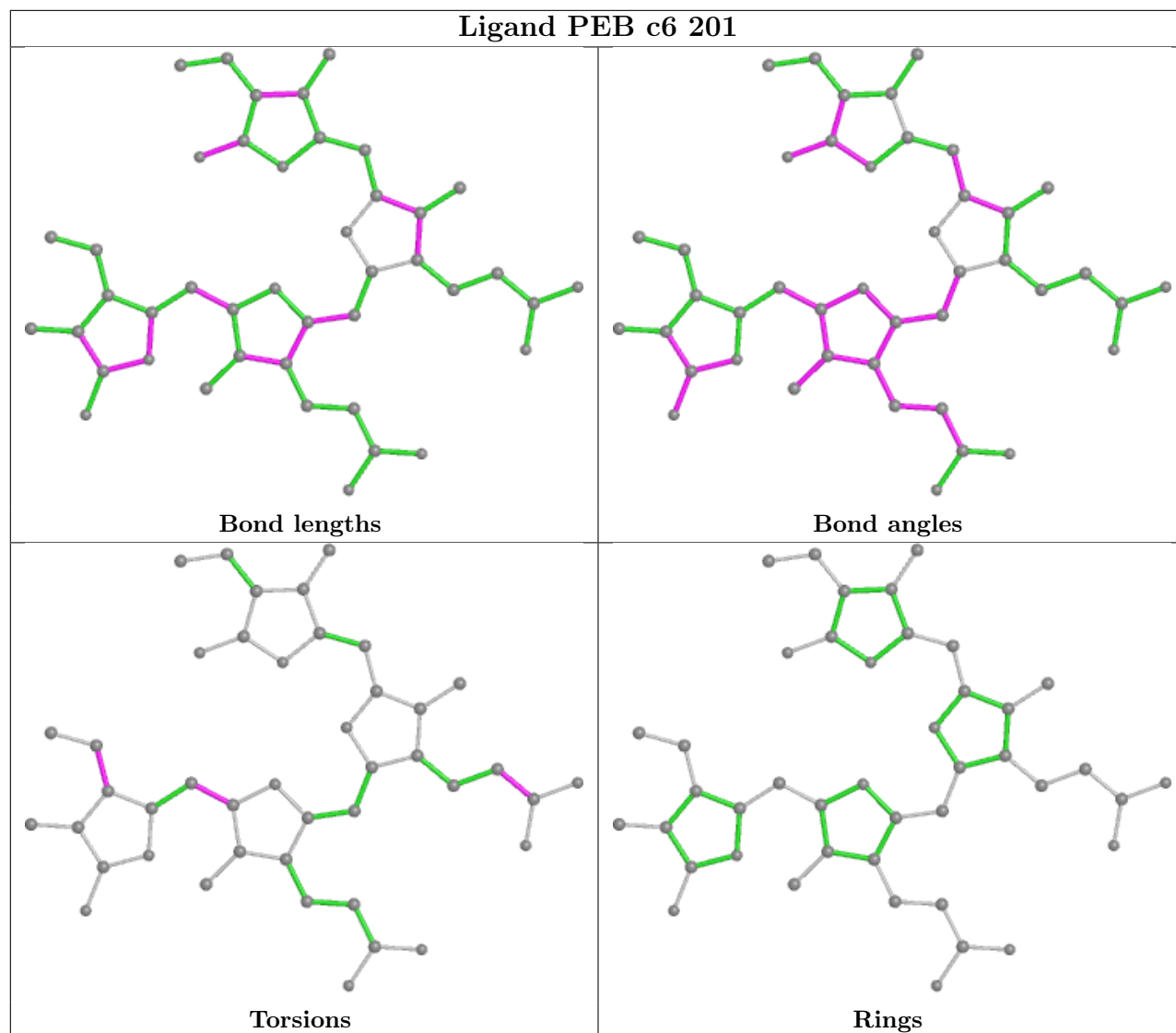


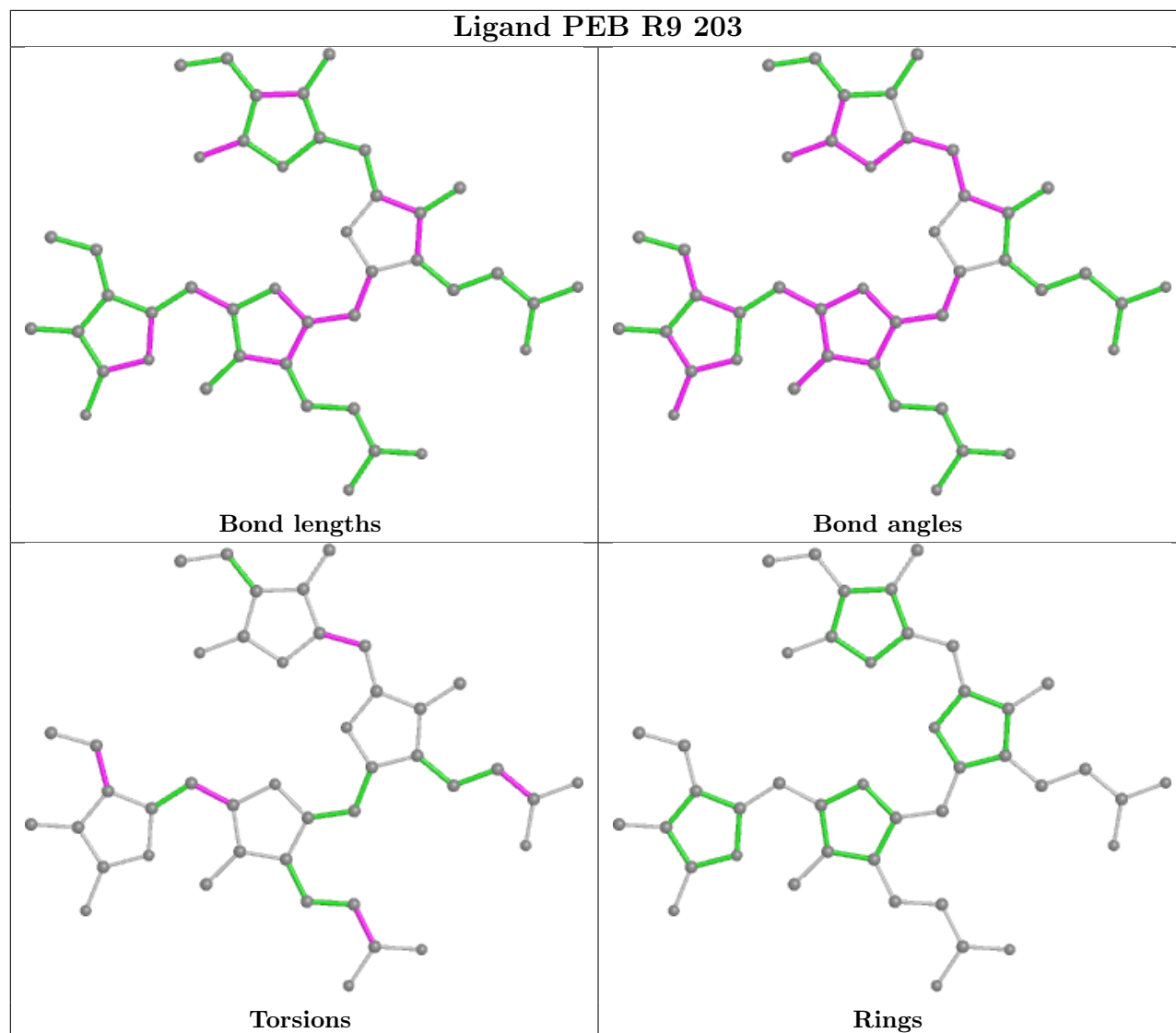


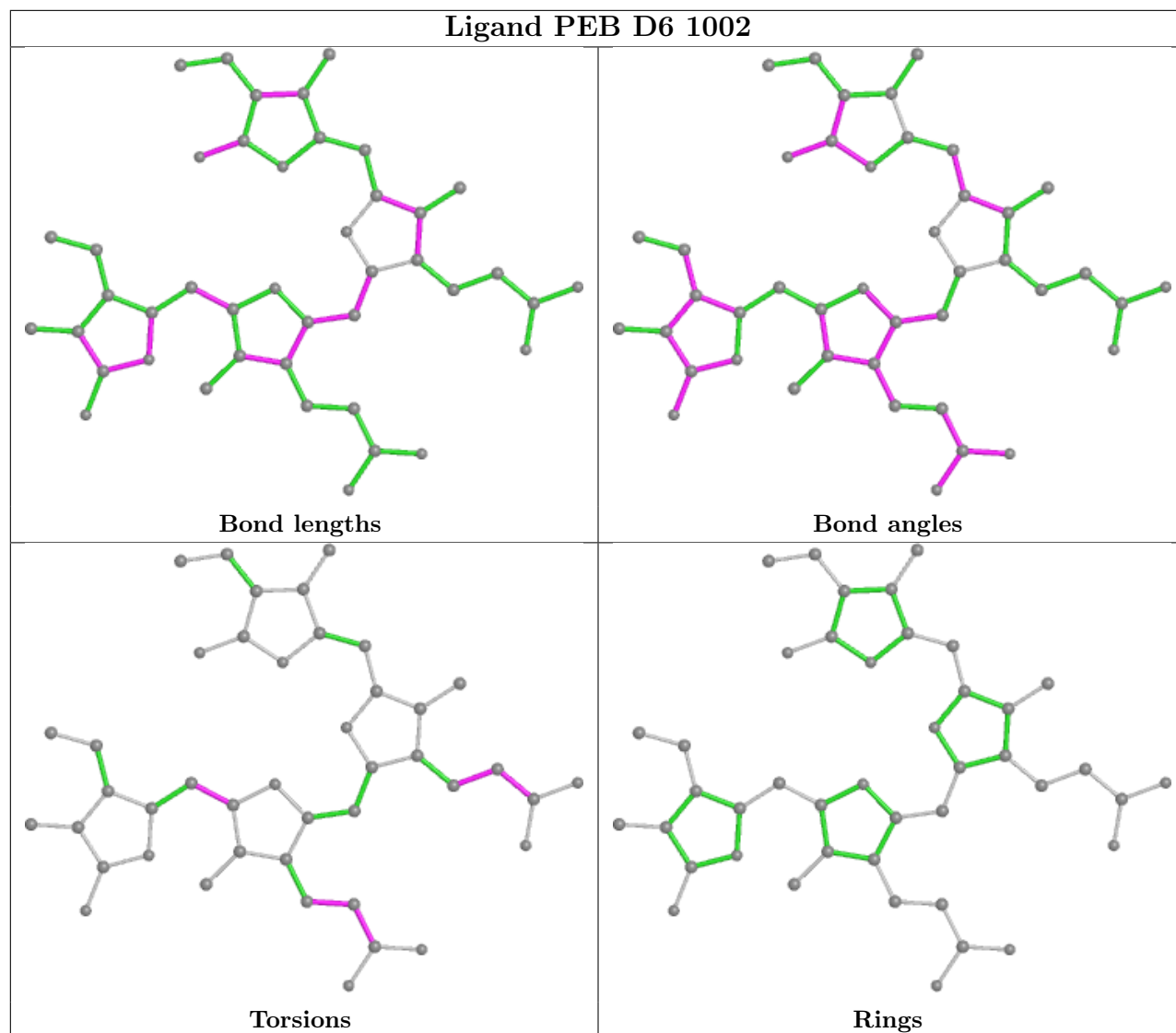


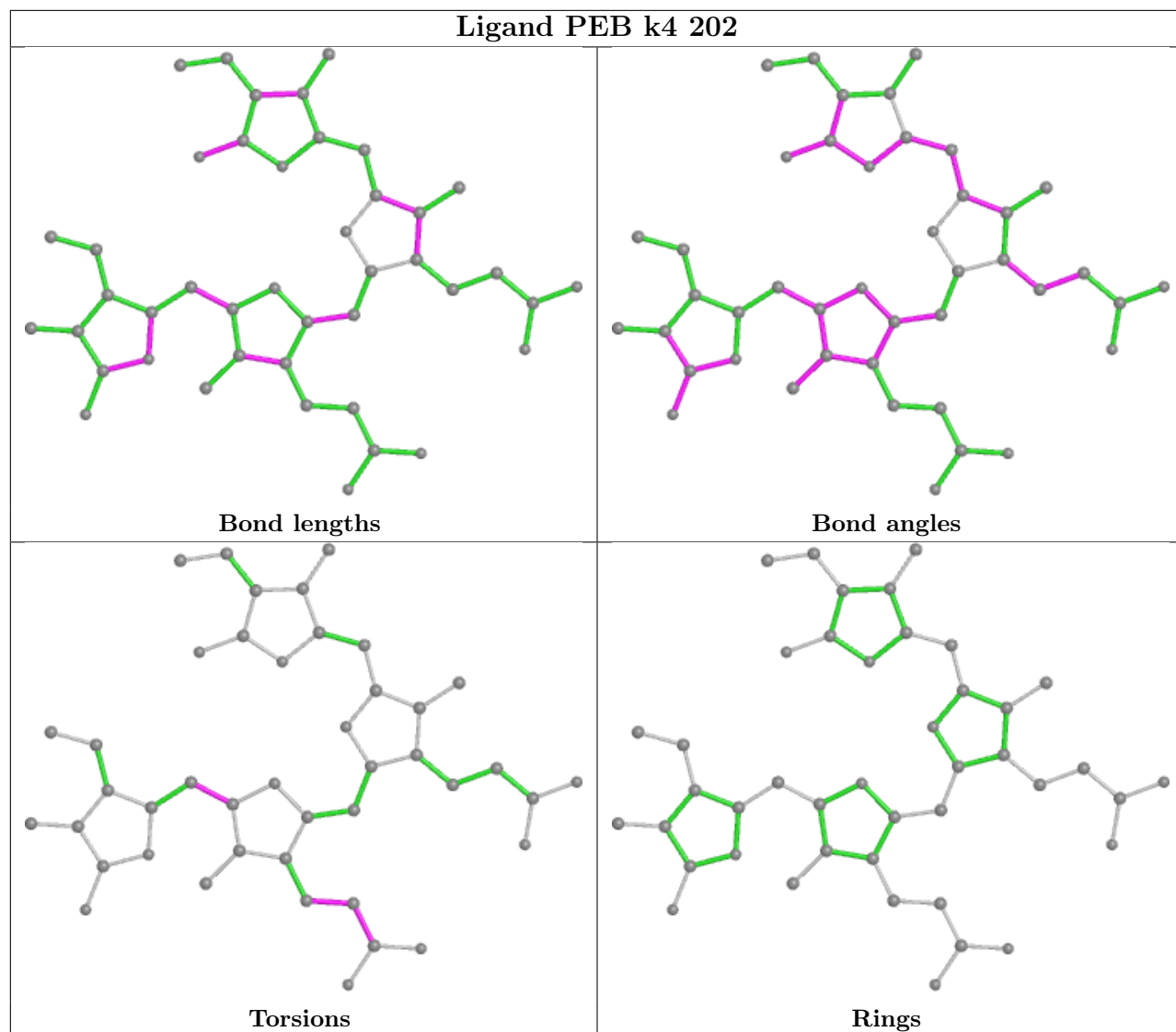


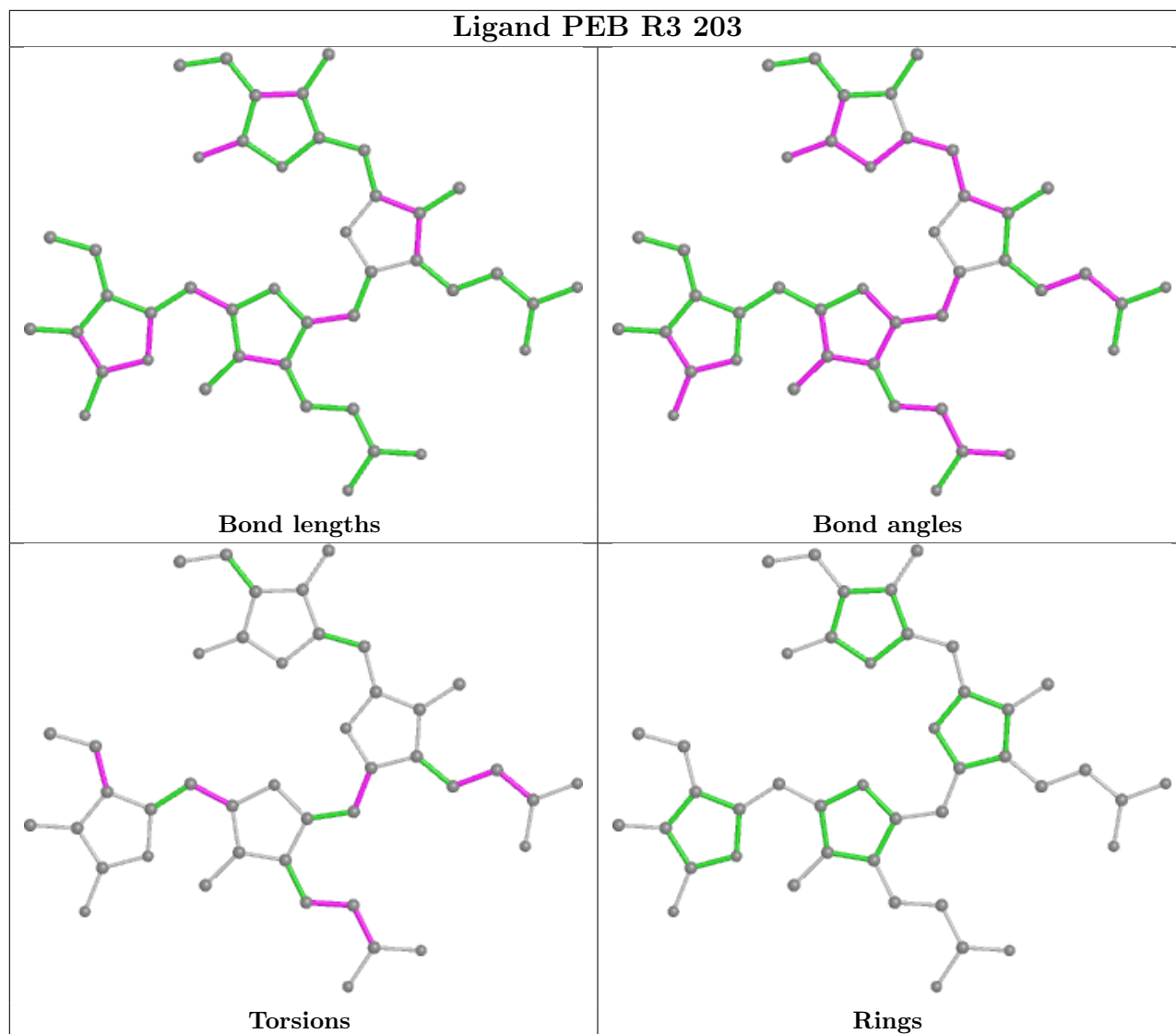


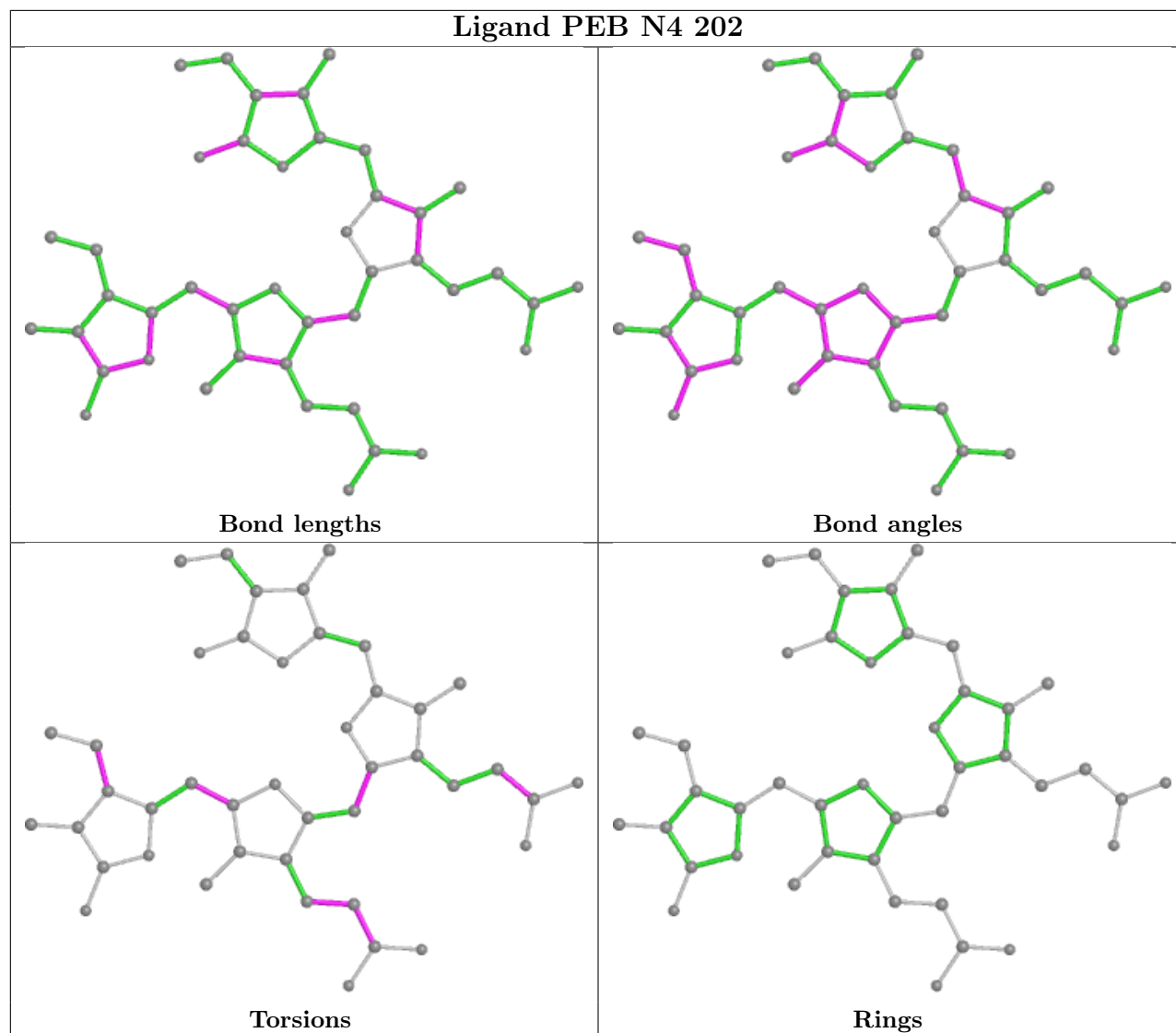


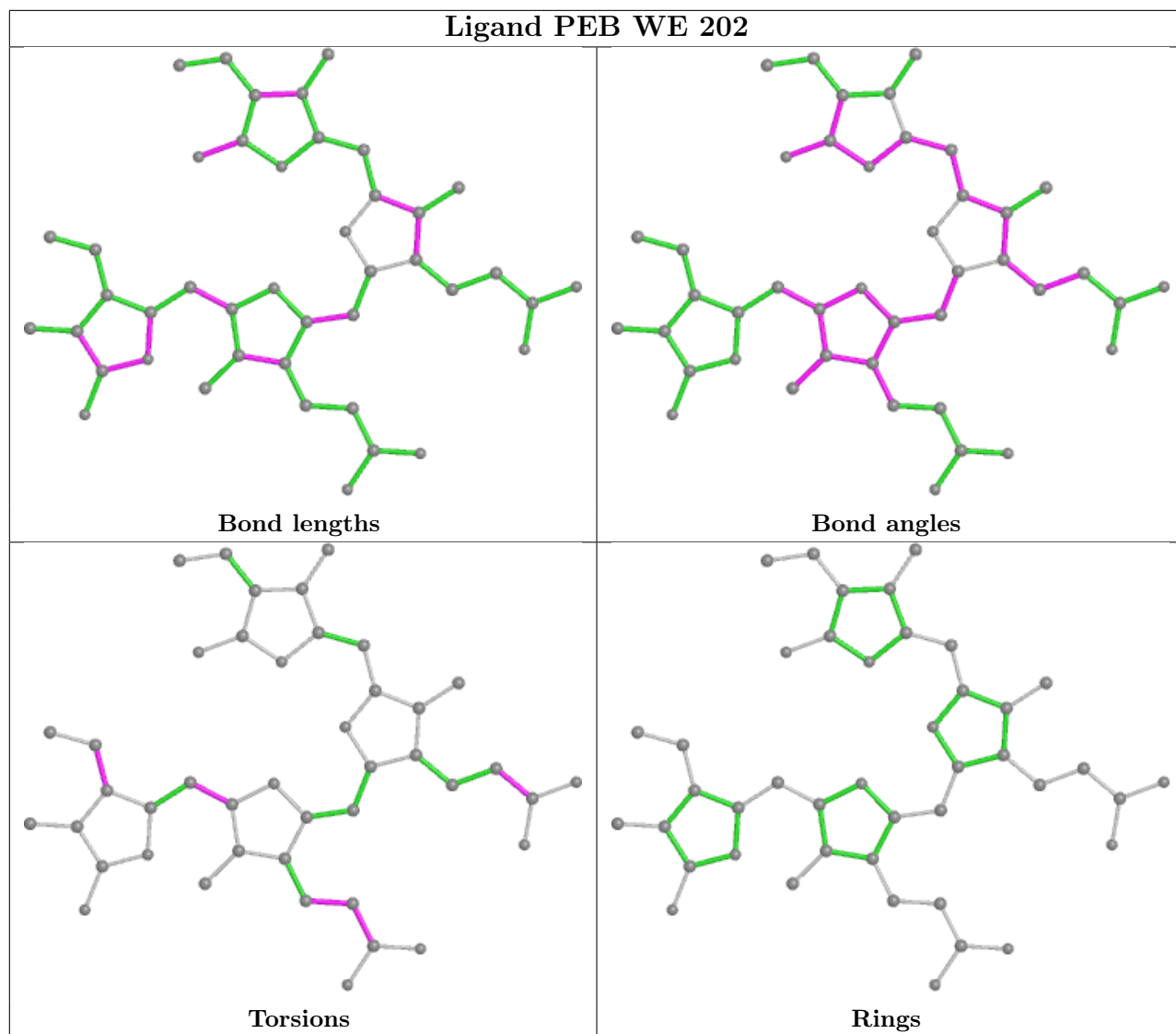


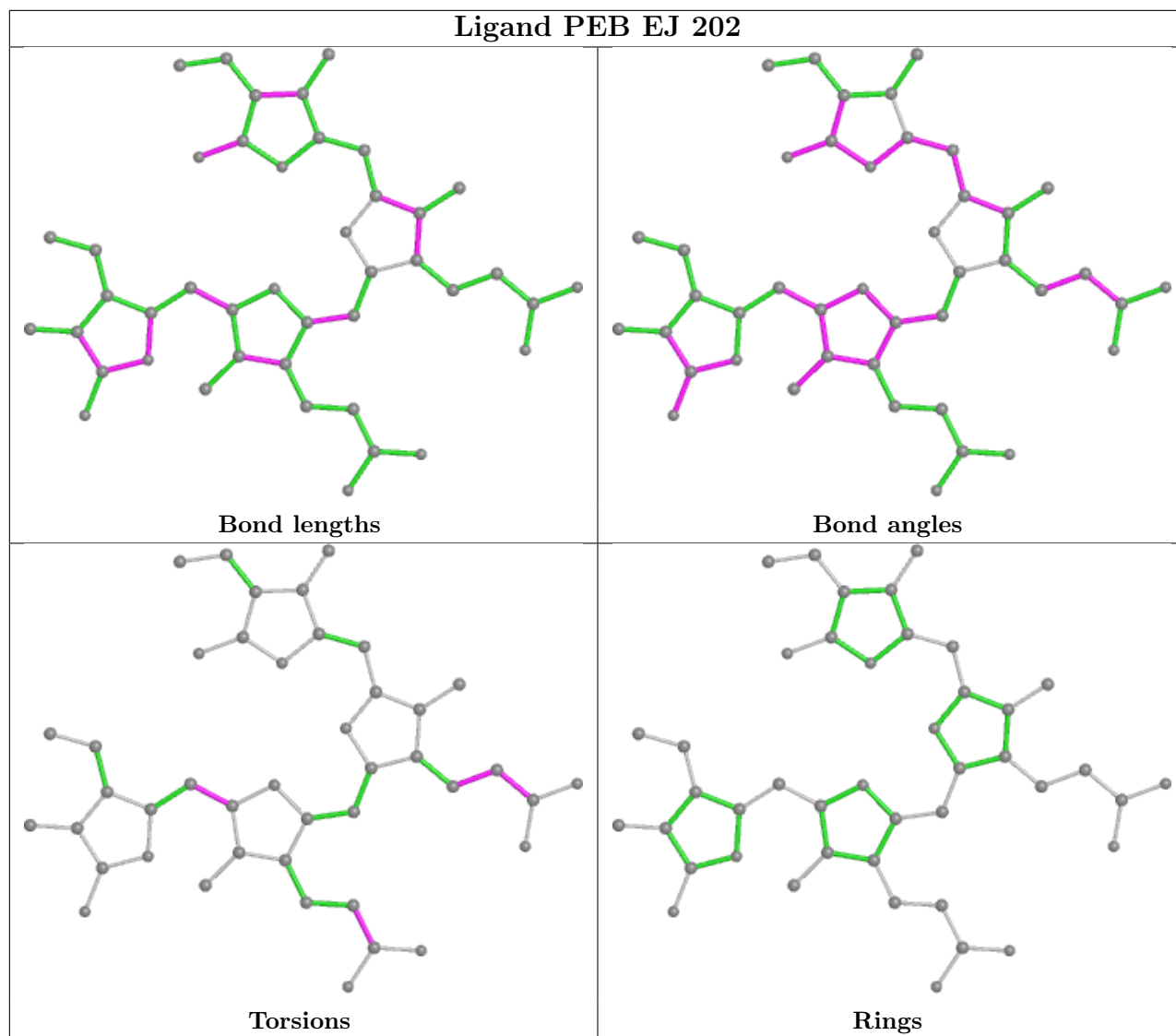


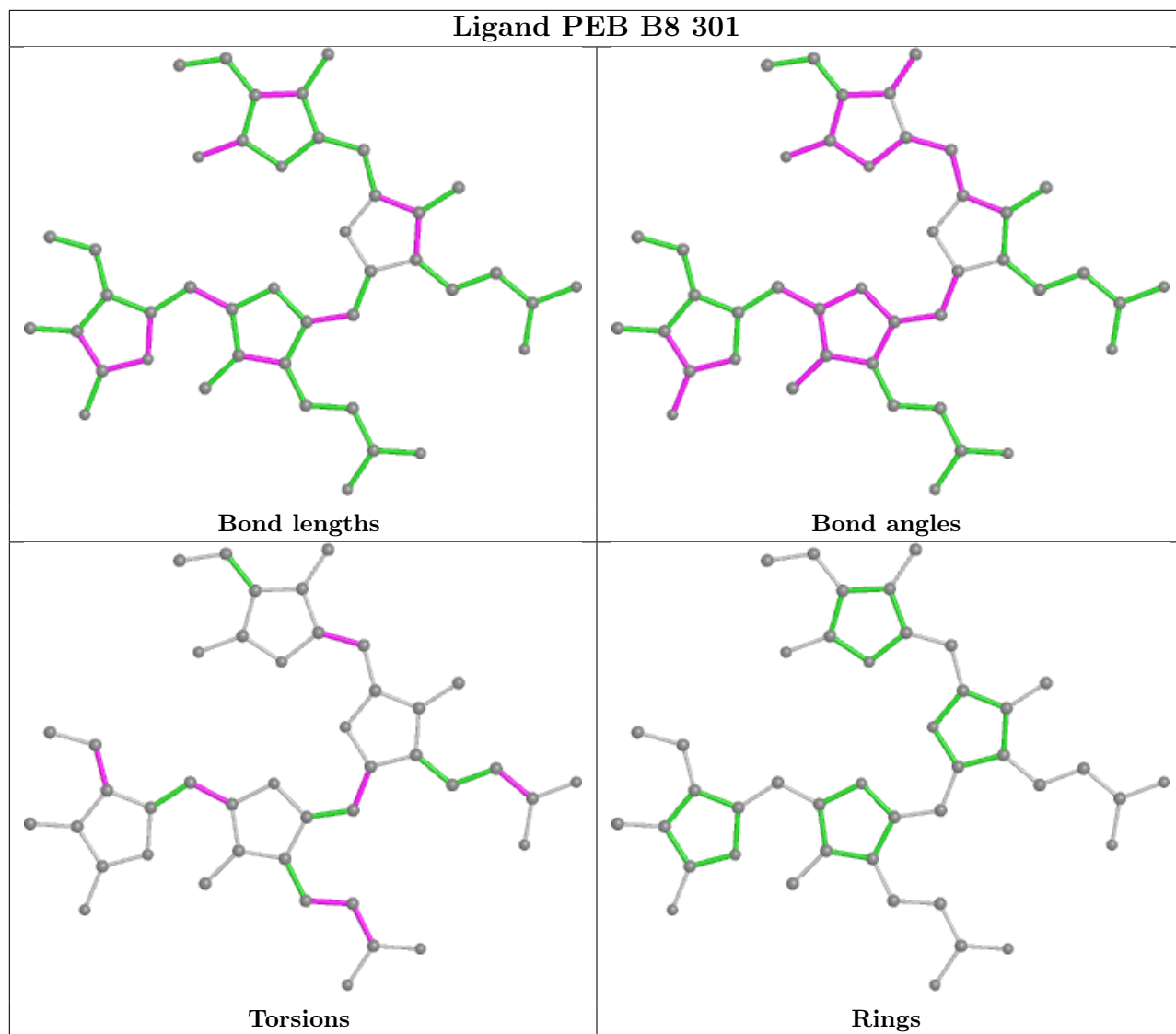


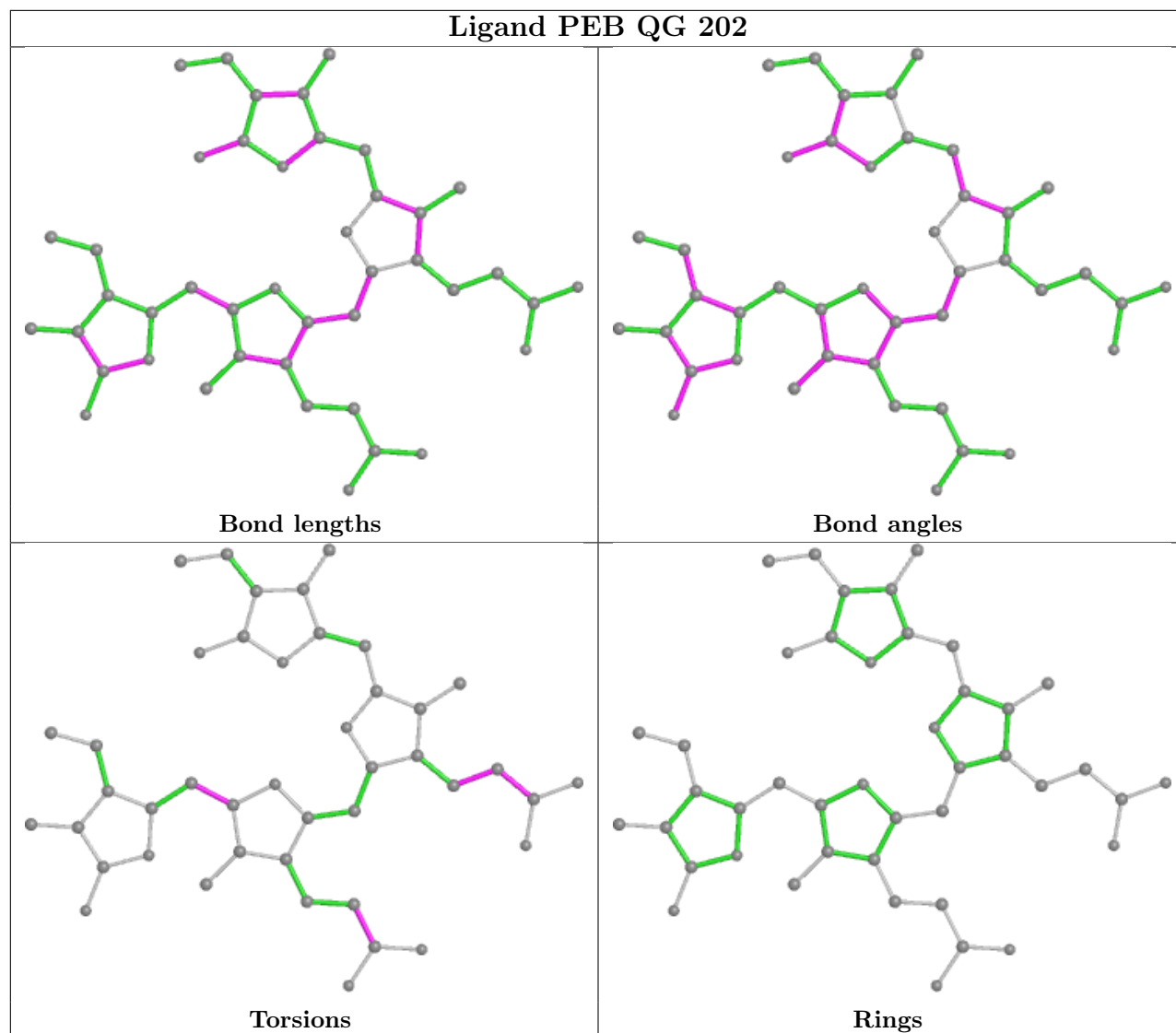


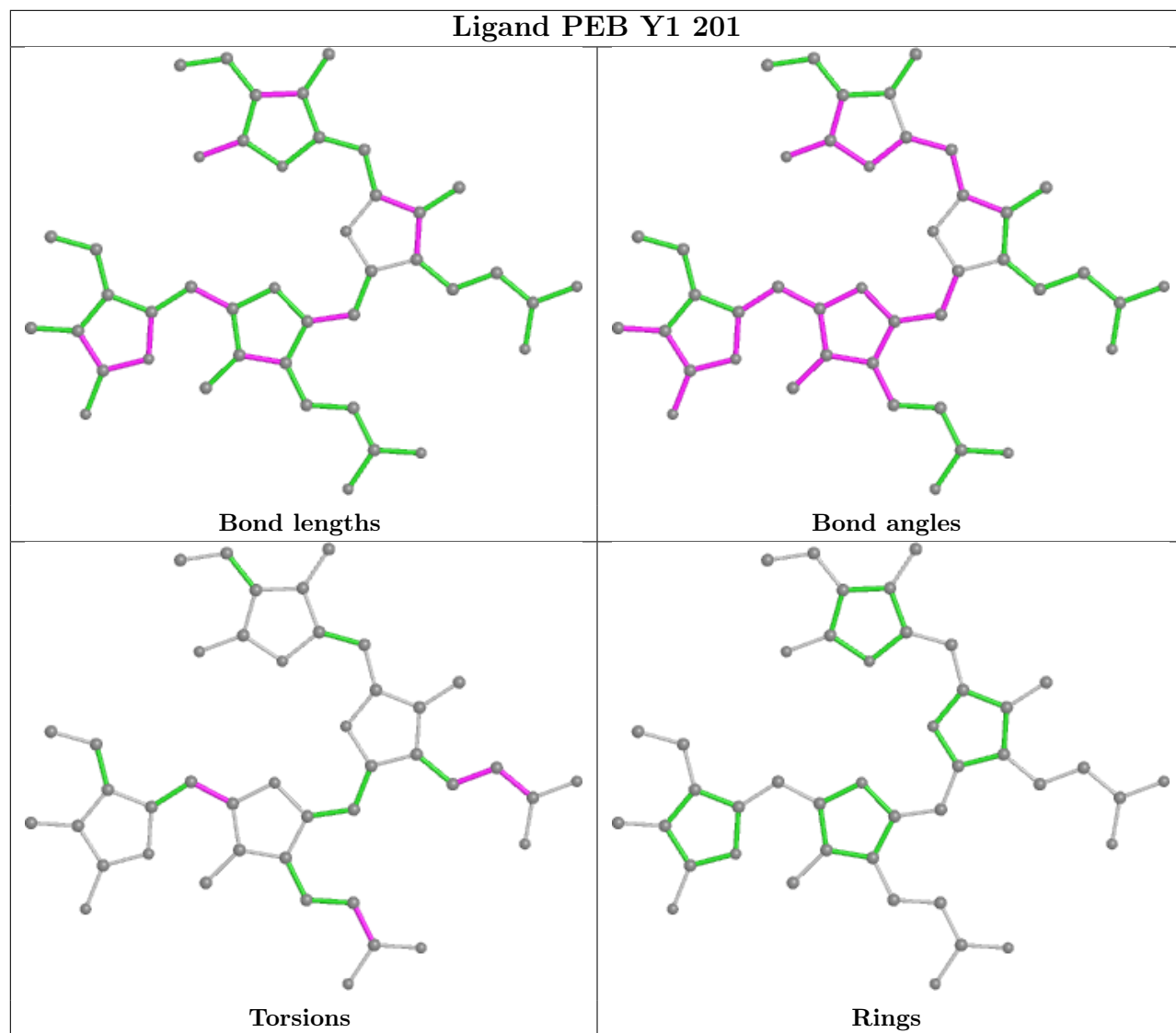


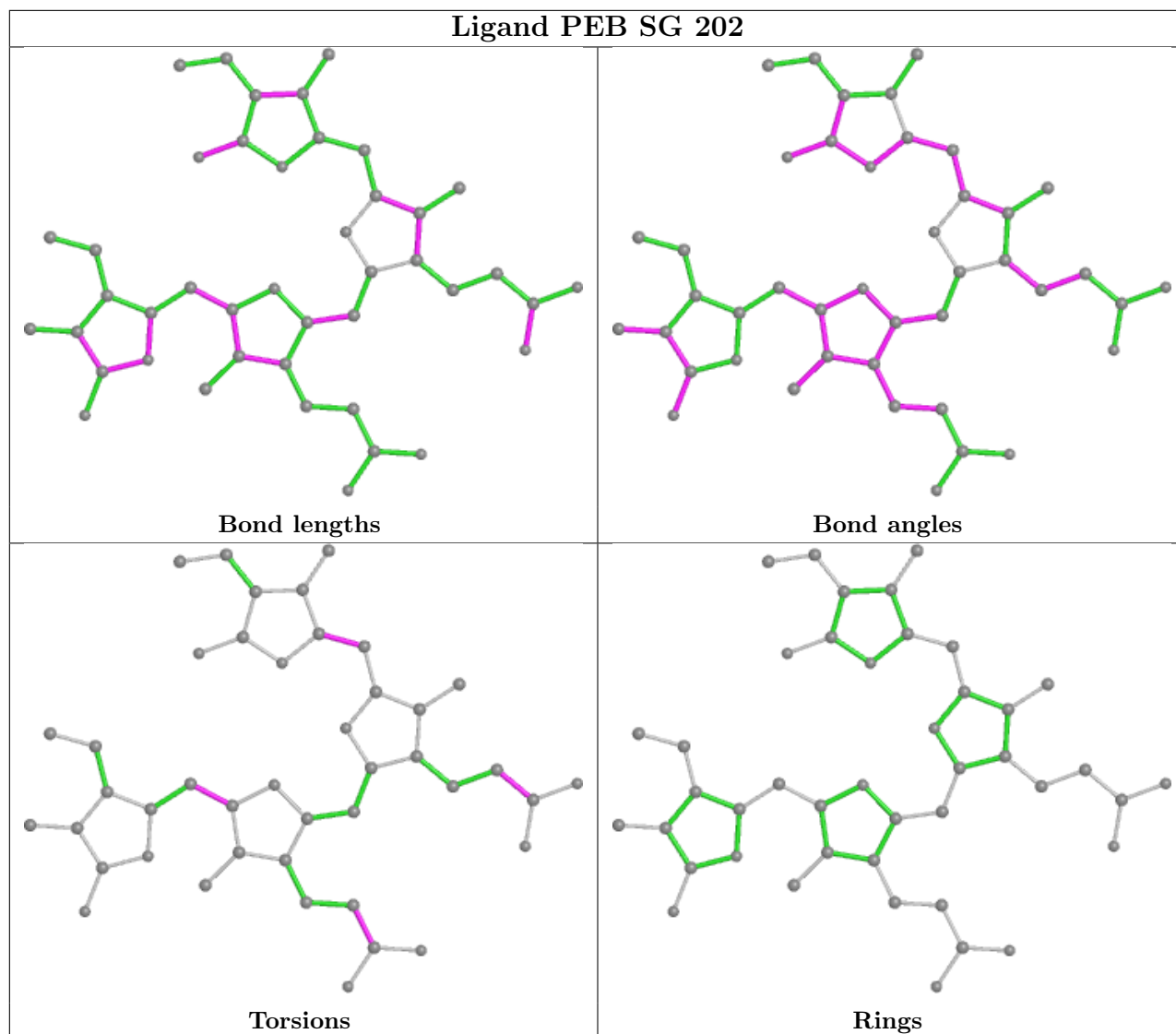


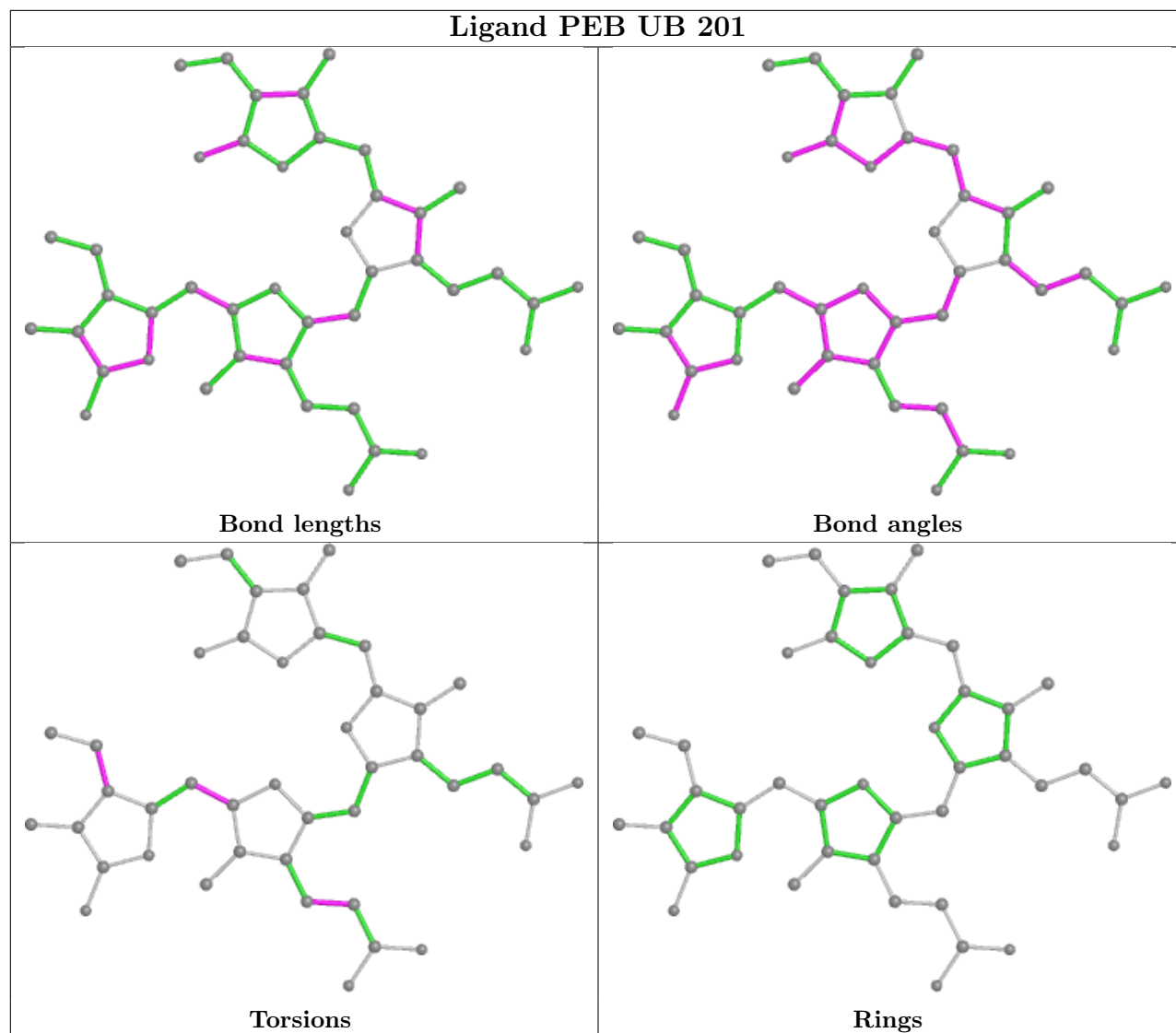


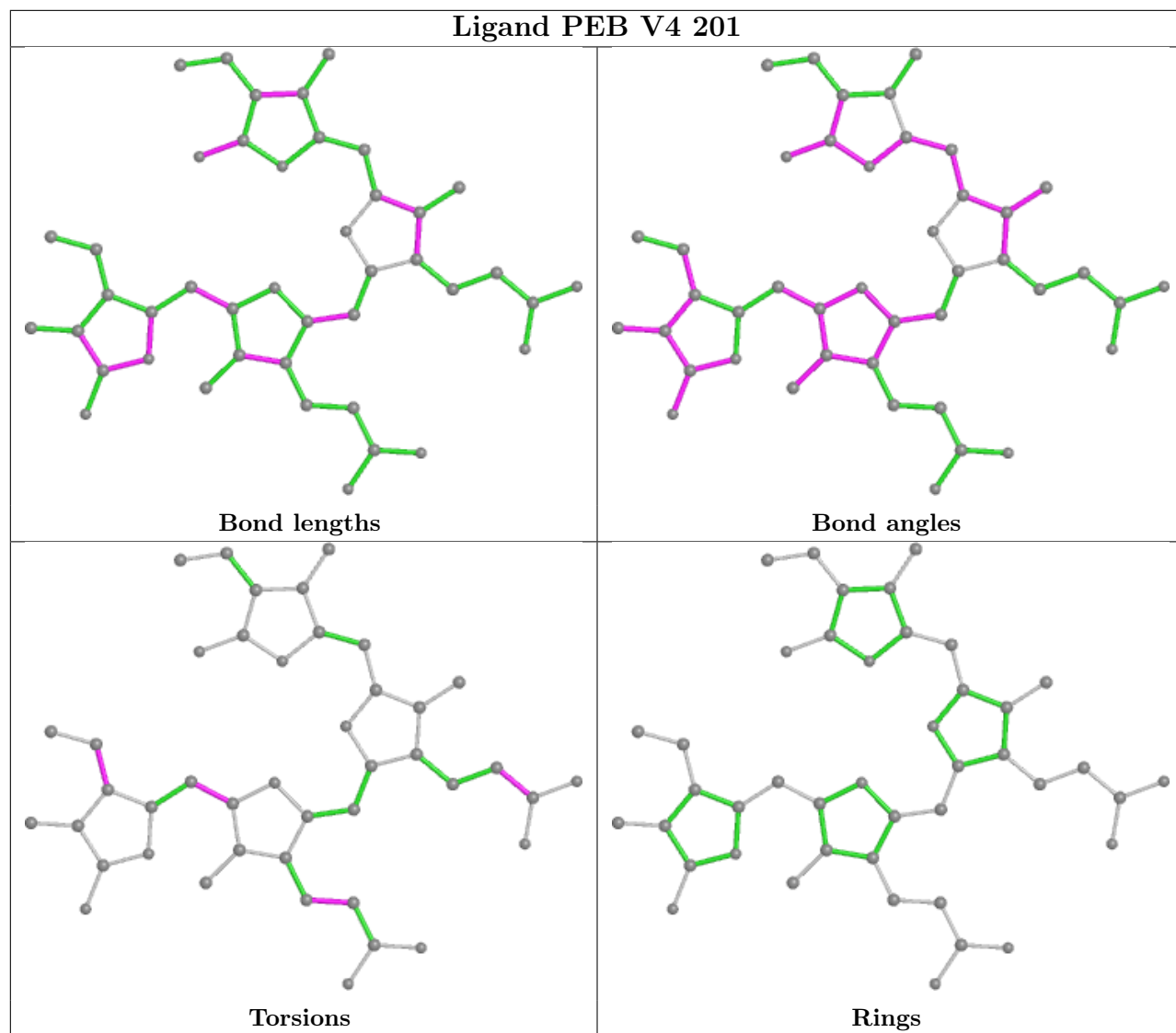


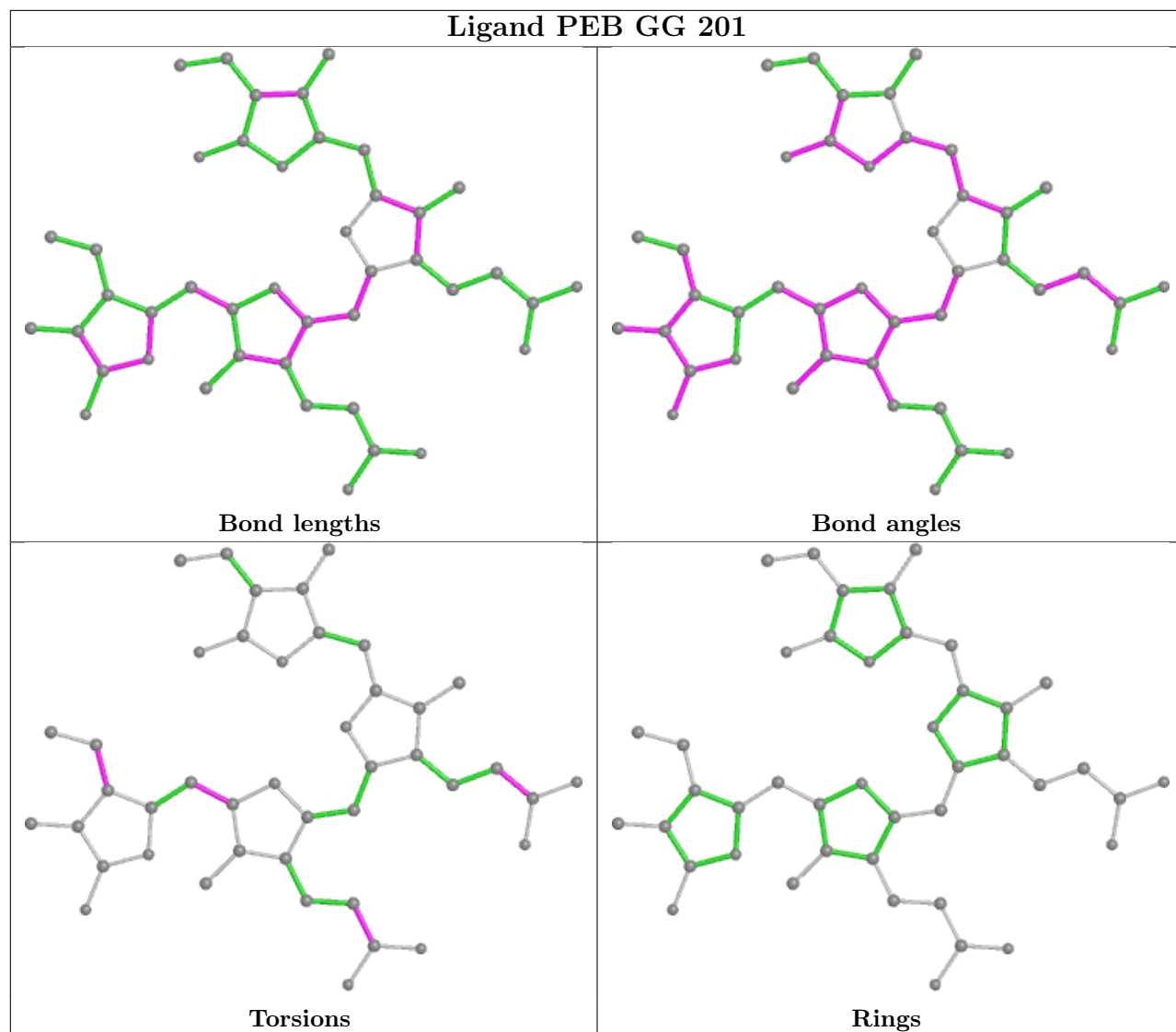


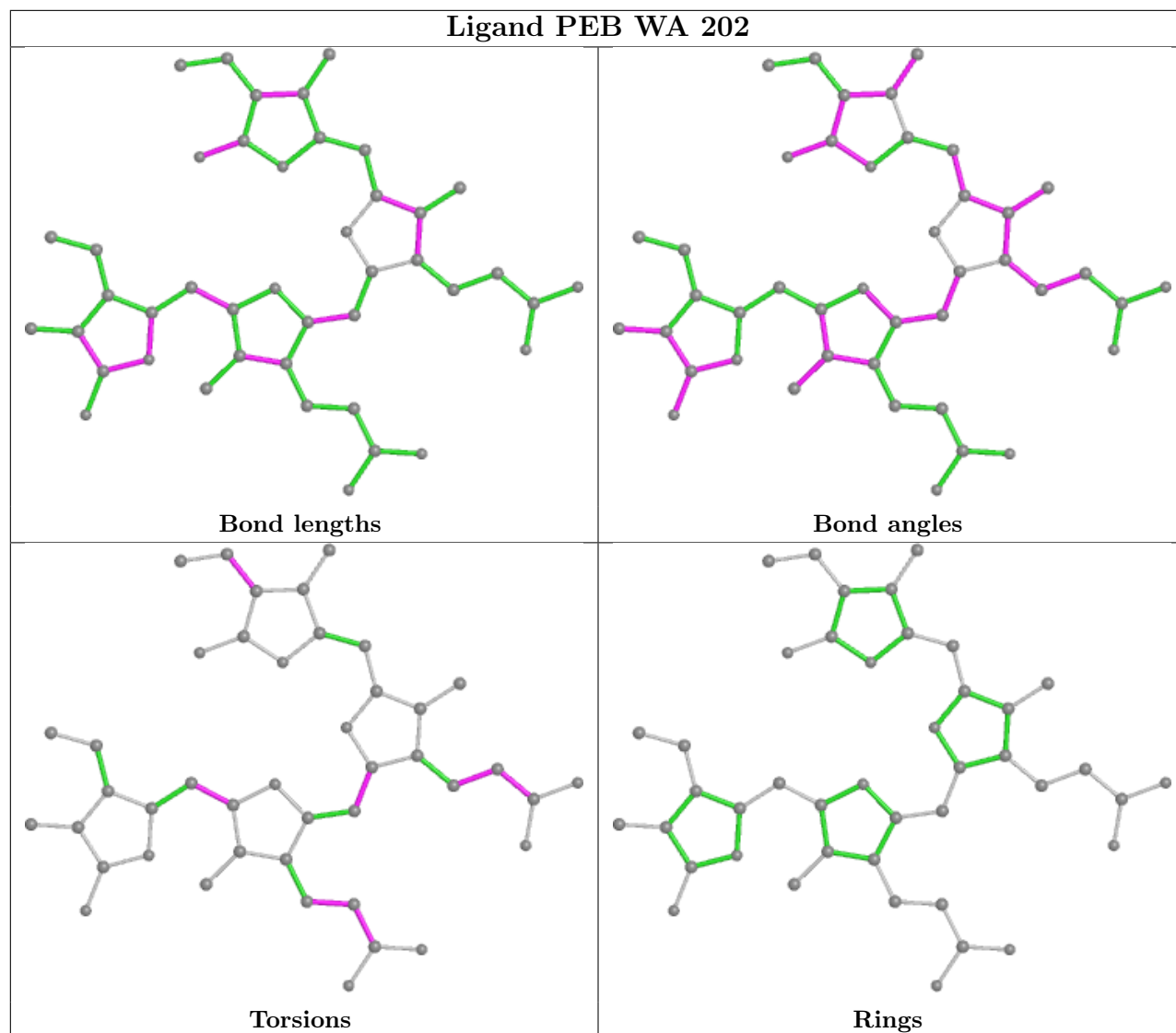


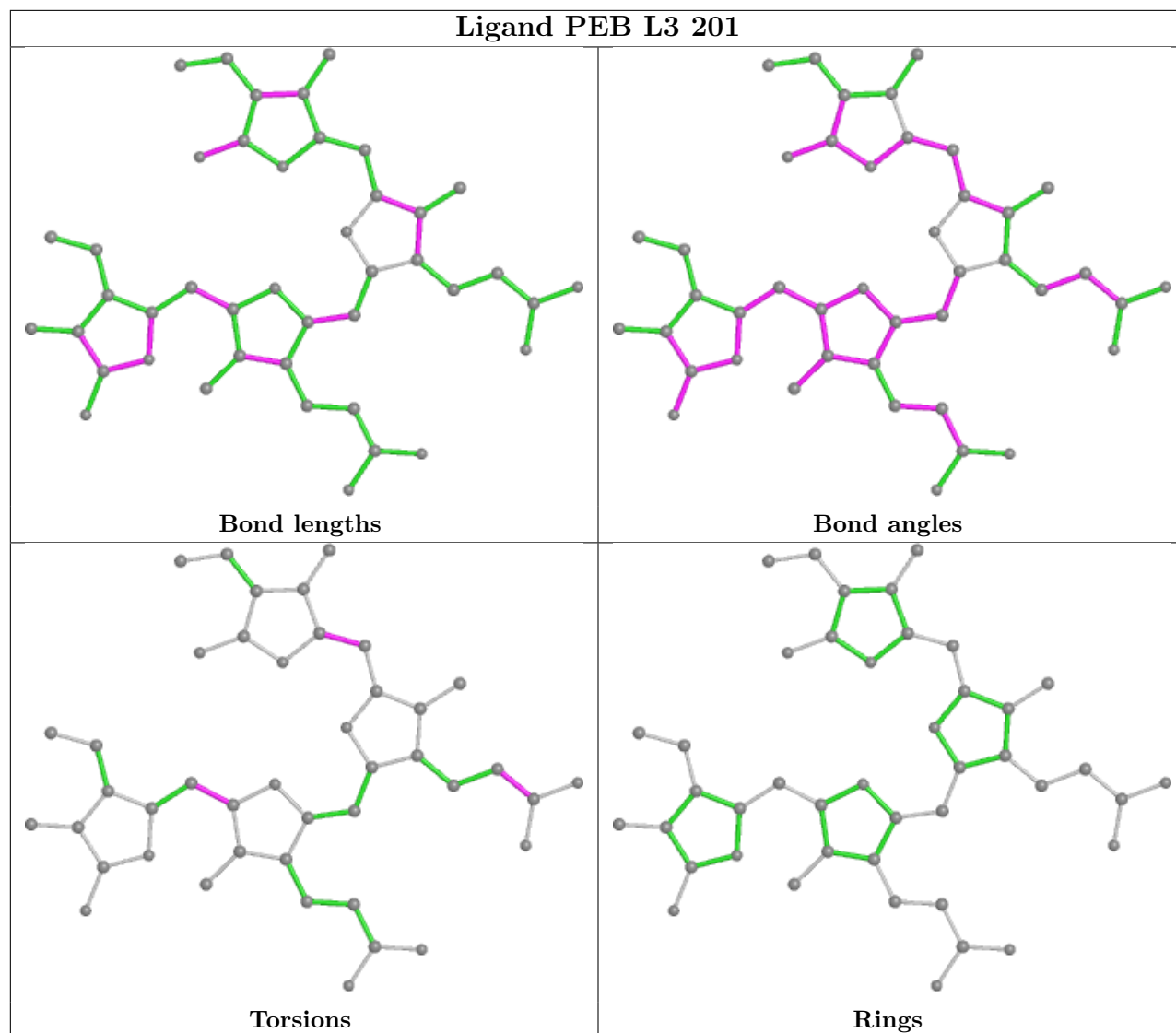


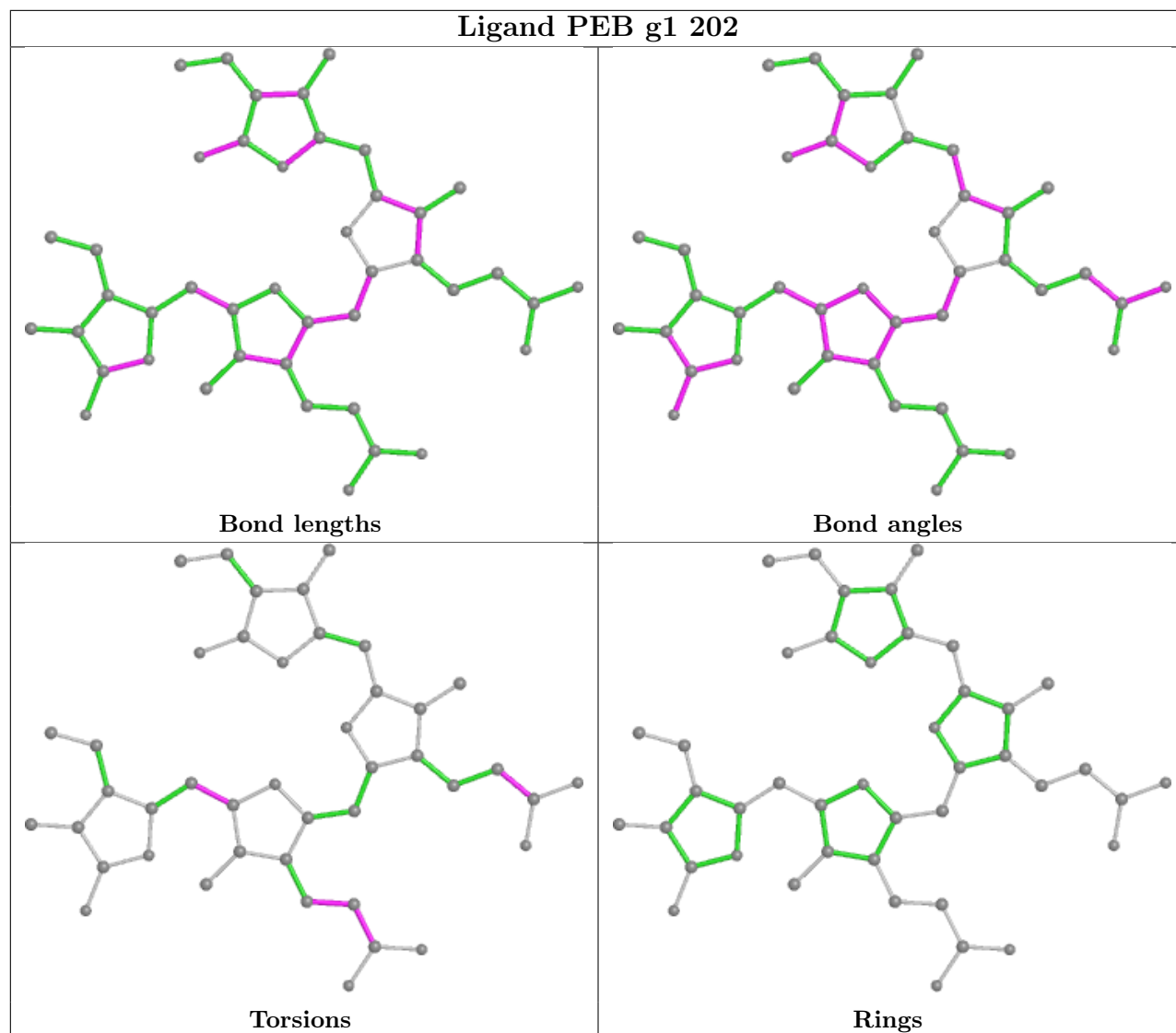


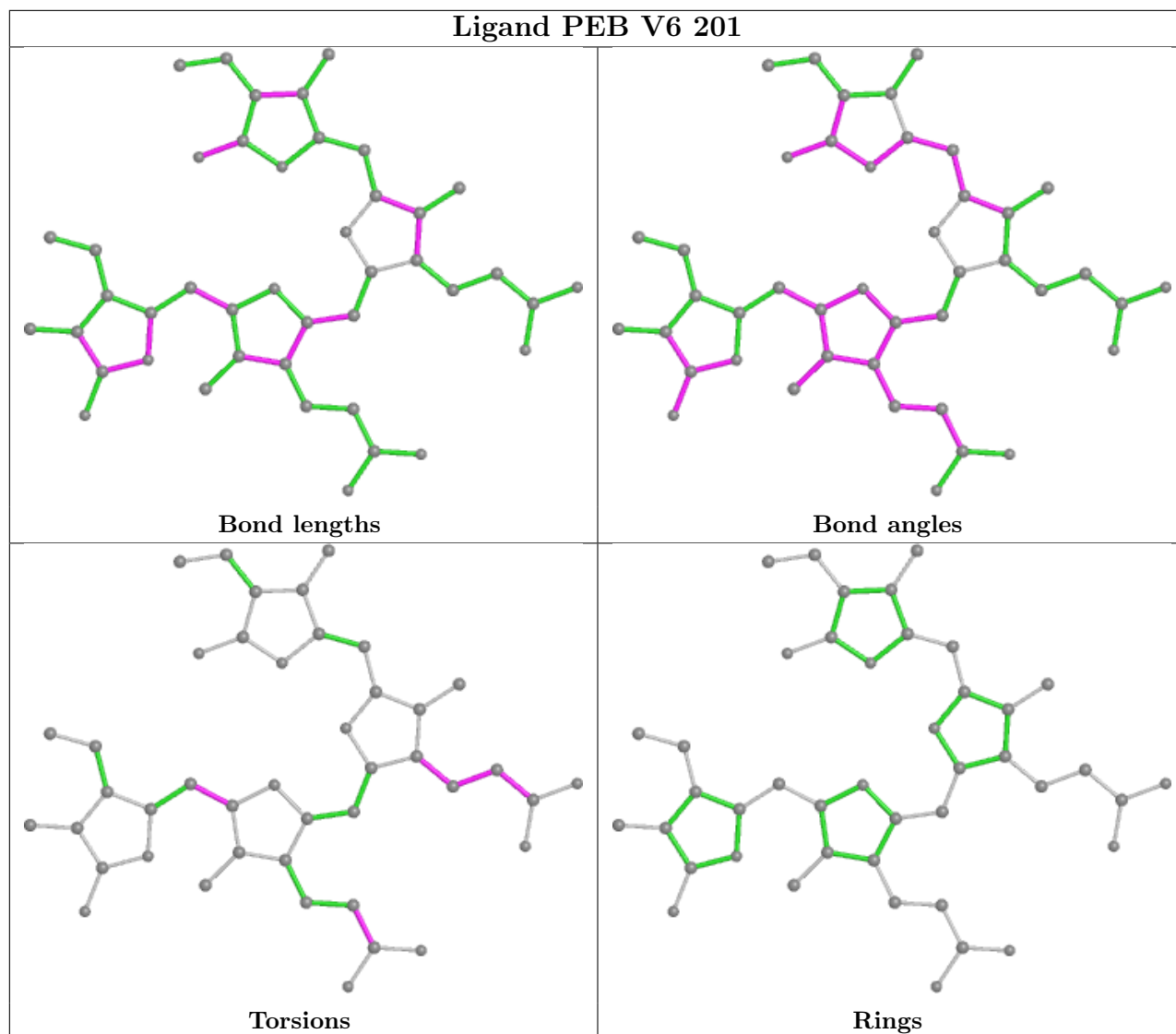


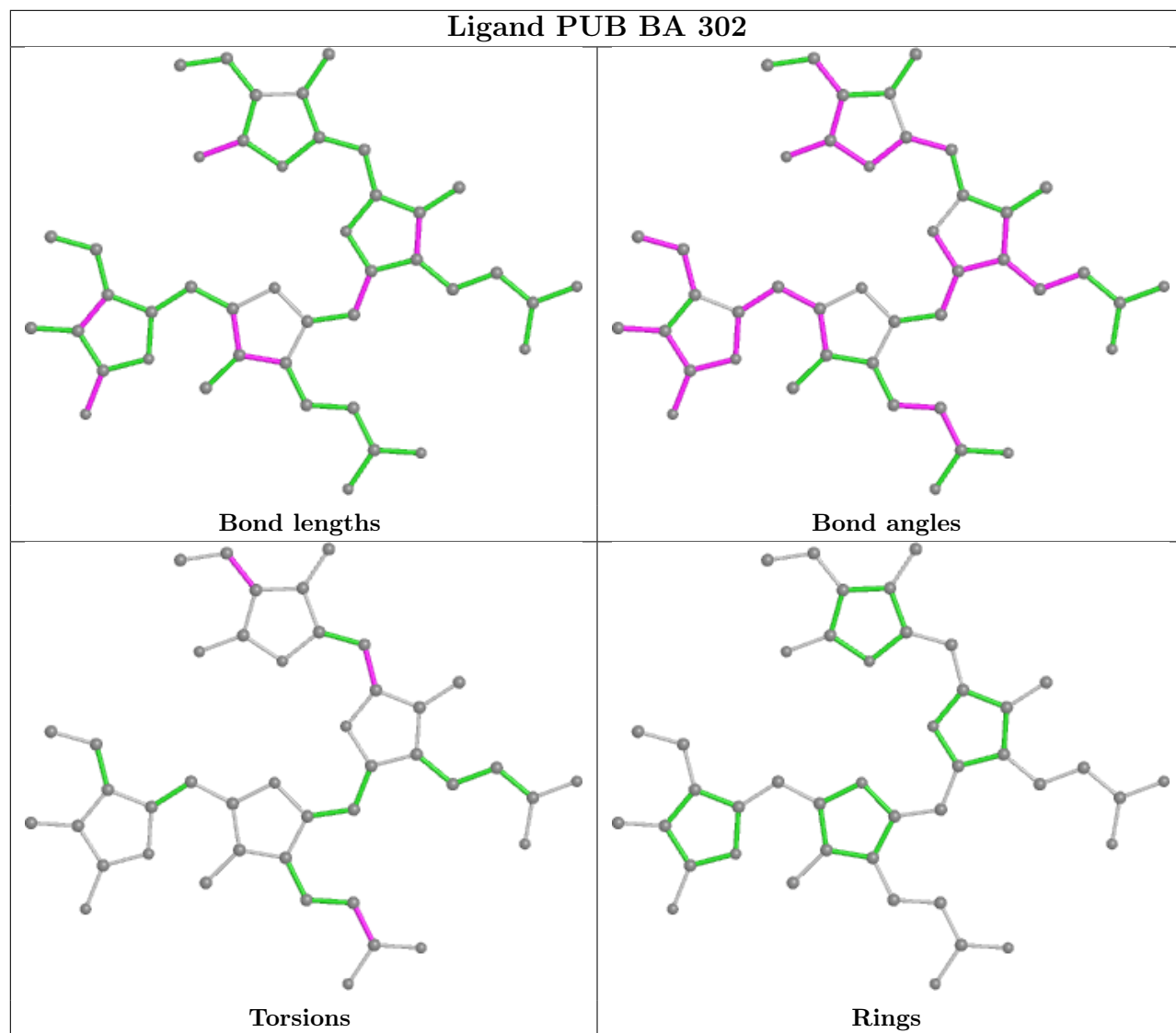


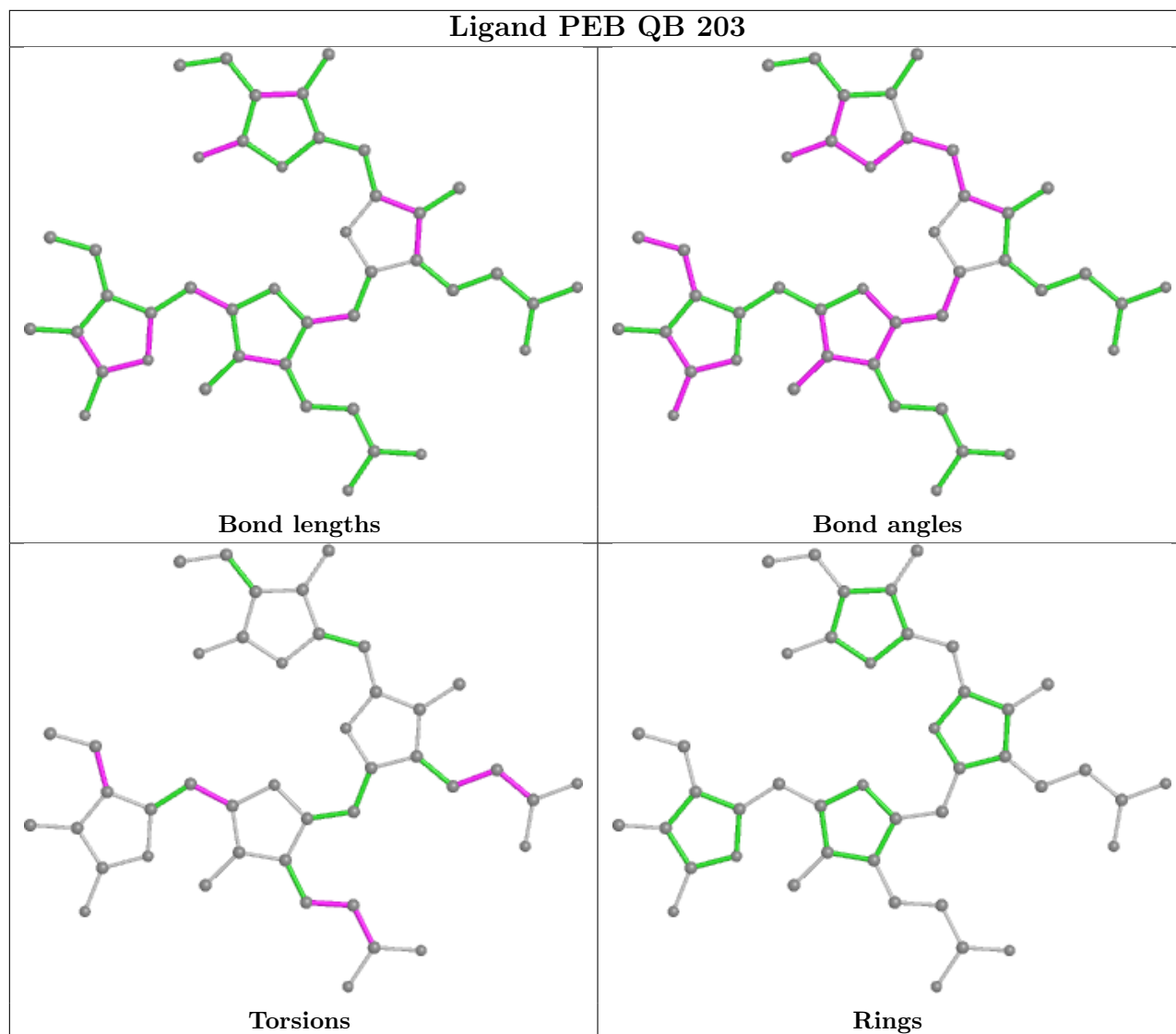


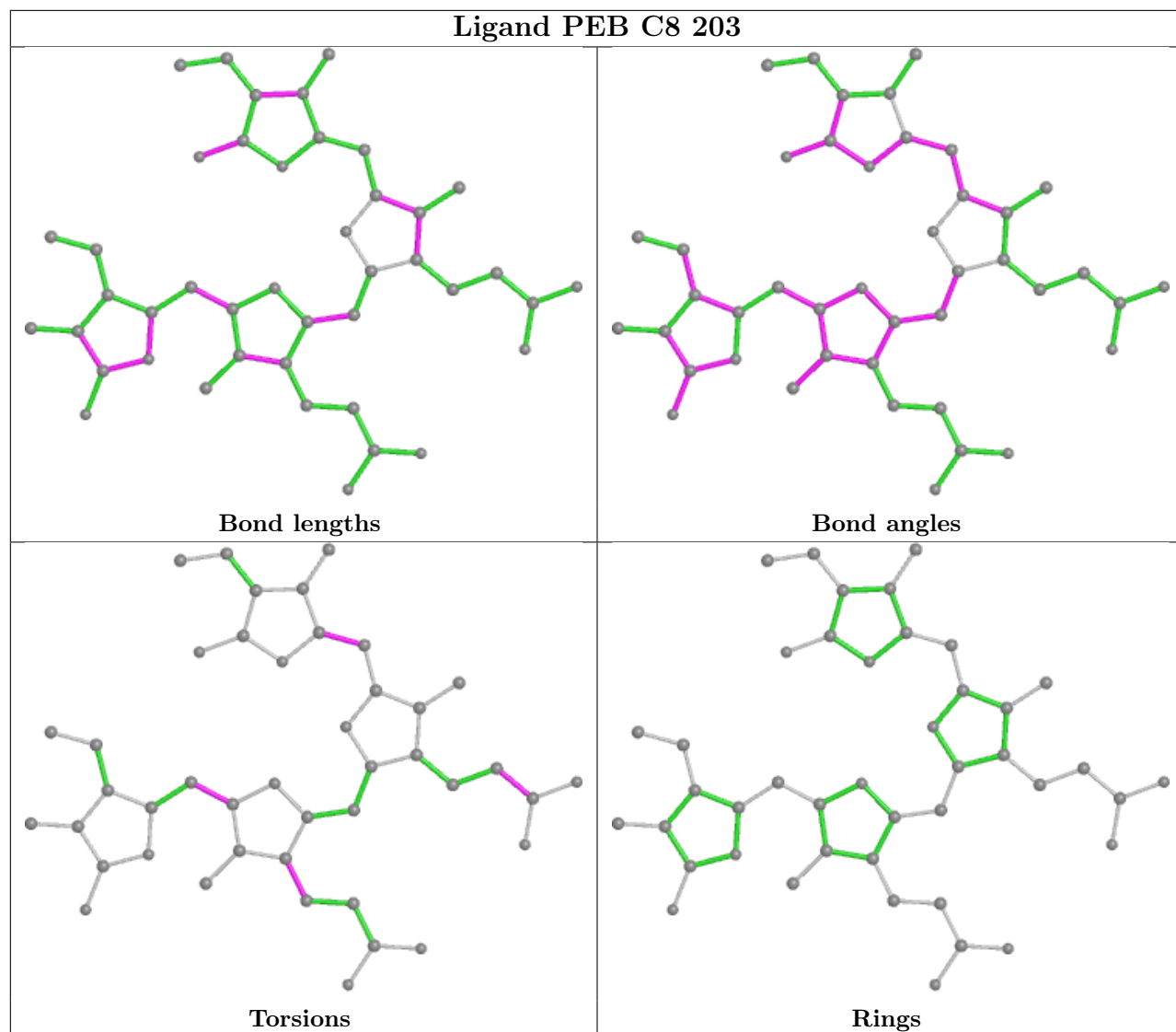


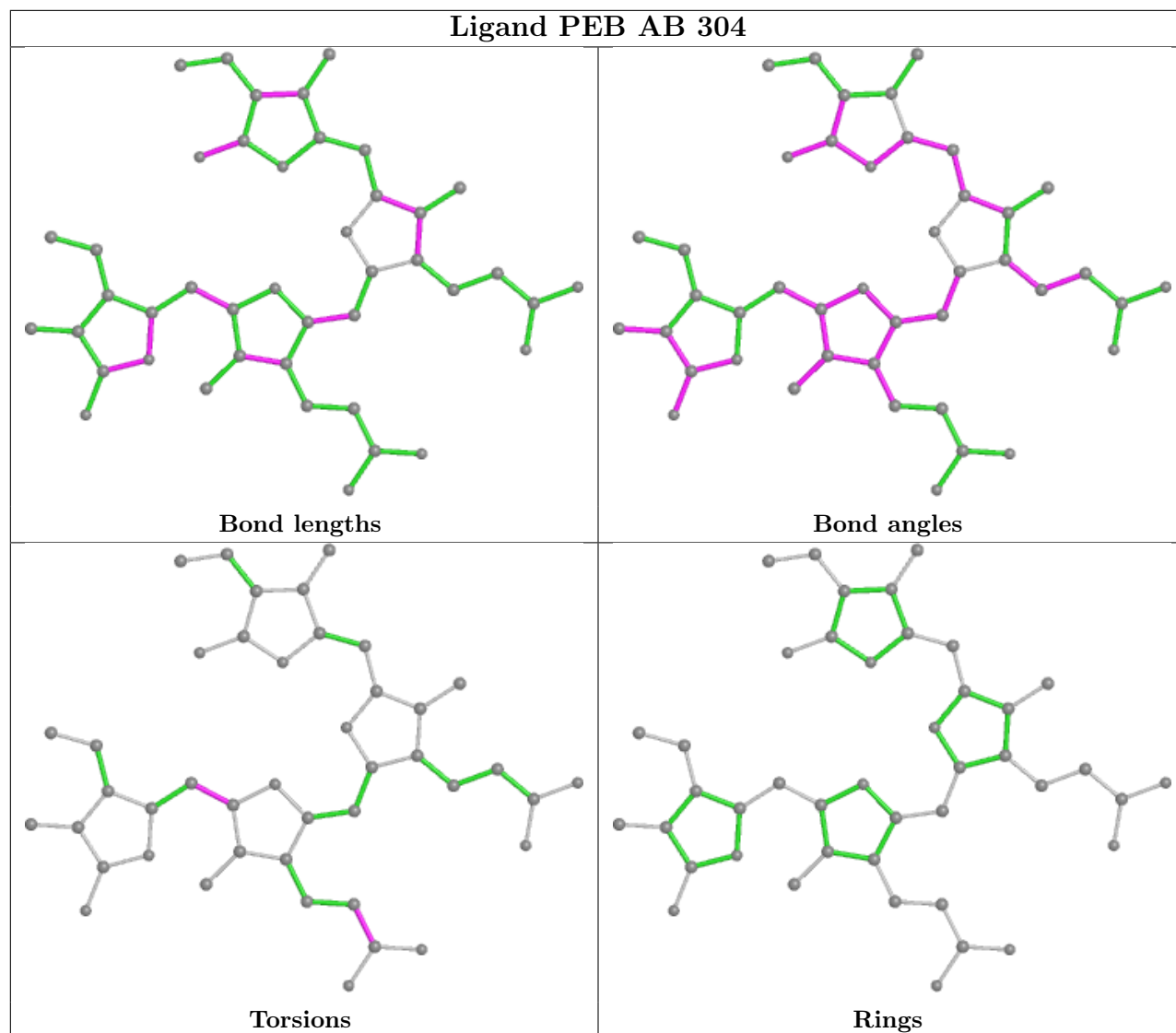


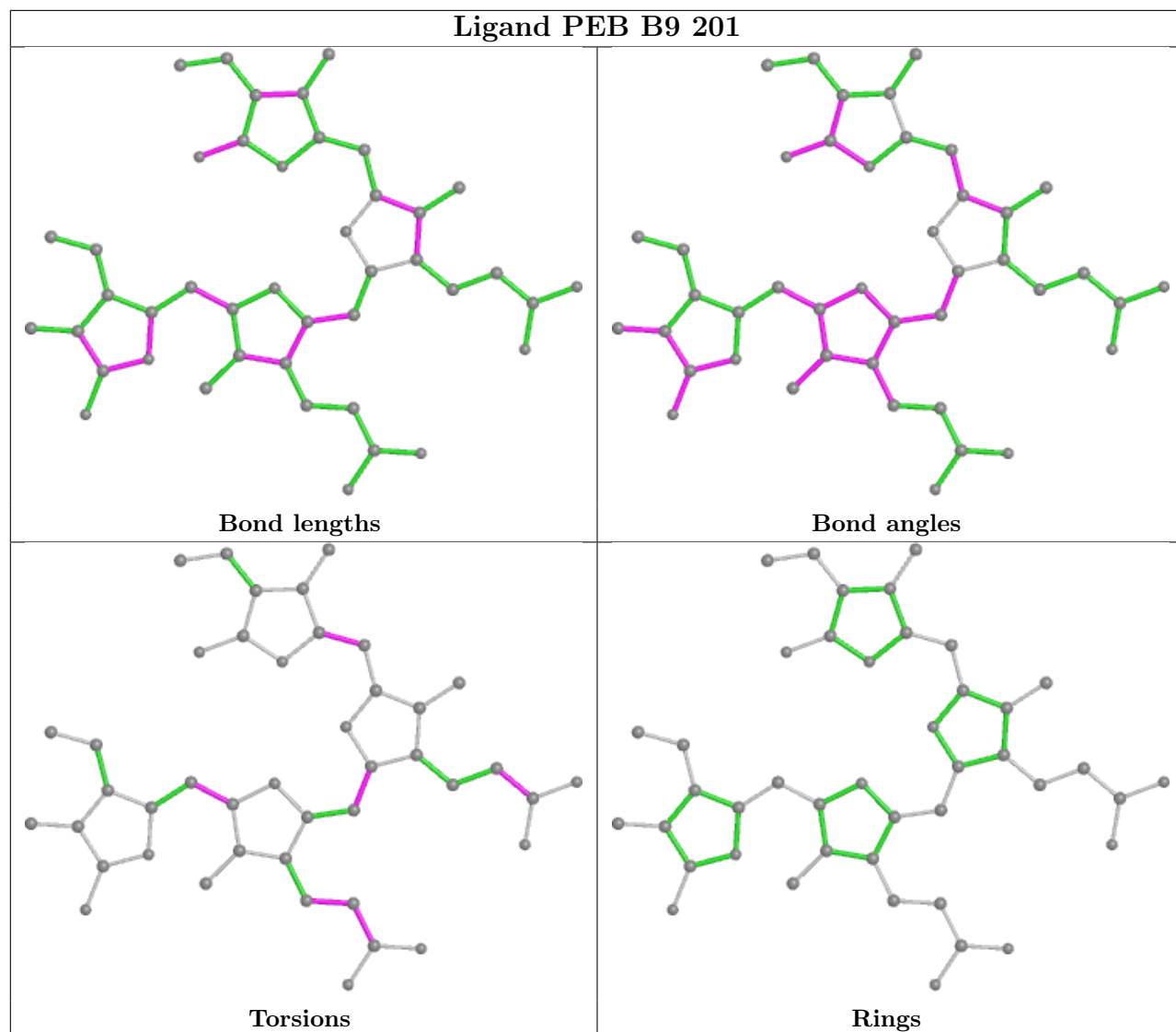


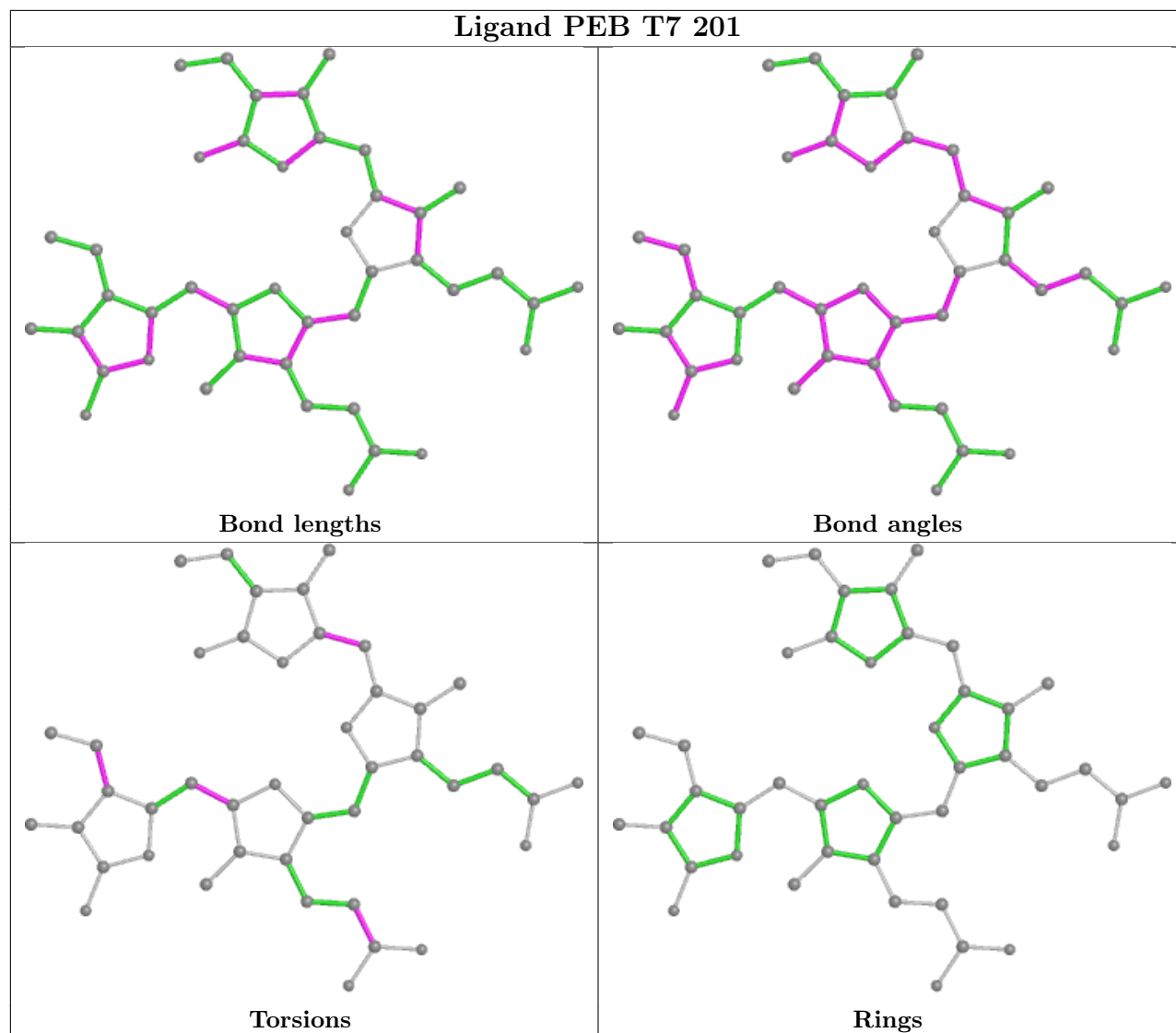


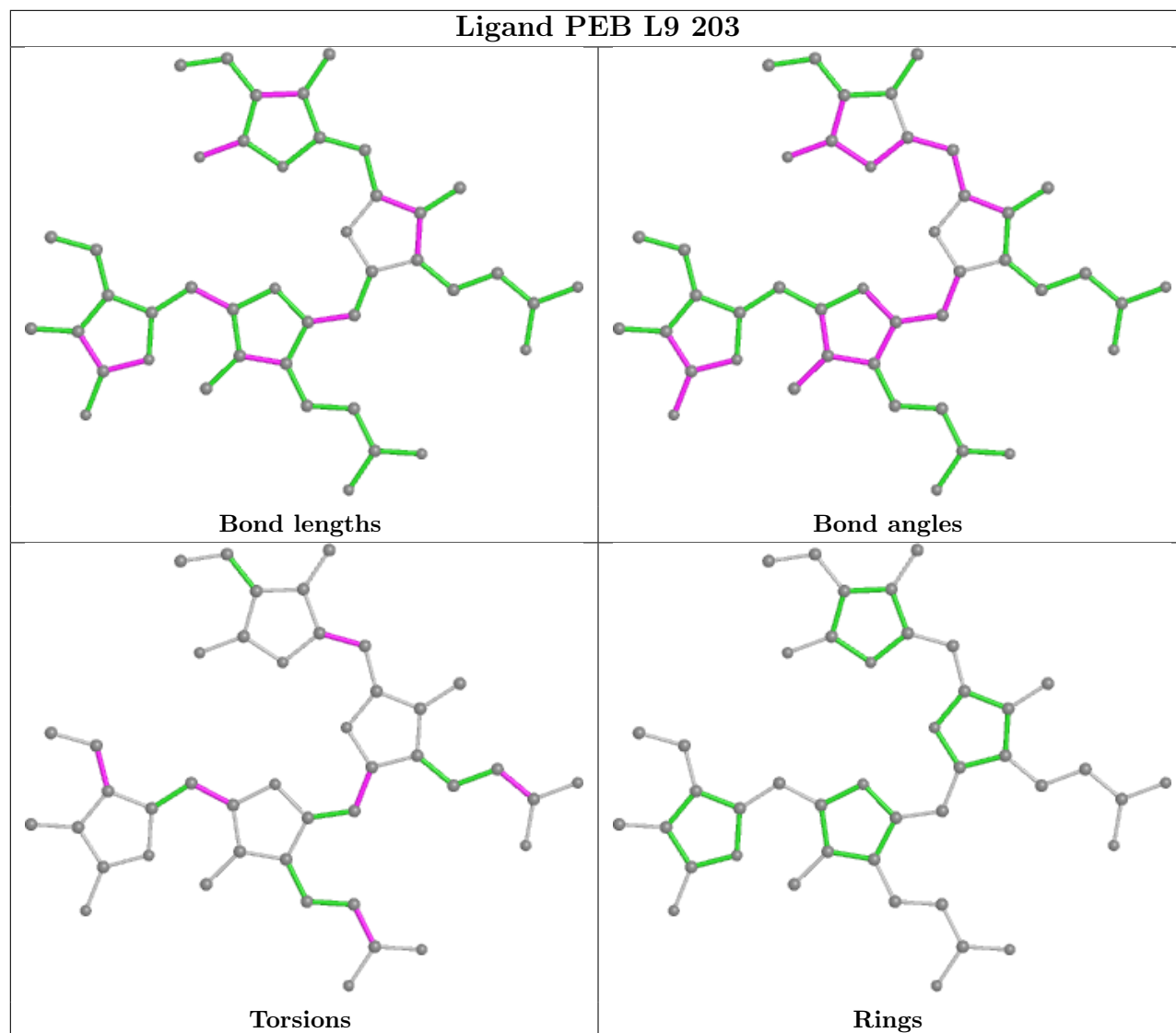


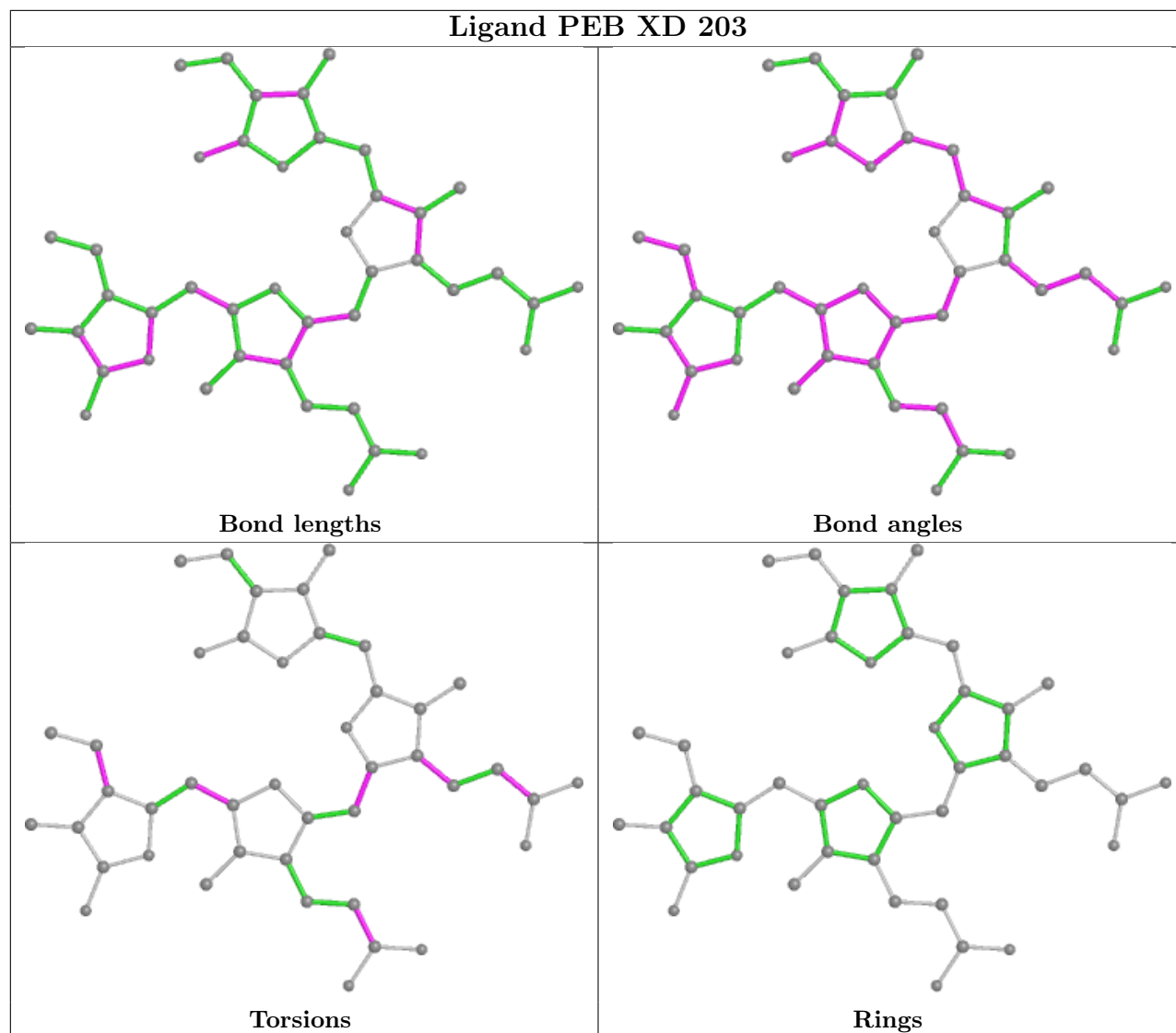


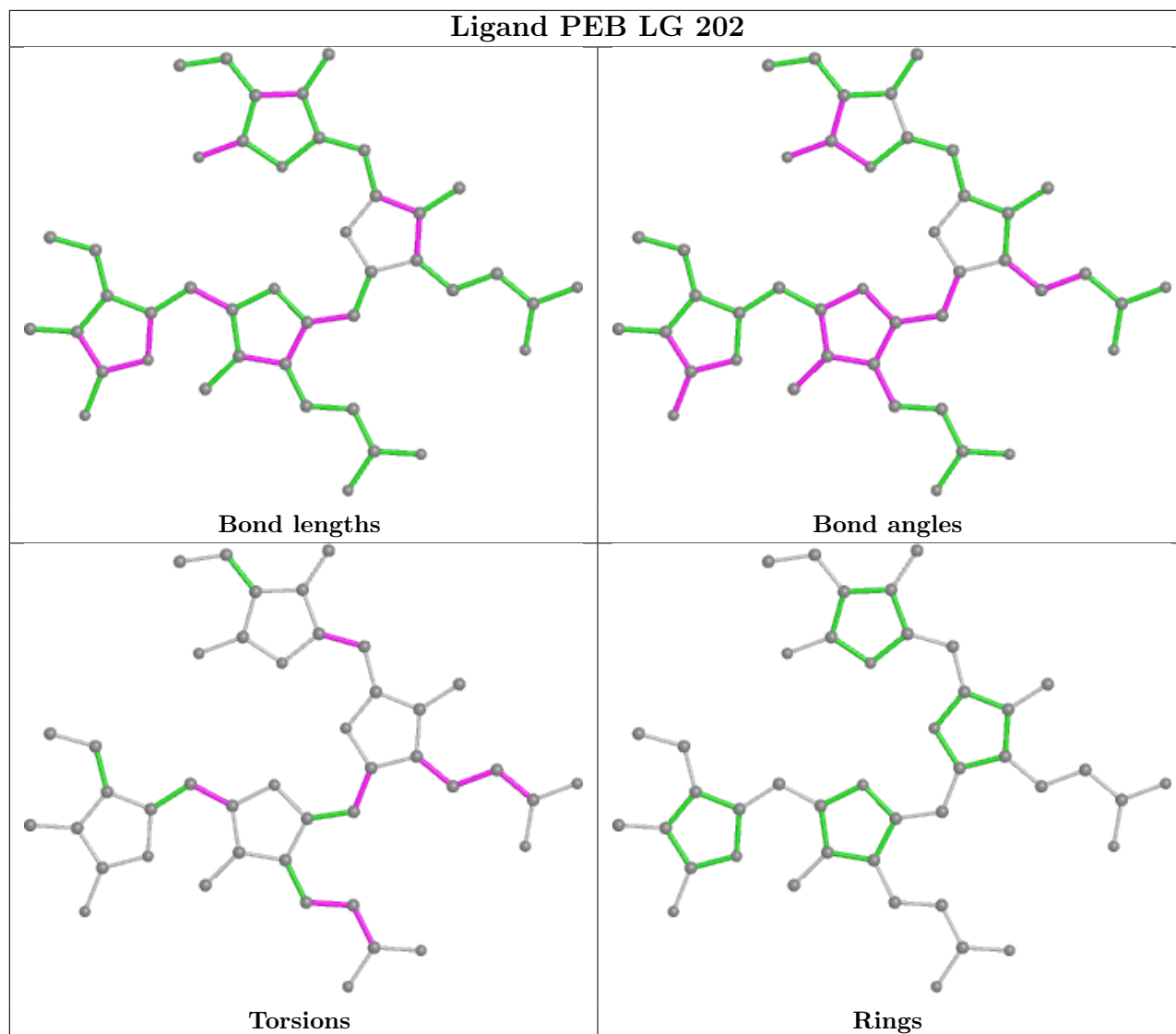


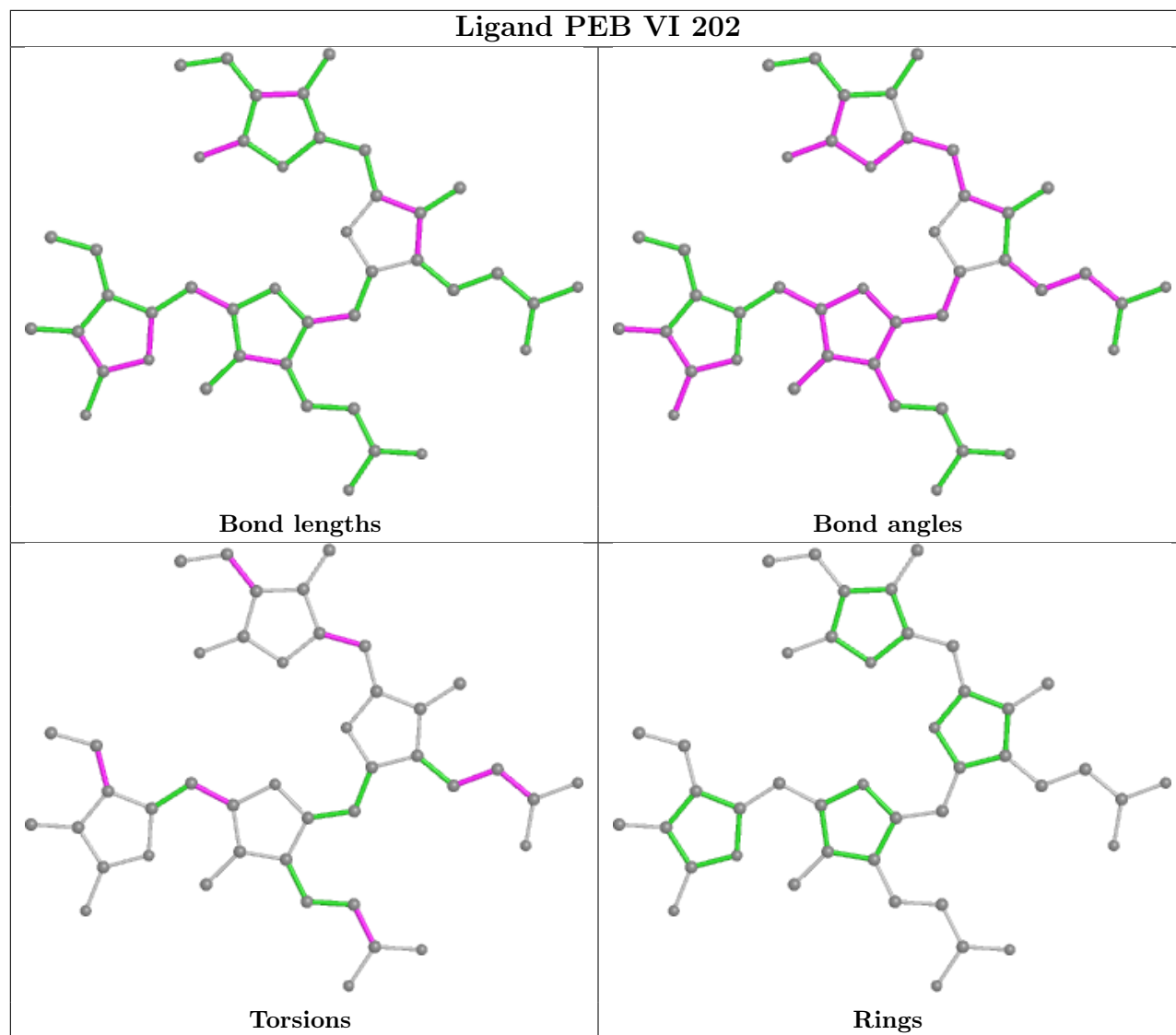


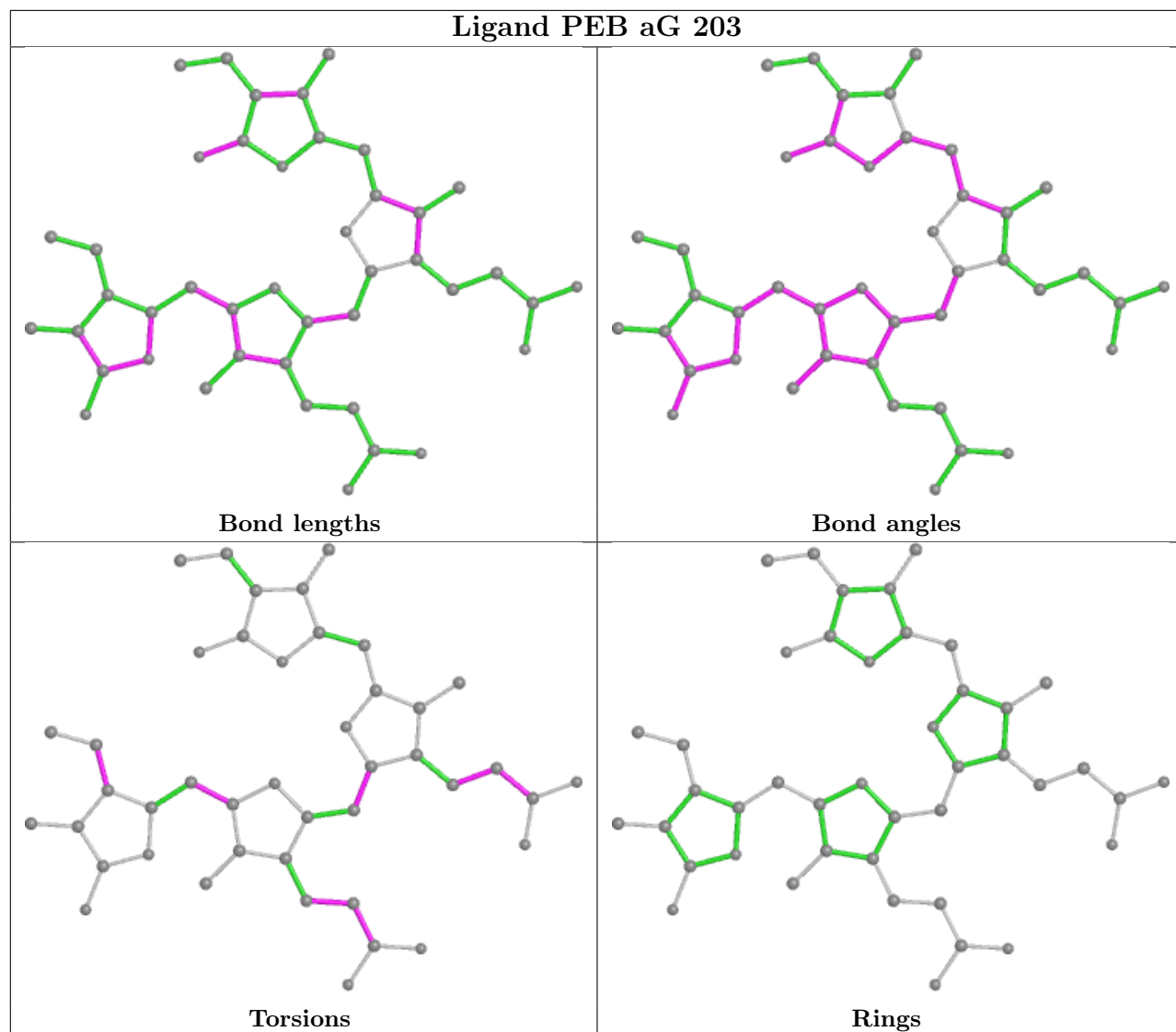


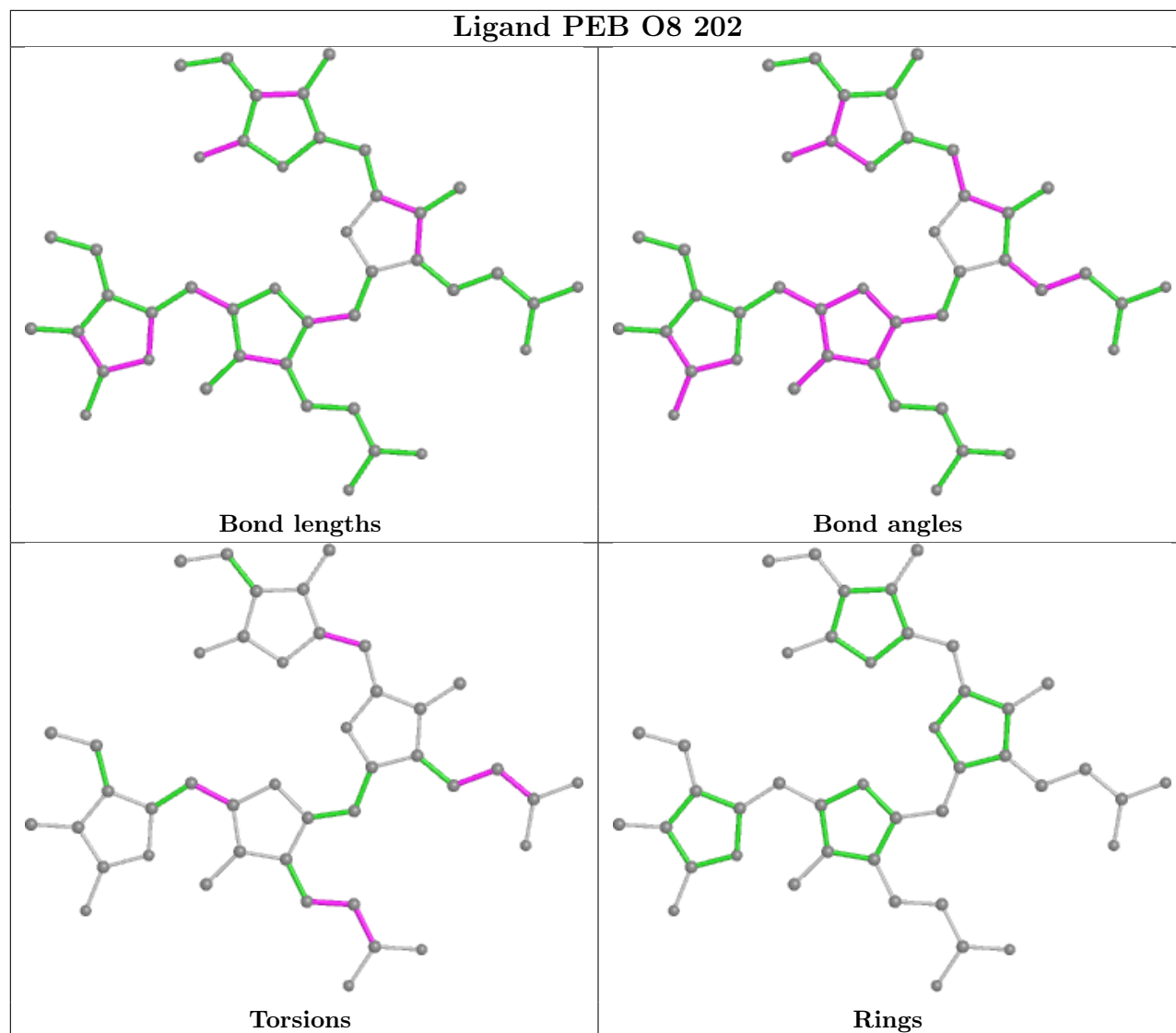


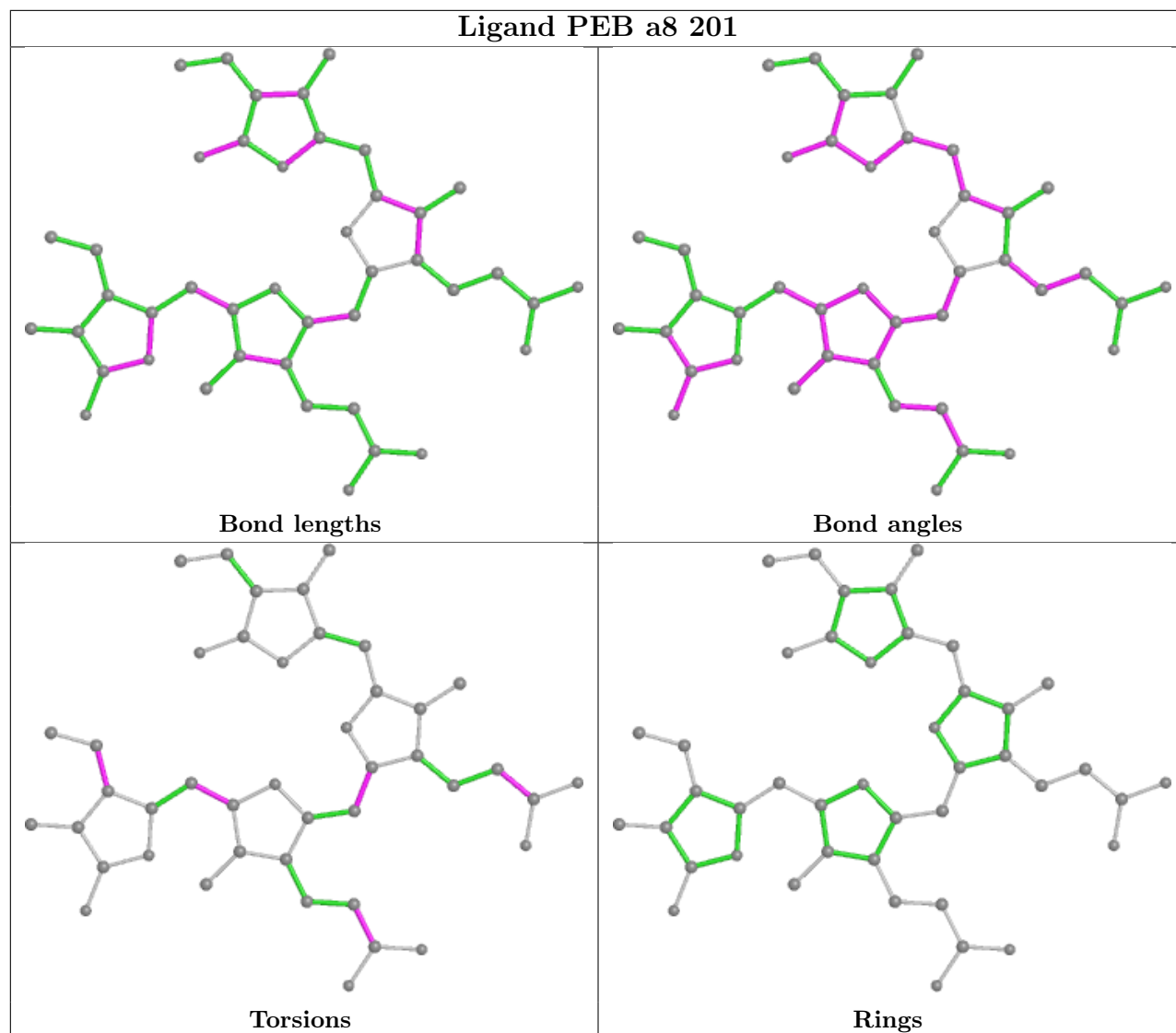


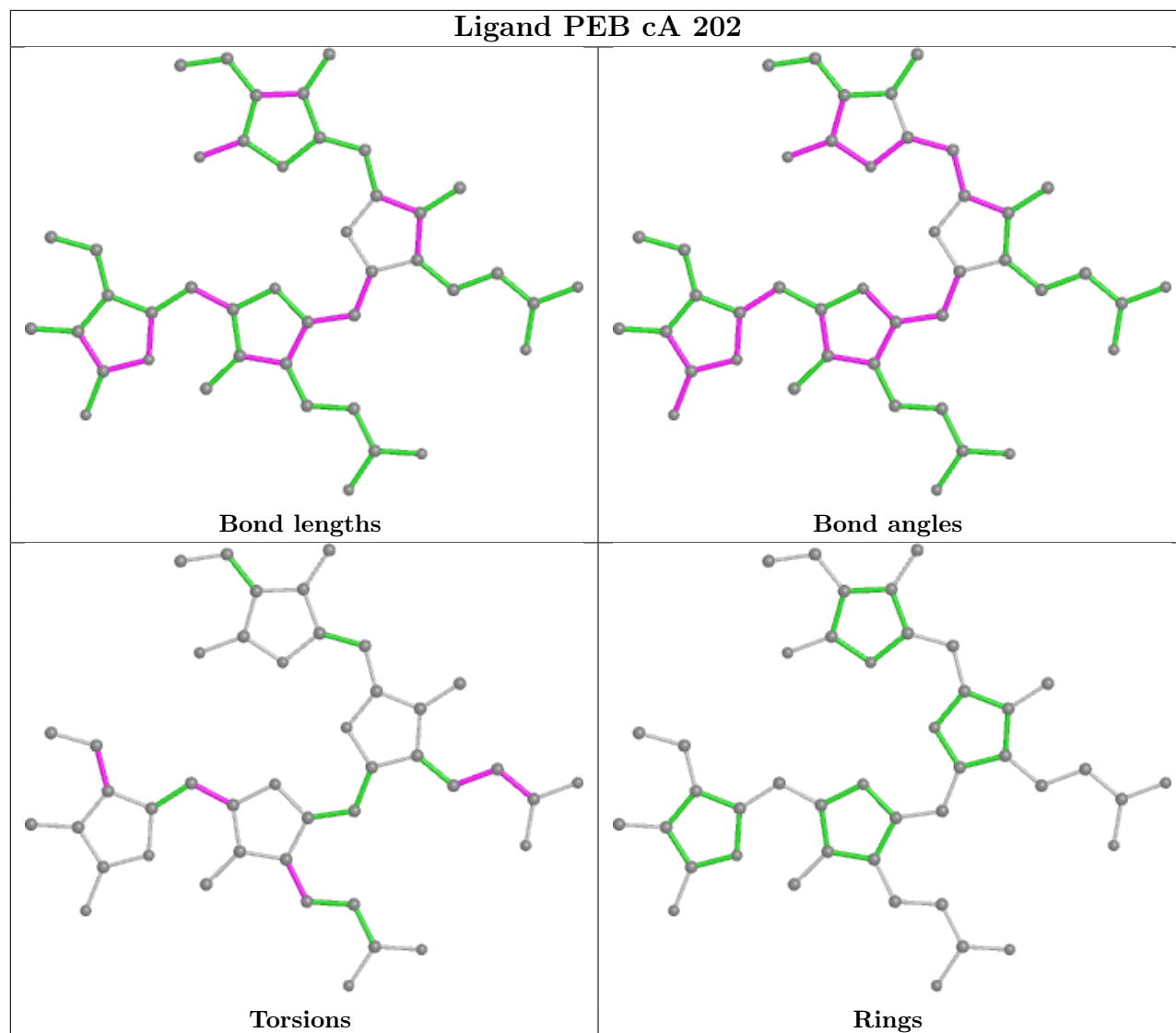


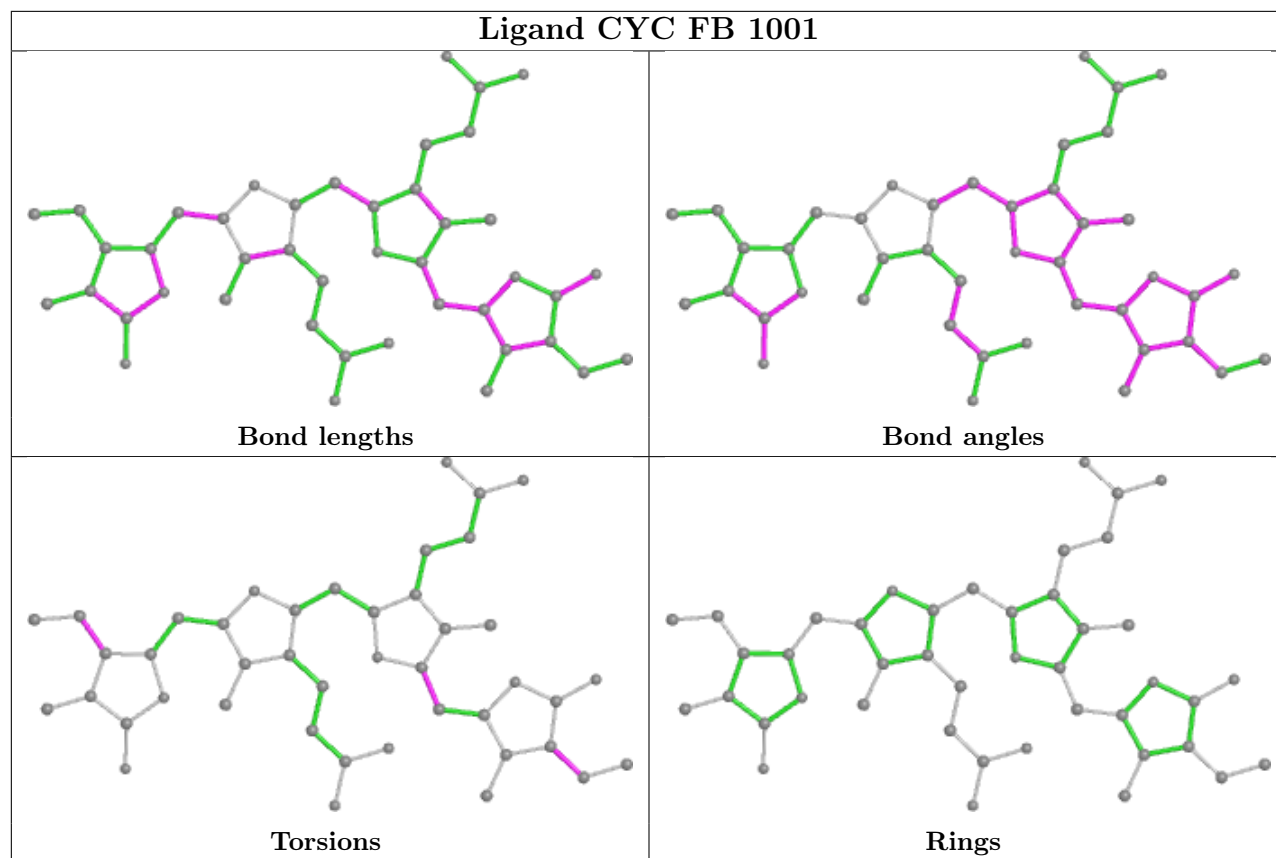


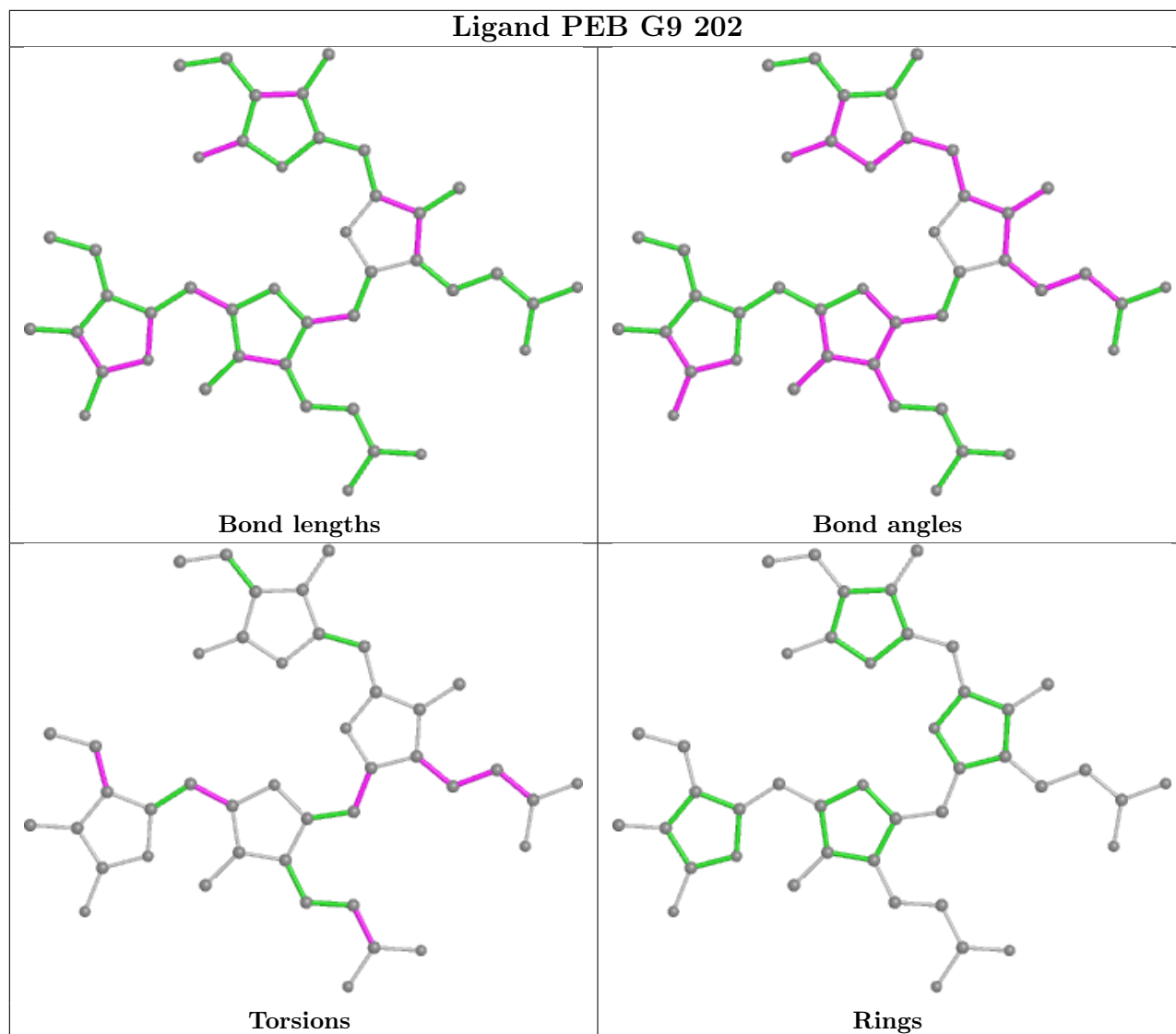


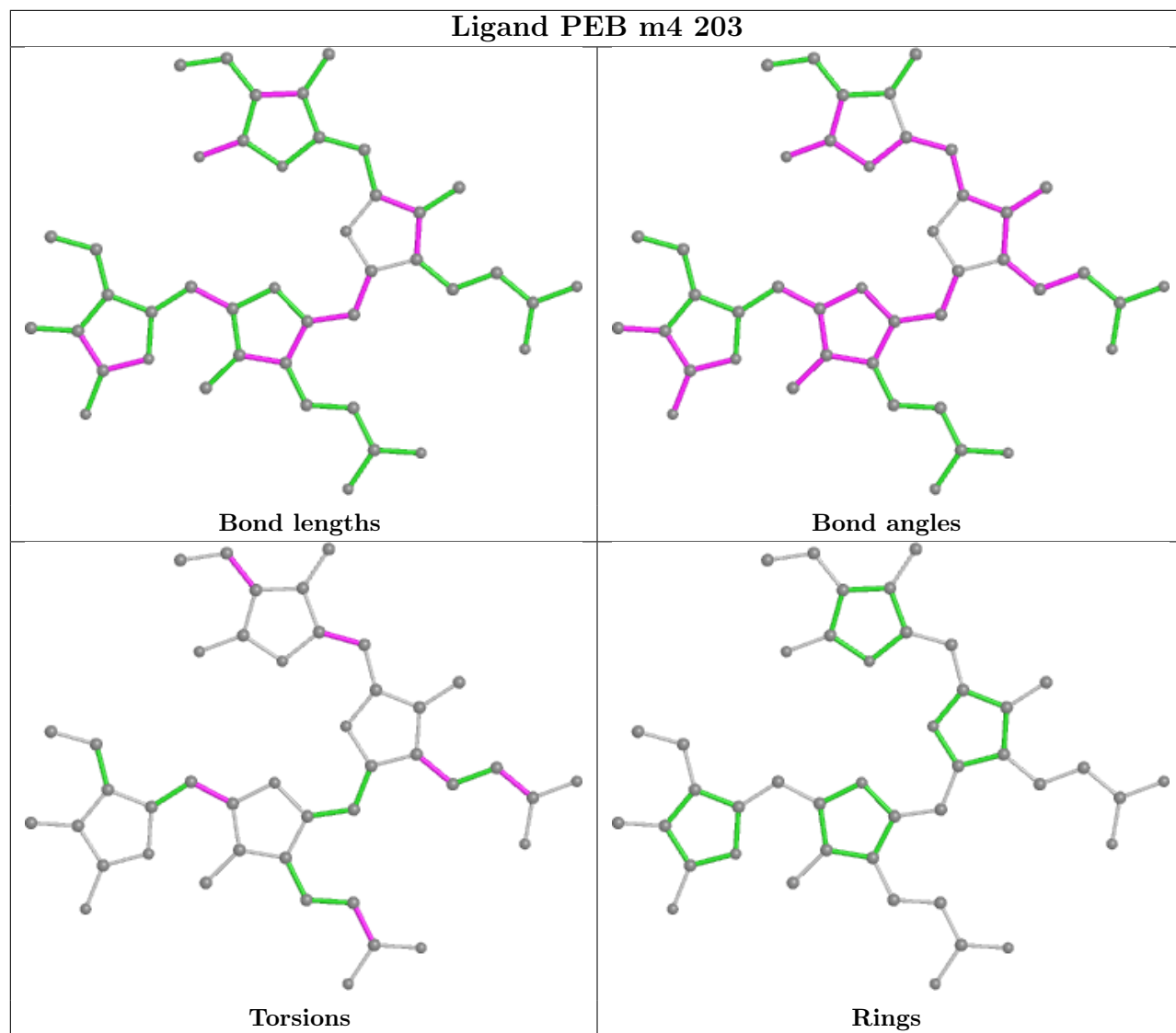


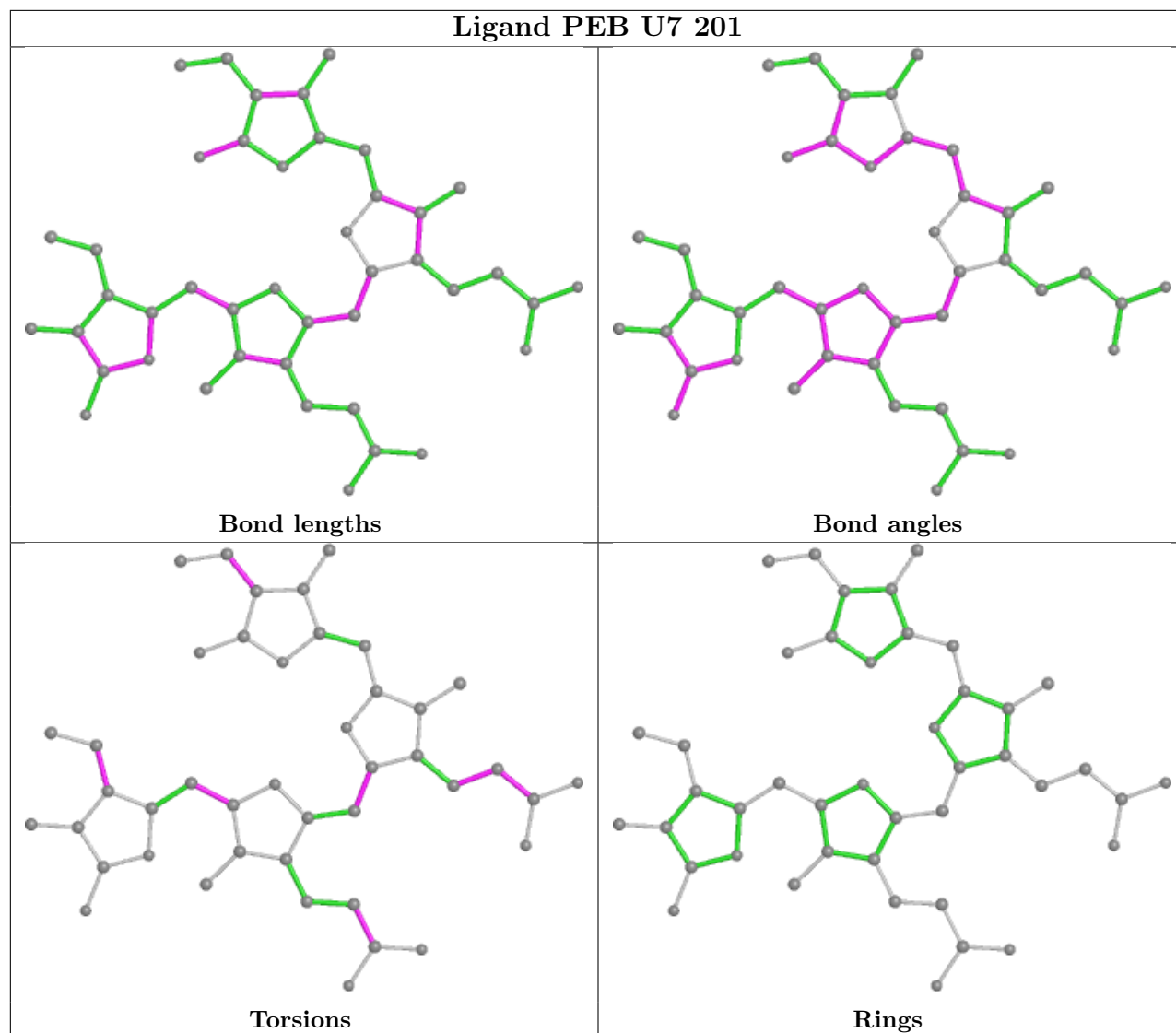


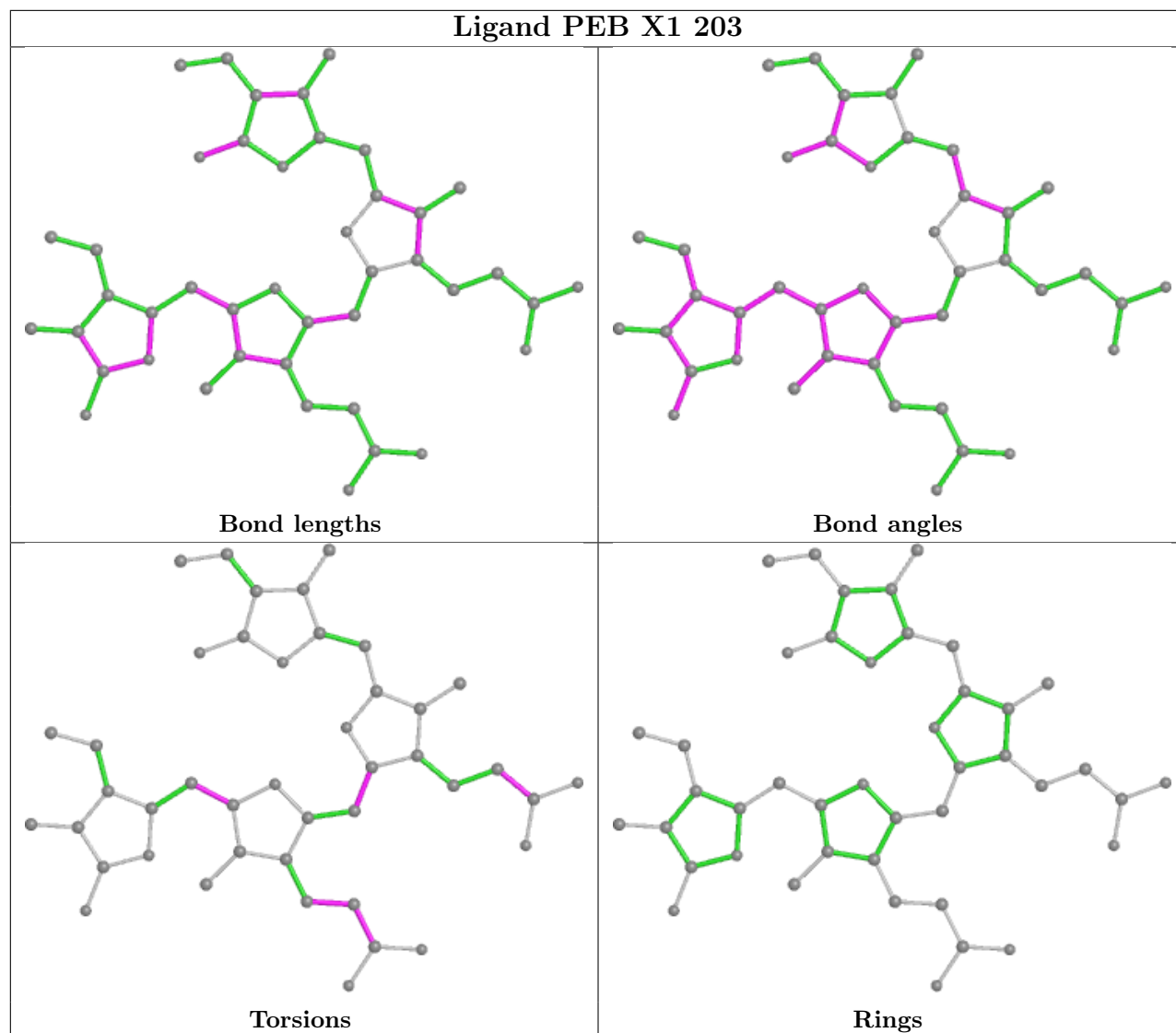


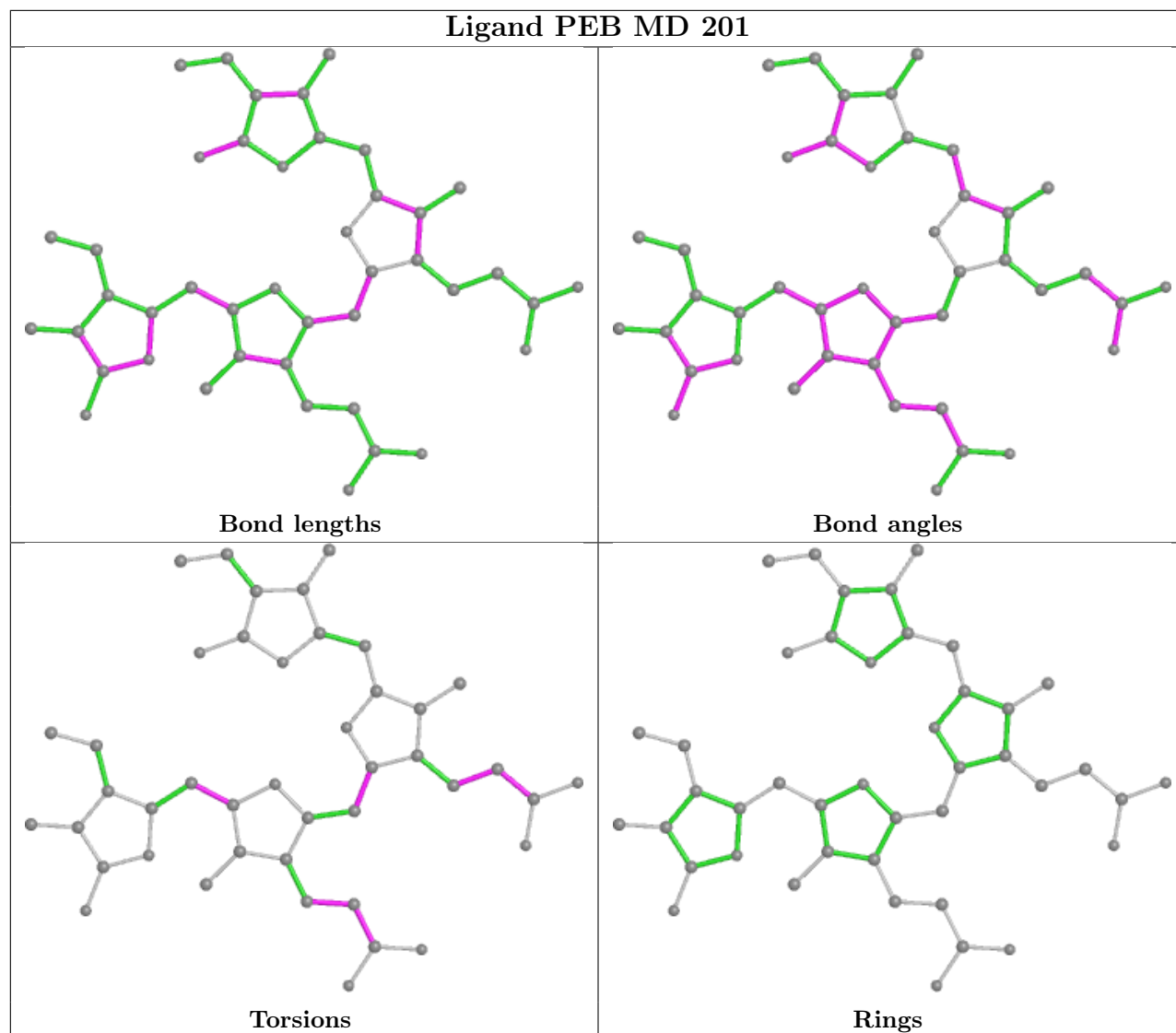


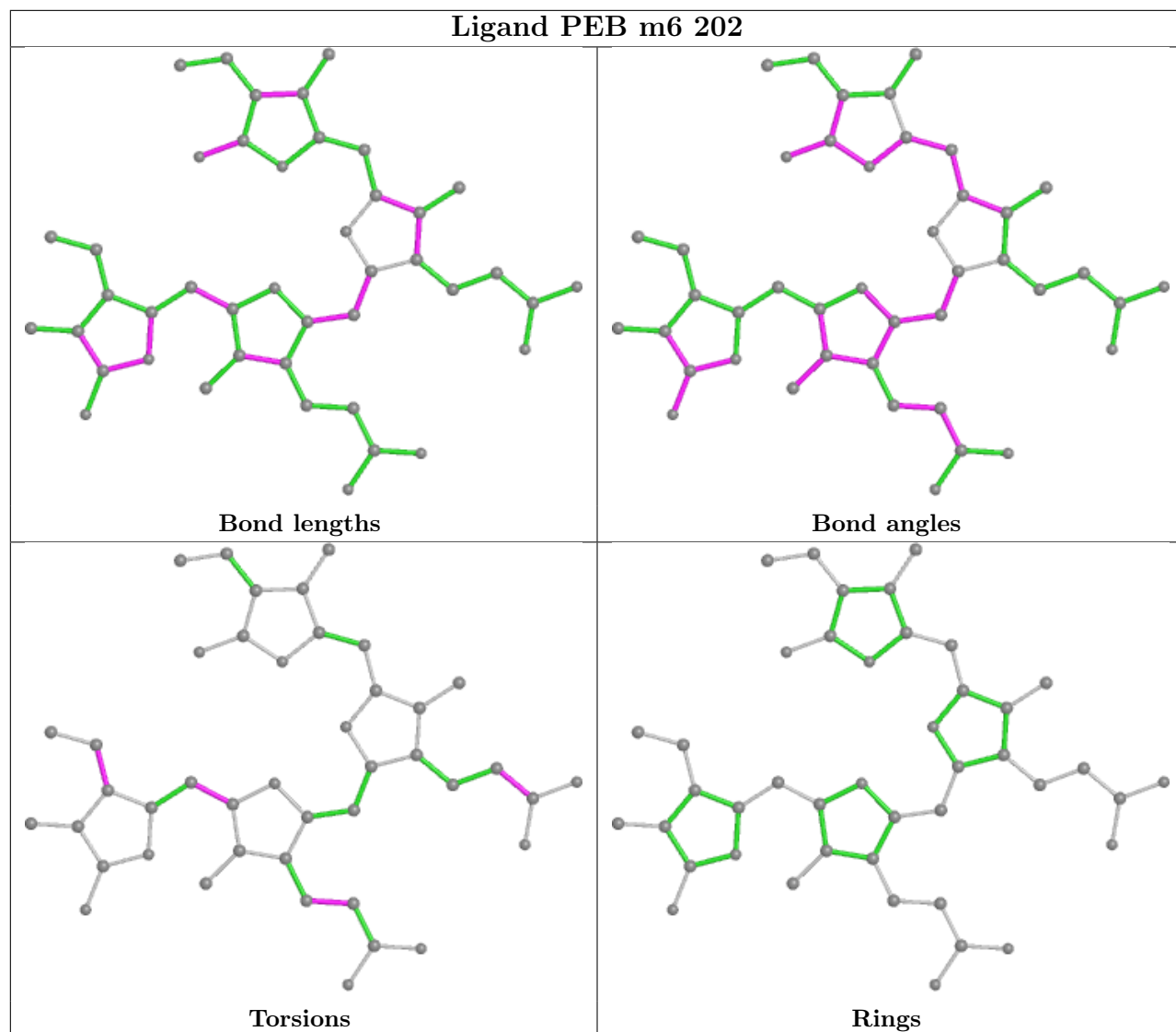


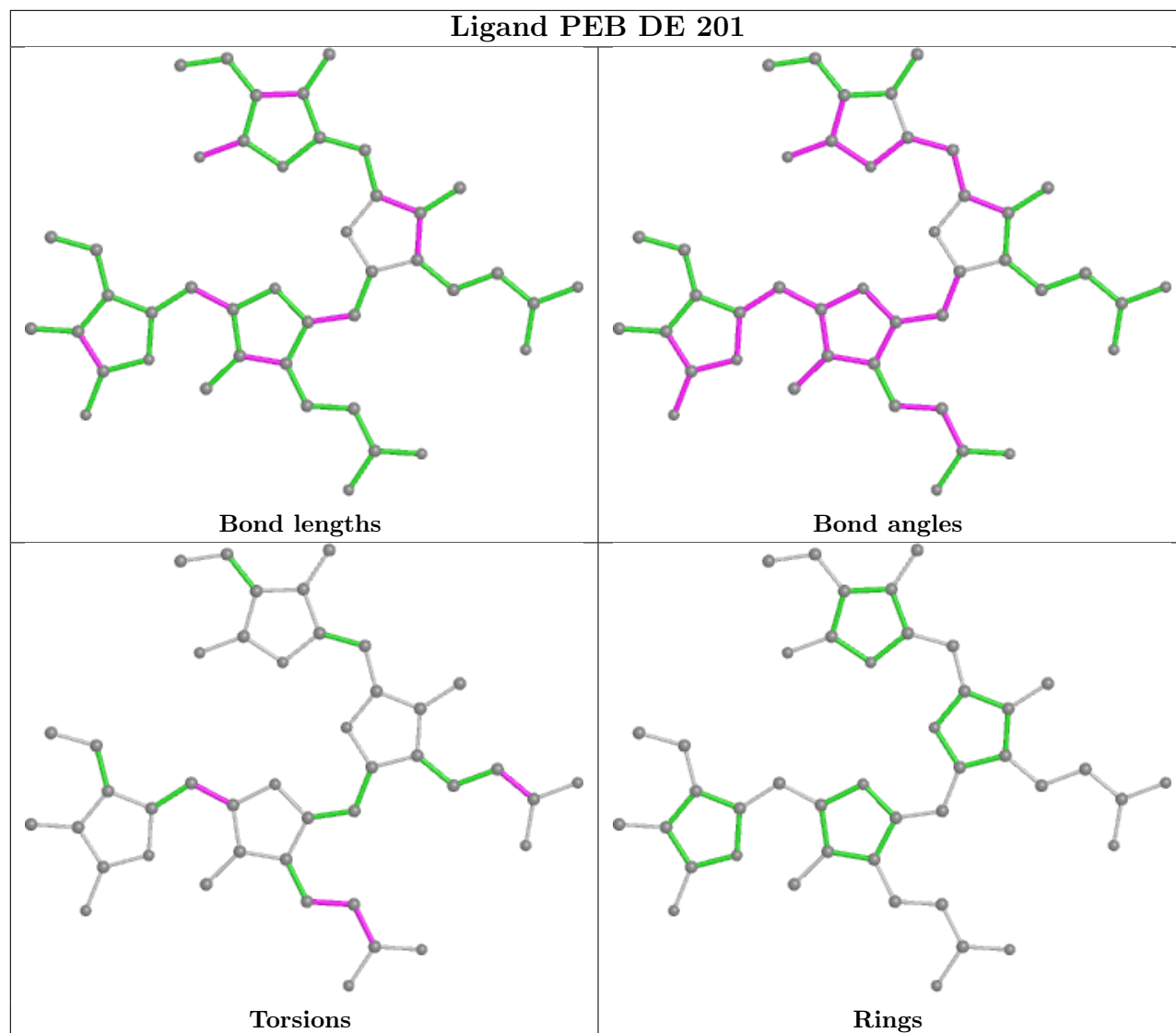


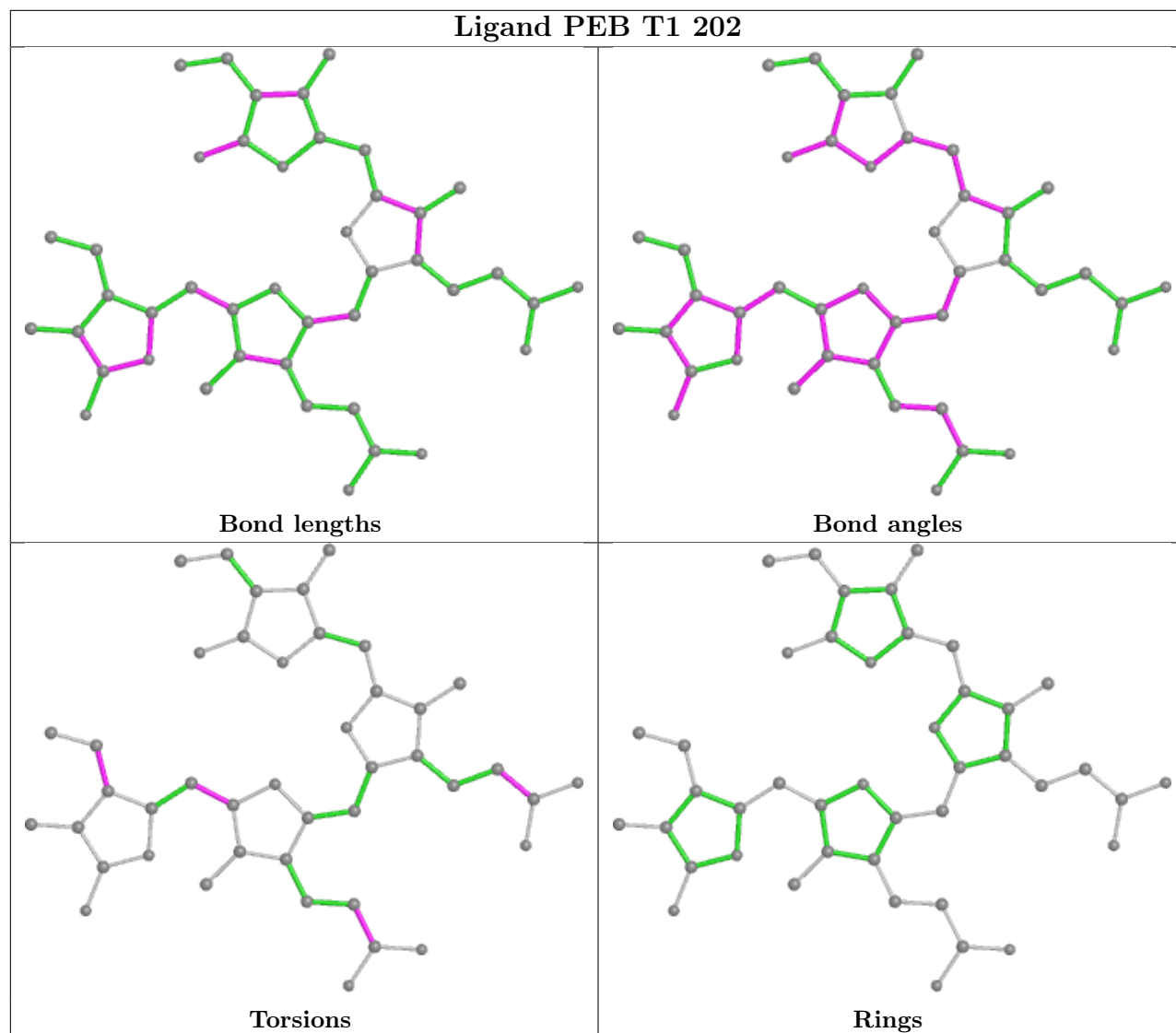


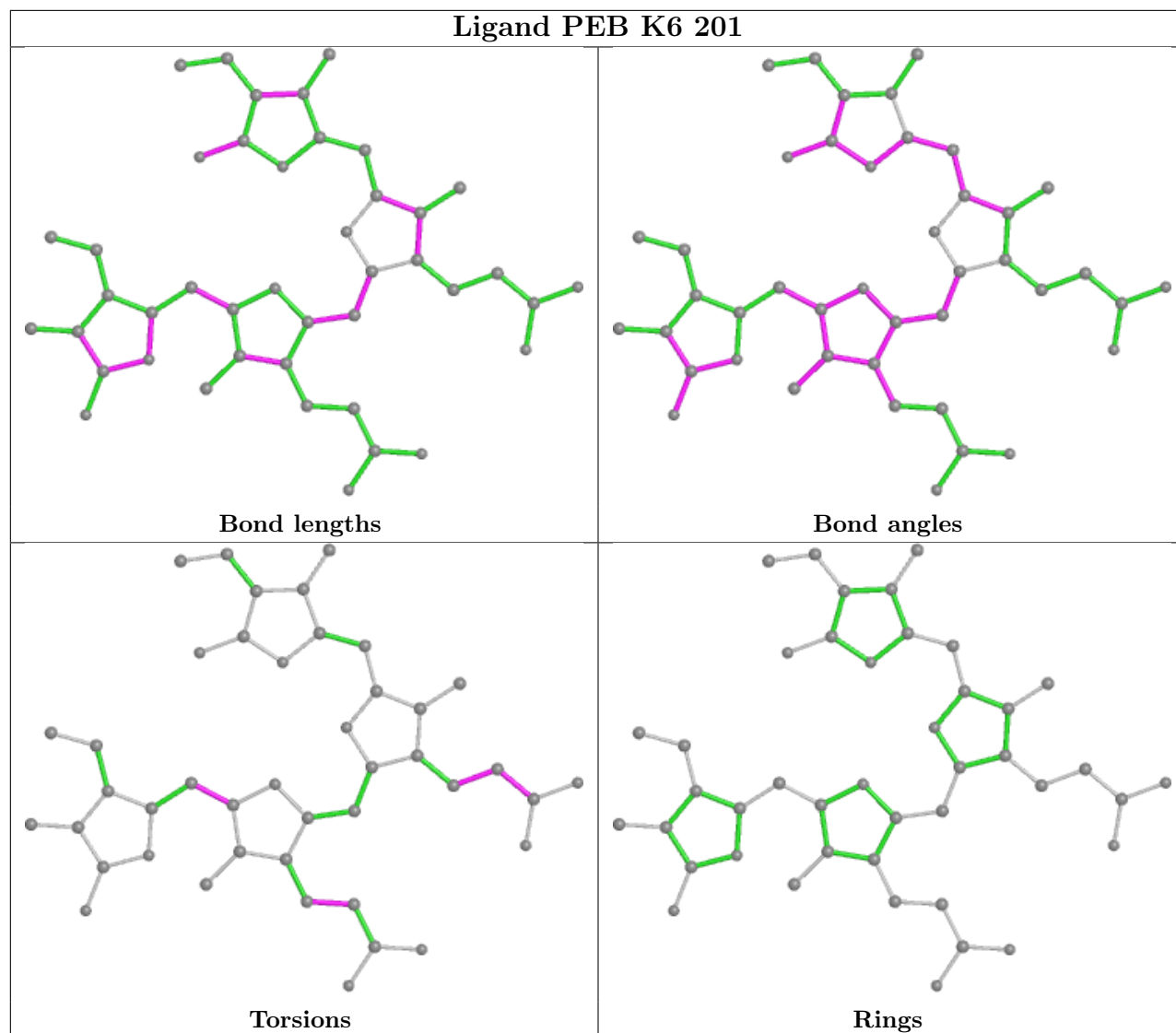


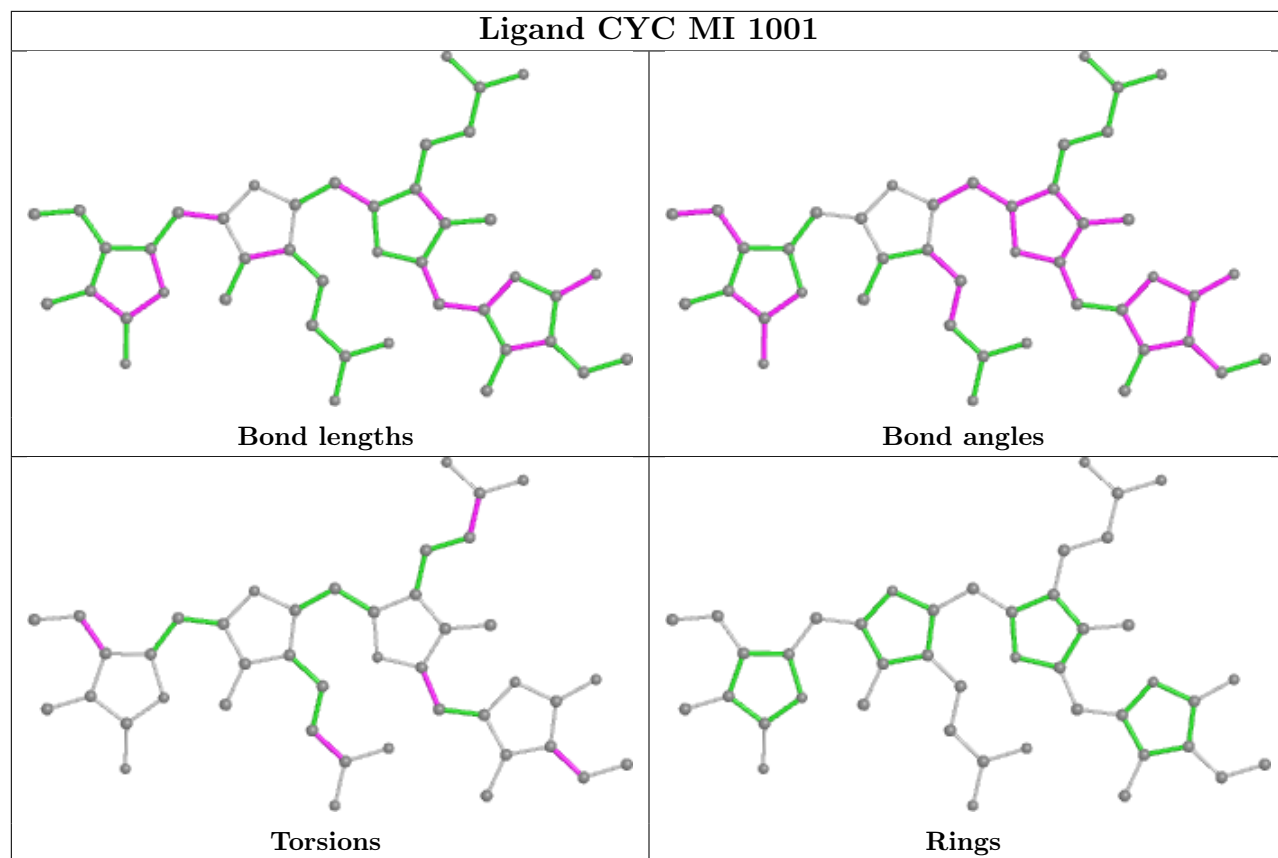


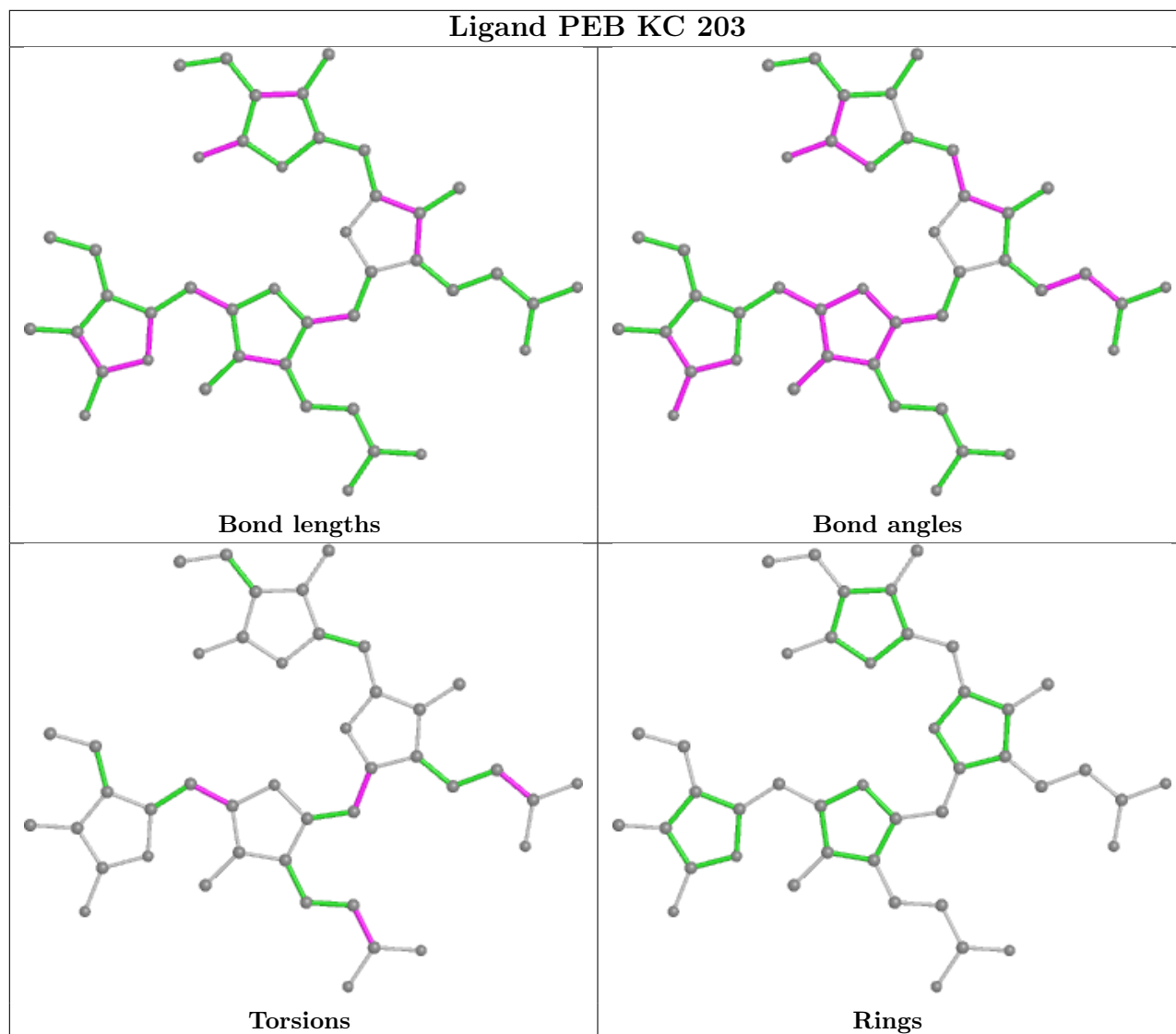


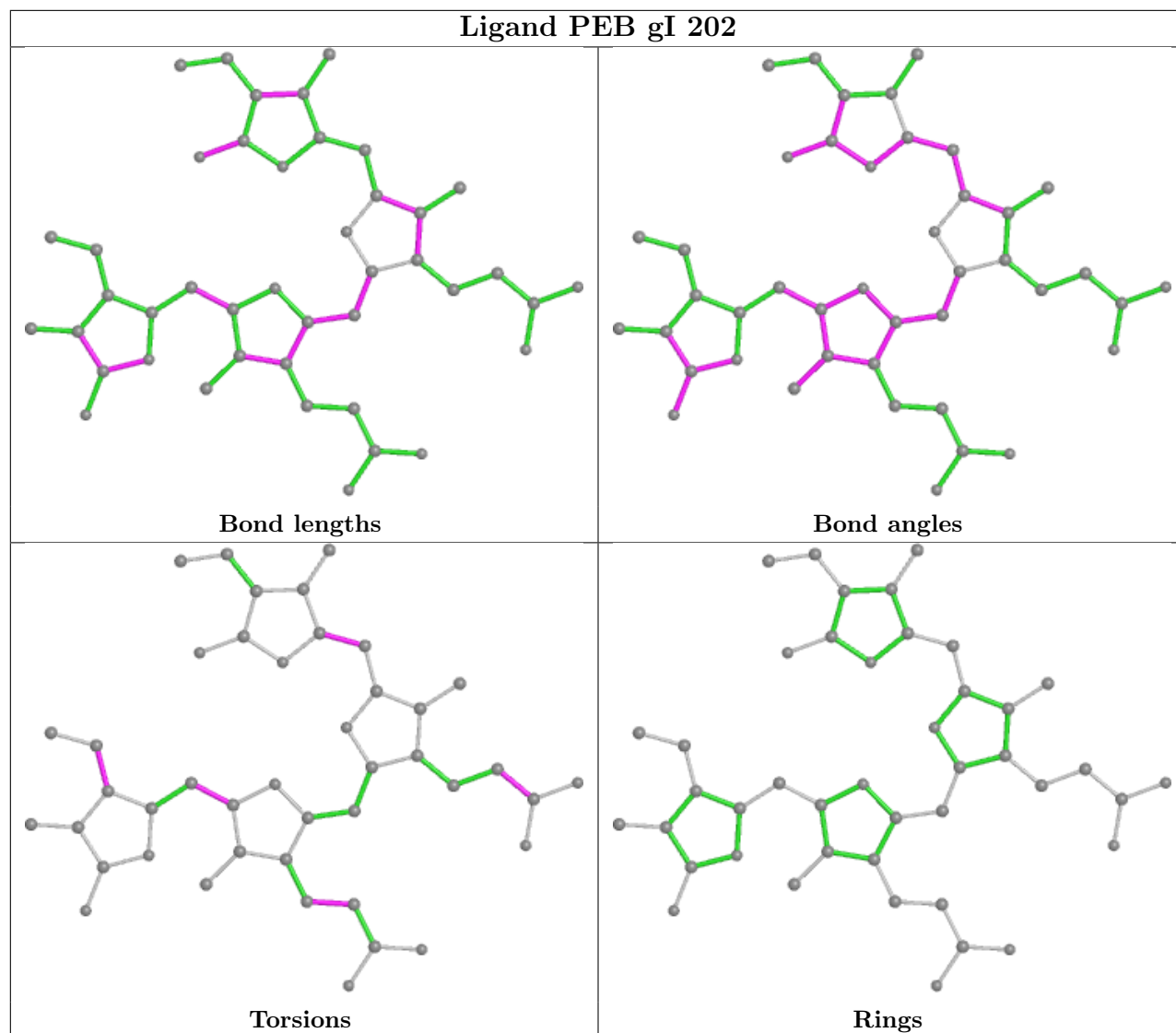


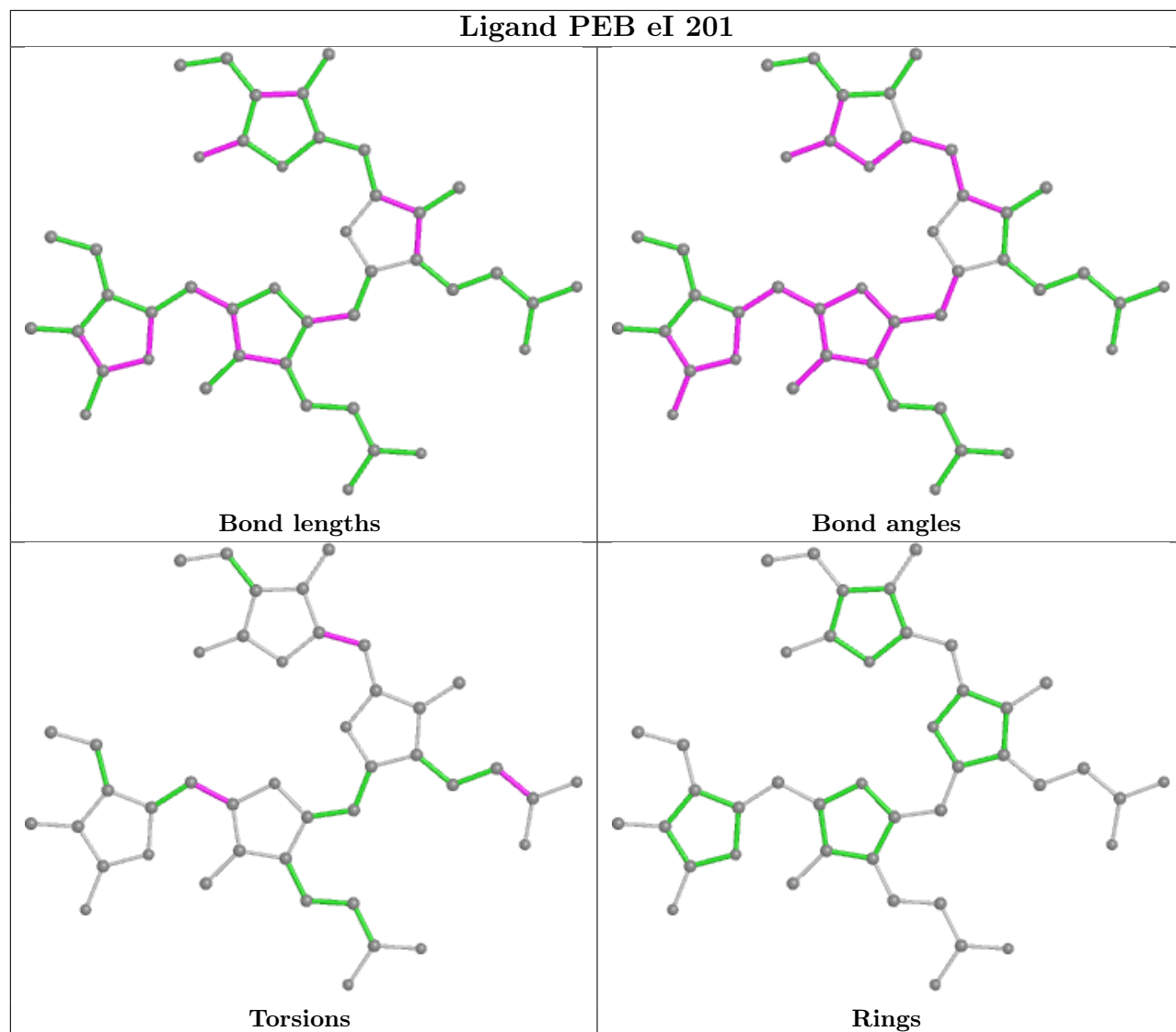


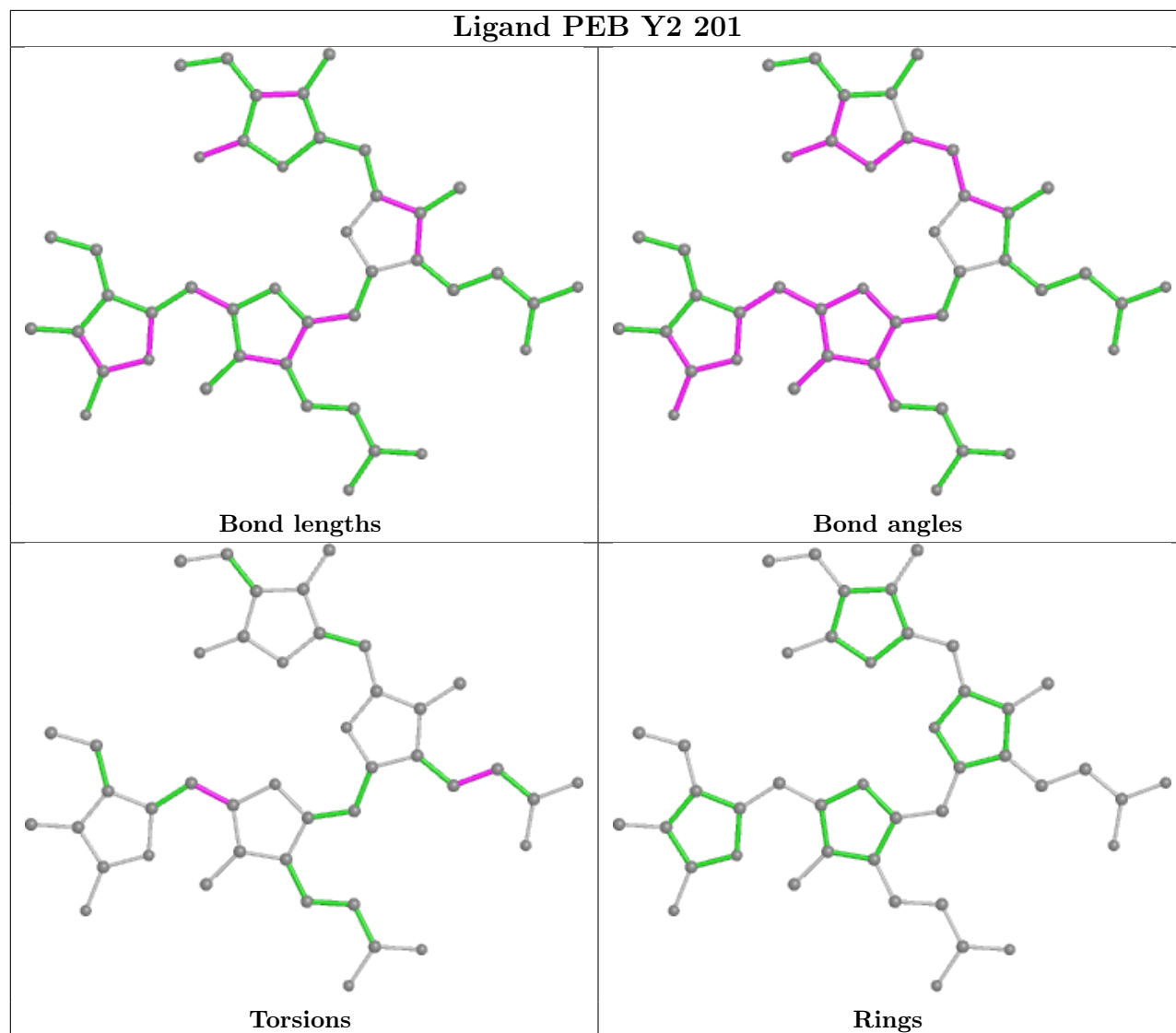


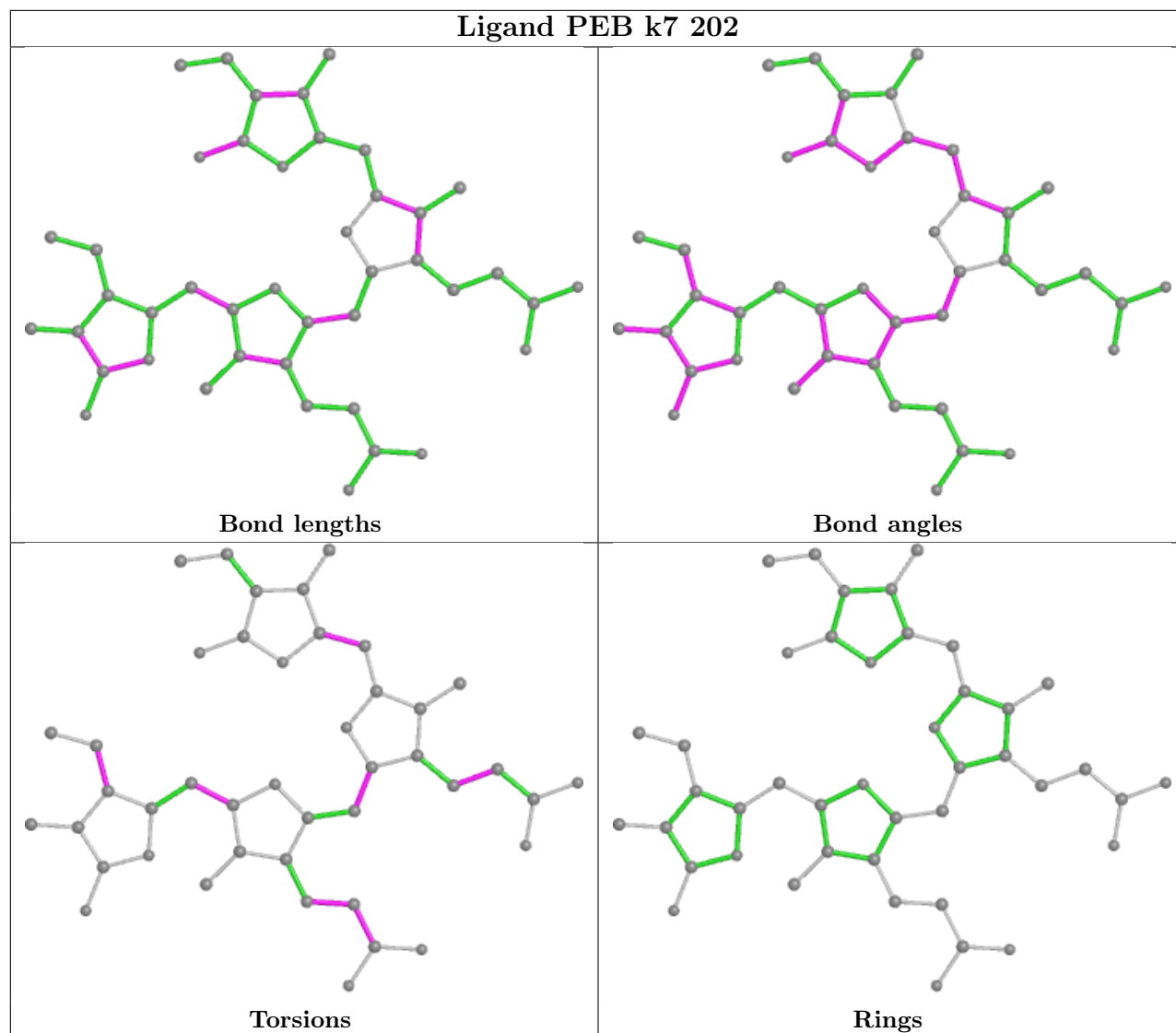


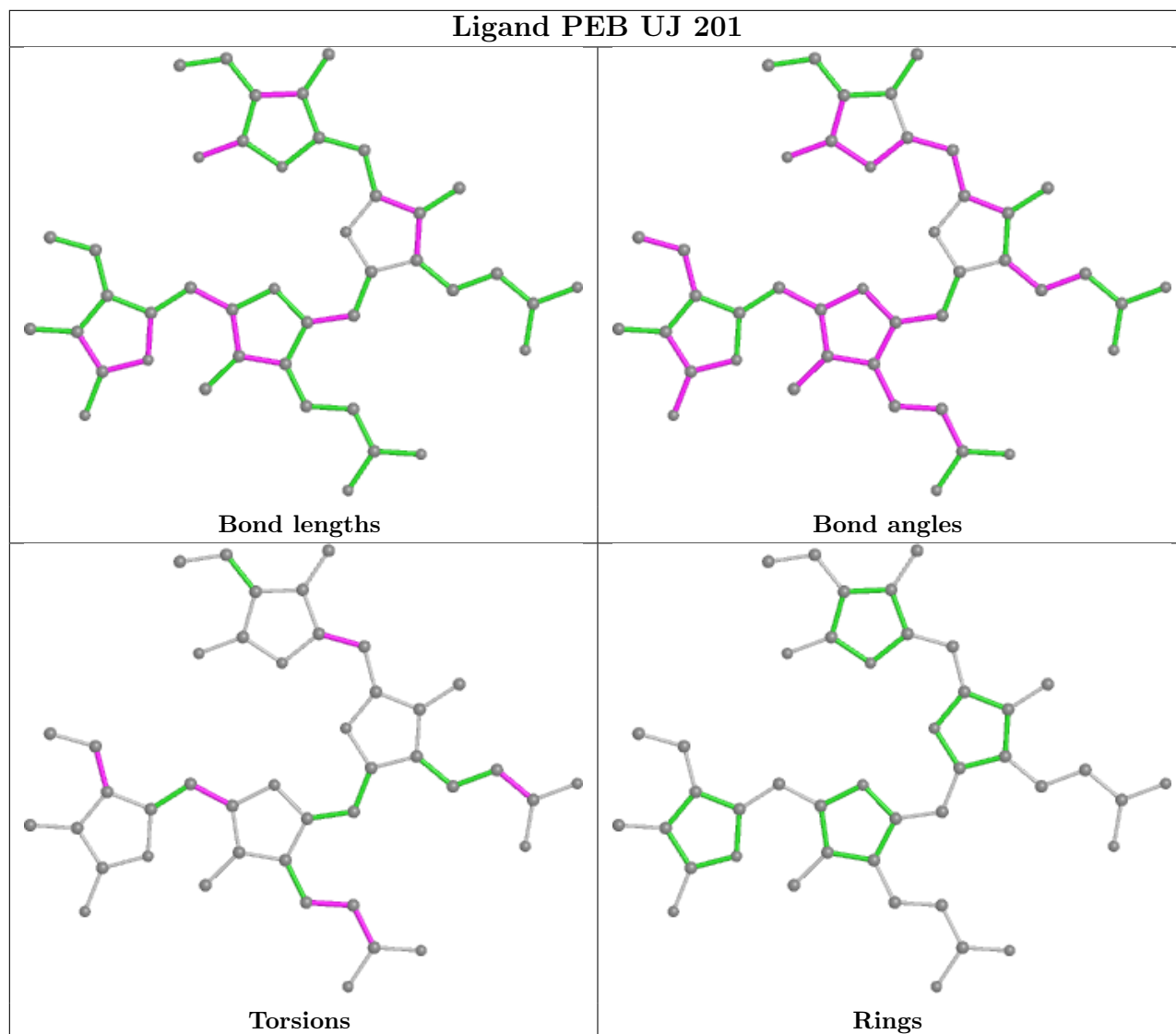


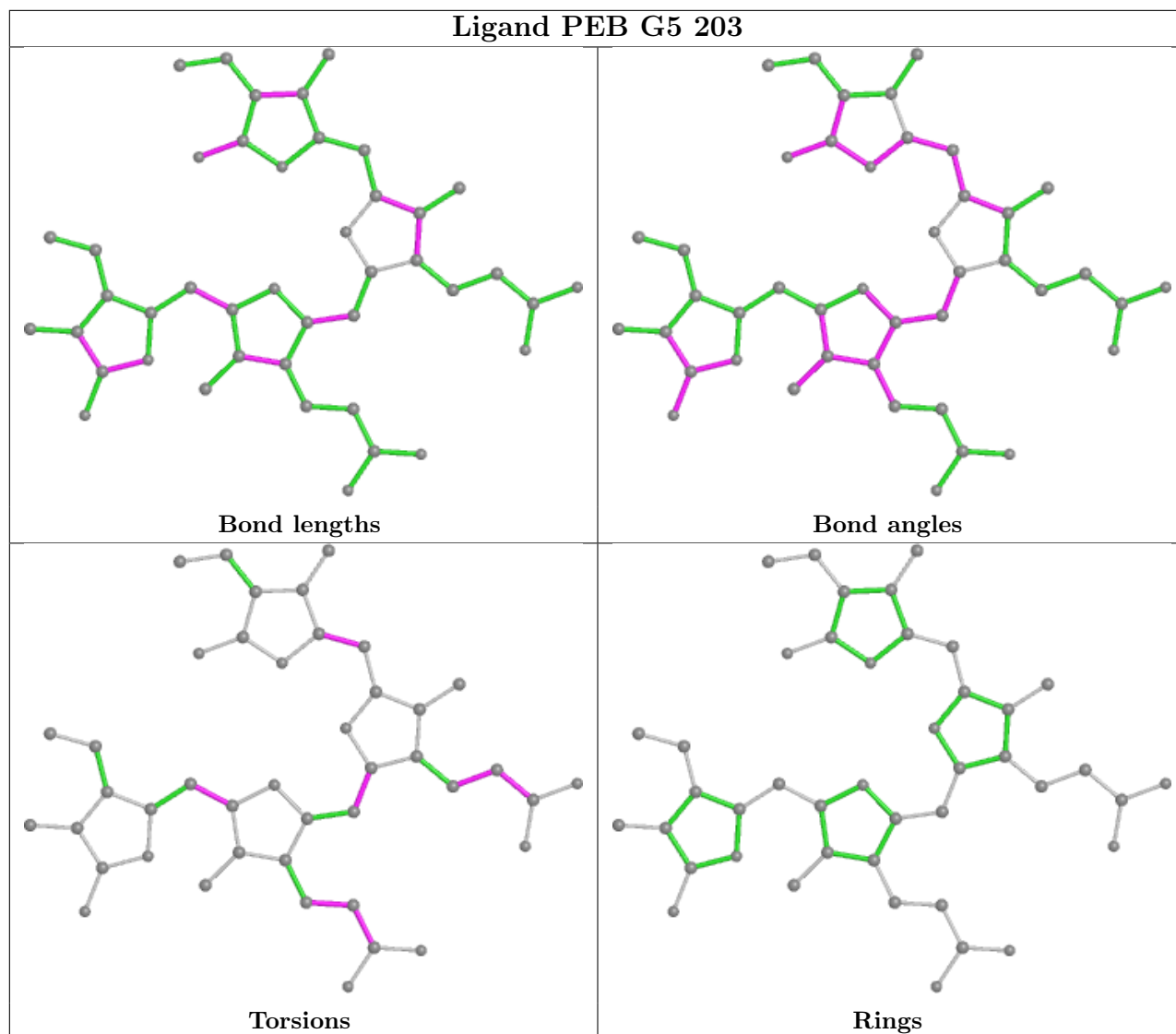


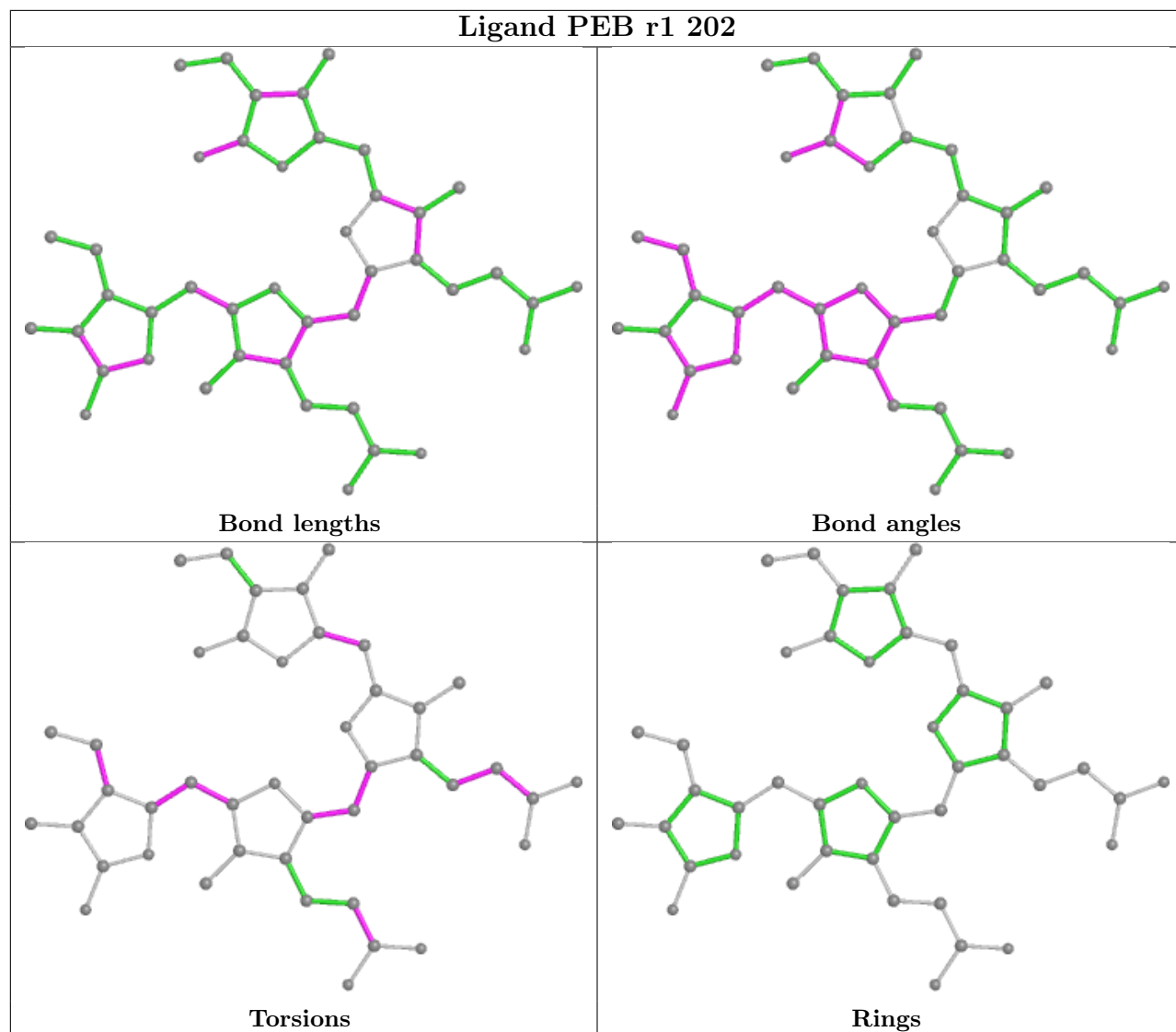


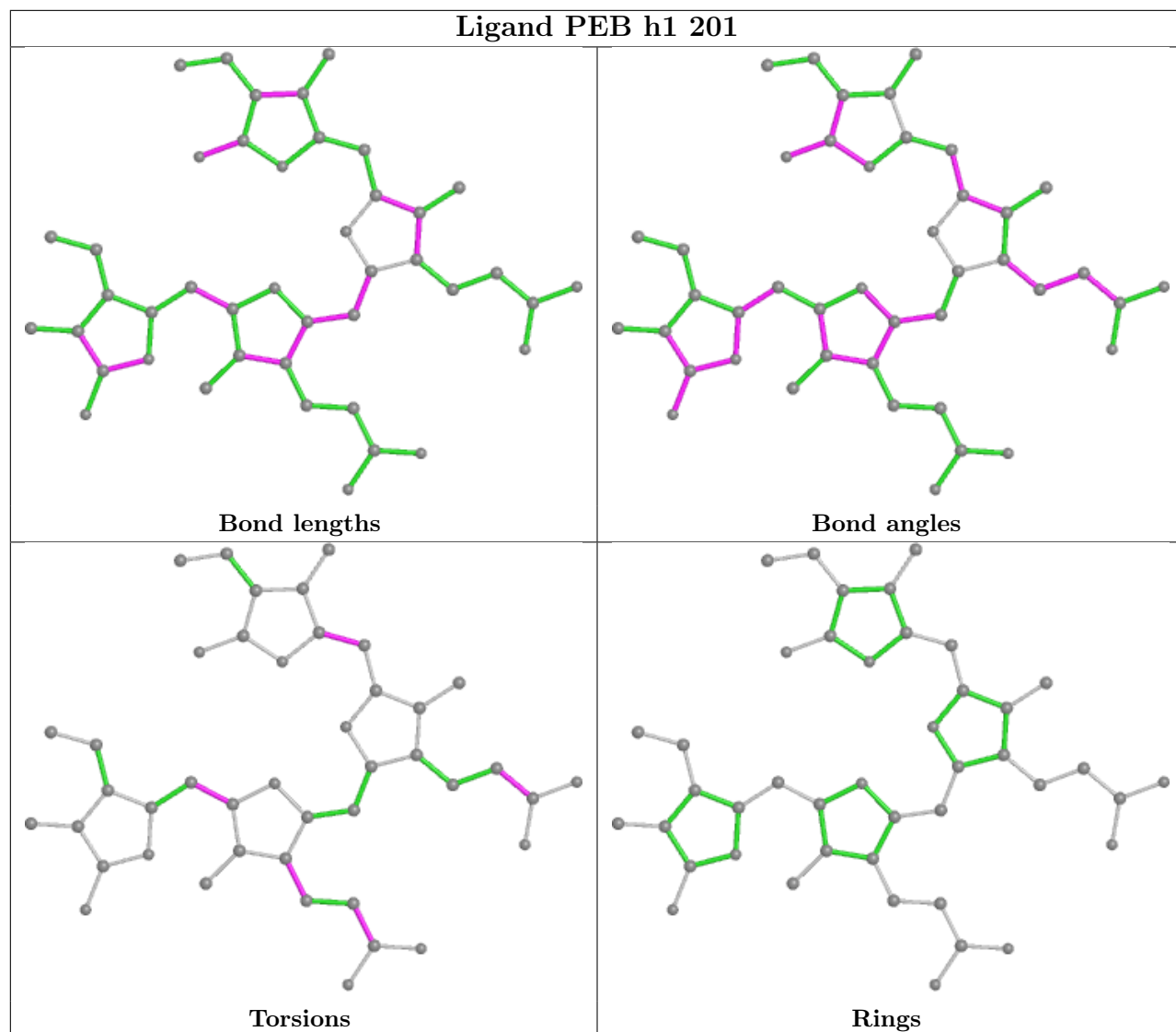


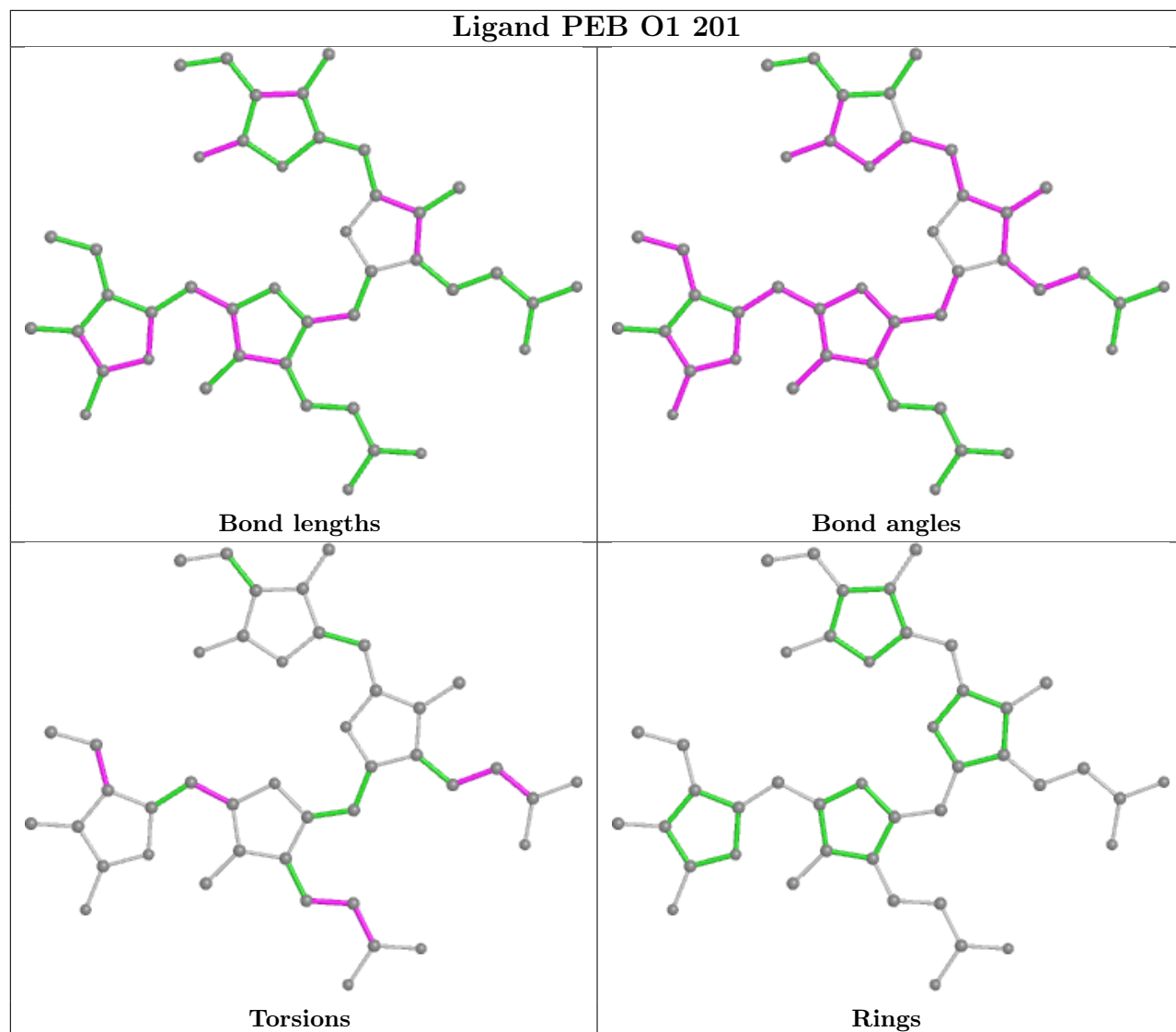


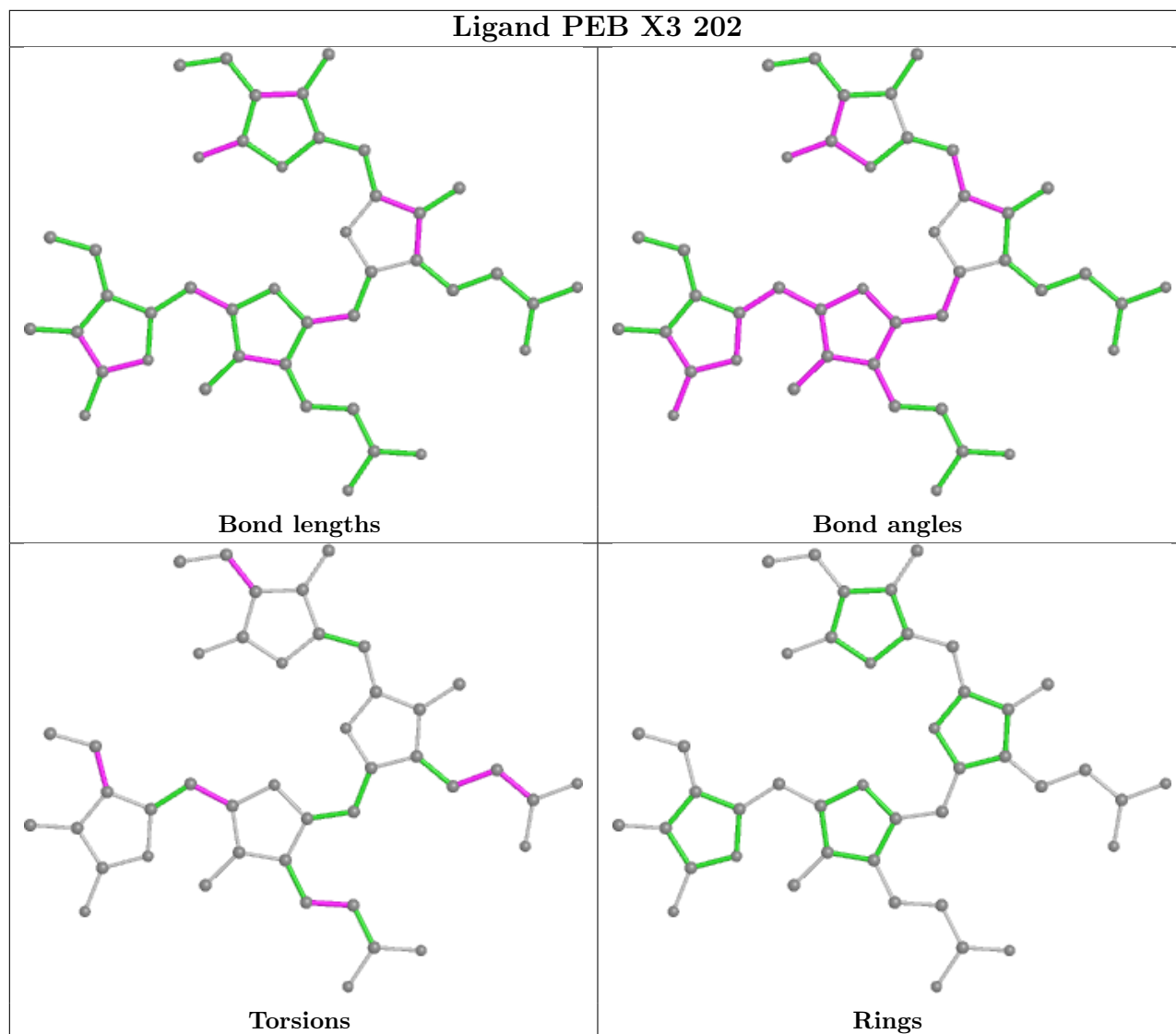


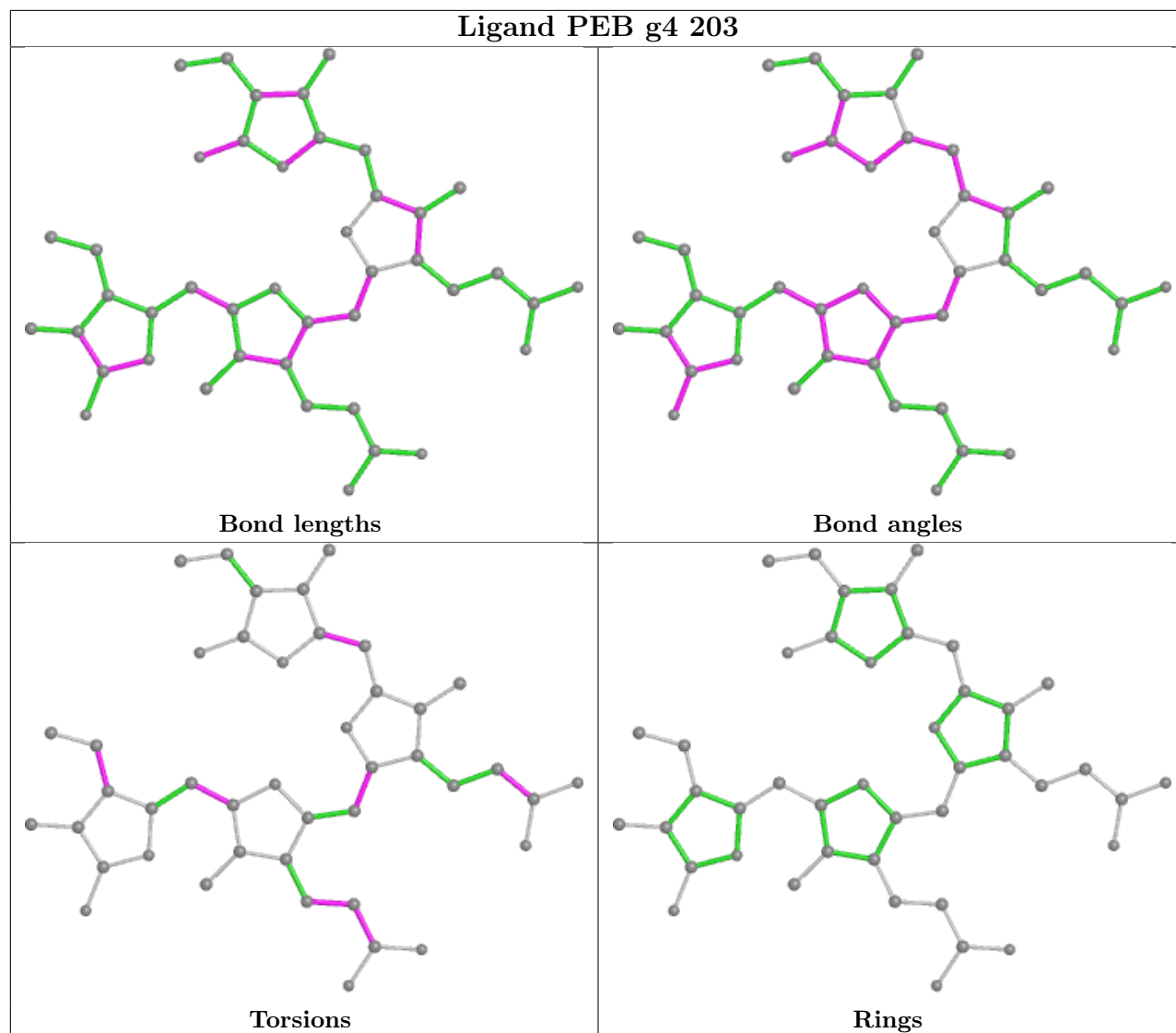


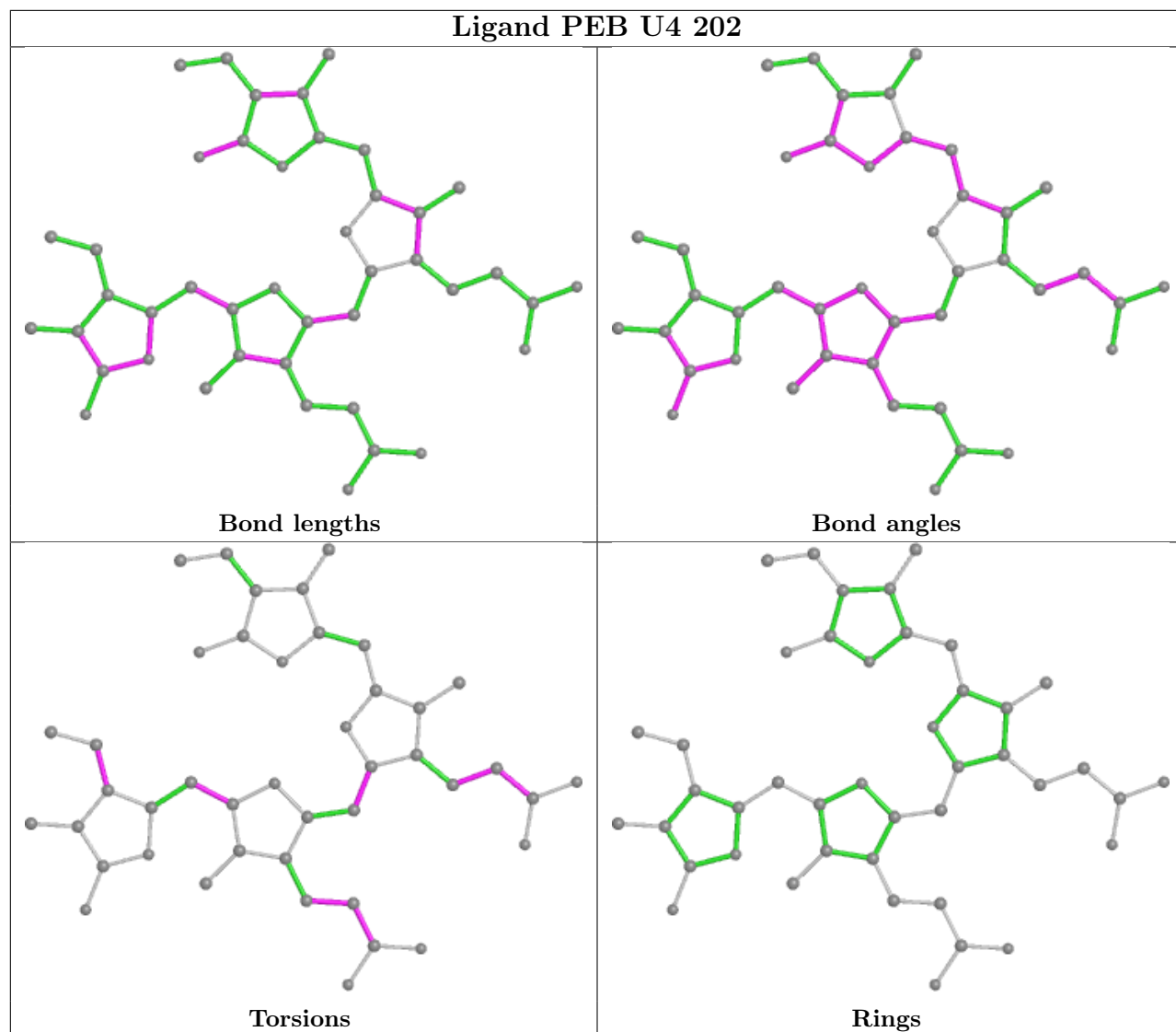


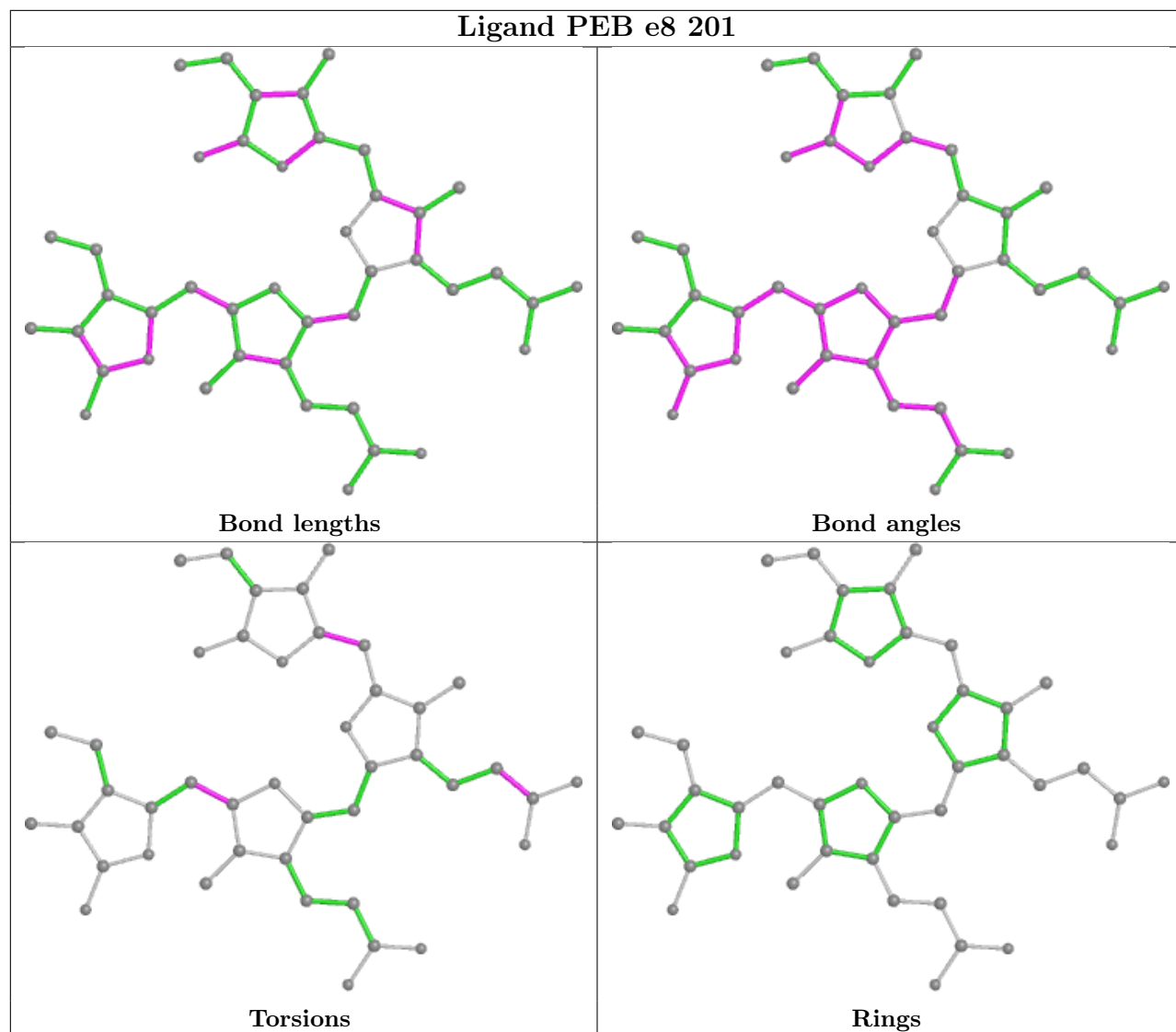


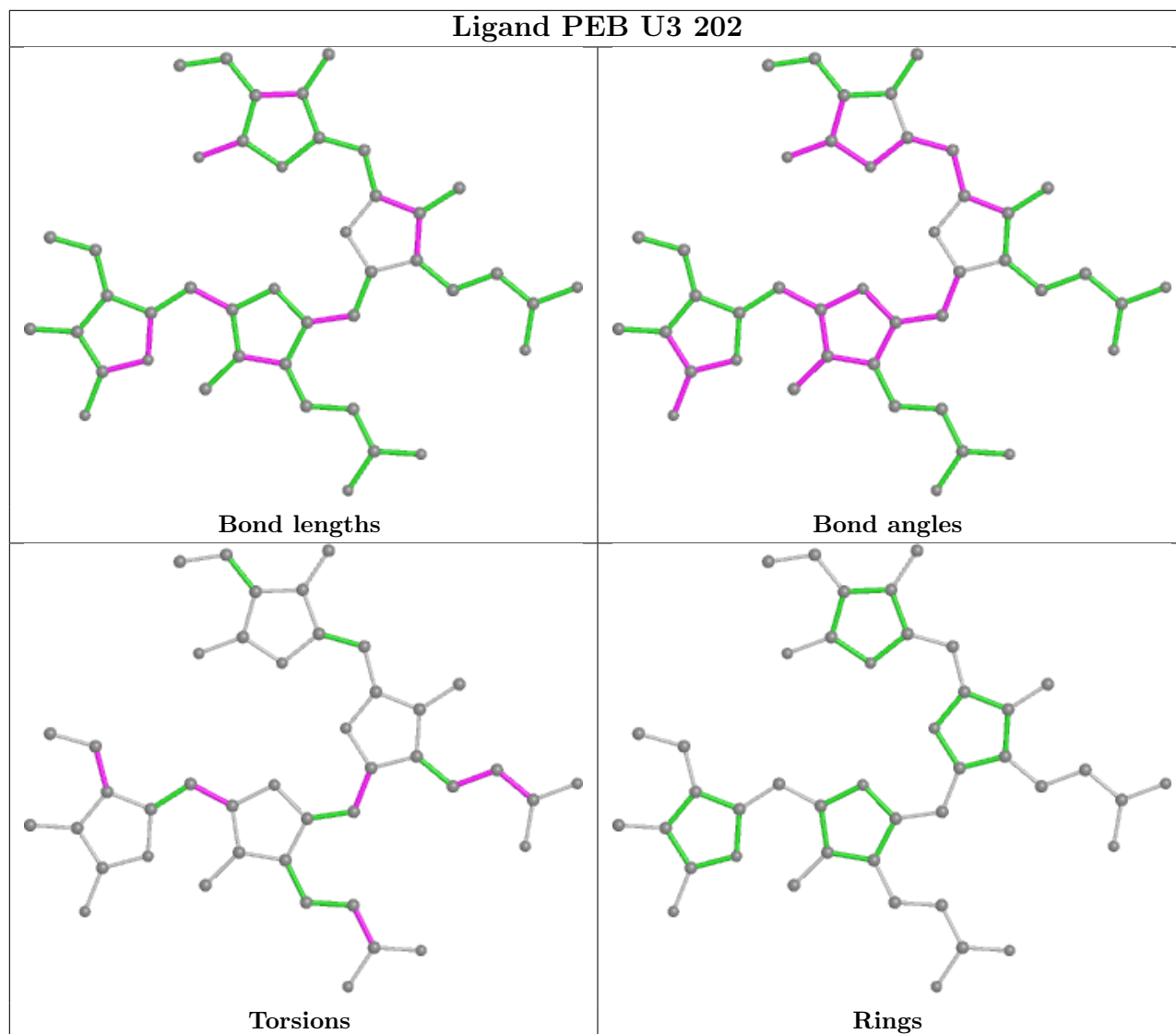


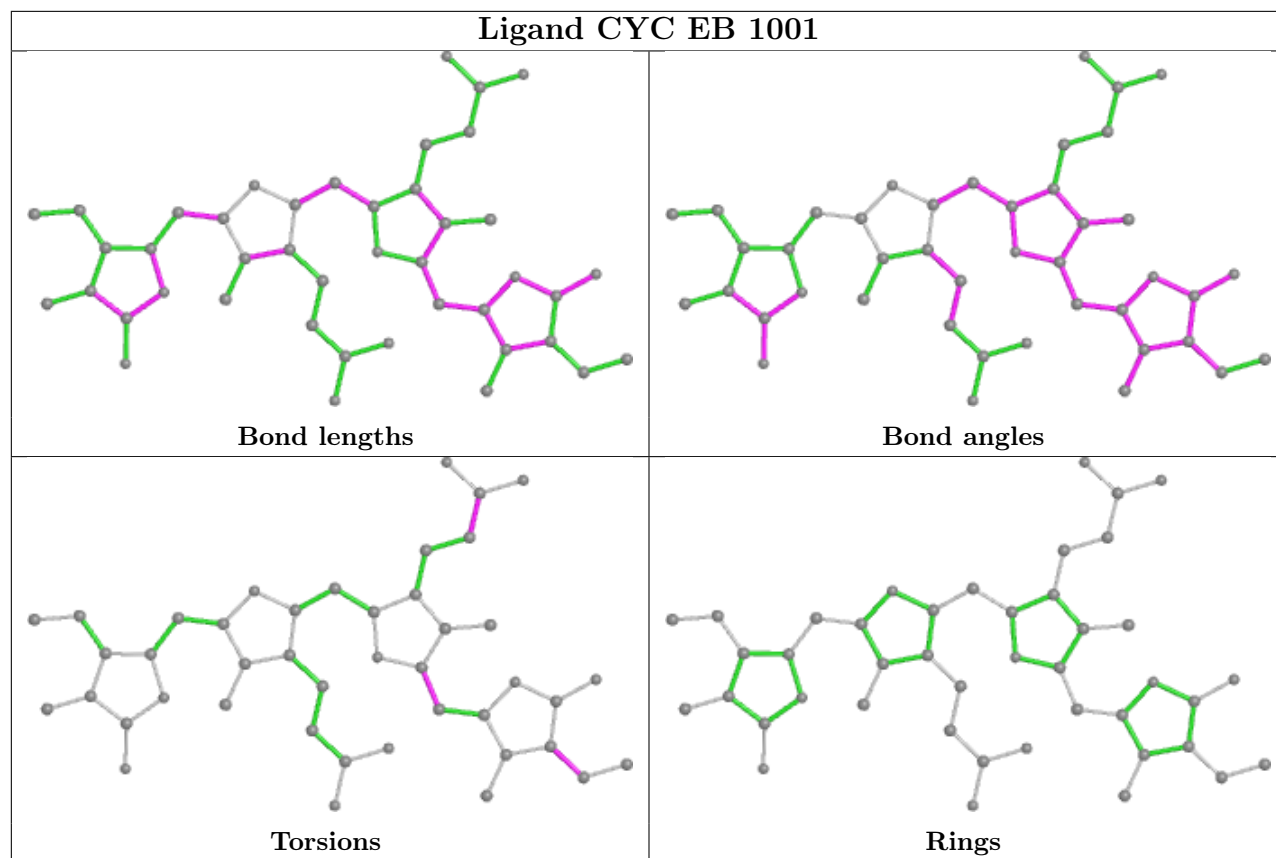


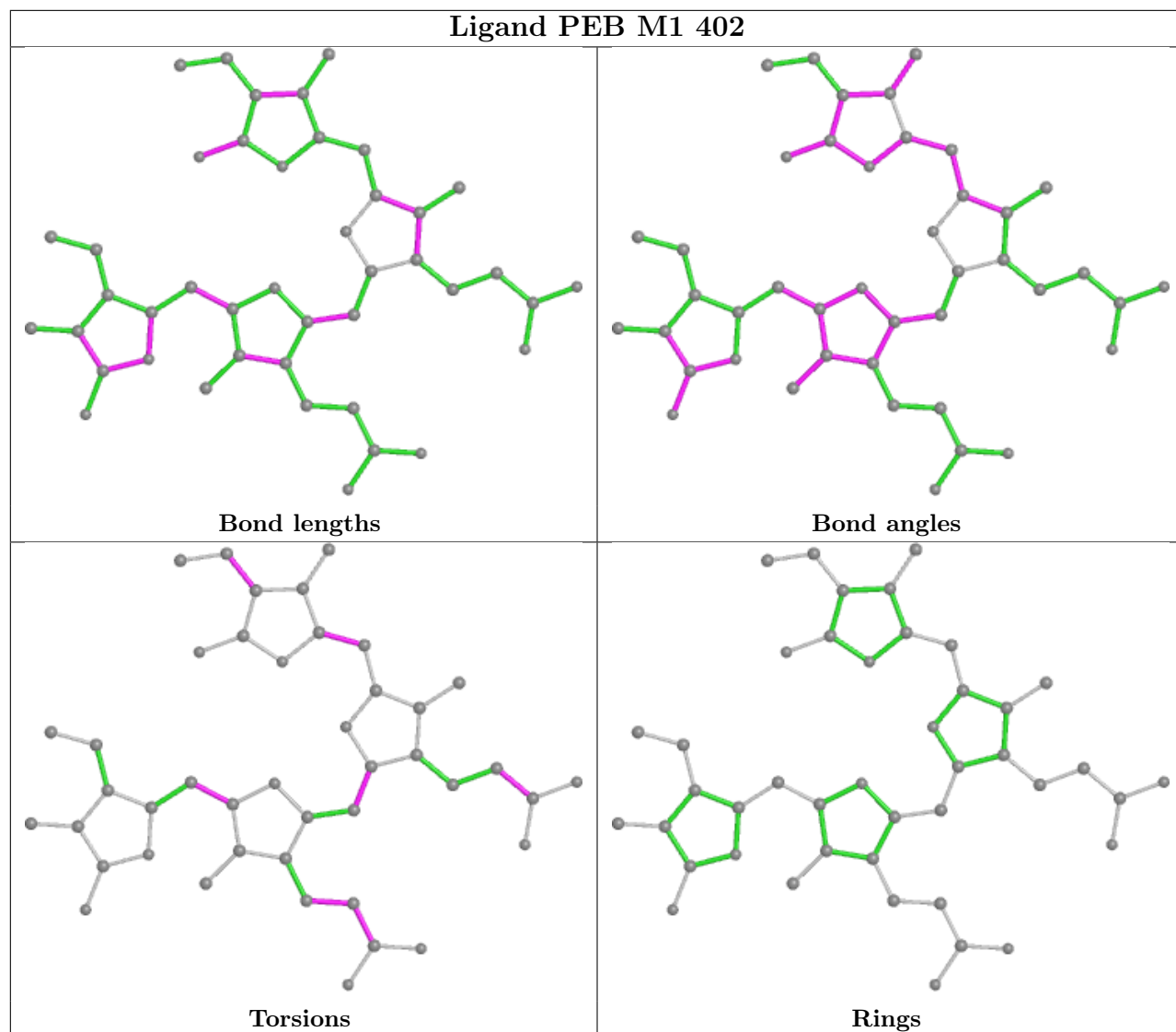


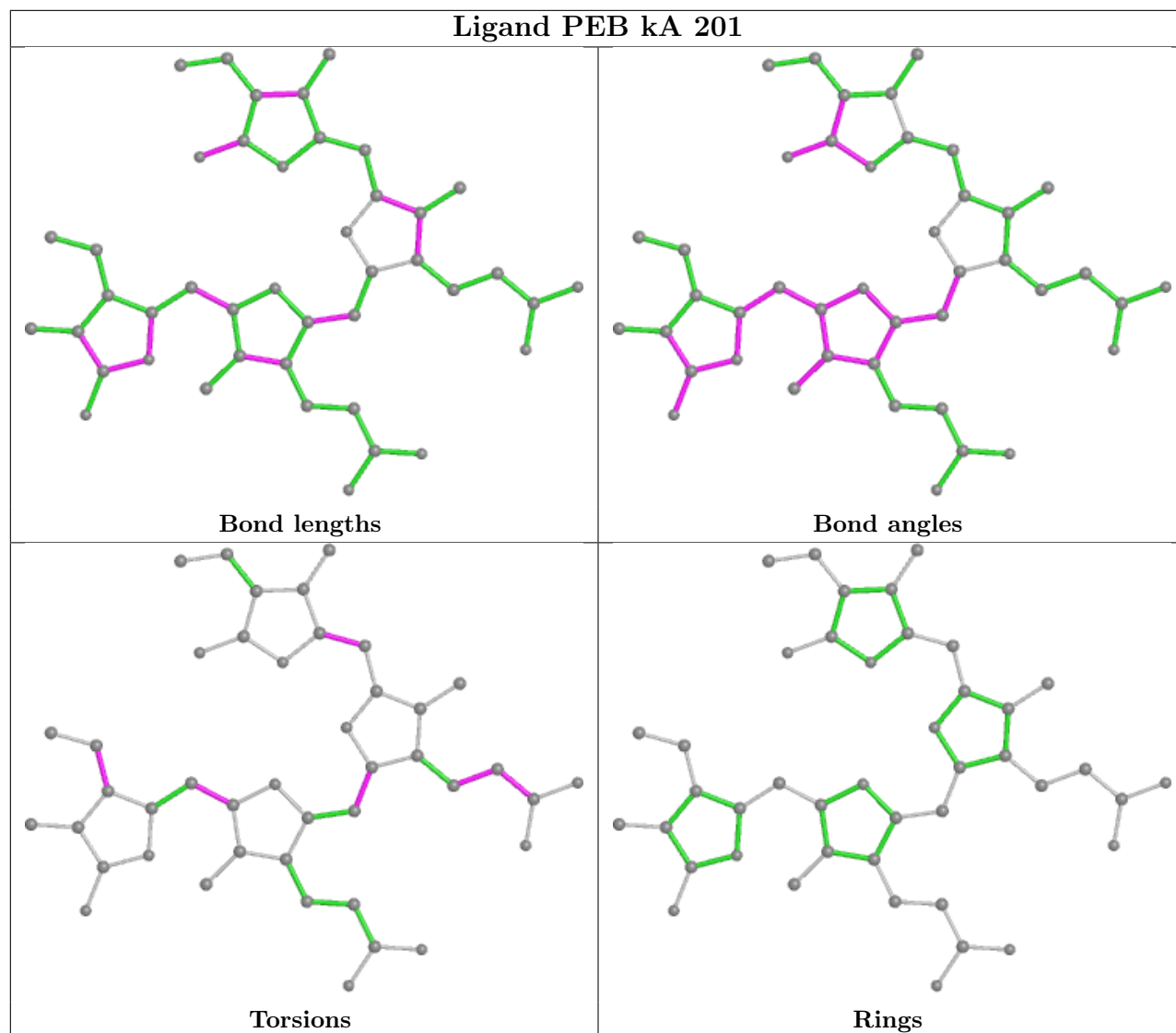


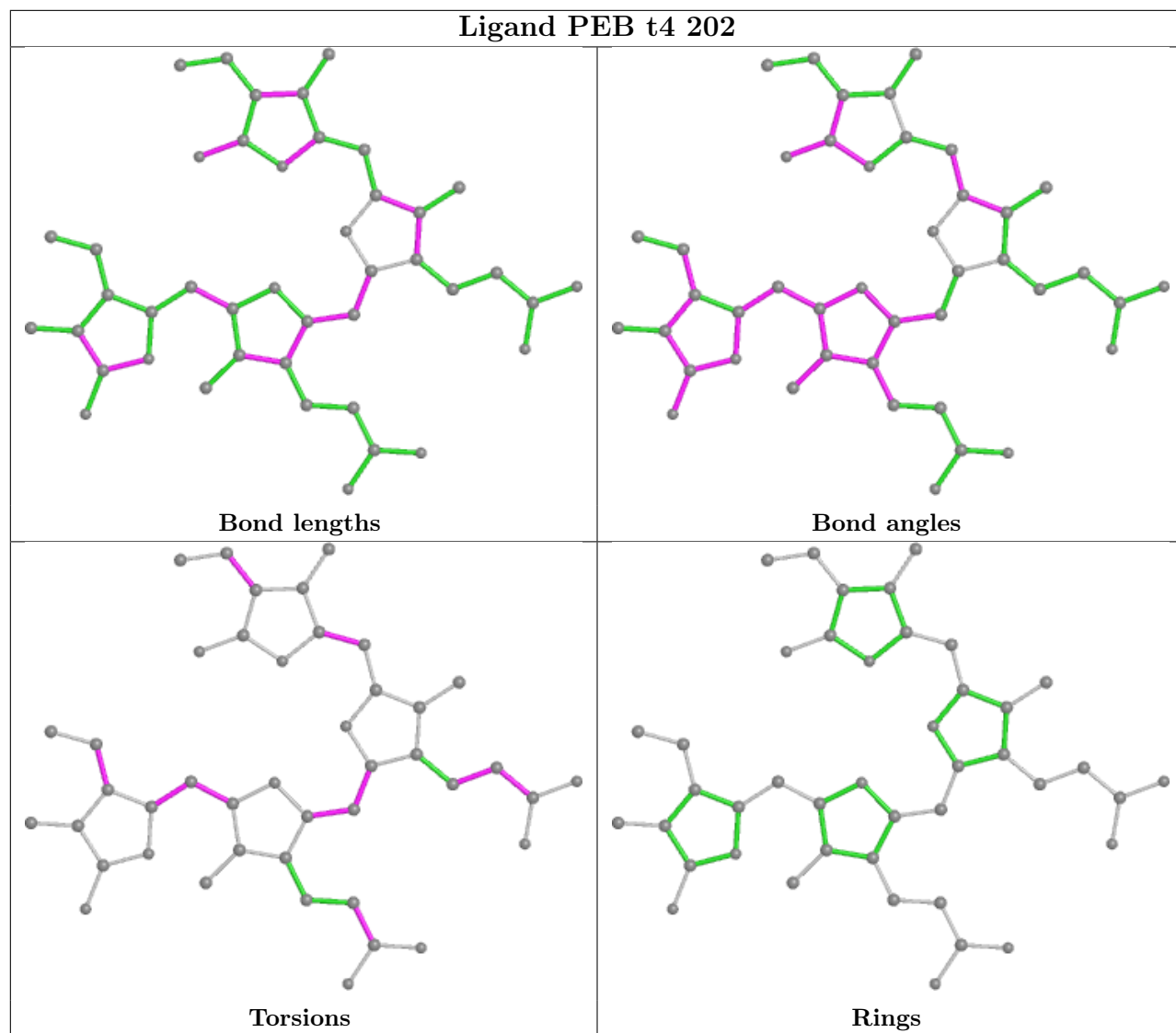


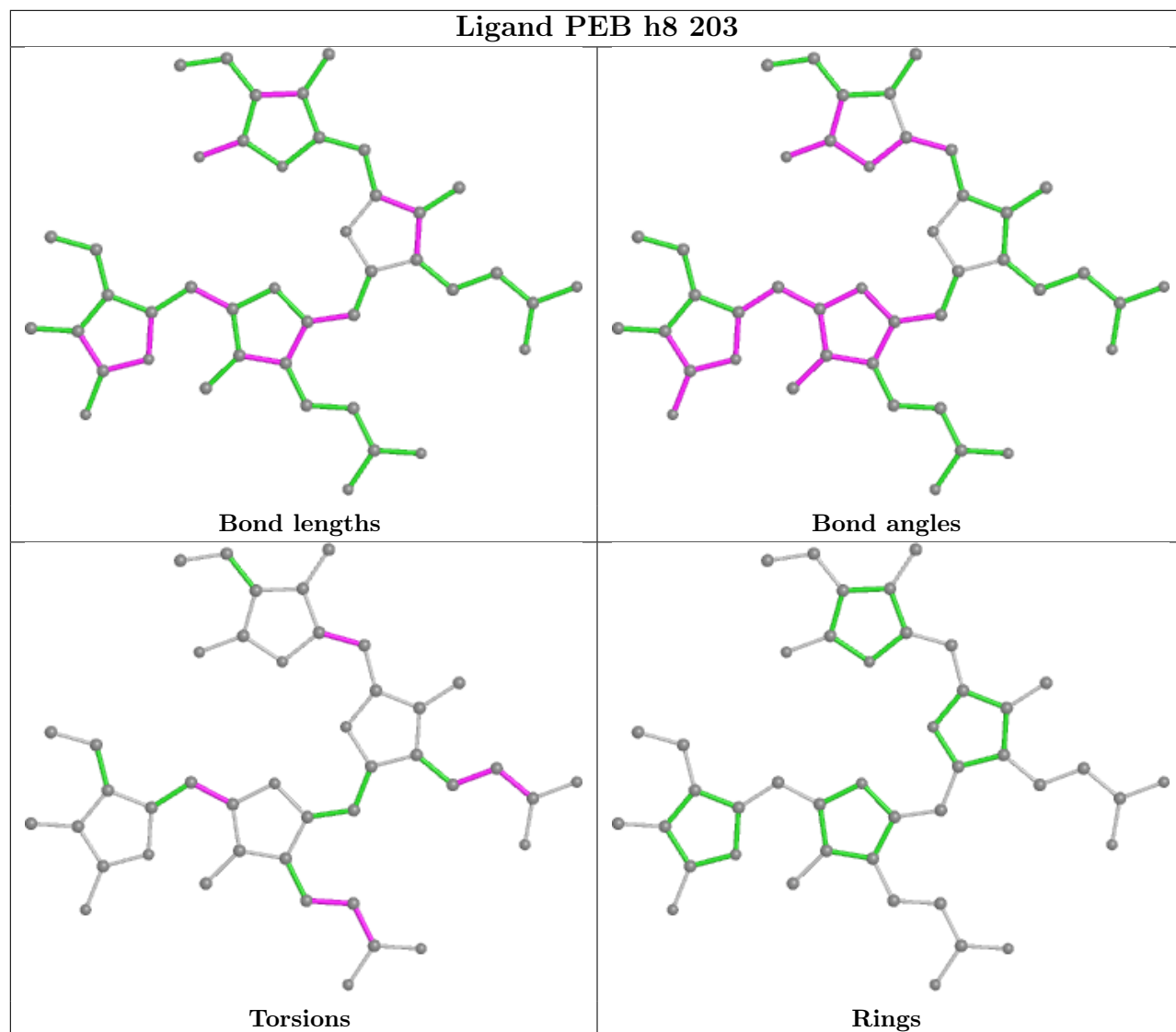


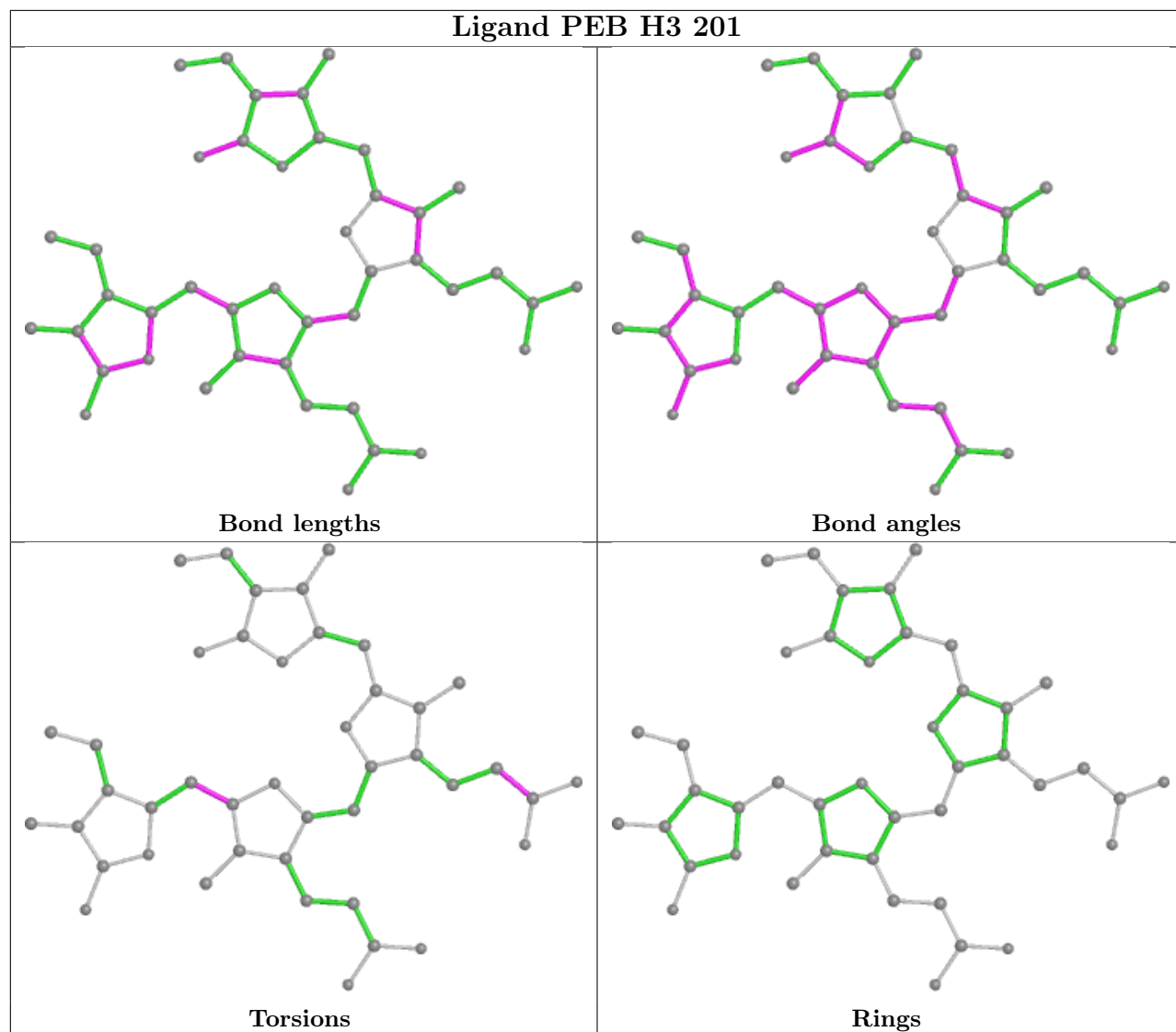


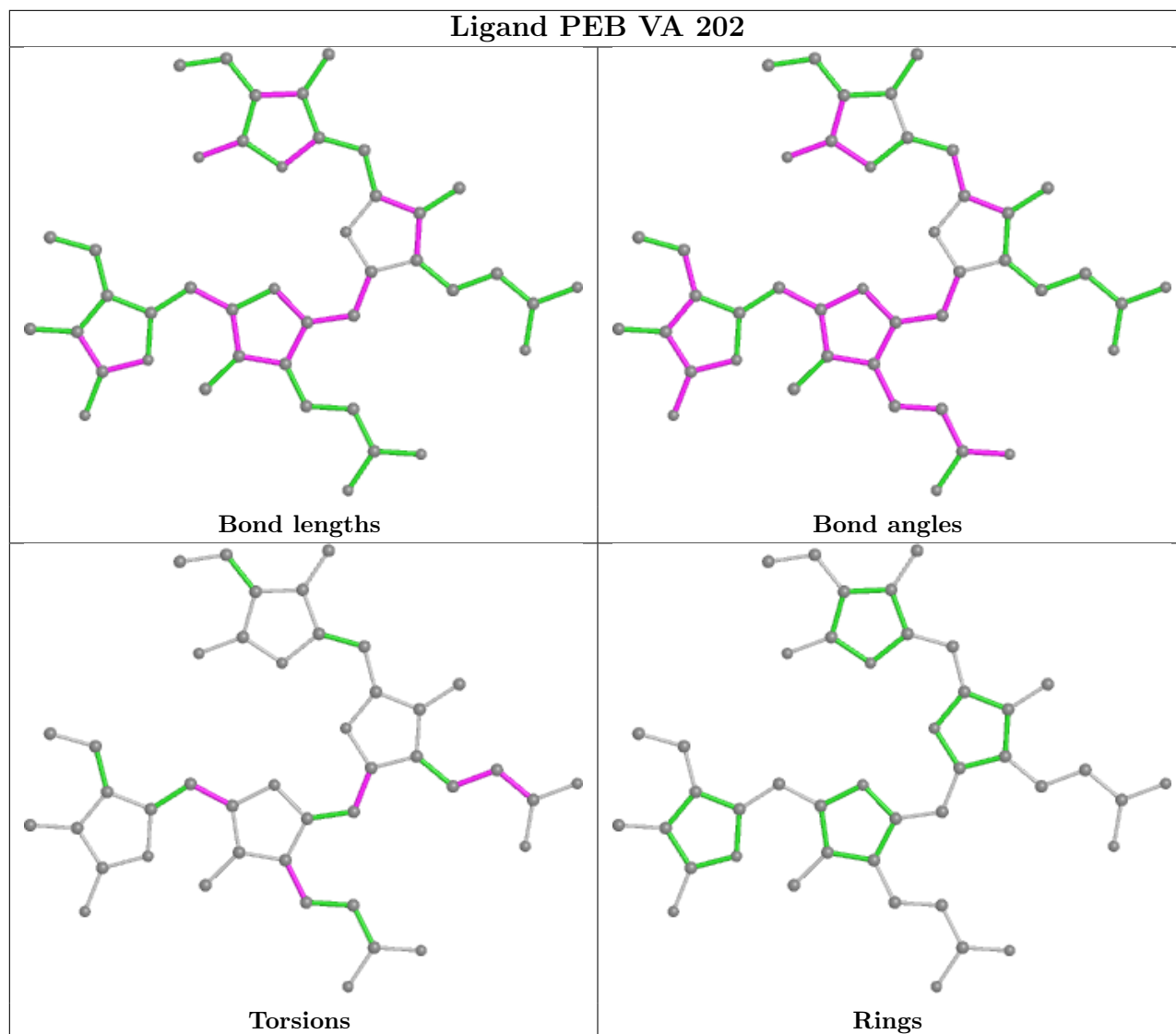


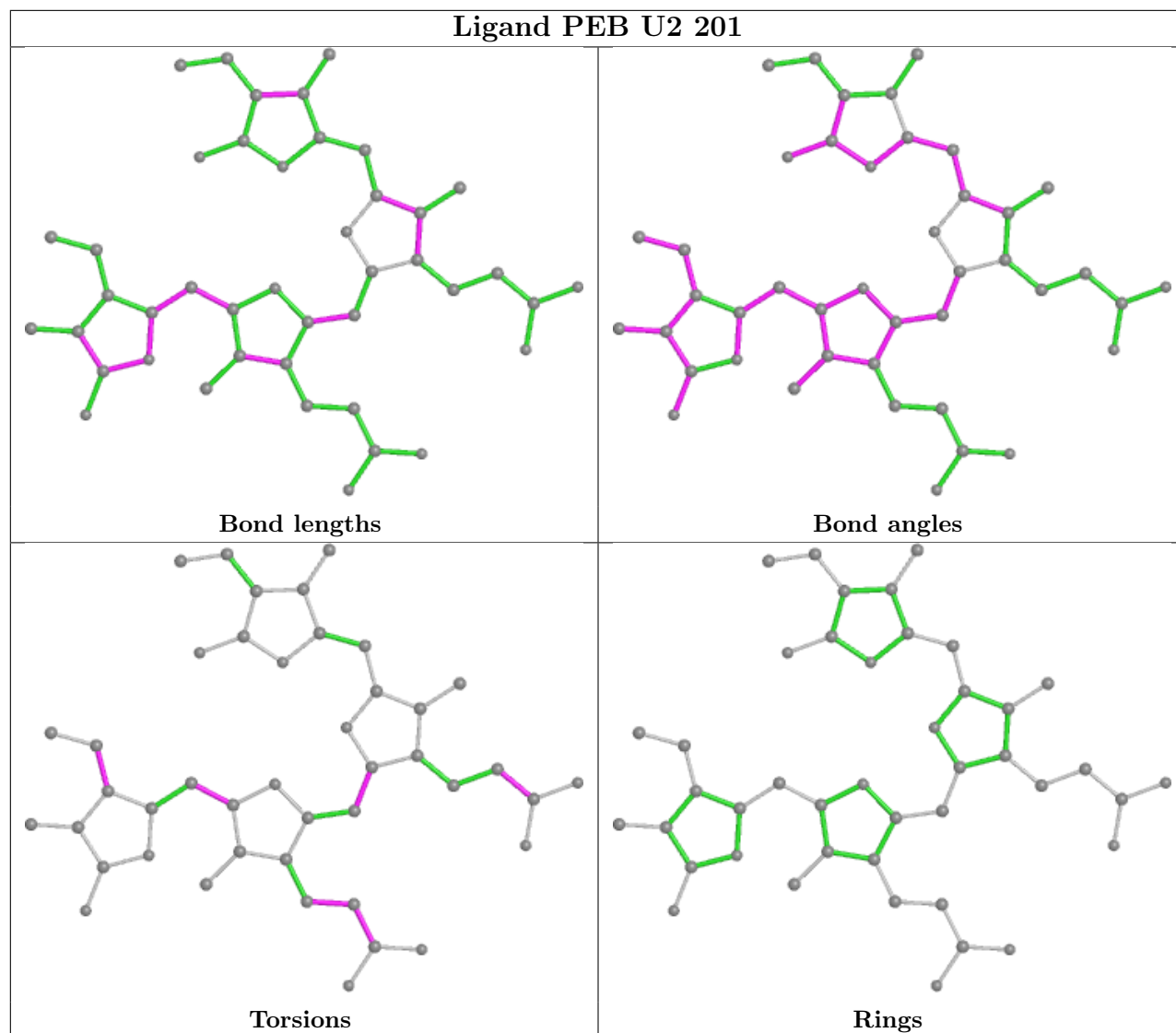


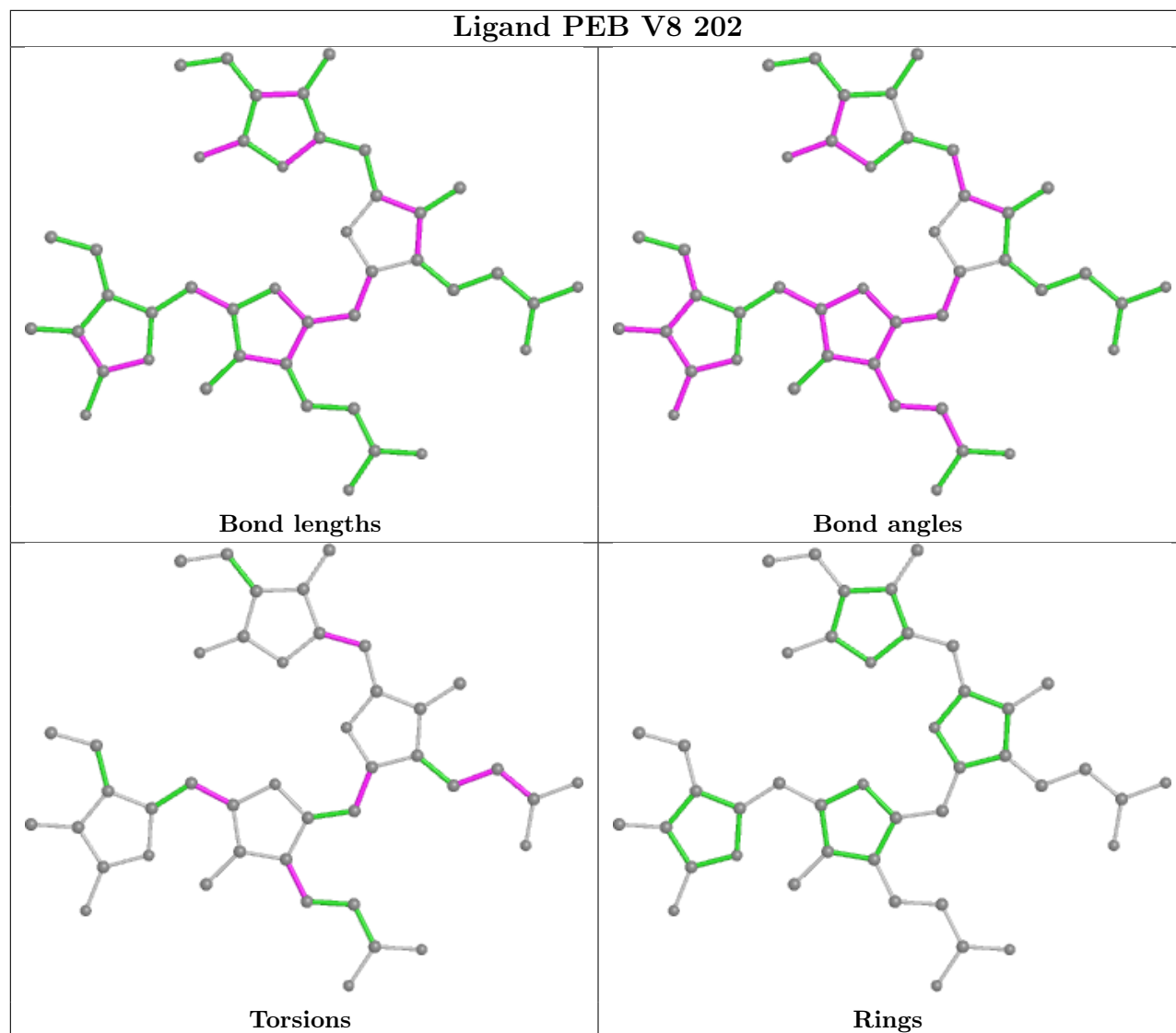


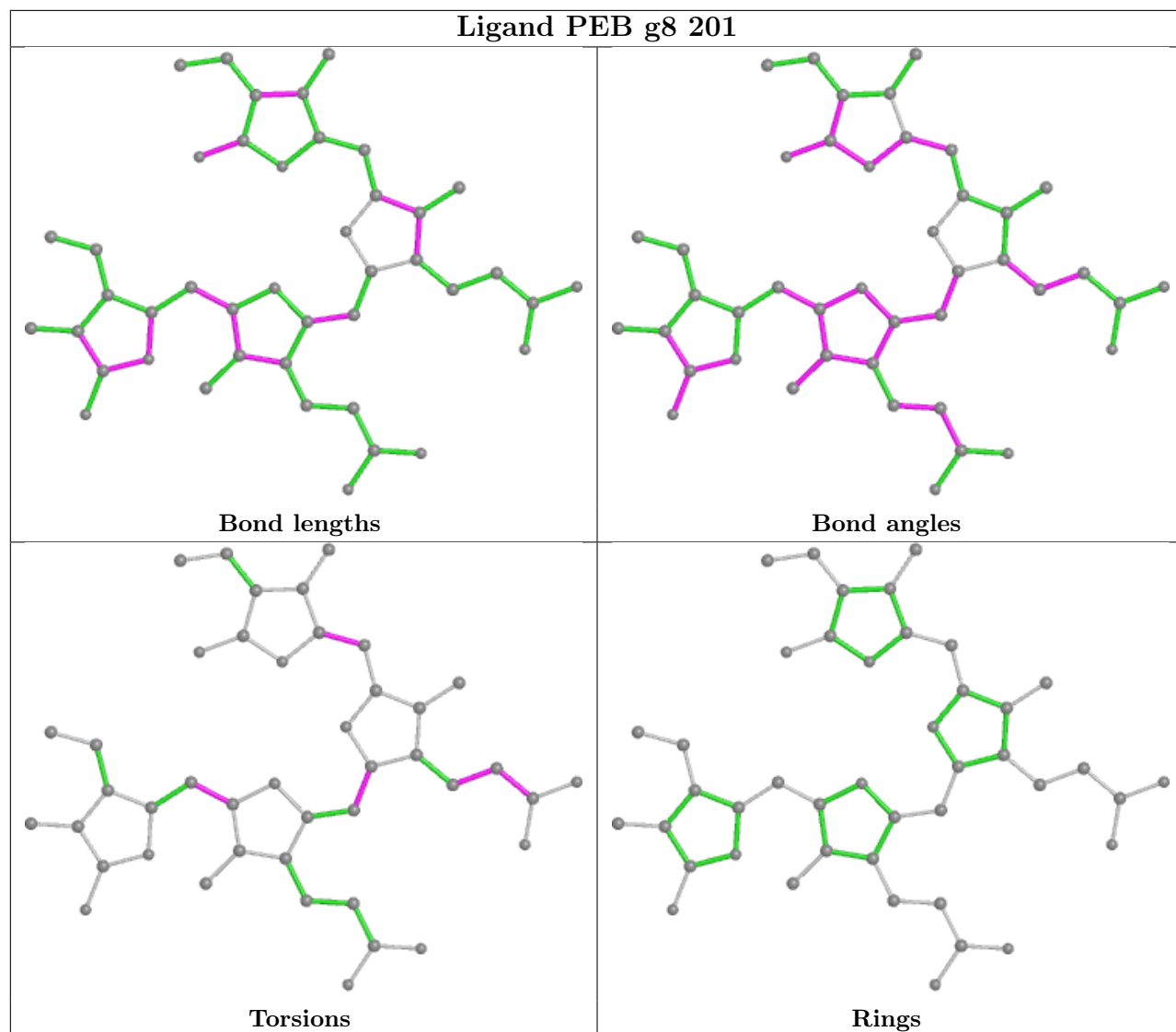


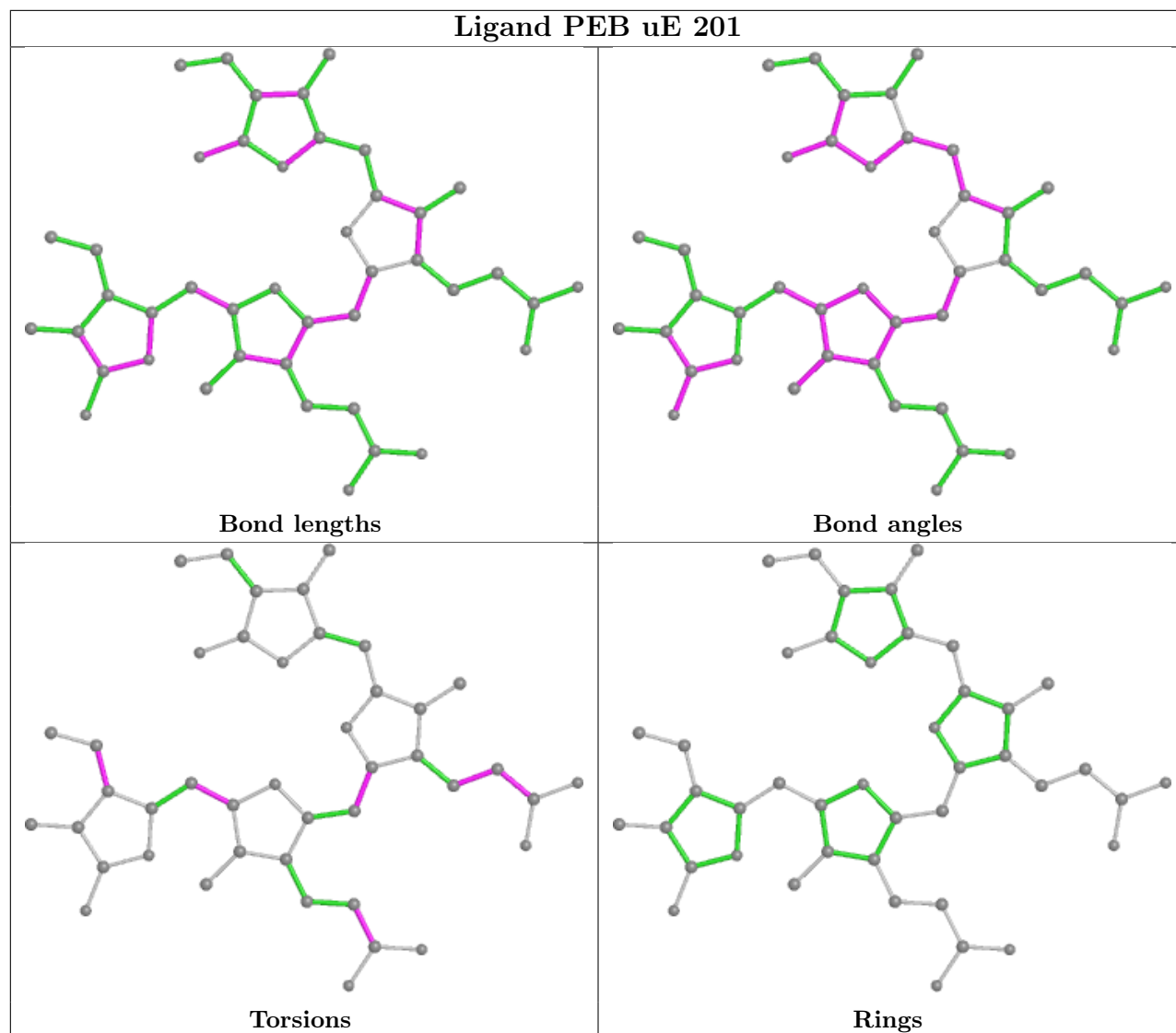


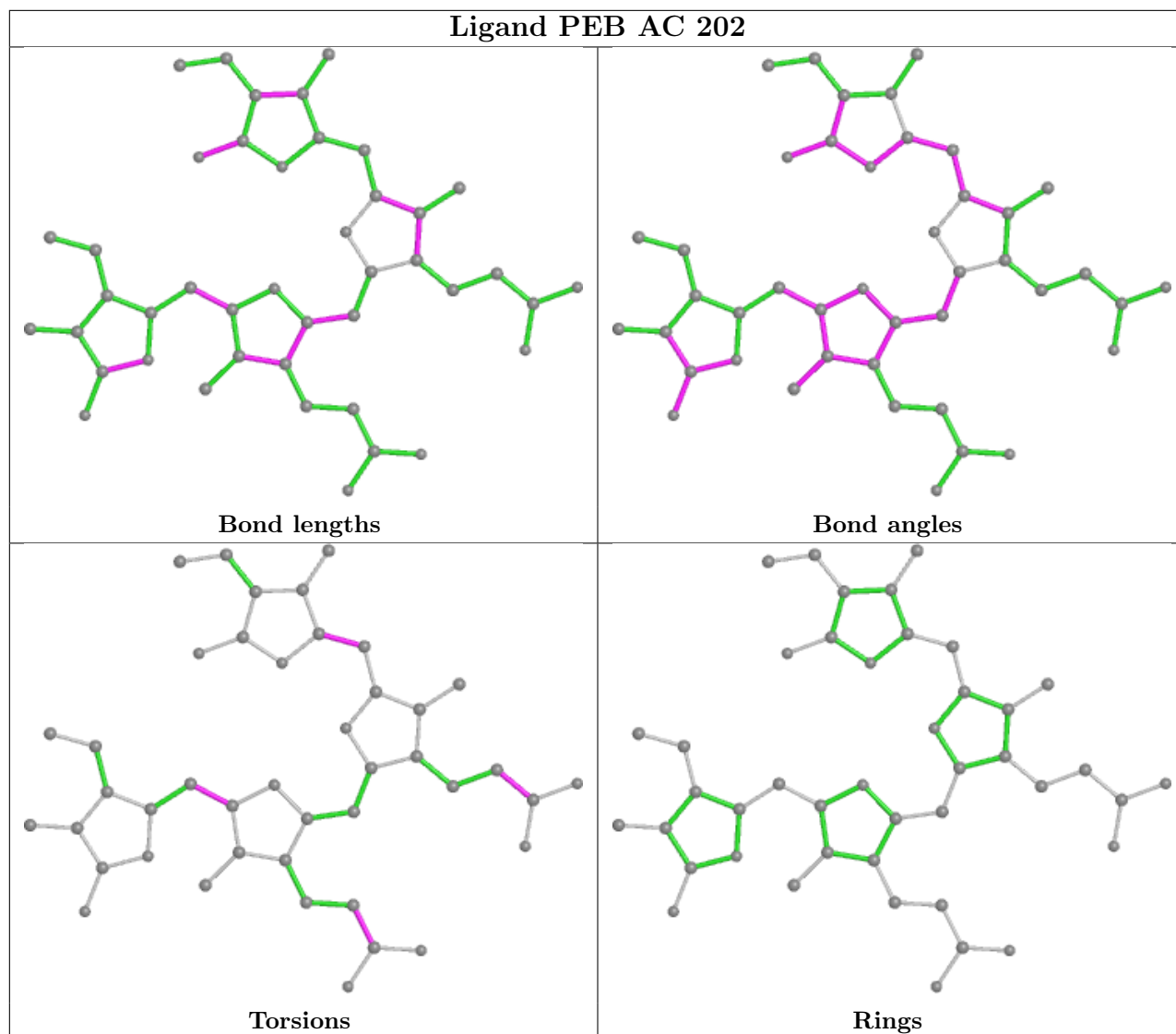


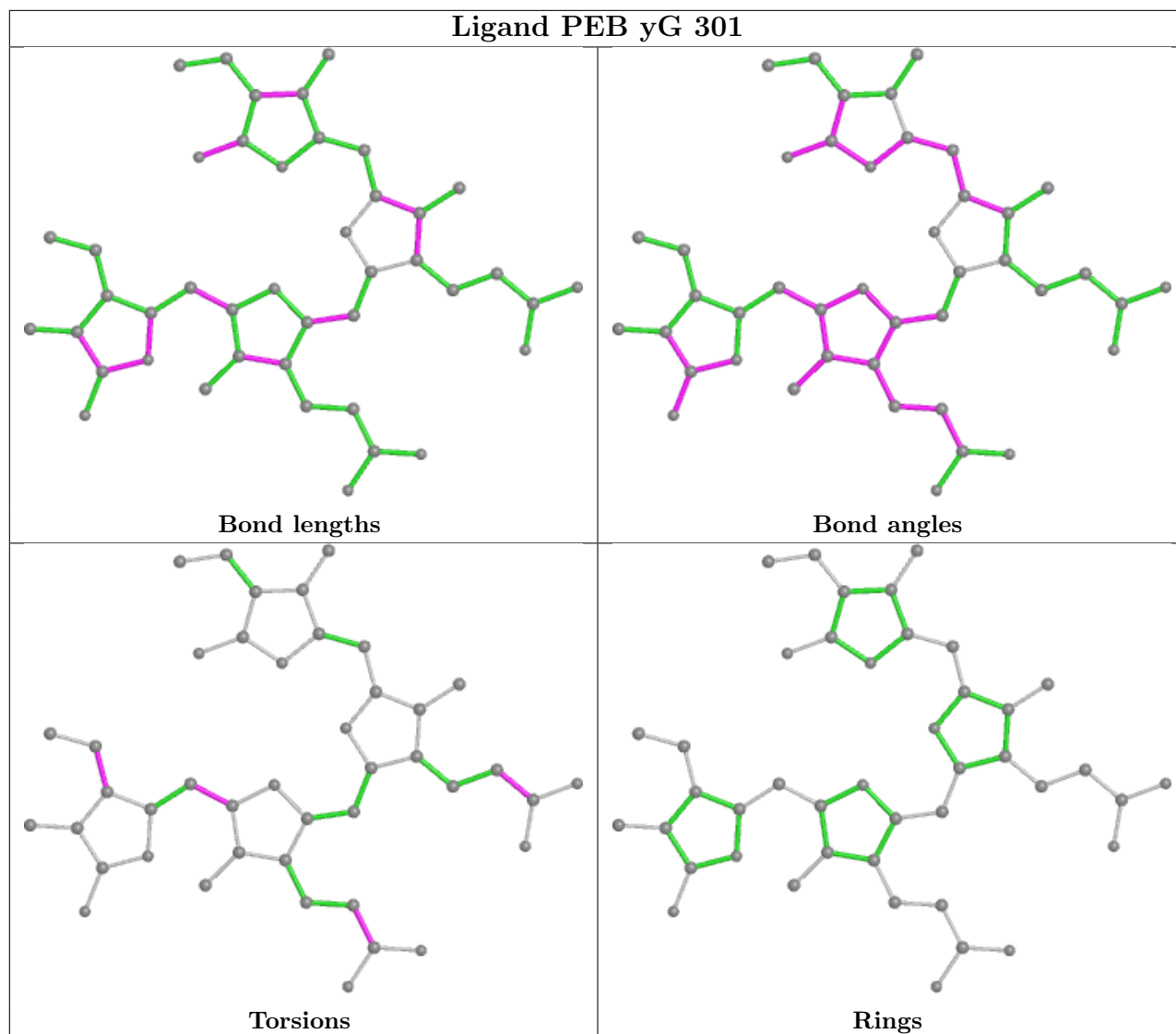


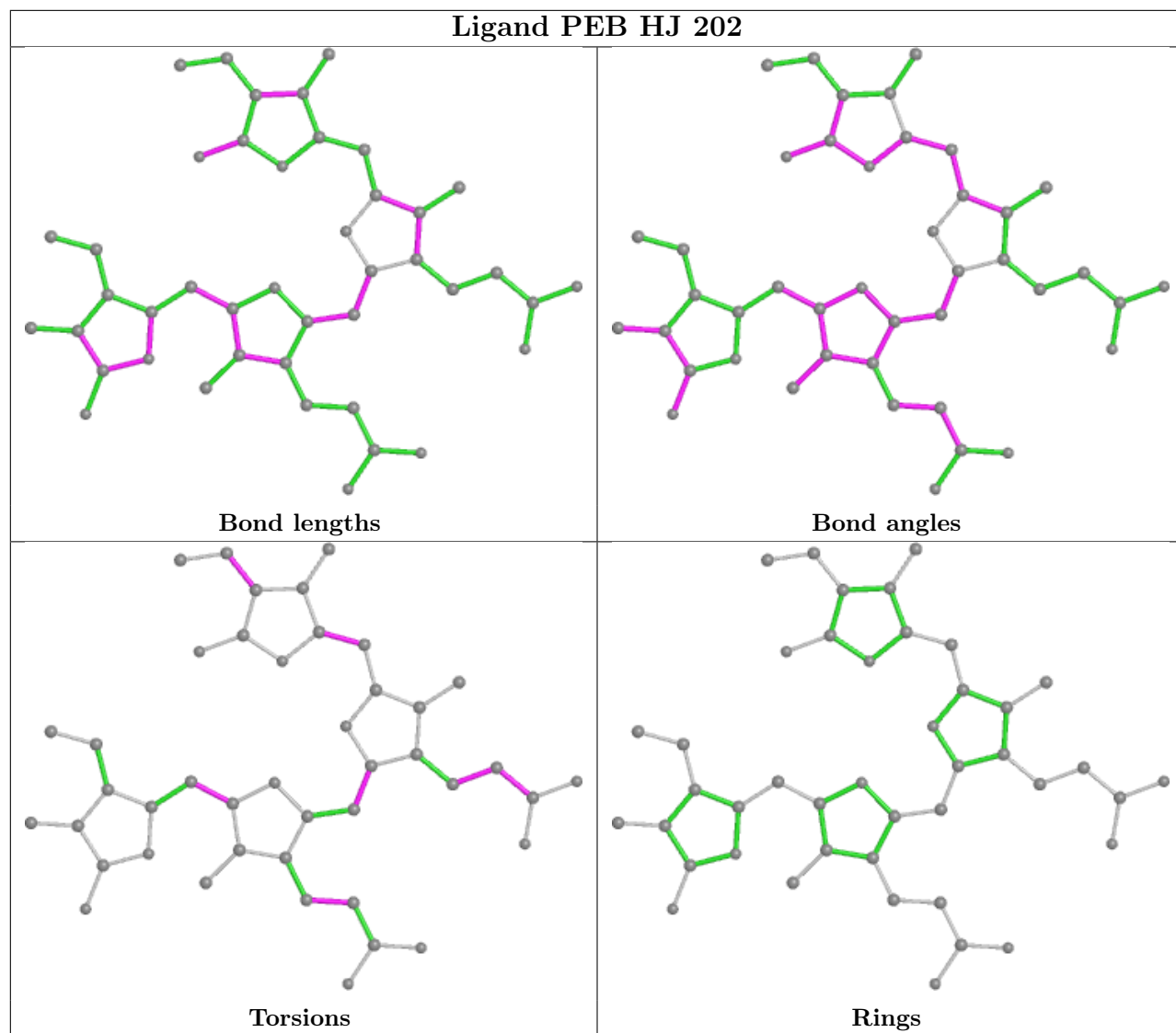


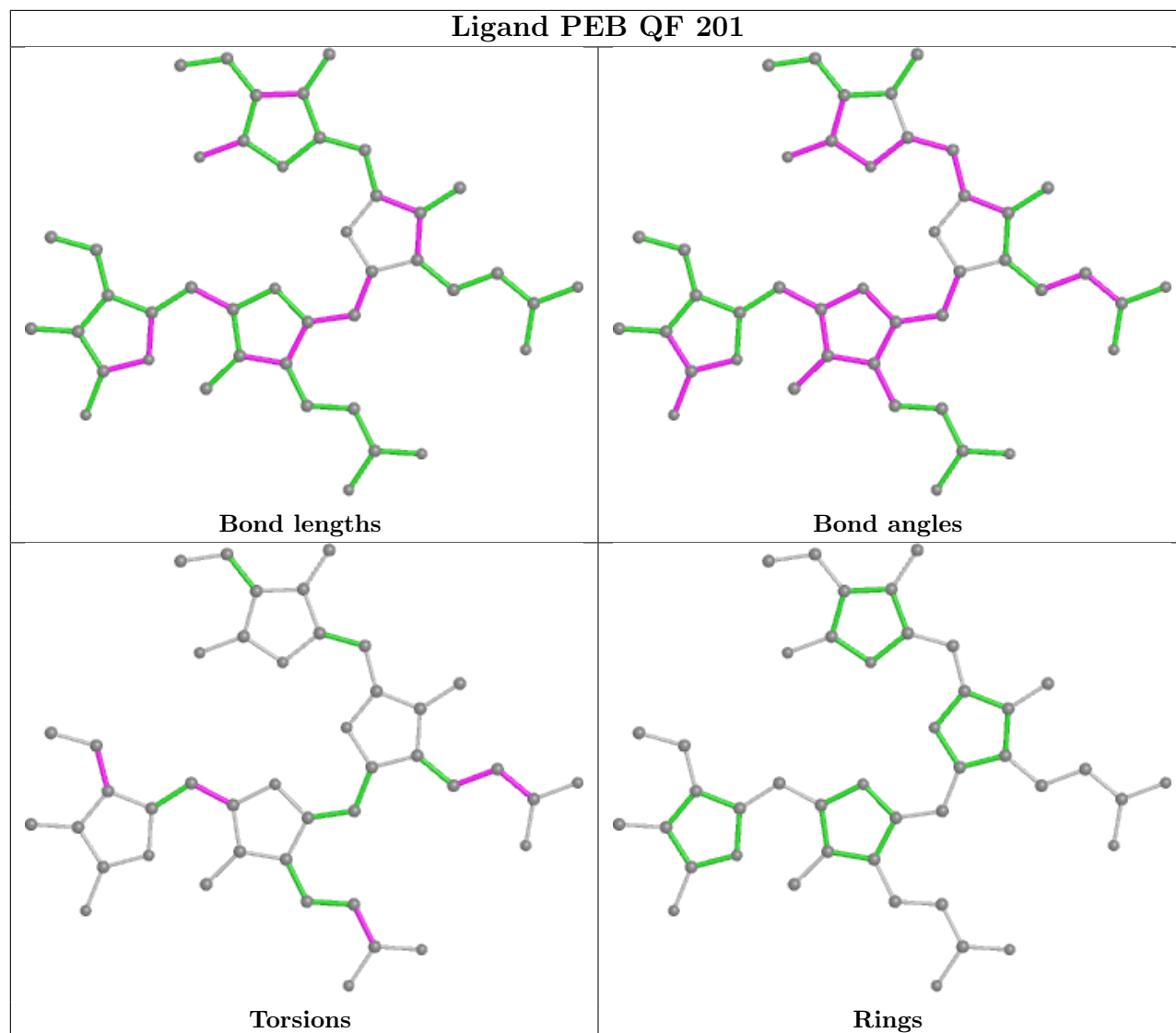


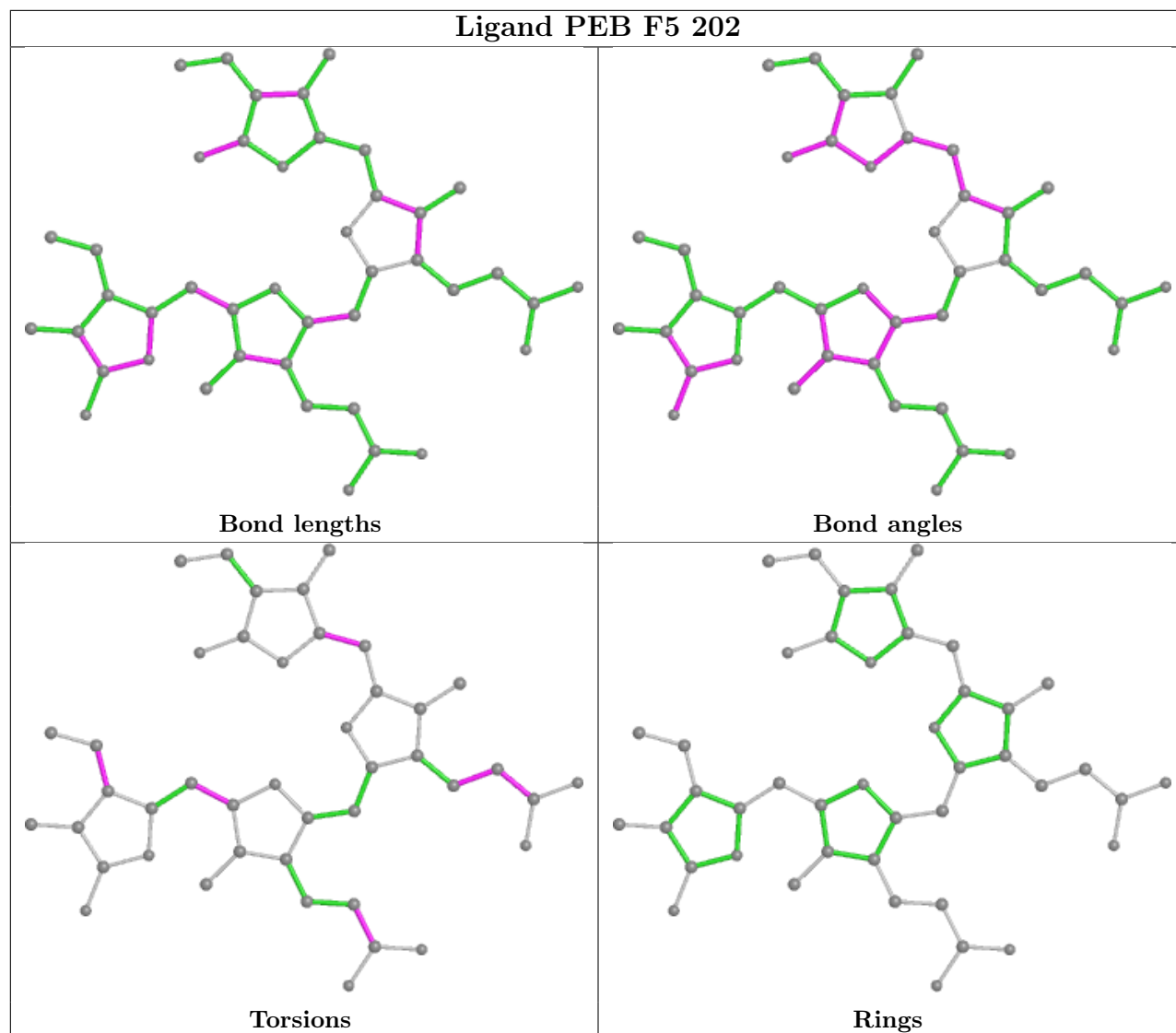


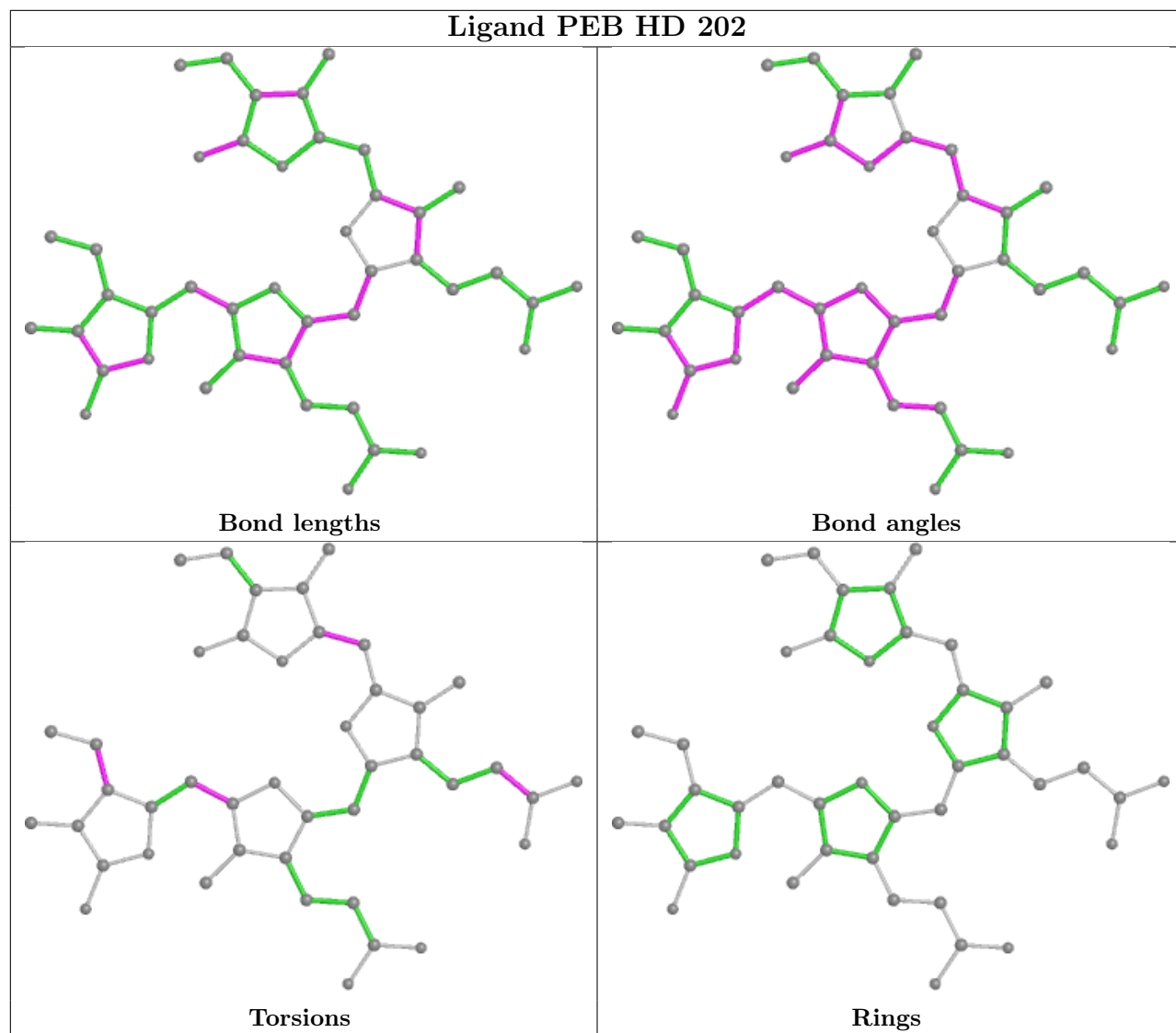


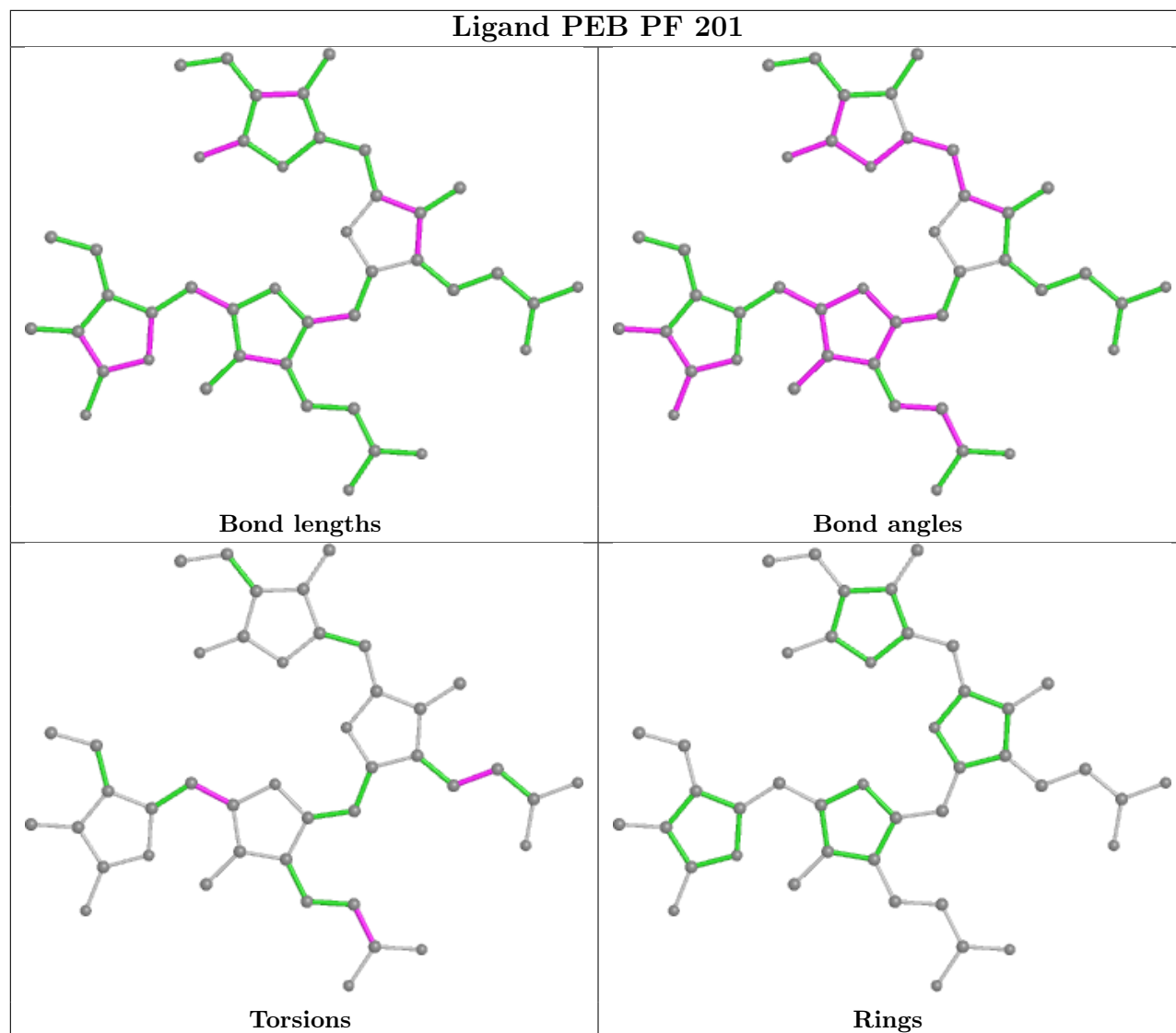


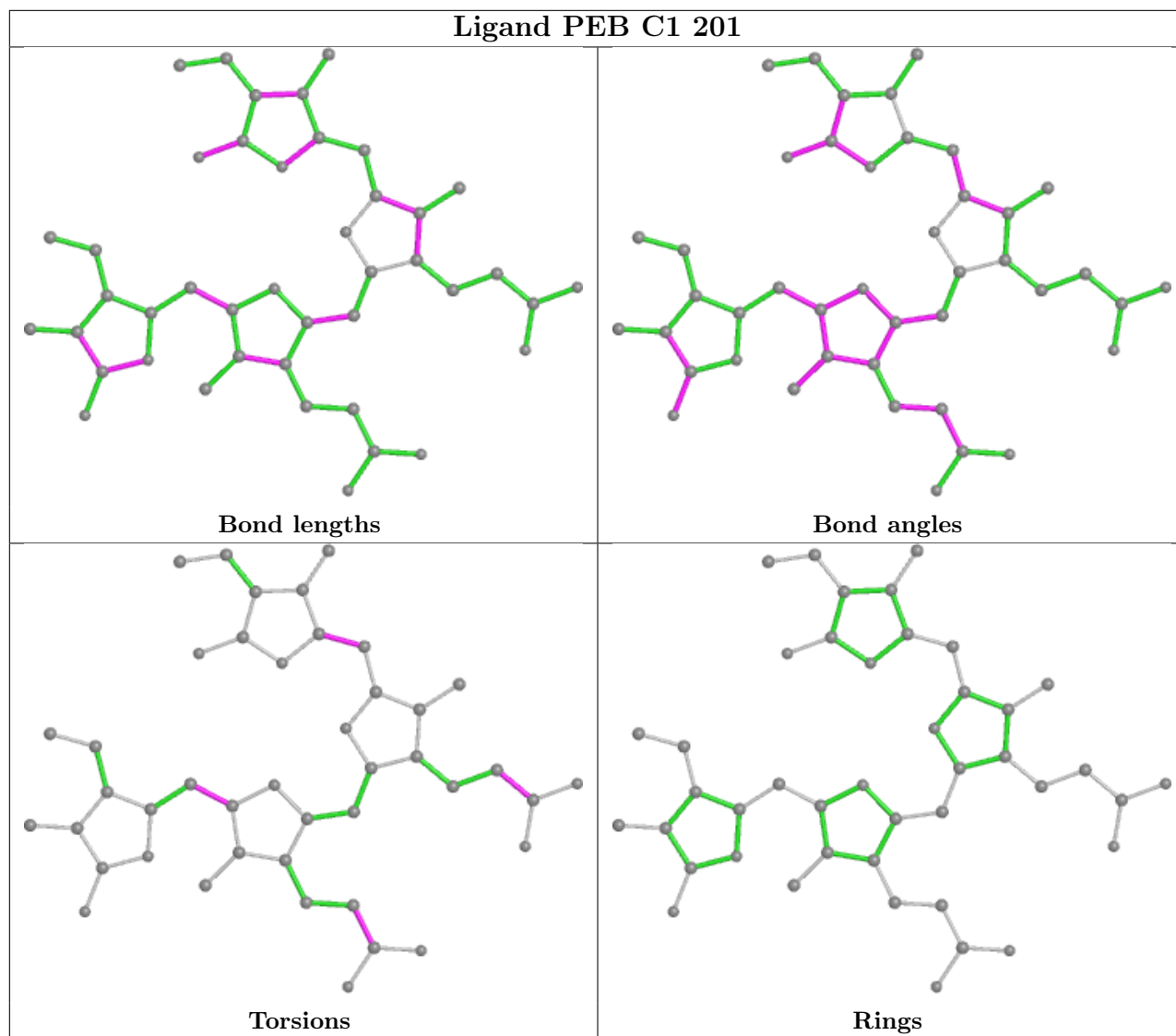


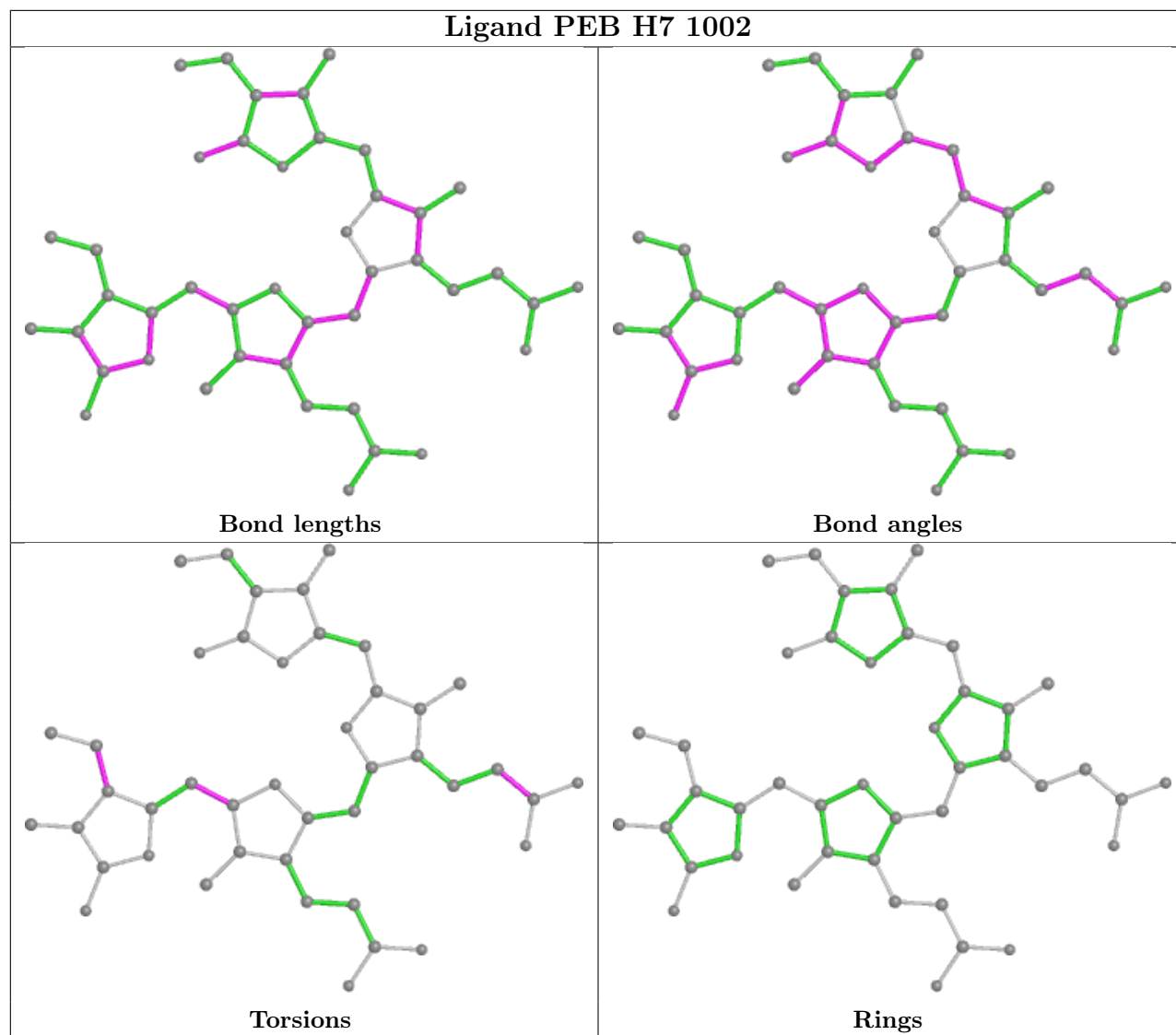


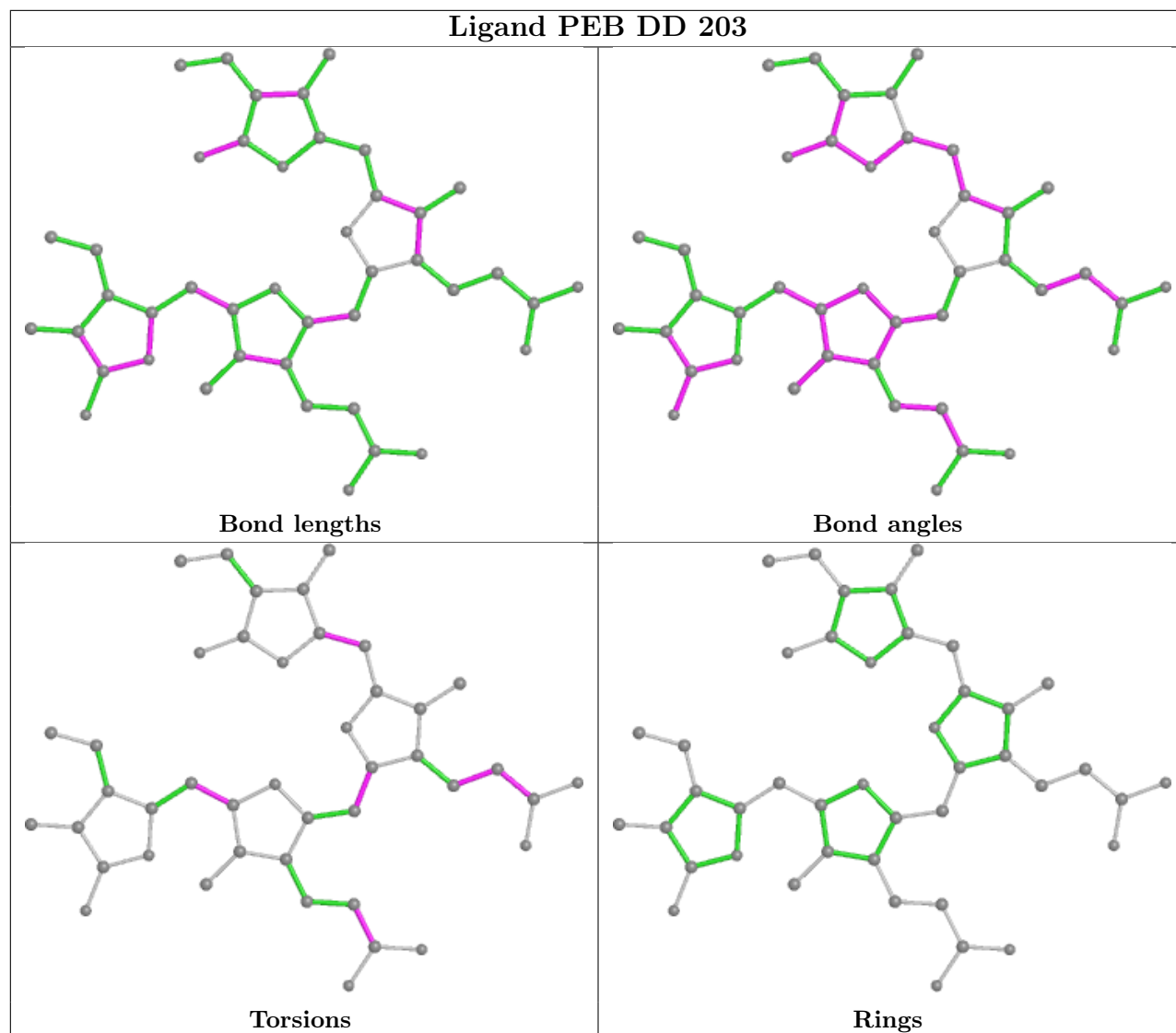


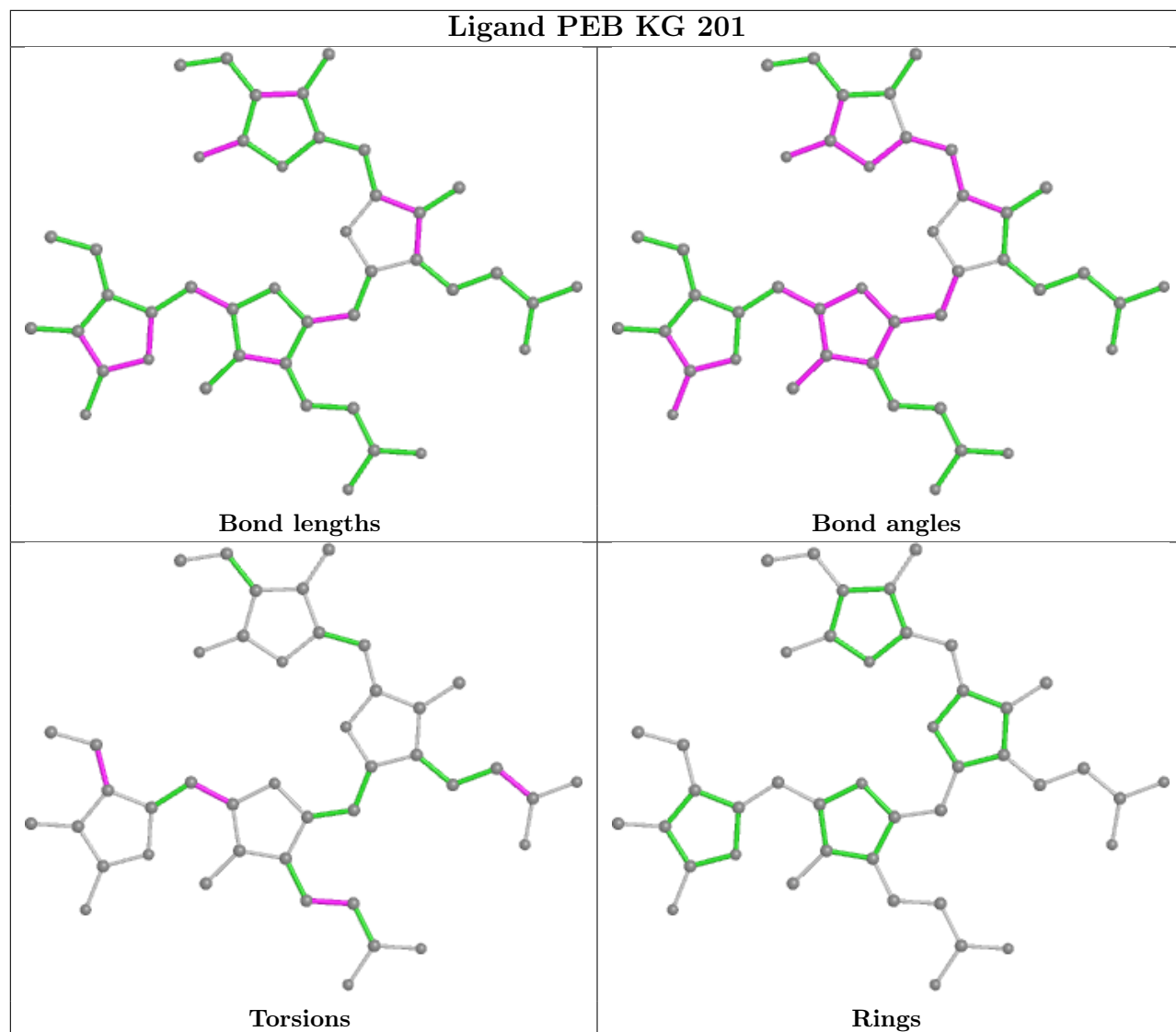


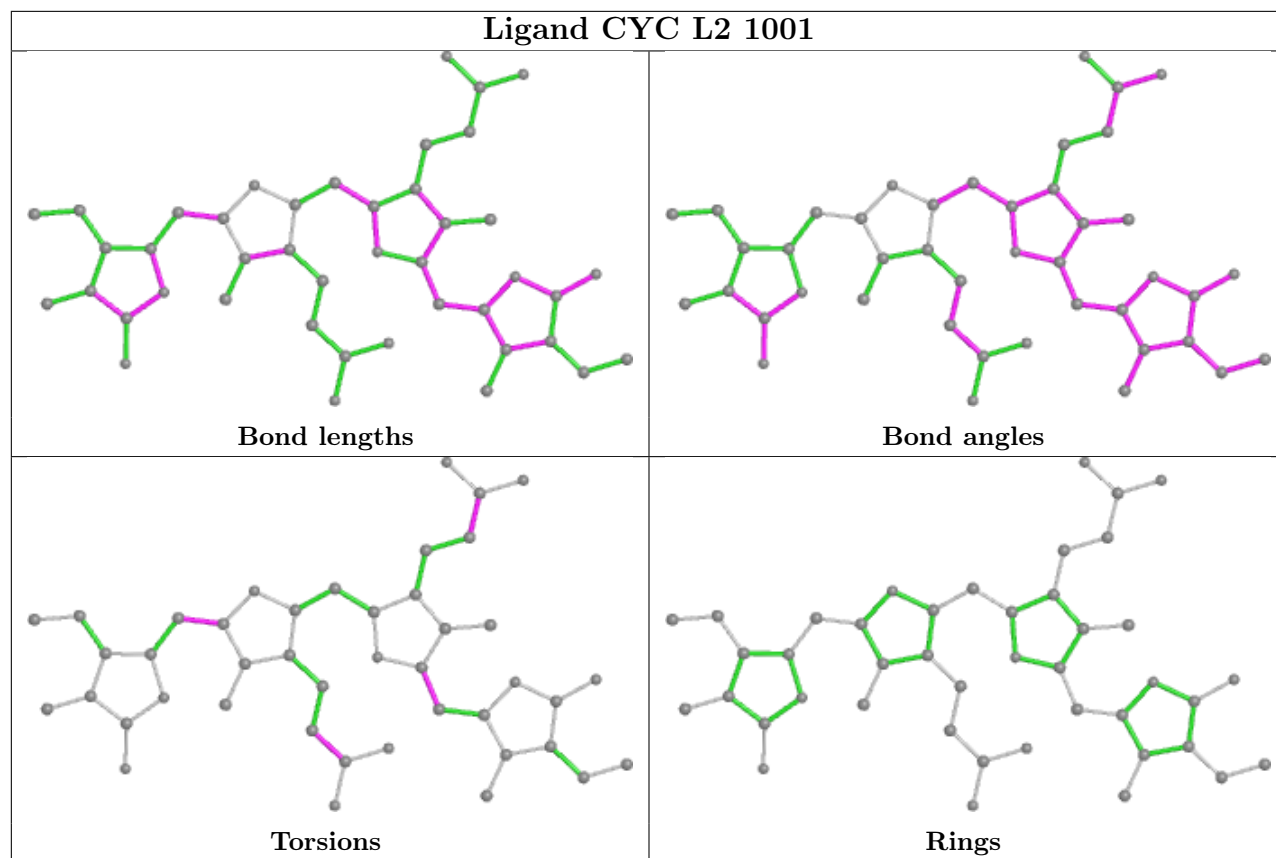


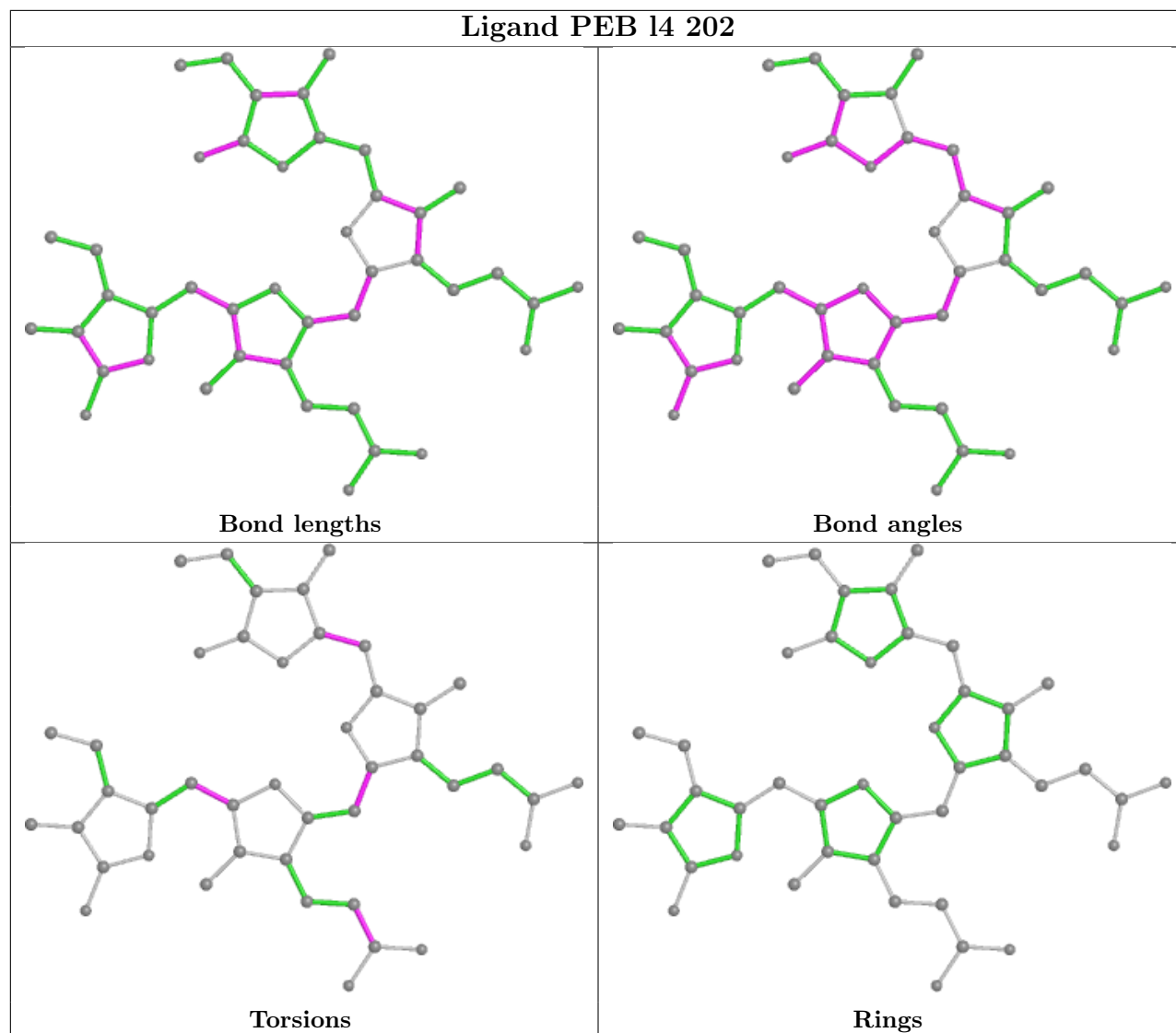


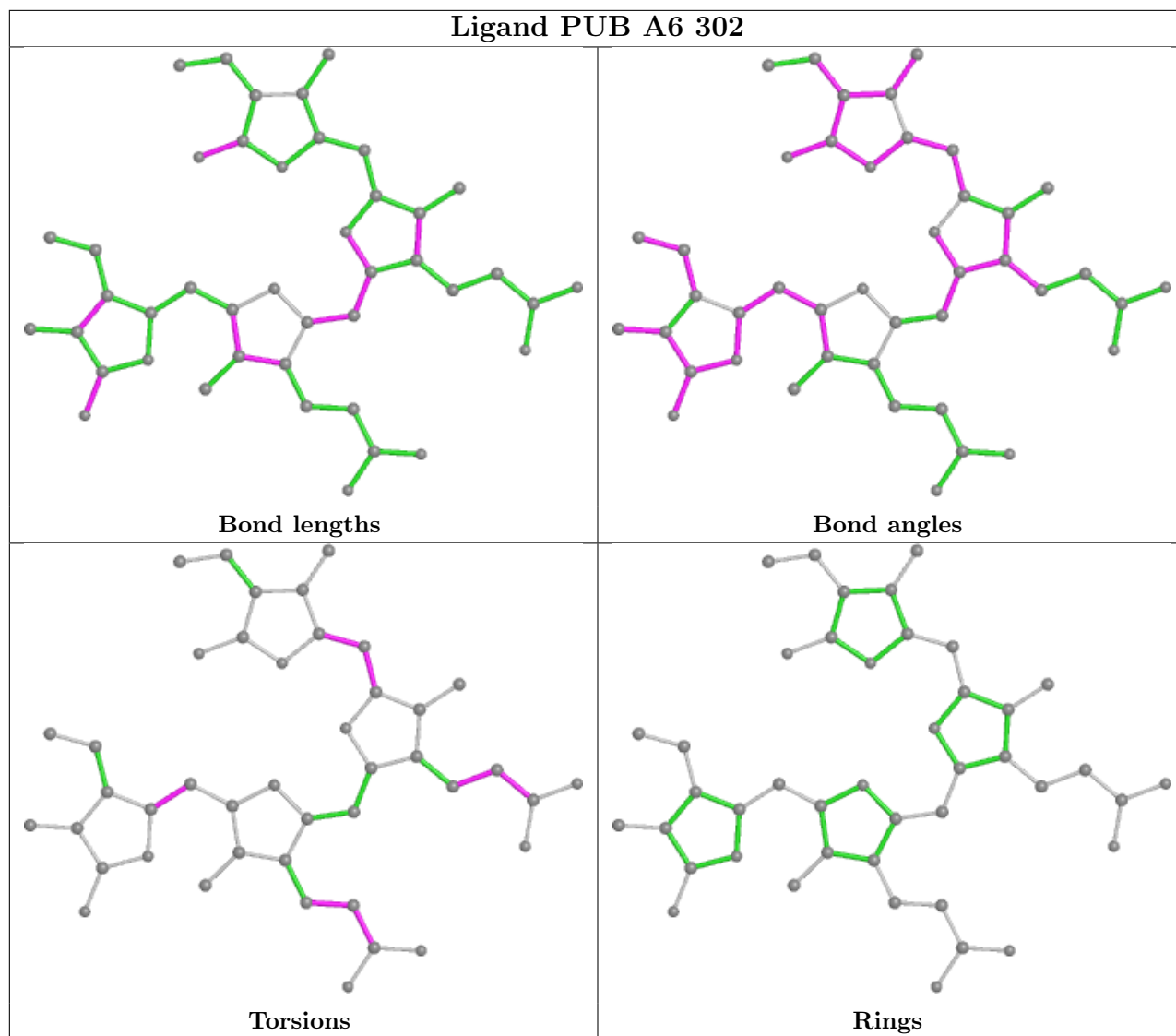


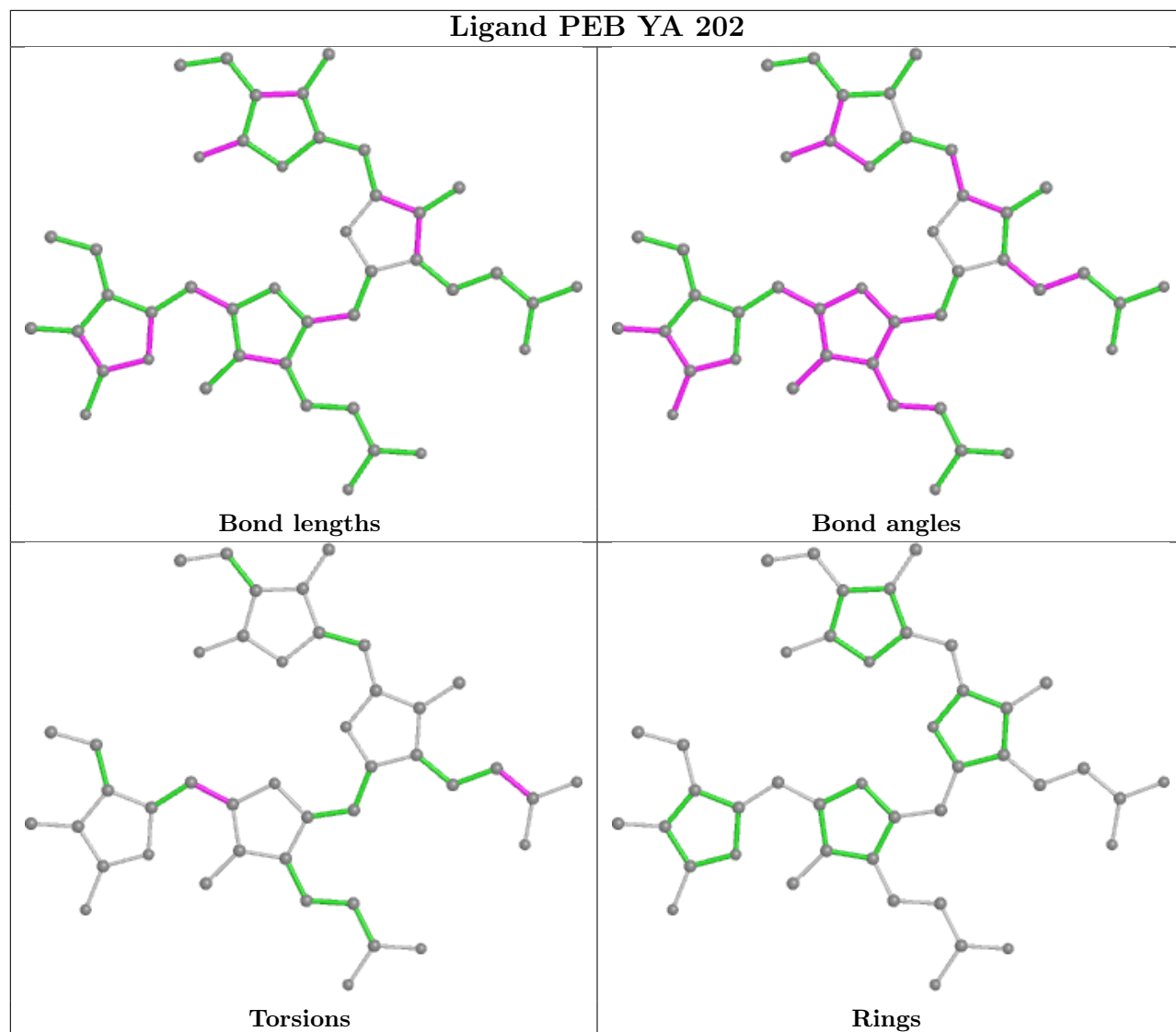


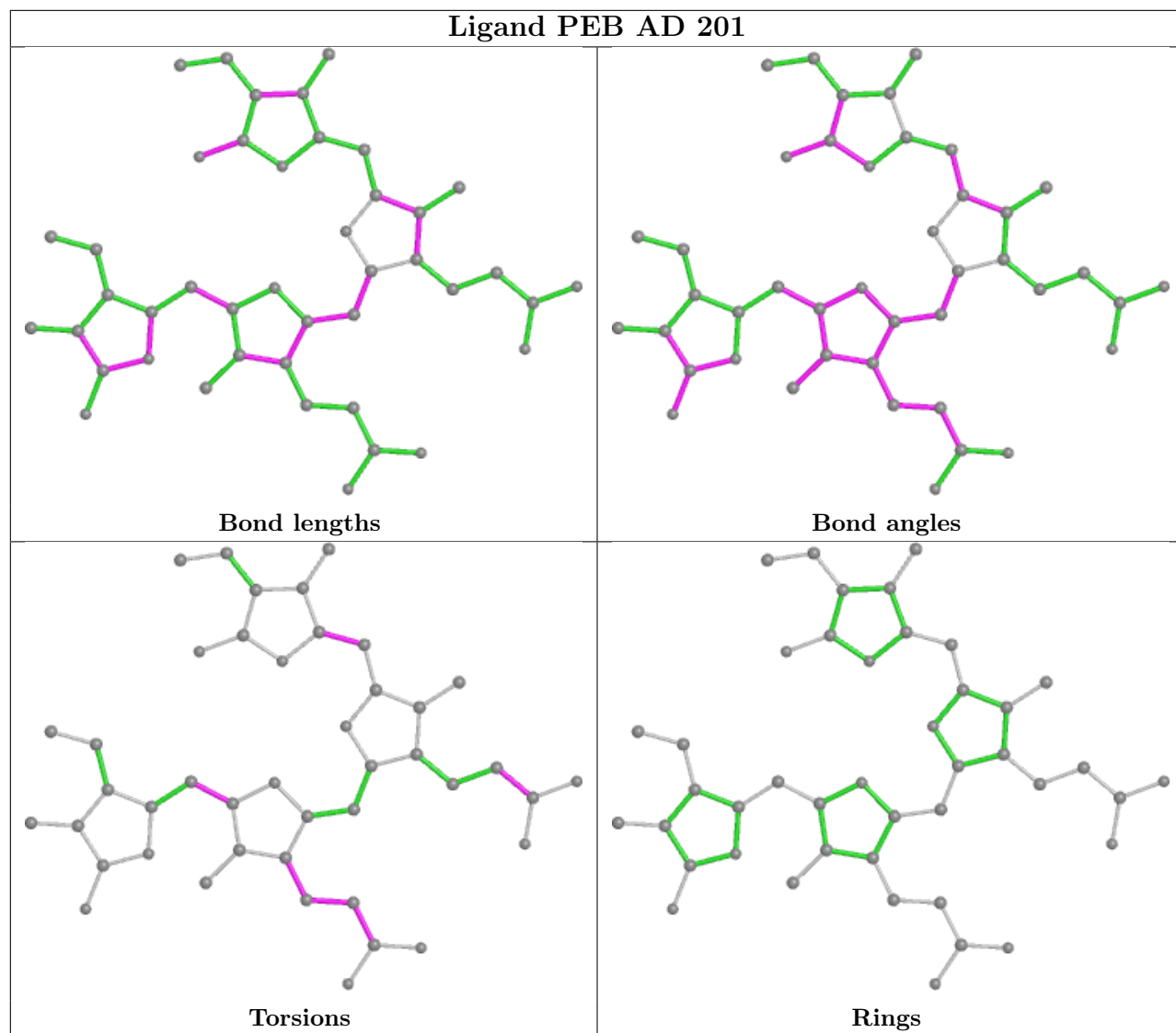


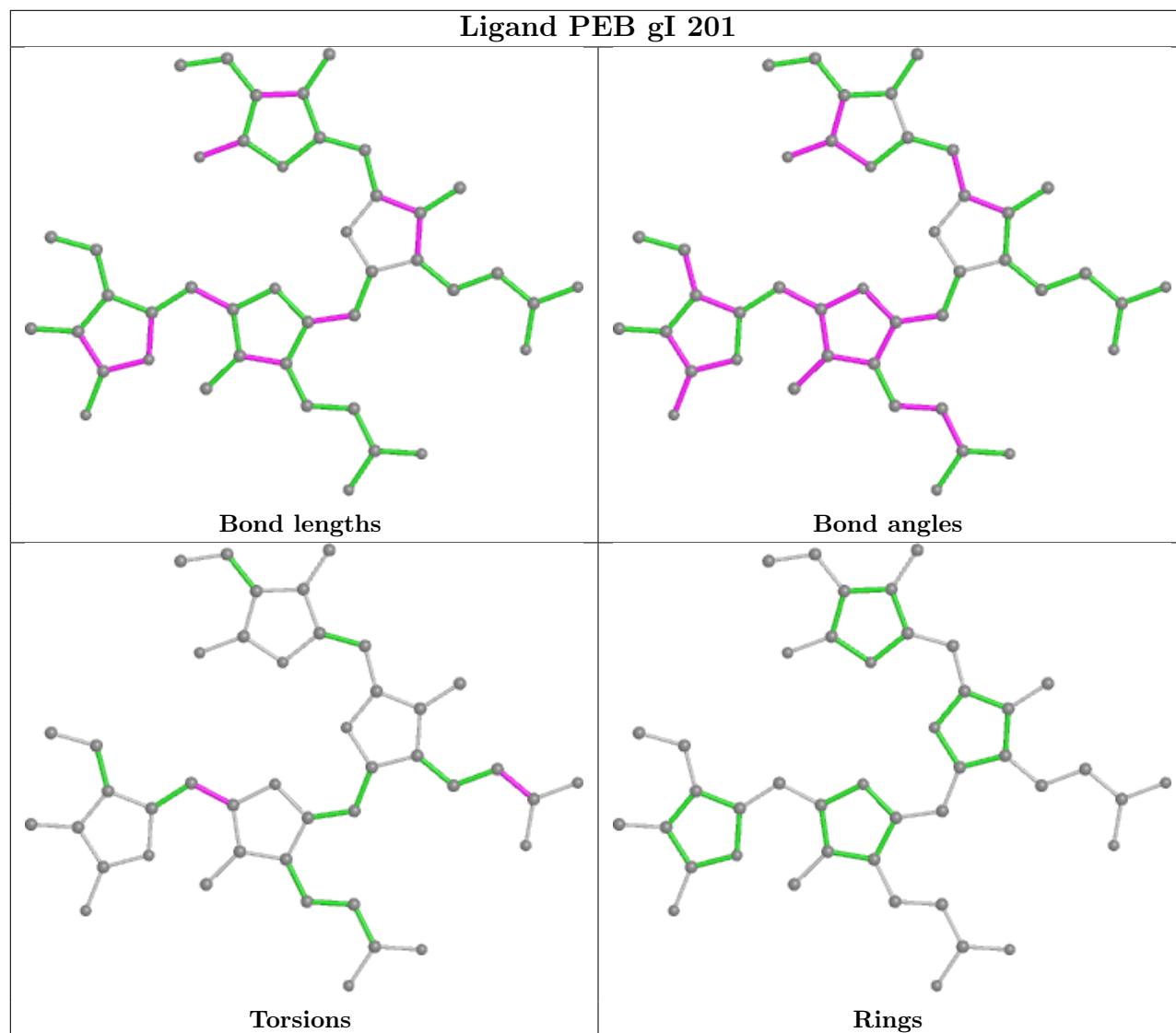


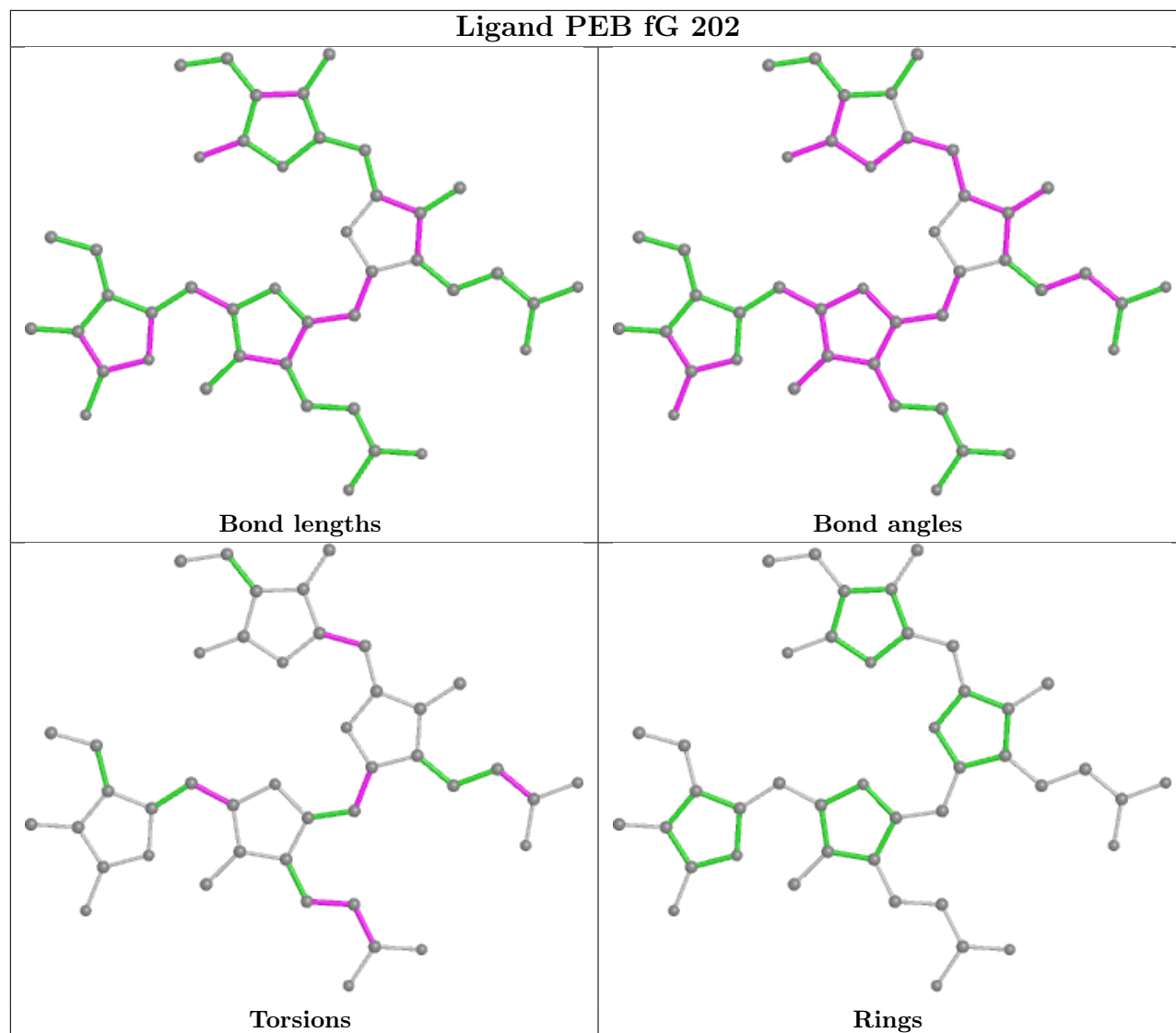


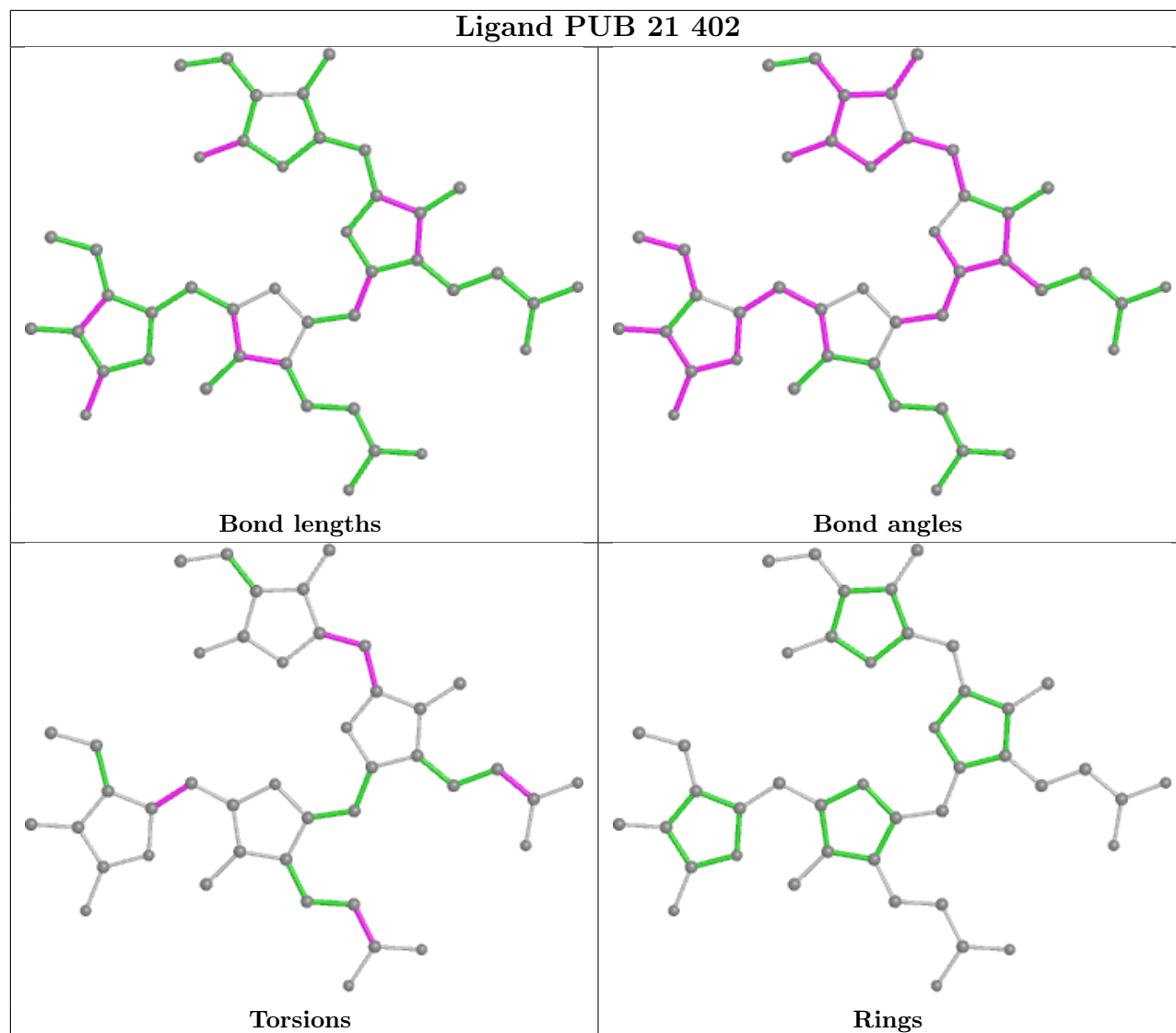


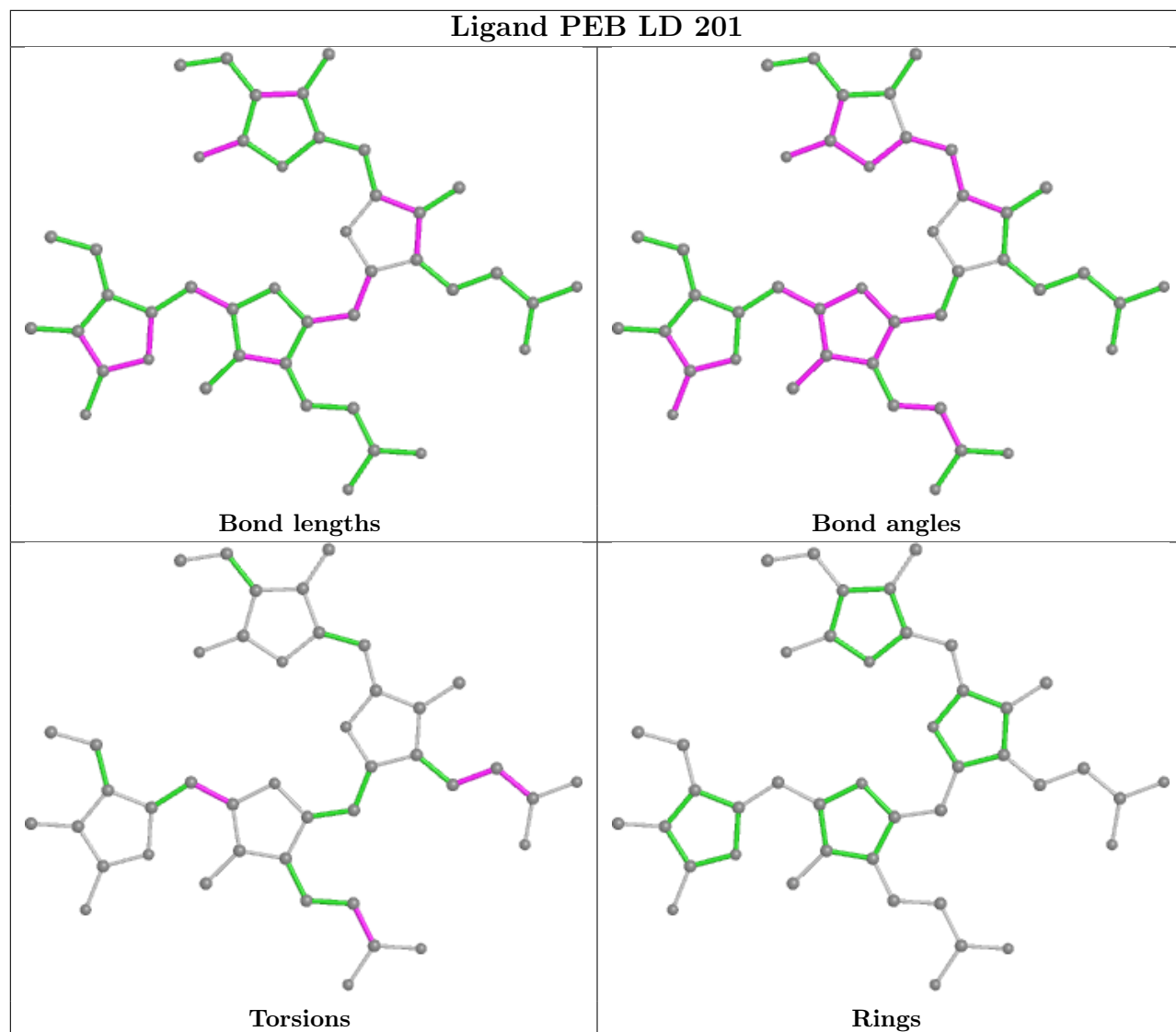


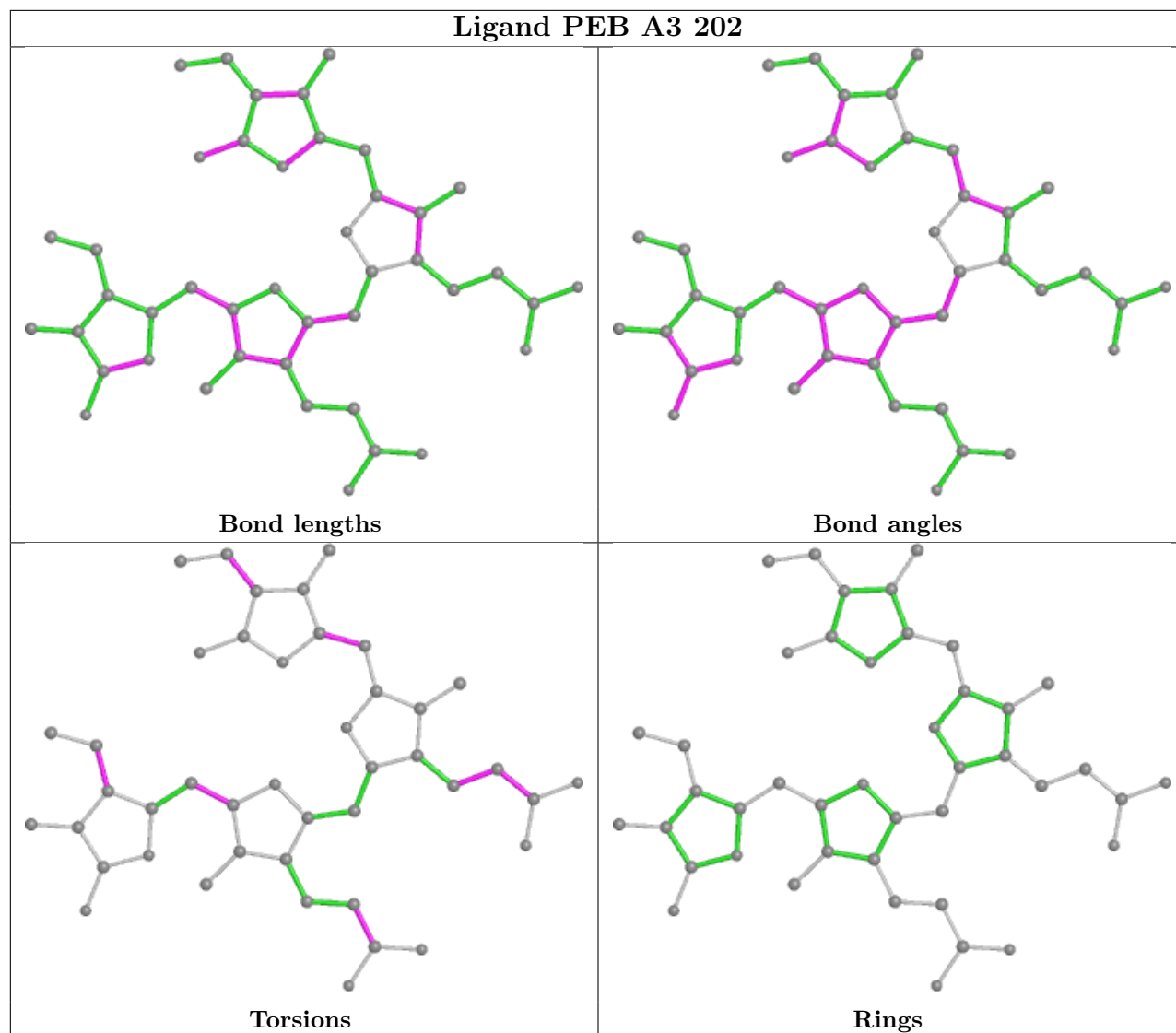


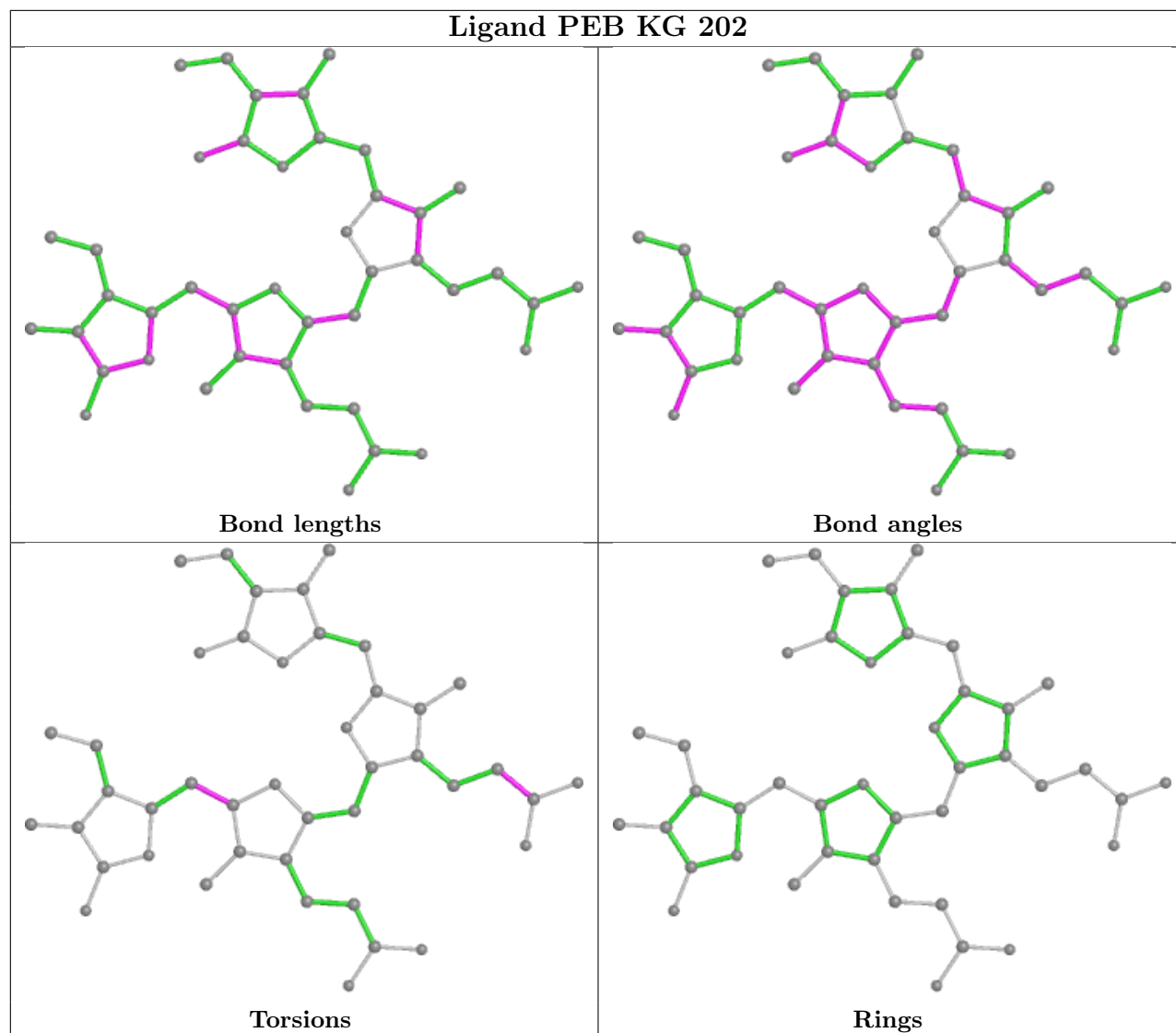


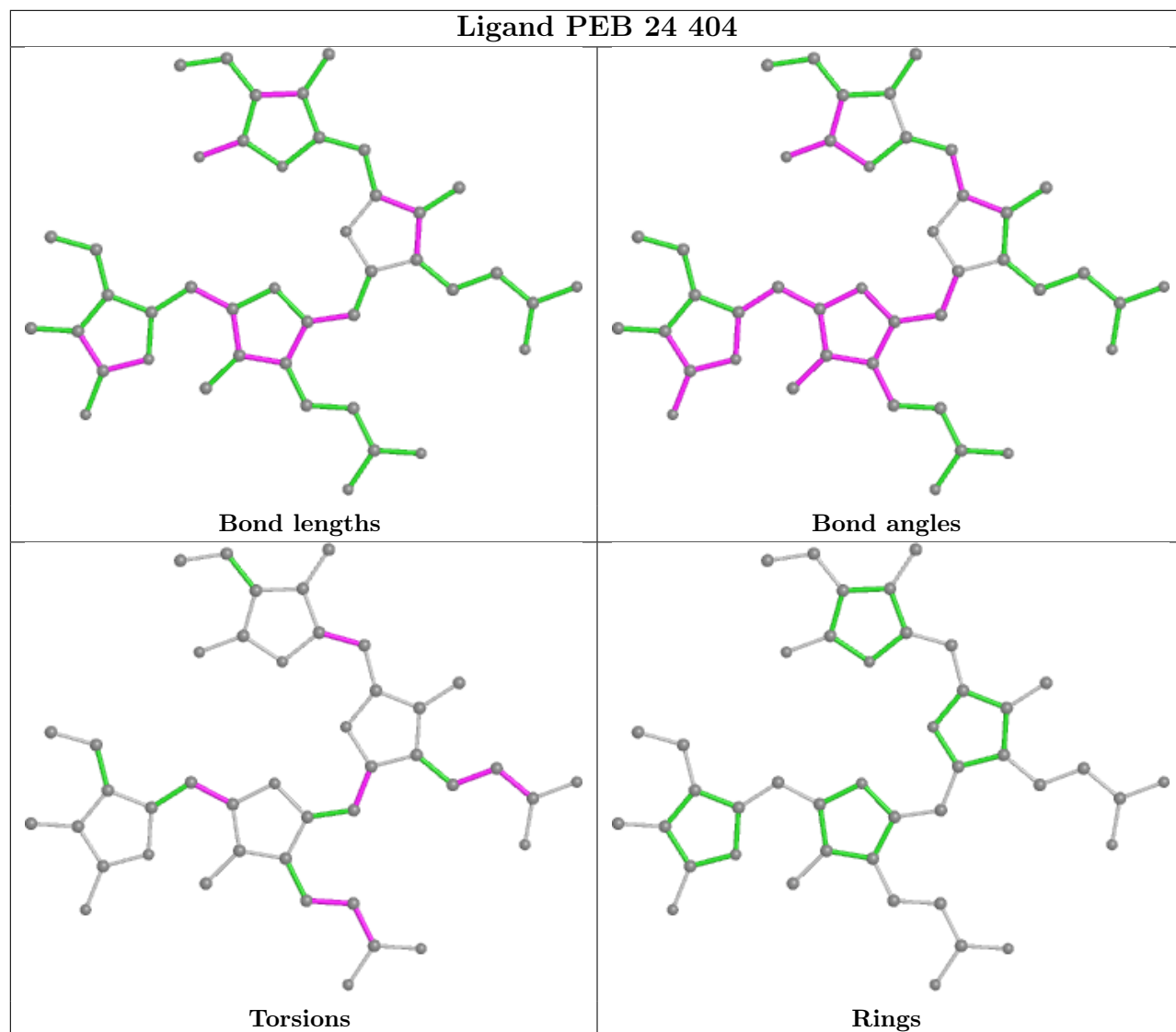


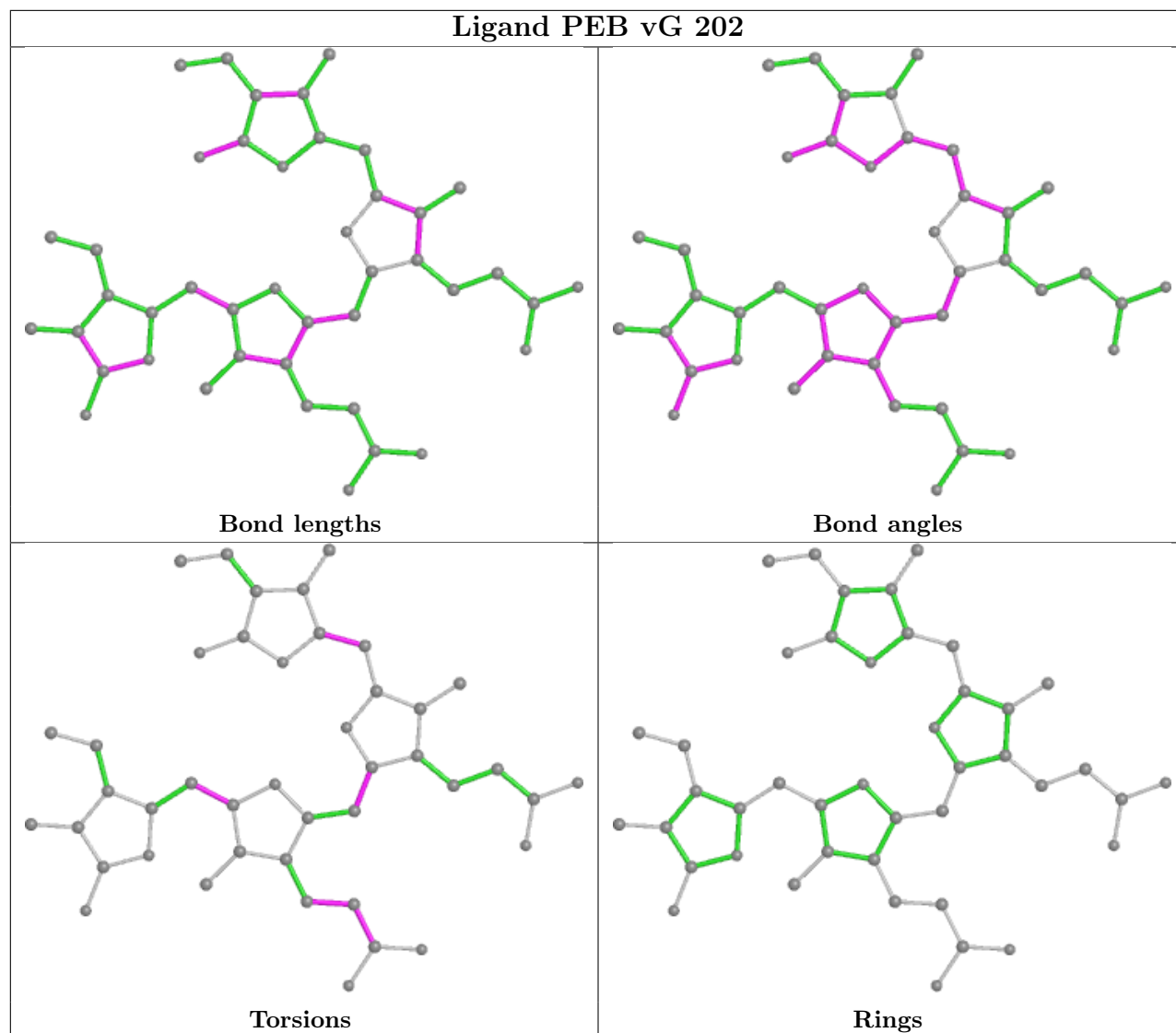


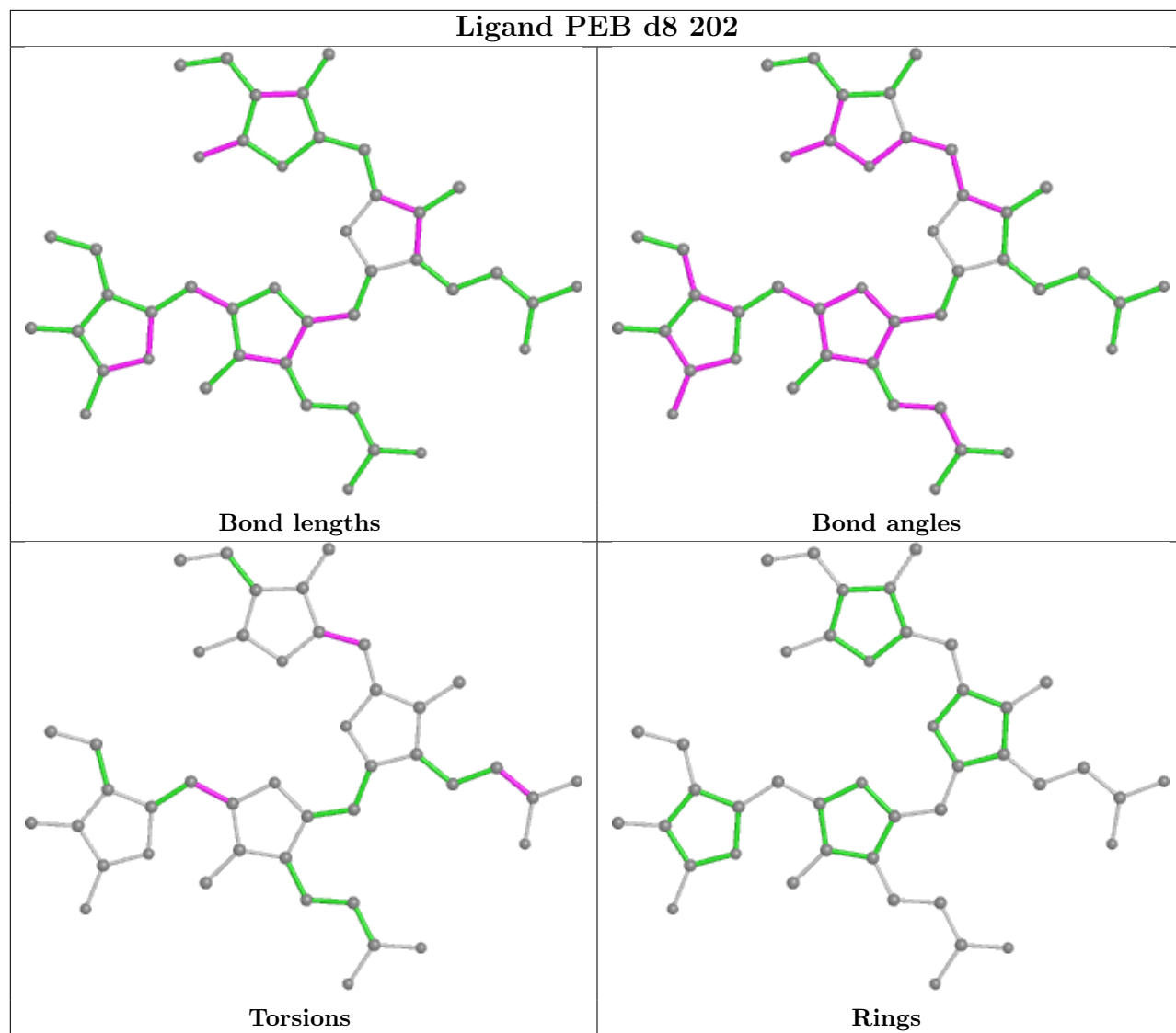


