



wwPDB EM Validation Summary Report ⓘ

Apr 10, 2023 – 05:07 AM JST

PDB ID : 7Y4L
EMDB ID : EMD-33605
Title : PBS of PBS-PSII-PSI-LHCs from *Porphyridium purpureum*.
Authors : You, X.; Zhang, X.; Cheng, J.; Xiao, Y.N.; Sun, S.; Sui, S.F.
Deposited on : 2022-06-15
Resolution : 3.30 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.dev50
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) : 2.32.2

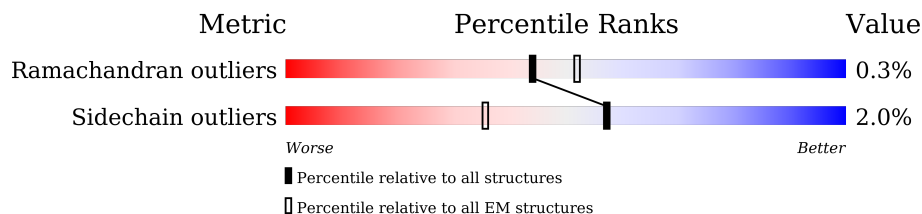
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	AA	138	
1	EA	138	
2	B1	177	
2	B7	177	
2	B8	177	
2	B9	177	
2	BA	177	
2	BF	177	
2	BG	177	

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Mol	Chain	Length	Quality of chain
2	BI	177	100%
2	BK	177	99%
2	C5	177	75%
2	CA	177	66%
2	CJ	177	79%
2	D1	177	98%
2	D4	177	55%
2	D7	177	29%
2	D8	177	62%
2	D9	177	100%
2	DA	177	25%
2	DF	177	64%
2	DG	177	98%
2	DH	177	50%
2	DI	177	100%
2	DK	177	100%
2	E5	177	79%
2	EJ	177	76%
2	F1	177	98%
2	F4	177	22%
2	F7	177	40%
2	F8	177	31%
2	F9	177	96%
2	FA	177	48%
2	FF	177	35%

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Mol	Chain	Length	Quality of chain
2	FG	177	99% 98%
2	FH	177	26% 98%
2	FI	177	99% 98%
2	FK	177	100% 98%
2	G5	177	93% 99%
2	GA	177	53% 99%
2	GJ	177	94% 99%
2	H1	177	95% 98%
2	H4	177	50% 98%
2	H7	177	60% 99%
2	H8	177	44% 99%
2	H9	177	99% 99%
2	HA	177	55% 94% 5%
2	HF	177	47% 99%
2	HG	177	98% 98%
2	HH	177	49% 99%
2	HI	177	100% 99%
2	HK	177	95% 98%
2	I5	177	59% 98%
2	IA	177	24% 97%
2	IJ	177	57% 98%
2	J1	177	99% 99%
2	J4	177	38% 99%
2	J7	177	23% 96%
2	J8	177	44% 98%

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Mol	Chain	Length	Quality of chain
2	J9	177	100% 99%
2	JF	177	47% 98%
2	JG	177	99% 99%
2	JH	177	44% 99%
2	JI	177	100% 98%
2	JK	177	99% 99%
2	K5	177	93% 99%
2	KJ	177	92% 99%
2	L1	177	98% 99%
2	L4	177	26% 99%
2	L7	177	36% 99%
2	L8	177	40% 98%
2	L9	177	99% 99%
2	LA	177	88% 95%
2	LF	177	41% 98%
2	LG	177	93% 98%
2	LH	177	24% 98%
2	LI	177	100% 99%
2	LK	177	99% 99%
2	M5	177	81% 99%
2	MA	177	59% 97%
2	MJ	177	83% 99%
2	N1	177	58% 99%
2	N4	177	17% 97%
2	N7	177	36% 98%

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Mol	Chain	Length	Quality of chain
2	N8	177	79% 99%
2	NA	177	25% 80% 18%
2	NF	177	76% 99%
2	NH	177	13% 97%
2	NK	177	53% 99%
2	O5	177	100% 98%
2	O9	177	99% 99%
2	OA	177	47% 99%
2	OG	177	99% 97%
2	OI	177	100% 98%
2	OJ	177	100% 98%
2	P1	177	59% 98%
2	P2	177	75% 98%
2	P4	177	79% 99%
2	P6	177	46% 100%
2	P7	177	32% 98%
2	P8	177	67% 99%
2	PA	177	34% 98%
2	PB	177	42% 100%
2	PC	177	71% 99%
2	PD	177	36% 98%
2	PE	177	33% 98%
2	PF	177	60% 99%
2	PH	177	75% 99%
2	PK	177	56% 97%

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Mol	Chain	Length	Quality of chain
2	Q5	177	100% 97%
2	Q9	177	100% 99%
2	QA	177	54% 97%
2	QG	177	99% 95%
2	QI	177	100% 98%
2	QJ	177	100% 97%
2	R1	177	50% 99%
2	R2	177	95% 99%
2	R4	177	51% 99%
2	R6	177	24% 99%
2	R7	177	44% 98%
2	R8	177	58% 99%
2	RA	177	88% 97%
2	RB	177	22% 99%
2	RC	177	96% 99%
2	RD	177	59% 99%
2	RE	177	51% 99%
2	RF	177	58% 99%
2	RH	177	51% 98%
2	RK	177	51% 99%
2	S5	177	100% 99%
2	S9	177	98% 98%
2	SA	177	24% 98%
2	SG	177	99% 97%
2	SI	177	100% 99%

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Mol	Chain	Length	Quality of chain
2	SJ	177	100% 99%
2	T1	177	32% 99%
2	T2	177	82% 99%
2	T4	177	56% 99%
2	T6	177	37% 99%
2	T7	177	60% 98%
2	T8	177	46% 99%
2	TB	177	40% 99%
2	TC	177	86% 99%
2	TD	177	36% 99%
2	TE	177	37% 99%
2	TF	177	44% 99%
2	TH	177	53% 98%
2	TK	177	28% 99%
2	U5	177	100% 98%
2	U9	177	100% 99%
2	UG	177	96% 98%
2	UI	177	100% 99%
2	UJ	177	100% 98%
2	V1	177	75% 99%
2	V2	177	90% 94% 5%
2	V4	177	77% 98%
2	V6	177	27% 97%
2	V7	177	23% 97%
2	V8	177	68% 98%

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Mol	Chain	Length	Quality of chain
2	VA	177	84% 97%
2	VB	177	21% 97%
2	VC	177	91% 93% 7%
2	VD	177	60% 98%
2	VE	177	64% 98%
2	VF	177	66% 98%
2	VH	177	75% 98%
2	VK	177	75% 99%
2	W5	177	100% 96%
2	W9	177	98% 99%
2	WG	177	100% 98%
2	WI	177	100% 98%
2	WJ	177	100% 96%
2	X1	177	55% 99%
2	X4	177	45% 98%
2	X7	177	37% 98%
2	X8	177	40% 99%
2	XA	177	77% 99%
2	XF	177	40% 99%
2	XH	177	44% 99%
2	XK	177	55% 99%
2	Y2	177	90% 99%
2	Y5	177	100% 99%
2	Y6	177	34% 99%
2	Y9	177	100% 99%

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Mol	Chain	Length	Quality of chain
2	YA	177	54% 97%
2	YB	177	34% 98%
2	YC	177	91% 99%
2	YD	177	30% 99%
2	YE	177	30% 99%
2	YG	177	91% 98%
2	YI	177	100% 99%
2	YJ	177	100% 99%
2	Z4	177	30% 99%
2	Z8	177	99% 97%
2	ZA	177	85% 85% 14%
2	ZF	177	98% 97%
2	ZH	177	28% 98%
2	a2	177	97% 99%
2	a6	177	20% 97%
2	aA	177	40% 97%
2	aB	177	19% 97%
2	aC	177	97% 99%
2	aD	177	58% 99%
2	aE	177	54% 99%
2	b8	177	92% 99%
2	bA	177	84% 99%
2	bF	177	90% 99%
2	c2	177	99% 98%
2	c4	177	95% 99%

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Mol	Chain	Length	Quality of chain
2	c6	177	82% 99%
2	cB	177	82% 99%
2	cC	177	99% 98%
2	cD	177	84% 99%
2	cE	177	81% 99%
2	cH	177	96% 99%
2	d8	177	98% 97%
2	dA	177	78% 99%
2	dF	177	96% 98%
2	e2	177	100% 98%
2	e4	177	69% 99%
2	e6	177	64% 99%
2	eA	177	62% 99%
2	eB	177	60% 99%
2	eC	177	100% 98%
2	eD	177	83% 98%
2	eE	177	85% 99%
2	eH	177	69% 99%
2	f8	177	89% 99%
2	fF	177	88% 99%
2	g2	177	100% 99%
2	g4	177	100% 99%
2	g6	177	83% 99%
2	gA	177	86% 77% 8% 14%
2	gB	177	84% 99%

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Mol	Chain	Length	Quality of chain
2	gC	177	99% 99%
2	gD	177	85% 98%
2	gE	177	84% 98%
2	gH	177	99% 99%
2	h8	177	99% 99%
2	hF	177	99% 99%
2	i2	177	100% 97%
2	i4	177	95% 99%
2	i6	177	69% 99%
2	iB	177	66% 99%
2	iC	177	100% 97%
2	iD	177	89% 99%
2	iE	177	89% 99%
2	iH	177	94% 99%
2	j8	177	88% 99%
2	jF	177	84% 99%
2	k2	177	100% 98%
2	k4	177	98% 99%
2	k6	177	84% 90% 10%
2	kB	177	76% 96%
2	kC	177	100% 98%
2	kD	177	78% 97%
2	kE	177	77% 99%
2	kH	177	95% 99%
2	l8	177	100% 97%

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Mol	Chain	Length	Quality of chain
2	lF	177	100% 97% .
2	m2	177	100% 97% ..
2	m4	177	89% 98% .
2	m6	177	68% 99% .
2	mB	177	67% 99% .
2	mC	177	100% 97% ..
2	mD	177	89% 99% .
2	mE	177	87% 99% .
2	mH	177	88% 99% .
2	n8	177	100% 97% .
2	nF	177	100% 97% .
2	p8	177	100% 98% .
2	pF	177	100% 98% .
2	r8	177	100% 97% .
2	rF	177	100% 97% .
2	t8	177	100% 99% .
2	tF	177	100% 99% .
2	v8	177	100% 98% .
2	vF	177	100% 98% .
3	A1	164	99% 98% .
3	A7	164	27% 100%
3	A8	164	65% 99% .
3	A9	164	100% 95% ..
3	AF	164	62% 99% .
3	AG	164	100% 99% .

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Mol	Chain	Length	Quality of chain
3	AI	164	100% 96%
3	AK	164	100% 98%
3	B5	164	85% 99%
3	BJ	164	83% 99%
3	C1	164	99% 100%
3	C4	164	35% 99%
3	C7	164	55% 100%
3	C8	164	57% 98%
3	C9	164	100% 95%
3	CF	164	62% 98%
3	CG	164	99% 99%
3	CH	164	32% 99%
3	CI	164	100% 96%
3	CK	164	99% 100%
3	D5	164	67% 98%
3	DJ	164	70% 98%
3	E1	164	99% 99%
3	E4	164	48% 100%
3	E7	164	63% 100%
3	E8	164	49% 99%
3	E9	164	99% 95%
3	EF	164	54% 98%
3	EG	164	100% 99%
3	EH	164	50% 100%
3	EI	164	100% 95%

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Mol	Chain	Length	Quality of chain
3	EK	164	99% 98%
3	F5	164	73% 99%
3	FJ	164	74% 99%
3	G1	164	100% 99%
3	G4	164	66% 99%
3	G7	164	59% 100%
3	G8	164	37% 98%
3	G9	164	99% 94% 5%
3	GF	164	38% 98%
3	GG	164	98% 99%
3	GH	164	63% 99%
3	GI	164	100% 96%
3	GK	164	99% 99%
3	H5	164	80% 100%
3	HJ	164	80% 100%
3	I1	164	98% 98%
3	I4	164	43% 100%
3	I7	164	40% 99%
3	I8	164	38% 96%
3	I9	164	99% 95%
3	IF	164	37% 96%
3	IG	164	99% 99%
3	IH	164	46% 99%
3	II	164	100% 96%
3	IK	164	99% 98%

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Mol	Chain	Length	Quality of chain
3	J5	164	91% 100%
3	JA	164	32% 93% 7%
3	JJ	164	92% 100%
3	K1	164	100% 99%
3	K4	164	38% 100%
3	K7	164	23% 99%
3	K8	164	52% 99%
3	K9	164	100% 95%
3	KF	164	53% 99%
3	KG	164	99% 99%
3	KH	164	31% 99%
3	KI	164	100% 96%
3	KK	164	99% 99%
3	L5	164	88% 99%
3	LJ	164	86% 99%
3	M1	164	74% 99%
3	M4	164	19% 99%
3	M7	164	27% 100%
3	M8	164	79% 100%
3	MF	164	77% 100%
3	MH	164	19% 99%
3	MK	164	68% 99%
3	N5	164	100% 99%
3	N9	164	100% 95%
3	NG	164	100% 99%

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Mol	Chain	Length	Quality of chain
3	NI	164	100% 96%
3	NJ	164	100% 99%
3	O1	164	41% 98%
3	O2	164	91% 99%
3	O4	164	68% 99%
3	O6	164	44% 100%
3	O7	164	55% 100%
3	O8	164	70% 100%
3	OB	164	40% 100%
3	OC	164	93% 99%
3	OD	164	40% 99%
3	OE	164	40% 99%
3	OF	164	68% 99%
3	OH	164	63% 99%
3	OK	164	48% 98%
3	P5	164	100% 100%
3	P9	164	100% 95%
3	PG	164	99% 99%
3	PI	164	100% 96%
3	PJ	164	100% 100%
3	Q1	164	39% 99%
3	Q2	164	88% 99%
3	Q4	164	73% 99%
3	Q6	164	29% 99%
3	Q7	164	58% 99%

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Mol	Chain	Length	Quality of chain
3	Q8	164	63% 99%
3	QB	164	29% 99%
3	QC	164	90% 99%
3	QD	164	54% 99%
3	QE	164	46% 99%
3	QF	164	63% 99%
3	QH	164	77% 99%
3	QK	164	41% 99%
3	R5	164	100% 99%
3	R9	164	100% 95%
3	RG	164	100% 99%
3	RI	164	100% 96%
3	RJ	164	100% 99%
3	S1	164	41% 100%
3	S2	164	83% 99%
3	S4	164	80% 99%
3	S6	164	33% 100%
3	S7	164	59% 99%
3	S8	164	50% 99%
3	SB	164	32% 100%
3	SC	164	84% 99%
3	SD	164	57% 99%
3	SE	164	55% 99%
3	SF	164	50% 99%
3	SH	164	83% 99%

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Mol	Chain	Length	Quality of chain
3	SK	164	46% 100%
3	T5	164	100% 98%
3	T9	164	99% 95%
3	TA	164	34% 93% 7%
3	TG	164	98% 99%
3	TI	164	100% 96%
3	TJ	164	100% 98%
3	U1	164	66% 99%
3	U2	164	94% 99%
3	U4	164	60% 99%
3	U6	164	30% 100%
3	U7	164	38% 100%
3	U8	164	57% 99%
3	UB	164	27% 100%
3	UC	164	94% 99%
3	UD	164	54% 100%
3	UE	164	52% 100%
3	UF	164	48% 99%
3	UH	164	56% 99%
3	UK	164	68% 99%
3	V5	164	100% 99%
3	V9	164	98% 95%
3	VG	164	99% 99%
3	VI	164	100% 96%
3	VJ	164	100% 99%

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Mol	Chain	Length	Quality of chain
3	W1	164	71% 100%
3	W2	164	95% 99%
3	W4	164	25% 99%
3	W6	164	37% 99%
3	W7	164	21% 98%
3	W8	164	63% 99%
3	WB	164	32% 99%
3	WC	164	96% 99%
3	WD	164	46% 100%
3	WE	164	44% 100%
3	WF	164	60% 99%
3	WH	164	27% 100%
3	WK	164	71% 100%
3	X5	164	100% 98%
3	X9	164	100% 95%
3	XG	164	100% 99%
3	XI	164	100% 96%
3	XJ	164	100% 98%
3	Y4	164	38% 99%
3	Y8	164	99% 100%
3	YF	164	98% 100%
3	YH	164	35% 98%
3	Z2	164	99% 99%
3	Z6	164	26% 100%
3	ZB	164	28% 100%

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Mol	Chain	Length	Quality of chain
3	ZC	164	96% 99%
3	ZD	164	43% 99%
3	ZE	164	43% 100%
3	a4	164	91% 99%
3	a8	164	95% 99%
3	aF	164	91% 99%
3	aH	164	93% 98%
3	b2	164	100% 99%
3	b6	164	80% 99%
3	bB	164	79% 99%
3	bC	164	100% 99%
3	bD	164	76% 95%
3	bE	164	81% 99%
3	c8	164	96% 98%
3	cF	164	93% 98%
3	d2	164	99% 97%
3	d4	164	95% 99%
3	d6	164	78% 100%
3	dB	164	77% 100%
3	dC	164	100% 97%
3	dD	164	88% 99%
3	dE	164	87% 99%
3	dH	164	91% 99%
3	e8	164	97% 98%
3	eF	164	93% 98%

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Mol	Chain	Length	Quality of chain
3	f2	164	99% 98%
3	f4	164	99% 99%
3	f6	164	82% 100%
3	fB	164	82% 100%
3	fC	164	100% 98%
3	fD	164	89% 99%
3	fE	164	87% 99%
3	fH	164	99% 99%
3	g8	164	92% 100%
3	gF	164	92% 99%
3	h2	164	99% 98%
3	h4	164	98% 99%
3	h6	164	73% 100%
3	hB	164	76% 100%
3	hC	164	100% 98%
3	hD	164	91% 99%
3	hE	164	88% 99%
3	hH	164	99% 99%
3	i8	164	93% 98%
3	iF	164	91% 98%
3	j2	164	100% 98%
3	j4	164	98% 99%
3	j6	164	81% 100%
3	jB	164	83% 100%
3	jC	164	100% 98%

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Mol	Chain	Length	Quality of chain
3	jD	164	85% 100%
3	jE	164	79% 100%
3	jH	164	99% 100%
3	k8	164	100% 99%
3	kF	164	100% 99%
3	l2	164	100% 96%
3	l4	164	73% 99%
3	l6	164	76% 95% 5%
3	lB	164	73% 99%
3	lC	164	100% 96%
3	lD	164	81% 85% 8% 5%
3	lE	164	82% 95% 5%
3	lH	164	77% 99%
3	m8	164	100% 98%
3	mF	164	100% 98%
3	o8	164	100% 99%
3	oF	164	100% 99%
3	q8	164	100% 98%
3	qF	164	100% 98%
3	s8	164	100% 98%
3	sF	164	100% 98%
3	u8	164	100% 99%
3	uF	164	100% 99%
4	KA	261	58% 66% 18% 13%
4	UA	261	57% 67% 18% 13%

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Mol	Chain	Length	Quality of chain
5	WA	317	36% 33% 9% 56%
5	cA	317	38% 35% 8% 56%
6	A2	290	89% 88% 11%
6	A5	290	88% 87% 12%
6	A6	290	67% 89% 11%
6	AB	290	60% 89% 11%
6	AC	290	88% 88% 11%
6	AD	290	68% 88% 11%
6	AE	290	68% 88% 11%
6	AJ	290	88% 87% 12%
6	Y1	290	80% 81% 18%
6	YK	290	80% 81% 18%
7	B2	232	53% 96% ..
7	B6	232	25% 89% 10% .
7	BB	232	23% 88% 9% ..
7	BC	232	57% 96% ..
7	BD	232	33% 95% ..
7	BE	232	27% 91% 7% ..
8	C2	162	81% 99% .
8	C6	162	21% 99% .
8	CB	162	21% 99% .
8	CC	162	83% 99% .
8	CD	162	38% 100%
8	CE	162	35% 100%
8	E2	162	34% 100%

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Mol	Chain	Length	Quality of chain
8	E6	162	28% 99%
8	EB	162	32% 100%
8	EC	162	33% 100%
8	ED	162	33% 100%
8	EE	162	33% 100%
8	G2	162	76% 99%
8	G6	162	21% 99%
8	GB	162	22% 99%
8	GC	162	75% 99%
8	GD	162	20% 100%
8	GE	162	20% 100%
8	I2	162	56% 100%
8	I6	162	38% 100%
8	IB	162	34% 100%
8	IC	162	59% 100%
8	ID	162	26% 100%
8	IE	162	26% 100%
8	K2	162	62% 99%
8	K6	162	40% 99%
8	KB	162	39% 99%
8	KC	162	62% 99%
8	KD	162	41% 99%
8	KE	162	43% 100%
8	M2	162	80% 99%
8	M6	162	25% 99%

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Mol	Chain	Length	Quality of chain
8	MB	162	22% 99%
8	MC	162	80% 99%
8	MD	162	27% 100%
8	ME	162	25% 100%
9	D2	172	84% 99%
9	D6	172	17% 98%
9	DB	172	15% 98%
9	DC	172	82% 99%
9	DD	172	28% 99%
9	DE	172	24% 99%
9	F2	172	60% 99%
9	F6	172	23% 98%
9	FB	172	24% 98%
9	FC	172	59% 99%
9	FD	172	31% 98%
9	FE	172	34% 98%
9	H2	172	60% 97%
9	H6	172	22% 98%
9	HB	172	22% 98%
9	HC	172	60% 93% 7%
9	HD	172	27% 99%
9	HE	172	22% 99%
9	J2	172	66% 94% 6%
9	J6	172	33% 99%
9	JB	172	33% 99%

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Mol	Chain	Length	Quality of chain
9	JC	172	61% 90% 9%
9	JD	172	30% 96% ..
9	JE	172	27% 94% 5%
9	L2	172	48% 99% .
9	L6	172	40% 93% 5% ..
9	LB	172	43% 98% .
9	LC	172	46% 99% .
9	LD	172	37% 98% .
9	LE	172	38% 98% .
9	N2	172	72% 99% .
9	N6	172	30% 97% ..
9	NB	172	31% 97% ...
9	NC	172	77% 99% .
9	ND	172	36% 96% .
9	NE	172	39% 99% .
10	X2	363	74% 88% 11%
10	X6	363	19% 88% 11%
10	XB	363	18% 88% 11%
10	XC	363	72% 88% 11%
10	XD	363	28% 88% 11%
10	XE	363	25% 88% 11%
11	MG	316	78% 74% 9% 16%
11	ZG	316	77% 75% 9% 16%
12	A4	273	82% 86% 13%
12	AH	273	81% 86% 13%

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Mol	Chain	Length	Quality of chain
12	w8	273	79% 87% 13%
12	wF	273	79% 87% 13%
12	x8	273	87% 87% 13%
12	xF	273	87% 87% 13%
13	B4	290	48% 86% 14%
13	BH	290	48% 86% 14%
13	y8	290	45% 86% 14%
13	yF	290	42% 86% 14%
14	M9	333	70% 66% 5% 29%
14	MI	333	80% 70% 9% 17%
14	Z9	333	70% 66% 5% 29%
14	ZI	333	79% 69% 11% 17%
15	e1	303	40% 82% 18%
15	eK	303	44% 82% 18%
16	23	159	28% 74% 9% 17%
16	Z3	159	33% 76% 6% 17%
17	33	288	24% 81% 7% 12%
17	a3	288	22% 79% 8% 12%
18	43	253	21% 74% 7% 19%
18	b3	253	22% 72% 9% 19%
19	A3	161	34% 93% 7%
19	C3	161	24% 93% 7%
19	E3	161	27% 93% 7%
19	G3	161	20% 93% 7%
19	J3	161	24% 92% 7%

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Mol	Chain	Length	Quality of chain
19	K3	161	28% 93% 7% .
19	N3	161	22% 93% 7% .
19	P3	161	20% 91% 8% ..
19	R3	161	24% 93% 7% .
19	T3	161	19% 93% 7% .
19	c3	161	35% 93% 7% .
19	e3	161	25% 93% 7% .
19	g3	161	23% 93% 7% .
19	i3	161	21% 93% 7% .
19	l3	161	24% 93% 7% .
19	m3	161	27% 92% 7% .
19	p3	161	21% 93% 7% .
19	r3	161	19% 89% 9% ...
19	t3	161	24% 93% 7% .
19	v3	161	14% 93% 6% .
20	B3	161	15% 94% 5% .
20	D3	161	21% 95% . .
20	F3	161	22% 95% . .
20	H3	161	20% 95% . .
20	I3	161	17% 95% . .
20	L3	161	16% 90% 8% .
20	M3	161	33% 94% 5% .
20	O3	161	20% 91% 7% ..
20	Q3	161	13% 91% 8% .
20	S3	161	14% 95% . .

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Mol	Chain	Length	Quality of chain
20	U3	161	13% 95%
20	d3	161	19% 95%
20	f3	161	24% 95%
20	h3	161	19% 95%
20	j3	161	17% 95%
20	k3	161	15% 95%
20	n3	161	19% 91% 6%
20	o3	161	31% 95%
20	q3	161	20% 94% 6%
20	s3	161	14% 93% 6%
20	u3	161	14% 95%
20	w3	161	11% 95%
21	V3	161	22% 96%
21	x3	161	22% 96%
22	W3	173	14% 96%
22	y3	173	14% 96%
23	X3	93	17% 97%
23	z3	93	18% 97%
24	63	879	22% 97%
24	73	879	24% 97%
25	b4	490	26% 81% 17%
25	bH	490	27% 81% 17%
26	d5	333	61% 81% 14%
26	dJ	333	60% 81% 5% 14%
27	Y7	420	33% 75% 11% 11%

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Mol	Chain	Length	Quality of chain
27	b7	420	
28	z8	498	
28	zF	498	
29	fA	288	
29	hA	288	
30	53	162	
30	Y3	162	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
20	MEN	B3	71	-	X	-	-
20	MEN	D3	71	-	X	-	-
20	MEN	F3	71	-	X	-	-
20	MEN	H3	71	-	X	-	-
20	MEN	I3	71	-	X	-	-
20	MEN	L3	71	-	X	-	-
20	MEN	M3	71	-	X	-	-
20	MEN	O3	71	-	X	-	-
20	MEN	Q3	71	-	X	-	-
20	MEN	S3	71	-	X	-	-
20	MEN	U3	71	-	X	-	-
20	MEN	d3	71	-	X	-	-
20	MEN	f3	71	-	X	-	-
20	MEN	h3	71	-	X	-	-
20	MEN	j3	71	-	X	-	-
20	MEN	k3	71	-	X	-	-
20	MEN	n3	71	-	X	-	-
20	MEN	o3	71	-	X	-	-
20	MEN	s3	71	-	X	-	-
20	MEN	u3	71	-	X	-	-
20	MEN	w3	71	-	X	-	-

2 Entry composition [i](#)

There are 33 unique types of molecules in this entry. The entry contains 1032373 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 Linker4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	103	774	492	129	150	3	0	0
1	EA	103	778	495	130	150	3	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BA	177	1294	800	225	257	12	0	0
2	CA	177	1294	800	225	257	12	0	0
2	DA	146	1065	654	187	213	11	0	0
2	FA	177	1294	800	225	257	12	0	0
2	GA	177	1294	800	225	257	12	0	0
2	HA	174	1270	785	222	252	11	0	0
2	IA	177	1294	800	225	257	12	0	0
2	LA	177	1290	797	224	257	12	0	0
2	MA	177	1294	800	225	257	12	0	0
2	NA	146	1056	650	184	211	11	0	0
2	OA	177	1294	800	225	257	12	0	0
2	PA	177	1294	800	225	257	12	0	0
2	QA	174	1270	785	222	252	11	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	RA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	SA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	XA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	ZA	152	Total 1111	C 687	N 194	O 219	S 11	0	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
2	VB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	PC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VC	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	YC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	PD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VD	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YD	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	PE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	TE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	VE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	YE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	BF	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	DF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	LF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	TF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	VF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	XF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	ZF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	BG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	DG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	FG	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	HG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	JG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	OG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	QG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	SG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	UG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	WG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	DH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	FH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	HH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	JH	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	LH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	NH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PH	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	RH	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	TH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XH	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	ZH	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	BI	177	Total 1291	C 799	N 224	O 256	S 12	0	0
2	DI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	FI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	HI	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	JI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	OI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	QI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	SI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	UI	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	WI	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	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
2	IJ	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	KJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	MJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	OJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	QJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	SJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	UJ	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	WJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	YJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	BK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	DK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	FK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	HK	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	JK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	LK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	NK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	PK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	RK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	TK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	VK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	XK	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	B1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H1	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J1	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L1	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	N1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	R1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	T1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	V1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X1	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	T2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V2	177	Total 1296	C 801	N 224	O 259	S 12	2	0
2	Y2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	g2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i2	177	Total 1300	C 804	N 225	O 259	S 12	2	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	a2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	c2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	e2	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	F4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	H4	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	J4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	L4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	N4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	P4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	R4	177	Total 1297	C 802	N 225	O 258	S 12	1	0
2	T4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	V4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	X4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	Z4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	c4	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	e4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	g4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	i4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	k4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	m4	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	M5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	O5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Q5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	S5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	U5	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	C5	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	G5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	I5	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	K5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	W5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	Y5	177	Total 1294	C 800	N 225	O 257	S 12	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 1294	C 800	N 225	O 257	S 12	0	0
2	Y6	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	i6	177	Total 1297	C 802	N 225	O 258	S 12	1	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
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	B7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F7	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	H7	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	N7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
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 1300	C 804	N 225	O 259	S 12	2	0
2	V7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	X7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	V8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	X8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	Z8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	B8	177	Total 1297	C 802	N 225	O 258	S 12	1	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 1303	C 806	N 225	O 260	S 12	3	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 1303	C 806	N 225	O 260	S 12	3	0
2	R8	177	Total 1300	C 804	N 225	O 259	S 12	2	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	b8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	d8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	f8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	h8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	j8	177	Total 1303	C 806	N 225	O 260	S 12	3	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 1303	C 806	N 225	O 260	S 12	3	0
2	r8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	t8	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	v8	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	B9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	D9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	F9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	H9	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	J9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	L9	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

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
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
2	aA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	bA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	dA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gA	152	Total 1101	C 678	N 193	O 219	S 11	0	0
2	iB	177	Total 1297	C 802	N 225	O 258	S 12	1	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	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	gC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iC	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cC	177	Total 1294	C 800	N 225	O 257	S 12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	eC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iD	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	aE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	cE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	eE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	gE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	iE	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	kE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	mE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
2	bF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	dF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	fF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	hF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	jF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	lF	177	Total 1303	C 806	N 225	O 260	S 12	3	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	nF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	pF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	rF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	tF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	vF	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	cH	177	Total 1300	C 804	N 225	O 259	S 12	2	0
2	eH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	gH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	iH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	kH	177	Total 1303	C 806	N 225	O 260	S 12	3	0
2	mH	177	Total 1303	C 806	N 225	O 260	S 12	3	0

- Molecule 3 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	JA	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	TA	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	OB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	QB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	SB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	UB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	WB	164	Total 1250	C 779	N 219	O 245	S 7	0	0
3	ZB	164	Total 1250	C 779	N 219	O 245	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	OC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	ZC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	OD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	ZD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	OE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	ZE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	AF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	CF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	EF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	GF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	IF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	KF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	MF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	YF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	AG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	CG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	EG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	GG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	IG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	KG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	NG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	PG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	RG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	TG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	VG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	XG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	CH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	EH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	GH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	IH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	KH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	MH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	OH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	YH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	AI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	CI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	EI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	GI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	II	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	KI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	NI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	PI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	RI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	TI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	VI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	XI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	BJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	DJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	FJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	HJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	JJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	LJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	NJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	PJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	RJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	TJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	VJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	XJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	AK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	CK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	EK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	GK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	IK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	KK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	MK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	OK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	QK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	SK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	UK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	WK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	A1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	C1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	E1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	G1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	I1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	K1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	M1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	S1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	W1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	S2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	W2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Z2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	f2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	h2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	j2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	l2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	b2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	d2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	C4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	E4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	G4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	I4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	K4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	M4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	S4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U4	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
3	W4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	Y4	164	Total	C	N	O	S	0	0
			1246	776	218	245	7		
3	a4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	d4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	f4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	h4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	j4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	l4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	L5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	N5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	P5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	R5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	T5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	B5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	D5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	F5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	H5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	J5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	V5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	X5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	S6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	W6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Z6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	j6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	l6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	b6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	d6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	f6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	h6	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	A7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	C7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	E7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	G7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	I7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	K7	164	Total	C	N	O	S	0	0
			1246	777	219	243	7		
3	M7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	W8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Y8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	A8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	C8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	E8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	G8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	I8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	K8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	M8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	O8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	Q8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	S8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	U8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	a8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	c8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	e8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	g8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	i8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	k8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	m8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	o8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	q8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	s8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	u8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	A9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	C9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	E9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	G9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	I9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	K9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	N9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	P9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	R9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	T9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	V9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	X9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	jB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	lB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	bB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	dB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	fB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	hB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	fC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	hC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	jC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	lC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	bC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	dC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	bD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	dD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	fD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	hD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	jD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	lD	164	Total	C	N	O	S	0	0
			1239	770	218	244	7		
3	bE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	dE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	fE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	hE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	jE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	lE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	aF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	cF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	eF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	gF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	iF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	kF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	mF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	oF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	qF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	sF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	uF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	aH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	dH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	fH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	hH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	jH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
3	lH	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 4 is a protein called CaRSPs1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	KA	226	Total	C	N	O	S	0	0
			1720	1084	305	322	9		
4	UA	226	Total	C	N	O	S	0	0
			1728	1090	305	325	8		

- Molecule 5 is a protein called CaRSPs2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	WA	139	Total	C	N	O	S	0	0
			1079	683	184	209	3		
5	cA	139	Total	C	N	O	S	0	0
			1085	686	184	213	2		

- Molecule 6 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	AB	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
6	AC	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
6	AD	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
6	AE	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
6	AJ	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
6	YK	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
6	Y1	237	Total	C	N	O	S	0	0
			1832	1132	339	346	15		
6	A2	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		
6	A5	256	Total	C	N	O	S	0	0
			1979	1220	367	377	15		
6	A6	257	Total	C	N	O	S	0	0
			1987	1226	368	378	15		

- Molecule 7 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	BB	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		
7	BC	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		
7	BD	231	Total	C	N	O	S	0	0
			1894	1211	331	348	4		
7	BE	231	Total	C	N	O	S	0	0
			1895	1210	332	349	4		
7	B2	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		
7	B6	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		

- Molecule 8 is a protein called C-phycoyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	EB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	GB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	IB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	KB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	MB	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	CC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	EC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	GC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	IC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	KC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	MC	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	CD	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	ED	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	GD	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	ID	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	KD	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	MD	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	CE	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	EE	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
8	GE	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	IE	162	1228	773	209	240	6	0	0
8	KE	162	1228	773	209	240	6	0	0
8	ME	162	1228	773	209	240	6	0	0
8	M2	162	1228	773	209	240	6	0	0
8	C2	162	1228	773	209	240	6	0	0
8	E2	162	1228	773	209	240	6	0	0
8	G2	162	1228	773	209	240	6	0	0
8	I2	162	1228	773	209	240	6	0	0
8	K2	162	1228	773	209	240	6	0	0
8	G6	162	1228	773	209	240	6	0	0
8	I6	162	1228	773	209	240	6	0	0
8	K6	162	1228	773	209	240	6	0	0
8	M6	162	1228	773	209	240	6	0	0
8	C6	162	1228	773	209	240	6	0	0
8	E6	162	1228	773	209	240	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	DB	172	1272	786	224	253	9	0	0
9	FB	172	1272	786	224	253	9	0	0
9	HB	172	1272	786	224	253	9	0	0
9	JB	172	1272	786	224	253	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	LB	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	NB	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	DC	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	FC	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	HC	172	Total 1268	C 784	N 224	O 251	S 9	0	0
9	JC	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	LC	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	NC	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	DD	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	FD	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	HD	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	JD	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	LD	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	ND	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	DE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	FE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	HE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	JE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	LE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	NE	172	Total 1272	C 786	N 224	O 253	S 9	0	0
9	L2	172	Total 1272	C 786	N 224	O 253	S 9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
9	N2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	D2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	F2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	H2	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	J2	172	Total	C	N	O	S	0	0
			1268	784	224	251	9		
9	F6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	H6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	J6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	L6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	N6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
9	D6	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

- Molecule 10 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	XB	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
10	XC	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
10	XD	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
10	XE	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
10	X2	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		
10	X6	324	Total	C	N	O	S	0	0
			2527	1603	431	486	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
XB	275	ALA	SER	conflict	UNP A0A5J4YM59
XC	275	ALA	SER	conflict	UNP A0A5J4YM59
XD	275	ALA	SER	conflict	UNP A0A5J4YM59
XE	275	ALA	SER	conflict	UNP A0A5J4YM59
X2	275	ALA	SER	conflict	UNP A0A5J4YM59
X6	275	ALA	SER	conflict	UNP A0A5J4YM59

- Molecule 11 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	MG	265	Total	C	N	O	S	0	0
			2079	1309	364	396	10		
11	ZG	265	Total	C	N	O	S	0	0
			2085	1313	364	398	10		

- Molecule 12 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	AH	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
12	A4	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
12	w8	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
12	x8	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
12	wF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		
12	xF	238	Total	C	N	O	S	0	0
			1814	1122	335	342	15		

- Molecule 13 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	BH	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
13	B4	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
13	y8	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		
13	yF	250	Total	C	N	O	S	0	0
			1902	1184	346	358	14		

- Molecule 14 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	MI	275	Total 2142	C 1324	N 401	O 401	S 16	0	0
14	ZI	275	Total 2148	C 1327	N 404	O 401	S 16	0	0
14	M9	238	Total 1851	C 1140	N 348	O 348	S 15	0	0
14	Z9	238	Total 1847	C 1137	N 347	O 348	S 15	0	0

- Molecule 15 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	eI	248	Total 1932	C 1217	N 336	O 369	S 10	0	0
15	eK	248	Total 1932	C 1217	N 336	O 369	S 10	0	0

- Molecule 16 is a protein called Lrc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	23	132	Total 1004	C 631	N 179	O 191	S 3	0	0
16	Z3	132	Total 1004	C 631	N 179	O 191	S 3	0	0

- Molecule 17 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	33	253	Total 1897	C 1190	N 325	O 375	S 7	0	0
17	a3	253	Total 1897	C 1190	N 325	O 375	S 7	0	0

- Molecule 18 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	43	206	Total 1532	C 982	N 259	O 286	S 5	0	0
18	b3	206	Total 1532	C 982	N 259	O 286	S 5	0	0

- Molecule 19 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	A3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	C3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	E3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	G3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	J3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	K3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	N3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	P3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	R3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	T3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	c3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	e3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	g3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	i3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	l3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	m3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	p3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	r3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	t3	160	Total	C	N	O	S	0	0
			1225	768	211	239	7		
19	v3	160	Total	C	N	O	S	0	0
			1217	764	211	235	7		

- Molecule 20 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	B3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	D3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	F3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	H3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	I3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	L3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	M3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
20	O3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	Q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	S3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	U3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	d3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	f3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	h3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	j3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	k3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	n3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	o3	161	Total	C	N	O	S	0	0
			1216	764	205	240	7		
20	q3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	s3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	u3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
20	w3	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 21 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	V3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
21	x3	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 22 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	W3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		
22	y3	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 23 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	X3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
23	z3	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 24 is a protein called Phycobiliprotein ApcE.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	63	868	Total	C	N	O	S	0	0
			6933	4434	1198	1286	15		
24	73	865	Total	C	N	O	S	0	0
			6910	4422	1195	1278	15		

- Molecule 25 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	b4	405	Total	C	N	O	S	0	0
			3086	1945	536	590	15		
25	bH	407	Total	C	N	O	S	0	0
			3089	1949	538	590	12		

- Molecule 26 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	d5	285	2203	1367	390	435	11	0	0
26	dJ	285	2203	1367	390	435	11	0	0

- Molecule 27 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	b7	372	2828	1778	483	555	12	0	0
27	Y7	372	2832	1779	483	557	13	0	0

- Molecule 28 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	z8	463	3622	2288	637	682	15	0	0
28	zF	462	3610	2281	636	678	15	0	0

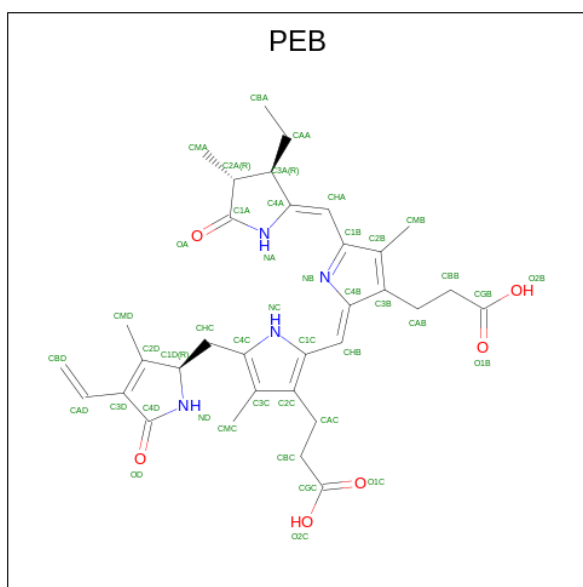
- Molecule 29 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	fA	285	2182	1399	369	404	10	0	0
29	hA	285	2178	1396	368	404	10	0	0

- Molecule 30 is a protein called LPP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	Y3	61	415	256	77	79	3	0	0
30	53	57	369	230	70	66	3	0	0

- Molecule 31 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	AA	1	Total	C	N	O	0
			43	33	4	6	
31	BA	1	Total	C	N	O	0
			43	33	4	6	
31	BA	1	Total	C	N	O	0
			43	33	4	6	
31	BA	1	Total	C	N	O	0
			43	33	4	6	
31	CA	1	Total	C	N	O	0
			43	33	4	6	
31	CA	1	Total	C	N	O	0
			43	33	4	6	
31	DA	1	Total	C	N	O	0
			43	33	4	6	
31	DA	1	Total	C	N	O	0
			43	33	4	6	
31	DA	1	Total	C	N	O	0
			43	33	4	6	
31	EA	1	Total	C	N	O	0
			43	33	4	6	
31	FA	1	Total	C	N	O	0
			43	33	4	6	
31	GA	1	Total	C	N	O	0
			43	33	4	6	
31	GA	1	Total	C	N	O	0
			43	33	4	6	
31	GA	1	Total	C	N	O	0
			43	33	4	6	