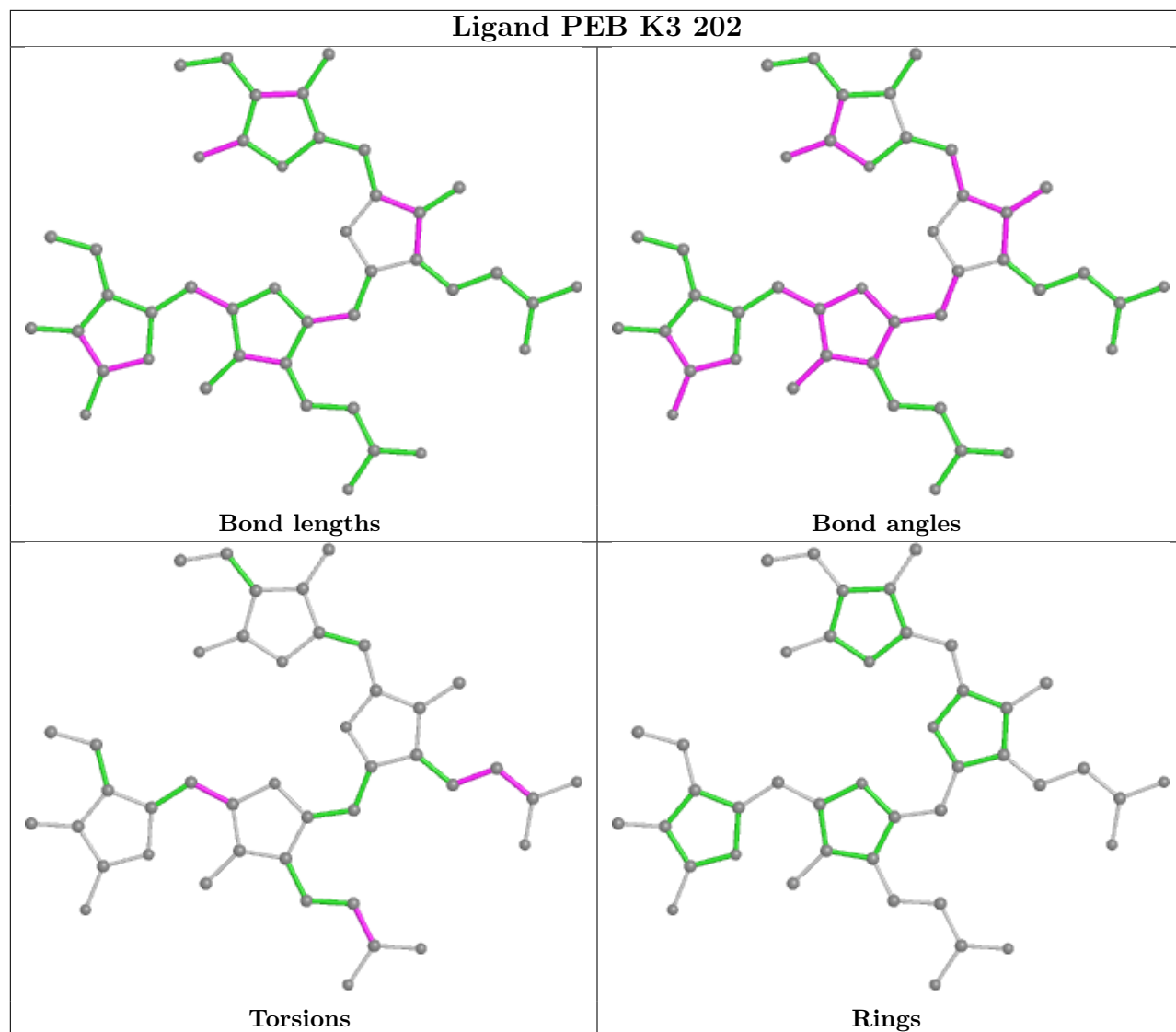


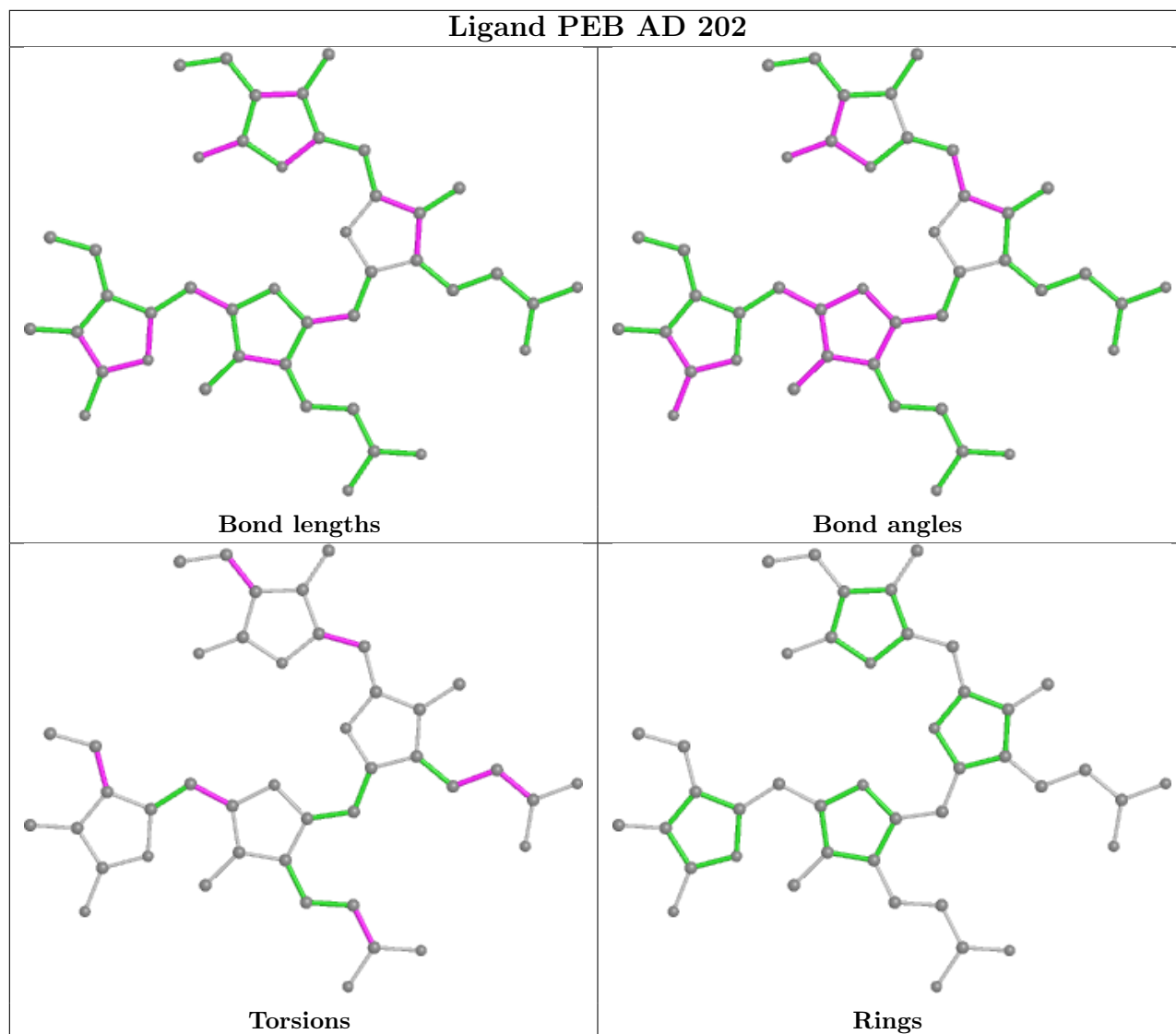


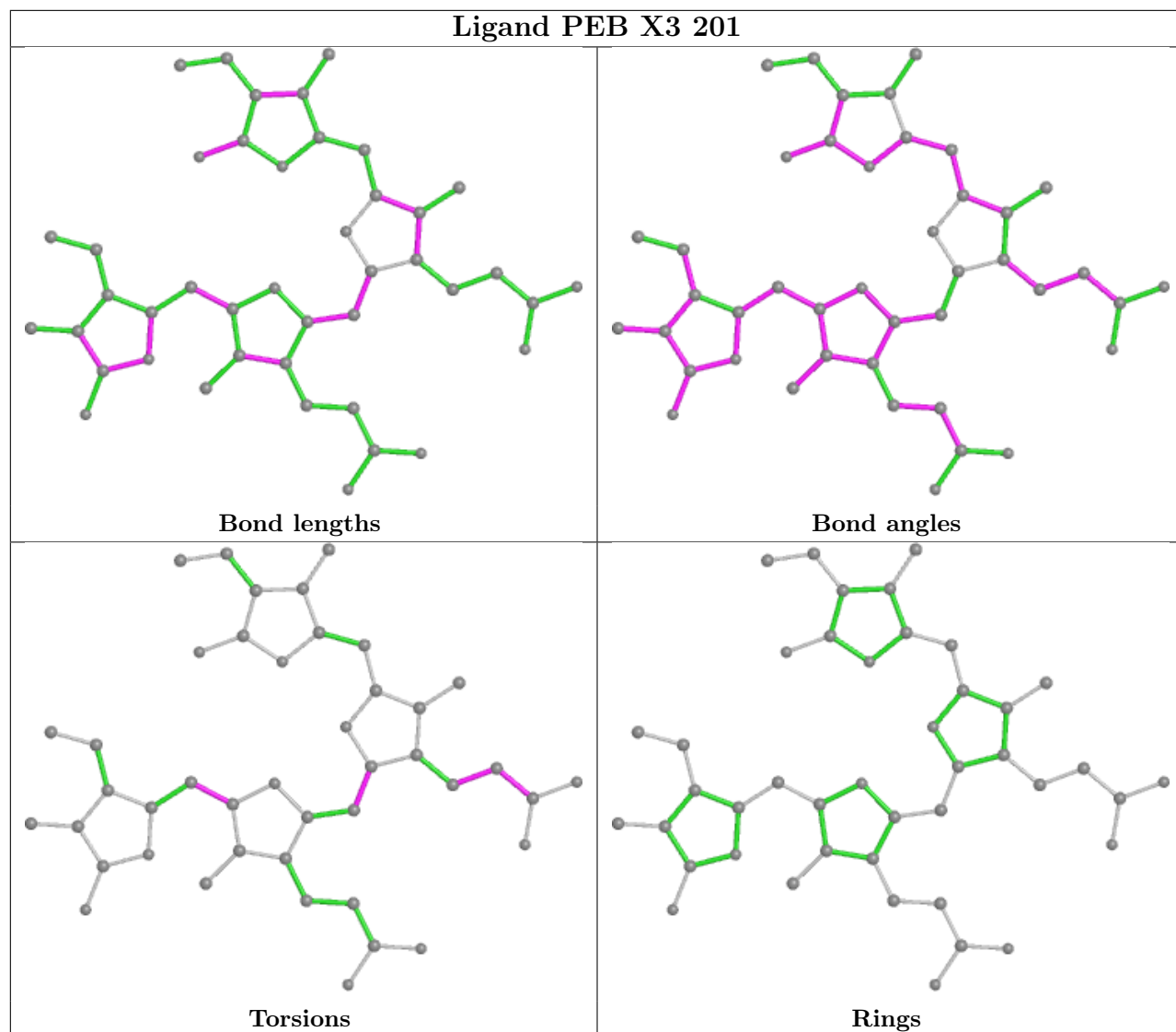


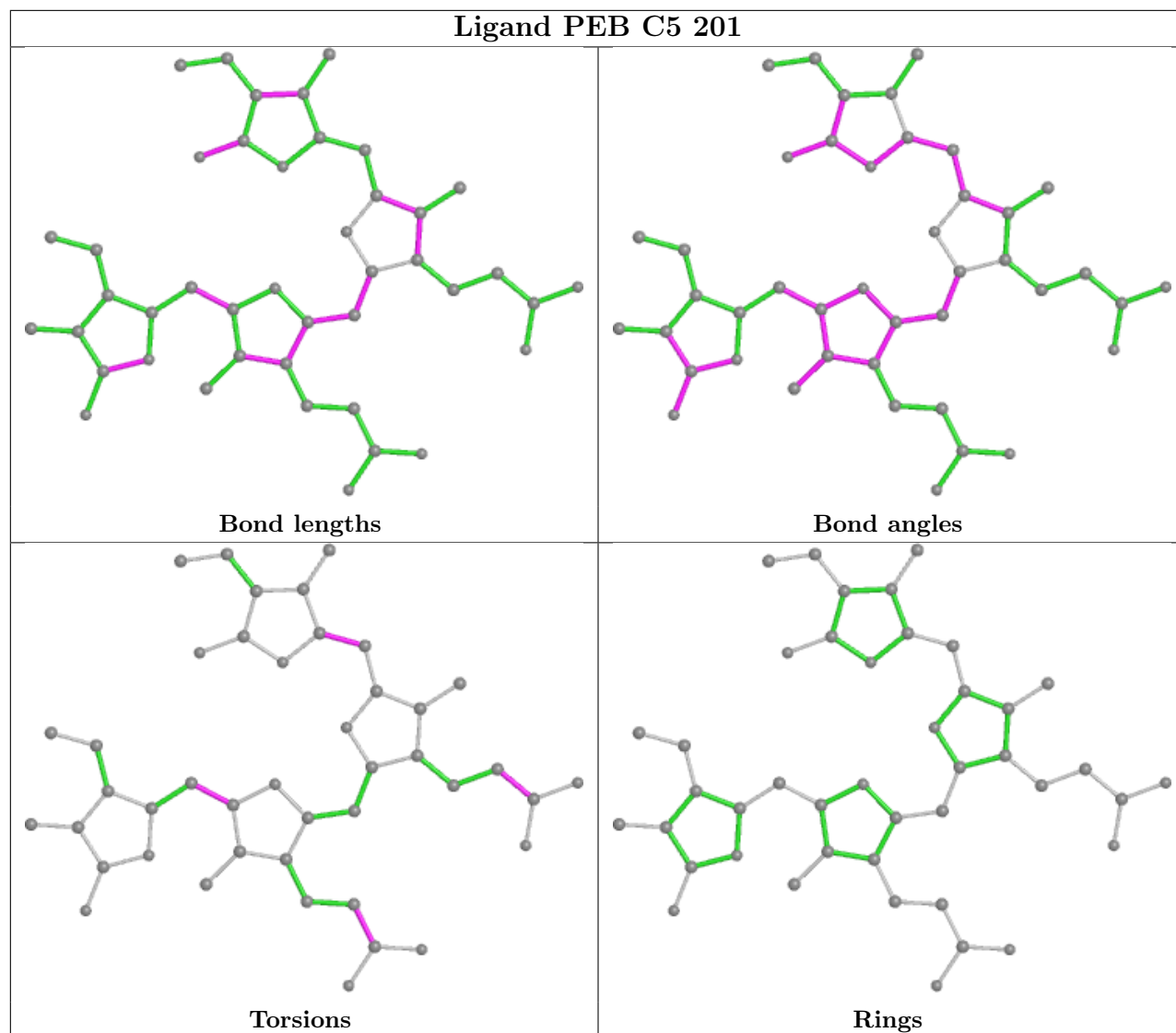


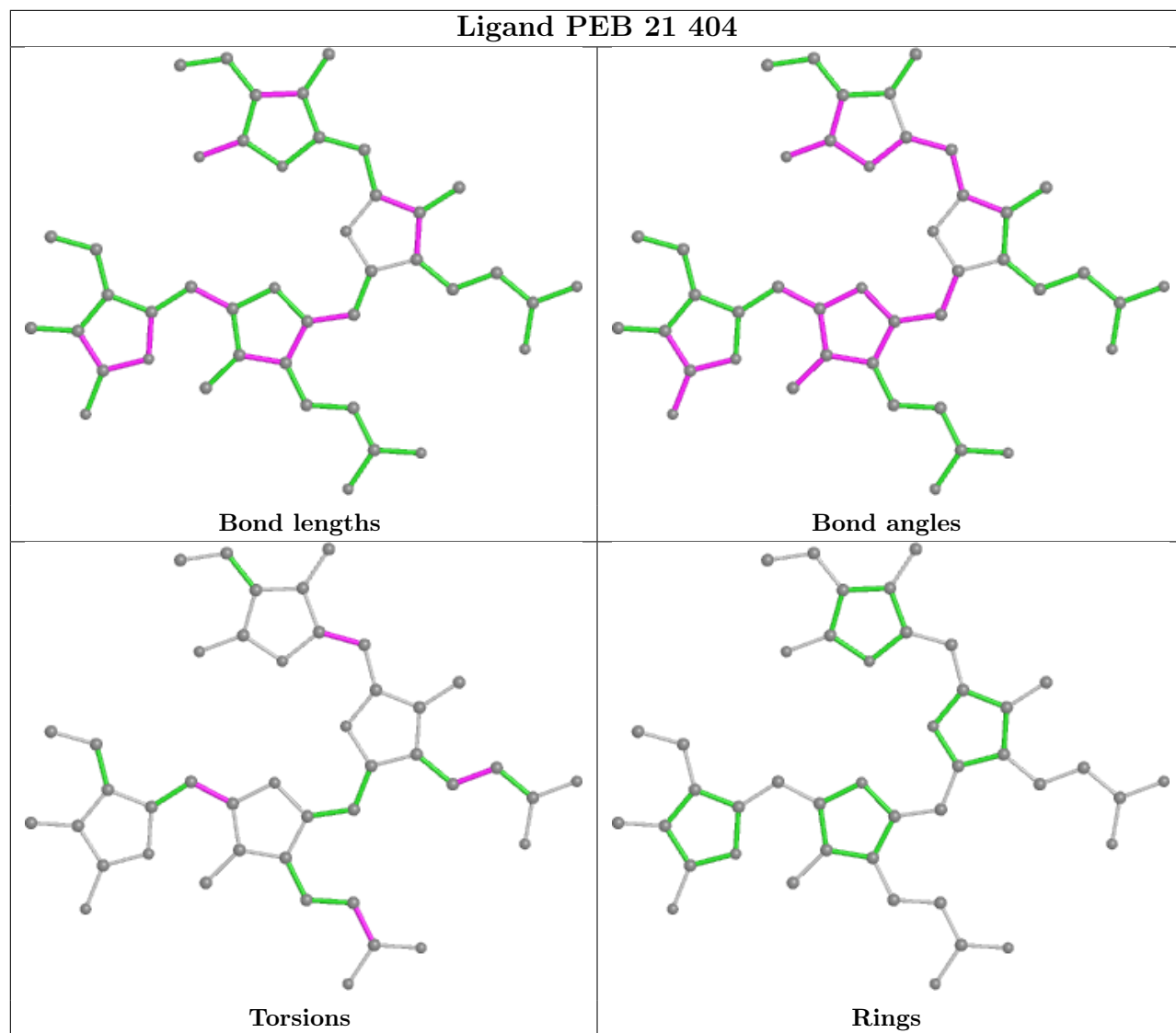


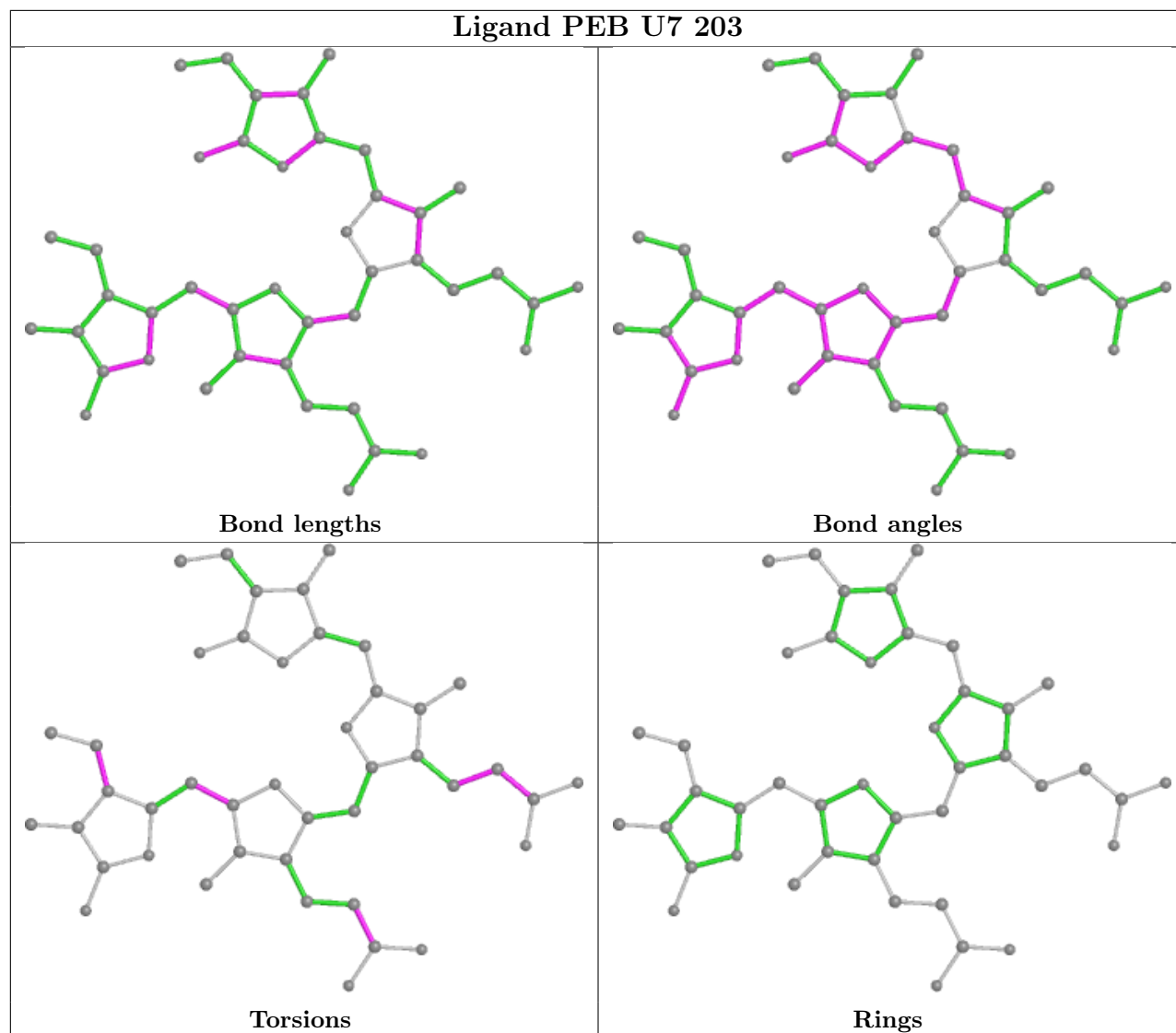


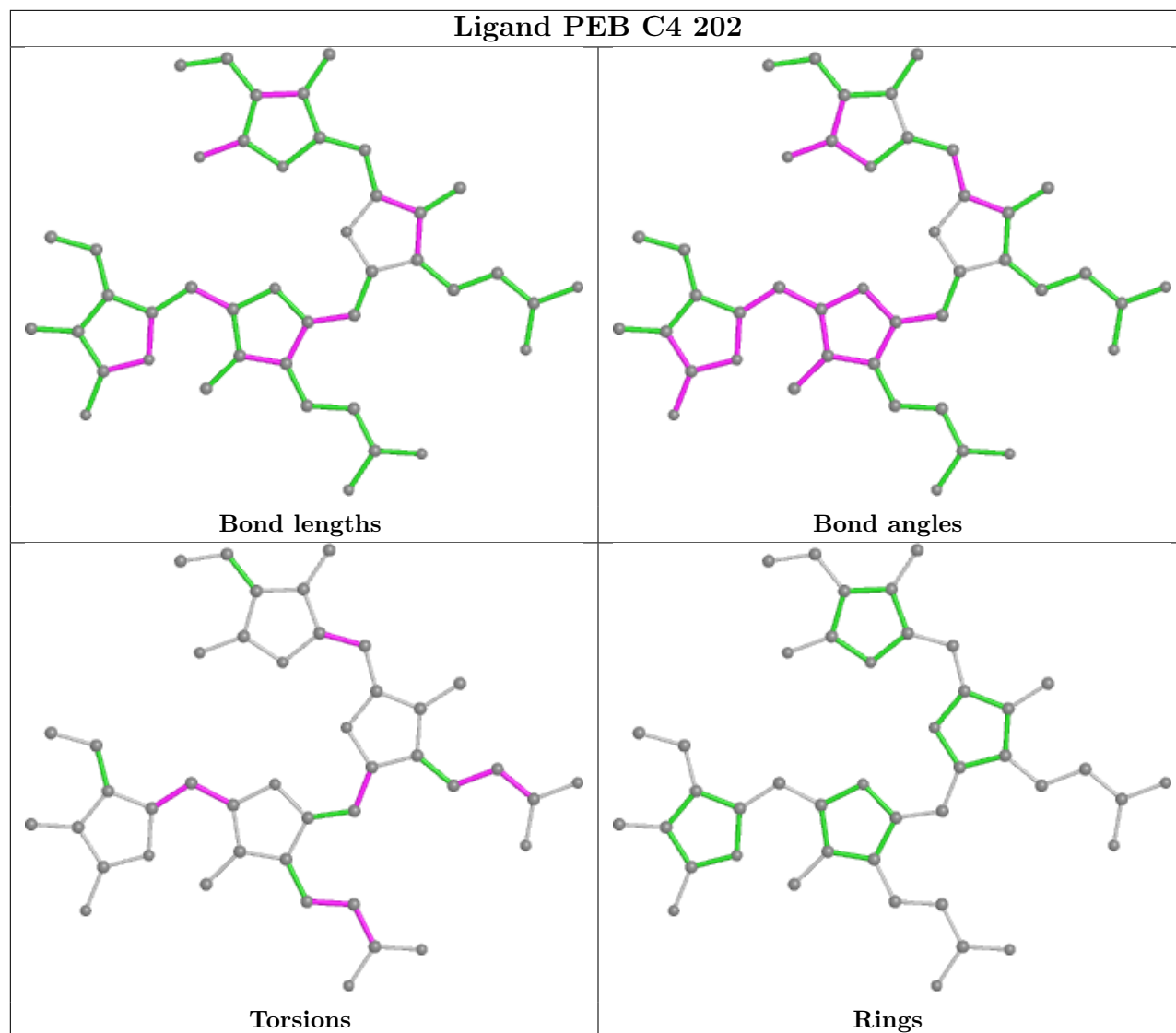


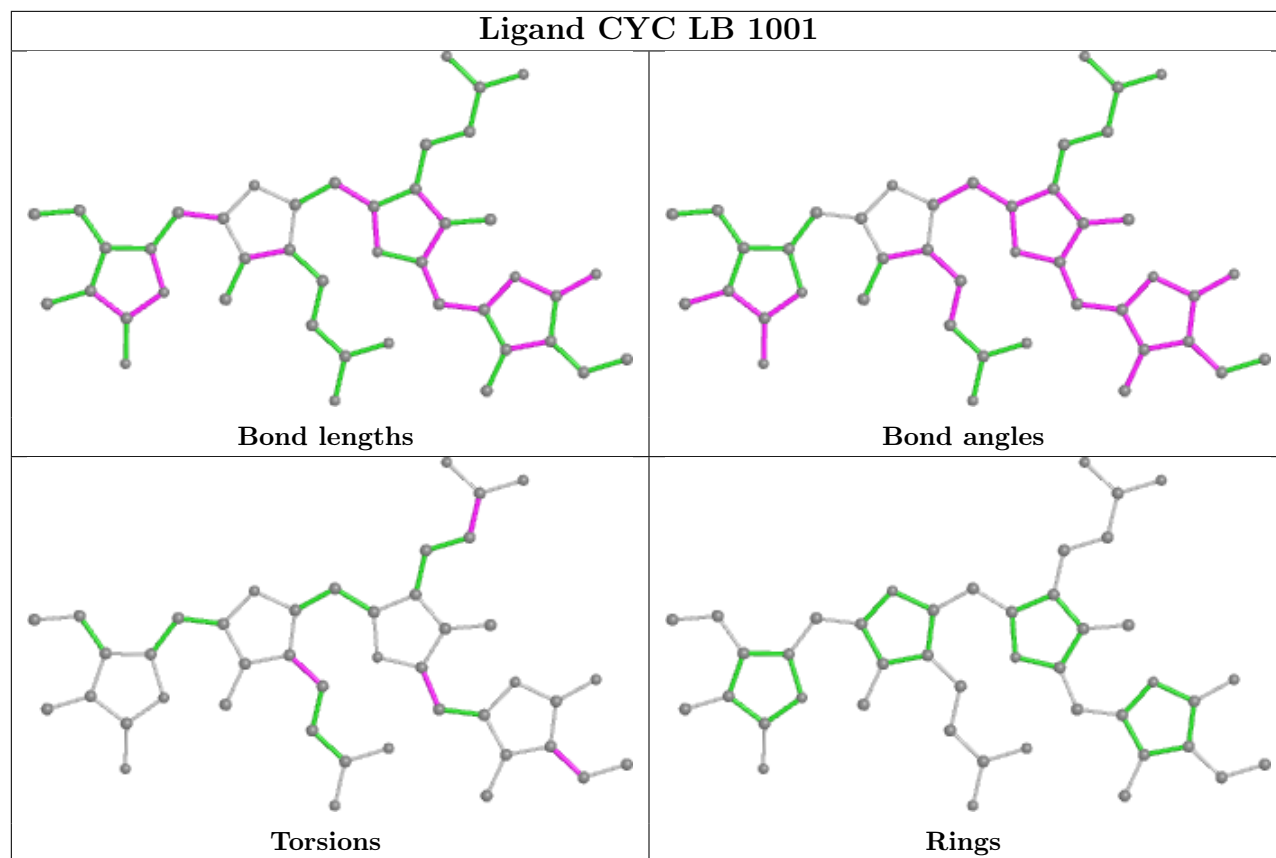


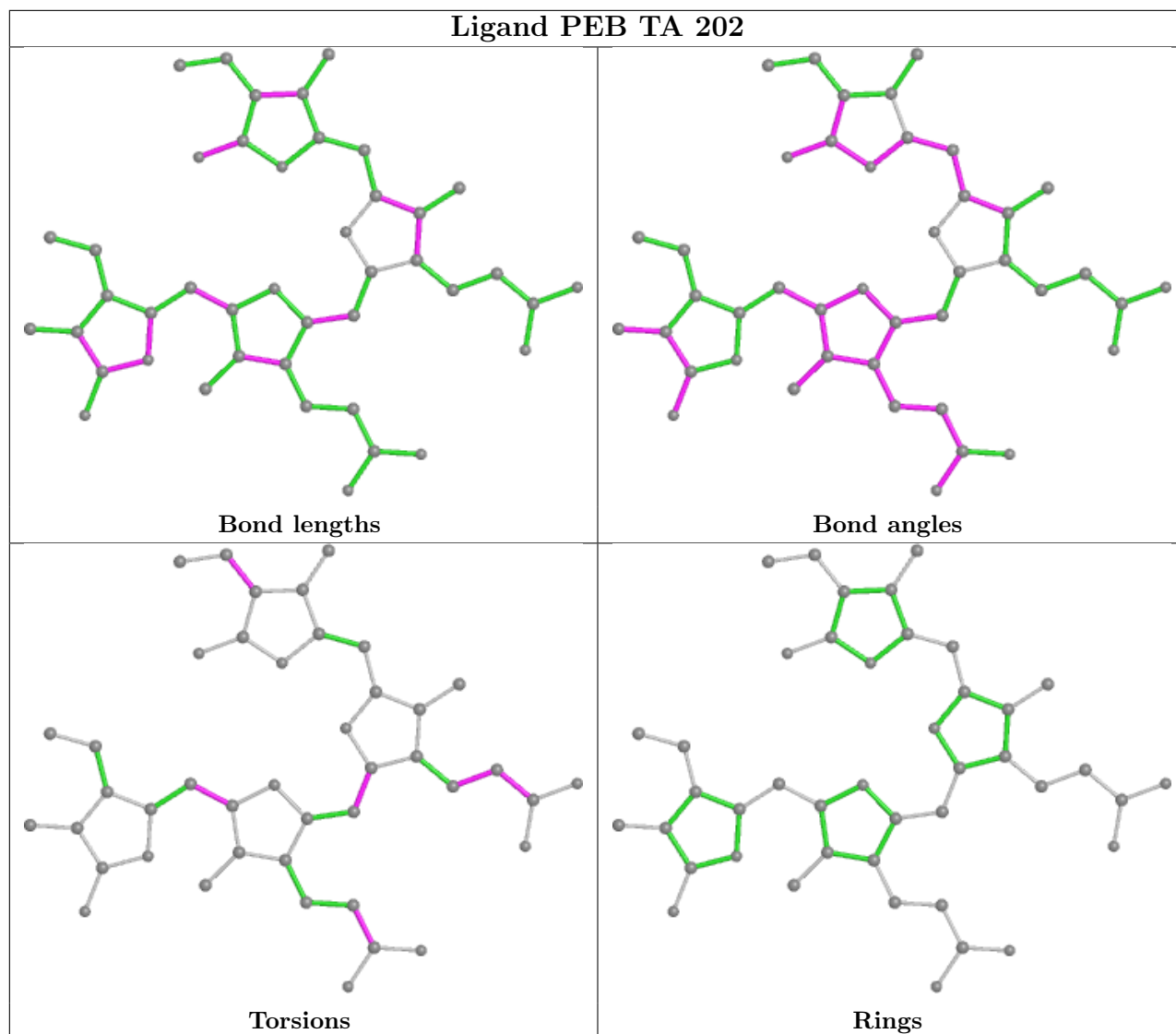


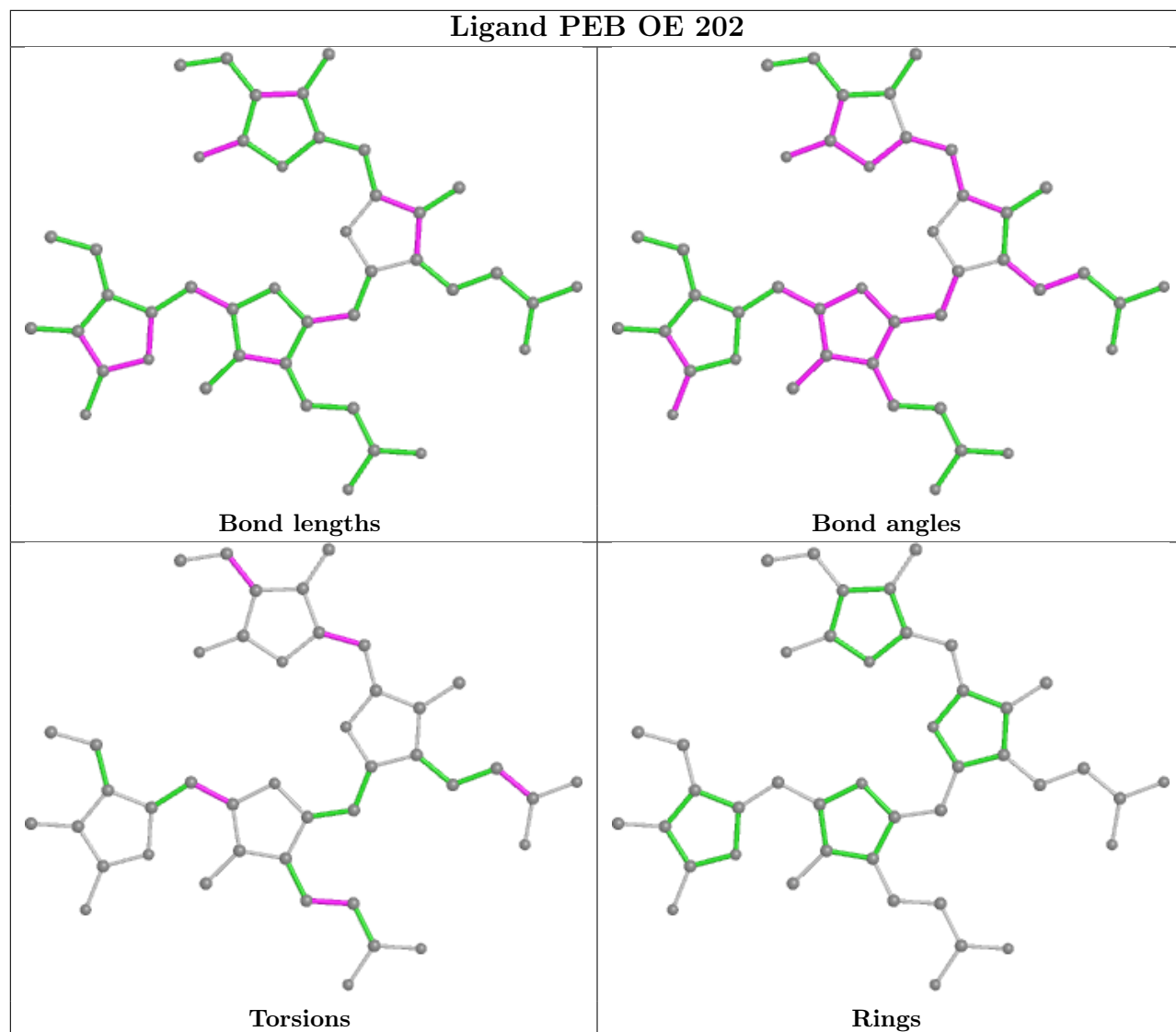


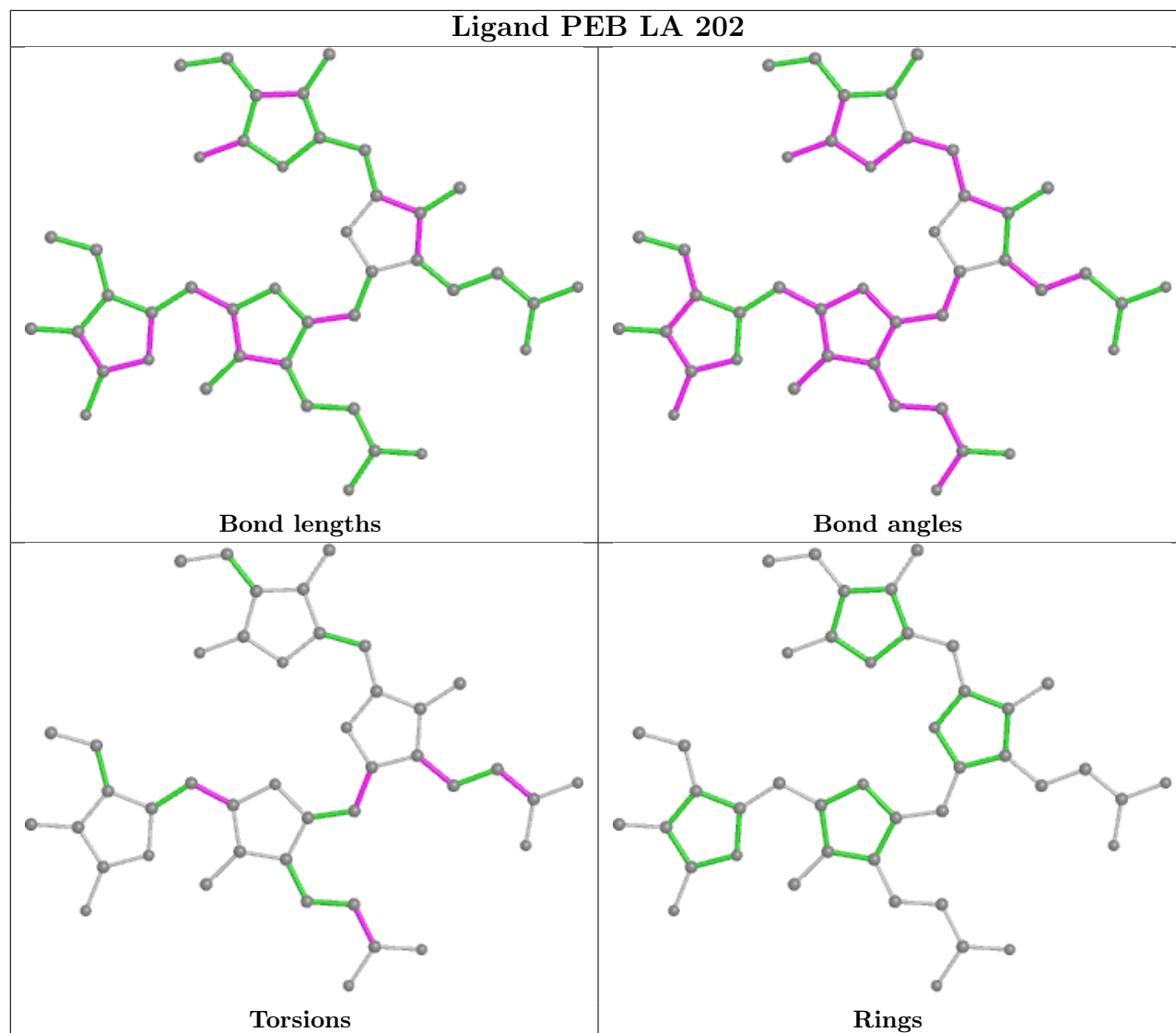


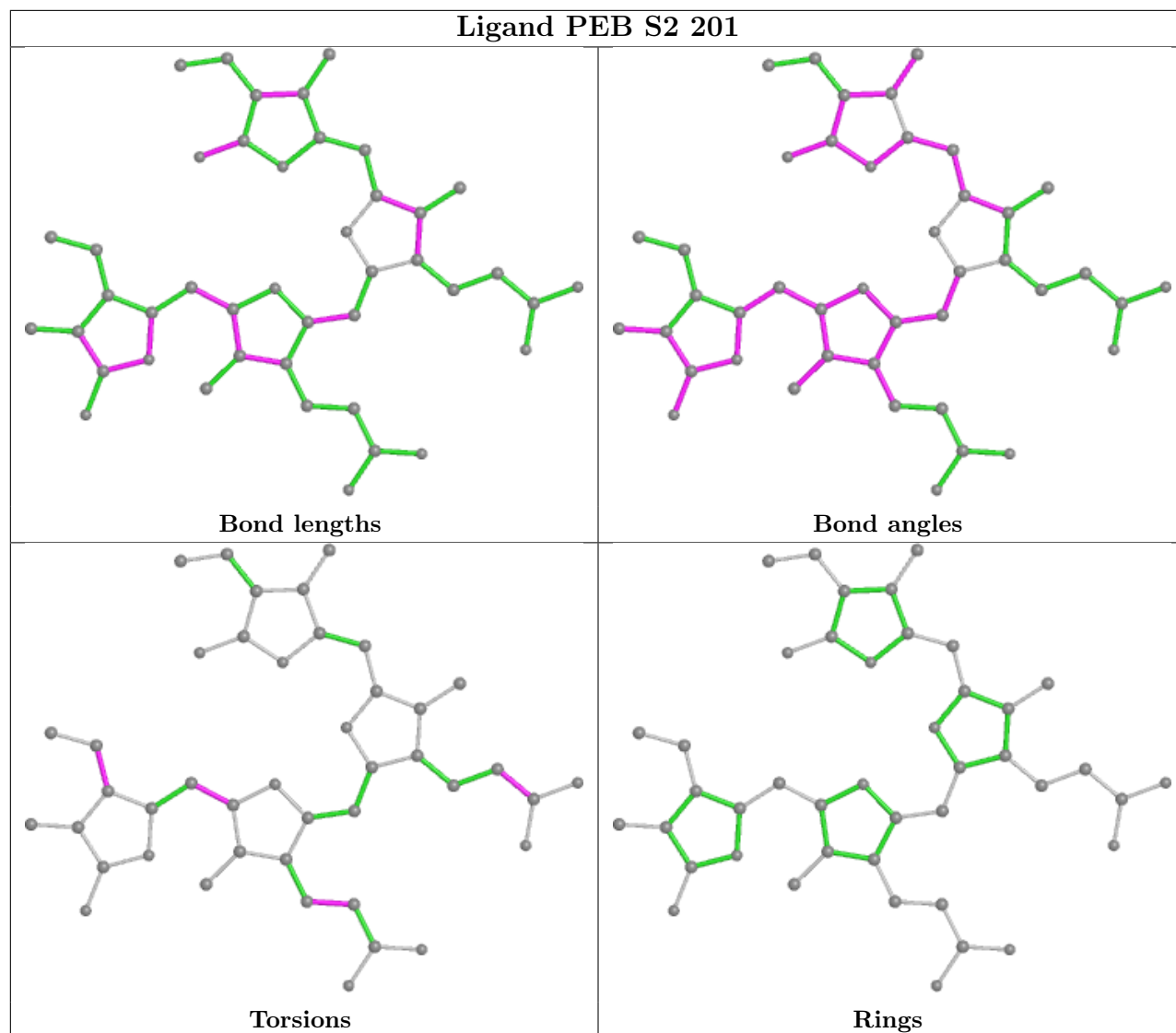


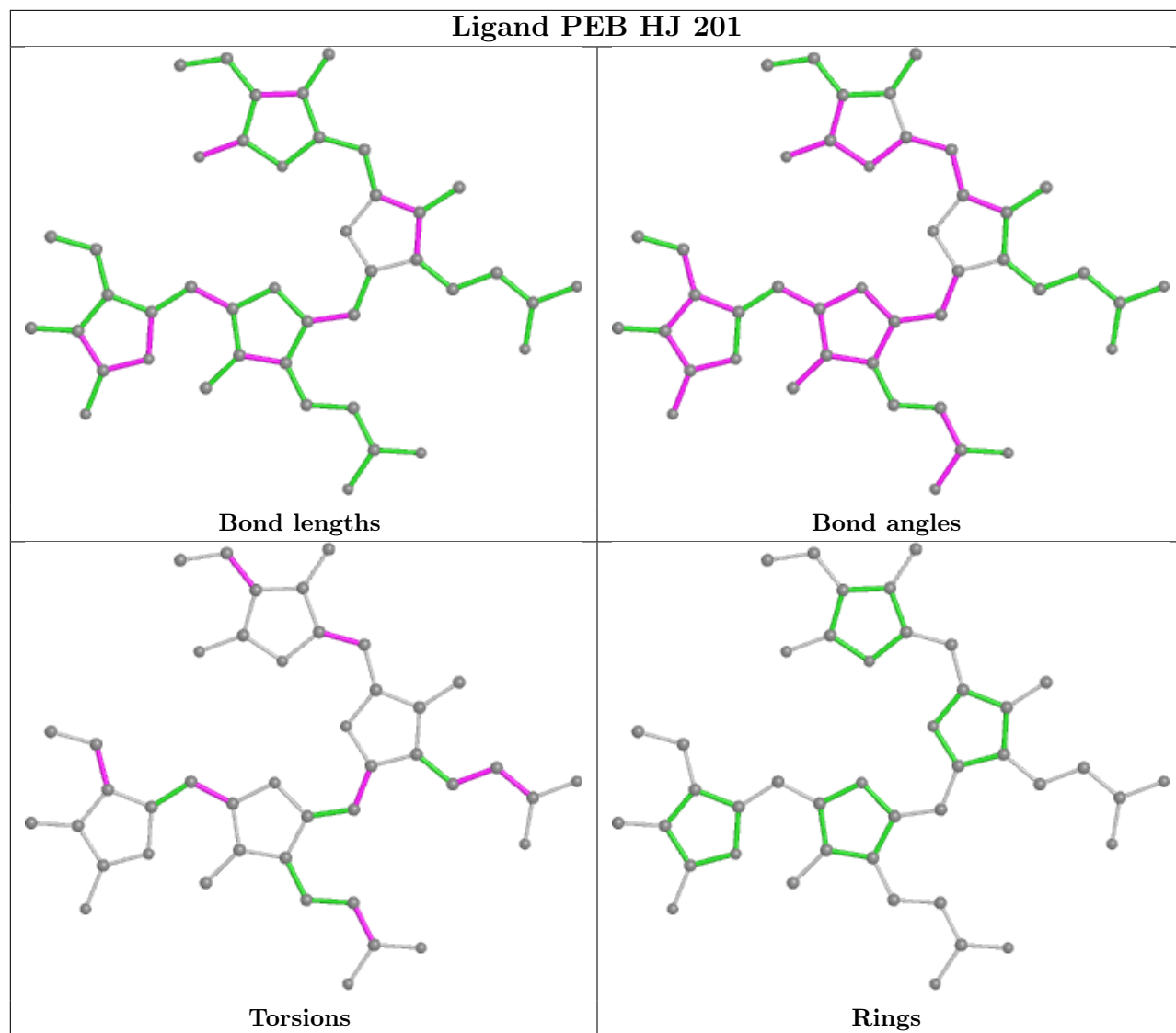


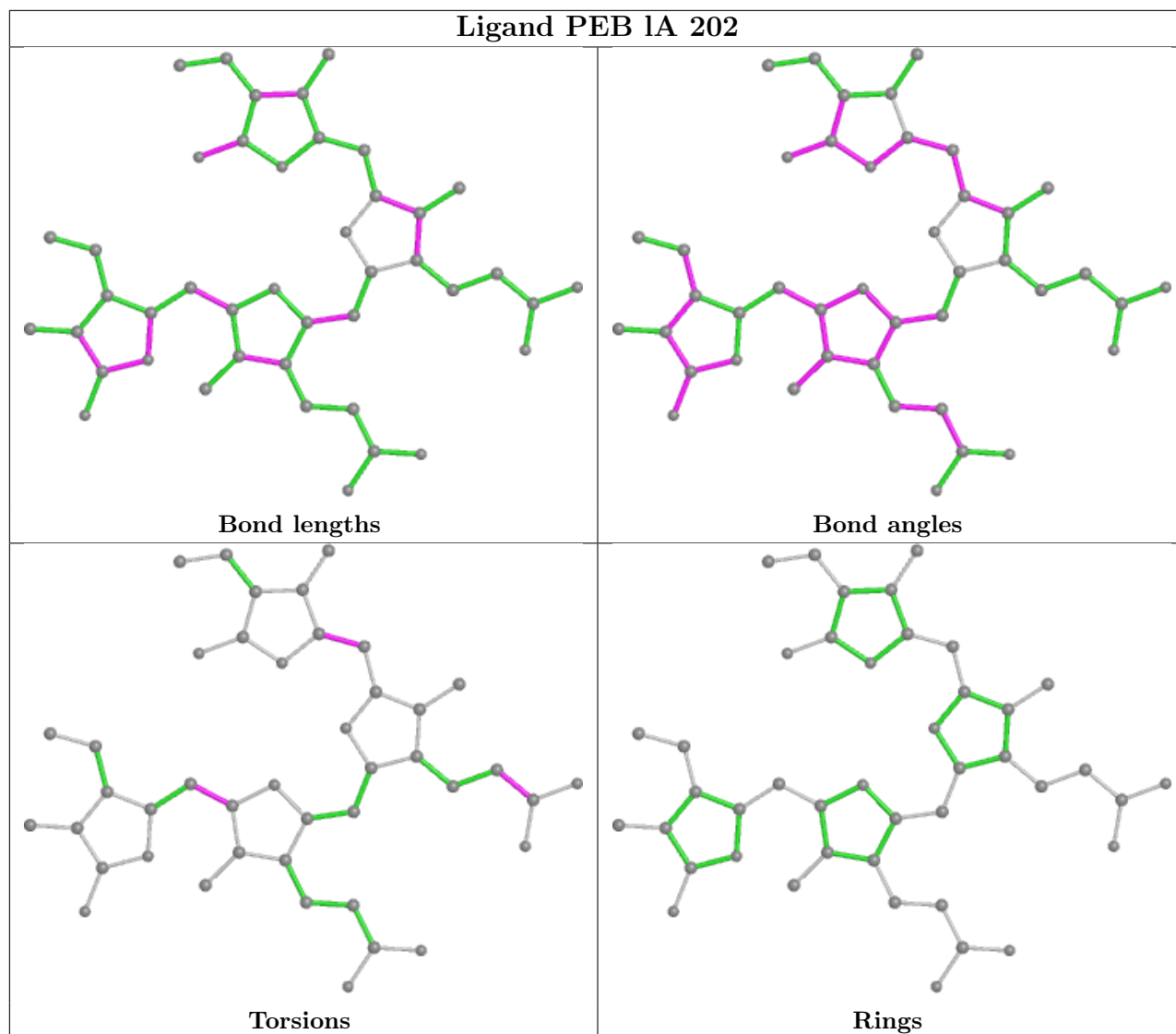


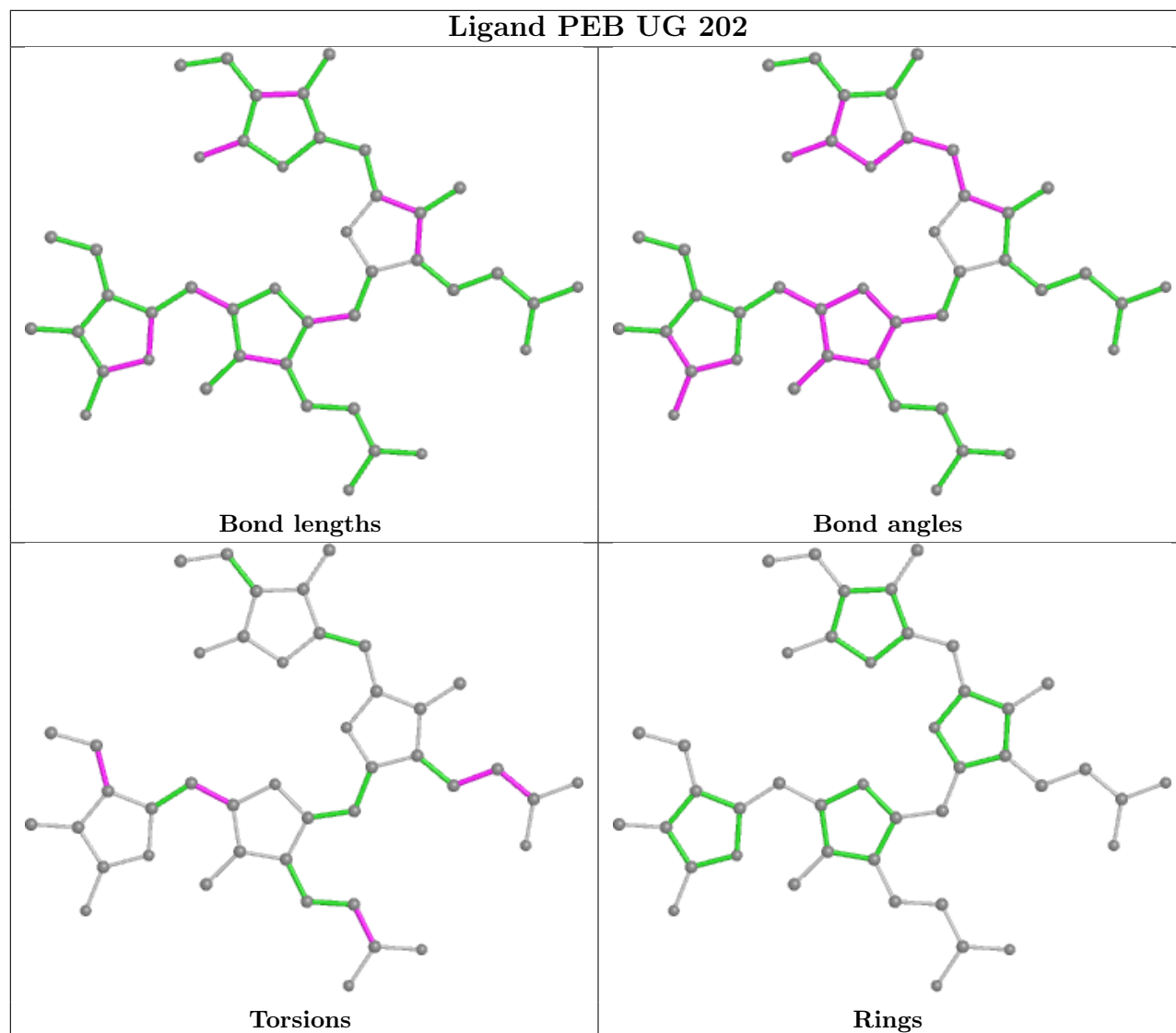


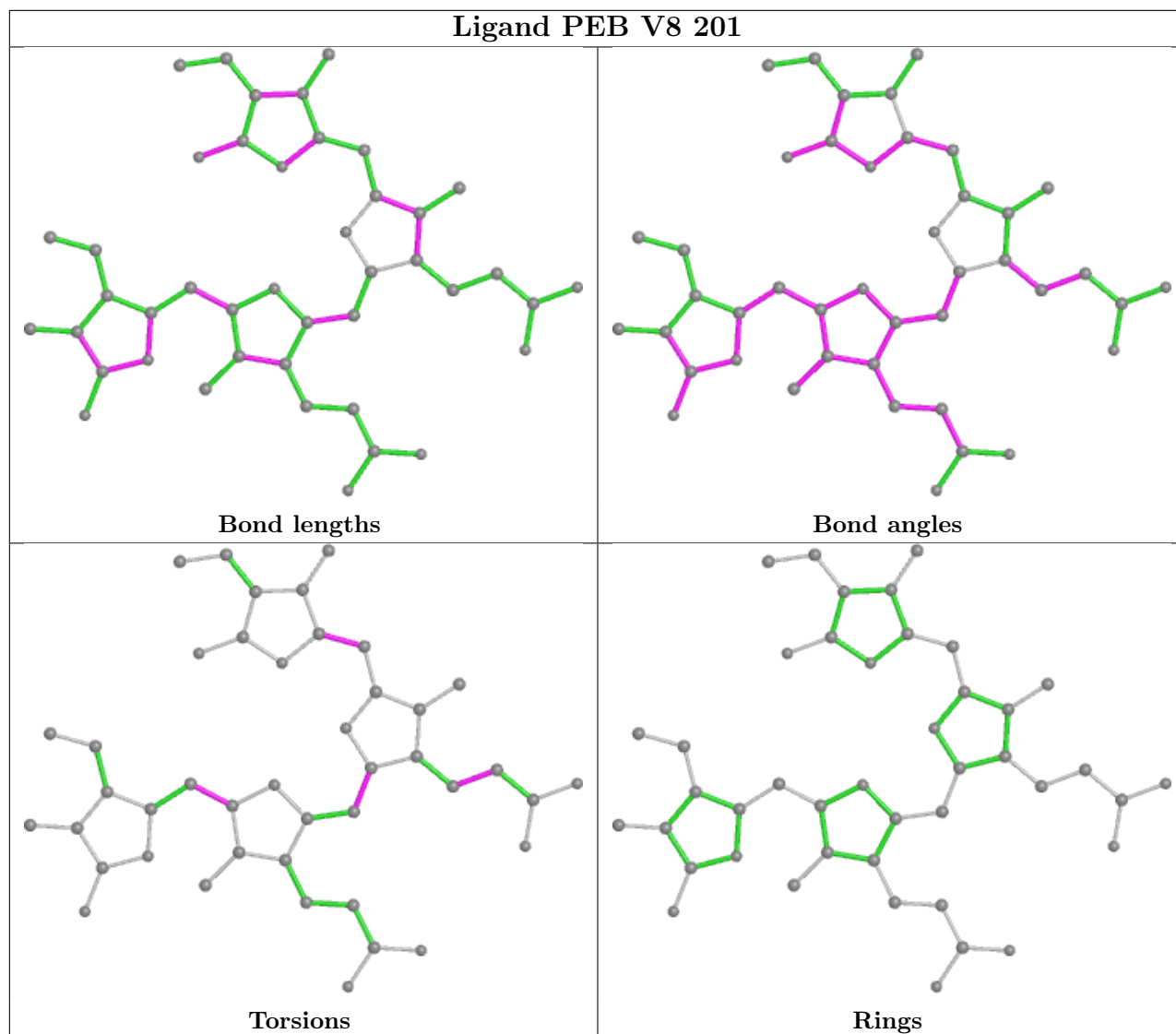


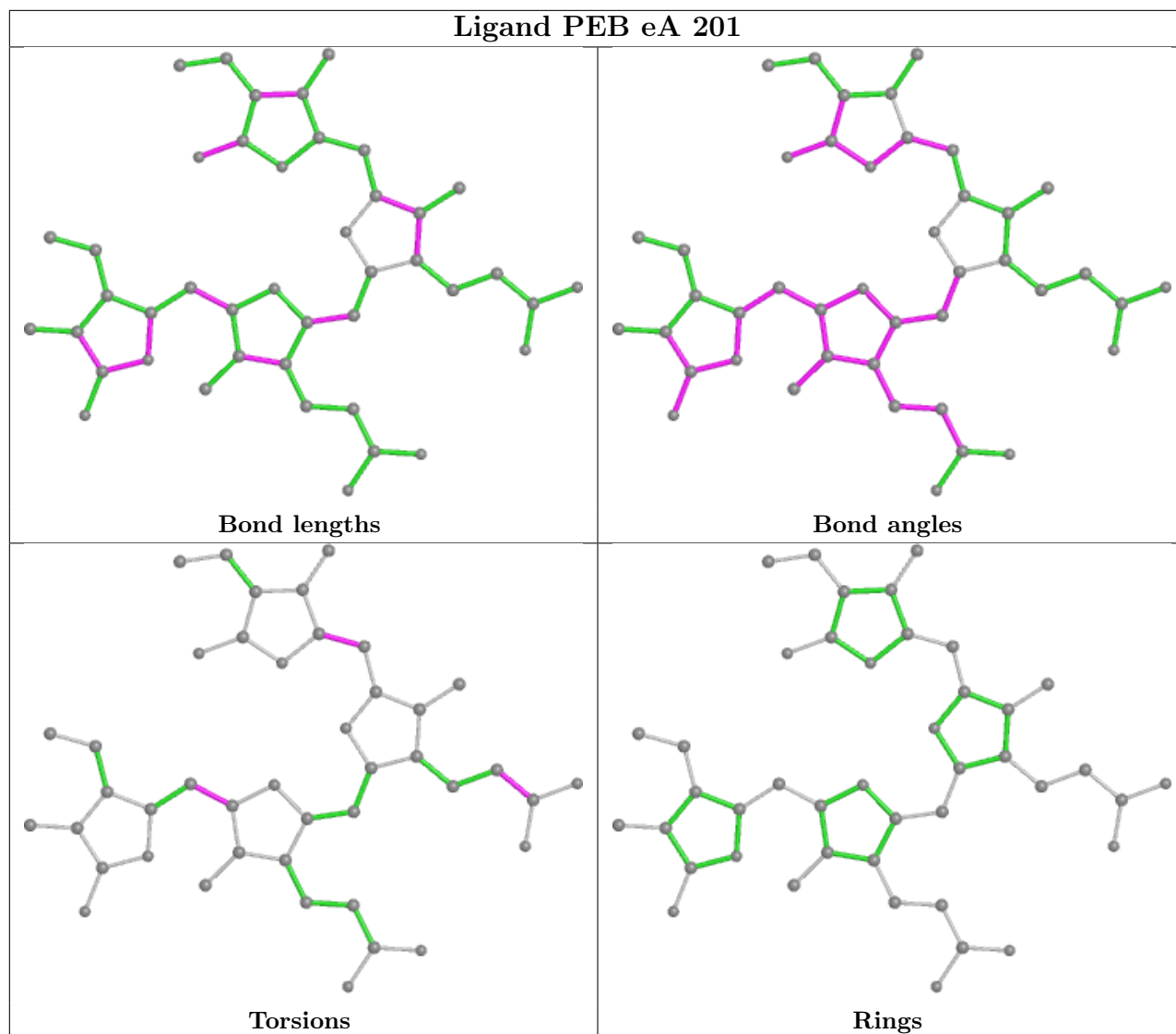


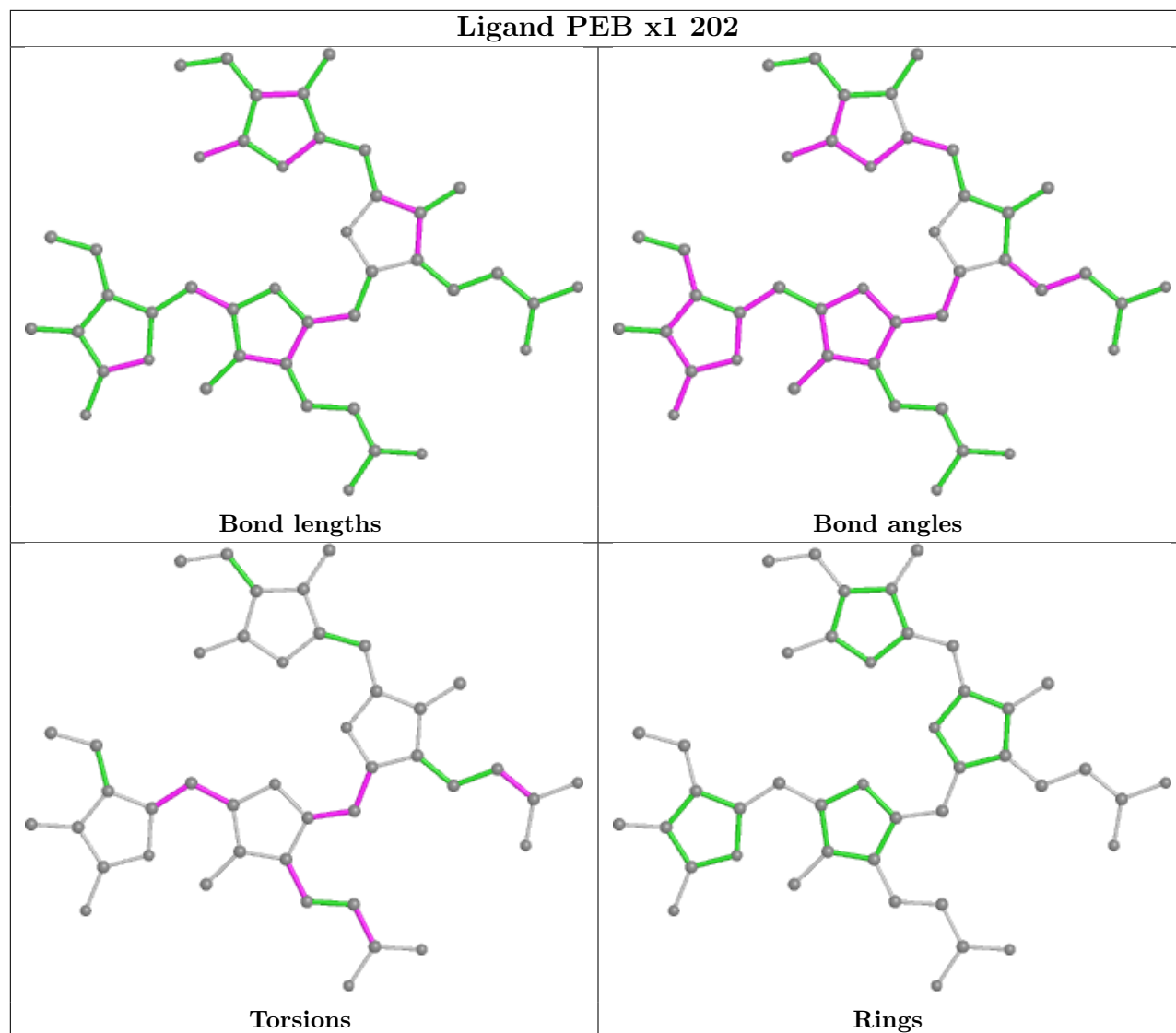


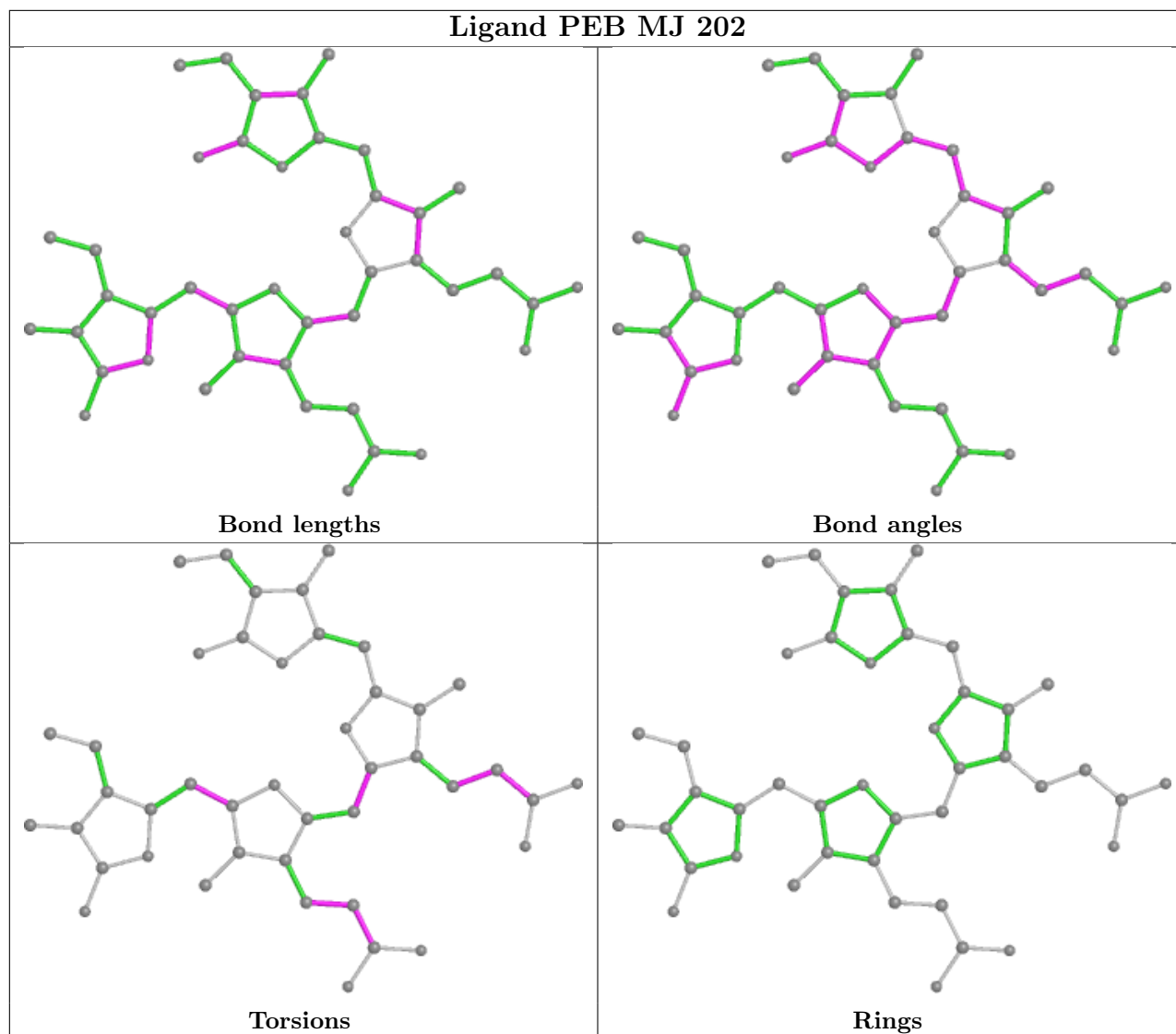


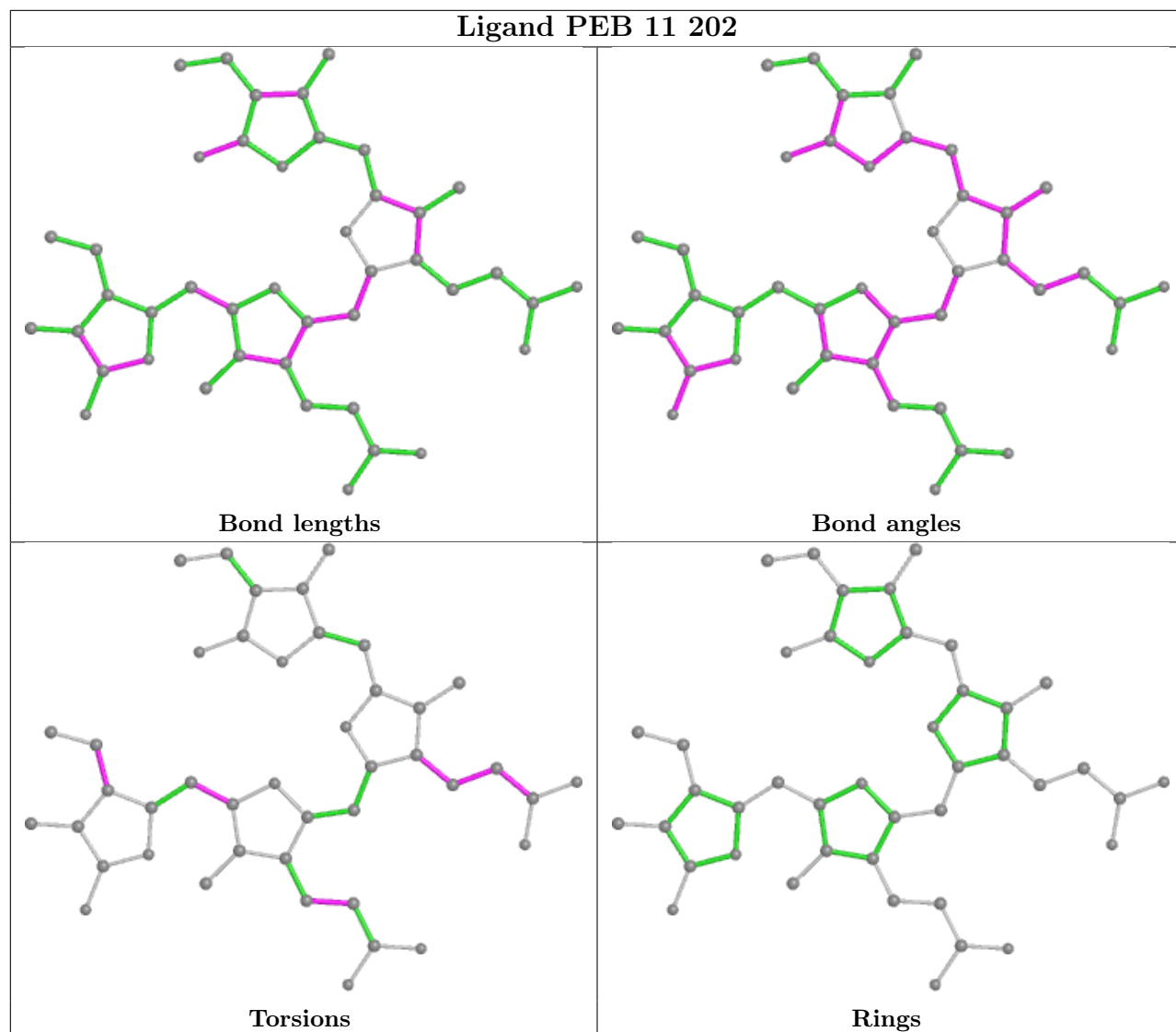


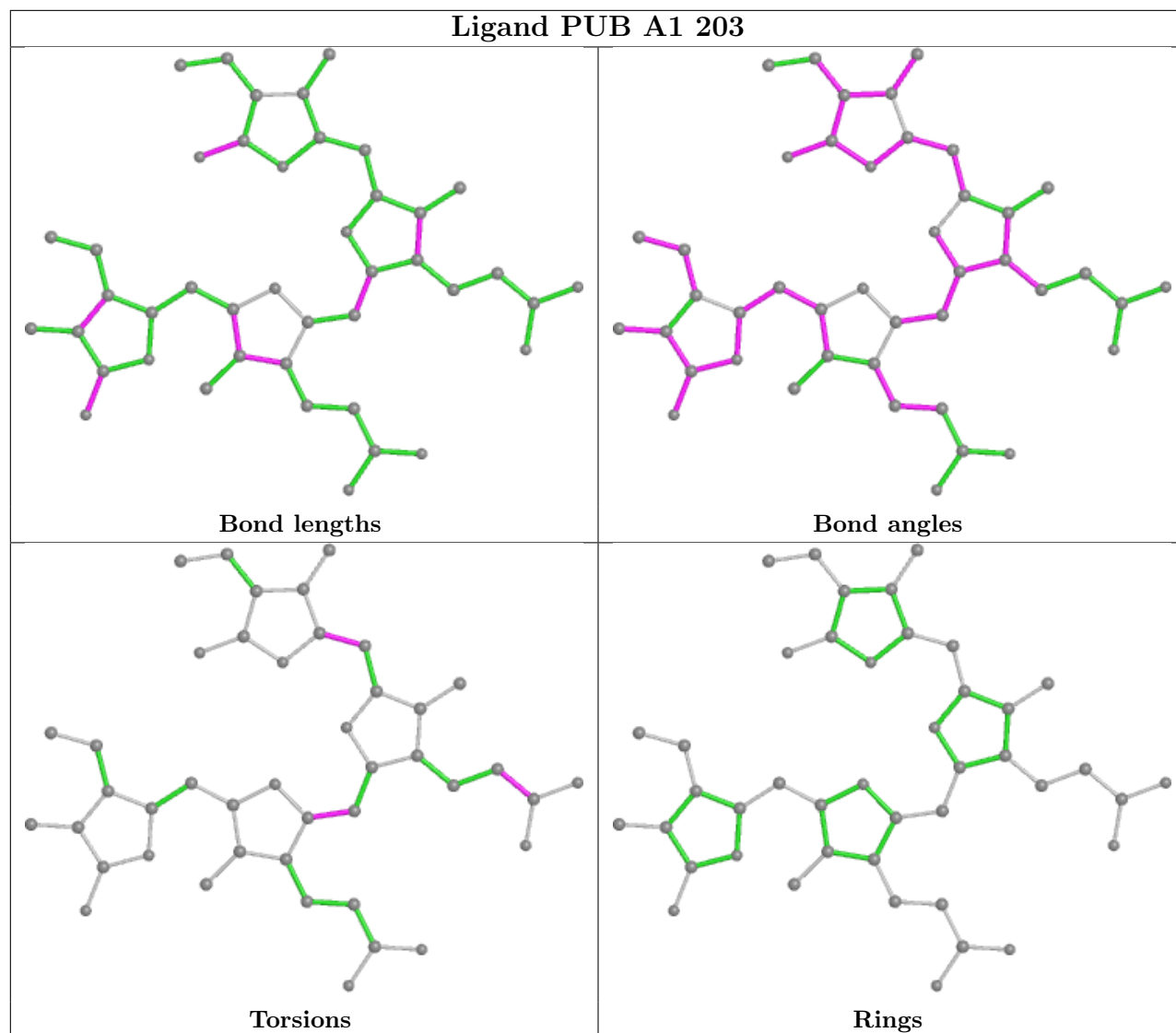


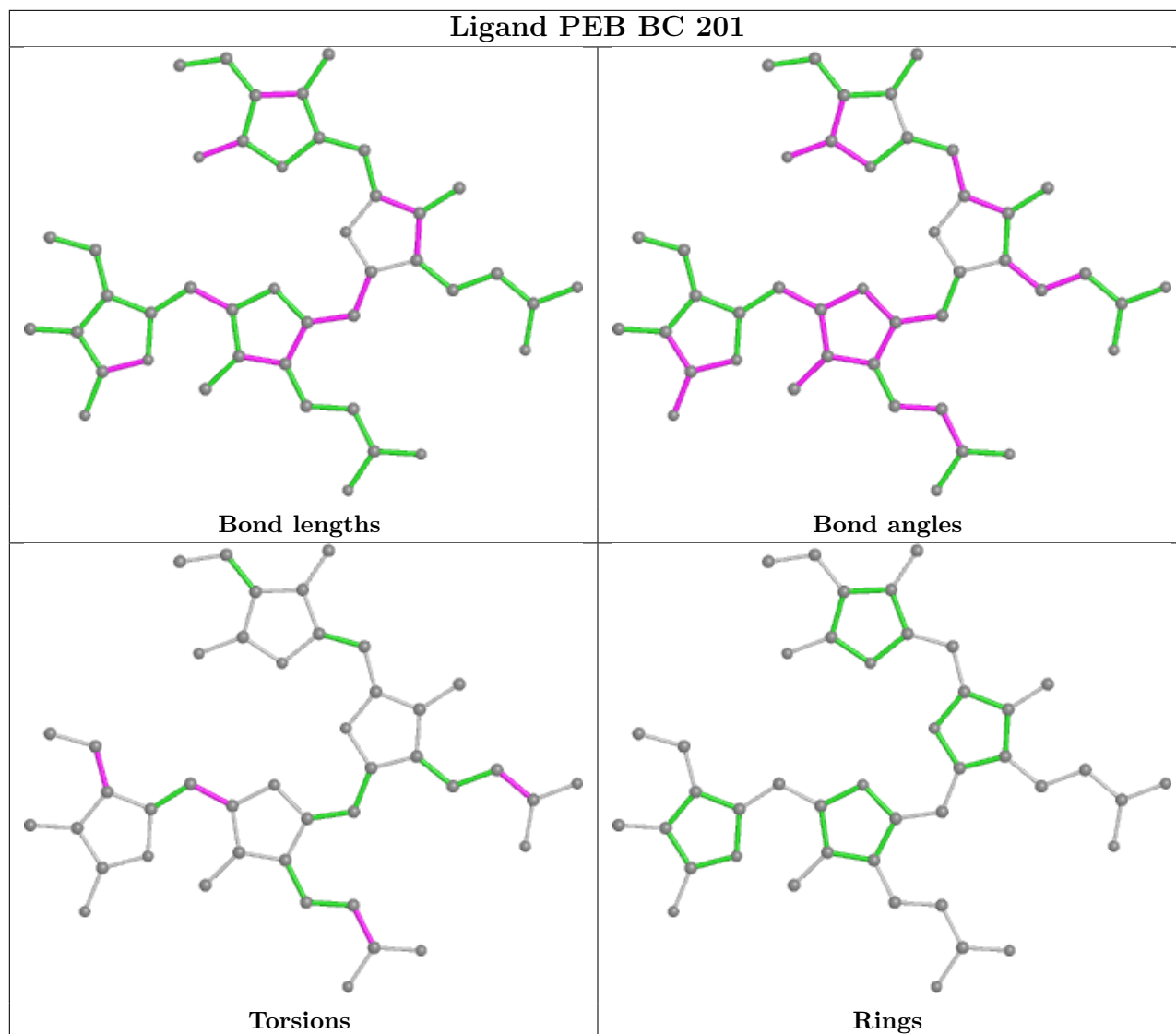


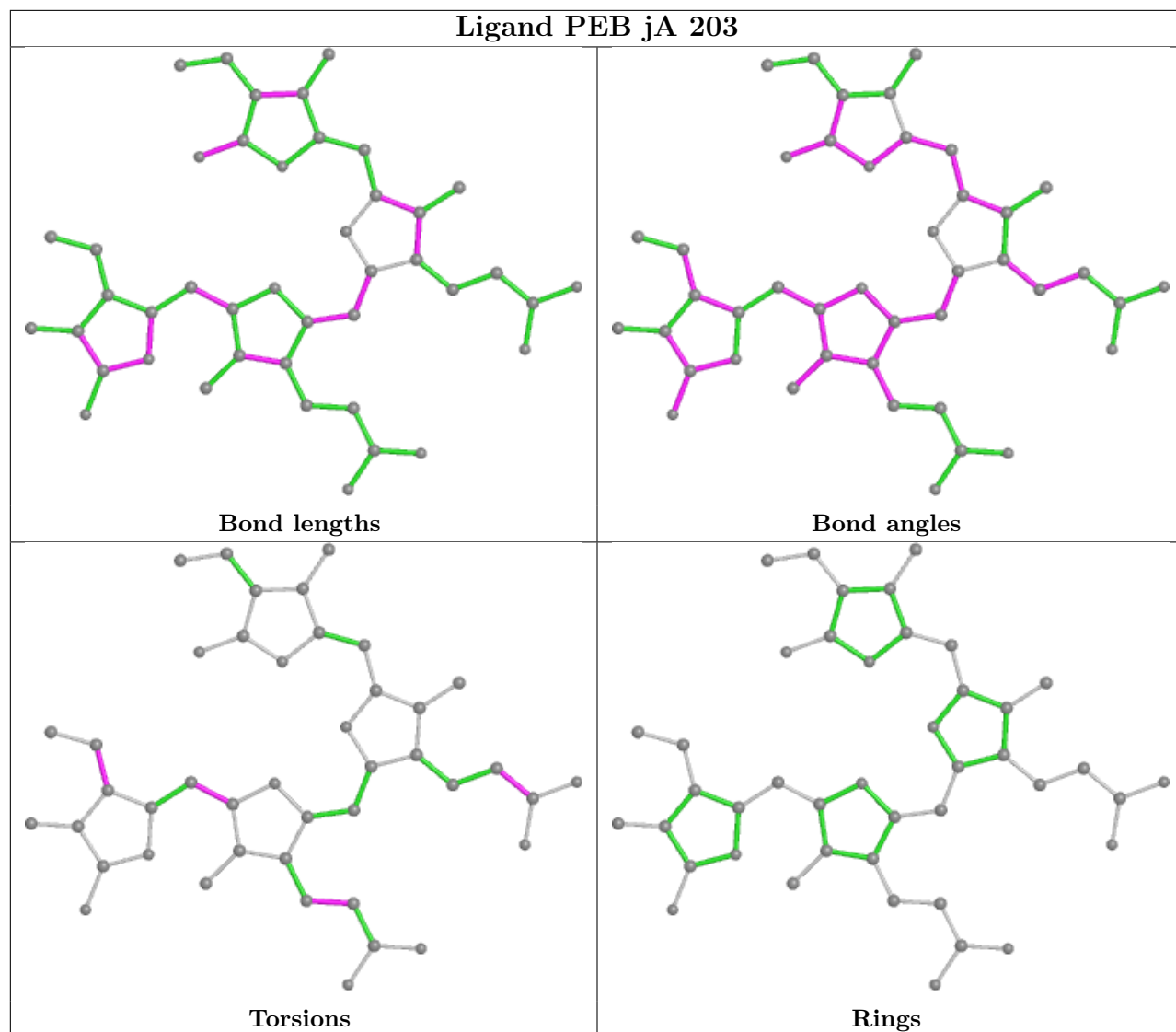


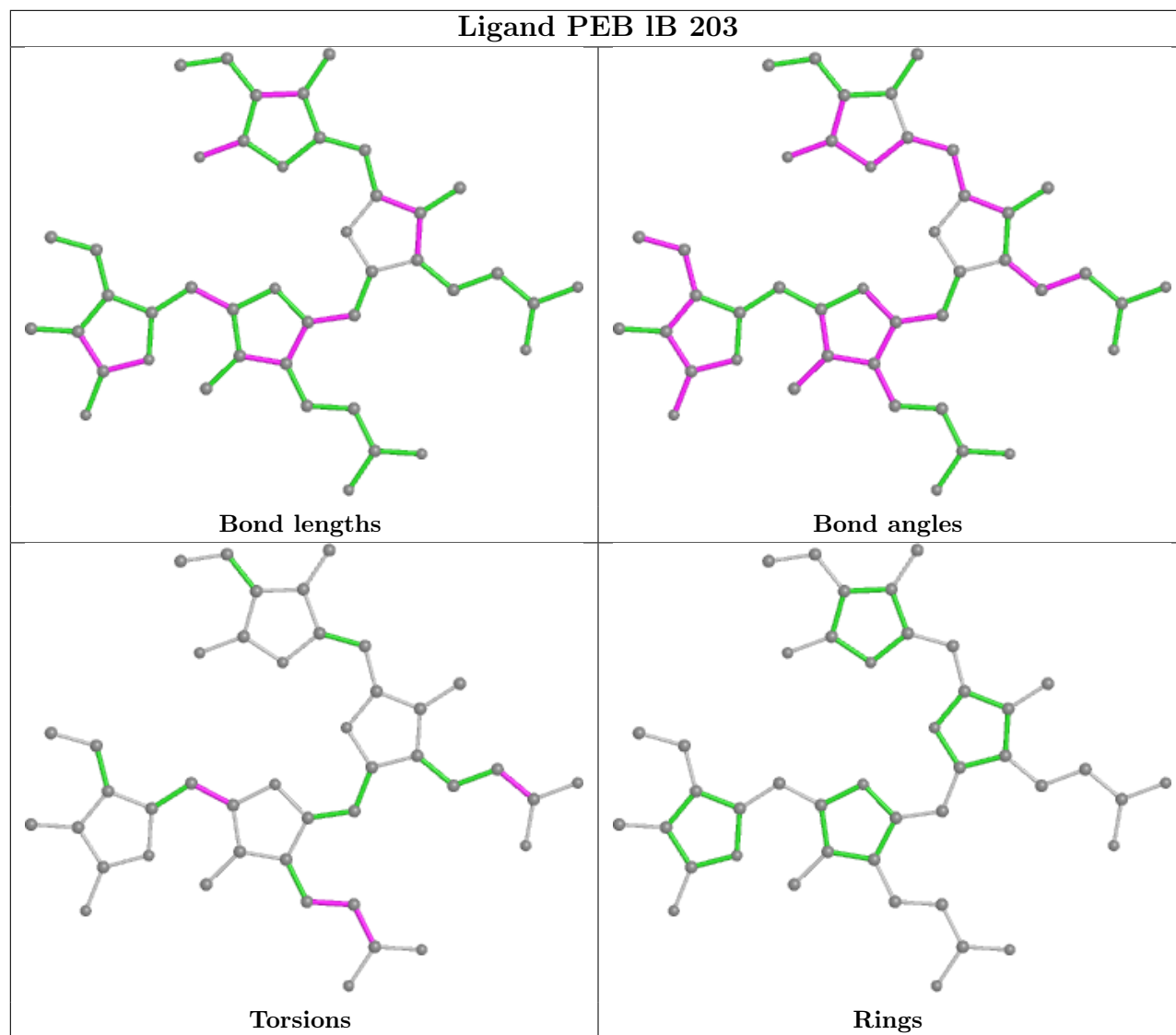


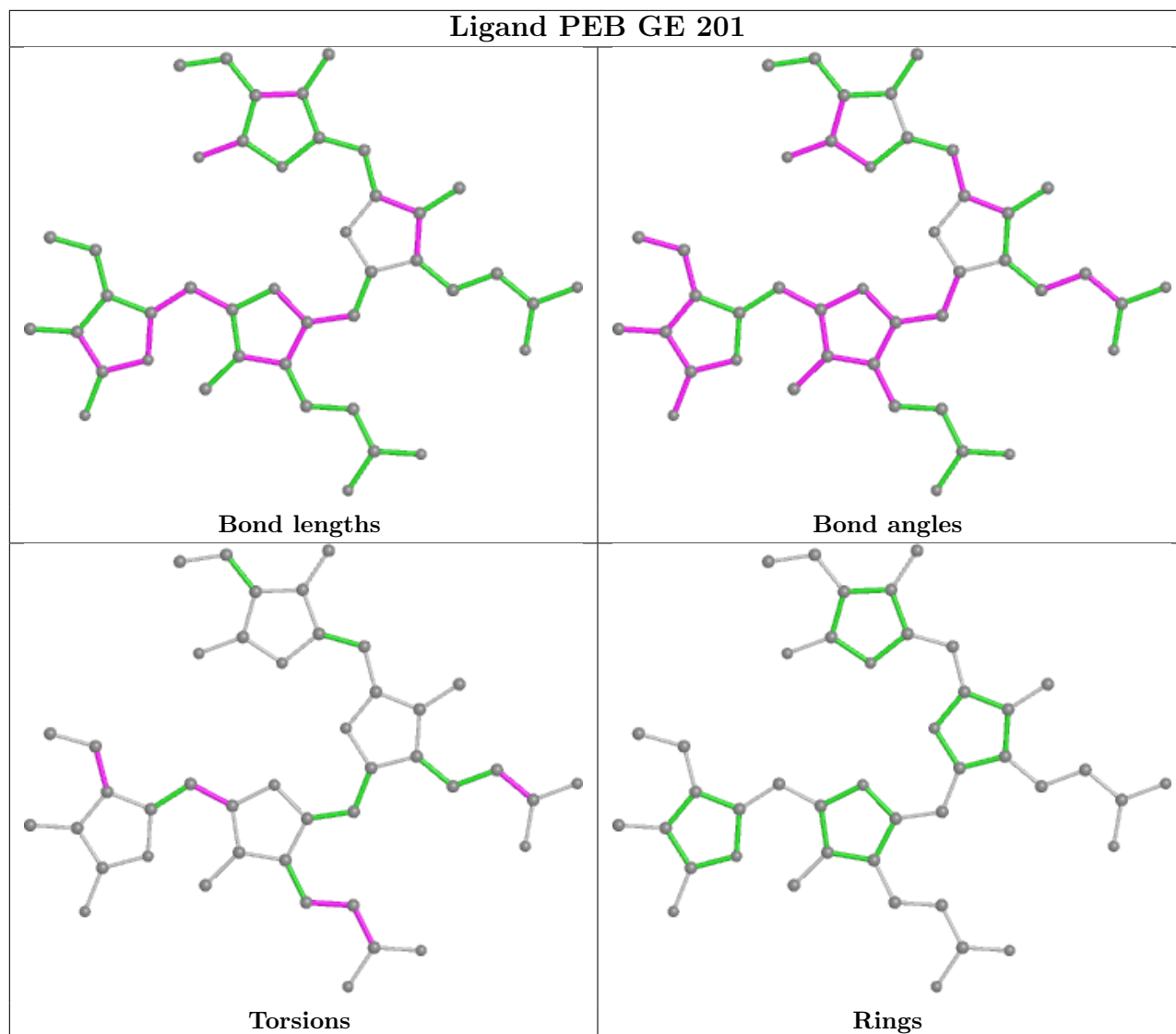


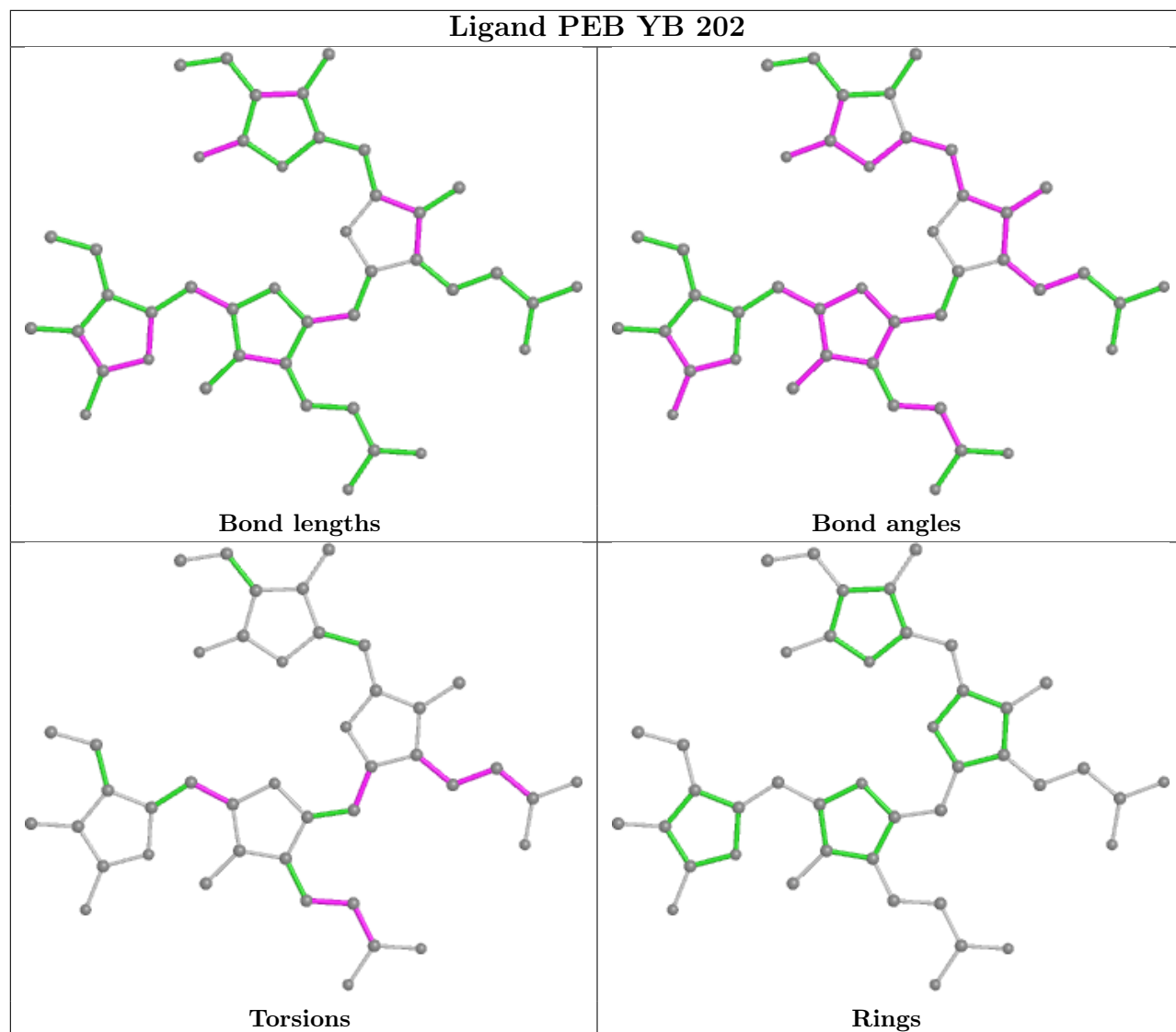


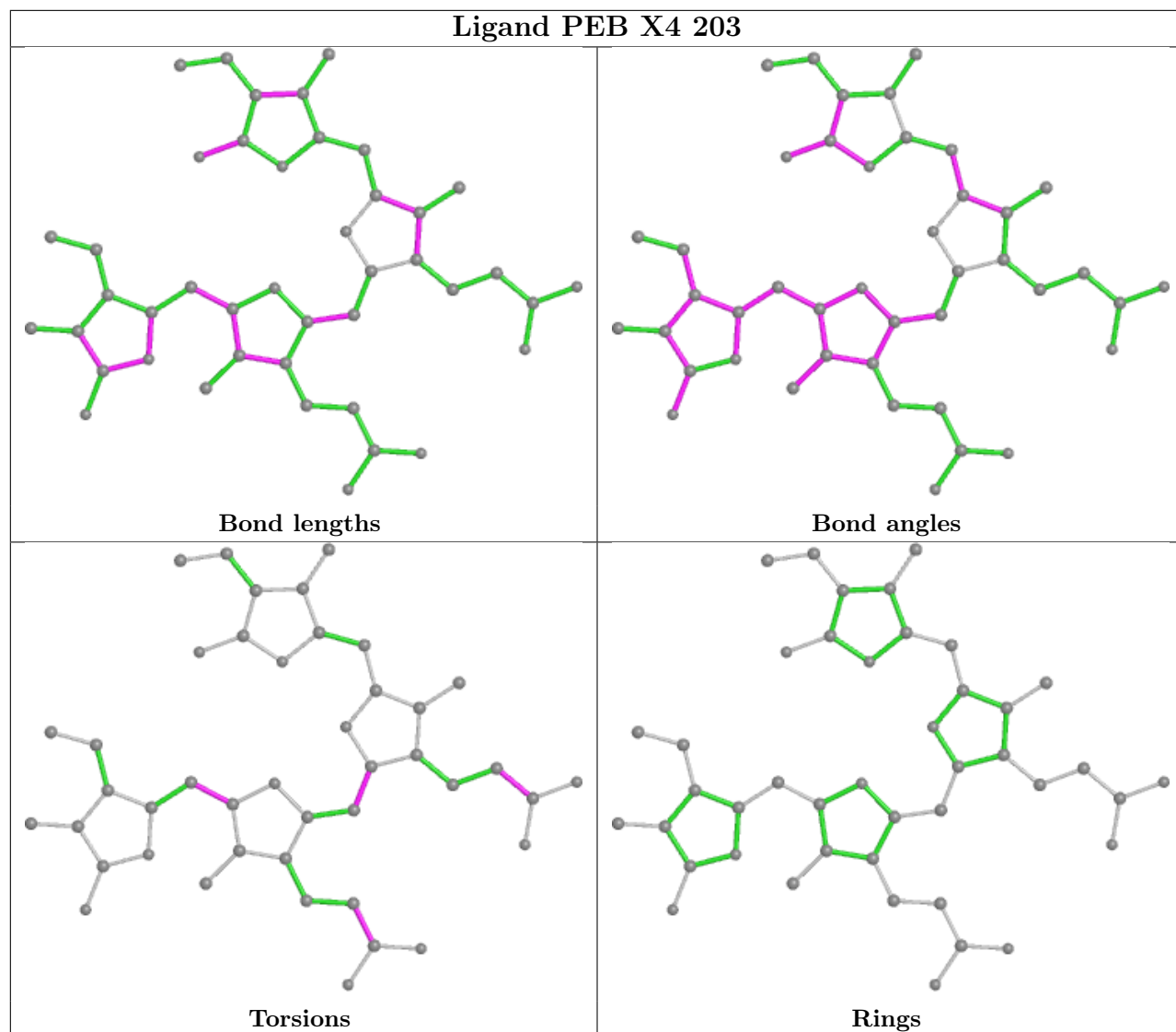


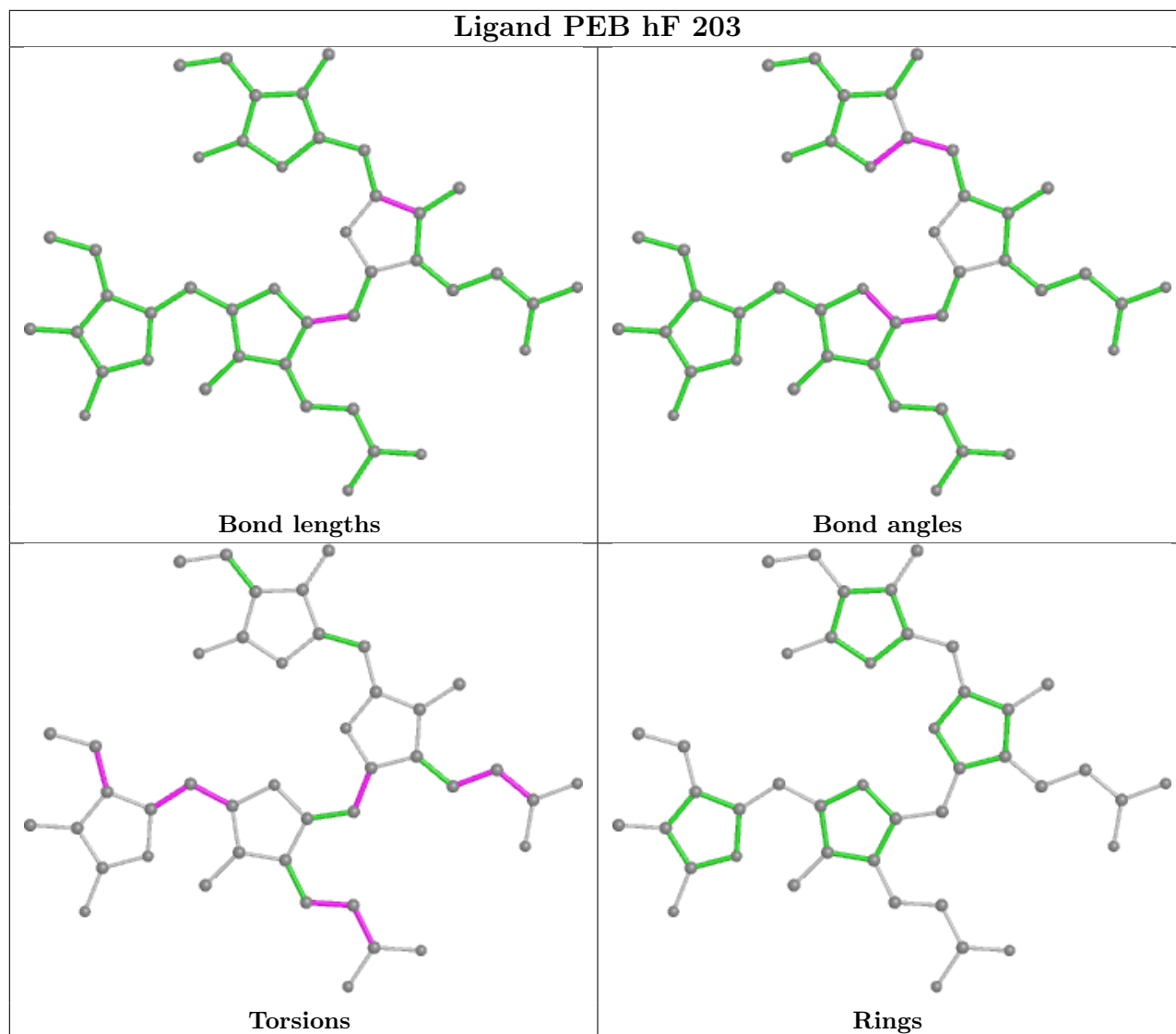


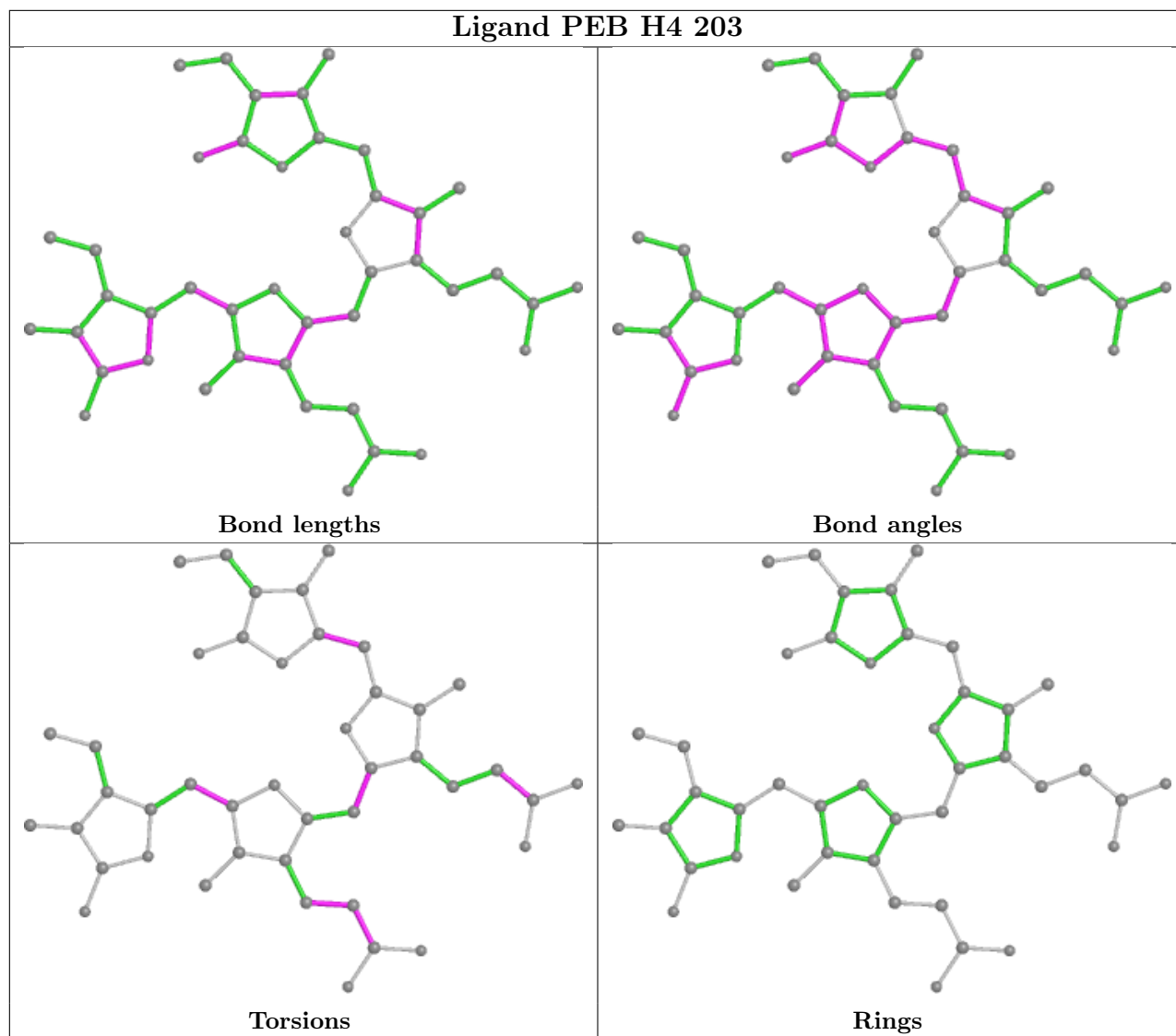


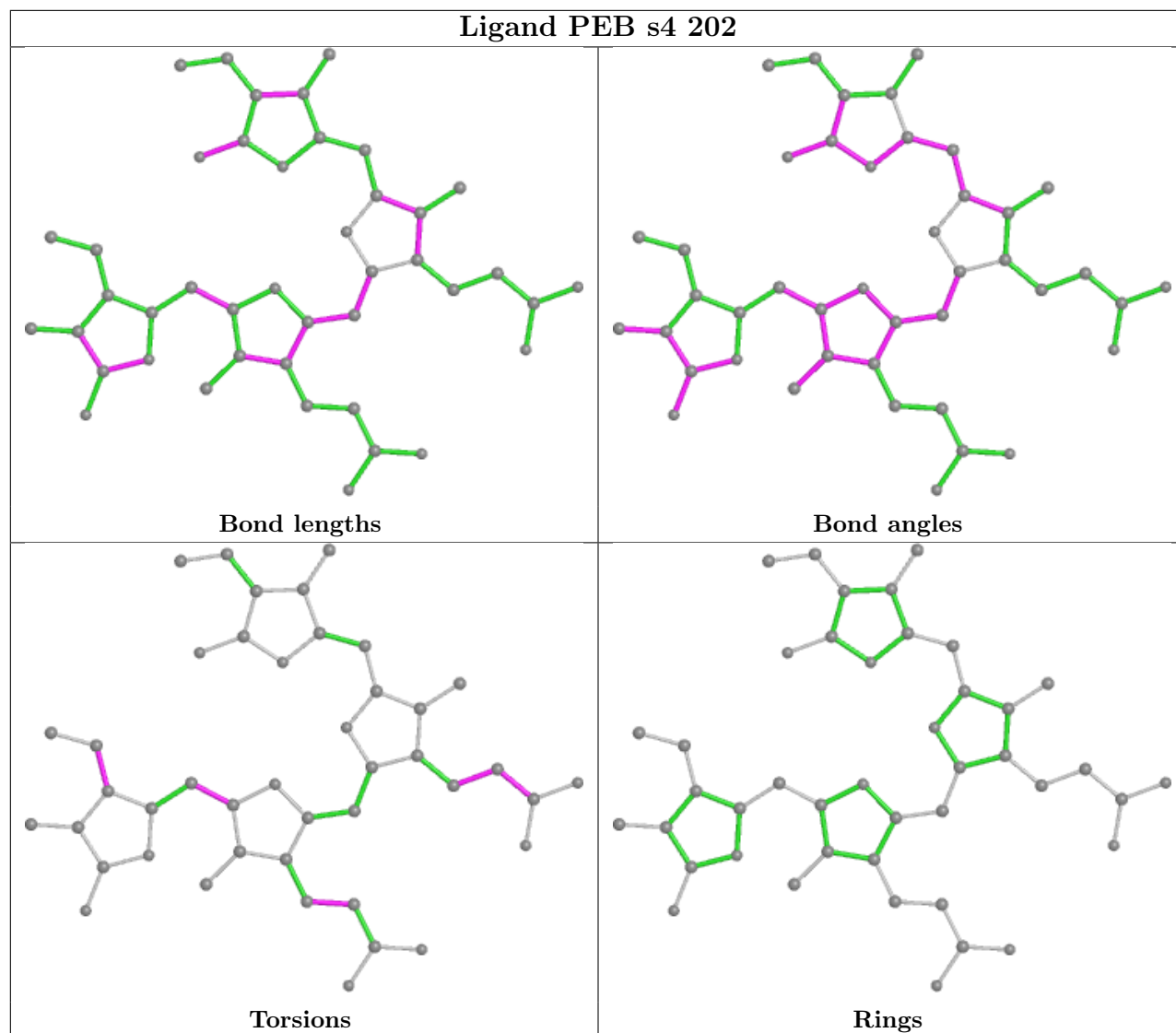


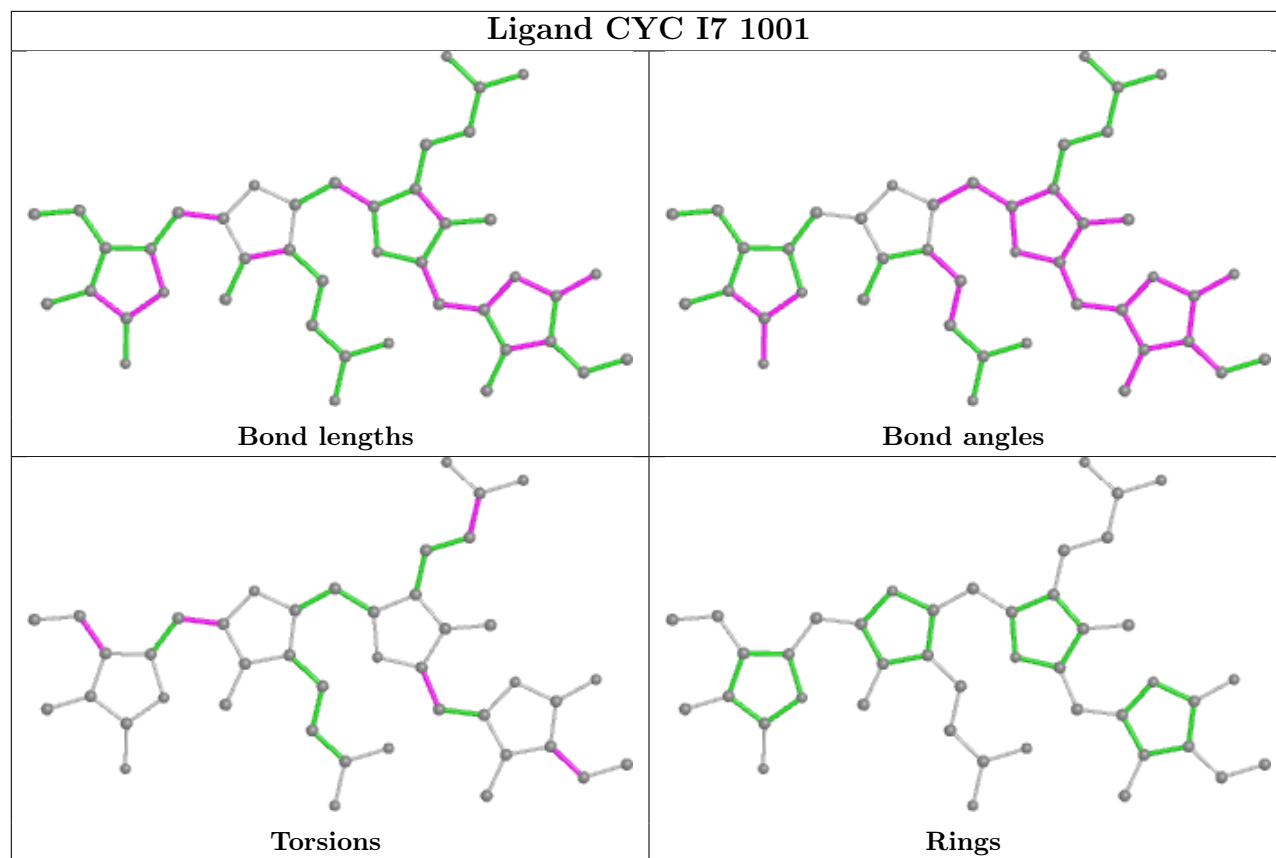


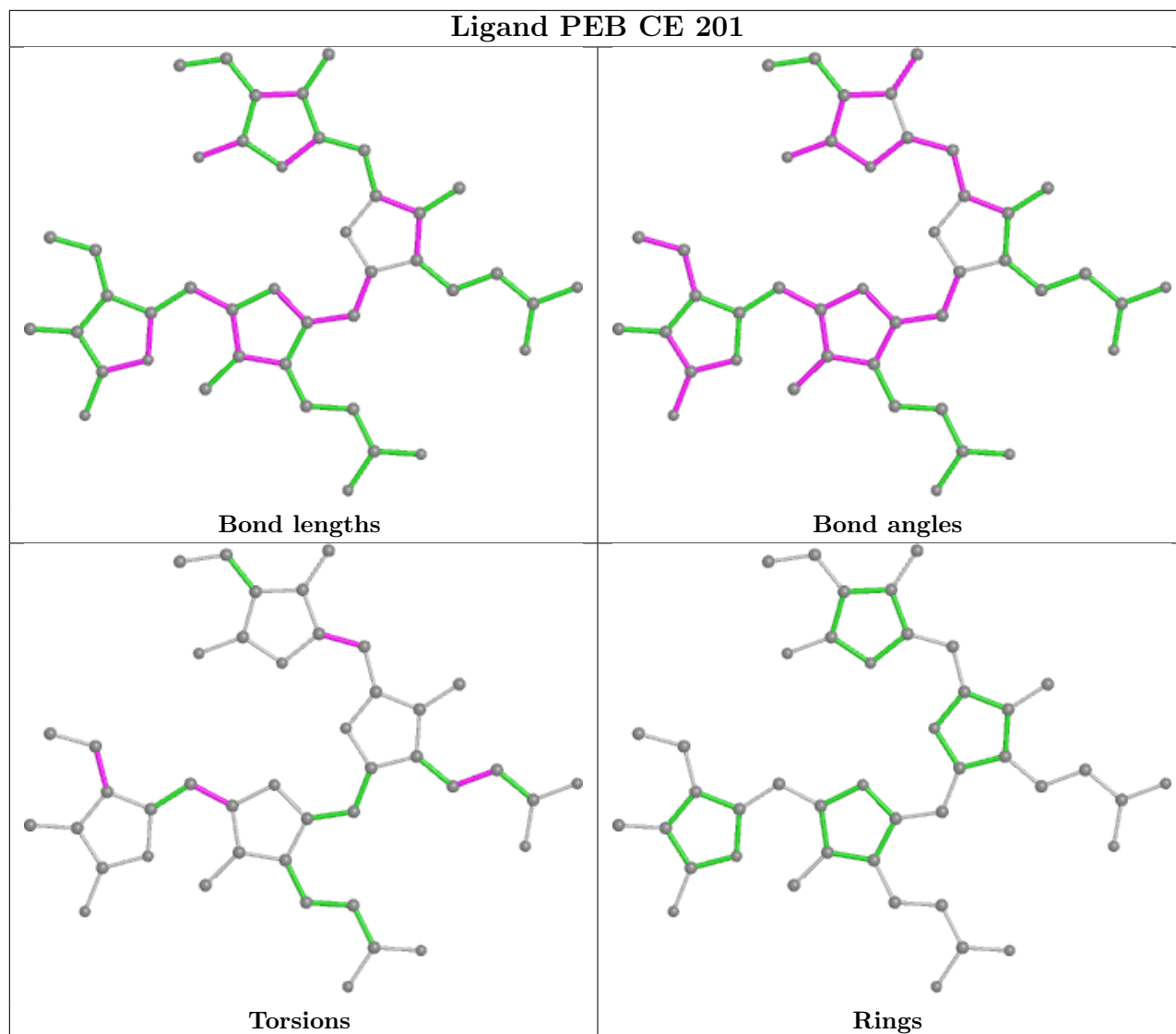


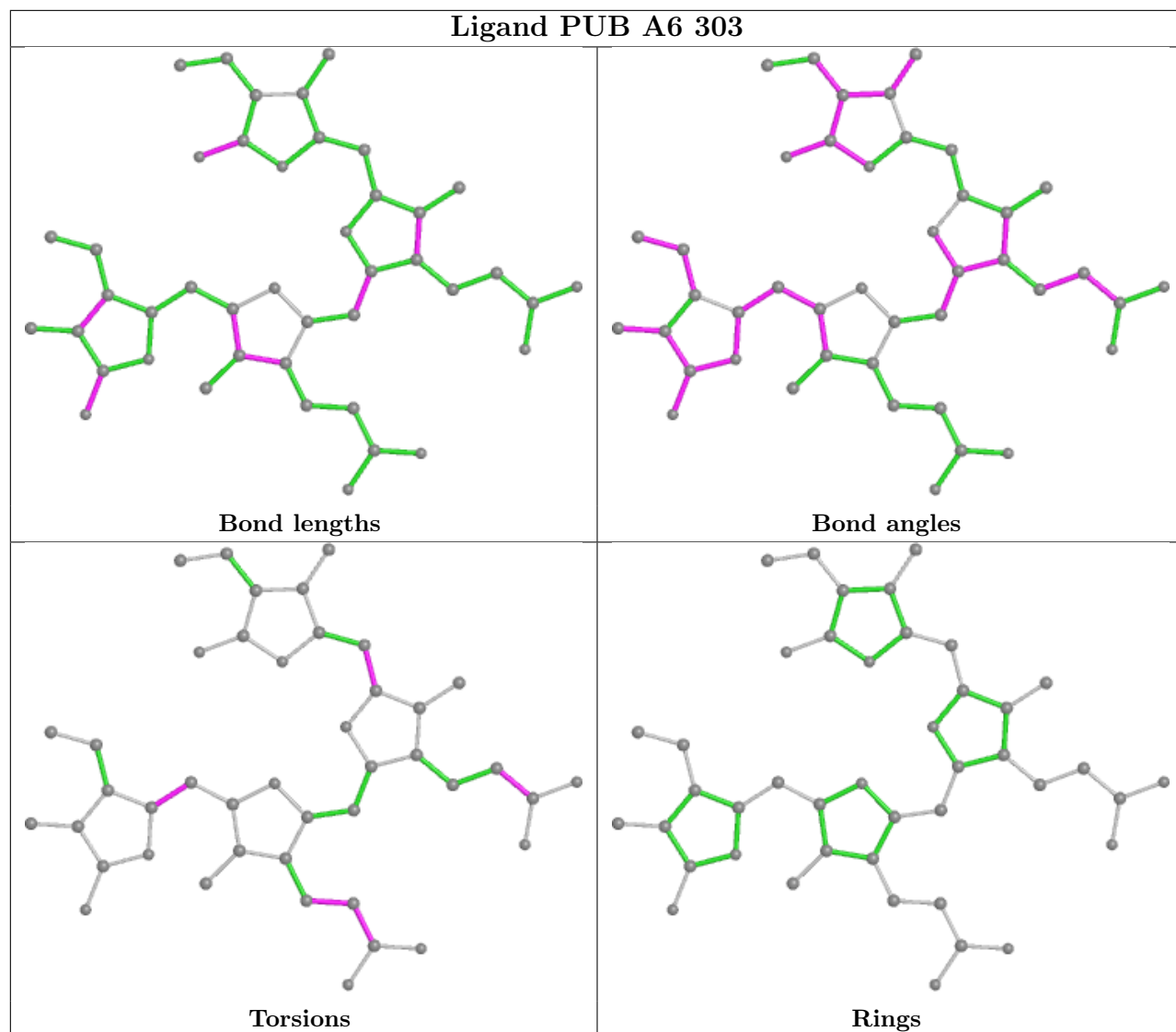


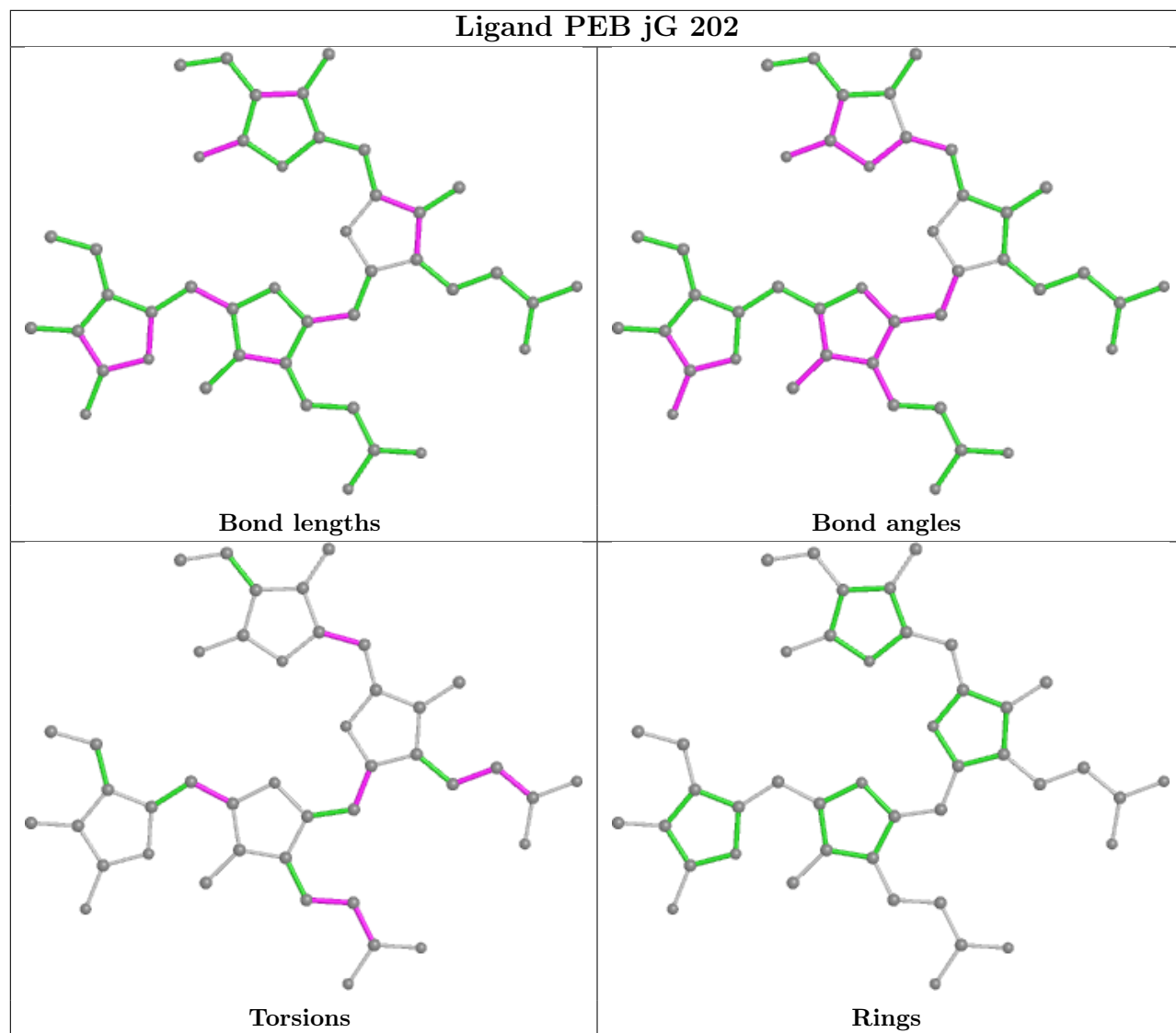


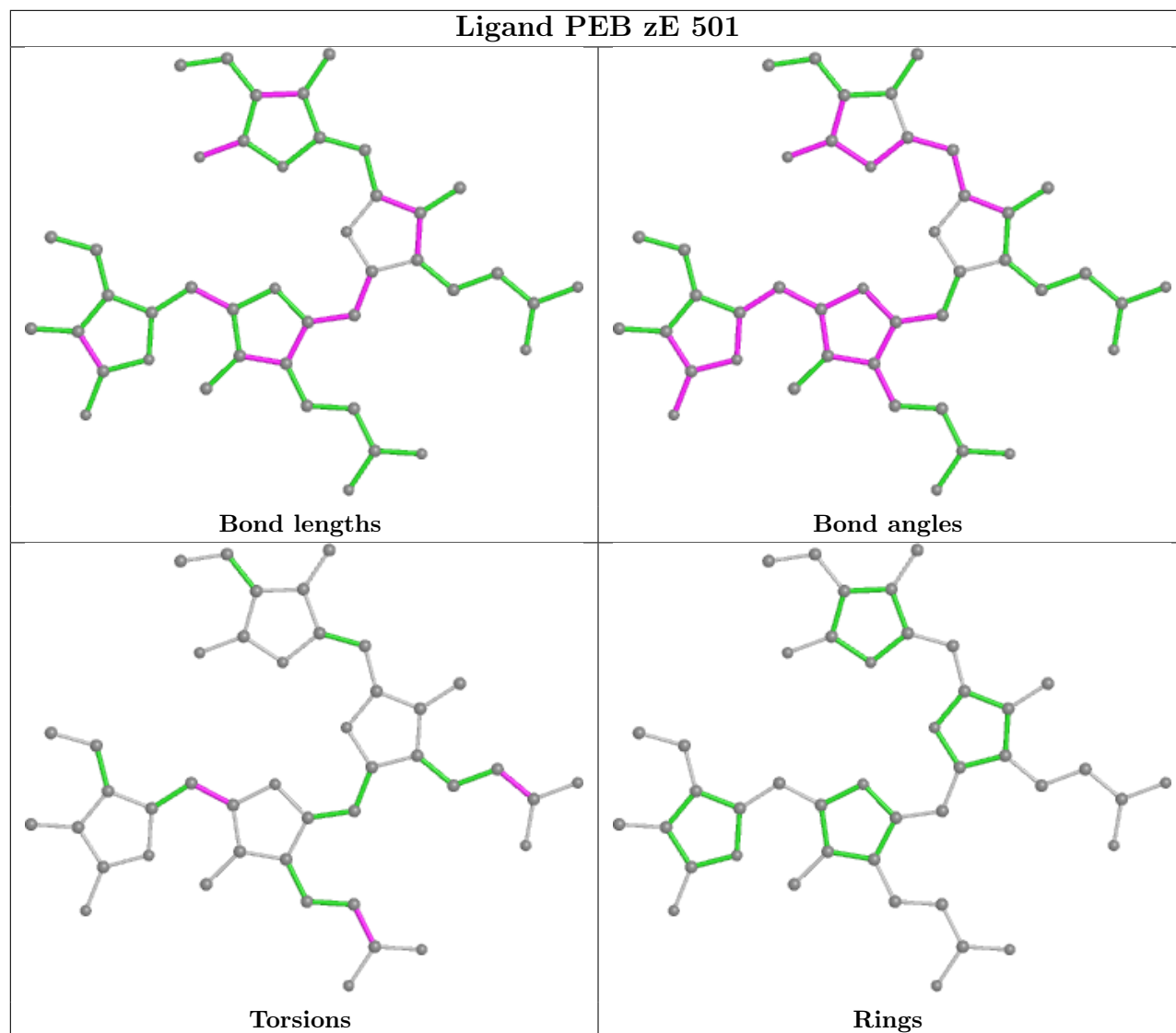


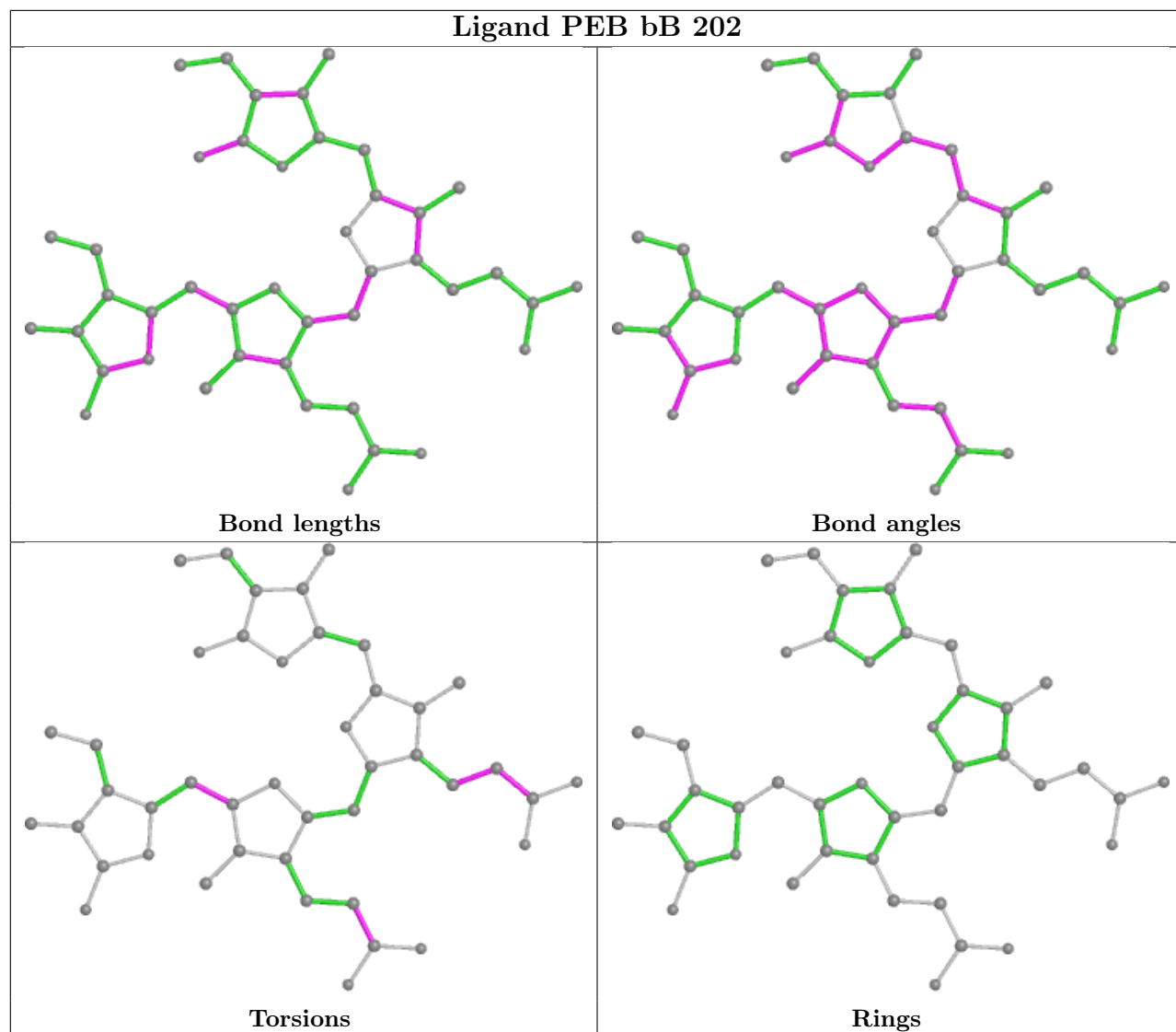


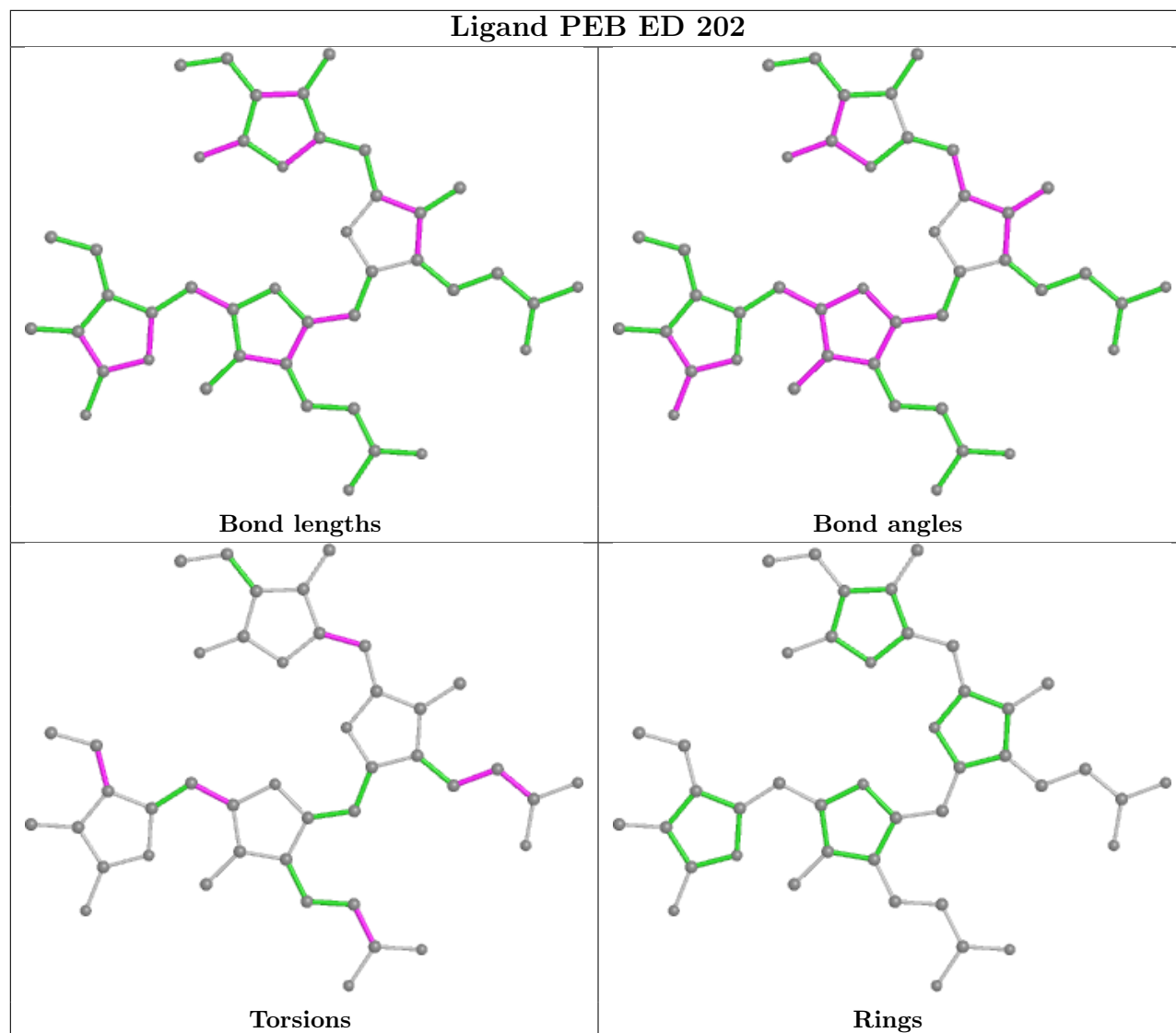


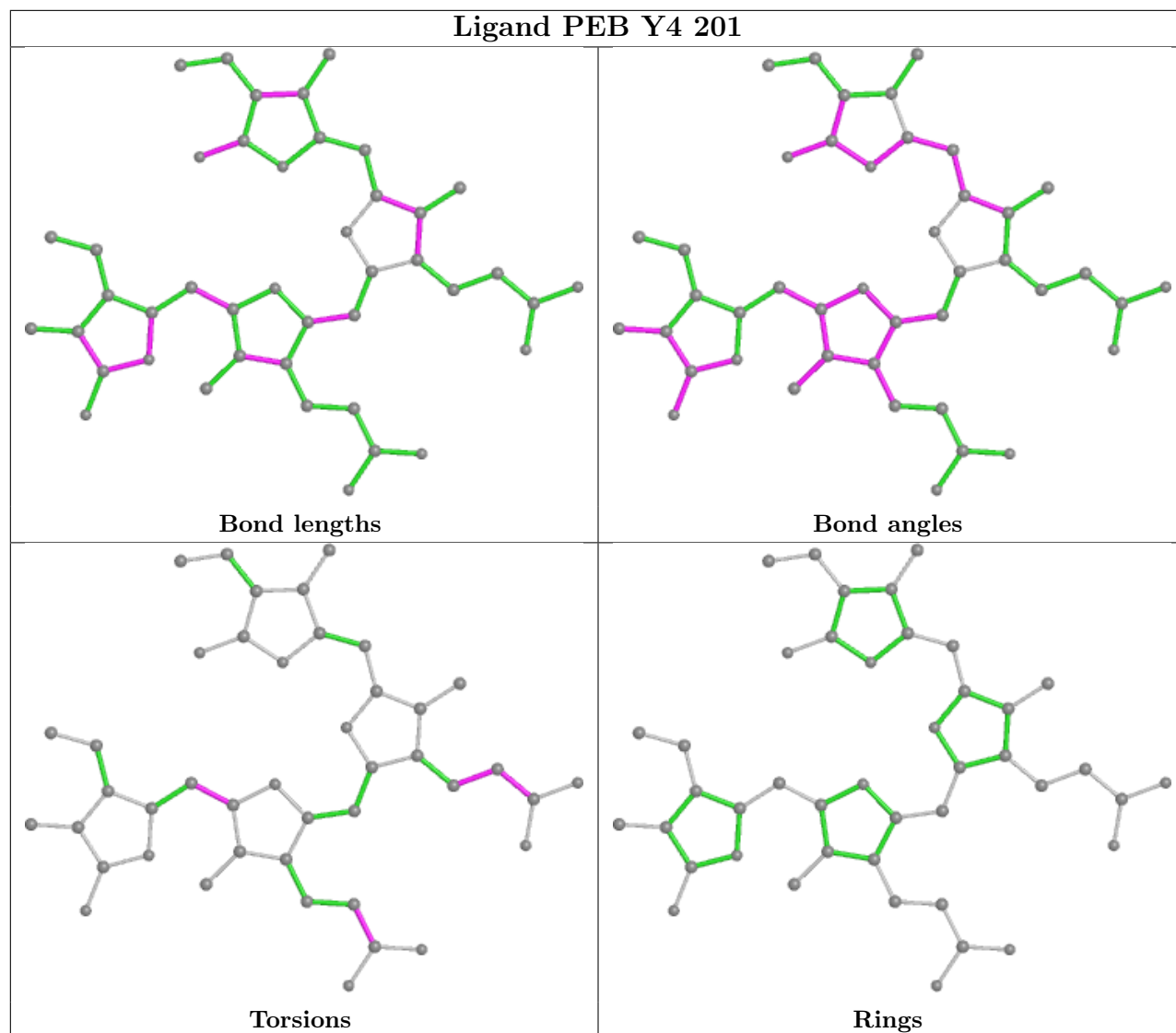


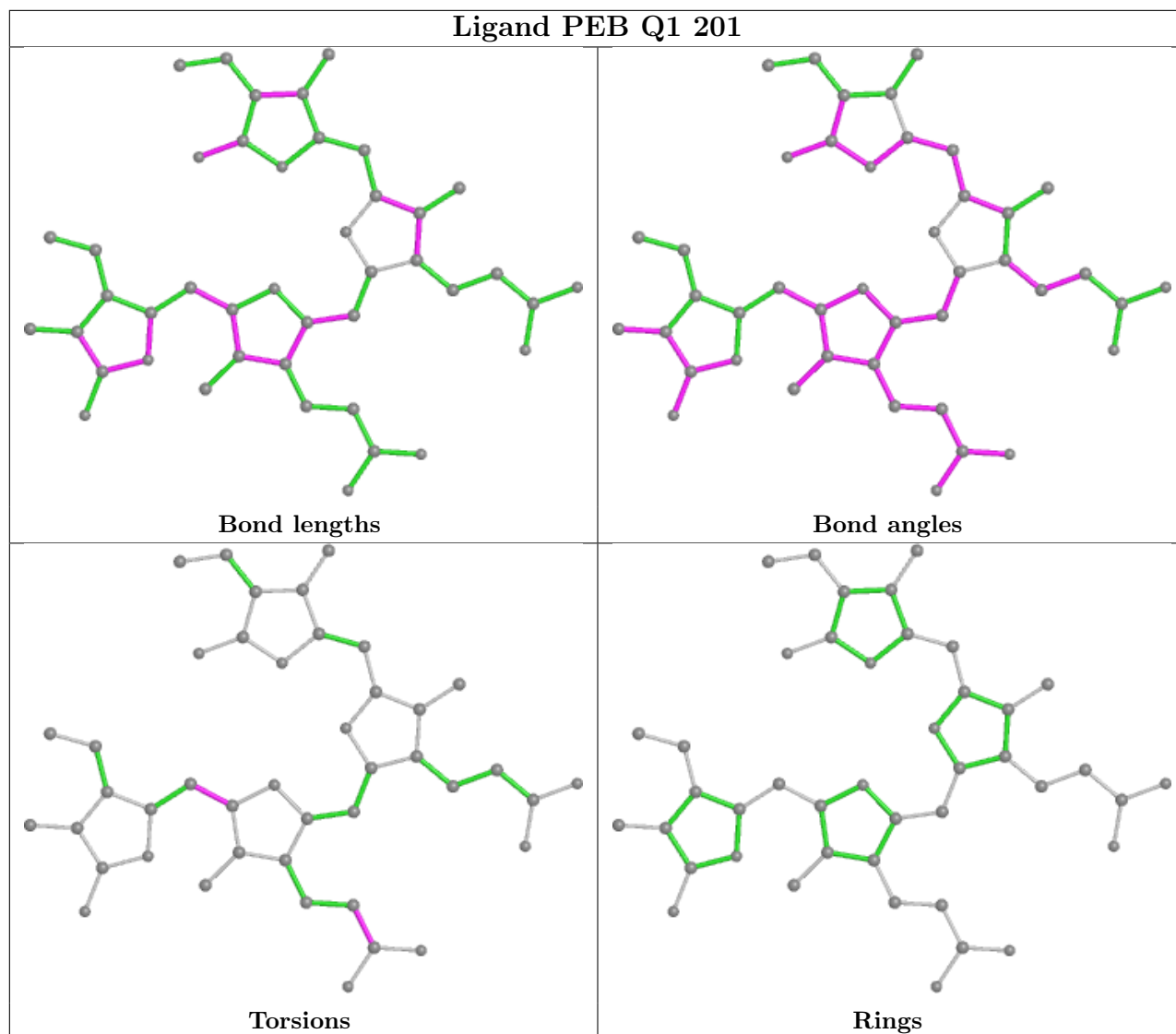


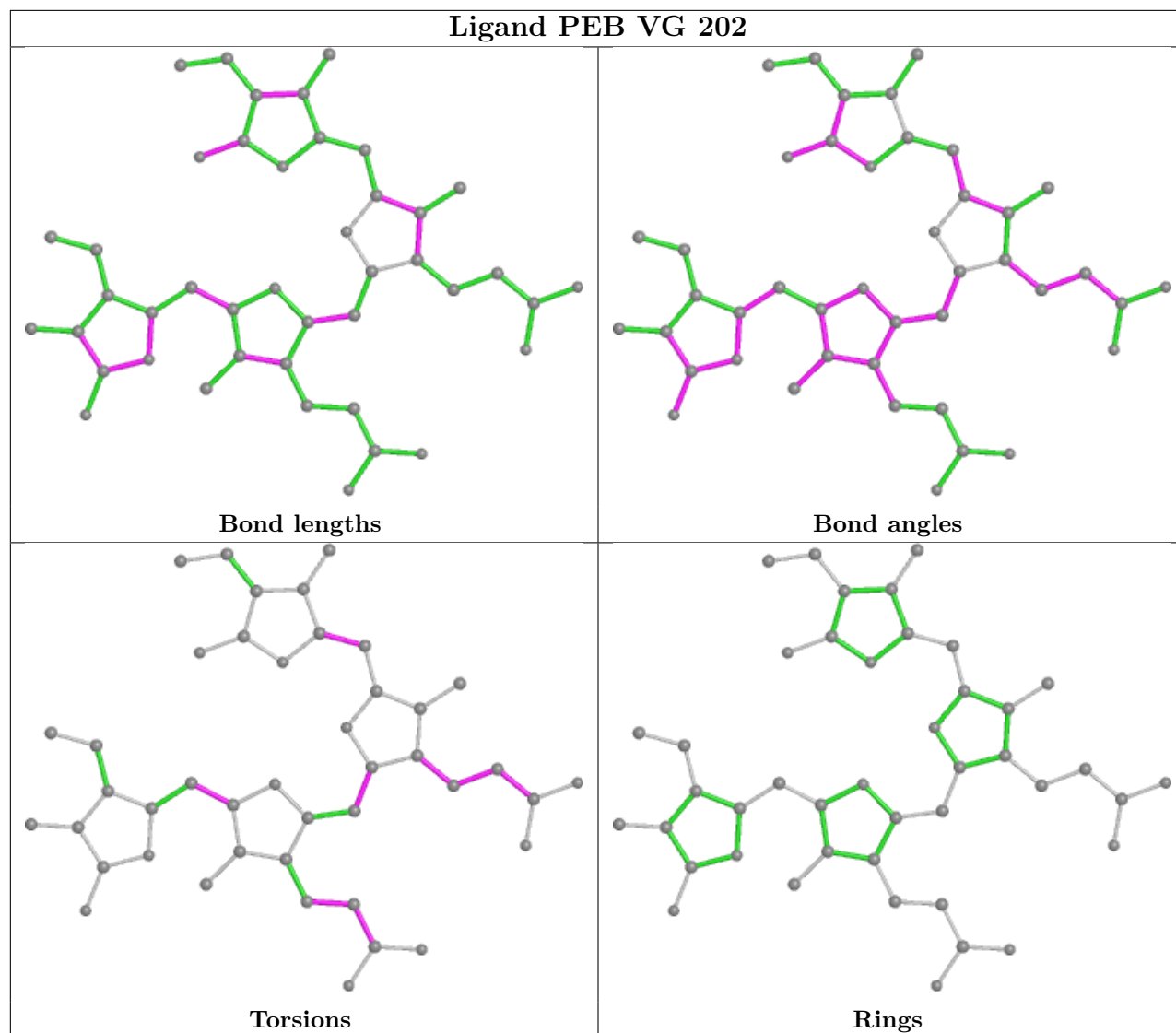


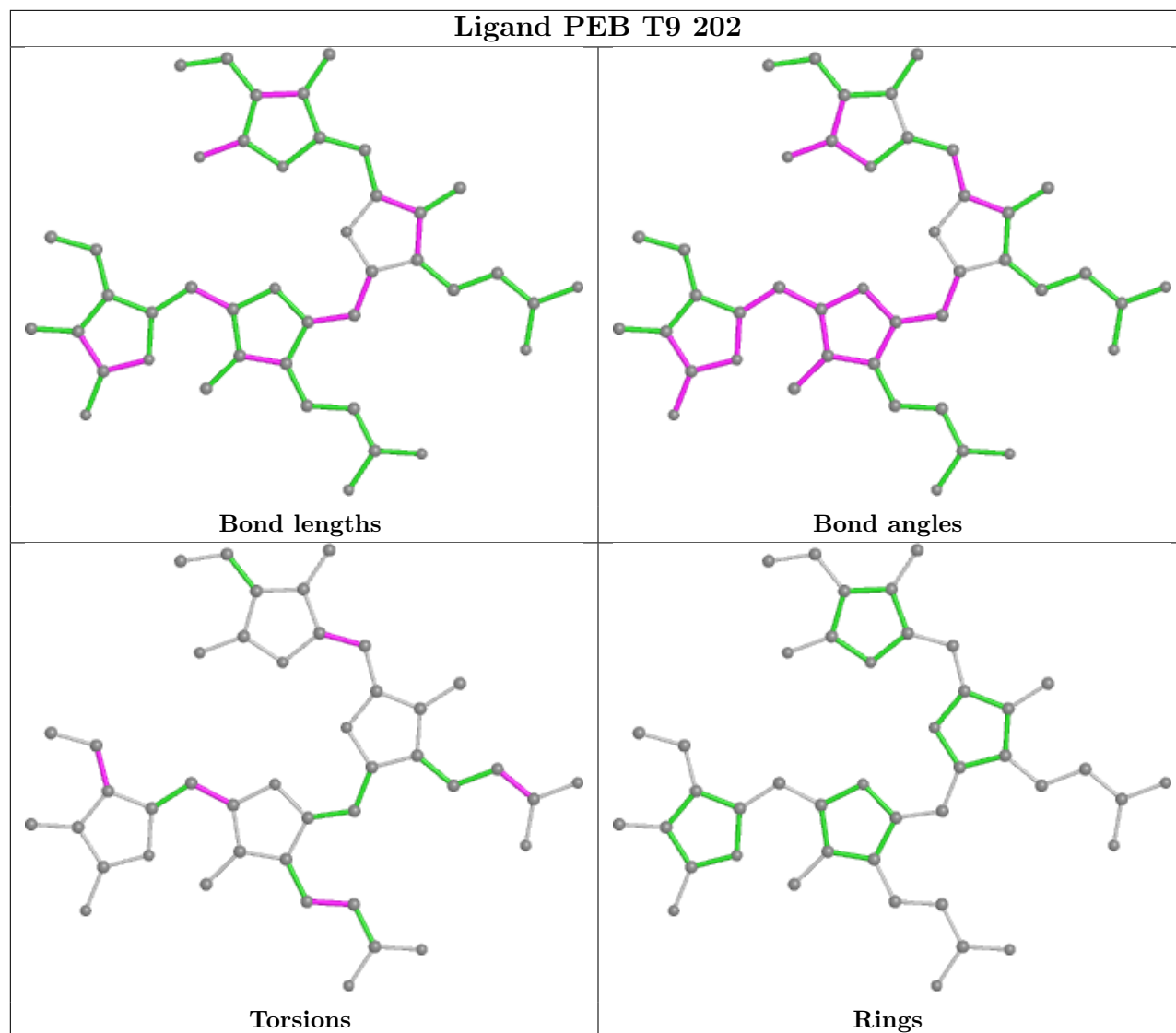


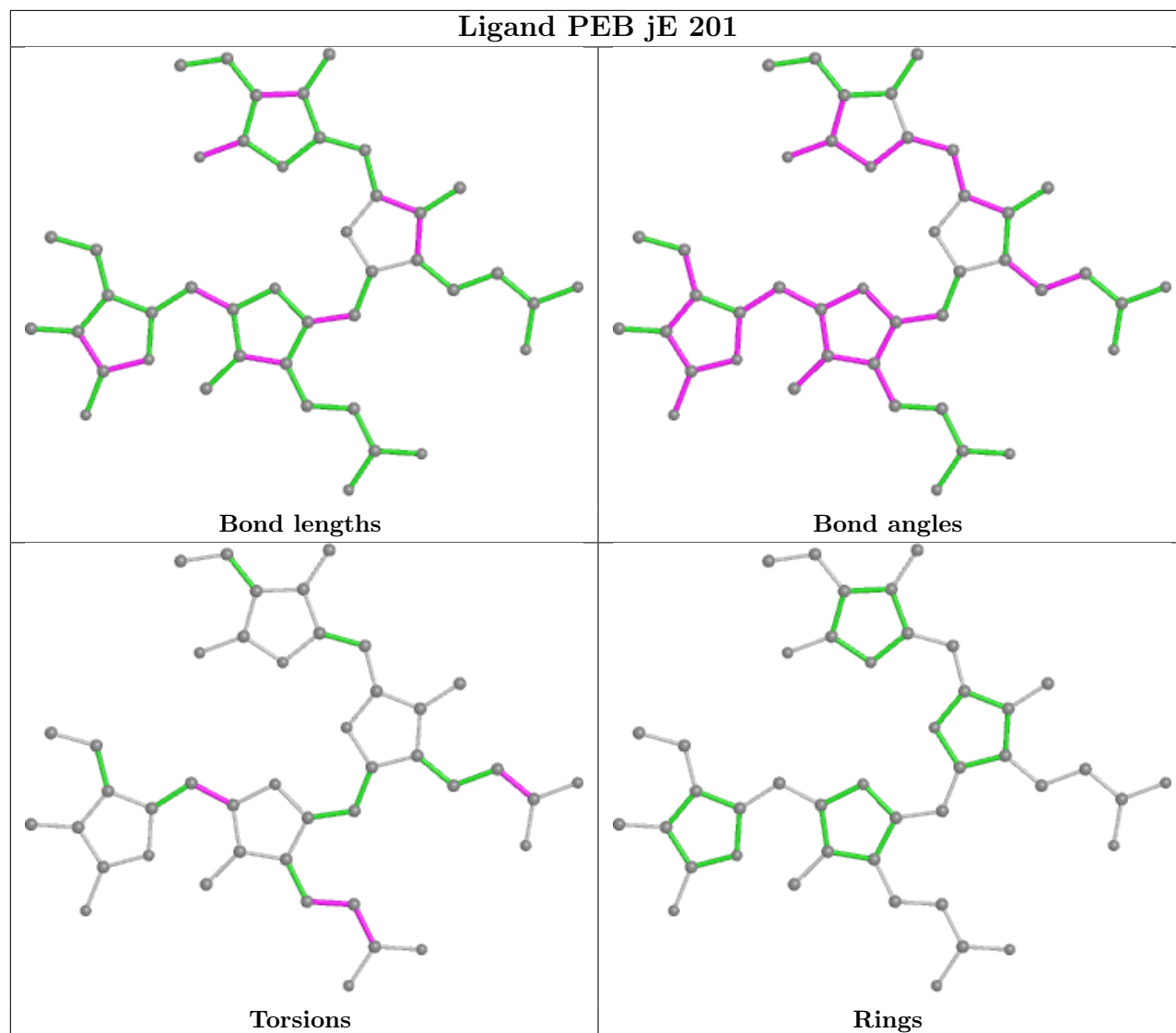


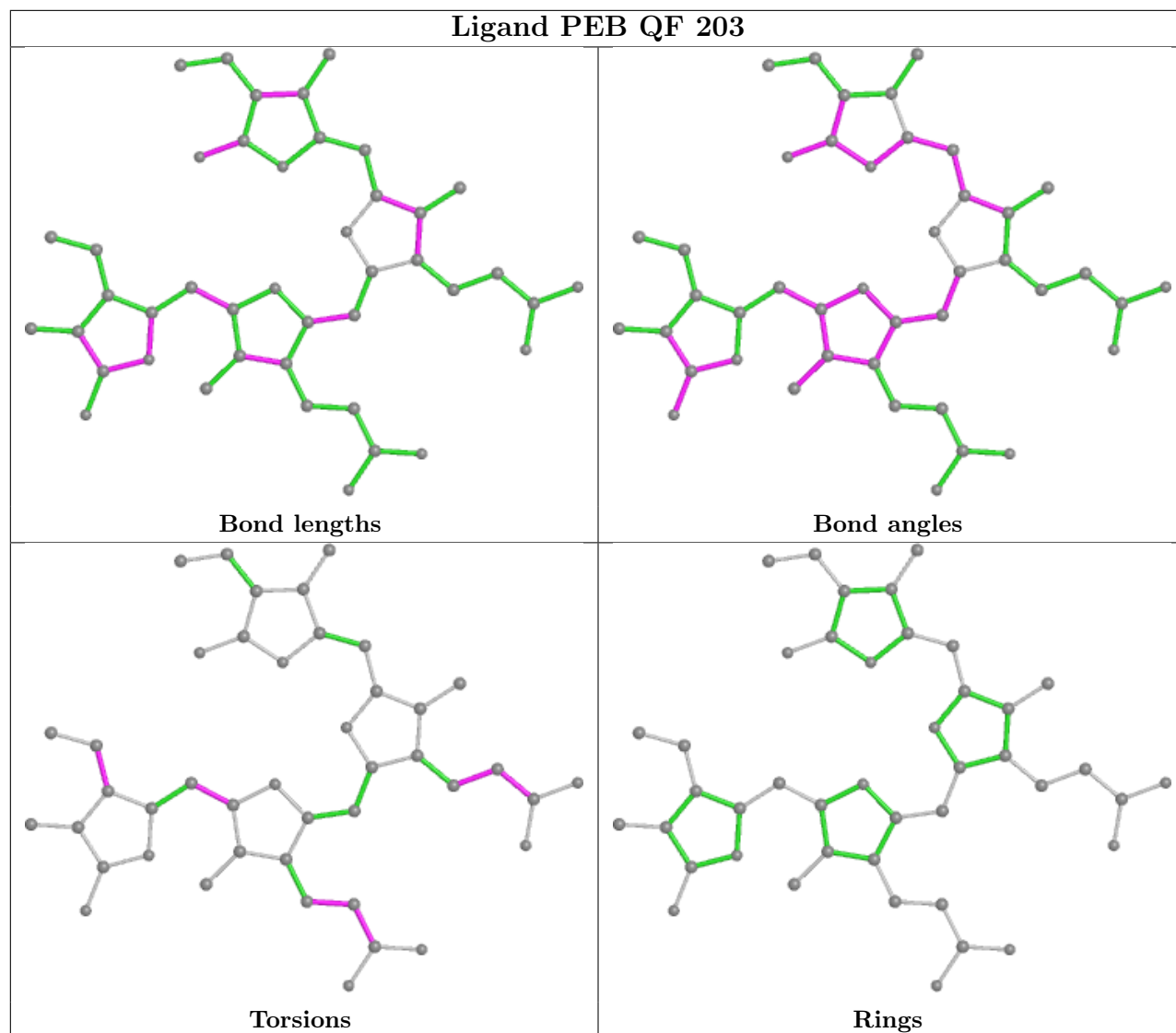


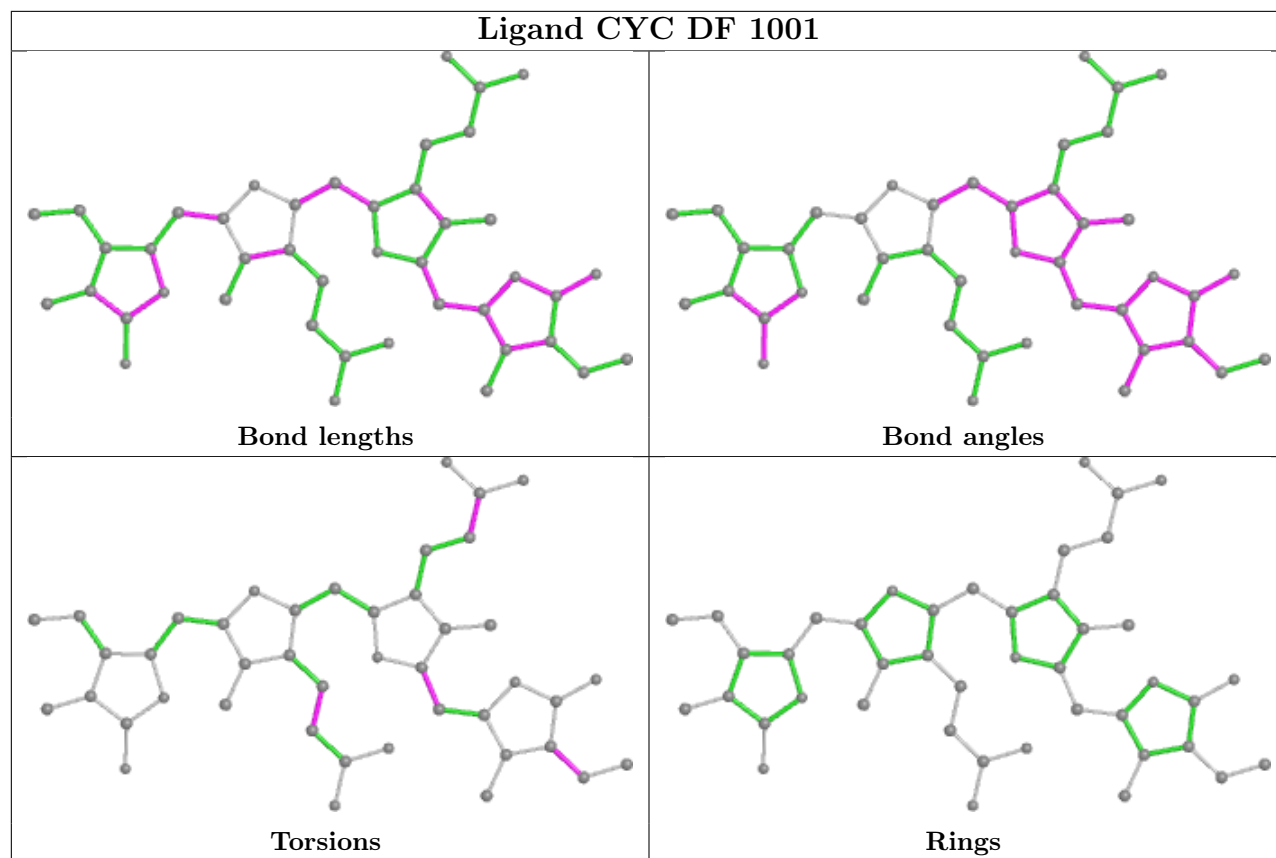


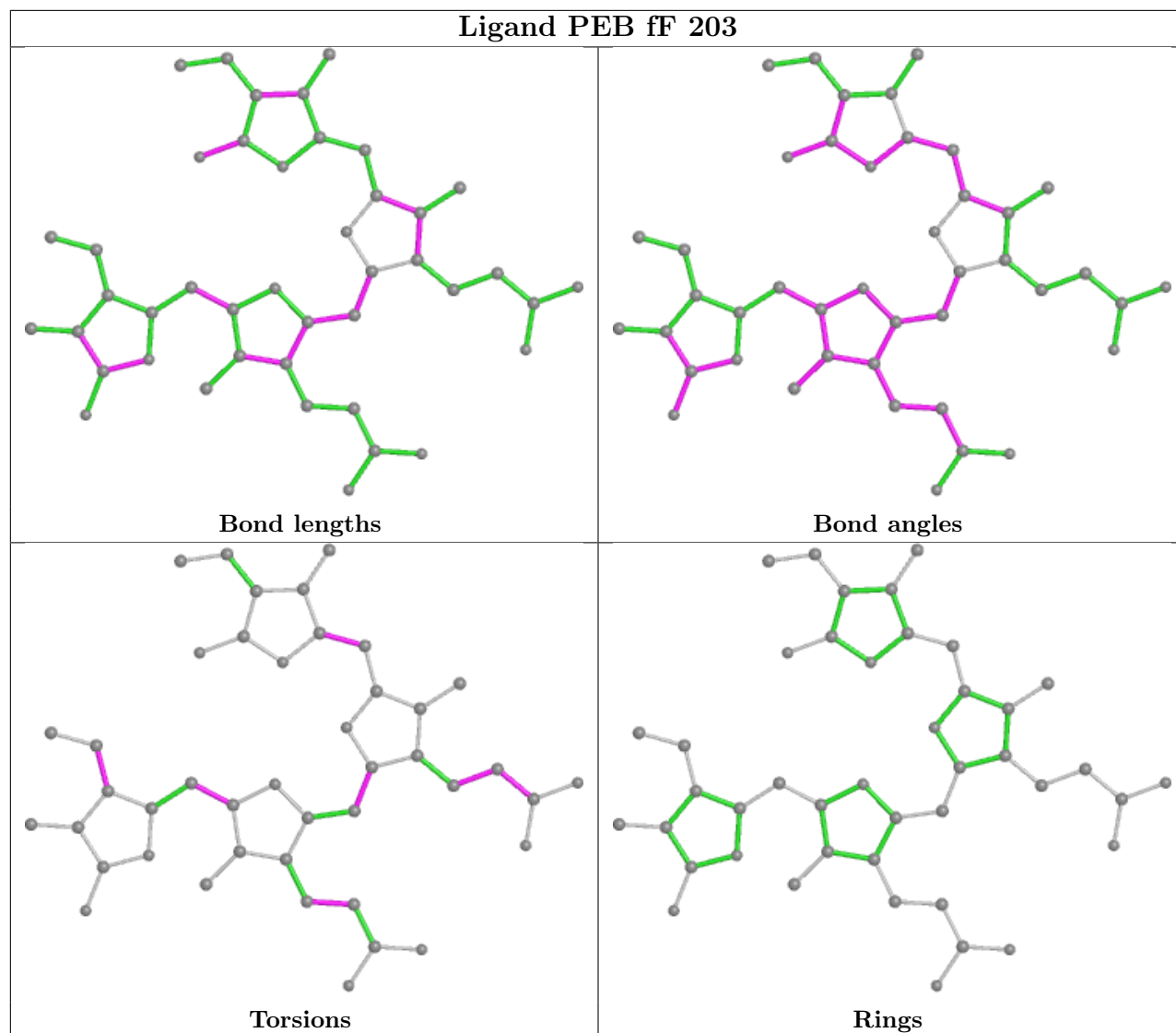


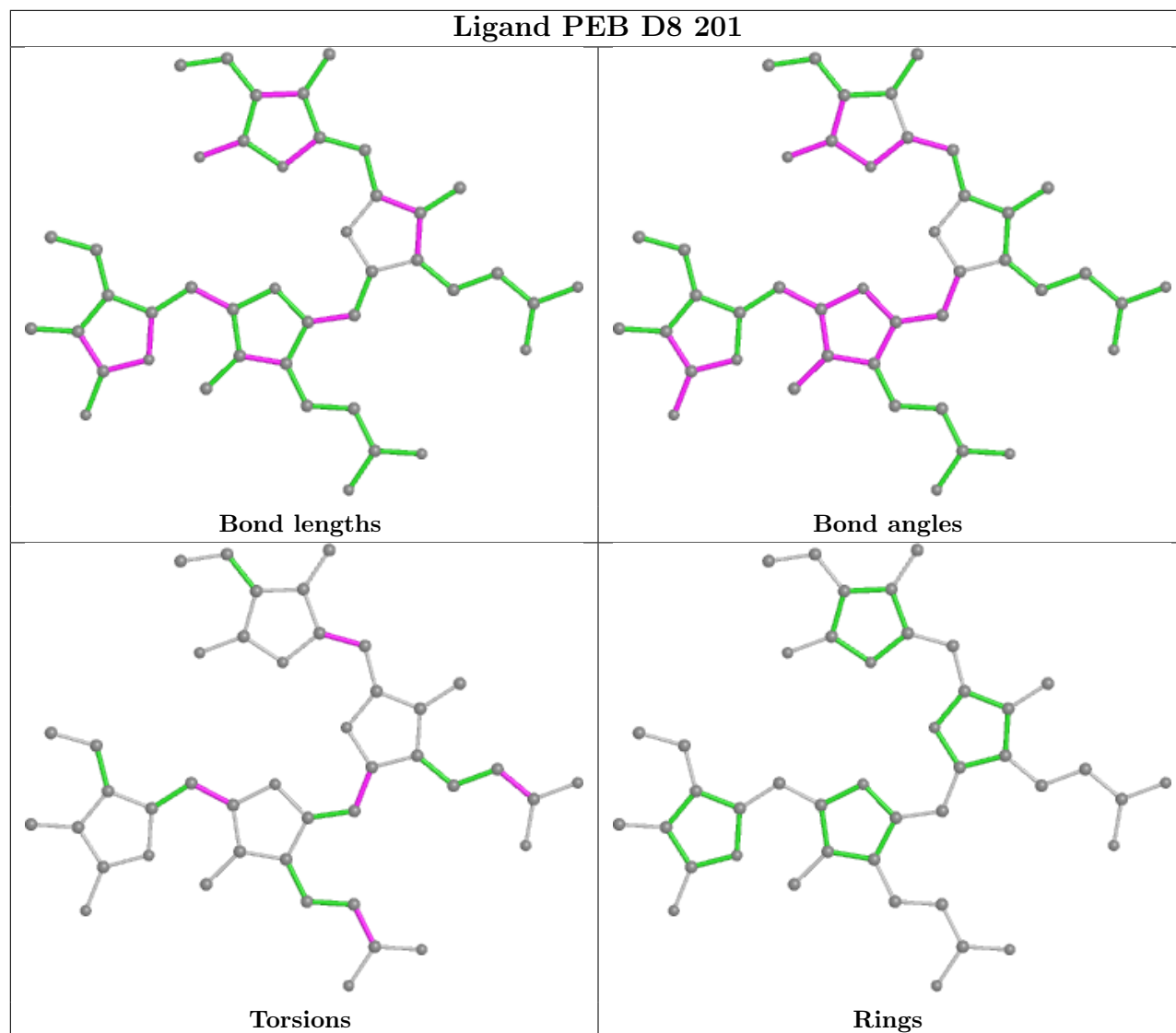


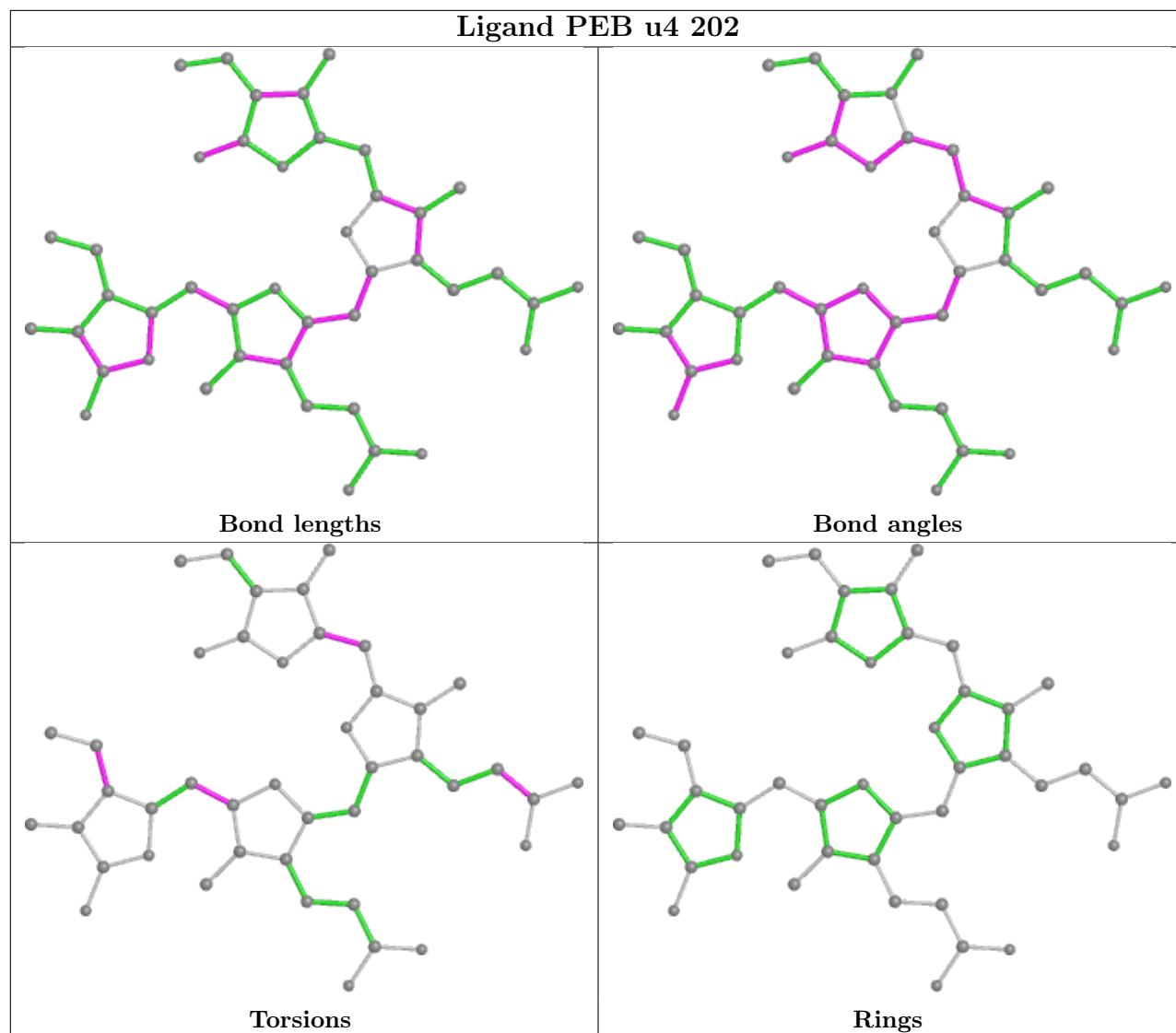


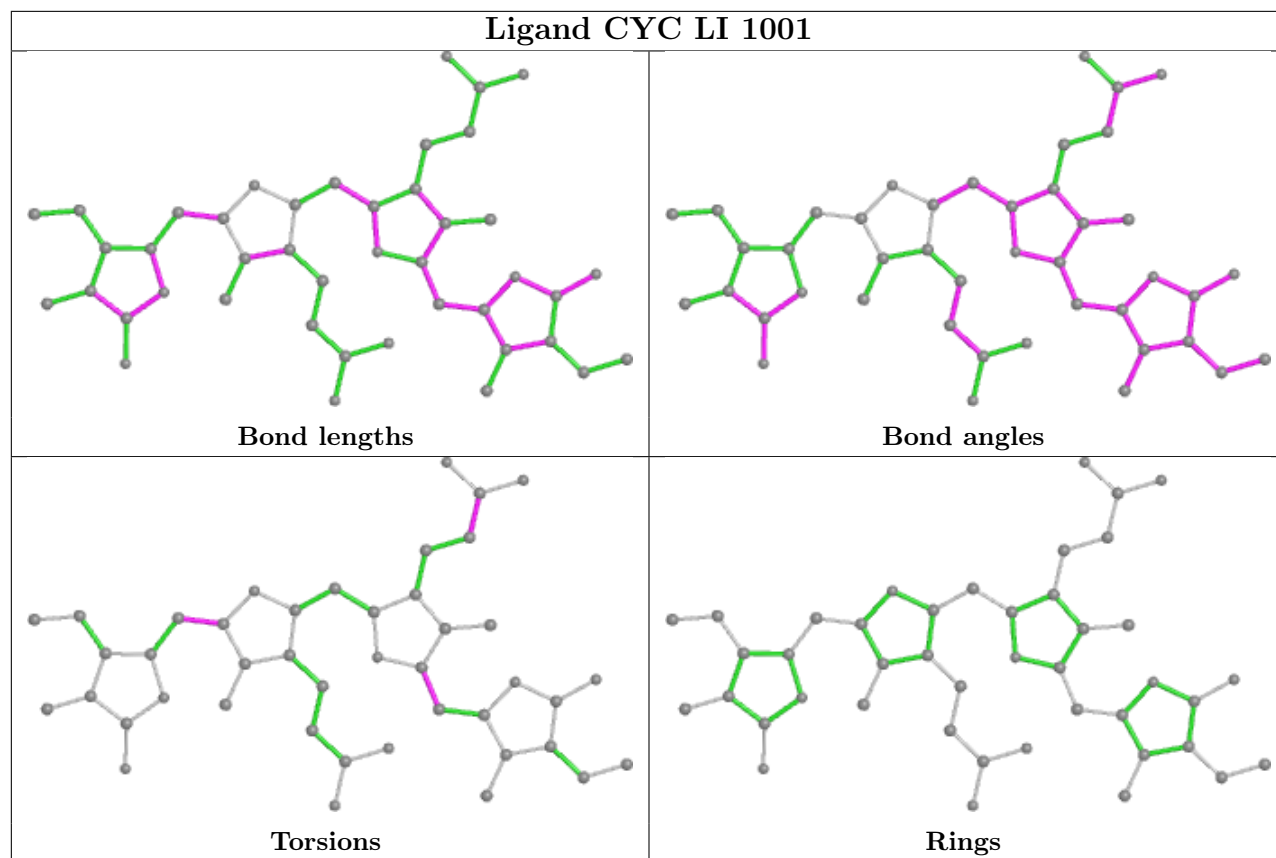


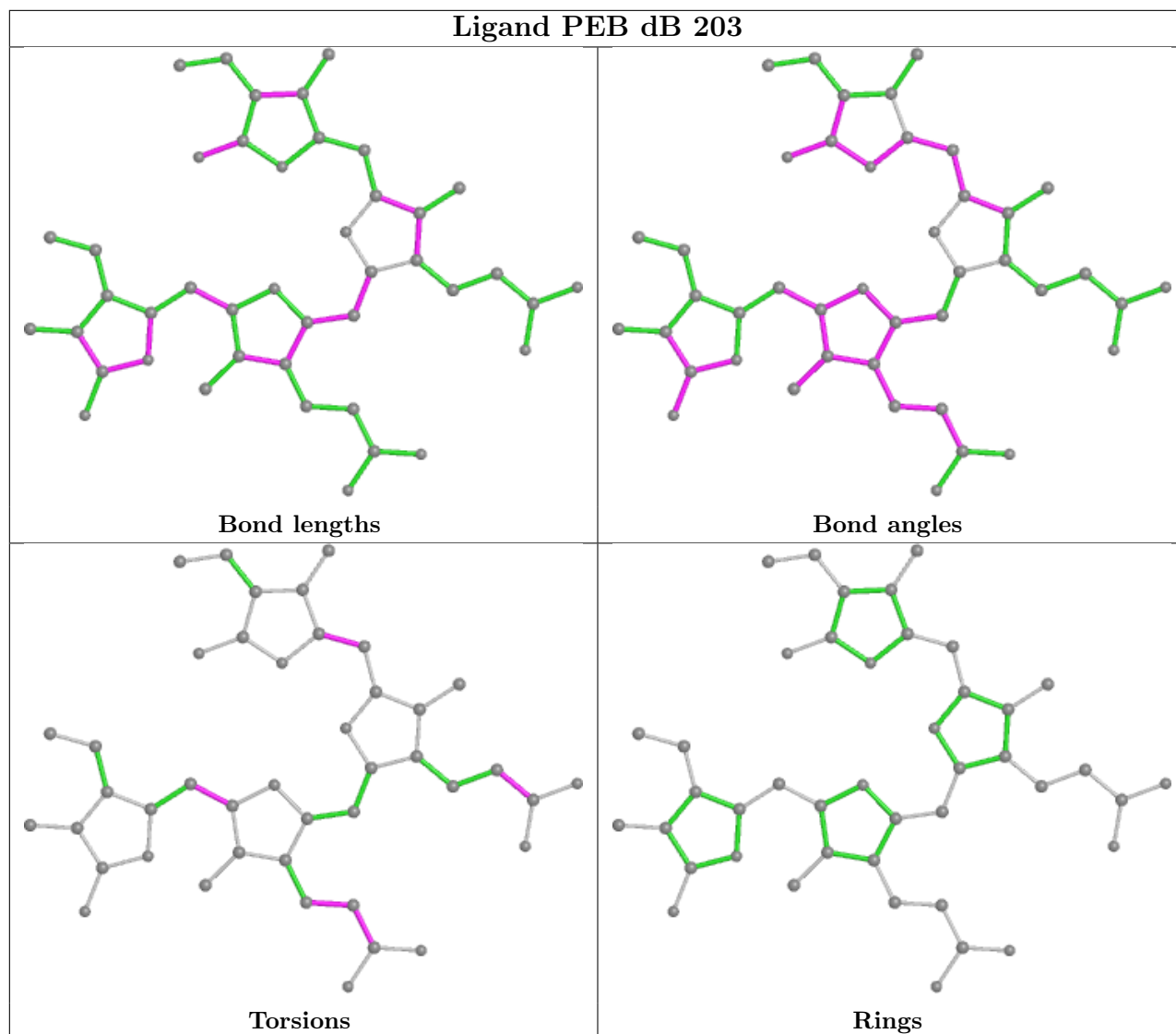


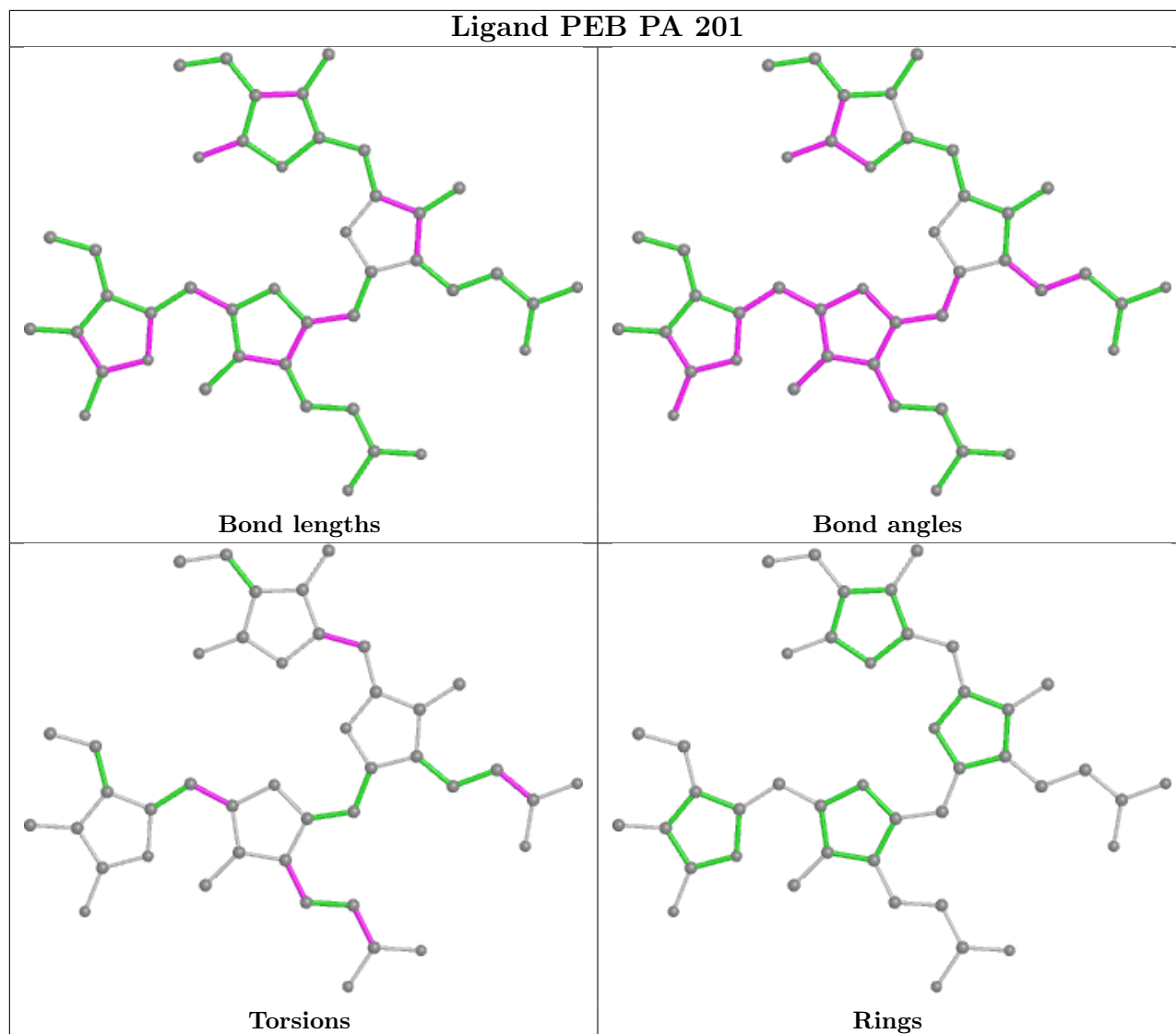


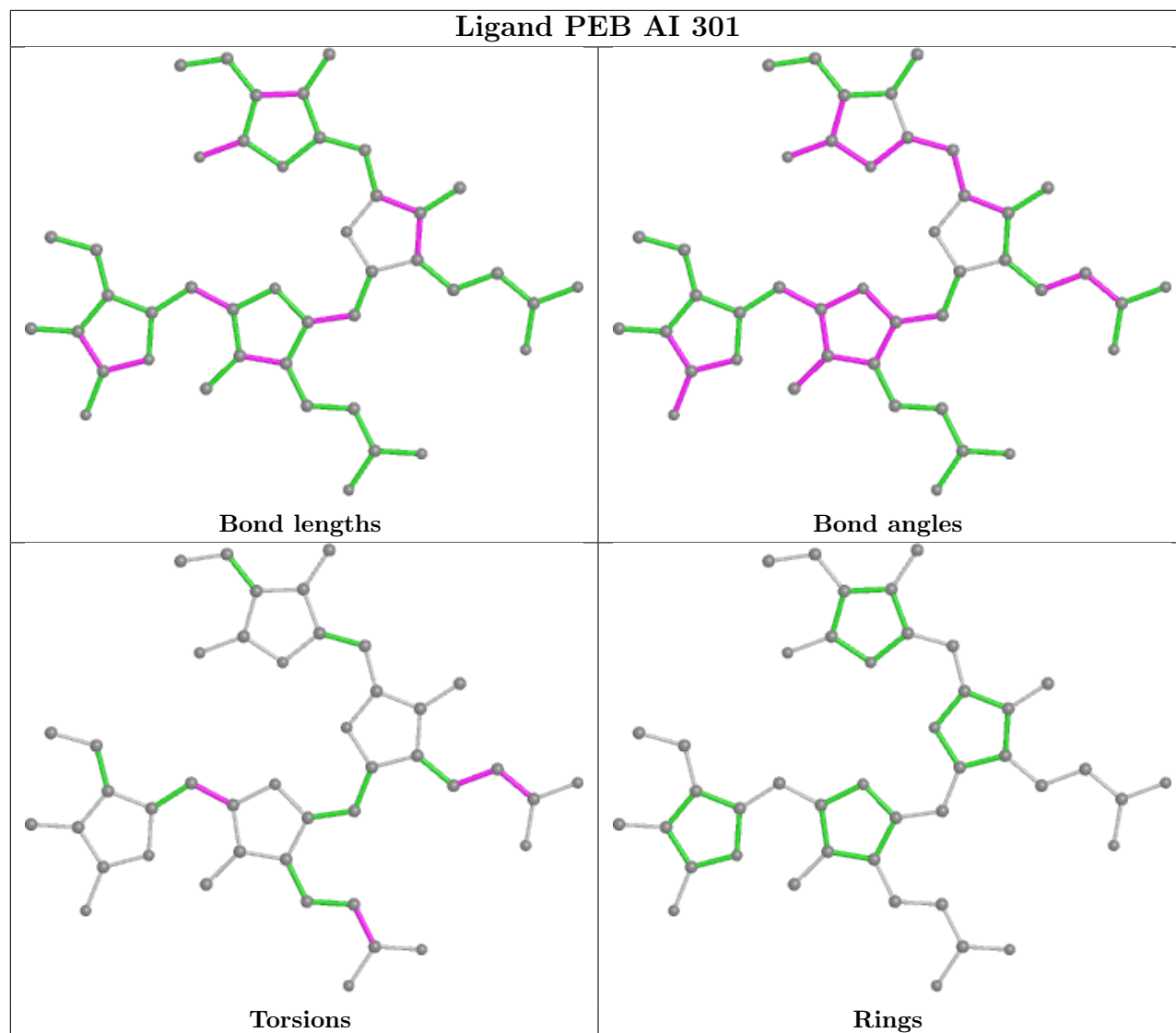


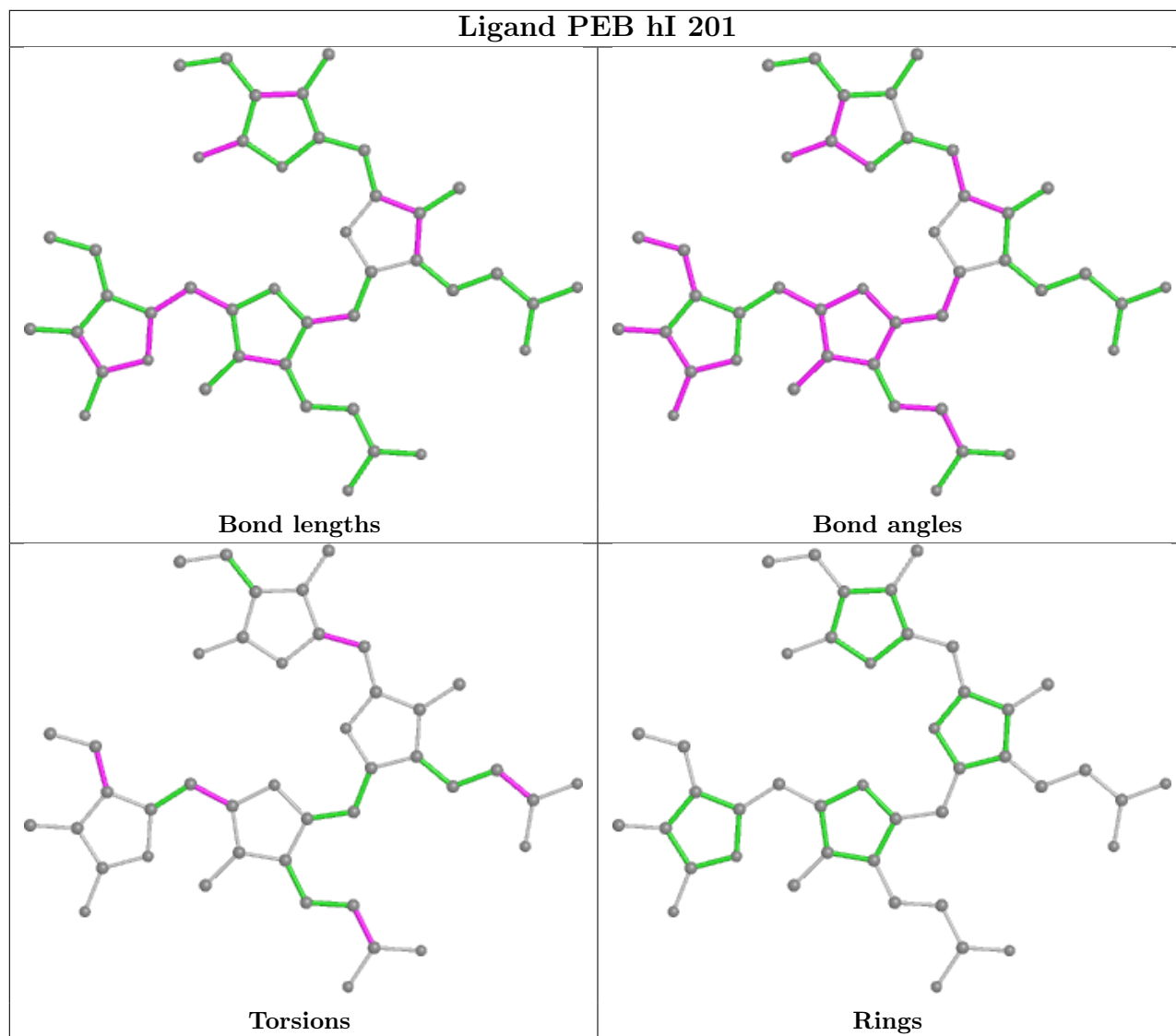


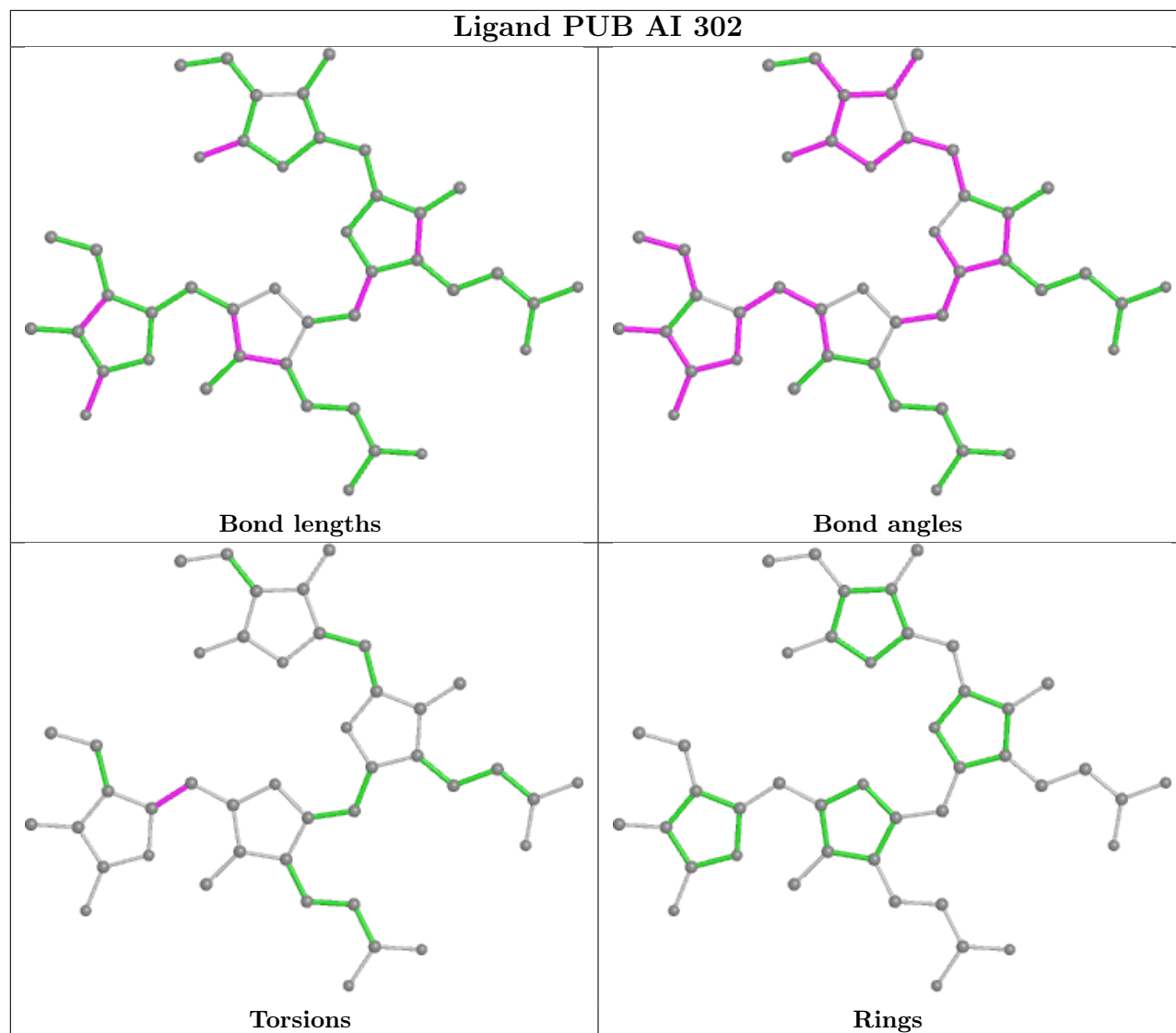


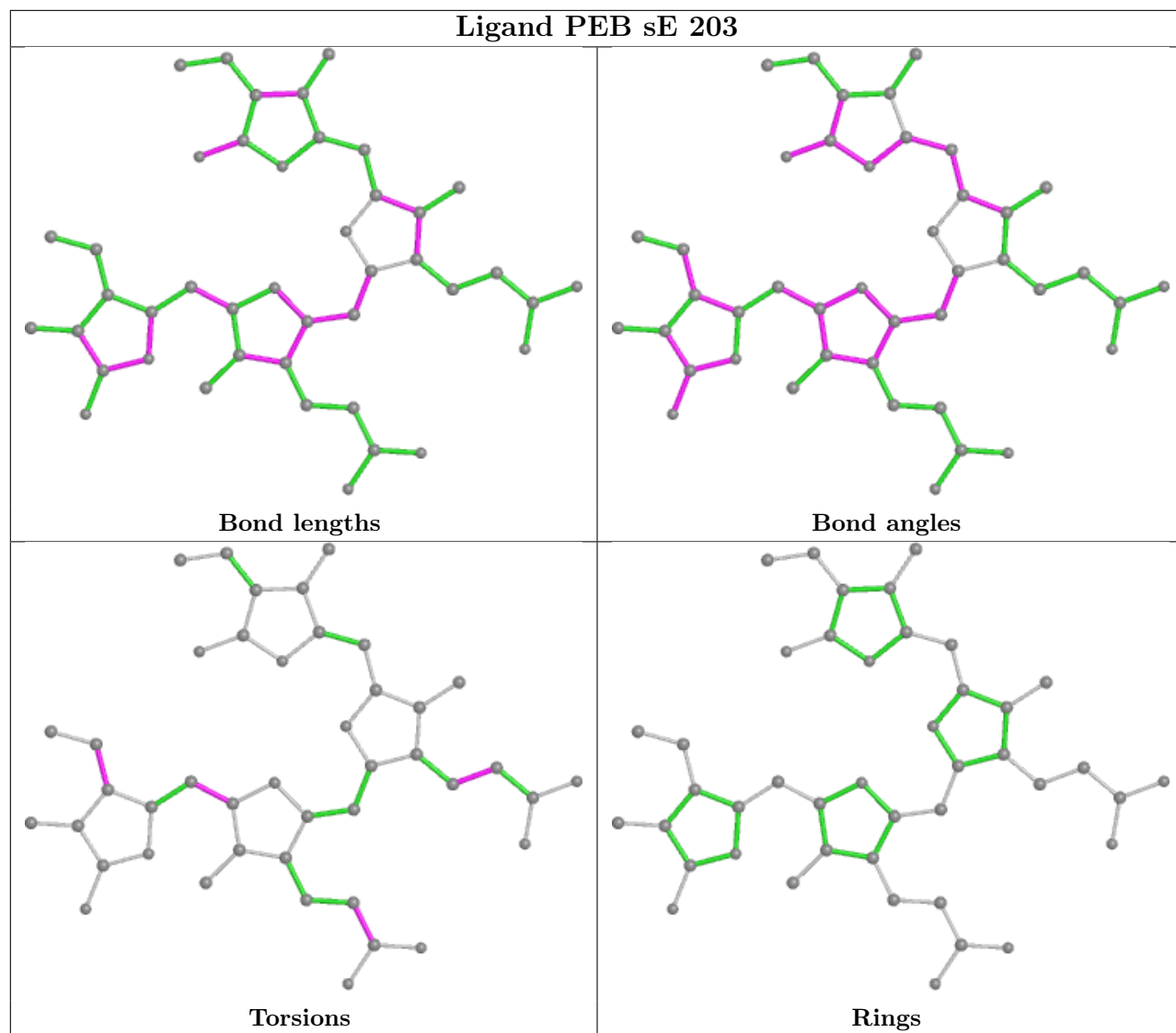


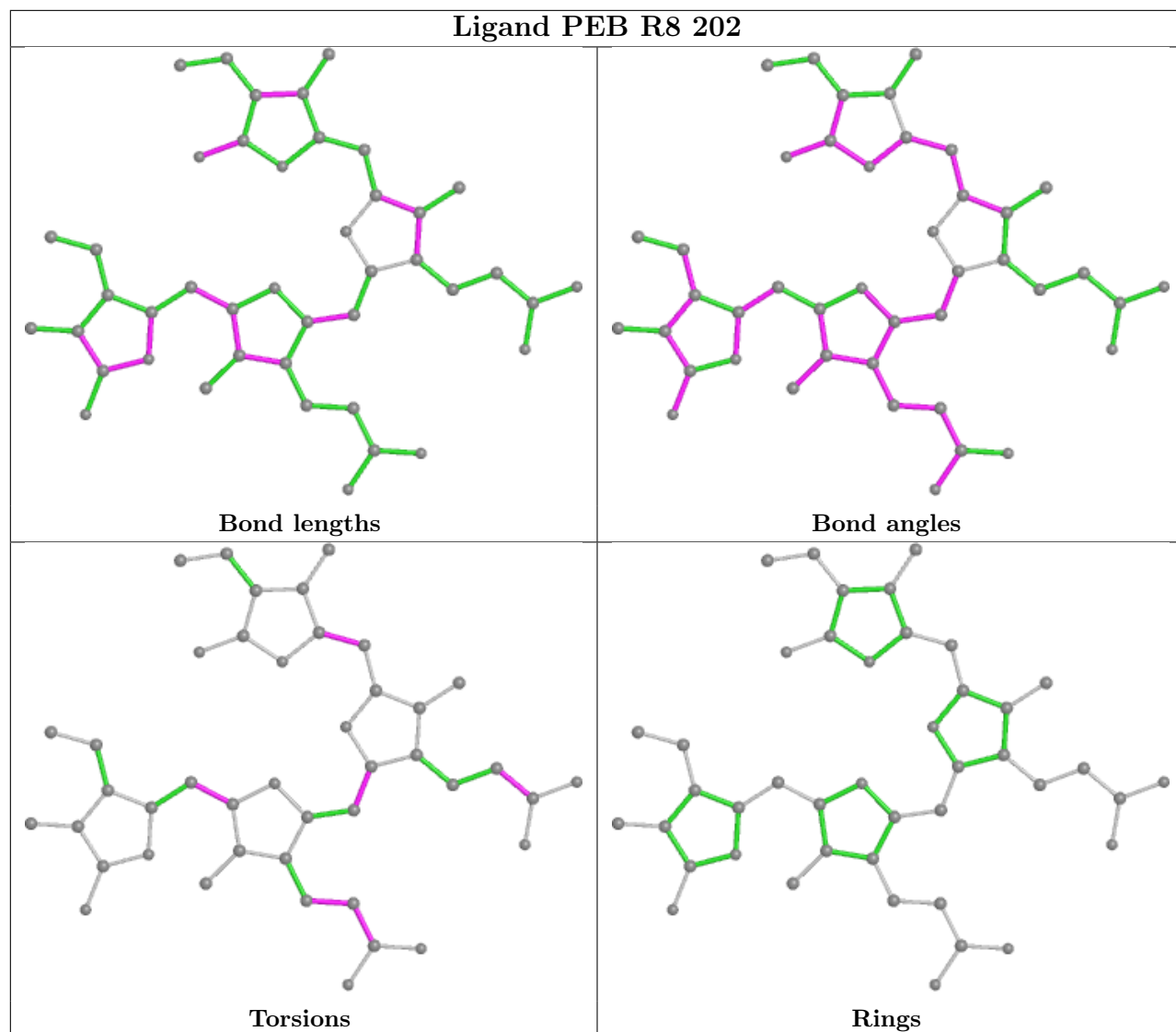


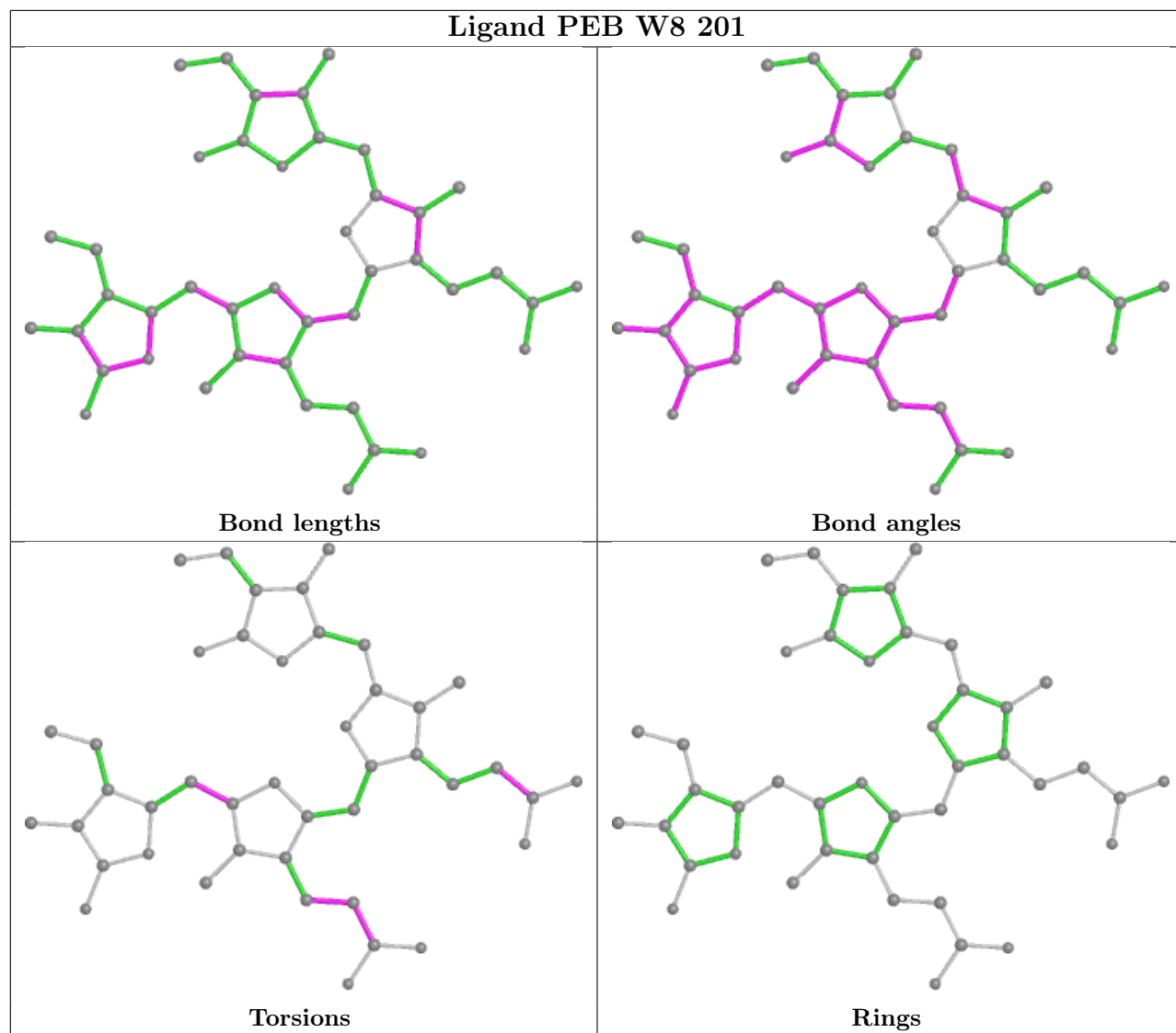


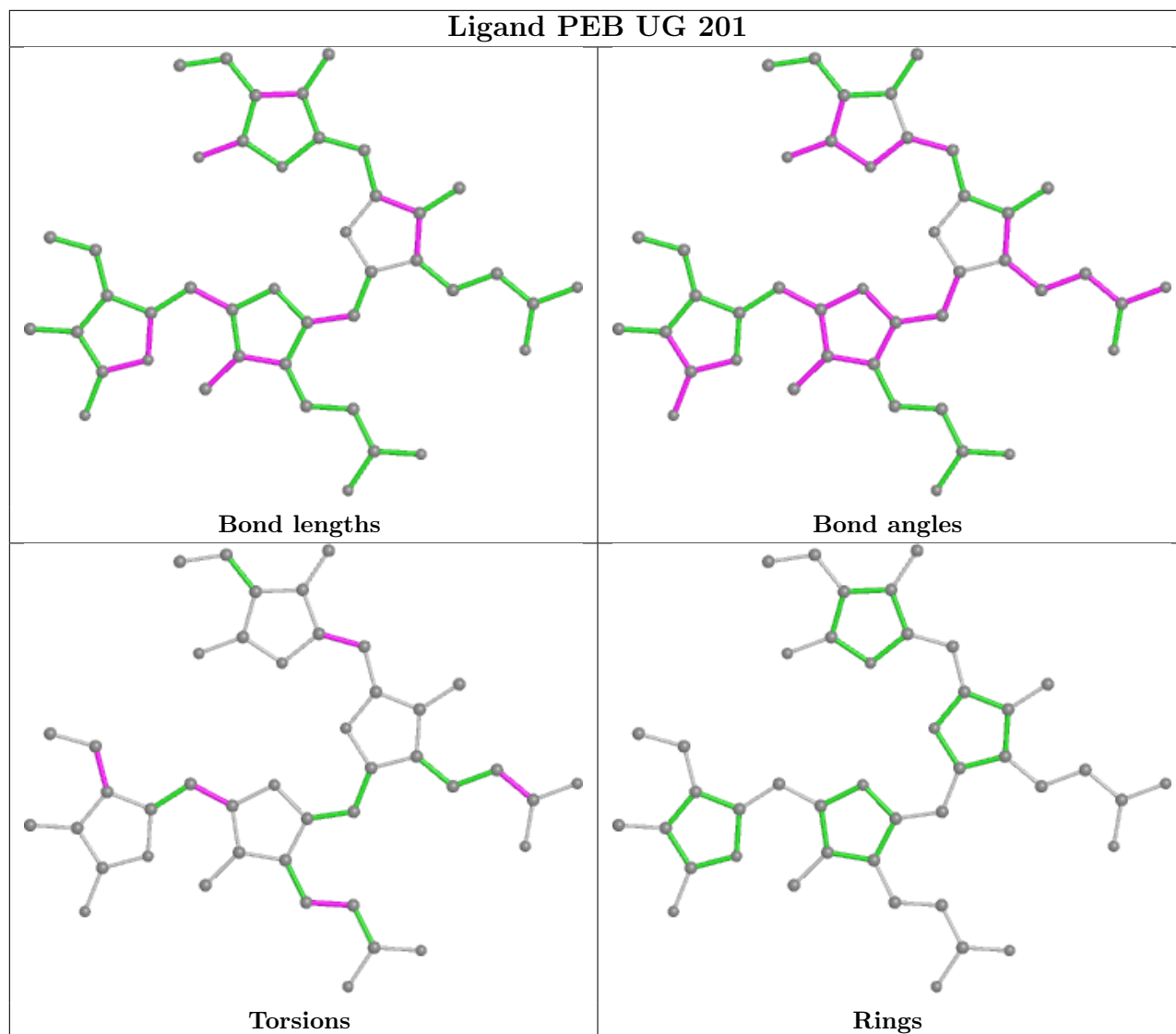


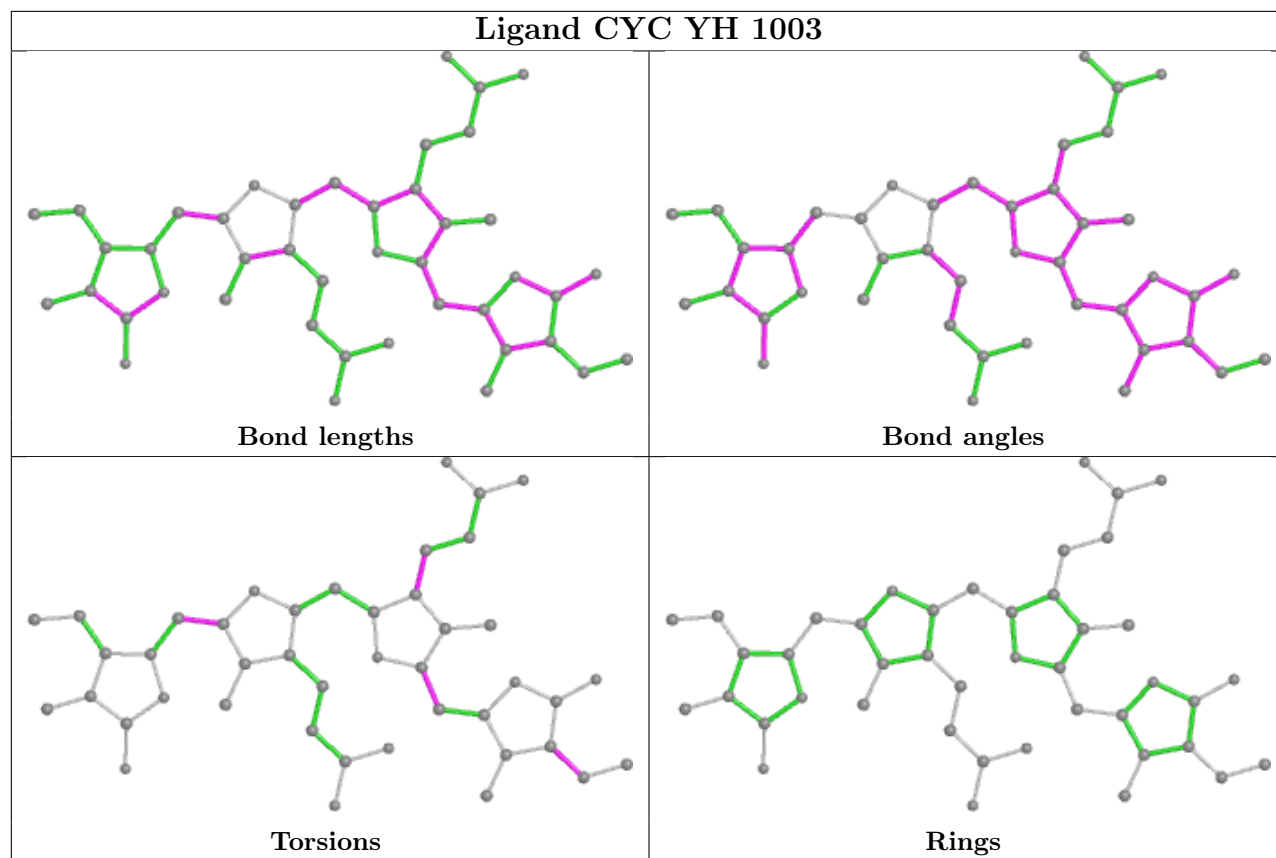


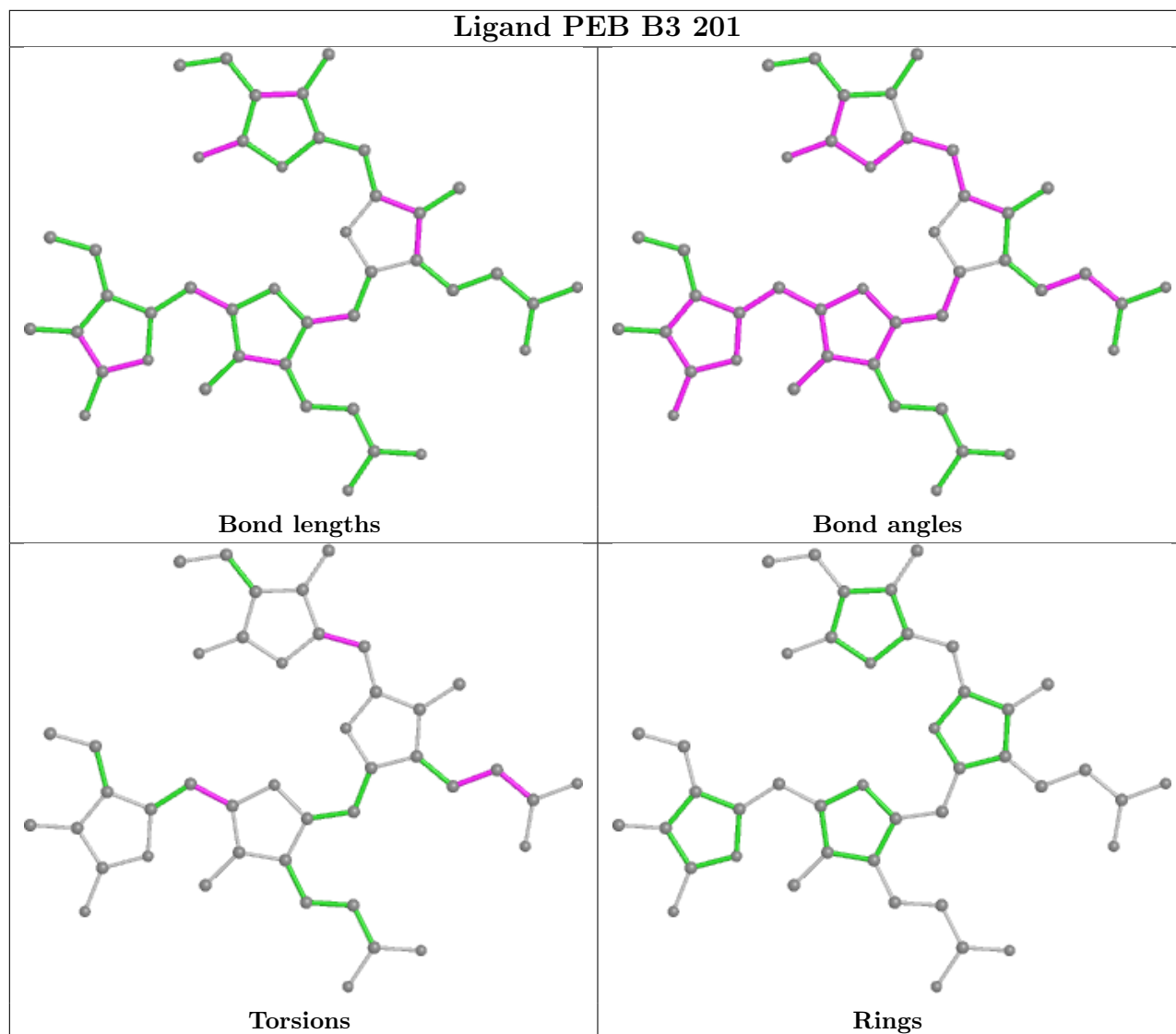


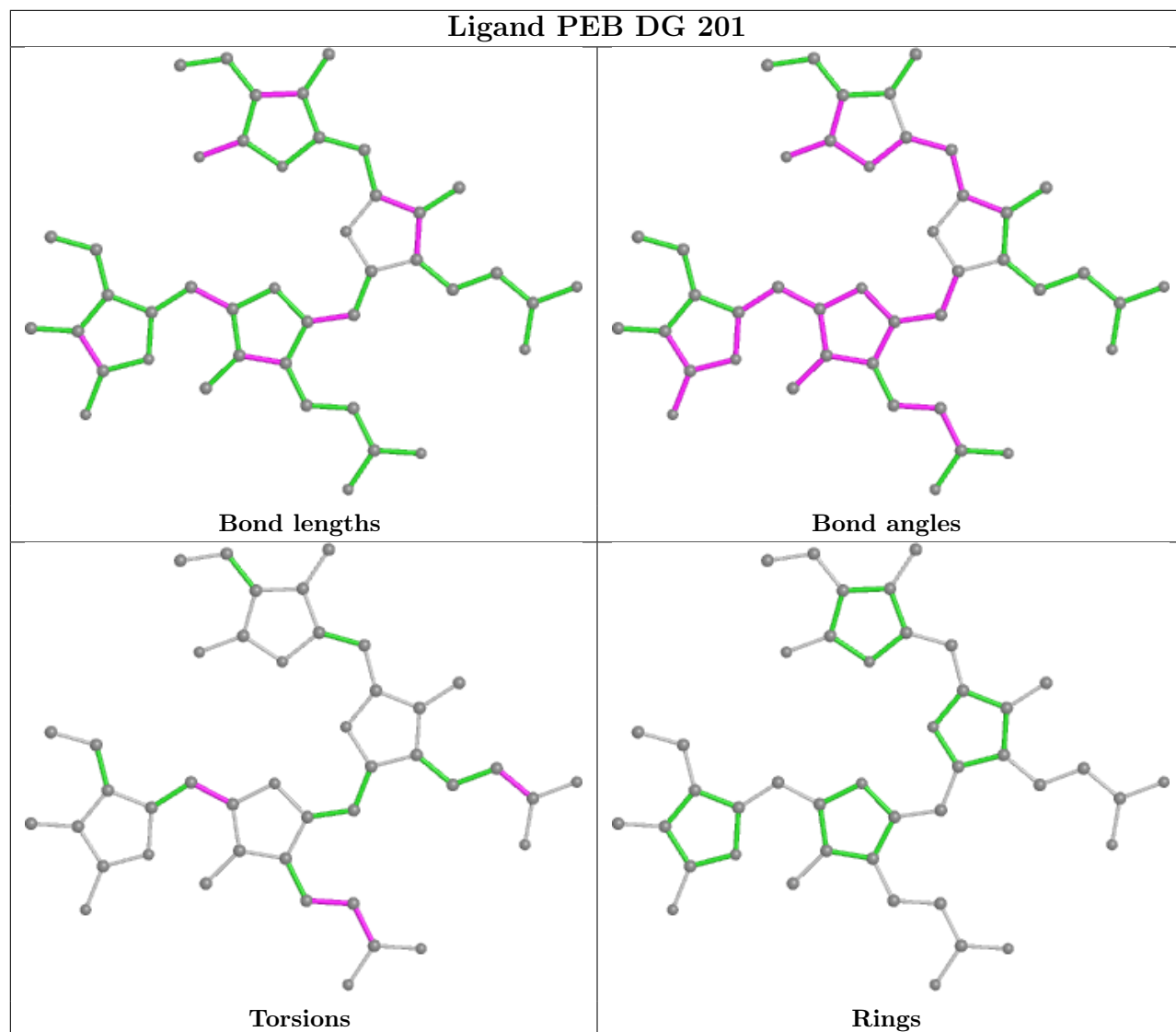


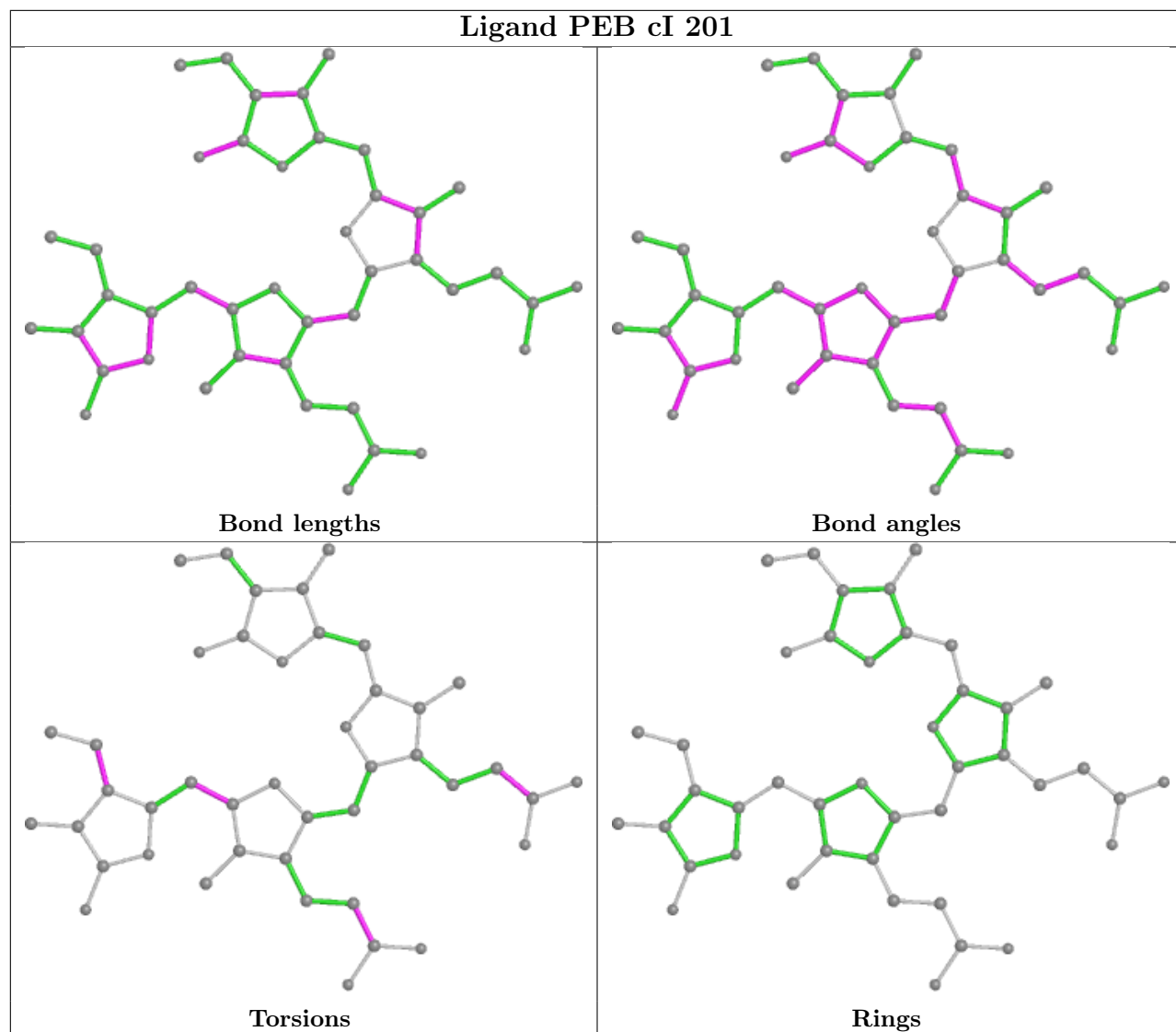


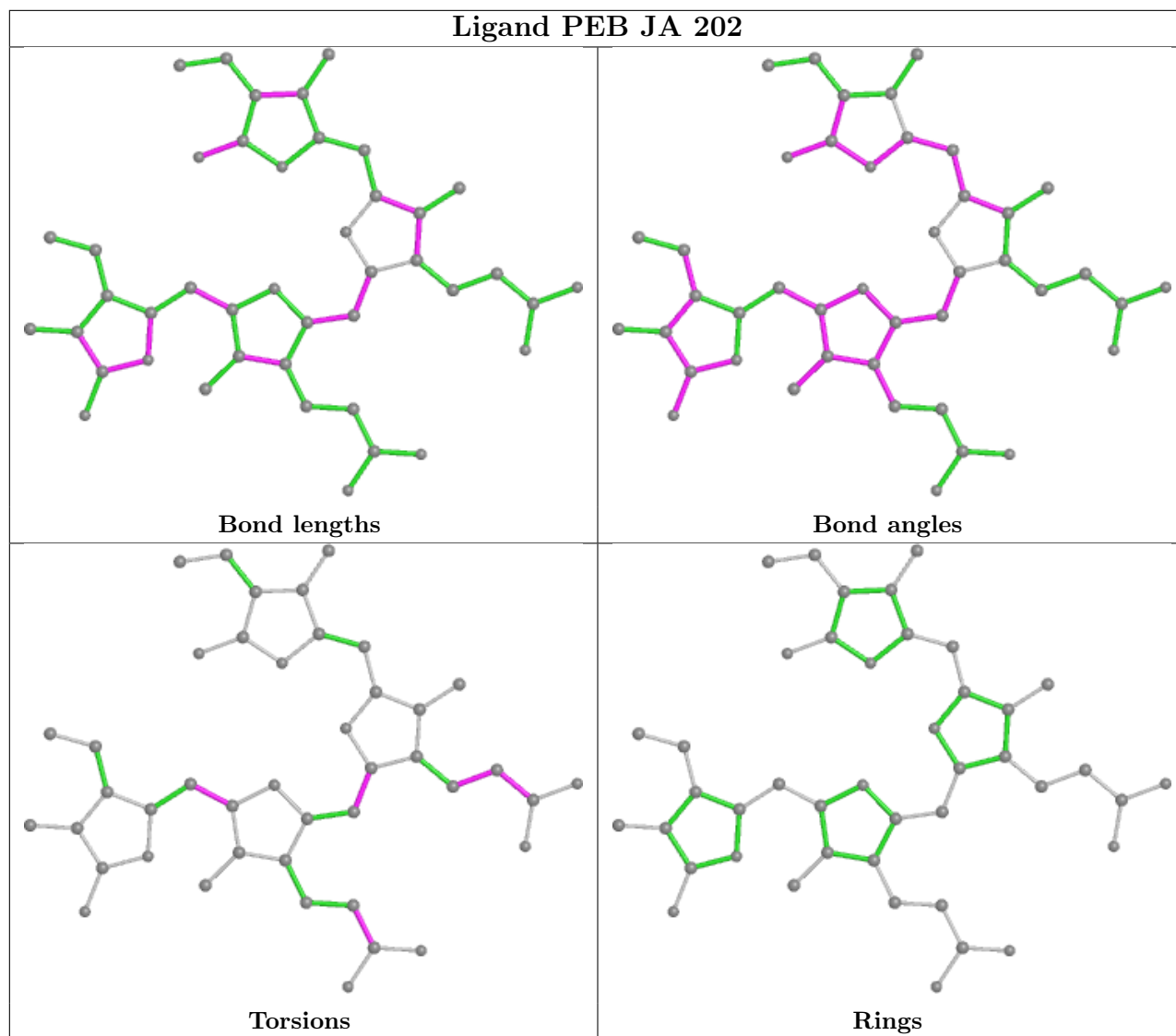


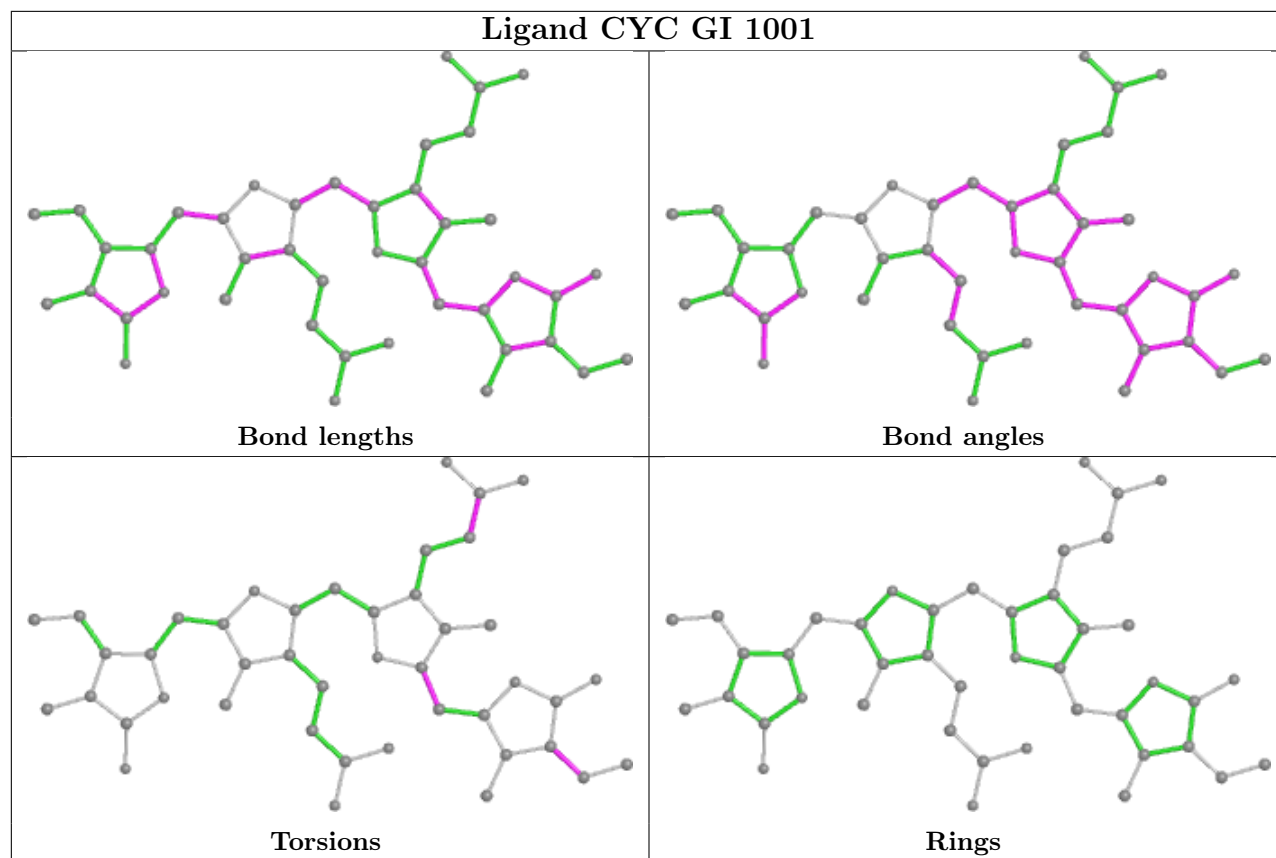


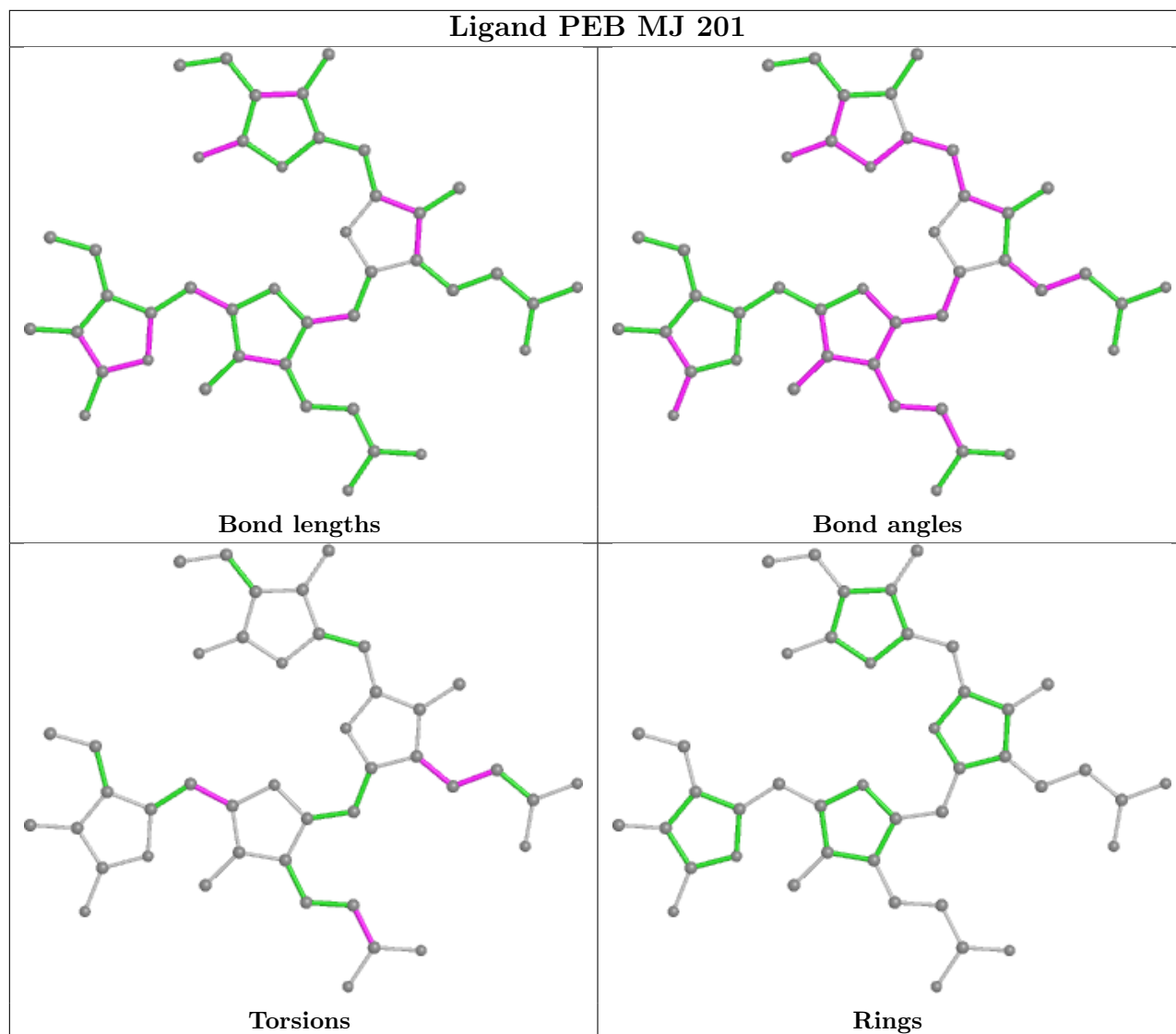


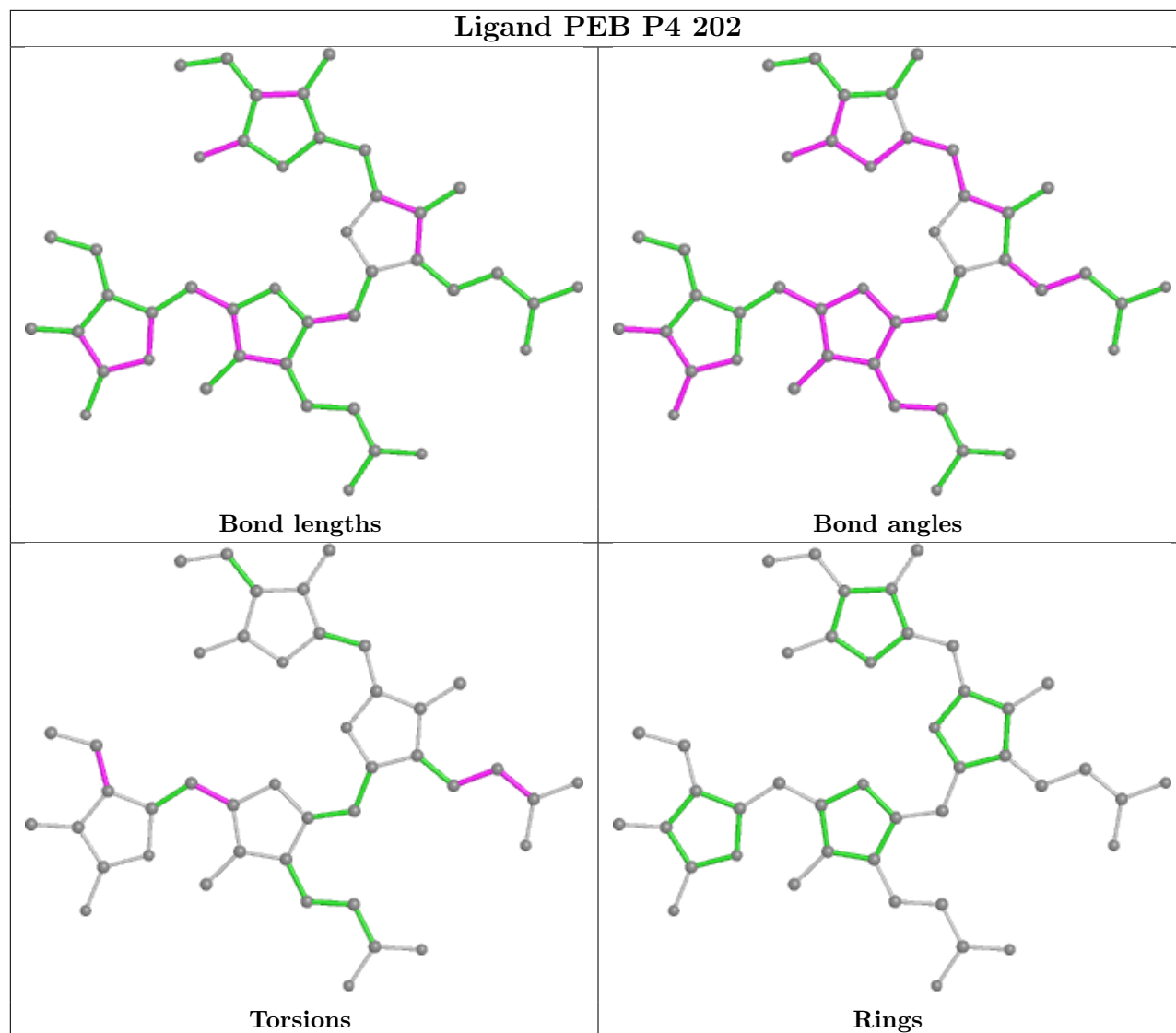


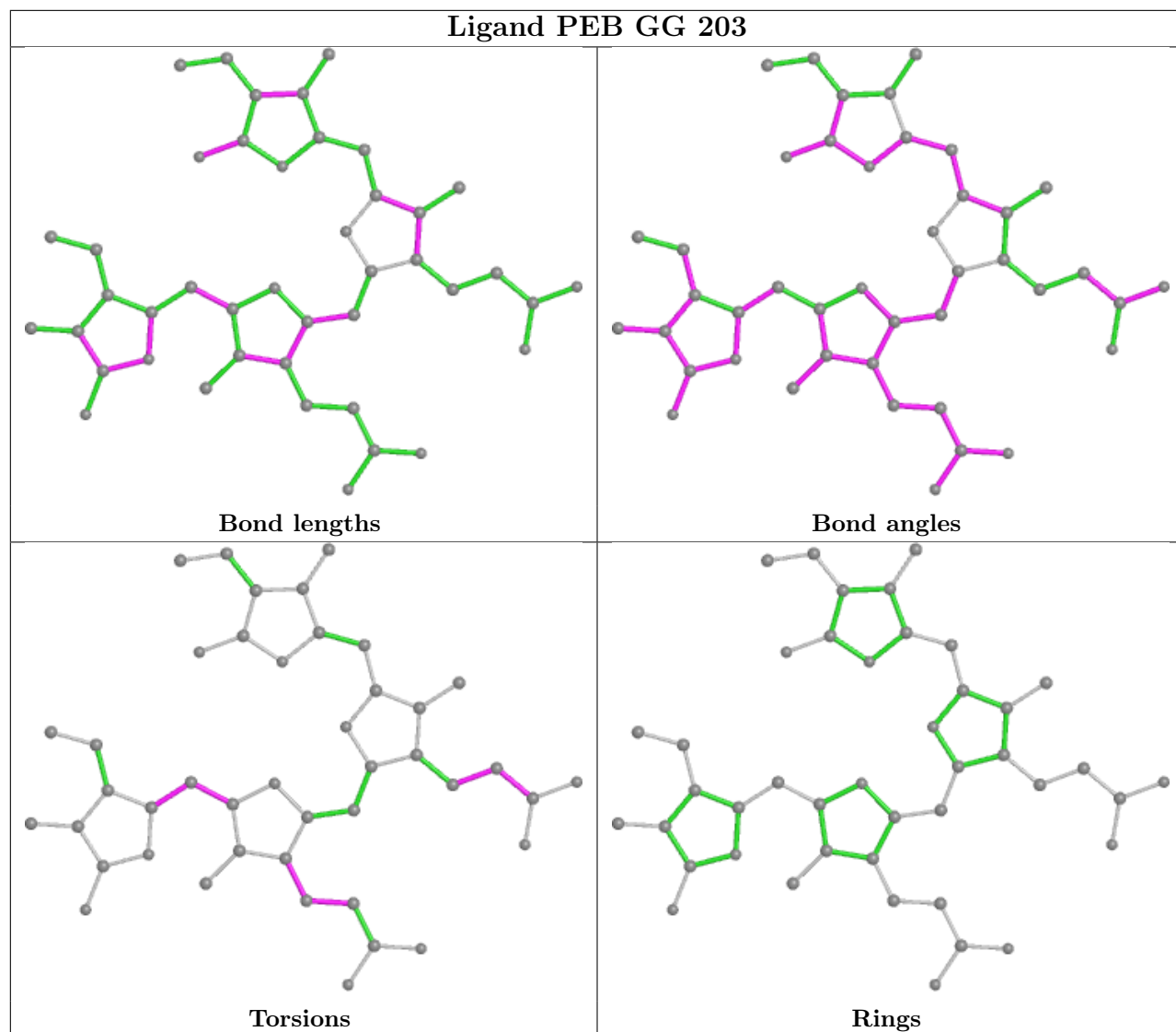


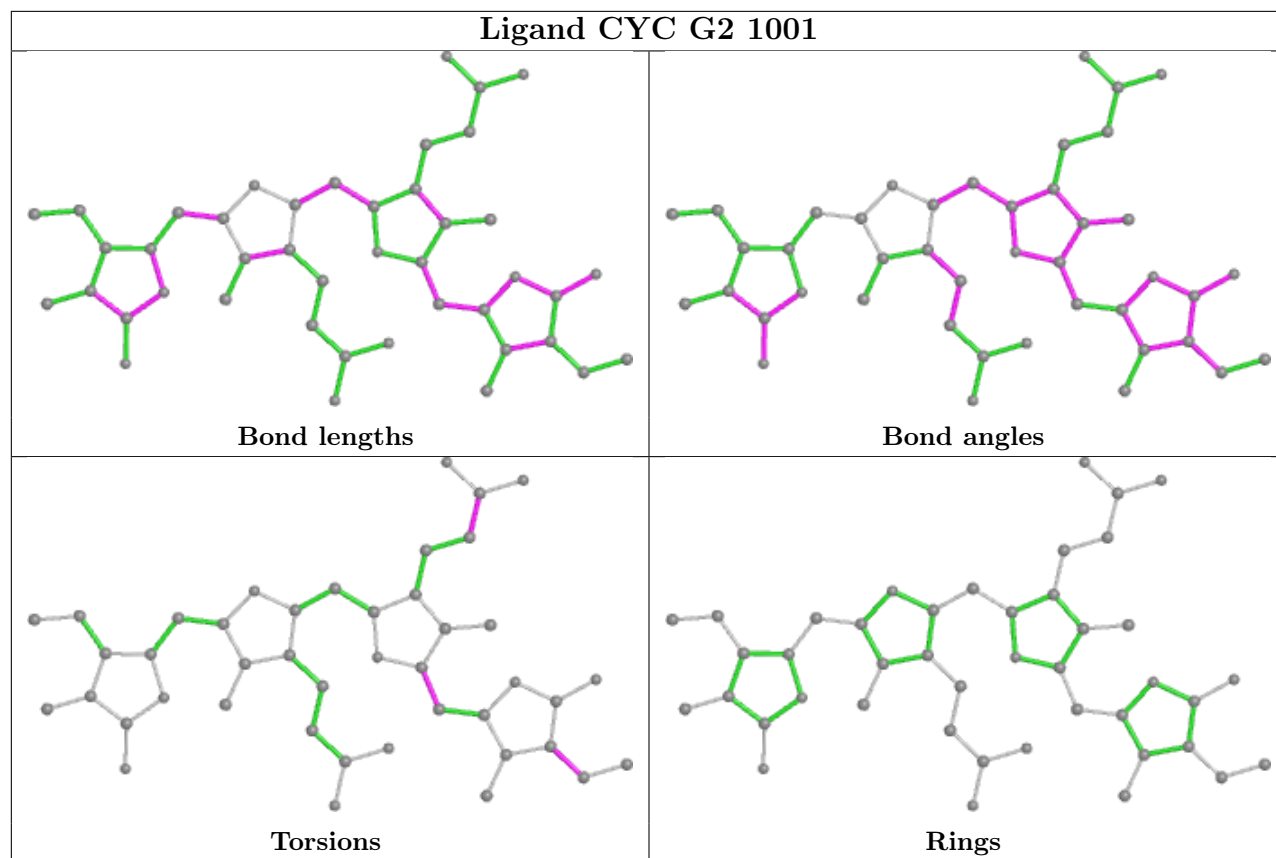


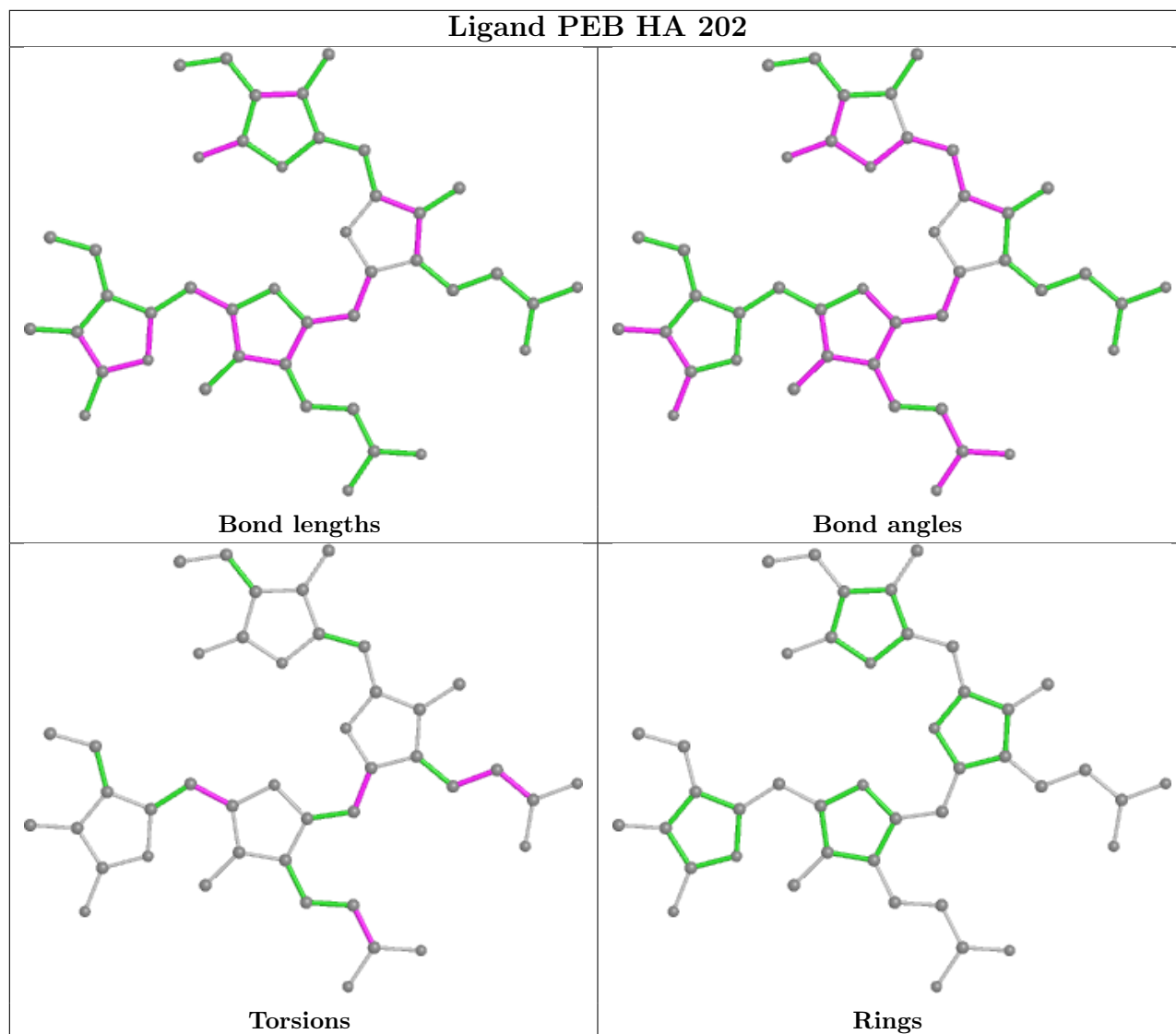


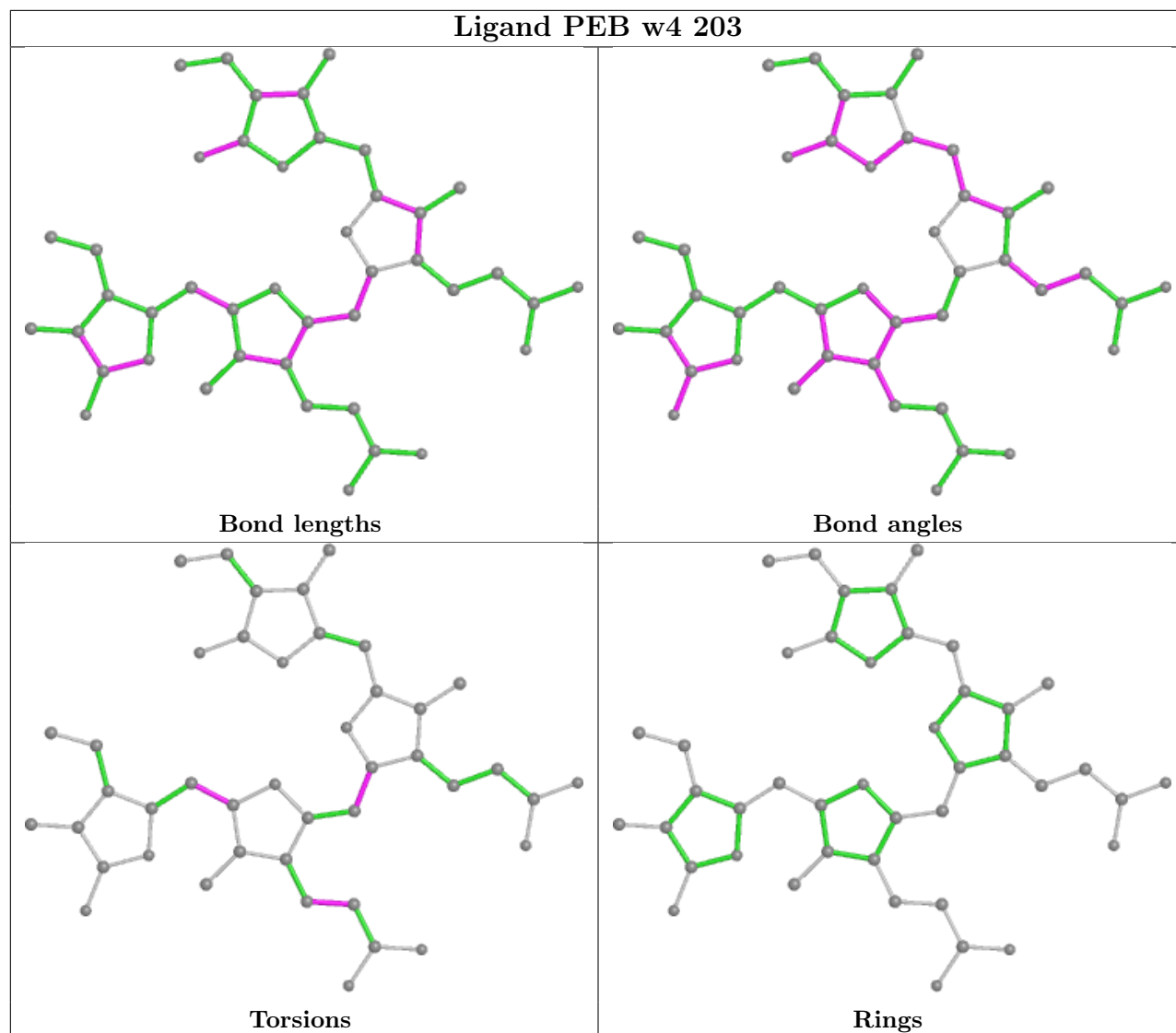


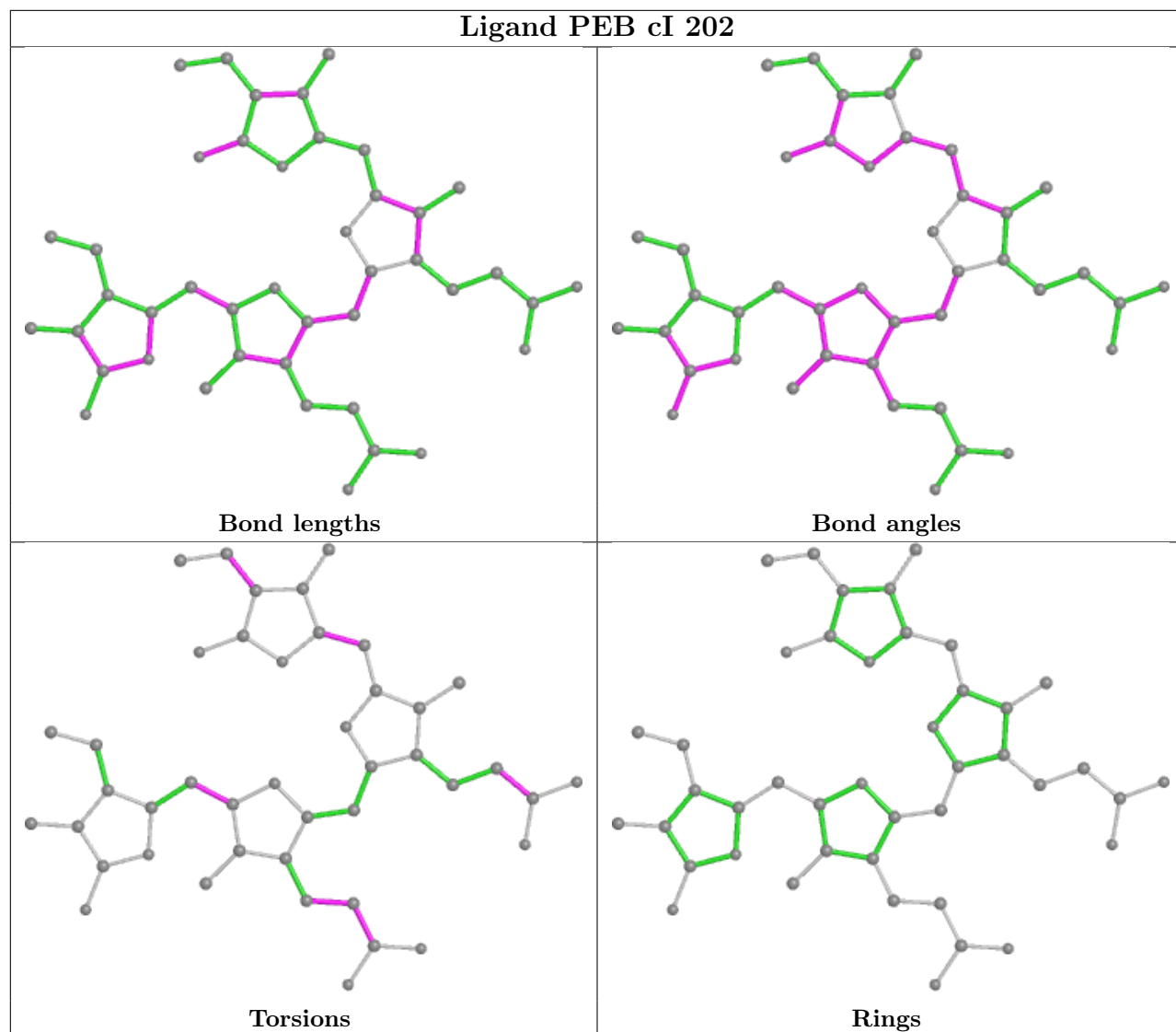


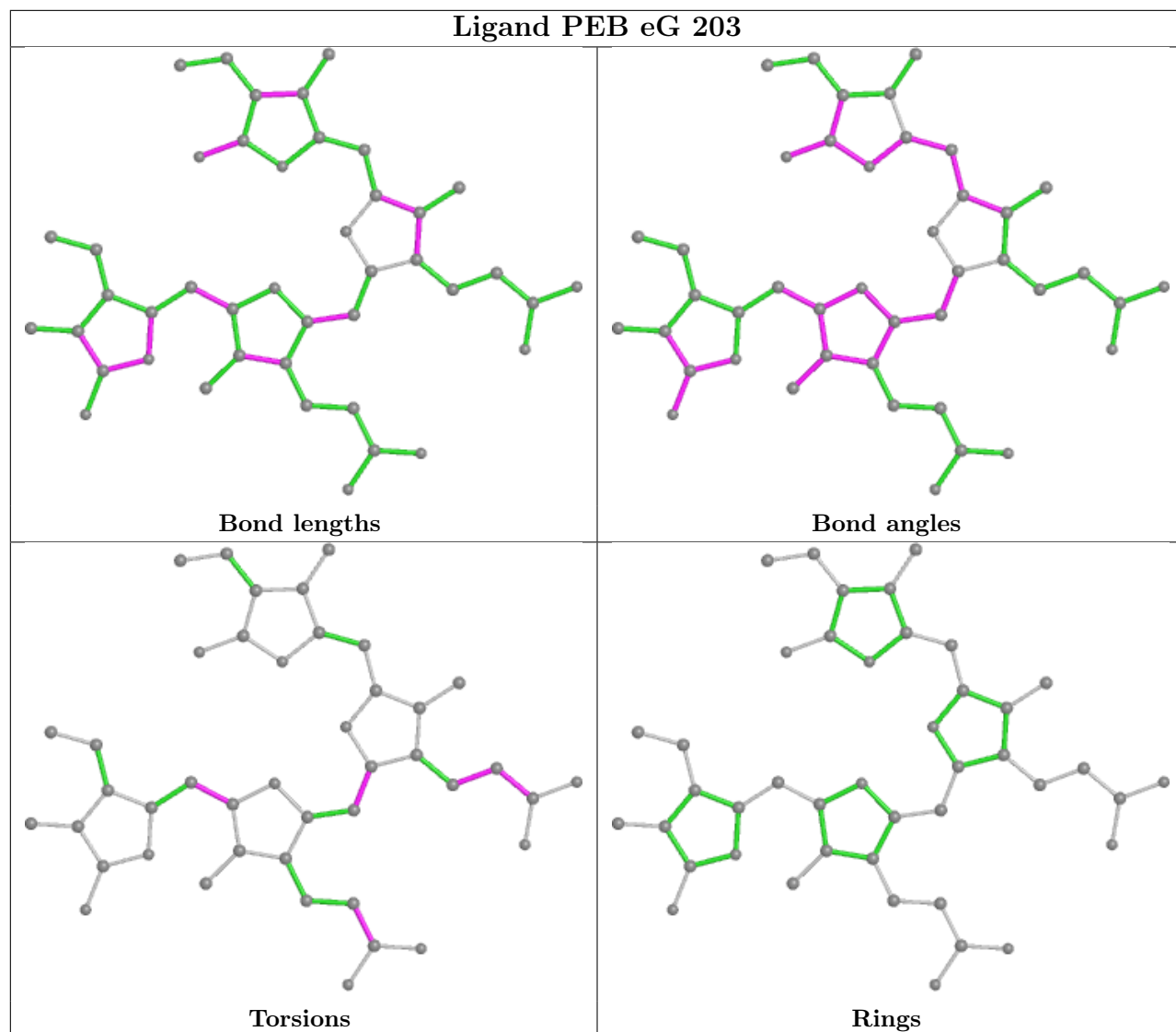


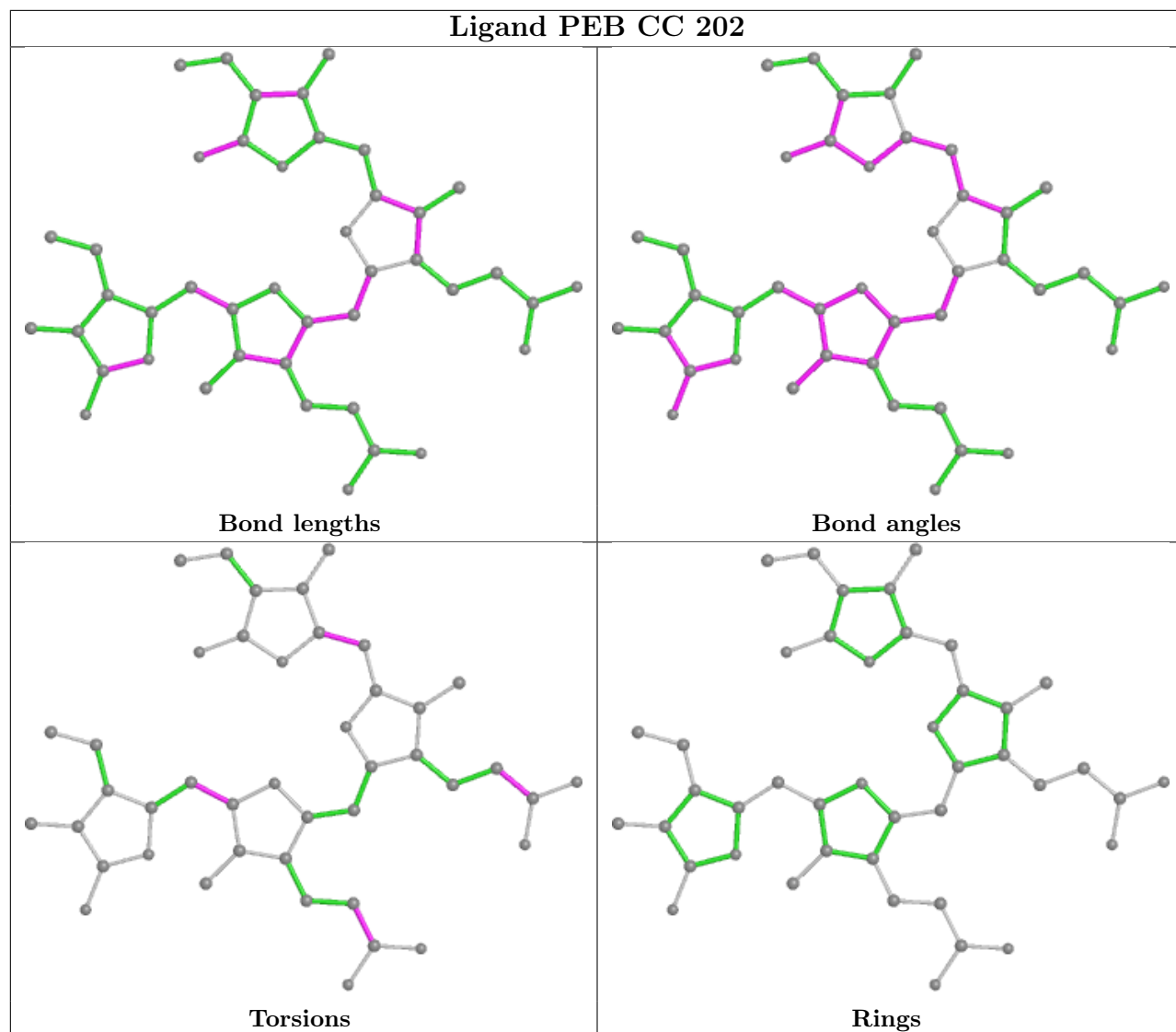


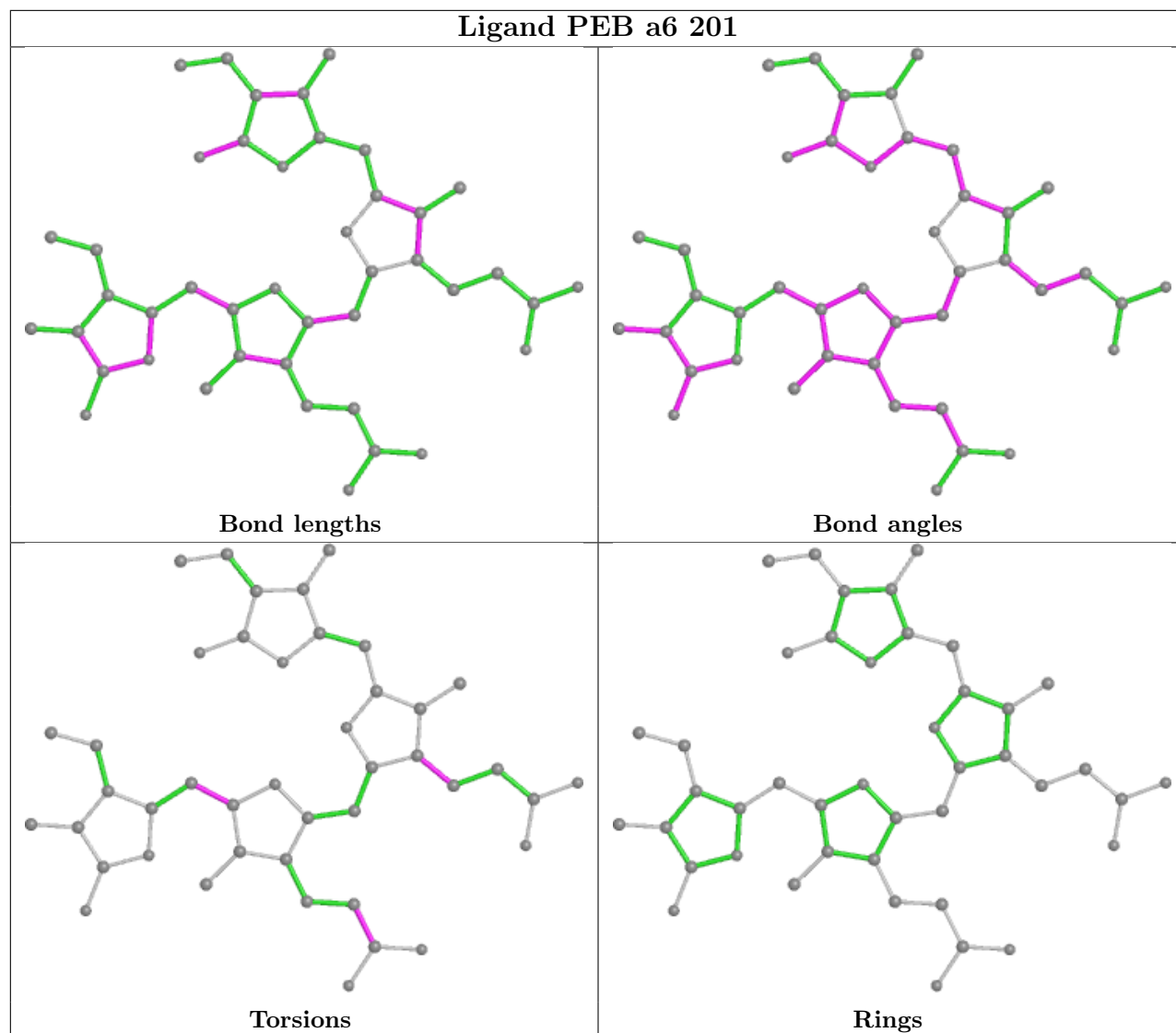


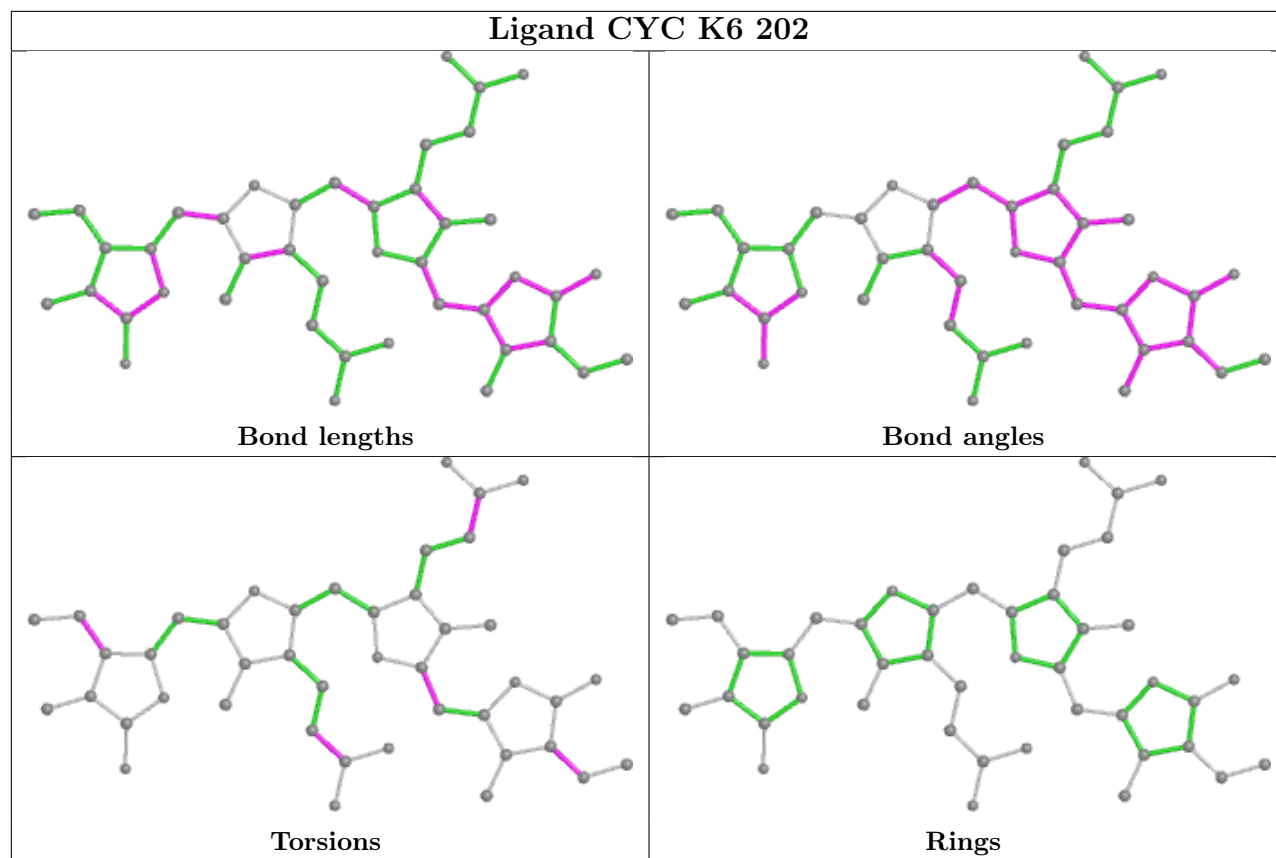


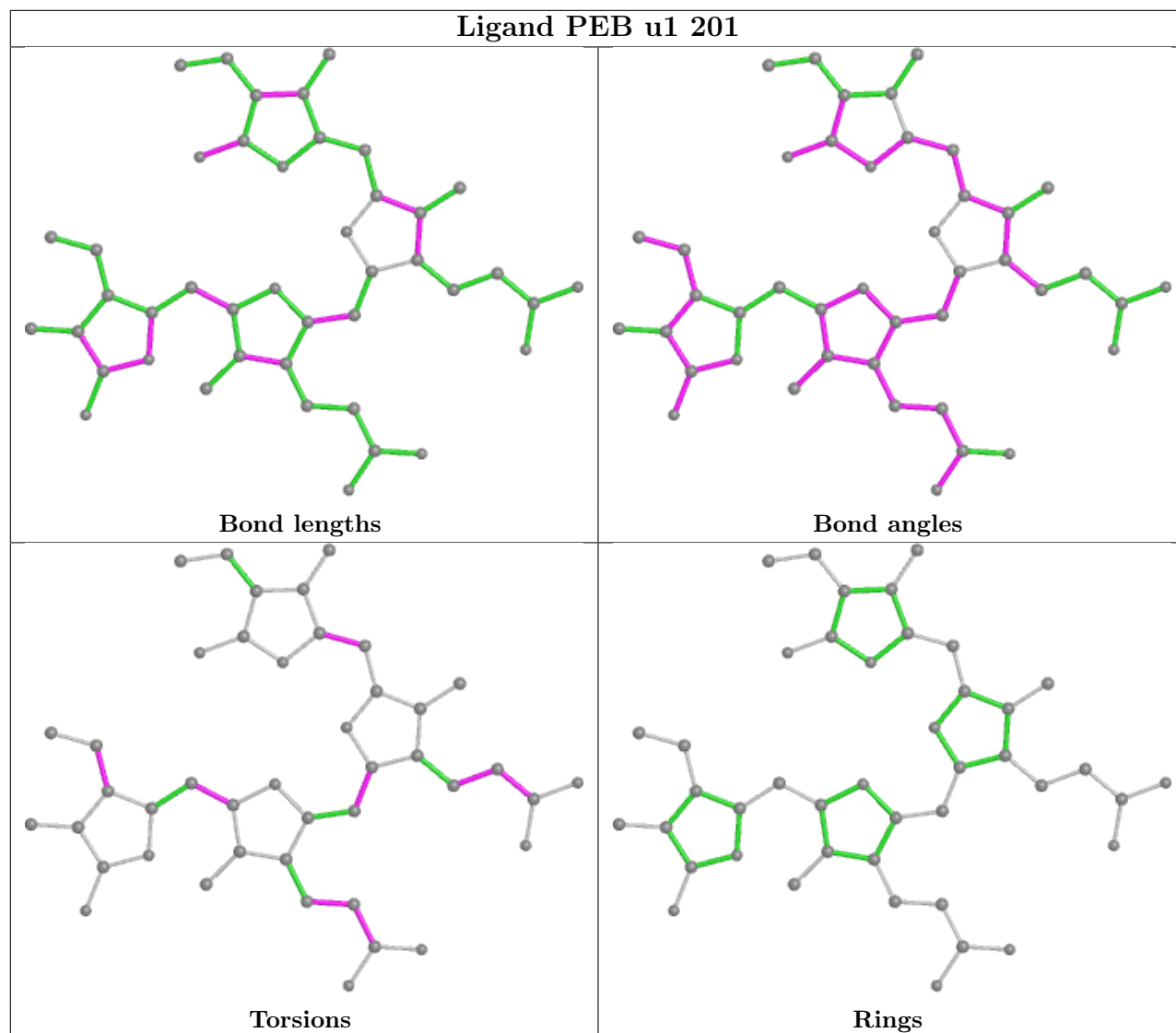


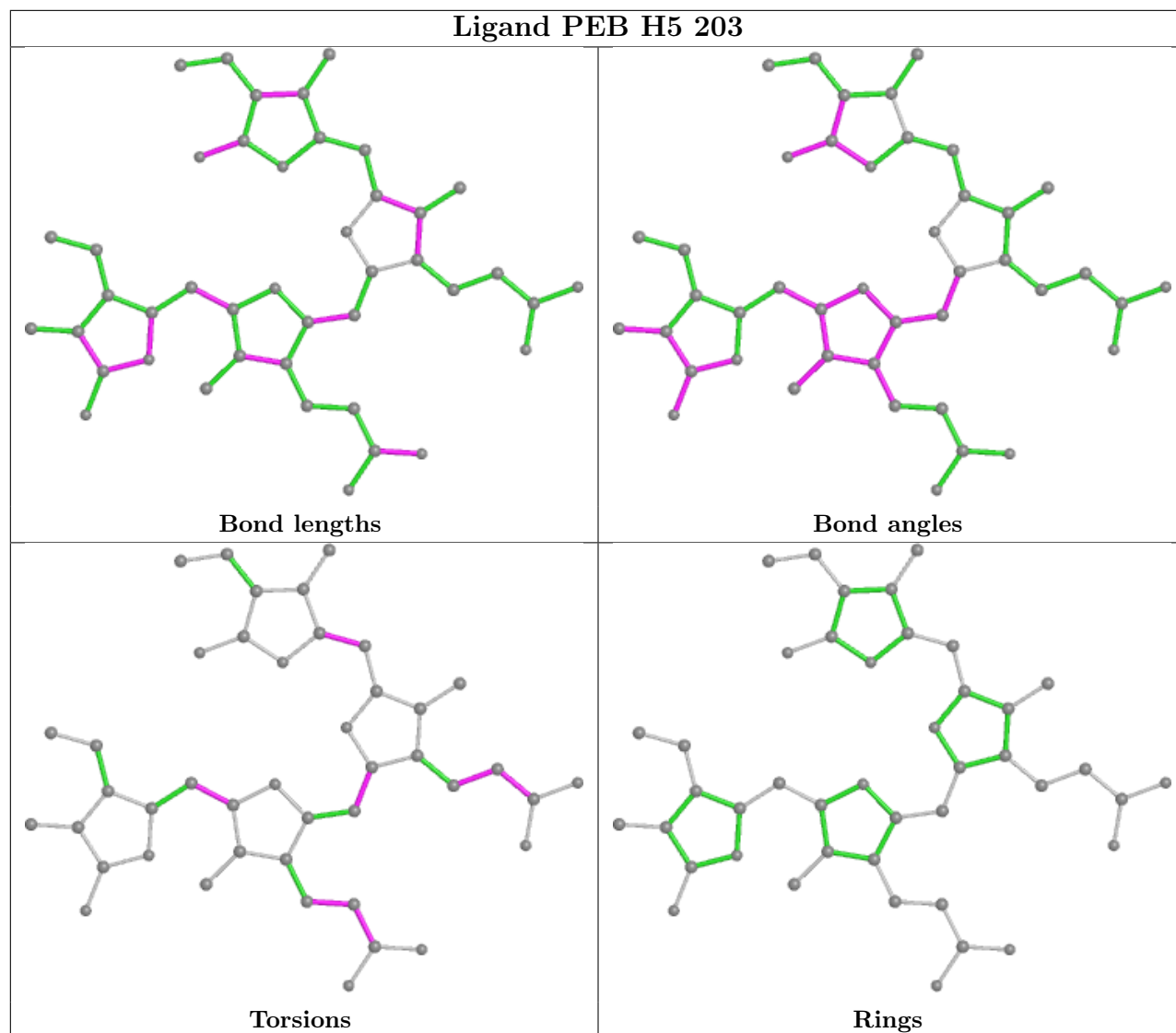


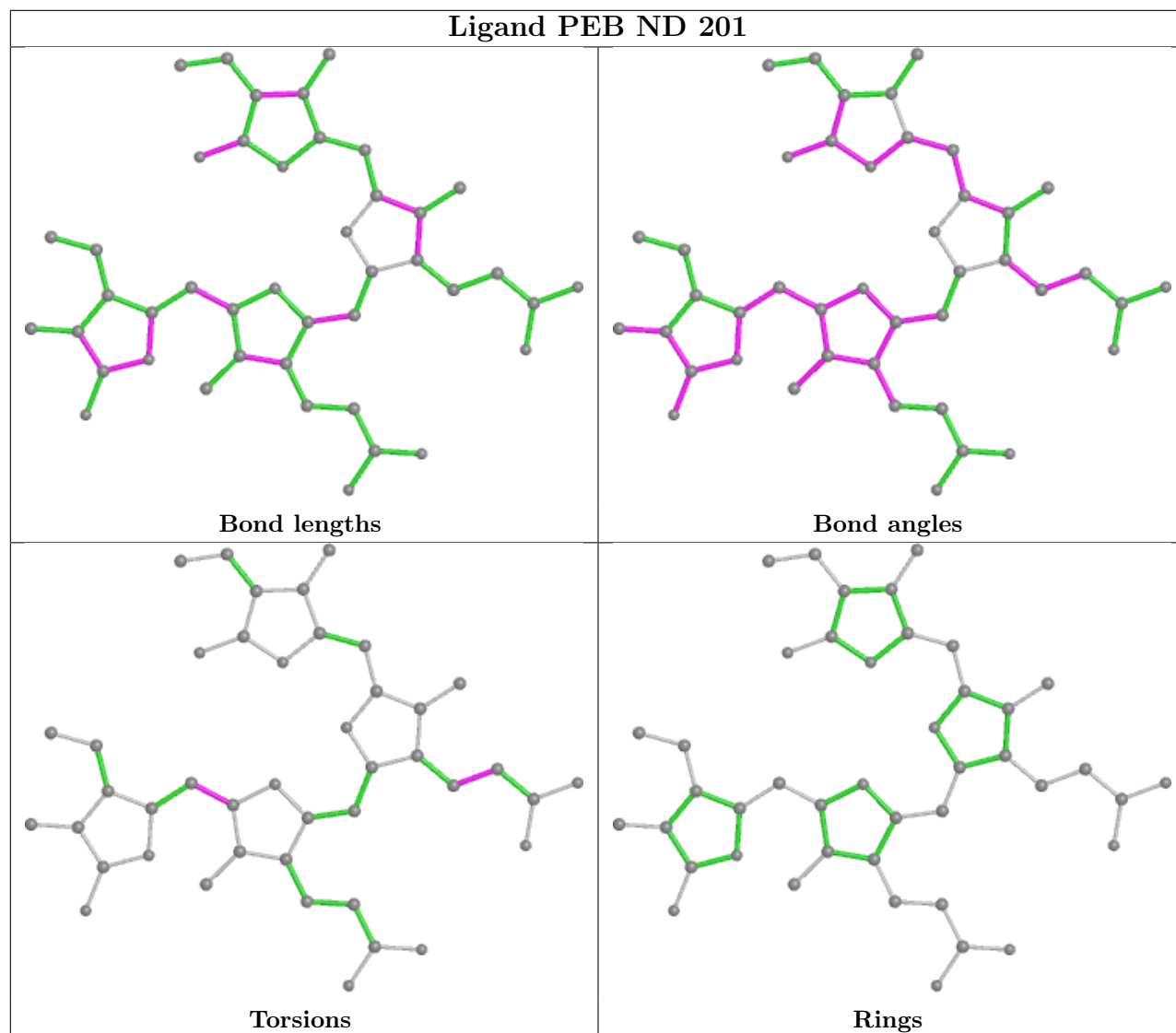


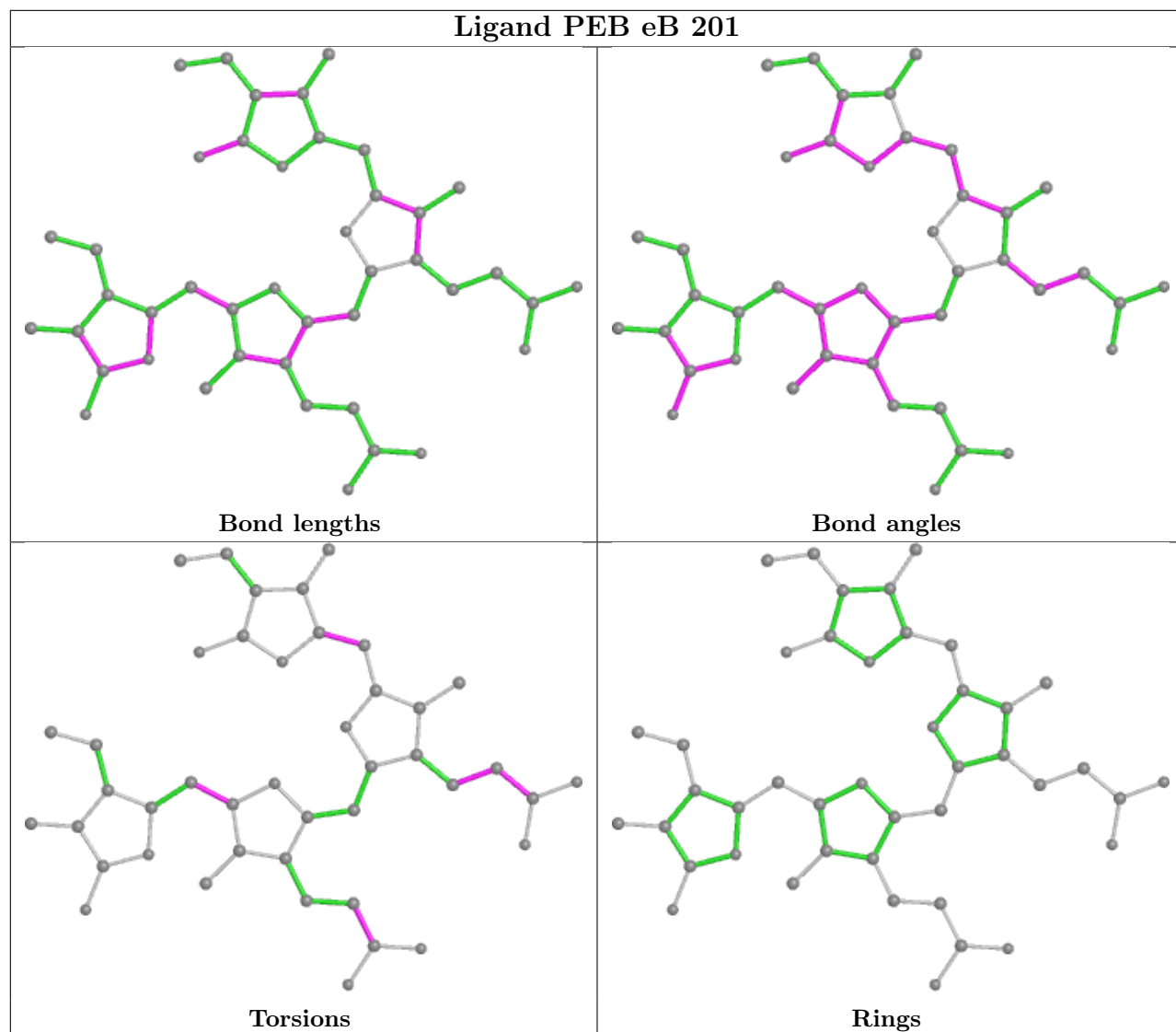


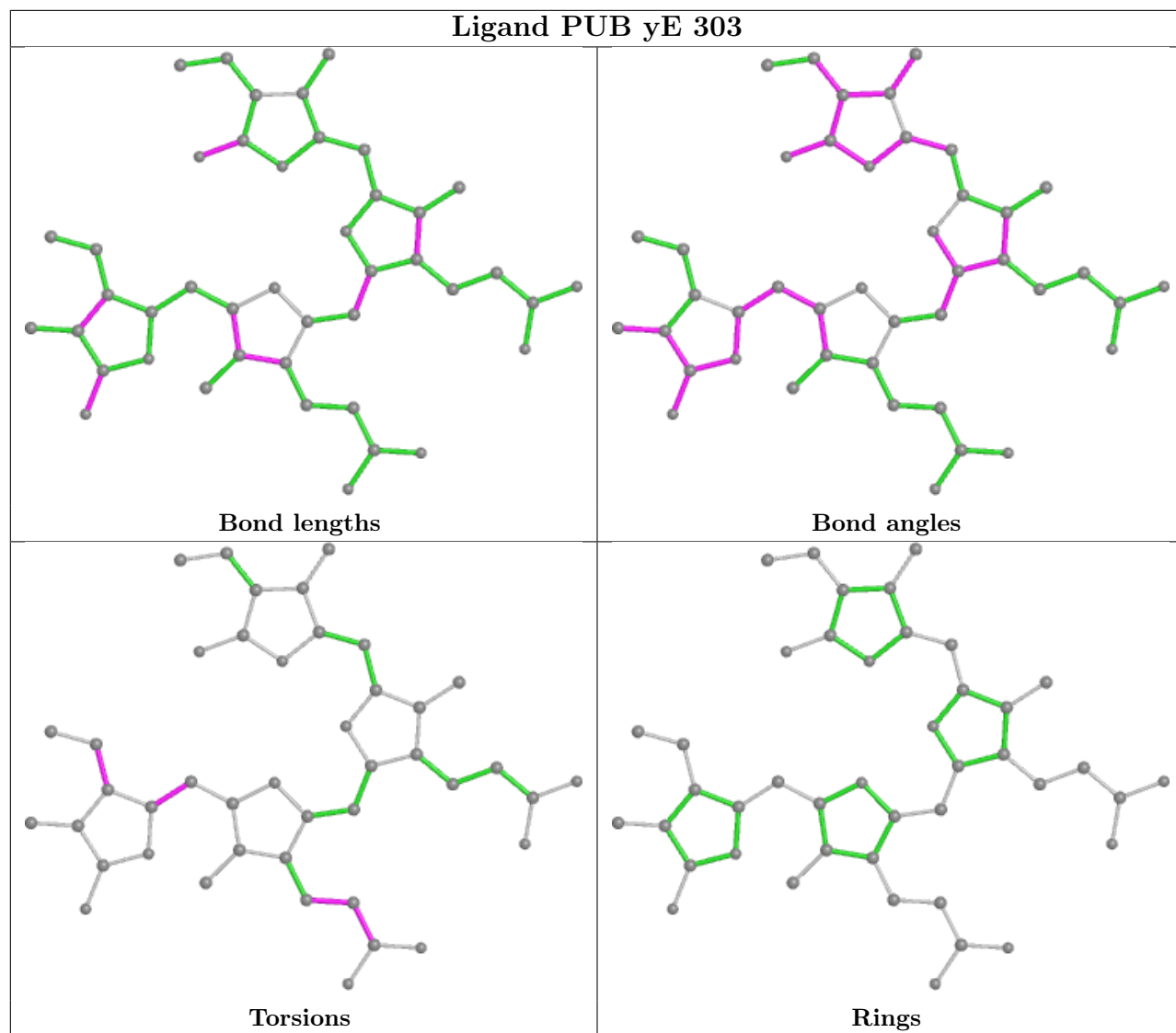


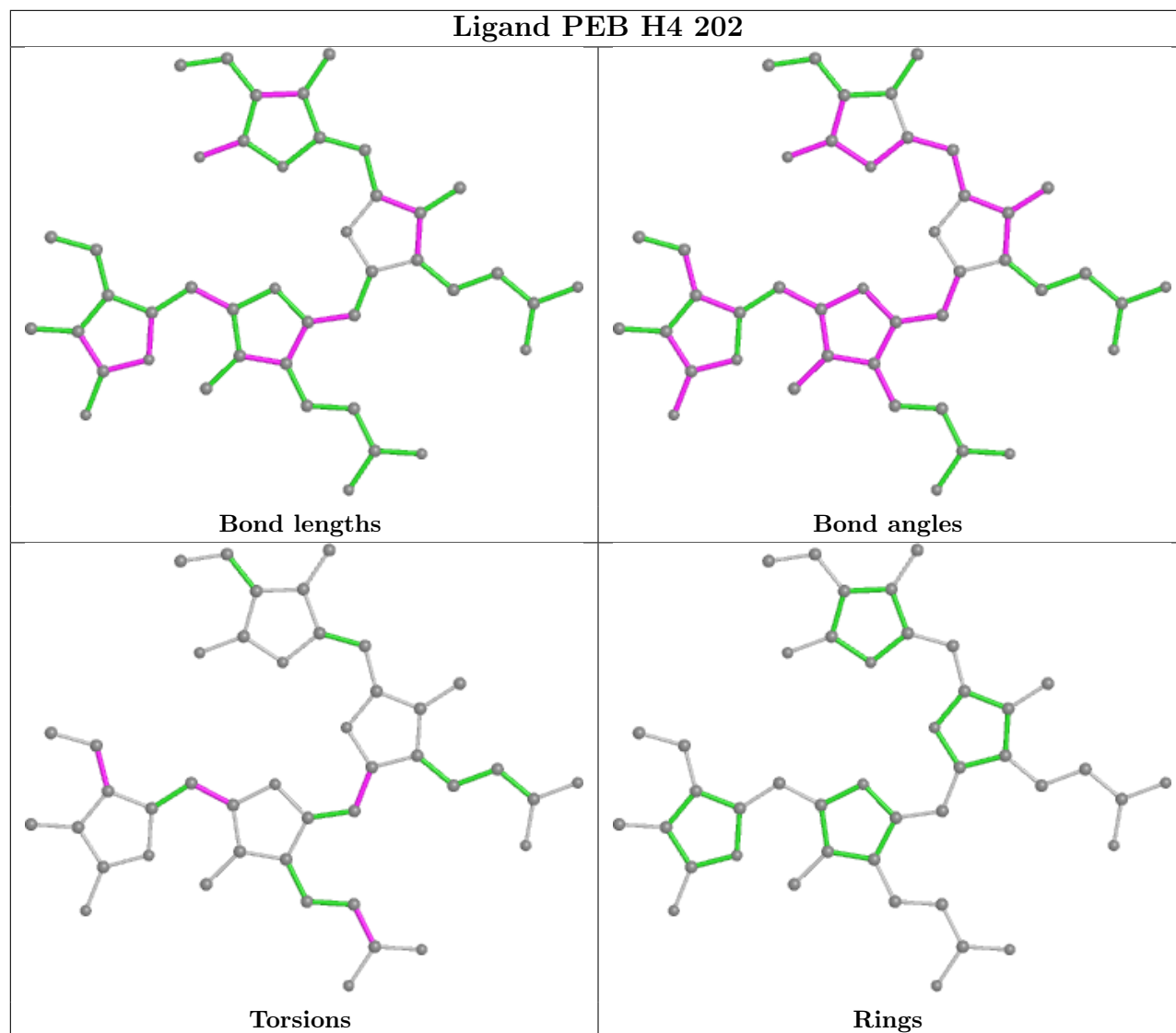


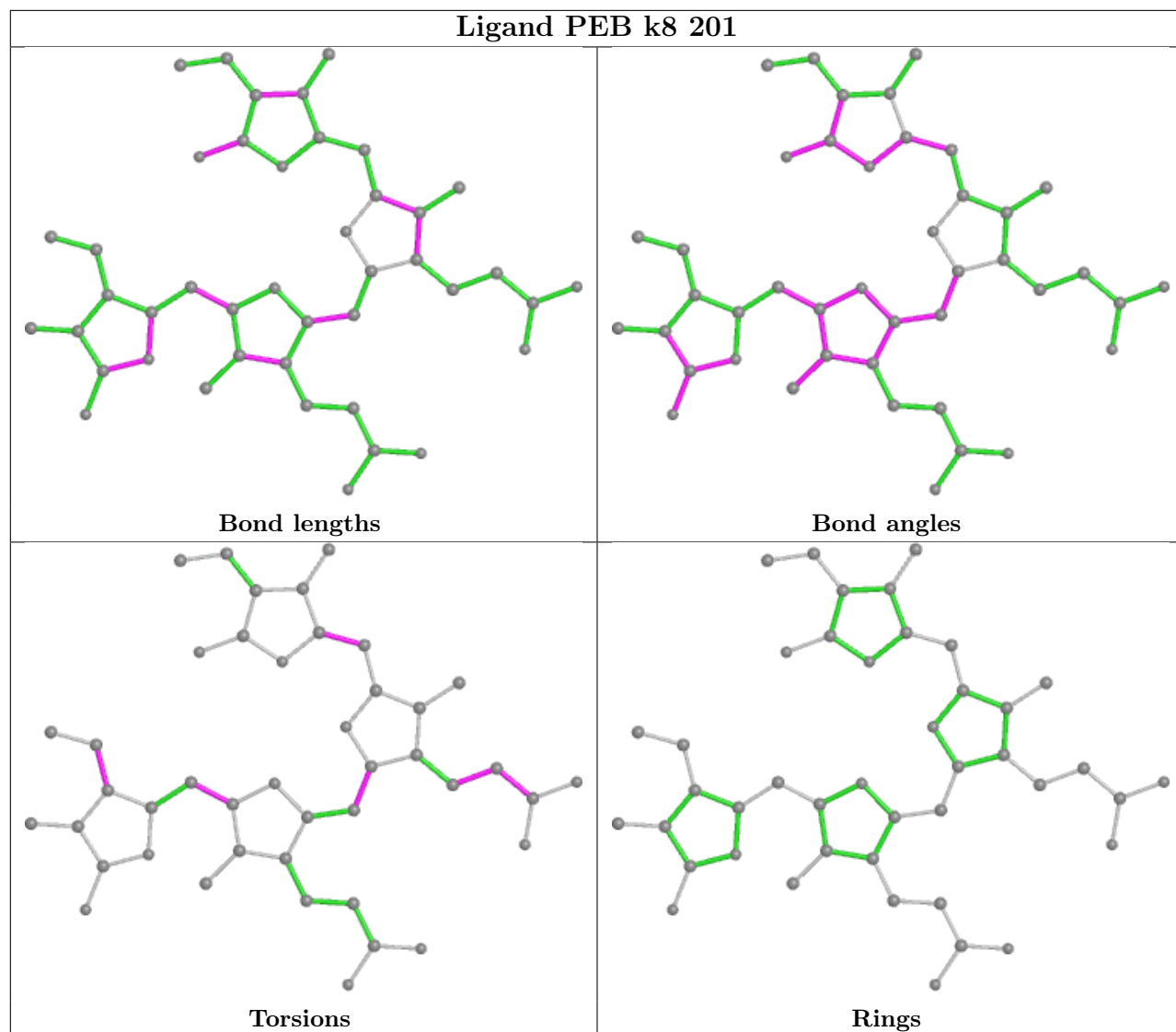


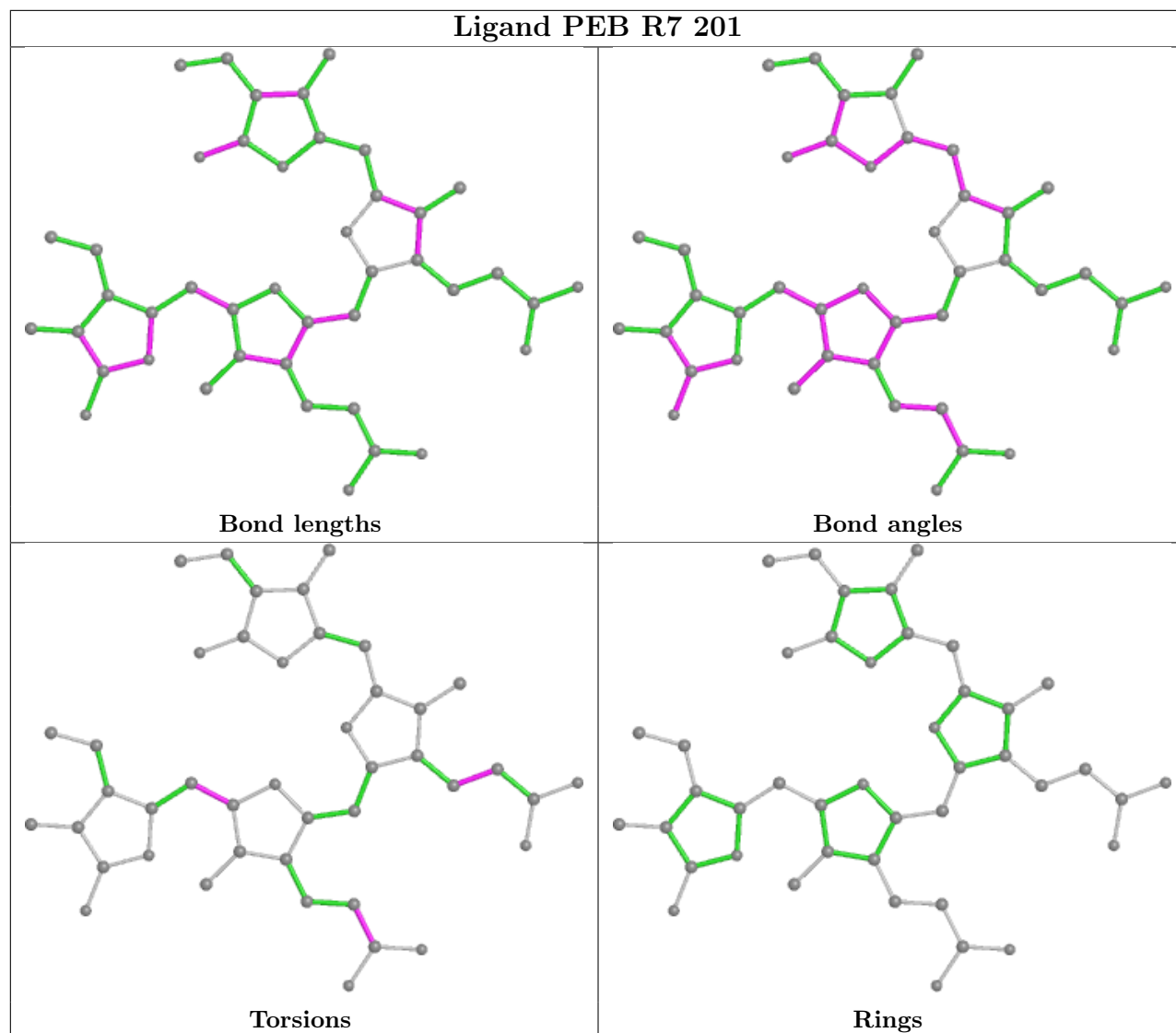


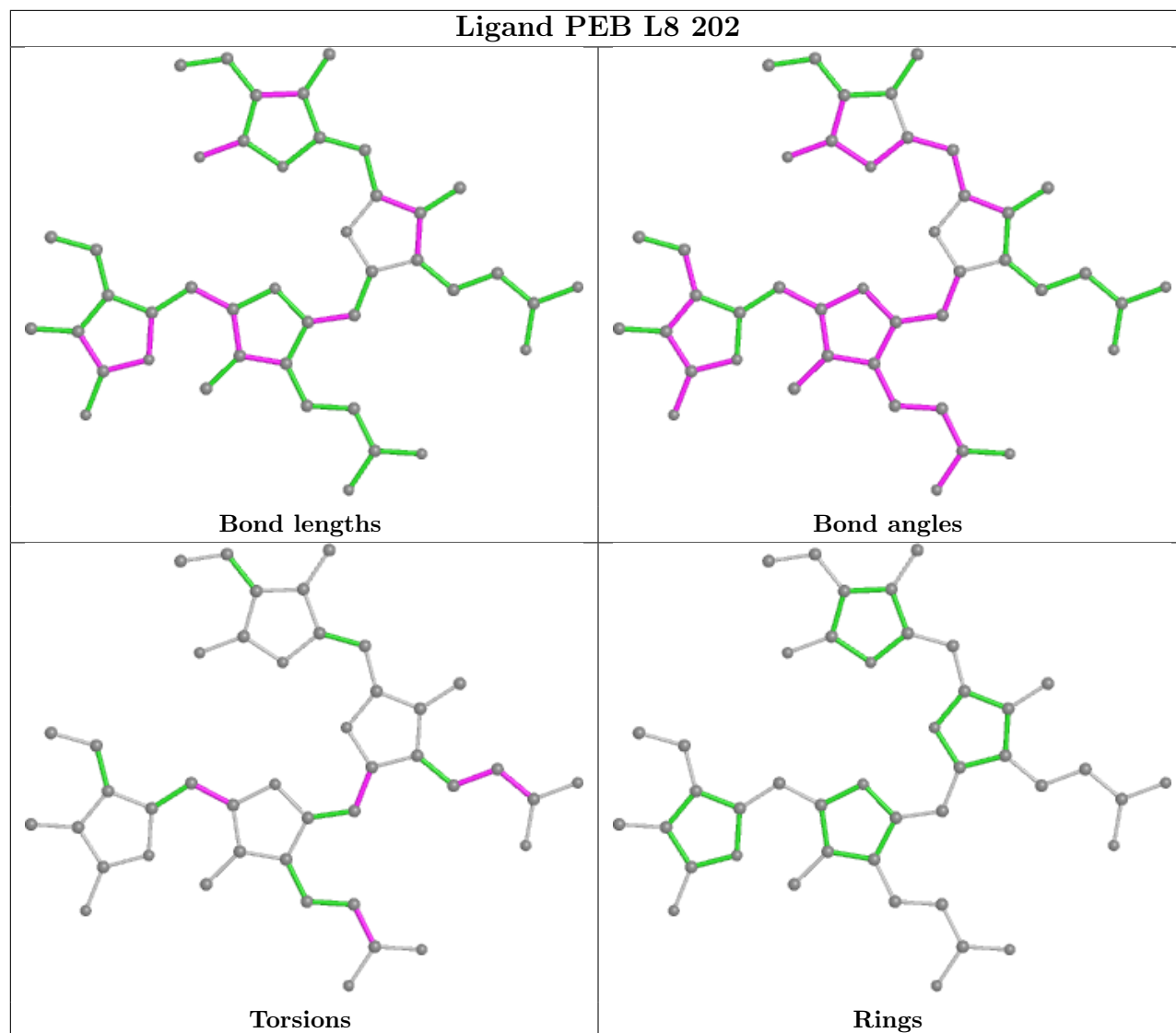


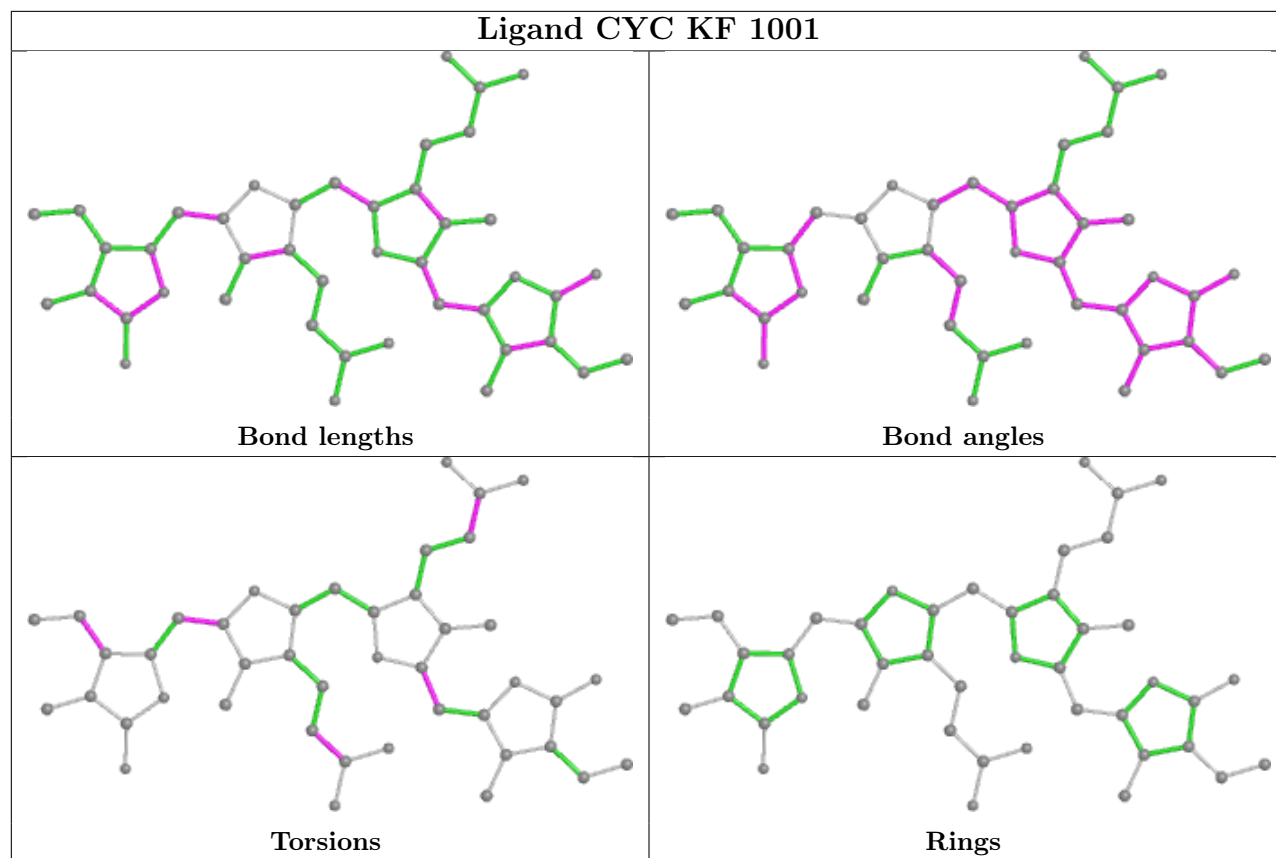


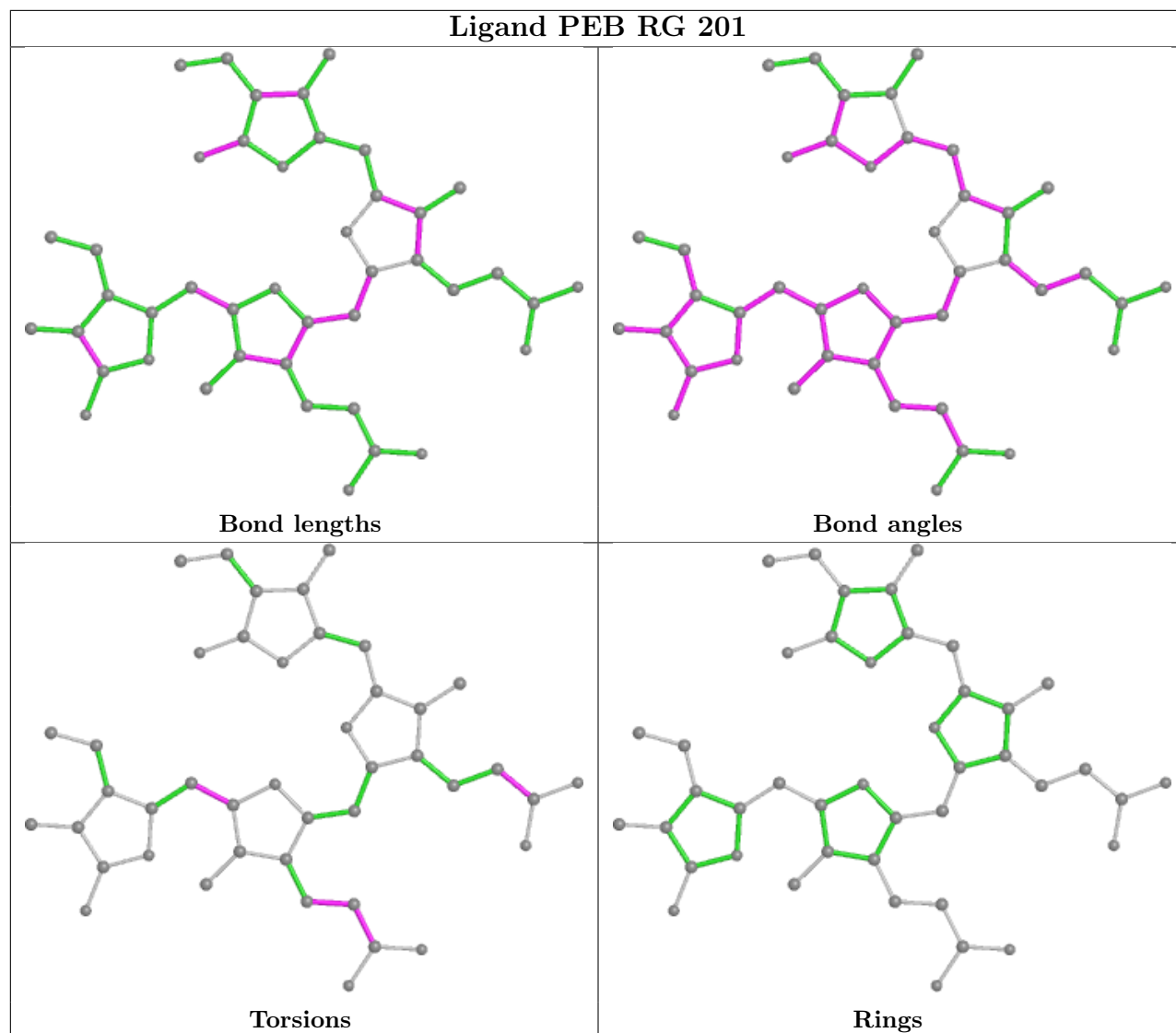


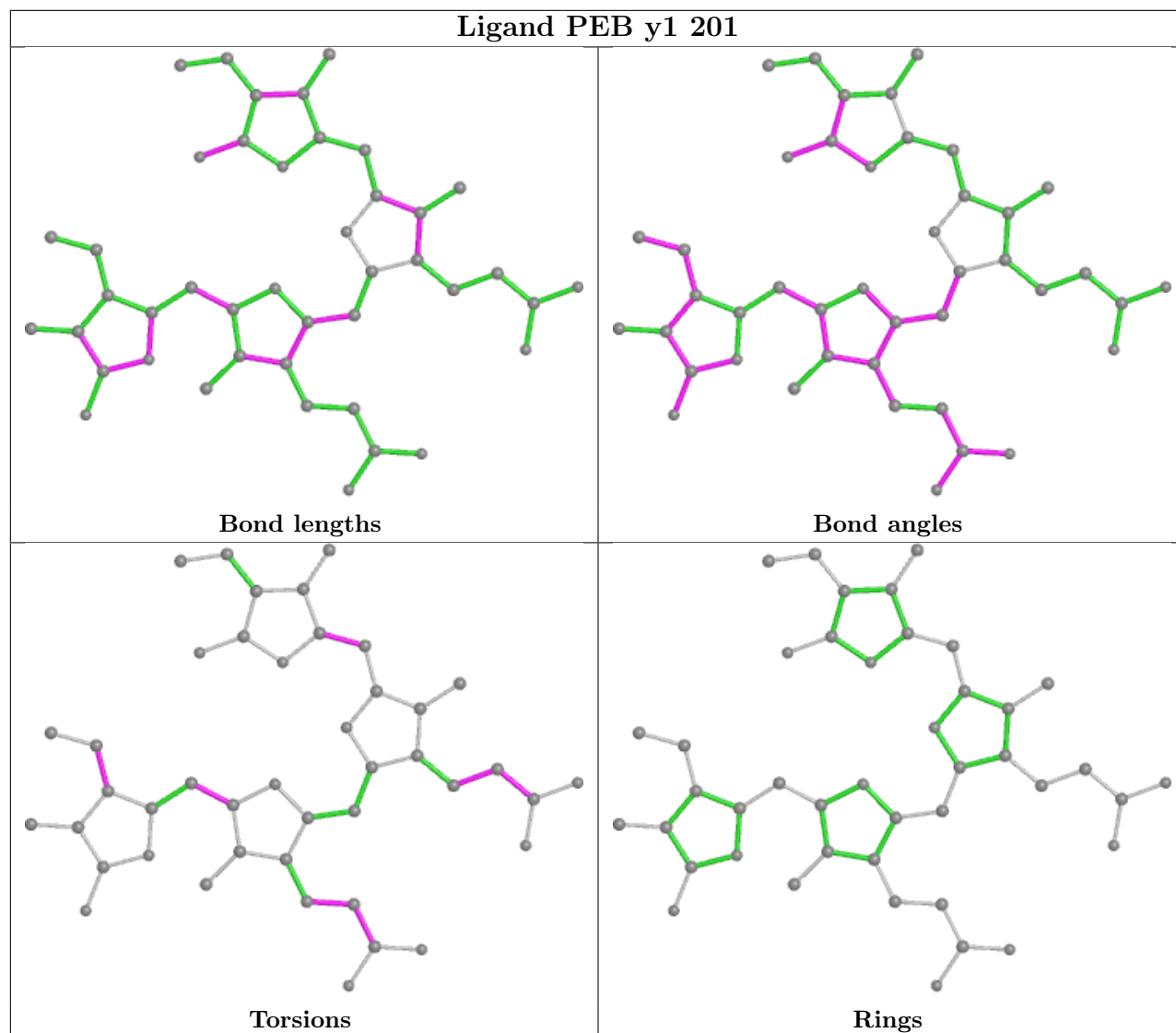


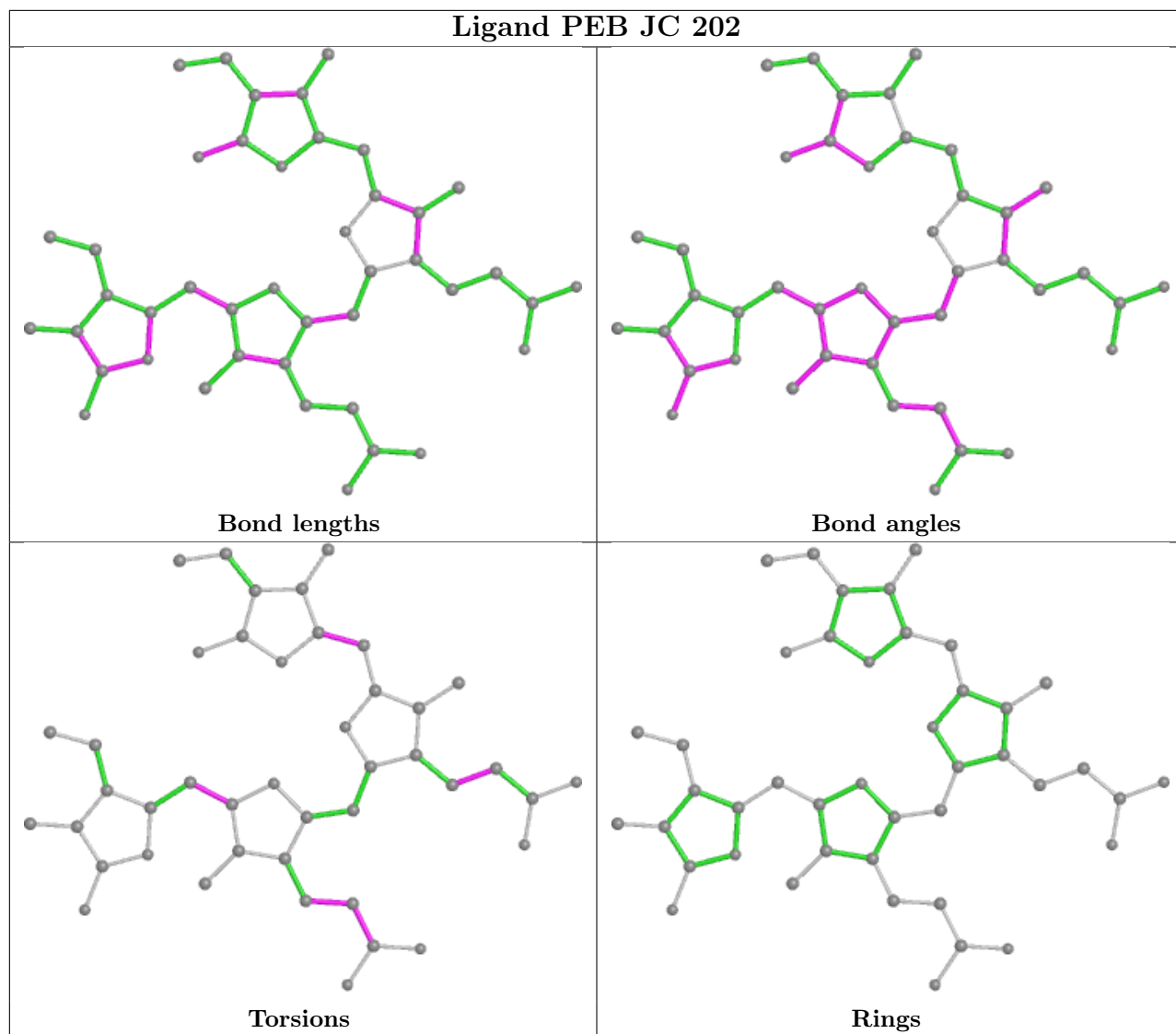


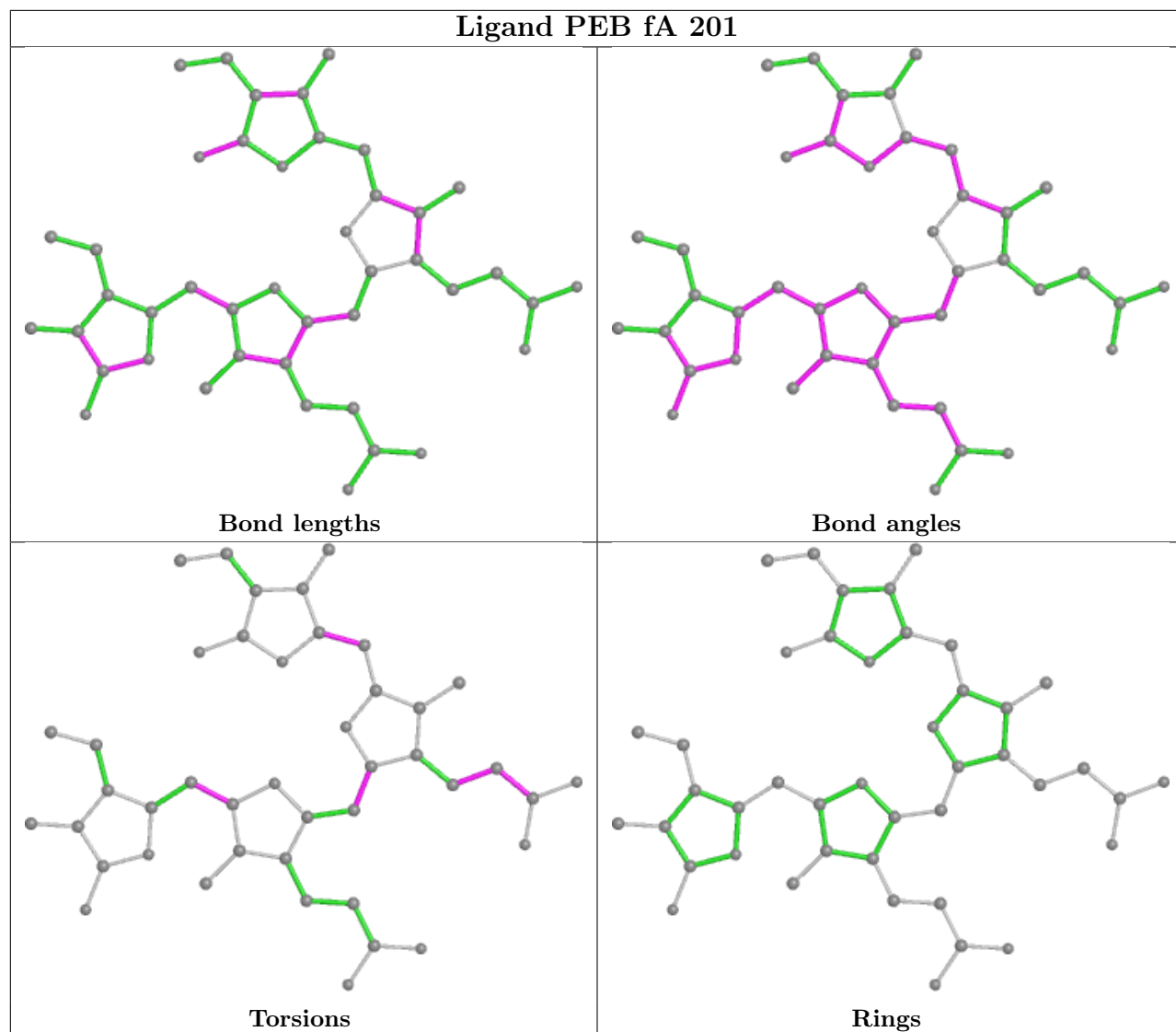


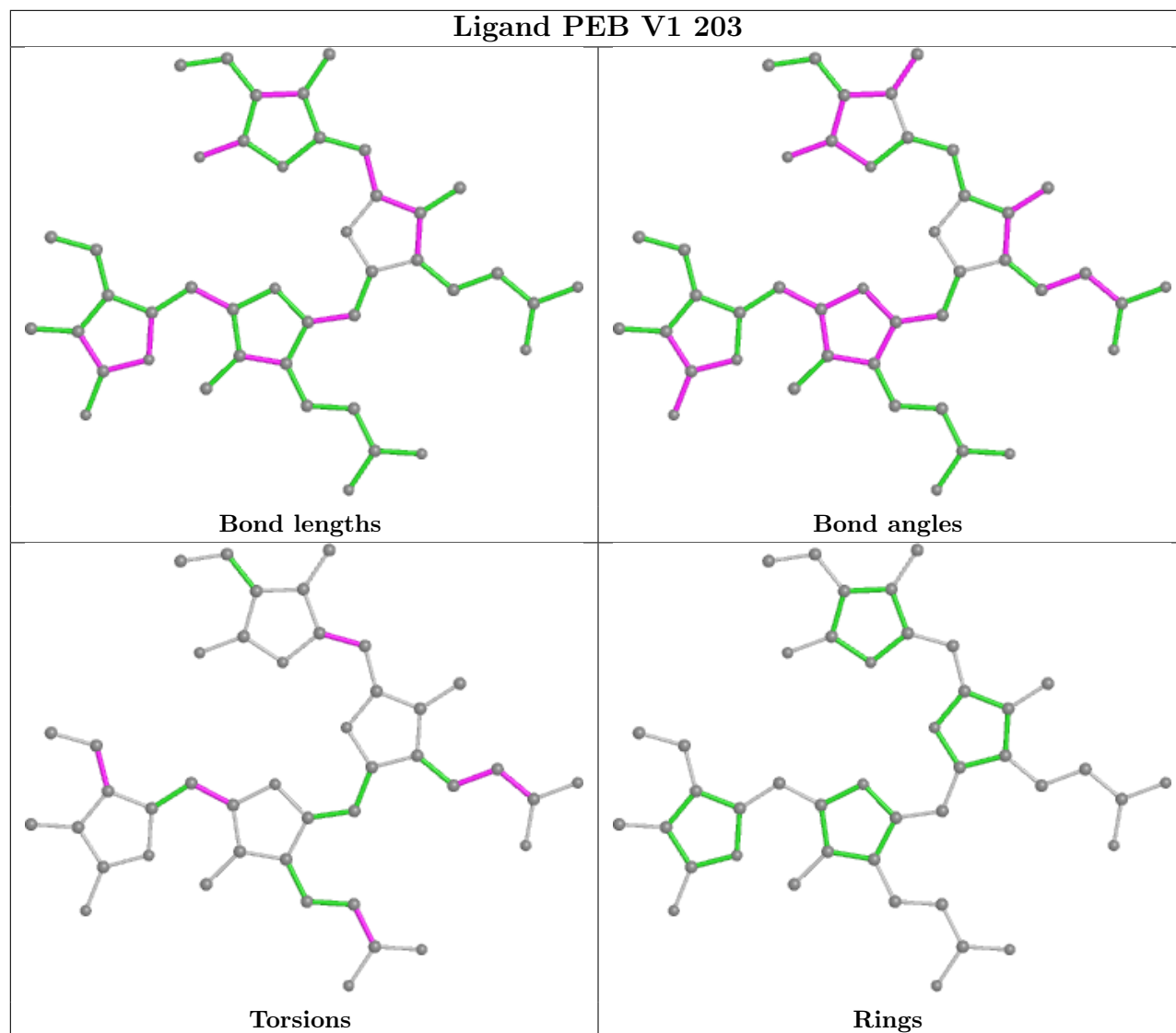


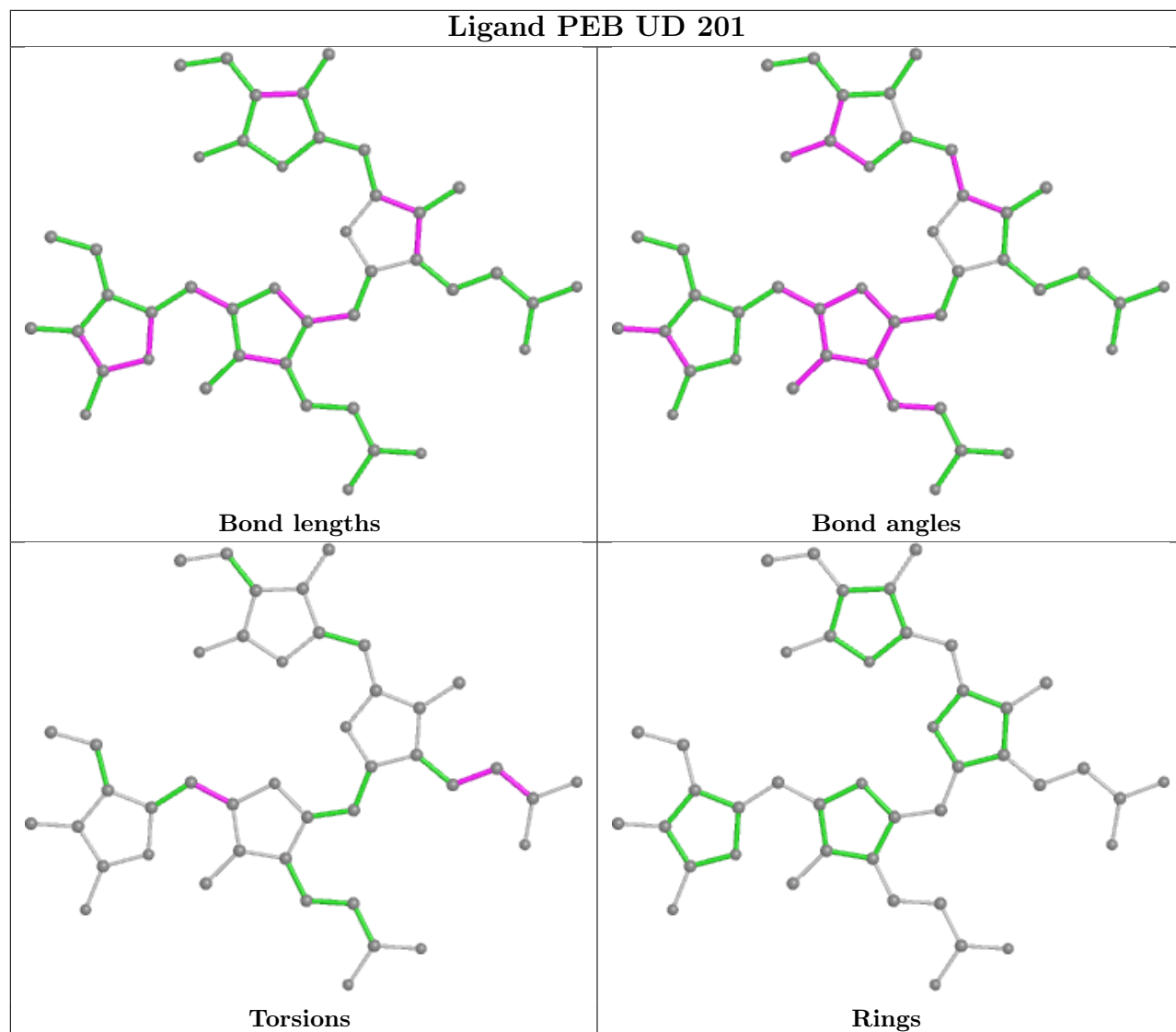


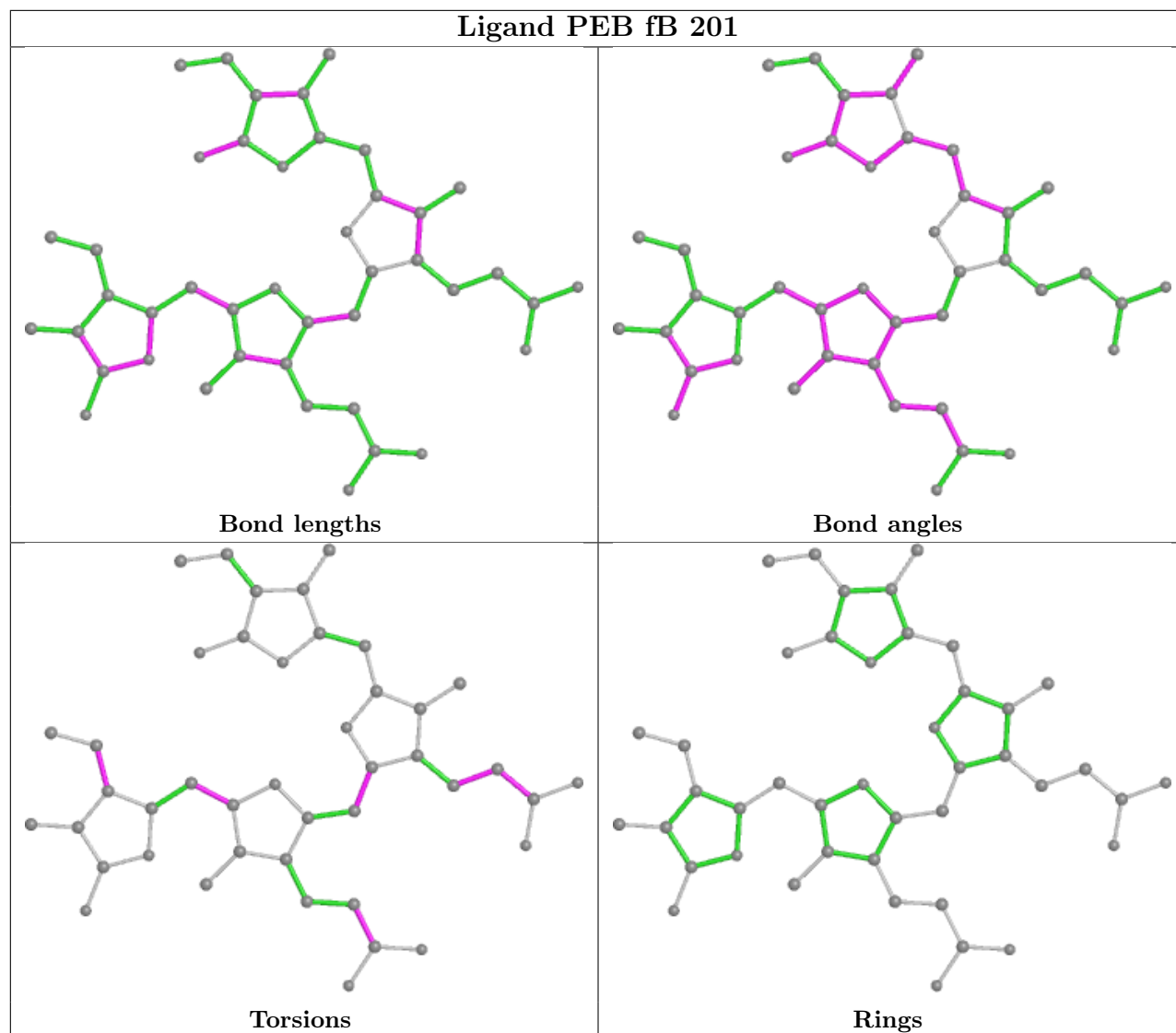


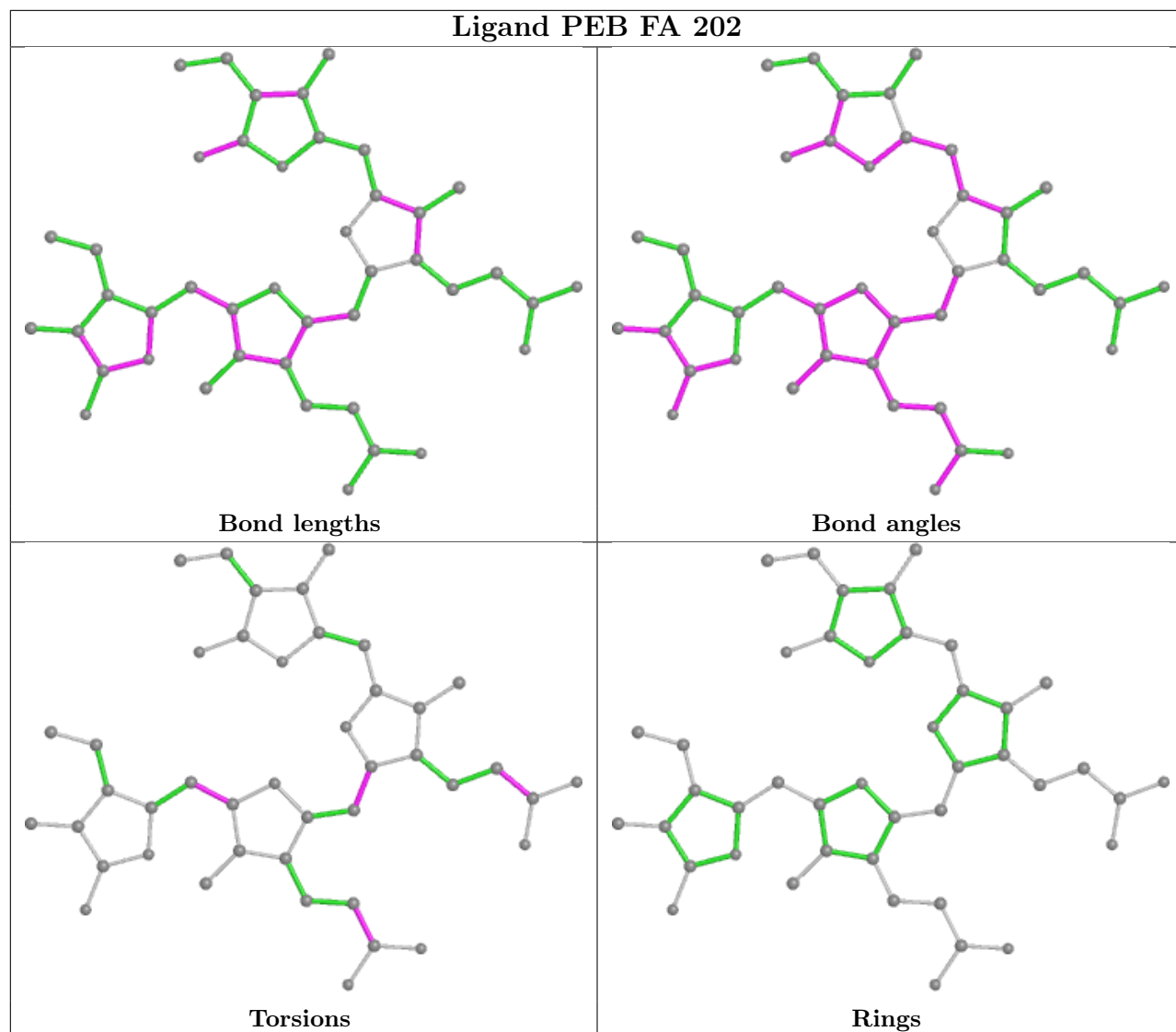


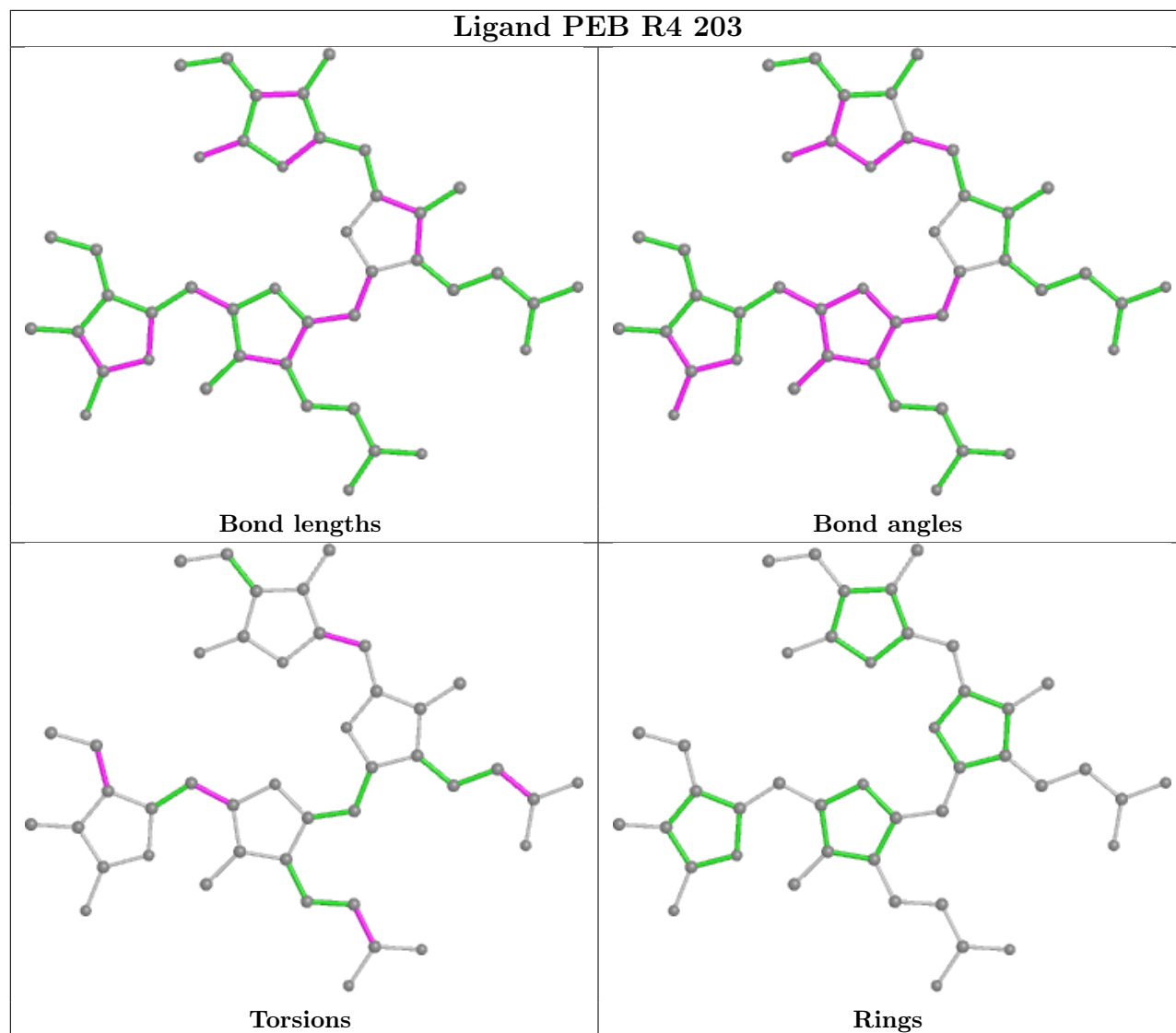


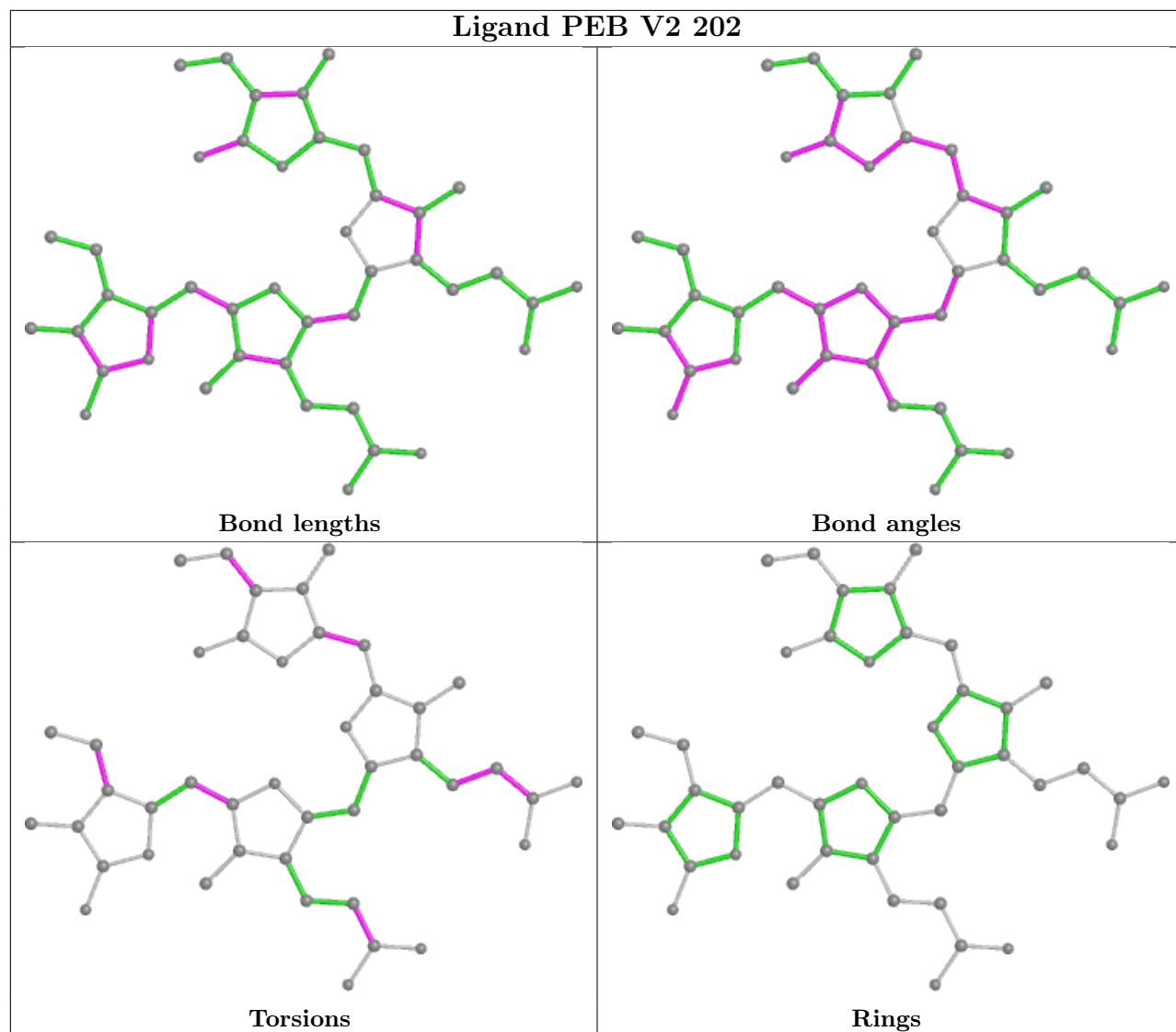


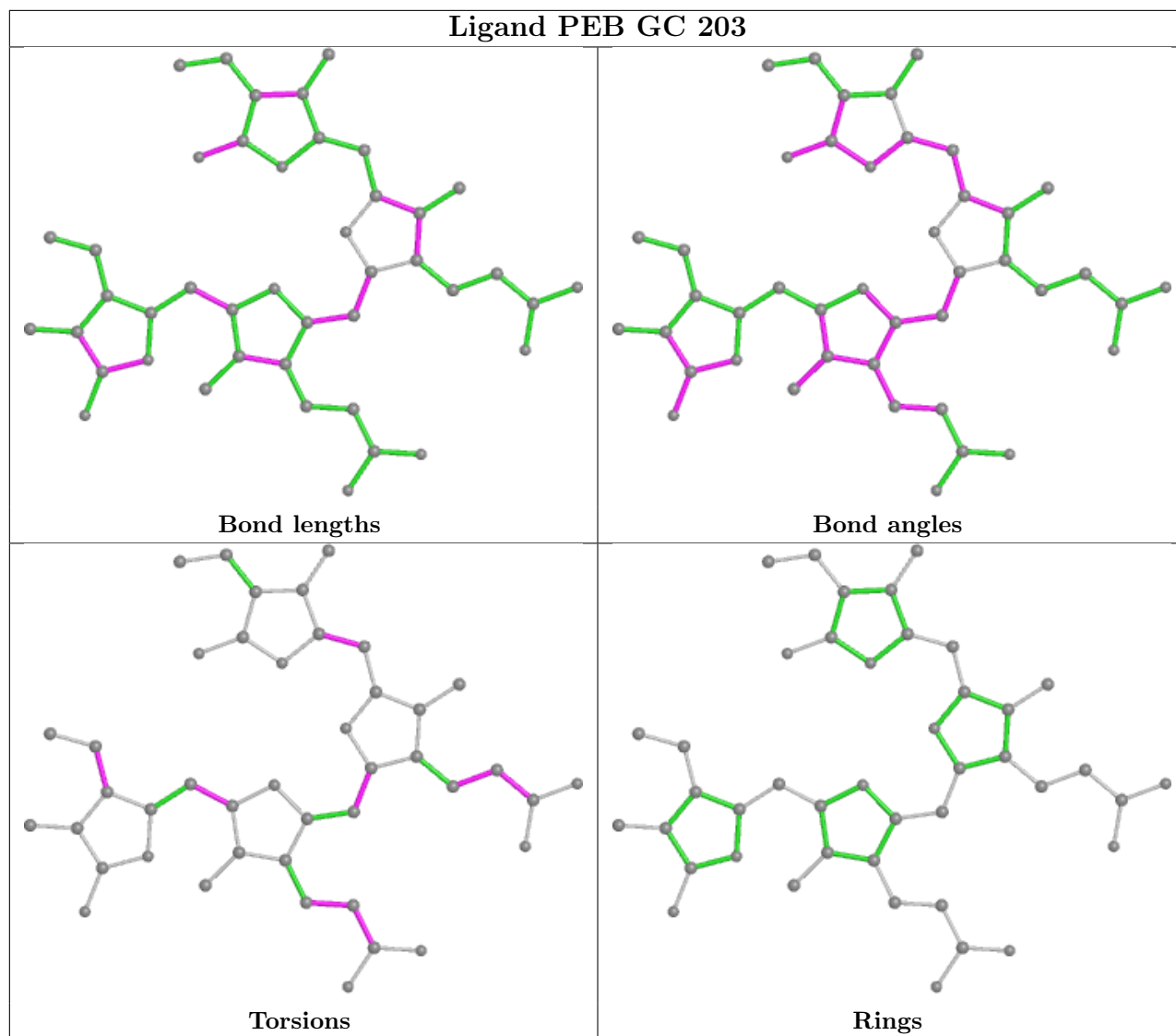


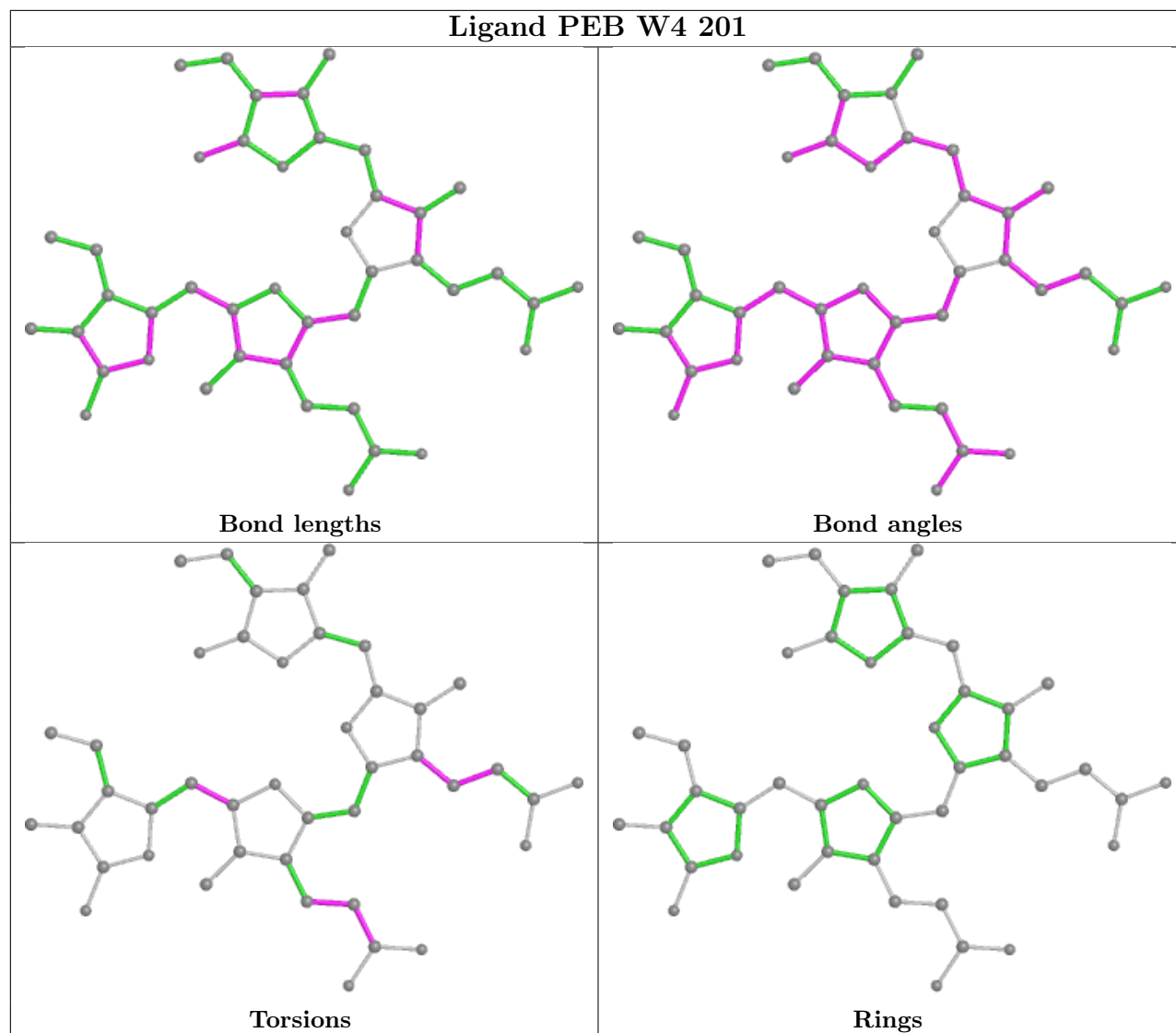