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	HA	1	43	33	4	6	0
31	HA	1	43	33	4	6	0
31	HA	1	43	33	4	6	0
31	IA	1	43	33	4	6	0
31	IA	1	43	33	4	6	0
31	IA	1	43	33	4	6	0
31	JA	1	43	33	4	6	0
31	JA	1	43	33	4	6	0
31	KA	1	43	33	4	6	0
31	KA	1	43	33	4	6	0
31	KA	1	43	33	4	6	0
31	KA	1	43	33	4	6	0
31	KA	1	43	33	4	6	0
31	LA	1	43	33	4	6	0
31	MA	1	43	33	4	6	0
31	MA	1	43	33	4	6	0
31	NA	1	43	33	4	6	0
31	NA	1	43	33	4	6	0
31	NA	1	43	33	4	6	0
31	OA	1	43	33	4	6	0
31	PA	1	43	33	4	6	0
31	QA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	QA	1	43	33	4	6	0
31	QA	1	43	33	4	6	0
31	QA	1	43	33	4	6	0
31	RA	1	43	33	4	6	0
31	RA	1	43	33	4	6	0
31	SA	1	43	33	4	6	0
31	SA	1	43	33	4	6	0
31	SA	1	43	33	4	6	0
31	TA	1	43	33	4	6	0
31	TA	1	43	33	4	6	0
31	UA	1	43	33	4	6	0
31	UA	1	43	33	4	6	0
31	UA	1	43	33	4	6	0
31	UA	1	43	33	4	6	0
31	VA	1	43	33	4	6	0
31	VA	1	43	33	4	6	0
31	WA	1	43	33	4	6	0
31	WA	1	43	33	4	6	0
31	XA	1	43	33	4	6	0
31	XA	1	43	33	4	6	0
31	YA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	ZA	1	43	33	4	6	0
31	ZA	1	43	33	4	6	0
31	ZA	1	43	33	4	6	0
31	AB	1	43	33	4	6	0
31	AB	1	43	33	4	6	0
31	AB	1	43	33	4	6	0
31	DB	1	43	33	4	6	0
31	FB	1	43	33	4	6	0
31	HB	1	43	33	4	6	0
31	JB	1	43	33	4	6	0
31	LB	1	43	33	4	6	0
31	NB	1	43	33	4	6	0
31	OB	1	43	33	4	6	0
31	OB	1	43	33	4	6	0
31	PB	1	43	33	4	6	0
31	PB	1	43	33	4	6	0
31	QB	1	43	33	4	6	0
31	QB	1	43	33	4	6	0
31	RB	1	43	33	4	6	0
31	RB	1	43	33	4	6	0
31	RB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	SB	1	43	33	4	6	0
31	SB	1	43	33	4	6	0
31	TB	1	43	33	4	6	0
31	TB	1	43	33	4	6	0
31	TB	1	43	33	4	6	0
31	UB	1	43	33	4	6	0
31	UB	1	43	33	4	6	0
31	VB	1	43	33	4	6	0
31	VB	1	43	33	4	6	0
31	WB	1	43	33	4	6	0
31	YB	1	43	33	4	6	0
31	YB	1	43	33	4	6	0
31	YB	1	43	33	4	6	0
31	ZB	1	43	33	4	6	0
31	ZB	1	43	33	4	6	0
31	AC	1	43	33	4	6	0
31	AC	1	43	33	4	6	0
31	AC	1	43	33	4	6	0
31	DC	1	43	33	4	6	0
31	FC	1	43	33	4	6	0
31	HC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	JC	1	43	33	4	6	0
31	LC	1	43	33	4	6	0
31	NC	1	43	33	4	6	0
31	OC	1	43	33	4	6	0
31	OC	1	43	33	4	6	0
31	OC	1	43	33	4	6	0
31	PC	1	43	33	4	6	0
31	PC	1	43	33	4	6	0
31	QC	1	43	33	4	6	0
31	QC	1	43	33	4	6	0
31	QC	1	43	33	4	6	0
31	RC	1	43	33	4	6	0
31	RC	1	43	33	4	6	0
31	SC	1	43	33	4	6	0
31	SC	1	43	33	4	6	0
31	TC	1	43	33	4	6	0
31	TC	1	43	33	4	6	0
31	UC	1	43	33	4	6	0
31	UC	1	43	33	4	6	0
31	UC	1	43	33	4	6	0
31	VC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	VC	1	43	33	4	6	0
31	VC	1	43	33	4	6	0
31	WC	1	43	33	4	6	0
31	WC	1	43	33	4	6	0
31	WC	1	43	33	4	6	0
31	YC	1	43	33	4	6	0
31	YC	1	43	33	4	6	0
31	ZC	1	43	33	4	6	0
31	ZC	1	43	33	4	6	0
31	ZC	1	43	33	4	6	0
31	AD	1	43	33	4	6	0
31	AD	1	43	33	4	6	0
31	DD	1	43	33	4	6	0
31	GD	1	43	33	4	6	0
31	HD	1	43	33	4	6	0
31	KD	1	43	33	4	6	0
31	LD	1	43	33	4	6	0
31	ND	1	43	33	4	6	0
31	OD	1	43	33	4	6	0
31	OD	1	43	33	4	6	0
31	OD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	PD	1	43	33	4	6	0
31	PD	1	43	33	4	6	0
31	QD	1	43	33	4	6	0
31	QD	1	43	33	4	6	0
31	QD	1	43	33	4	6	0
31	RD	1	43	33	4	6	0
31	RD	1	43	33	4	6	0
31	SD	1	43	33	4	6	0
31	SD	1	43	33	4	6	0
31	TD	1	43	33	4	6	0
31	UD	1	43	33	4	6	0
31	UD	1	43	33	4	6	0
31	UD	1	43	33	4	6	0
31	VD	1	43	33	4	6	0
31	VD	1	43	33	4	6	0
31	WD	1	43	33	4	6	0
31	WD	1	43	33	4	6	0
31	WD	1	43	33	4	6	0
31	YD	1	43	33	4	6	0
31	YD	1	43	33	4	6	0
31	ZD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	ZD	1	43	33	4	6	0
31	ZD	1	43	33	4	6	0
31	AE	1	43	33	4	6	0
31	AE	1	43	33	4	6	0
31	DE	1	43	33	4	6	0
31	HE	1	43	33	4	6	0
31	JE	1	43	33	4	6	0
31	KE	1	43	33	4	6	0
31	LE	1	43	33	4	6	0
31	NE	1	43	33	4	6	0
31	OE	1	43	33	4	6	0
31	OE	1	43	33	4	6	0
31	OE	1	43	33	4	6	0
31	PE	1	43	33	4	6	0
31	PE	1	43	33	4	6	0
31	QE	1	43	33	4	6	0
31	QE	1	43	33	4	6	0
31	QE	1	43	33	4	6	0
31	RE	1	43	33	4	6	0
31	RE	1	43	33	4	6	0
31	SE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	SE	1	Total 43	C 33	N 4	O 6	0
31	SE	1	Total 43	C 33	N 4	O 6	0
31	TE	1	Total 43	C 33	N 4	O 6	0
31	UE	1	Total 43	C 33	N 4	O 6	0
31	UE	1	Total 43	C 33	N 4	O 6	0
31	UE	1	Total 43	C 33	N 4	O 6	0
31	VE	1	Total 43	C 33	N 4	O 6	0
31	VE	1	Total 43	C 33	N 4	O 6	0
31	WE	1	Total 43	C 33	N 4	O 6	0
31	WE	1	Total 43	C 33	N 4	O 6	0
31	WE	1	Total 43	C 33	N 4	O 6	0
31	WE	1	Total 43	C 33	N 4	O 6	0
31	YE	1	Total 43	C 33	N 4	O 6	0
31	YE	1	Total 43	C 33	N 4	O 6	0
31	ZE	1	Total 43	C 33	N 4	O 6	0
31	ZE	1	Total 43	C 33	N 4	O 6	0
31	ZE	1	Total 43	C 33	N 4	O 6	0
31	AF	1	Total 43	C 33	N 4	O 6	0
31	AF	1	Total 43	C 33	N 4	O 6	0
31	BF	1	Total 43	C 33	N 4	O 6	0
31	BF	1	Total 43	C 33	N 4	O 6	0
31	CF	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	CF	1	Total 43	C 33	N 4	O 6	0
31	CF	1	Total 43	C 33	N 4	O 6	0
31	DF	1	Total 43	C 33	N 4	O 6	0
31	DF	1	Total 43	C 33	N 4	O 6	0
31	DF	1	Total 43	C 33	N 4	O 6	0
31	EF	1	Total 43	C 33	N 4	O 6	0
31	EF	1	Total 43	C 33	N 4	O 6	0
31	FF	1	Total 43	C 33	N 4	O 6	0
31	FF	1	Total 43	C 33	N 4	O 6	0
31	GF	1	Total 43	C 33	N 4	O 6	0
31	GF	1	Total 43	C 33	N 4	O 6	0
31	GF	1	Total 43	C 33	N 4	O 6	0
31	HF	1	Total 43	C 33	N 4	O 6	0
31	HF	1	Total 43	C 33	N 4	O 6	0
31	IF	1	Total 43	C 33	N 4	O 6	0
31	IF	1	Total 43	C 33	N 4	O 6	0
31	IF	1	Total 43	C 33	N 4	O 6	0
31	JF	1	Total 43	C 33	N 4	O 6	0
31	JF	1	Total 43	C 33	N 4	O 6	0
31	KF	1	Total 43	C 33	N 4	O 6	0
31	KF	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	KF	1	43	33	4	6	0
31	LF	1	43	33	4	6	0
31	LF	1	43	33	4	6	0
31	MF	1	43	33	4	6	0
31	MF	1	43	33	4	6	0
31	MF	1	43	33	4	6	0
31	NF	1	43	33	4	6	0
31	NF	1	43	33	4	6	0
31	OF	1	43	33	4	6	0
31	OF	1	43	33	4	6	0
31	OF	1	43	33	4	6	0
31	PF	1	43	33	4	6	0
31	PF	1	43	33	4	6	0
31	QF	1	43	33	4	6	0
31	QF	1	43	33	4	6	0
31	QF	1	43	33	4	6	0
31	RF	1	43	33	4	6	0
31	RF	1	43	33	4	6	0
31	SF	1	43	33	4	6	0
31	SF	1	43	33	4	6	0
31	SF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	TF	1	43	33	4	6	0
31	TF	1	43	33	4	6	0
31	UF	1	43	33	4	6	0
31	UF	1	43	33	4	6	0
31	VF	1	43	33	4	6	0
31	VF	1	43	33	4	6	0
31	WF	1	43	33	4	6	0
31	WF	1	43	33	4	6	0
31	WF	1	43	33	4	6	0
31	XF	1	43	33	4	6	0
31	XF	1	43	33	4	6	0
31	XF	1	43	33	4	6	0
31	YF	1	43	33	4	6	0
31	YF	1	43	33	4	6	0
31	YF	1	43	33	4	6	0
31	ZF	1	43	33	4	6	0
31	ZF	1	43	33	4	6	0
31	AG	1	43	33	4	6	0
31	AG	1	43	33	4	6	0
31	AG	1	43	33	4	6	0
31	BG	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	BG	1	43	33	4	6	0
31	BG	1	43	33	4	6	0
31	CG	1	43	33	4	6	0
31	CG	1	43	33	4	6	0
31	DG	1	43	33	4	6	0
31	DG	1	43	33	4	6	0
31	EG	1	43	33	4	6	0
31	EG	1	43	33	4	6	0
31	FG	1	43	33	4	6	0
31	FG	1	43	33	4	6	0
31	GG	1	43	33	4	6	0
31	GG	1	43	33	4	6	0
31	GG	1	43	33	4	6	0
31	HG	1	43	33	4	6	0
31	HG	1	43	33	4	6	0
31	HG	1	43	33	4	6	0
31	IG	1	43	33	4	6	0
31	IG	1	43	33	4	6	0
31	IG	1	43	33	4	6	0
31	JG	1	43	33	4	6	0
31	JG	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	KG	1	43	33	4	6	0
31	KG	1	43	33	4	6	0
31	KG	1	43	33	4	6	0
31	LG	1	43	33	4	6	0
31	LG	1	43	33	4	6	0
31	MG	1	43	33	4	6	0
31	NG	1	43	33	4	6	0
31	NG	1	43	33	4	6	0
31	NG	1	43	33	4	6	0
31	OG	1	43	33	4	6	0
31	OG	1	43	33	4	6	0
31	OG	1	43	33	4	6	0
31	PG	1	43	33	4	6	0
31	PG	1	43	33	4	6	0
31	QG	1	43	33	4	6	0
31	RG	1	43	33	4	6	0
31	RG	1	43	33	4	6	0
31	RG	1	43	33	4	6	0
31	SG	1	43	33	4	6	0
31	SG	1	43	33	4	6	0
31	TG	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	TG	1	43	33	4	6	0
31	TG	1	43	33	4	6	0
31	UG	1	43	33	4	6	0
31	UG	1	43	33	4	6	0
31	VG	1	43	33	4	6	0
31	VG	1	43	33	4	6	0
31	VG	1	43	33	4	6	0
31	WG	1	43	33	4	6	0
31	WG	1	43	33	4	6	0
31	WG	1	43	33	4	6	0
31	XG	1	43	33	4	6	0
31	XG	1	43	33	4	6	0
31	YG	1	43	33	4	6	0
31	YG	1	43	33	4	6	0
31	ZG	1	43	33	4	6	0
31	AH	1	43	33	4	6	0
31	AH	1	43	33	4	6	0
31	BH	1	43	33	4	6	0
31	CH	1	43	33	4	6	0
31	CH	1	43	33	4	6	0
31	CH	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	DH	1	43	33	4	6	0
31	DH	1	43	33	4	6	0
31	EH	1	43	33	4	6	0
31	EH	1	43	33	4	6	0
31	EH	1	43	33	4	6	0
31	FH	1	43	33	4	6	0
31	FH	1	43	33	4	6	0
31	GH	1	43	33	4	6	0
31	GH	1	43	33	4	6	0
31	GH	1	43	33	4	6	0
31	HH	1	43	33	4	6	0
31	HH	1	43	33	4	6	0
31	IH	1	43	33	4	6	0
31	IH	1	43	33	4	6	0
31	IH	1	43	33	4	6	0
31	JH	1	43	33	4	6	0
31	JH	1	43	33	4	6	0
31	KH	1	43	33	4	6	0
31	KH	1	43	33	4	6	0
31	KH	1	43	33	4	6	0
31	LH	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	LH	1	43	33	4	6	0
31	MH	1	43	33	4	6	0
31	MH	1	43	33	4	6	0
31	MH	1	43	33	4	6	0
31	NH	1	43	33	4	6	0
31	NH	1	43	33	4	6	0
31	OH	1	43	33	4	6	0
31	OH	1	43	33	4	6	0
31	OH	1	43	33	4	6	0
31	PH	1	43	33	4	6	0
31	PH	1	43	33	4	6	0
31	QH	1	43	33	4	6	0
31	QH	1	43	33	4	6	0
31	QH	1	43	33	4	6	0
31	RH	1	43	33	4	6	0
31	RH	1	43	33	4	6	0
31	SH	1	43	33	4	6	0
31	SH	1	43	33	4	6	0
31	SH	1	43	33	4	6	0
31	TH	1	43	33	4	6	0
31	TH	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	UH	1	43	33	4	6	0
31	UH	1	43	33	4	6	0
31	UH	1	43	33	4	6	0
31	VH	1	43	33	4	6	0
31	VH	1	43	33	4	6	0
31	WH	1	43	33	4	6	0
31	WH	1	43	33	4	6	0
31	WH	1	43	33	4	6	0
31	XH	1	43	33	4	6	0
31	XH	1	43	33	4	6	0
31	YH	1	43	33	4	6	0
31	YH	1	43	33	4	6	0
31	YH	1	43	33	4	6	0
31	ZH	1	43	33	4	6	0
31	ZH	1	43	33	4	6	0
31	AI	1	43	33	4	6	0
31	AI	1	43	33	4	6	0
31	BI	1	43	33	4	6	0
31	BI	1	43	33	4	6	0
31	BI	1	43	33	4	6	0
31	CI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	CI	1	43	33	4	6	0
31	DI	1	43	33	4	6	0
31	DI	1	43	33	4	6	0
31	DI	1	43	33	4	6	0
31	EI	1	43	33	4	6	0
31	EI	1	43	33	4	6	0
31	FI	1	43	33	4	6	0
31	FI	1	43	33	4	6	0
31	FI	1	43	33	4	6	0
31	GI	1	43	33	4	6	0
31	GI	1	43	33	4	6	0
31	HI	1	43	33	4	6	0
31	HI	1	43	33	4	6	0
31	HI	1	43	33	4	6	0
31	II	1	43	33	4	6	0
31	II	1	43	33	4	6	0
31	JI	1	43	33	4	6	0
31	JI	1	43	33	4	6	0
31	JI	1	43	33	4	6	0
31	KI	1	43	33	4	6	0
31	KI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	LI	1	43	33	4	6	0
31	LI	1	43	33	4	6	0
31	LI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	NI	1	43	33	4	6	0
31	NI	1	43	33	4	6	0
31	OI	1	43	33	4	6	0
31	OI	1	43	33	4	6	0
31	OI	1	43	33	4	6	0
31	PI	1	43	33	4	6	0
31	PI	1	43	33	4	6	0
31	QI	1	43	33	4	6	0
31	QI	1	43	33	4	6	0
31	QI	1	43	33	4	6	0
31	RI	1	43	33	4	6	0
31	RI	1	43	33	4	6	0
31	SI	1	43	33	4	6	0
31	SI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	SI	1	43	33	4	6	0
31	TI	1	43	33	4	6	0
31	TI	1	43	33	4	6	0
31	UI	1	43	33	4	6	0
31	UI	1	43	33	4	6	0
31	UI	1	43	33	4	6	0
31	UI	1	43	33	4	6	0
31	VI	1	43	33	4	6	0
31	VI	1	43	33	4	6	0
31	WI	1	43	33	4	6	0
31	WI	1	43	33	4	6	0
31	WI	1	43	33	4	6	0
31	XI	1	43	33	4	6	0
31	XI	1	43	33	4	6	0
31	YI	1	43	33	4	6	0
31	YI	1	43	33	4	6	0
31	YI	1	43	33	4	6	0
31	ZI	1	43	33	4	6	0
31	ZI	1	43	33	4	6	0
31	ZI	1	43	33	4	6	0
31	AJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	AJ	1	43	33	4	6	0
31	AJ	1	43	33	4	6	0
31	BJ	1	43	33	4	6	0
31	BJ	1	43	33	4	6	0
31	BJ	1	43	33	4	6	0
31	CJ	1	43	33	4	6	0
31	CJ	1	43	33	4	6	0
31	DJ	1	43	33	4	6	0
31	DJ	1	43	33	4	6	0
31	DJ	1	43	33	4	6	0
31	EJ	1	43	33	4	6	0
31	EJ	1	43	33	4	6	0
31	FJ	1	43	33	4	6	0
31	FJ	1	43	33	4	6	0
31	FJ	1	43	33	4	6	0
31	GJ	1	43	33	4	6	0
31	GJ	1	43	33	4	6	0
31	HJ	1	43	33	4	6	0
31	HJ	1	43	33	4	6	0
31	HJ	1	43	33	4	6	0
31	IJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	IJ	1	43	33	4	6	0
31	JJ	1	43	33	4	6	0
31	JJ	1	43	33	4	6	0
31	JJ	1	43	33	4	6	0
31	KJ	1	43	33	4	6	0
31	KJ	1	43	33	4	6	0
31	LJ	1	43	33	4	6	0
31	LJ	1	43	33	4	6	0
31	LJ	1	43	33	4	6	0
31	MJ	1	43	33	4	6	0
31	MJ	1	43	33	4	6	0
31	NJ	1	43	33	4	6	0
31	NJ	1	43	33	4	6	0
31	NJ	1	43	33	4	6	0
31	OJ	1	43	33	4	6	0
31	OJ	1	43	33	4	6	0
31	PJ	1	43	33	4	6	0
31	PJ	1	43	33	4	6	0
31	PJ	1	43	33	4	6	0
31	QJ	1	43	33	4	6	0
31	QJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	RJ	1	43	33	4	6	0
31	RJ	1	43	33	4	6	0
31	RJ	1	43	33	4	6	0
31	SJ	1	43	33	4	6	0
31	SJ	1	43	33	4	6	0
31	TJ	1	43	33	4	6	0
31	TJ	1	43	33	4	6	0
31	TJ	1	43	33	4	6	0
31	UJ	1	43	33	4	6	0
31	UJ	1	43	33	4	6	0
31	VJ	1	43	33	4	6	0
31	VJ	1	43	33	4	6	0
31	VJ	1	43	33	4	6	0
31	WJ	1	43	33	4	6	0
31	WJ	1	43	33	4	6	0
31	XJ	1	43	33	4	6	0
31	XJ	1	43	33	4	6	0
31	XJ	1	43	33	4	6	0
31	YJ	1	43	33	4	6	0
31	YJ	1	43	33	4	6	0
31	AK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	AK	1	43	33	4	6	0
31	BK	1	43	33	4	6	0
31	BK	1	43	33	4	6	0
31	BK	1	43	33	4	6	0
31	CK	1	43	33	4	6	0
31	CK	1	43	33	4	6	0
31	DK	1	43	33	4	6	0
31	DK	1	43	33	4	6	0
31	DK	1	43	33	4	6	0
31	EK	1	43	33	4	6	0
31	EK	1	43	33	4	6	0
31	FK	1	43	33	4	6	0
31	FK	1	43	33	4	6	0
31	FK	1	43	33	4	6	0
31	GK	1	43	33	4	6	0
31	GK	1	43	33	4	6	0
31	HK	1	43	33	4	6	0
31	HK	1	43	33	4	6	0
31	HK	1	43	33	4	6	0
31	IK	1	43	33	4	6	0
31	IK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	JK	1	43	33	4	6	0
31	JK	1	43	33	4	6	0
31	JK	1	43	33	4	6	0
31	KK	1	43	33	4	6	0
31	KK	1	43	33	4	6	0
31	LK	1	43	33	4	6	0
31	LK	1	43	33	4	6	0
31	LK	1	43	33	4	6	0
31	MK	1	43	33	4	6	0
31	MK	1	43	33	4	6	0
31	NK	1	43	33	4	6	0
31	NK	1	43	33	4	6	0
31	NK	1	43	33	4	6	0
31	OK	1	43	33	4	6	0
31	OK	1	43	33	4	6	0
31	PK	1	43	33	4	6	0
31	PK	1	43	33	4	6	0
31	PK	1	43	33	4	6	0
31	QK	1	43	33	4	6	0
31	QK	1	43	33	4	6	0
31	RK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	RK	1	43	33	4	6	0
31	RK	1	43	33	4	6	0
31	SK	1	43	33	4	6	0
31	SK	1	43	33	4	6	0
31	TK	1	43	33	4	6	0
31	TK	1	43	33	4	6	0
31	TK	1	43	33	4	6	0
31	UK	1	43	33	4	6	0
31	UK	1	43	33	4	6	0
31	VK	1	43	33	4	6	0
31	VK	1	43	33	4	6	0
31	VK	1	43	33	4	6	0
31	WK	1	43	33	4	6	0
31	WK	1	43	33	4	6	0
31	XK	1	43	33	4	6	0
31	XK	1	43	33	4	6	0
31	XK	1	43	33	4	6	0
31	YK	1	43	33	4	6	0
31	YK	1	43	33	4	6	0
31	YK	1	43	33	4	6	0
31	A1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	A1	1	43	33	4	6	0
31	B1	1	43	33	4	6	0
31	B1	1	43	33	4	6	0
31	B1	1	43	33	4	6	0
31	C1	1	43	33	4	6	0
31	C1	1	43	33	4	6	0
31	D1	1	43	33	4	6	0
31	D1	1	43	33	4	6	0
31	D1	1	43	33	4	6	0
31	E1	1	43	33	4	6	0
31	E1	1	43	33	4	6	0
31	F1	1	43	33	4	6	0
31	F1	1	43	33	4	6	0
31	F1	1	43	33	4	6	0
31	G1	1	43	33	4	6	0
31	G1	1	43	33	4	6	0
31	H1	1	43	33	4	6	0
31	H1	1	43	33	4	6	0
31	H1	1	43	33	4	6	0
31	I1	1	43	33	4	6	0
31	I1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	J1	1	43	33	4	6	0
31	J1	1	43	33	4	6	0
31	J1	1	43	33	4	6	0
31	K1	1	43	33	4	6	0
31	K1	1	43	33	4	6	0
31	L1	1	43	33	4	6	0
31	L1	1	43	33	4	6	0
31	L1	1	43	33	4	6	0
31	M1	1	43	33	4	6	0
31	M1	1	43	33	4	6	0
31	N1	1	43	33	4	6	0
31	N1	1	43	33	4	6	0
31	N1	1	43	33	4	6	0
31	O1	1	43	33	4	6	0
31	O1	1	43	33	4	6	0
31	P1	1	43	33	4	6	0
31	P1	1	43	33	4	6	0
31	P1	1	43	33	4	6	0
31	Q1	1	43	33	4	6	0
31	Q1	1	43	33	4	6	0
31	R1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	R1	1	43	33	4	6	0
31	R1	1	43	33	4	6	0
31	S1	1	43	33	4	6	0
31	S1	1	43	33	4	6	0
31	T1	1	43	33	4	6	0
31	T1	1	43	33	4	6	0
31	T1	1	43	33	4	6	0
31	U1	1	43	33	4	6	0
31	U1	1	43	33	4	6	0
31	V1	1	43	33	4	6	0
31	V1	1	43	33	4	6	0
31	V1	1	43	33	4	6	0
31	W1	1	43	33	4	6	0
31	W1	1	43	33	4	6	0
31	X1	1	43	33	4	6	0
31	X1	1	43	33	4	6	0
31	X1	1	43	33	4	6	0
31	Y1	1	43	33	4	6	0
31	Y1	1	43	33	4	6	0
31	Y1	1	43	33	4	6	0
31	e1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	L2	1	43	33	4	6	0
31	N2	1	43	33	4	6	0
31	O2	1	43	33	4	6	0
31	O2	1	43	33	4	6	0
31	O2	1	43	33	4	6	0
31	P2	1	43	33	4	6	0
31	P2	1	43	33	4	6	0
31	Q2	1	43	33	4	6	0
31	Q2	1	43	33	4	6	0
31	Q2	1	43	33	4	6	0
31	R2	1	43	33	4	6	0
31	R2	1	43	33	4	6	0
31	S2	1	43	33	4	6	0
31	S2	1	43	33	4	6	0
31	T2	1	43	33	4	6	0
31	T2	1	43	33	4	6	0
31	U2	1	43	33	4	6	0
31	U2	1	43	33	4	6	0
31	U2	1	43	33	4	6	0
31	A2	1	43	33	4	6	0
31	A2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	A2	1	43	33	4	6	0
31	D2	1	43	33	4	6	0
31	F2	1	43	33	4	6	0
31	H2	1	43	33	4	6	0
31	J2	1	43	33	4	6	0
31	V2	1	43	33	4	6	0
31	V2	1	43	33	4	6	0
31	V2	1	43	33	4	6	0
31	W2	1	43	33	4	6	0
31	W2	1	43	33	4	6	0
31	W2	1	43	33	4	6	0
31	Y2	1	43	33	4	6	0
31	Y2	1	43	33	4	6	0
31	Z2	1	43	33	4	6	0
31	Z2	1	43	33	4	6	0
31	Z2	1	43	33	4	6	0
31	f2	1	43	33	4	6	0
31	f2	1	43	33	4	6	0
31	f2	1	43	33	4	6	0
31	g2	1	43	33	4	6	0
31	g2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	h2	1	43	33	4	6	0
31	h2	1	43	33	4	6	0
31	h2	1	43	33	4	6	0
31	i2	1	43	33	4	6	0
31	i2	1	43	33	4	6	0
31	j2	1	43	33	4	6	0
31	j2	1	43	33	4	6	0
31	j2	1	43	33	4	6	0
31	k2	1	43	33	4	6	0
31	k2	1	43	33	4	6	0
31	l2	1	43	33	4	6	0
31	l2	1	43	33	4	6	0
31	l2	1	43	33	4	6	0
31	m2	1	43	33	4	6	0
31	m2	1	43	33	4	6	0
31	a2	1	43	33	4	6	0
31	a2	1	43	33	4	6	0
31	b2	1	43	33	4	6	0
31	b2	1	43	33	4	6	0
31	b2	1	43	33	4	6	0
31	c2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	c2	1	43	33	4	6	0
31	d2	1	43	33	4	6	0
31	d2	1	43	33	4	6	0
31	d2	1	43	33	4	6	0
31	e2	1	43	33	4	6	0
31	e2	1	43	33	4	6	0
31	A4	1	43	33	4	6	0
31	A4	1	43	33	4	6	0
31	B4	1	43	33	4	6	0
31	C4	1	43	33	4	6	0
31	C4	1	43	33	4	6	0
31	C4	1	43	33	4	6	0
31	D4	1	43	33	4	6	0
31	D4	1	43	33	4	6	0
31	E4	1	43	33	4	6	0
31	E4	1	43	33	4	6	0
31	E4	1	43	33	4	6	0
31	F4	1	43	33	4	6	0
31	F4	1	43	33	4	6	0
31	G4	1	43	33	4	6	0
31	G4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	G4	1	43	33	4	6	0
31	H4	1	43	33	4	6	0
31	H4	1	43	33	4	6	0
31	I4	1	43	33	4	6	0
31	I4	1	43	33	4	6	0
31	I4	1	43	33	4	6	0
31	J4	1	43	33	4	6	0
31	J4	1	43	33	4	6	0
31	K4	1	43	33	4	6	0
31	K4	1	43	33	4	6	0
31	K4	1	43	33	4	6	0
31	L4	1	43	33	4	6	0
31	L4	1	43	33	4	6	0
31	M4	1	43	33	4	6	0
31	M4	1	43	33	4	6	0
31	M4	1	43	33	4	6	0
31	N4	1	43	33	4	6	0
31	N4	1	43	33	4	6	0
31	O4	1	43	33	4	6	0
31	O4	1	43	33	4	6	0
31	O4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	P4	1	43	33	4	6	0
31	P4	1	43	33	4	6	0
31	Q4	1	43	33	4	6	0
31	Q4	1	43	33	4	6	0
31	Q4	1	43	33	4	6	0
31	R4	1	43	33	4	6	0
31	R4	1	43	33	4	6	0
31	S4	1	43	33	4	6	0
31	S4	1	43	33	4	6	0
31	S4	1	43	33	4	6	0
31	T4	1	43	33	4	6	0
31	T4	1	43	33	4	6	0
31	U4	1	43	33	4	6	0
31	U4	1	43	33	4	6	0
31	U4	1	43	33	4	6	0
31	V4	1	43	33	4	6	0
31	V4	1	43	33	4	6	0
31	W4	1	43	33	4	6	0
31	W4	1	43	33	4	6	0
31	W4	1	43	33	4	6	0
31	X4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	X4	1	43	33	4	6	0
31	Y4	1	43	33	4	6	0
31	Y4	1	43	33	4	6	0
31	Y4	1	43	33	4	6	0
31	Z4	1	43	33	4	6	0
31	Z4	1	43	33	4	6	0
31	a4	1	43	33	4	6	0
31	a4	1	43	33	4	6	0
31	a4	1	43	33	4	6	0
31	a4	1	43	33	4	6	0
31	c4	1	43	33	4	6	0
31	c4	1	43	33	4	6	0
31	d4	1	43	33	4	6	0
31	d4	1	43	33	4	6	0
31	d4	1	43	33	4	6	0
31	e4	1	43	33	4	6	0
31	e4	1	43	33	4	6	0
31	f4	1	43	33	4	6	0
31	f4	1	43	33	4	6	0
31	f4	1	43	33	4	6	0
31	g4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	g4	1	Total 43	C 33	N 4	O 6	0
31	h4	1	Total 43	C 33	N 4	O 6	0
31	h4	1	Total 43	C 33	N 4	O 6	0
31	h4	1	Total 43	C 33	N 4	O 6	0
31	i4	1	Total 43	C 33	N 4	O 6	0
31	i4	1	Total 43	C 33	N 4	O 6	0
31	j4	1	Total 43	C 33	N 4	O 6	0
31	j4	1	Total 43	C 33	N 4	O 6	0
31	j4	1	Total 43	C 33	N 4	O 6	0
31	k4	1	Total 43	C 33	N 4	O 6	0
31	k4	1	Total 43	C 33	N 4	O 6	0
31	l4	1	Total 43	C 33	N 4	O 6	0
31	l4	1	Total 43	C 33	N 4	O 6	0
31	l4	1	Total 43	C 33	N 4	O 6	0
31	m4	1	Total 43	C 33	N 4	O 6	0
31	m4	1	Total 43	C 33	N 4	O 6	0
31	L5	1	Total 43	C 33	N 4	O 6	0
31	L5	1	Total 43	C 33	N 4	O 6	0
31	L5	1	Total 43	C 33	N 4	O 6	0
31	M5	1	Total 43	C 33	N 4	O 6	0
31	M5	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	N5	1	43	33	4	6	0
31	N5	1	43	33	4	6	0
31	N5	1	43	33	4	6	0
31	O5	1	43	33	4	6	0
31	O5	1	43	33	4	6	0
31	P5	1	43	33	4	6	0
31	P5	1	43	33	4	6	0
31	P5	1	43	33	4	6	0
31	Q5	1	43	33	4	6	0
31	Q5	1	43	33	4	6	0
31	R5	1	43	33	4	6	0
31	R5	1	43	33	4	6	0
31	R5	1	43	33	4	6	0
31	S5	1	43	33	4	6	0
31	S5	1	43	33	4	6	0
31	T5	1	43	33	4	6	0
31	T5	1	43	33	4	6	0
31	T5	1	43	33	4	6	0
31	U5	1	43	33	4	6	0
31	U5	1	43	33	4	6	0
31	d5	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	A5	1	43	33	4	6	0
31	A5	1	43	33	4	6	0
31	A5	1	43	33	4	6	0
31	B5	1	43	33	4	6	0
31	B5	1	43	33	4	6	0
31	B5	1	43	33	4	6	0
31	C5	1	43	33	4	6	0
31	C5	1	43	33	4	6	0
31	D5	1	43	33	4	6	0
31	D5	1	43	33	4	6	0
31	D5	1	43	33	4	6	0
31	E5	1	43	33	4	6	0
31	E5	1	43	33	4	6	0
31	F5	1	43	33	4	6	0
31	F5	1	43	33	4	6	0
31	F5	1	43	33	4	6	0
31	G5	1	43	33	4	6	0
31	G5	1	43	33	4	6	0
31	H5	1	43	33	4	6	0
31	H5	1	43	33	4	6	0
31	H5	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	I5	1	43	33	4	6	0
31	I5	1	43	33	4	6	0
31	J5	1	43	33	4	6	0
31	J5	1	43	33	4	6	0
31	J5	1	43	33	4	6	0
31	K5	1	43	33	4	6	0
31	K5	1	43	33	4	6	0
31	V5	1	43	33	4	6	0
31	V5	1	43	33	4	6	0
31	V5	1	43	33	4	6	0
31	W5	1	43	33	4	6	0
31	W5	1	43	33	4	6	0
31	X5	1	43	33	4	6	0
31	X5	1	43	33	4	6	0
31	X5	1	43	33	4	6	0
31	Y5	1	43	33	4	6	0
31	Y5	1	43	33	4	6	0
31	F6	1	43	33	4	6	0
31	H6	1	43	33	4	6	0
31	J6	1	43	33	4	6	0
31	L6	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	N6	1	43	33	4	6	0
31	O6	1	43	33	4	6	0
31	O6	1	43	33	4	6	0
31	A6	1	43	33	4	6	0
31	A6	1	43	33	4	6	0
31	A6	1	43	33	4	6	0
31	D6	1	43	33	4	6	0
31	P6	1	43	33	4	6	0
31	P6	1	43	33	4	6	0
31	P6	1	43	33	4	6	0
31	Q6	1	43	33	4	6	0
31	Q6	1	43	33	4	6	0
31	R6	1	43	33	4	6	0
31	R6	1	43	33	4	6	0
31	R6	1	43	33	4	6	0
31	S6	1	43	33	4	6	0
31	S6	1	43	33	4	6	0
31	T6	1	43	33	4	6	0
31	T6	1	43	33	4	6	0
31	T6	1	43	33	4	6	0
31	U6	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	U6	1	43	33	4	6	0
31	V6	1	43	33	4	6	0
31	V6	1	43	33	4	6	0
31	W6	1	43	33	4	6	0
31	Y6	1	43	33	4	6	0
31	Y6	1	43	33	4	6	0
31	Y6	1	43	33	4	6	0
31	Z6	1	43	33	4	6	0
31	Z6	1	43	33	4	6	0
31	i6	1	43	33	4	6	0
31	i6	1	43	33	4	6	0
31	i6	1	43	33	4	6	0
31	j6	1	43	33	4	6	0
31	j6	1	43	33	4	6	0
31	k6	1	43	33	4	6	0
31	k6	1	43	33	4	6	0
31	k6	1	43	33	4	6	0
31	l6	1	43	33	4	6	0
31	l6	1	43	33	4	6	0
31	m6	1	43	33	4	6	0
31	m6	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	m6	1	43	33	4	6	0
31	a6	1	43	33	4	6	0
31	a6	1	43	33	4	6	0
31	a6	1	43	33	4	6	0
31	b6	1	43	33	4	6	0
31	b6	1	43	33	4	6	0
31	c6	1	43	33	4	6	0
31	c6	1	43	33	4	6	0
31	c6	1	43	33	4	6	0
31	d6	1	43	33	4	6	0
31	d6	1	43	33	4	6	0
31	e6	1	43	33	4	6	0
31	e6	1	43	33	4	6	0
31	e6	1	43	33	4	6	0
31	f6	1	43	33	4	6	0
31	f6	1	43	33	4	6	0
31	g6	1	43	33	4	6	0
31	g6	1	43	33	4	6	0
31	g6	1	43	33	4	6	0
31	h6	1	43	33	4	6	0
31	h6	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	A7	1	43	33	4	6	0
31	A7	1	43	33	4	6	0
31	A7	1	43	33	4	6	0
31	B7	1	43	33	4	6	0
31	B7	1	43	33	4	6	0
31	C7	1	43	33	4	6	0
31	C7	1	43	33	4	6	0
31	C7	1	43	33	4	6	0
31	D7	1	43	33	4	6	0
31	D7	1	43	33	4	6	0
31	E7	1	43	33	4	6	0
31	E7	1	43	33	4	6	0
31	E7	1	43	33	4	6	0
31	F7	1	43	33	4	6	0
31	F7	1	43	33	4	6	0
31	G7	1	43	33	4	6	0
31	G7	1	43	33	4	6	0
31	G7	1	43	33	4	6	0
31	H7	1	43	33	4	6	0
31	H7	1	43	33	4	6	0
31	I7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	I7	1	43	33	4	6	0
31	I7	1	43	33	4	6	0
31	J7	1	43	33	4	6	0
31	J7	1	43	33	4	6	0
31	K7	1	43	33	4	6	0
31	K7	1	43	33	4	6	0
31	L7	1	43	33	4	6	0
31	L7	1	43	33	4	6	0
31	b7	1	43	33	4	6	0
31	b7	1	43	33	4	6	0
31	b7	1	43	33	4	6	0
31	M7	1	43	33	4	6	0
31	M7	1	43	33	4	6	0
31	M7	1	43	33	4	6	0
31	N7	1	43	33	4	6	0
31	N7	1	43	33	4	6	0
31	O7	1	43	33	4	6	0
31	O7	1	43	33	4	6	0
31	O7	1	43	33	4	6	0
31	P7	1	43	33	4	6	0
31	P7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	Q7	1	43	33	4	6	0
31	Q7	1	43	33	4	6	0
31	Q7	1	43	33	4	6	0
31	R7	1	43	33	4	6	0
31	R7	1	43	33	4	6	0
31	S7	1	43	33	4	6	0
31	S7	1	43	33	4	6	0
31	S7	1	43	33	4	6	0
31	T7	1	43	33	4	6	0
31	T7	1	43	33	4	6	0
31	U7	1	43	33	4	6	0
31	U7	1	43	33	4	6	0
31	U7	1	43	33	4	6	0
31	V7	1	43	33	4	6	0
31	V7	1	43	33	4	6	0
31	W7	1	43	33	4	6	0
31	W7	1	43	33	4	6	0
31	X7	1	43	33	4	6	0
31	X7	1	43	33	4	6	0
31	Y7	1	43	33	4	6	0
31	Y7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	Y7	1	43	33	4	6	0
31	Y7	1	43	33	4	6	0
31	V8	1	43	33	4	6	0
31	V8	1	43	33	4	6	0
31	W8	1	43	33	4	6	0
31	W8	1	43	33	4	6	0
31	W8	1	43	33	4	6	0
31	X8	1	43	33	4	6	0
31	X8	1	43	33	4	6	0
31	X8	1	43	33	4	6	0
31	Y8	1	43	33	4	6	0
31	Y8	1	43	33	4	6	0
31	Y8	1	43	33	4	6	0
31	Z8	1	43	33	4	6	0
31	Z8	1	43	33	4	6	0
31	A8	1	43	33	4	6	0
31	A8	1	43	33	4	6	0
31	B8	1	43	33	4	6	0
31	B8	1	43	33	4	6	0
31	C8	1	43	33	4	6	0
31	C8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	C8	1	43	33	4	6	0
31	D8	1	43	33	4	6	0
31	D8	1	43	33	4	6	0
31	D8	1	43	33	4	6	0
31	E8	1	43	33	4	6	0
31	E8	1	43	33	4	6	0
31	F8	1	43	33	4	6	0
31	F8	1	43	33	4	6	0
31	G8	1	43	33	4	6	0
31	G8	1	43	33	4	6	0
31	G8	1	43	33	4	6	0
31	H8	1	43	33	4	6	0
31	H8	1	43	33	4	6	0
31	I8	1	43	33	4	6	0
31	I8	1	43	33	4	6	0
31	I8	1	43	33	4	6	0
31	J8	1	43	33	4	6	0
31	J8	1	43	33	4	6	0
31	K8	1	43	33	4	6	0
31	K8	1	43	33	4	6	0
31	K8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	L8	1	43	33	4	6	0
31	L8	1	43	33	4	6	0
31	M8	1	43	33	4	6	0
31	M8	1	43	33	4	6	0
31	M8	1	43	33	4	6	0
31	N8	1	43	33	4	6	0
31	N8	1	43	33	4	6	0
31	O8	1	43	33	4	6	0
31	O8	1	43	33	4	6	0
31	O8	1	43	33	4	6	0
31	P8	1	43	33	4	6	0
31	P8	1	43	33	4	6	0
31	Q8	1	43	33	4	6	0
31	Q8	1	43	33	4	6	0
31	Q8	1	43	33	4	6	0
31	R8	1	43	33	4	6	0
31	R8	1	43	33	4	6	0
31	S8	1	43	33	4	6	0
31	S8	1	43	33	4	6	0
31	S8	1	43	33	4	6	0
31	T8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	T8	1	43	33	4	6	0
31	U8	1	43	33	4	6	0
31	U8	1	43	33	4	6	0
31	a8	1	43	33	4	6	0
31	a8	1	43	33	4	6	0
31	a8	1	43	33	4	6	0
31	b8	1	43	33	4	6	0
31	b8	1	43	33	4	6	0
31	c8	1	43	33	4	6	0
31	c8	1	43	33	4	6	0
31	c8	1	43	33	4	6	0
31	d8	1	43	33	4	6	0
31	d8	1	43	33	4	6	0
31	e8	1	43	33	4	6	0
31	e8	1	43	33	4	6	0
31	e8	1	43	33	4	6	0
31	f8	1	43	33	4	6	0
31	f8	1	43	33	4	6	0
31	g8	1	43	33	4	6	0
31	g8	1	43	33	4	6	0
31	g8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	h8	1	Total 43	C 33	N 4	O 6	0
31	h8	1	Total 43	C 33	N 4	O 6	0
31	i8	1	Total 43	C 33	N 4	O 6	0
31	i8	1	Total 43	C 33	N 4	O 6	0
31	i8	1	Total 43	C 33	N 4	O 6	0
31	j8	1	Total 43	C 33	N 4	O 6	0
31	j8	1	Total 43	C 33	N 4	O 6	0
31	k8	1	Total 43	C 33	N 4	O 6	0
31	k8	1	Total 43	C 33	N 4	O 6	0
31	k8	1	Total 43	C 33	N 4	O 6	0
31	l8	1	Total 43	C 33	N 4	O 6	0
31	l8	1	Total 43	C 33	N 4	O 6	0
31	l8	1	Total 43	C 33	N 4	O 6	0
31	m8	1	Total 43	C 33	N 4	O 6	0
31	m8	1	Total 43	C 33	N 4	O 6	0
31	n8	1	Total 43	C 33	N 4	O 6	0
31	n8	1	Total 43	C 33	N 4	O 6	0
31	o8	1	Total 43	C 33	N 4	O 6	0
31	o8	1	Total 43	C 33	N 4	O 6	0
31	o8	1	Total 43	C 33	N 4	O 6	0
31	p8	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	p8	1	43	33	4	6	0
31	q8	1	43	33	4	6	0
31	q8	1	43	33	4	6	0
31	q8	1	43	33	4	6	0
31	r8	1	43	33	4	6	0
31	r8	1	43	33	4	6	0
31	s8	1	43	33	4	6	0
31	s8	1	43	33	4	6	0
31	s8	1	43	33	4	6	0
31	t8	1	43	33	4	6	0
31	t8	1	43	33	4	6	0
31	t8	1	43	33	4	6	0
31	u8	1	43	33	4	6	0
31	u8	1	43	33	4	6	0
31	v8	1	43	33	4	6	0
31	v8	1	43	33	4	6	0
31	w8	1	43	33	4	6	0
31	w8	1	43	33	4	6	0
31	w8	1	43	33	4	6	0
31	x8	1	43	33	4	6	0
31	x8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	x8	1	43	33	4	6	0
31	y8	1	43	33	4	6	0
31	z8	1	43	33	4	6	0
31	A9	1	43	33	4	6	0
31	A9	1	43	33	4	6	0
31	B9	1	43	33	4	6	0
31	B9	1	43	33	4	6	0
31	B9	1	43	33	4	6	0
31	C9	1	43	33	4	6	0
31	C9	1	43	33	4	6	0
31	D9	1	43	33	4	6	0
31	D9	1	43	33	4	6	0
31	D9	1	43	33	4	6	0
31	E9	1	43	33	4	6	0
31	E9	1	43	33	4	6	0
31	F9	1	43	33	4	6	0
31	F9	1	43	33	4	6	0
31	F9	1	43	33	4	6	0
31	G9	1	43	33	4	6	0
31	G9	1	43	33	4	6	0
31	H9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	H9	1	43	33	4	6	0
31	H9	1	43	33	4	6	0
31	I9	1	43	33	4	6	0
31	I9	1	43	33	4	6	0
31	J9	1	43	33	4	6	0
31	J9	1	43	33	4	6	0
31	J9	1	43	33	4	6	0
31	J9	1	43	33	4	6	0
31	K9	1	43	33	4	6	0
31	K9	1	43	33	4	6	0
31	L9	1	43	33	4	6	0
31	L9	1	43	33	4	6	0
31	L9	1	43	33	4	6	0
31	M9	1	43	33	4	6	0
31	M9	1	43	33	4	6	0
31	M9	1	43	33	4	6	0
31	N9	1	43	33	4	6	0
31	N9	1	43	33	4	6	0
31	O9	1	43	33	4	6	0
31	O9	1	43	33	4	6	0
31	O9	1	43	33	4	6	0
31	P9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	P9	1	43	33	4	6	0
31	Q9	1	43	33	4	6	0
31	Q9	1	43	33	4	6	0
31	Q9	1	43	33	4	6	0
31	R9	1	43	33	4	6	0
31	R9	1	43	33	4	6	0
31	S9	1	43	33	4	6	0
31	S9	1	43	33	4	6	0
31	S9	1	43	33	4	6	0
31	T9	1	43	33	4	6	0
31	T9	1	43	33	4	6	0
31	U9	1	43	33	4	6	0
31	U9	1	43	33	4	6	0
31	U9	1	43	33	4	6	0
31	V9	1	43	33	4	6	0
31	V9	1	43	33	4	6	0
31	W9	1	43	33	4	6	0
31	W9	1	43	33	4	6	0
31	W9	1	43	33	4	6	0
31	X9	1	43	33	4	6	0
31	X9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	Y9	1	43	33	4	6	0
31	Y9	1	43	33	4	6	0
31	Y9	1	43	33	4	6	0
31	Z9	1	43	33	4	6	0
31	Z9	1	43	33	4	6	0
31	Z9	1	43	33	4	6	0
31	fA	1	43	33	4	6	0
31	aA	1	43	33	4	6	0
31	aA	1	43	33	4	6	0
31	bA	1	43	33	4	6	0
31	cA	1	43	33	4	6	0
31	cA	1	43	33	4	6	0
31	cA	1	43	33	4	6	0
31	dA	1	43	33	4	6	0
31	dA	1	43	33	4	6	0
31	eA	1	43	33	4	6	0
31	gA	1	43	33	4	6	0
31	gA	1	43	33	4	6	0
31	gA	1	43	33	4	6	0
31	hA	1	43	33	4	6	0
31	iB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	iB	1	43	33	4	6	0
31	iB	1	43	33	4	6	0
31	jB	1	43	33	4	6	0
31	jB	1	43	33	4	6	0
31	kB	1	43	33	4	6	0
31	kB	1	43	33	4	6	0
31	kB	1	43	33	4	6	0
31	lB	1	43	33	4	6	0
31	lB	1	43	33	4	6	0
31	mB	1	43	33	4	6	0
31	mB	1	43	33	4	6	0
31	mB	1	43	33	4	6	0
31	aB	1	43	33	4	6	0
31	aB	1	43	33	4	6	0
31	aB	1	43	33	4	6	0
31	bB	1	43	33	4	6	0
31	bB	1	43	33	4	6	0
31	cB	1	43	33	4	6	0
31	cB	1	43	33	4	6	0
31	cB	1	43	33	4	6	0
31	dB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	dB	1	43	33	4	6	0
31	eB	1	43	33	4	6	0
31	eB	1	43	33	4	6	0
31	eB	1	43	33	4	6	0
31	fB	1	43	33	4	6	0
31	fB	1	43	33	4	6	0
31	gB	1	43	33	4	6	0
31	gB	1	43	33	4	6	0
31	gB	1	43	33	4	6	0
31	hB	1	43	33	4	6	0
31	hB	1	43	33	4	6	0
31	fC	1	43	33	4	6	0
31	fC	1	43	33	4	6	0
31	fC	1	43	33	4	6	0
31	gC	1	43	33	4	6	0
31	gC	1	43	33	4	6	0
31	gC	1	43	33	4	6	0
31	hC	1	43	33	4	6	0
31	hC	1	43	33	4	6	0
31	iC	1	43	33	4	6	0
31	iC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	jC	1	43	33	4	6	0
31	jC	1	43	33	4	6	0
31	jC	1	43	33	4	6	0
31	kC	1	43	33	4	6	0
31	kC	1	43	33	4	6	0
31	kC	1	43	33	4	6	0
31	lC	1	43	33	4	6	0
31	lC	1	43	33	4	6	0
31	mC	1	43	33	4	6	0
31	mC	1	43	33	4	6	0
31	aC	1	43	33	4	6	0
31	aC	1	43	33	4	6	0
31	bC	1	43	33	4	6	0
31	bC	1	43	33	4	6	0
31	cC	1	43	33	4	6	0
31	cC	1	43	33	4	6	0
31	dC	1	43	33	4	6	0
31	dC	1	43	33	4	6	0
31	dC	1	43	33	4	6	0
31	eC	1	43	33	4	6	0
31	eC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	eC	1	43	33	4	6	0
31	aD	1	43	33	4	6	0
31	aD	1	43	33	4	6	0
31	bD	1	43	33	4	6	0
31	bD	1	43	33	4	6	0
31	cD	1	43	33	4	6	0
31	cD	1	43	33	4	6	0
31	dD	1	43	33	4	6	0
31	dD	1	43	33	4	6	0
31	dD	1	43	33	4	6	0
31	dD	1	43	33	4	6	0
31	eD	1	43	33	4	6	0
31	eD	1	43	33	4	6	0
31	eD	1	43	33	4	6	0
31	fD	1	43	33	4	6	0
31	fD	1	43	33	4	6	0
31	fD	1	43	33	4	6	0
31	gD	1	43	33	4	6	0
31	gD	1	43	33	4	6	0
31	hD	1	43	33	4	6	0
31	hD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	hD	1	43	33	4	6	0
31	iD	1	43	33	4	6	0
31	iD	1	43	33	4	6	0
31	jD	1	43	33	4	6	0
31	jD	1	43	33	4	6	0
31	kD	1	43	33	4	6	0
31	kD	1	43	33	4	6	0
31	lD	1	43	33	4	6	0
31	lD	1	43	33	4	6	0
31	lD	1	43	33	4	6	0
31	mD	1	43	33	4	6	0
31	mD	1	43	33	4	6	0
31	mD	1	43	33	4	6	0
31	aE	1	43	33	4	6	0
31	aE	1	43	33	4	6	0
31	bE	1	43	33	4	6	0
31	cE	1	43	33	4	6	0
31	cE	1	43	33	4	6	0
31	dE	1	43	33	4	6	0
31	dE	1	43	33	4	6	0
31	dE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	dE	1	43	33	4	6	0
31	eE	1	43	33	4	6	0
31	eE	1	43	33	4	6	0
31	fE	1	43	33	4	6	0
31	fE	1	43	33	4	6	0
31	fE	1	43	33	4	6	0
31	gE	1	43	33	4	6	0
31	gE	1	43	33	4	6	0
31	hE	1	43	33	4	6	0
31	hE	1	43	33	4	6	0
31	hE	1	43	33	4	6	0
31	iE	1	43	33	4	6	0
31	iE	1	43	33	4	6	0
31	jE	1	43	33	4	6	0
31	jE	1	43	33	4	6	0
31	kE	1	43	33	4	6	0
31	kE	1	43	33	4	6	0
31	lE	1	43	33	4	6	0
31	lE	1	43	33	4	6	0
31	lE	1	43	33	4	6	0
31	mE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	mE	1	43	33	4	6	0
31	mE	1	43	33	4	6	0
31	aF	1	43	33	4	6	0
31	aF	1	43	33	4	6	0
31	aF	1	43	33	4	6	0
31	bF	1	43	33	4	6	0
31	bF	1	43	33	4	6	0
31	cF	1	43	33	4	6	0
31	cF	1	43	33	4	6	0
31	cF	1	43	33	4	6	0
31	dF	1	43	33	4	6	0
31	dF	1	43	33	4	6	0
31	eF	1	43	33	4	6	0
31	eF	1	43	33	4	6	0
31	eF	1	43	33	4	6	0
31	fF	1	43	33	4	6	0
31	fF	1	43	33	4	6	0
31	gF	1	43	33	4	6	0
31	gF	1	43	33	4	6	0
31	gF	1	43	33	4	6	0
31	hF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	hF	1	43	33	4	6	0
31	iF	1	43	33	4	6	0
31	iF	1	43	33	4	6	0
31	iF	1	43	33	4	6	0
31	jF	1	43	33	4	6	0
31	jF	1	43	33	4	6	0
31	kF	1	43	33	4	6	0
31	kF	1	43	33	4	6	0
31	kF	1	43	33	4	6	0
31	lF	1	43	33	4	6	0
31	lF	1	43	33	4	6	0
31	lF	1	43	33	4	6	0
31	mF	1	43	33	4	6	0
31	mF	1	43	33	4	6	0
31	nF	1	43	33	4	6	0
31	nF	1	43	33	4	6	0
31	oF	1	43	33	4	6	0
31	oF	1	43	33	4	6	0
31	oF	1	43	33	4	6	0
31	pF	1	43	33	4	6	0
31	pF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	qF	1	43	33	4	6	0
31	qF	1	43	33	4	6	0
31	qF	1	43	33	4	6	0
31	rF	1	43	33	4	6	0
31	rF	1	43	33	4	6	0
31	sF	1	43	33	4	6	0
31	sF	1	43	33	4	6	0
31	sF	1	43	33	4	6	0
31	tF	1	43	33	4	6	0
31	tF	1	43	33	4	6	0
31	uF	1	43	33	4	6	0
31	uF	1	43	33	4	6	0
31	uF	1	43	33	4	6	0
31	vF	1	43	33	4	6	0
31	vF	1	43	33	4	6	0
31	wF	1	43	33	4	6	0
31	wF	1	43	33	4	6	0
31	wF	1	43	33	4	6	0
31	xF	1	43	33	4	6	0
31	xF	1	43	33	4	6	0
31	xF	1	43	33	4	6	0

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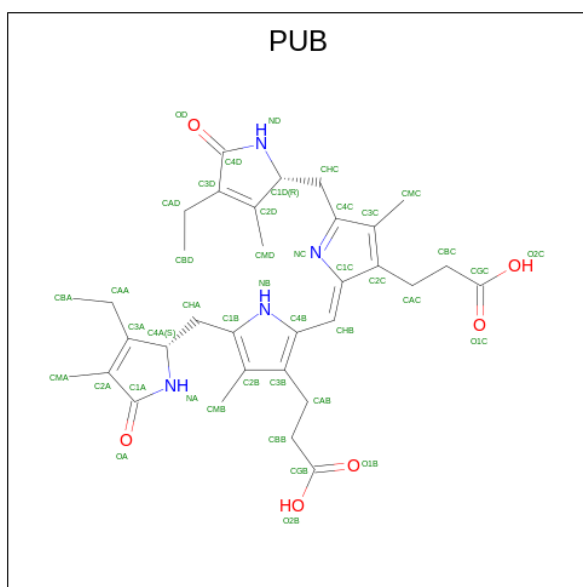
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	yF	1	43	33	4	6	0
31	zF	1	43	33	4	6	0
31	aH	1	43	33	4	6	0
31	aH	1	43	33	4	6	0
31	aH	1	43	33	4	6	0
31	aH	1	43	33	4	6	0
31	cH	1	43	33	4	6	0
31	cH	1	43	33	4	6	0
31	dH	1	43	33	4	6	0
31	dH	1	43	33	4	6	0
31	eH	1	43	33	4	6	0
31	eH	1	43	33	4	6	0
31	fH	1	43	33	4	6	0
31	fH	1	43	33	4	6	0
31	fH	1	43	33	4	6	0
31	gH	1	43	33	4	6	0
31	gH	1	43	33	4	6	0
31	hH	1	43	33	4	6	0
31	hH	1	43	33	4	6	0
31	hH	1	43	33	4	6	0
31	iH	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	iH	1	Total 43	C 33	N 4	O 6	0
31	jH	1	Total 43	C 33	N 4	O 6	0
31	jH	1	Total 43	C 33	N 4	O 6	0
31	jH	1	Total 43	C 33	N 4	O 6	0
31	kH	1	Total 43	C 33	N 4	O 6	0
31	kH	1	Total 43	C 33	N 4	O 6	0
31	lH	1	Total 43	C 33	N 4	O 6	0
31	lH	1	Total 43	C 33	N 4	O 6	0
31	lH	1	Total 43	C 33	N 4	O 6	0
31	mH	1	Total 43	C 33	N 4	O 6	0
31	mH	1	Total 43	C 33	N 4	O 6	0
31	dJ	1	Total 43	C 33	N 4	O 6	0
31	eK	1	Total 43	C 33	N 4	O 6	0

- Molecule 32 is PHYCOUROBILIN (three-letter code: PUB) (formula: $C_{33}H_{42}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
32	AB	1	43	33	4	6	0
32	AB	1	43	33	4	6	0
32	AC	1	43	33	4	6	0
32	AC	1	43	33	4	6	0
32	AD	1	43	33	4	6	0
32	AD	1	43	33	4	6	0
32	AE	1	43	33	4	6	0
32	AE	1	43	33	4	6	0
32	AH	1	43	33	4	6	0
32	AH	1	43	33	4	6	0
32	BH	1	43	33	4	6	0
32	QH	1	43	33	4	6	0
32	CI	1	43	33	4	6	0
32	MI	1	43	33	4	6	0

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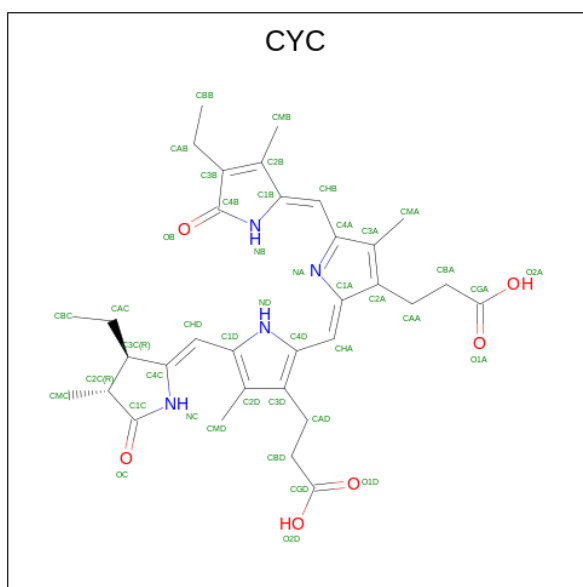
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
32	ZI	1	43	33	4	6	0
32	ZI	1	43	33	4	6	0
32	AJ	1	43	33	4	6	0
32	NJ	1	43	33	4	6	0
32	KK	1	43	33	4	6	0
32	YK	1	43	33	4	6	0
32	K1	1	43	33	4	6	0
32	Y1	1	43	33	4	6	0
32	A2	1	43	33	4	6	0
32	A2	1	43	33	4	6	0
32	A4	1	43	33	4	6	0
32	A4	1	43	33	4	6	0
32	B4	1	43	33	4	6	0
32	Q4	1	43	33	4	6	0
32	N5	1	43	33	4	6	0
32	A5	1	43	33	4	6	0
32	A6	1	43	33	4	6	0
32	A6	1	43	33	4	6	0
32	w8	1	43	33	4	6	0
32	x8	1	43	33	4	6	0
32	x8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
32	x8	1	Total 43	C 33	N 4	O 6	0
32	y8	1	Total 43	C 33	N 4	O 6	0
32	y8	1	Total 43	C 33	N 4	O 6	0
32	M9	1	Total 43	C 33	N 4	O 6	0
32	M9	1	Total 43	C 33	N 4	O 6	0
32	Z9	1	Total 43	C 33	N 4	O 6	0
32	Z9	1	Total 43	C 33	N 4	O 6	0
32	wF	1	Total 43	C 33	N 4	O 6	0
32	xF	1	Total 43	C 33	N 4	O 6	0
32	xF	1	Total 43	C 33	N 4	O 6	0
32	xF	1	Total 43	C 33	N 4	O 6	0
32	yF	1	Total 43	C 33	N 4	O 6	0
32	yF	1	Total 43	C 33	N 4	O 6	0

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



Mol	Chain	Residues	Atoms				AltConf	
			Total	C	N	O		
33	CB	1	Total	43	33	4	6	0
33	DB	1	Total	43	33	4	6	0
33	EB	1	Total	43	33	4	6	0
33	FB	1	Total	43	33	4	6	0
33	GB	1	Total	43	33	4	6	0
33	HB	1	Total	43	33	4	6	0
33	IB	1	Total	43	33	4	6	0
33	JB	1	Total	43	33	4	6	0
33	KB	1	Total	43	33	4	6	0
33	LB	1	Total	43	33	4	6	0
33	MB	1	Total	43	33	4	6	0
33	NB	1	Total	43	33	4	6	0
33	CC	1	Total	43	33	4	6	0
33	DC	1	Total	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	DC	1	43	33	4	6	0
33	EC	1	43	33	4	6	0
33	FC	1	43	33	4	6	0
33	HC	1	43	33	4	6	0
33	JC	1	43	33	4	6	0
33	JC	1	43	33	4	6	0
33	KC	1	43	33	4	6	0
33	LC	1	43	33	4	6	0
33	LC	1	43	33	4	6	0
33	NC	1	43	33	4	6	0
33	BD	1	43	33	4	6	0
33	BD	1	43	33	4	6	0
33	DD	1	43	33	4	6	0
33	ED	1	43	33	4	6	0
33	FD	1	43	33	4	6	0
33	FD	1	43	33	4	6	0
33	GD	1	43	33	4	6	0
33	HD	1	43	33	4	6	0
33	ID	1	43	33	4	6	0
33	KD	1	43	33	4	6	0
33	LD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	MD	1	43	33	4	6	0
33	BE	1	43	33	4	6	0
33	BE	1	43	33	4	6	0
33	CE	1	43	33	4	6	0
33	DE	1	43	33	4	6	0
33	EE	1	43	33	4	6	0
33	FE	1	43	33	4	6	0
33	GE	1	43	33	4	6	0
33	HE	1	43	33	4	6	0
33	IE	1	43	33	4	6	0
33	KE	1	43	33	4	6	0
33	LE	1	43	33	4	6	0
33	ME	1	43	33	4	6	0
33	L2	1	43	33	4	6	0
33	M2	1	43	33	4	6	0
33	N2	1	43	33	4	6	0
33	C2	1	43	33	4	6	0
33	D2	1	43	33	4	6	0
33	D2	1	43	33	4	6	0
33	E2	1	43	33	4	6	0
33	F2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
33	H2	1	43	33	4	6	0
33	I2	1	43	33	4	6	0
33	J2	1	43	33	4	6	0
33	K2	1	43	33	4	6	0
33	A3	1	81	33	38	4	6
33	B3	1	81	33	38	4	6
33	C3	1	81	33	38	4	6
33	D3	1	81	33	38	4	6
33	E3	1	81	33	38	4	6
33	F3	1	81	33	38	4	6
33	G3	1	81	33	38	4	6
33	H3	1	81	33	38	4	6
33	I3	1	81	33	38	4	6
33	J3	1	81	33	38	4	6
33	K3	1	81	33	38	4	6
33	L3	1	81	33	38	4	6
33	M3	1	81	33	38	4	6
33	N3	1	81	33	38	4	6
33	O3	1	81	33	38	4	6
33	P3	1	81	33	38	4	6
33	Q3	1	81	33	38	4	6

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
33	R3	1	81	33	38	4	6	0
33	S3	1	81	33	38	4	6	0
33	T3	1	81	33	38	4	6	0
33	U3	1	81	33	38	4	6	0
33	V3	1	81	33	38	4	6	0
33	W3	1	81	33	38	4	6	0
33	c3	1	81	33	38	4	6	0
33	d3	1	81	33	38	4	6	0
33	e3	1	81	33	38	4	6	0
33	f3	1	81	33	38	4	6	0
33	g3	1	81	33	38	4	6	0
33	h3	1	81	33	38	4	6	0
33	i3	1	81	33	38	4	6	0
33	j3	1	81	33	38	4	6	0
33	k3	1	81	33	38	4	6	0
33	l3	1	81	33	38	4	6	0
33	m3	1	81	33	38	4	6	0
33	n3	1	81	33	38	4	6	0
33	o3	1	81	33	38	4	6	0
33	p3	1	81	33	38	4	6	0
33	q3	1	81	33	38	4	6	0

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Mol	Chain	Residues	Atoms					AltConf
			Total	C	H	N	O	
33	r3	1	Total 81	C 33	H 38	N 4	O 6	0
33	t3	1	Total 81	C 33	H 38	N 4	O 6	0
33	u3	1	Total 81	C 33	H 38	N 4	O 6	0
33	v3	1	Total 81	C 33	H 38	N 4	O 6	0
33	w3	1	Total 81	C 33	H 38	N 4	O 6	0
33	x3	1	Total 81	C 33	H 38	N 4	O 6	0
33	y3	1	Total 81	C 33	H 38	N 4	O 6	0
33	63	1	Total 81	C 33	H 38	N 4	O 6	0
33	73	1	Total 81	C 33	H 38	N 4	O 6	0
33	73	1	Total 81	C 33	H 38	N 4	O 6	0
33	F6	1	Total 43	C 33	N 4	O 6		0
33	G6	1	Total 43	C 33	N 4	O 6		0
33	H6	1	Total 43	C 33	N 4	O 6		0
33	I6	1	Total 43	C 33	N 4	O 6		0
33	J6	1	Total 43	C 33	N 4	O 6		0
33	K6	1	Total 43	C 33	N 4	O 6		0
33	L6	1	Total 43	C 33	N 4	O 6		0
33	M6	1	Total 43	C 33	N 4	O 6		0
33	N6	1	Total 43	C 33	N 4	O 6		0
33	C6	1	Total 43	C 33	N 4	O 6		0
33	D6	1	Total 43	C 33	N 4	O 6		0

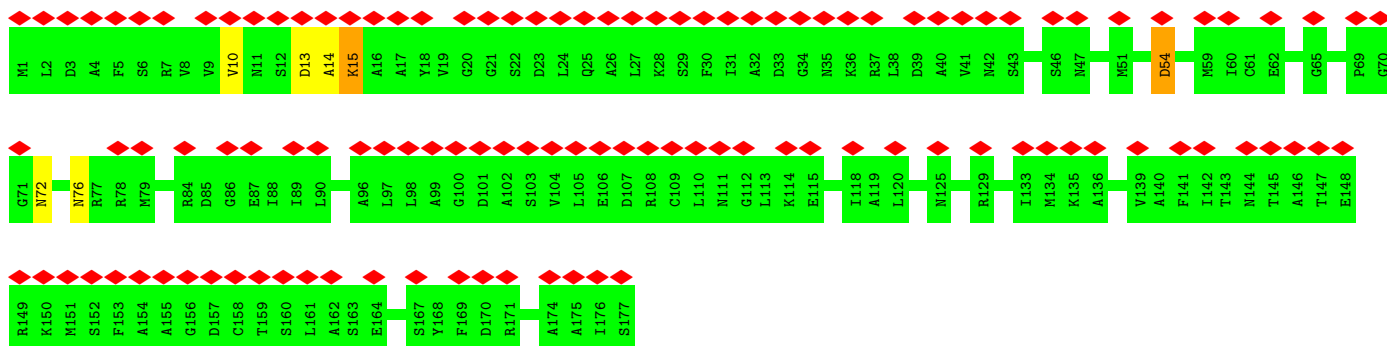
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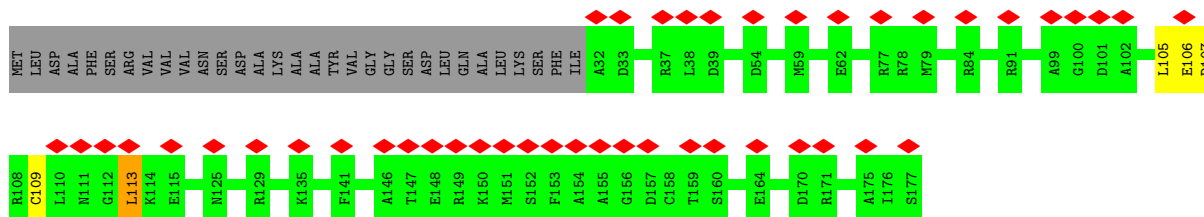
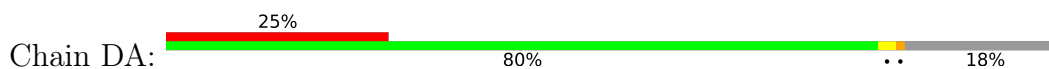
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			Total	C	N	O	
33	E6	1	43	33	4	6	0



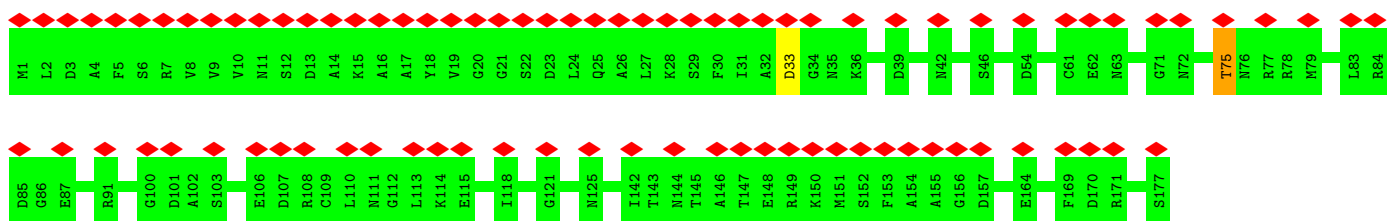
- Molecule 2: B-phycoerythrin beta chain



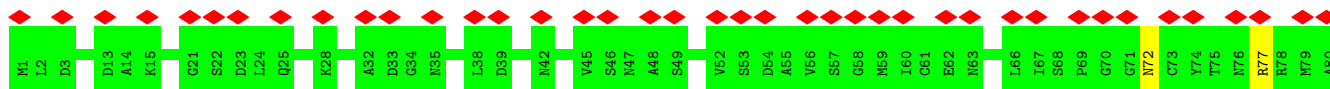
- Molecule 2: B-phycoerythrin beta chain

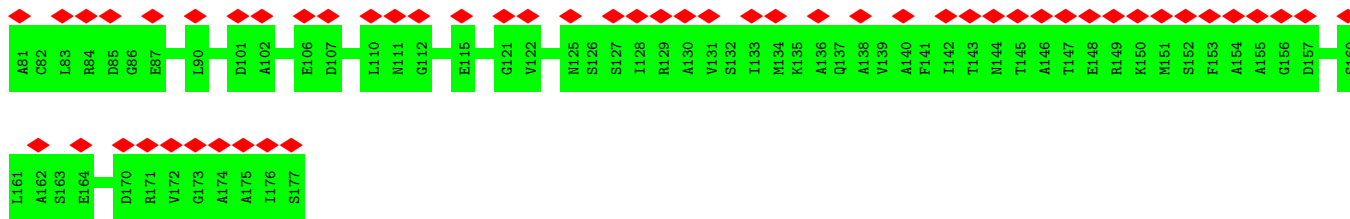


- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

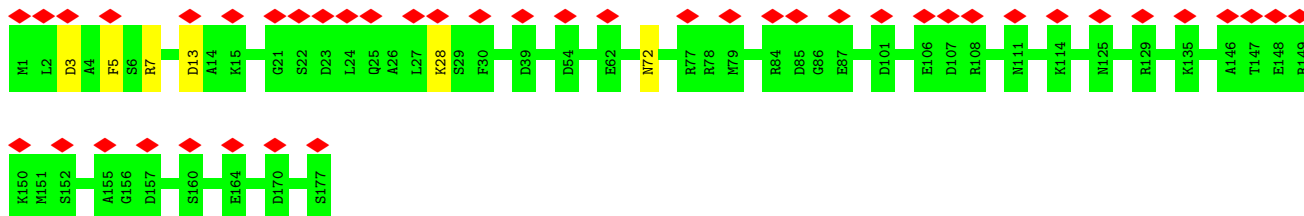




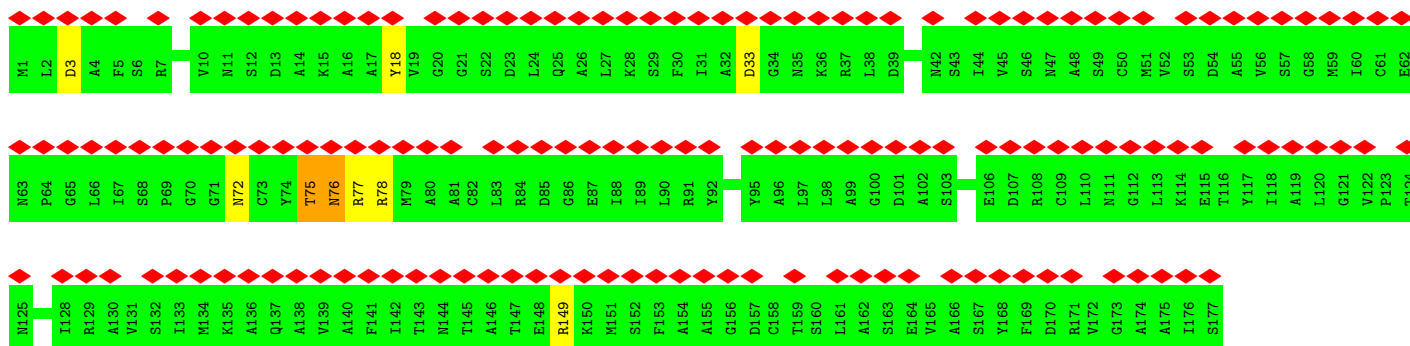
• Molecule 2: B-phycoerythrin beta chain



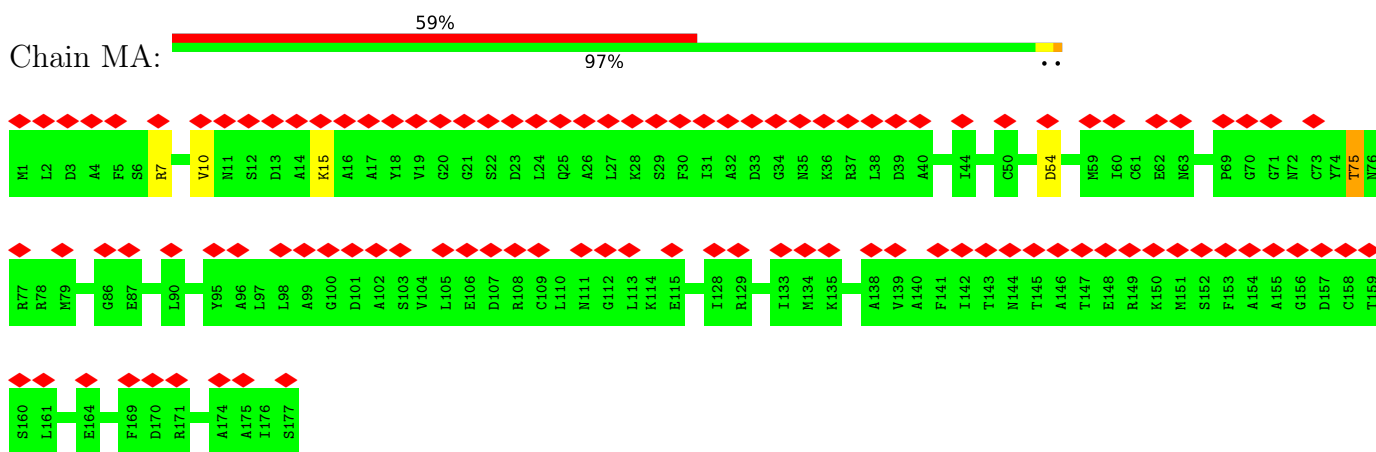
• Molecule 2: B-phycoerythrin beta chain



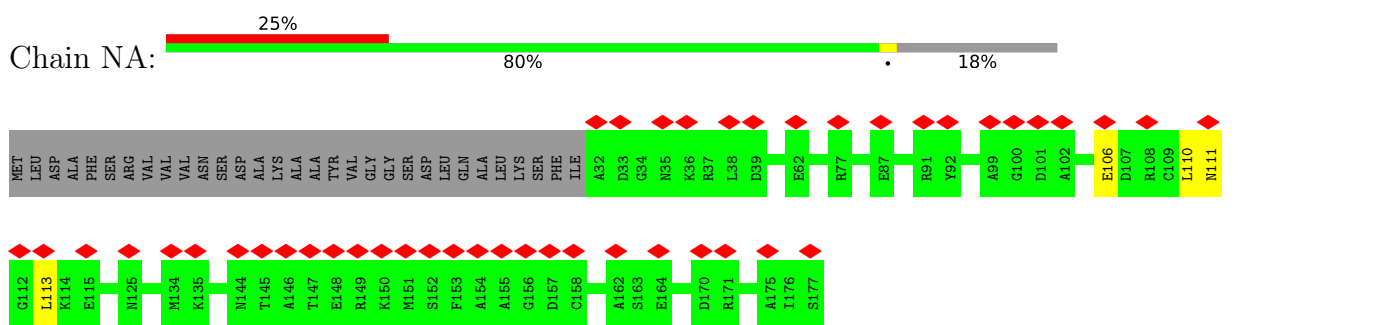
• Molecule 2: B-phycoerythrin beta chain



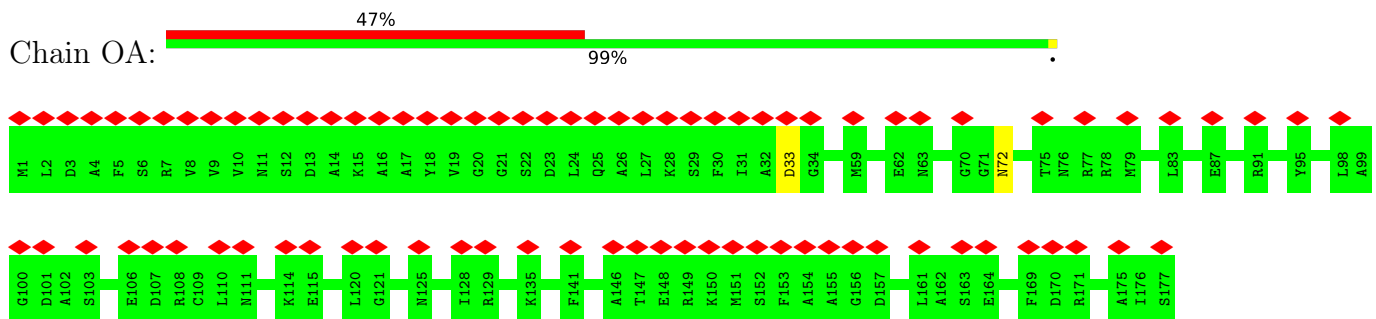
• Molecule 2: B-phycoerythrin beta chain



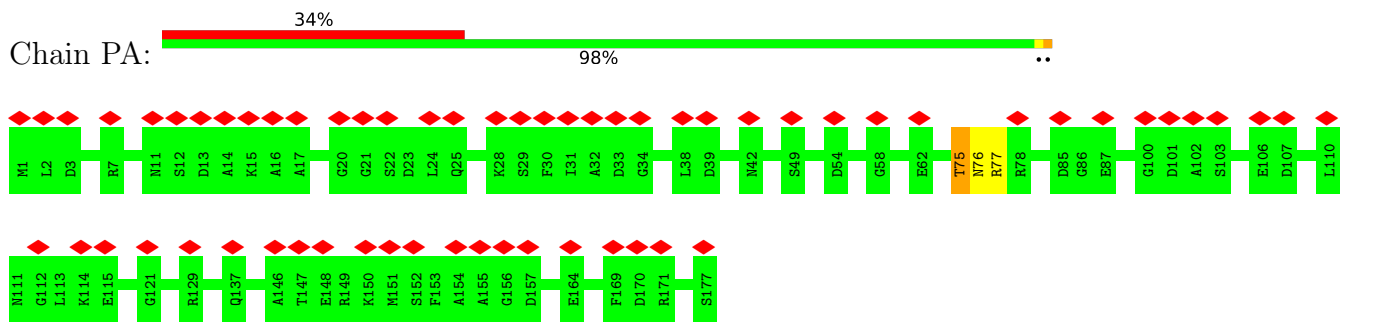
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

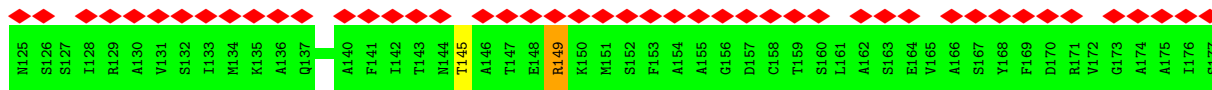


- Molecule 2: B-phycoerythrin beta chain

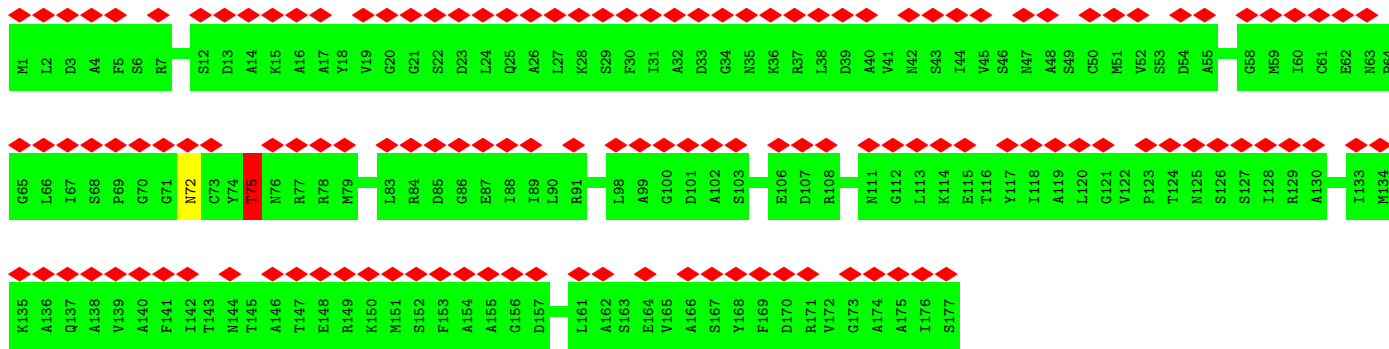
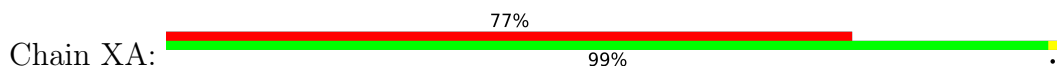


- Molecule 2: B-phycoerythrin beta chain

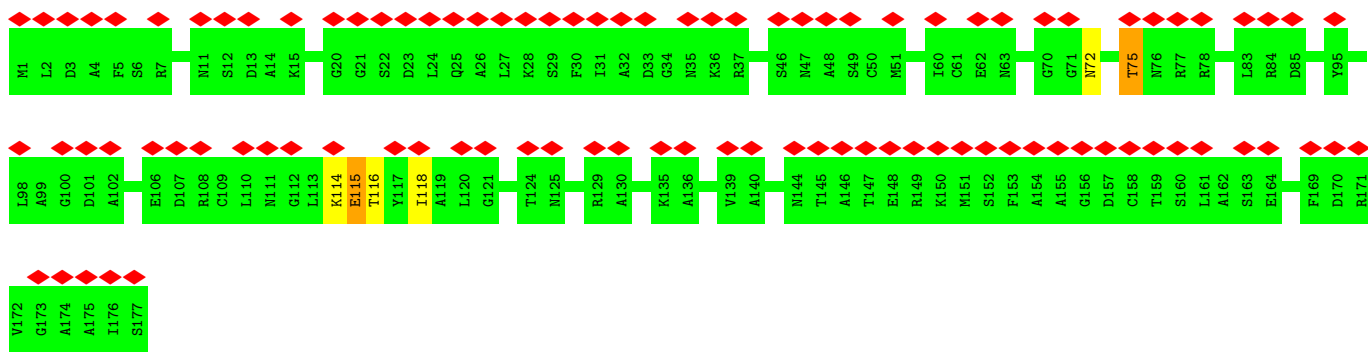




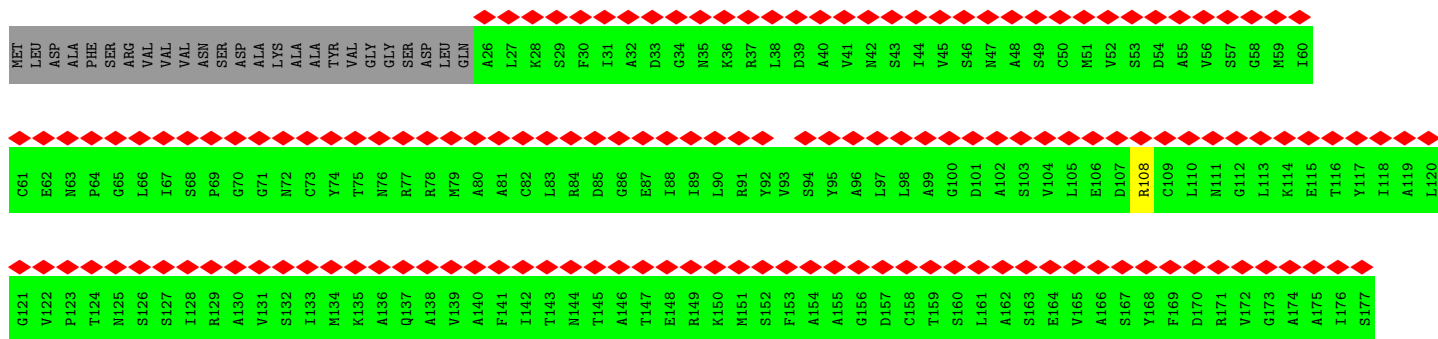
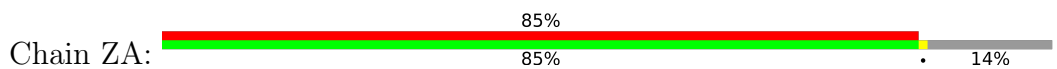
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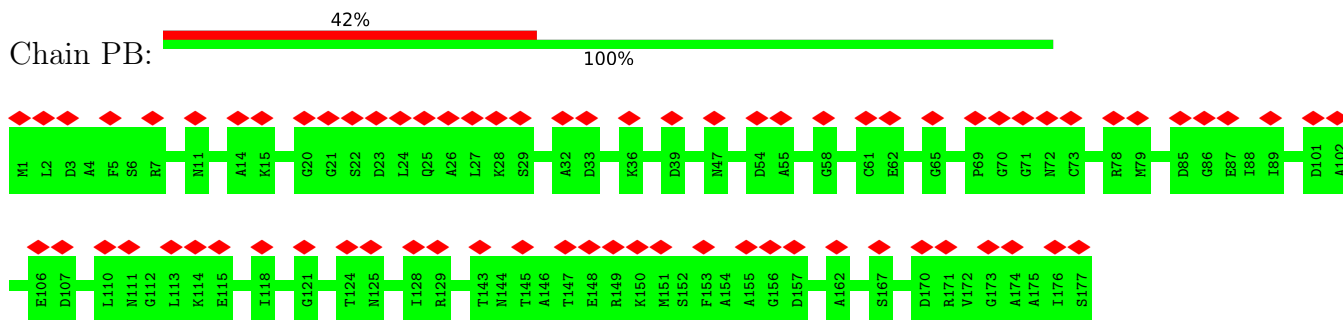
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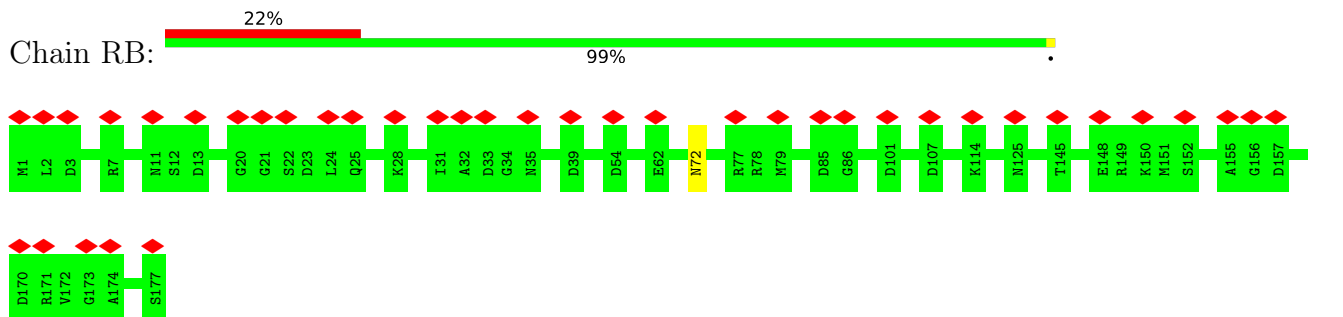
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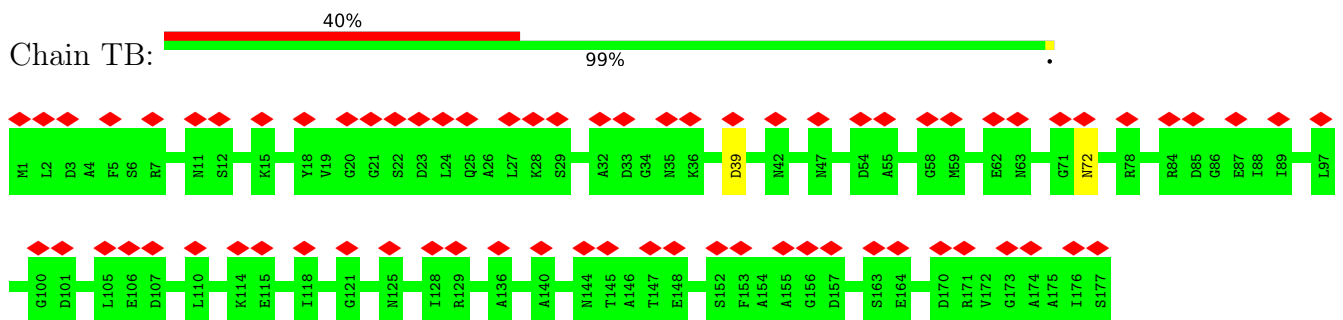
• Molecule 2: B-phycoerythrin beta chain



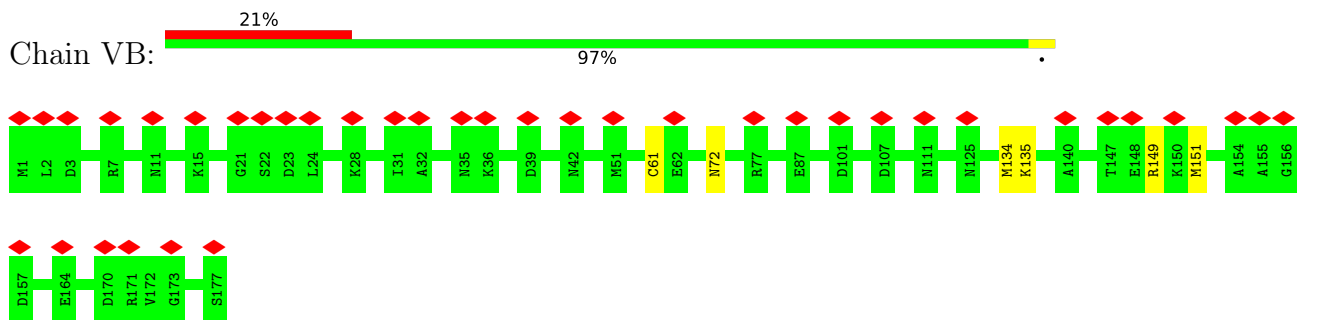
• Molecule 2: B-phycoerythrin beta chain



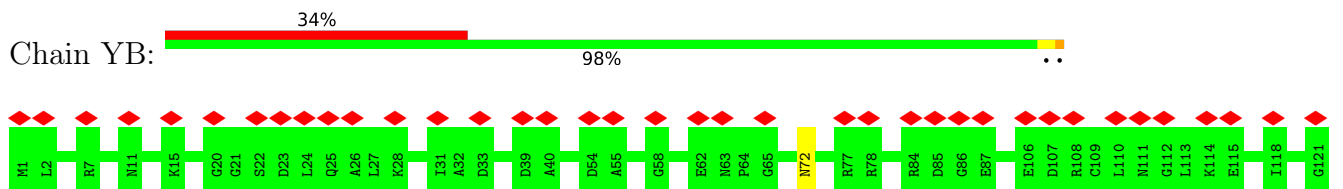
• Molecule 2: B-phycoerythrin beta chain