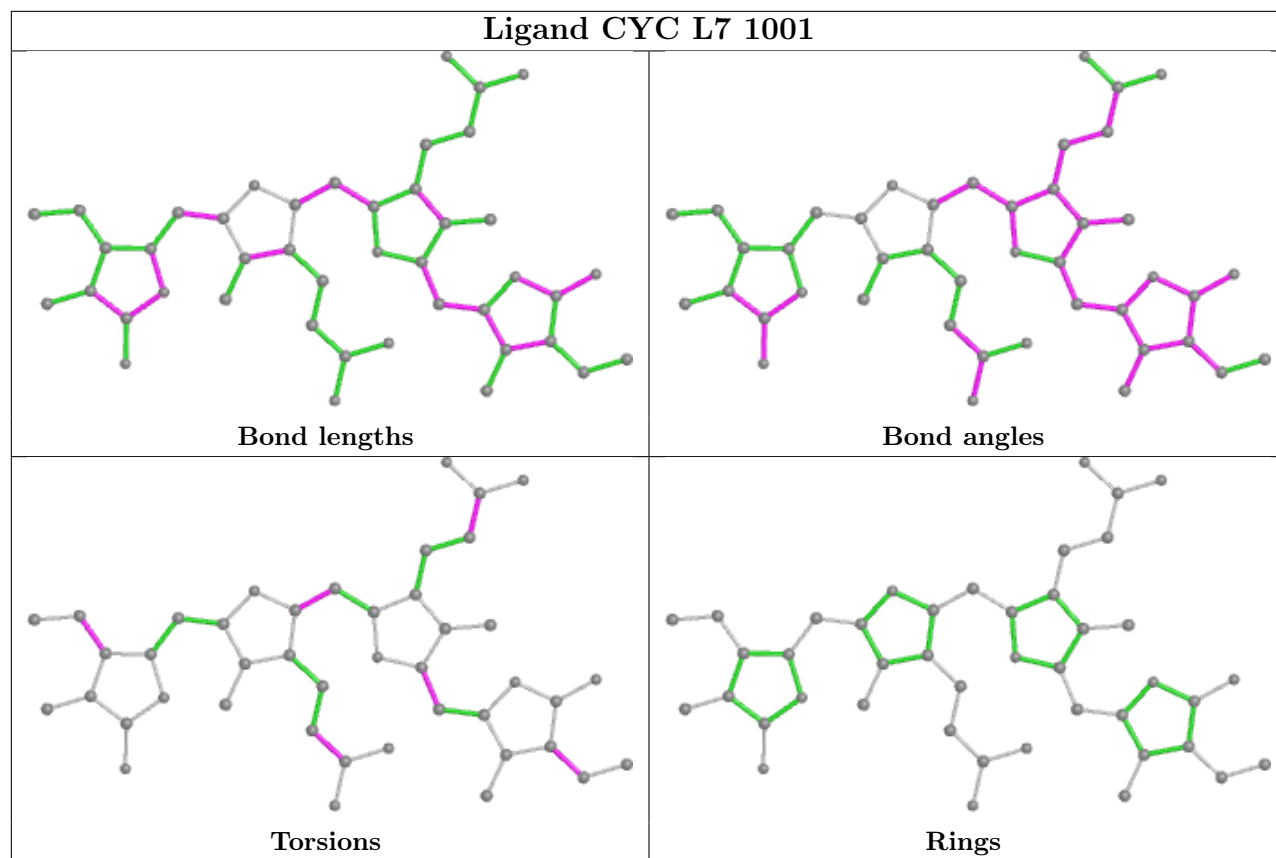


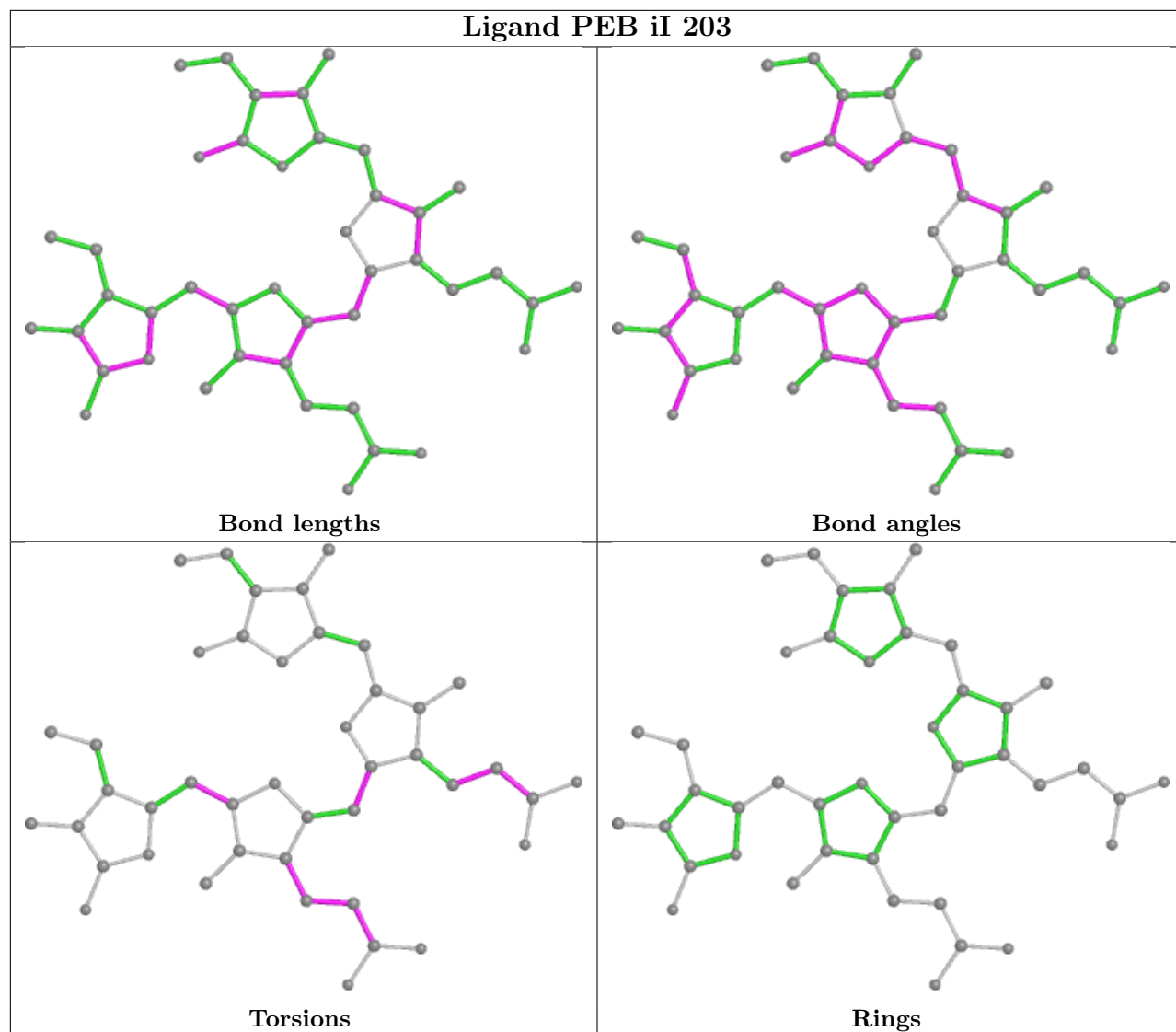


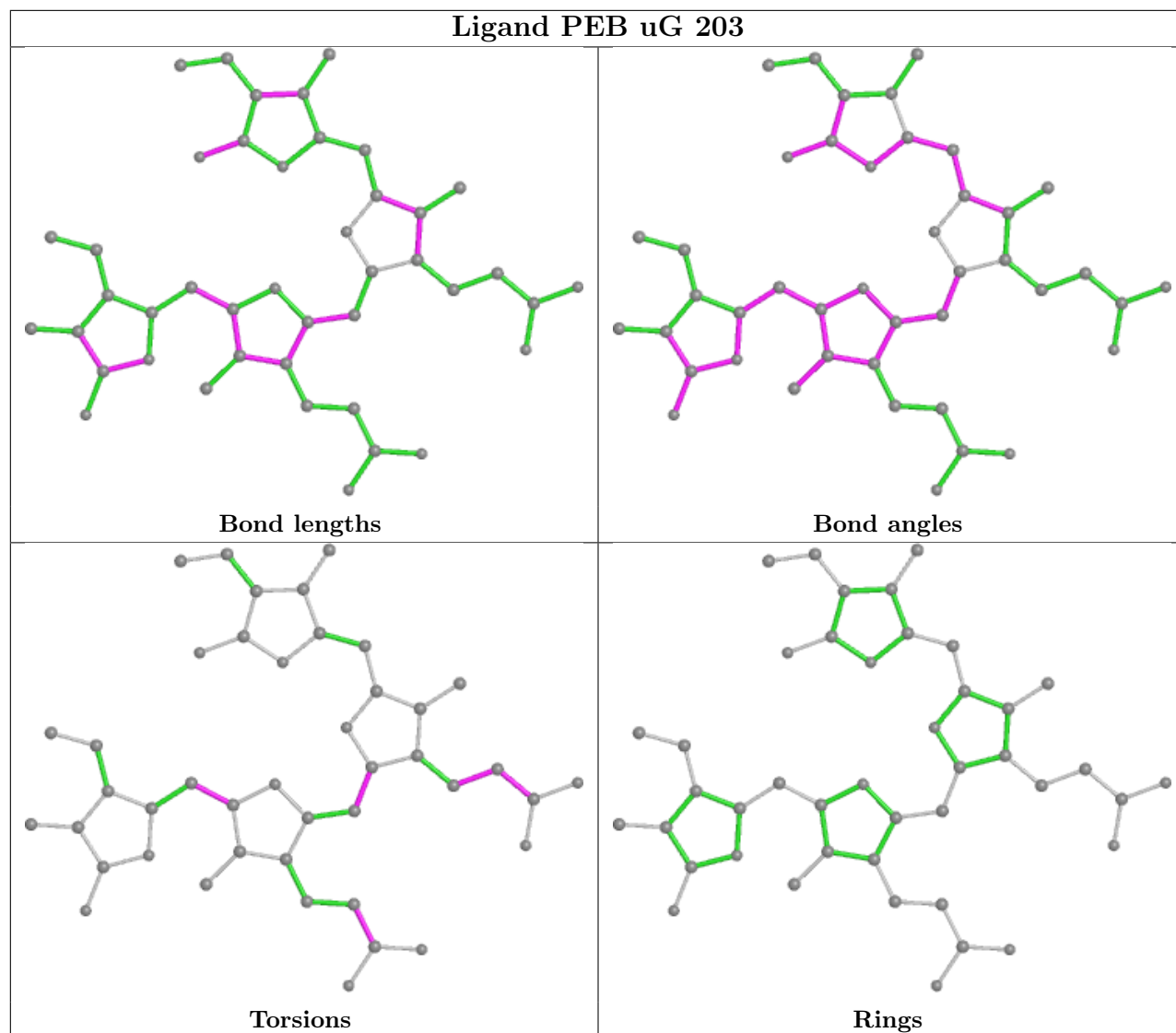


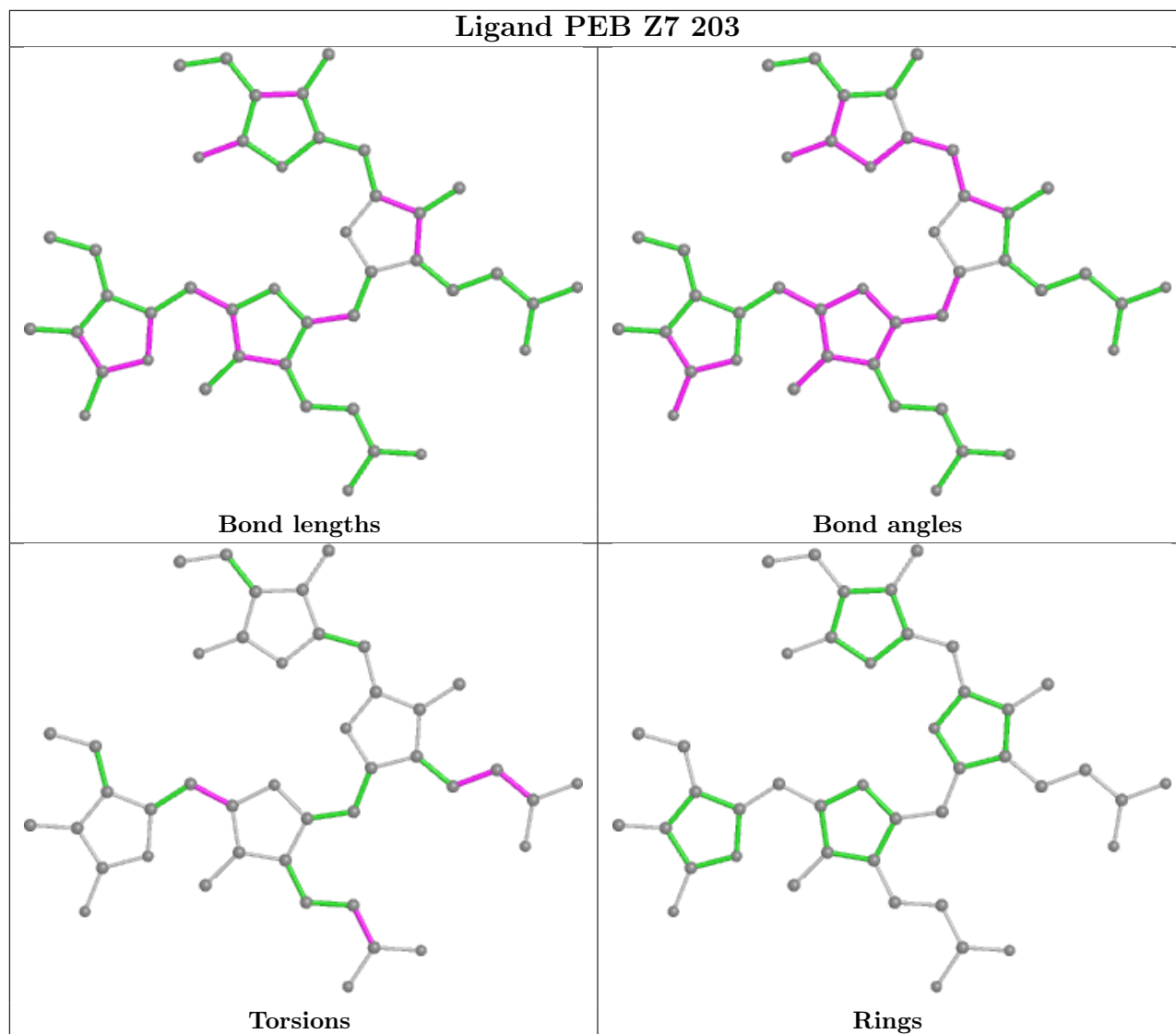


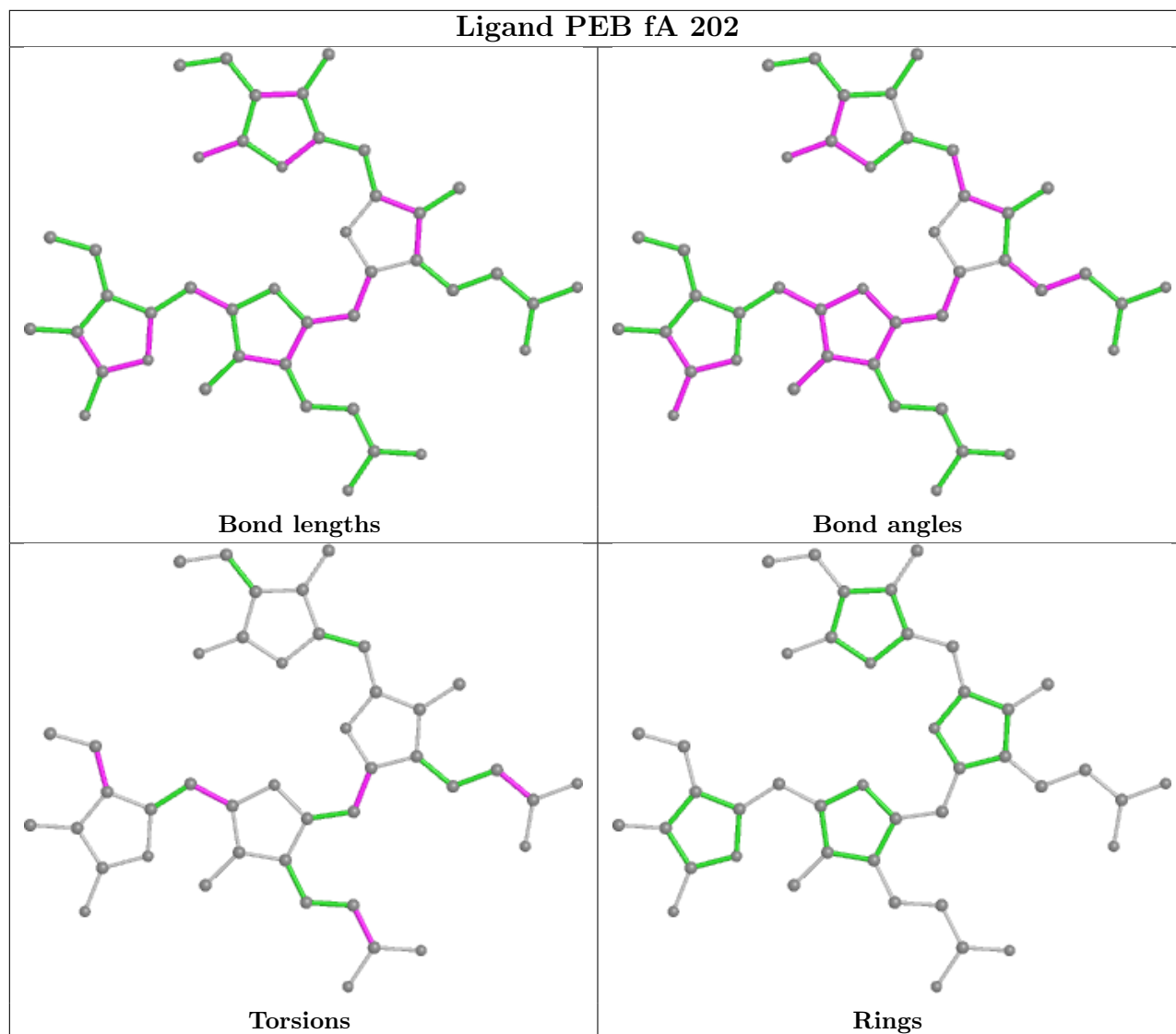


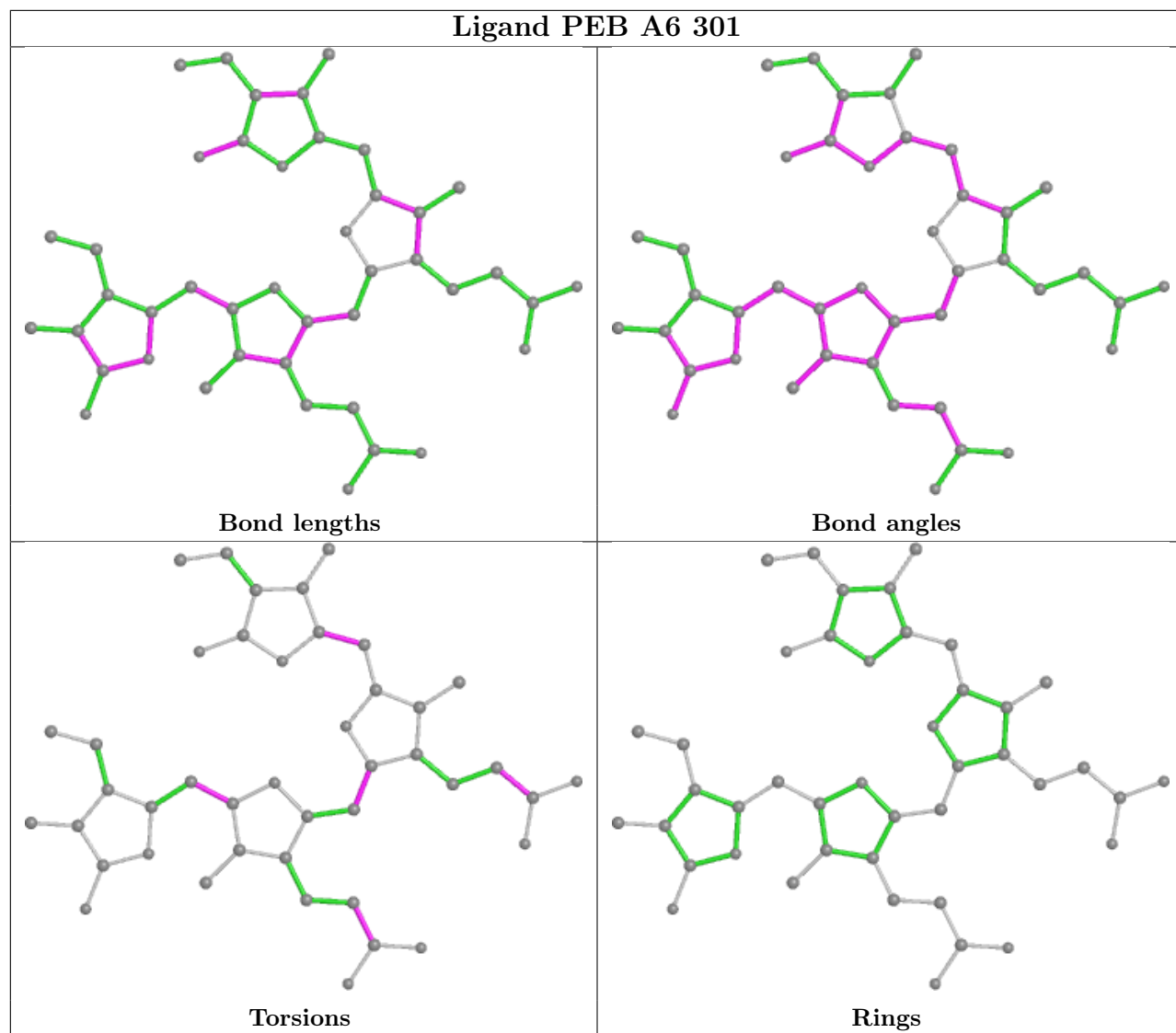


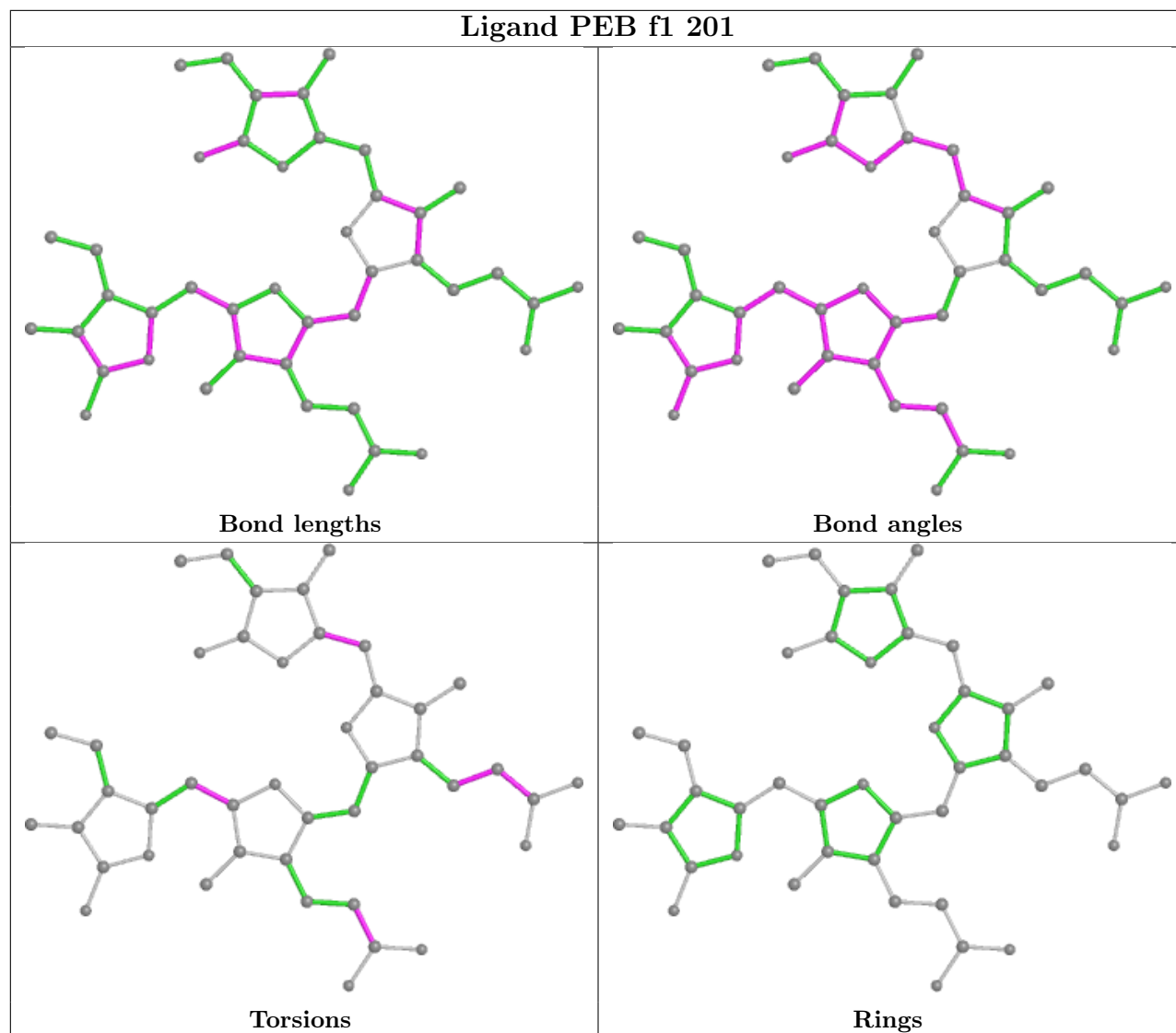


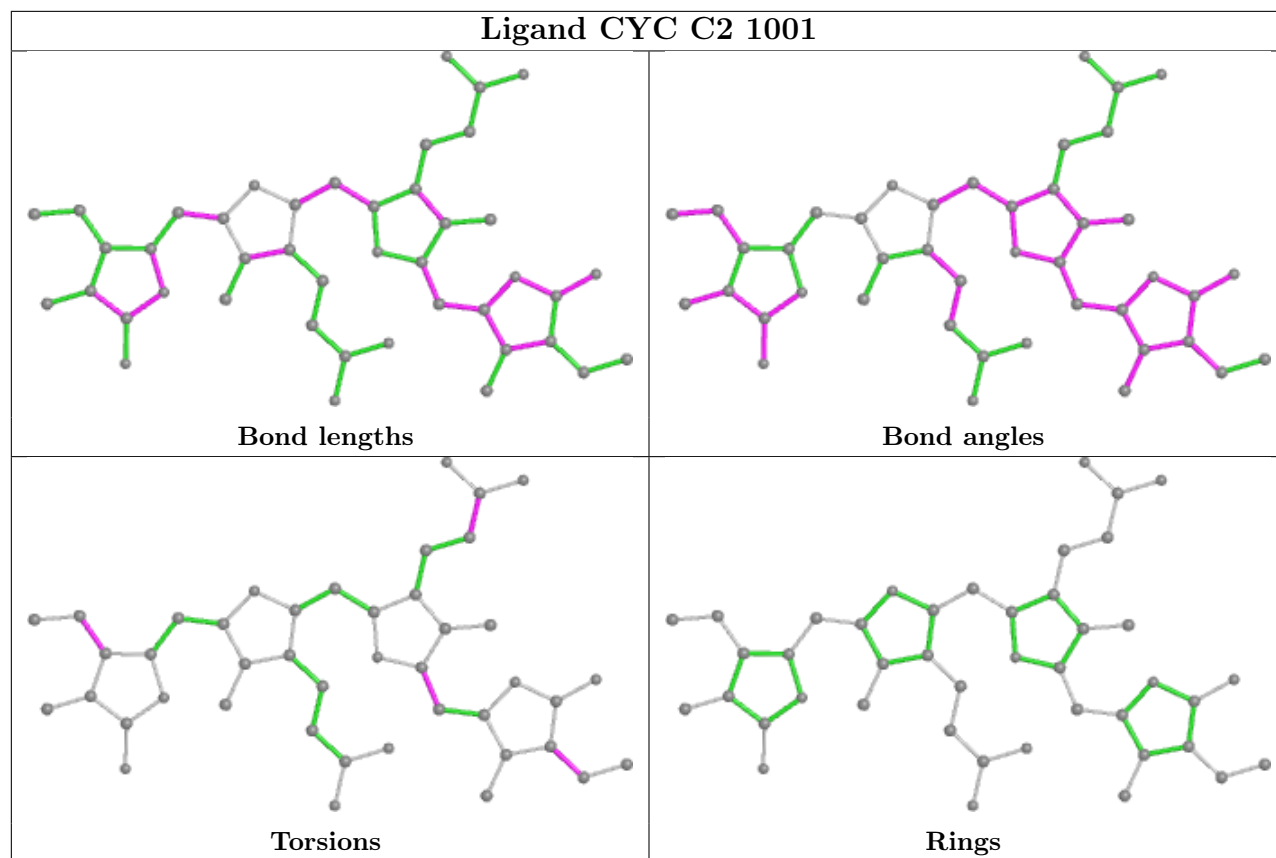


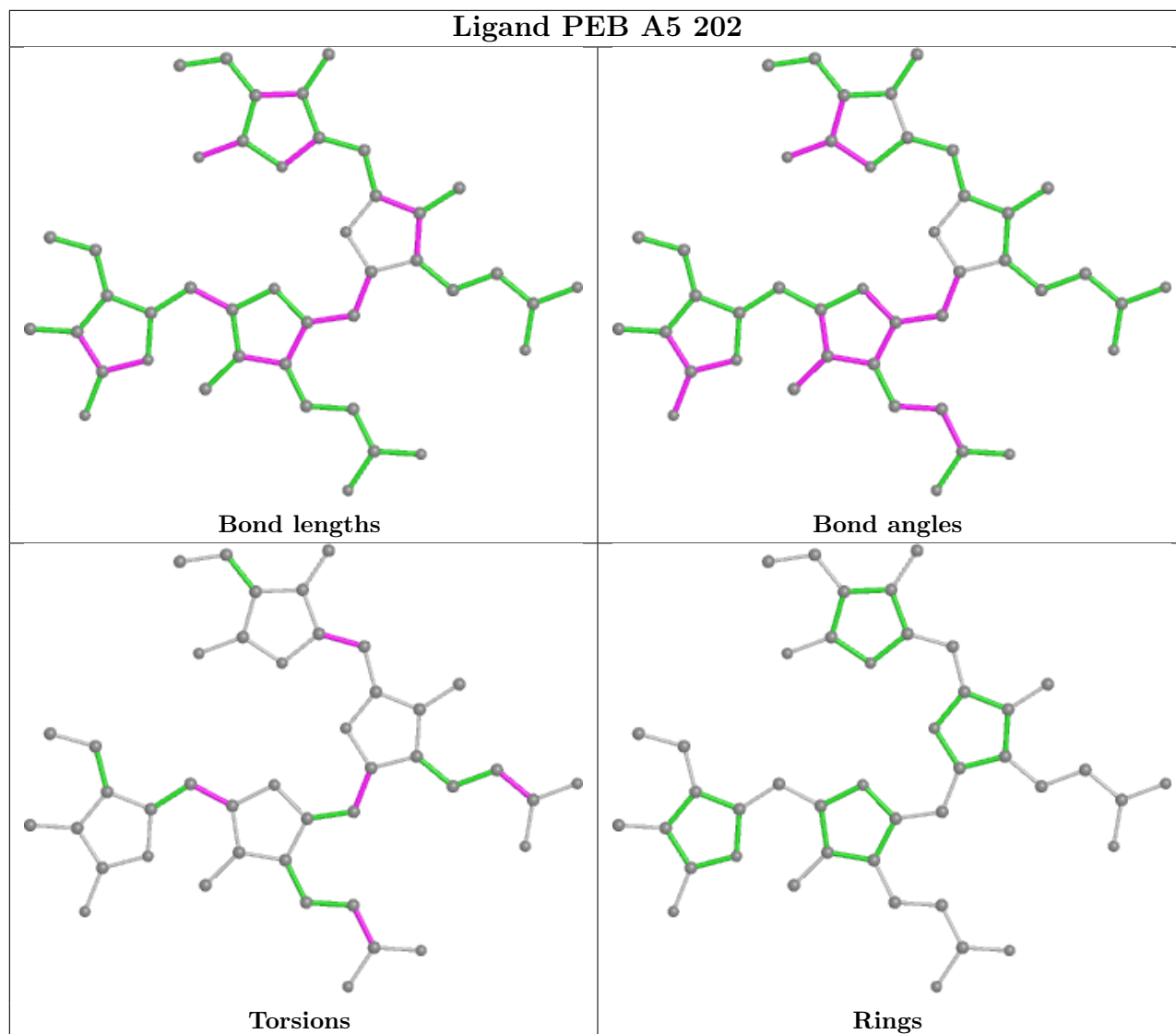


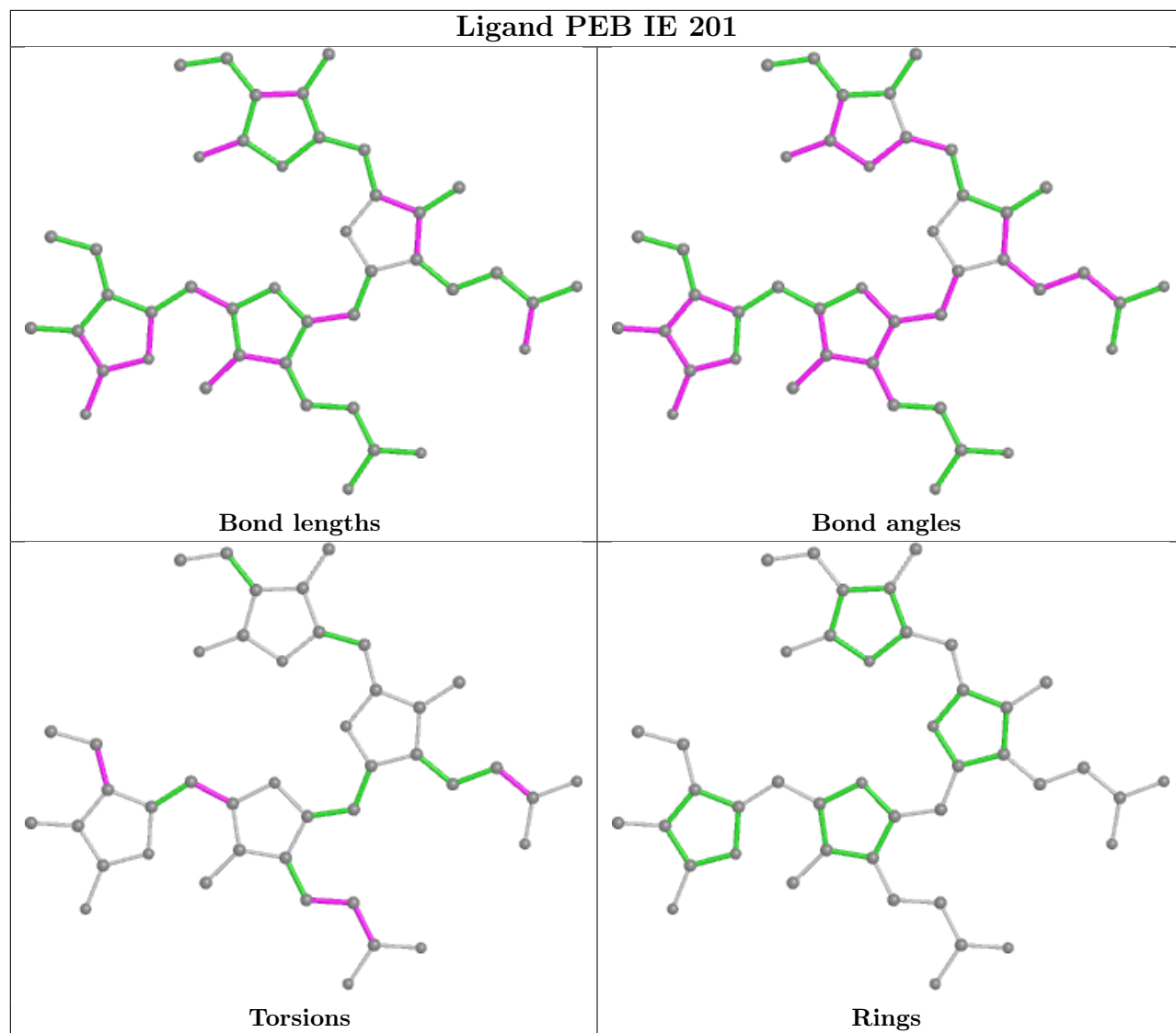


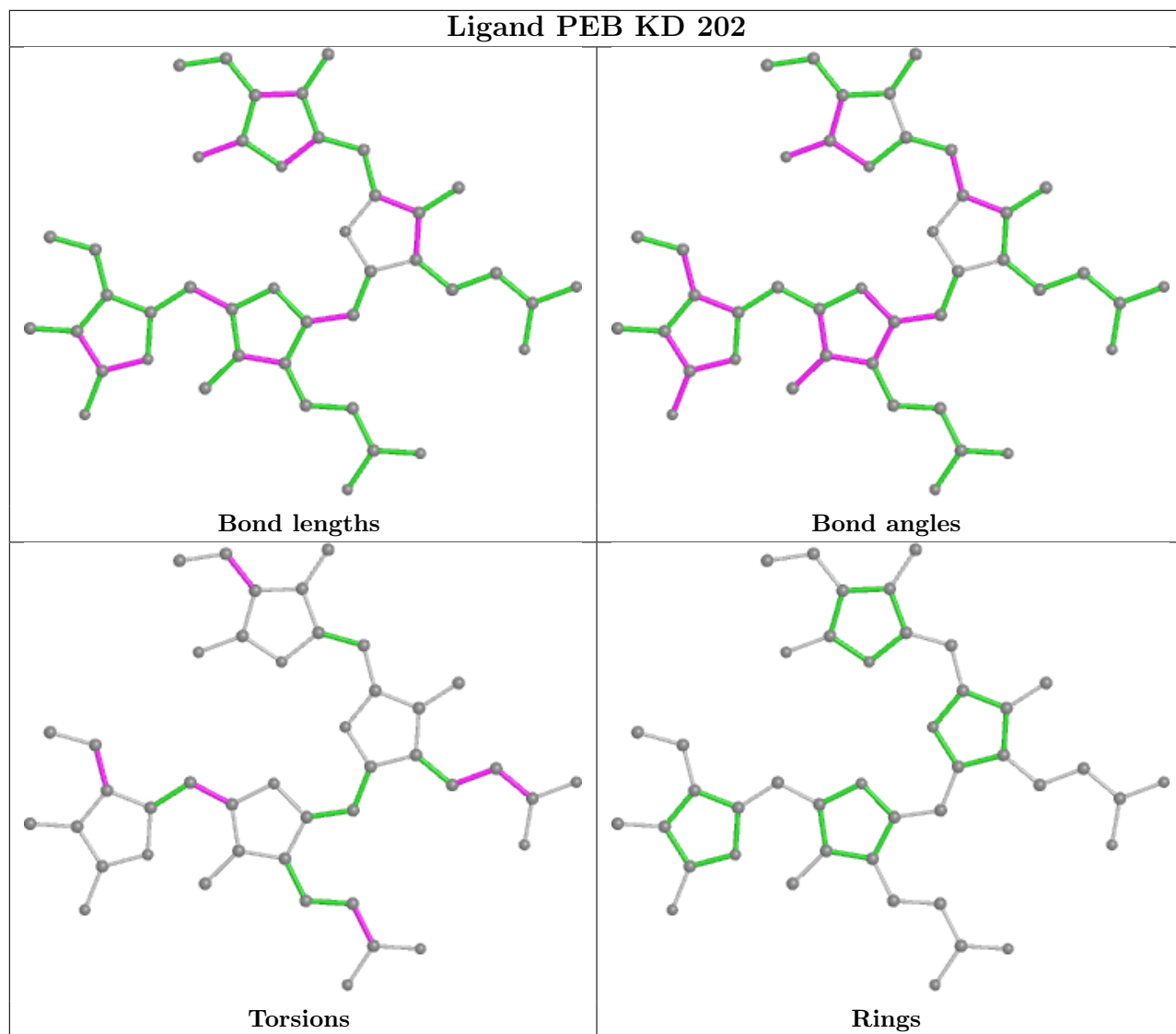


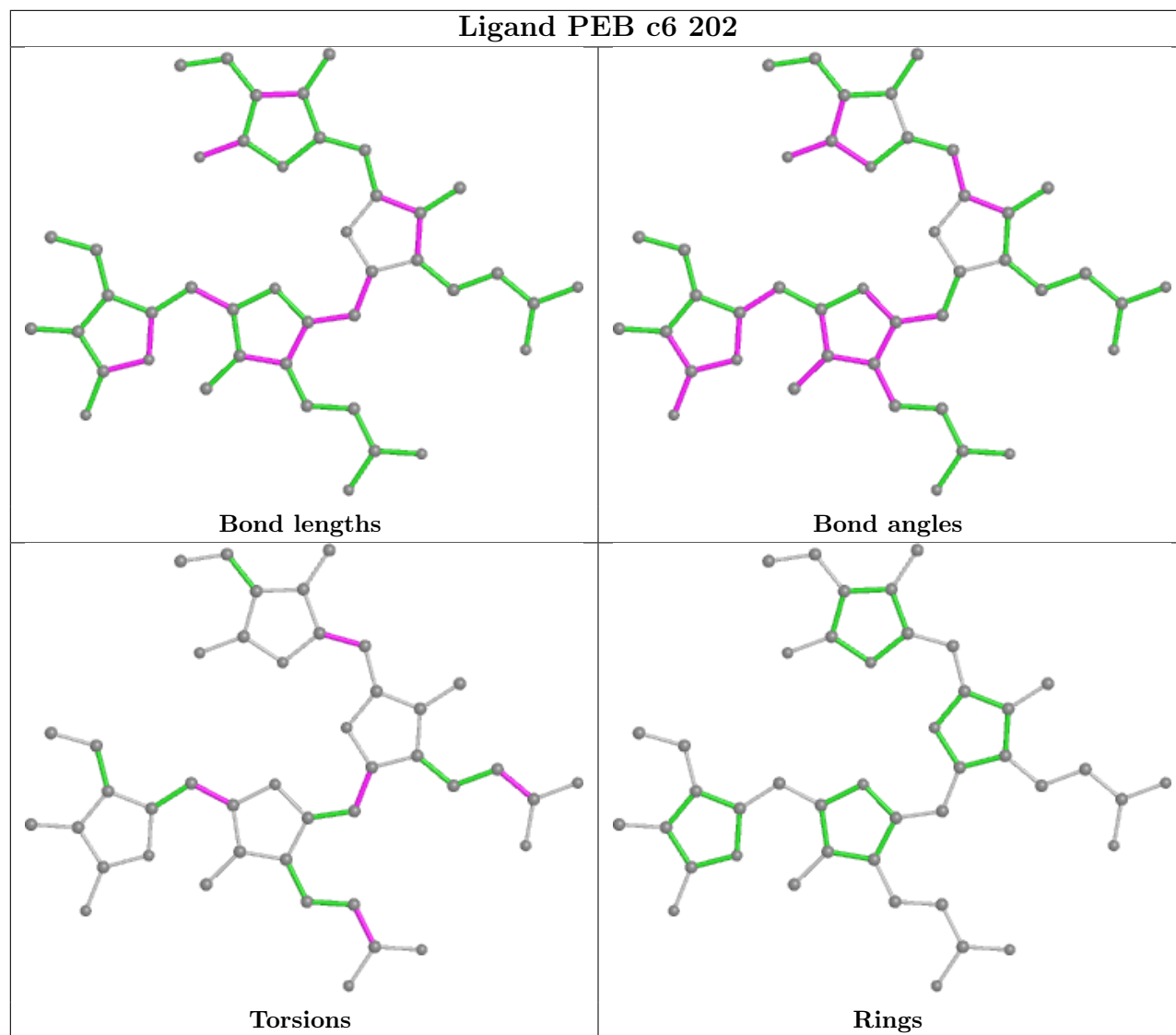


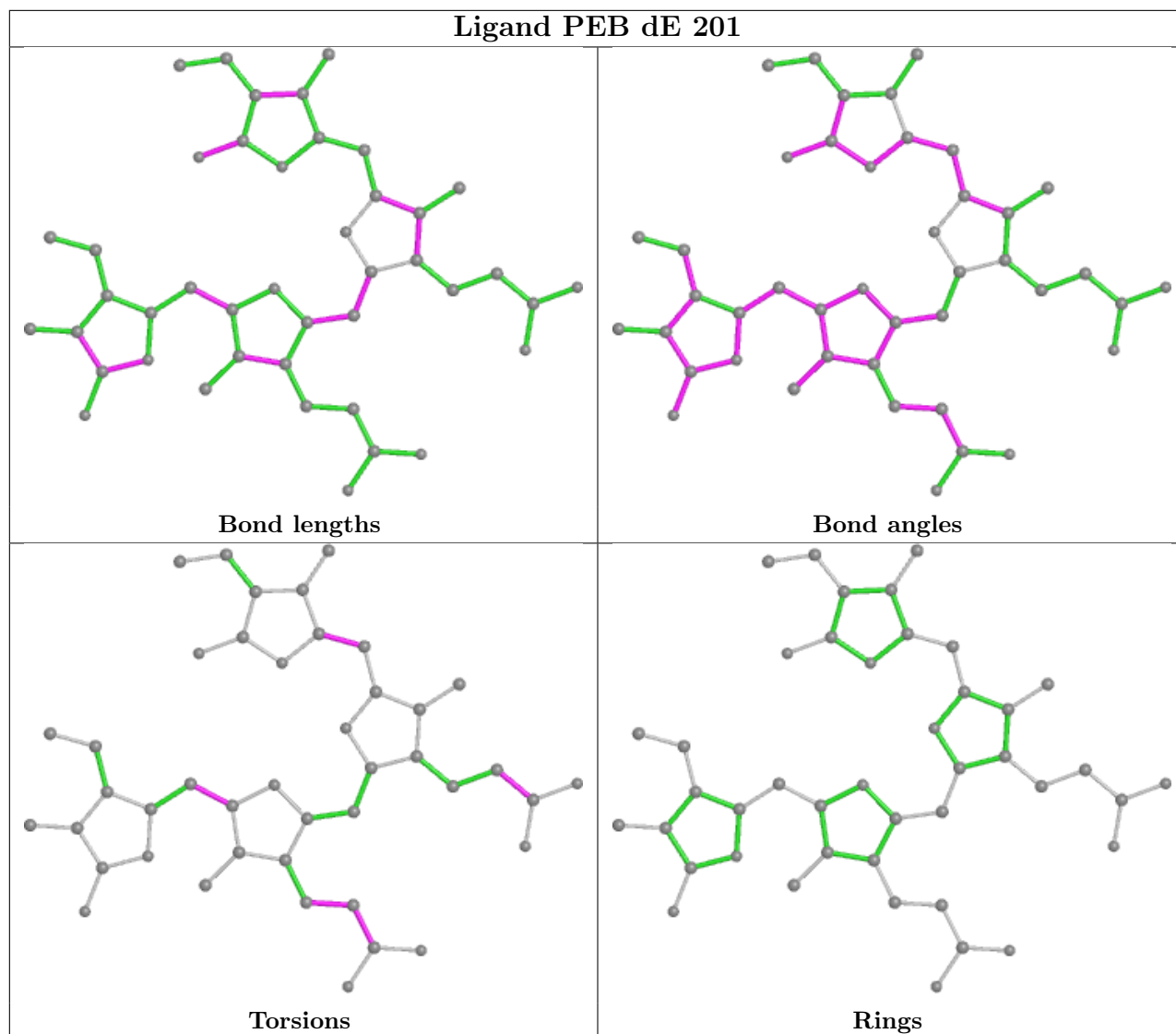


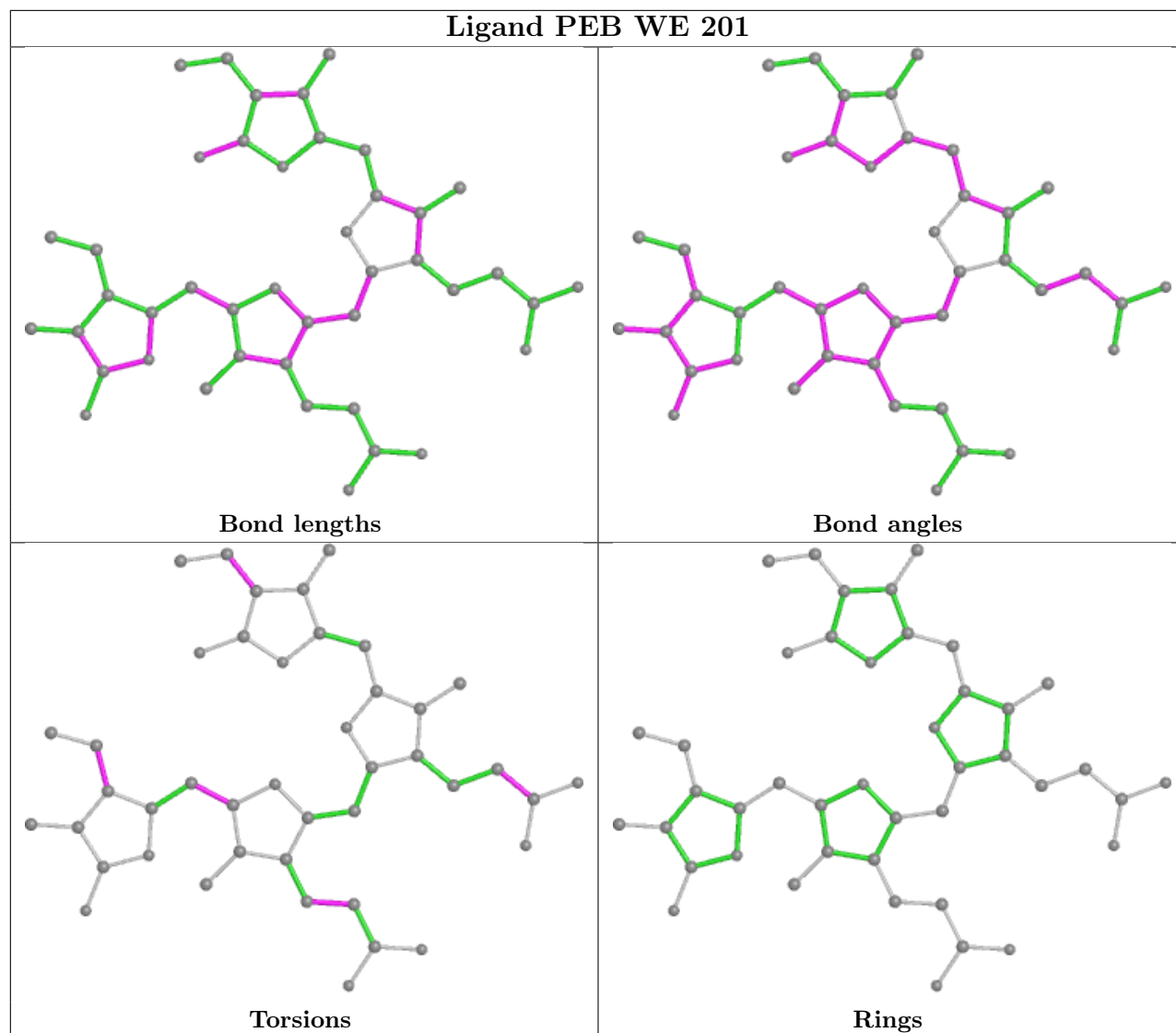


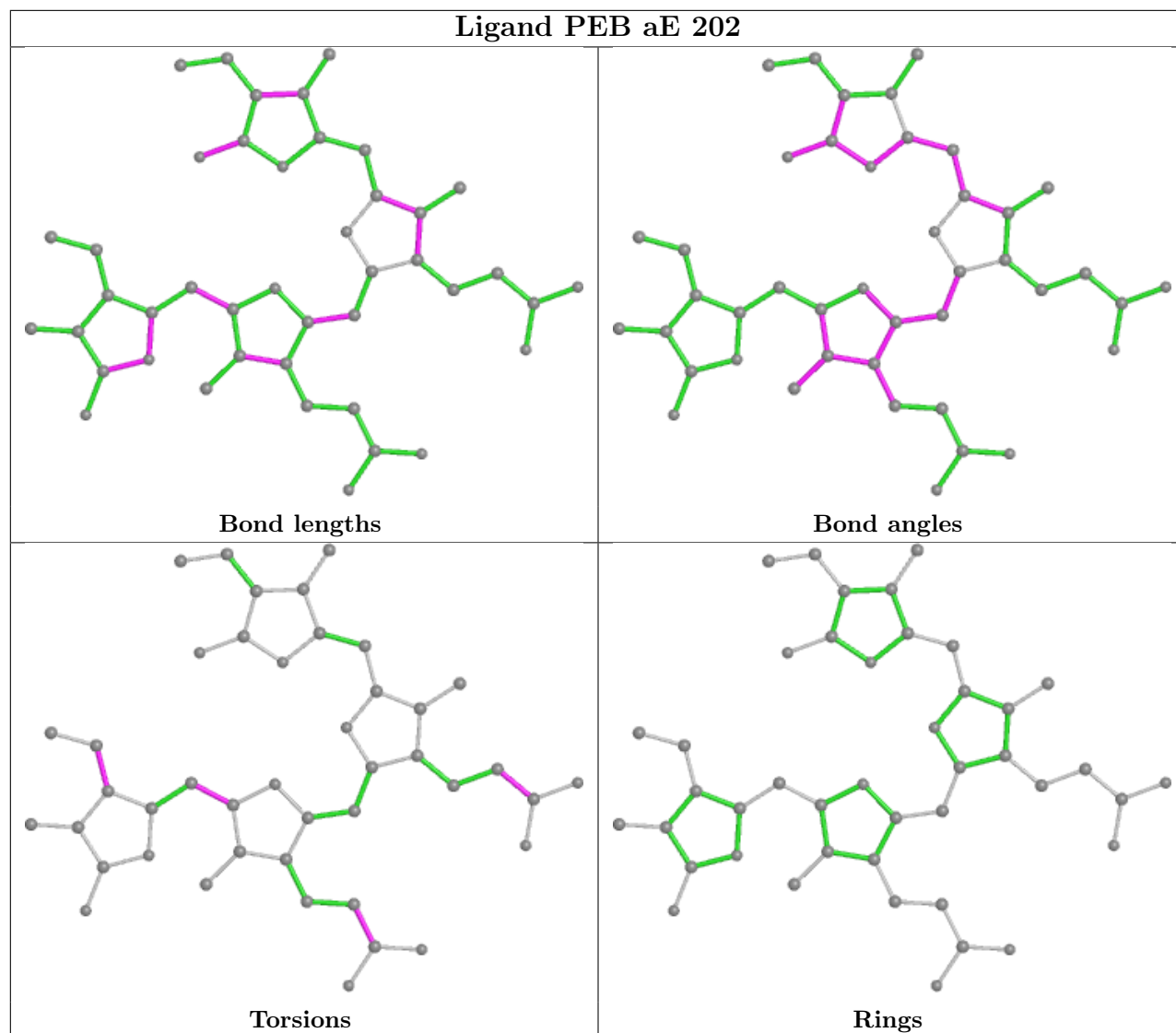


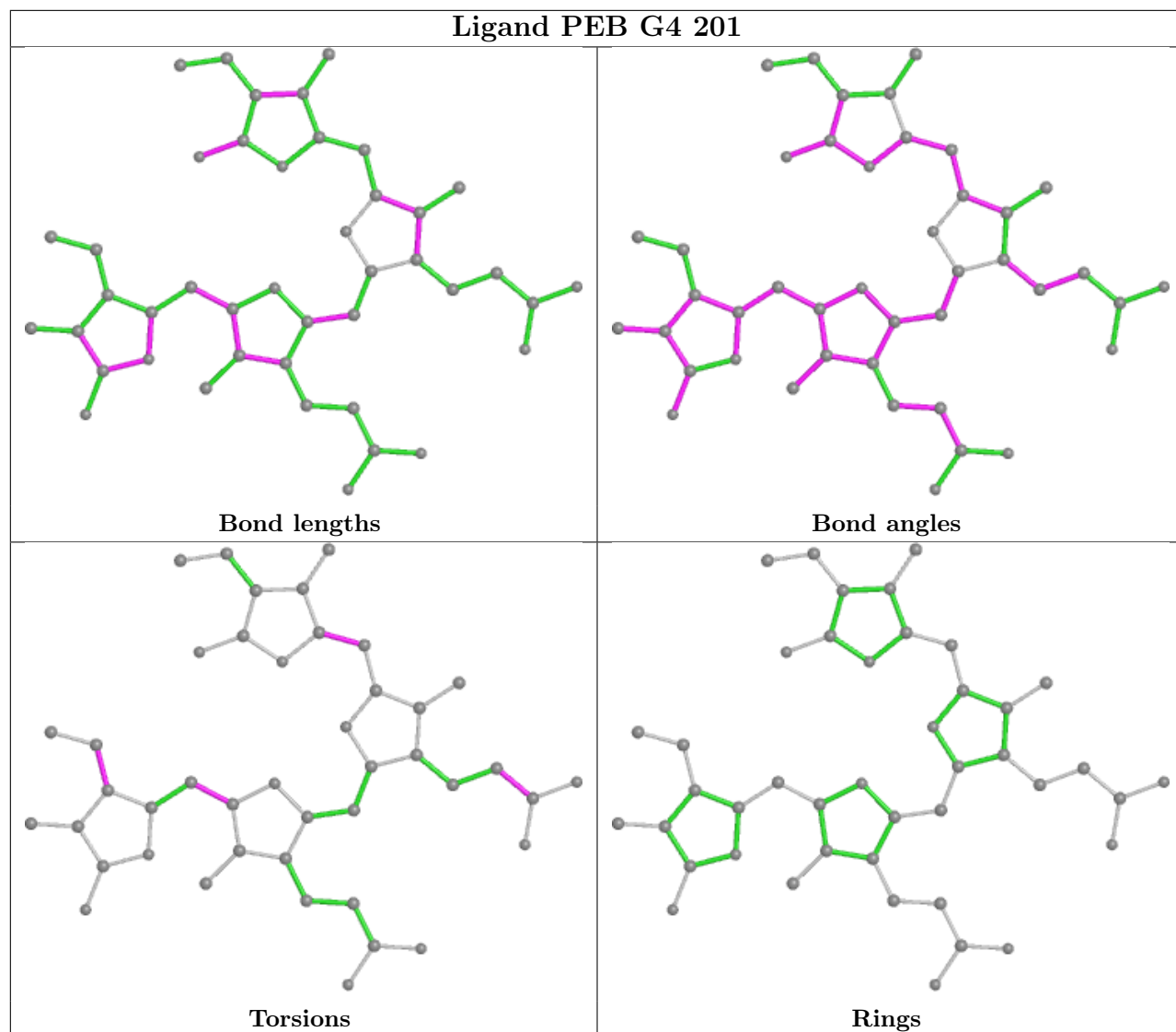


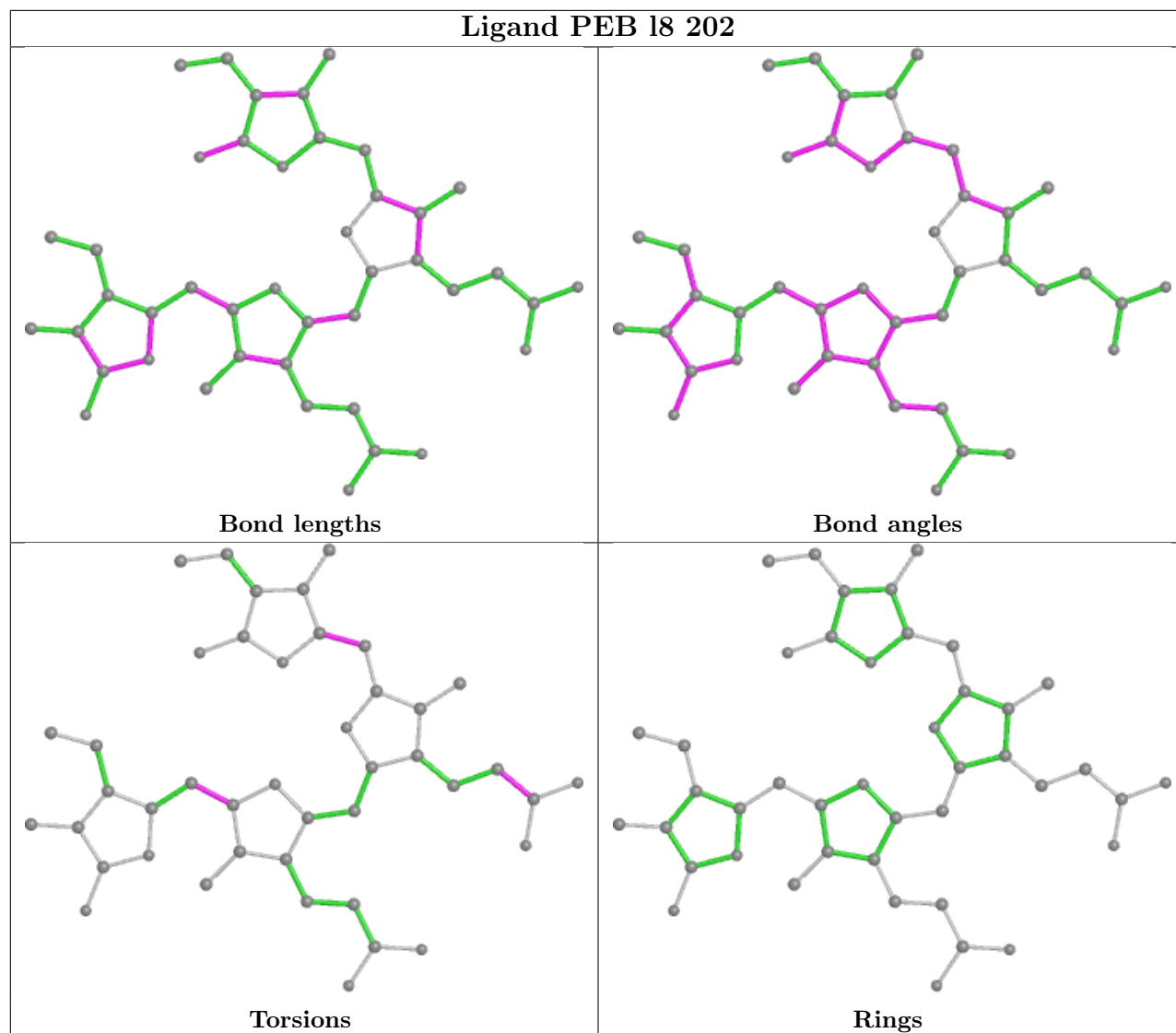


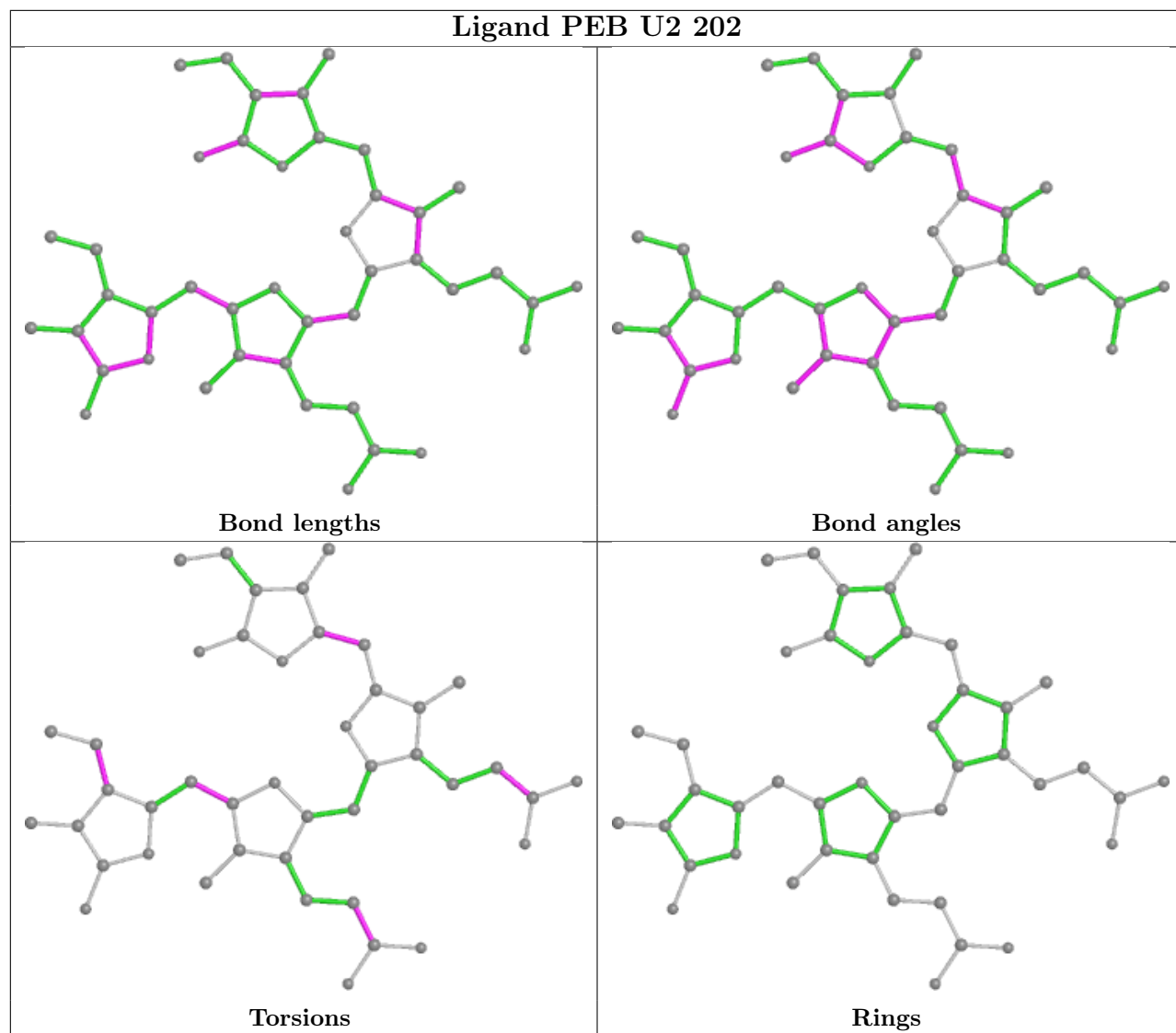


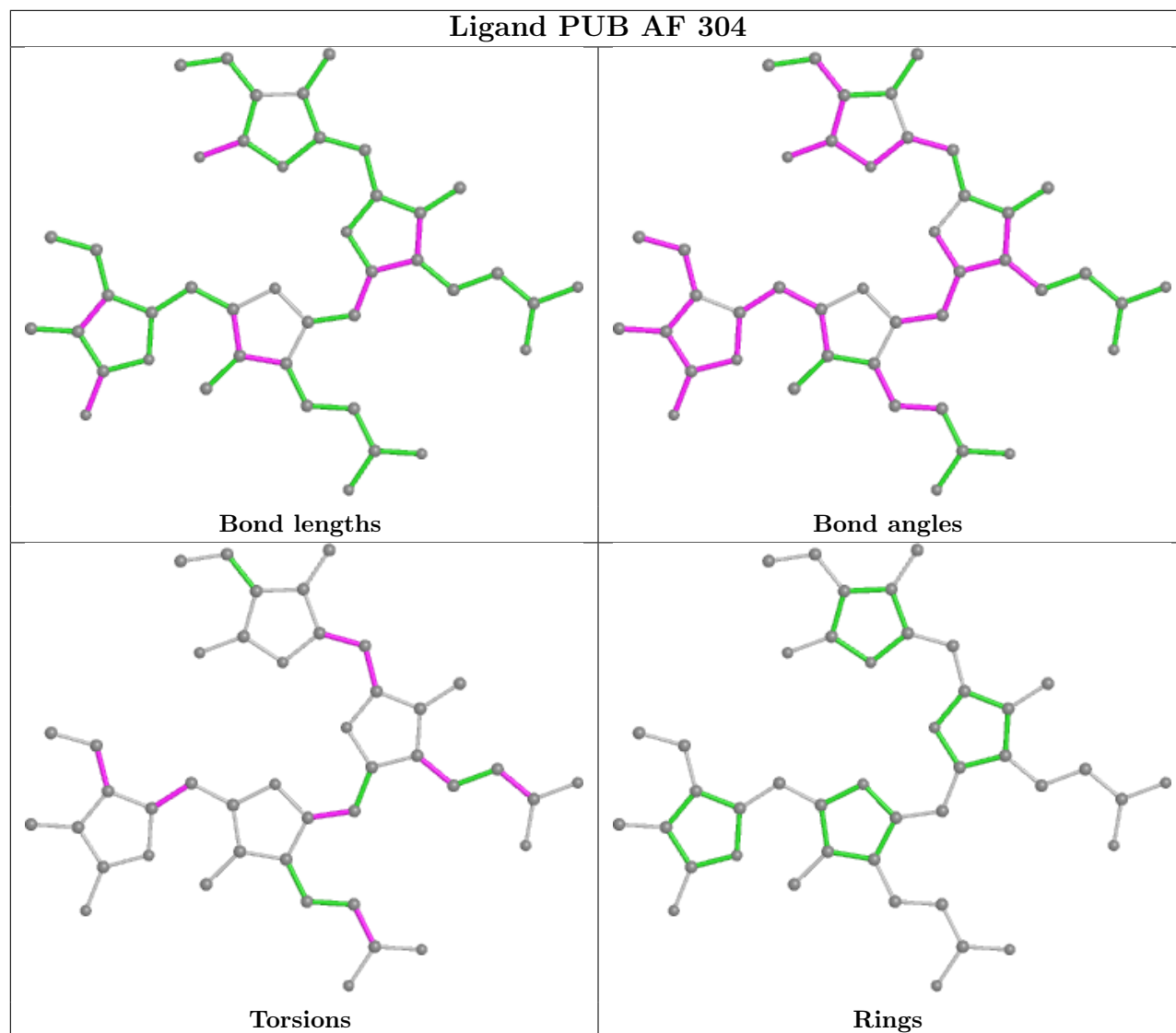


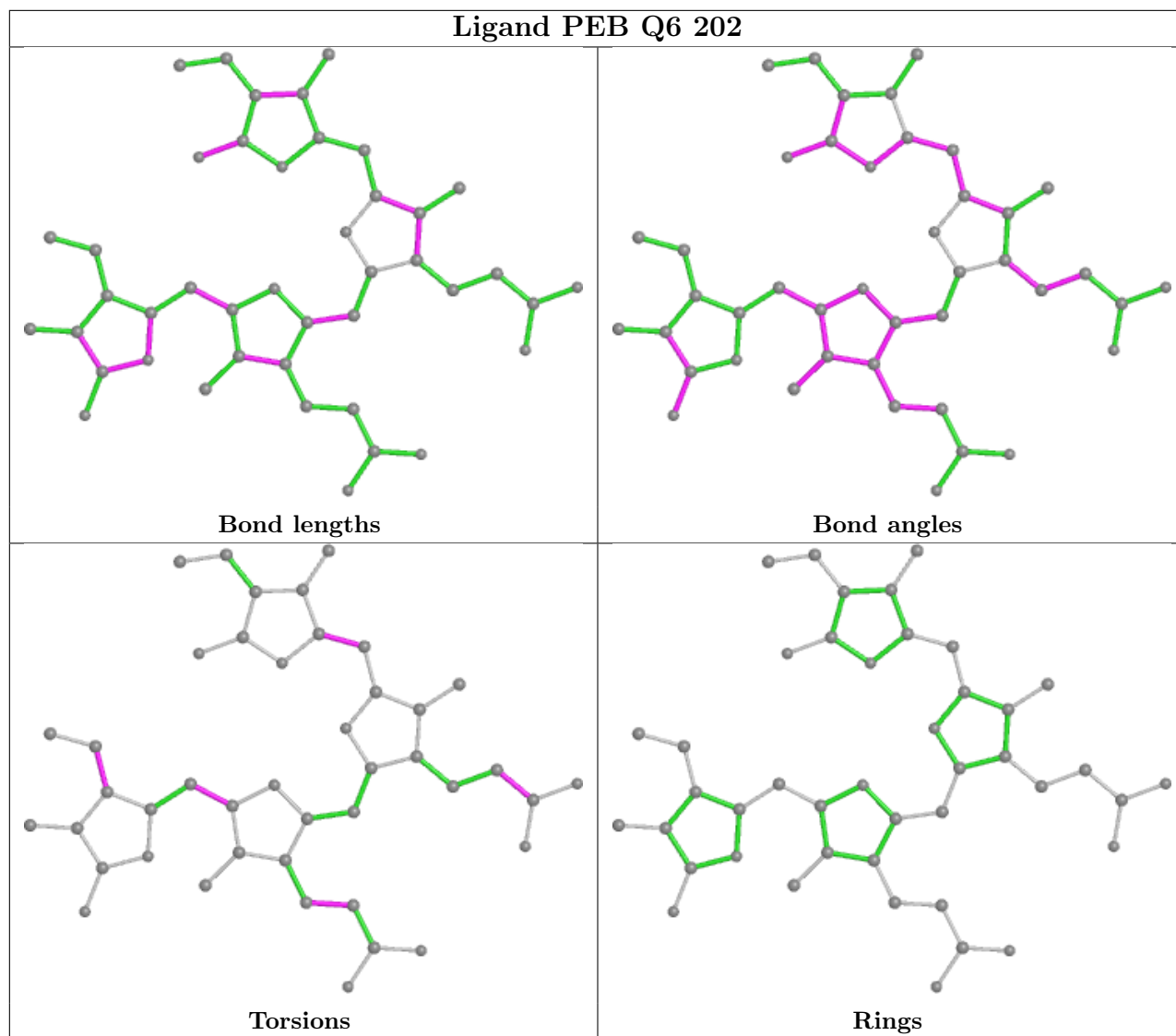


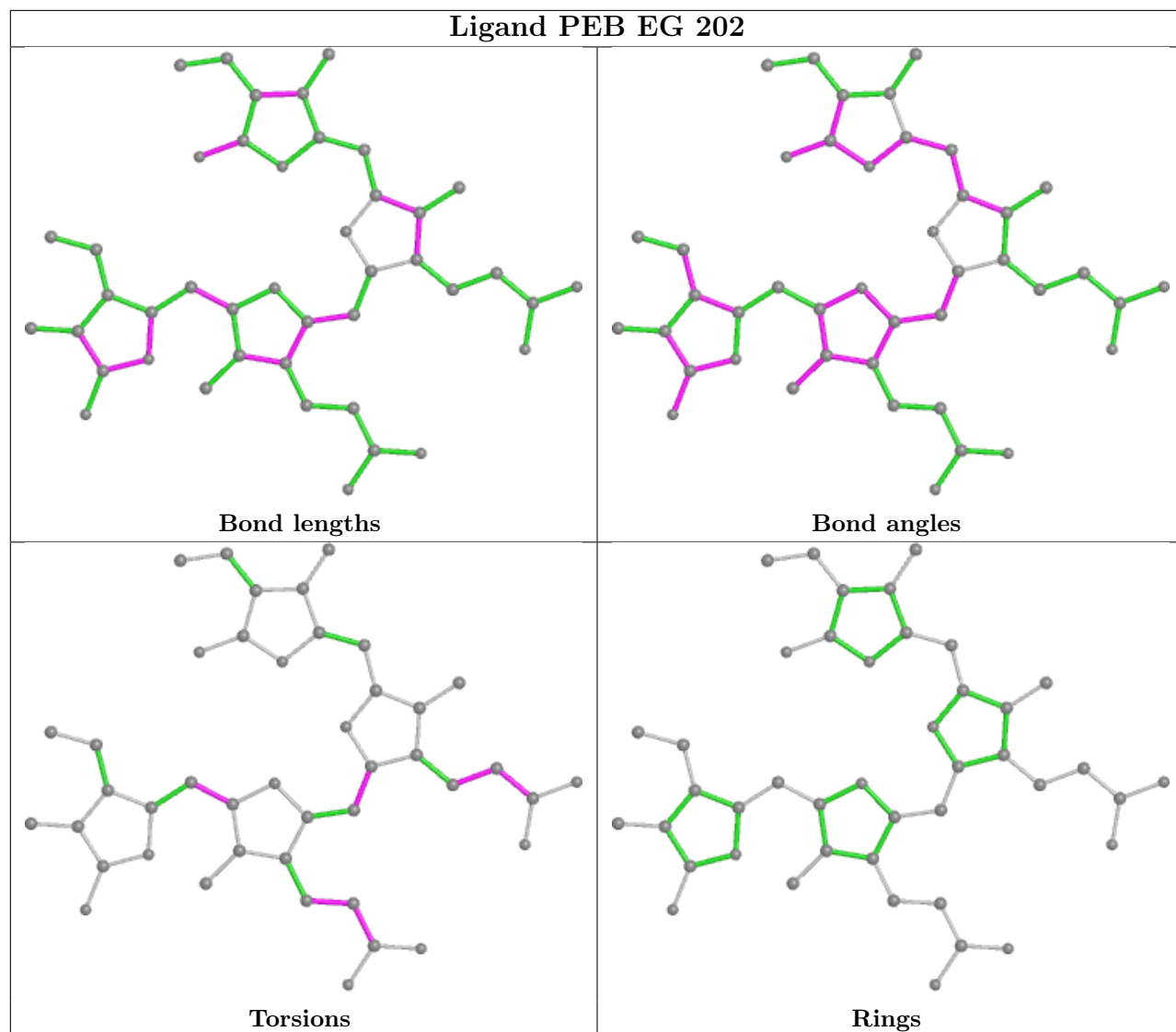


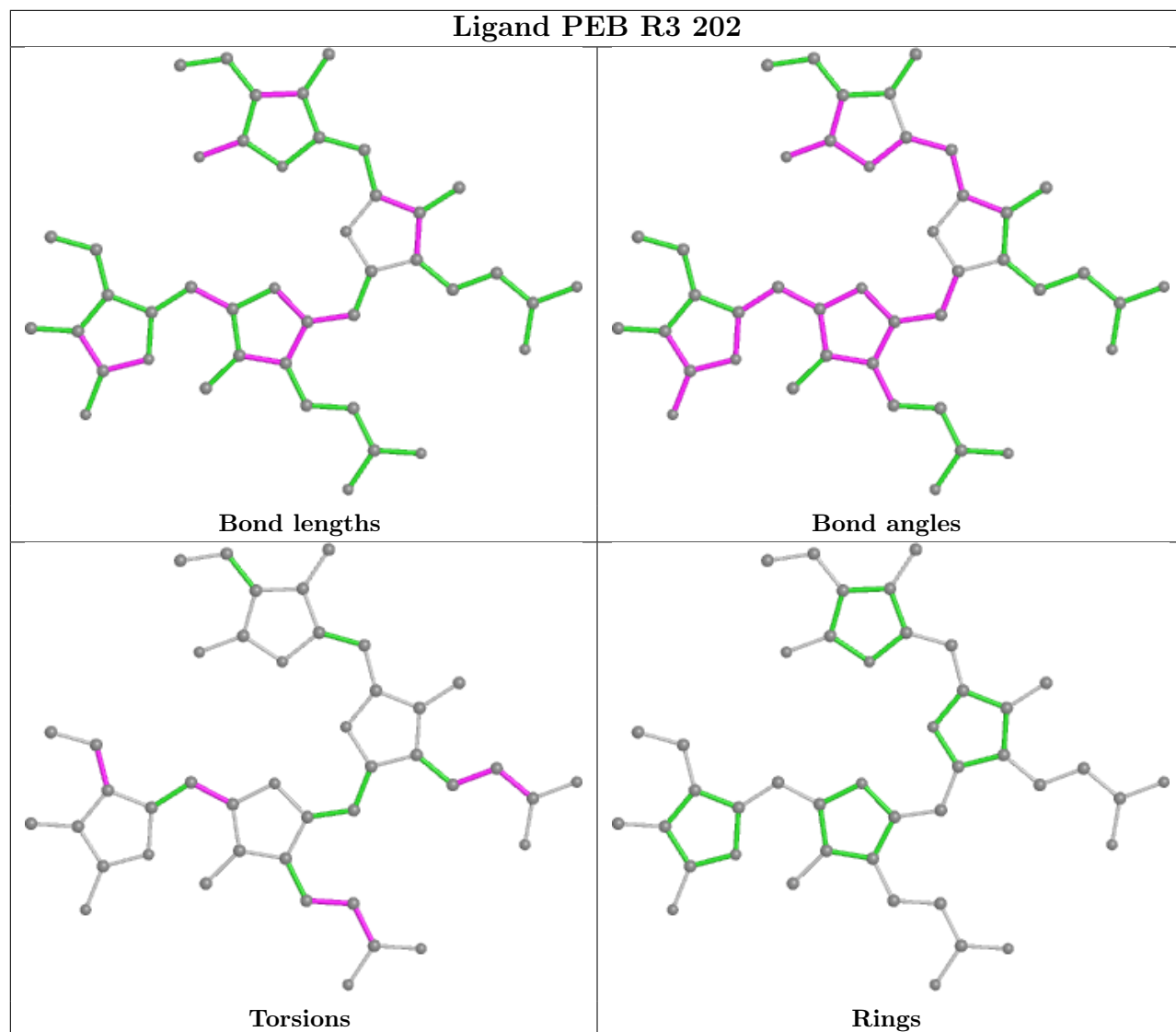


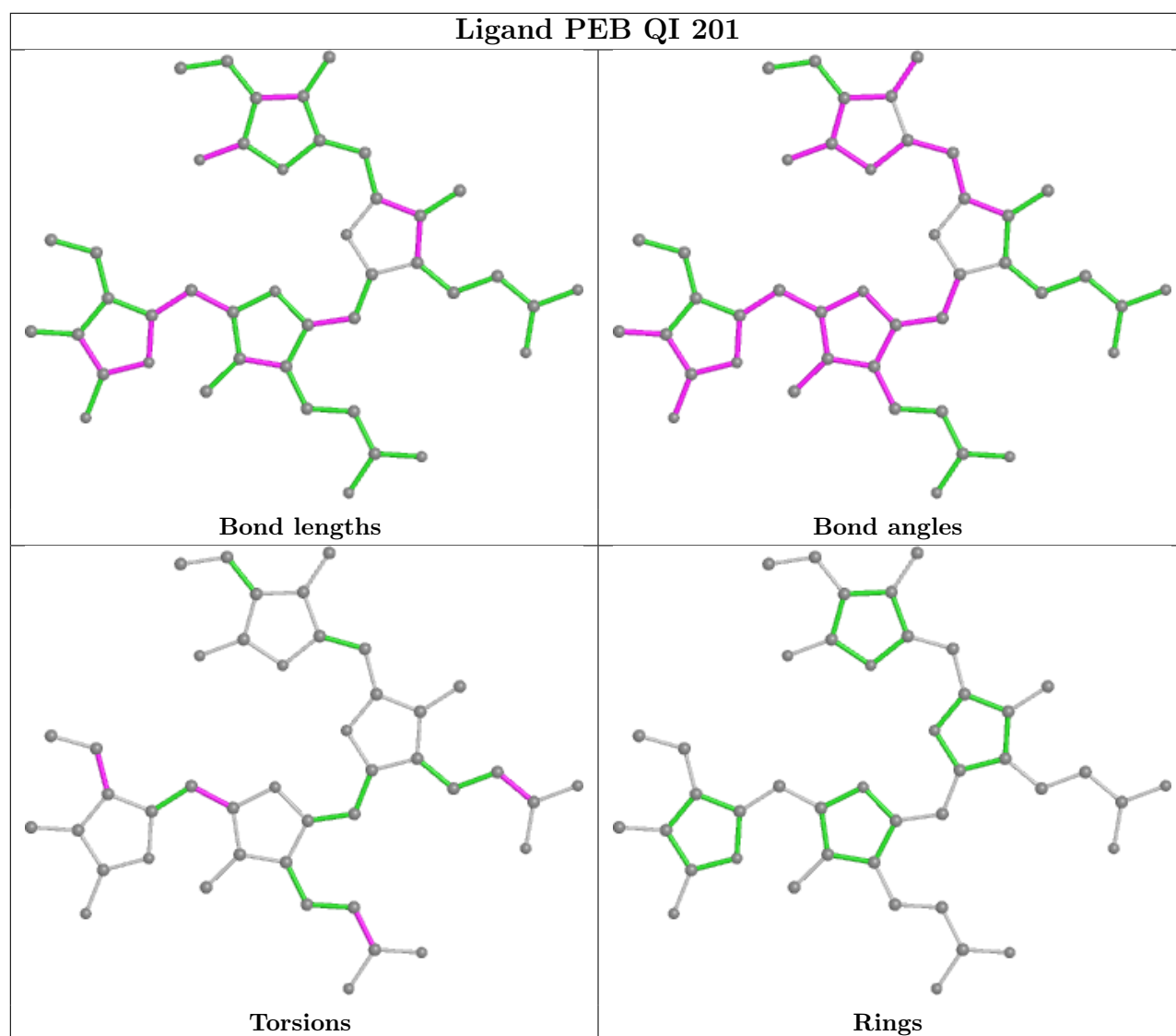


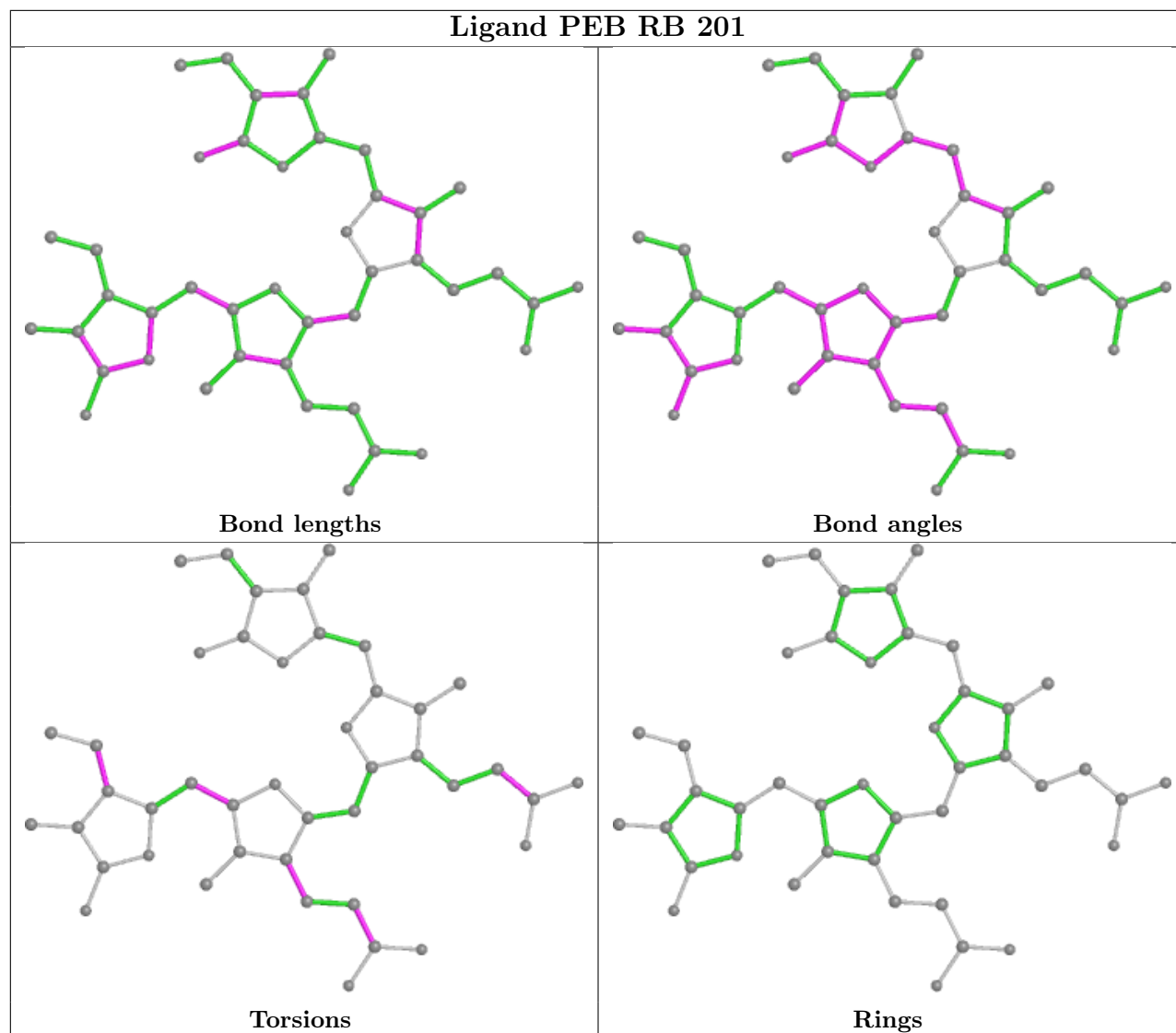


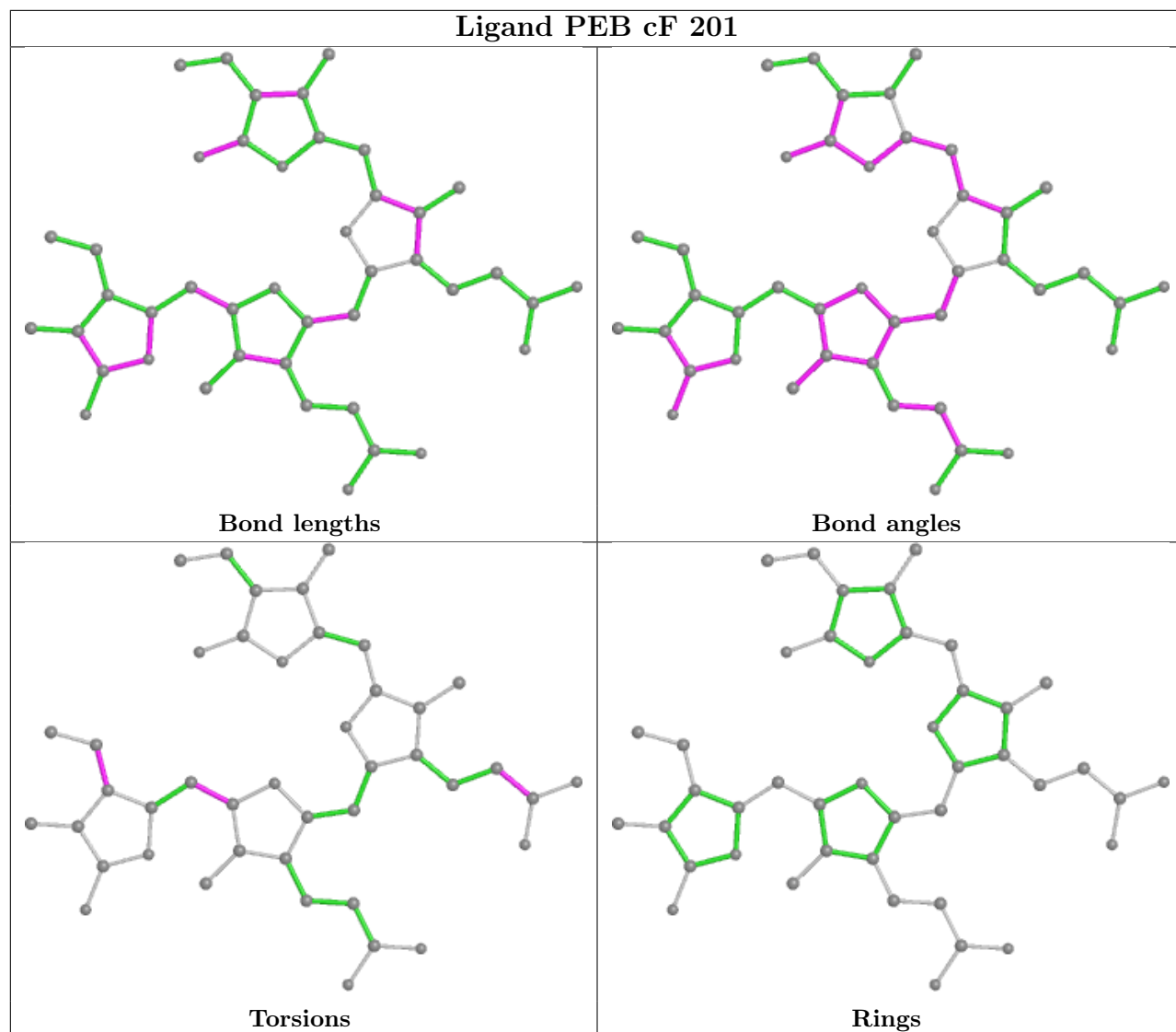


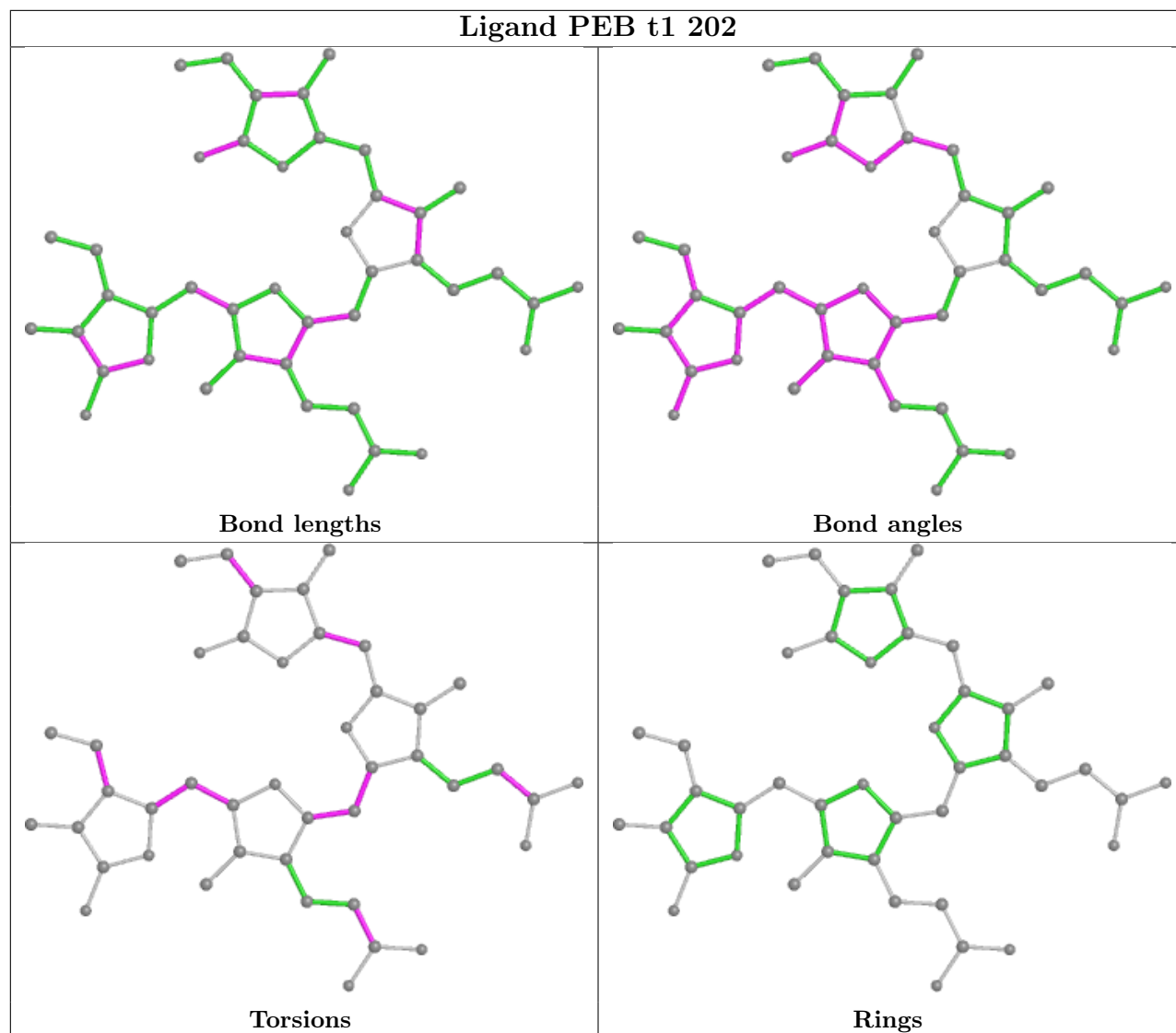


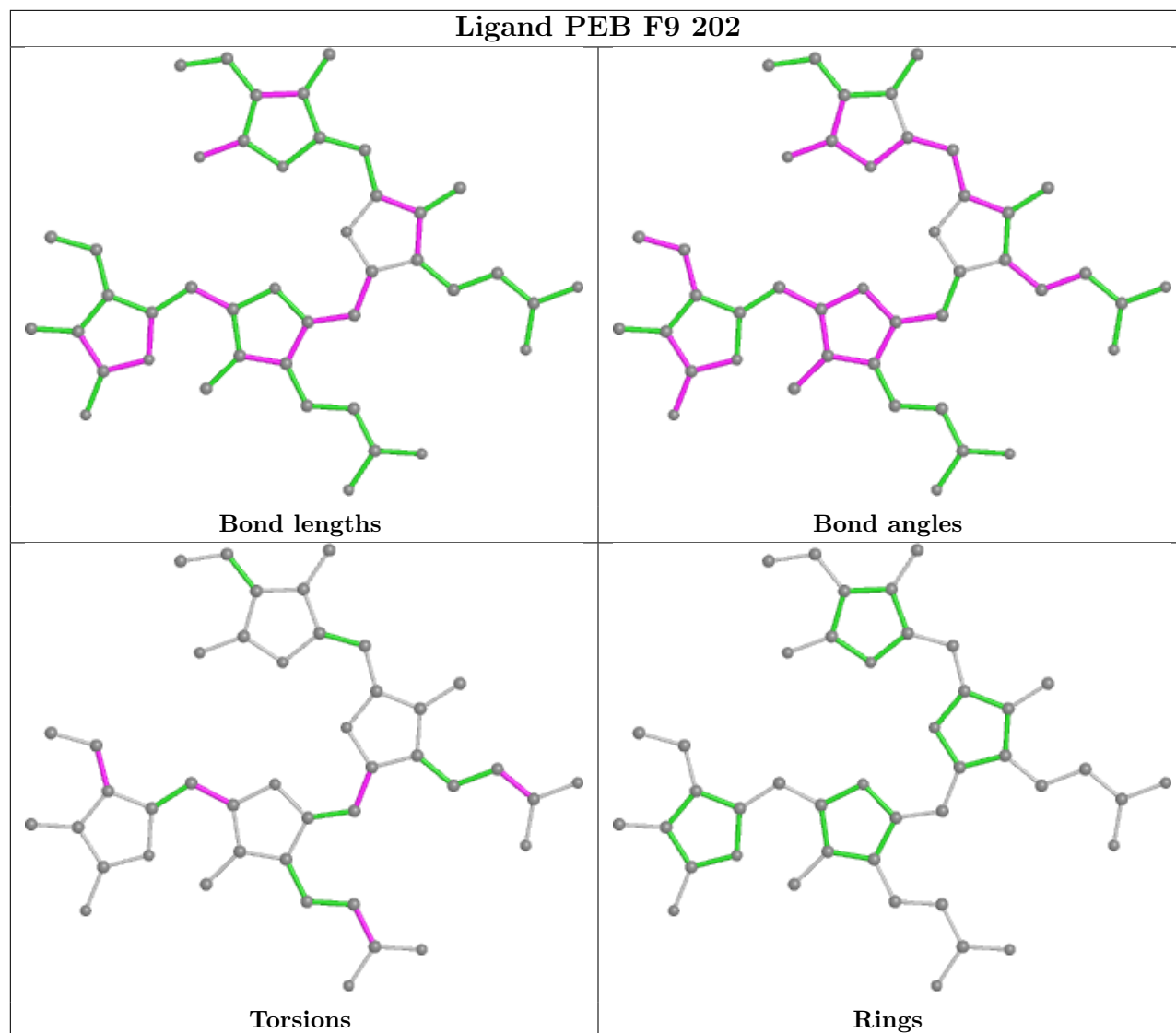


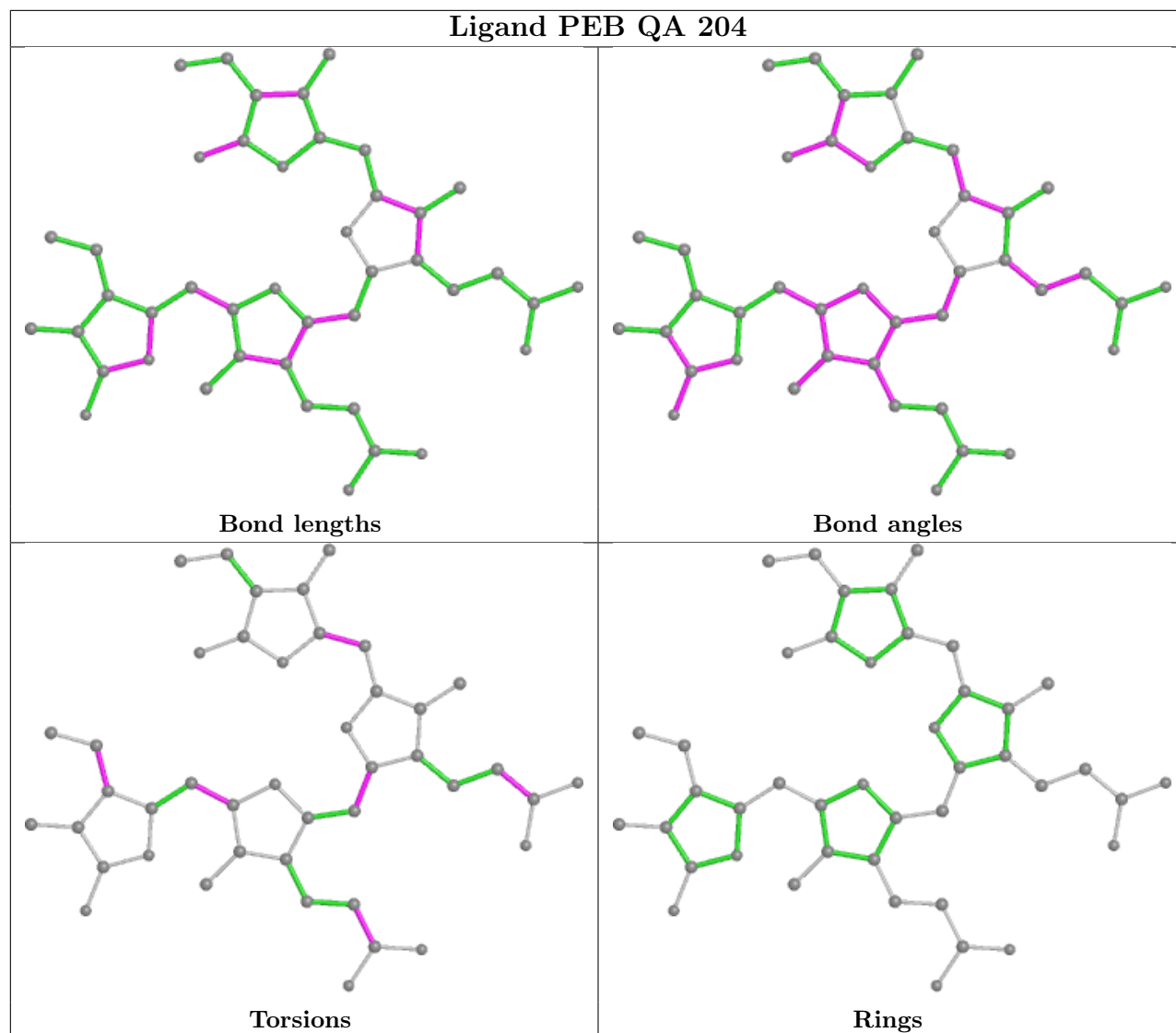


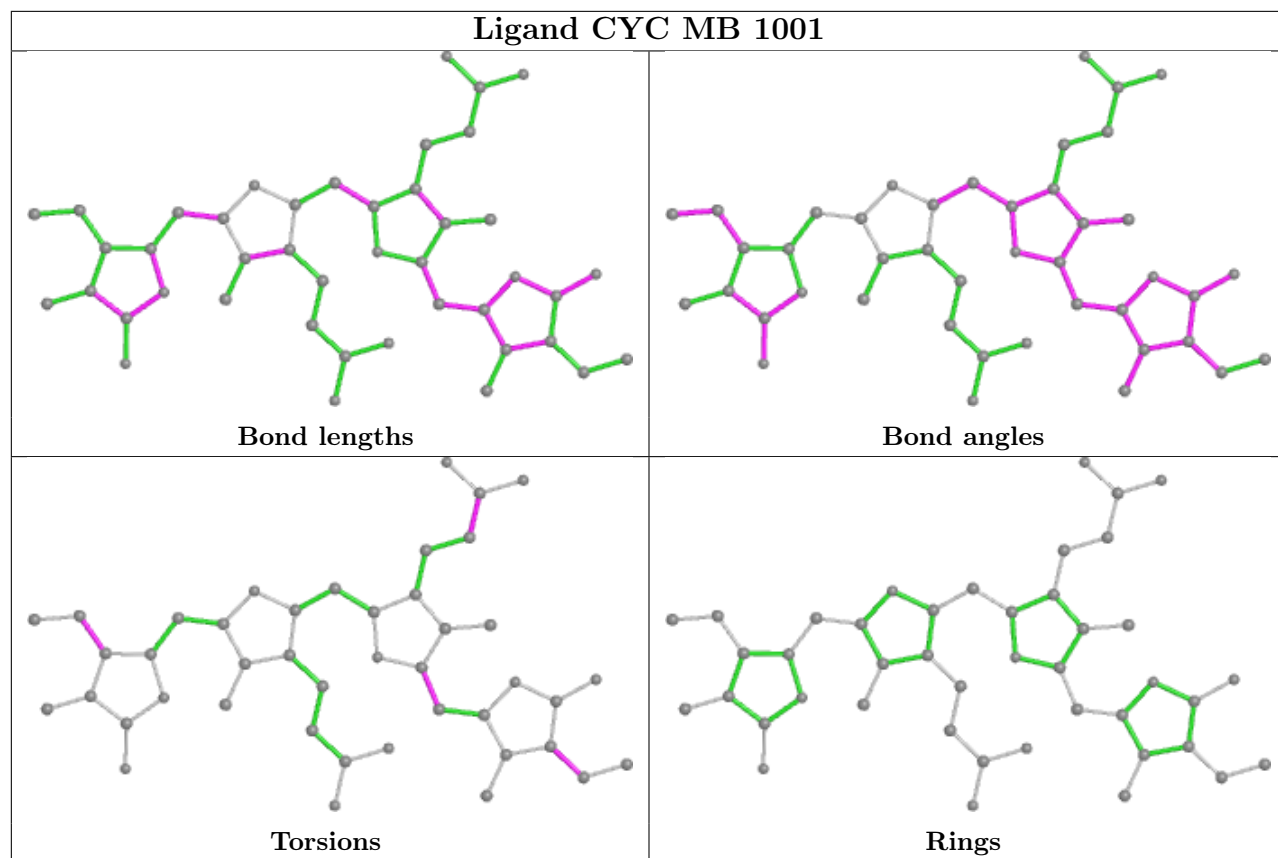


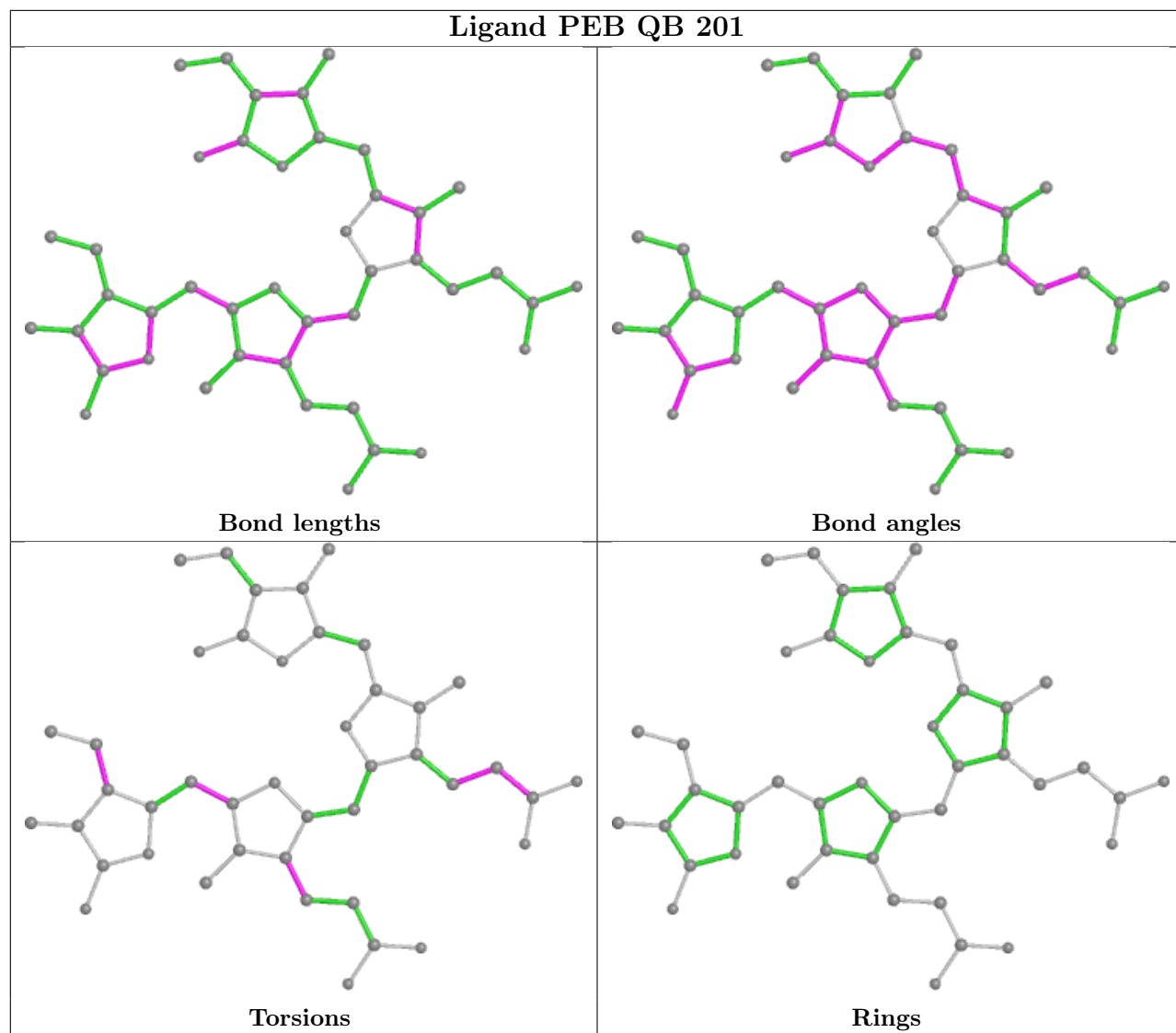


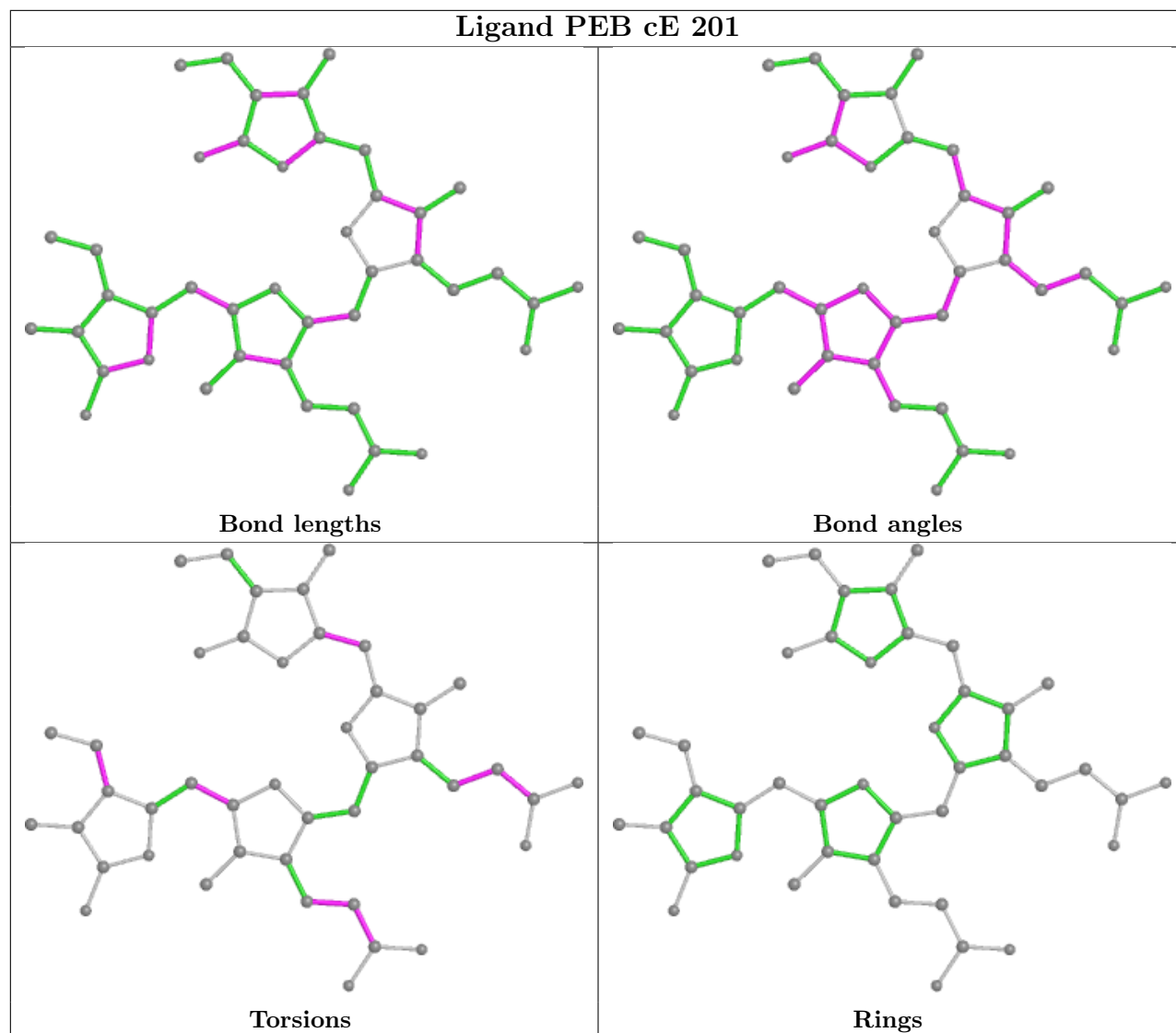


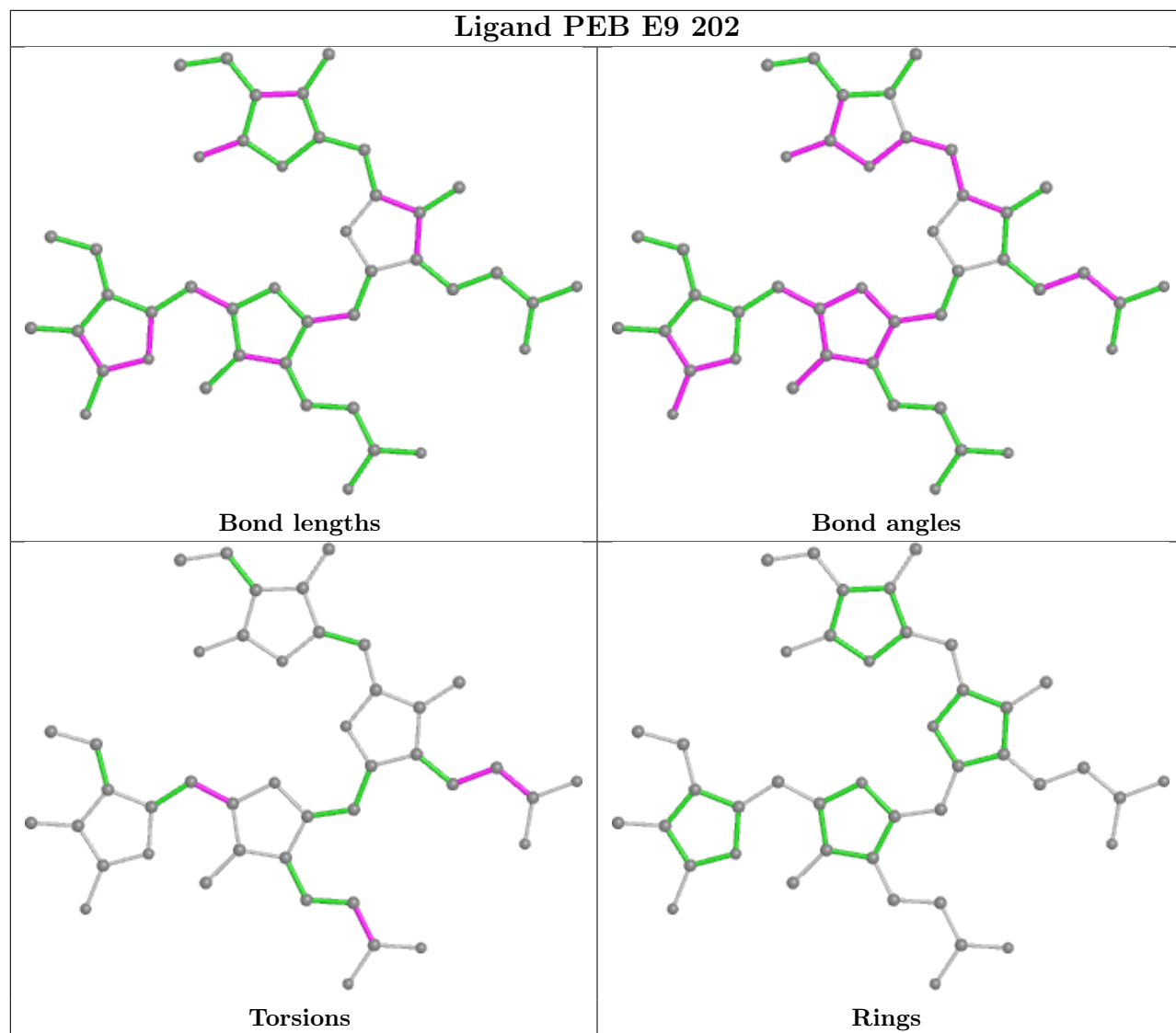


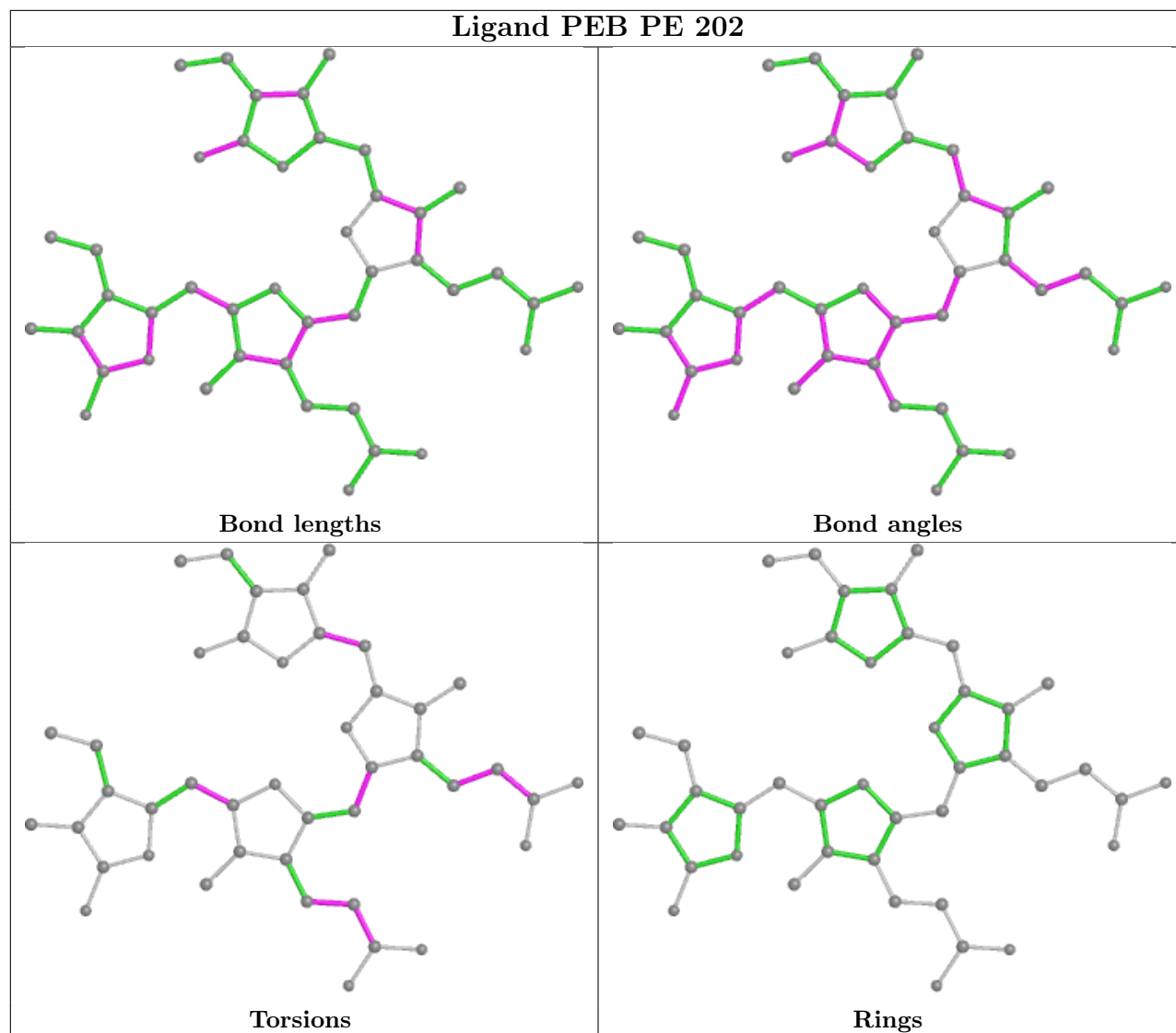


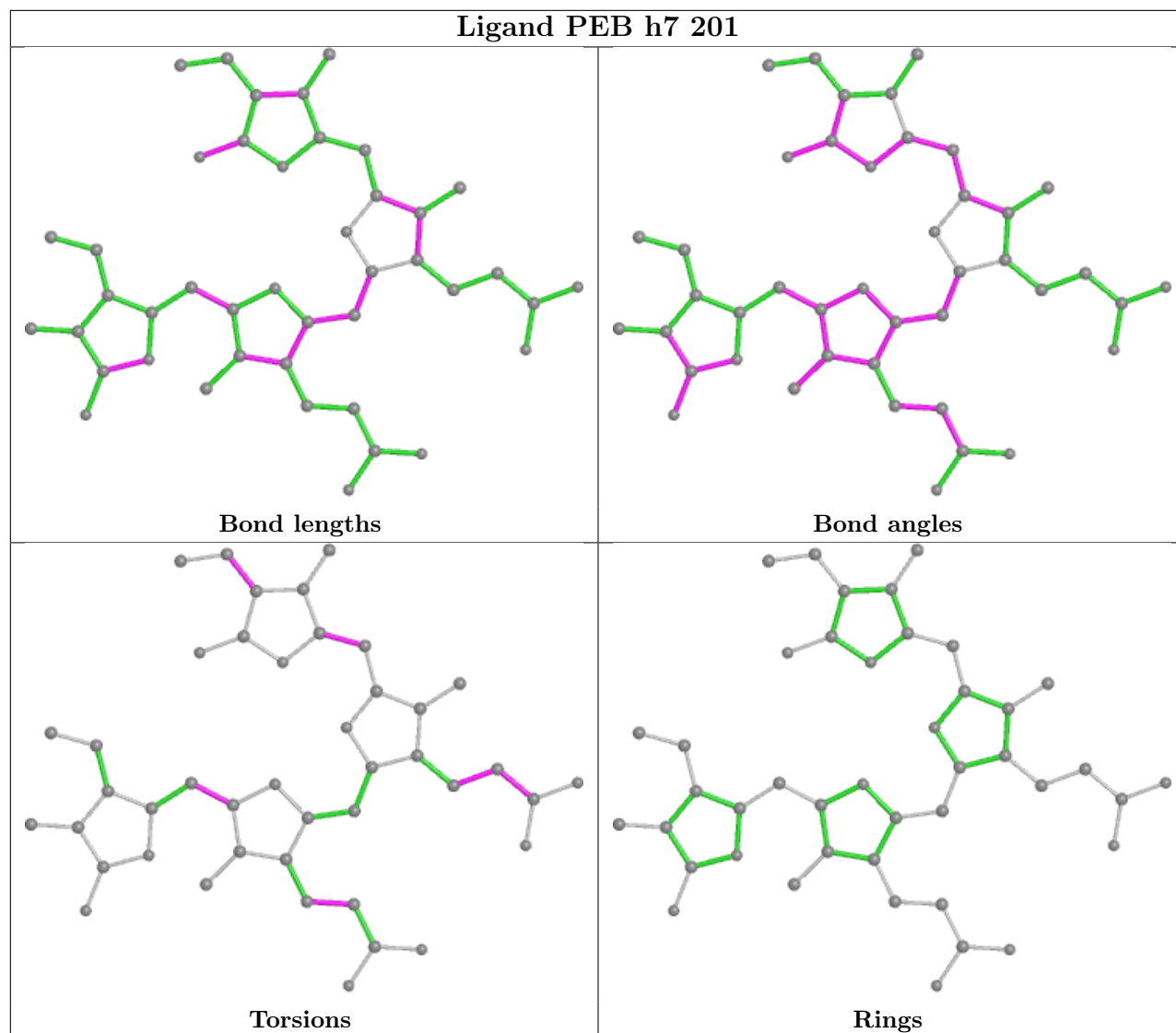


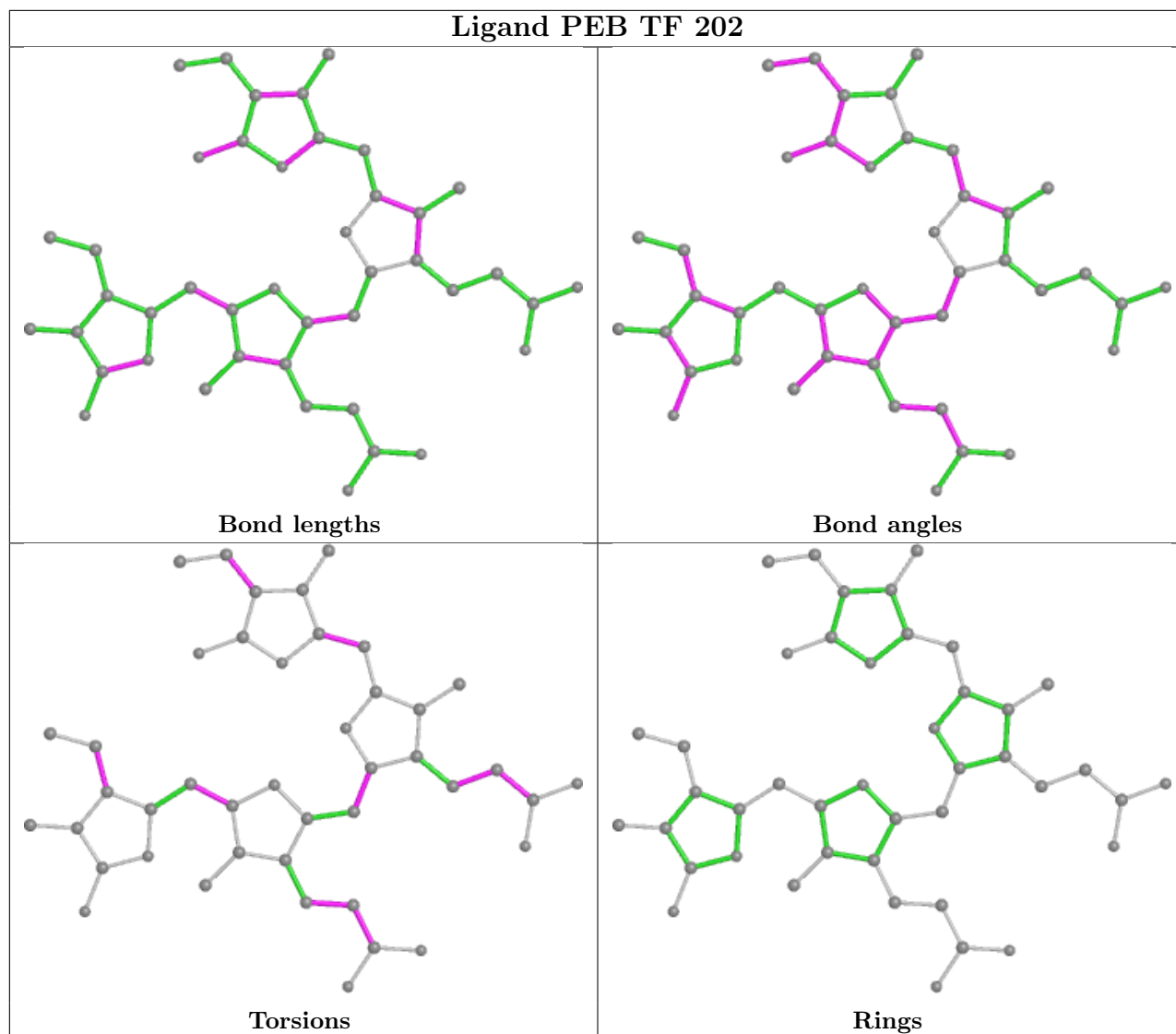


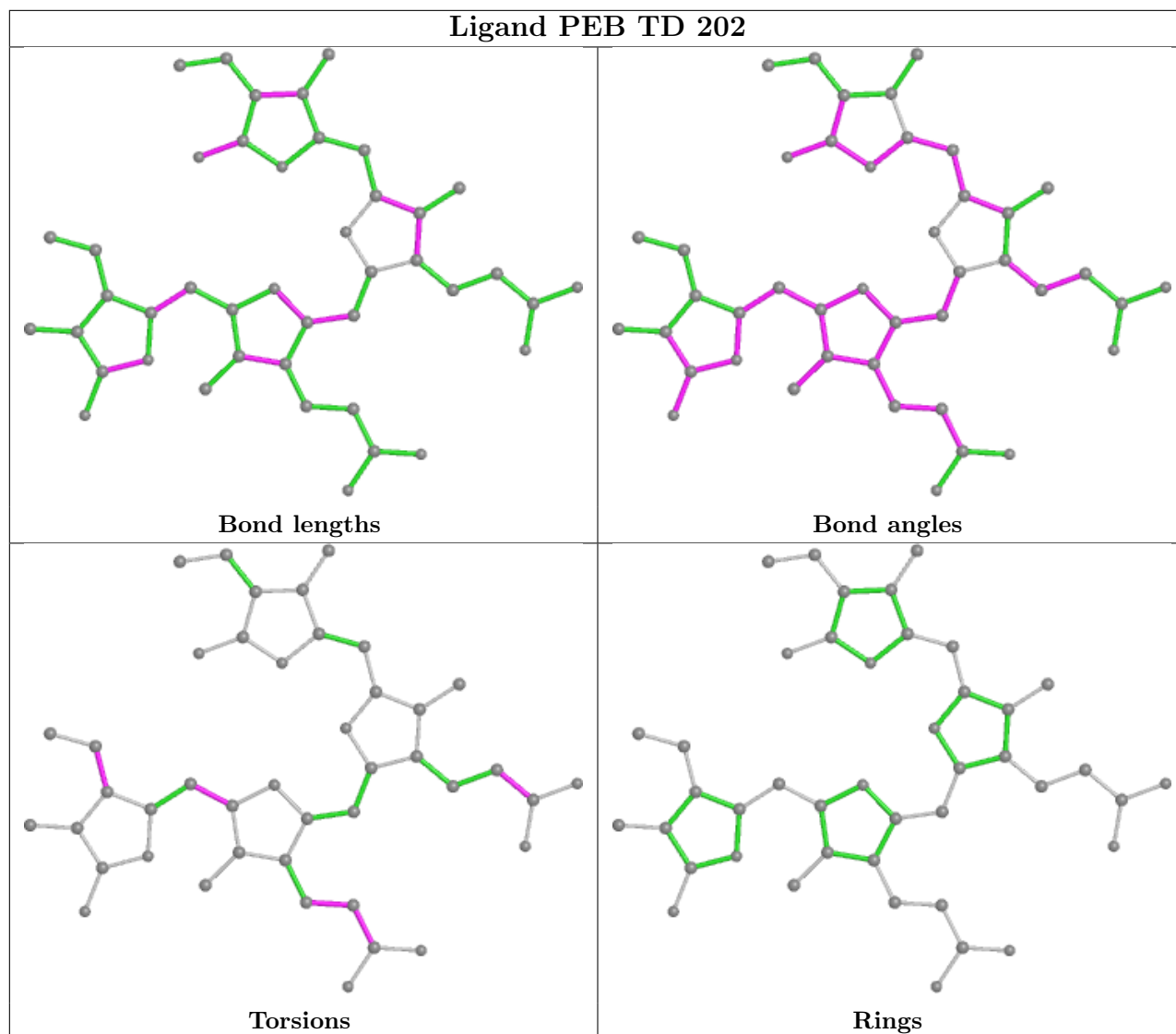


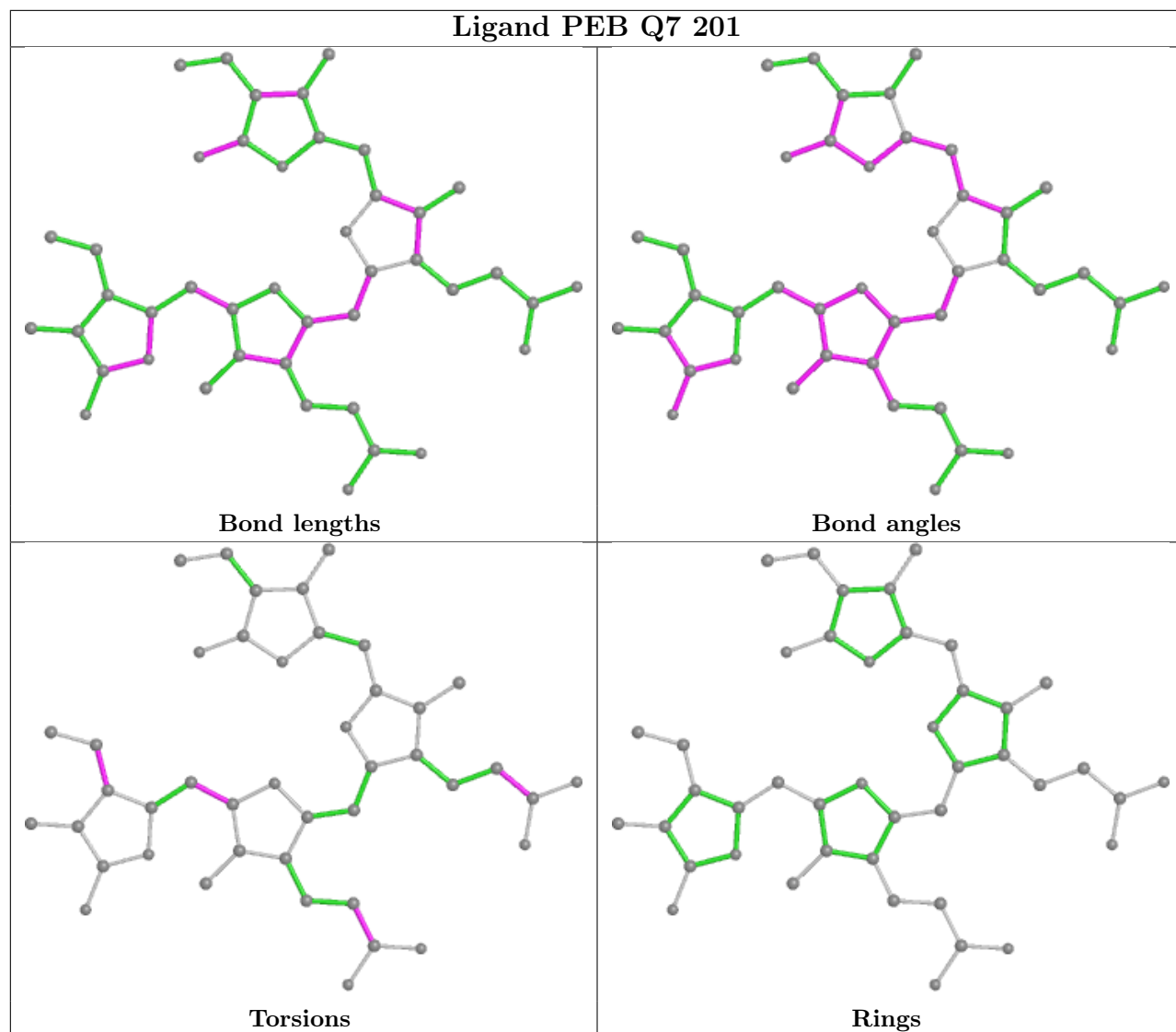


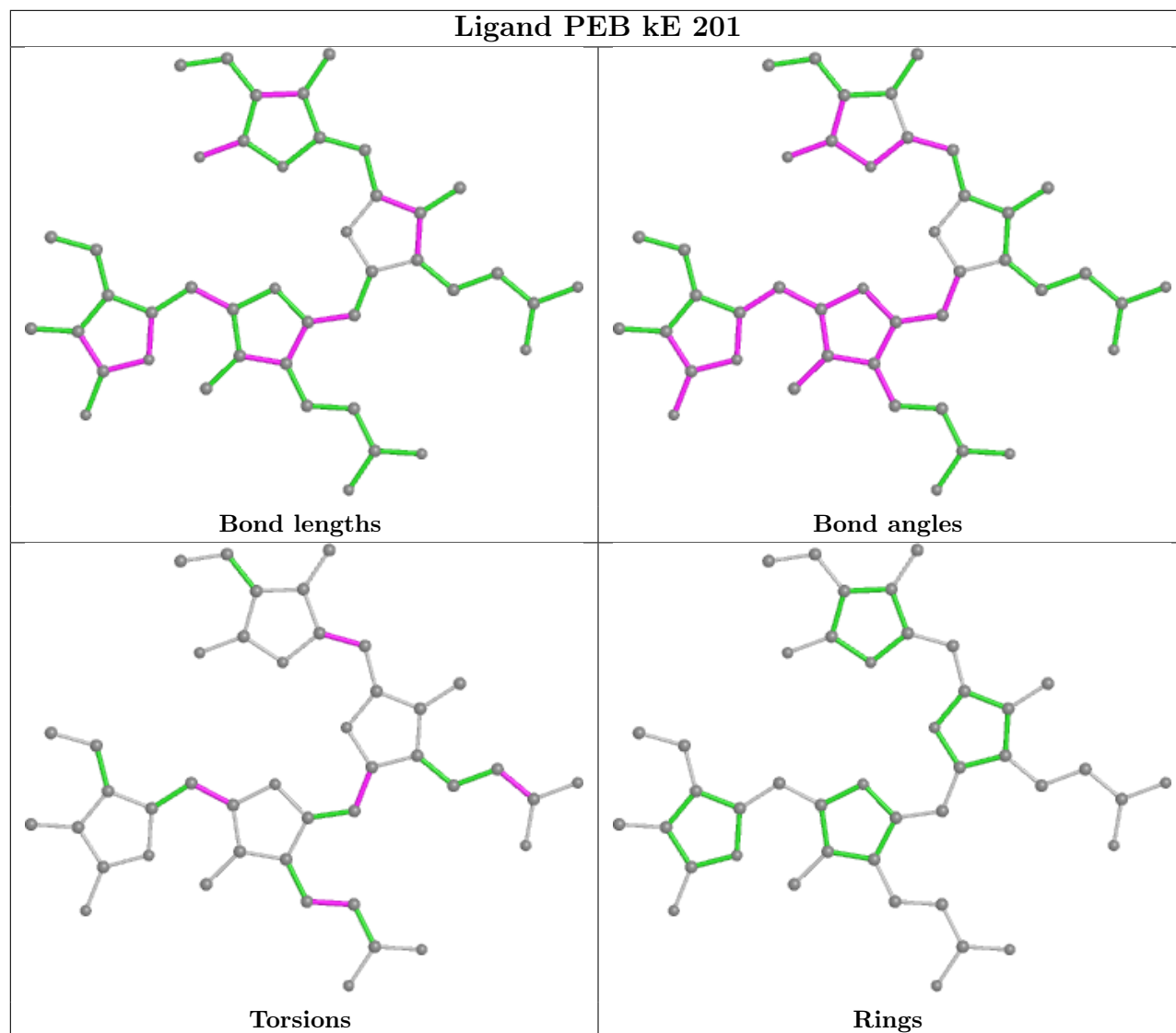


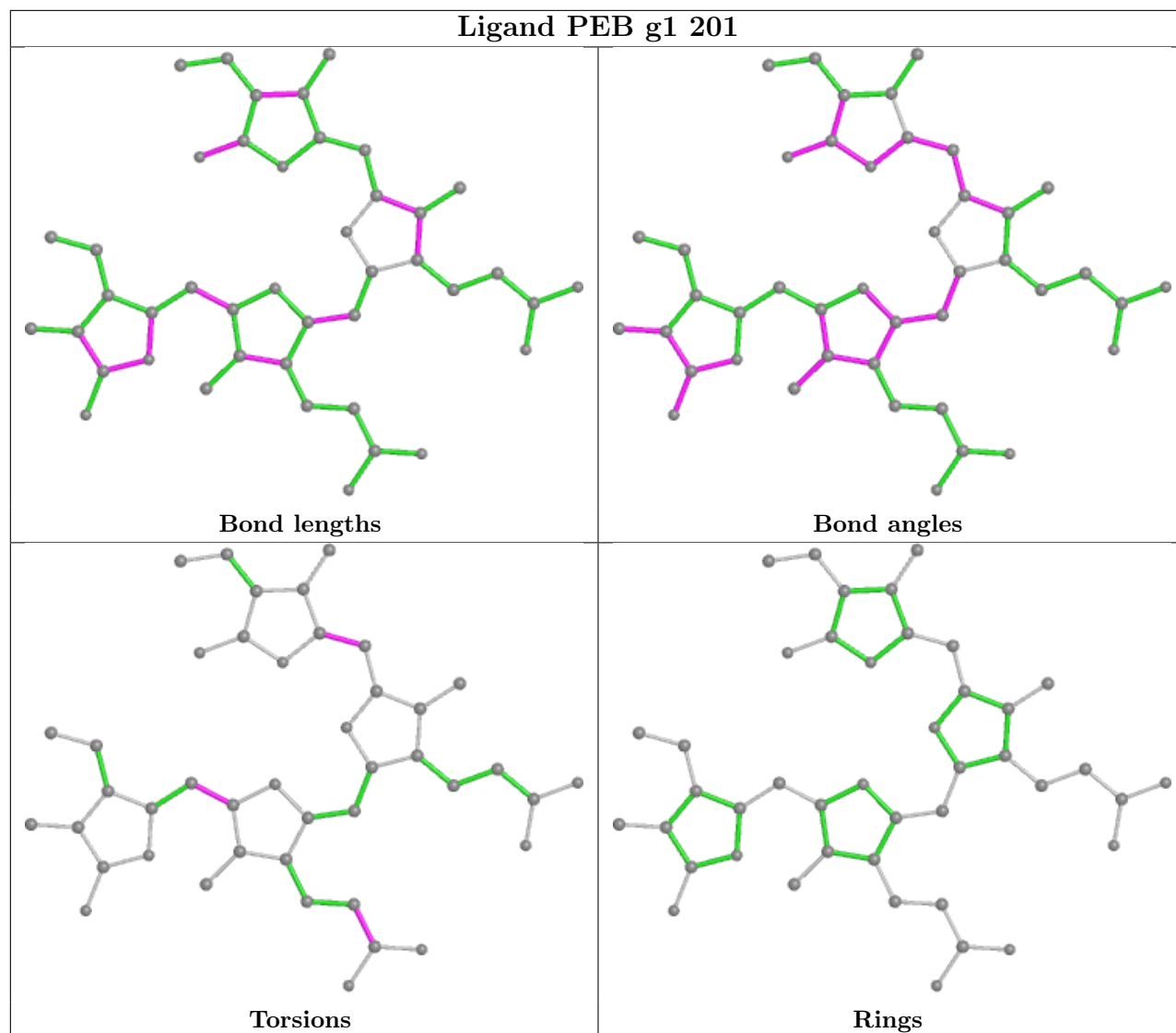


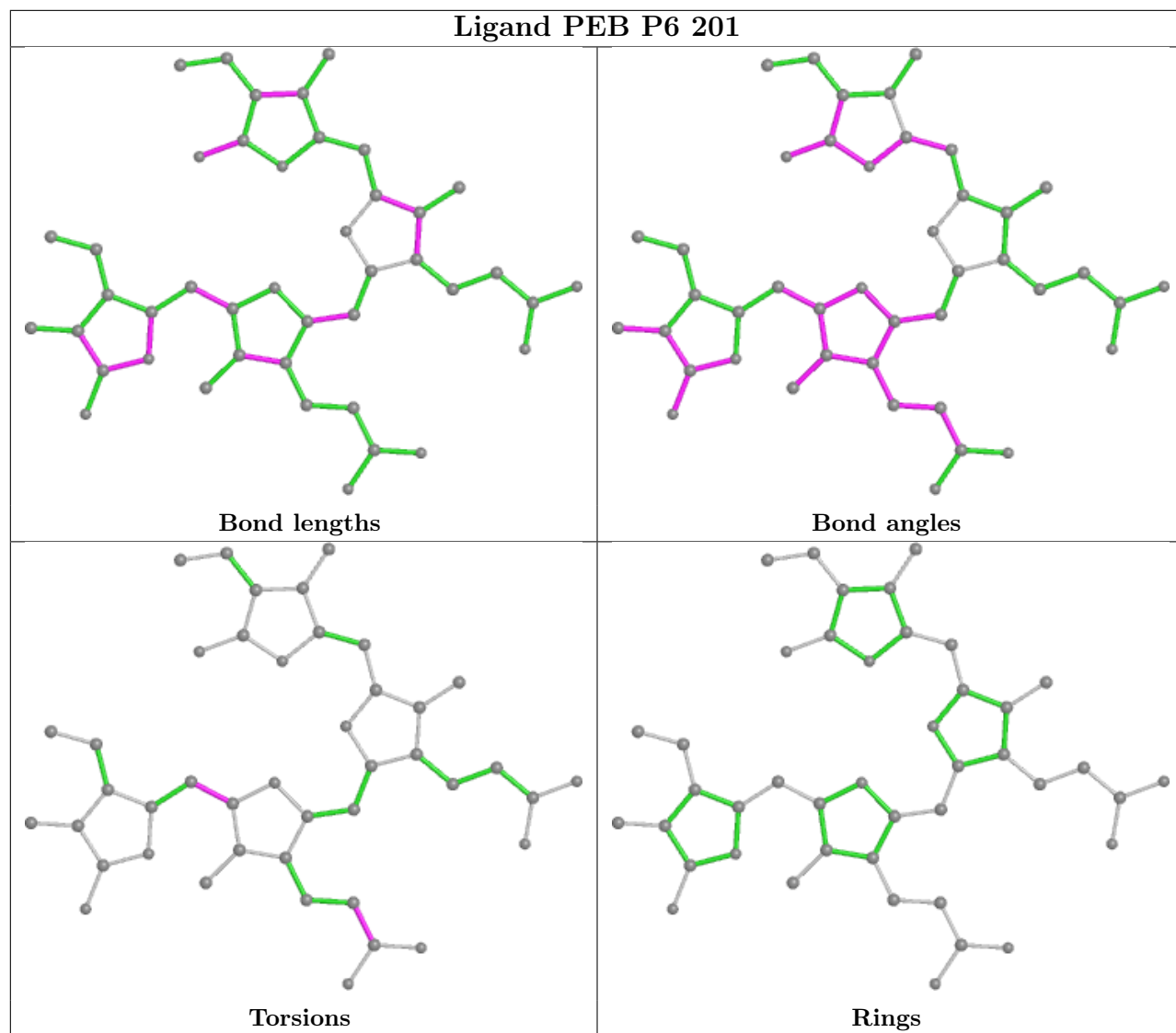


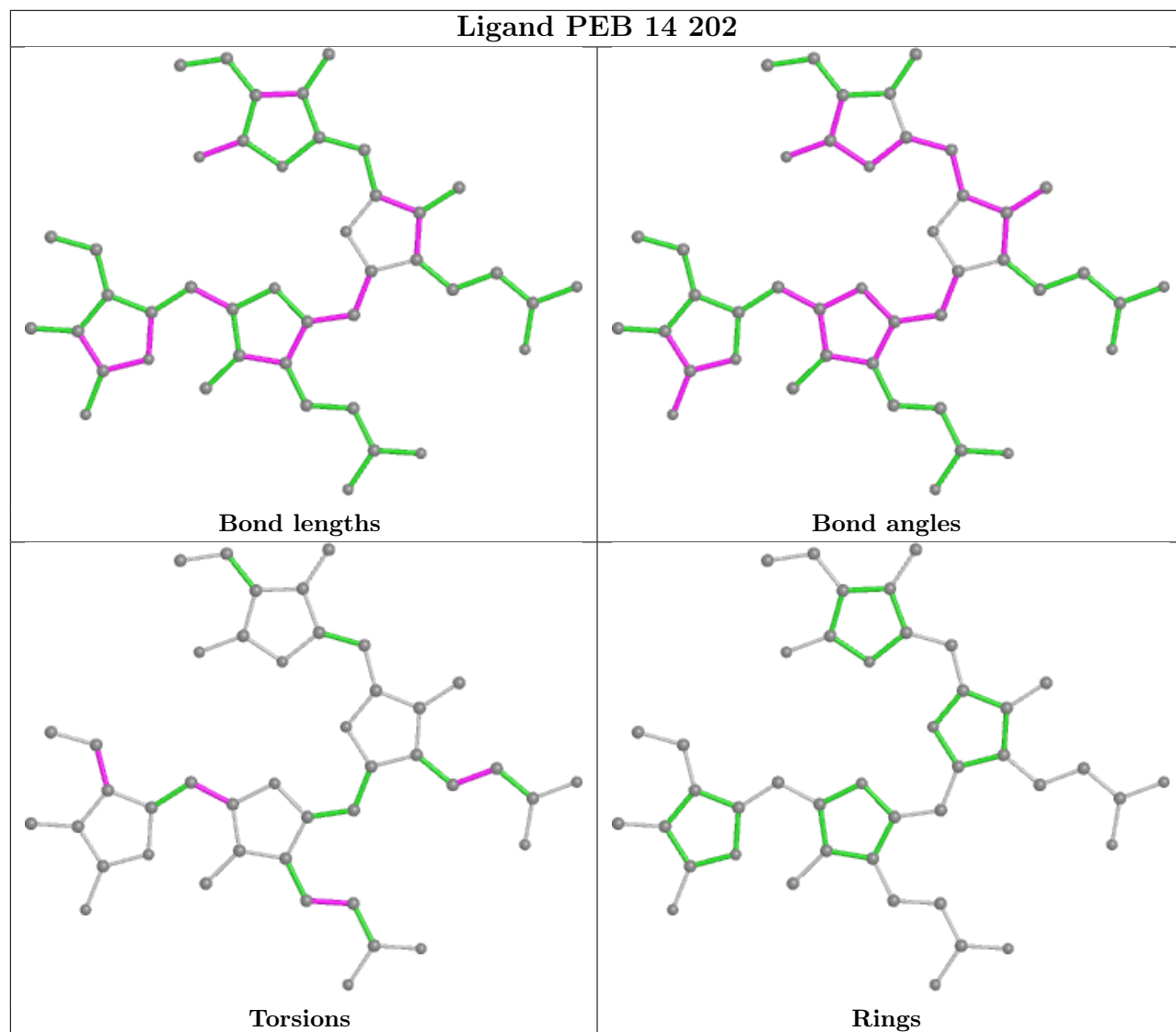


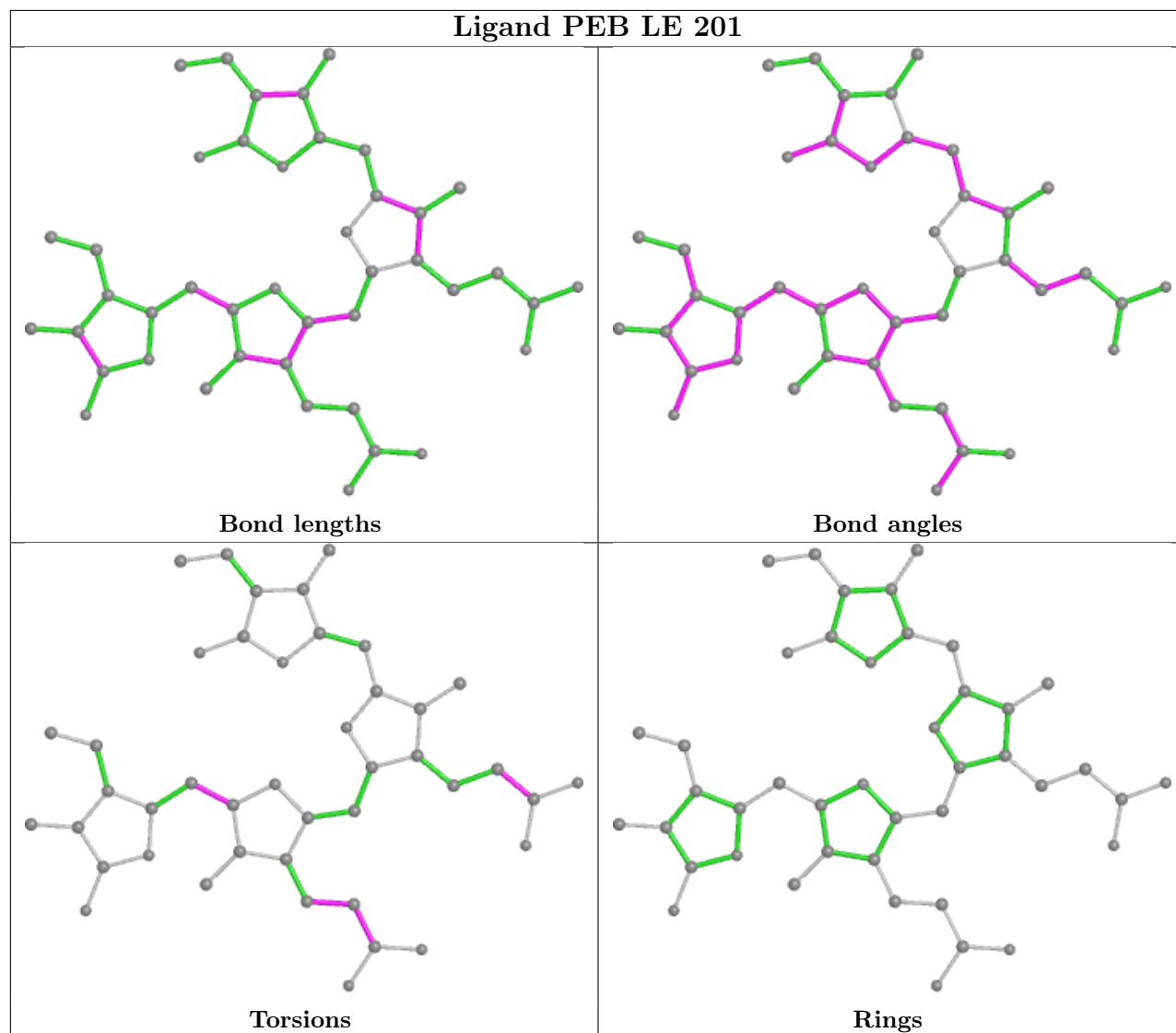


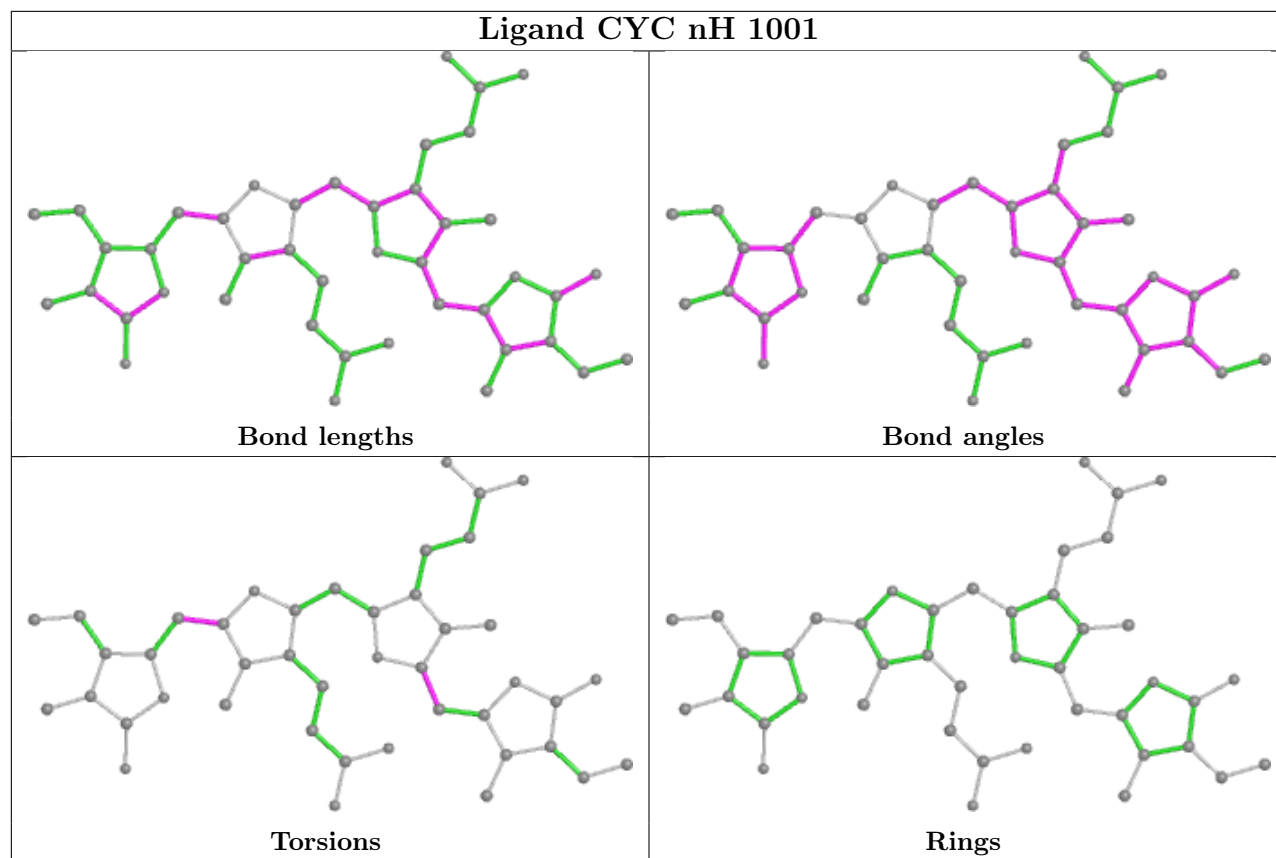


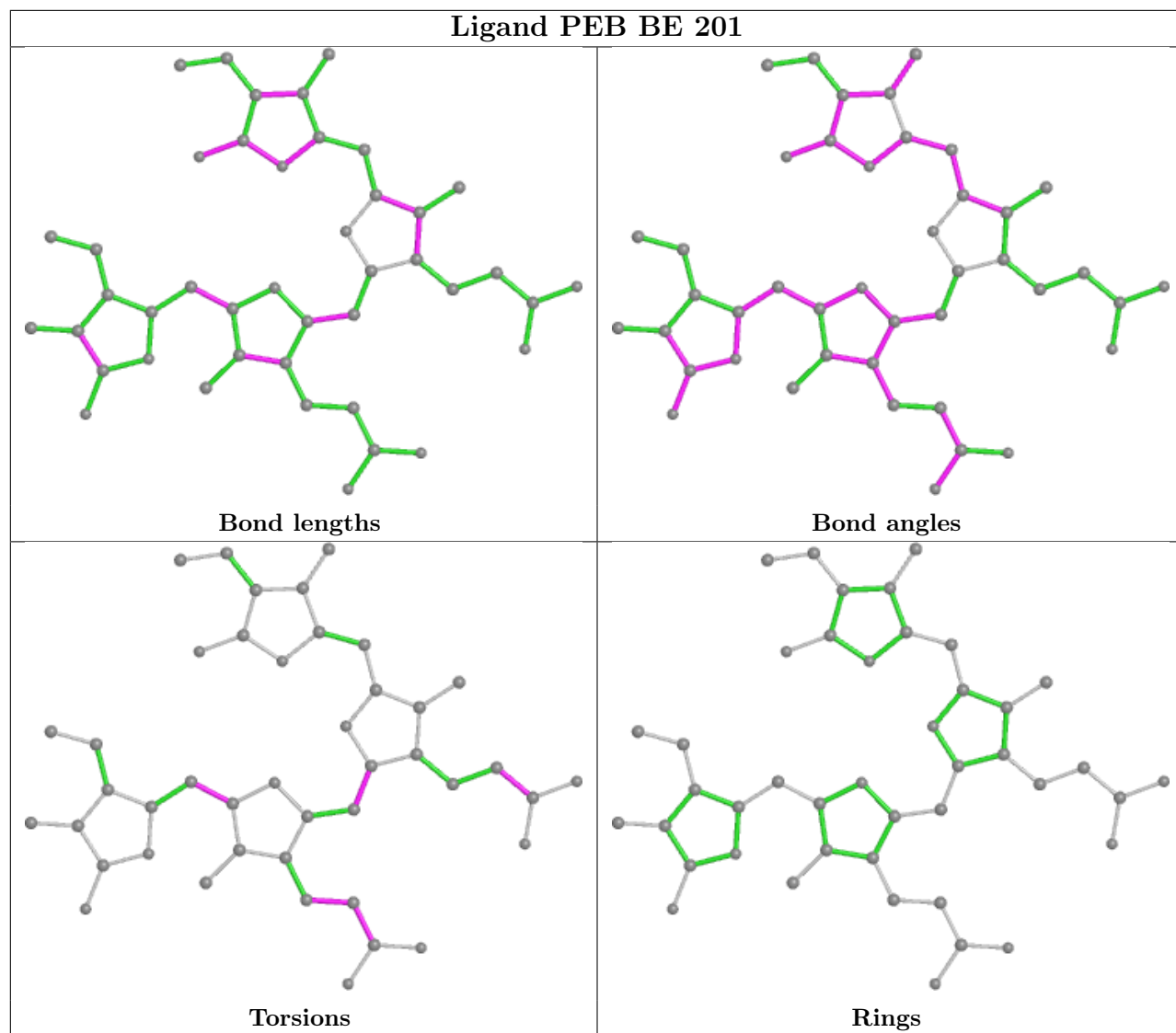


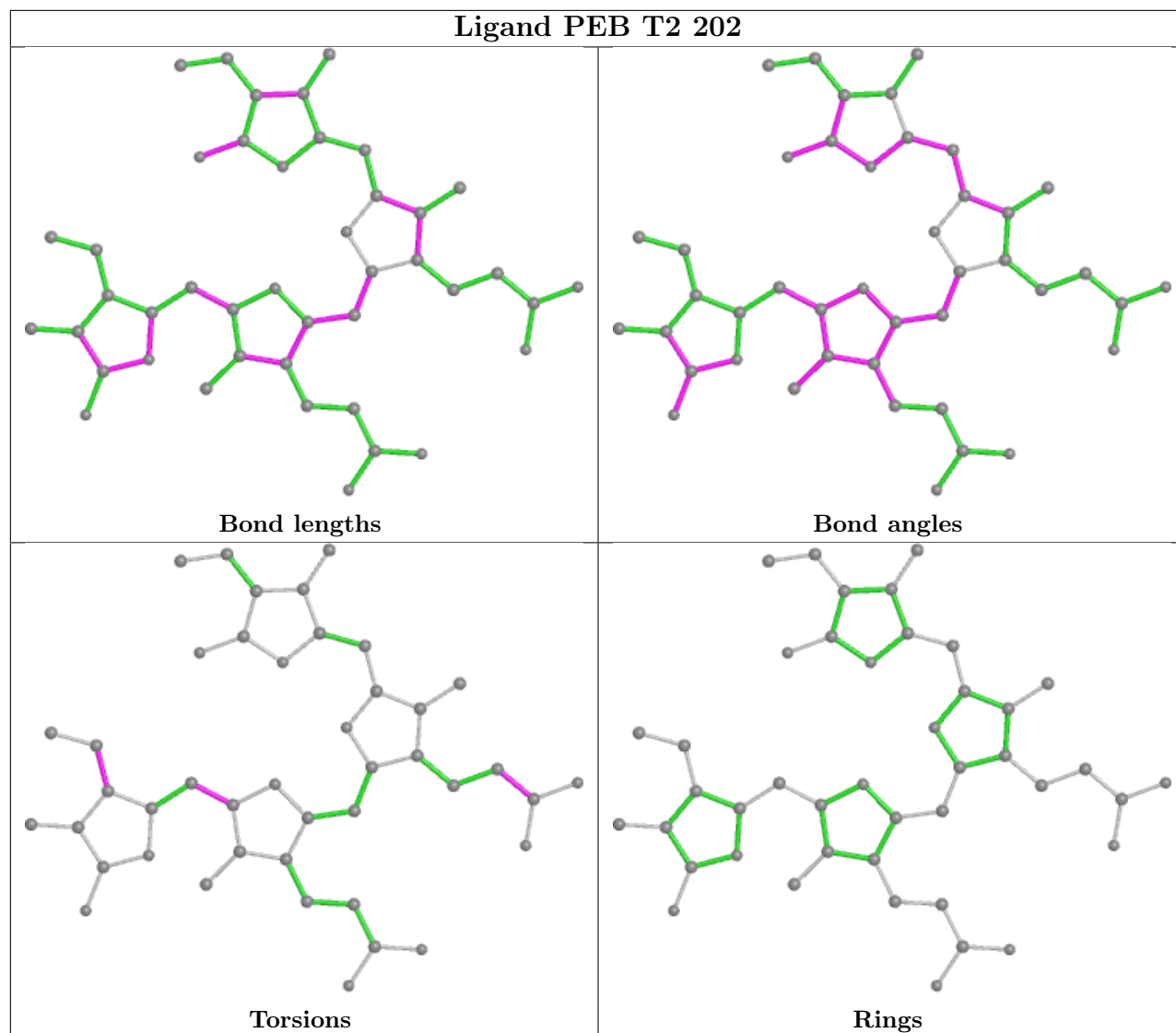


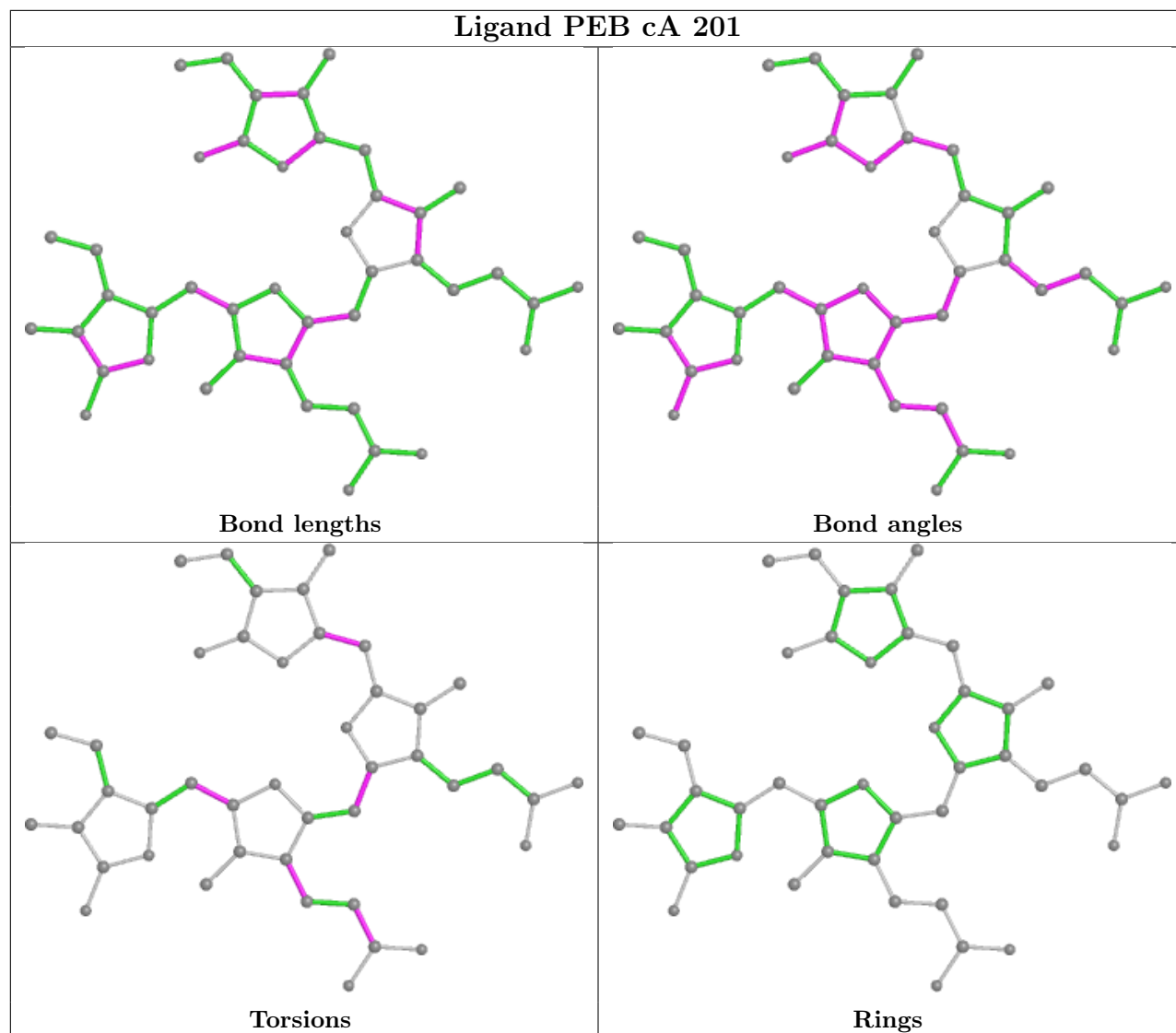


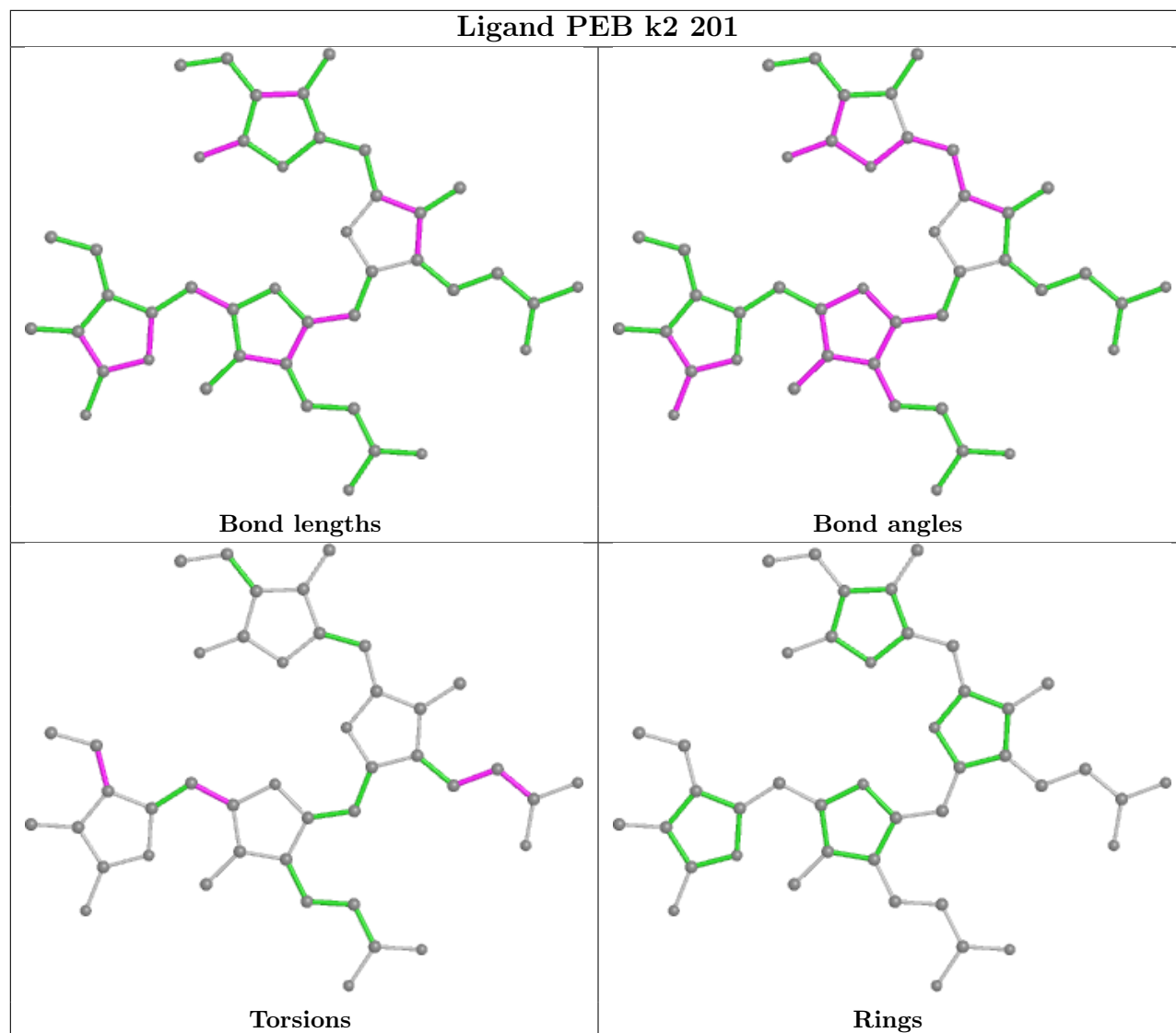


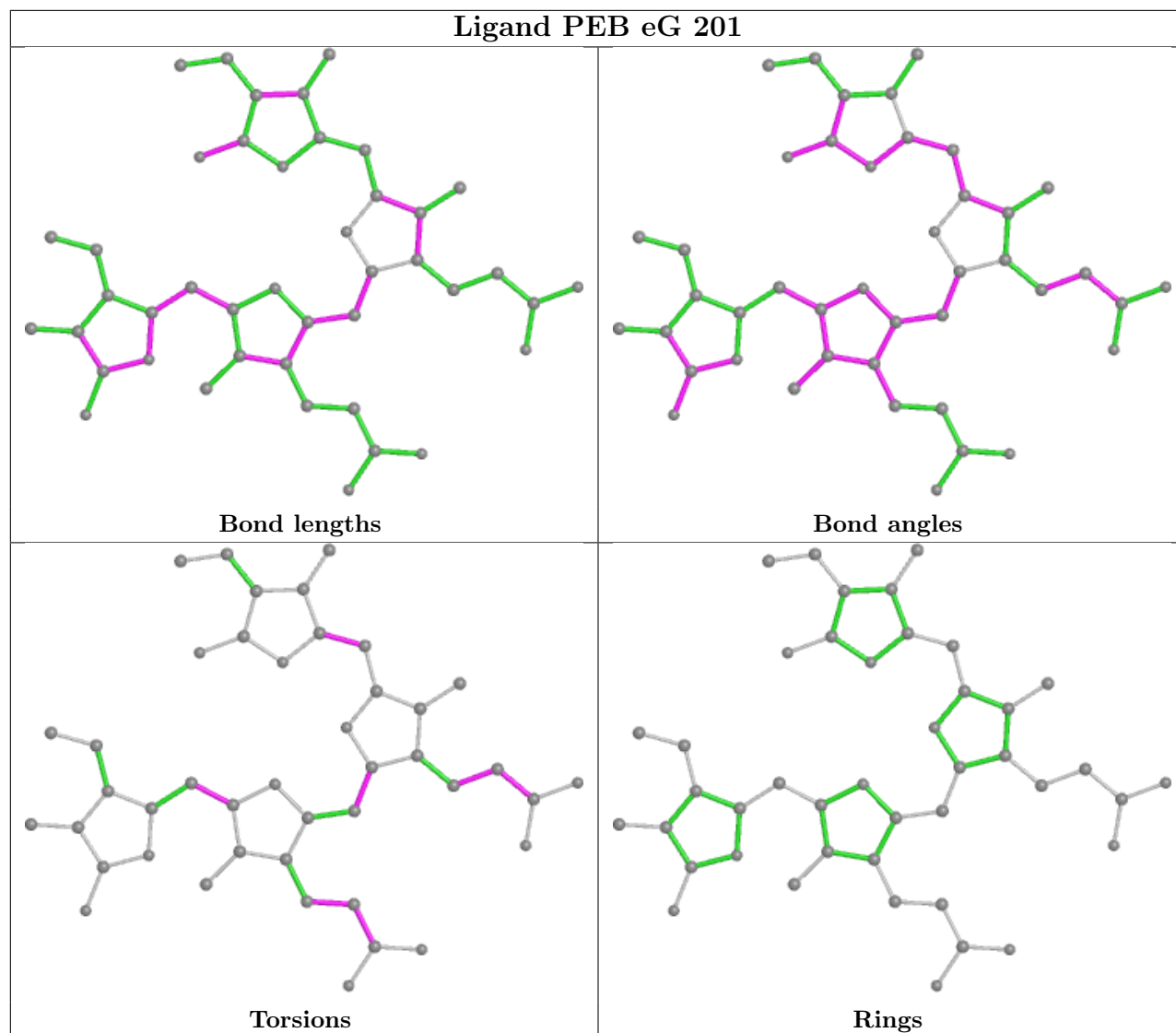


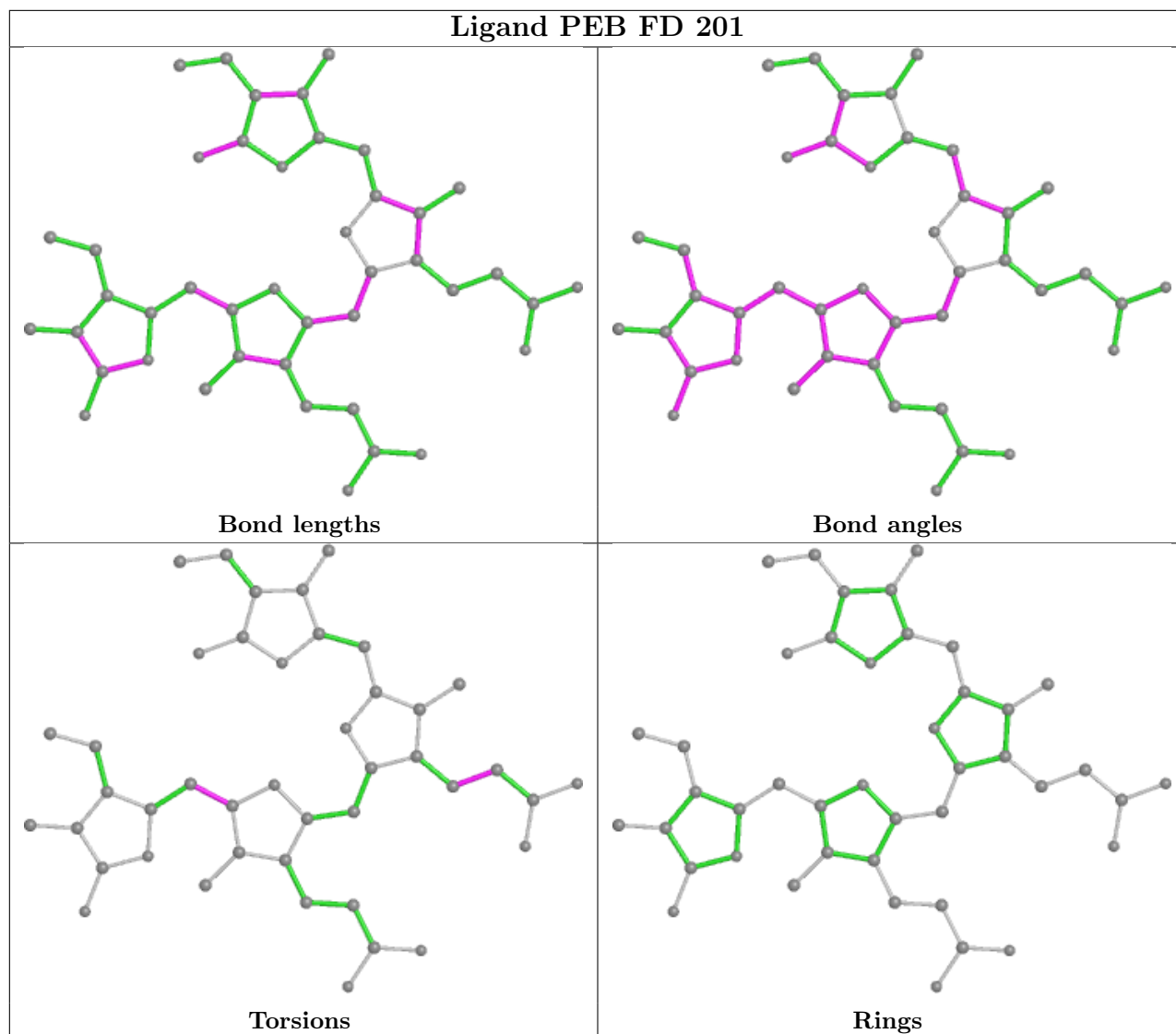


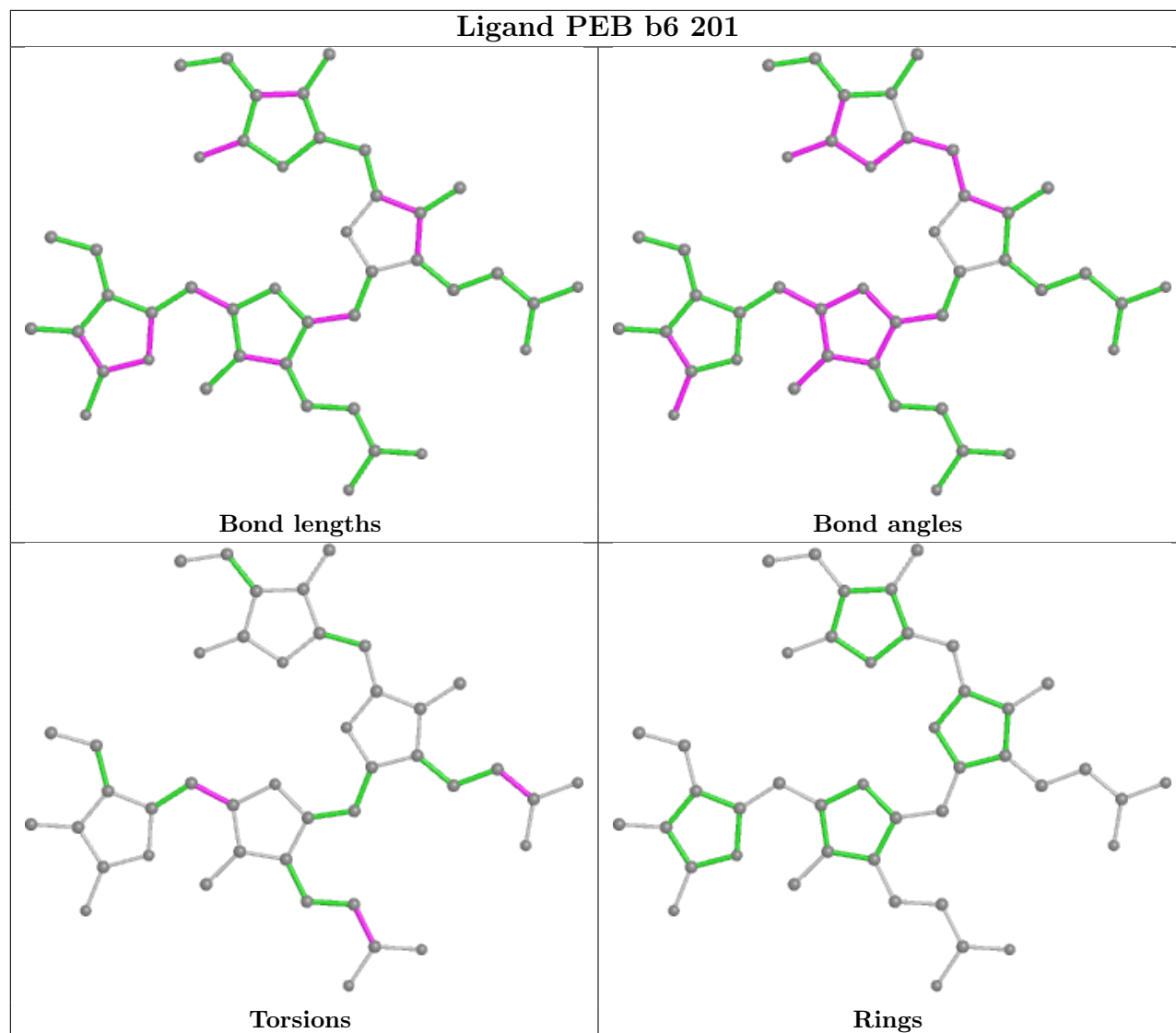


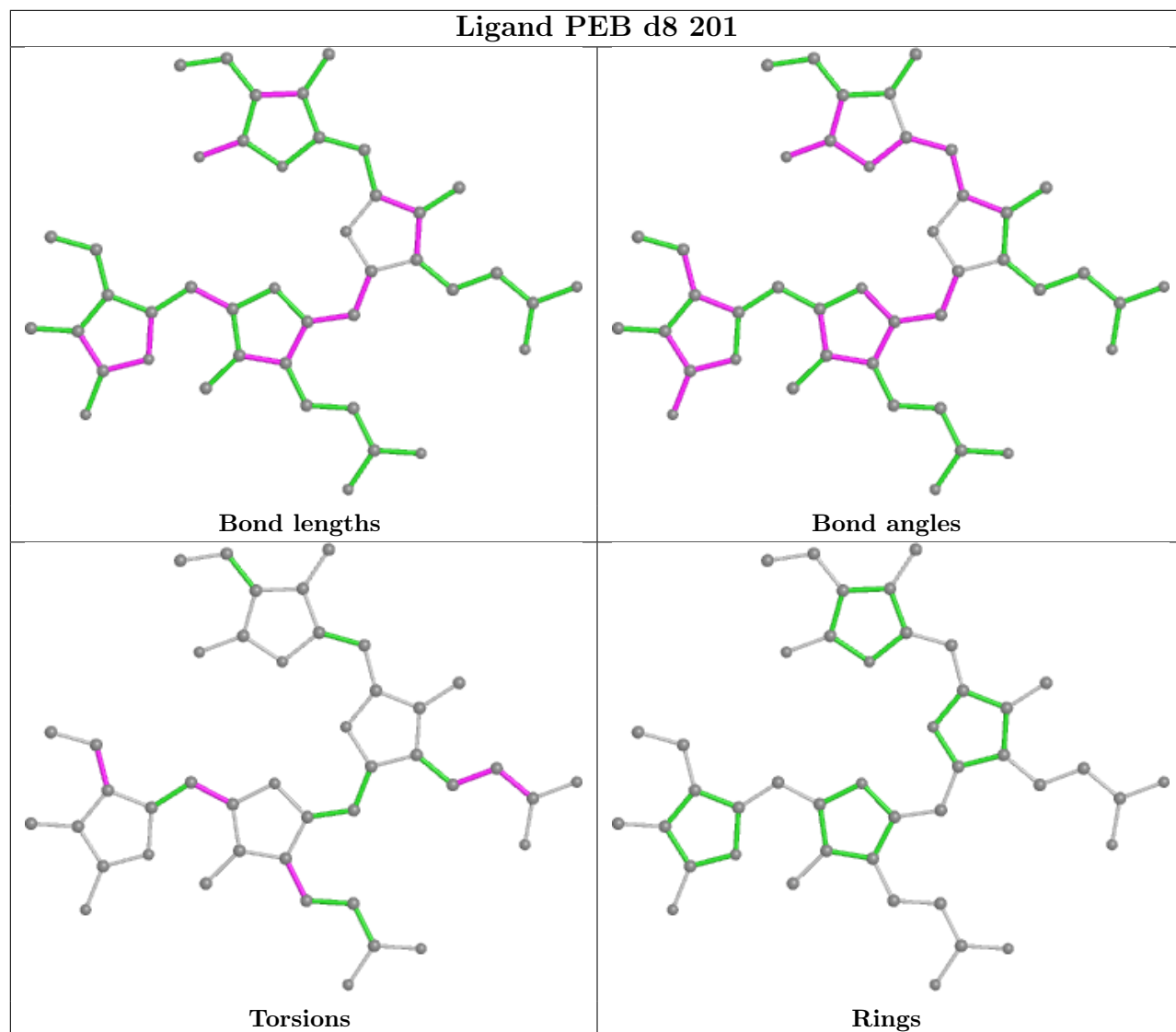


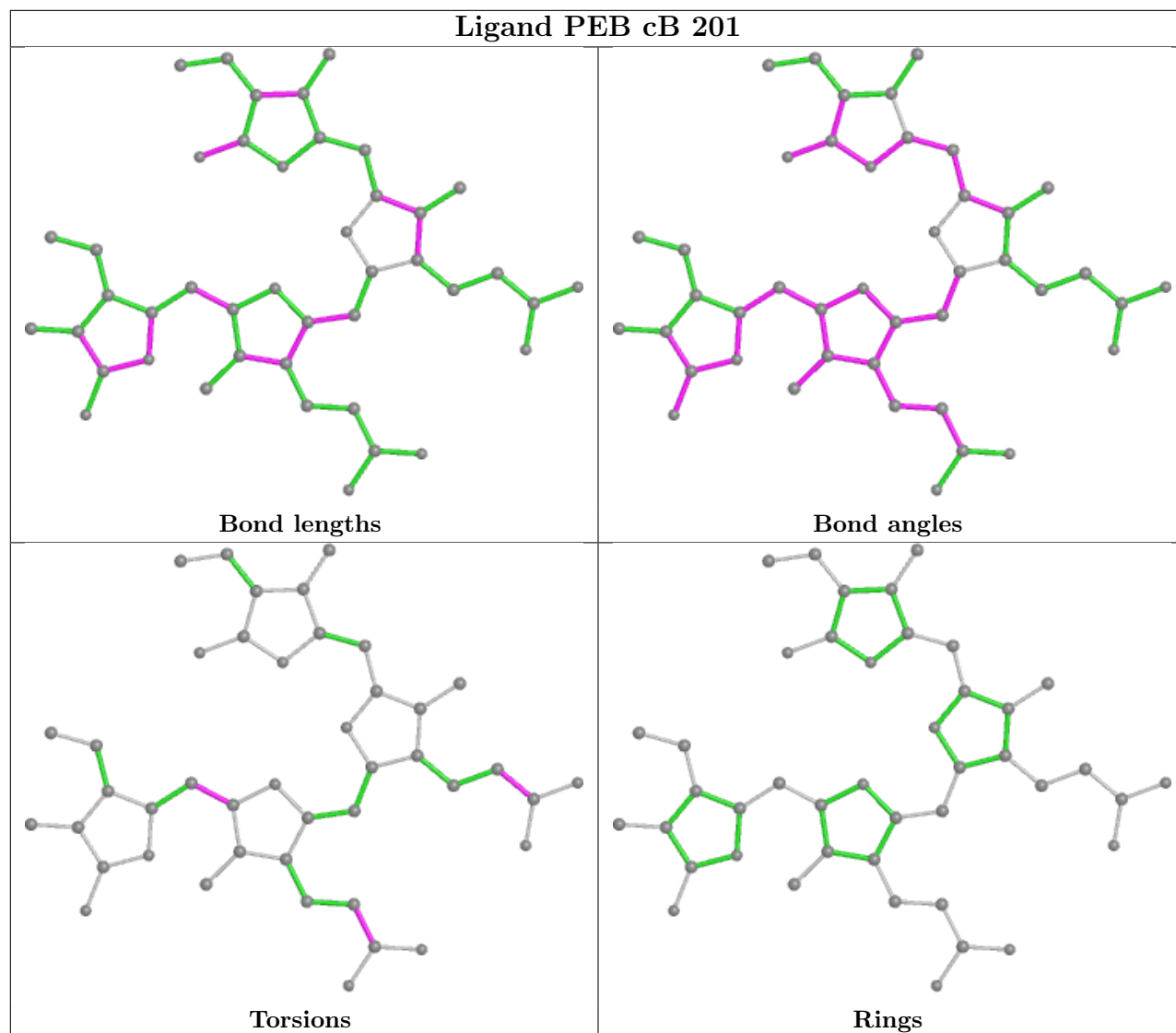


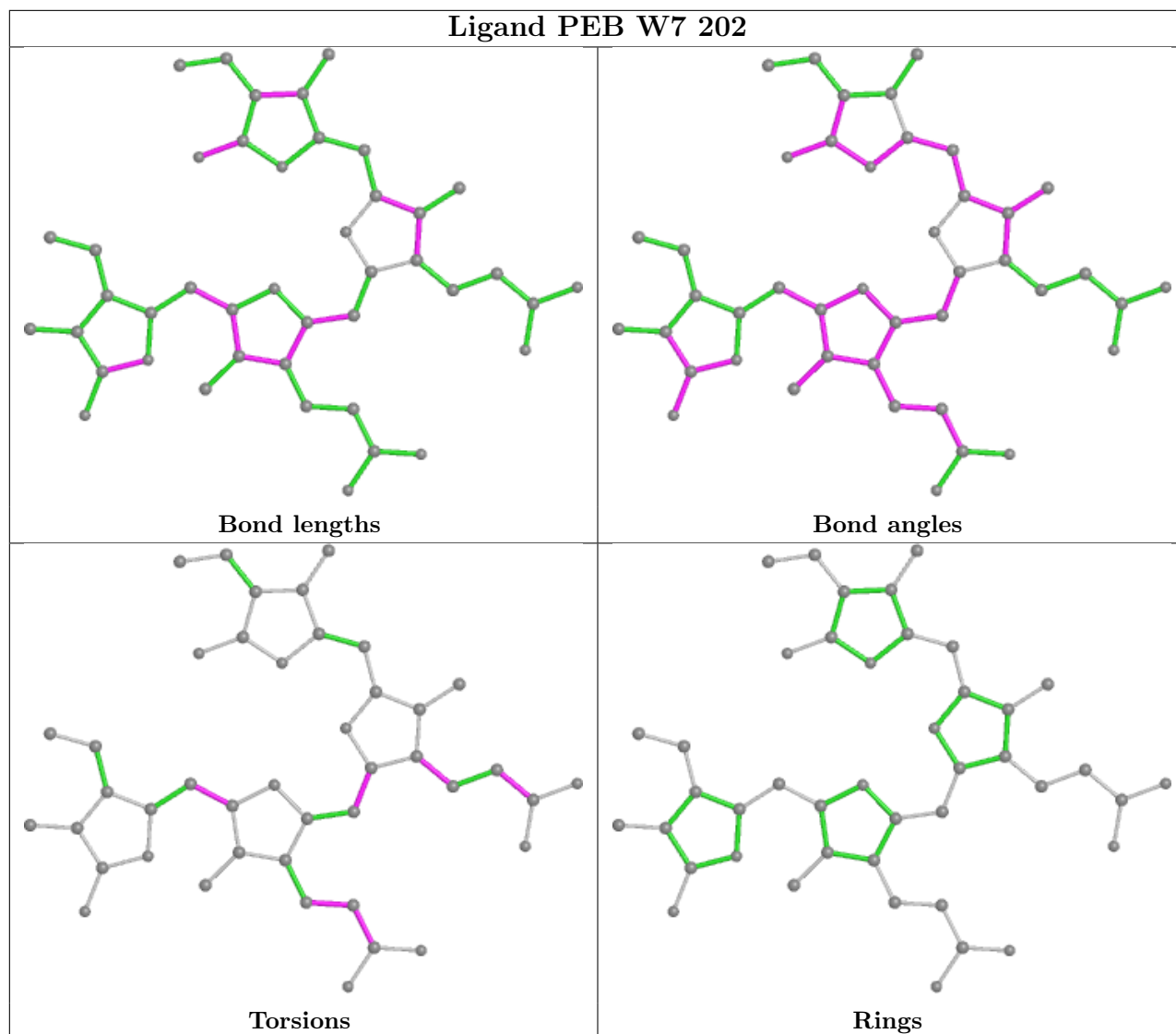


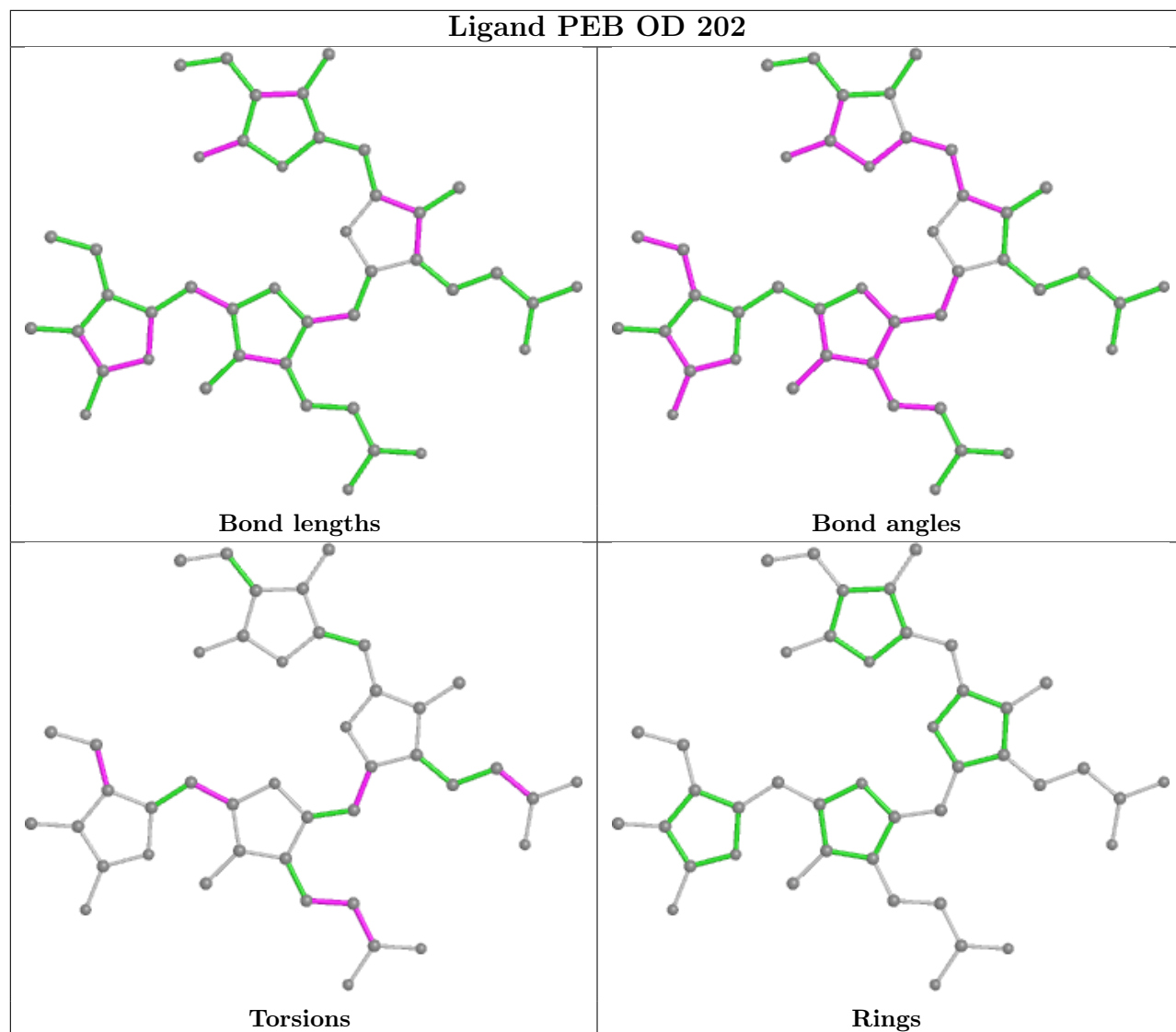


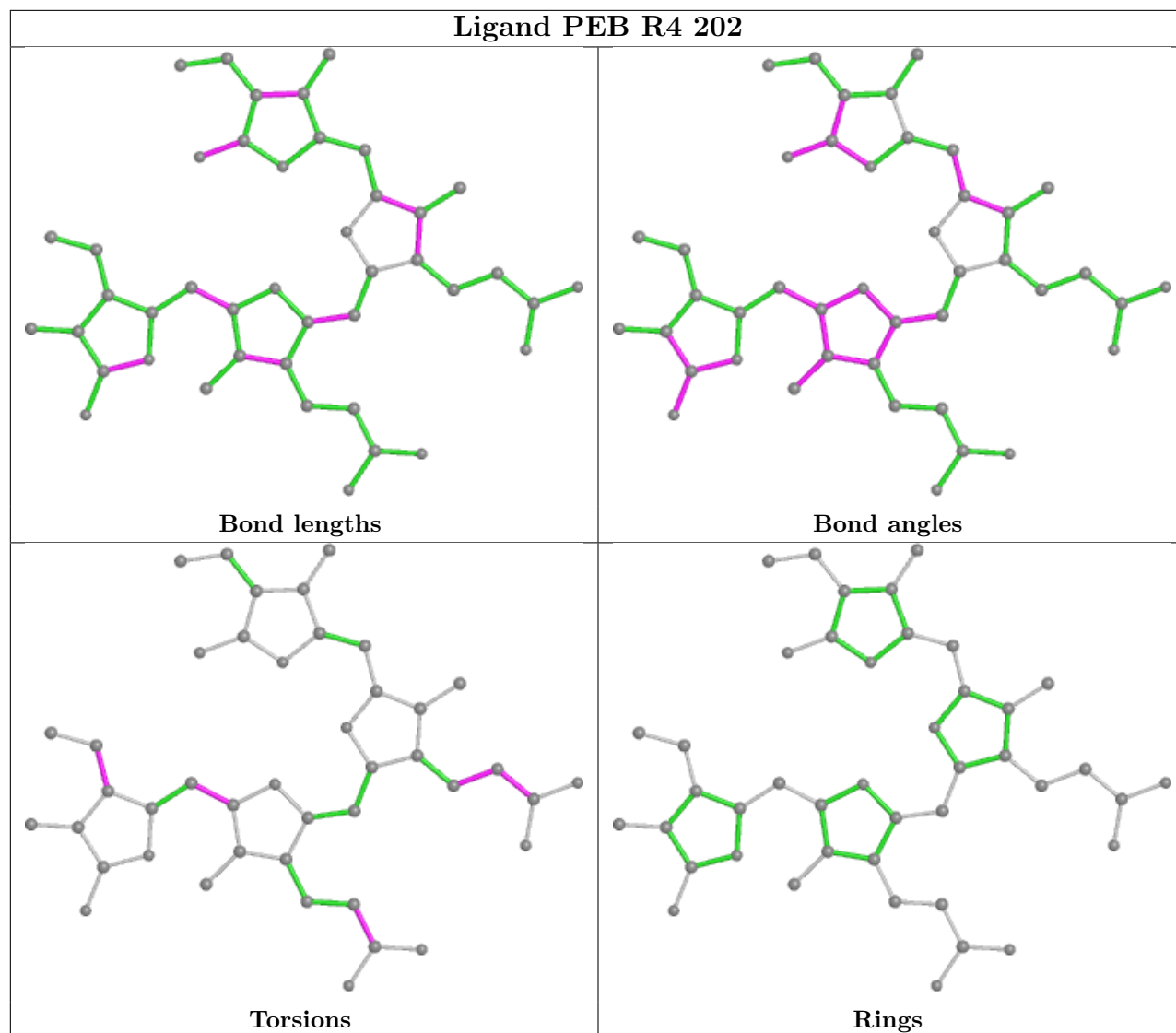


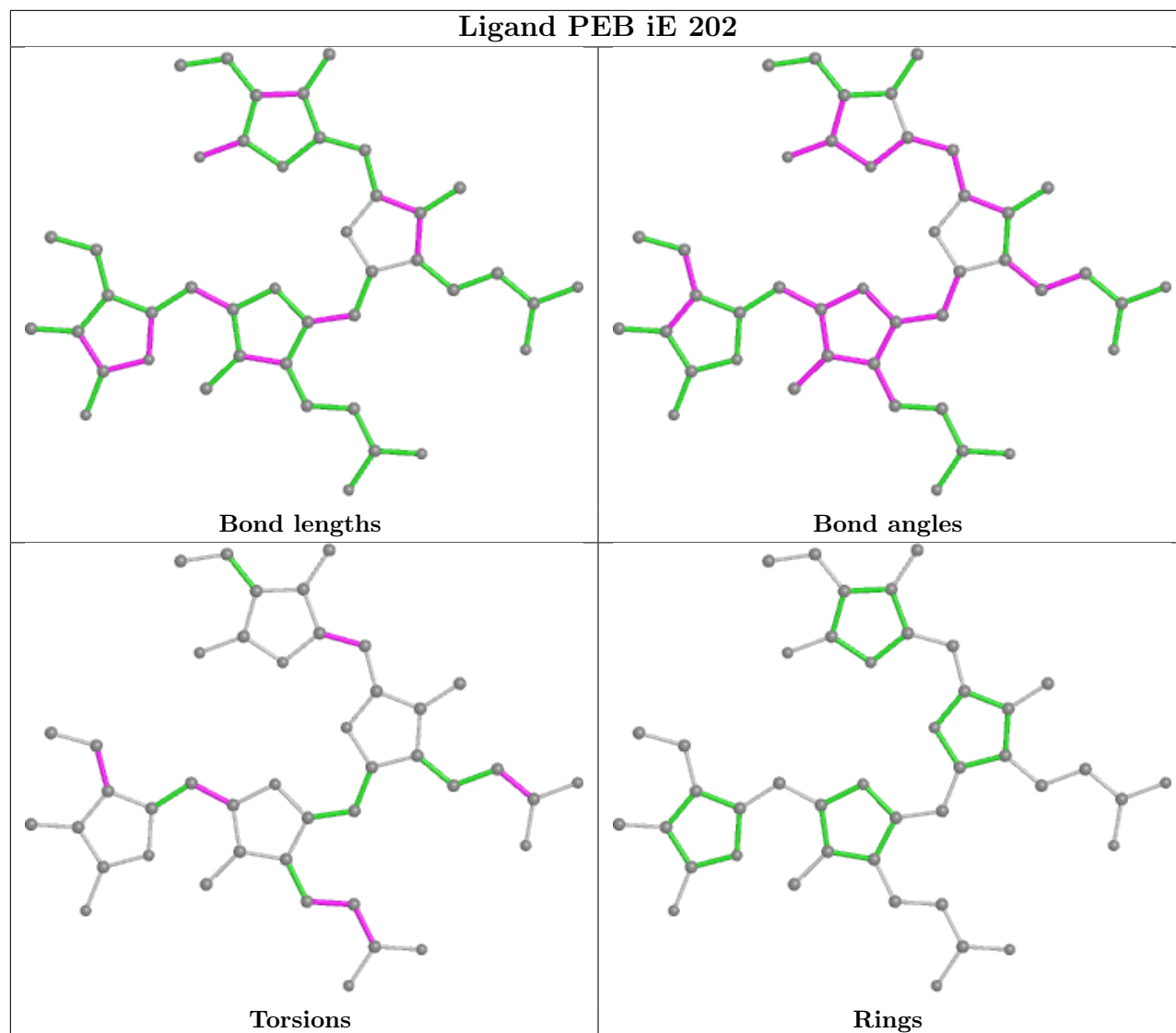


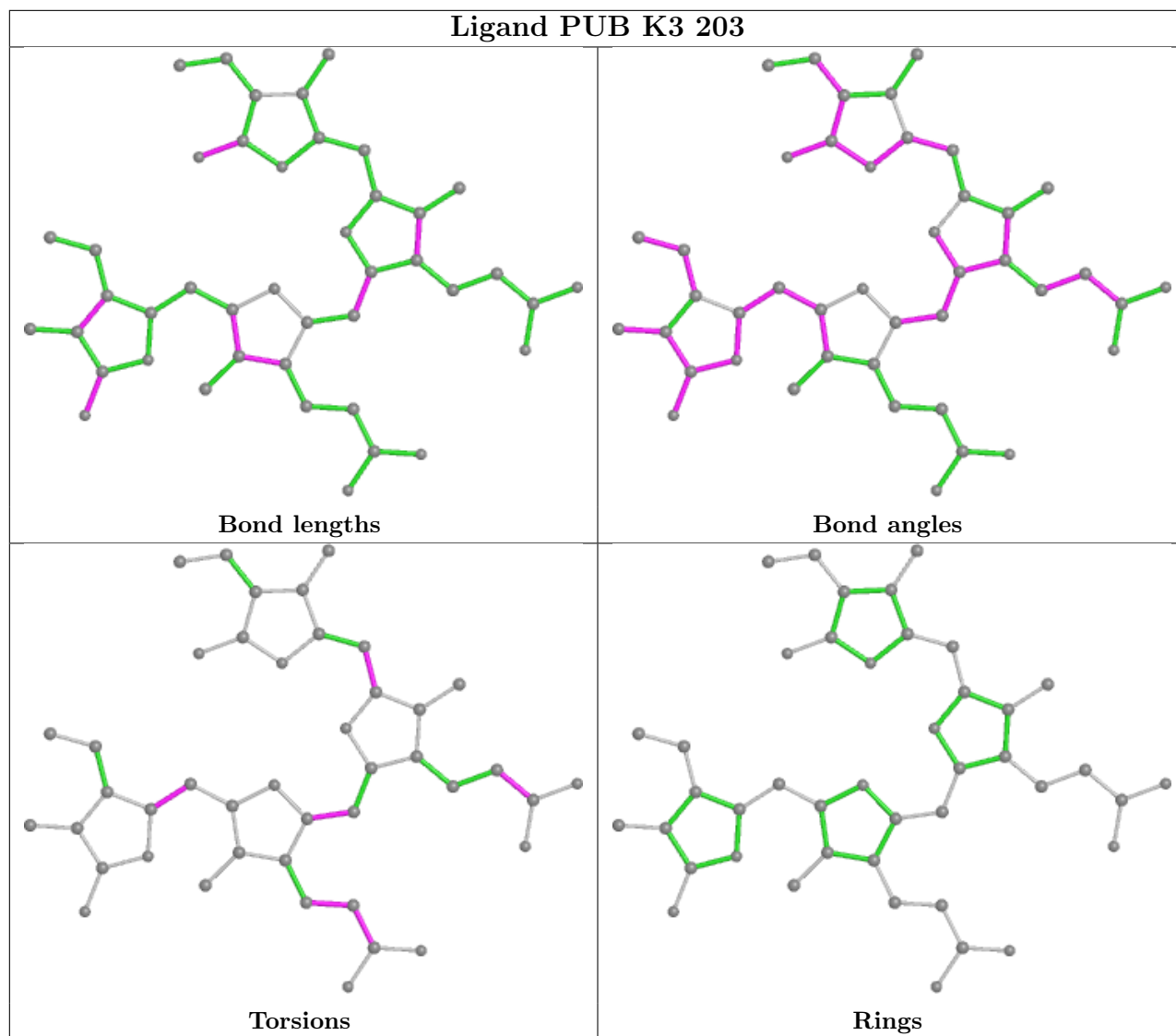


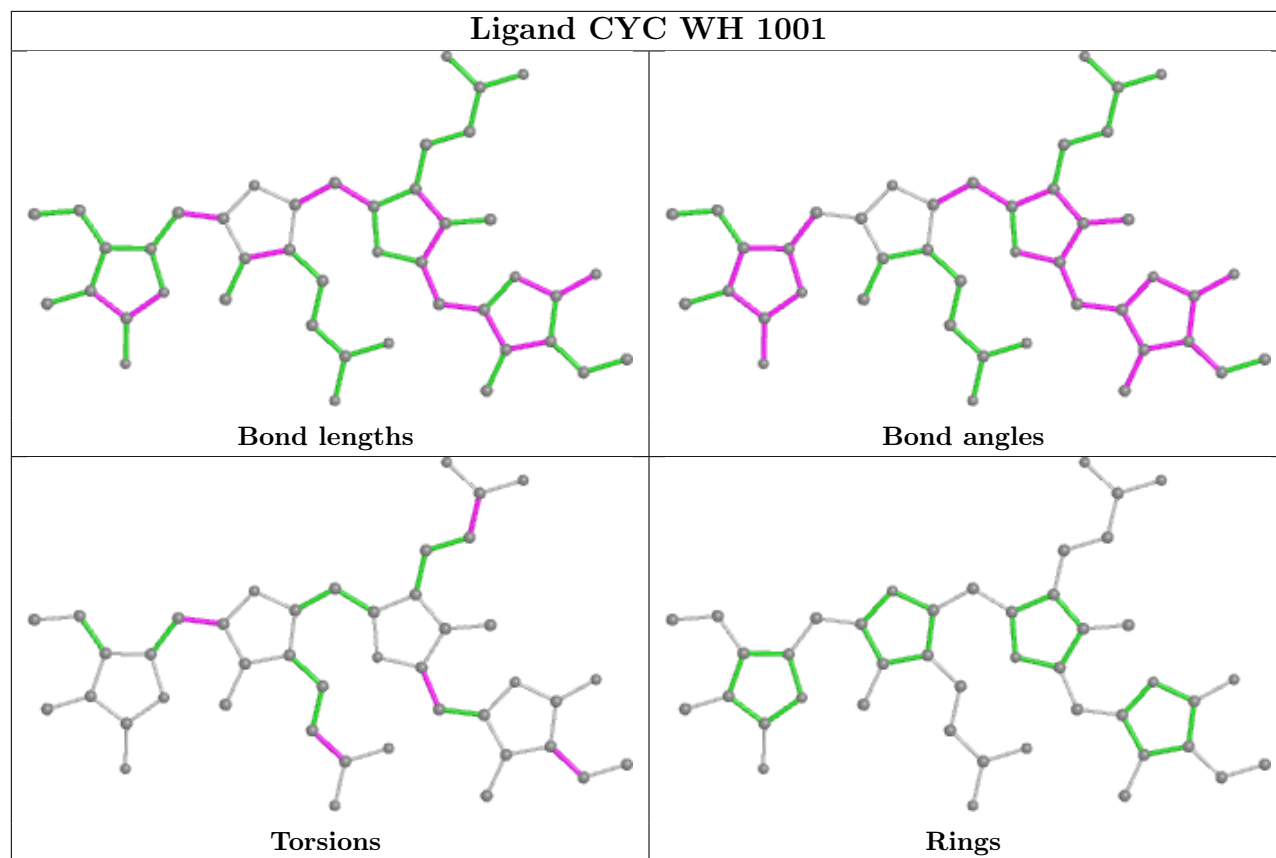


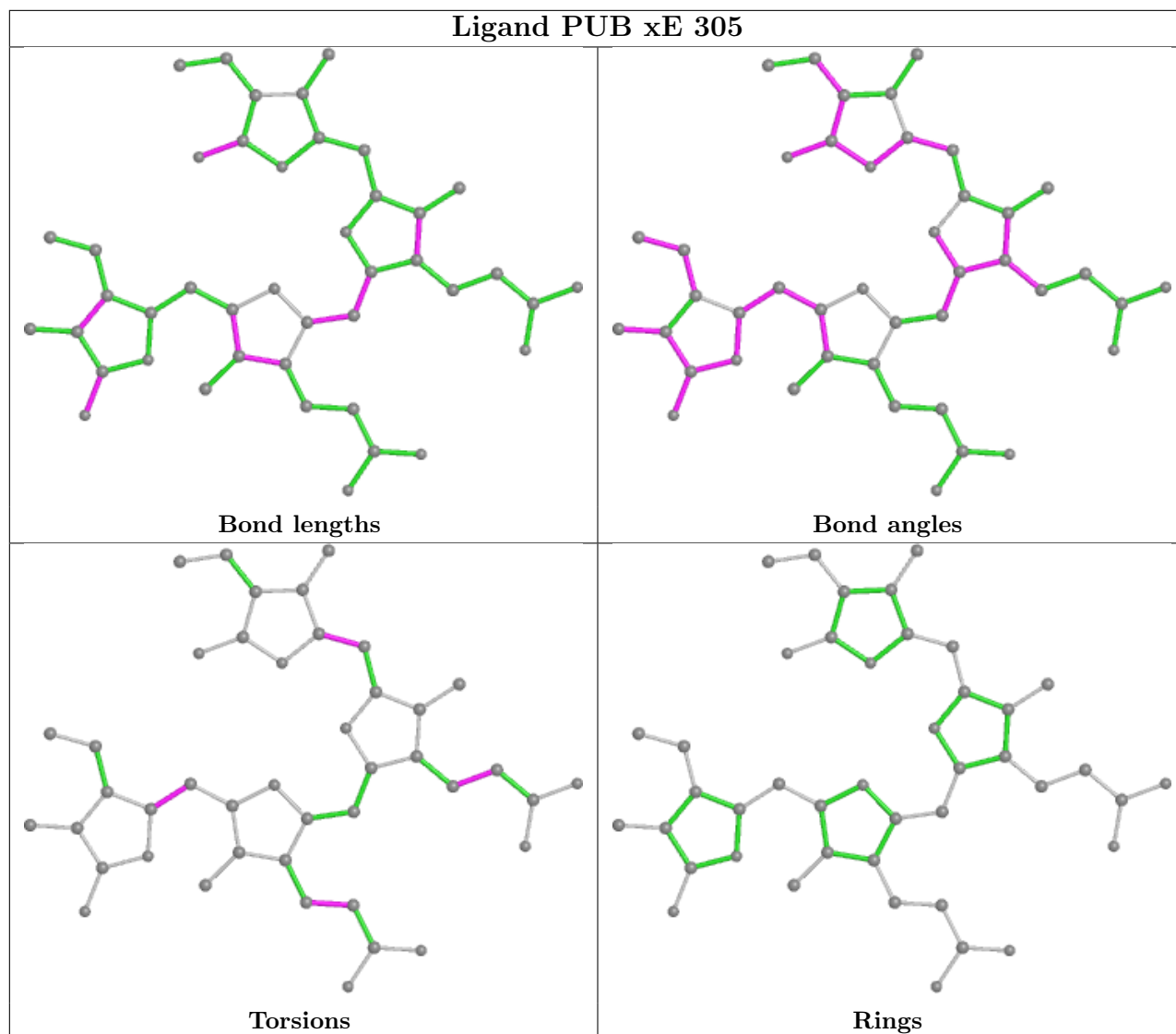


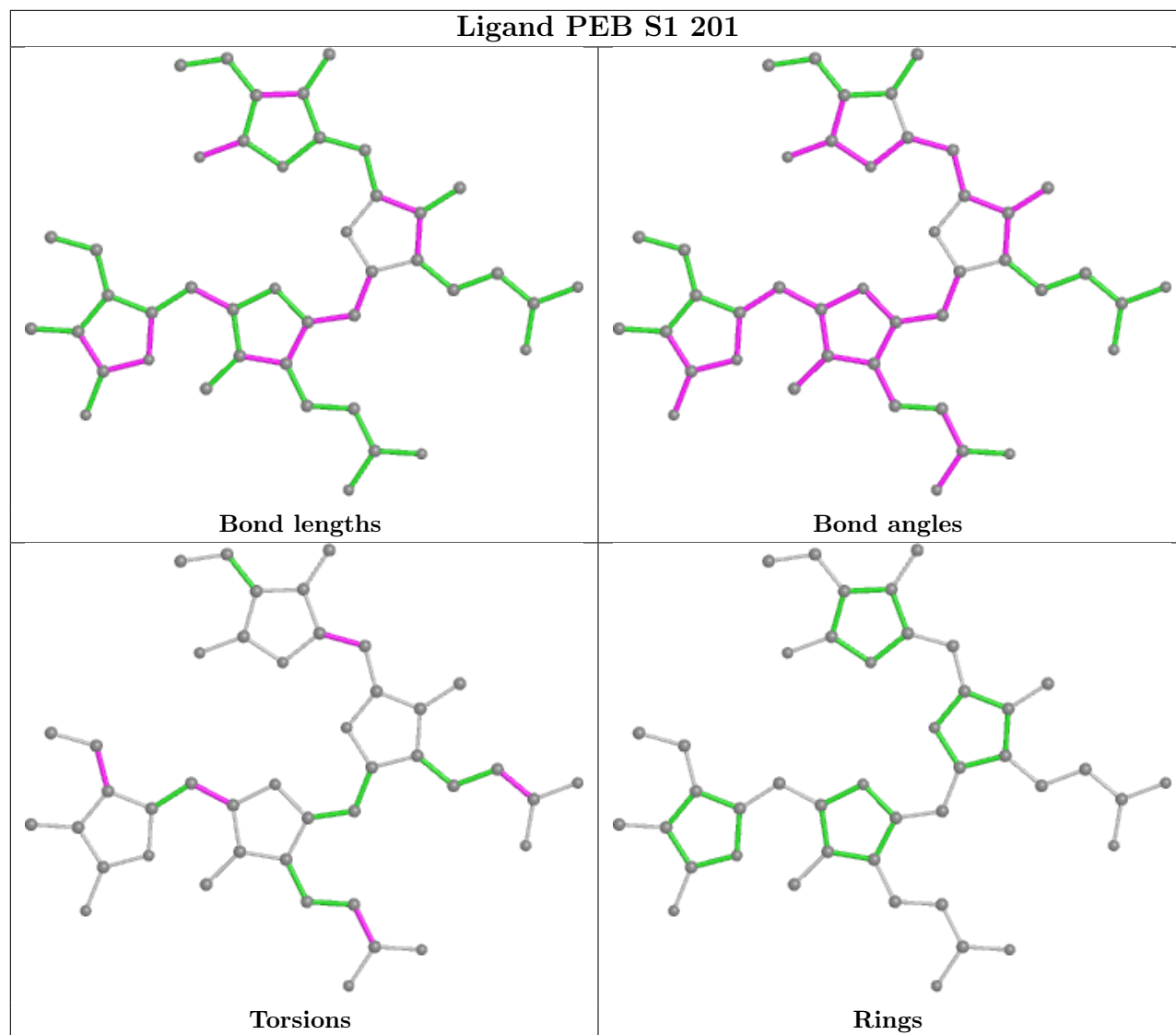


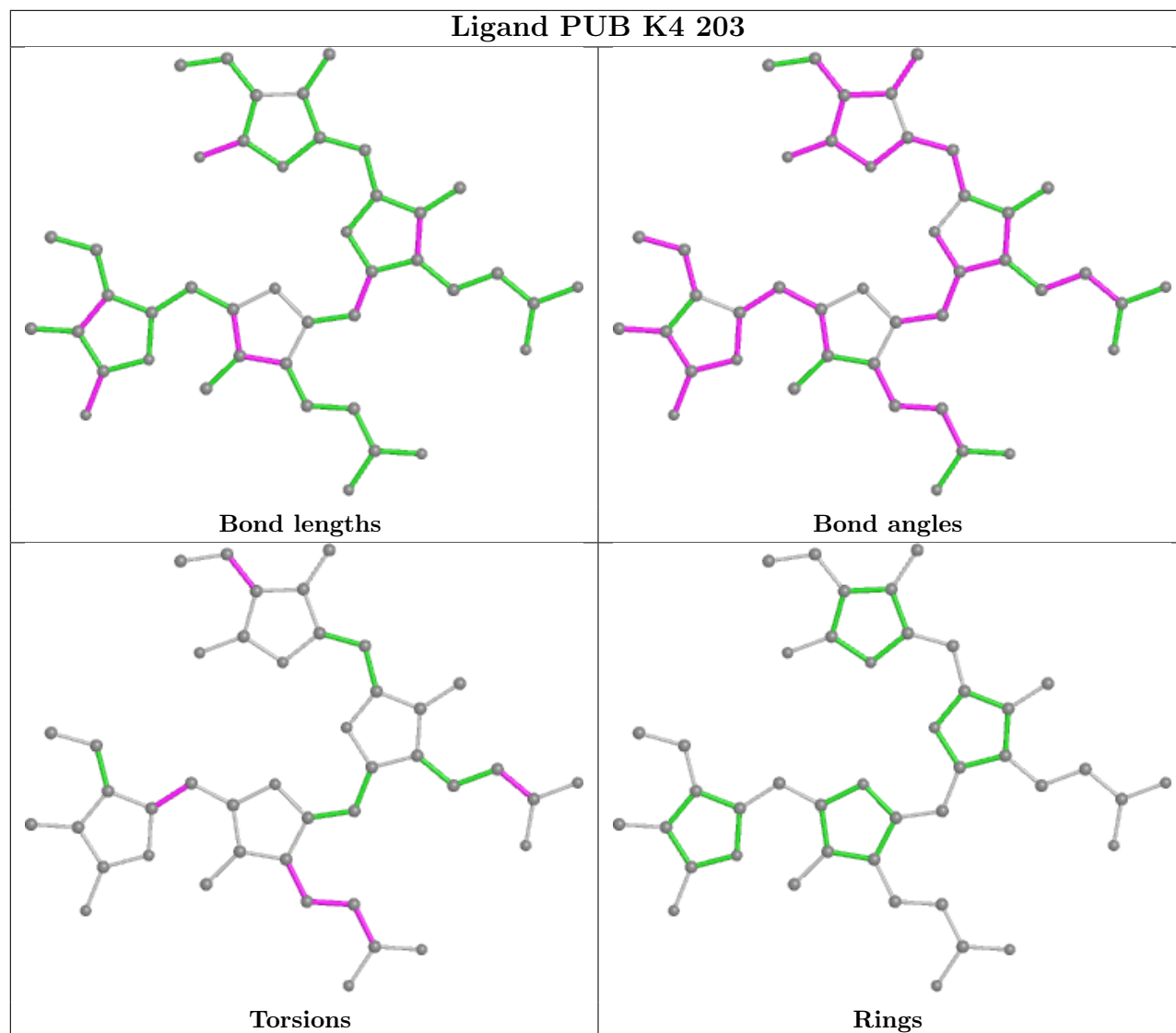


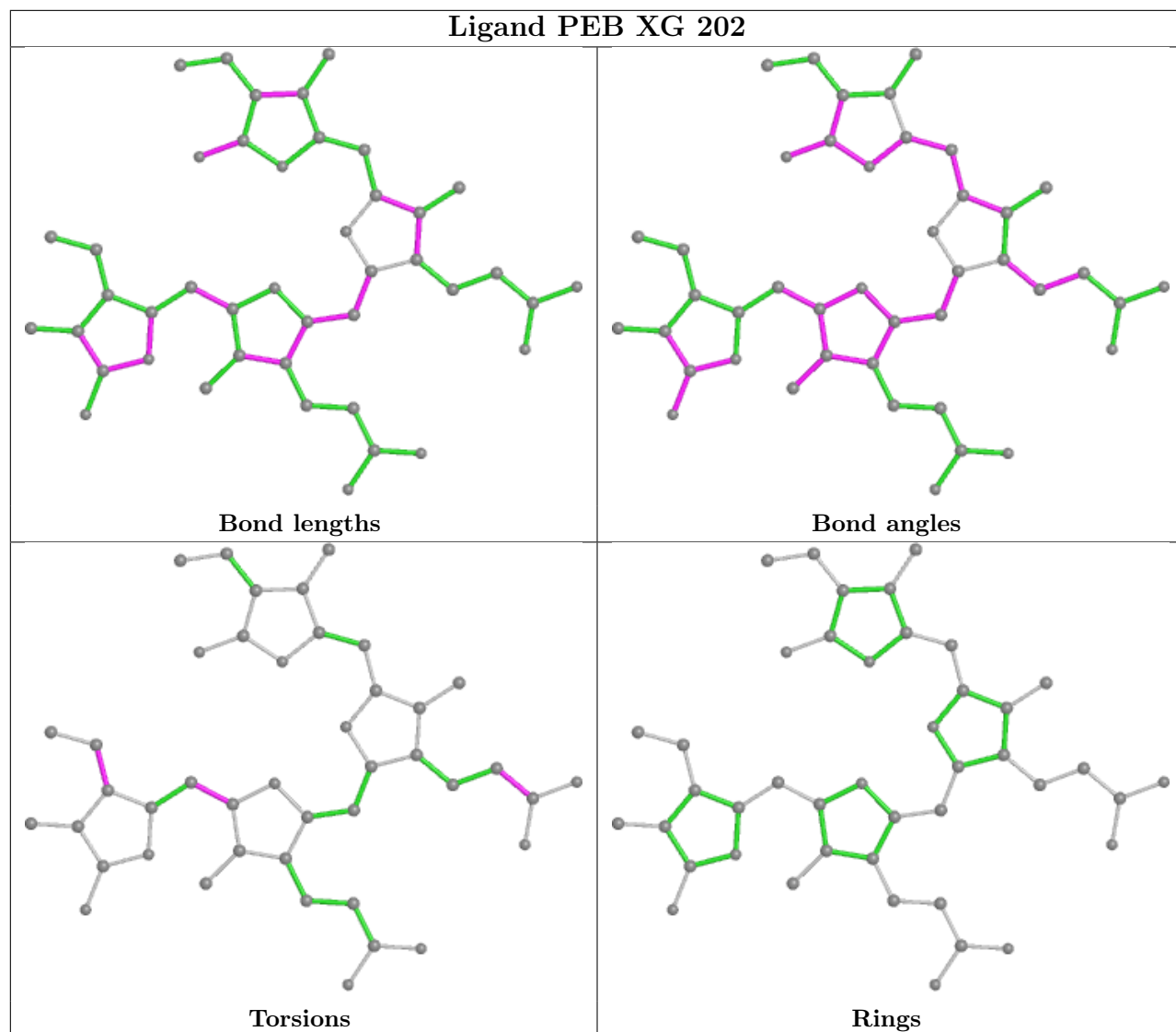


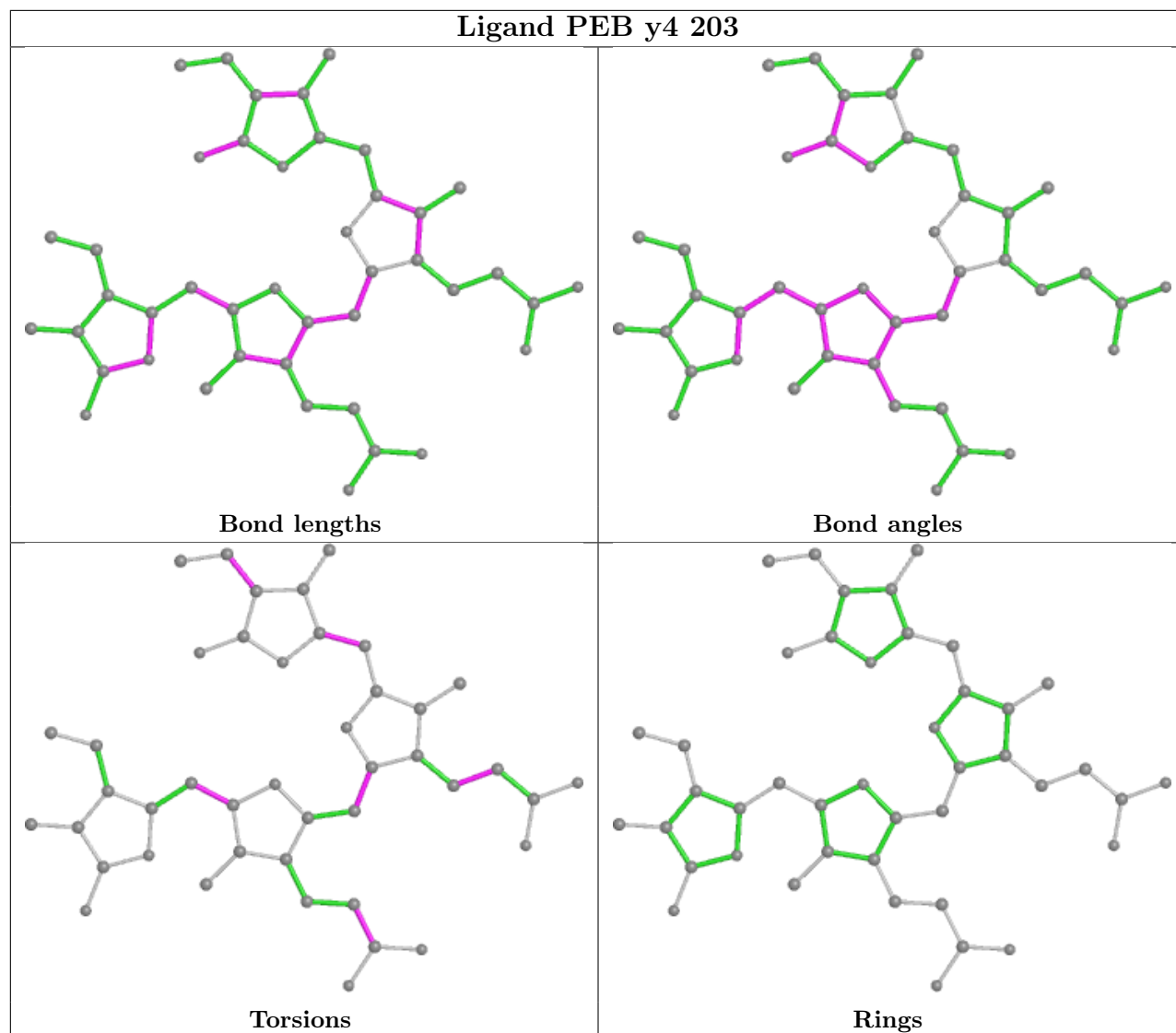


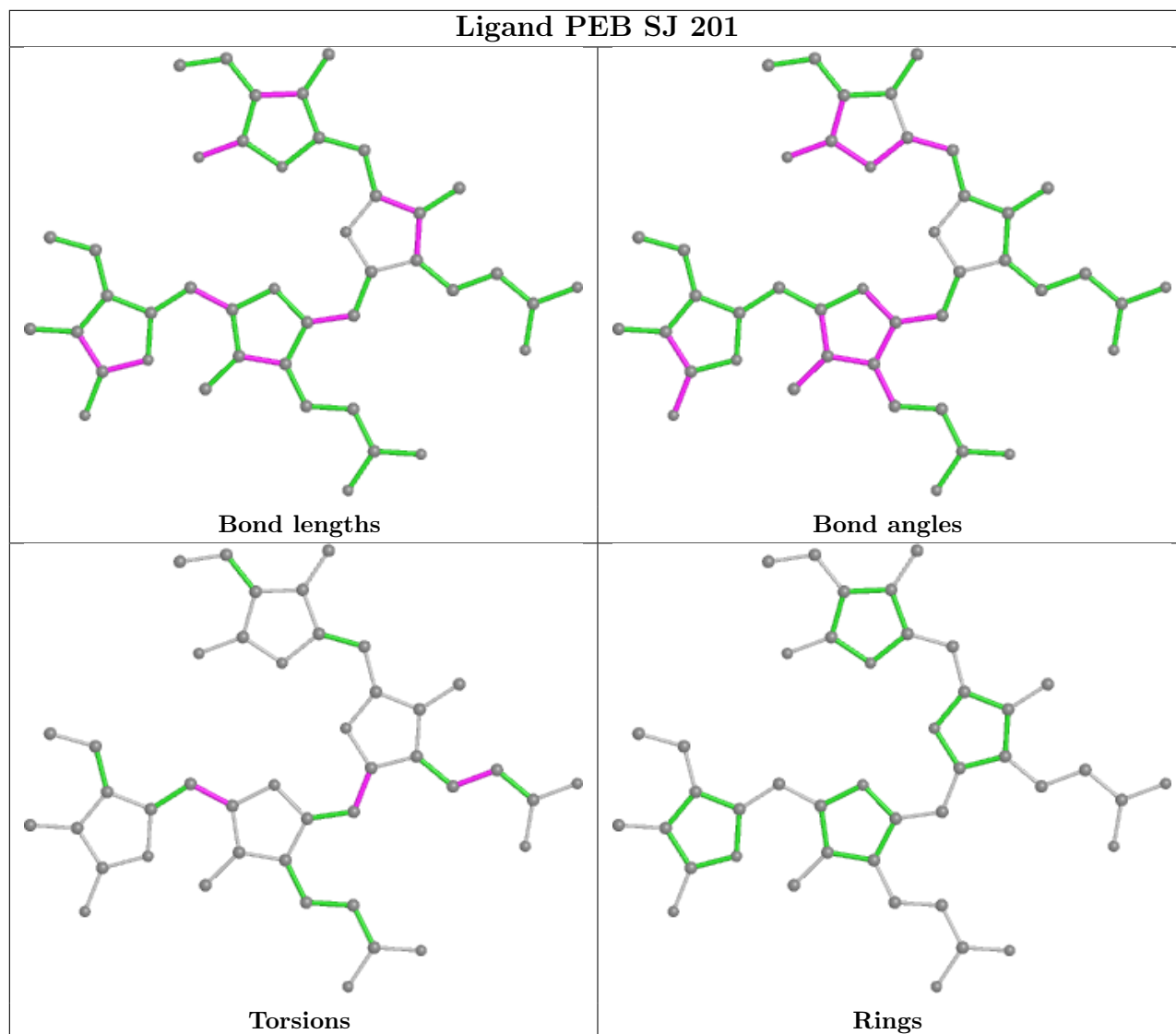


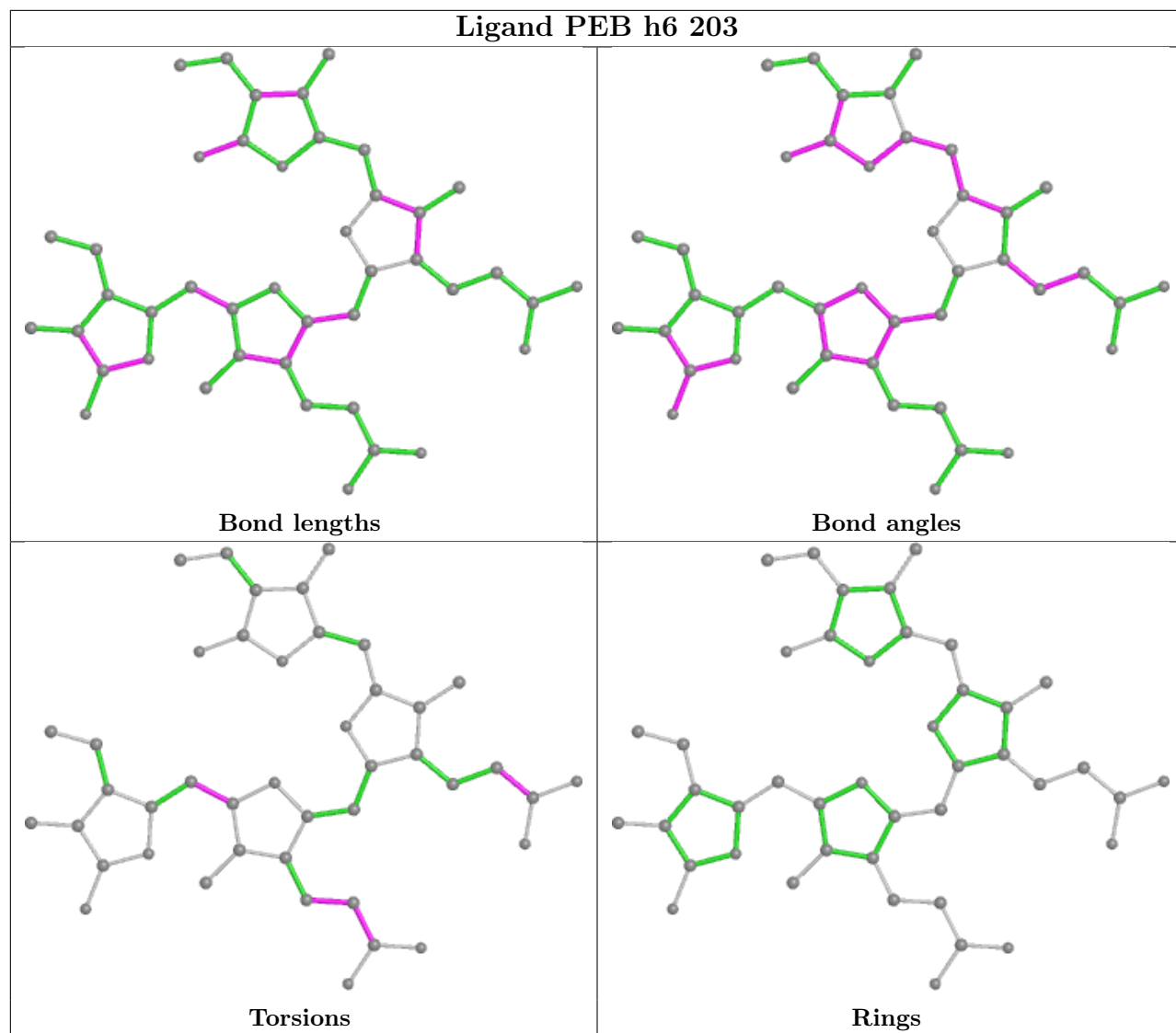


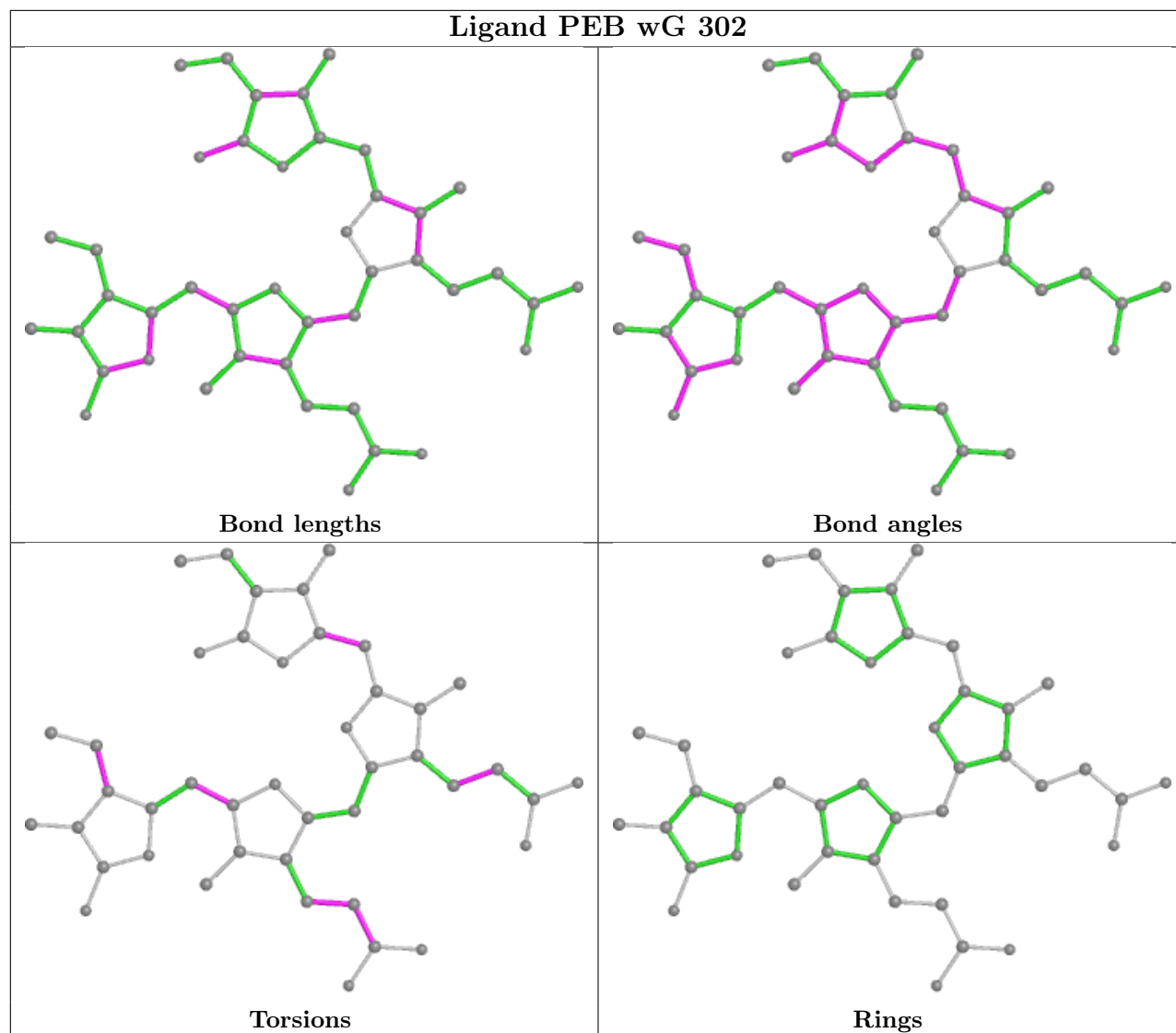


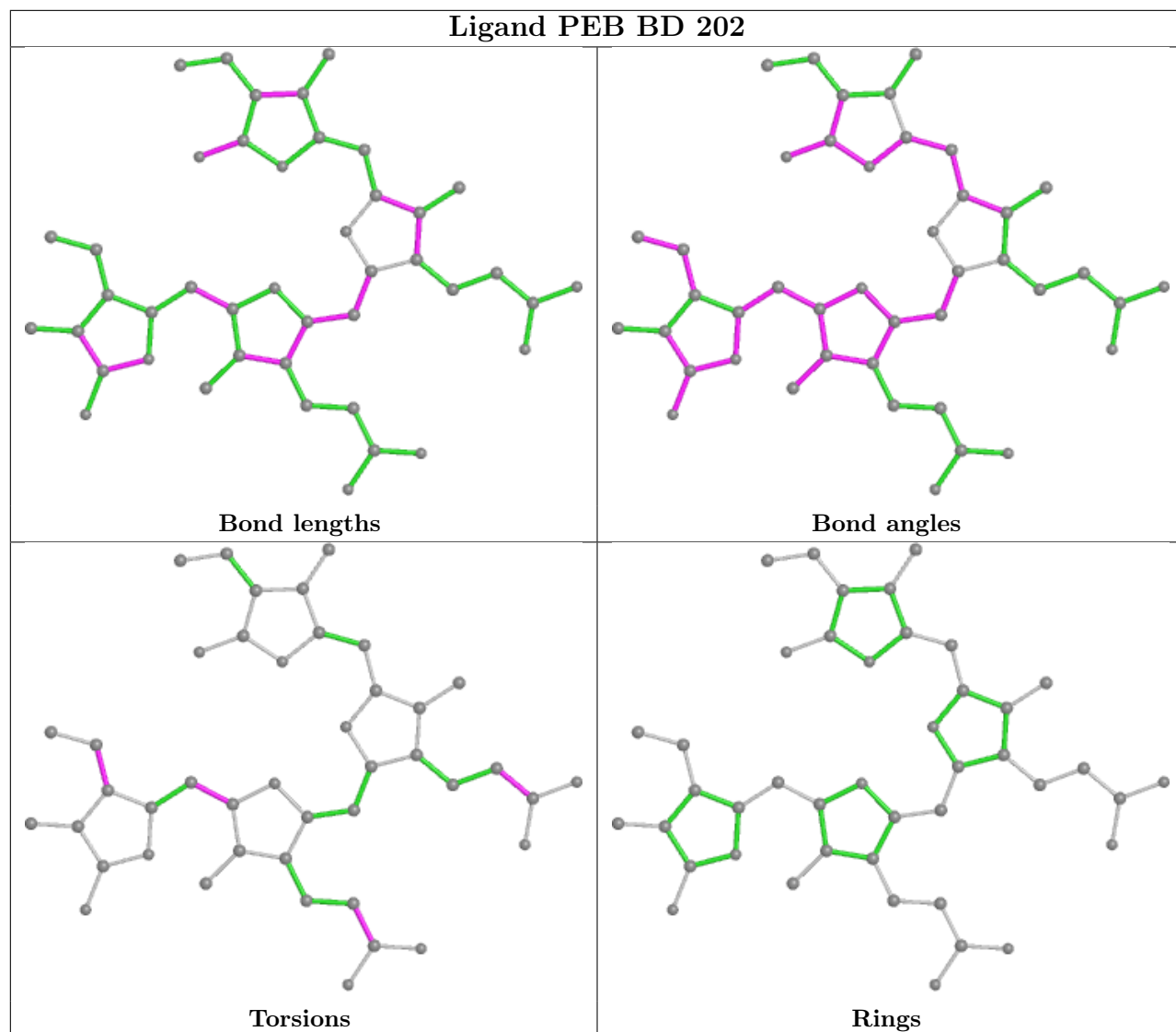


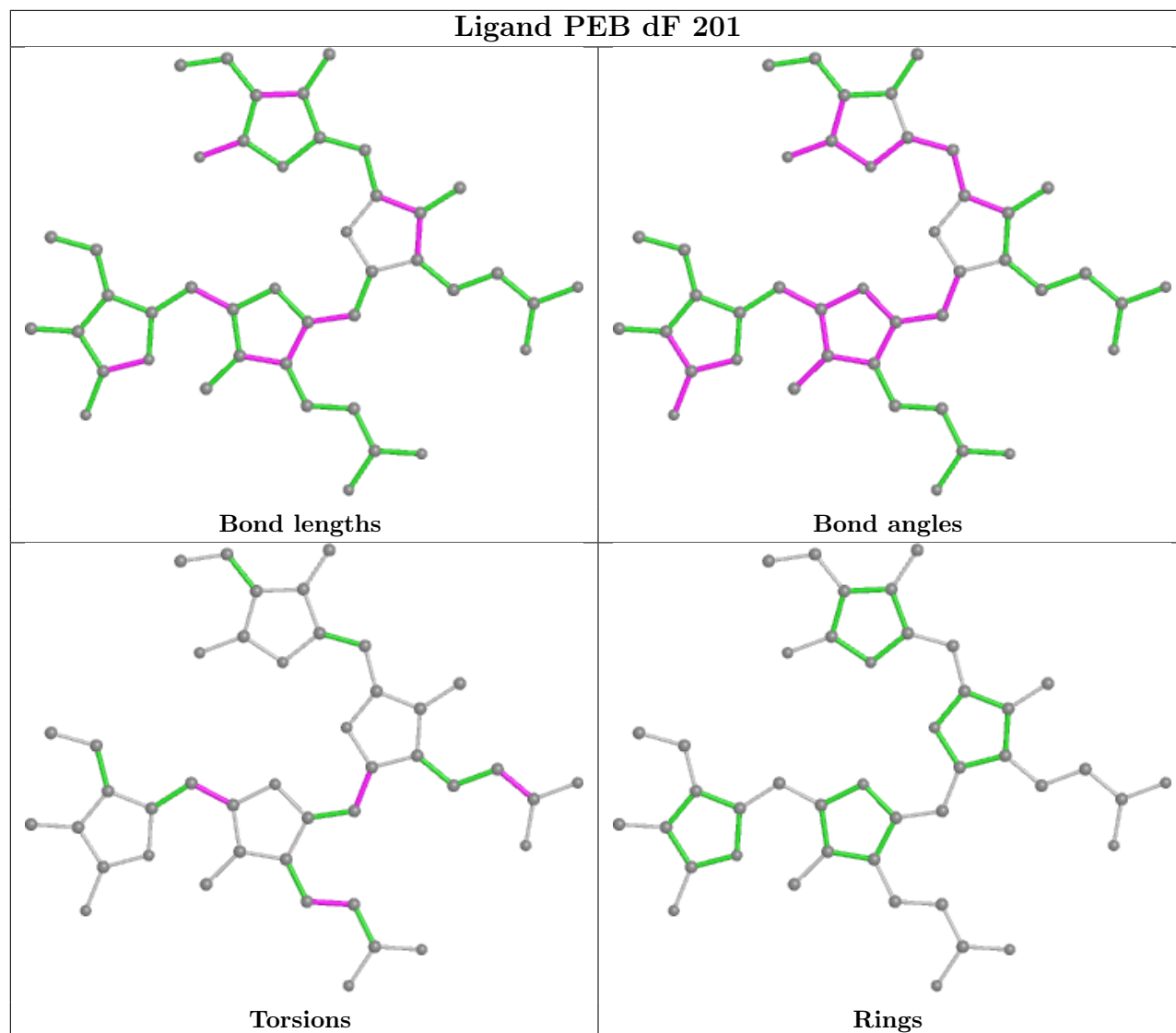


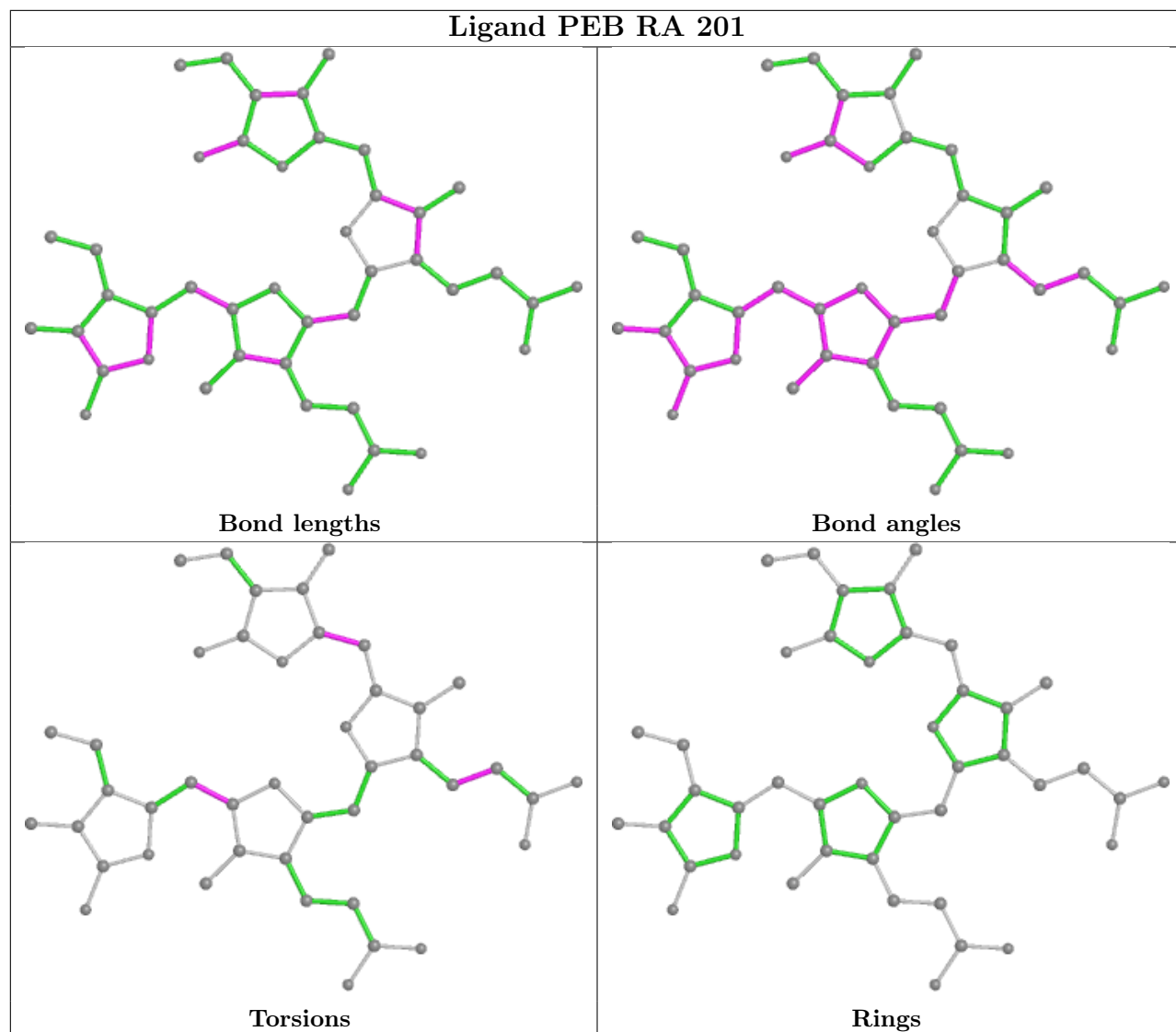


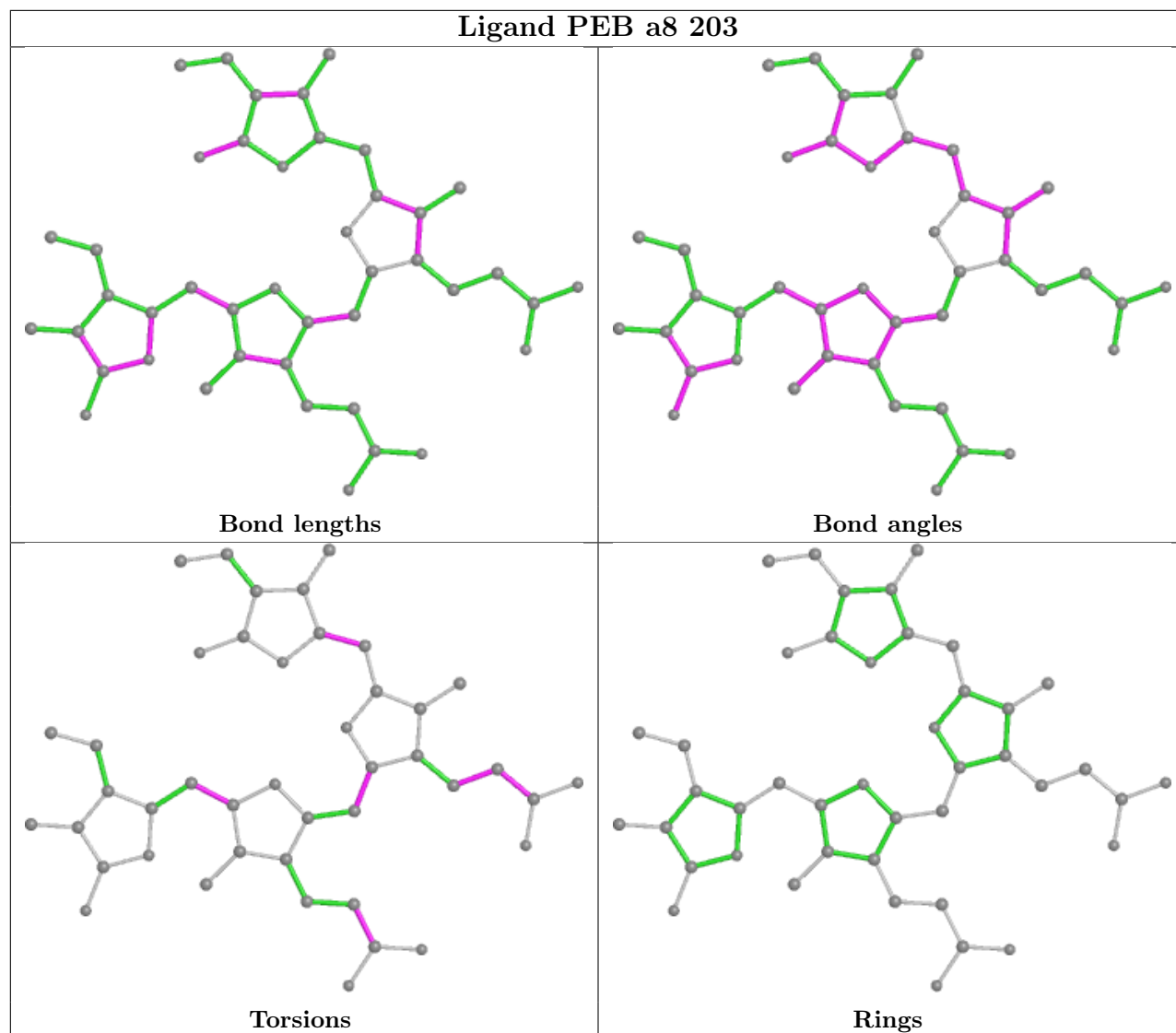


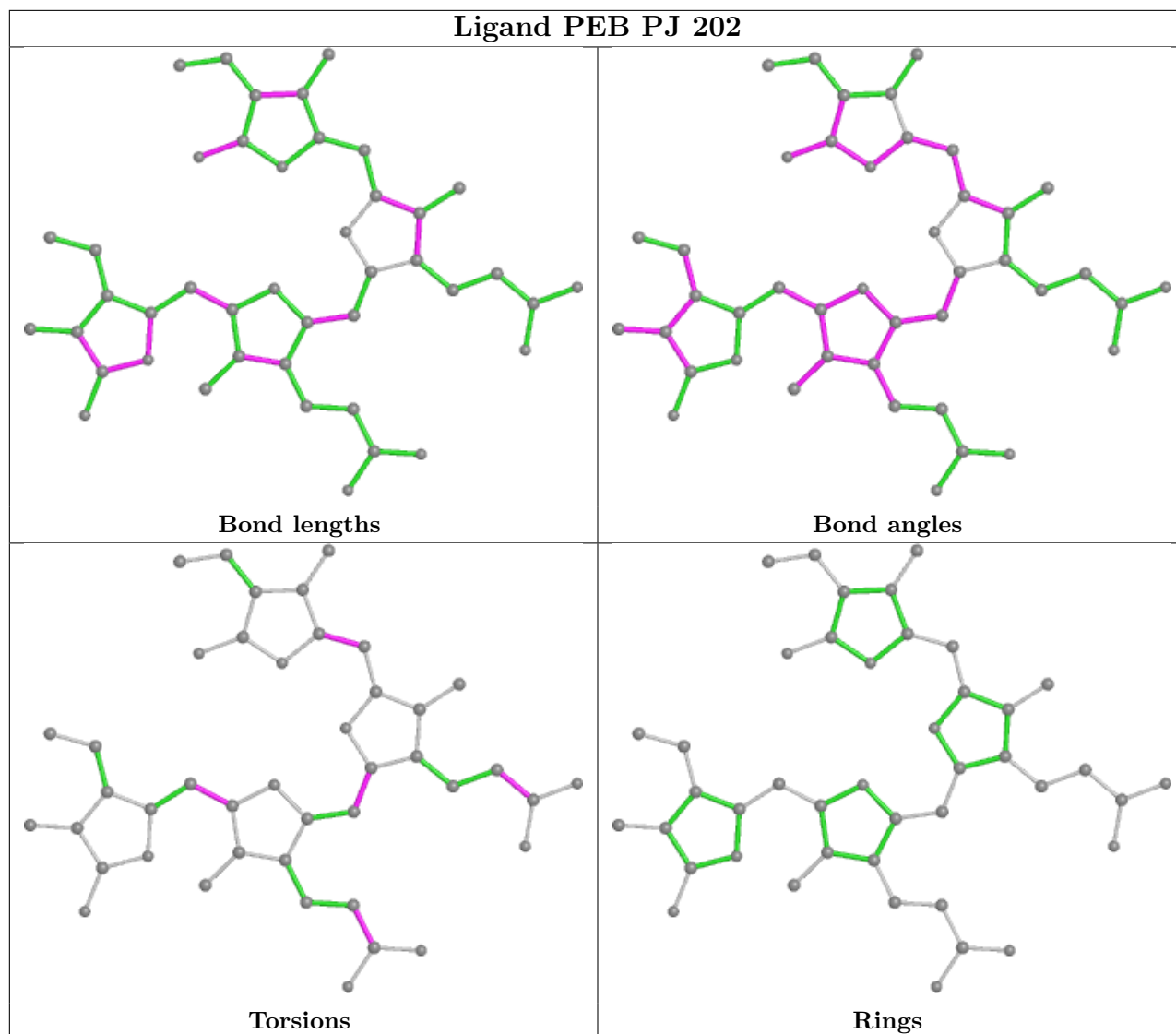


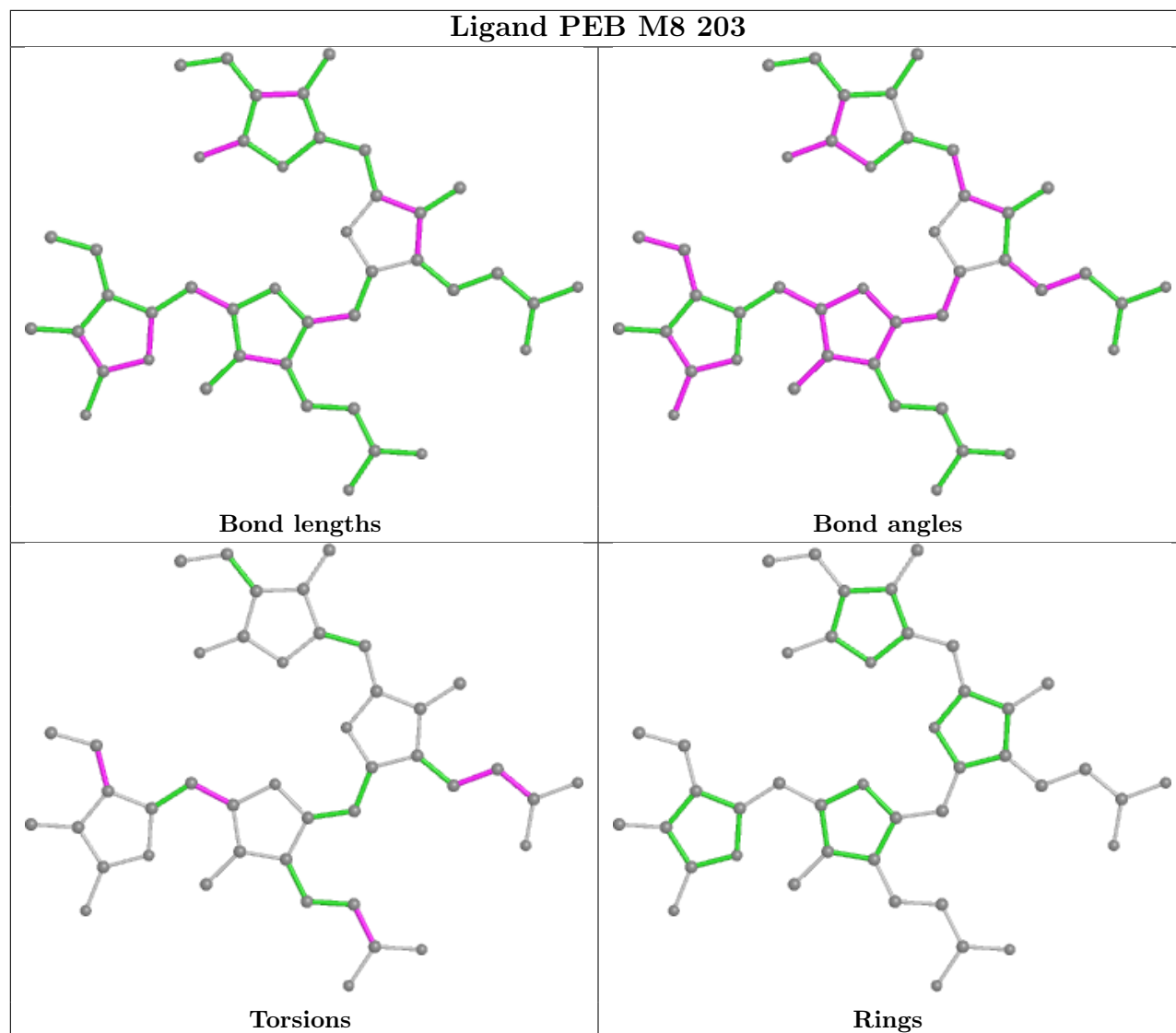


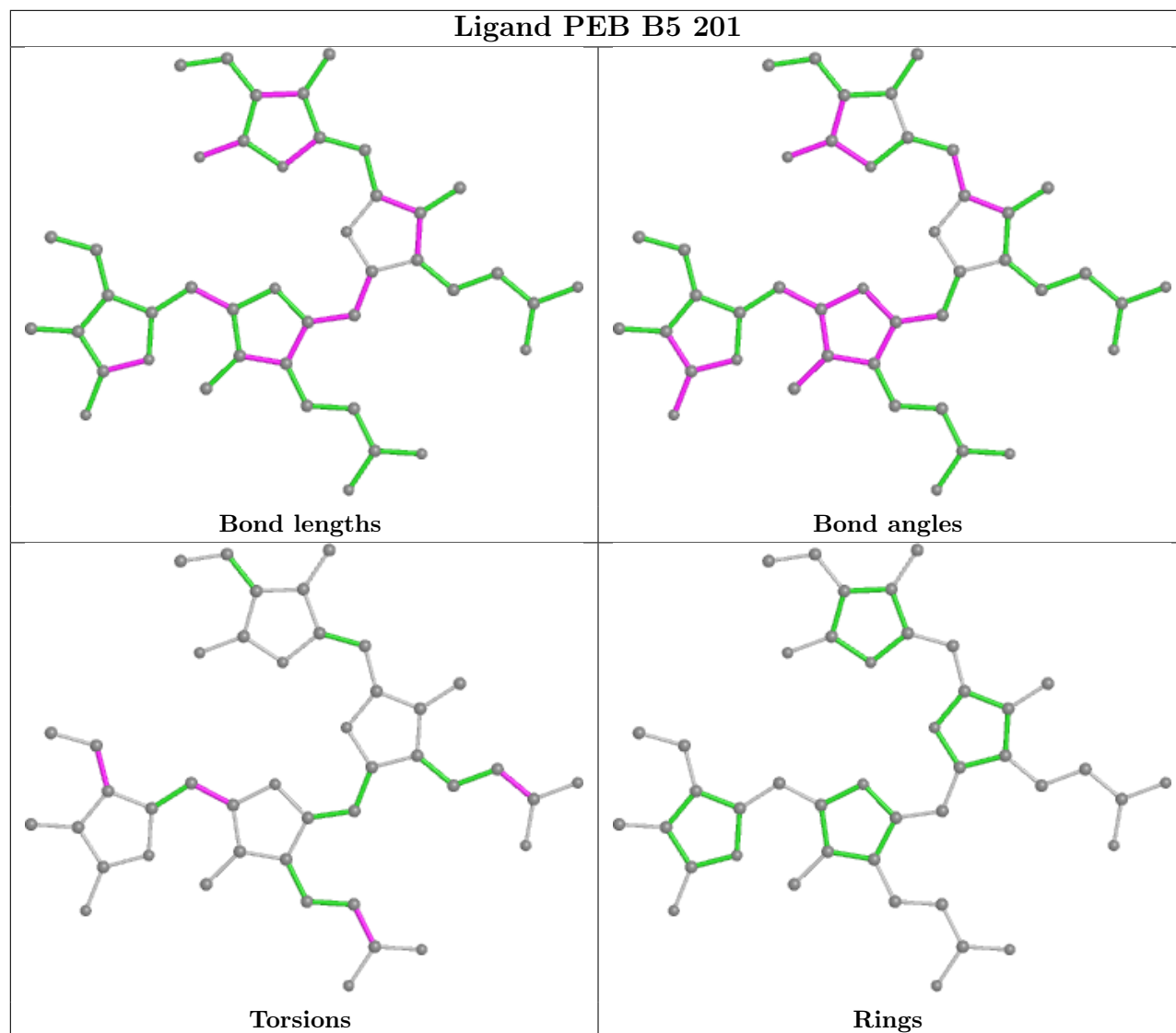


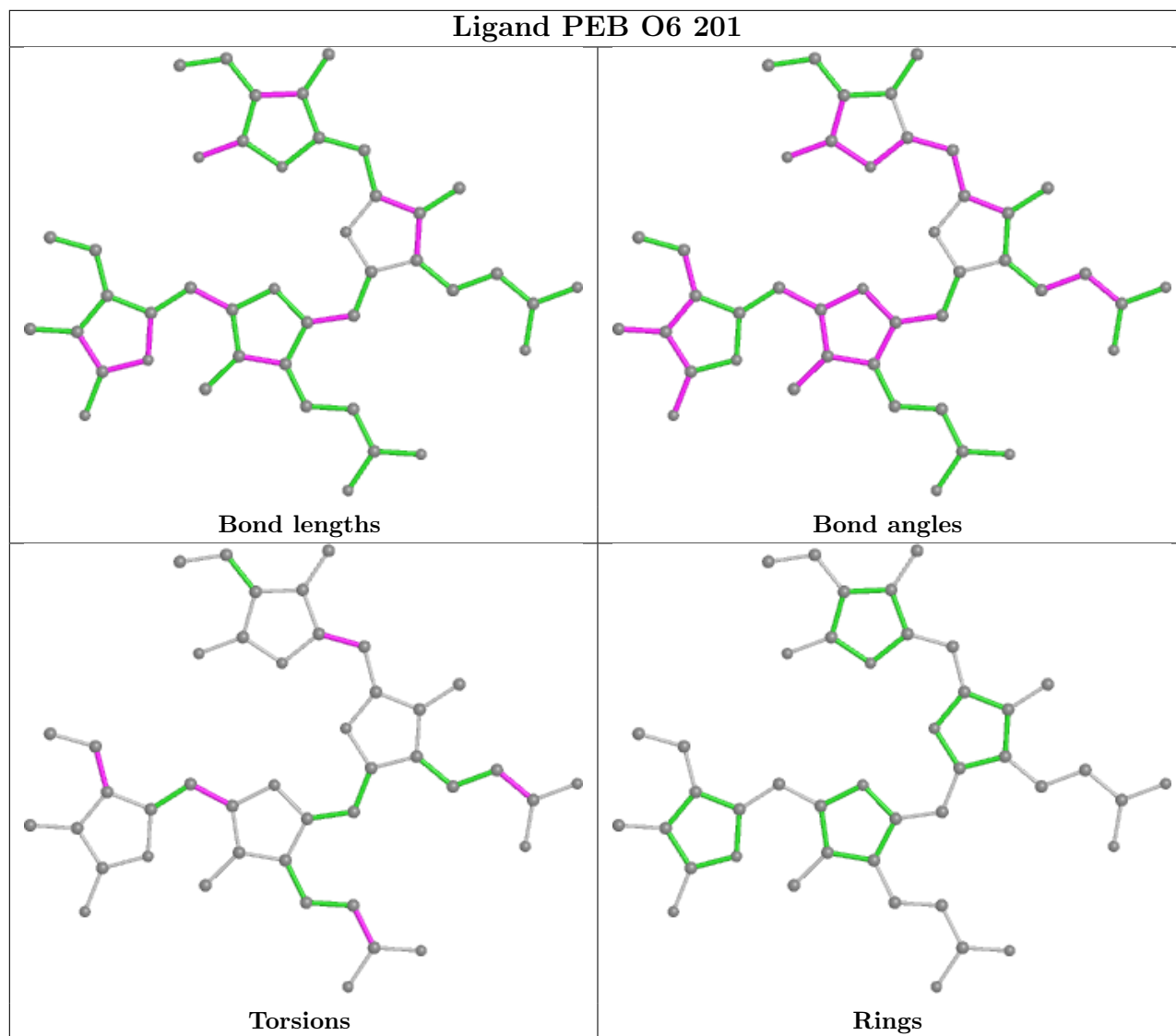


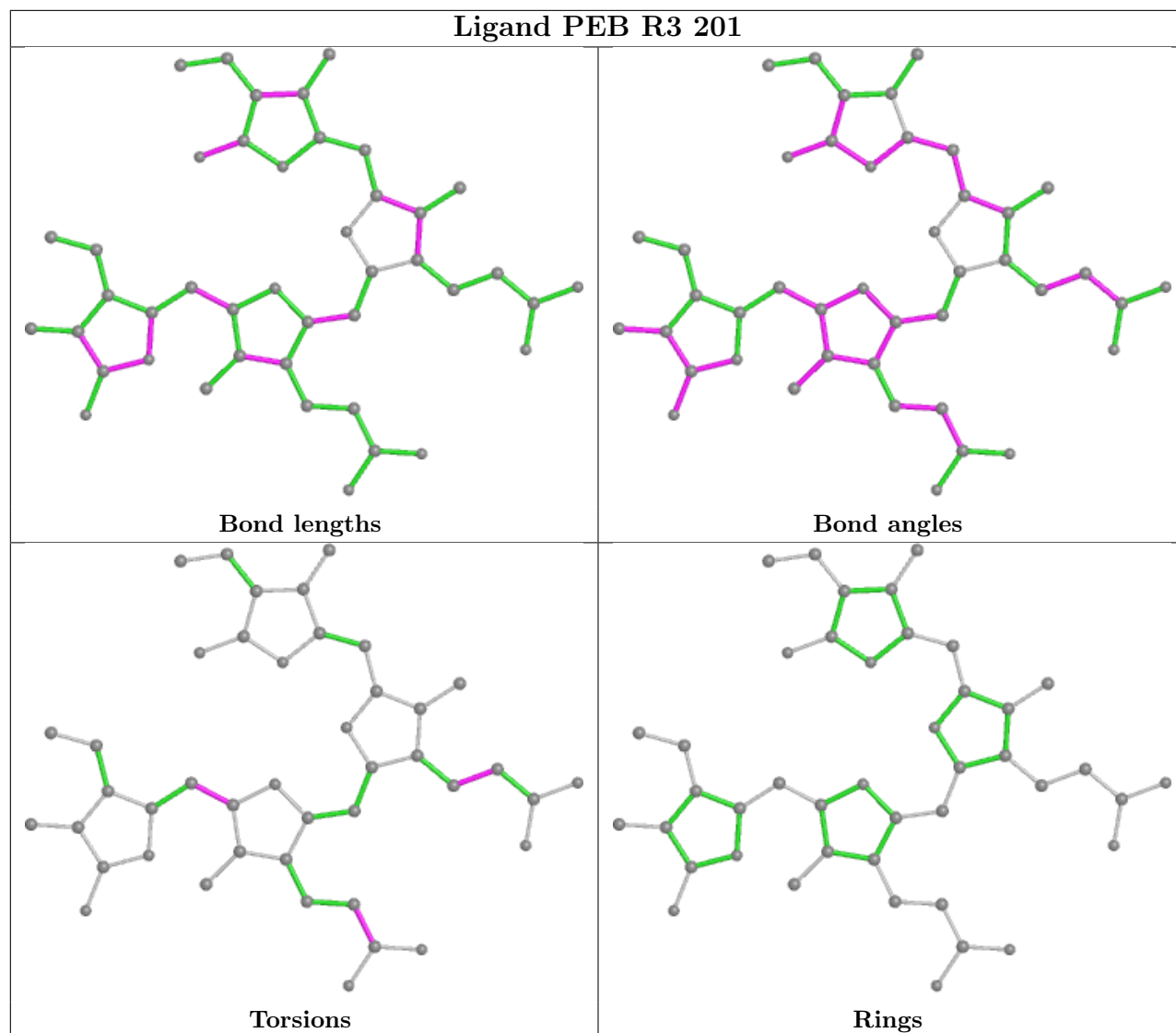


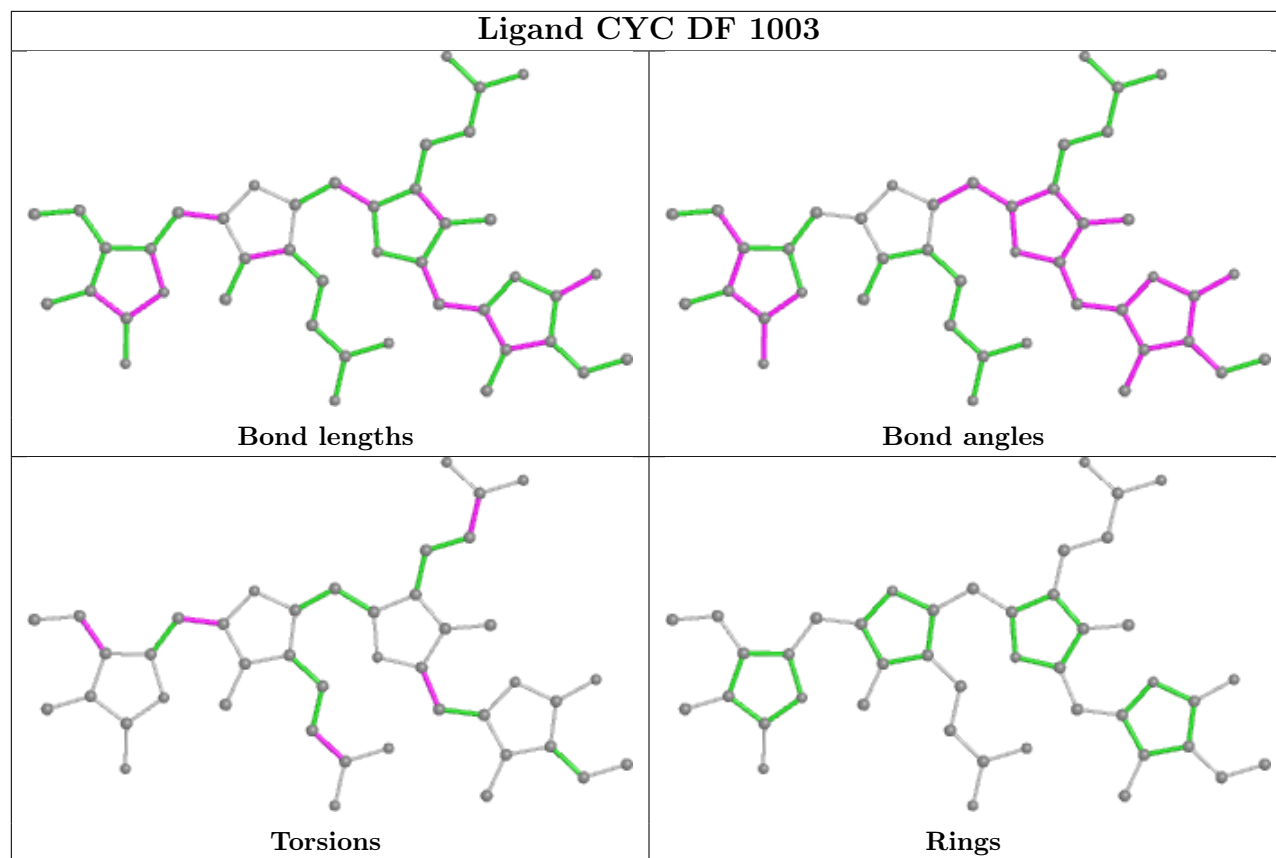


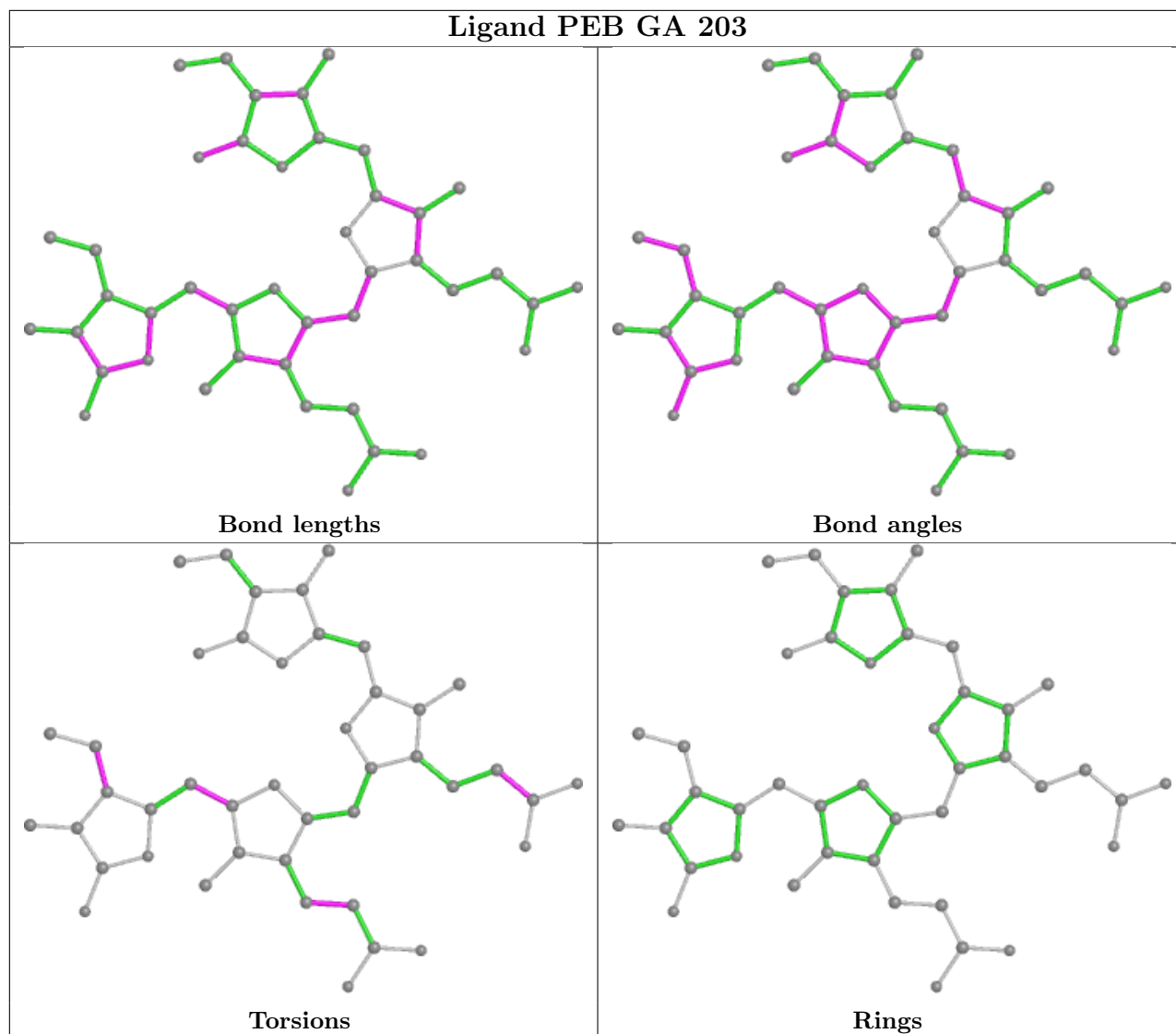


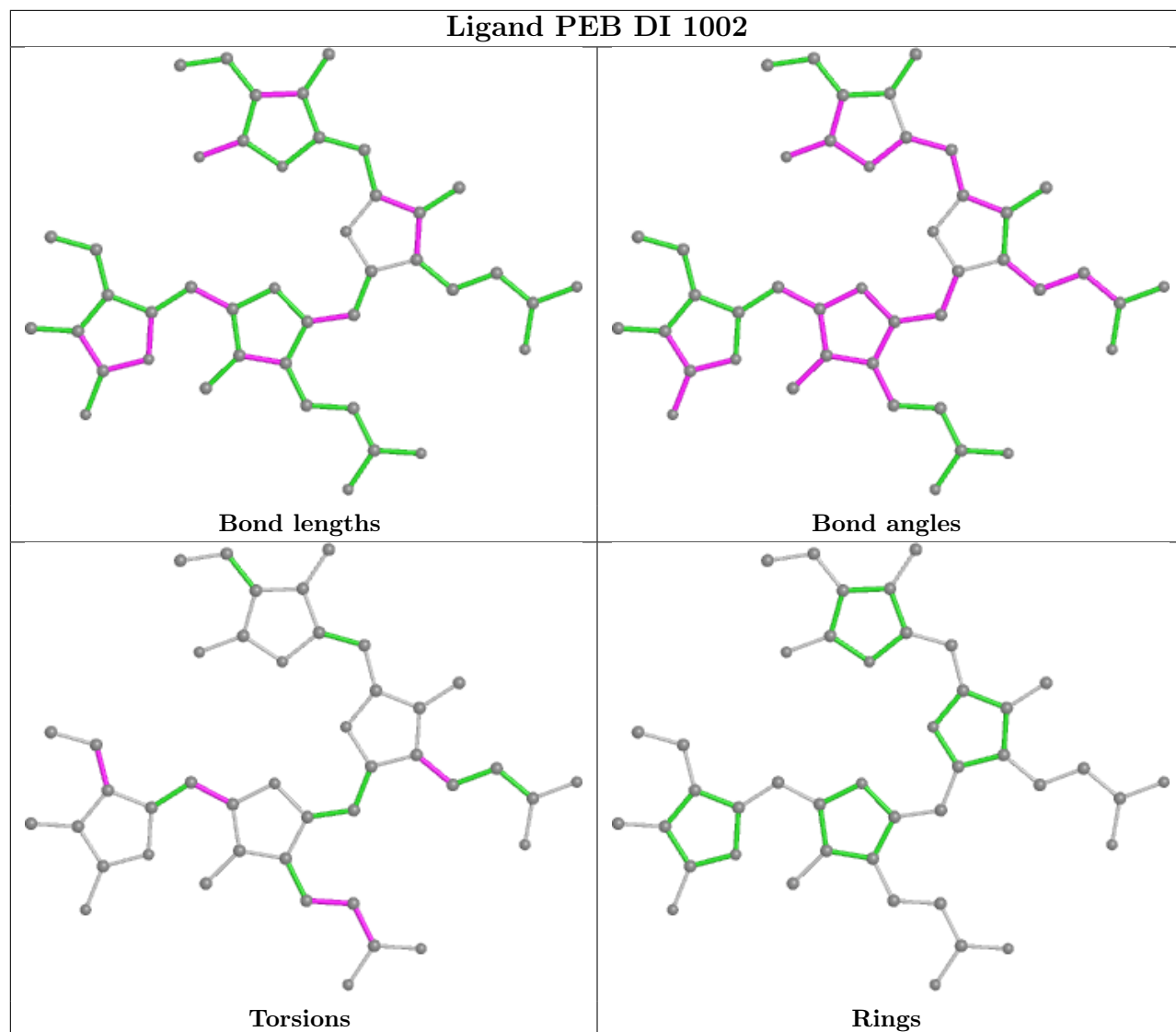


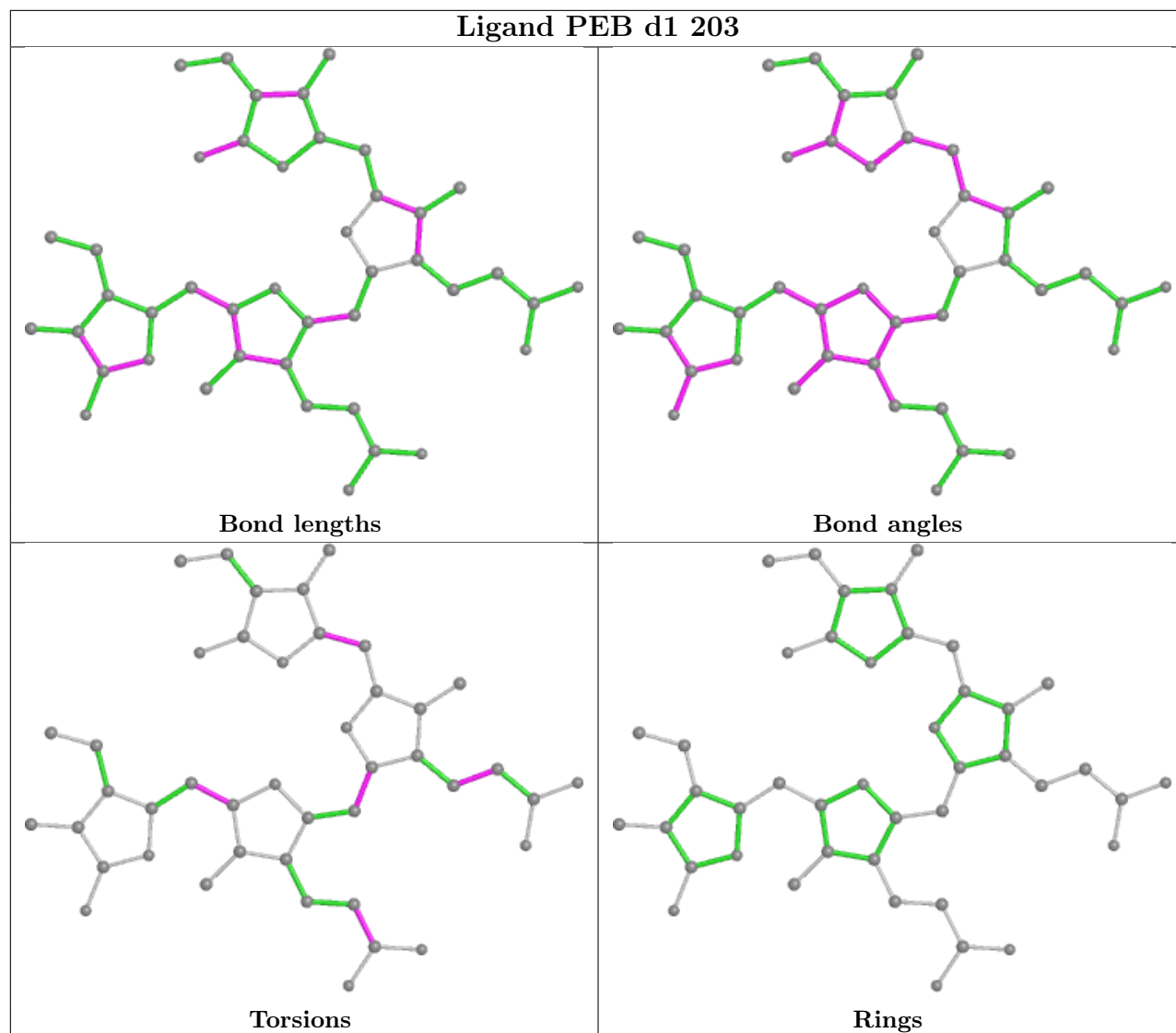


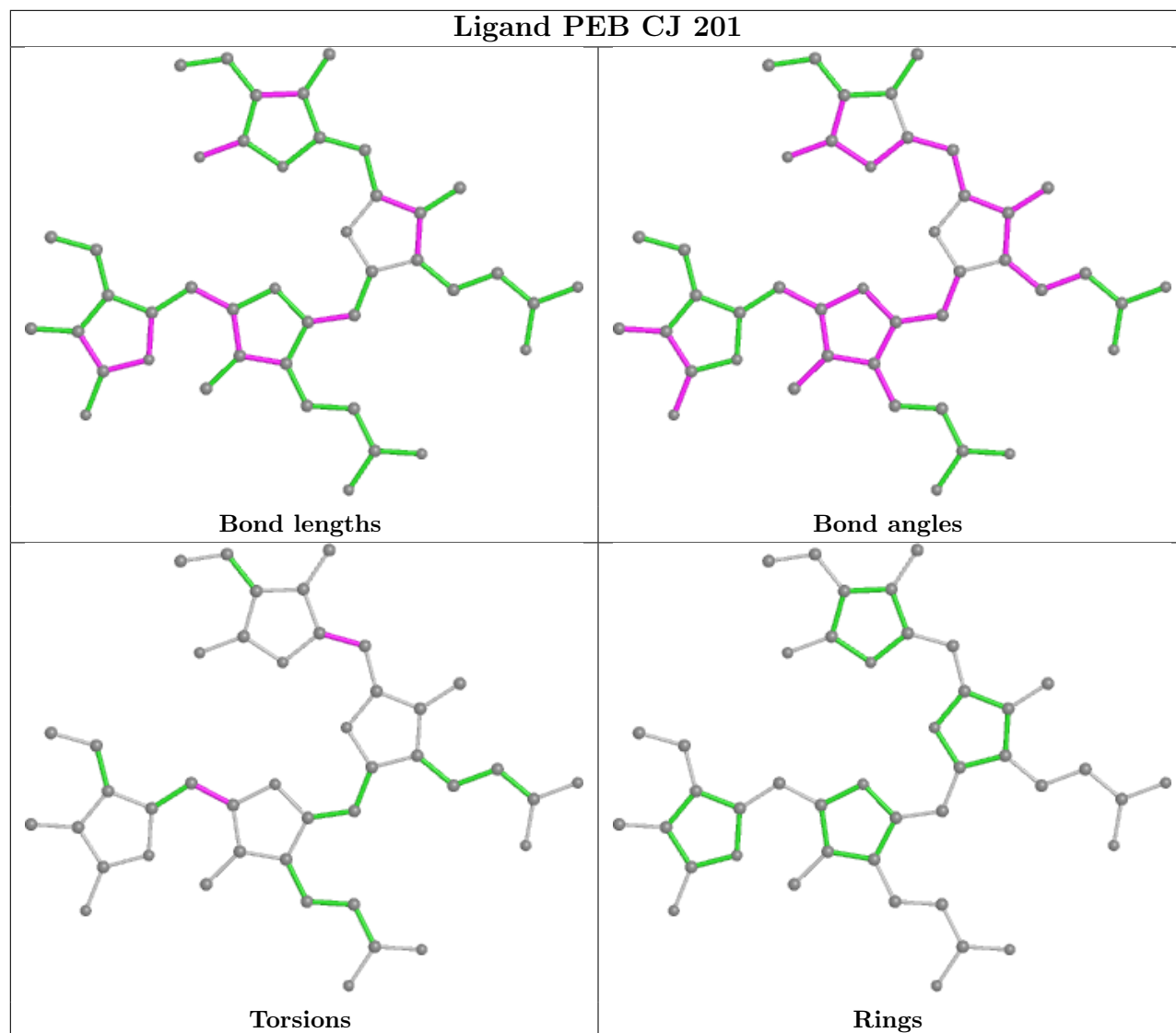


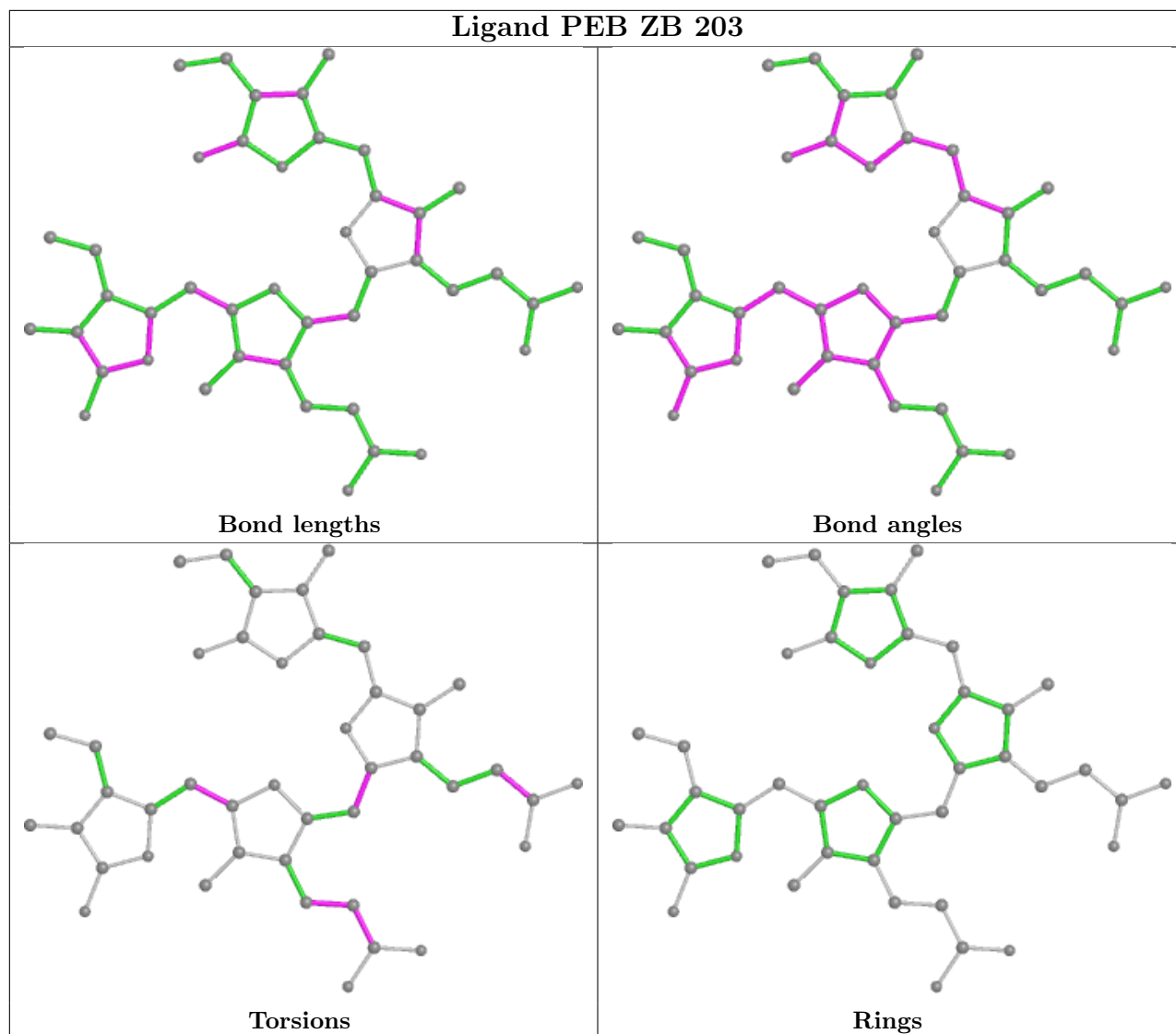


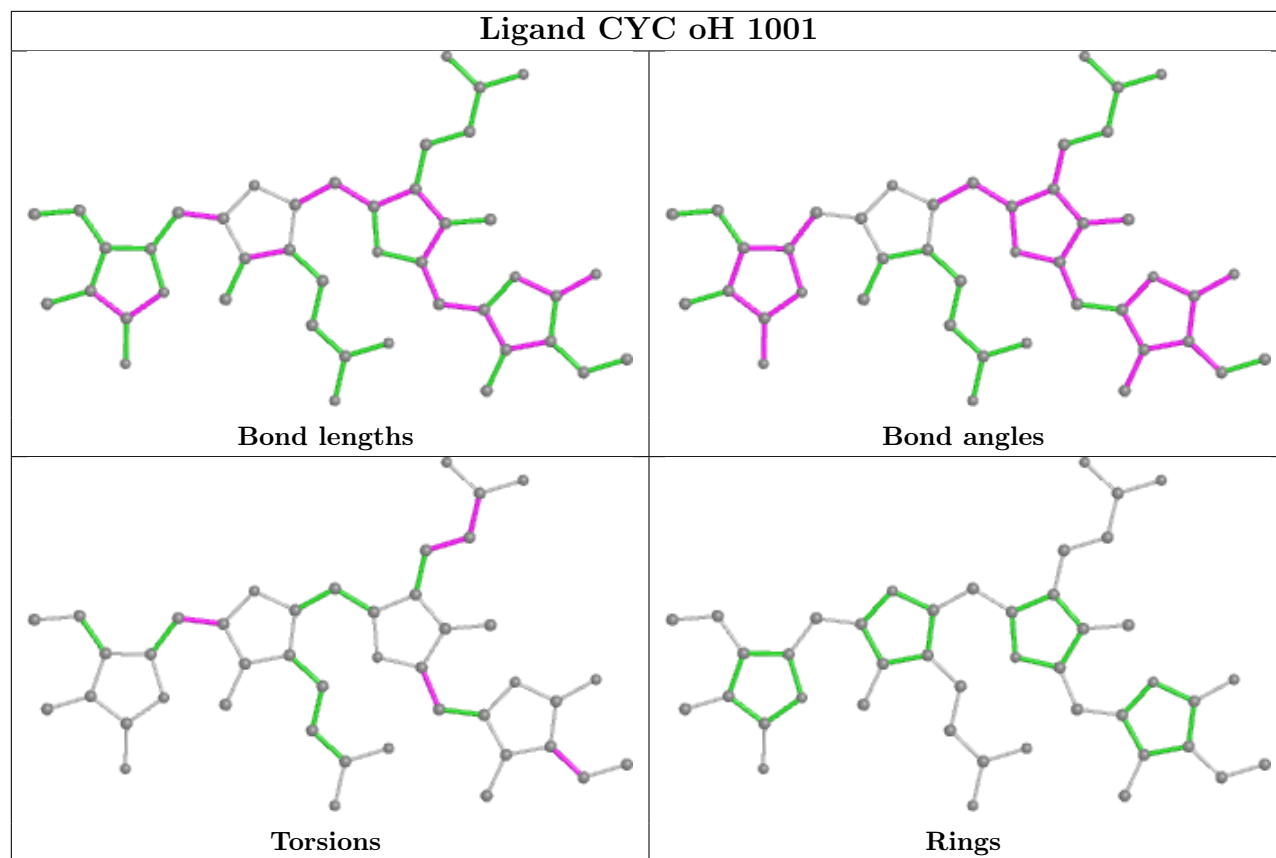


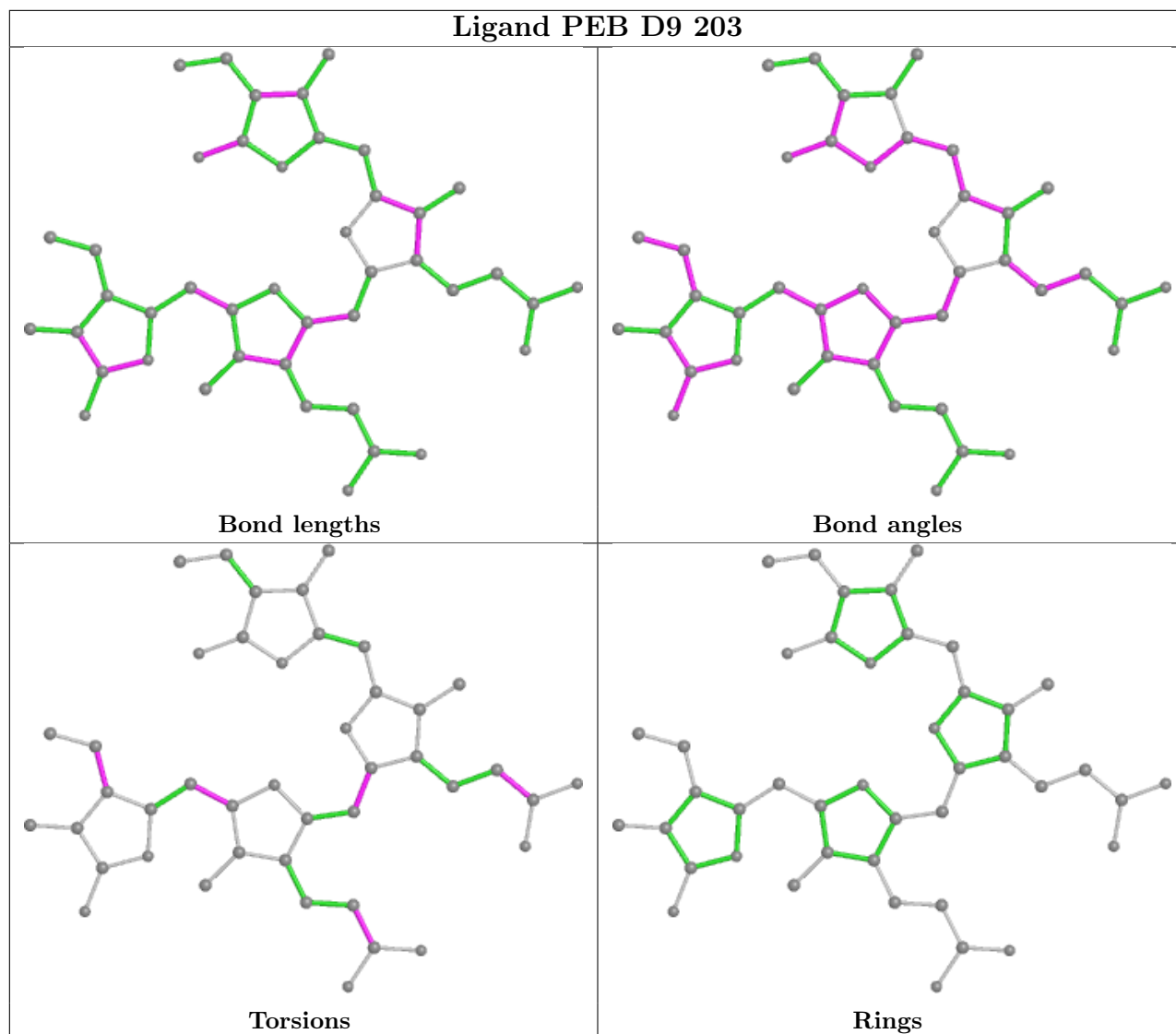


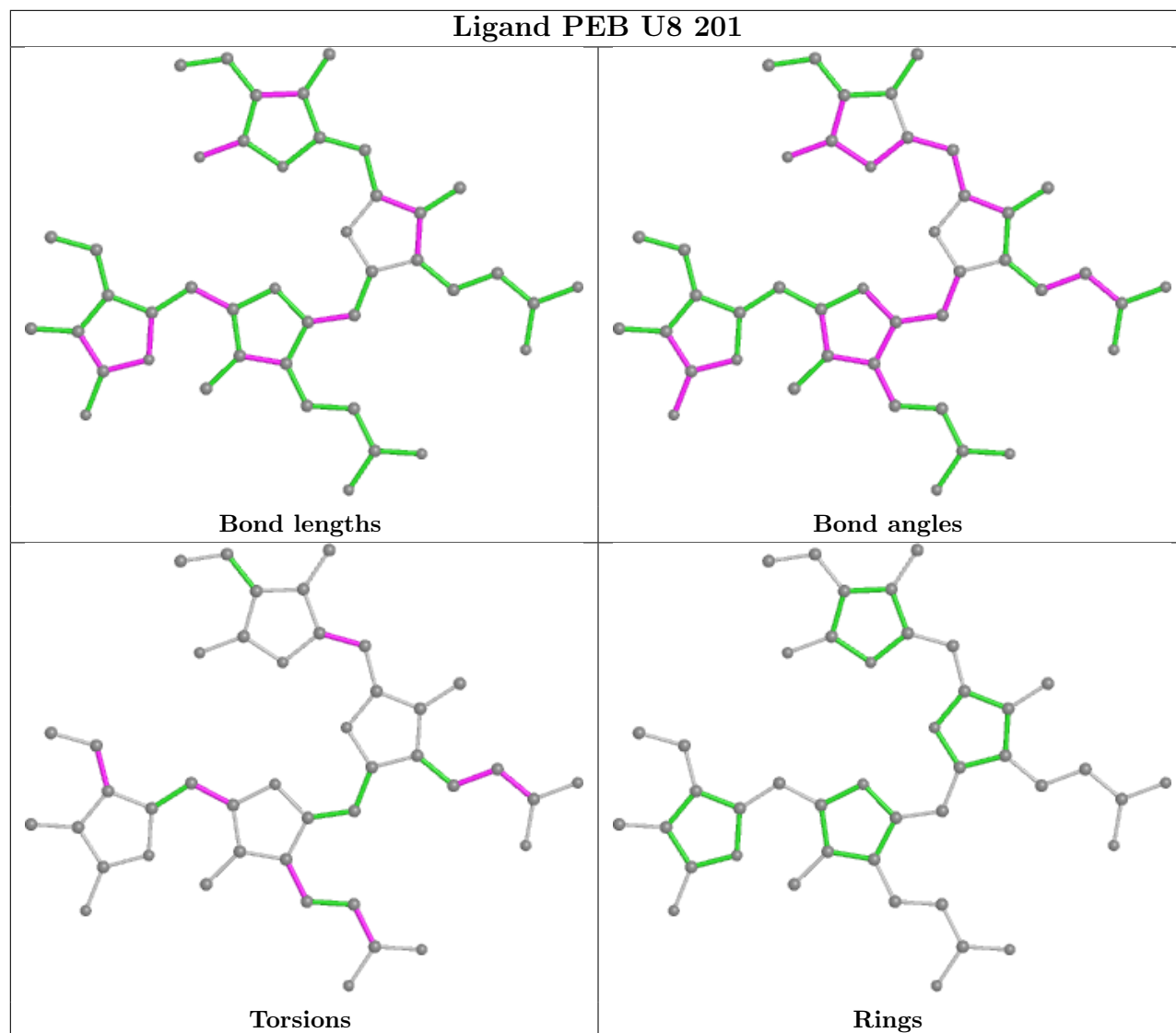


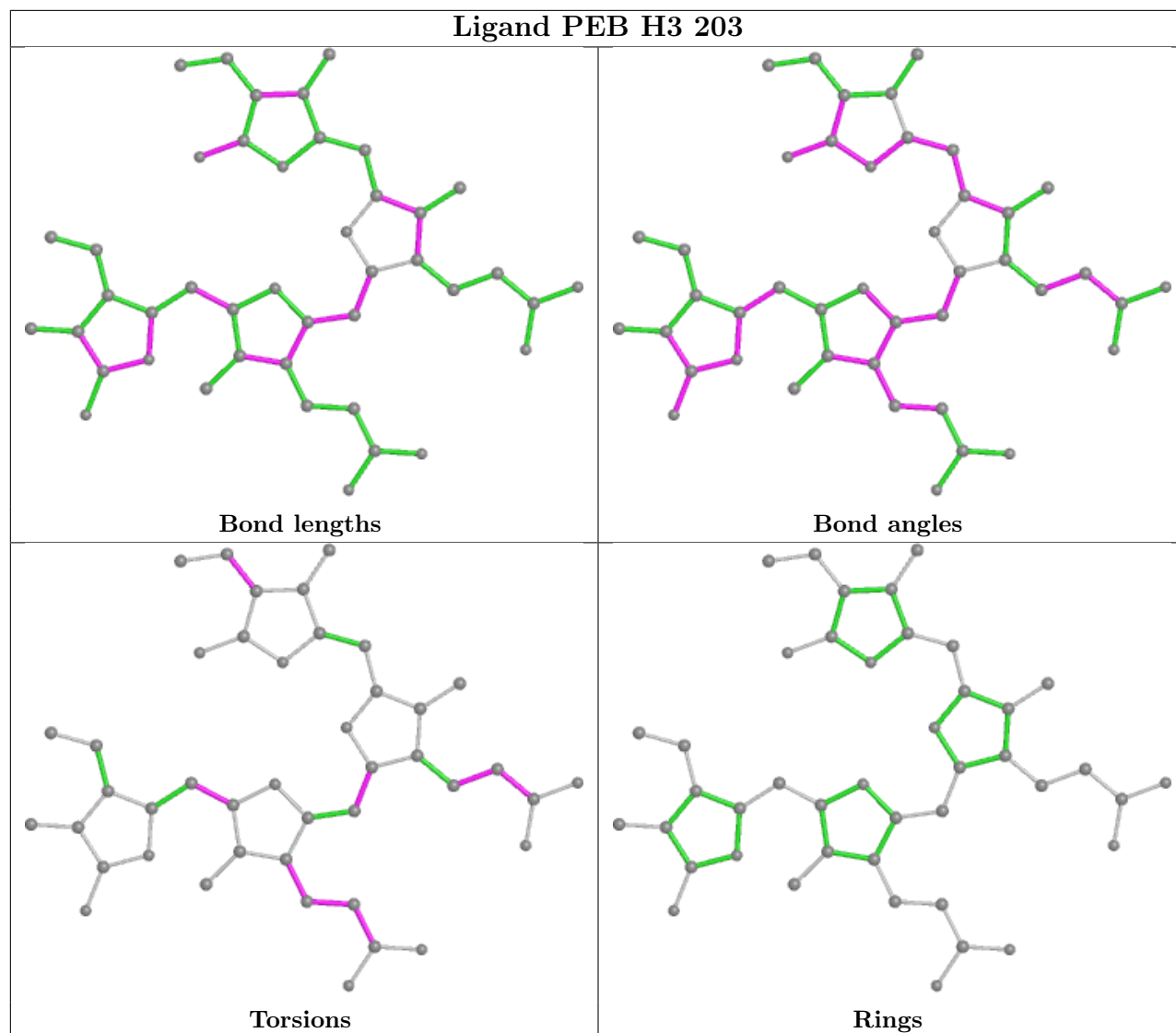


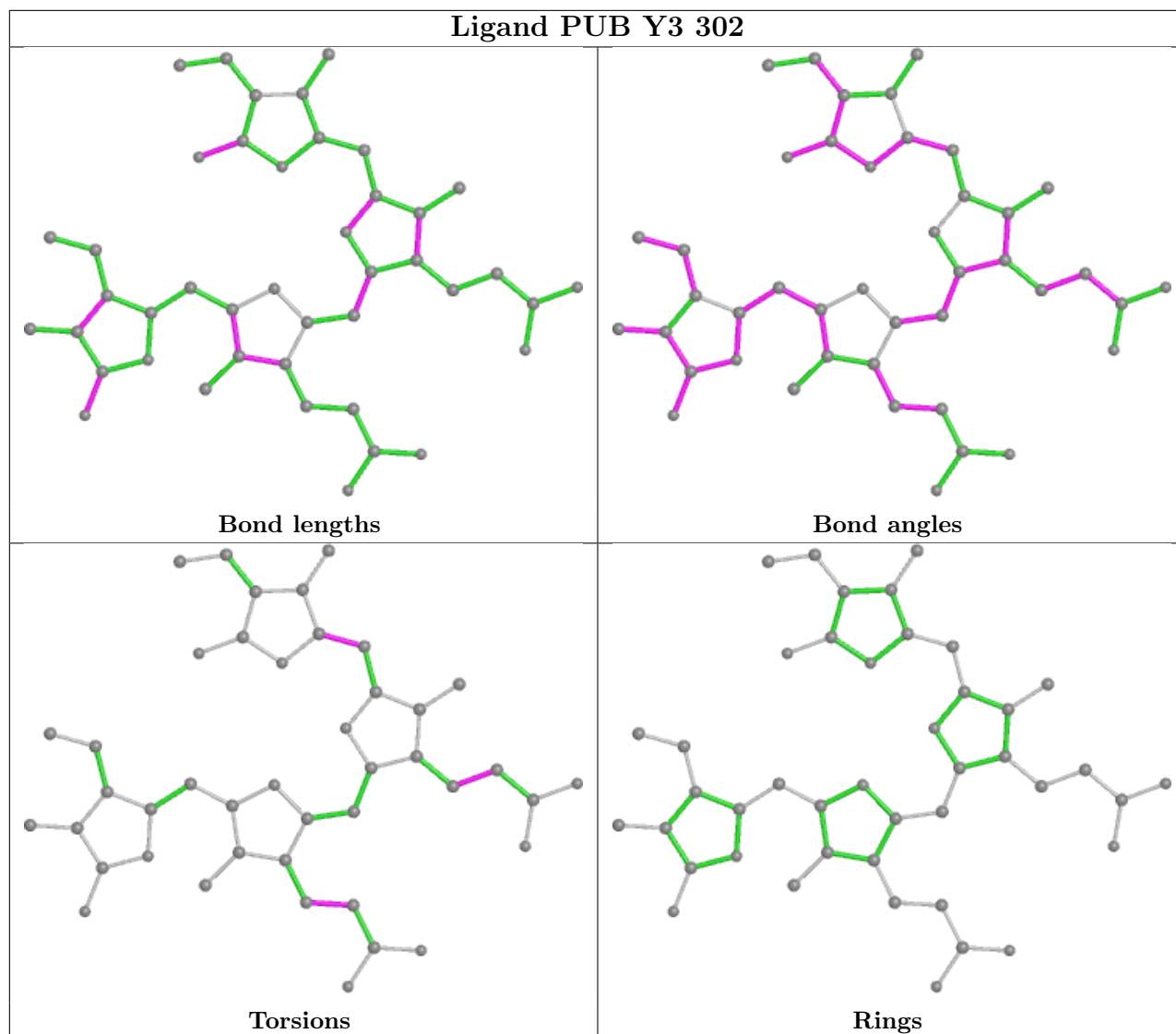


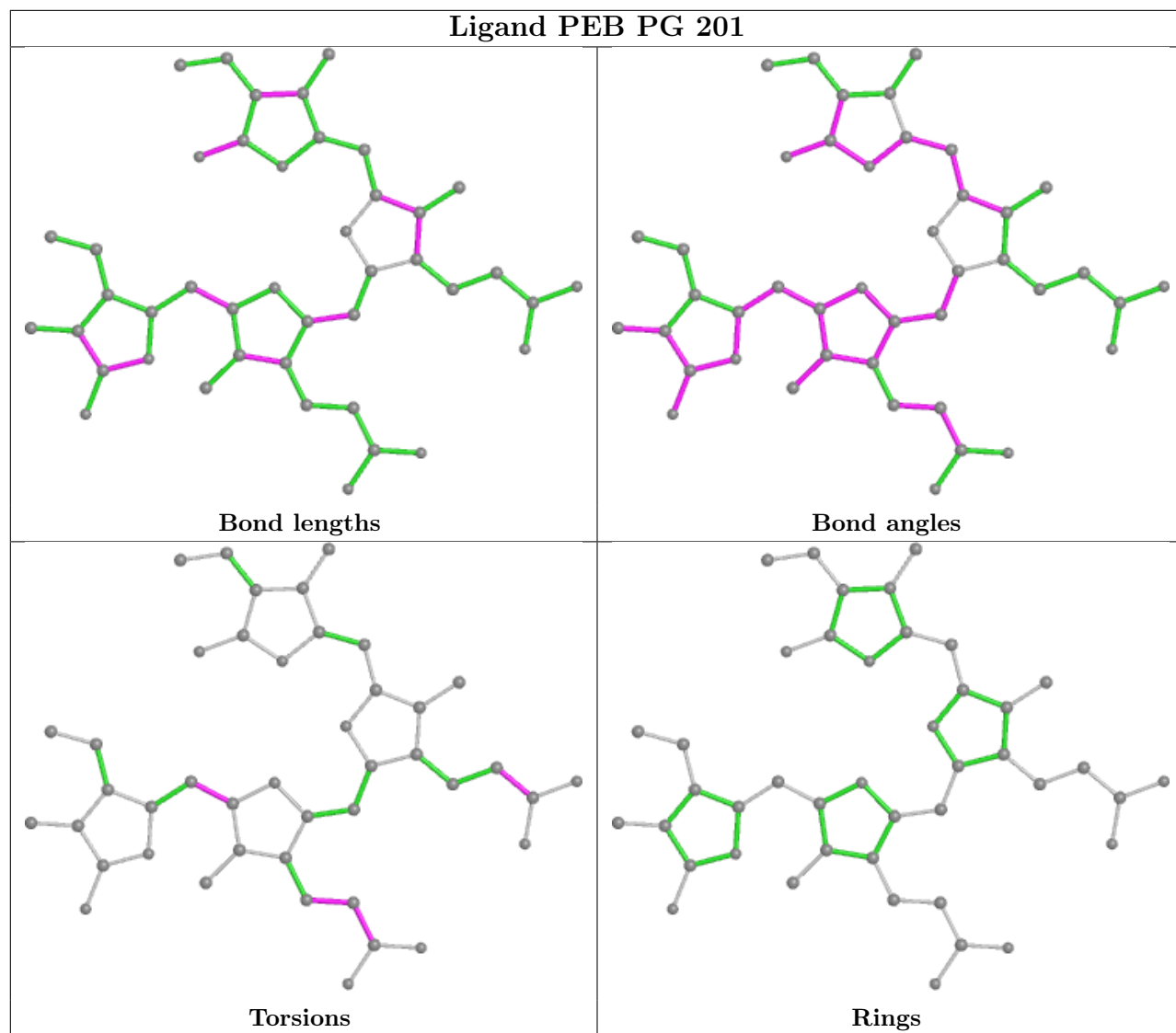


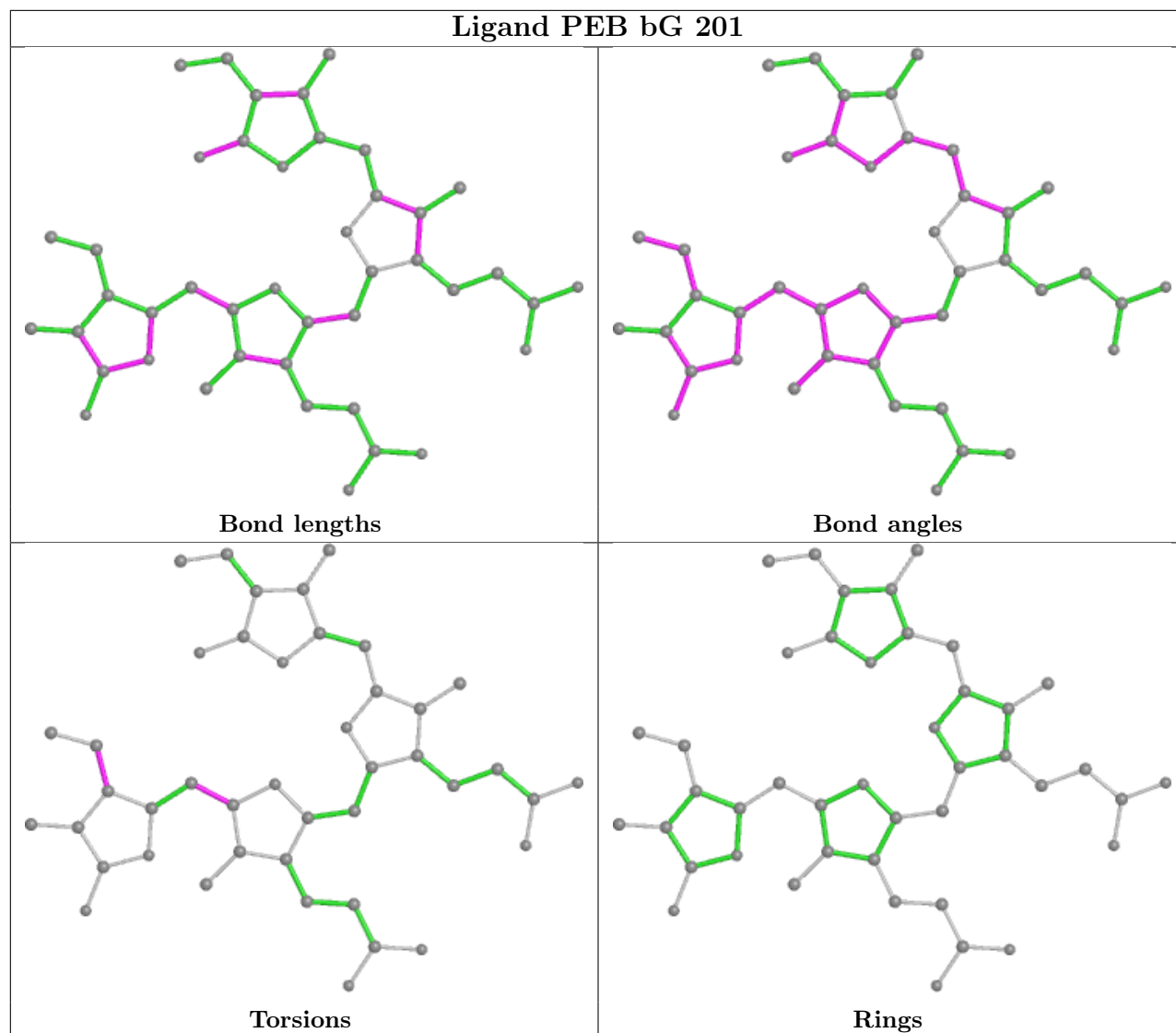


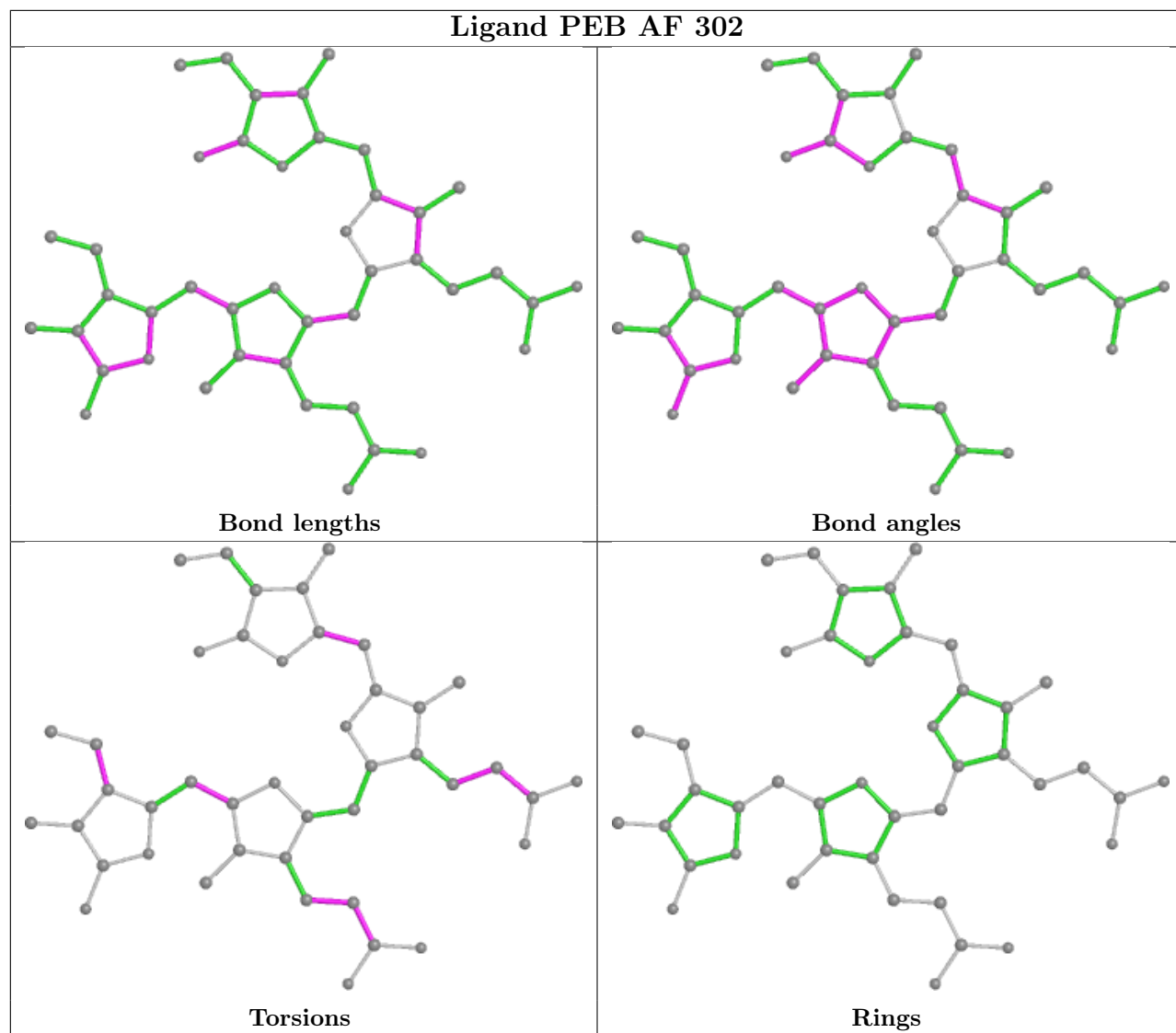


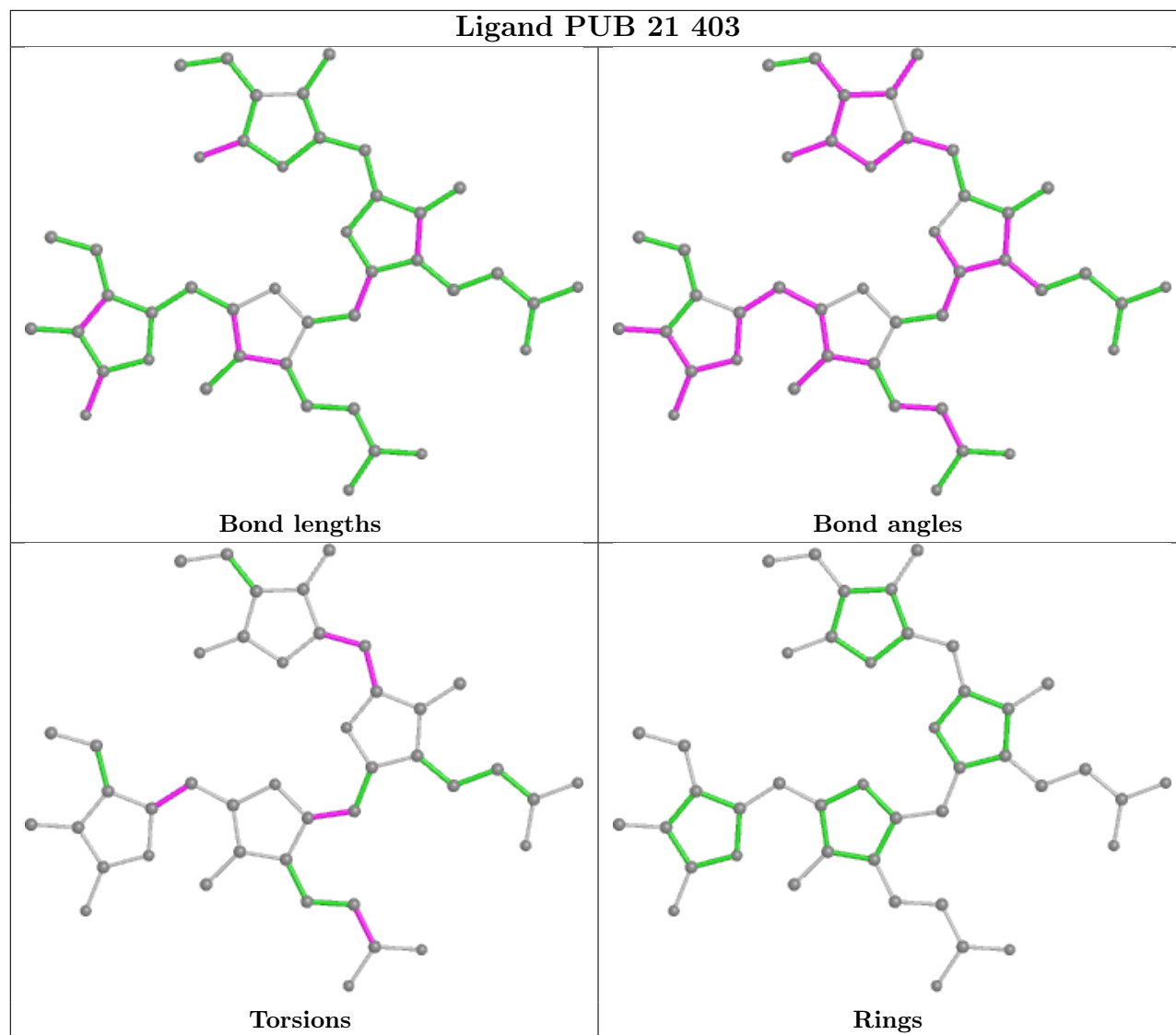


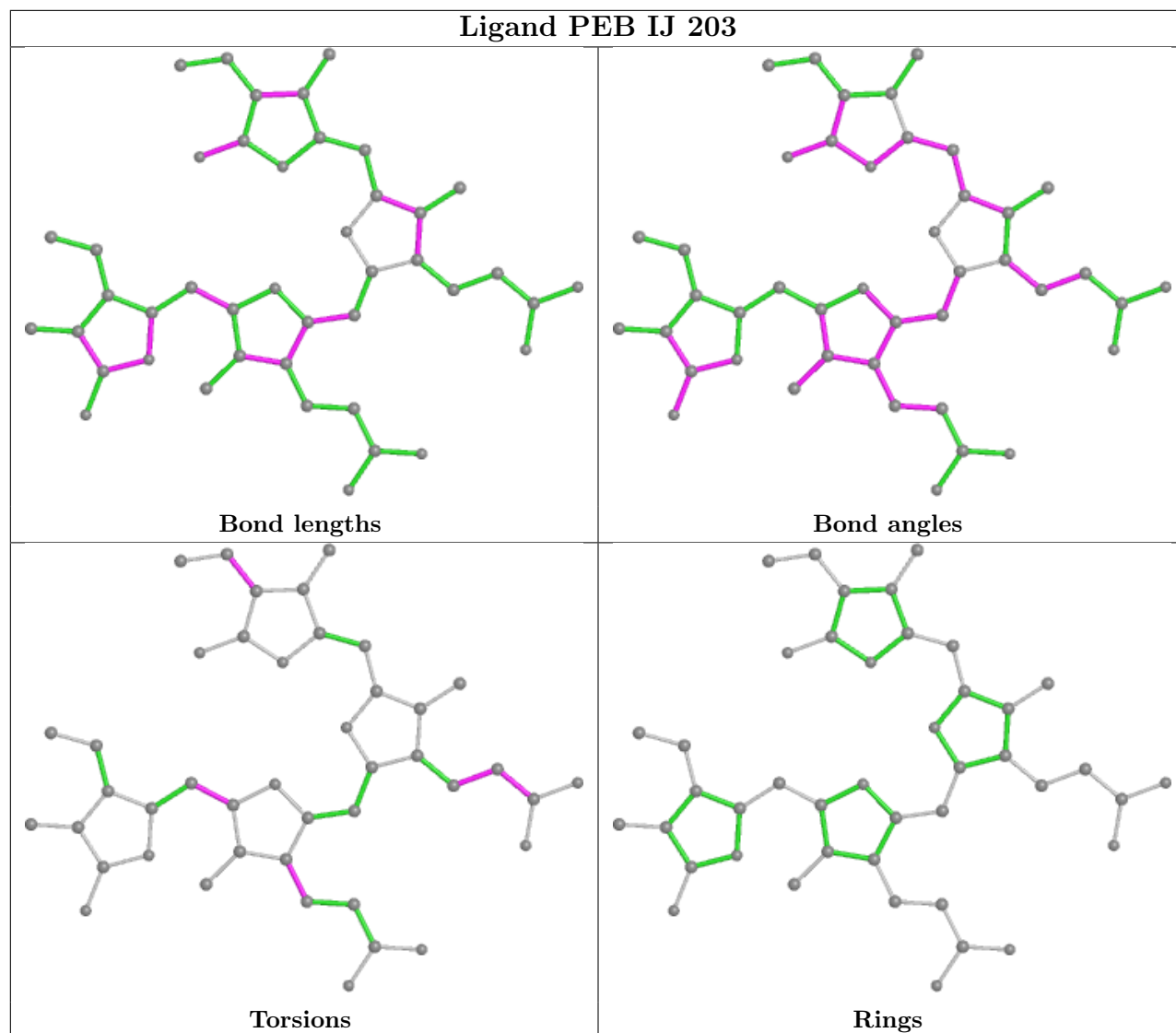


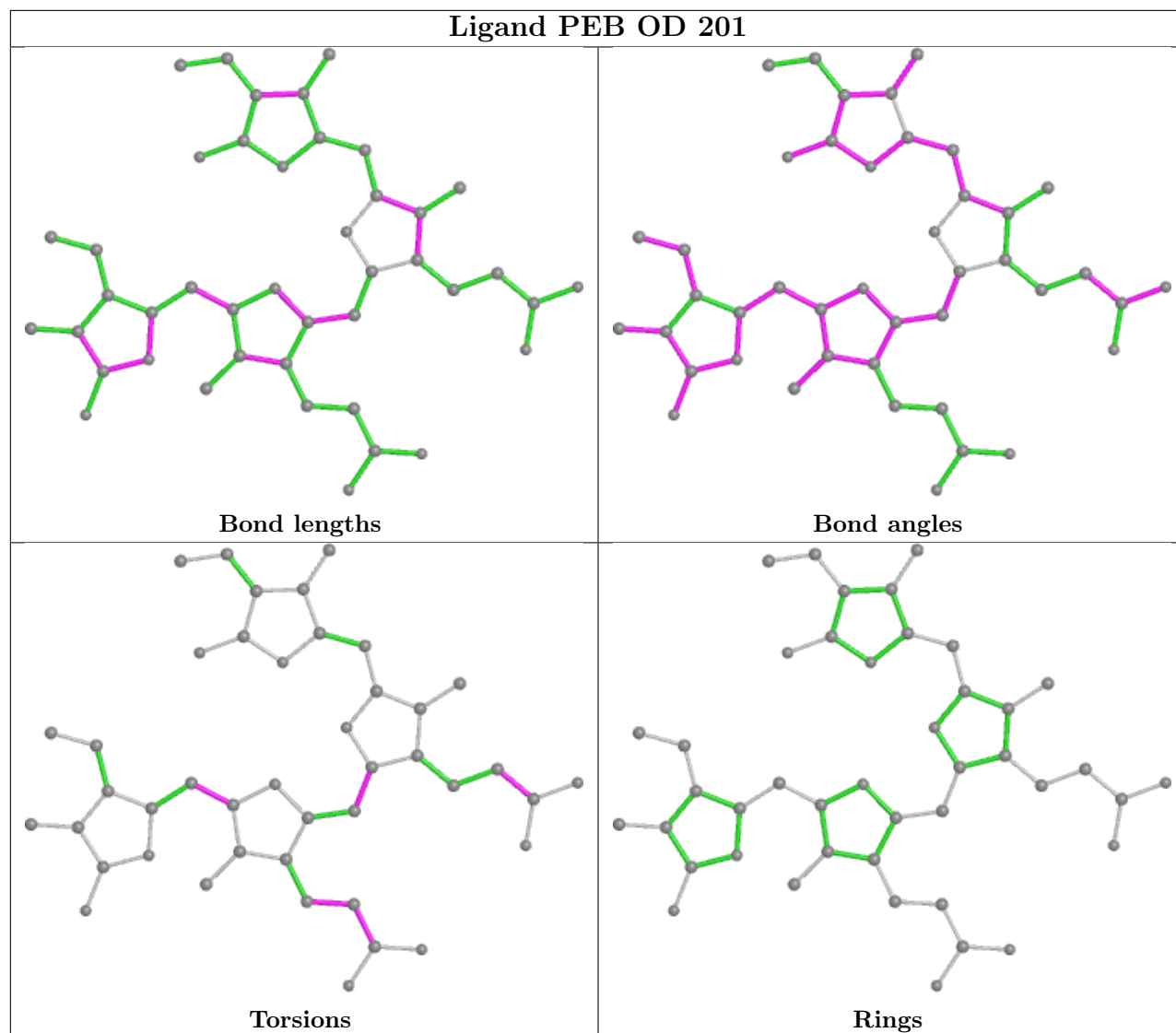


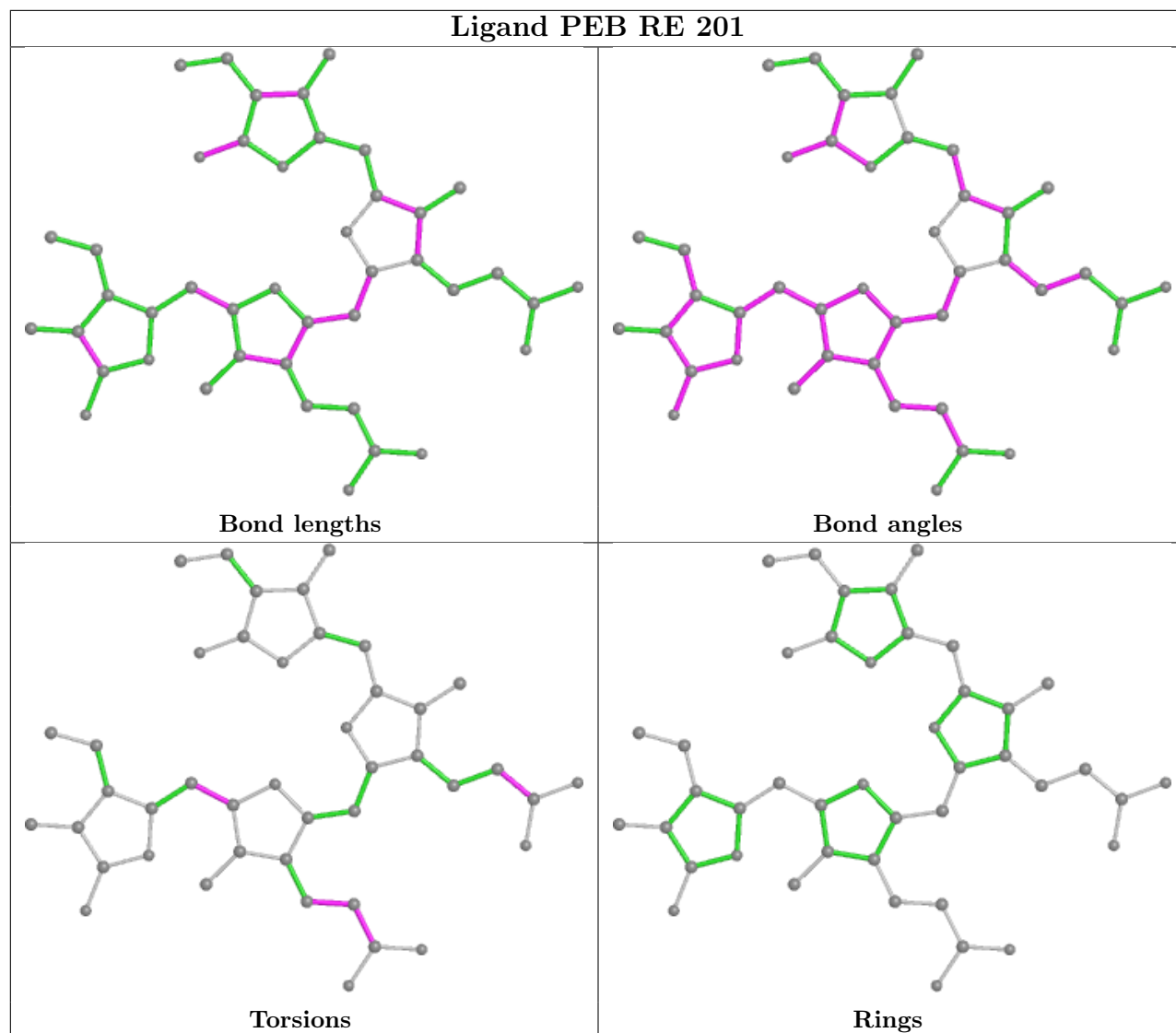


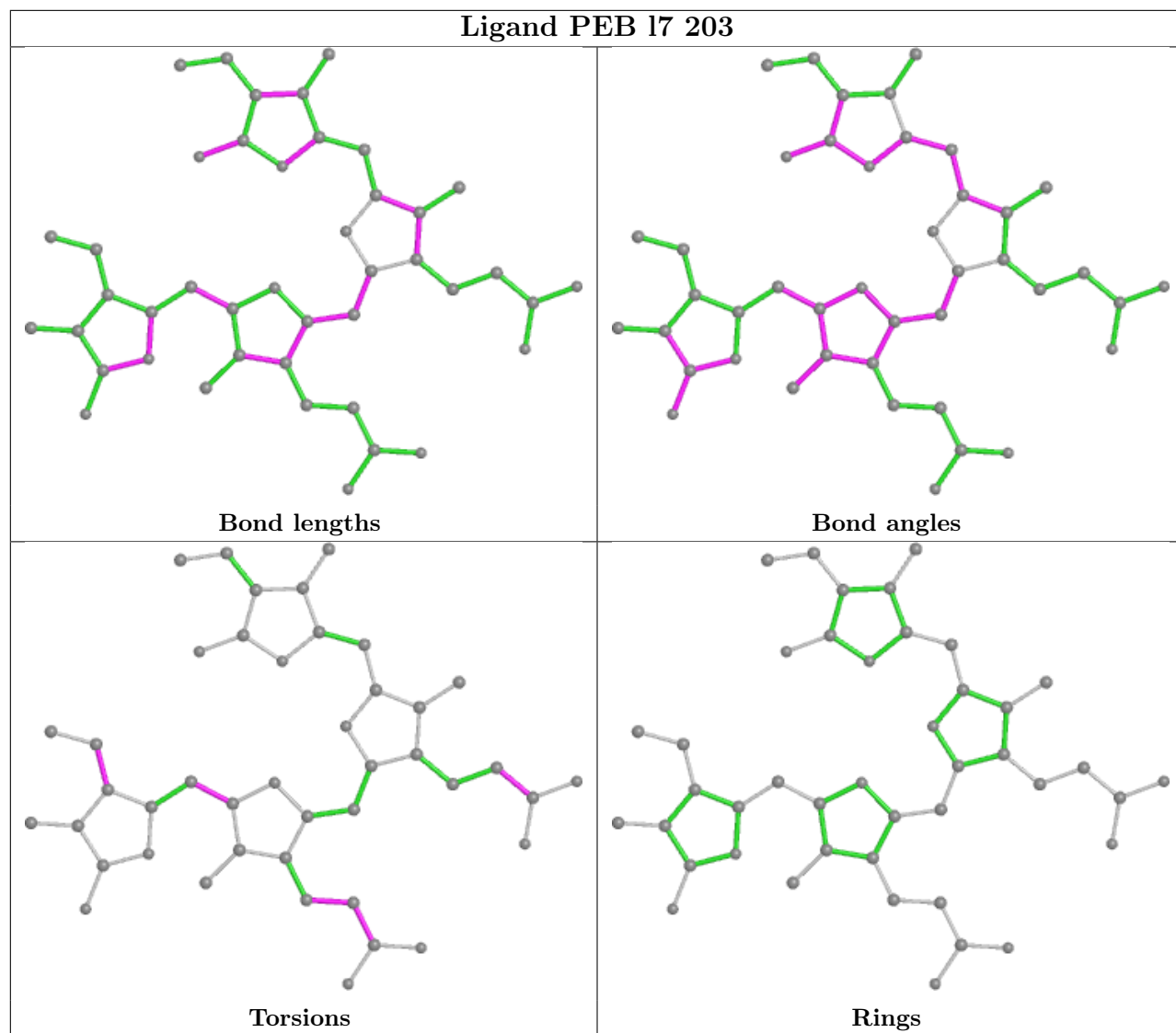


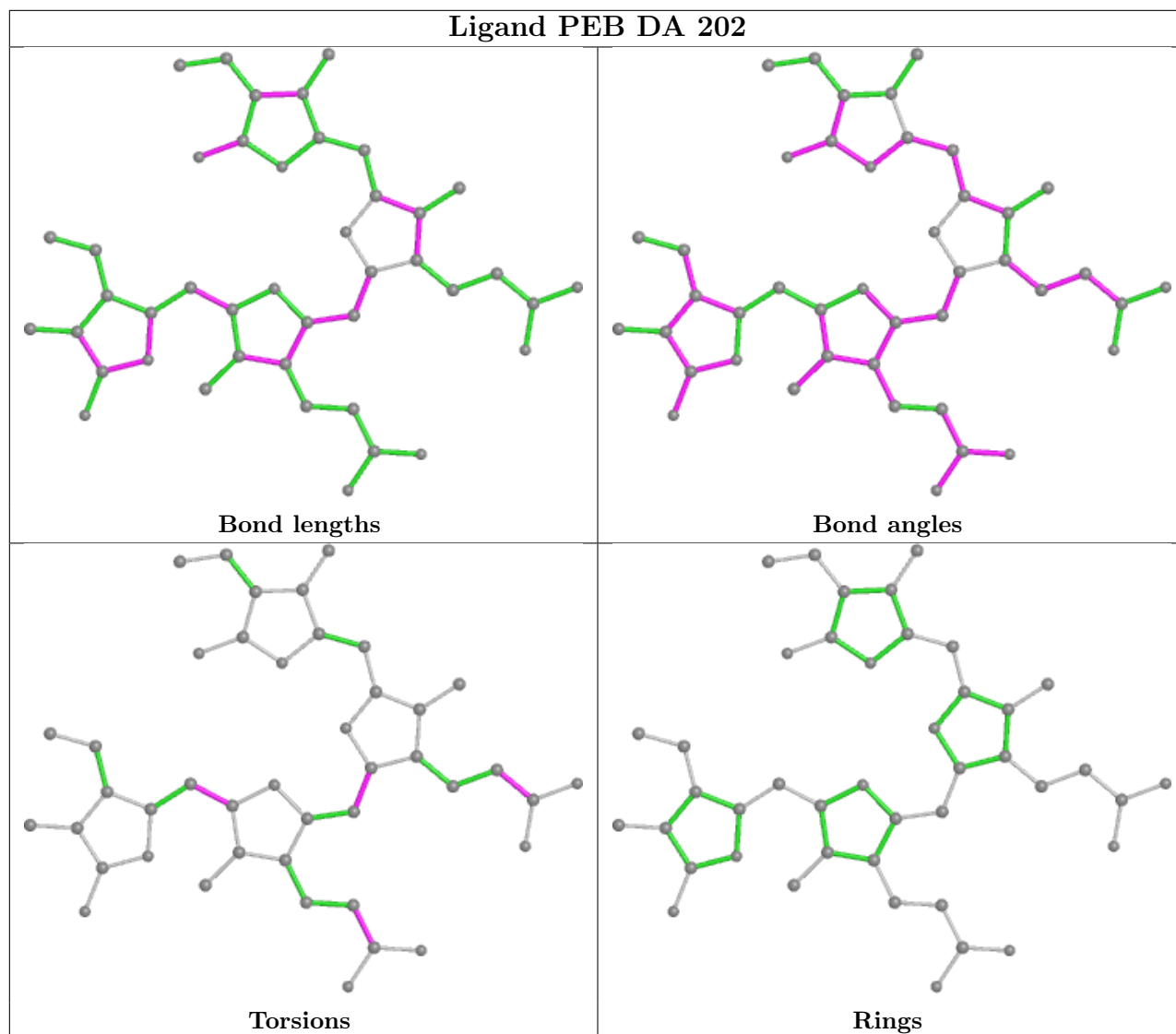