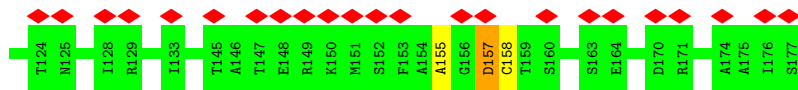


• Molecule 2: B-phycoerythrin beta chain

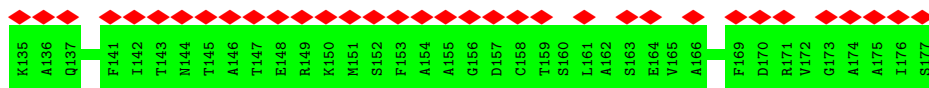
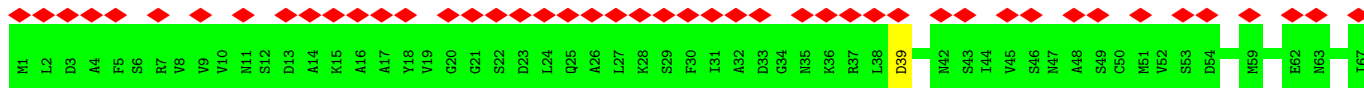
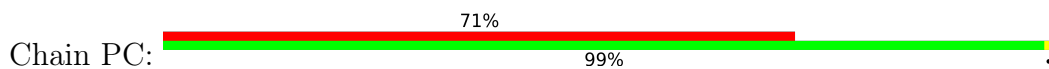


• Molecule 2: B-phycoerythrin beta chain

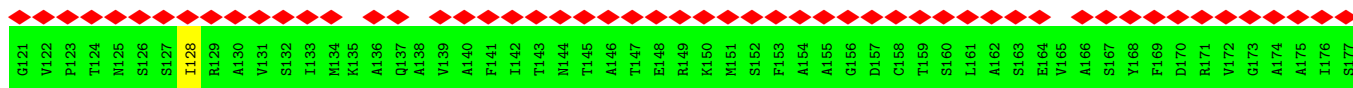
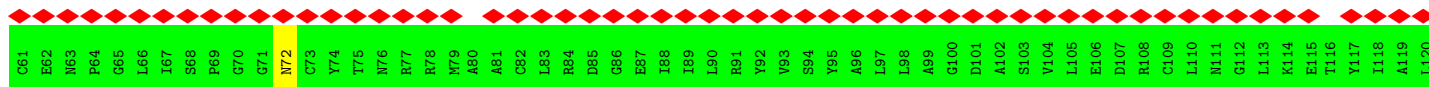
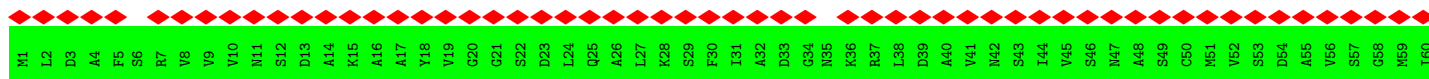




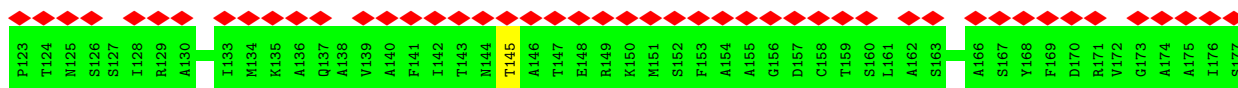
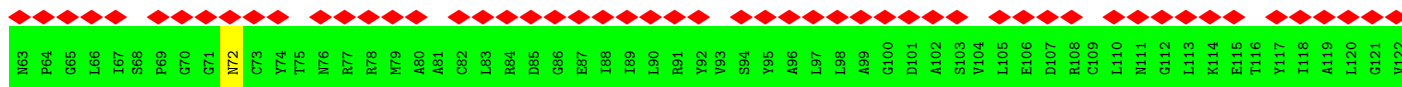
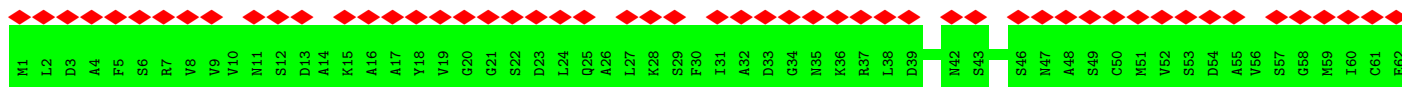
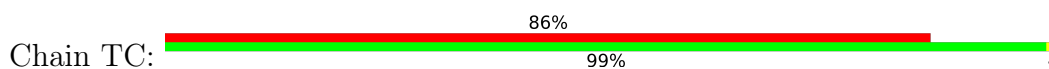
• Molecule 2: B-phycoerythrin beta chain



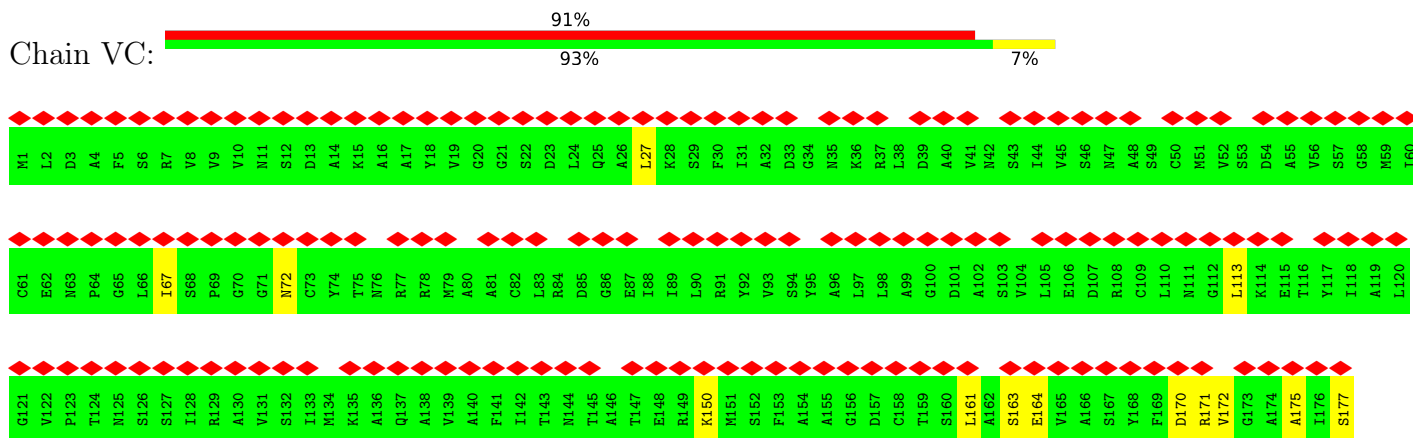
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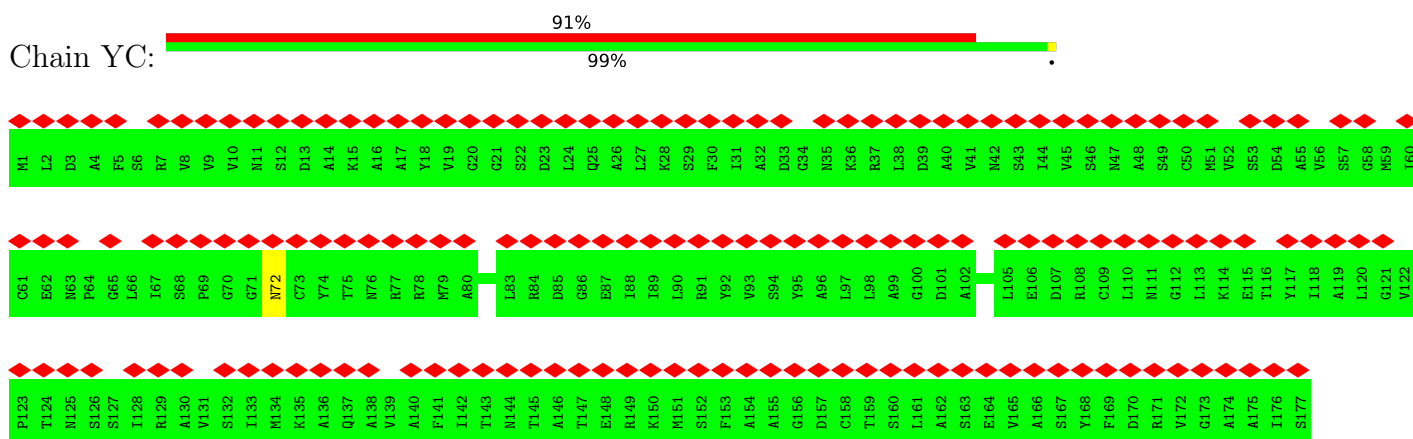
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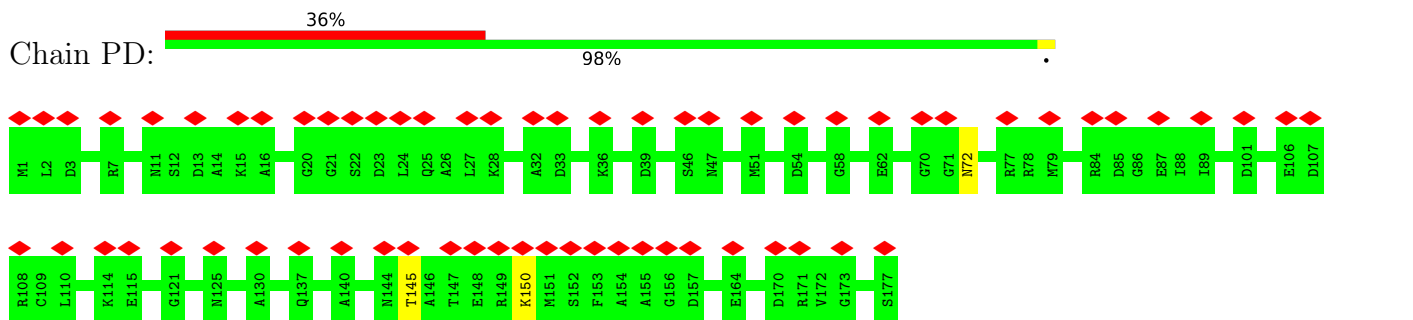
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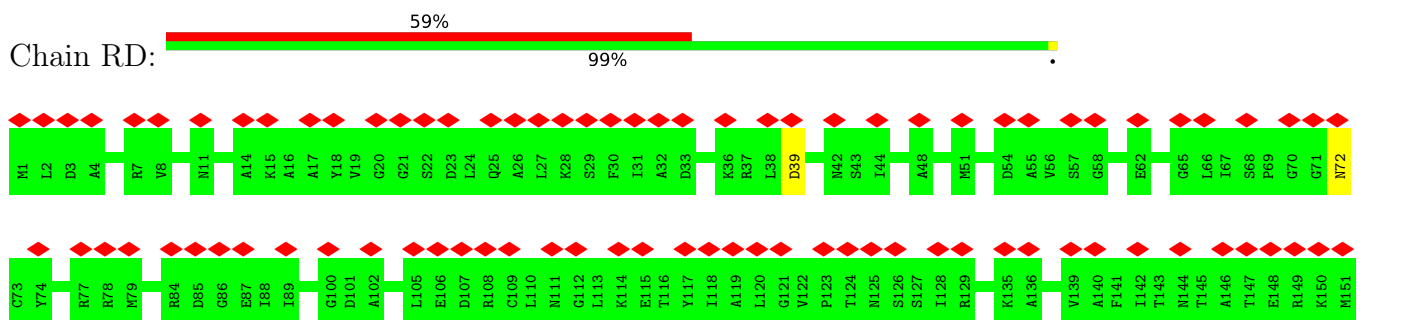
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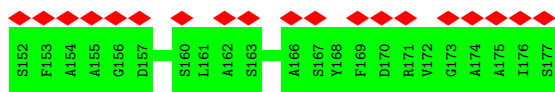


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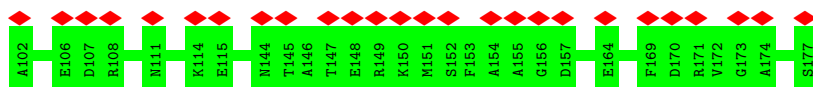
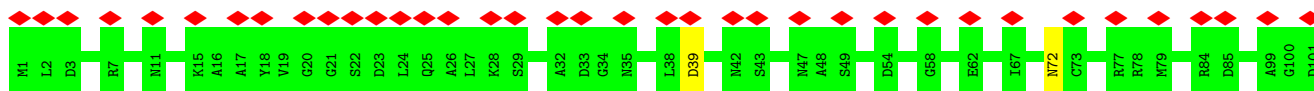


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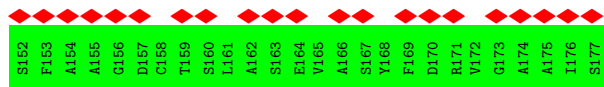
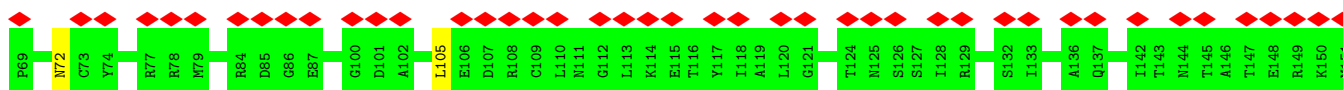
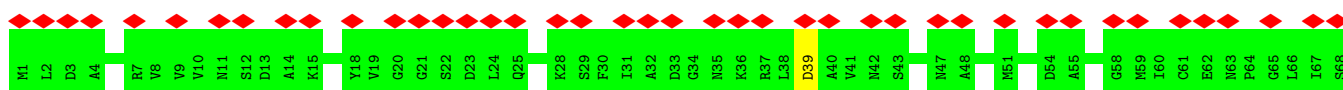




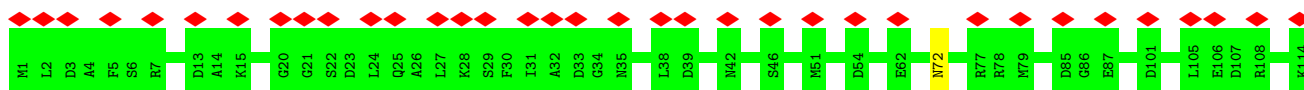
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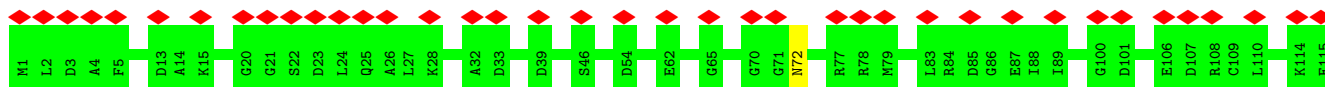
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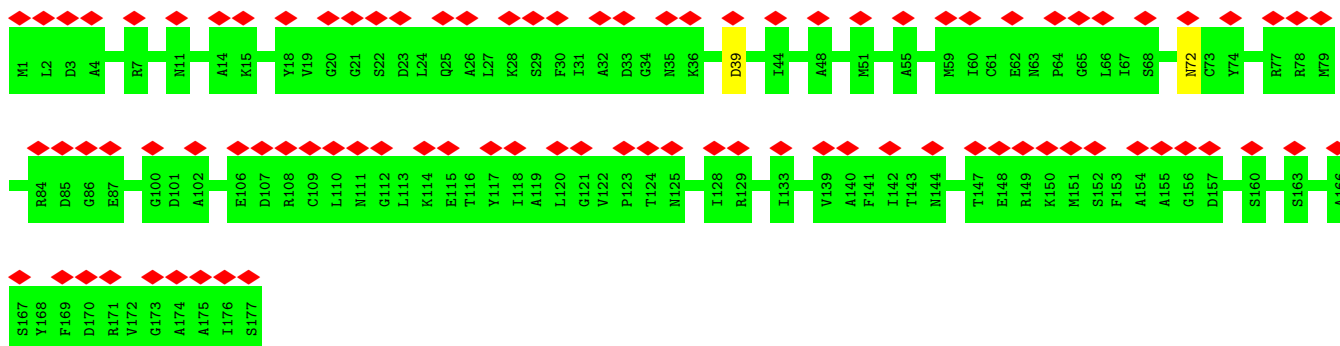


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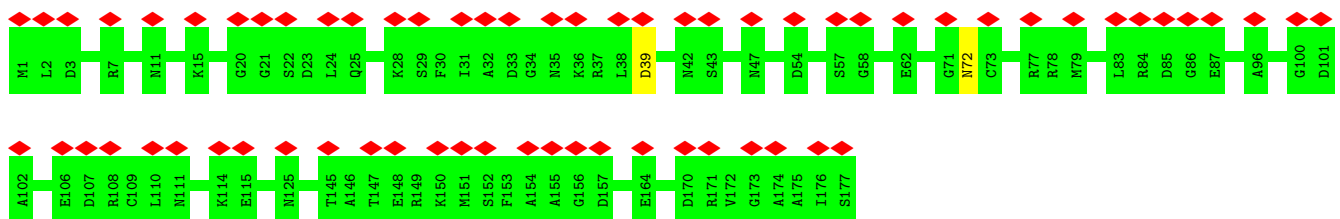
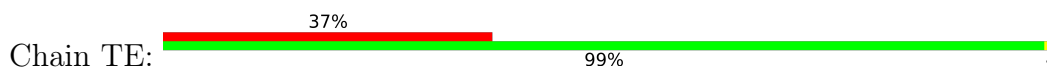




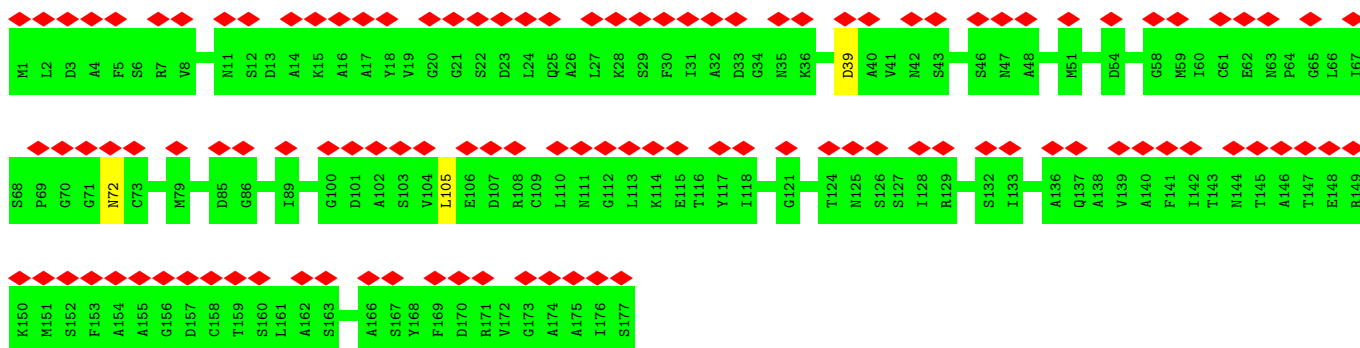
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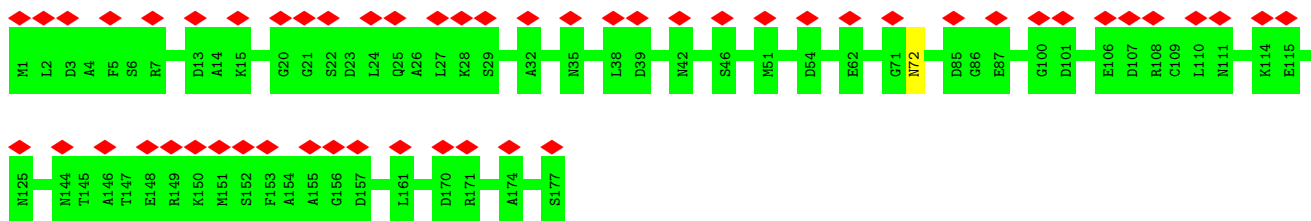


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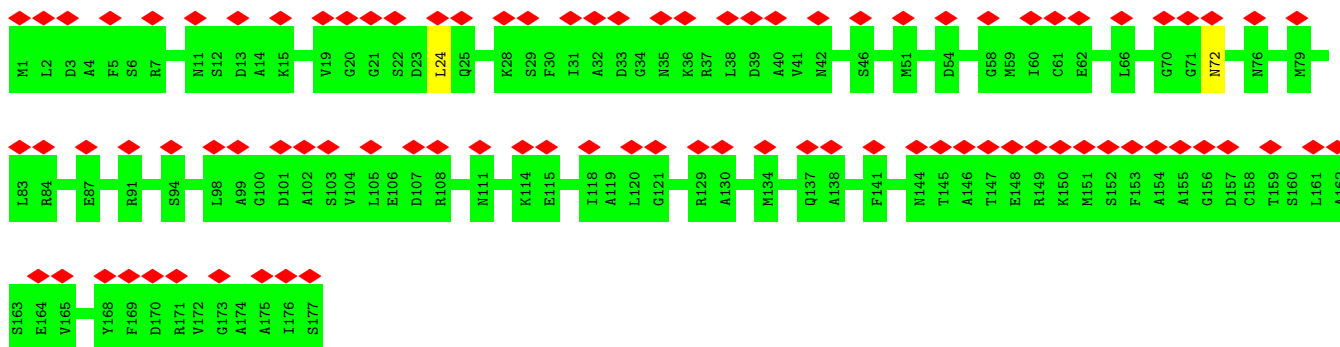


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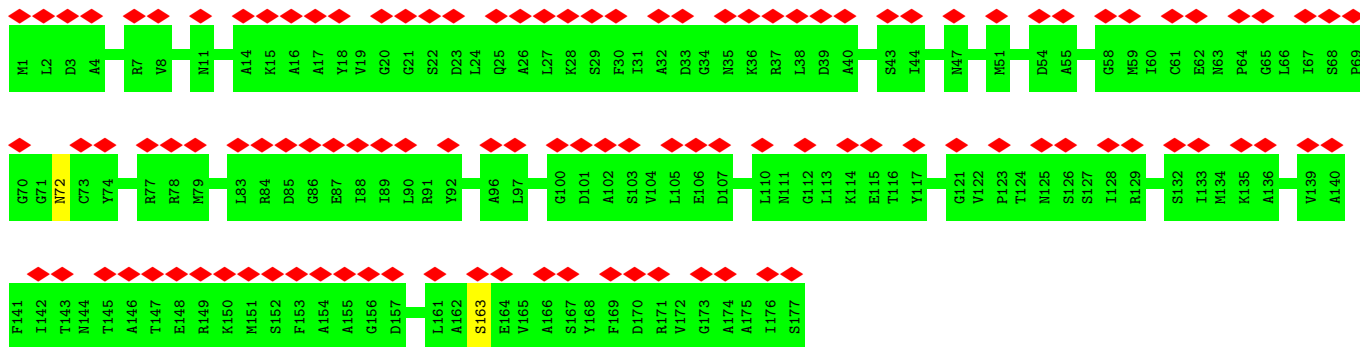




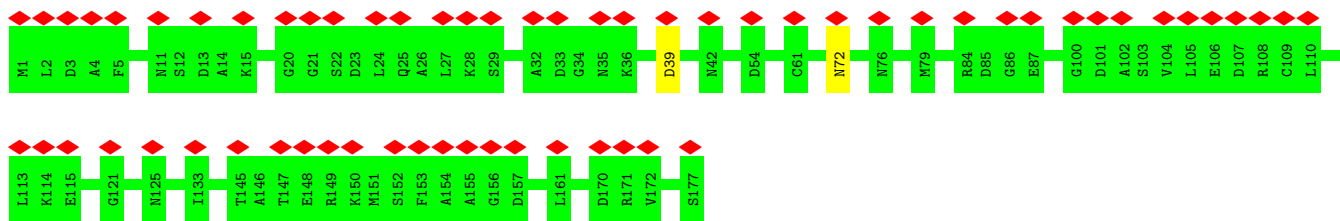
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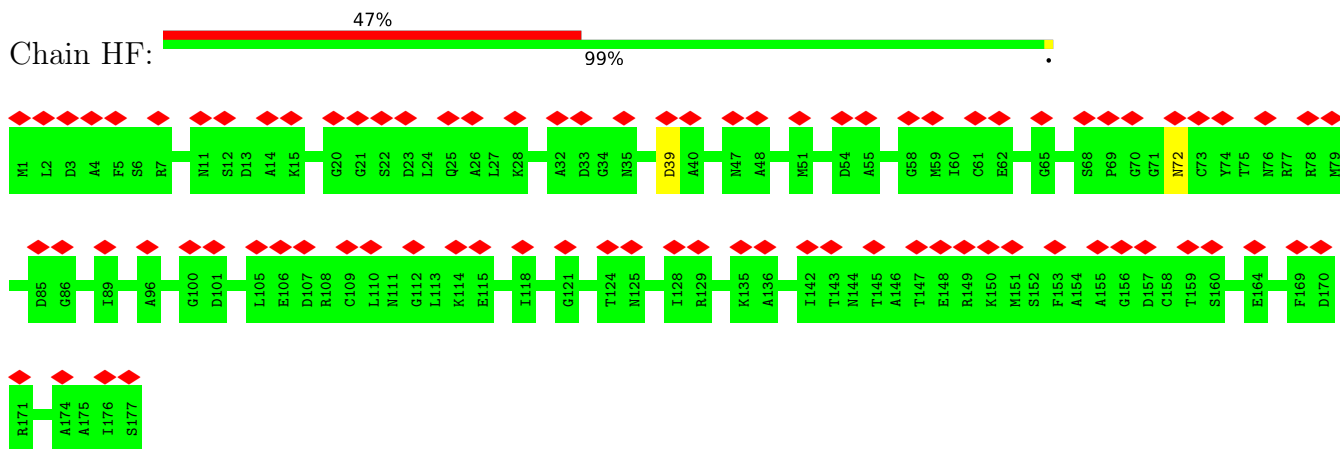
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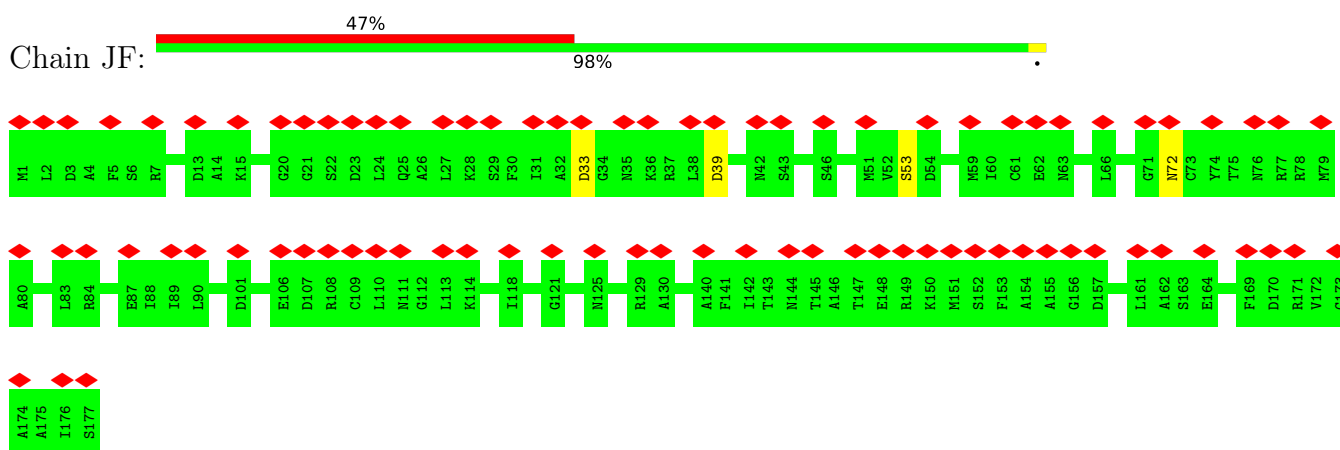
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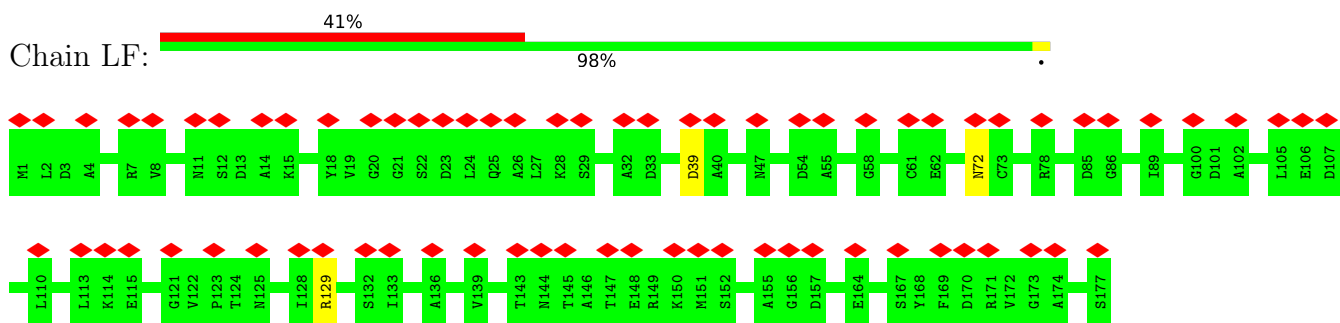
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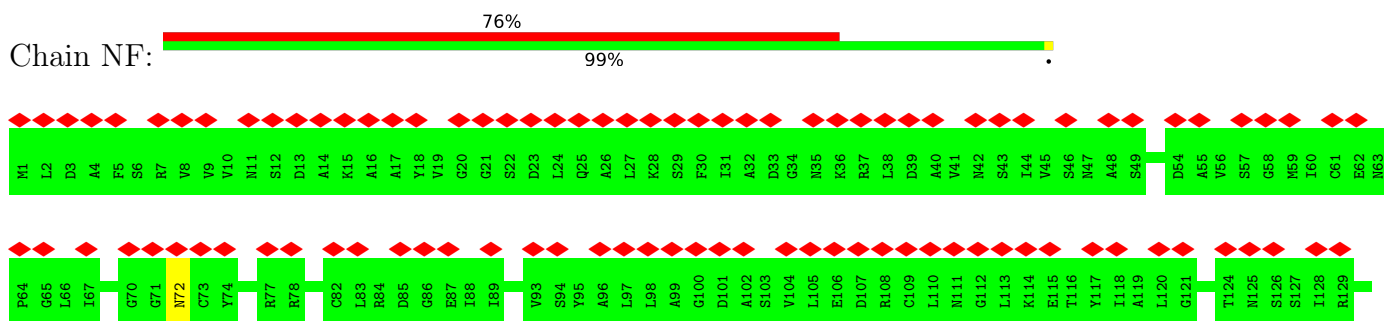
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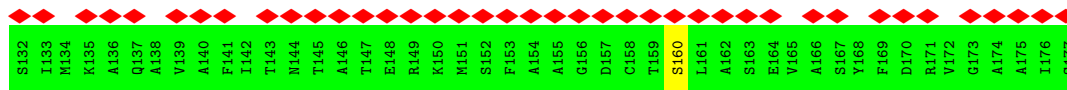


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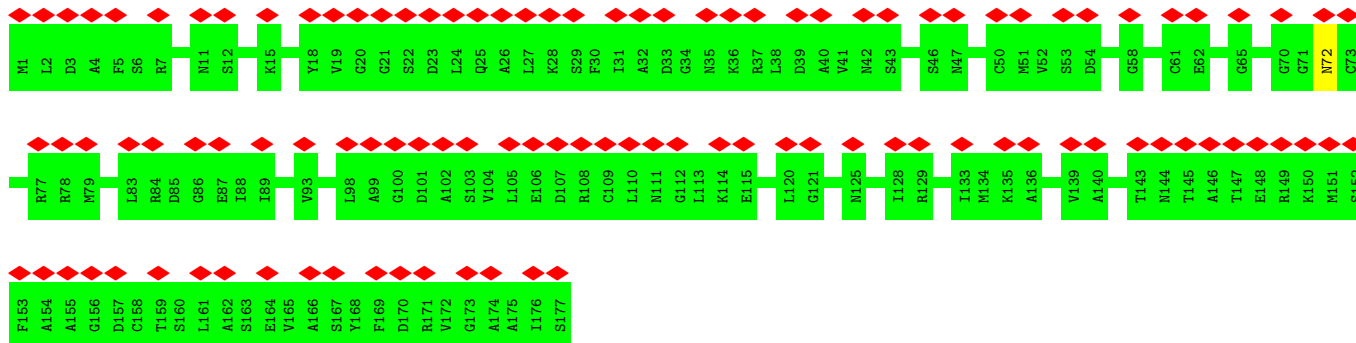


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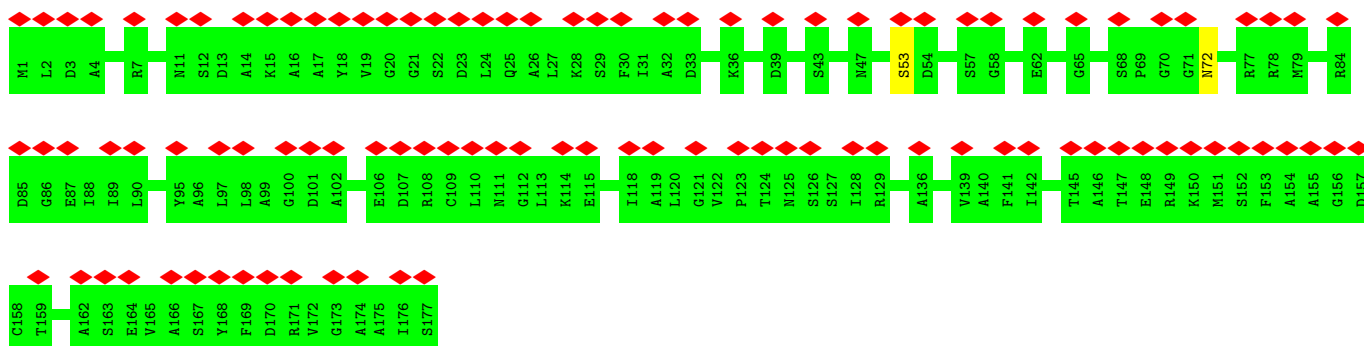




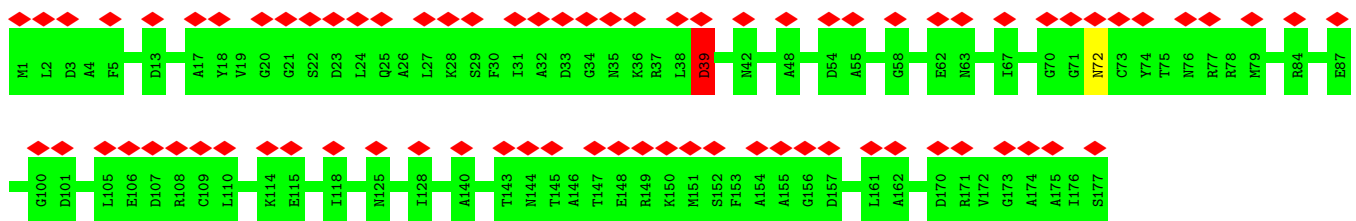
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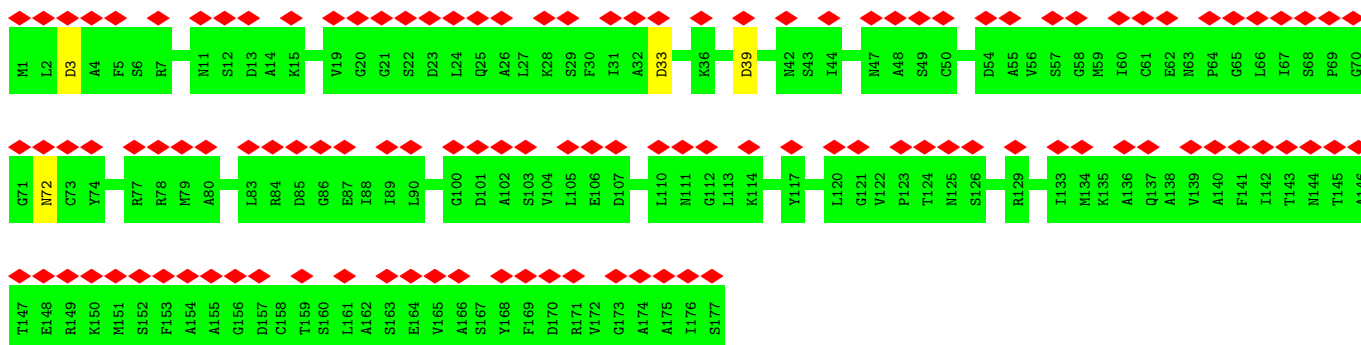


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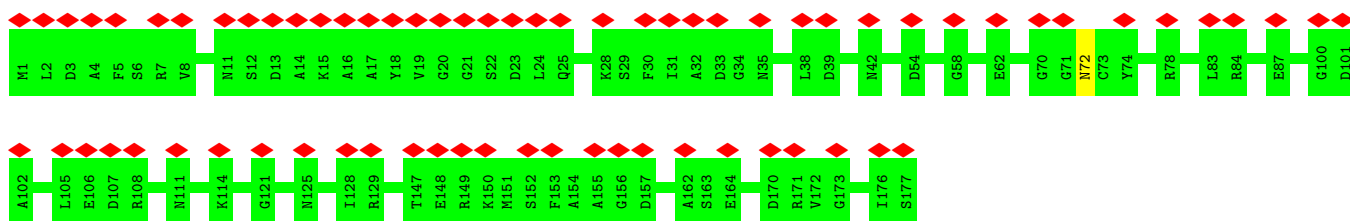
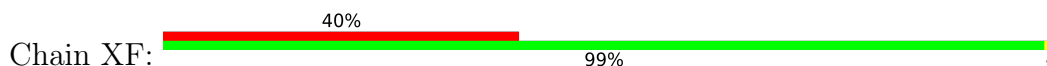


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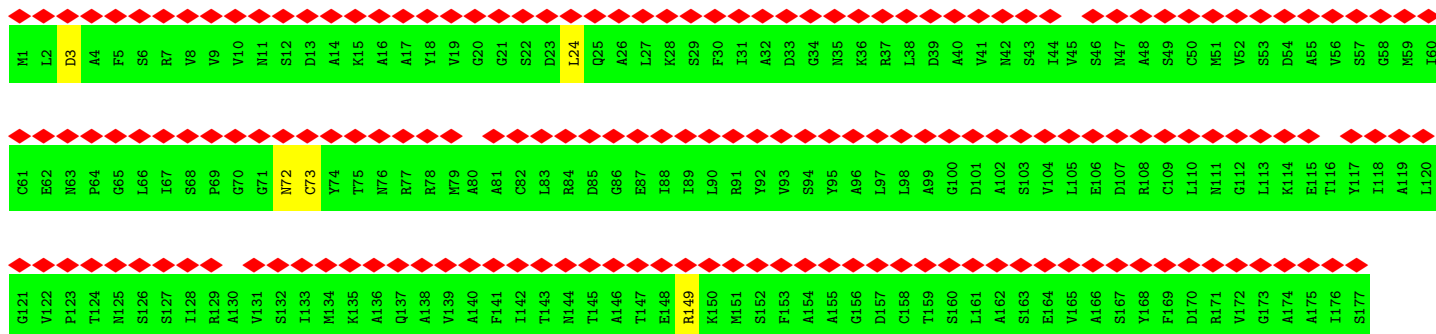




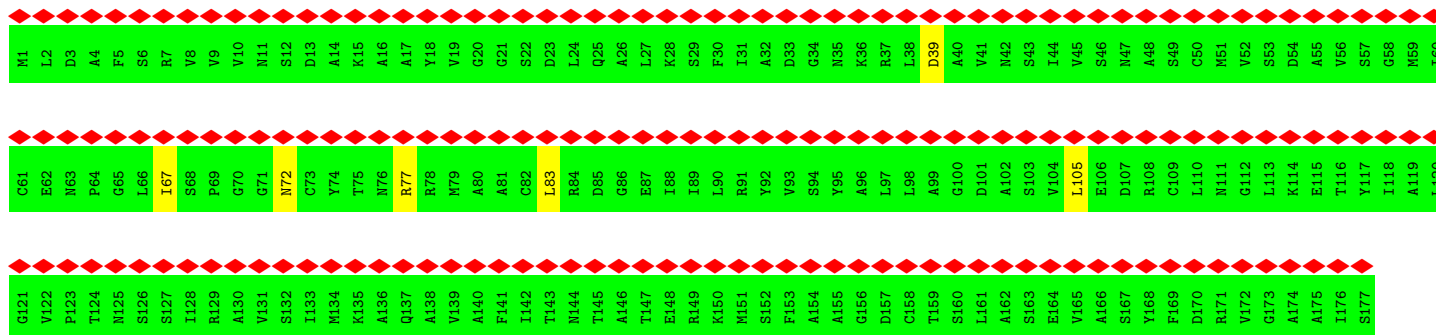
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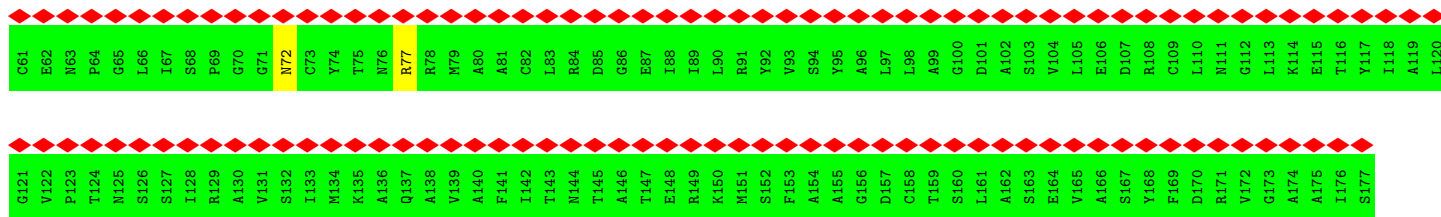


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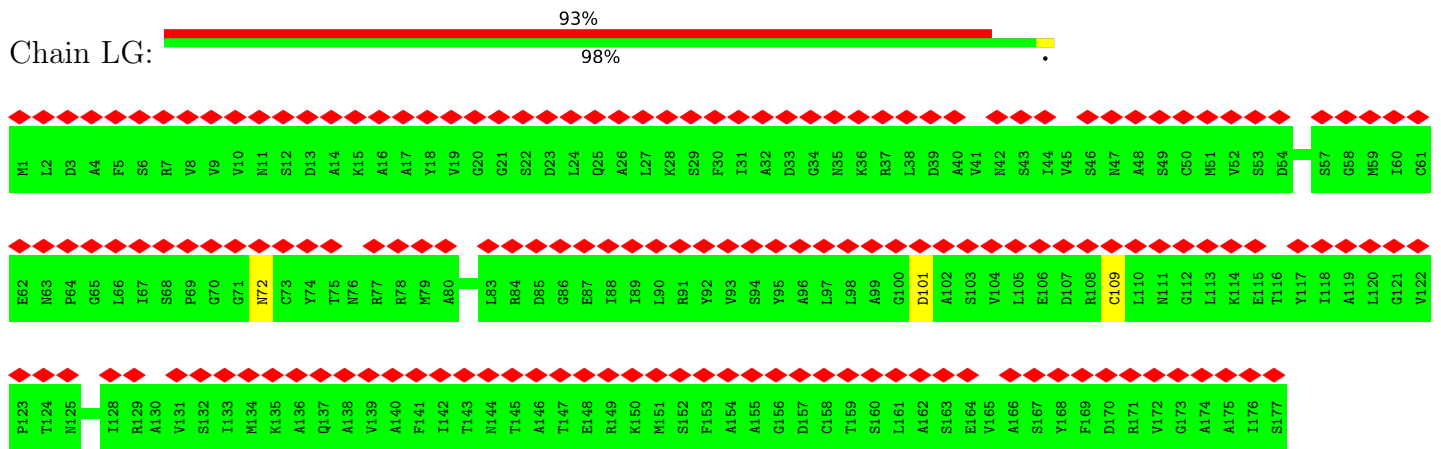


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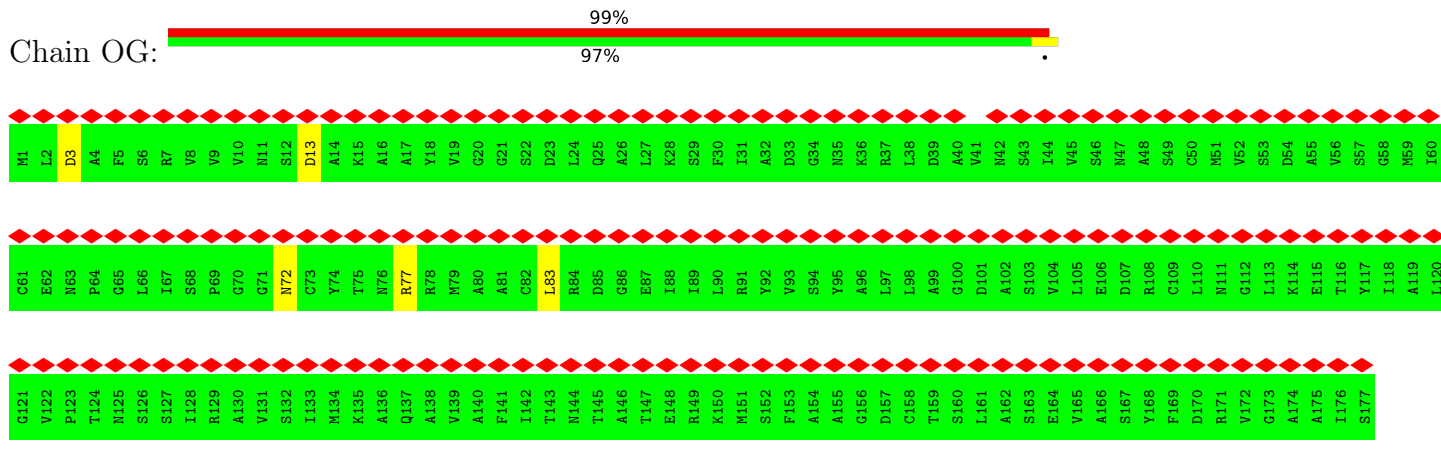




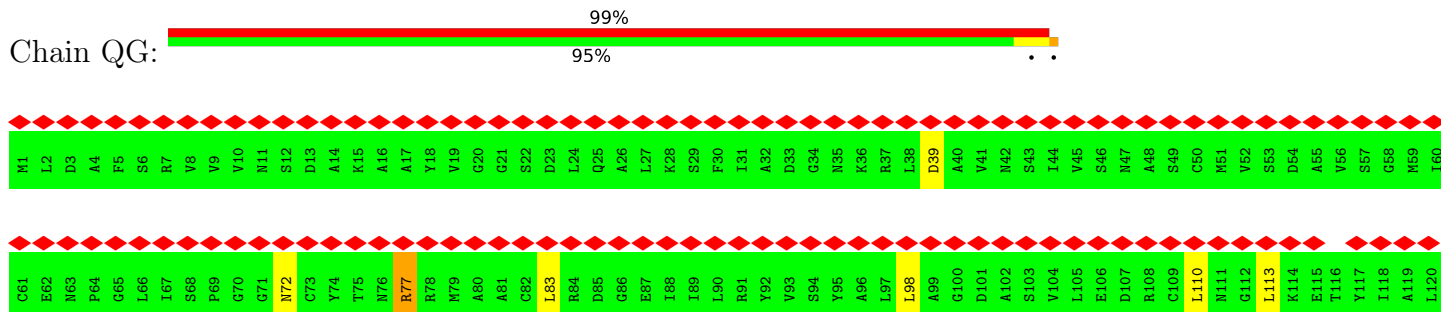
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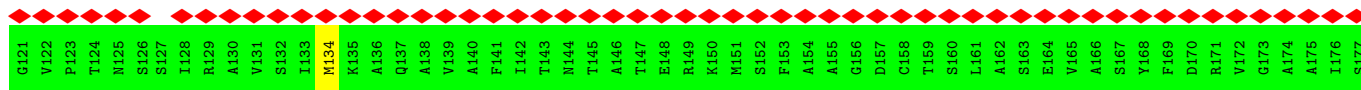


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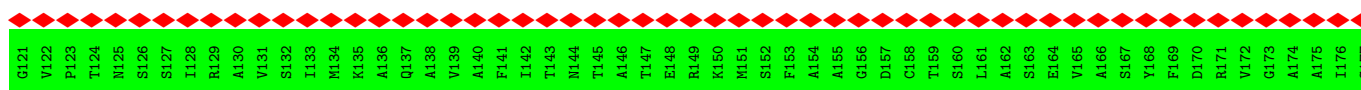
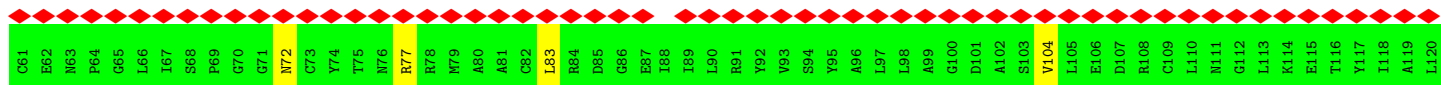
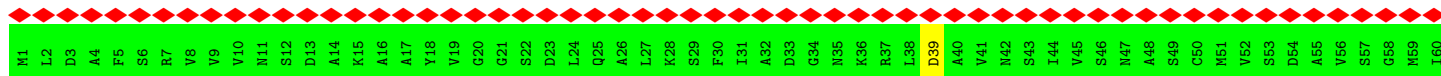


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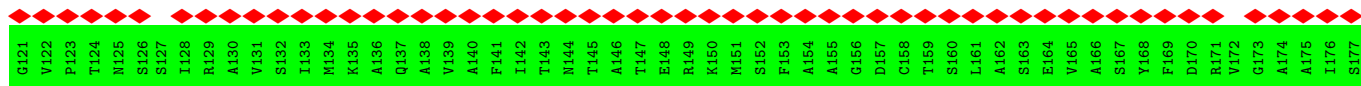
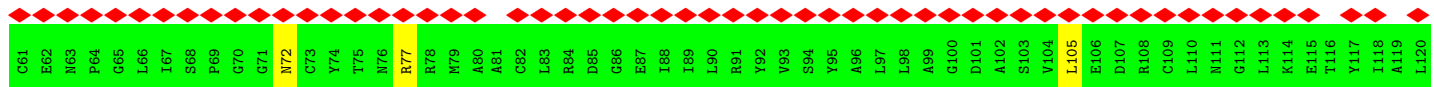
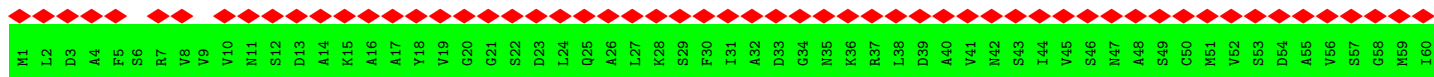




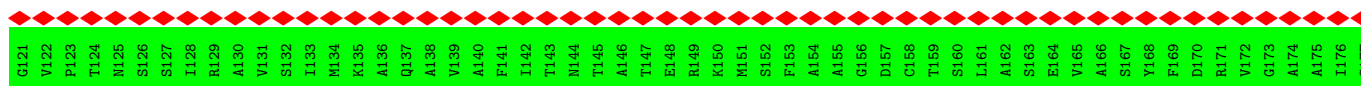
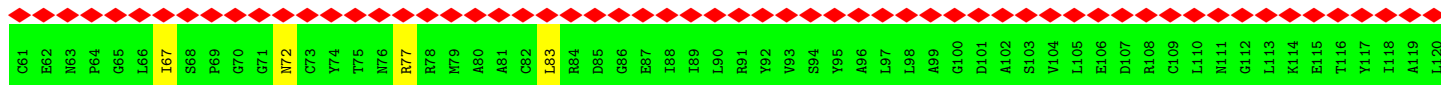
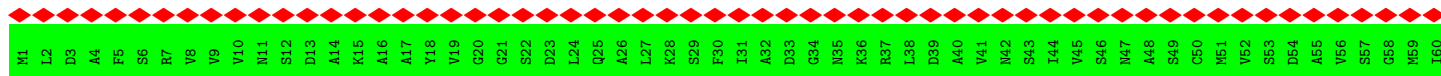
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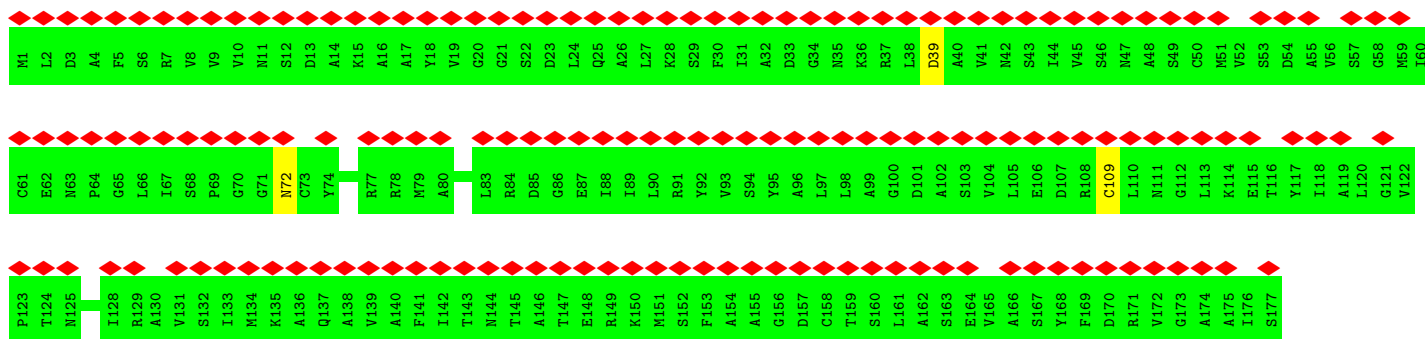


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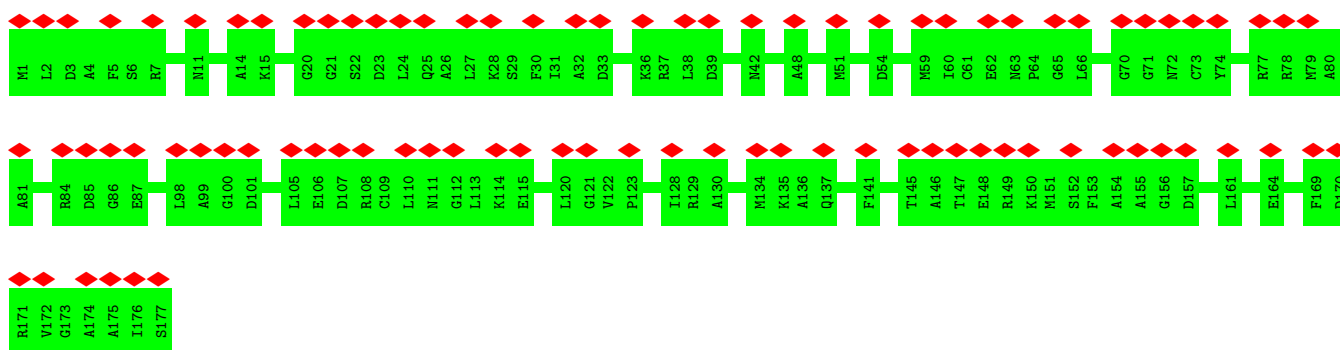


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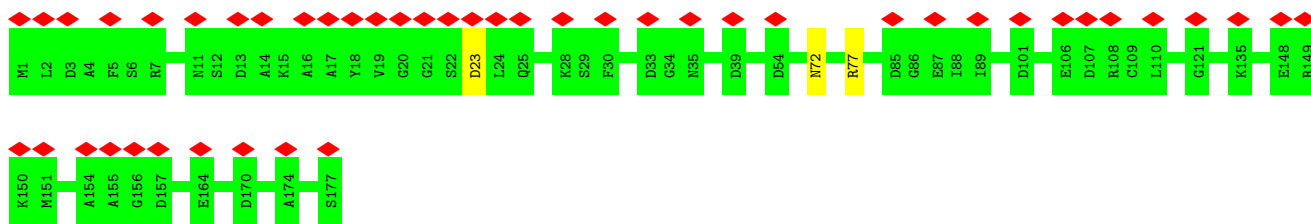




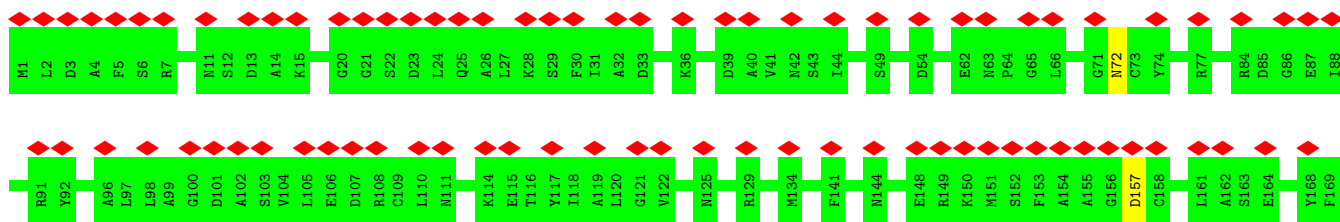
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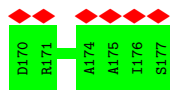


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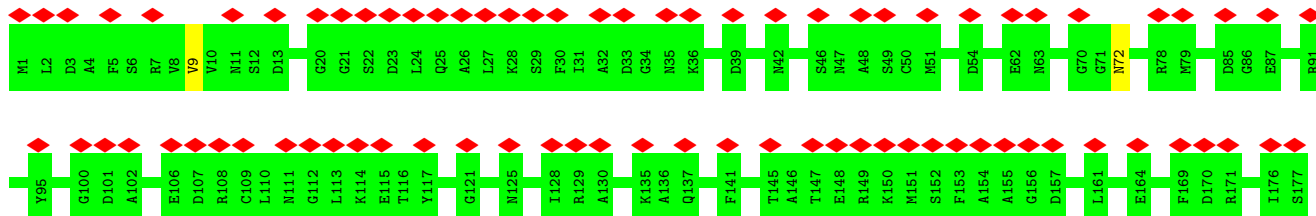
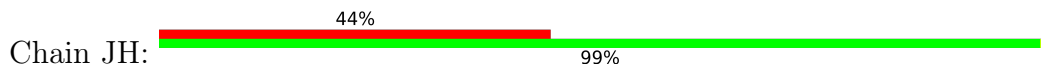


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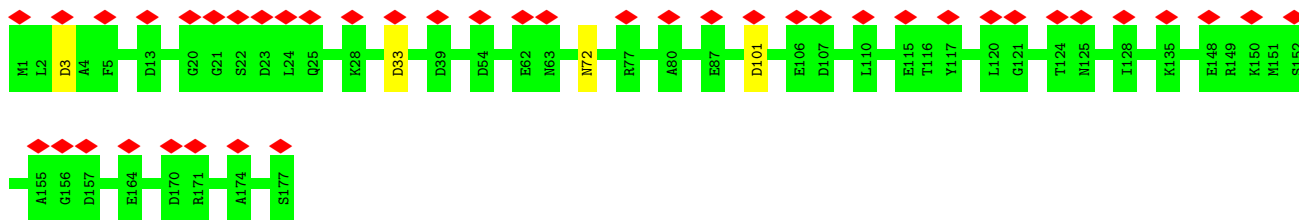




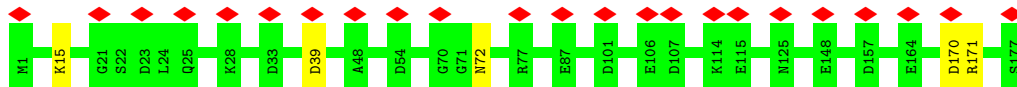
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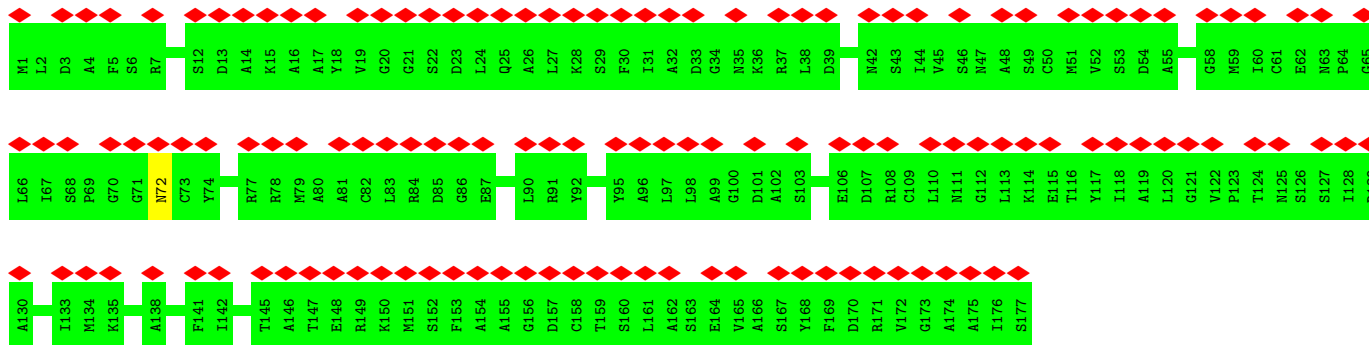
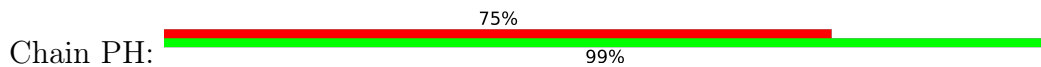
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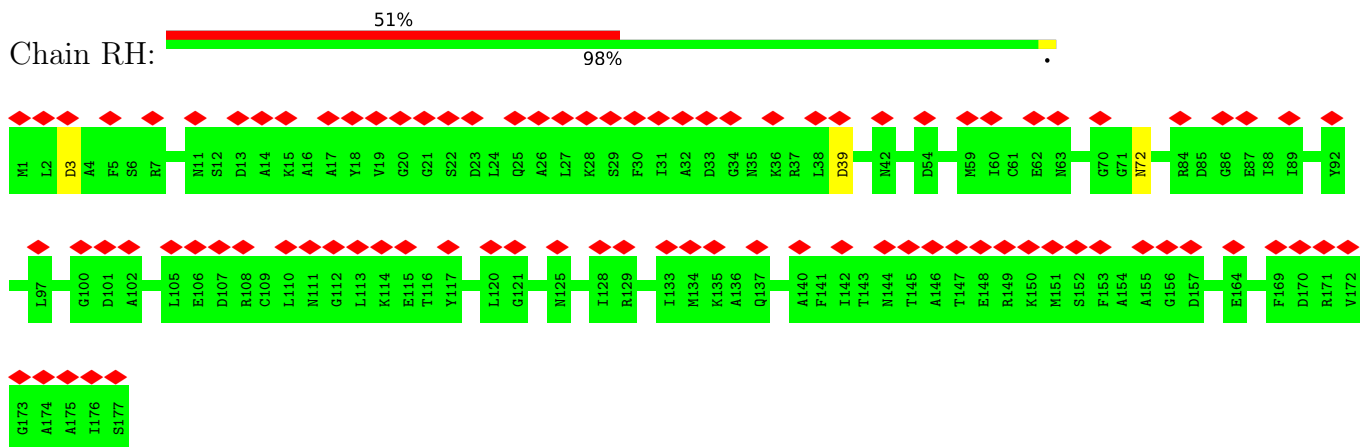
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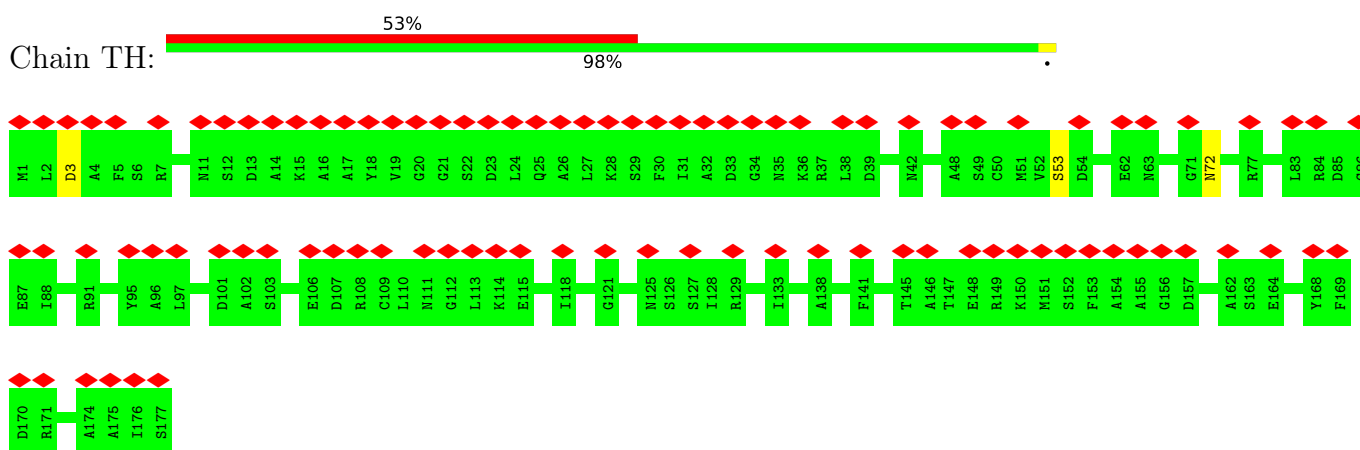
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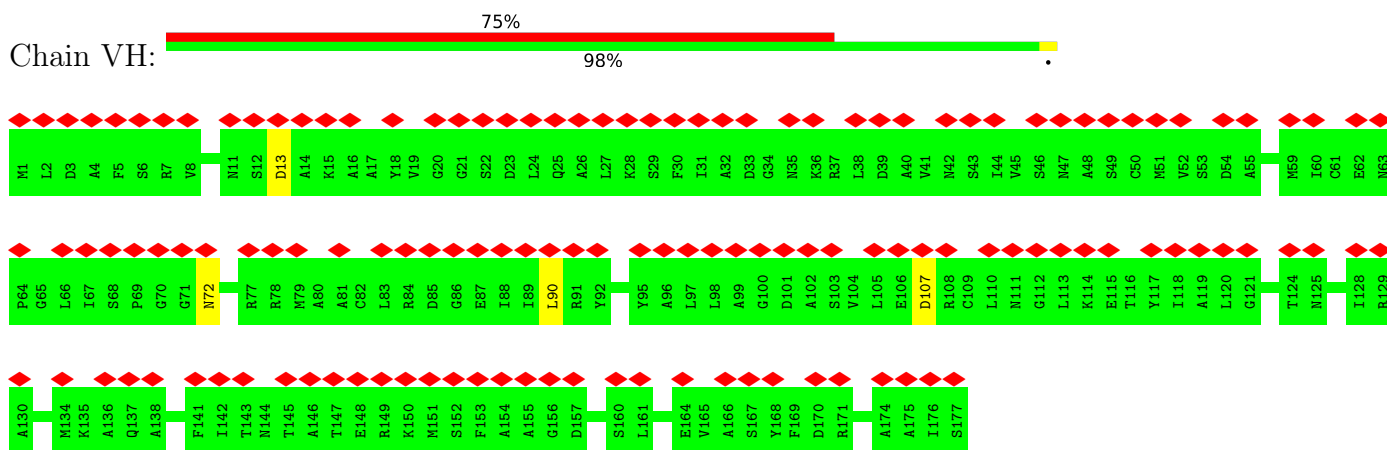
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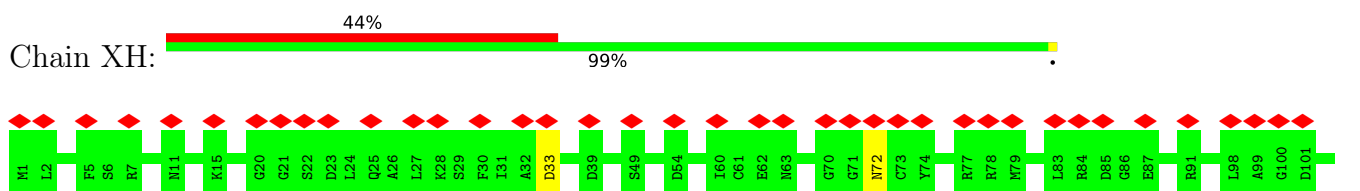
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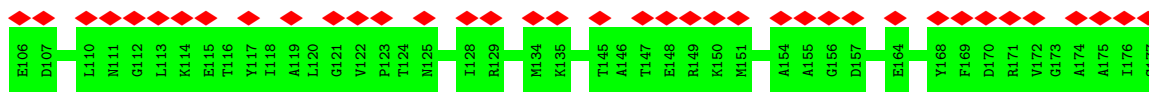


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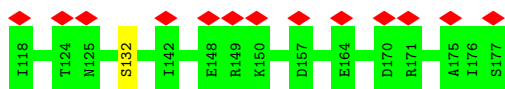
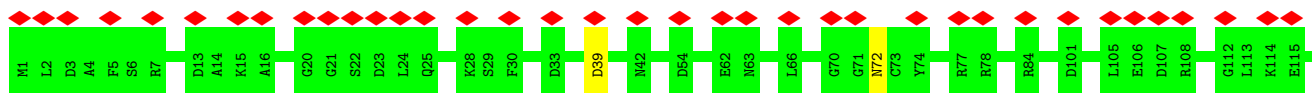


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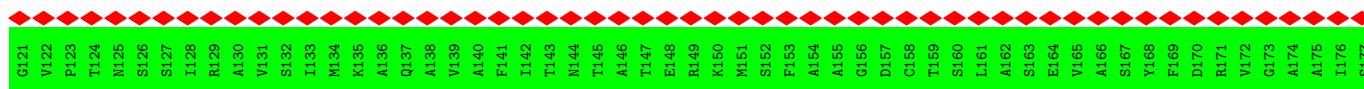
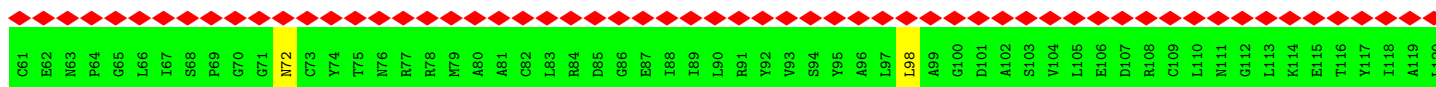




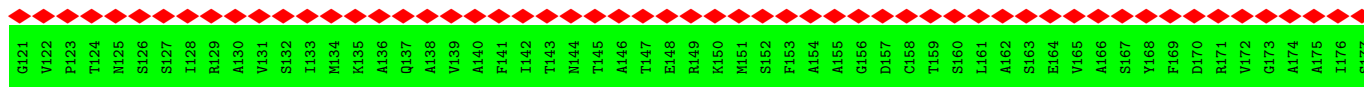
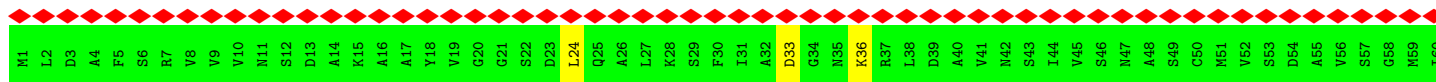
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M1	L2	D3	A4	F5	S6	R7	V8	V9	V10	M11	S12	D13	A14	K15	A16	A17	Y18	V19	G20	G21	S22	D23	L24	Q25	A26	L27	K28	S29	F30	I31	A32	D33	G34	N35	K36	R37	L38	D39	A40	V41	N42	S43	I44	V45	S46	N47	A48	S49	C50	M51	V52	S53	D54	A55	V56	S57	G58	M59	I60
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C61	E62	N63	P64	G65	L66	I67	S68	P69	G70	G71	N72	C73	Y74	T75	N76	R77	R78	M79	A80	A81	C82	L83	R84	D85	A86	E87	I88	I89	L90	R91	Y92	V93	S94	Y95	A96	L97	L98	A99	G100	D101	A102	S103	V104	L105	E106	D107	R108	C109	D110	M111	G112	L113	K114	E115	T116	I117	I118	A119	L120
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G121	V122	P123	T124	N125	S126	S127	I128	R129	A130	V131	S132	I133	M134	K135	A136	Q137	A138	V139	A140	F141	I142	T143	N144	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	G172	G173	A174	A175	I176	S177
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• Molecule 2: B-phycoerythrin beta chain



M1	L2	D3	A4	F5	S6	R7	V8	V9	V10	M11	S12	D13	A14	K15	A16	A17	Y18	V19	G20	G21	S22	D23	L24	Q25	A26	L27	K28	S29	F30	I31	A32	D33	G34	N35	K36	R37	L38	D39	A40	V41	N42	S43	I44	V45	S46	N47	A48	S49	C50	M51	V52	S53	D54	A55	V56	S57	G58	M59	I60
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C61	E62	N63	P64	G65	L66	I67	S68	P69	G70	G71	N72	C73	Y74	T75	N76	R77	R78	M79	A80	A81	C82	L83	R84	D85	A86	E87	I88	I89	L90	R91	Y92	V93	S94	Y95	A96	L97	L98	A99	G100	D101	A102	S103	V104	L105	E106	D107	R108	C109	D110	M111	G112	L113	K114	E115	T116	I117	I118	A119	L120
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G121	V122	P123	T124	N125	S126	S127	I128	R129	A130	V131	S132	I133	M134	K135	A136	Q137	A138	V139	A140	F141	I142	T143	N144	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	G172	G173	A174	A175	I176	S177
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• Molecule 2: B-phycoerythrin beta chain



M1	L2	D3	A4	F5	S6	R7	V8	V9	V10	M11	S12	D13	A14	K15	A16	A17	Y18	V19	G20	G21	S22	D23	L24	Q25	A26	L27	K28	S29	F30	I31	A32	D33	G34	N35	K36	R37	L38	D39	A40	V41	N42	S43	I44	V45	S46	N47	A48	S49	C50	M51	V52	S53	D54	A55	V56	S57	G58	M59	I60
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C61	E62	N63	P64	G65	L66	I67	S68	P69	G70	G71	N72	C73	Y74	T75	N76	R77	R78	M79	A80	A81	C82	L83	R84	D85	A86	E87	I88	I89	L90	R91	Y92	V93	S94	Y95	A96	L97	L98	A99	G100	D101	A102	S103	V104	L105	E106	D107	R108	C109	D110	M111	G112	L113	K114	E115	T116	I117	I118	A119	L120
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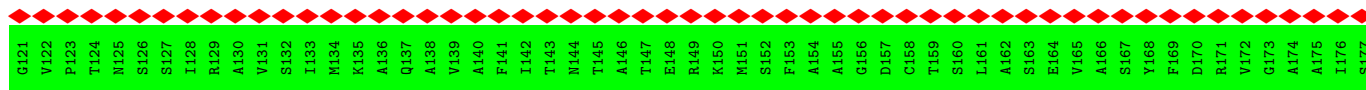
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• Molecule 2: B-phycoerythrin beta chain

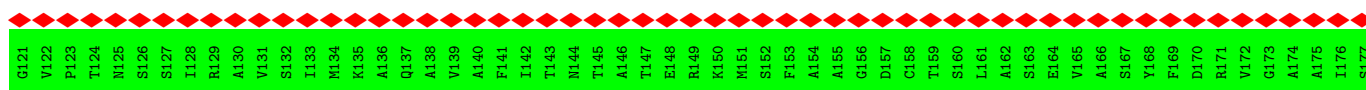
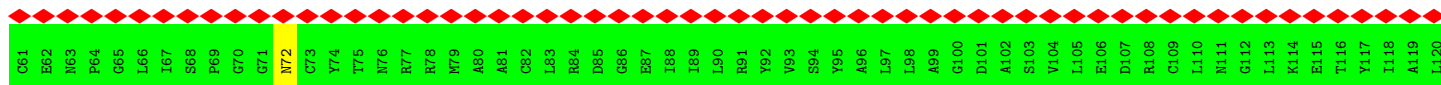


M1	L2	D3	A4	F5	S6	R7	V8	V9	V10	M11	S12	D13	A14	K15	A16	A17	Y18	V19	G20	G21	S22	D23	L24	Q25	A26	L27	K28	S29	F30	I31	A32	D33	G34	N35	K36	R37	L38	D39	A40	V41	N42	S43	I44	V45	S46	N47	A48	S49	C50	M51	V52	S53	D54	A55	V56	S57	G58	M59	I60
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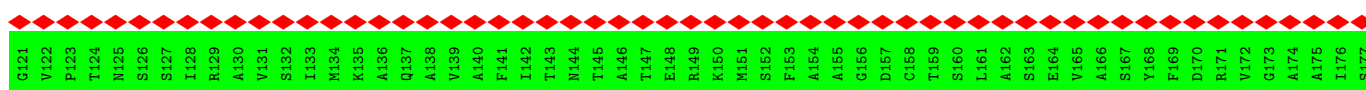
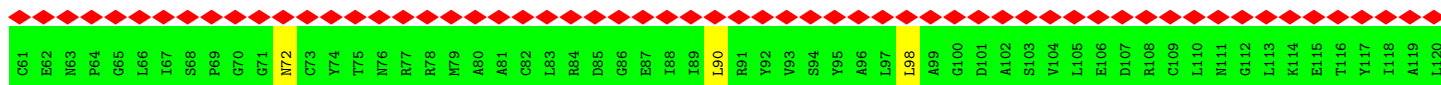
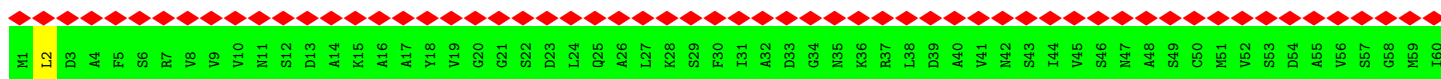
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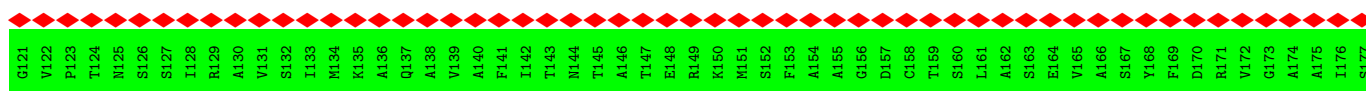
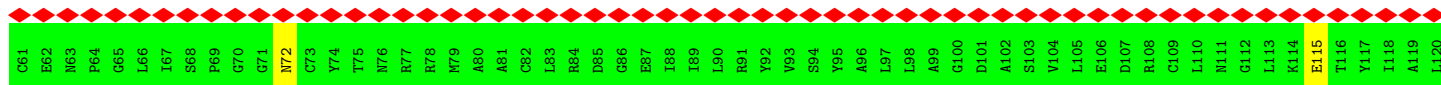
• Molecule 2: B-phycoerythrin beta chain



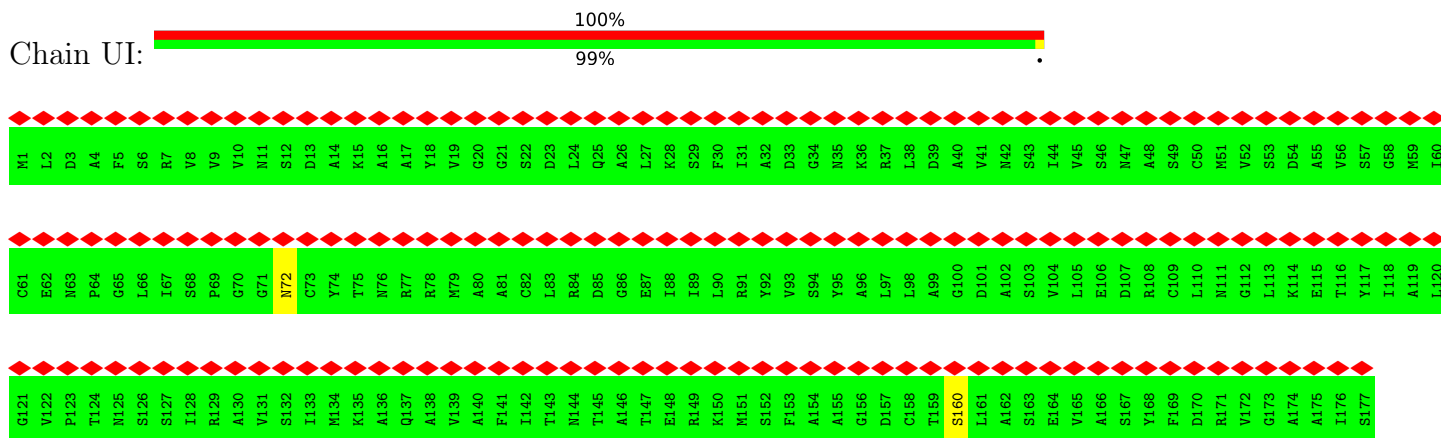
• Molecule 2: B-phycoerythrin beta chain



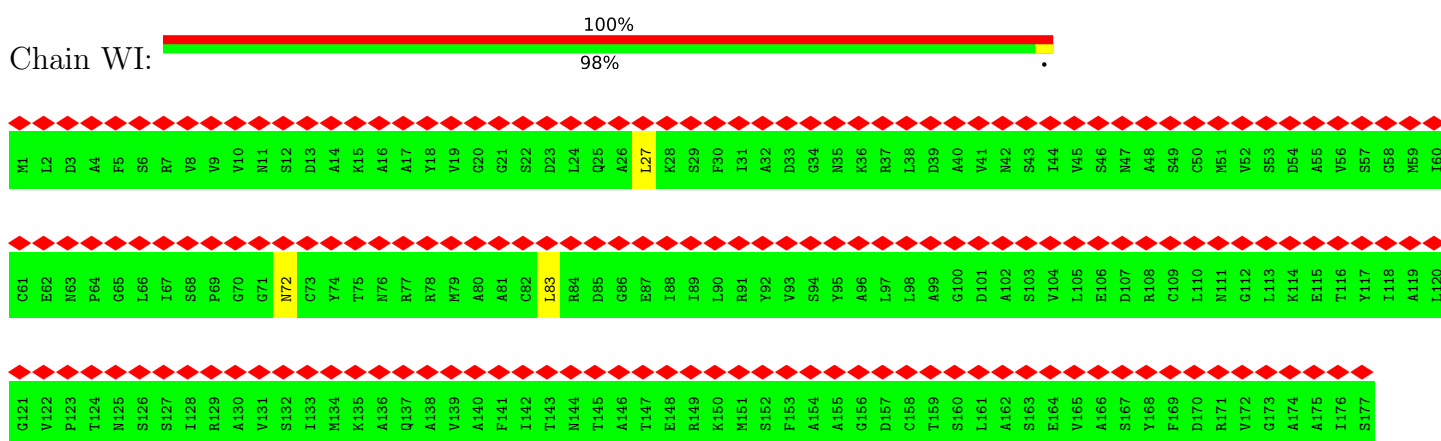
• Molecule 2: B-phycoerythrin beta chain



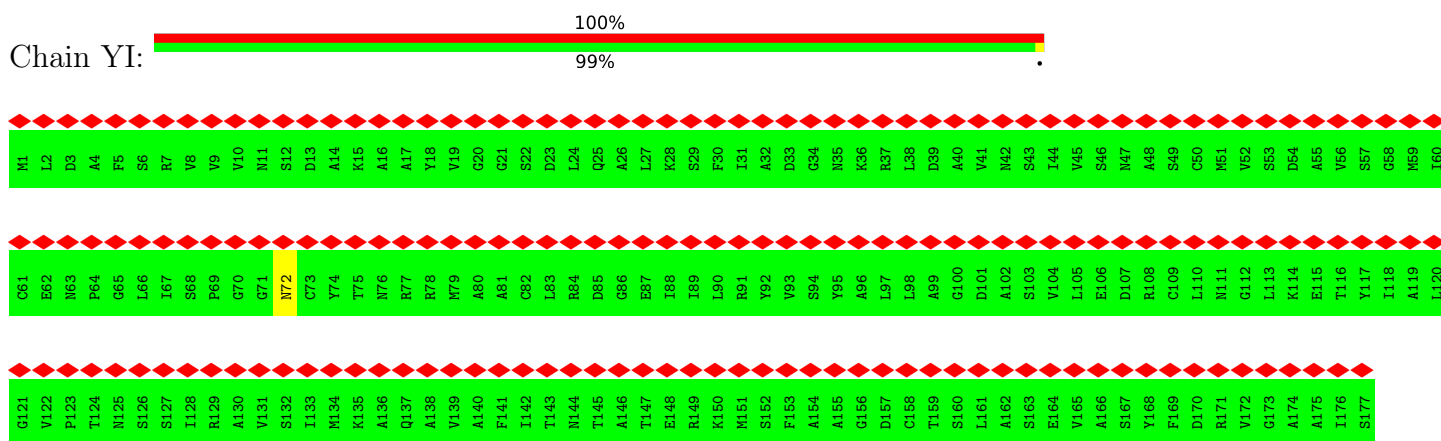
• Molecule 2: B-phycoerythrin beta chain



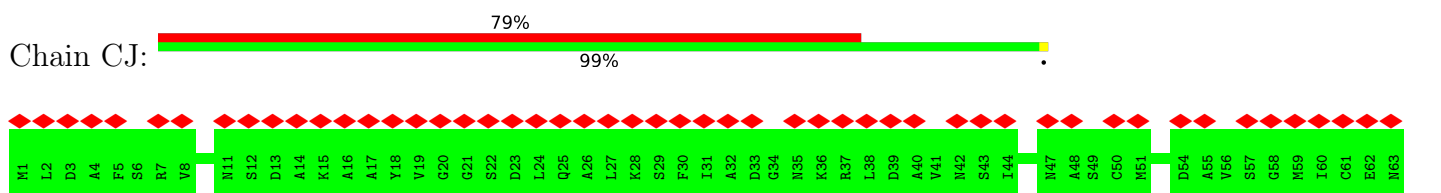
• Molecule 2: B-phycoerythrin beta chain

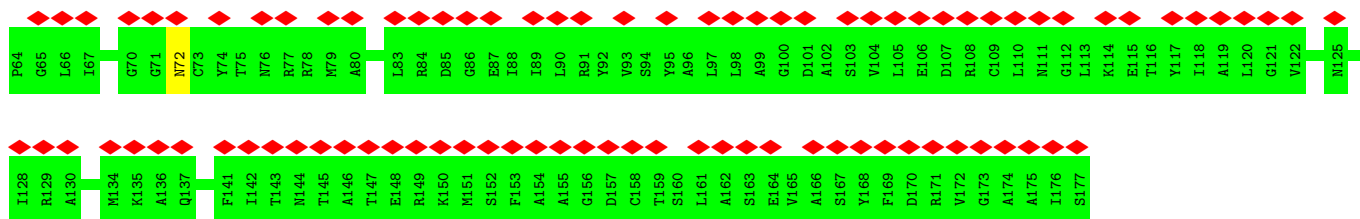


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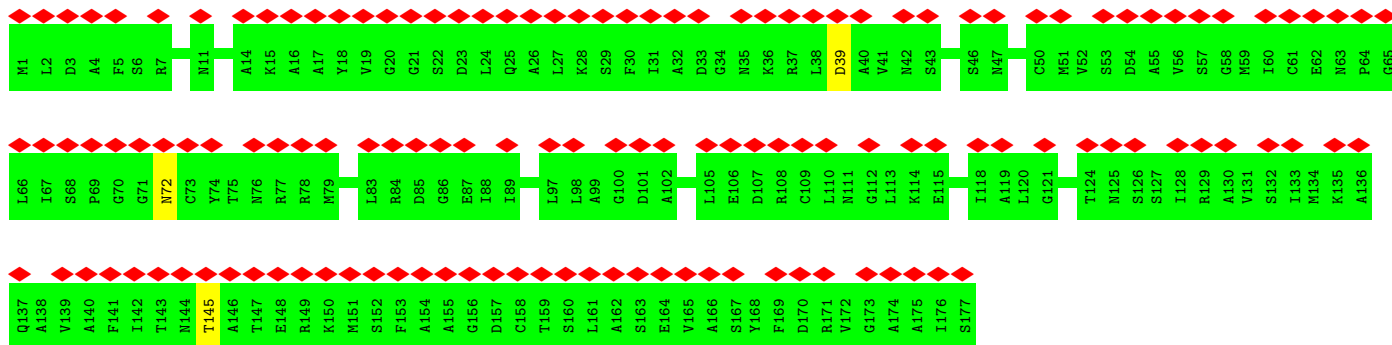
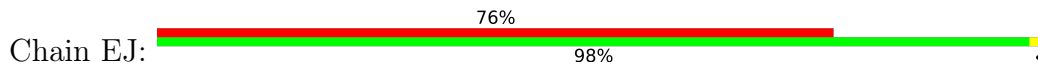


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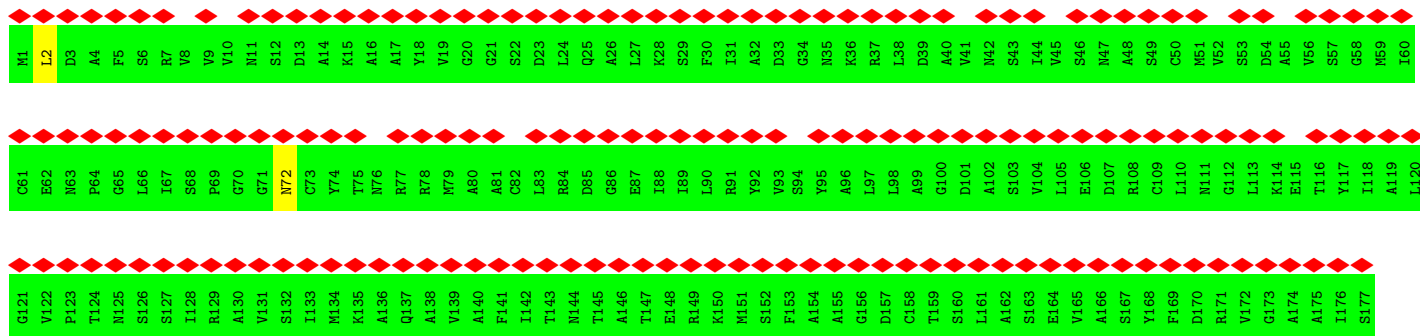




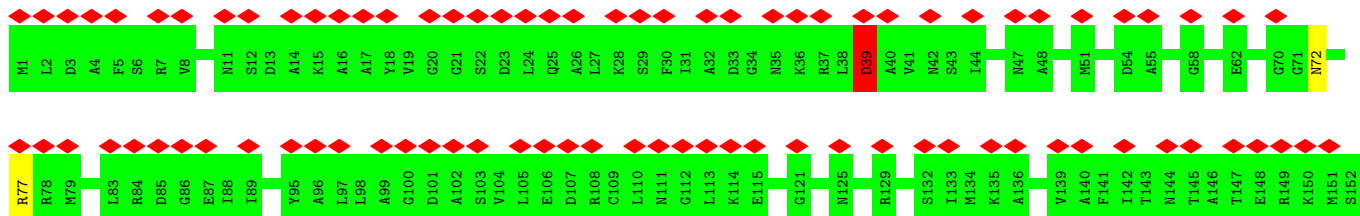
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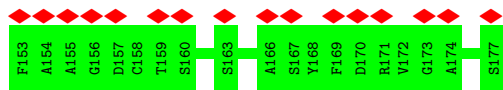


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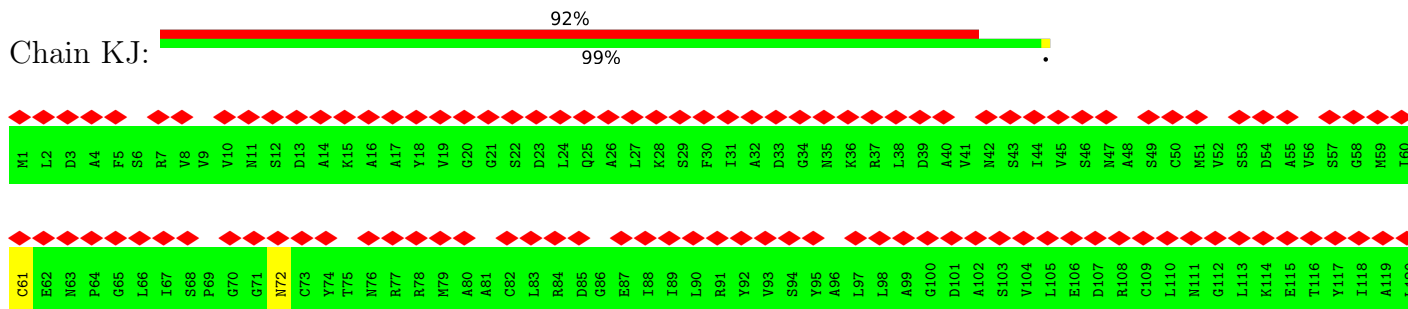


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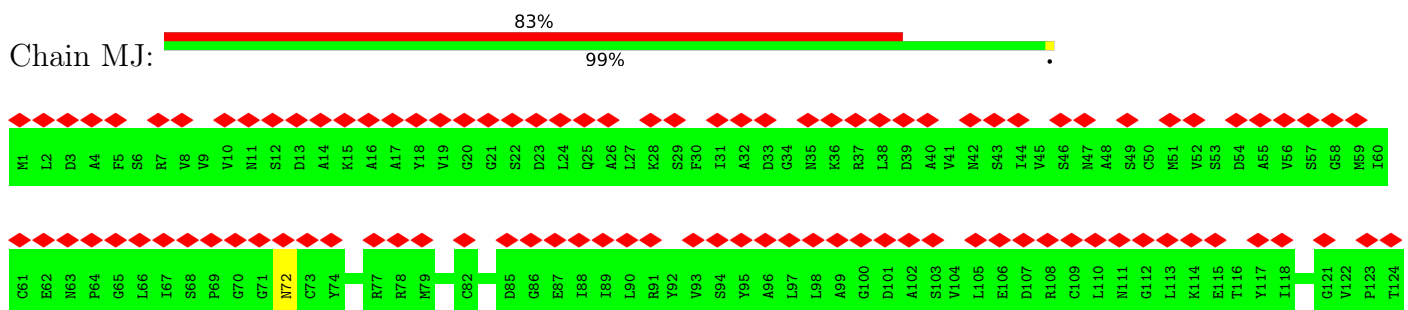




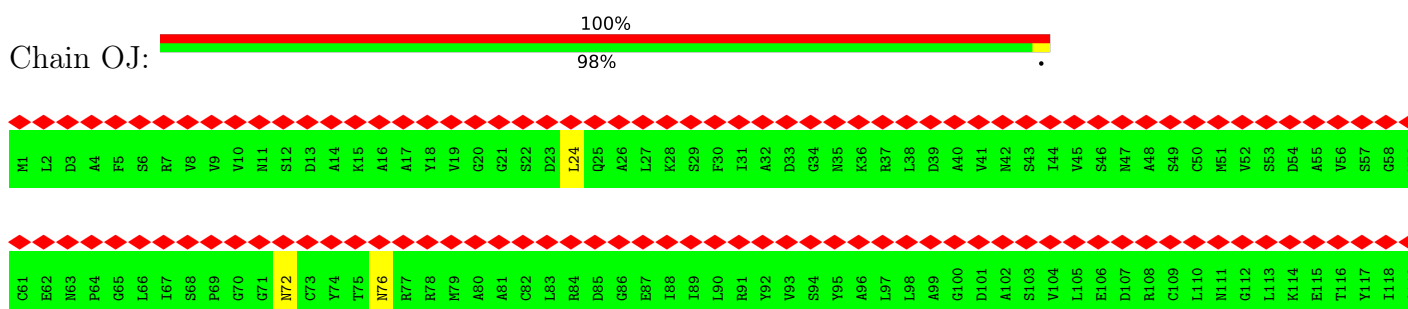
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• Molecule 2: B-phycoerythrin beta chain

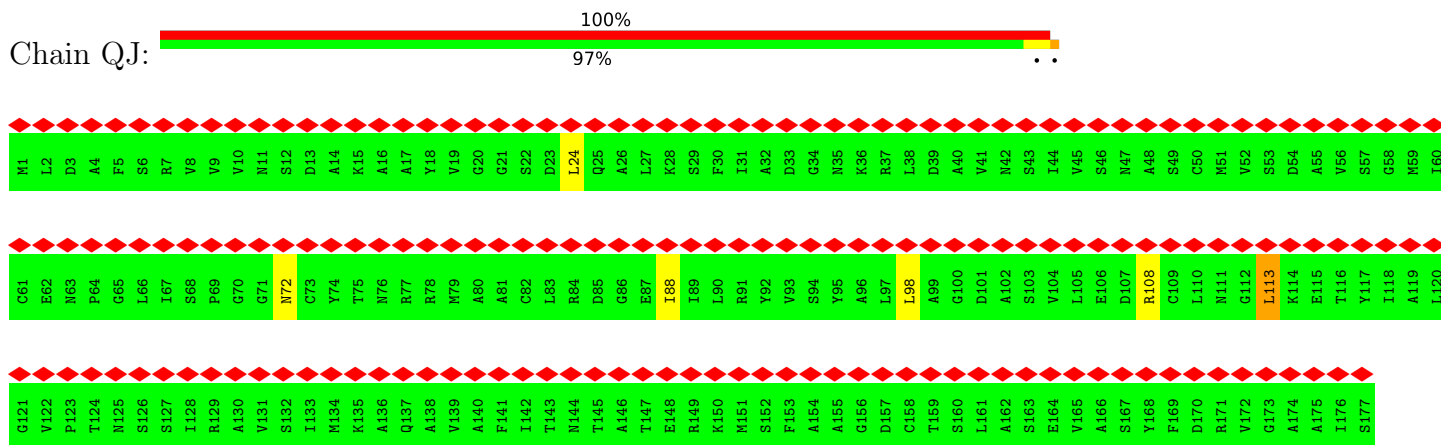


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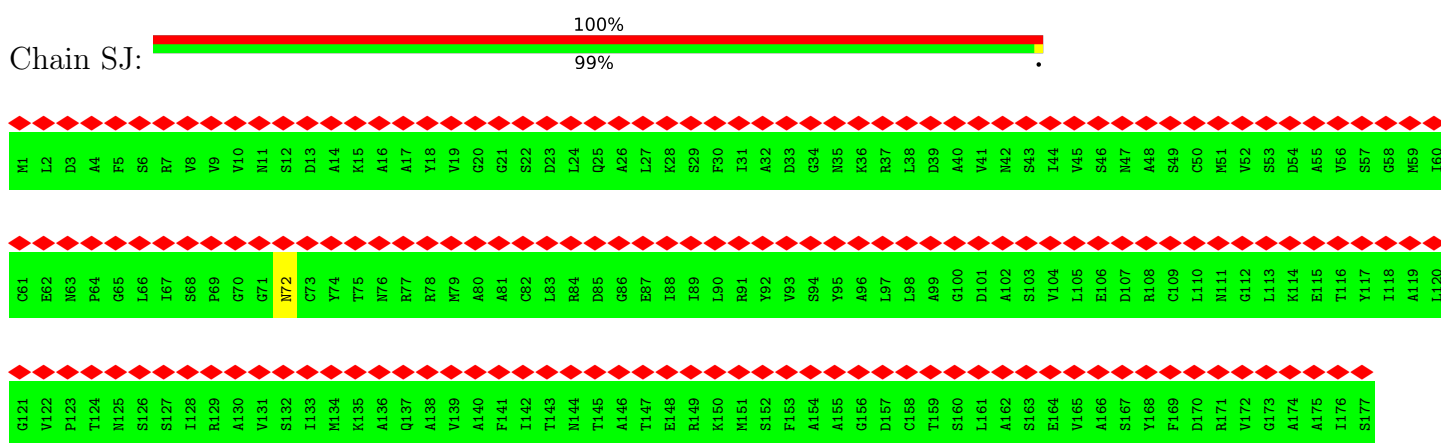


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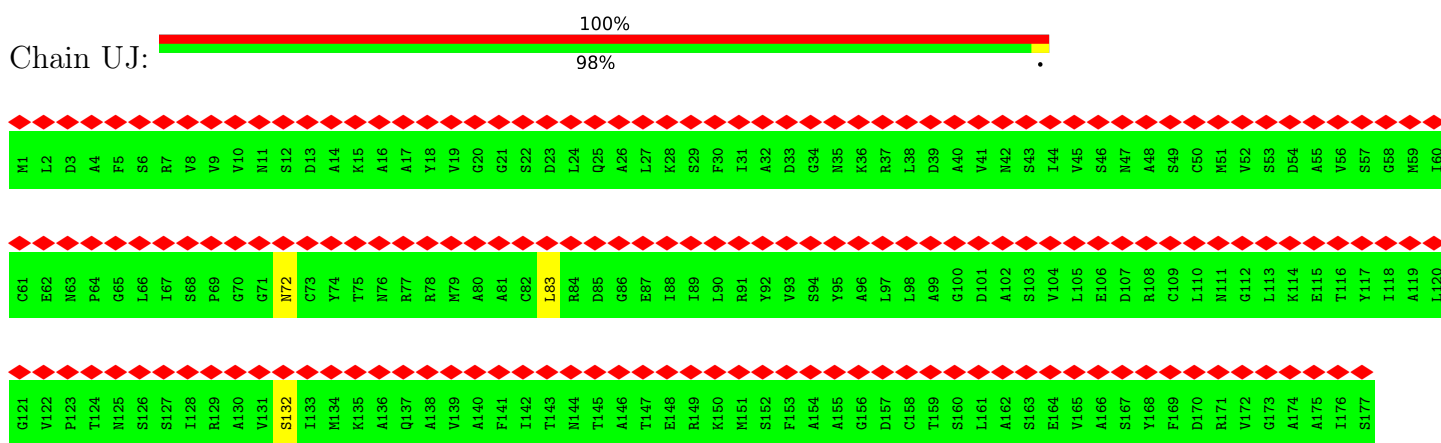




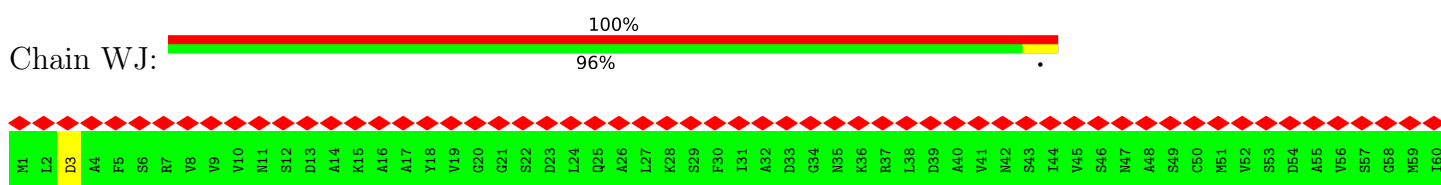
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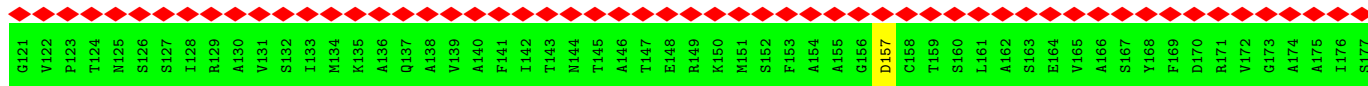
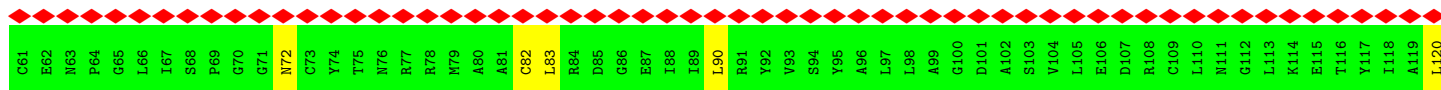


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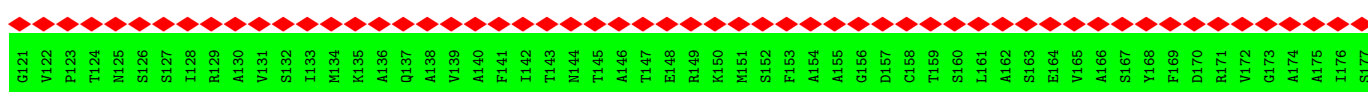
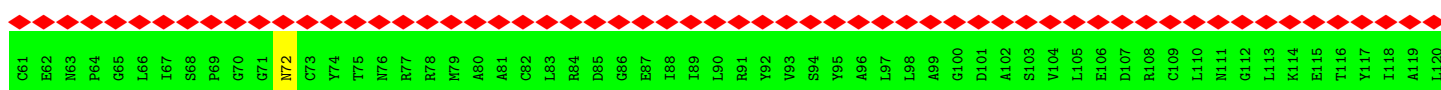


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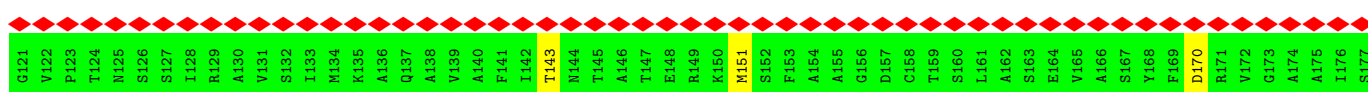
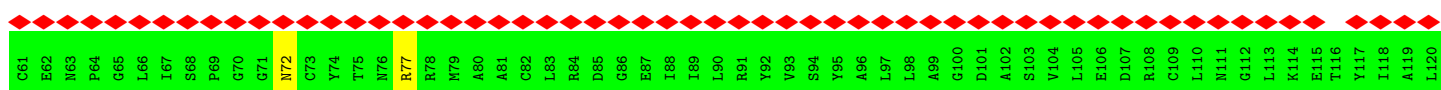
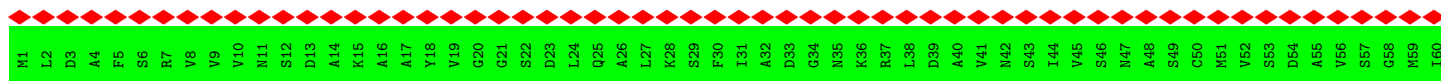




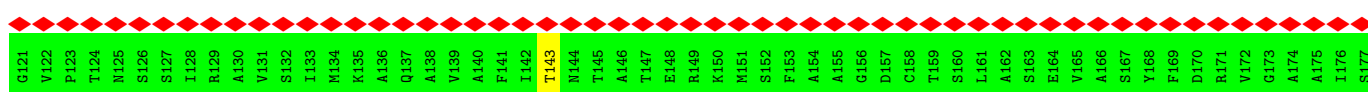
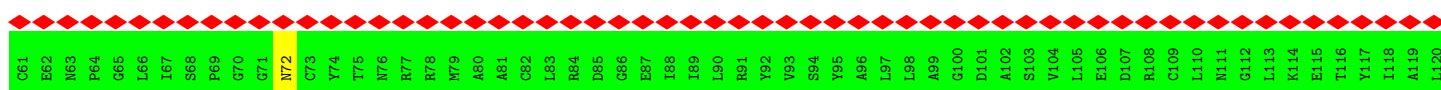
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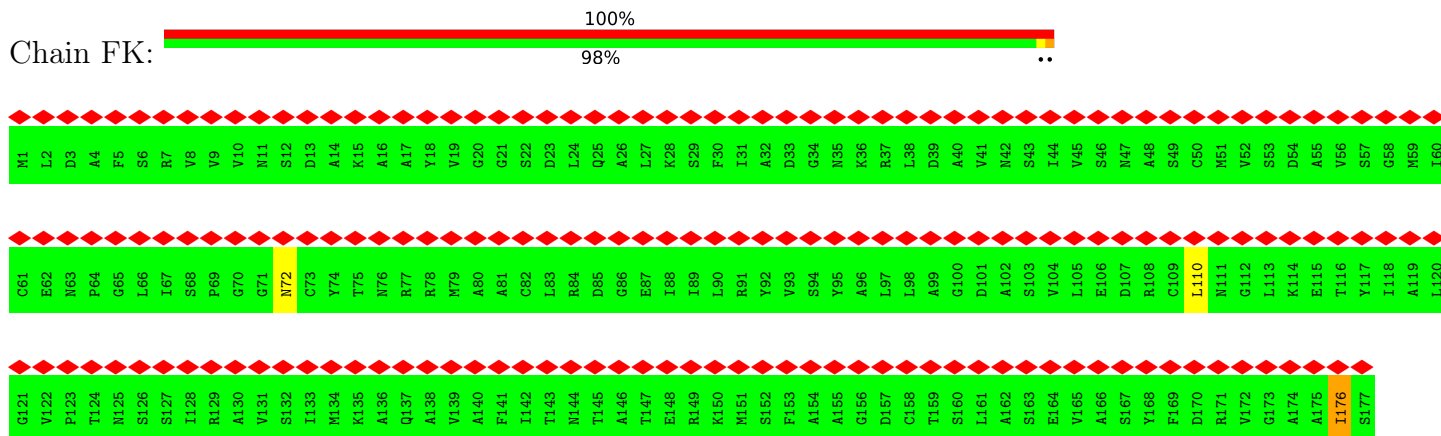
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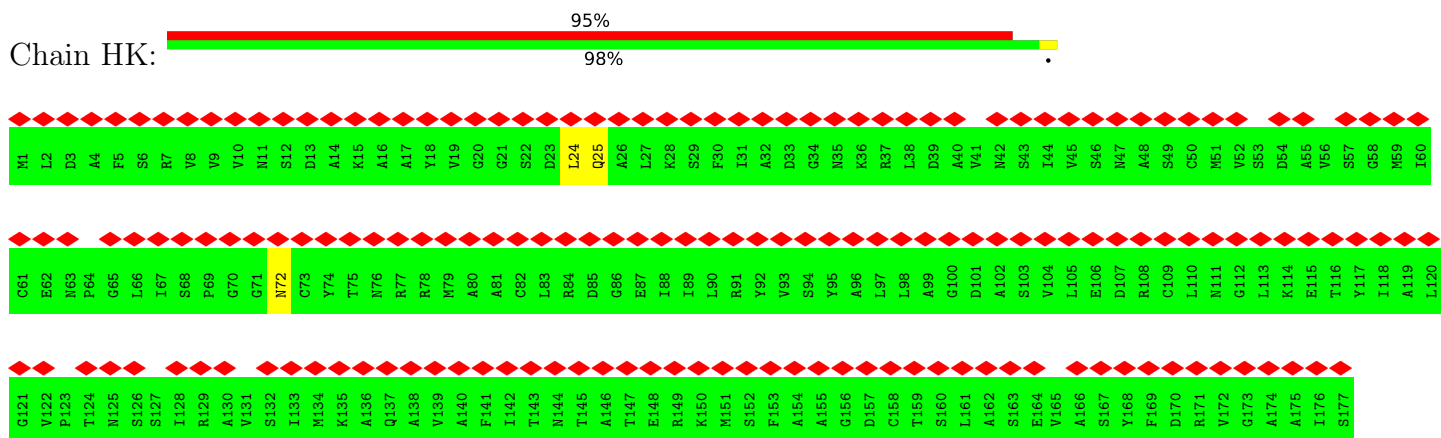
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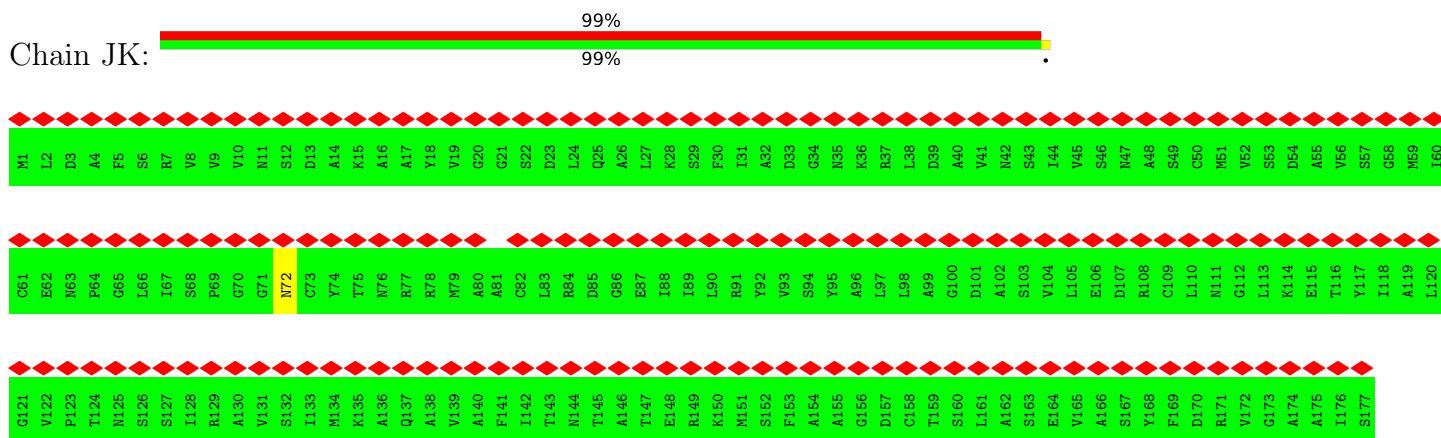
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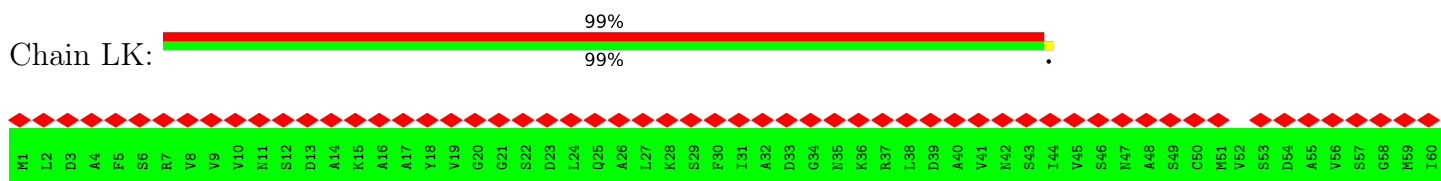
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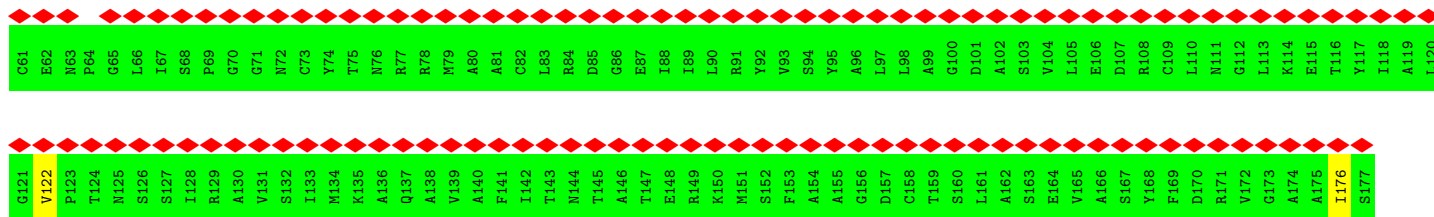


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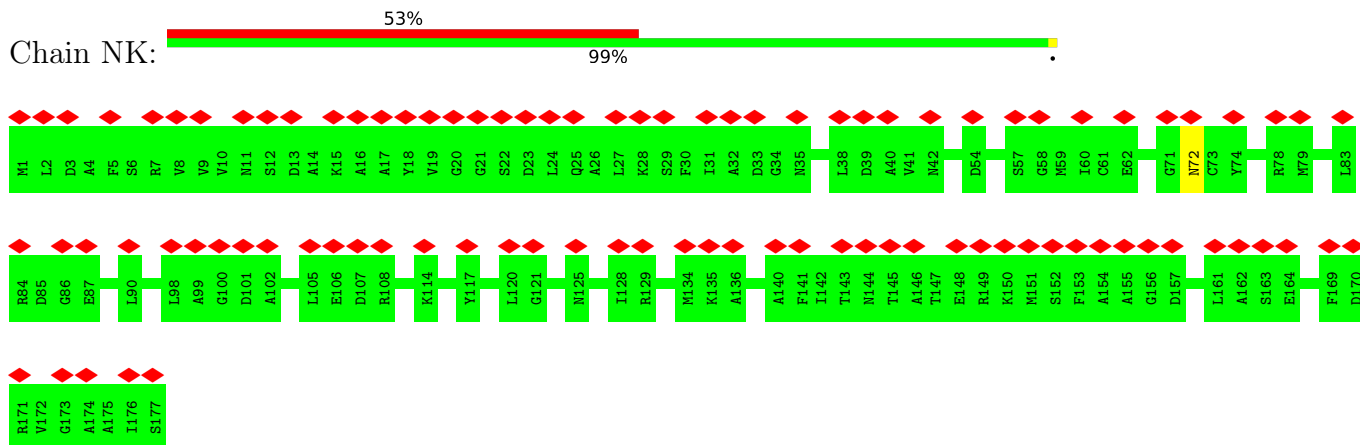


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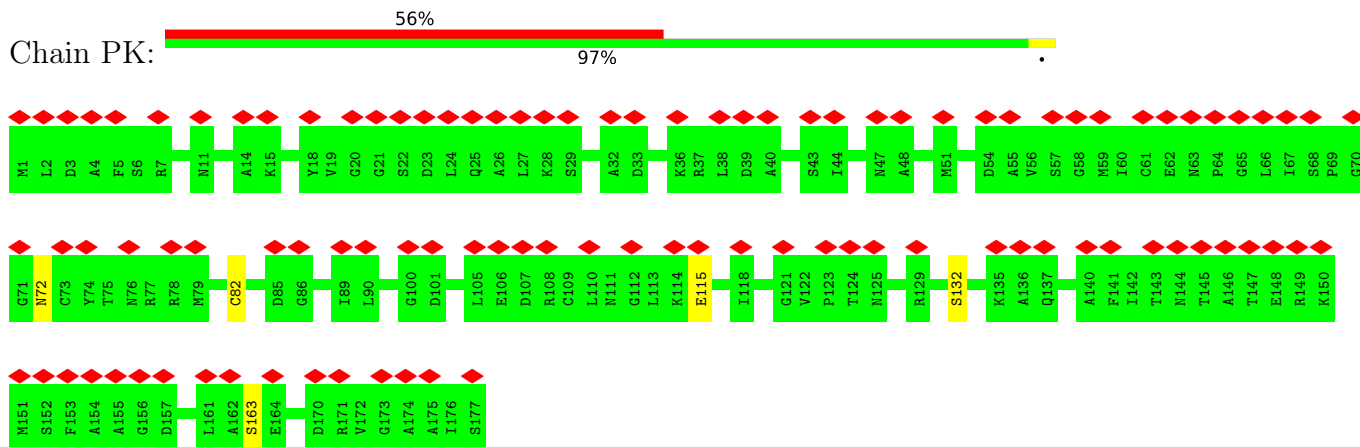




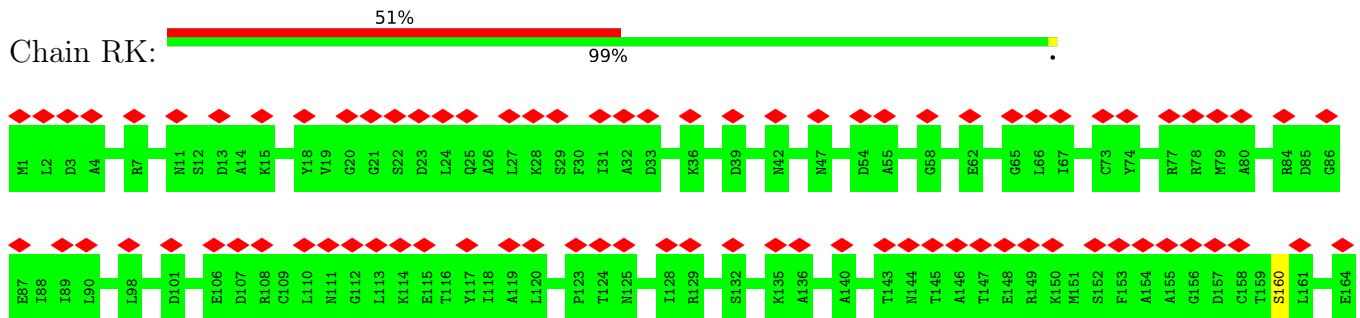
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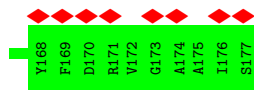


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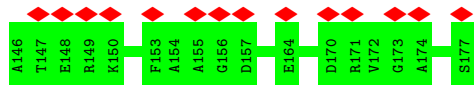
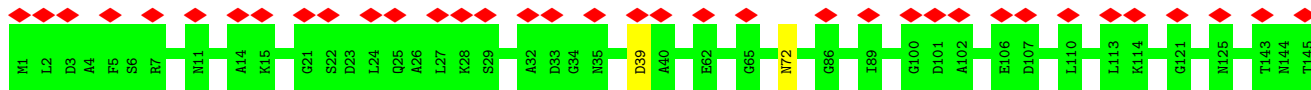


• Molecule 2: B-phycoerythrin beta chain

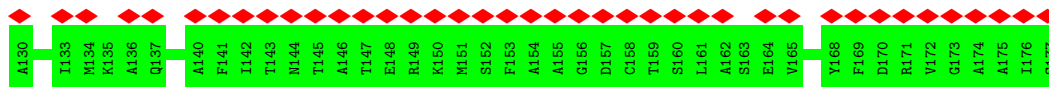
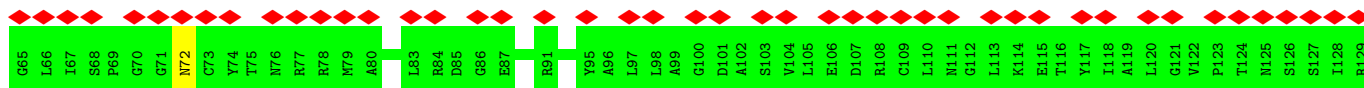
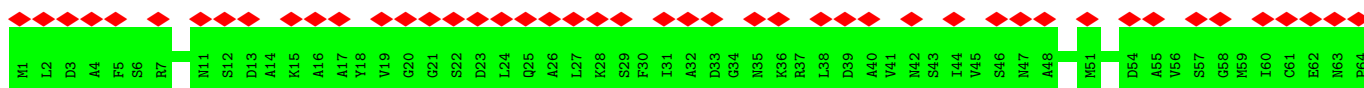
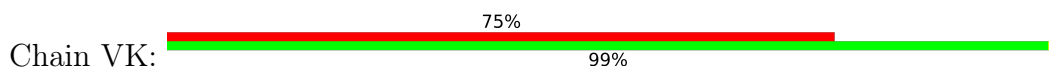




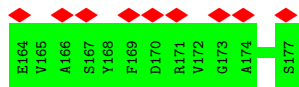
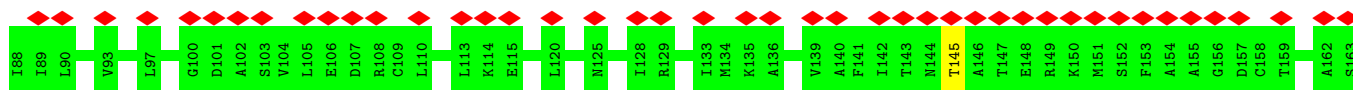
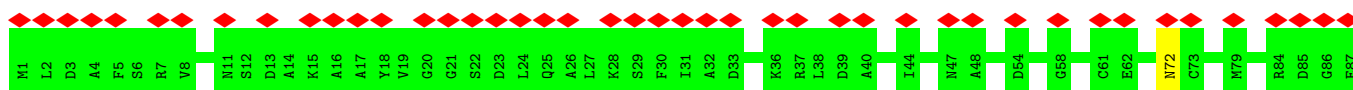
• Molecule 2: B-phycoerythrin beta chain



• Molecule 2: B-phycoerythrin beta chain

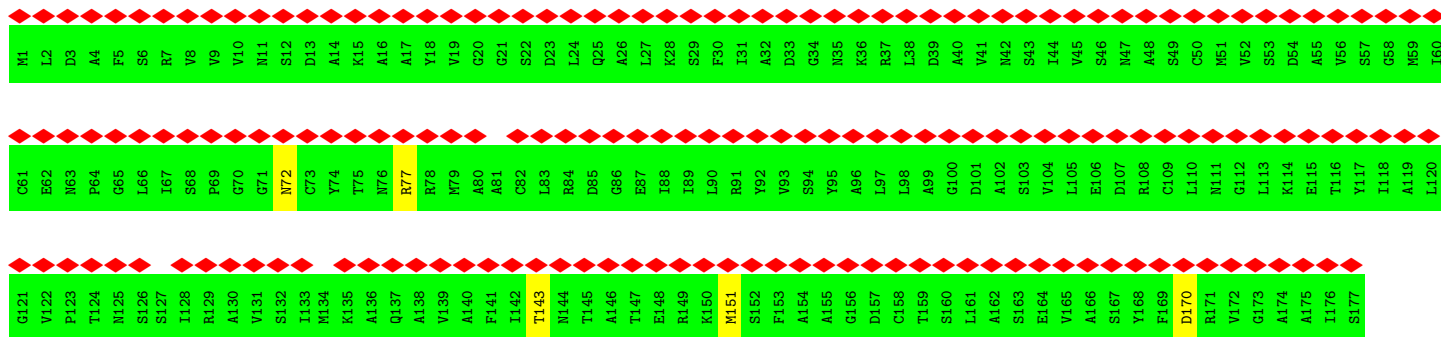


• Molecule 2: B-phycoerythrin beta chain

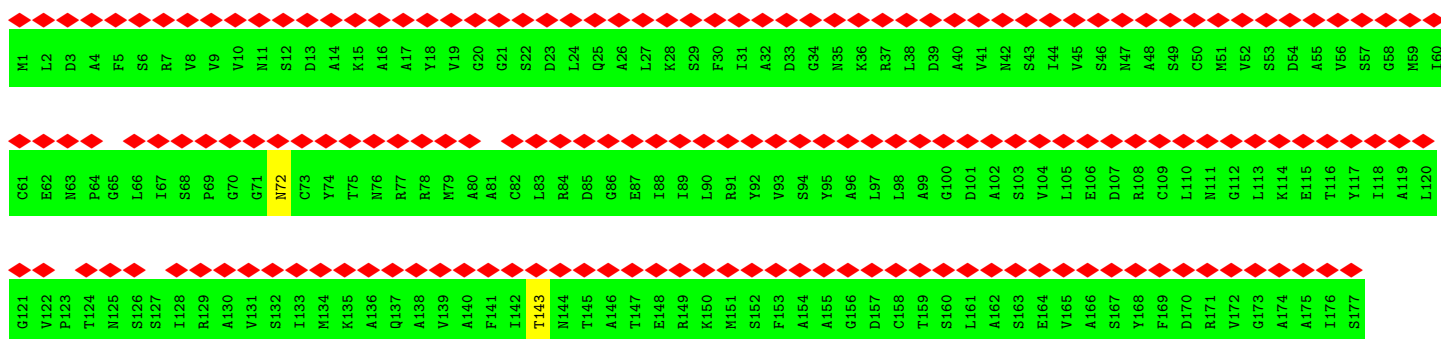


• Molecule 2: B-phycoerythrin beta chain

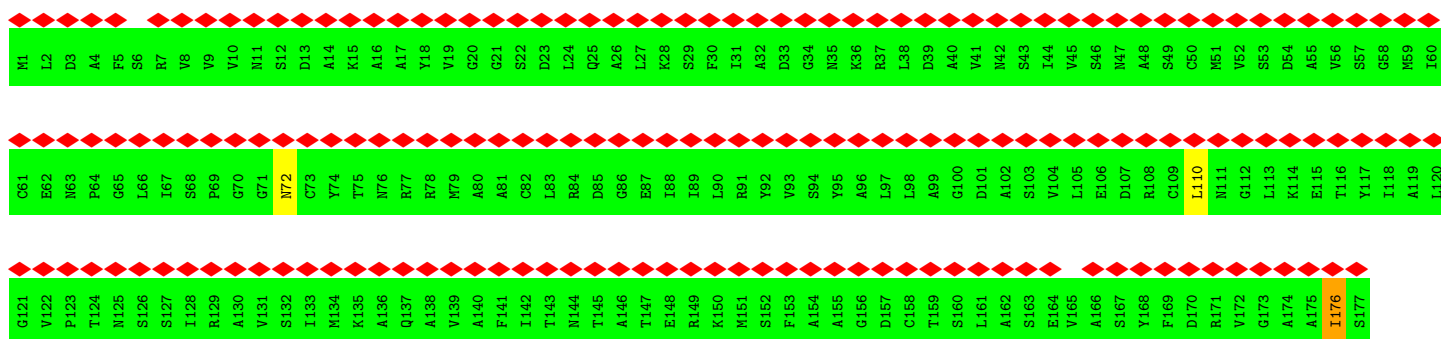




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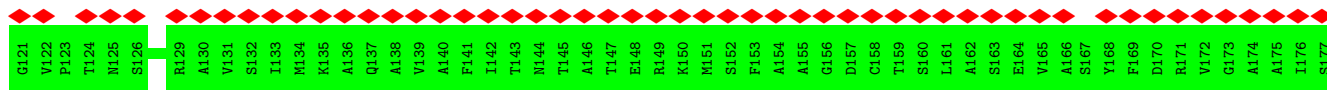


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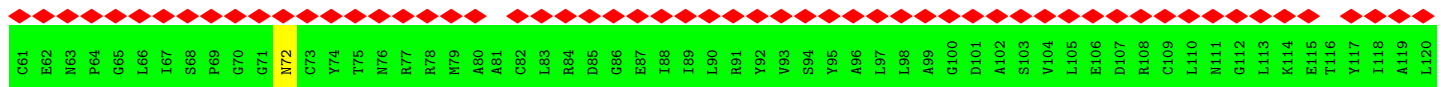
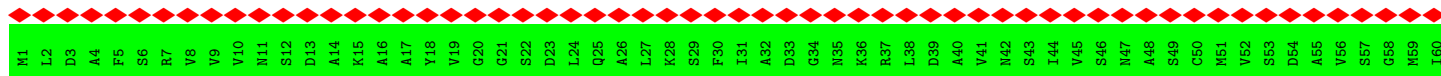


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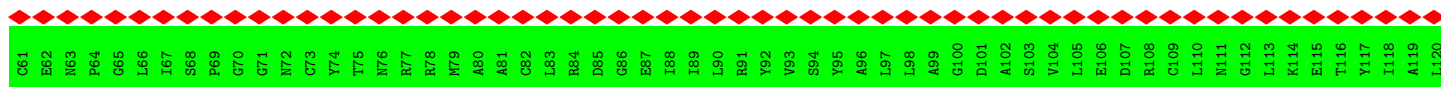
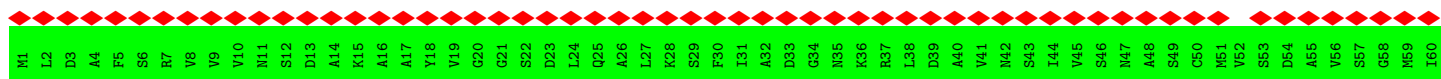




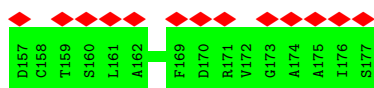
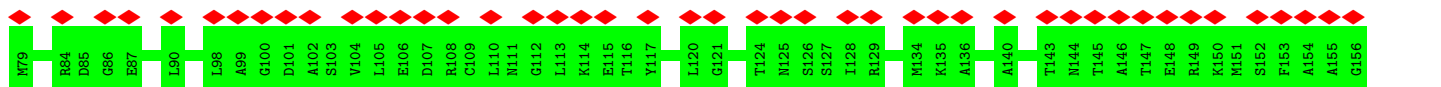
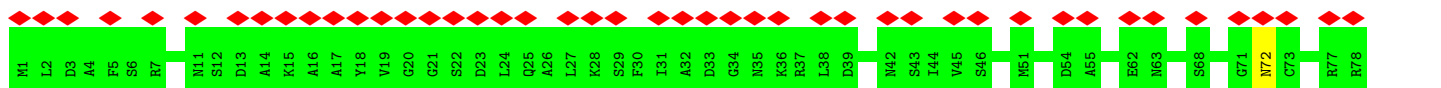
• Molecule 2: B-phycoerythrin beta chain



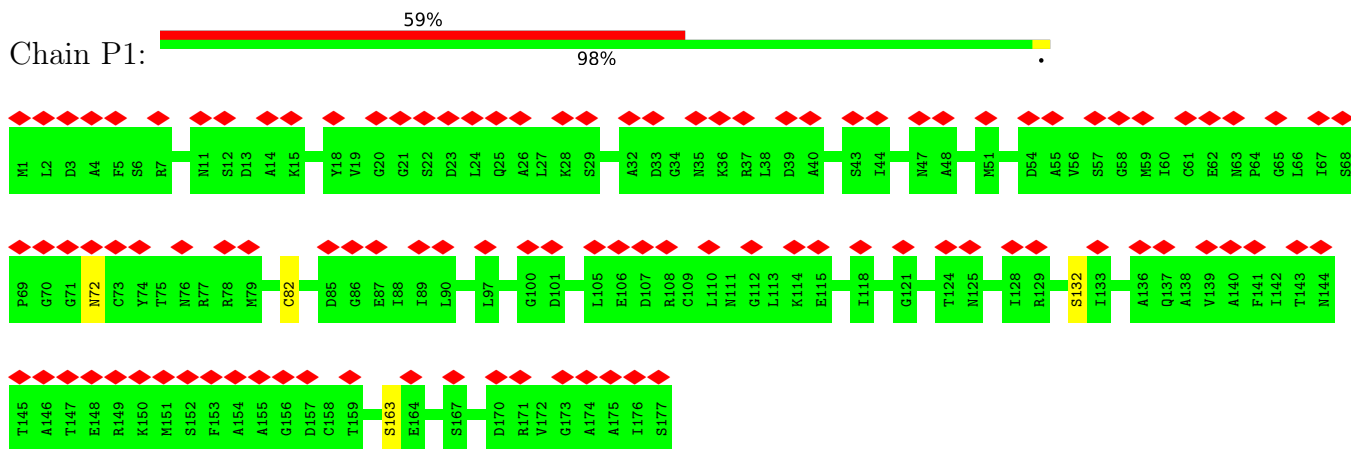
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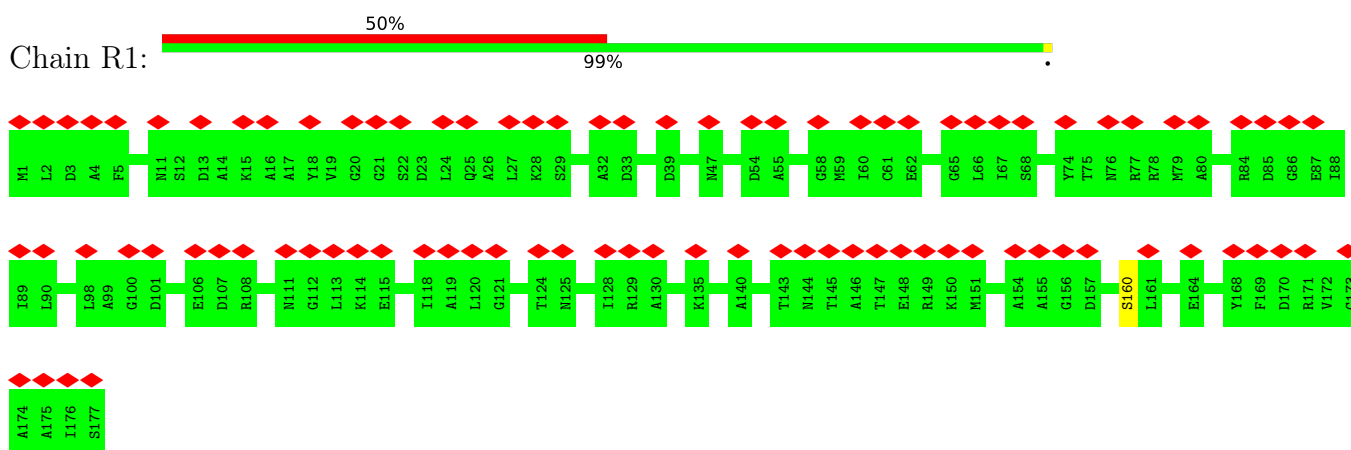
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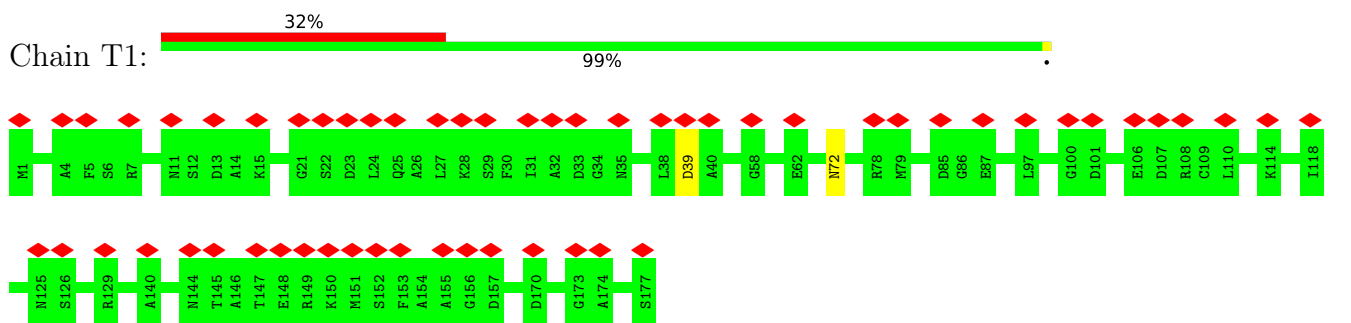
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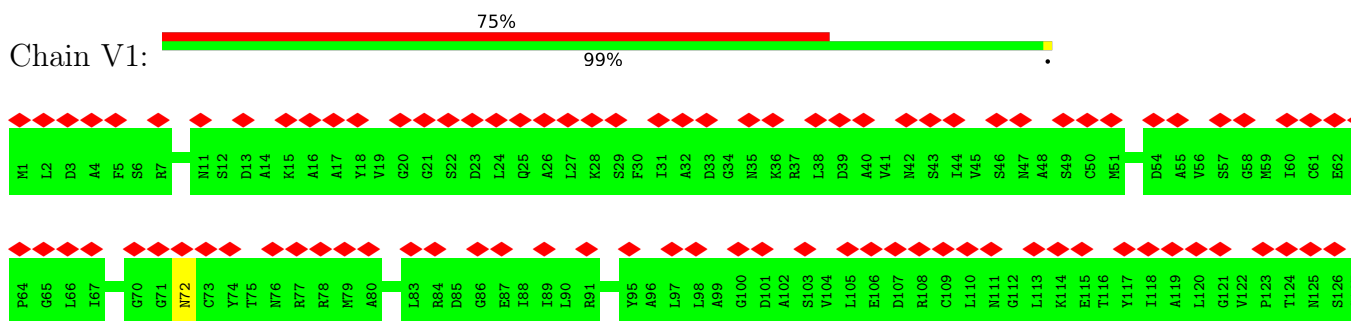
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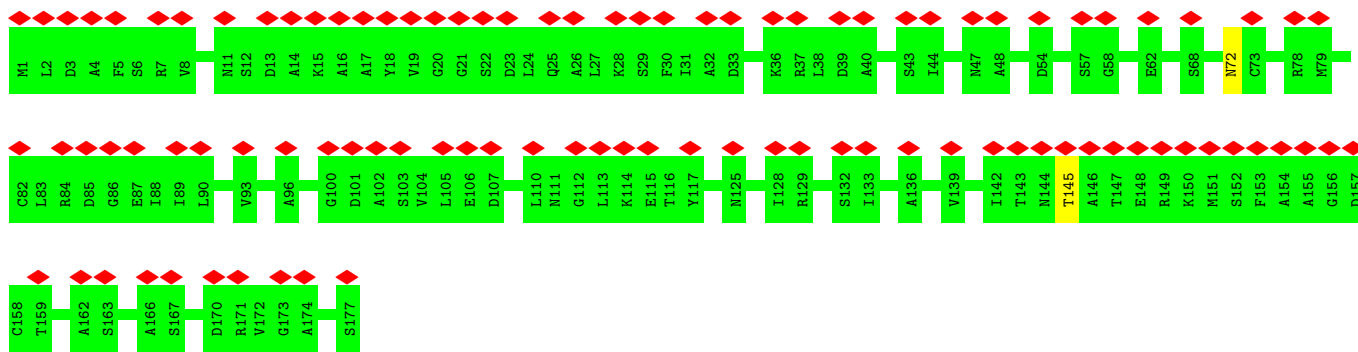