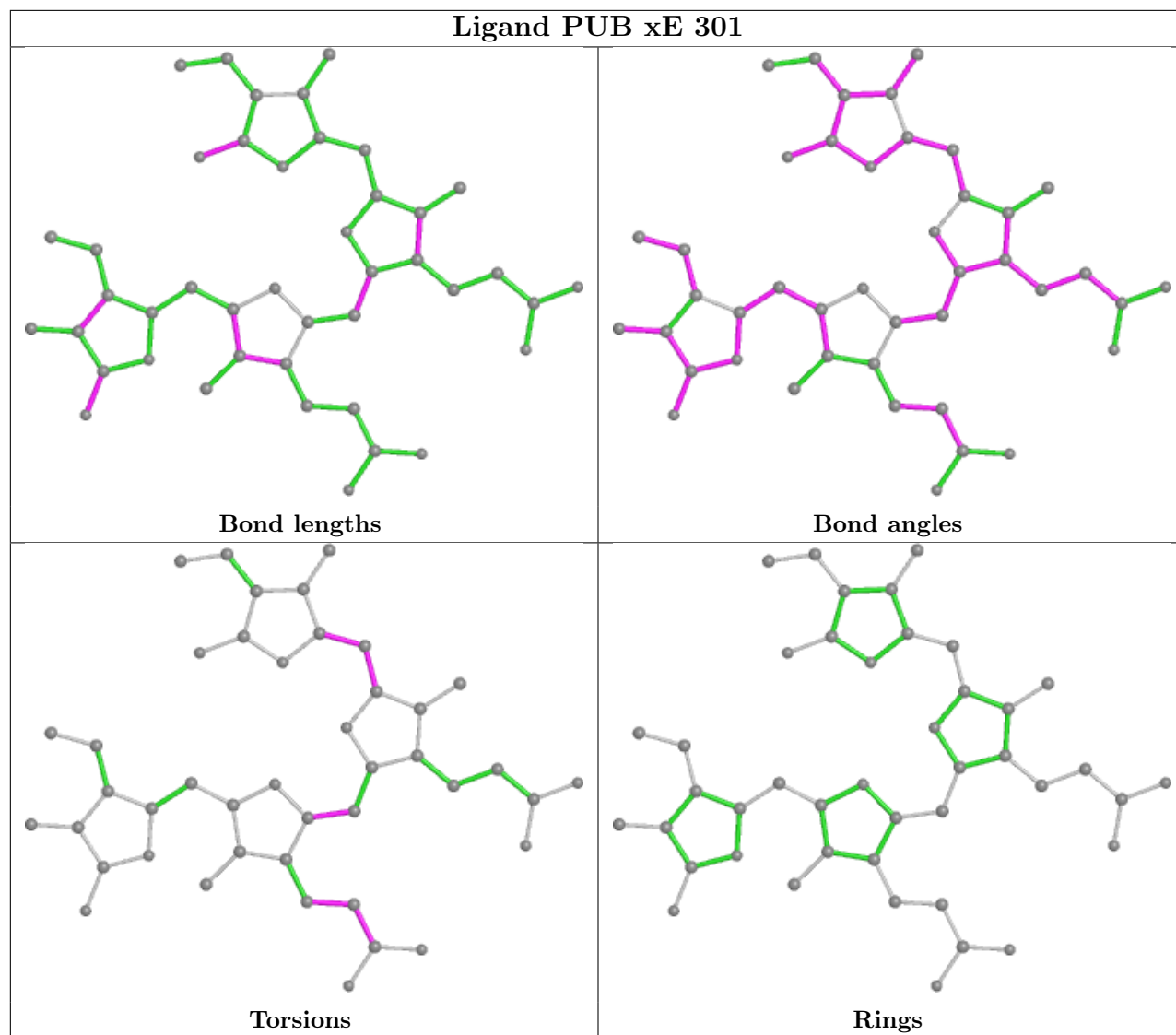


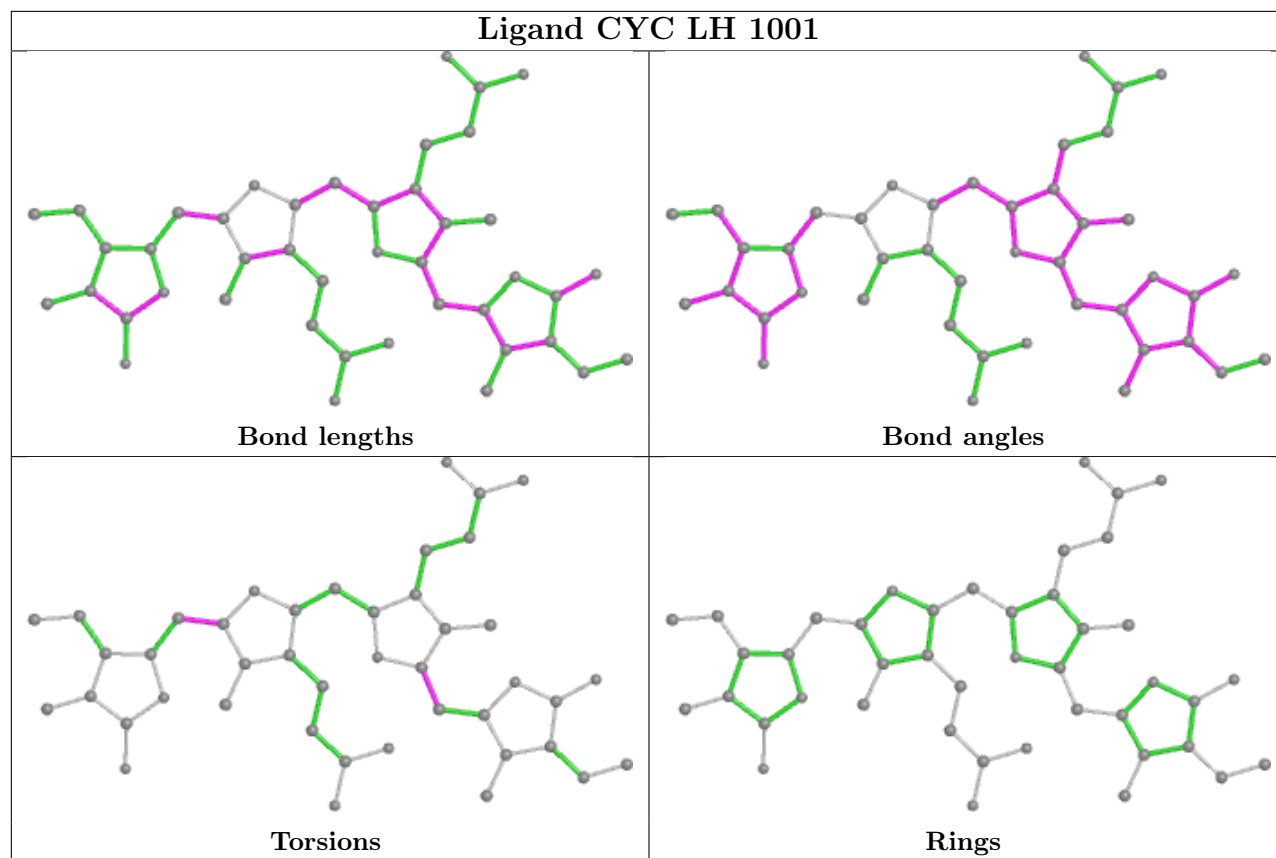


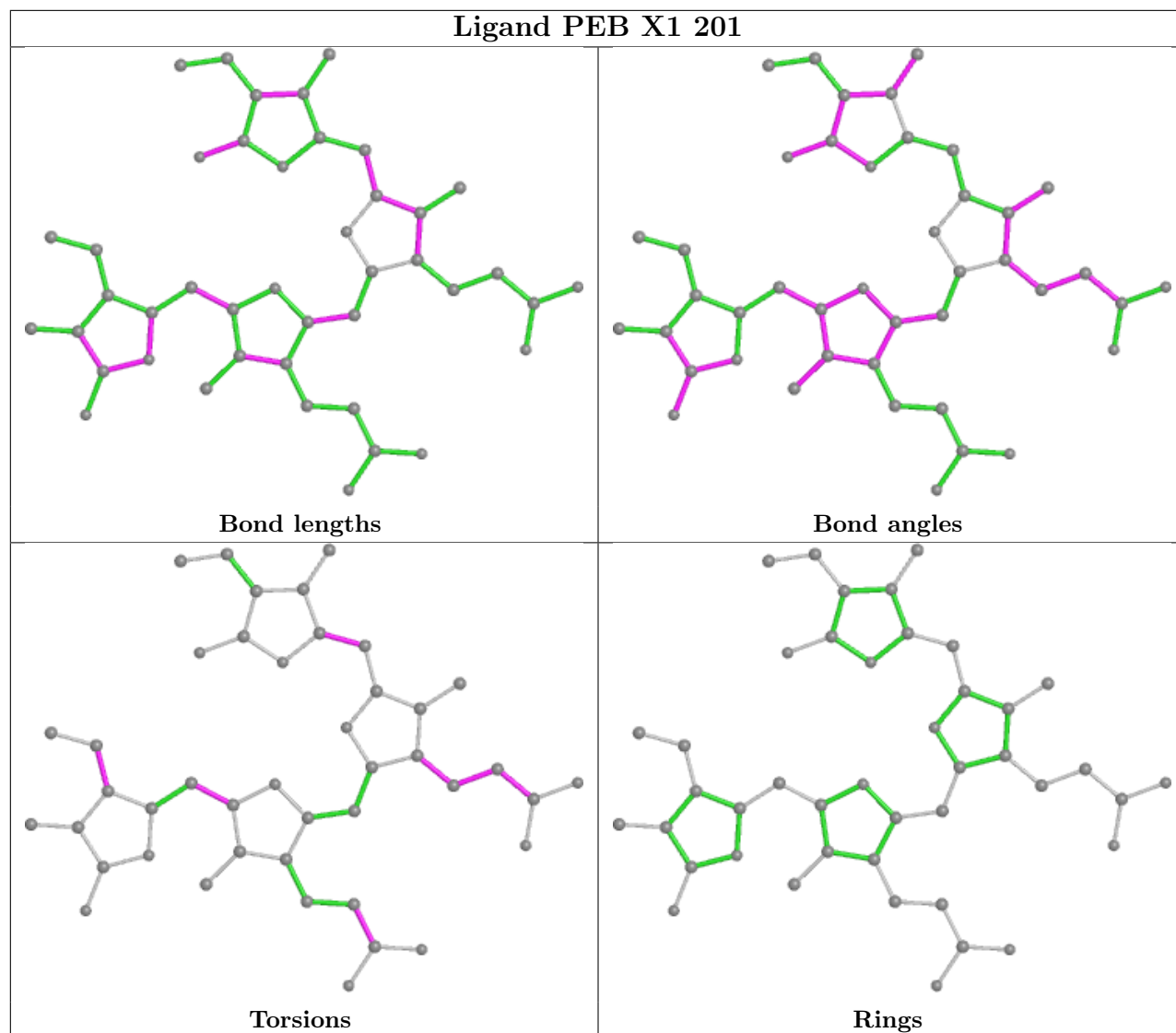


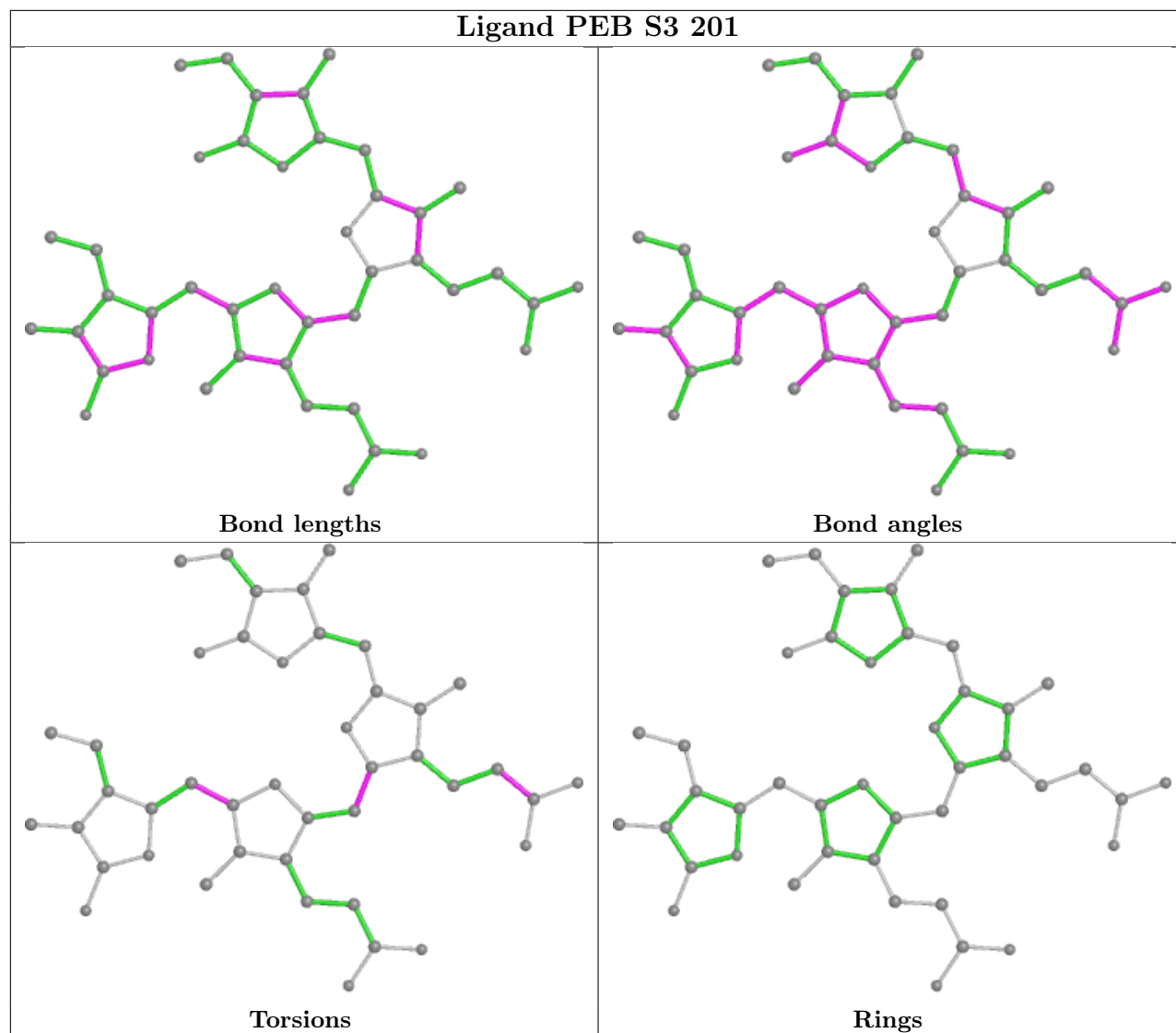


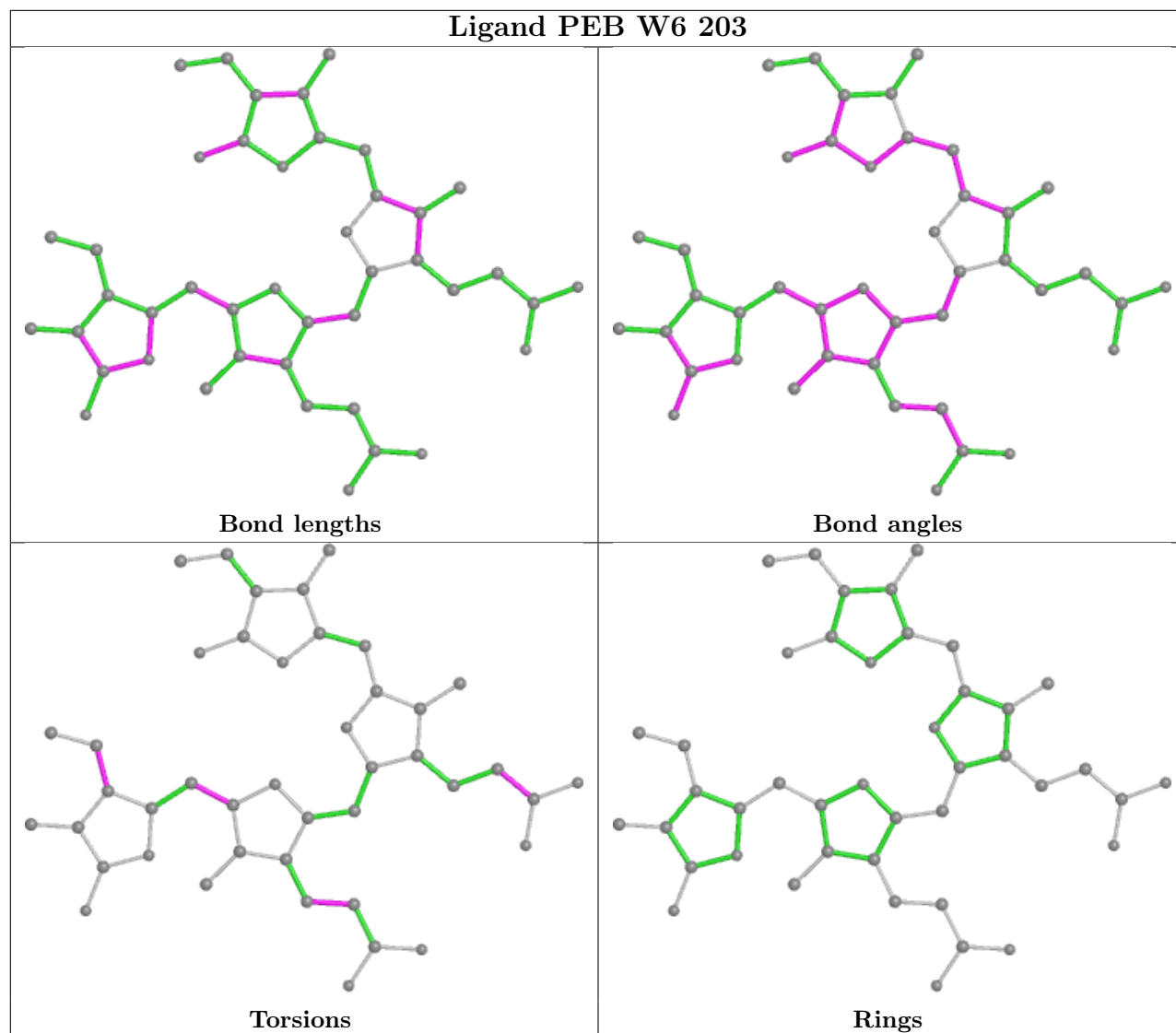


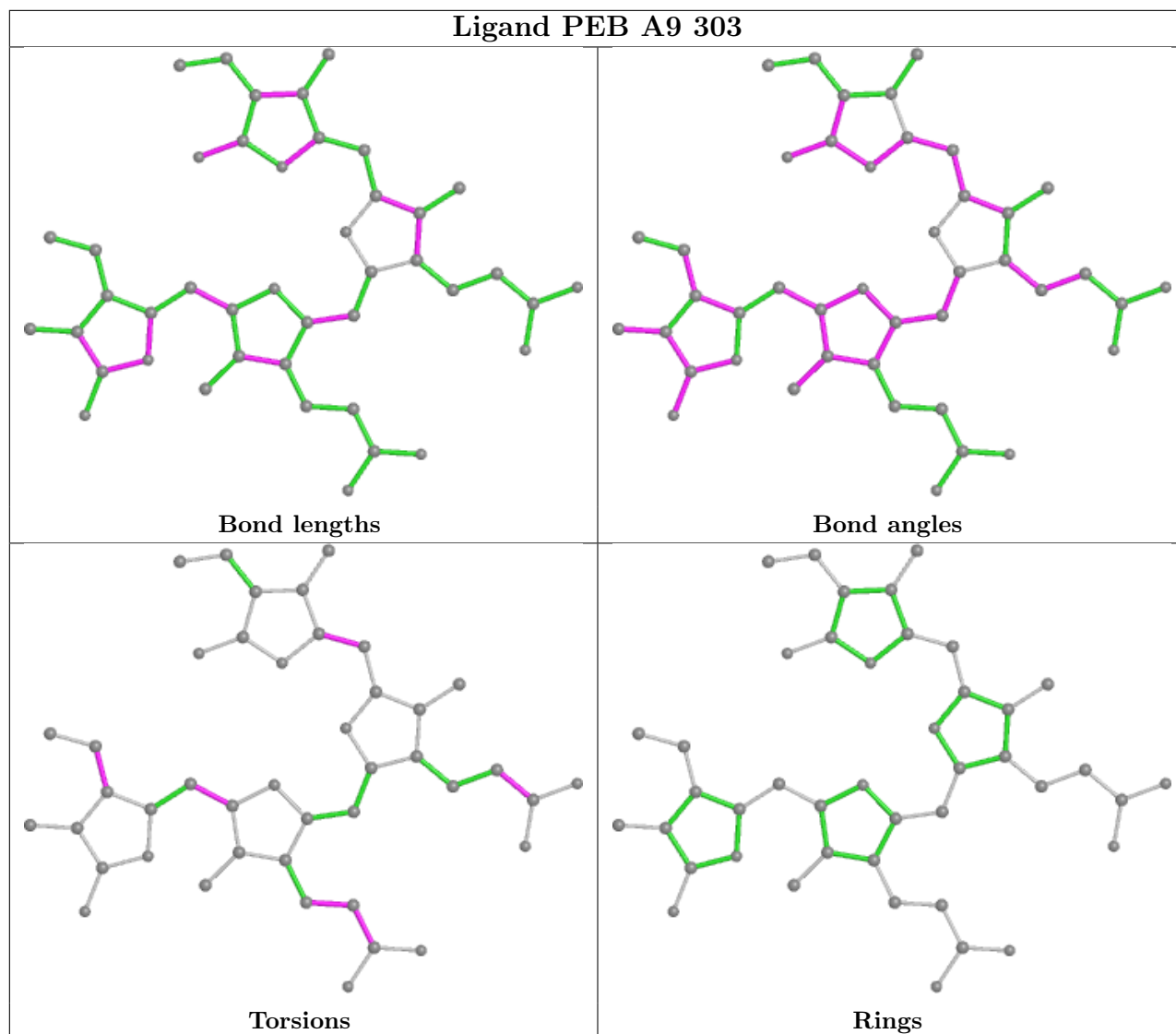


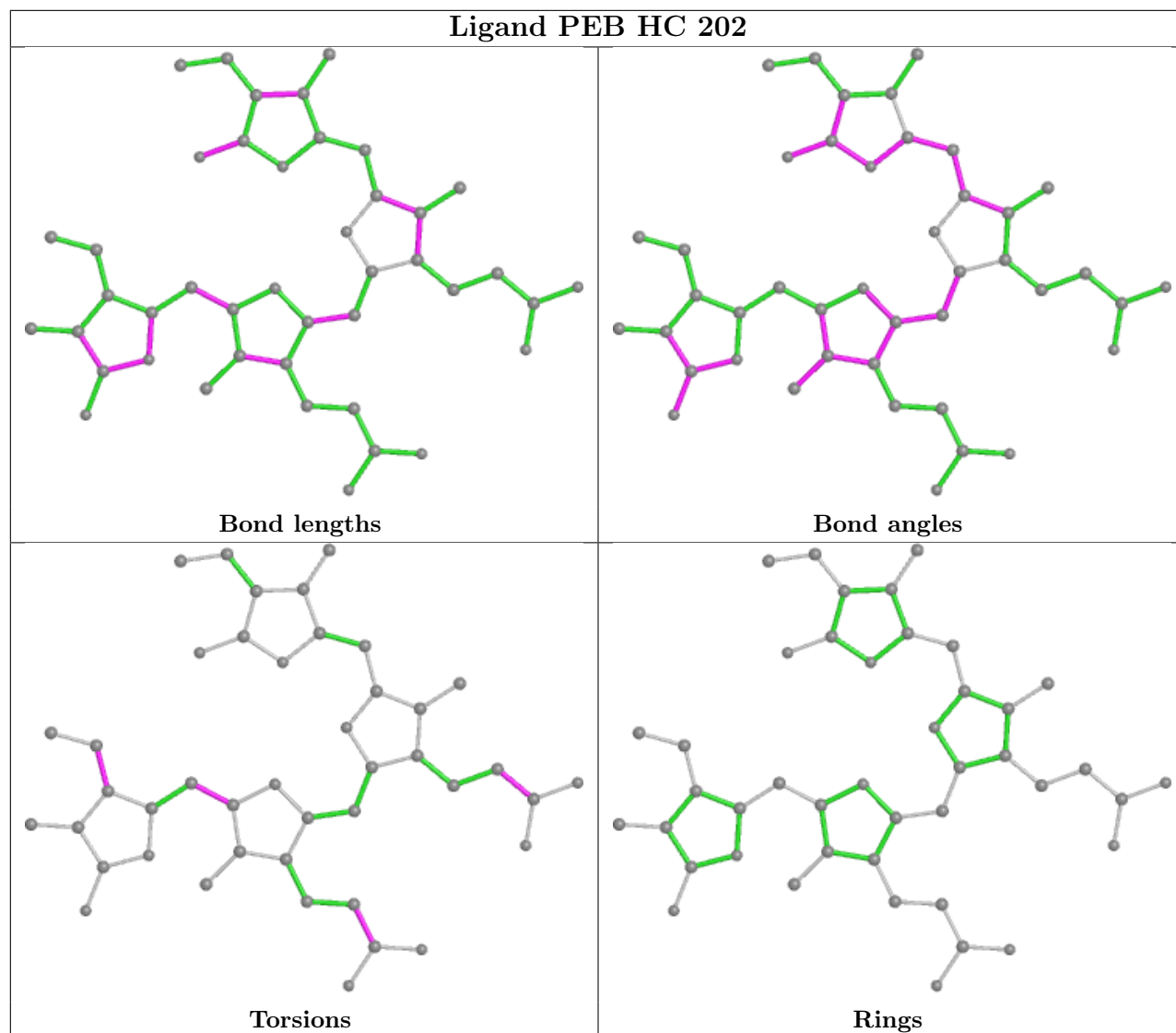


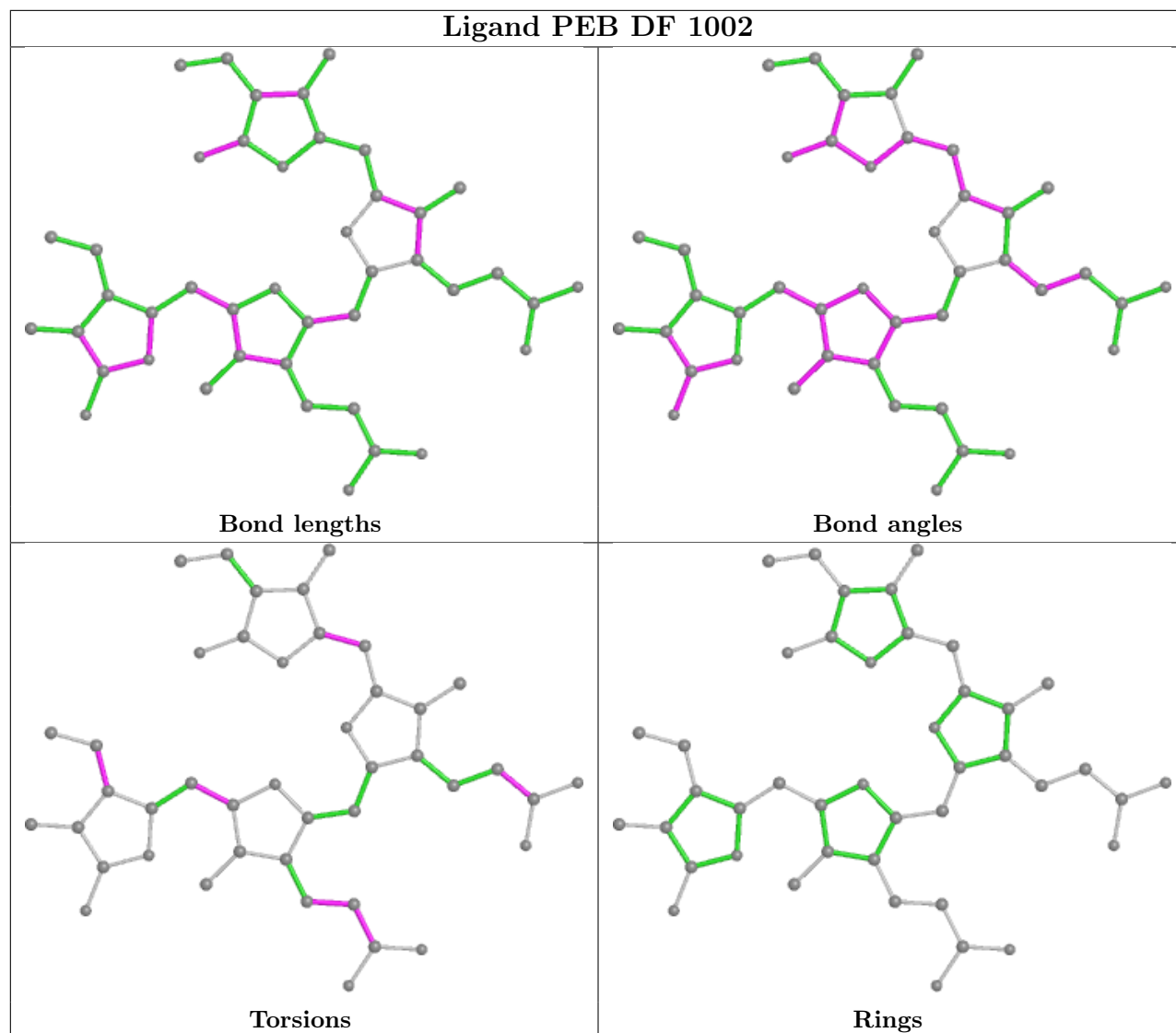


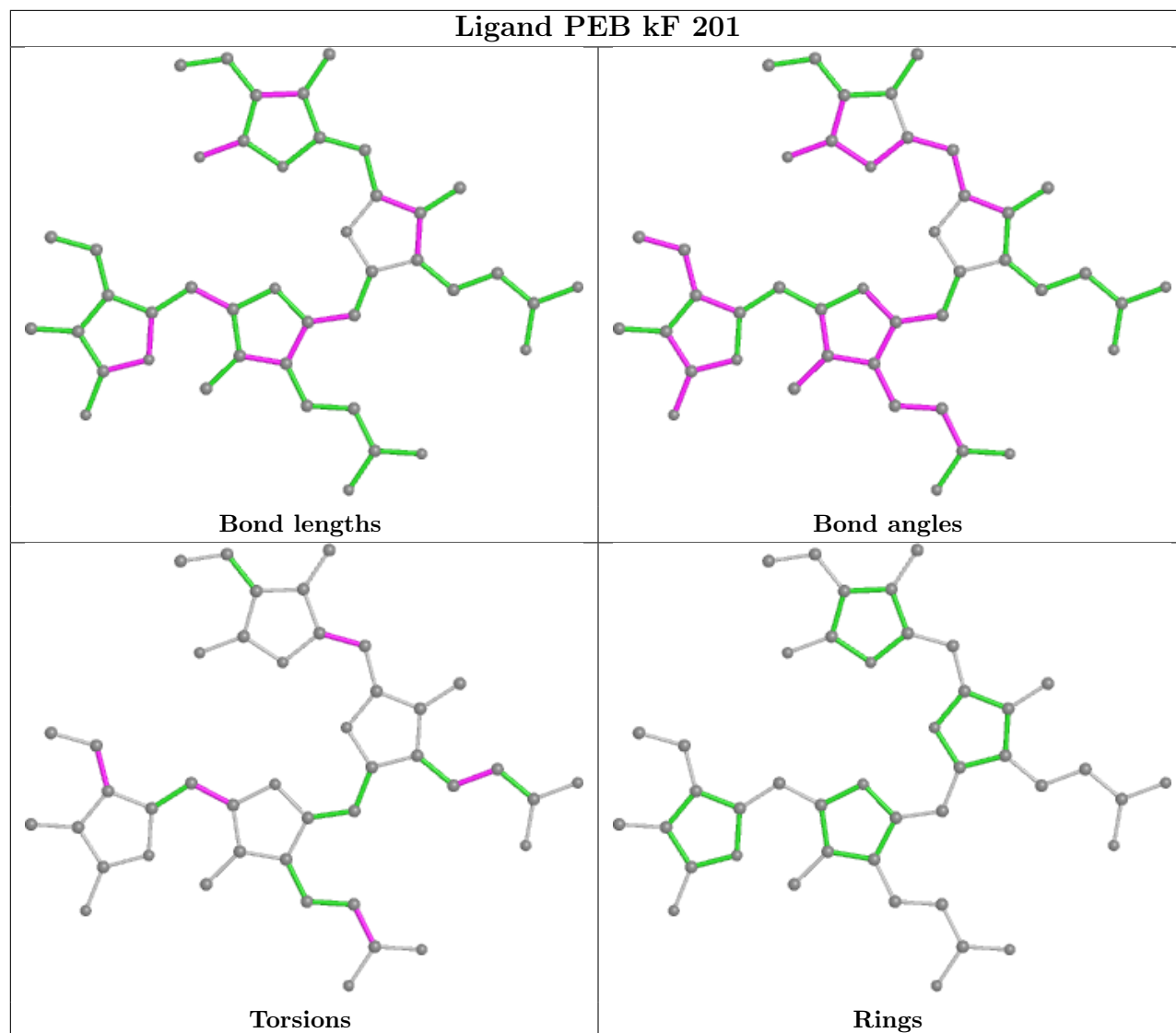


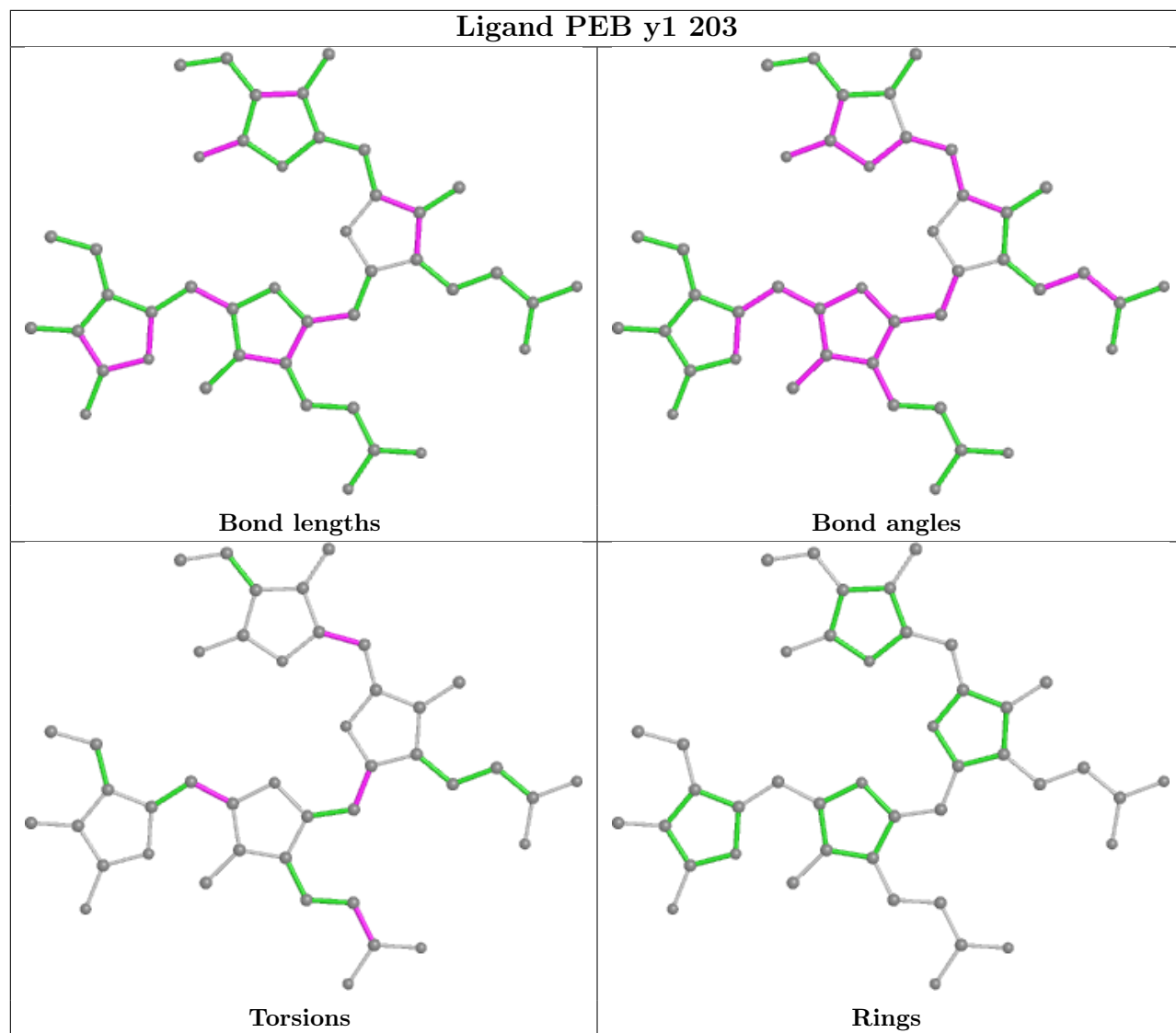


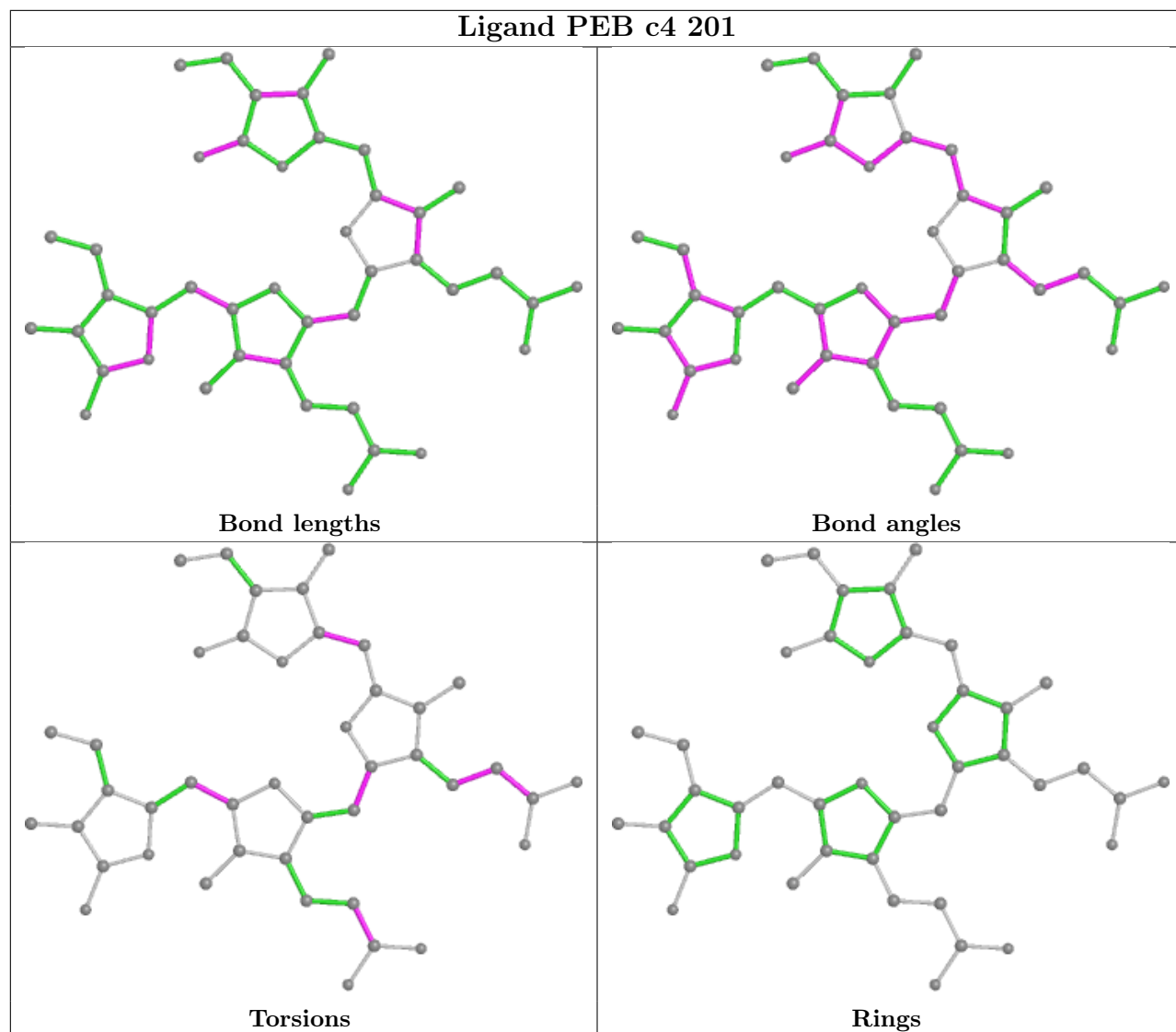


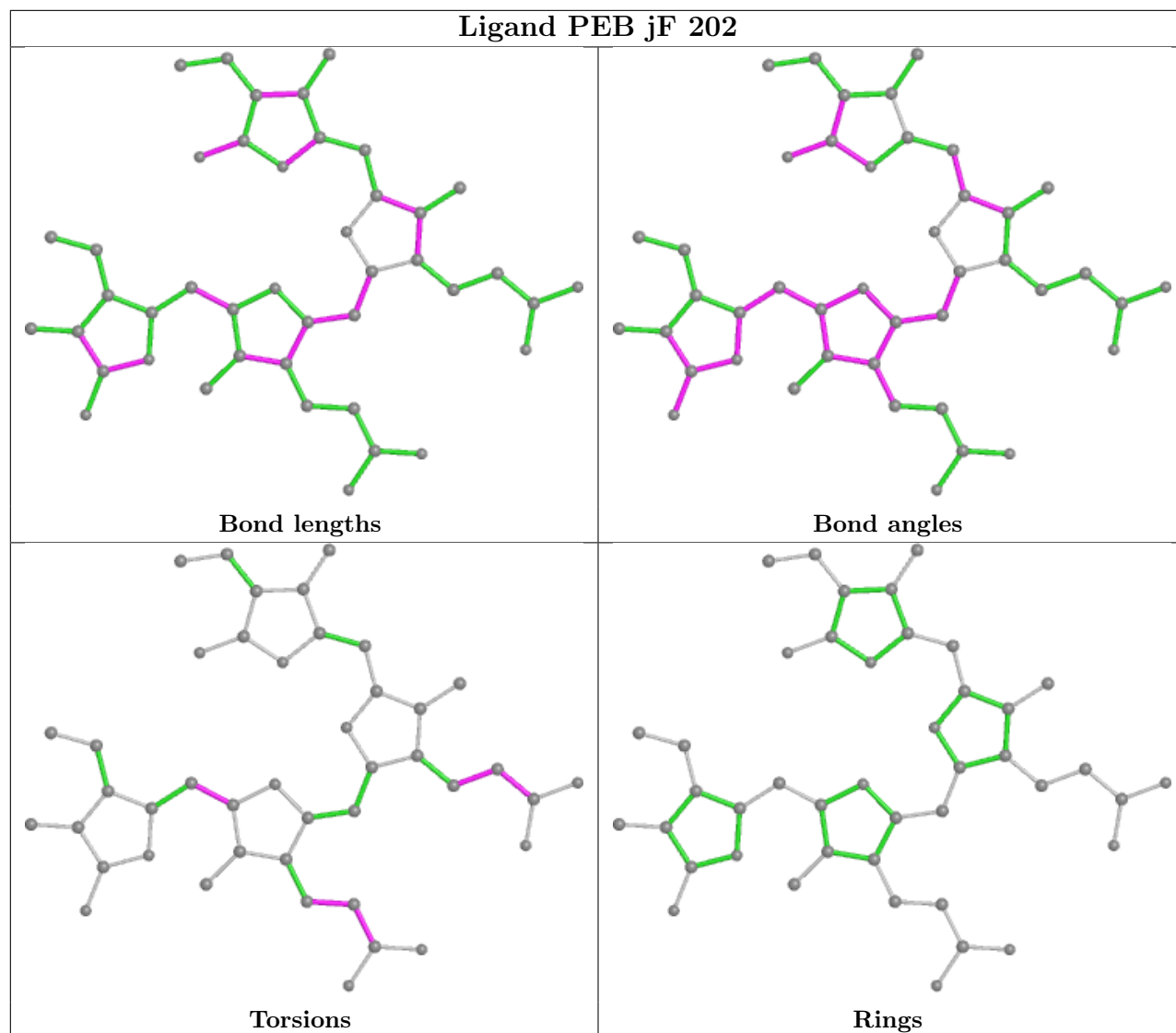


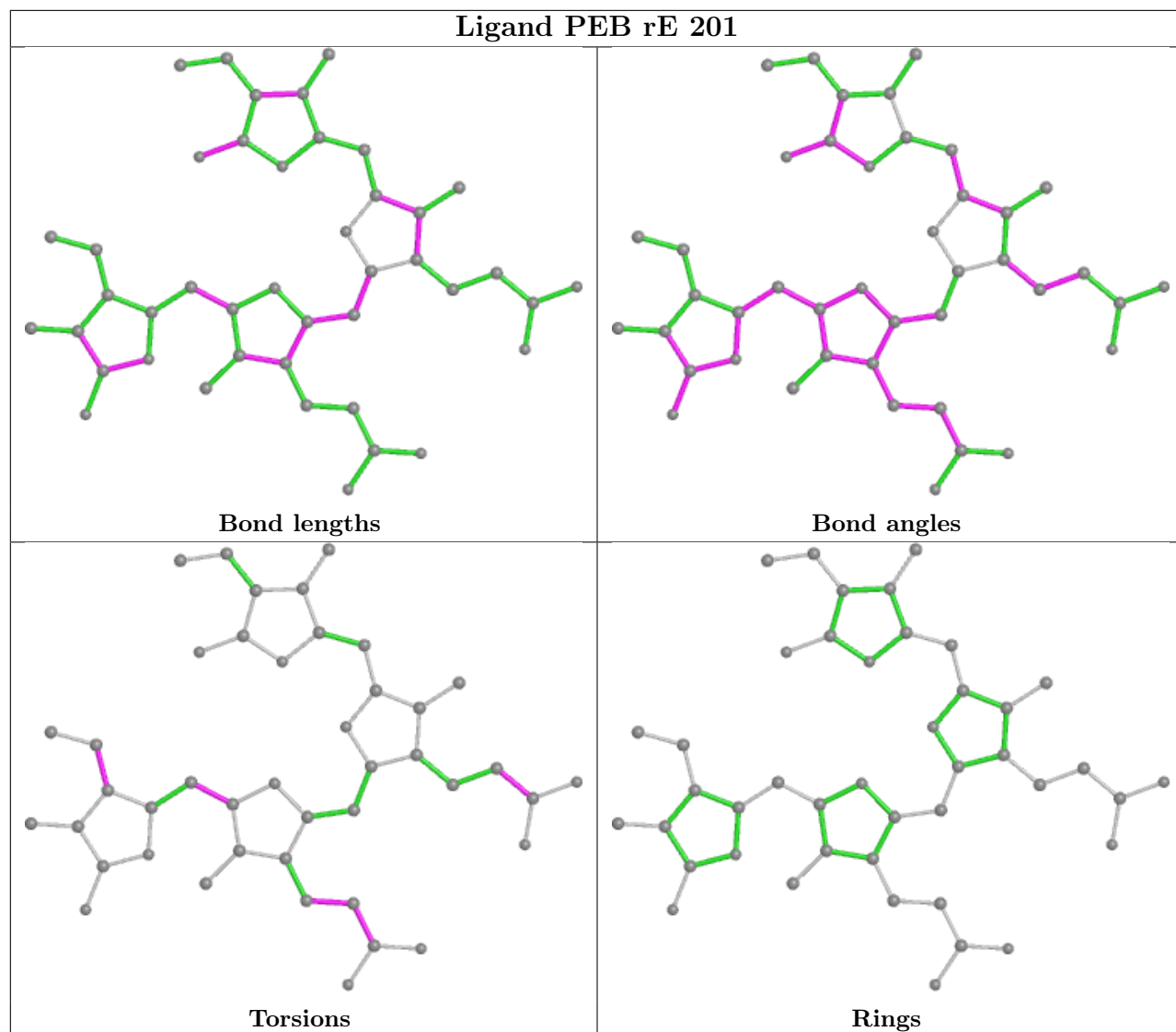


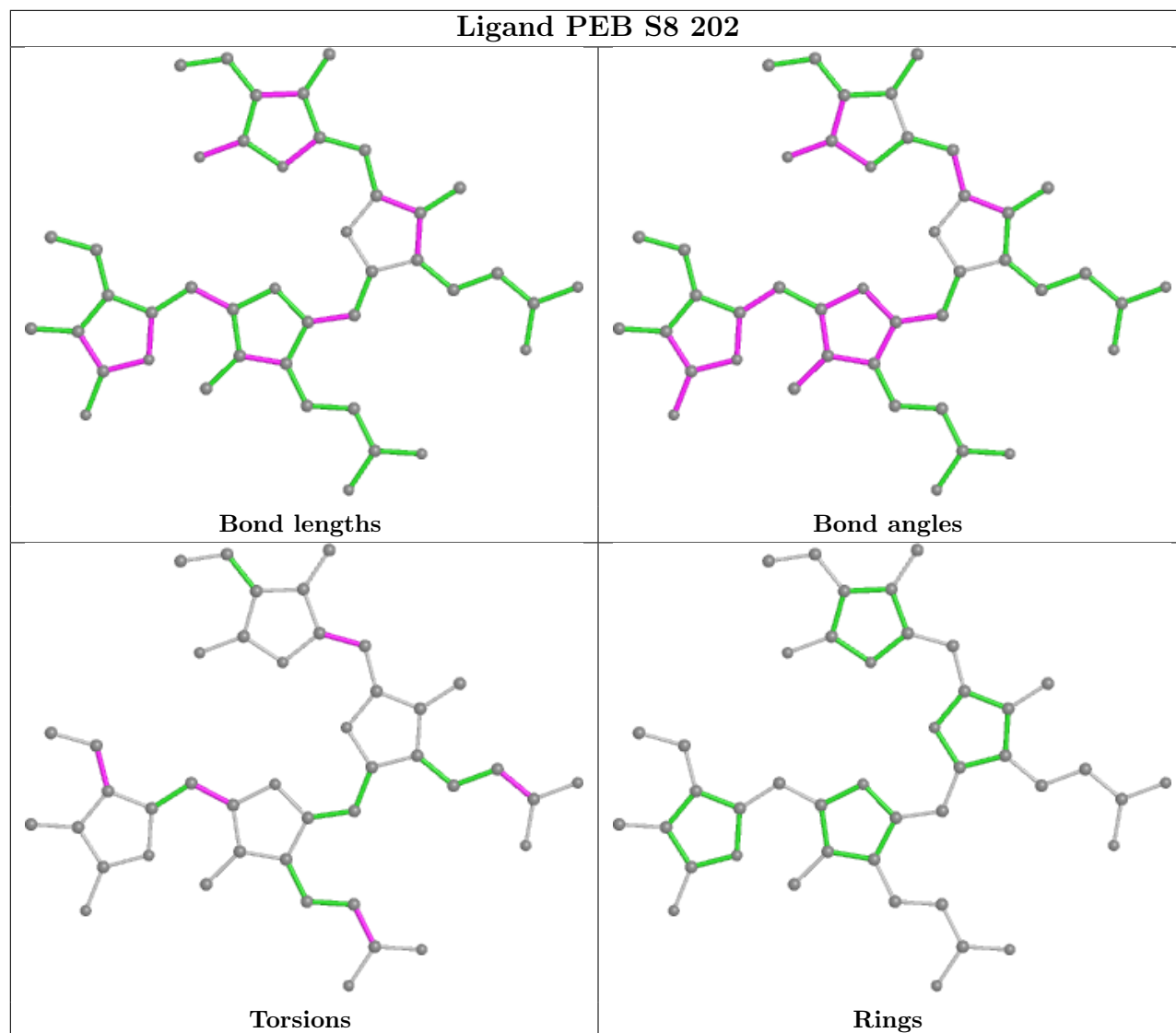


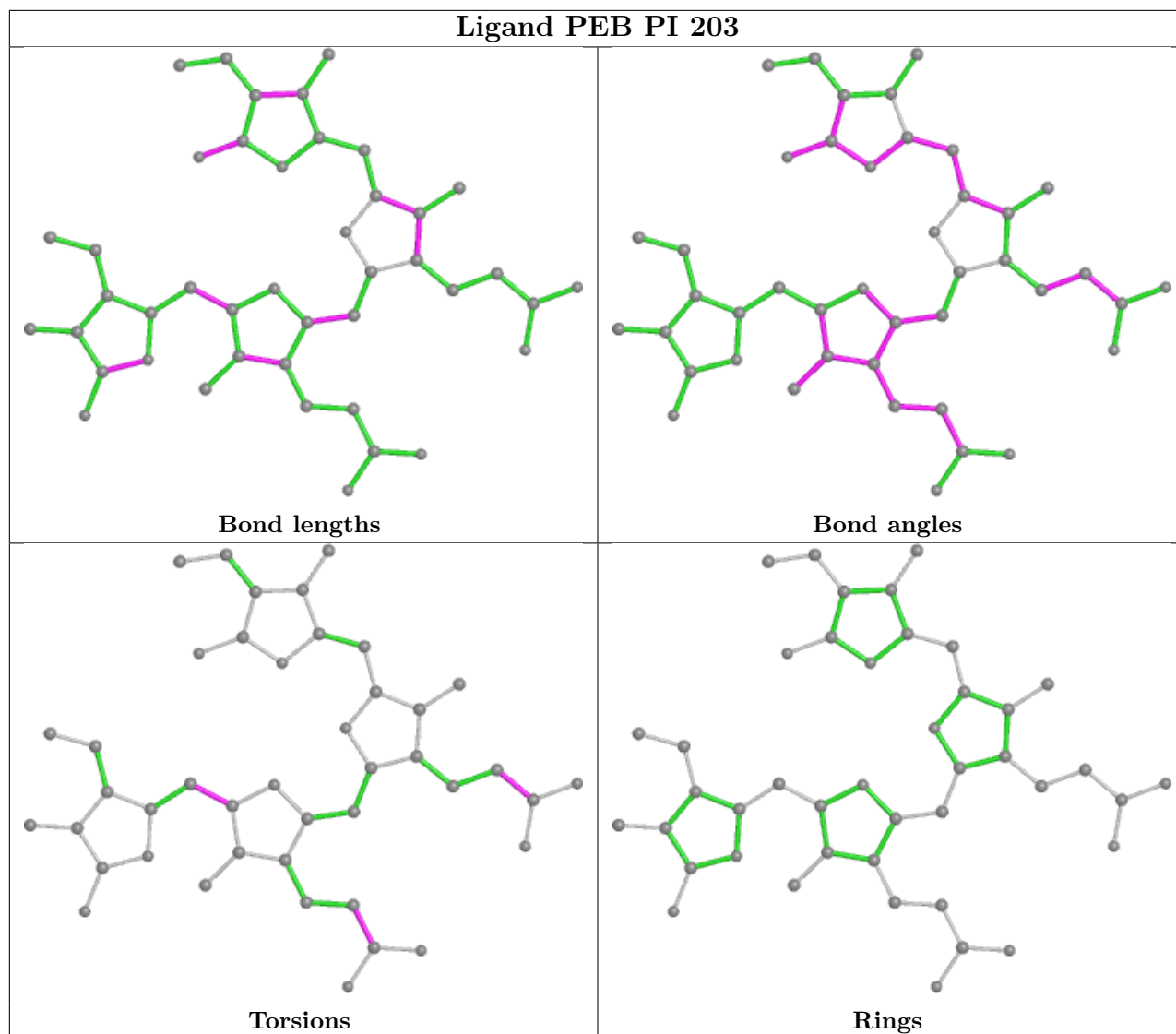


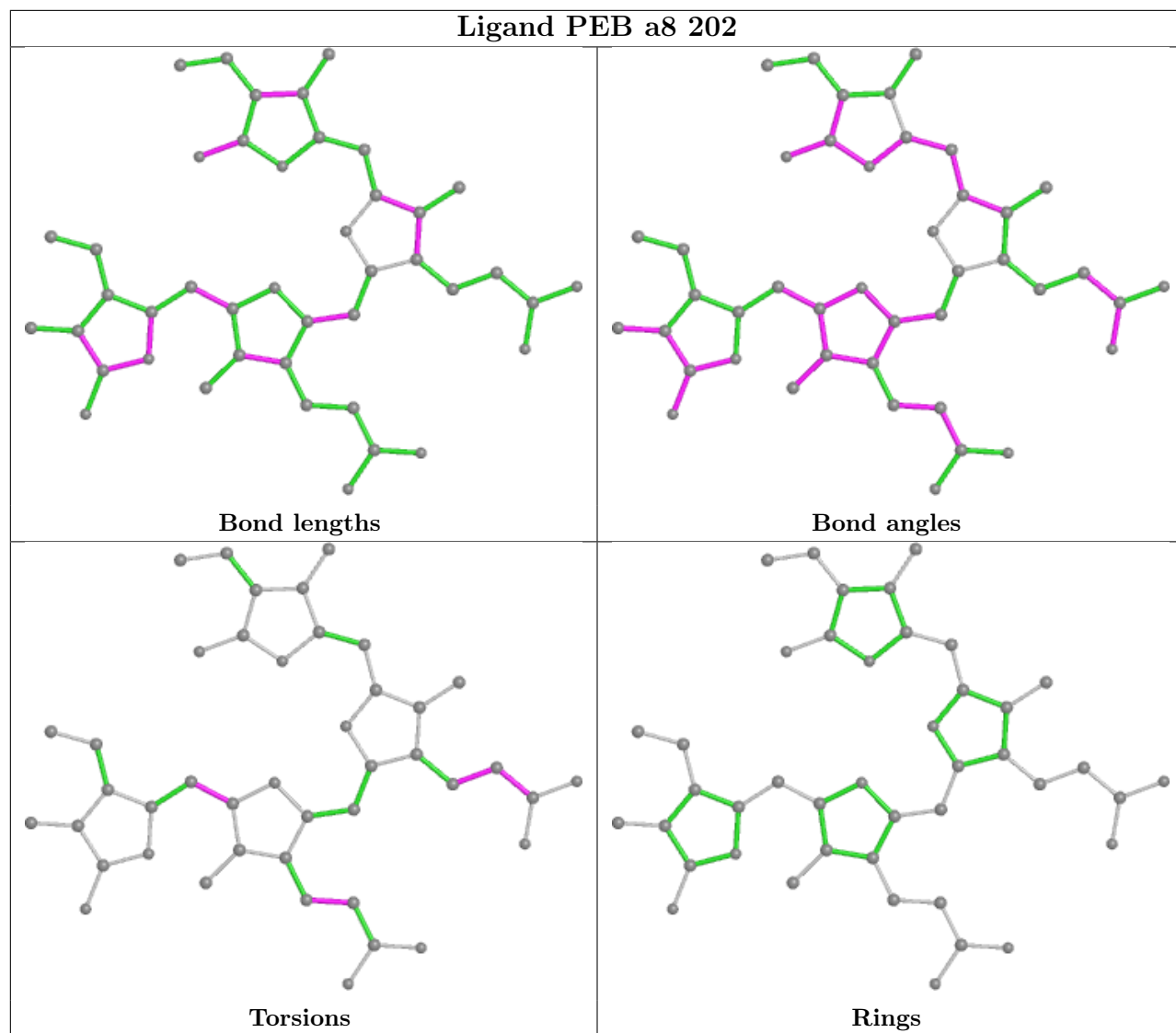


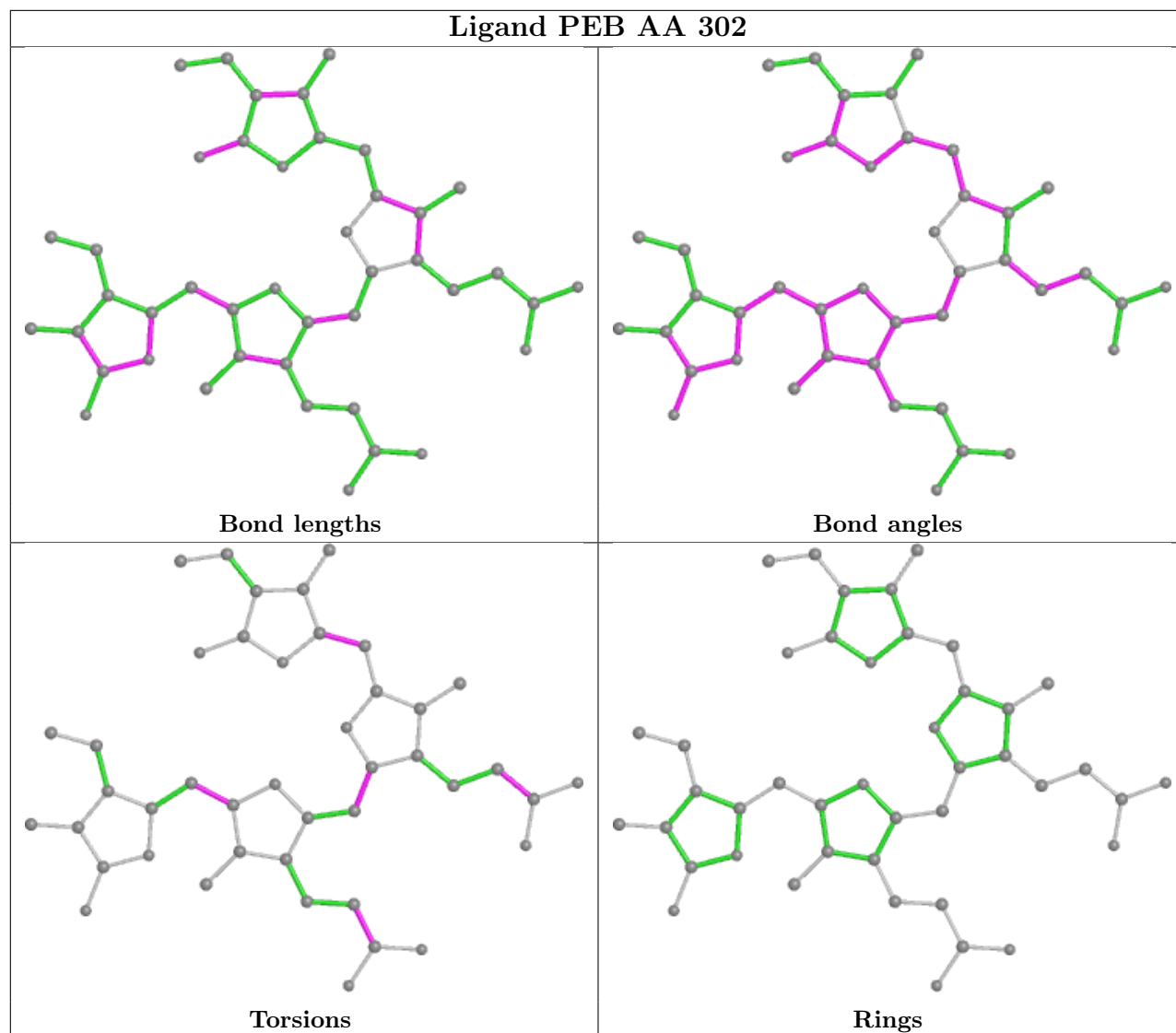


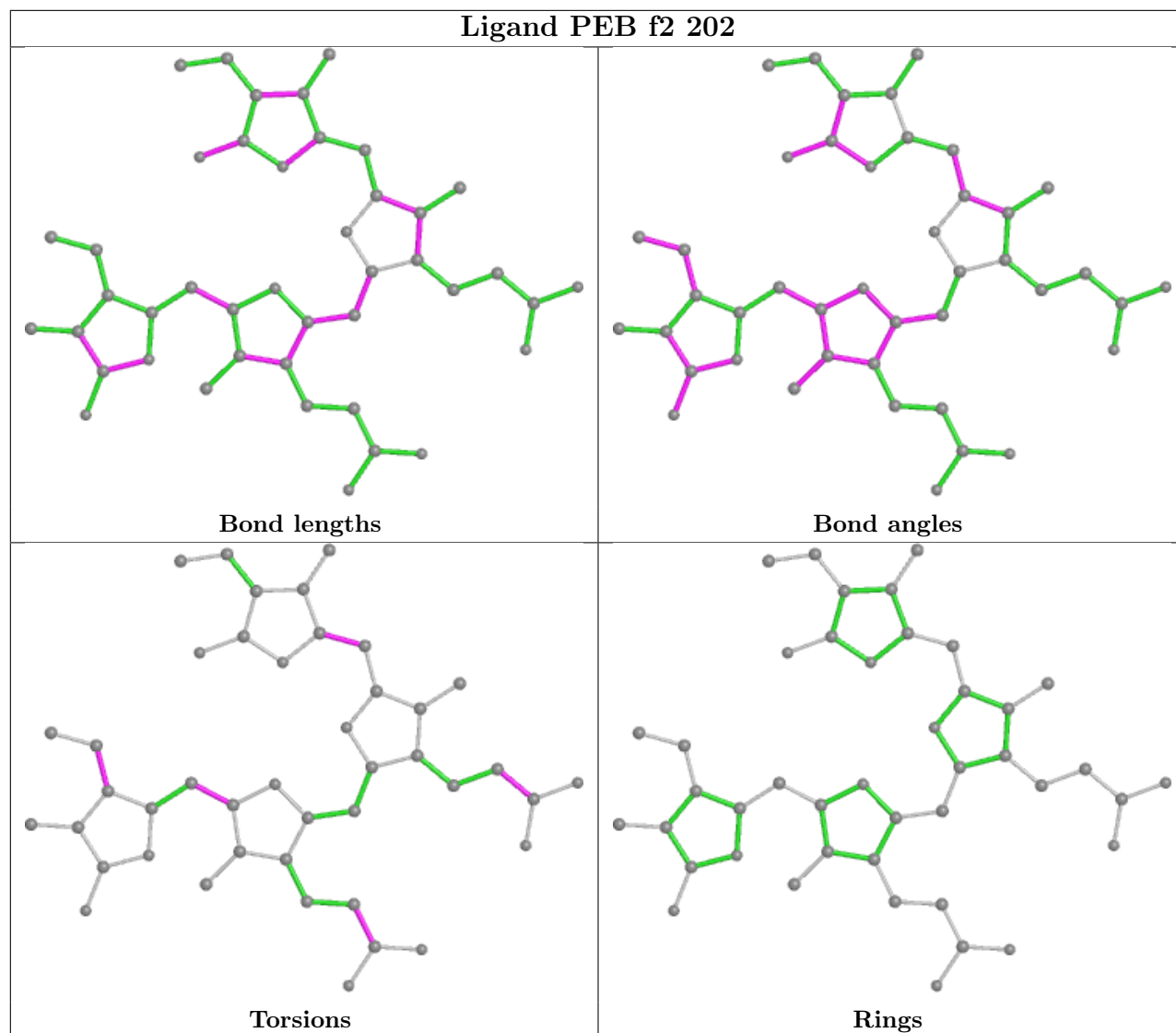


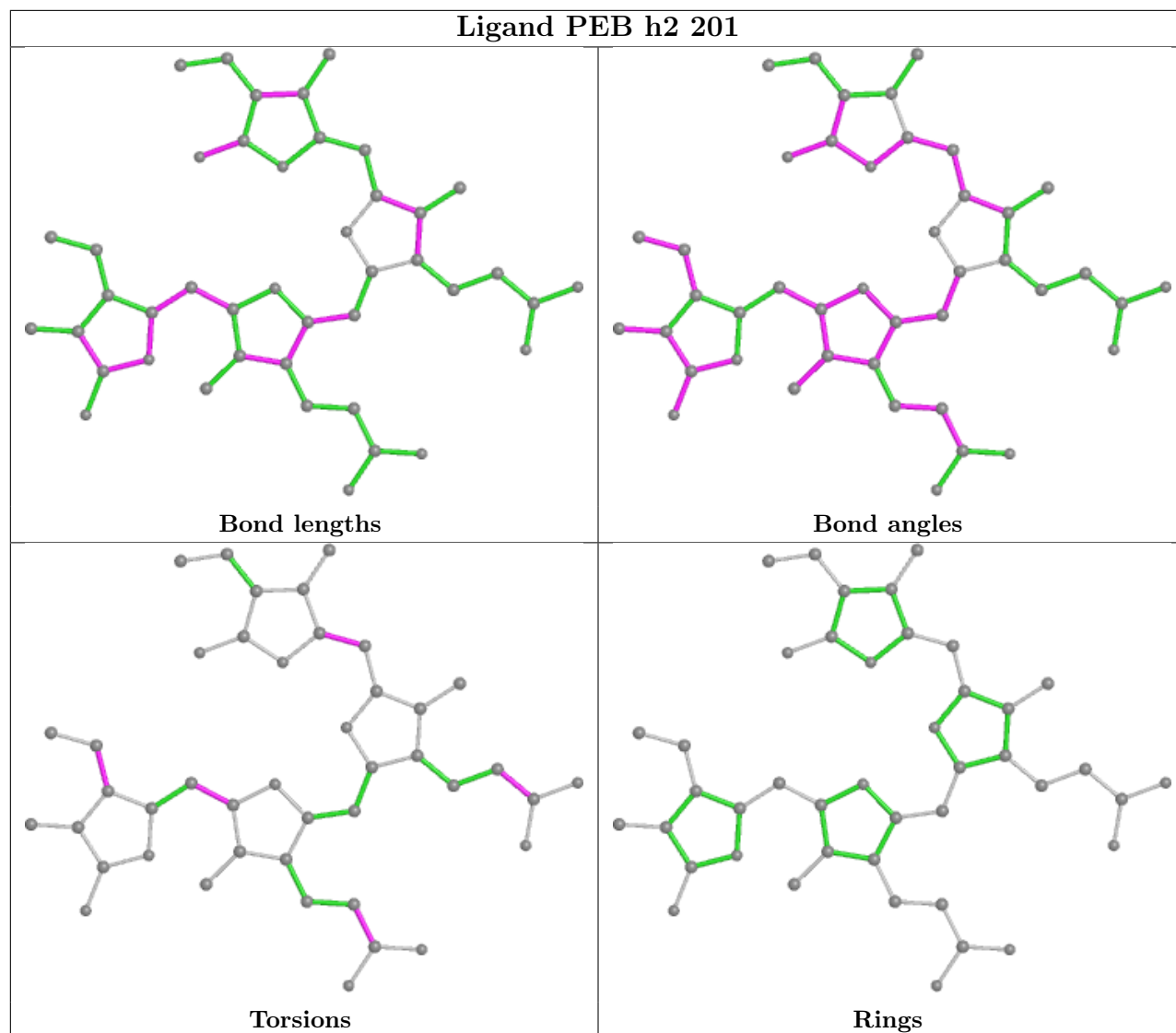


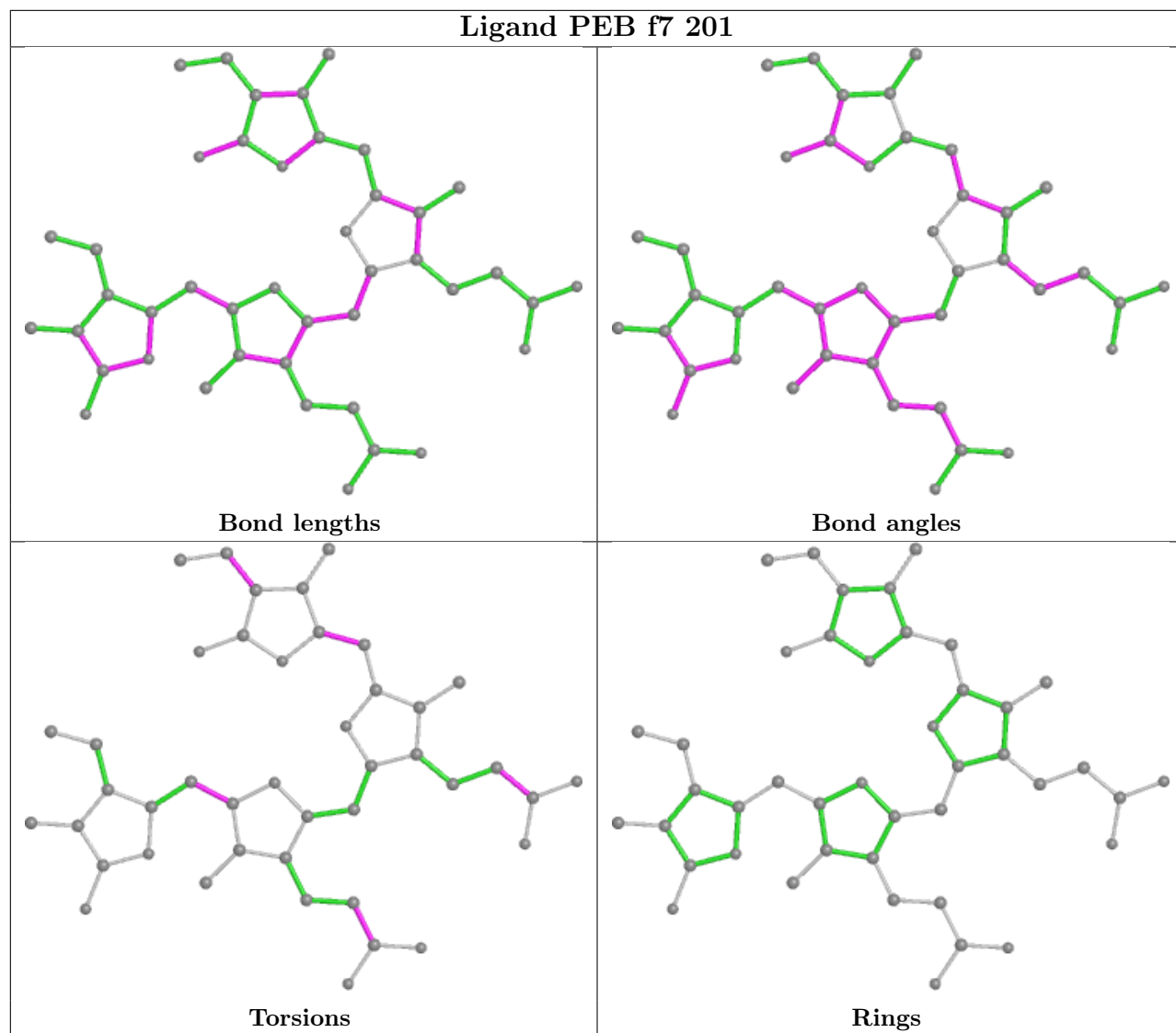


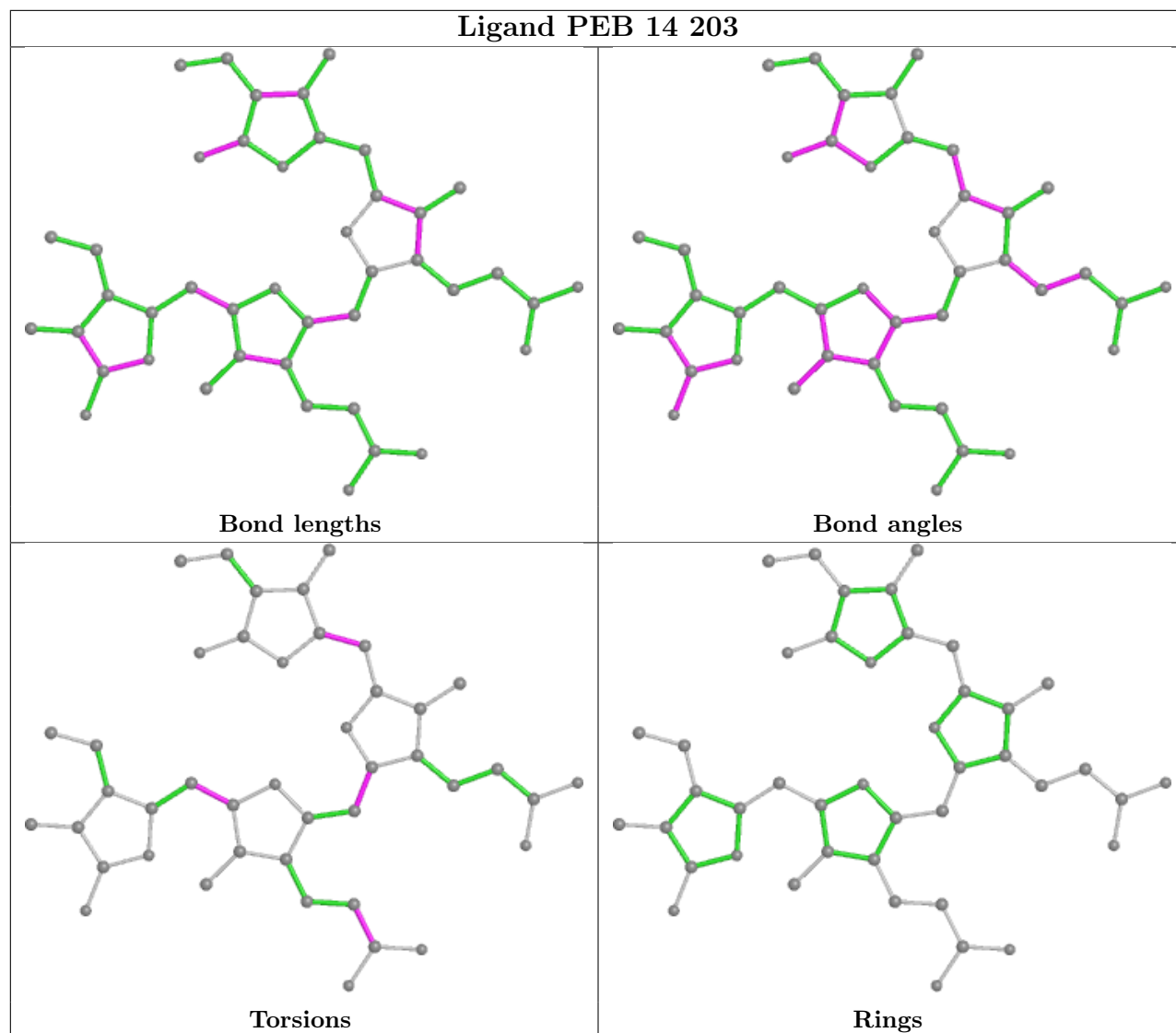


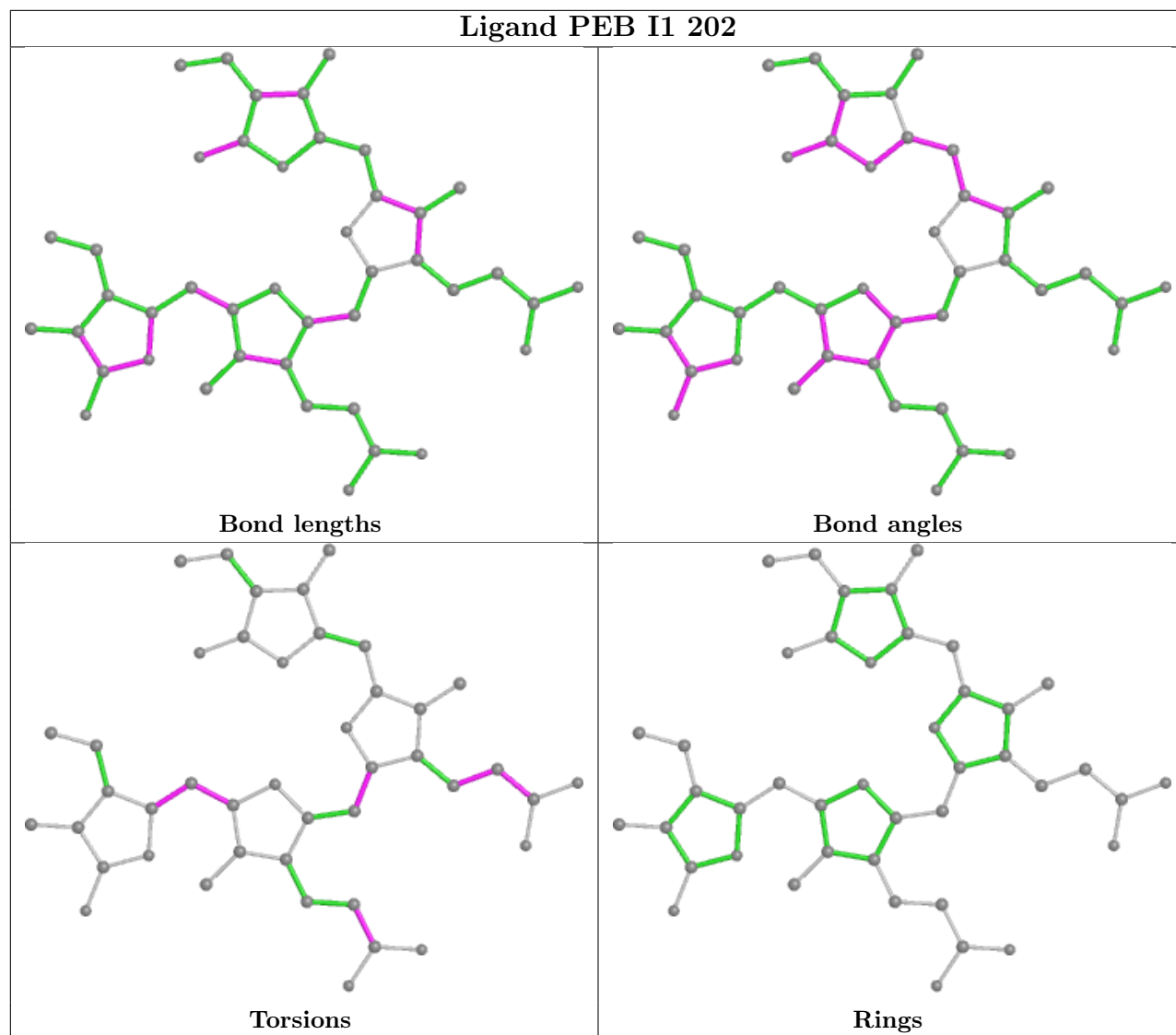


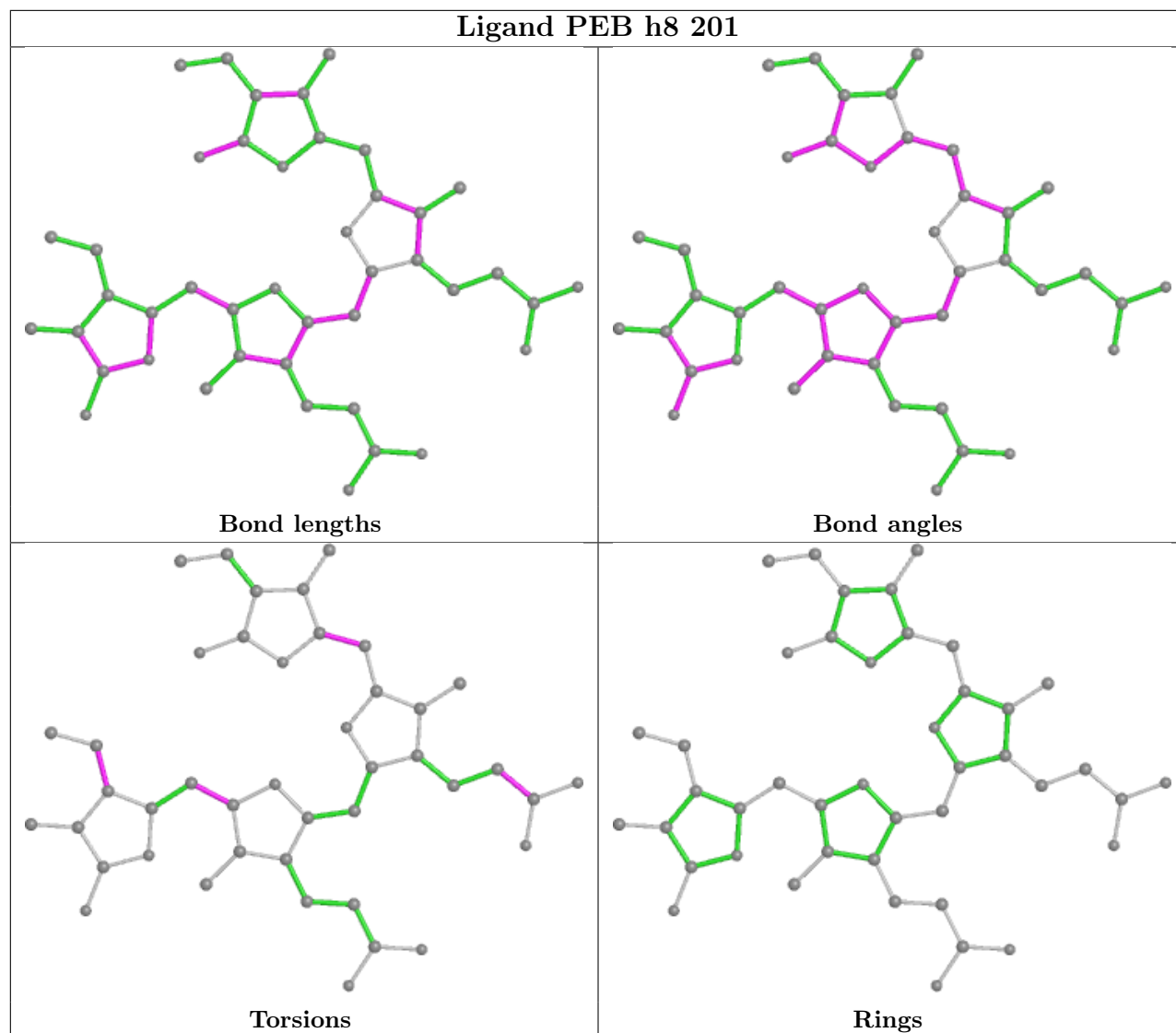


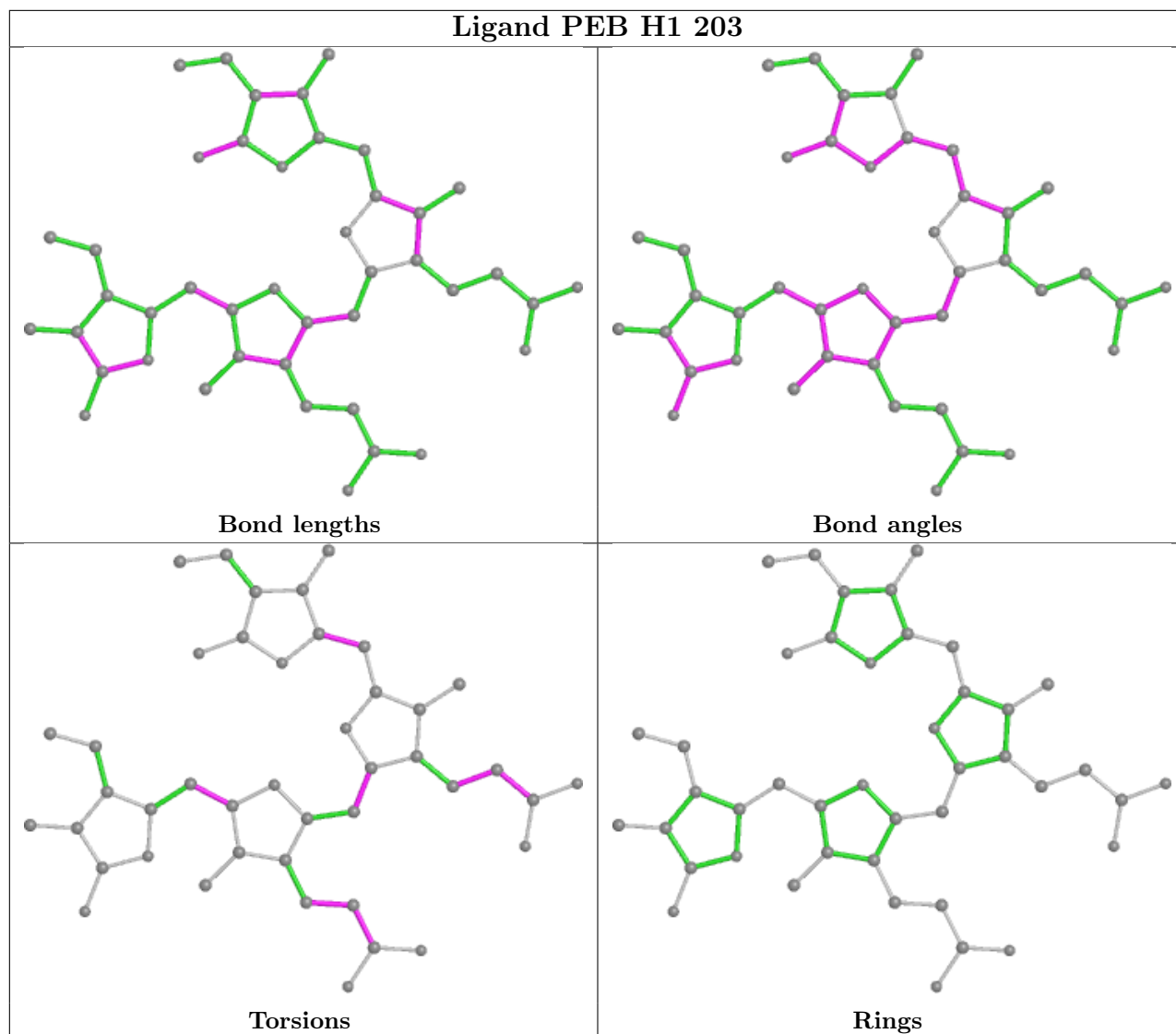


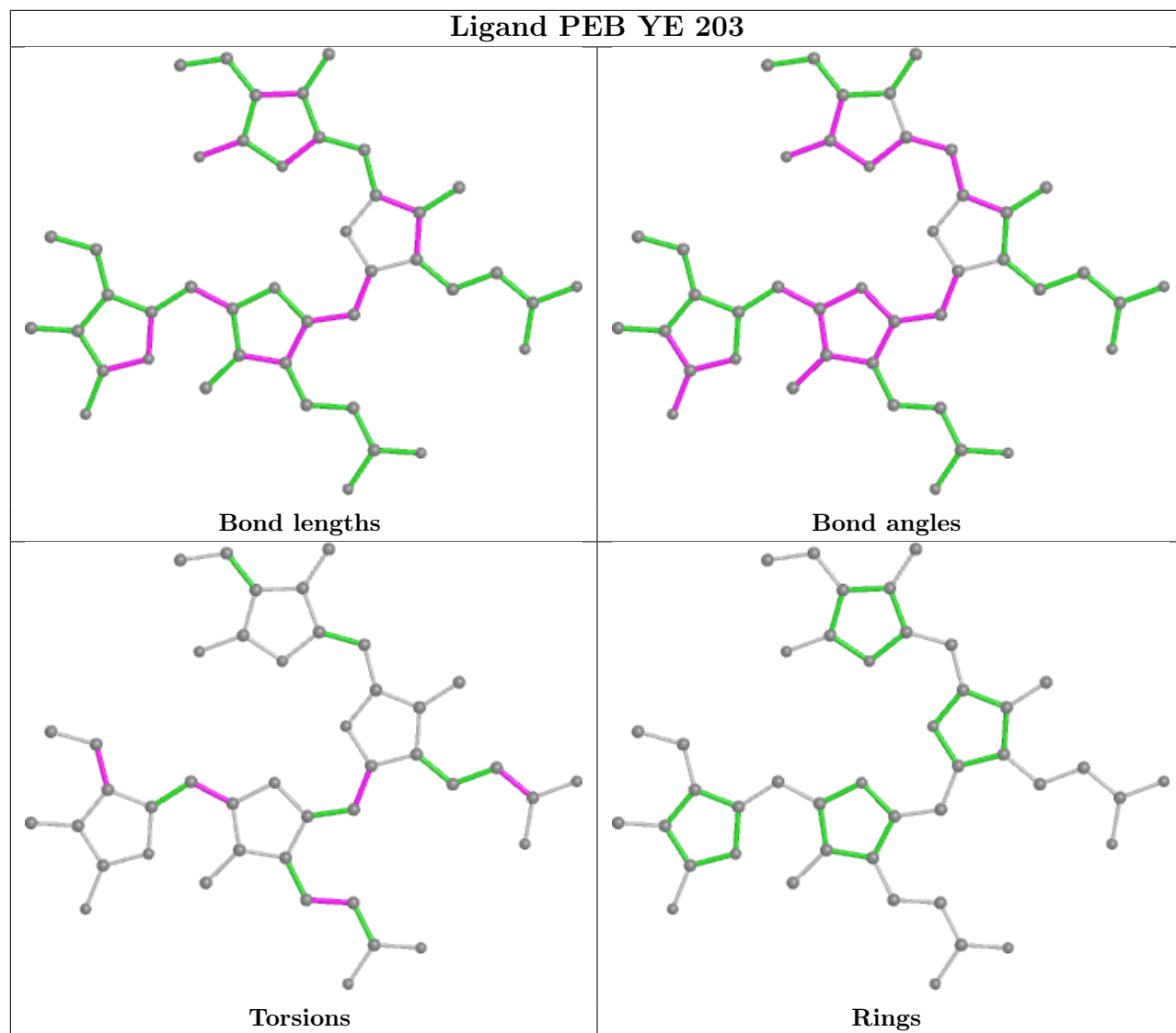


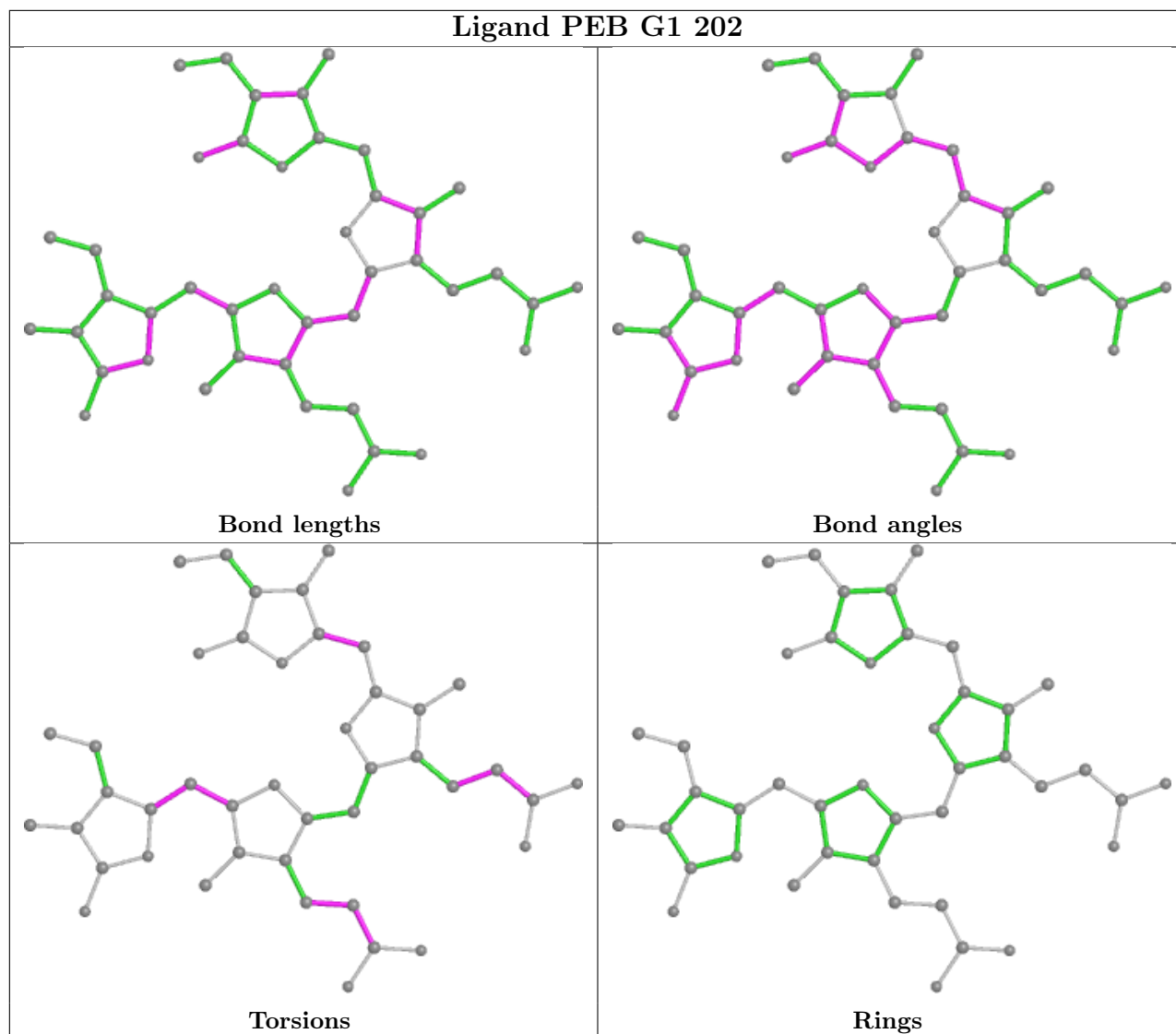


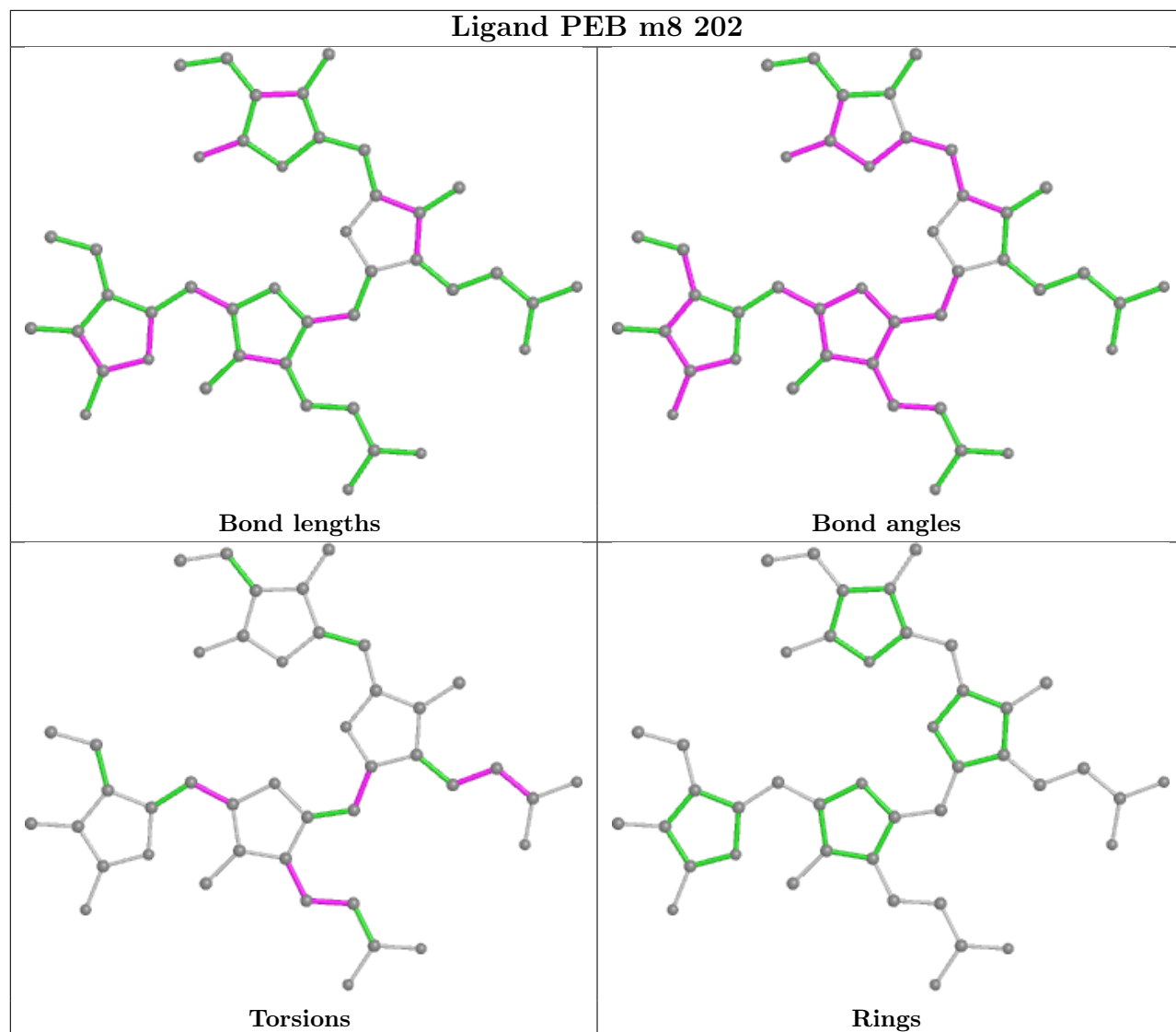


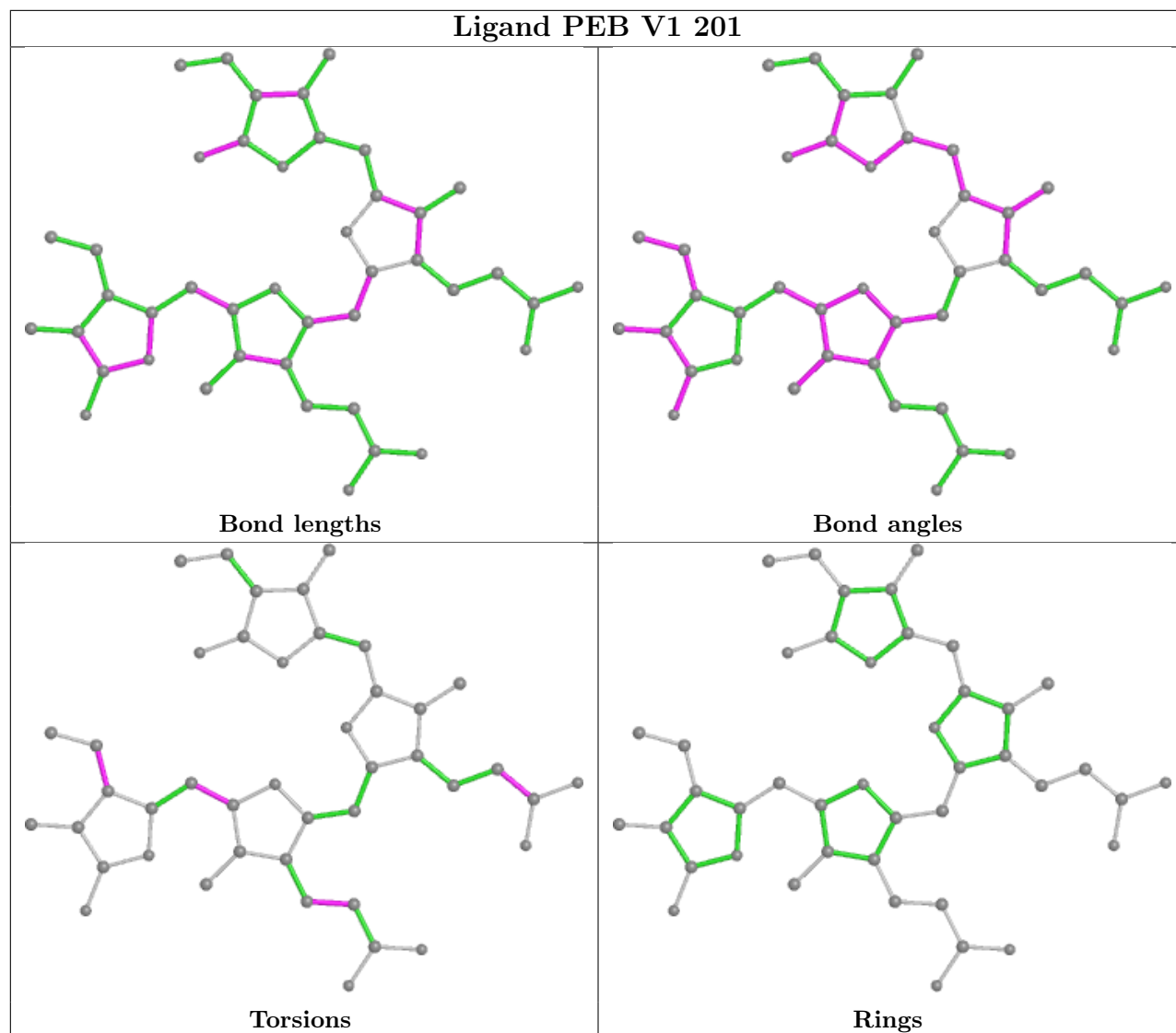


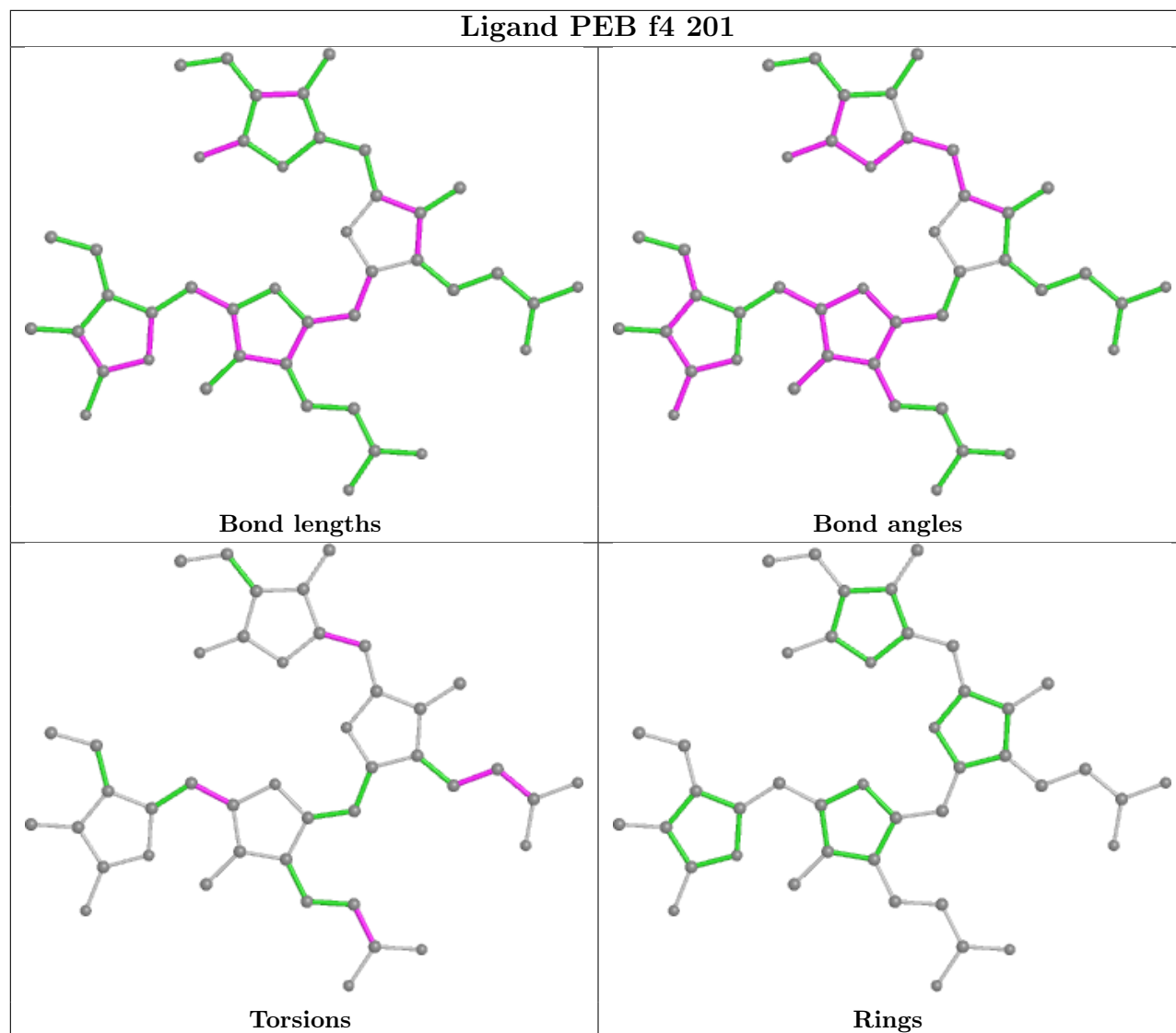


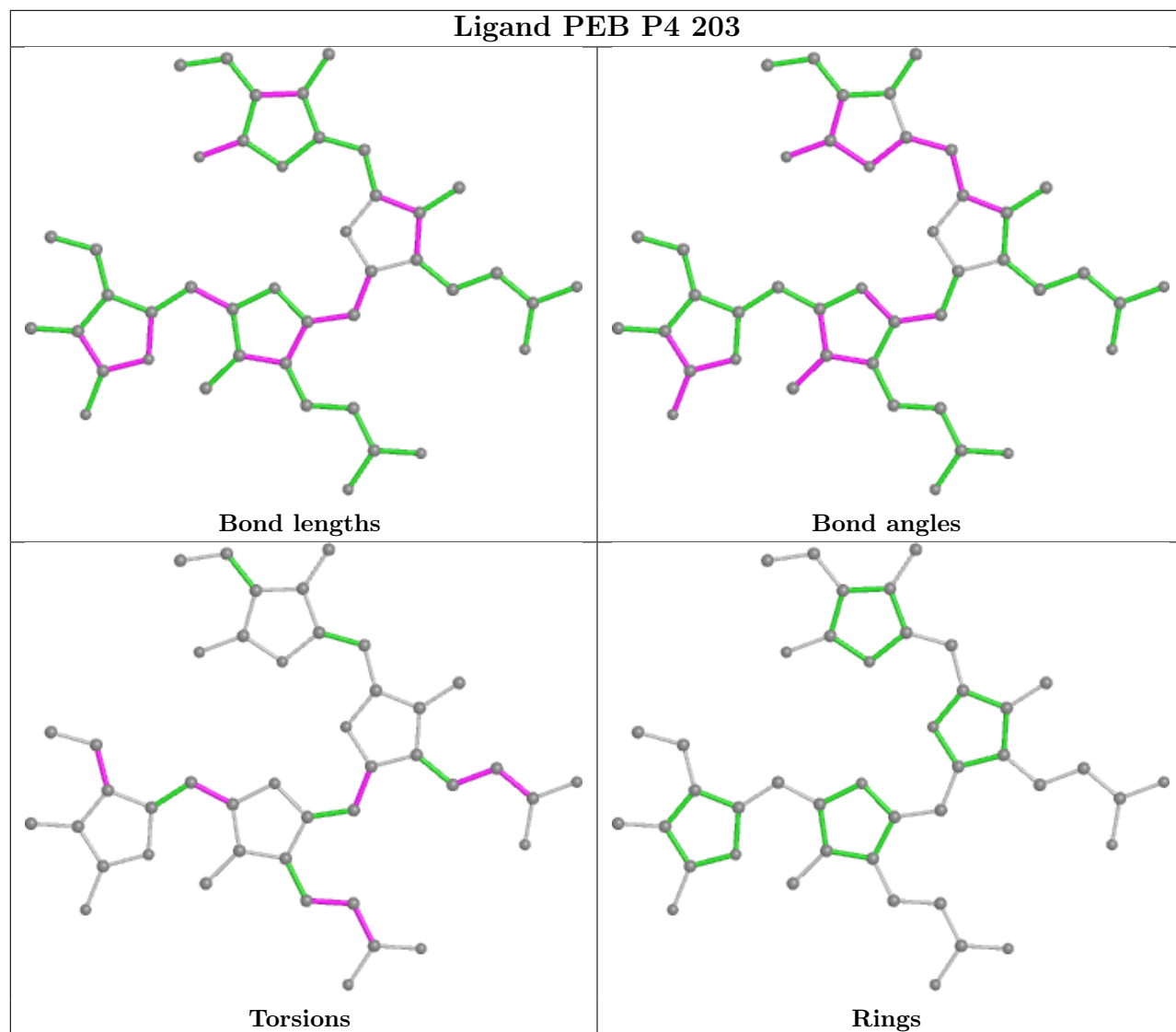


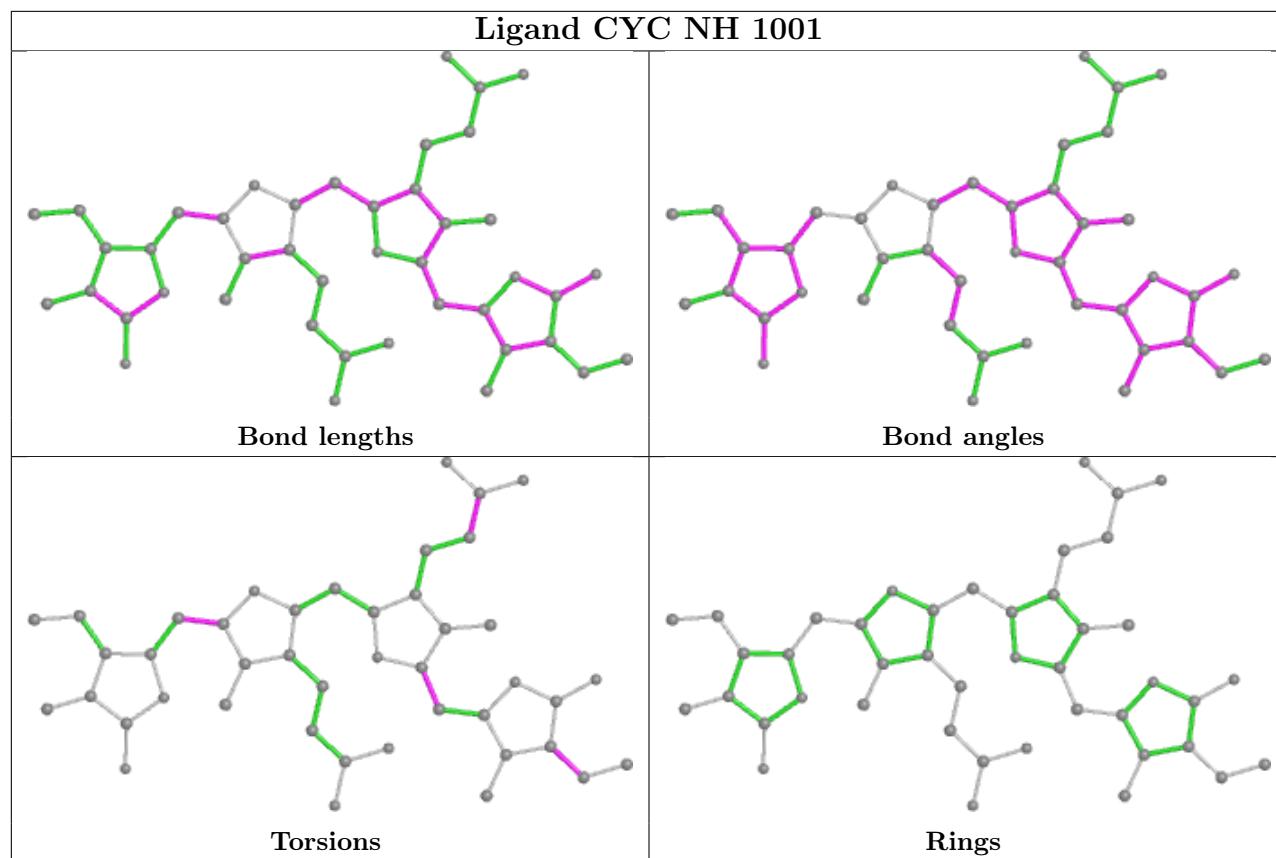


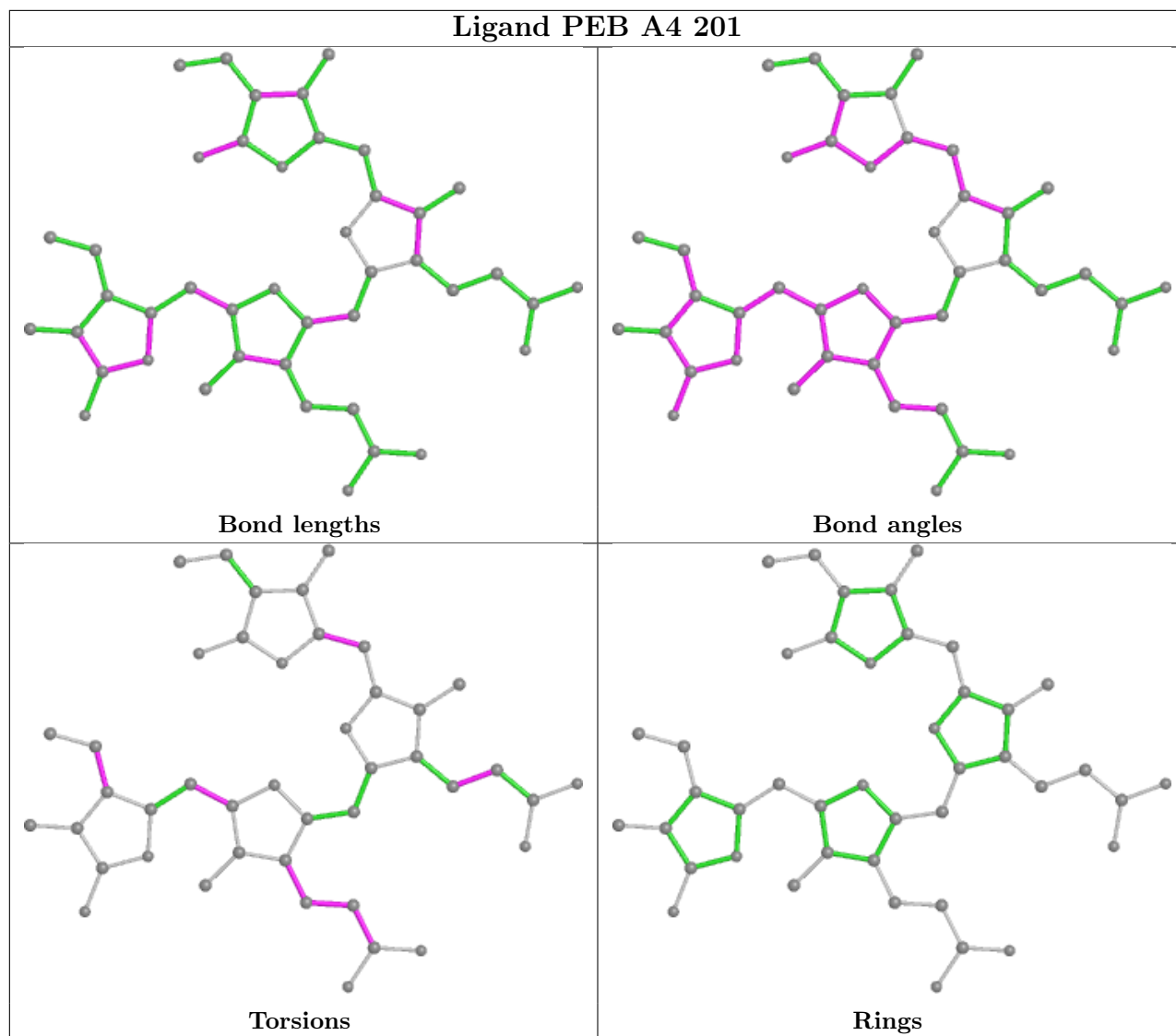


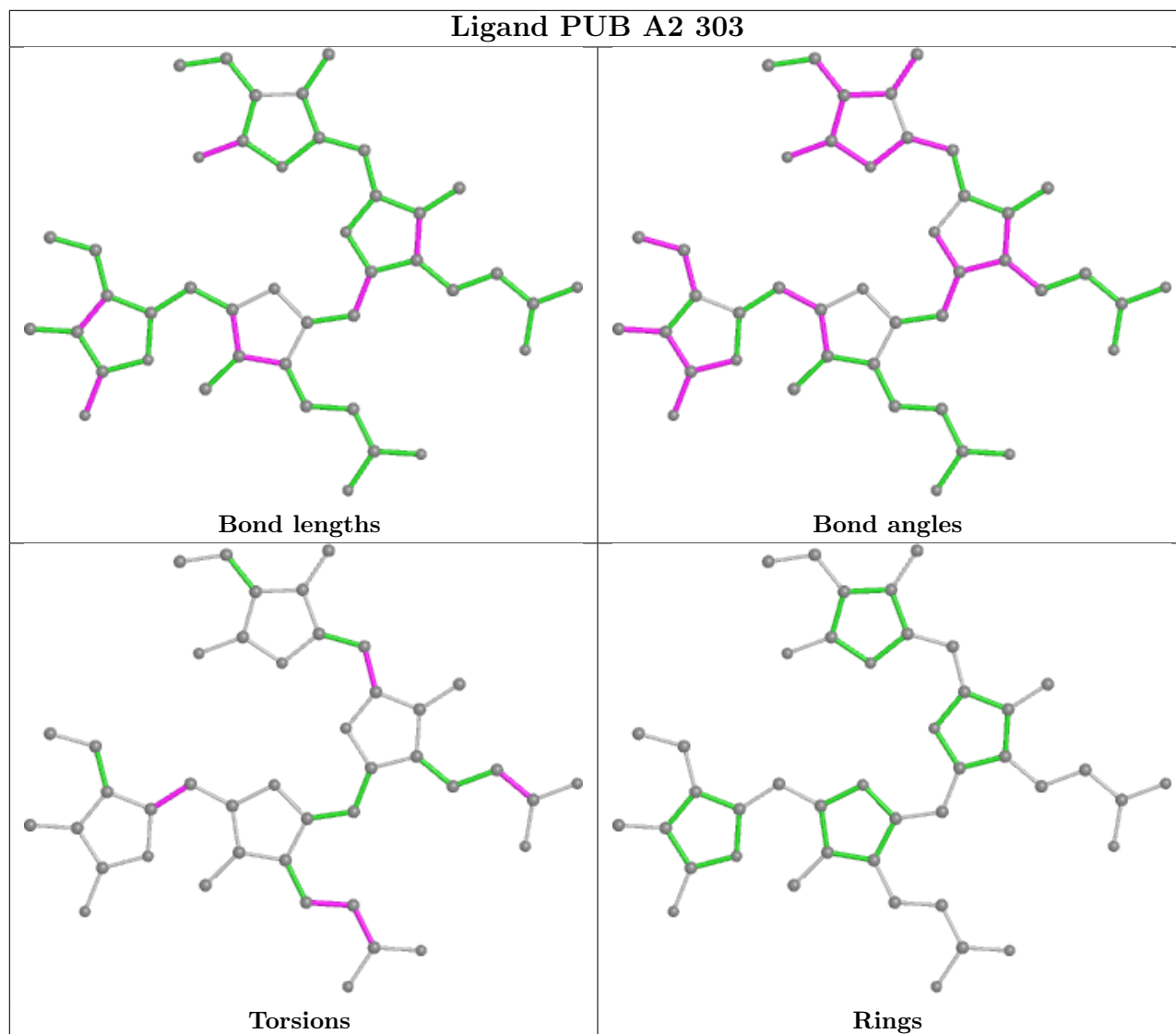


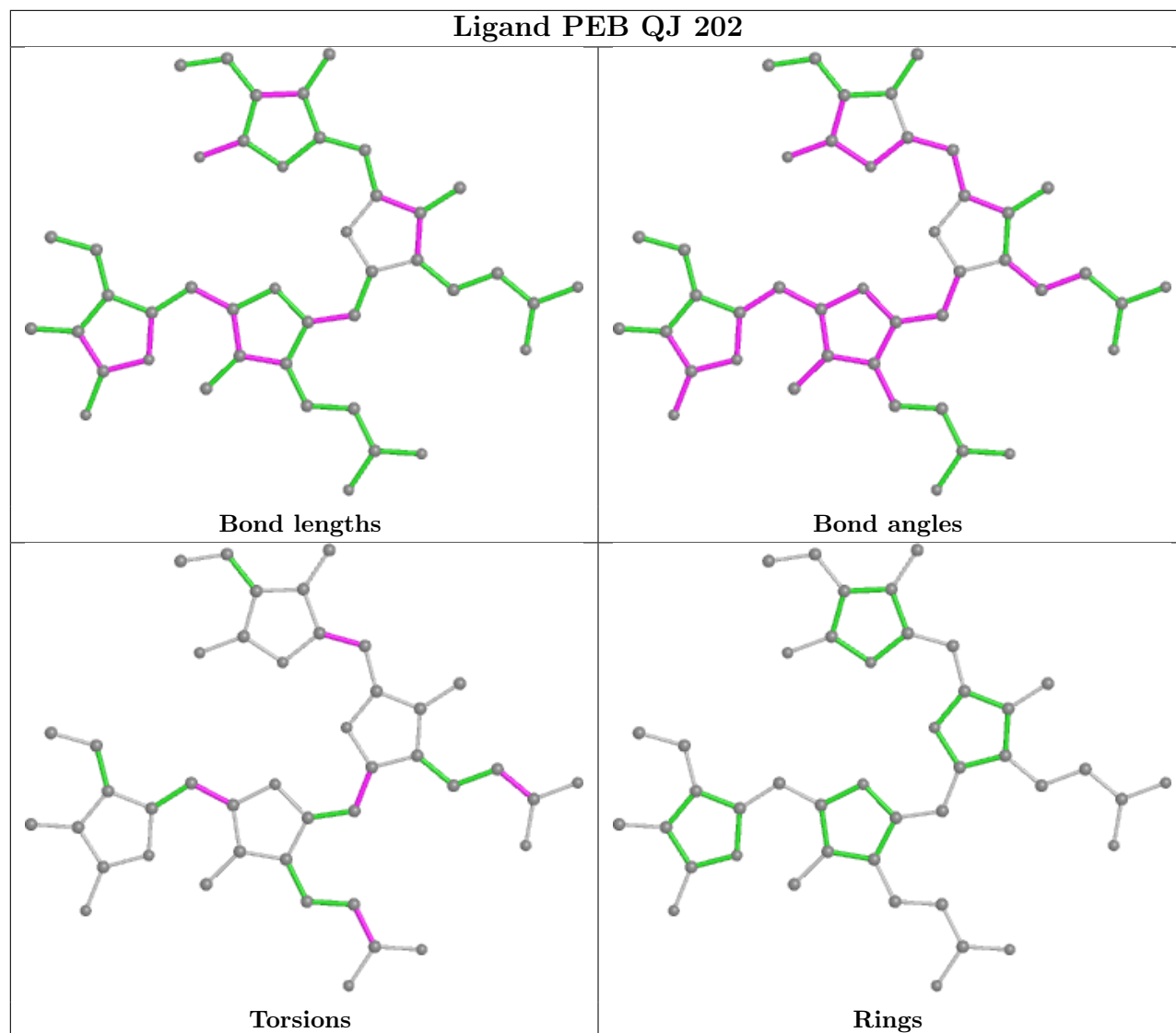


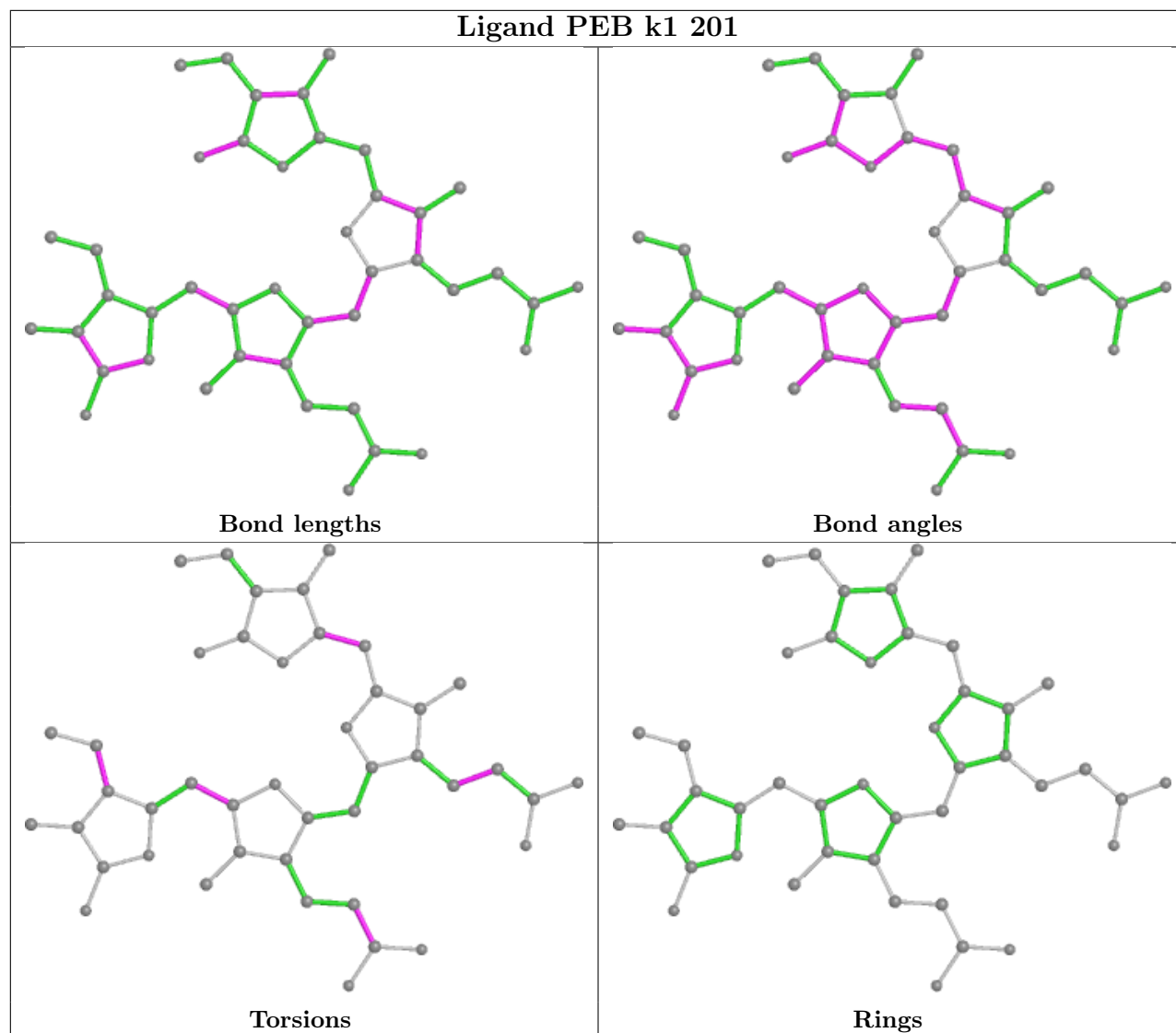


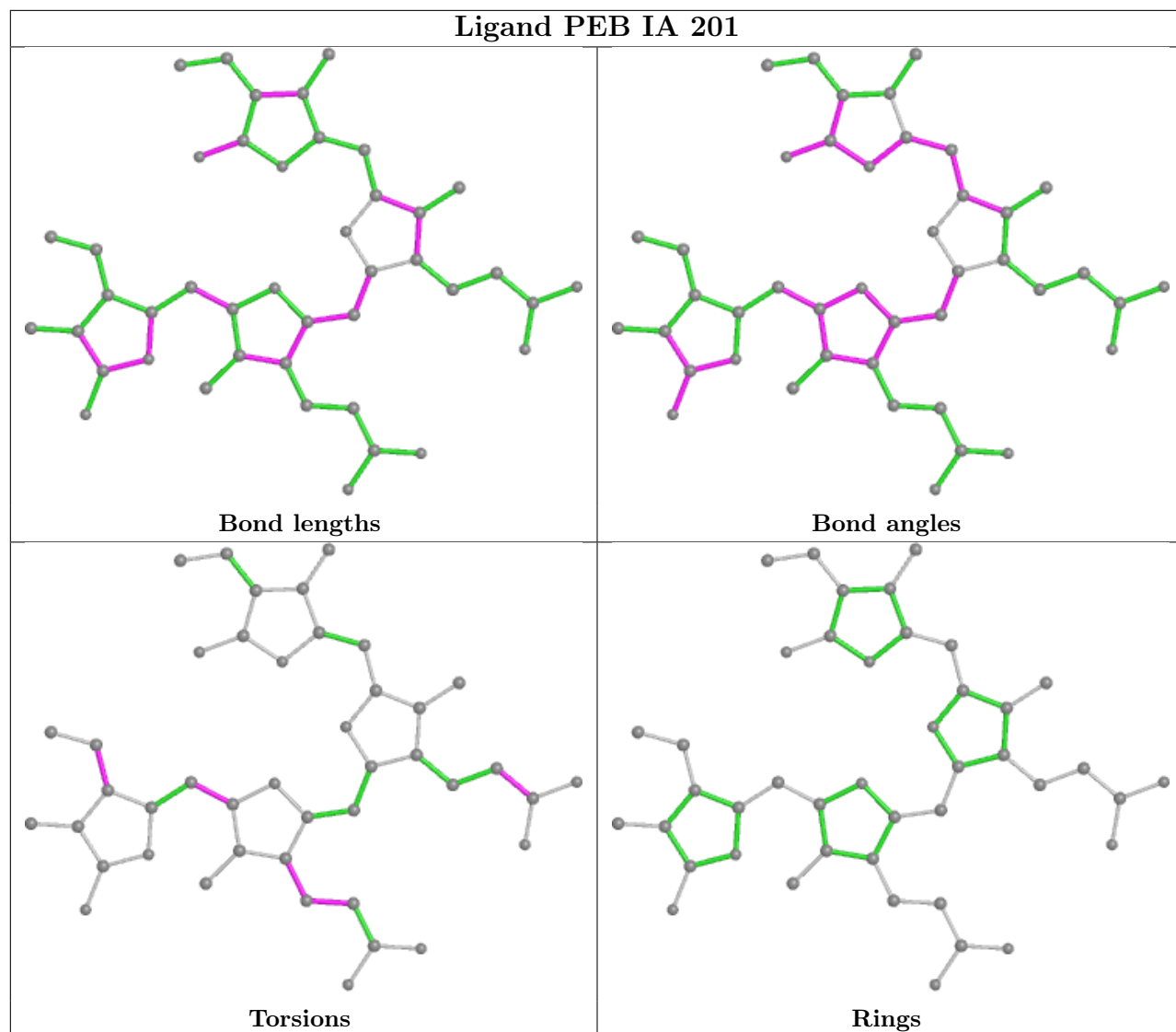


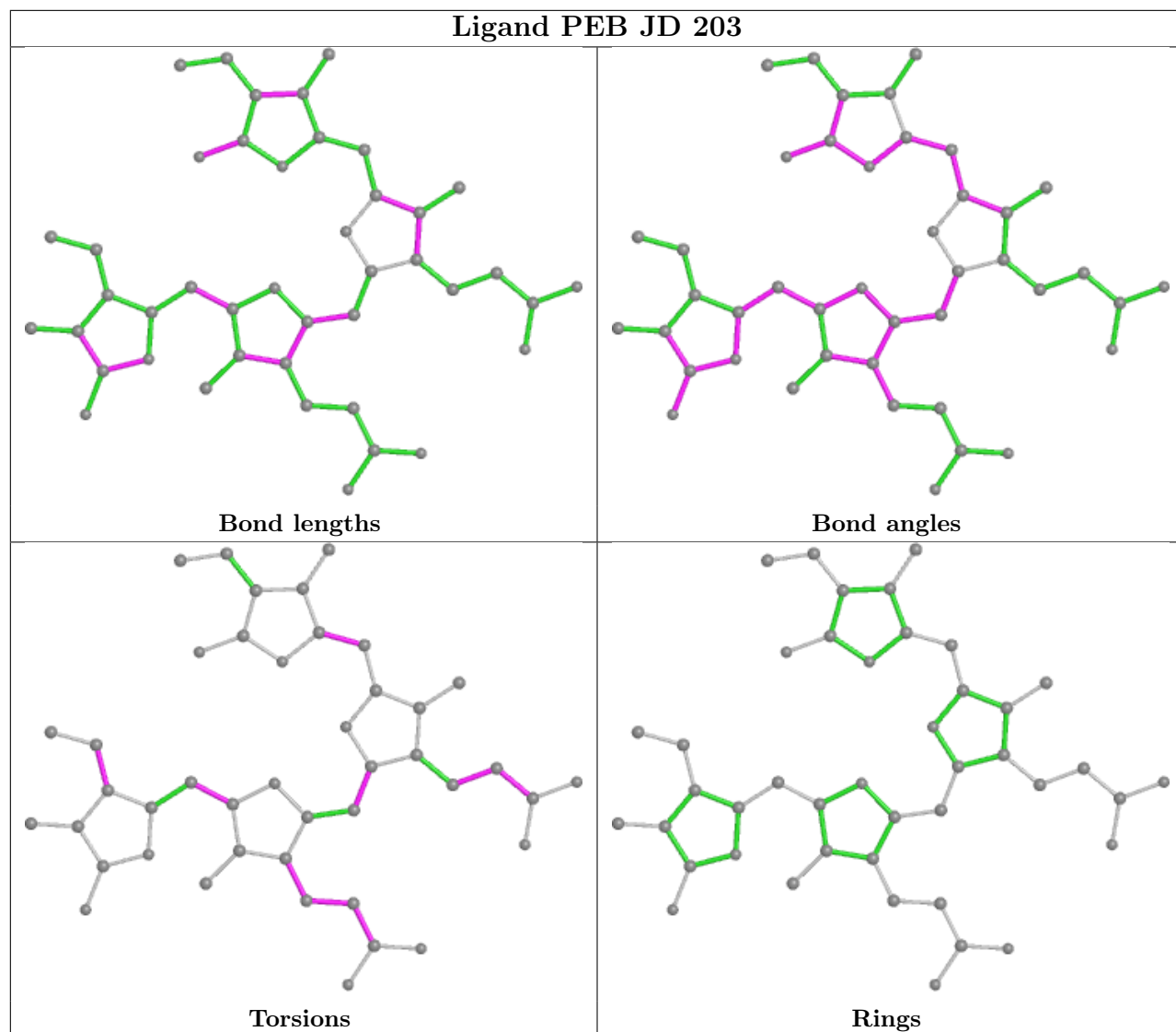


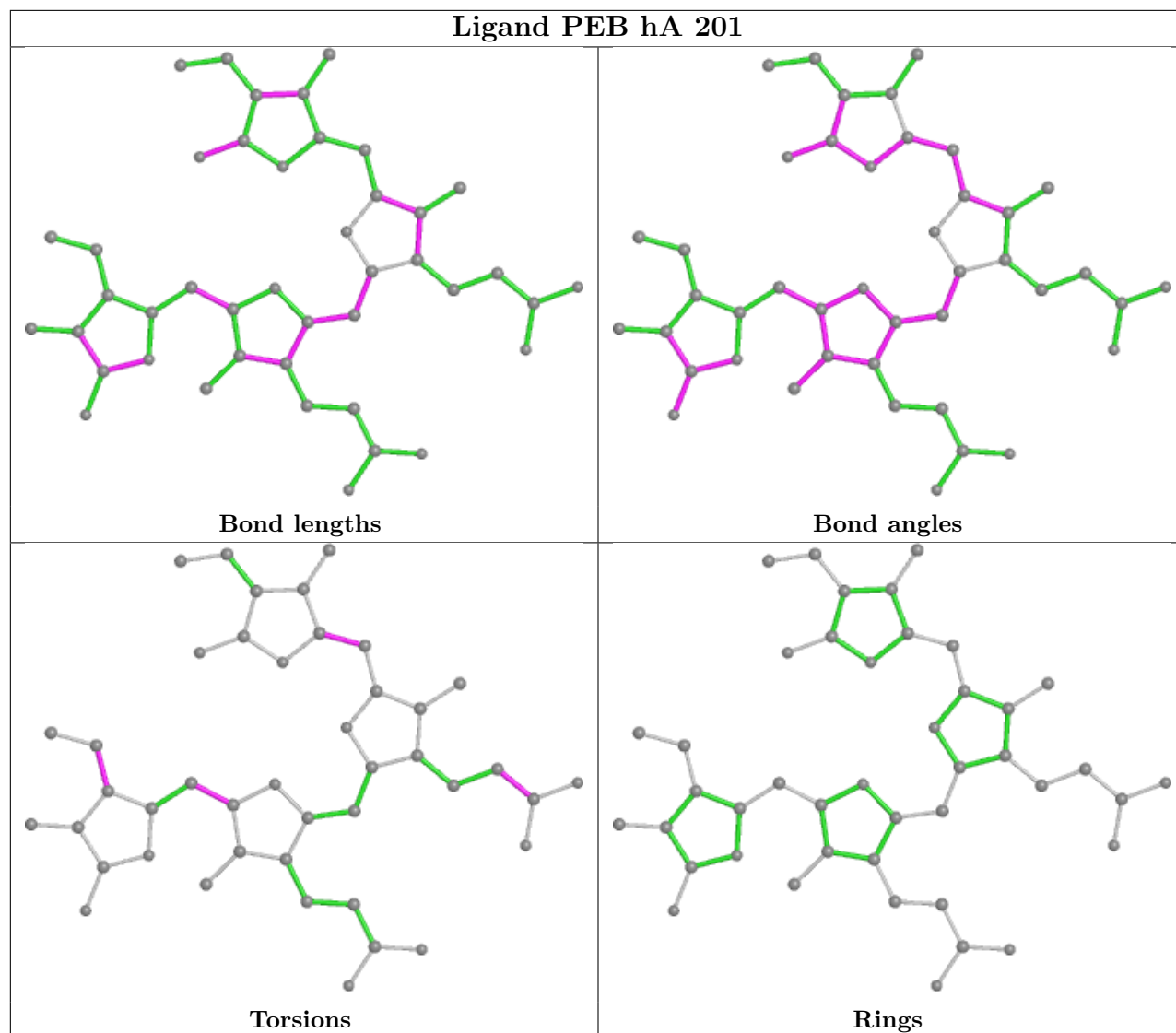


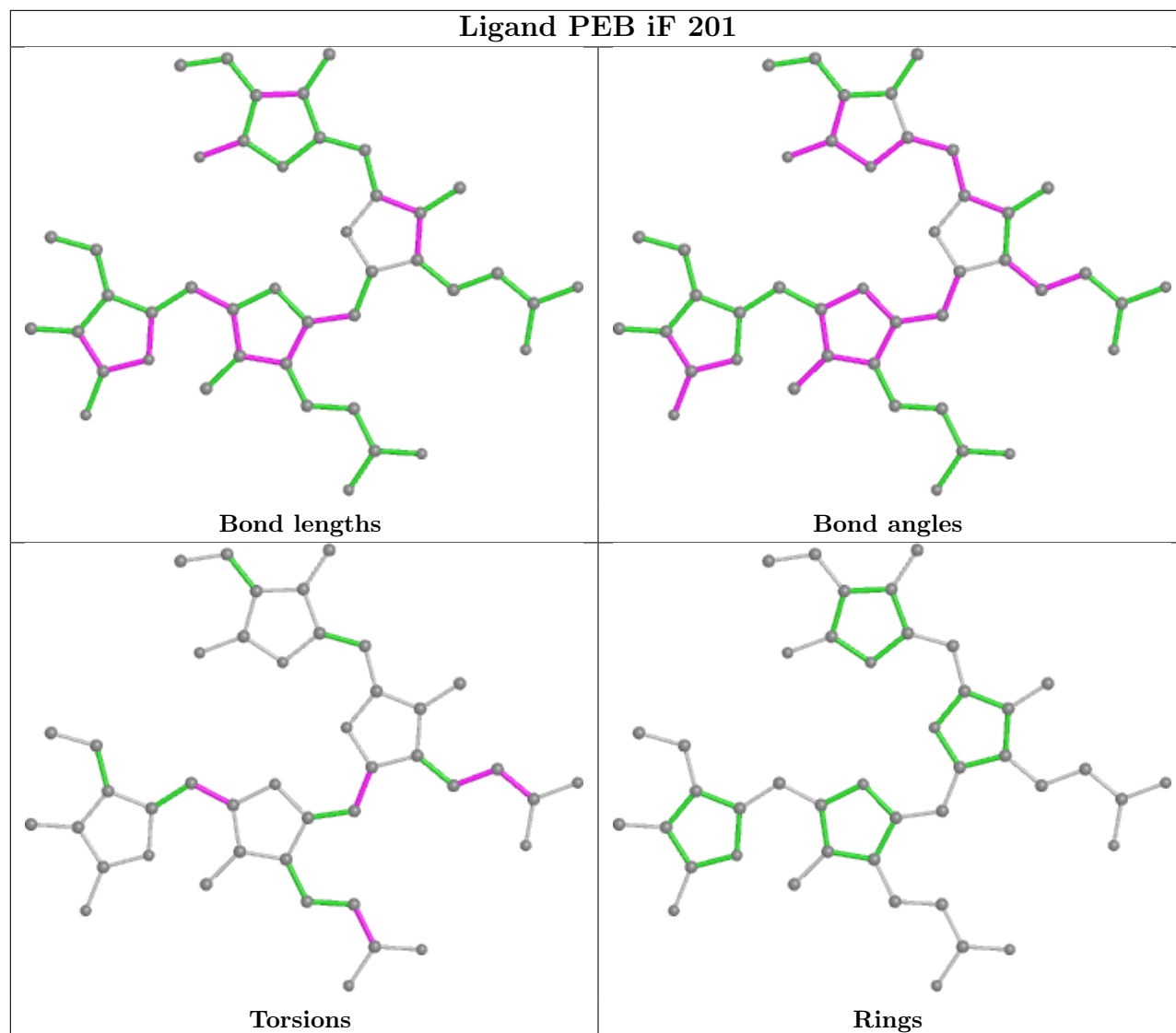


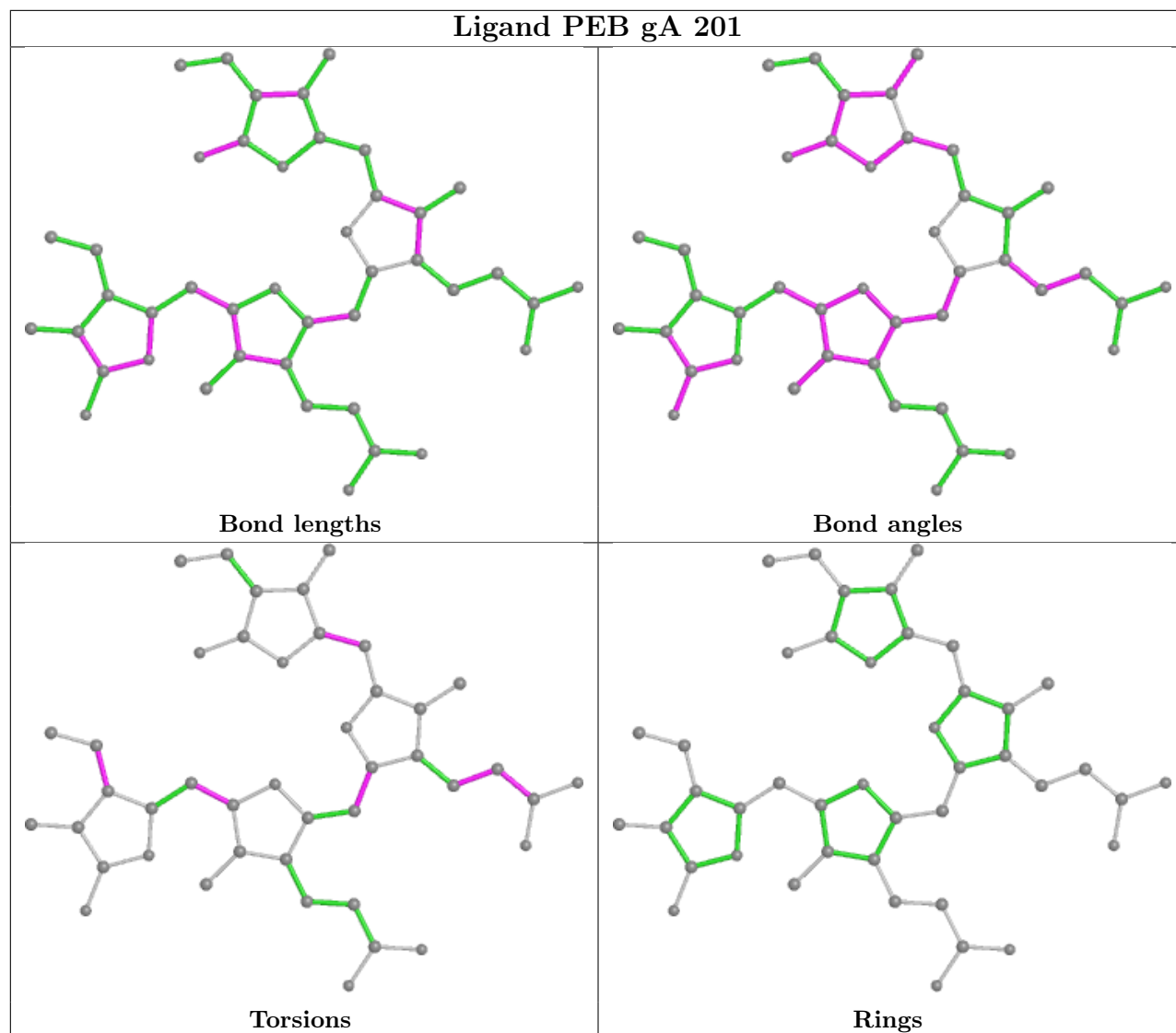


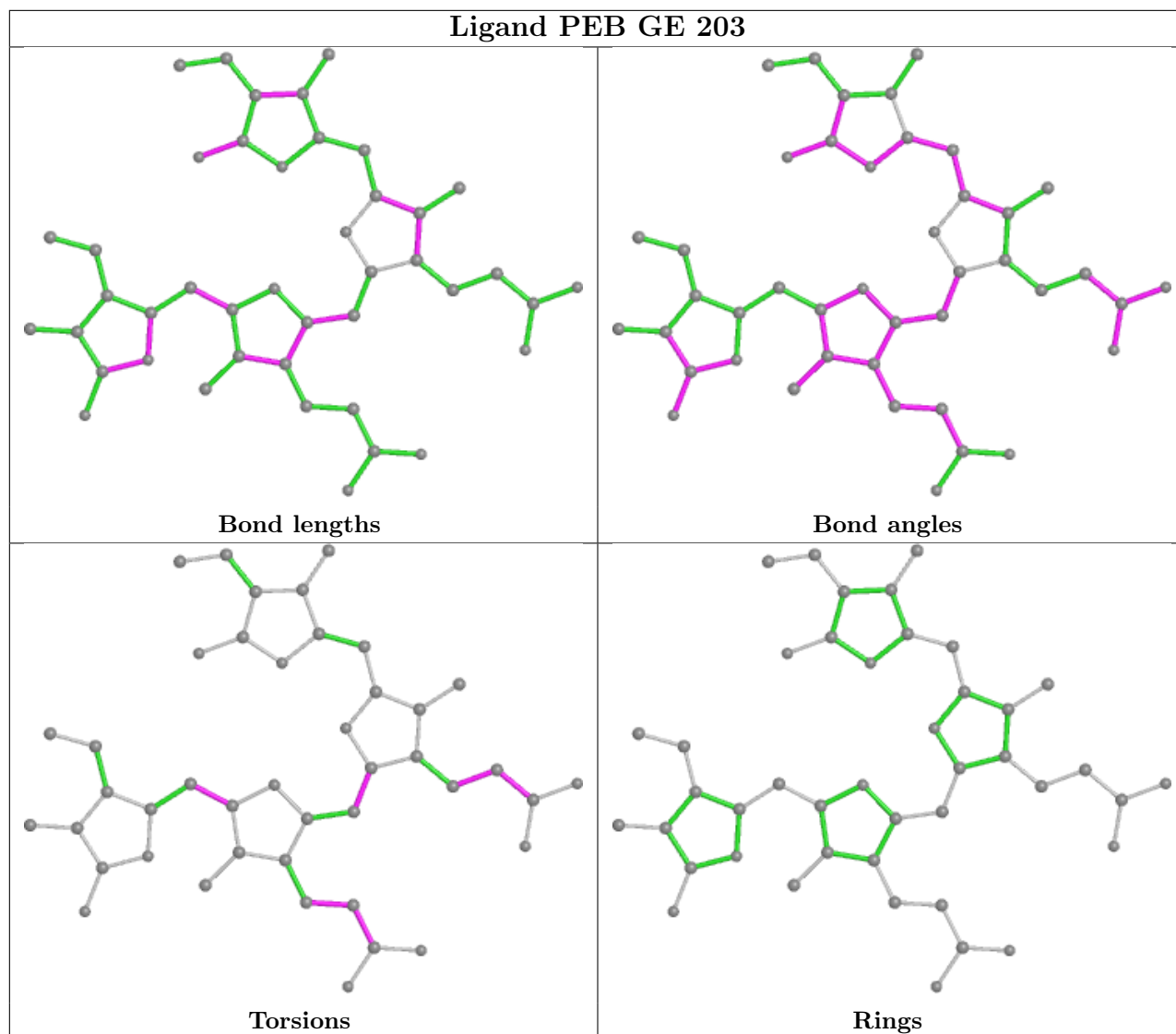


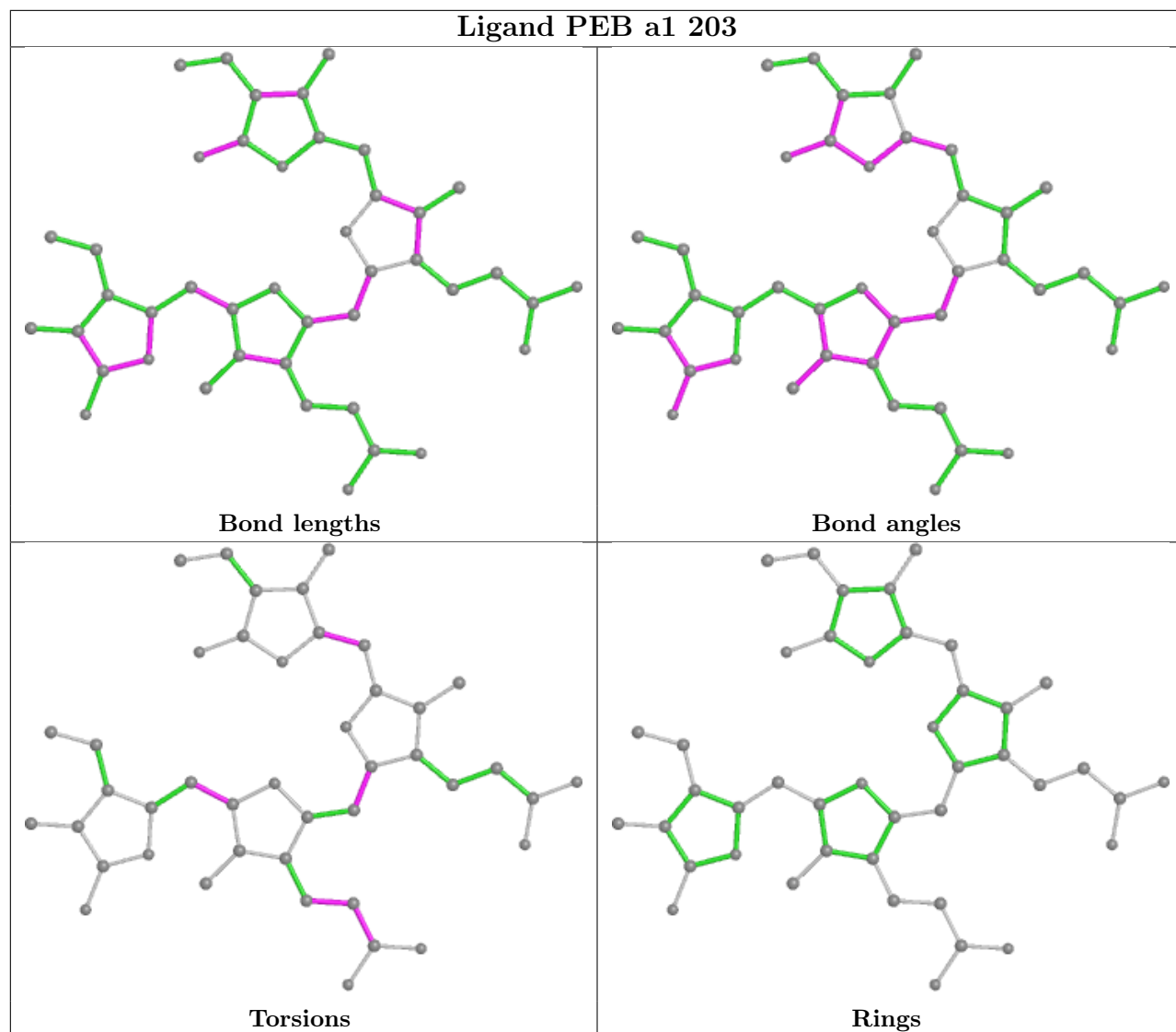


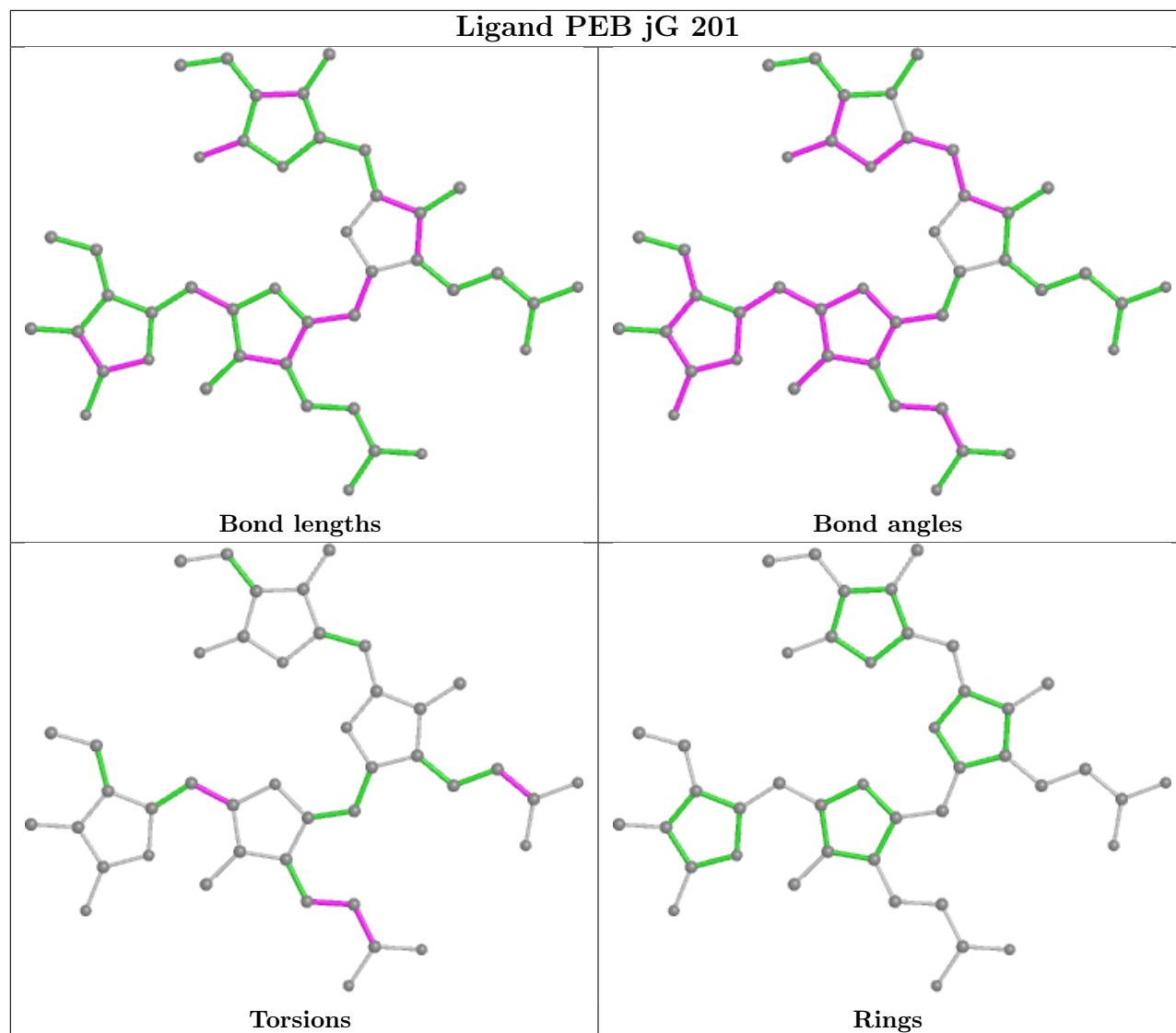


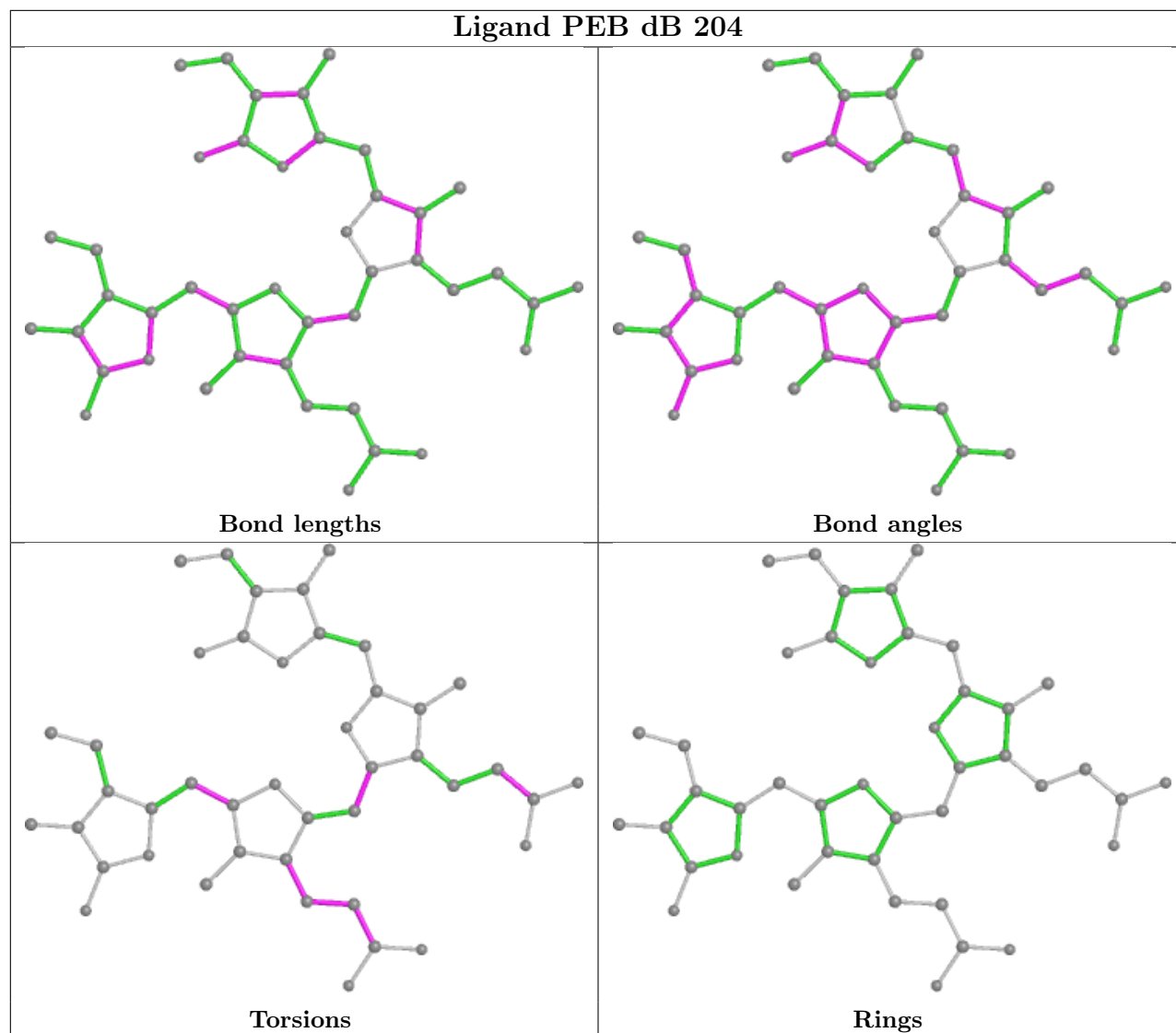


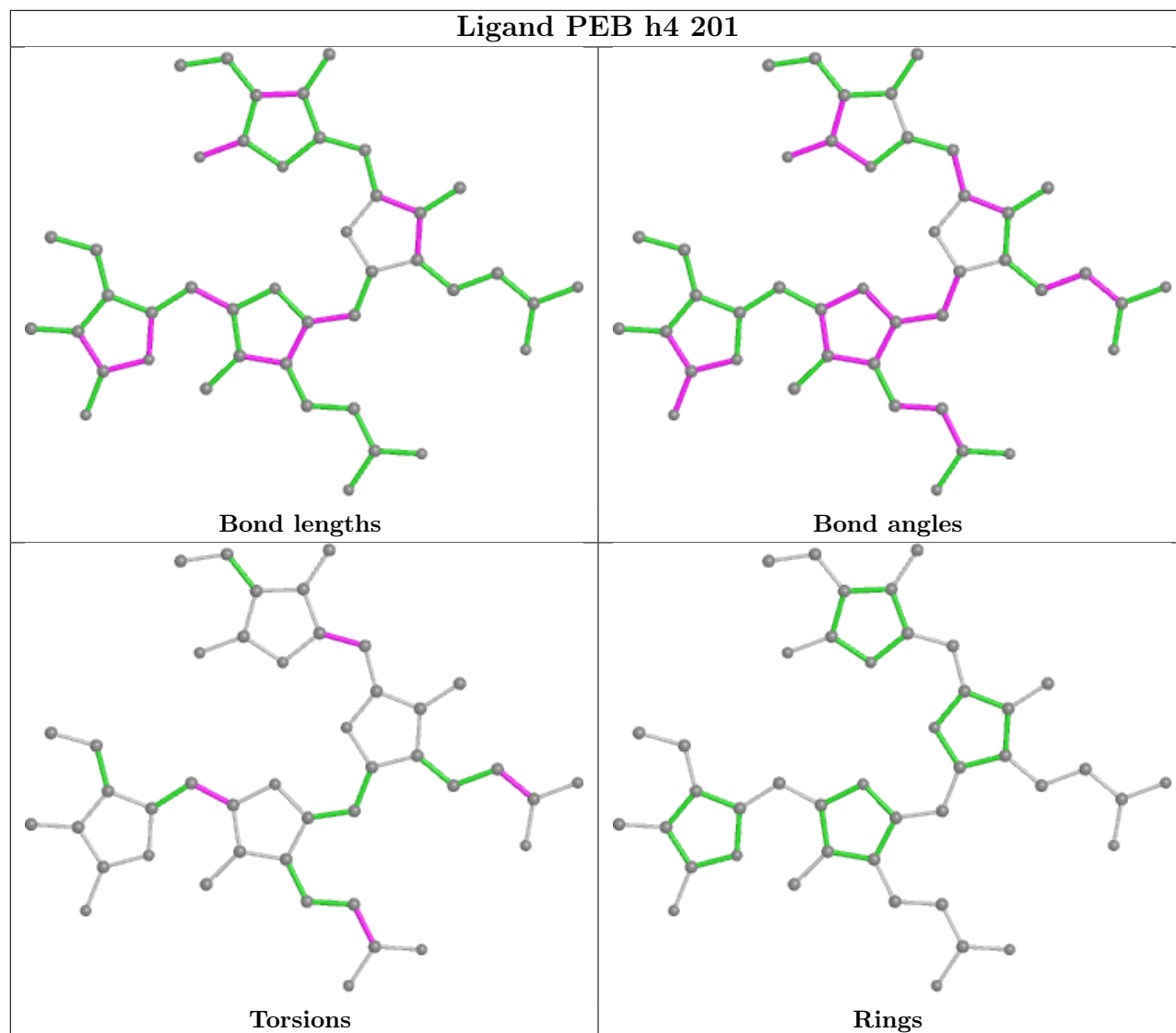


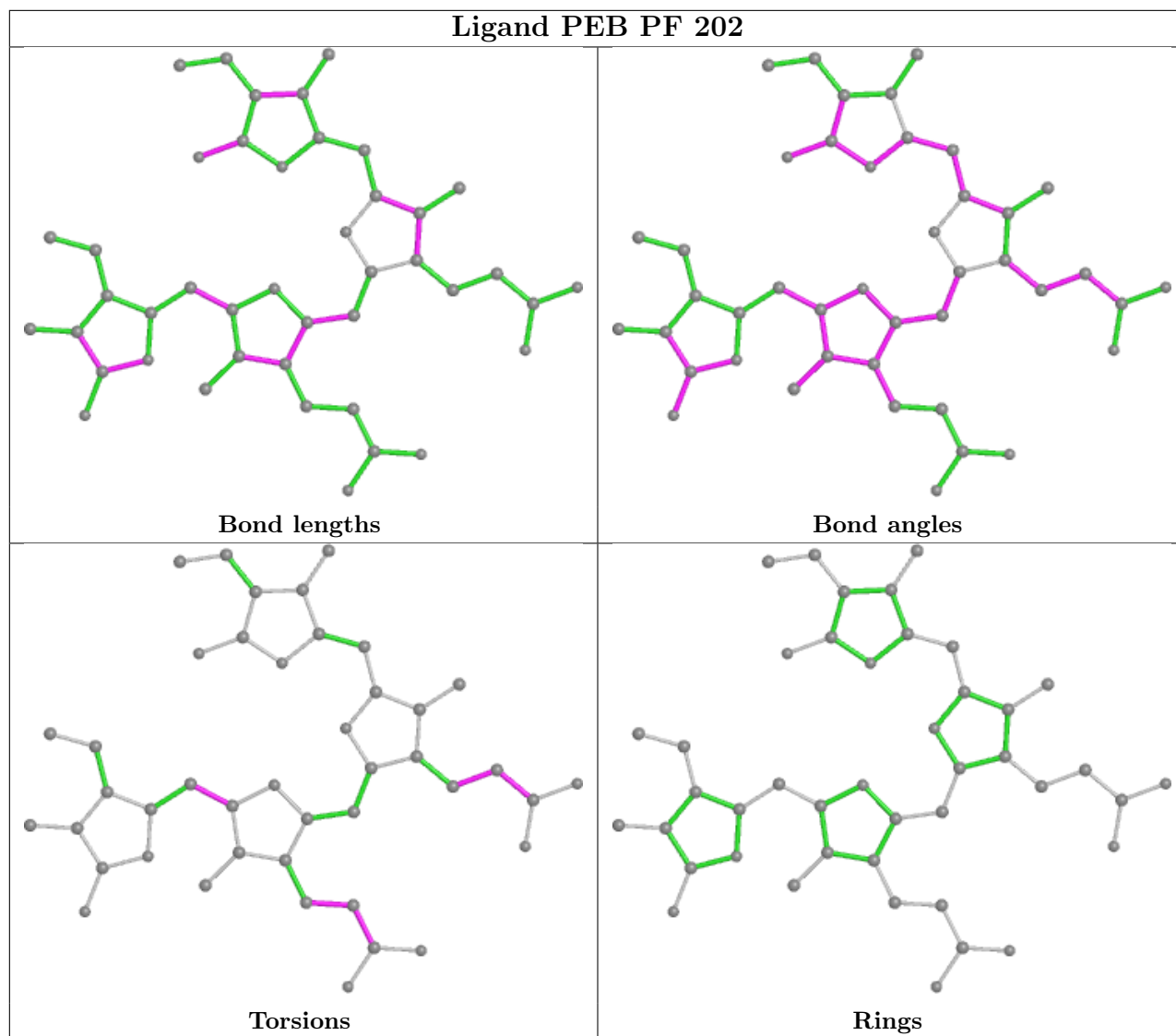


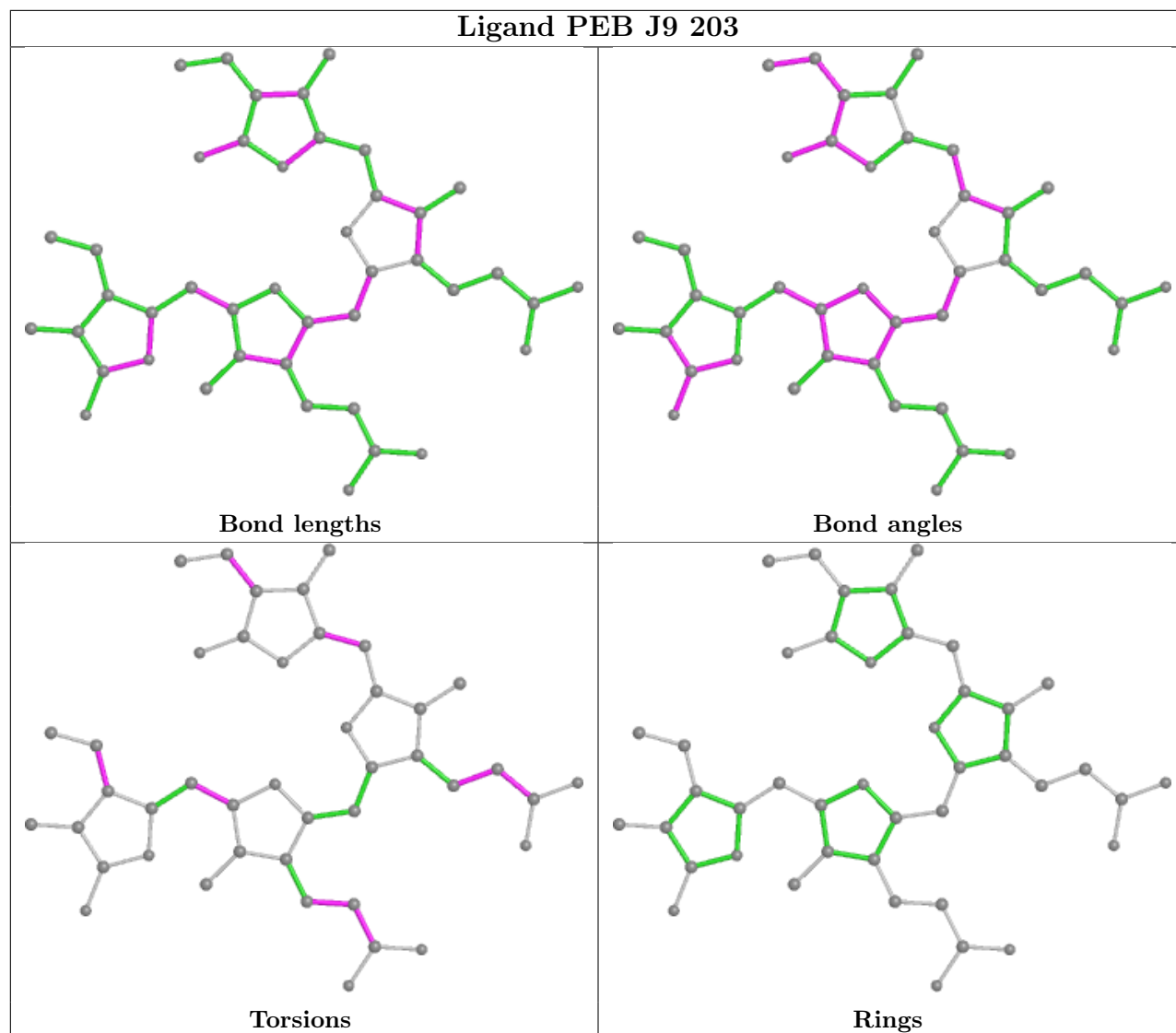


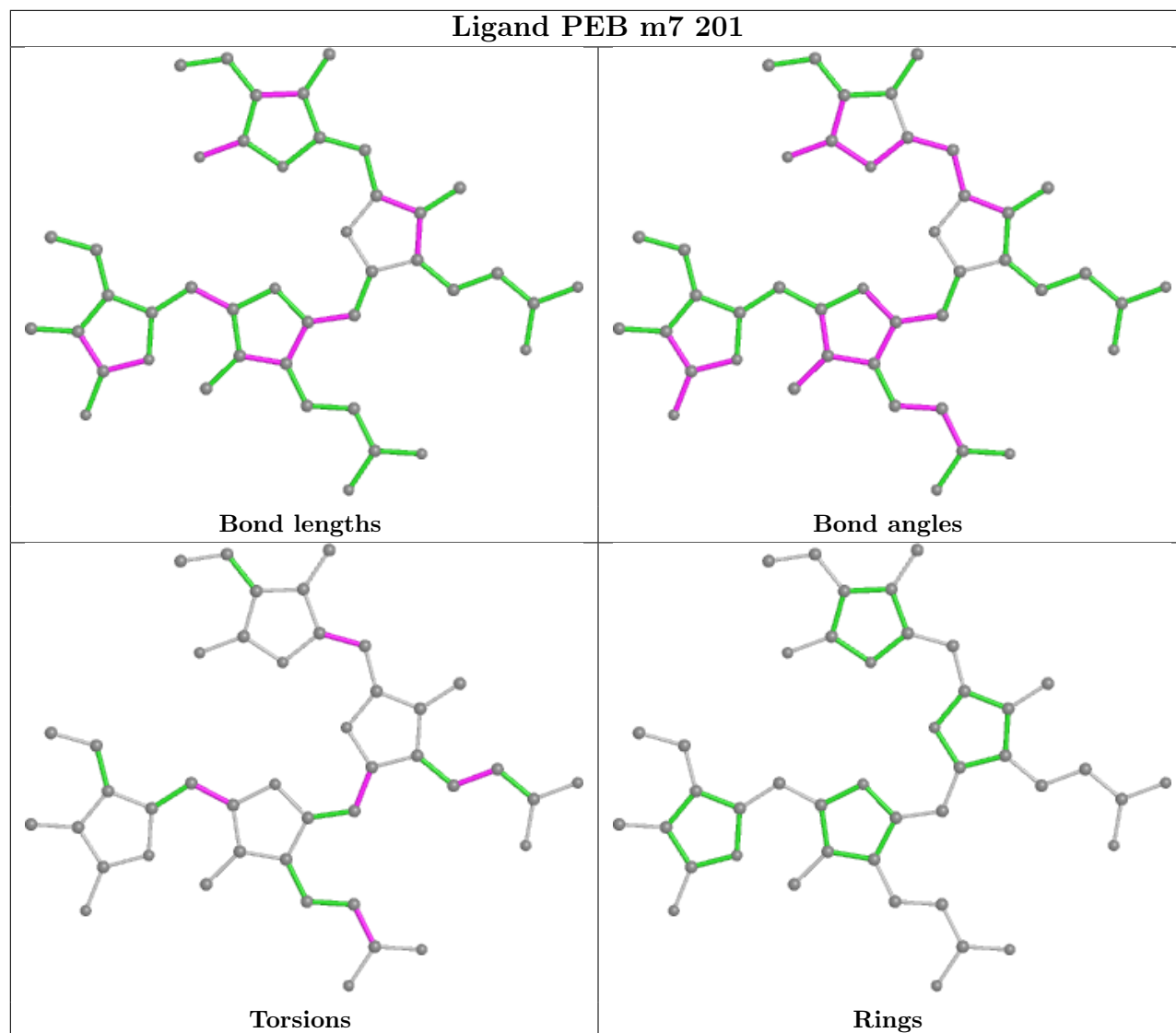


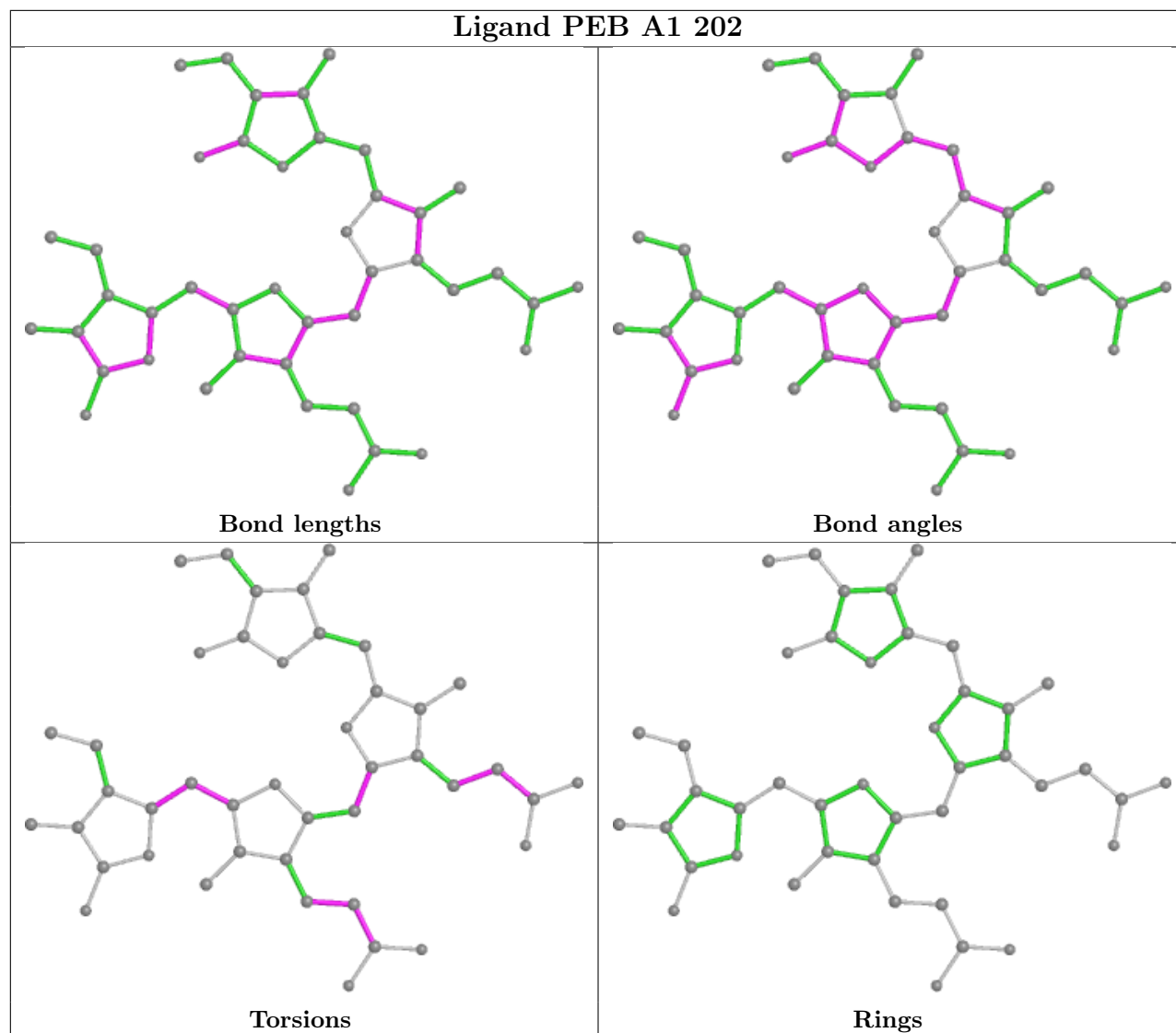


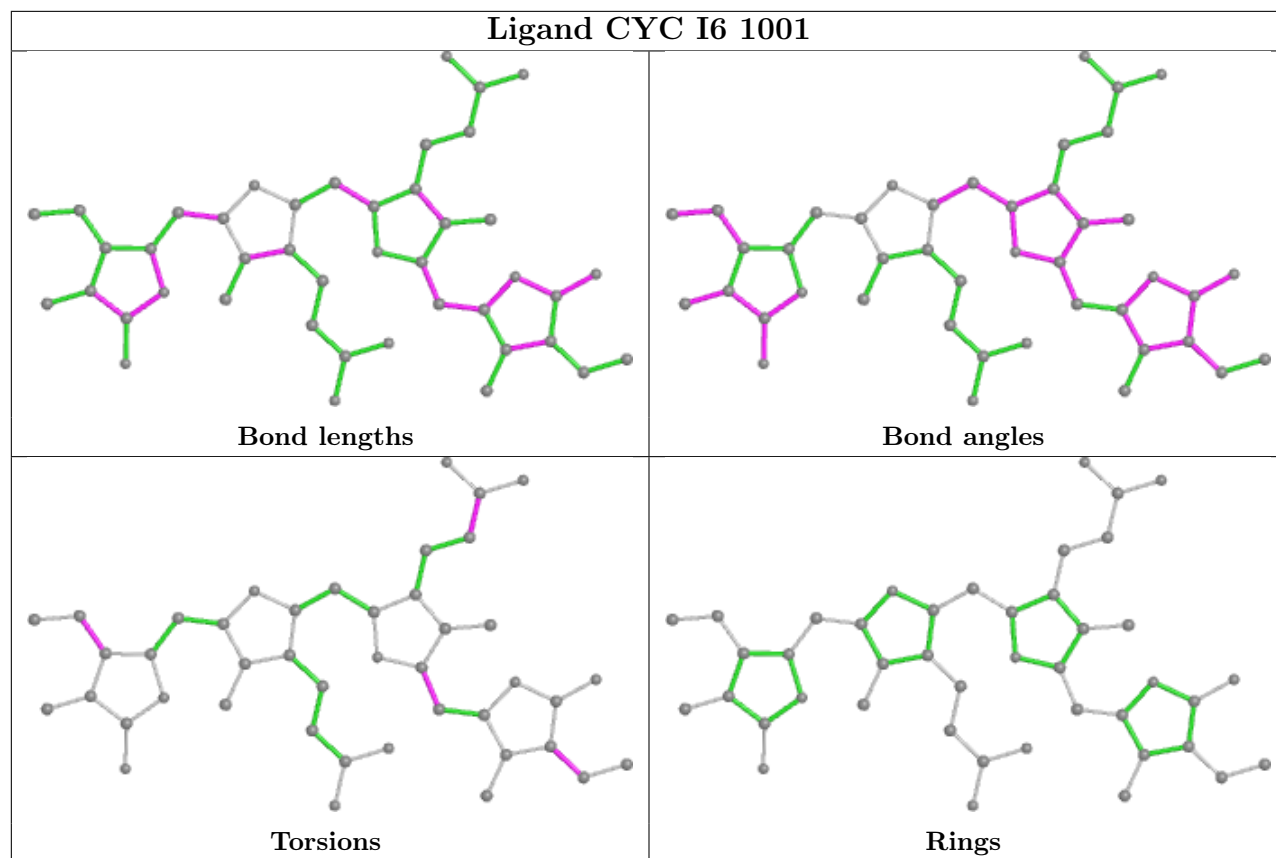


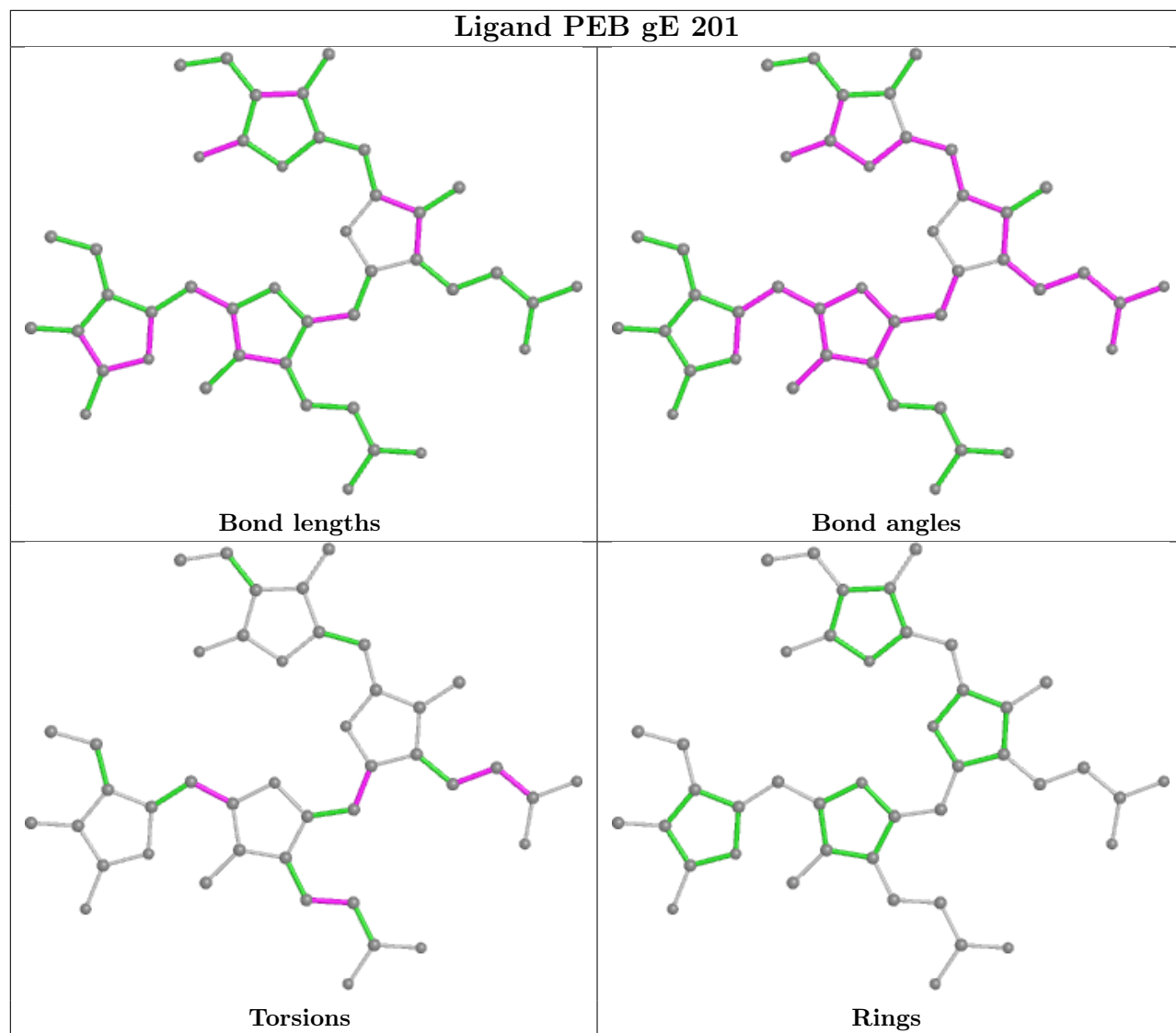


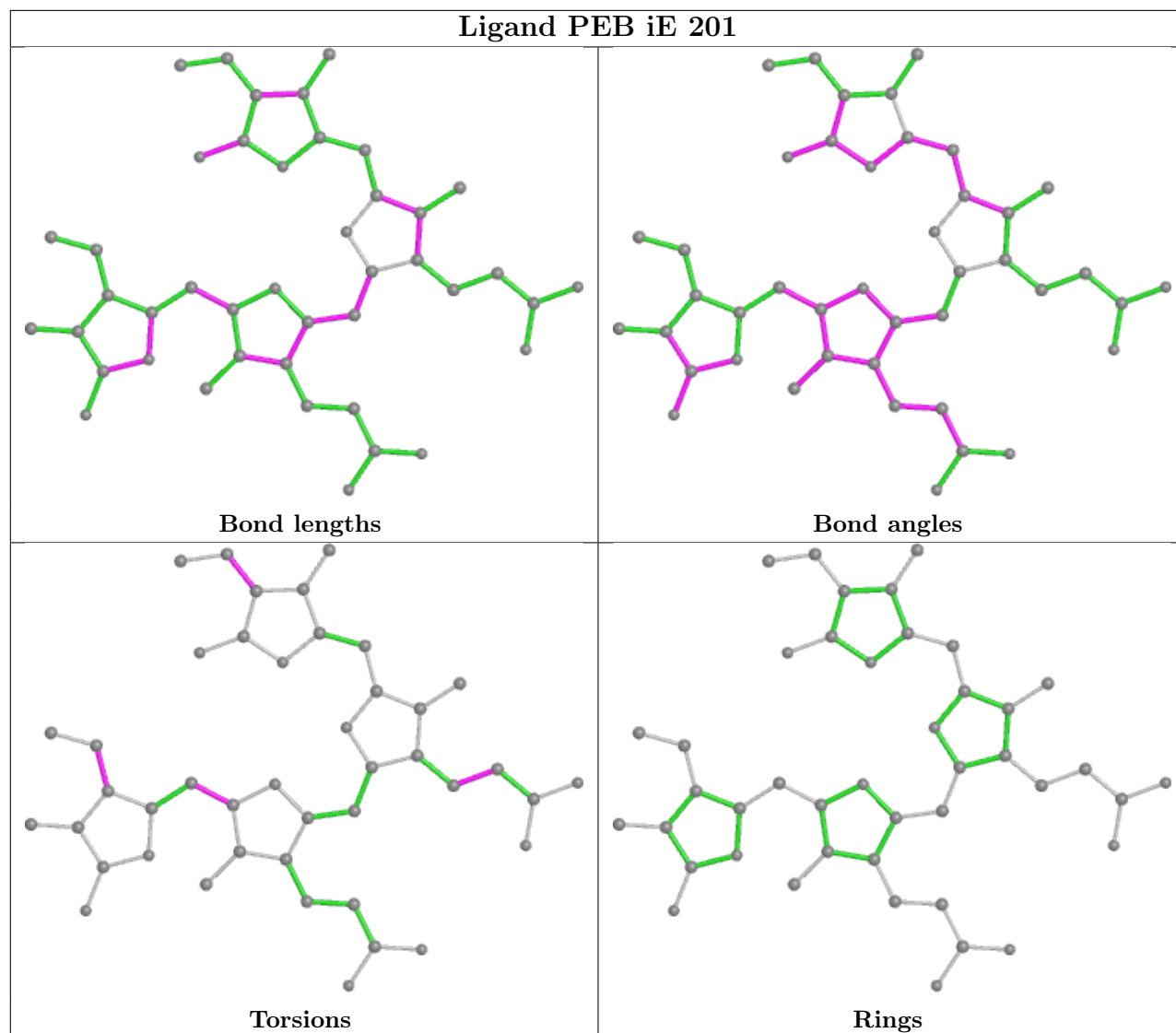


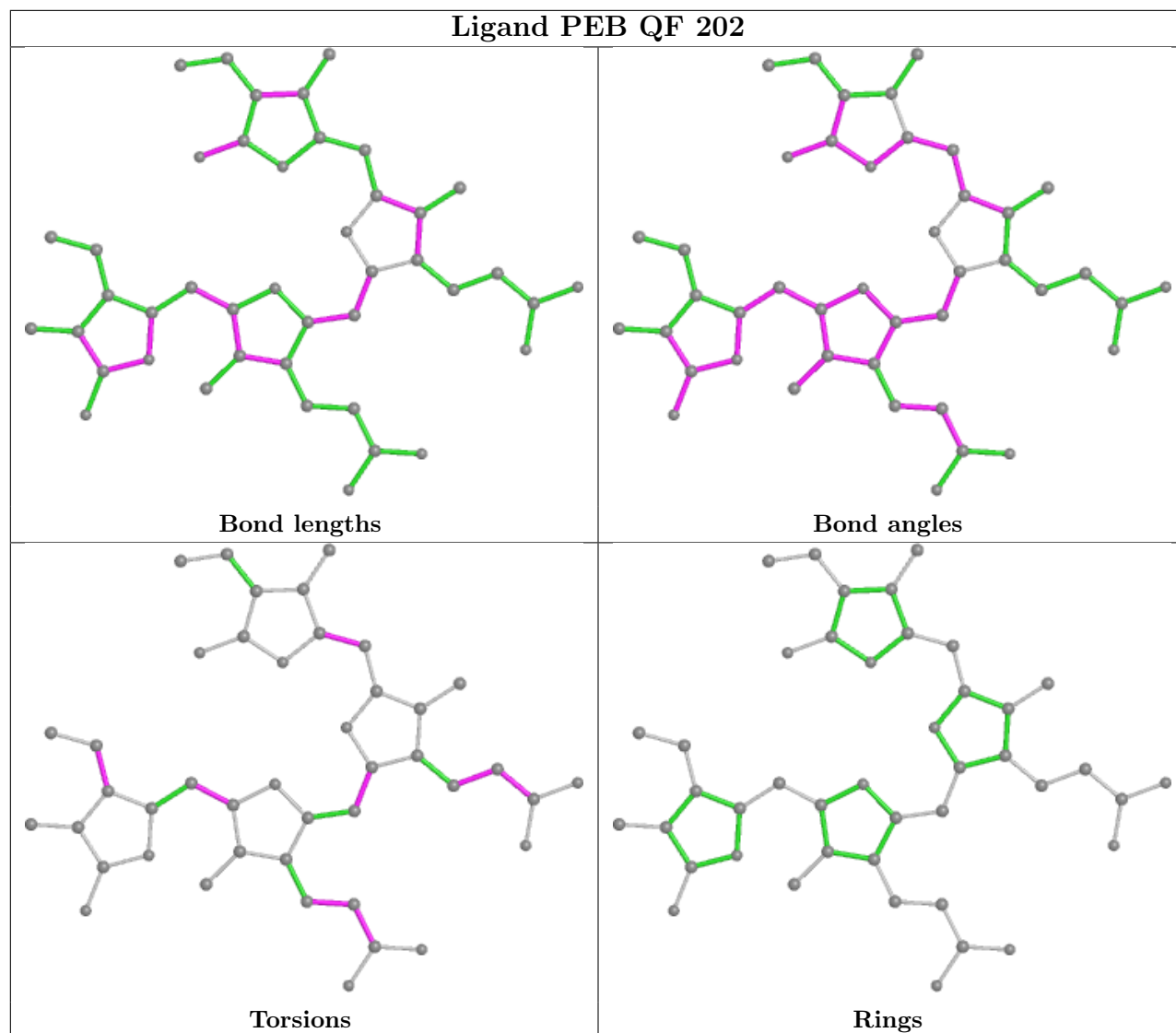


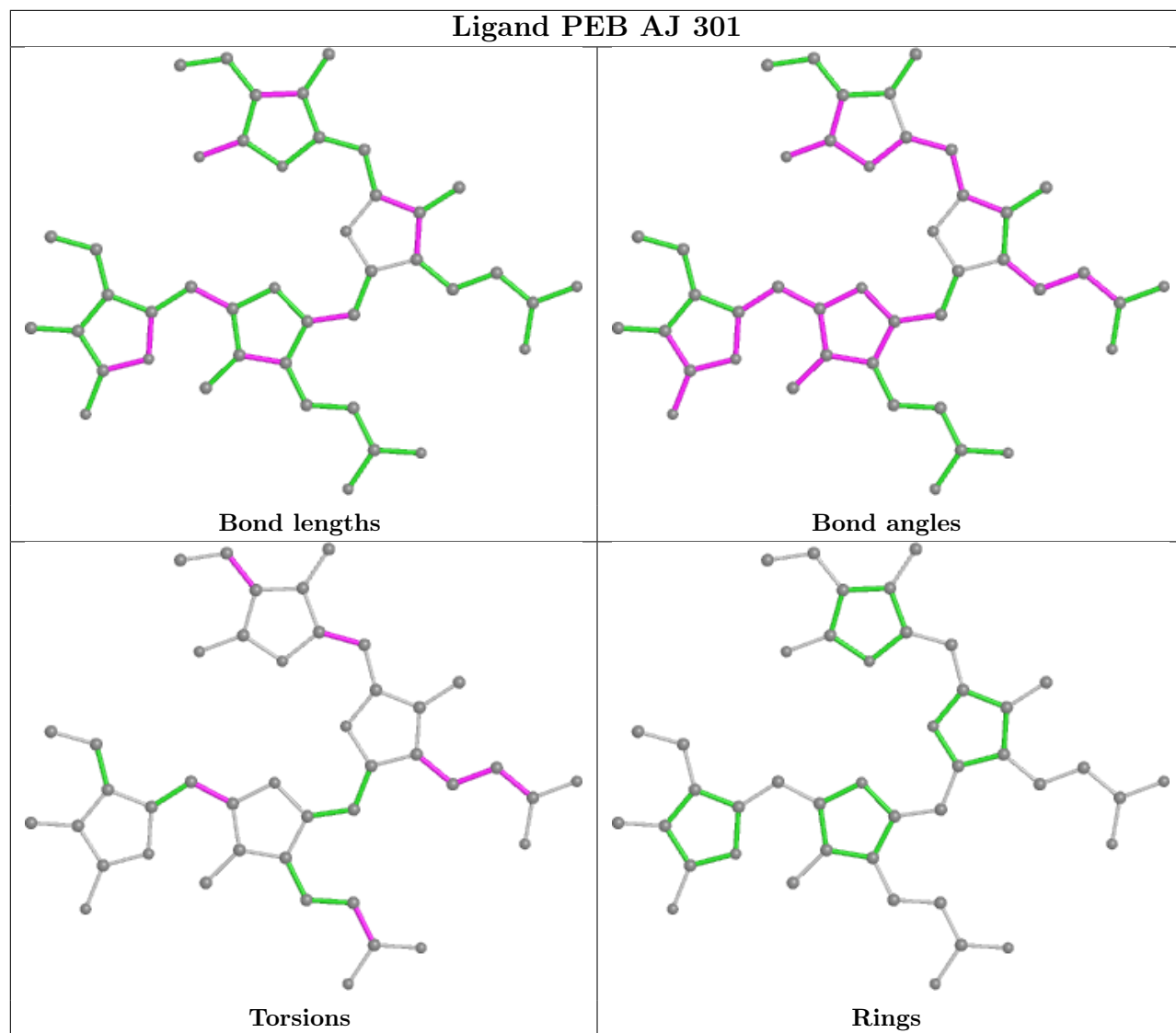


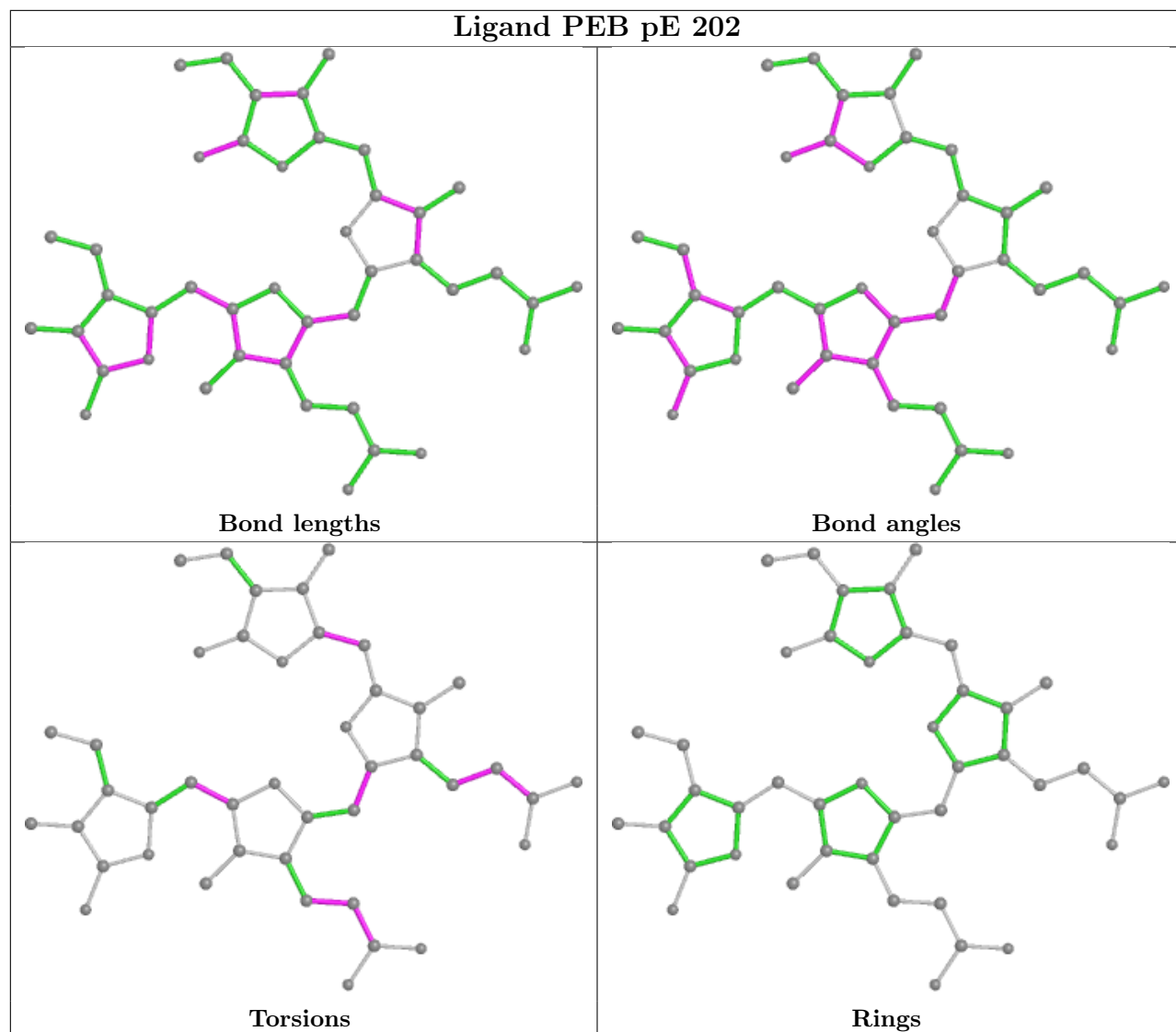


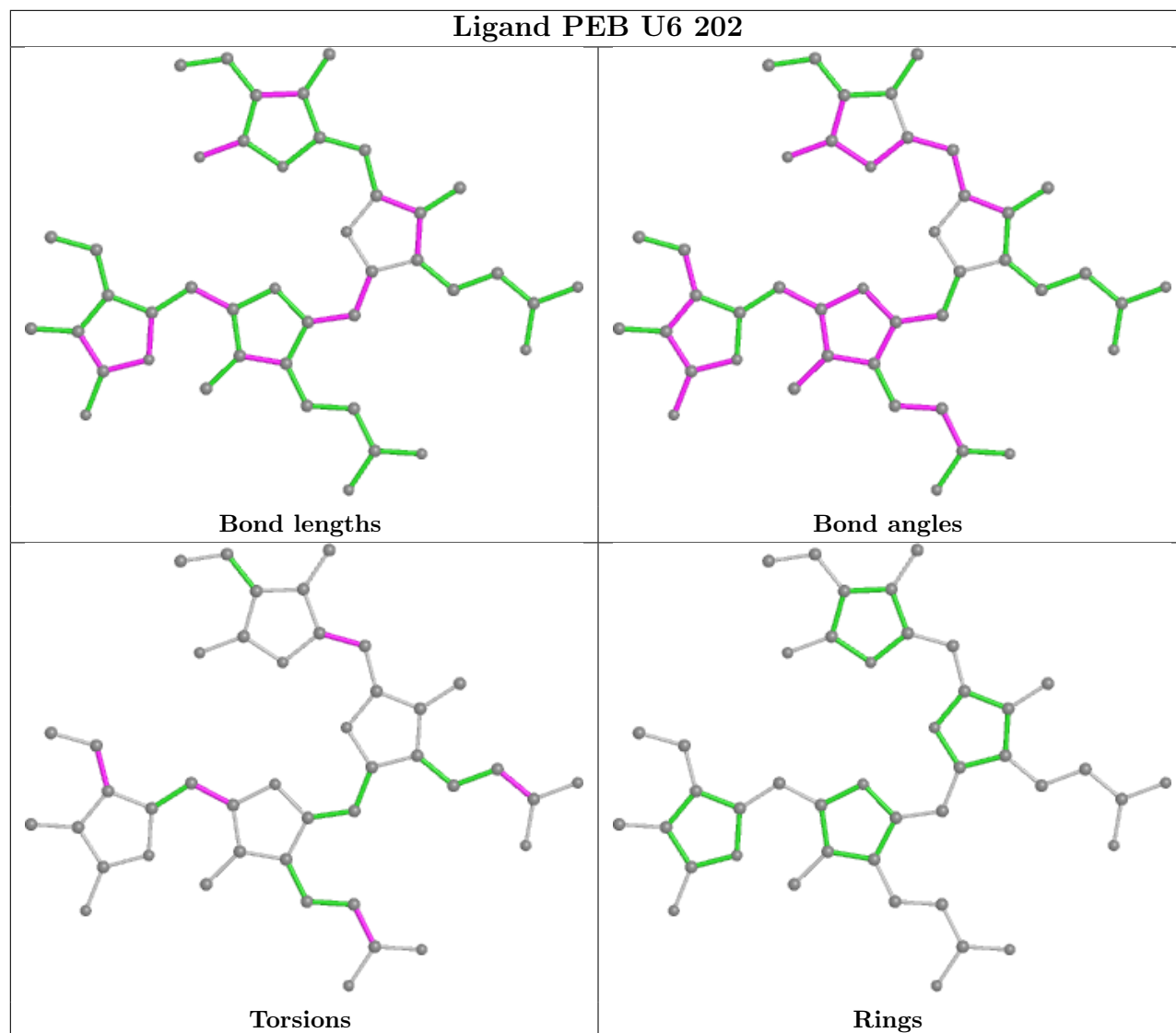


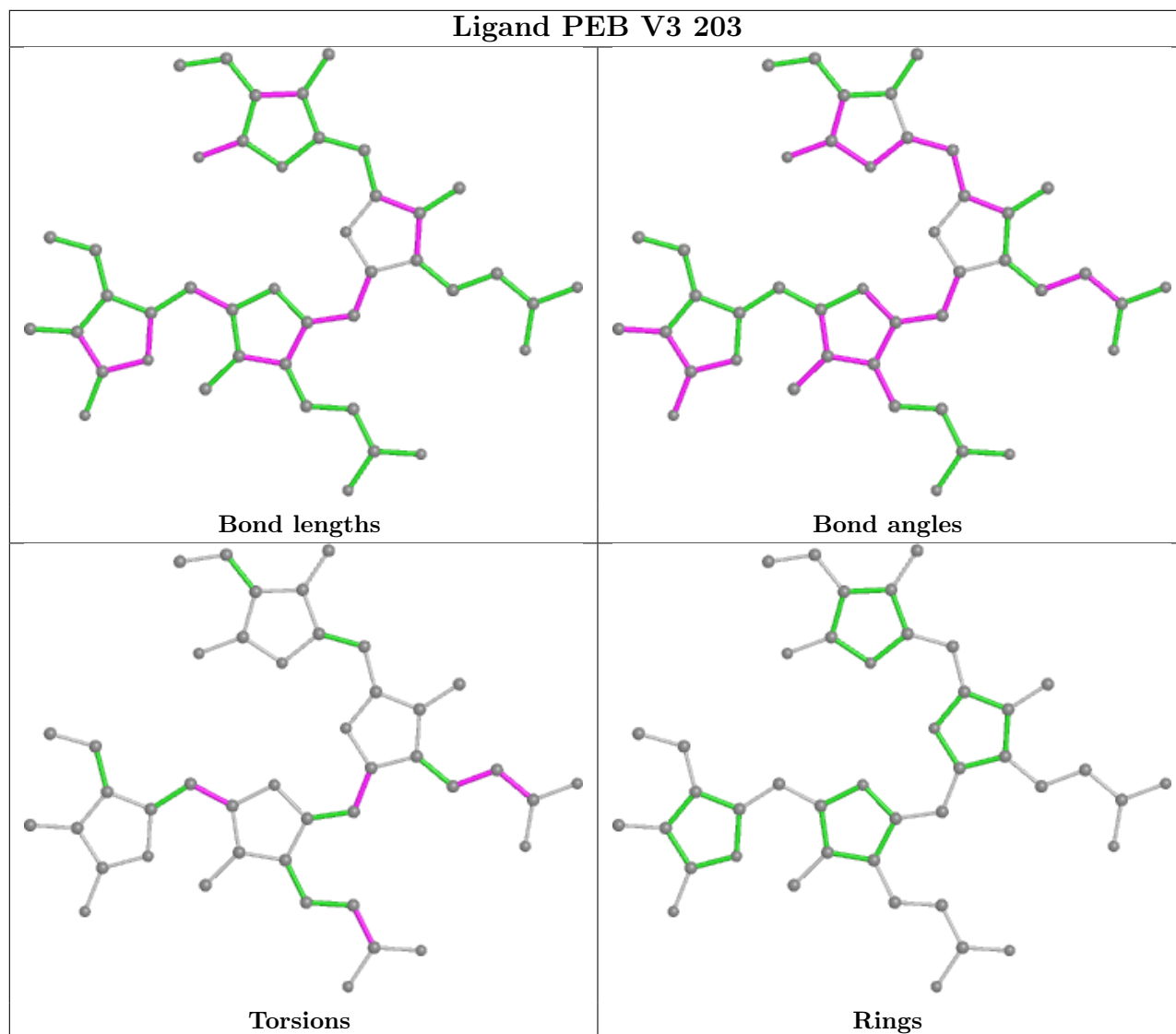


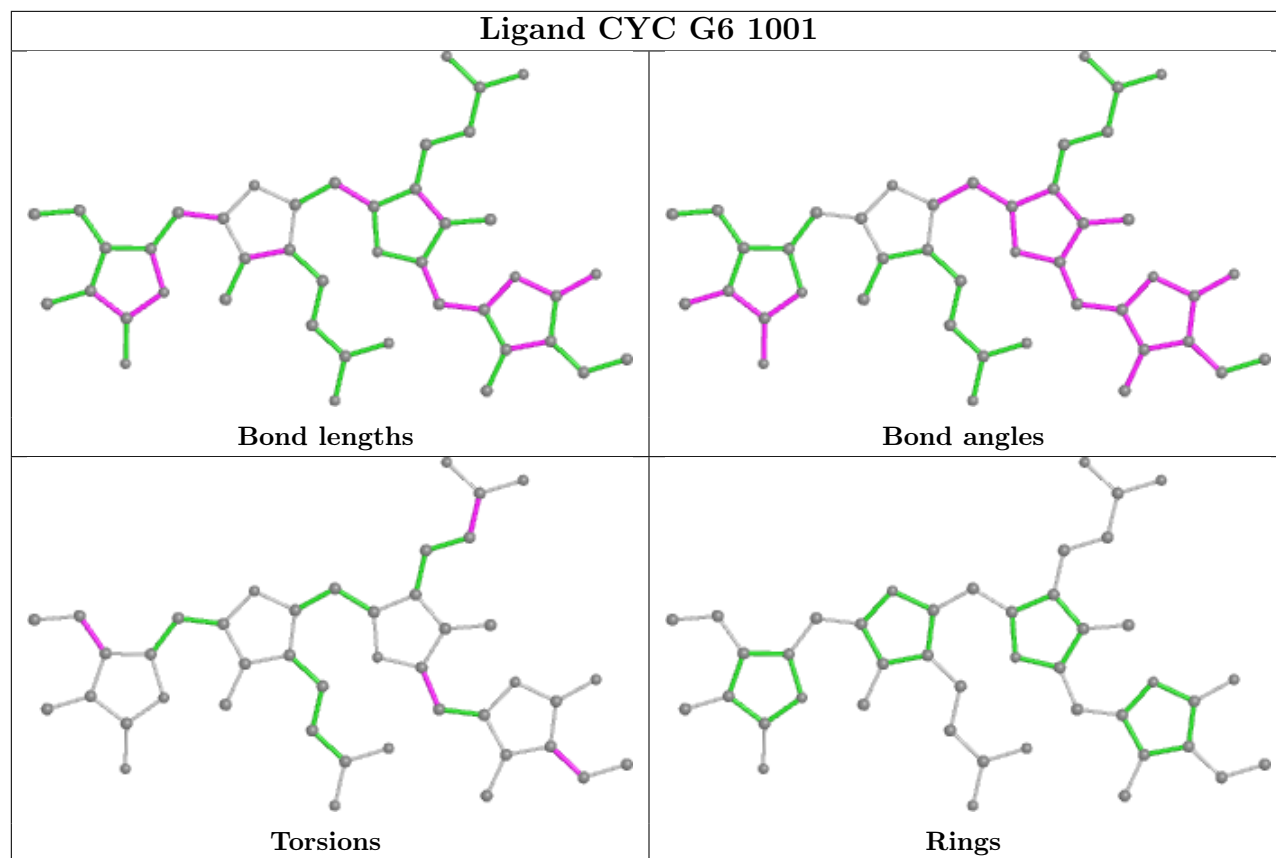


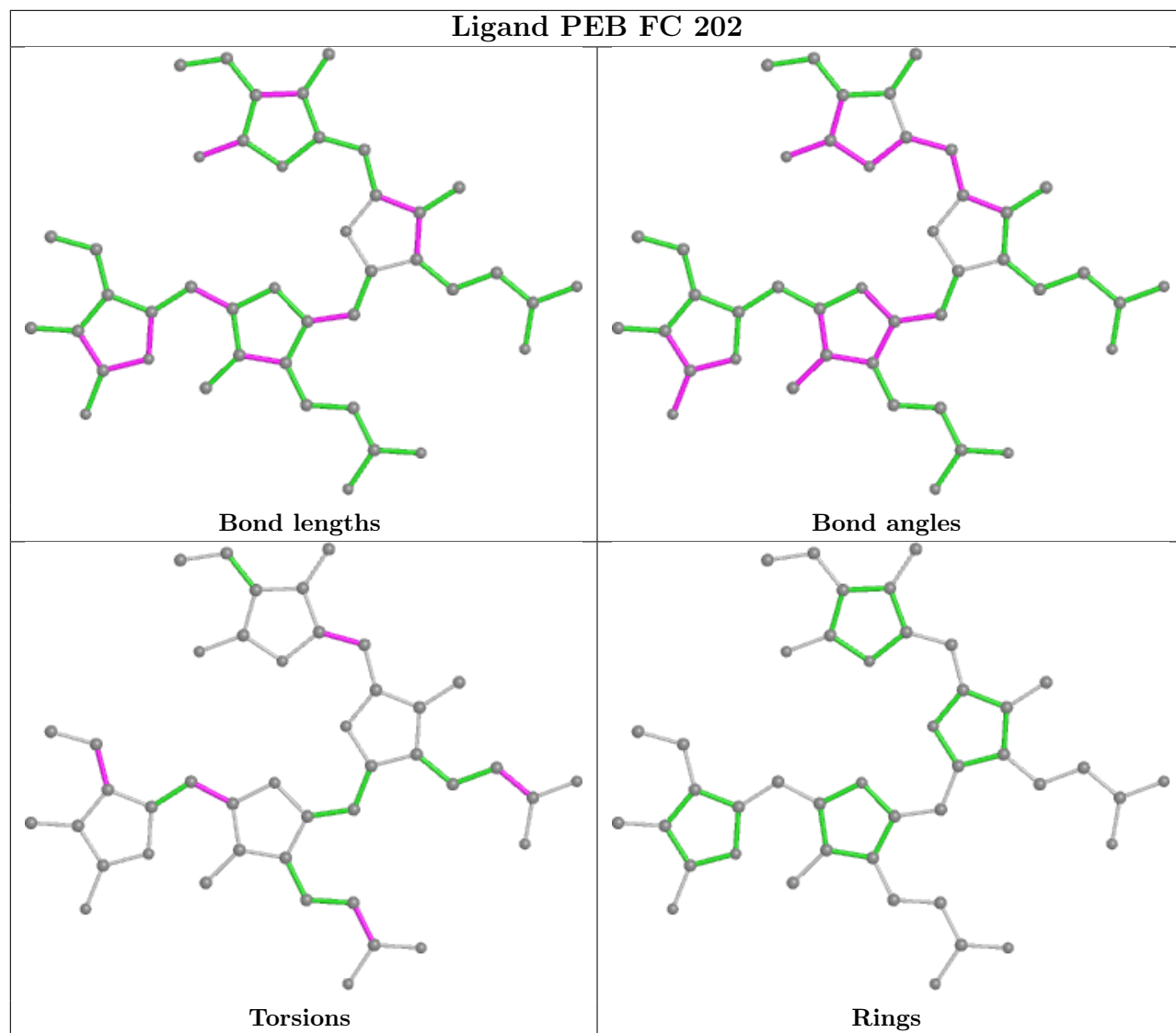


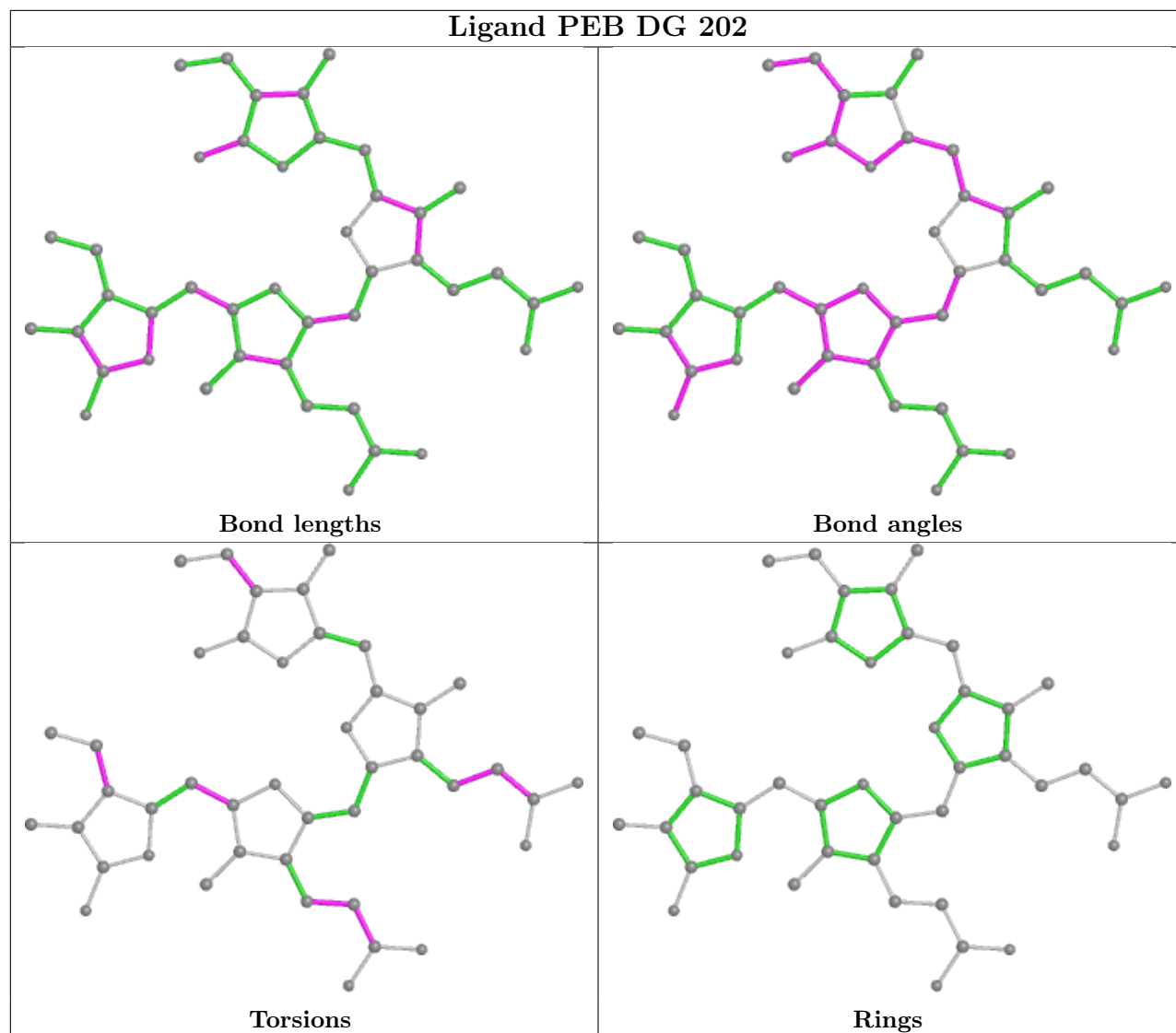


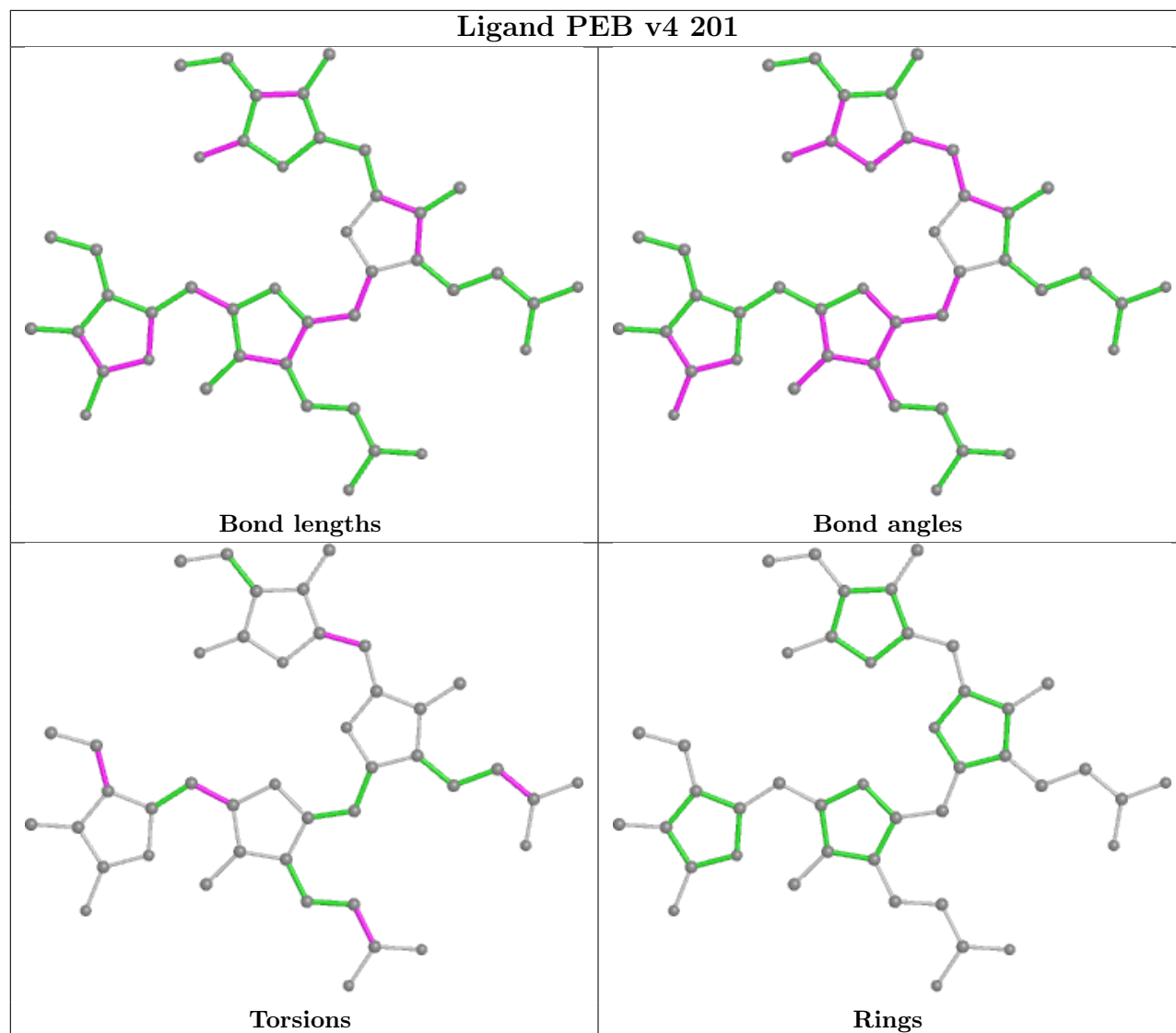


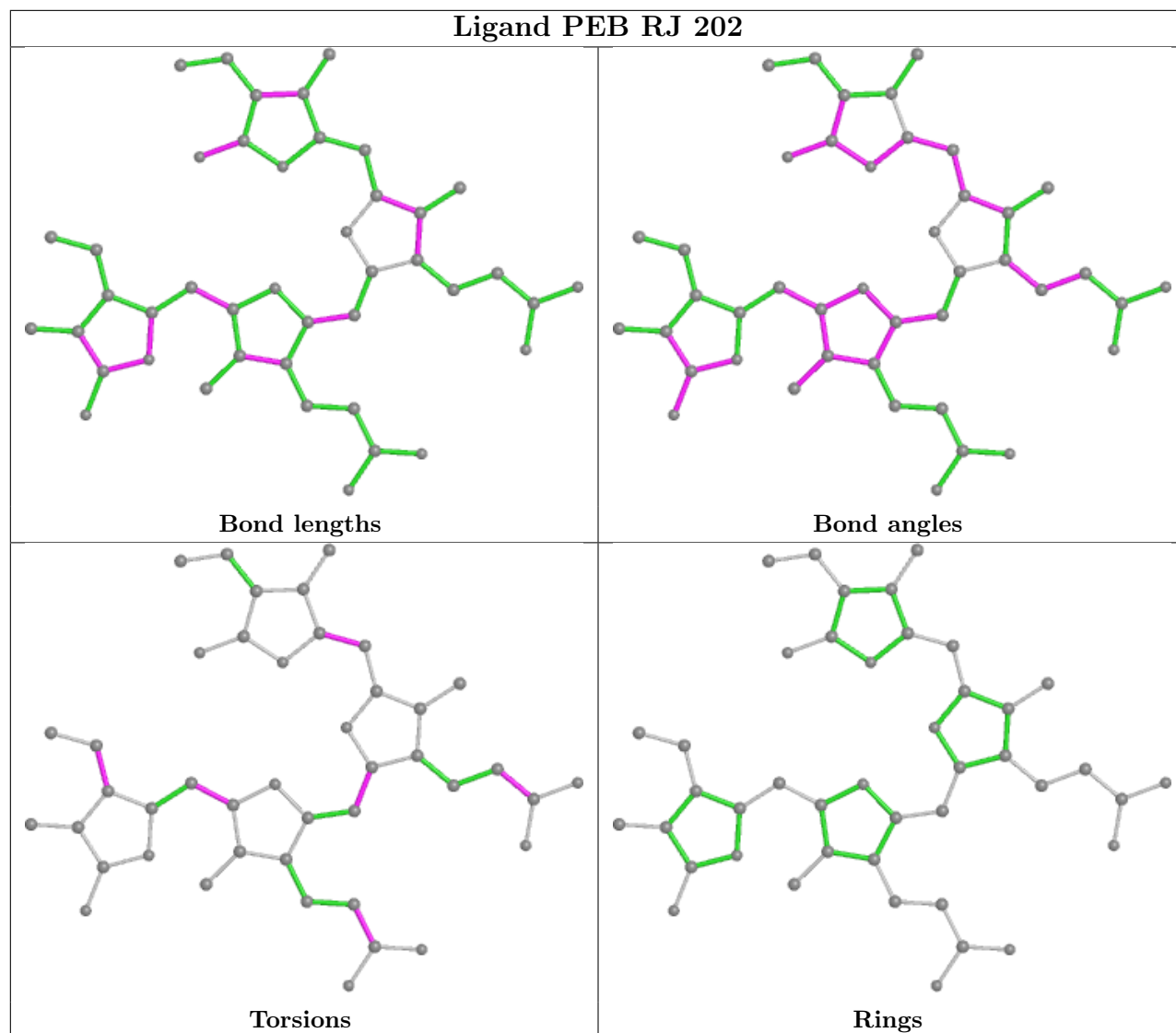


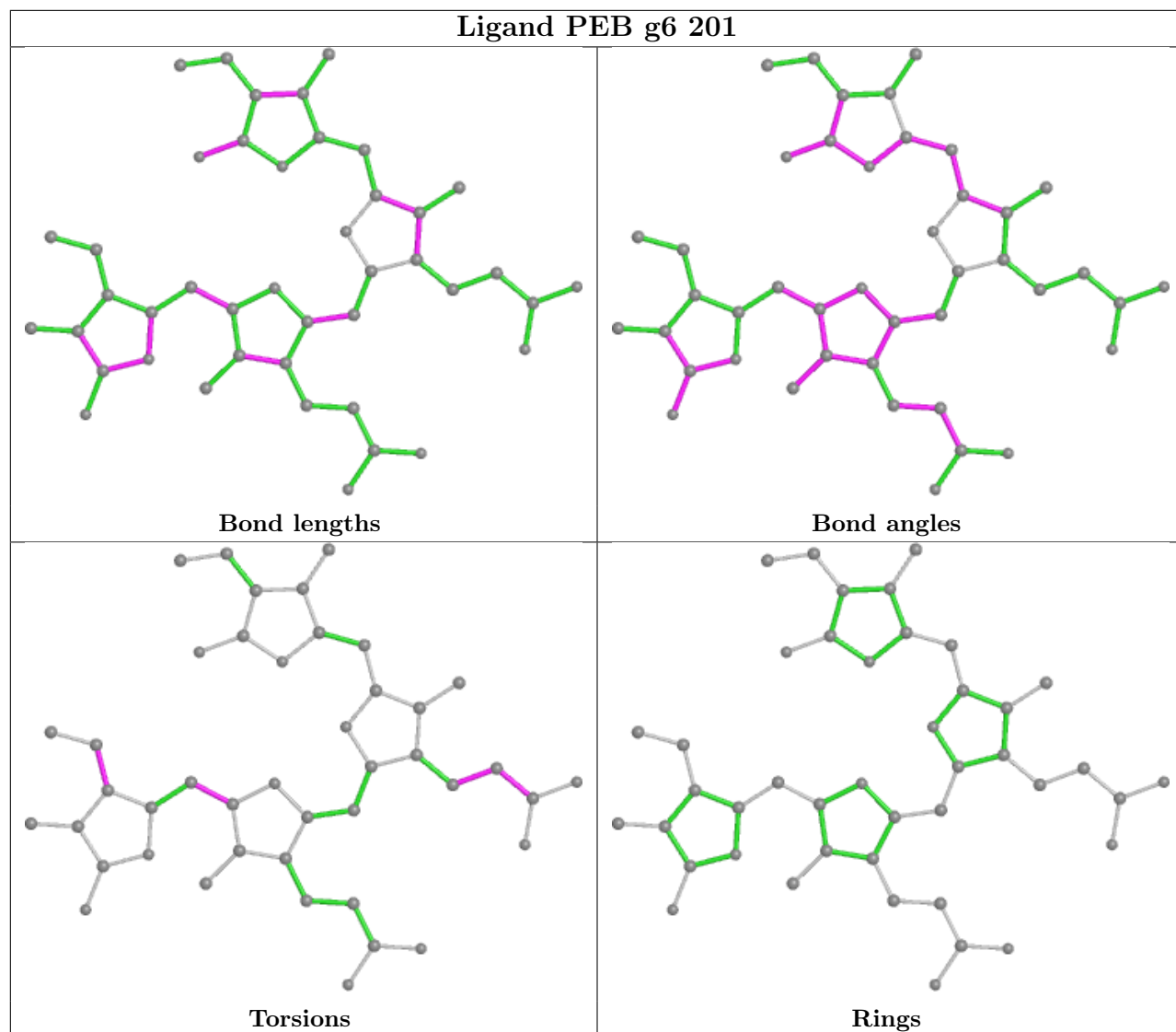


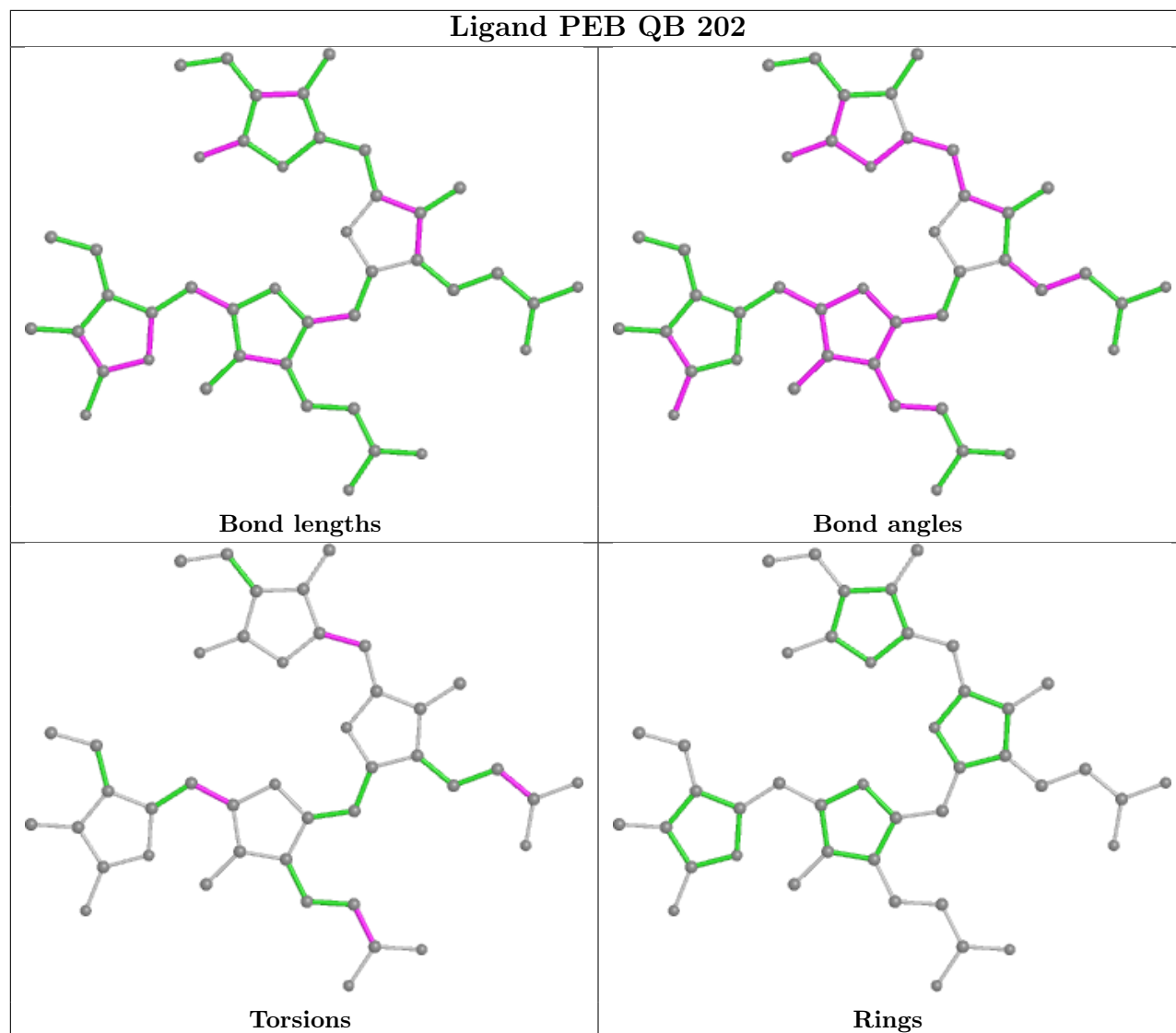


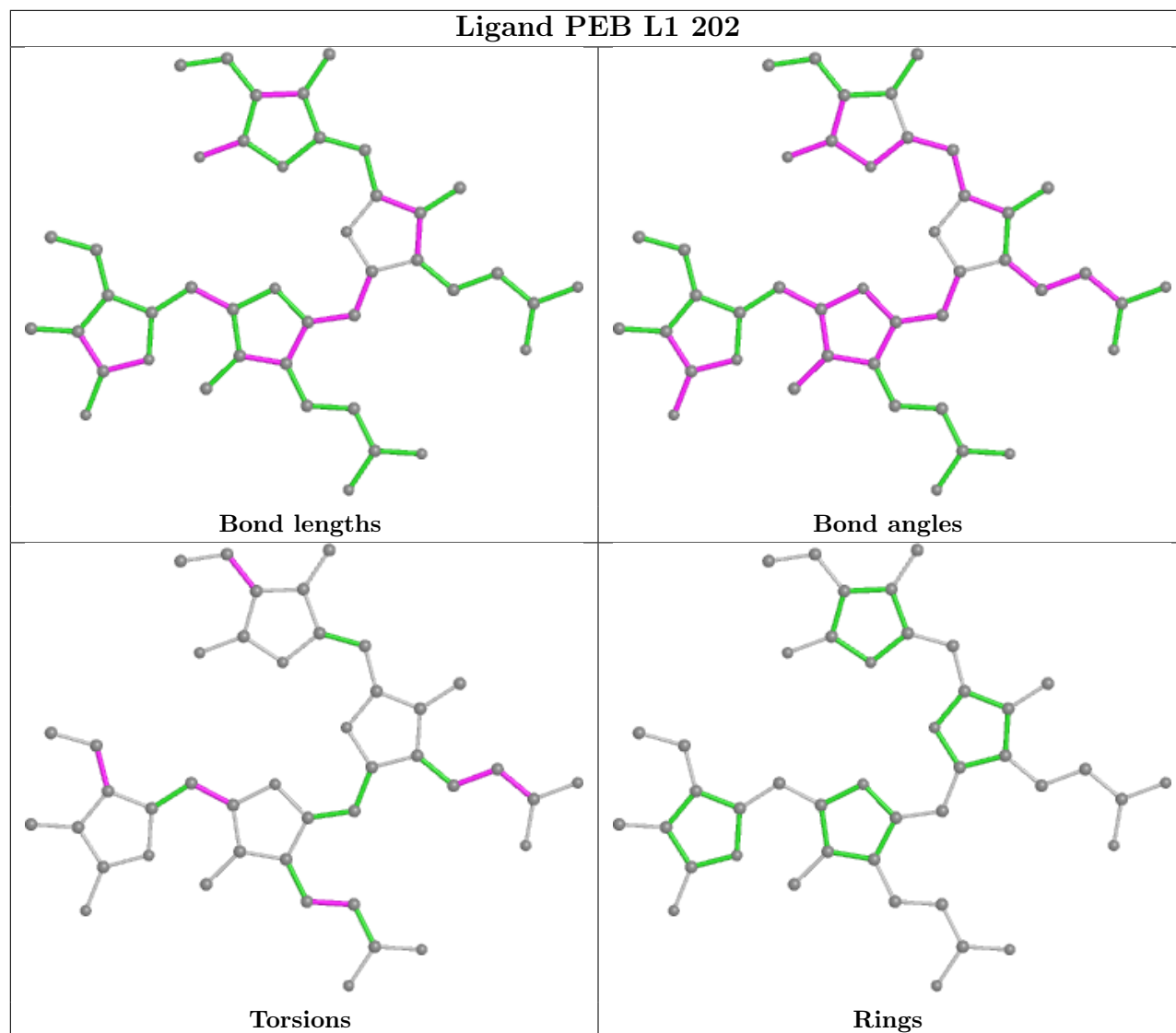


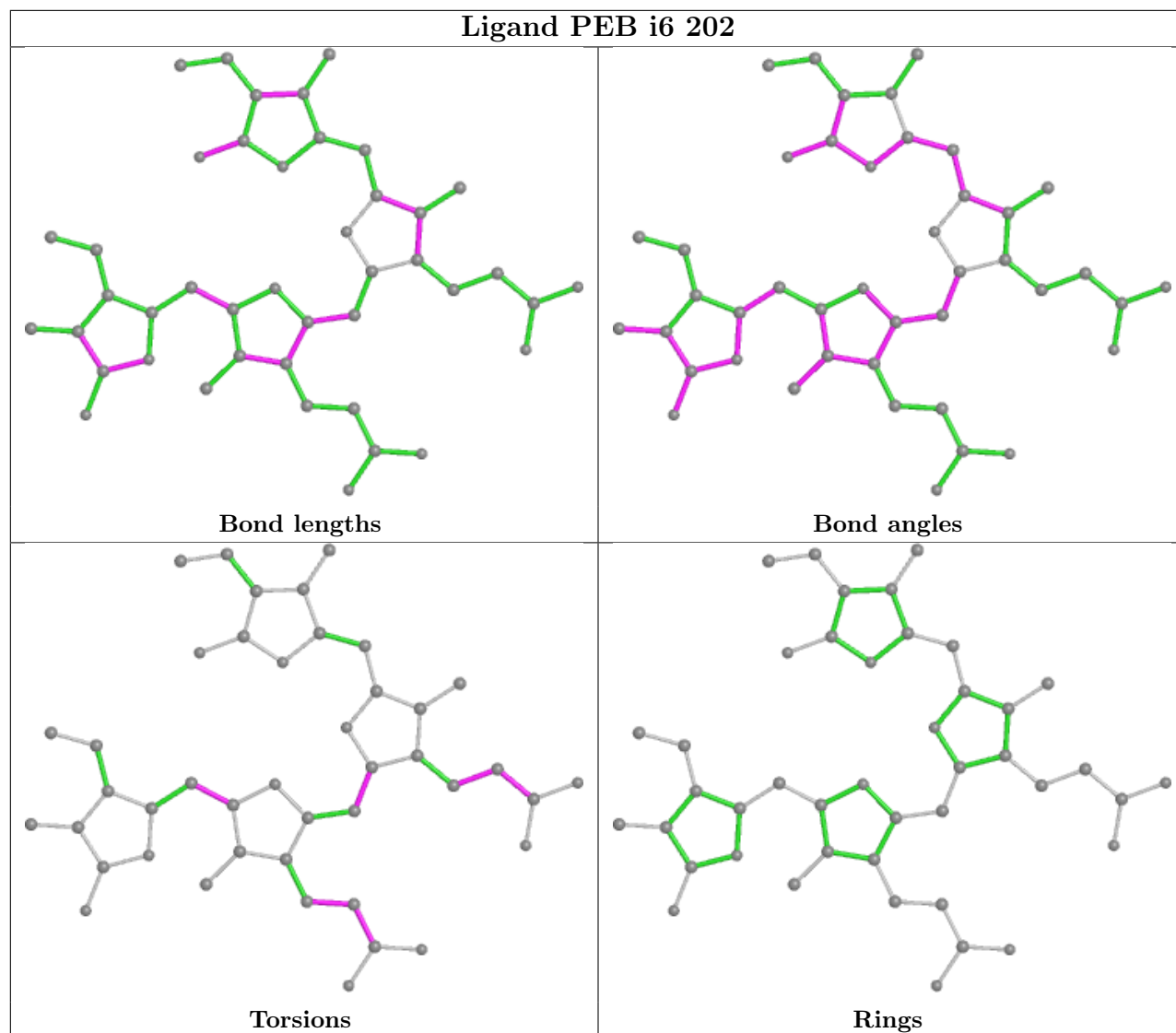


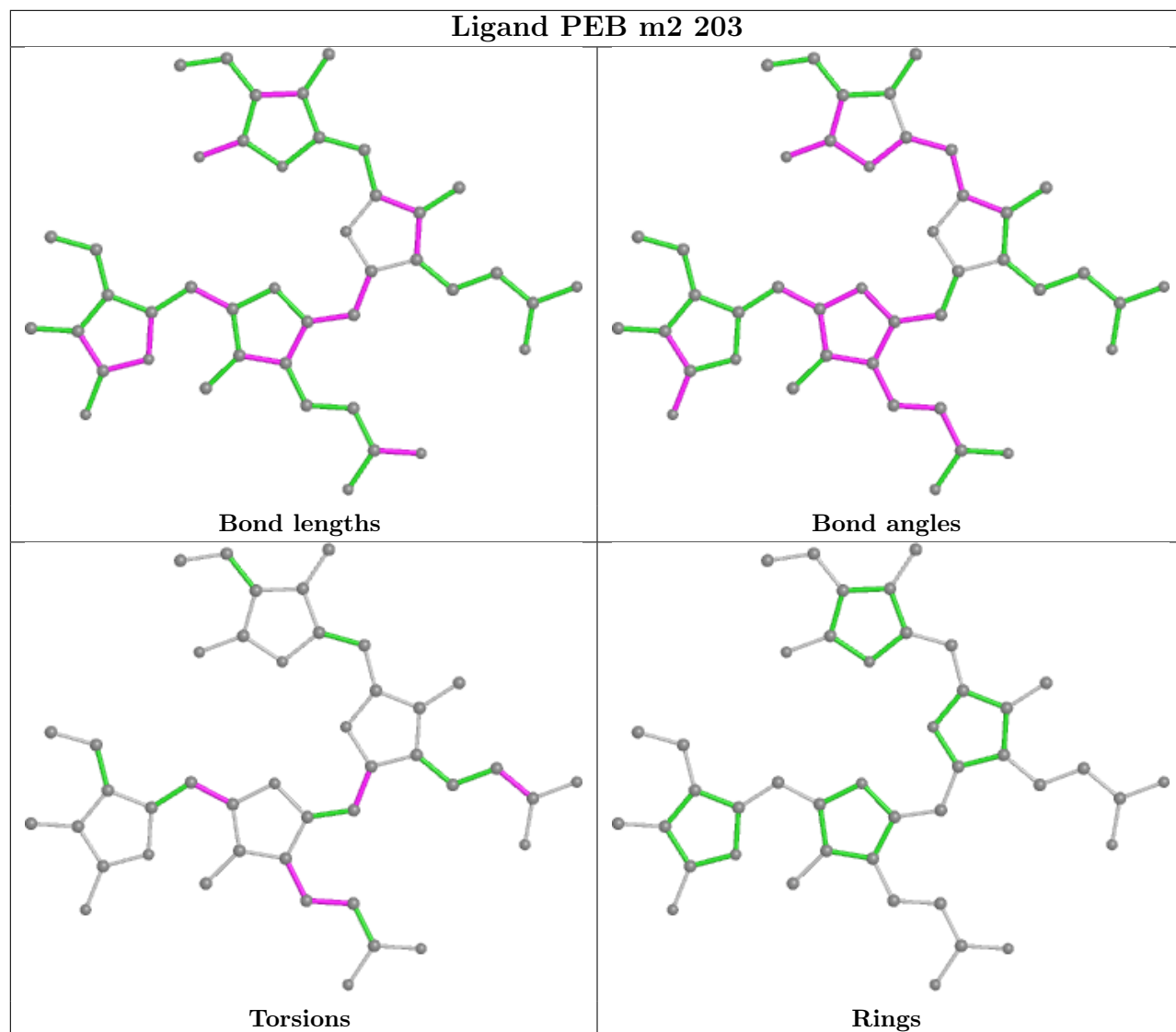


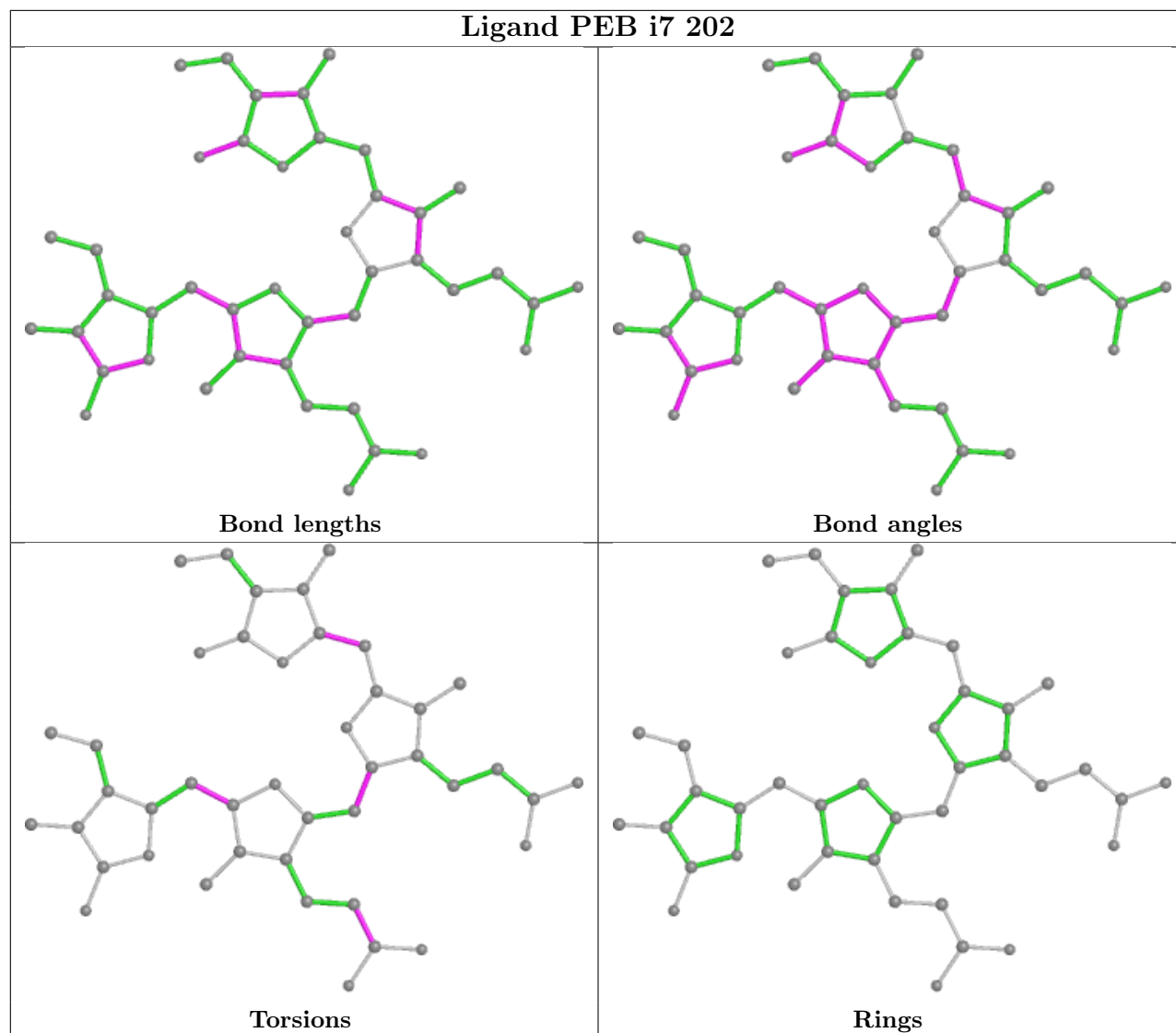


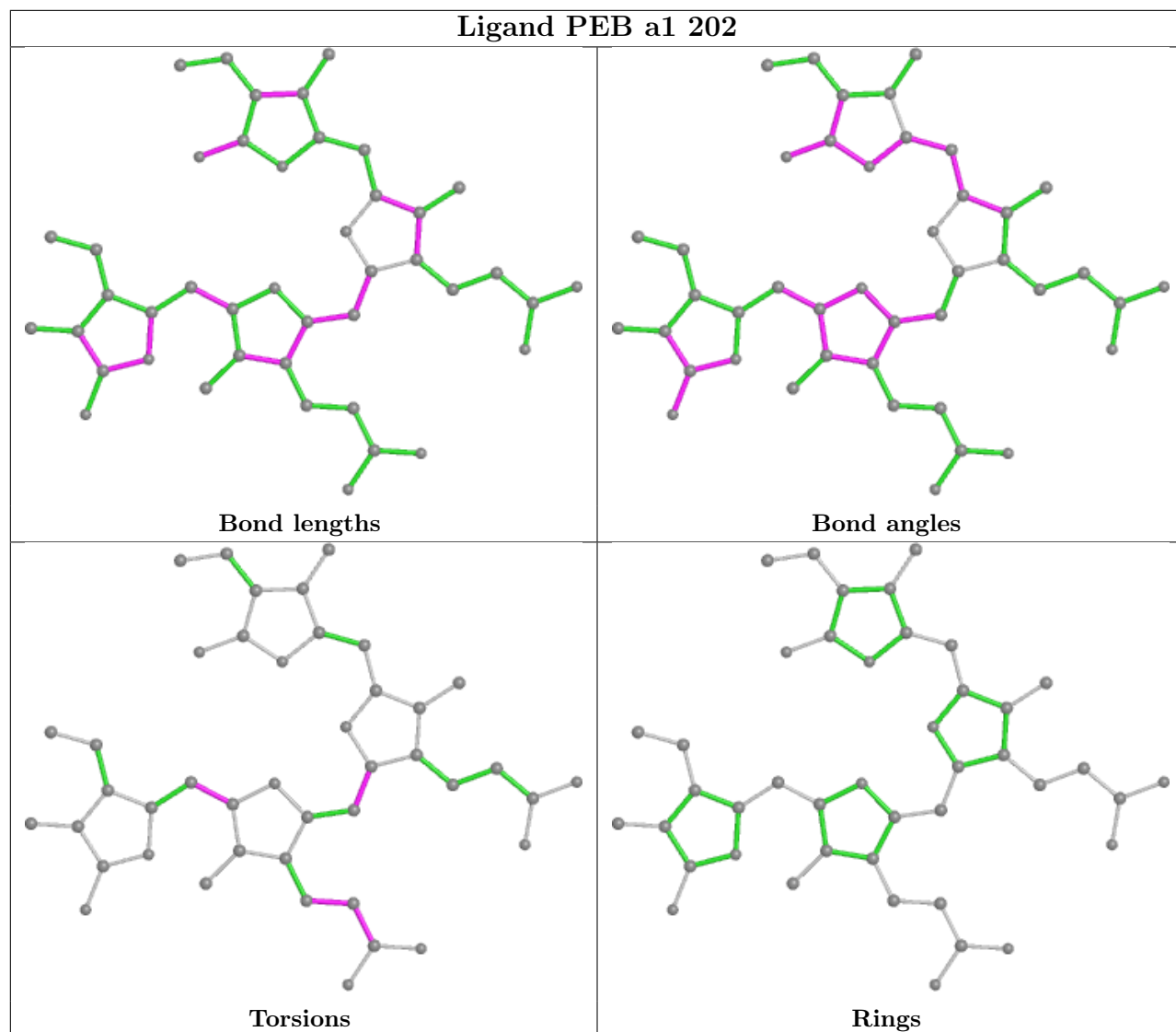


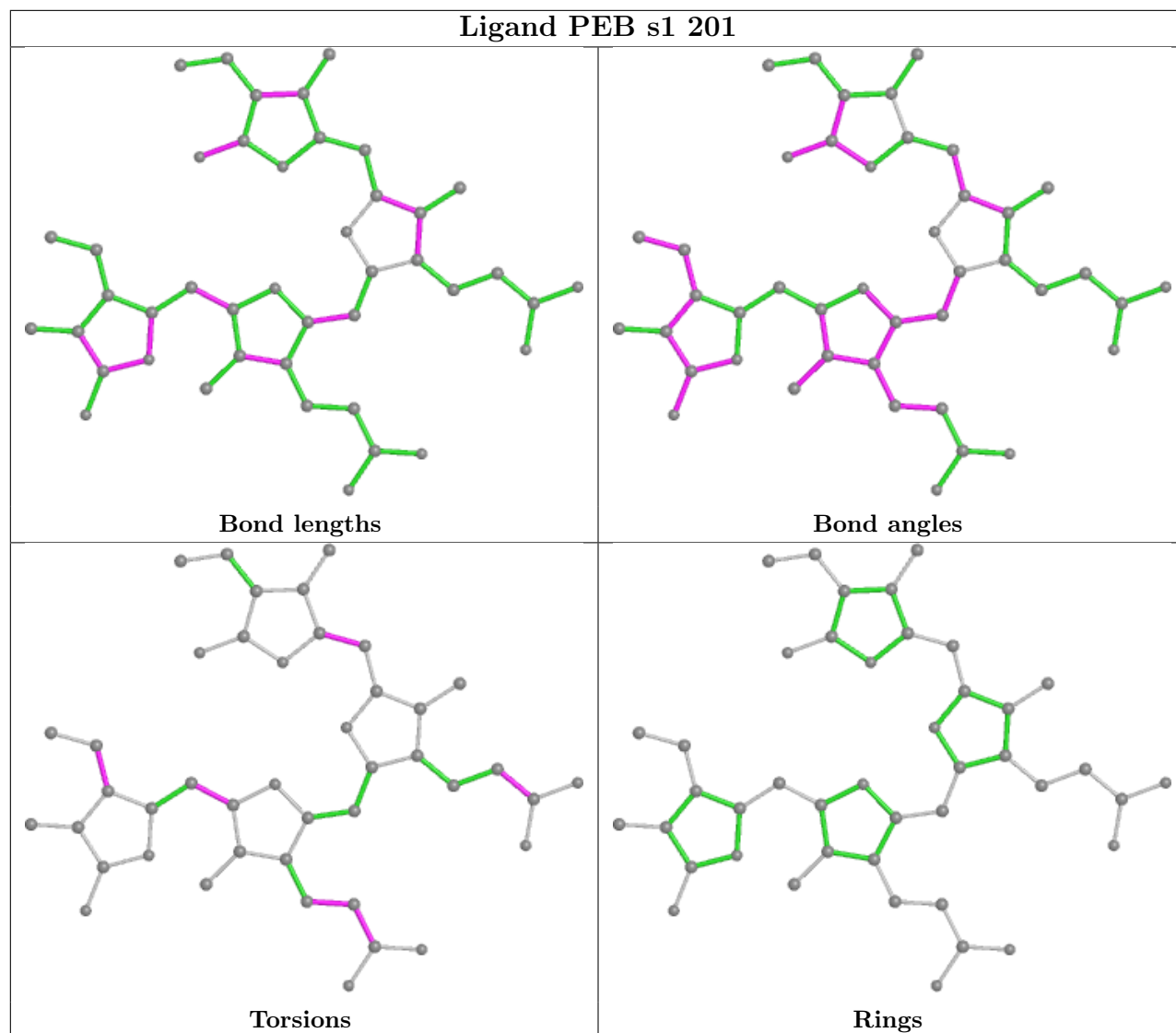


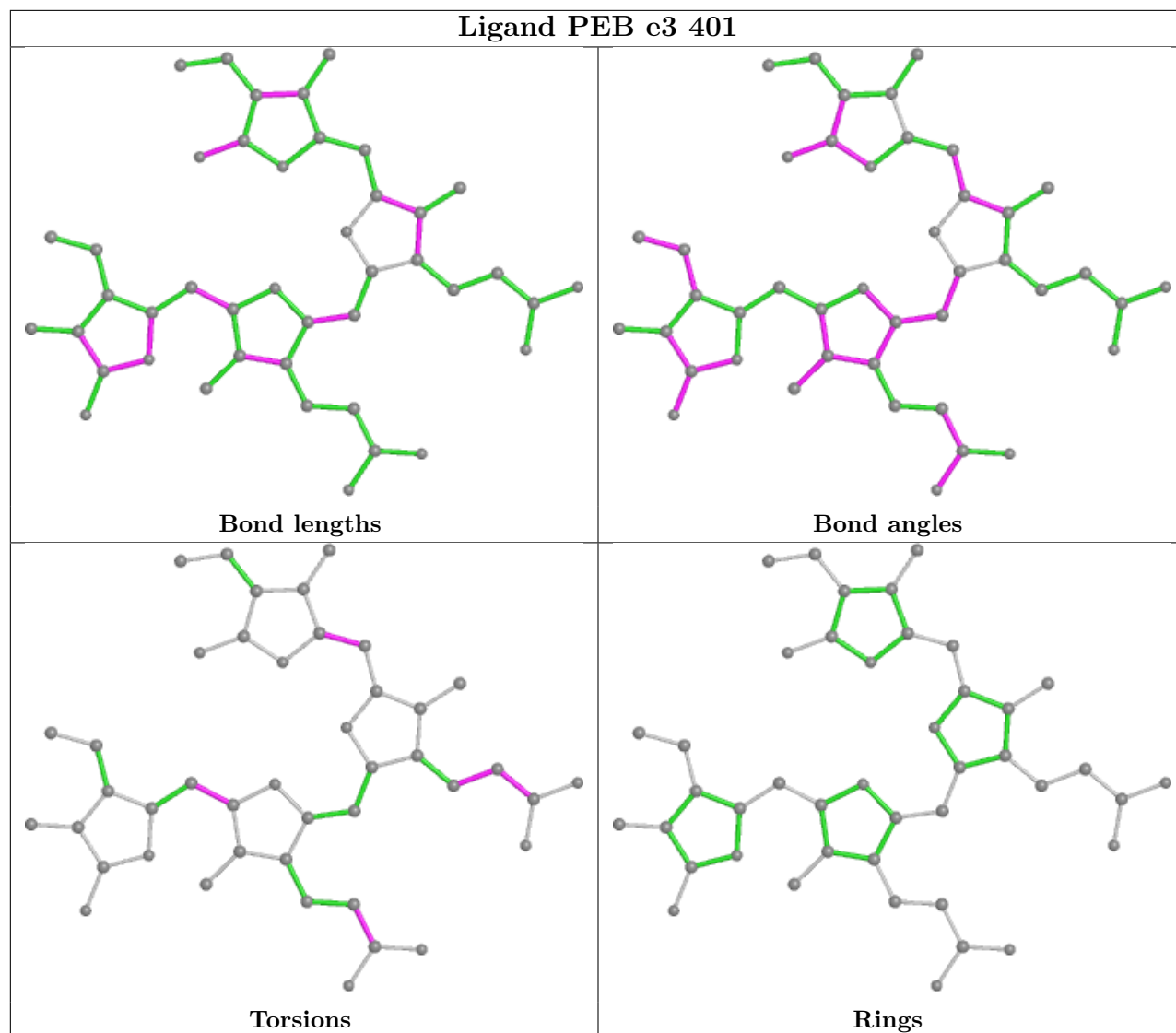


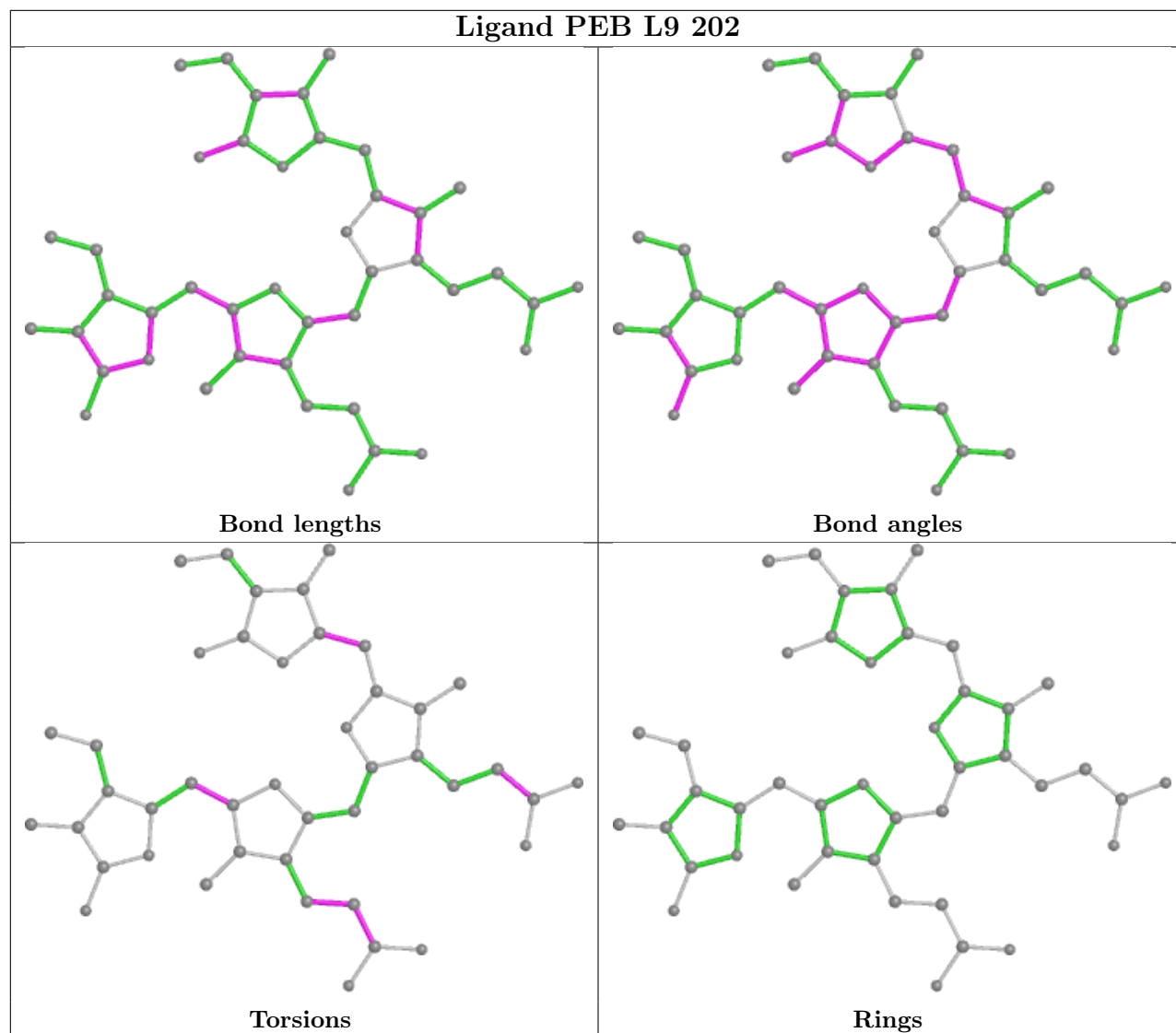


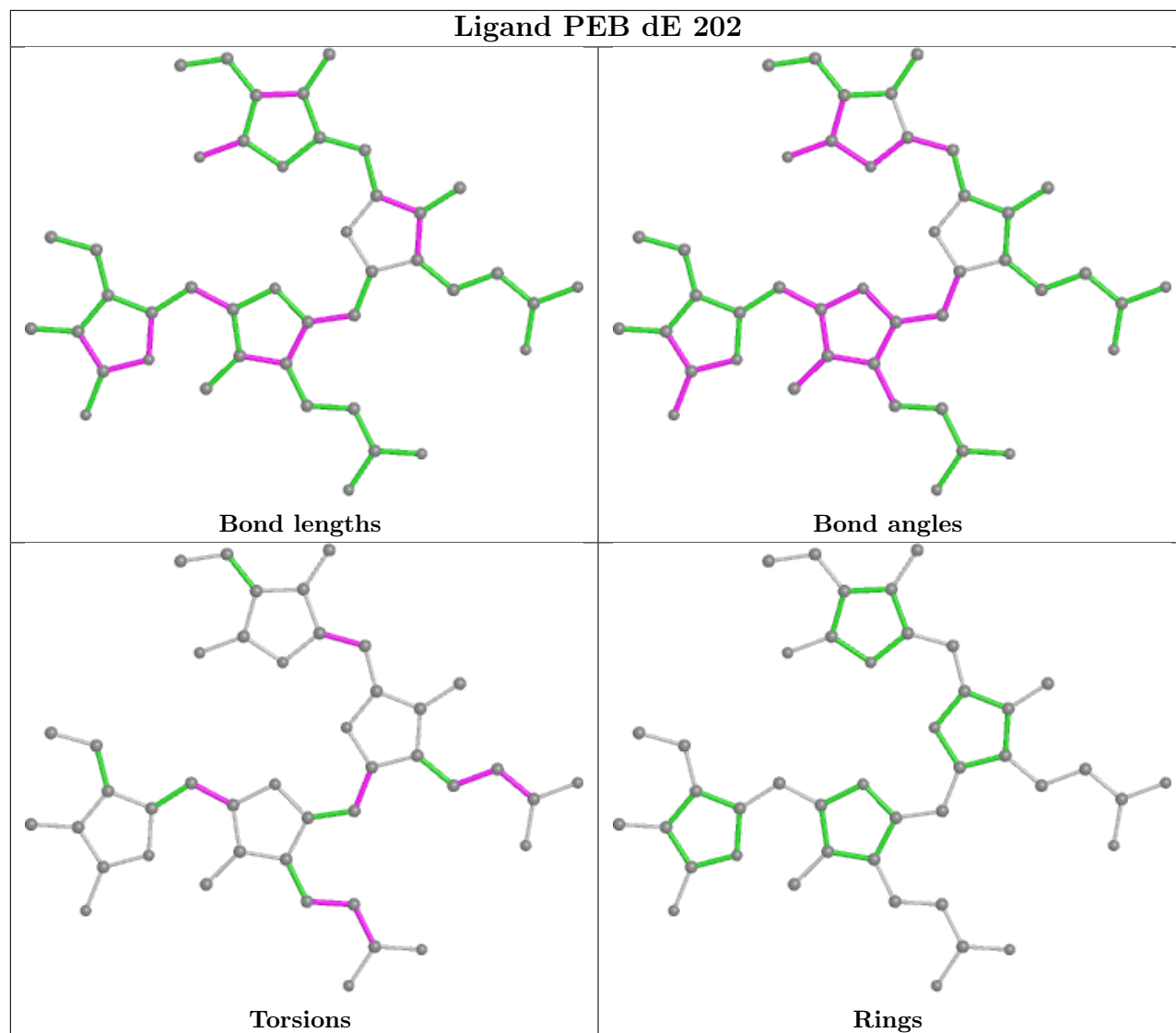


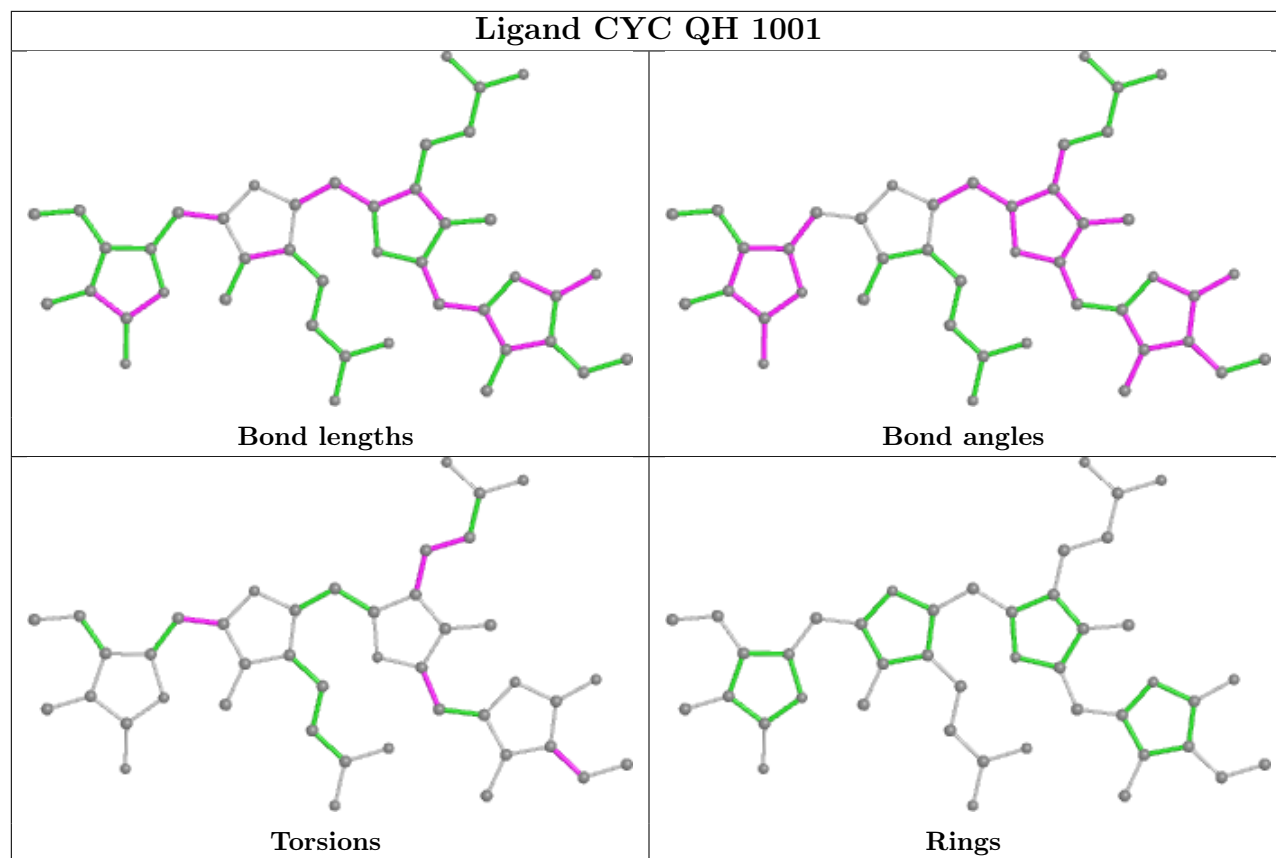


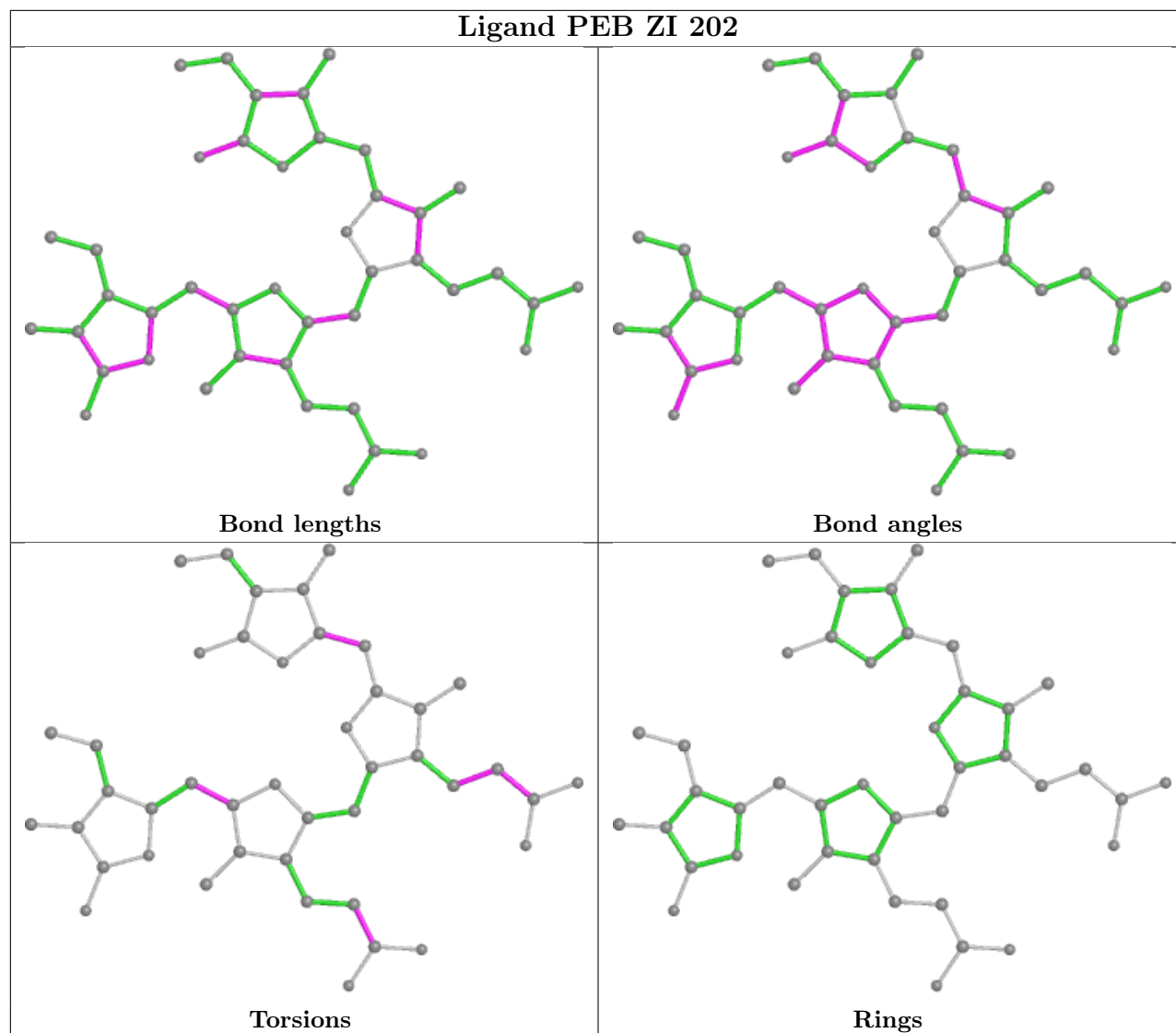


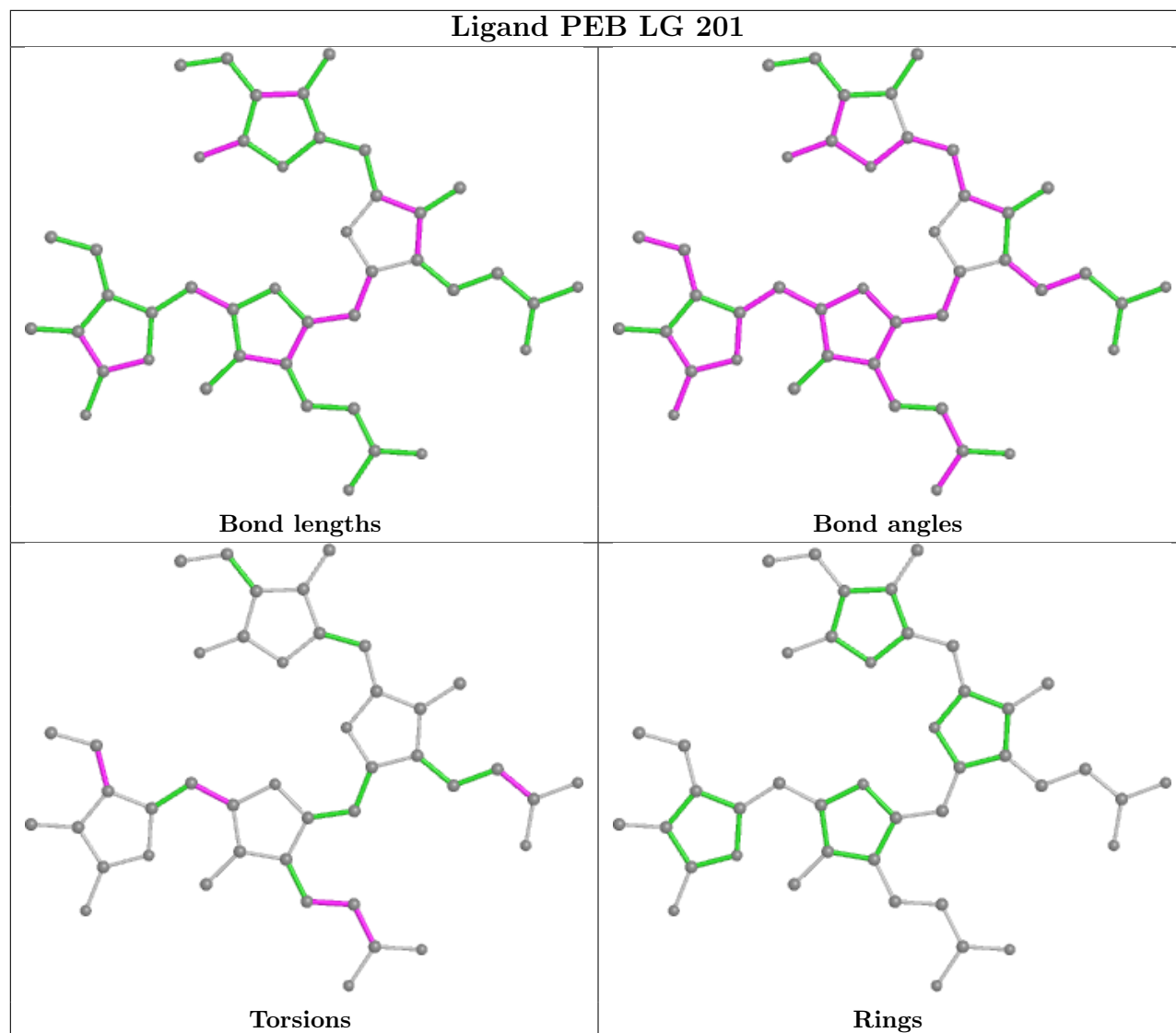


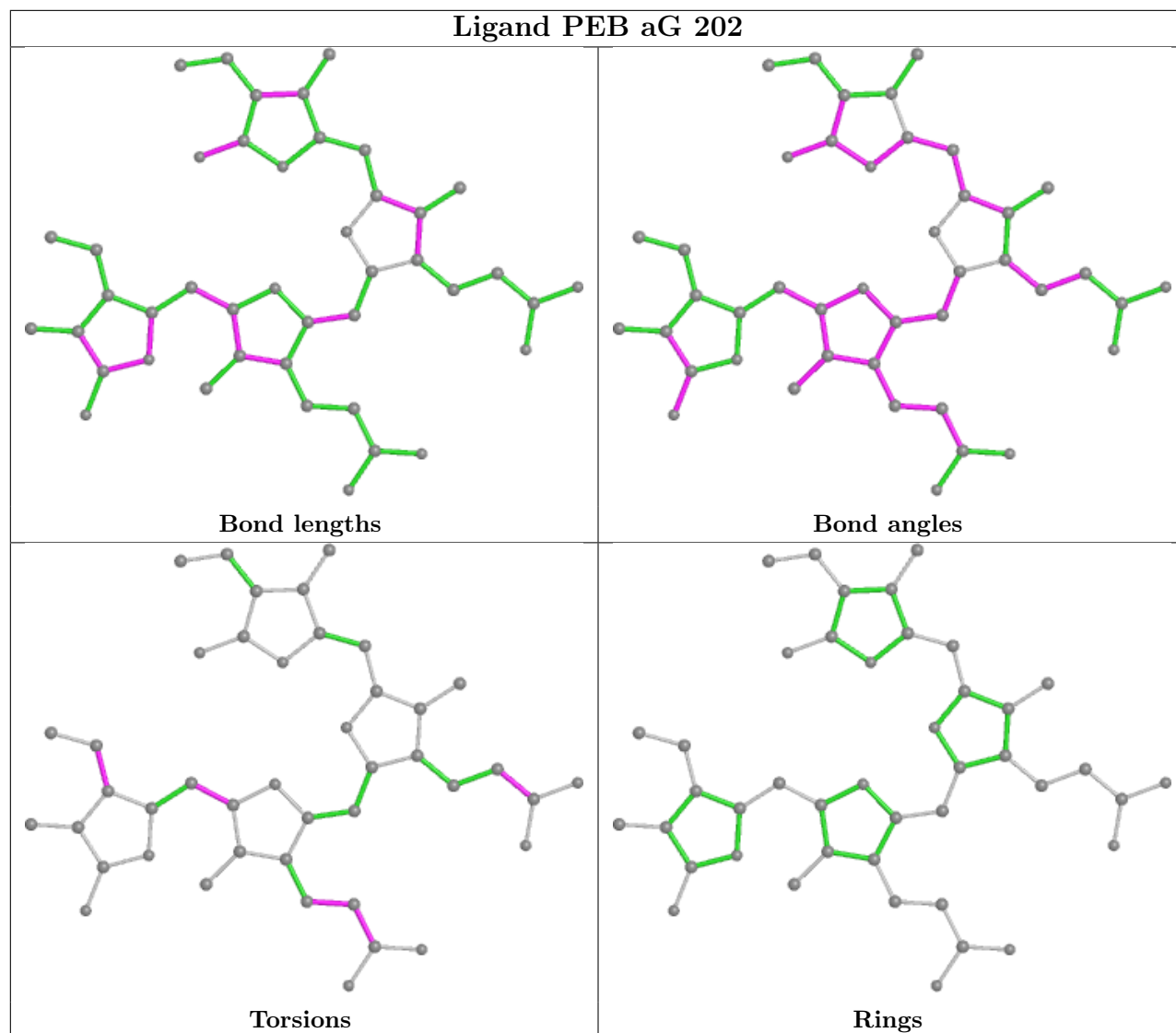


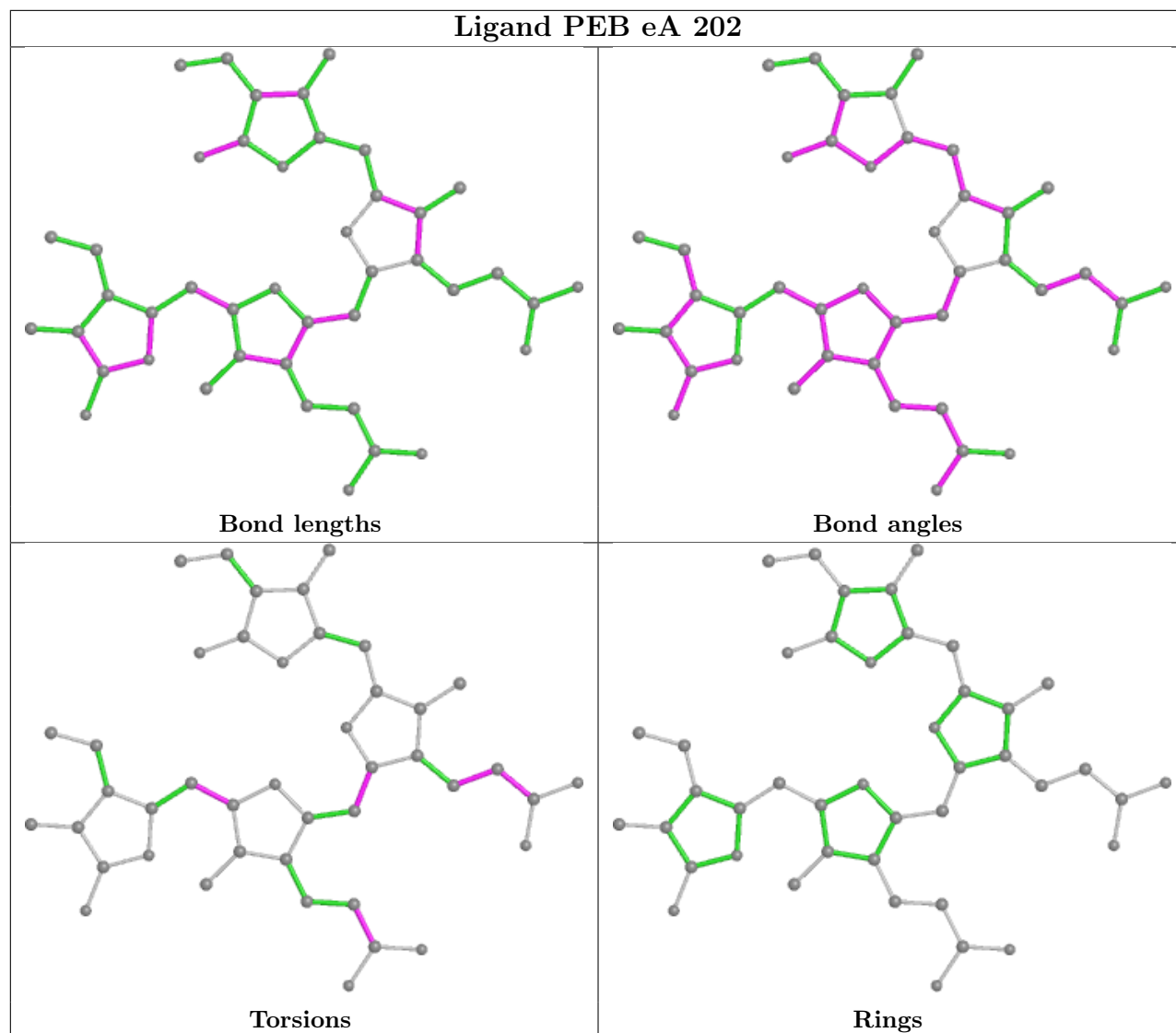


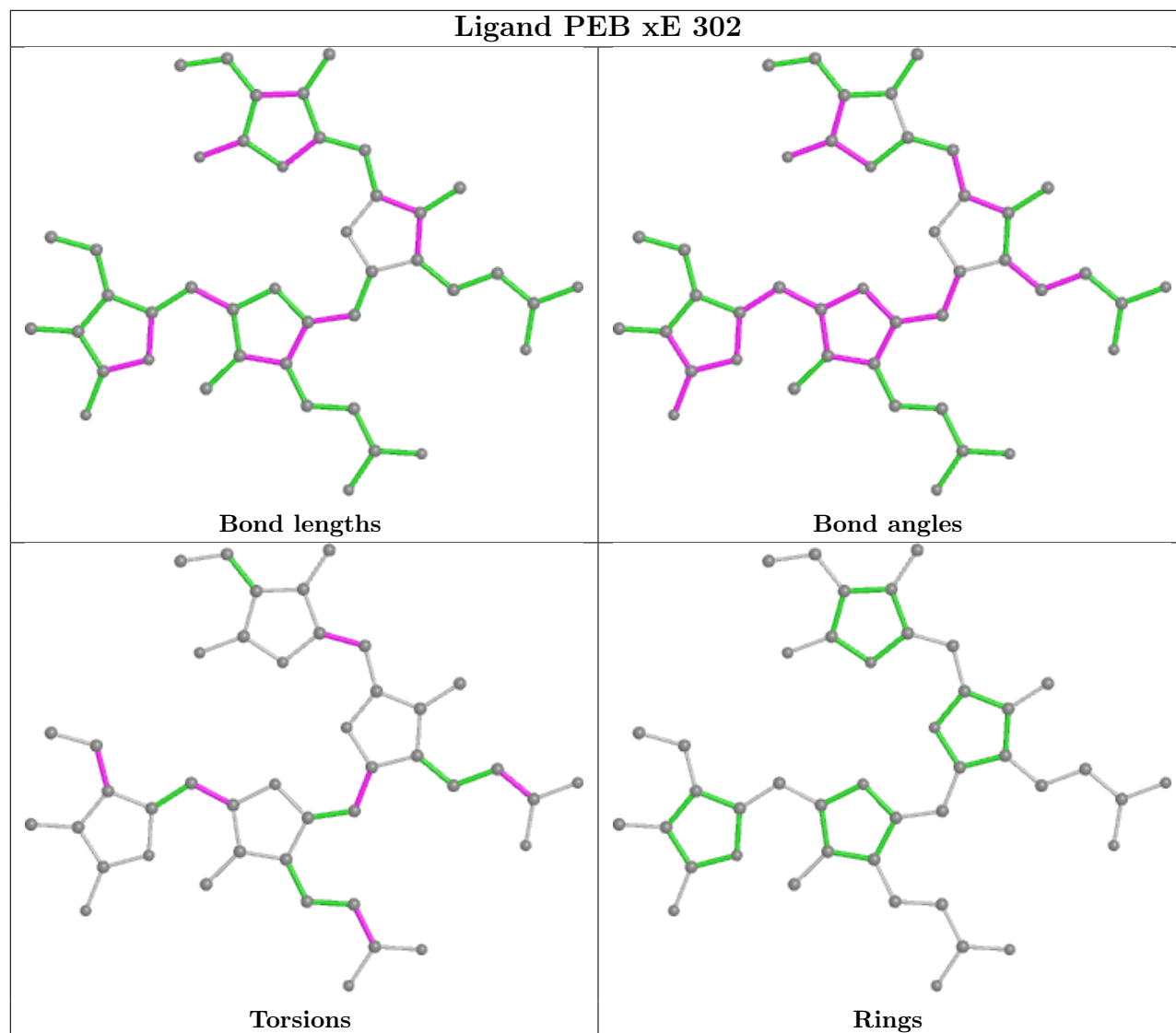


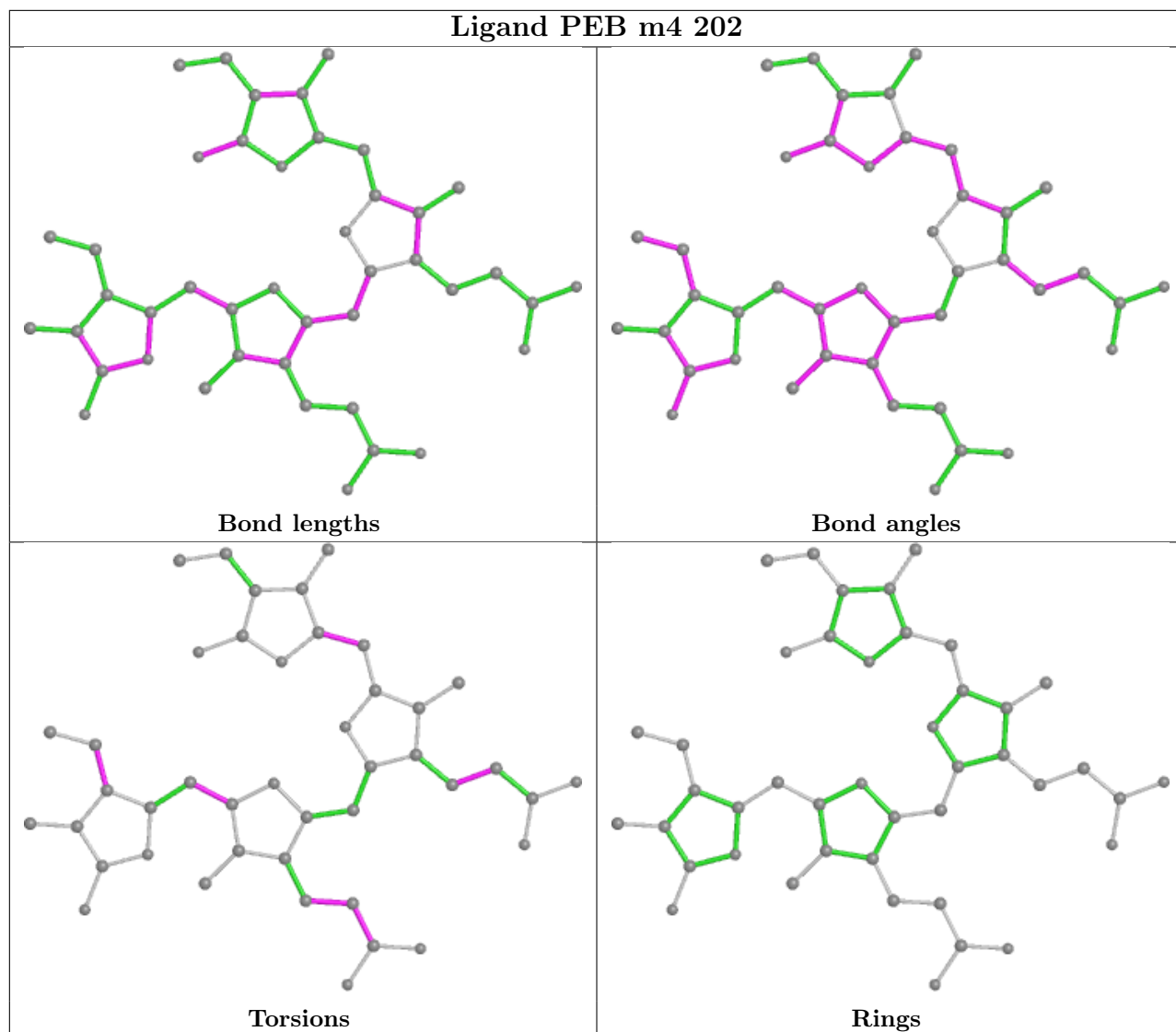


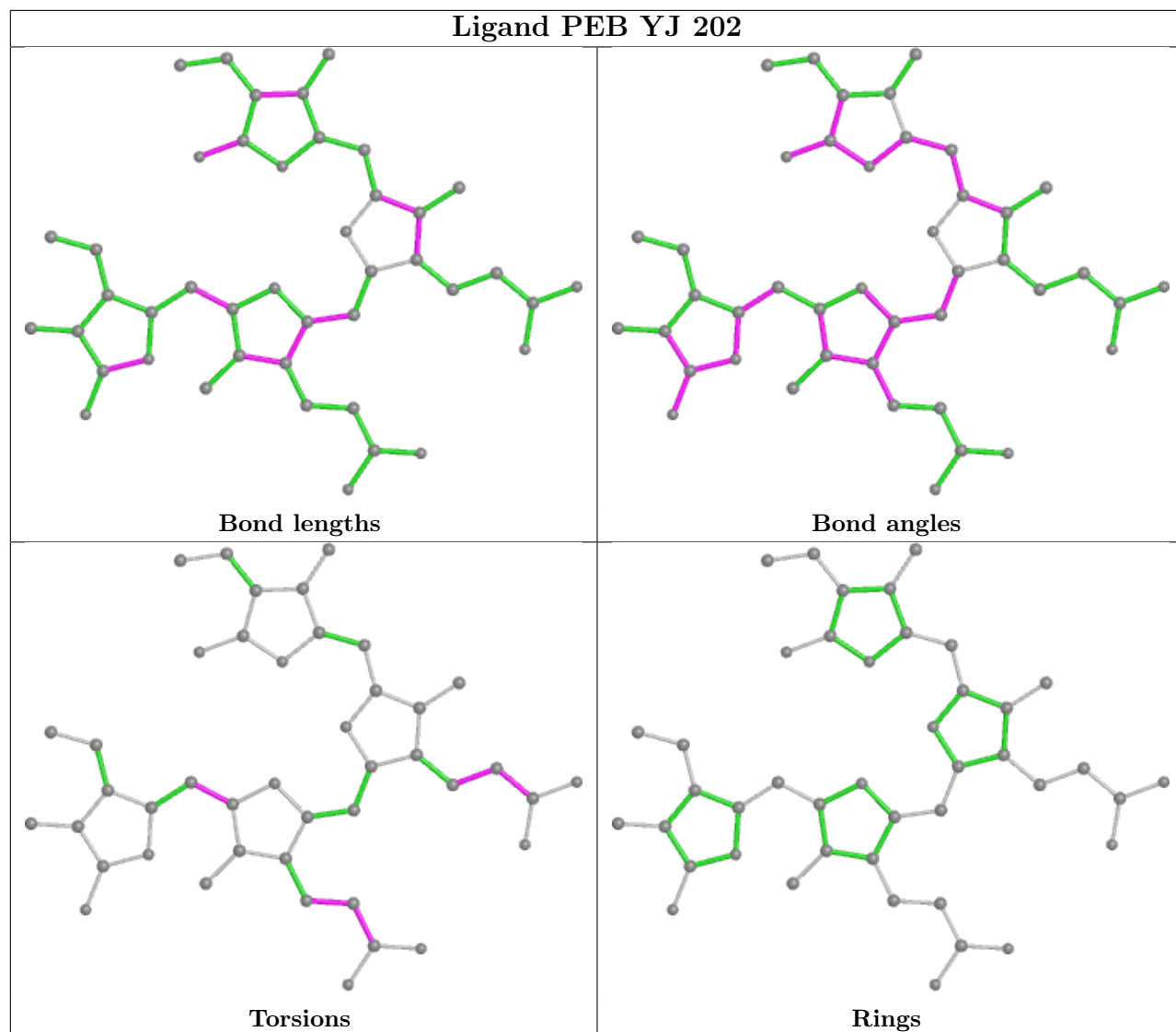


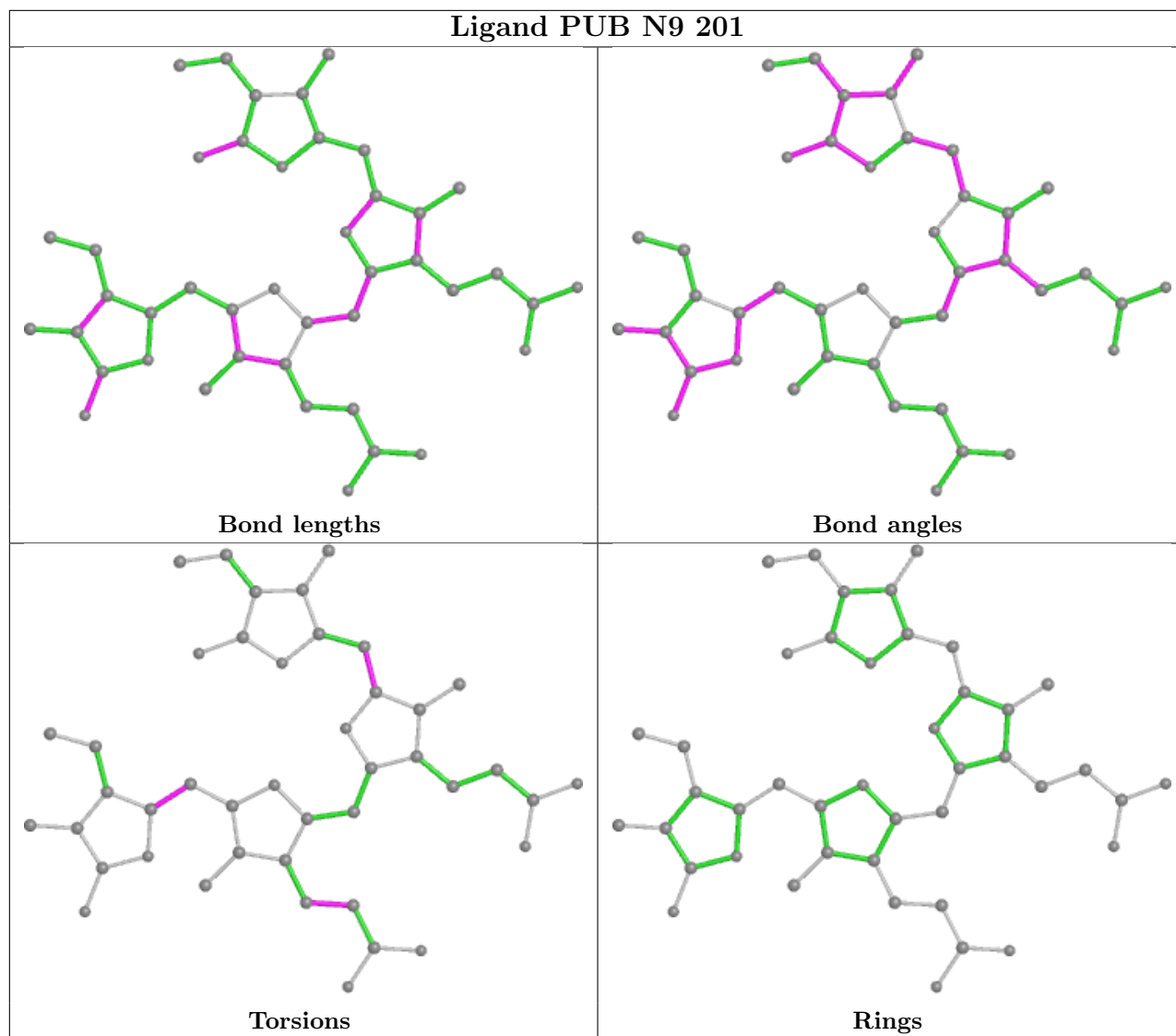


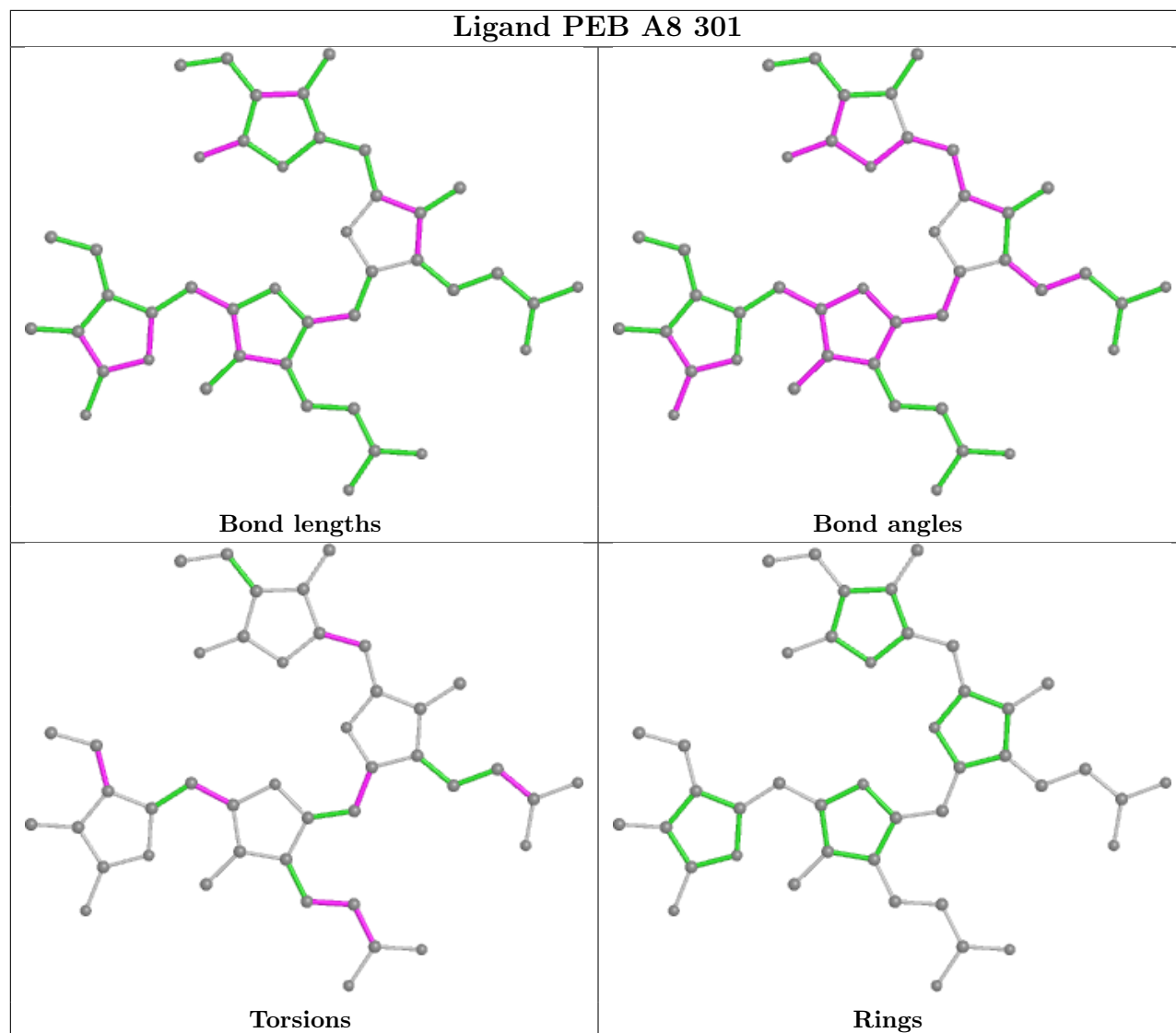


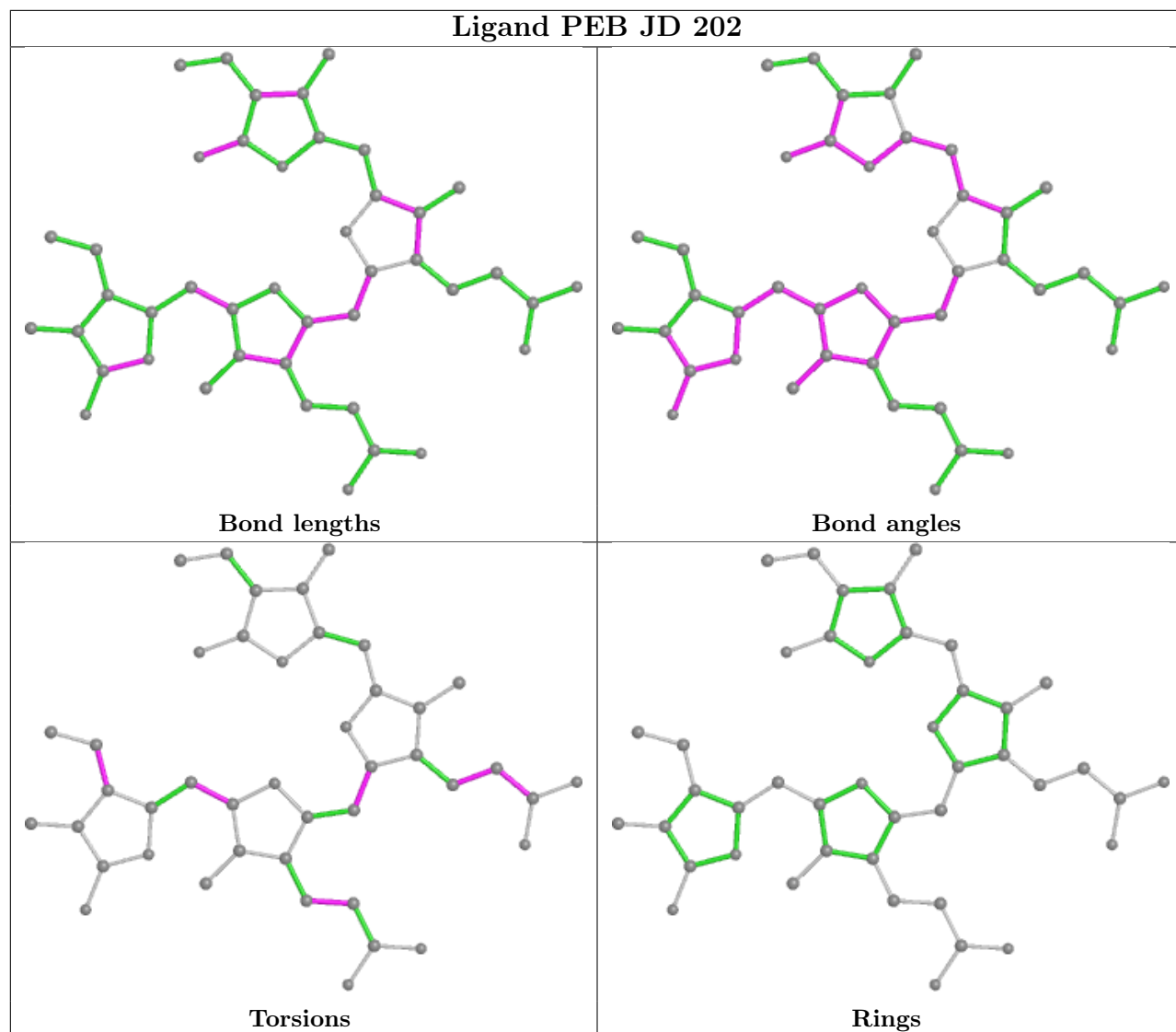


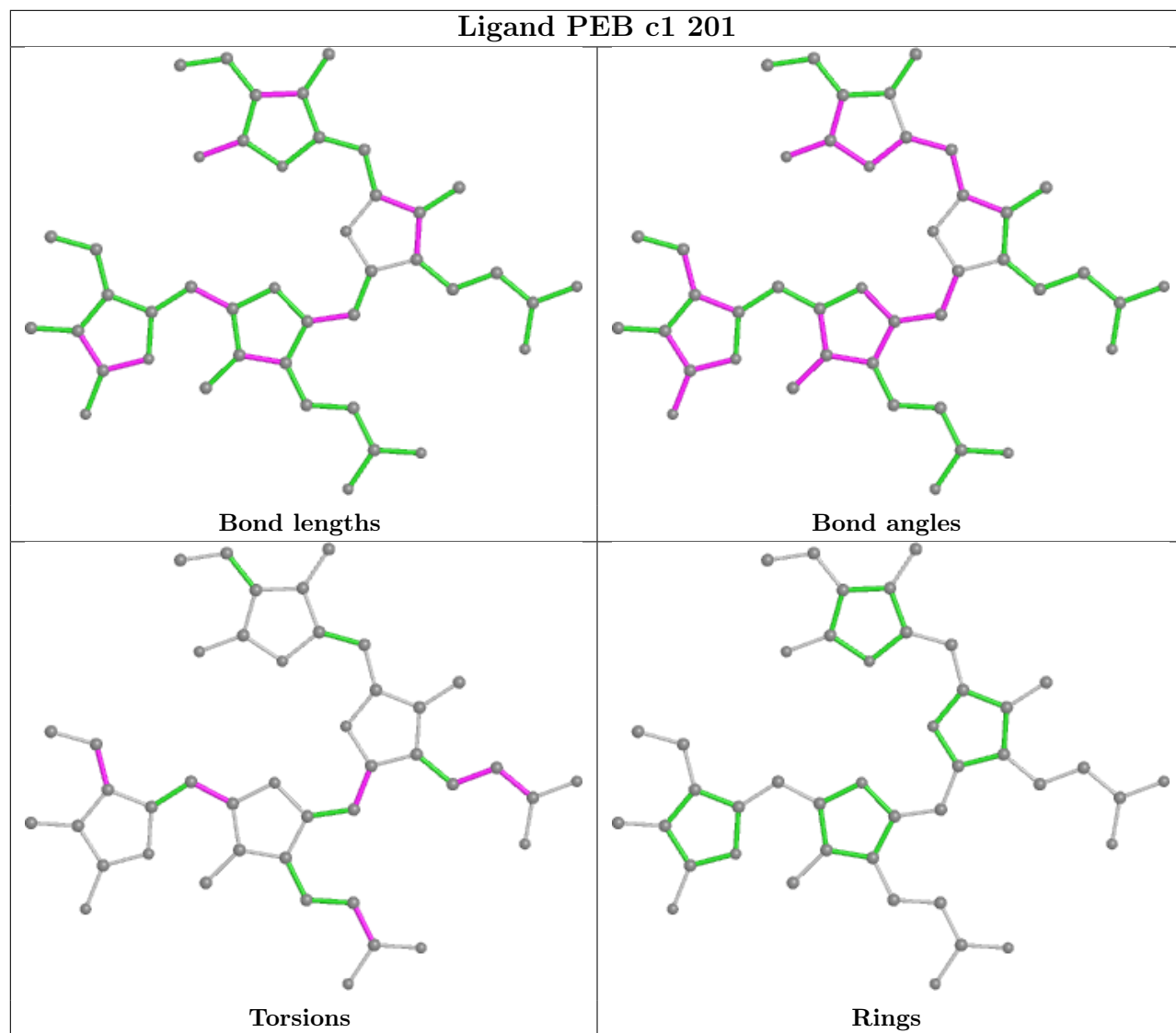


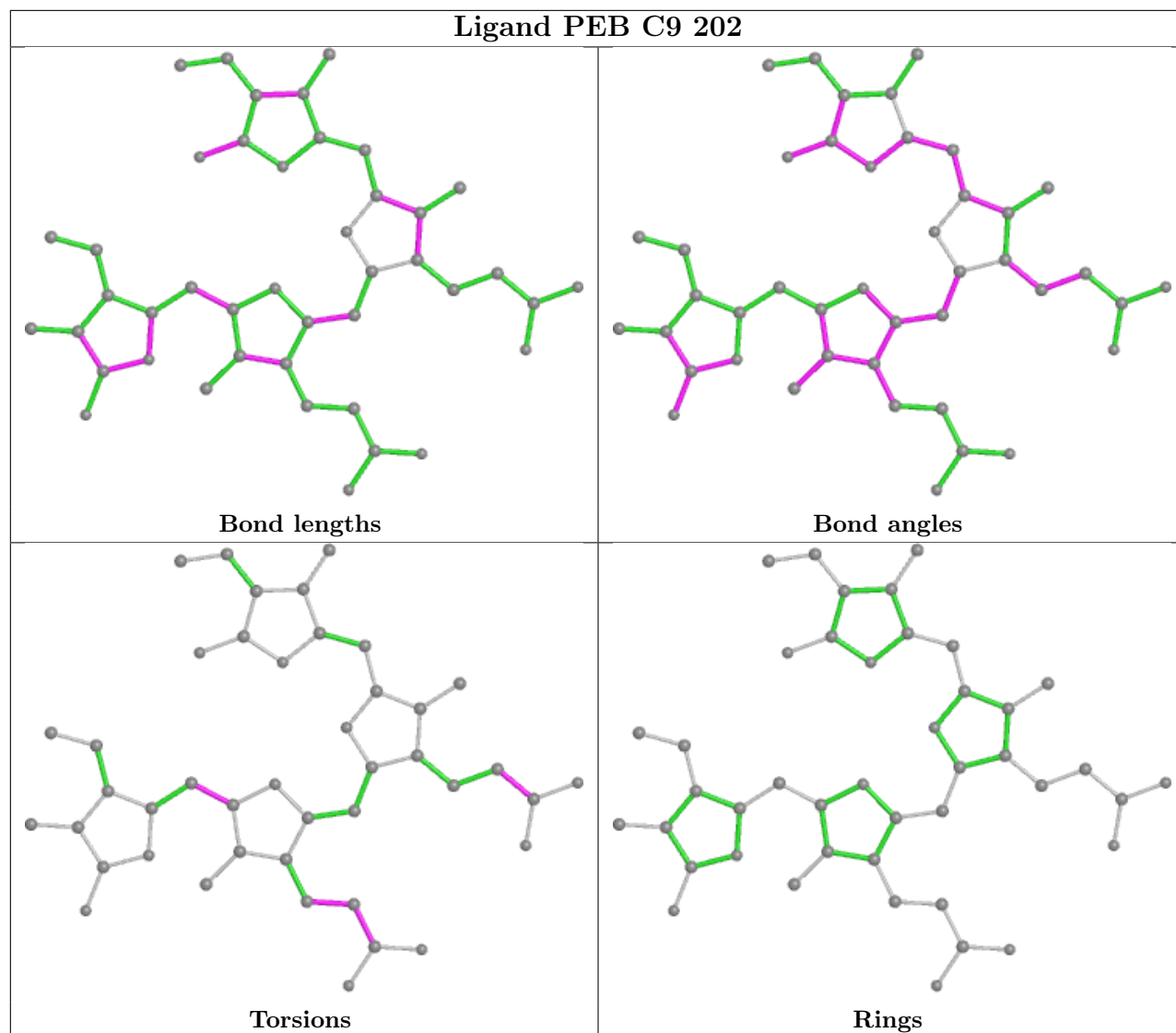


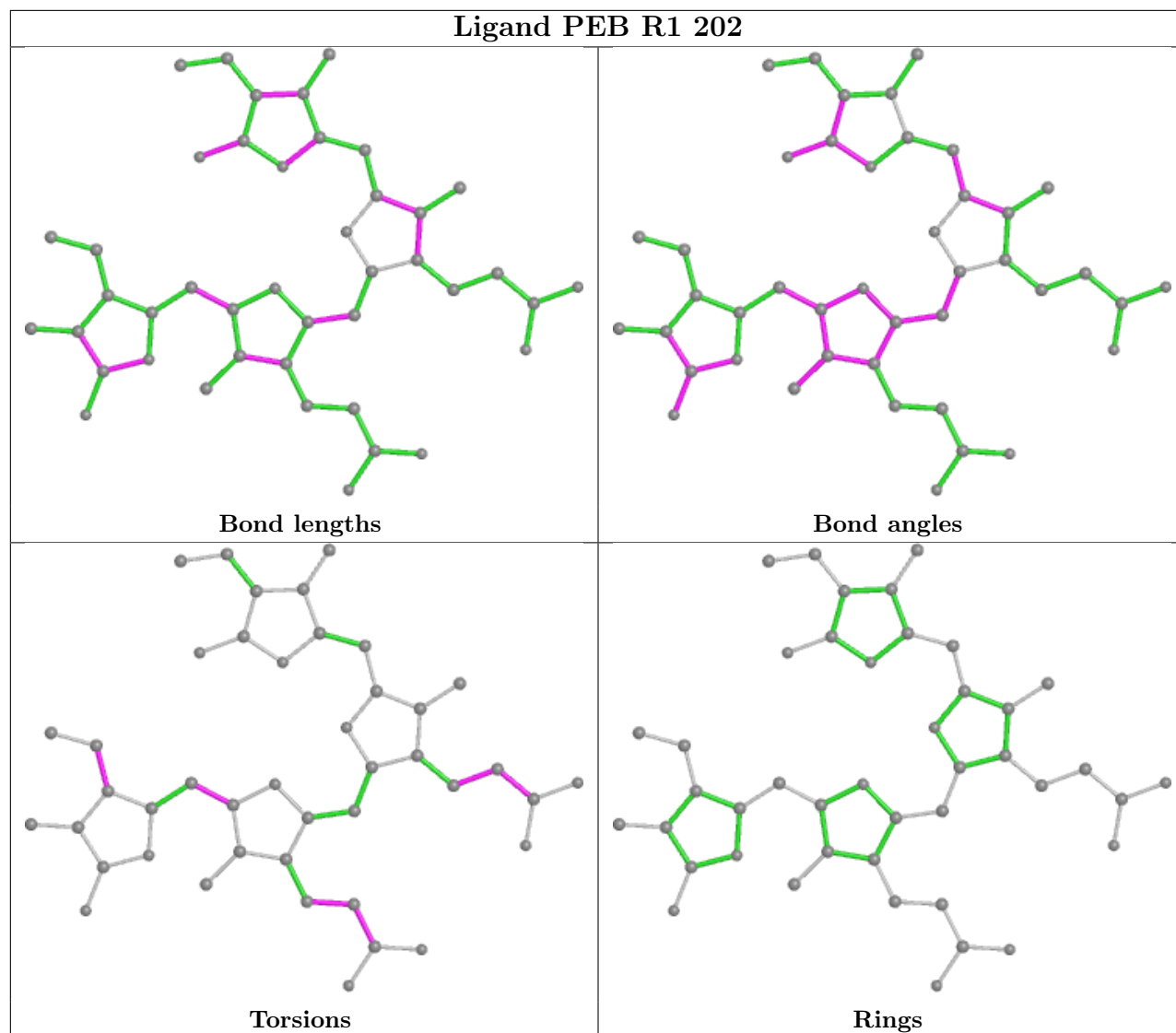


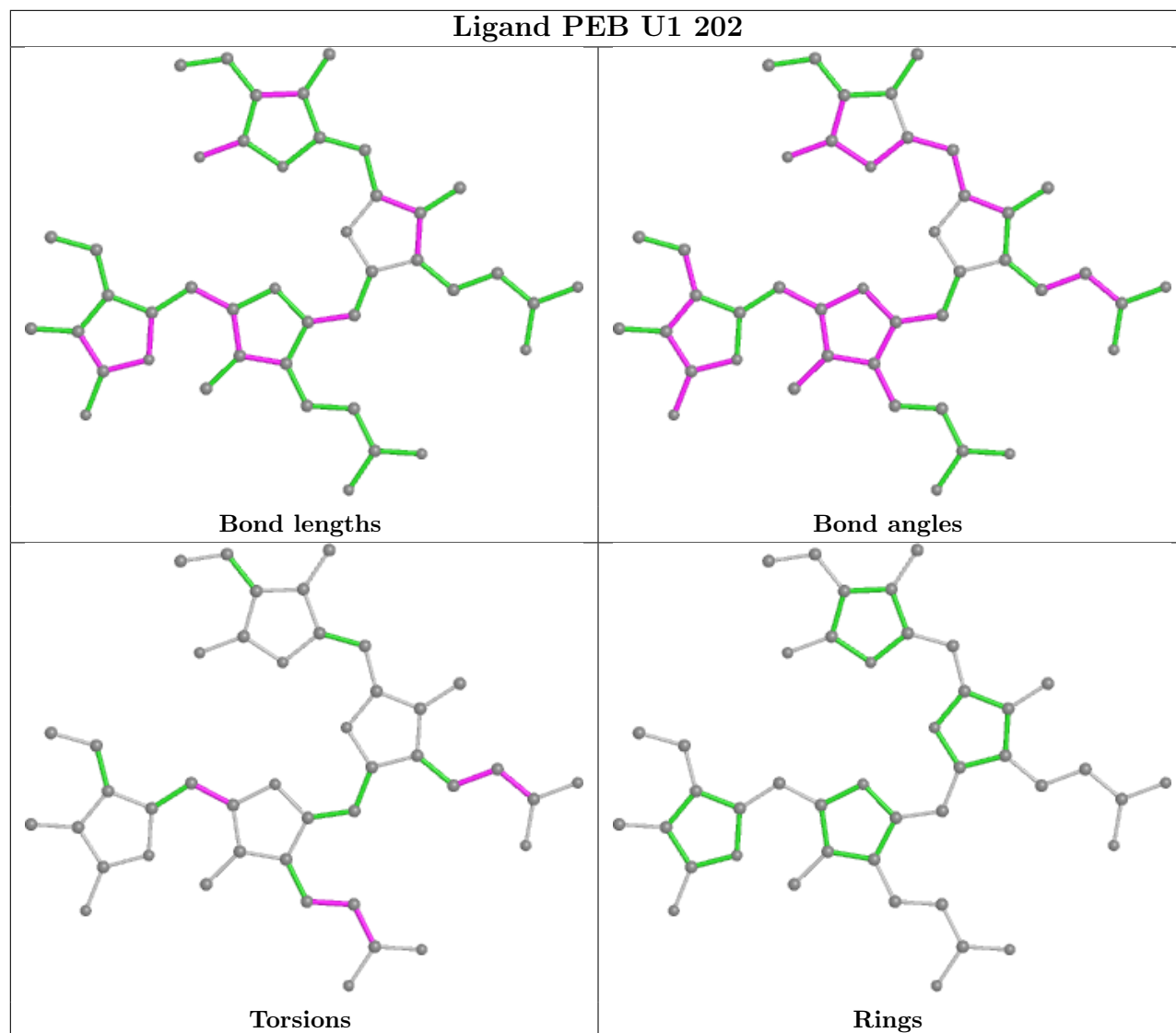


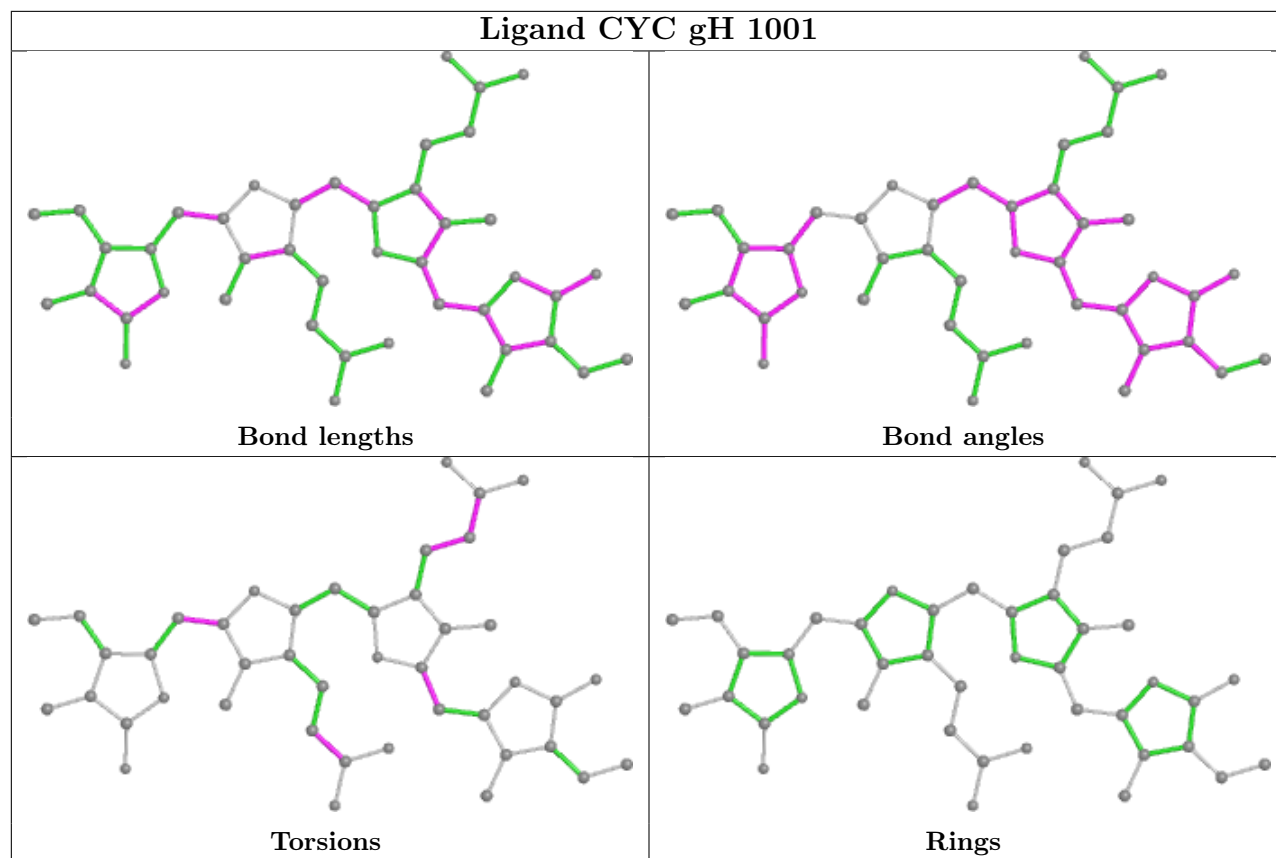


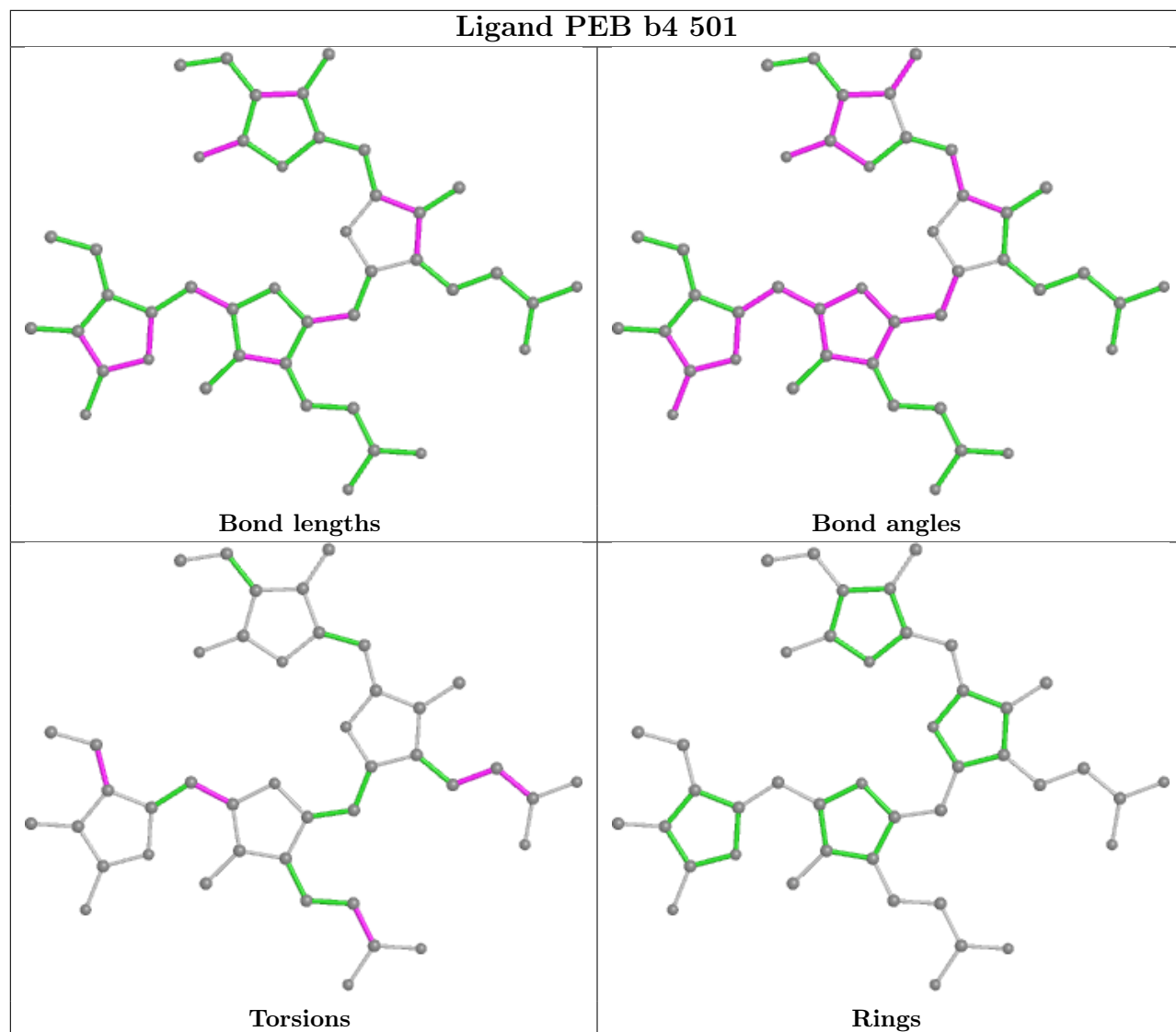


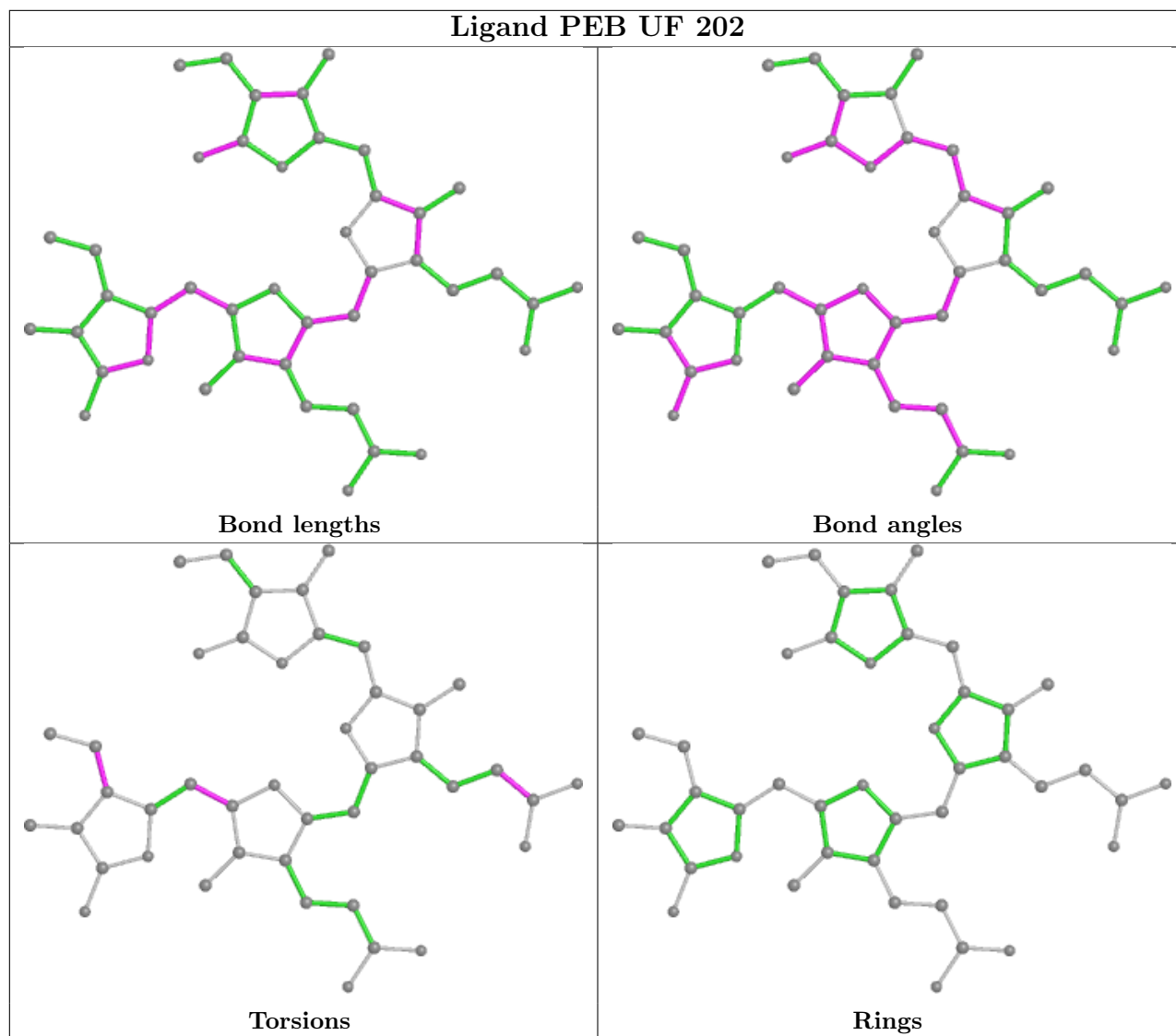


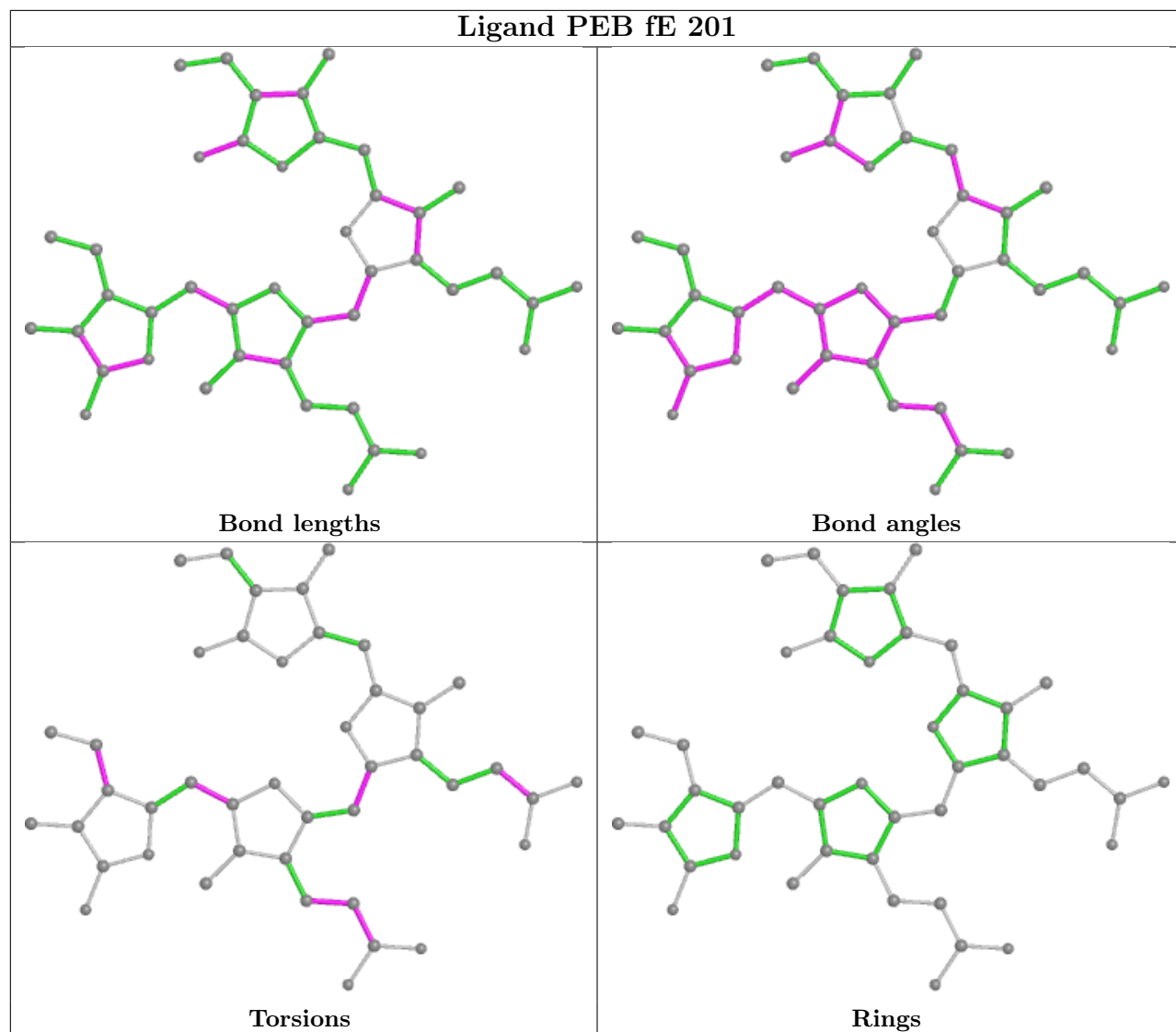


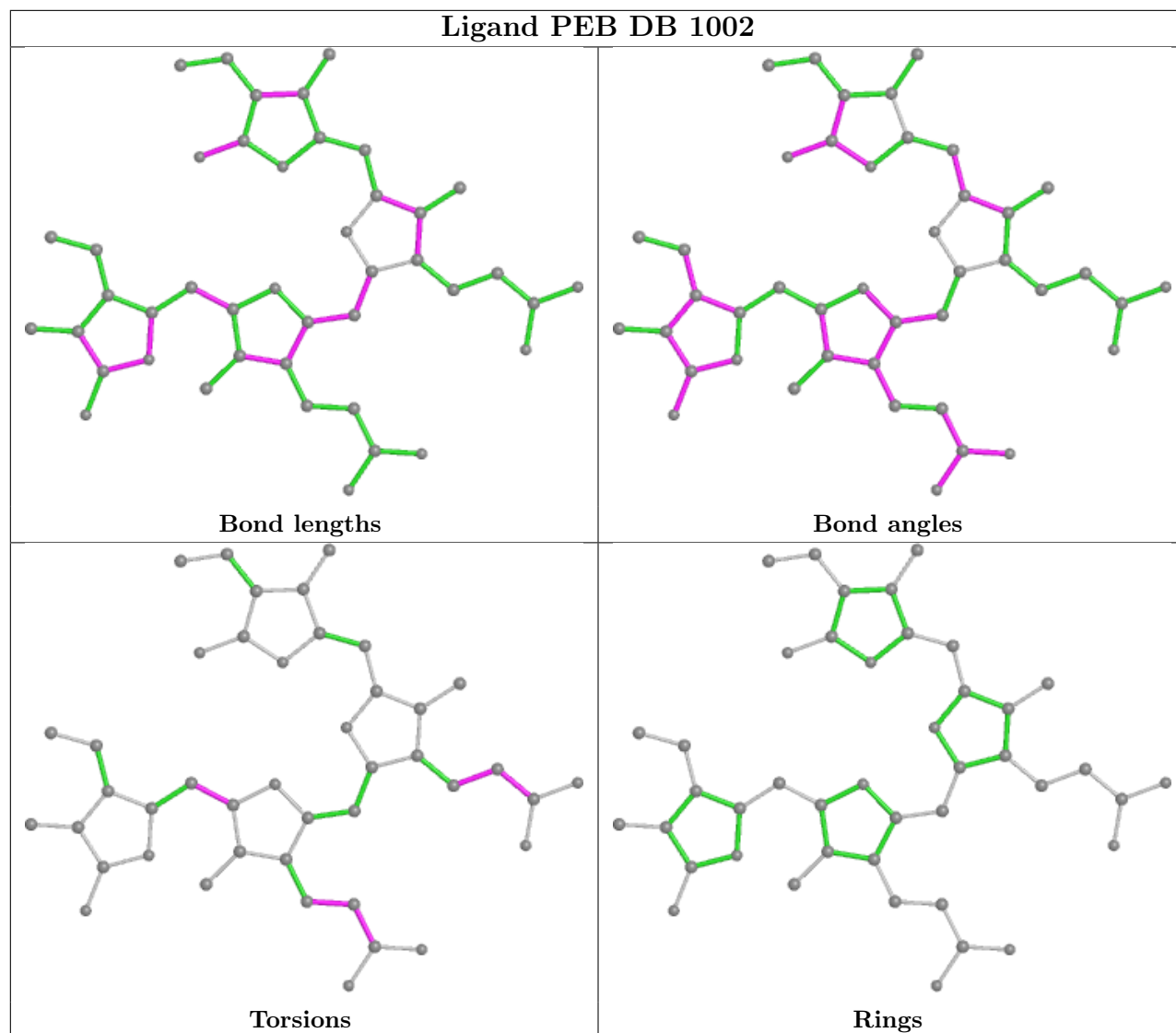


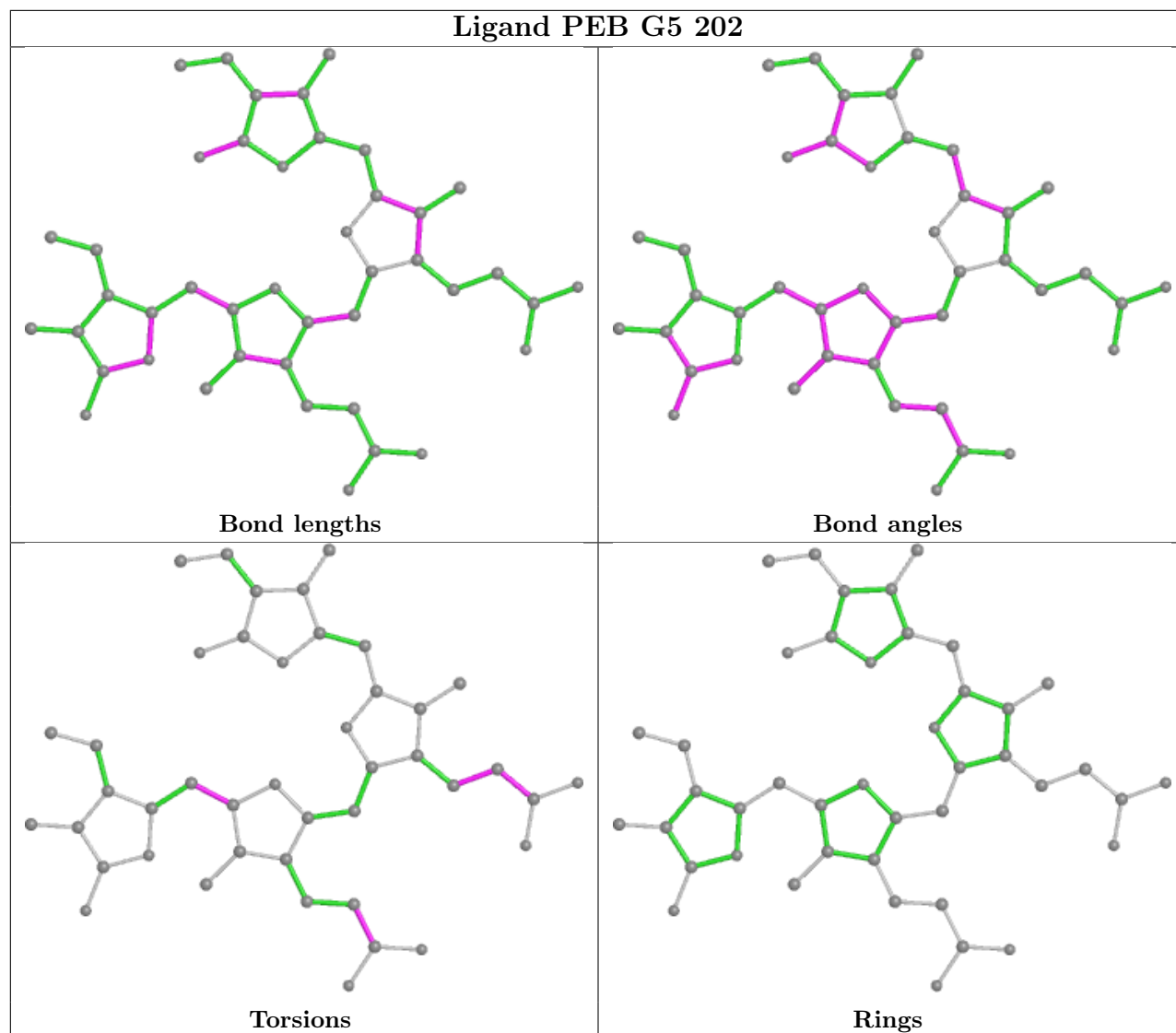


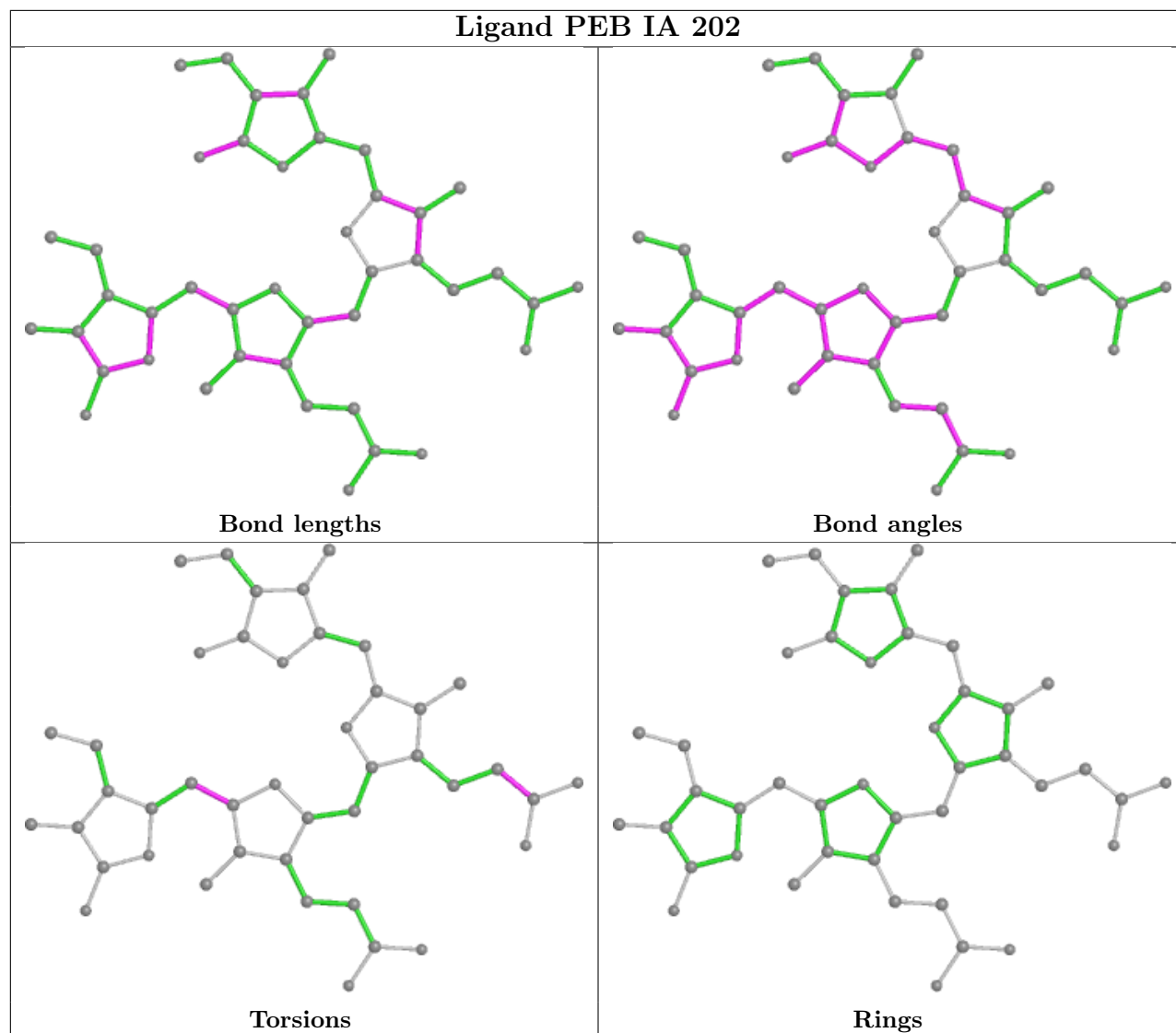


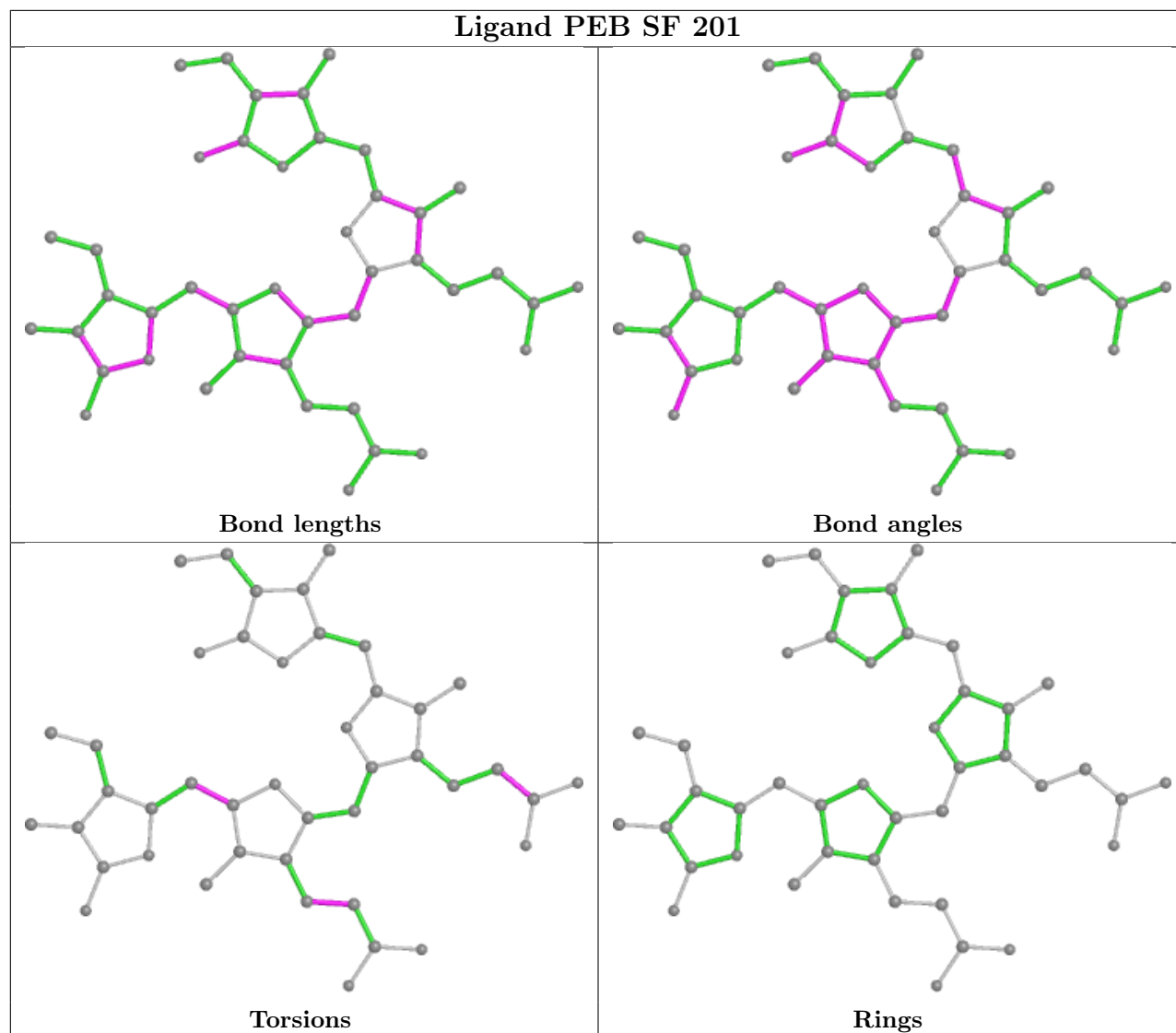