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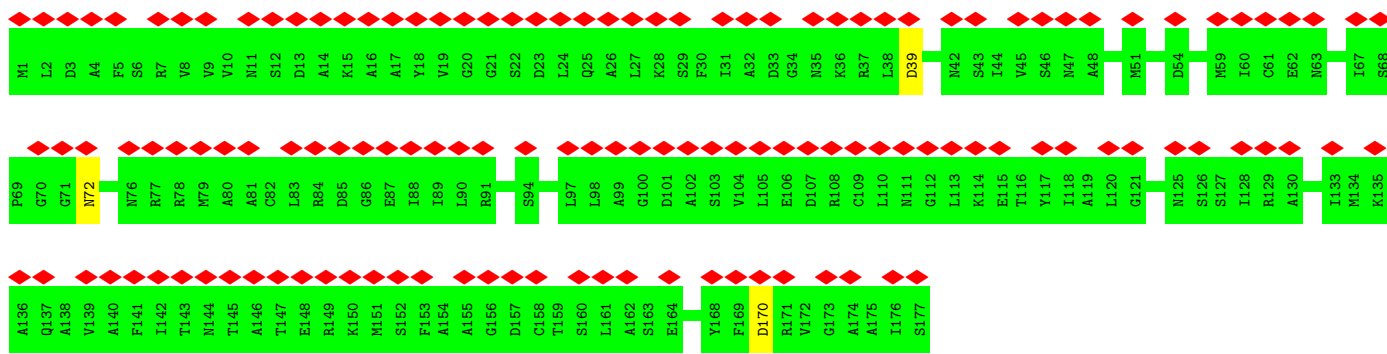
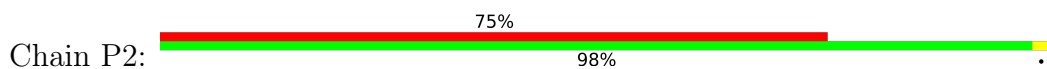




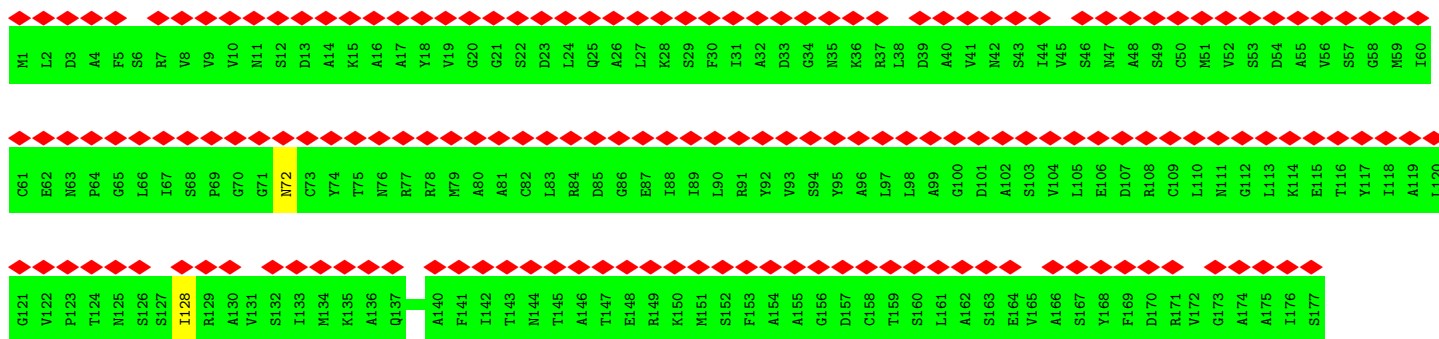
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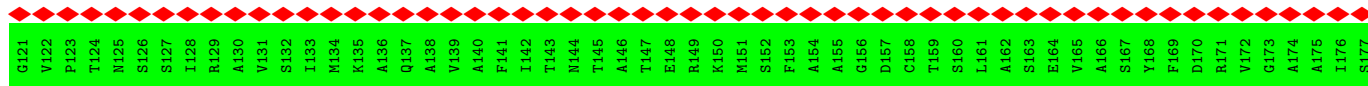
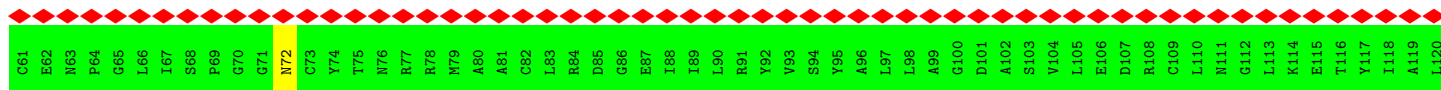
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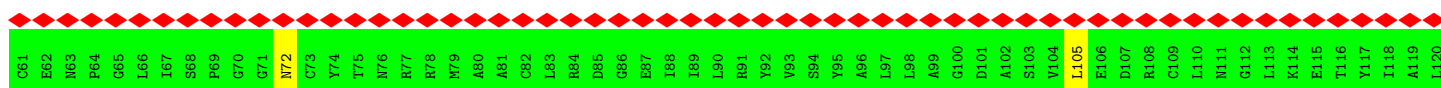
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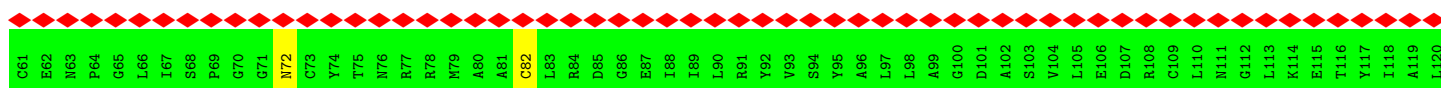
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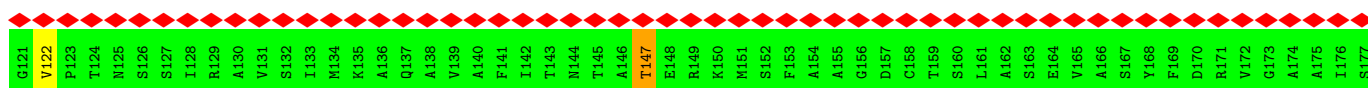
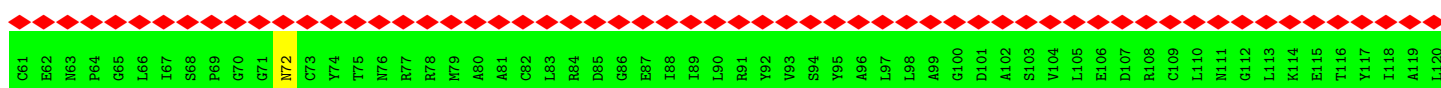
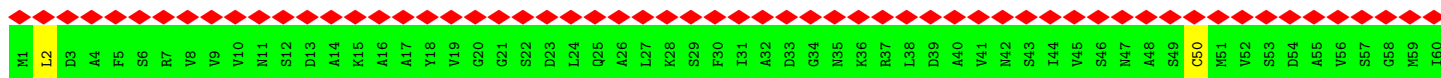
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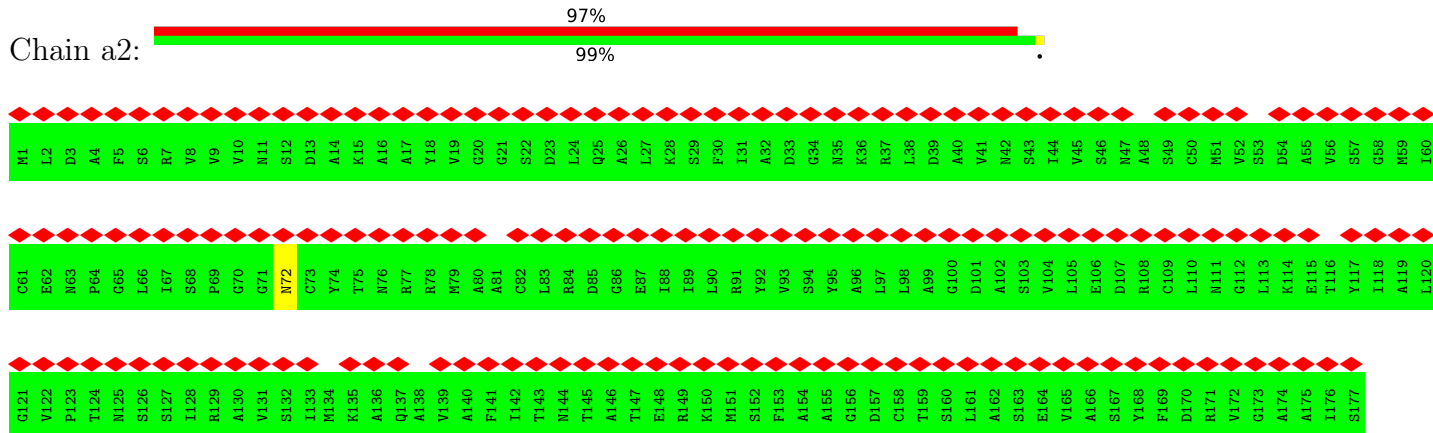
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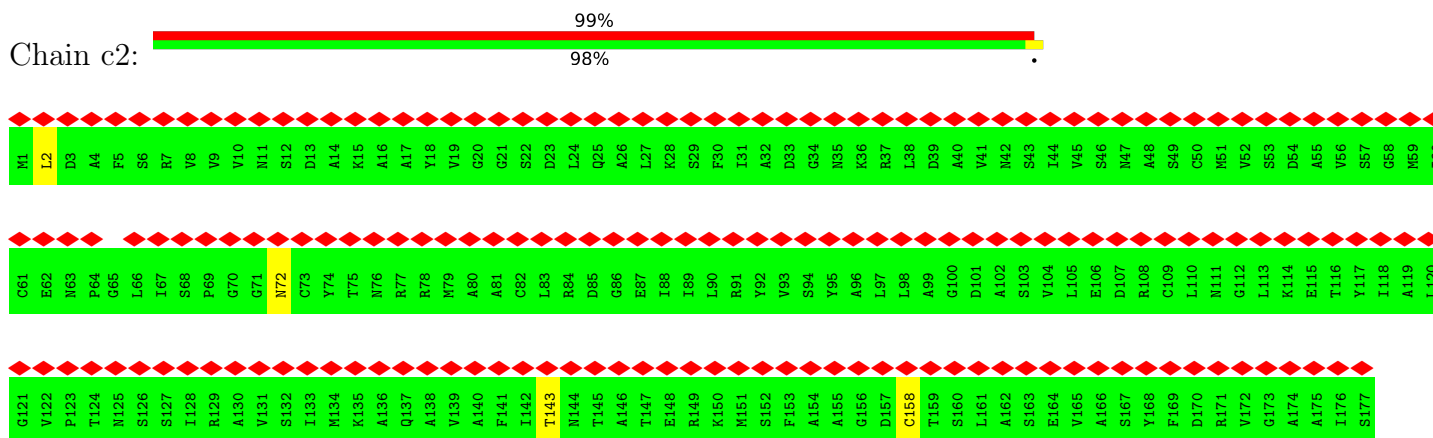
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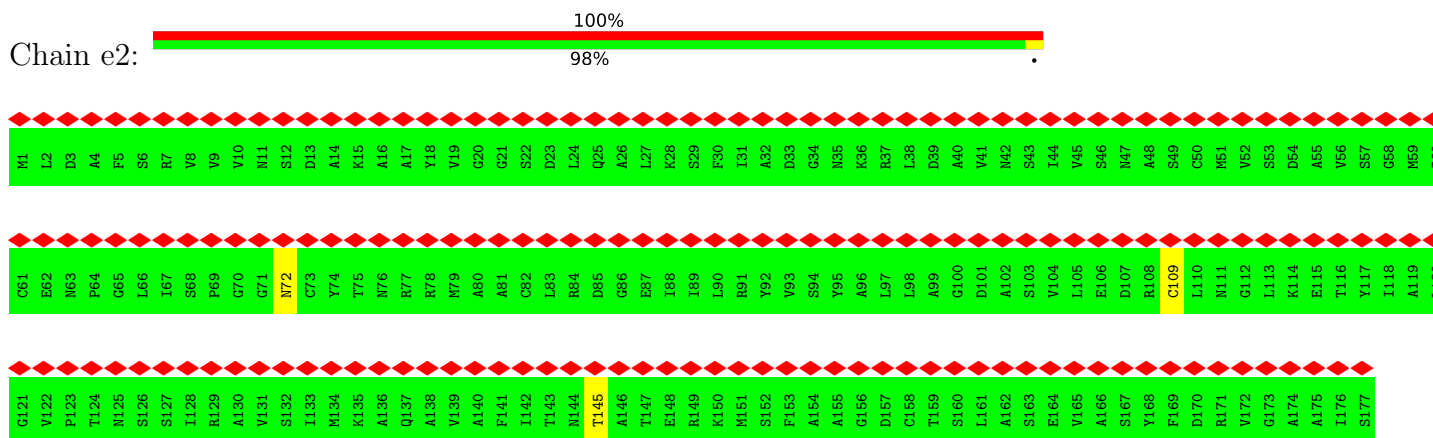
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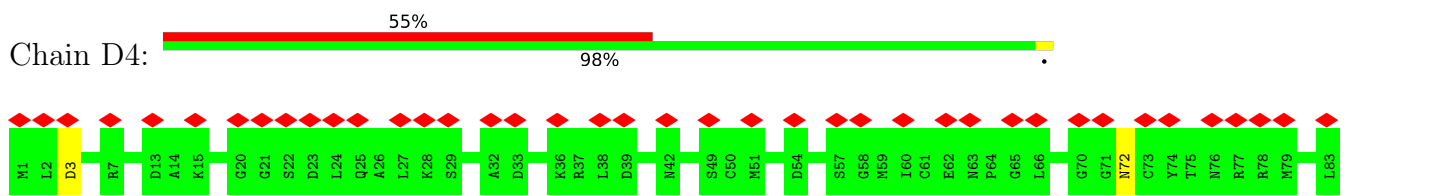
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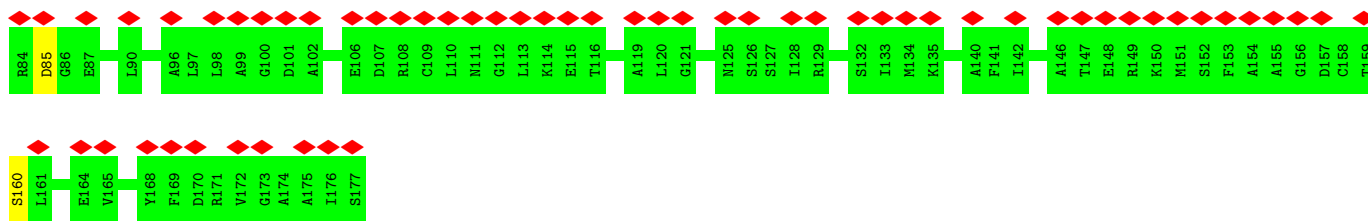


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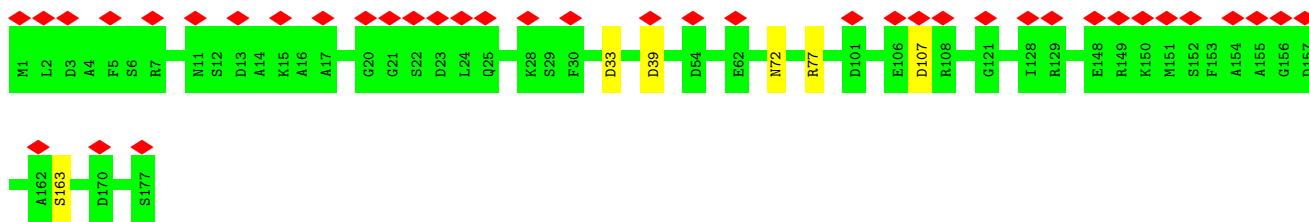


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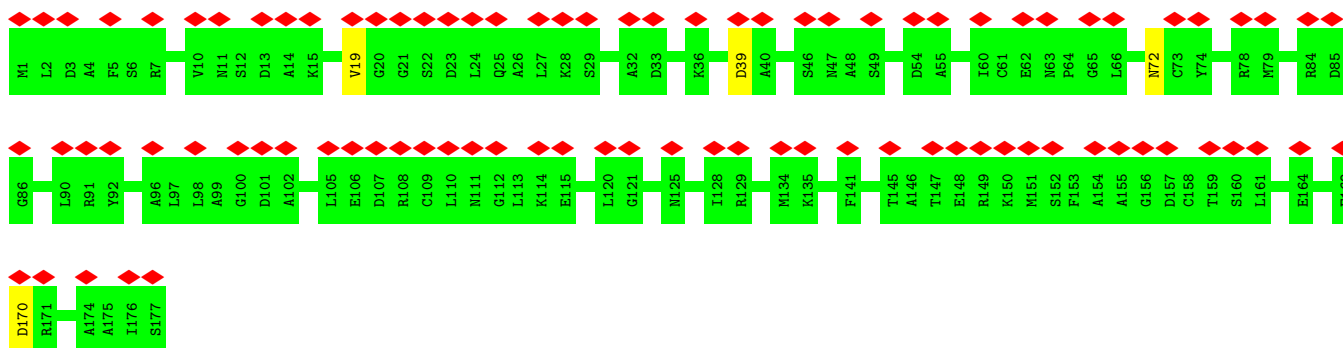




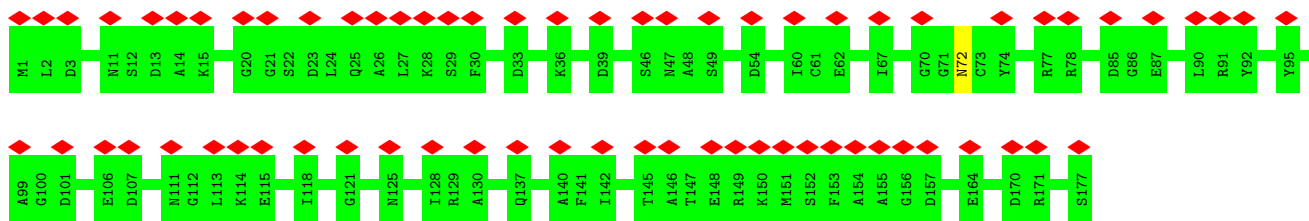
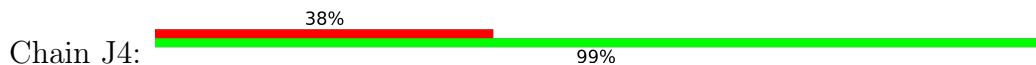
- Molecule 2: B-phycoerythrin beta chain



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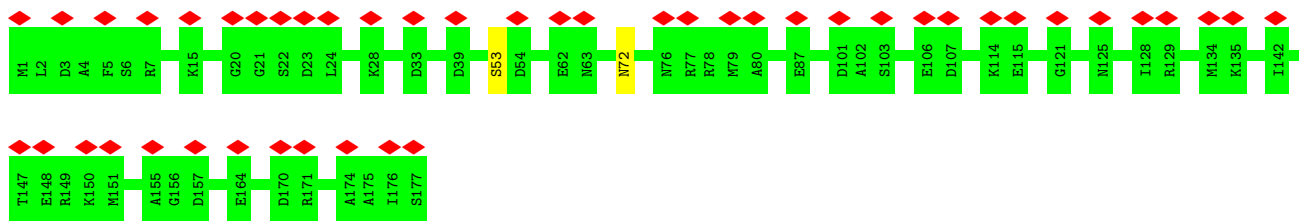


- Molecule 2: B-phycoerythrin beta chain

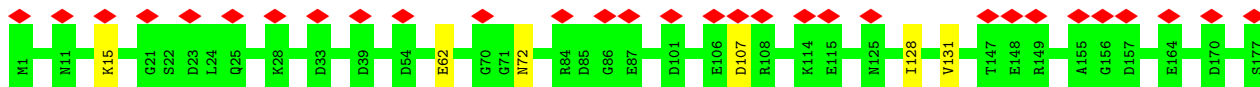


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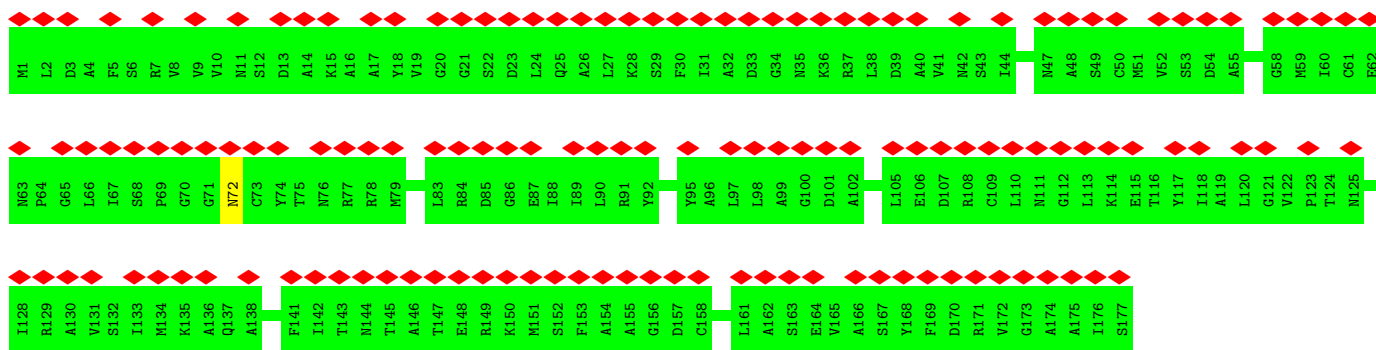
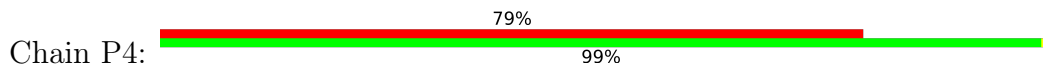




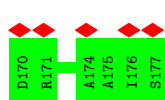
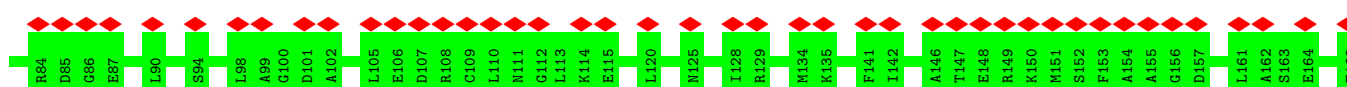
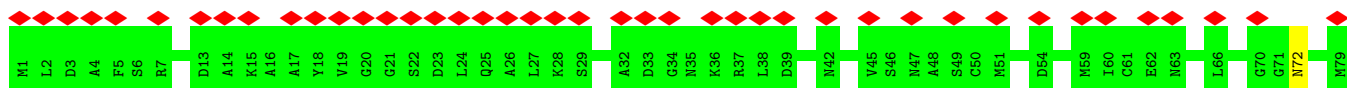
• Molecule 2: B-phycoerythrin beta chain



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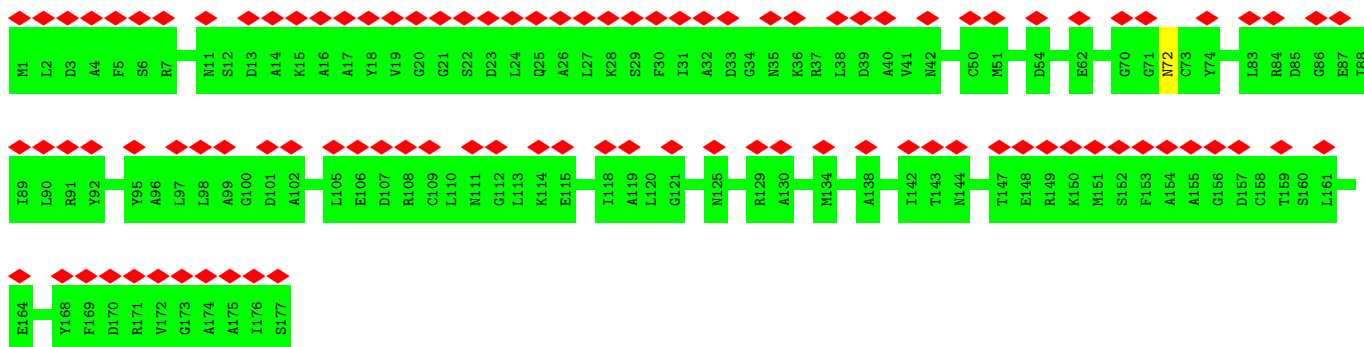


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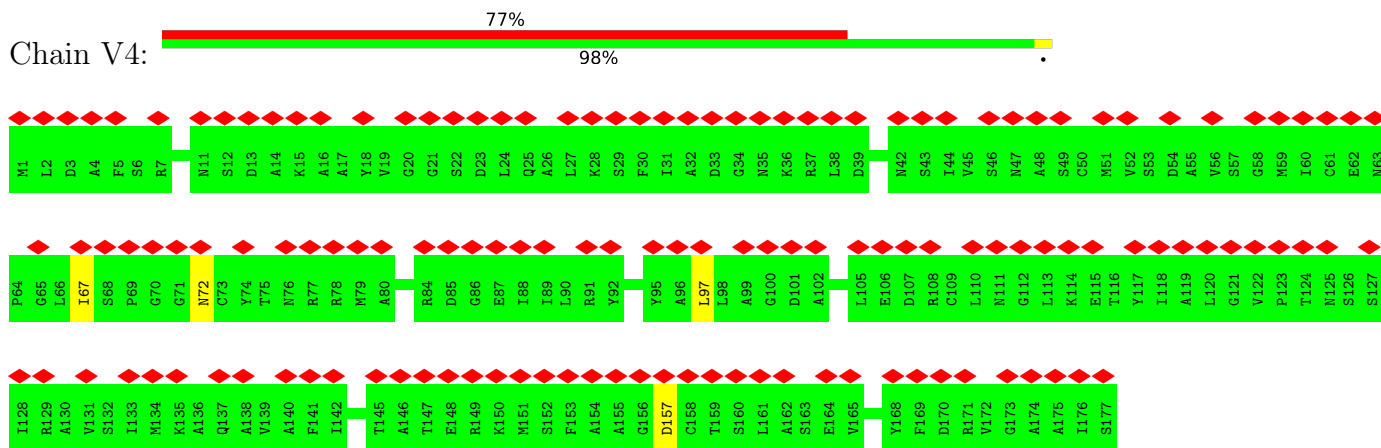


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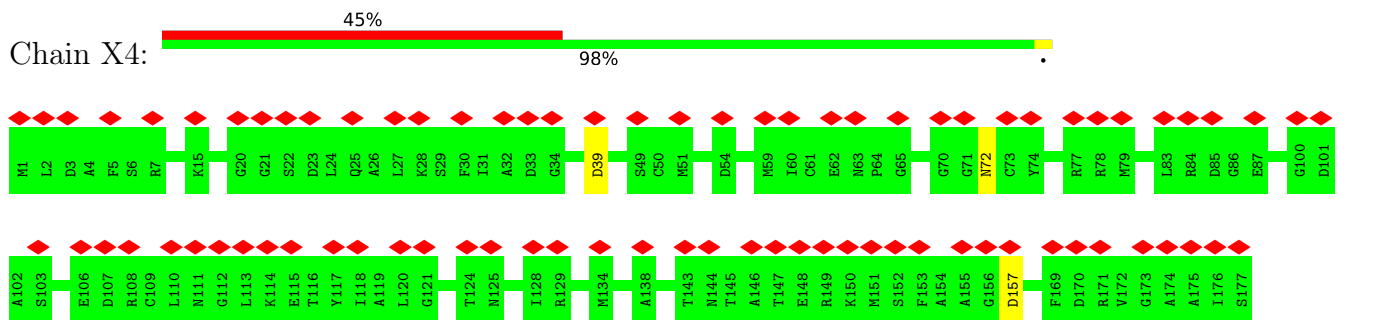




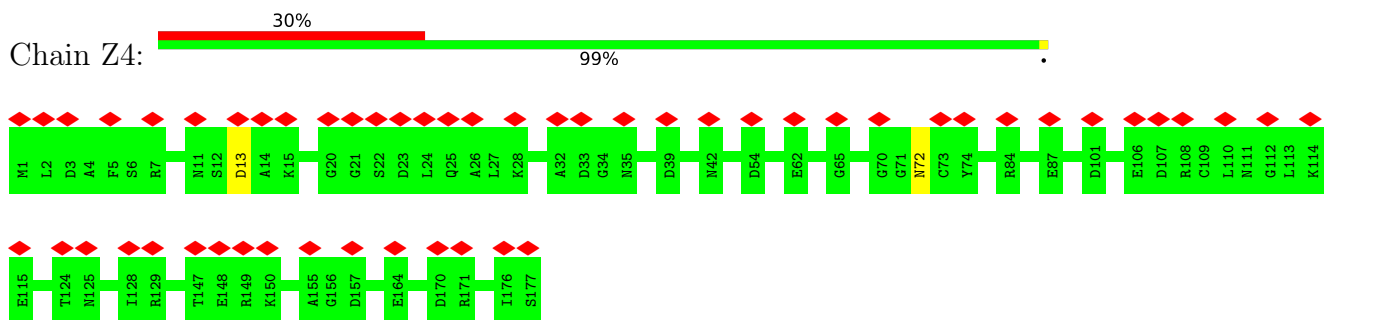
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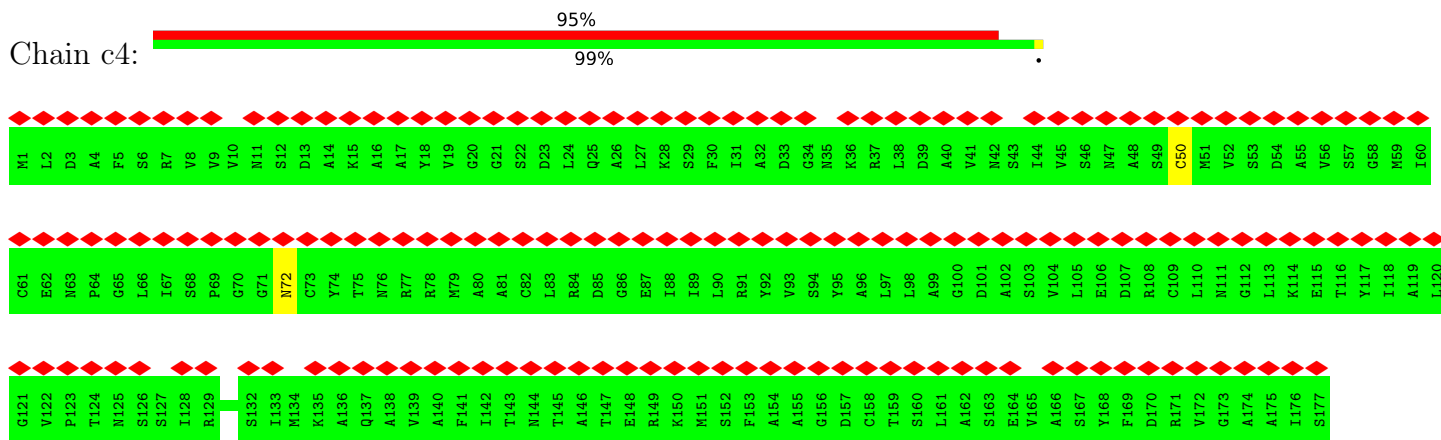
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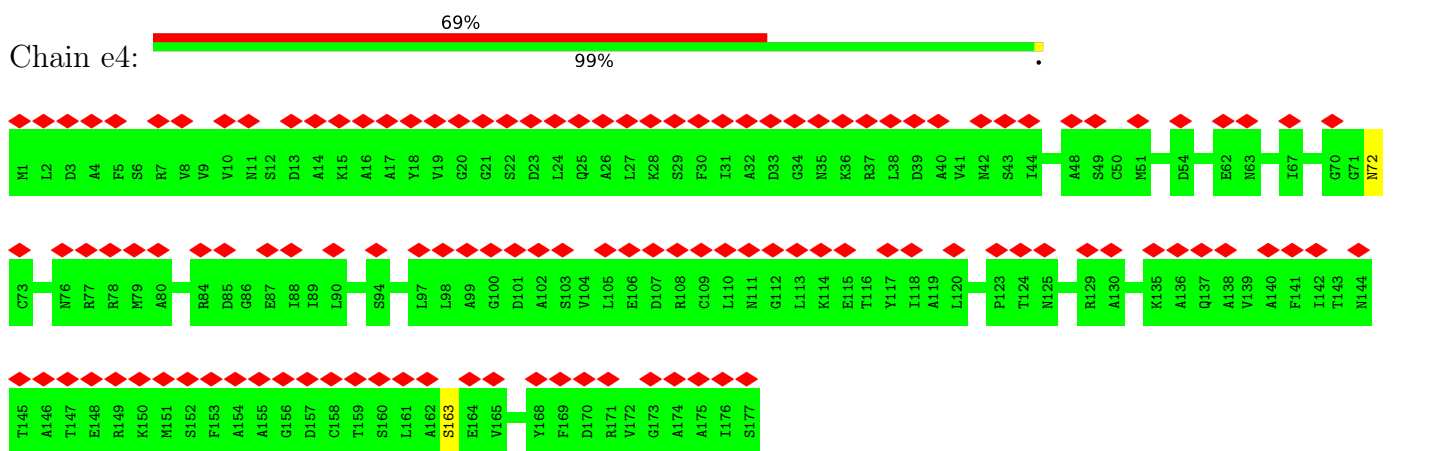
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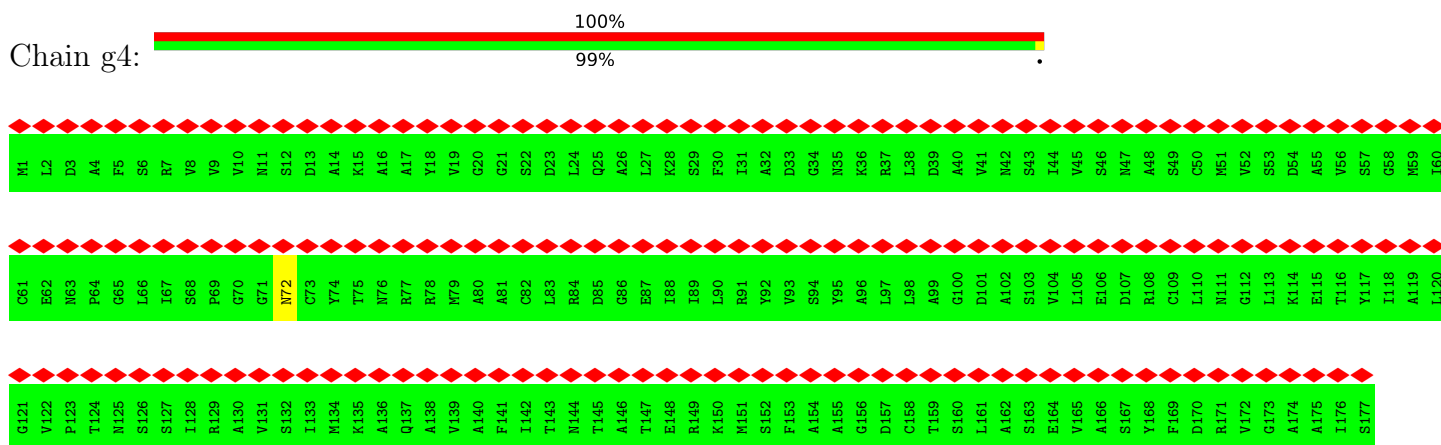
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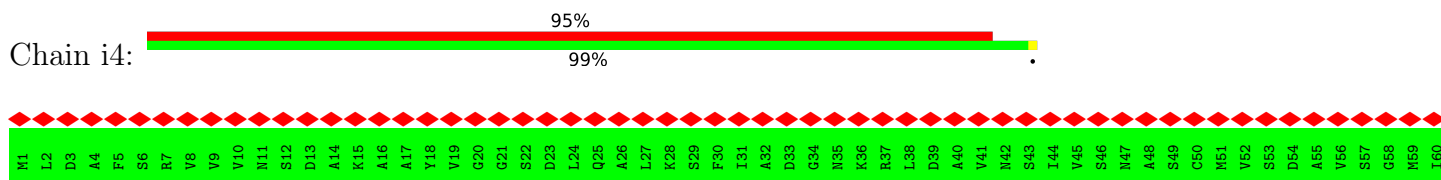
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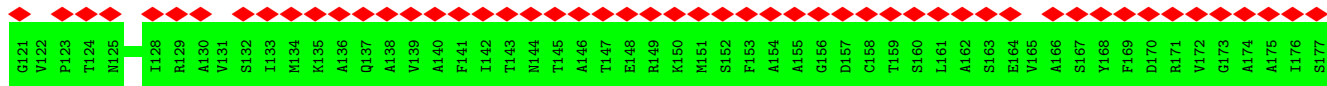
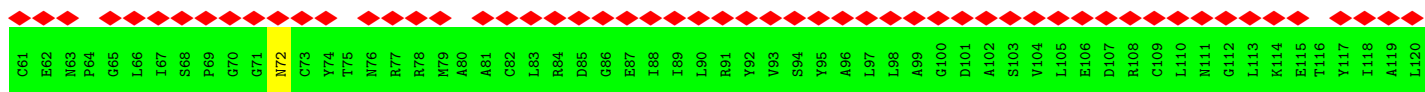


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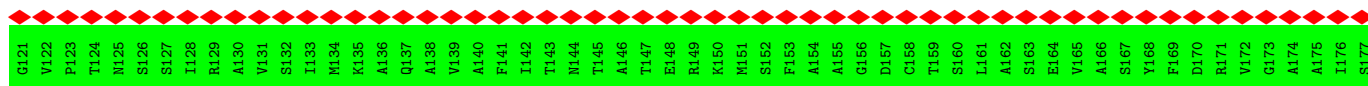
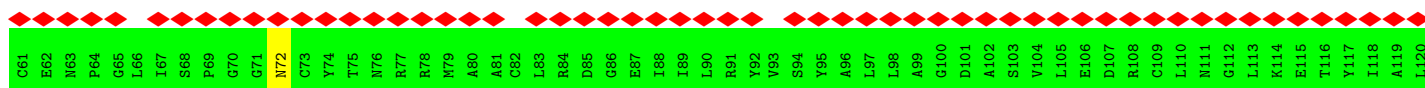
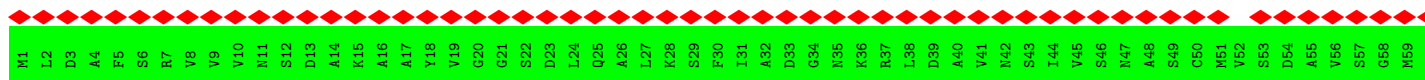


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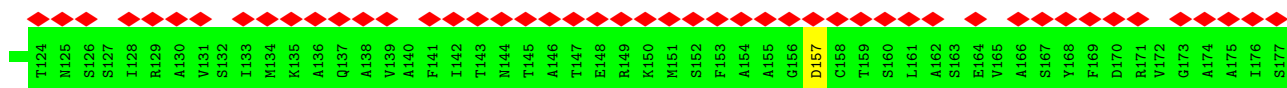
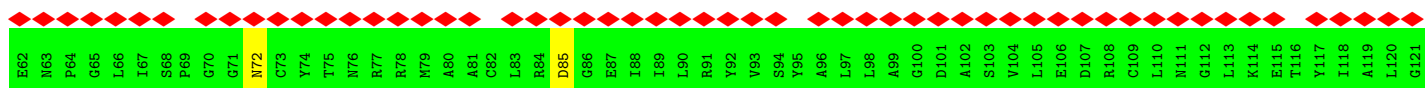
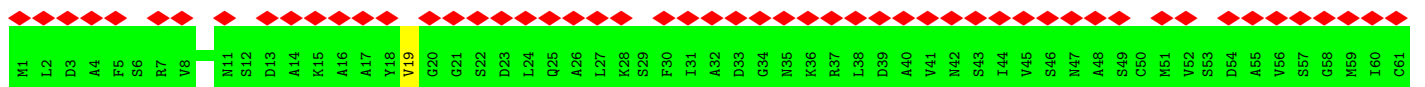




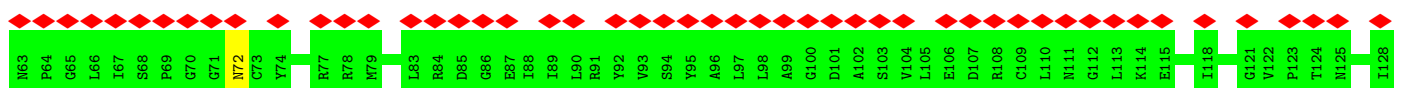
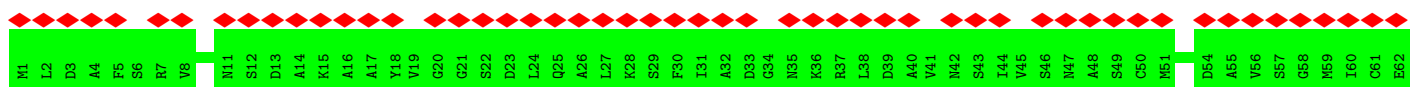
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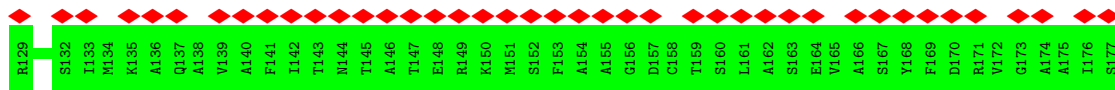


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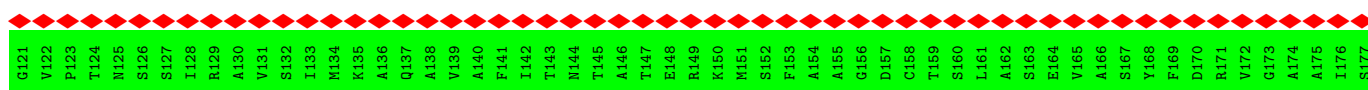
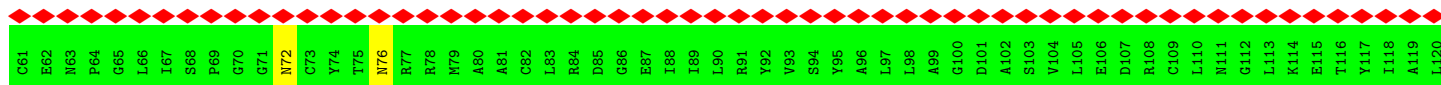


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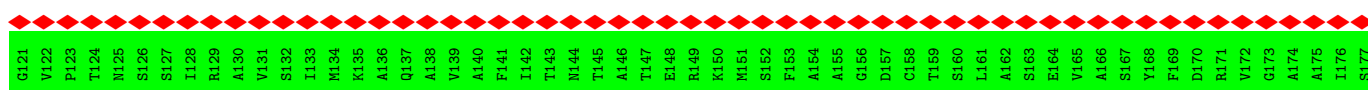




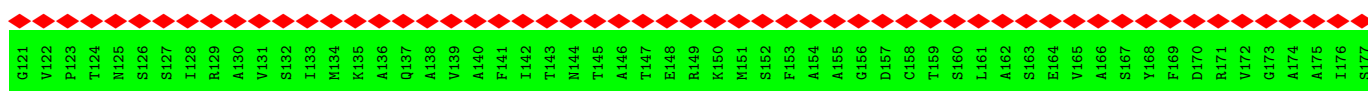
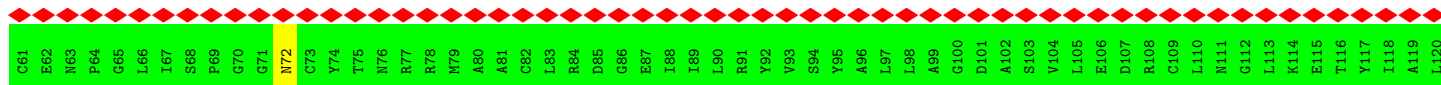
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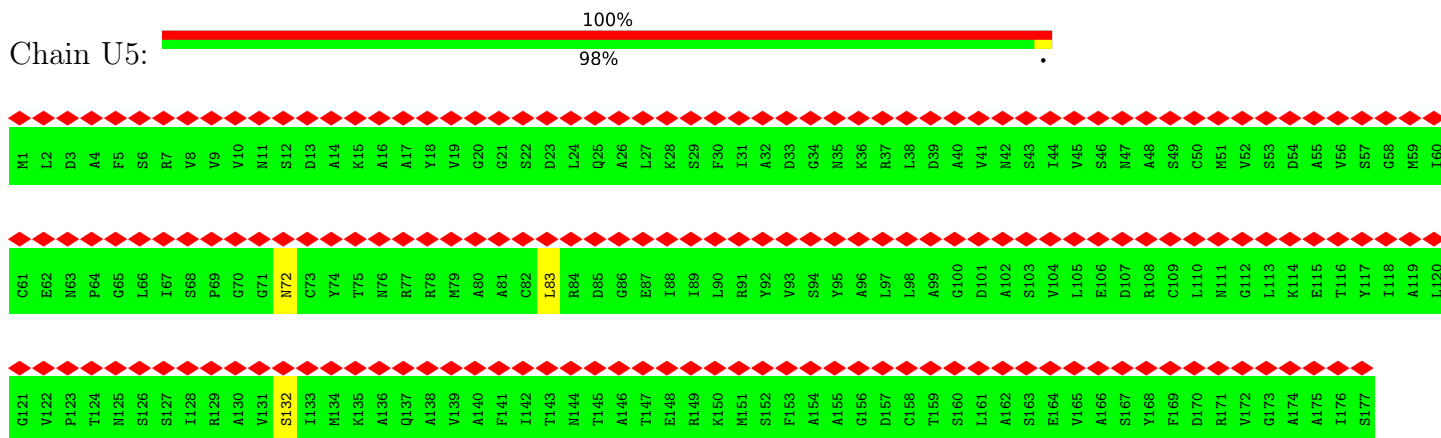
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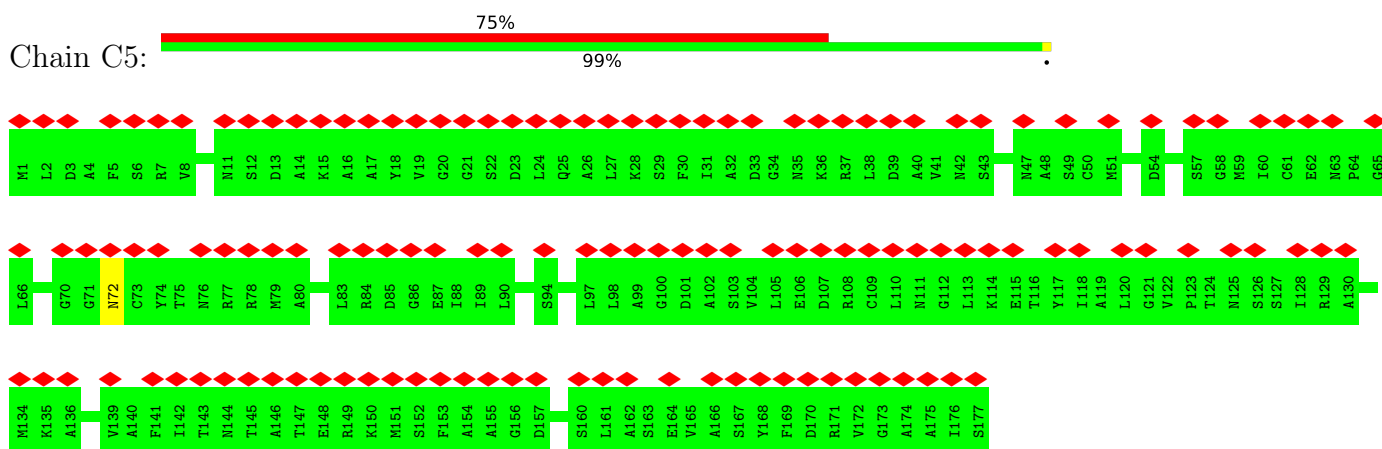
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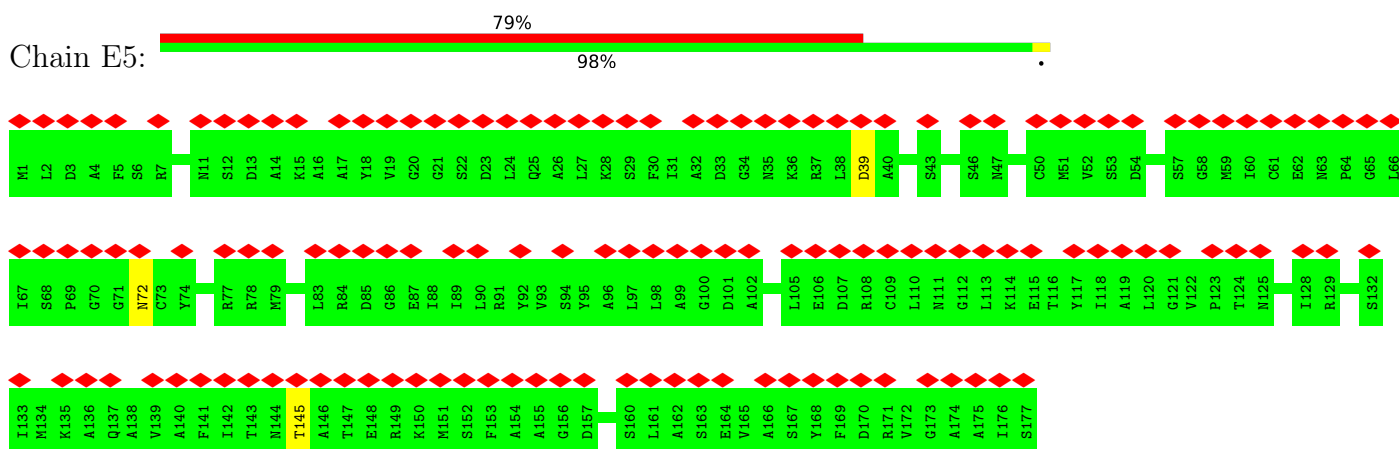
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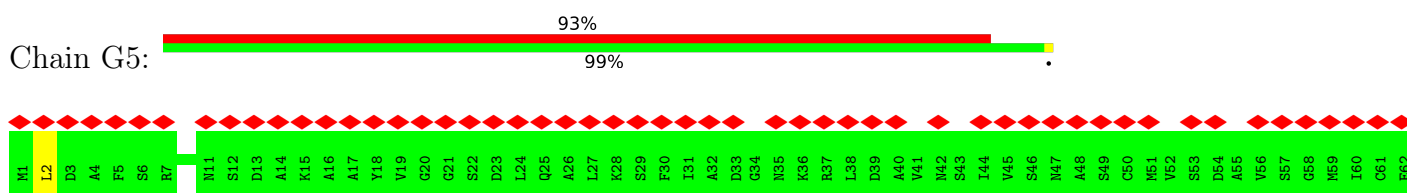
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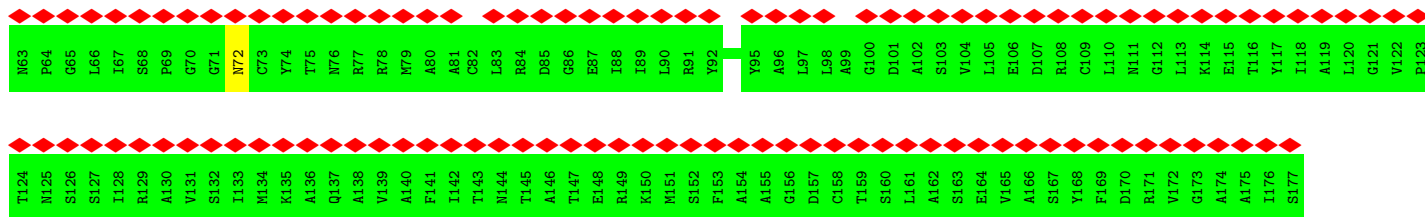


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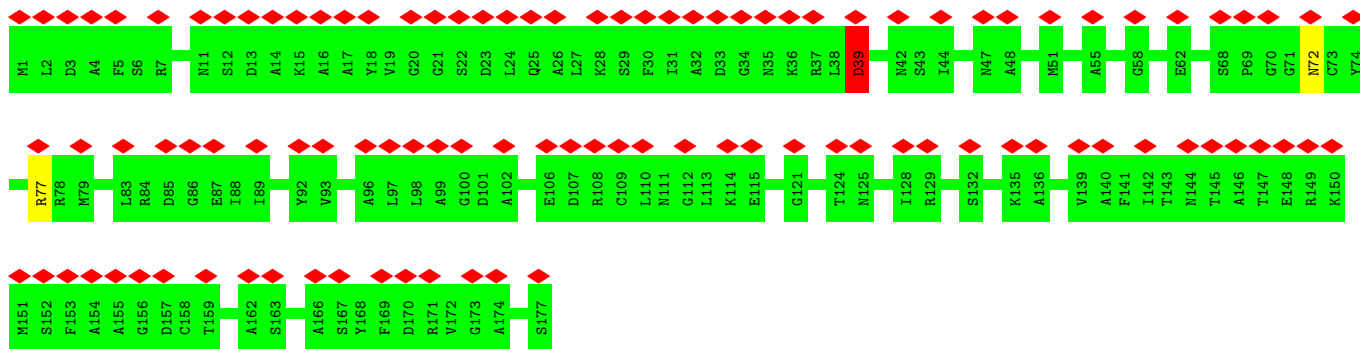


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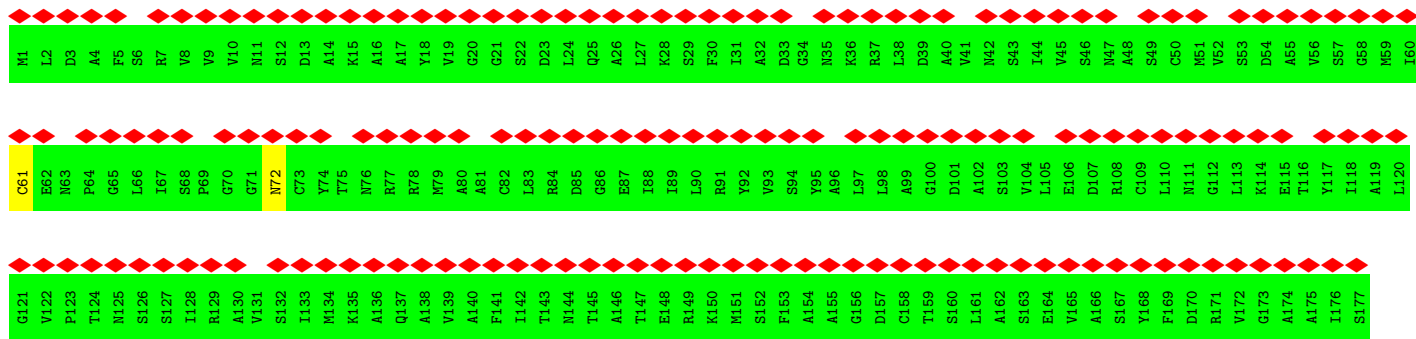




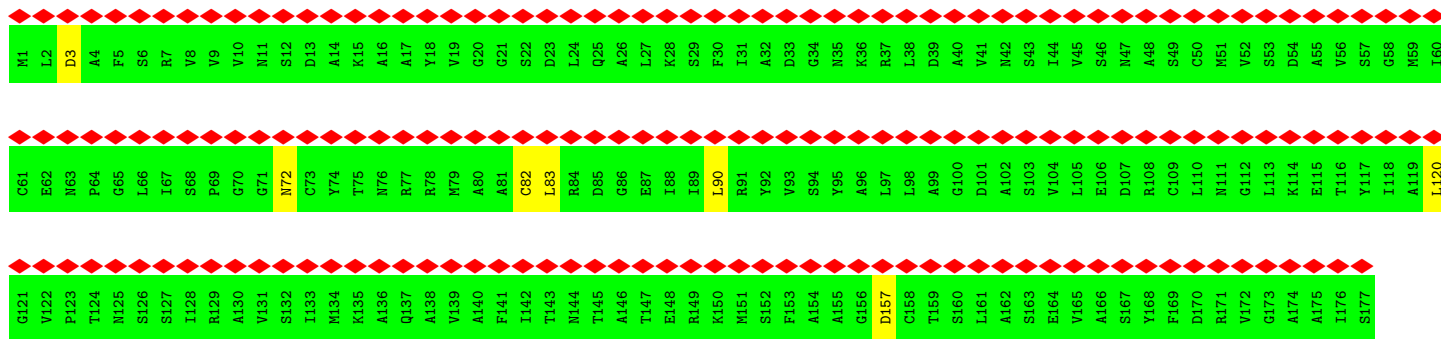
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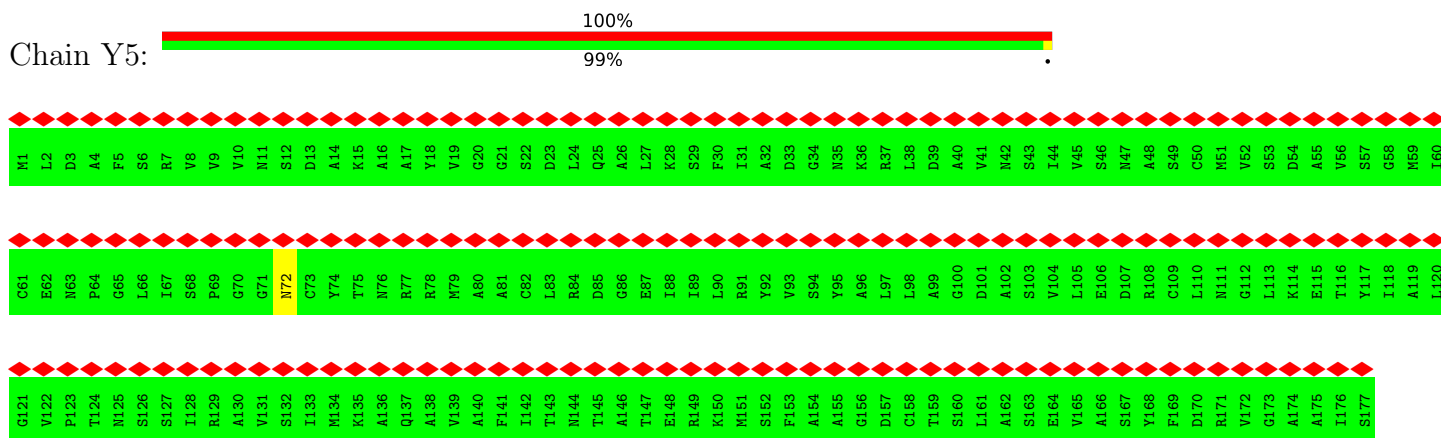
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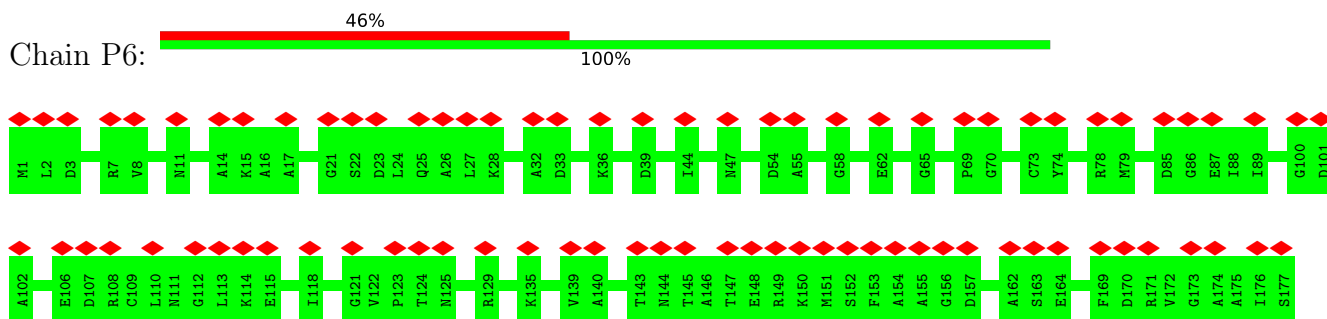
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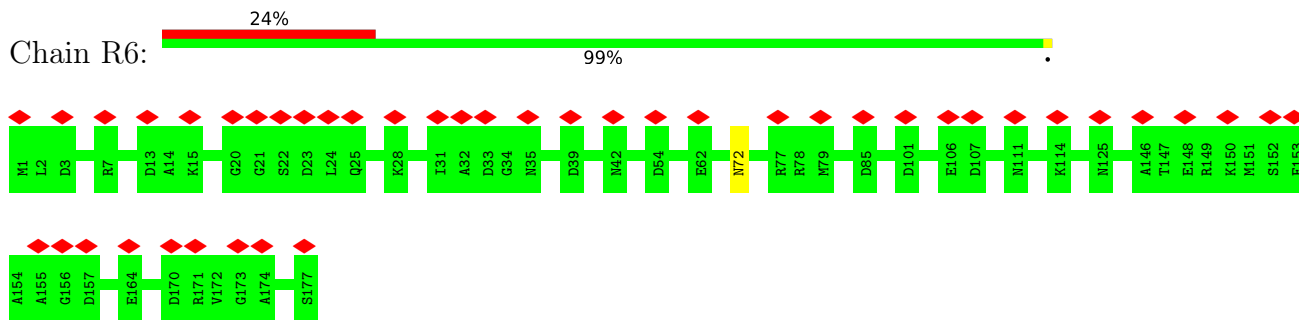
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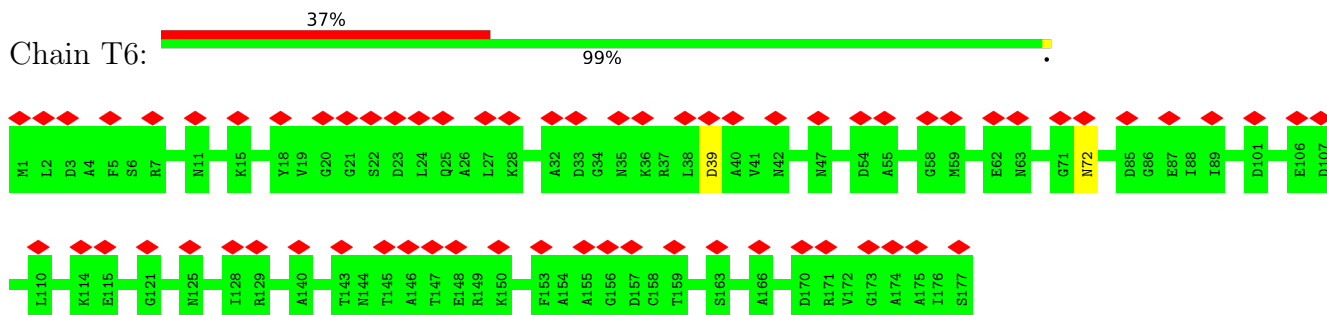
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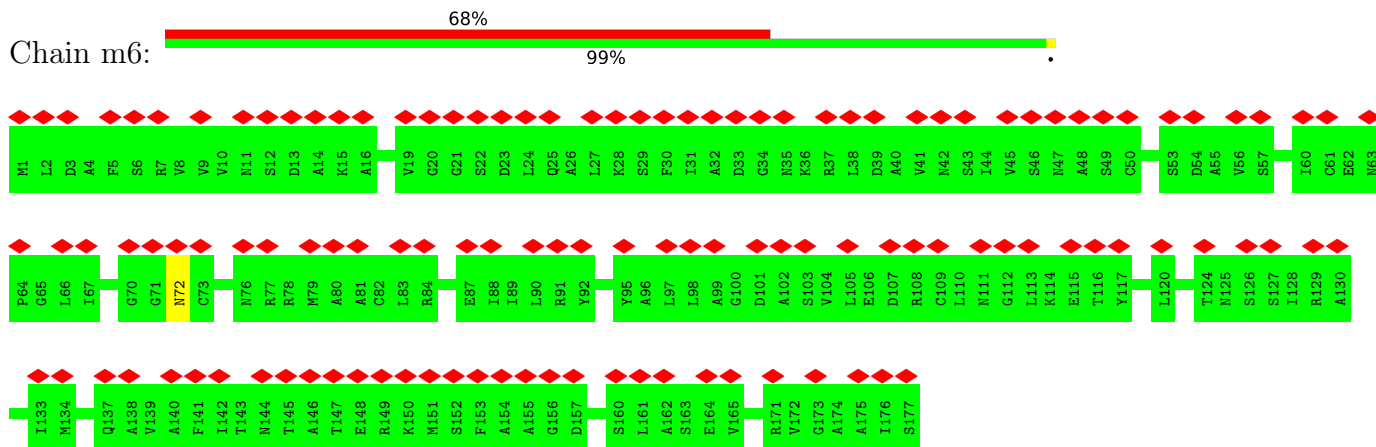


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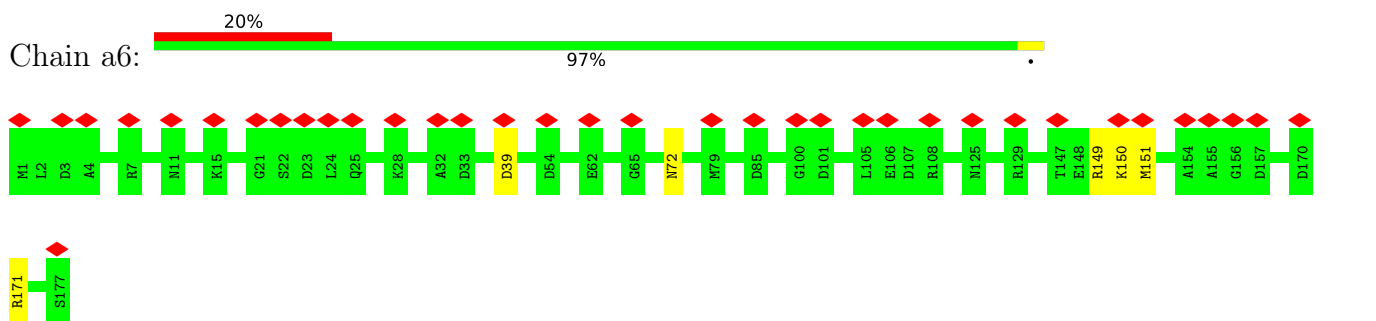


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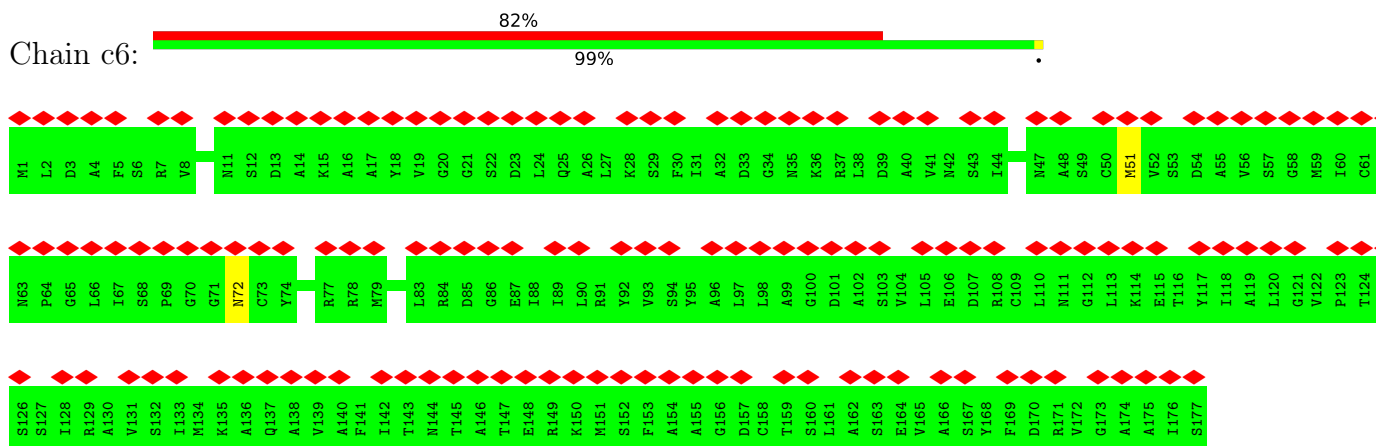
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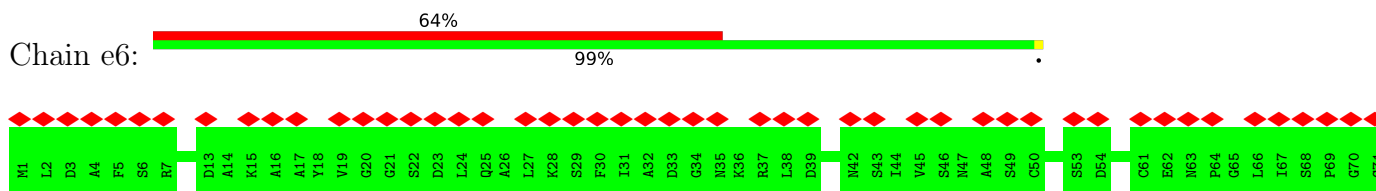
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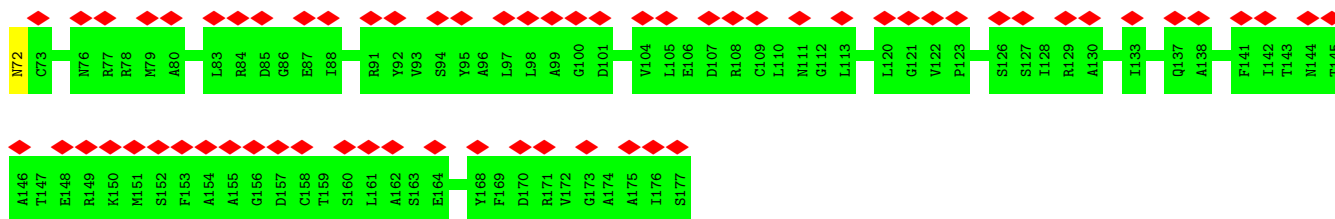


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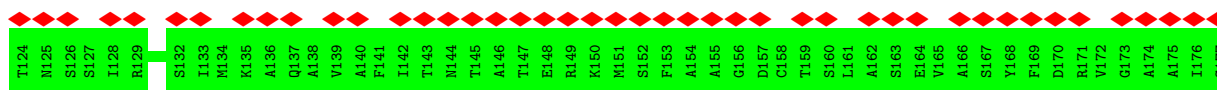
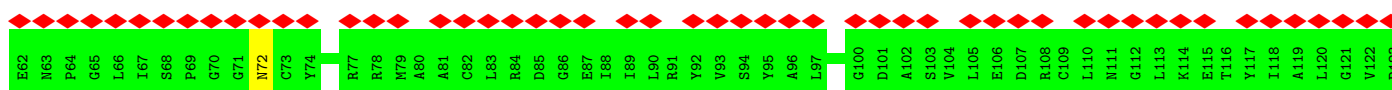
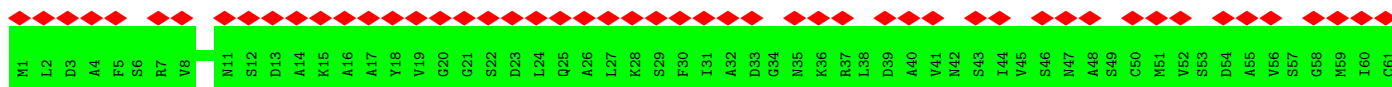
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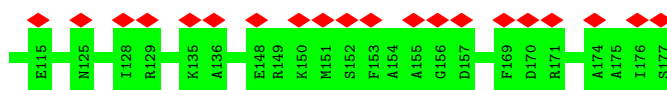
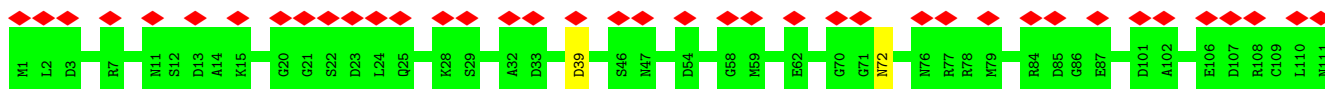
- Molecule 2: B-phycoerythrin beta chain

Chain g6: 99% 83%



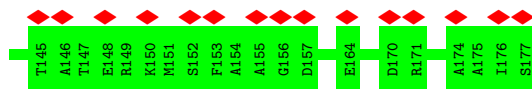
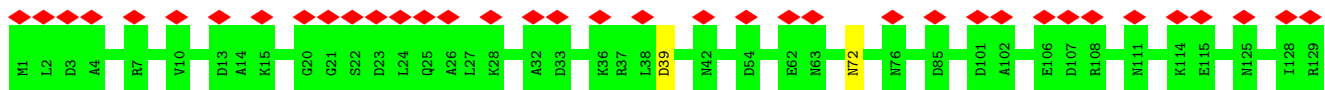
- Molecule 2: B-phycoerythrin beta chain

Chain B7: 99% 33%



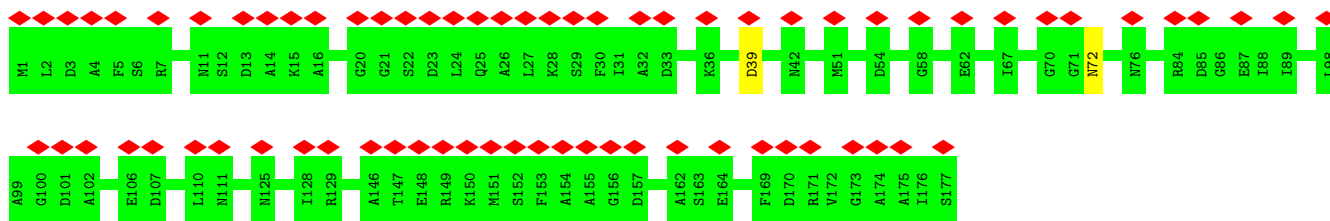
- Molecule 2: B-phycoerythrin beta chain

Chain D7: 99% 29%

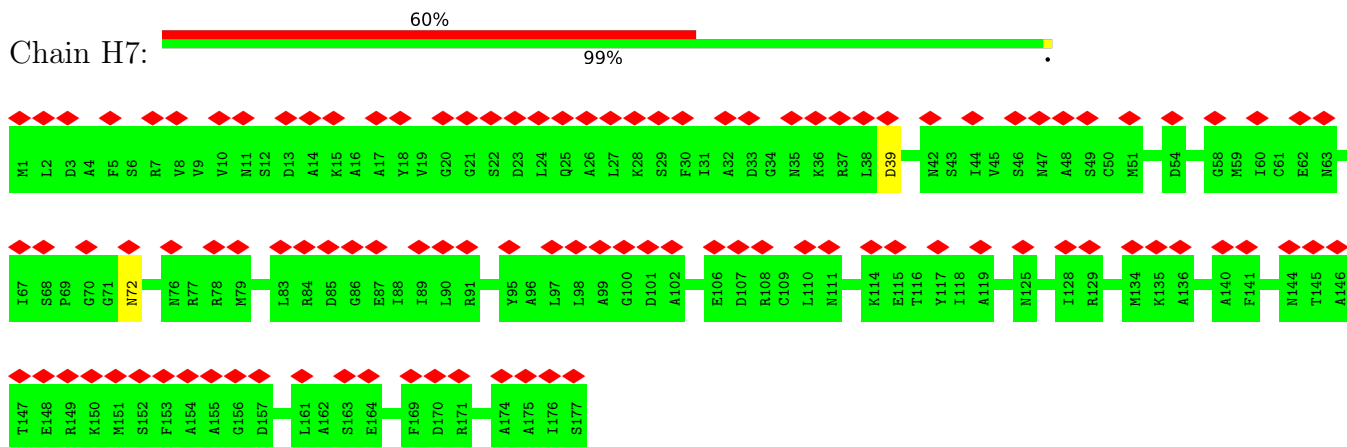


- Molecule 2: B-phycoerythrin beta chain

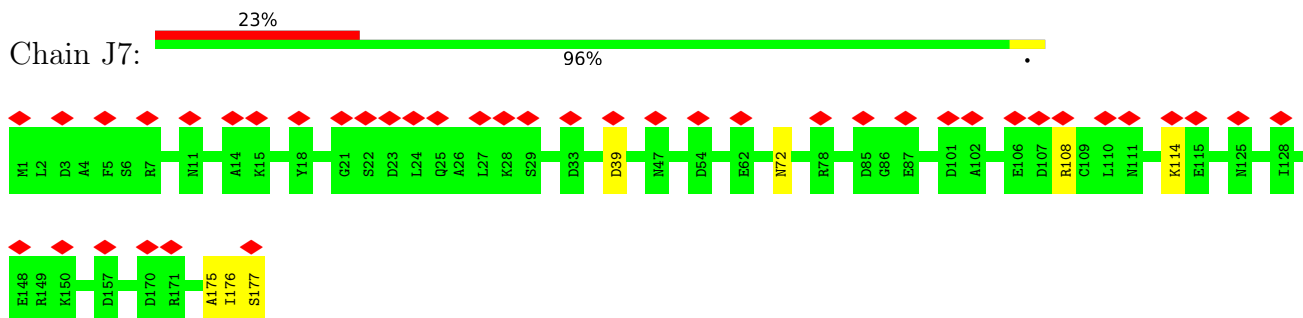
Chain F7: 99% 40%



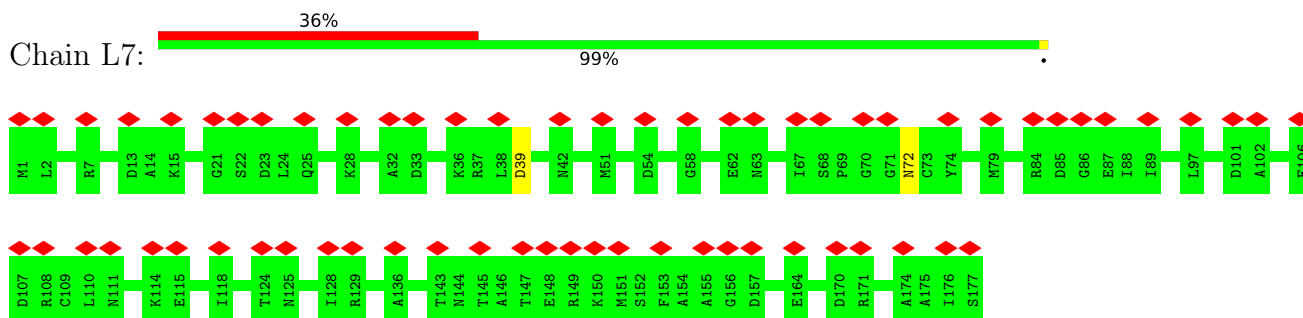
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

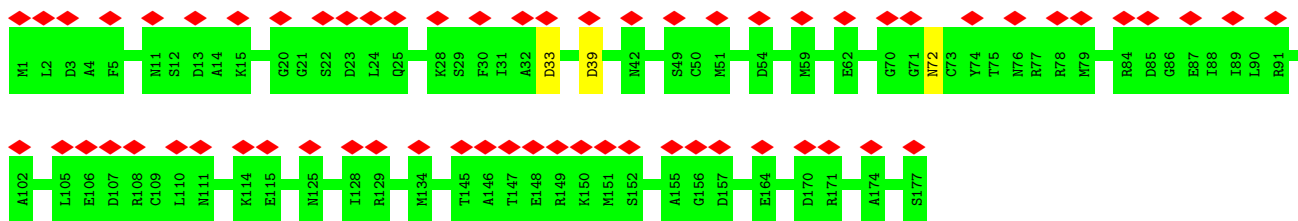


- Molecule 2: B-phycoerythrin beta chain

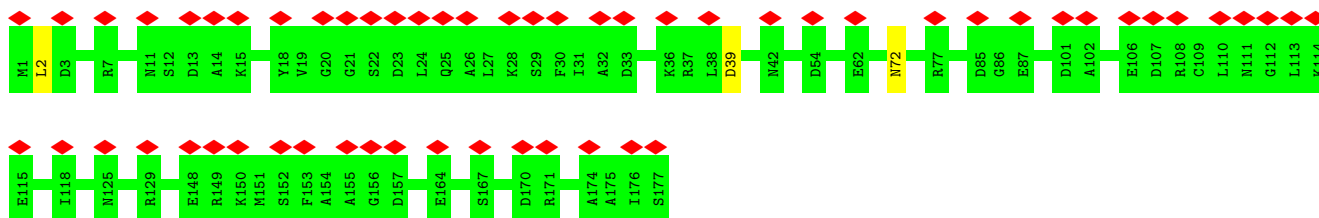


- Molecule 2: B-phycoerythrin beta chain

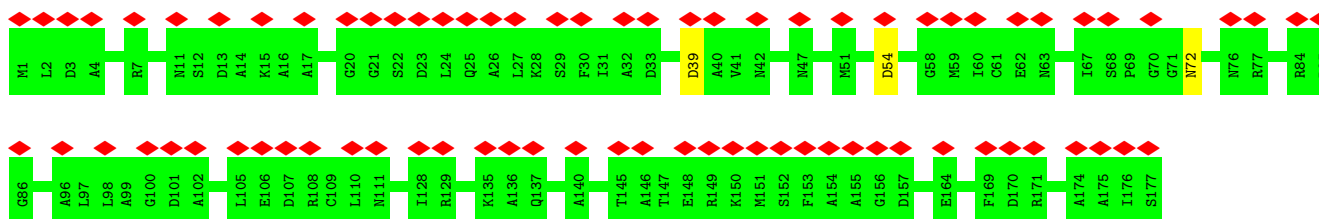




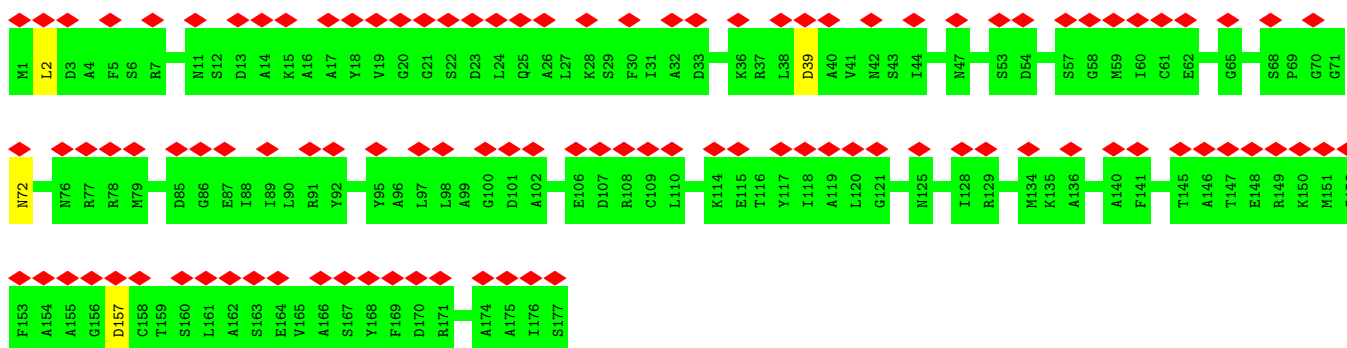
- Molecule 2: B-phycoerythrin beta chain



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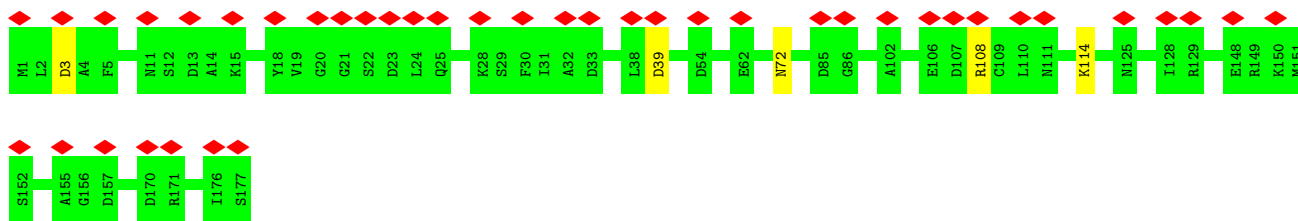


- Molecule 2: B-phycoerythrin beta chain

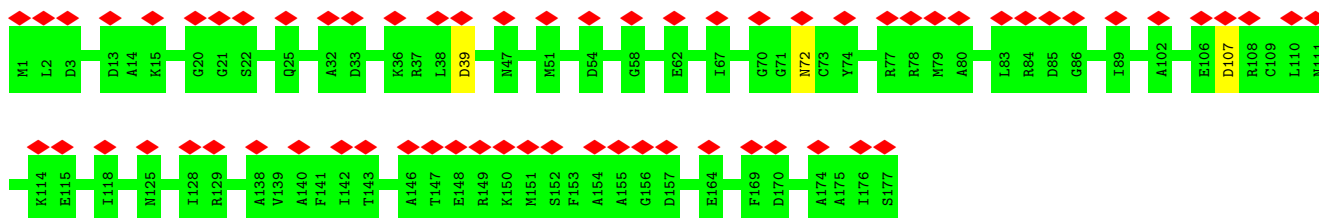


- Molecule 2: B-phycoerythrin beta chain

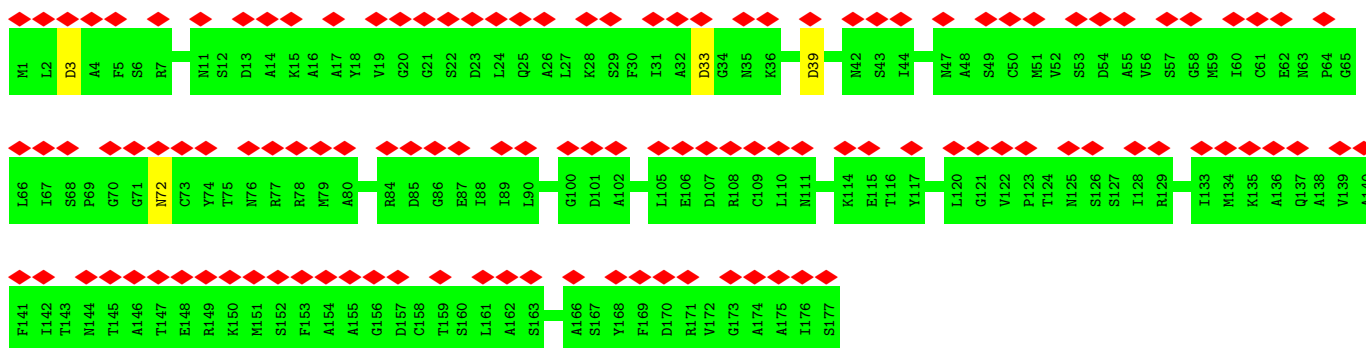




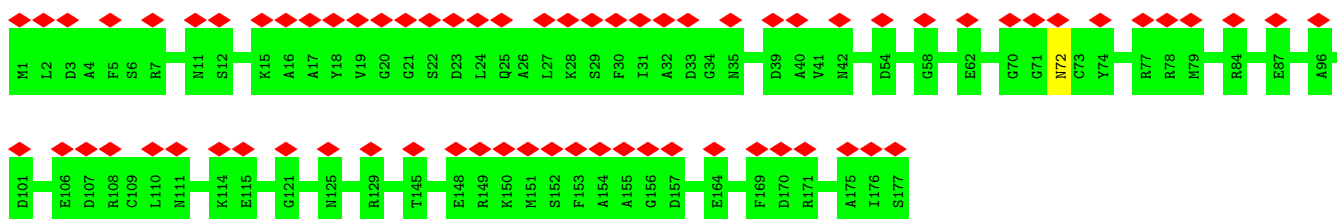
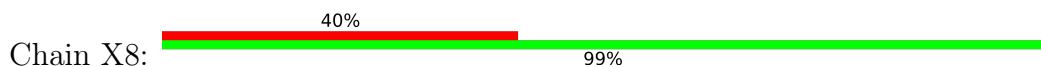
- Molecule 2: B-phycoerythrin beta chain



- Molecule 2: B-phycoerythrin beta chain

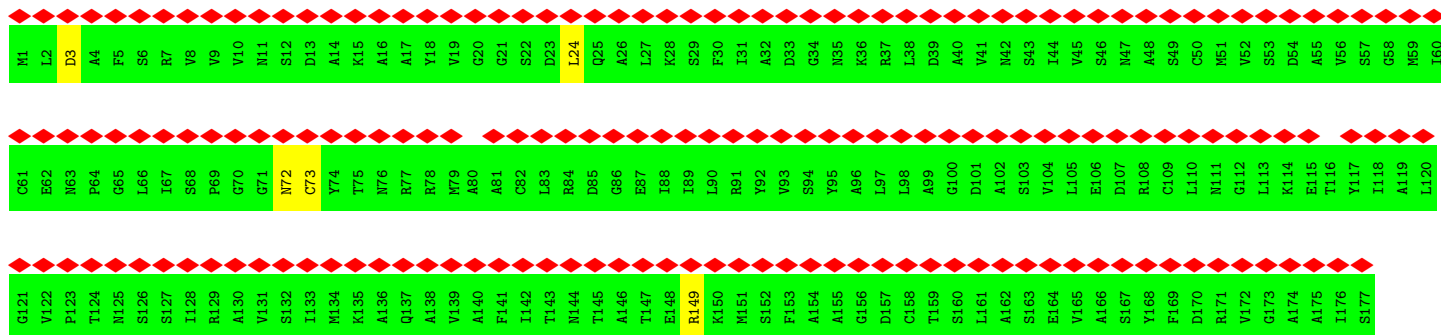


- Molecule 2: B-phycoerythrin beta chain

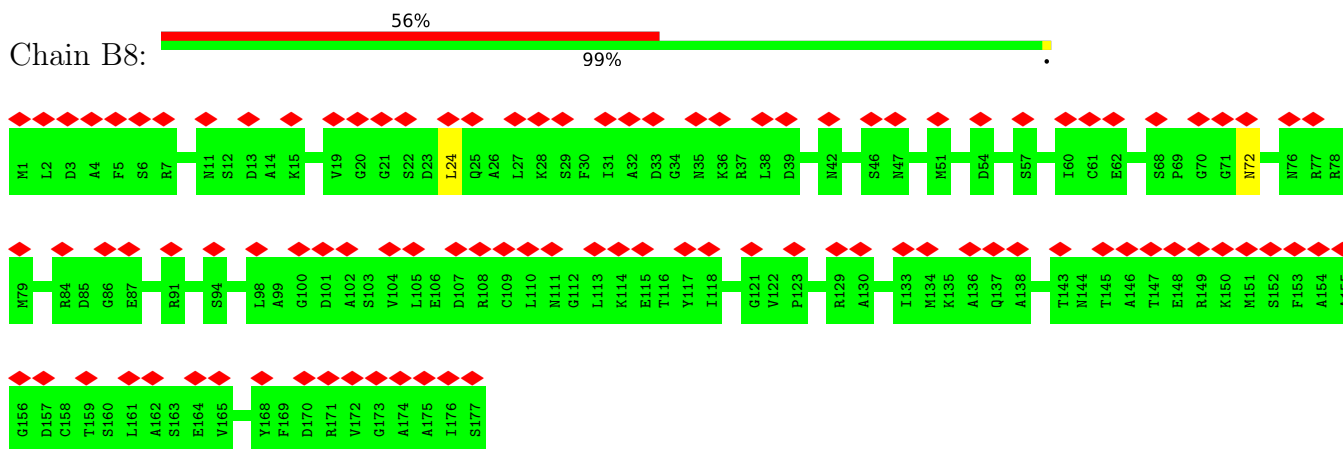


- Molecule 2: B-phycoerythrin beta chain

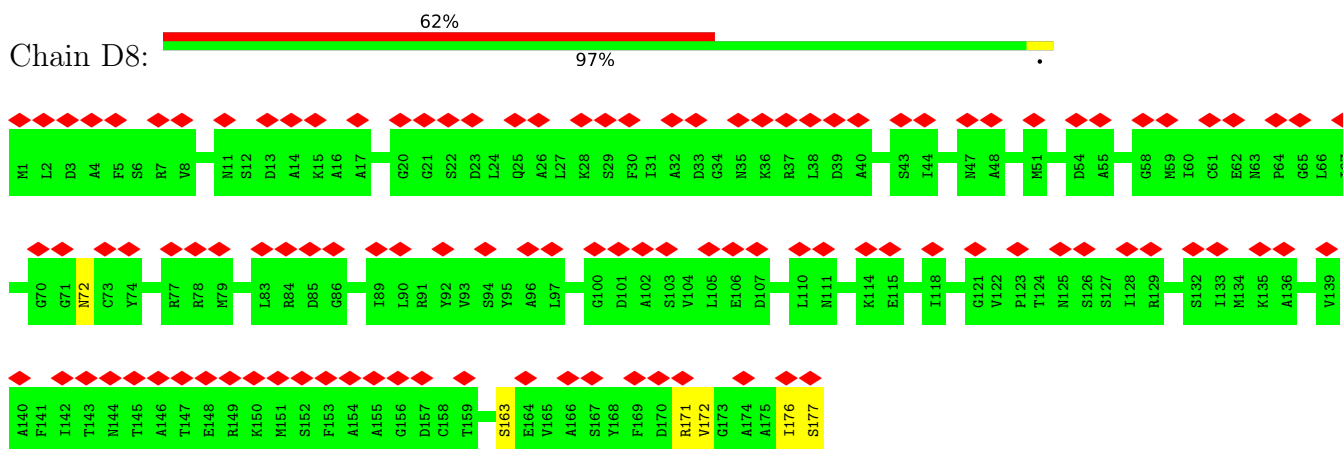




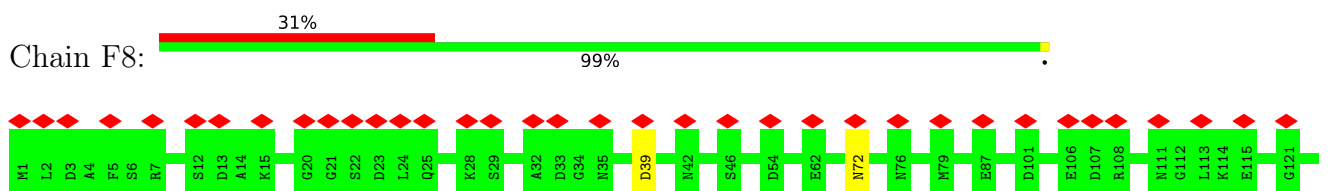
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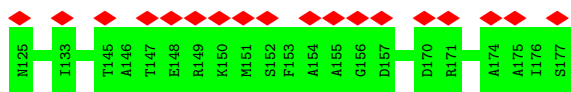


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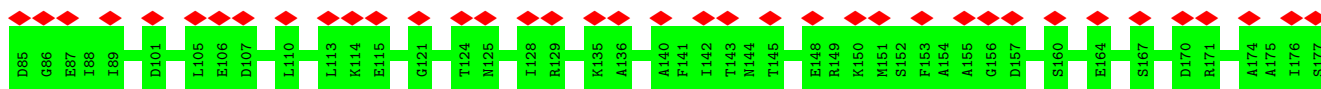
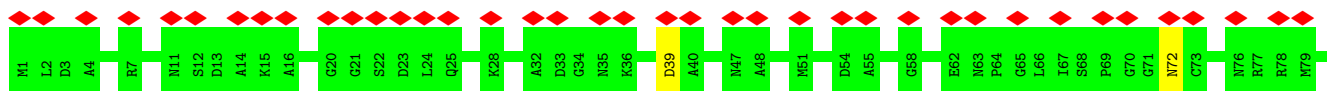
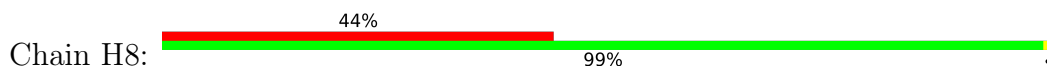


• Molecule 2: B-phycoerythrin beta chain

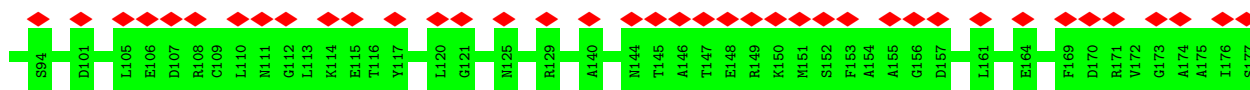
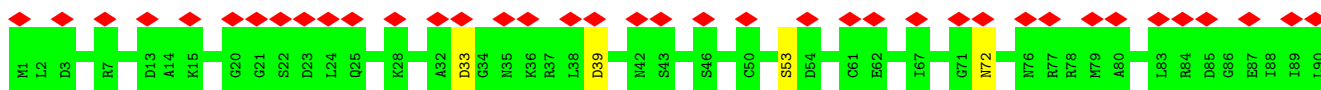
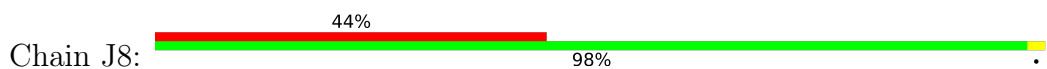




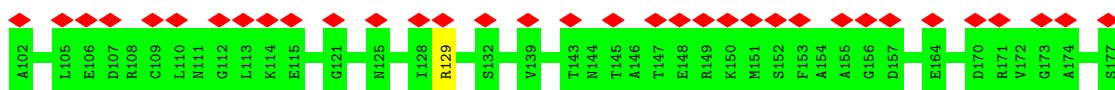
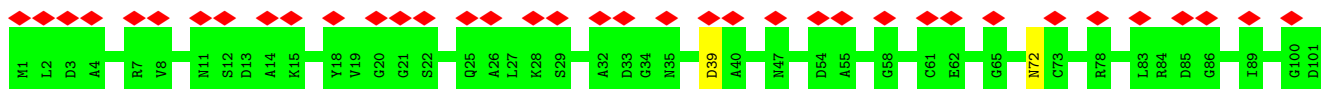
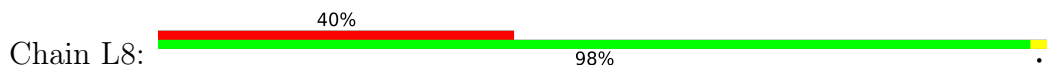
- Molecule 2: B-phycoerythrin beta chain



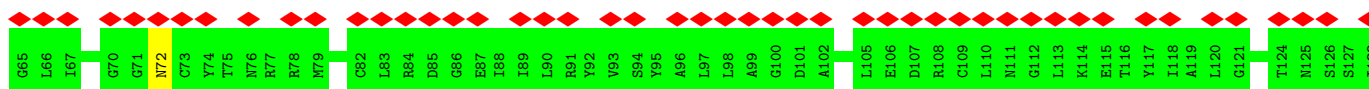
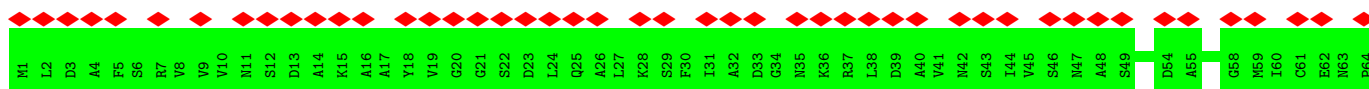
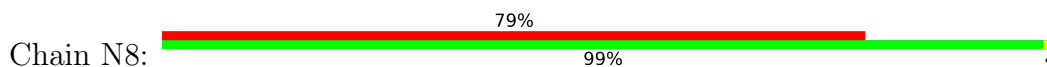
- Molecule 2: B-phycoerythrin beta chain

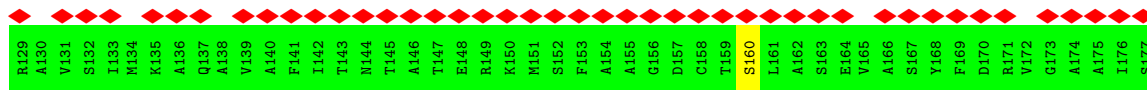


- Molecule 2: B-phycoerythrin beta chain

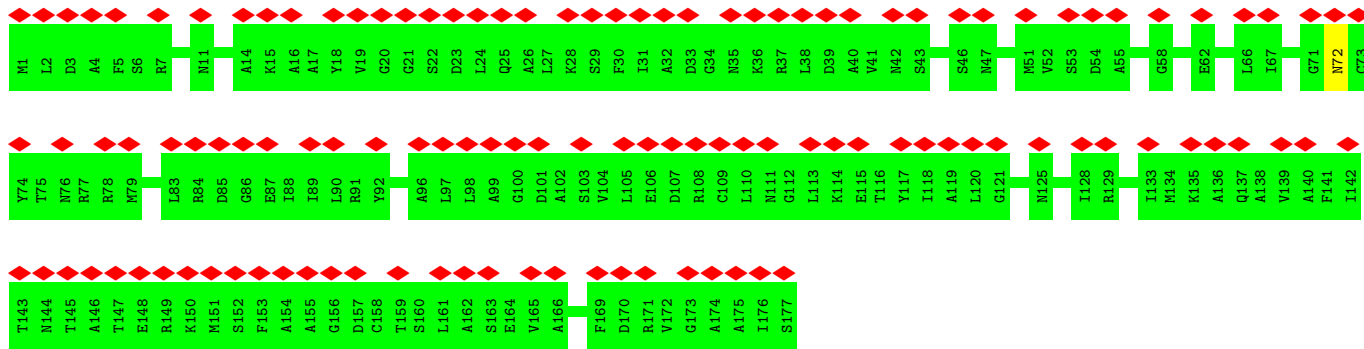


- Molecule 2: B-phycoerythrin beta chain

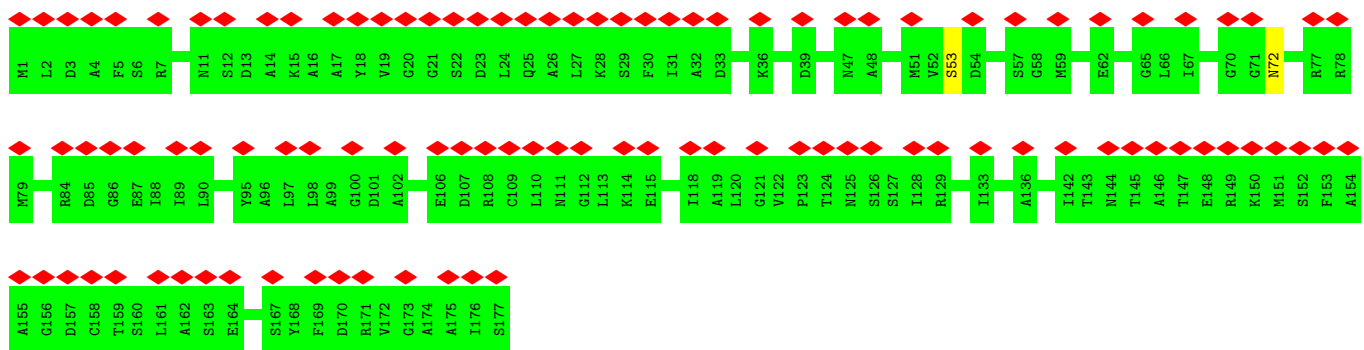




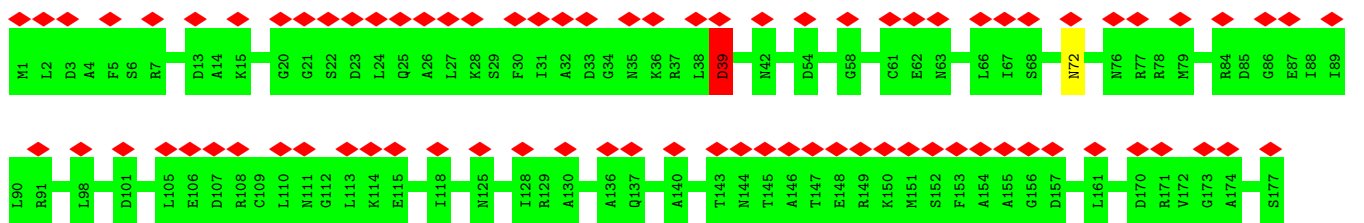
• Molecule 2: B-phycoerythrin beta chain



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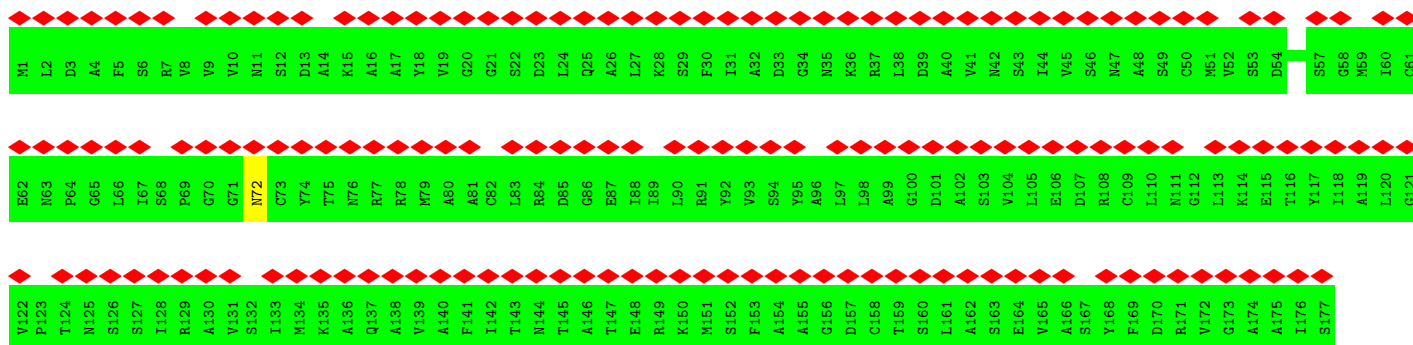


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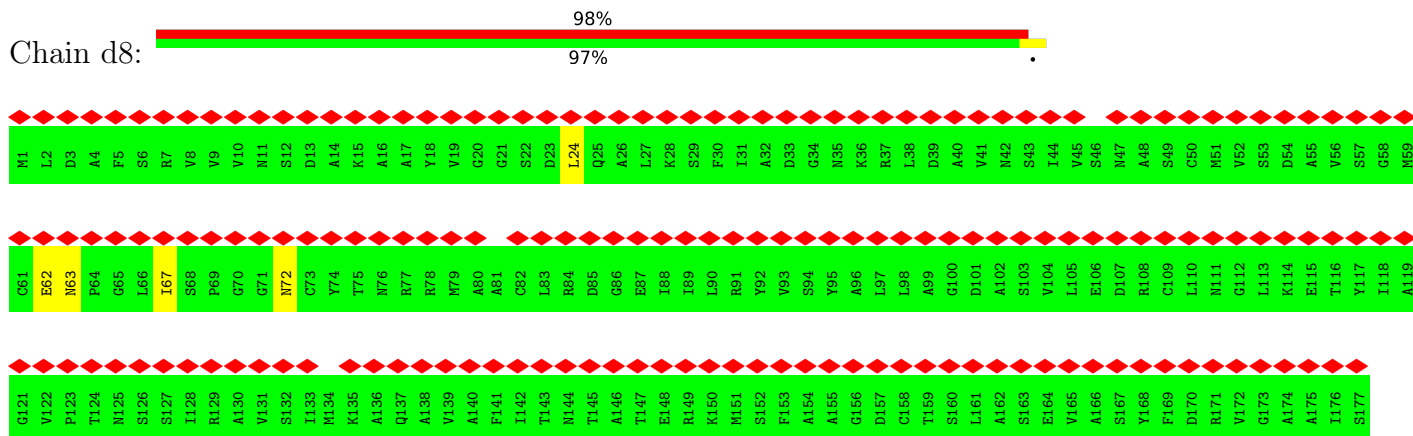


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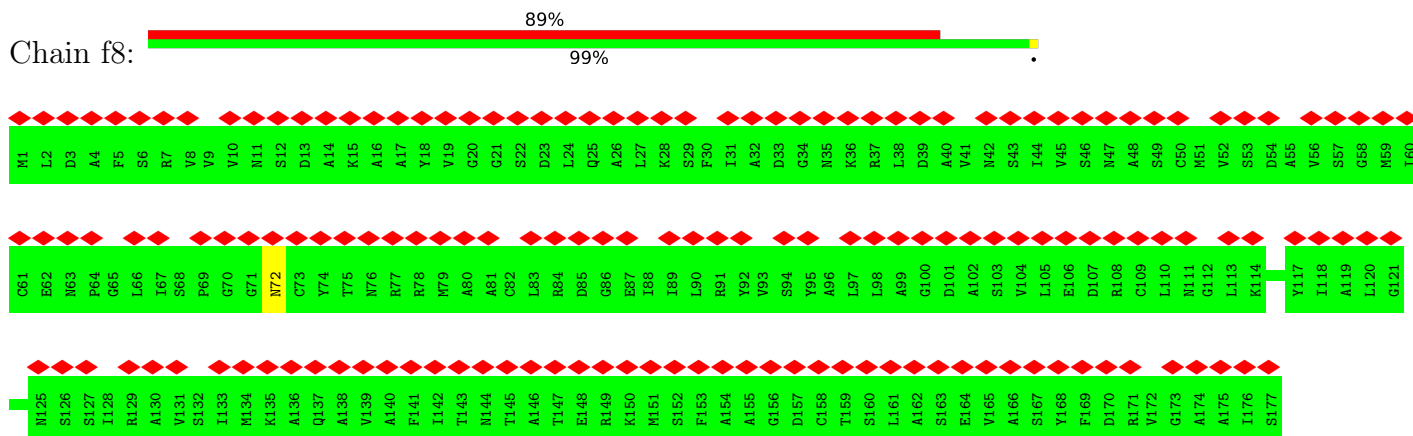




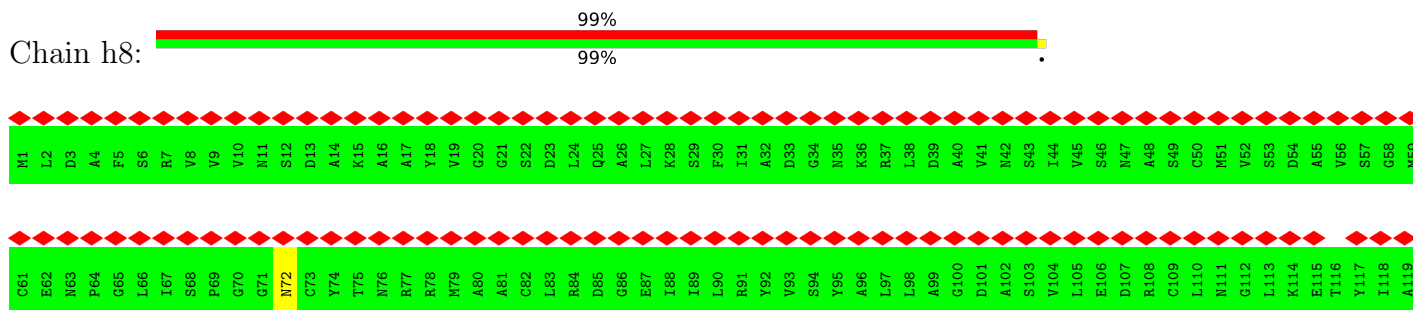
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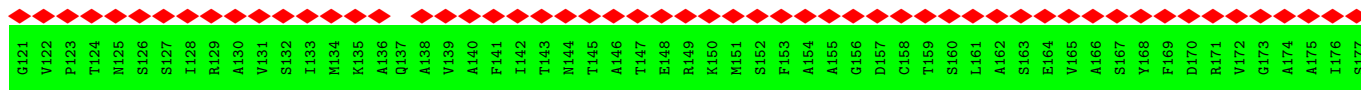


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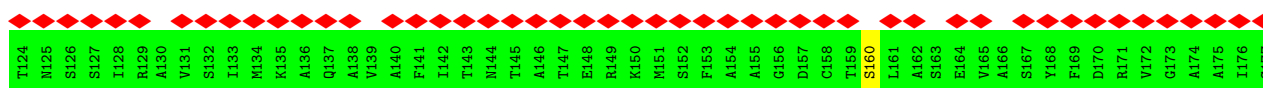
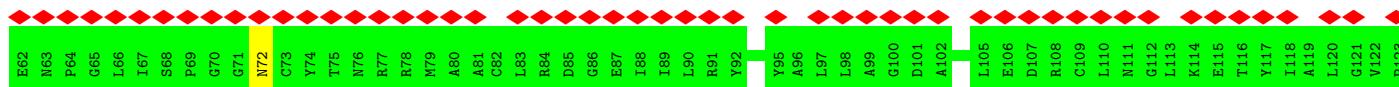
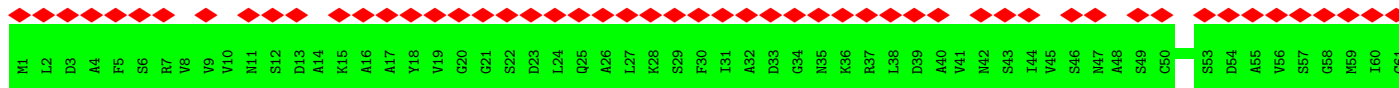


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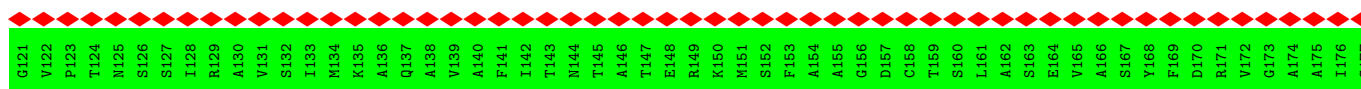
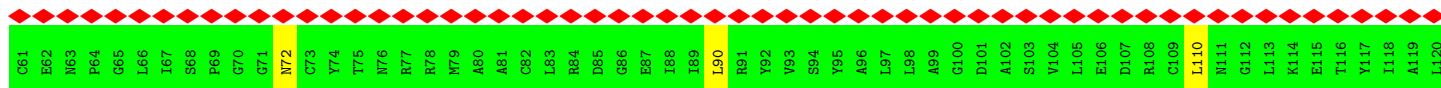
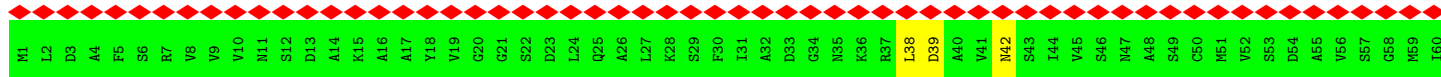




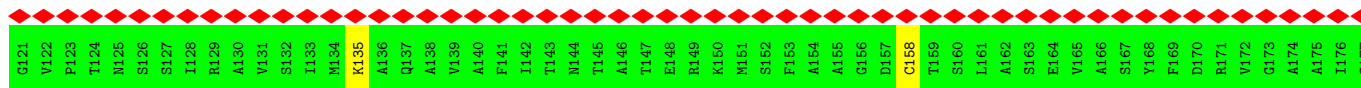
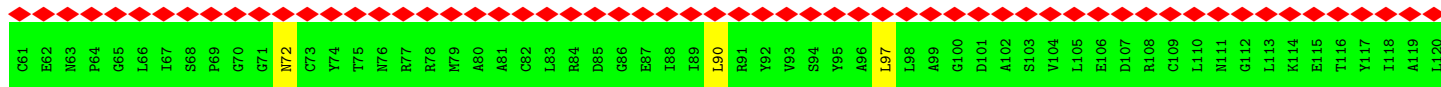
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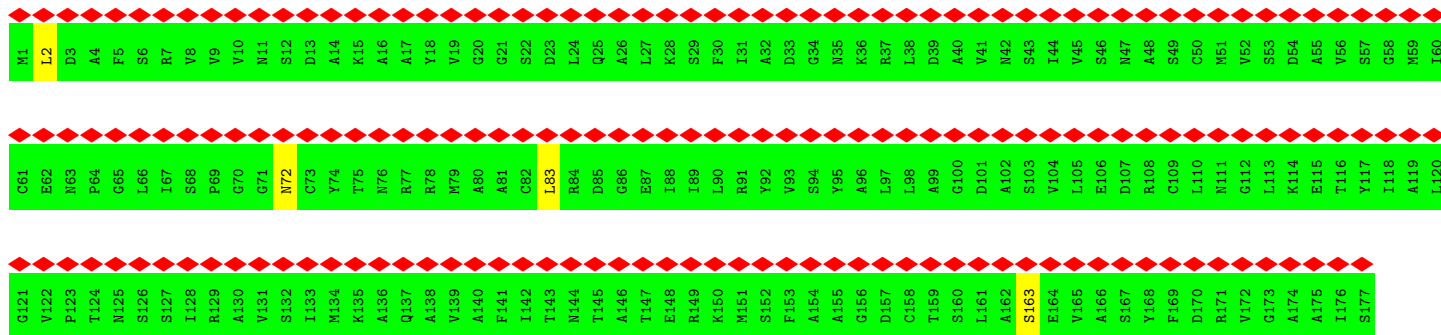
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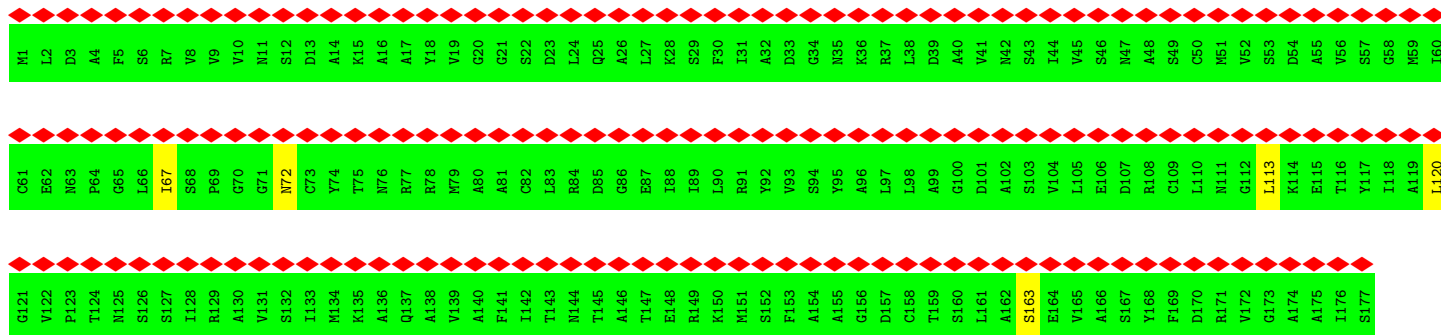
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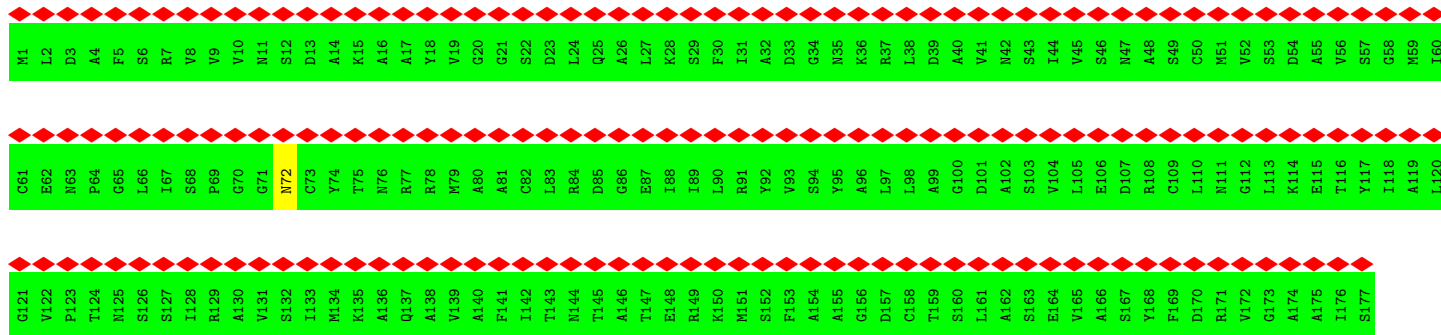
• Molecule 2: B-phycoerythrin beta chain



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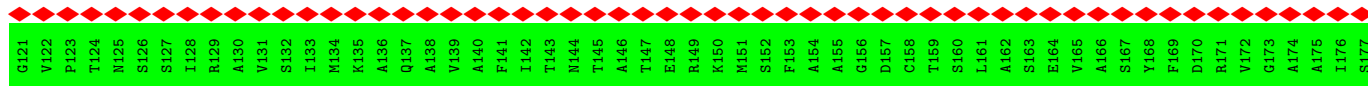
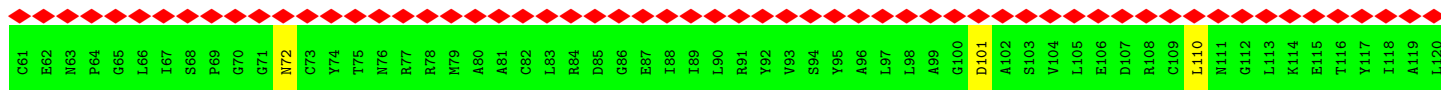


• Molecule 2: B-phycoerythrin beta chain



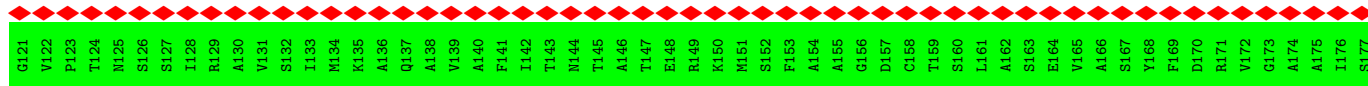
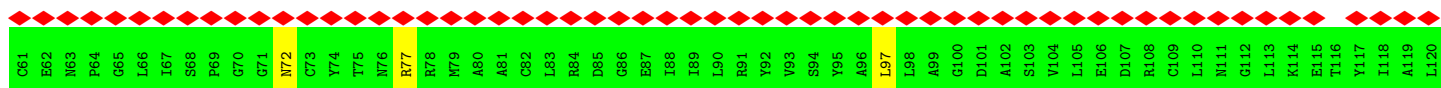
• Molecule 2: B-phycoerythrin beta chain





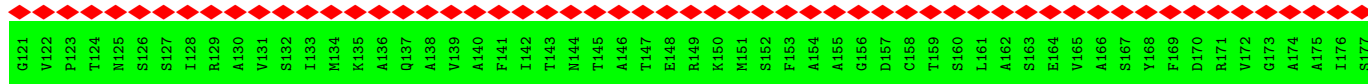
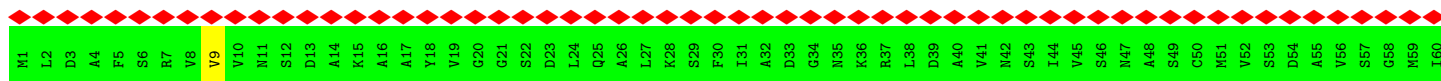
• Molecule 2: B-phycoerythrin beta chain

Chain B9:



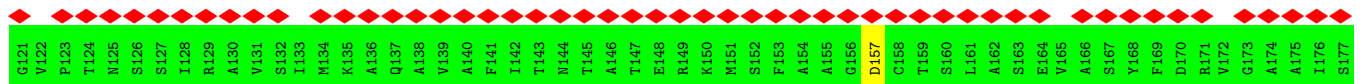
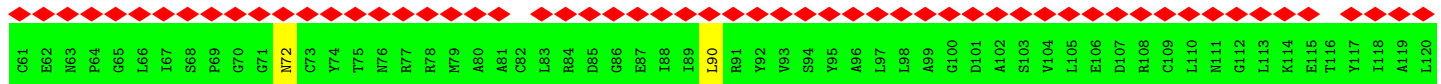
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Chain D9:

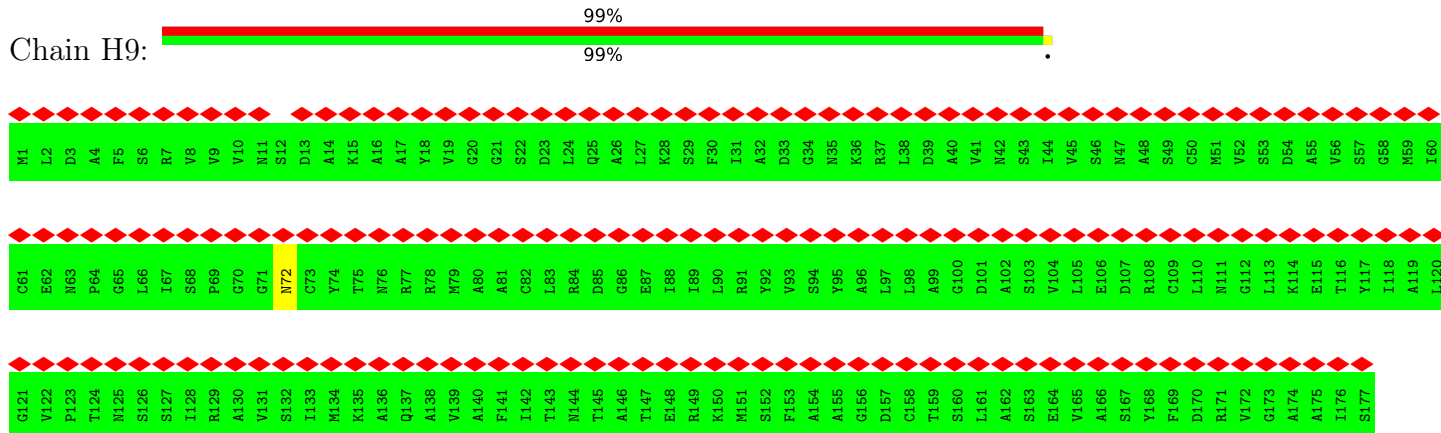


• Molecule 2: B-phycoerythrin beta chain

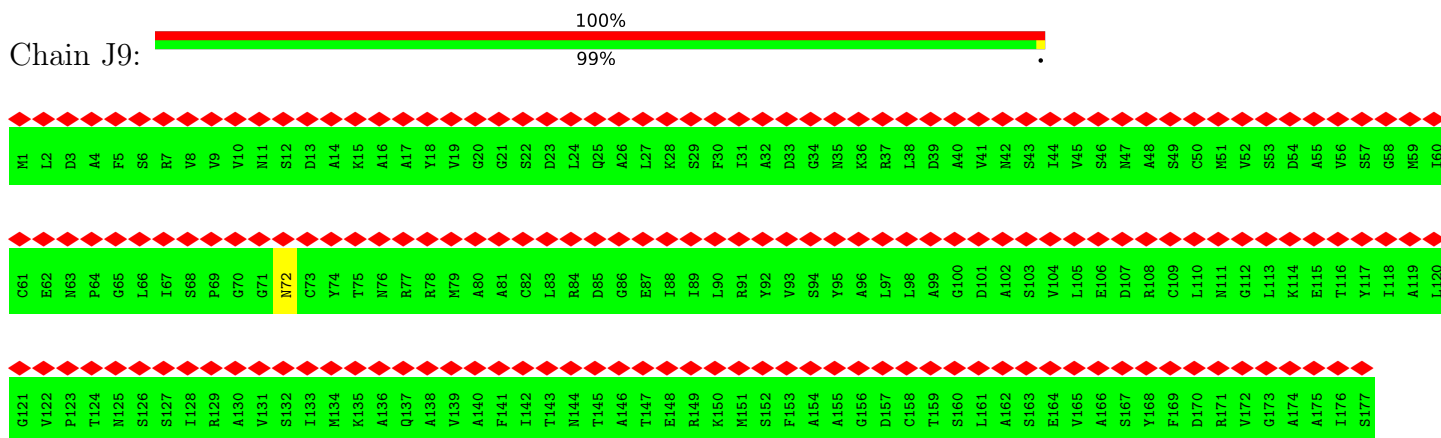
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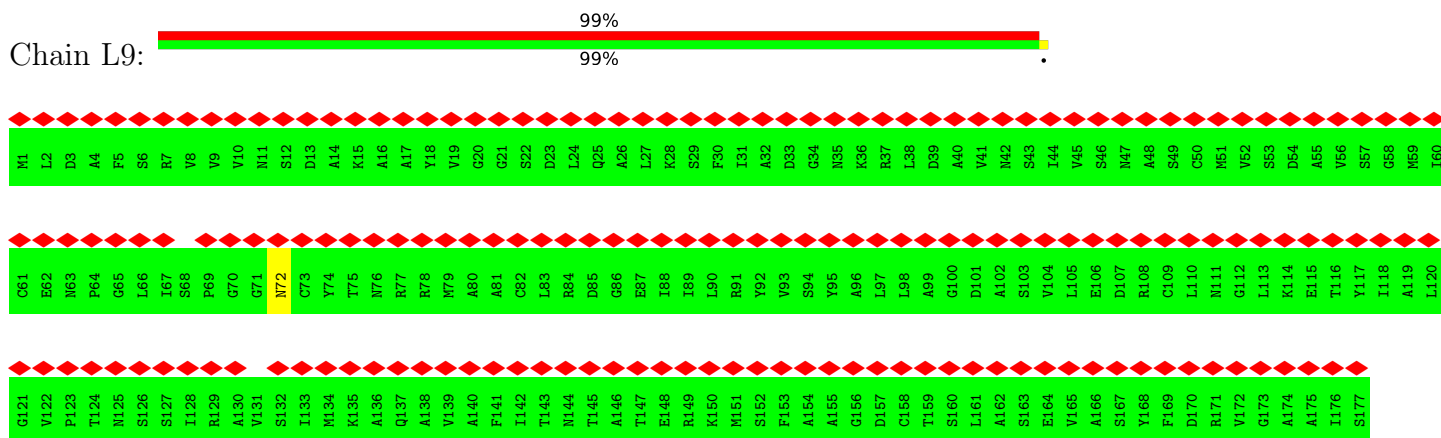
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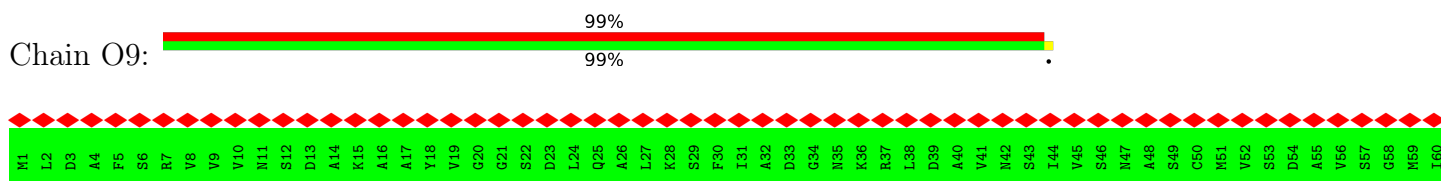
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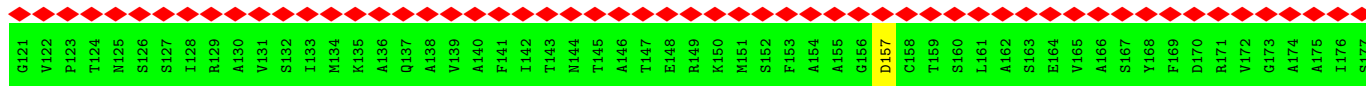
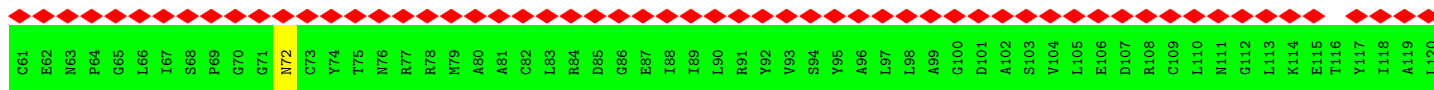


• Molecule 2: B-phycoerythrin beta chain

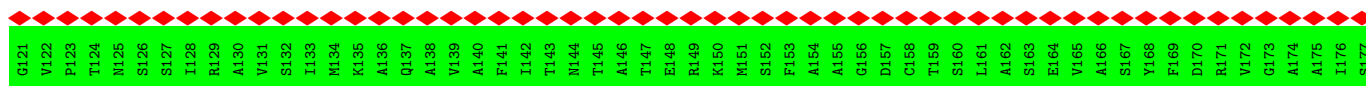
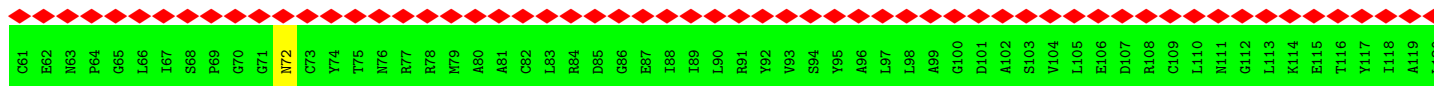
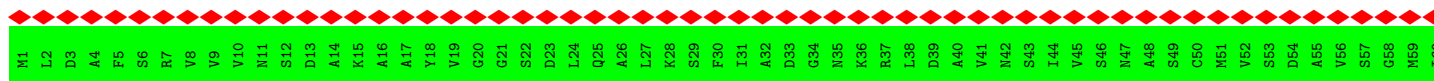


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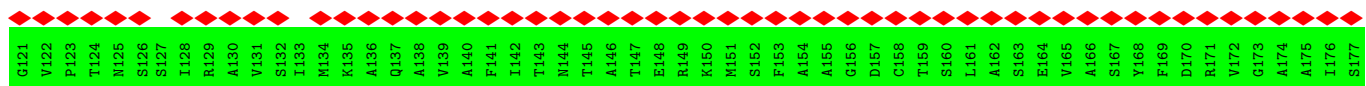
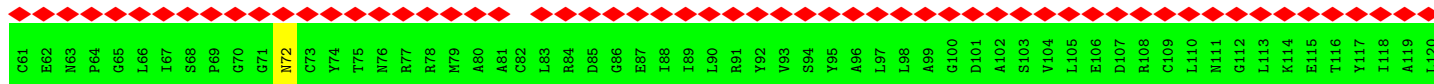
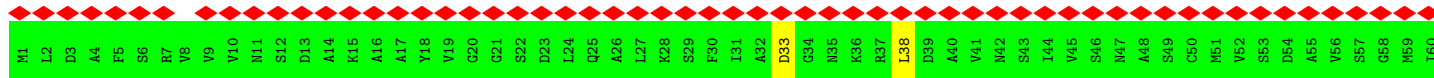