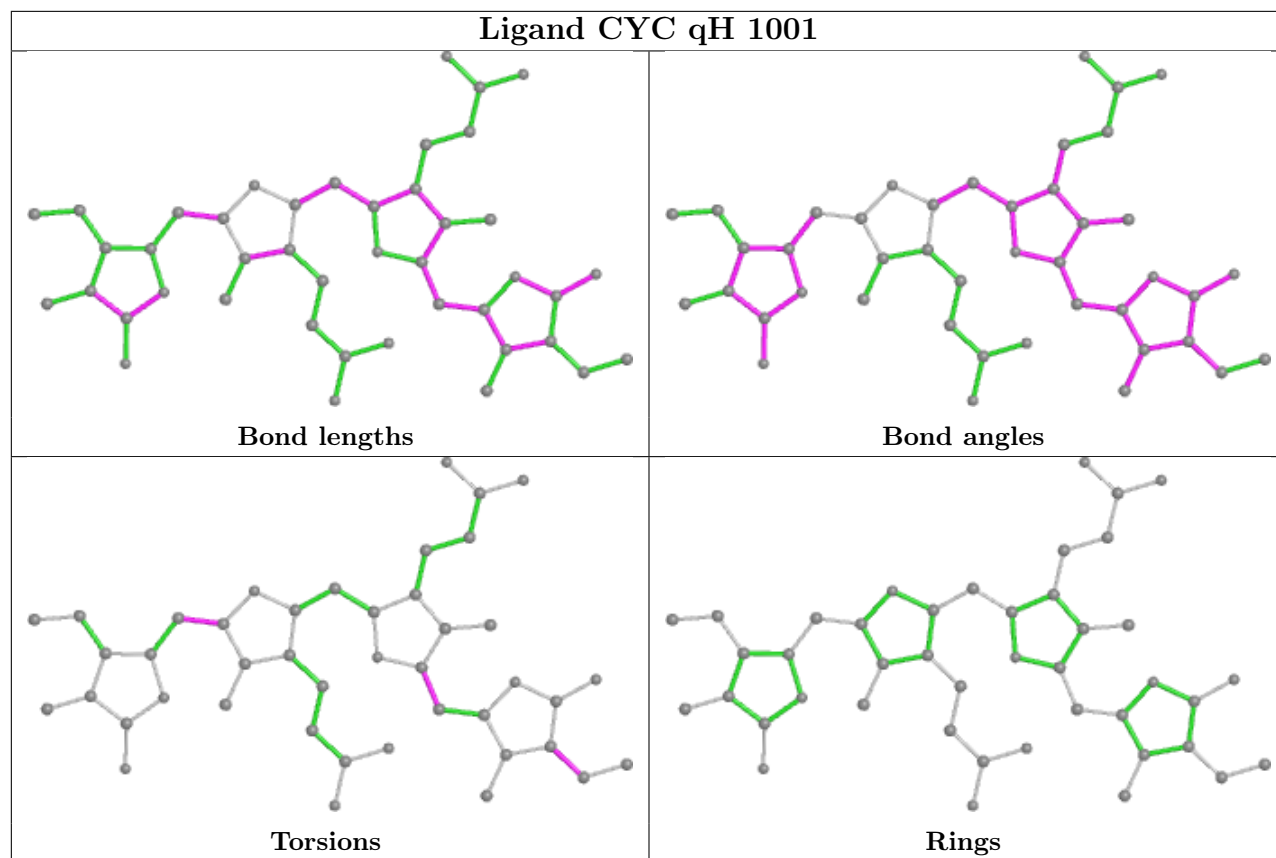


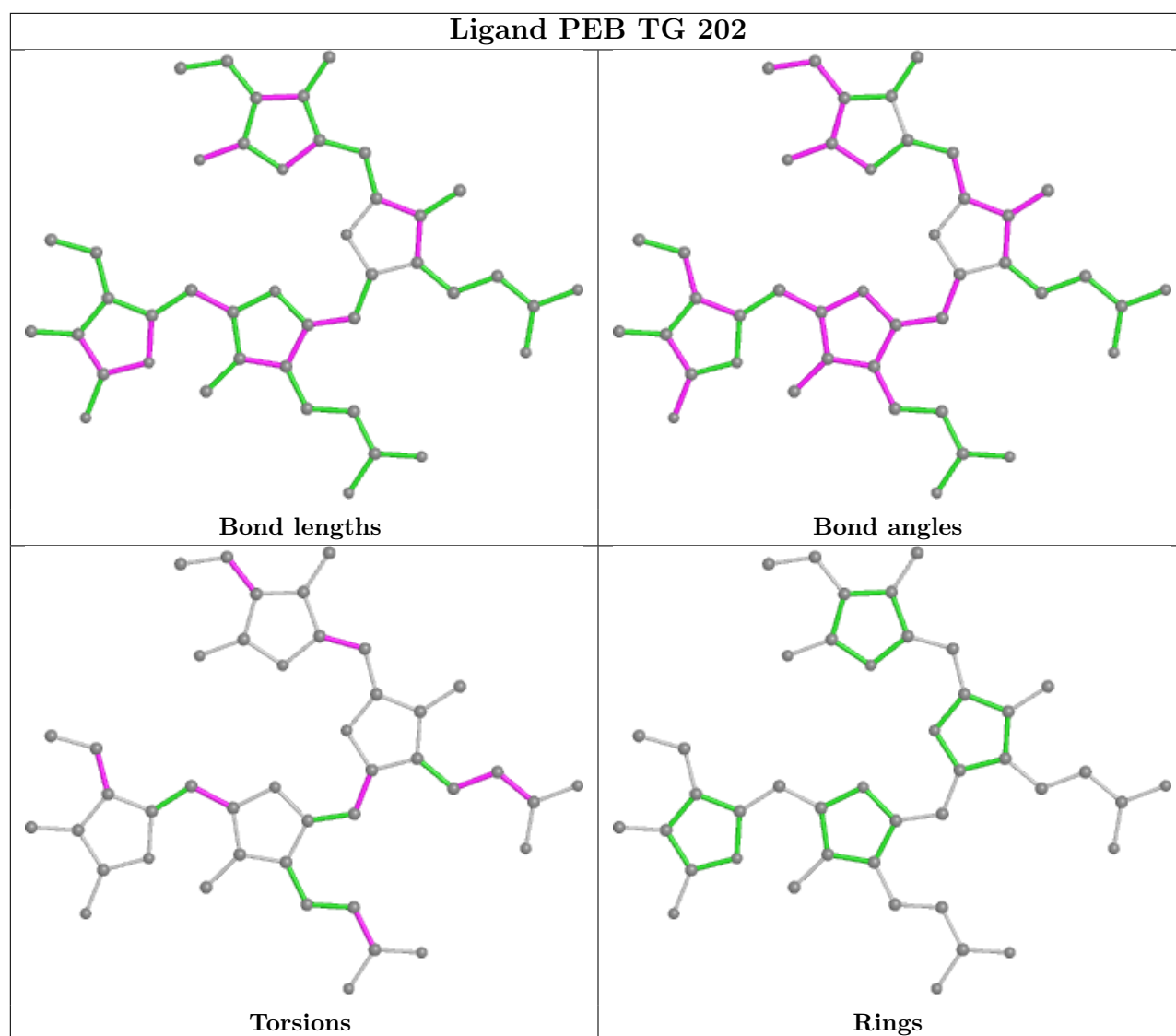


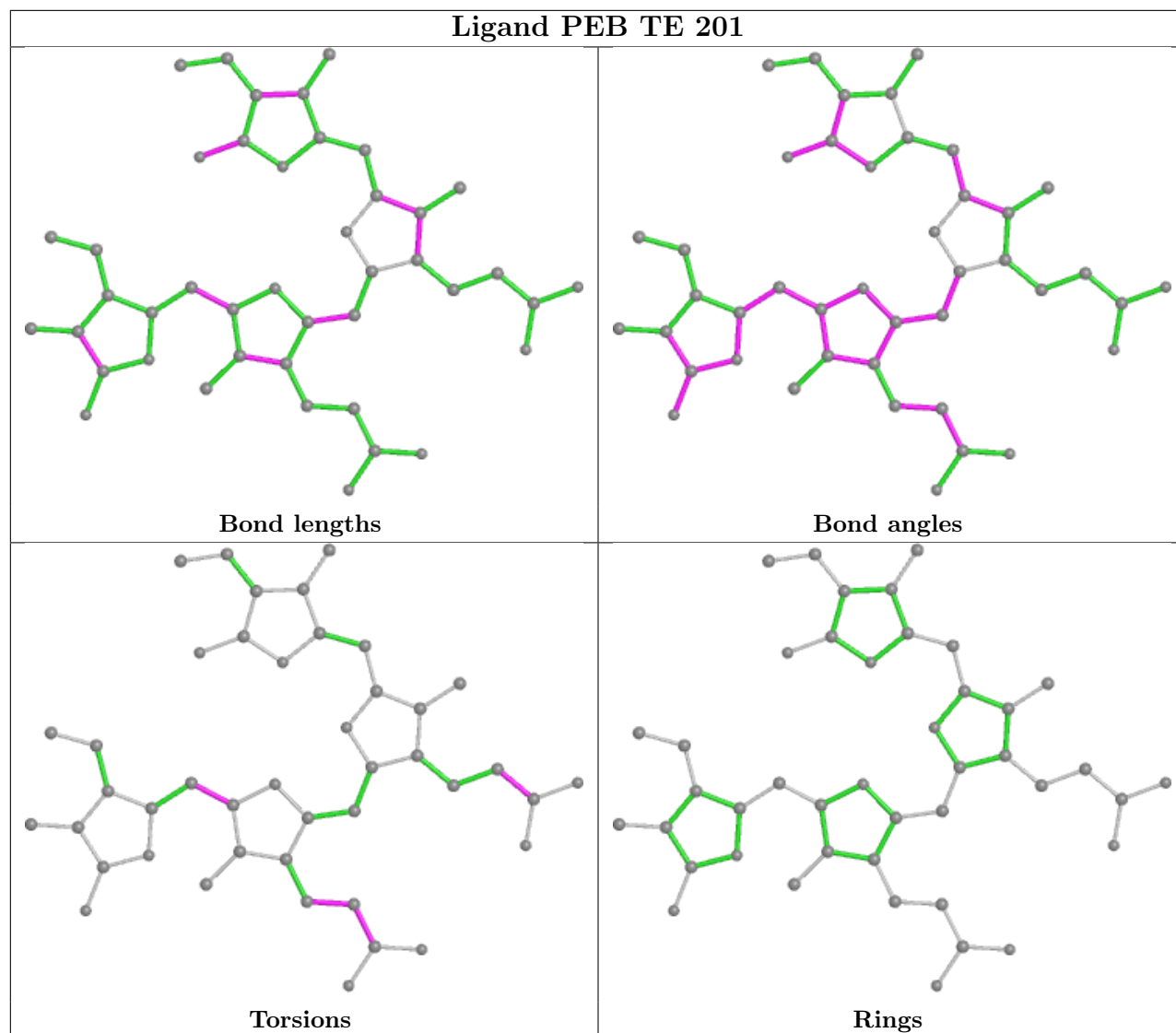


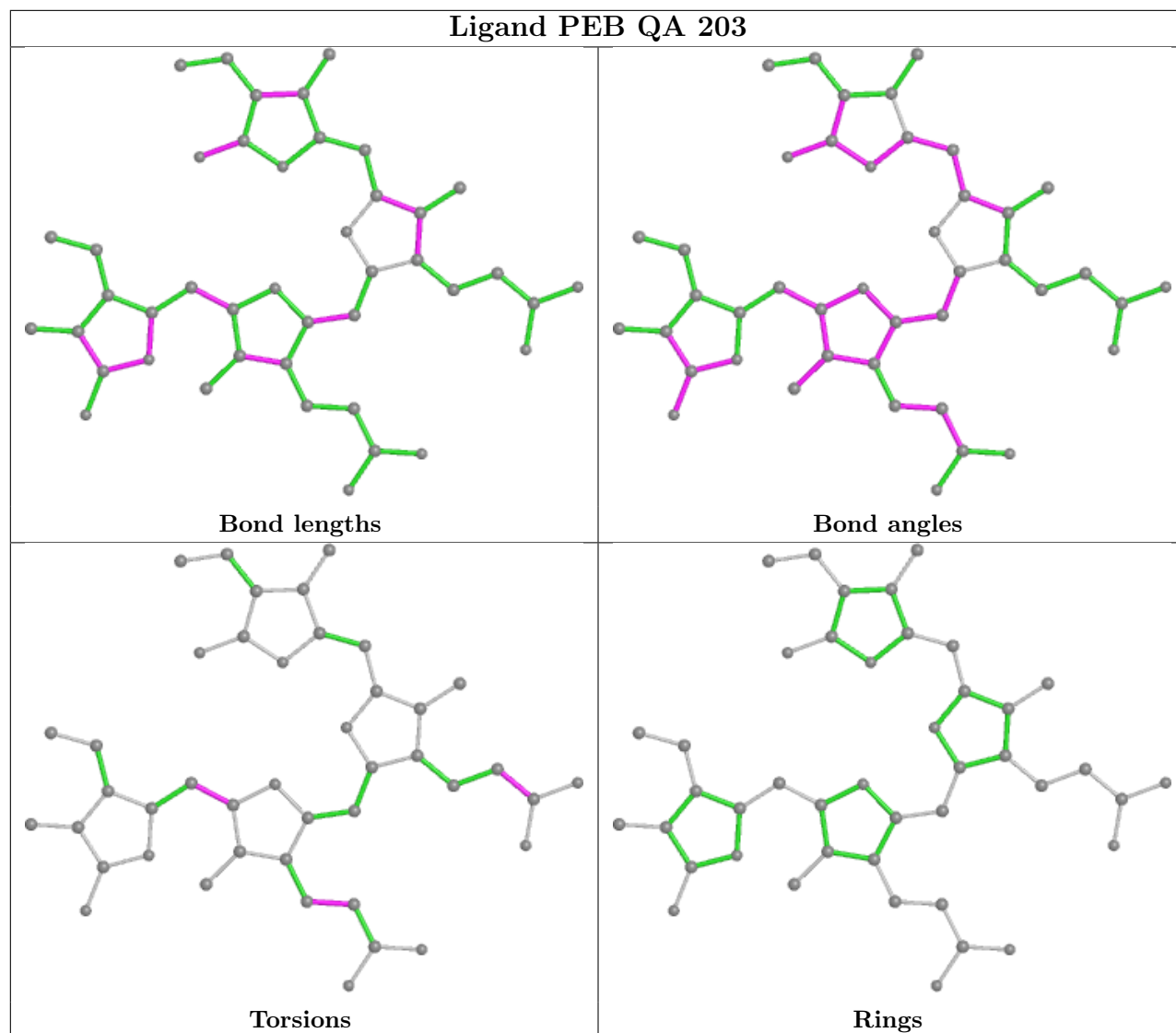


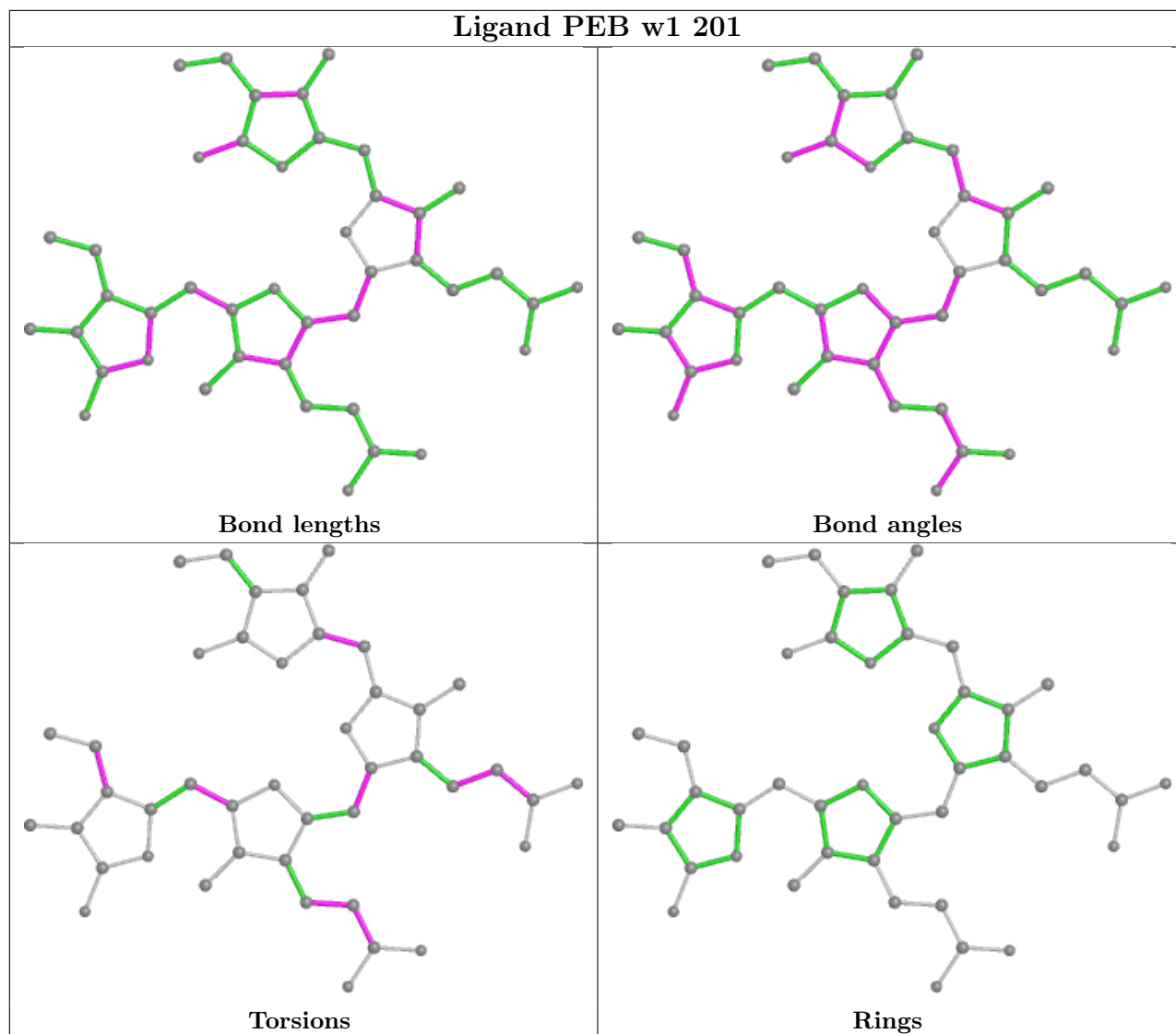


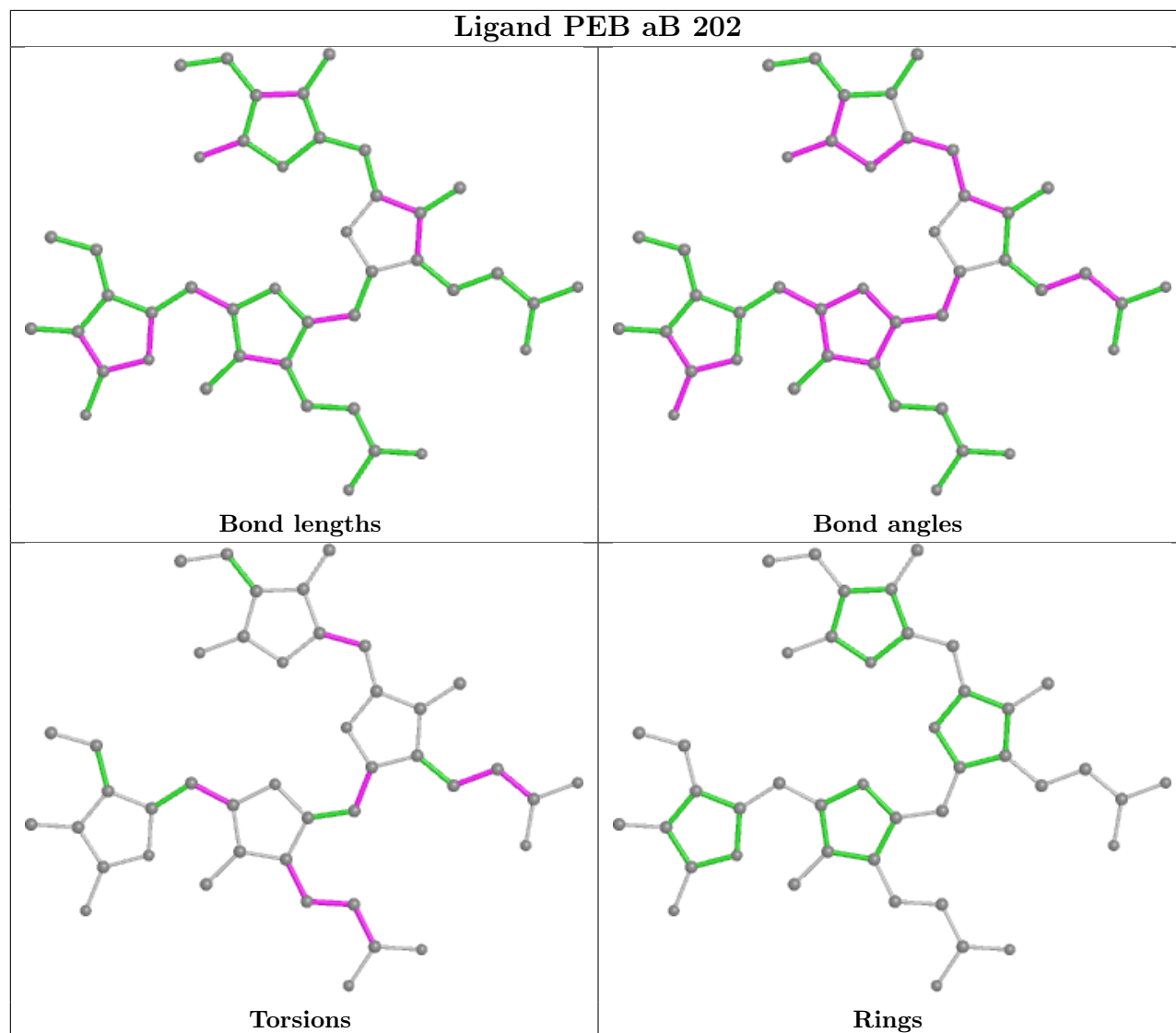


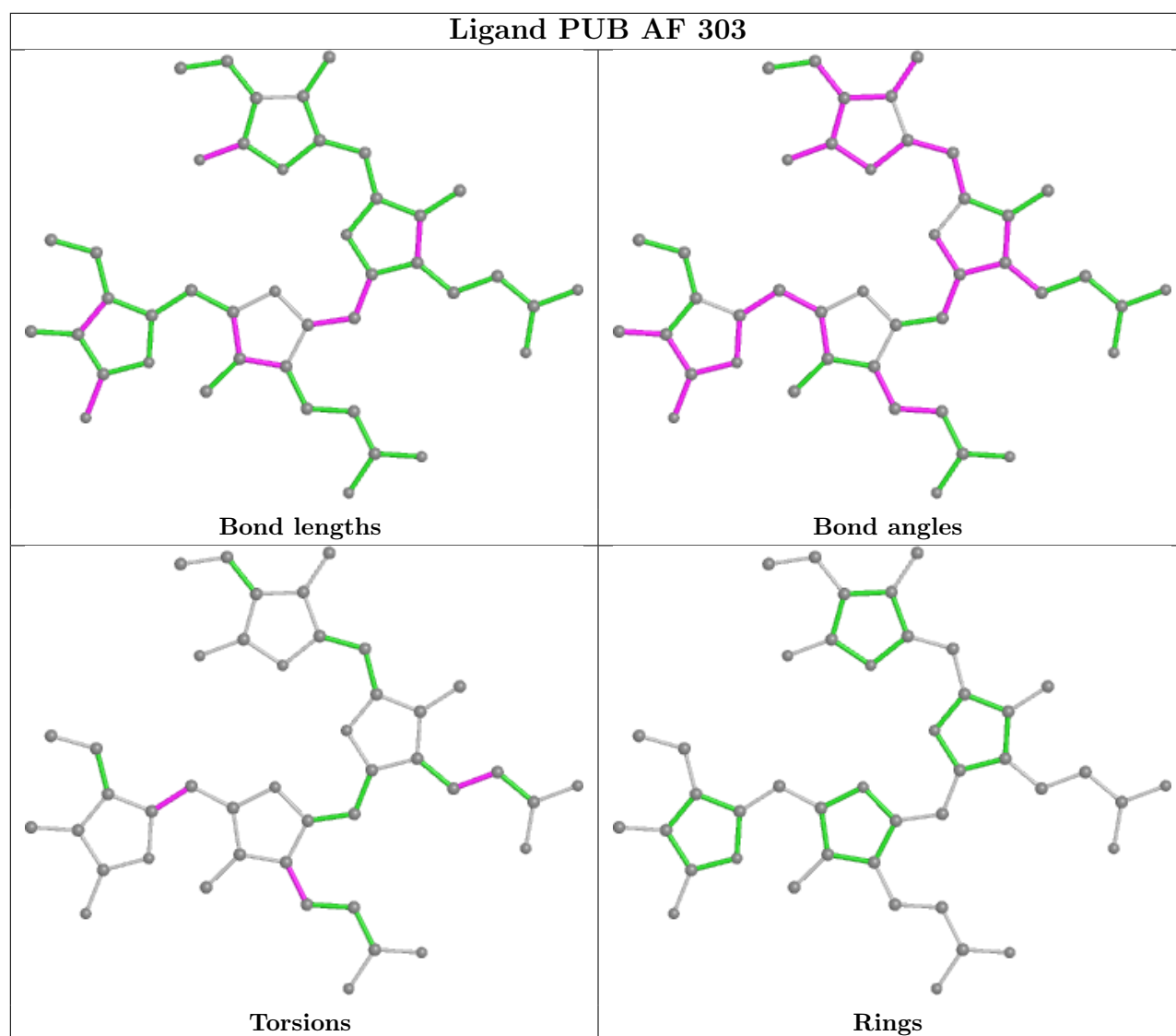


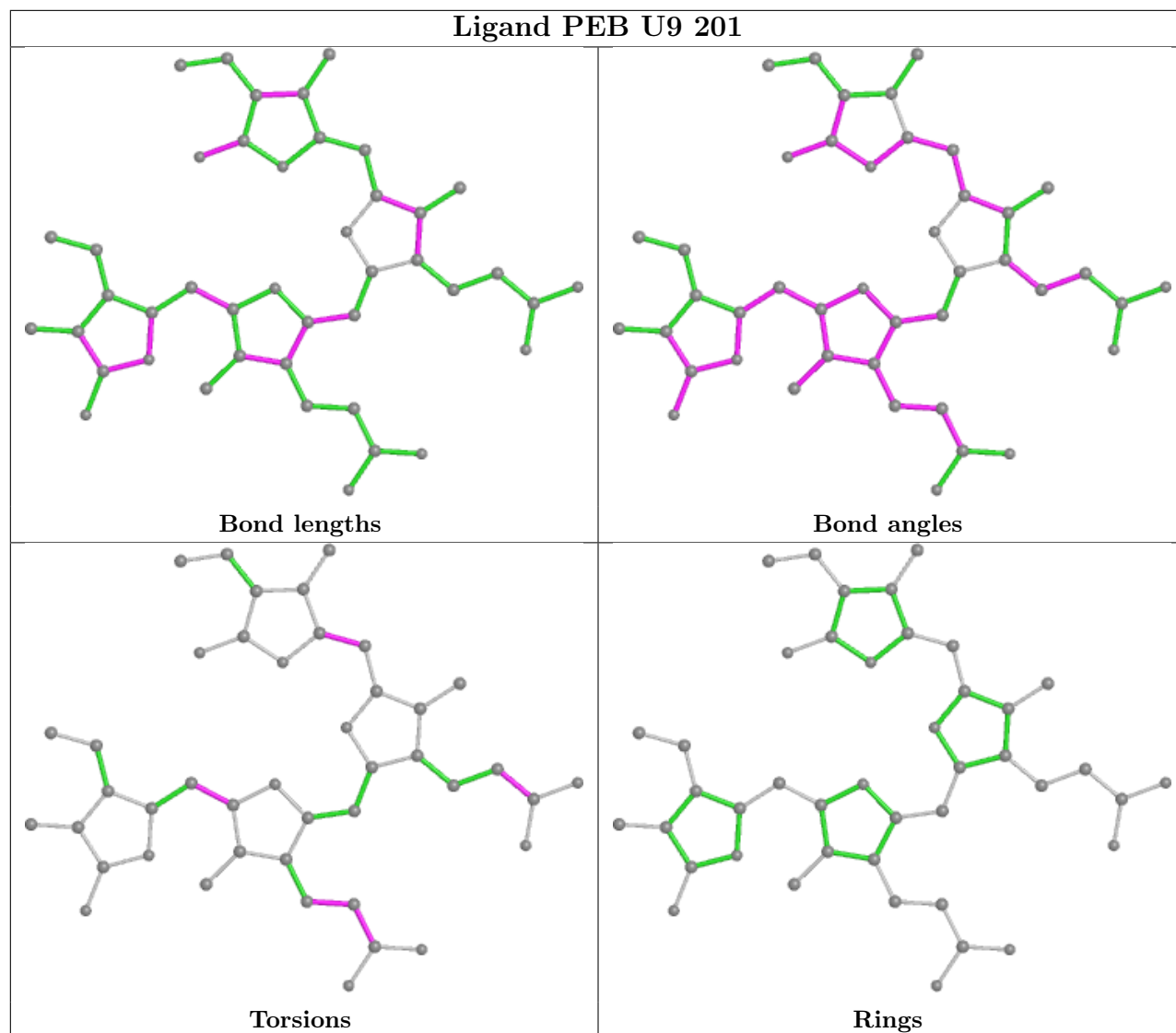


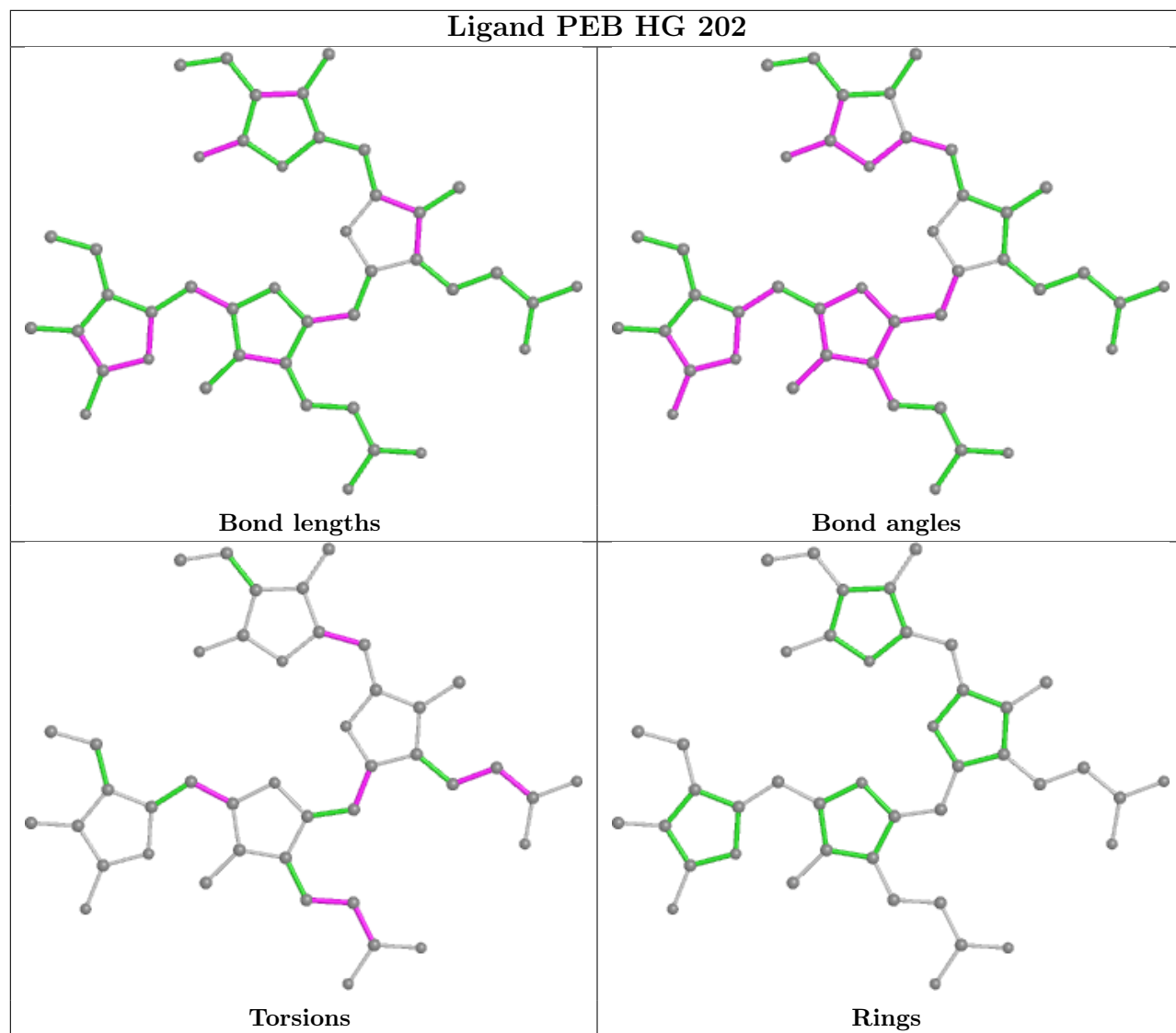


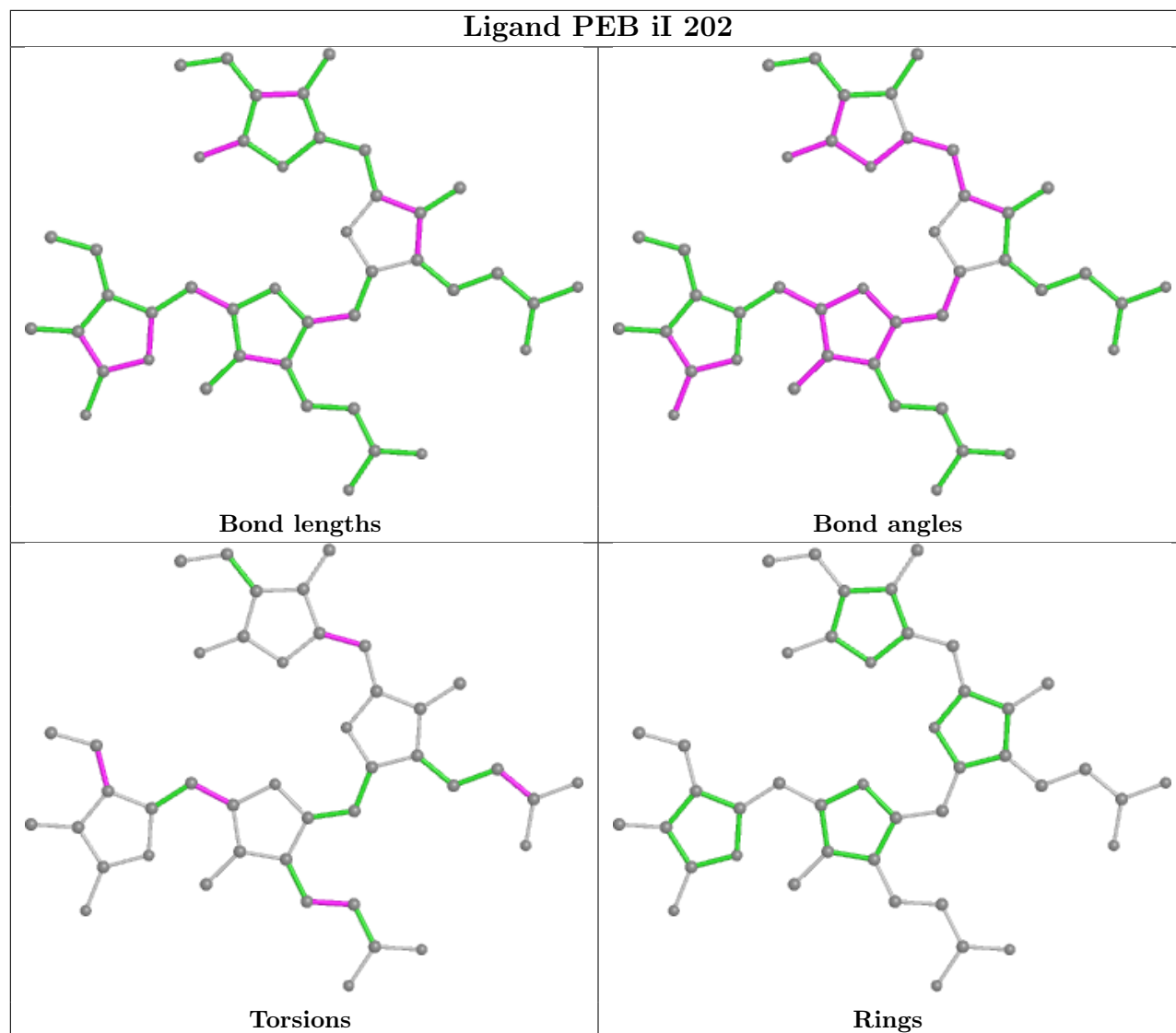


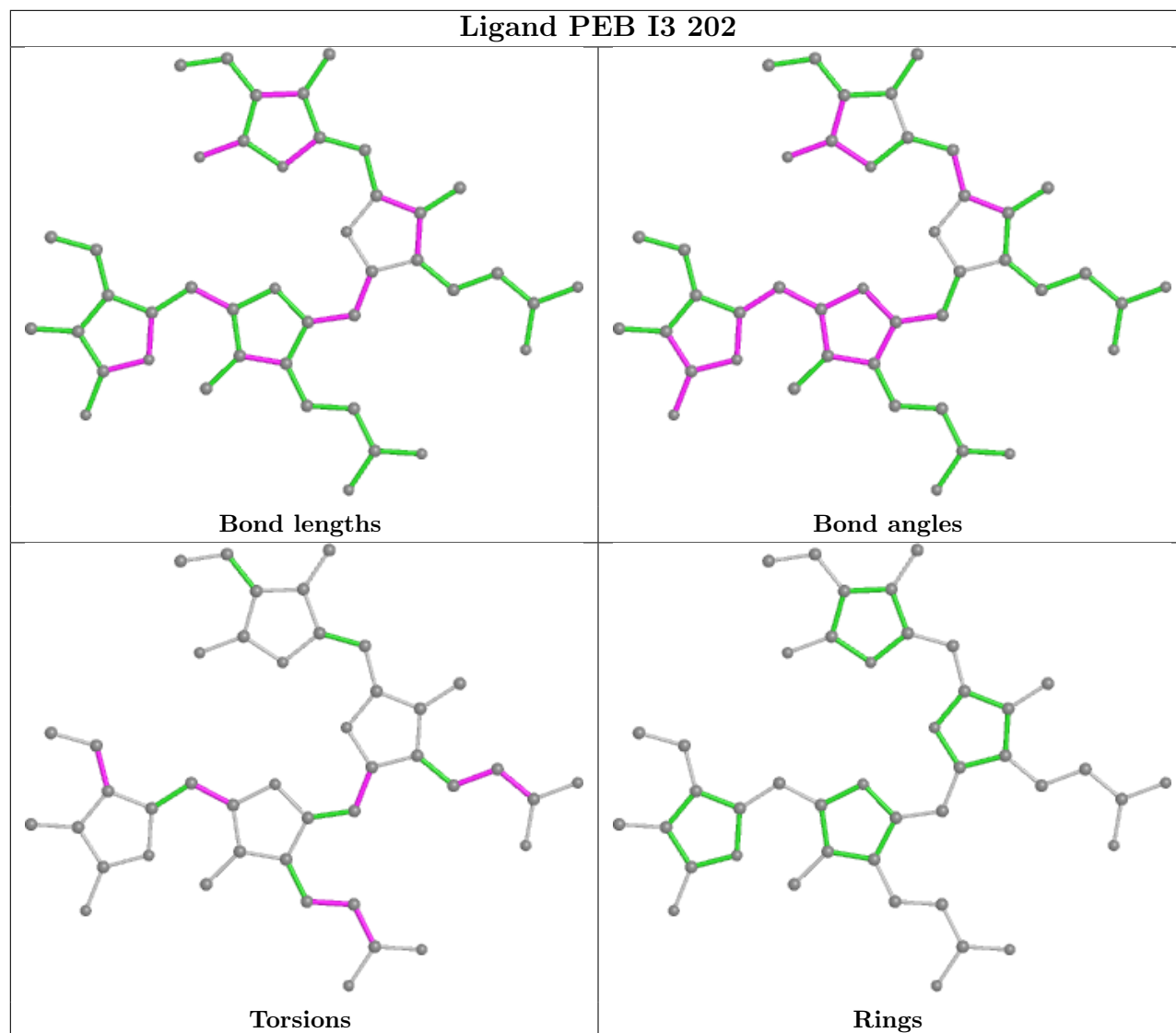


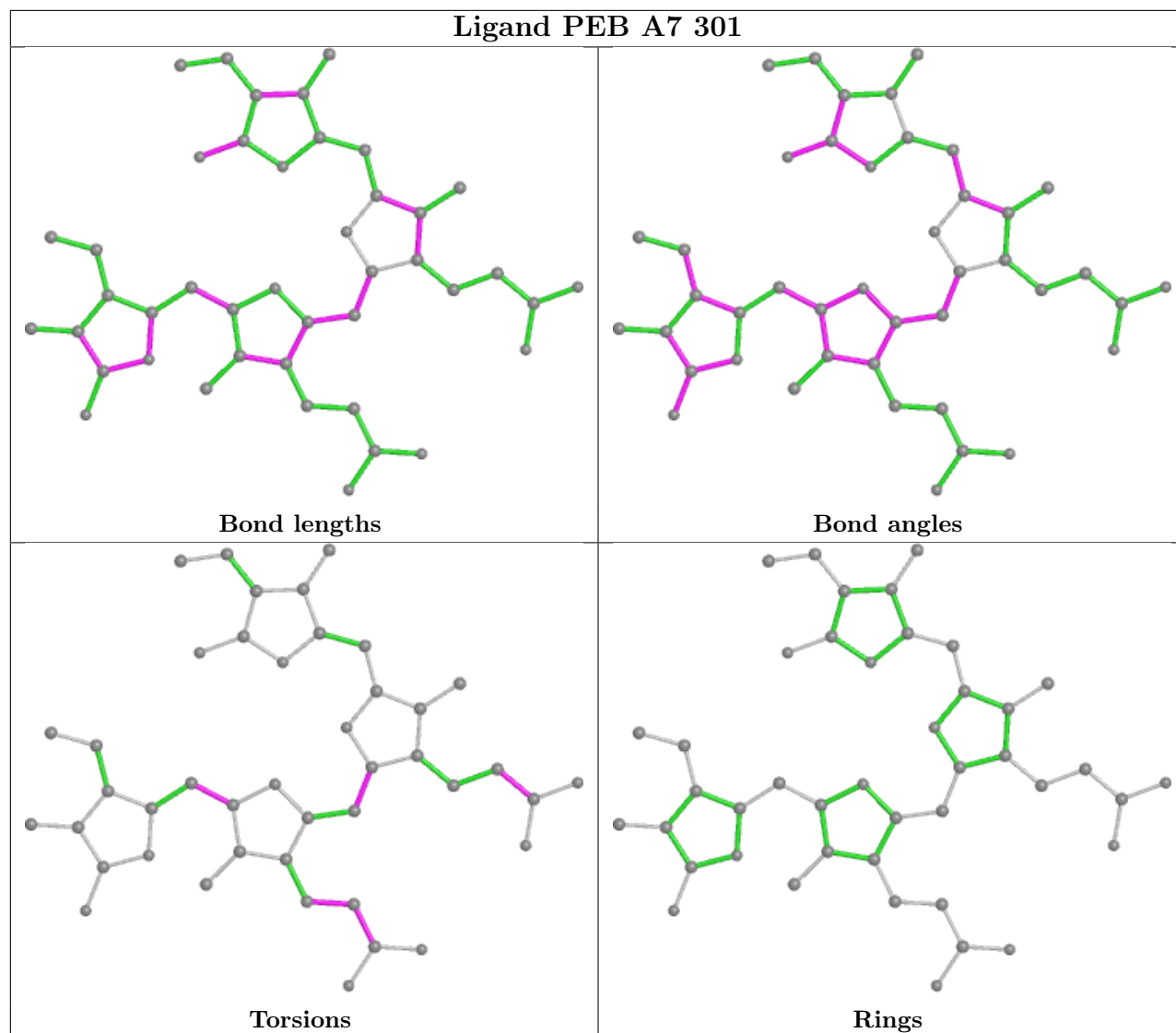


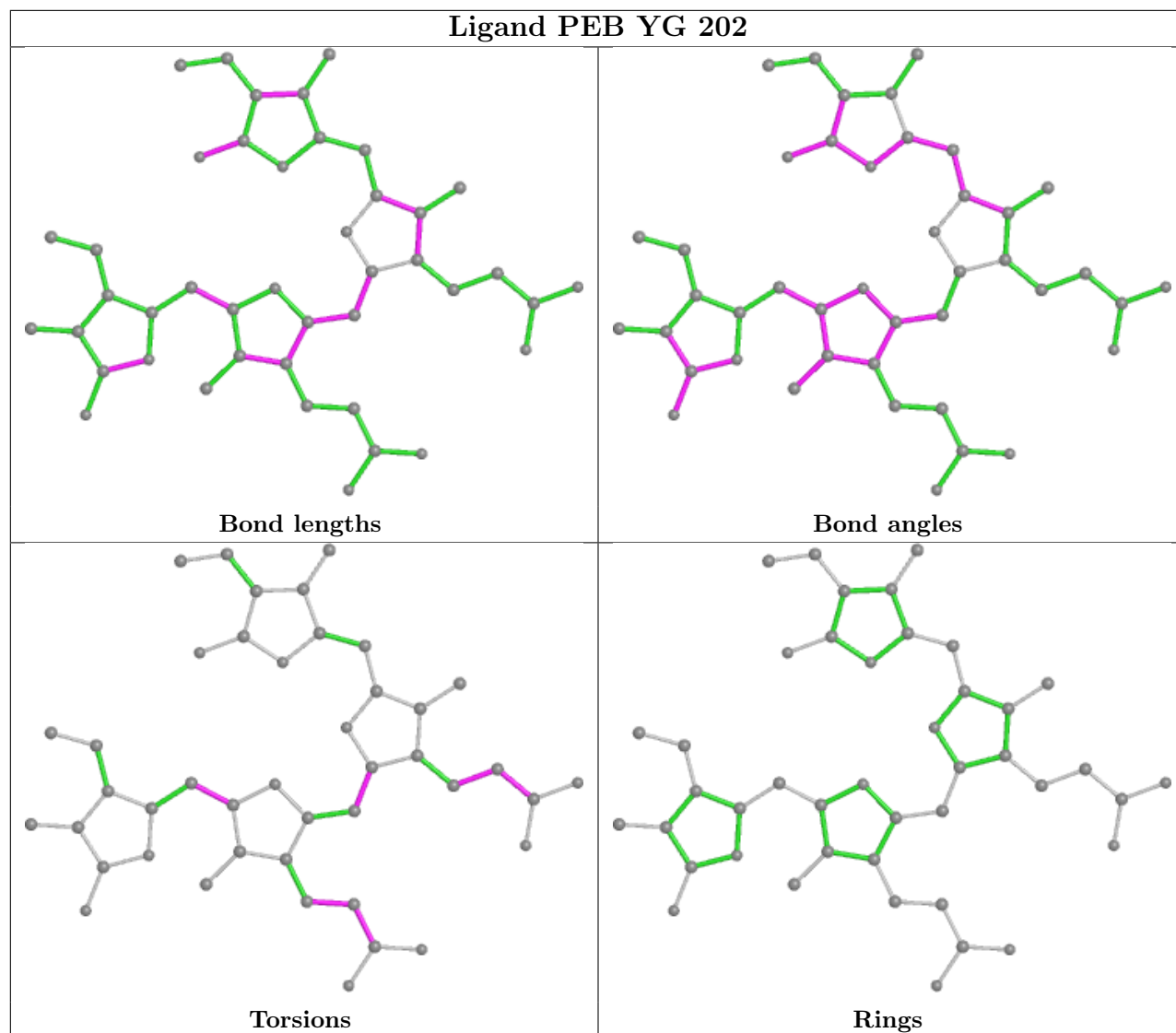


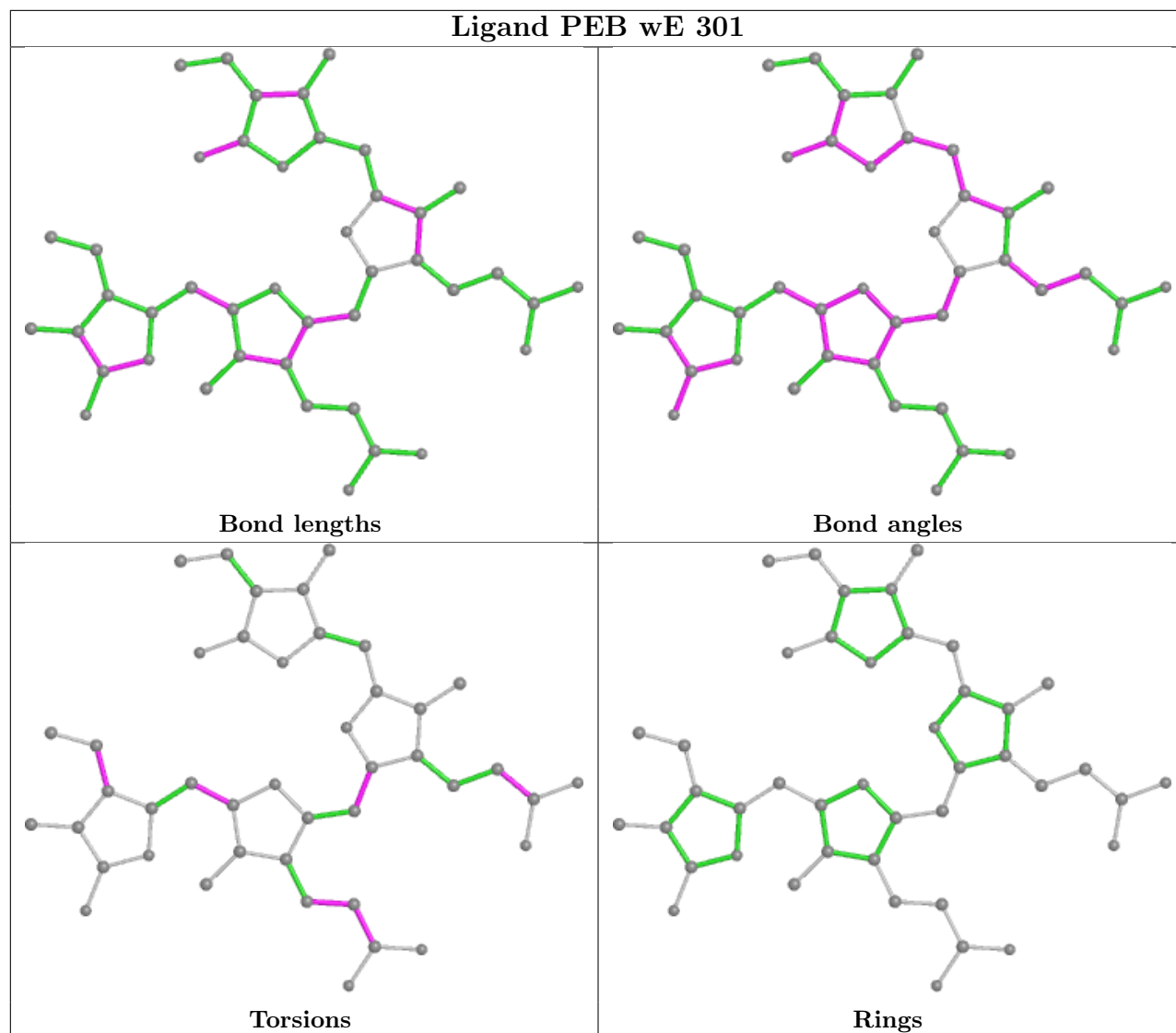


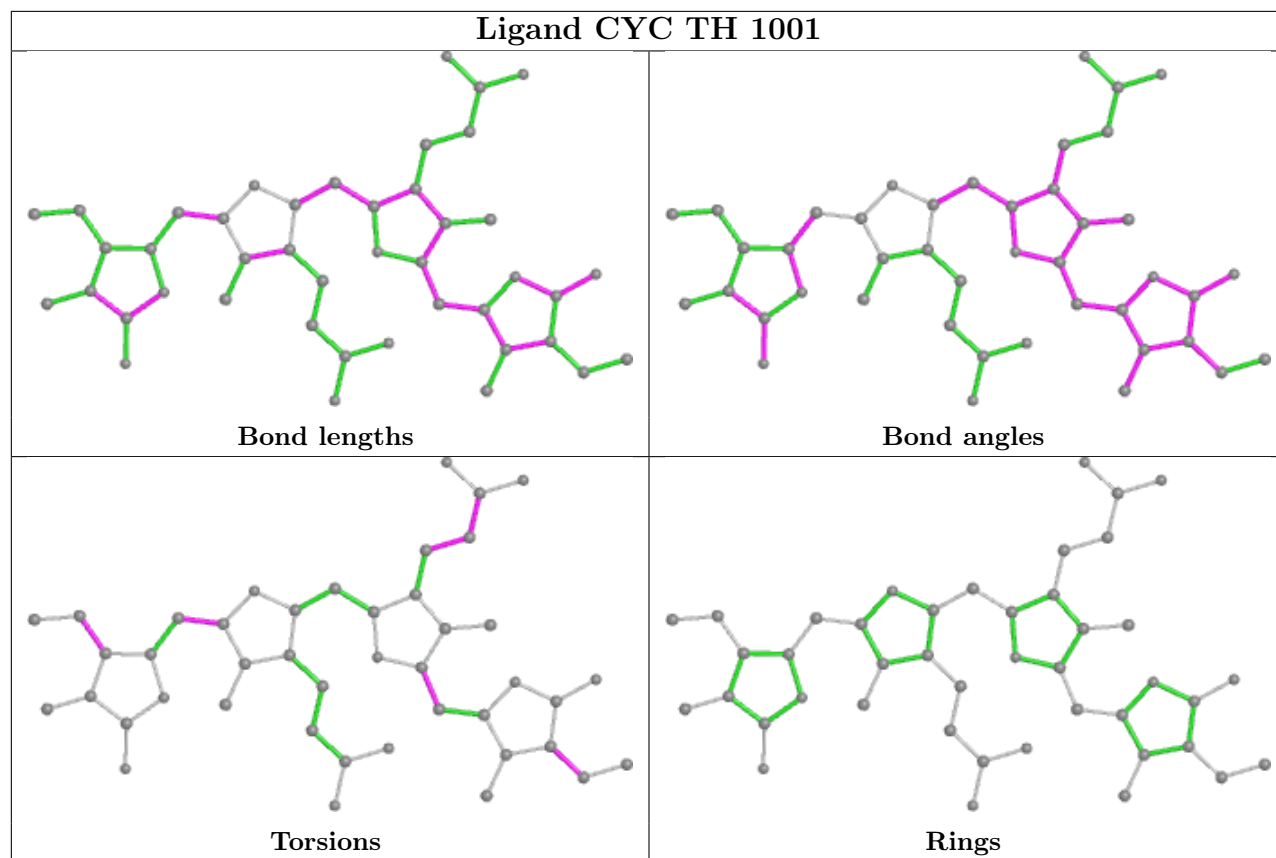


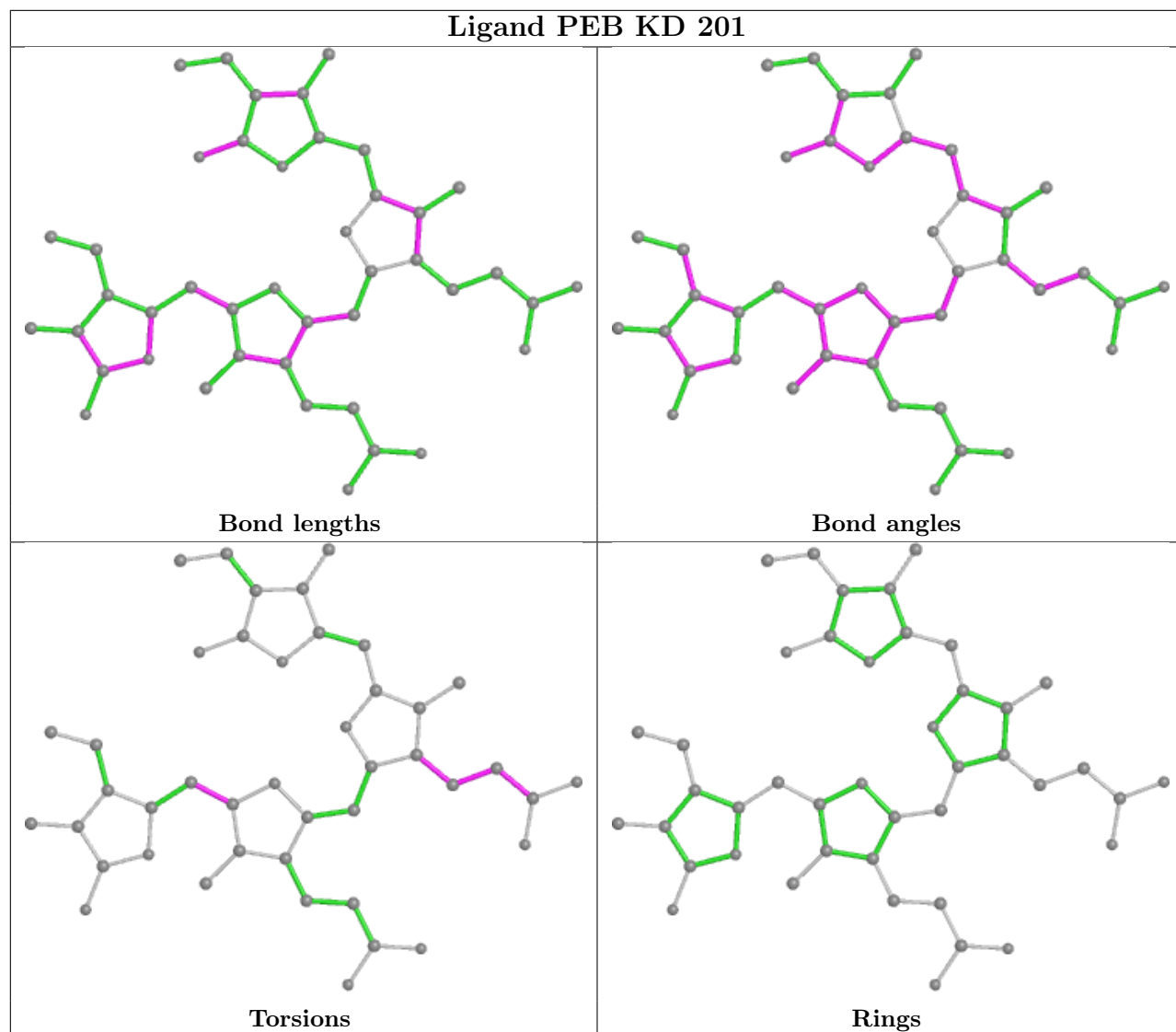


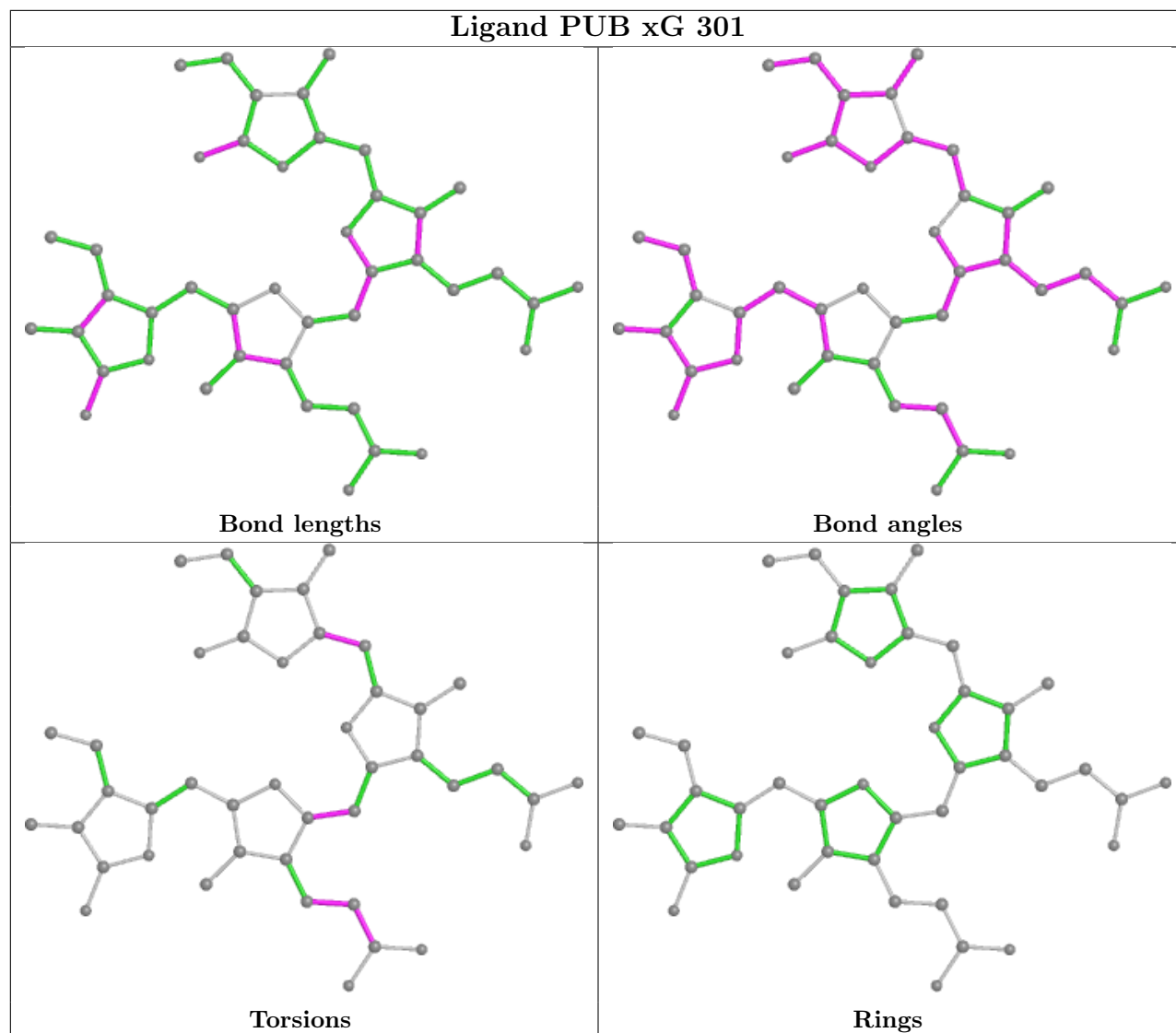


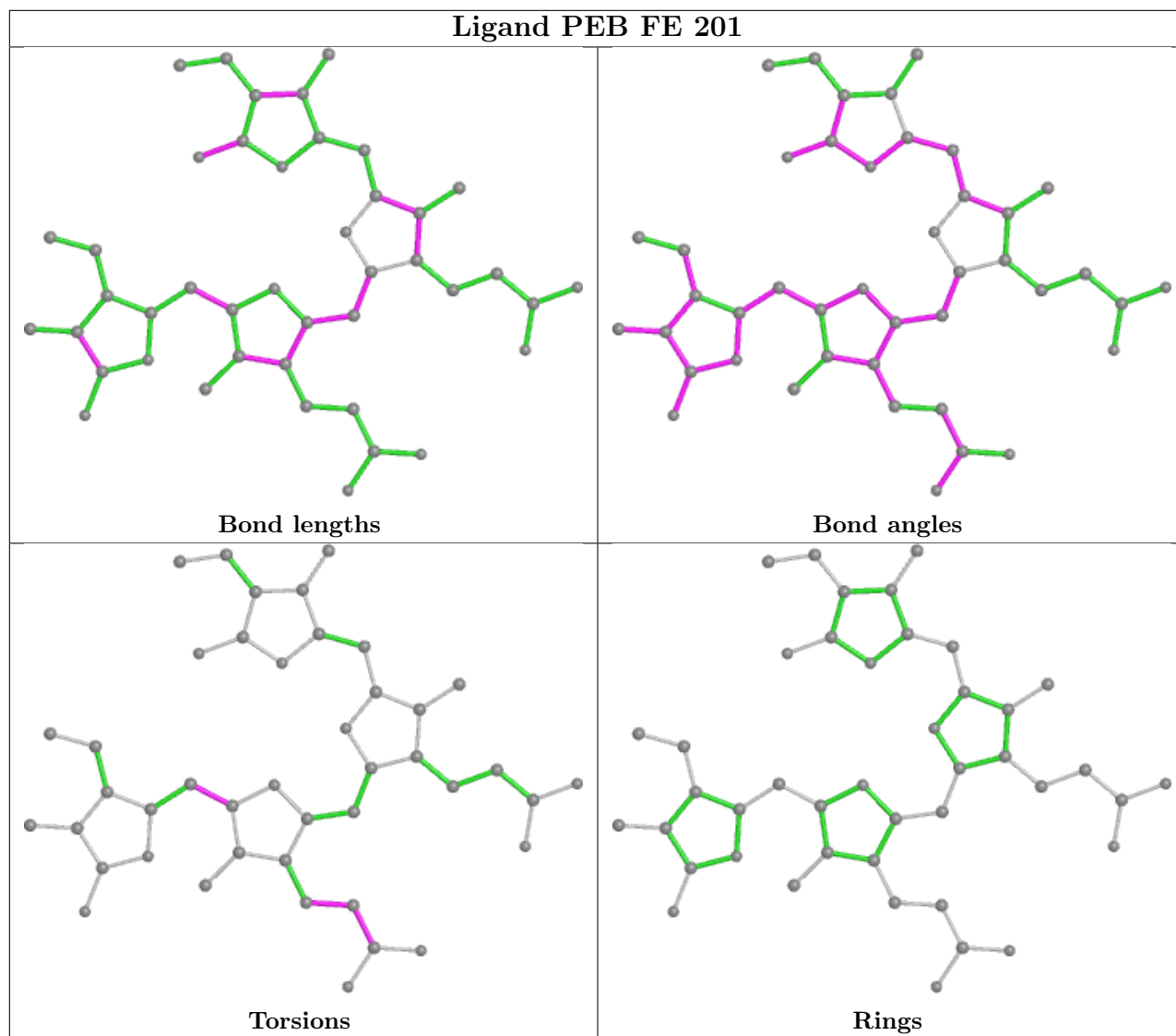


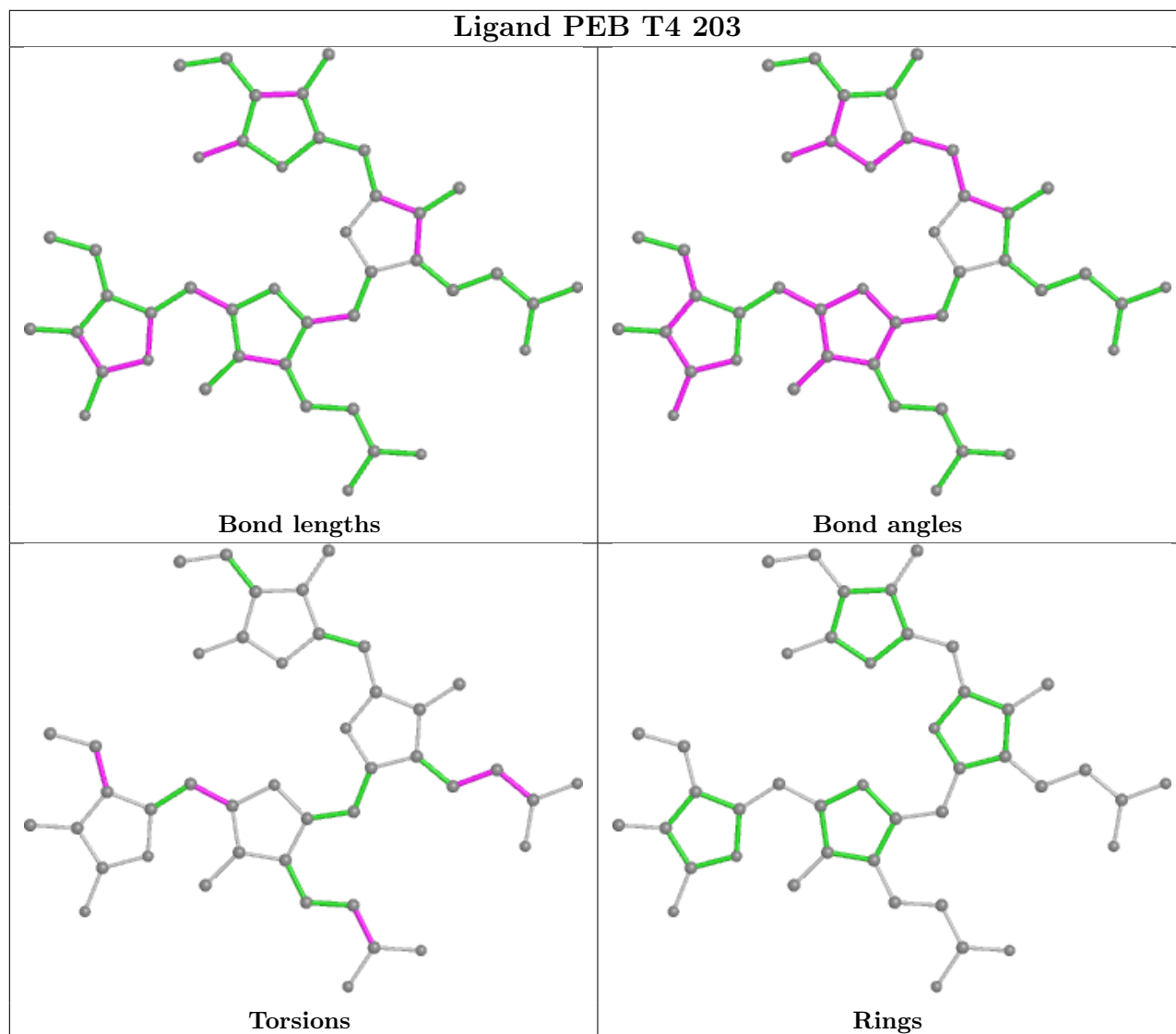


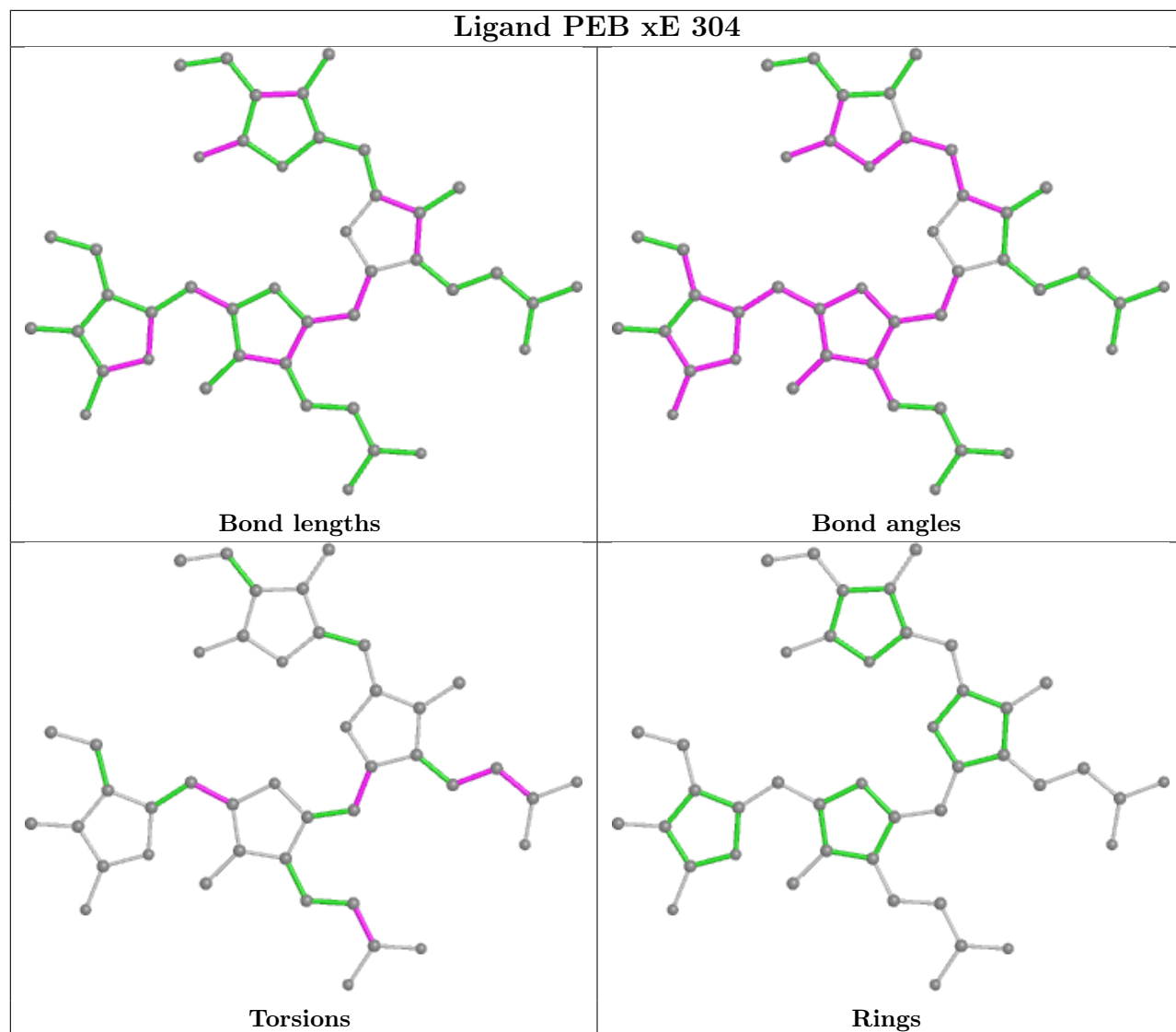


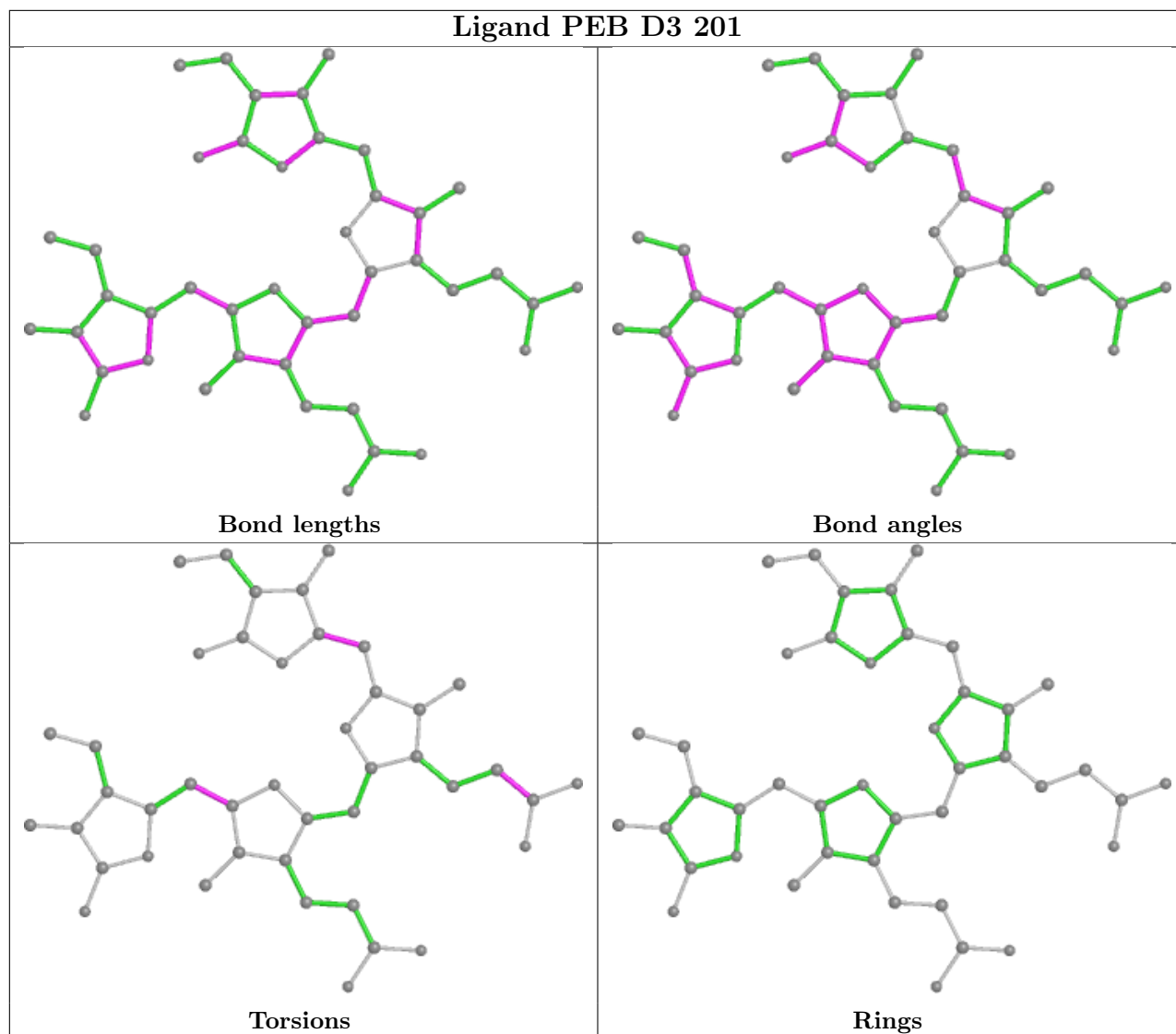


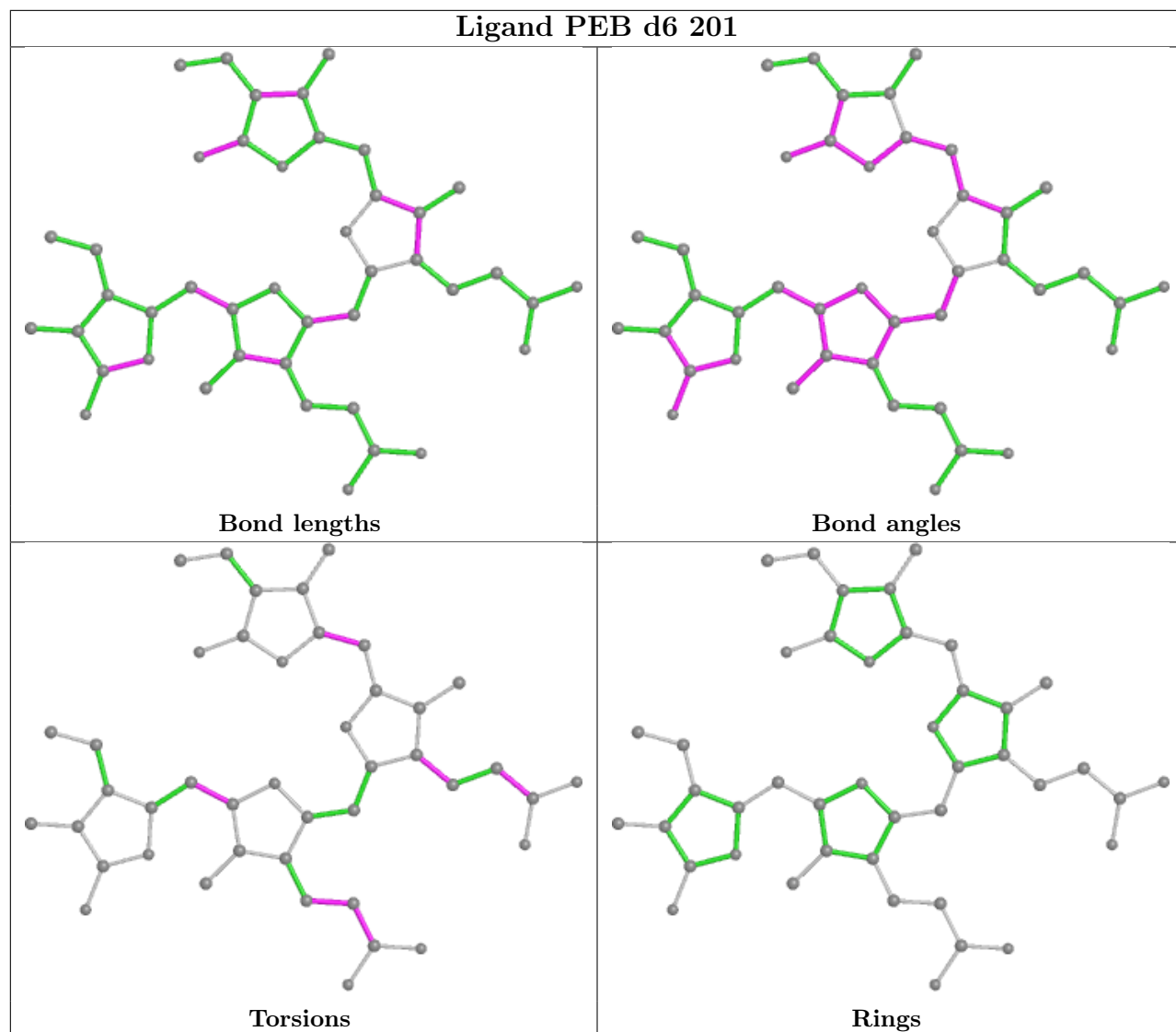


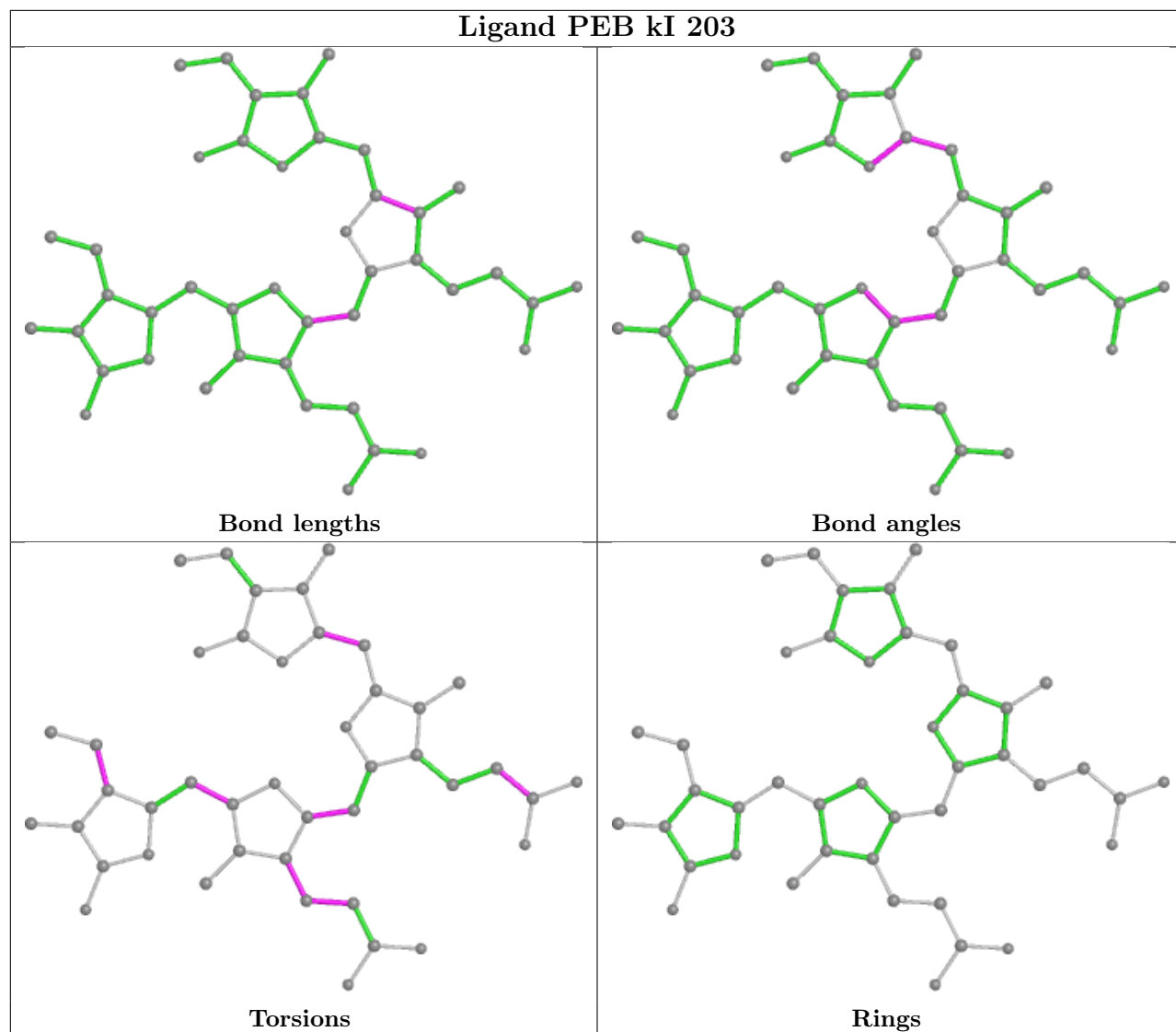


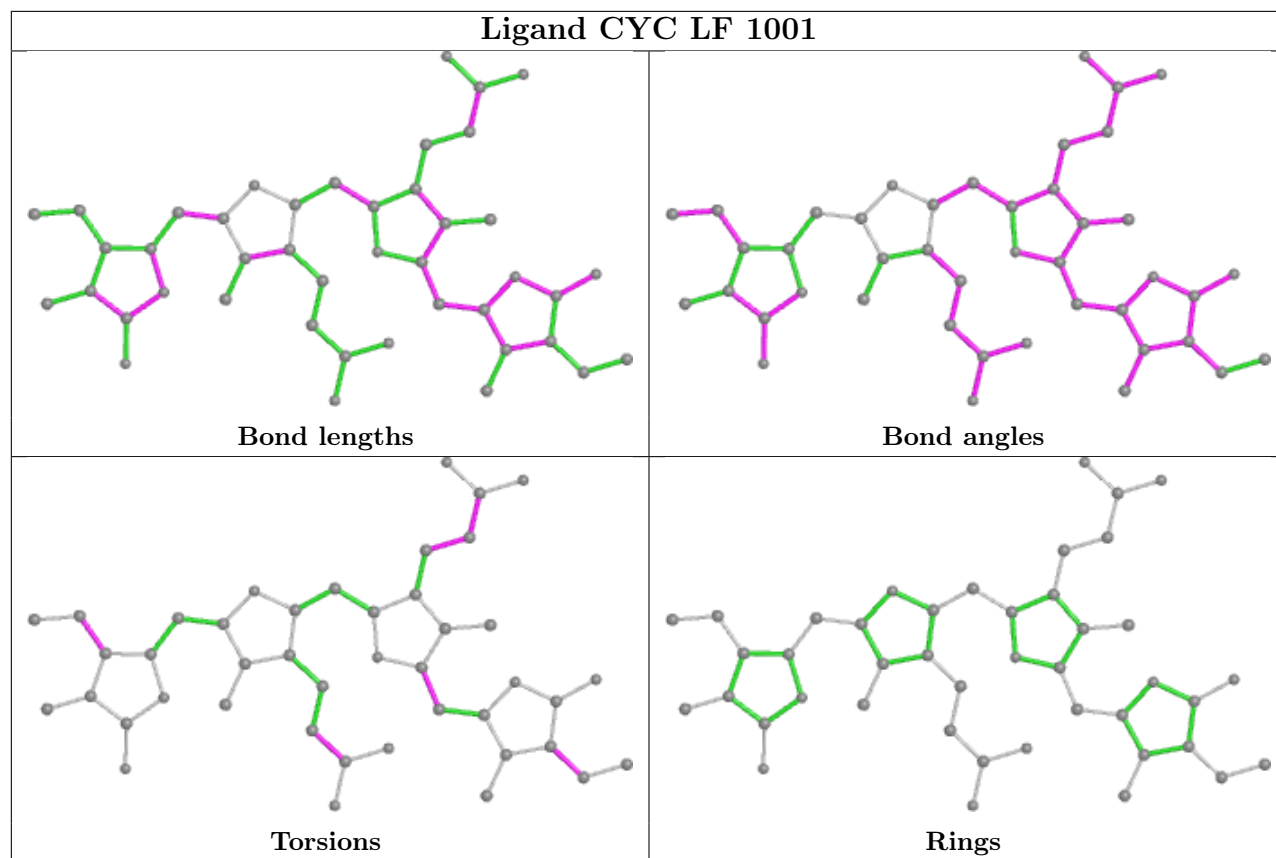


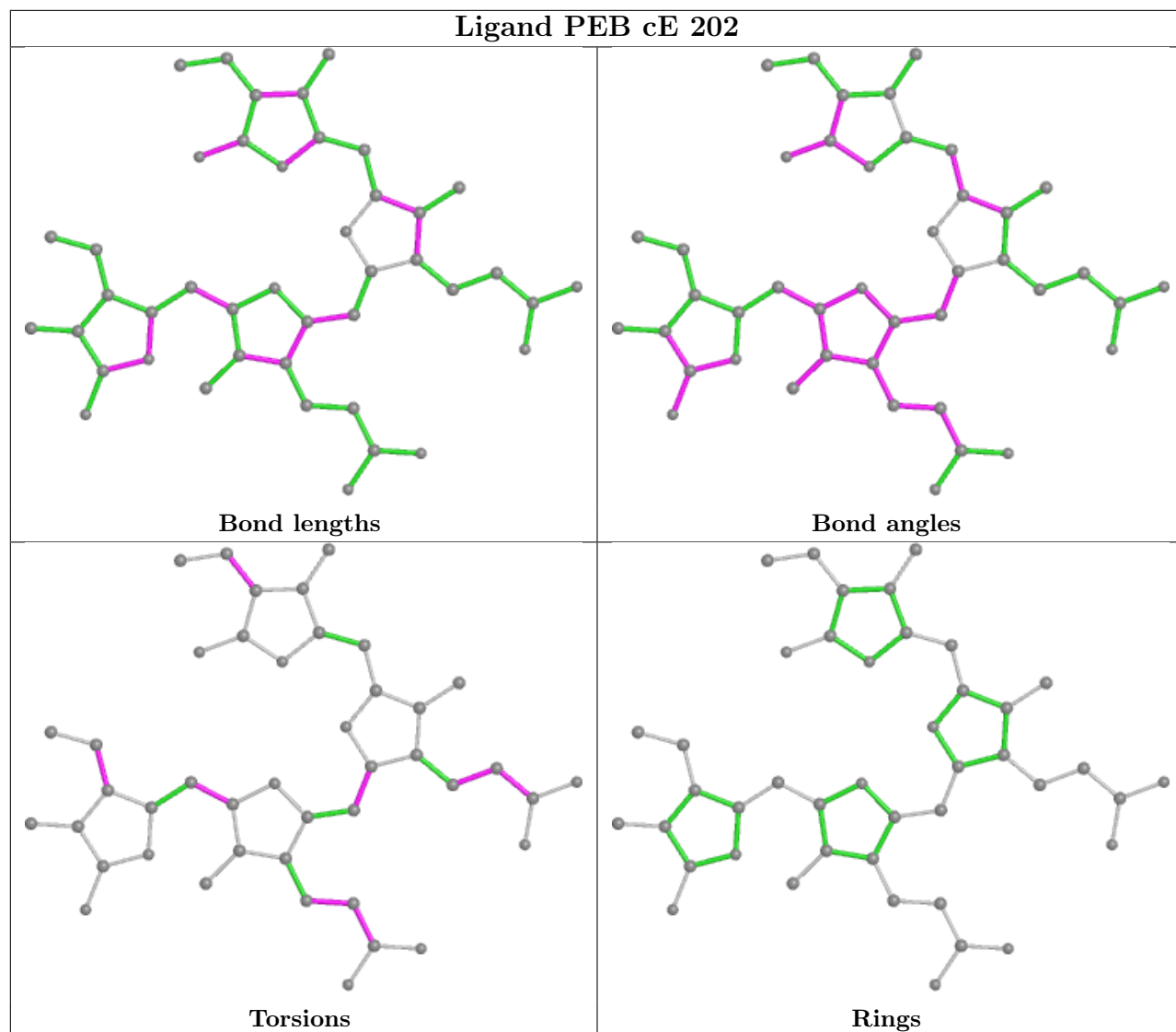


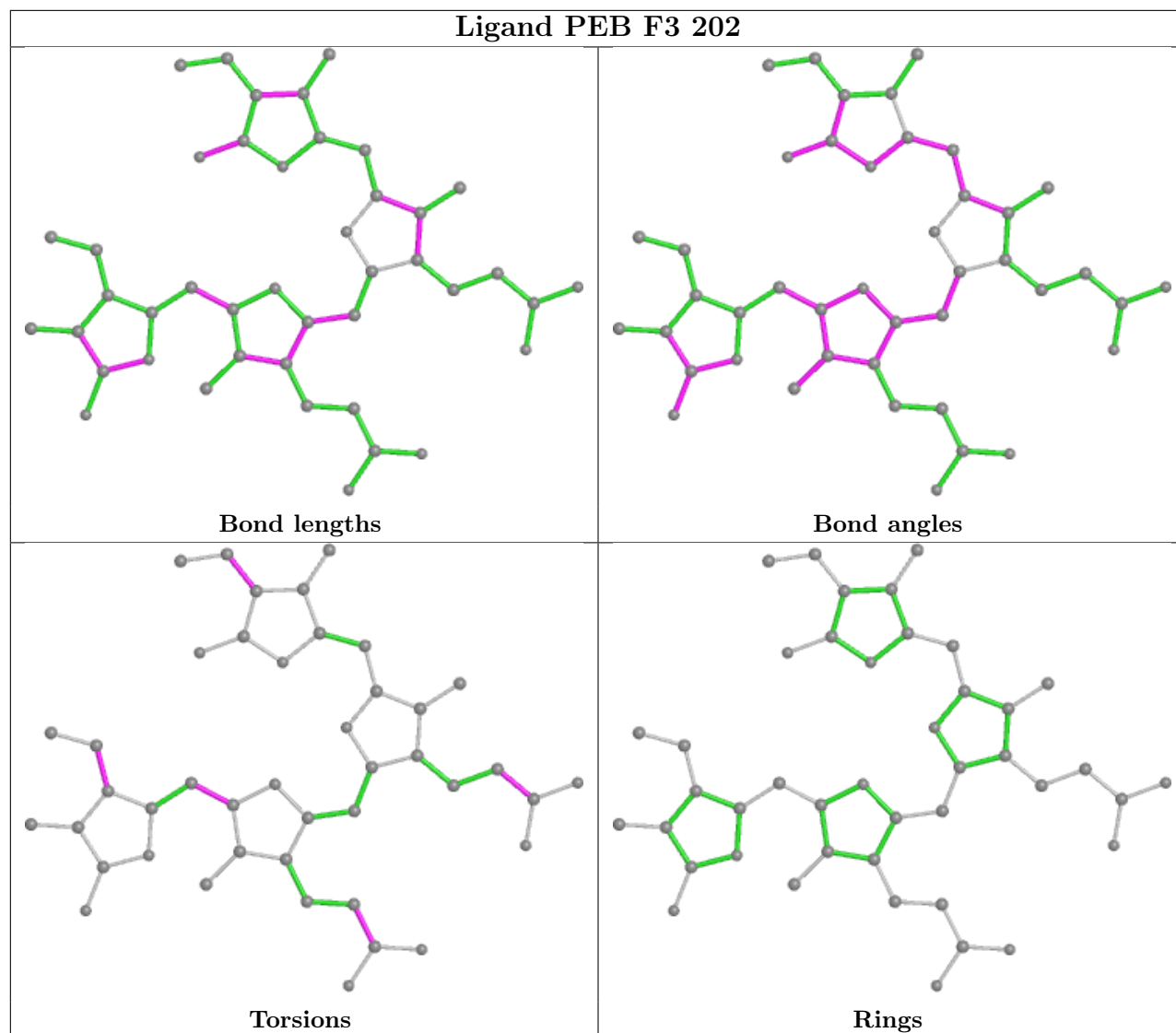


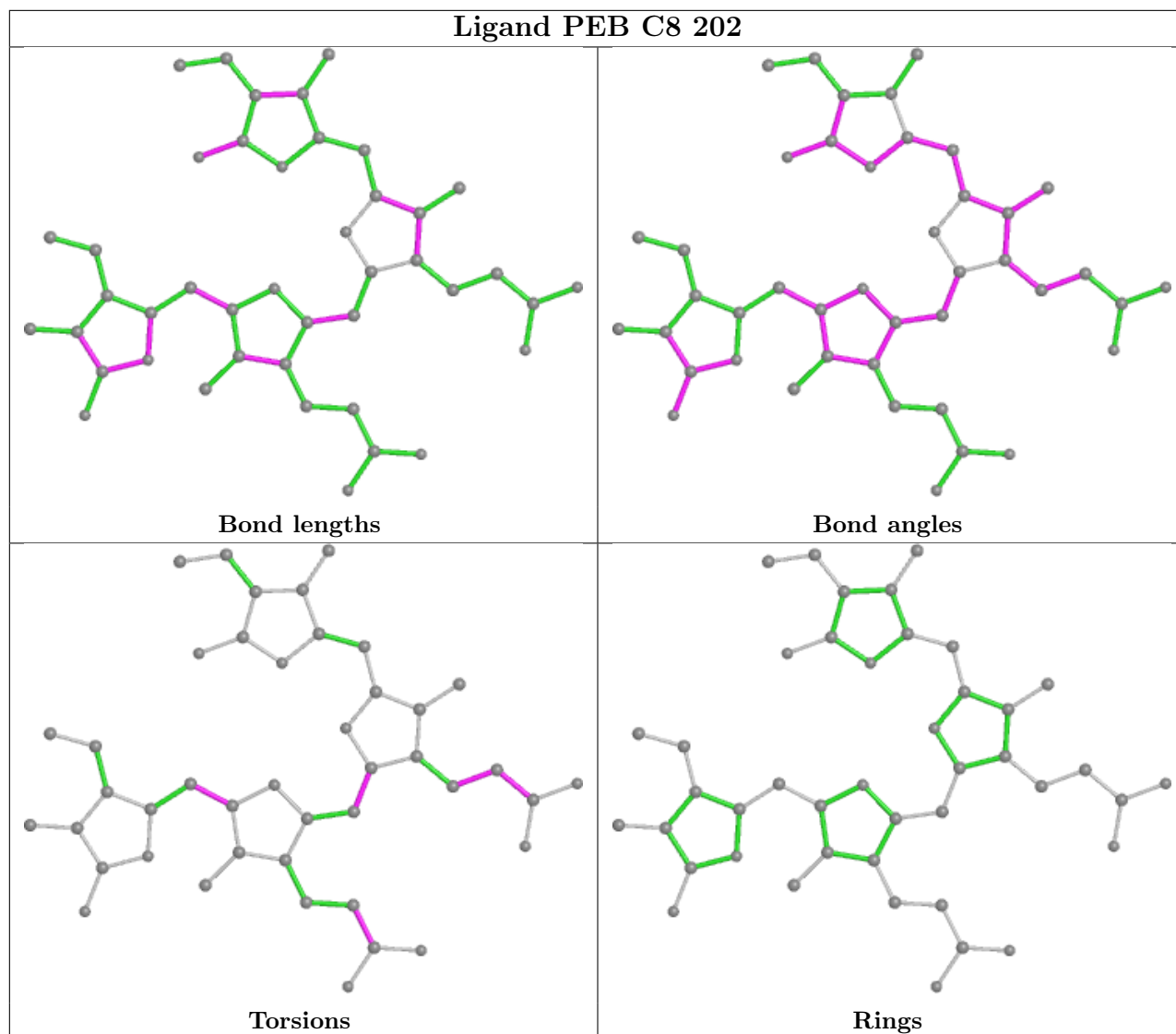


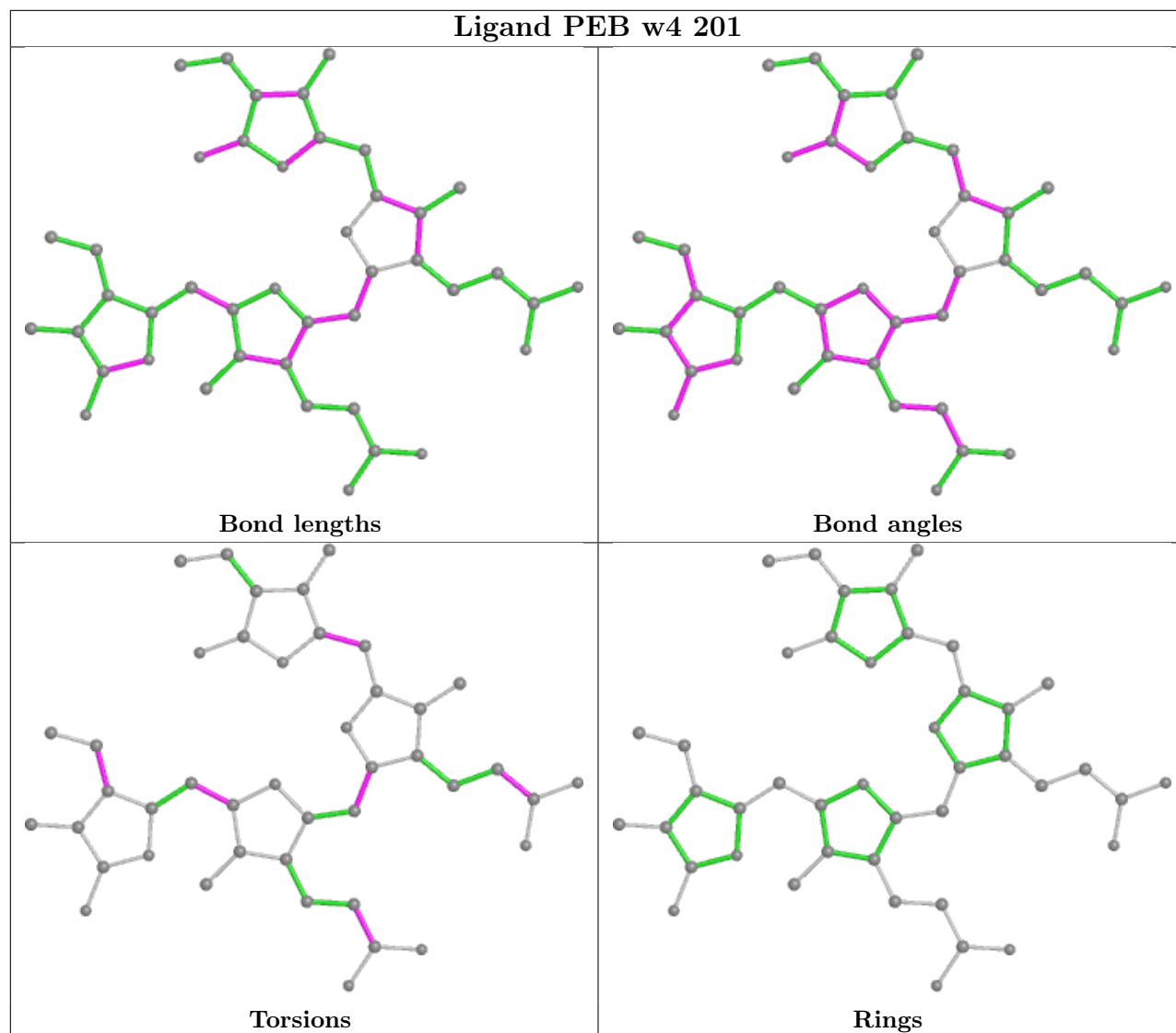


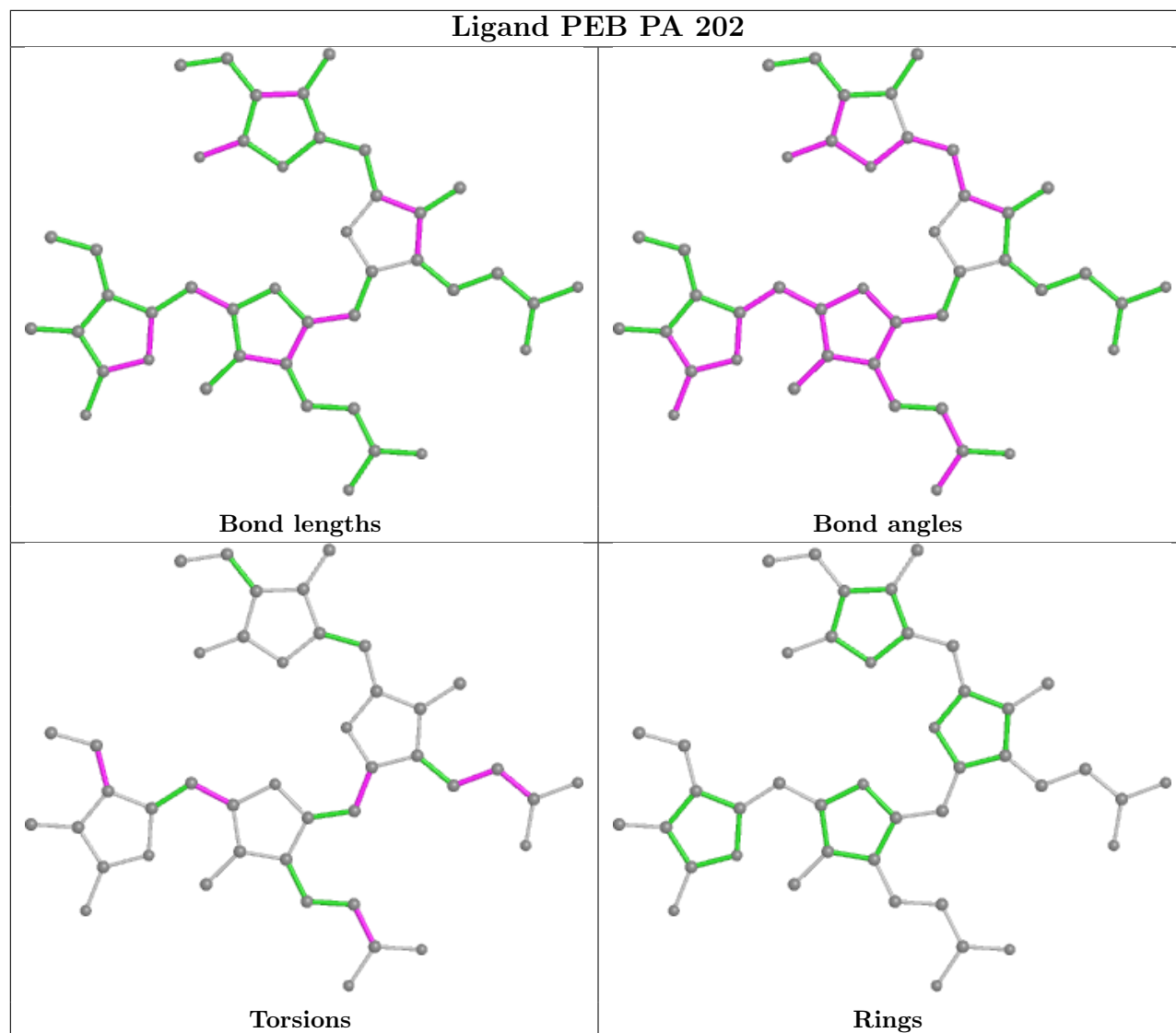


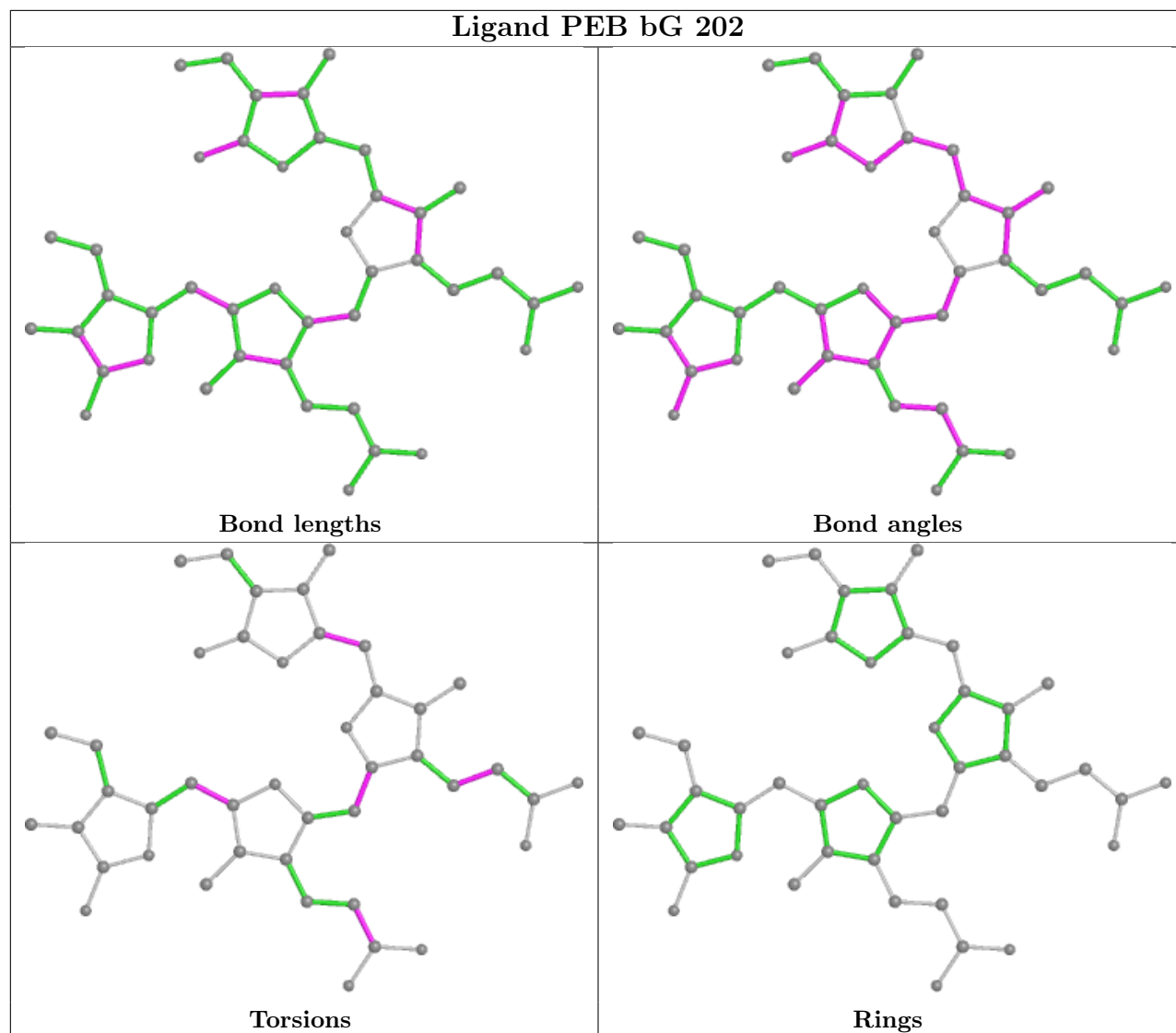


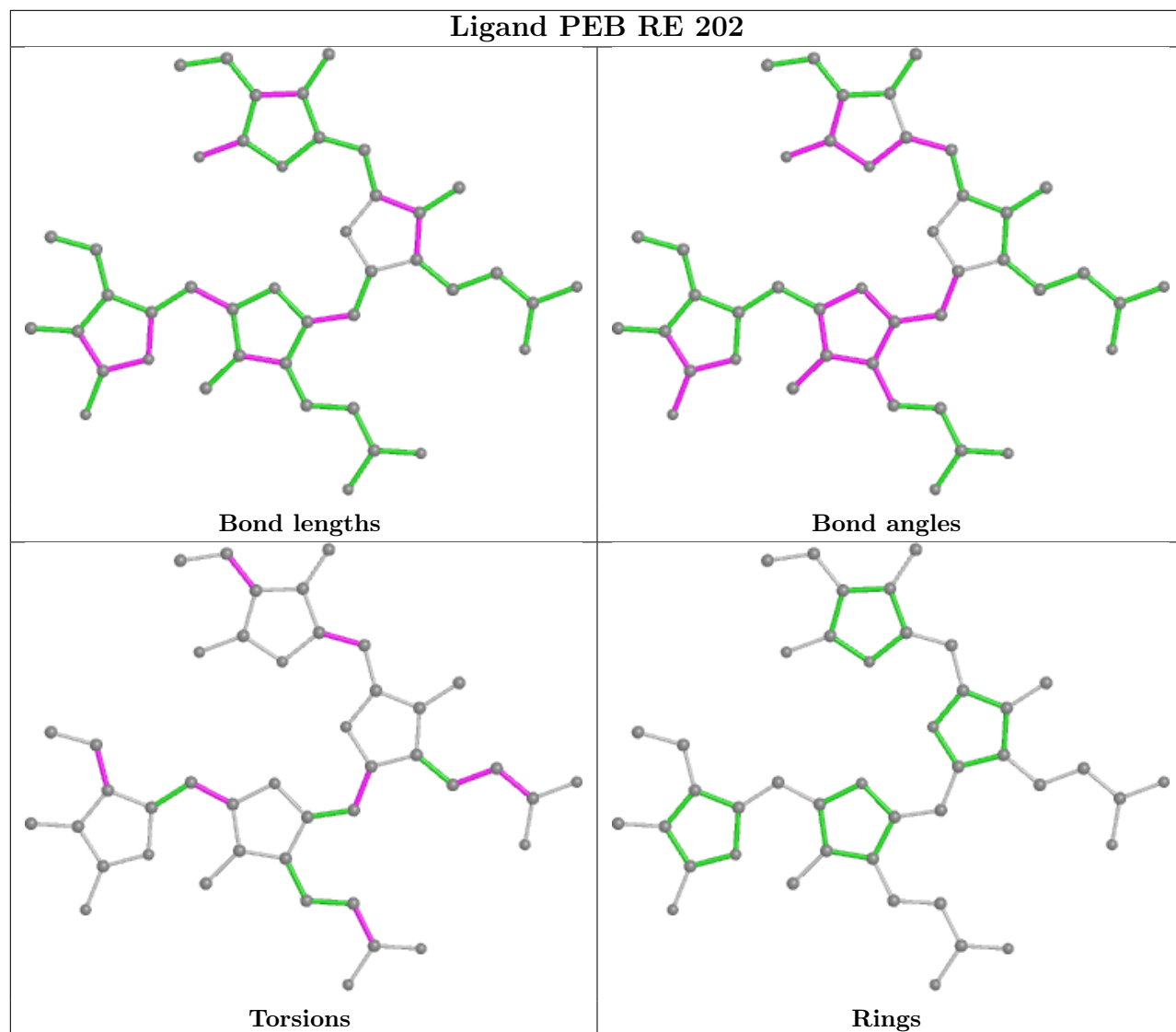


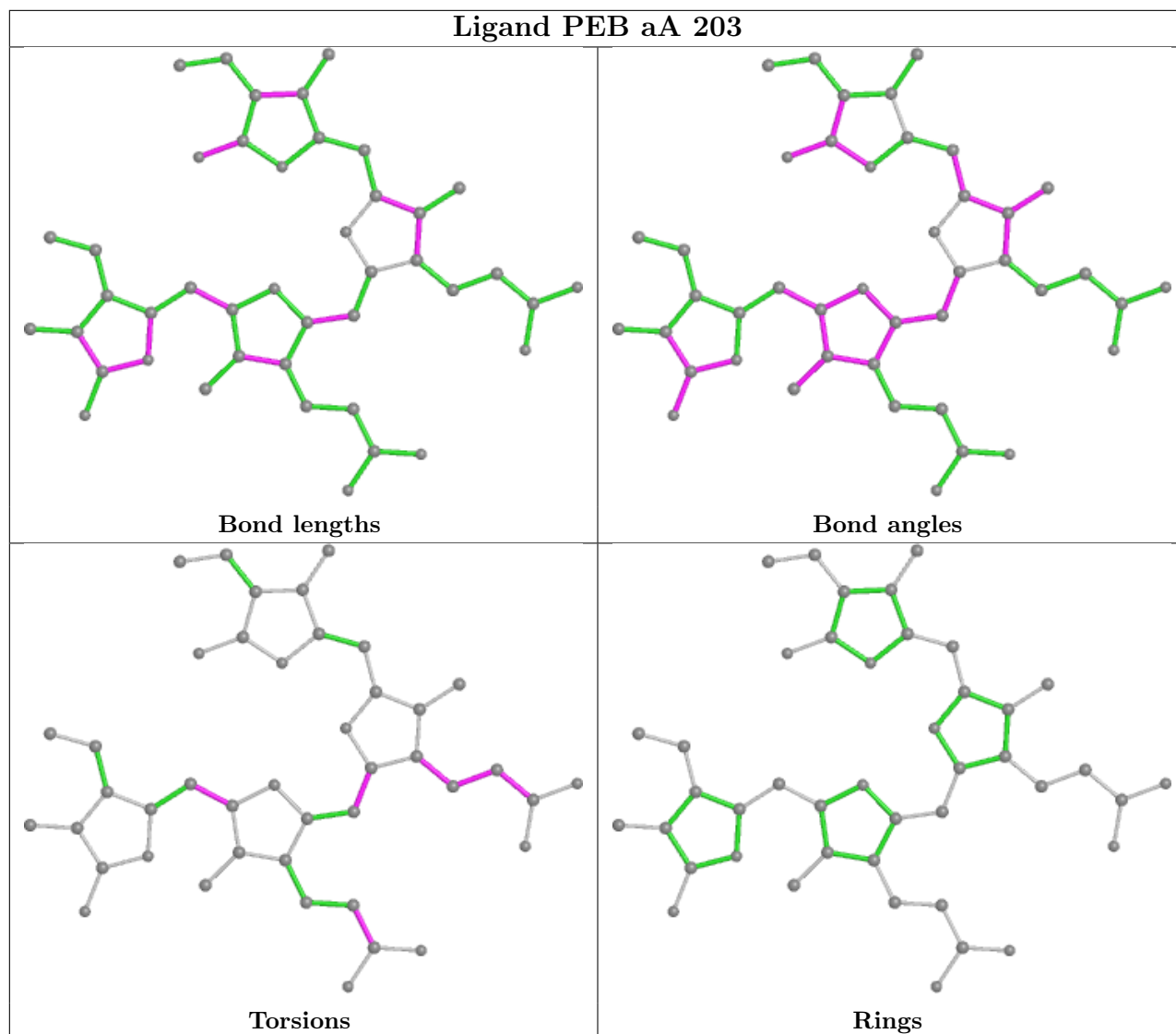


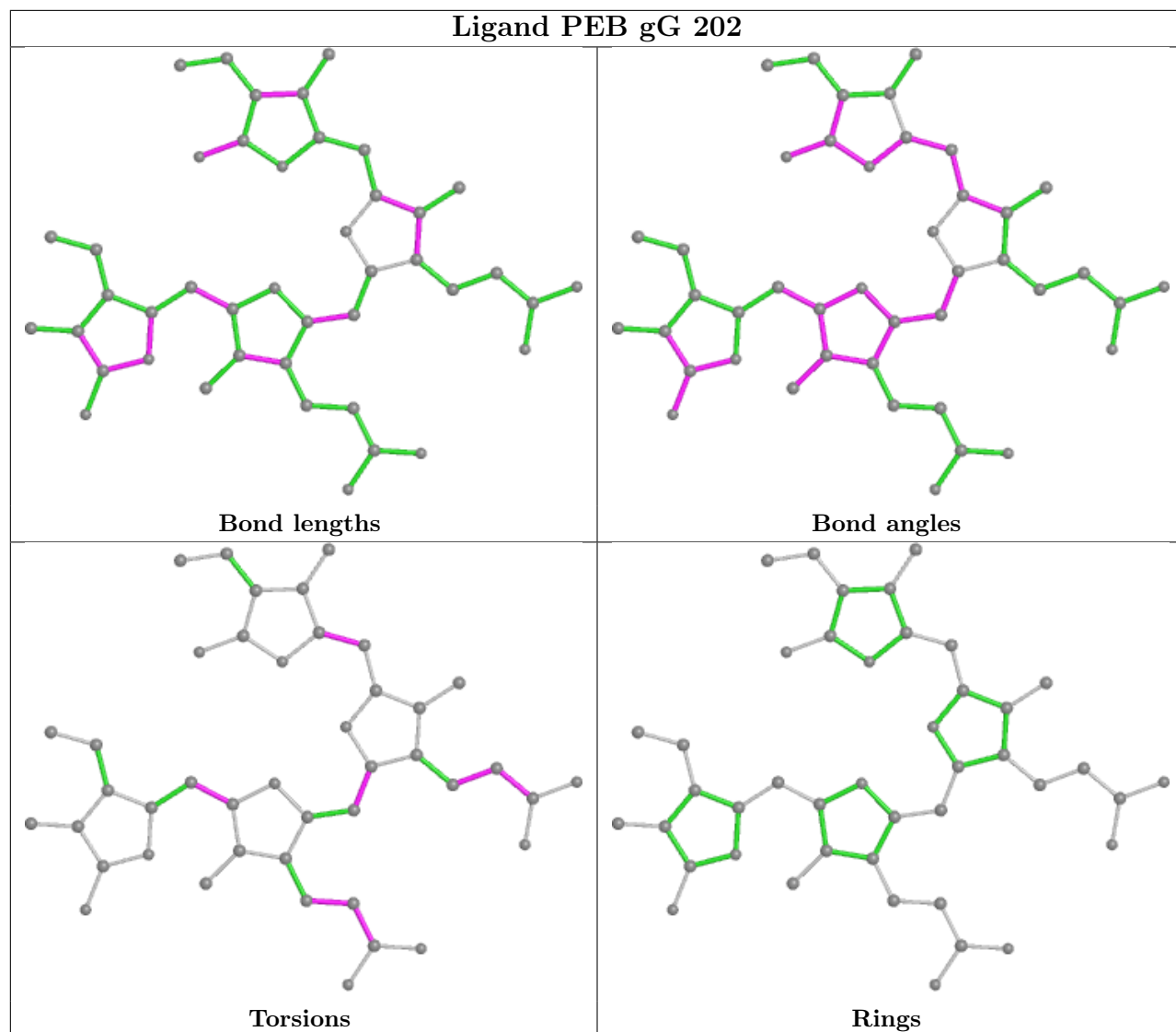


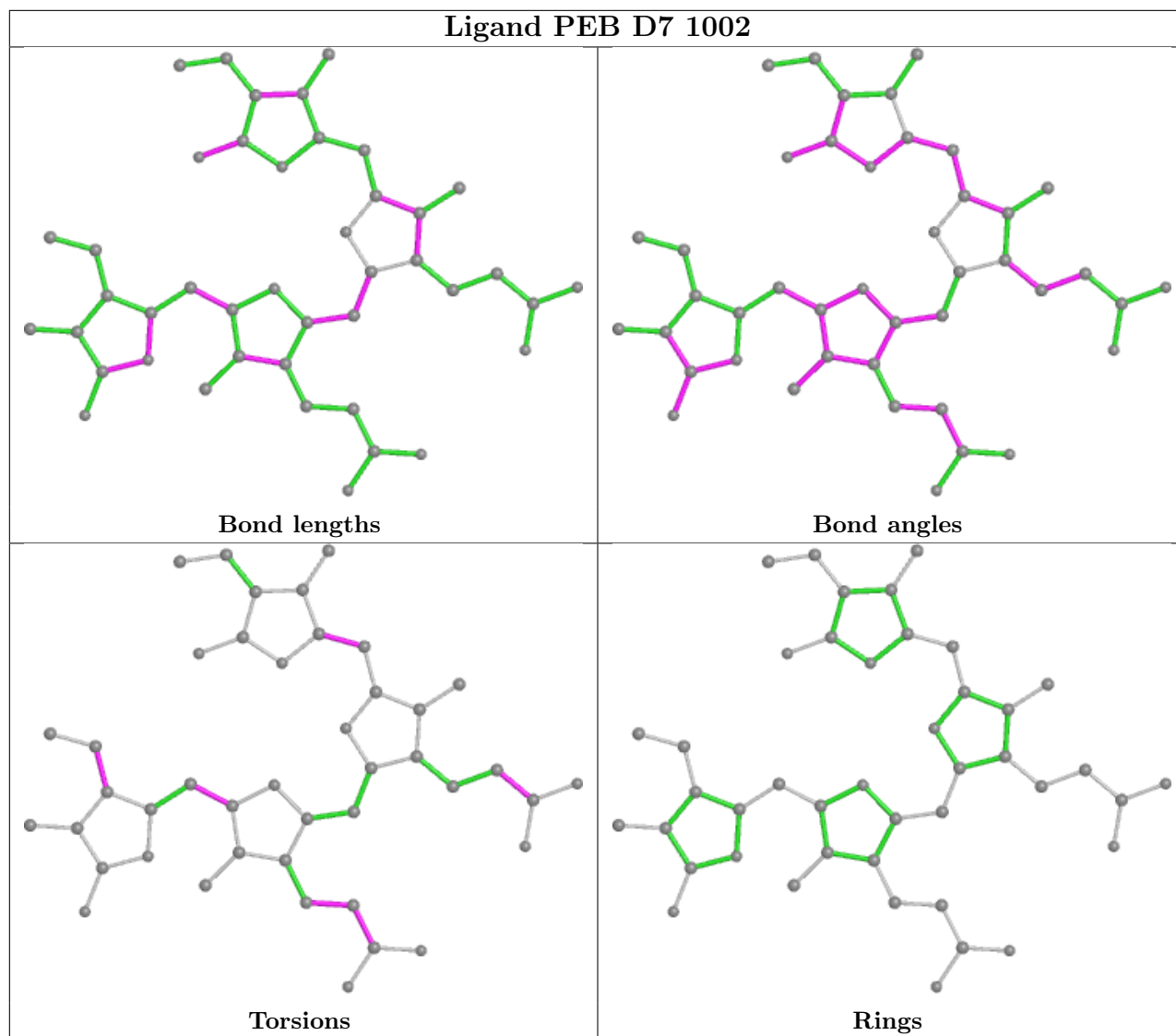


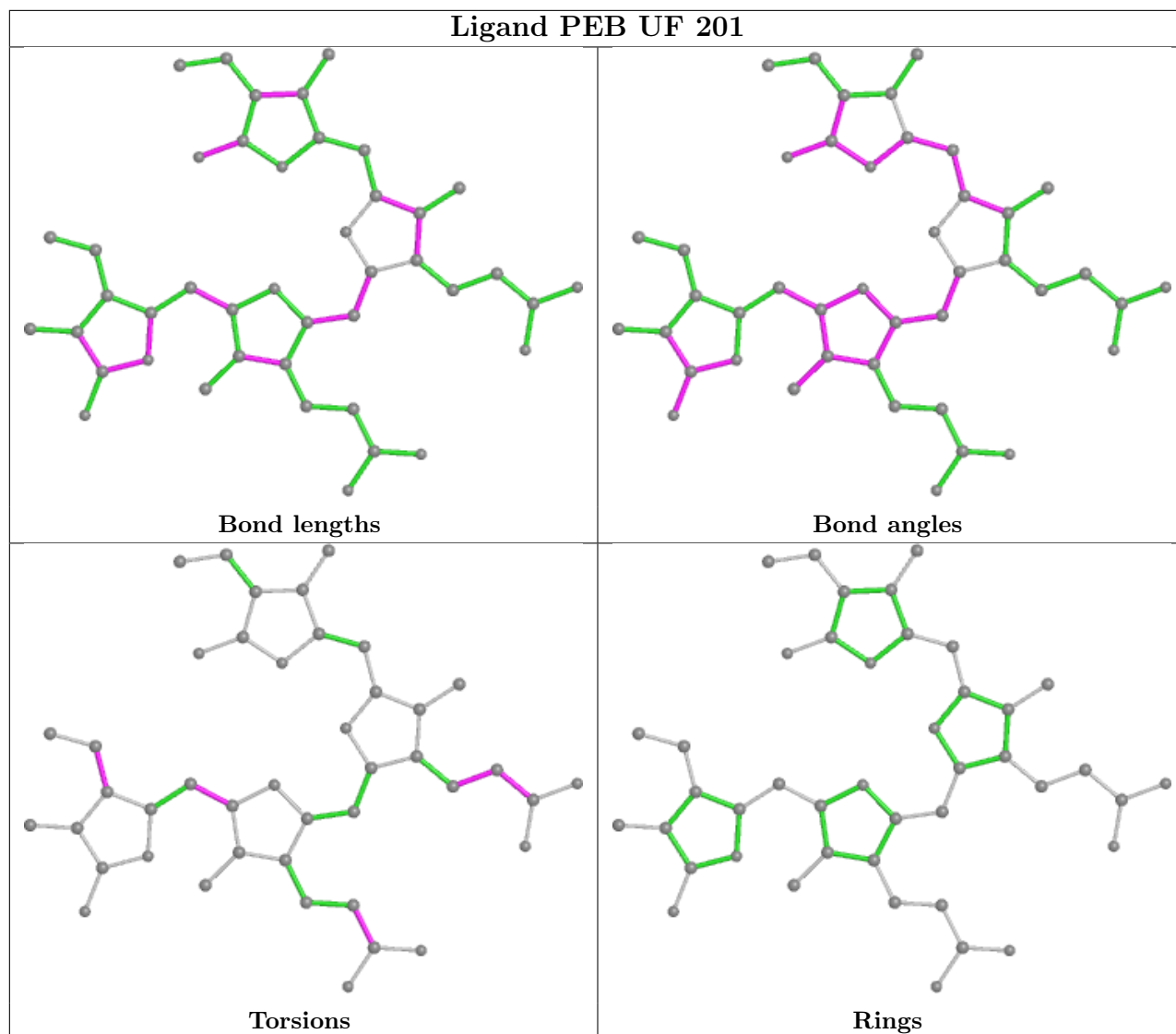


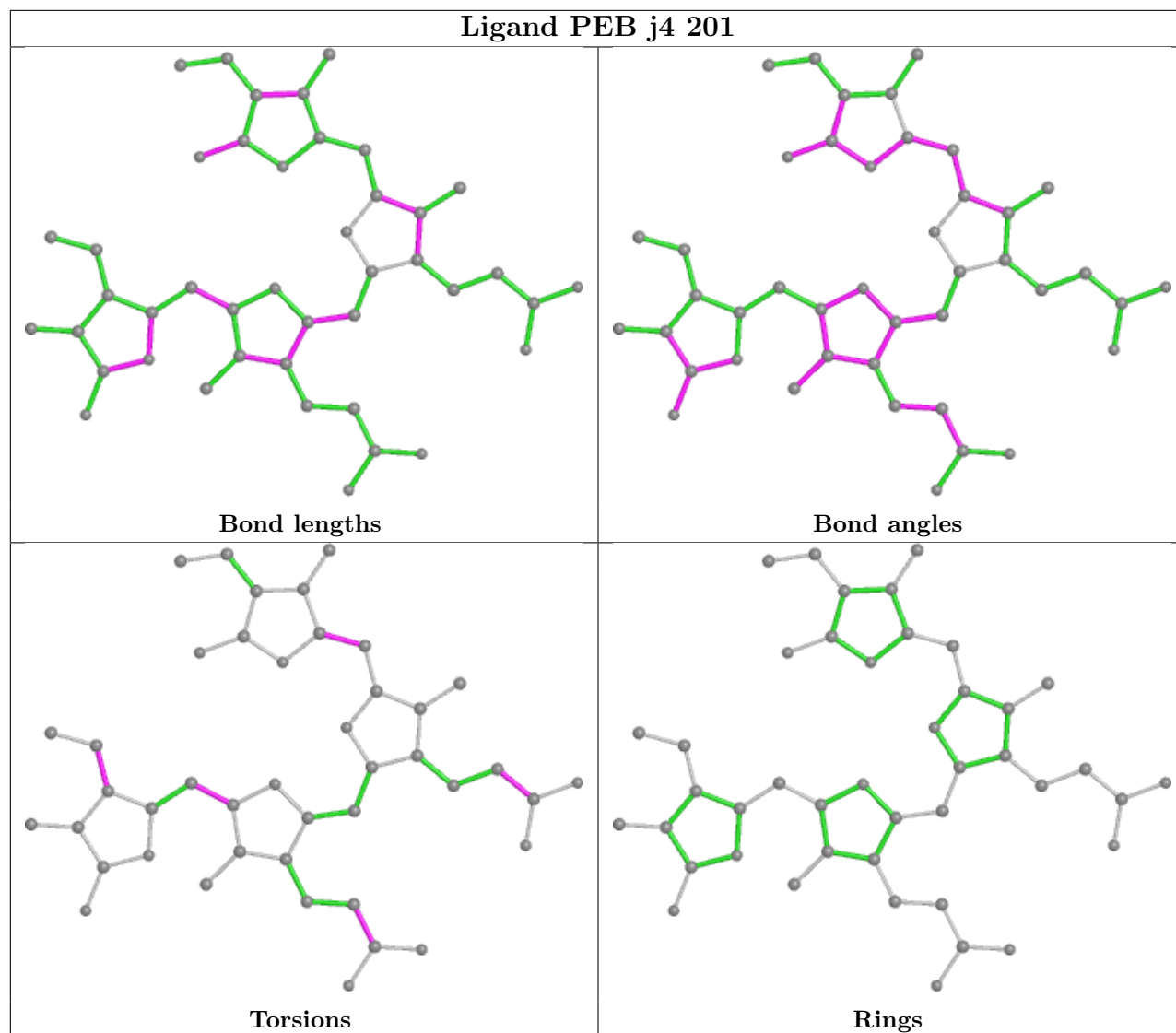


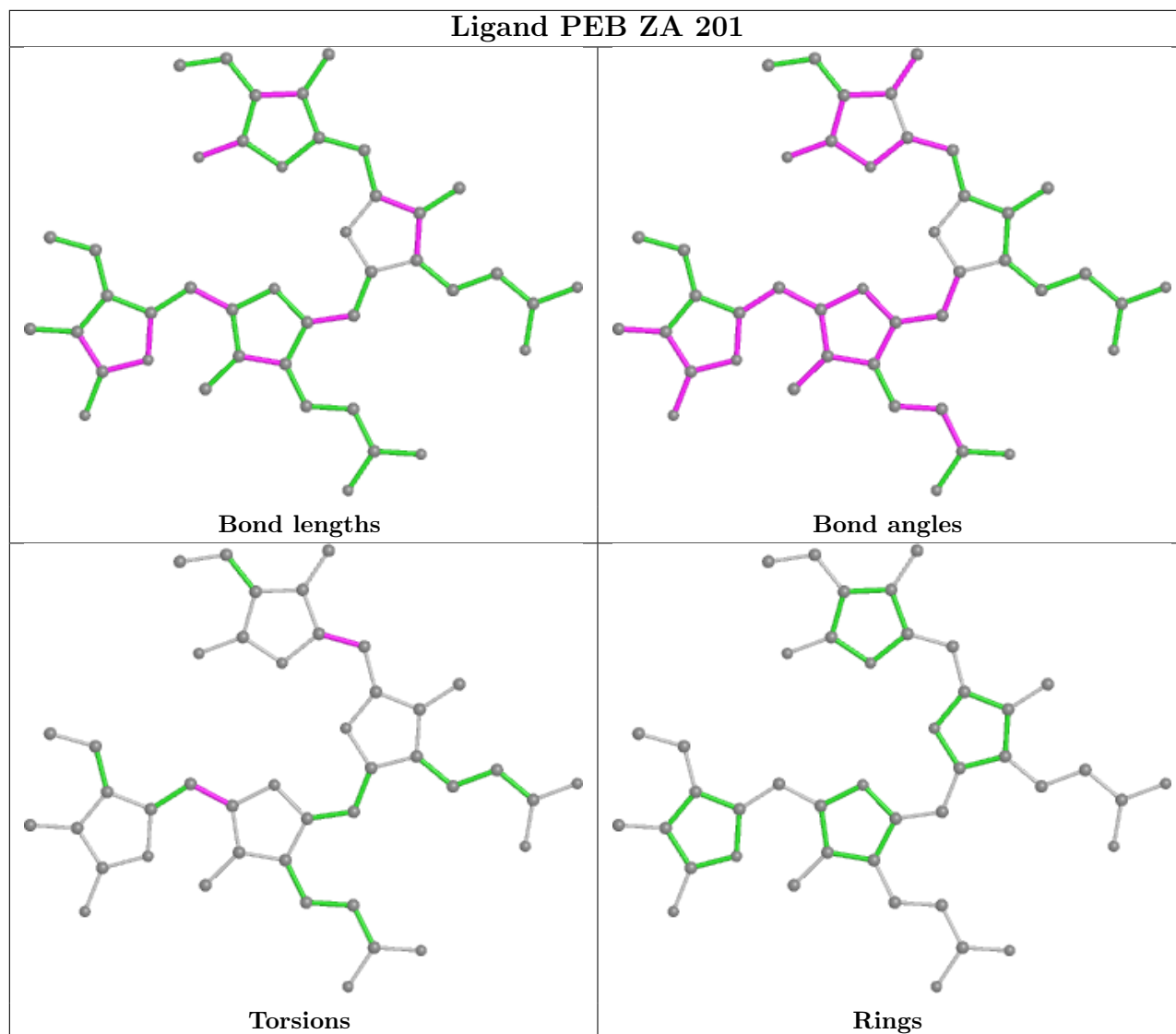


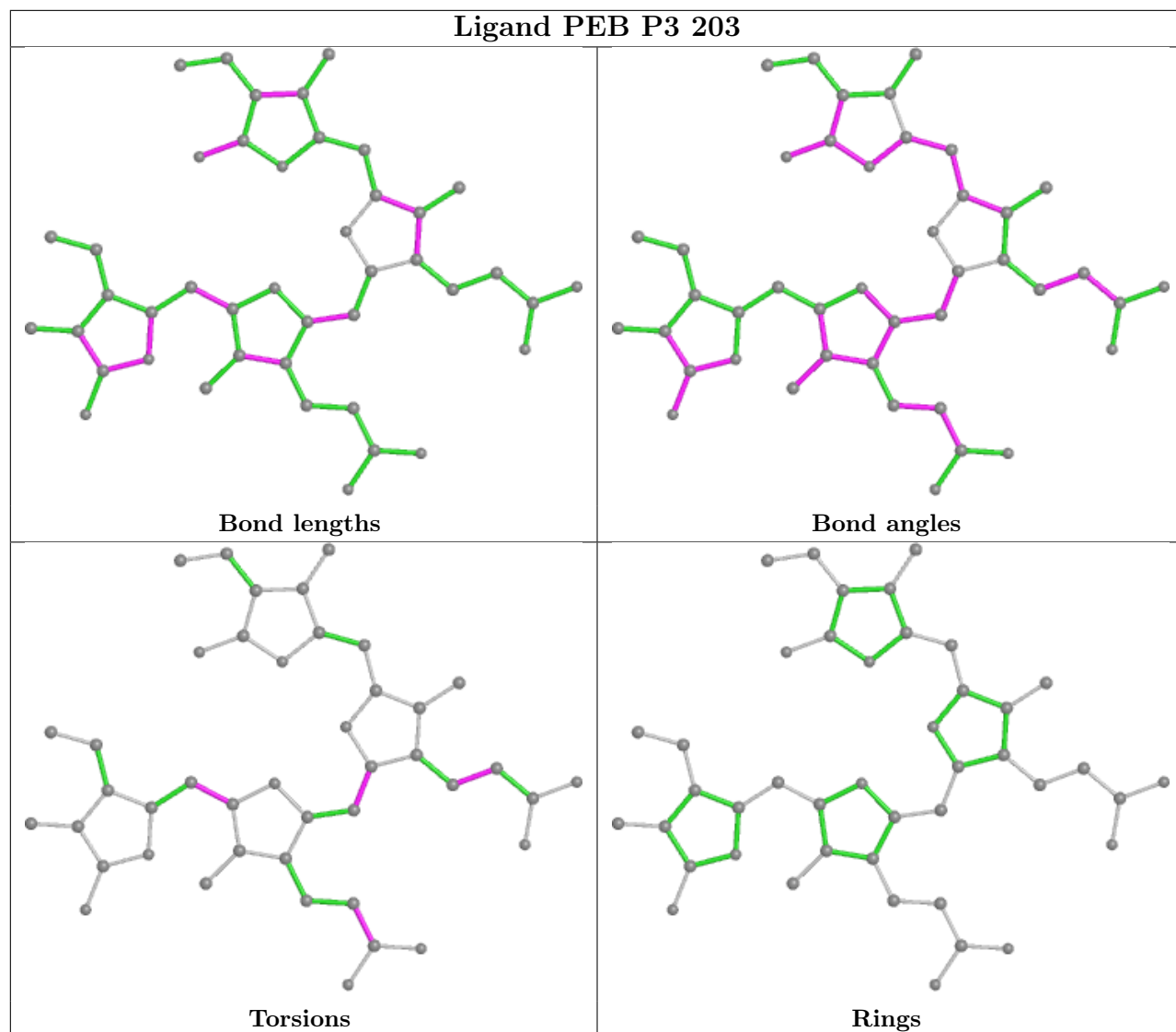


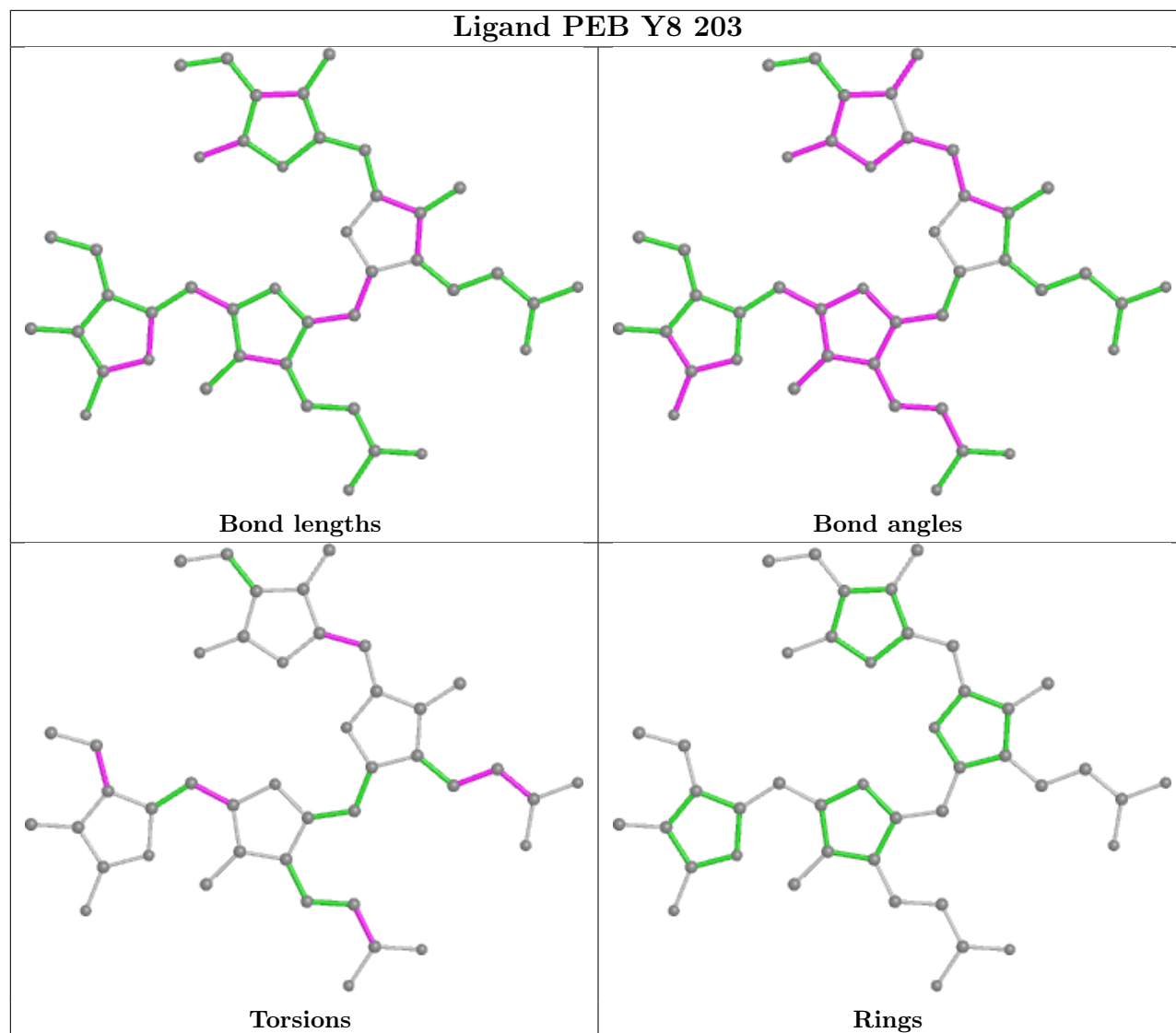


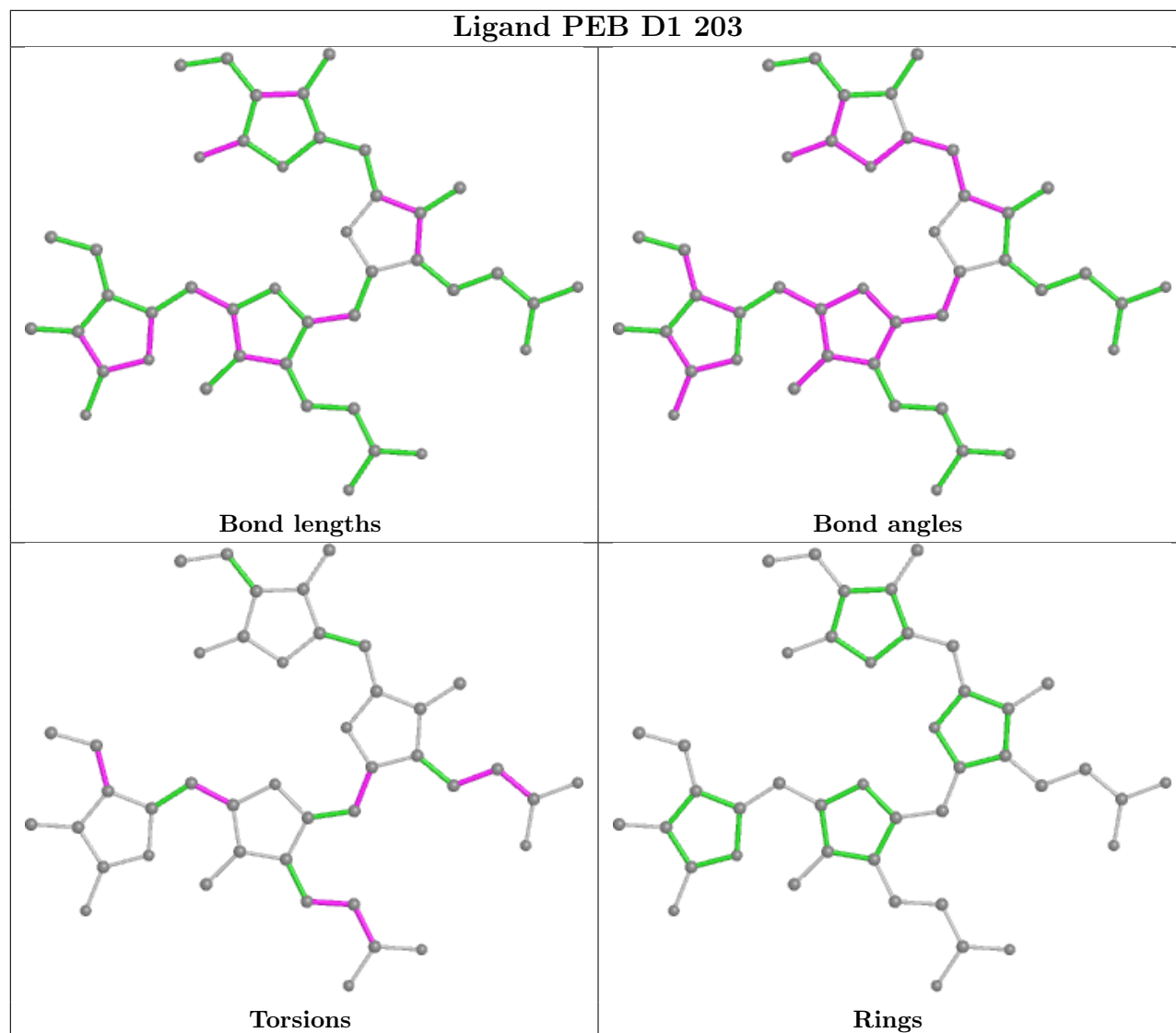


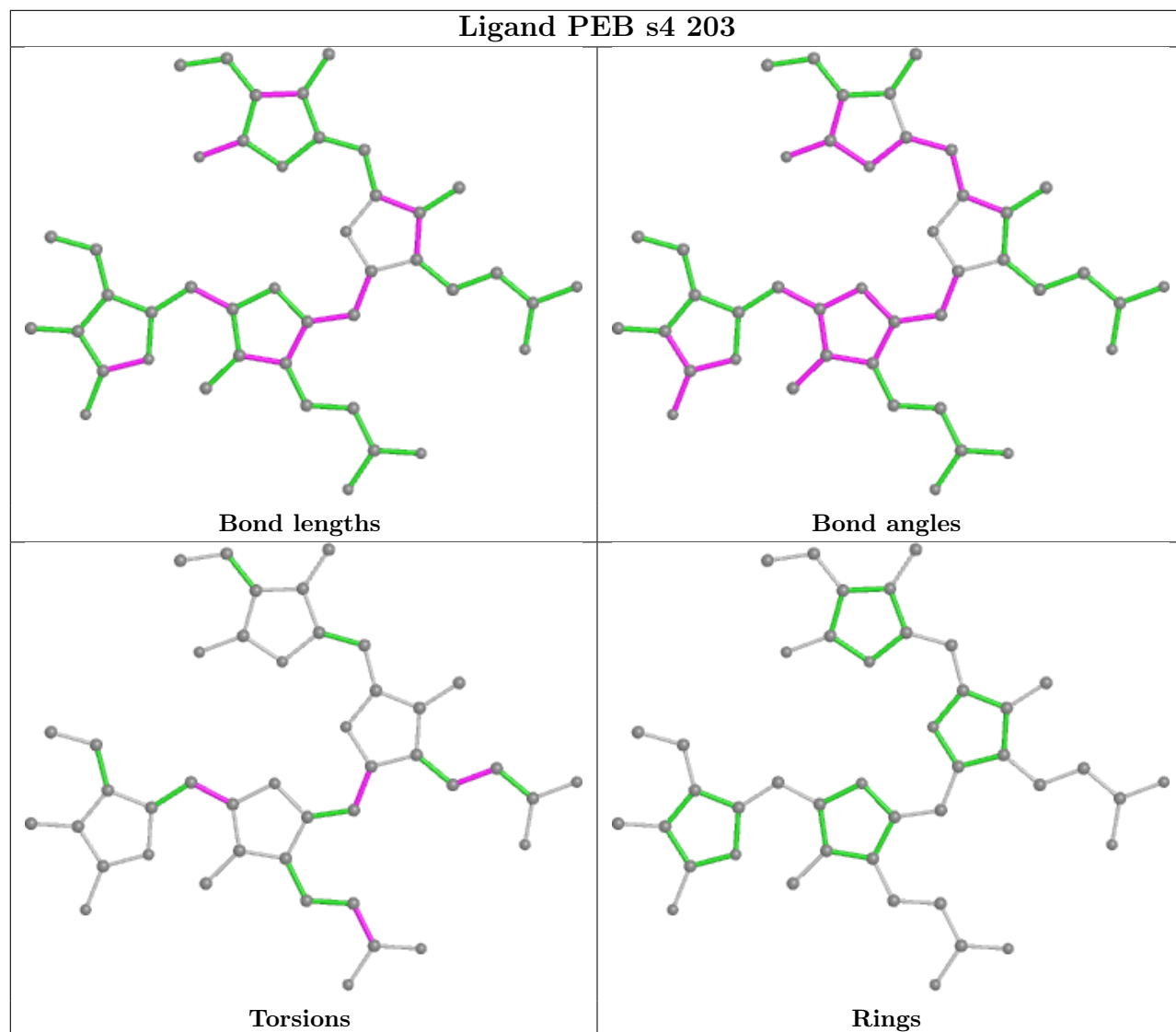


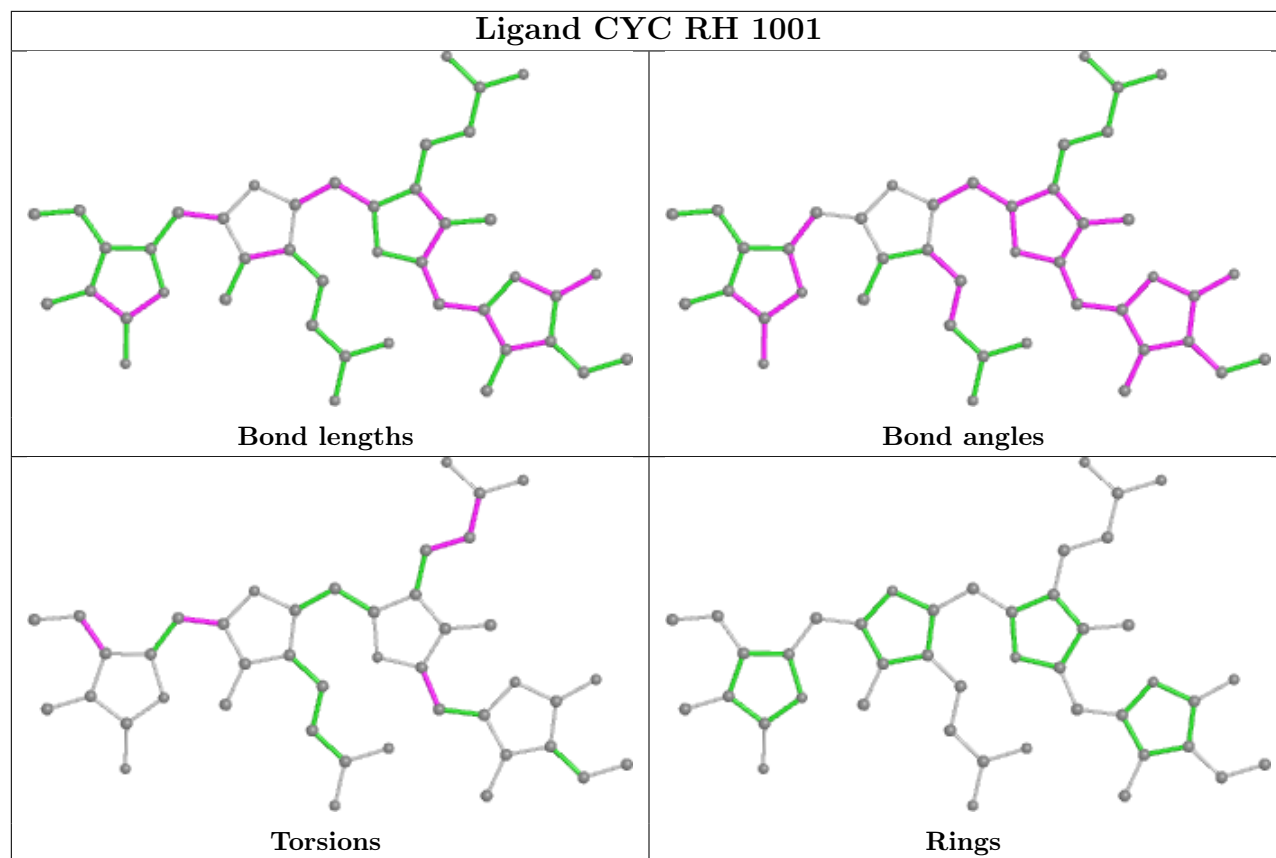


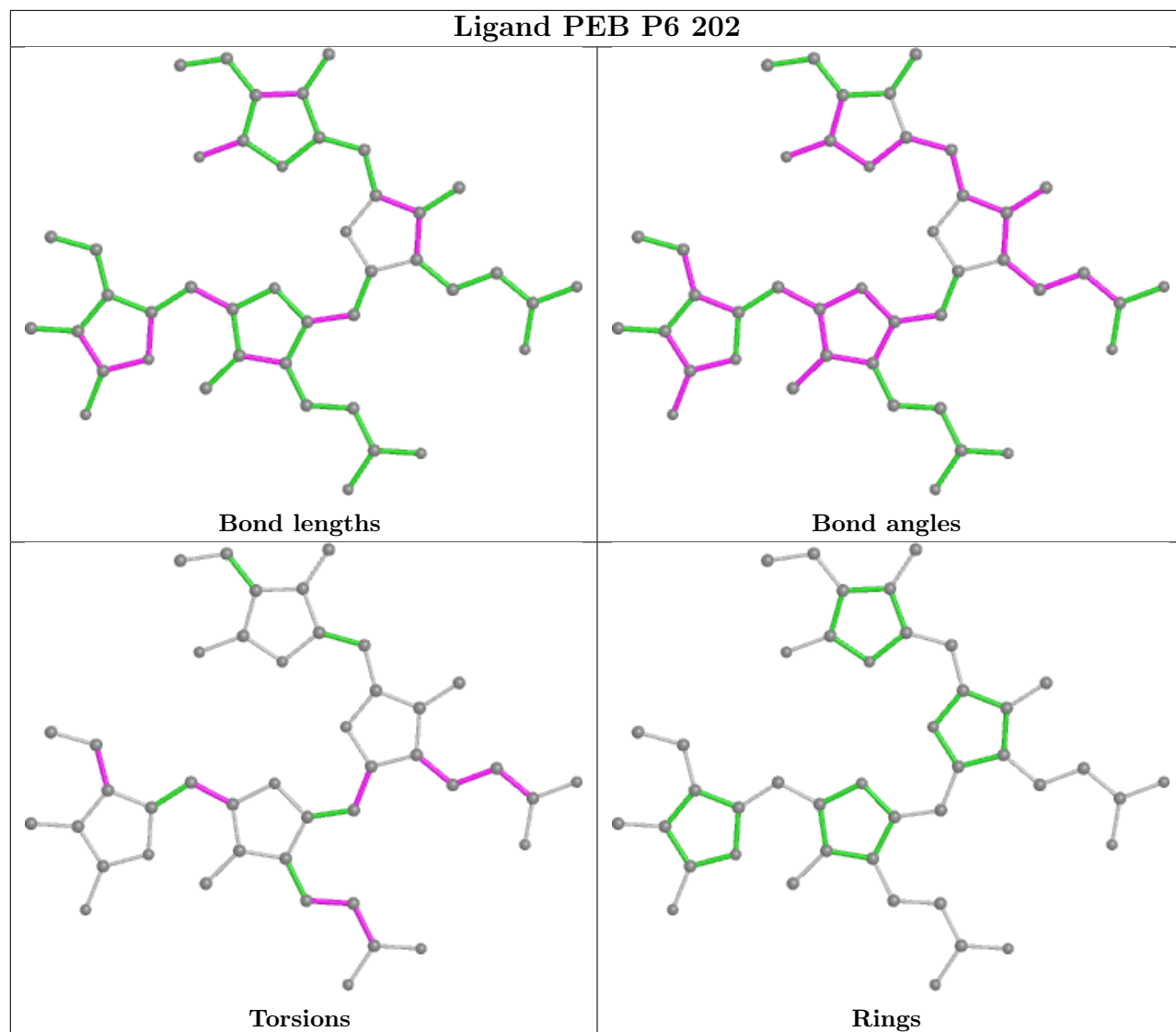


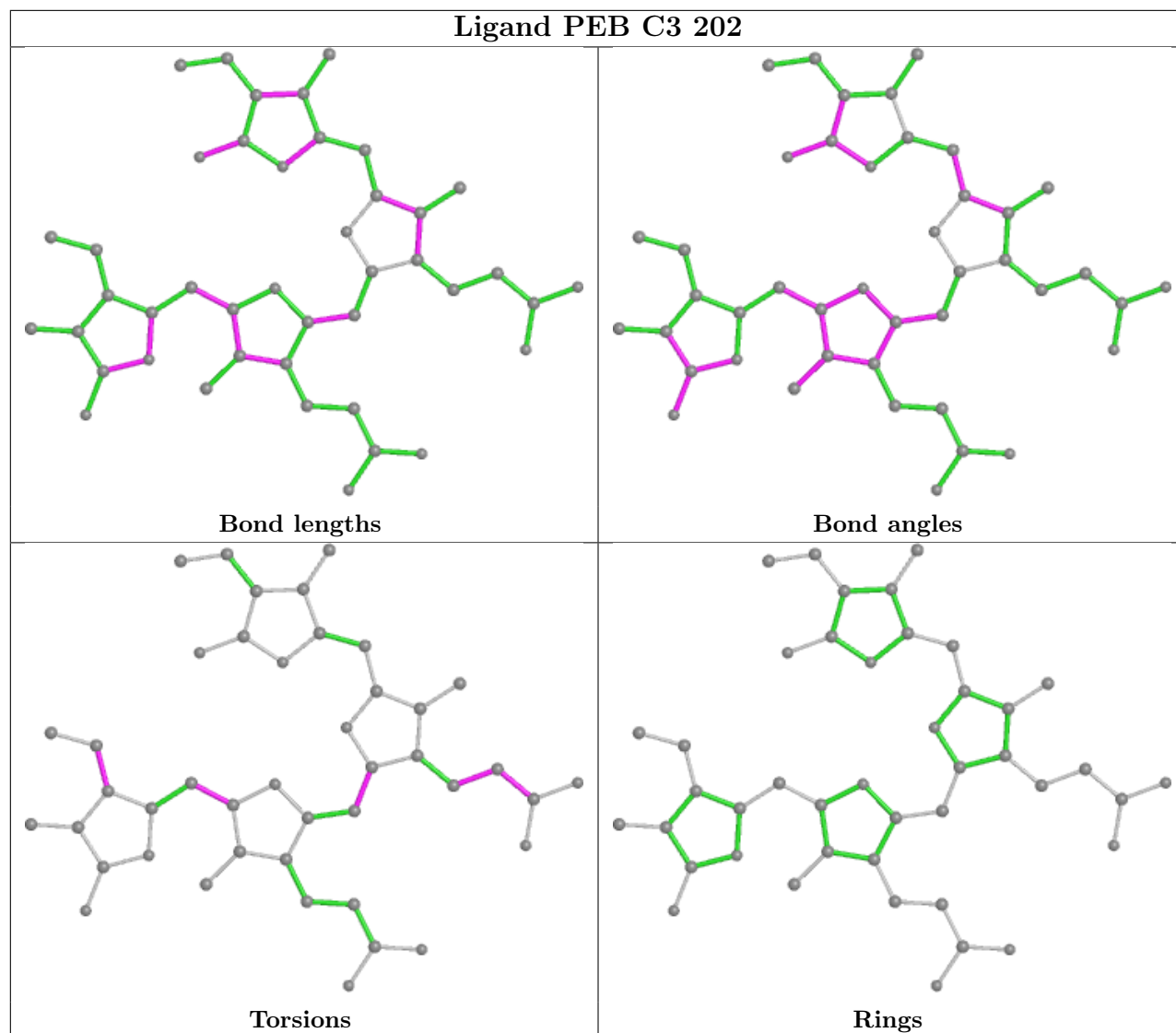


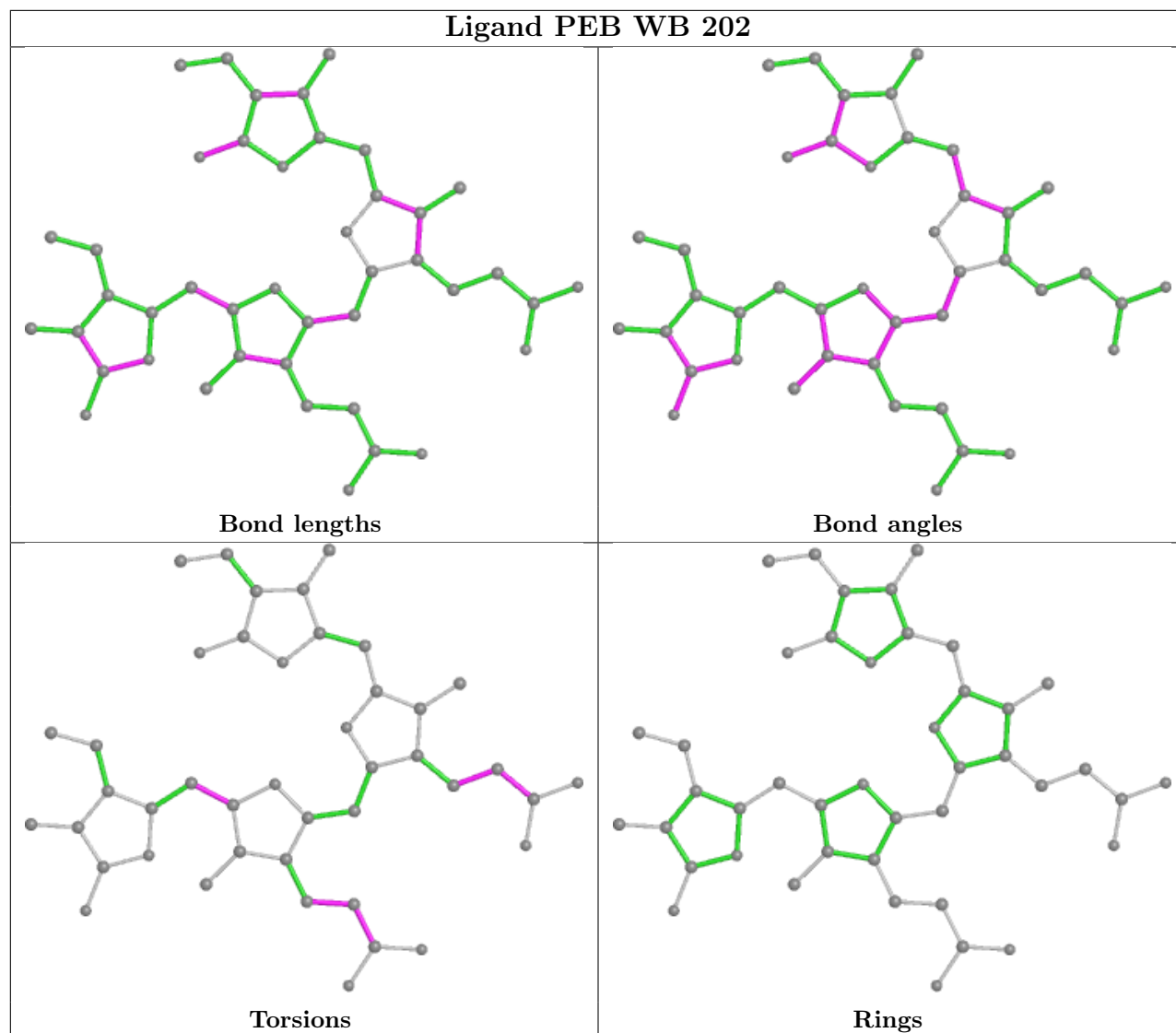


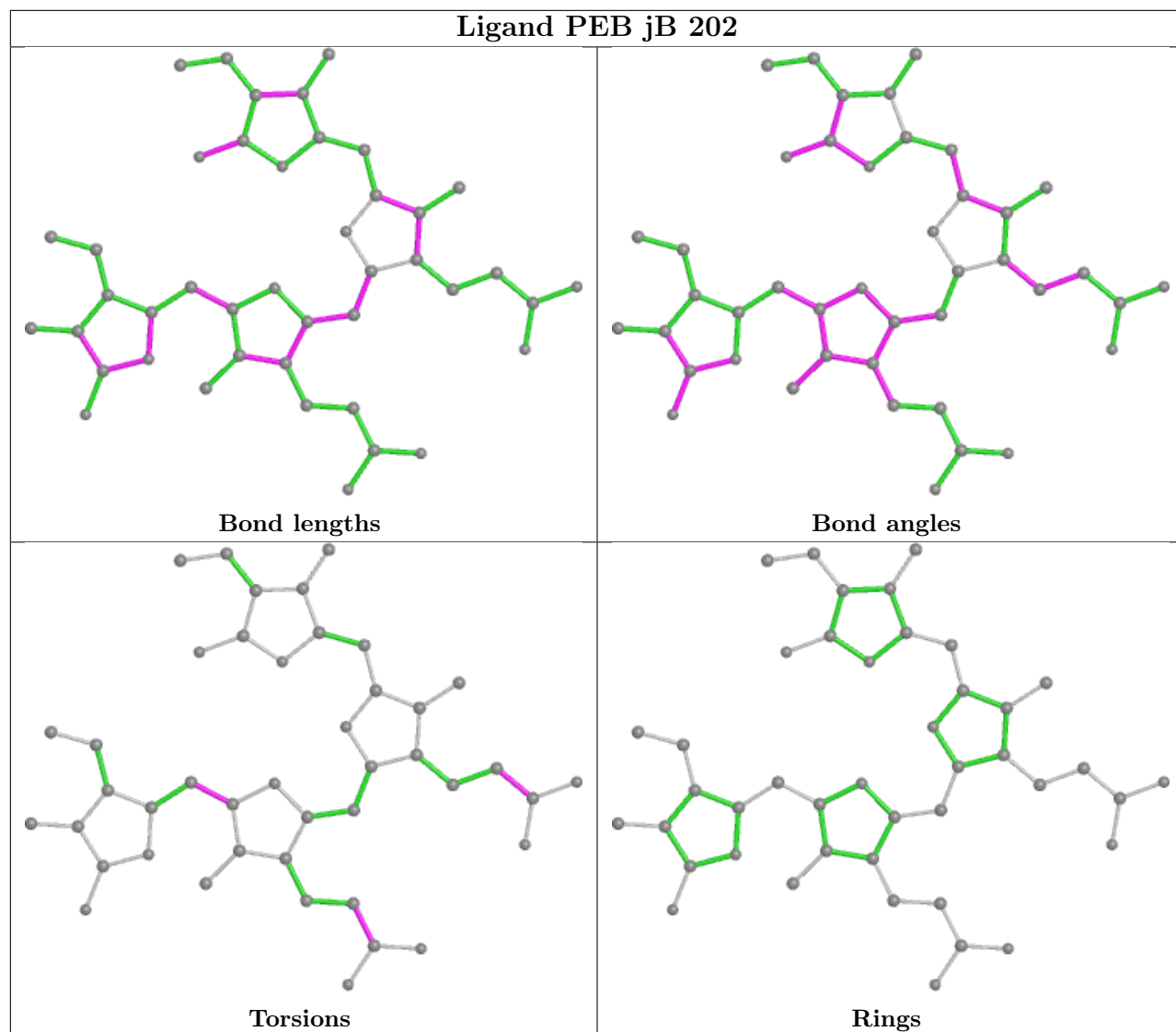


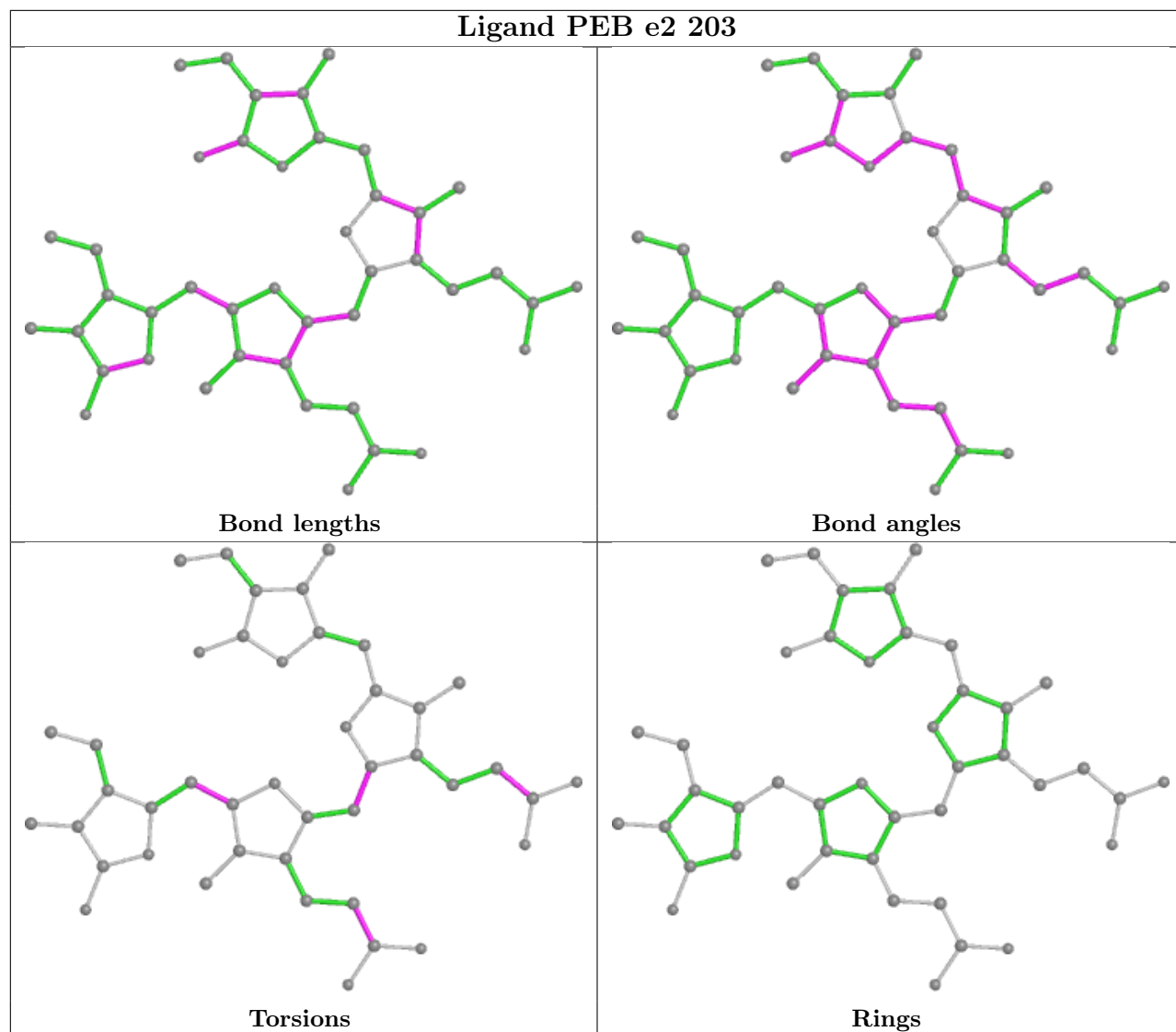


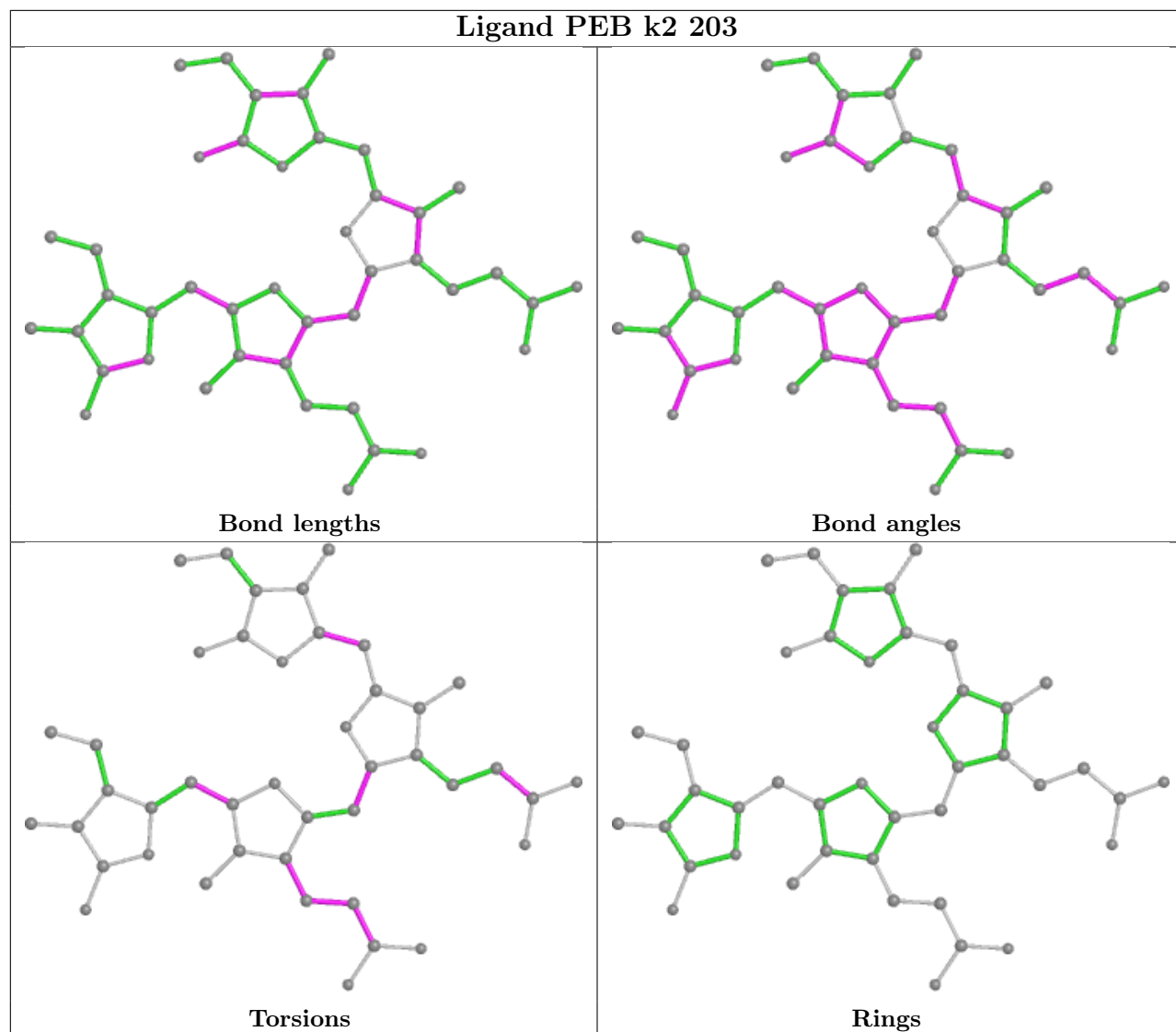


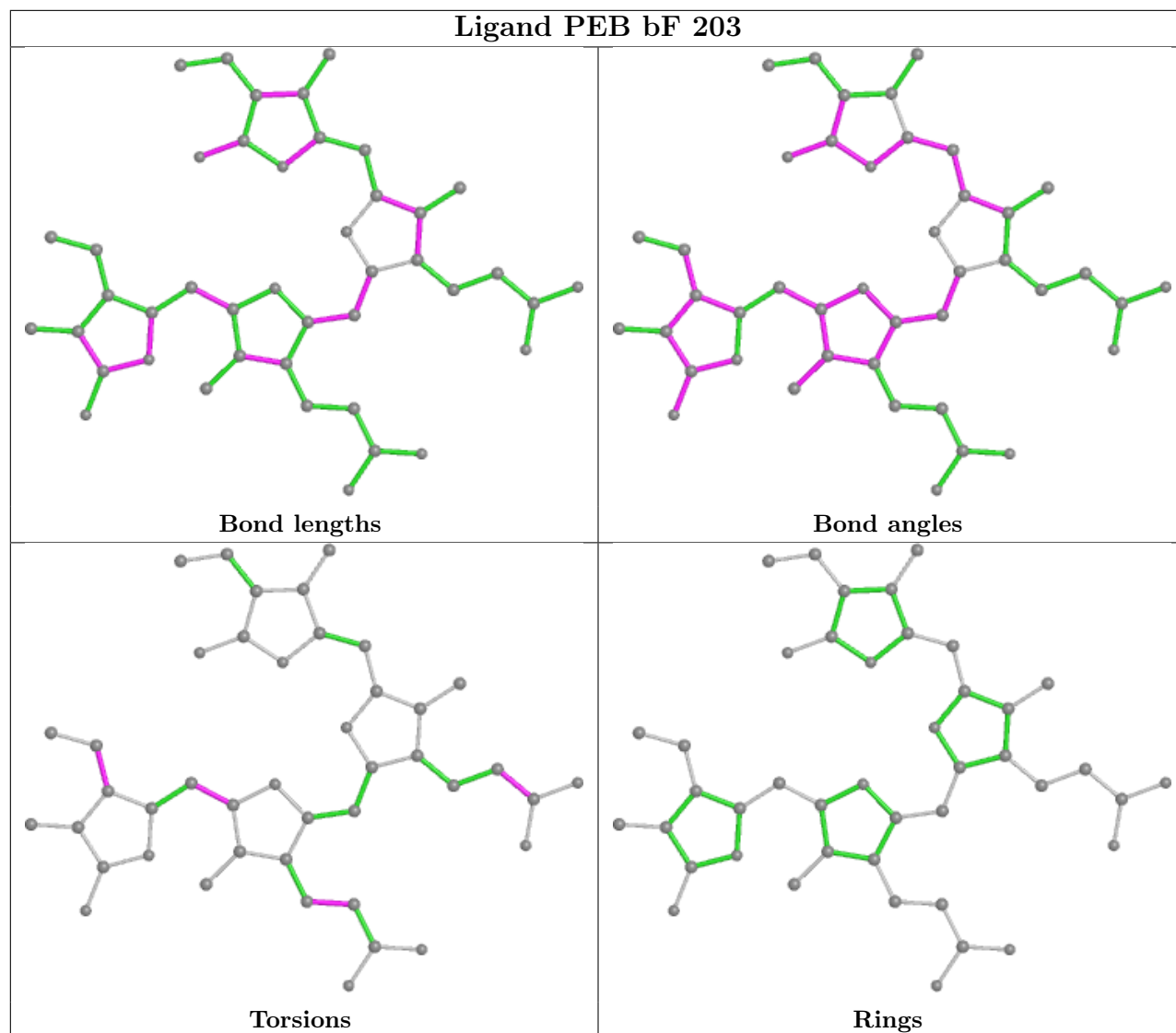


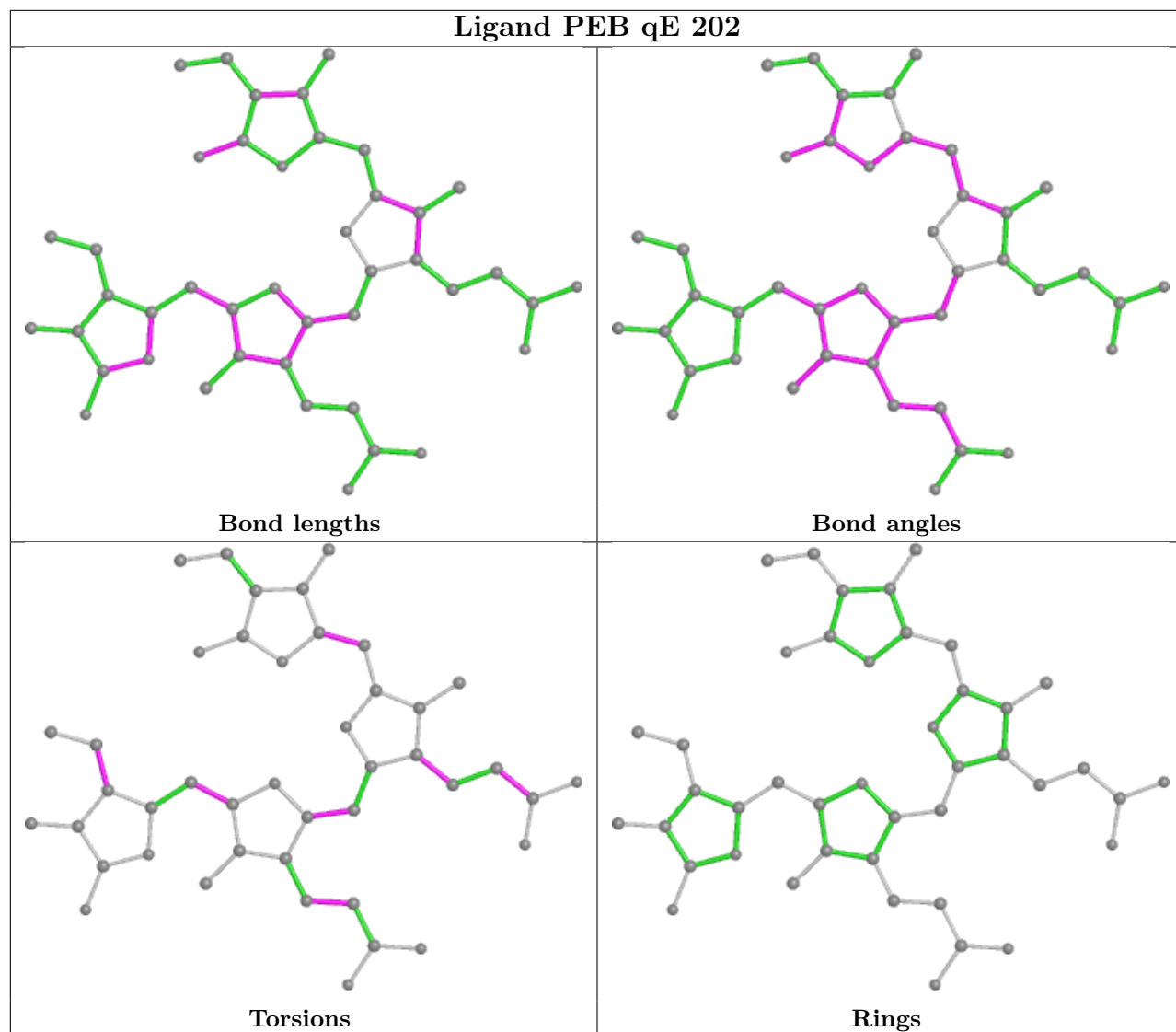


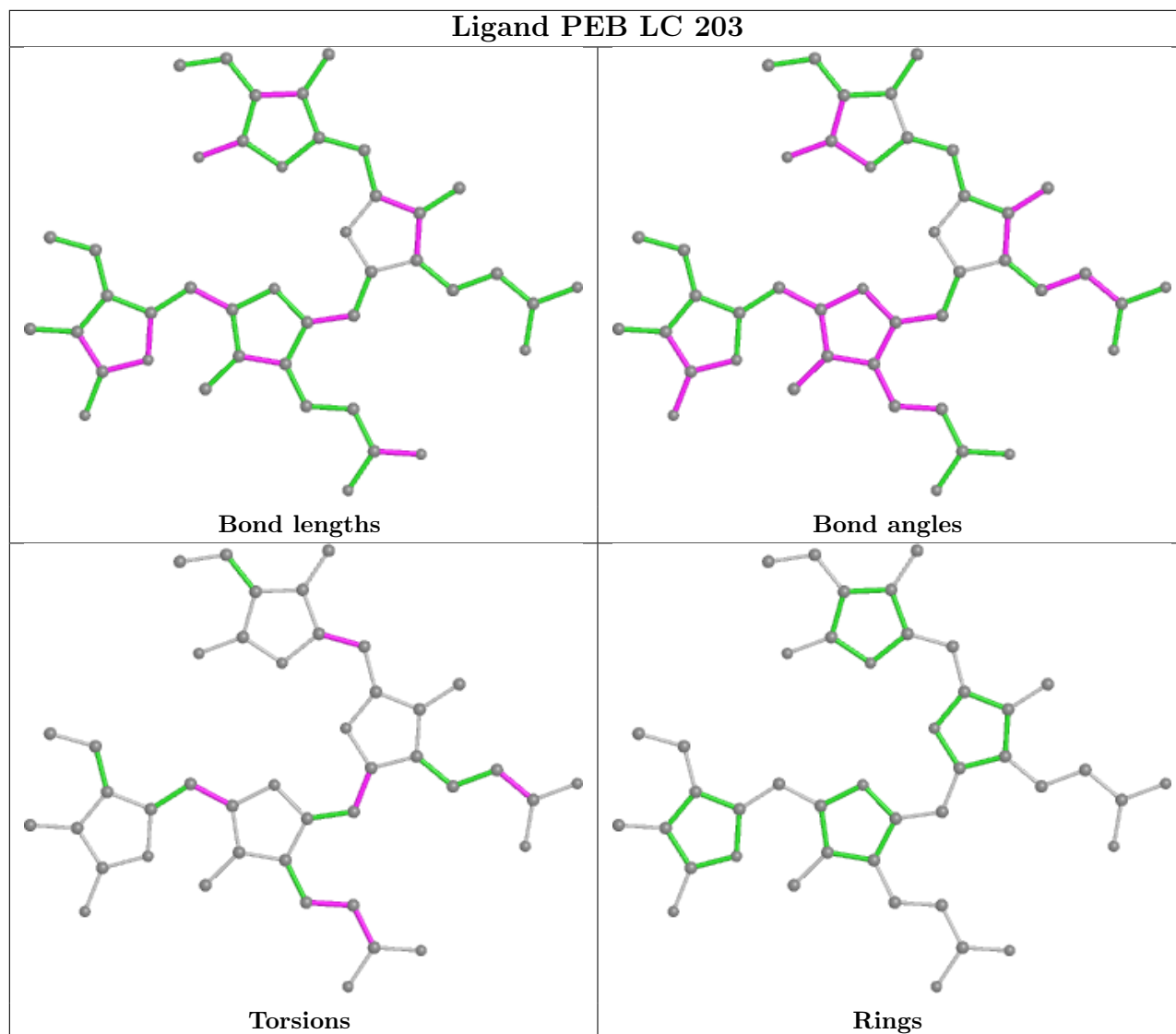


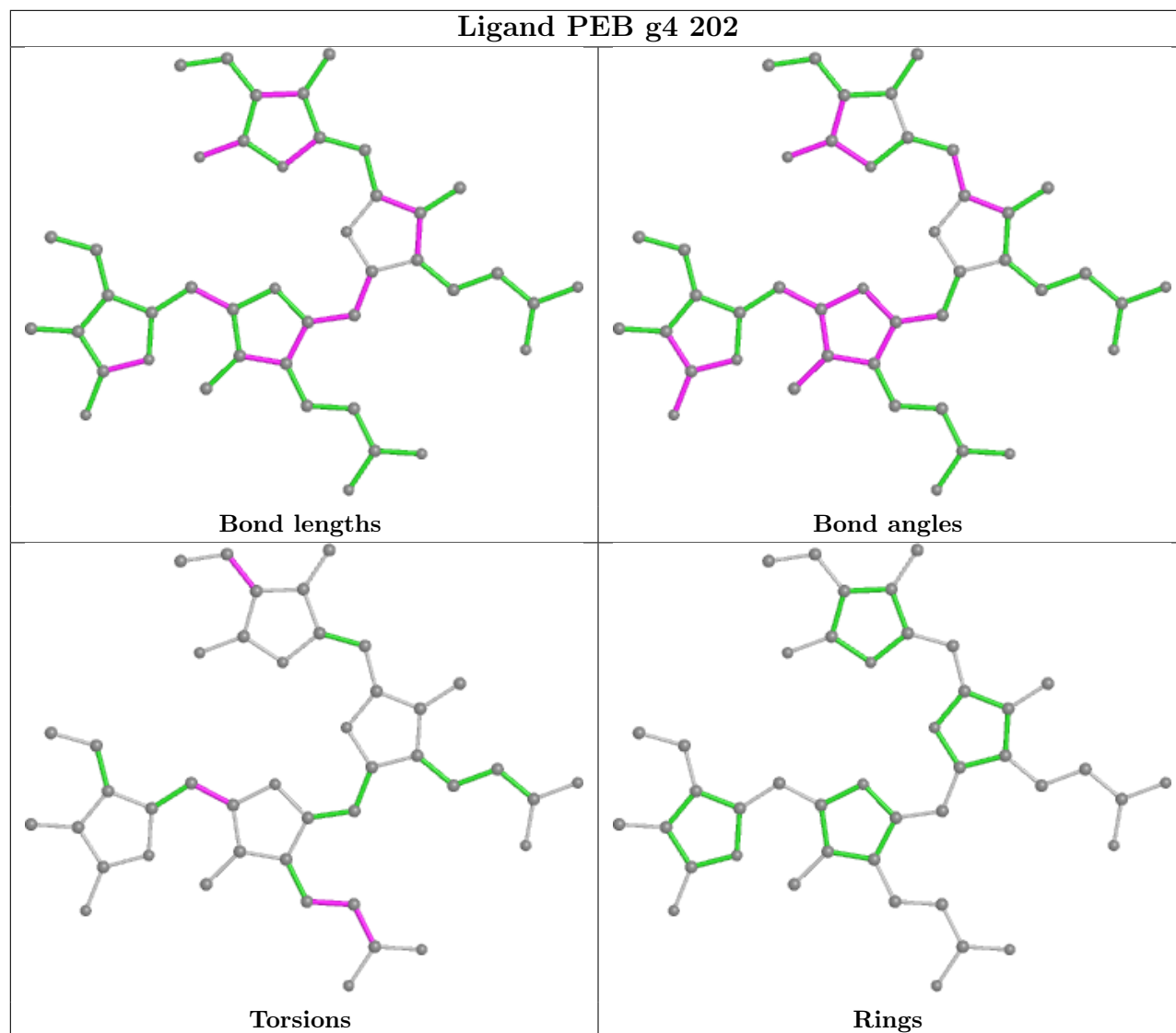


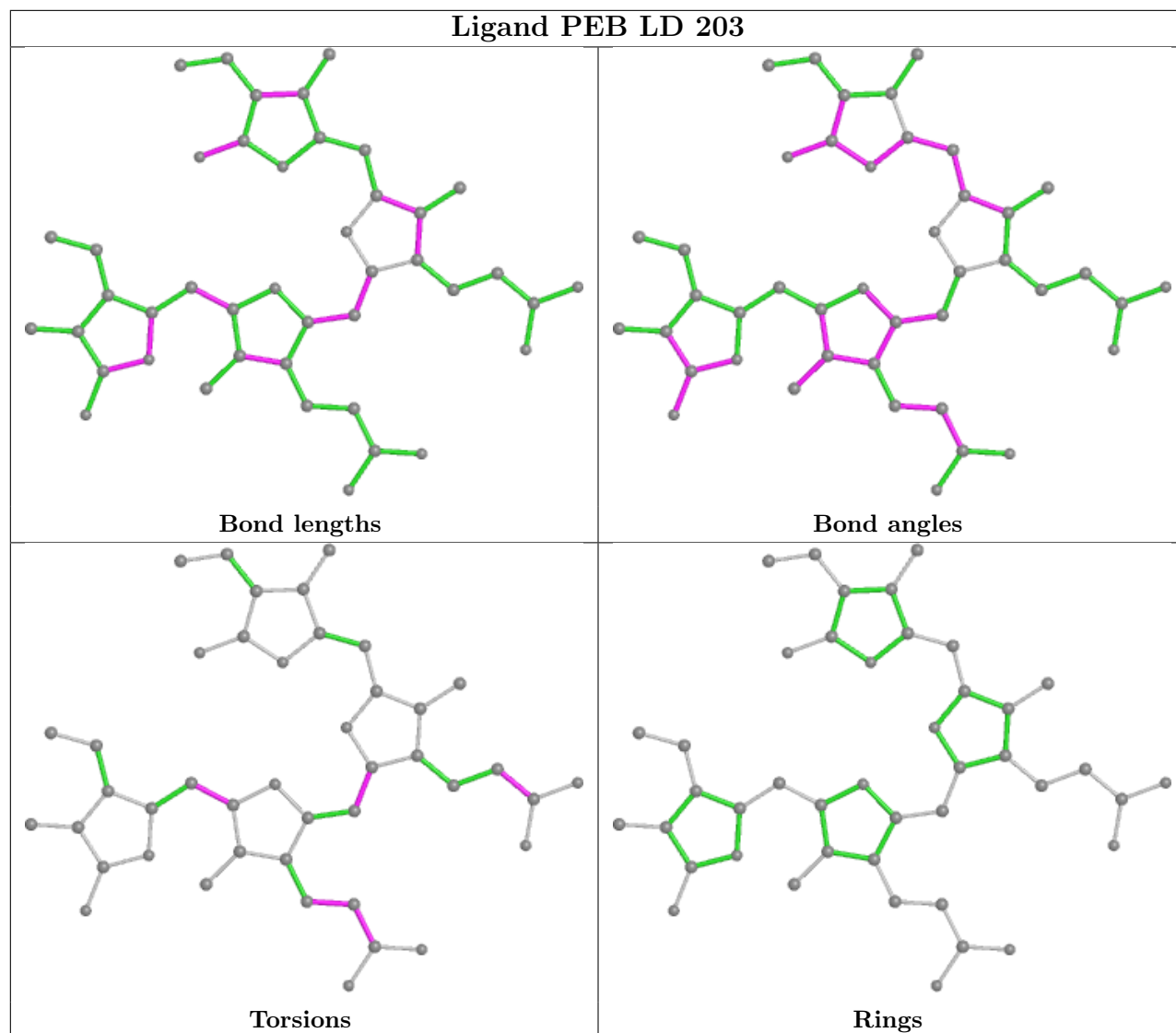


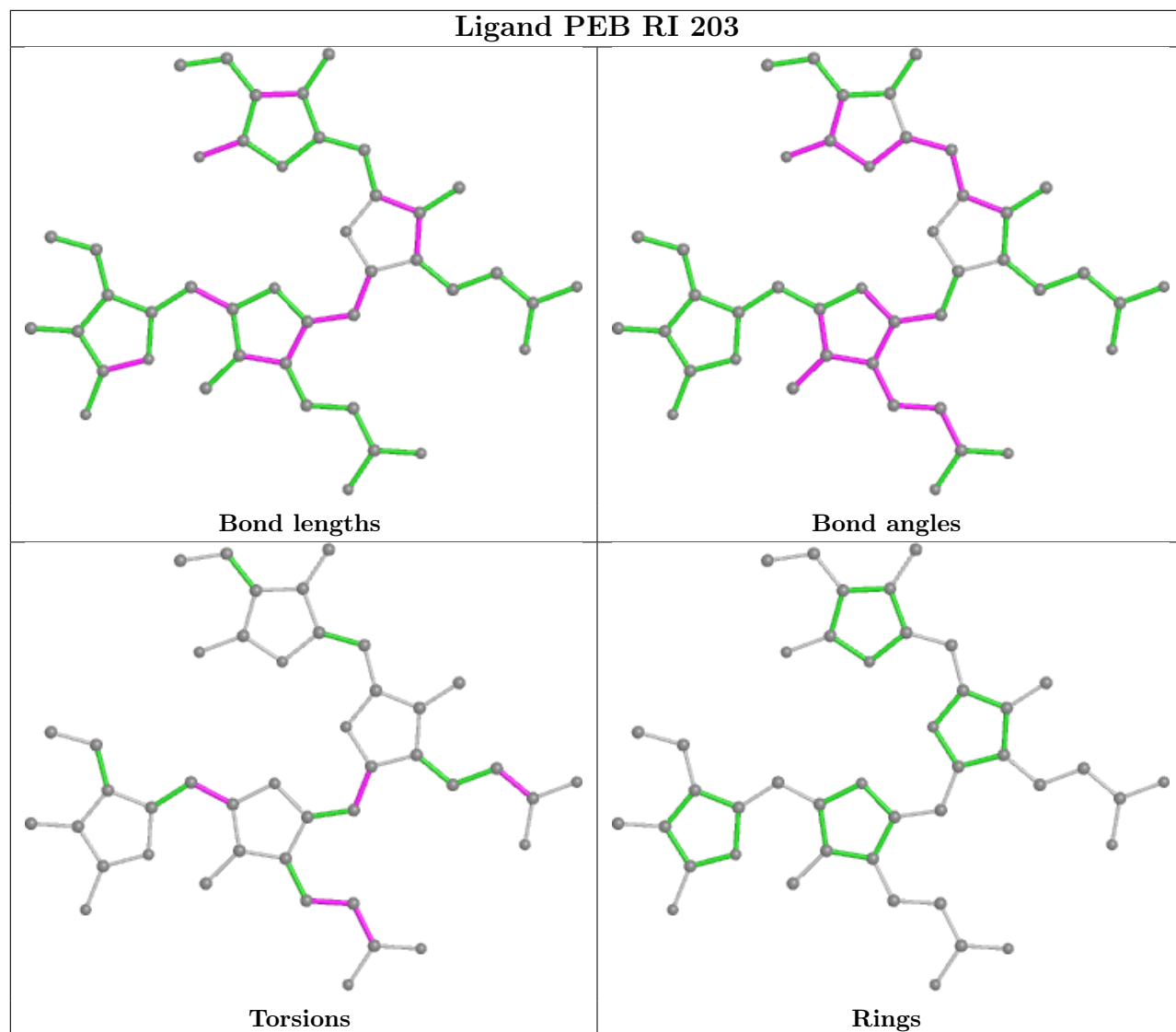


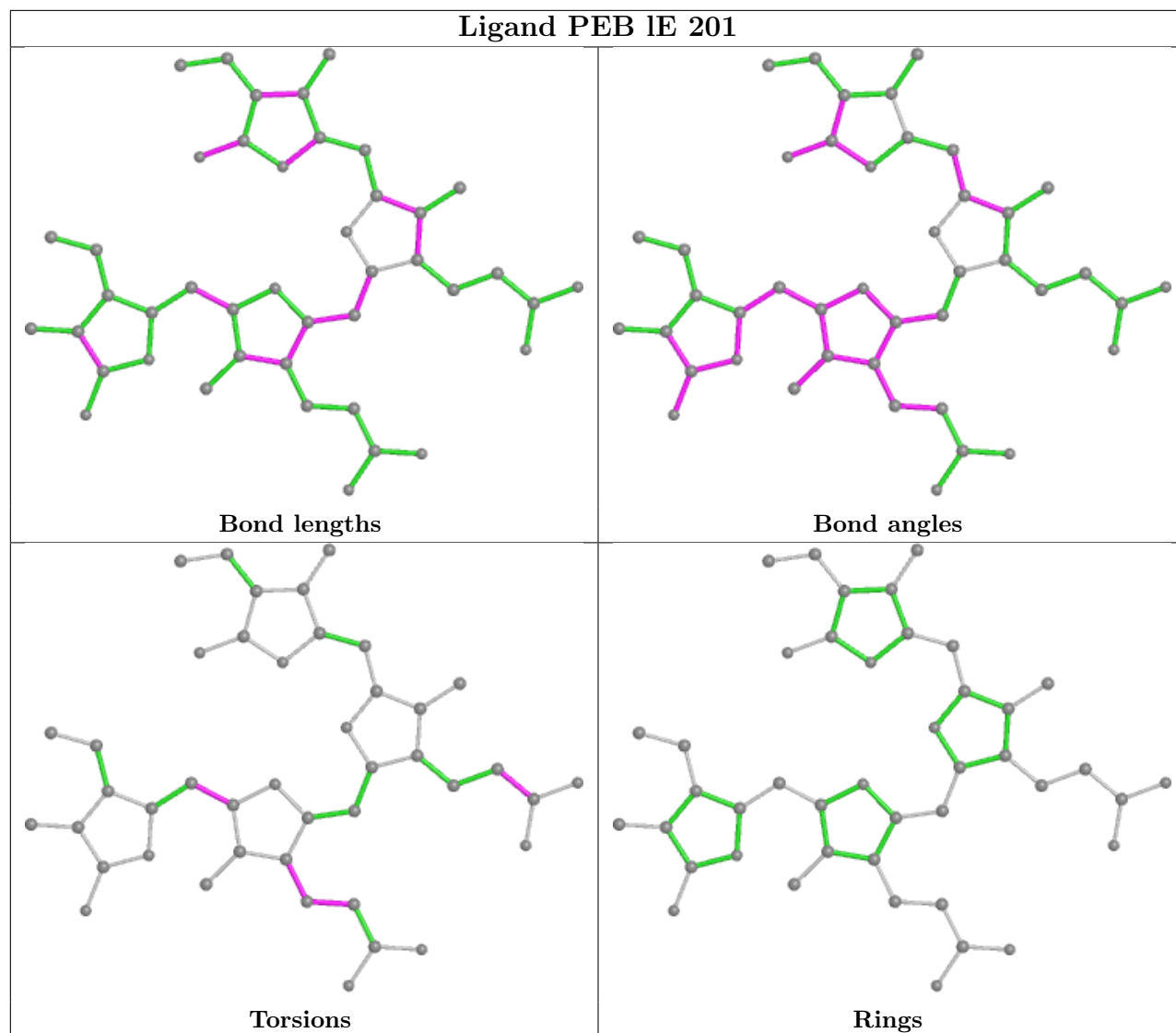


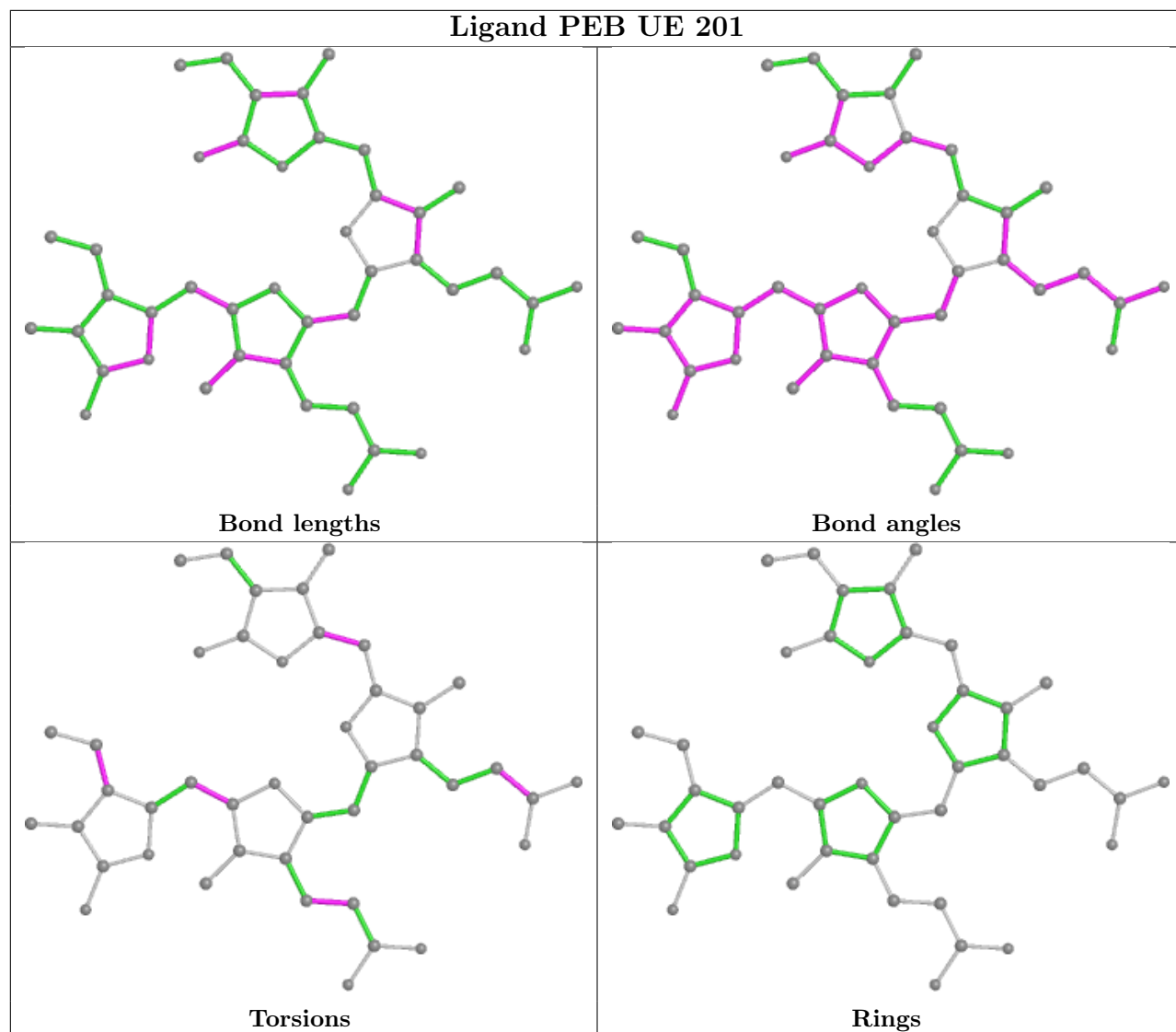


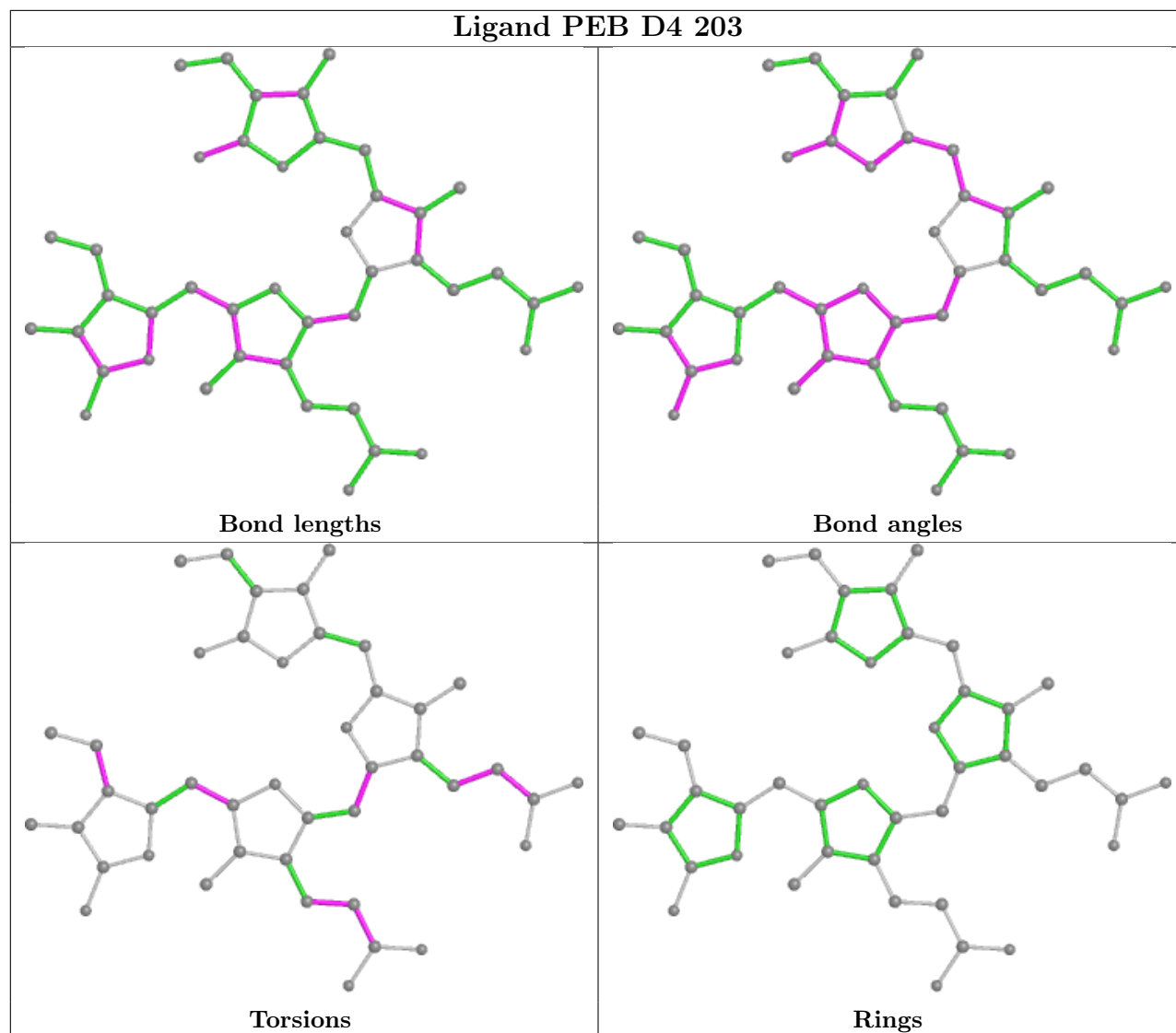


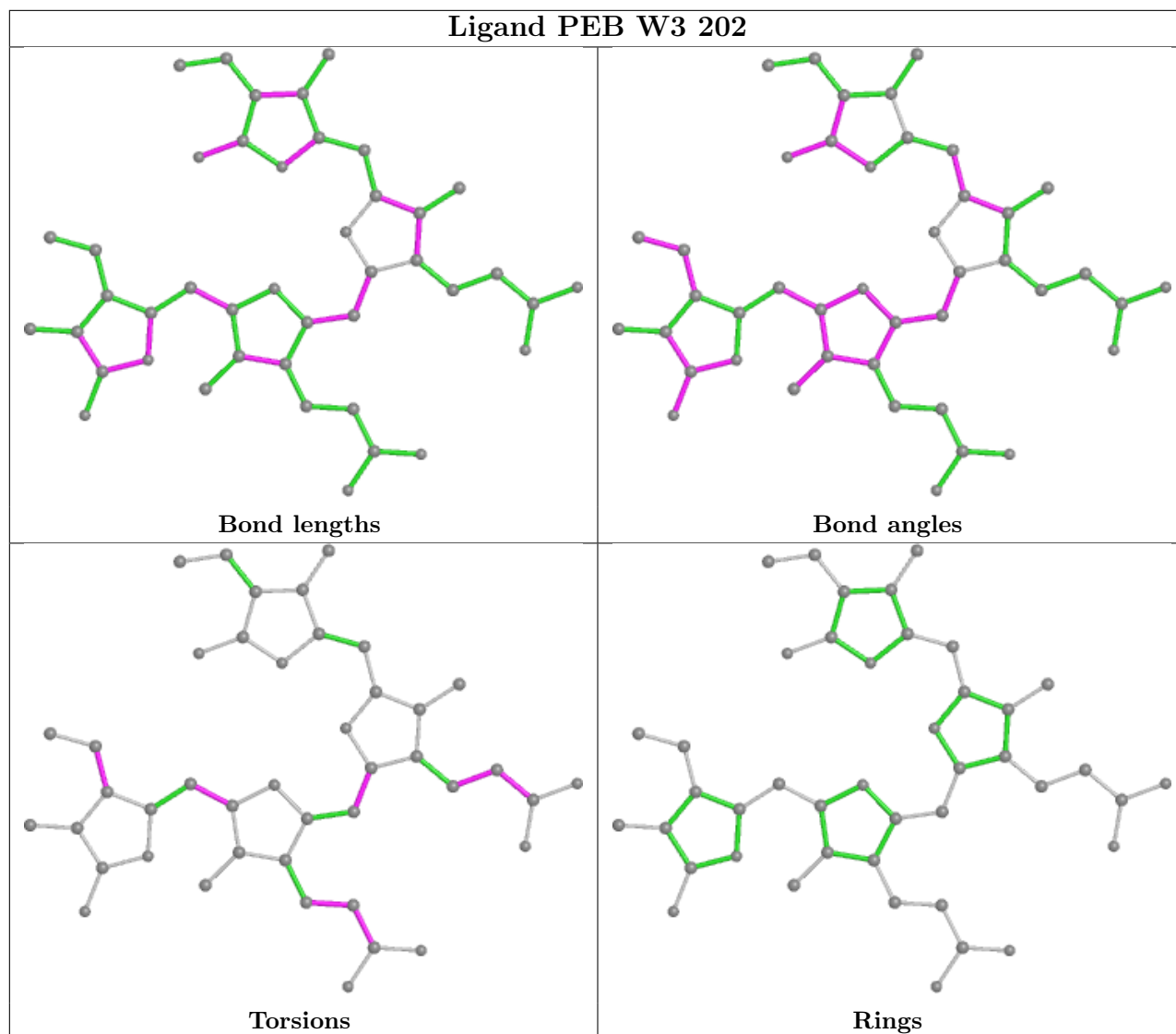


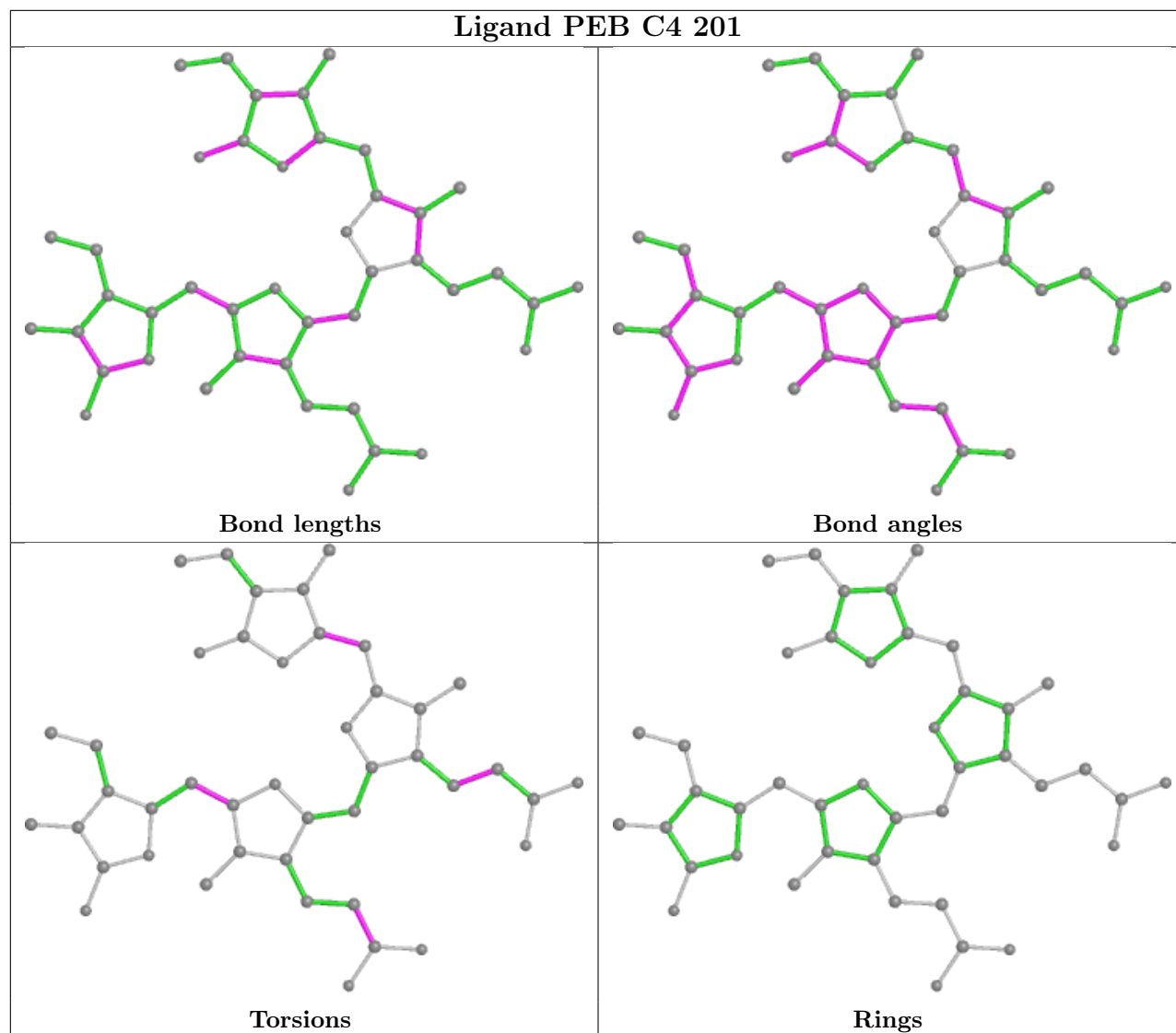


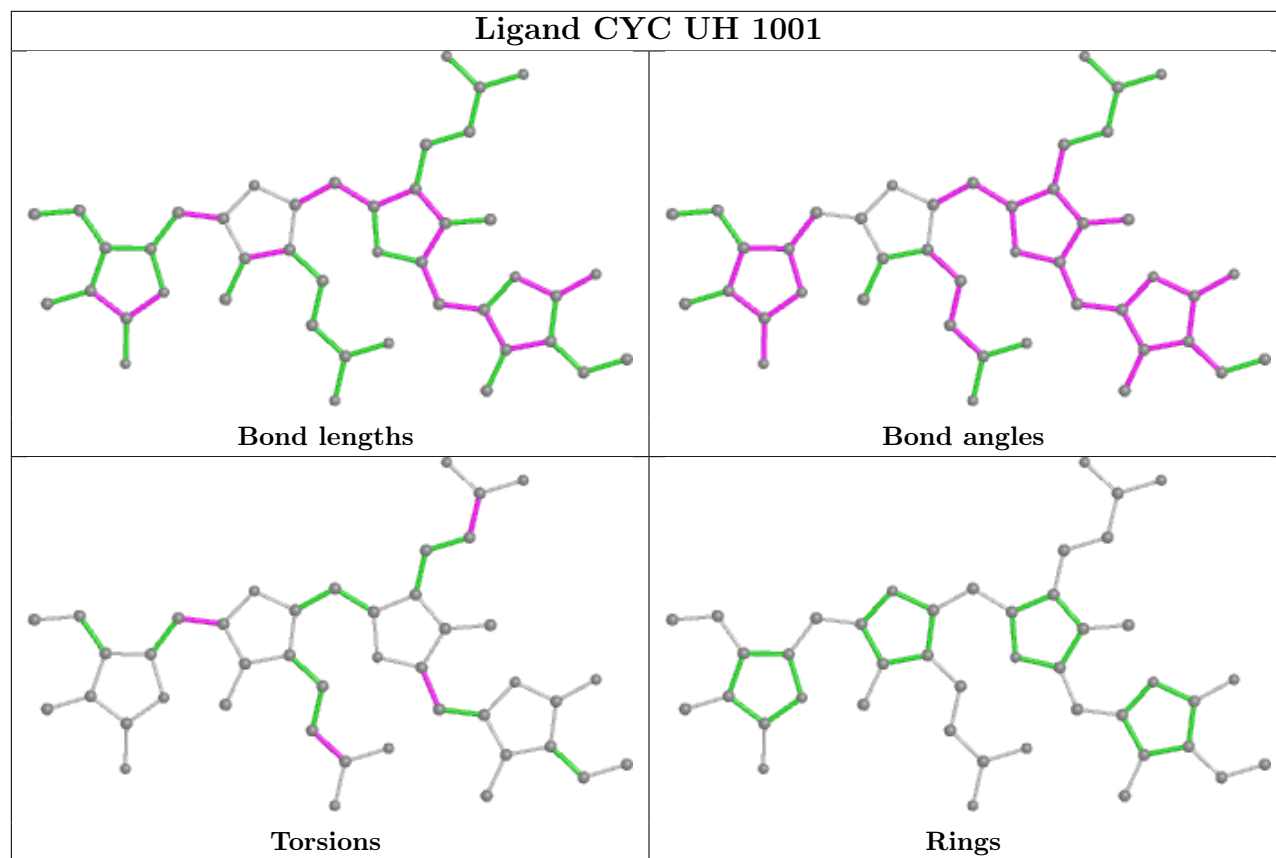


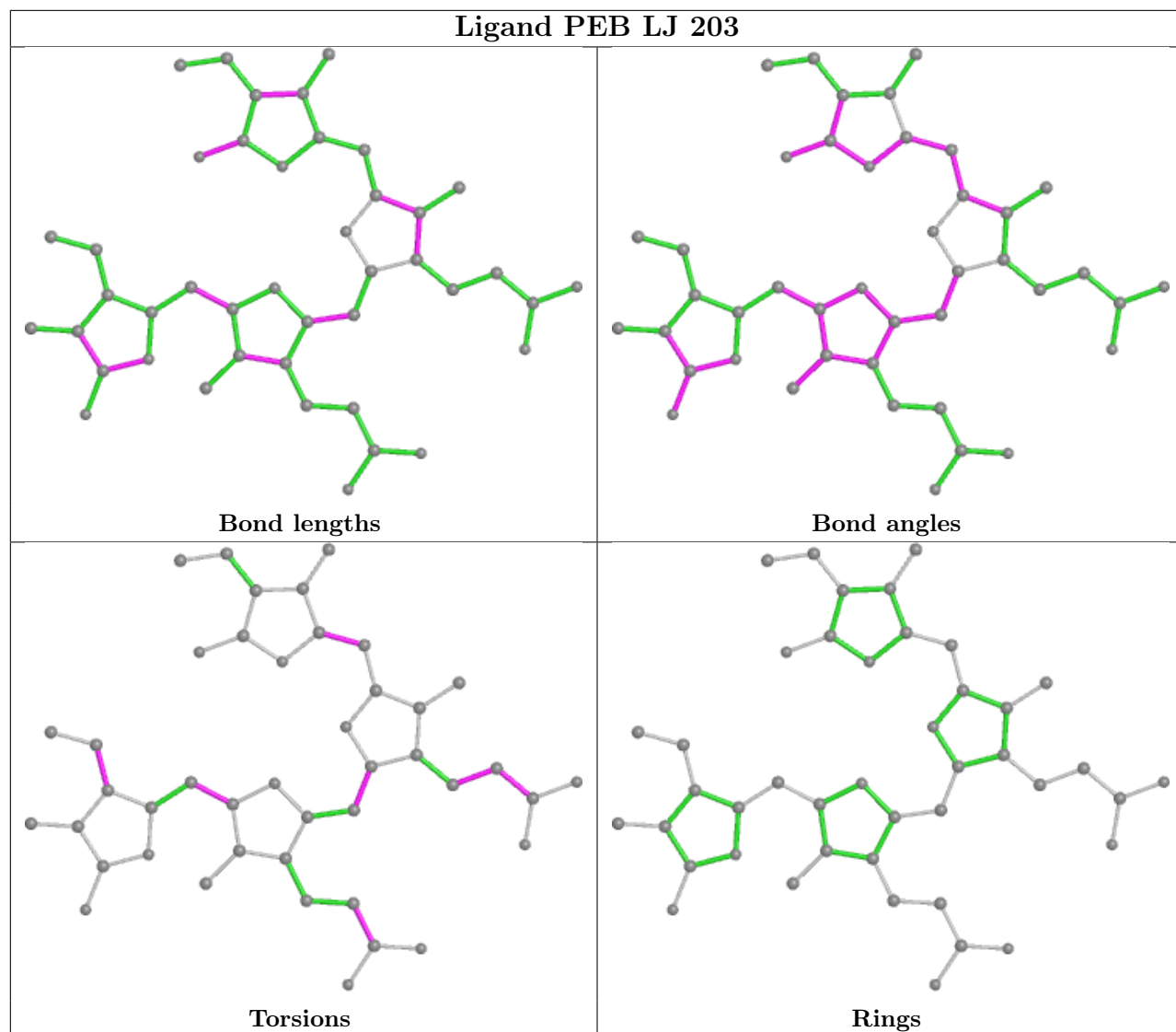


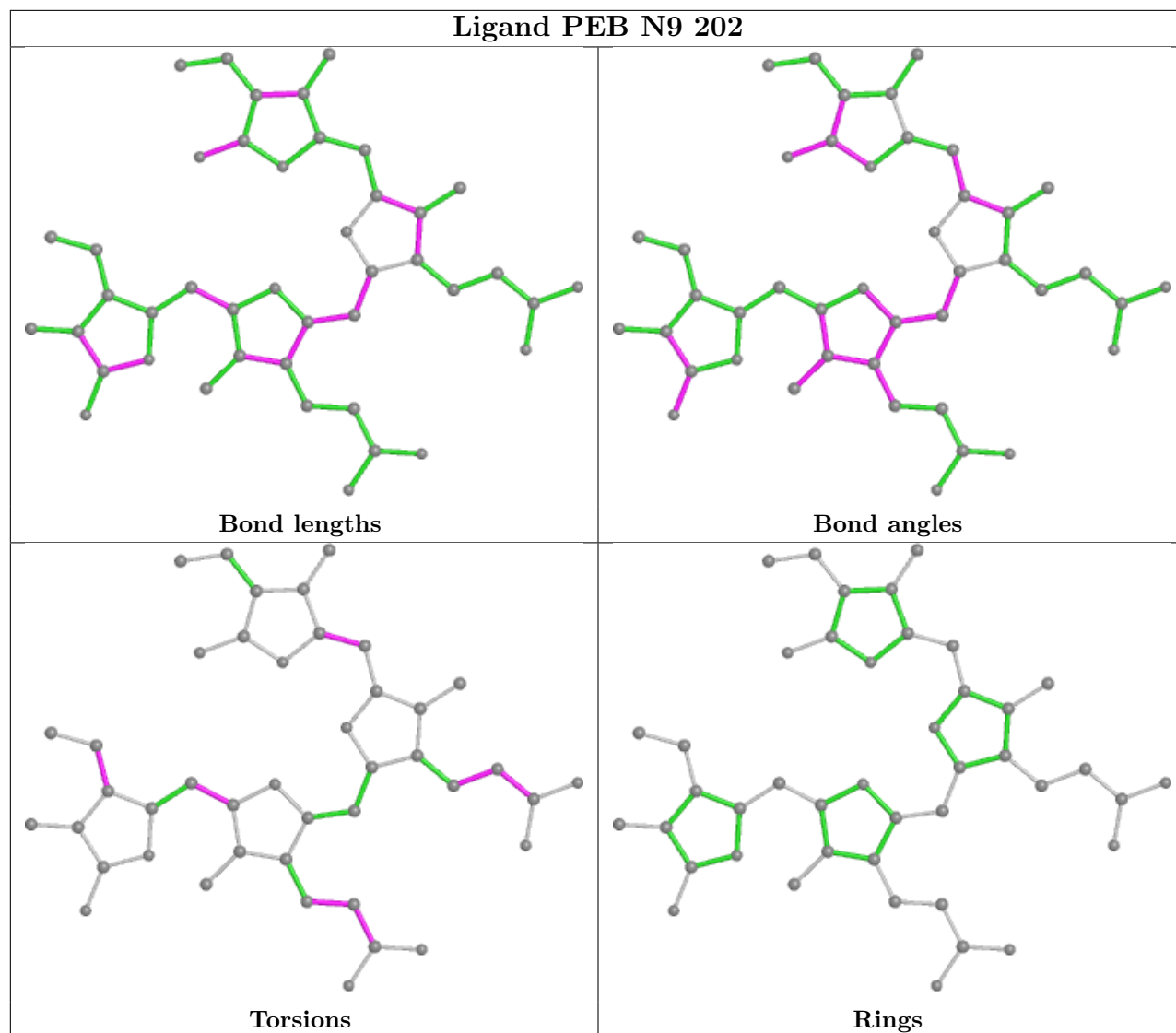


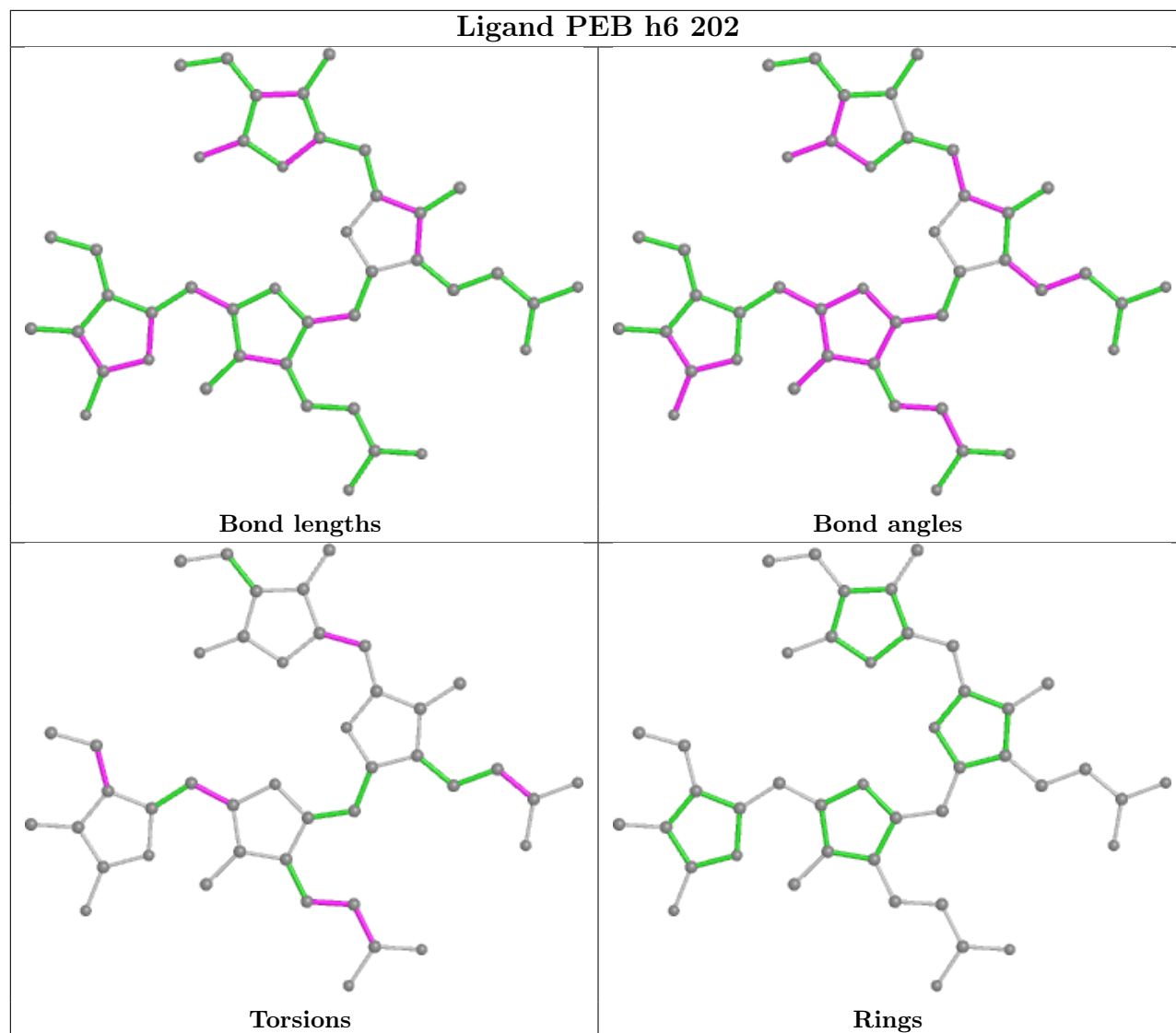


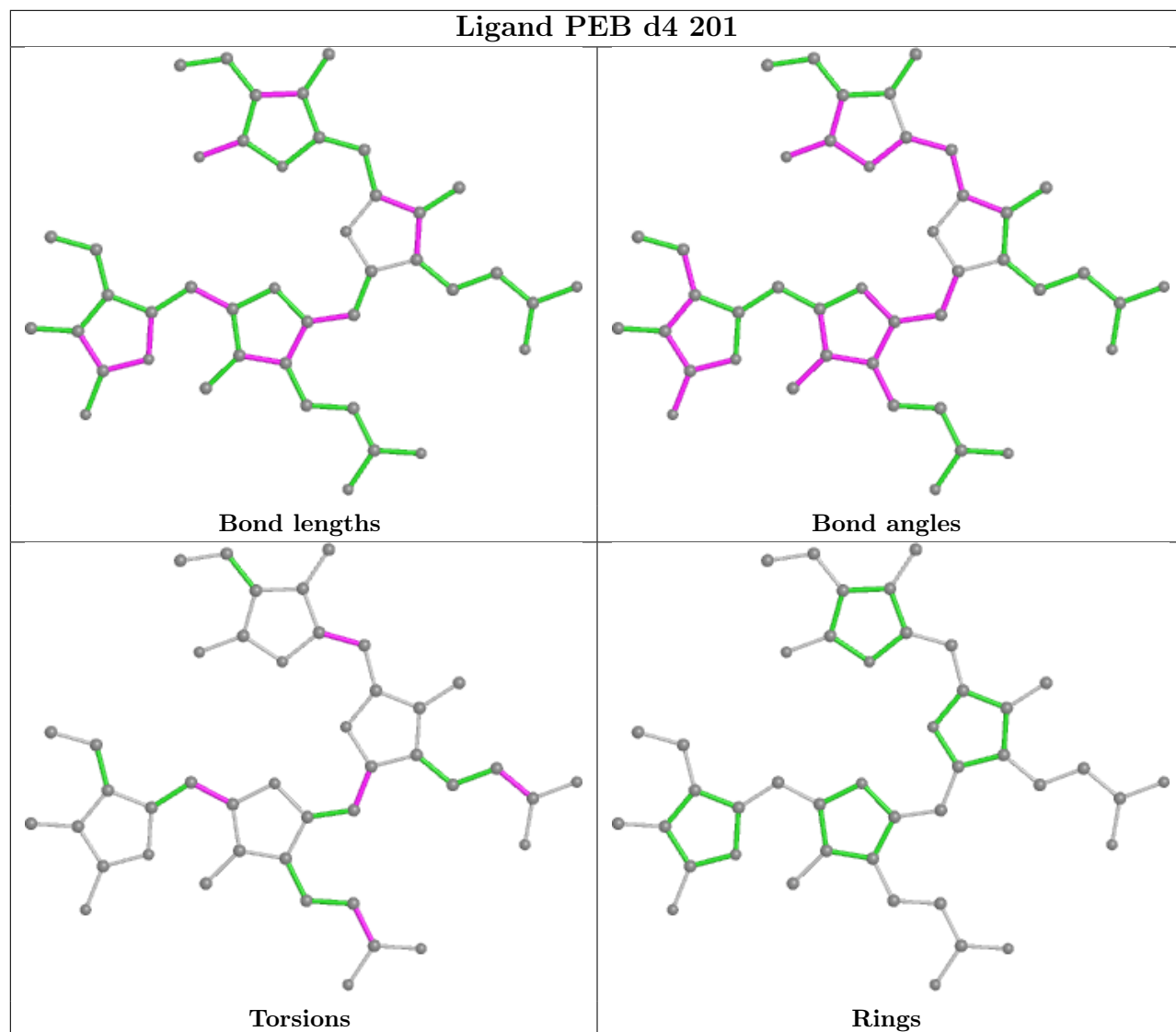


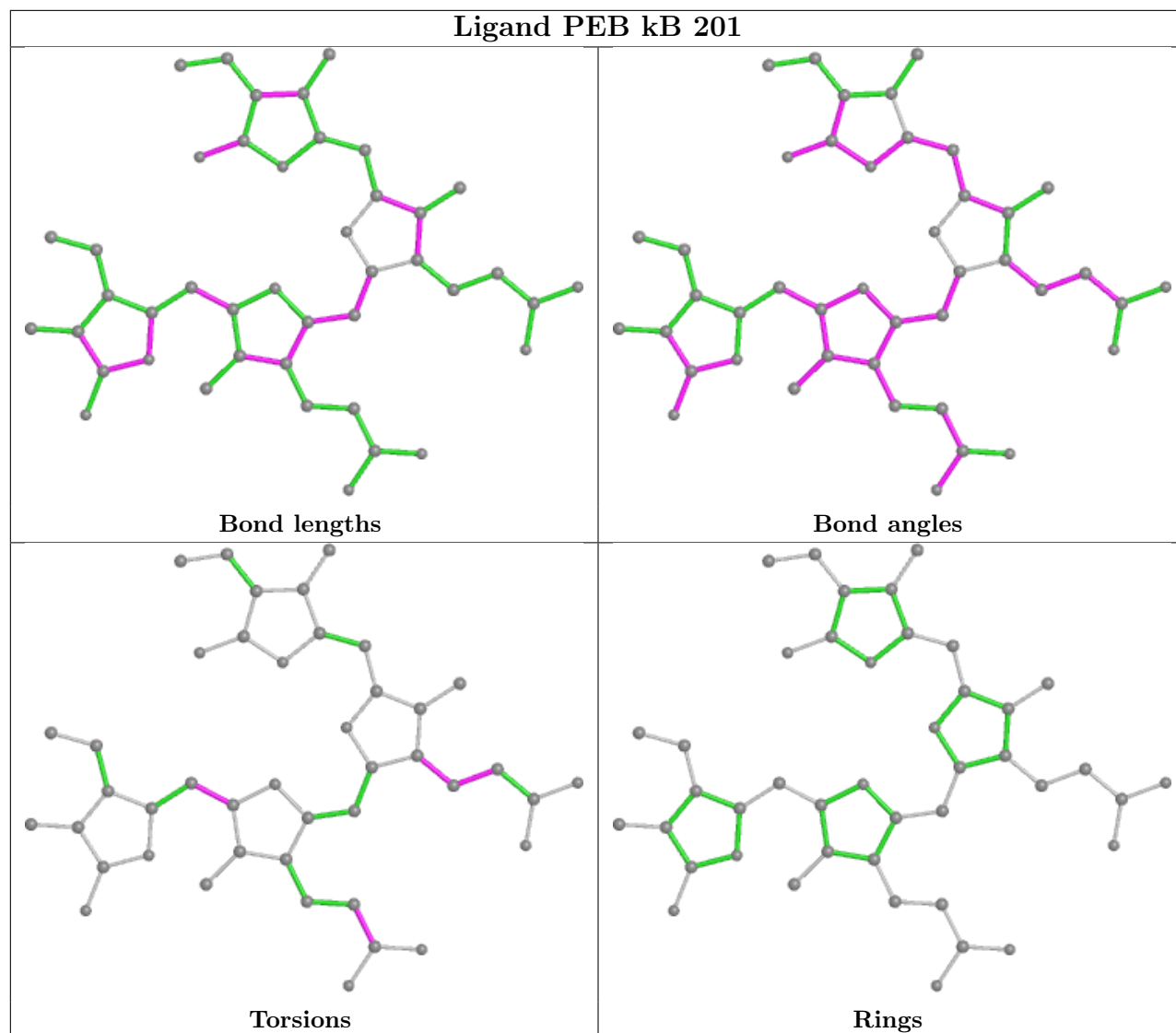


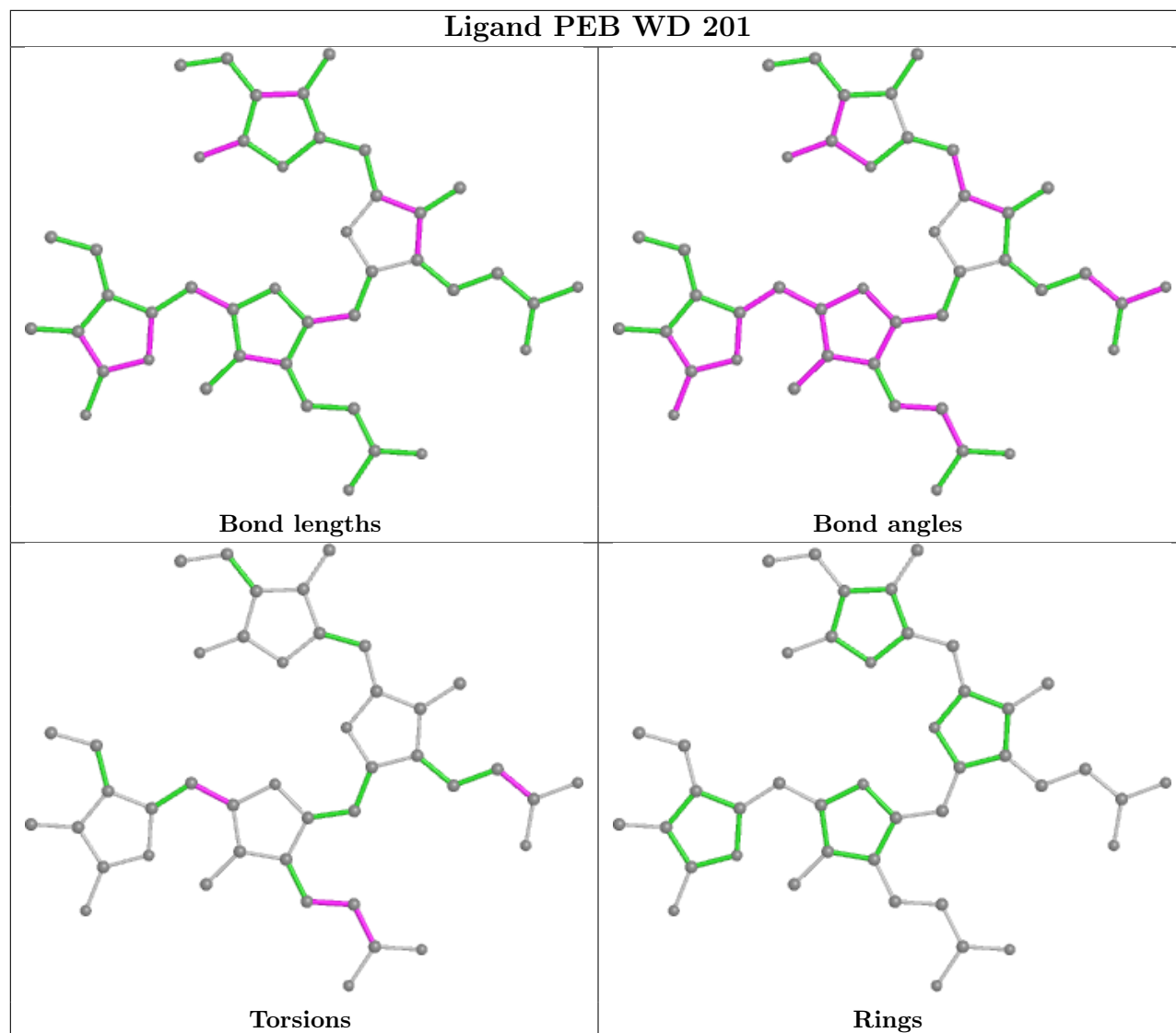


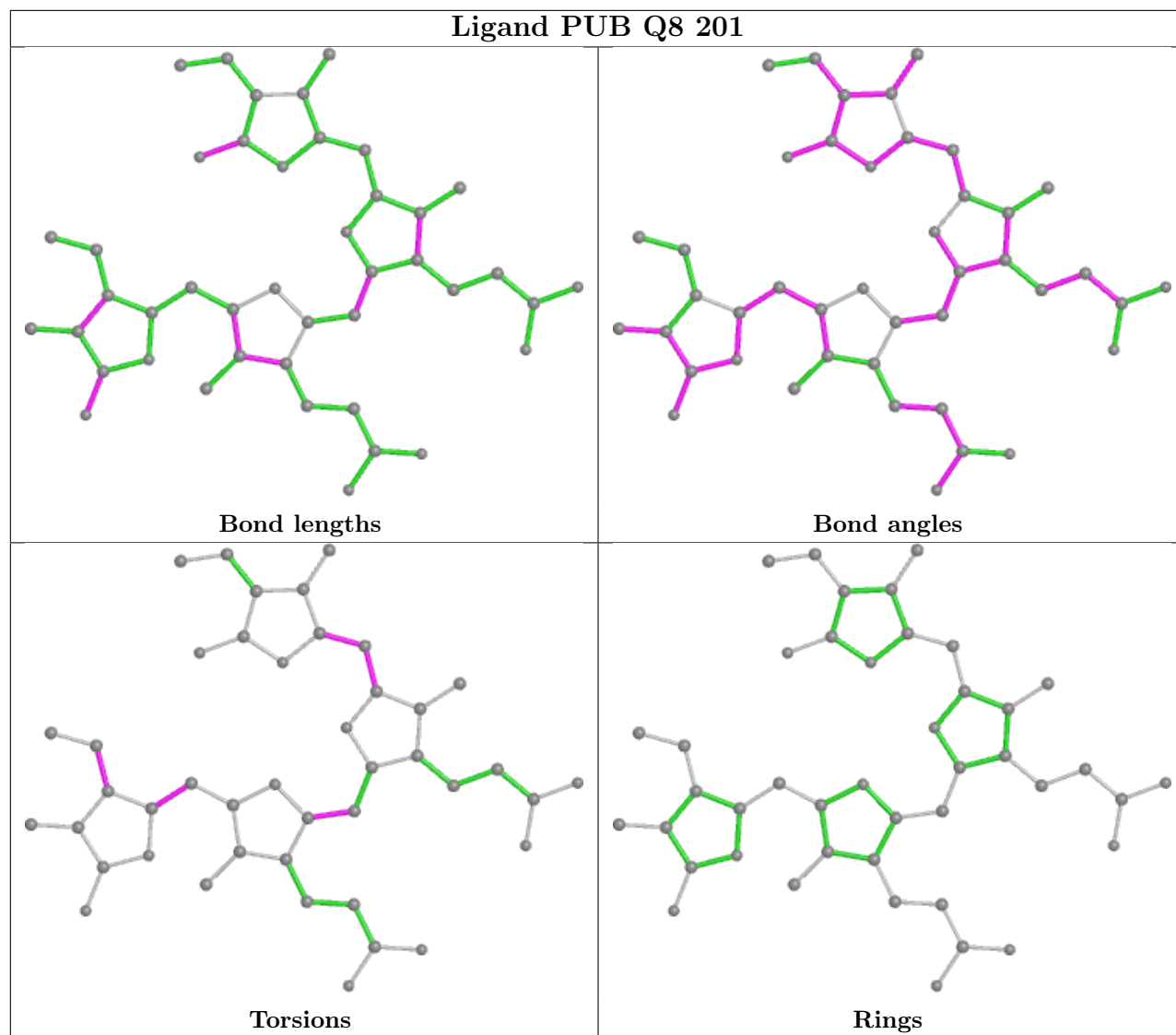


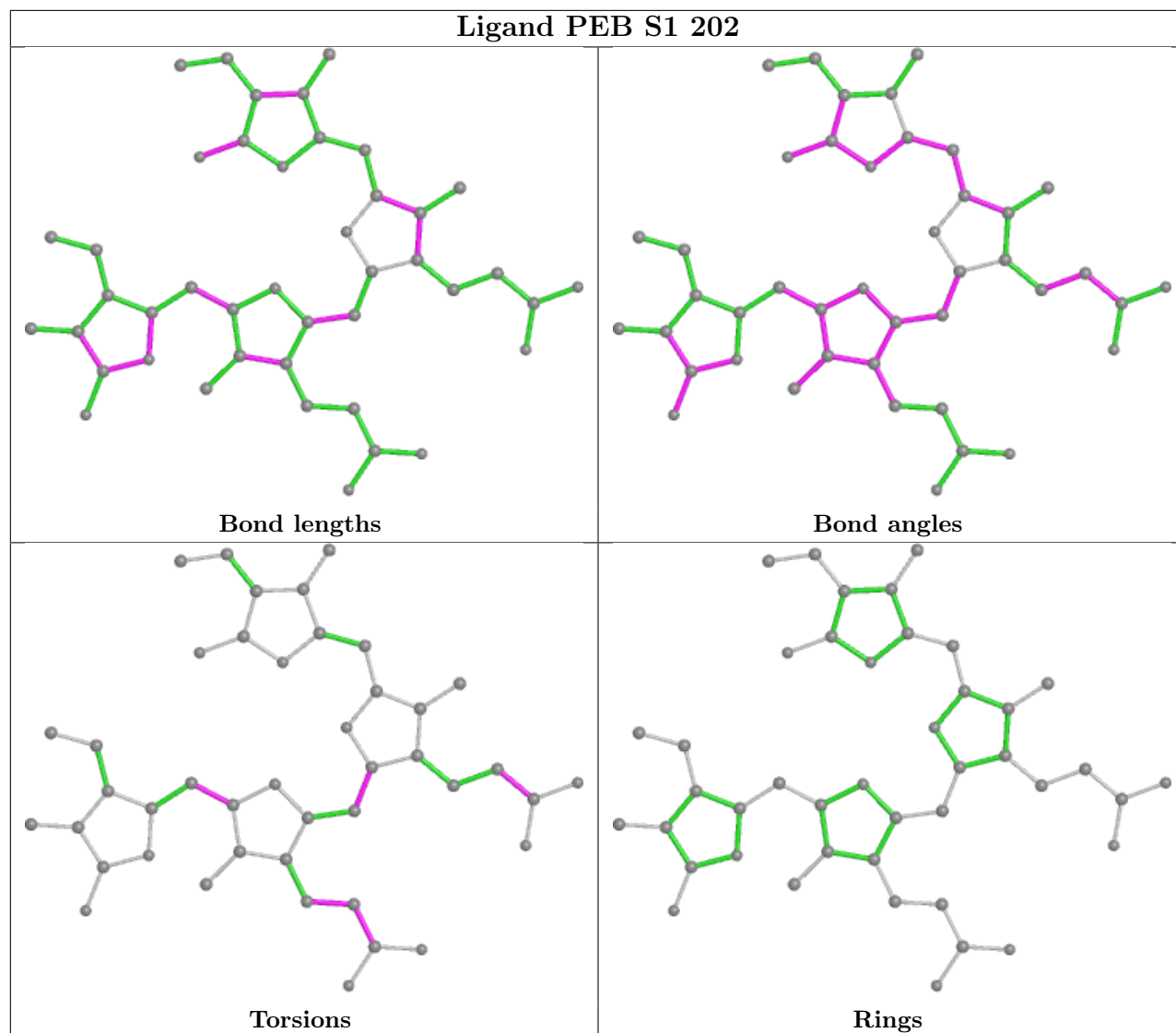


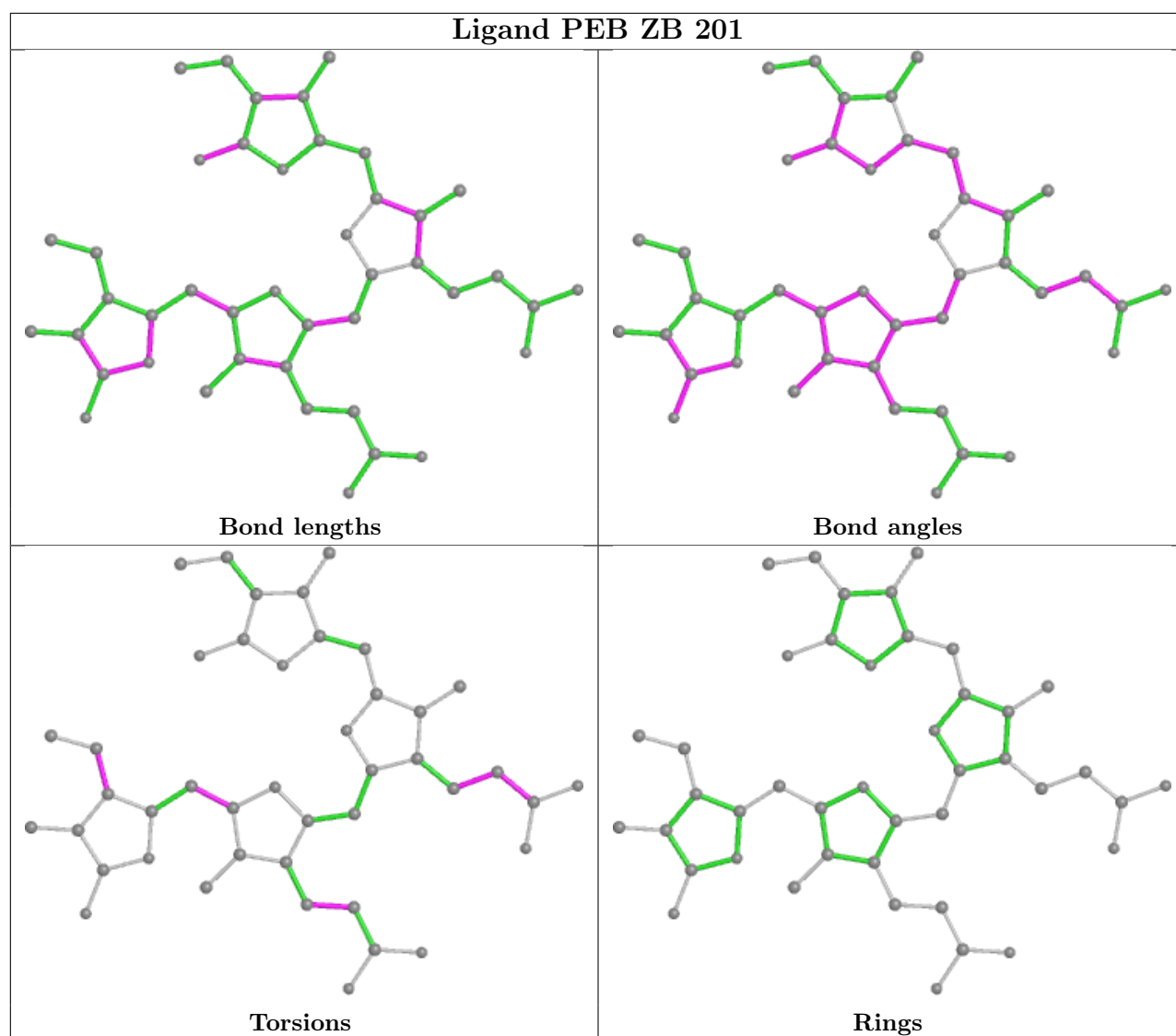


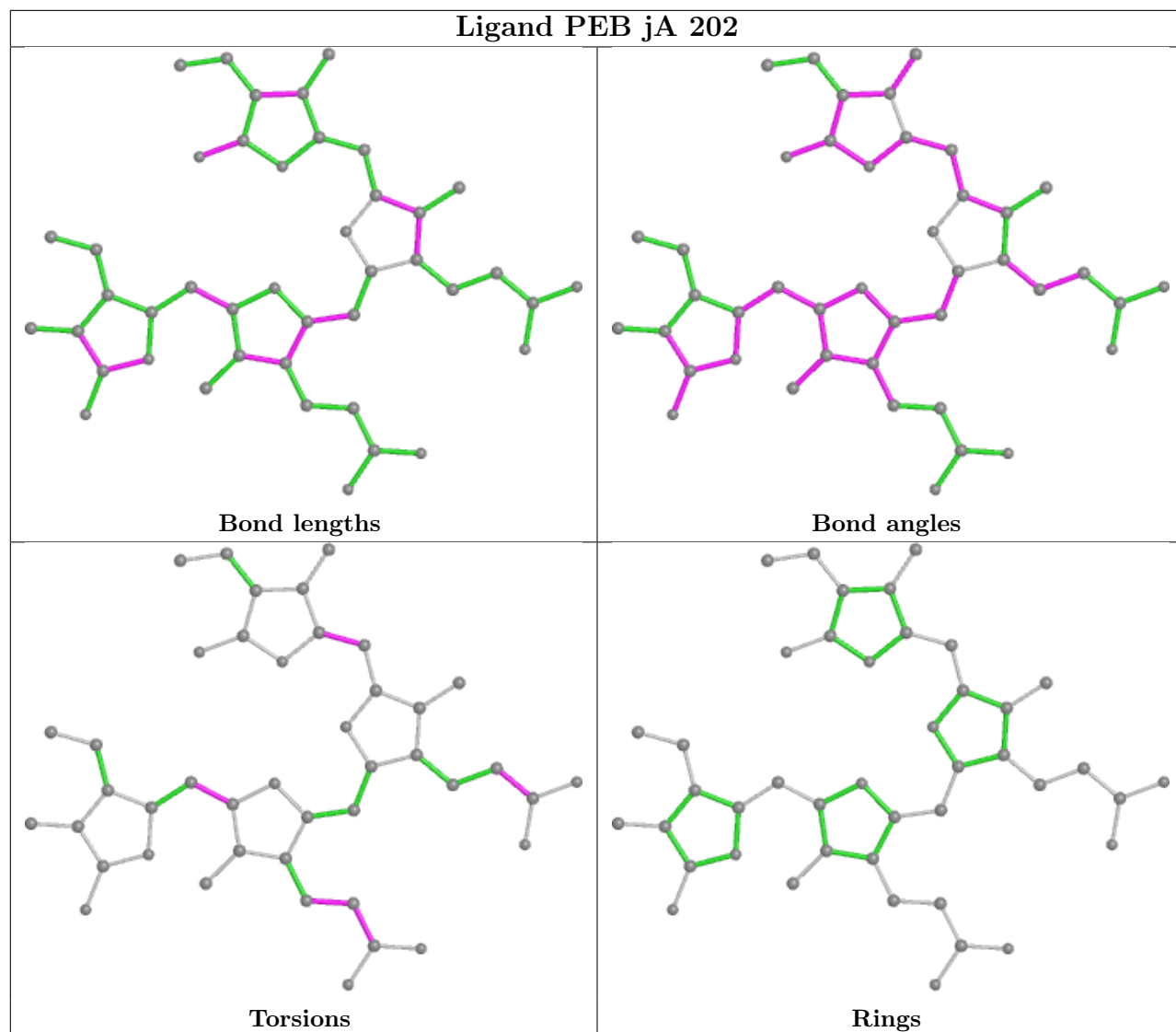


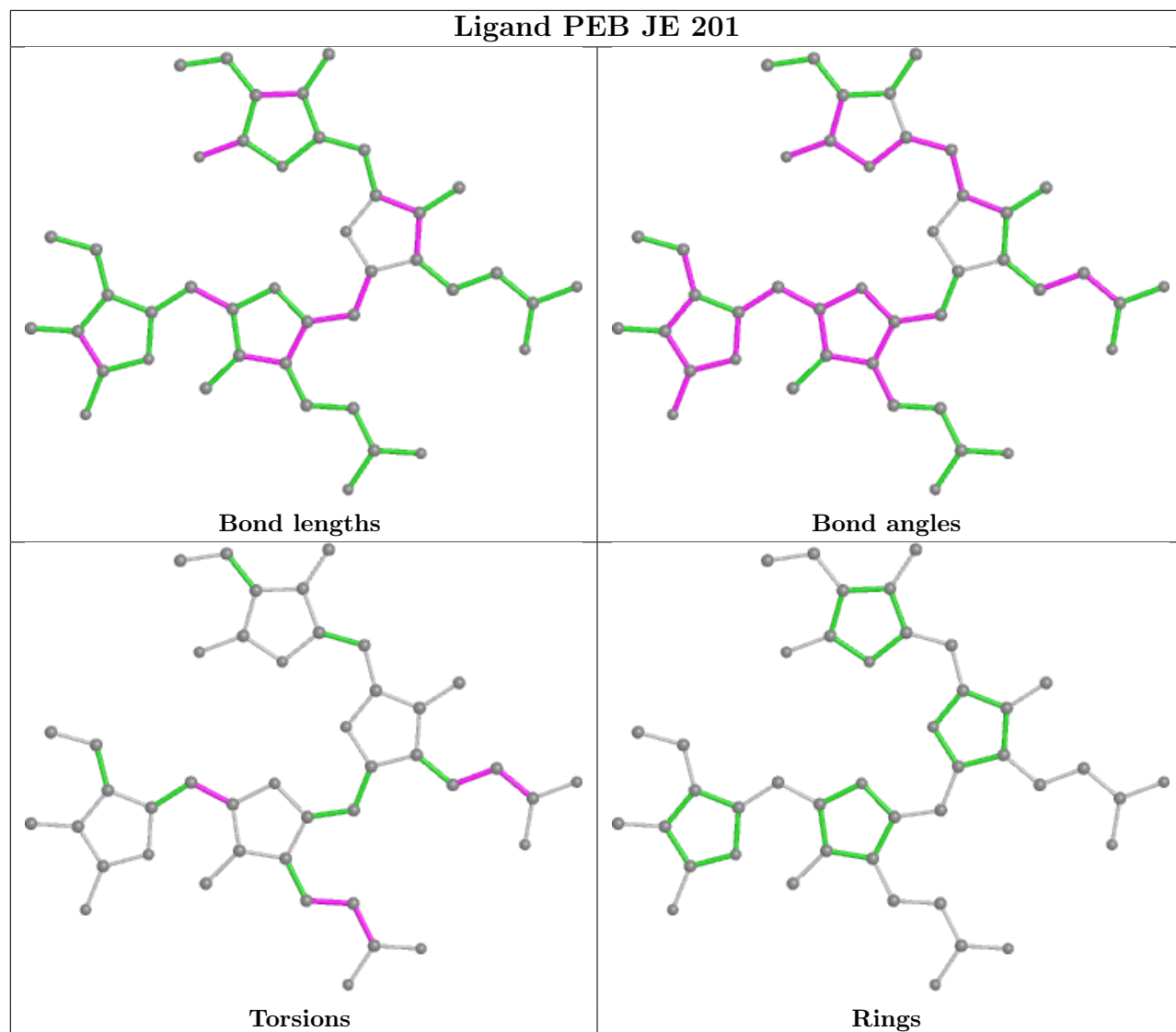


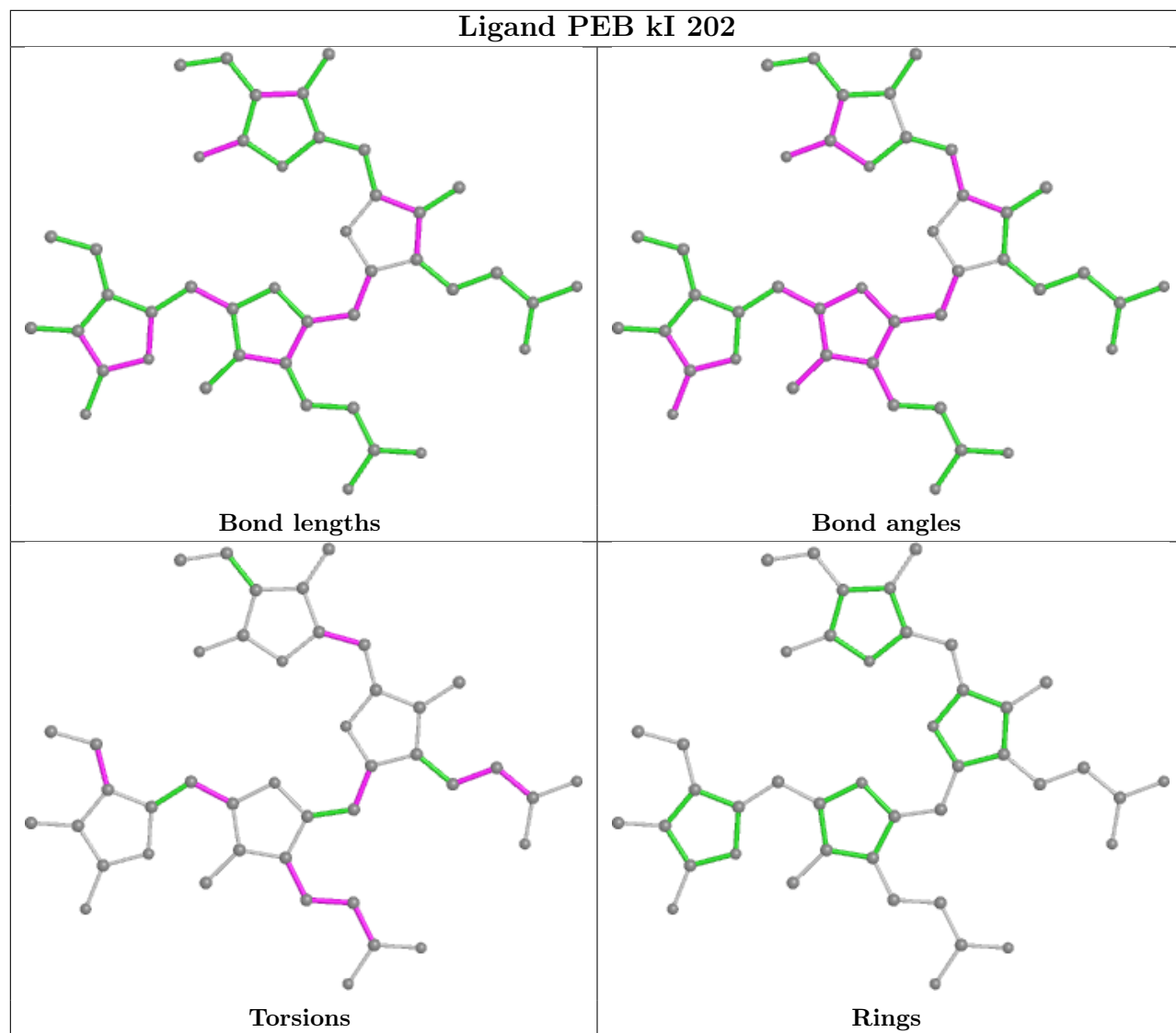


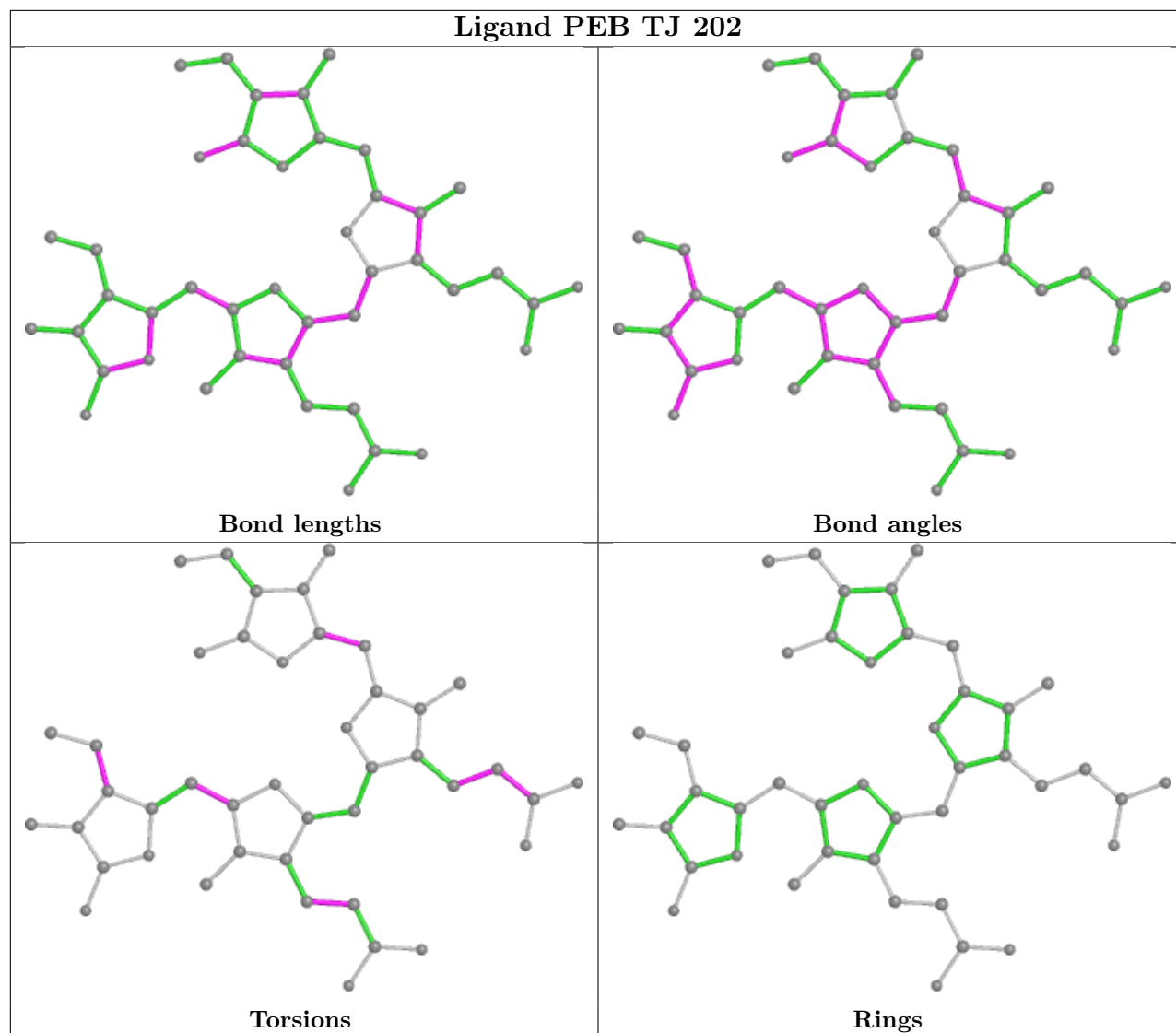


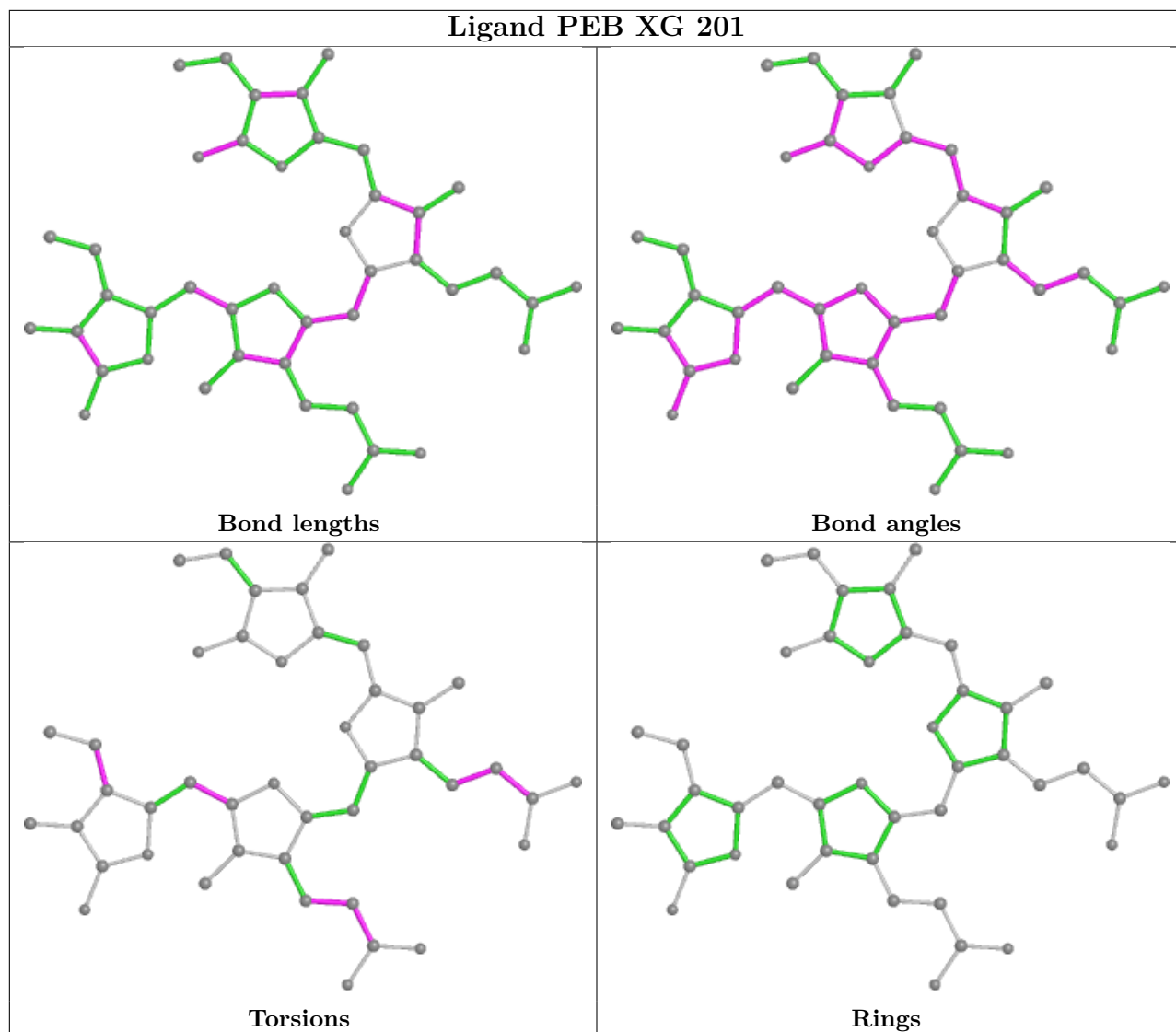


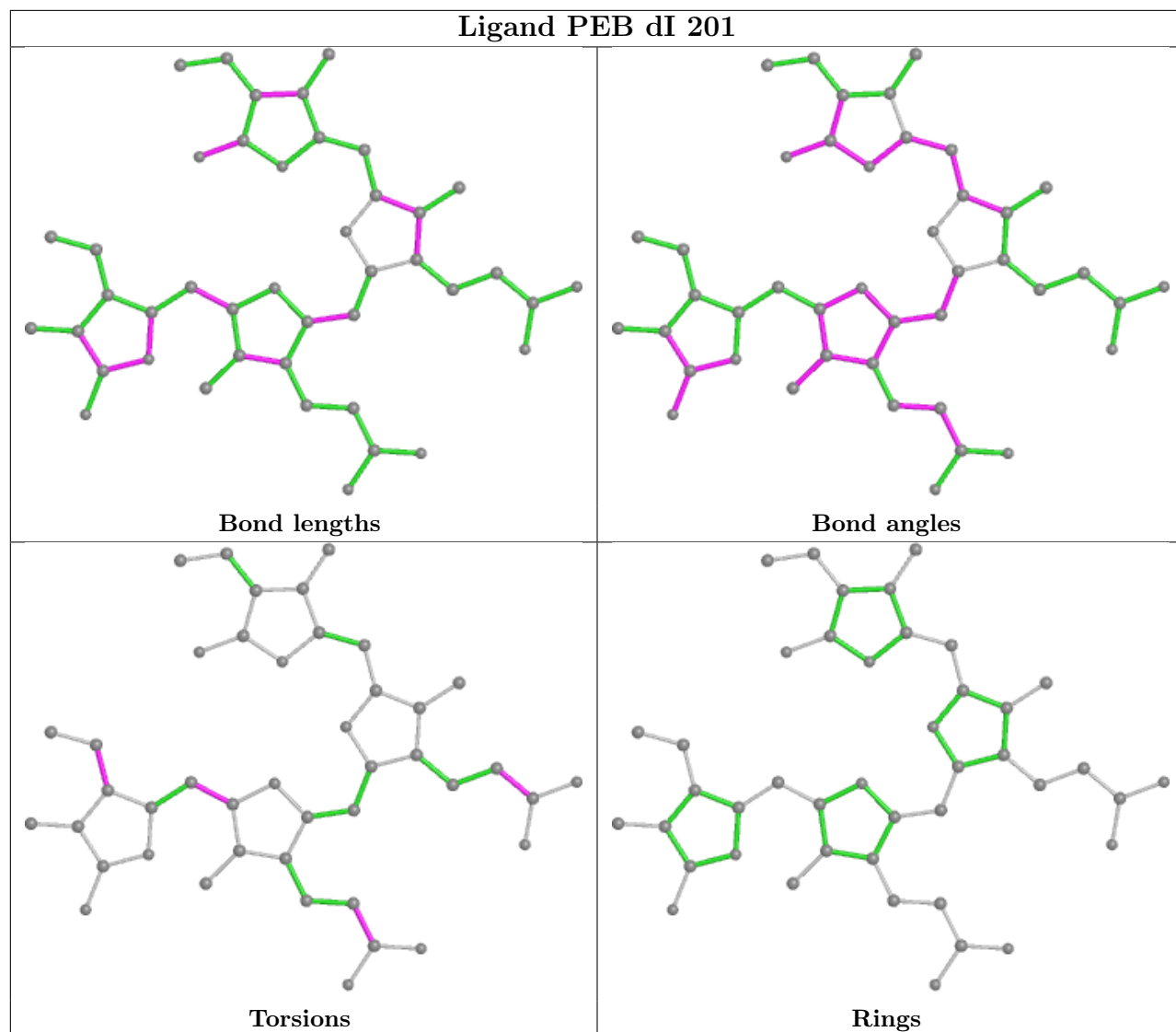


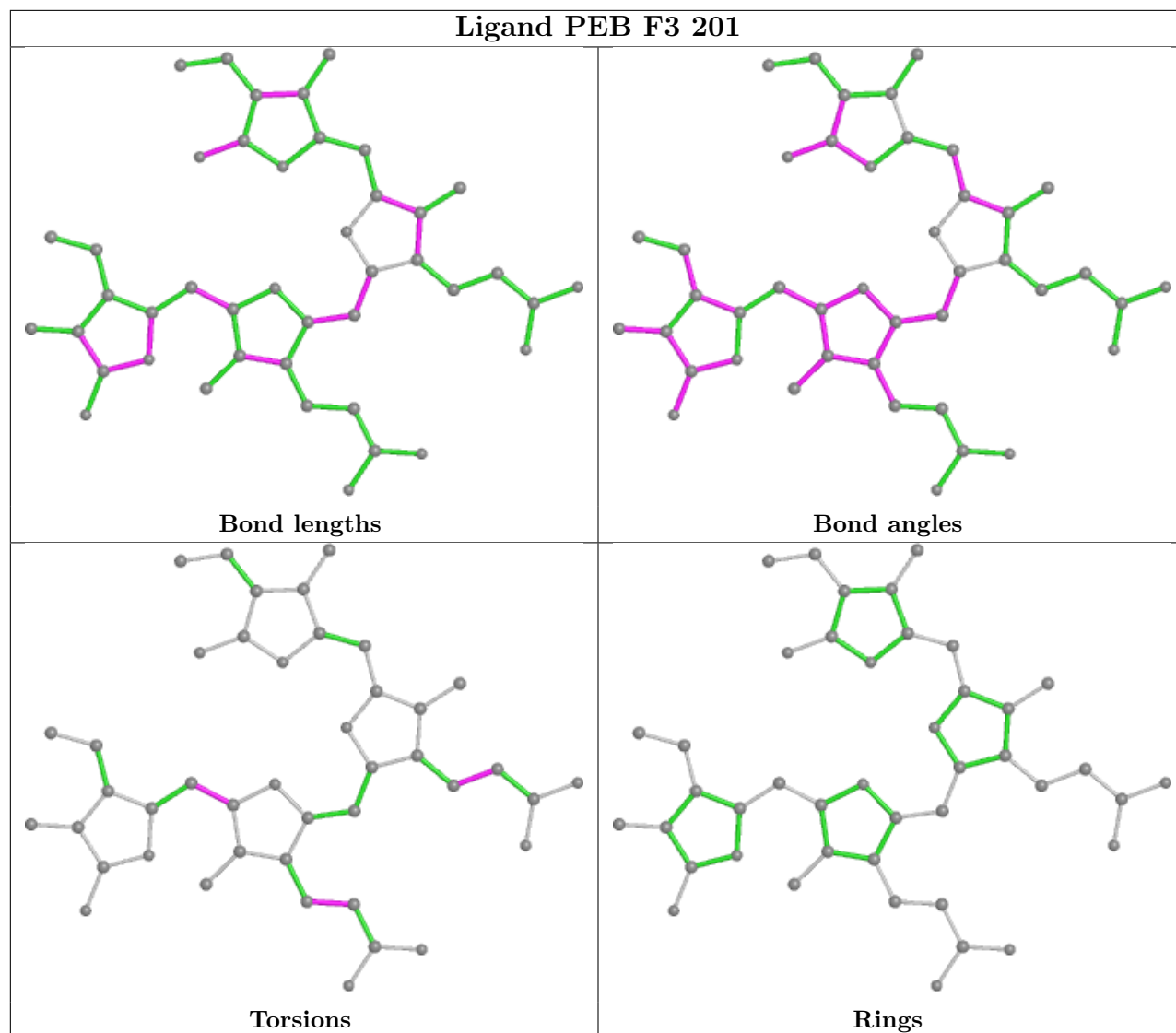


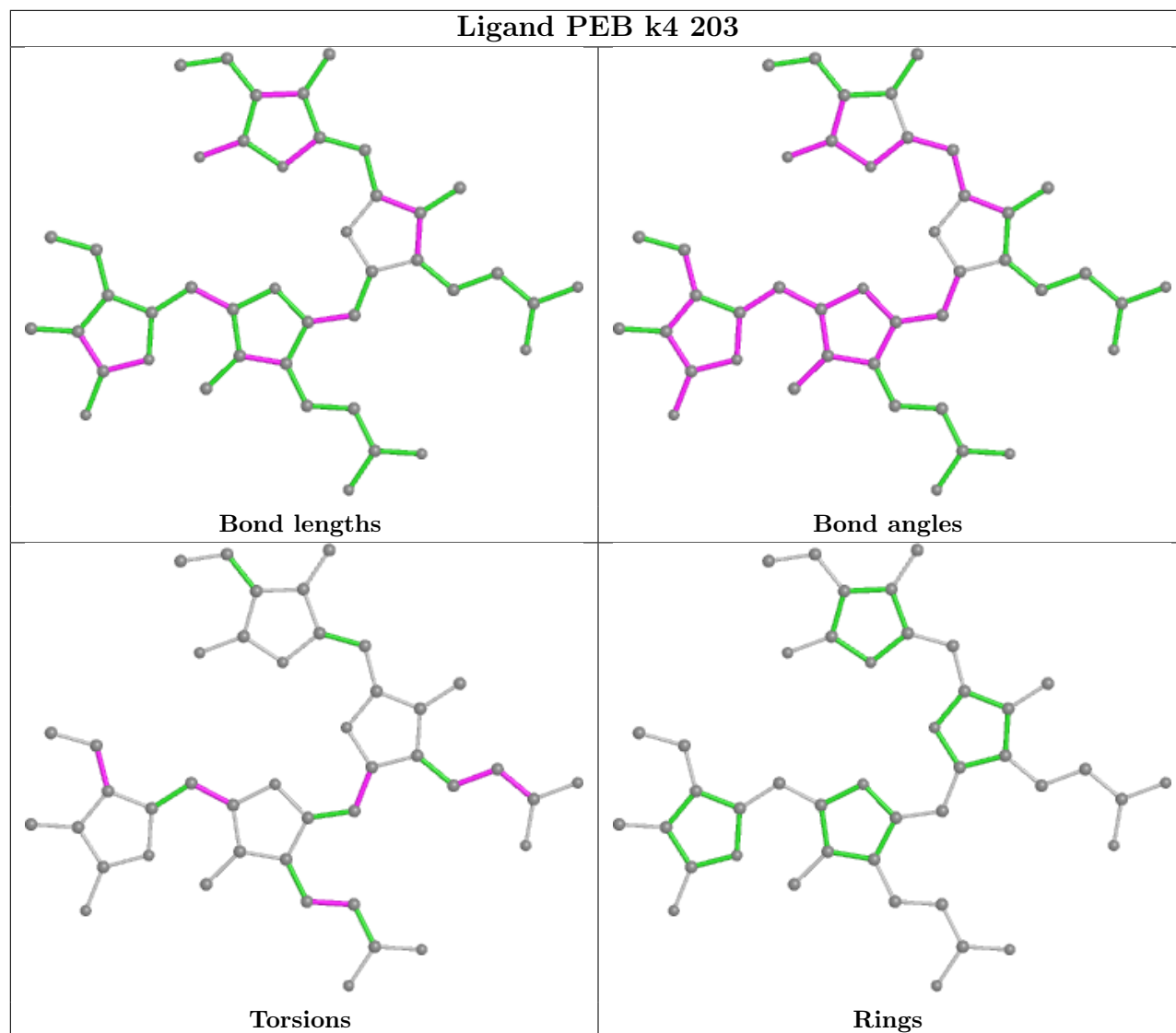


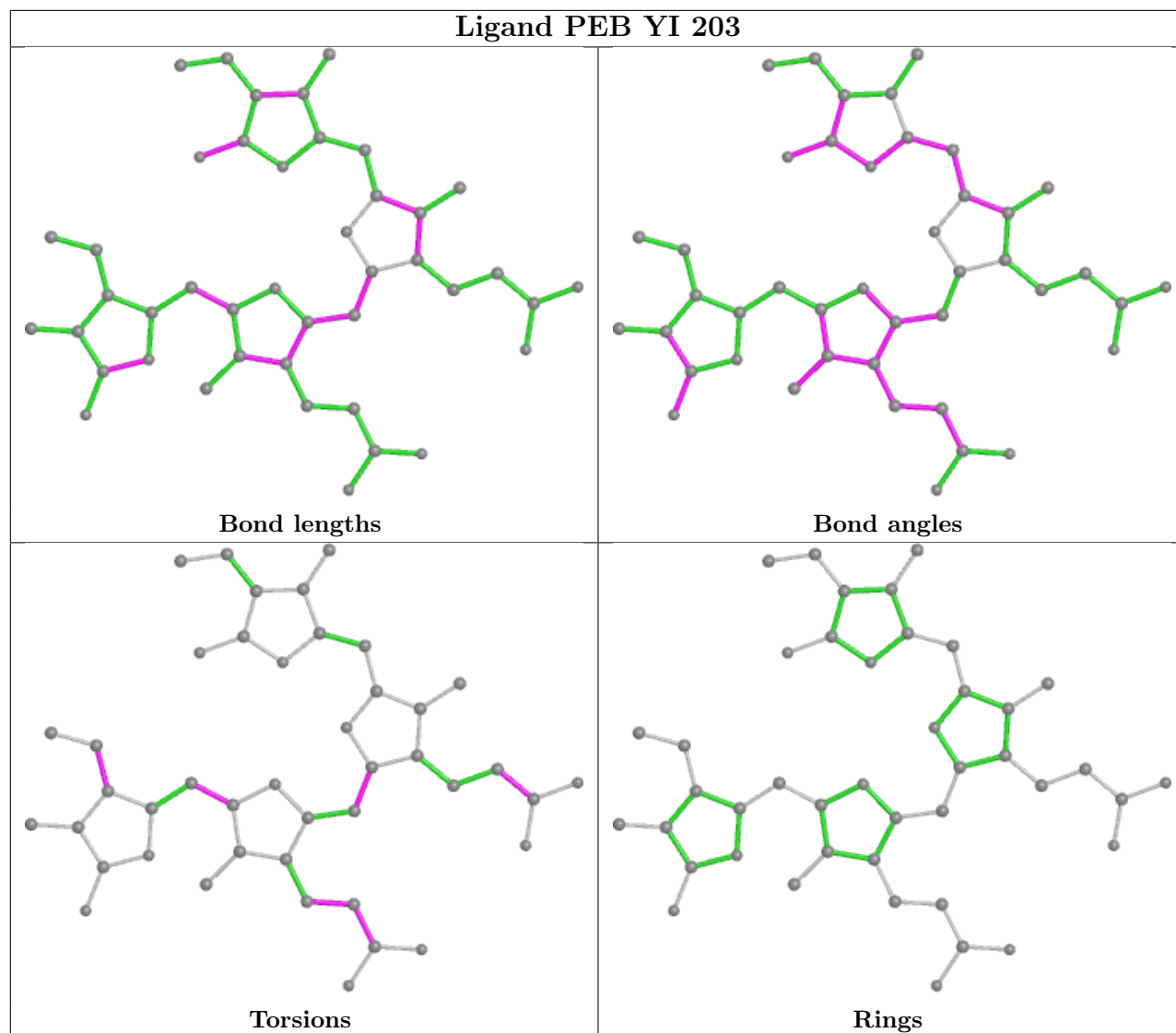


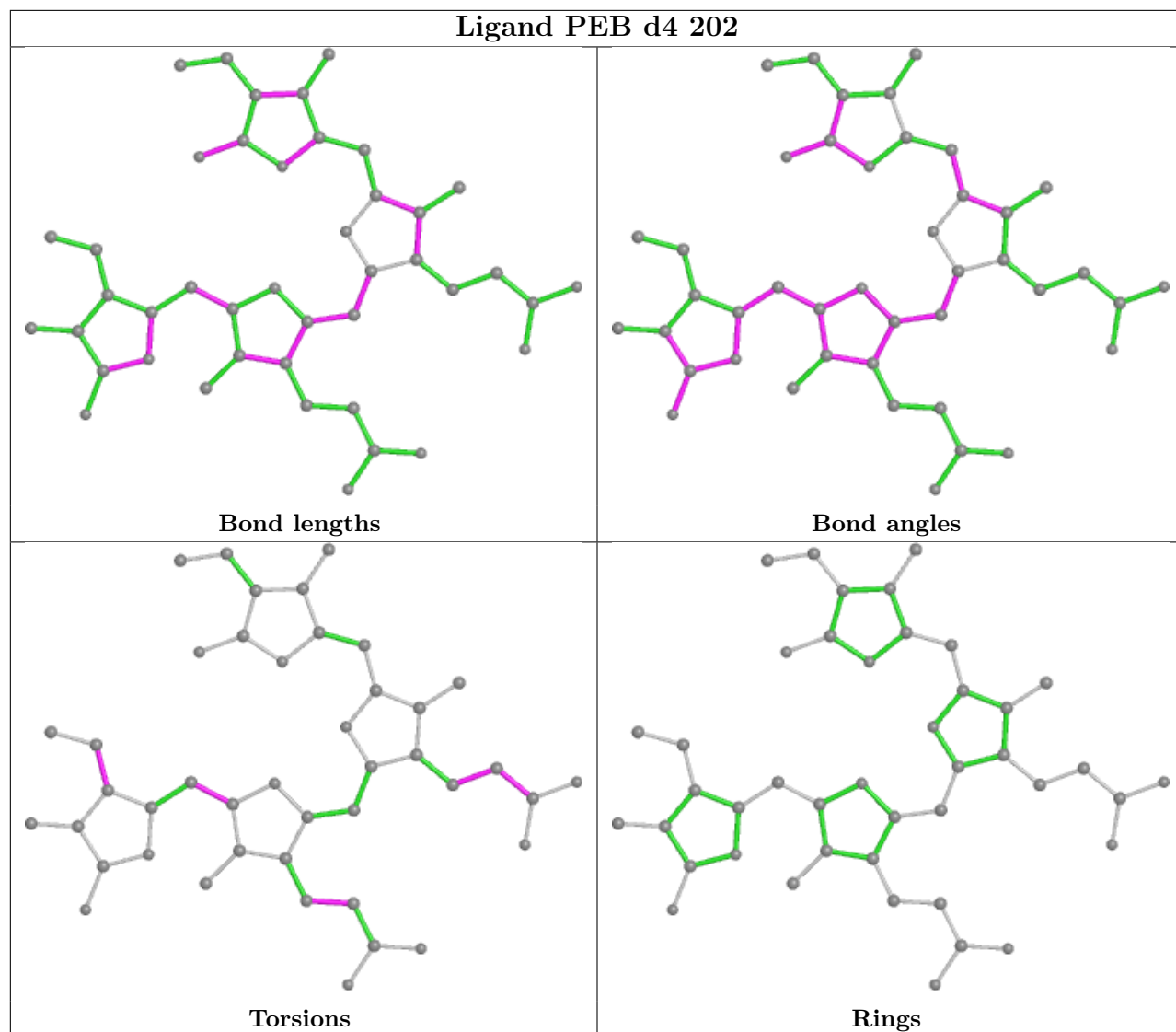


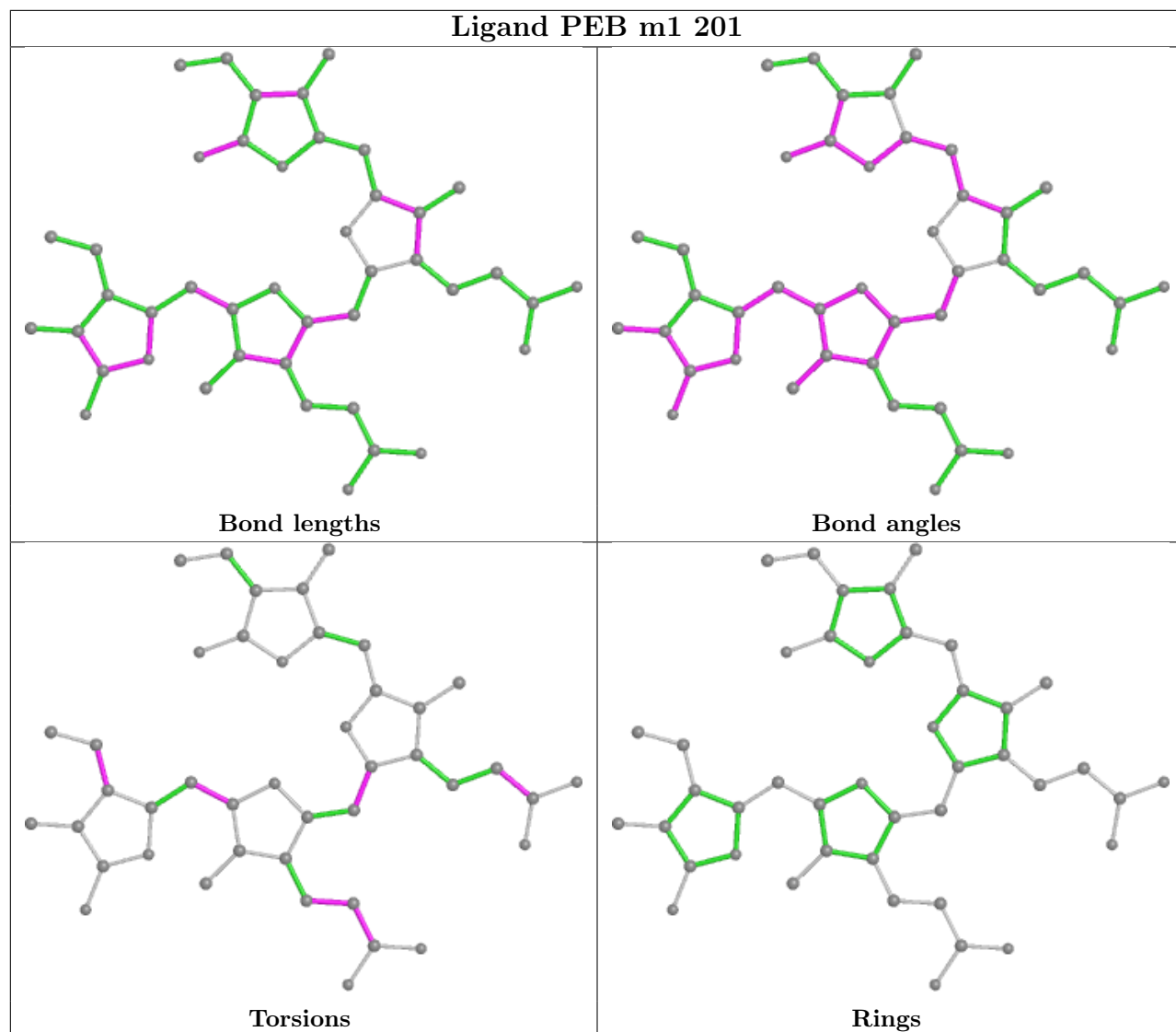


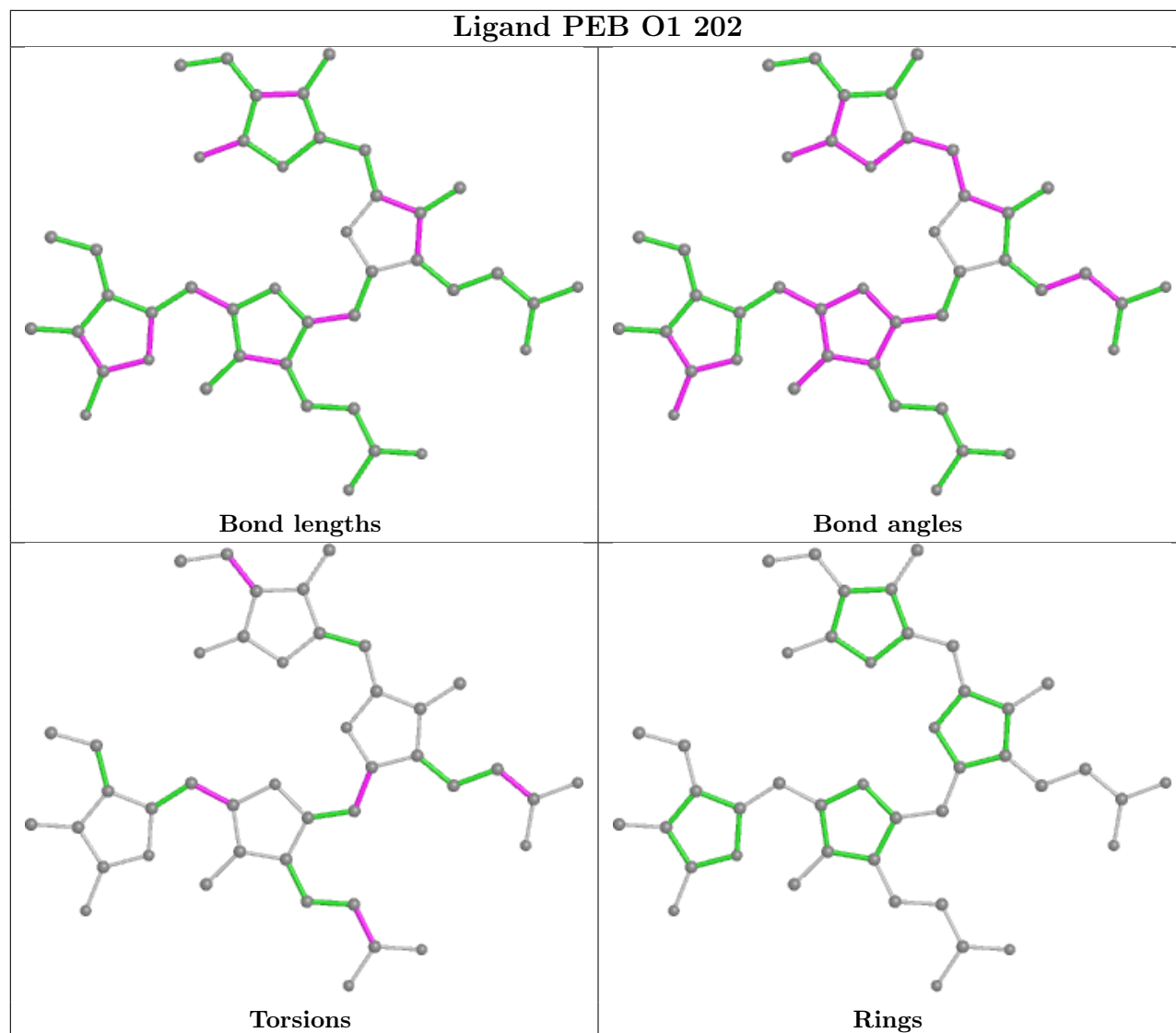


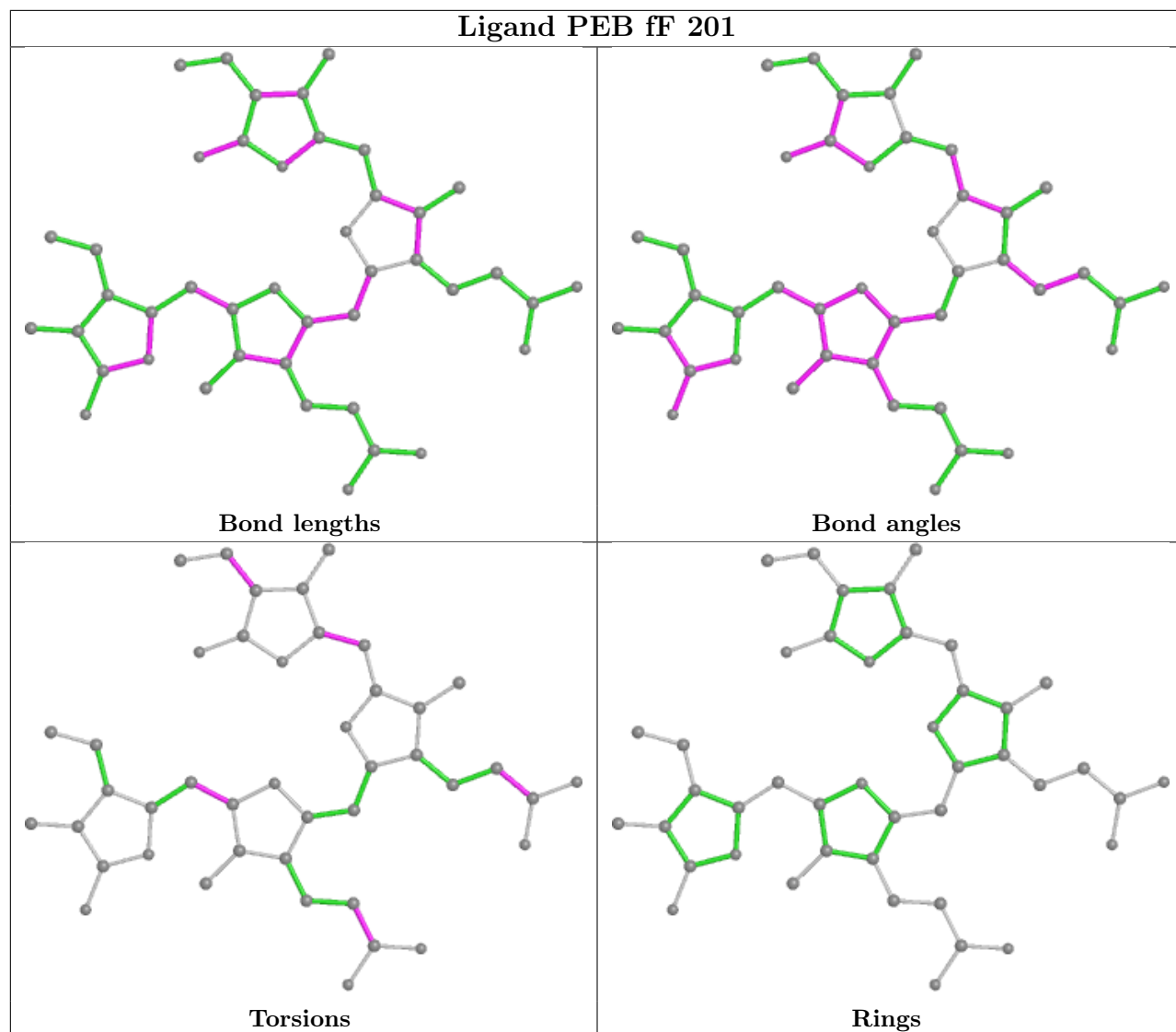


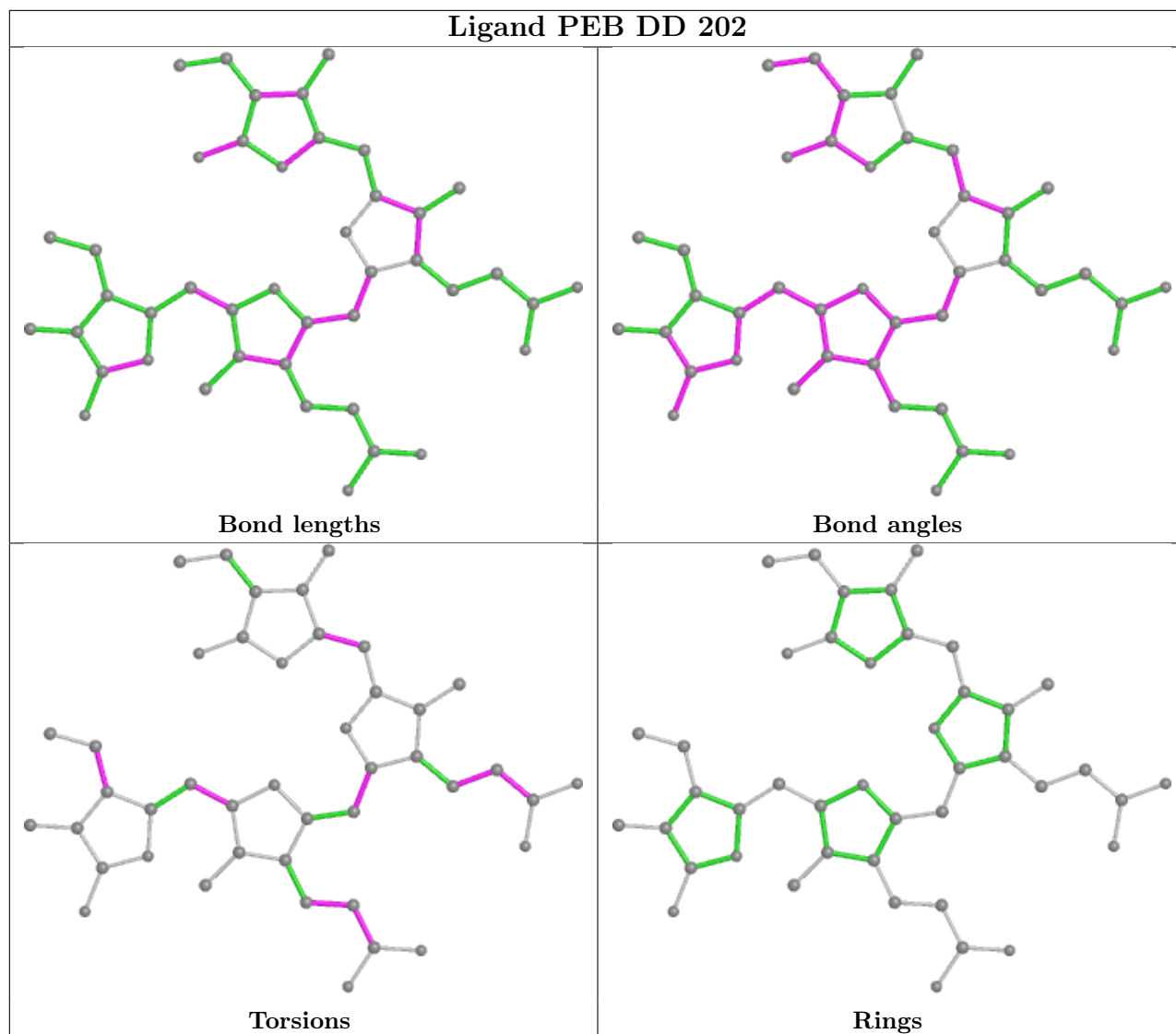


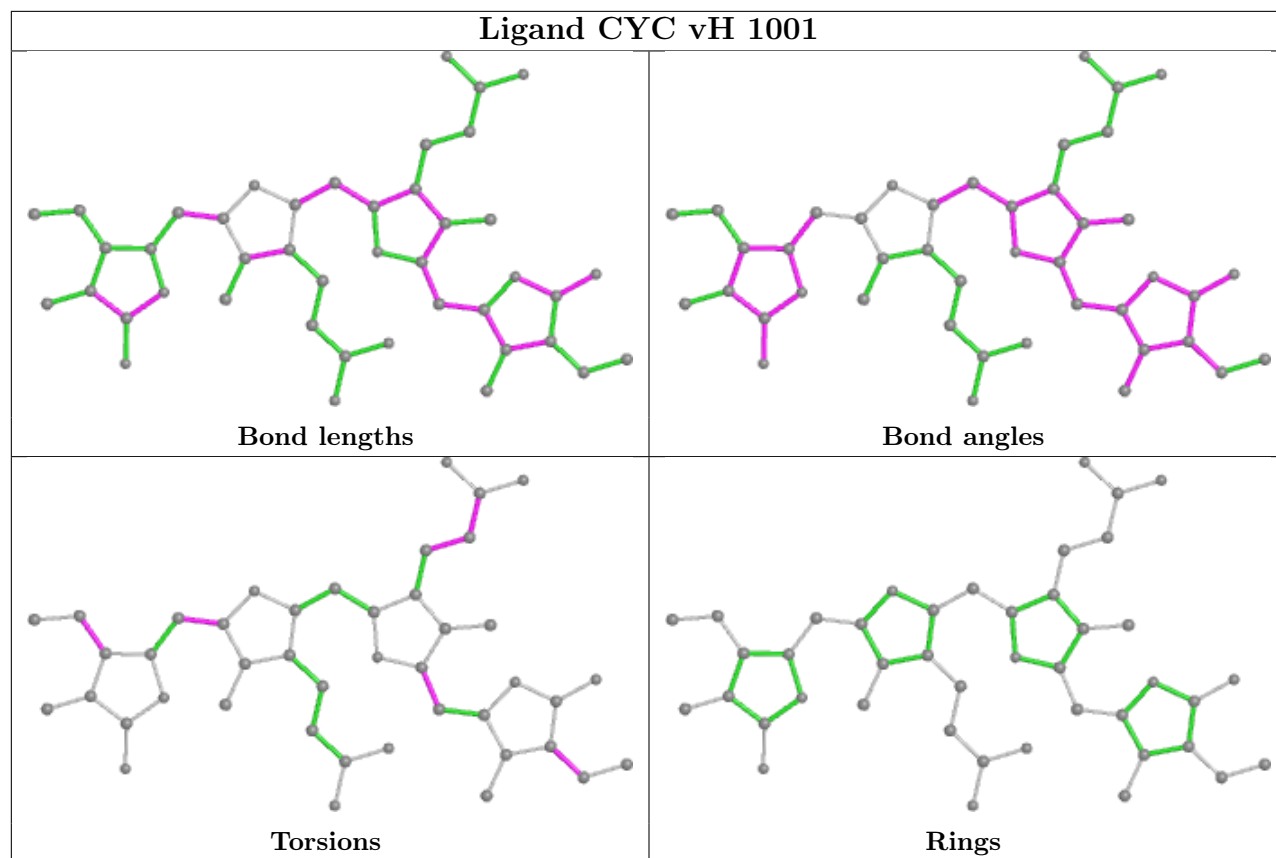


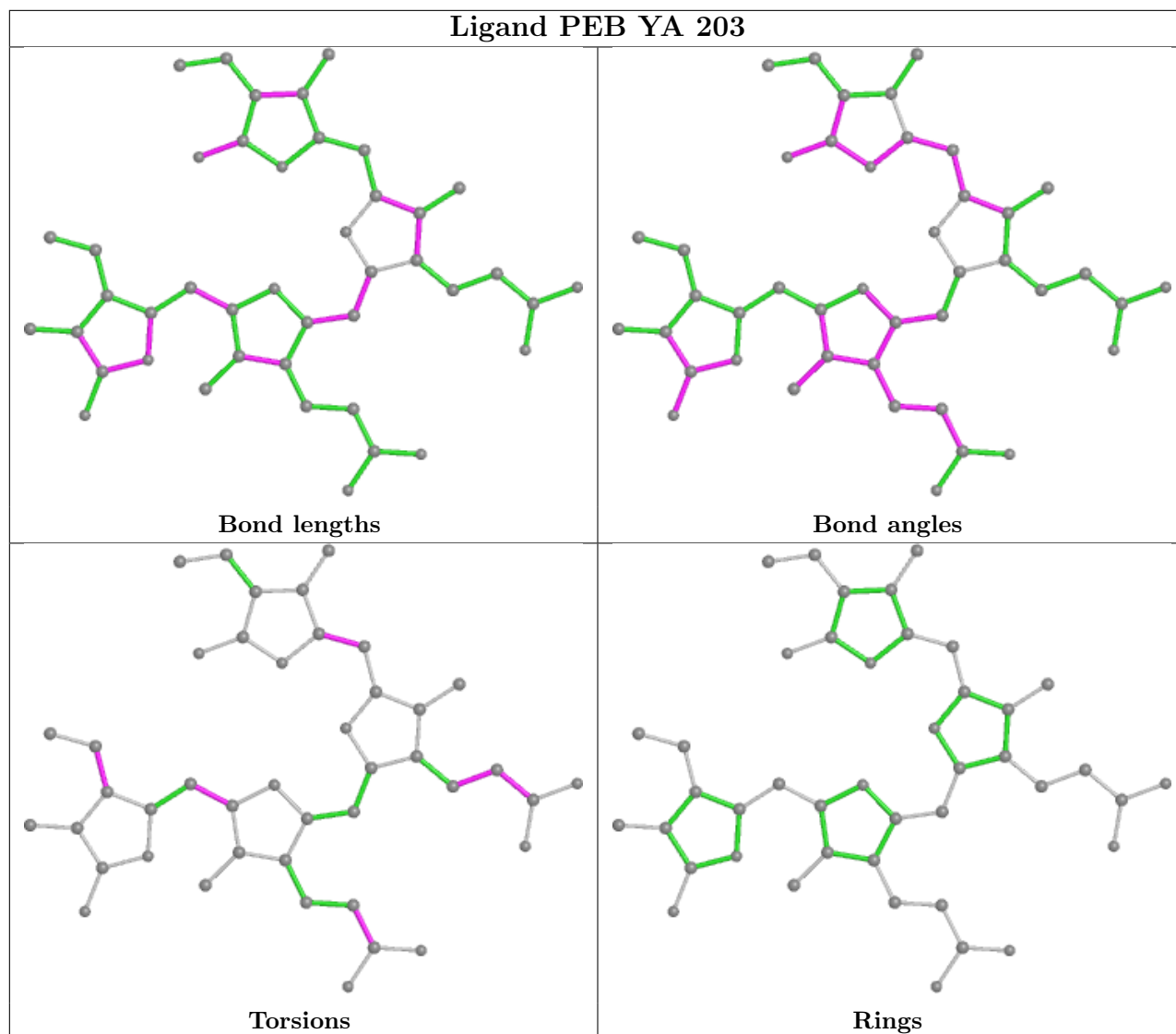


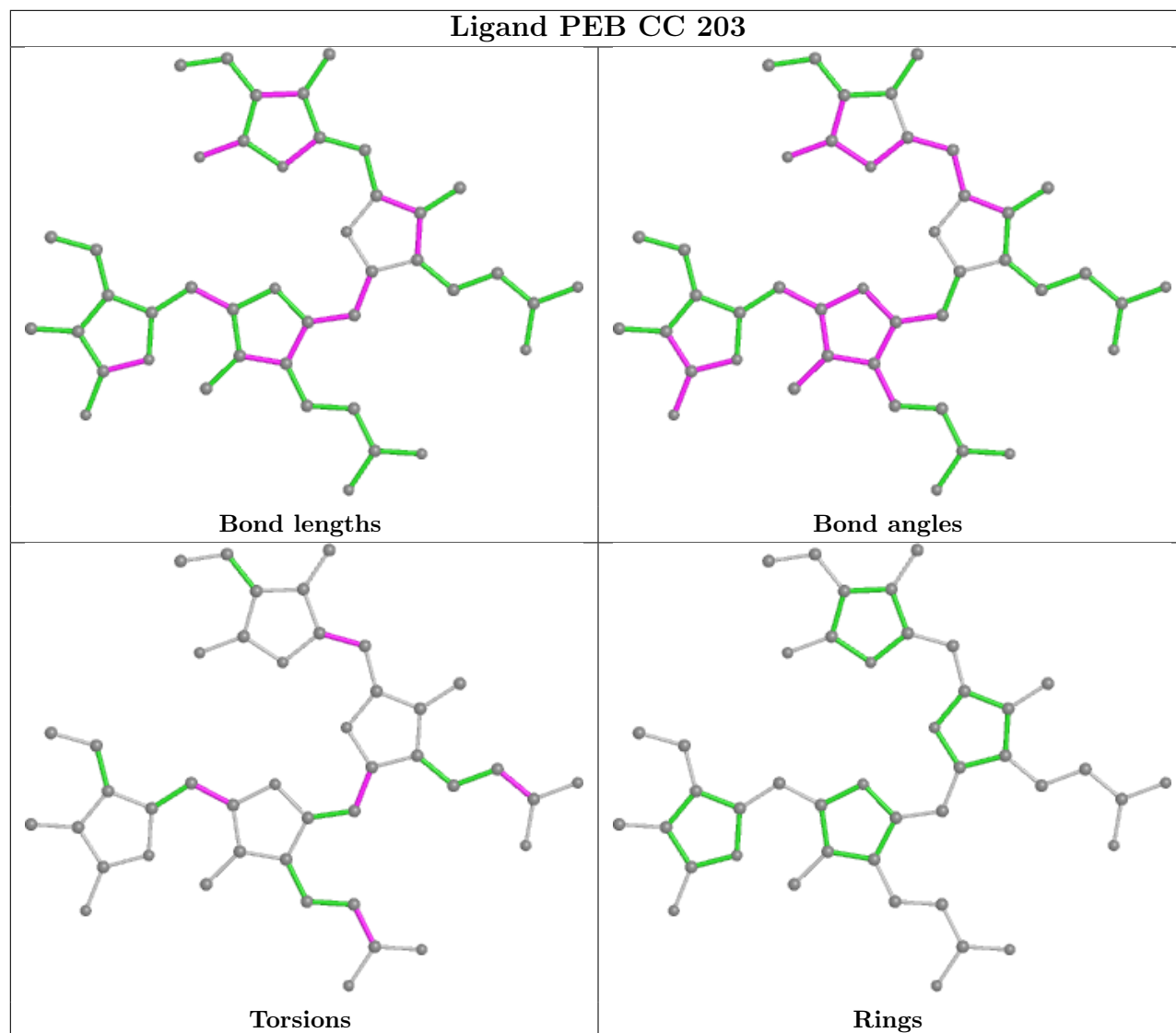


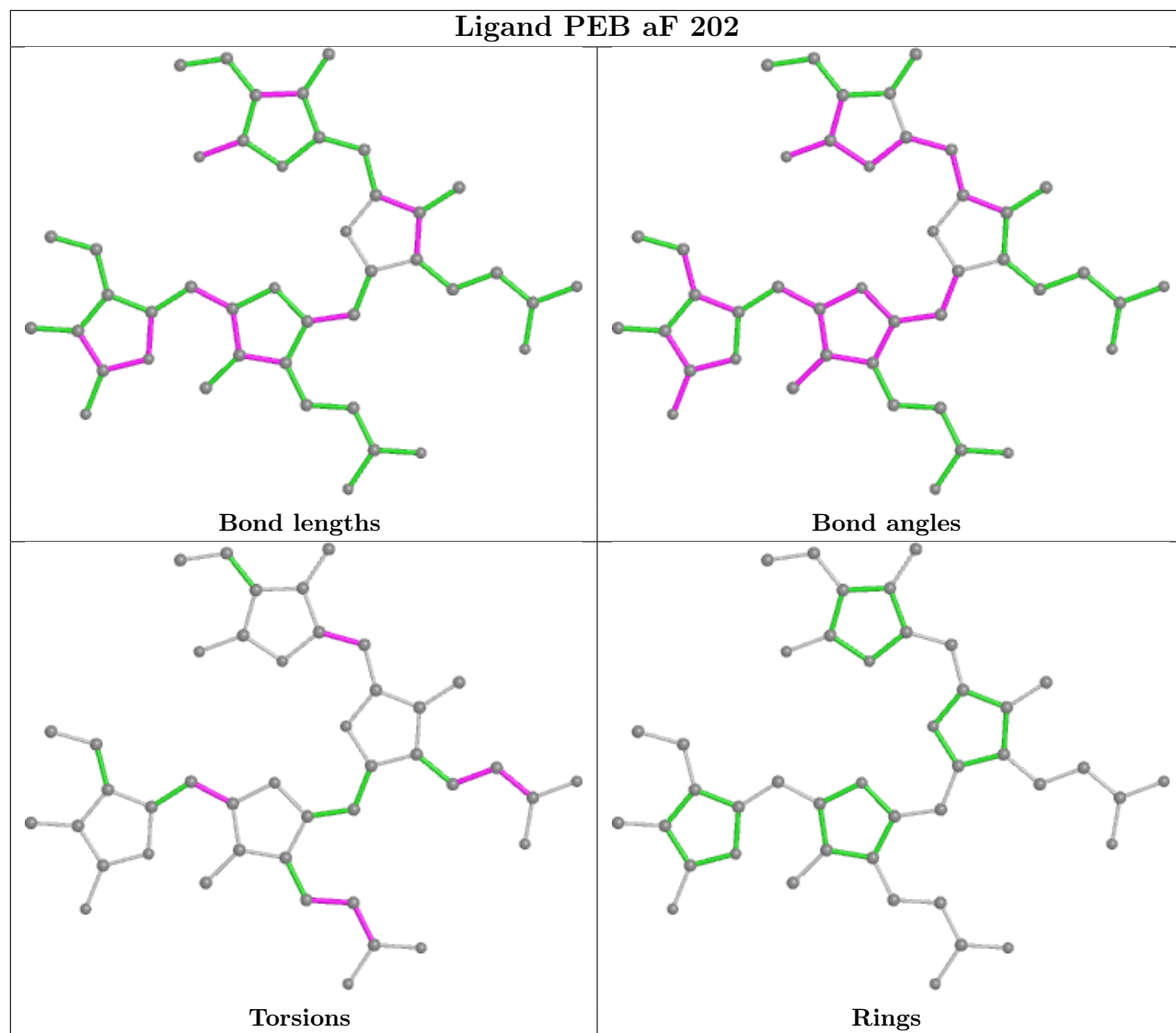


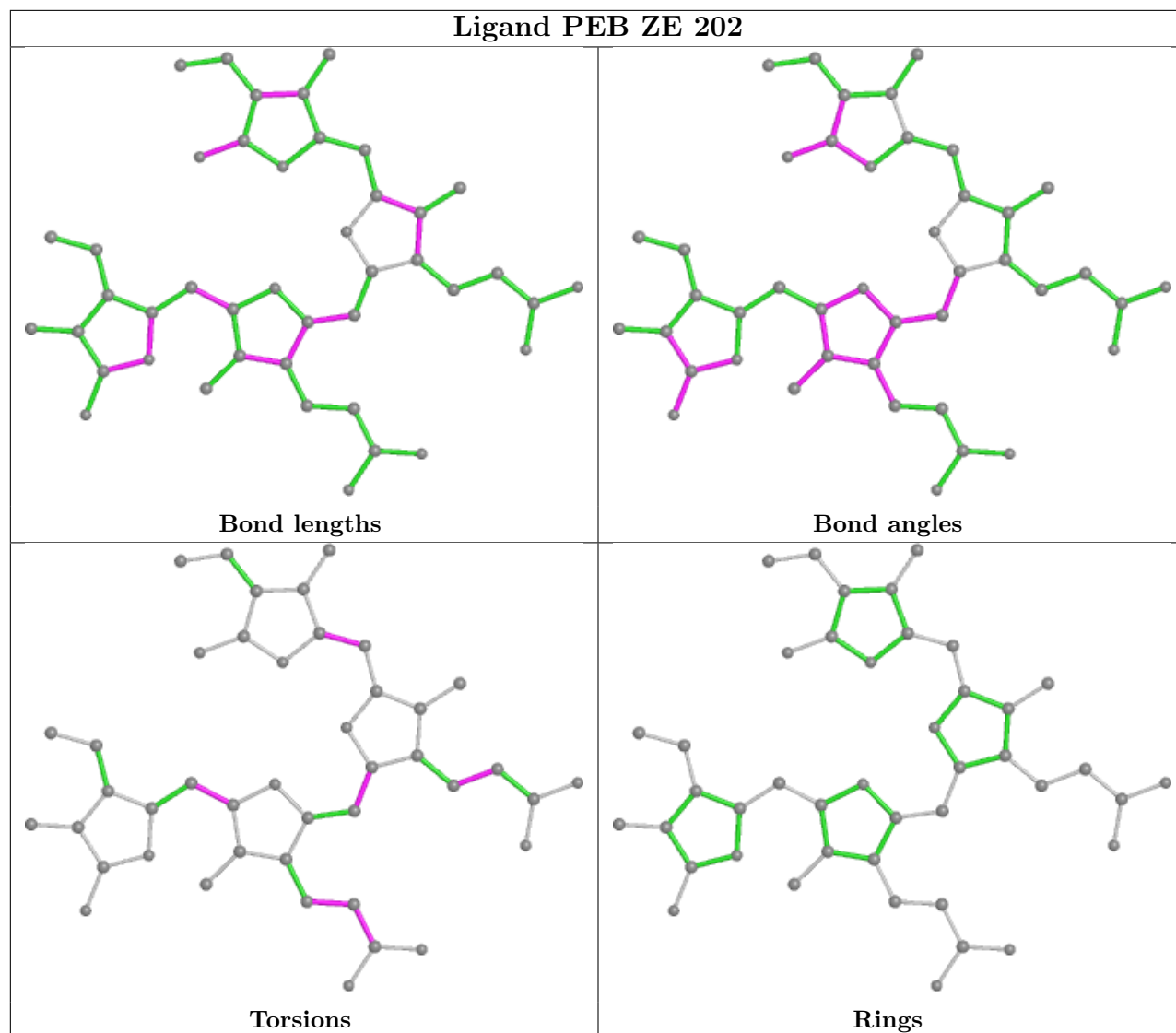


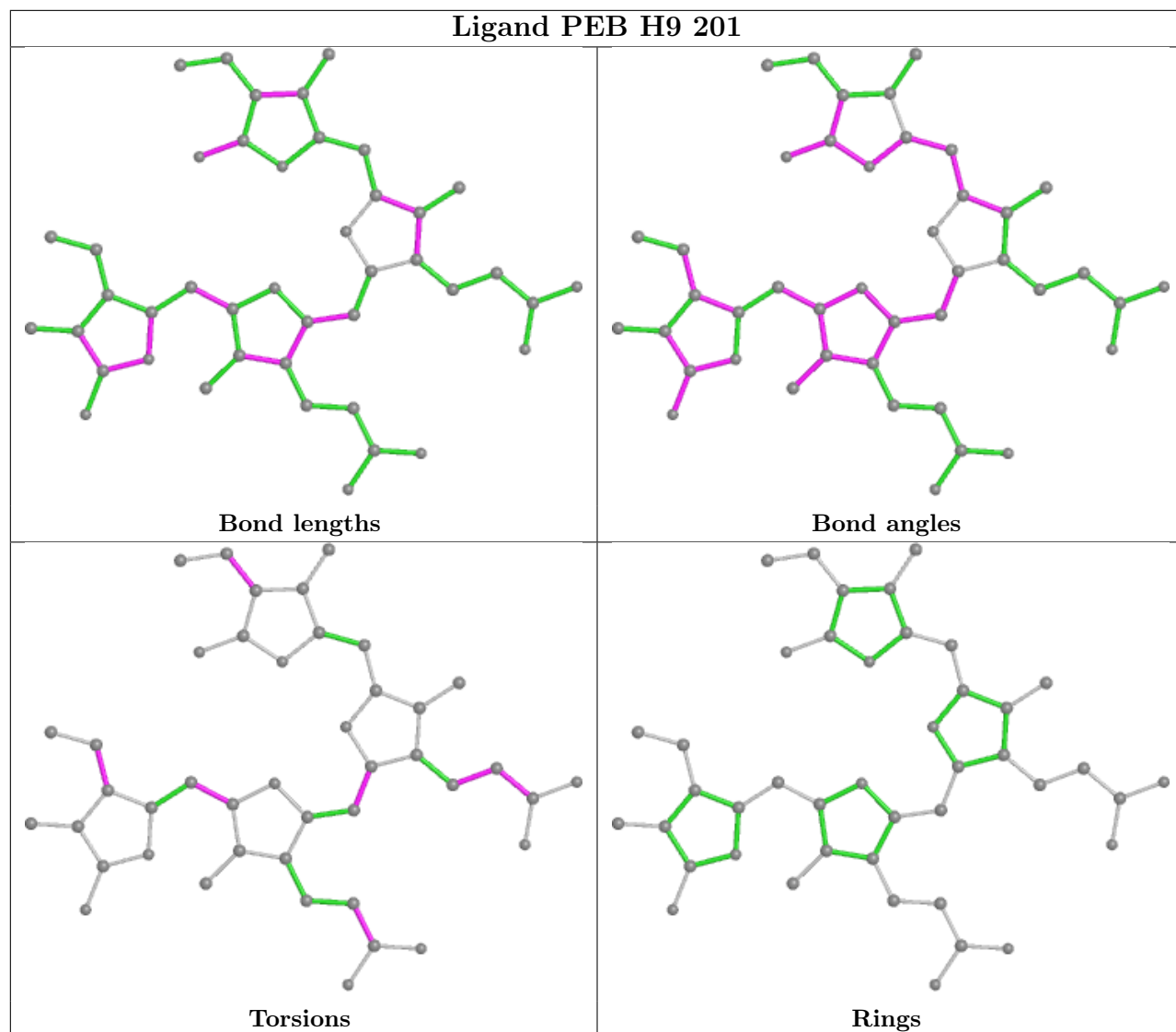


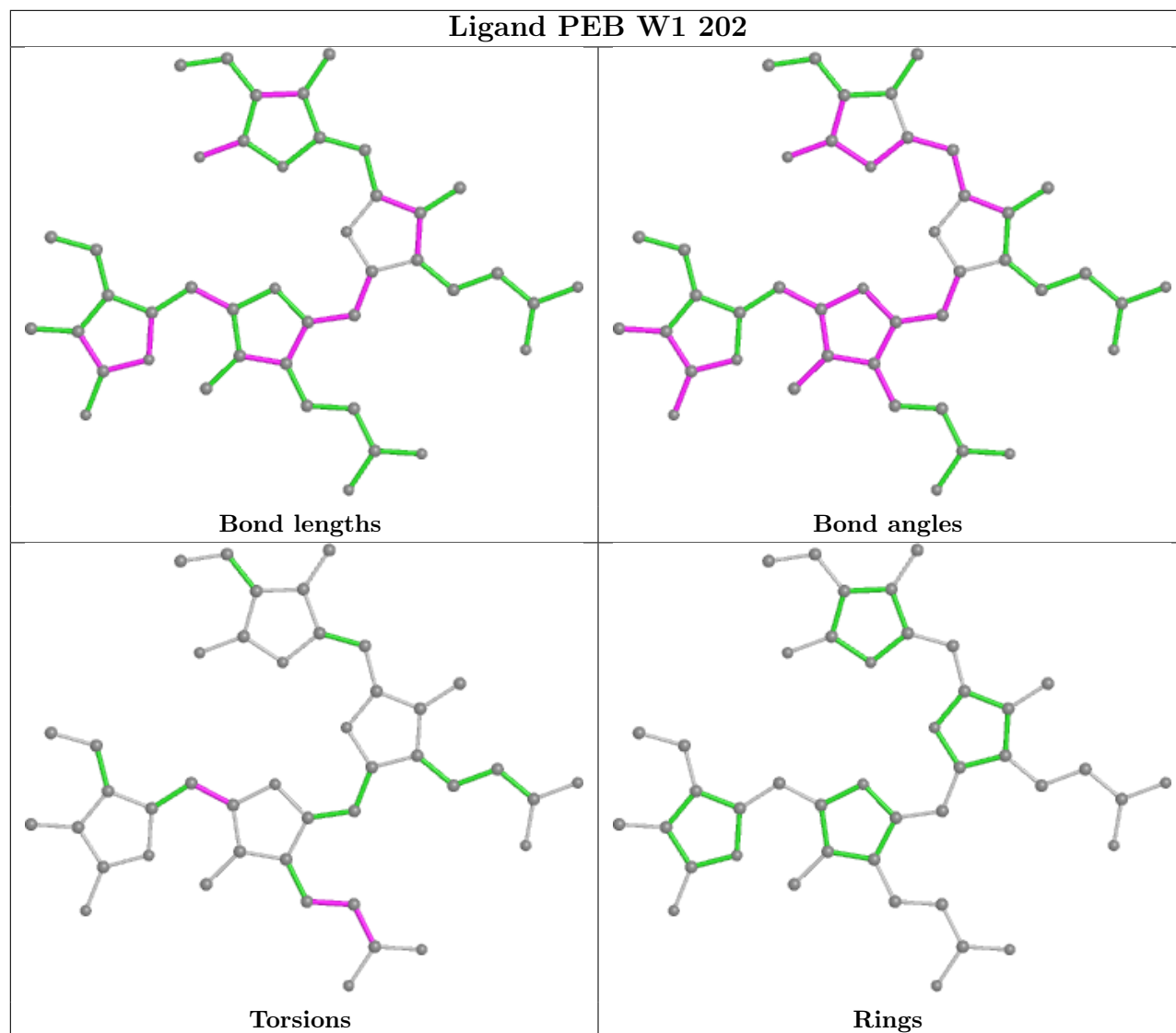


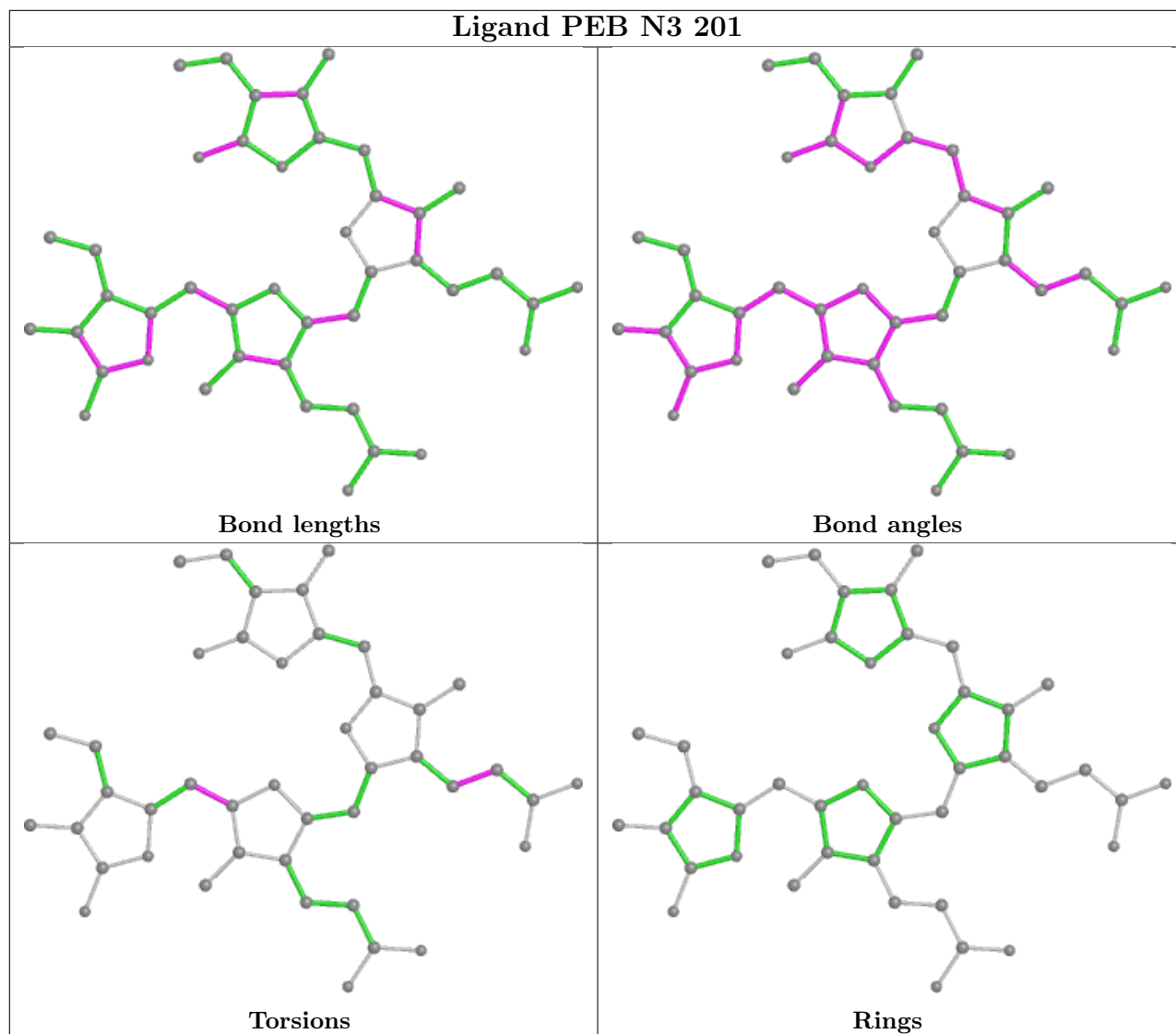


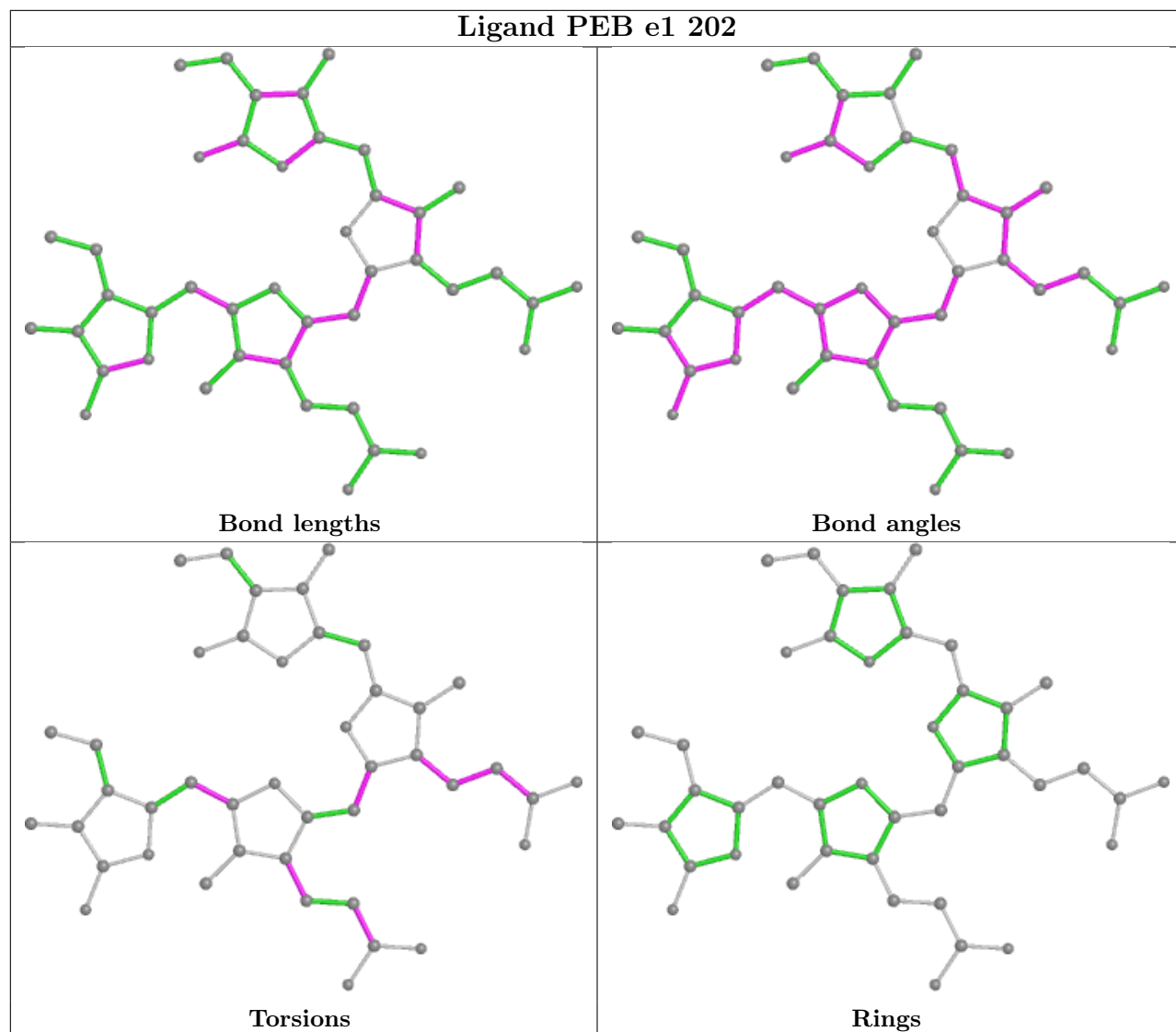


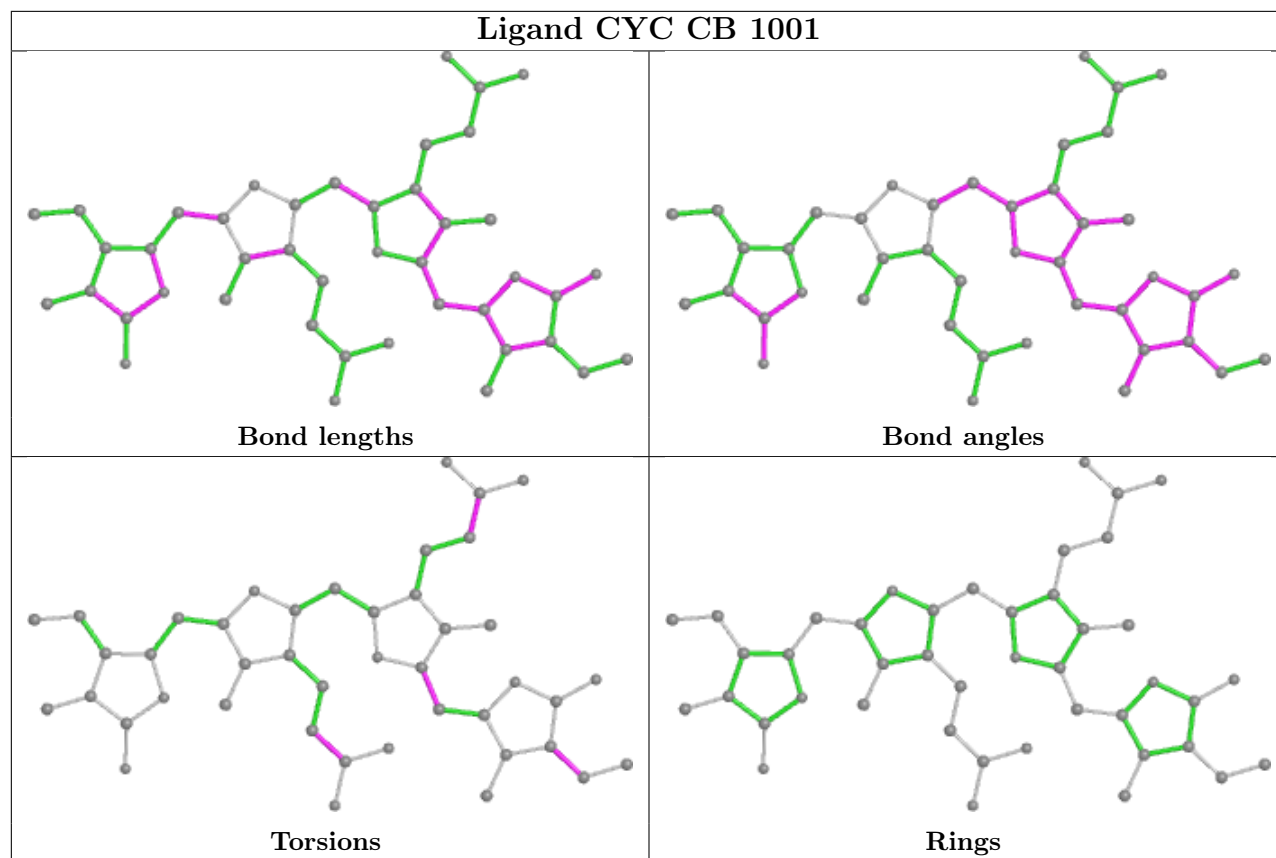


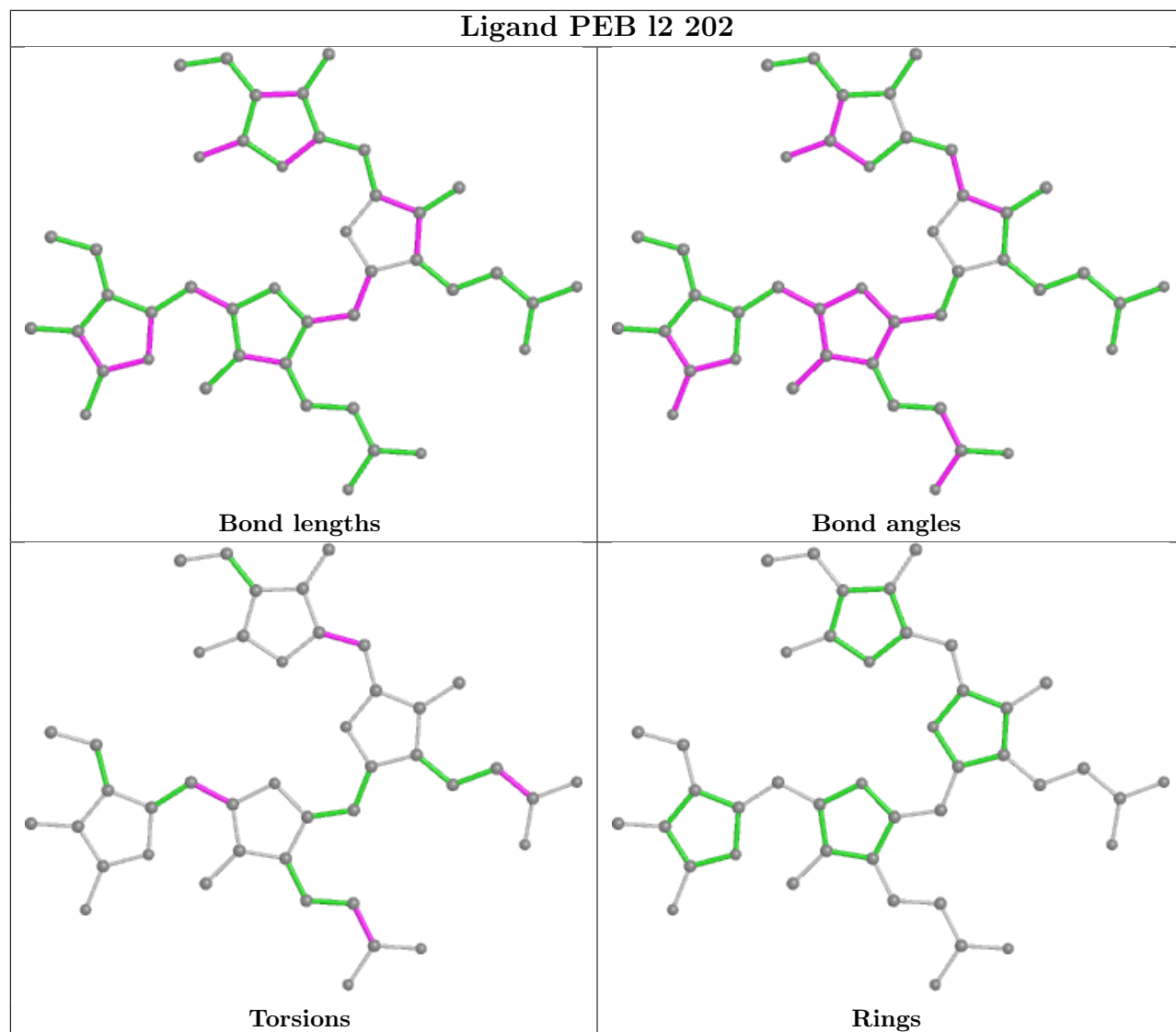


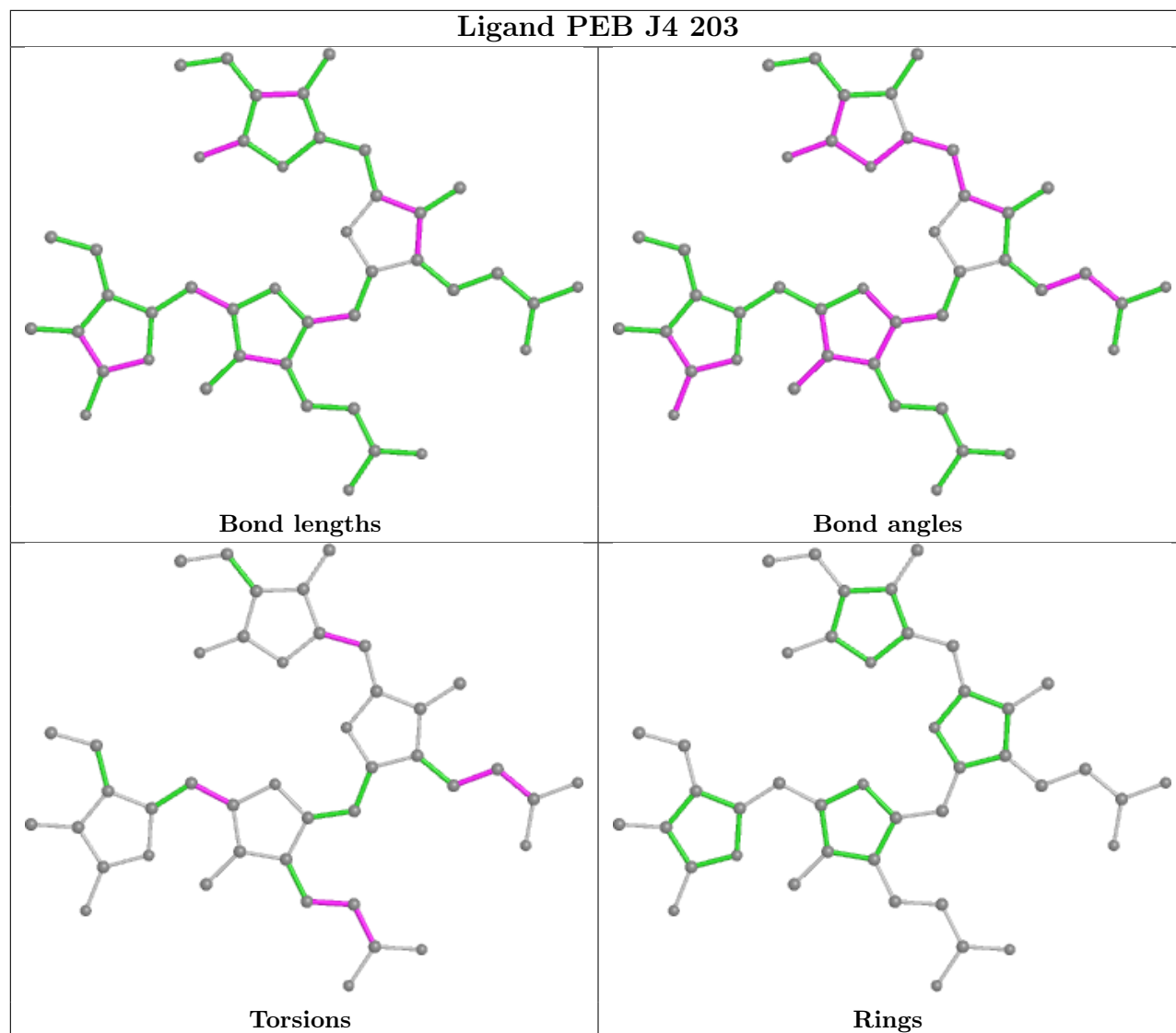