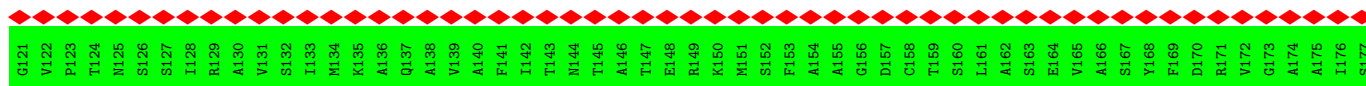
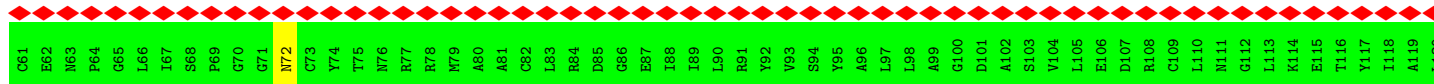
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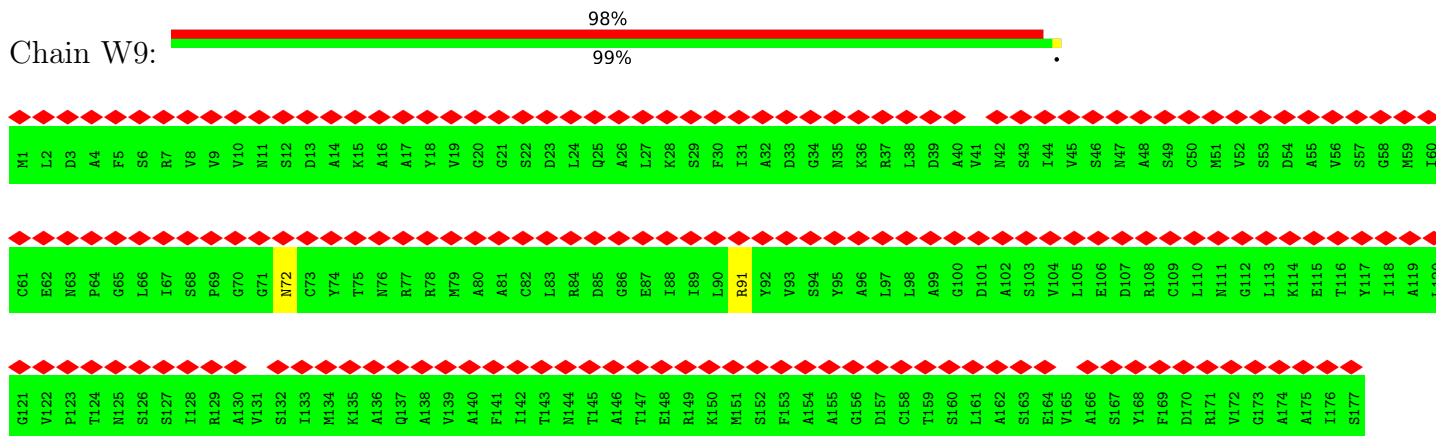
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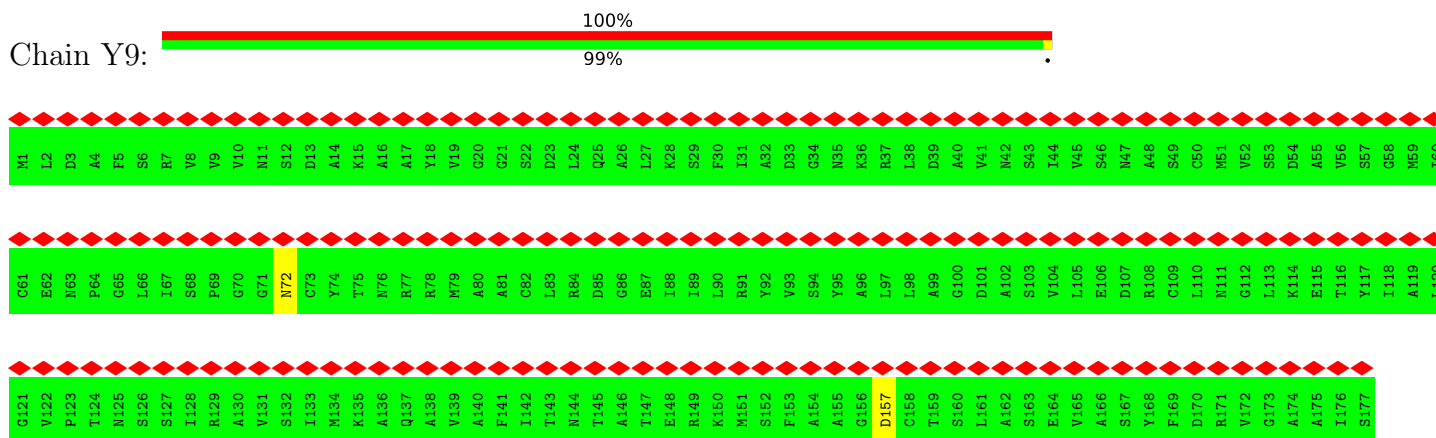
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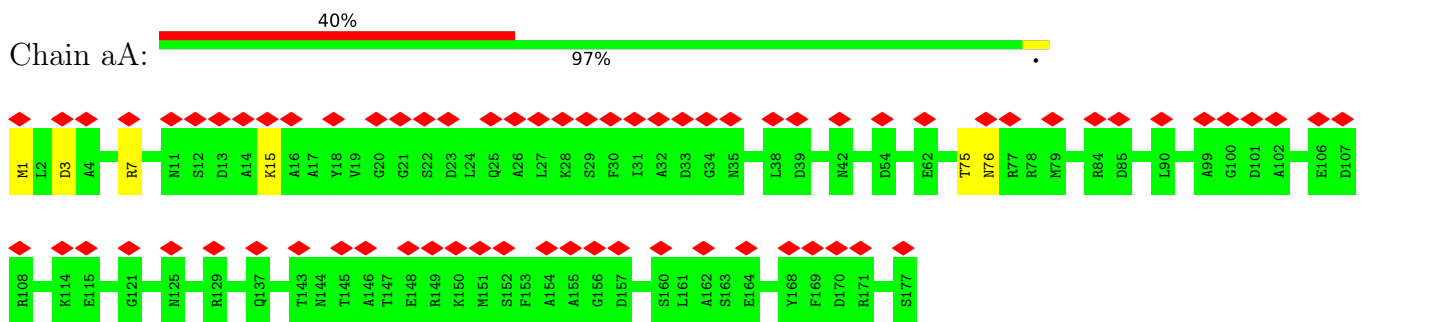
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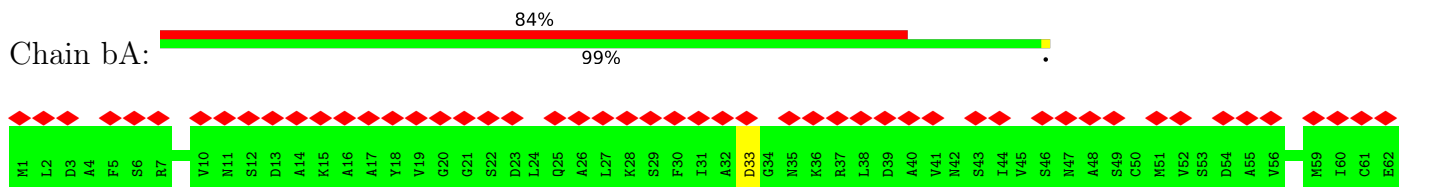
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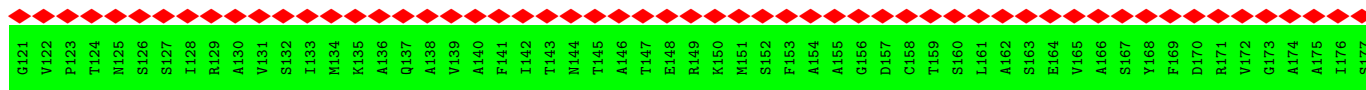


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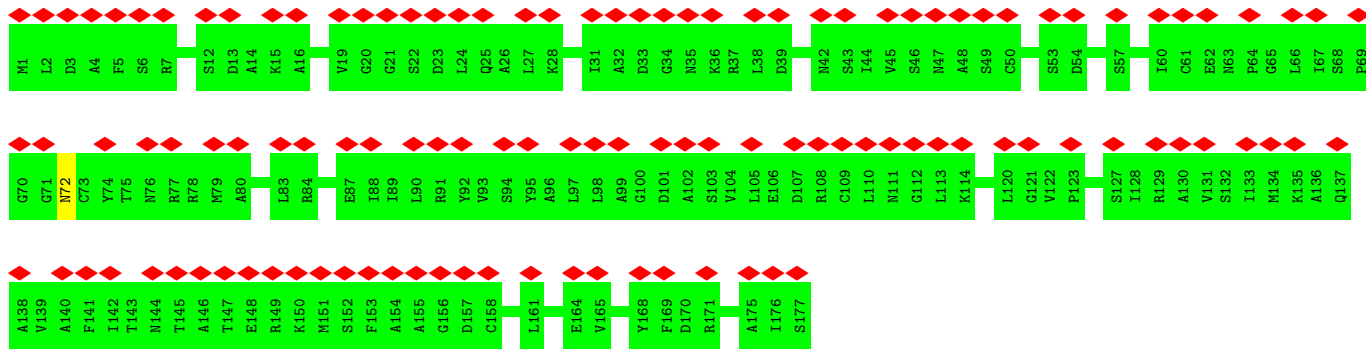




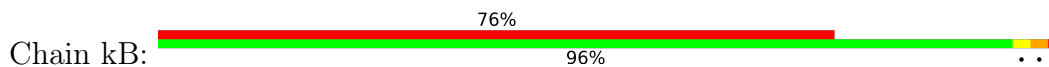
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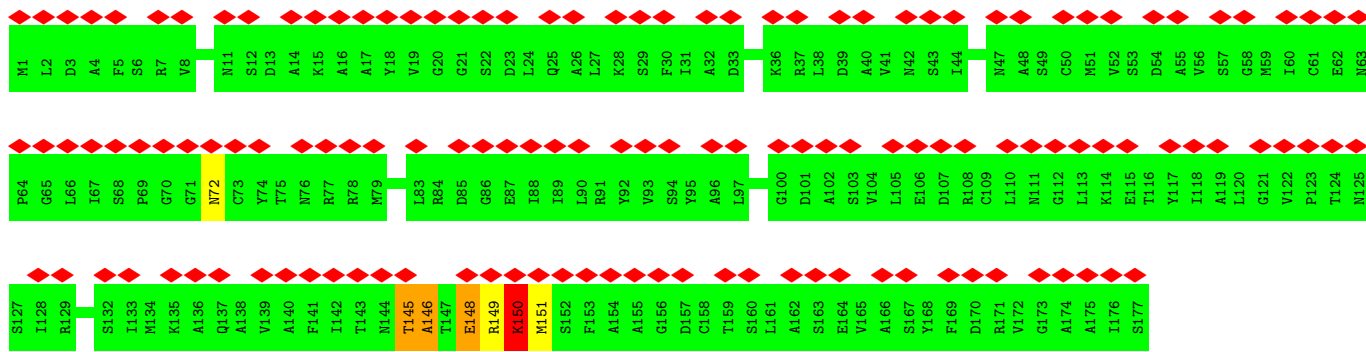
Chain iB:



• Molecule 2: B-phycoerythrin beta chain



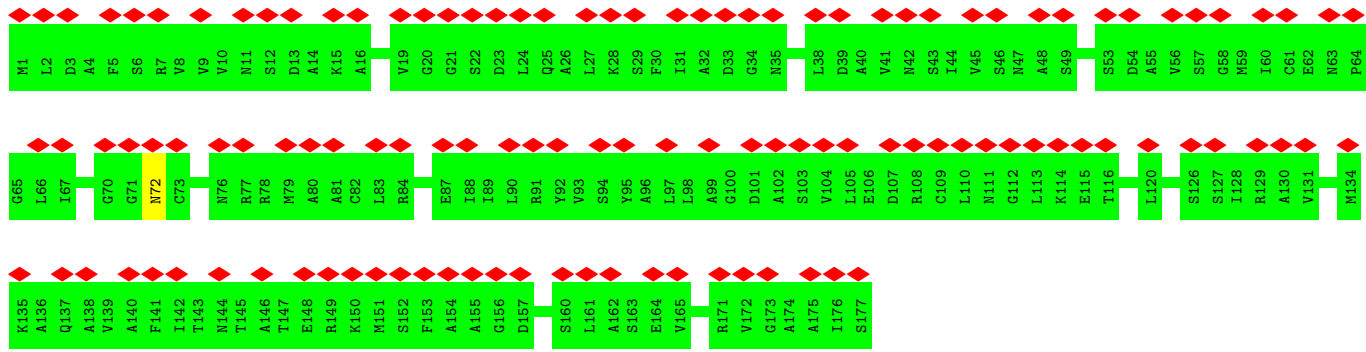
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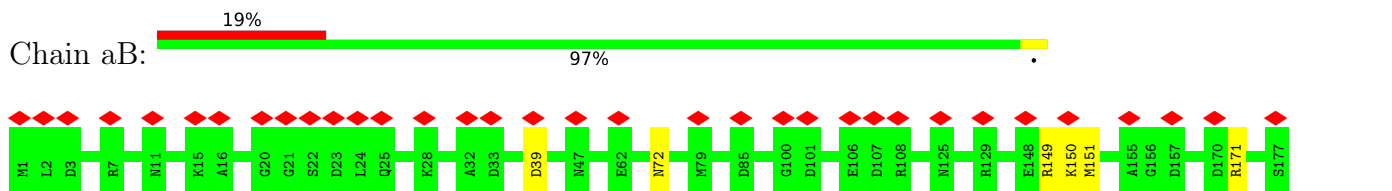
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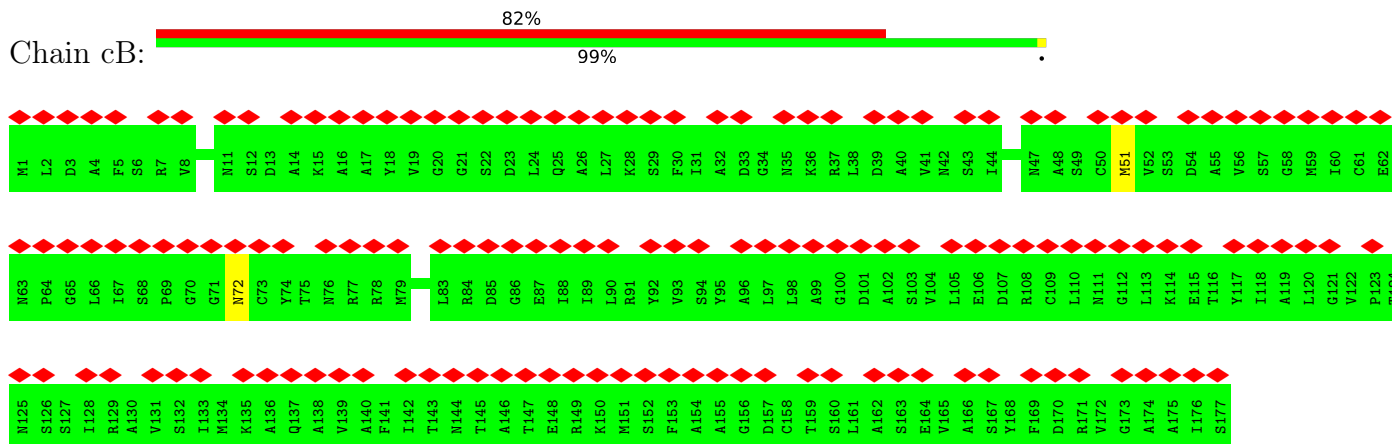
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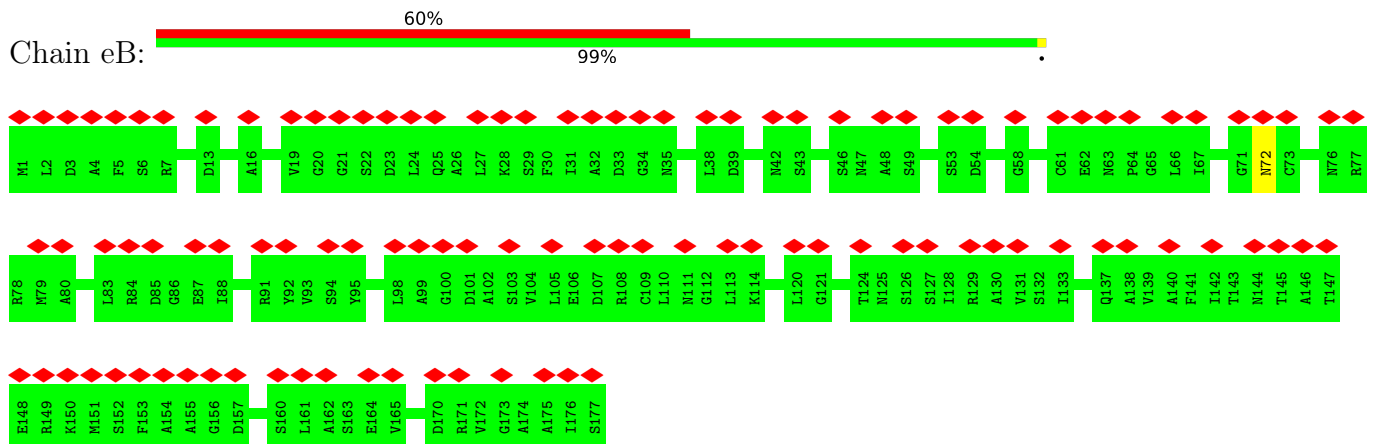
• Molecule 2: B-phycoerythrin beta chain



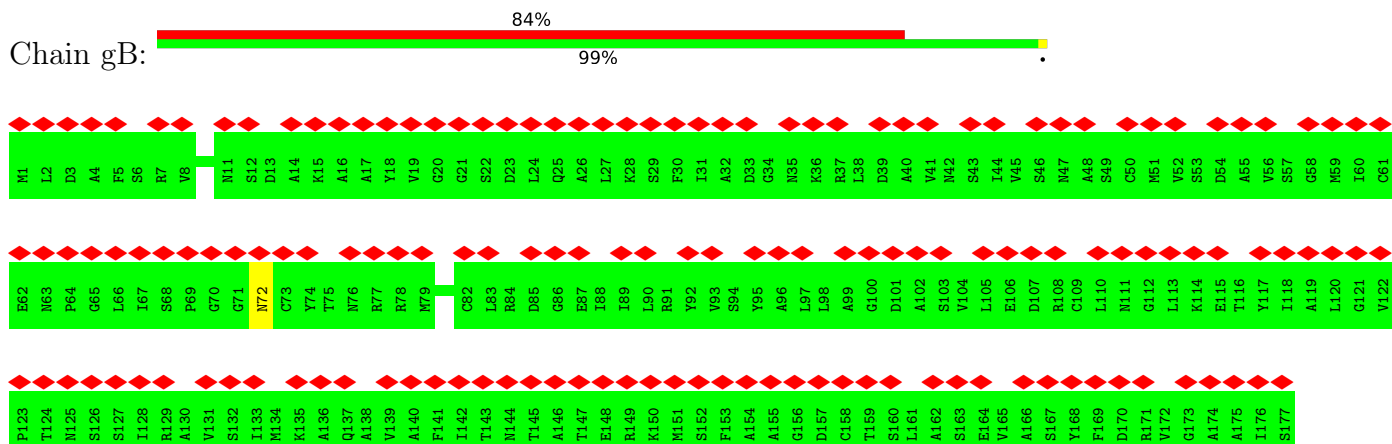
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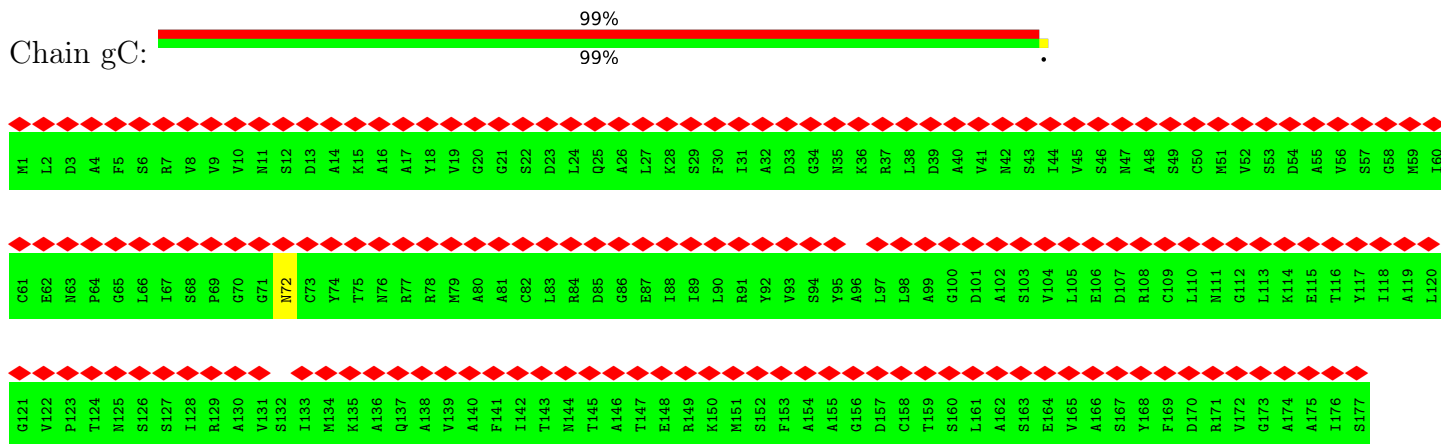
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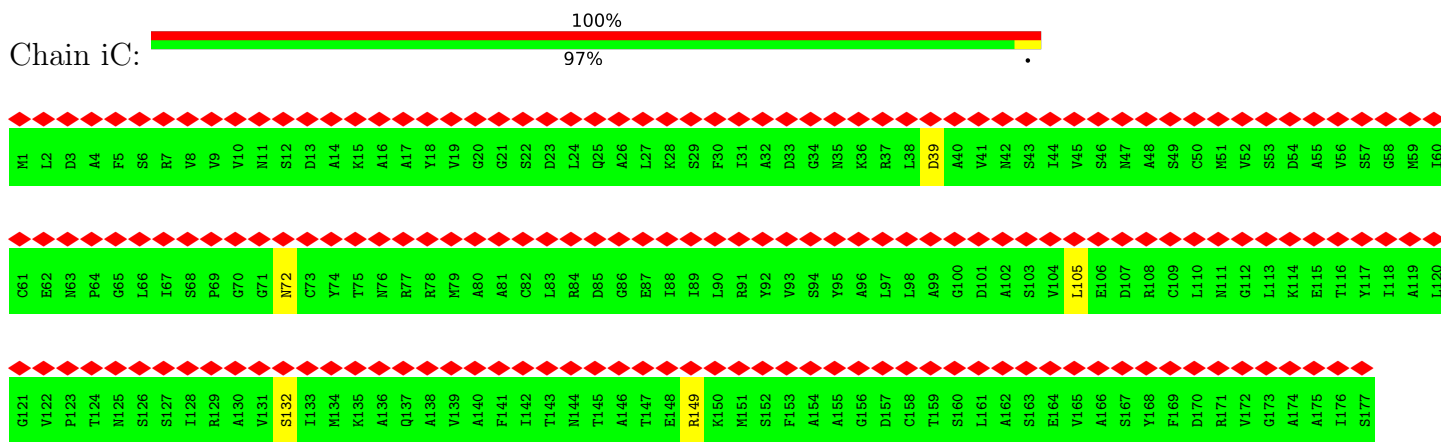
• Molecule 2: B-phycoerythrin beta chain



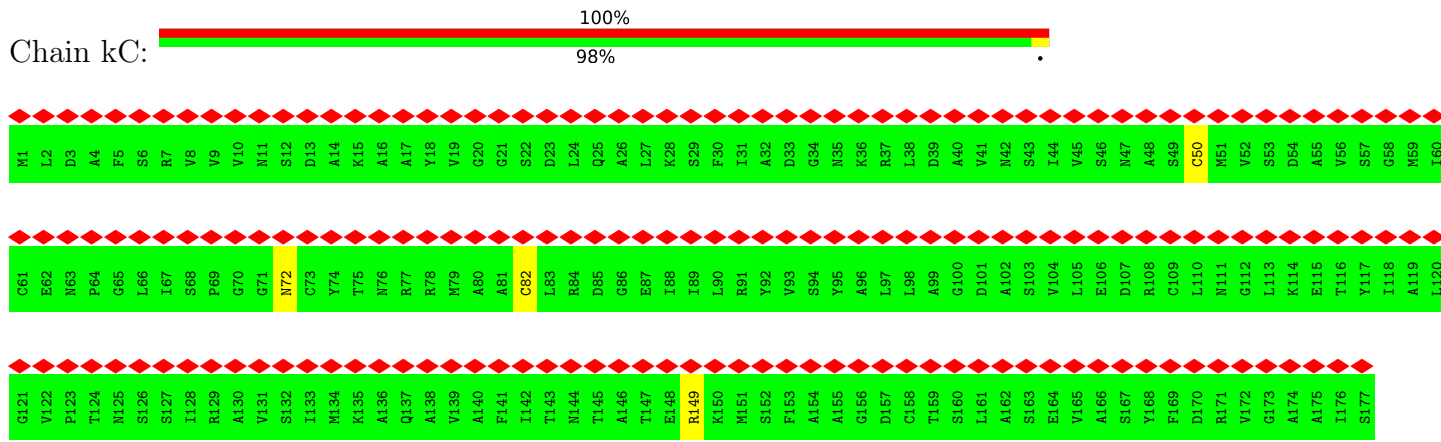
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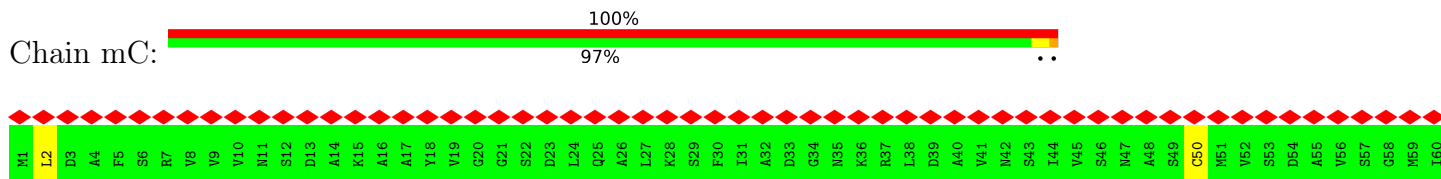
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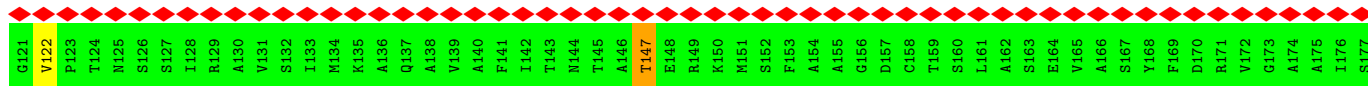
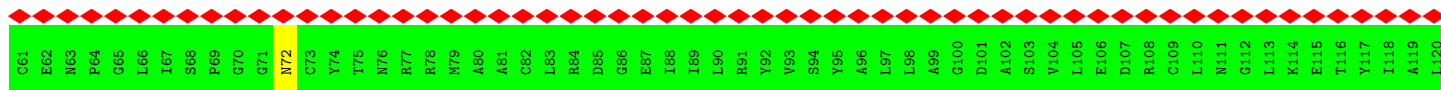


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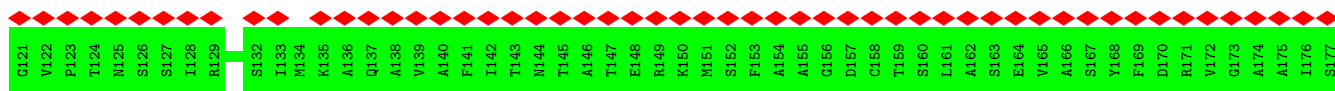
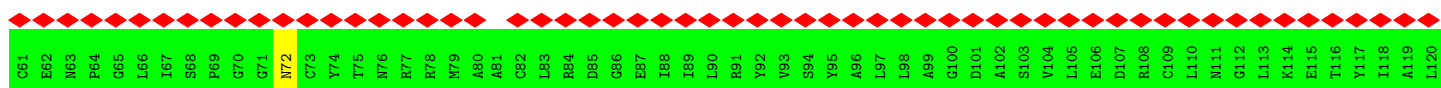
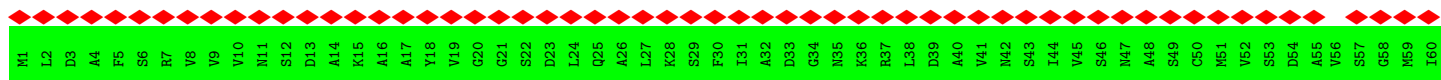


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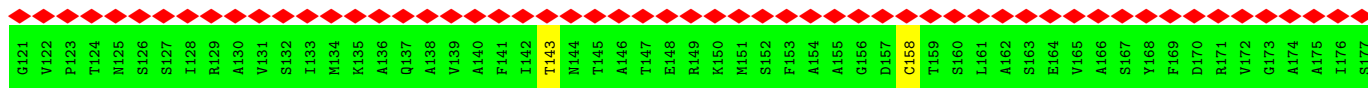
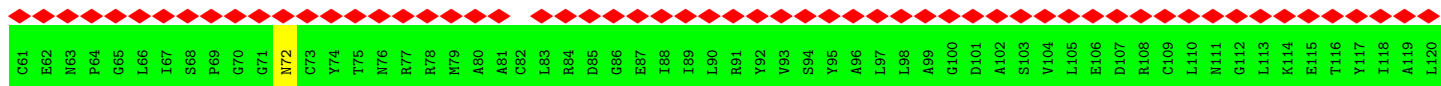
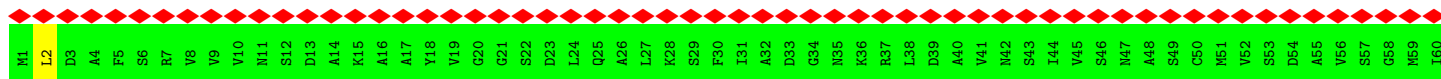




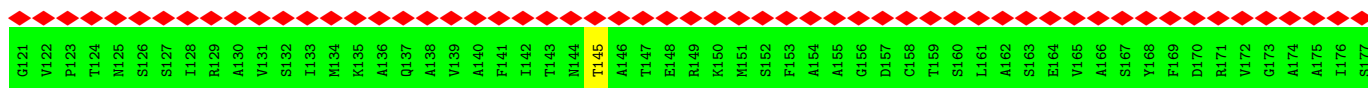
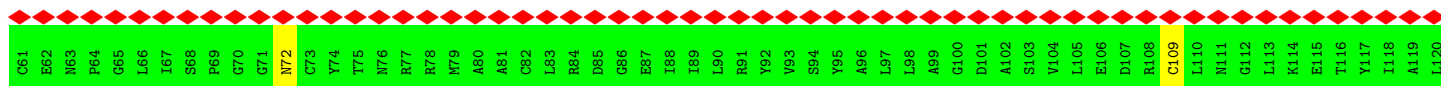
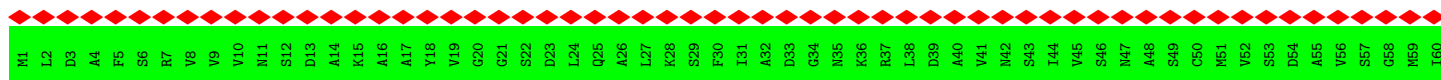
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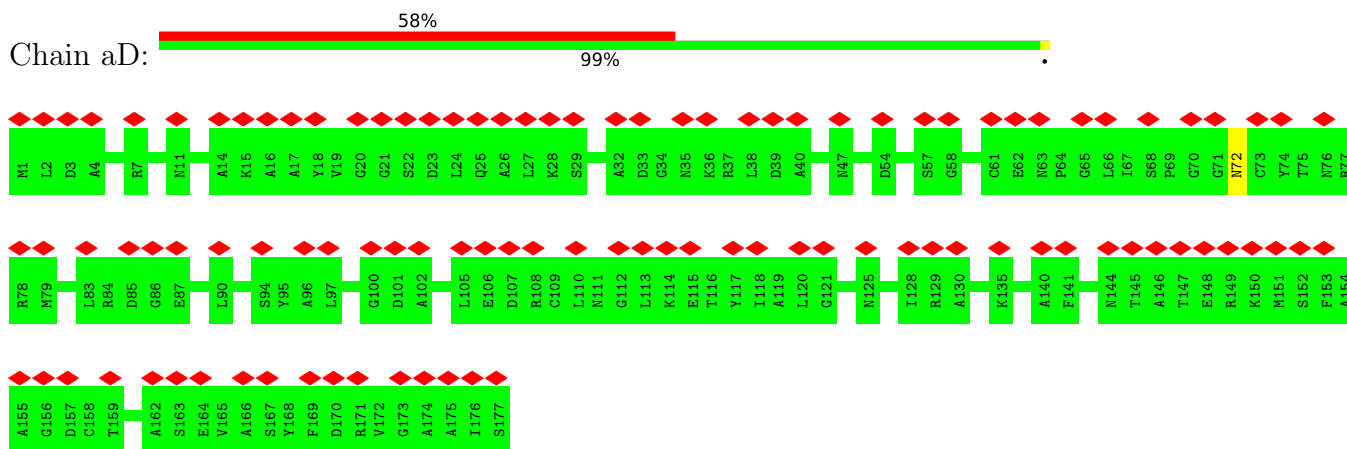
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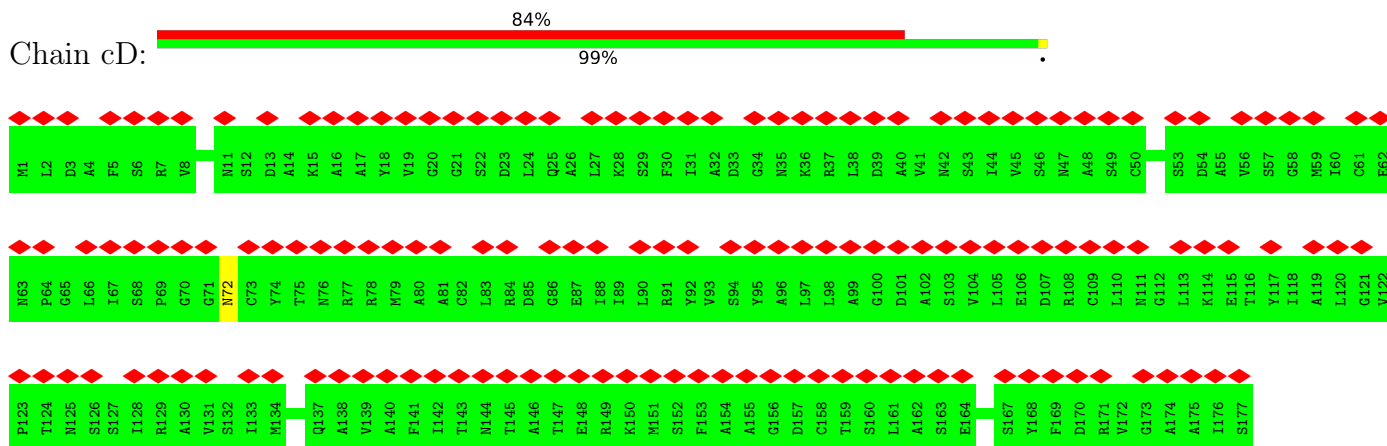
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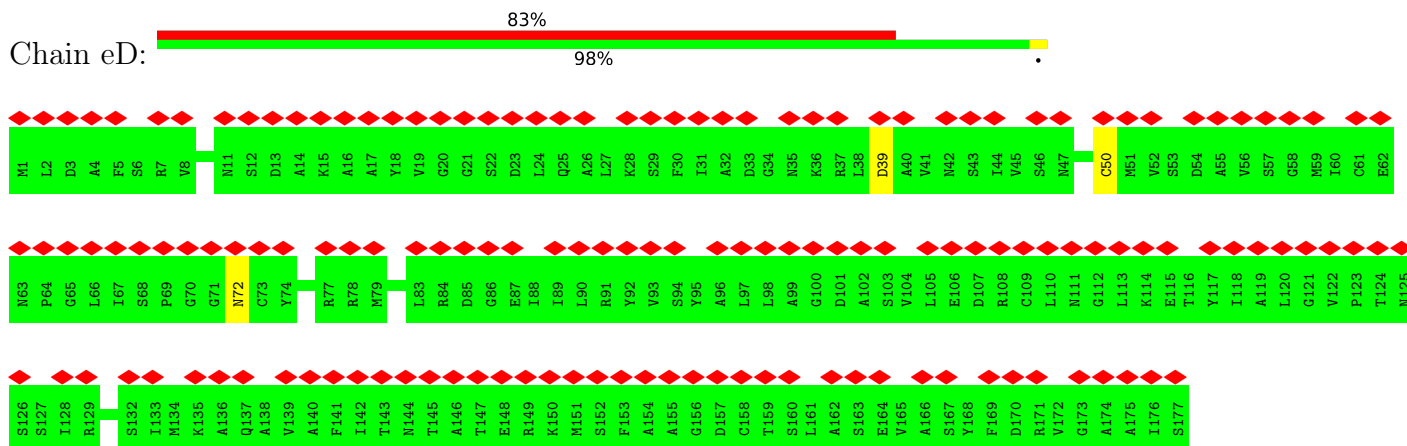
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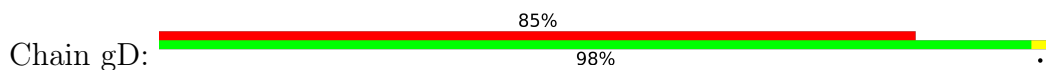
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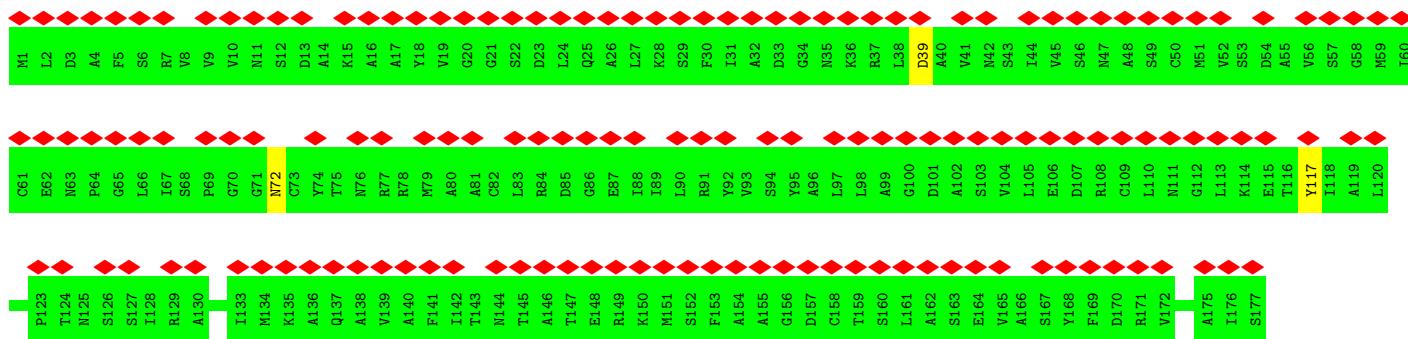


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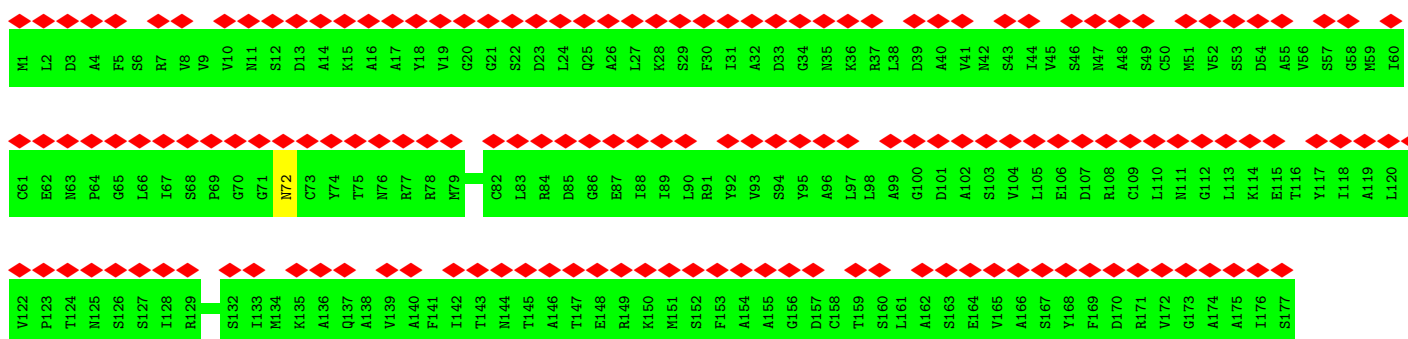


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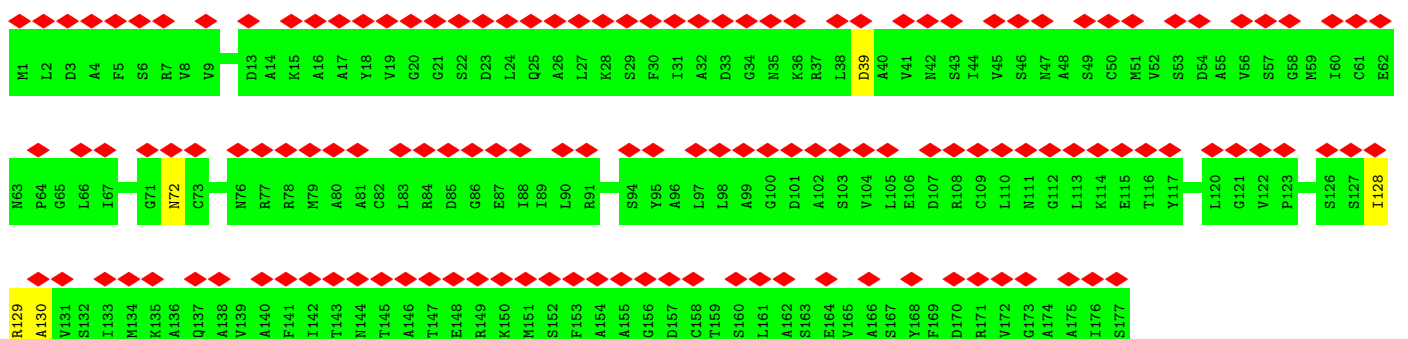
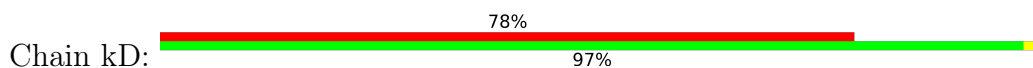




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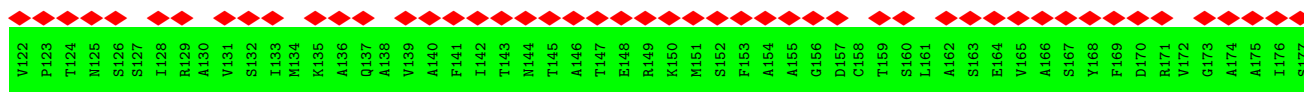


• Molecule 2: B-phycoerythrin beta chain

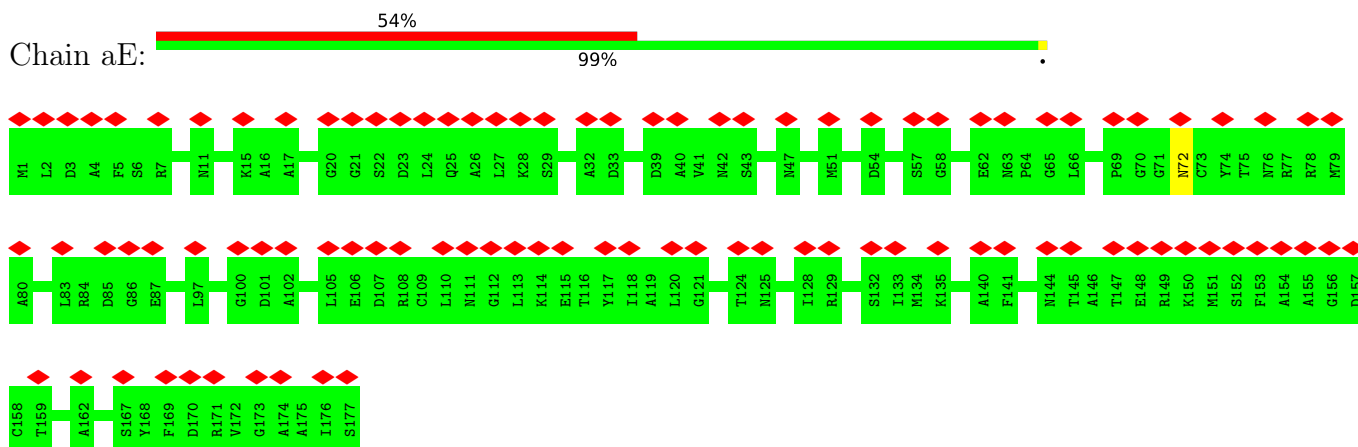


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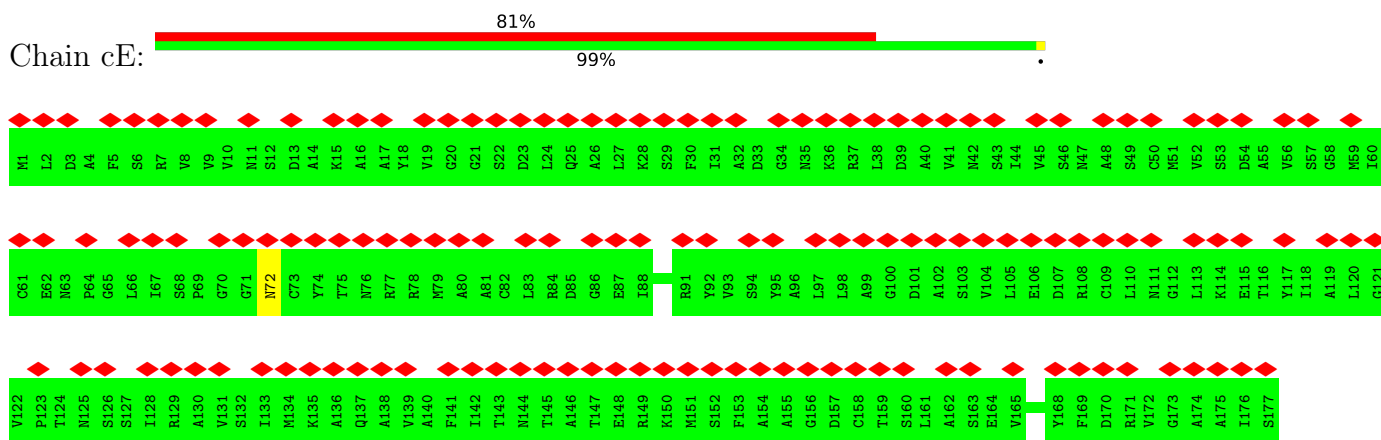




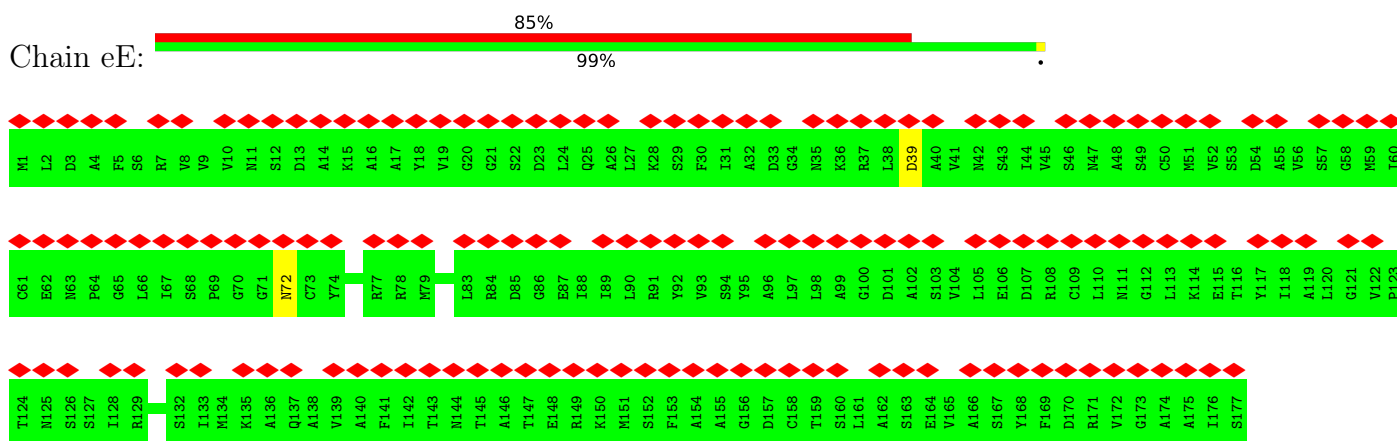
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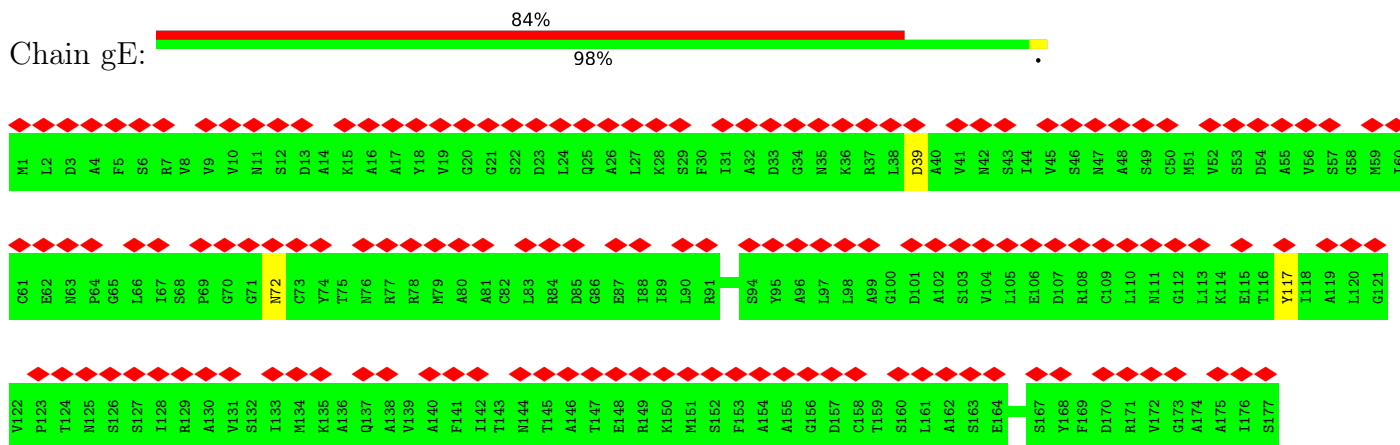
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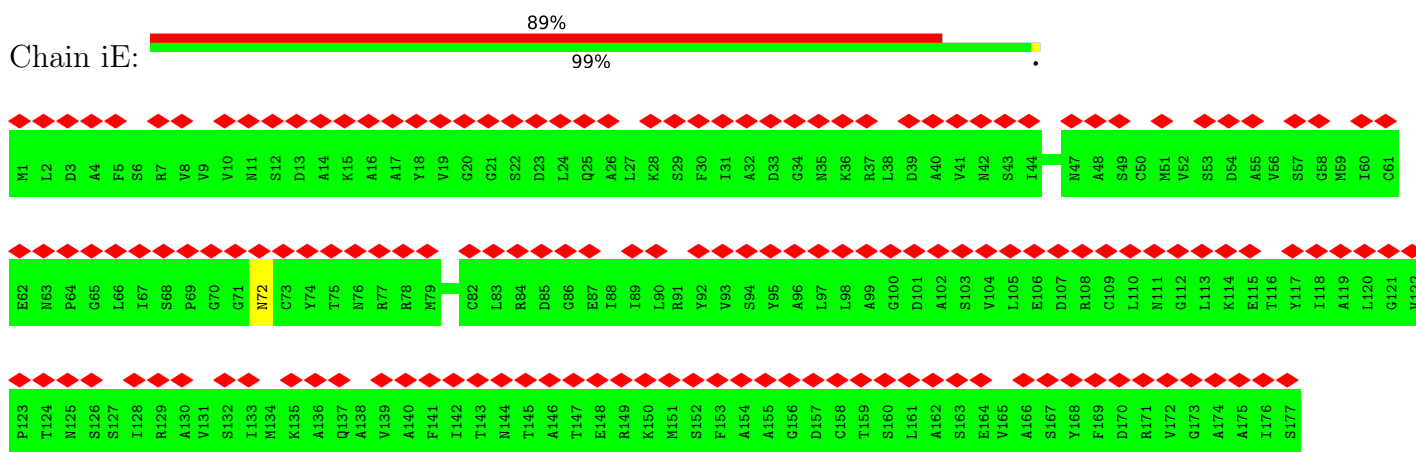
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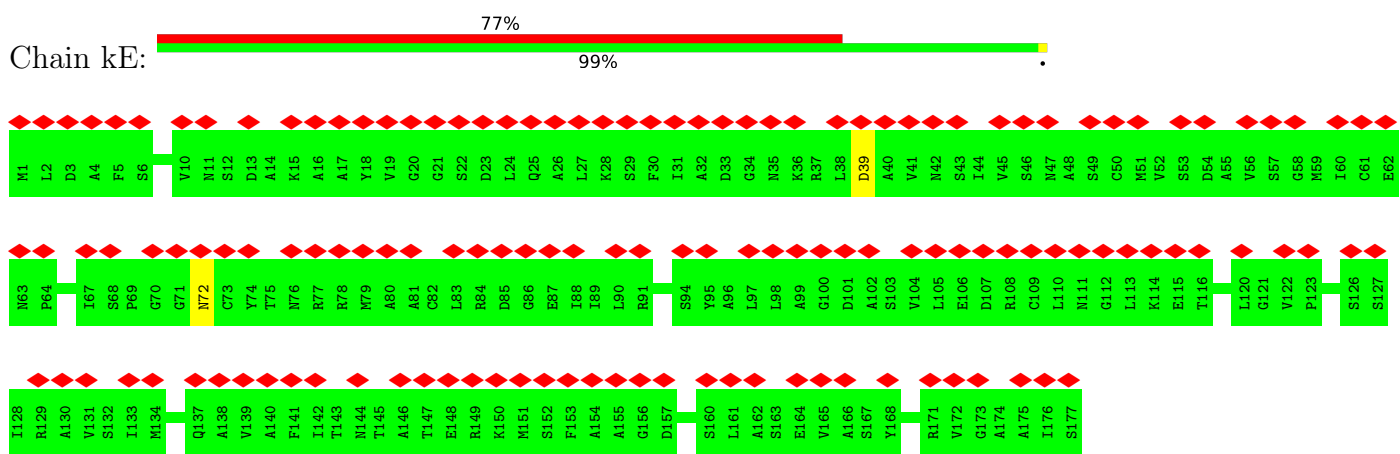
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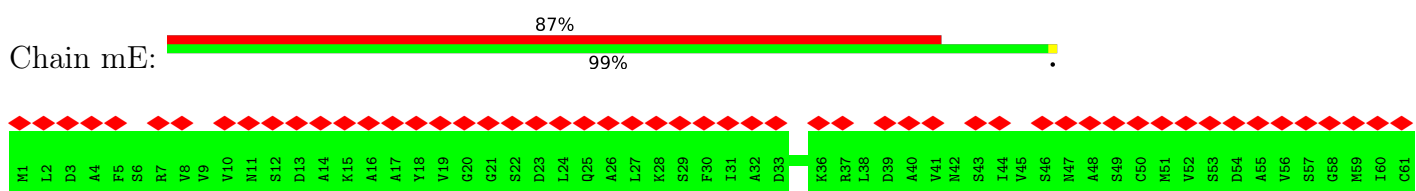
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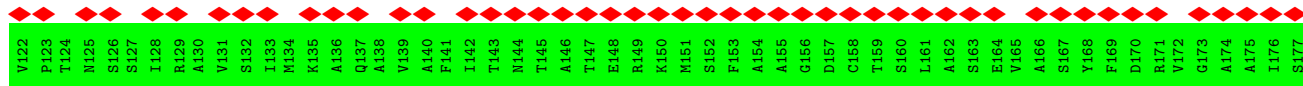
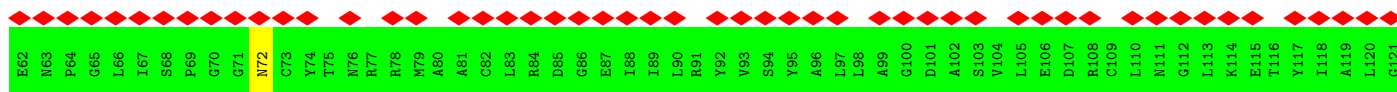


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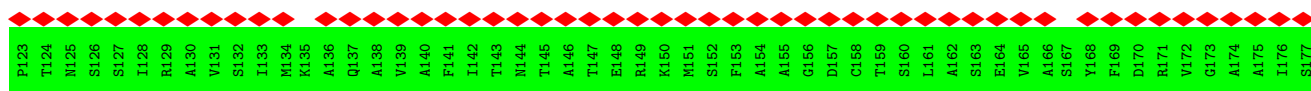
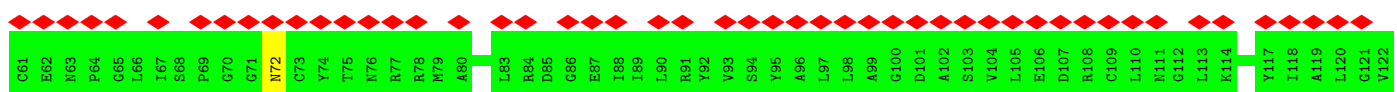
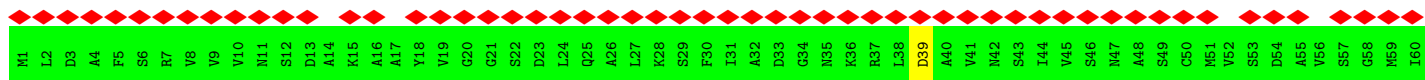


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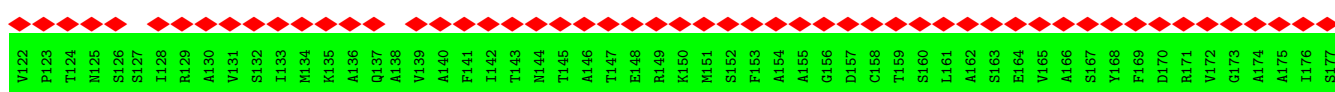
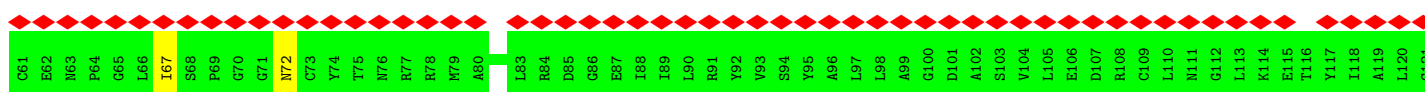
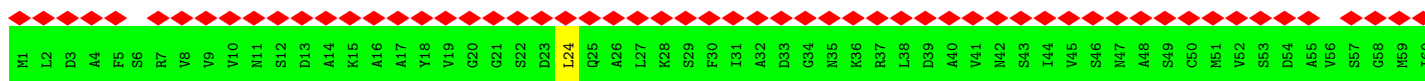




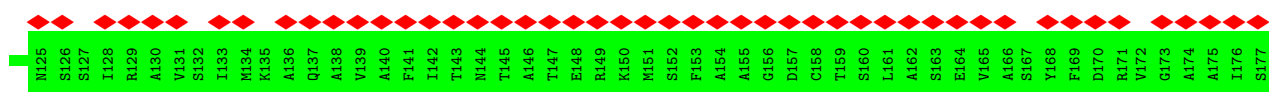
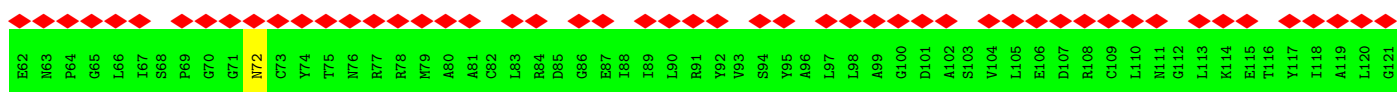
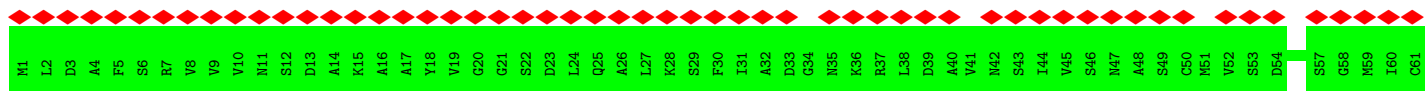
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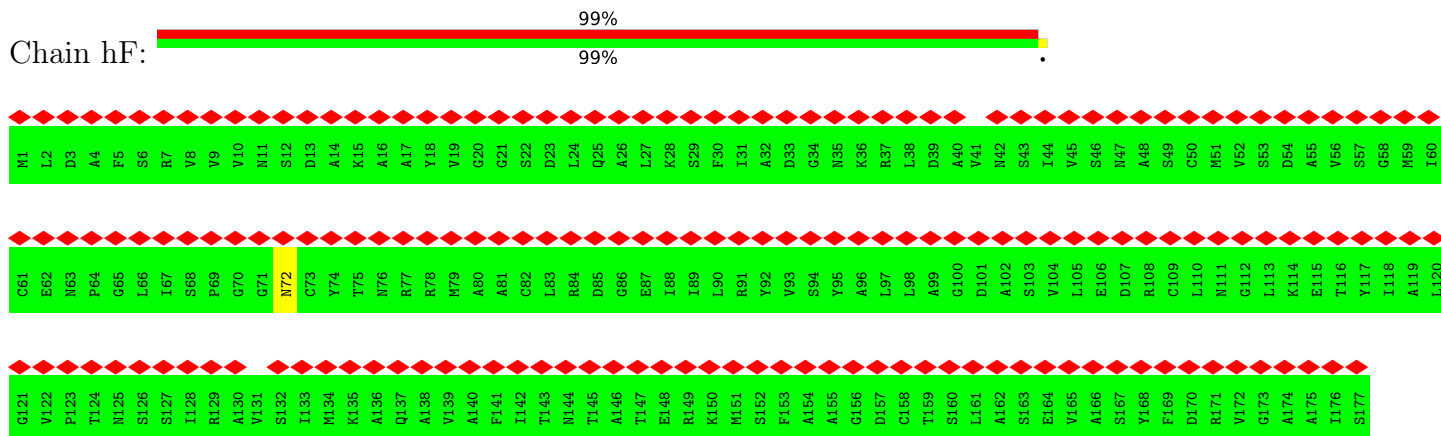
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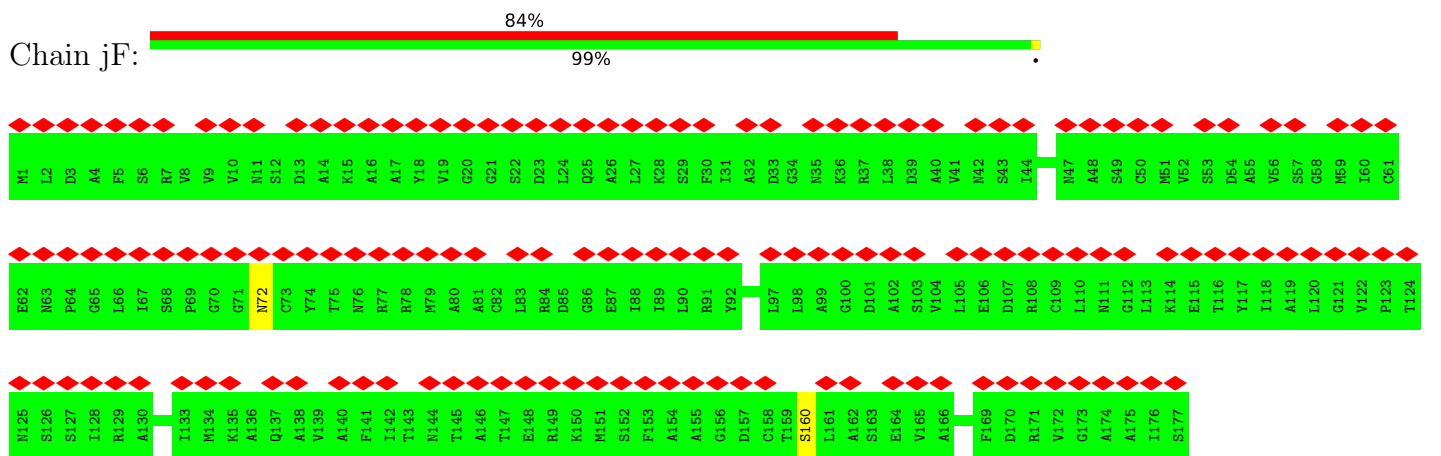
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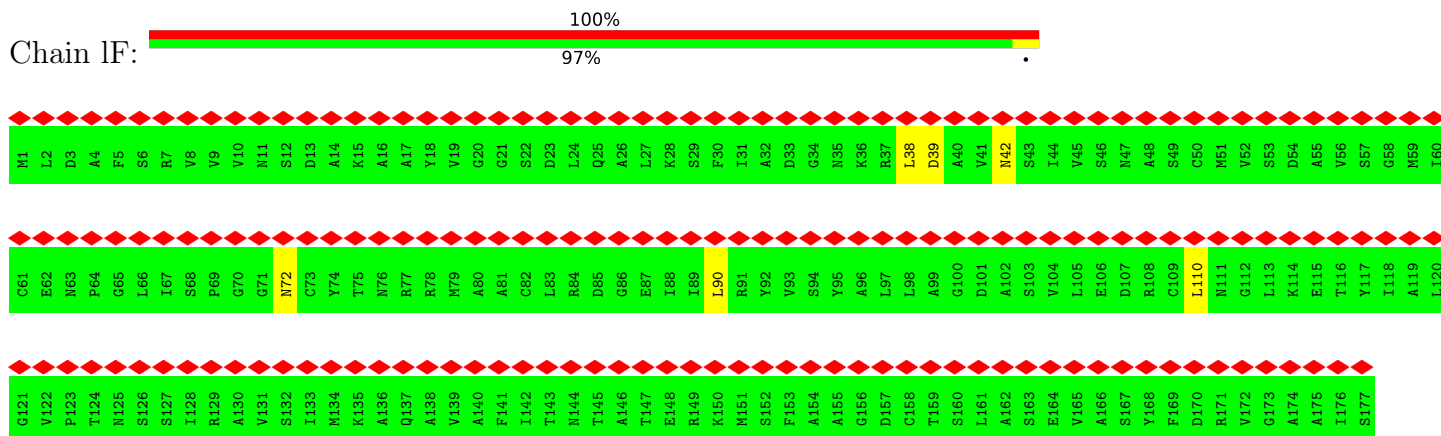
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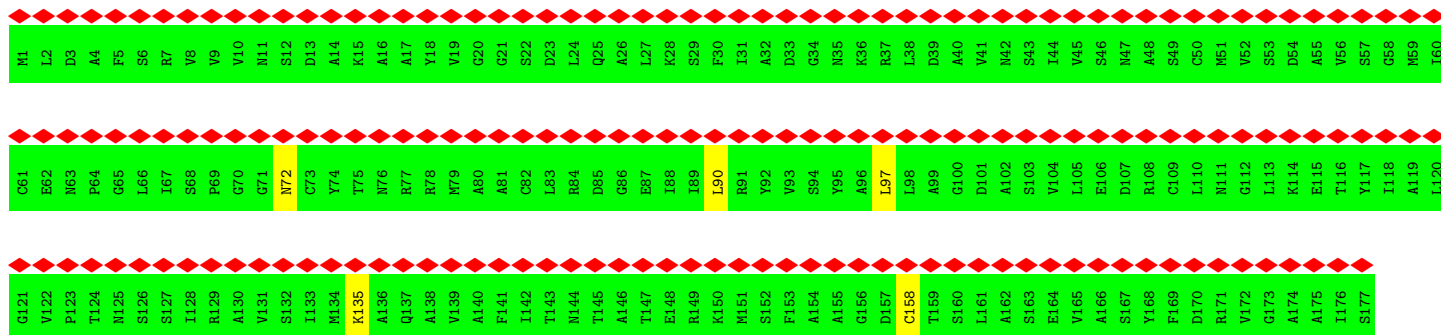


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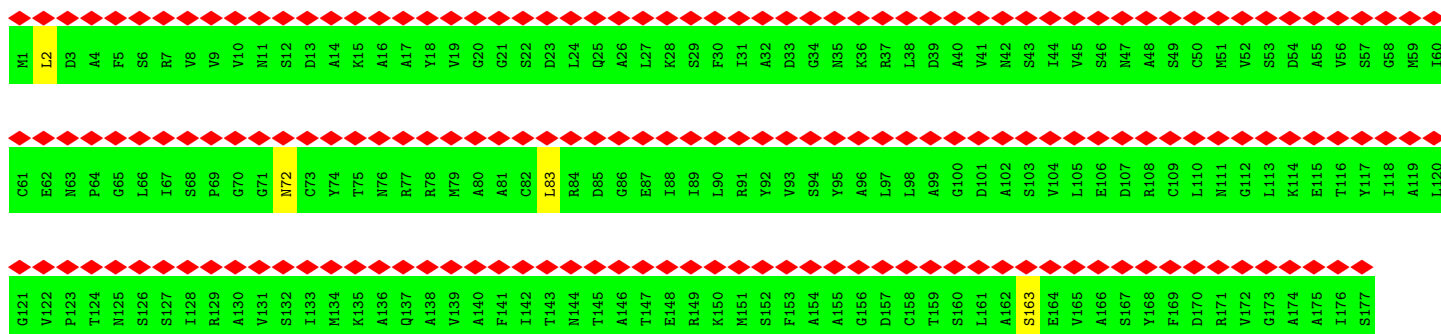


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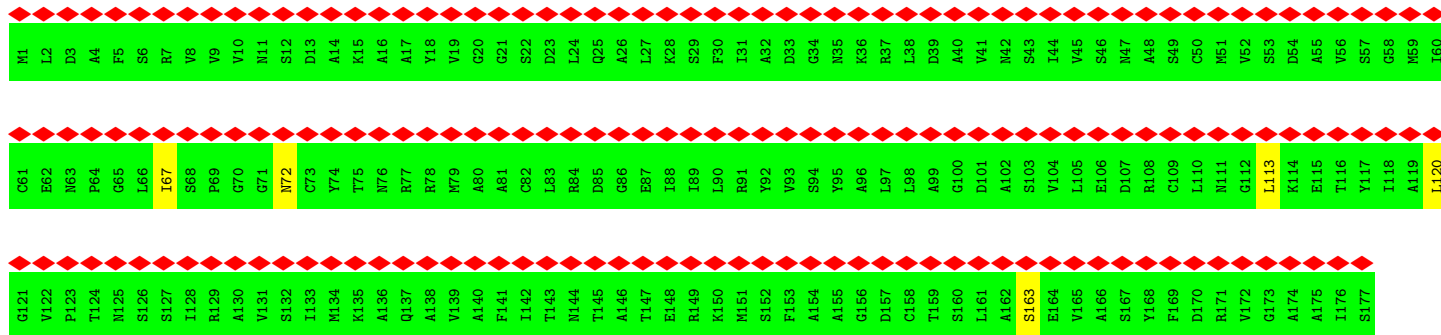