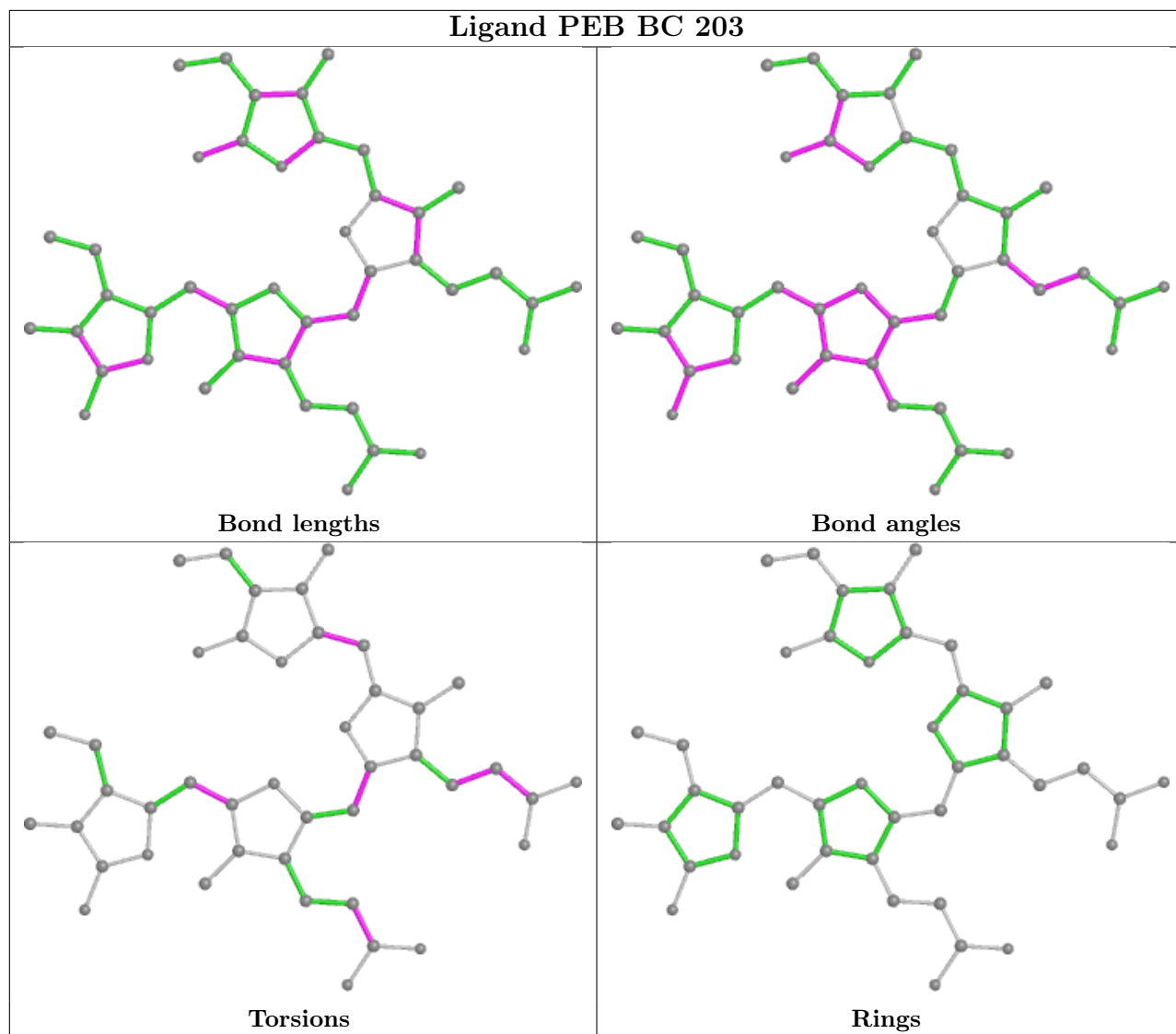


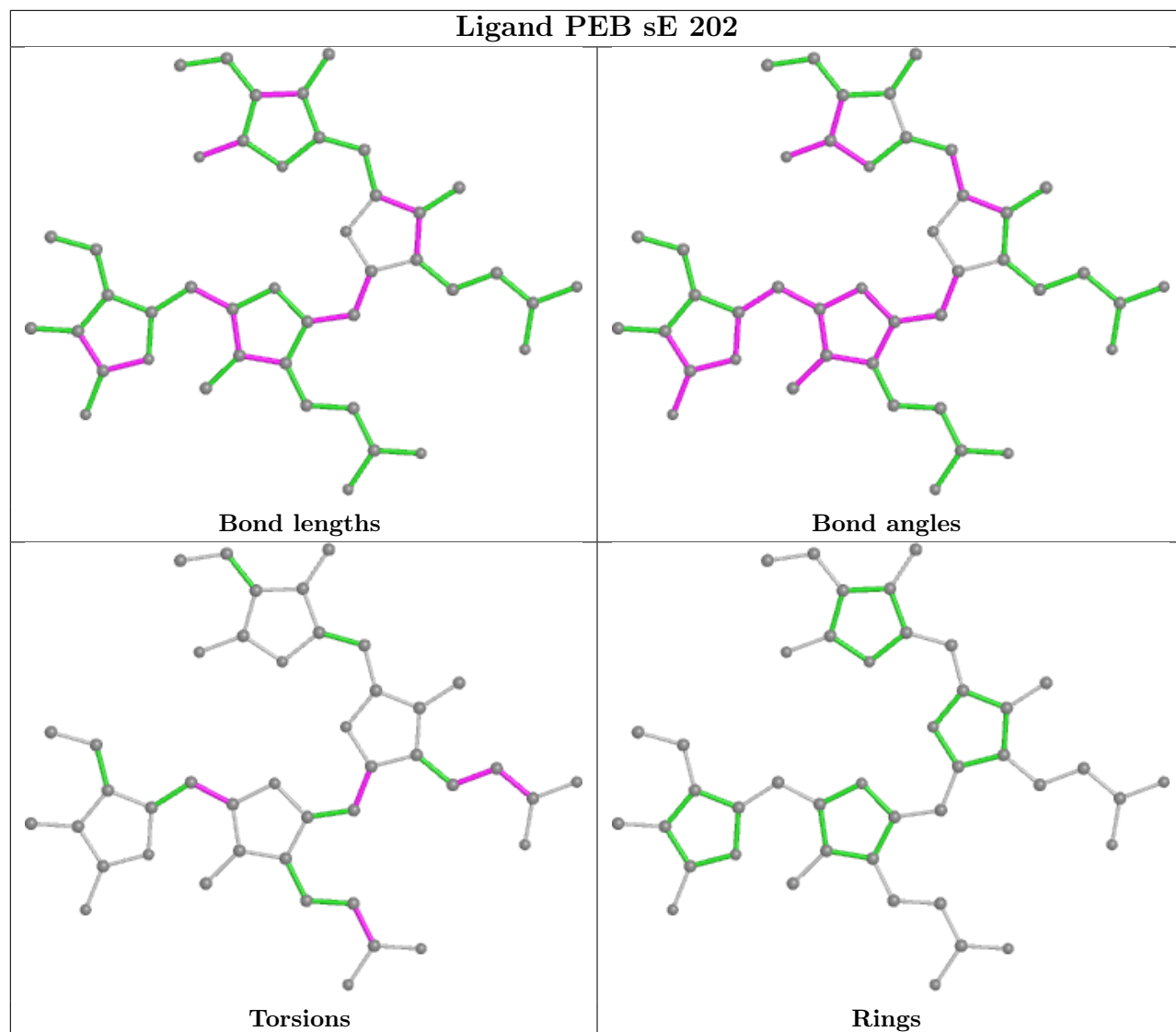


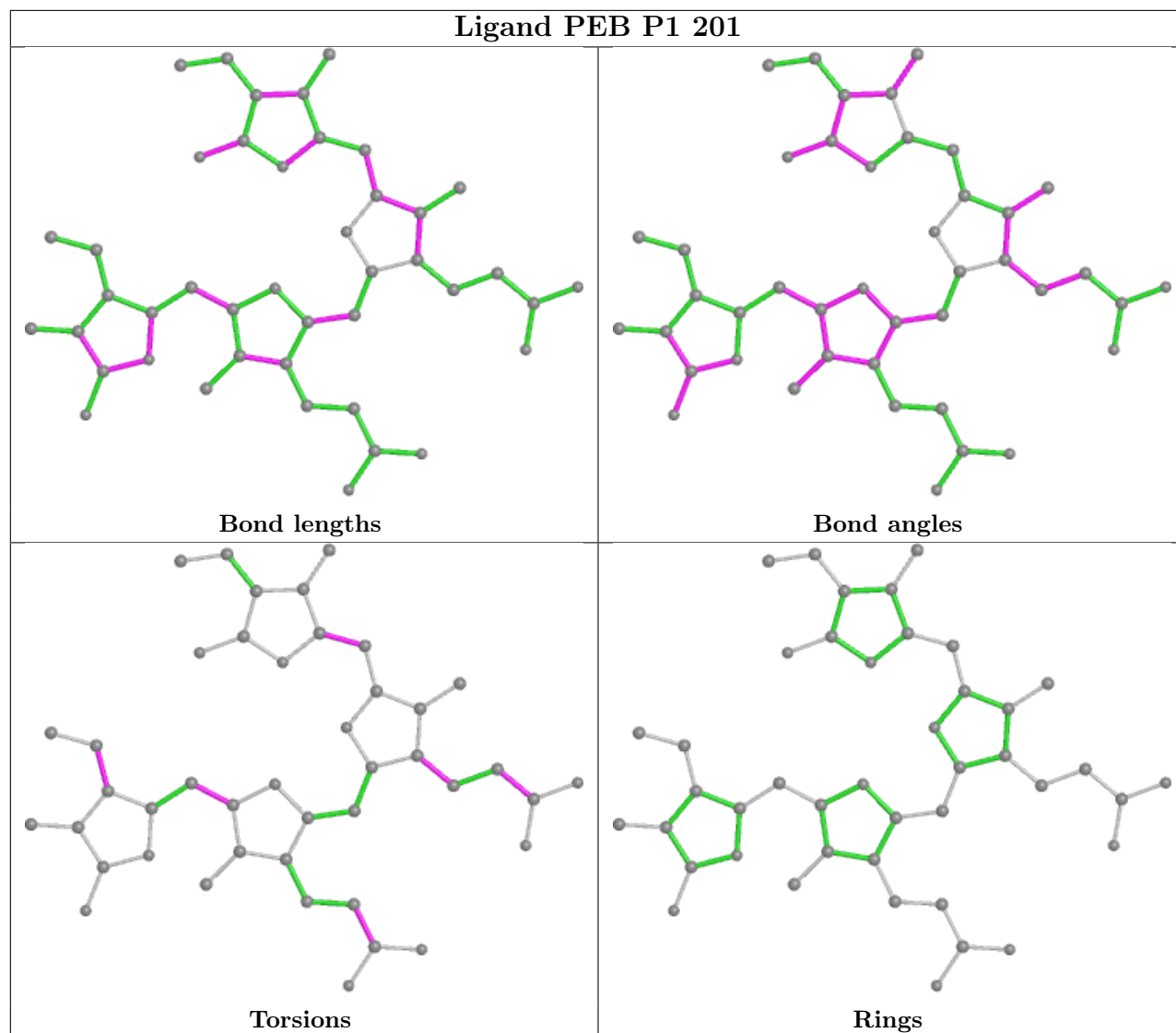


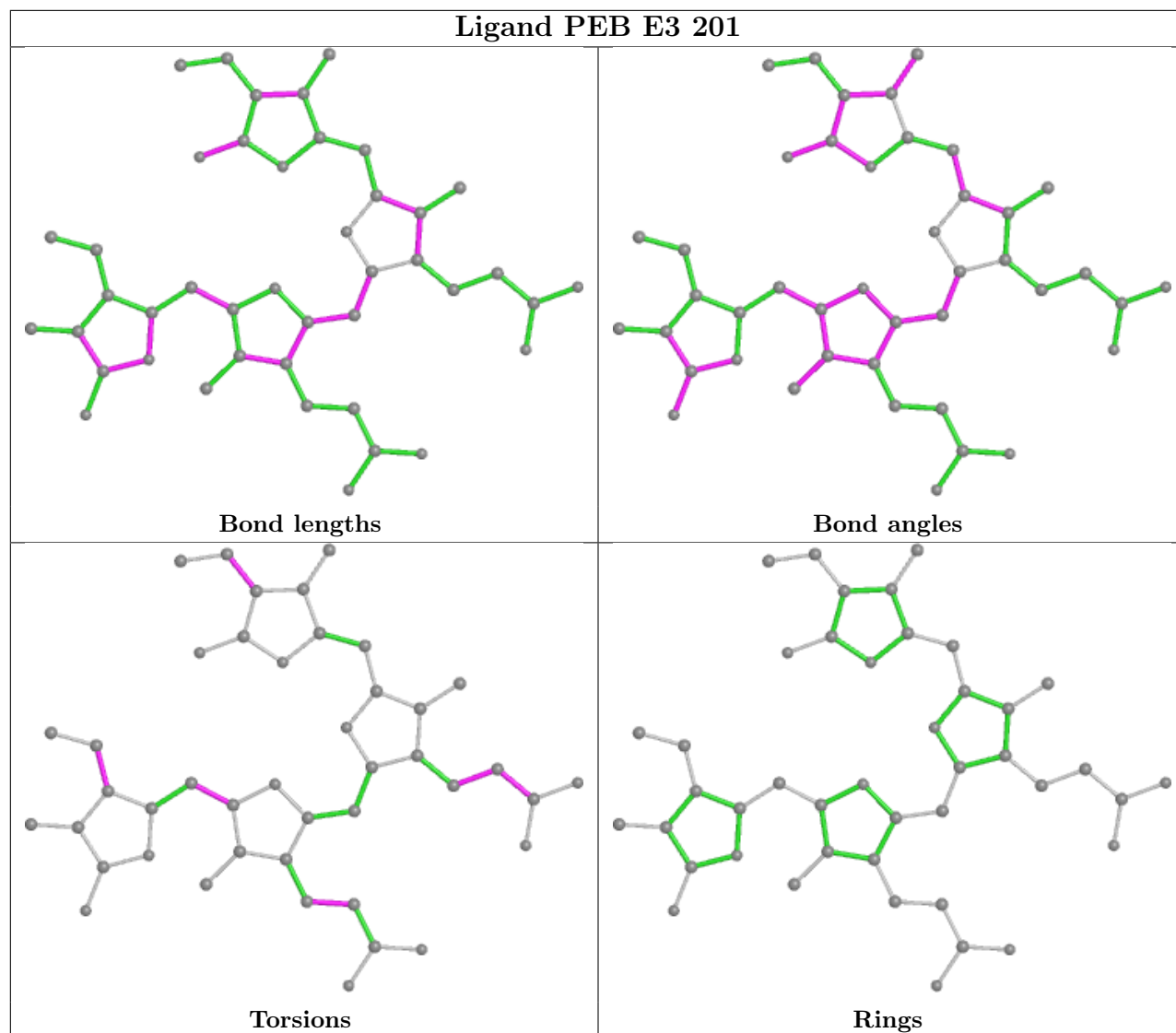


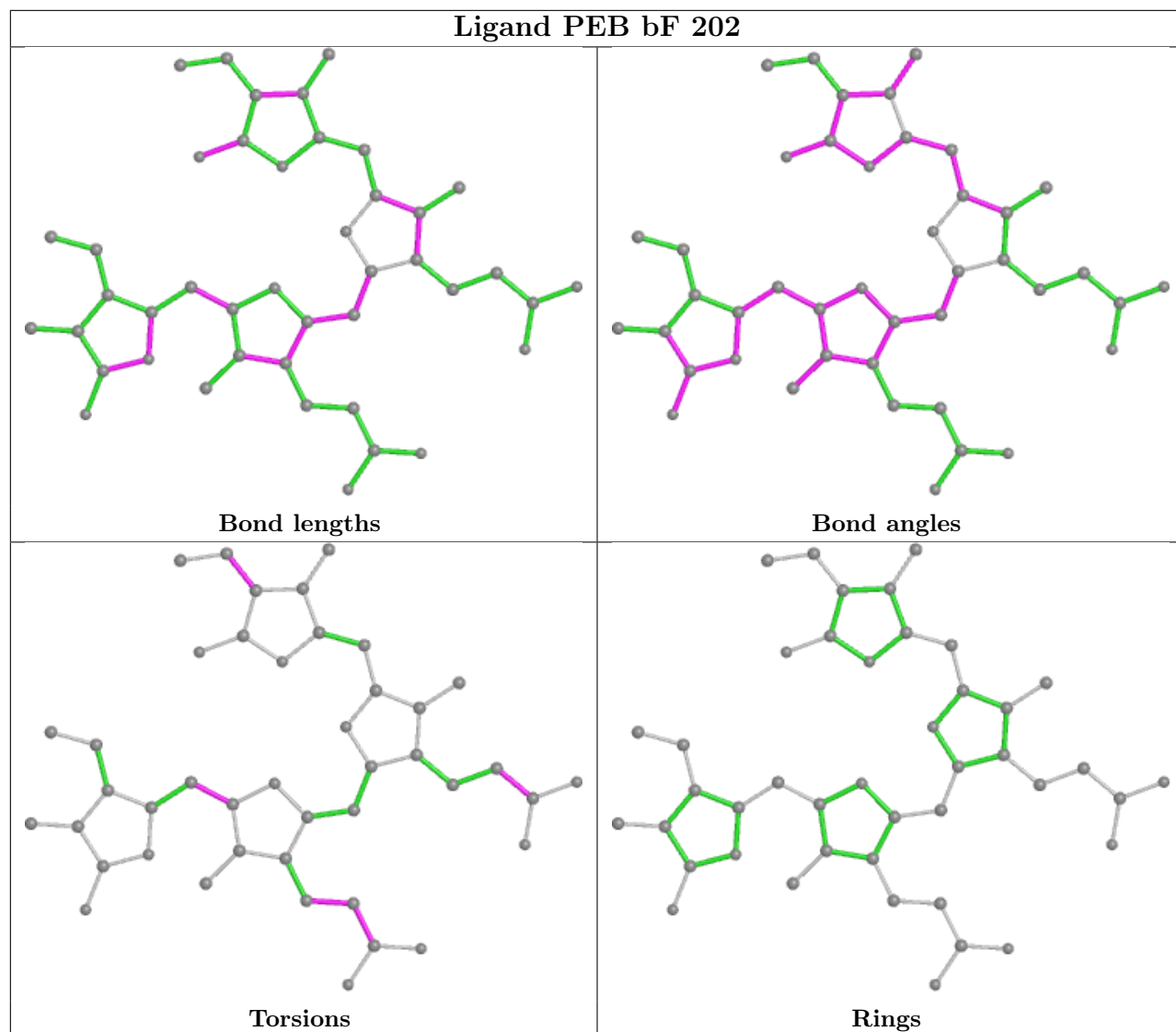


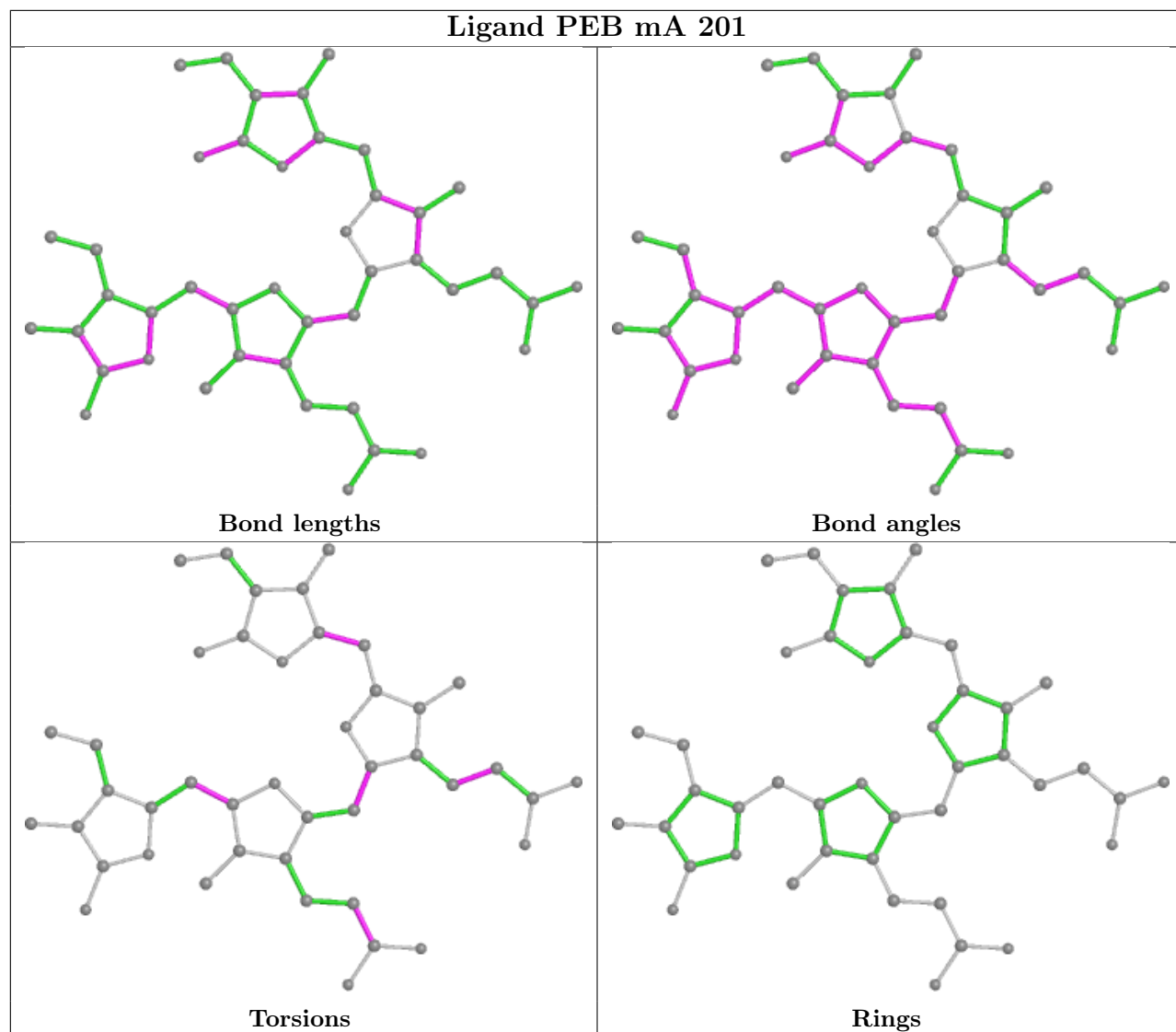


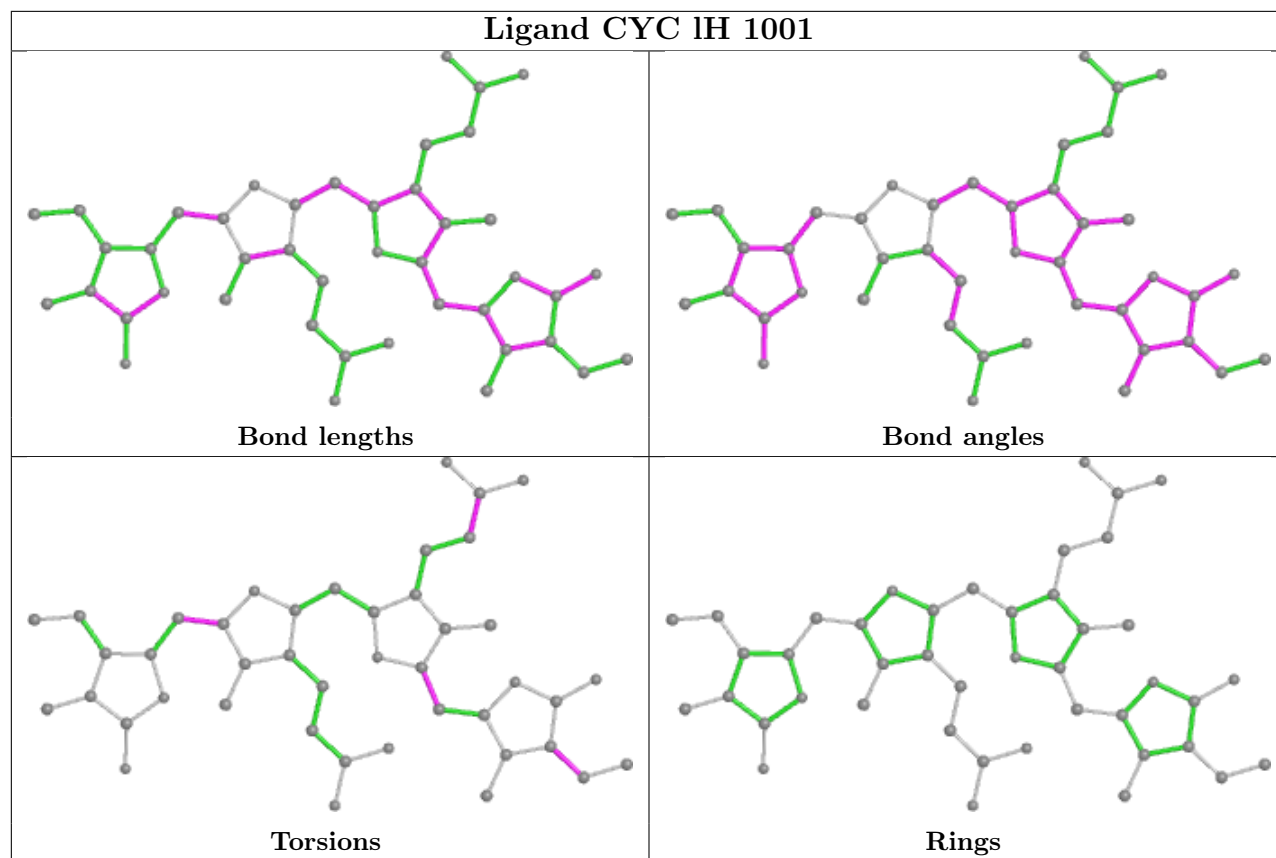


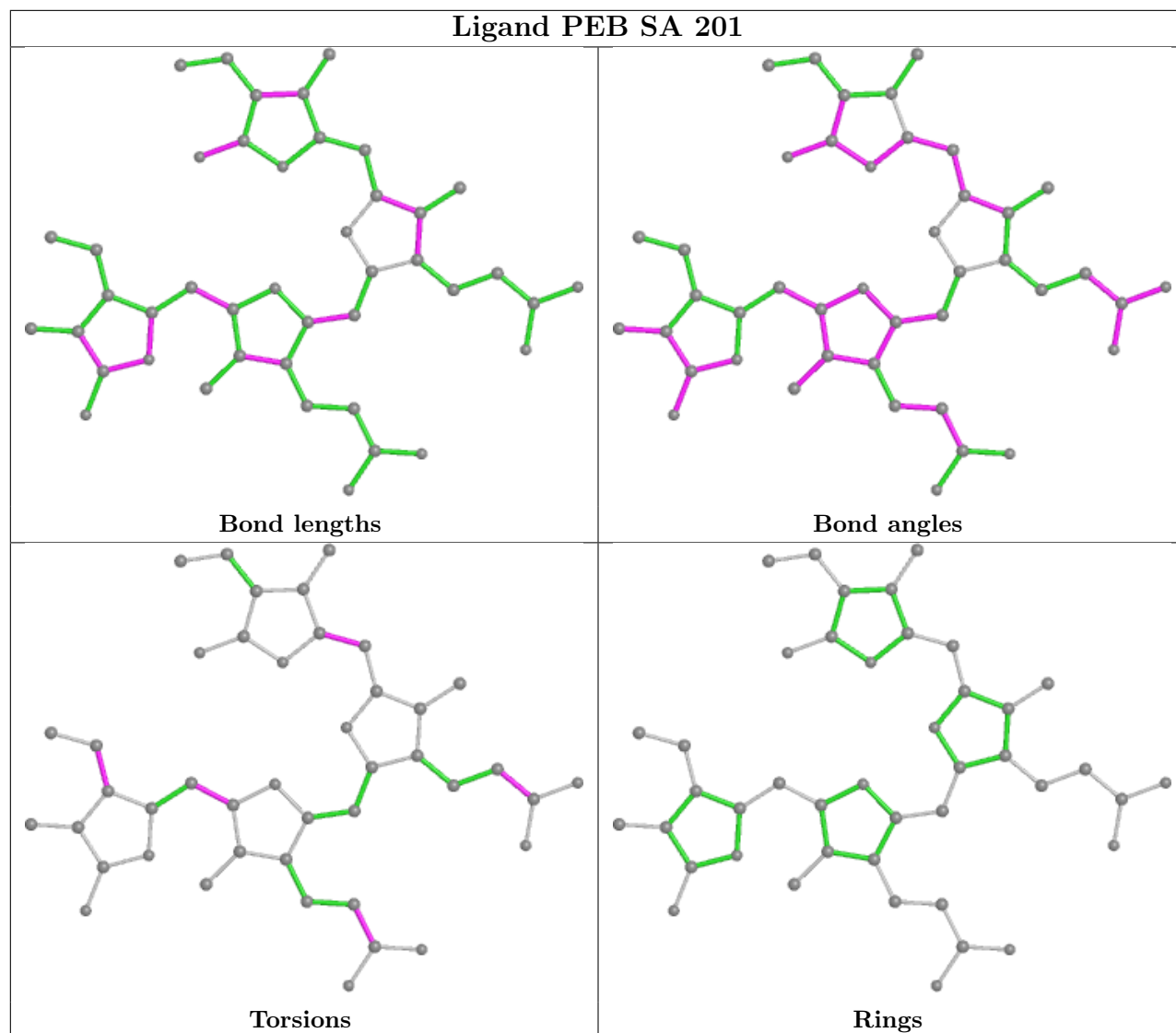


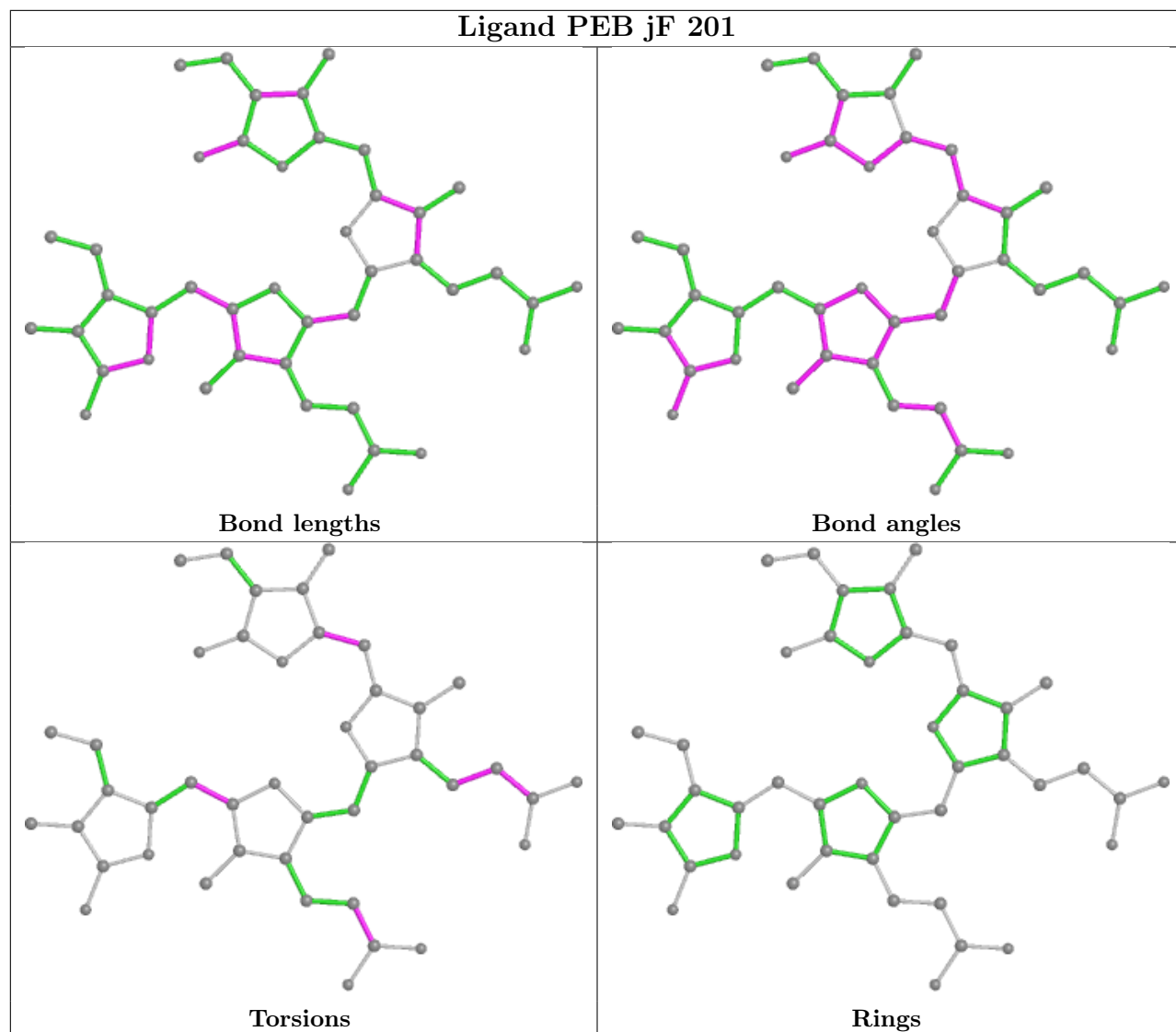


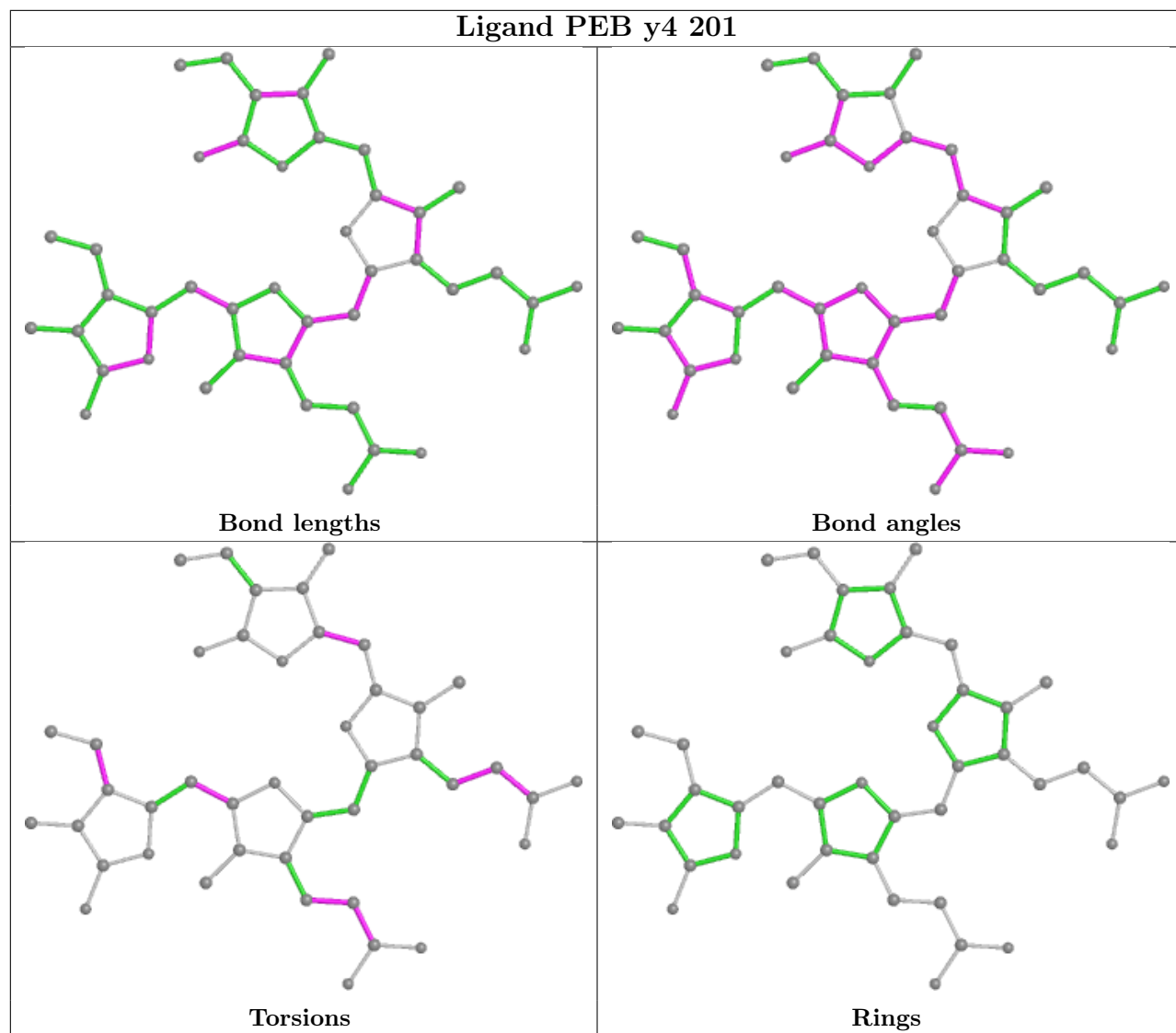


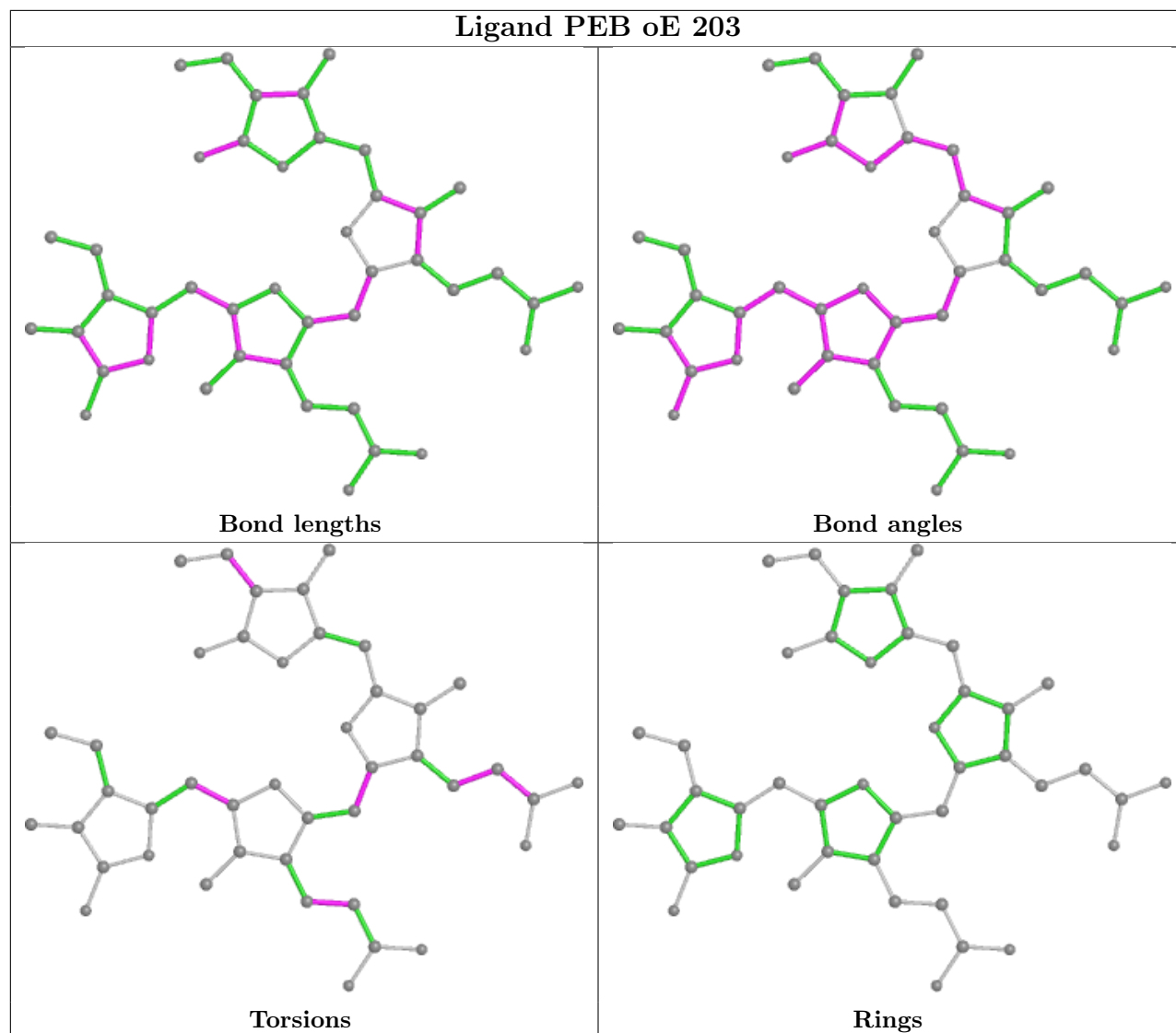


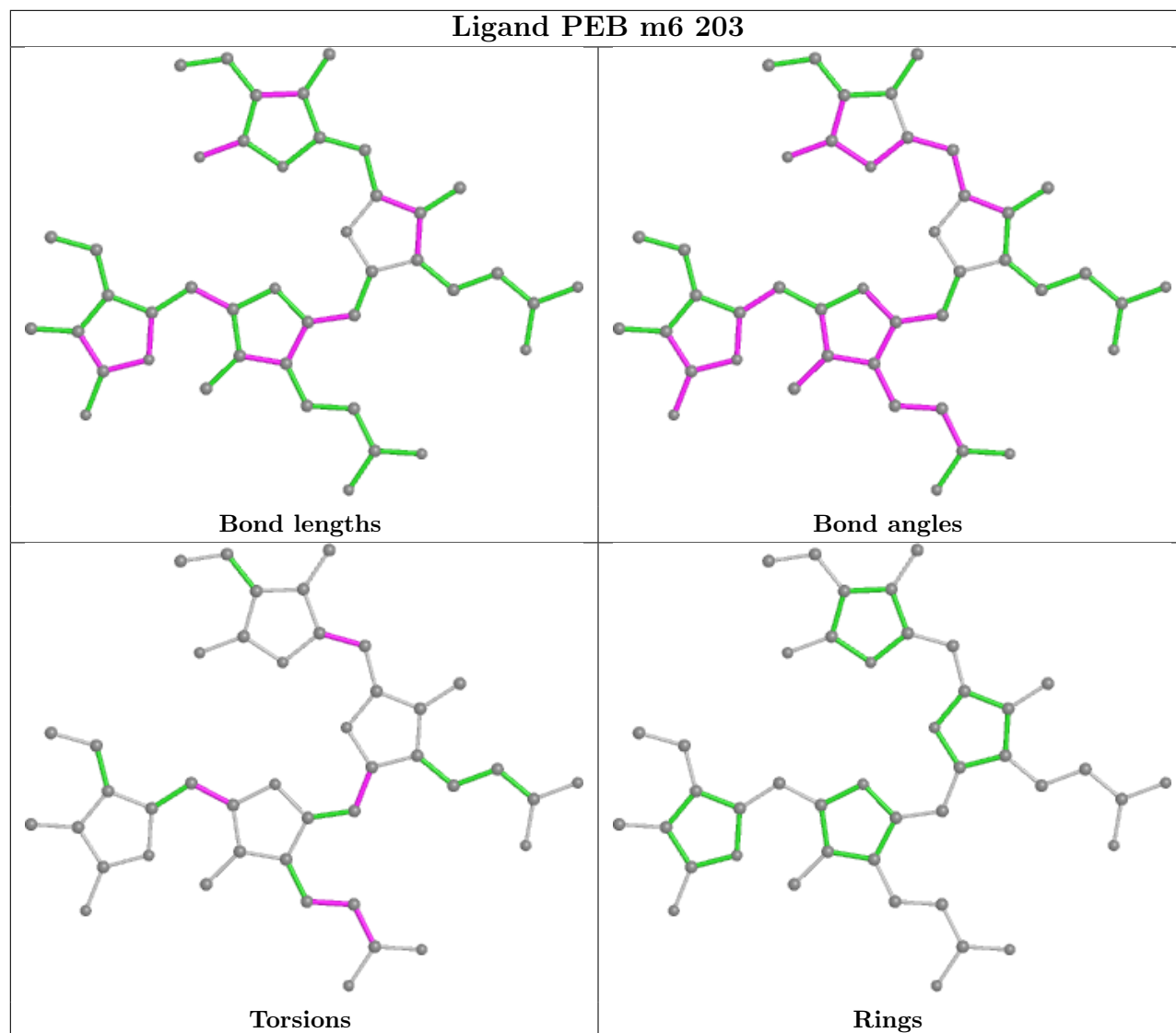


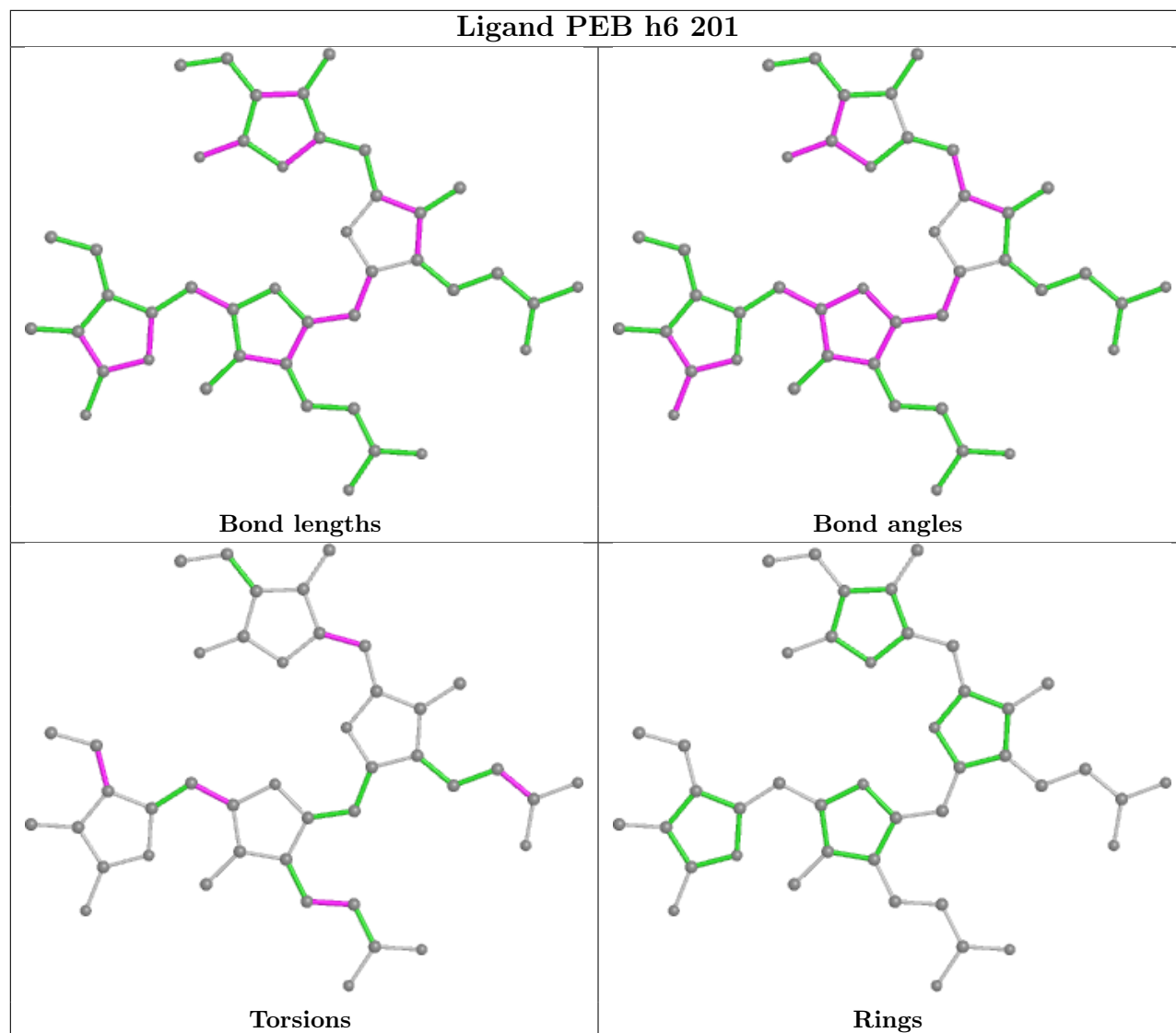


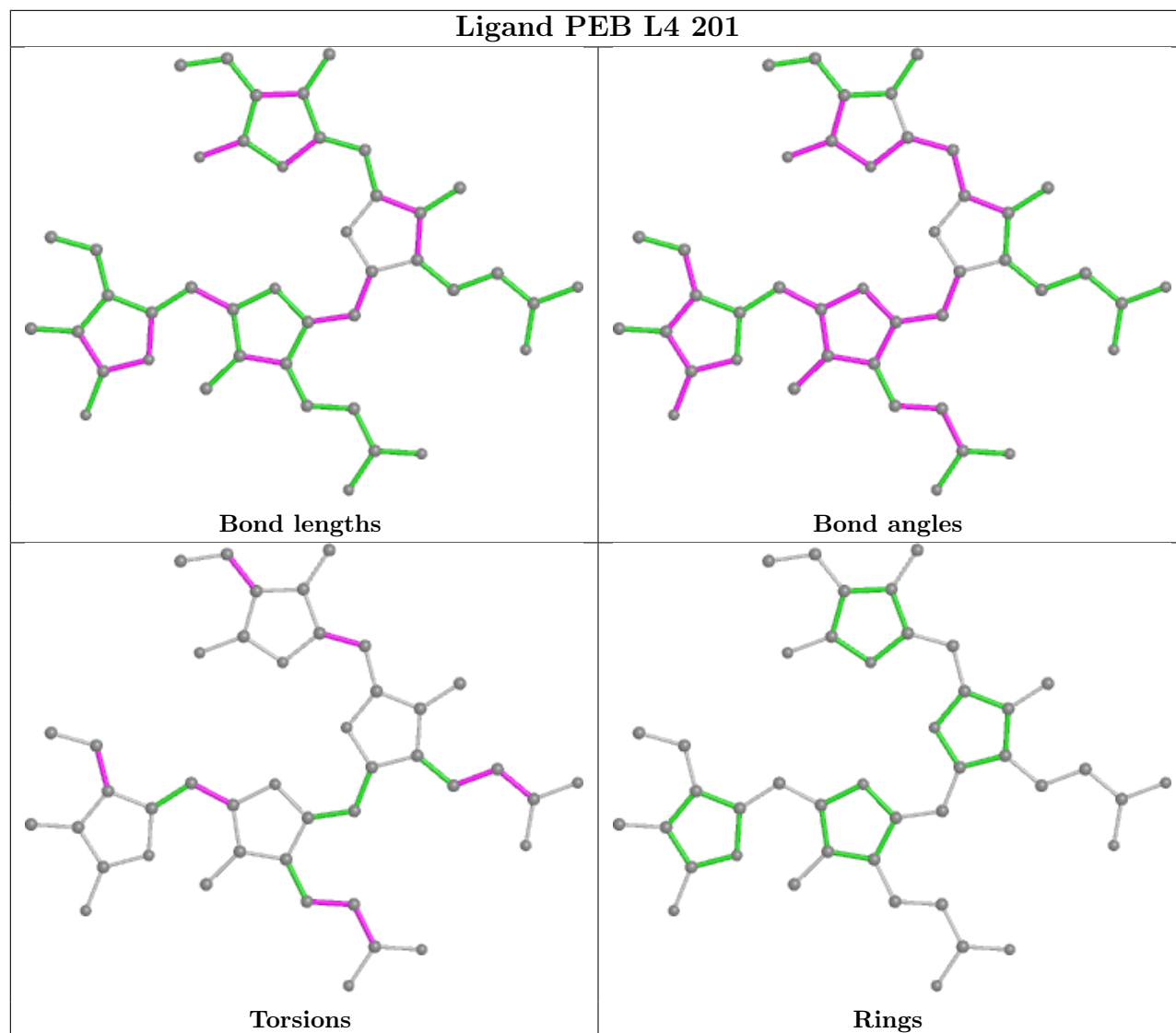


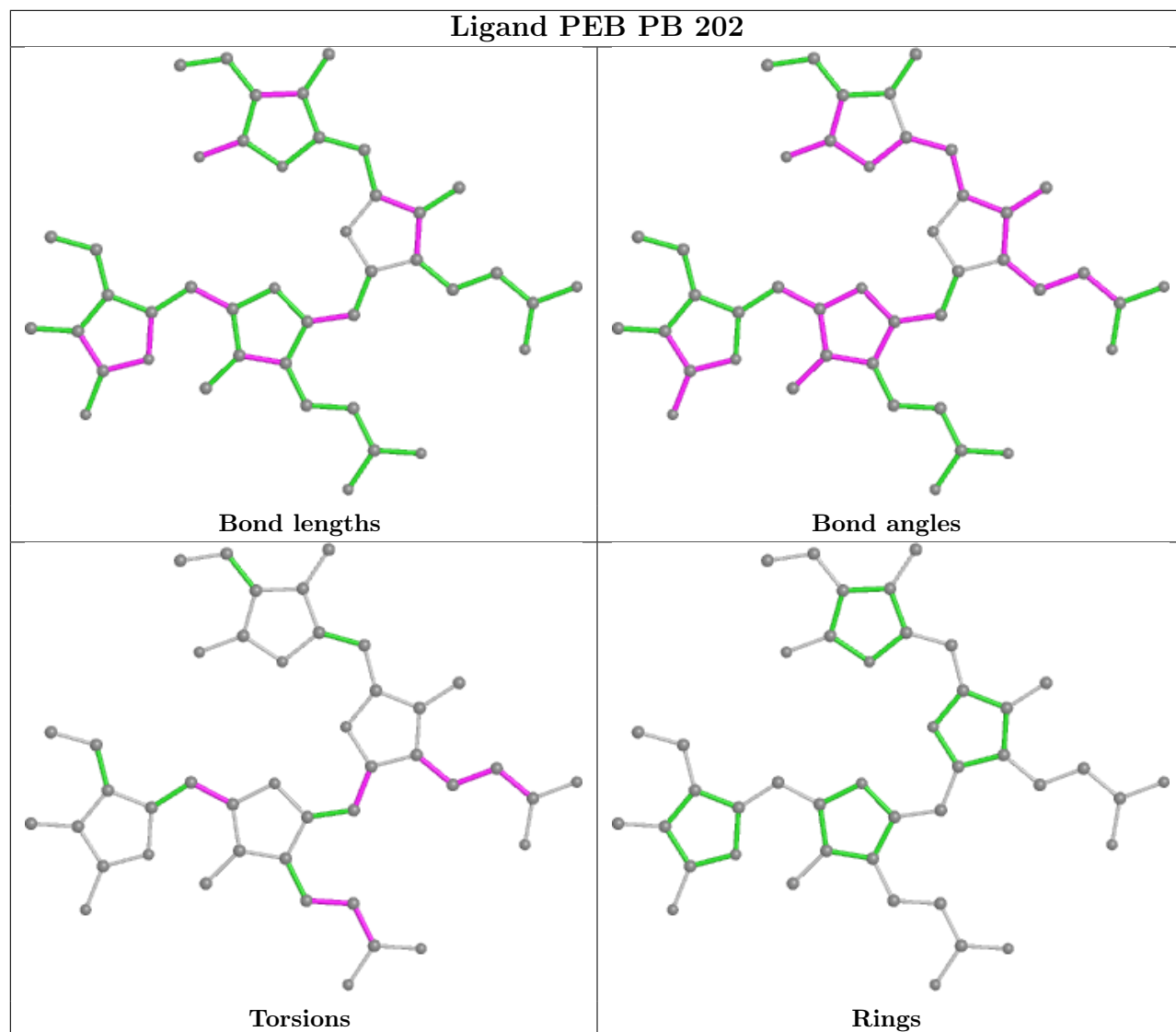


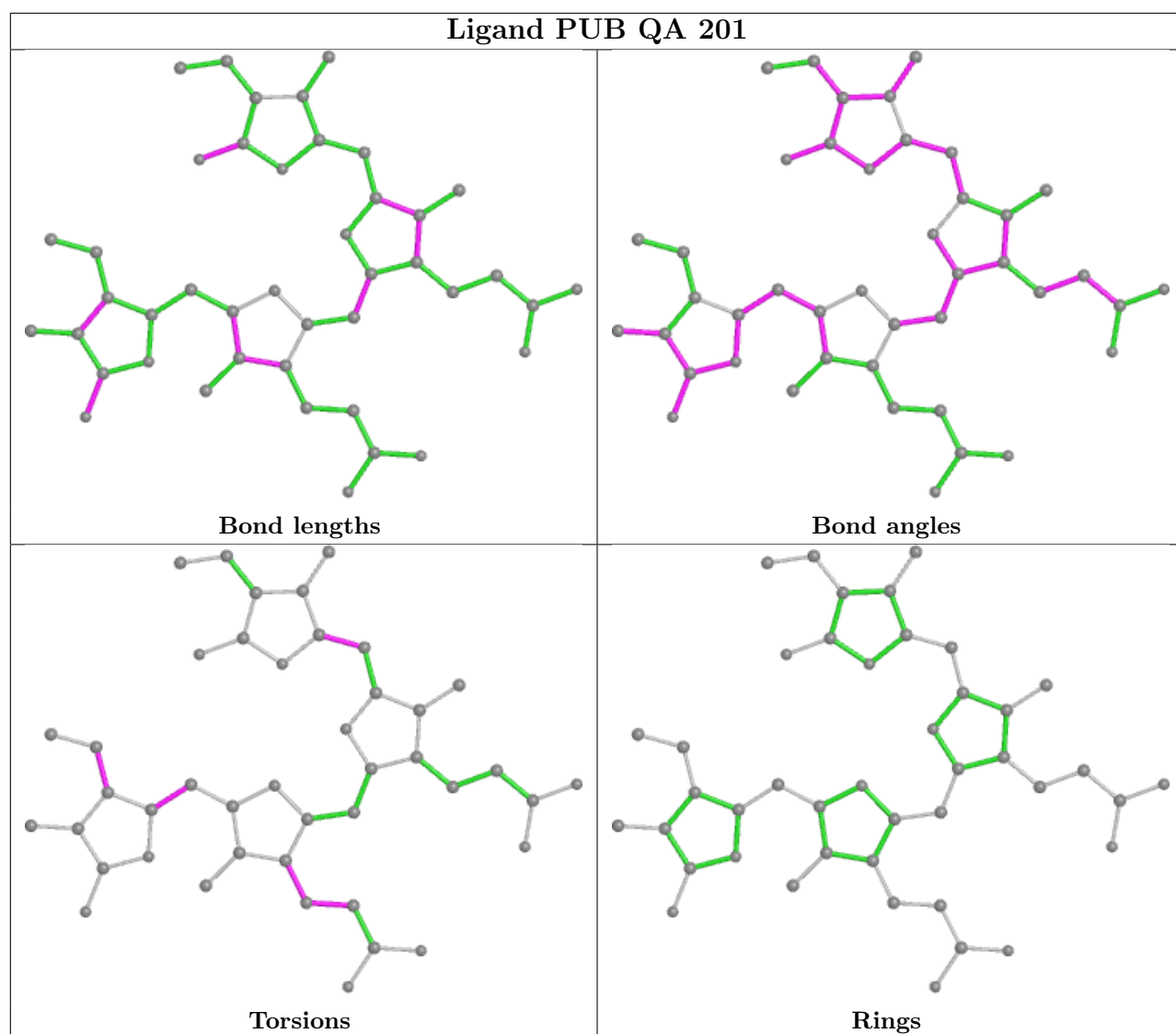


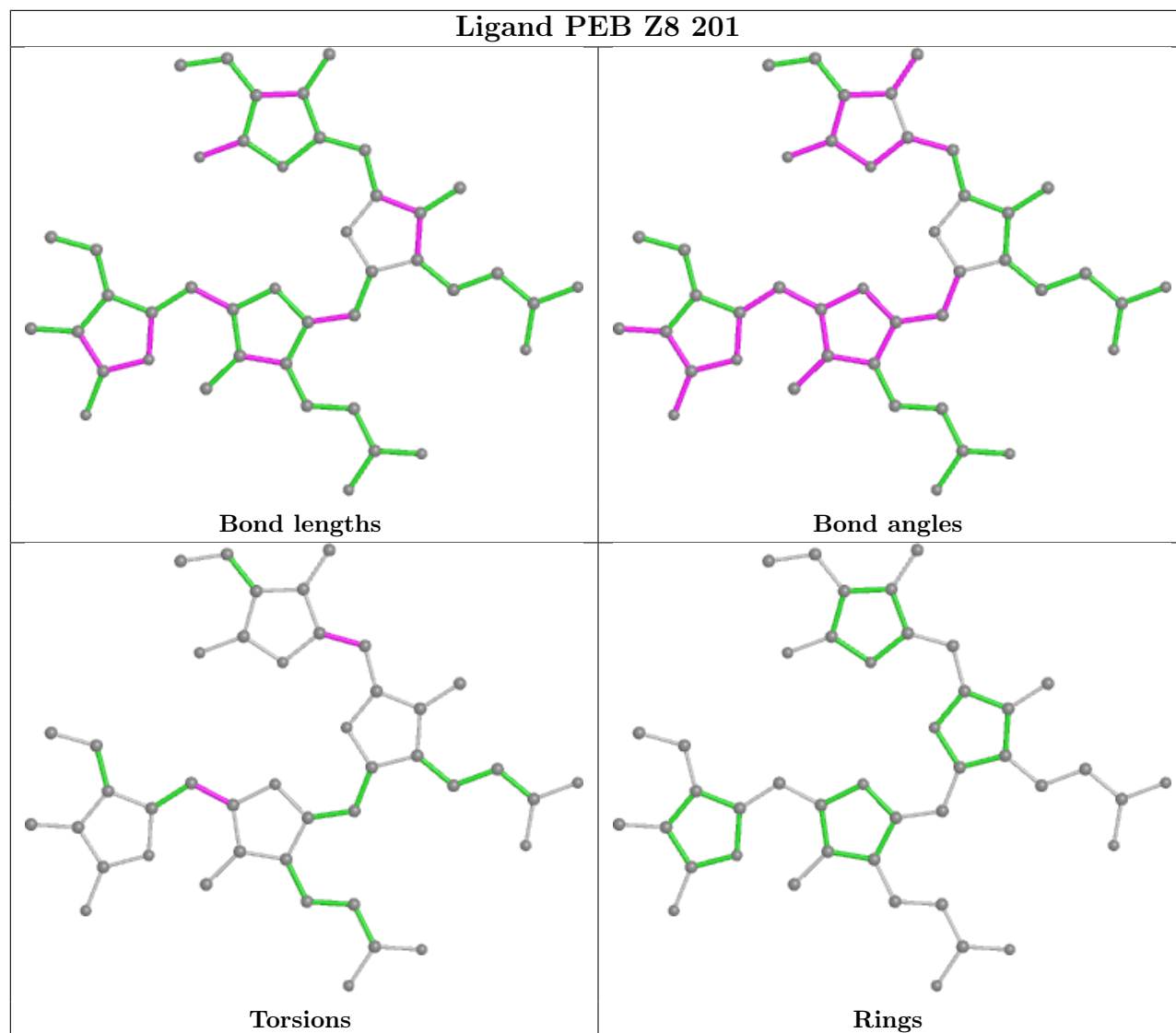


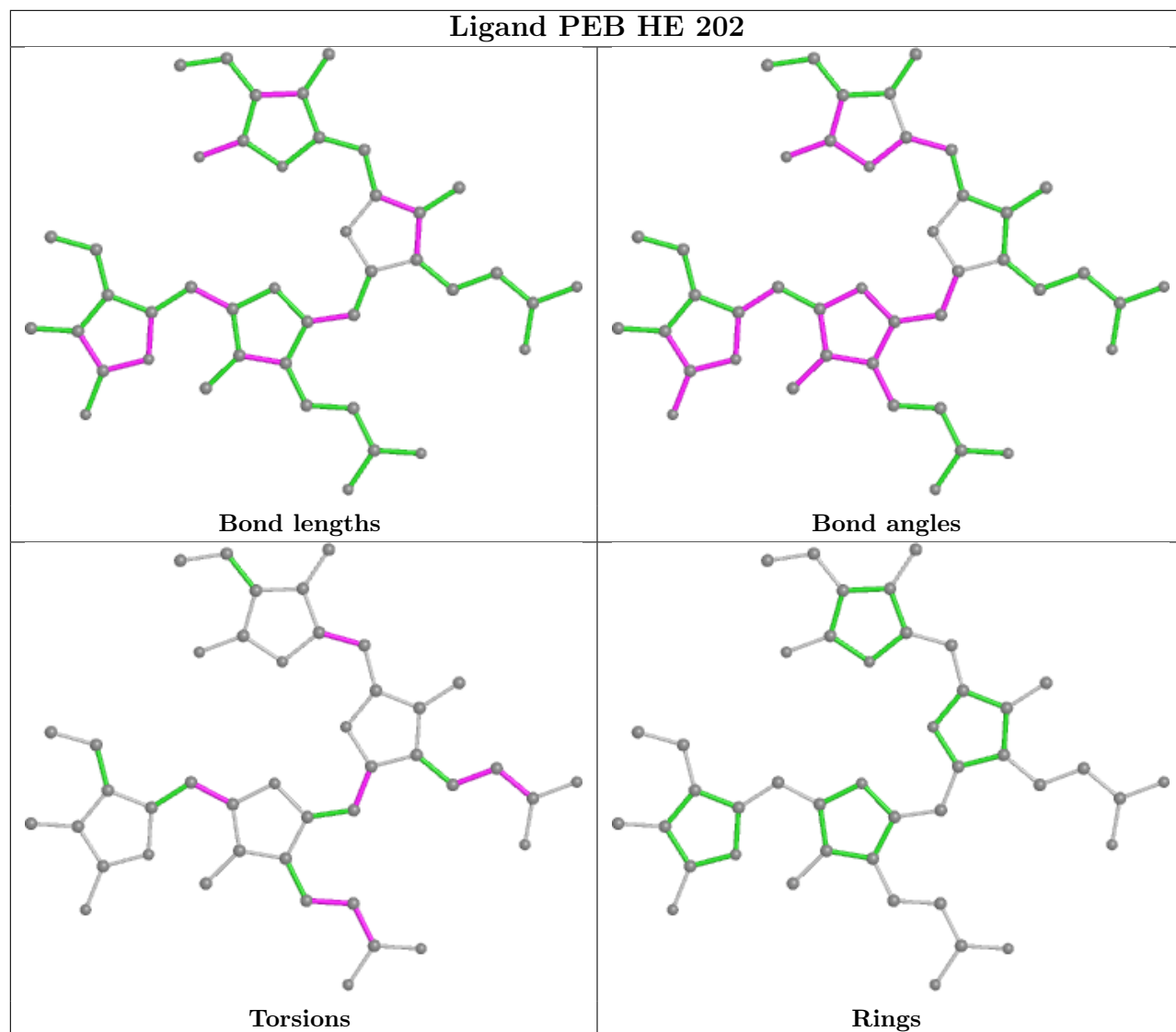


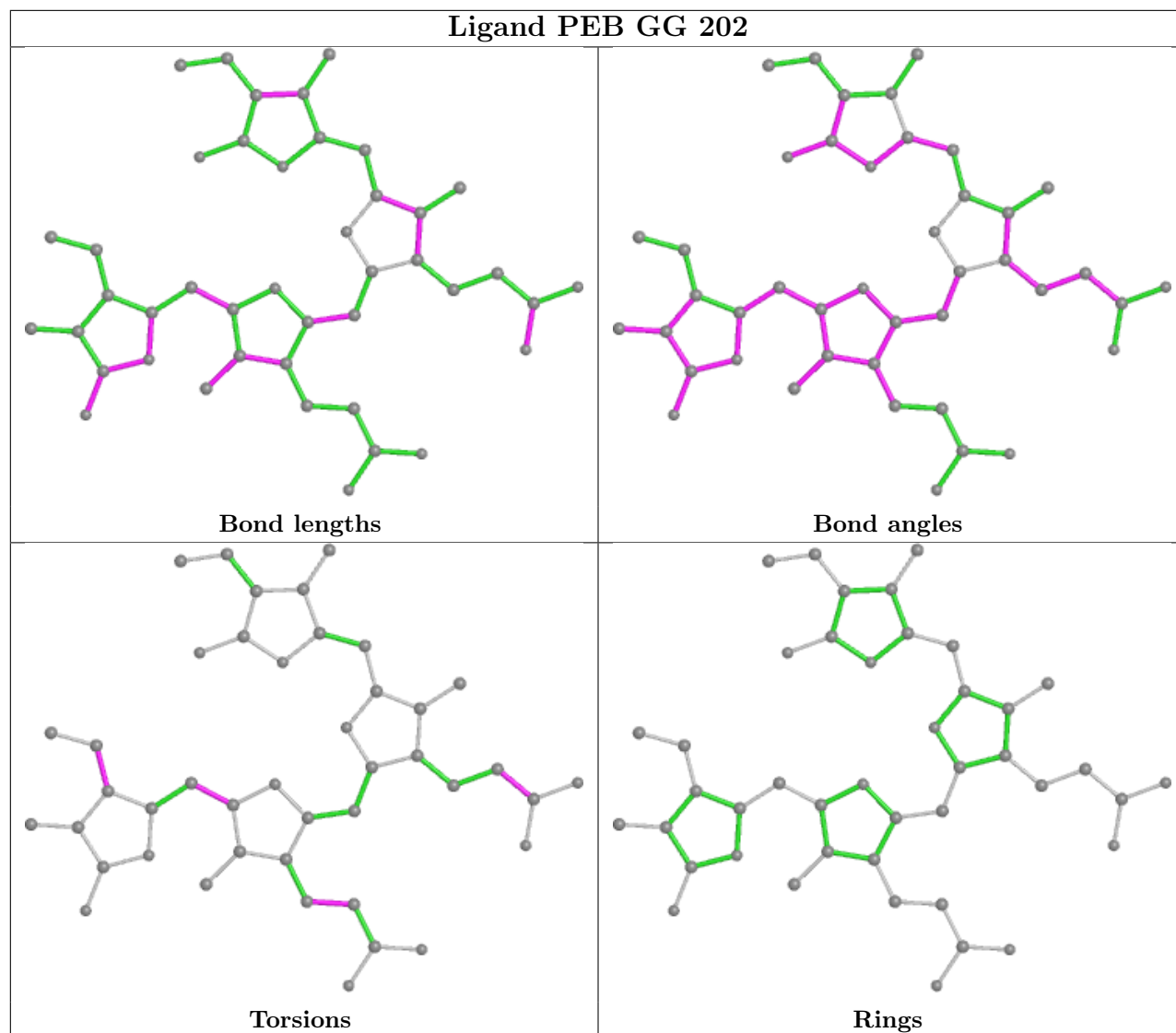


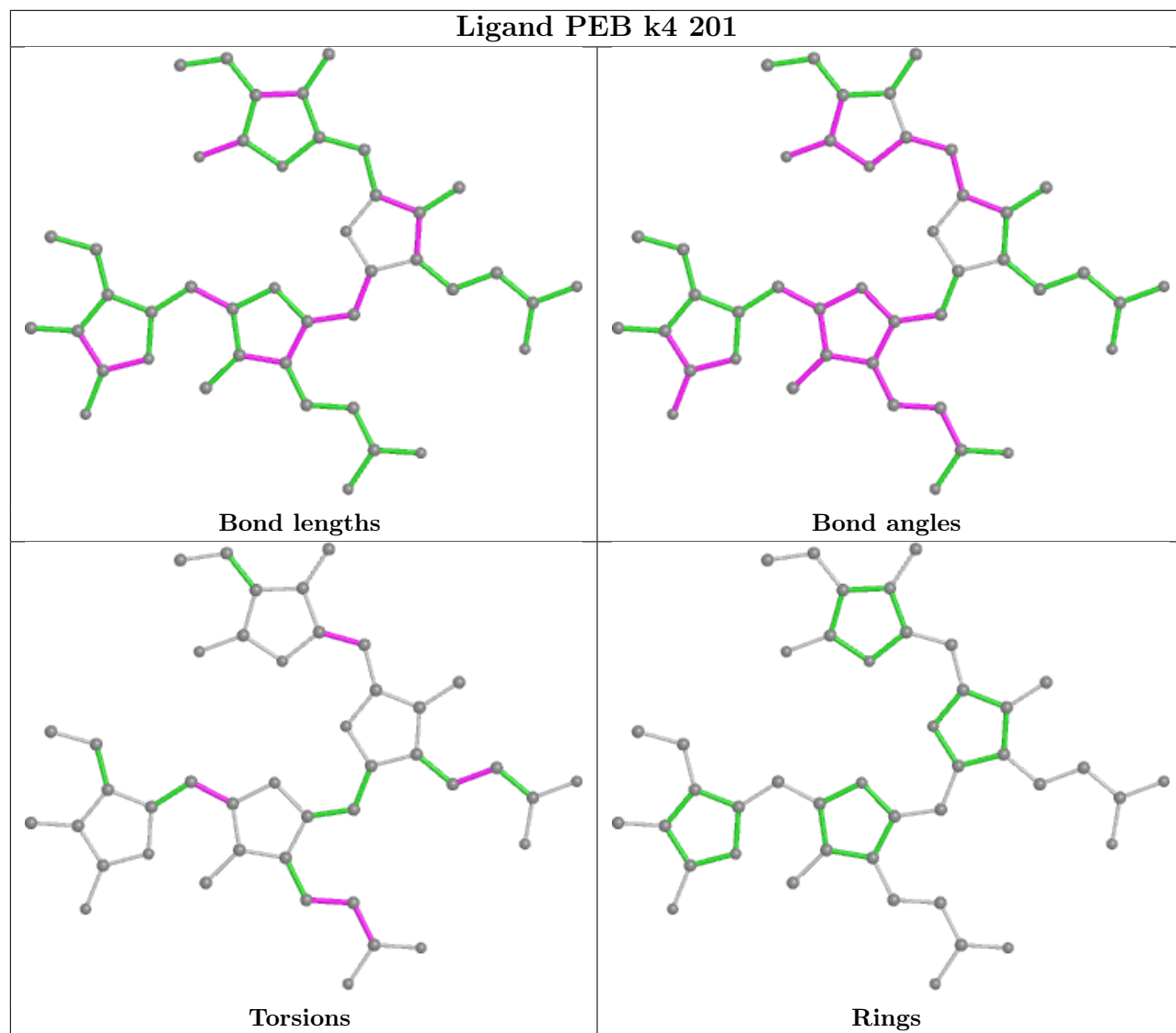


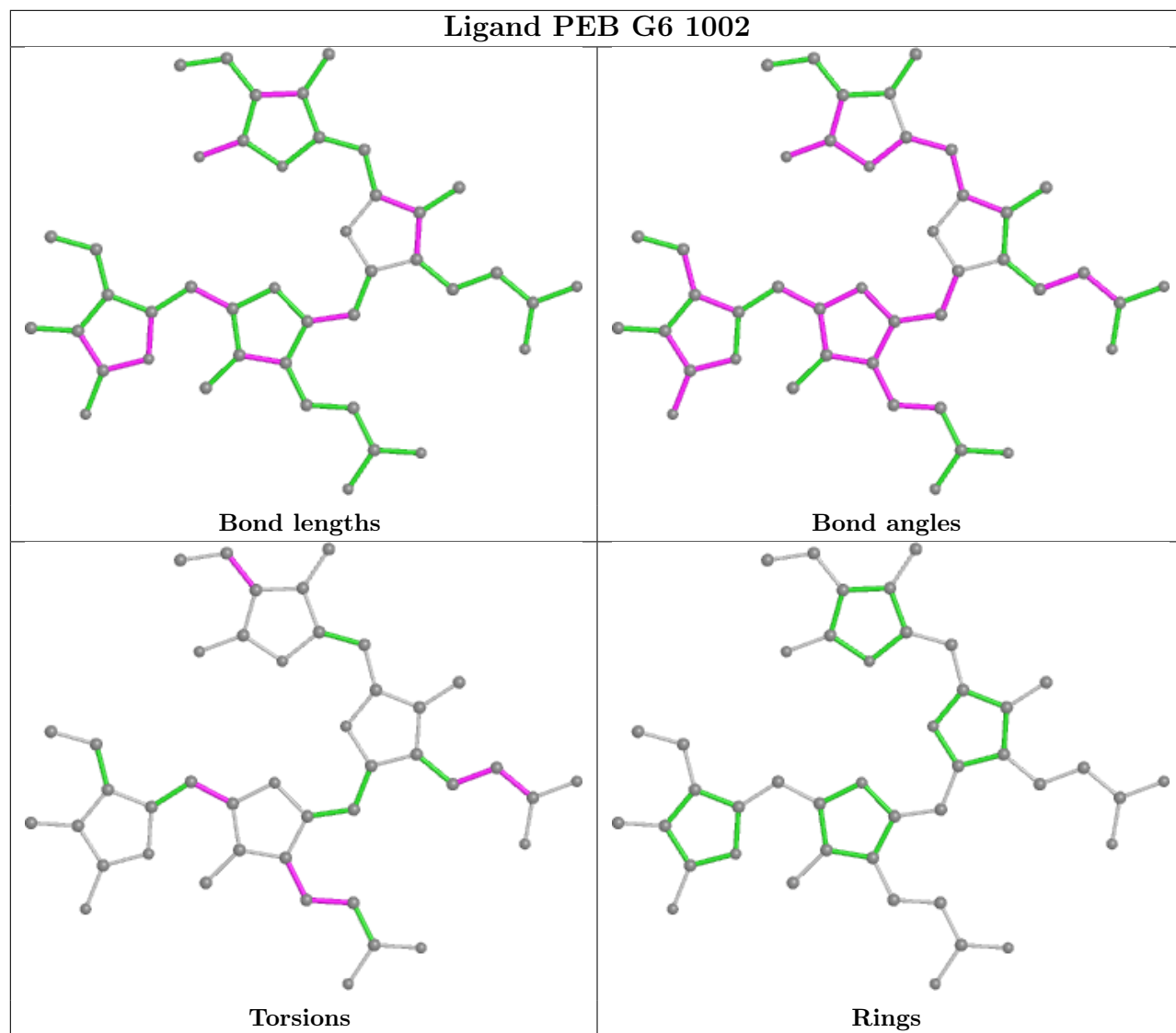


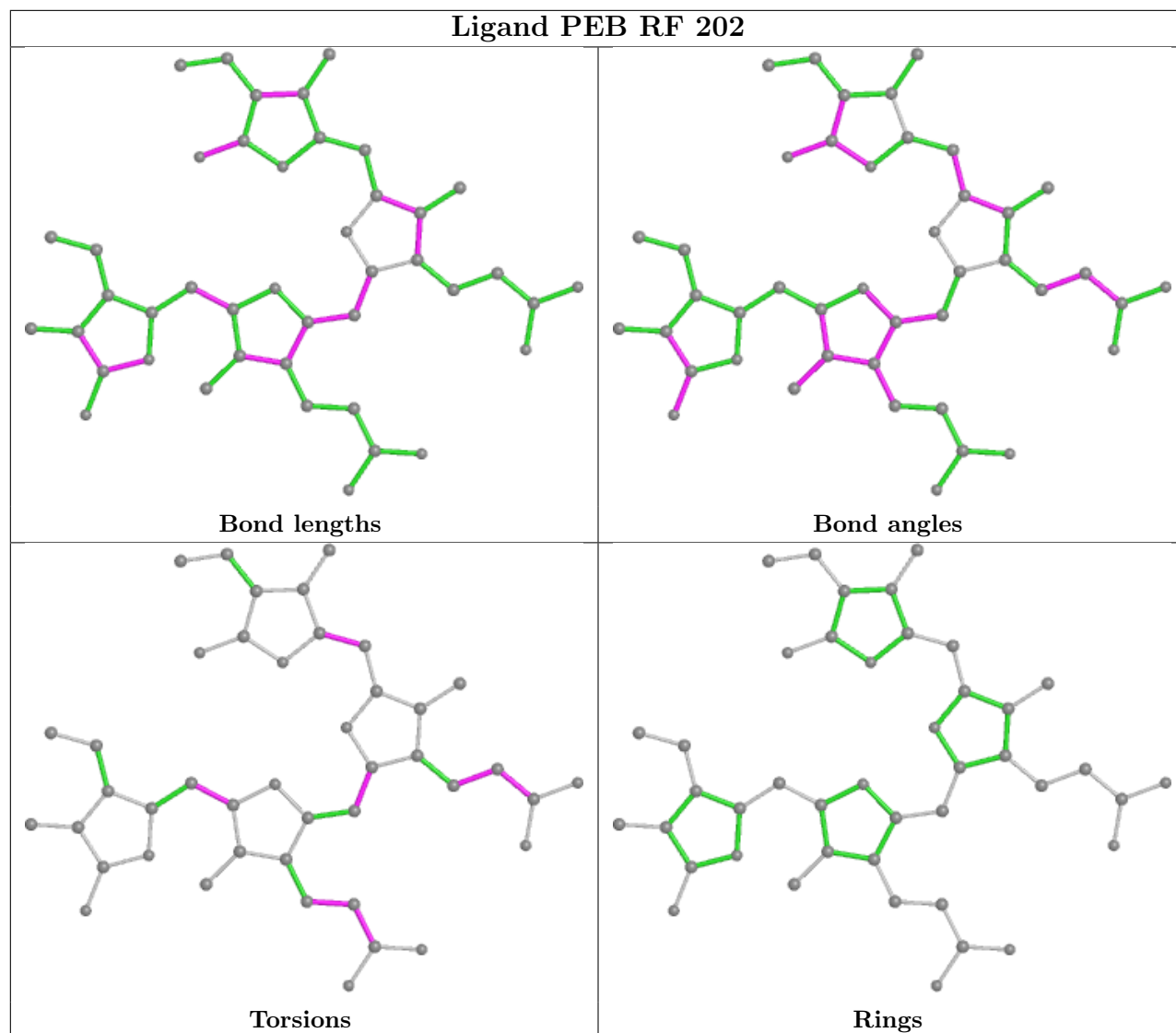


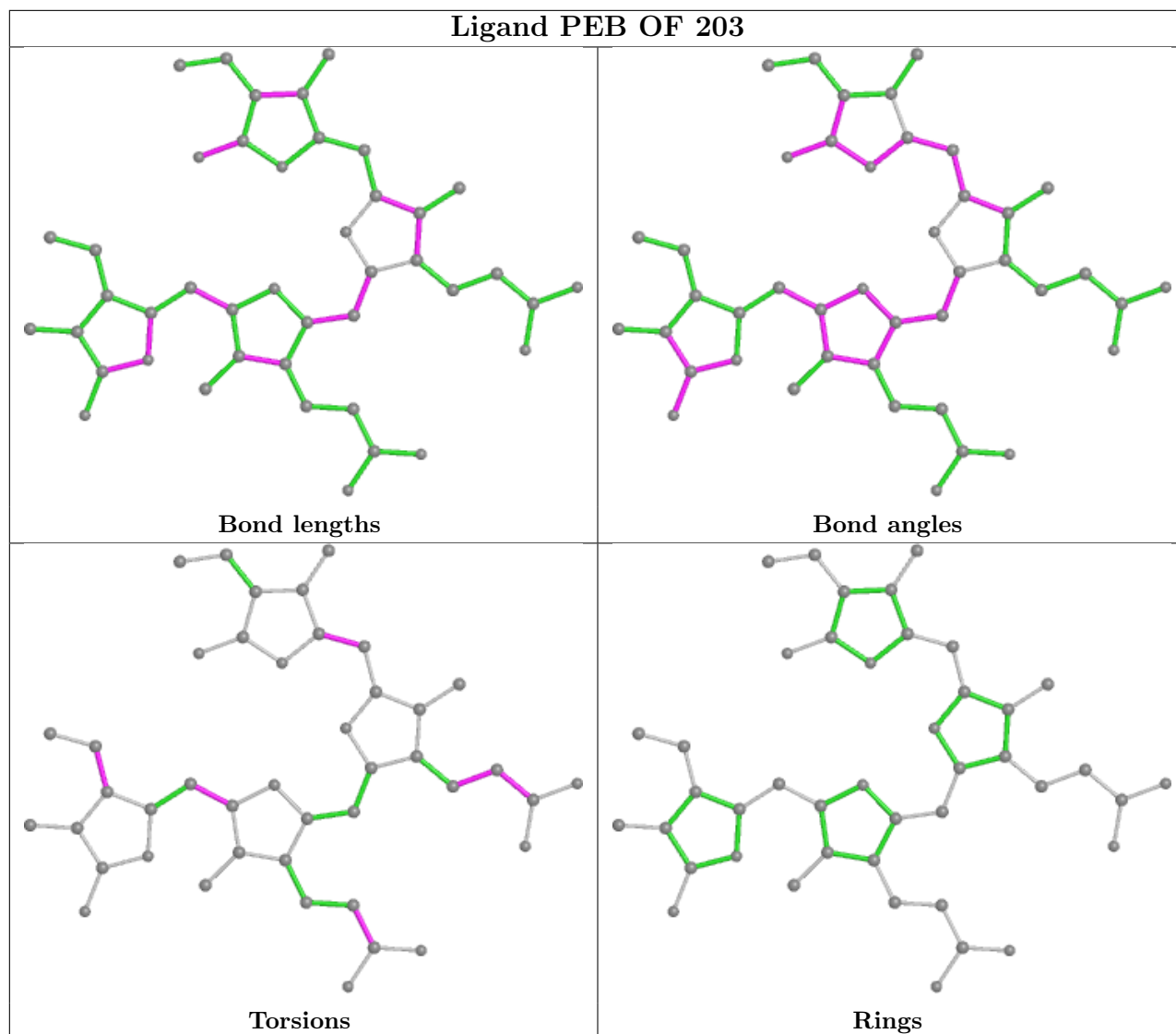


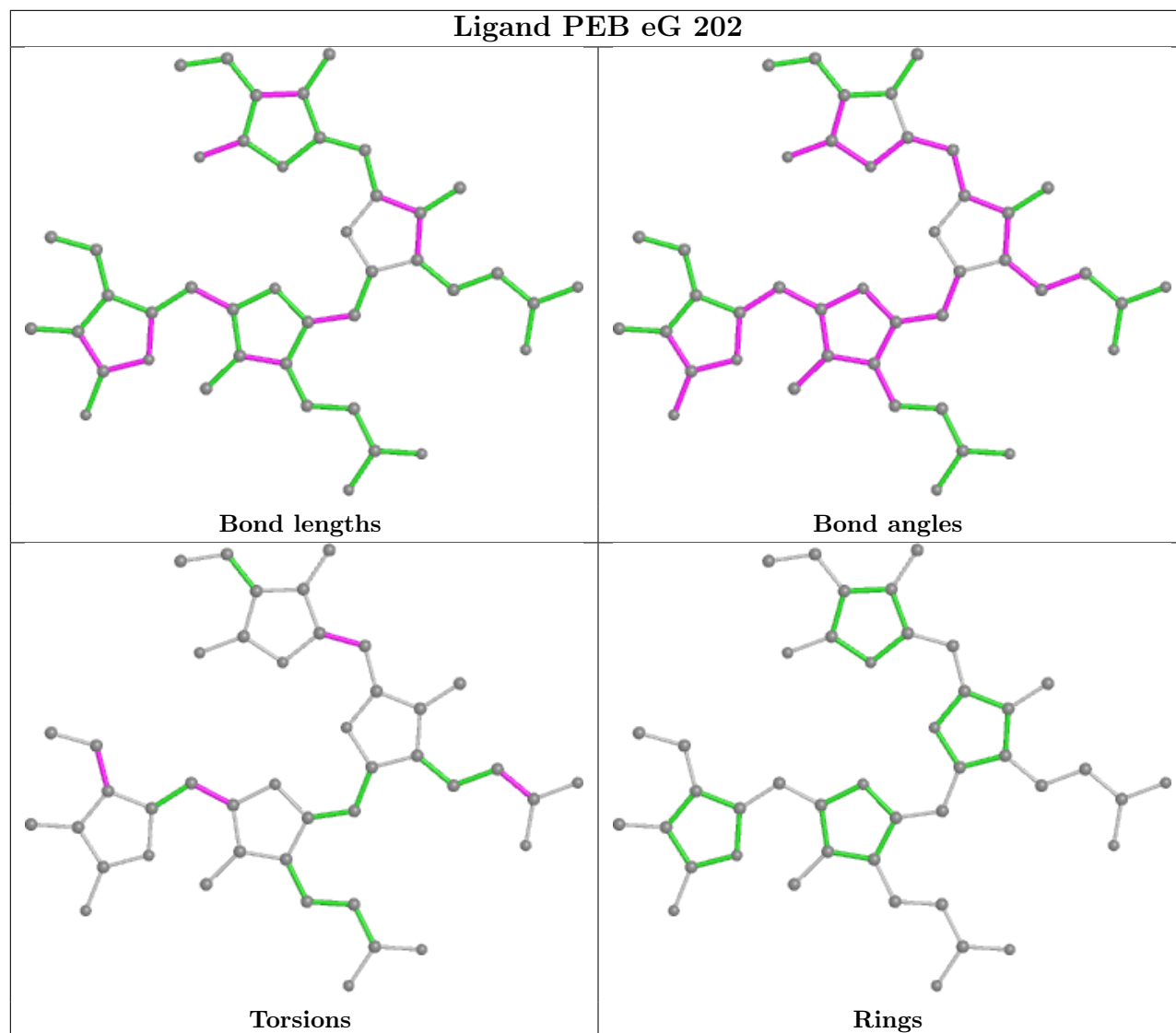


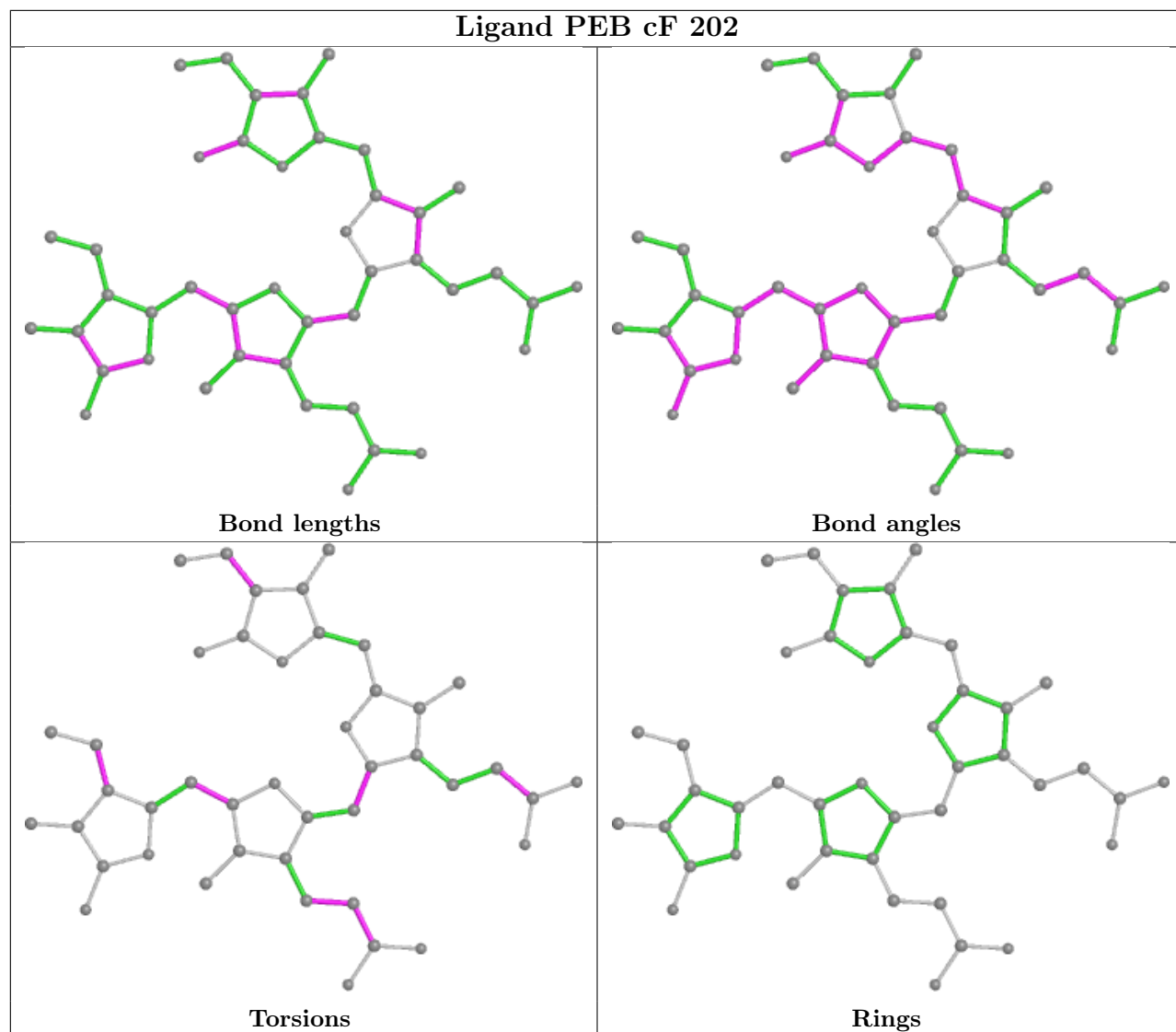


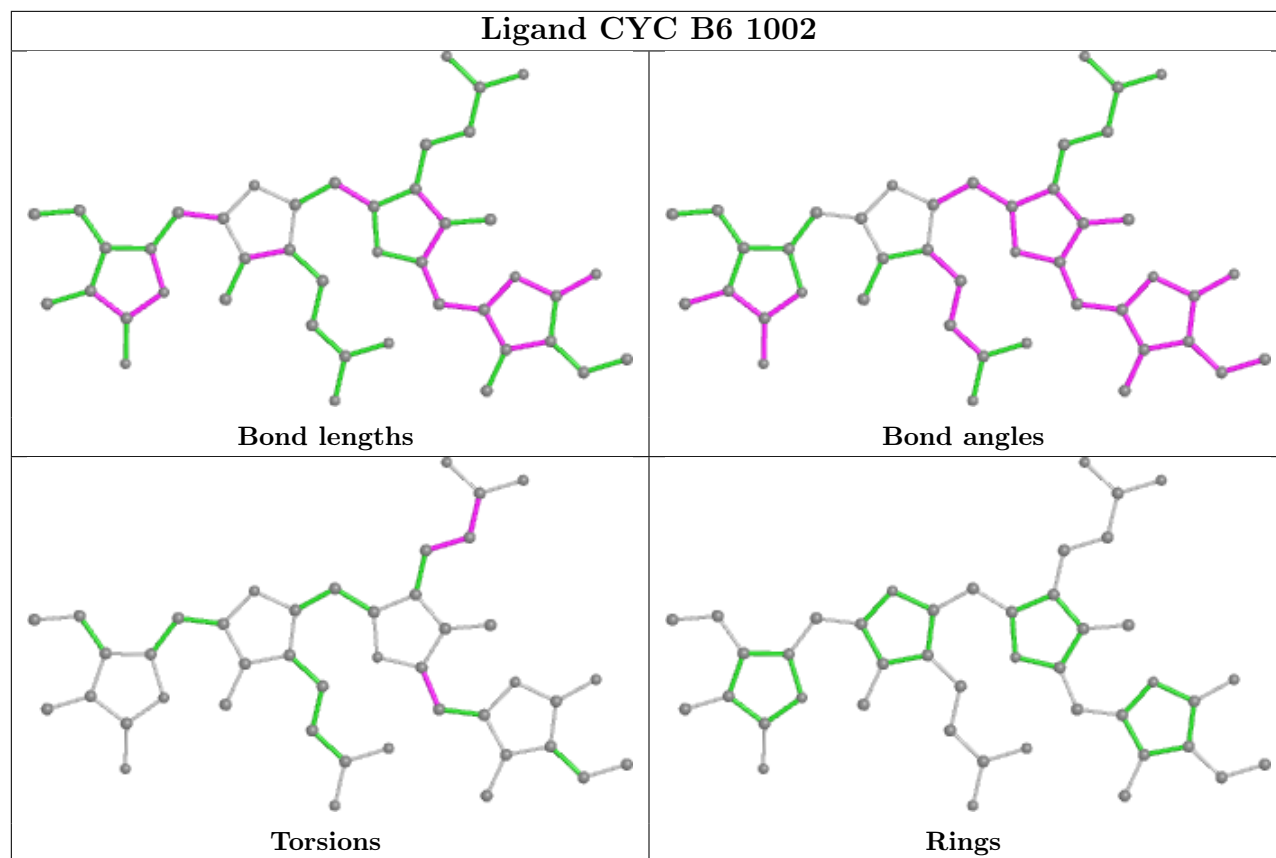


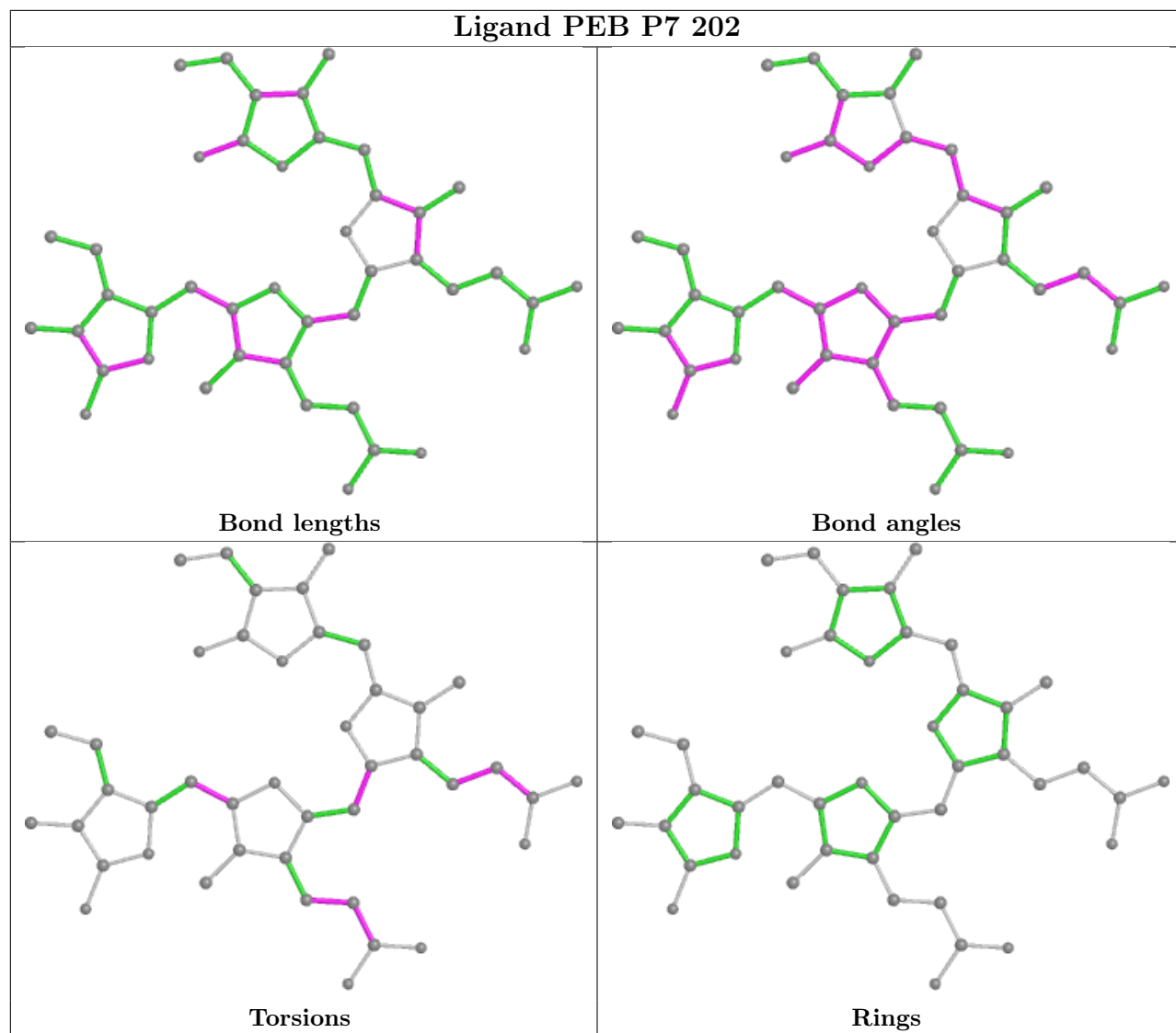


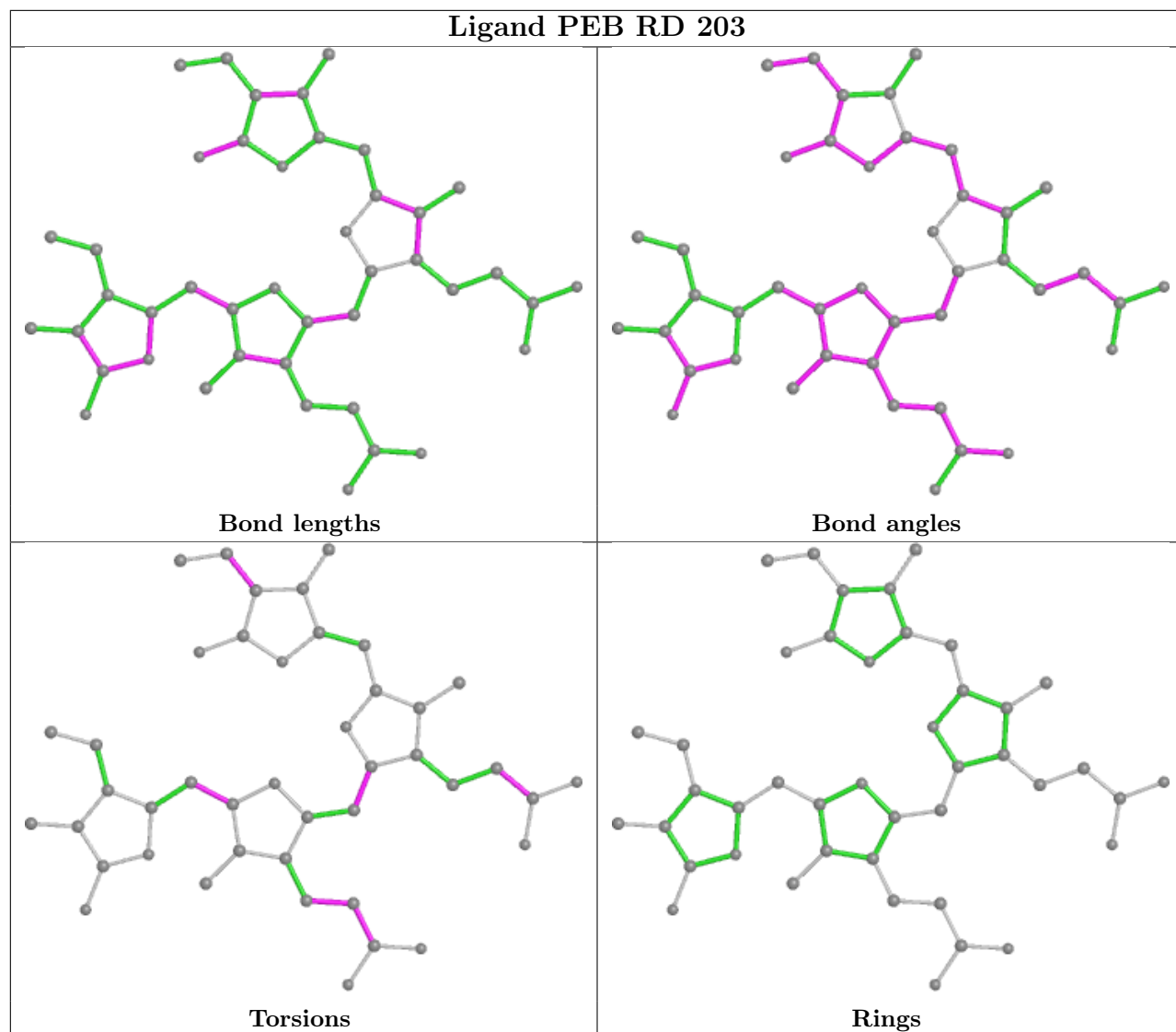


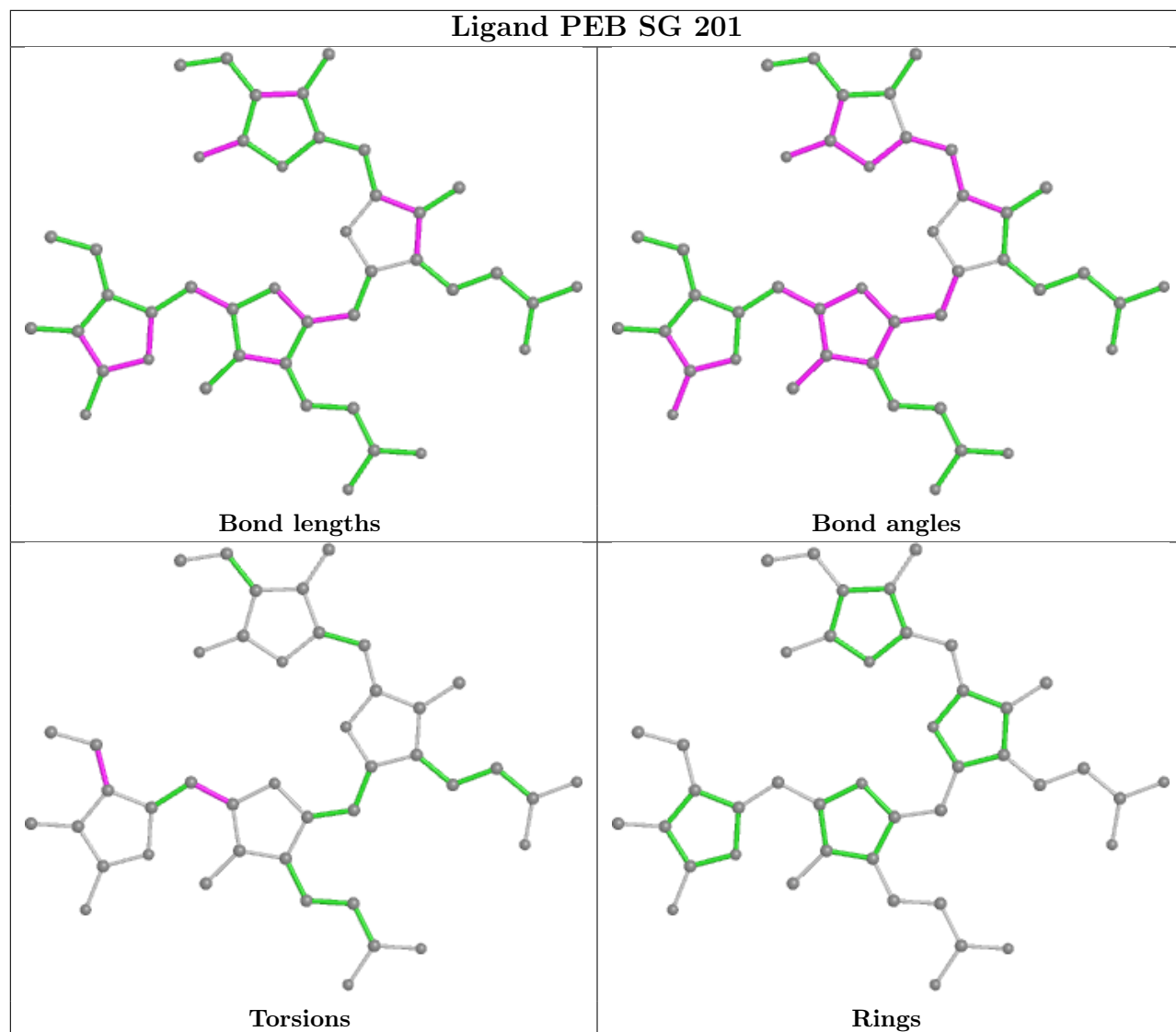


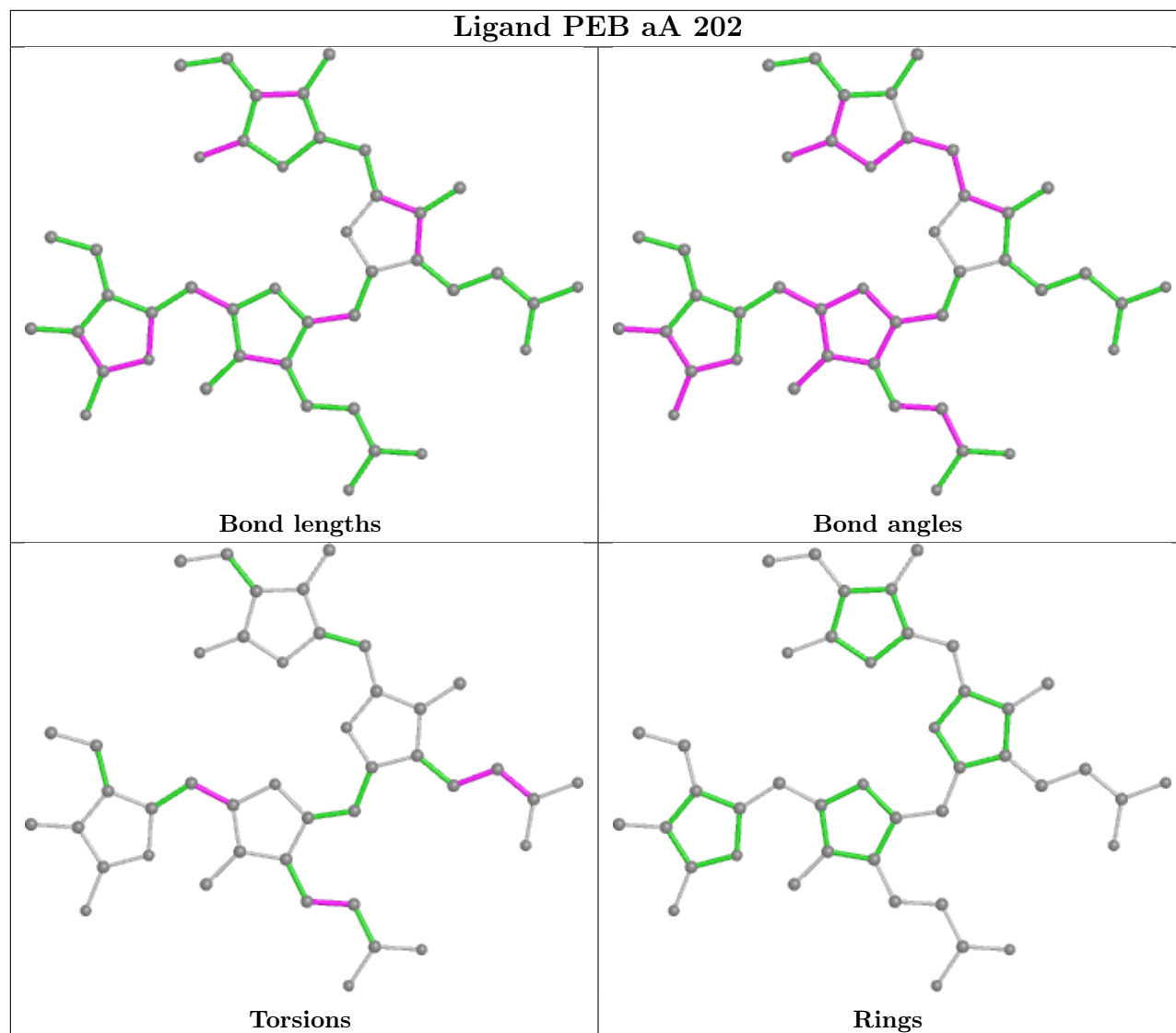


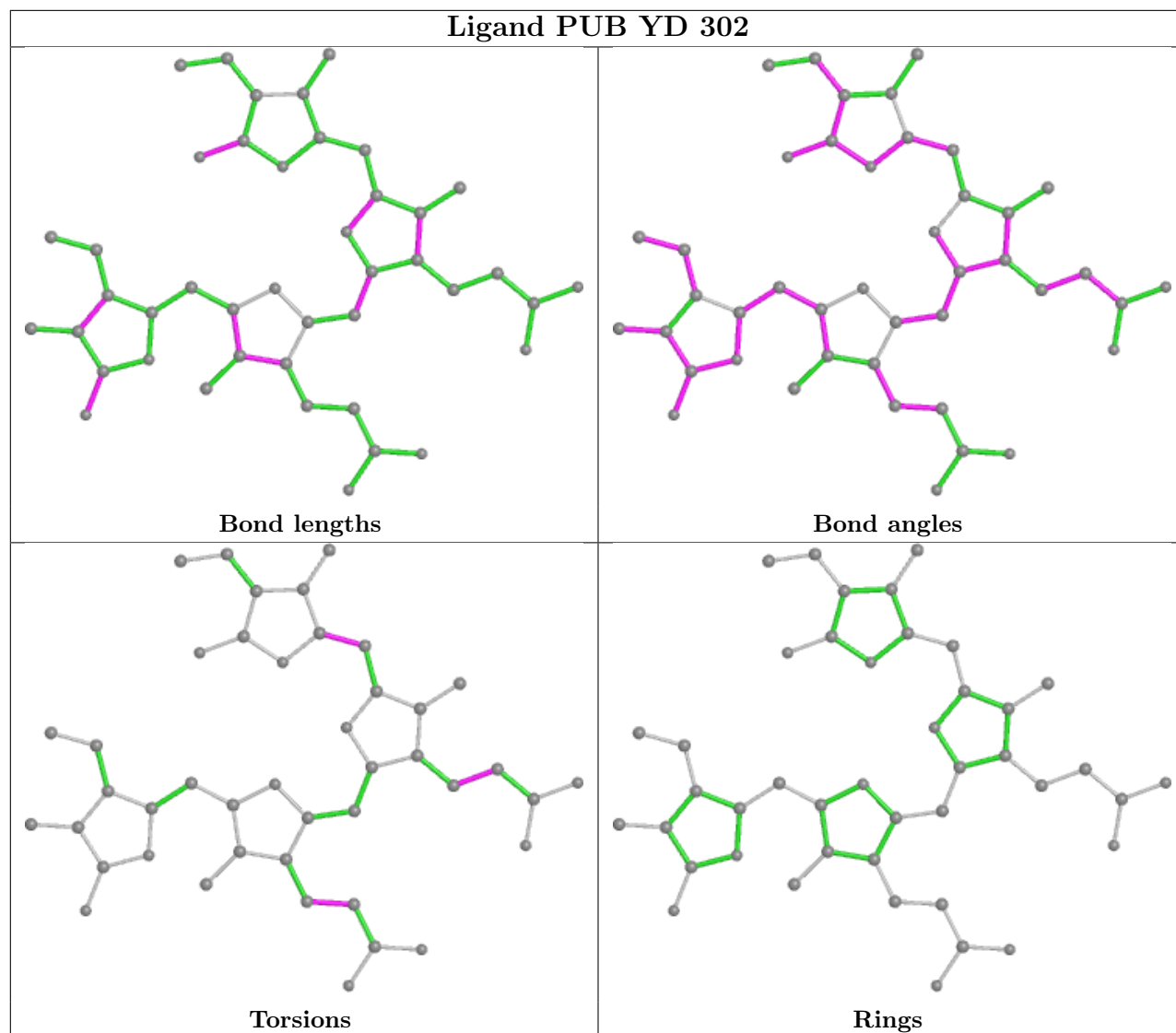


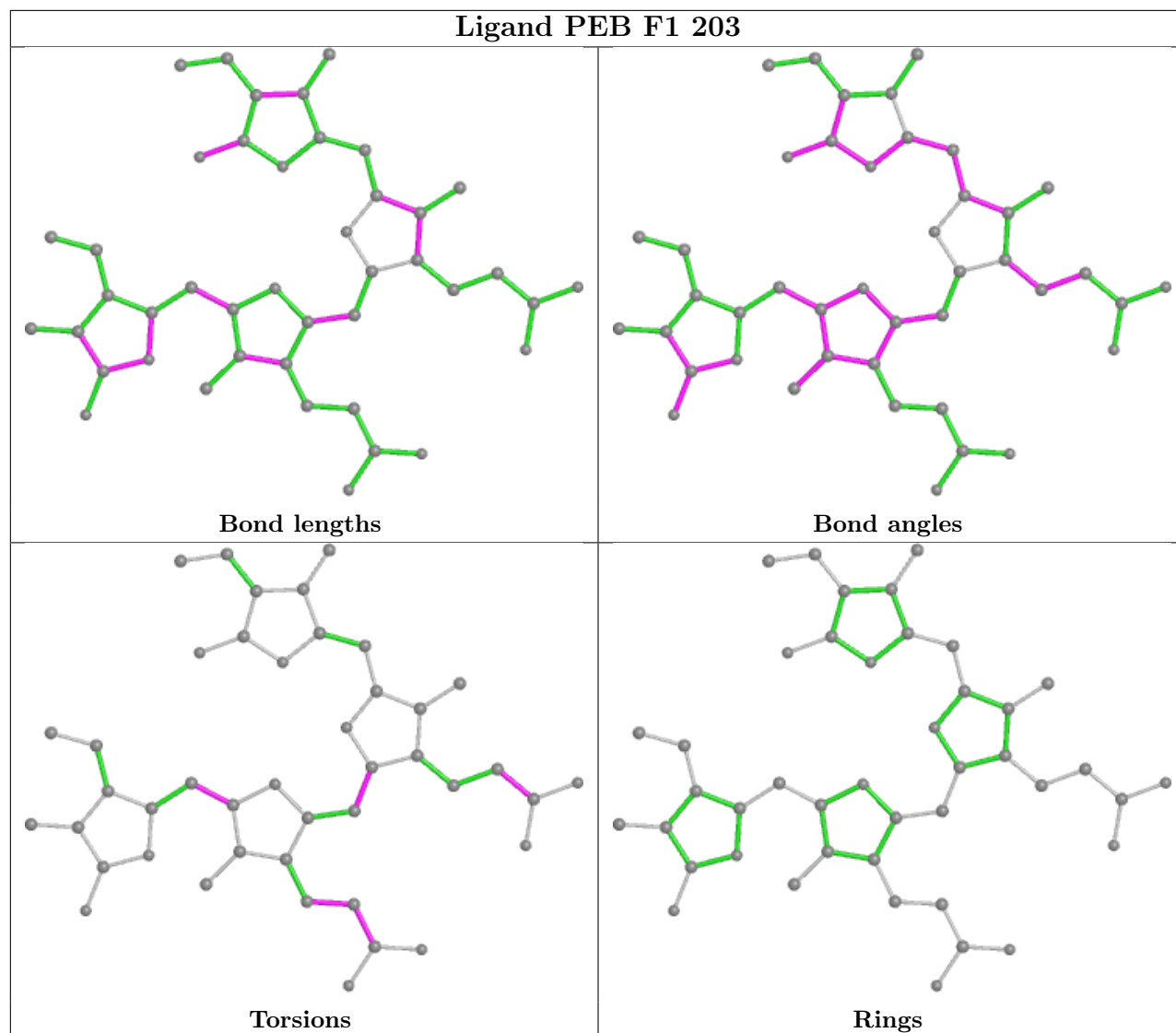


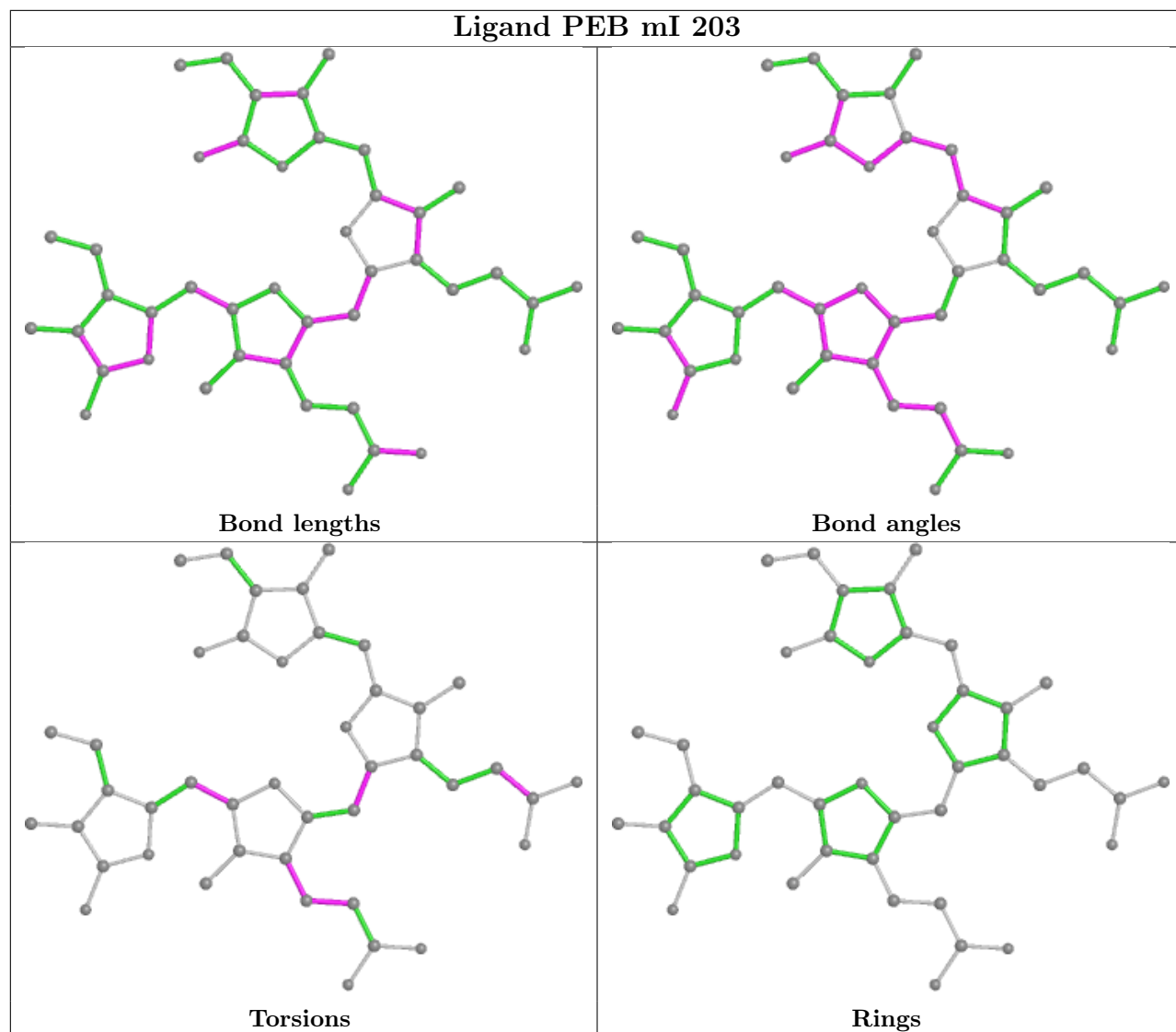


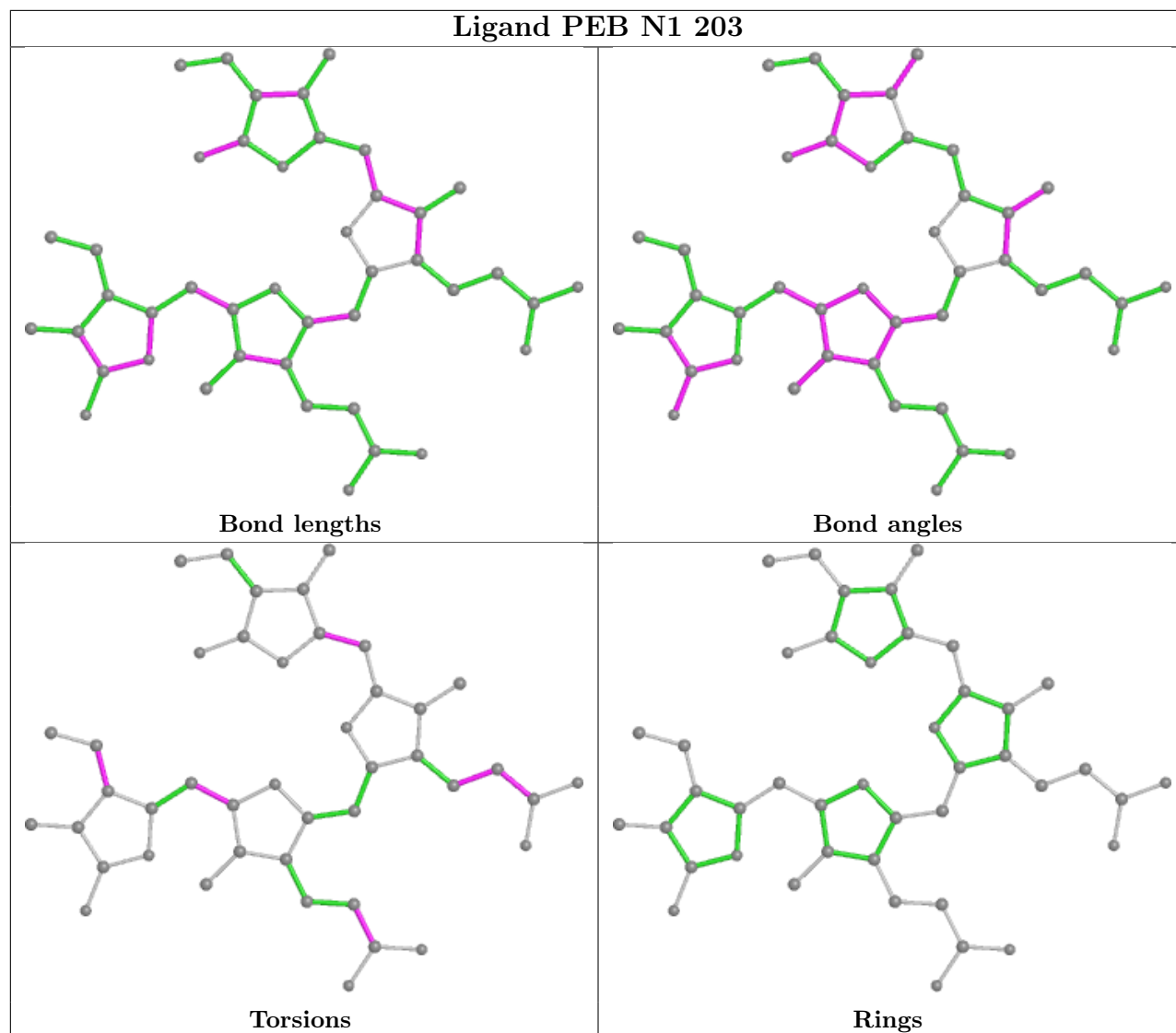


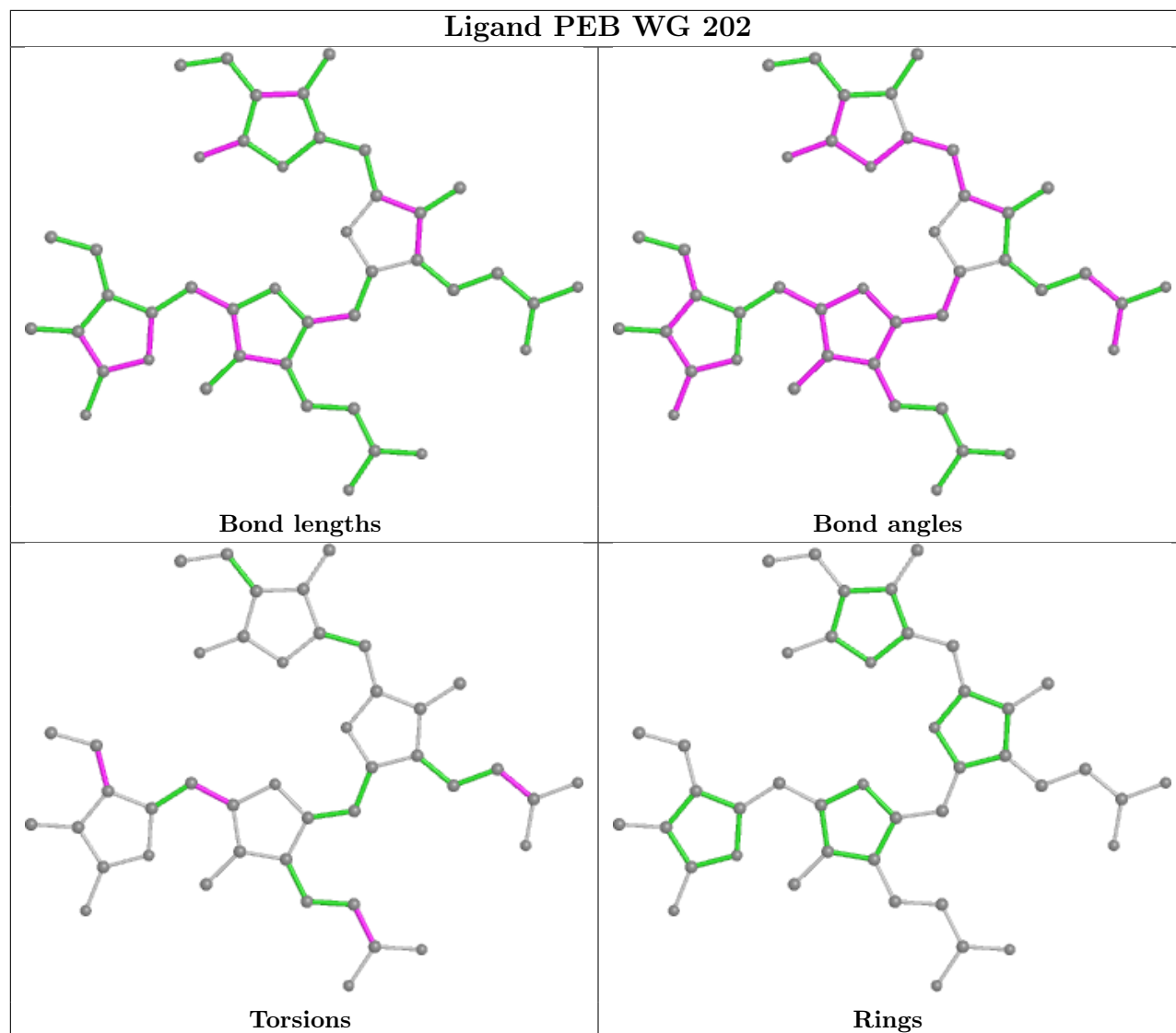


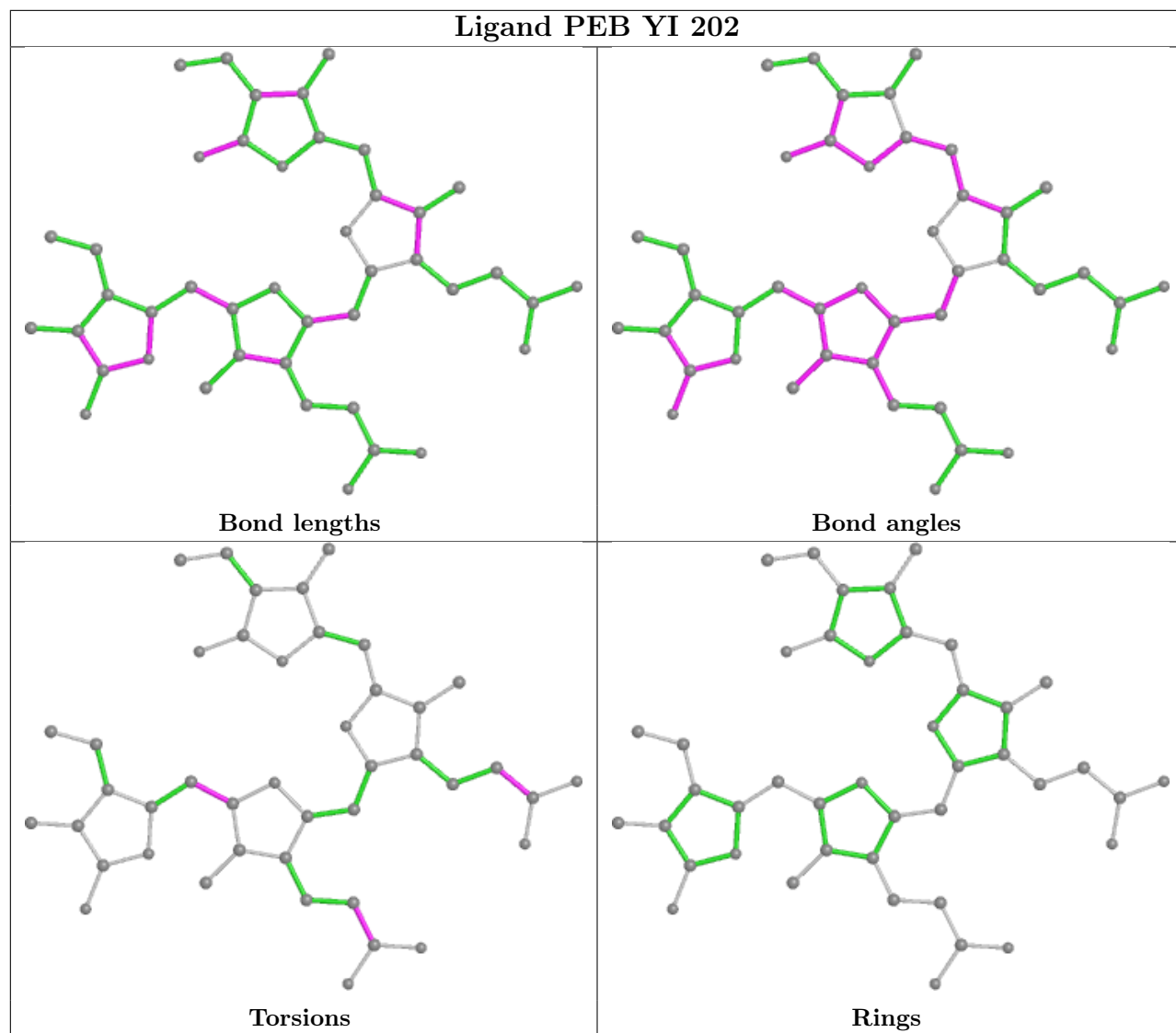


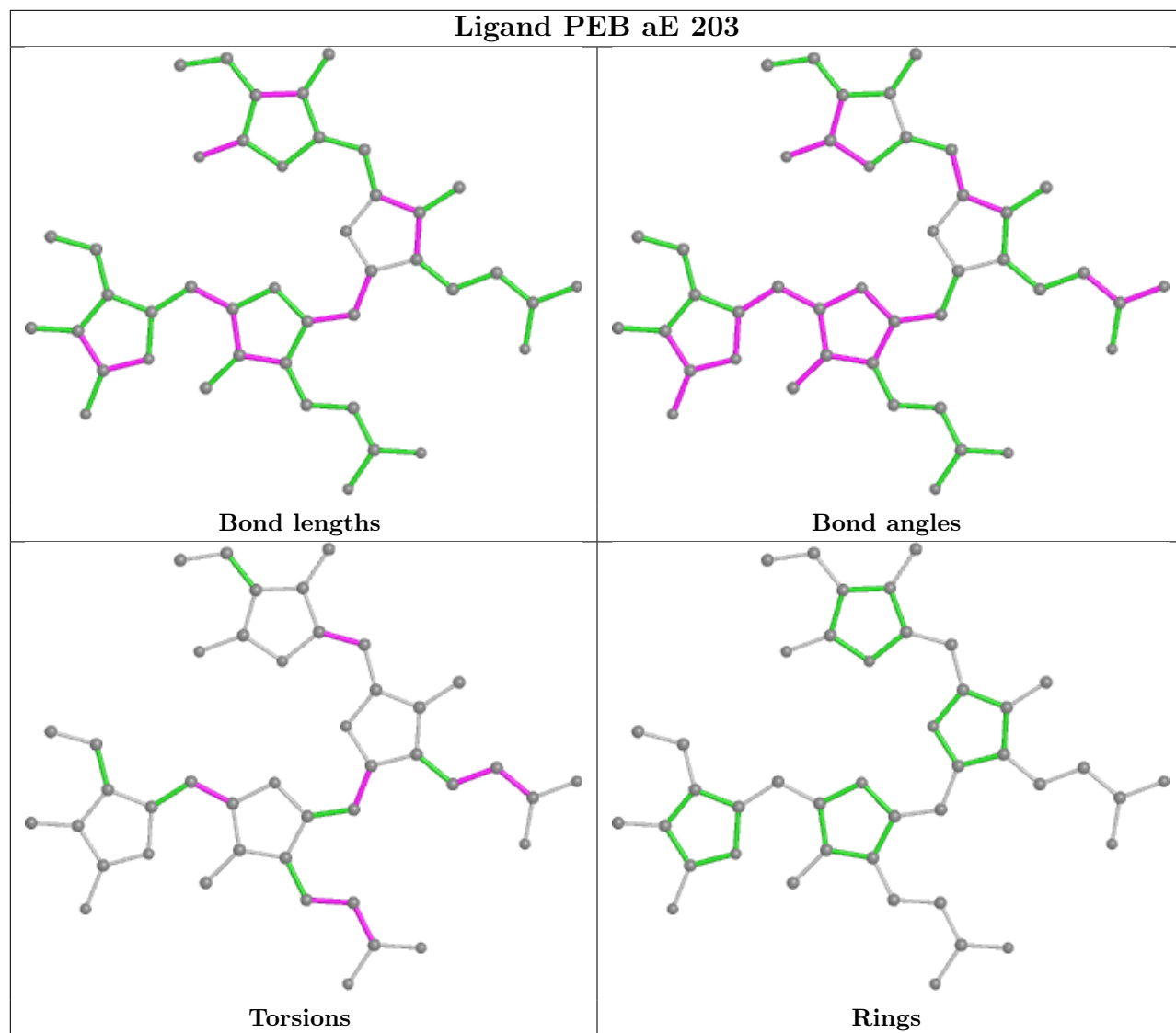


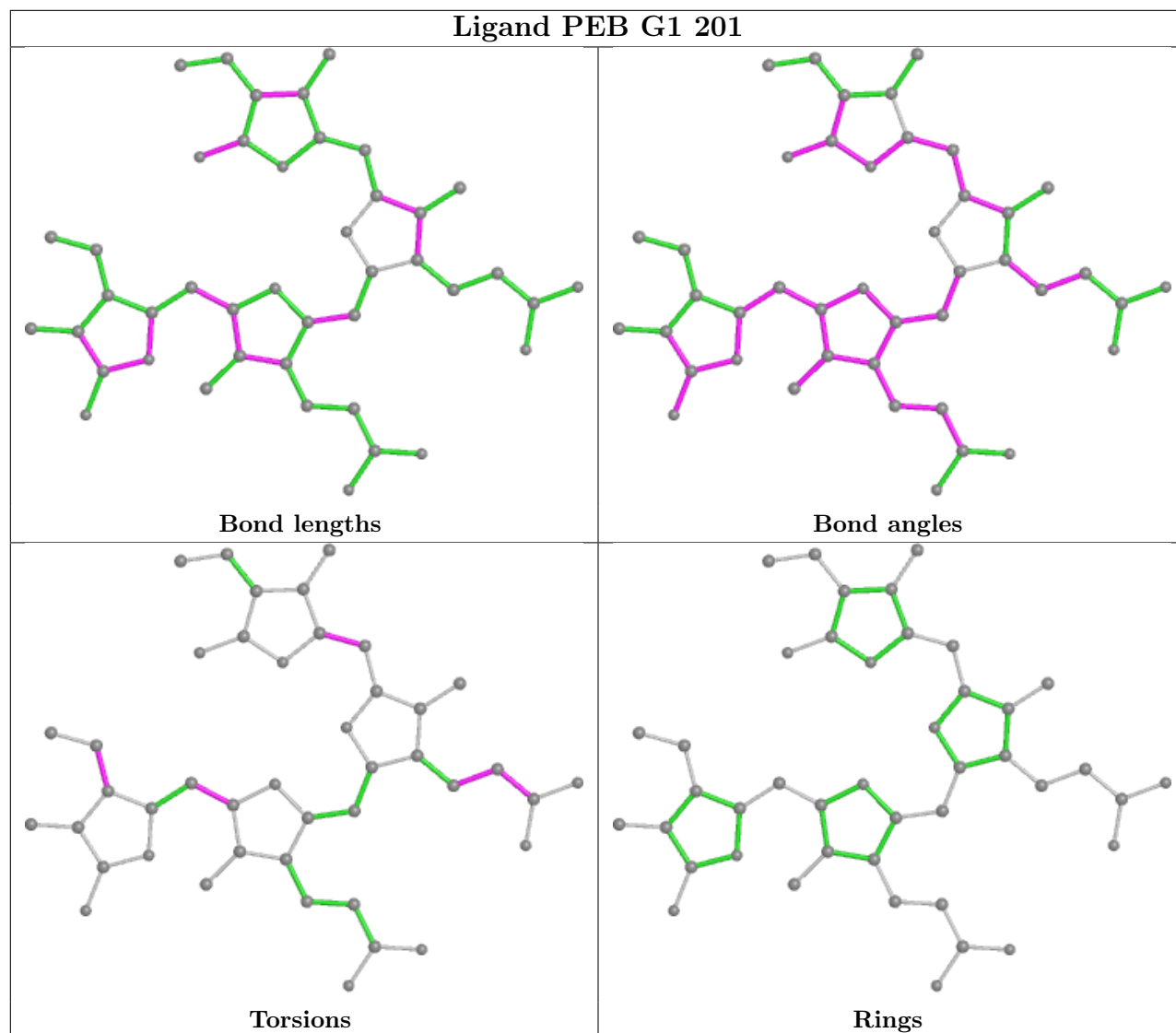


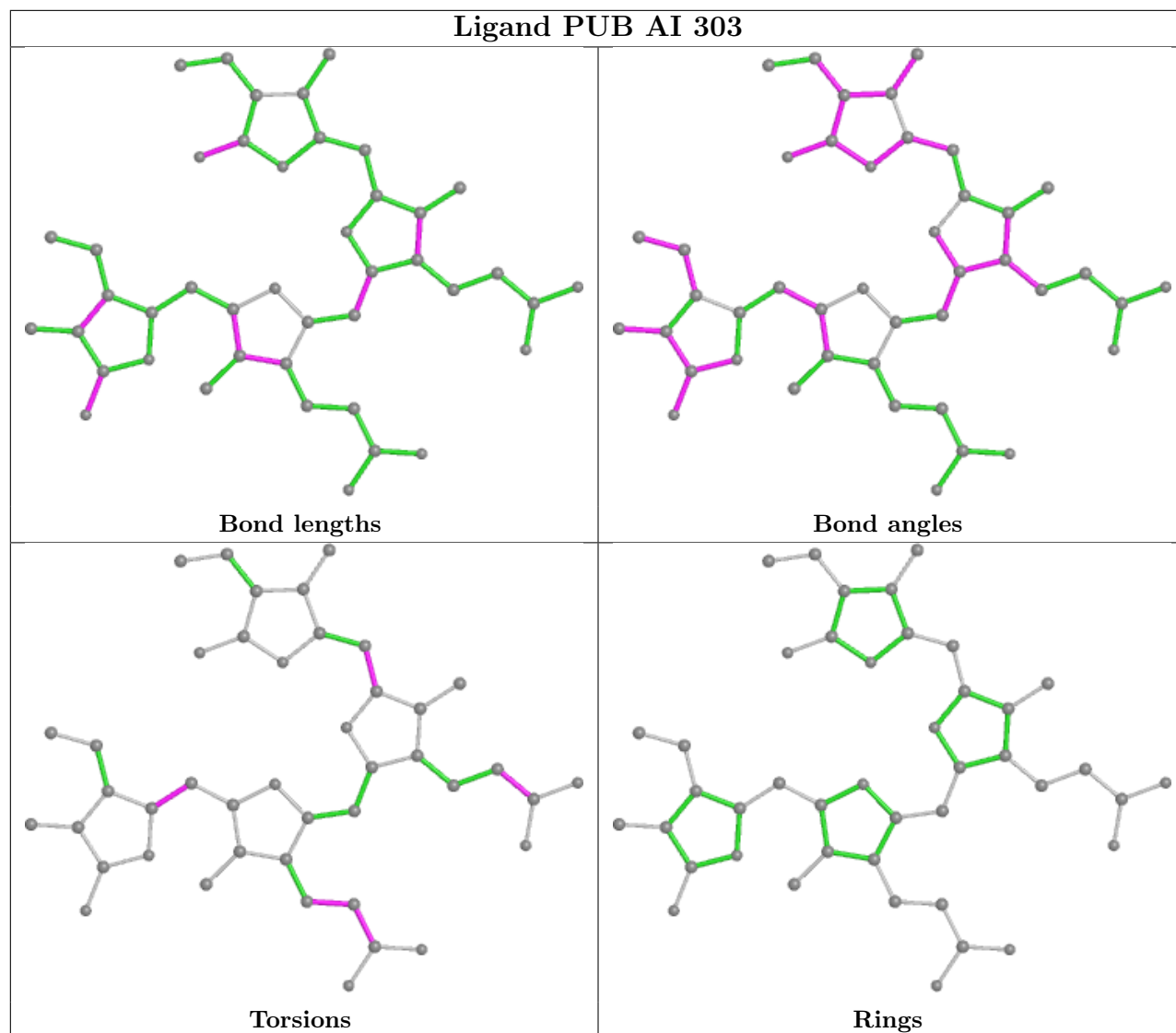


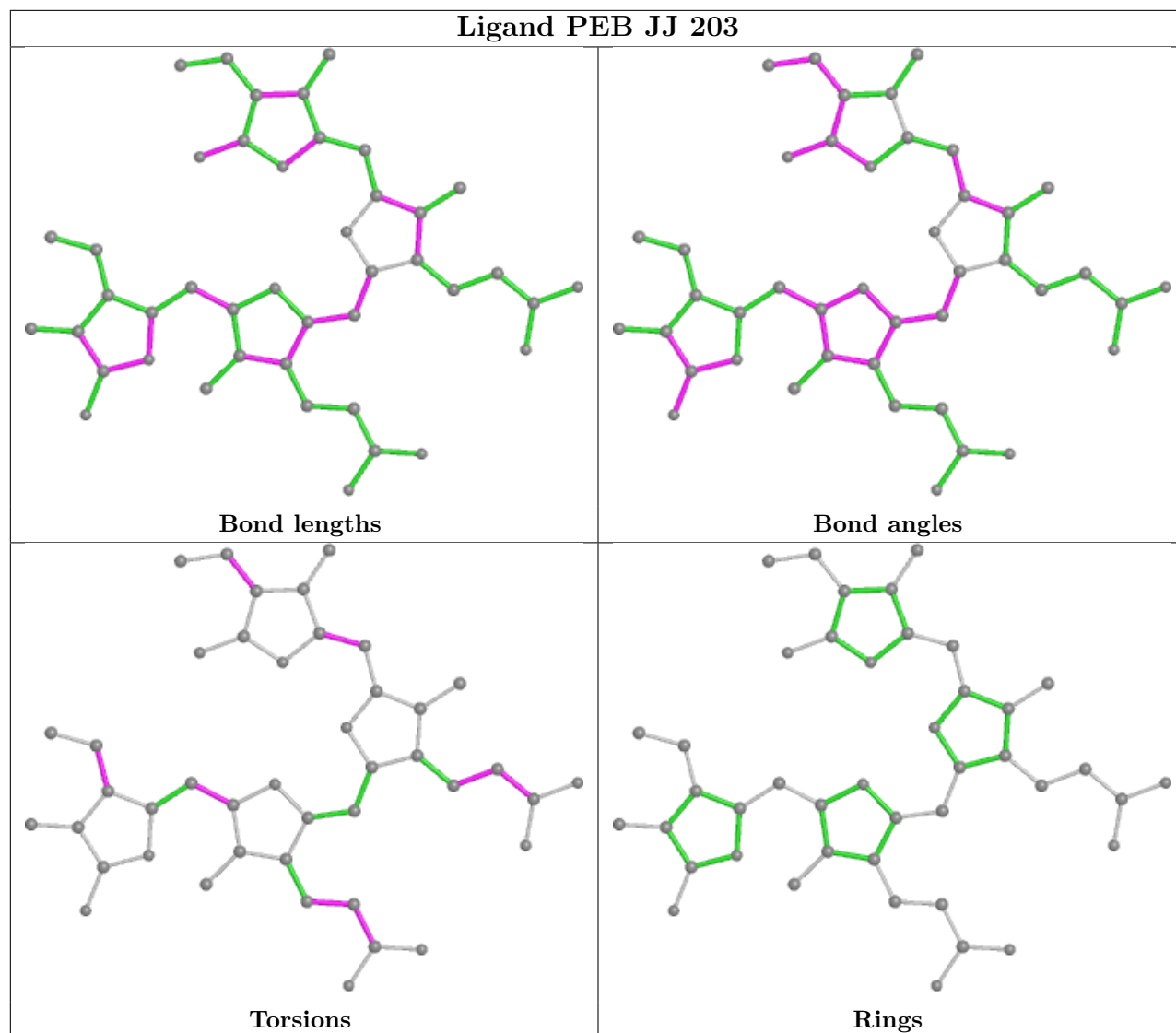


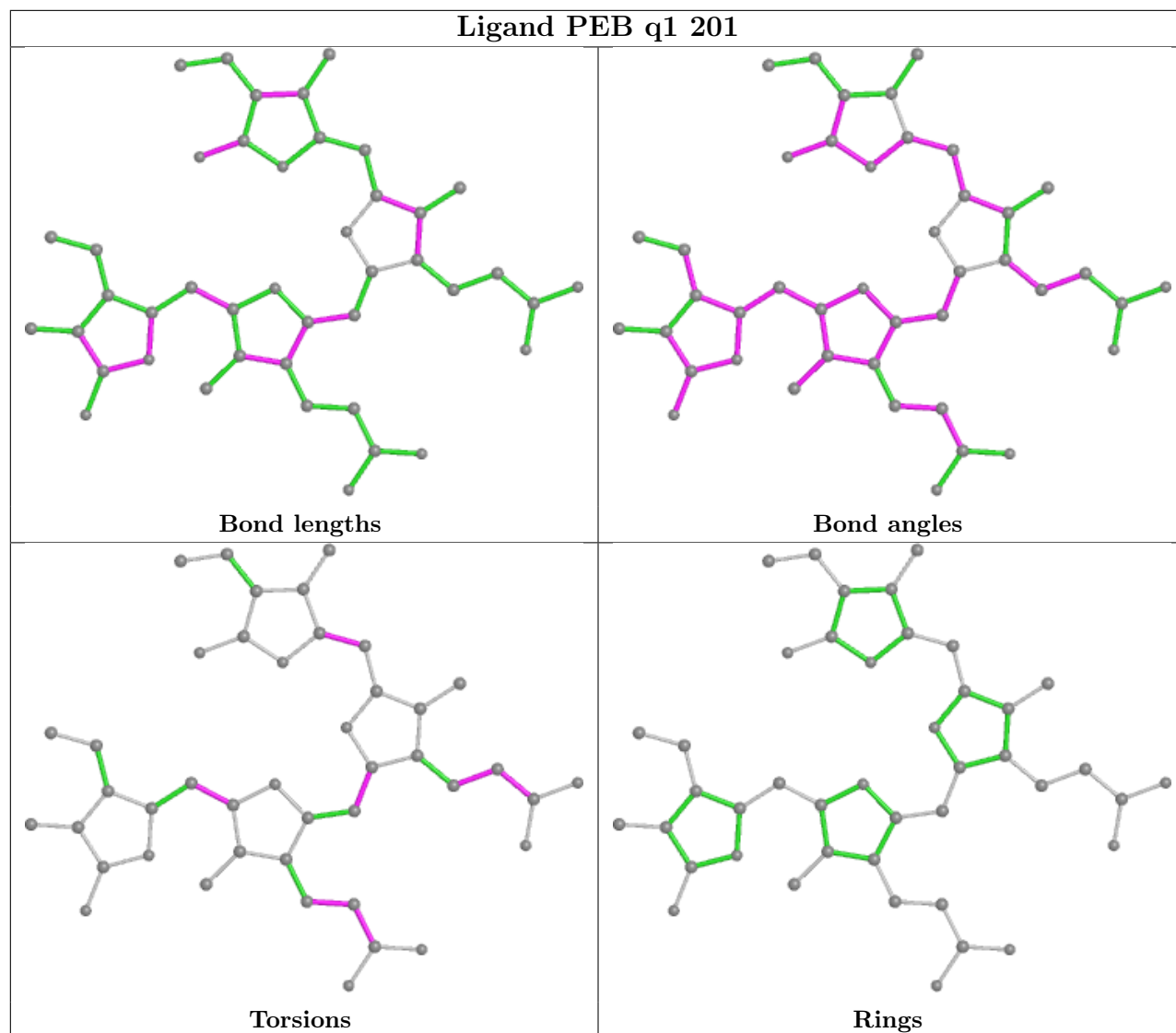


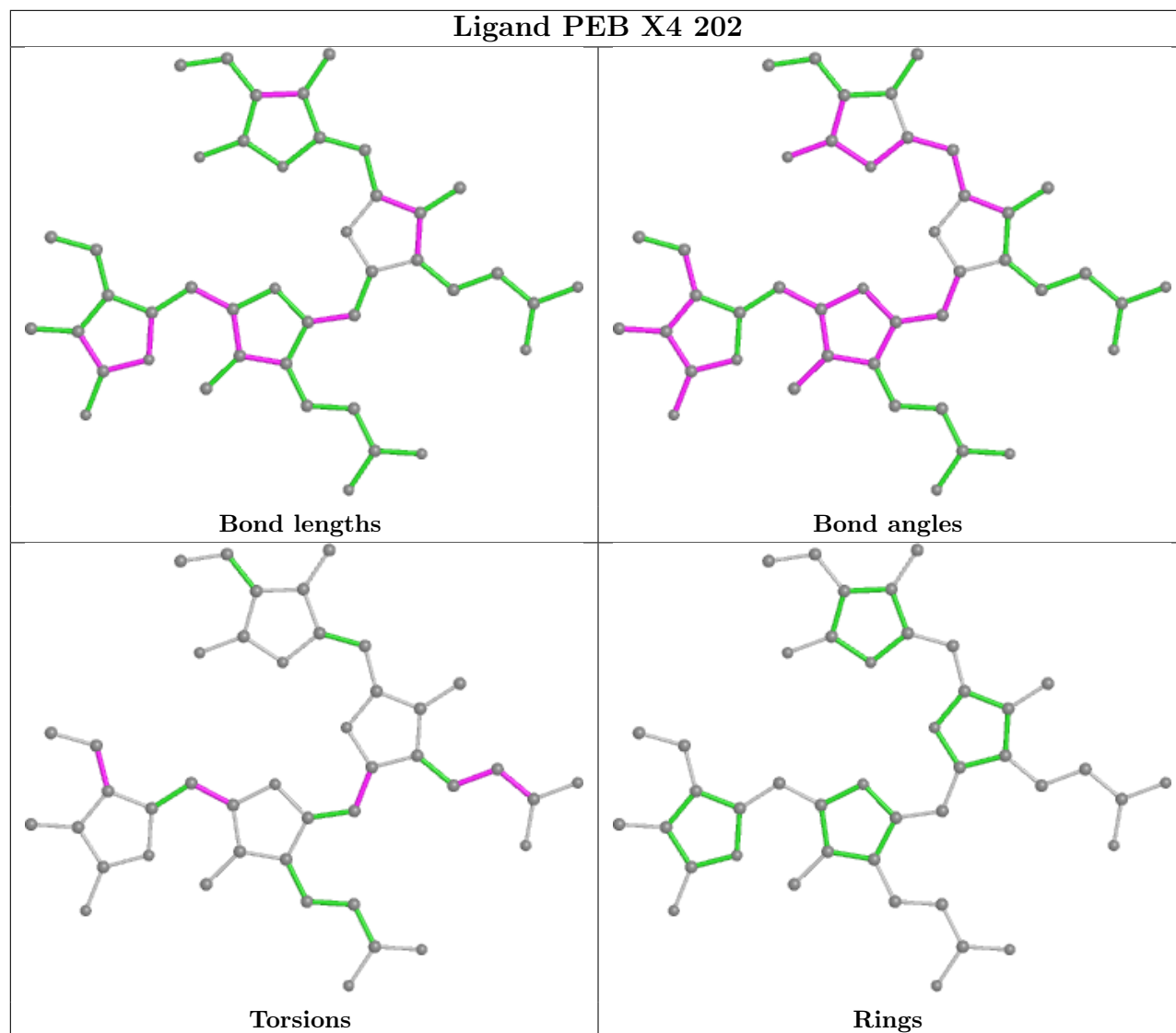


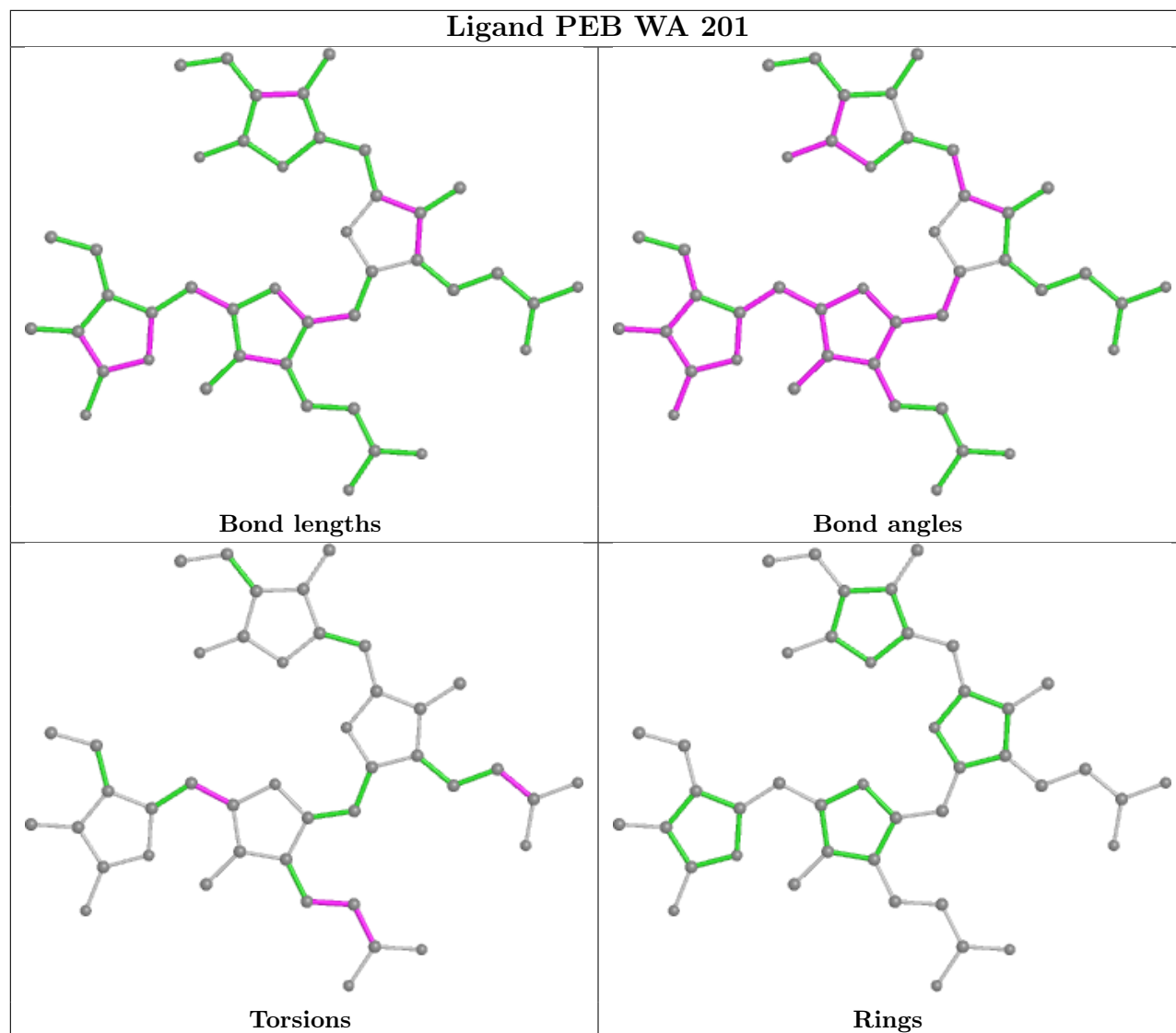


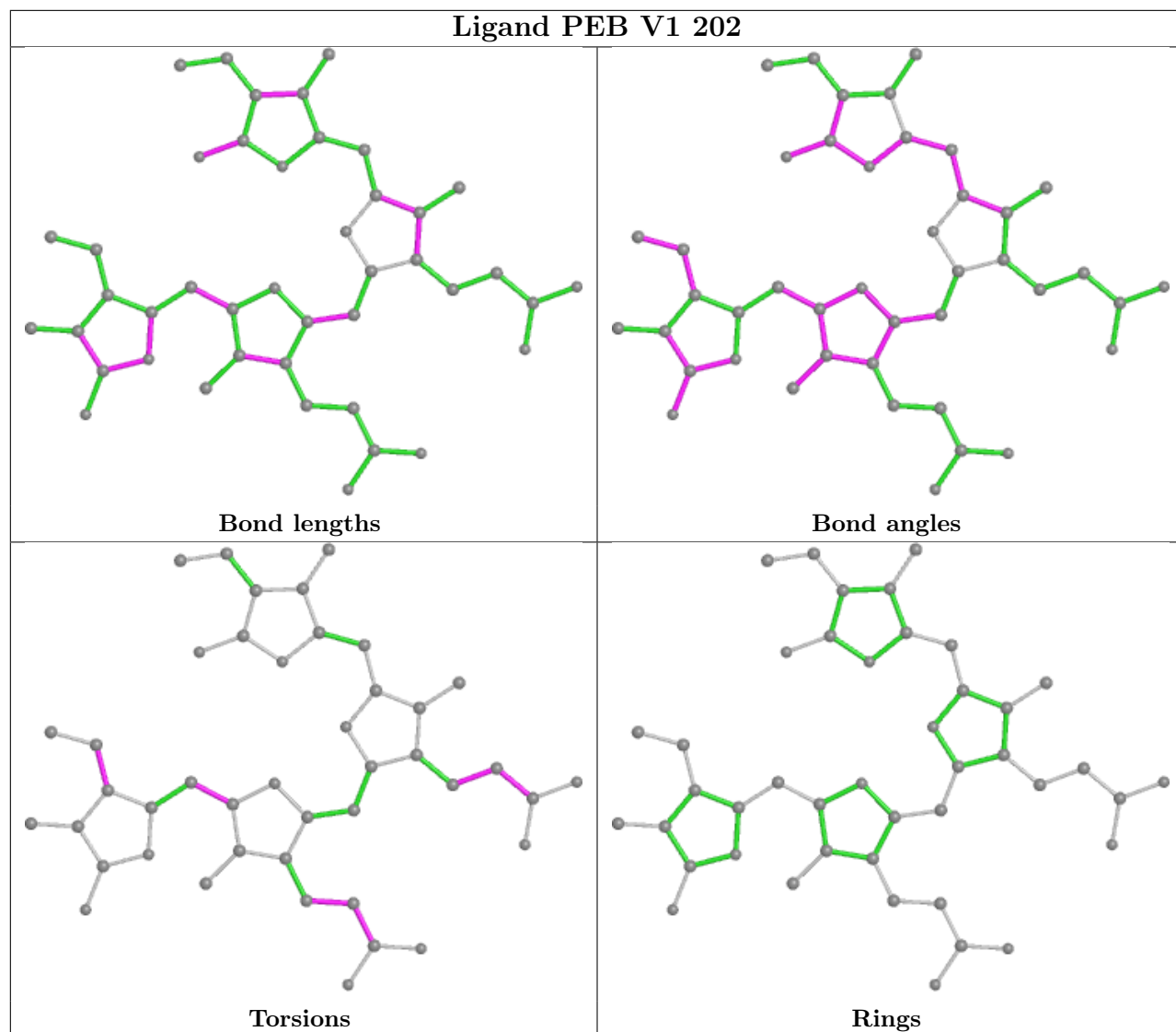


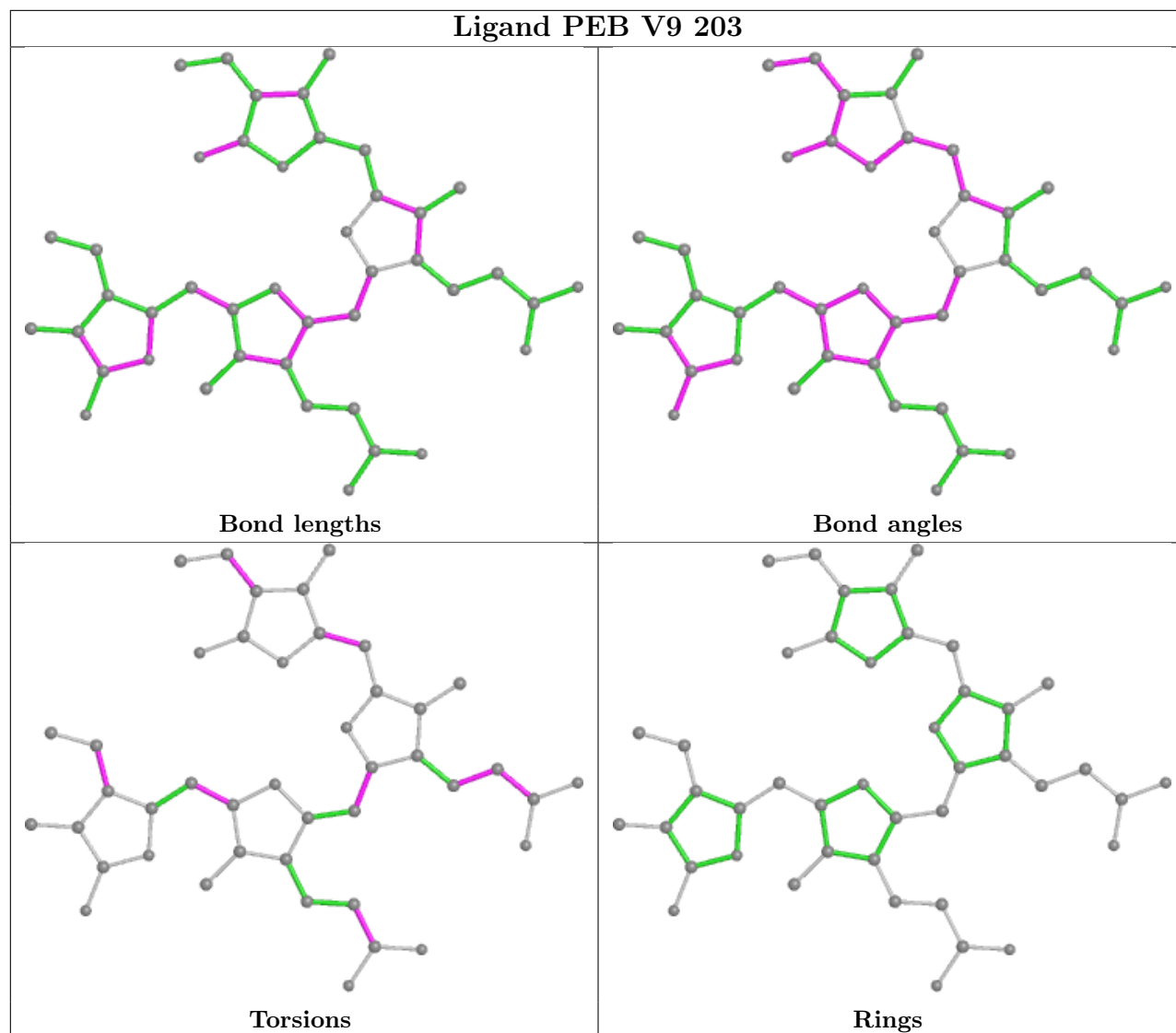


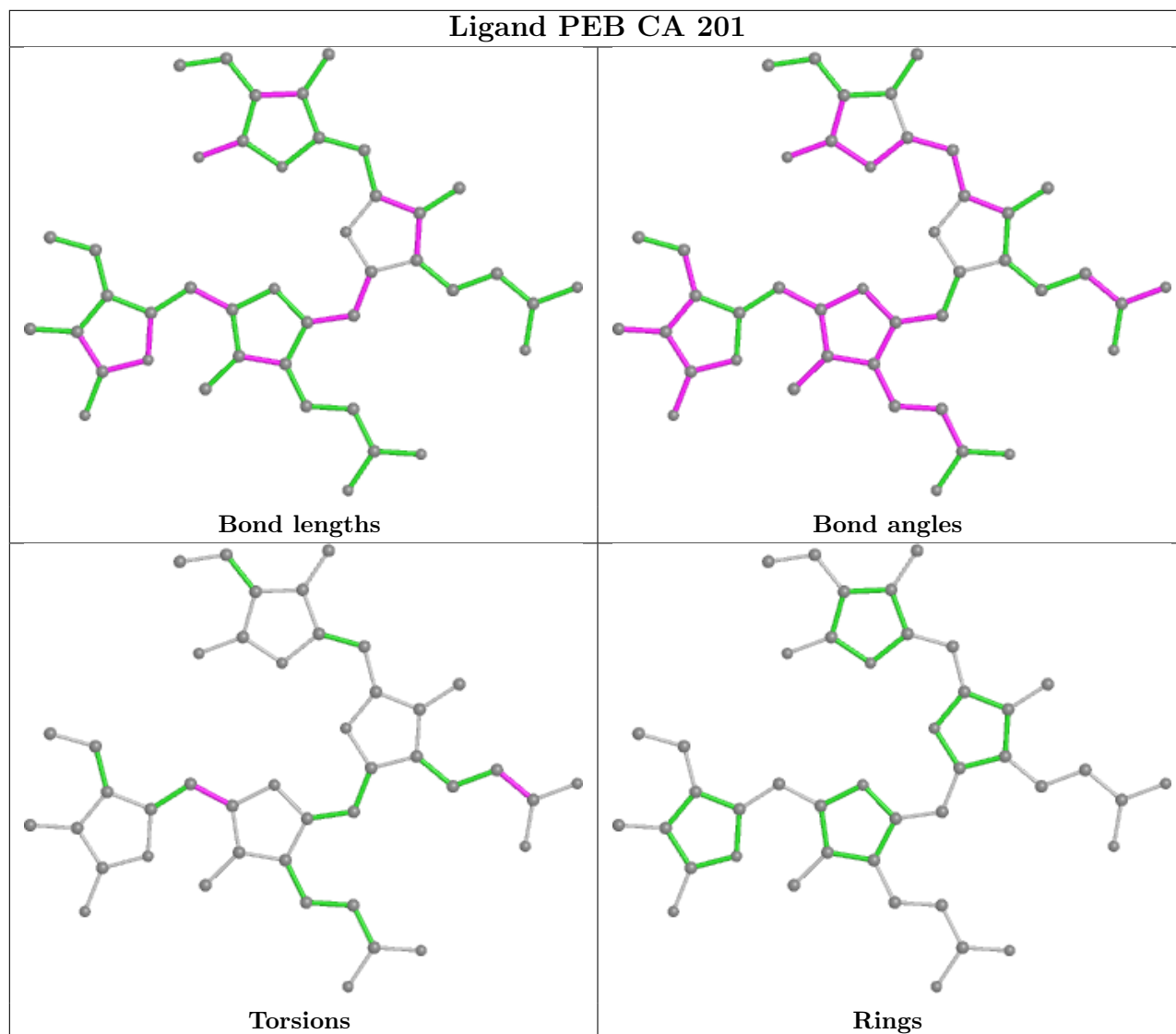


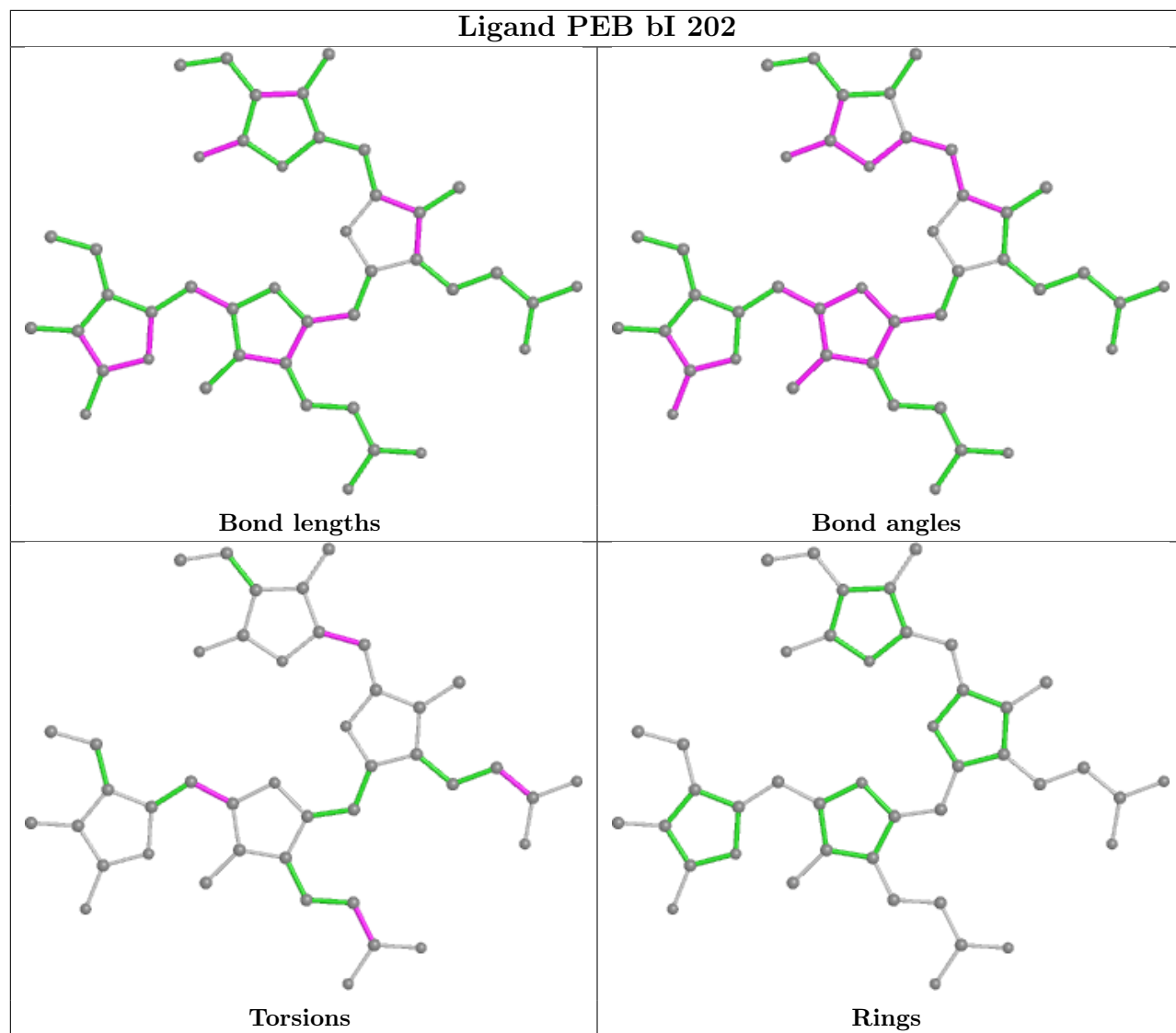


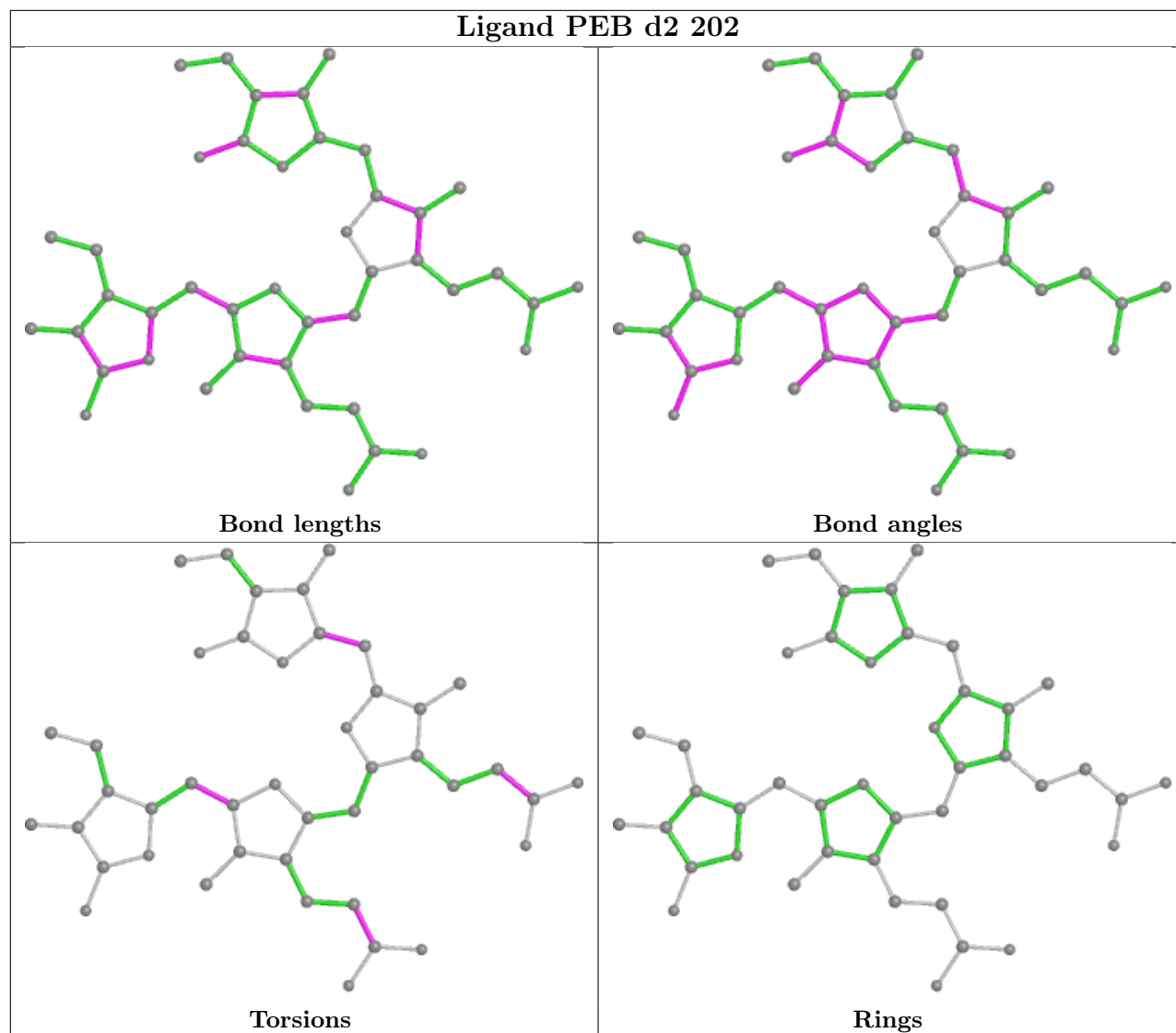


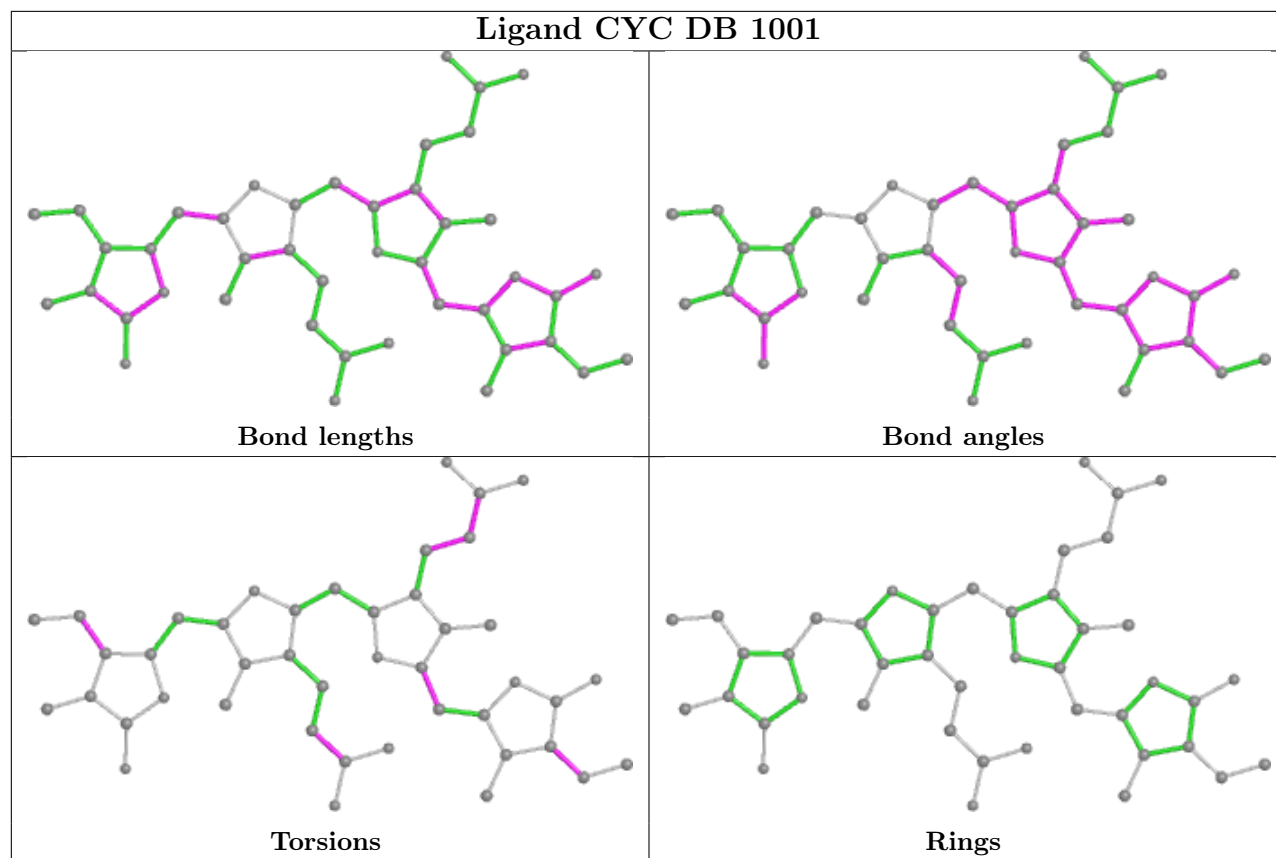


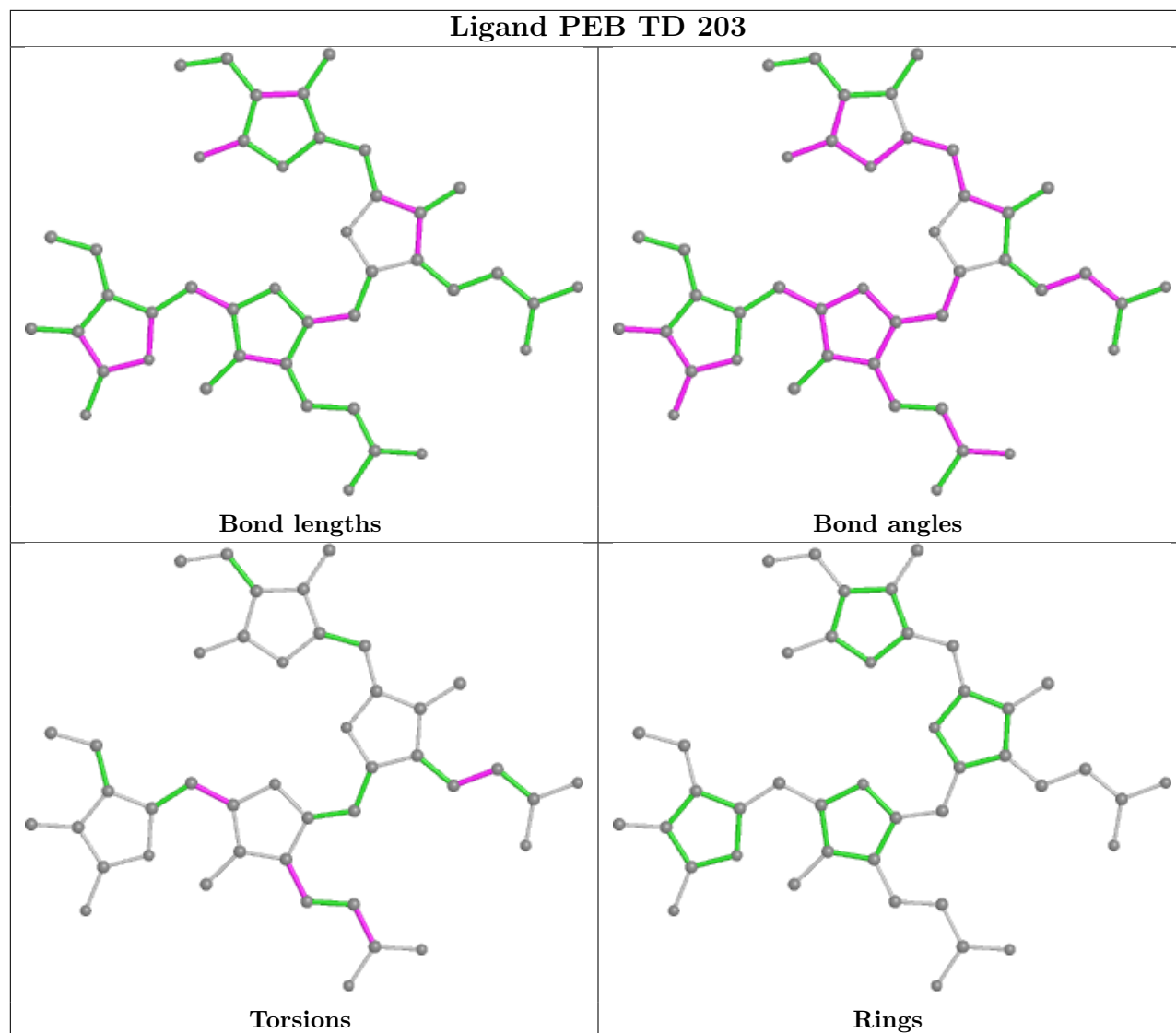


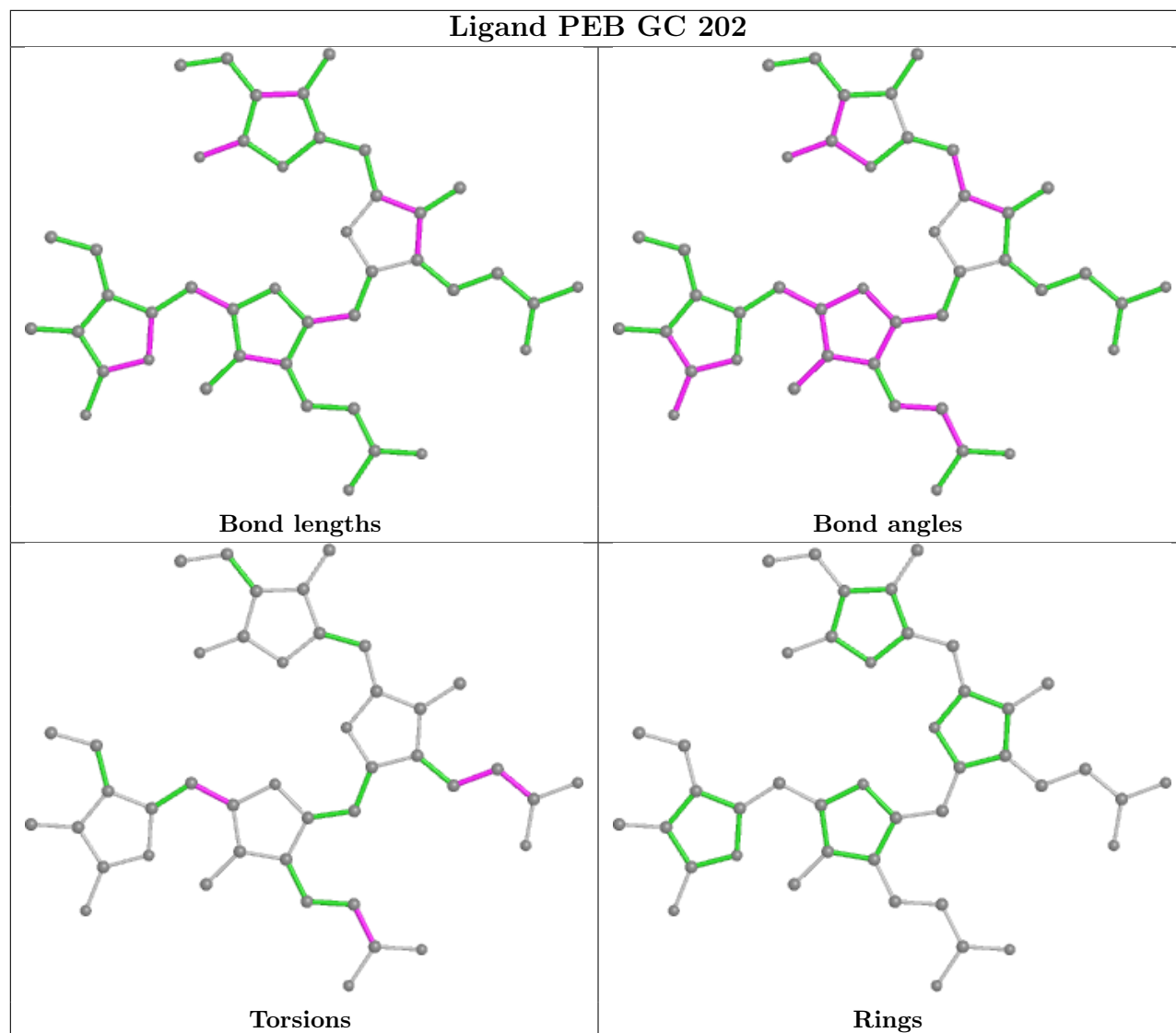


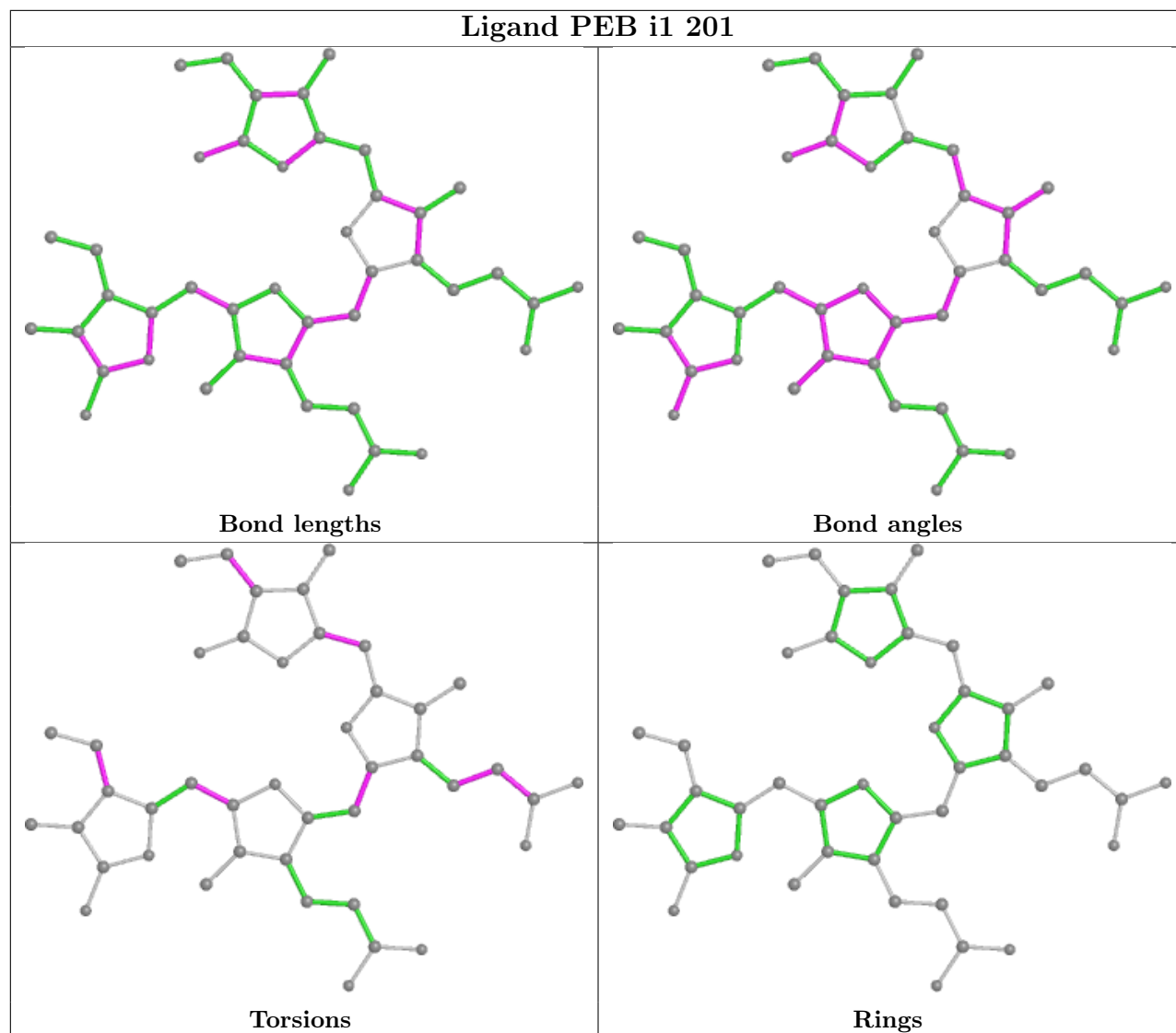


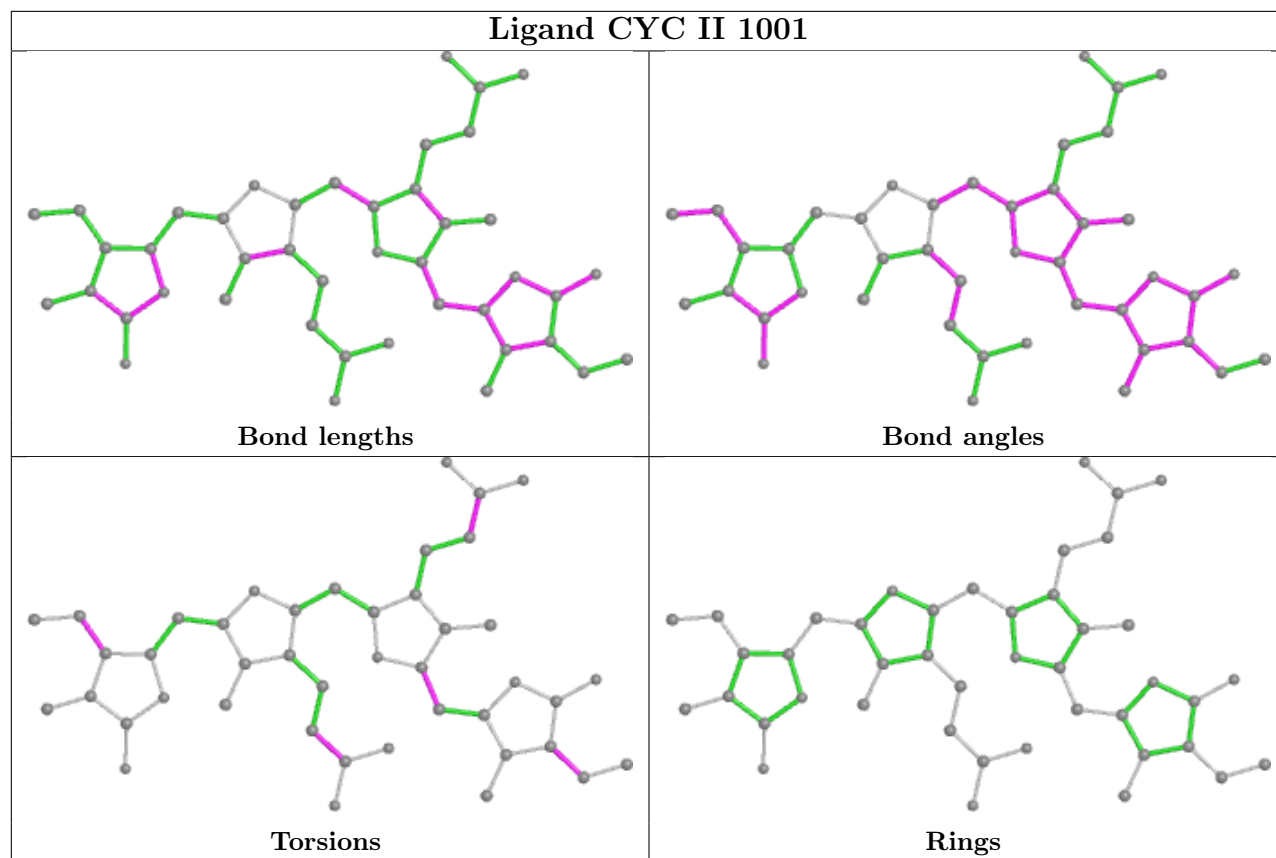


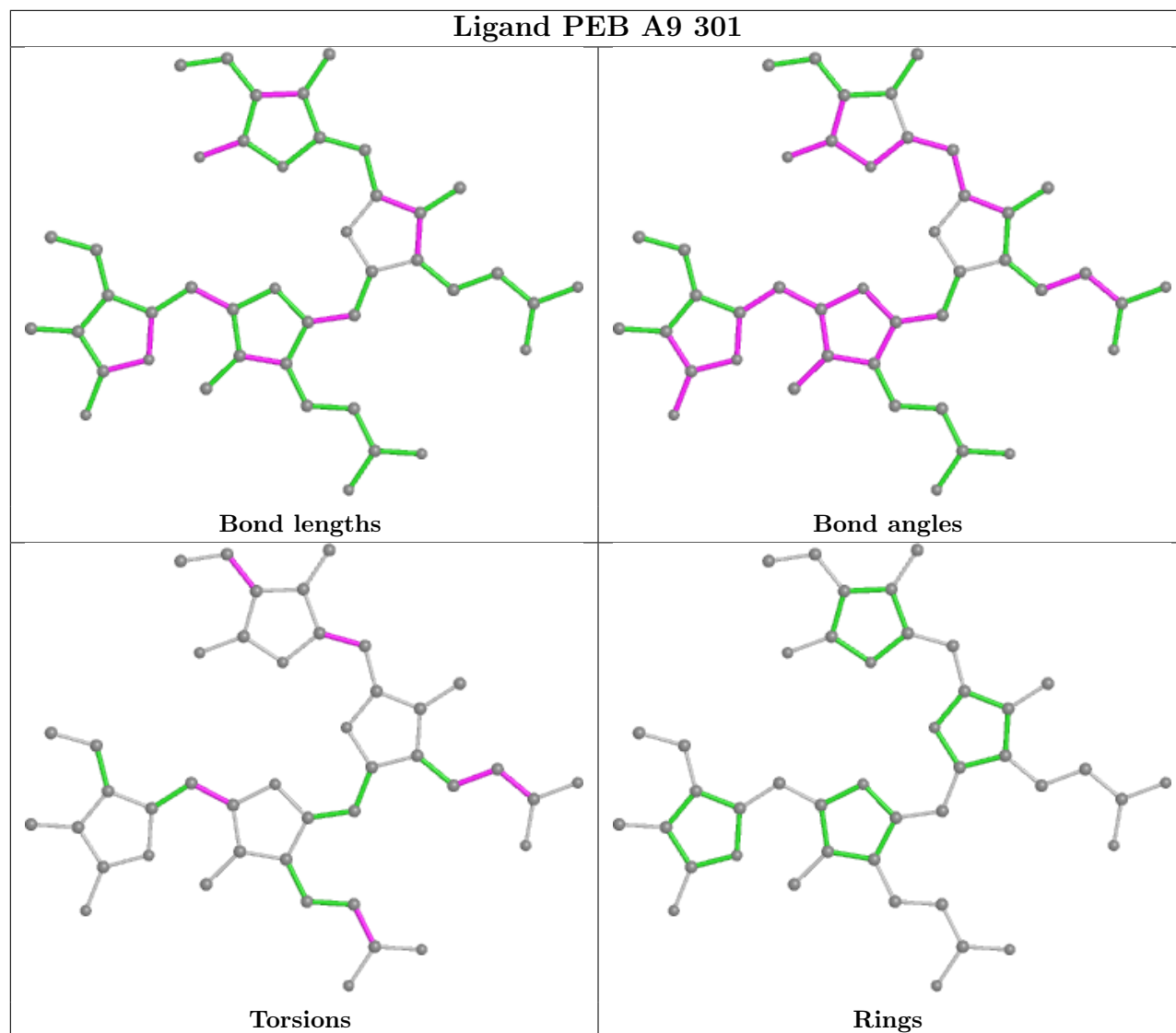


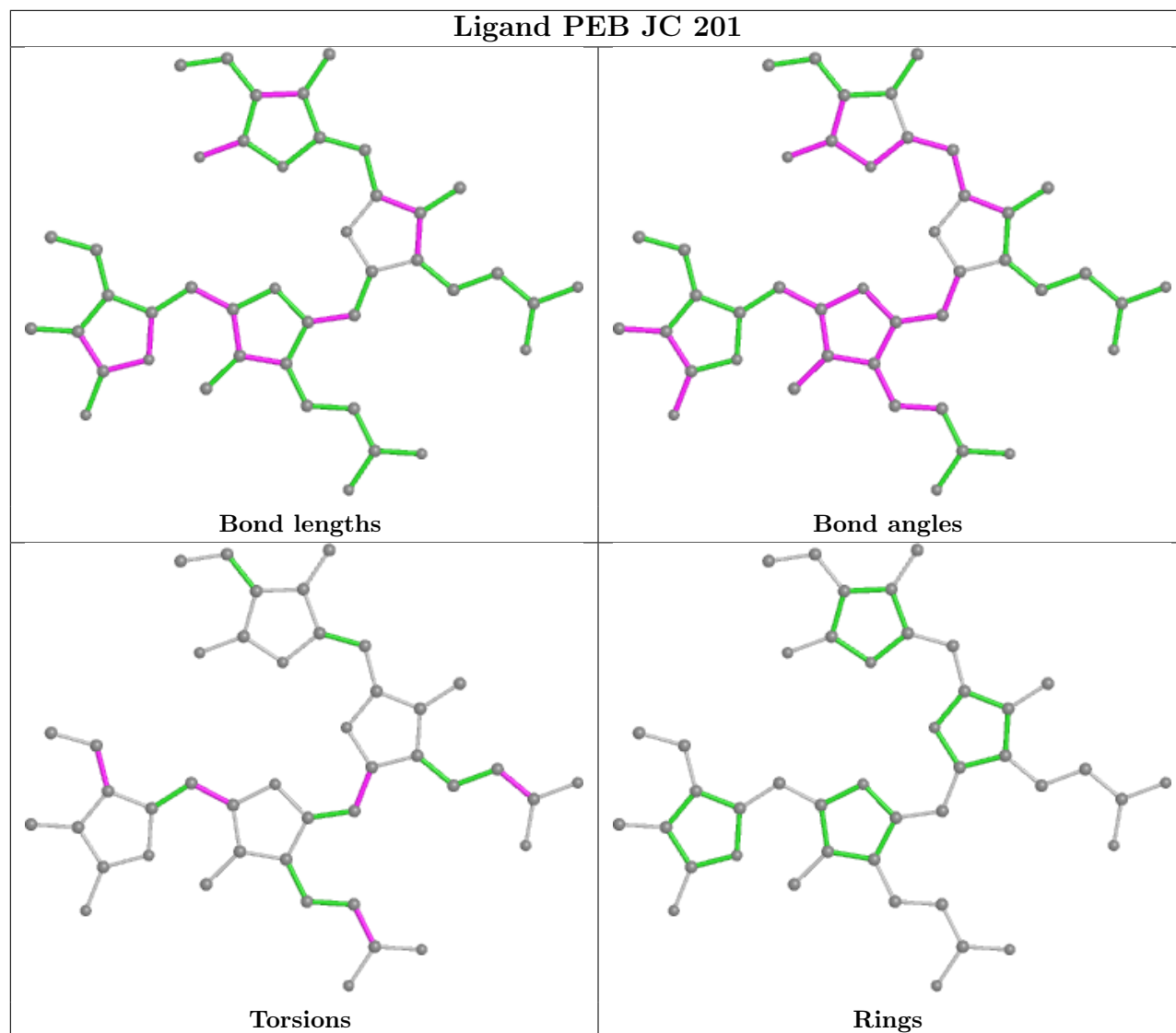


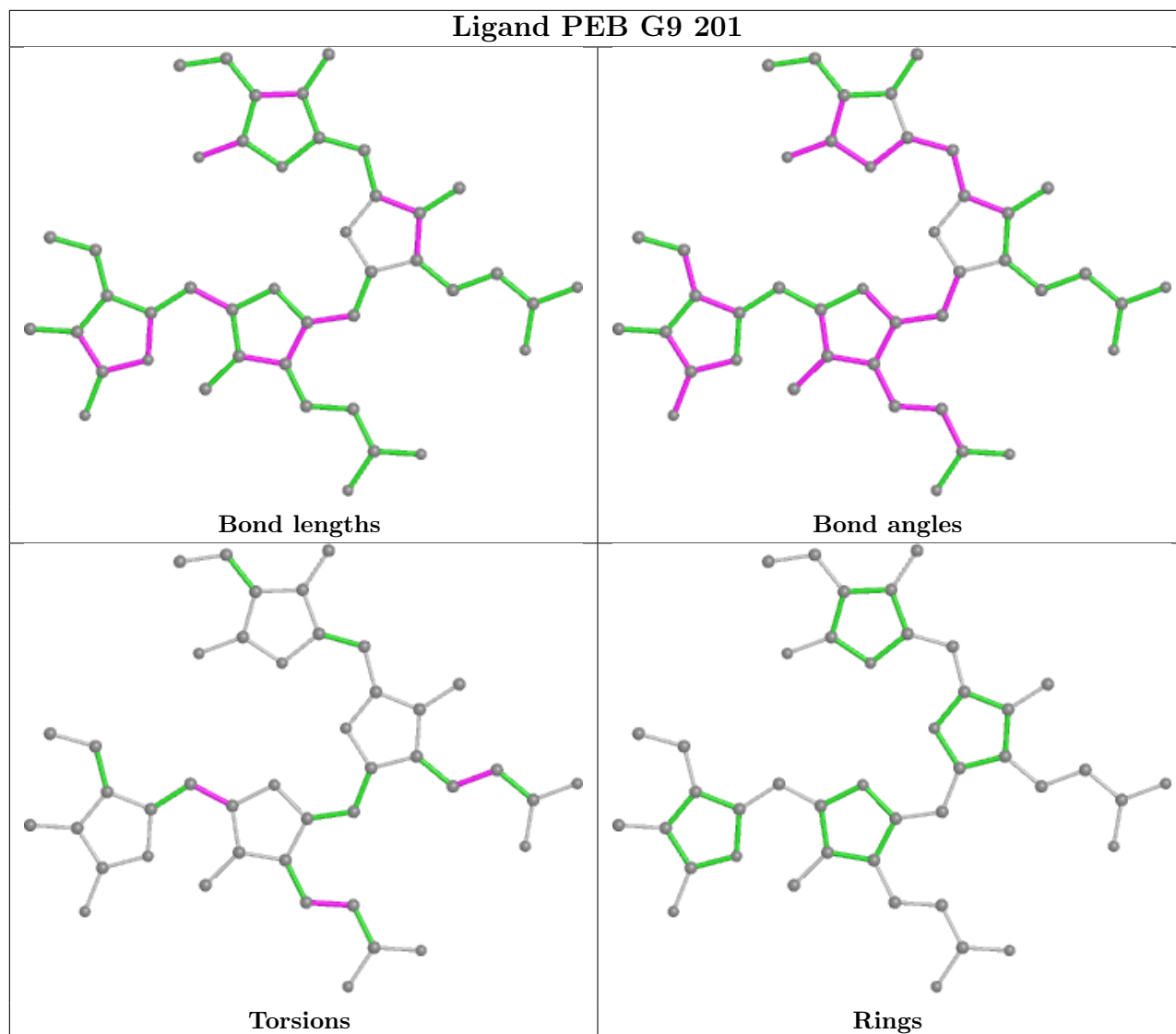


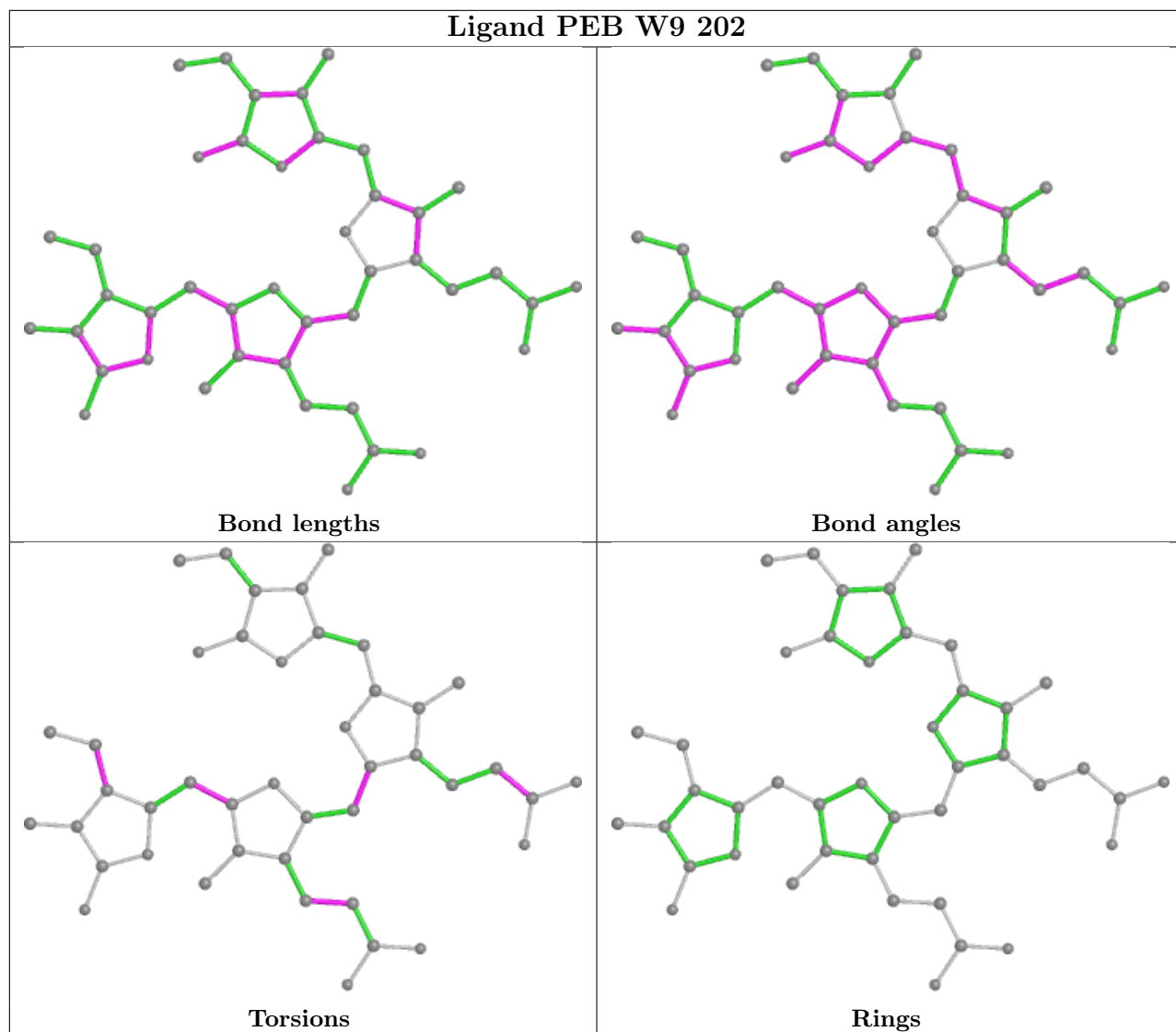


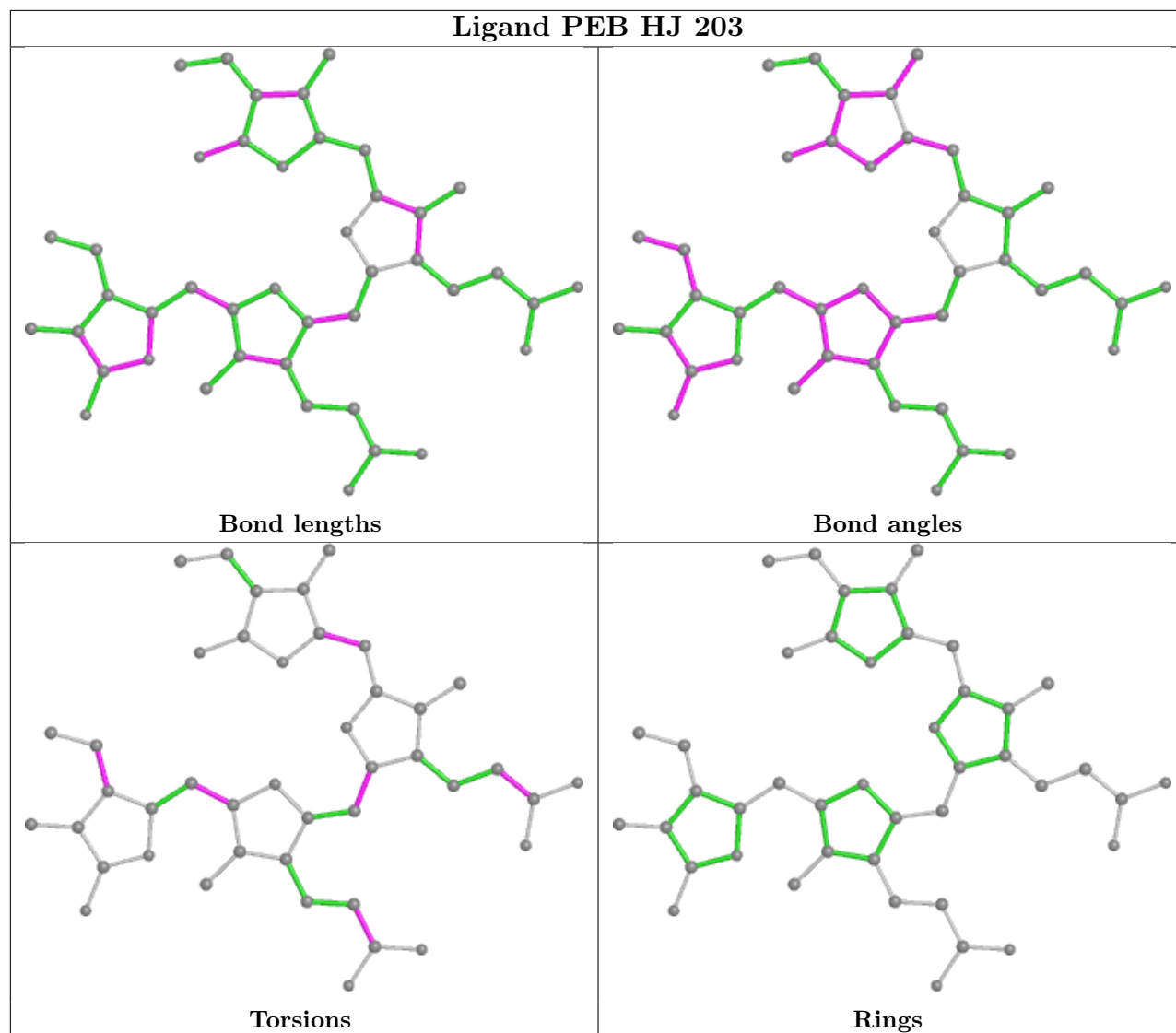


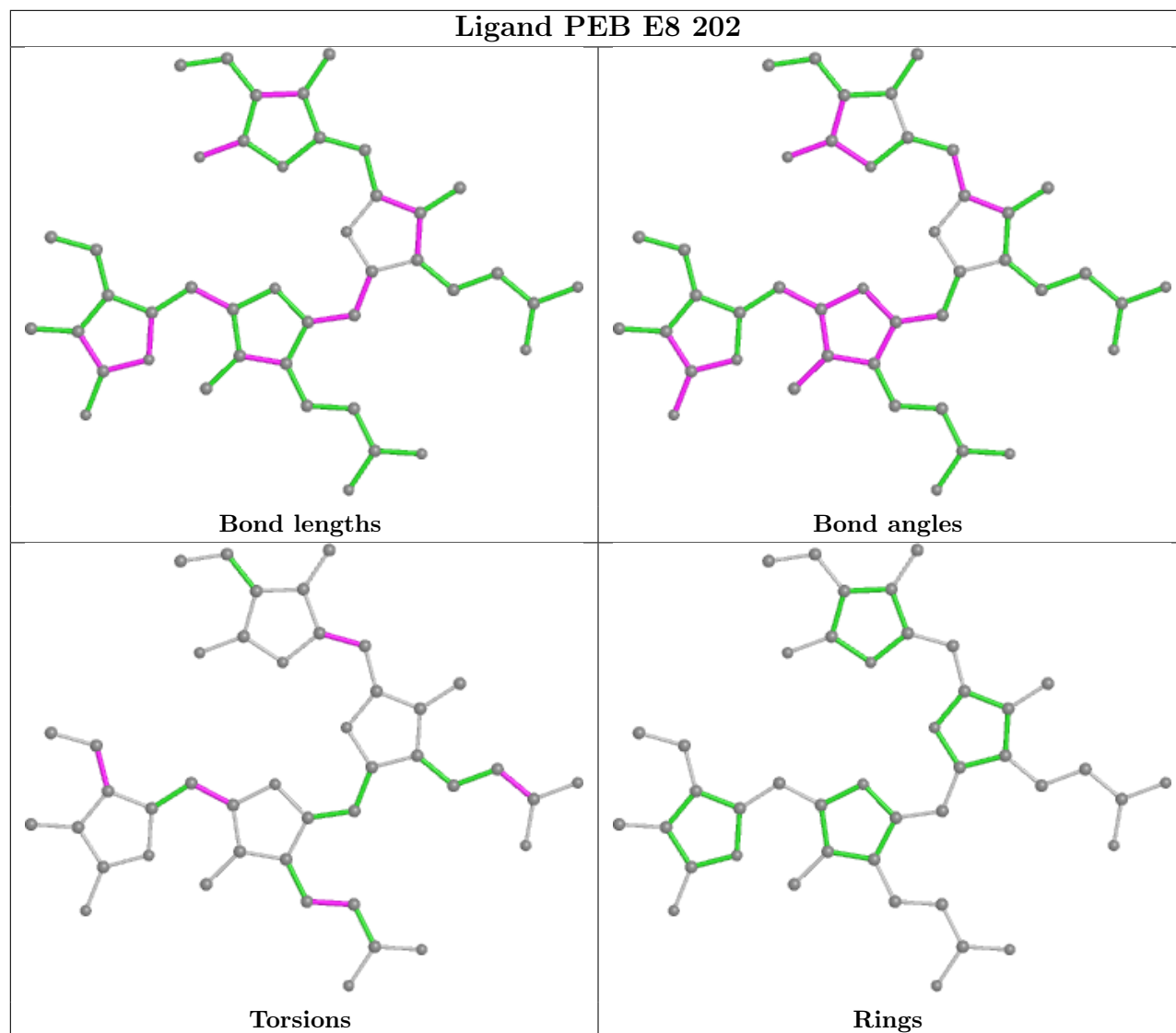


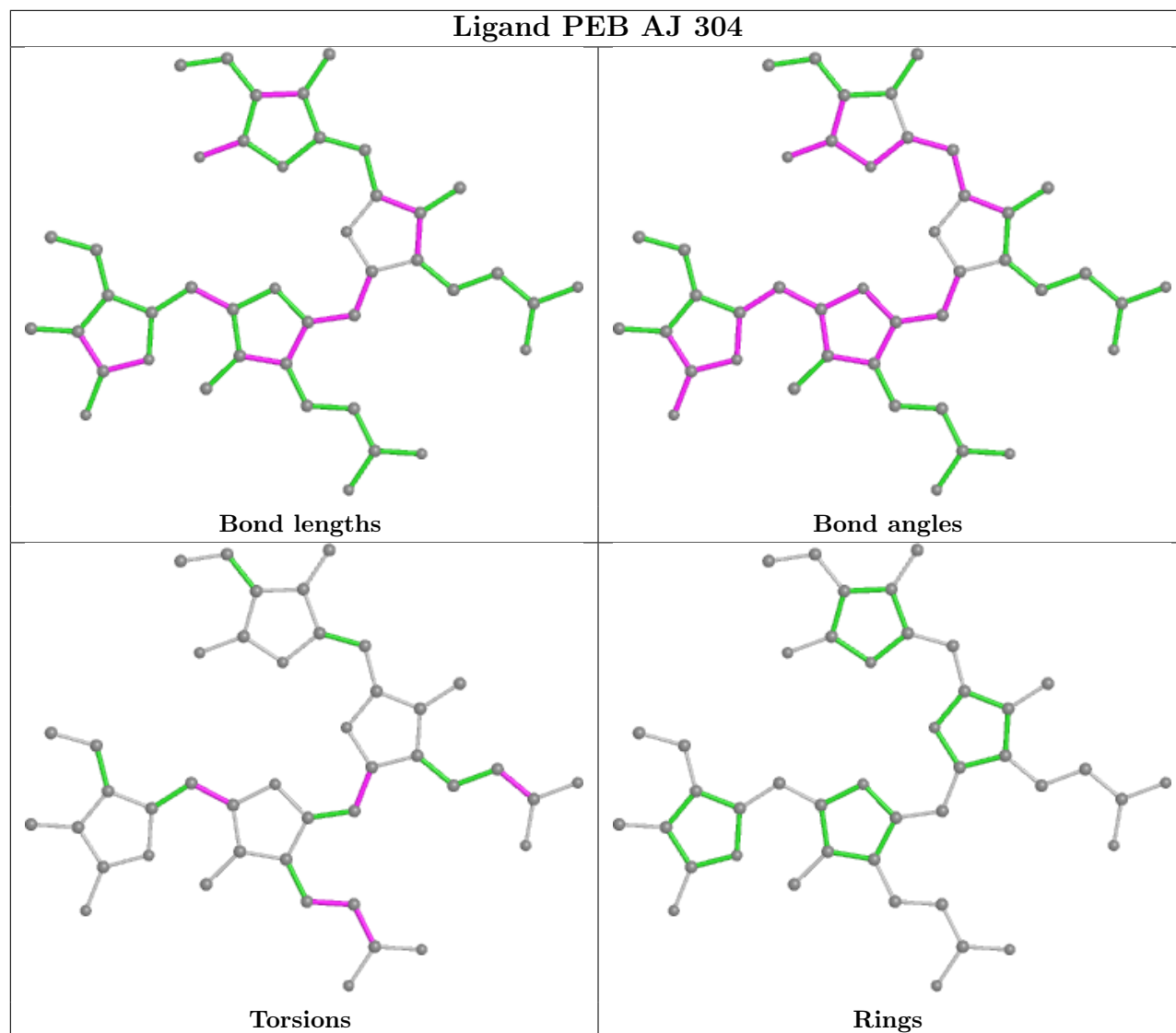


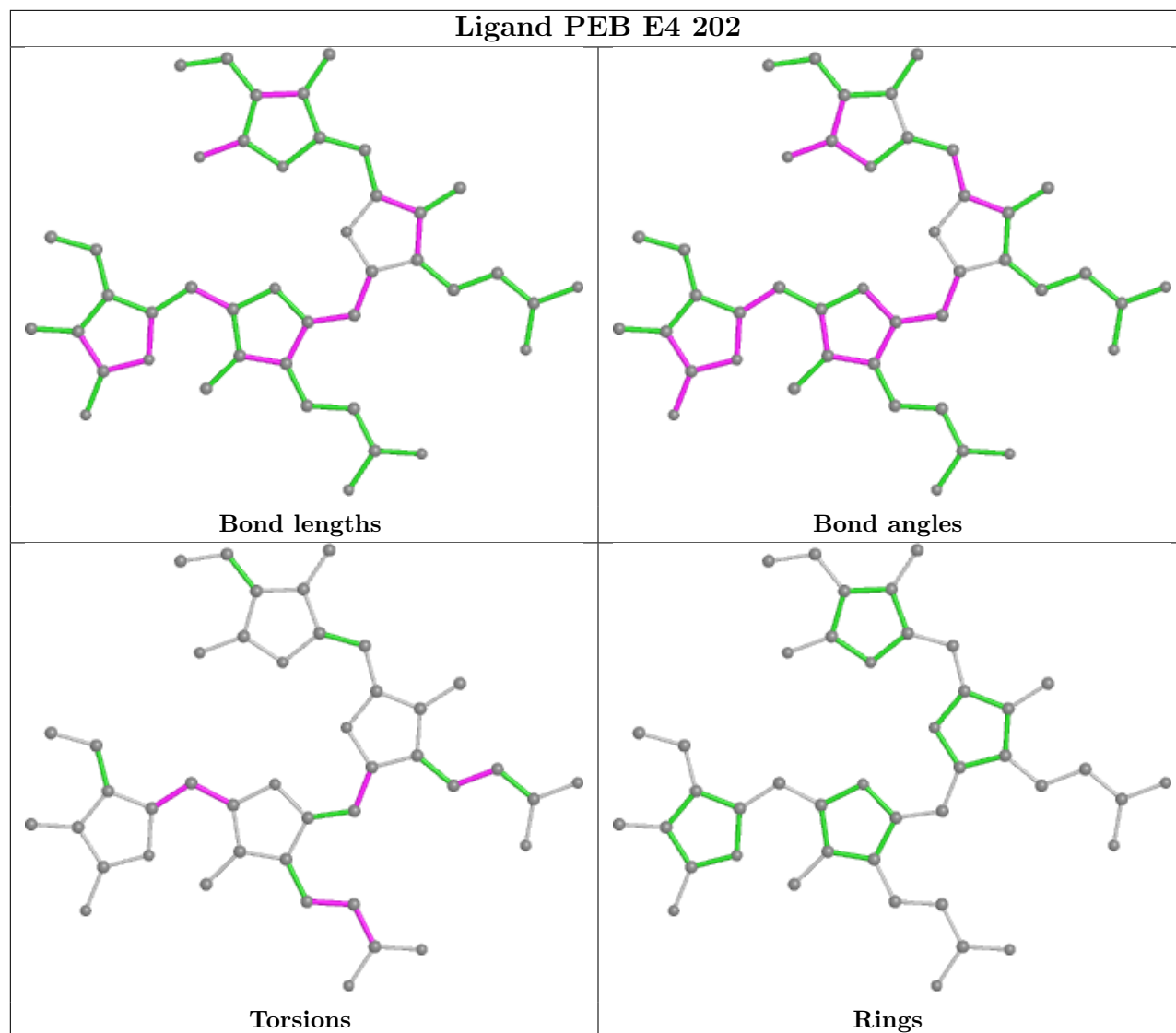


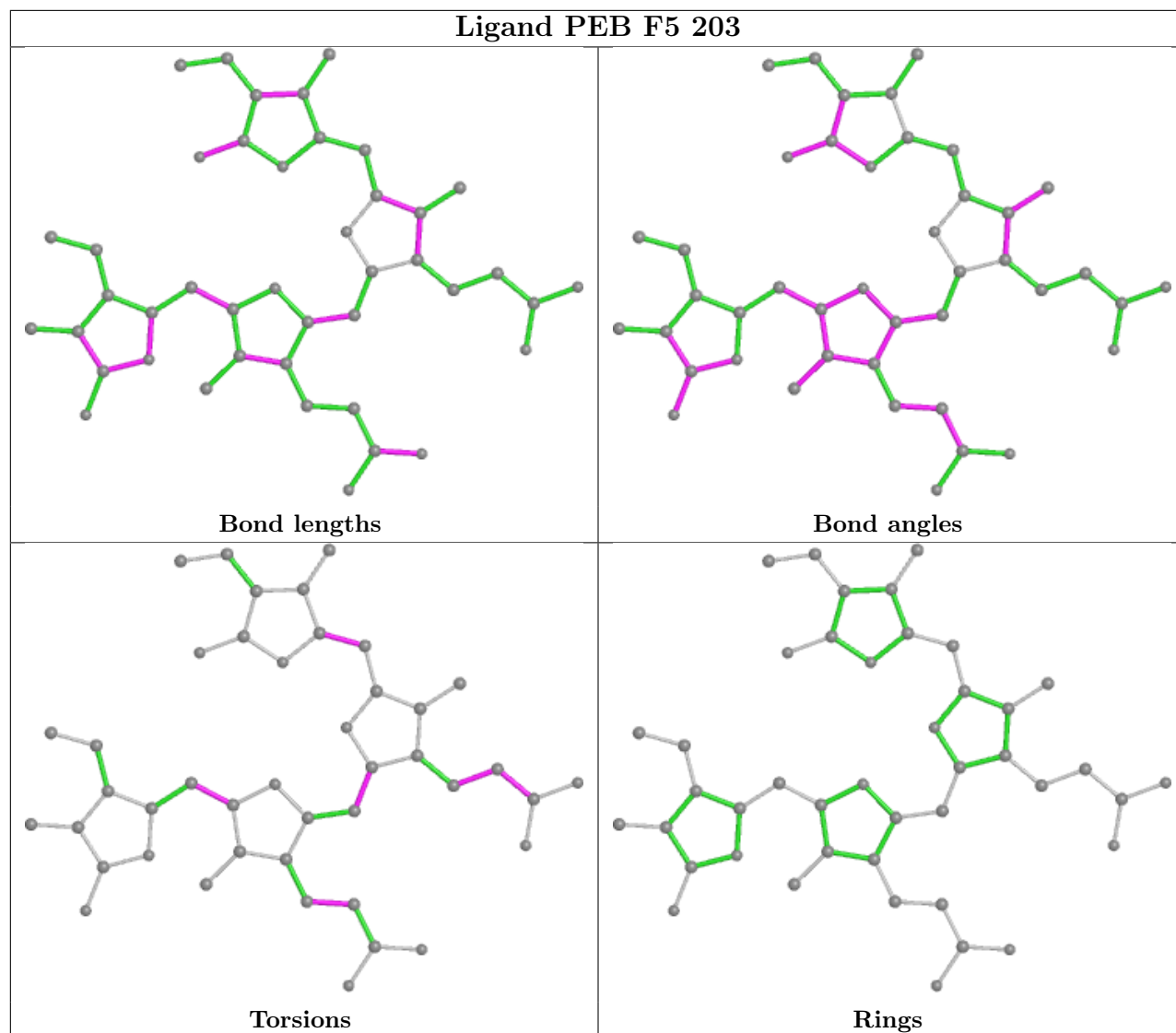


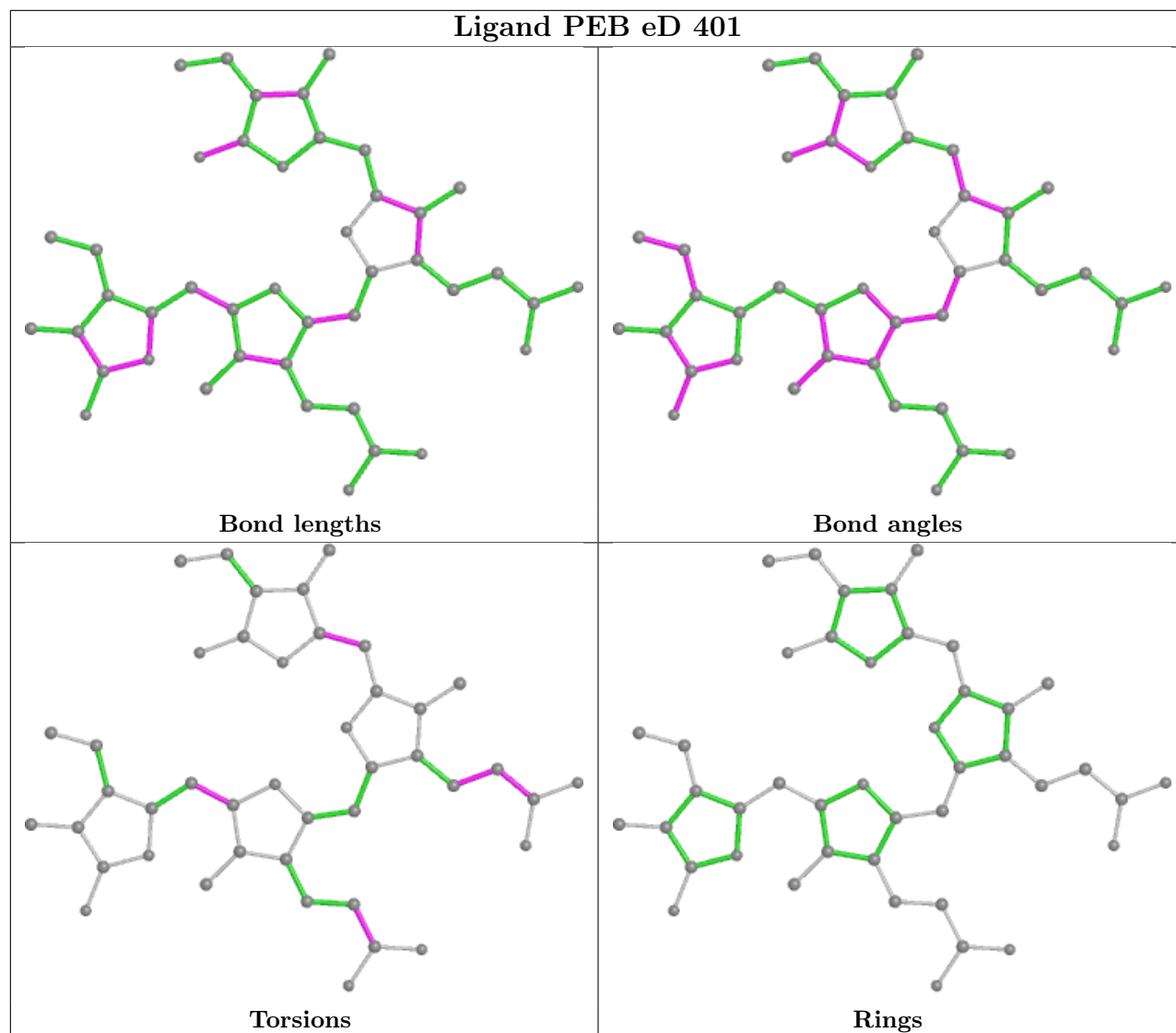


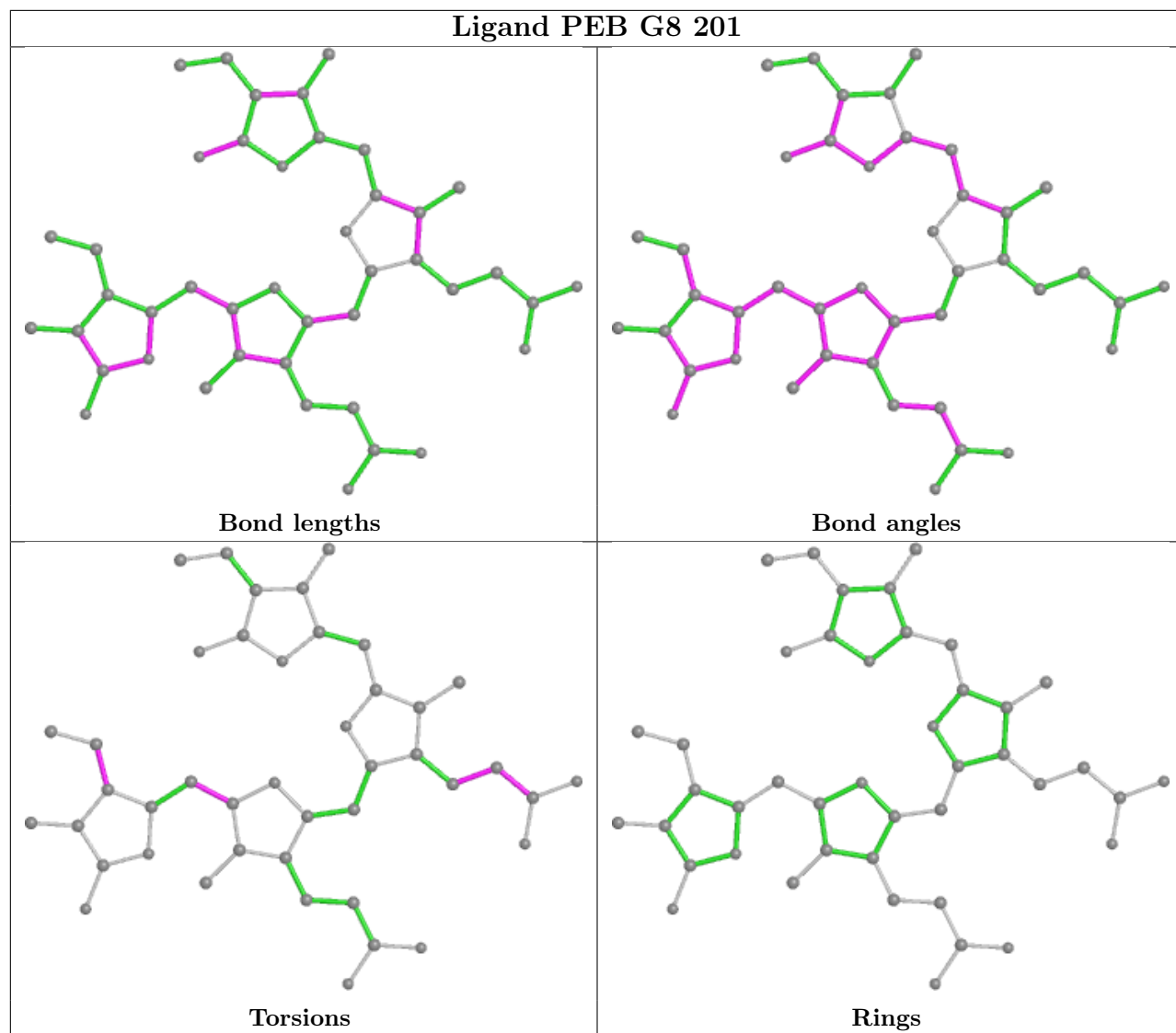


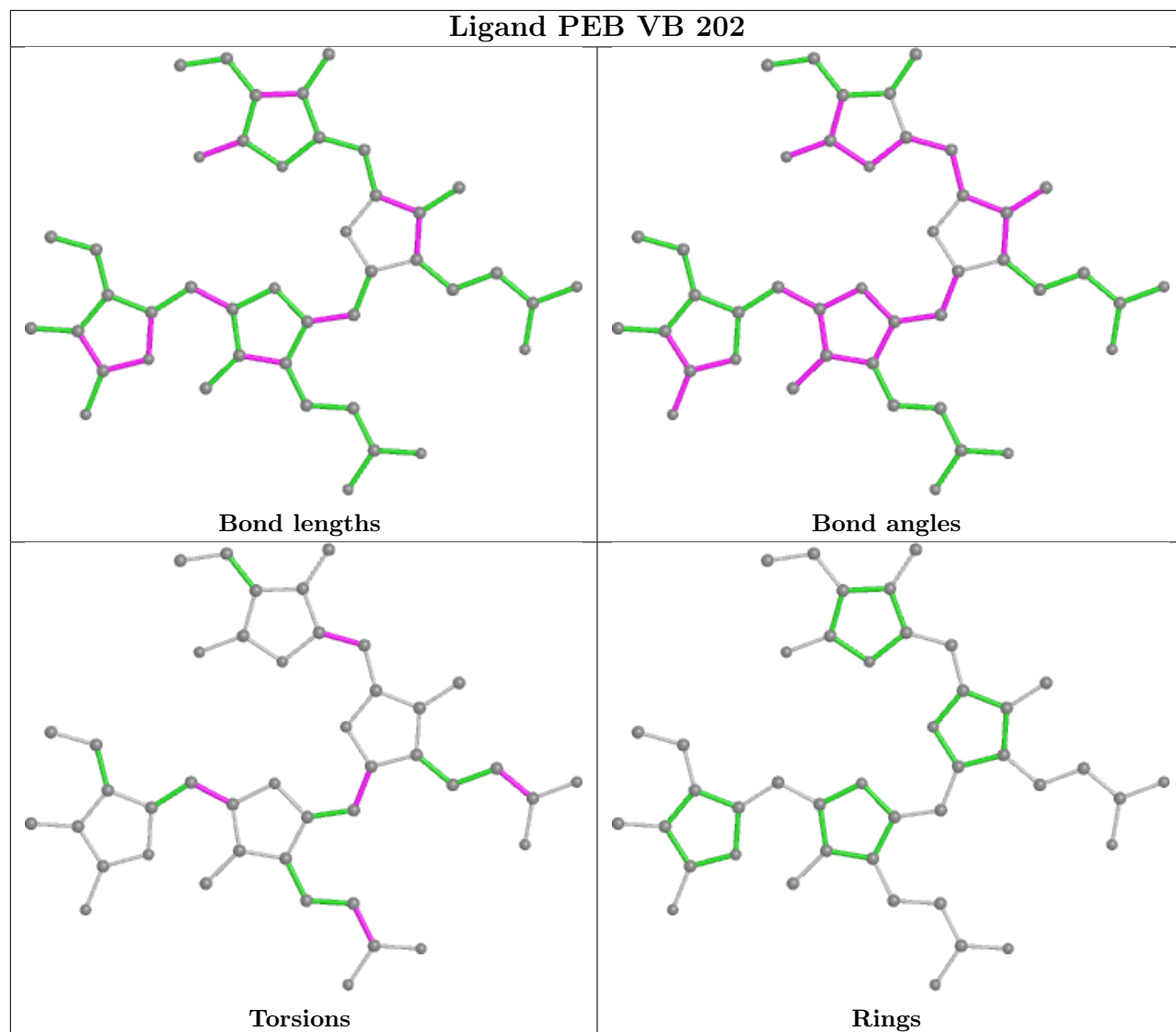


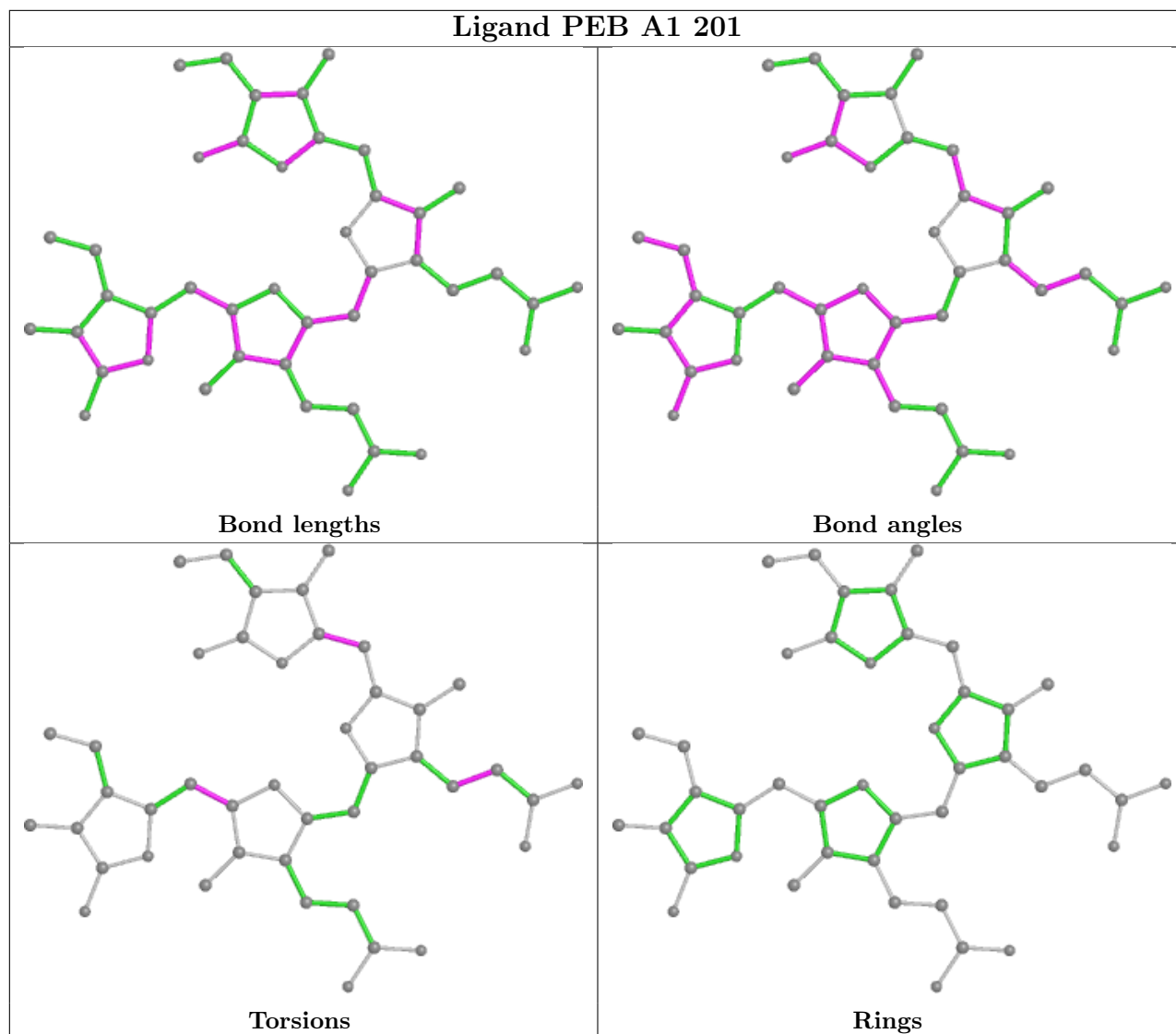


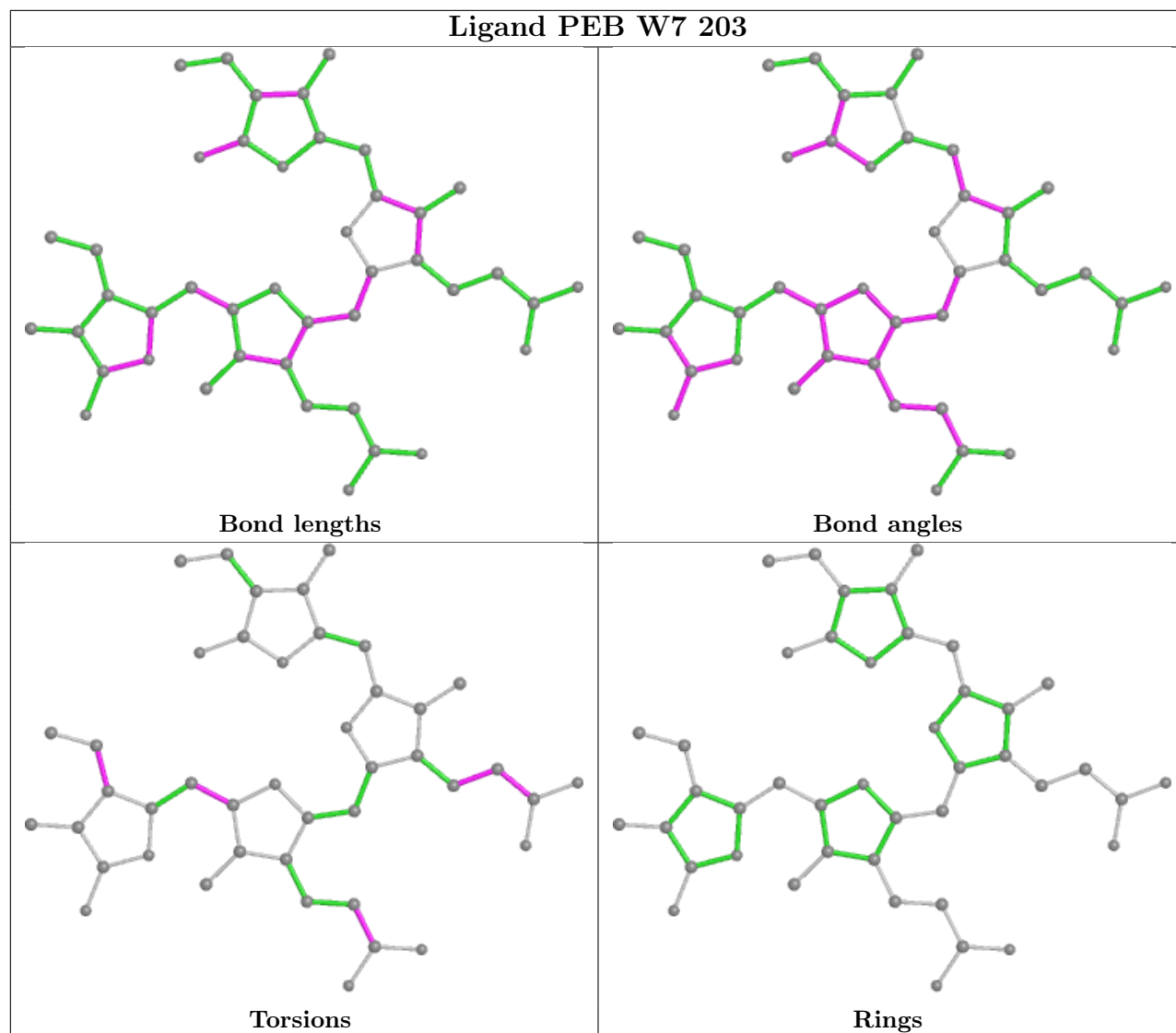


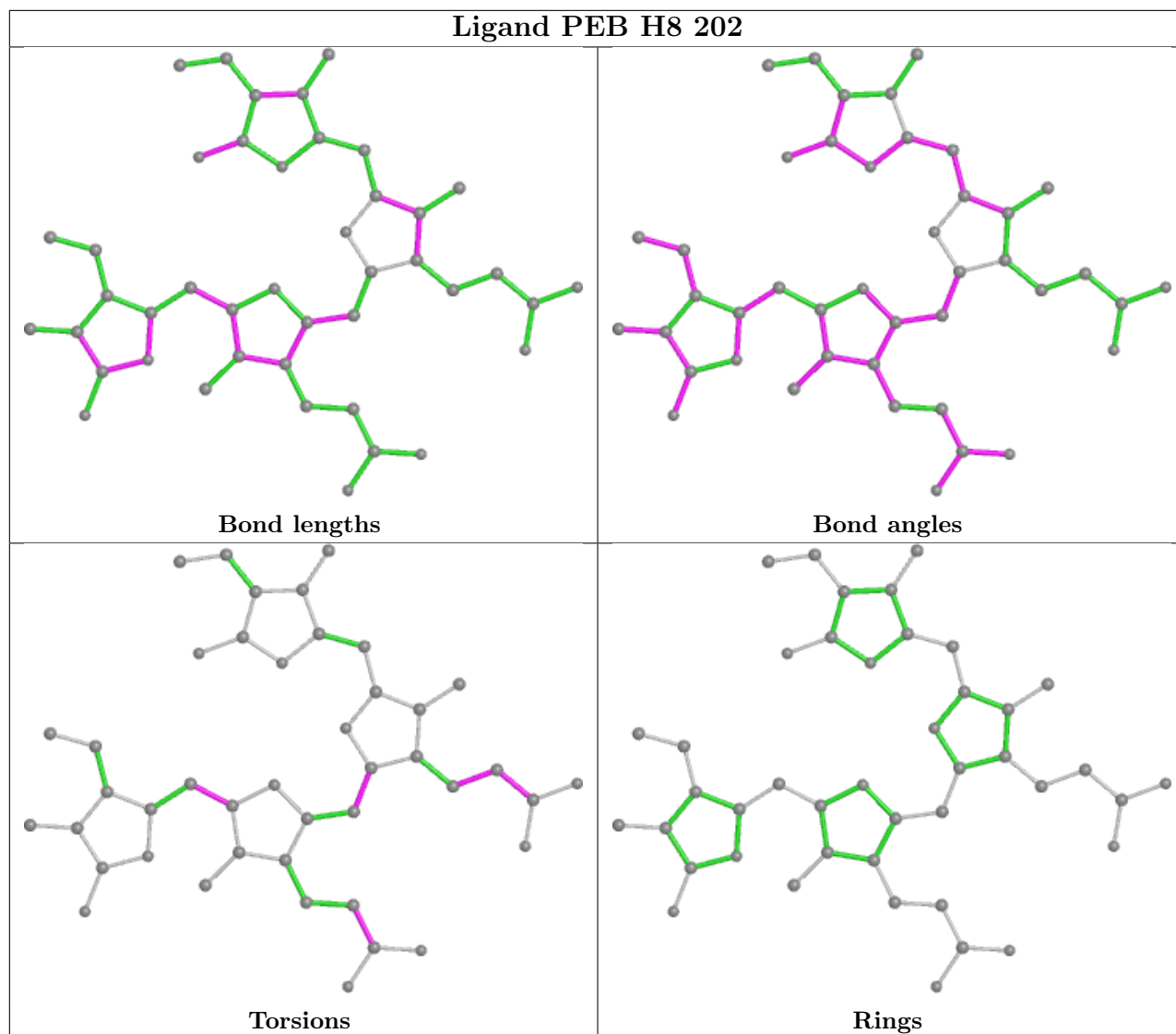


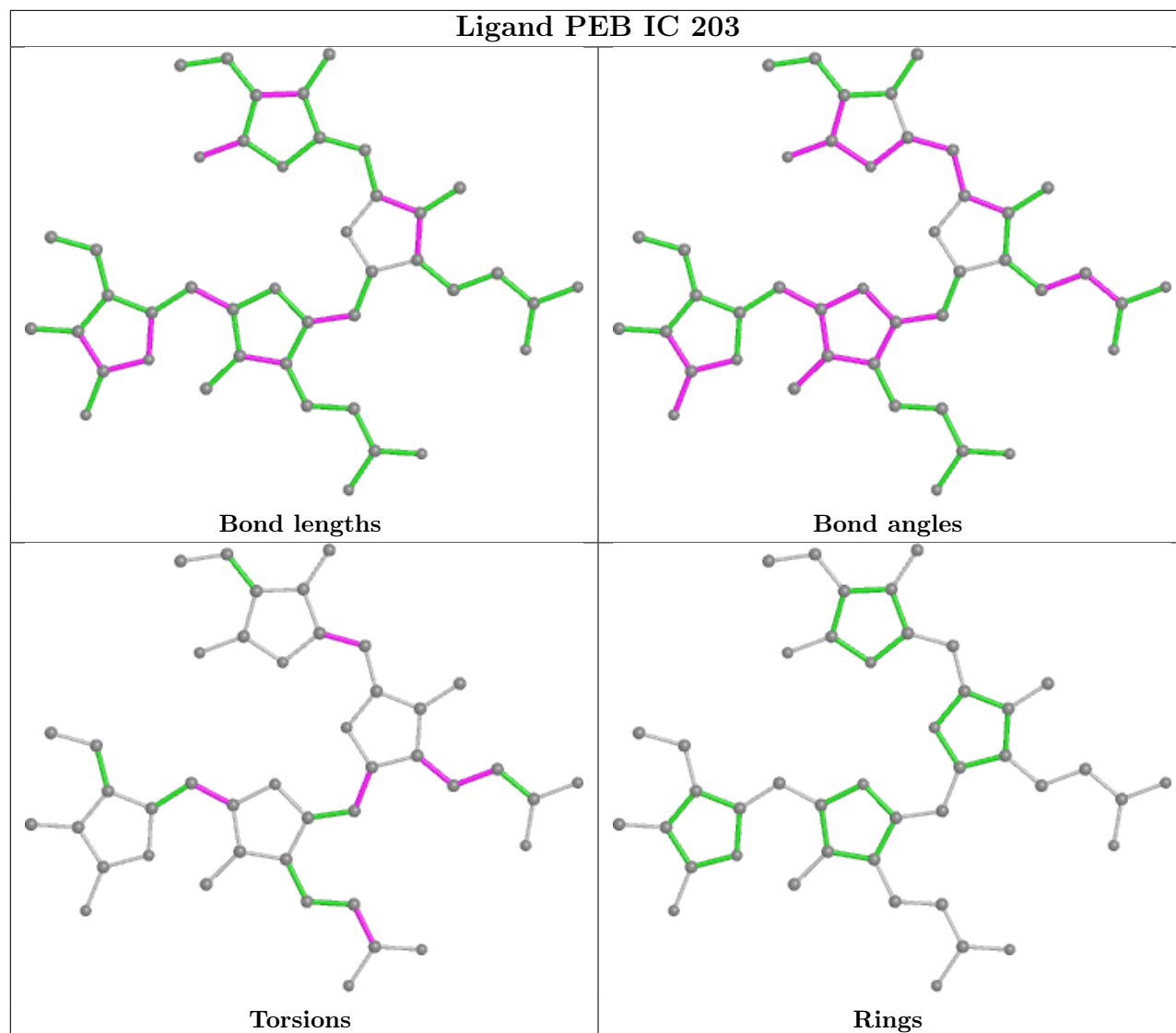


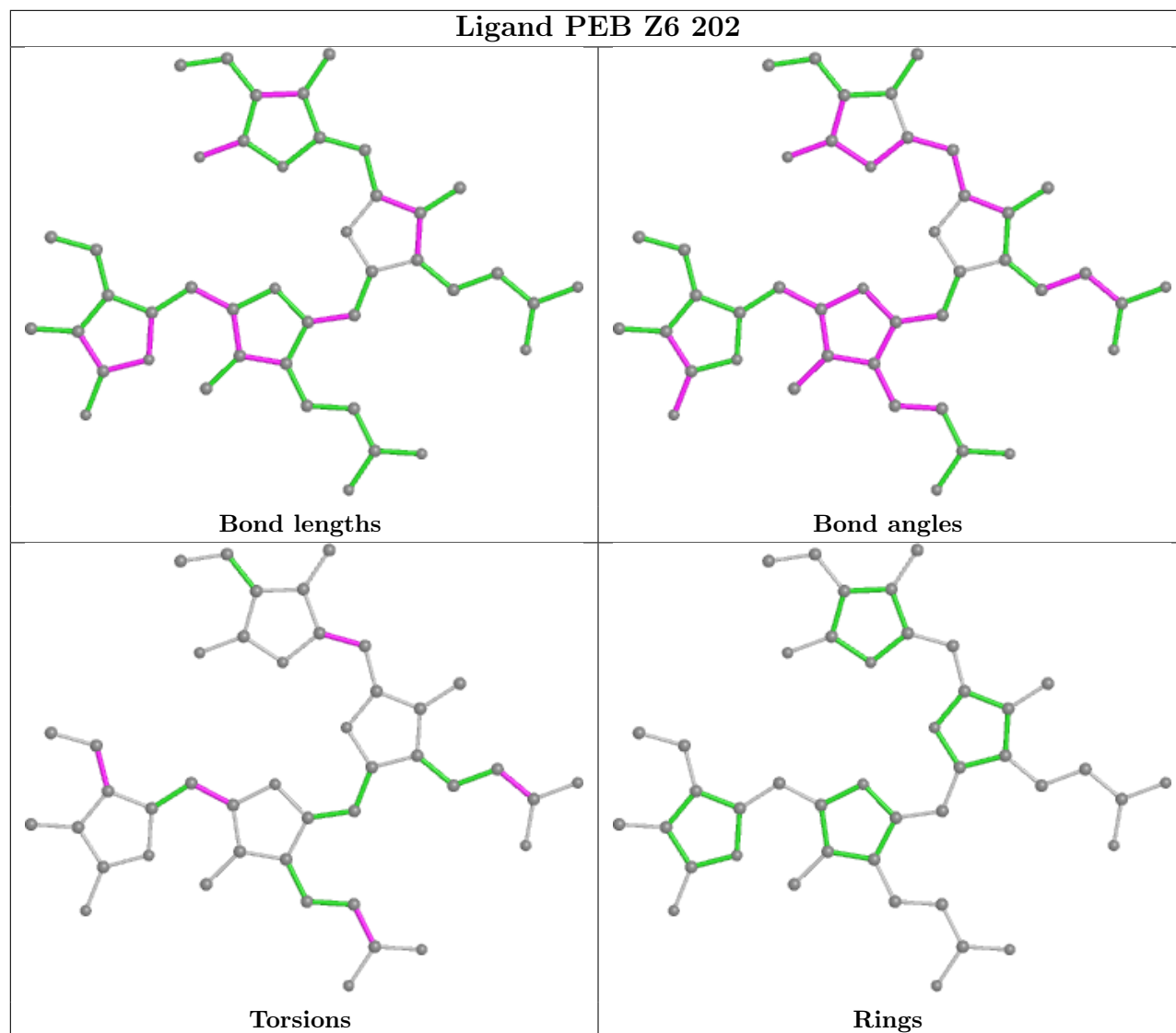


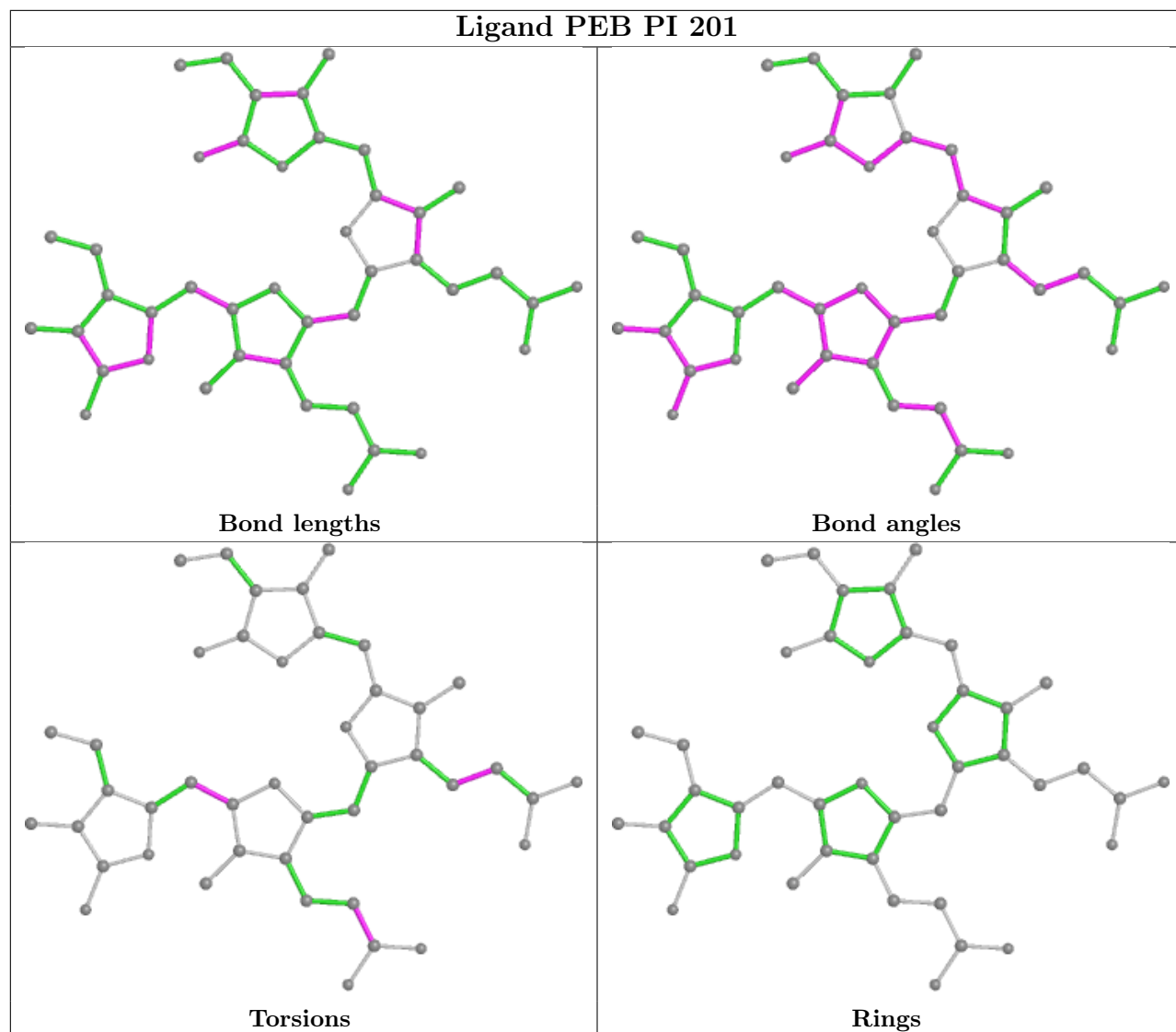


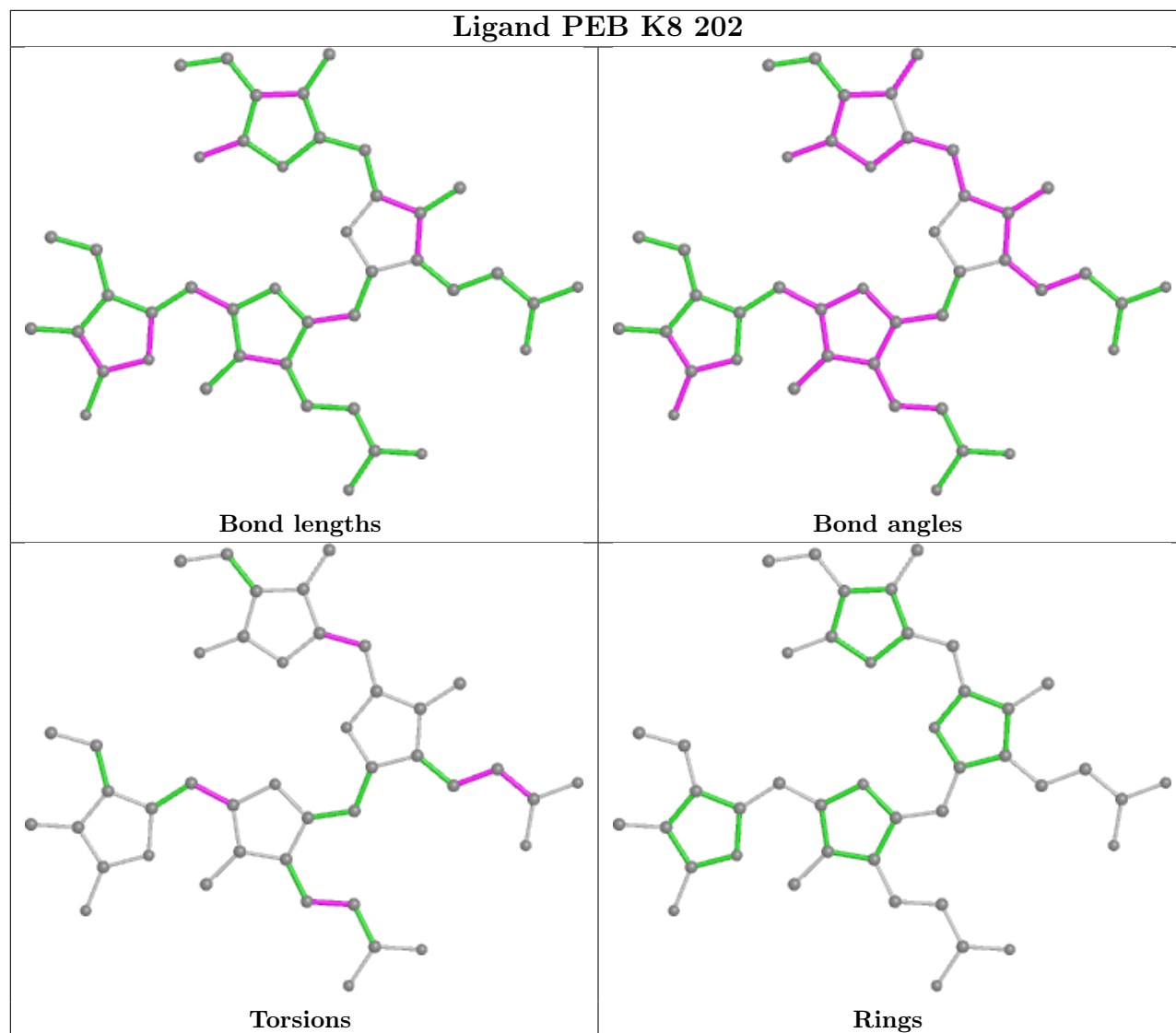


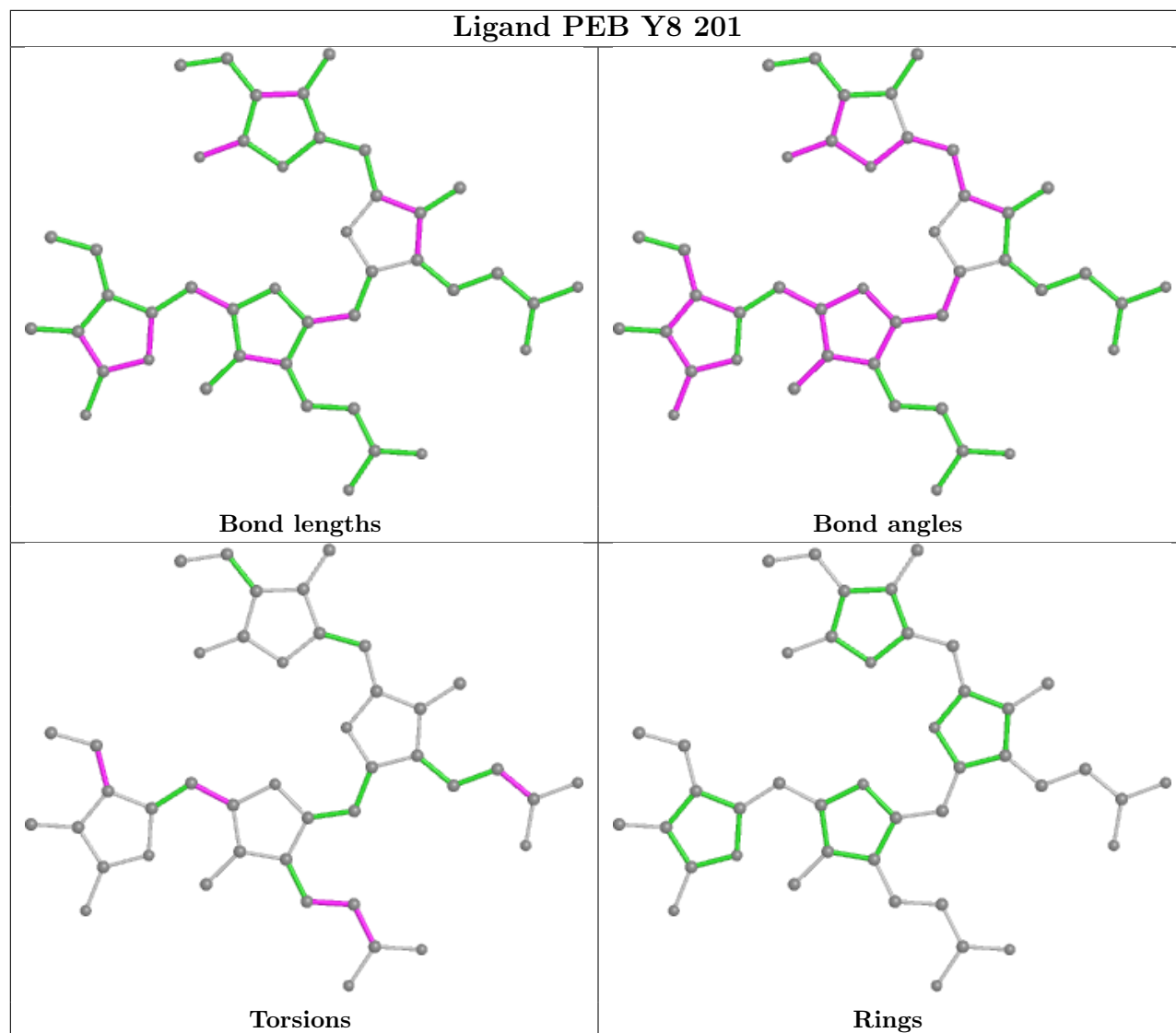


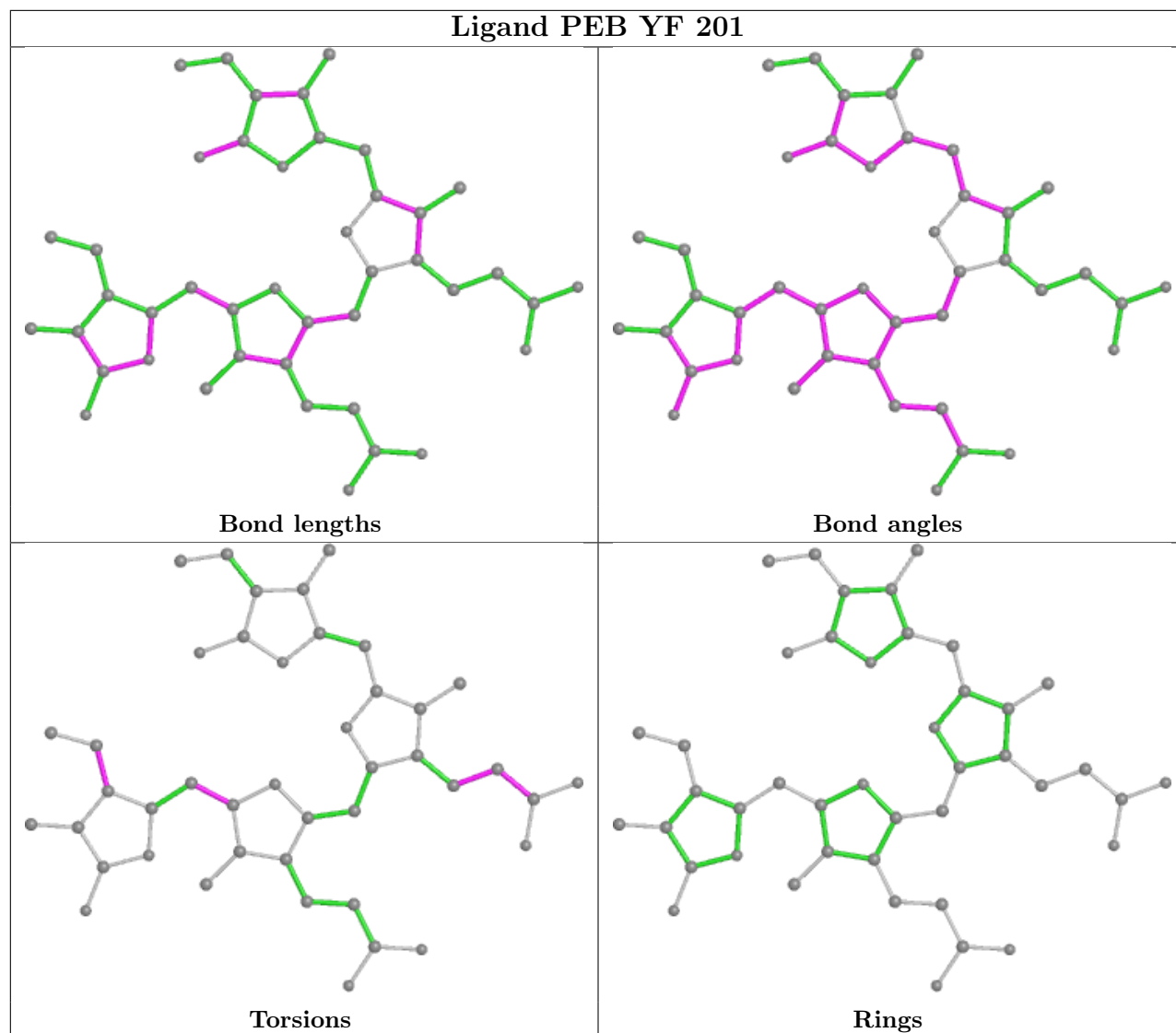


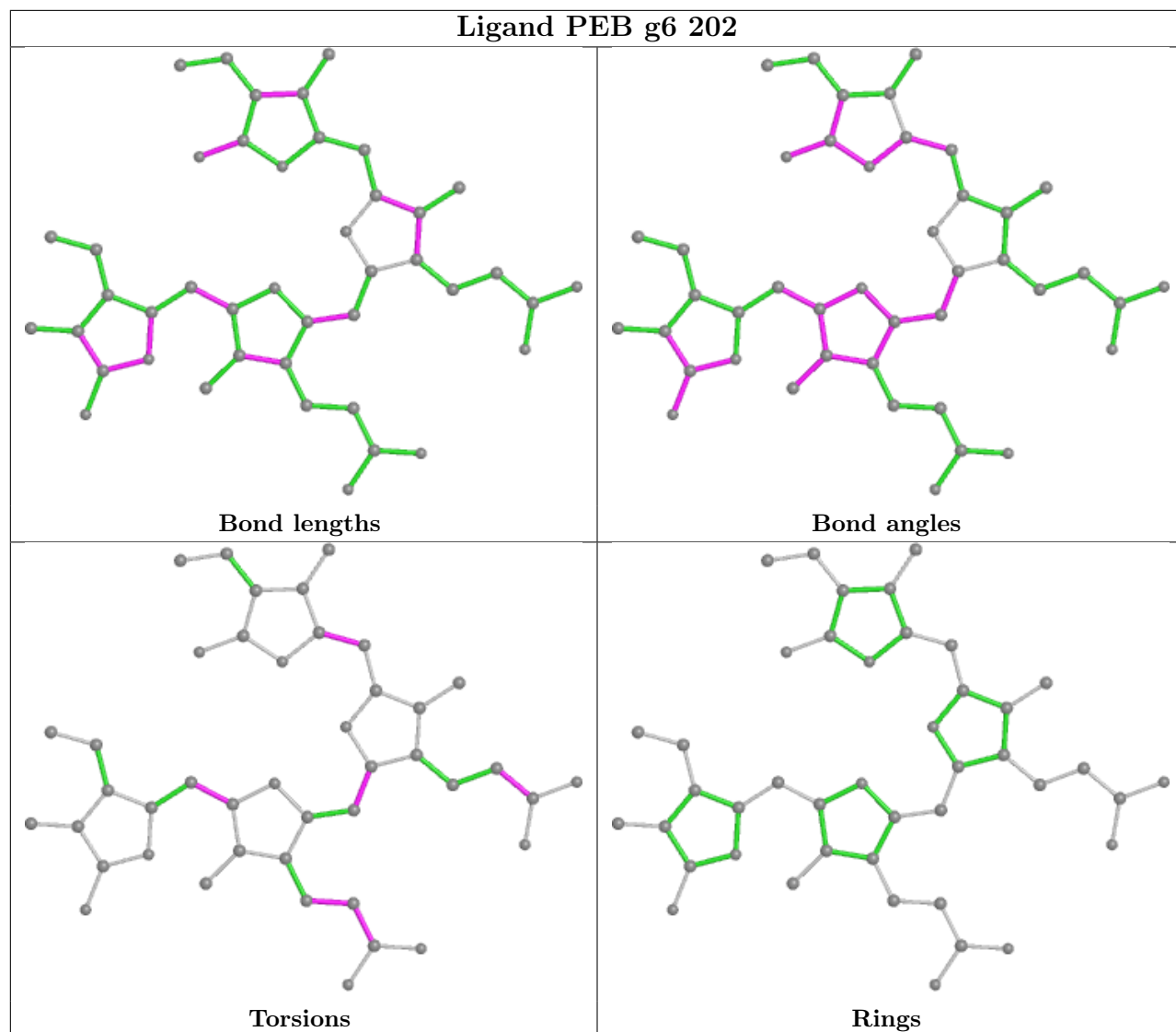


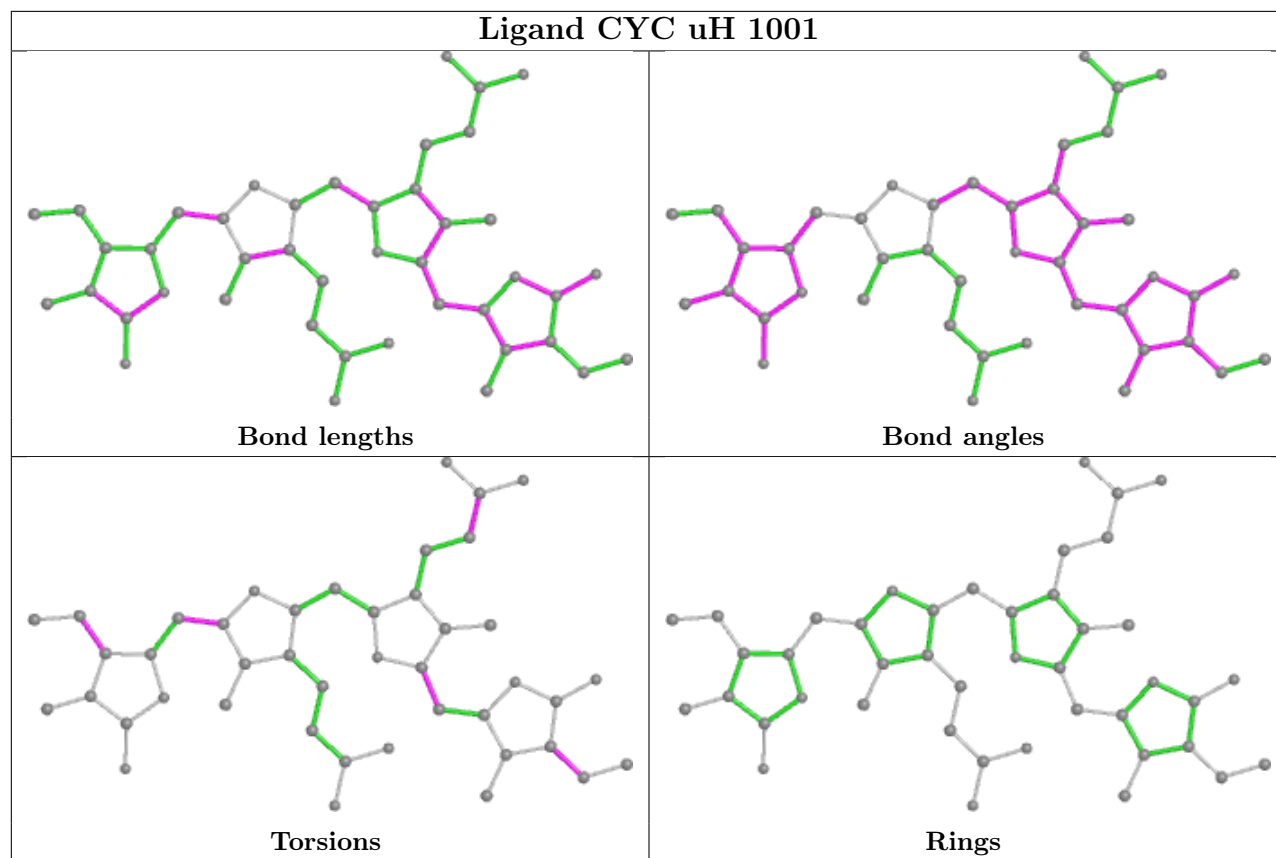


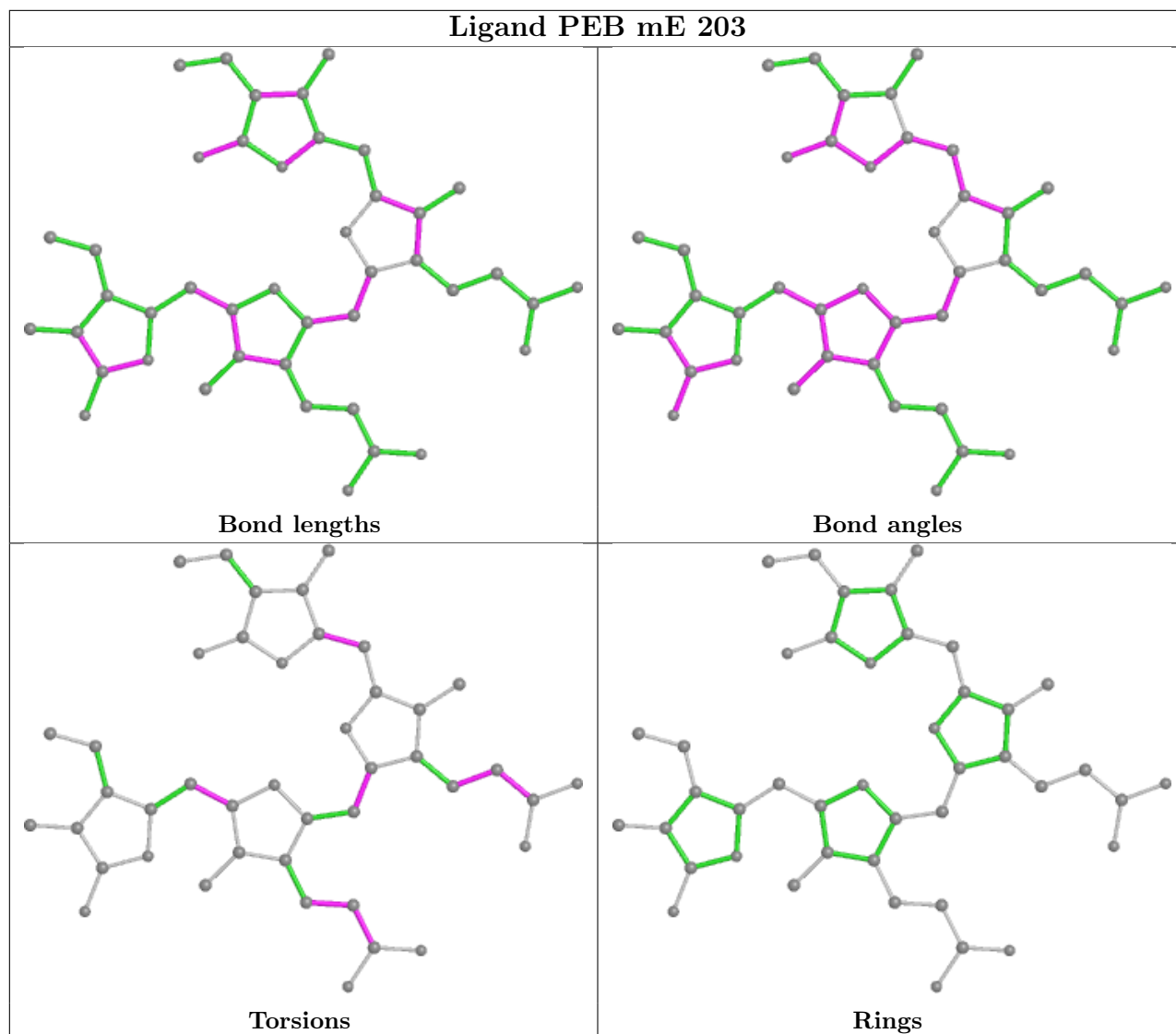


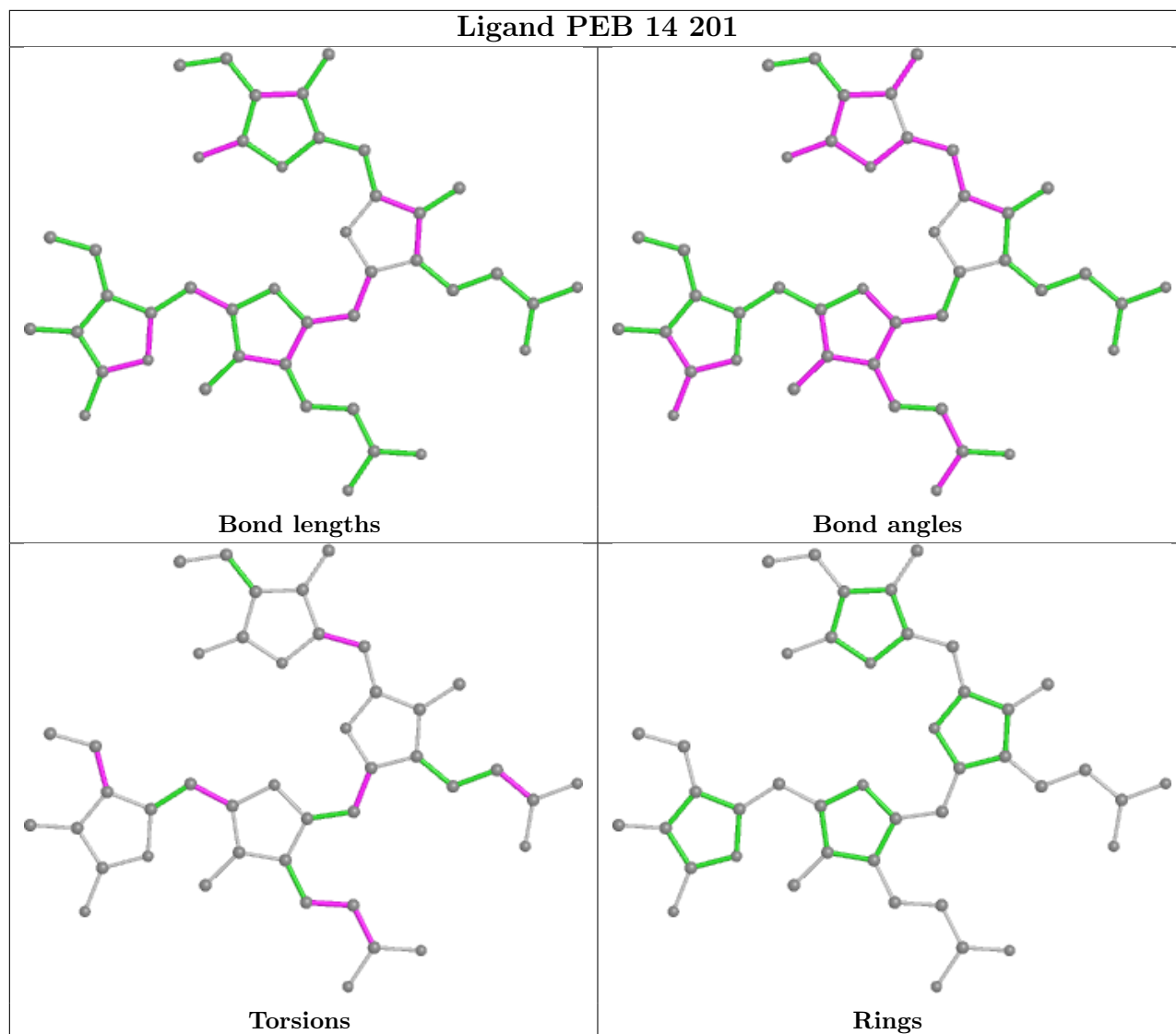


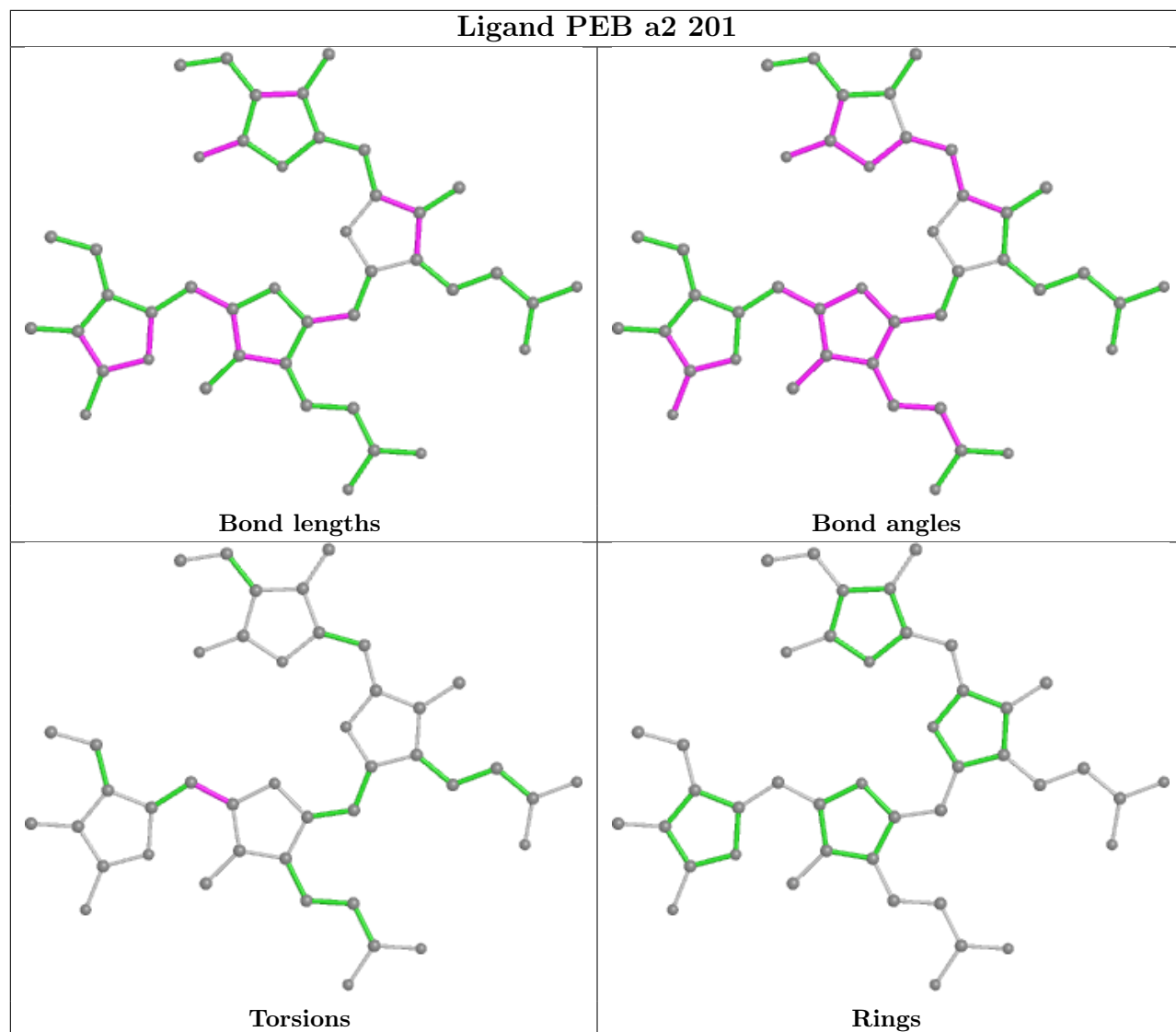


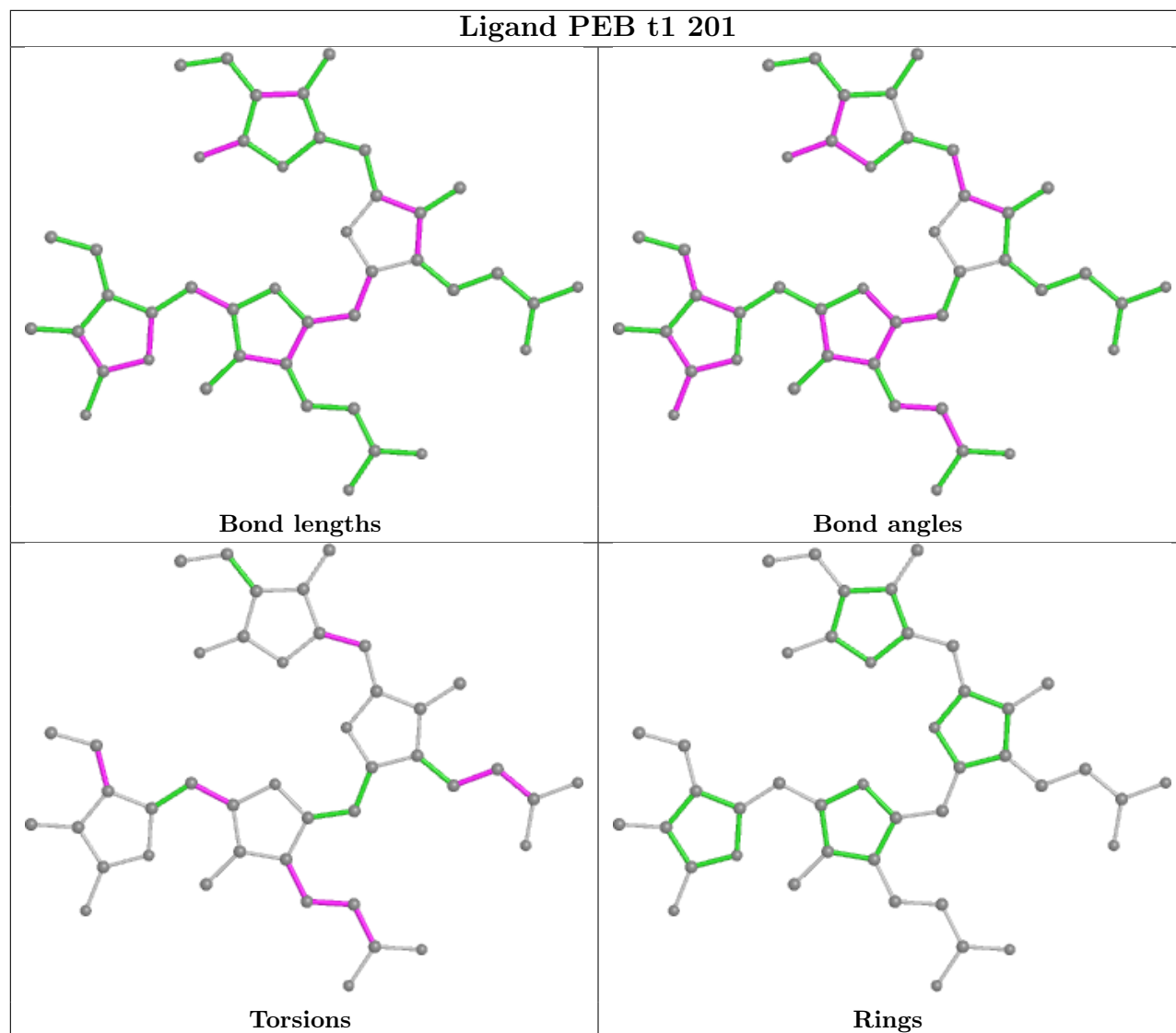


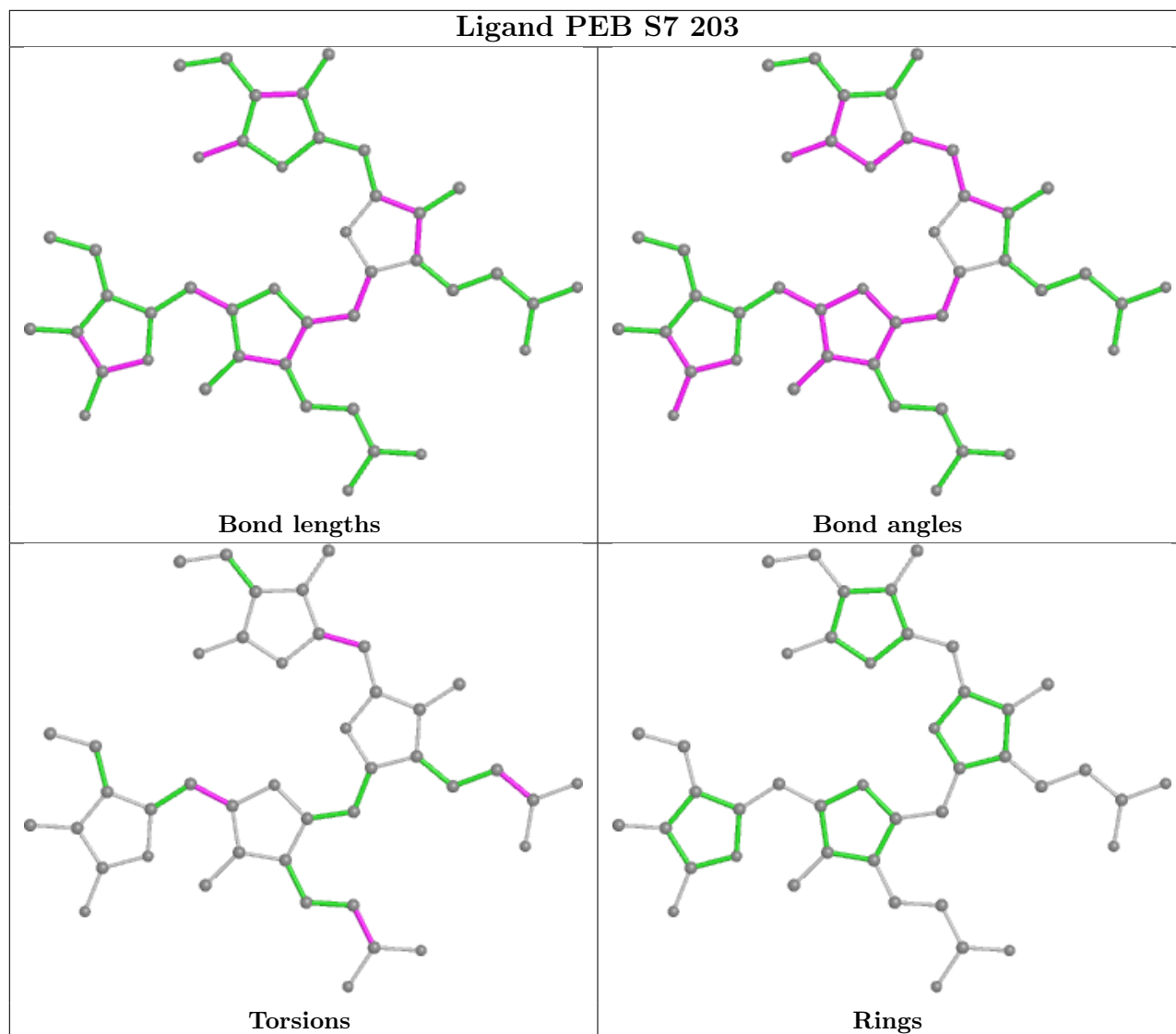


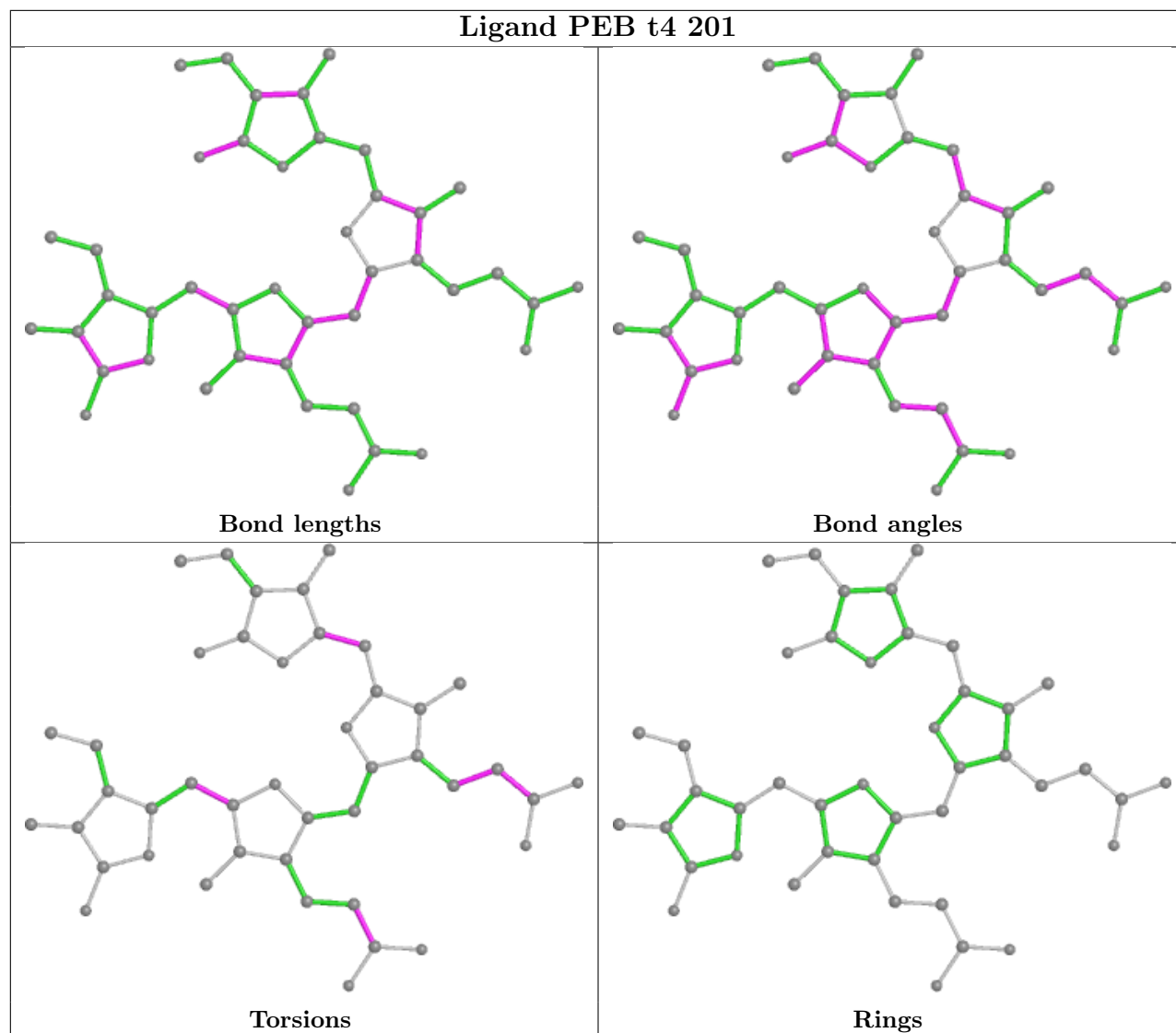


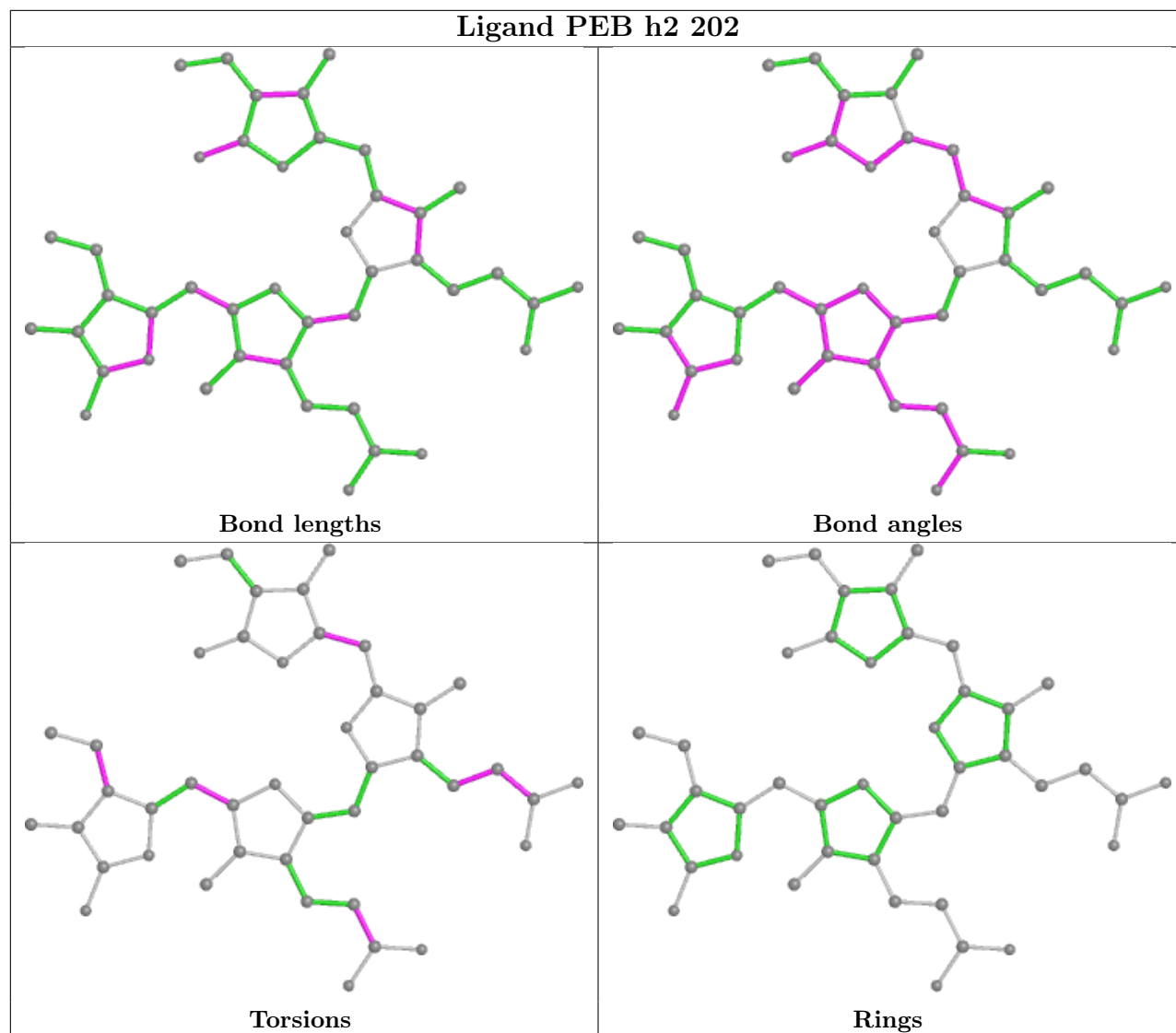


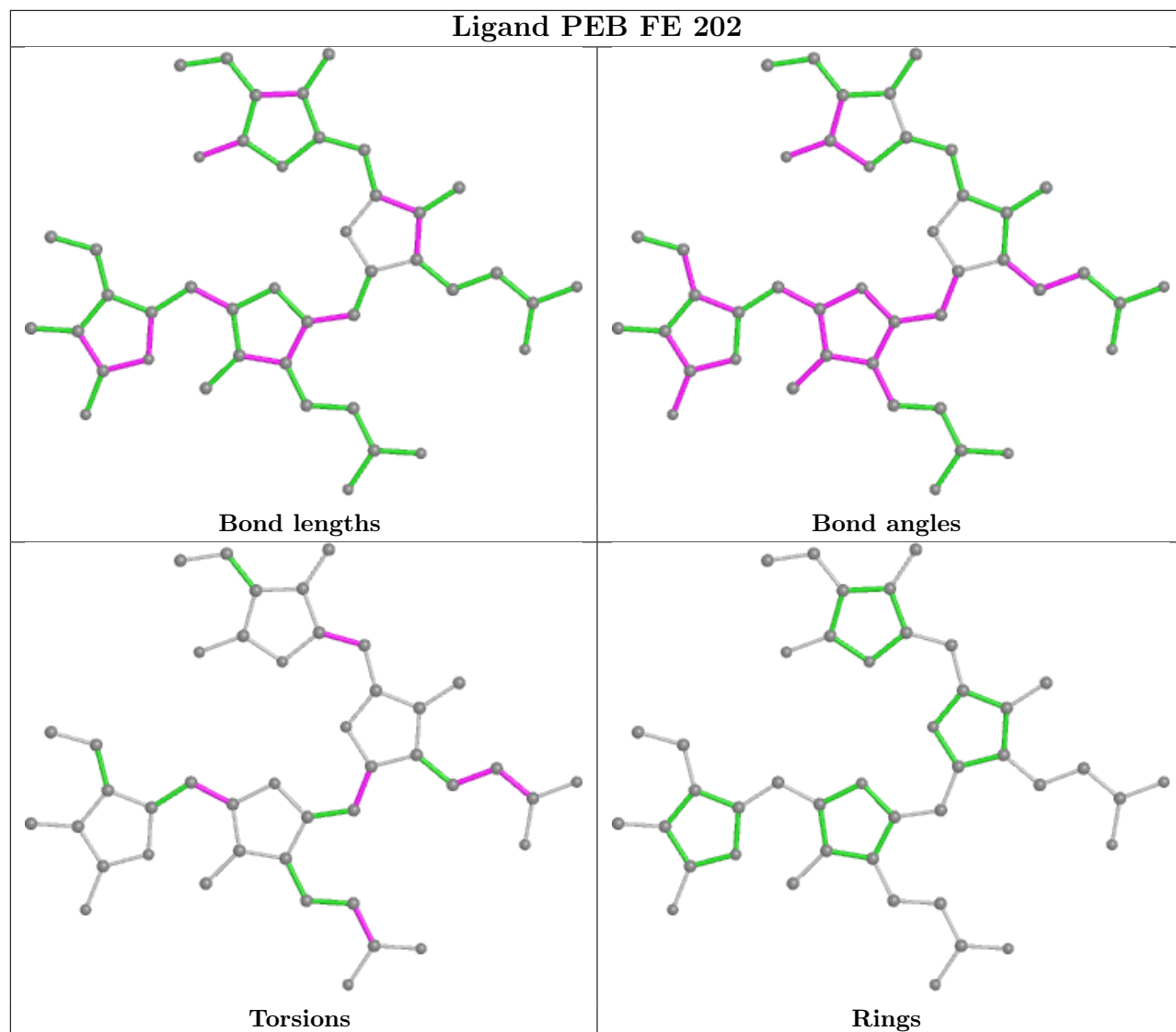


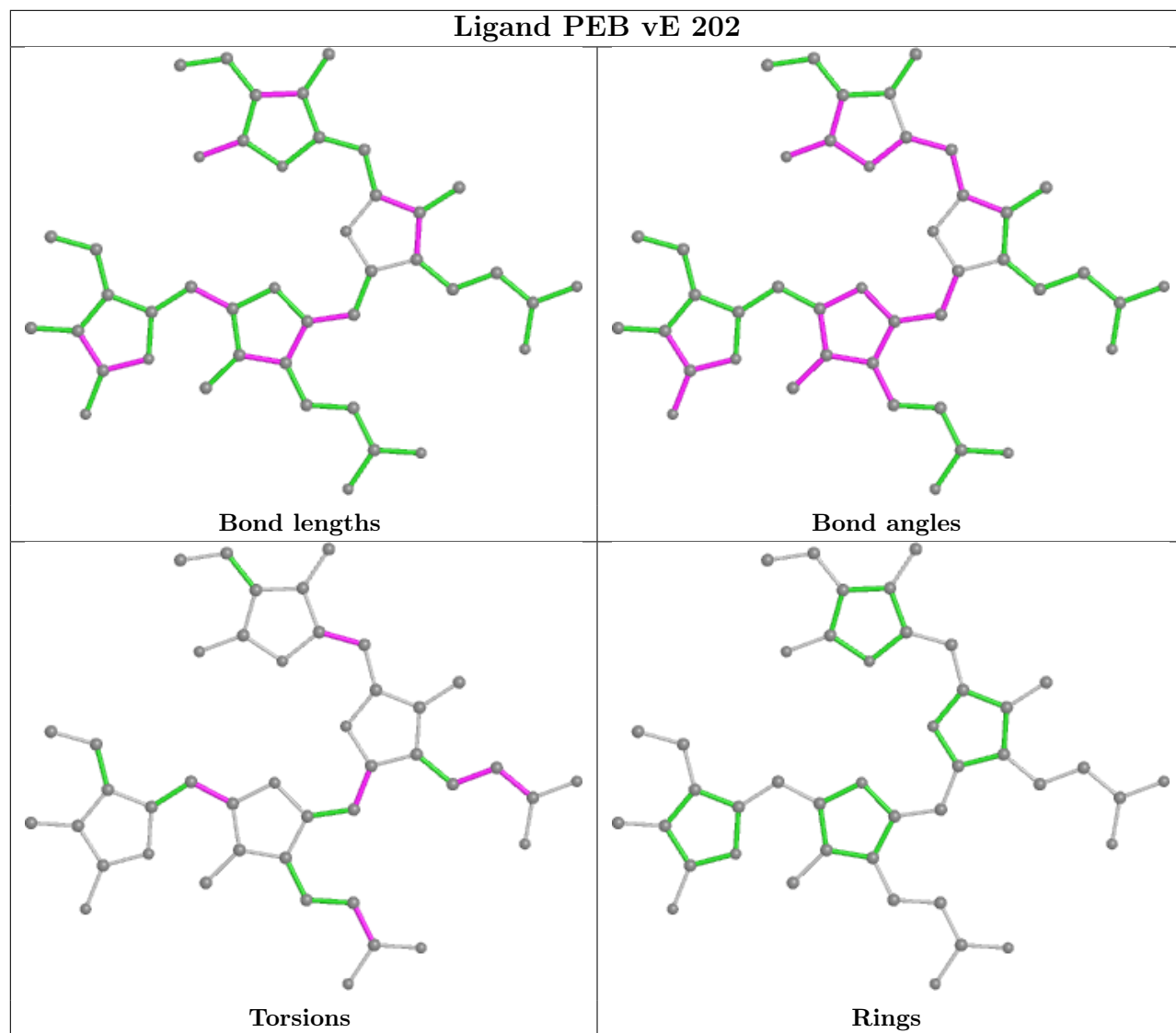


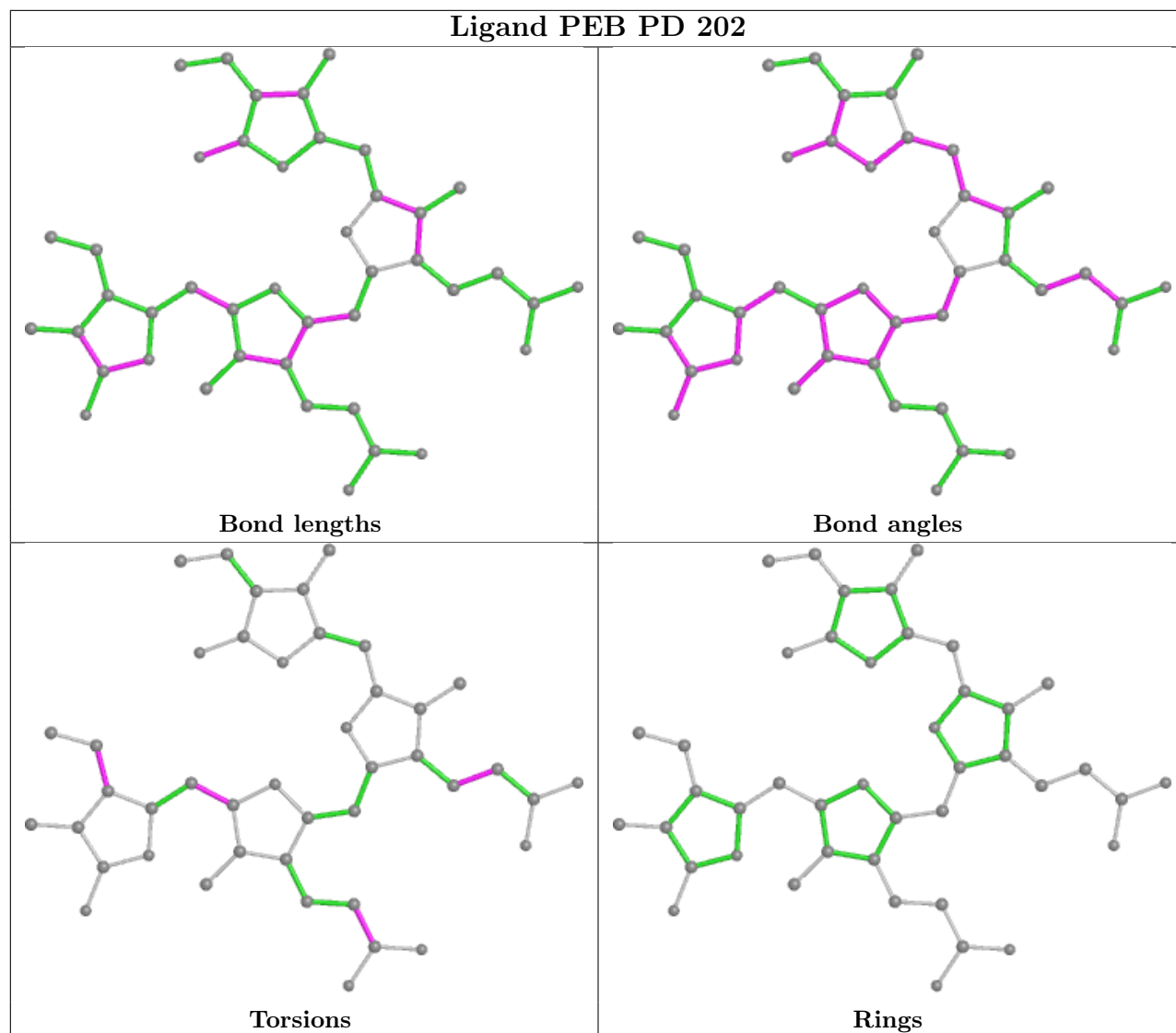


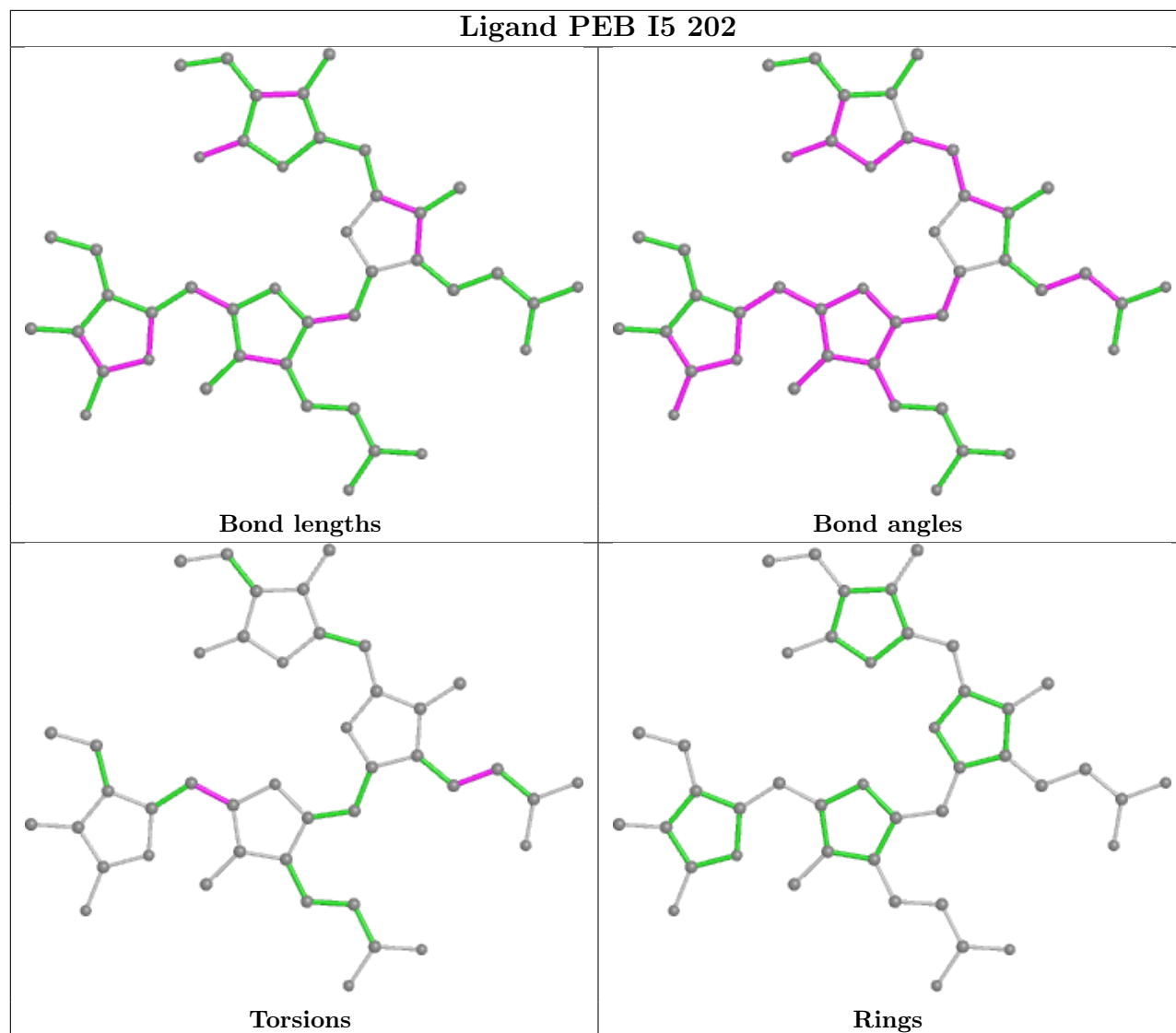


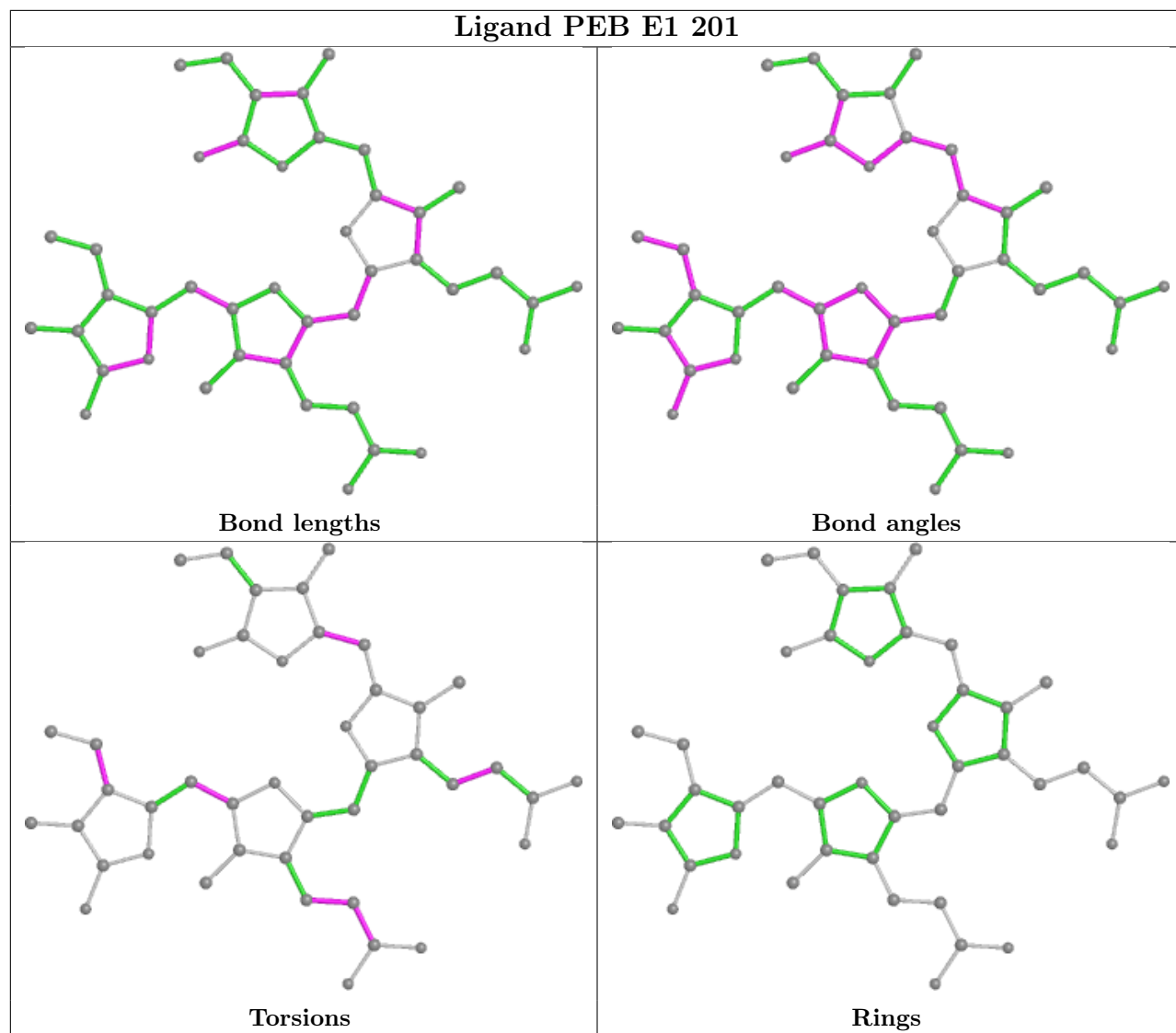


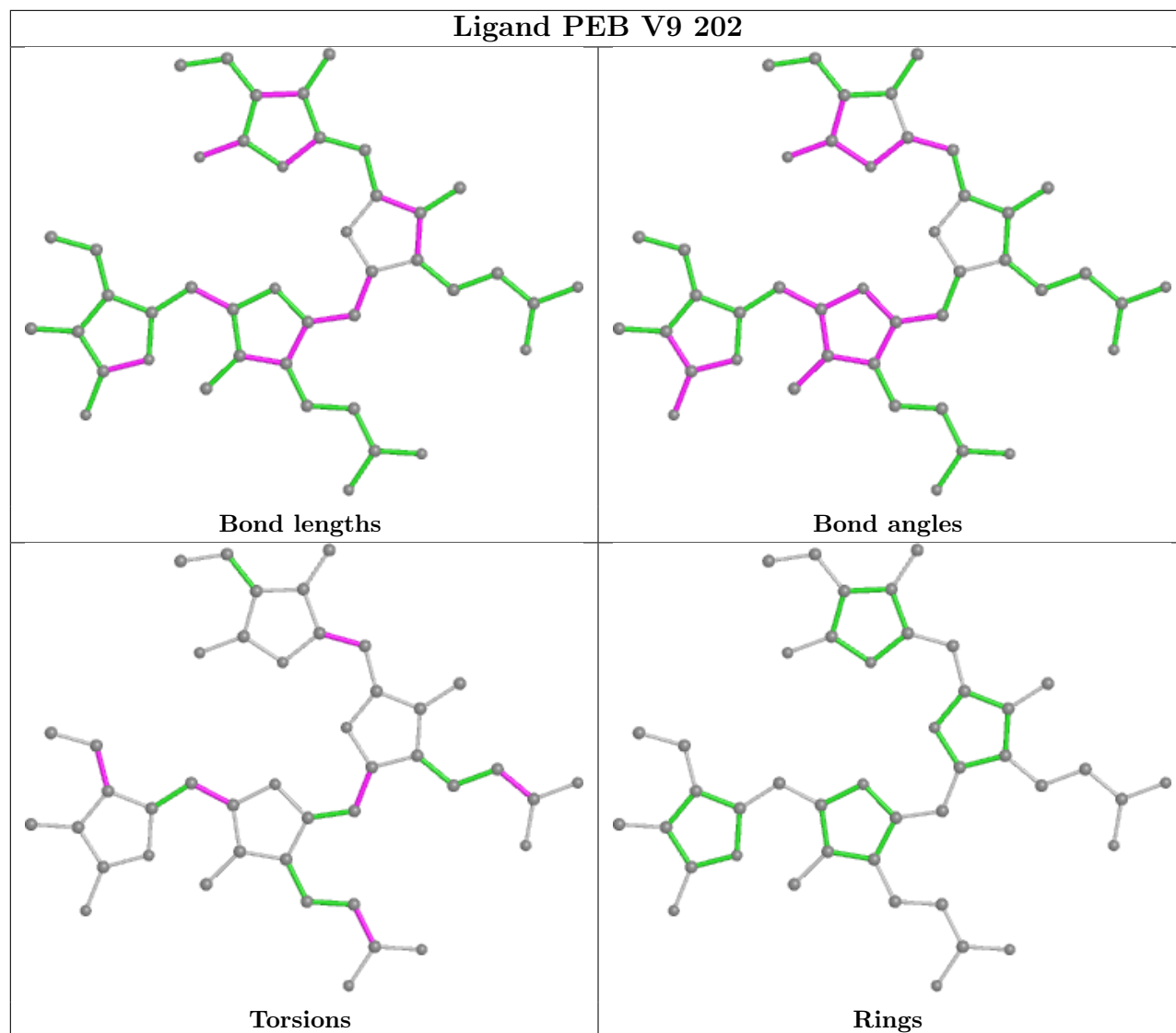


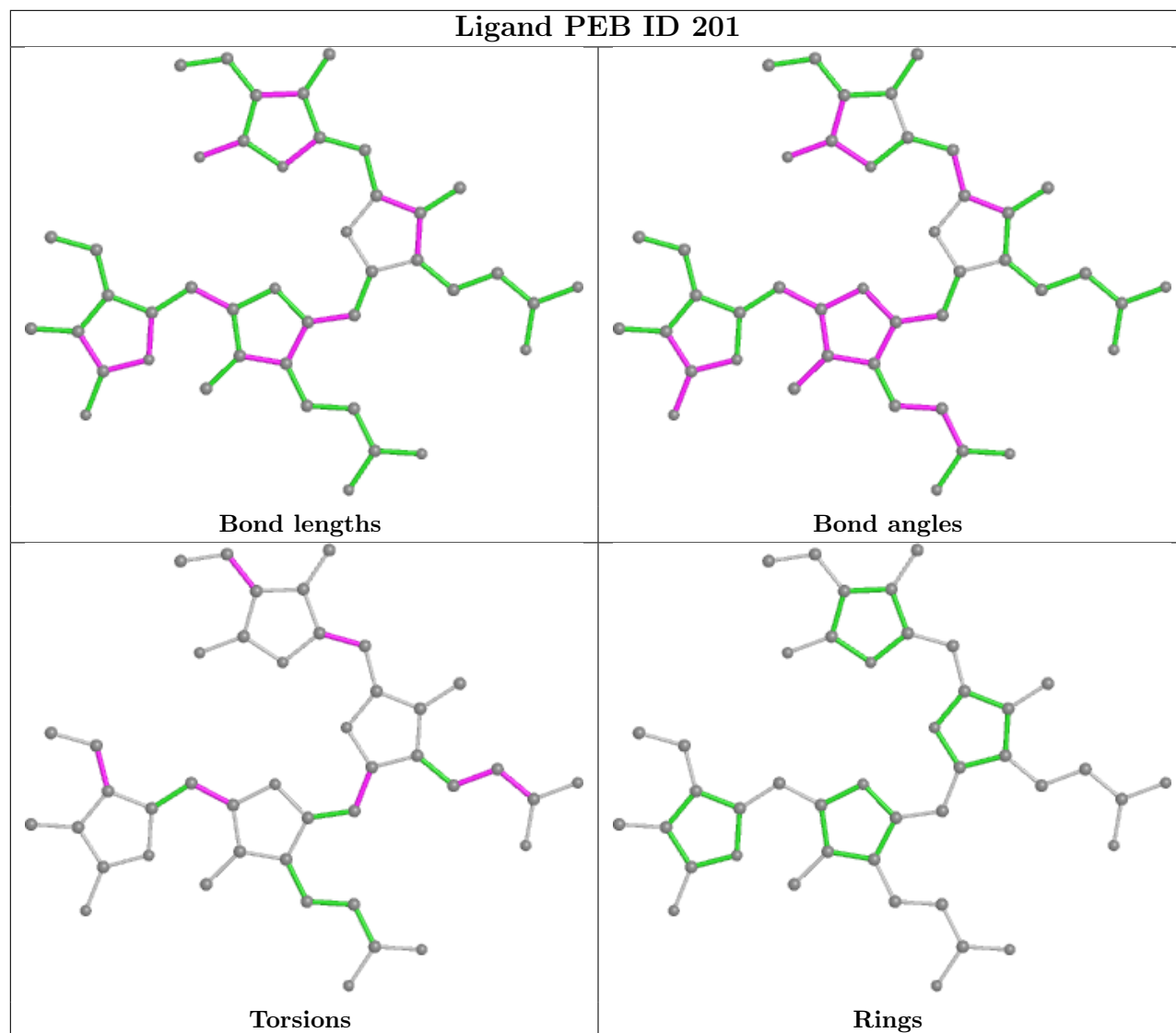


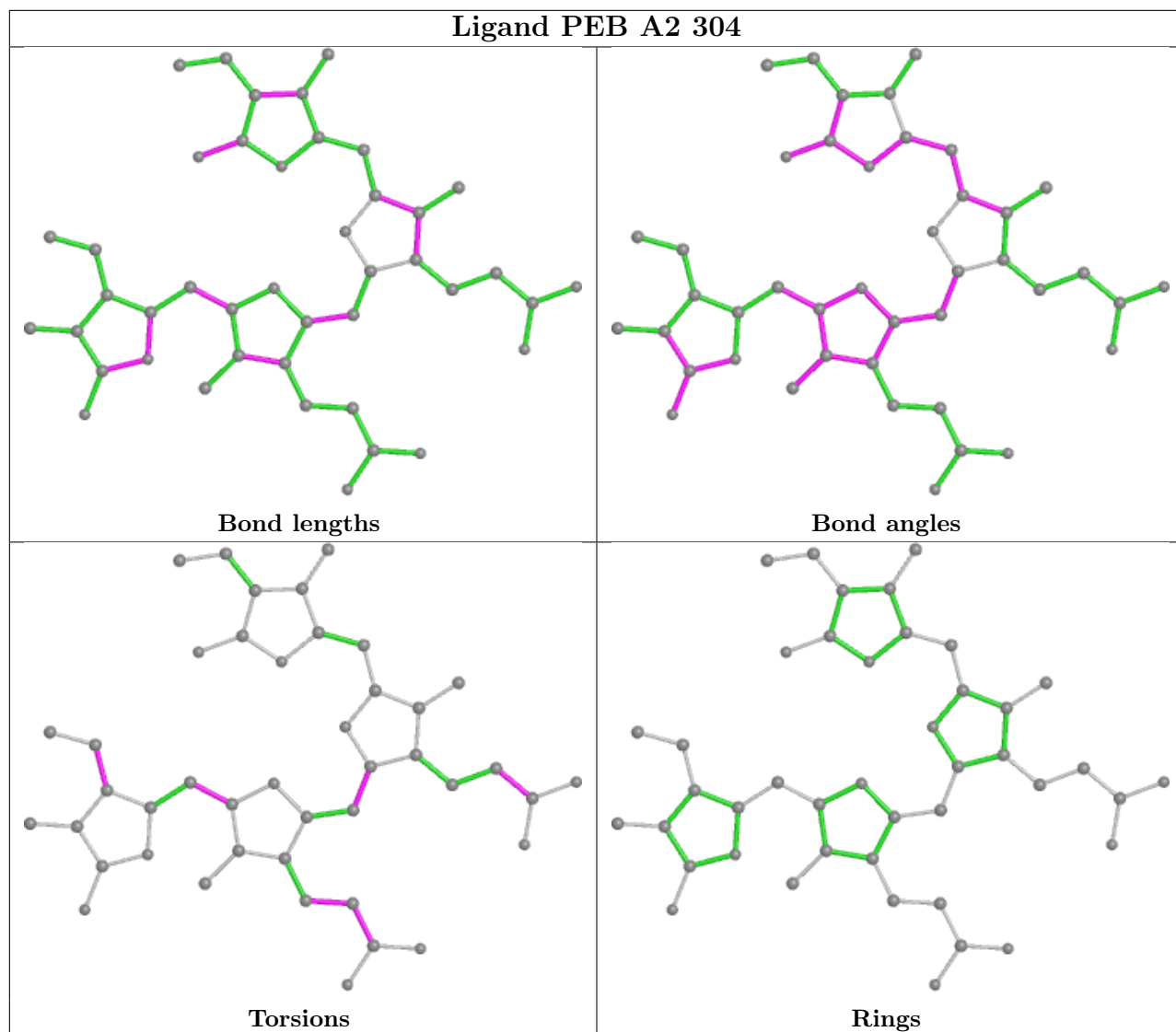


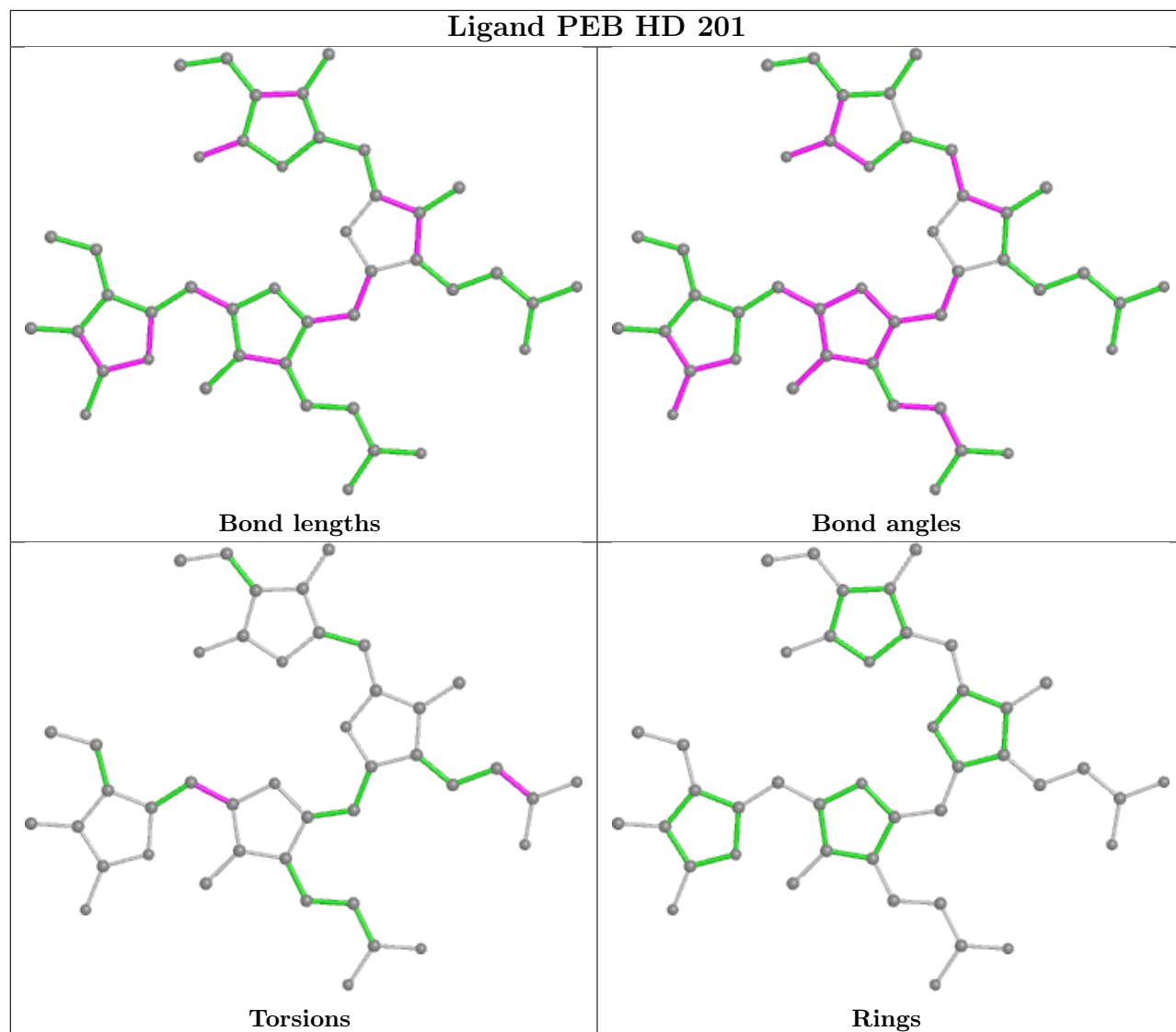


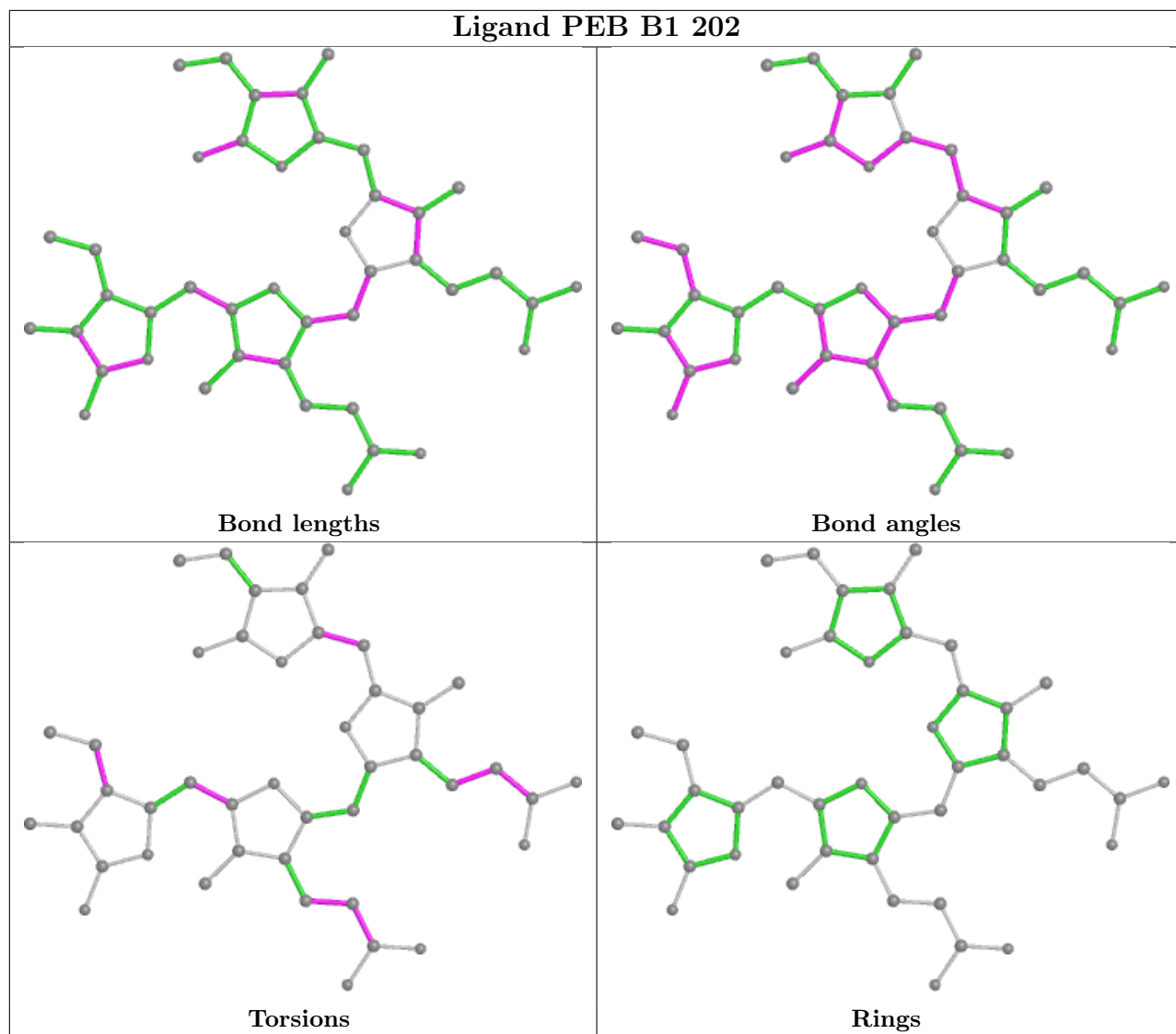


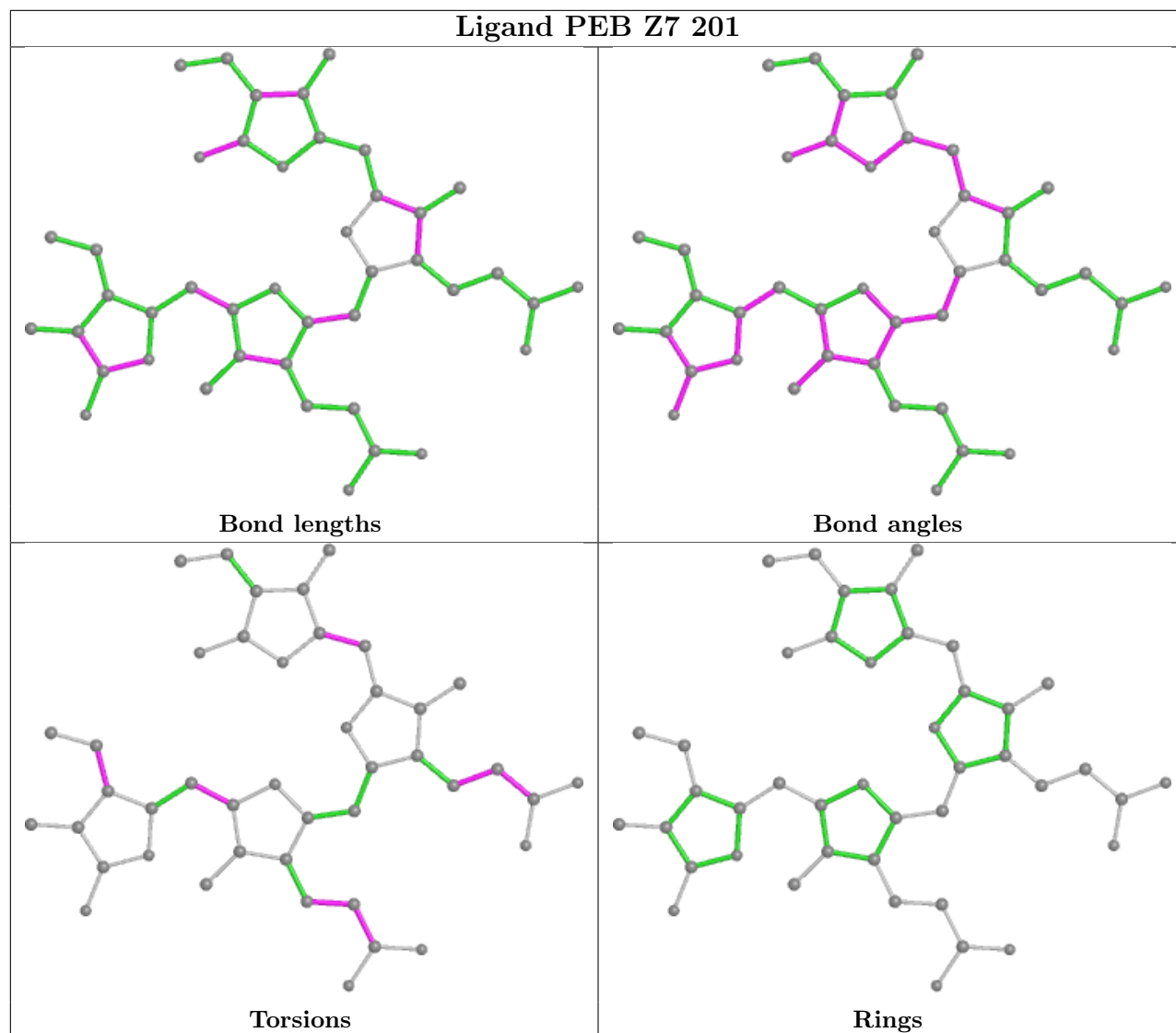


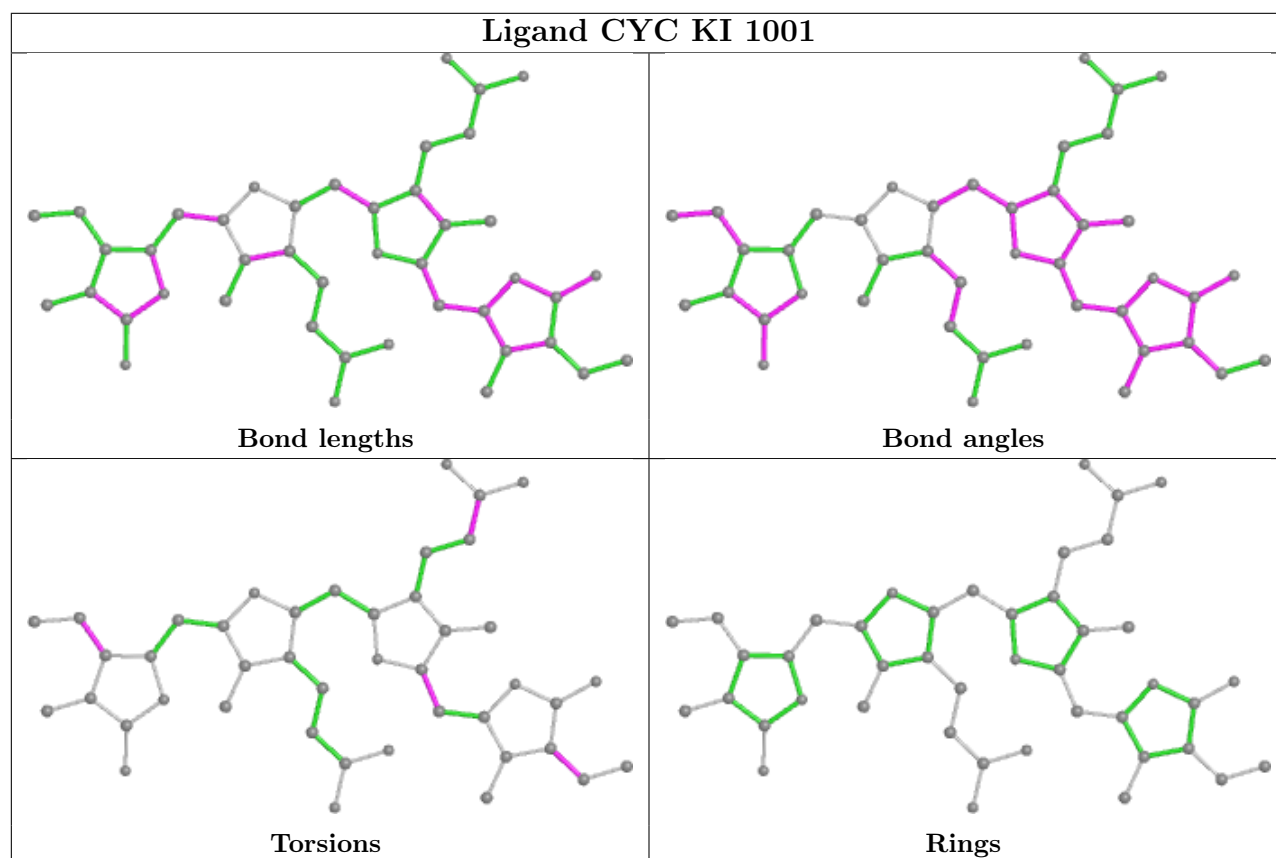
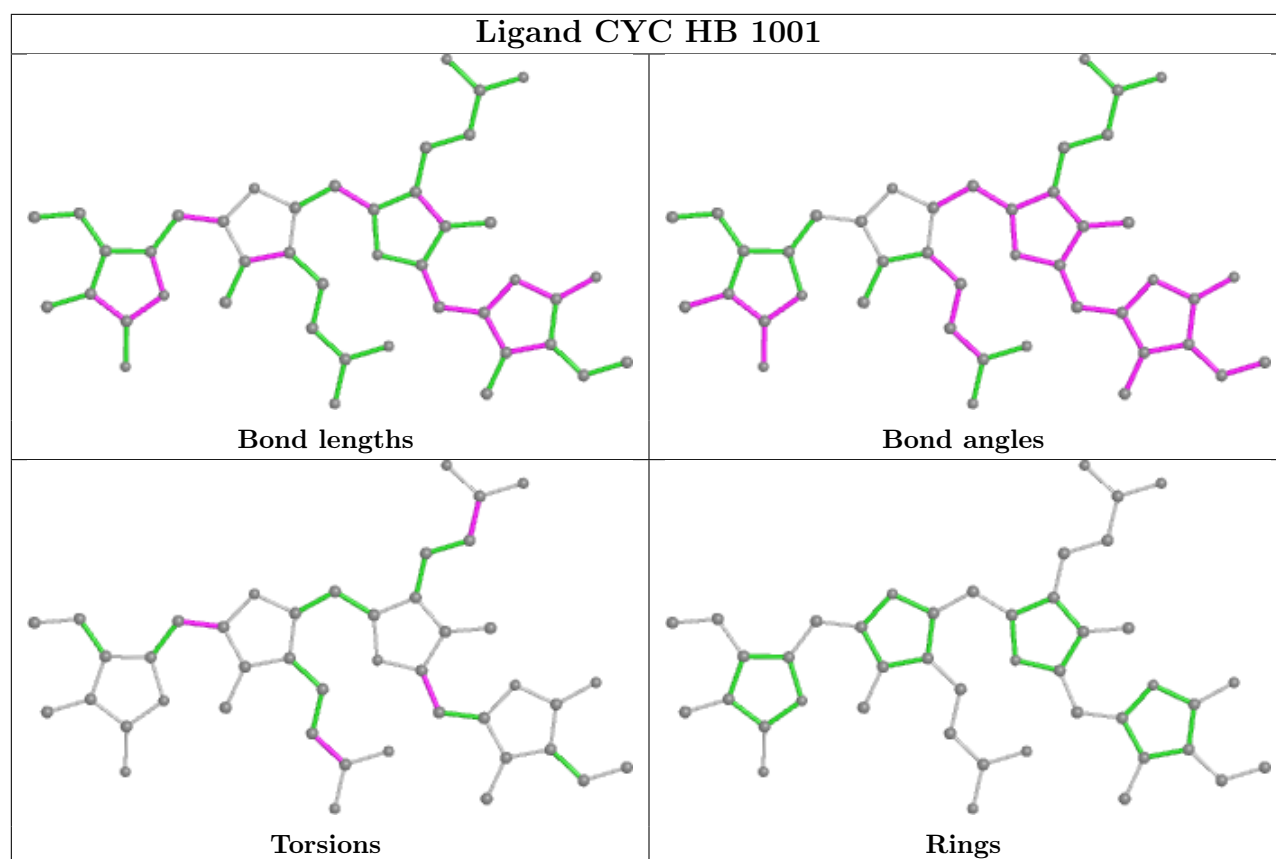


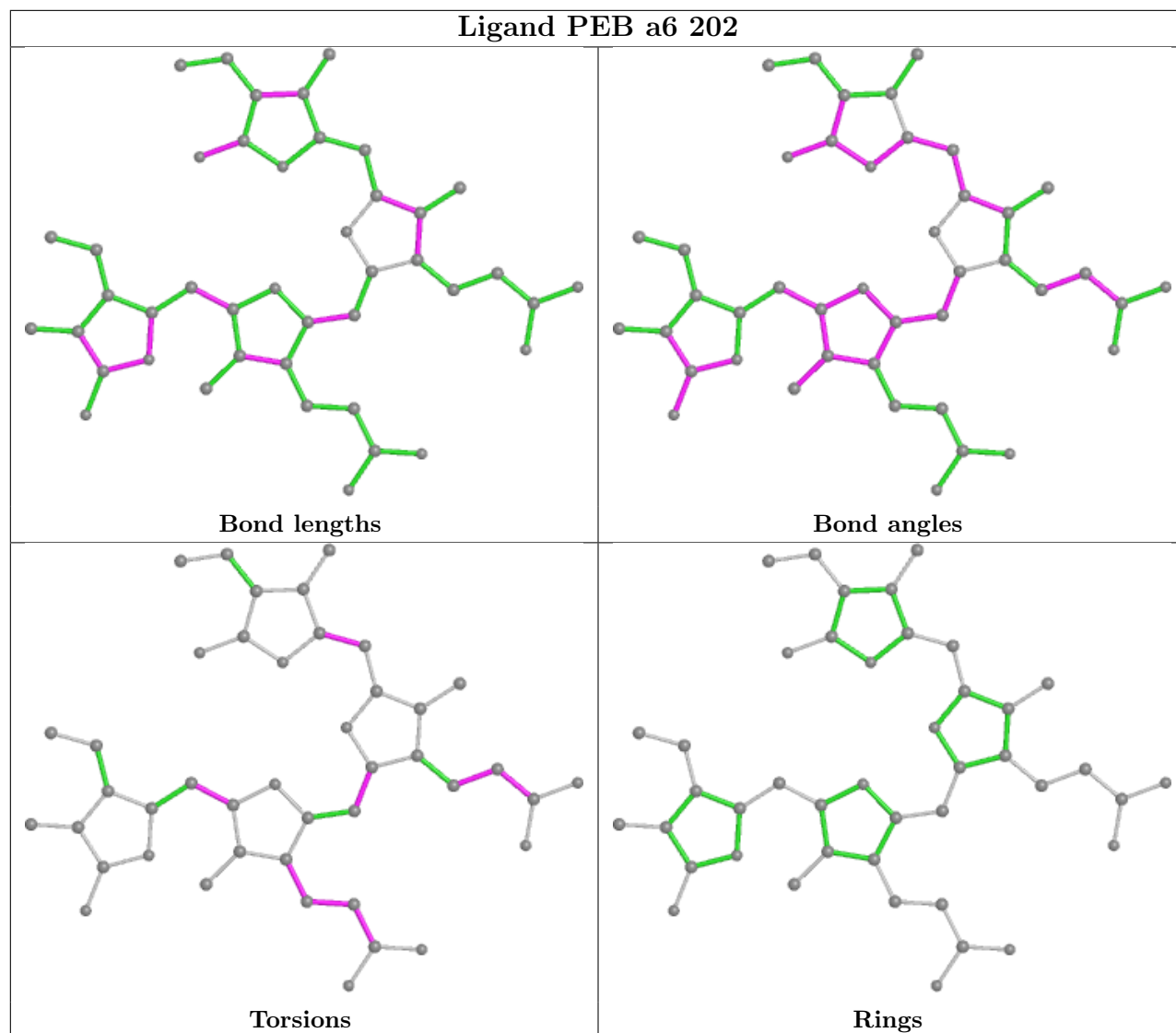


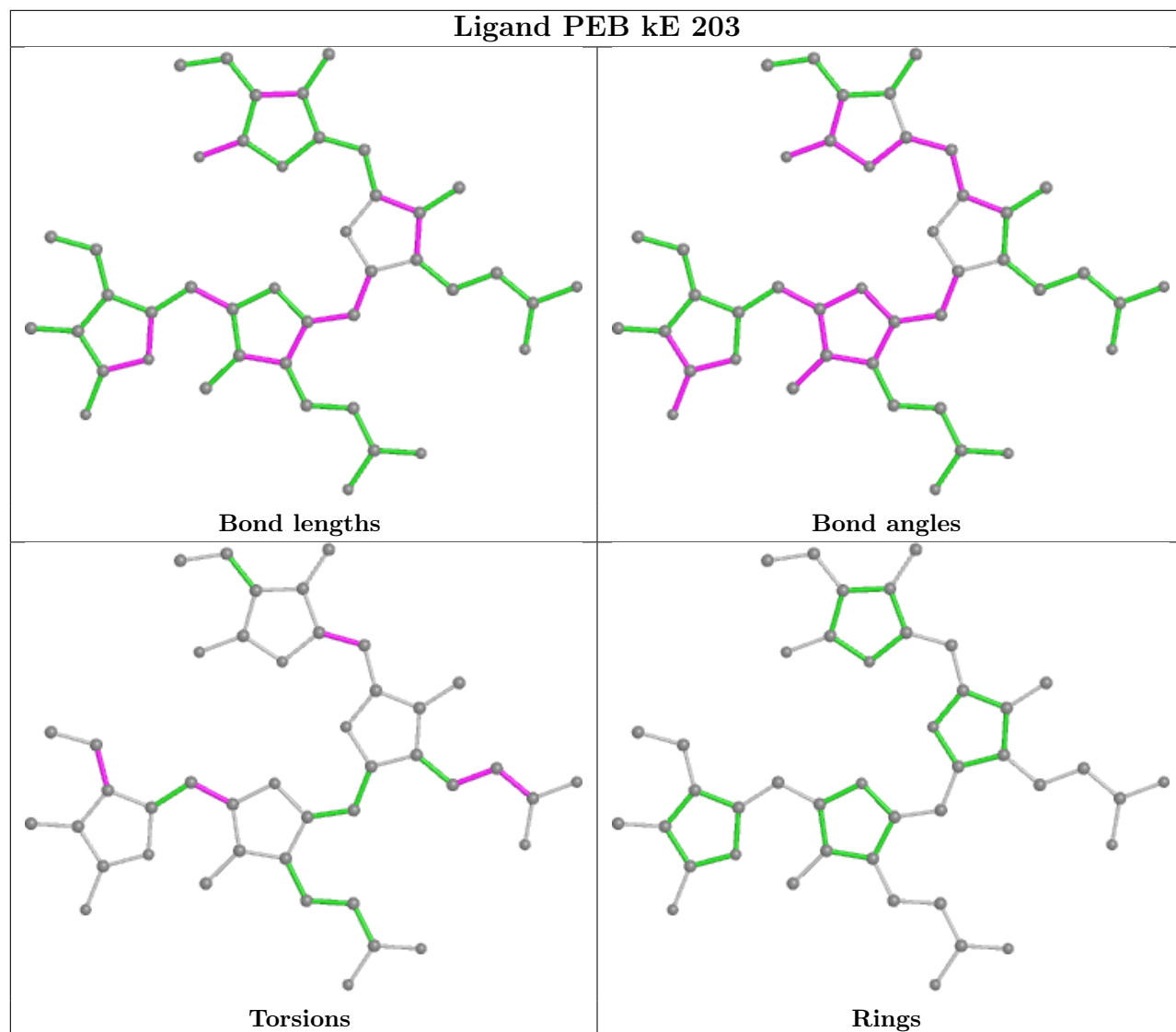


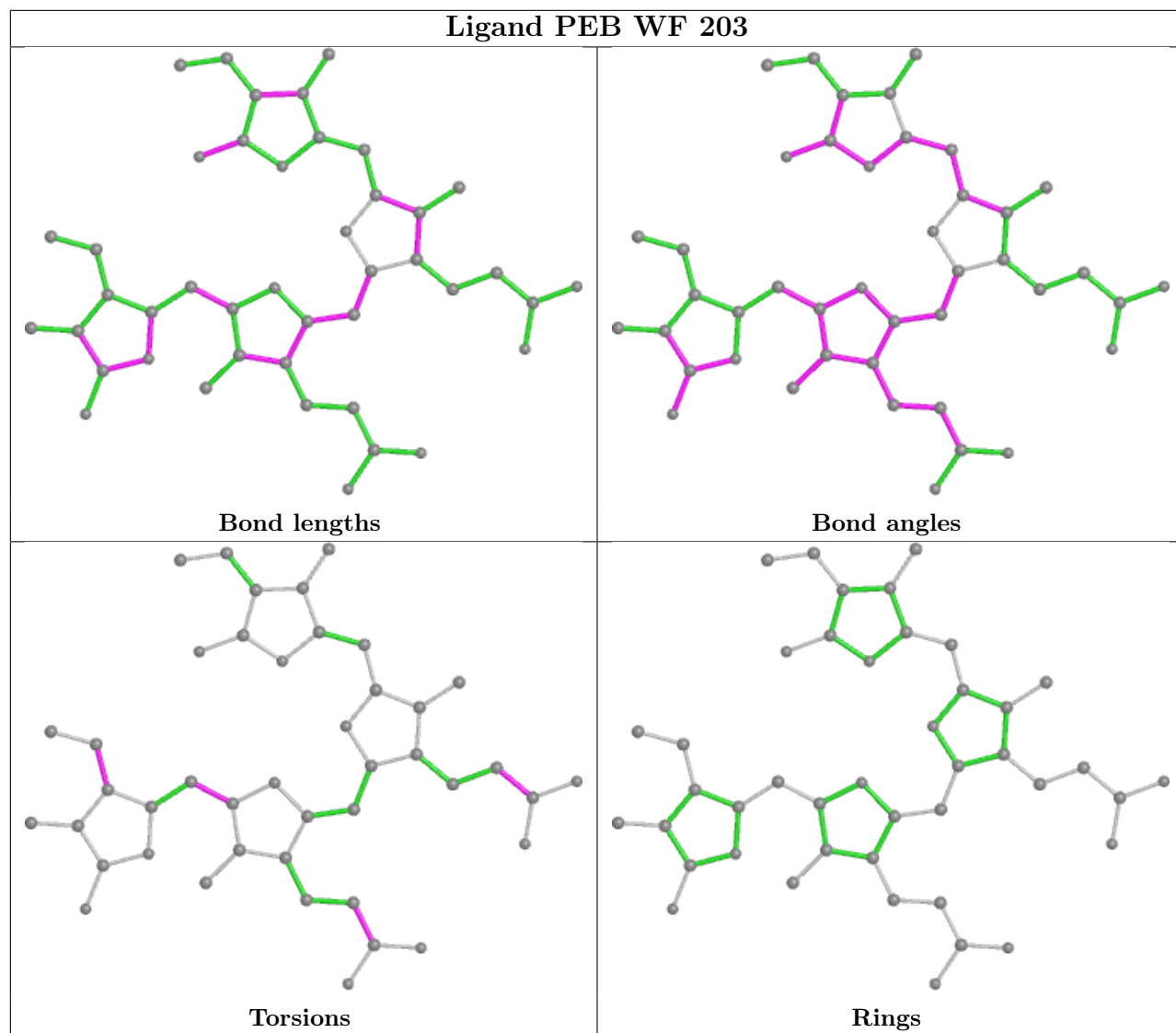


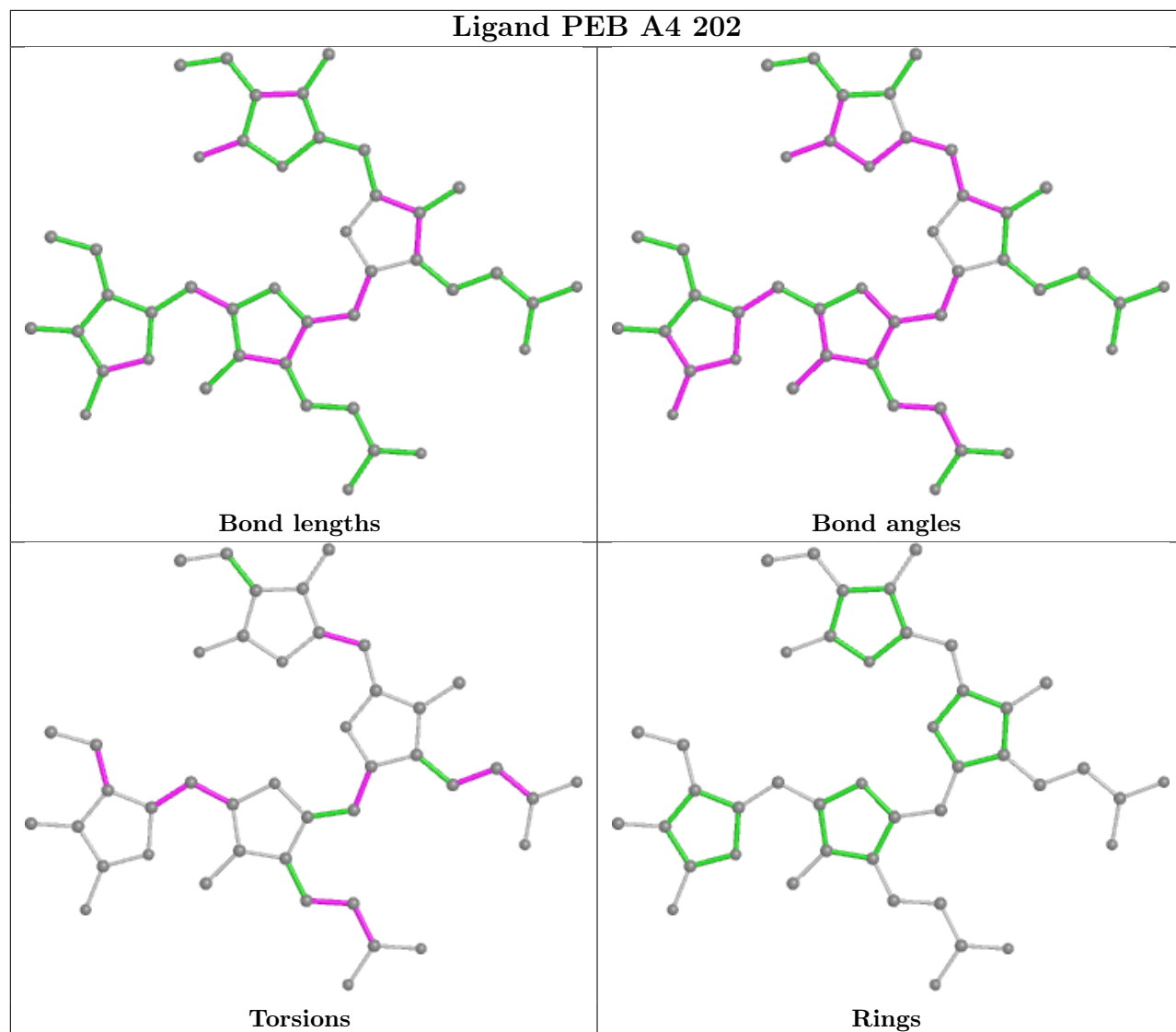


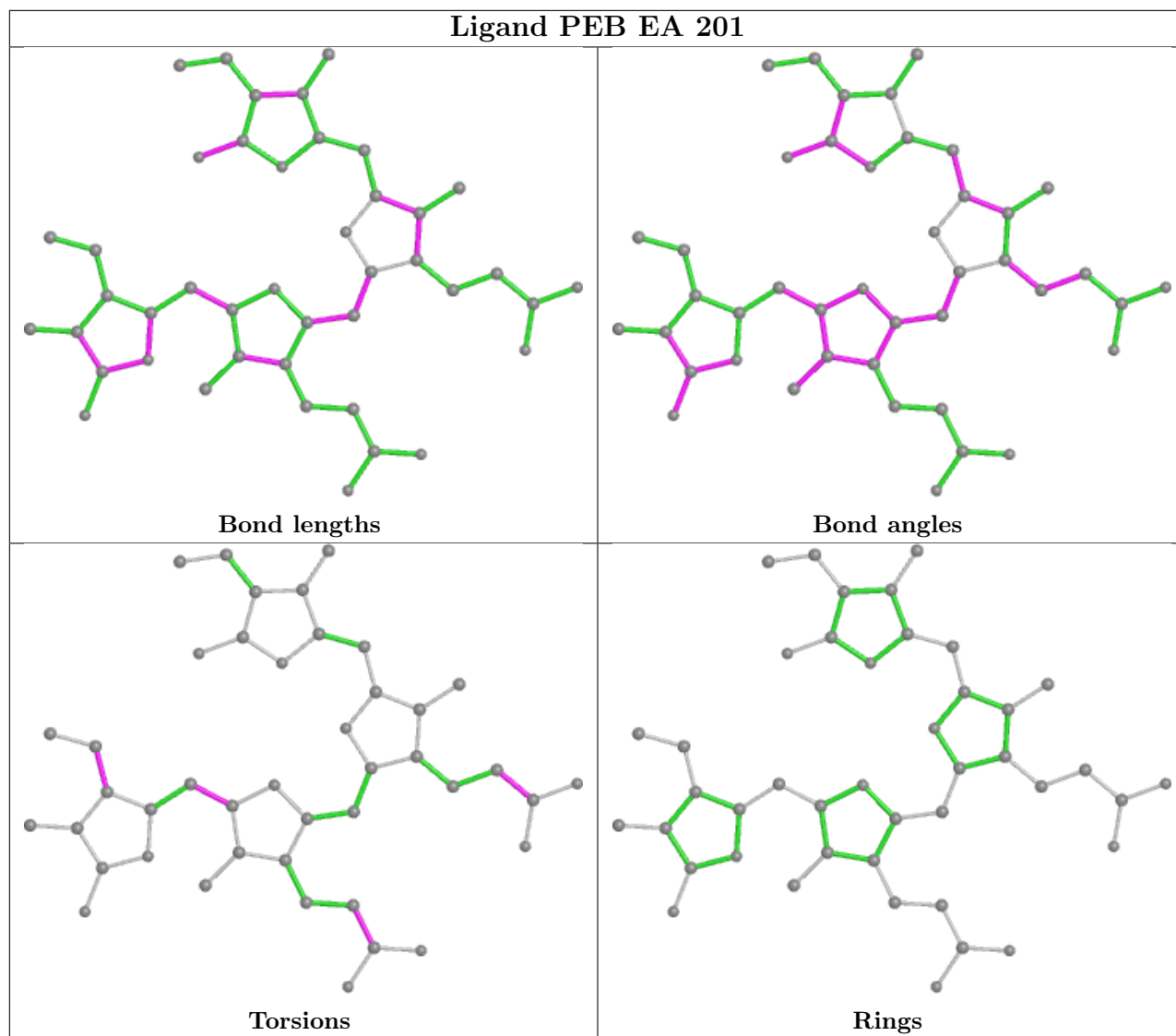


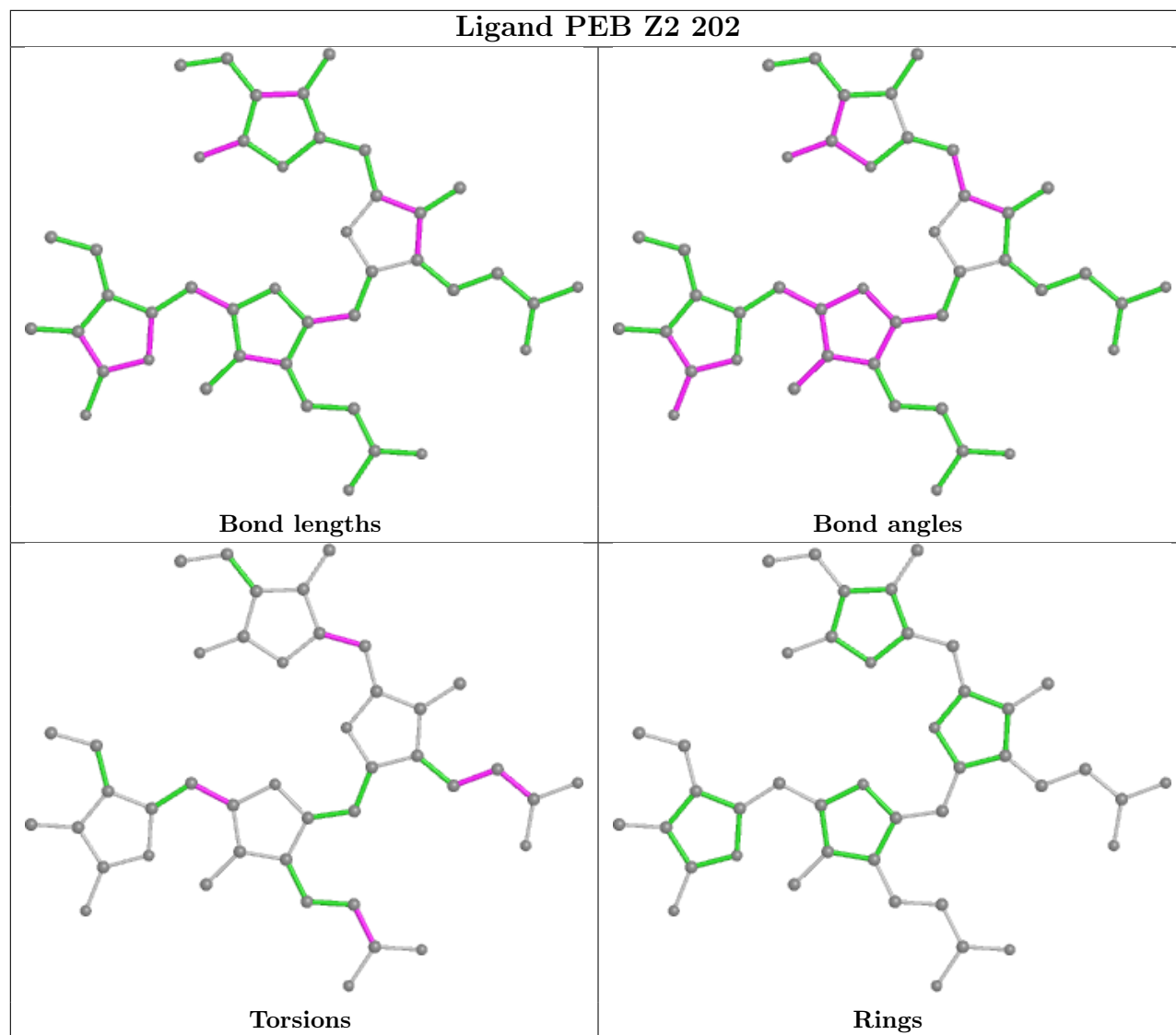


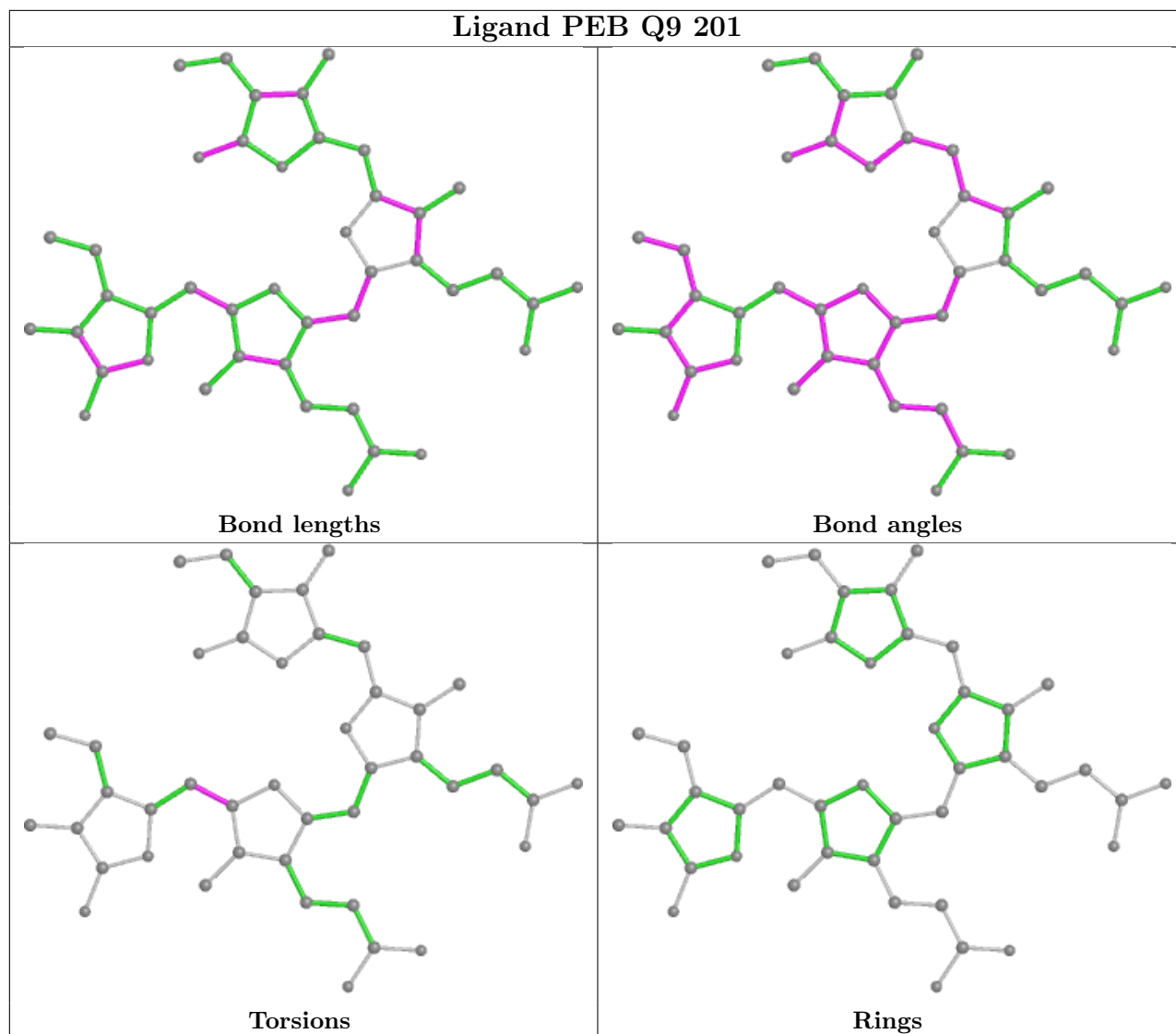


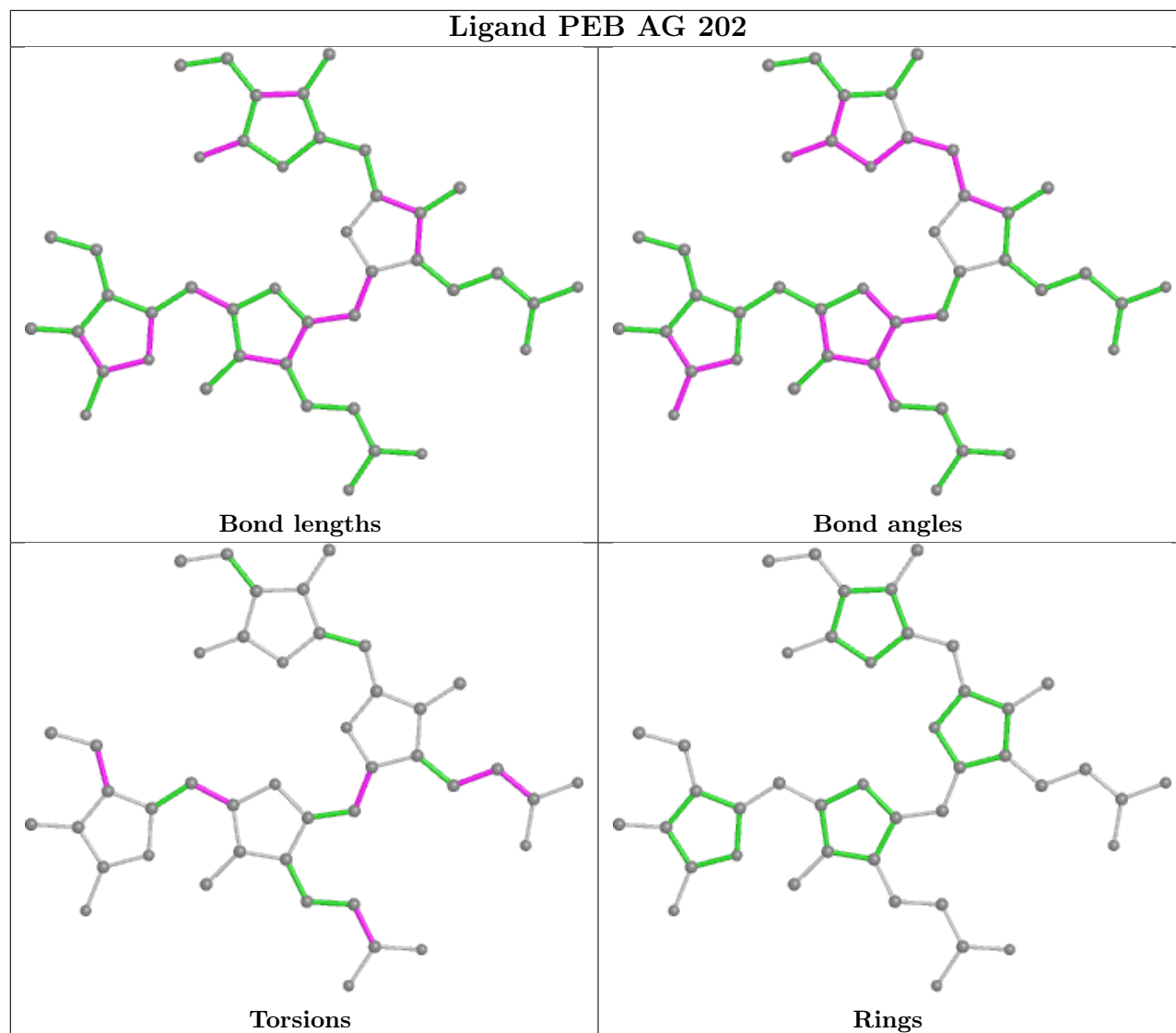


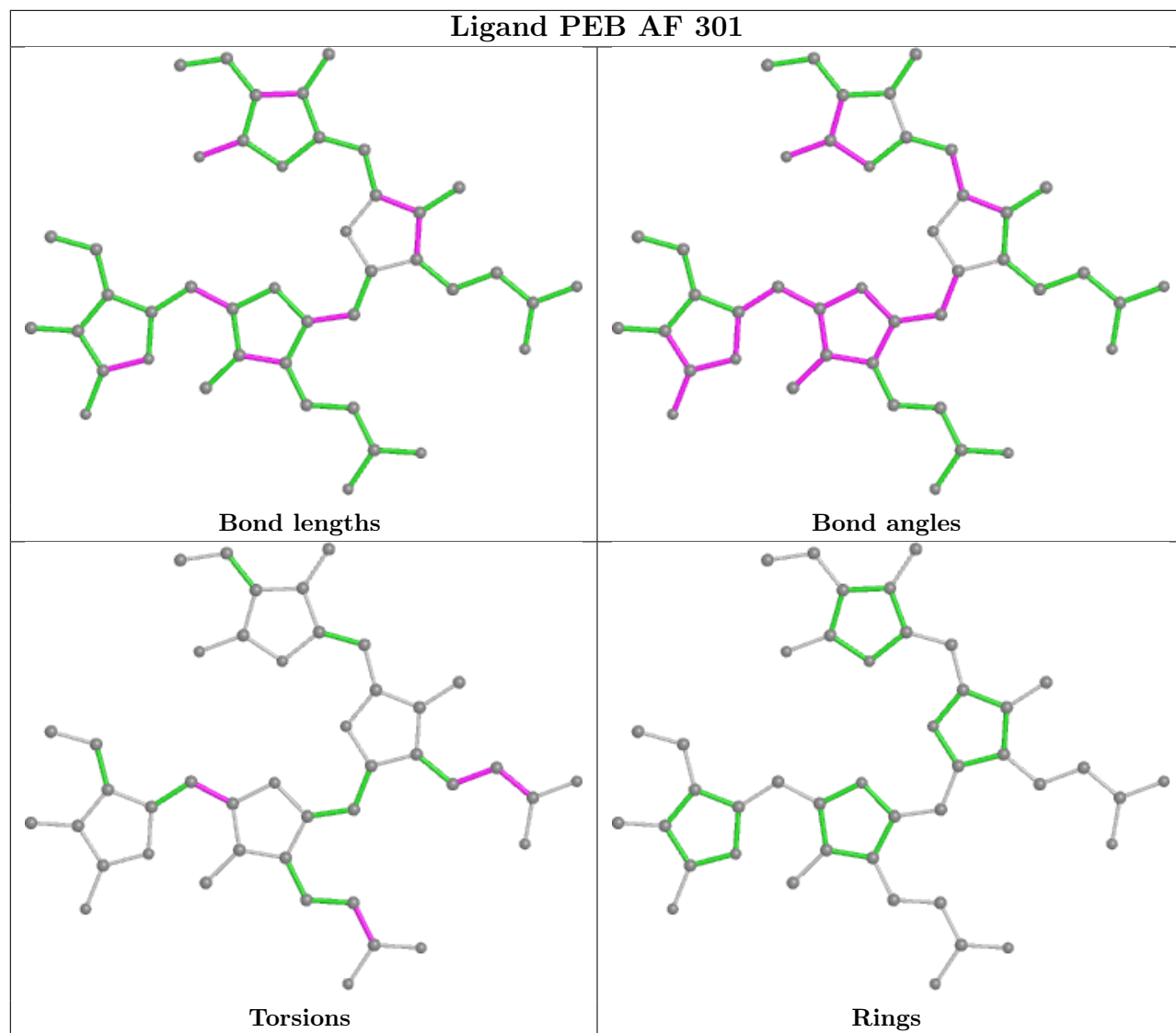


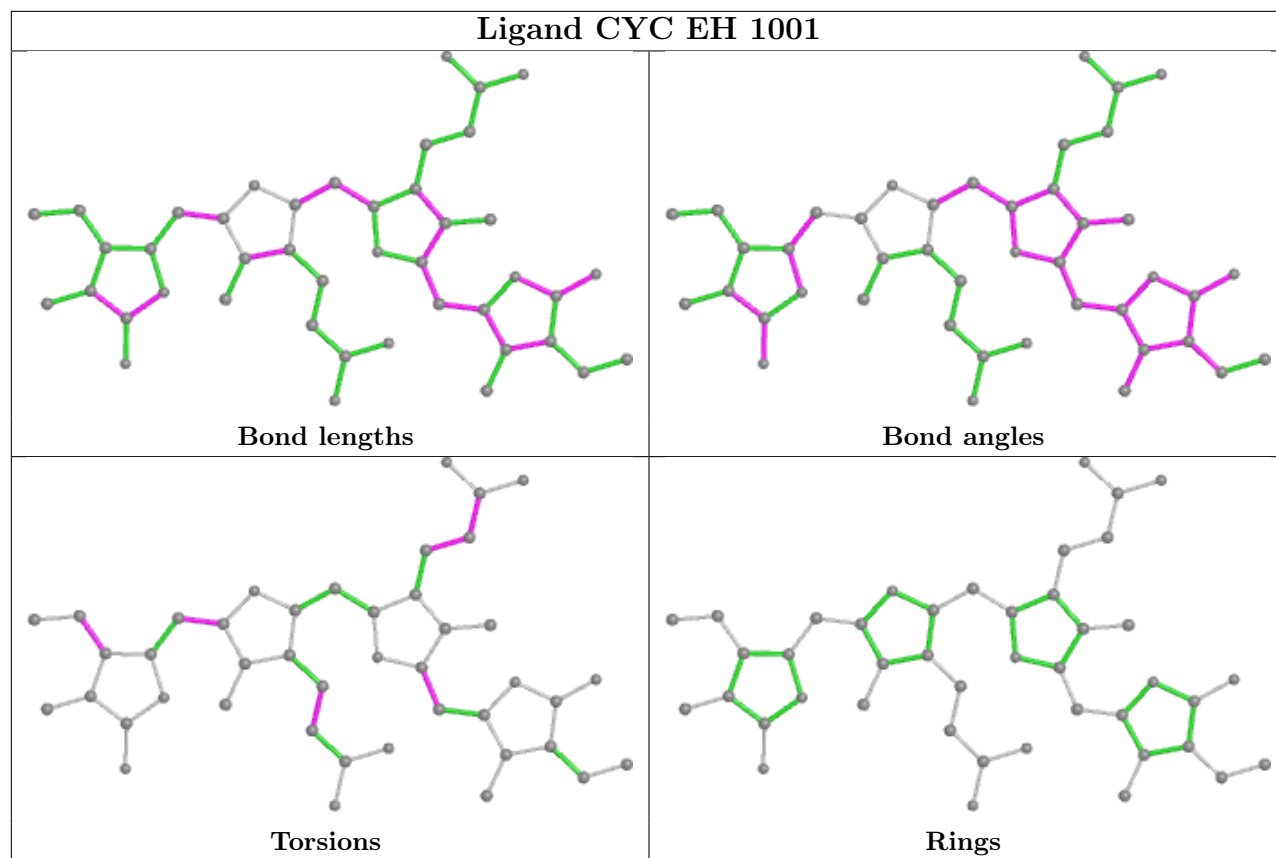


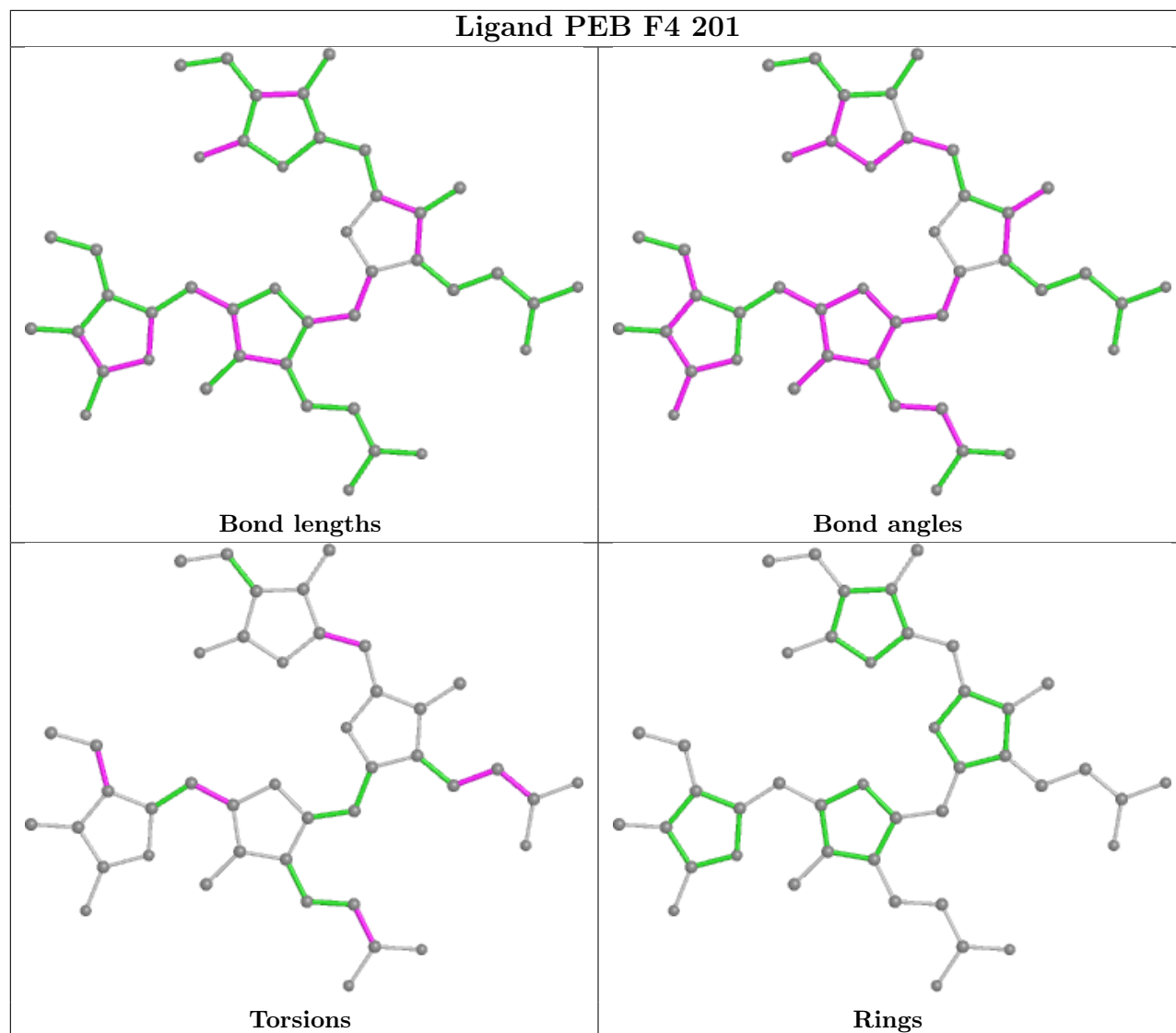


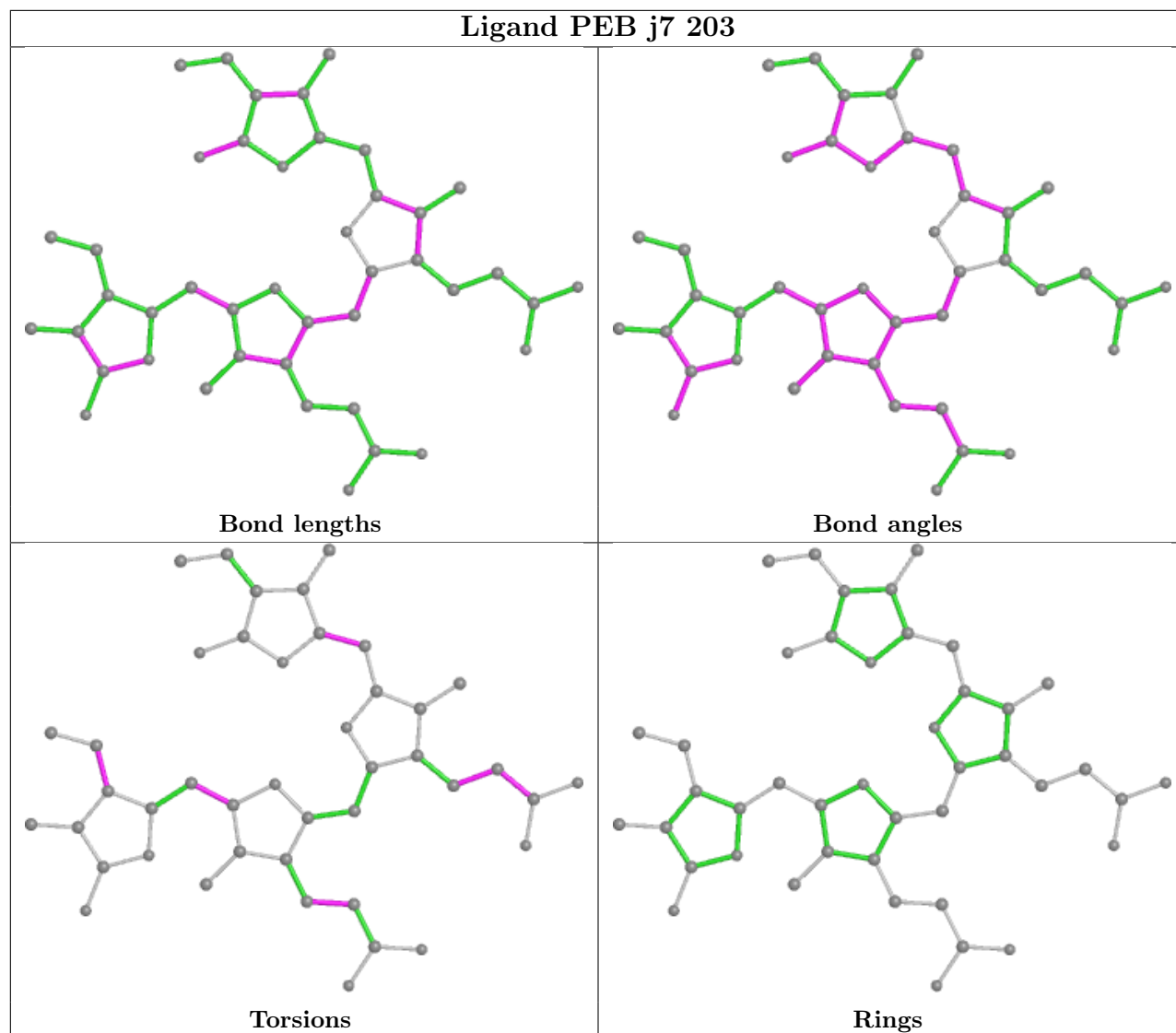


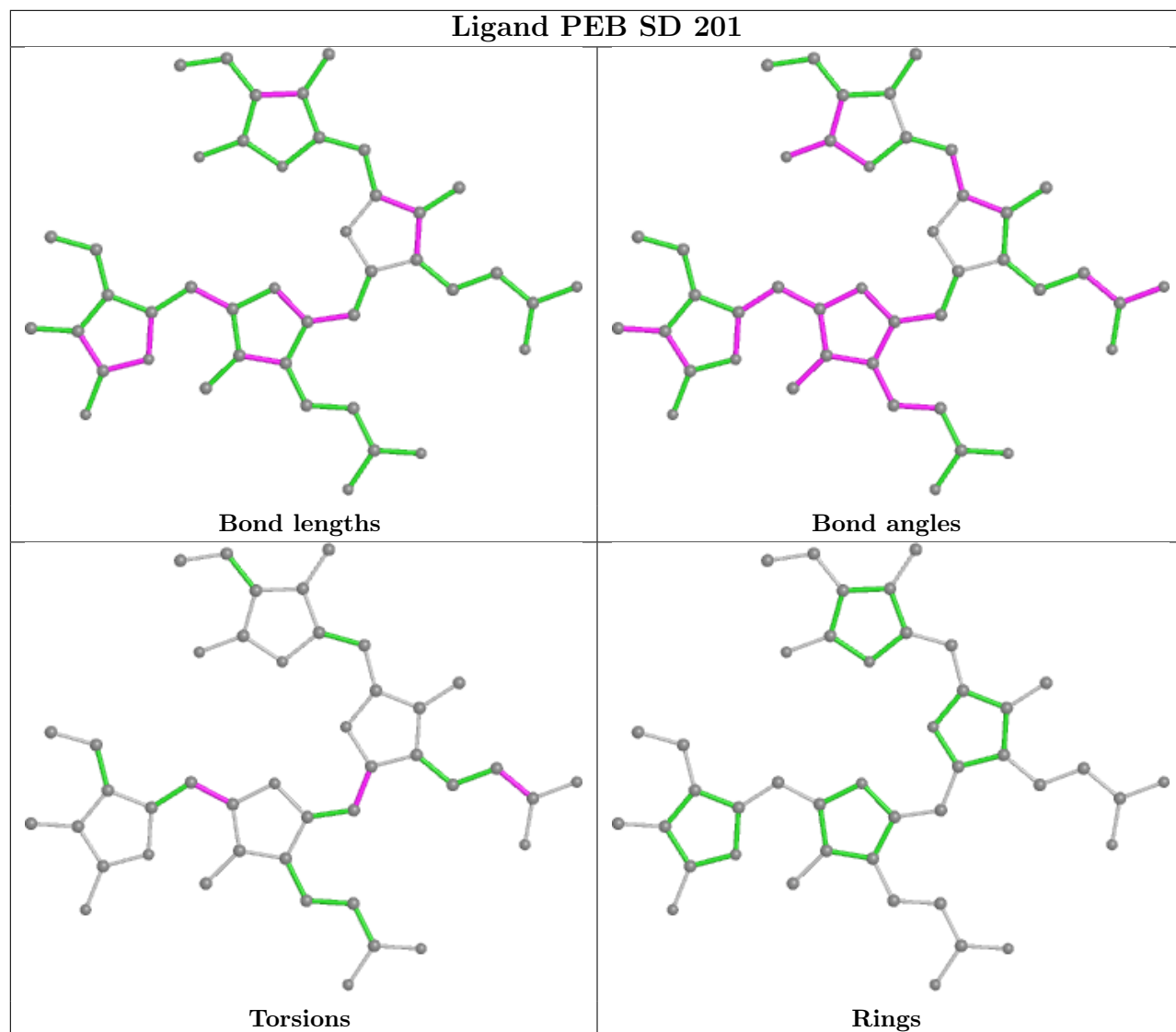


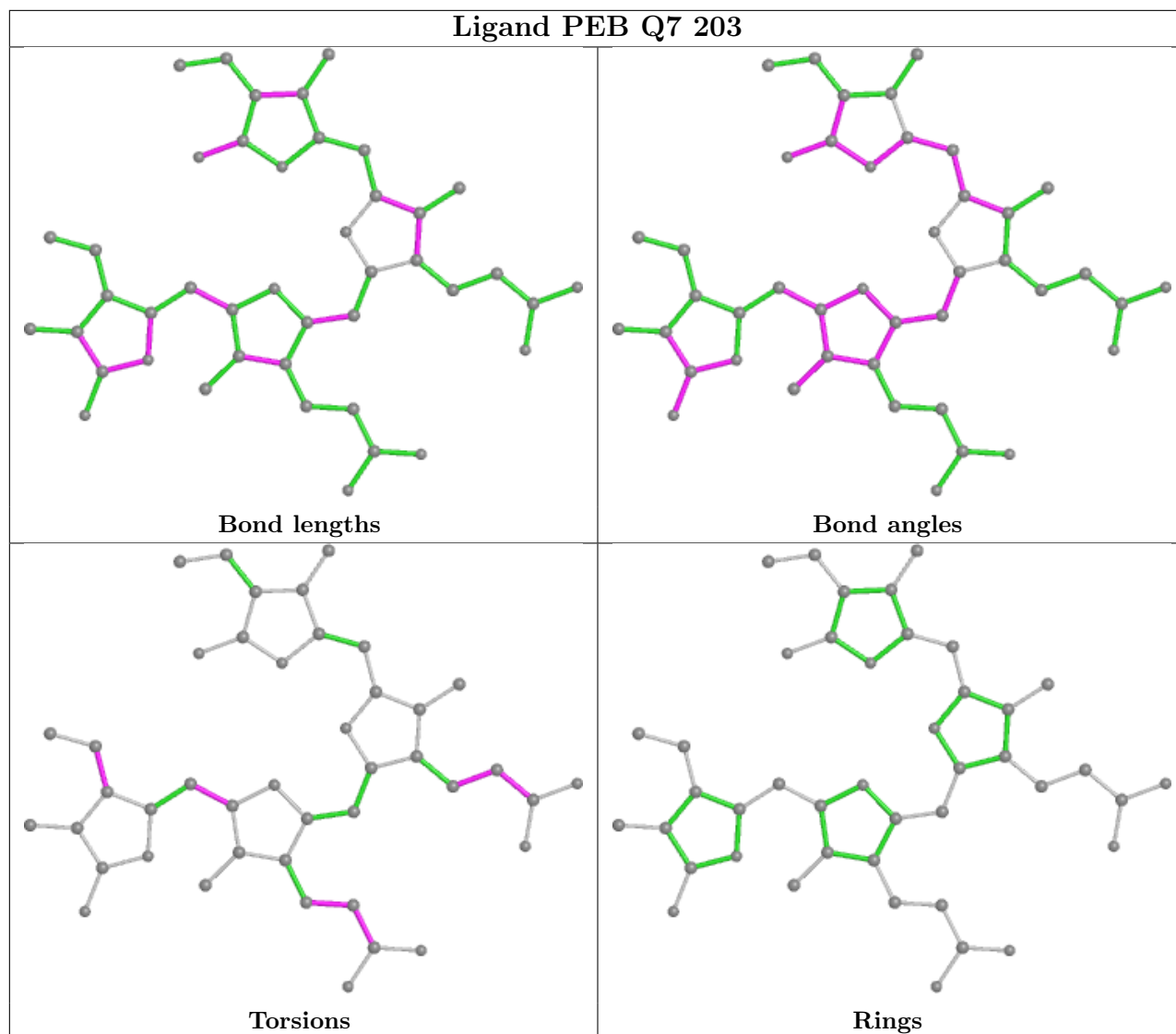


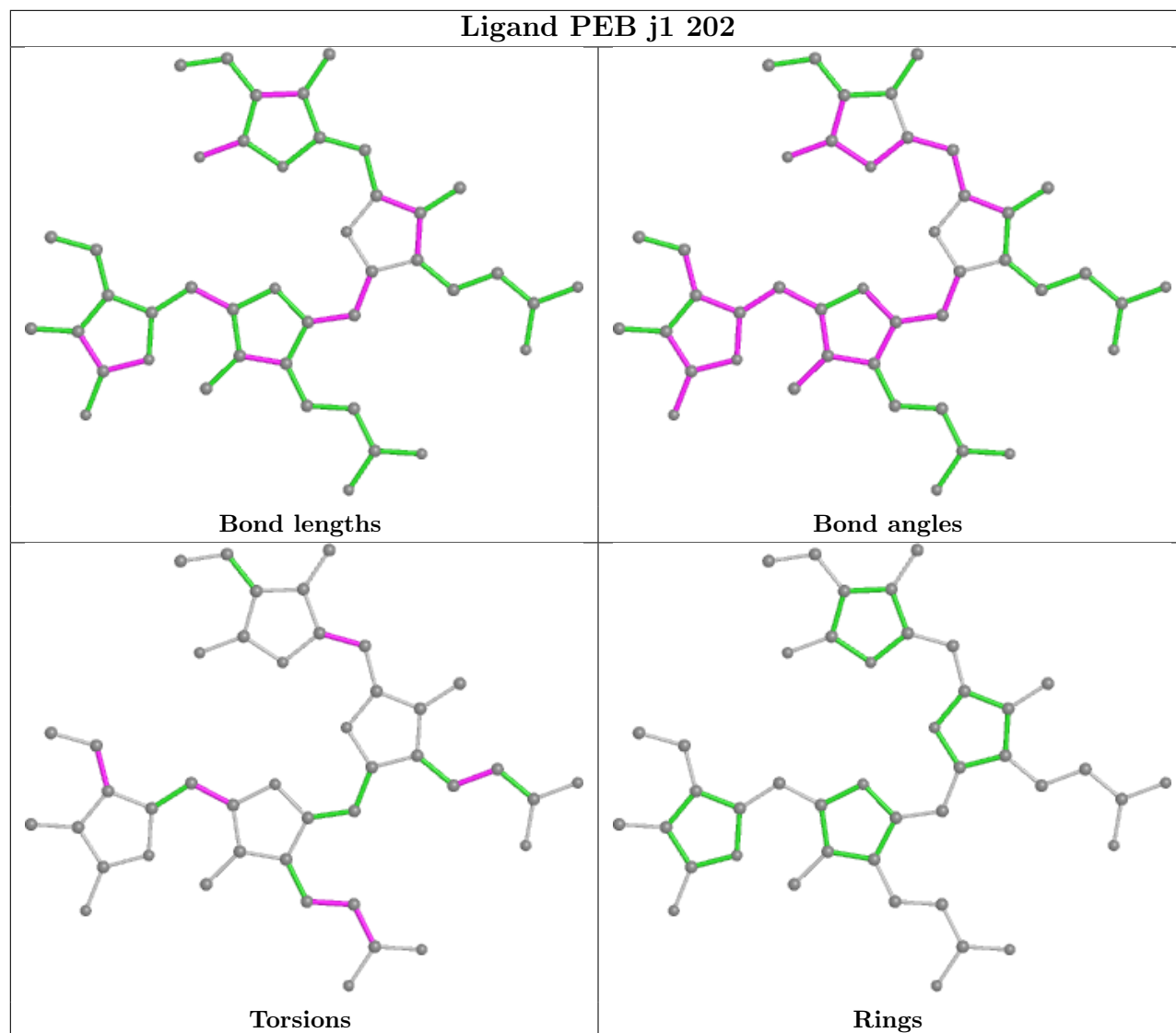


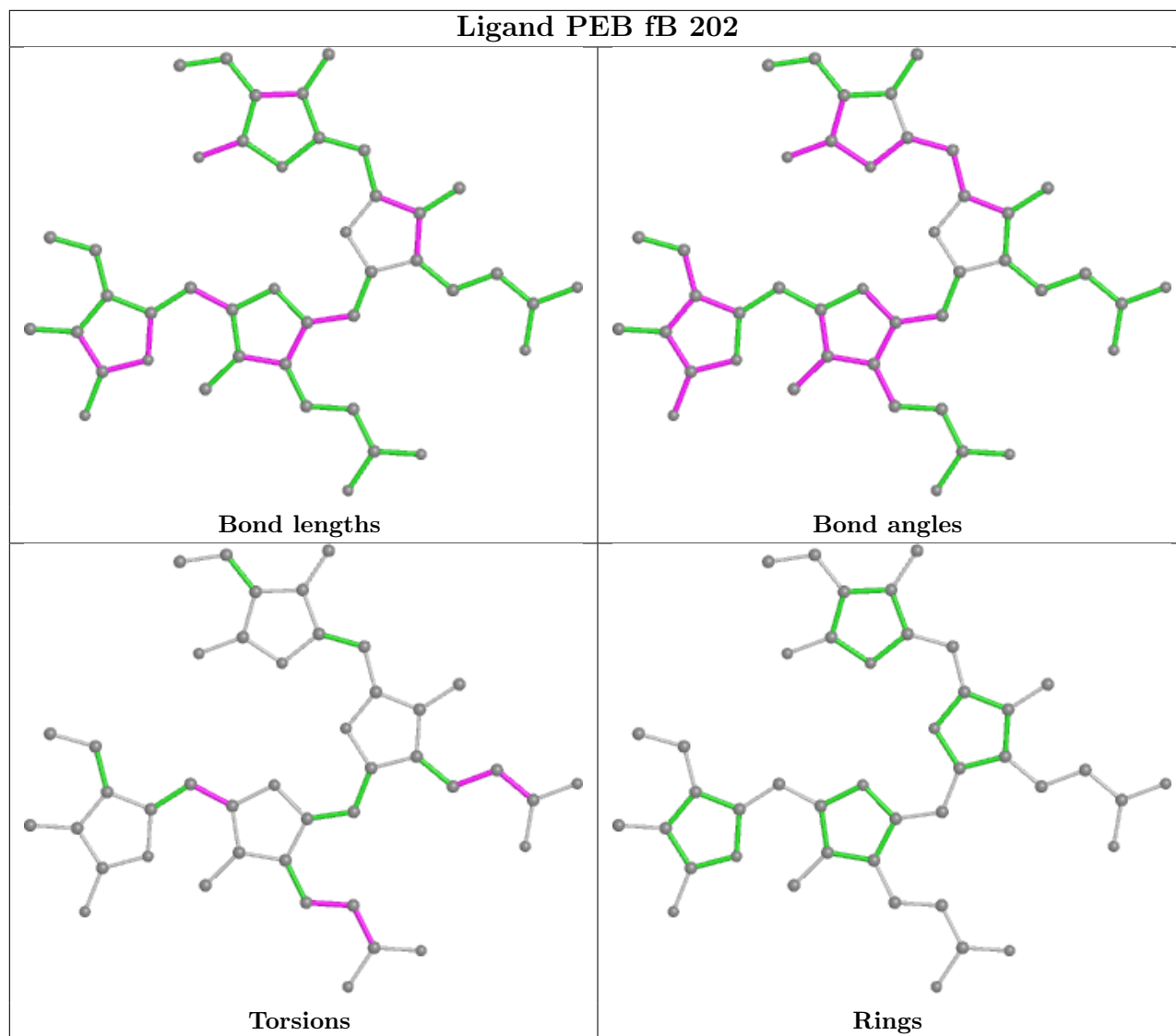


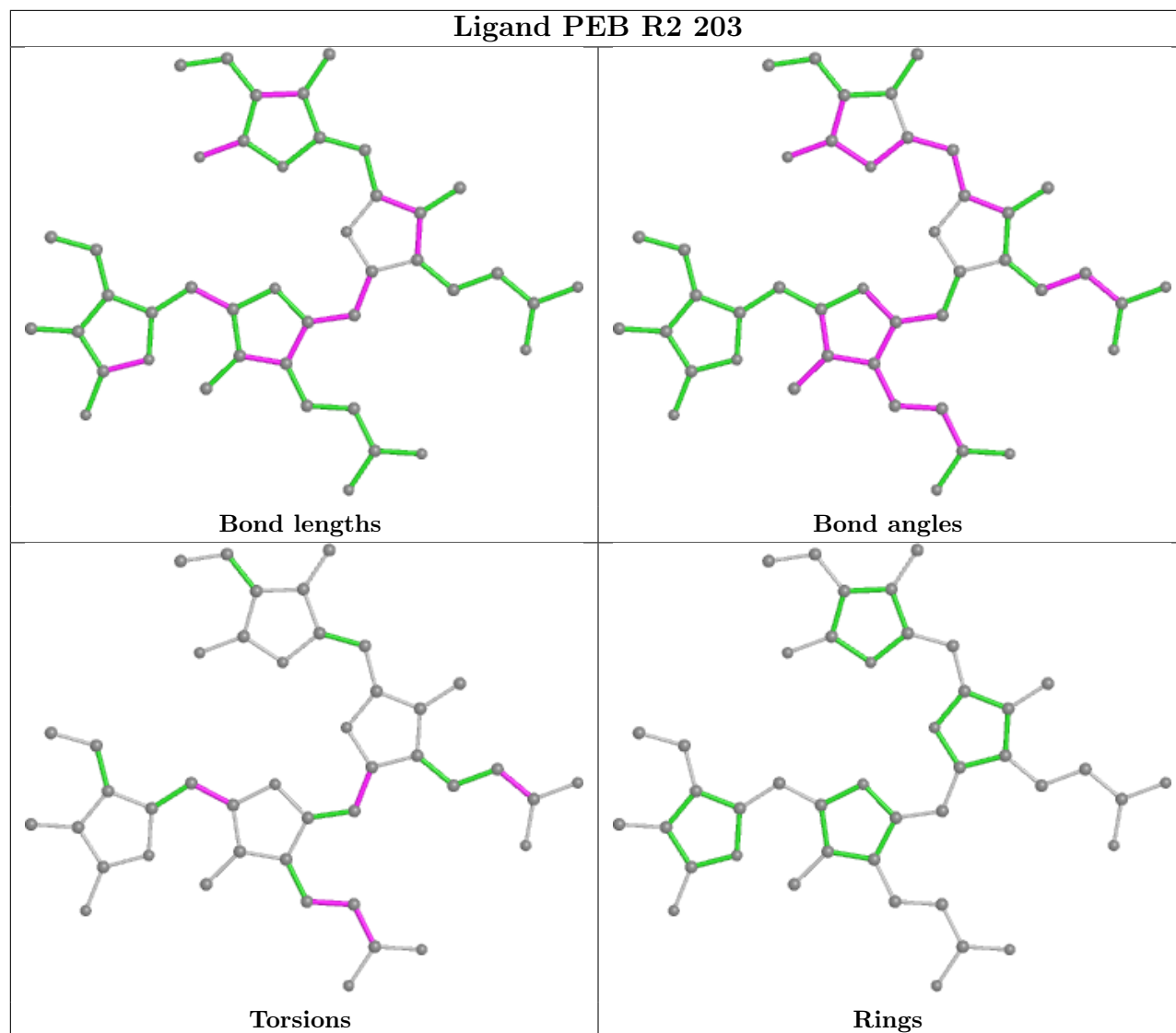


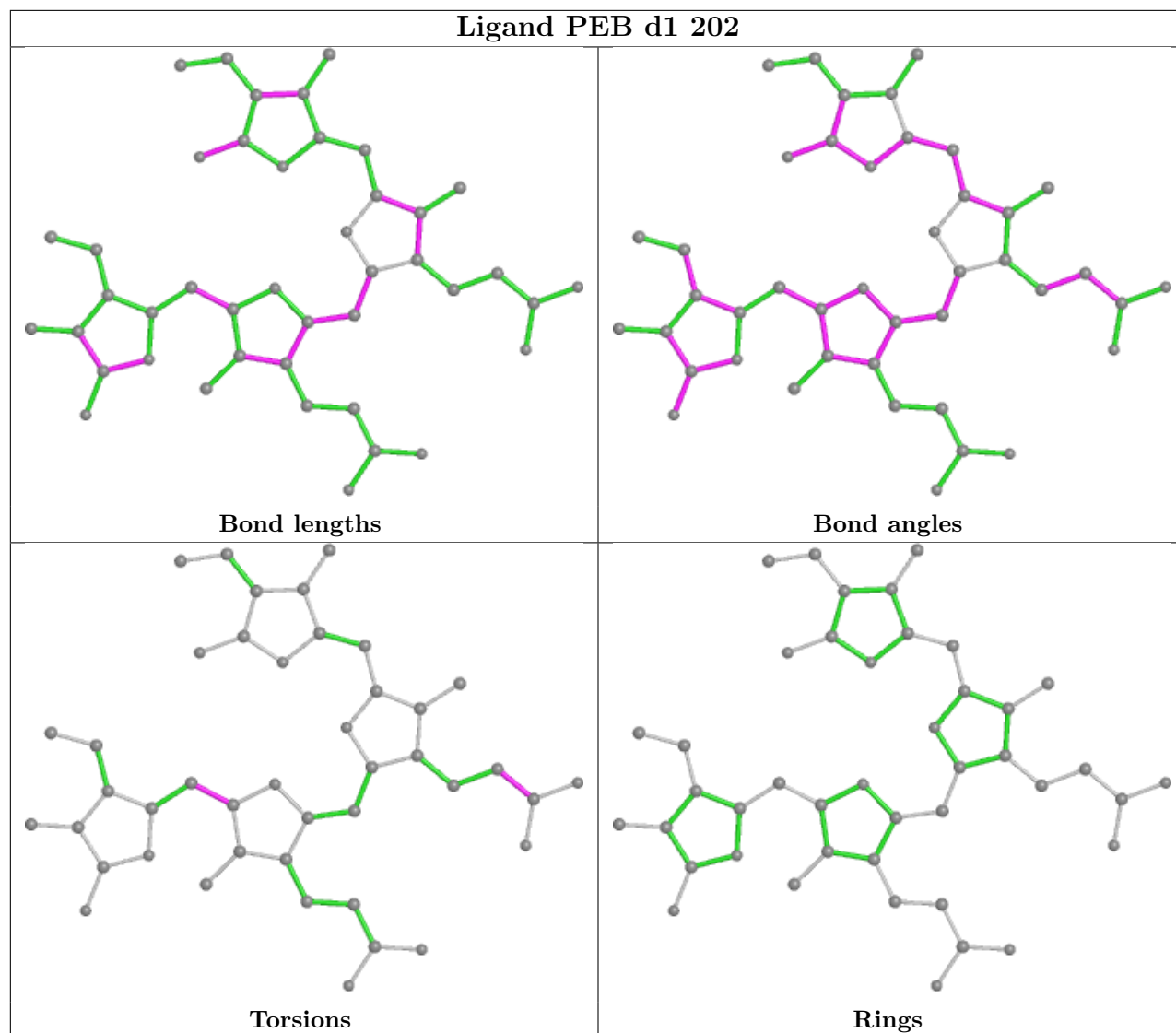


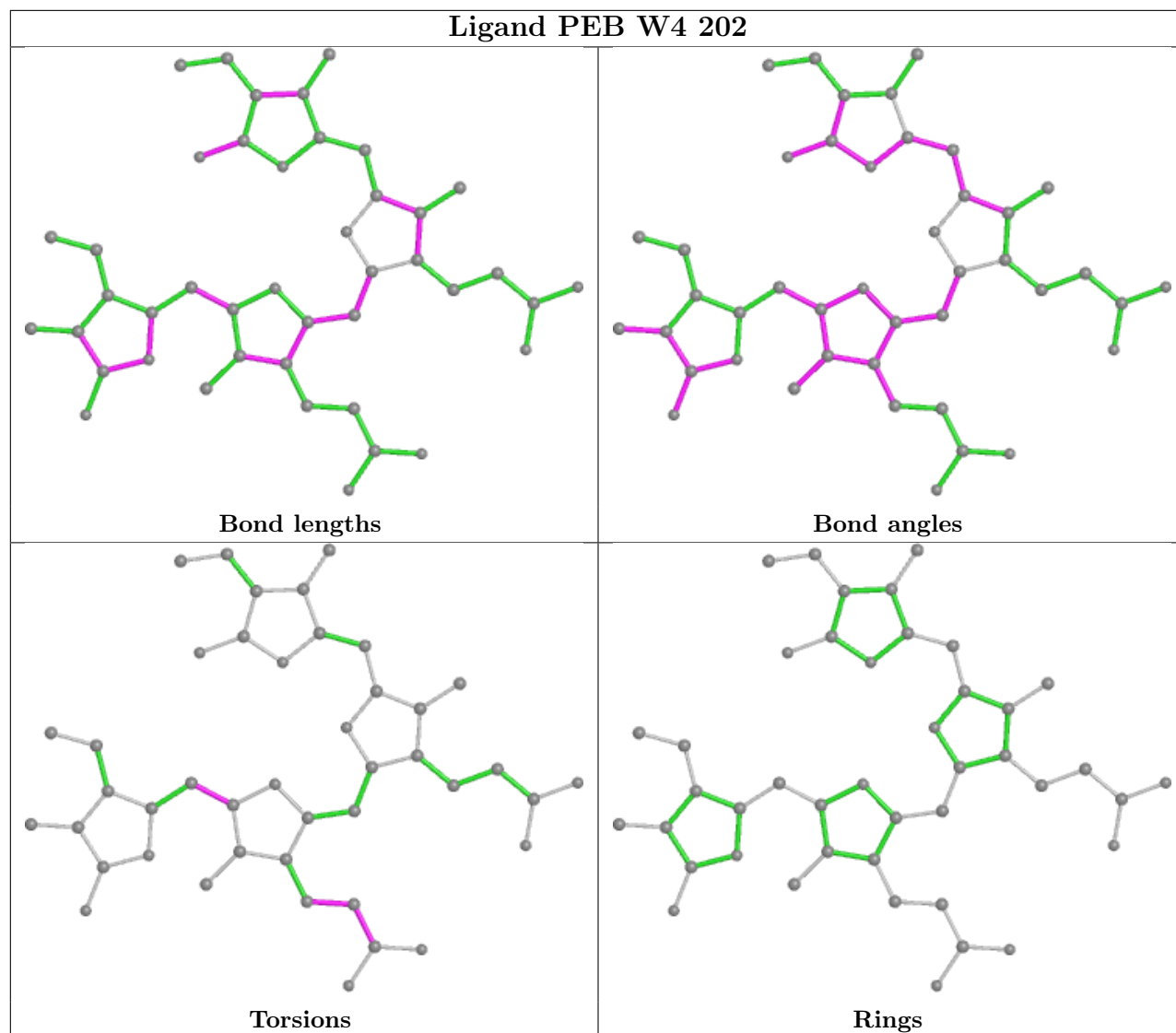


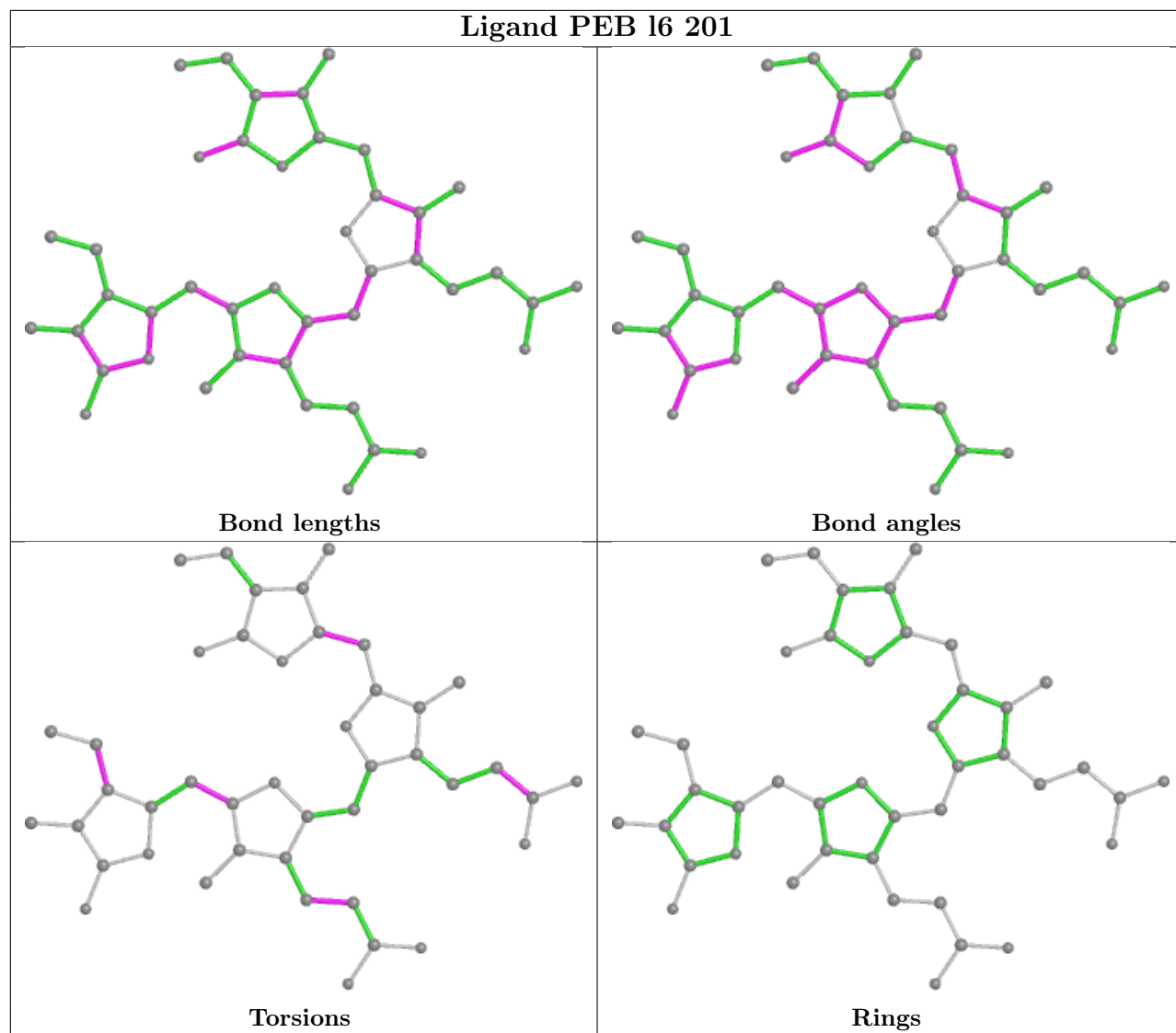


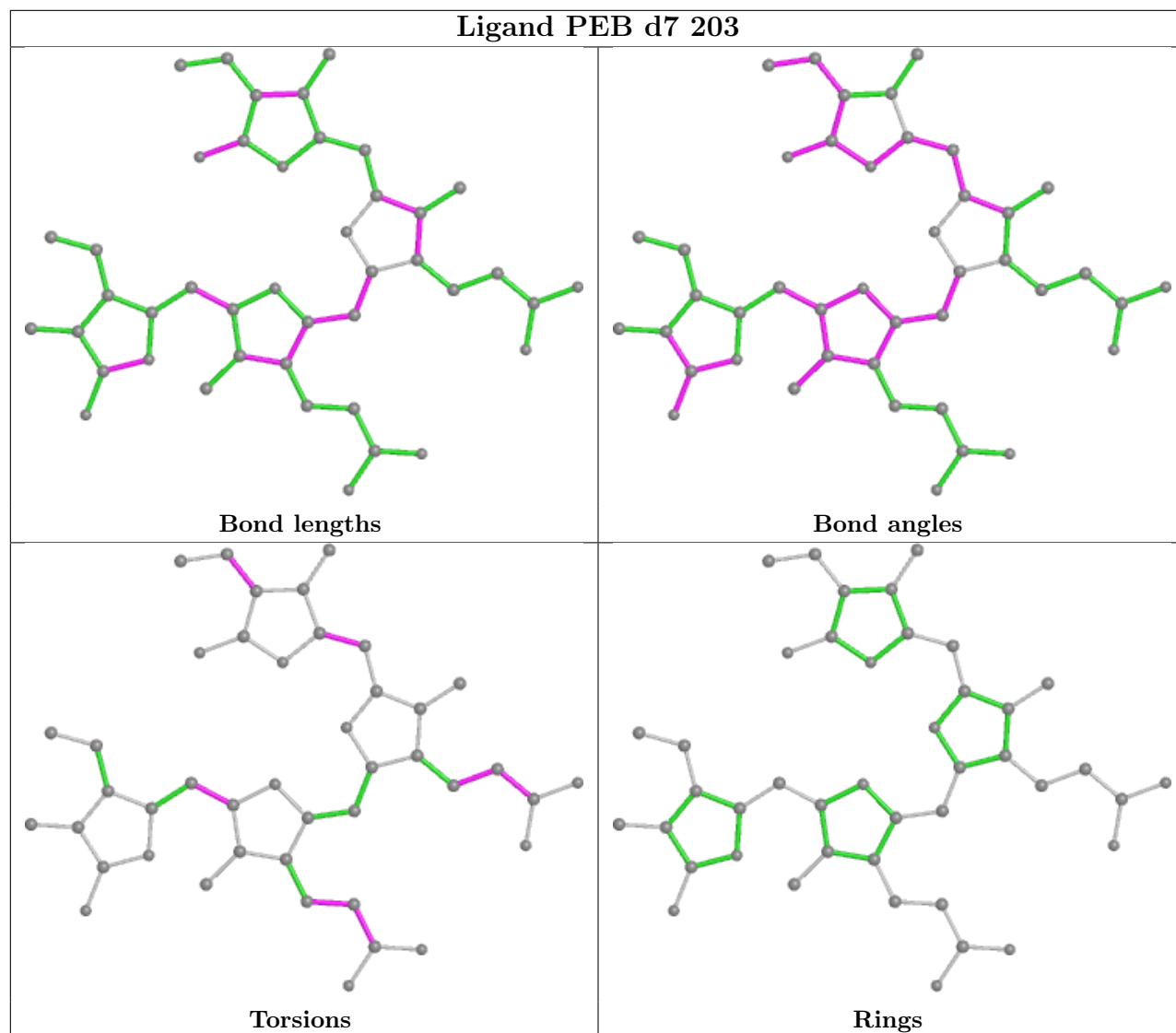


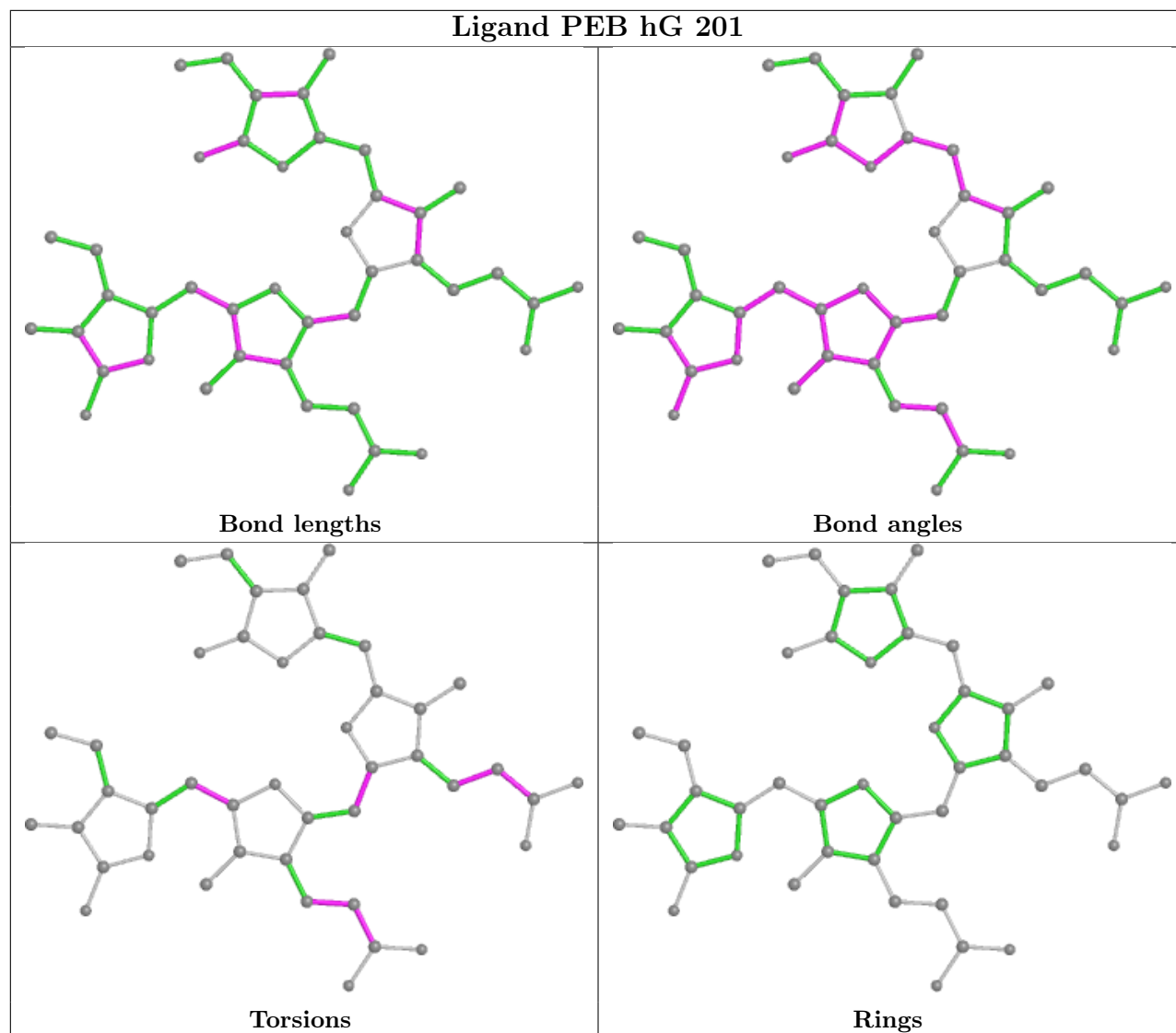


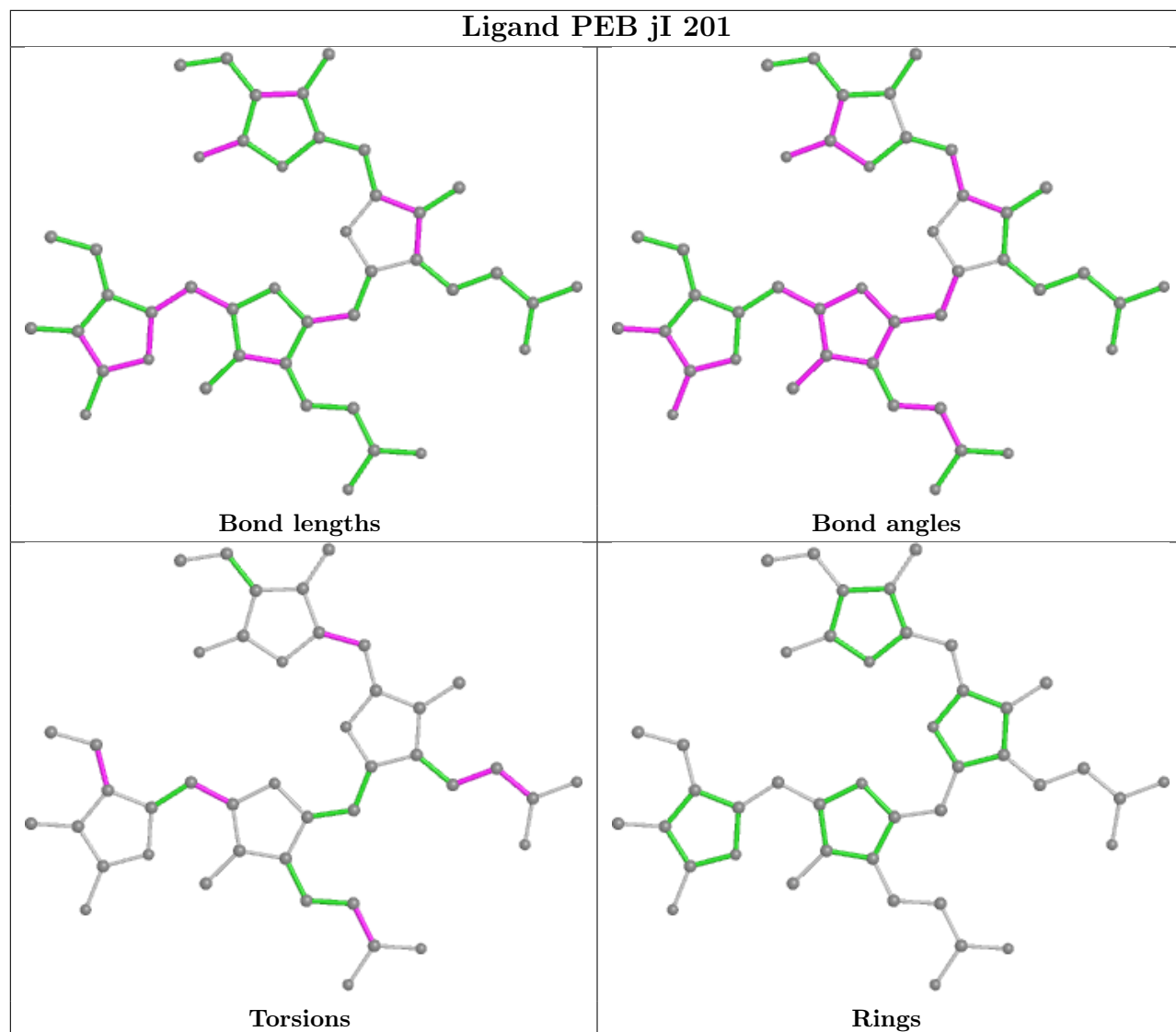


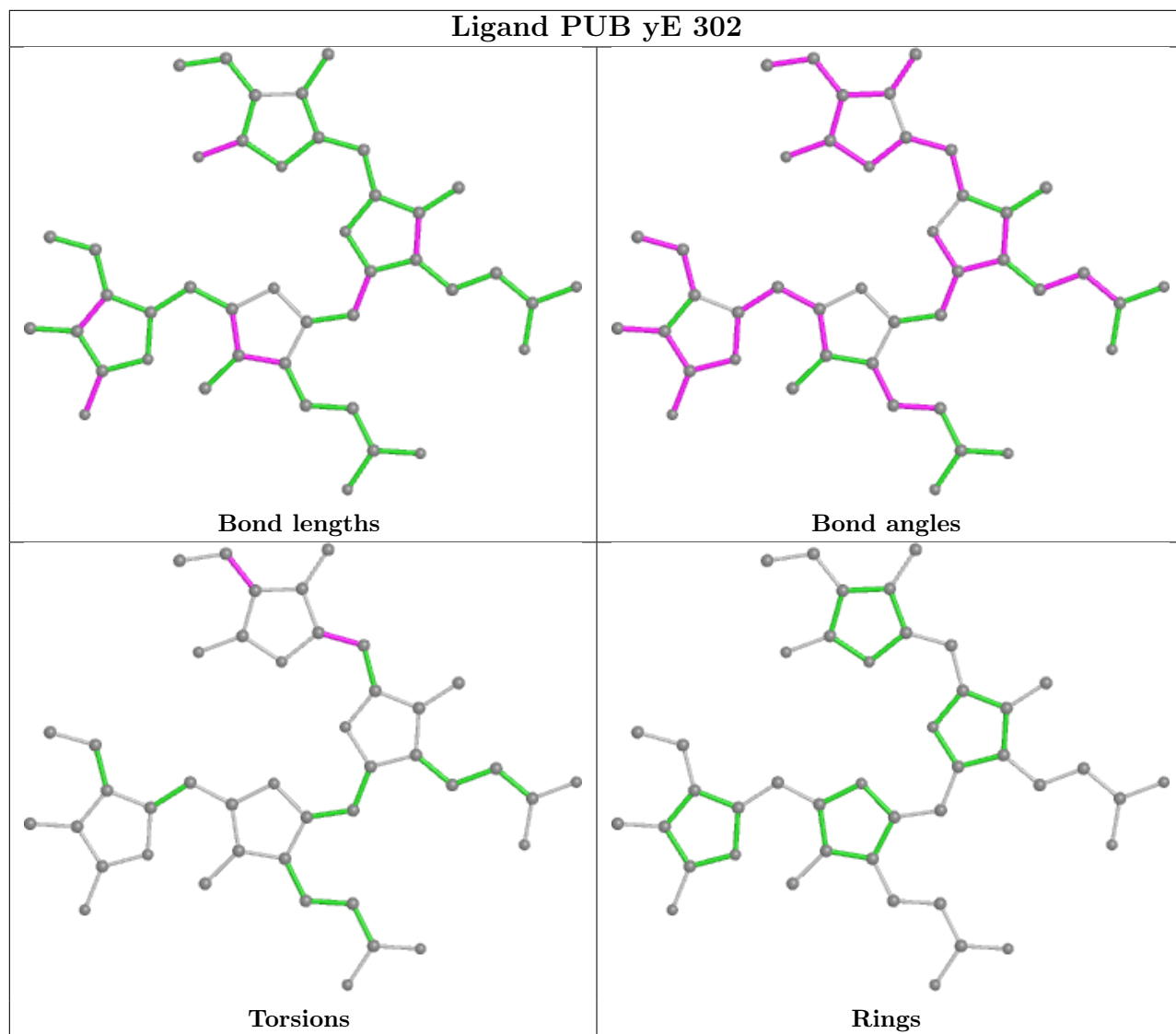


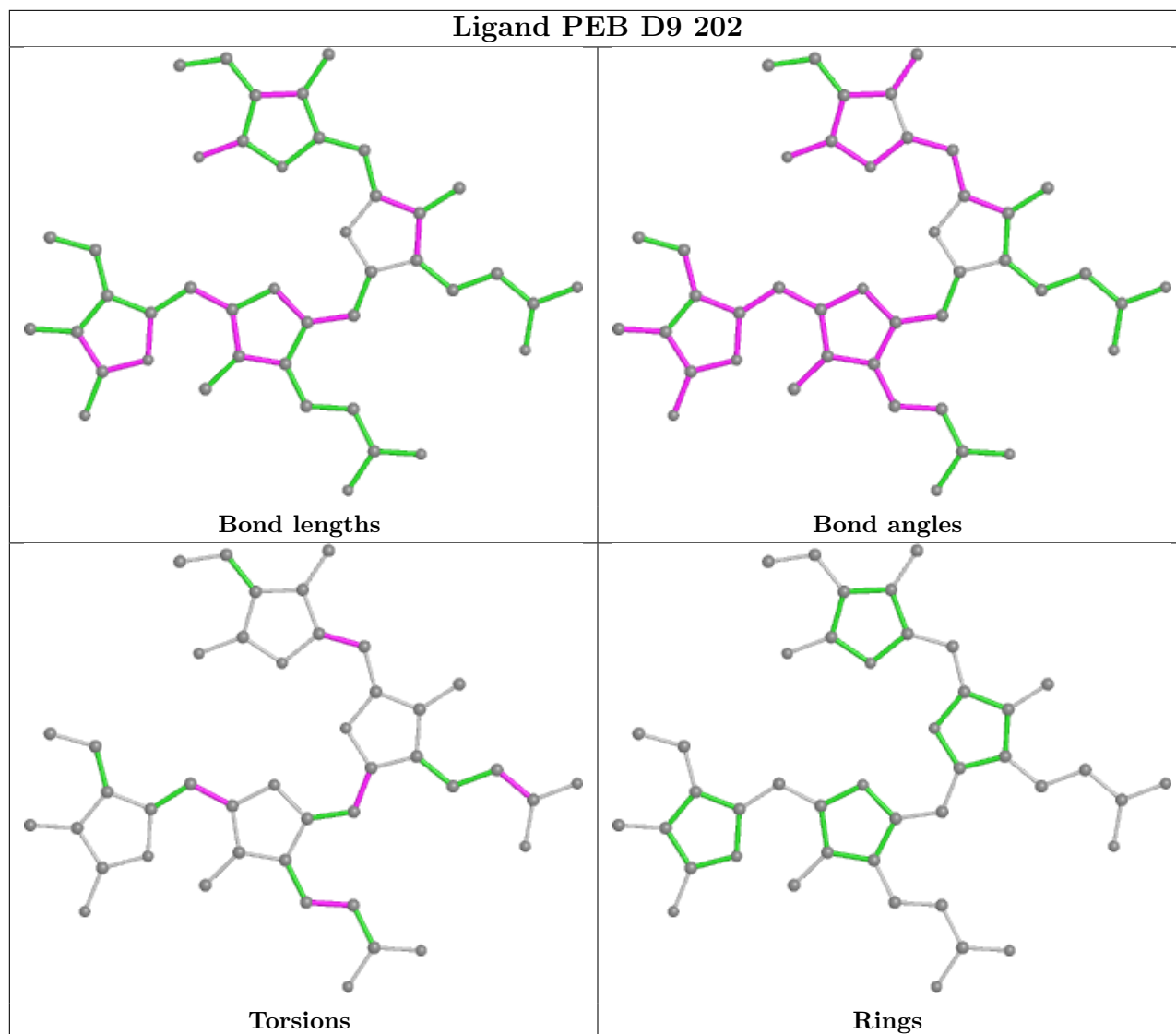


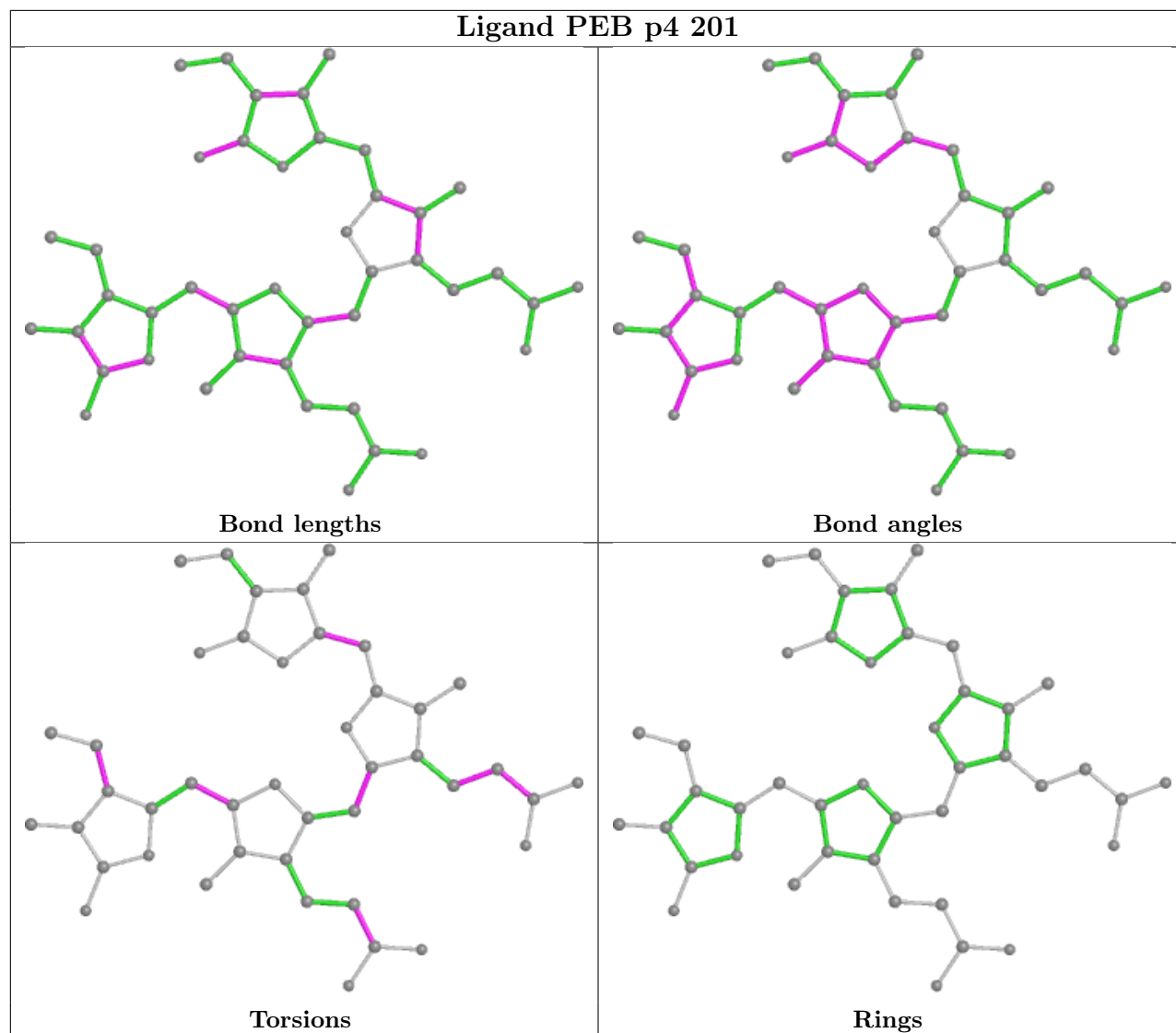


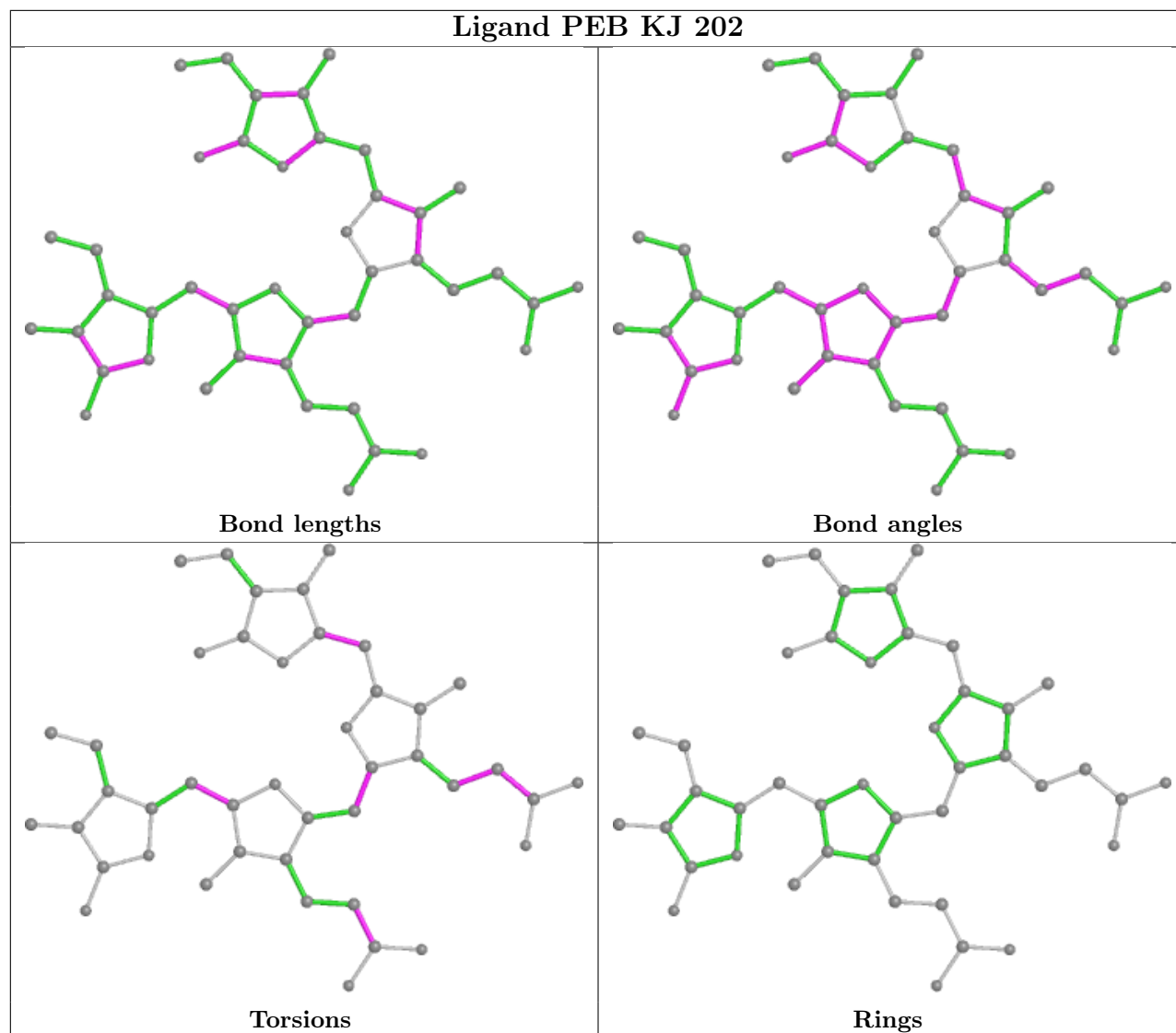


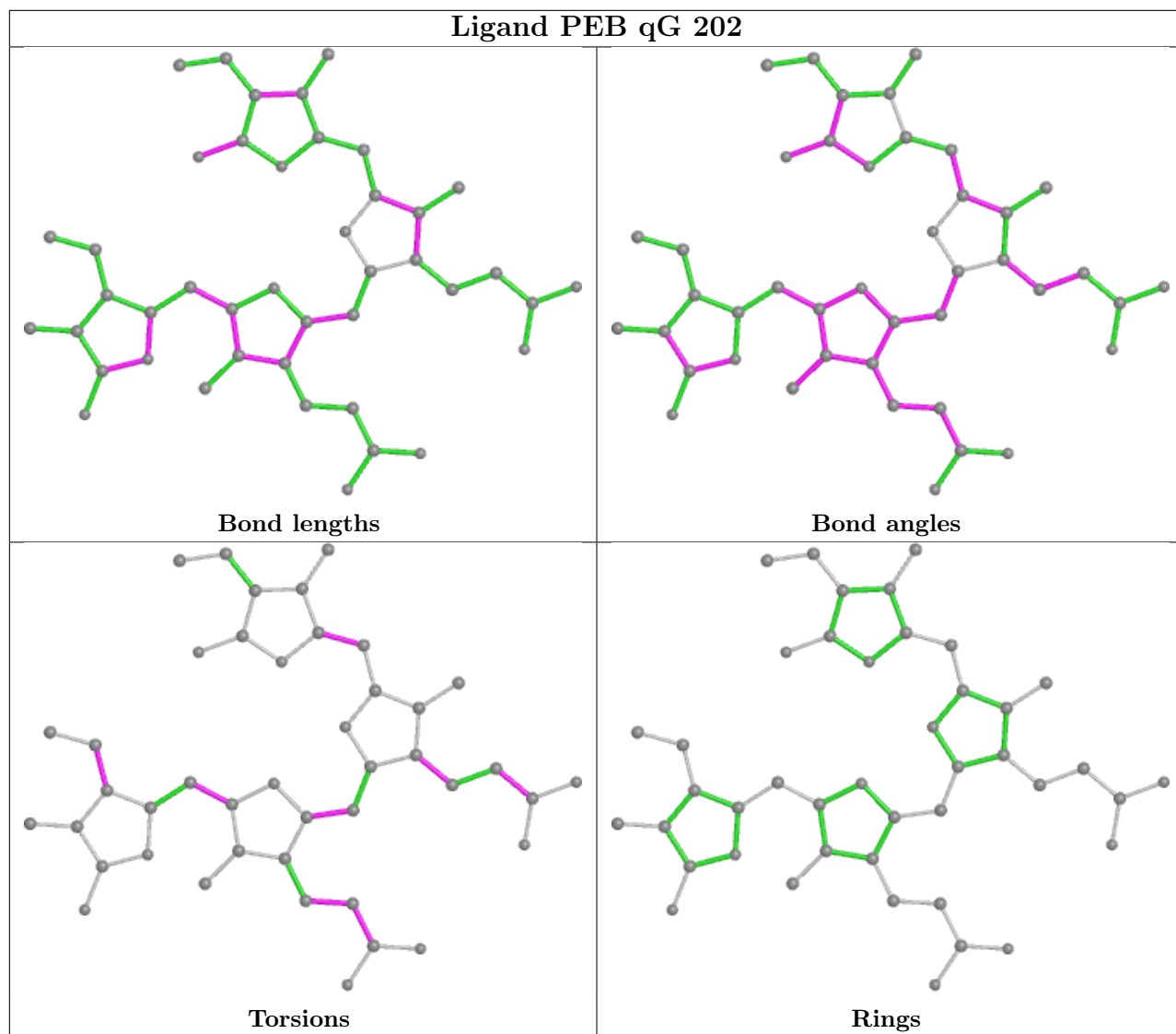


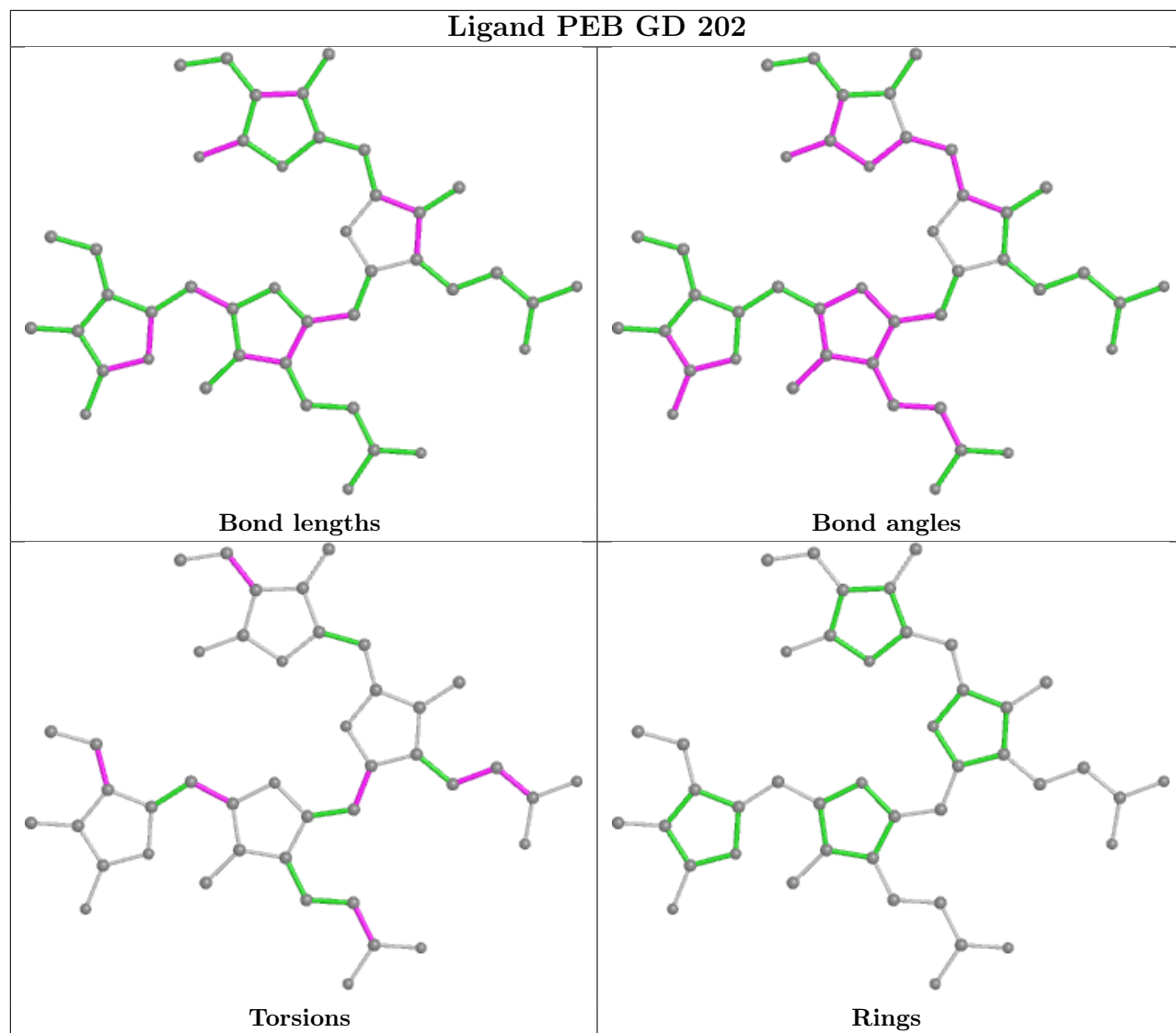


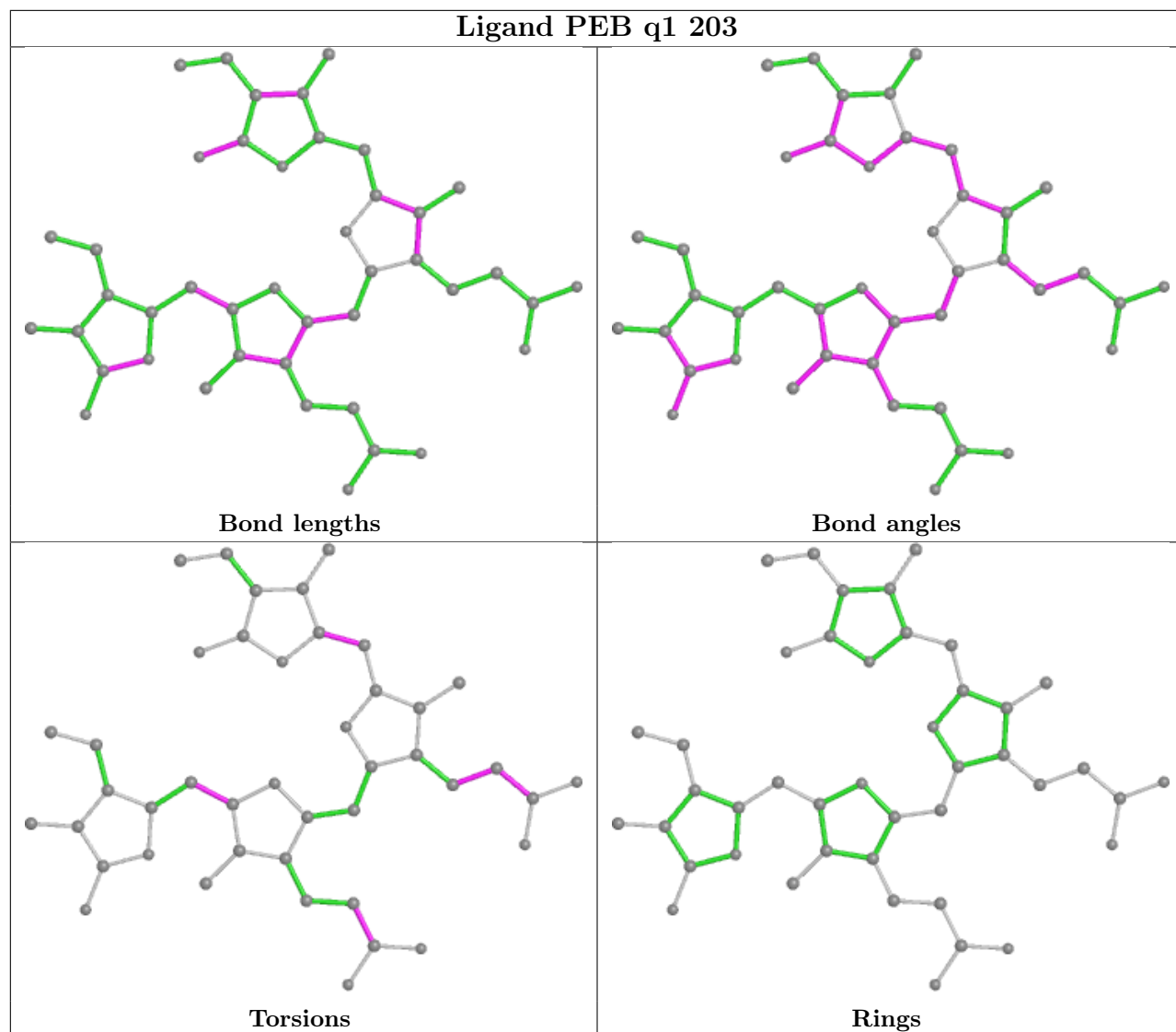


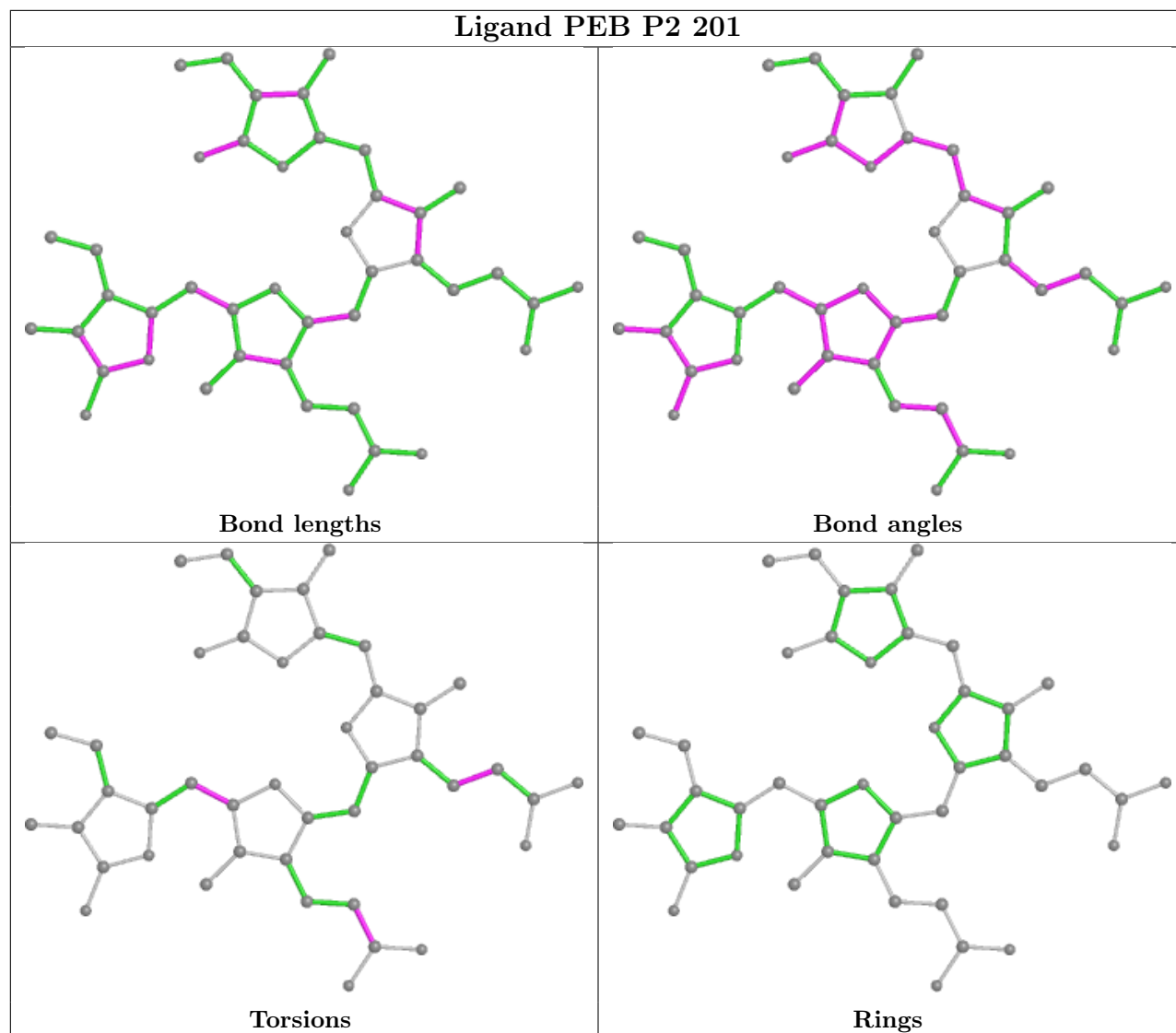


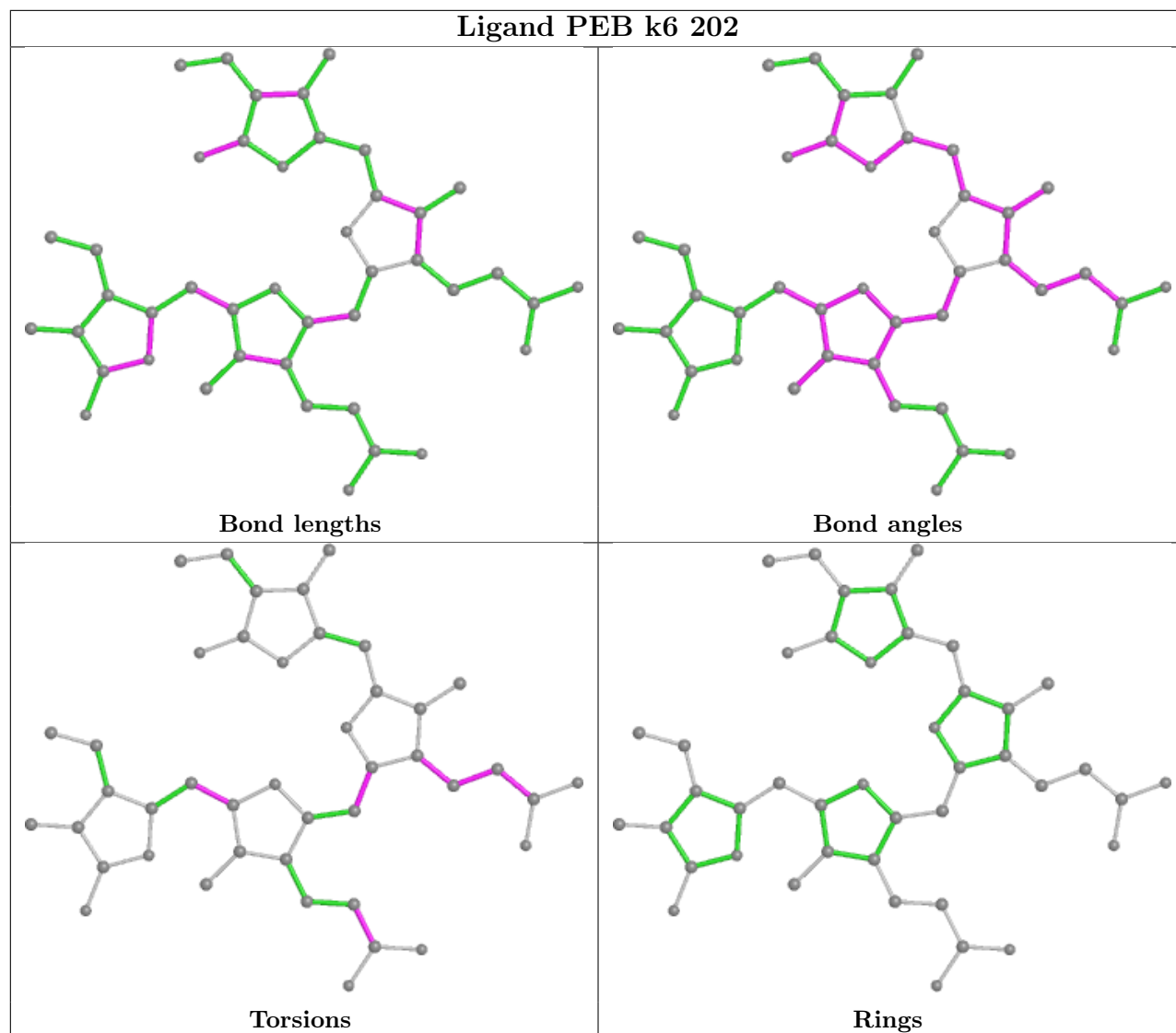


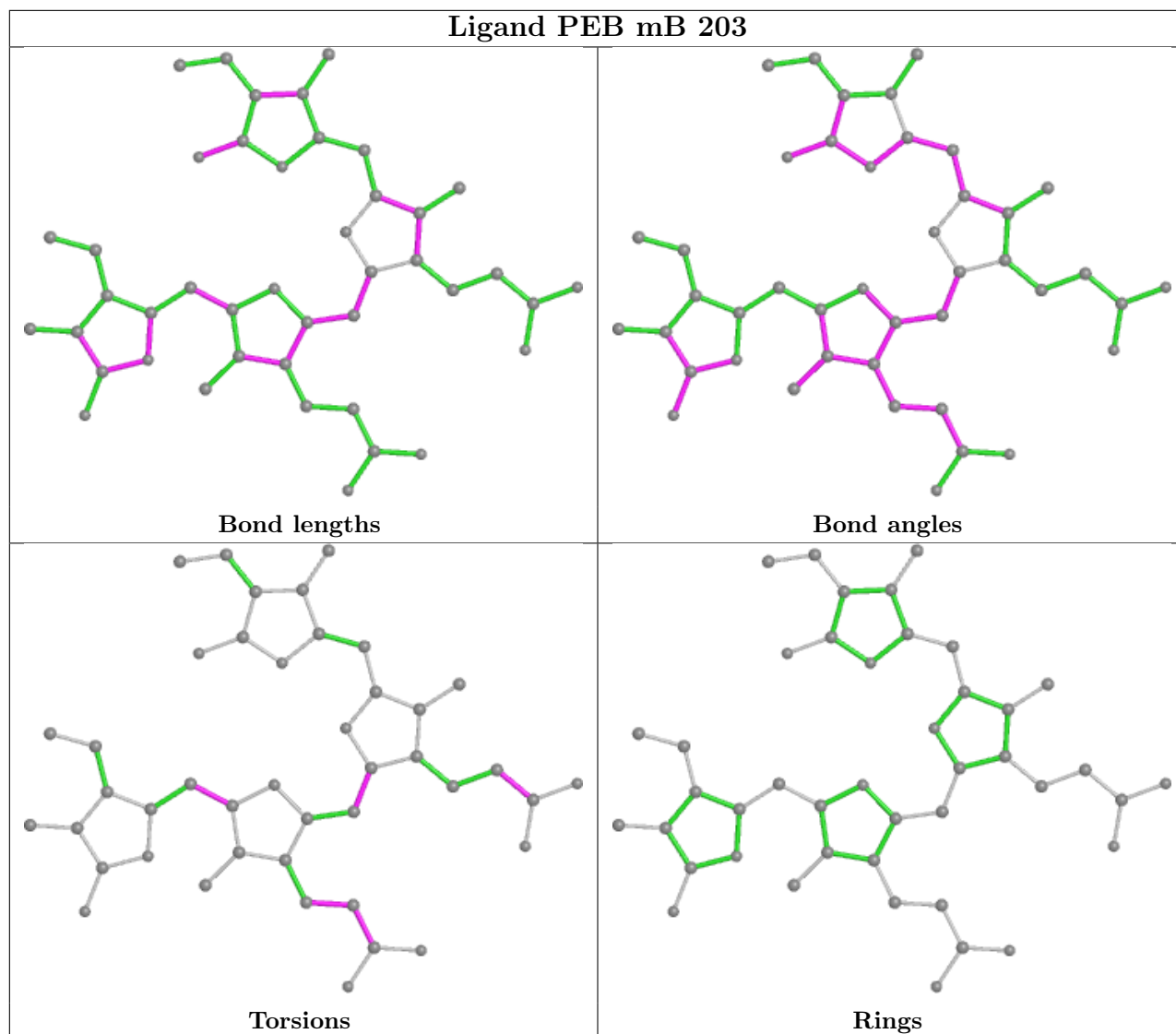


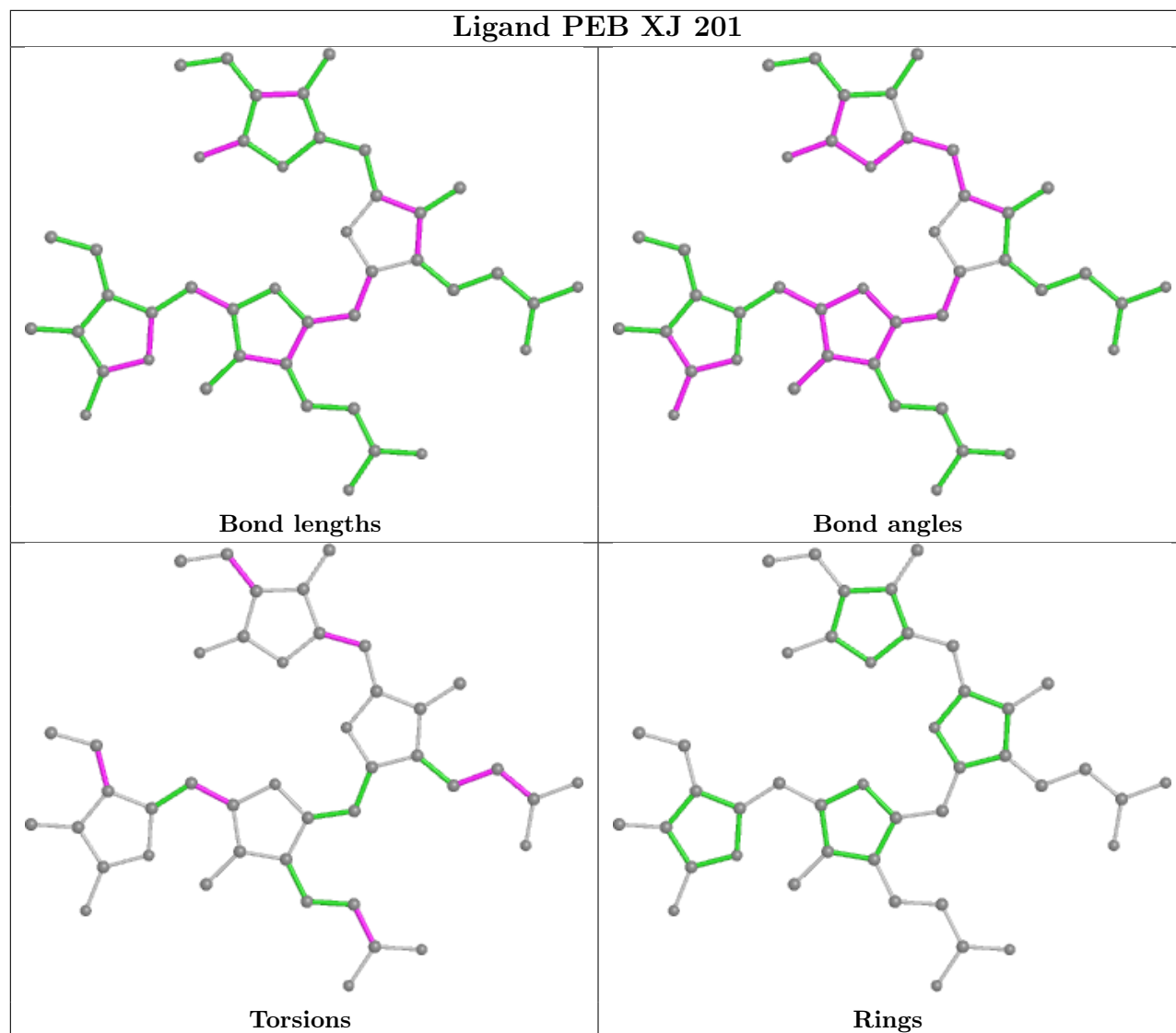


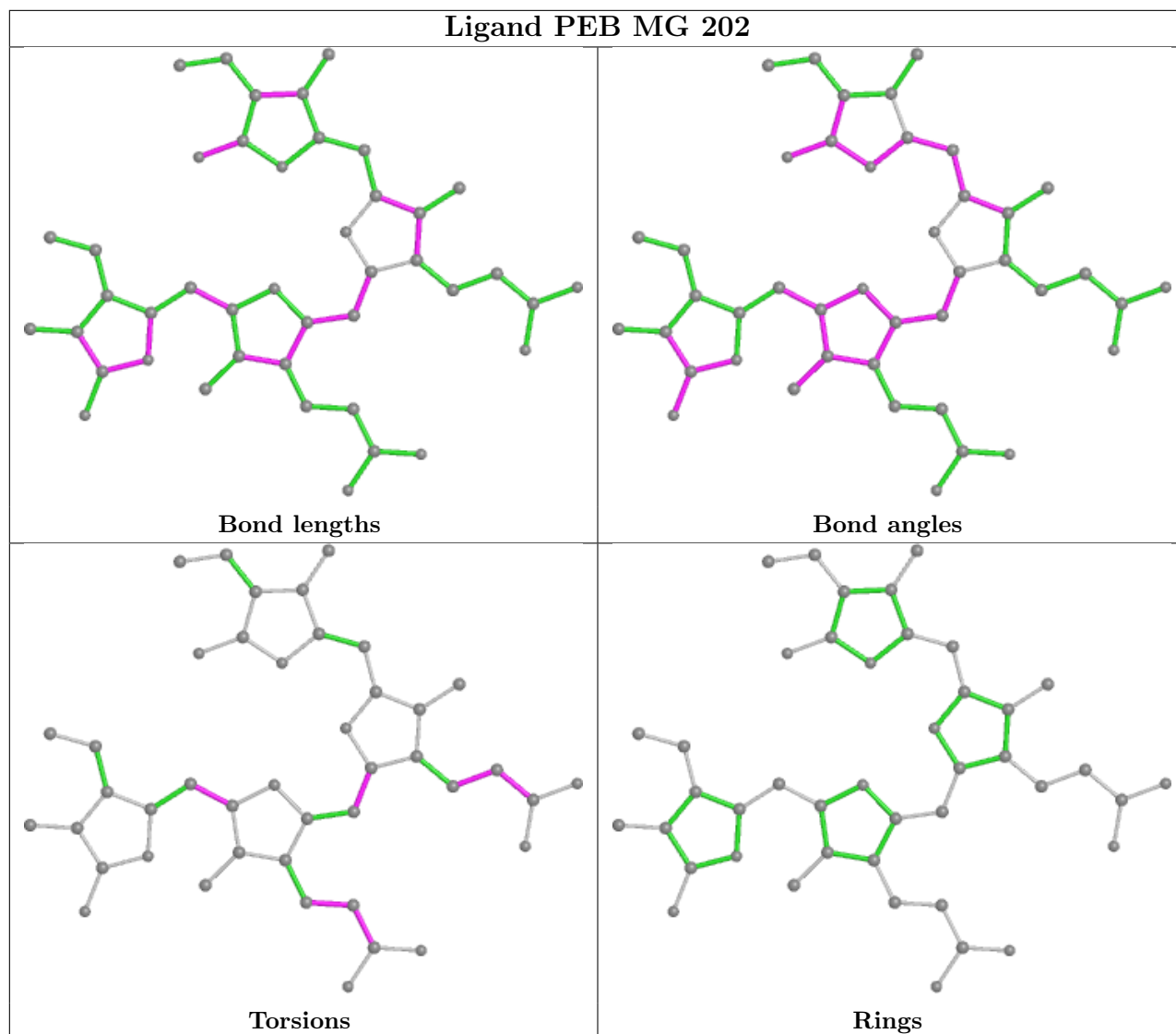


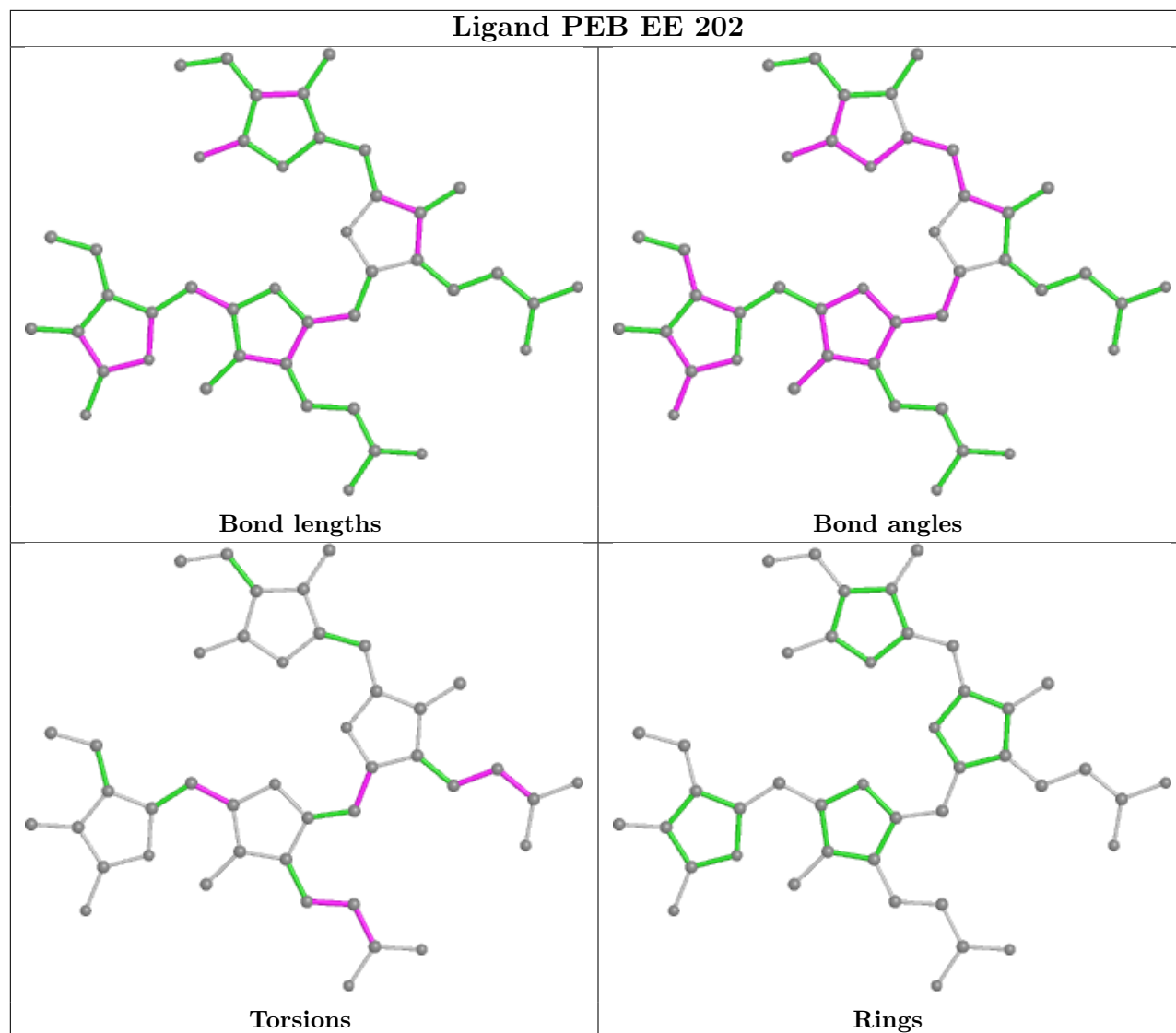


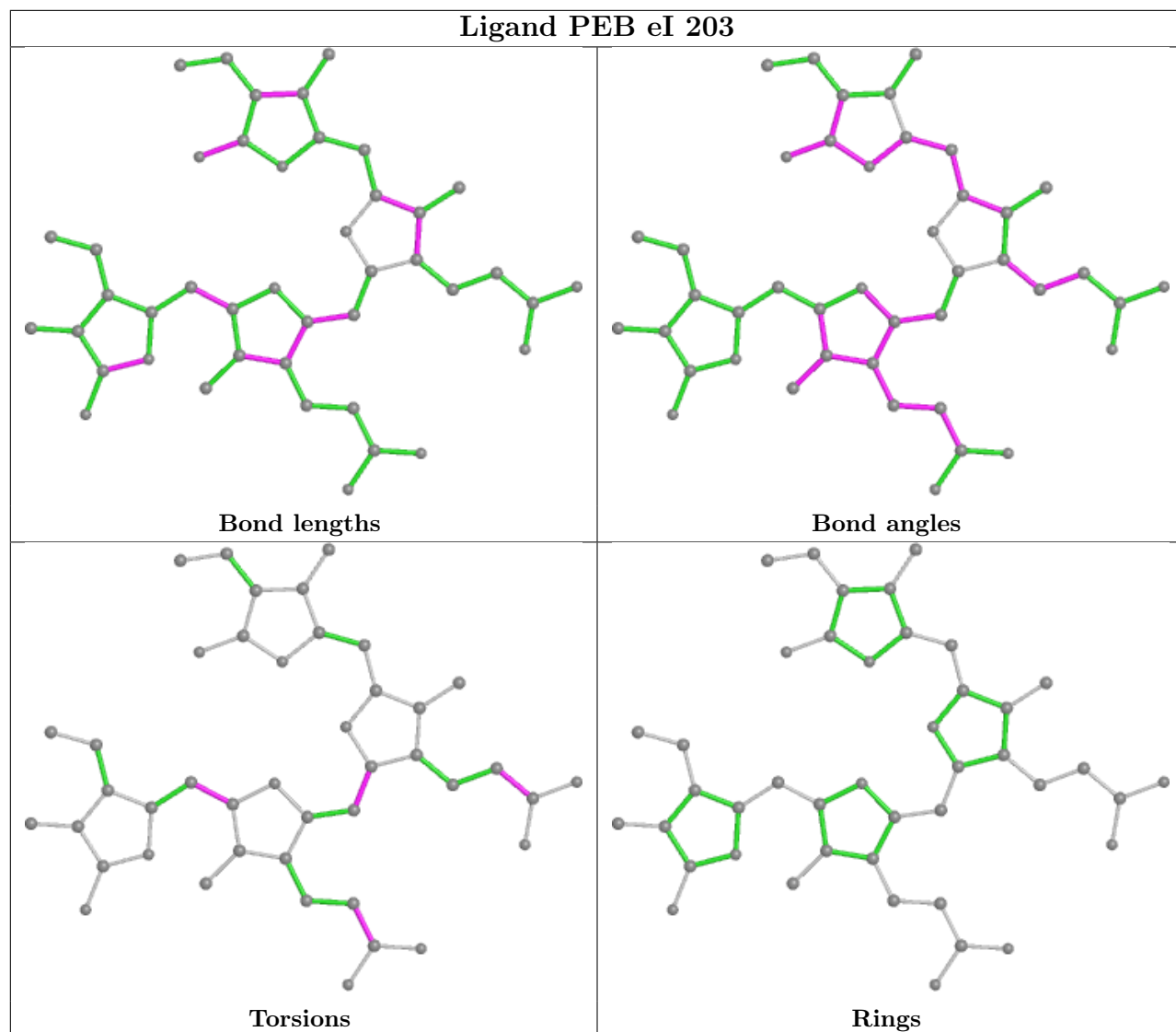


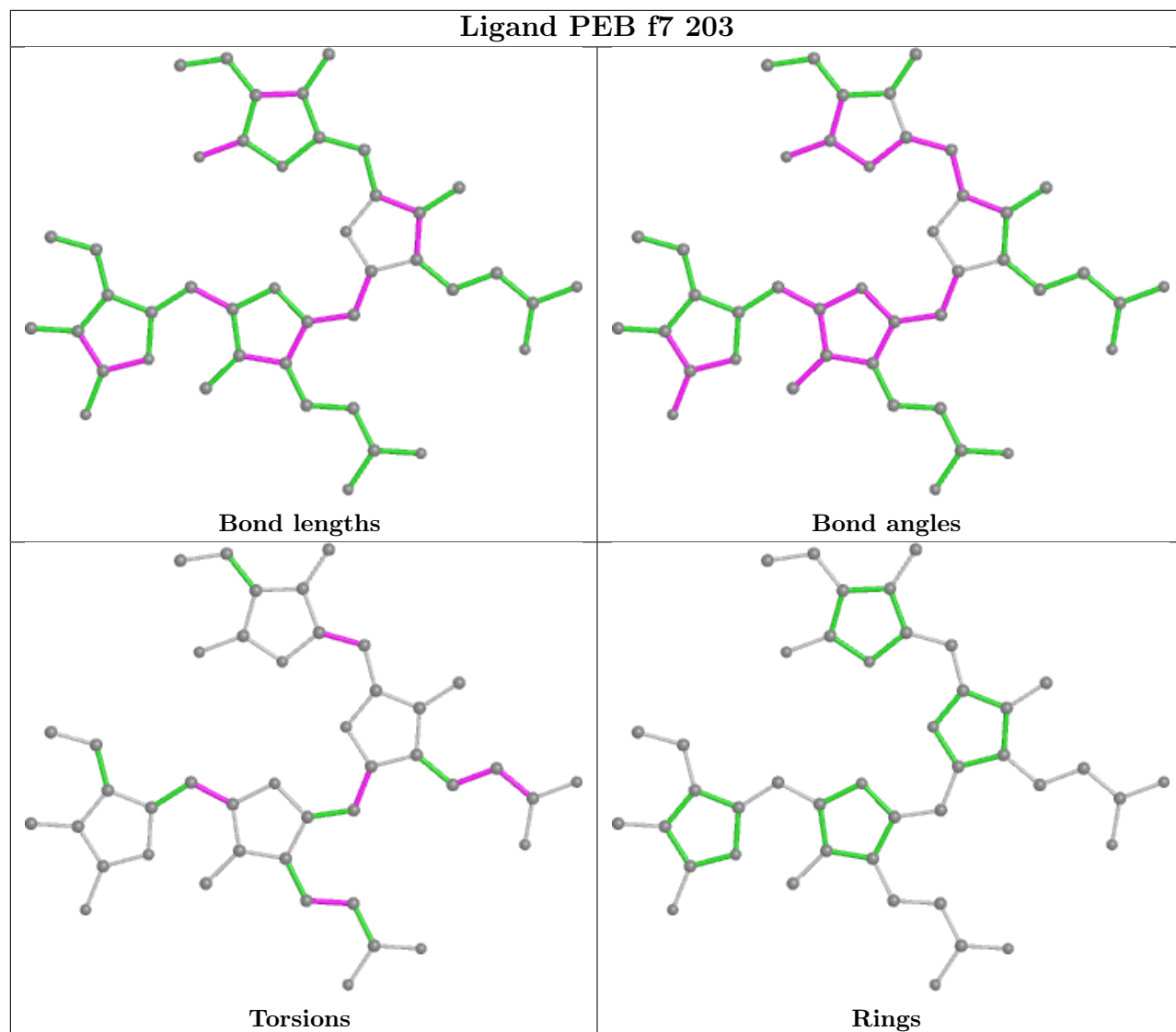


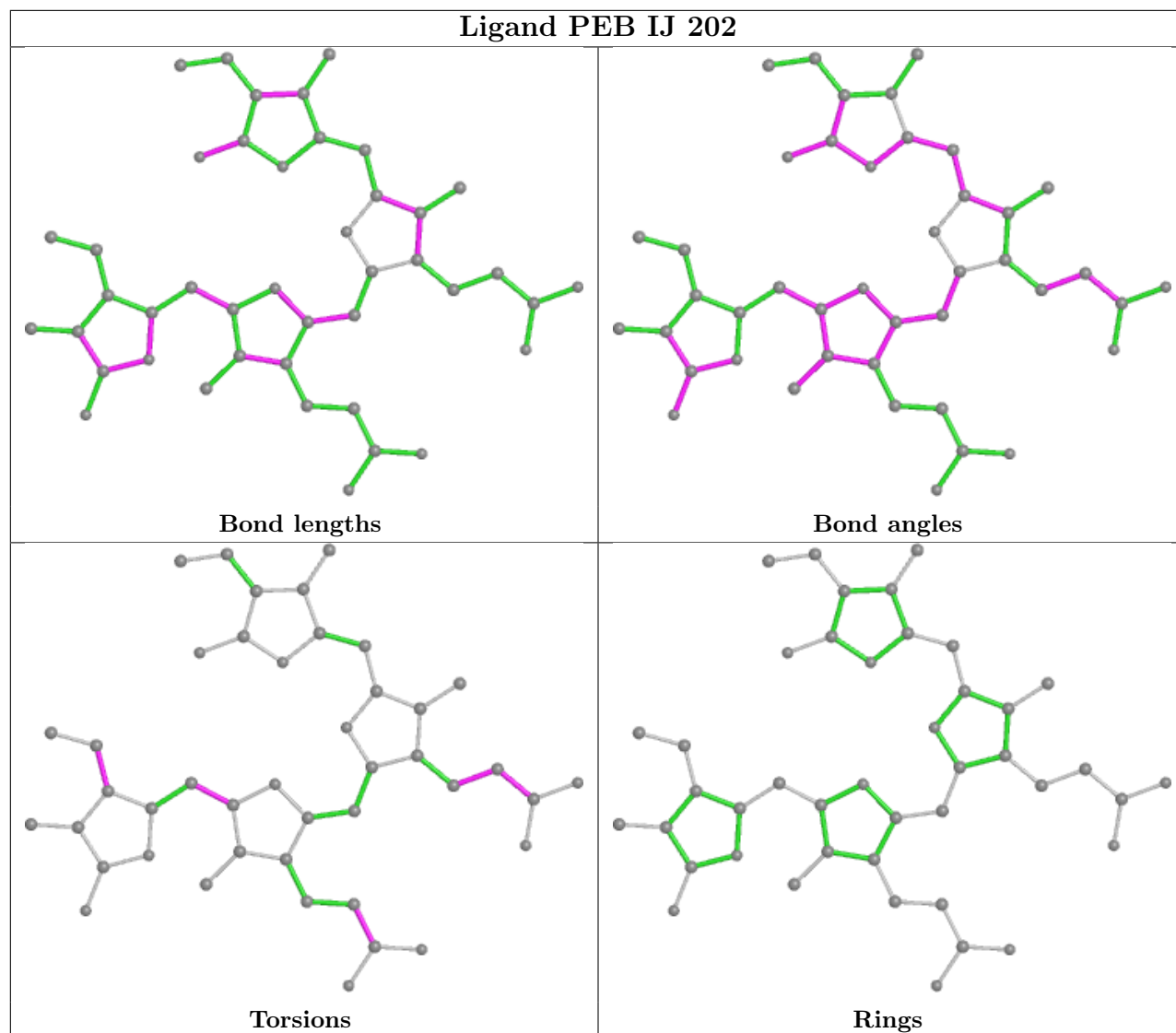


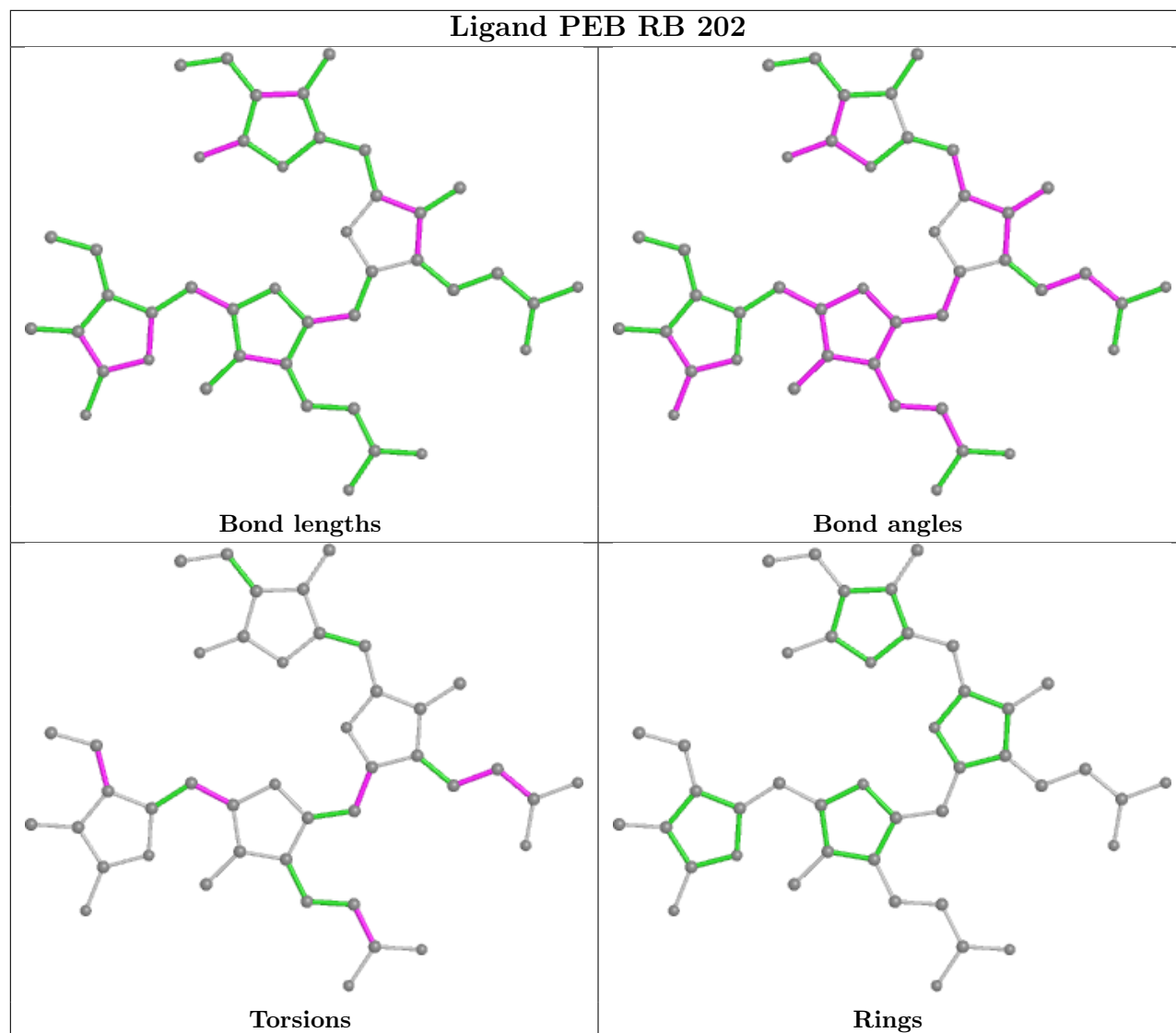


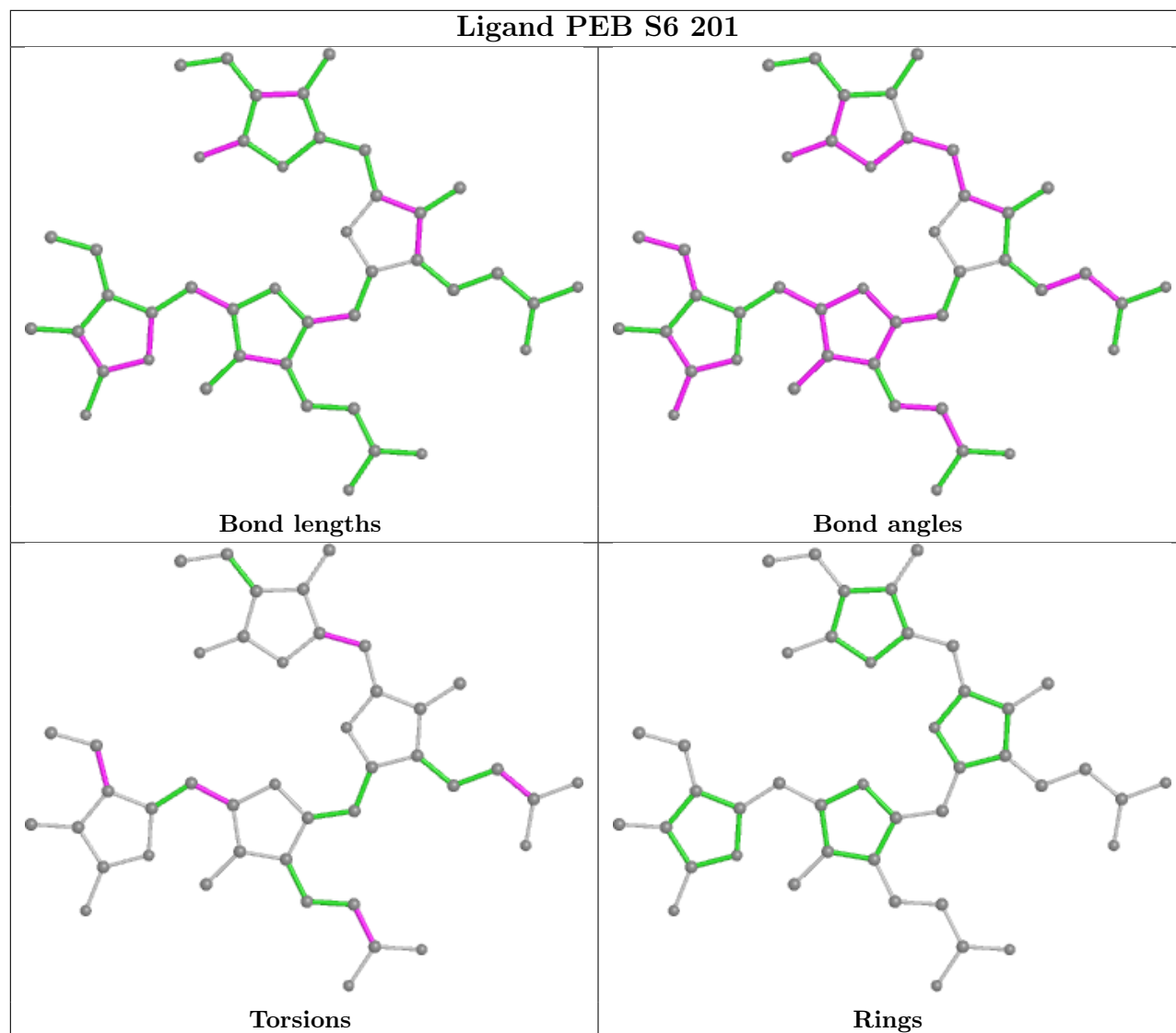


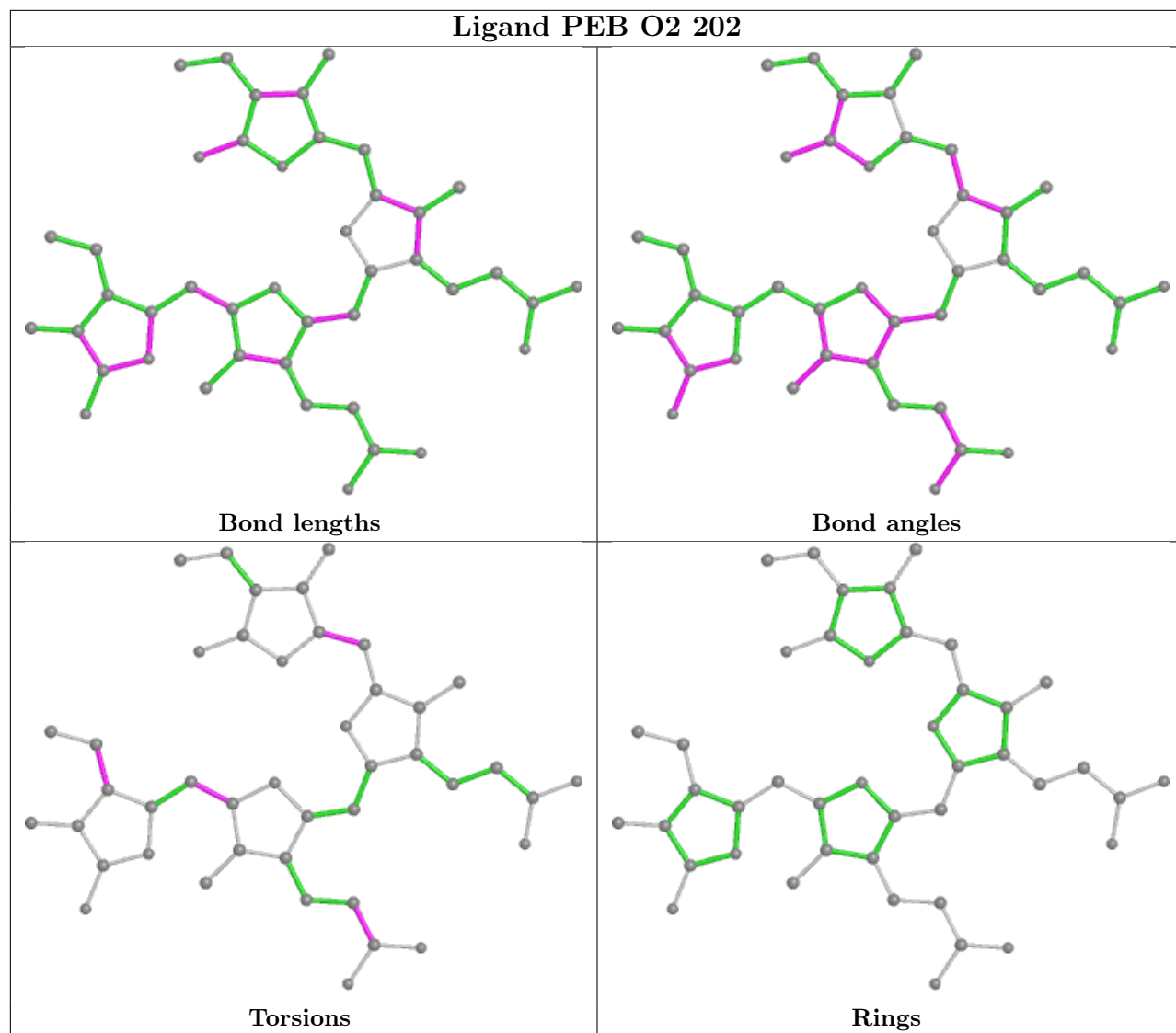


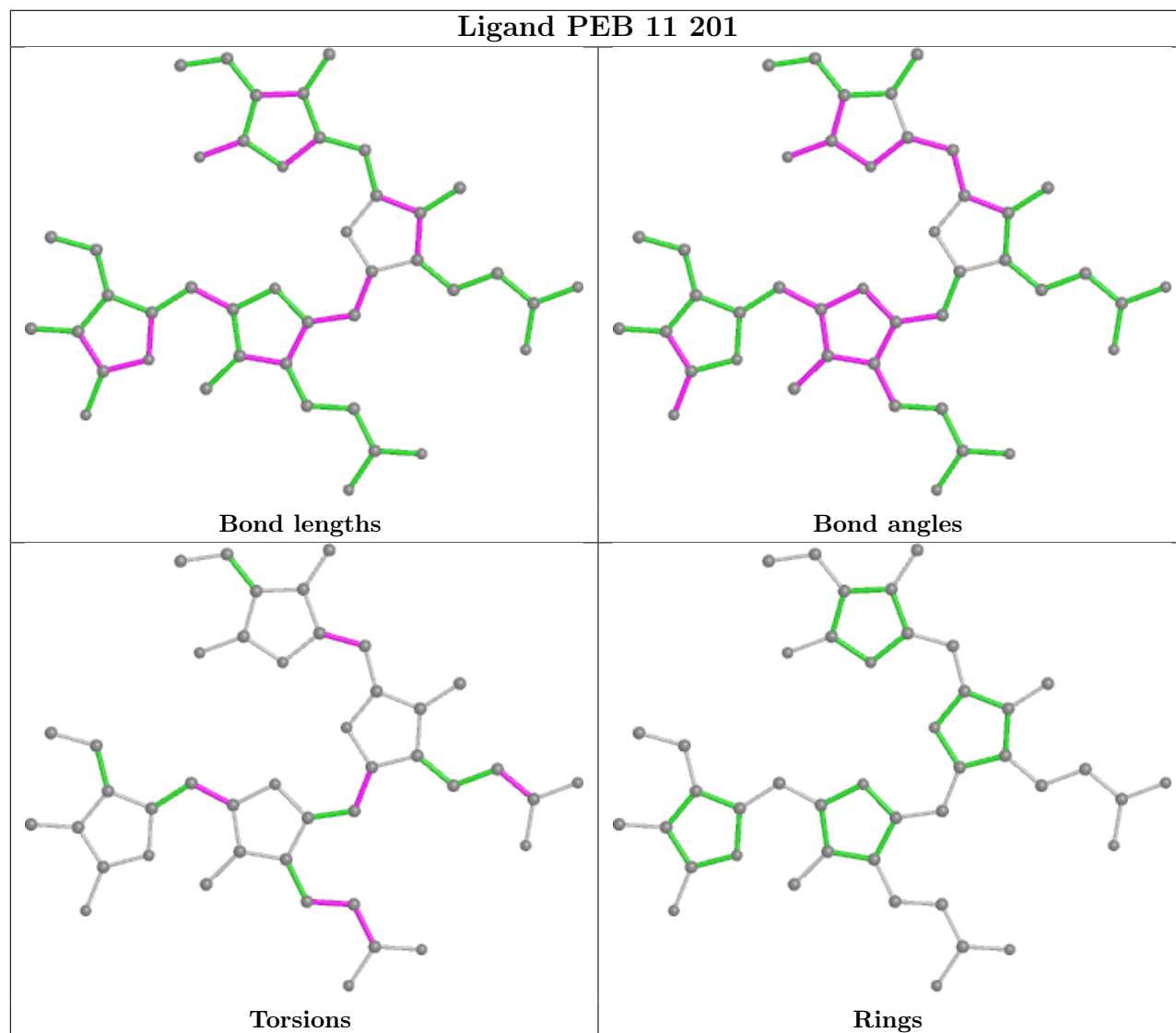


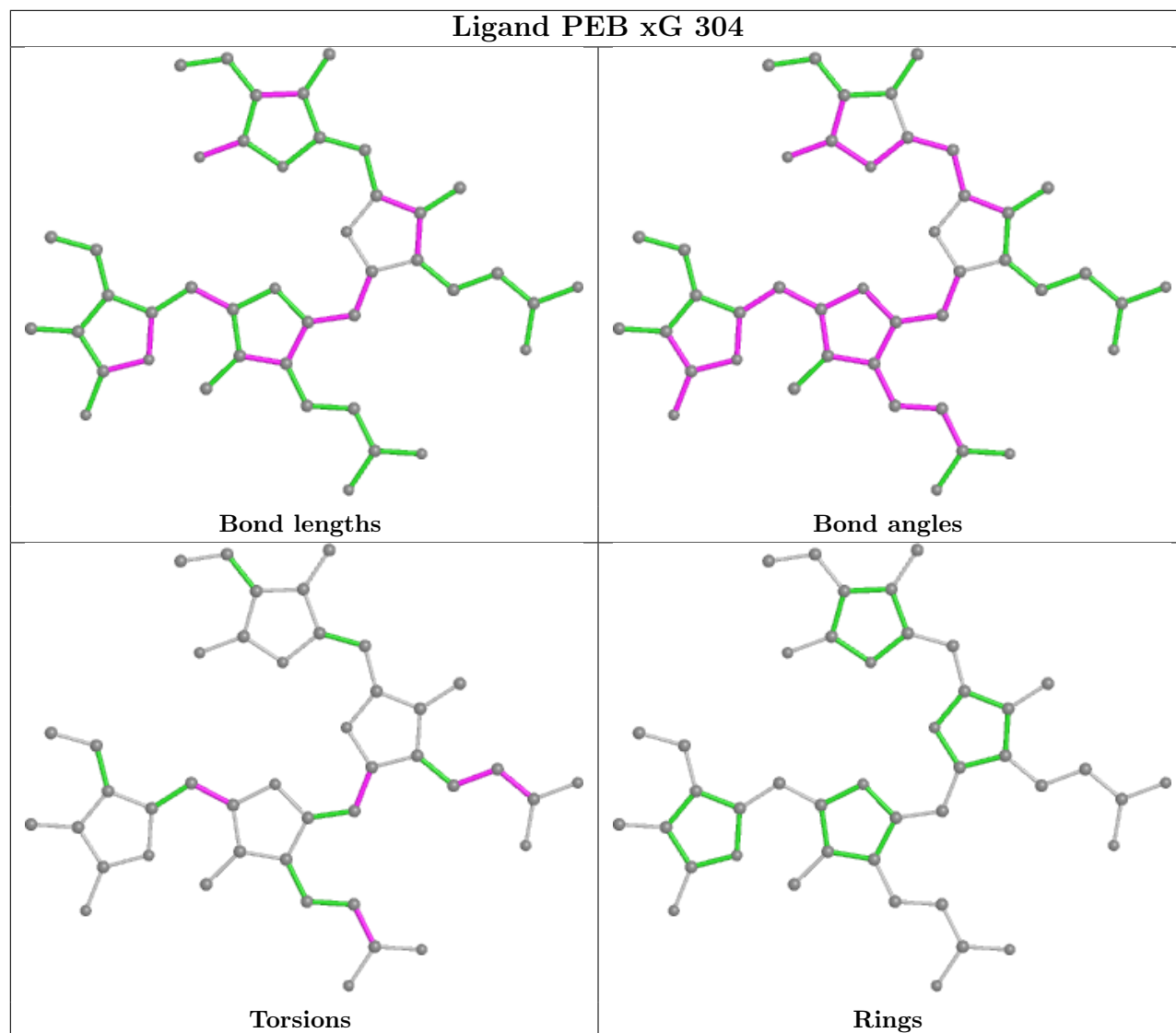


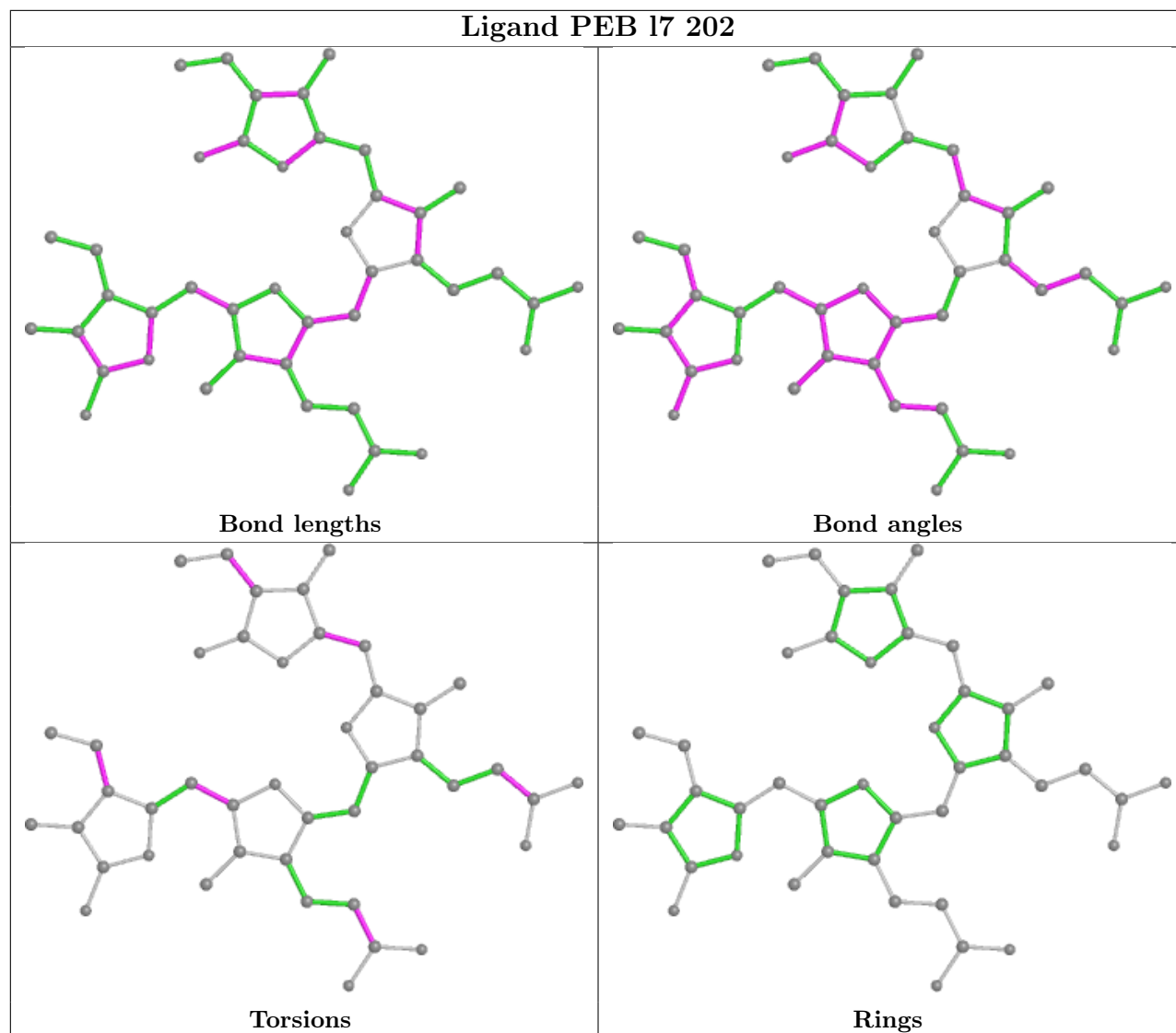


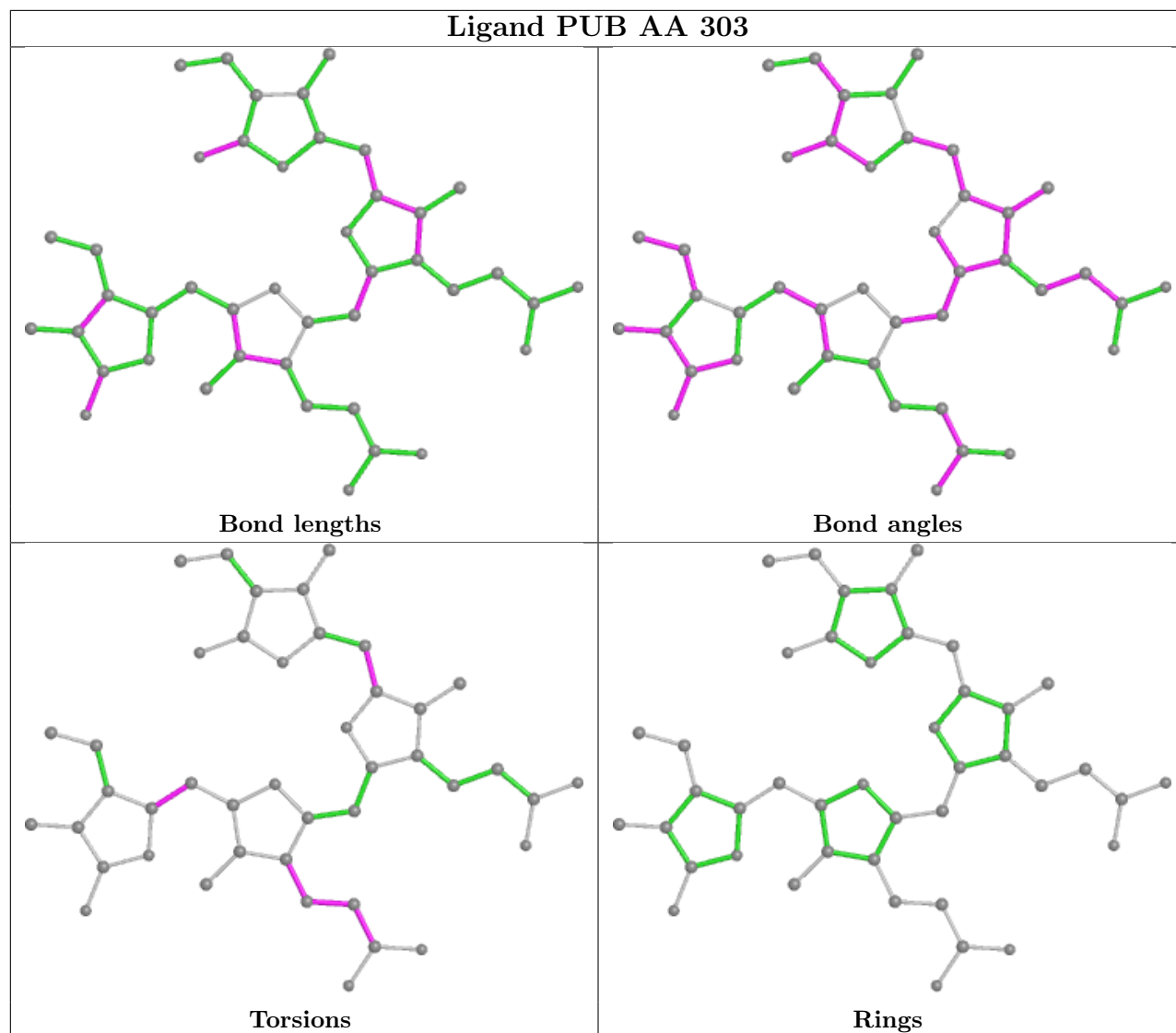


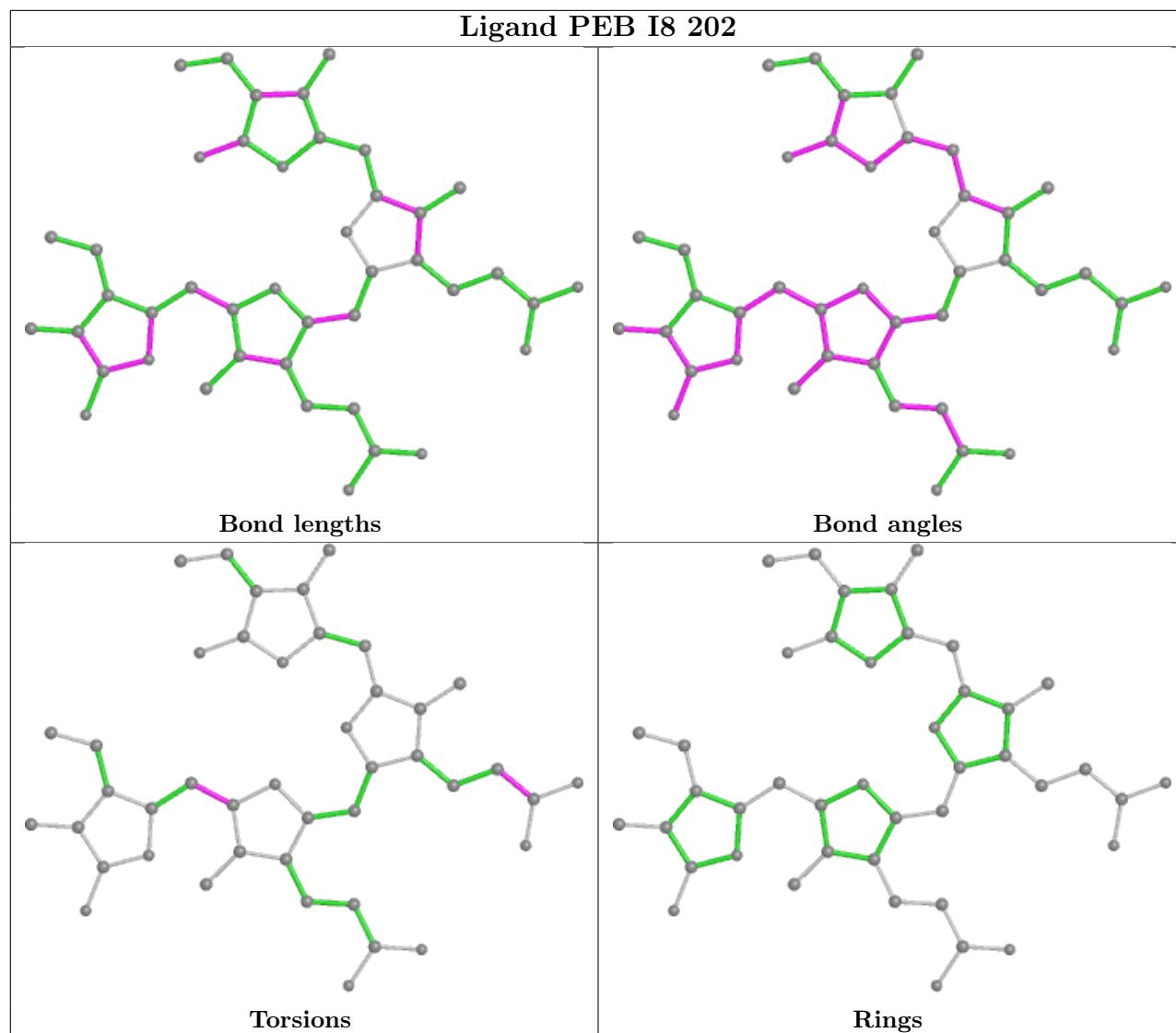


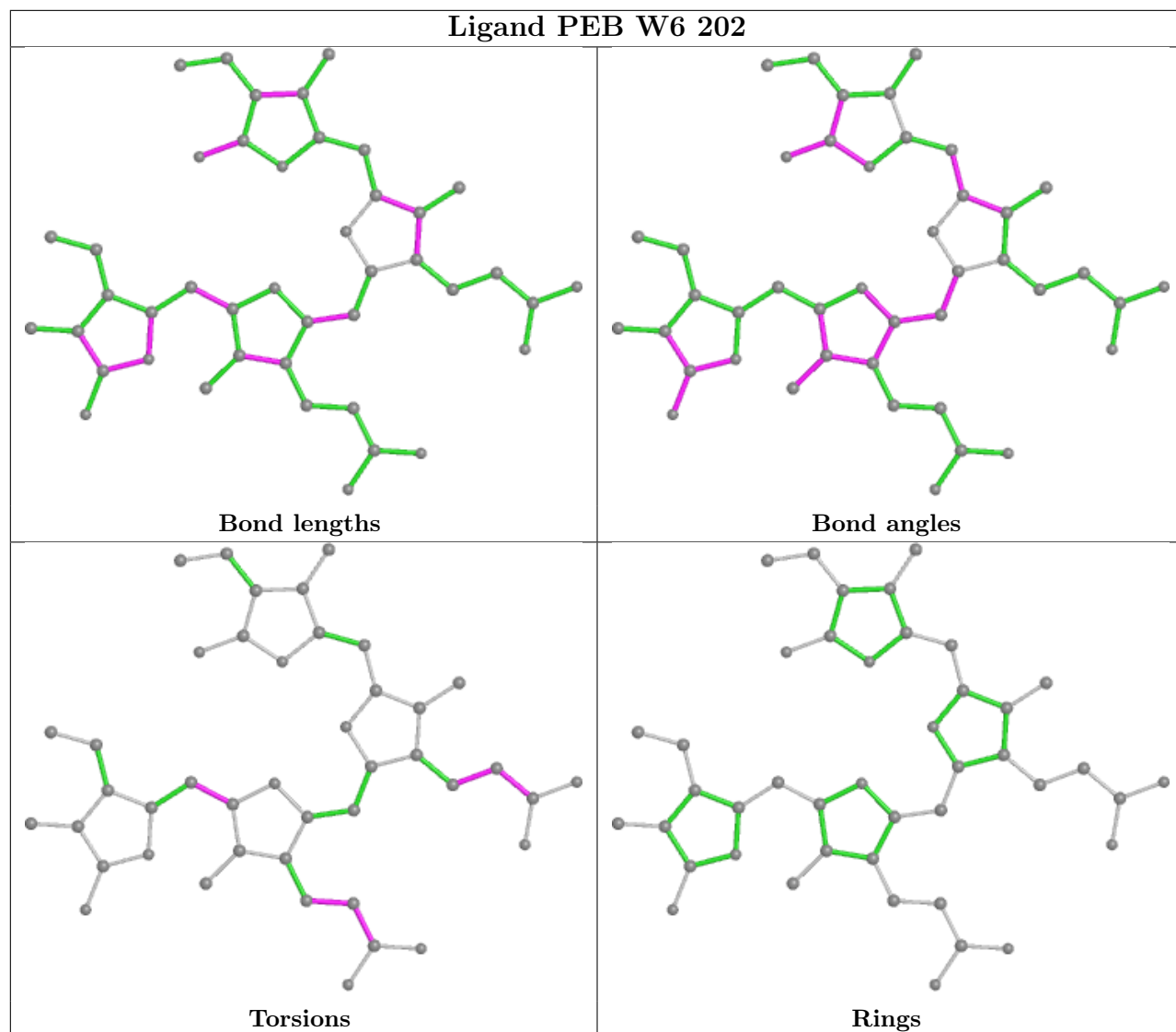


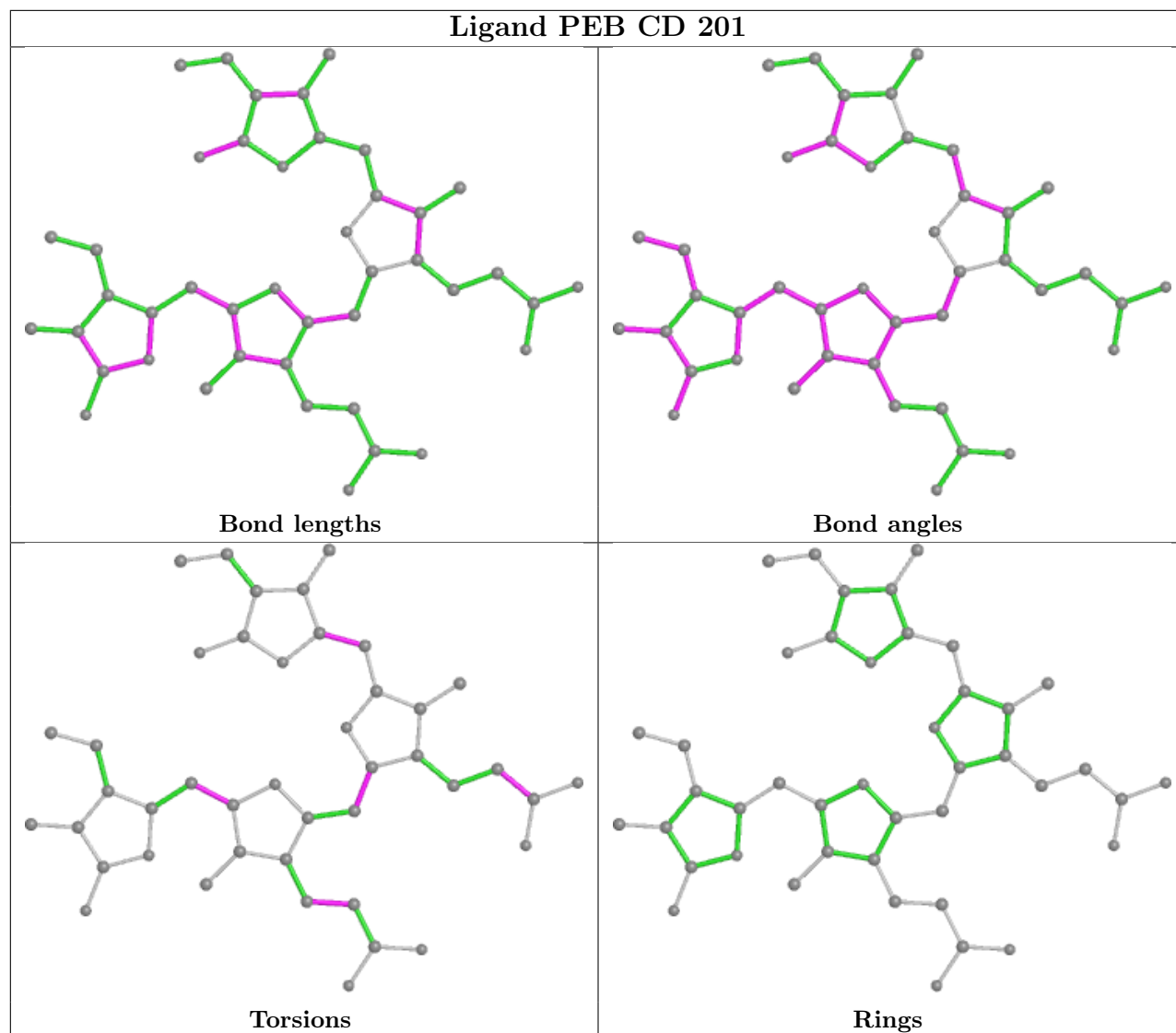


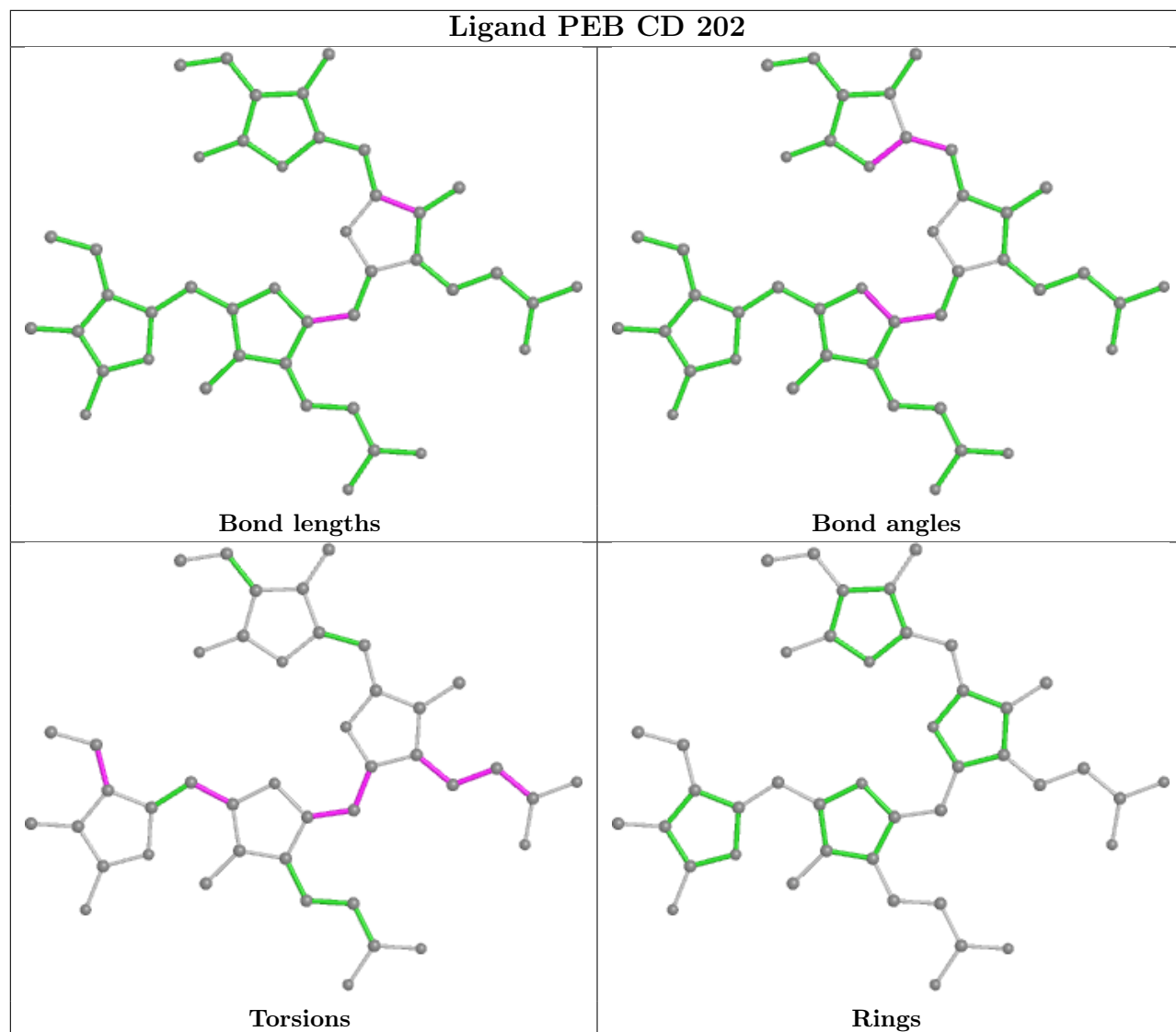


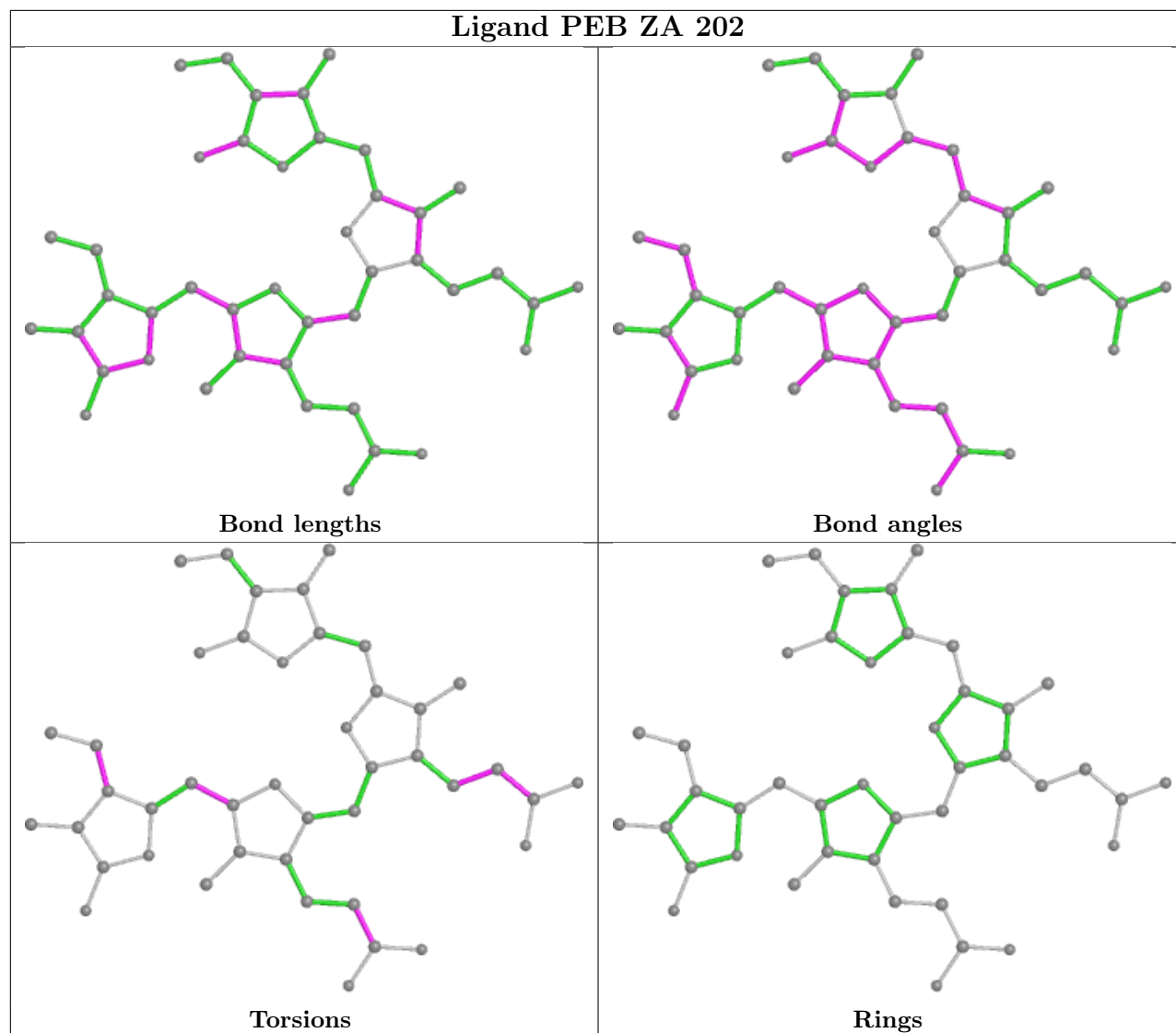


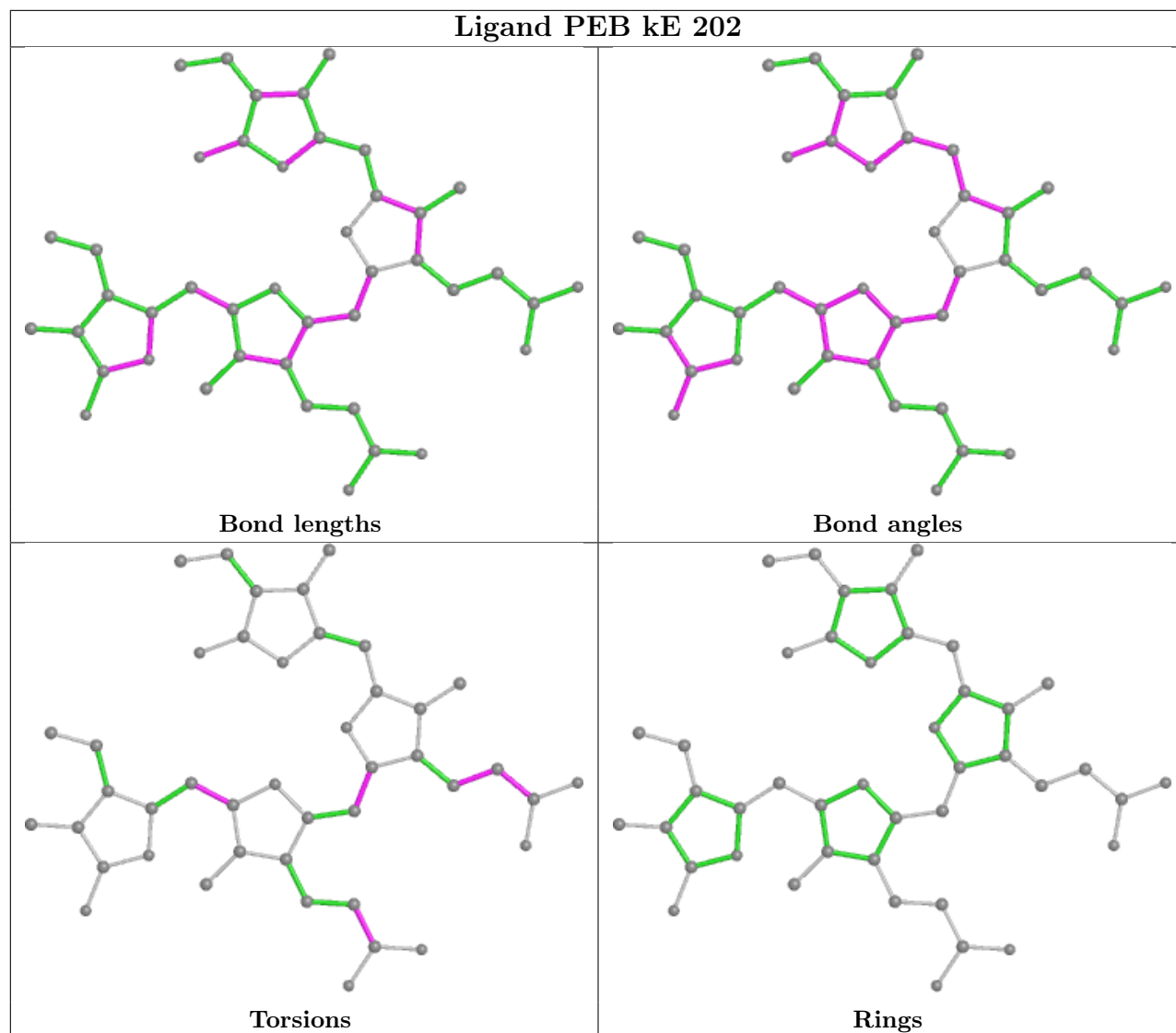


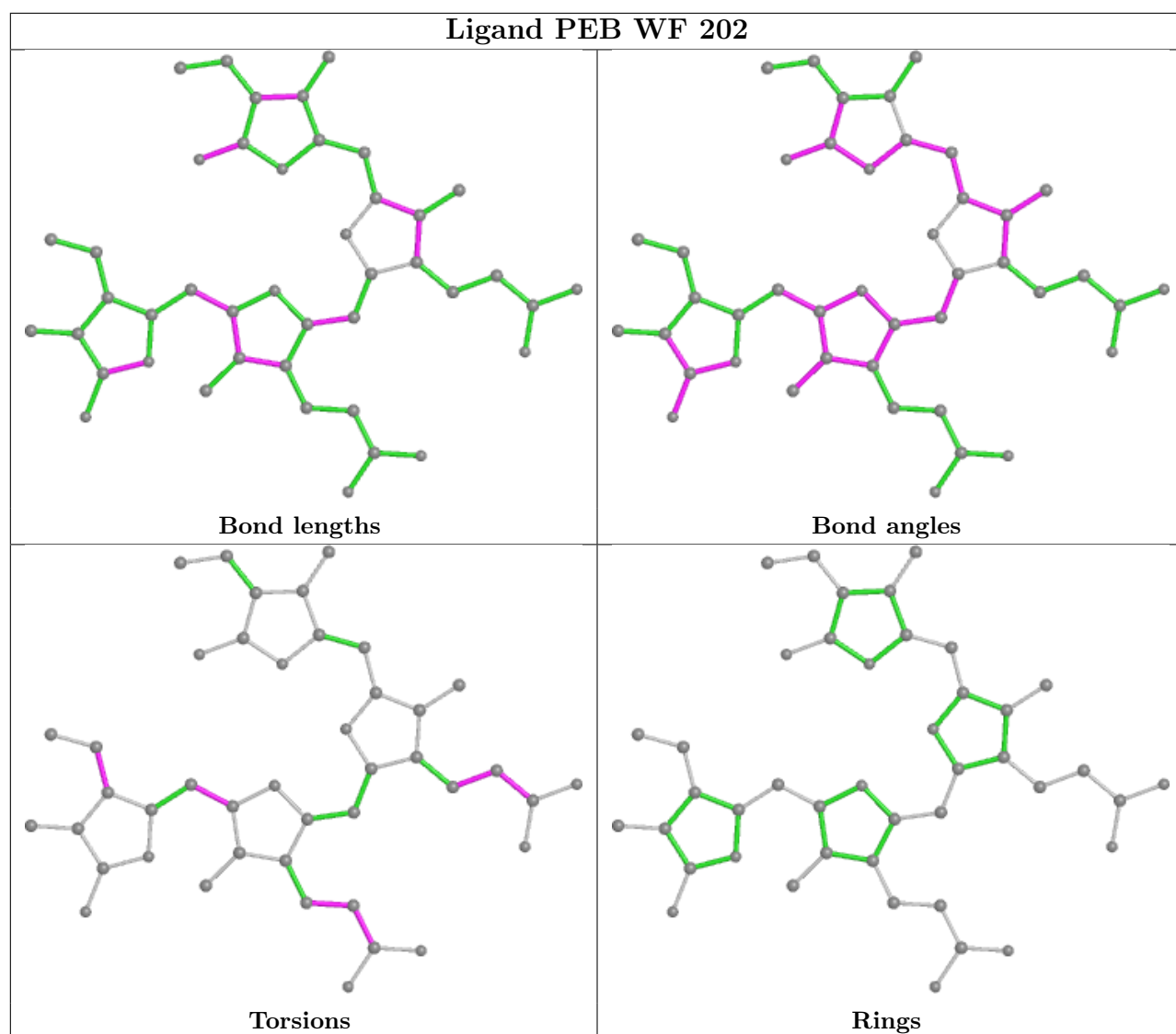


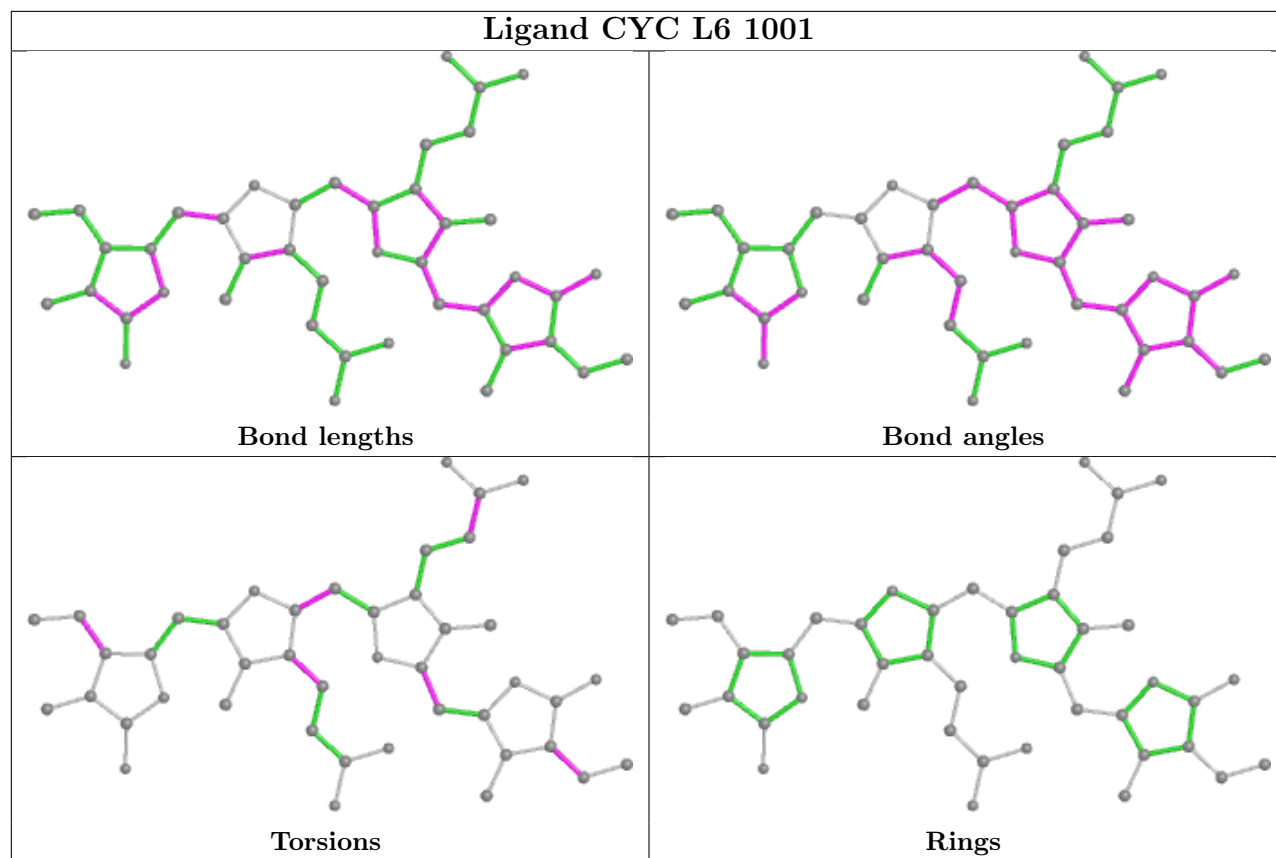


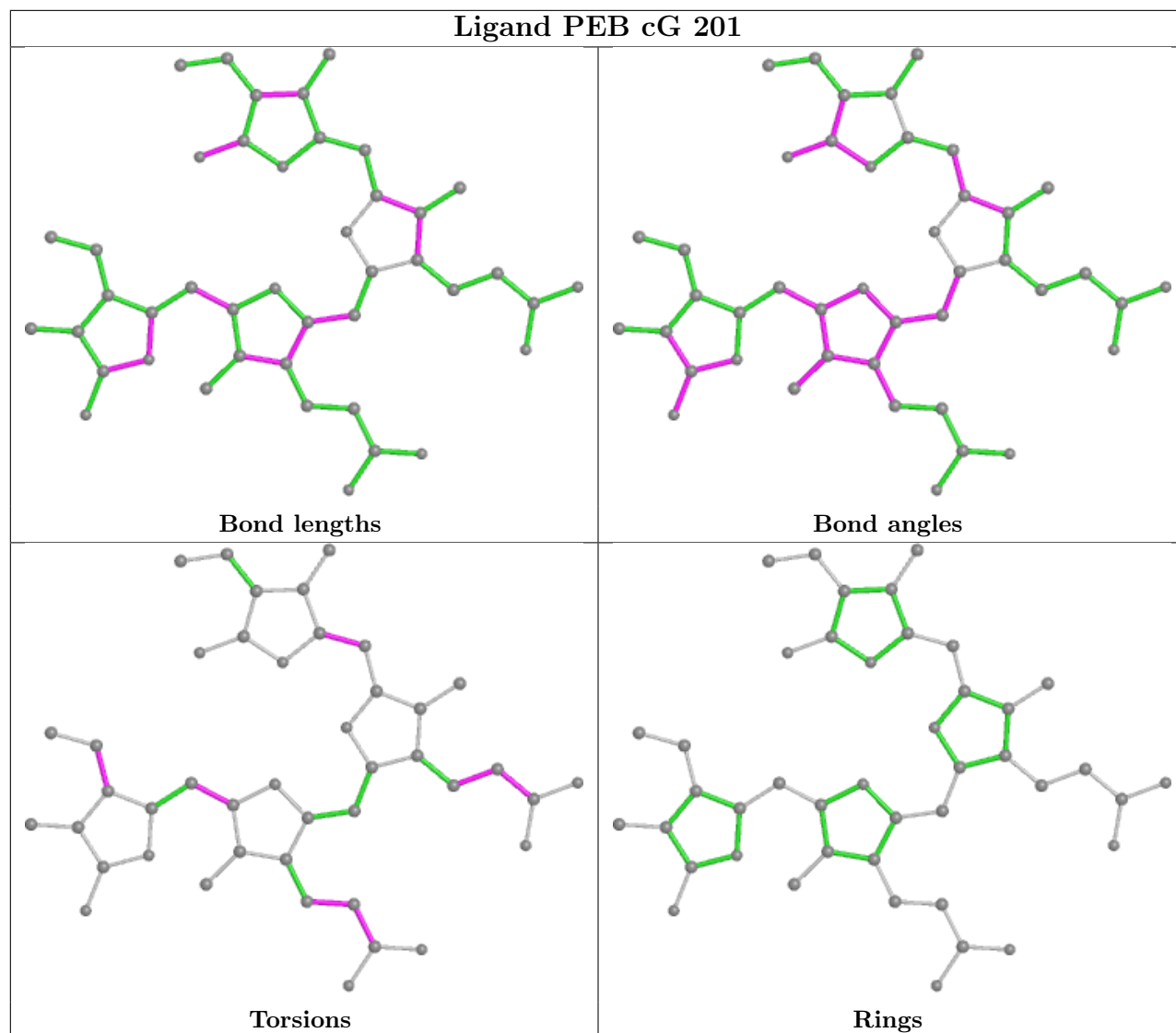


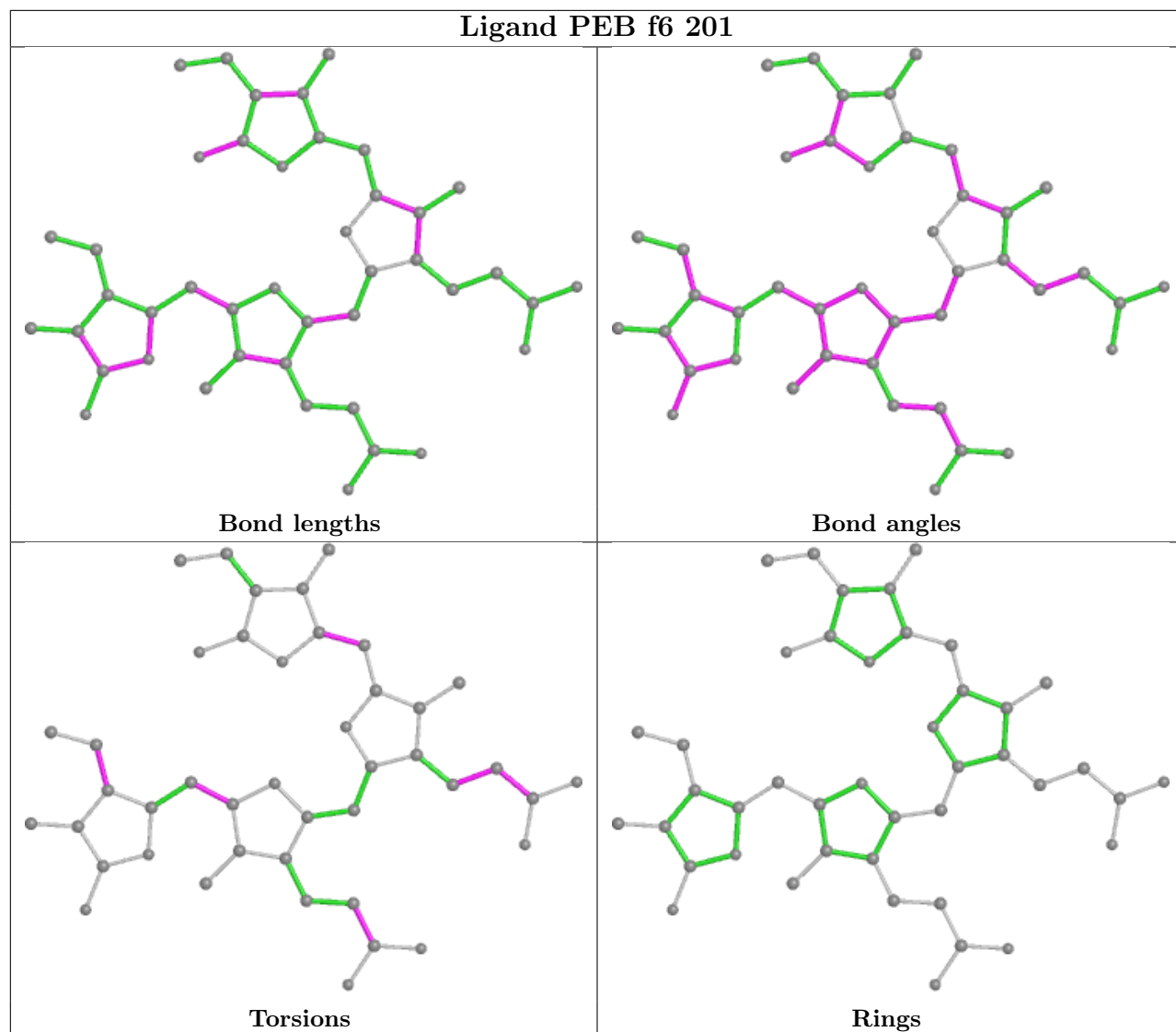


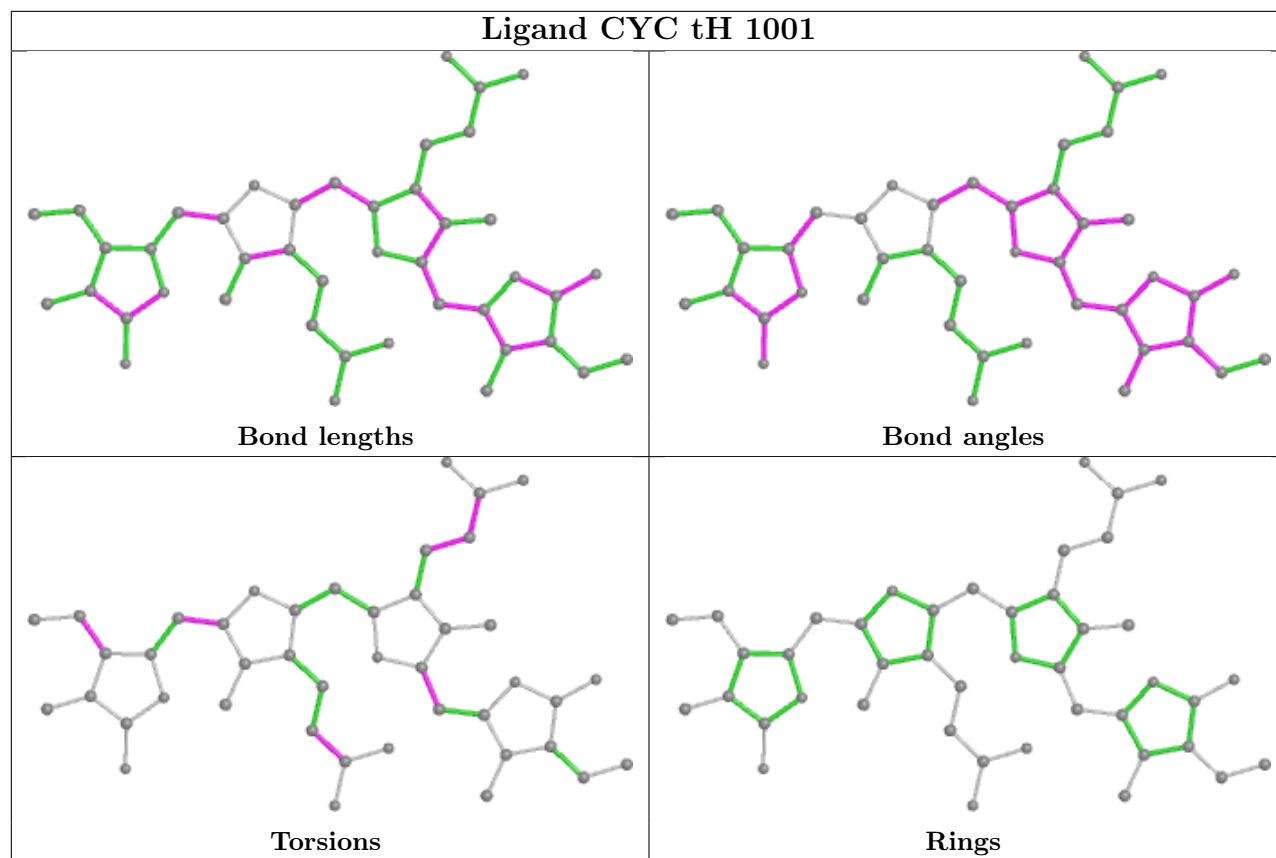


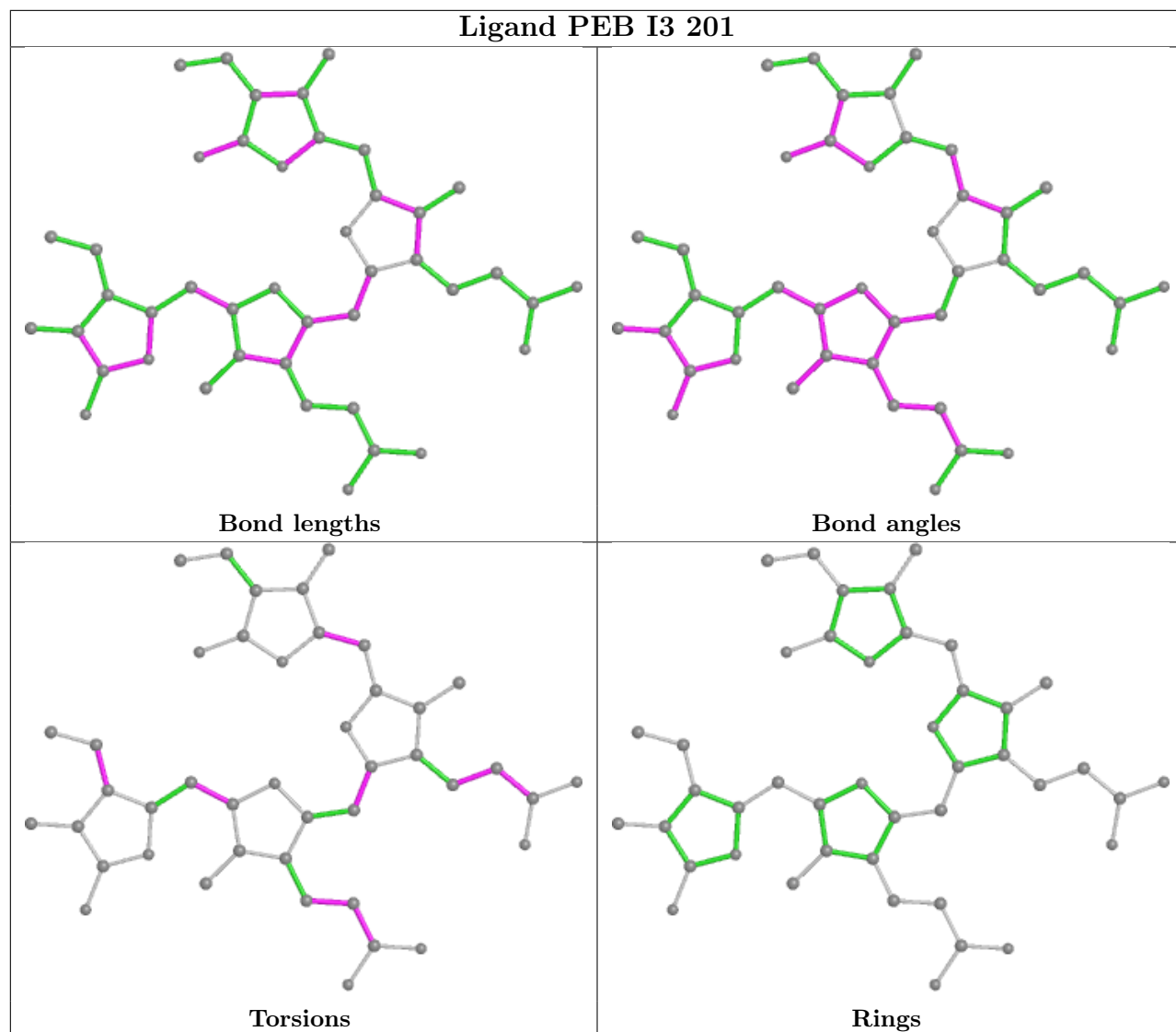


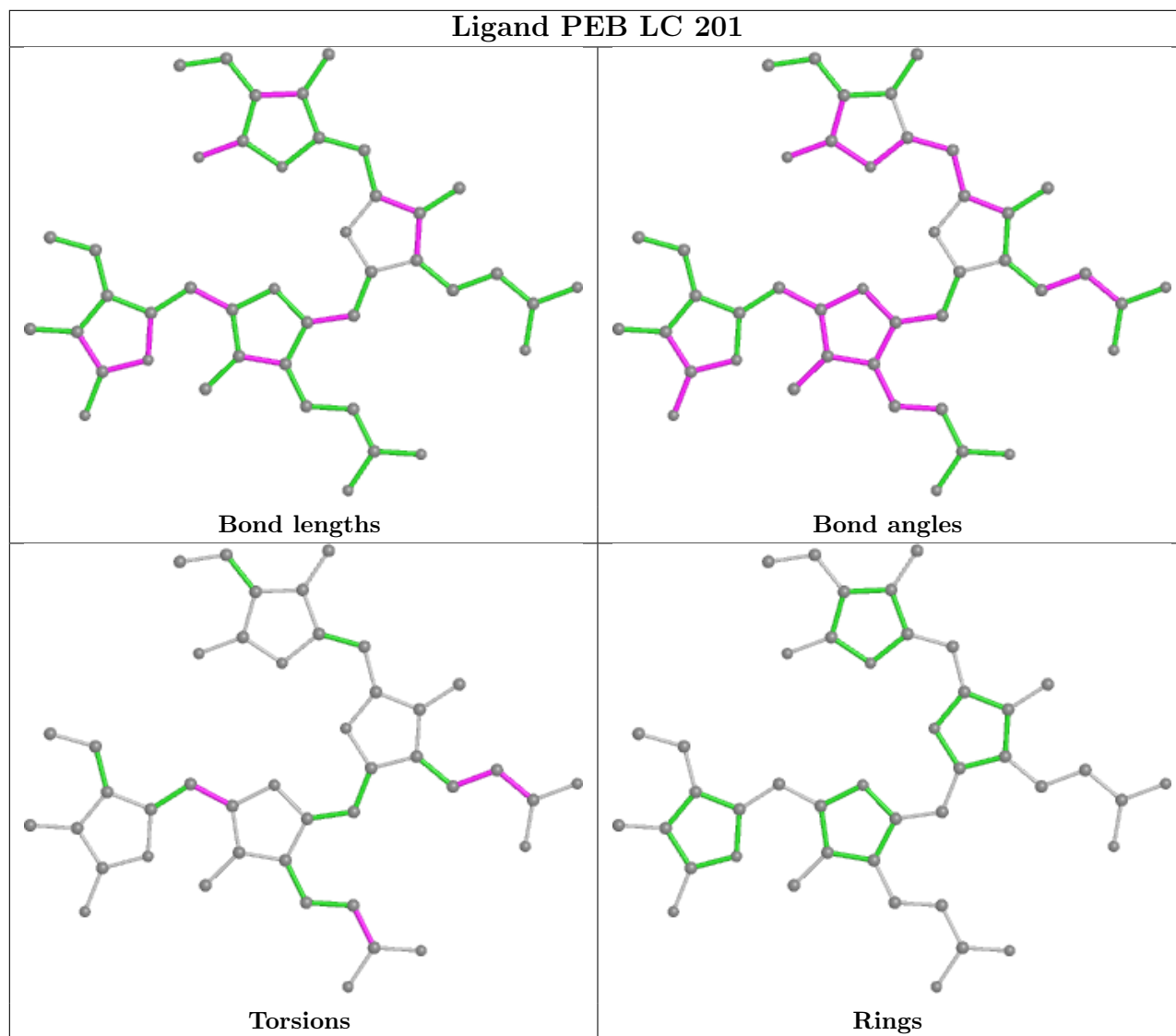


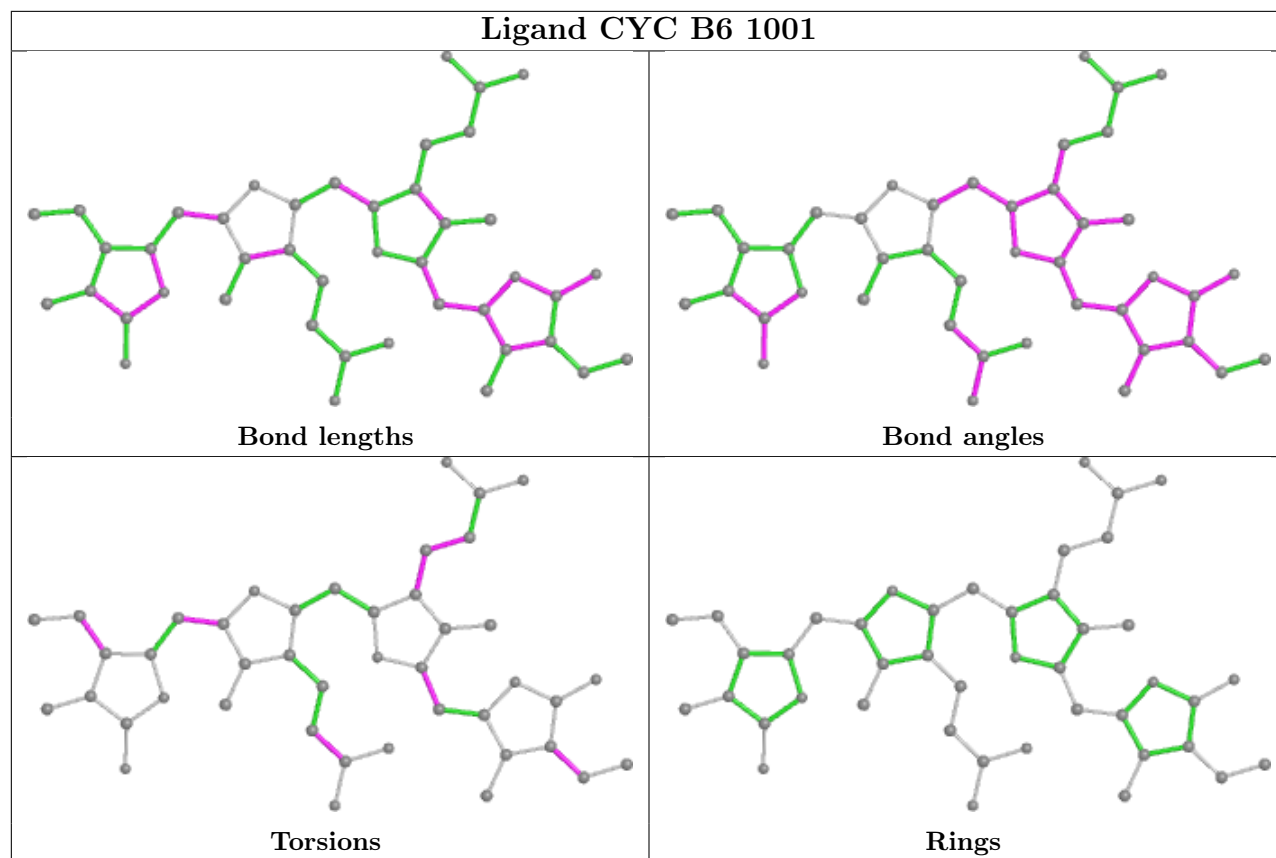


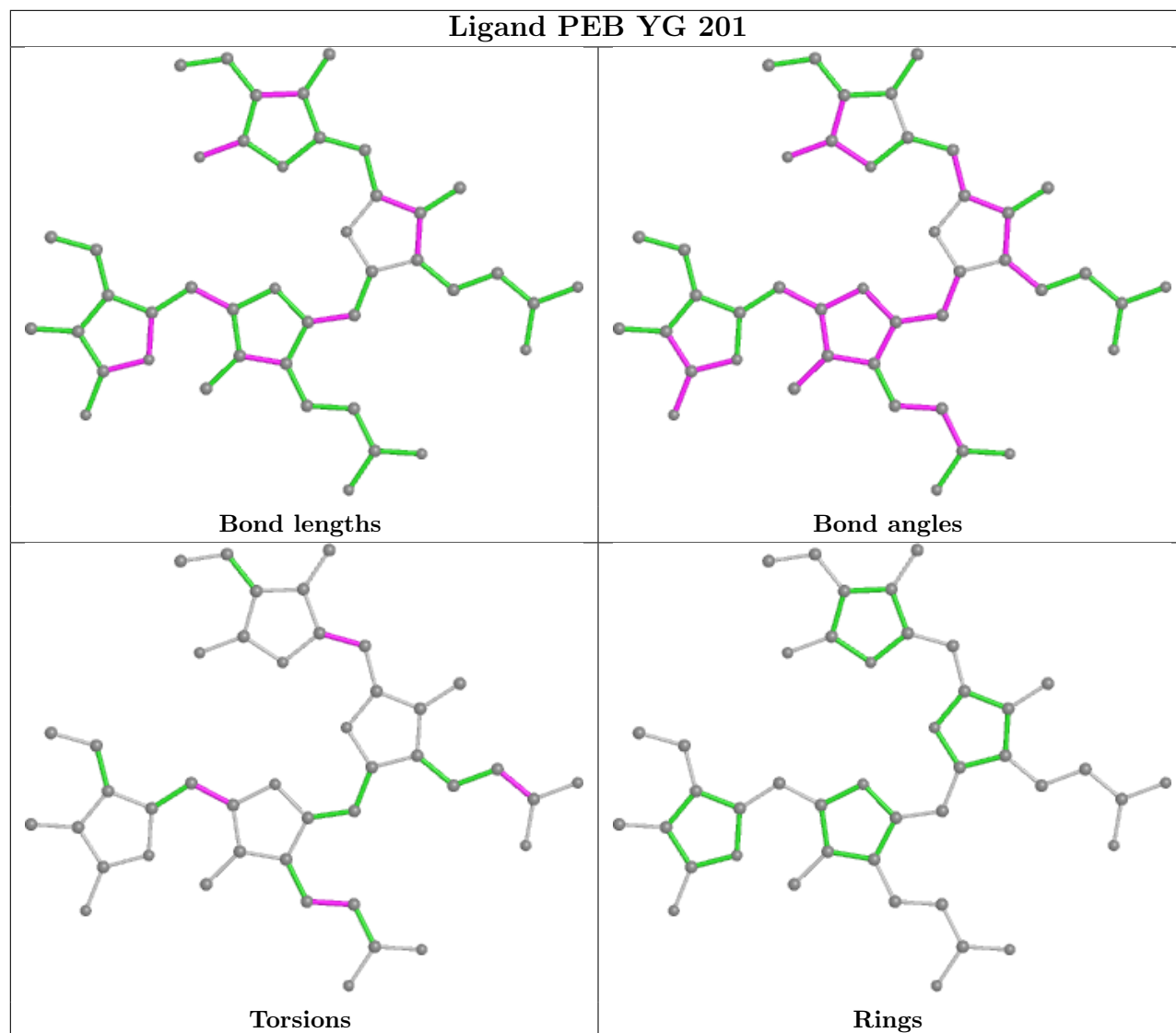


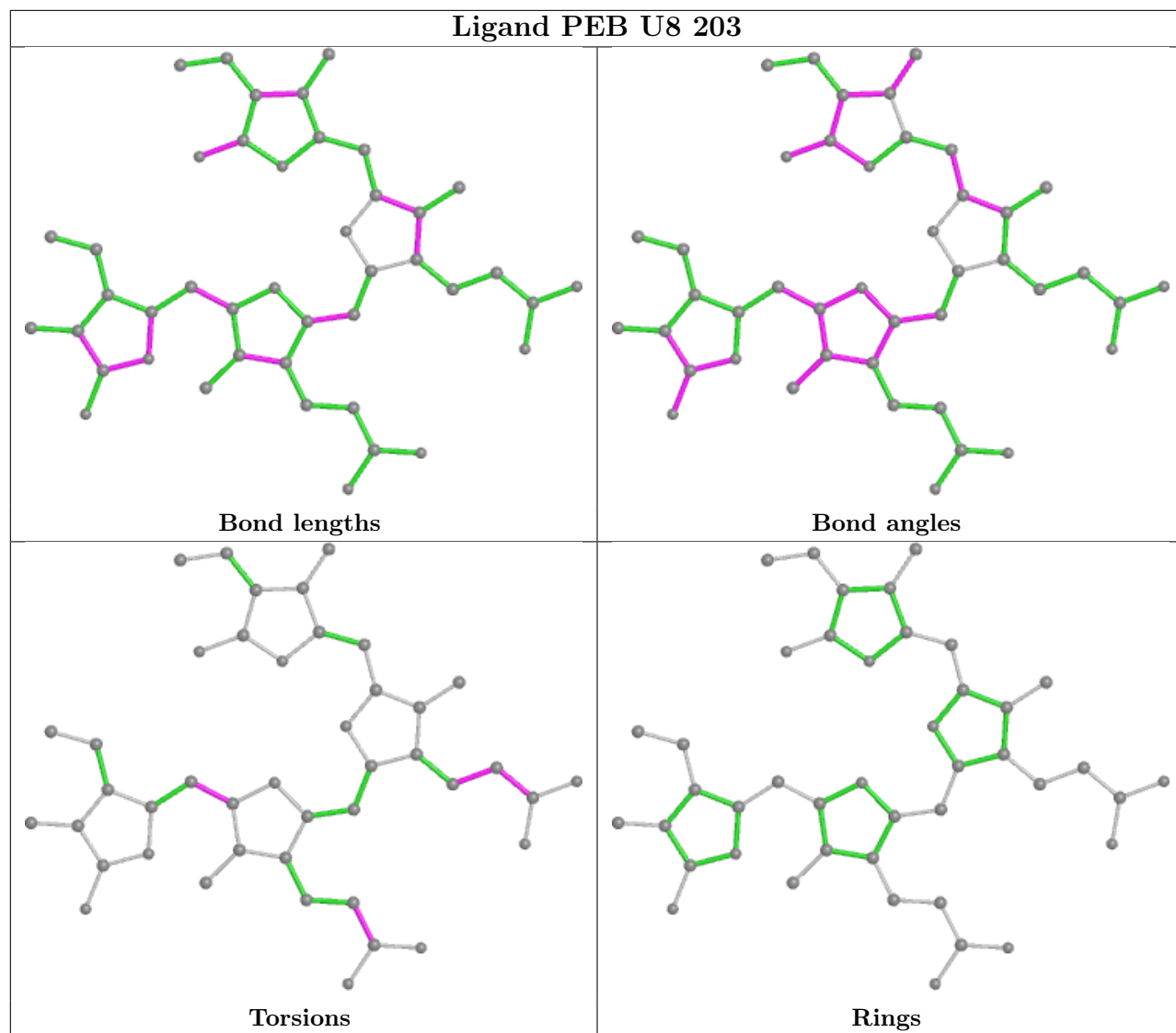


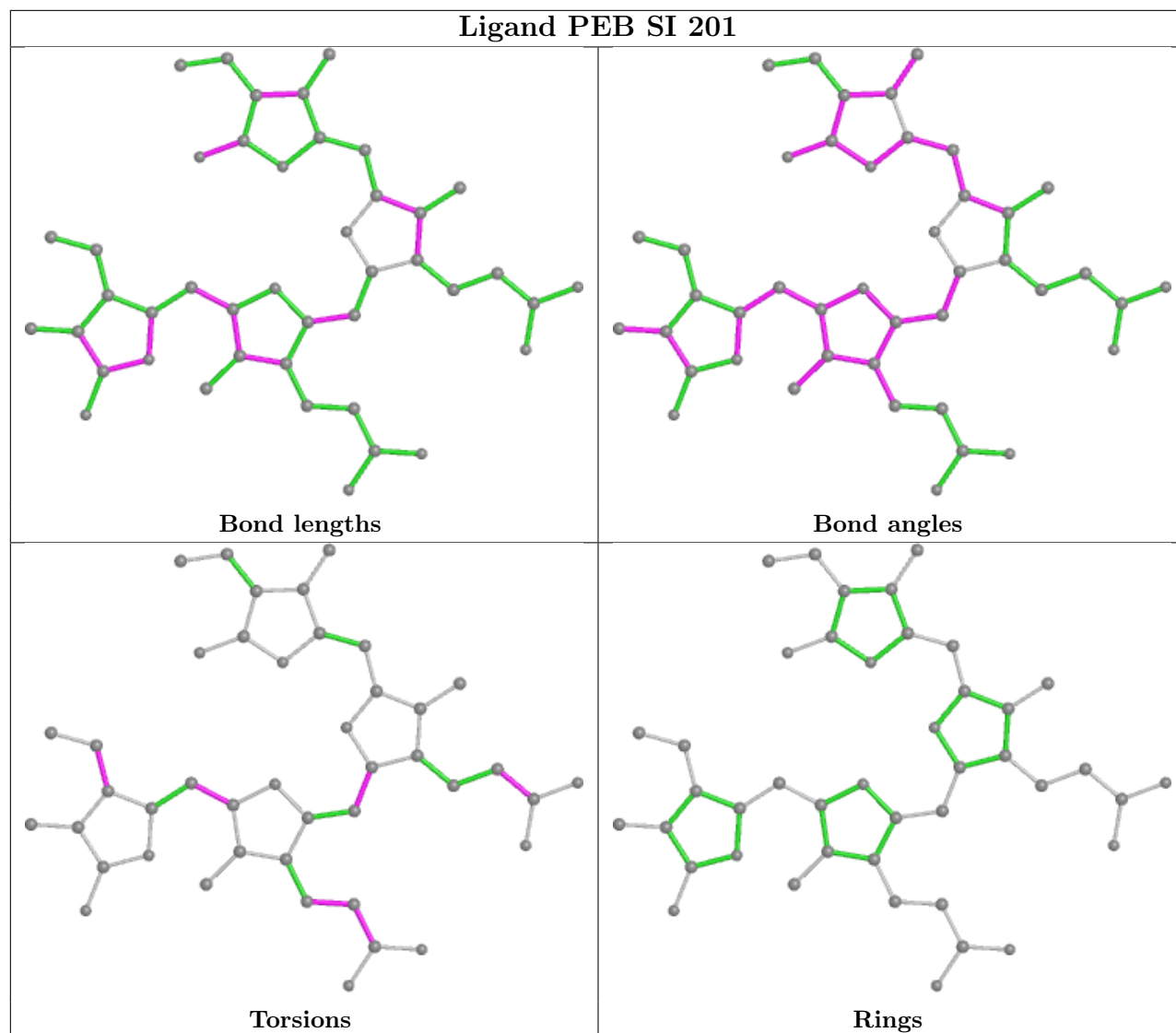


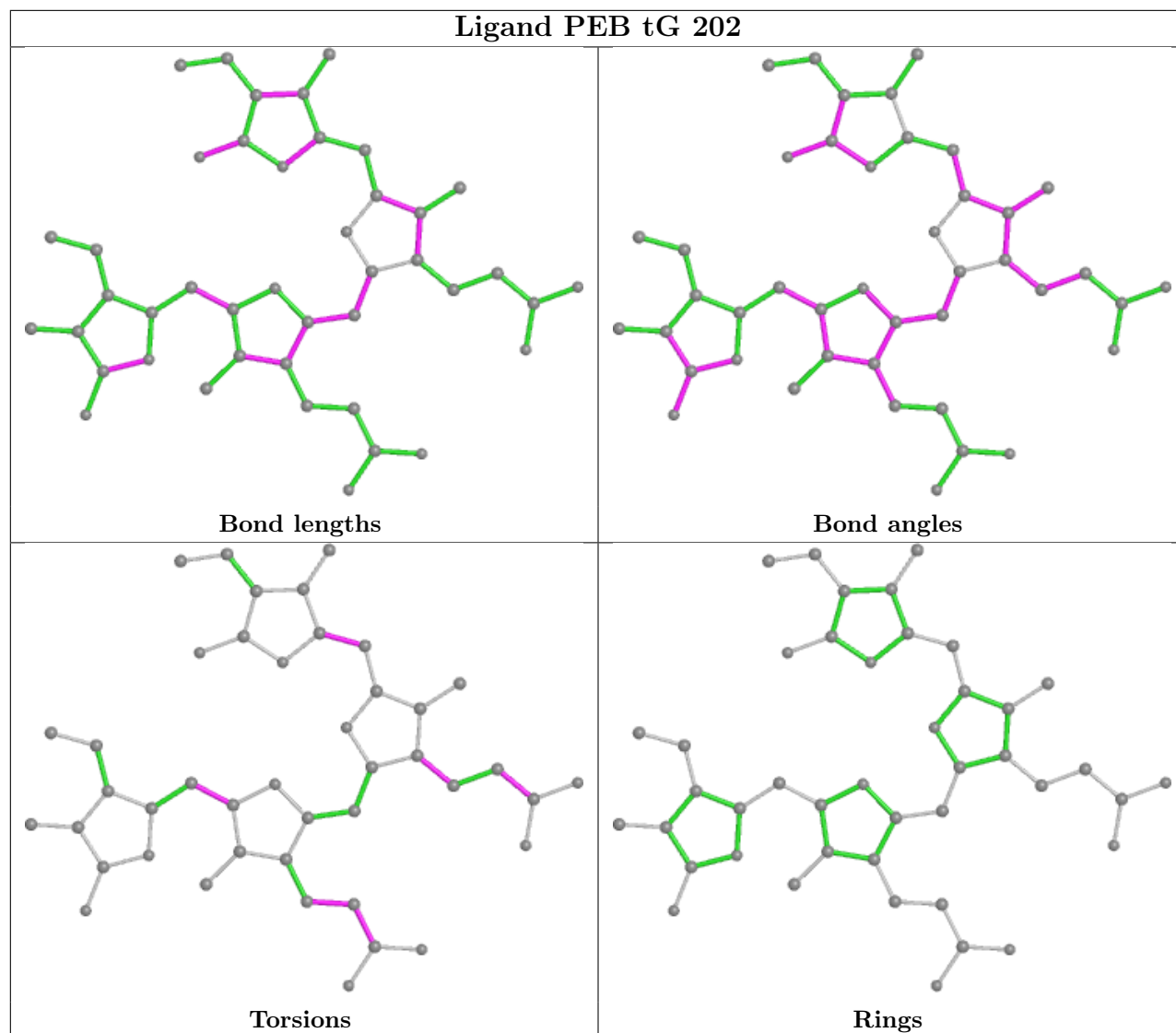


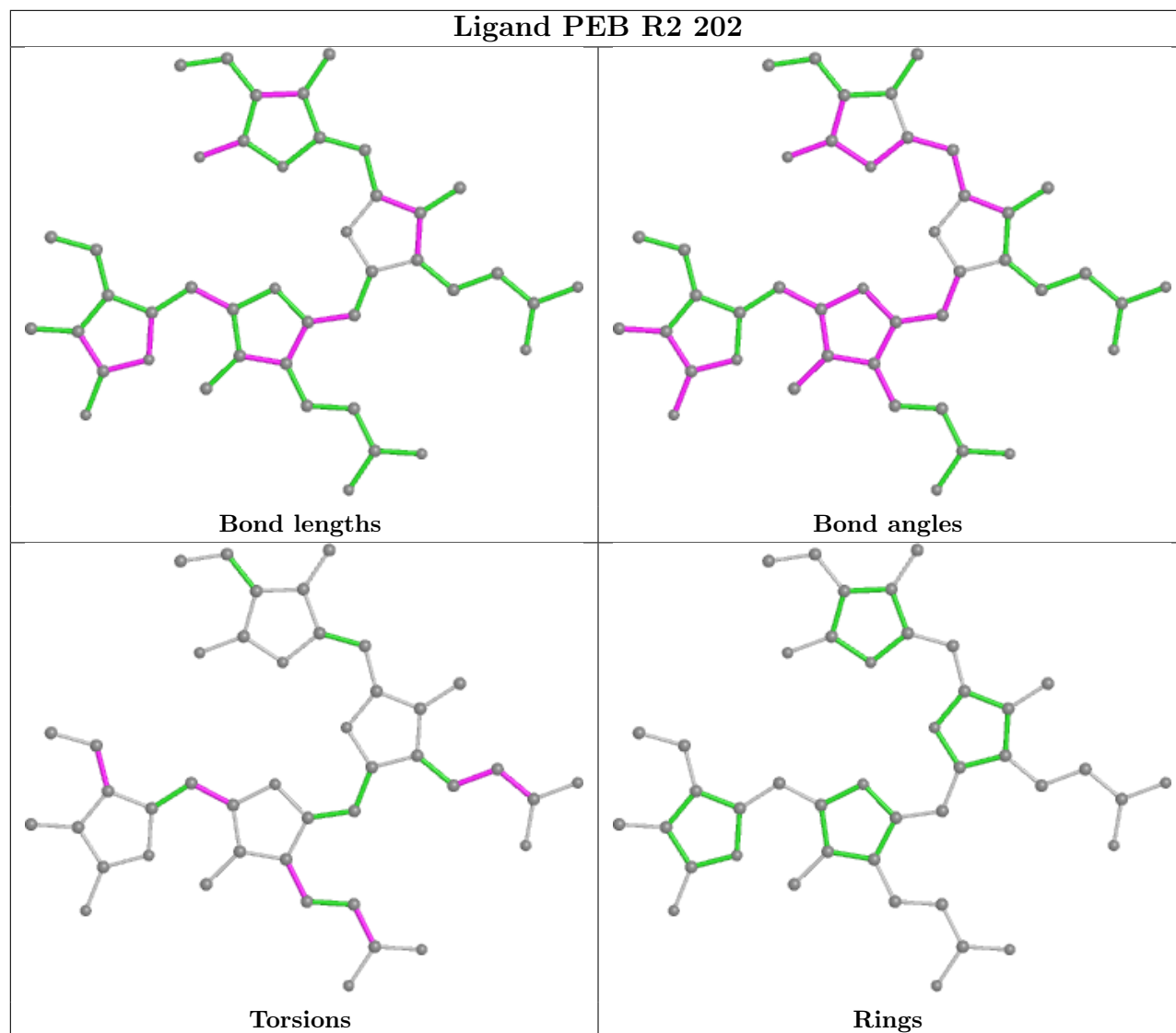


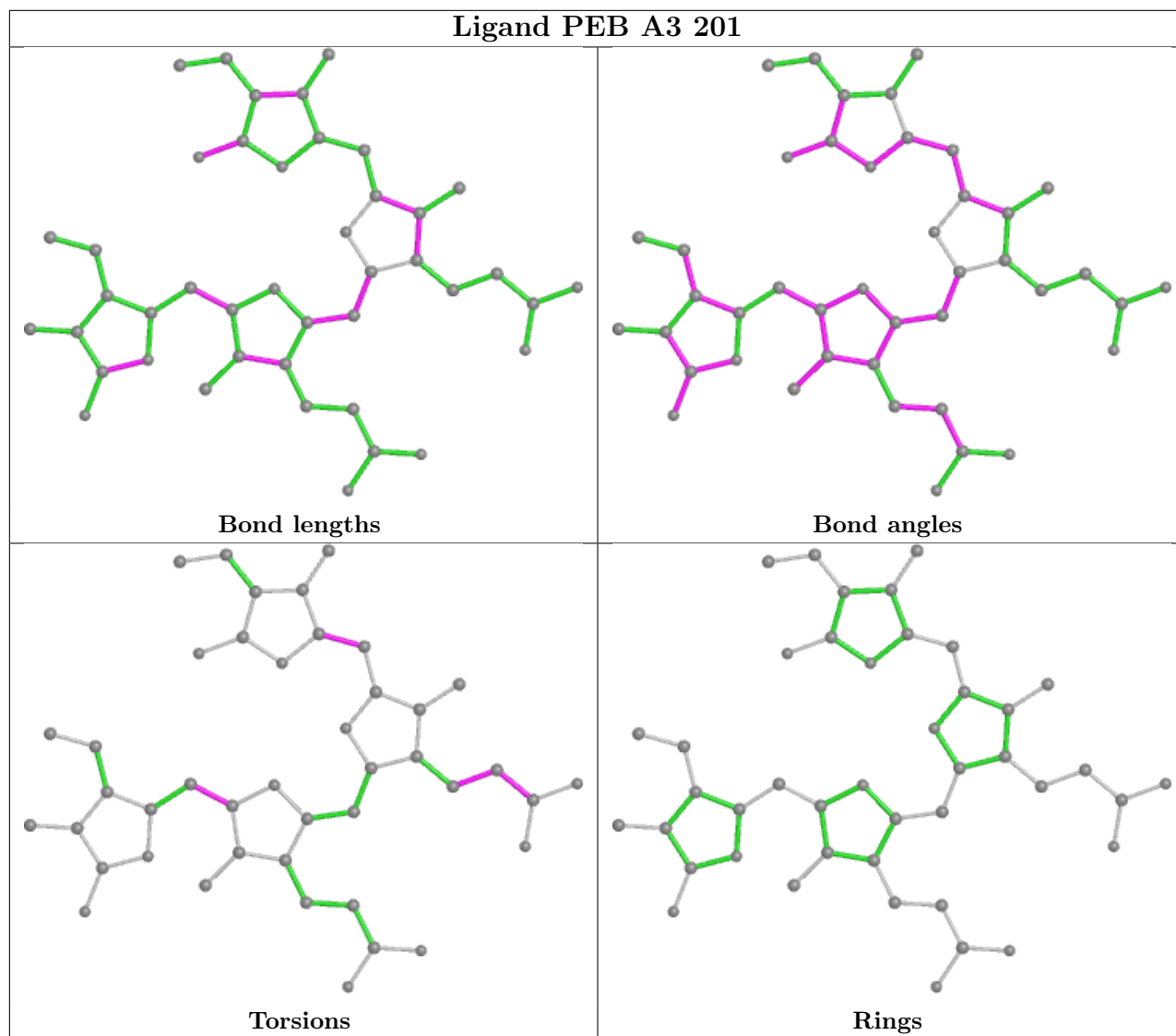


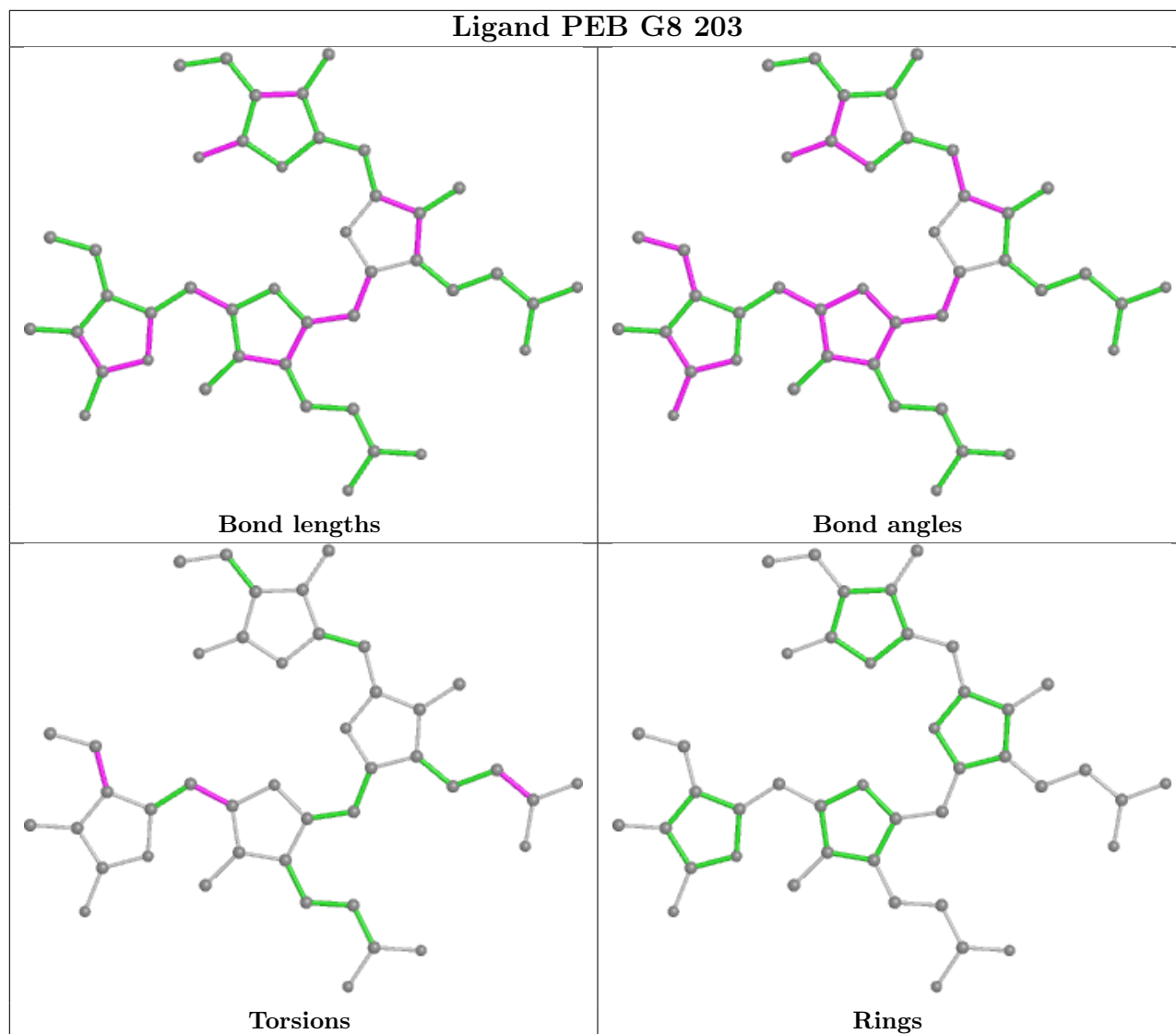


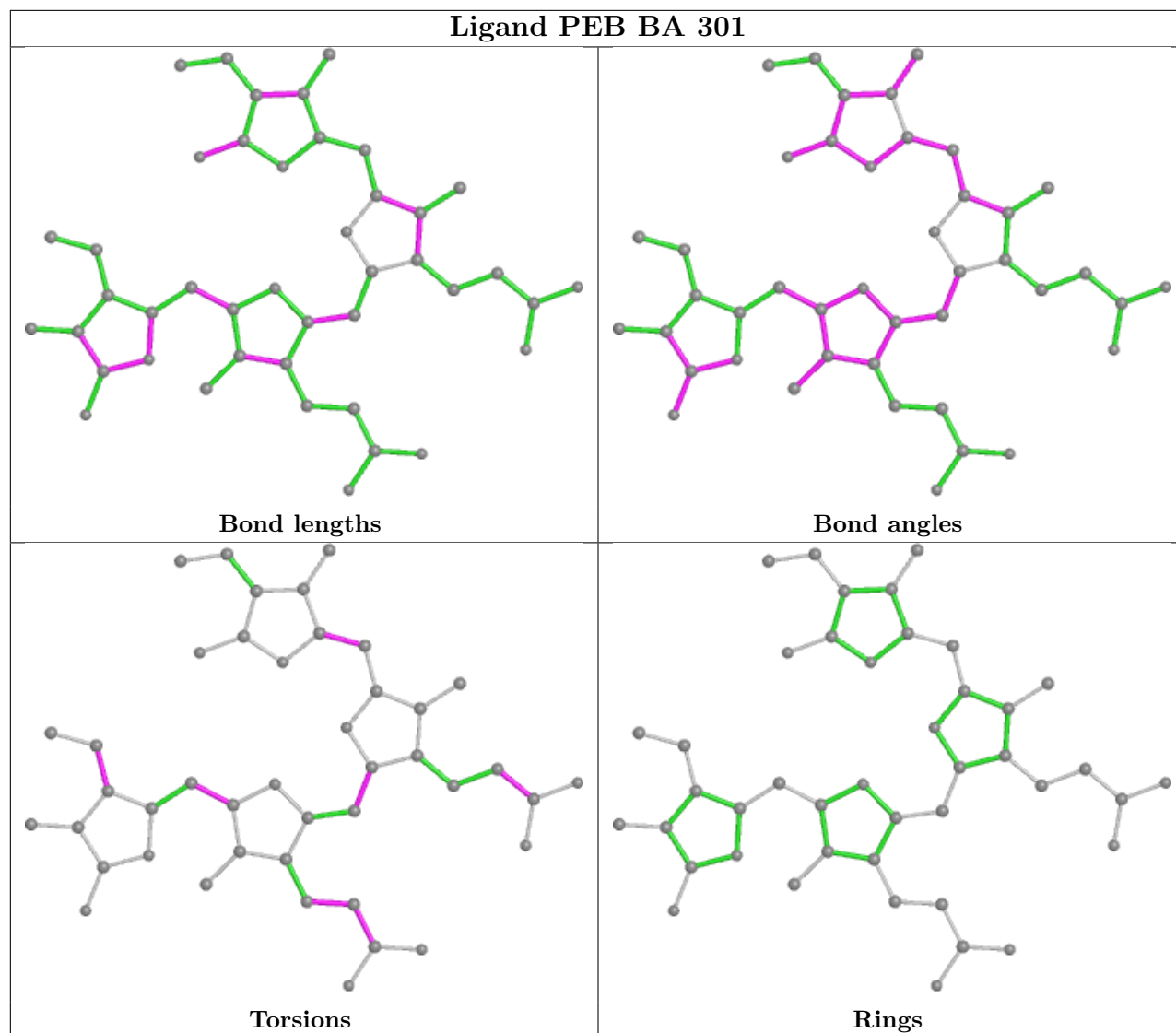


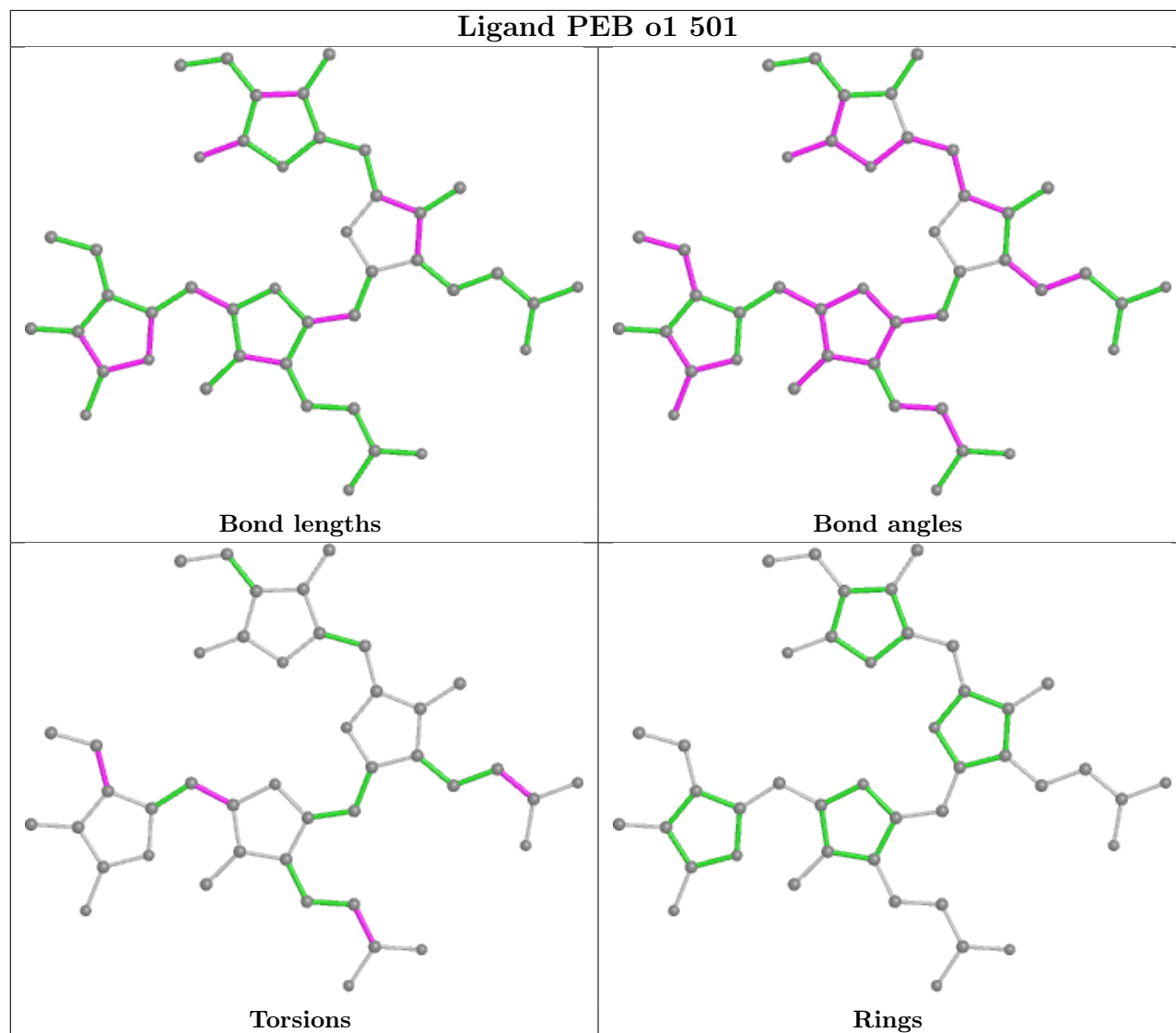


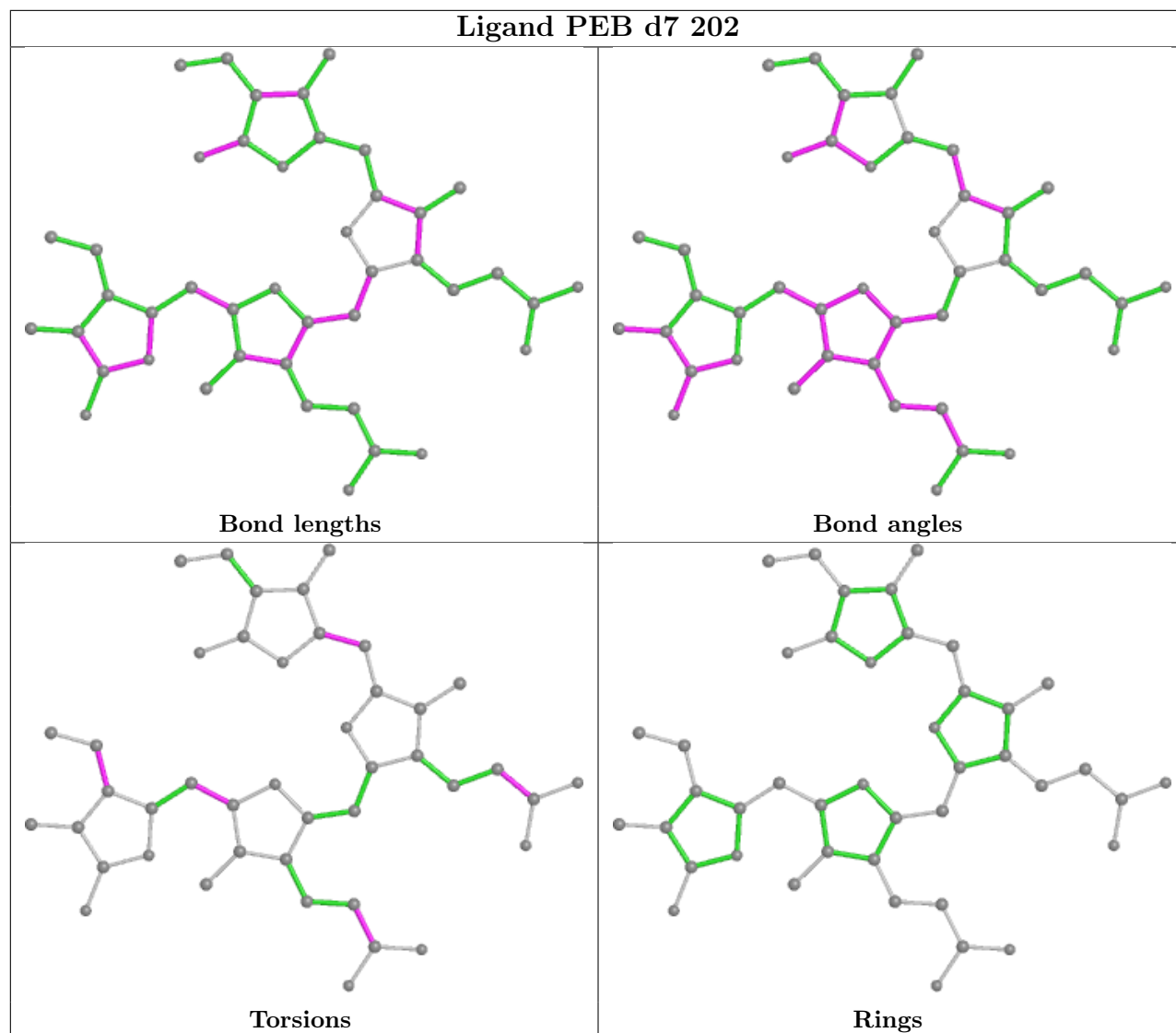


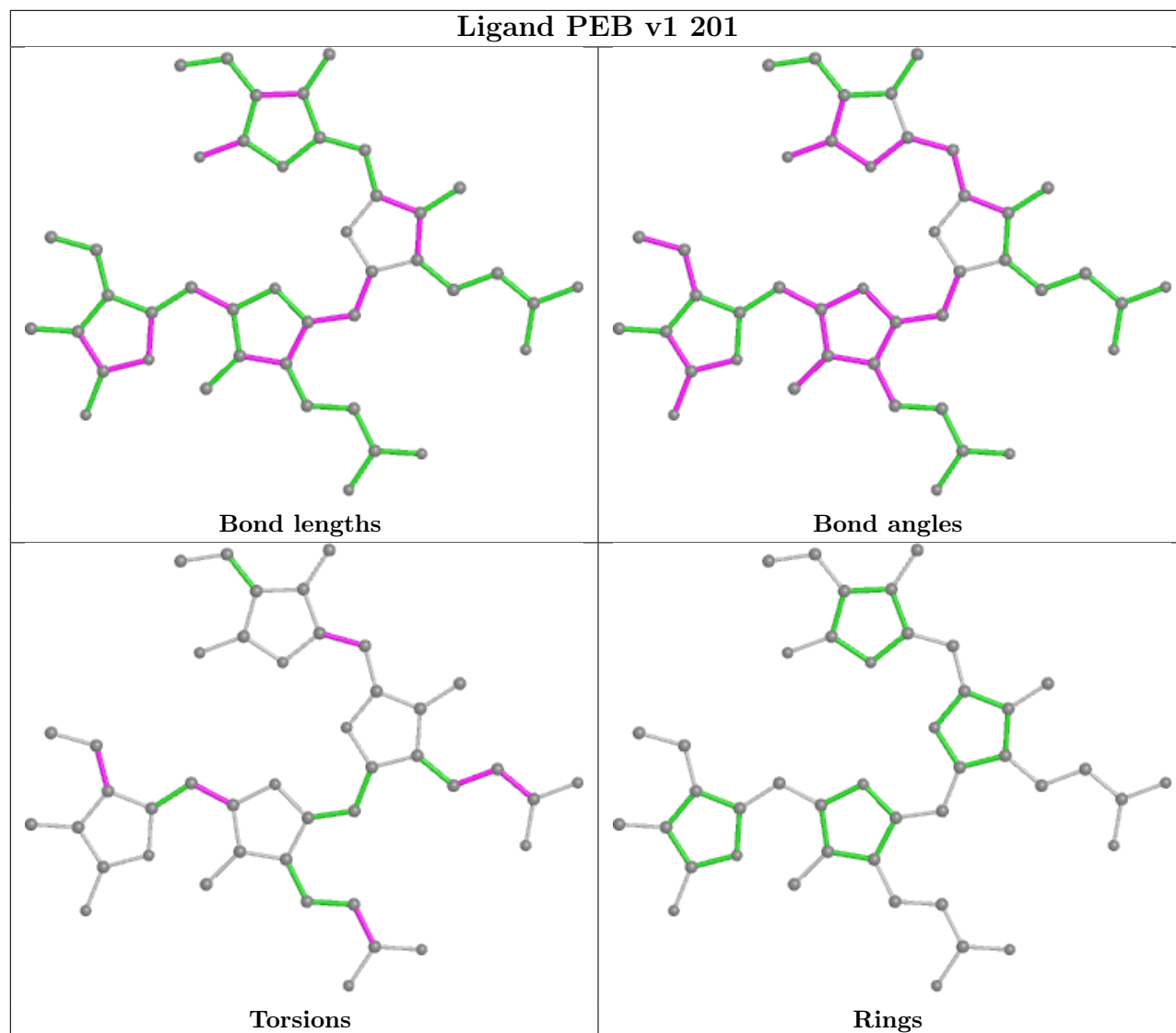


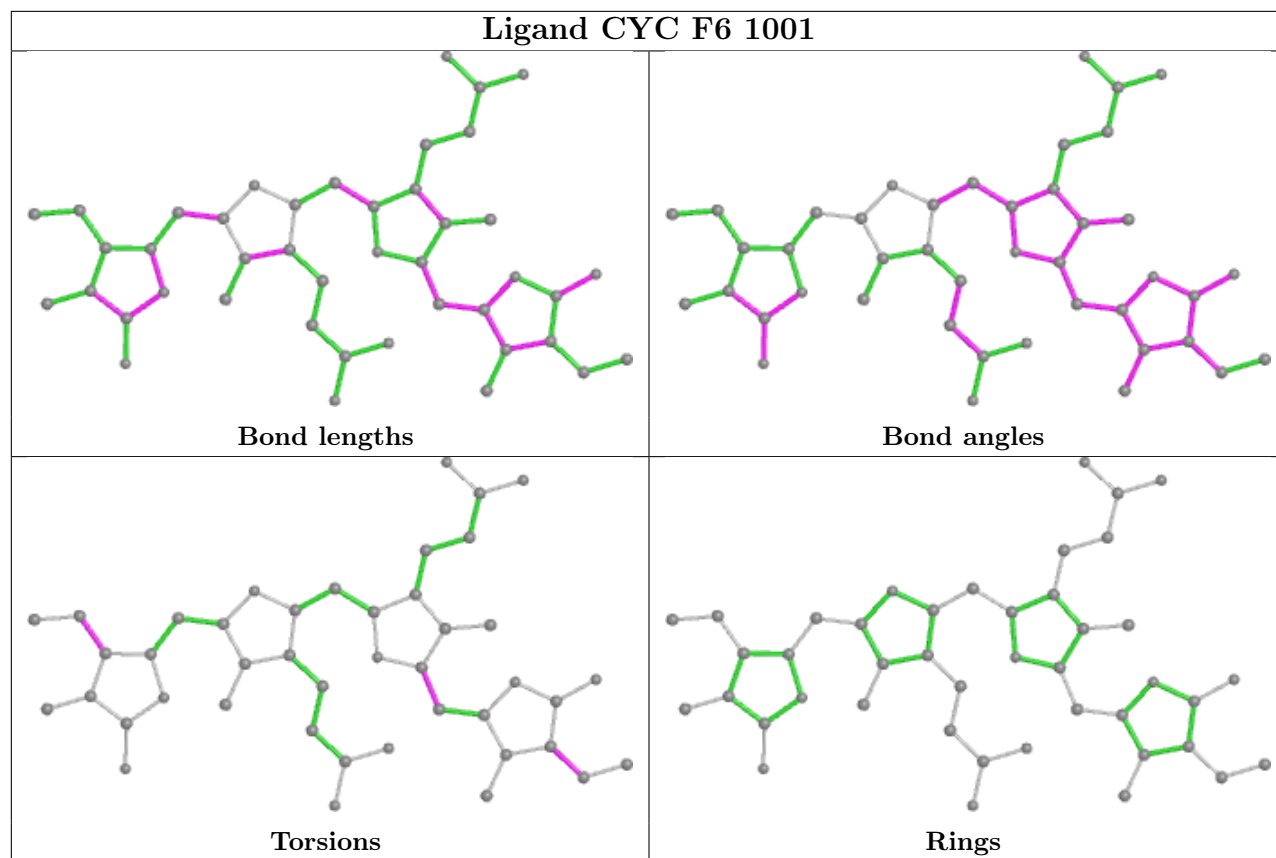


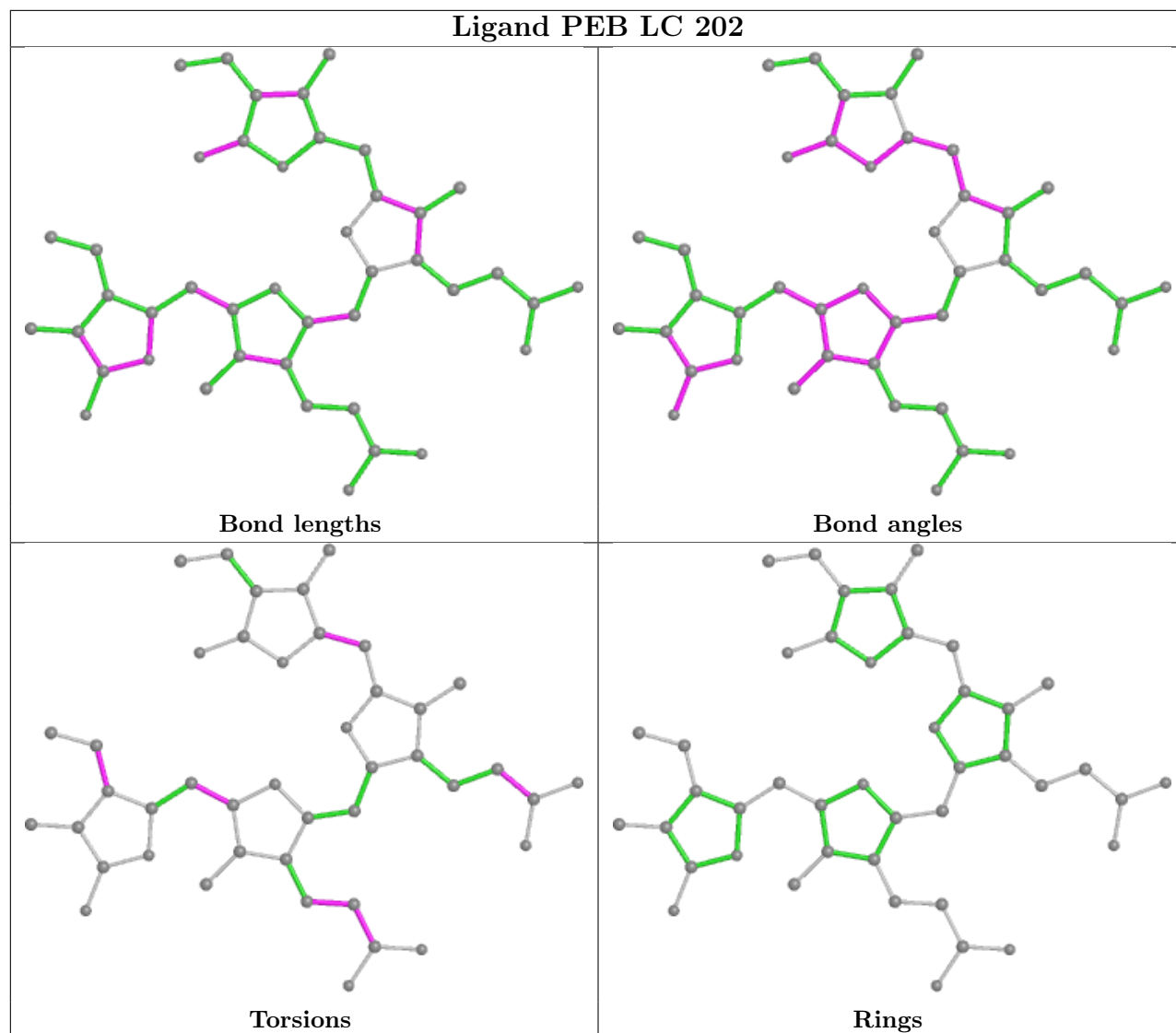


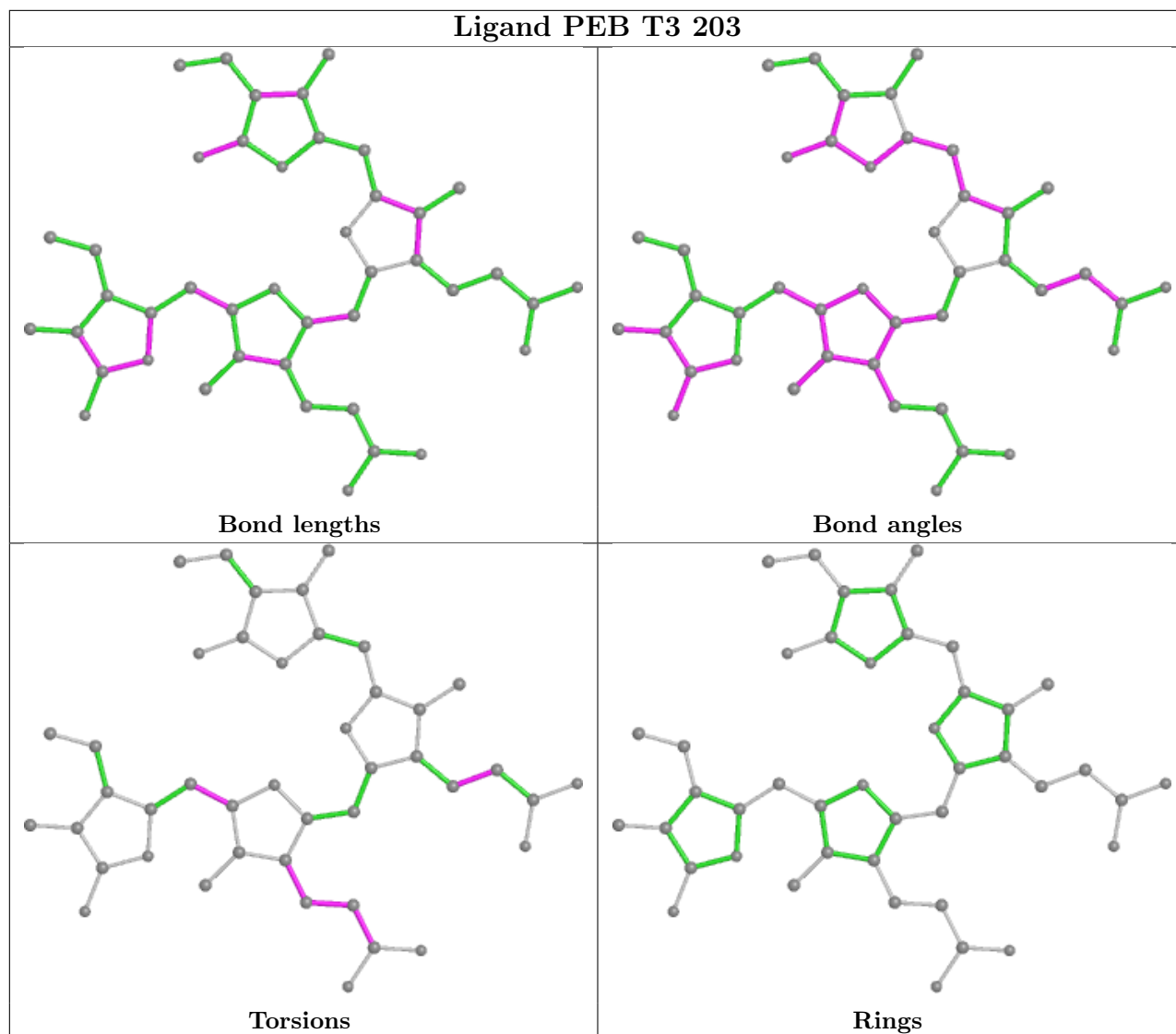


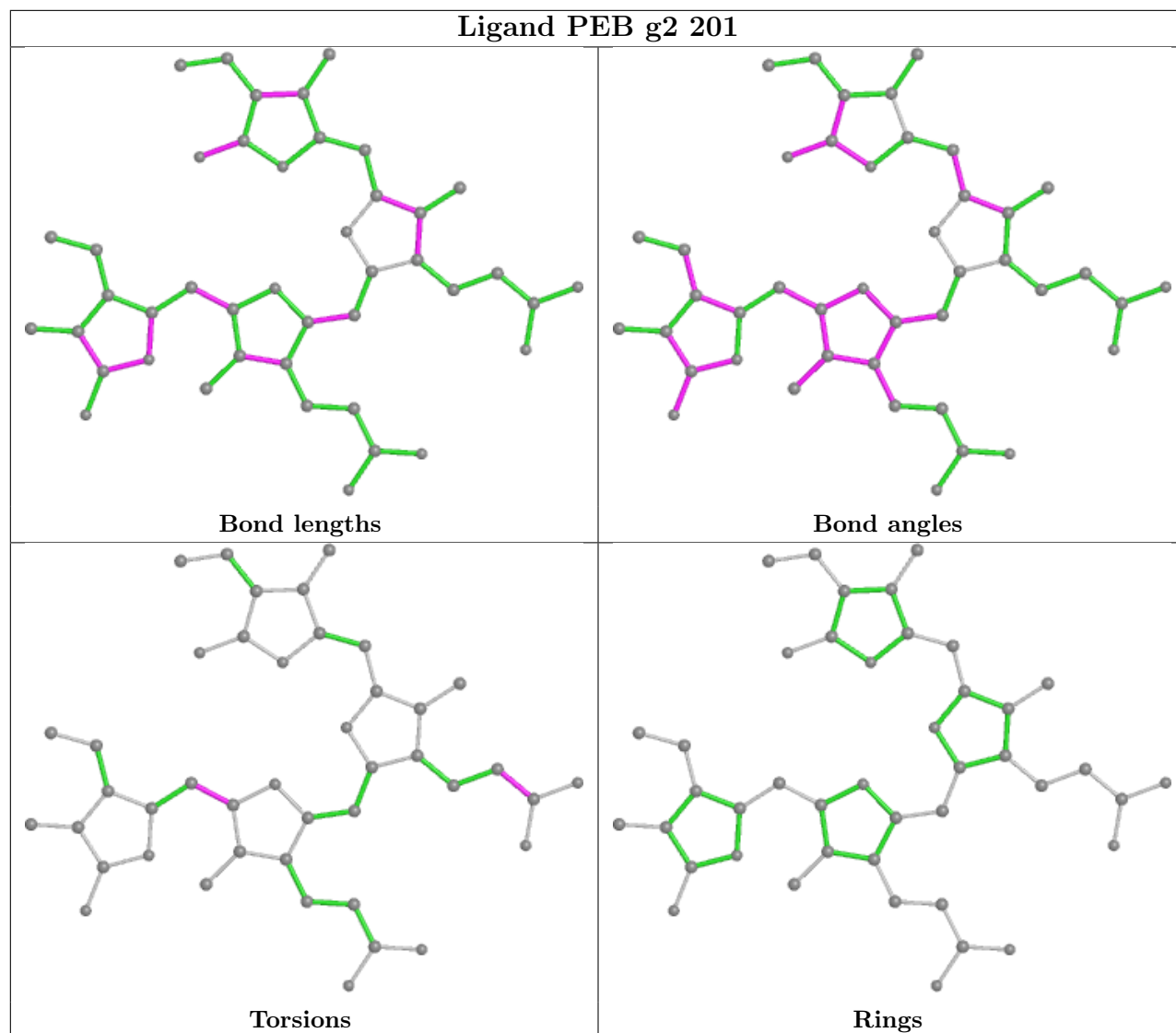


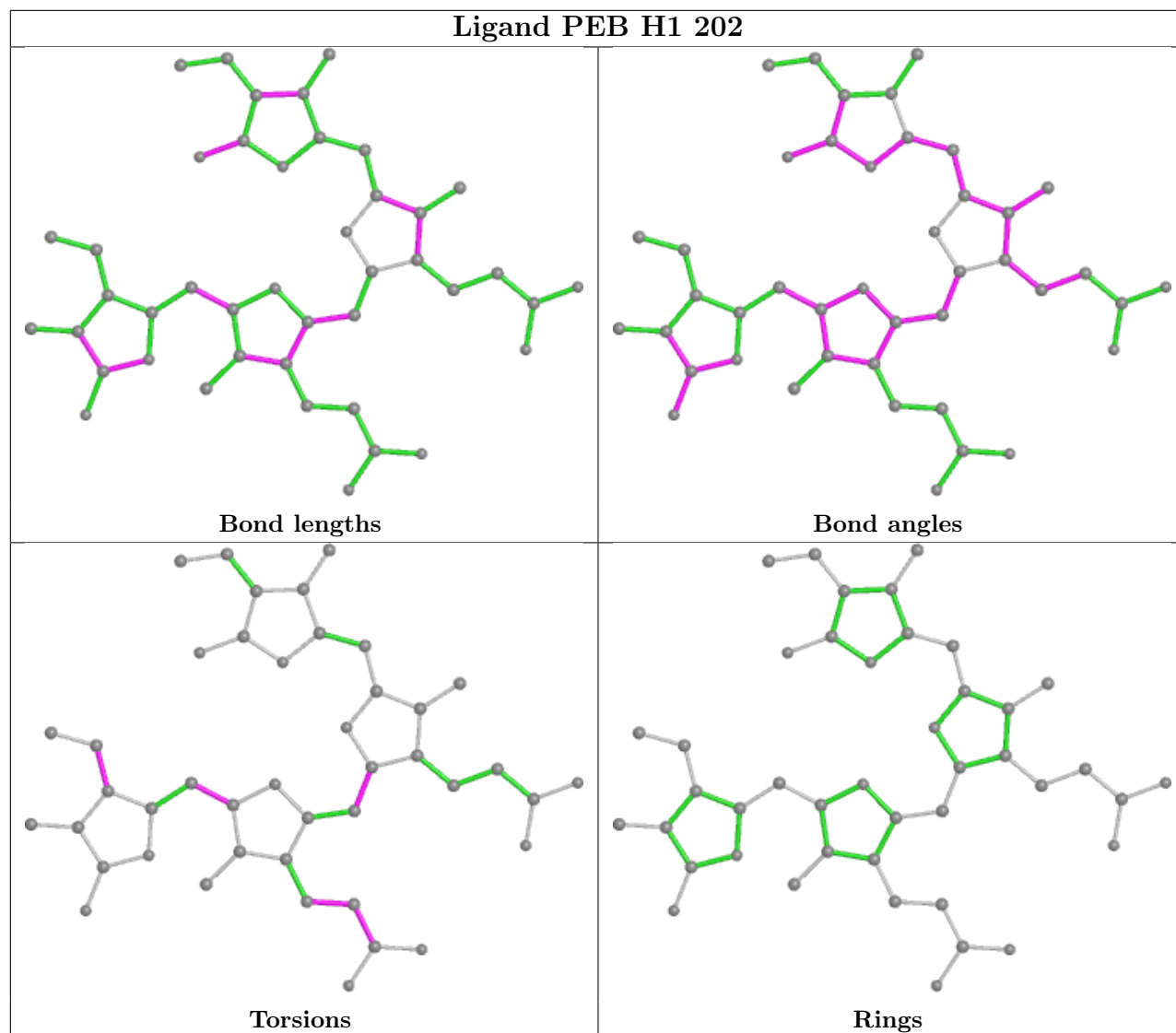


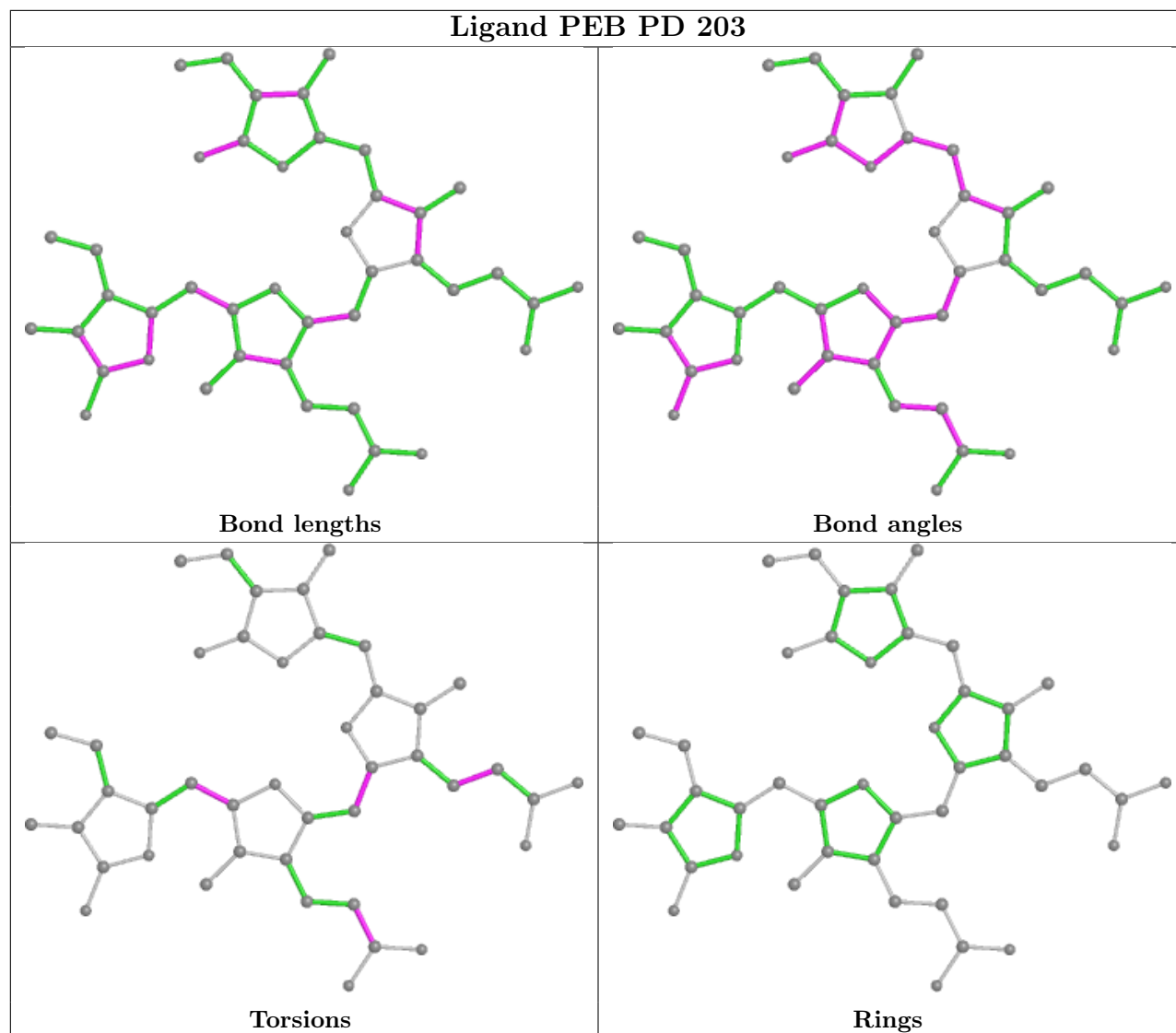


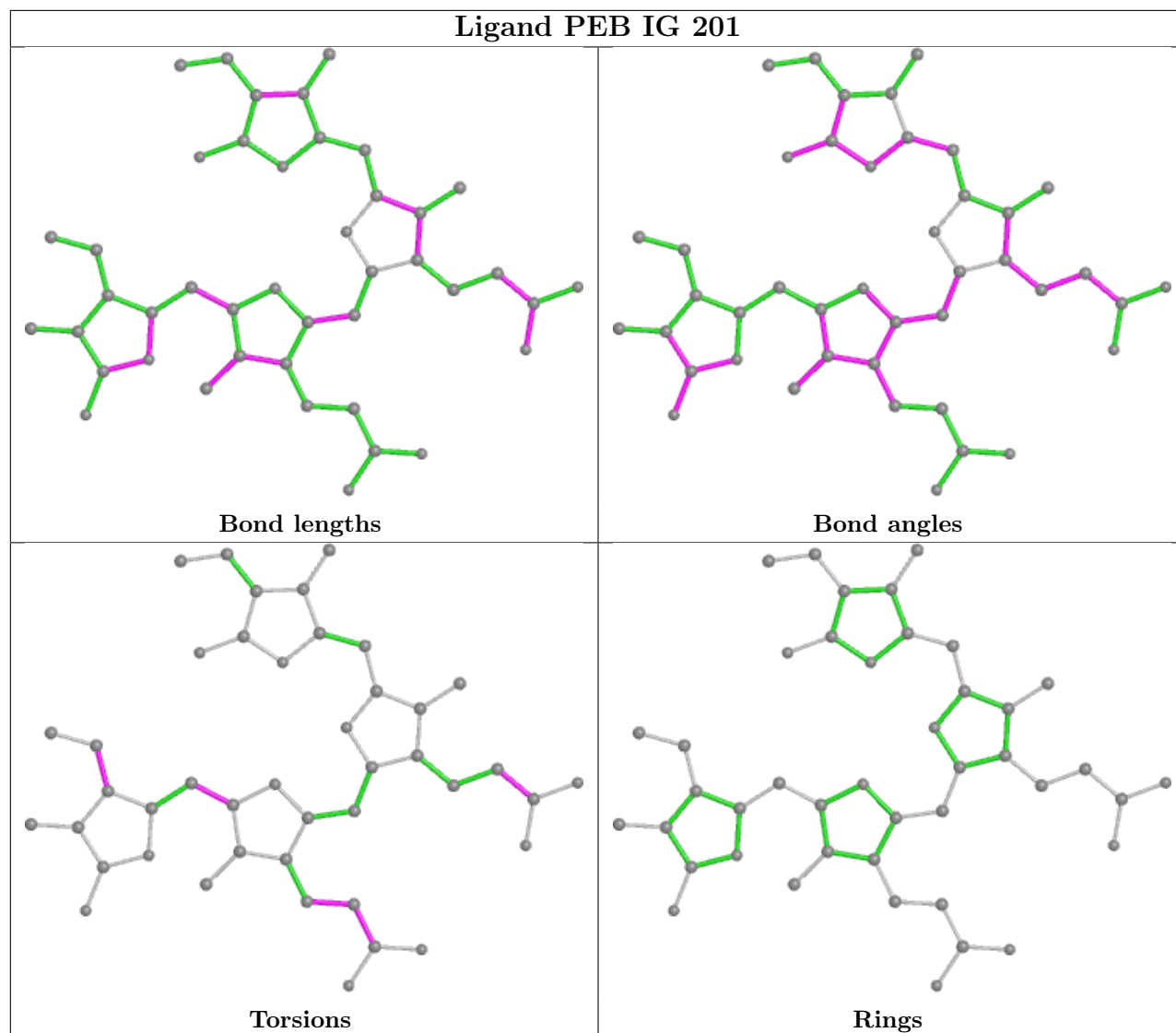


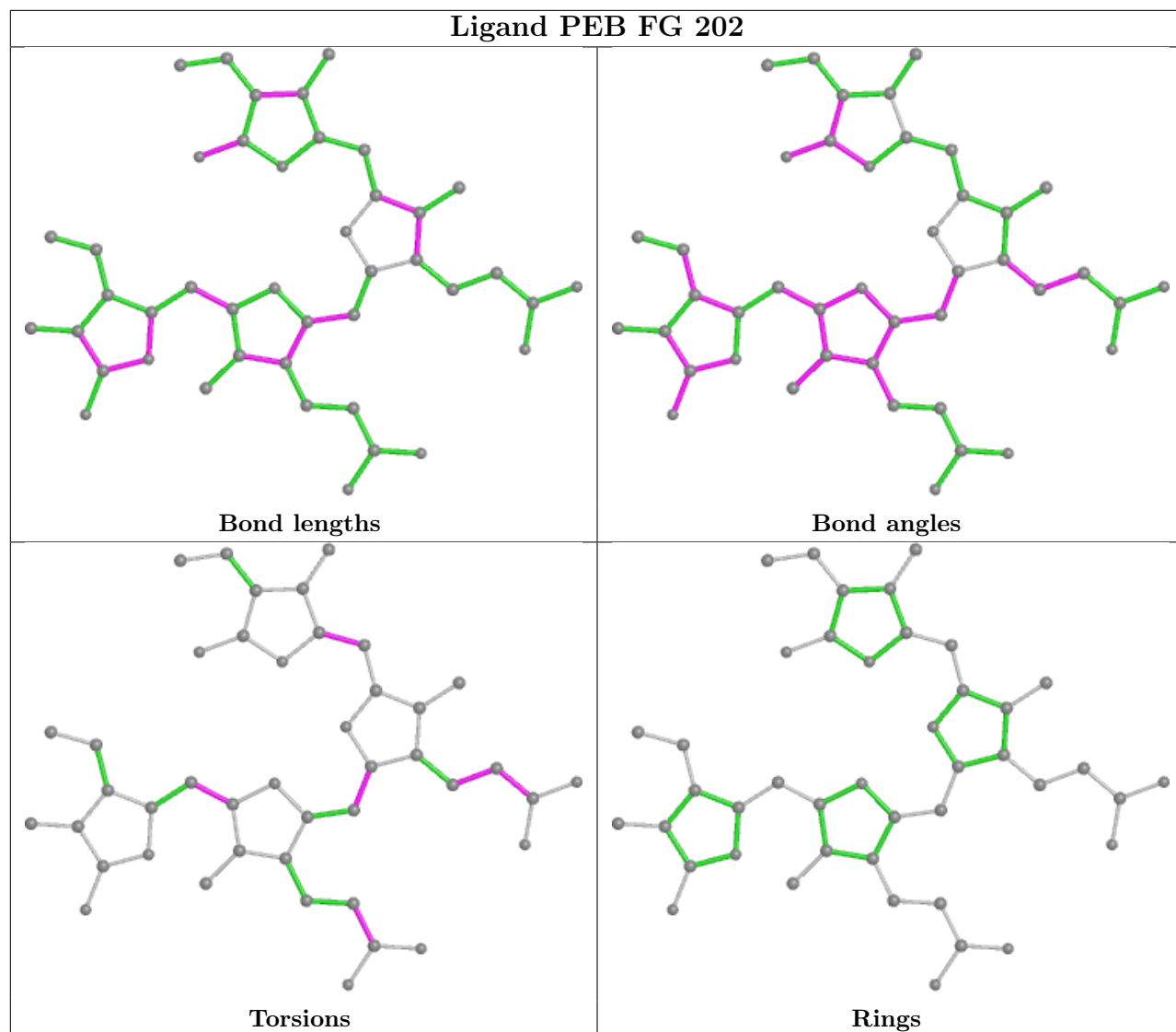


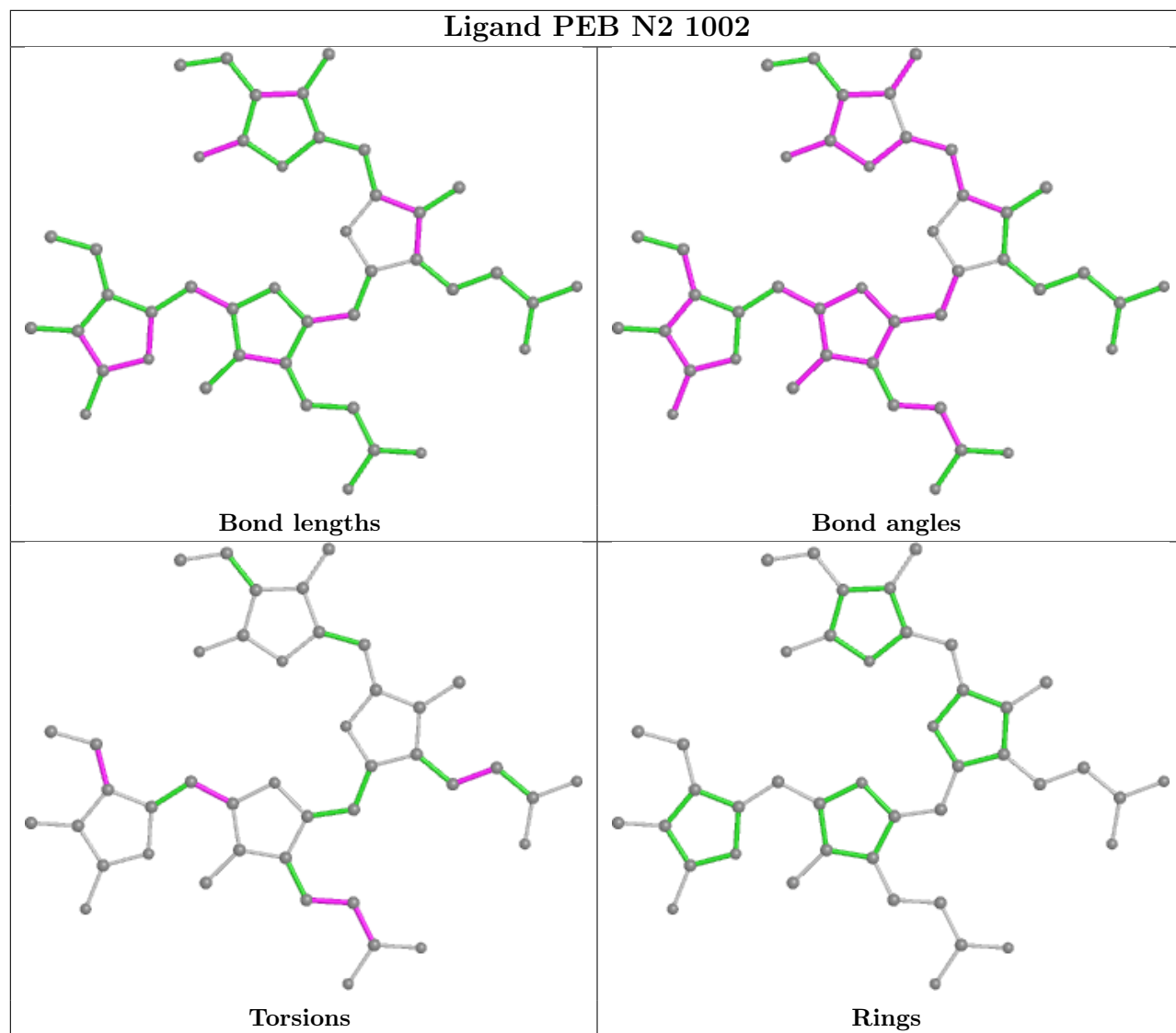


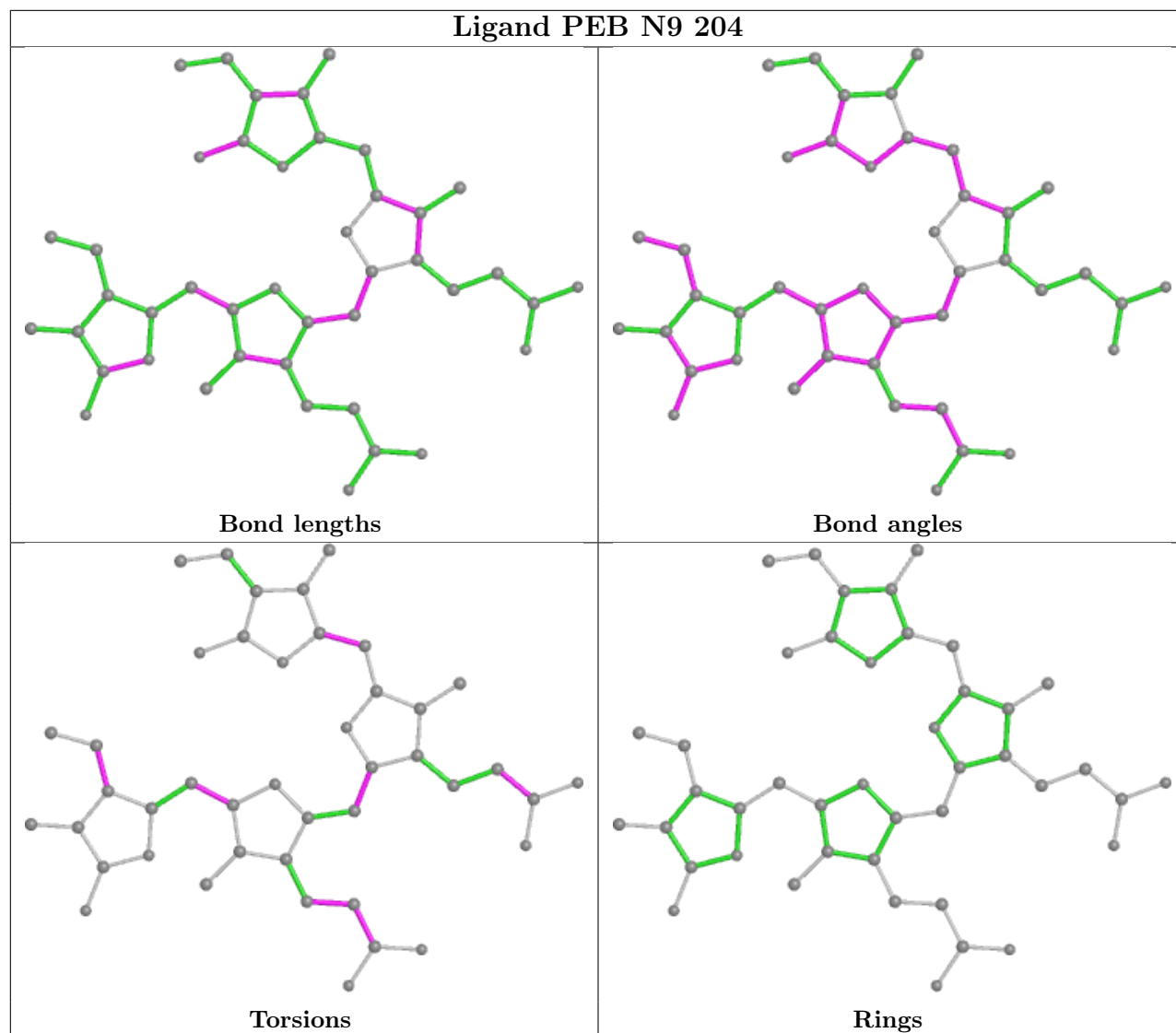


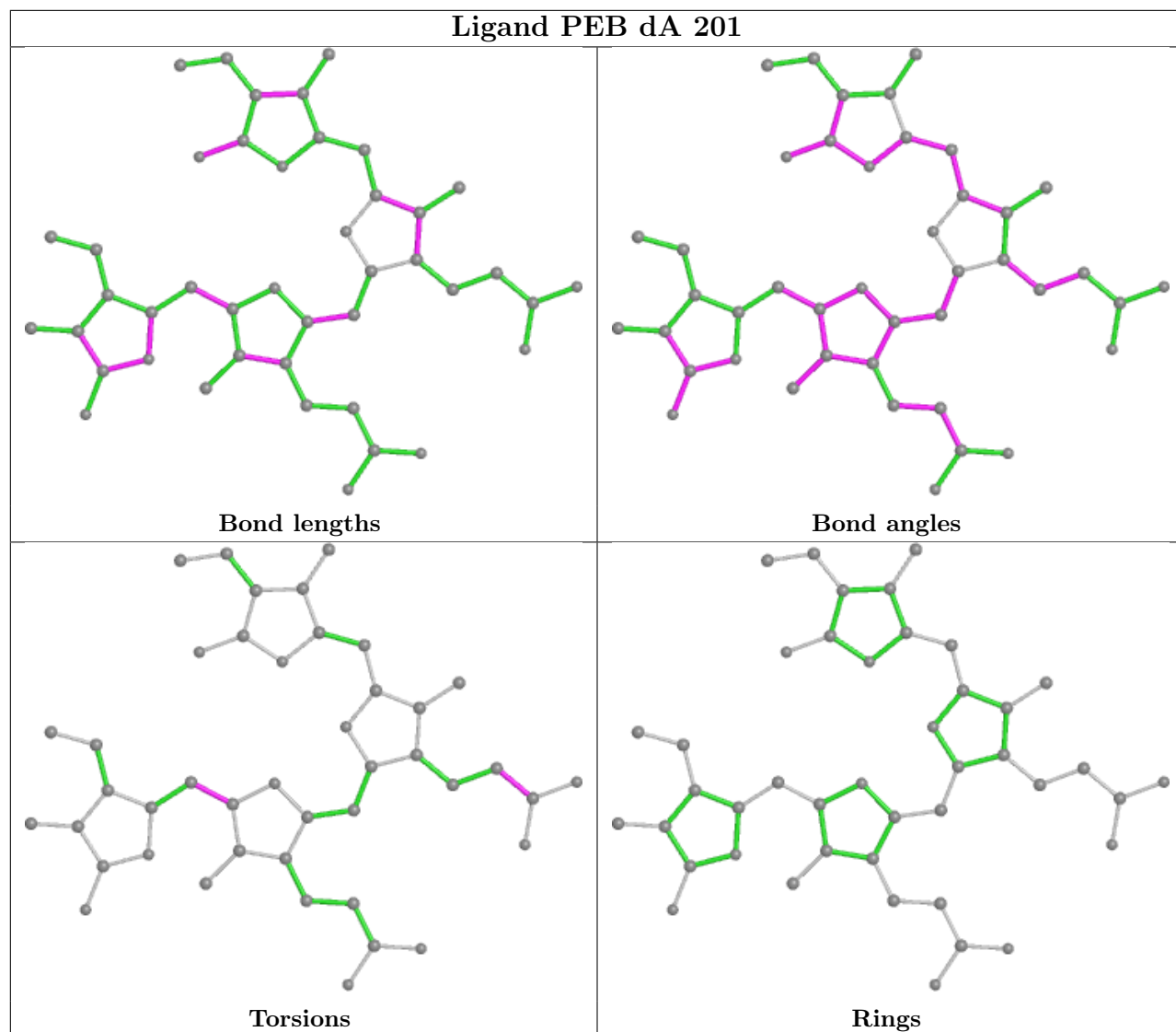


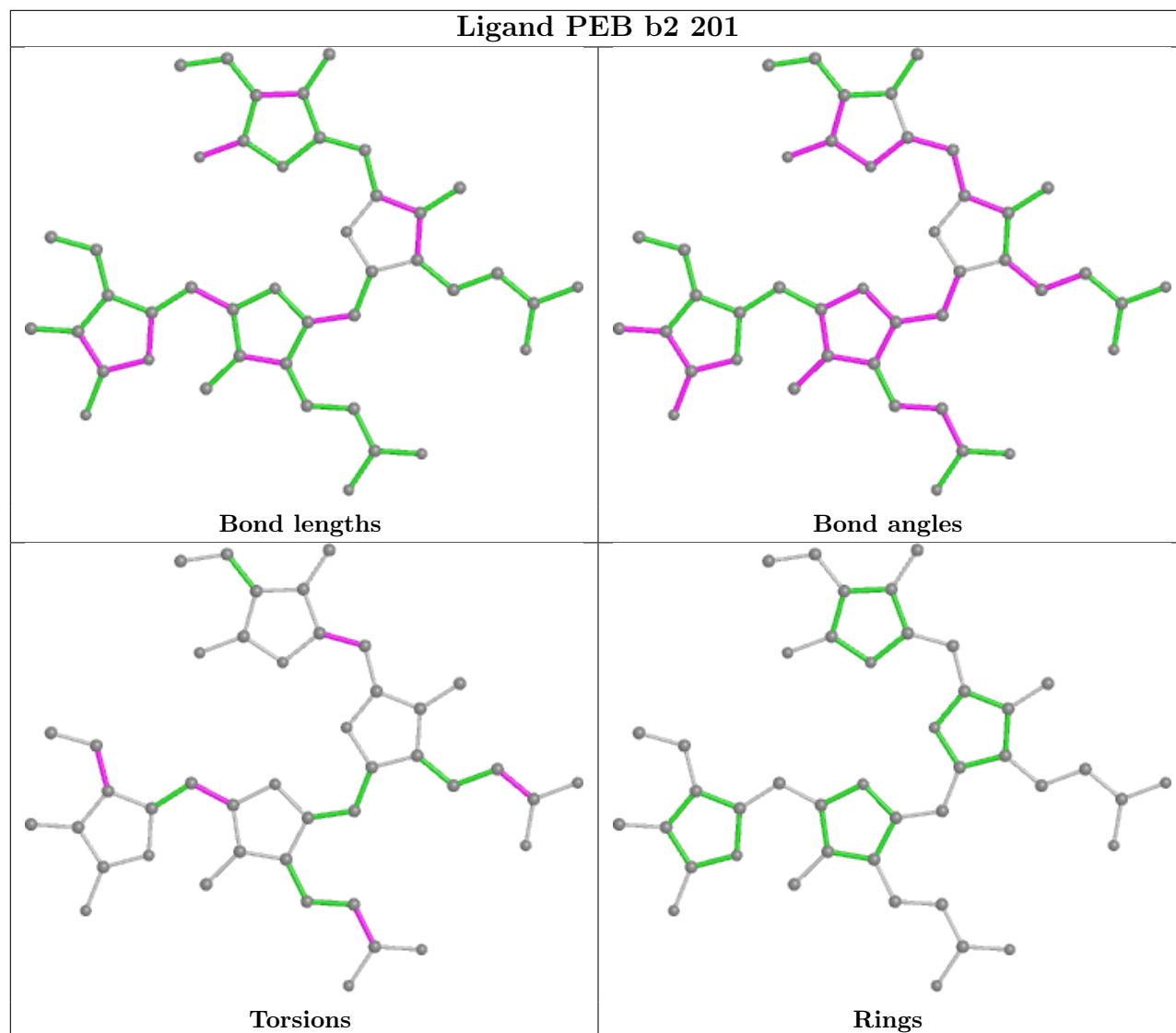


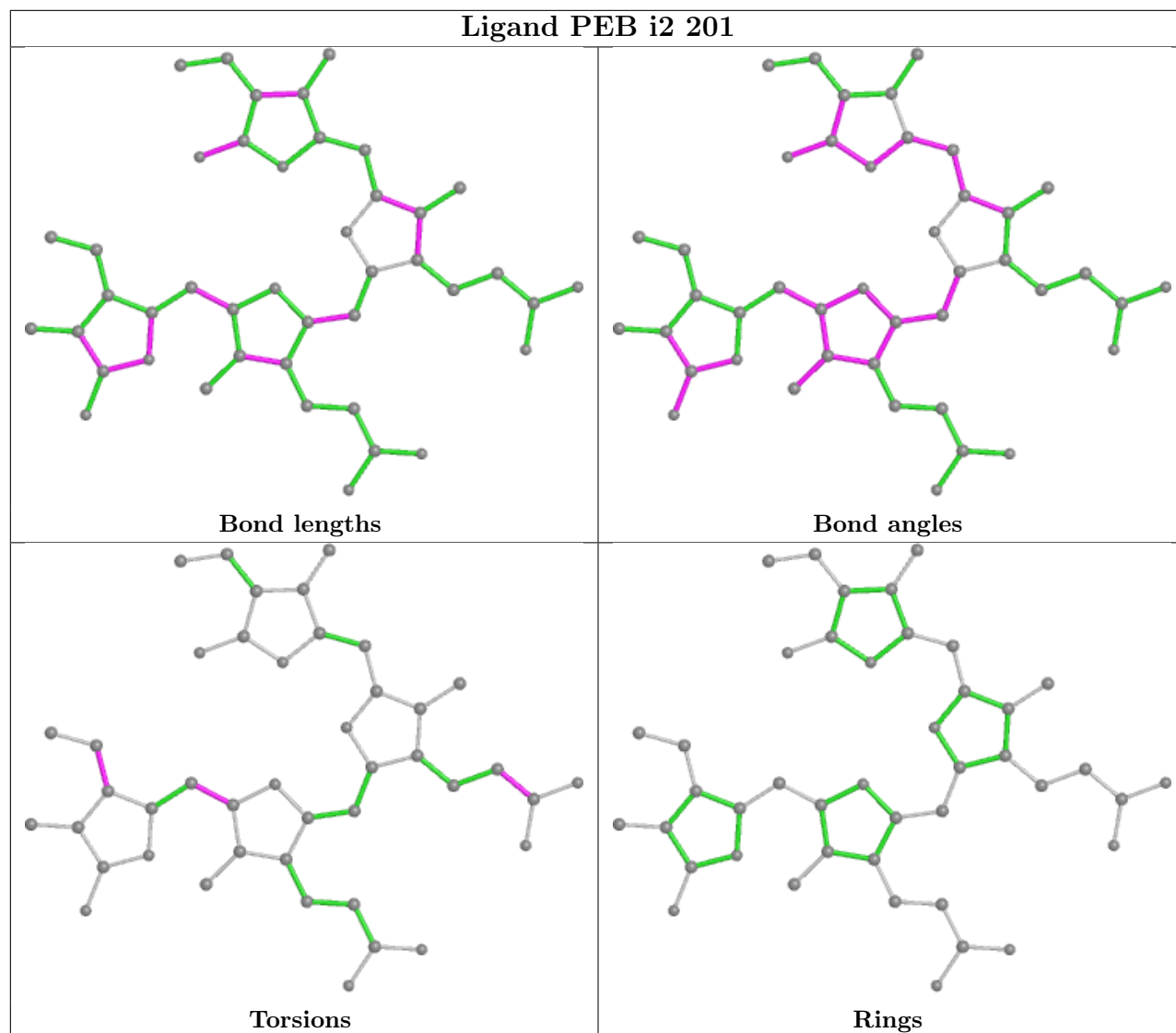


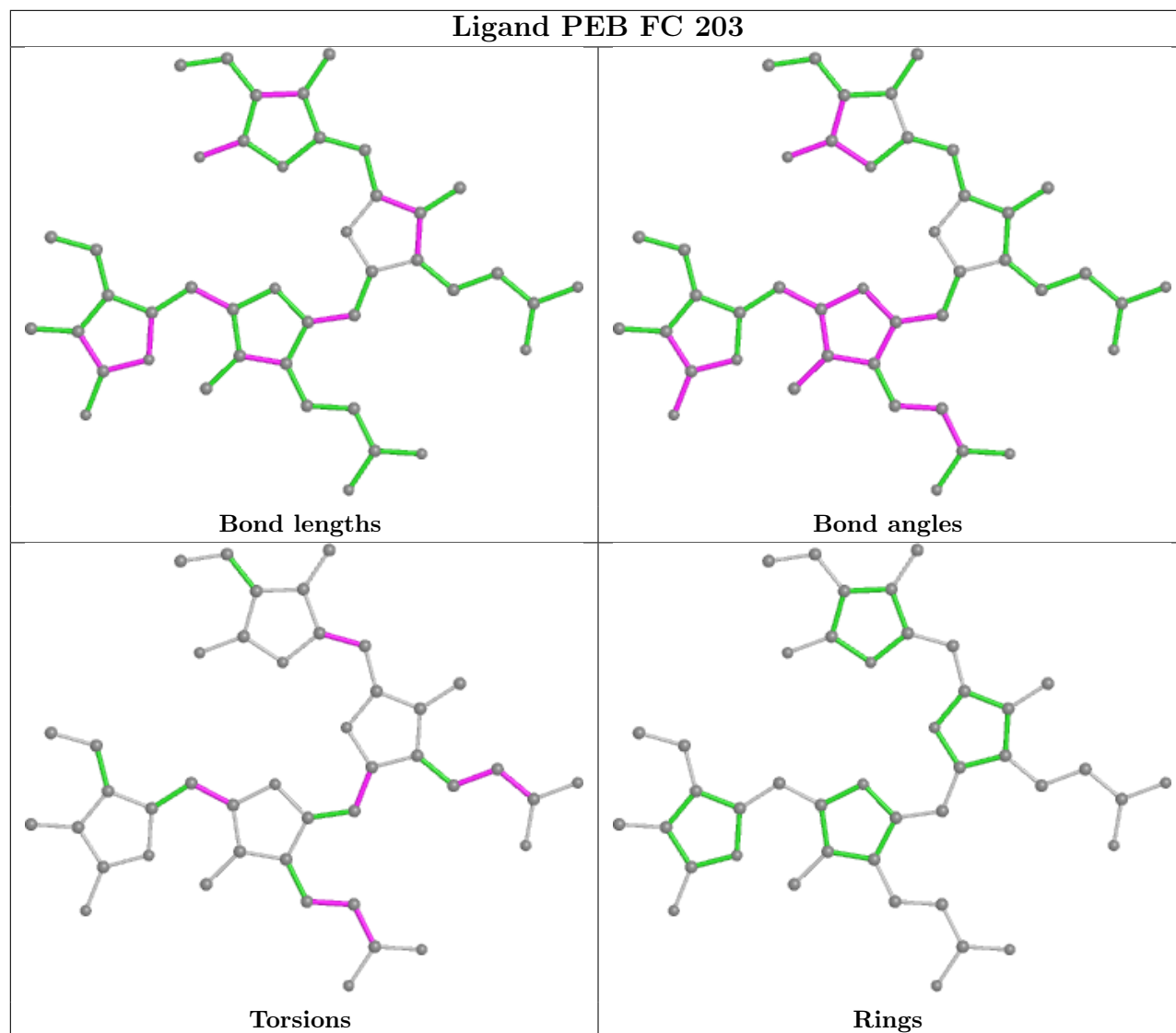


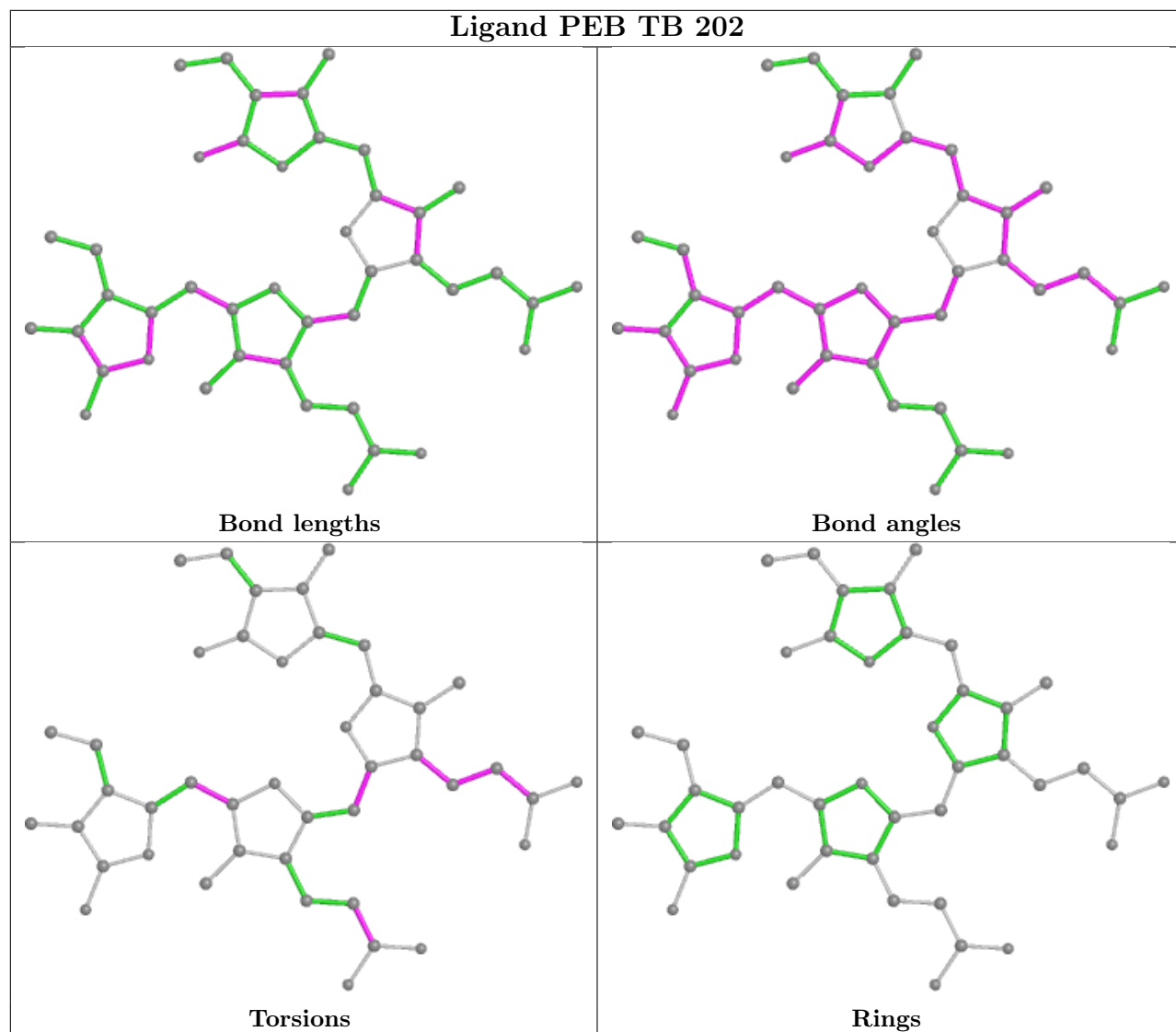


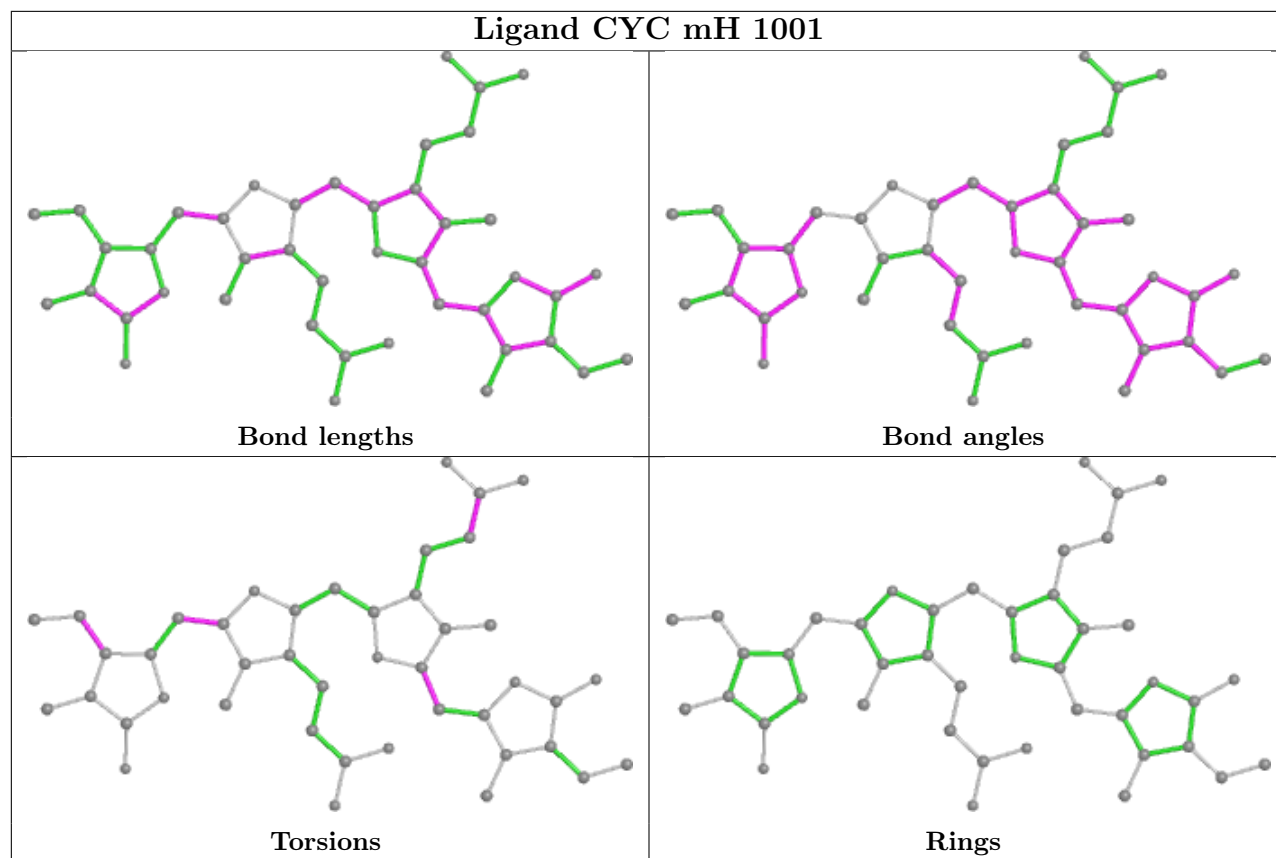


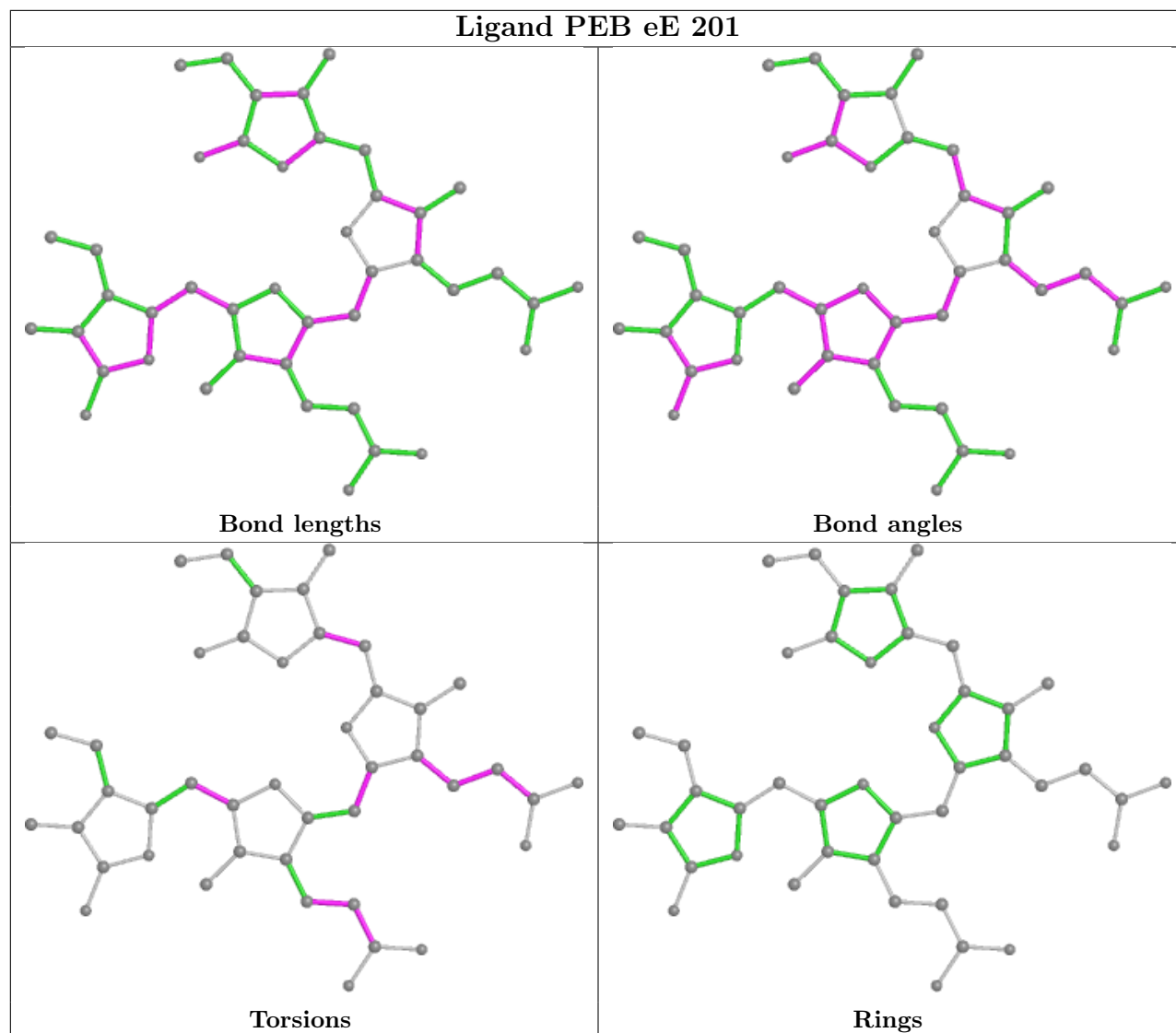


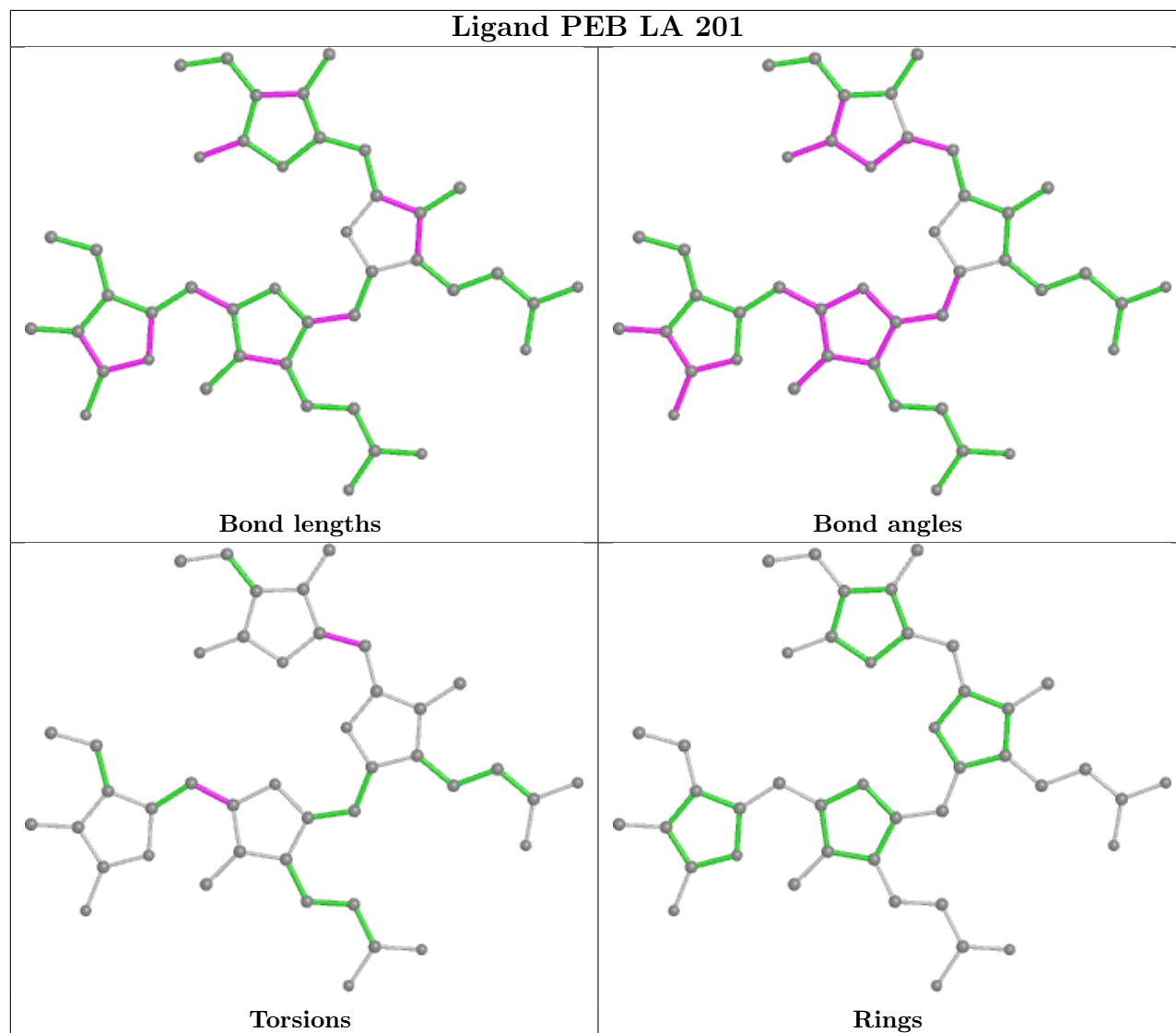


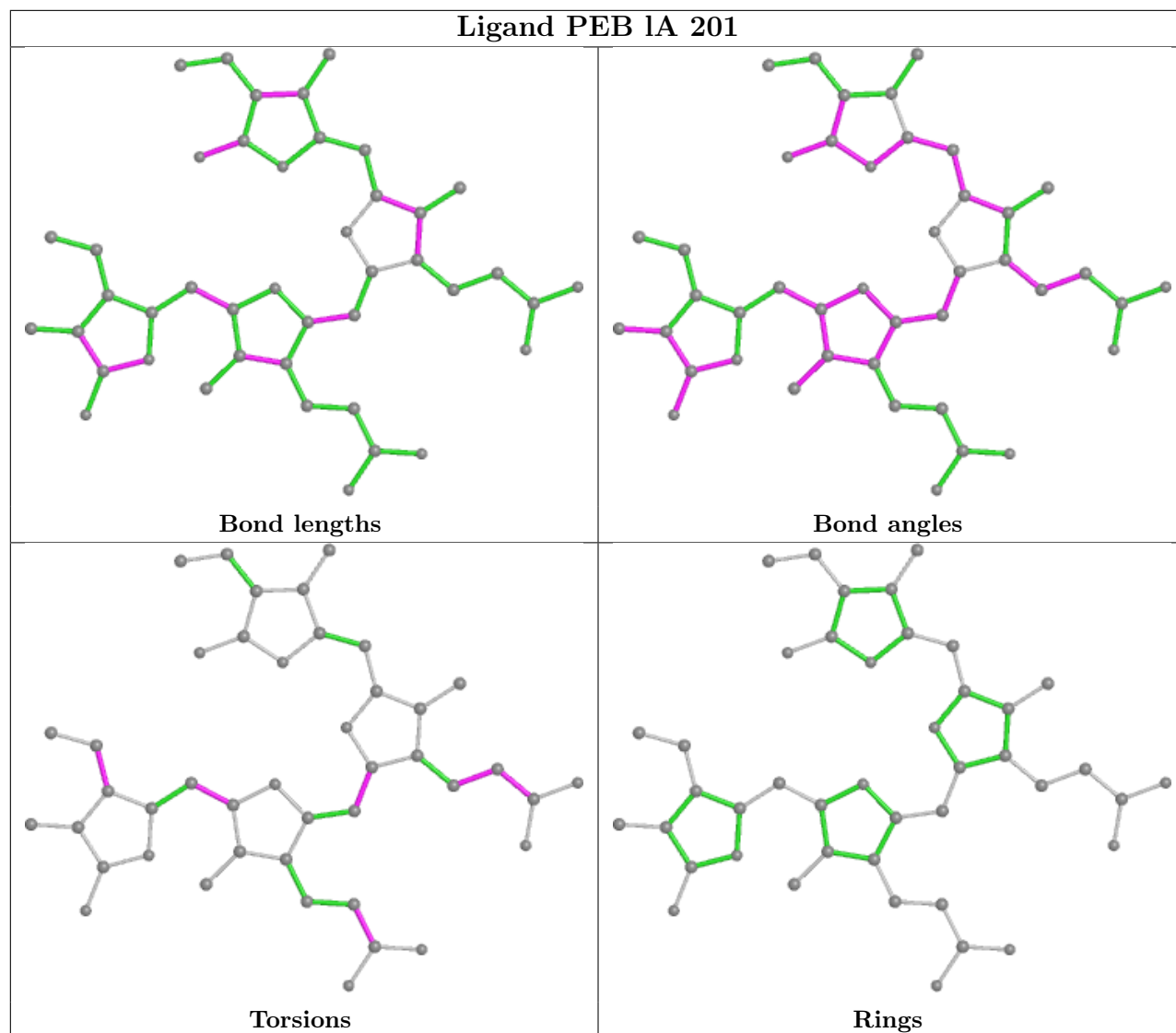


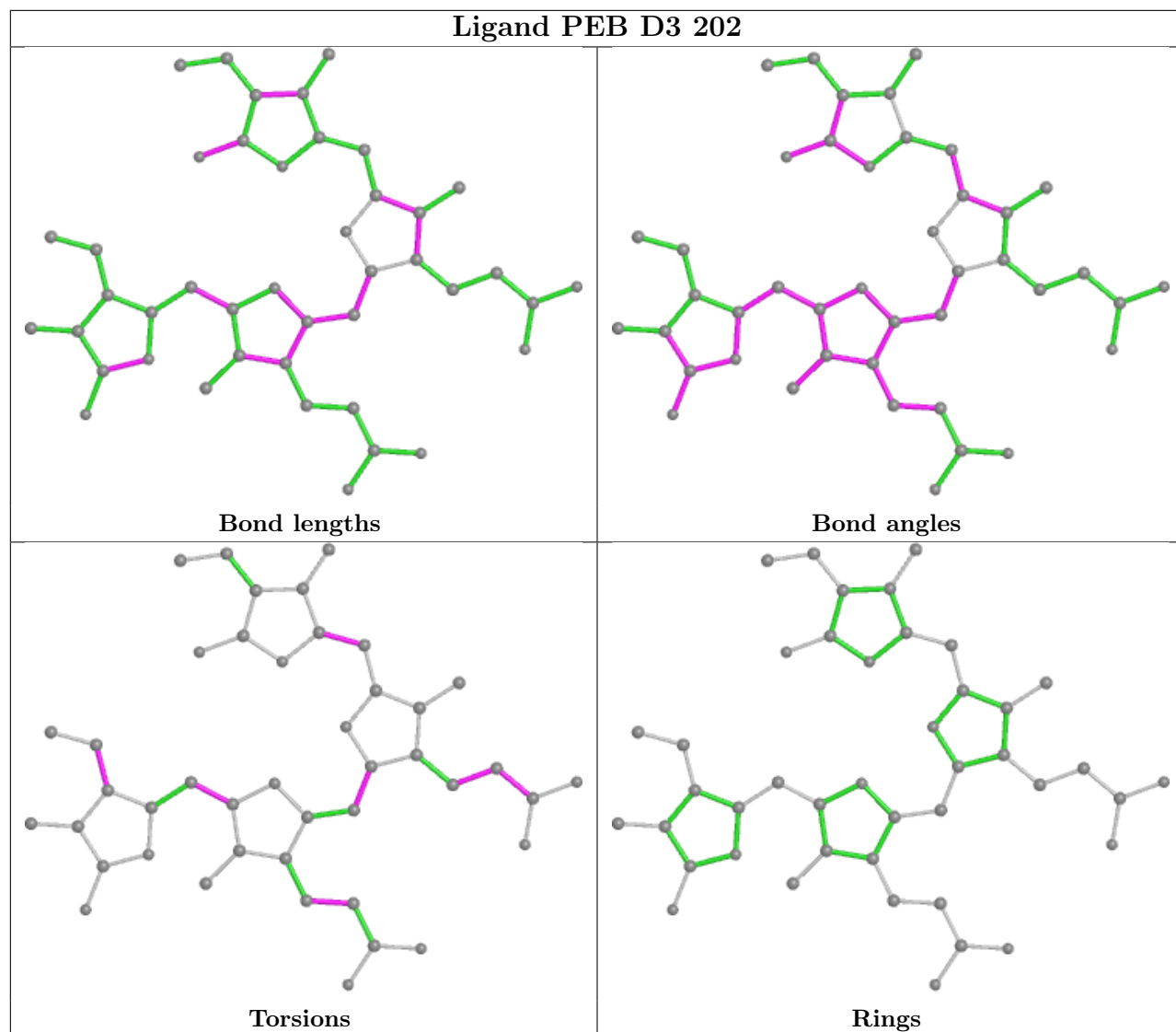


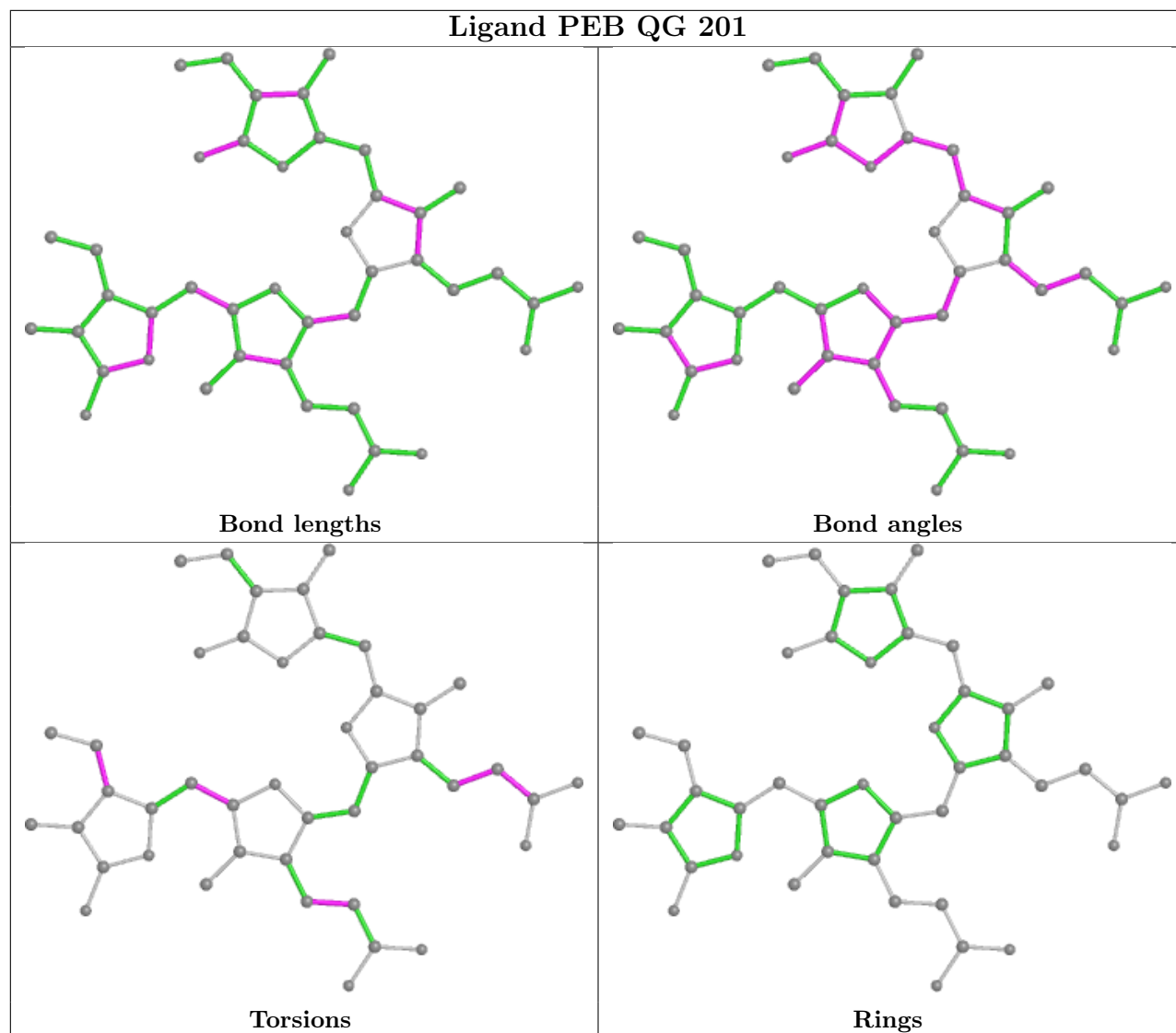


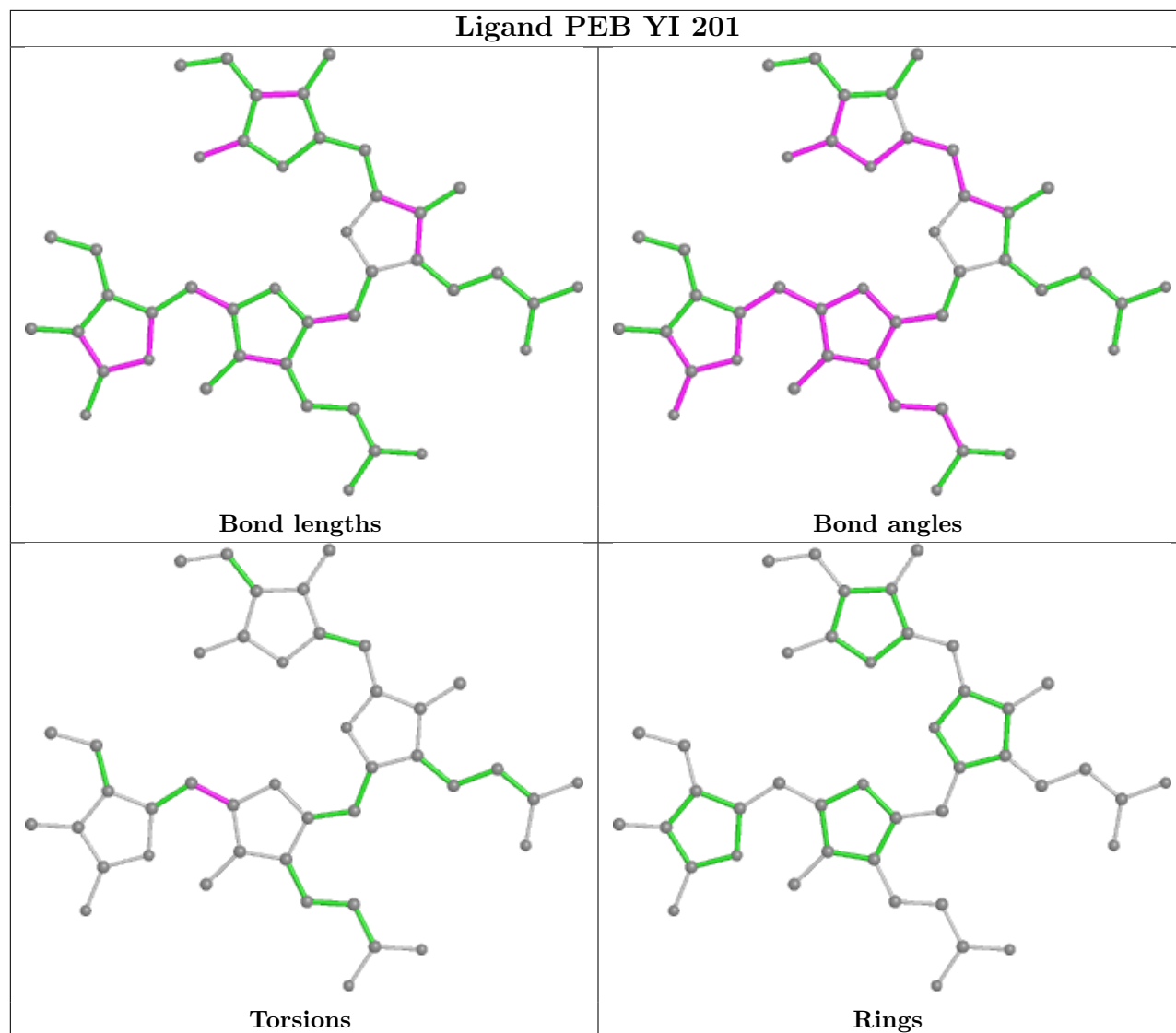


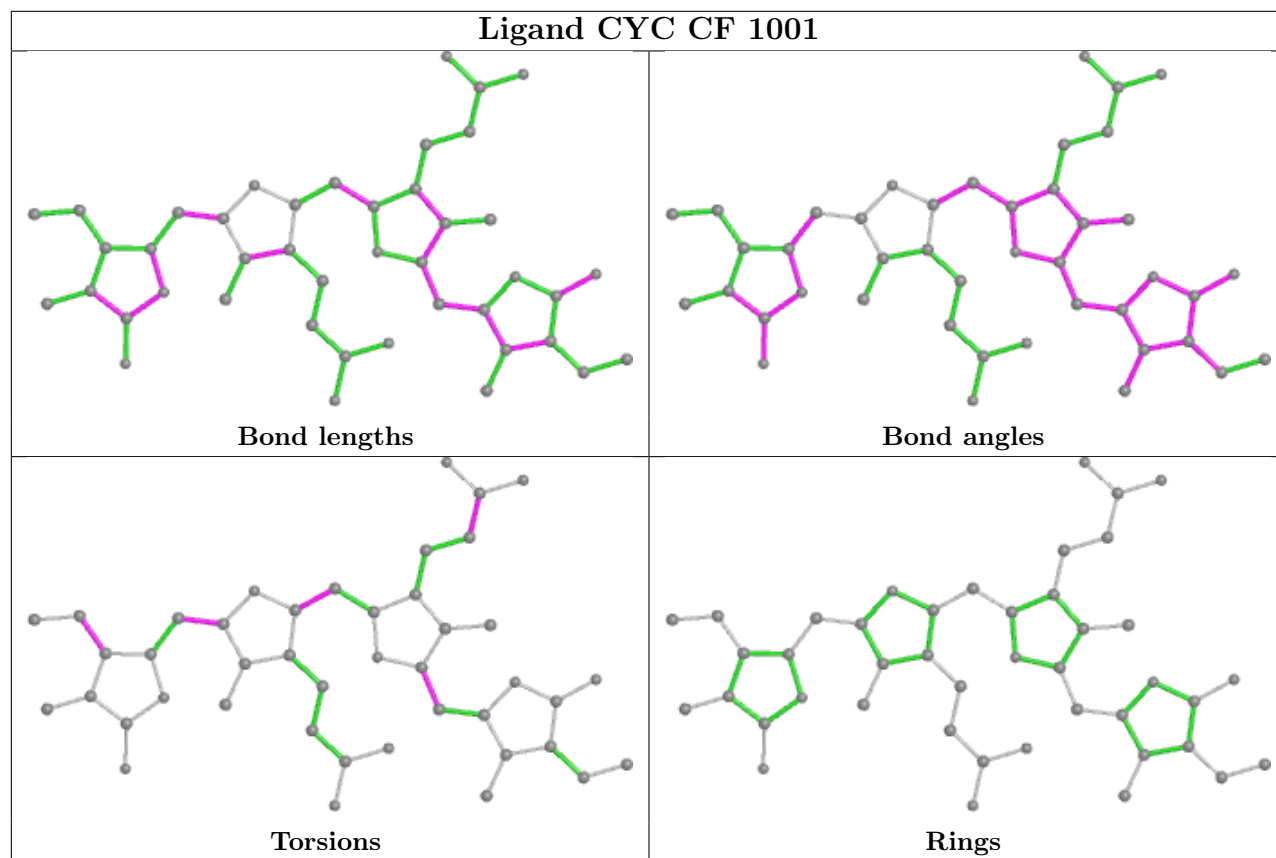


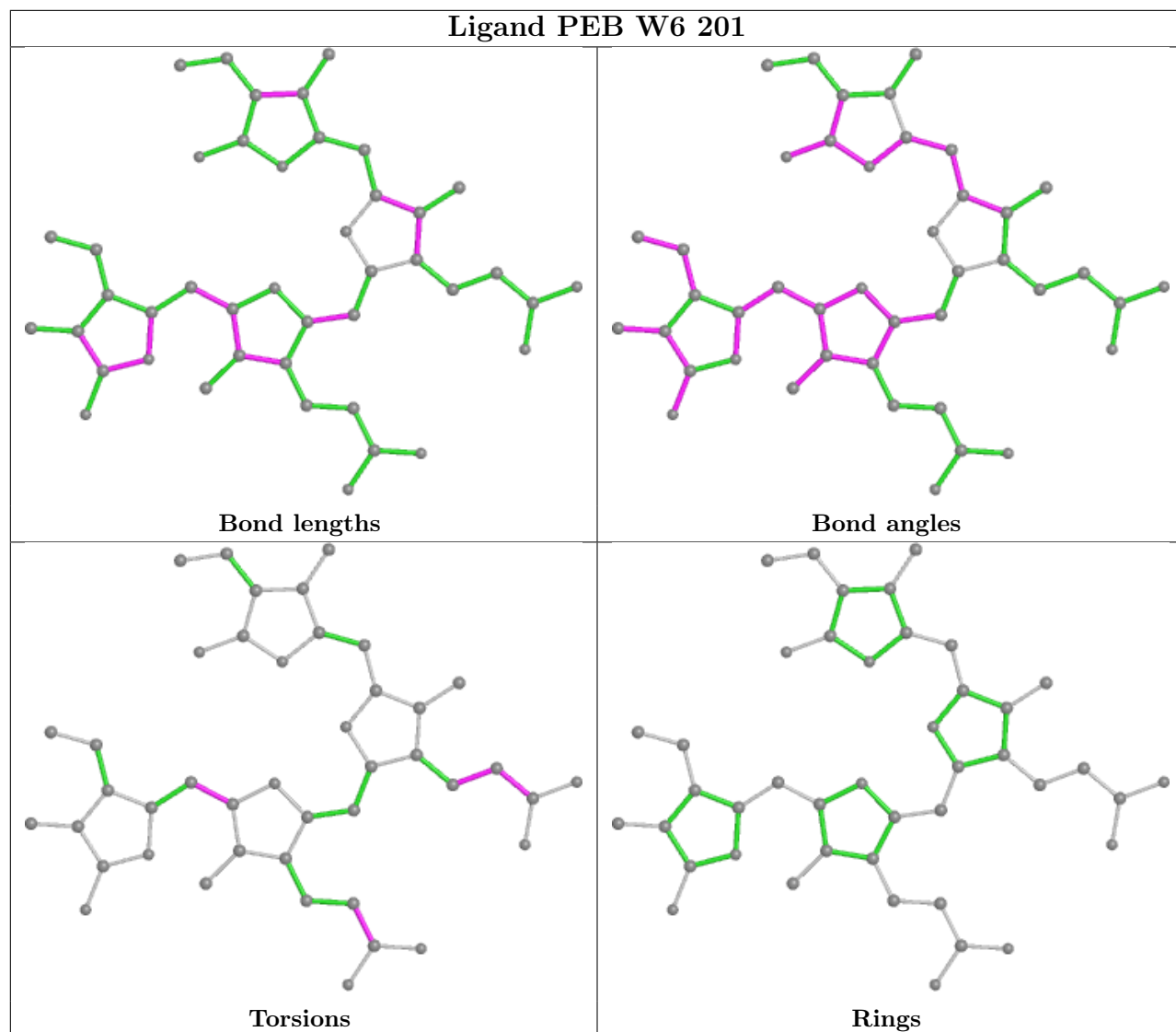


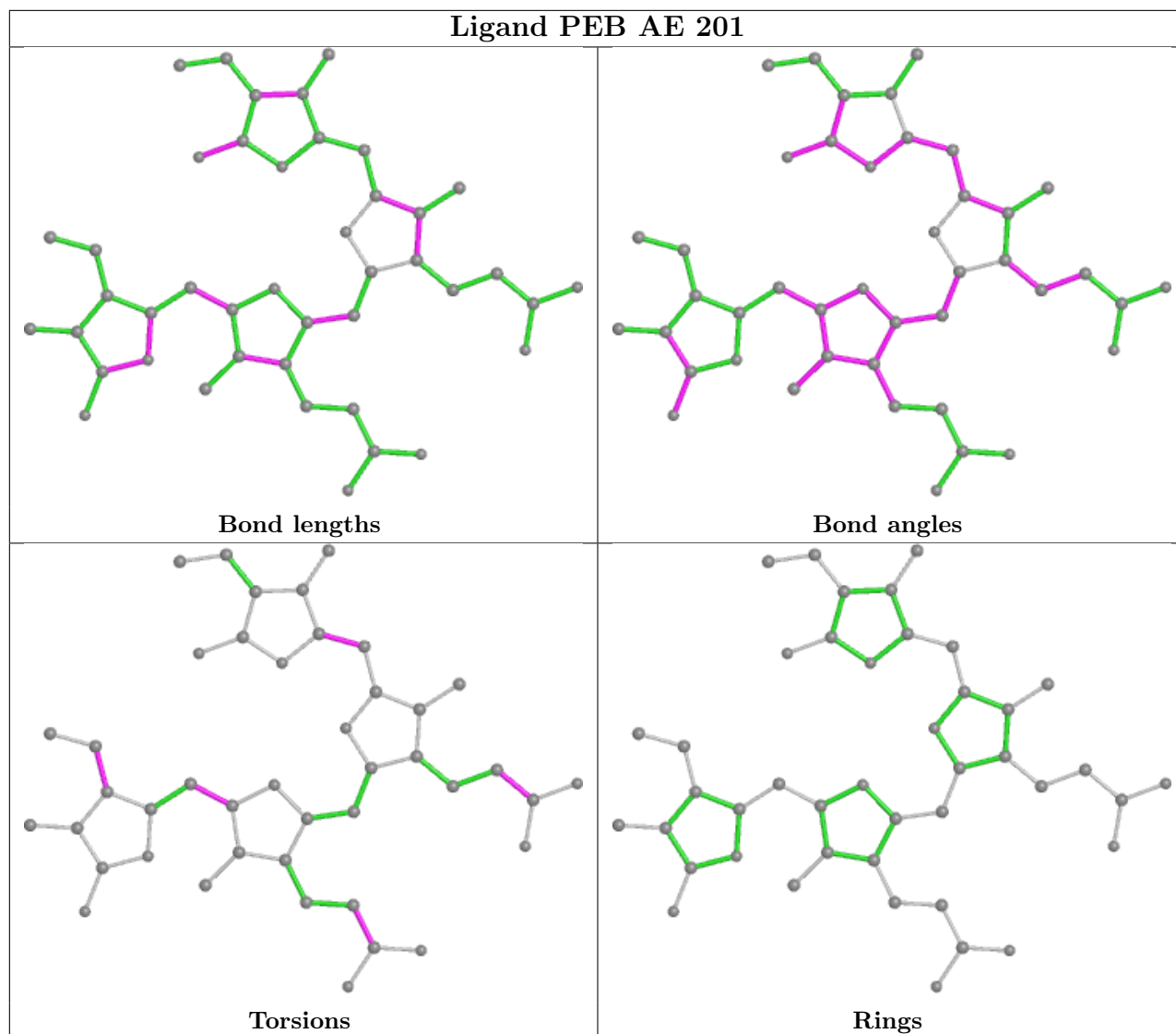


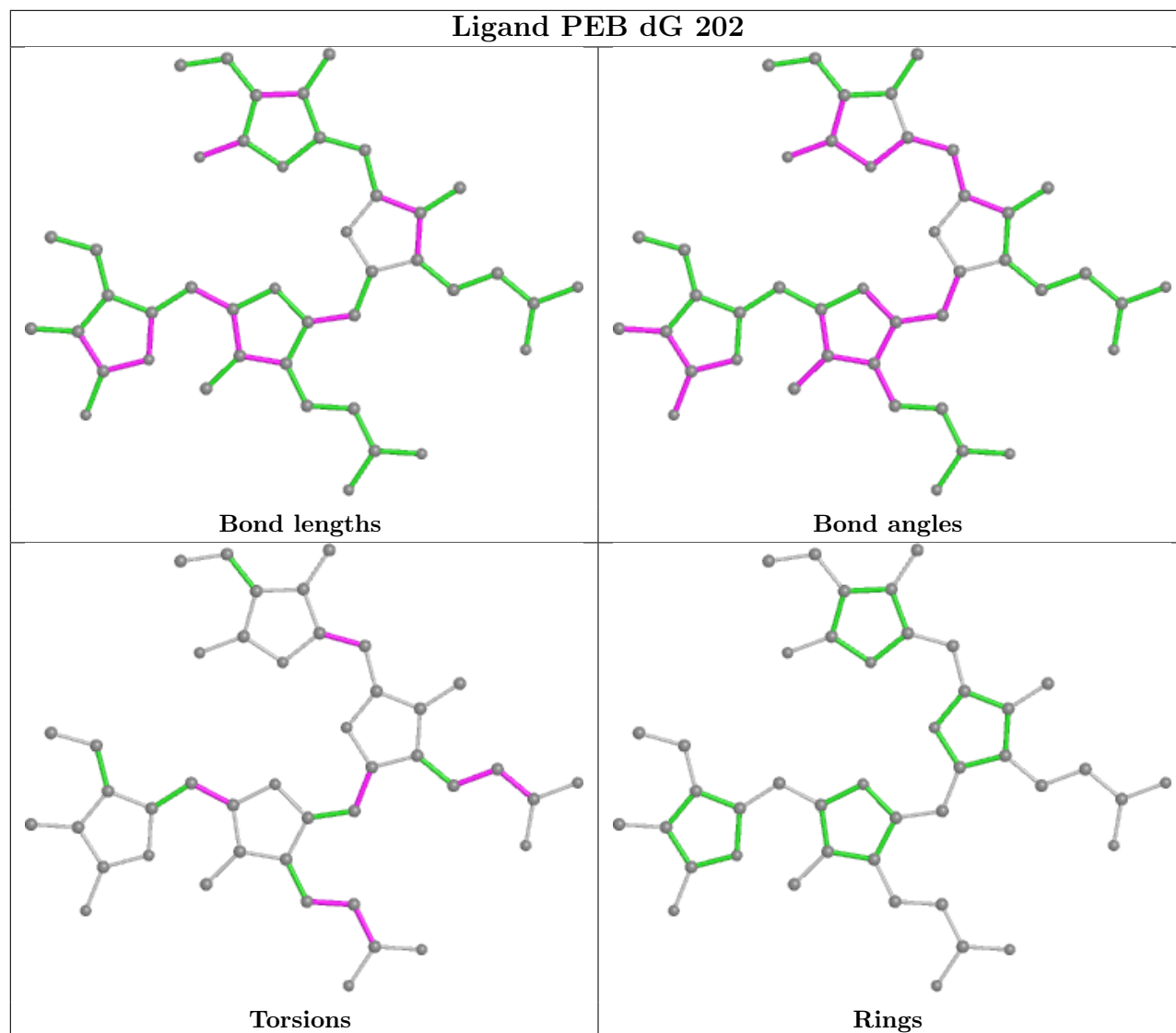


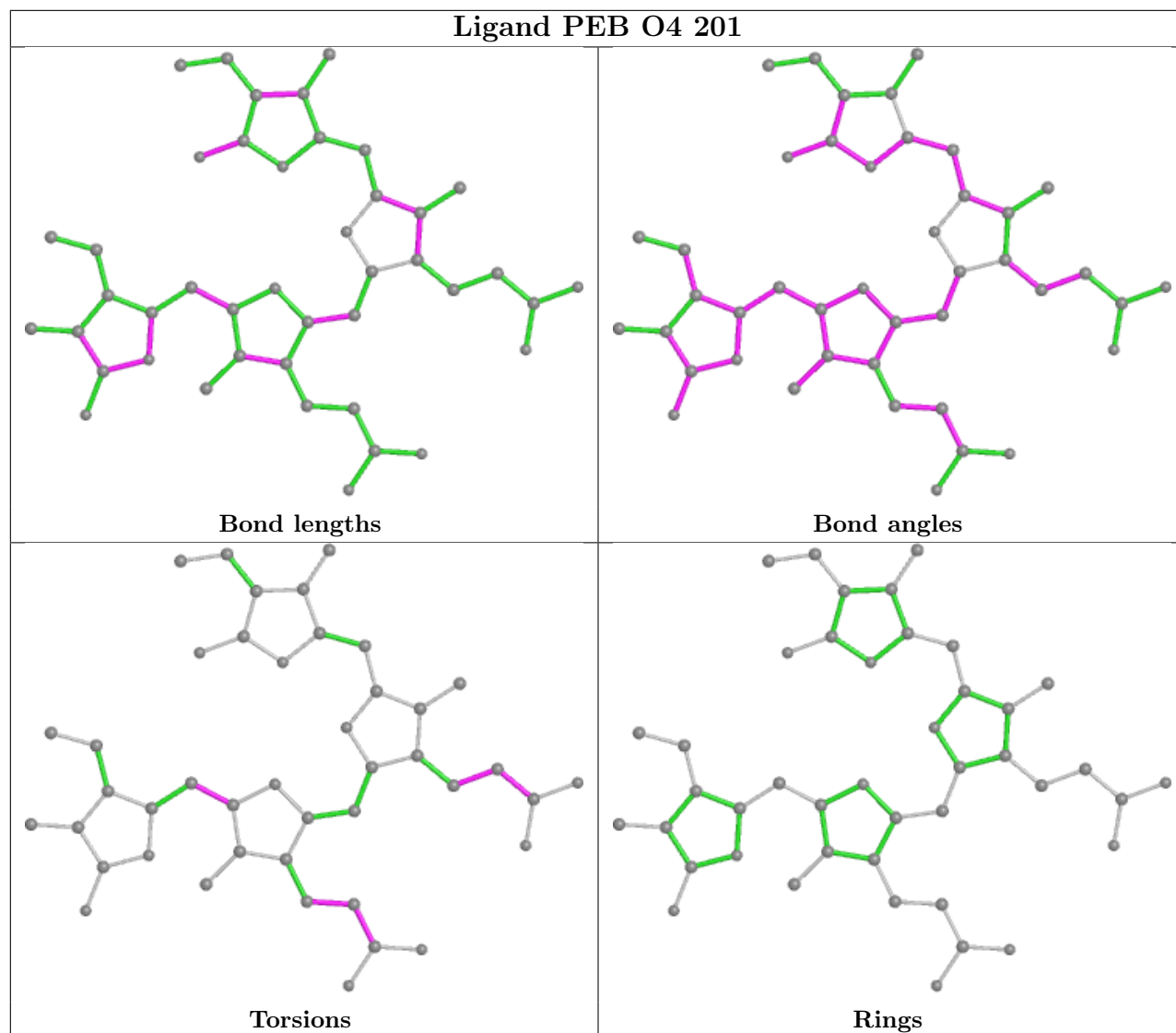


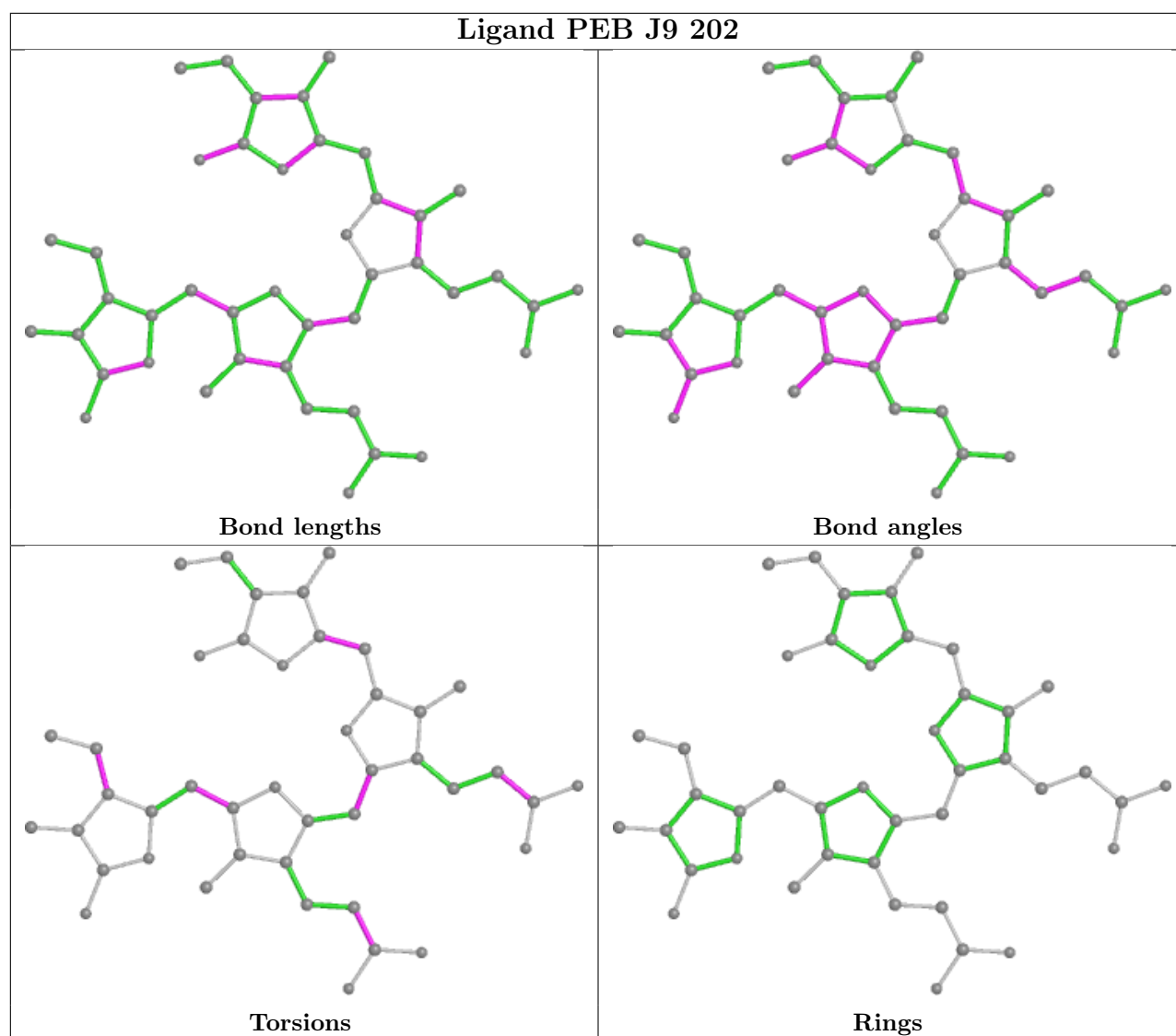


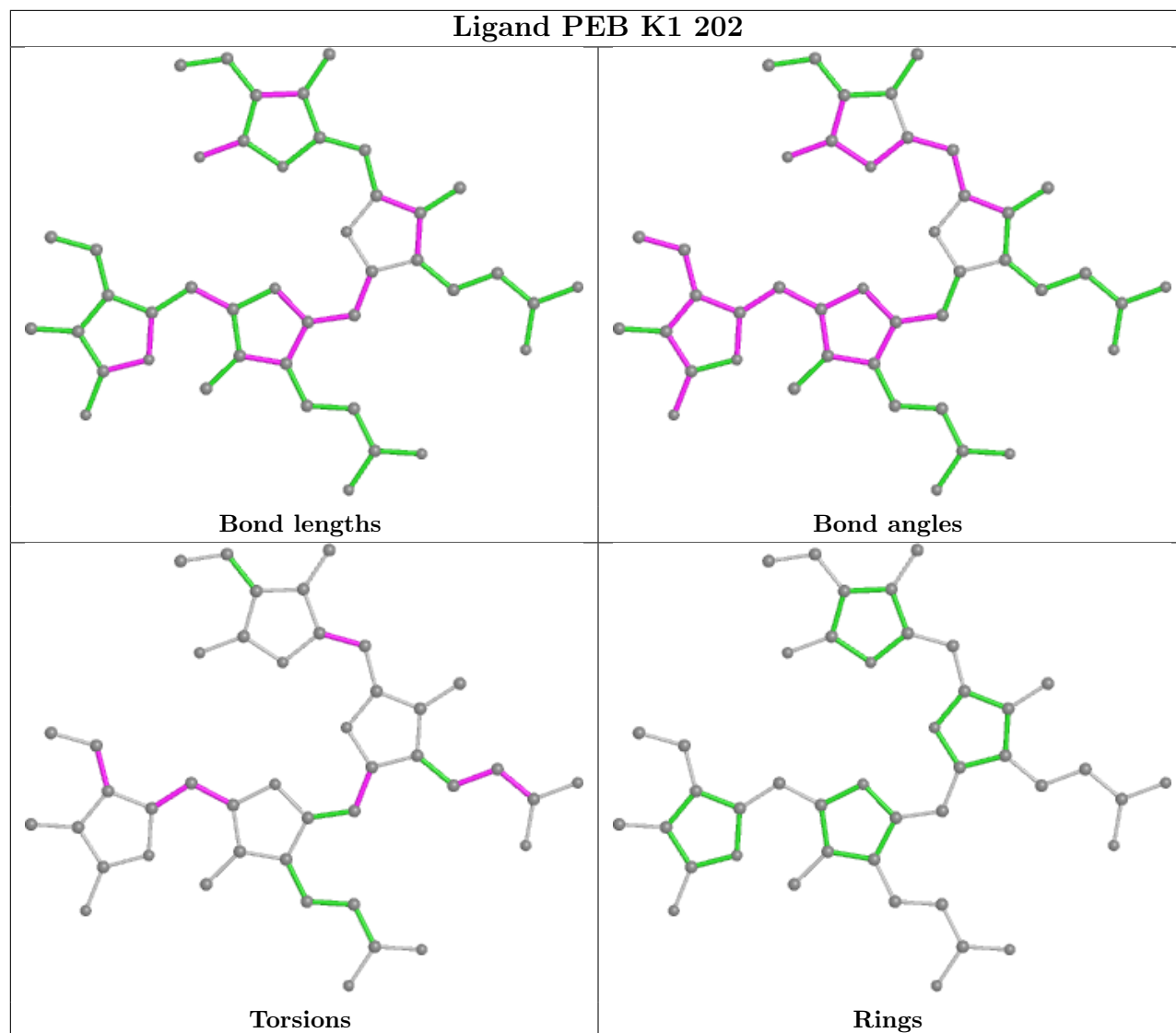


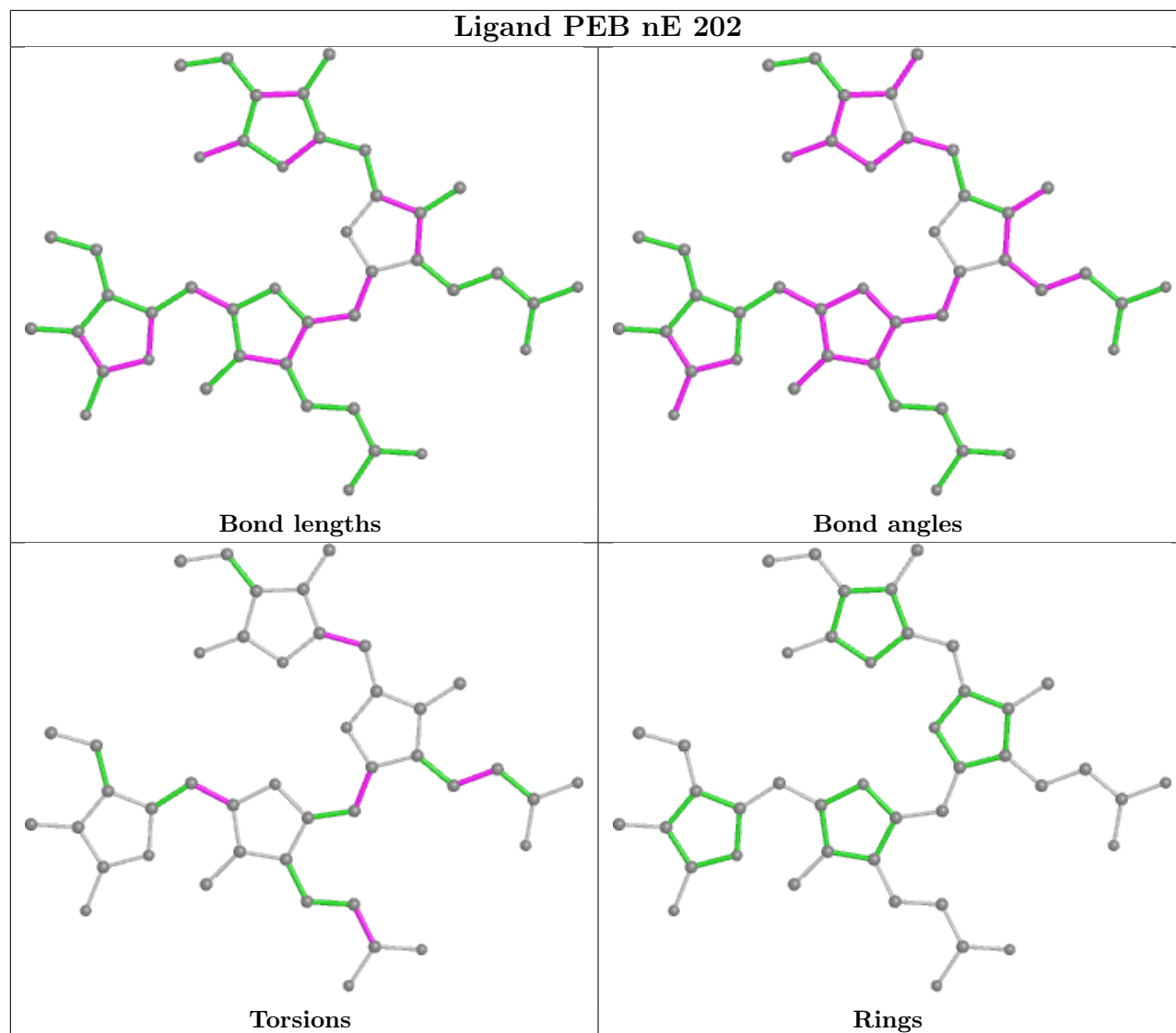


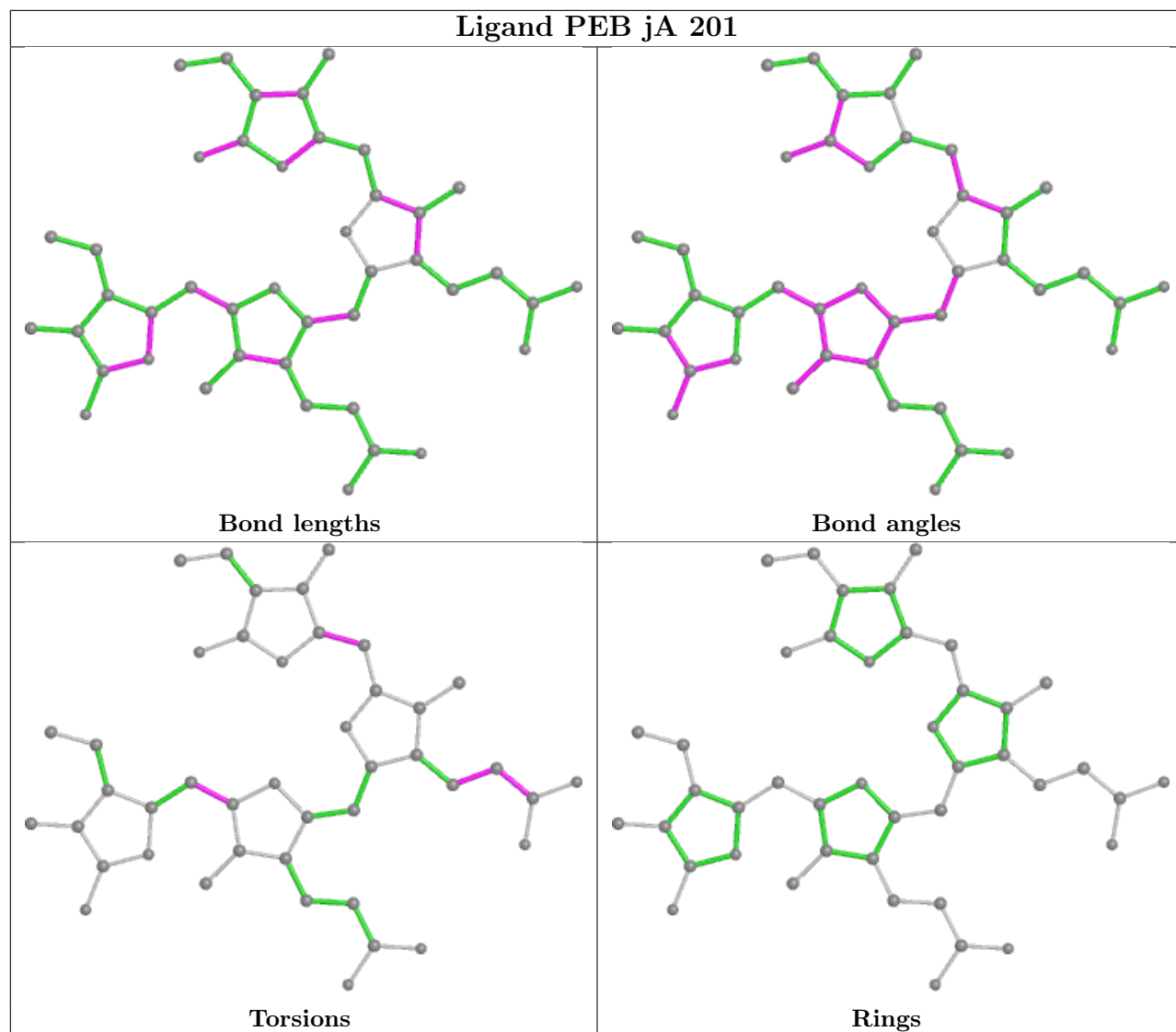


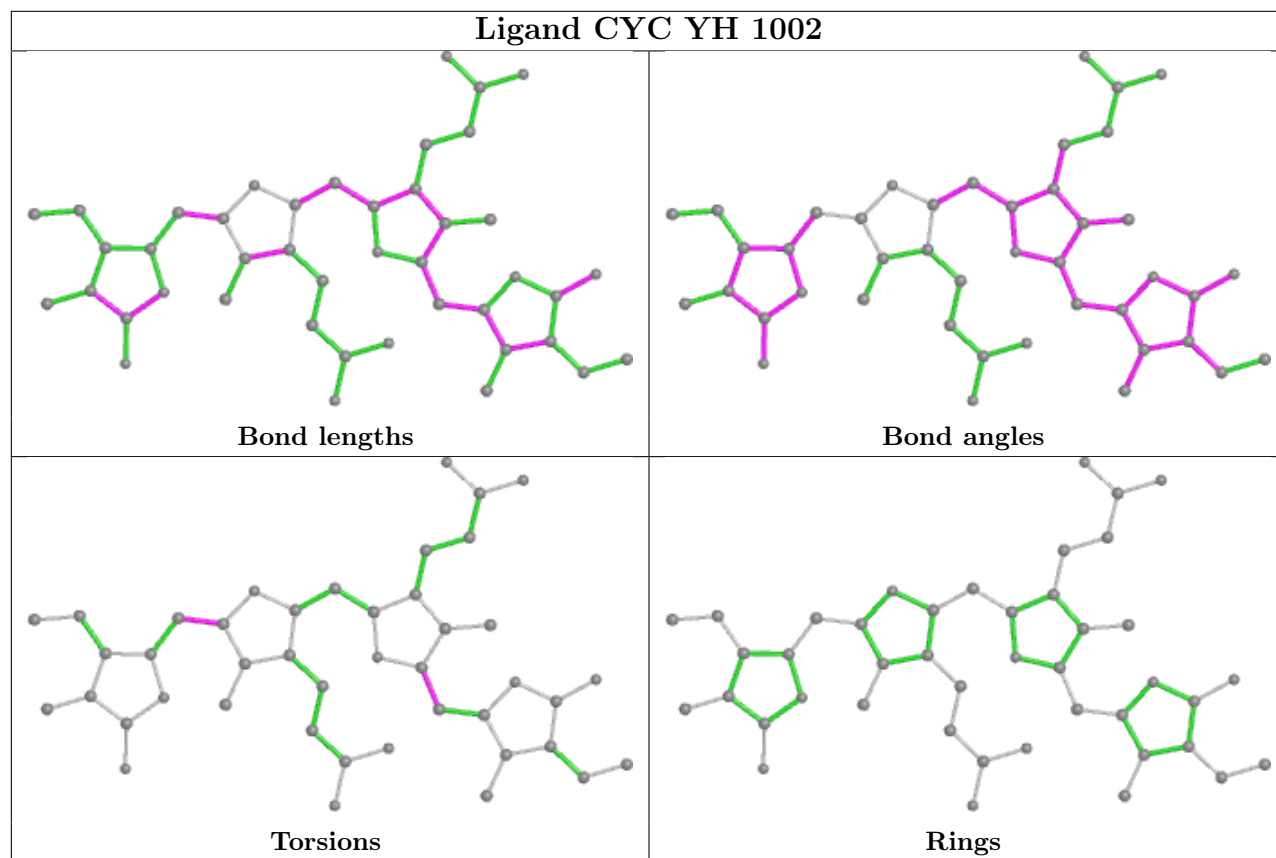


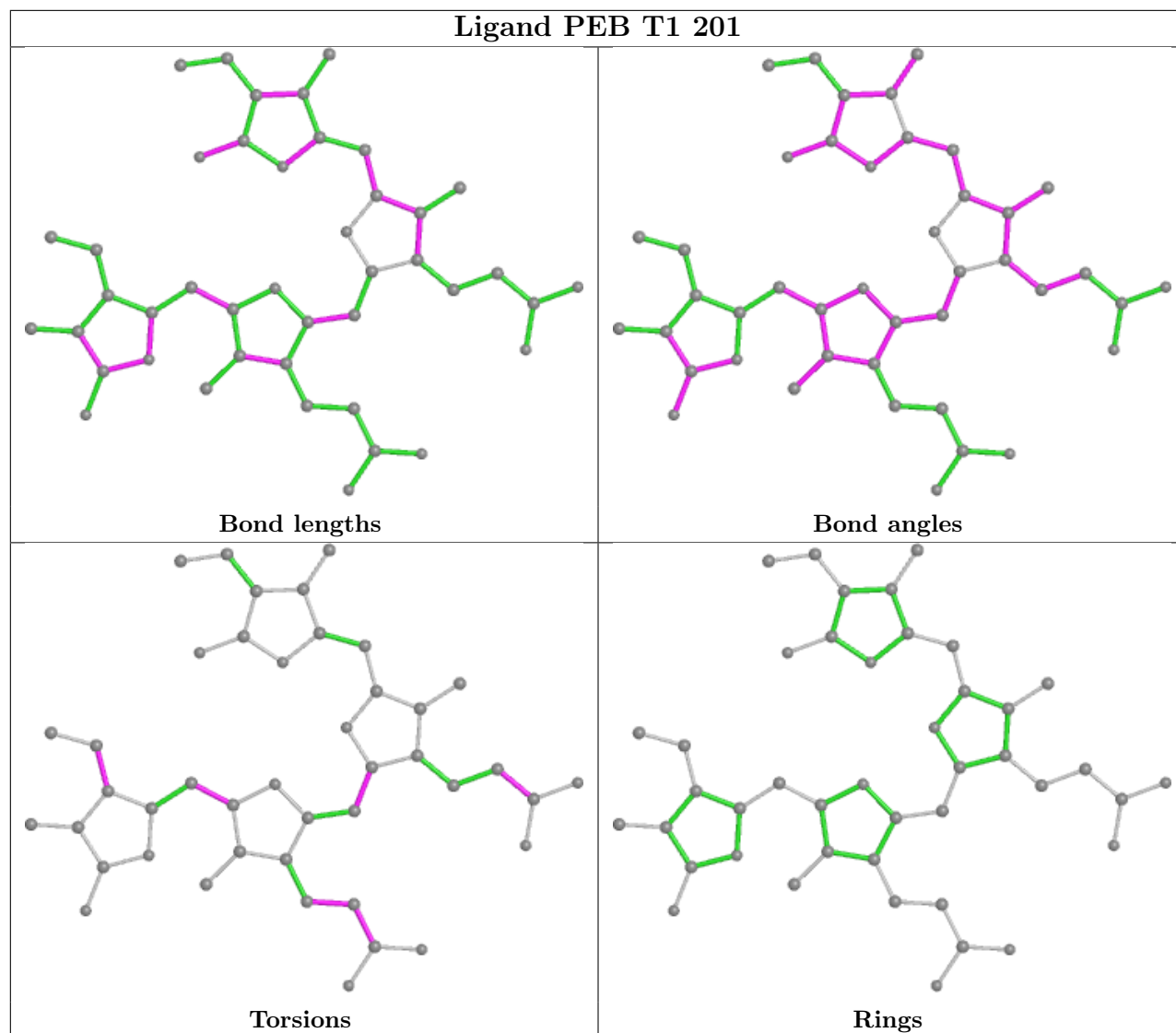


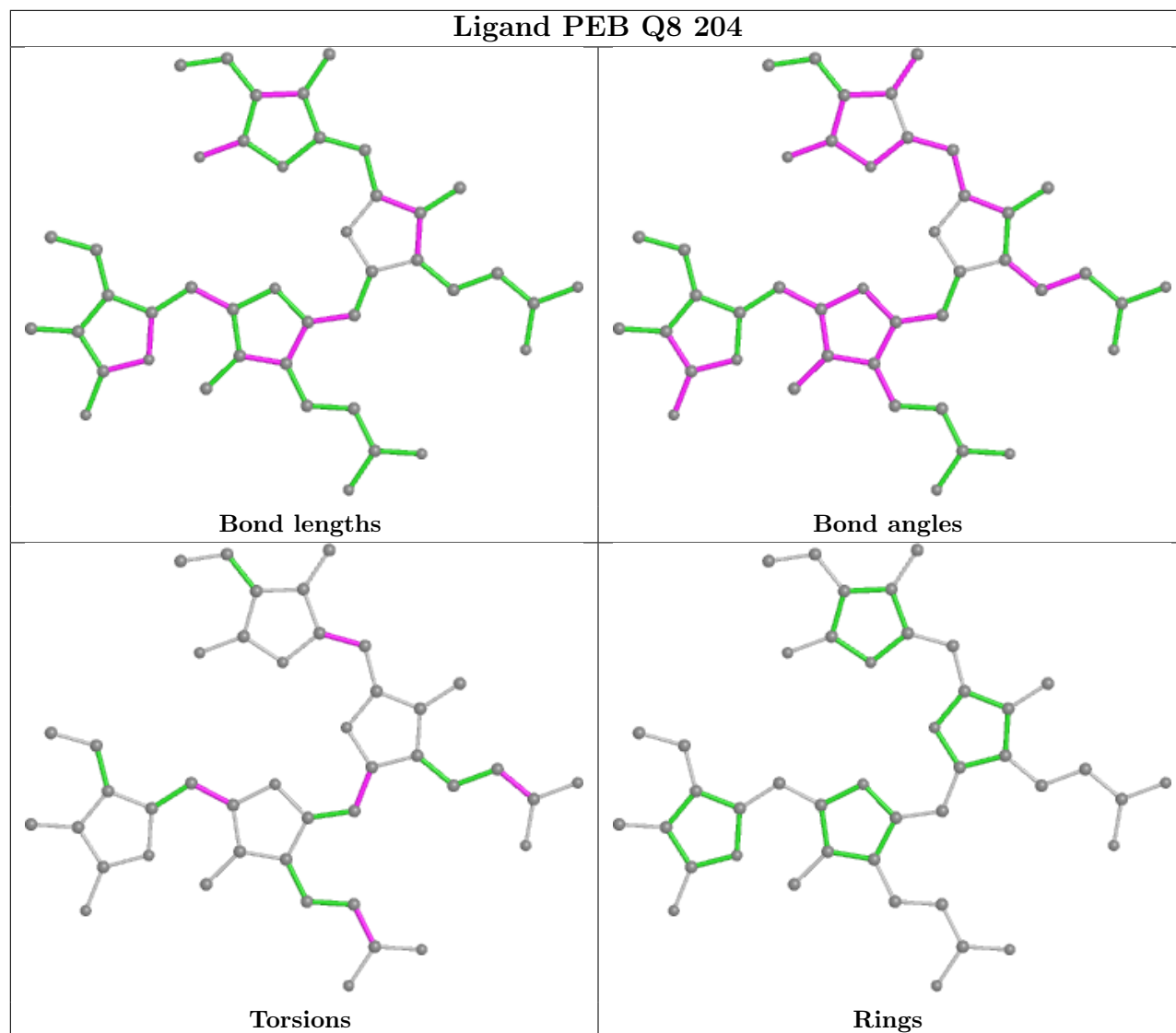


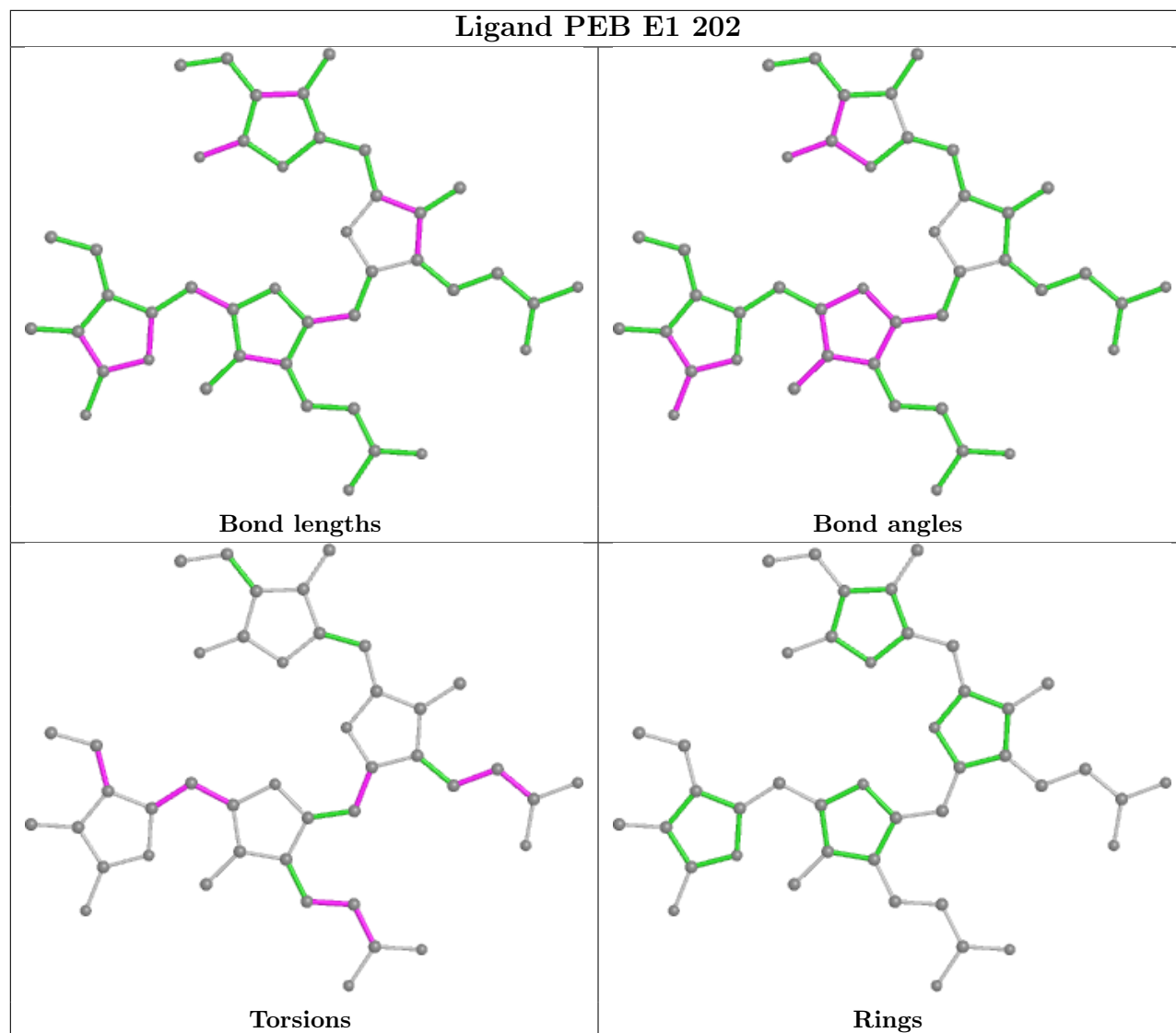


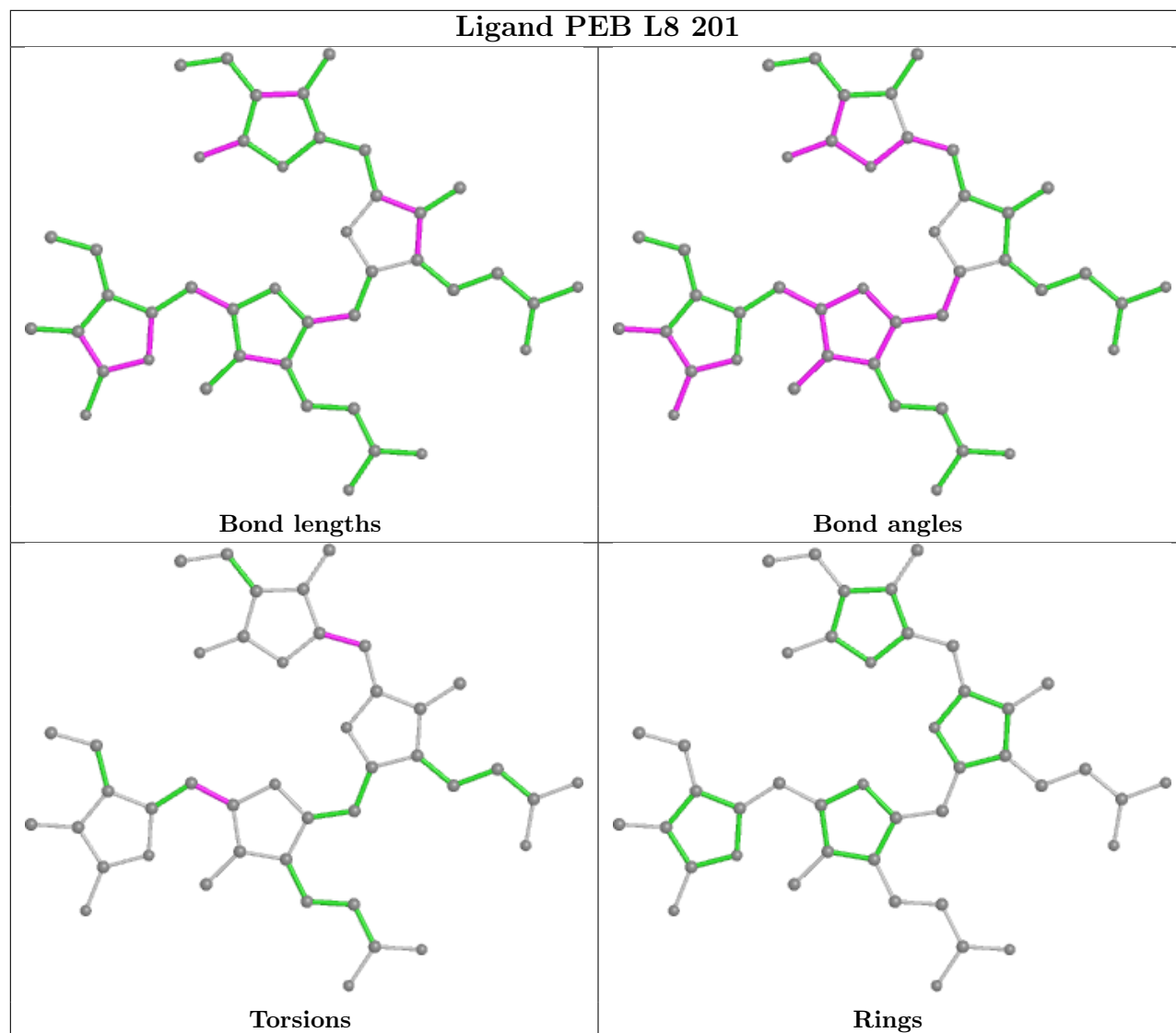


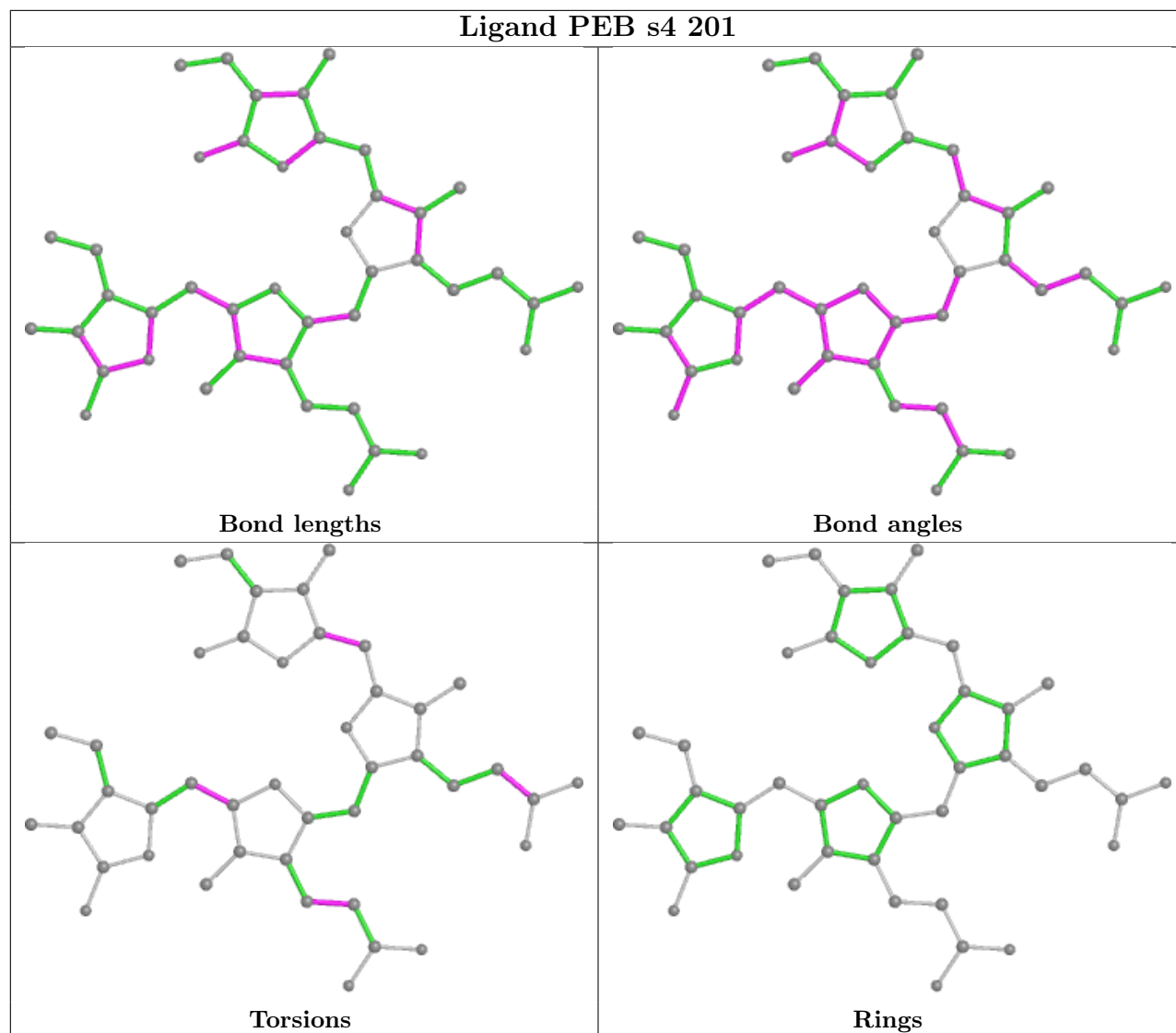


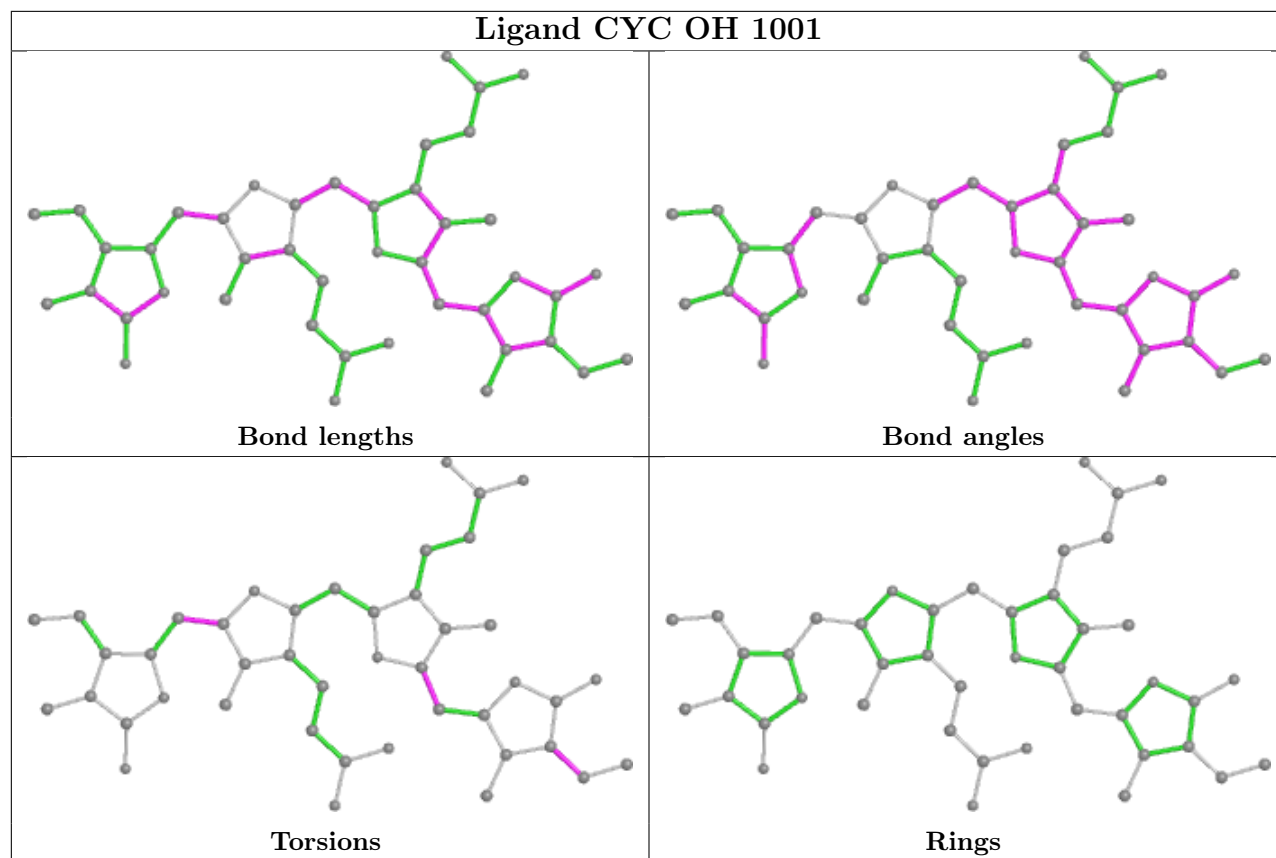


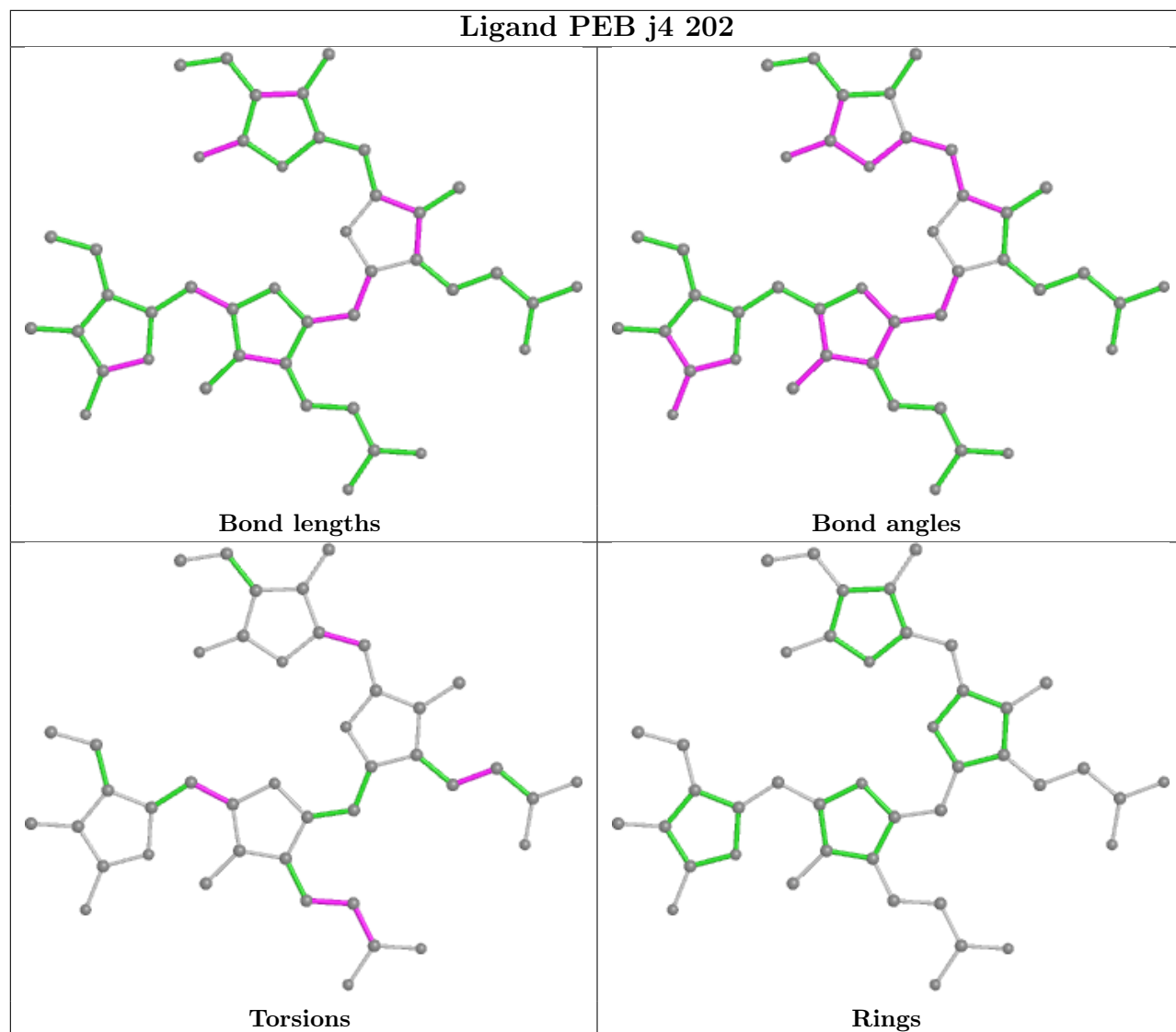


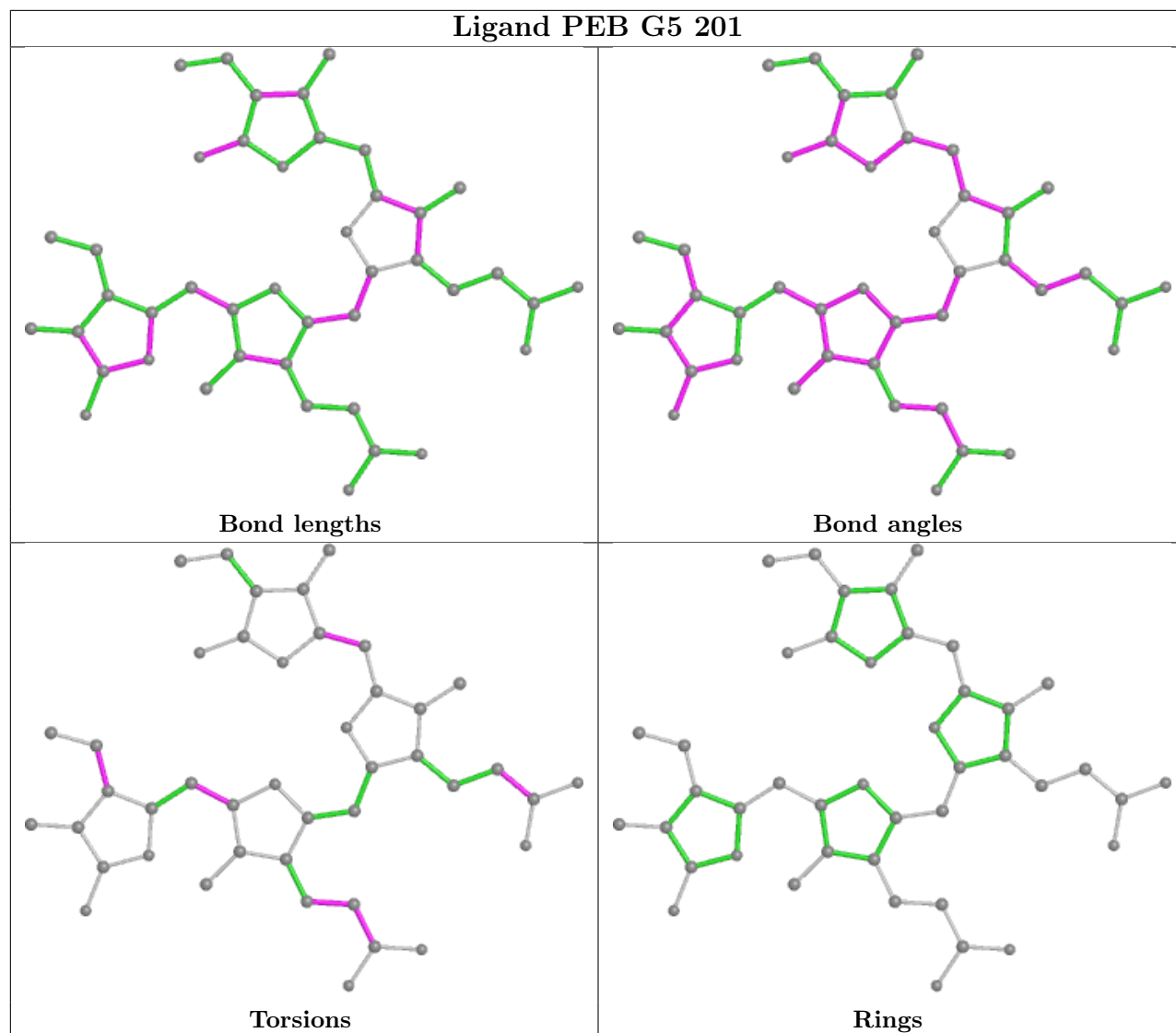


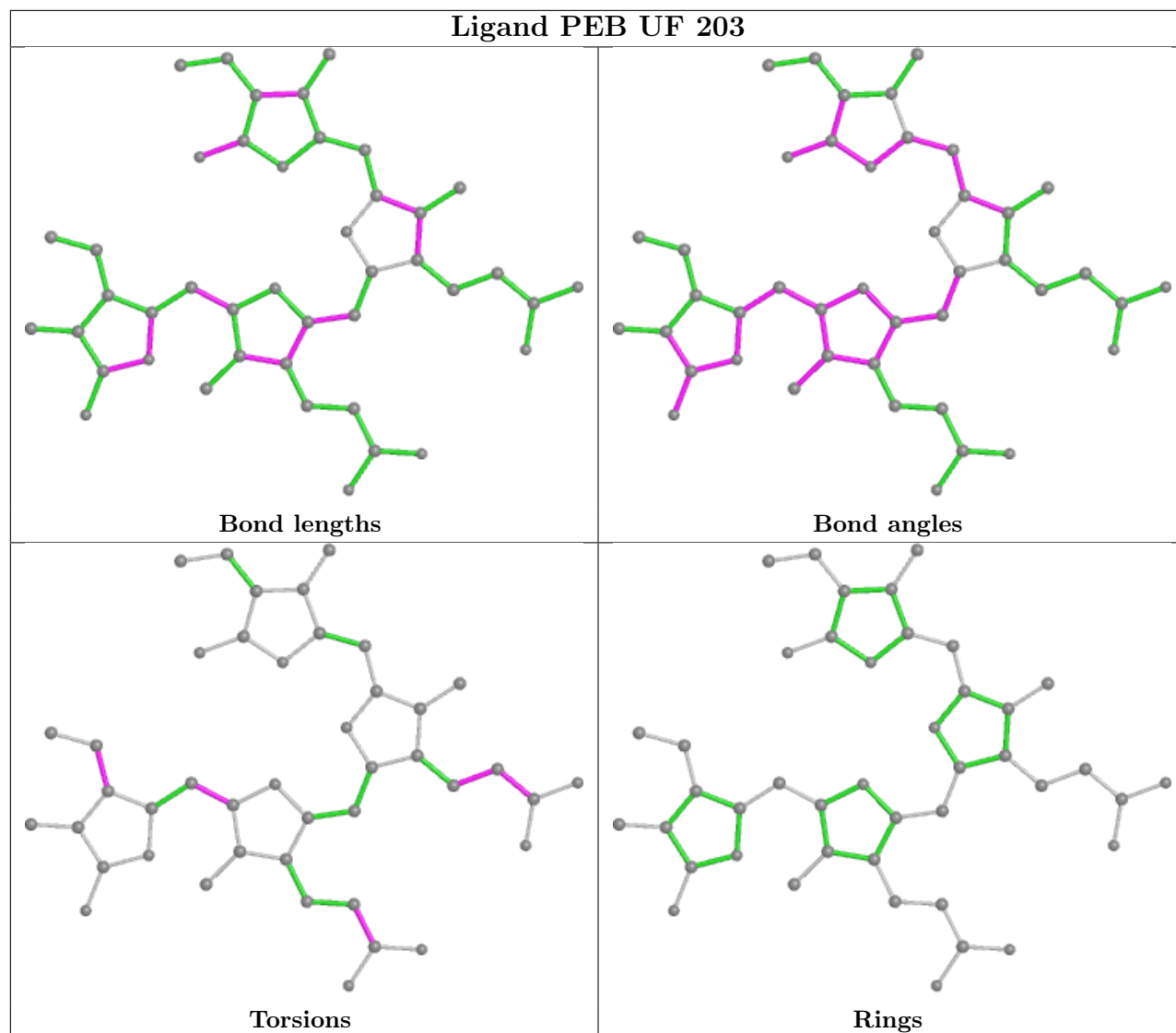


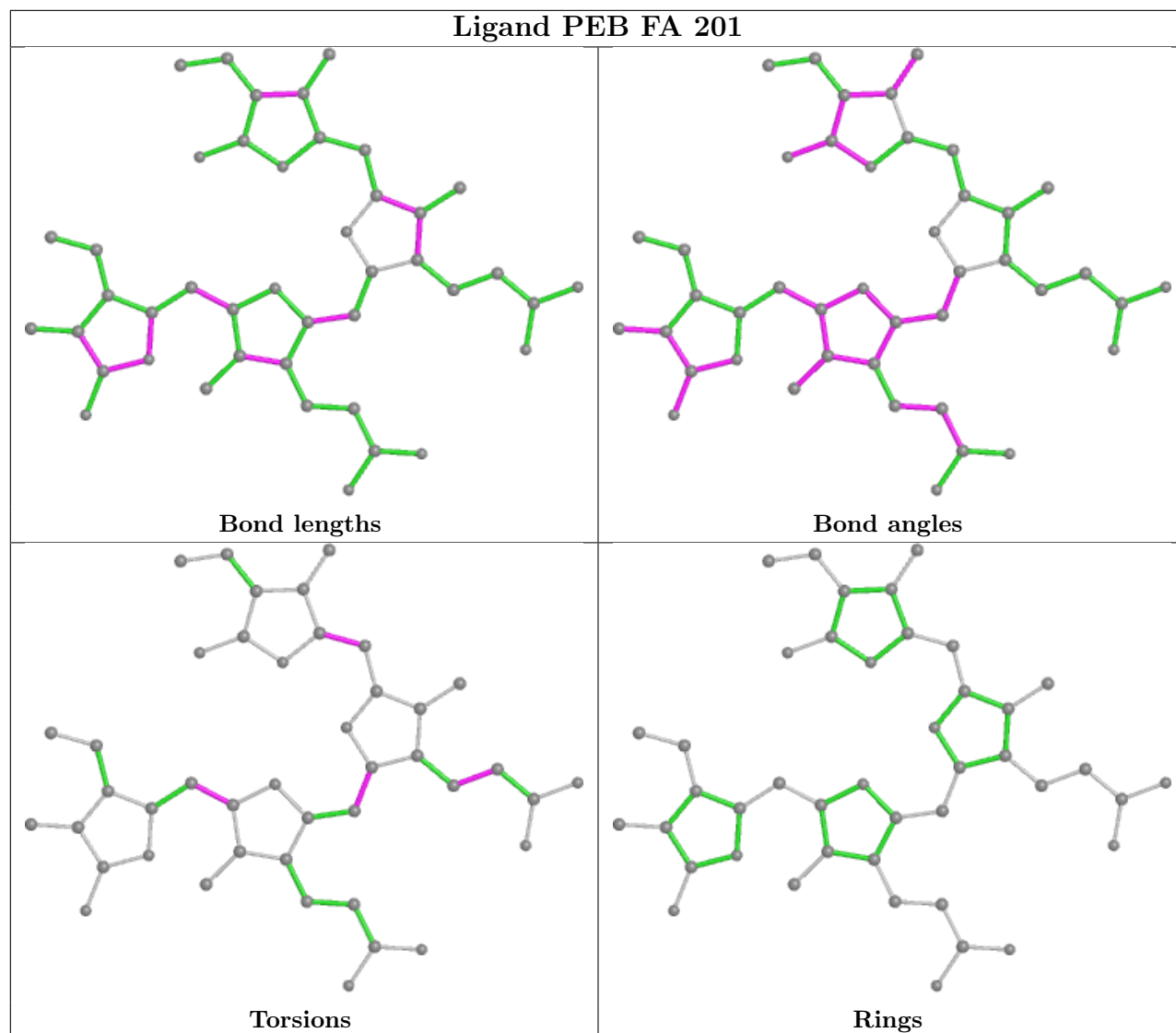


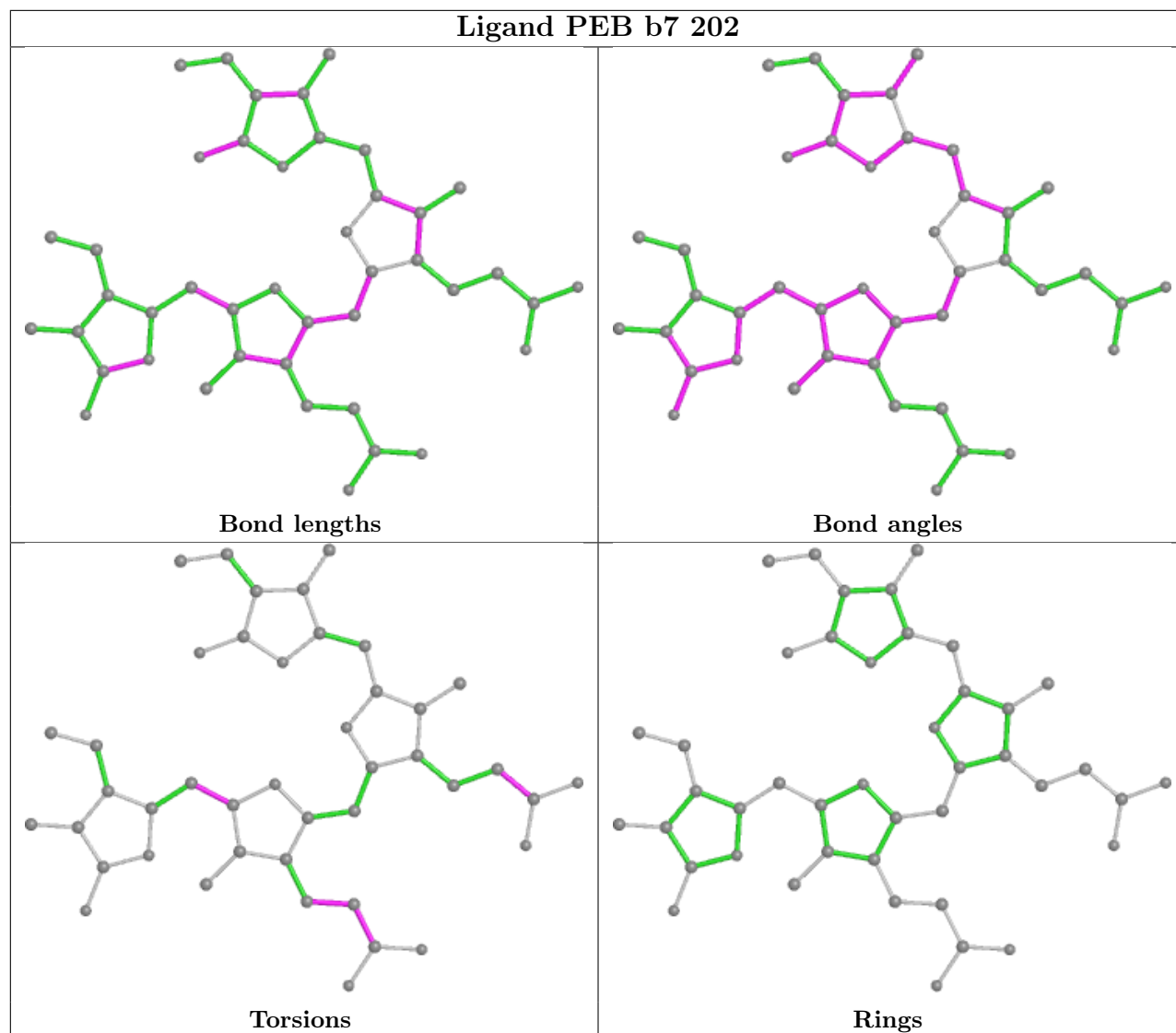


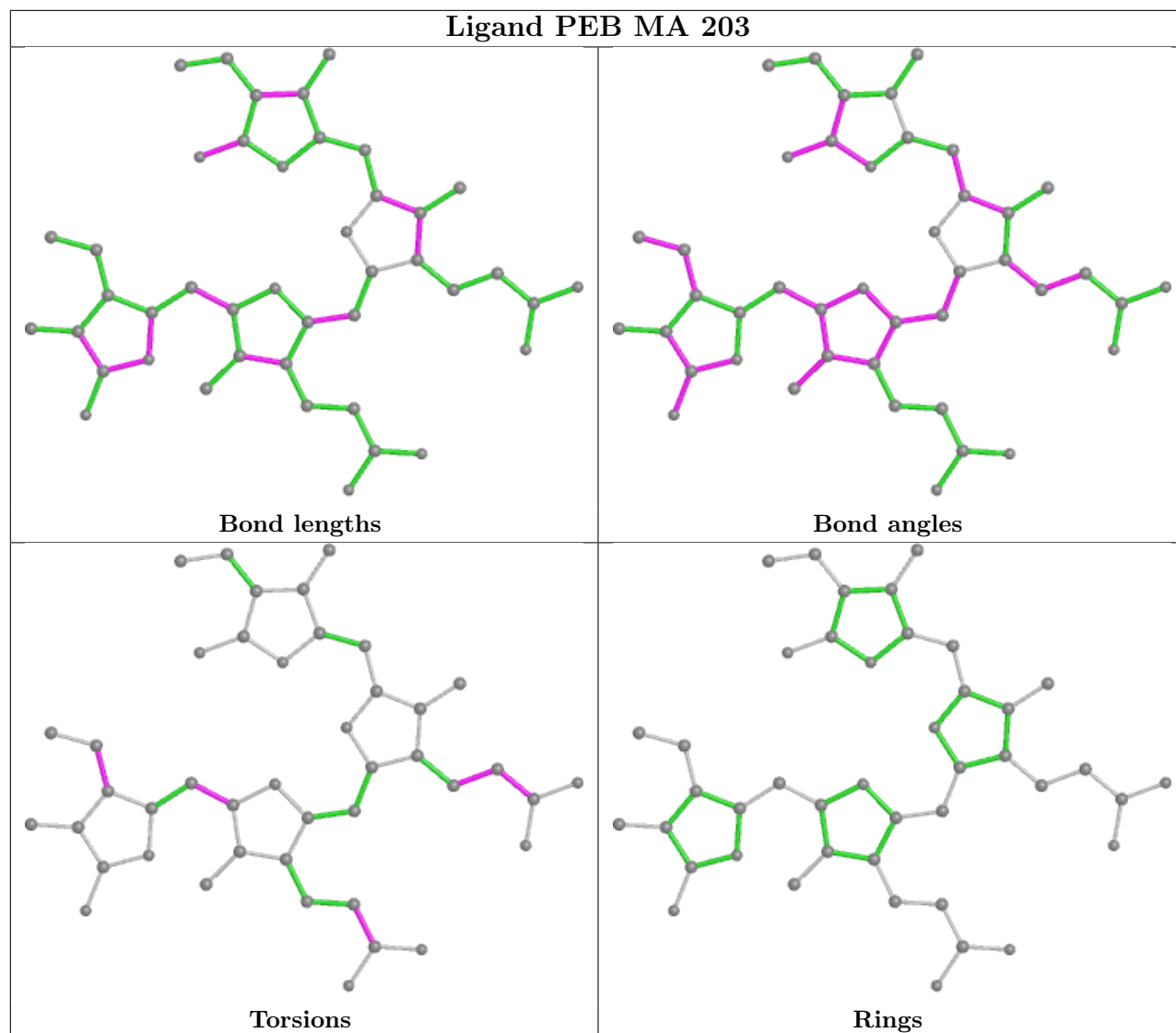


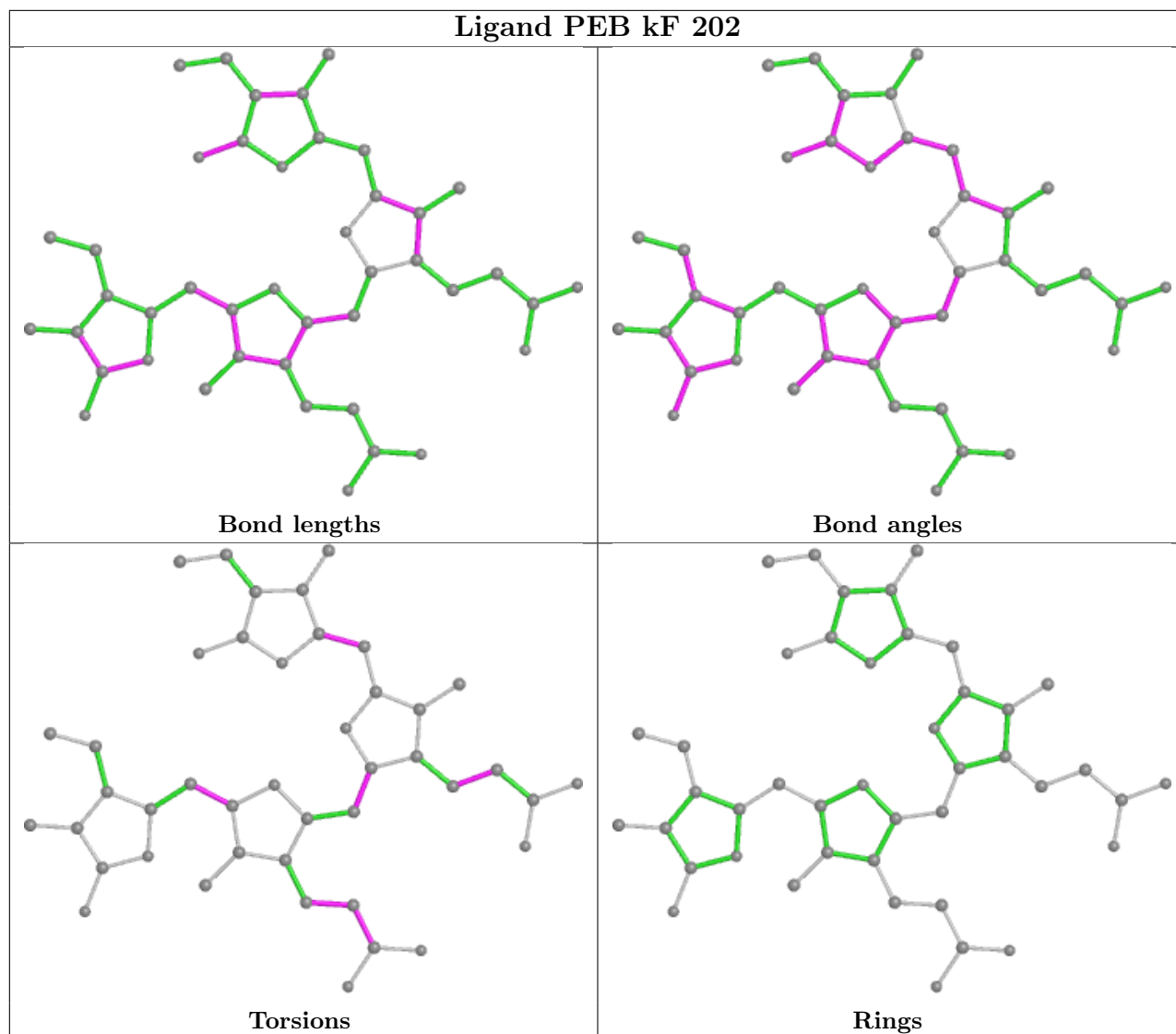


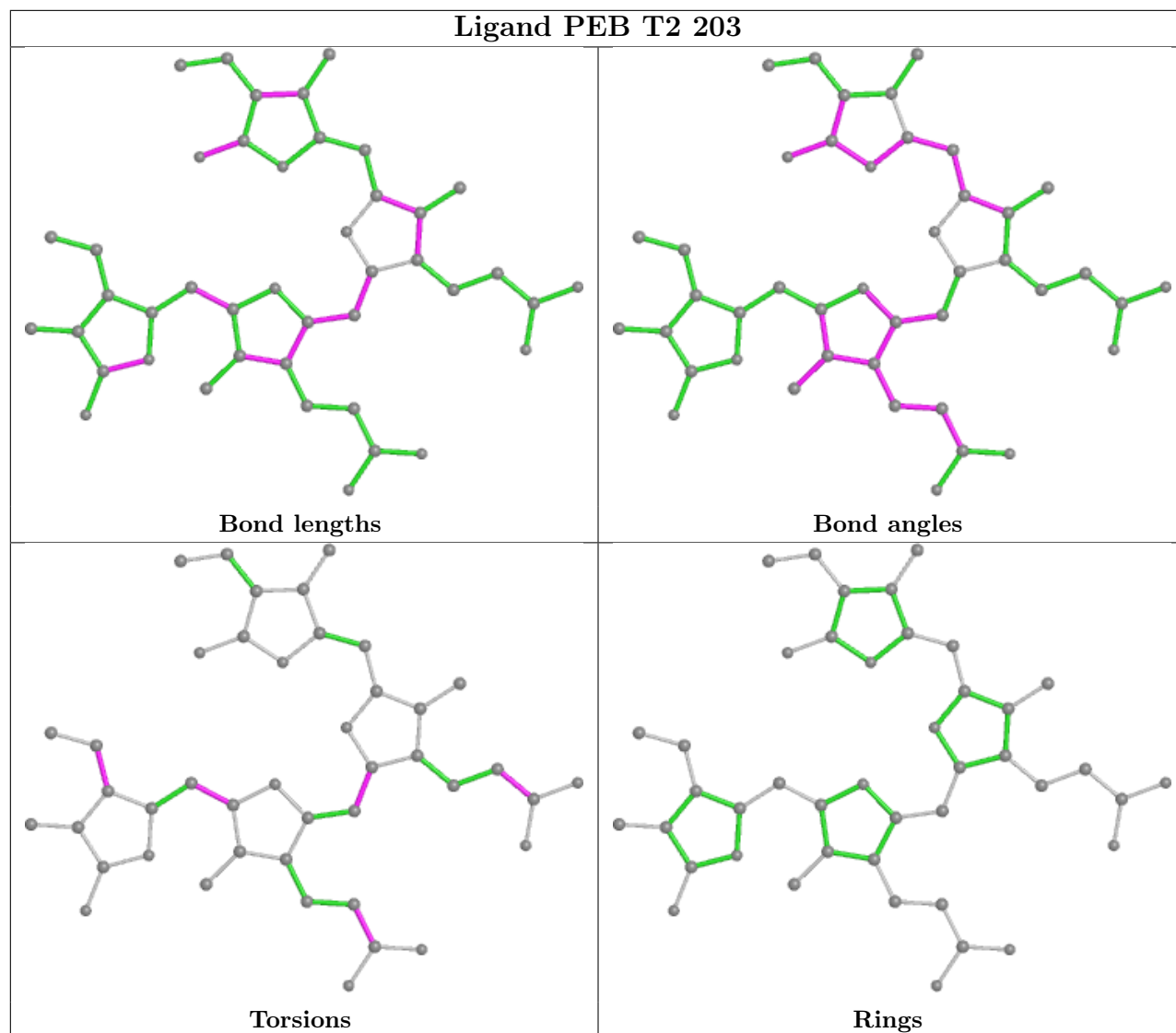


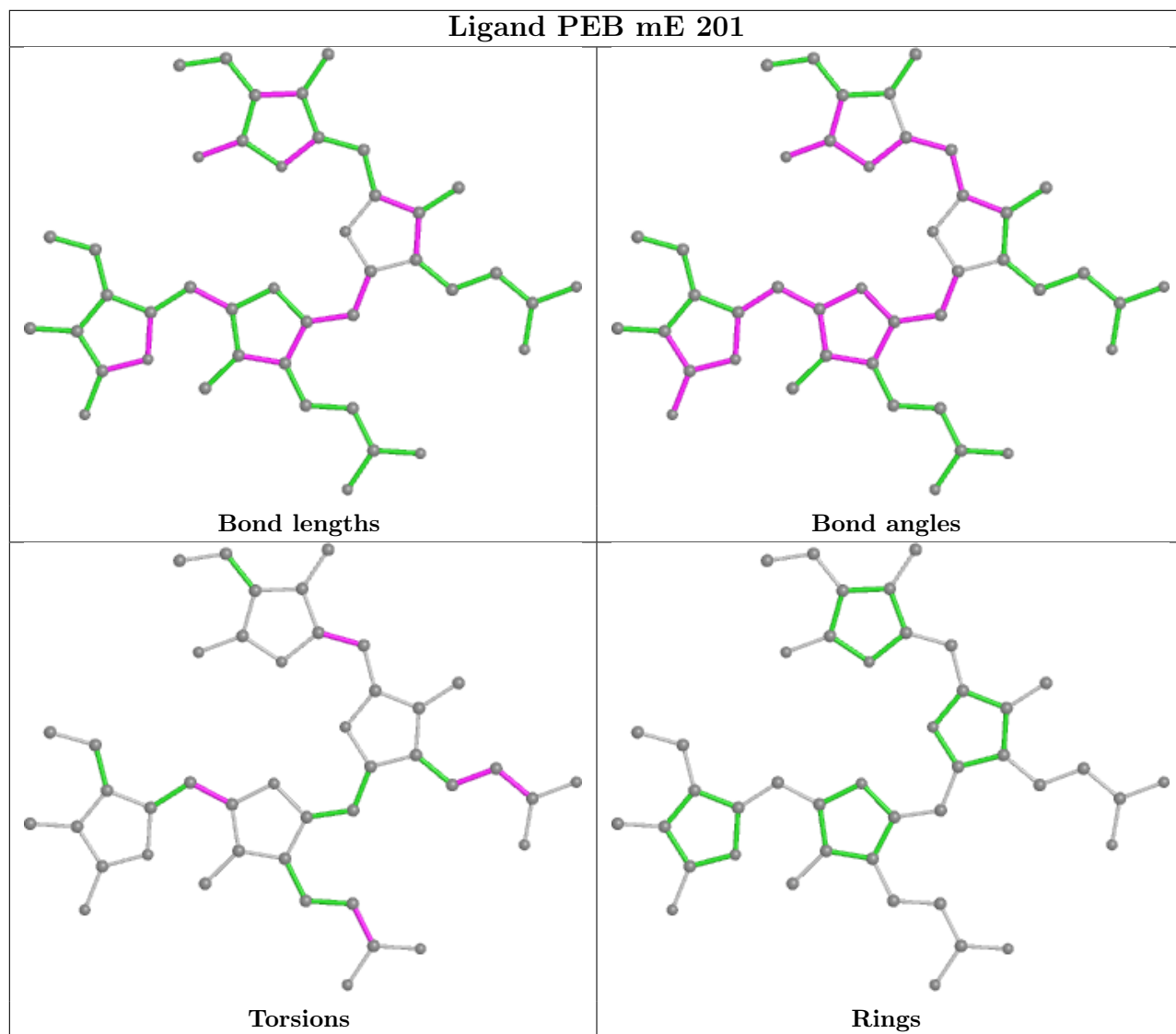


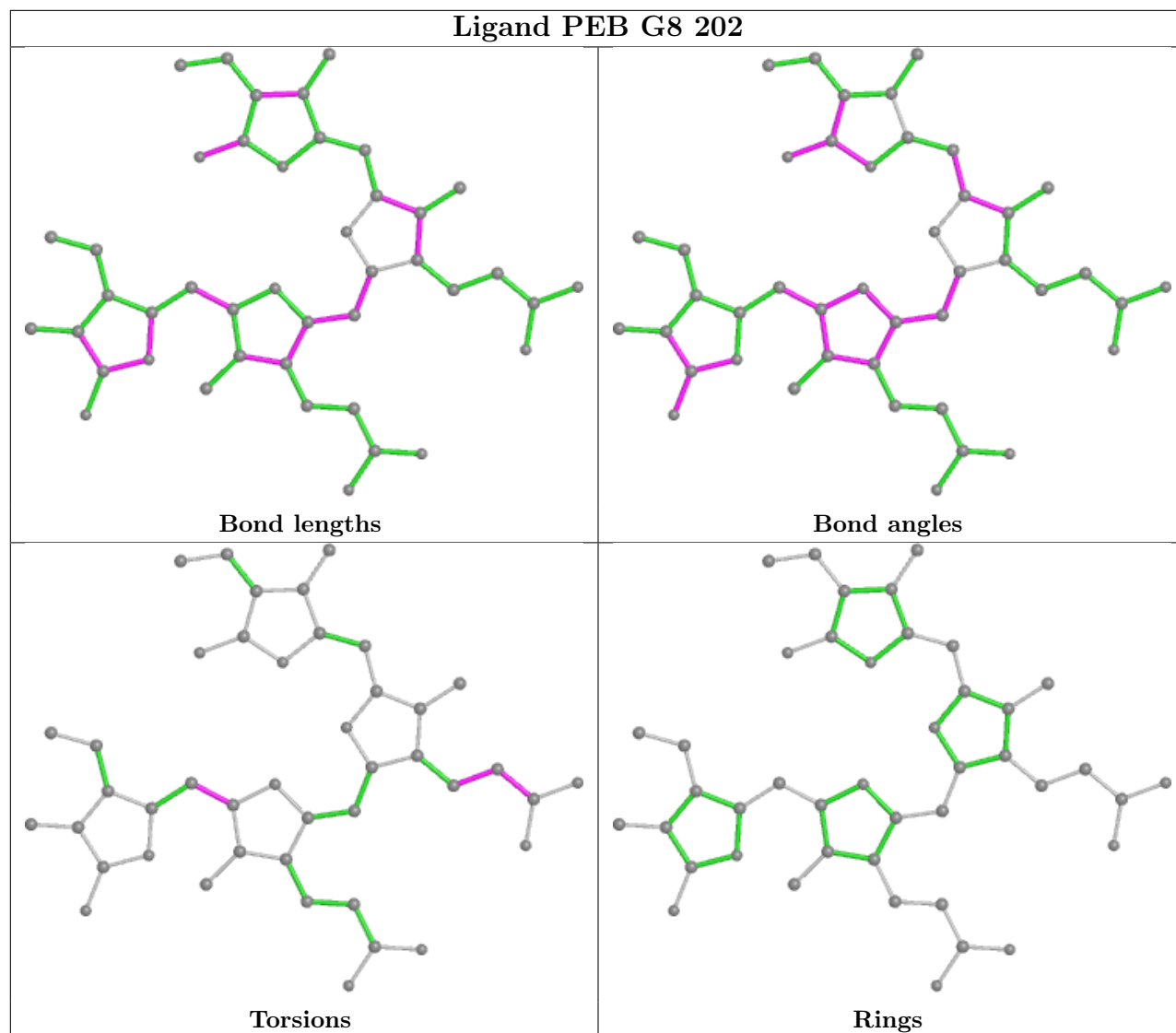


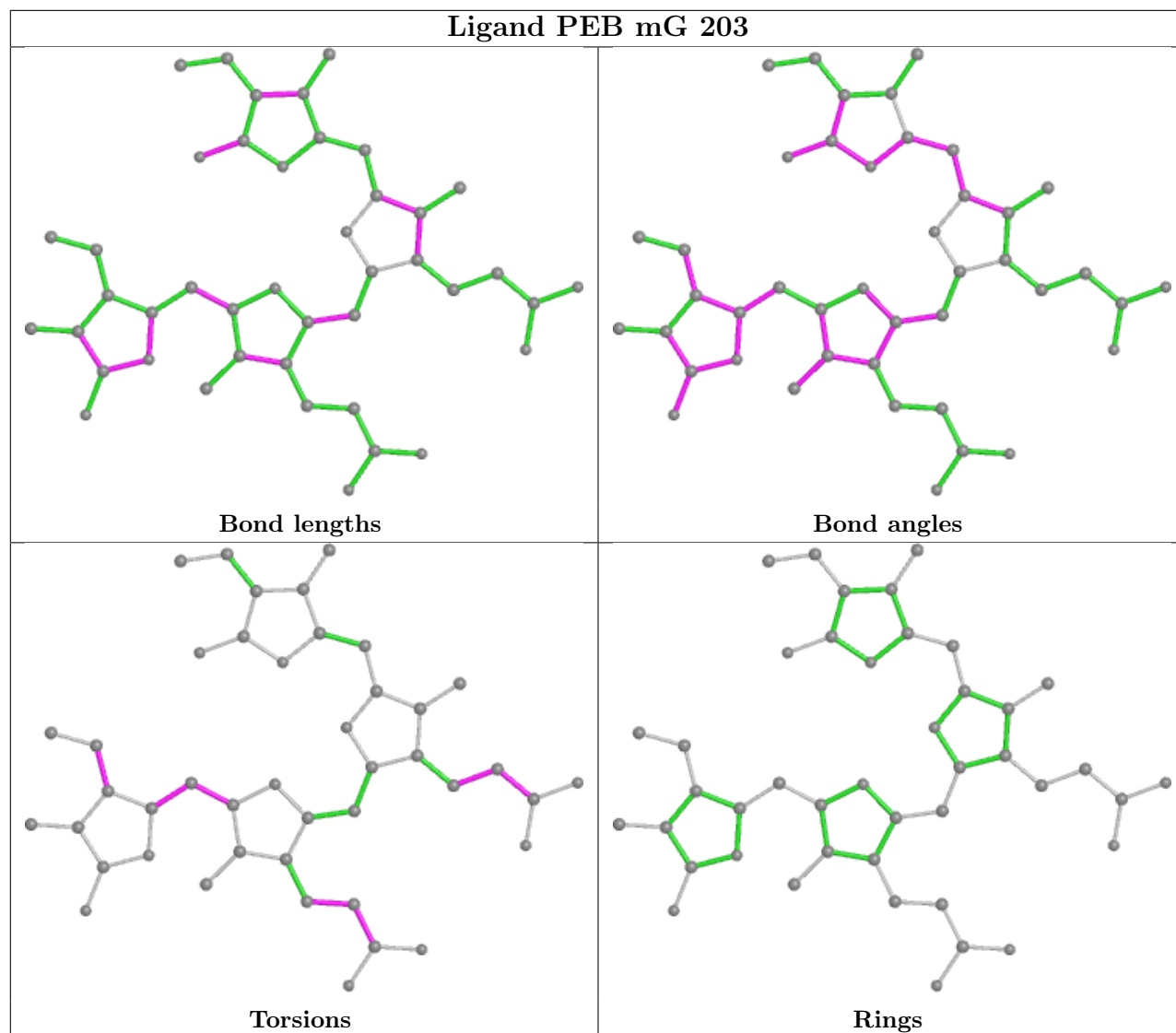


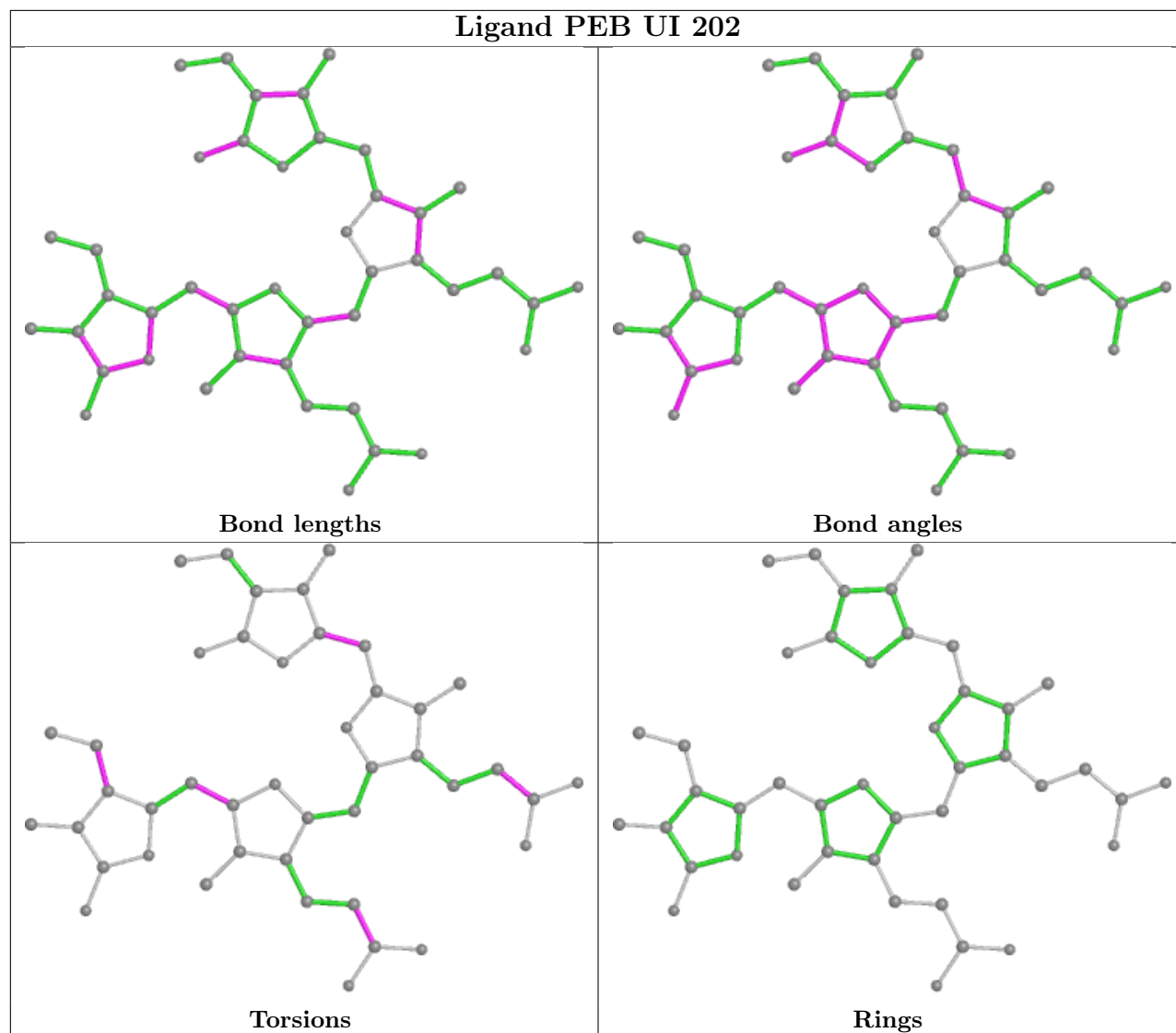


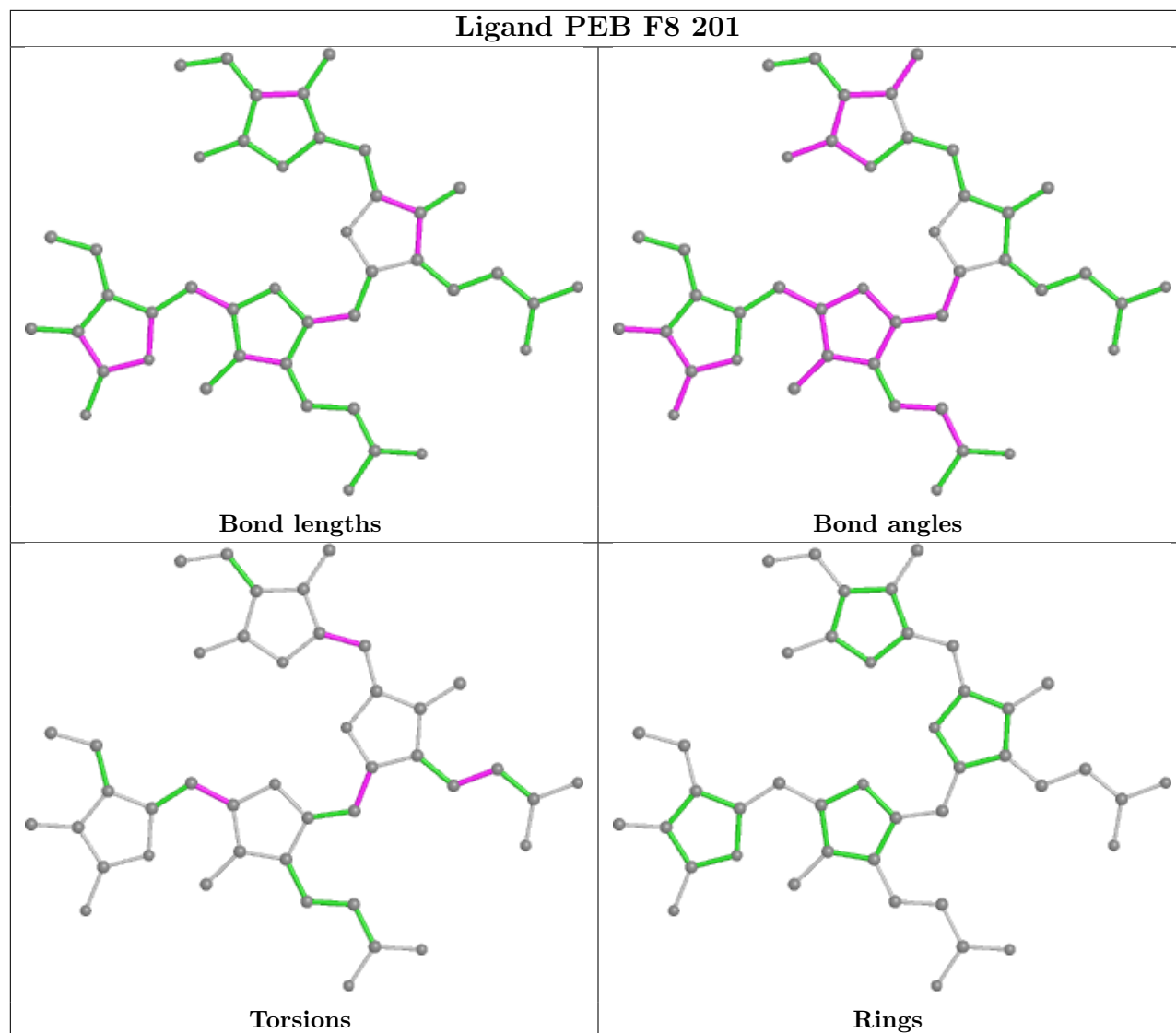


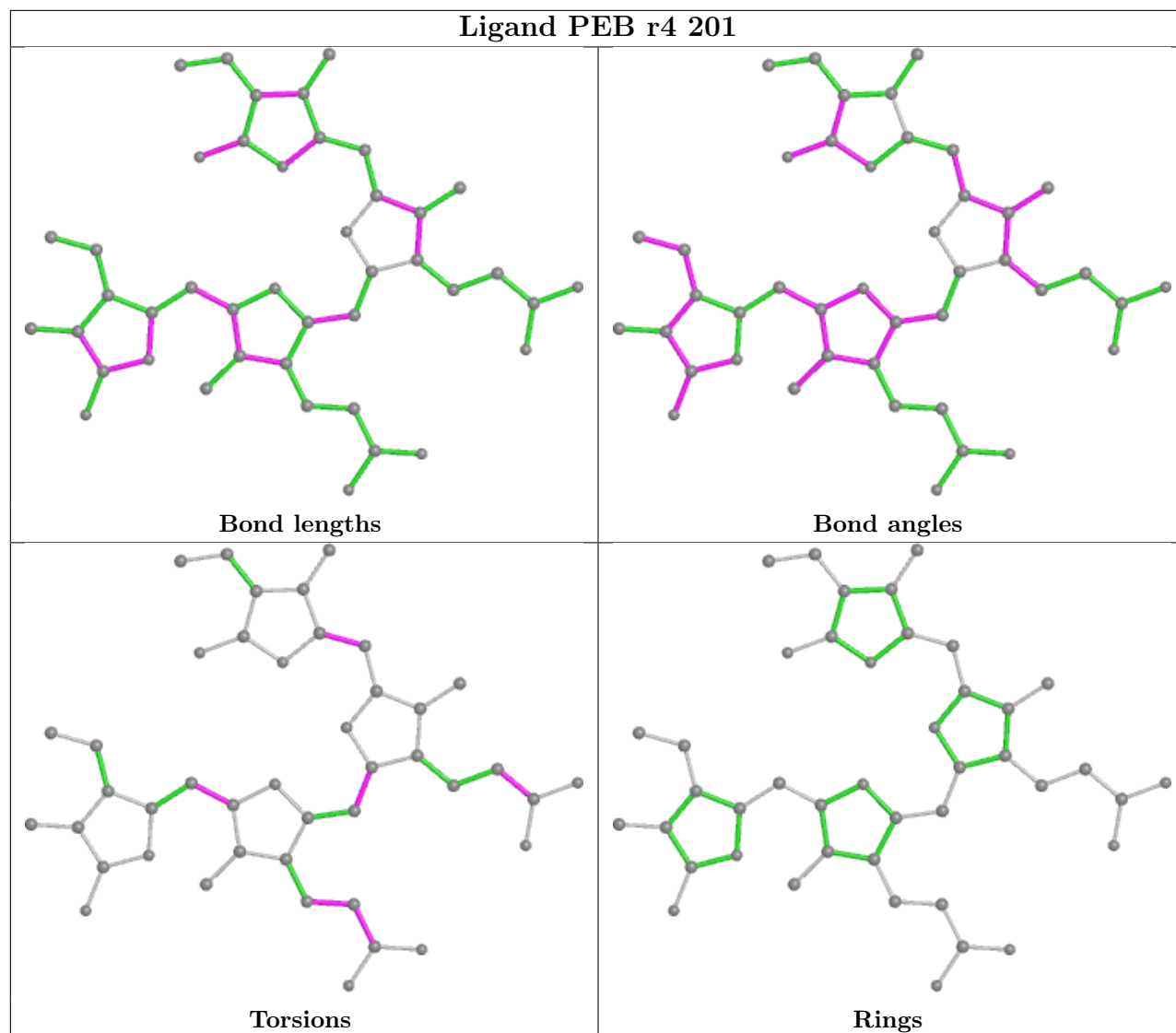


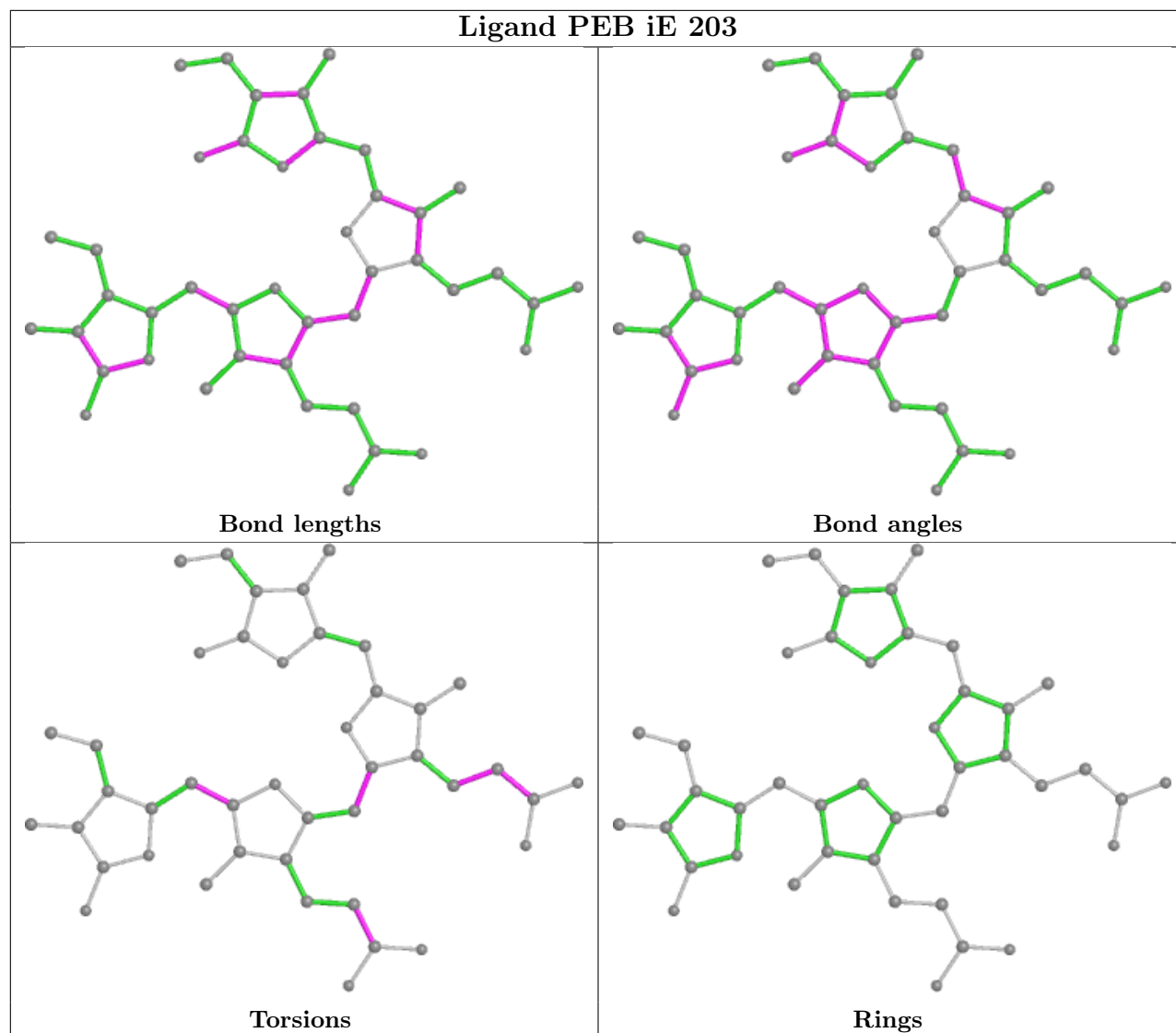


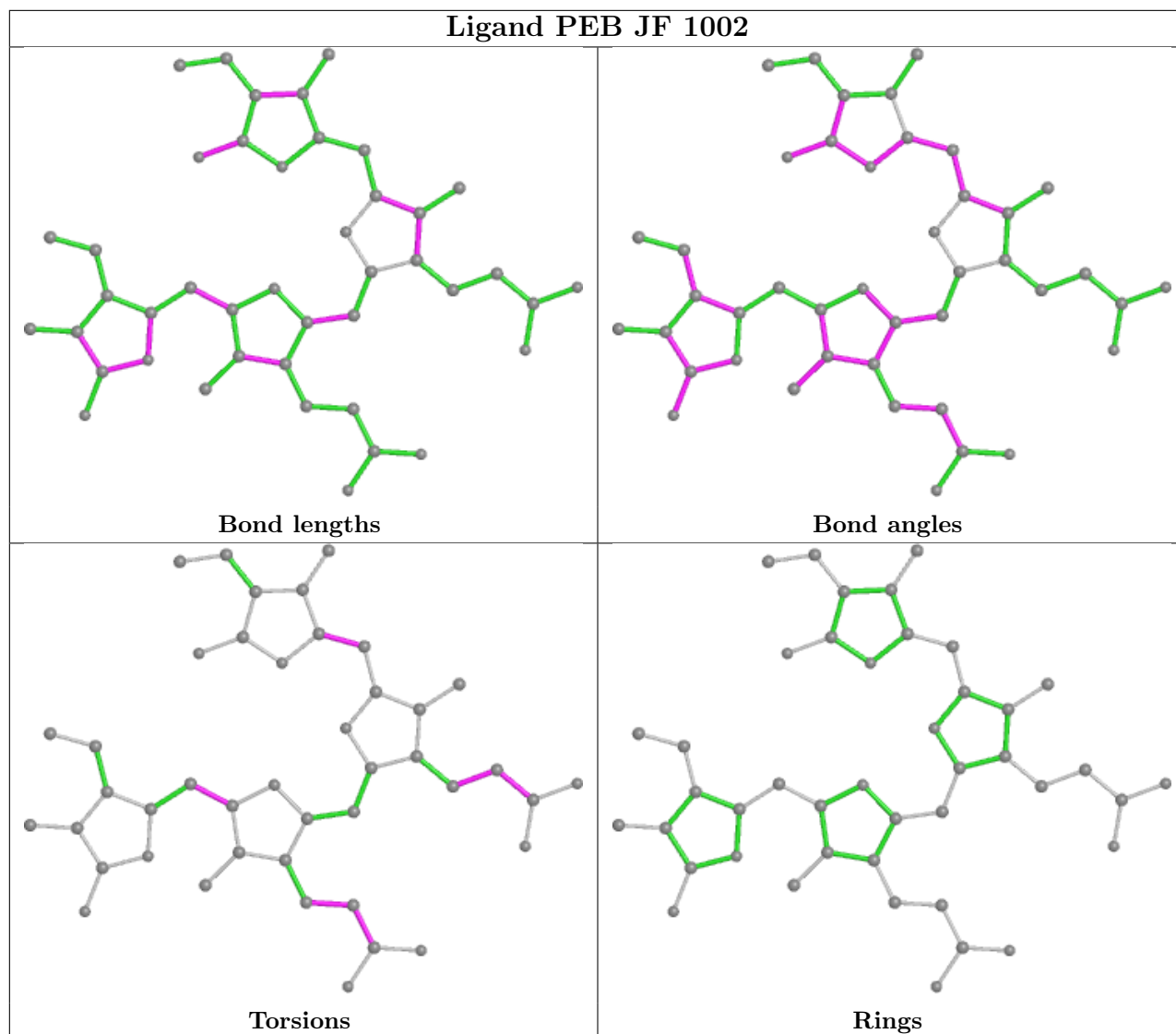


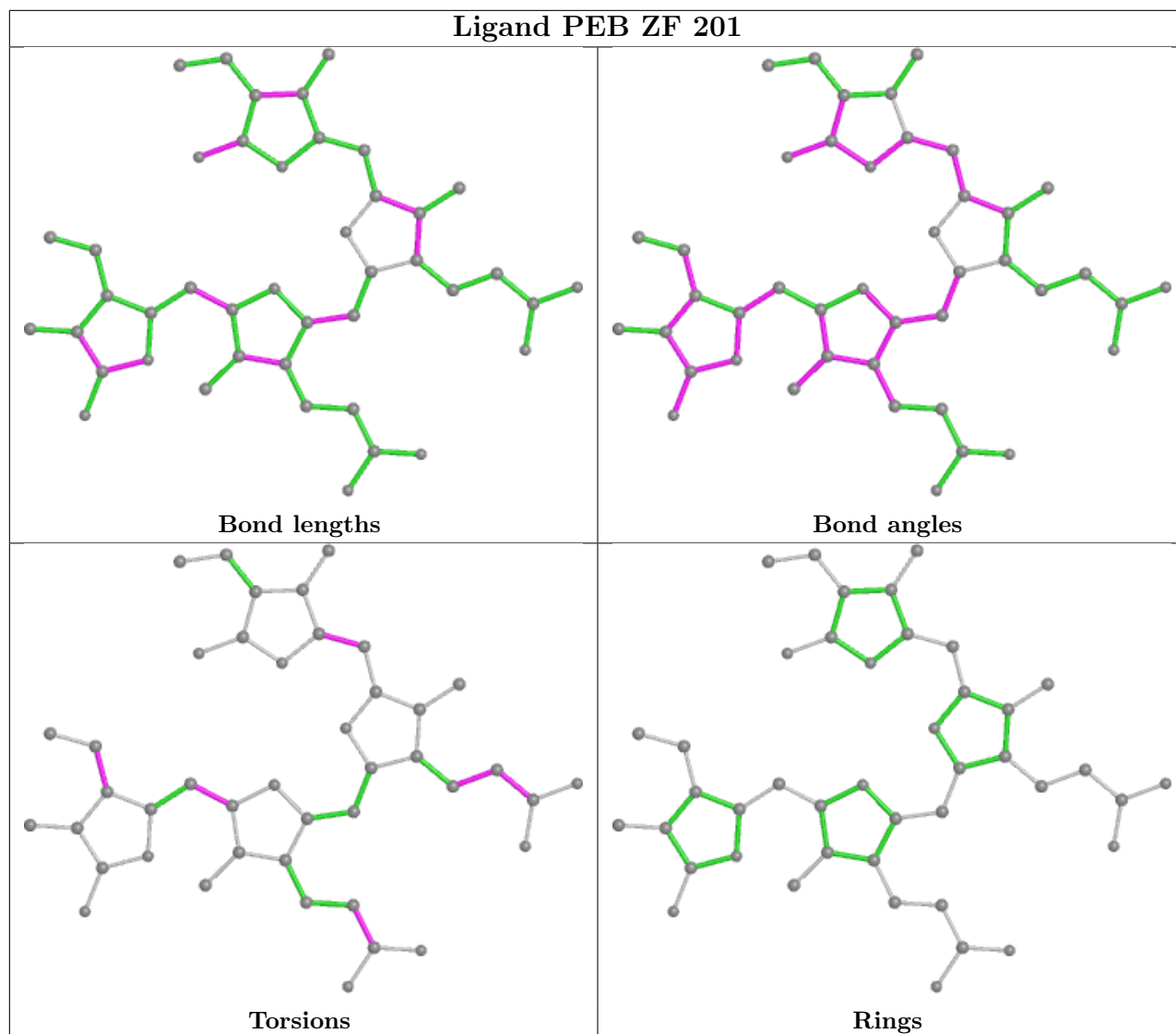


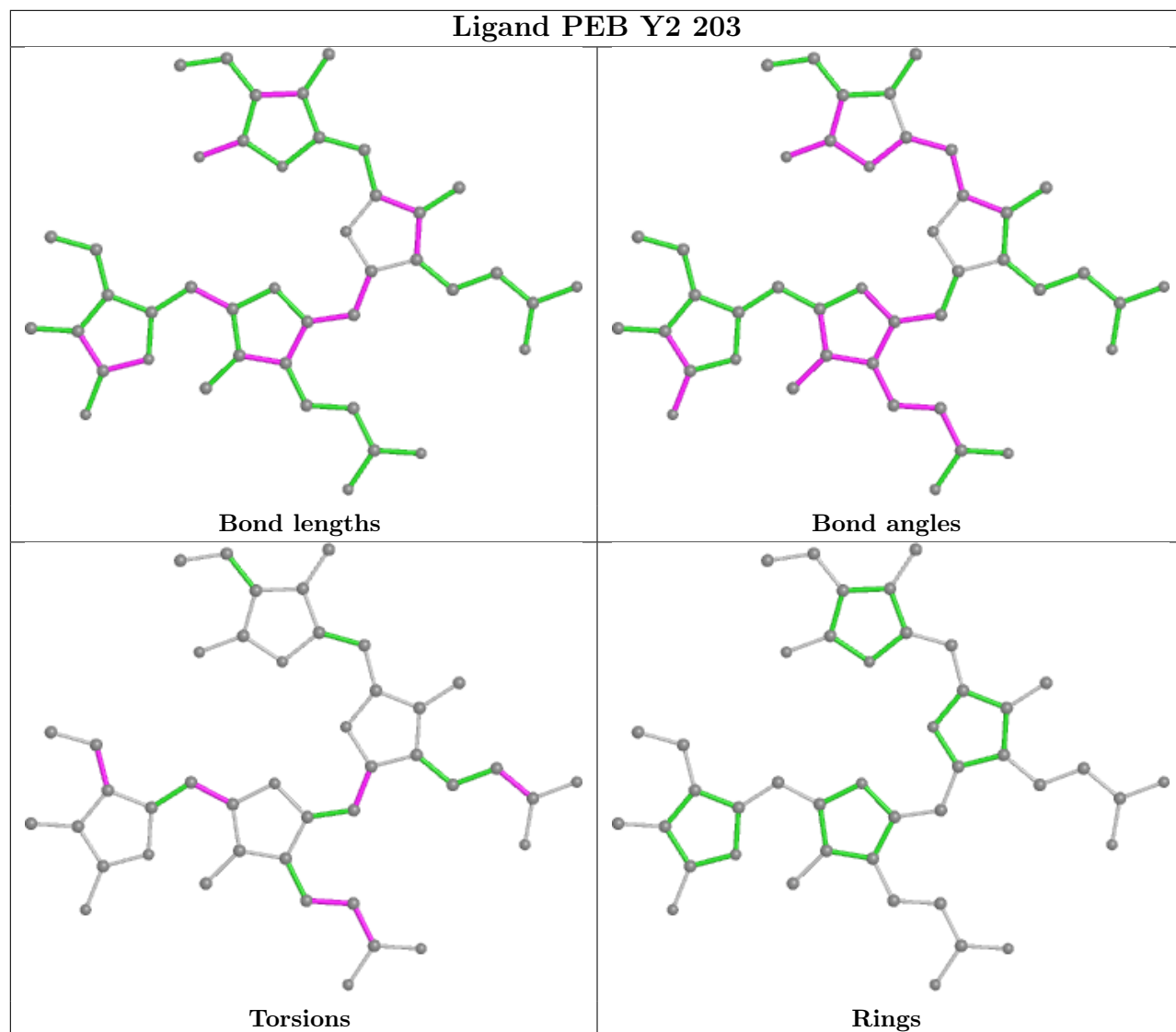


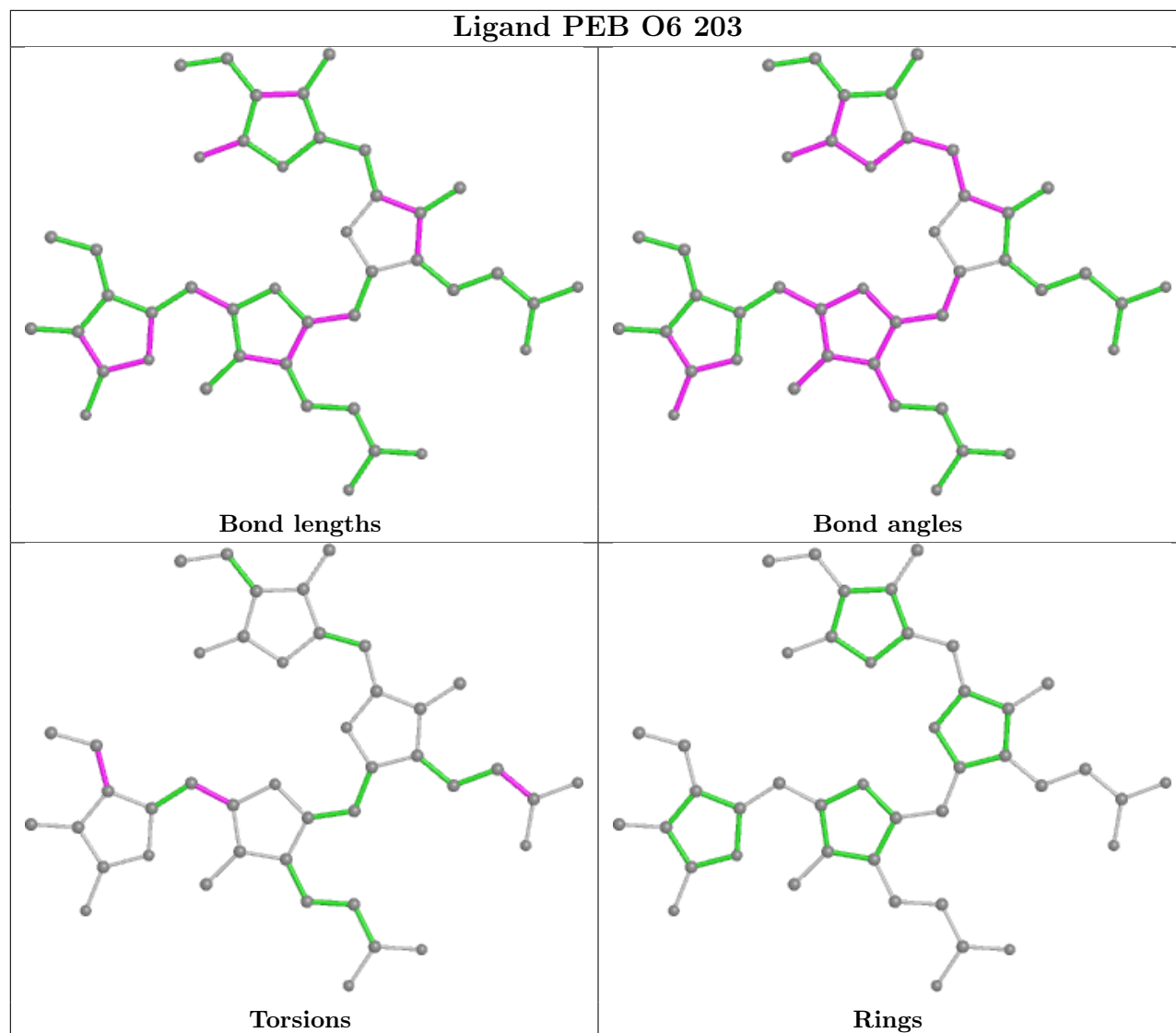


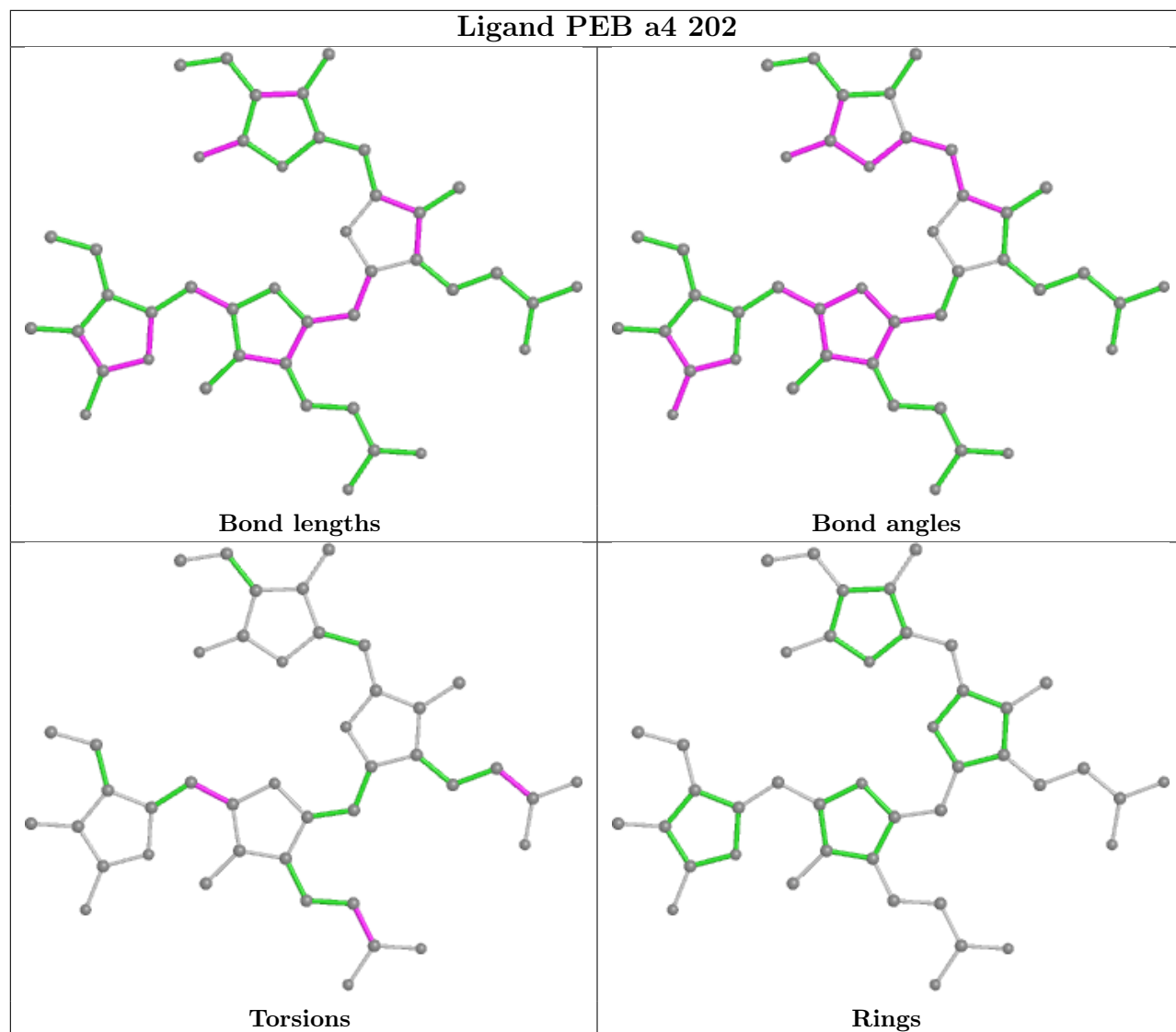


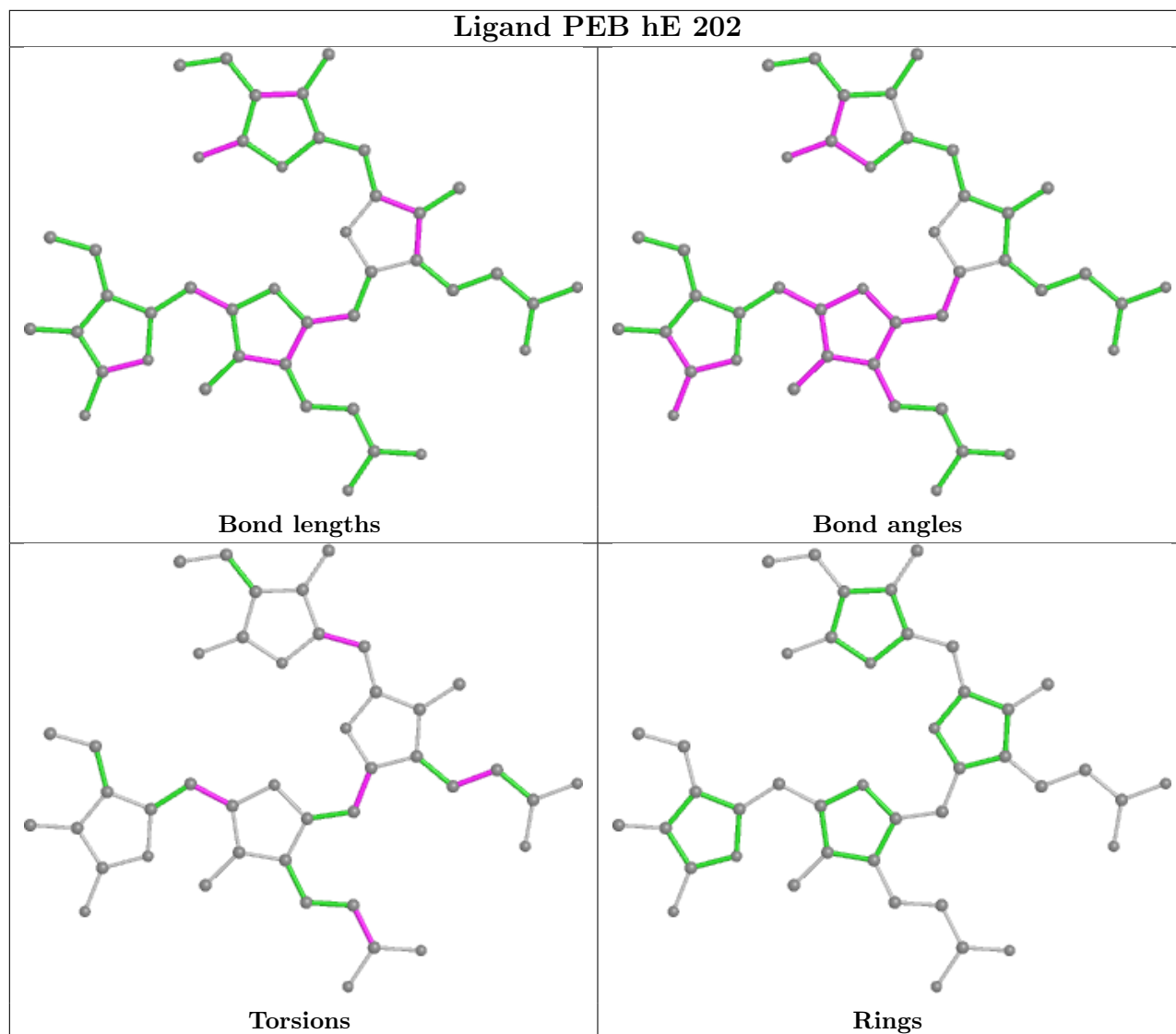


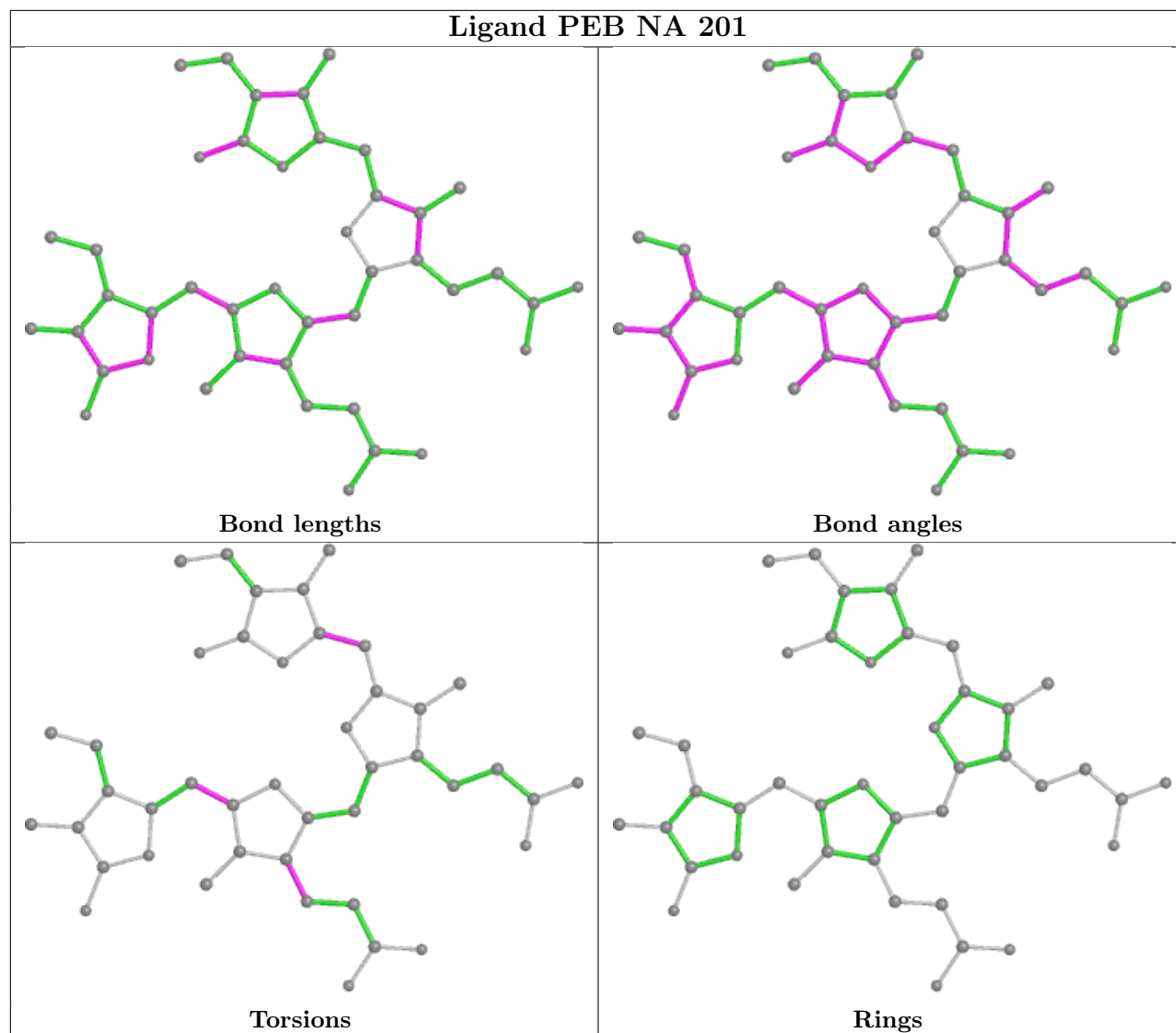


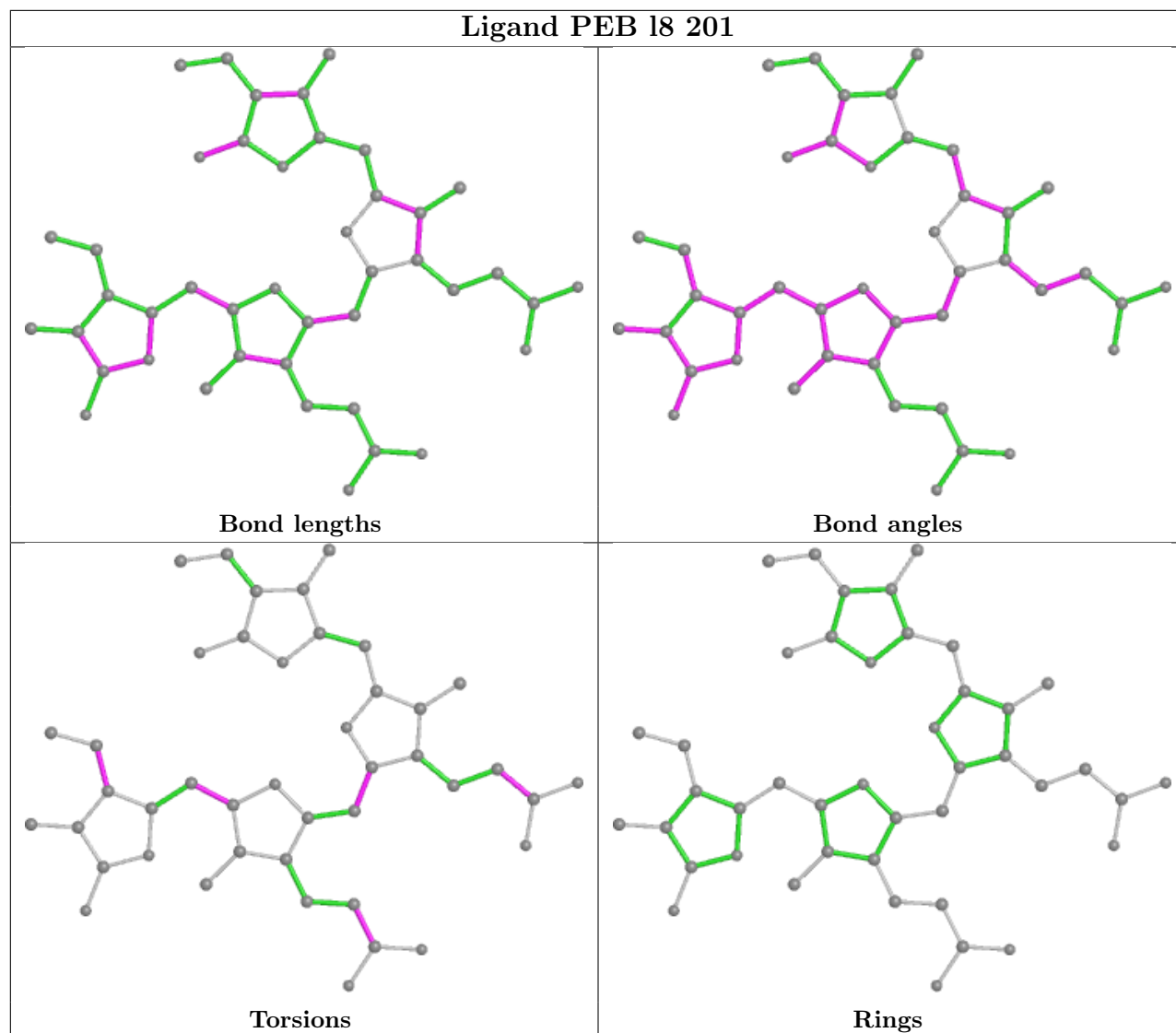


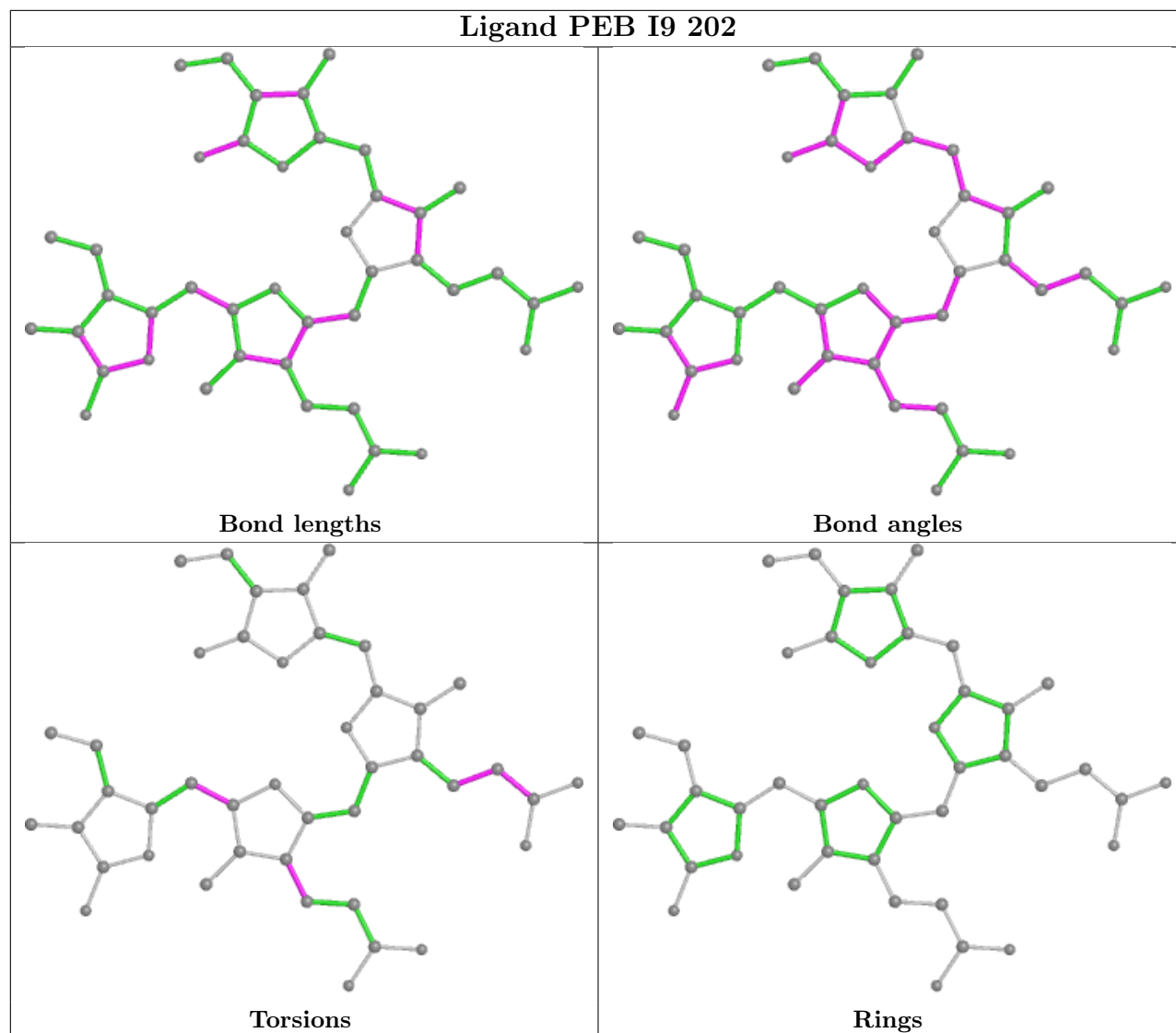


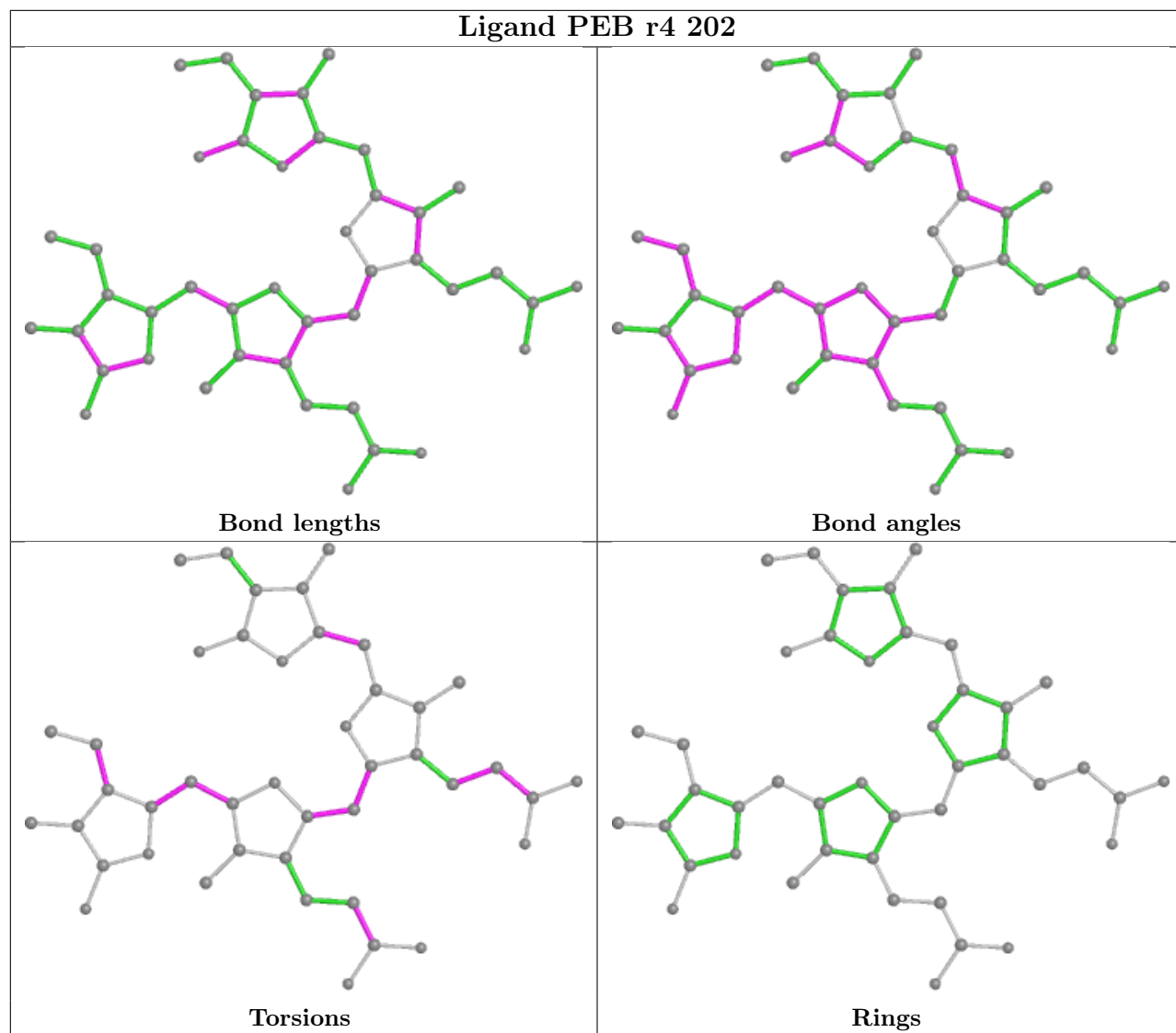


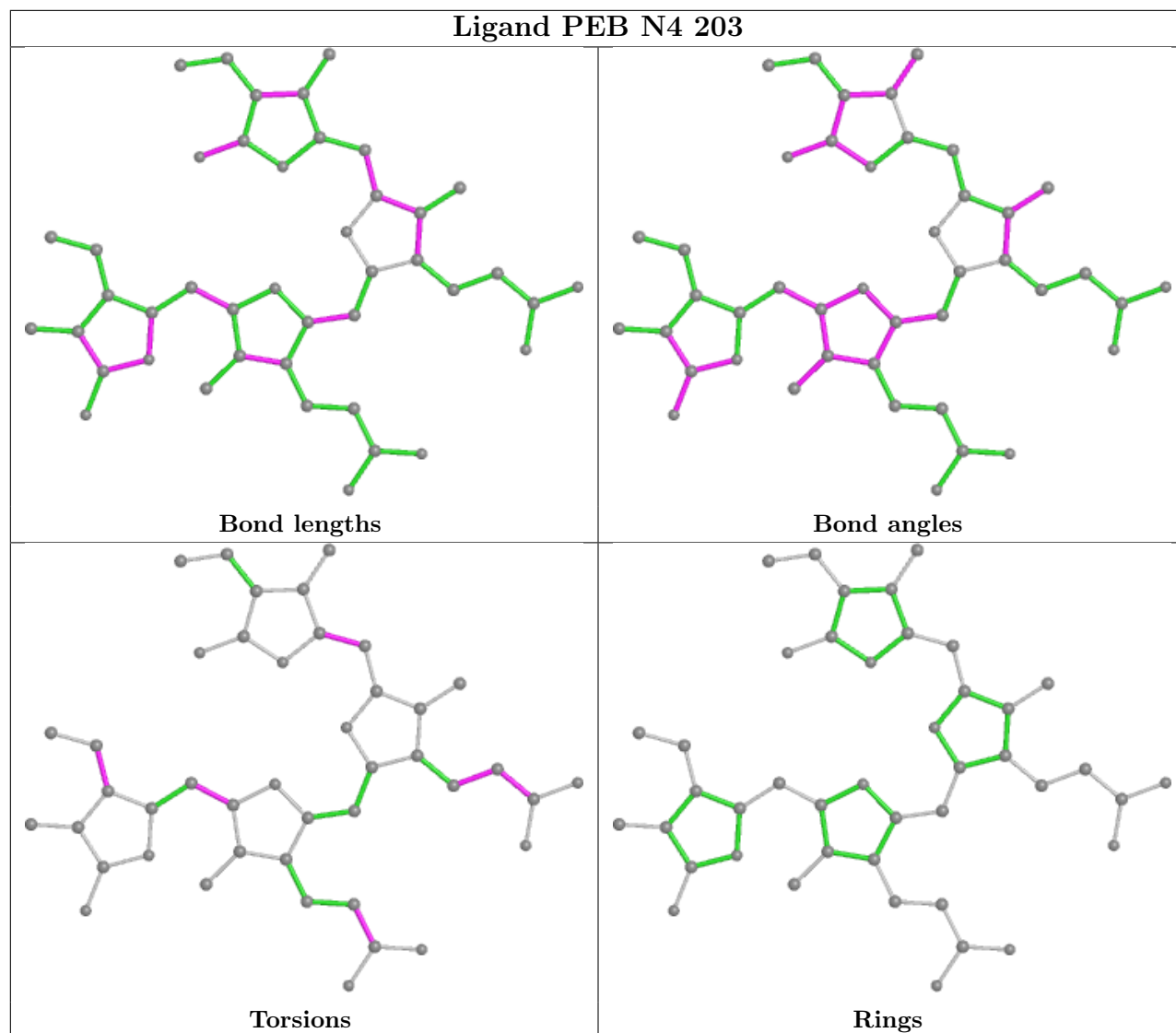


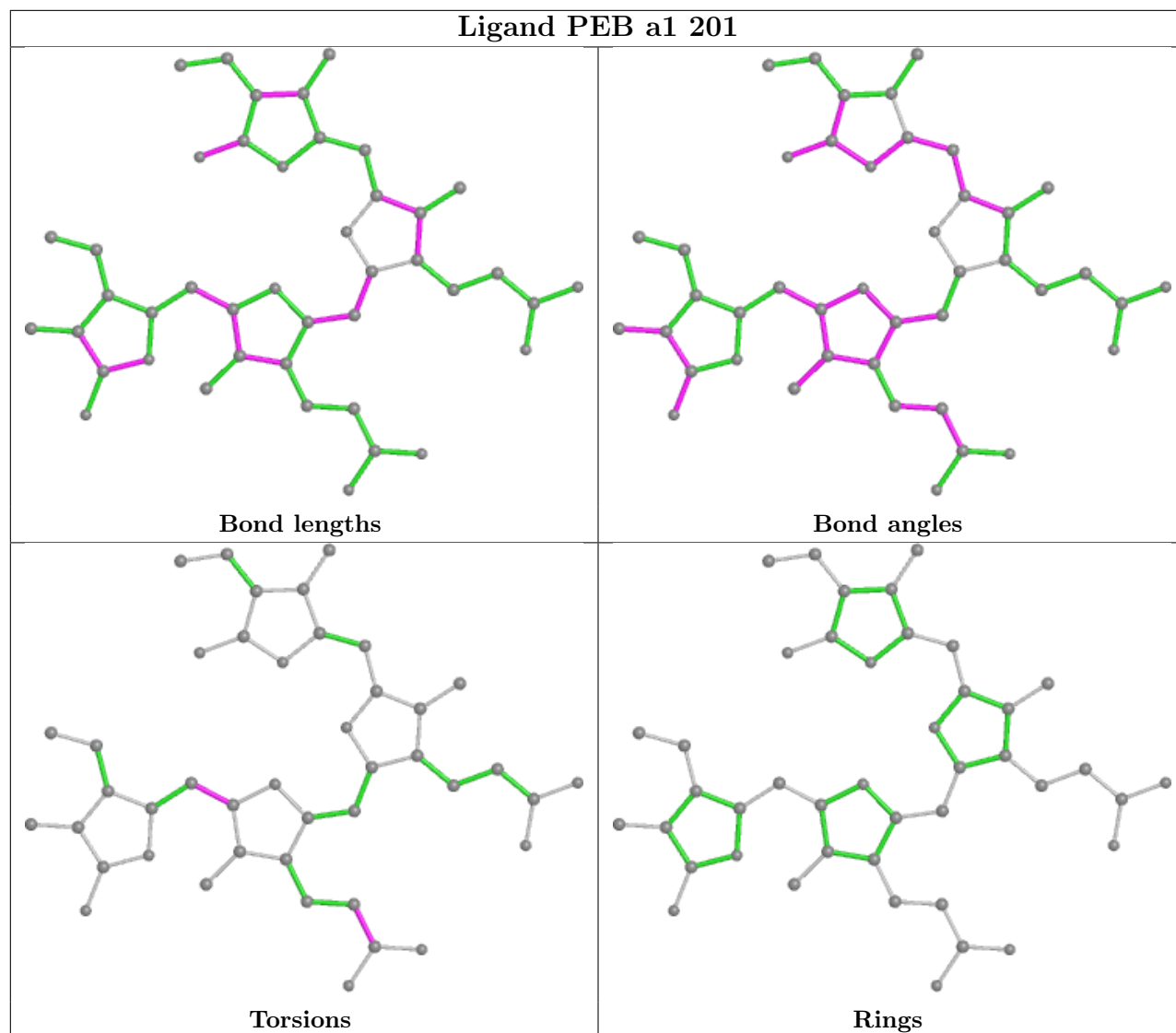


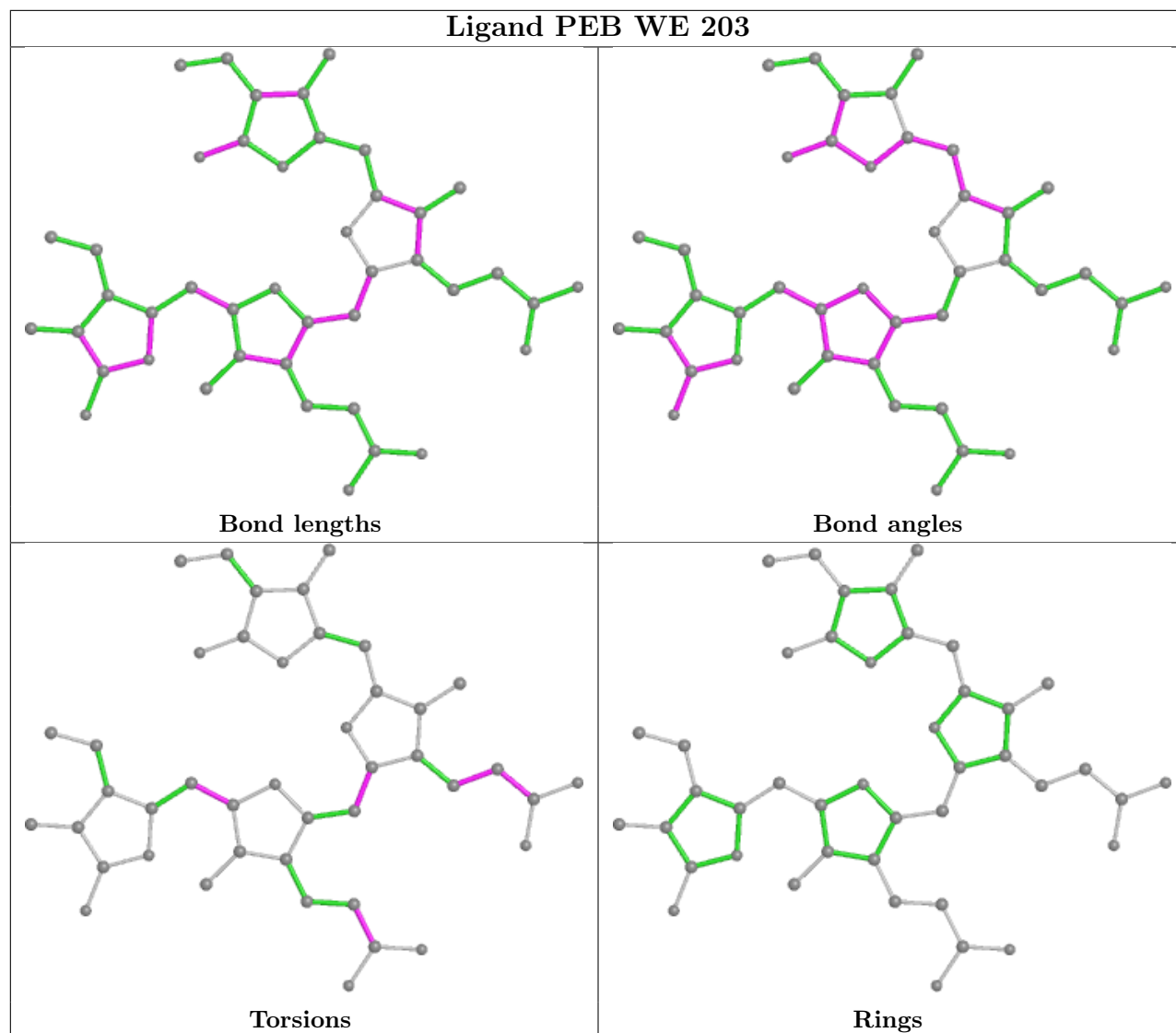


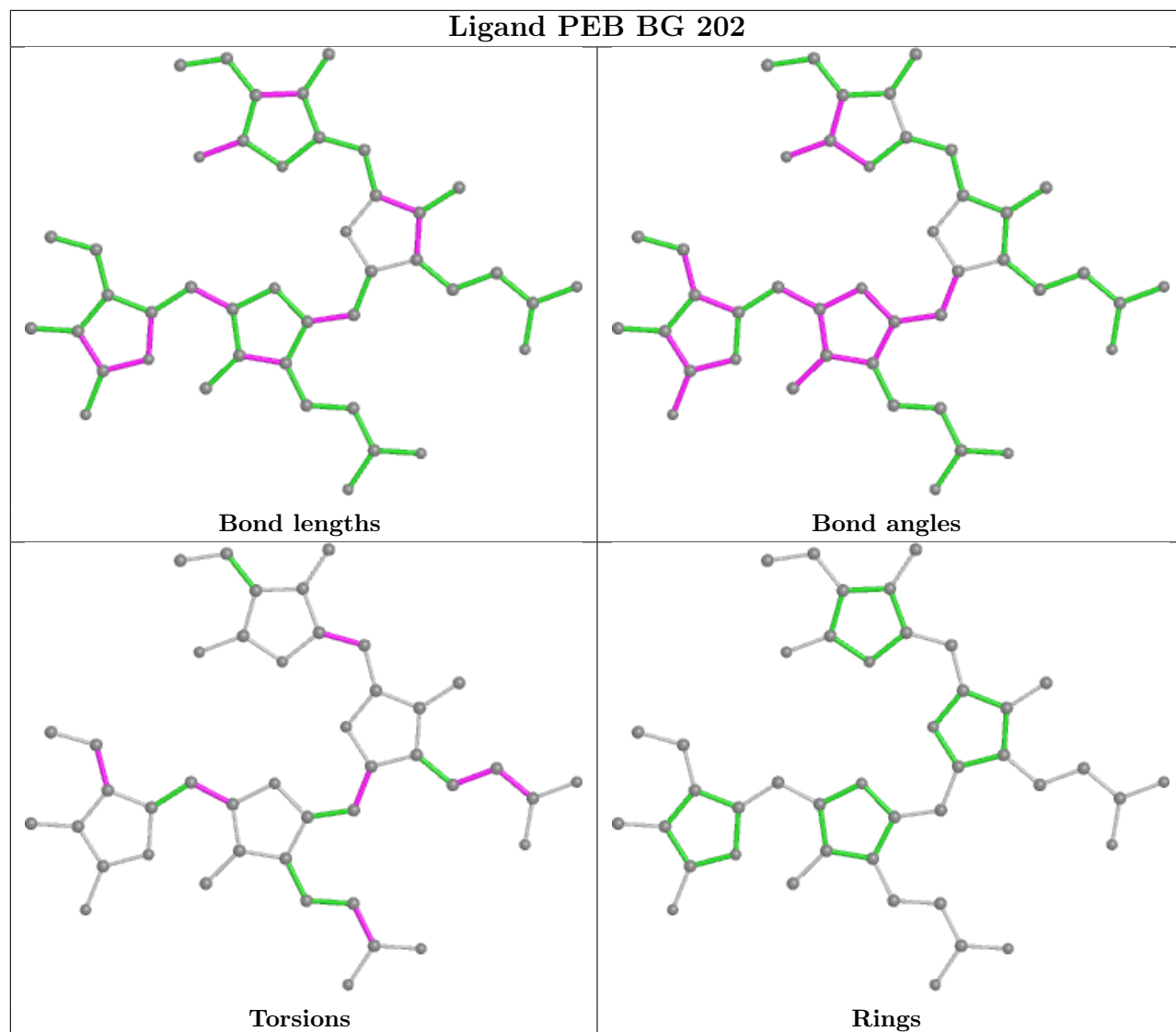


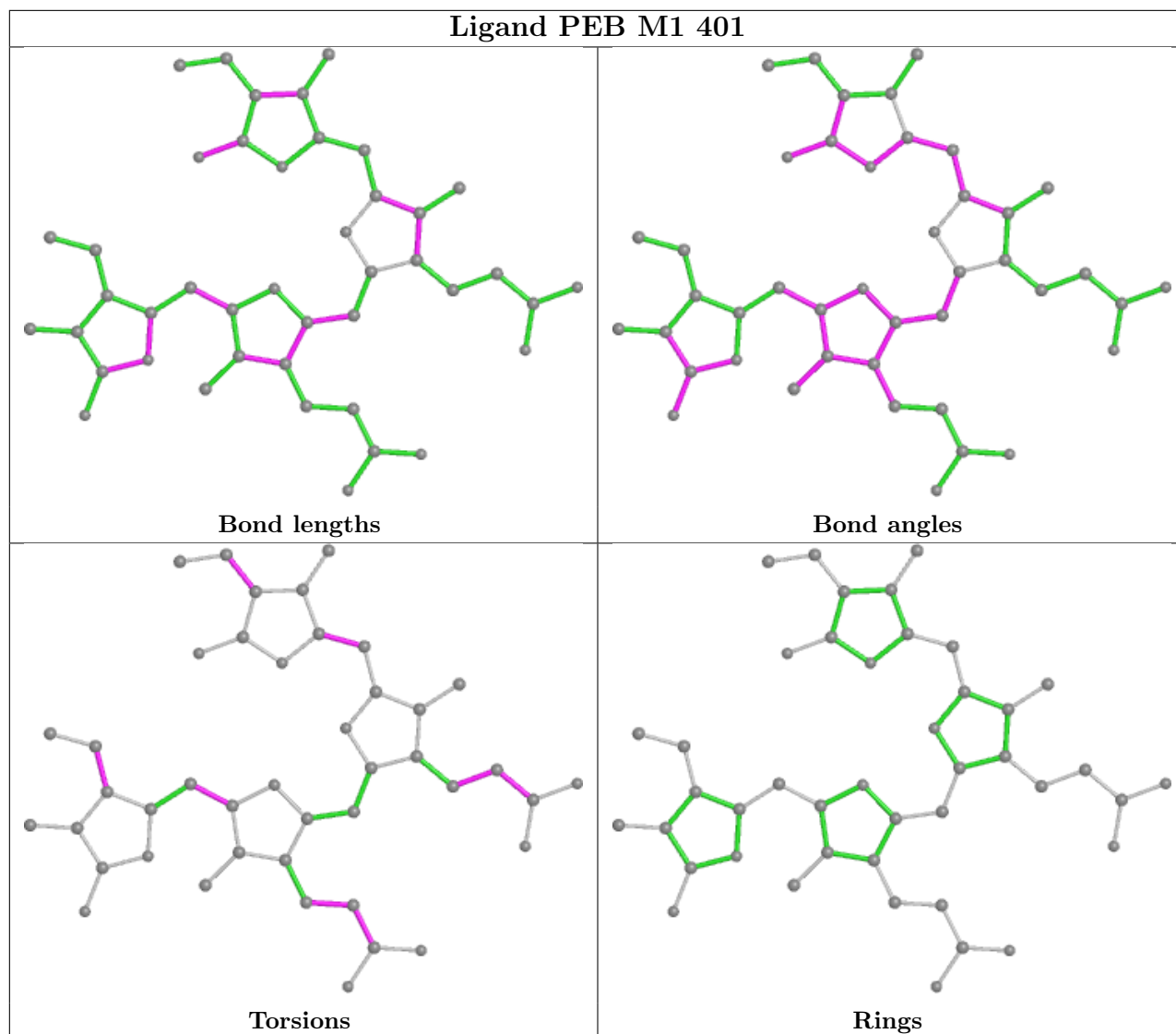


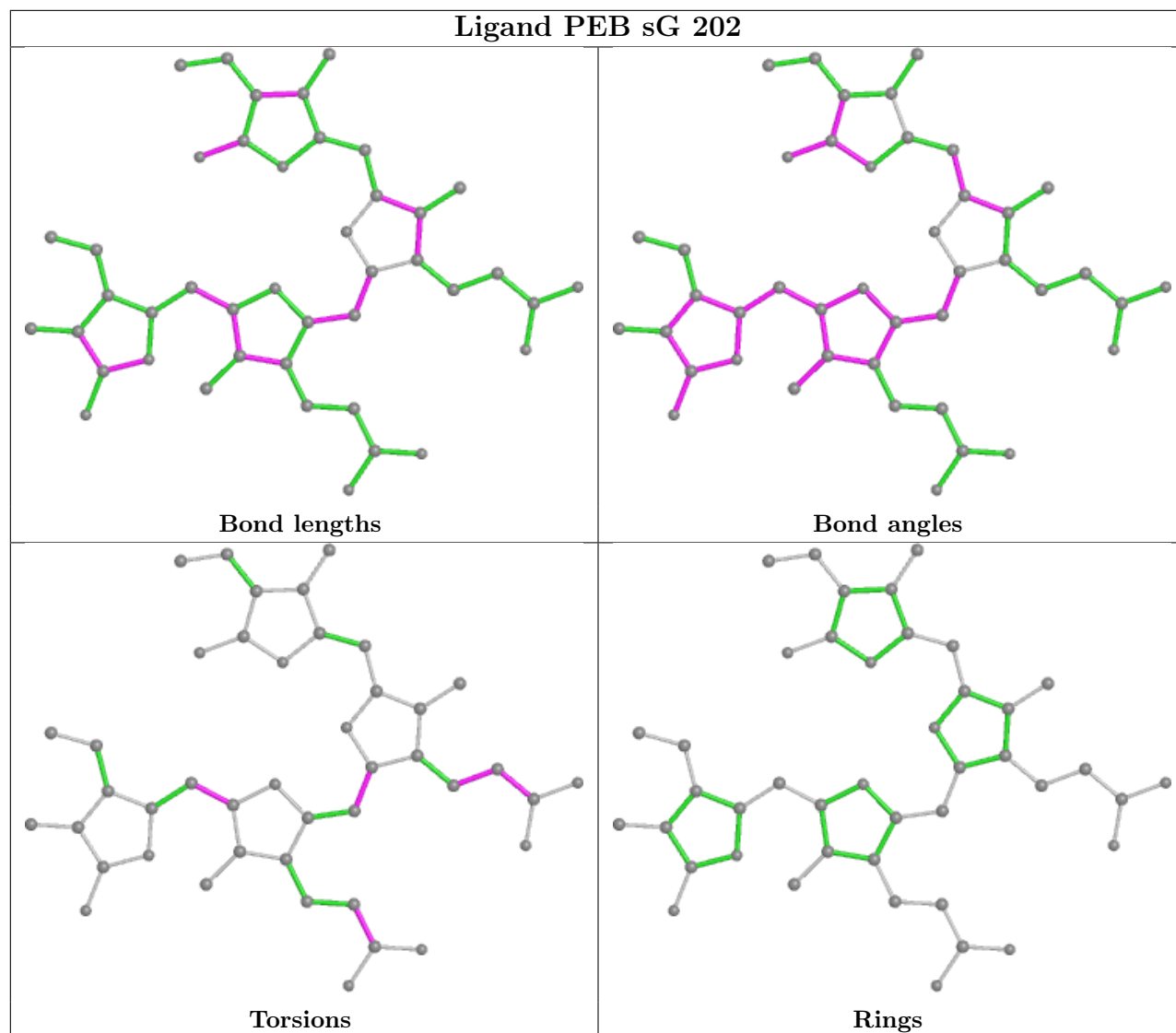


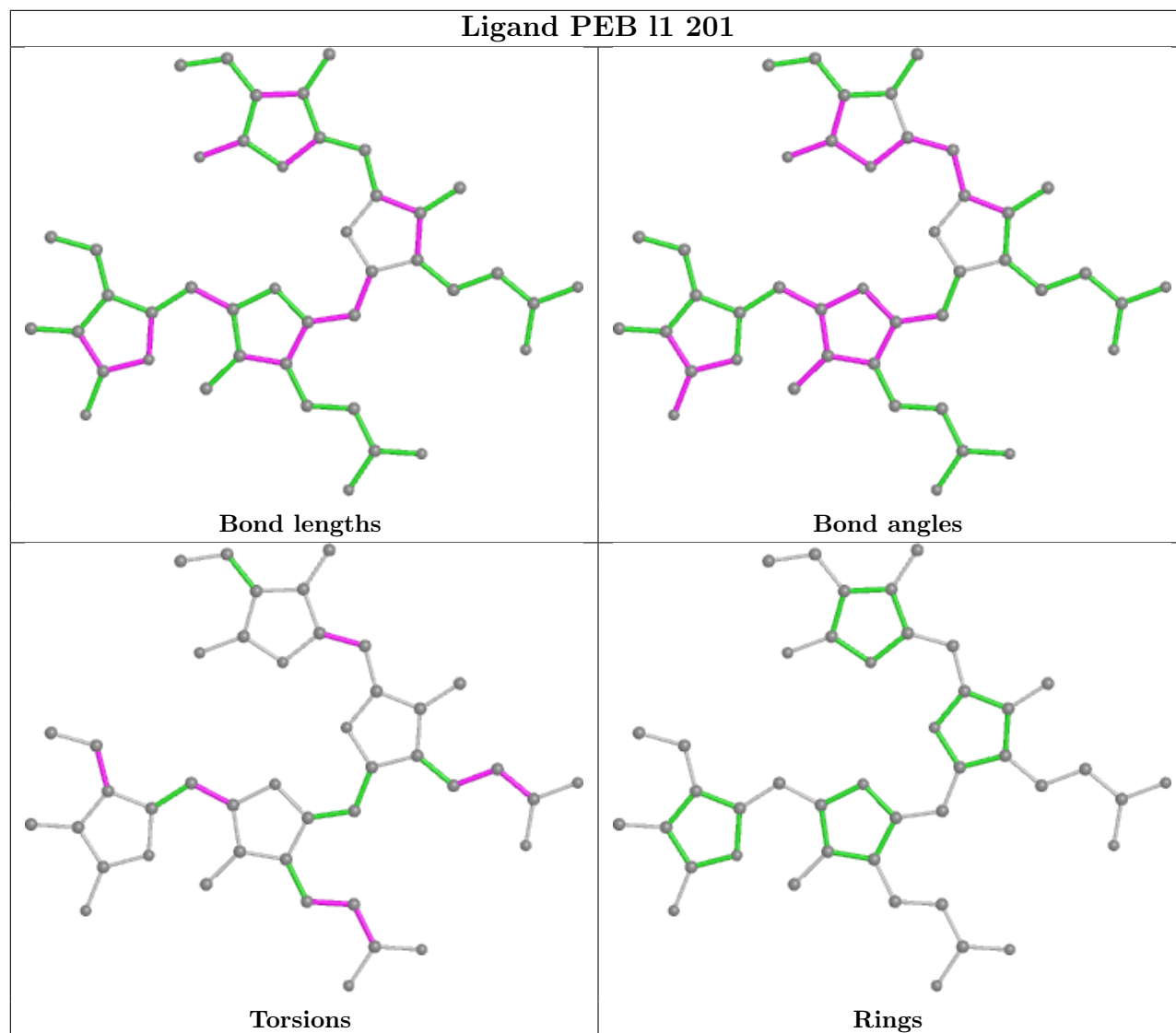


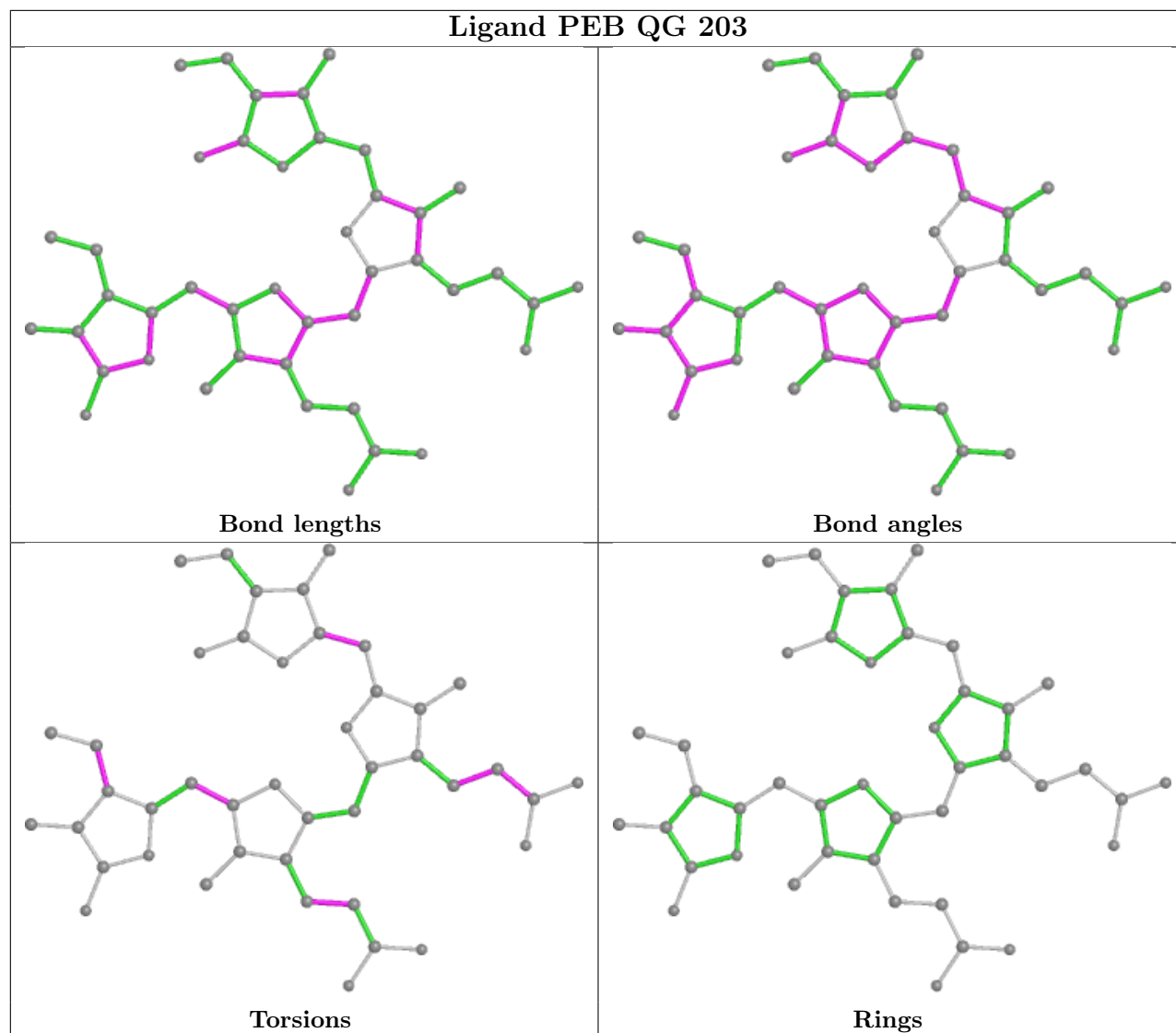


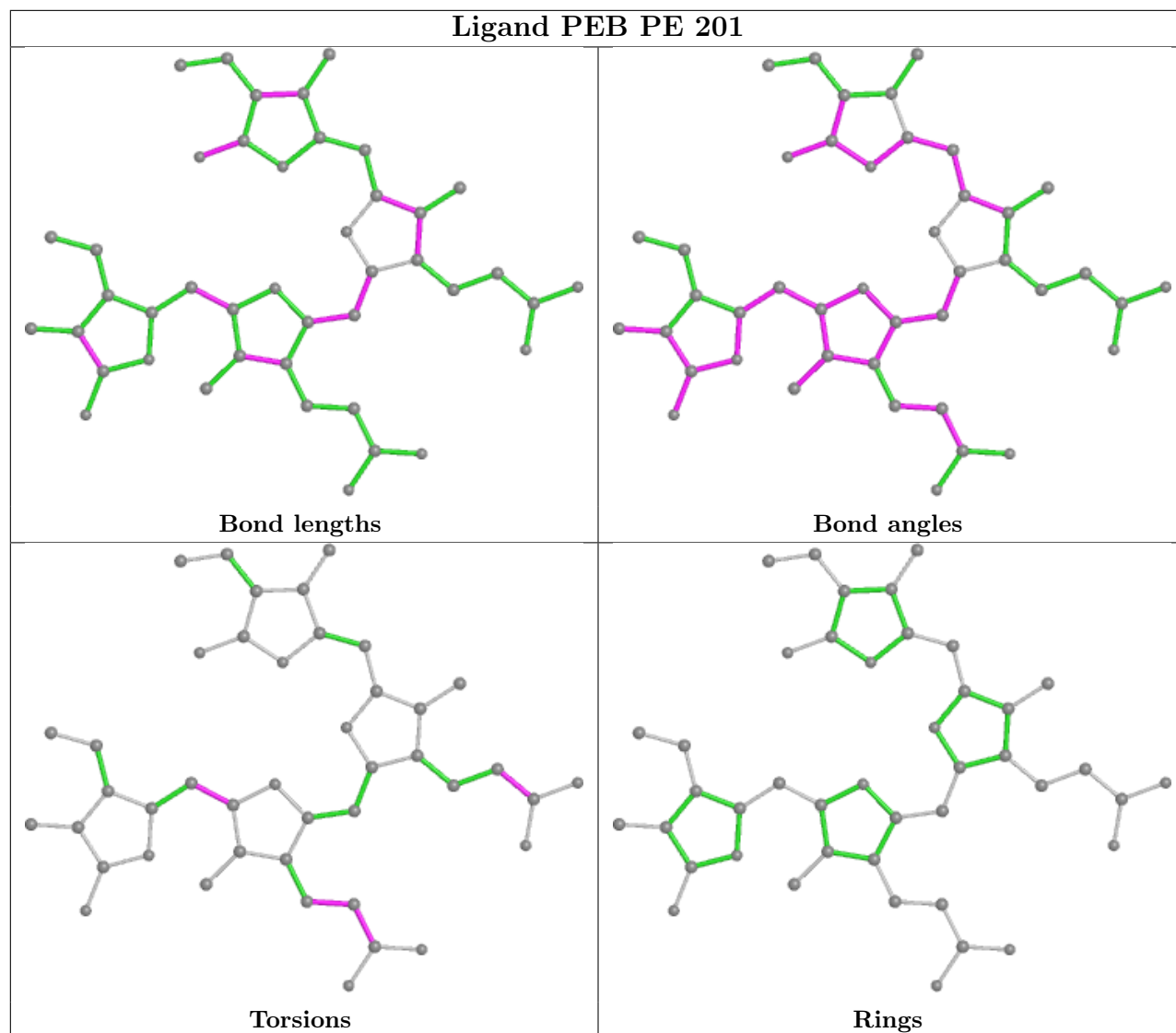


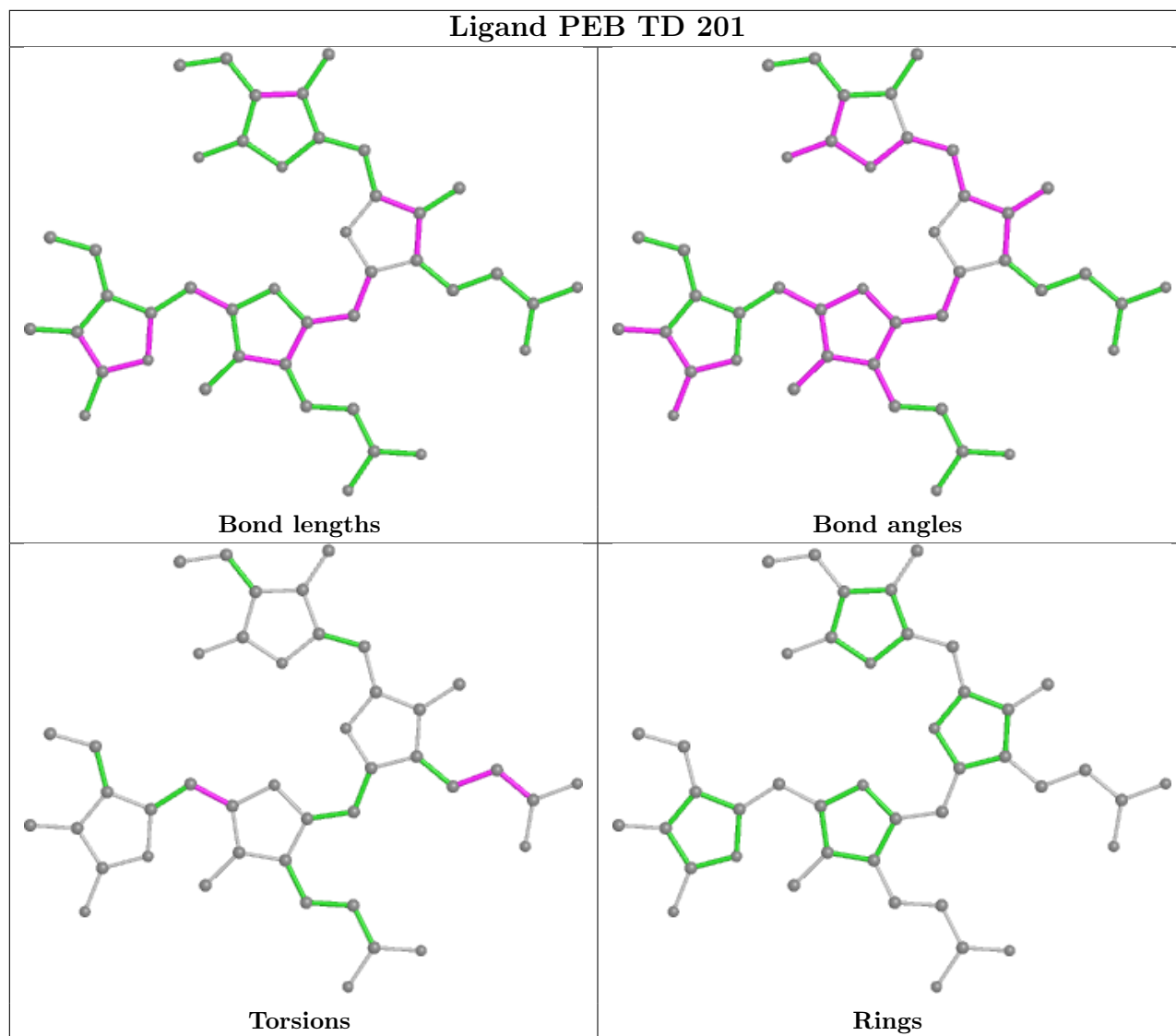


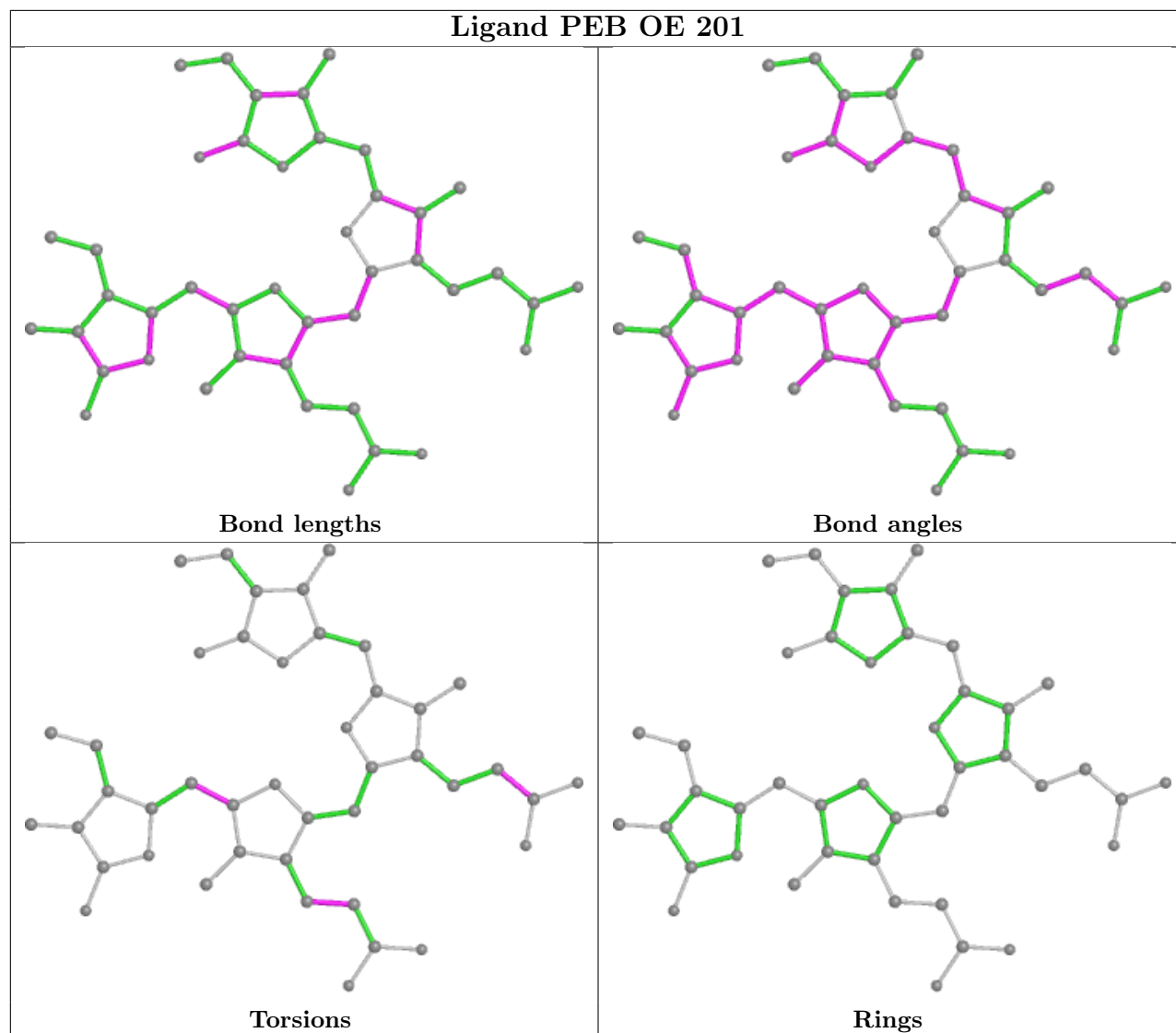


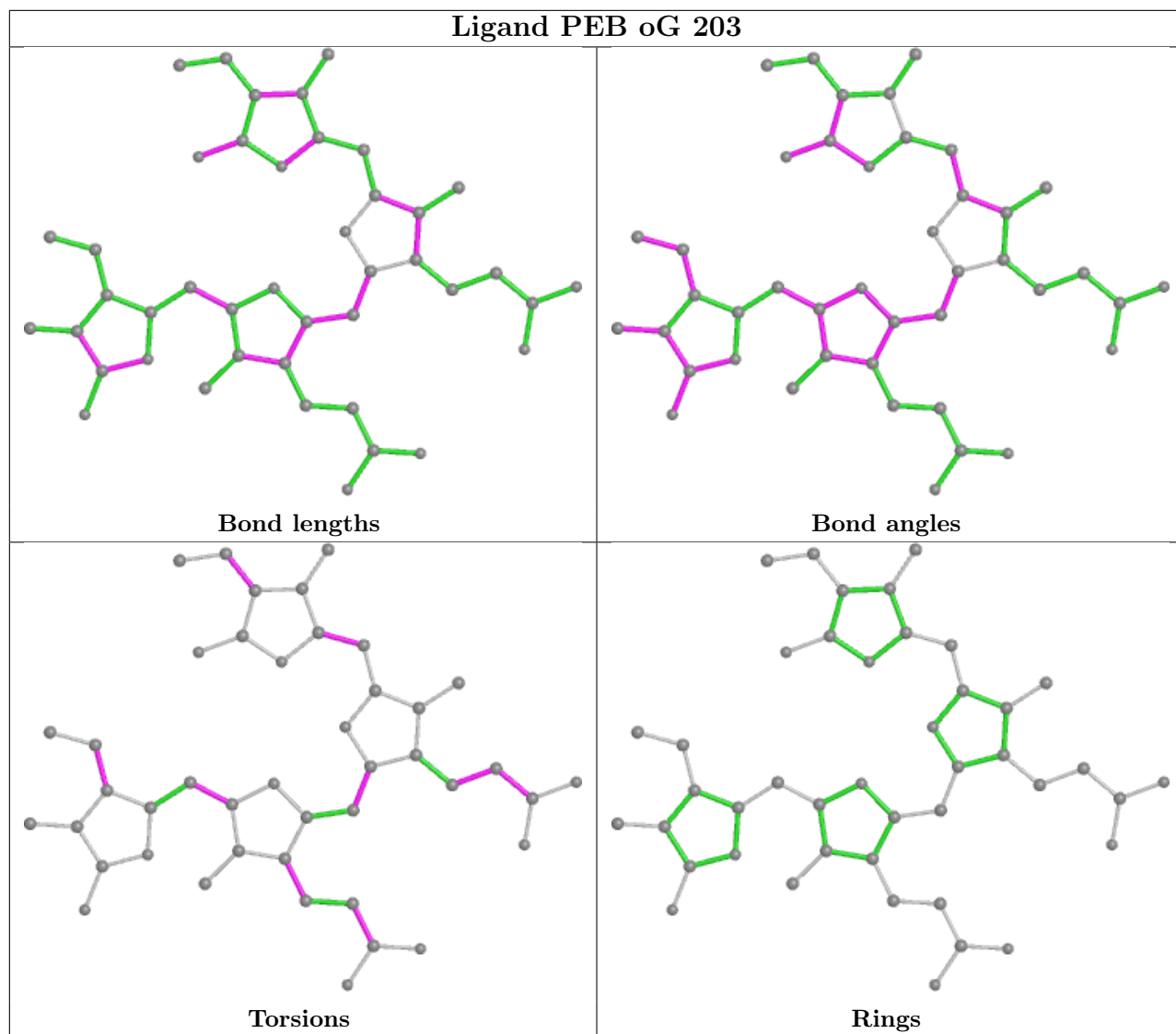


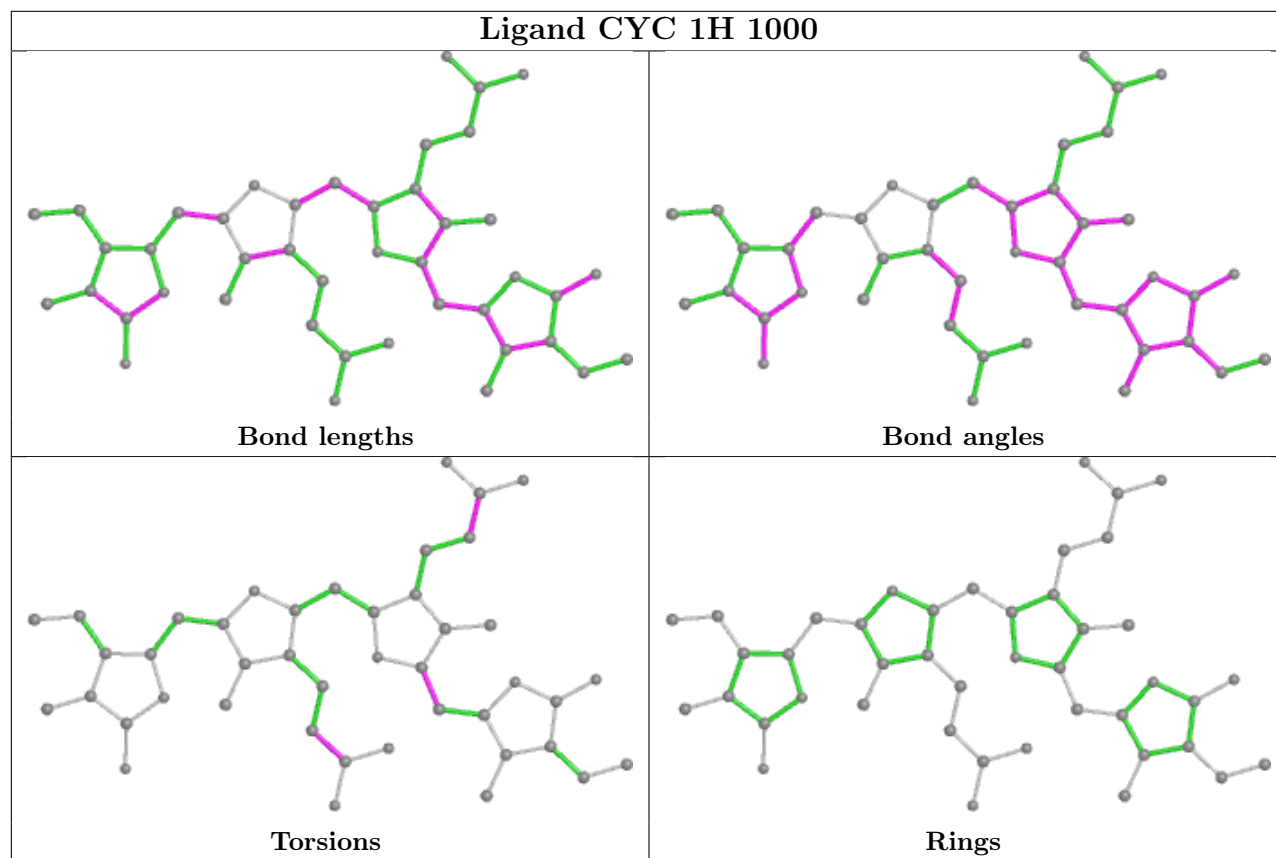


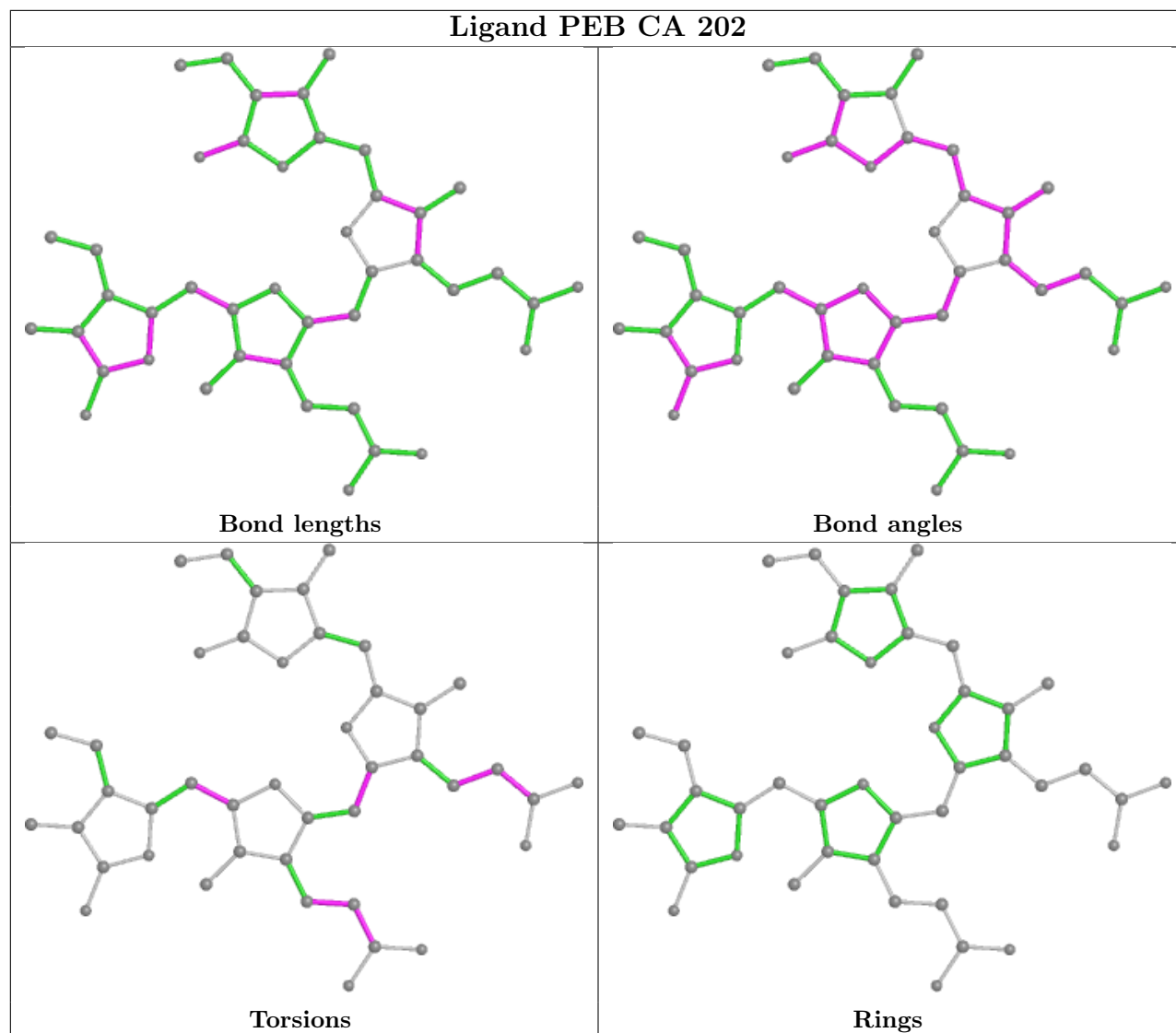


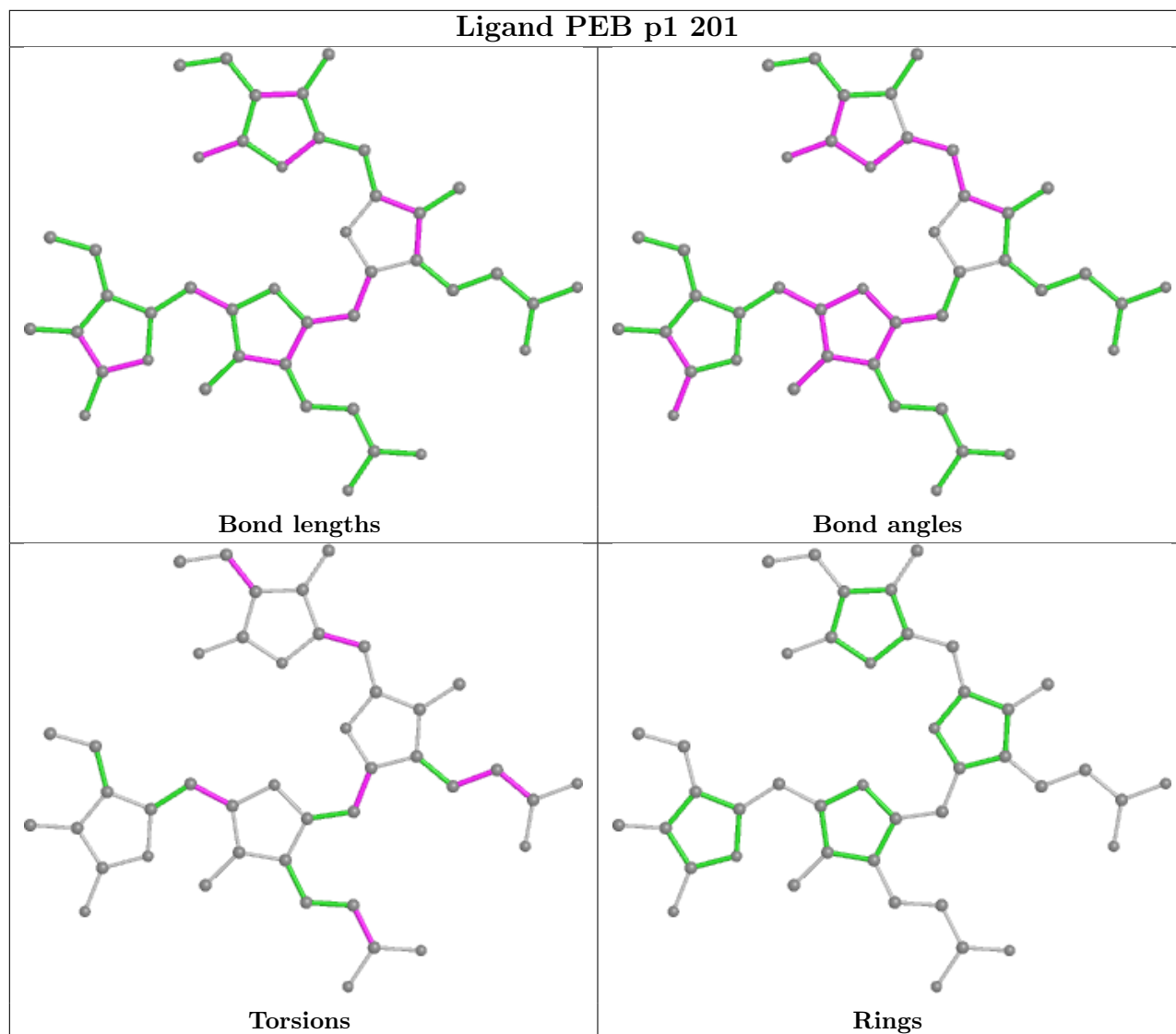


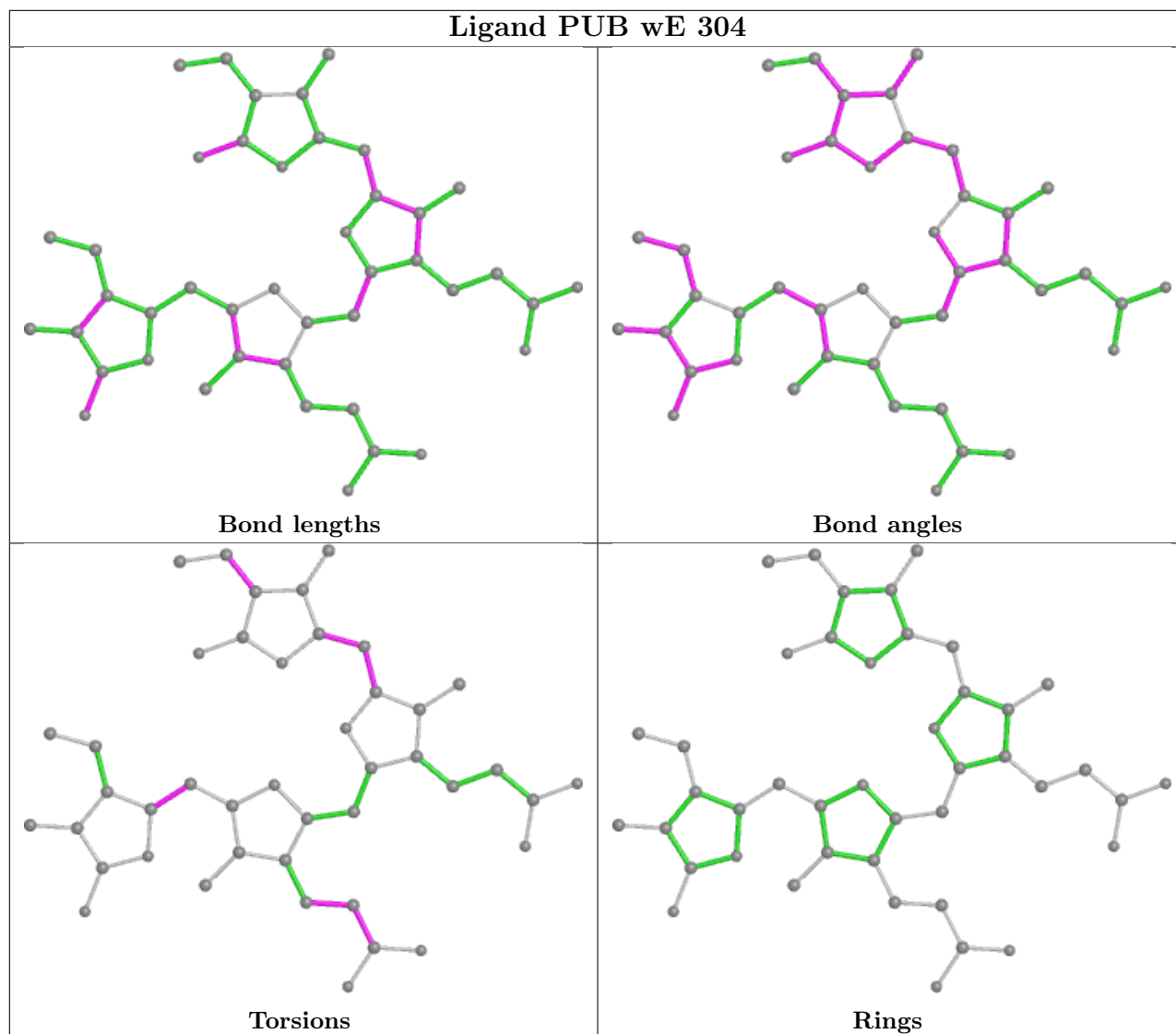


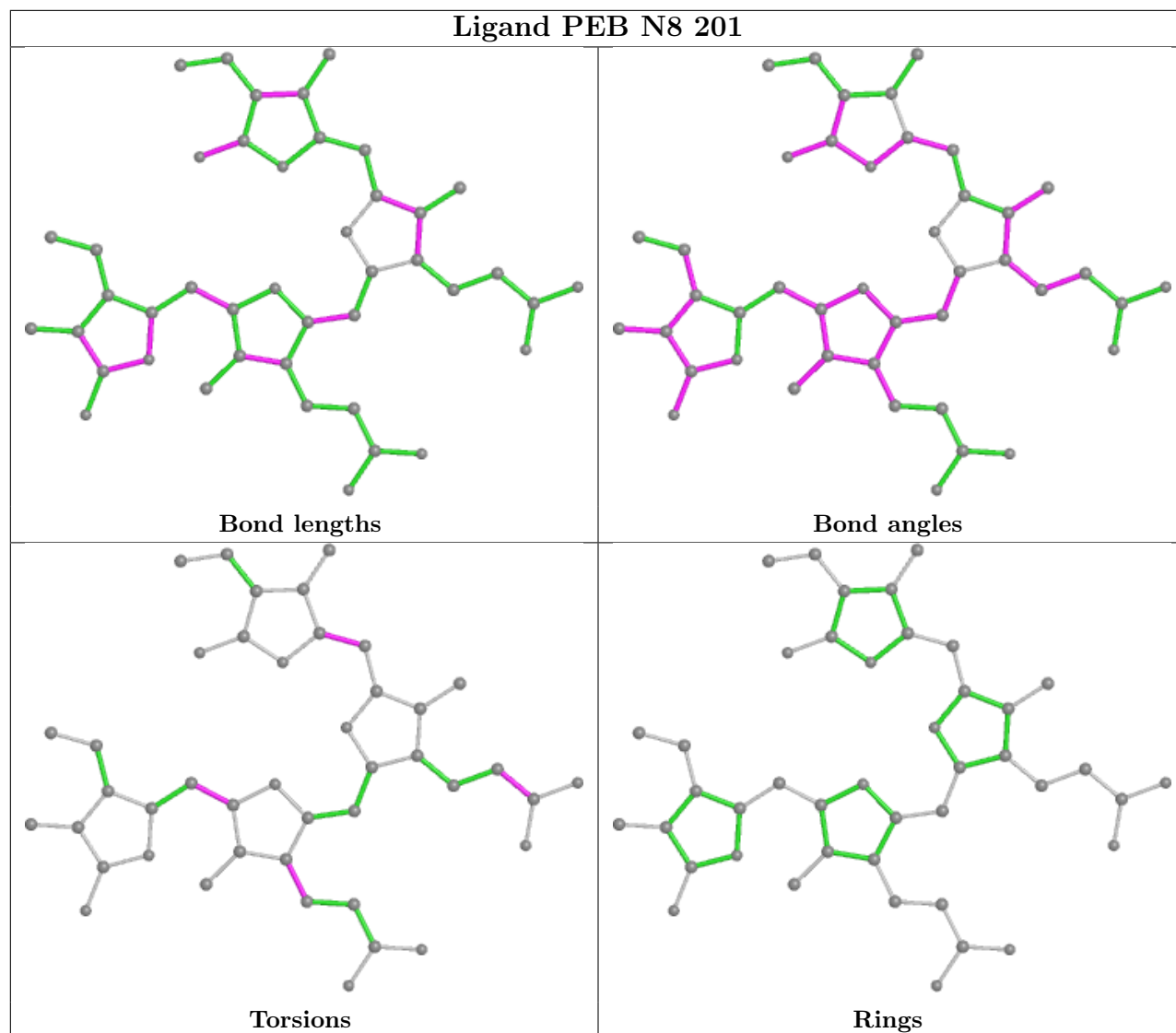


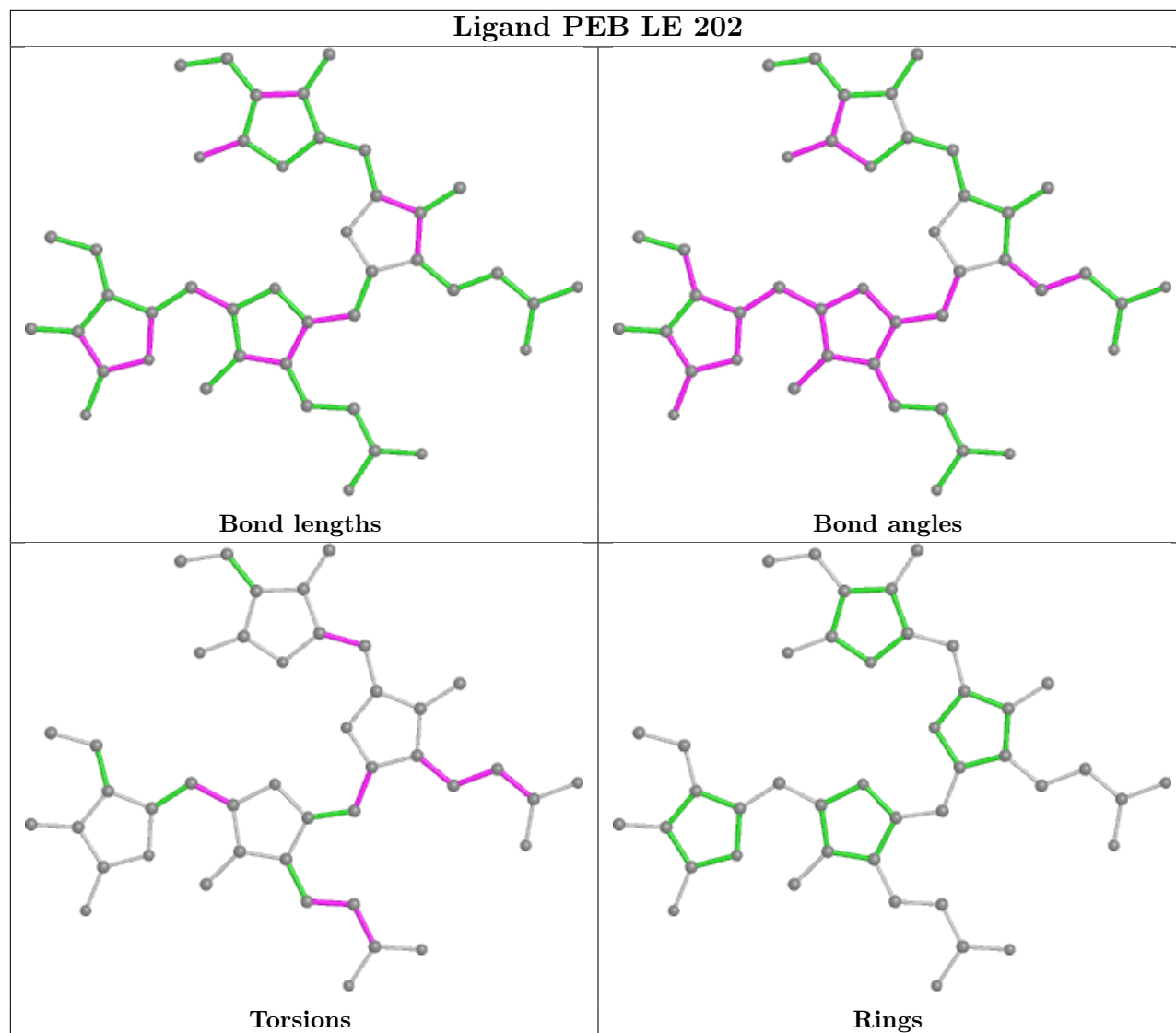


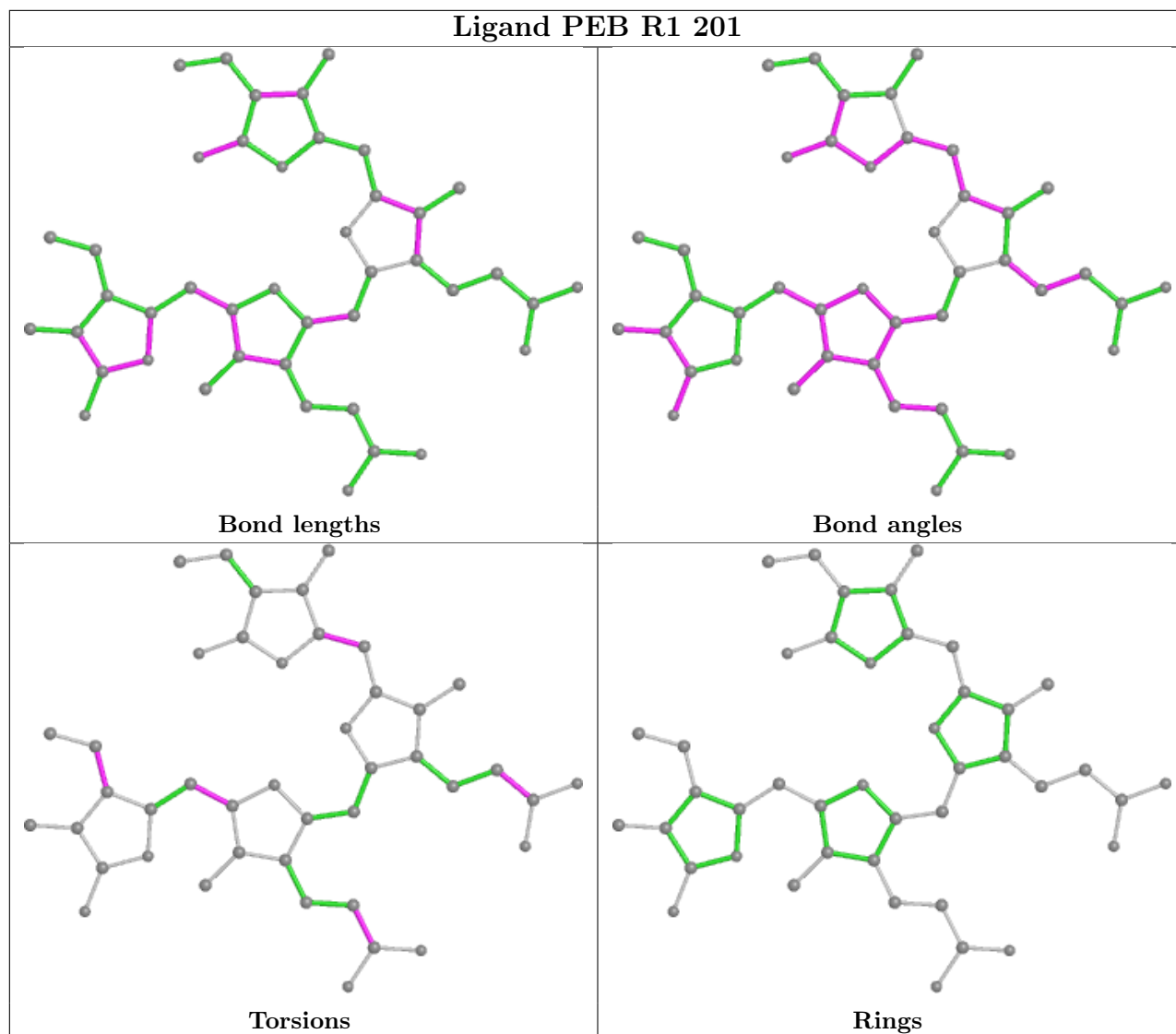


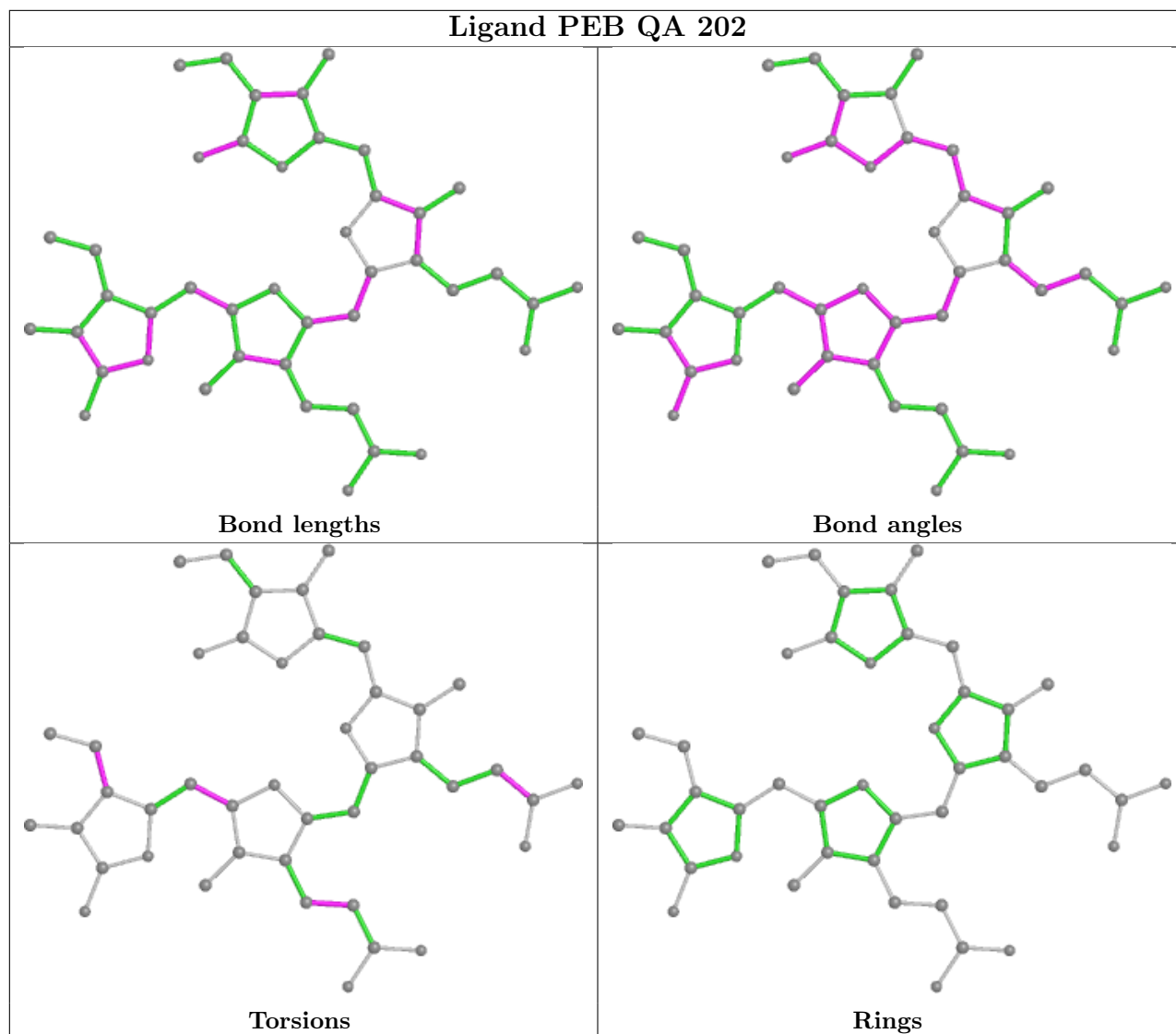


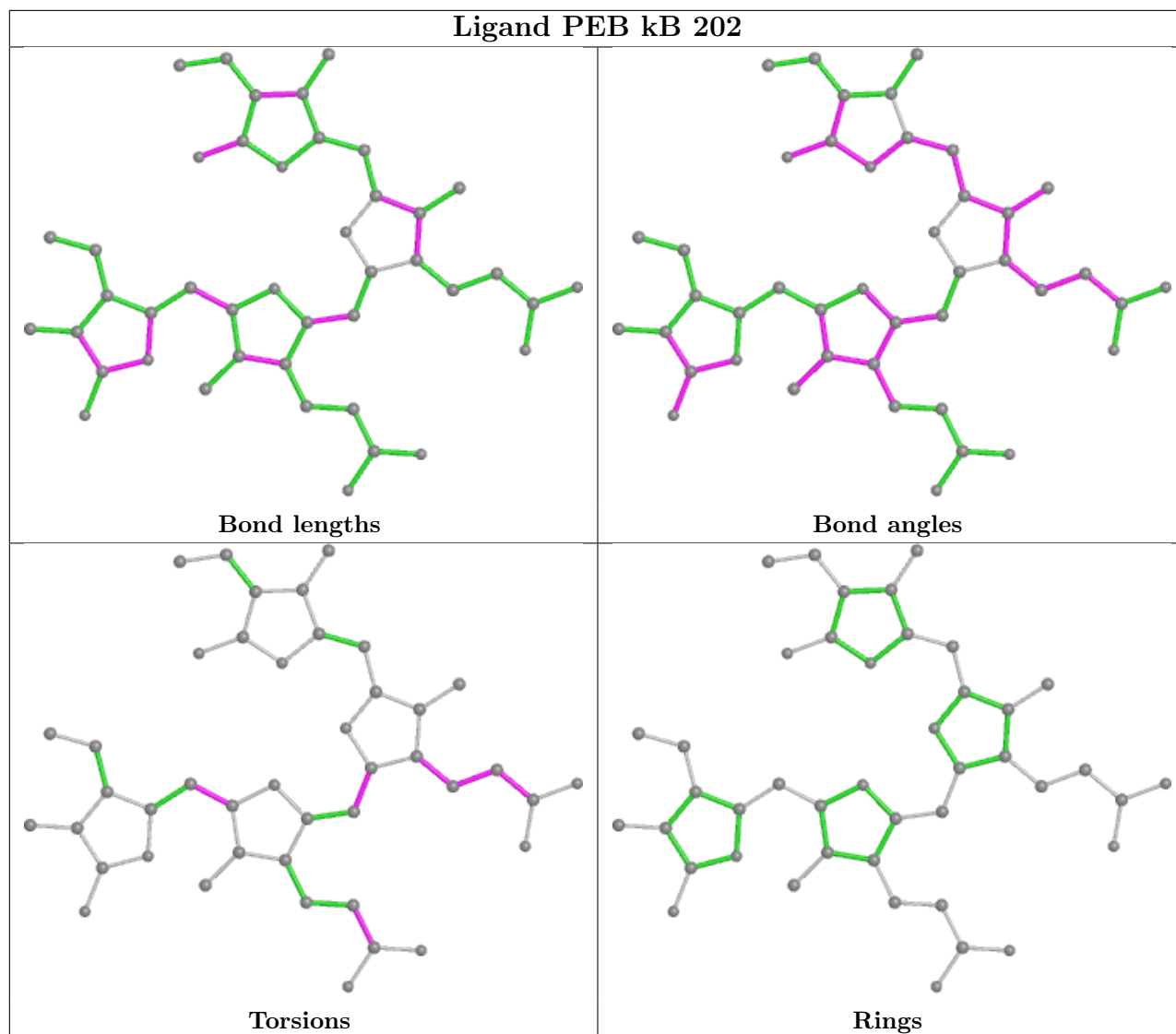


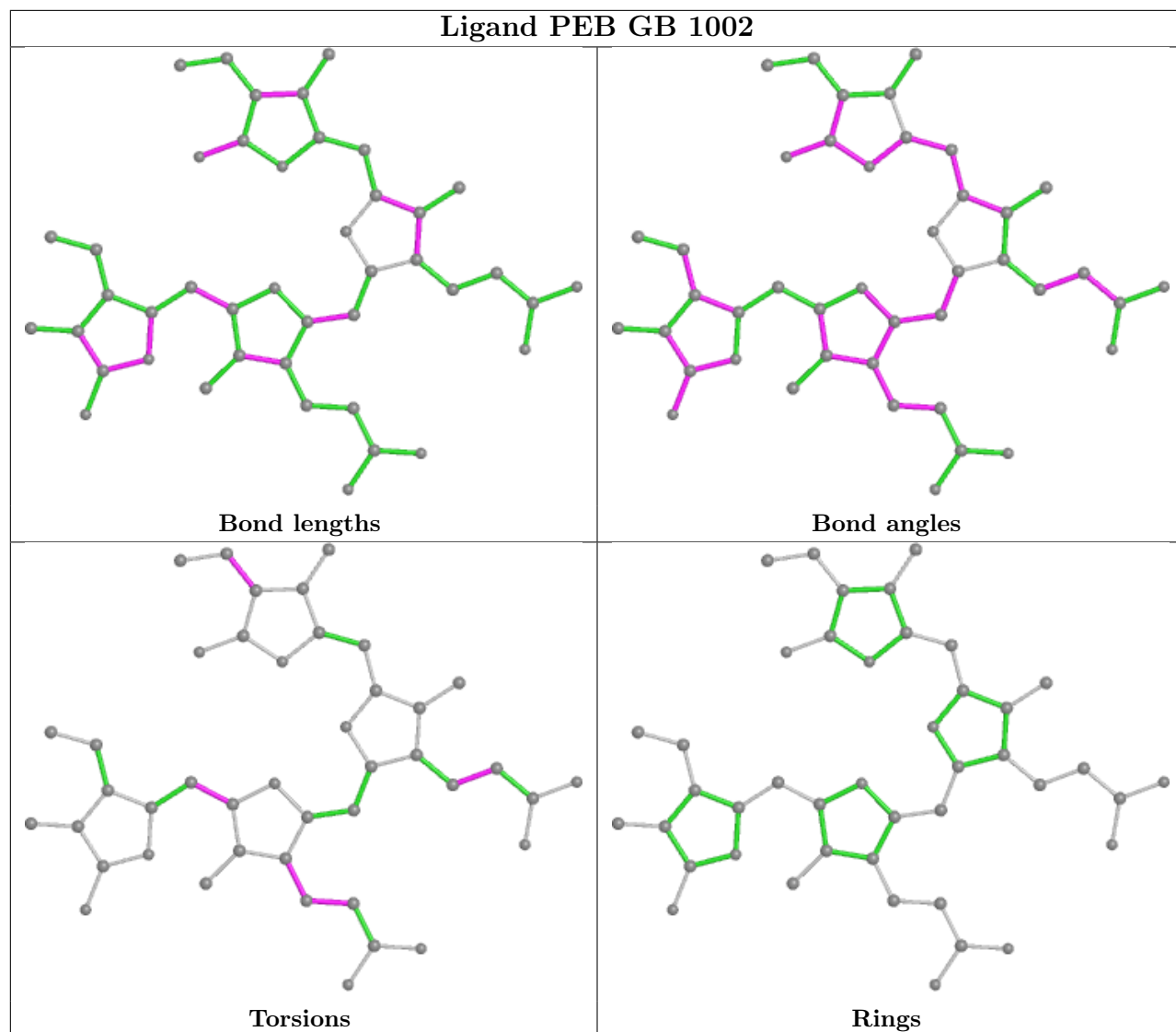


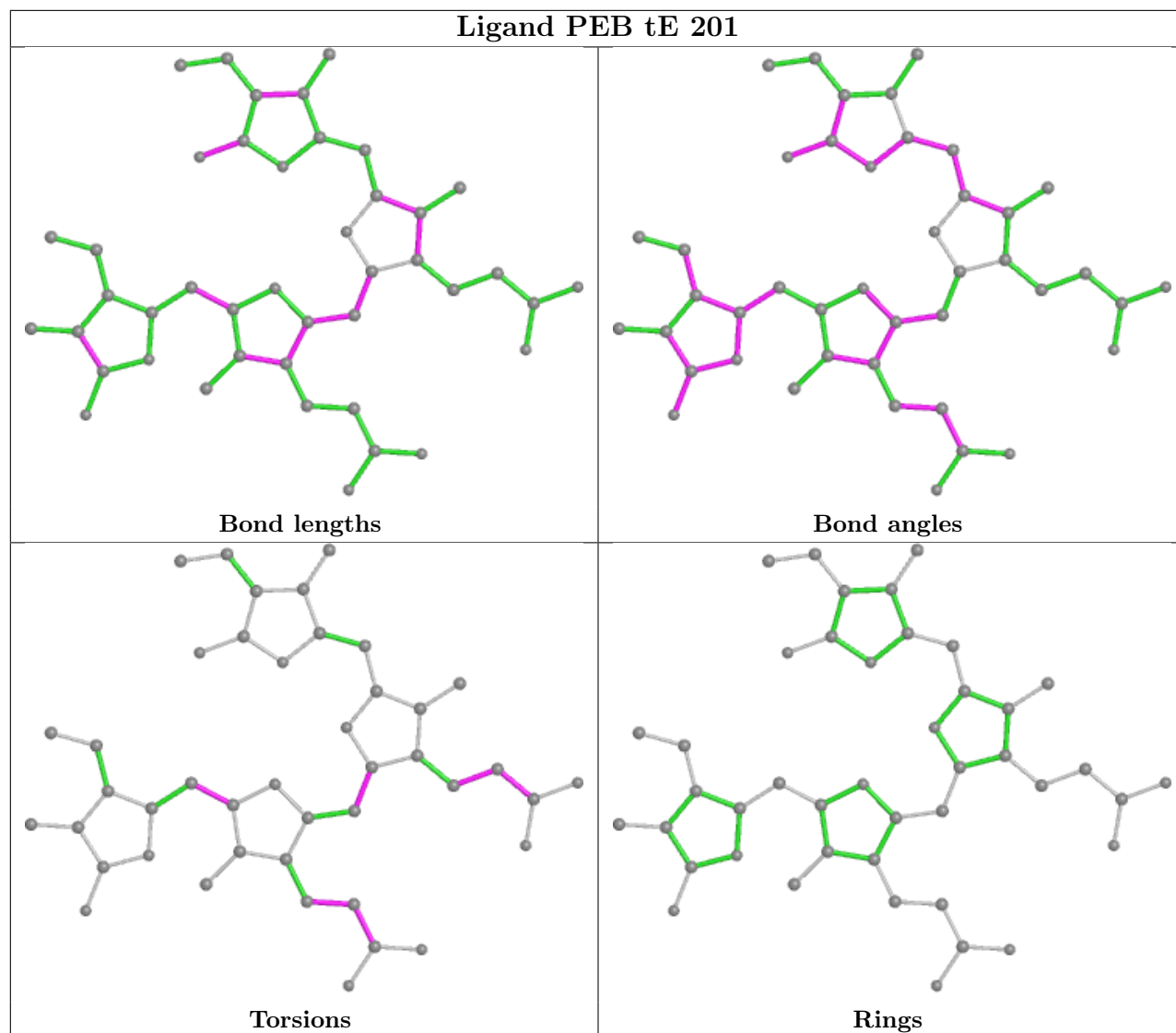


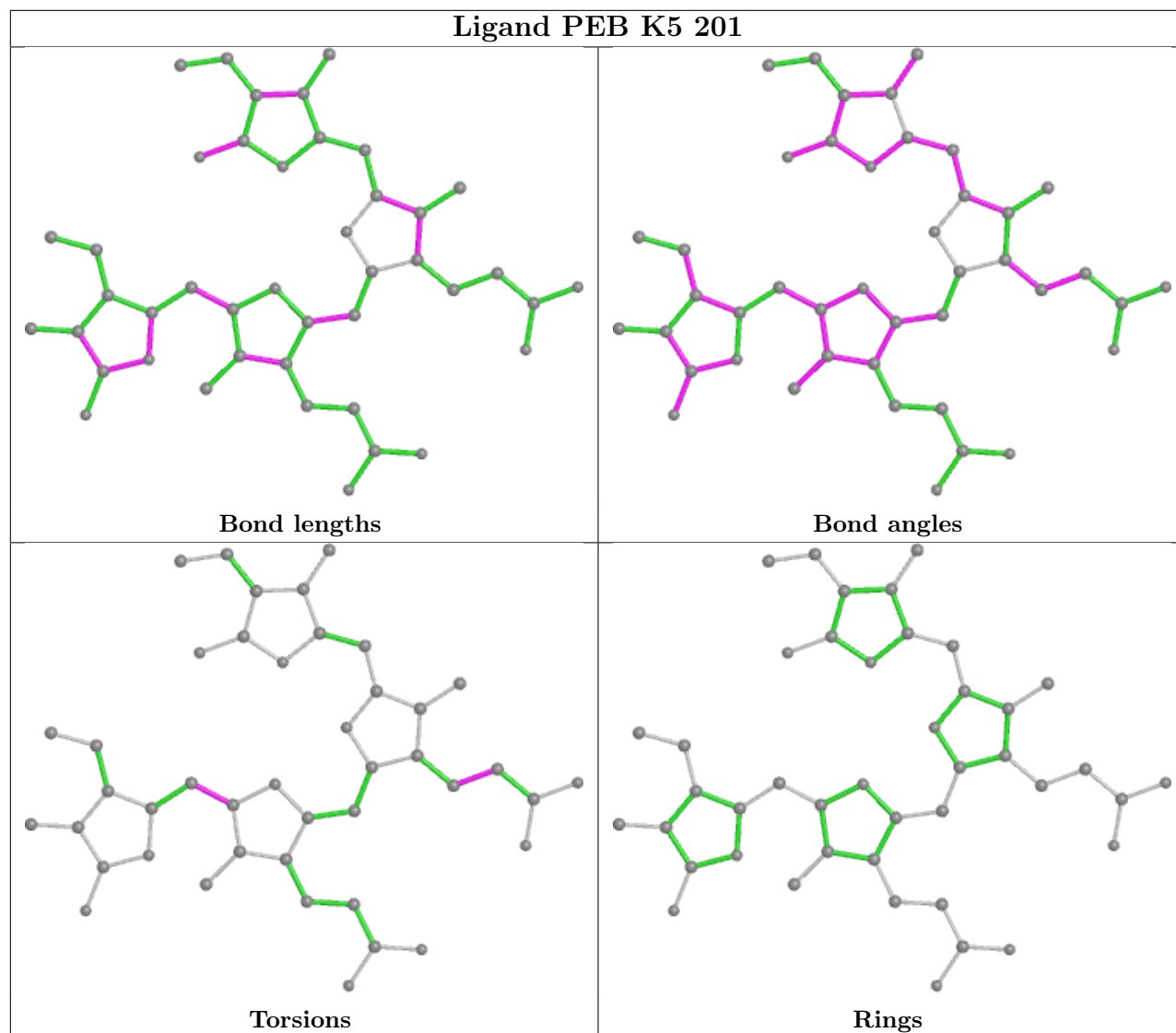


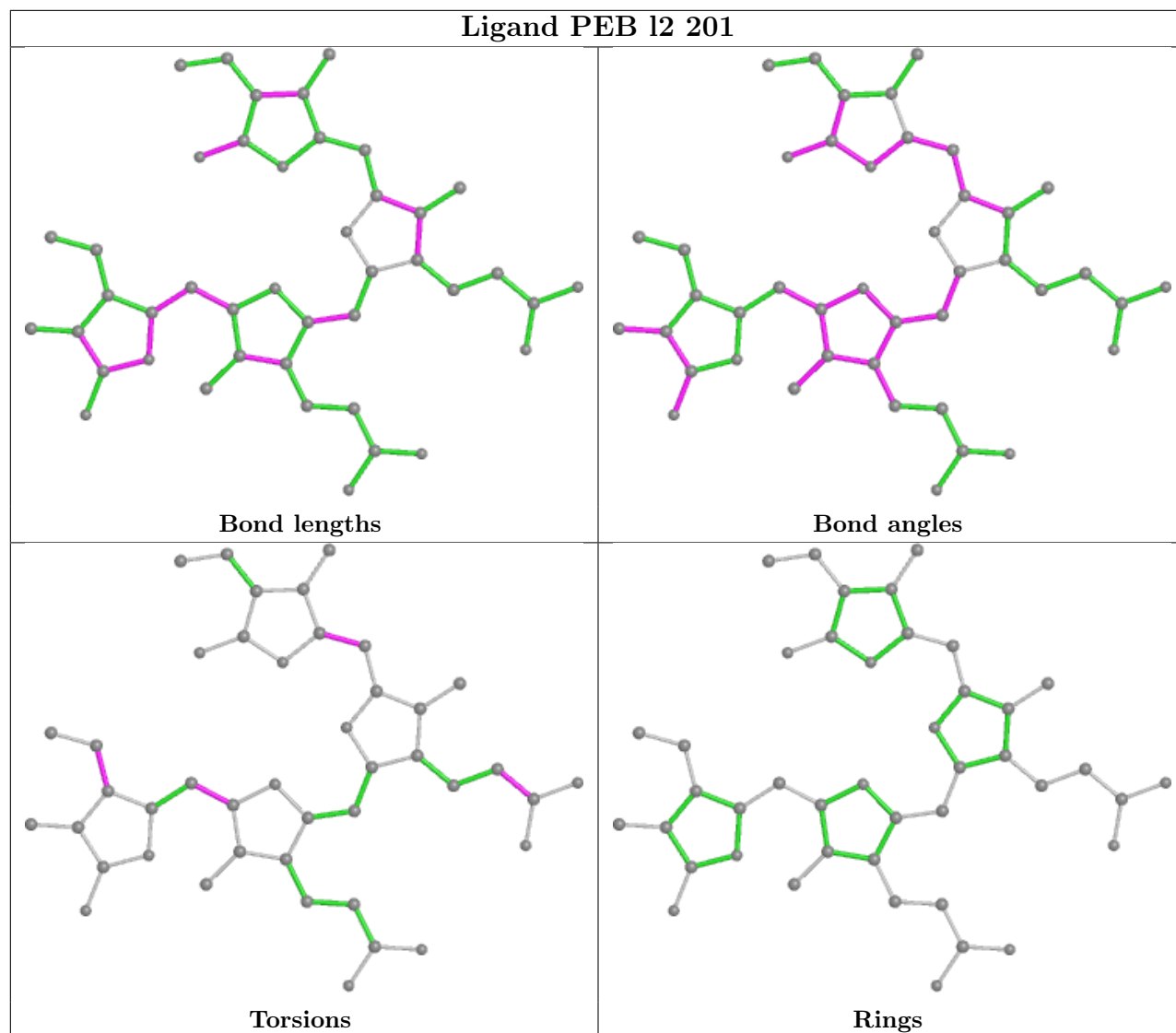


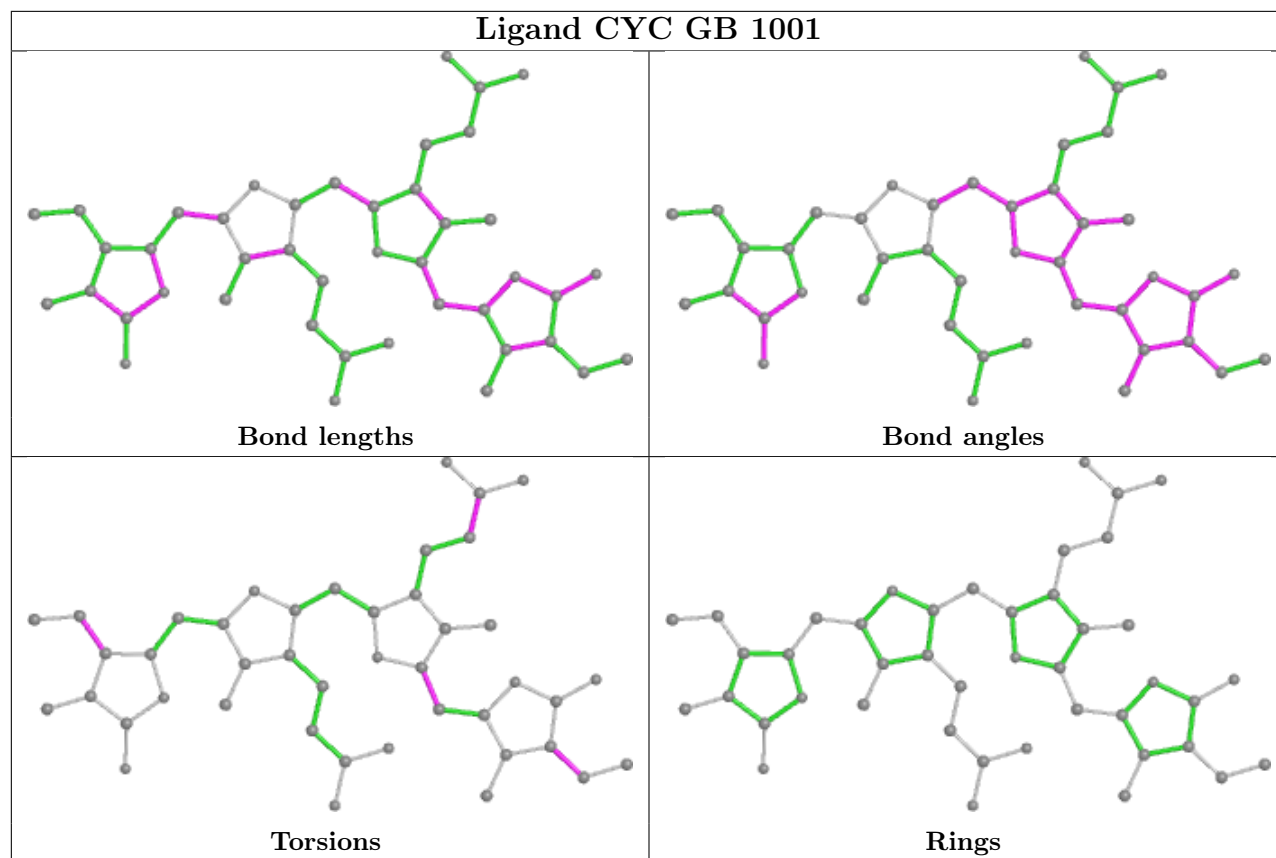


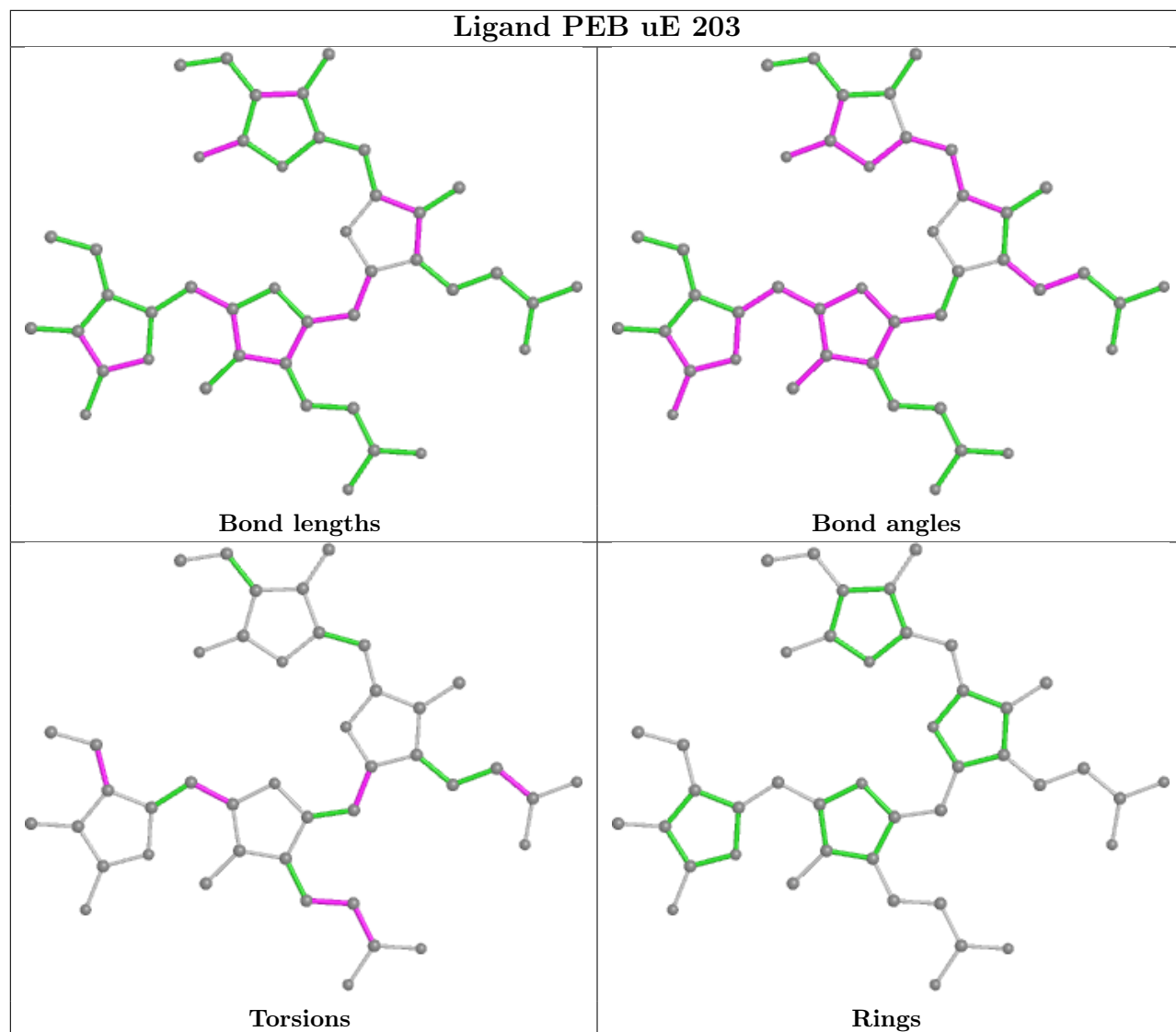


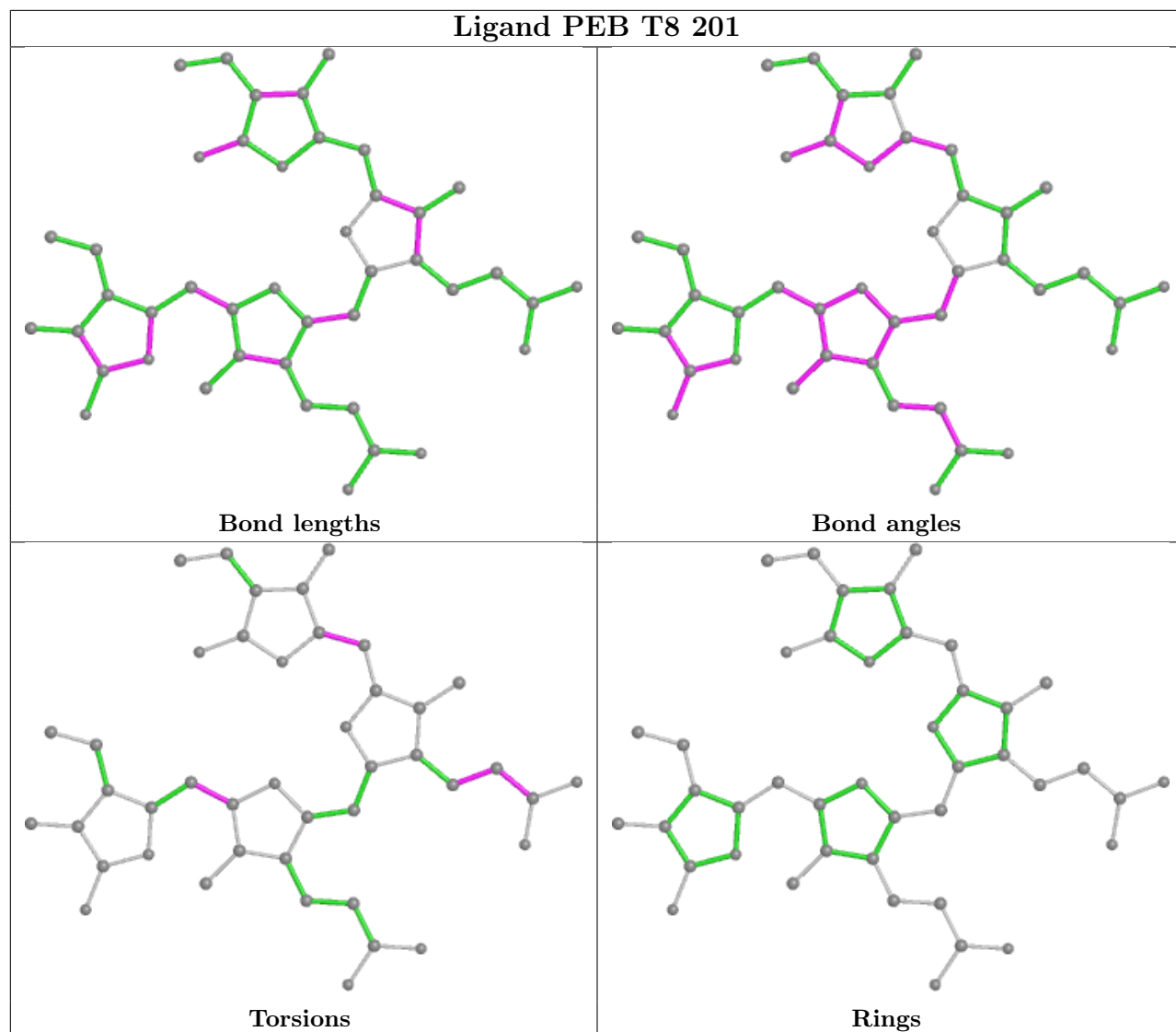


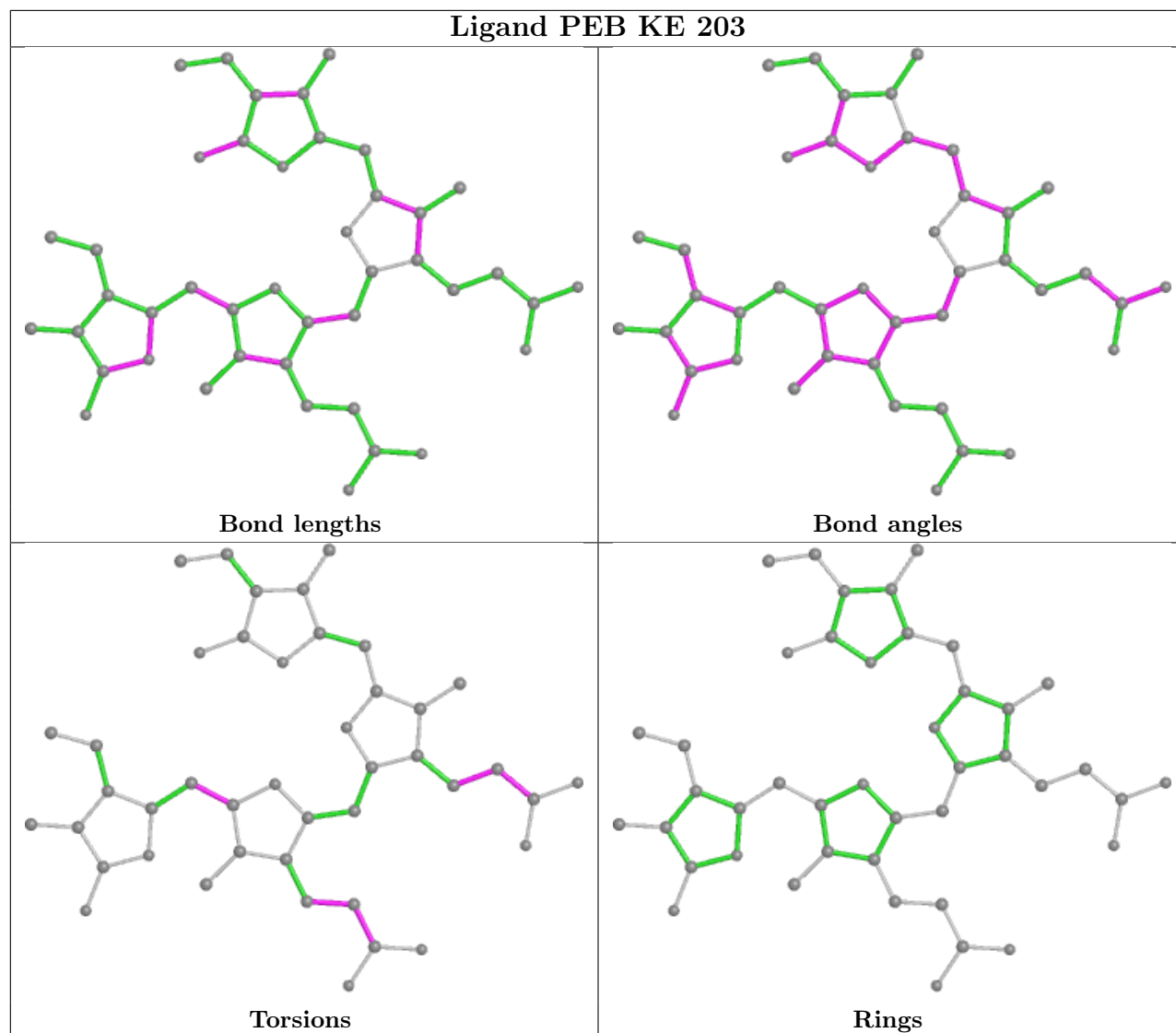


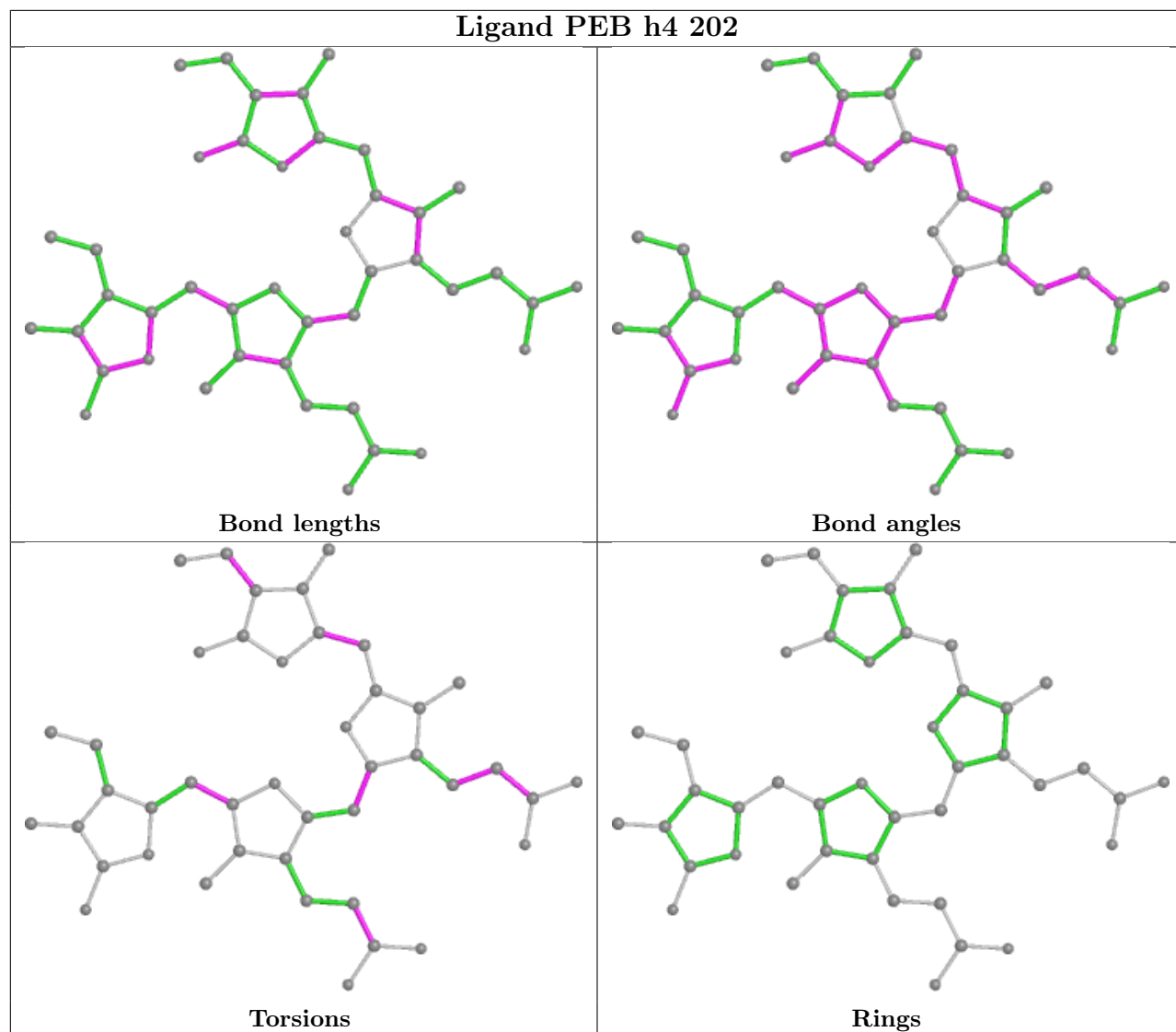


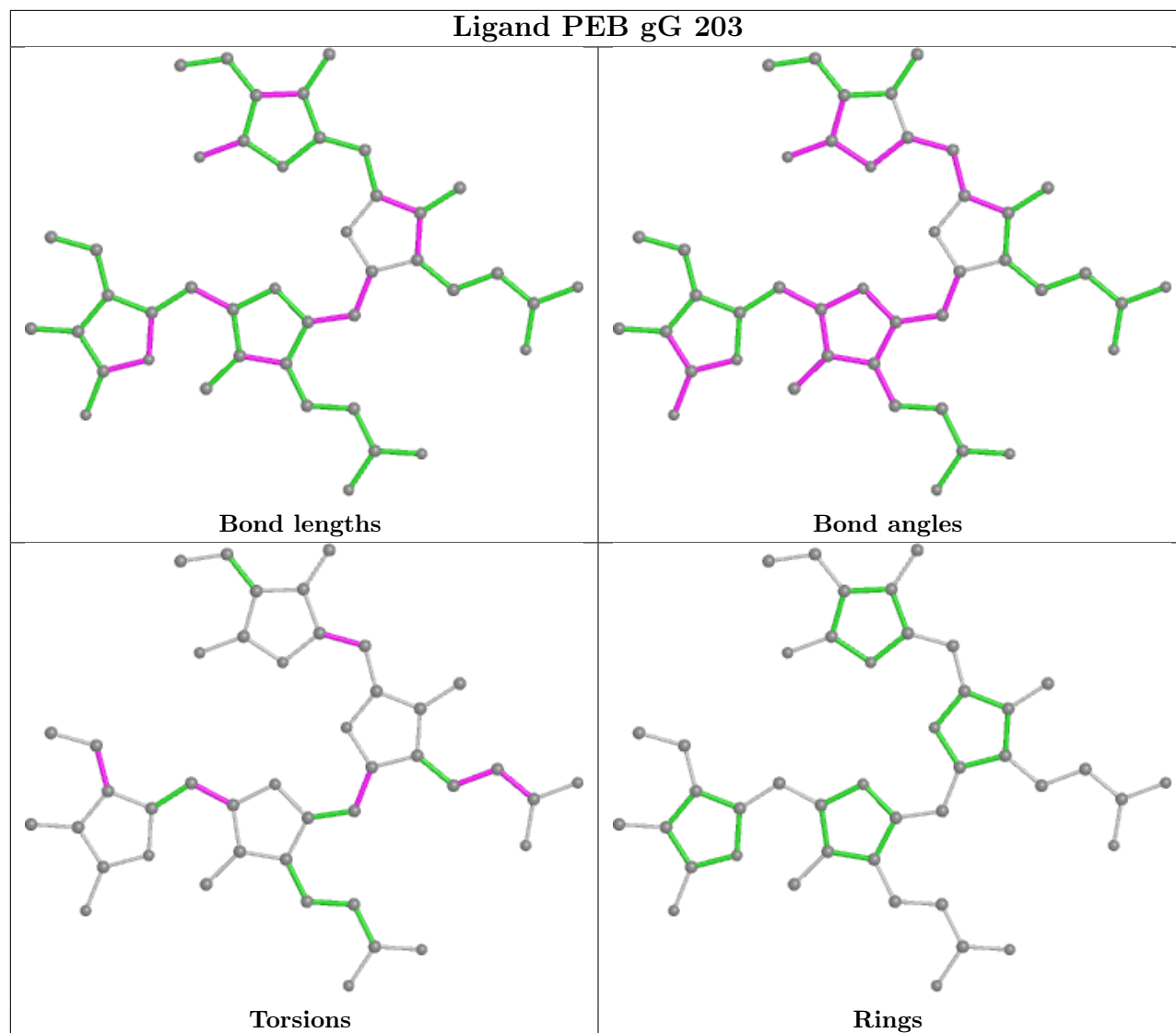


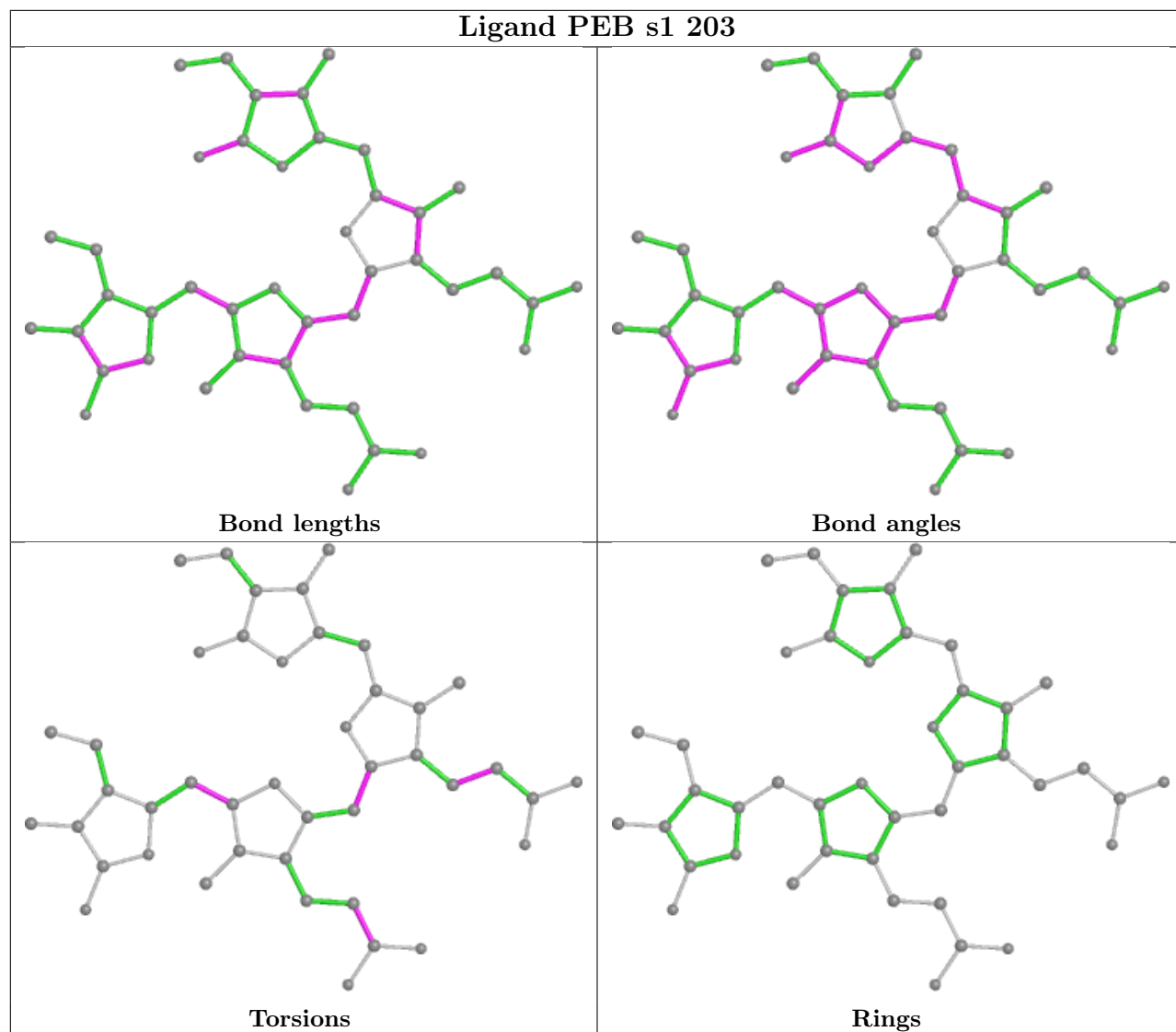


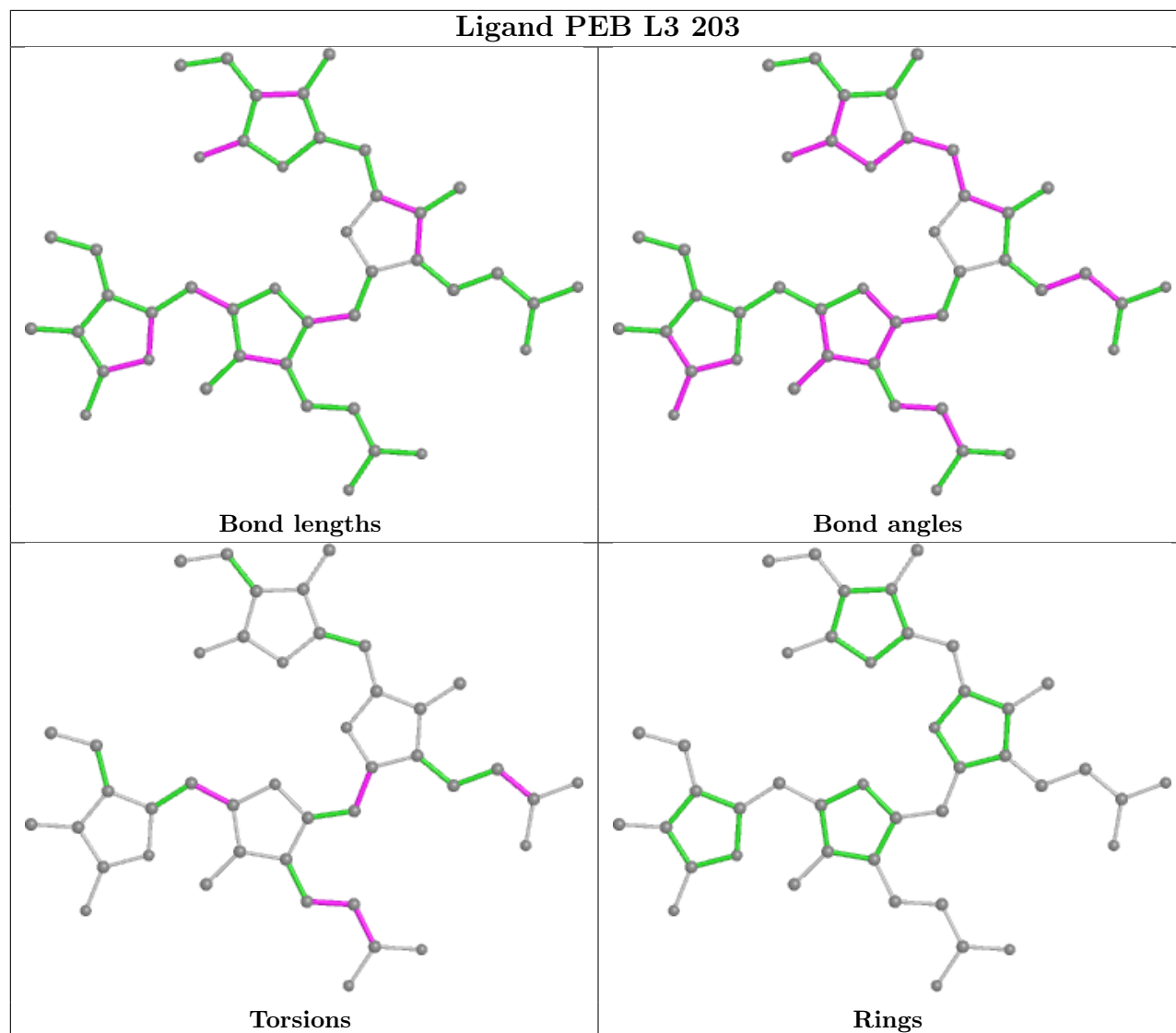


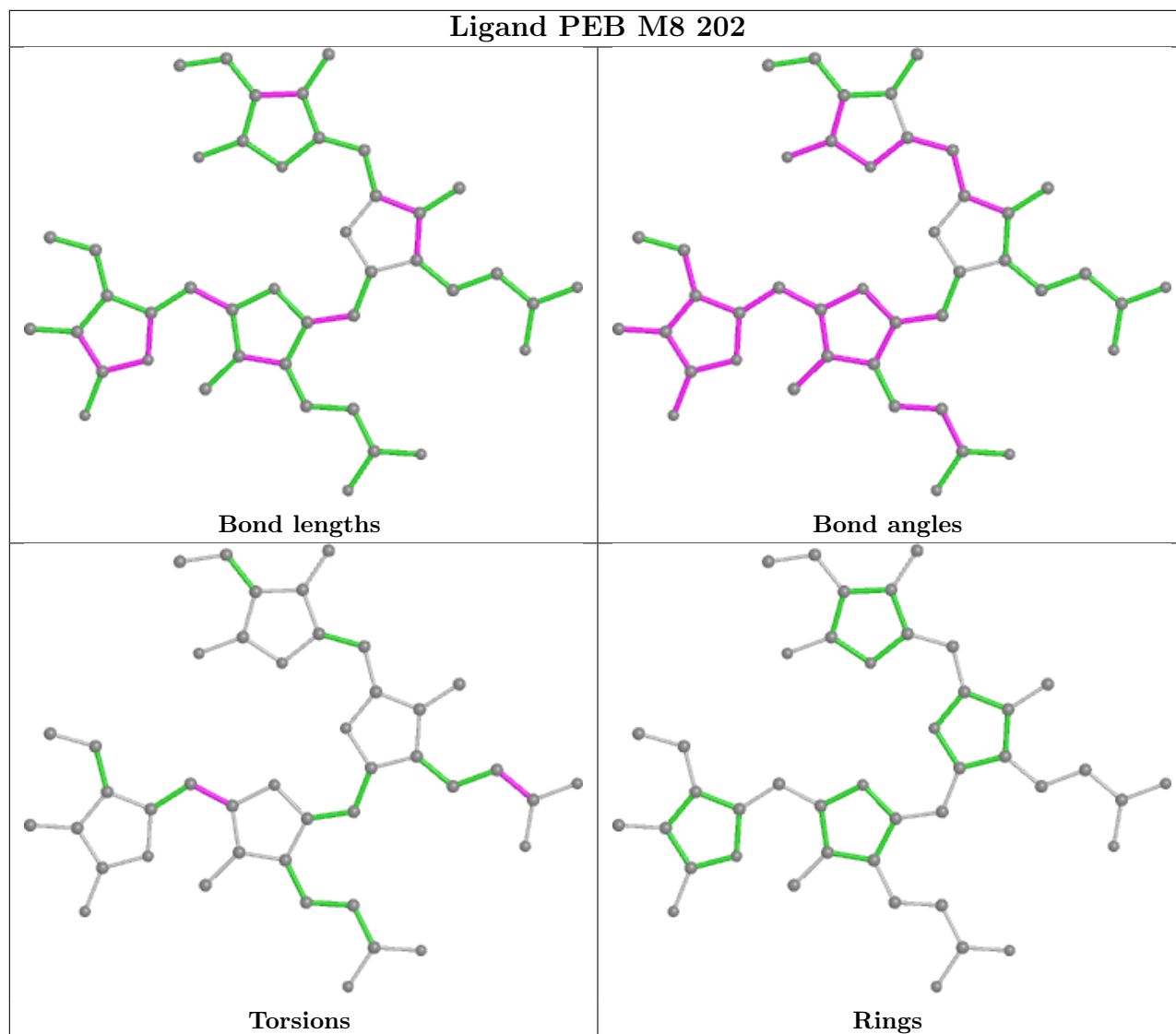


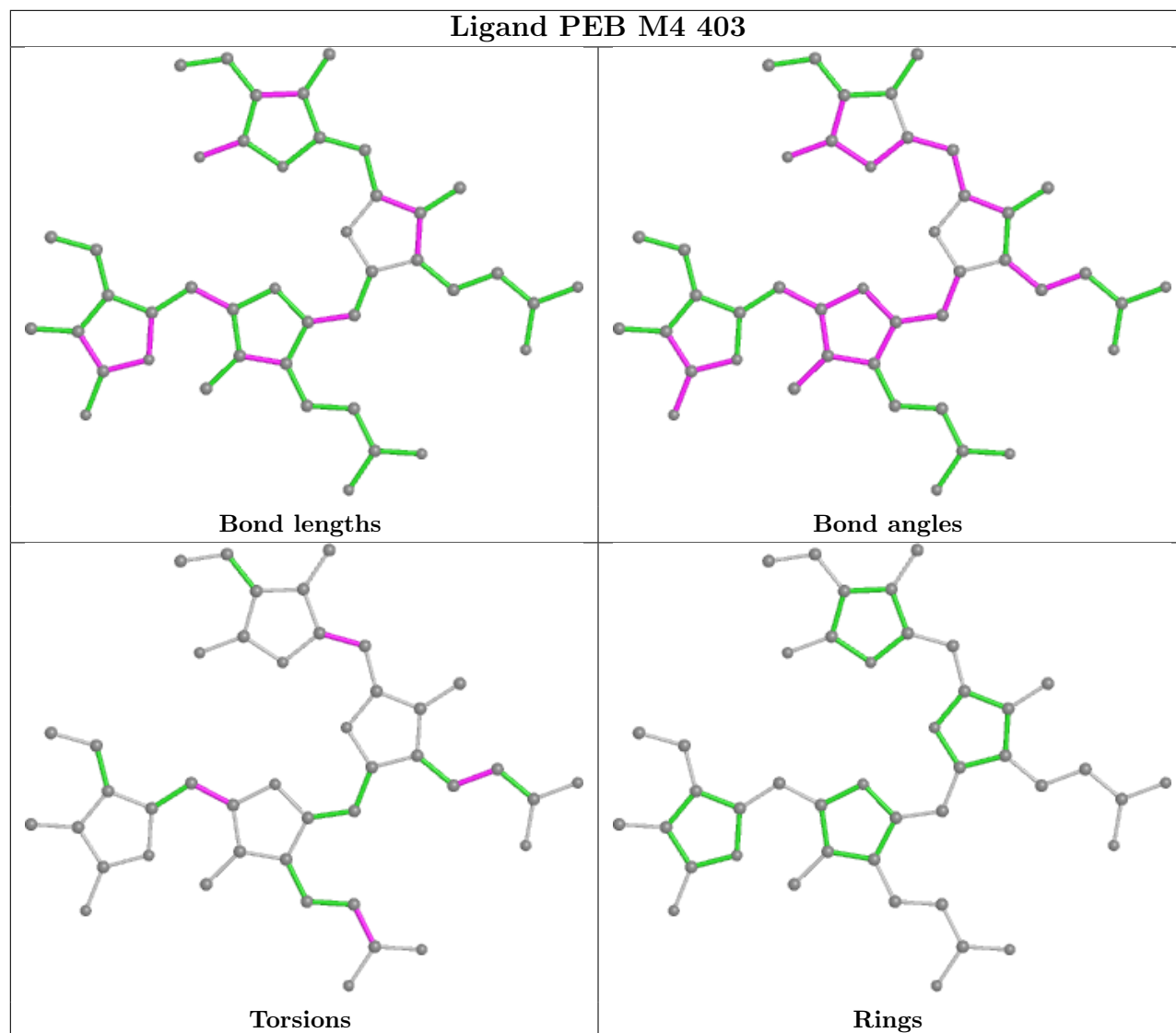


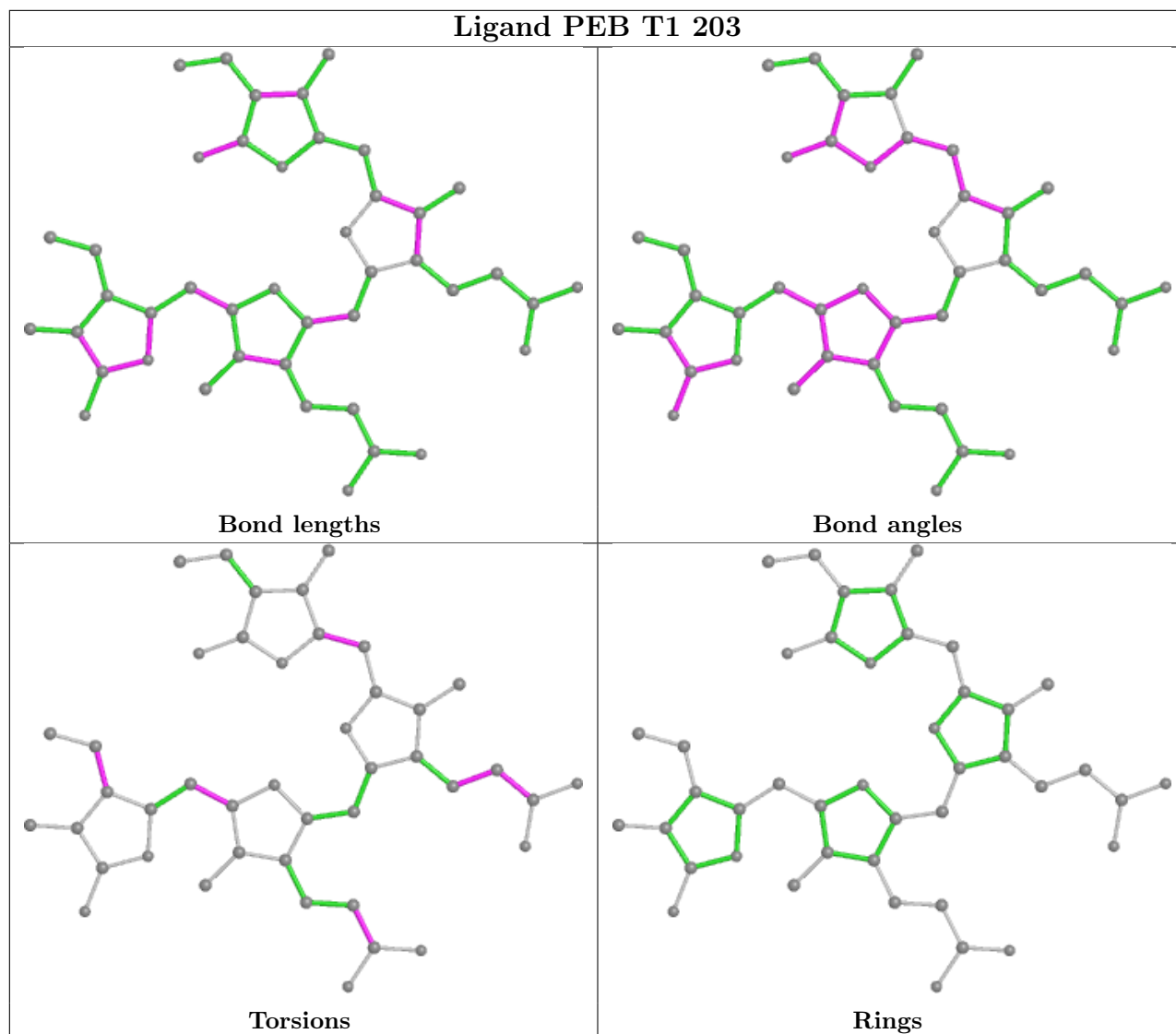


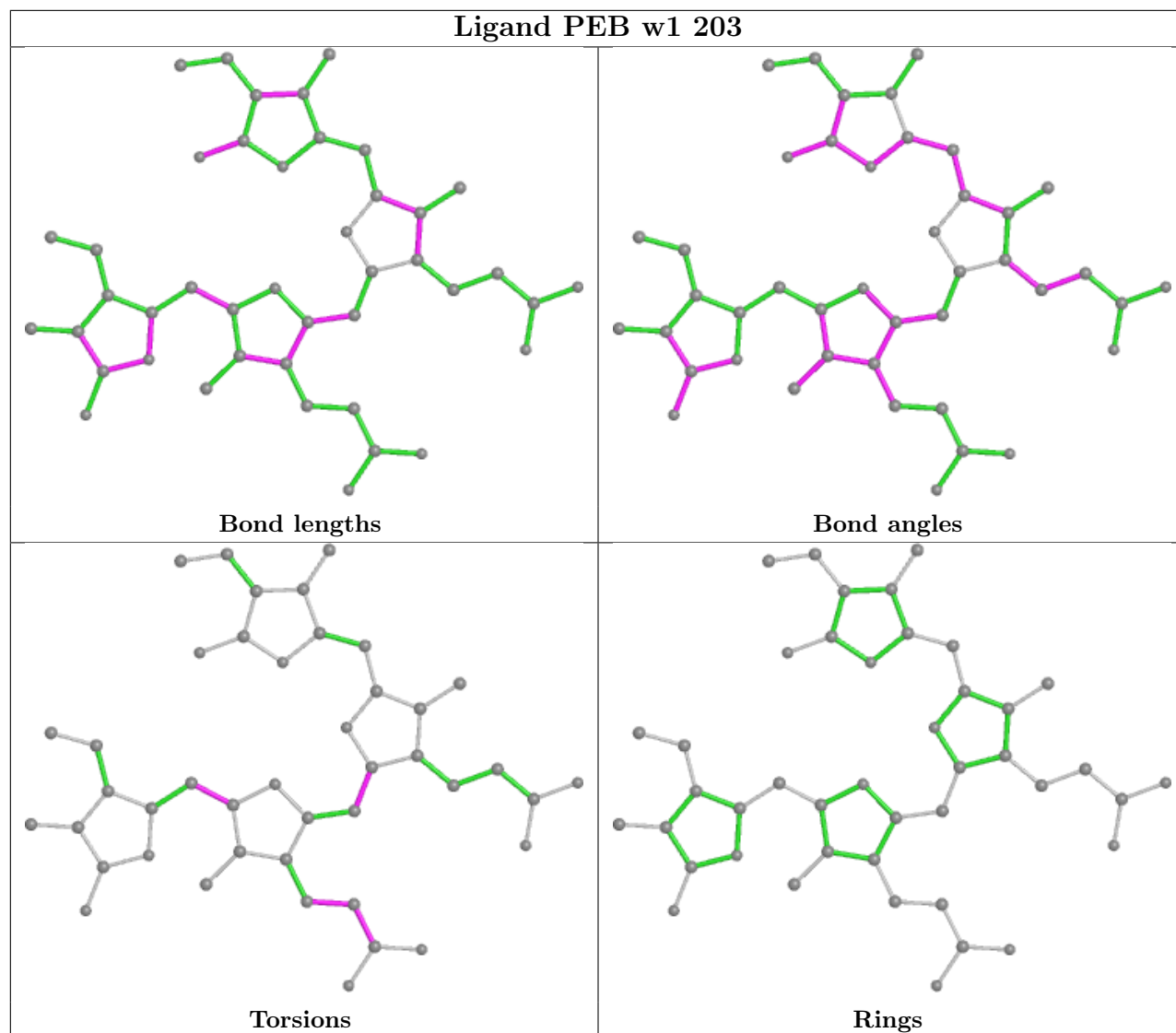


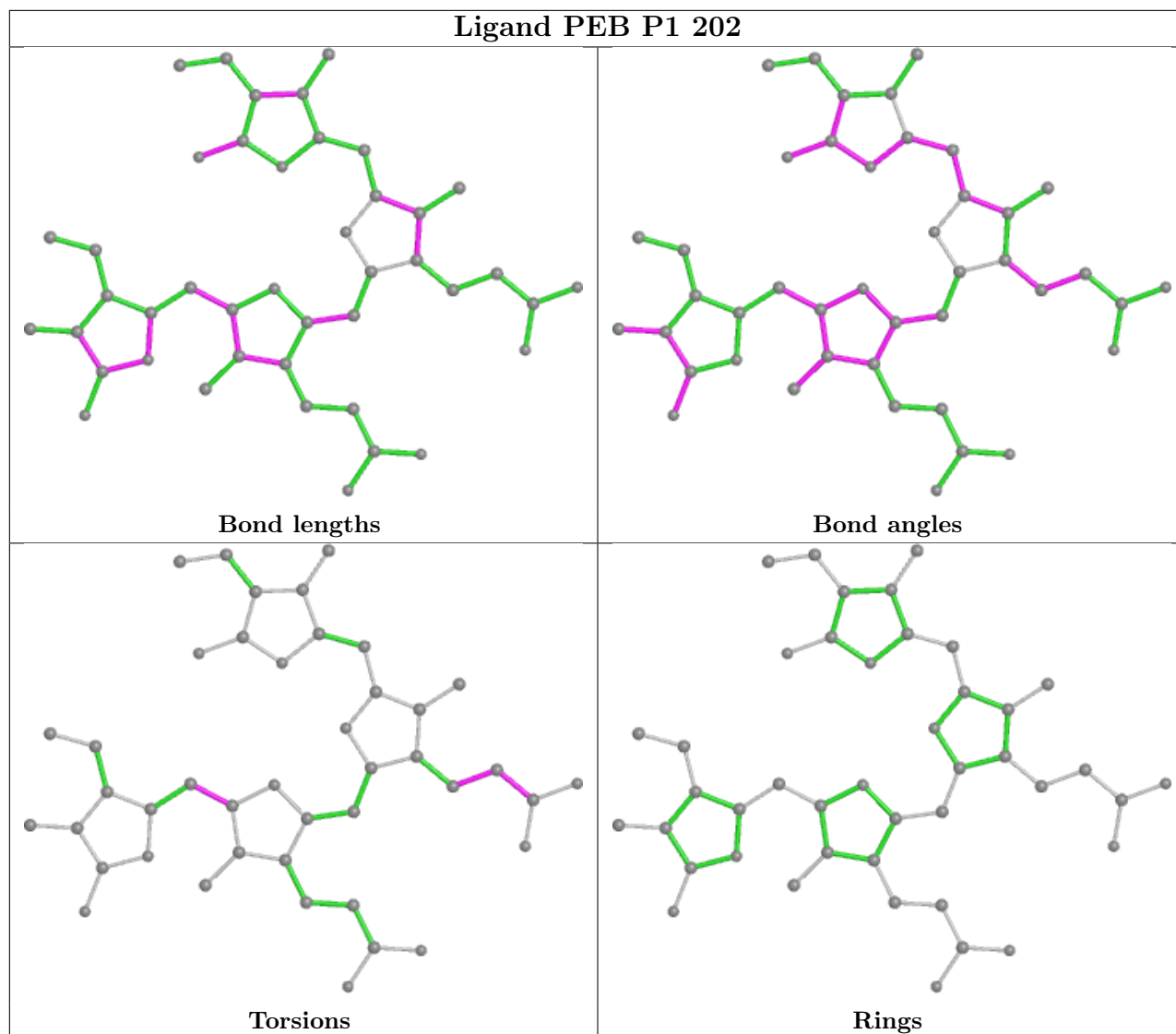


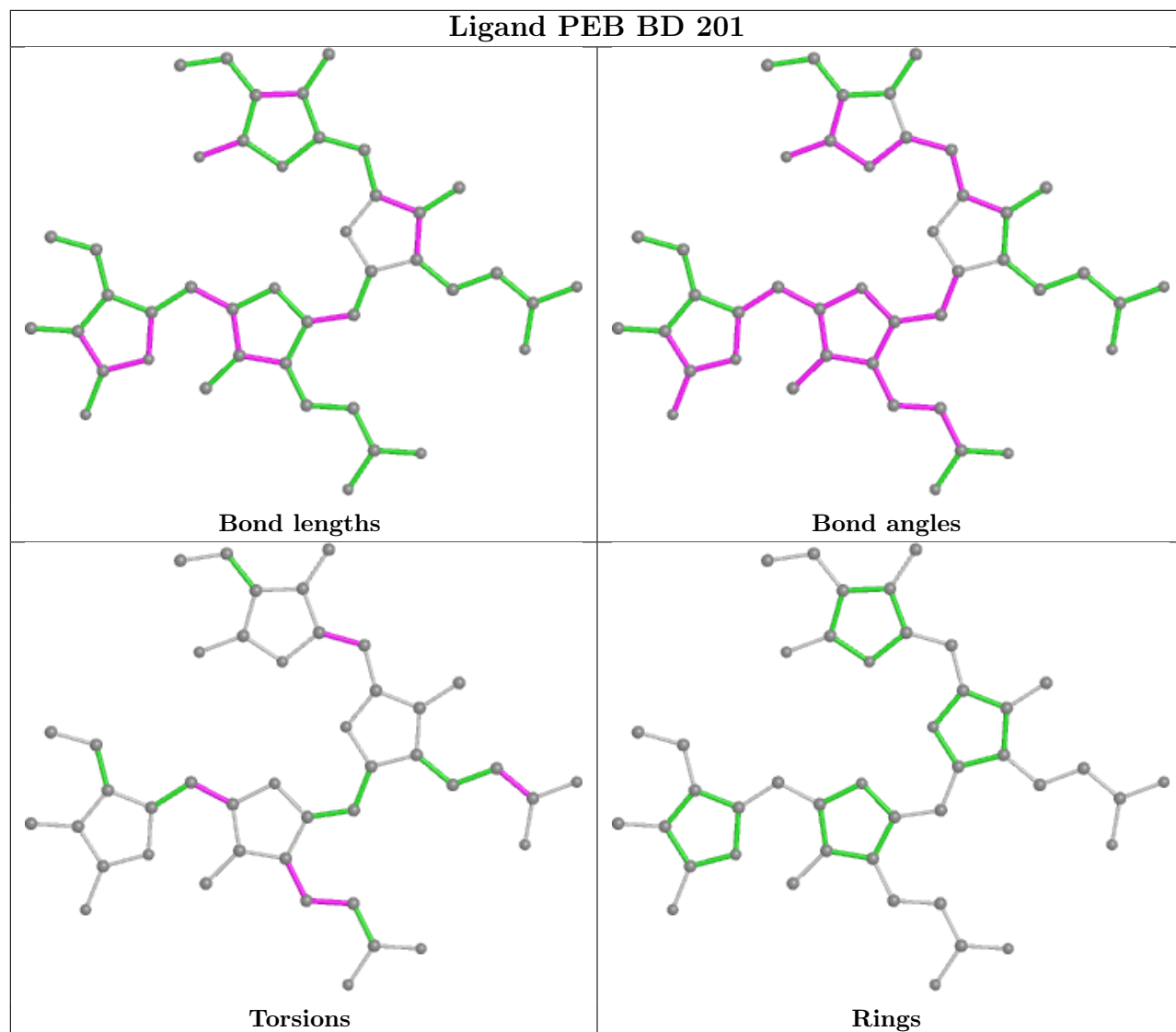


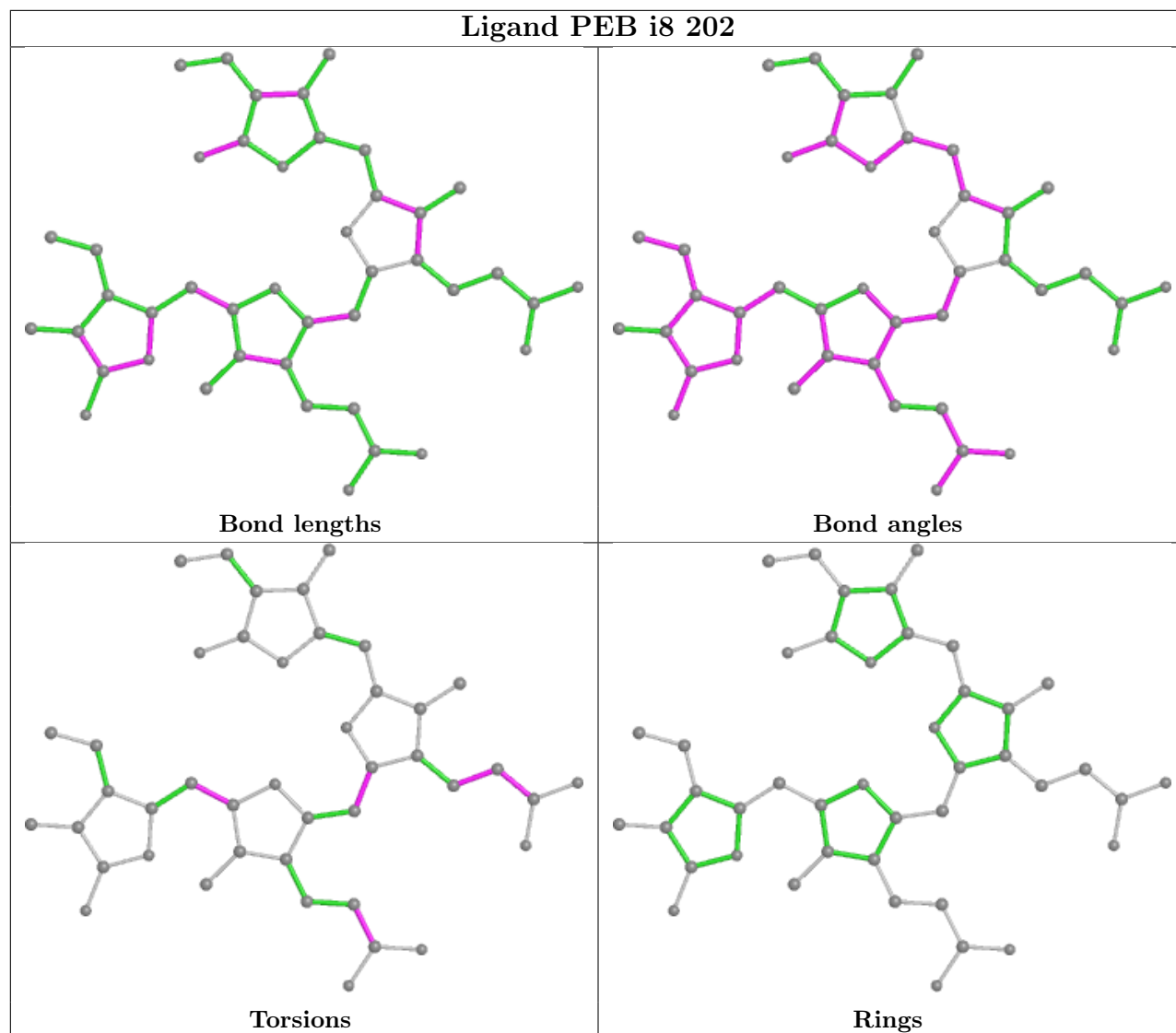


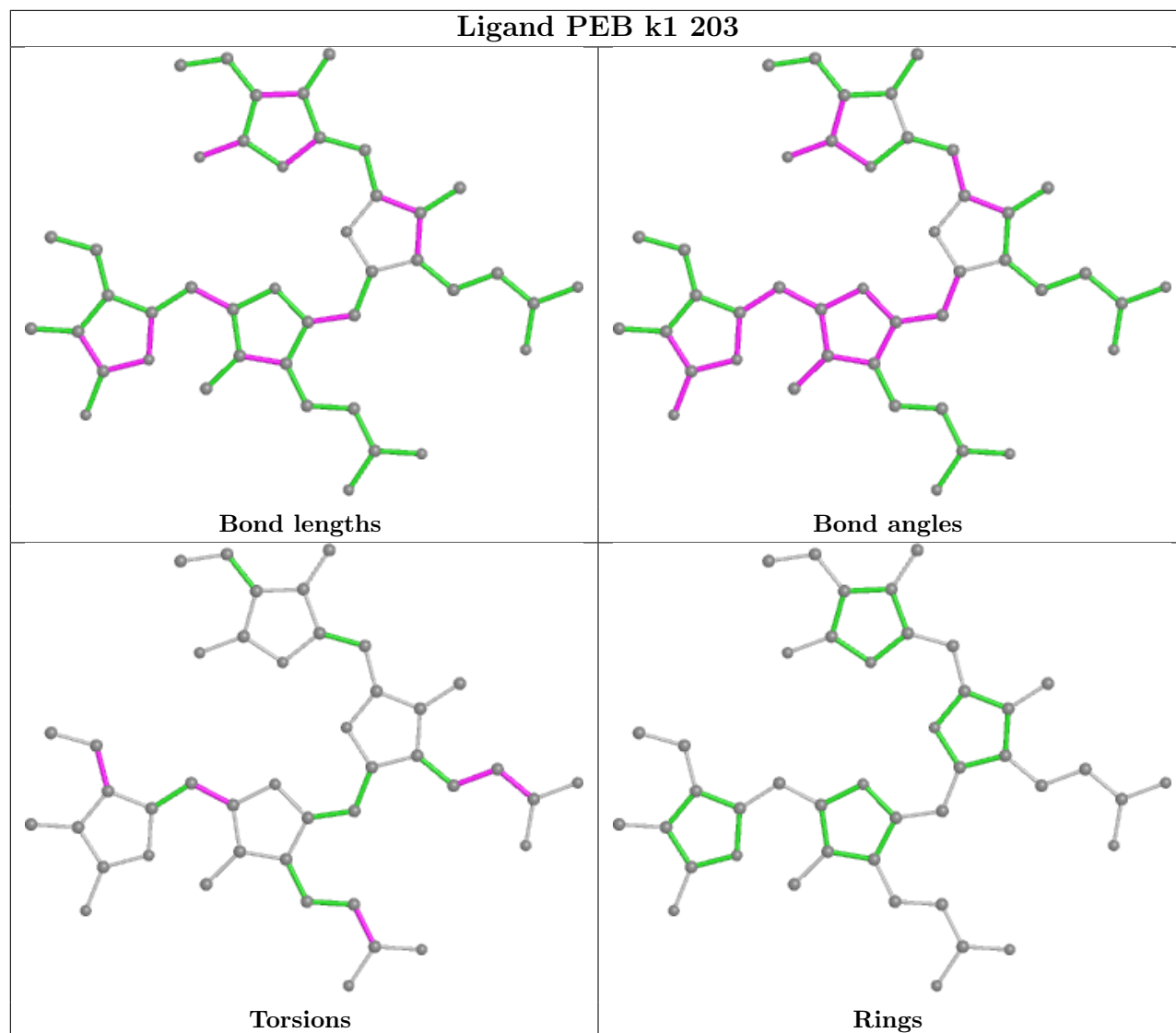


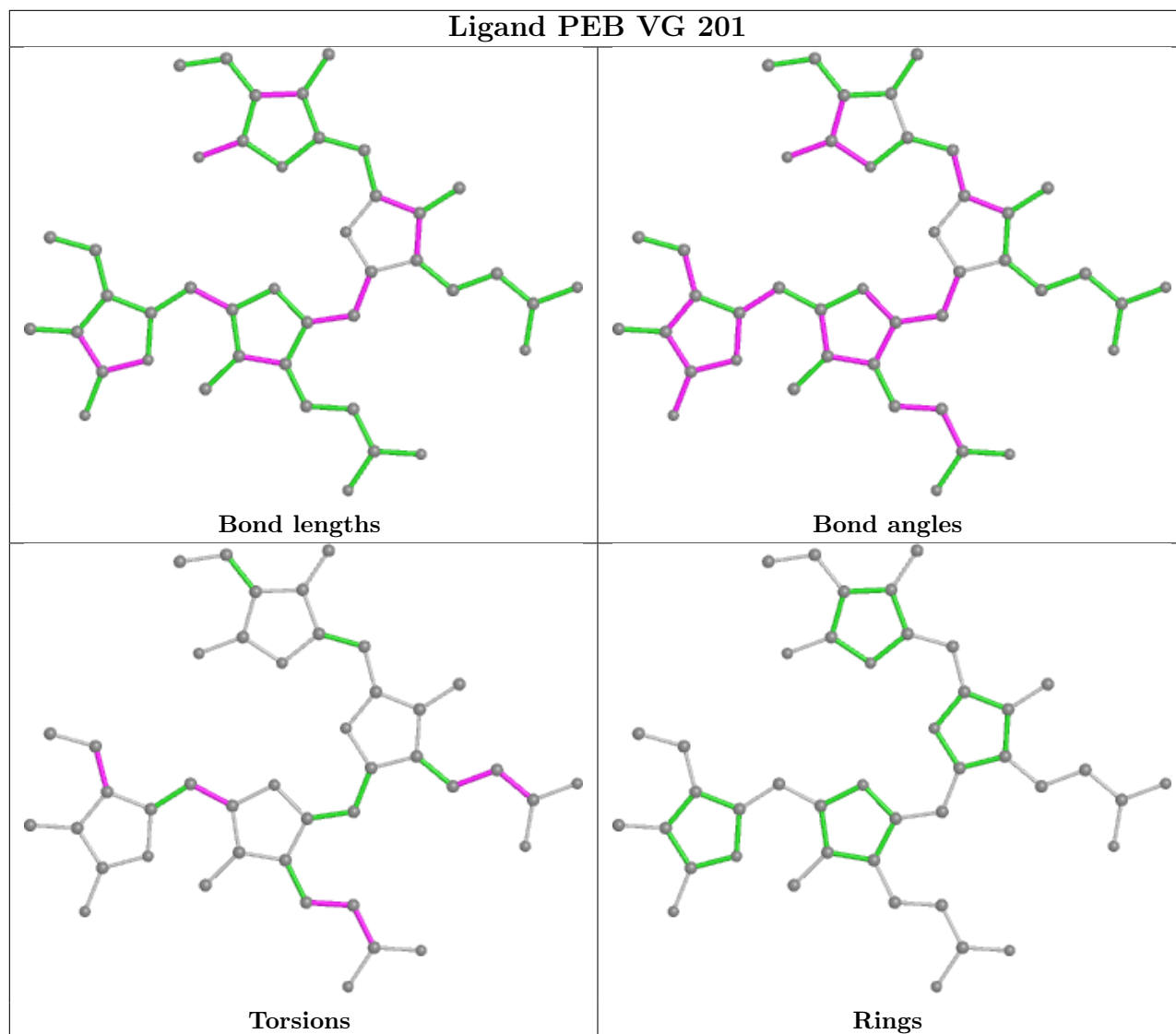


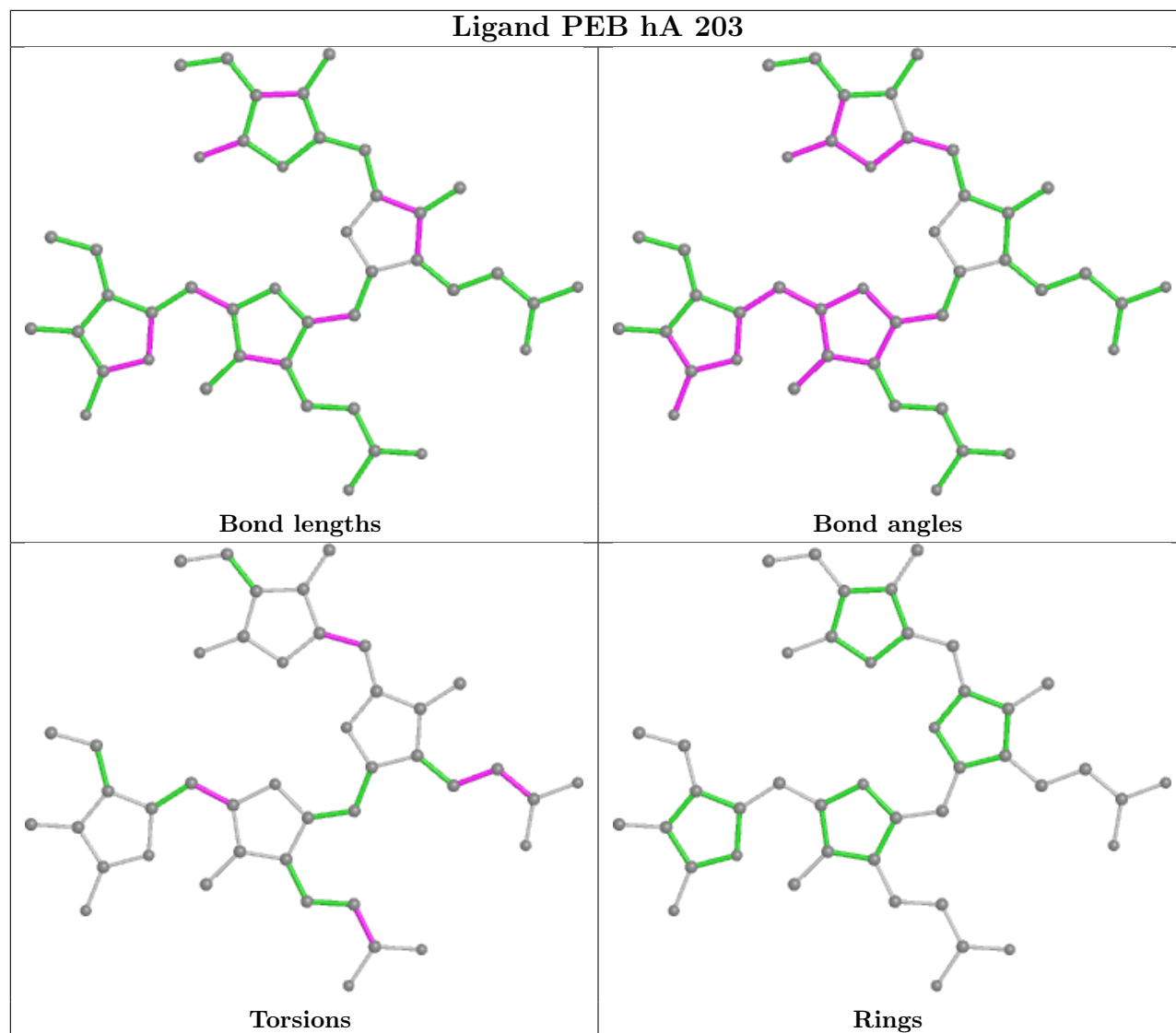


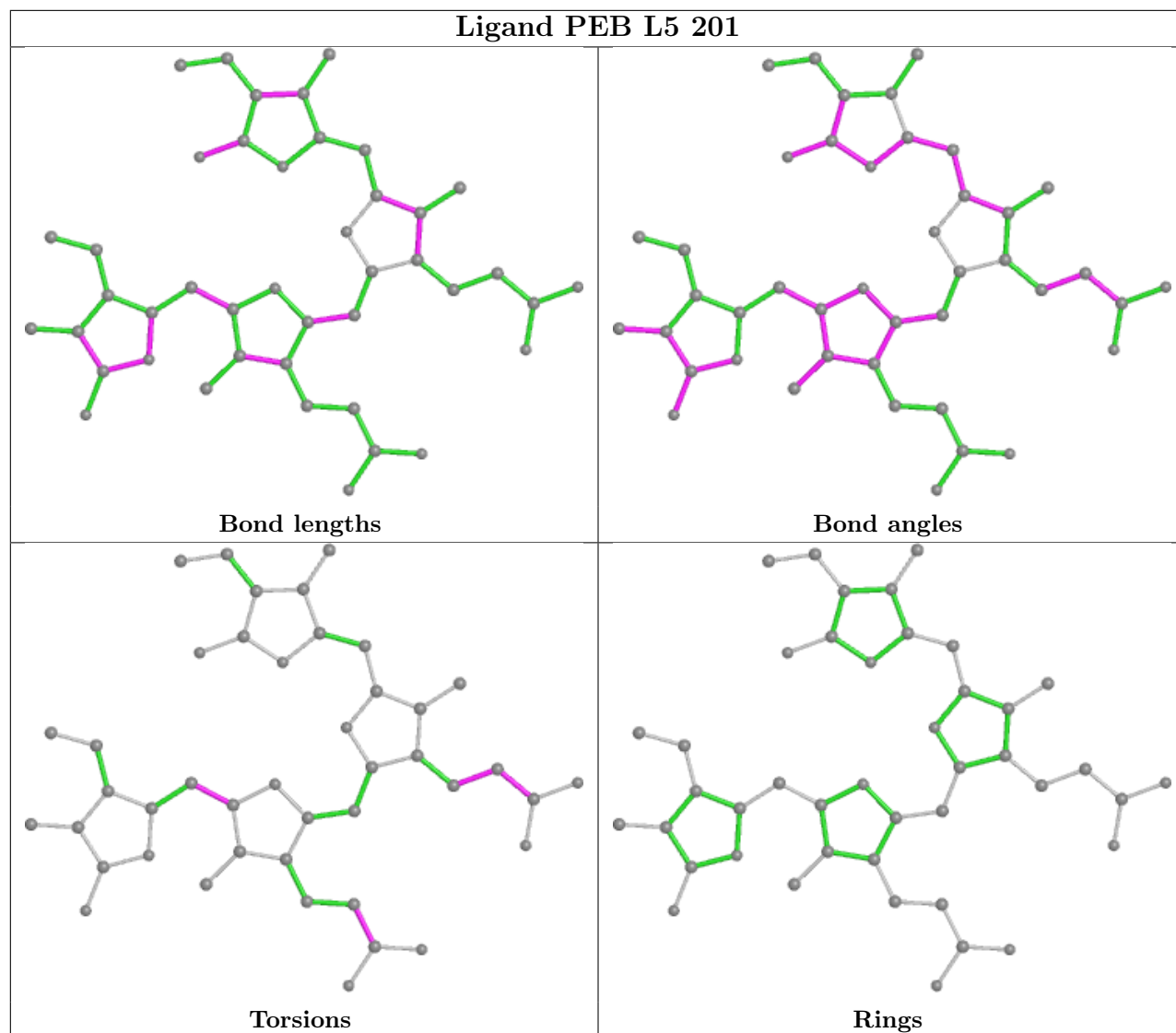


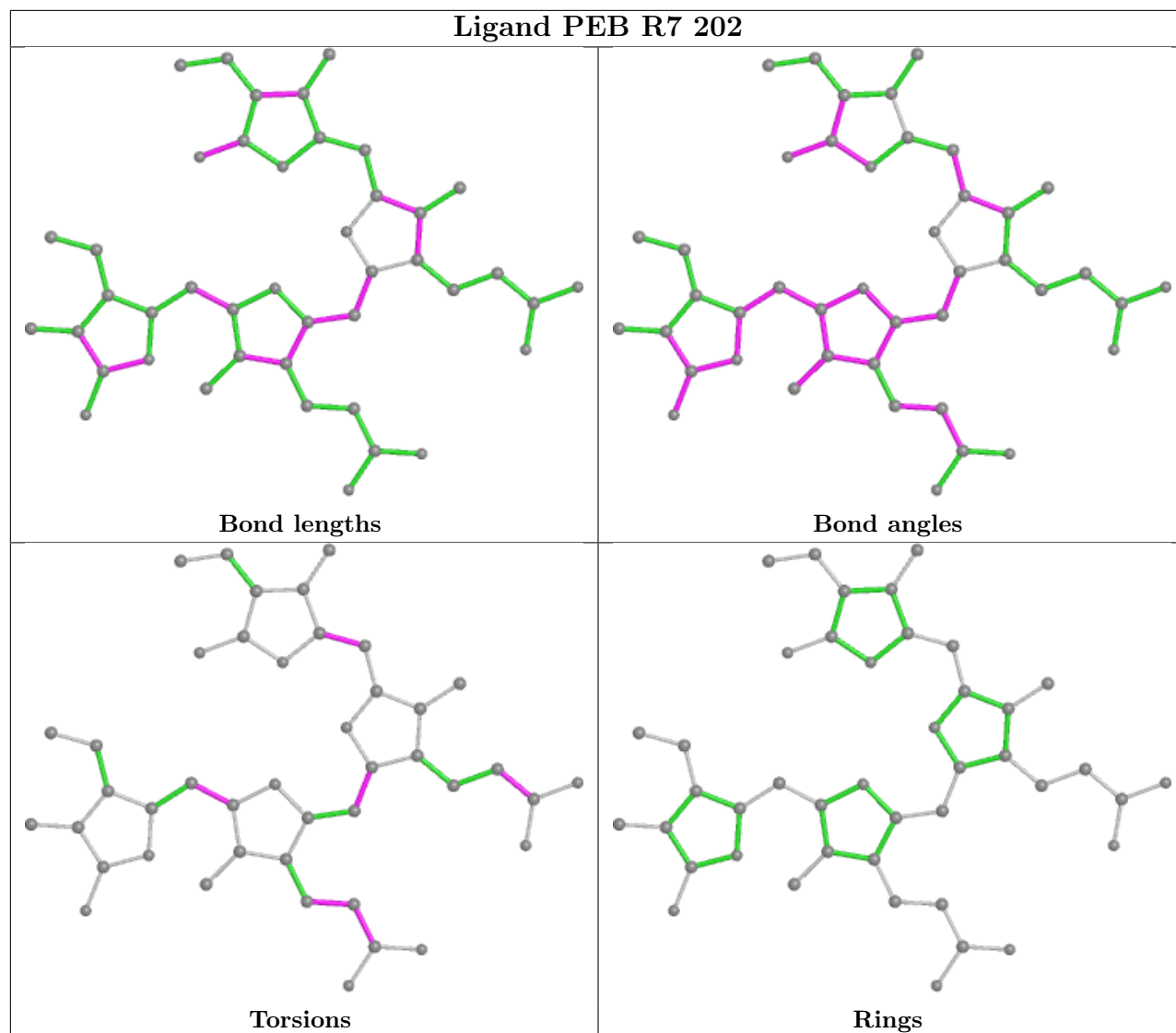


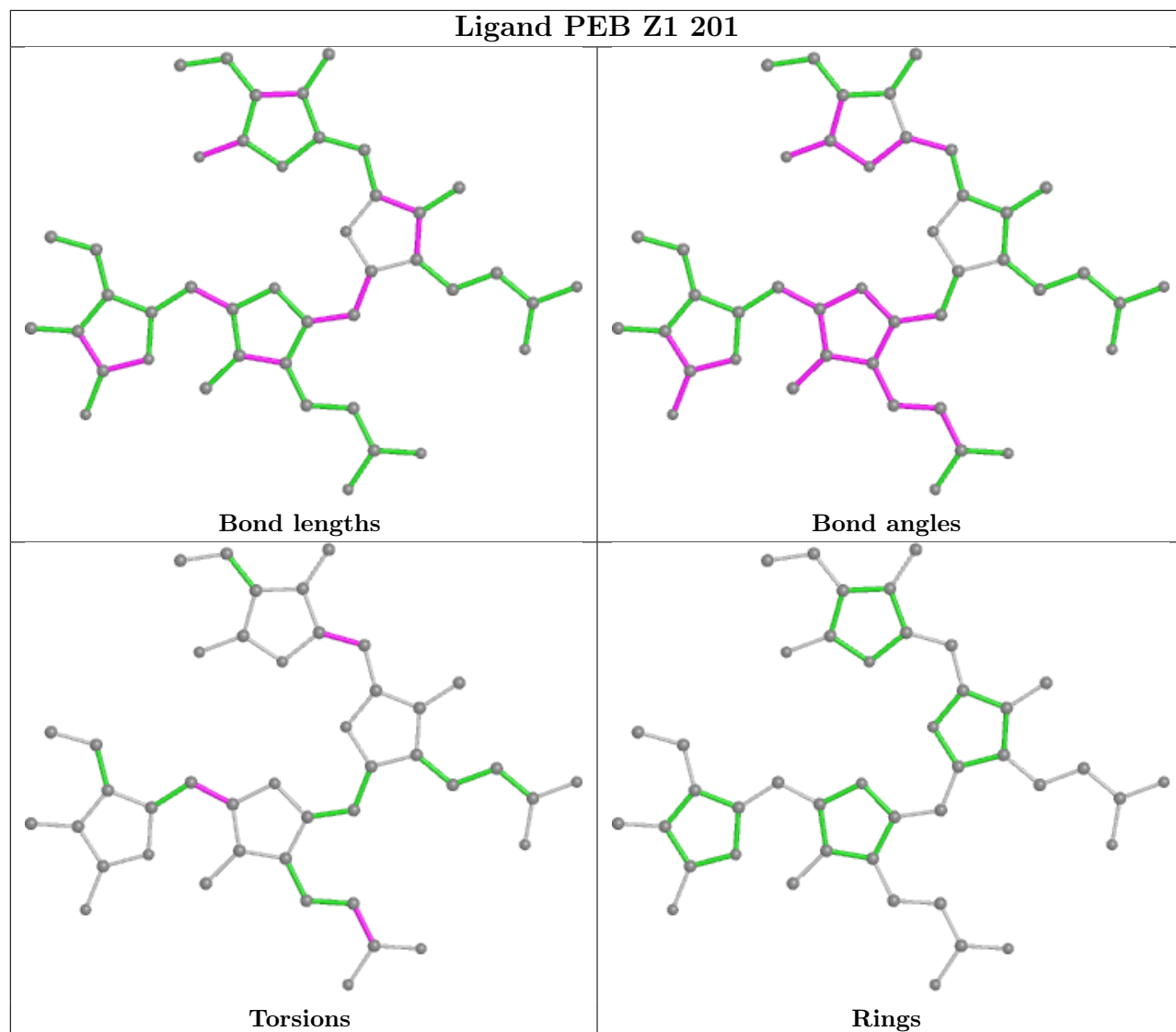


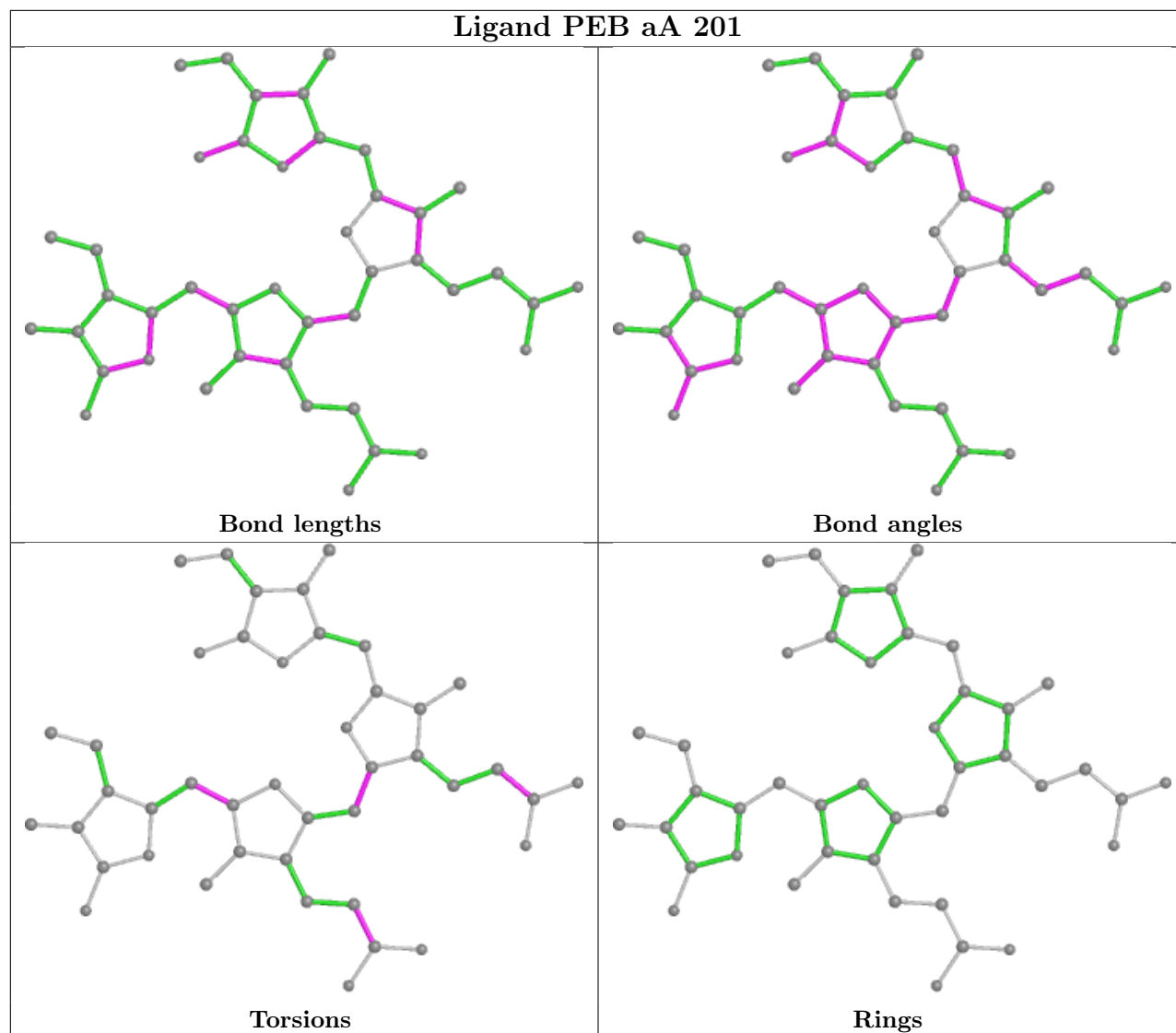


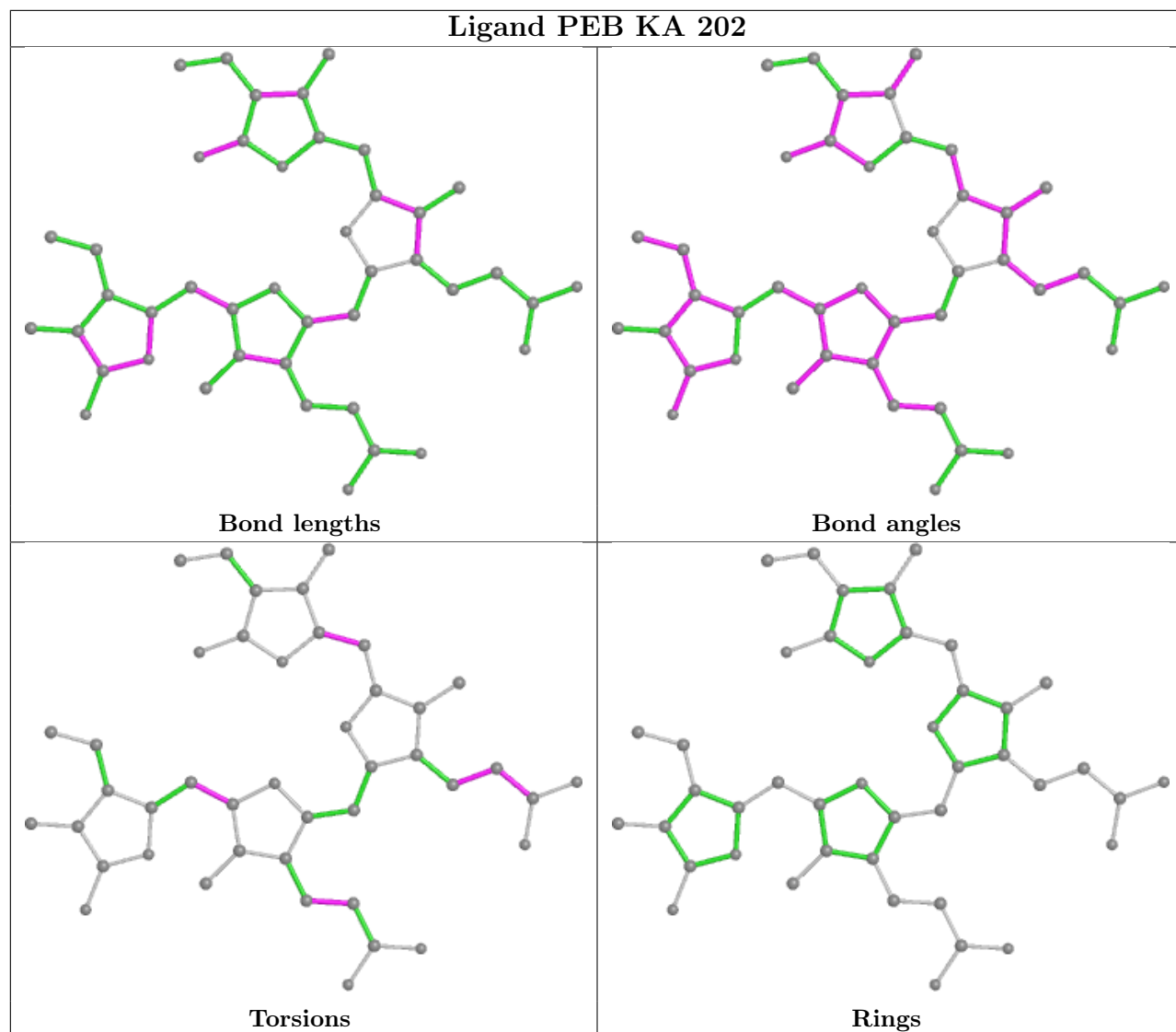


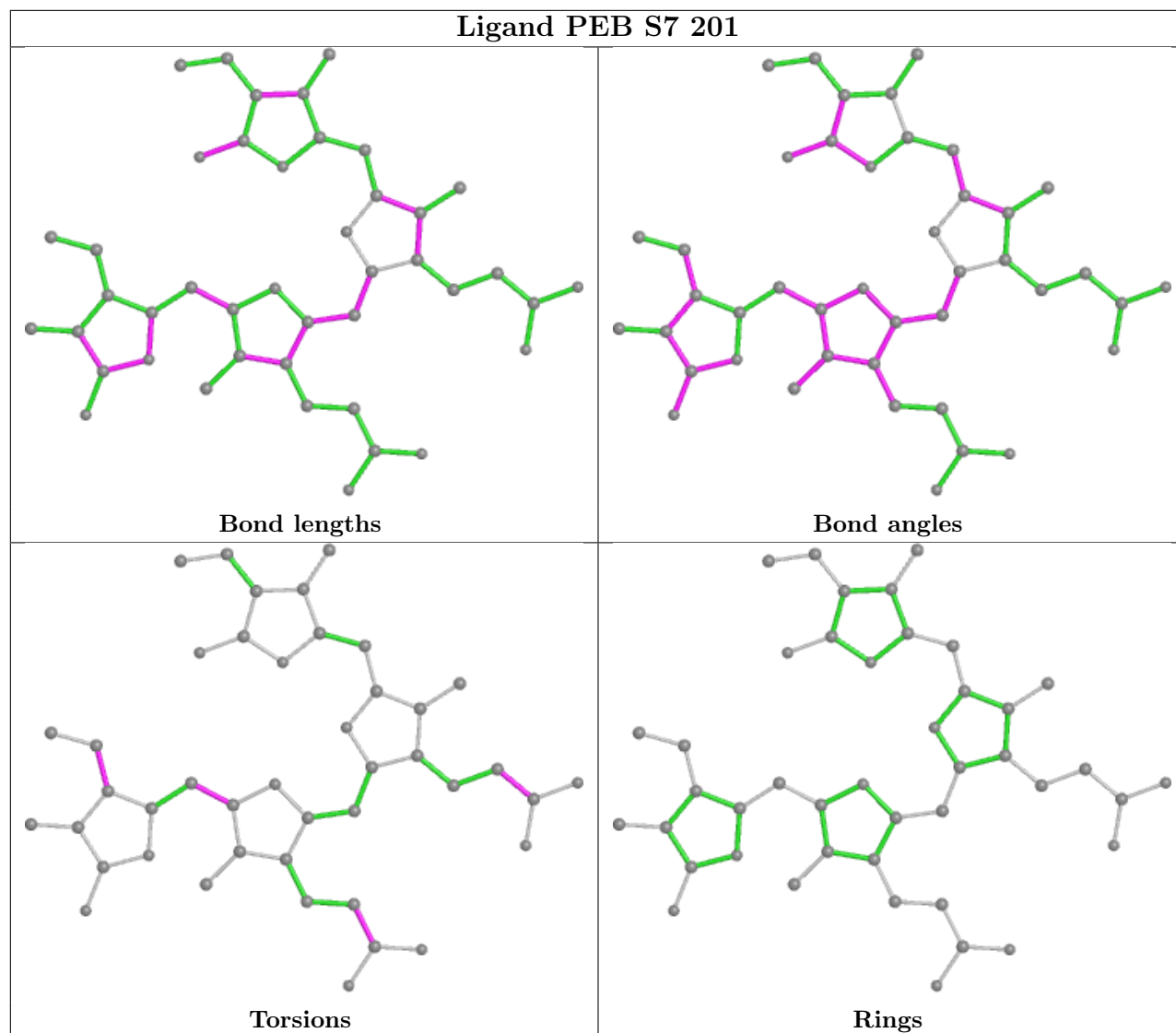


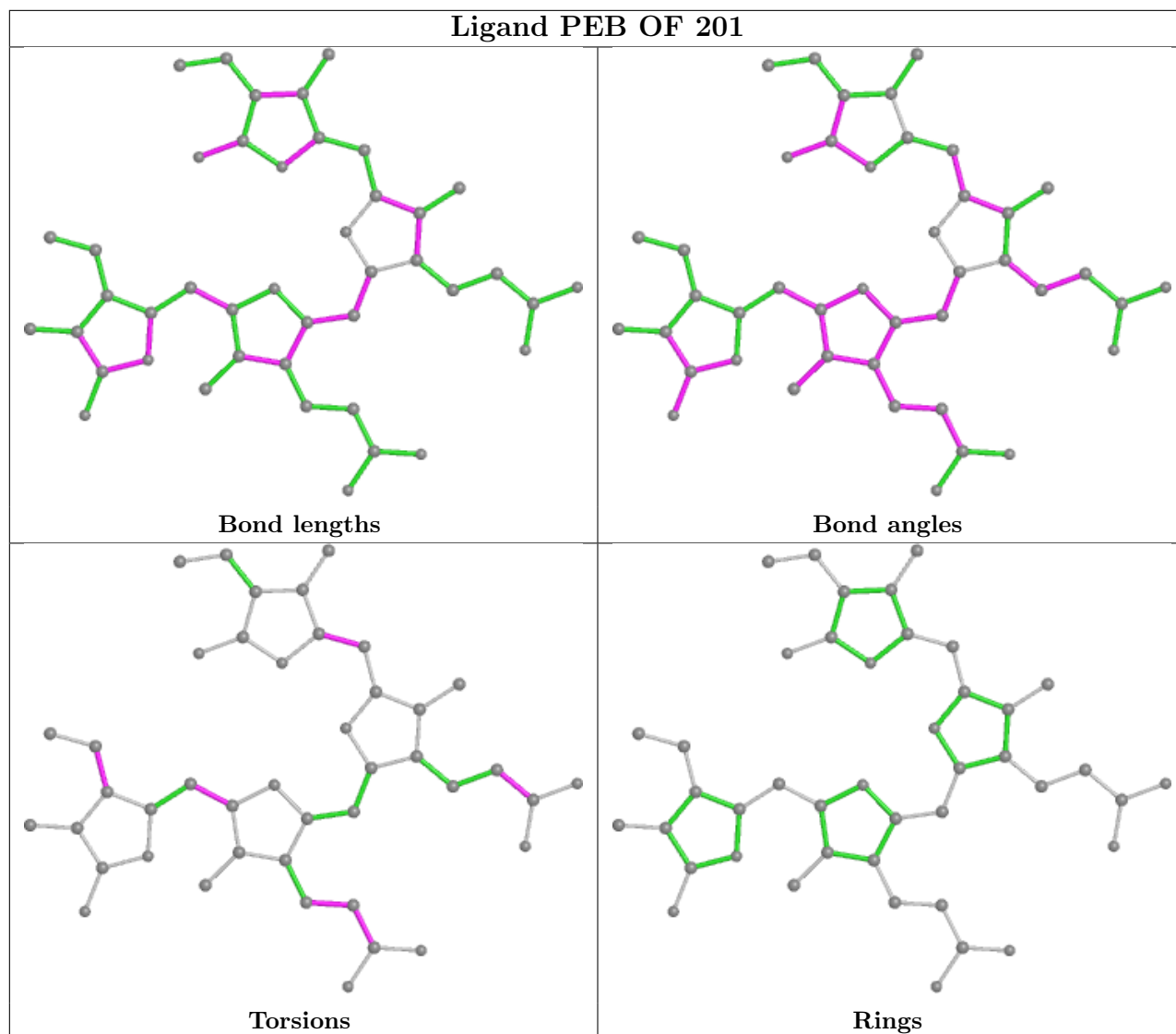


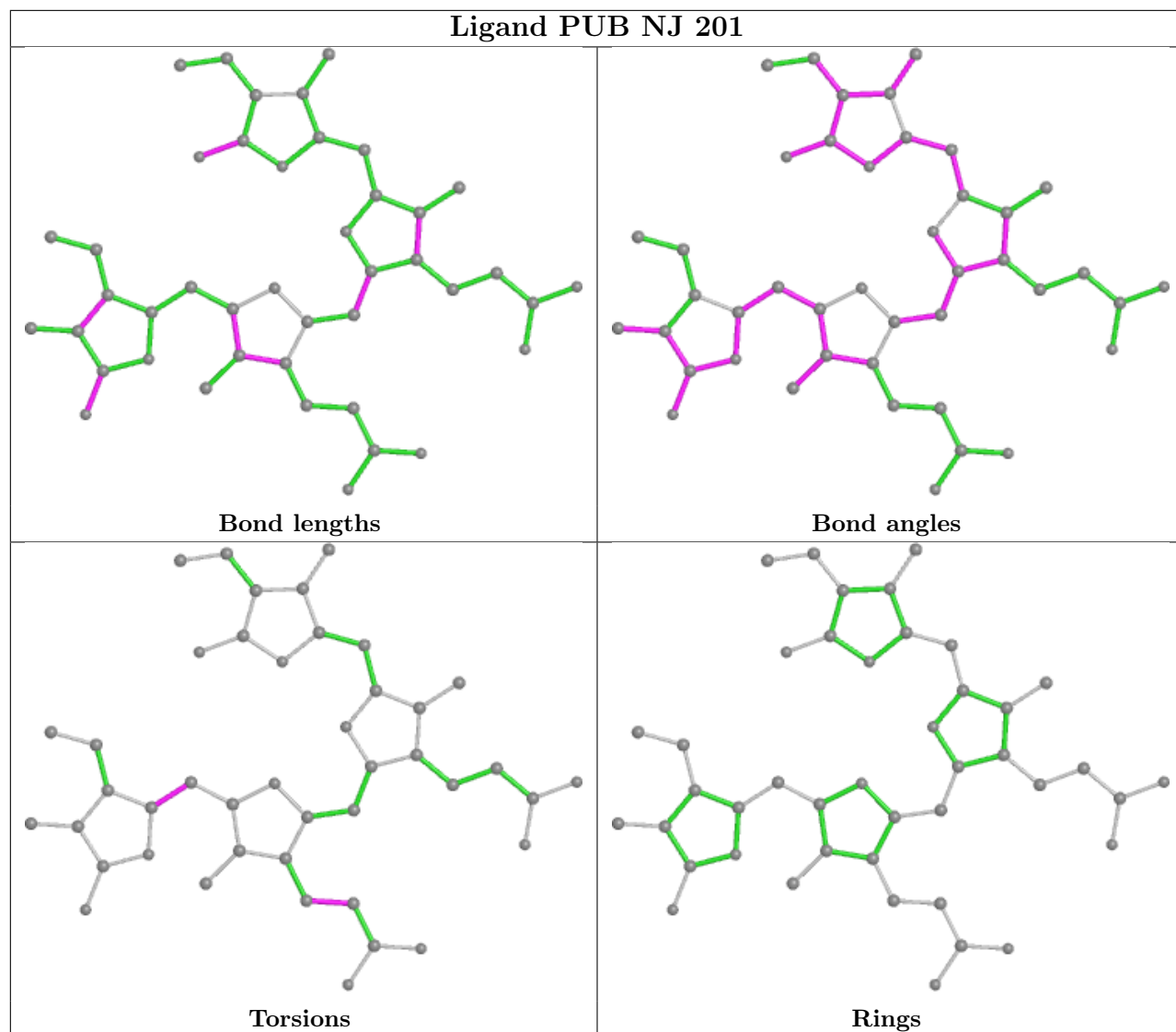


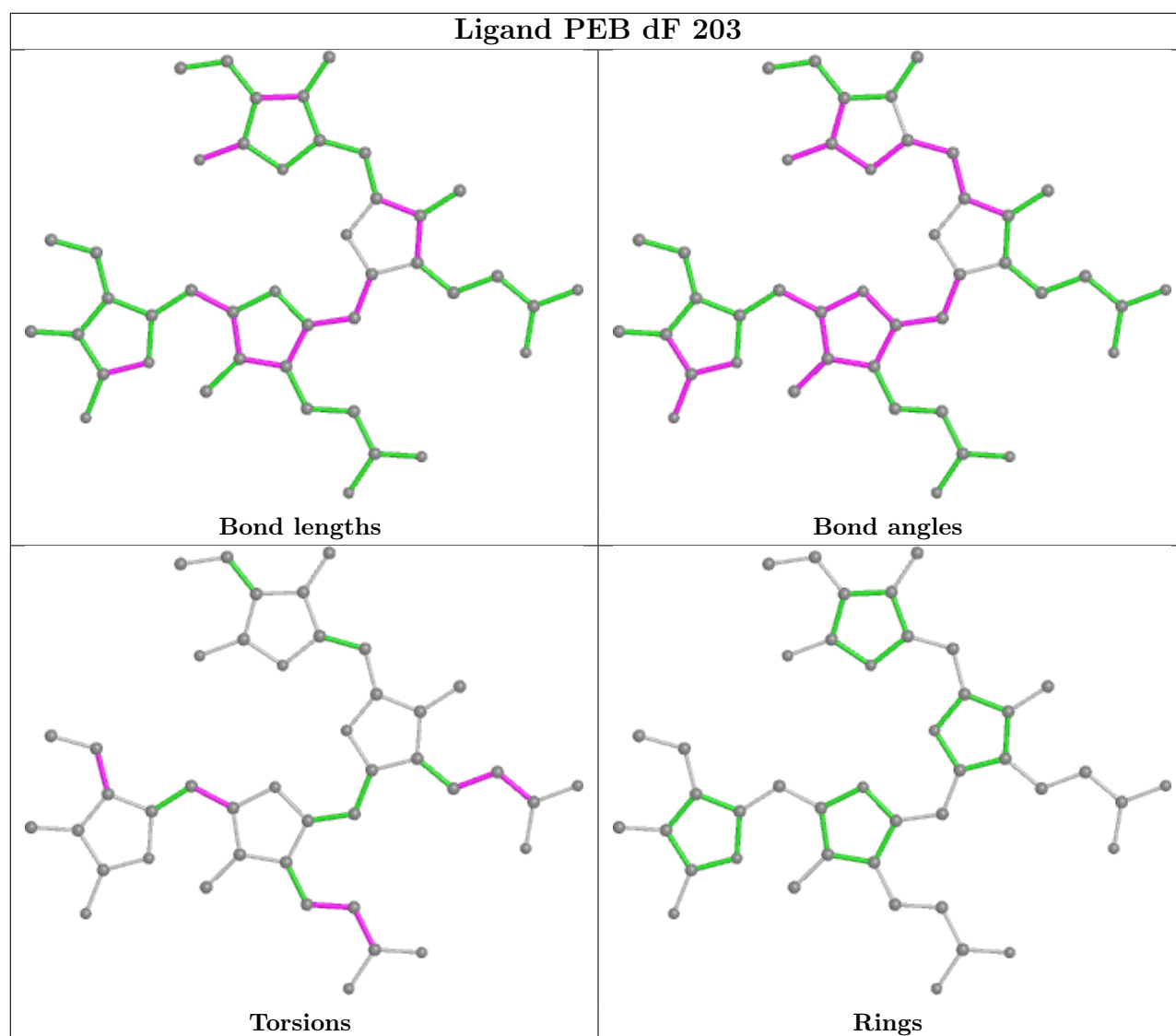


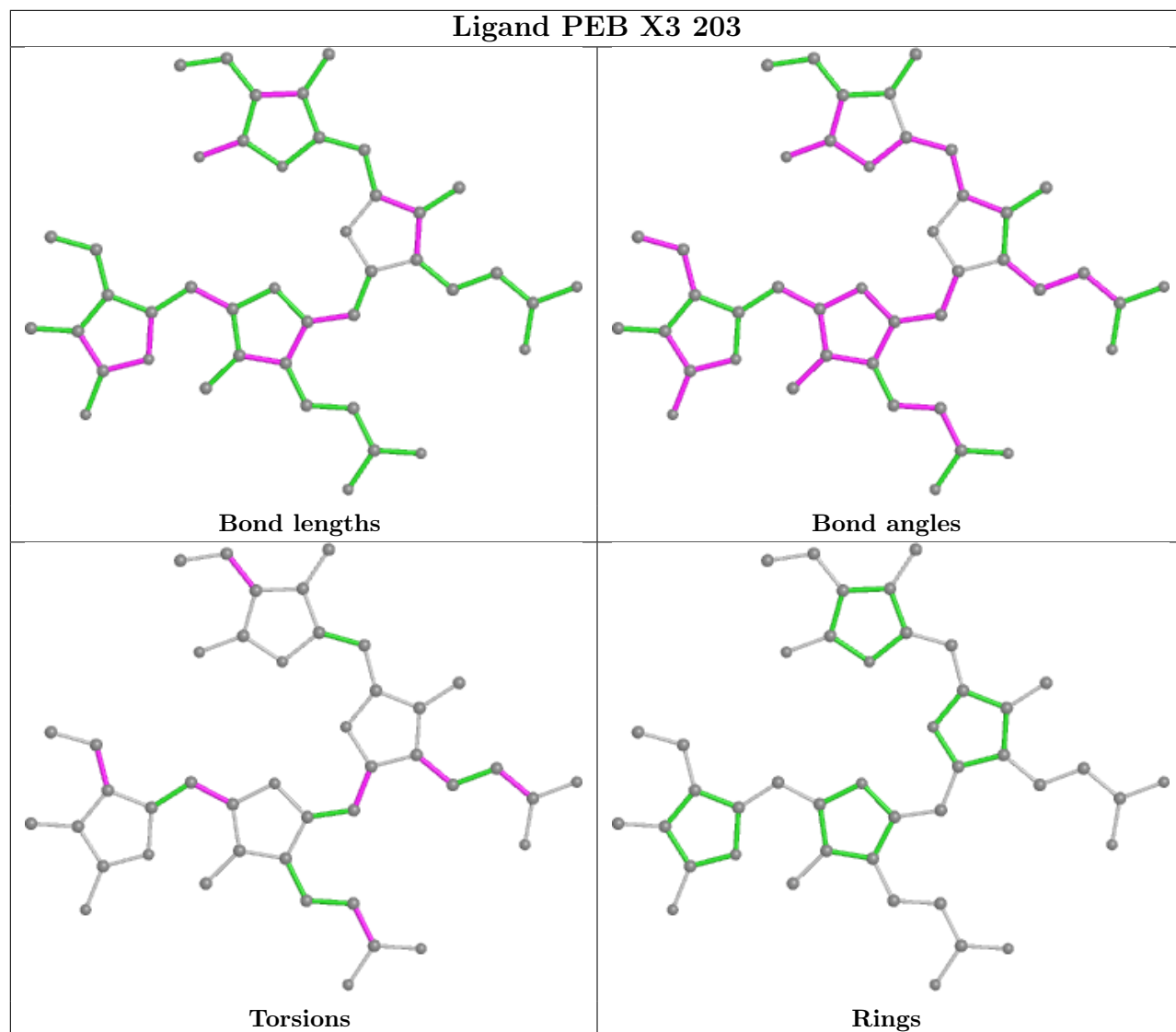


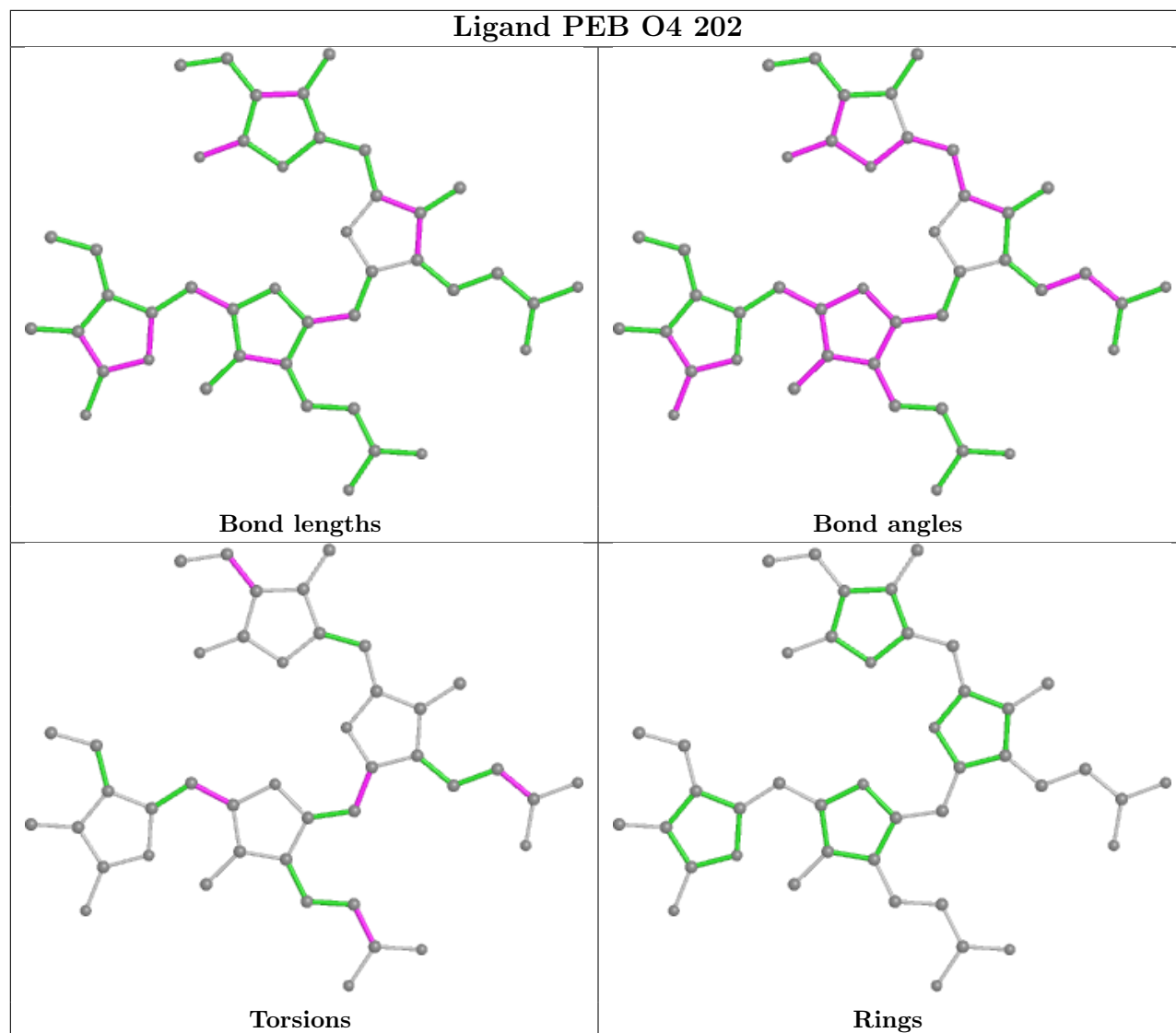


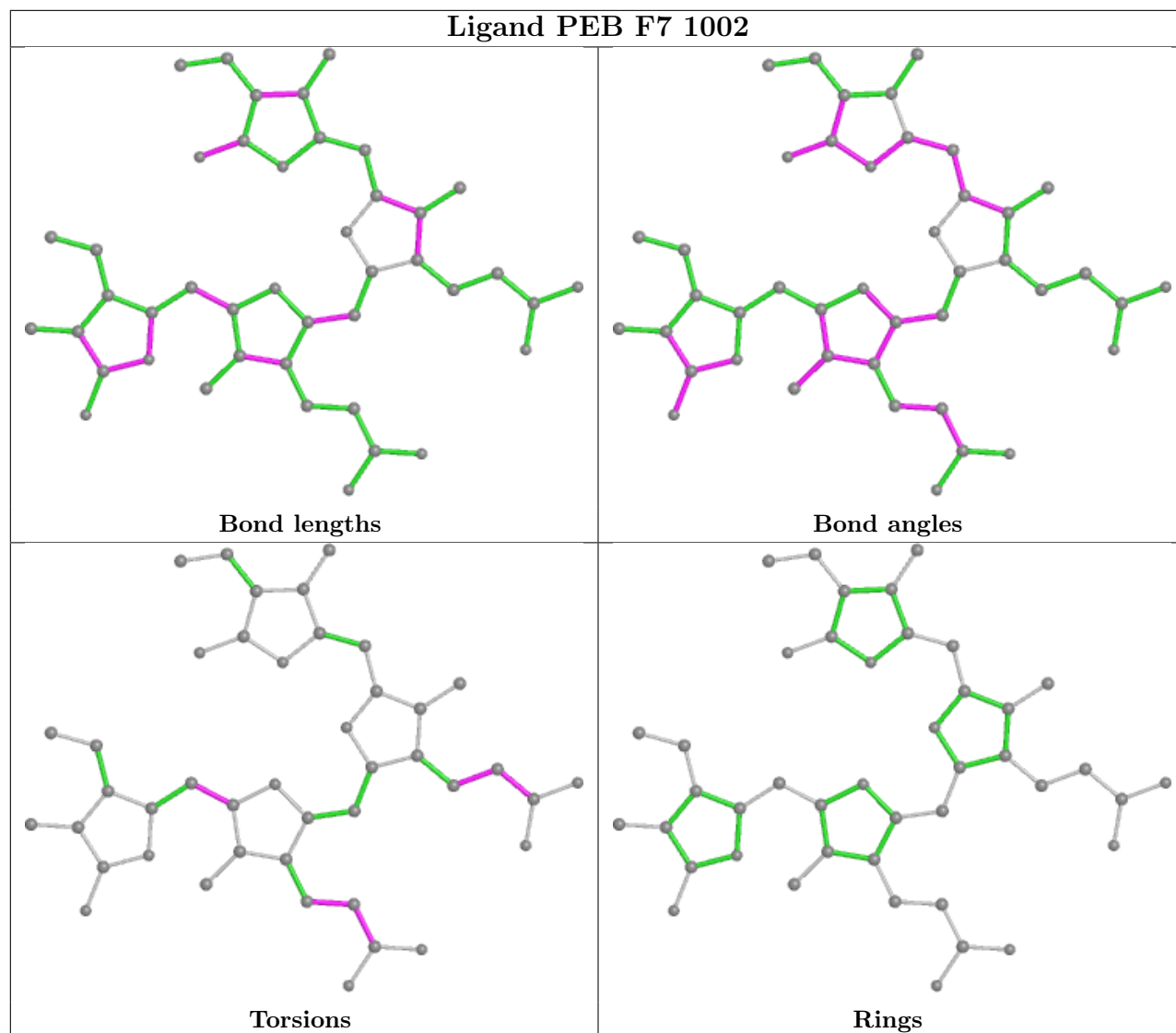


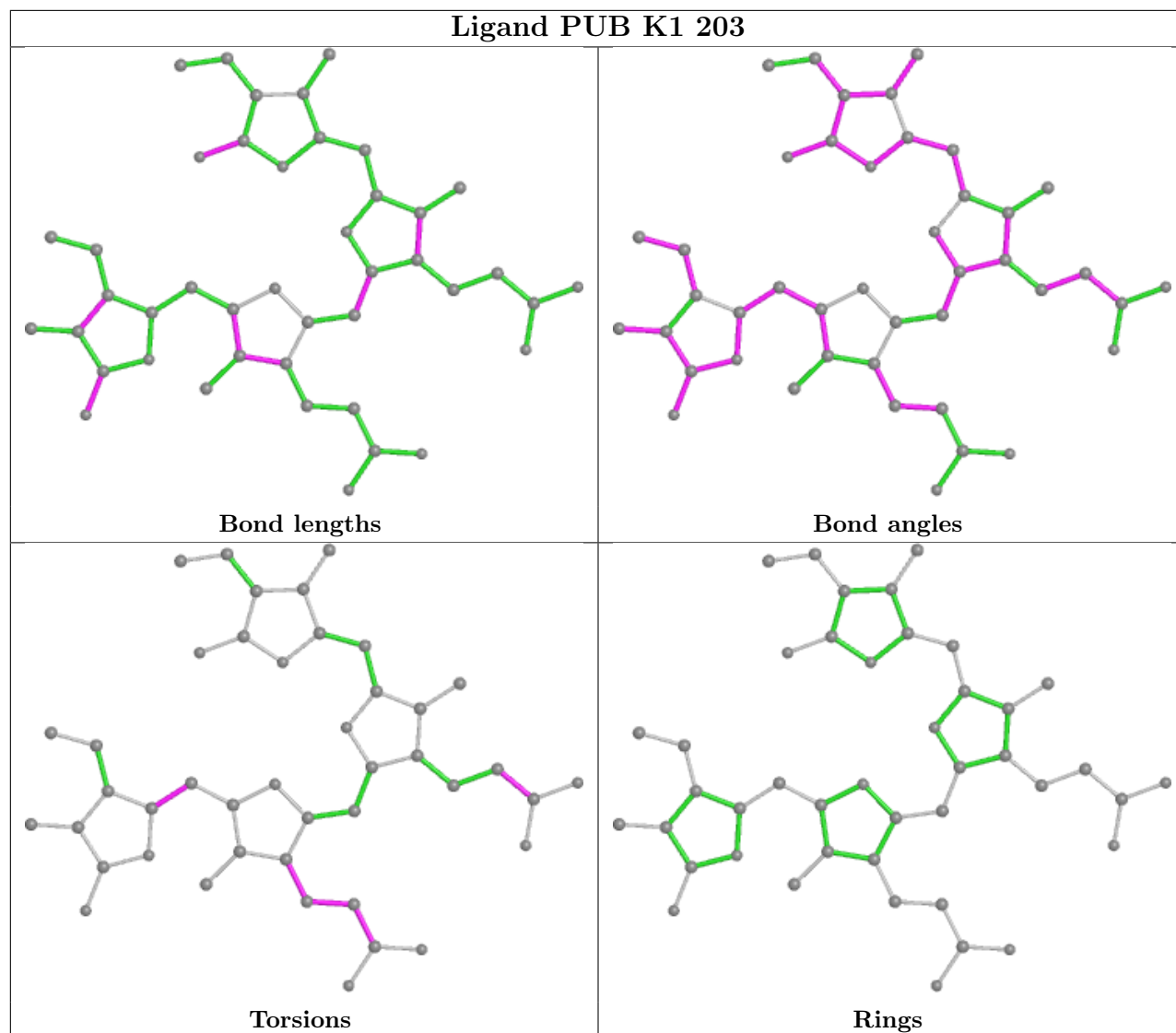


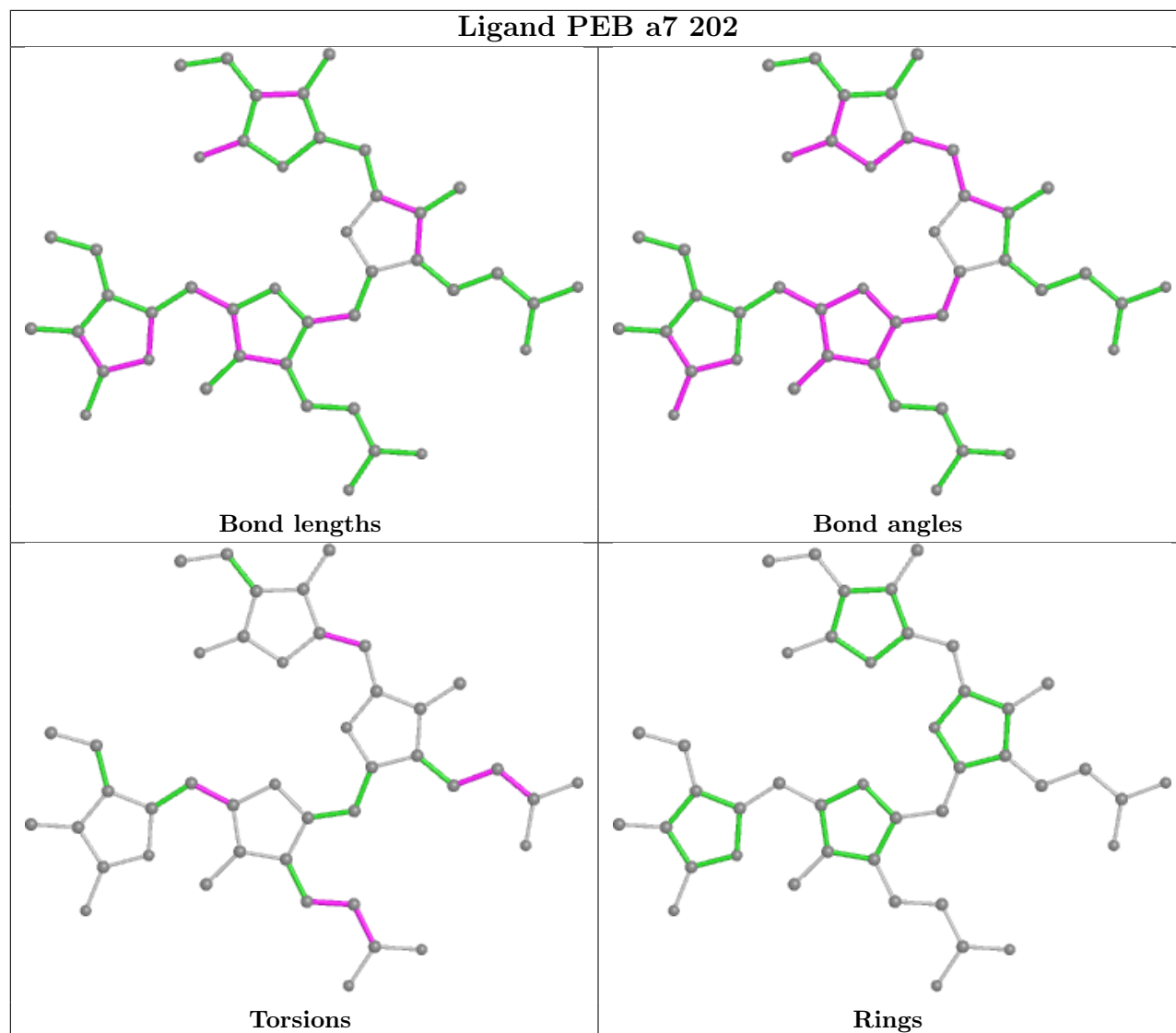


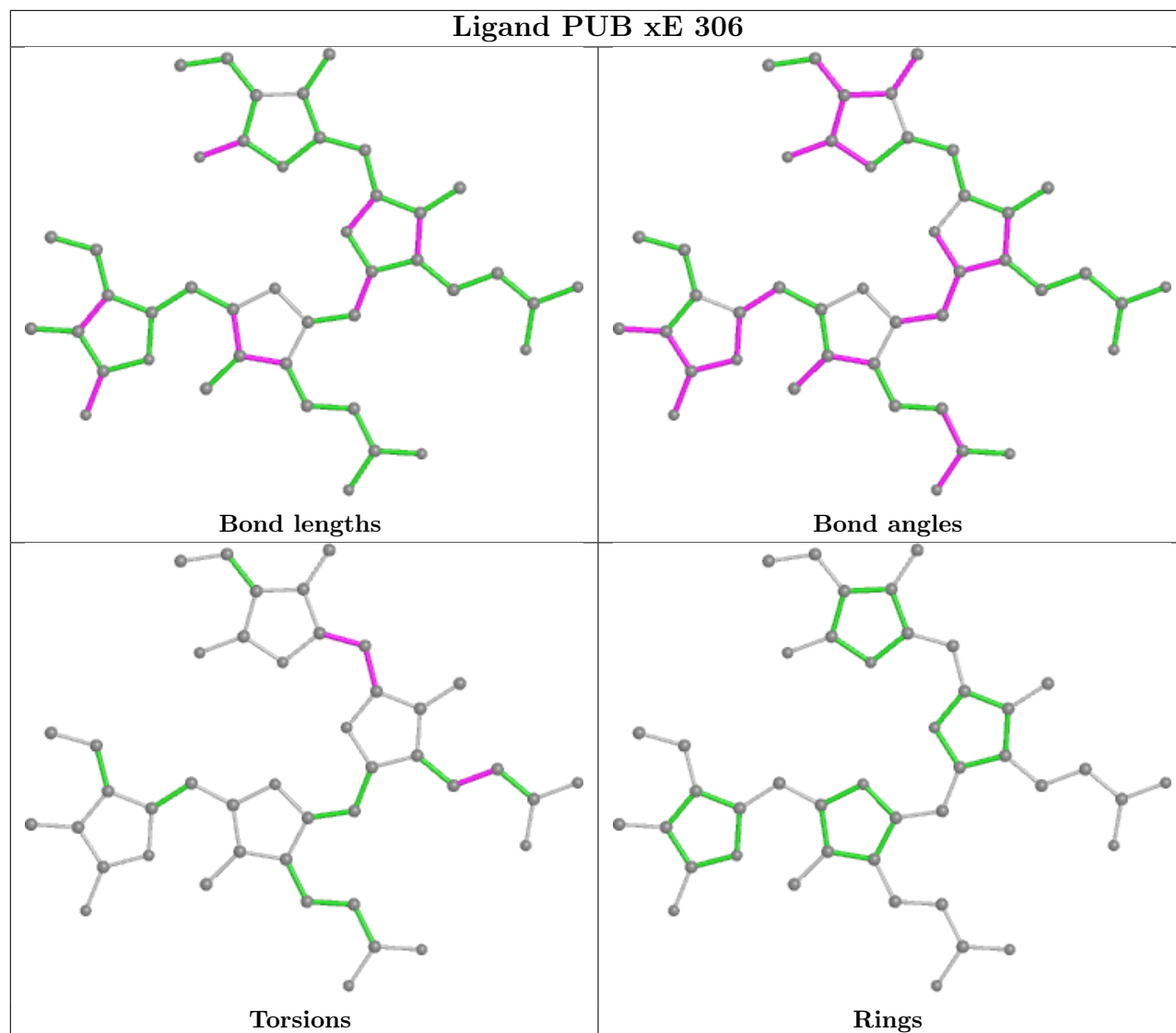


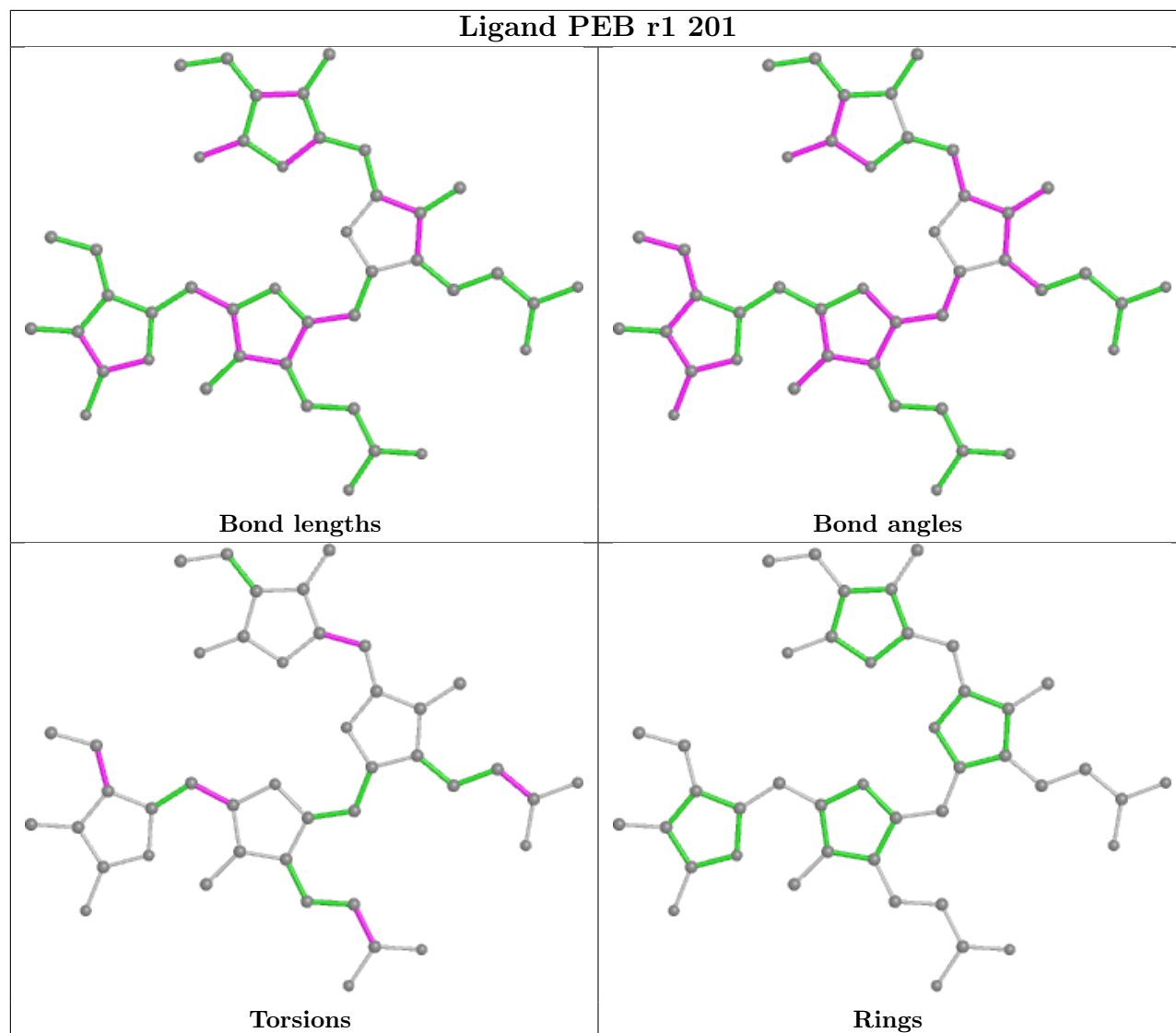


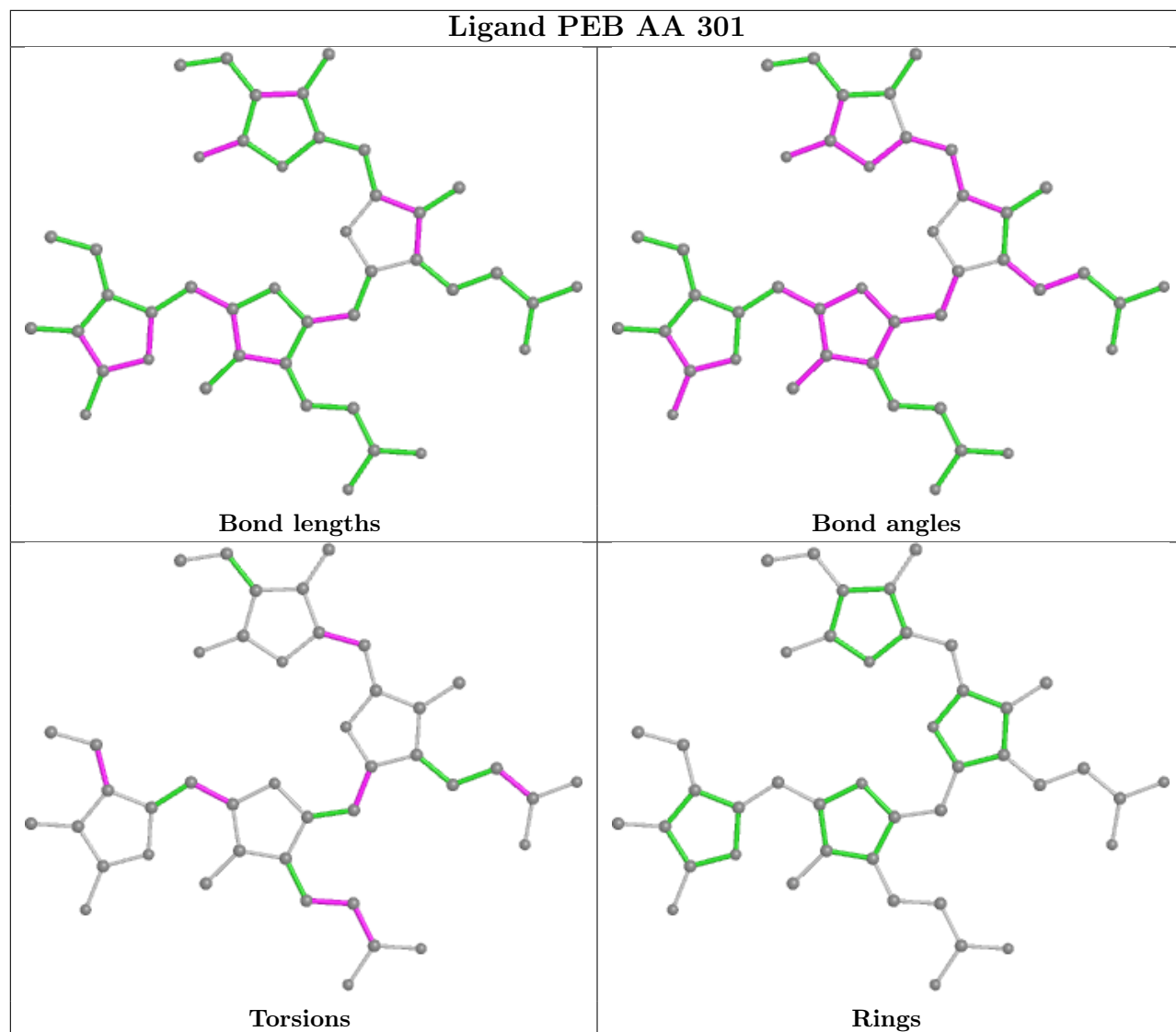


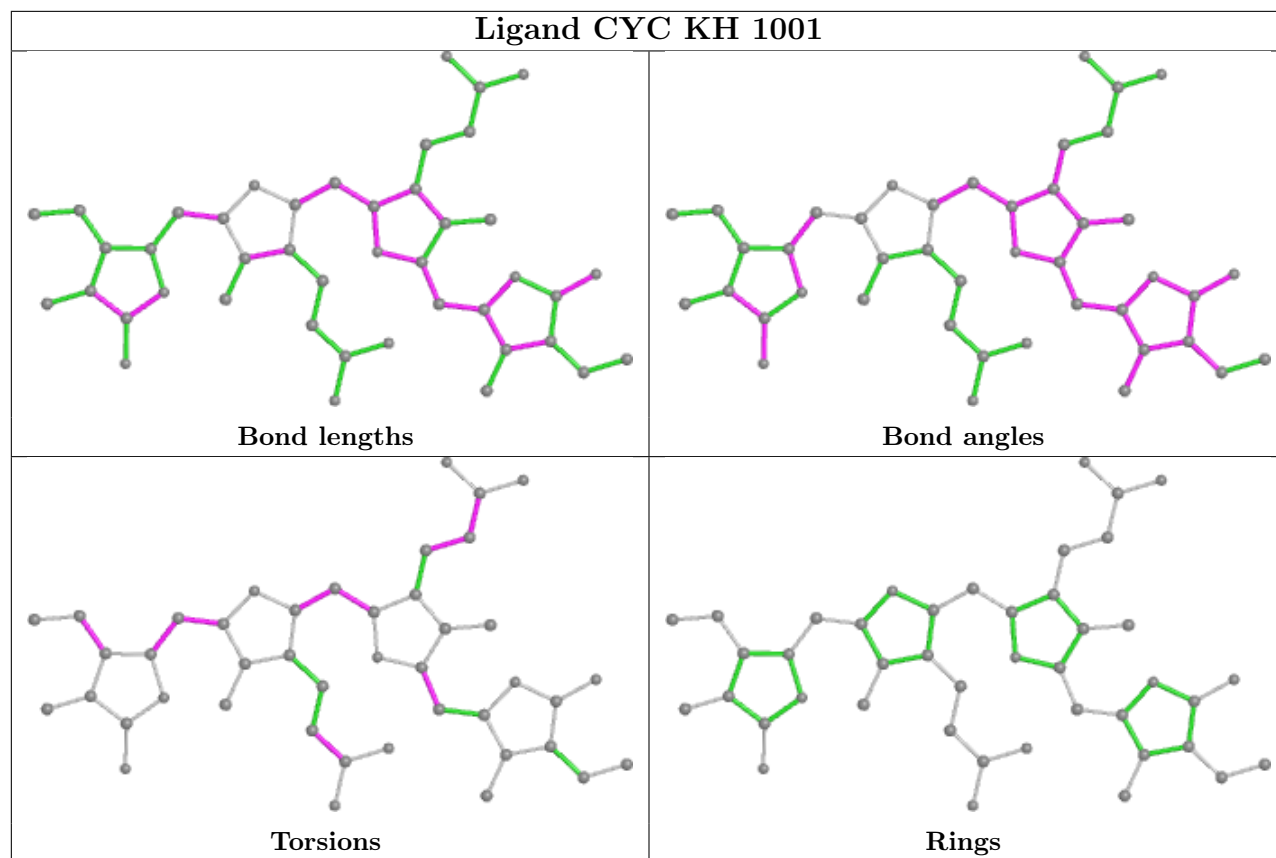


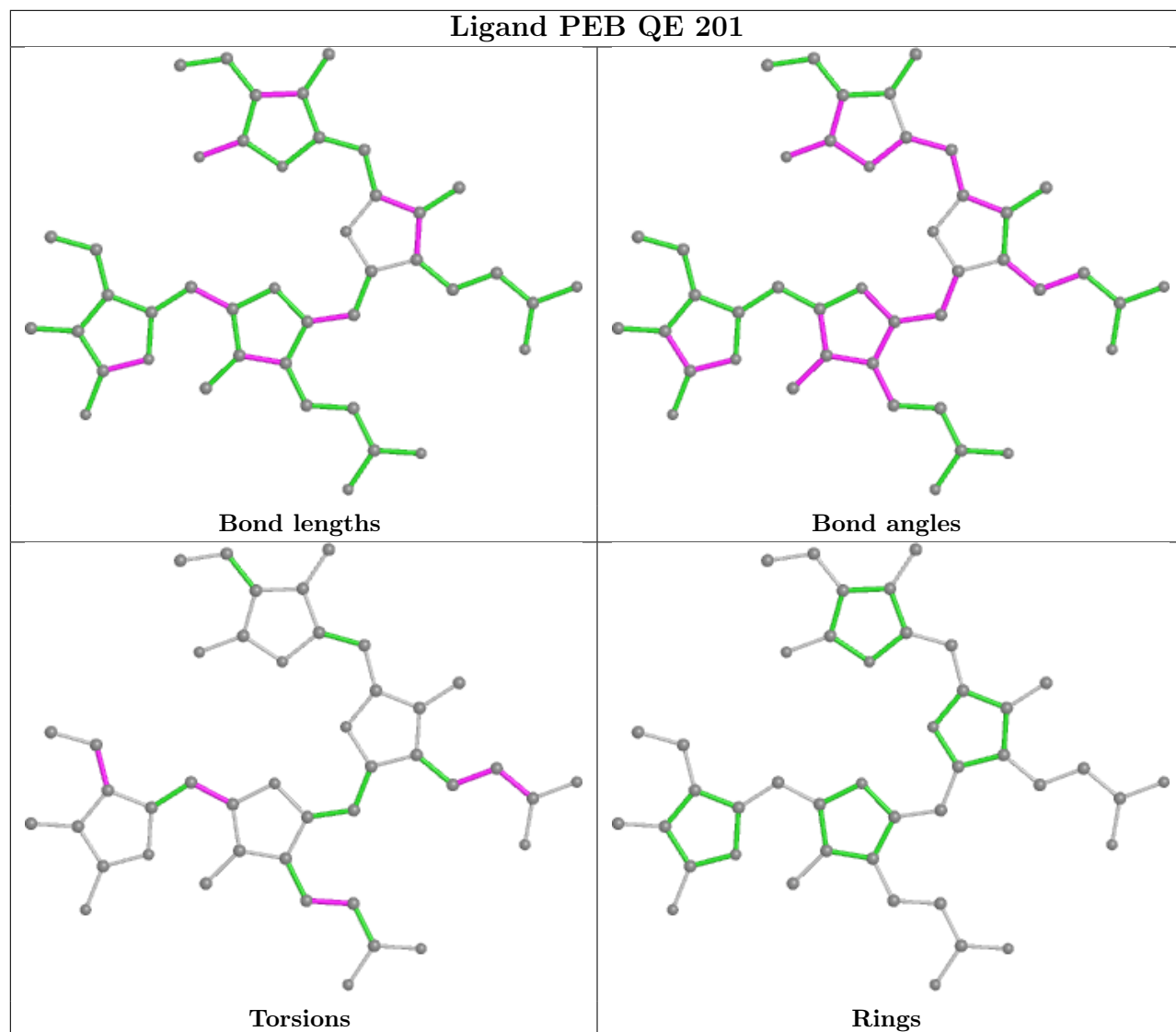


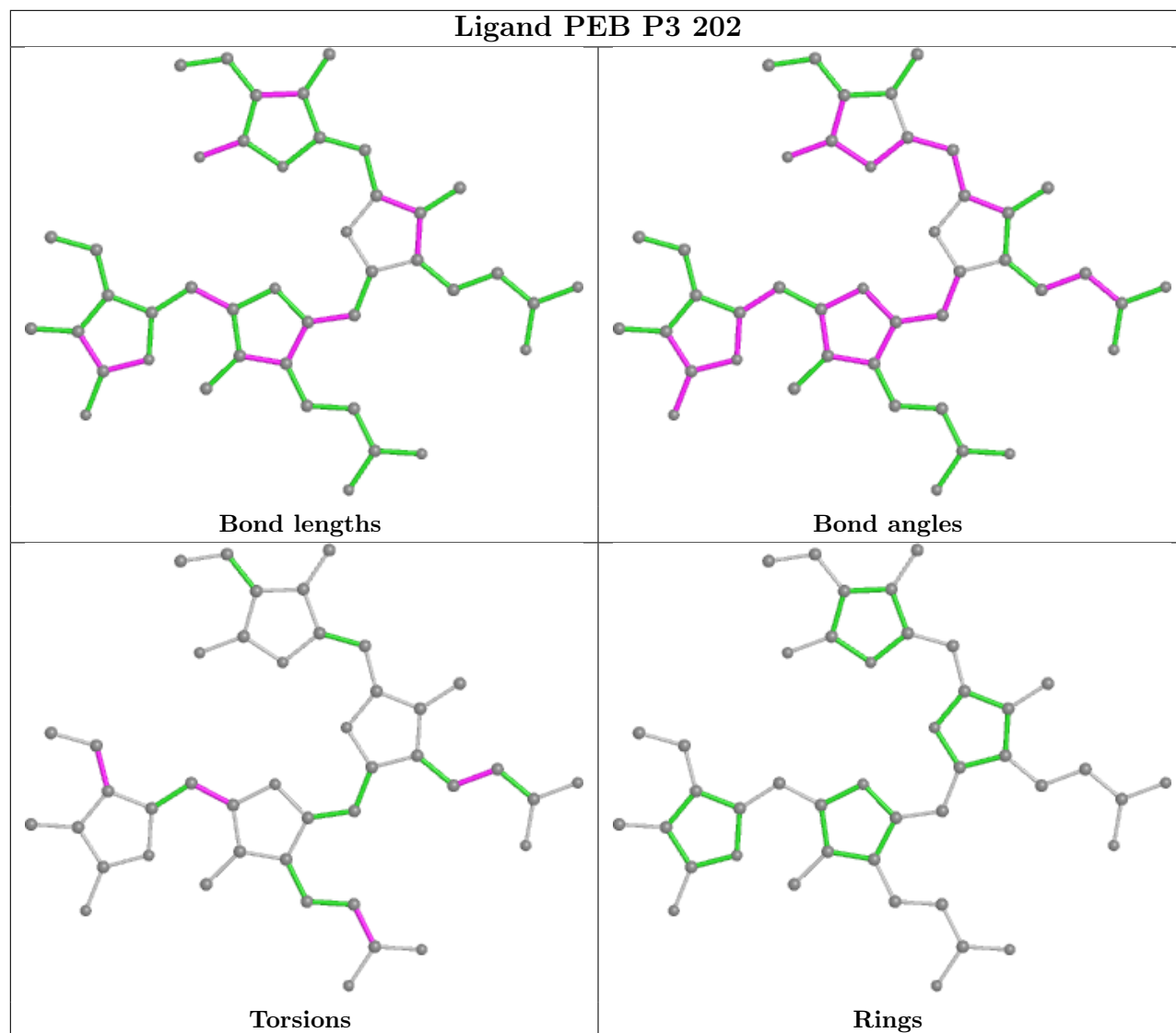


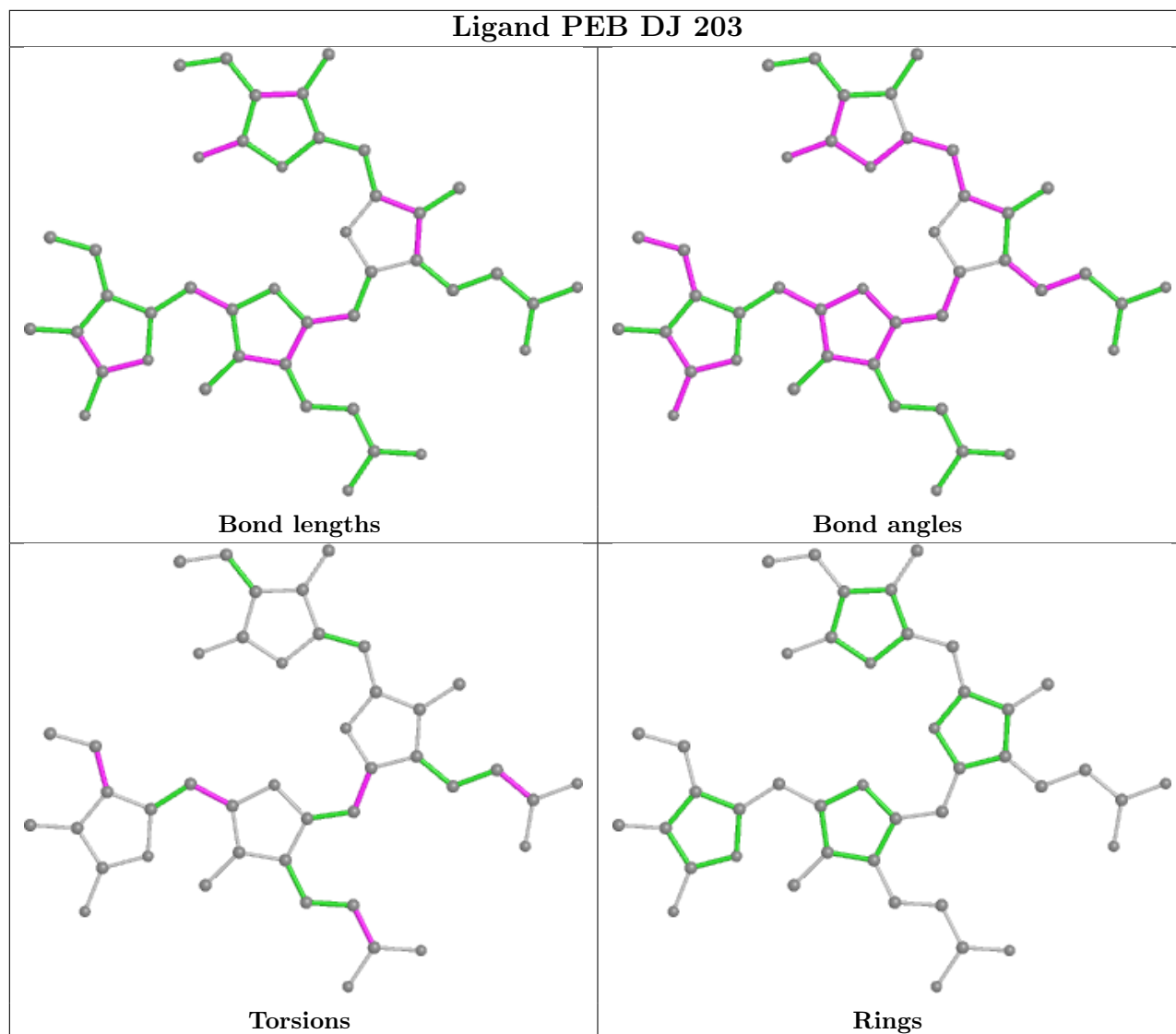


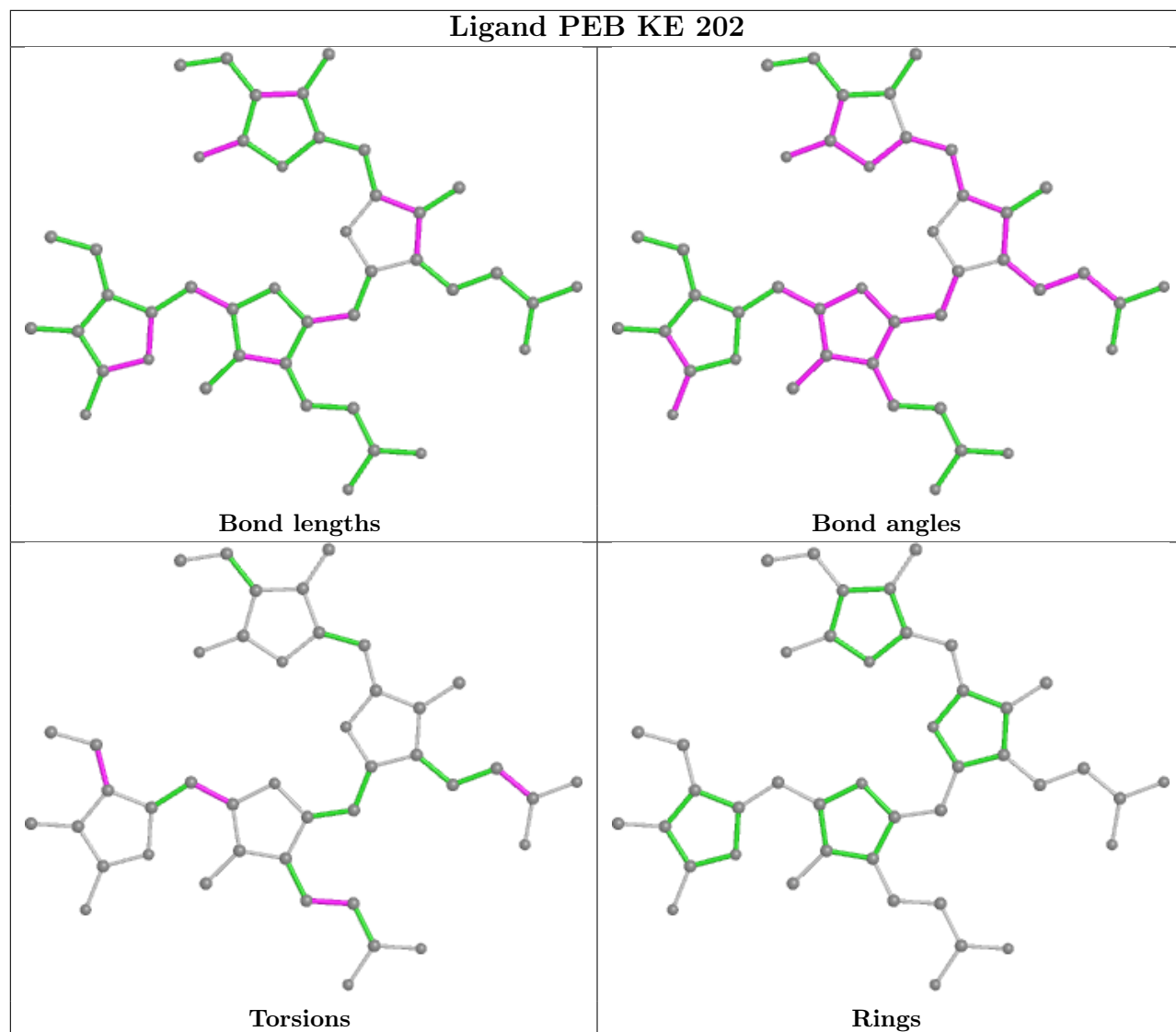


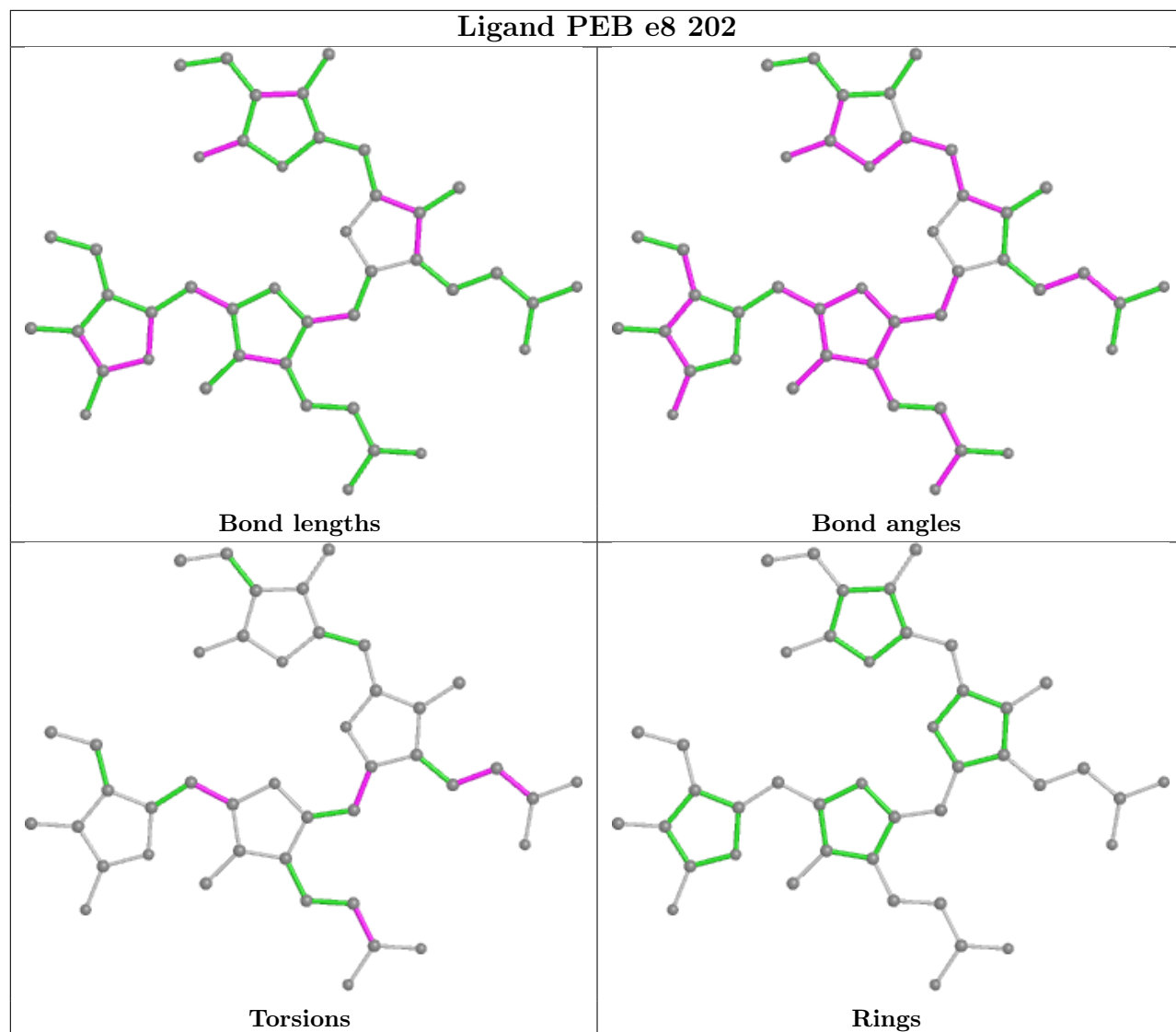


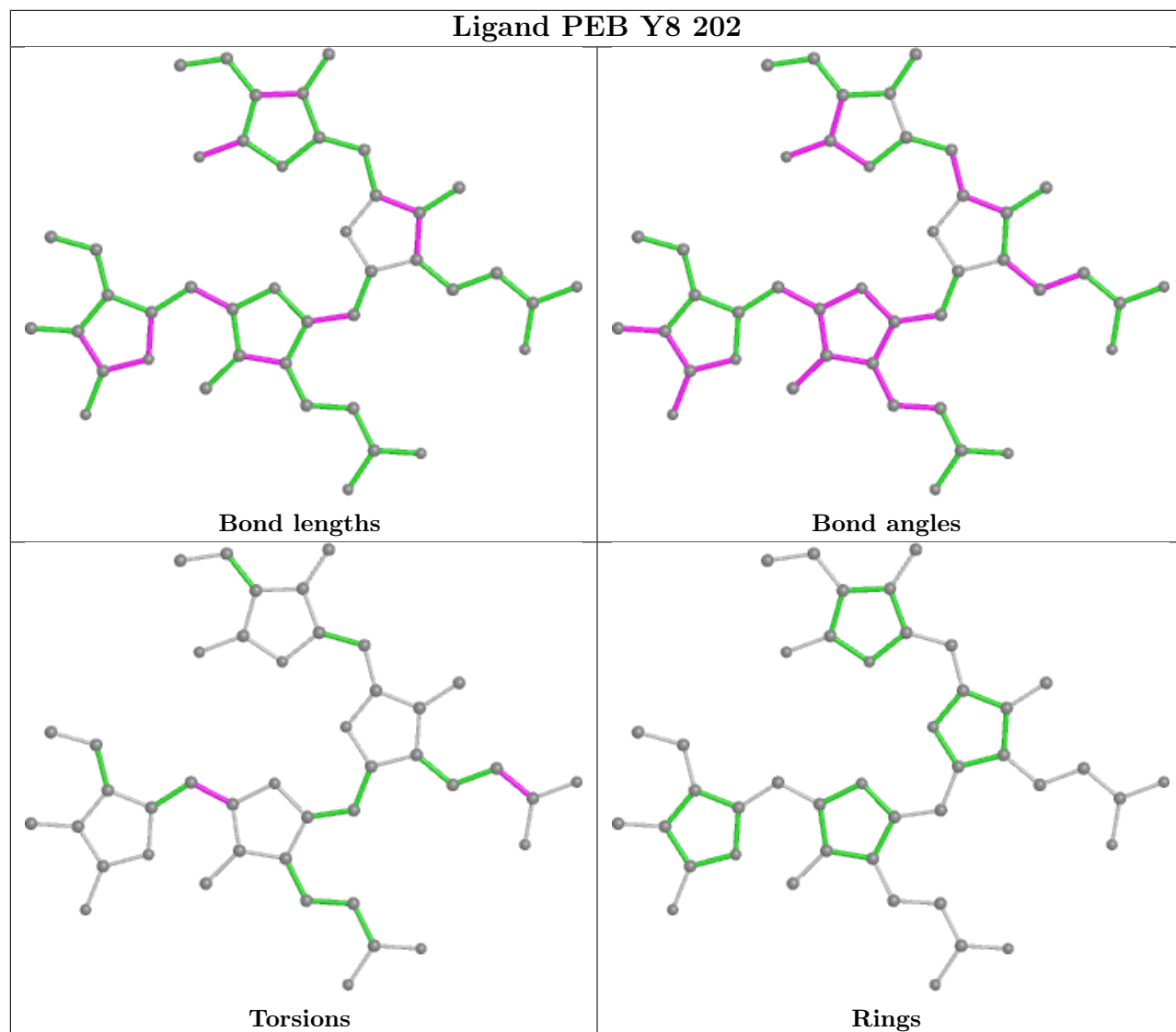


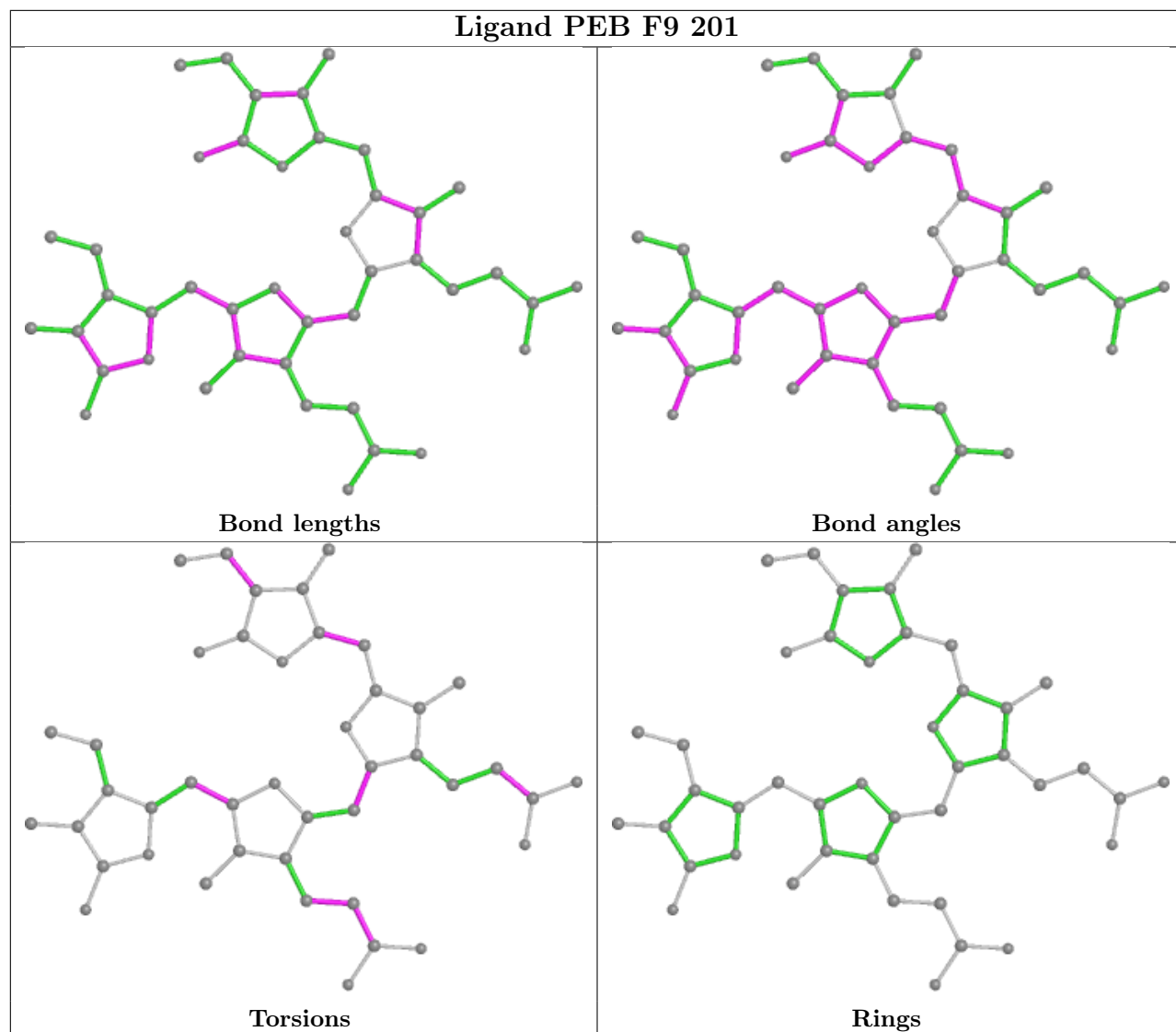


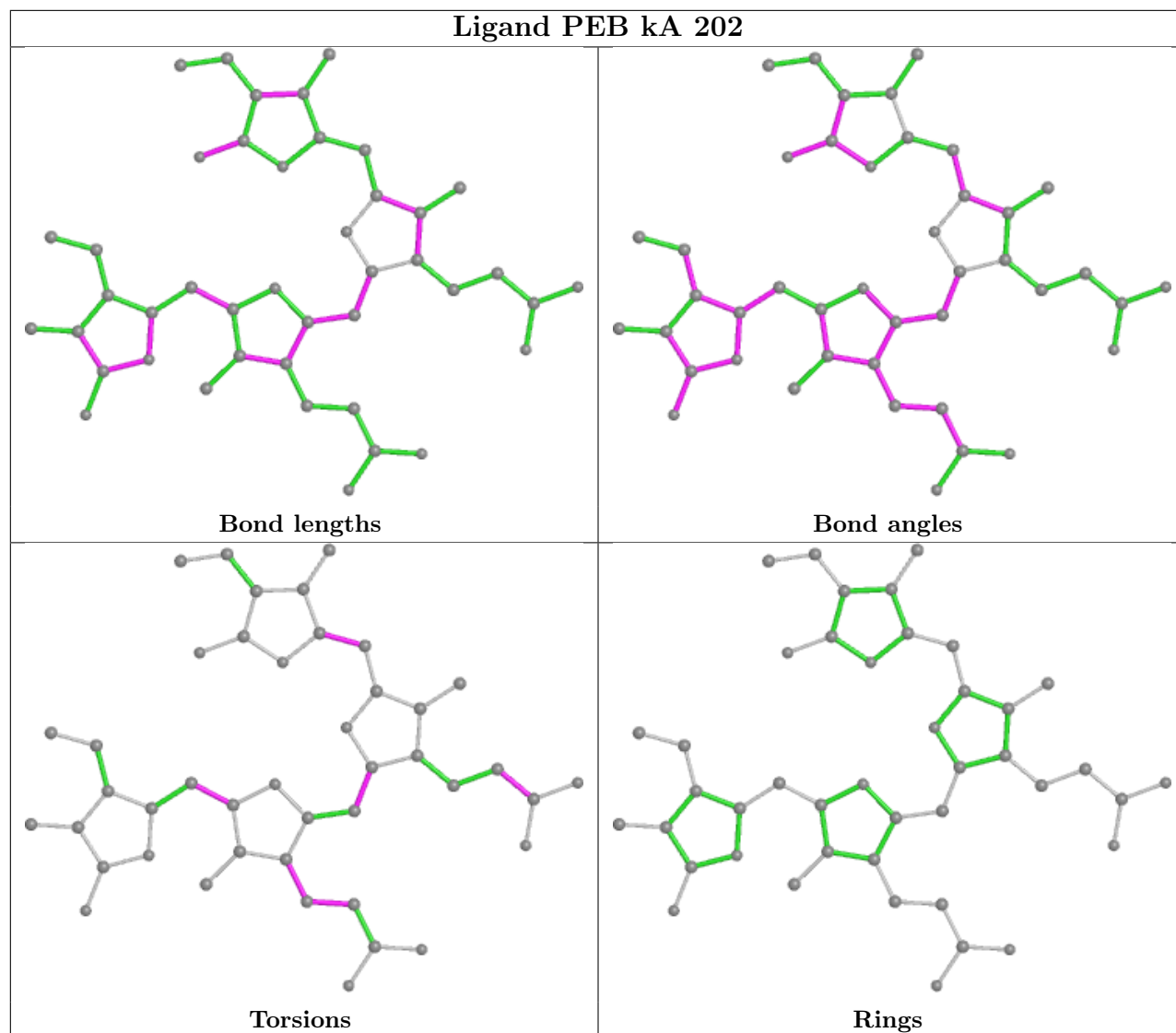


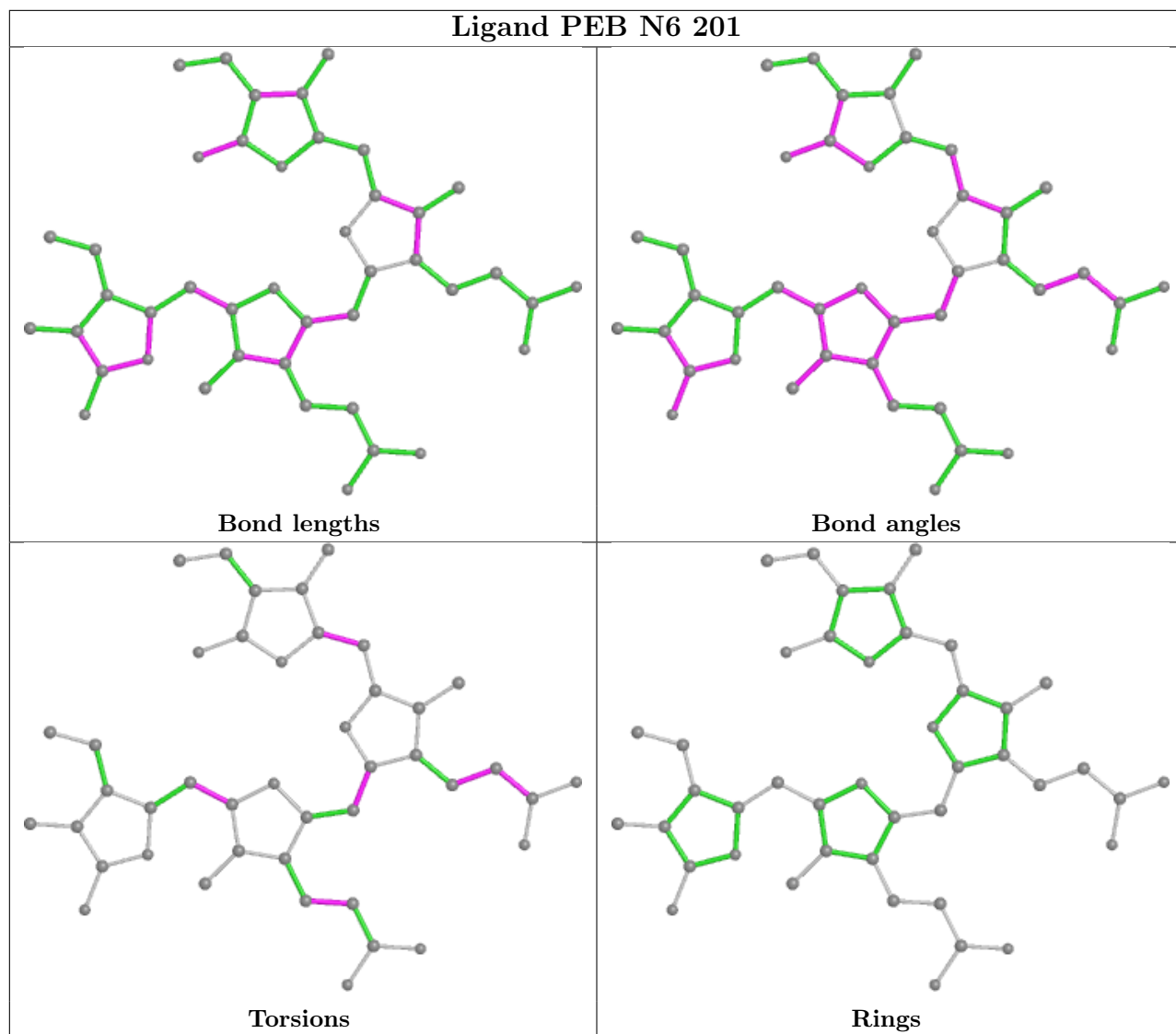


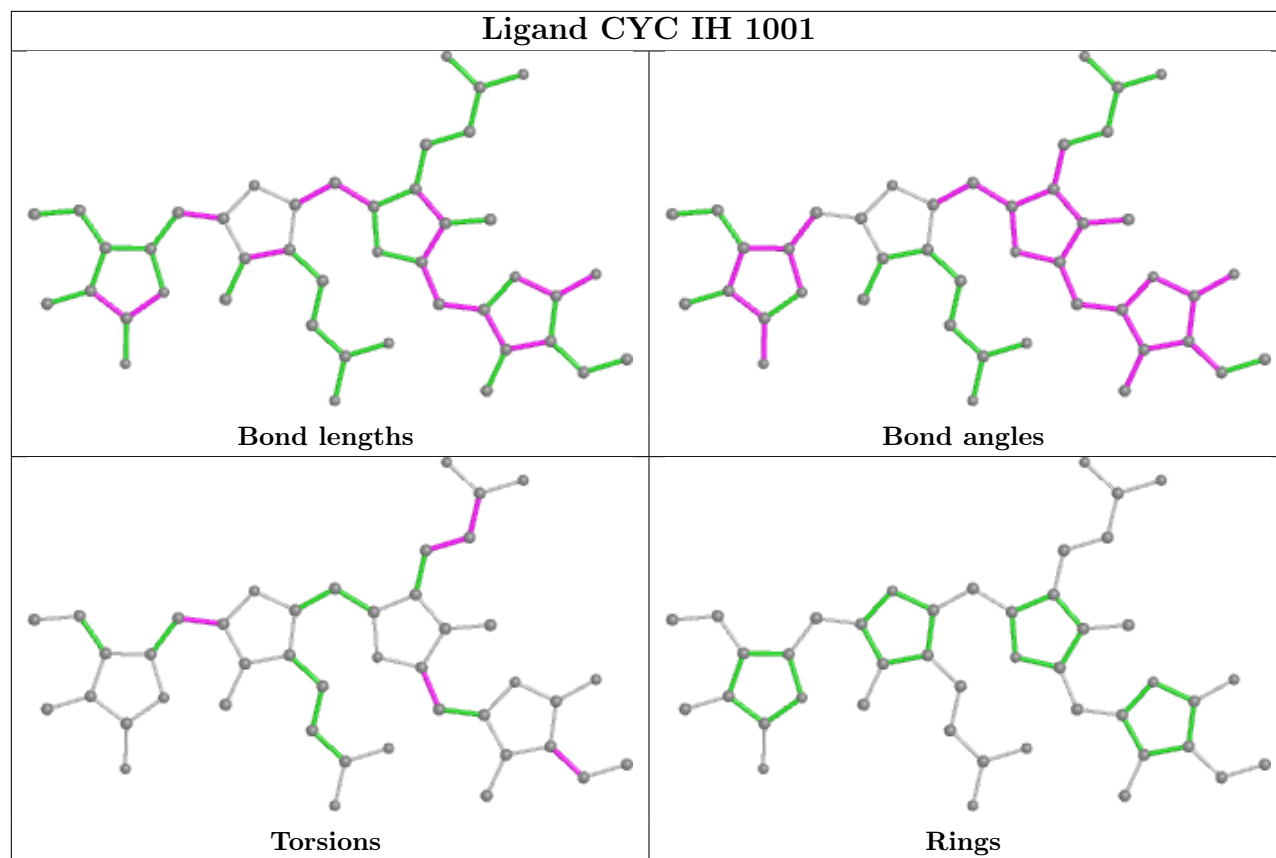


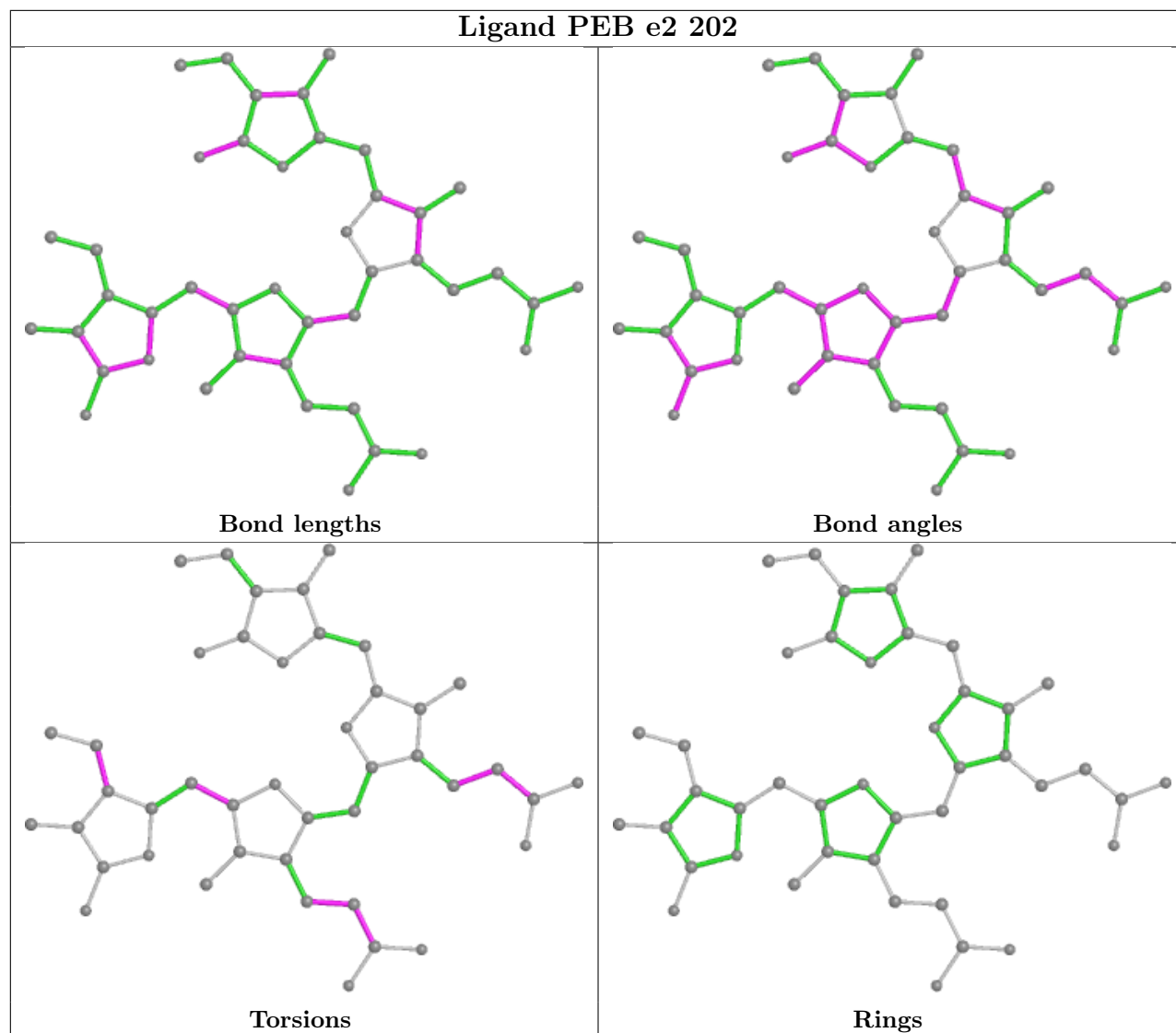


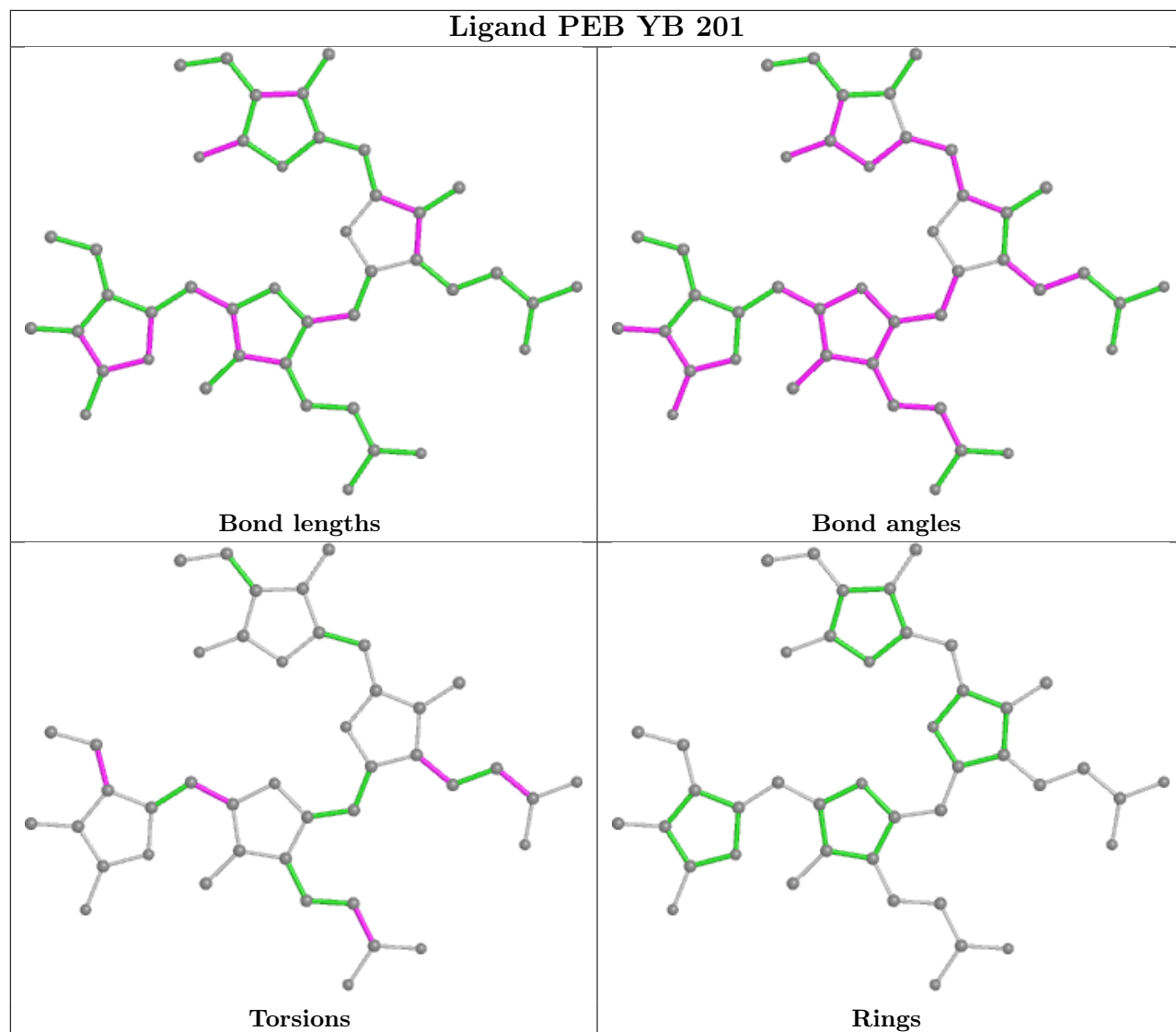


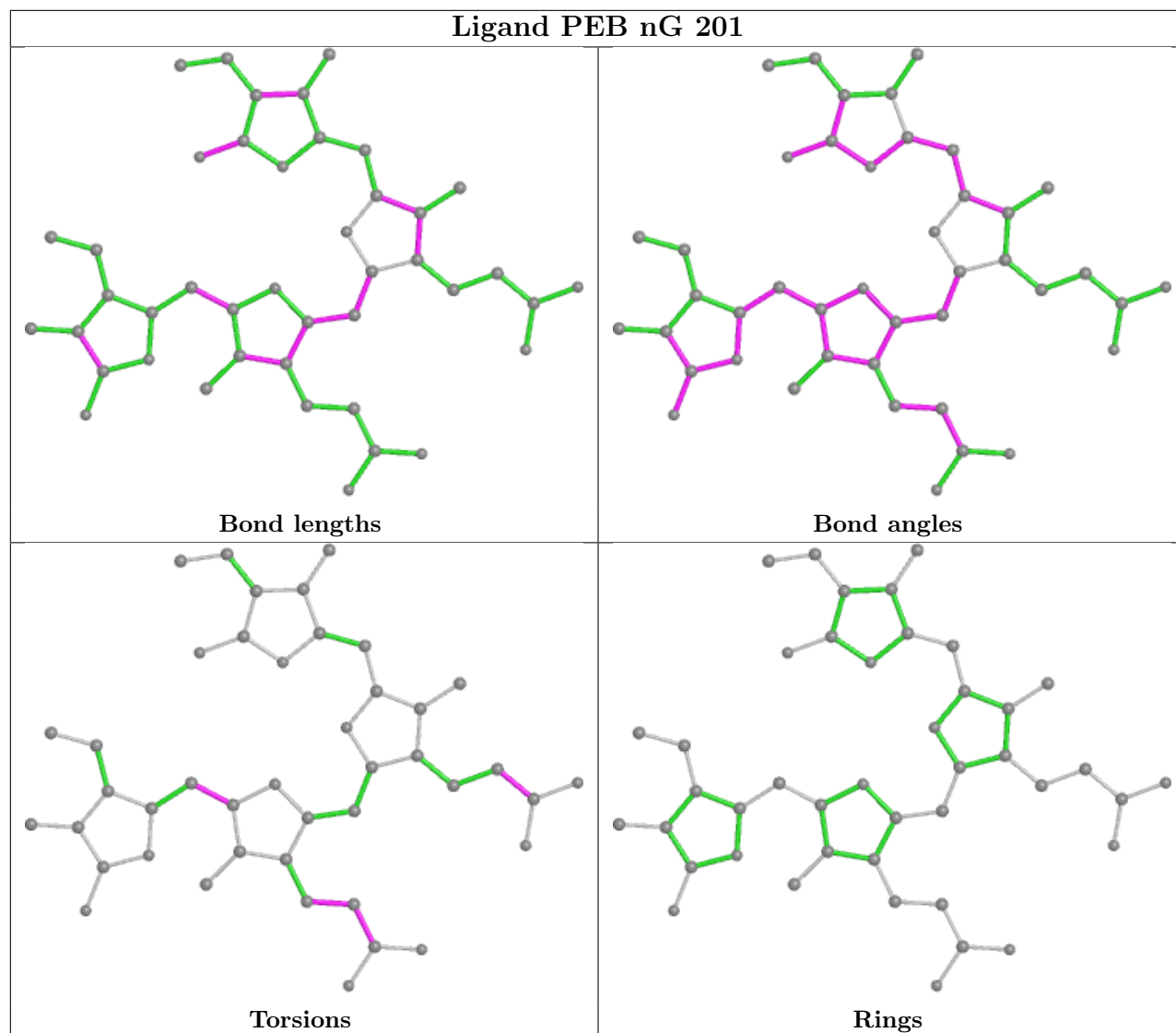


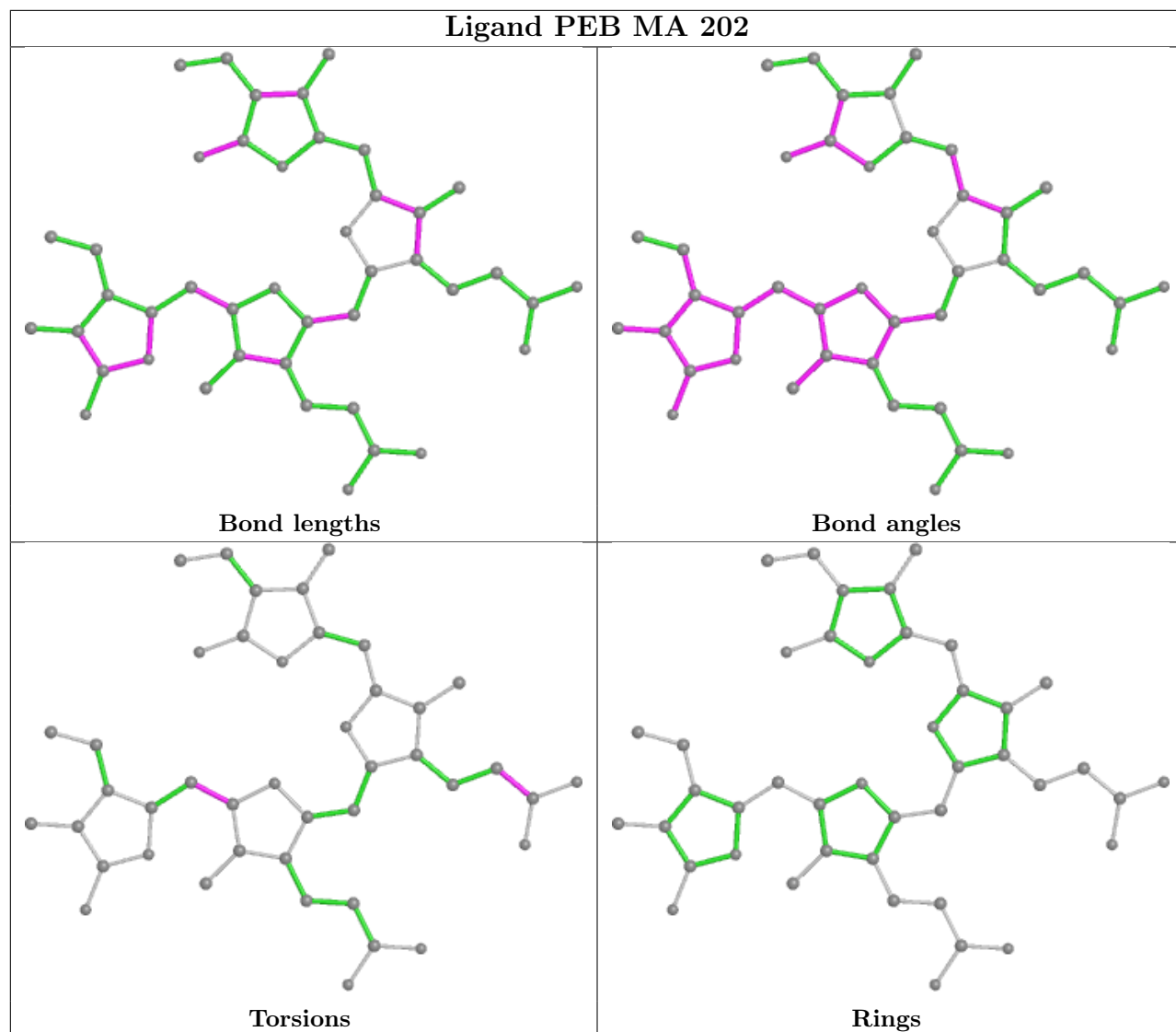


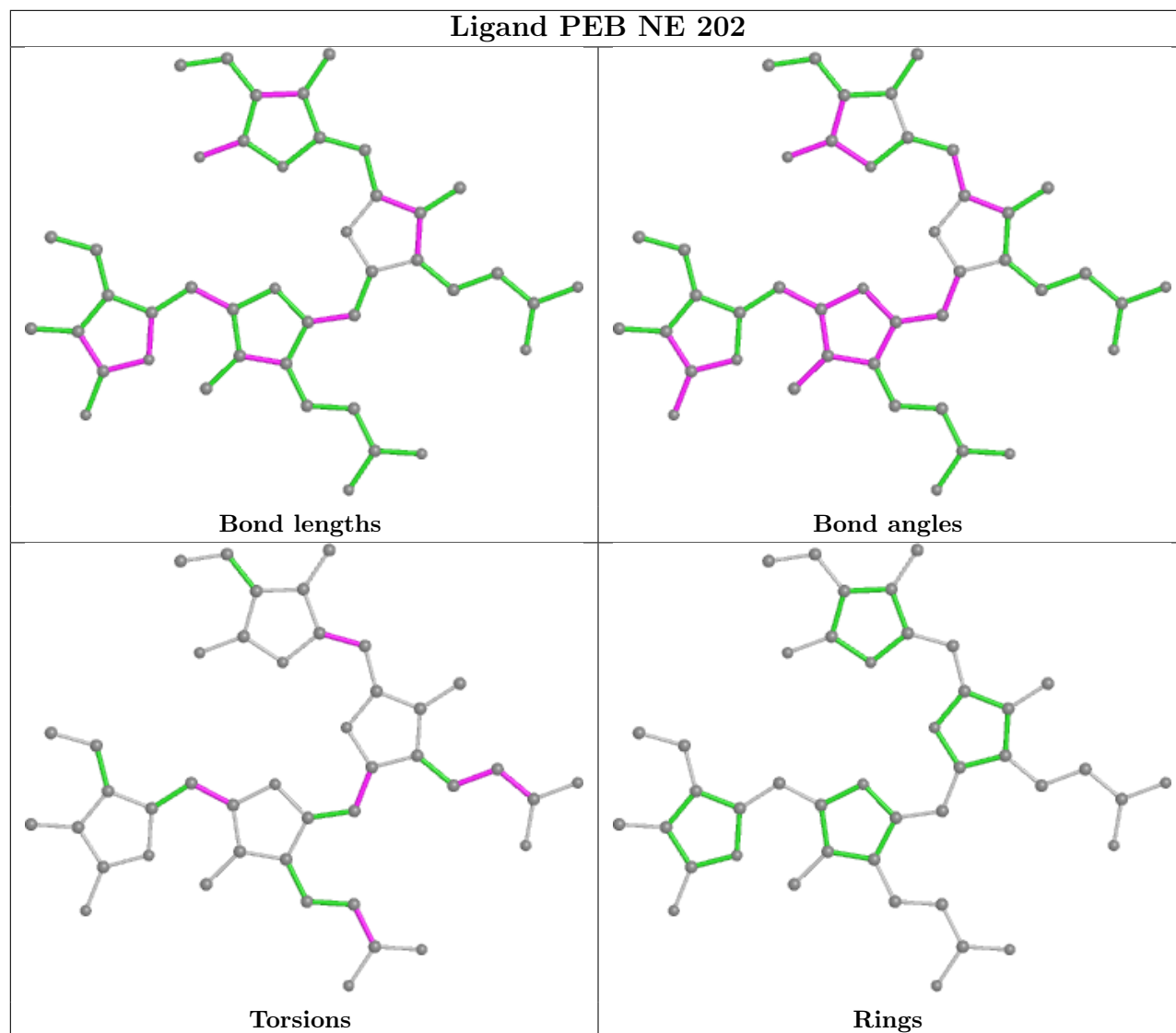


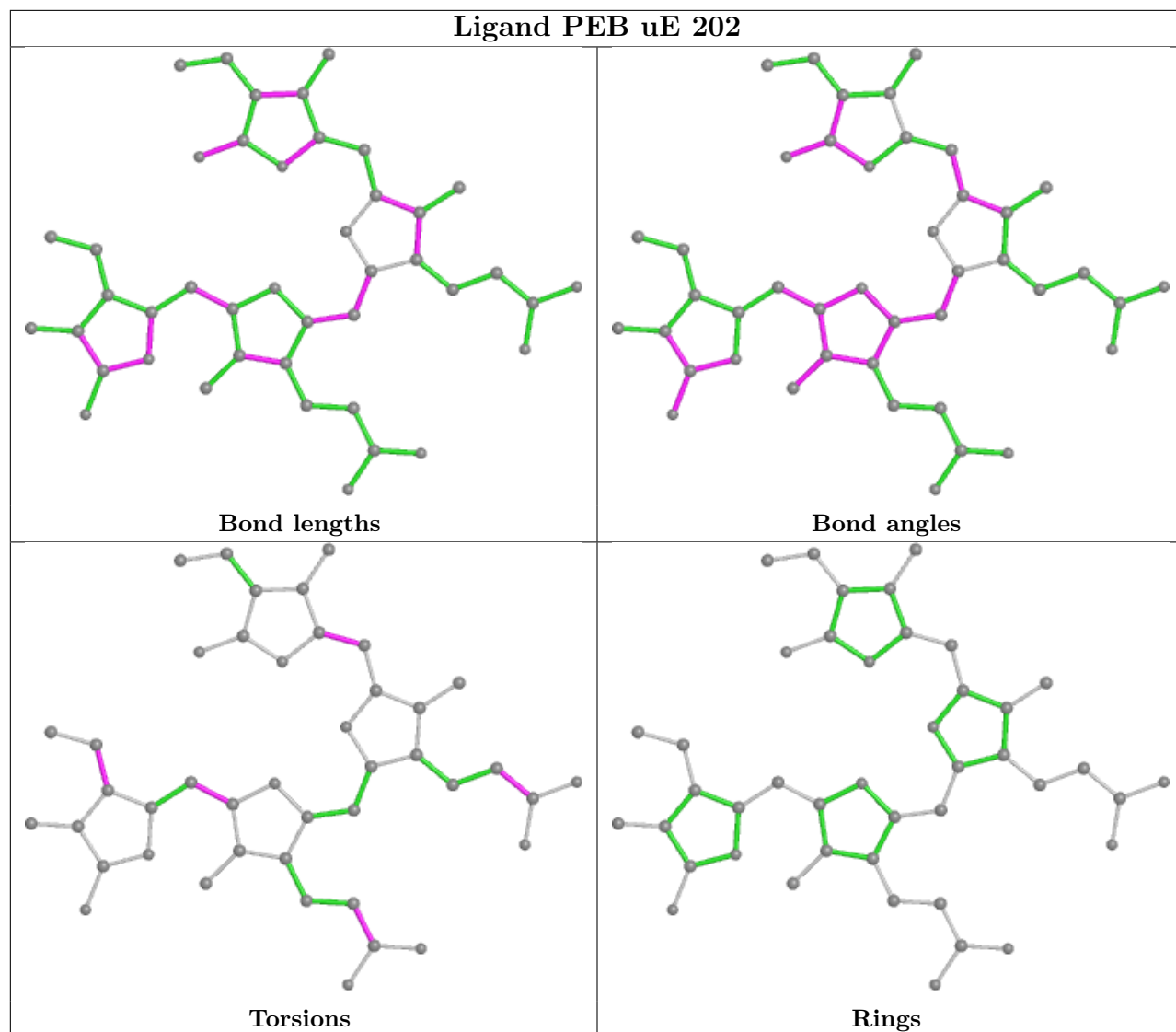


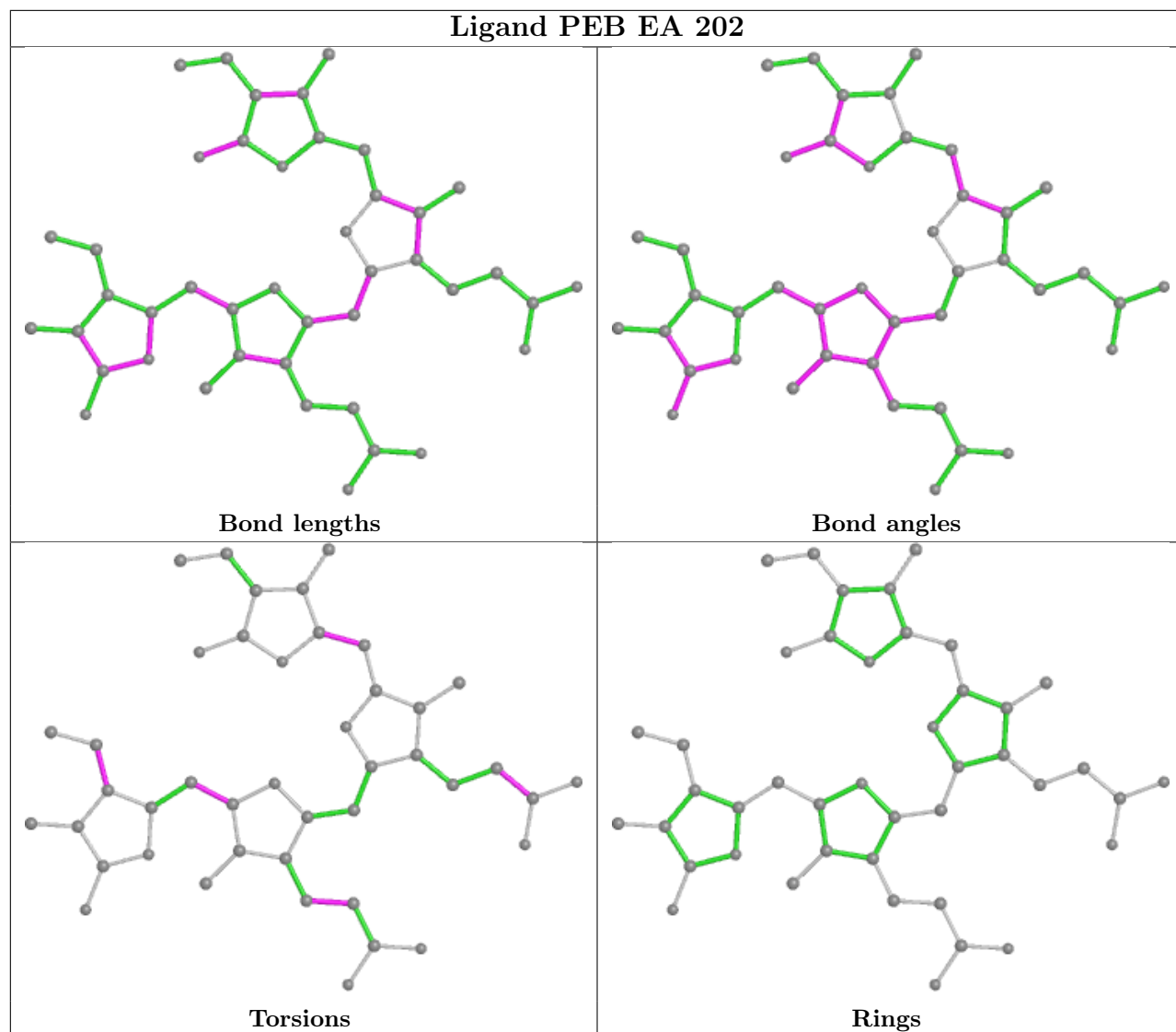


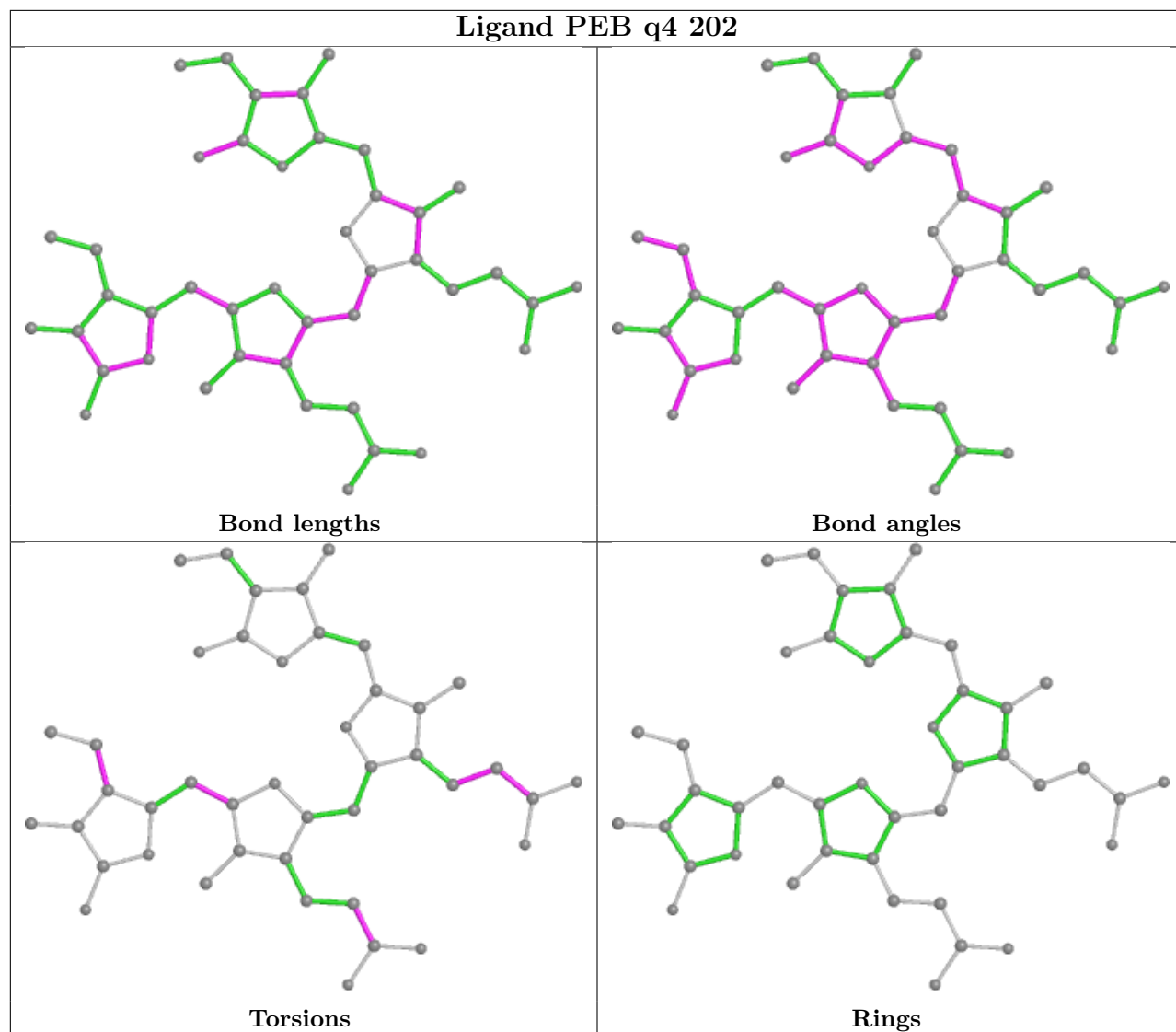


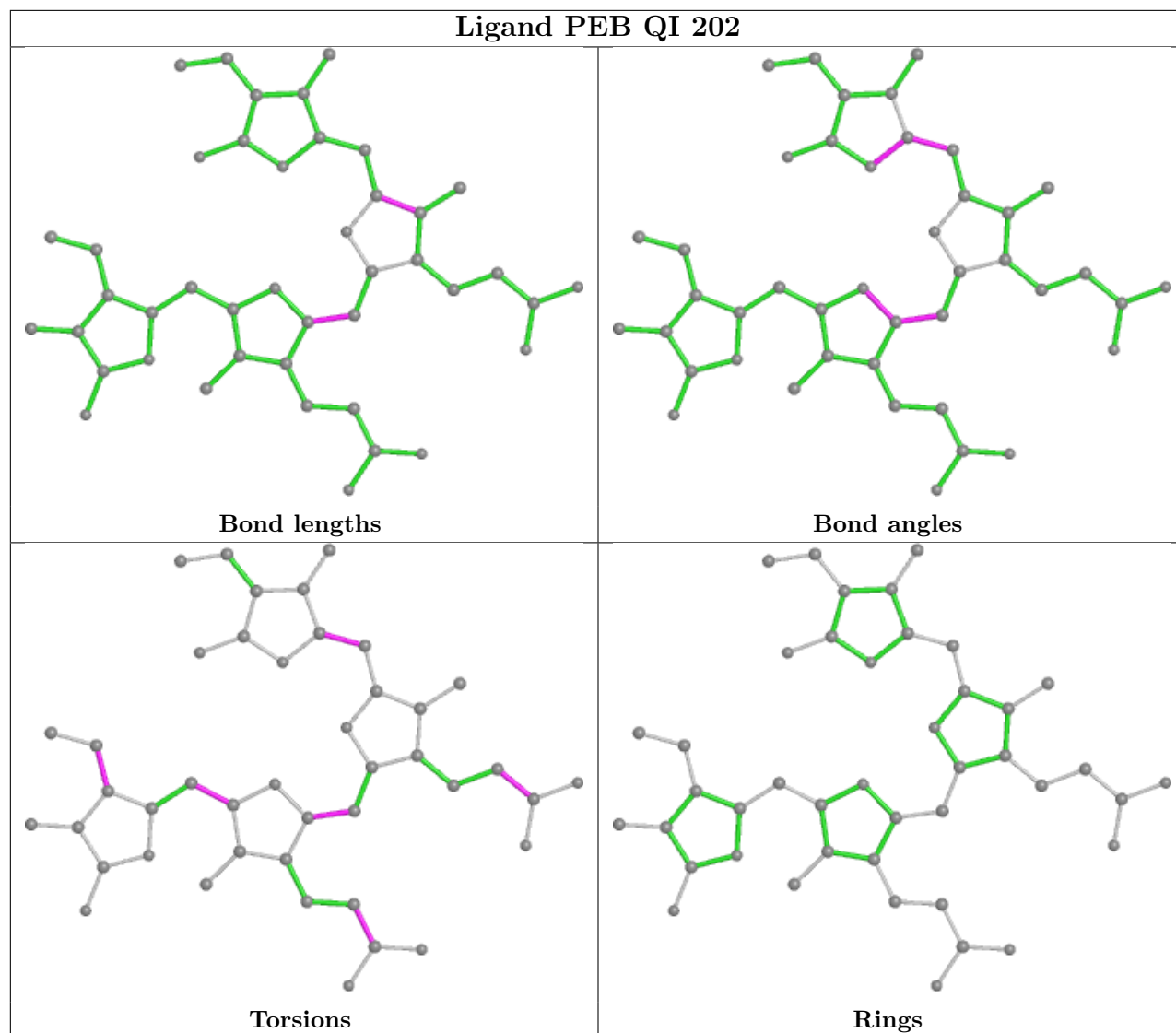


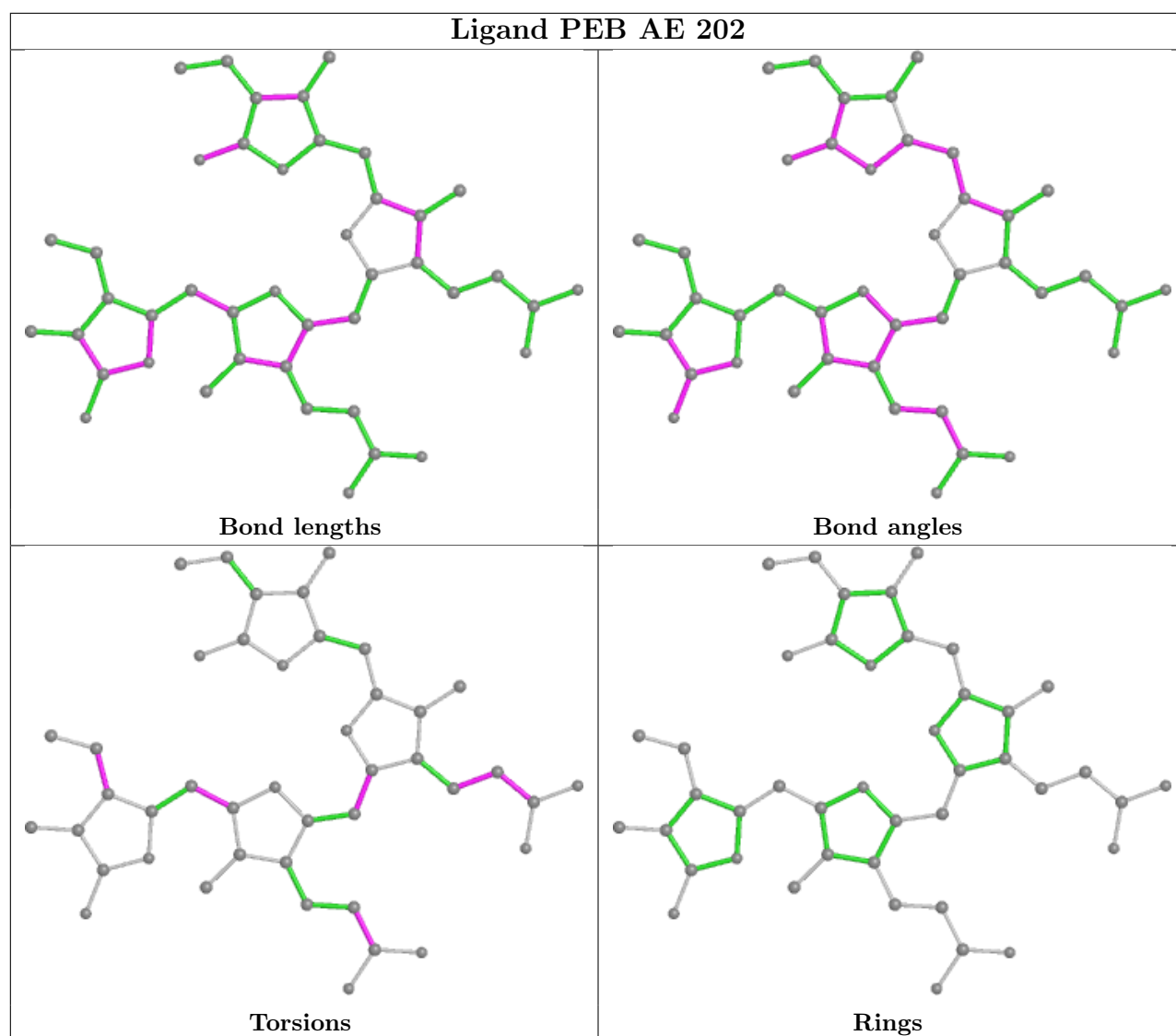












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

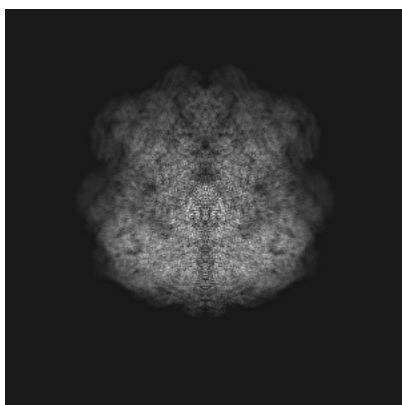
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9976. These allow visual inspection of the internal detail of the map and identification of artifacts.

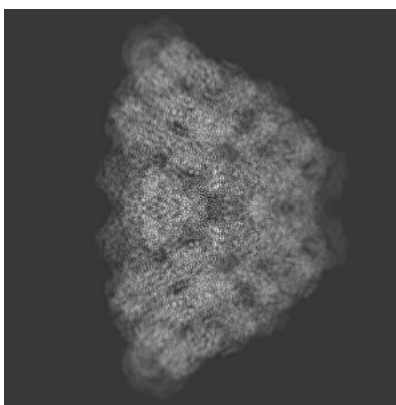
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

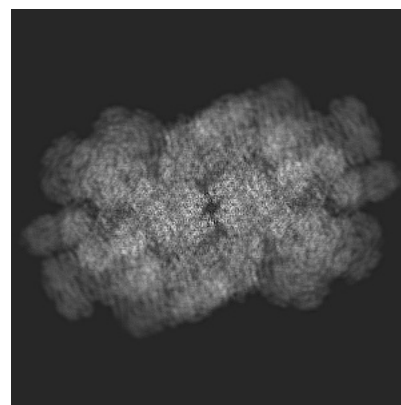
6.1.1 Primary map



X



Y

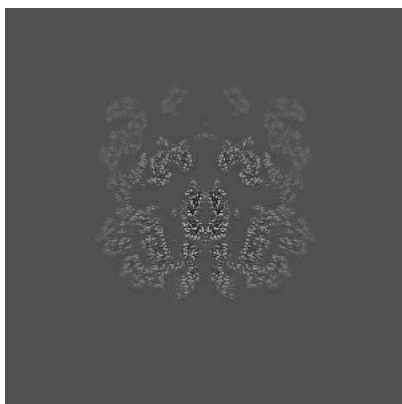


Z

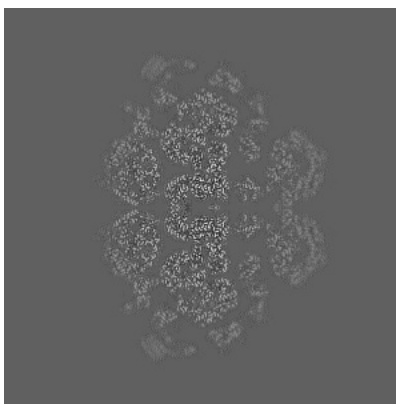
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

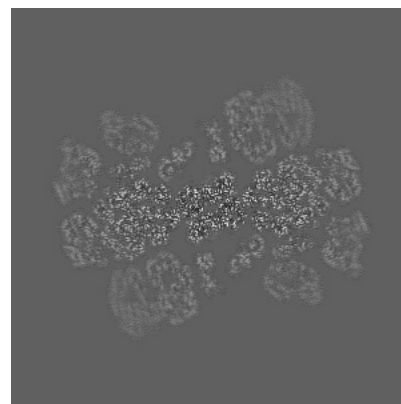
6.2.1 Primary map



X Index: 280



Y Index: 280

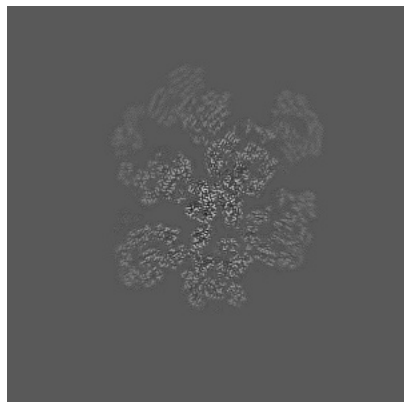


Z Index: 280

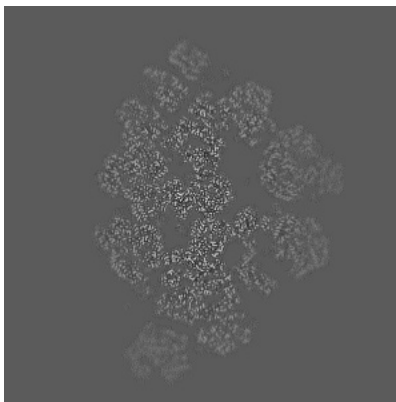
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

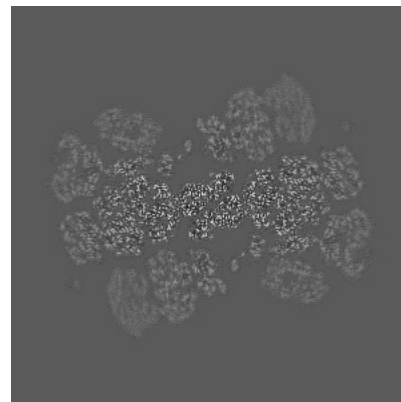
6.3.1 Primary map



X Index: 305



Y Index: 268



Z Index: 275

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

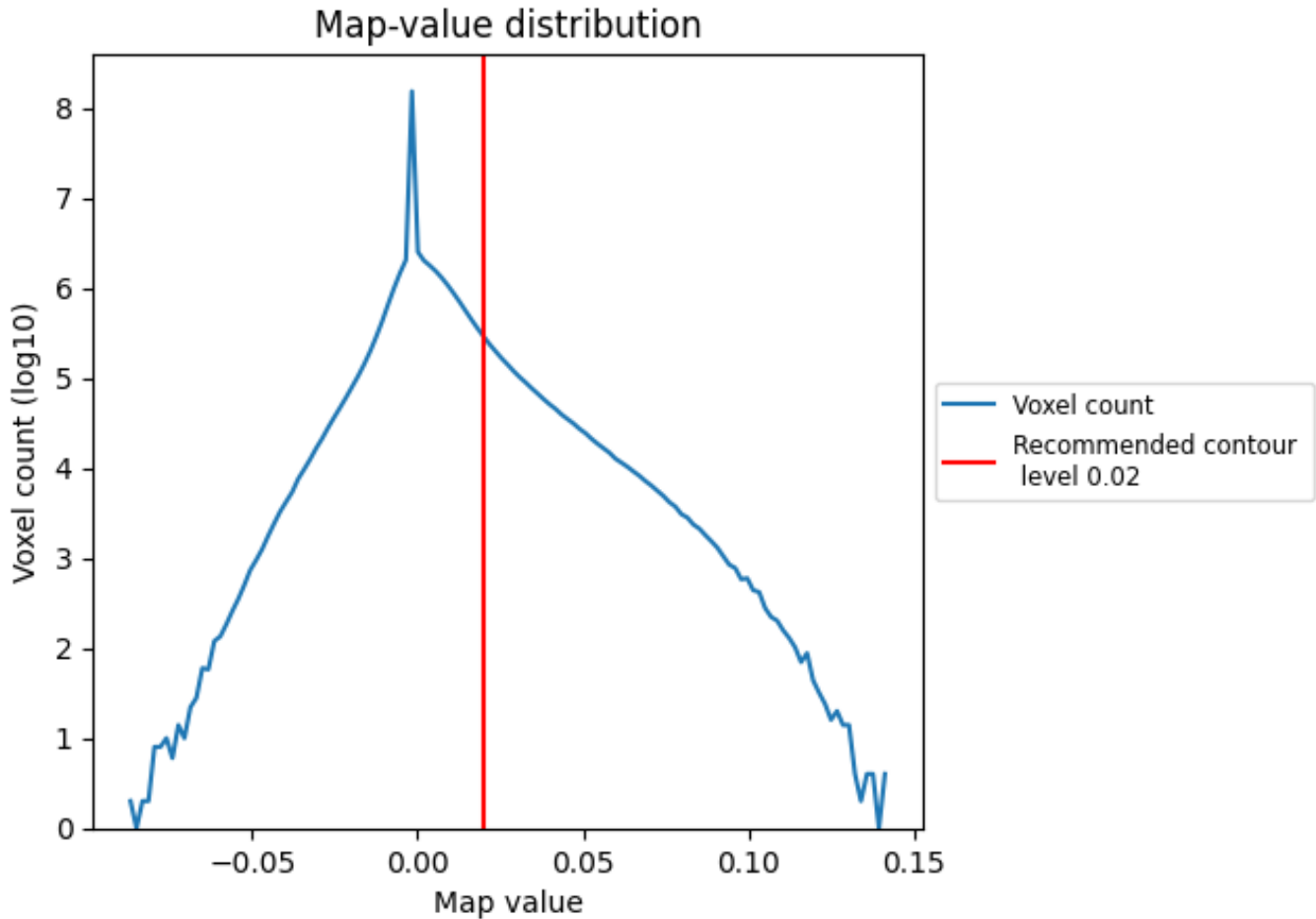
6.5 Mask visualisation

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

7 Map analysis [i](#)

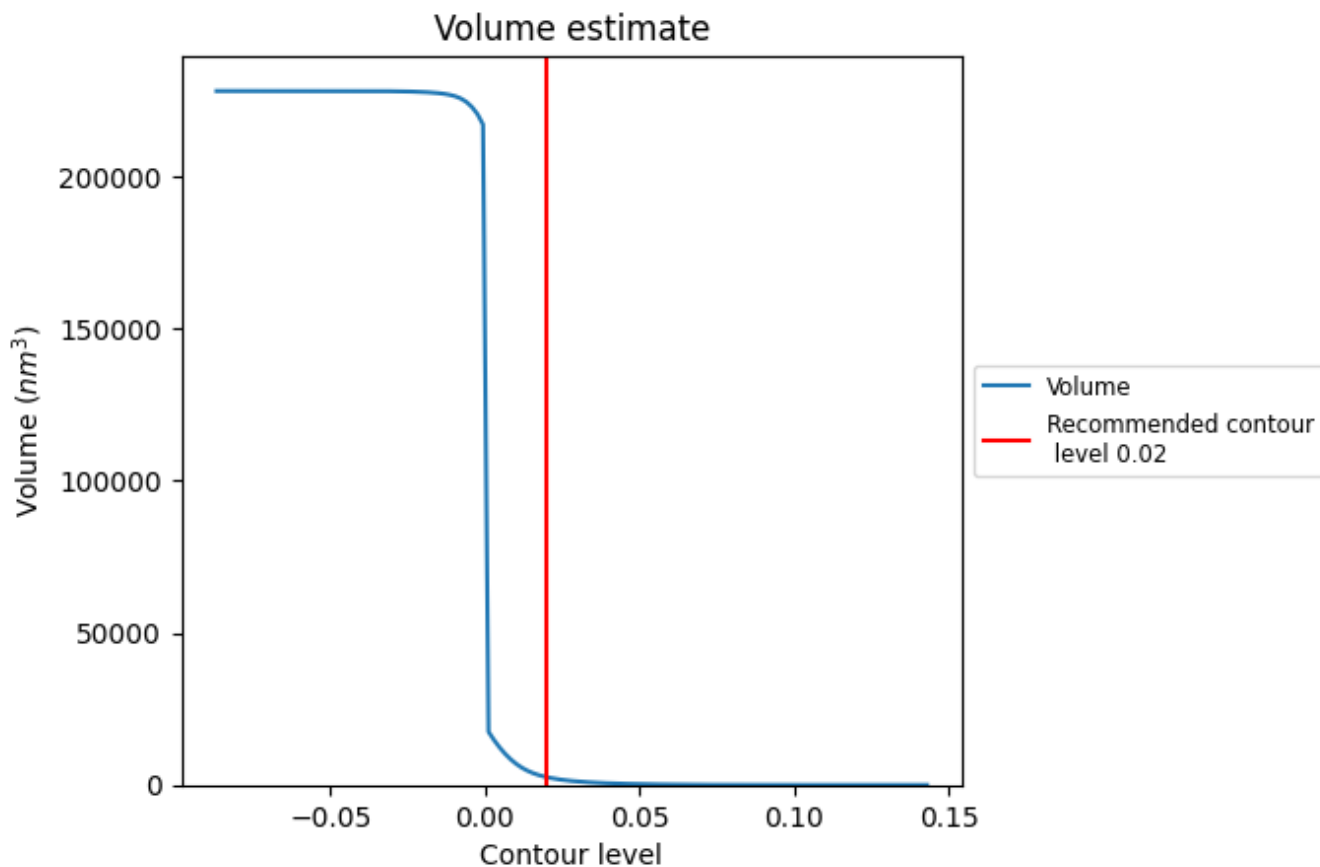
This section contains the results of statistical analysis of the map.

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.

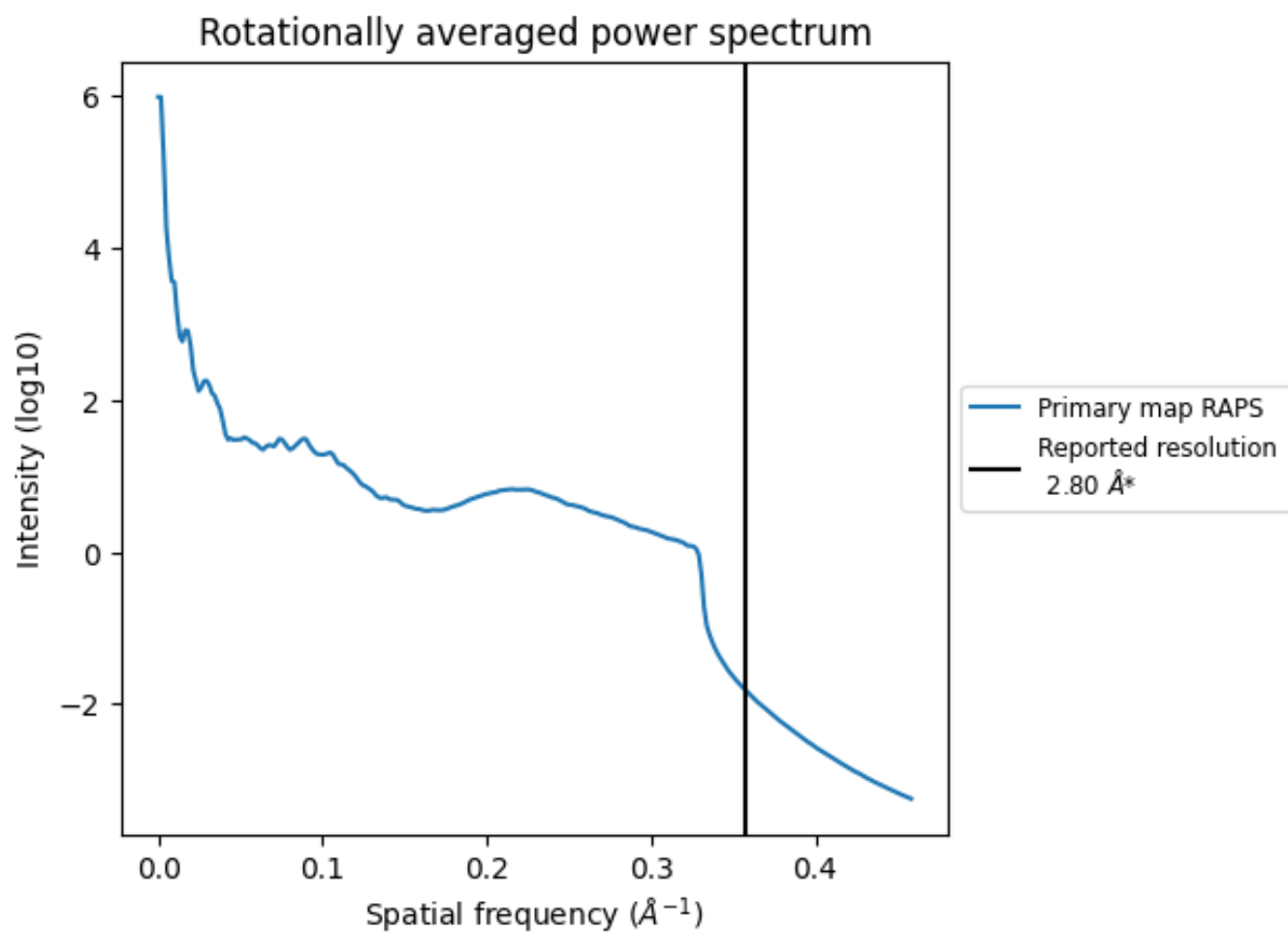
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2573 nm^3 ; this corresponds to an approximate mass of 2324 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.357 Å⁻¹

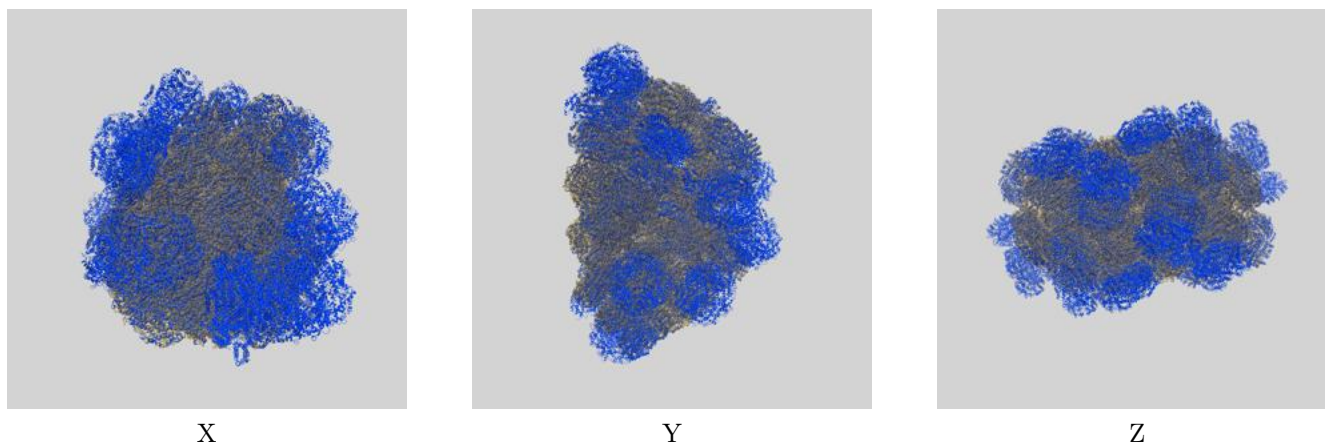
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

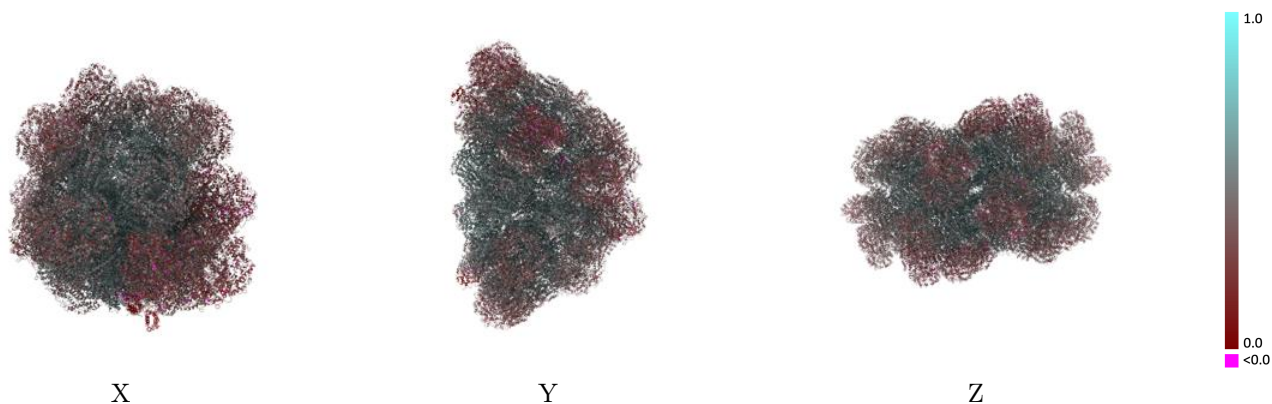
This section contains information regarding the fit between EMDB map EMD-9976 and PDB model 6KGX. Per-residue inclusion information can be found in section [3](#) on page [145](#).

9.1 Map-model overlay [i](#)



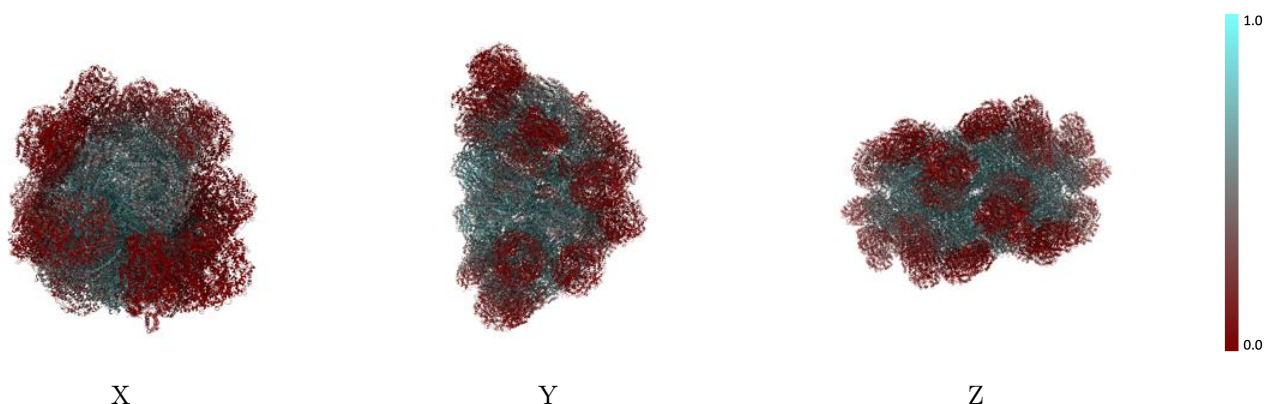
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



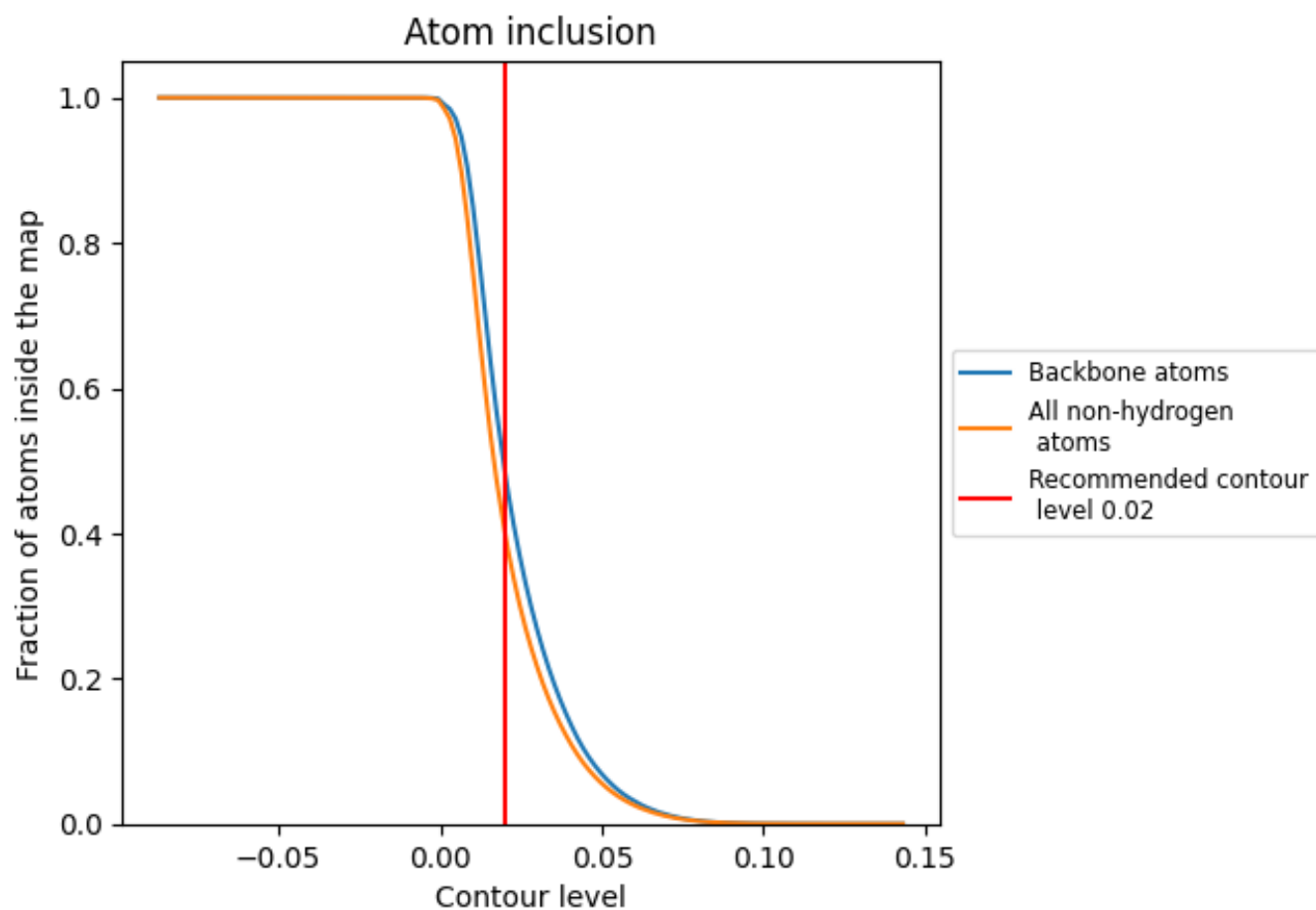
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 49% of all backbone atoms, 40% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4018	 0.4550
11	 0.0014	 0.2860
14	 0.0036	 0.2720
1H	 0.7734	 0.5840
21	 0.0100	 0.2690
24	 0.0080	 0.2650
2H	 0.7276	 0.5700
31	 0.7462	 0.5720
34	 0.7457	 0.5740
3H	 0.8233	 0.5980
4H	 0.6788	 0.5760
A1	 0.0299	 0.3560
A2	 0.5533	 0.4990
A3	 0.0077	 0.3530
A4	 0.0261	 0.3500
A5	 0.0000	 -0.0070
A6	 0.2494	 0.4250
A7	 0.0193	 0.3250
A8	 0.1939	 0.4300
A9	 0.0048	 0.3270
AA	 0.1959	 0.4270
AB	 0.2504	 0.4240
AC	 0.0000	 0.0030
AD	 0.0054	 0.3350
AE	 0.4888	 0.4690
AF	 0.0155	 0.3290
AG	 0.4865	 0.4750
AH	 0.6983	 0.5630
AI	 0.5575	 0.5000
AJ	 0.0052	 0.3350
B1	 0.0468	 0.3710
B2	 0.9125	 0.6200
B3	 0.0115	 0.3600
B4	 0.0548	 0.3660
B5	 0.0052	 0.2100























































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
B6	 0.8331	 0.5950
B7	 0.5465	 0.5370
B8	 0.4997	 0.5200
B9	 0.2666	 0.4540
BA	 0.4951	 0.5170
BB	 0.8311	 0.5950
BC	 0.0034	 0.1960
BD	 0.0137	 0.3500
BE	 0.4800	 0.4880
BF	 0.5433	 0.5380
BG	 0.4829	 0.4960
BH	 0.7368	 0.5640
BI	 0.9169	 0.6200
BJ	 0.2659	 0.4580
C1	 0.0139	 0.3120
C2	 0.9186	 0.6240
C3	 0.0339	 0.4040
C4	 0.0123	 0.3050
C5	 0.0000	 -0.0000
C6	 0.7317	 0.5820
C7	 0.1716	 0.3940
C8	 0.5400	 0.5220
C9	 0.3516	 0.4790
CA	 0.5385	 0.5200
CB	 0.7301	 0.5780
CC	 0.0000	 -0.0050
CD	 0.0339	 0.3980
CE	 0.4384	 0.4610
CF	 0.1684	 0.3950
CG	 0.4421	 0.4650
CH	 0.6780	 0.5500
CI	 0.9186	 0.6260
CJ	 0.3561	 0.4790
D1	 0.0209	 0.3510
D2	 0.8696	 0.6110
D3	 0.0231	 0.4000
D4	 0.0202	 0.3390
D6	 0.7438	 0.5860
D7	 0.1341	 0.3700
D8	 0.3650	 0.4680
D9	 0.5161	 0.5270
DA	 0.3657	 0.4680





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
DB	 0.7423	 0.5860
DD	 0.0281	 0.3990
DE	 0.5281	 0.5010
DF	 0.1361	 0.3670
DG	 0.5267	 0.5060
DH	 0.8066	 0.5950
DI	 0.8711	 0.6120
DJ	 0.5116	 0.5300
E1	 0.0277	 0.3380
E2	 0.8928	 0.6220
E3	 0.0177	 0.3850
E4	 0.0293	 0.3340
E6	 0.8187	 0.5950
E7	 0.7260	 0.5840
E8	 0.3256	 0.4390
E9	 0.4533	 0.5120
EA	 0.3286	 0.4430
EB	 0.8203	 0.5930
ED	 0.0146	 0.3780
EE	 0.5774	 0.5100
EF	 0.7228	 0.5860
EG	 0.5720	 0.5120
EH	 0.8654	 0.6100
EI	 0.8936	 0.6230
EJ	 0.4599	 0.5190
F1	 0.1477	 0.4320
F2	 0.8742	 0.6140
F3	 0.0036	 0.3450
F4	 0.1455	 0.4280
F5	 0.4406	 0.5120
F6	 0.7234	 0.5730
F7	 0.4333	 0.4900
F8	 0.5809	 0.5210
F9	 0.4205	 0.4880
FA	 0.5823	 0.5210
FB	 0.7226	 0.5720
FC	 0.4355	 0.5030
FD	 0.0029	 0.3310
FE	 0.7589	 0.5820
FF	 0.4348	 0.4970
FG	 0.7656	 0.5830
FH	 0.8324	 0.6000





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
FI	 0.8772	 0.6120
FJ	 0.4196	 0.4930
G1	 0.0739	 0.3820
G2	 0.9025	 0.6190
G3	 0.0185	 0.3860
G4	 0.0708	 0.3760
G5	 0.0947	 0.3870
G6	 0.8931	 0.6220
G7	 0.2853	 0.4260
G8	 0.2704	 0.4300
G9	 0.1869	 0.4080
GA	 0.2681	 0.4270
GB	 0.8907	 0.6220
GC	 0.0921	 0.3790
GD	 0.0169	 0.3810
GE	 0.7976	 0.5880
GF	 0.2889	 0.4240
GG	 0.8051	 0.5930
GH	 0.8337	 0.6010
GI	 0.9033	 0.6200
GJ	 0.1847	 0.4090
H1	 0.0317	 0.3460
H2	 0.8659	 0.6110
H3	 0.0605	 0.4420
H4	 0.0281	 0.3290
H5	 0.6119	 0.5690
H6	 0.8199	 0.6000
H7	 0.4906	 0.4960
H8	 0.4228	 0.4900
H9	 0.2524	 0.4240
HA	 0.4295	 0.4930
HB	 0.8199	 0.6020
HC	 0.6033	 0.5640
HD	 0.0634	 0.4360
HE	 0.6669	 0.5420
HF	 0.4928	 0.4950
HG	 0.6677	 0.5470
HH	 0.7124	 0.5640
HI	 0.8644	 0.6100
HJ	 0.2524	 0.4270
I1	 0.1432	 0.4330
I2	 0.8920	 0.6250

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
I3	 0.0069	 0.3510
I4	 0.1393	 0.4270
I5	 0.5591	 0.5540
I6	 0.8977	 0.6180
I7	 0.6970	 0.5660
I8	 0.4981	 0.5210
I9	 0.5593	 0.5340
IA	 0.4974	 0.5200
IB	 0.8993	 0.6180
IC	 0.5529	 0.5520
ID	 0.0023	 0.3410
IE	 0.7931	 0.5900
IF	 0.6946	 0.5660
IG	 0.7909	 0.5910
IH	 0.8535	 0.6050
II	 0.8912	 0.6210
IJ	 0.5605	 0.5400
J1	 0.1037	 0.4350
J2	 0.8998	 0.6190
J3	 0.0029	 0.3520
J4	 0.1059	 0.4310
J5	 0.8068	 0.5960
J6	 0.9118	 0.6290
J7	 0.4587	 0.4790
J8	 0.3865	 0.4770
J9	 0.1001	 0.3530
JA	 0.3828	 0.4770
JB	 0.9086	 0.6290
JC	 0.7914	 0.5940
JD	 0.0022	 0.3330
JE	 0.7025	 0.5590
JF	 0.4565	 0.4790
JG	 0.7033	 0.5610
JH	 0.8005	 0.5900
JI	 0.8990	 0.6190
JJ	 0.0934	 0.3540
K1	 0.0702	 0.3770
K2	 0.9291	 0.6330
K3	 0.0052	 0.3480
K4	 0.0702	 0.3740
K5	 0.6707	 0.5730
K6	 0.7721	 0.5890

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
K7	0.4488	0.4920
K8	0.6632	0.5630
K9	0.1417	0.3900
KA	0.6624	0.5650
KB	0.7705	0.5860
KC	0.6693	0.5700
KD	0.0067	0.3360
KE	0.6535	0.5370
KF	0.4553	0.4950
KG	0.6587	0.5450
KH	0.6626	0.5520
KI	0.9251	0.6340
KJ	0.1432	0.3920
L1	0.0807	0.3890
L2	0.9013	0.6230
L3	0.0259	0.3890
L4	0.0836	0.3830
L5	0.6411	0.5550
L6	0.8320	0.6030
L7	0.6895	0.5710
L8	0.6625	0.5690
L9	0.1822	0.4090
LA	0.6617	0.5690
LB	0.8320	0.6040
LC	0.6429	0.5540
LD	0.0238	0.3800
LE	0.7975	0.5900
LF	0.6895	0.5750
LG	0.7990	0.5940
LH	0.7893	0.5900
LI	0.9035	0.6240
LJ	0.1792	0.4150
M1	0.1031	0.4080
M2	0.9041	0.6210
M3	0.4488	0.4610
M4	0.1099	0.3970
M6	0.8582	0.6130
M7	0.1749	0.3870
M8	0.7438	0.5870
M9	0.2136	0.4280
MA	0.7476	0.5870
MB	0.8630	0.6140





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
MD	0.4450	0.4580
ME	0.3391	0.4370
MF	0.1707	0.3900
MG	0.3413	0.4420
MH	0.7705	0.5780
MI	0.9049	0.6220
MJ	0.2159	0.4310
N1	0.7715	0.5920
N2	0.9073	0.6230
N3	0.5843	0.5170
N4	0.7737	0.5910
N6	0.8104	0.5990
N7	0.2743	0.4180
N8	0.7322	0.5870
N9	0.0000	0.3080
NA	0.7315	0.5840
NB	0.8124	0.6000
ND	0.5836	0.5160
NE	0.3947	0.4530
NF	0.2645	0.4260
NG	0.3976	0.4560
NH	0.8475	0.6120
NI	0.9088	0.6230
NJ	0.0015	0.3160
O1	0.6387	0.5470
O2	0.7290	0.5560
O3	0.7067	0.5600
O4	0.6358	0.5450
O6	0.6714	0.5490
O7	0.1105	0.3840
O8	0.4571	0.4750
O9	0.0015	0.2870
OA	0.4571	0.4730
OB	0.6774	0.5500
OD	0.6975	0.5580
OE	0.4683	0.4630
OF	0.1083	0.3880
OG	0.4683	0.4690
OH	0.6509	0.5480
OI	0.7267	0.5560
OJ	0.0015	0.2900
P1	0.5302	0.5080

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
P2	 0.7003	 0.5560
P3	 0.6045	 0.5290
P4	 0.5310	 0.5030
P6	 0.6424	 0.5560
P7	 0.3464	 0.4770
P8	 0.3375	 0.4490
P9	 0.0119	 0.3540
PA	 0.3316	 0.4430
PB	 0.6461	 0.5580
PD	 0.5980	 0.5290
PE	 0.4711	 0.4800
PF	 0.3464	 0.4810
PG	 0.4748	 0.4830
PH	 0.8921	 0.6120
PI	 0.7017	 0.5540
PJ	 0.0075	 0.3540
Q1	 0.7122	 0.5760
Q2	 0.7490	 0.5650
Q3	 0.6975	 0.5700
Q4	 0.7122	 0.5720
Q6	 0.4959	 0.4850
Q7	 0.2181	 0.4250
Q8	 0.3452	 0.4410
Q9	 0.0163	 0.3480
QA	 0.3474	 0.4430
QB	 0.4974	 0.4890
QD	 0.6913	 0.5660
QE	 0.5474	 0.4880
QF	 0.2143	 0.4280
QG	 0.5467	 0.4940
QH	 0.9146	 0.6160
QI	 0.7560	 0.5660
QJ	 0.0141	 0.3580
R1	 0.4406	 0.4590
R2	 0.8213	 0.5910
R3	 0.6427	 0.5430
R4	 0.4406	 0.4620
R6	 0.5586	 0.5100
R7	 0.0660	 0.3560
R8	 0.4985	 0.4980
R9	 0.0030	 0.3030
RA	 0.4948	 0.4950

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
RB	0.5564	0.5100
RD	0.6398	0.5380
RE	0.6157	0.5390
RF	0.0690	0.3620
RG	0.6202	0.5400
RH	0.9051	0.6150
RI	0.8249	0.5920
RJ	0.0037	0.3070
S1	0.5312	0.5140
S2	0.7475	0.5600
S3	0.7206	0.5730
S4	0.5319	0.5130
S6	0.5235	0.4950
S7	0.1710	0.4110
S8	0.3323	0.4370
S9	0.0007	0.2820
SA	0.3331	0.4350
SB	0.5250	0.4950
SD	0.7182	0.5690
SE	0.7184	0.5650
SF	0.1694	0.4110
SG	0.7282	0.5740
SH	0.9195	0.6240
SI	0.7444	0.5580
SJ	0.0015	0.2800
T1	0.4518	0.4680
T2	0.7320	0.5670
T3	0.7889	0.6000
T4	0.4548	0.4700
T6	0.6907	0.5550
T7	0.1261	0.3680
T8	0.5289	0.4970
T9	0.0045	0.3070
TA	0.5289	0.4980
TB	0.6936	0.5570
TD	0.7824	0.5960
TE	0.6766	0.5560
TF	0.1269	0.3670
TG	0.6758	0.5570
TH	0.9108	0.6190
TI	0.7370	0.5670
TJ	0.0022	0.3090





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
U1	0.4651	0.4850
U2	0.8029	0.5860
U3	0.5912	0.5110
U4	0.4666	0.4820
U6	0.5497	0.4920
U7	0.0515	0.3330
U8	0.5489	0.5200
U9	0.0245	0.3590
UA	0.5444	0.5230
UB	0.5497	0.4890
UD	0.5843	0.5090
UE	0.6826	0.5480
UF	0.0485	0.3260
UG	0.6882	0.5560
UH	0.9081	0.6190
UI	0.8045	0.5890
UJ	0.0245	0.3650
V1	0.6527	0.5470
V2	0.8343	0.5960
V3	0.4171	0.4520
V4	0.6542	0.5500
V6	0.4310	0.4710
V7	0.1009	0.3790
V8	0.4058	0.4670
V9	0.0030	0.2740
VA	0.4028	0.4670
VB	0.4295	0.4730
VD	0.4186	0.4520
VE	0.5245	0.4910
VF	0.1016	0.3810
VG	0.5274	0.4990
VH	0.6591	0.5510
VI	0.8307	0.5970
VJ	0.0045	0.2720
W1	0.7886	0.5980
W2	0.7768	0.5790
W3	0.4965	0.4840
W4	0.7938	0.5970
W6	0.6781	0.5530
W7	0.0530	0.3280
W8	0.7095	0.5700
W9	0.0022	0.2820





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
WA	 0.7087	 0.5670
WB	 0.6781	 0.5530
WD	 0.4927	 0.4830
WE	 0.5235	 0.4880
WF	 0.0530	 0.3240
WG	 0.5190	 0.4940
WH	 0.7282	 0.5830
WI	 0.7760	 0.5770
WJ	 0.0015	 0.2820
X1	 0.8297	 0.6030
X2	 0.8532	 0.6040
X3	 0.6383	 0.5410
X4	 0.8364	 0.6040
X6	 0.7393	 0.5740
X7	 0.1914	 0.4470
X8	 0.5964	 0.5300
X9	 0.0015	 0.2970
XA	 0.5972	 0.5310
XB	 0.7413	 0.5750
XD	 0.6390	 0.5380
XE	 0.7077	 0.5650
XF	 0.1955	 0.4460
XG	 0.7097	 0.5700
XH	 0.8151	 0.6100
XI	 0.8516	 0.6040
XJ	 0.0037	 0.2980
Y1	 0.6721	 0.5660
Y2	 0.7378	 0.5680
Y3	 0.0397	 0.4090
Y4	 0.6795	 0.5660
Y6	 0.7641	 0.5880
Y7	 0.0675	 0.3630
Y8	 0.6438	 0.5440
Y9	 0.0015	 0.3150
YA	 0.6415	 0.5460
YB	 0.7671	 0.5900
YD	 0.0428	 0.4050
YE	 0.0993	 0.3130
YF	 0.0697	 0.3640
YG	 0.1001	 0.3190
YH	 0.7735	 0.5840
YI	 0.7363	 0.5680





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
YJ	 0.0030	 0.3190
Z1	 0.3565	 0.5110
Z2	 0.7991	 0.5780
Z4	 0.3565	 0.5040
Z6	 0.6916	 0.5520
Z7	 0.0254	 0.3010
Z8	 0.6855	 0.5670
ZA	 0.6862	 0.5690
ZB	 0.6960	 0.5520
ZE	 0.1343	 0.3150
ZF	 0.0194	 0.3090
ZG	 0.1335	 0.3220
ZH	 0.7276	 0.5760
ZI	 0.7983	 0.5780
a1	 0.0981	 0.4560
a2	 0.8314	 0.5990
a4	 0.0990	 0.4460
a6	 0.5757	 0.5170
a7	 0.0364	 0.3110
a8	 0.2828	 0.4430
aA	 0.2857	 0.4430
aB	 0.5757	 0.5210
aE	 0.1964	 0.3610
aF	 0.0364	 0.3090
aG	 0.2009	 0.3750
aH	 0.8200	 0.5960
aI	 0.8293	 0.6010
b1	 0.5932	 0.5320
b2	 0.4503	 0.4370
b4	 0.5900	 0.5300
b6	 0.3795	 0.4490
b7	 0.0134	 0.3070
b8	 0.6324	 0.5450
bA	 0.6300	 0.5440
bB	 0.3857	 0.4470
bE	 0.2448	 0.3890
bF	 0.0119	 0.3060
bG	 0.2500	 0.3950
bH	 0.6828	 0.5760
bI	 0.4480	 0.4400
c1	 0.0060	 0.2740
c2	 0.3977	 0.4150





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
c4	 0.0022	 0.2560
c6	 0.2930	 0.4300
c7	 0.0289	 0.3320
c8	 0.1335	 0.3740
cA	 0.1304	 0.3750
cB	 0.3027	 0.4330
cE	 0.2054	 0.3580
cF	 0.0312	 0.3340
cG	 0.2270	 0.3750
cH	 0.6983	 0.5590
cI	 0.3991	 0.4230
d1	 0.0029	 0.2940
d2	 0.5035	 0.4600
d4	 0.0036	 0.2720
d6	 0.1762	 0.3580
d7	 0.0172	 0.2950
d8	 0.2091	 0.4090
d9	 0.4597	 0.5030
dA	 0.2176	 0.4140
dB	 0.1668	 0.3620
dE	 0.2418	 0.4080
dF	 0.0209	 0.2950
dG	 0.2374	 0.4160
dH	 0.7966	 0.5900
dI	 0.5019	 0.4620
dJ	 0.4573	 0.5020
e1	 0.0069	 0.2900
e2	 0.5720	 0.5070
e3	 0.6824	 0.5560
e4	 0.0085	 0.2910
e6	 0.2032	 0.3710
e7	 0.0126	 0.2740
e8	 0.4384	 0.4980
eA	 0.4369	 0.5000
eB	 0.2046	 0.3700
eD	 0.6798	 0.5560
eE	 0.2517	 0.4140
eF	 0.0104	 0.2840
eG	 0.2502	 0.4220
eH	 0.6788	 0.5530
eI	 0.5648	 0.5110
f1	 0.0200	 0.3310





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
f2	 0.4273	 0.4260
f4	 0.0163	 0.3060
f6	 0.1501	 0.3440
f7	 0.0284	 0.3240
f8	 0.1001	 0.3430
fA	 0.1023	 0.3440
fB	 0.1486	 0.3540
fE	 0.3086	 0.4280
fF	 0.0321	 0.3170
fG	 0.3093	 0.4340
fH	 0.8340	 0.6000
fI	 0.4249	 0.4280
g1	 0.0022	 0.2940
g2	 0.4114	 0.4290
g4	 0.0015	 0.2860
g6	 0.2596	 0.4140
g7	 0.0163	 0.3090
g8	 0.0519	 0.3340
gA	 0.0512	 0.3320
gB	 0.2648	 0.4160
gE	 0.3032	 0.4430
gF	 0.0185	 0.3140
gG	 0.3122	 0.4510
gH	 0.8605	 0.6070
gI	 0.4193	 0.4340
h1	 0.0134	 0.3020
h2	 0.5258	 0.4760
h4	 0.0144	 0.2970
h6	 0.1232	 0.3390
h7	 0.0112	 0.2780
h8	 0.1031	 0.3590
hA	 0.0926	 0.3520
hB	 0.1180	 0.3420
hE	 0.1610	 0.3640
hF	 0.0112	 0.2860
hG	 0.1588	 0.3720
hH	 0.7331	 0.5620
hI	 0.5281	 0.4710
i1	 0.0381	 0.3480
i2	 0.5742	 0.5010
i4	 0.0339	 0.3440
i6	 0.0935	 0.3300





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i7	 0.0119	 0.2920
i8	 0.2070	 0.3980
iA	 0.2047	 0.3970
iB	 0.0987	 0.3340
iE	 0.2263	 0.3680
iF	 0.0104	 0.2920
iG	 0.2270	 0.3760
iH	 0.8345	 0.5970
iI	 0.5713	 0.5030
j1	 0.0274	 0.3410
j2	 0.4796	 0.4540
j4	 0.0252	 0.3400
j6	 0.2510	 0.3900
j7	 0.0127	 0.2630
j8	 0.1255	 0.3710
jA	 0.1217	 0.3700
jB	 0.2494	 0.3970
jE	 0.3828	 0.4640
jF	 0.0105	 0.2710
jG	 0.3850	 0.4680
jH	 0.7095	 0.5620
jI	 0.4804	 0.4560
k1	 0.0164	 0.3180
k2	 0.4316	 0.4300
k4	 0.0127	 0.3070
k6	 0.4473	 0.4730
k7	 0.0037	 0.3000
k8	 0.1877	 0.3820
kA	 0.1936	 0.3840
kB	 0.4444	 0.4730
kE	 0.0037	 0.2160
kF	 0.0030	 0.2910
kG	 0.0015	 0.2380
kH	 0.8552	 0.6040
kI	 0.4337	 0.4290
l1	 0.0059	 0.2950
l2	 0.5473	 0.4750
l4	 0.0067	 0.2900
l6	 0.2726	 0.4040
l7	 0.0030	 0.2470
l8	 0.3883	 0.4630
lA	 0.3883	 0.4660





















































































Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
lB	 0.2763	 0.4030
lE	 0.0007	 0.2300
lF	 0.0015	 0.2480
lG	 0.0037	 0.2440
lH	 0.8021	 0.5910
lI	 0.5450	 0.4710
m1	 0.0112	 0.2870
m2	 0.6001	 0.5240
m4	 0.0112	 0.2810
m6	 0.1455	 0.3380
m7	 0.0052	 0.2550
m8	 0.2507	 0.4450
mA	 0.2463	 0.4450
mB	 0.1513	 0.3470
mE	 0.0134	 0.2350
mF	 0.0037	 0.2560
mG	 0.0134	 0.2710
mH	 0.6618	 0.5580
mI	 0.6102	 0.5230
n1	 0.0635	 0.3760
n4	 0.0645	 0.3610
nE	 0.0059	 0.2510
nG	 0.0067	 0.2680
nH	 0.7925	 0.5910
o1	 0.0383	 0.3390
o4	 0.0380	 0.3230
oE	 0.0022	 0.2340
oG	 0.0060	 0.2500
oH	 0.7730	 0.5790
p1	 0.0015	 0.2710
p4	 0.0038	 0.2510
pE	 0.0134	 0.2540
pG	 0.0111	 0.2720
pH	 0.8443	 0.6100
q1	 0.0022	 0.2650
q4	 0.0014	 0.2680
qE	 0.0224	 0.2950
qG	 0.0246	 0.3120
qH	 0.6446	 0.5320
r1	 0.0031	 0.2610
r4	 0.0023	 0.2340
rE	 0.0178	 0.2830

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
rG	 0.0193	 0.2960
rH	 0.8897	 0.6080
s1	 0.0000	 0.2580
s4	 0.0007	 0.2370
sE	 0.0052	 0.2580
sG	 0.0075	 0.2750
sH	 0.9211	 0.6220
t1	 0.0054	 0.3010
t4	 0.0054	 0.2680
tE	 0.0022	 0.2210
tG	 0.0007	 0.2430
tH	 0.9002	 0.6160
u1	 0.0339	 0.3320
u4	 0.0310	 0.3290
uE	 0.0037	 0.2300
uG	 0.0022	 0.2410
uH	 0.9138	 0.6200
v1	 0.0192	 0.3270
v4	 0.0154	 0.3080
vE	 0.0438	 0.3110
vG	 0.0460	 0.3220
vH	 0.9148	 0.6210
w1	 0.0072	 0.2790
w4	 0.0063	 0.2650
wE	 0.3316	 0.4490
wG	 0.3337	 0.4540
wH	 0.9073	 0.6190
x1	 0.0177	 0.3110
x4	 0.0154	 0.2940
xE	 0.0140	 0.2790
xG	 0.0125	 0.2900
xH	 0.5935	 0.4930
y1	 0.0036	 0.2740
y4	 0.0014	 0.2580
yE	 0.6287	 0.5480
yG	 0.6328	 0.5480
yH	 0.7253	 0.5770
z1	 0.0000	 0.2640
z4	 0.0000	 0.2490
zE	 0.7216	 0.5710
zG	 0.7219	 0.5760
zH	 0.8137	 0.6050