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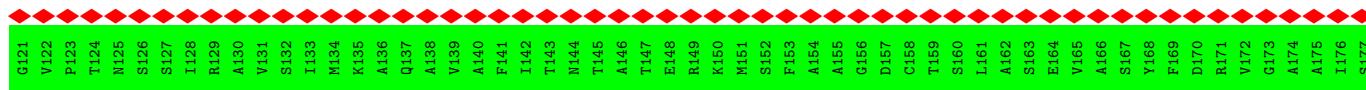


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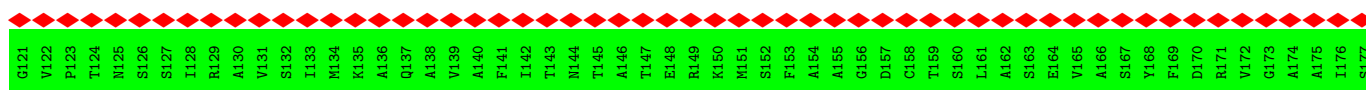
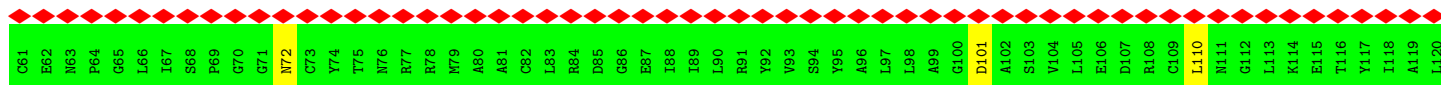


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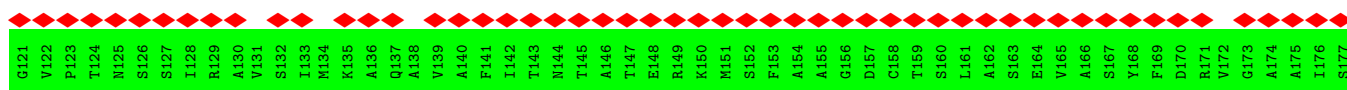
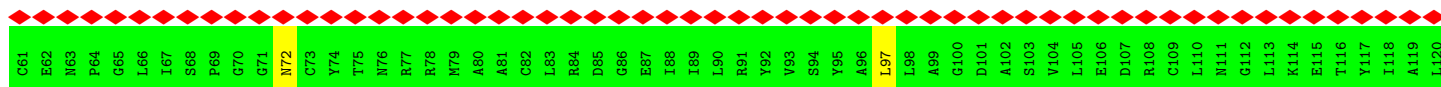
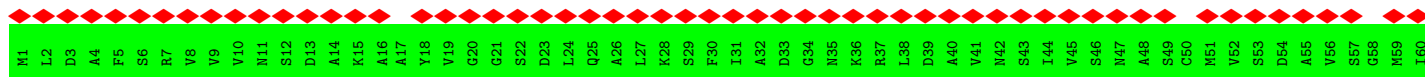




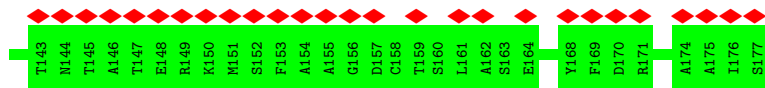
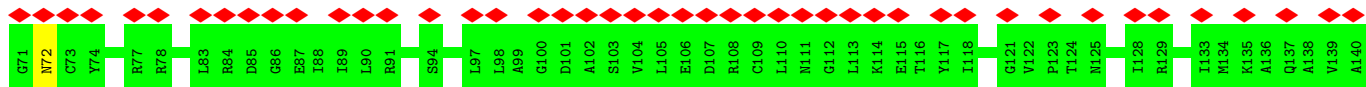
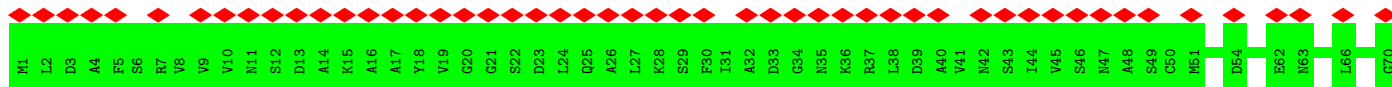
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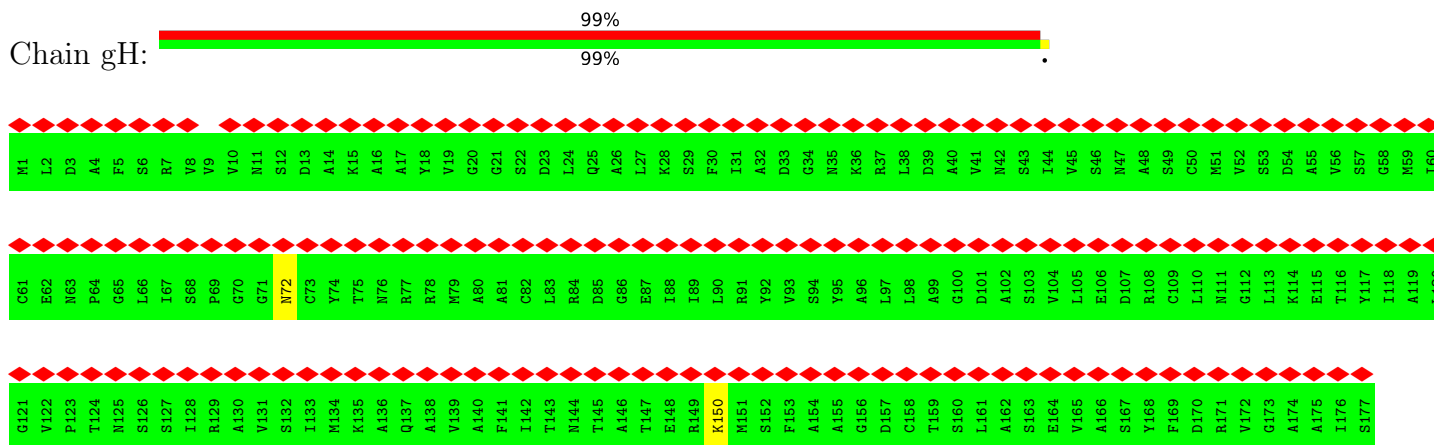
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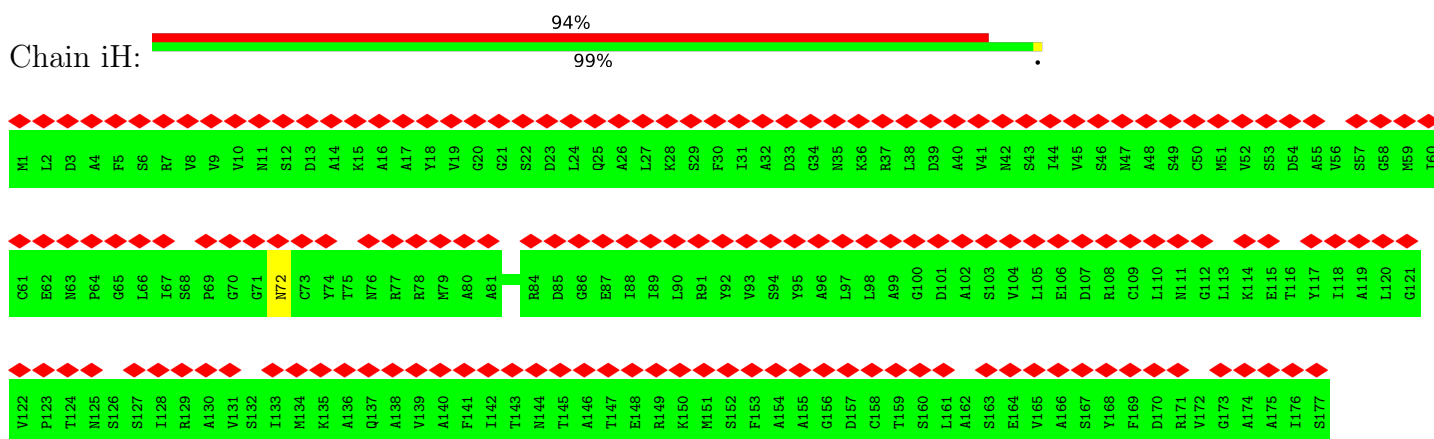
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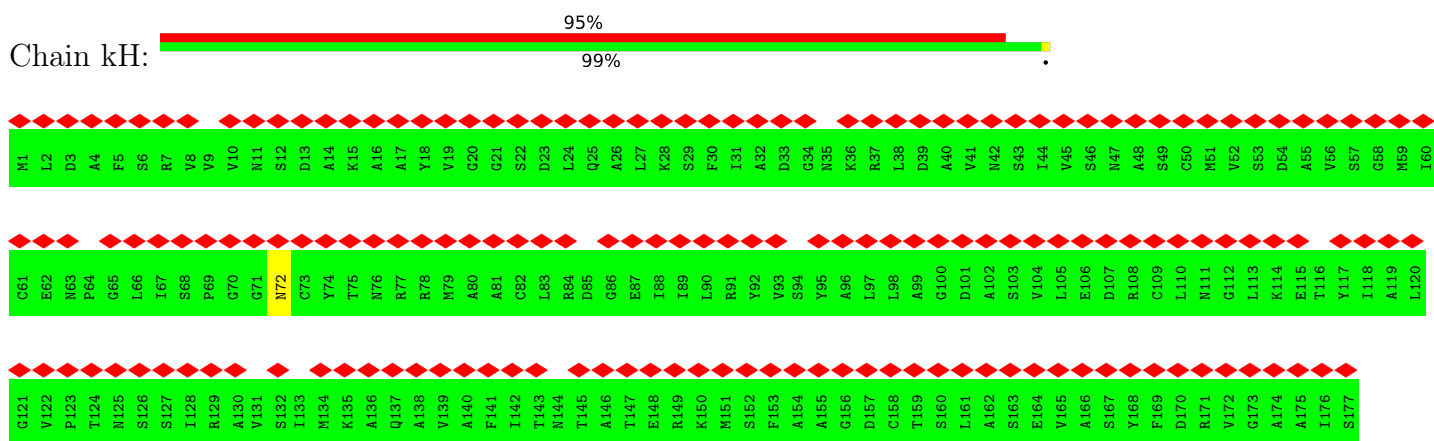
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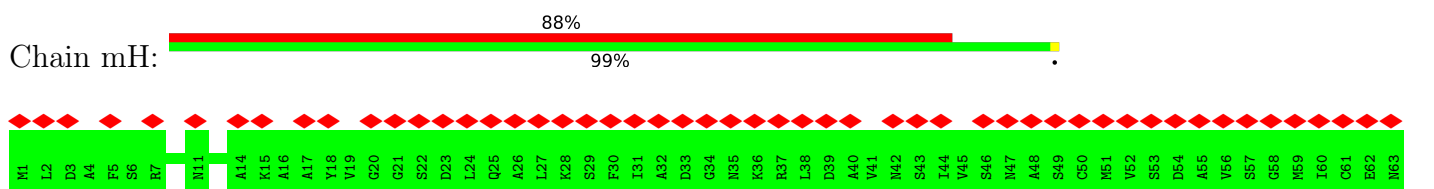
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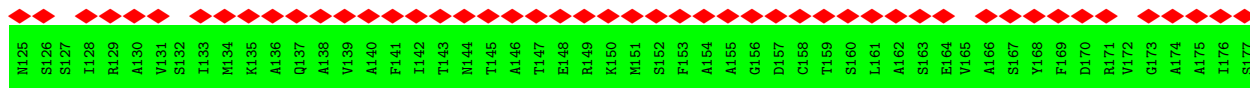
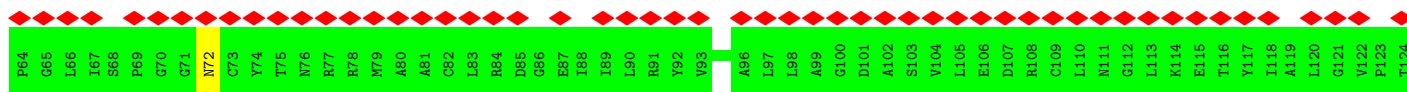


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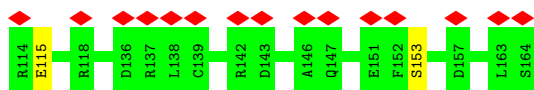
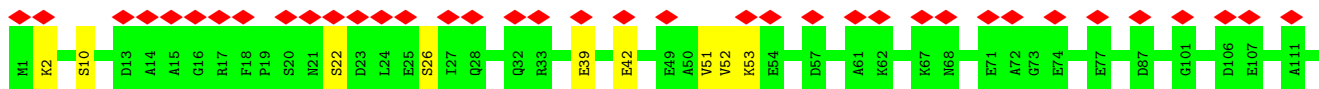


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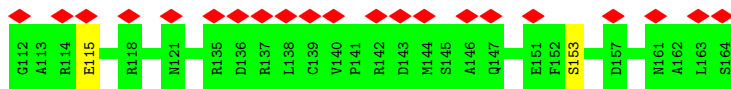
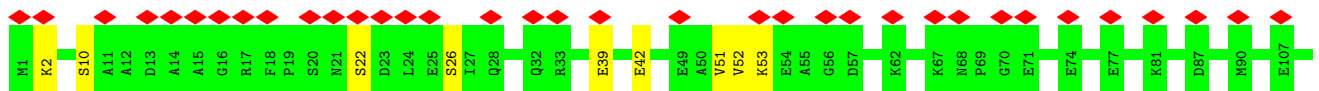




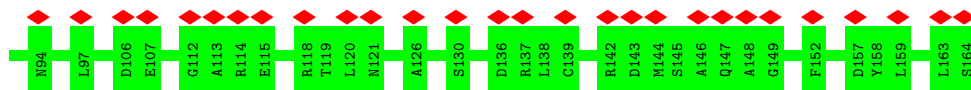
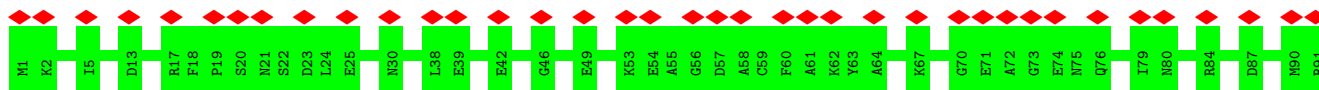
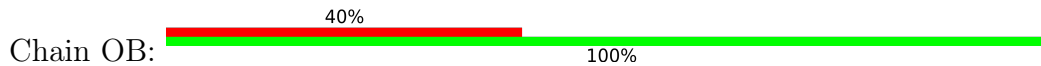
- Molecule 3: Phycoerythrin alpha subunit



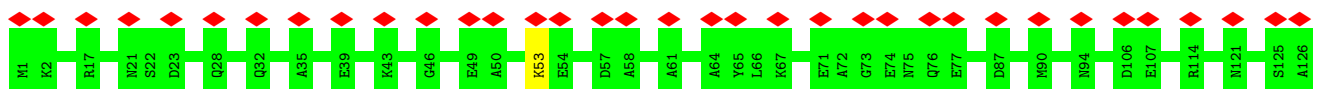
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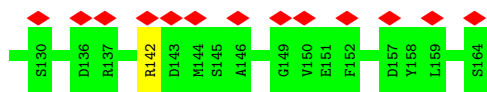


- Molecule 3: Phycoerythrin alpha subunit

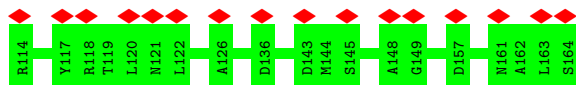
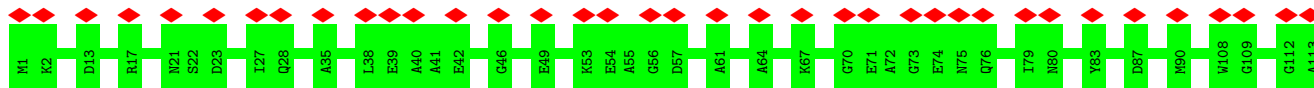


- Molecule 3: Phycoerythrin alpha subunit

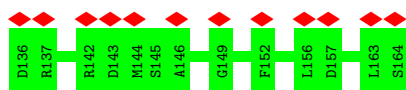
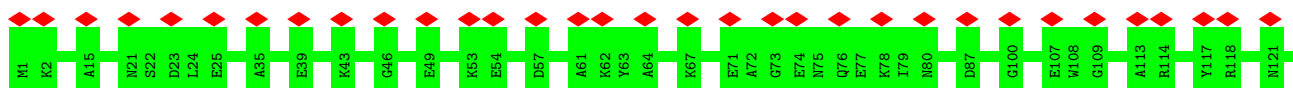




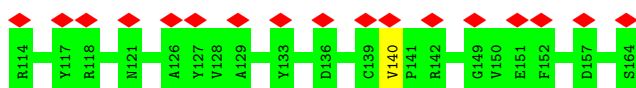
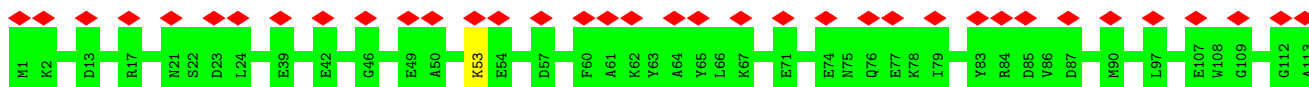
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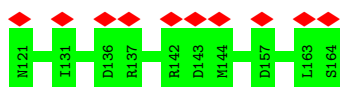
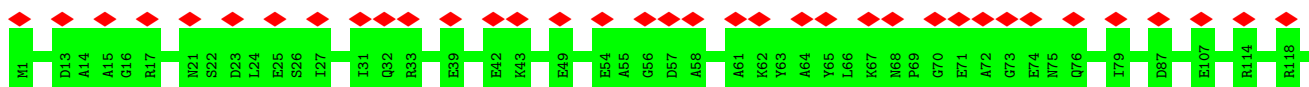
- Molecule 3: Phycoerythrin alpha subunit



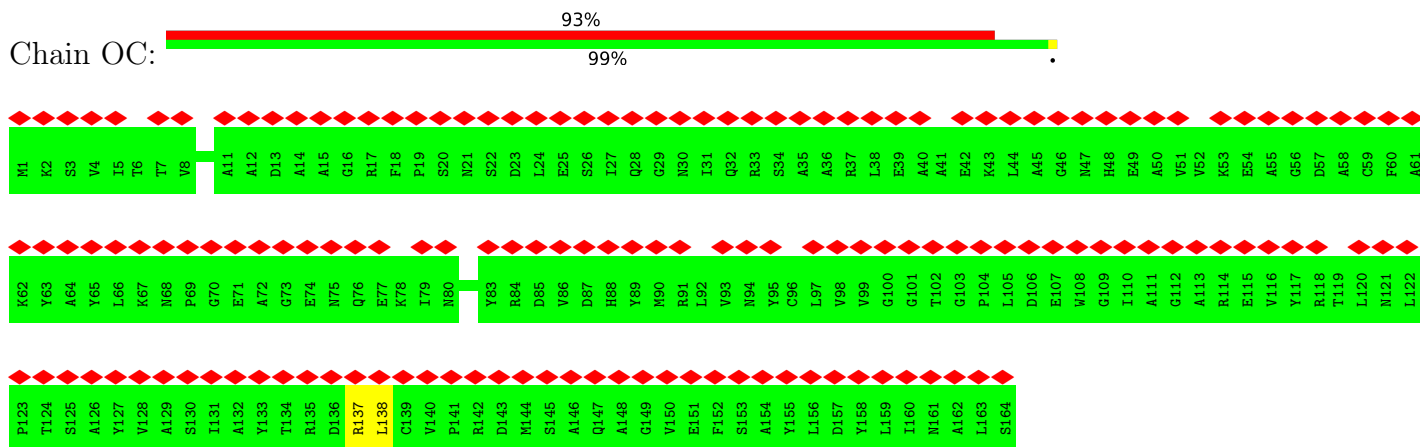
- Molecule 3: Phycoerythrin alpha subunit



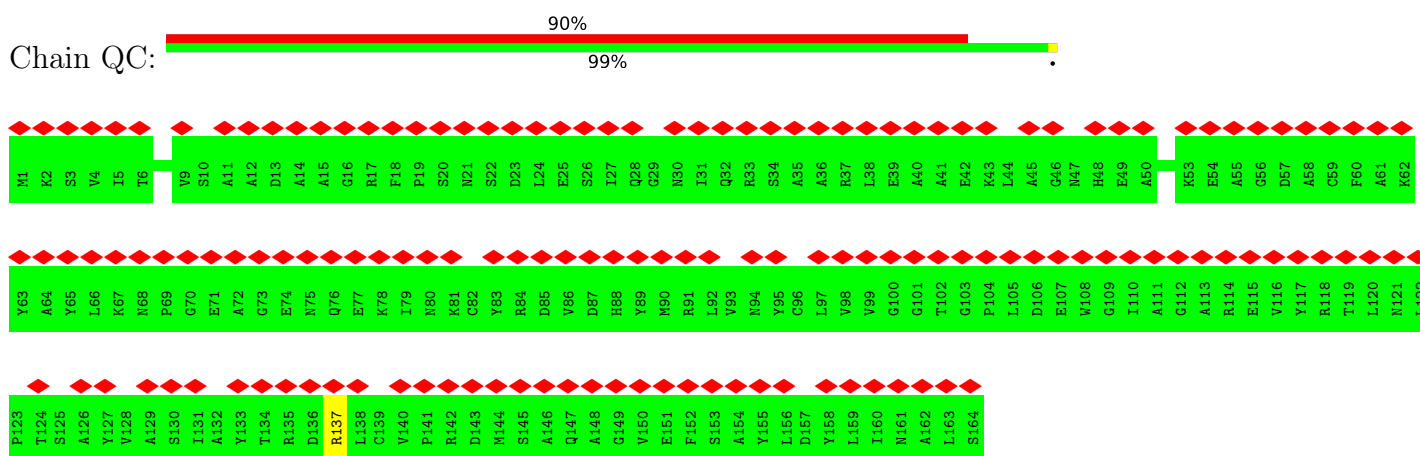
- Molecule 3: Phycoerythrin alpha subunit



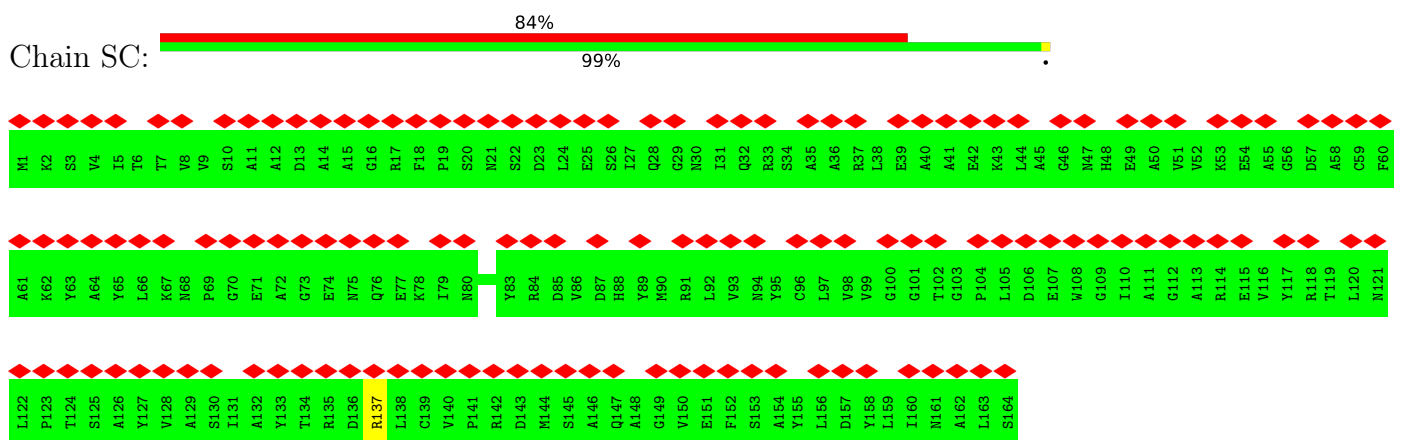
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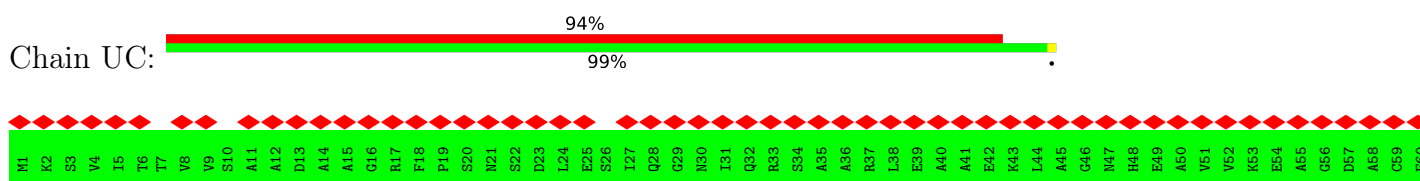
• Molecule 3: Phycoerythrin alpha subunit

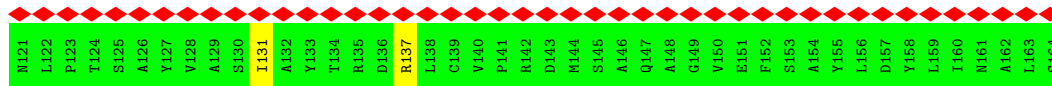


• Molecule 3: Phycoerythrin alpha subunit

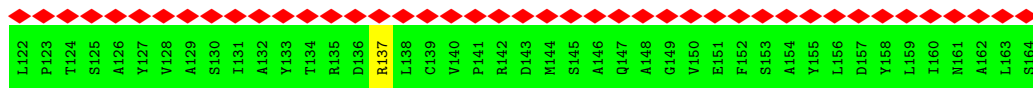
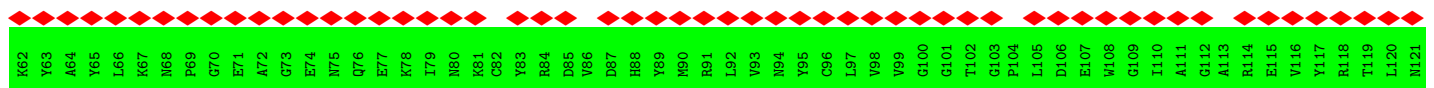
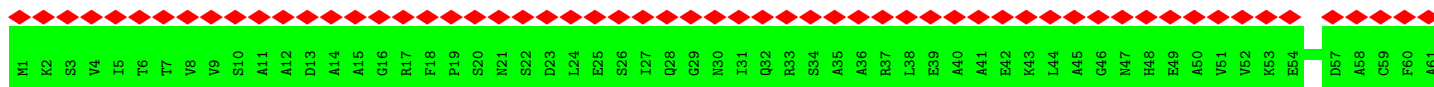


• Molecule 3: Phycoerythrin alpha subunit

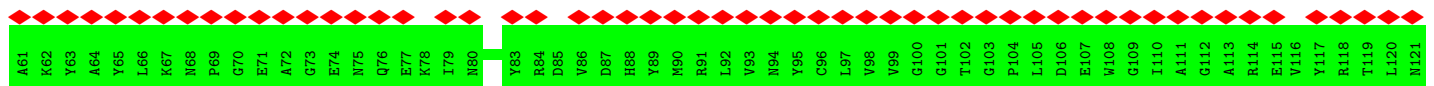
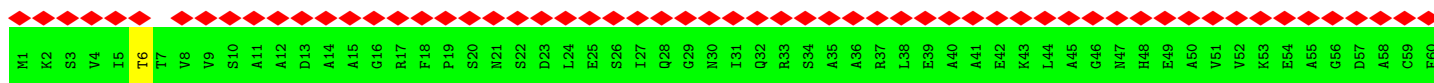




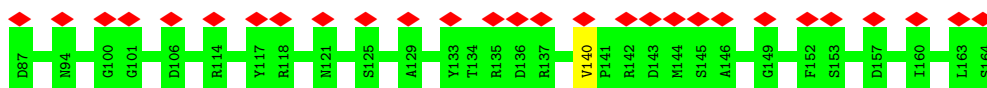
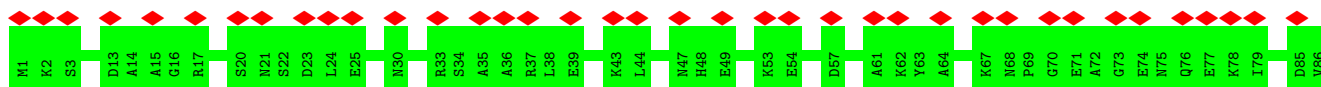
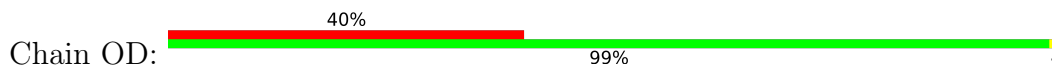
• Molecule 3: Phycoerythrin alpha subunit



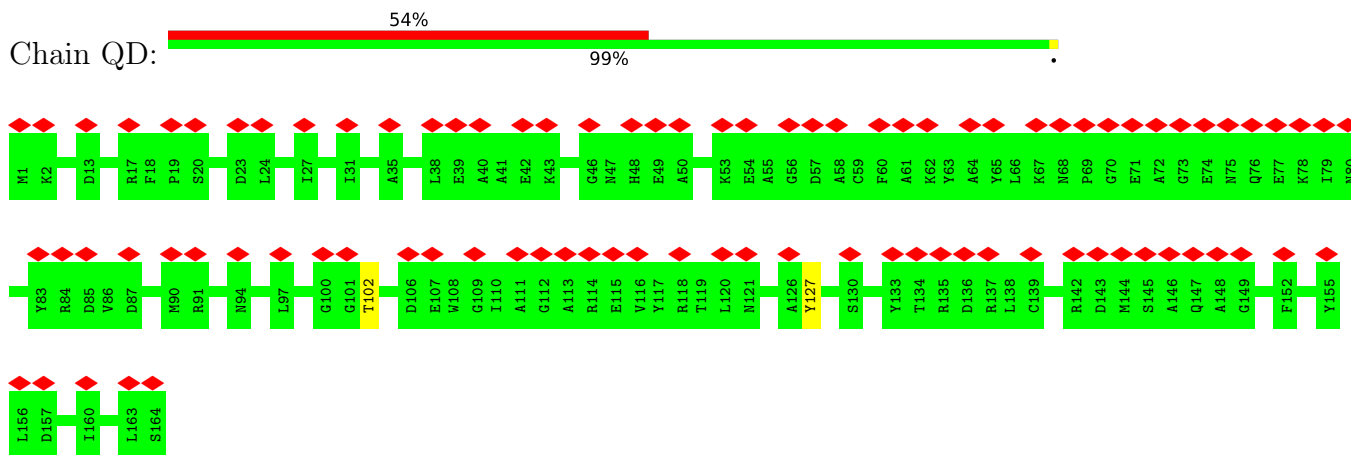
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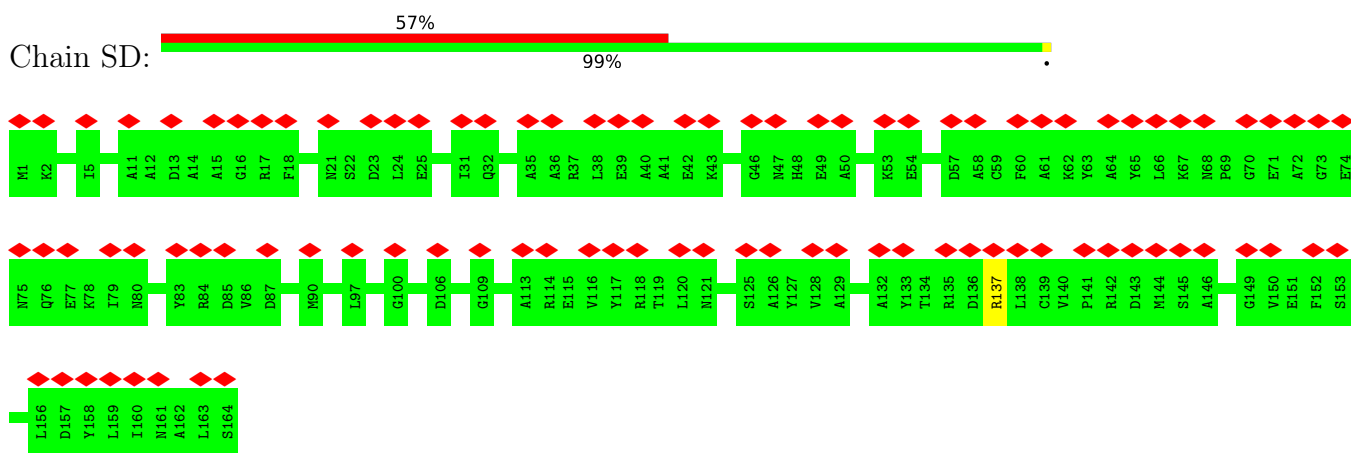
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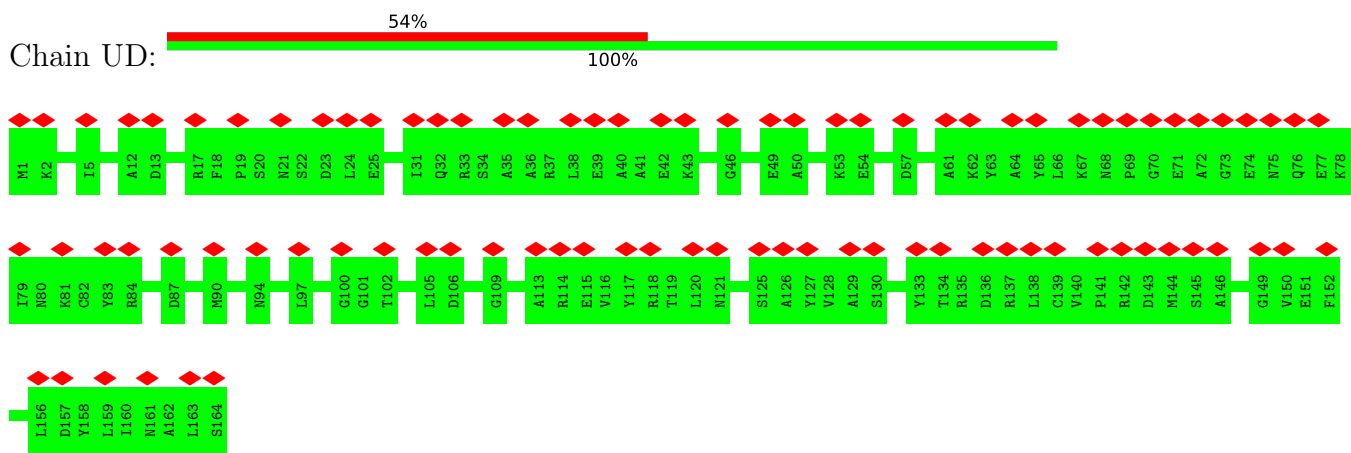
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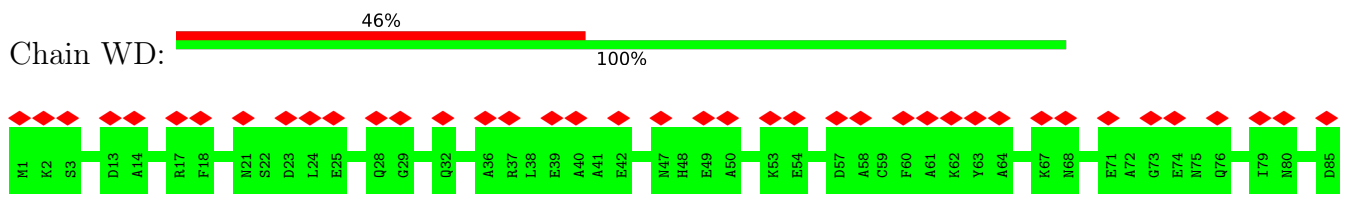
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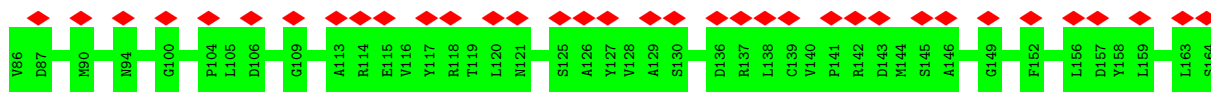


• Molecule 3: Phycoerythrin alpha subunit

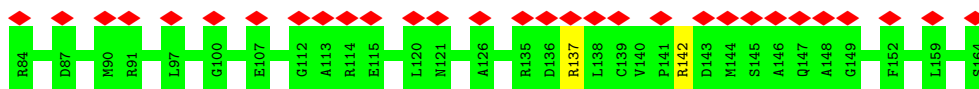
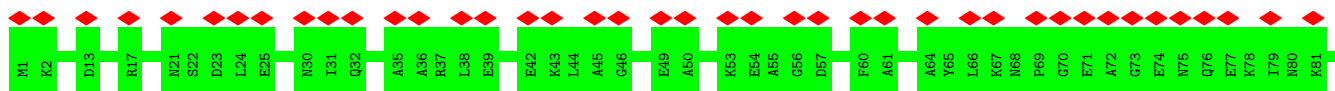
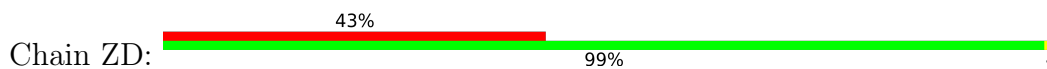


• Molecule 3: Phycoerythrin alpha subunit

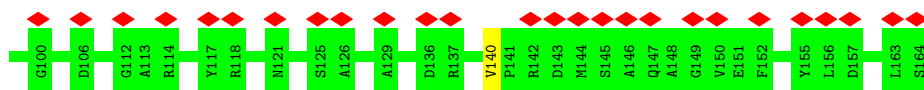
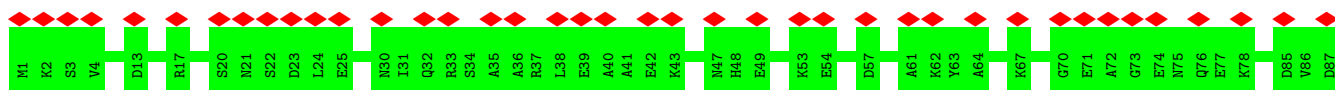
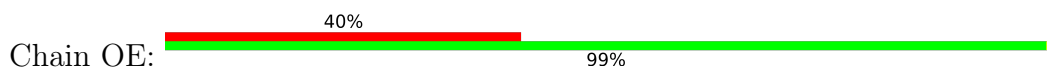




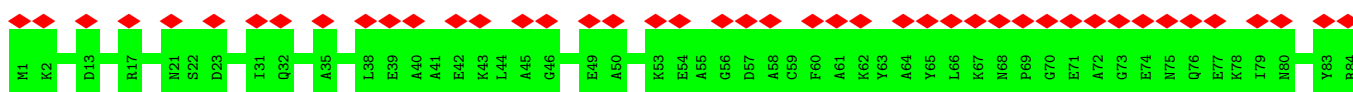
- Molecule 3: Phycoerythrin alpha subunit



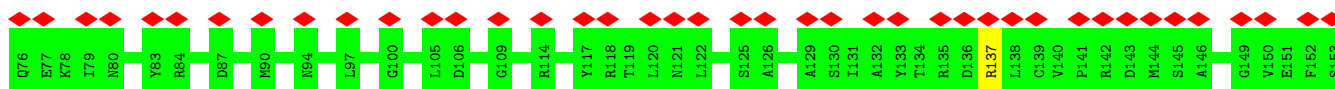
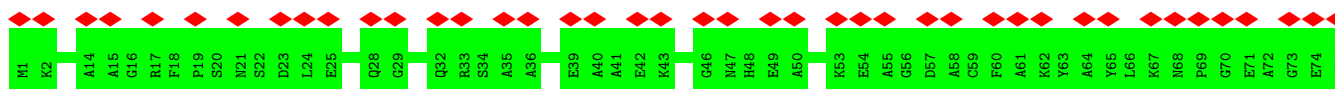
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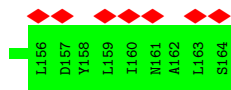


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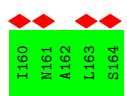
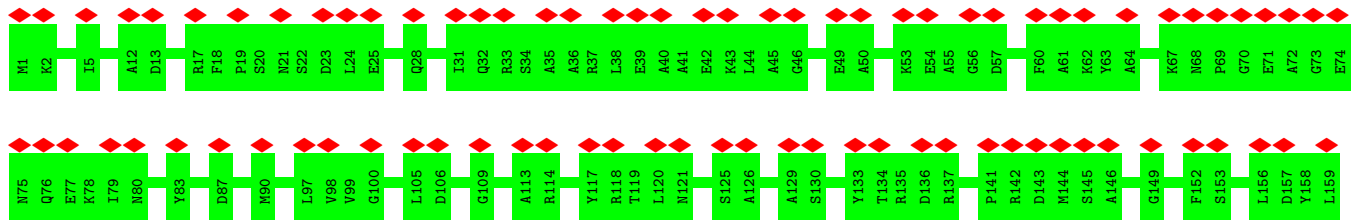


- Molecule 3: Phycoerythrin alpha subunit

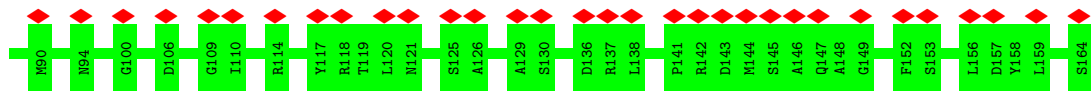
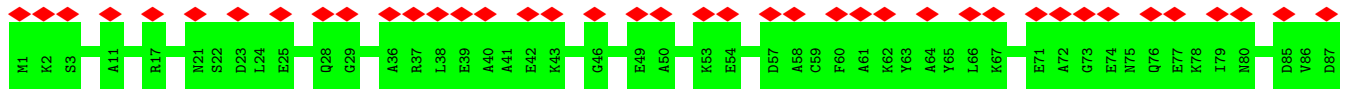




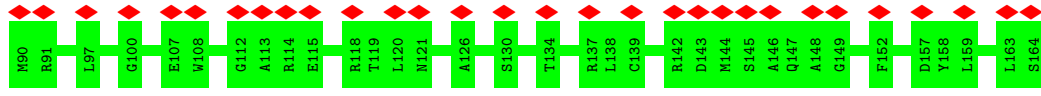
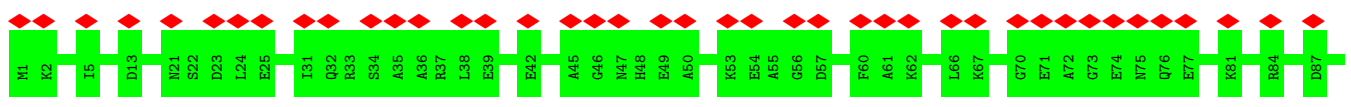
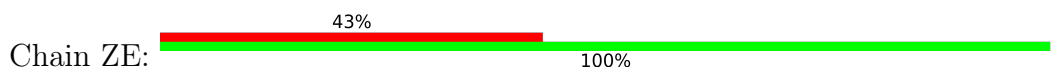
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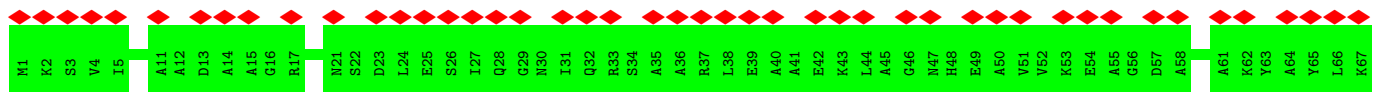
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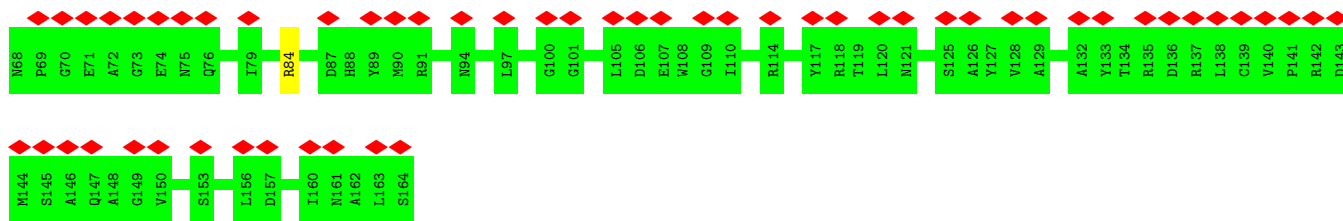


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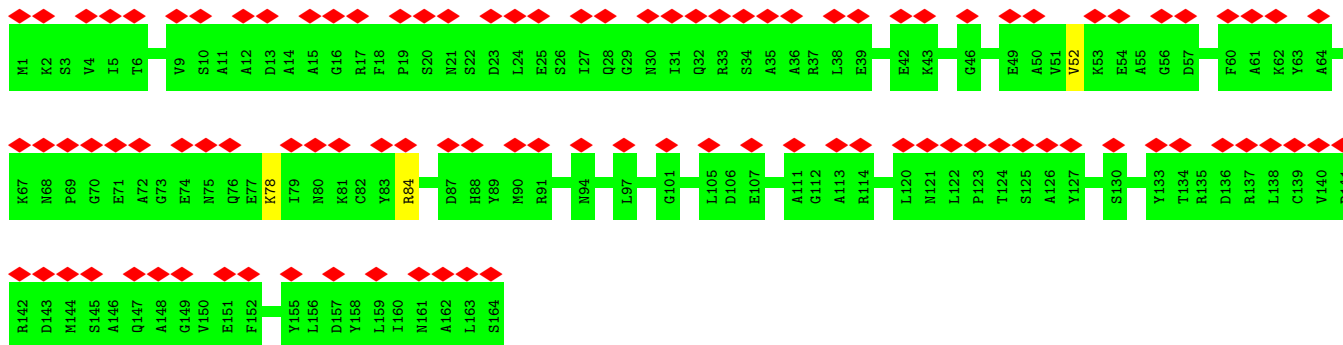


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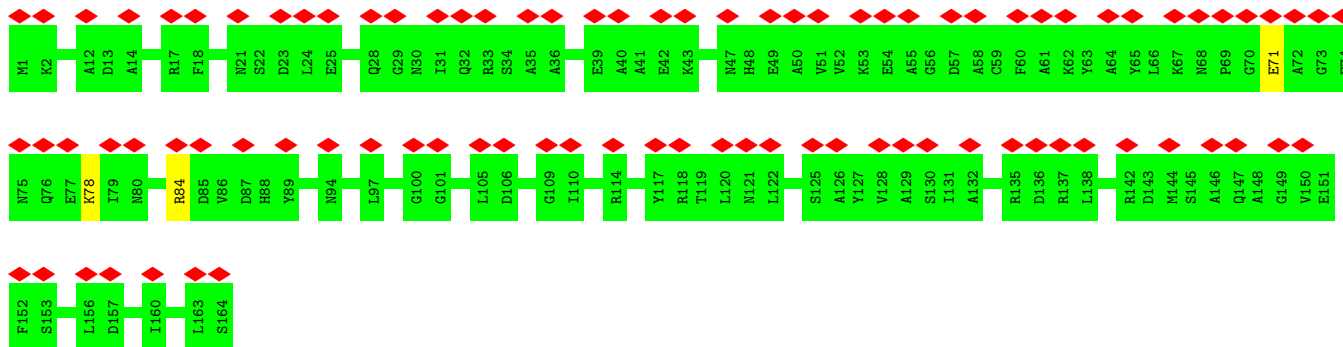




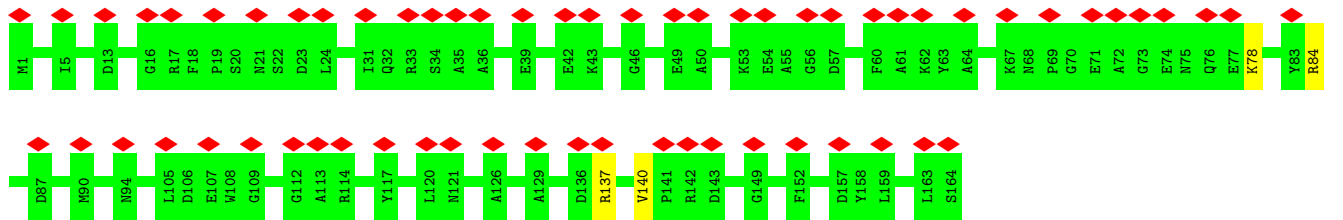
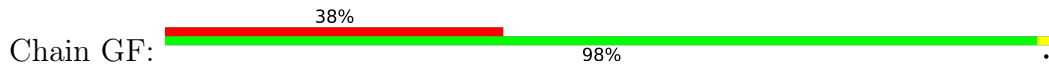
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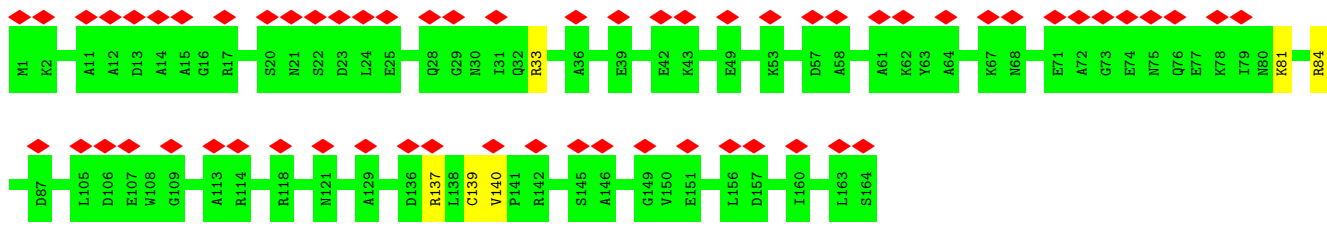
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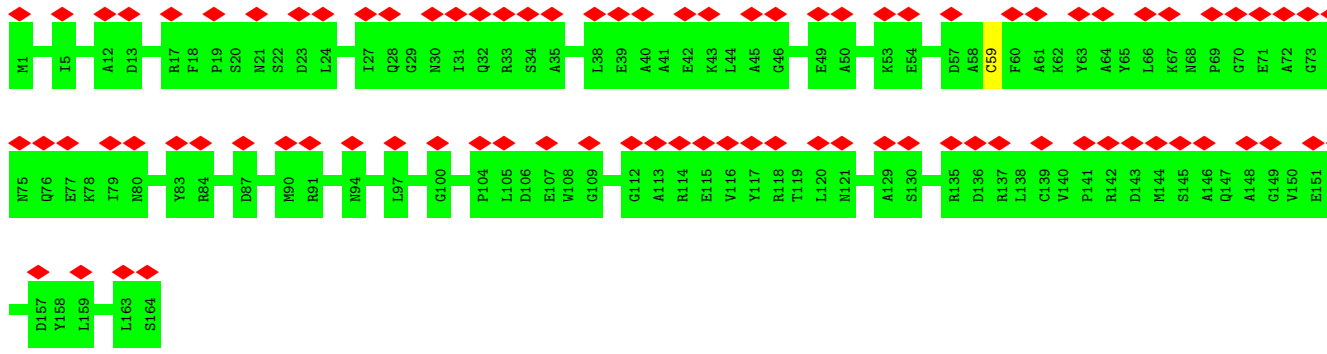
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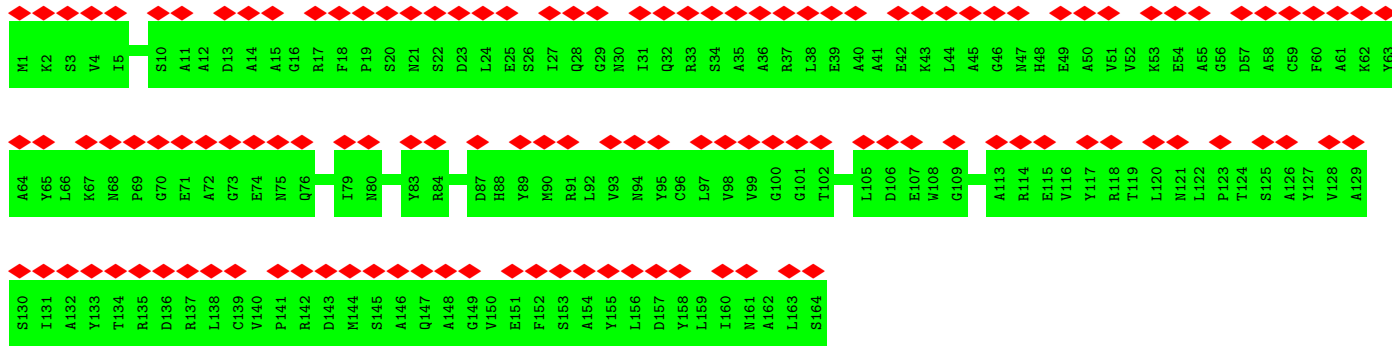
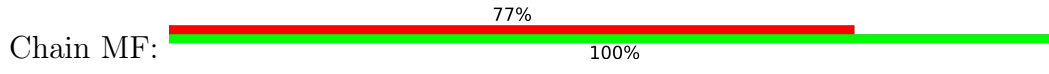
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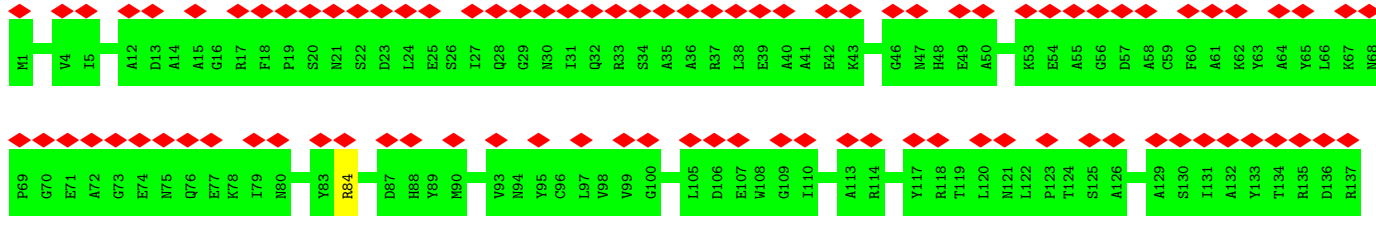
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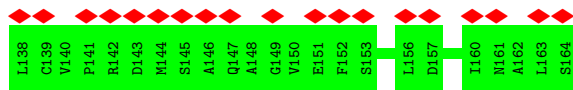


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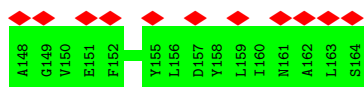
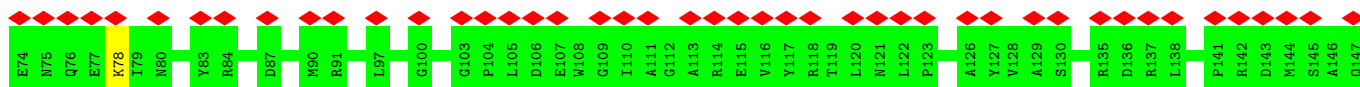


• Molecule 3: Phycoerythrin alpha subunit

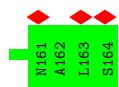
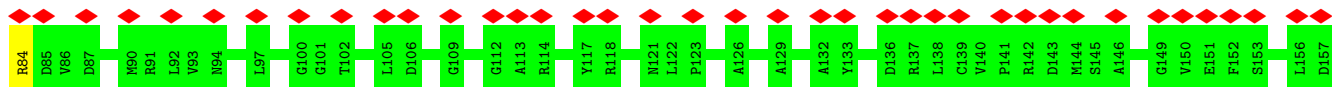
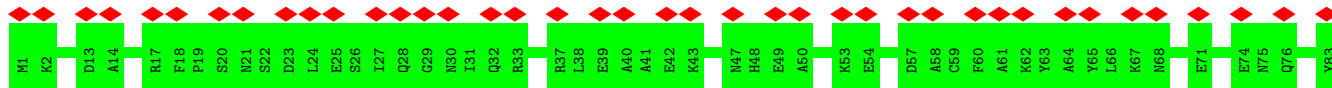




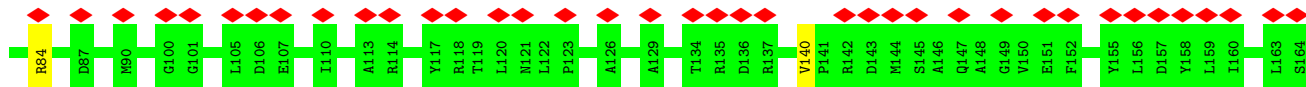
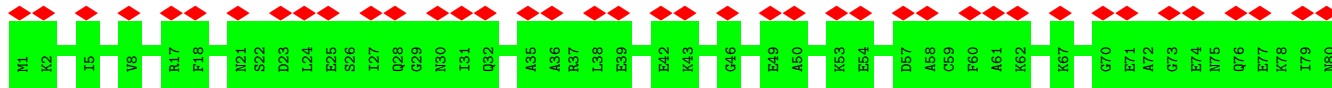
• Molecule 3: Phycoerythrin alpha subunit



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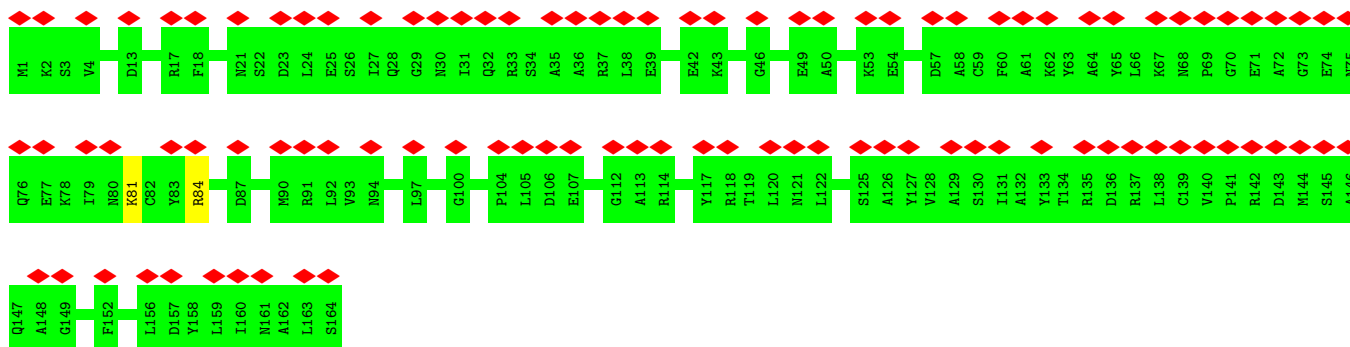


• Molecule 3: Phycoerythrin alpha subunit

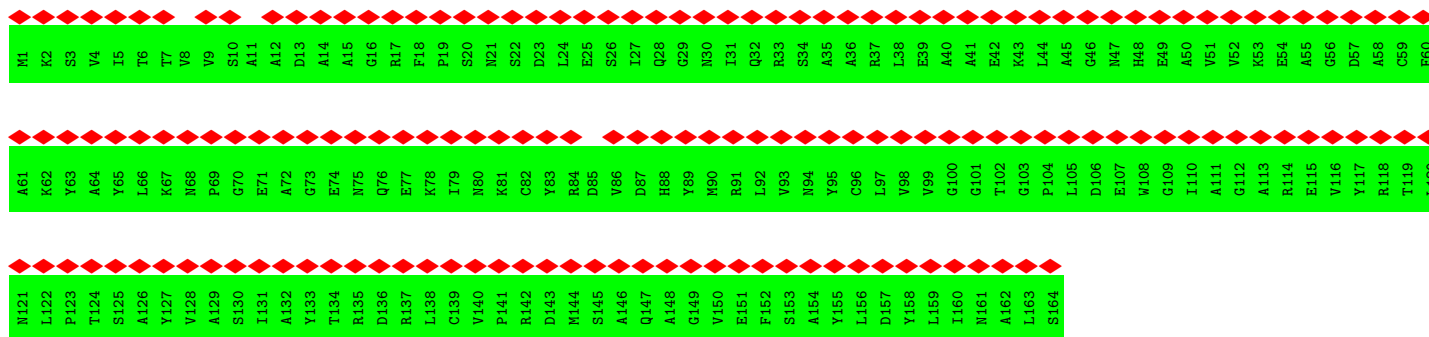


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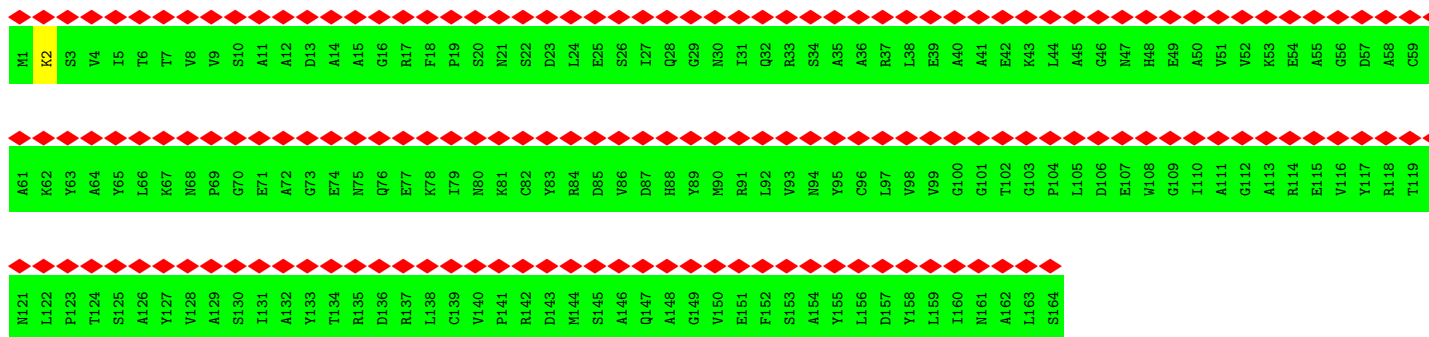




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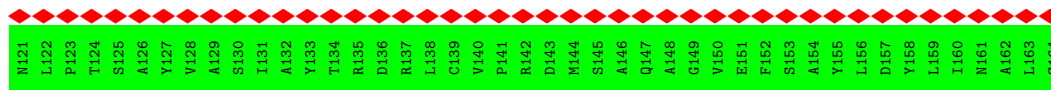


• Molecule 3: Phycoerythrin alpha subunit

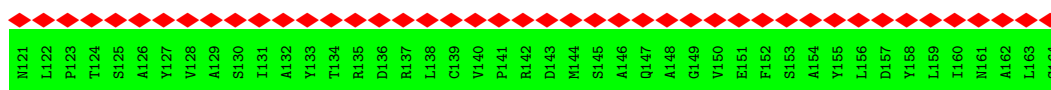
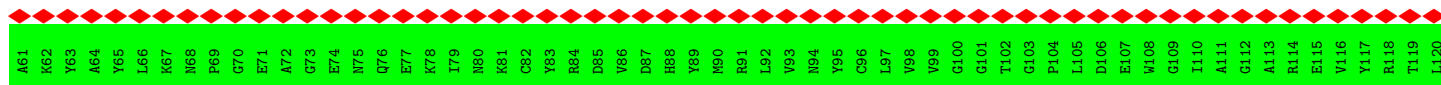
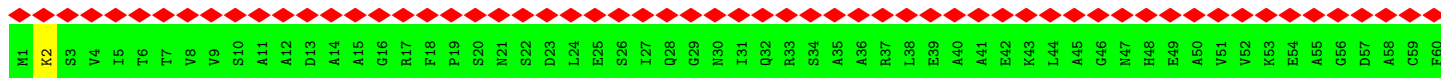


• Molecule 3: Phycoerythrin alpha subunit

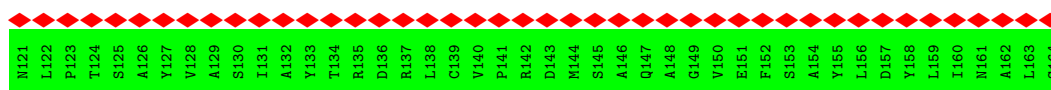
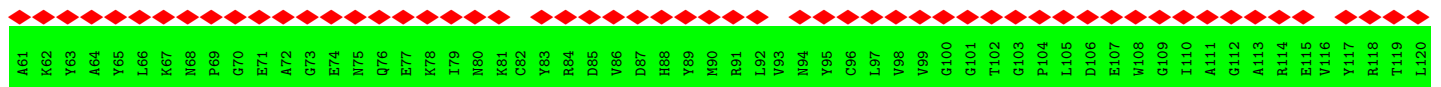
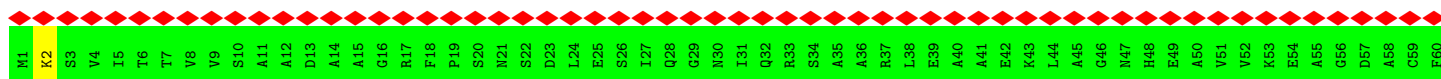




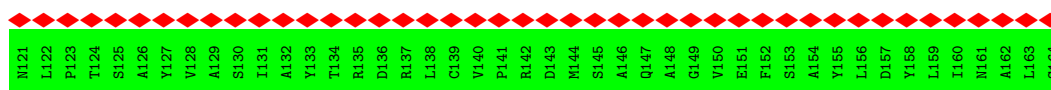
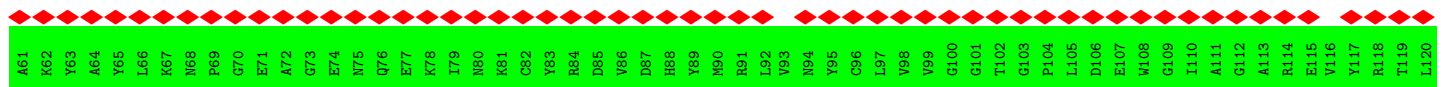
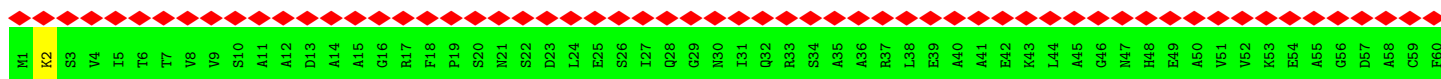
• Molecule 3: Phycoerythrin alpha subunit



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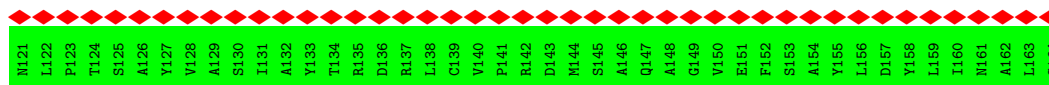
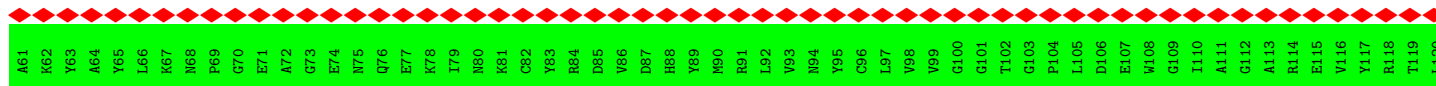
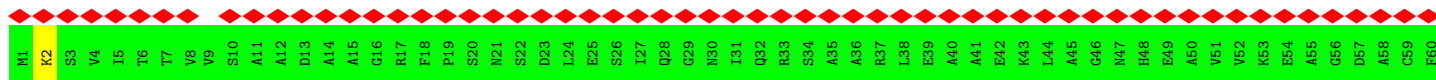


• Molecule 3: Phycoerythrin alpha subunit

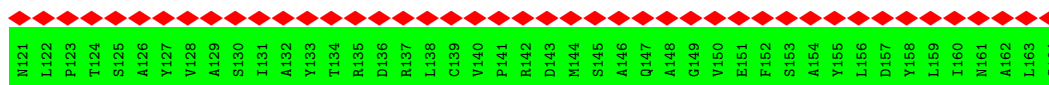
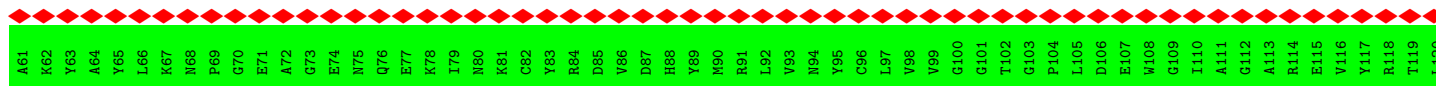
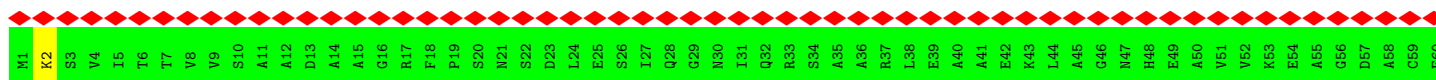


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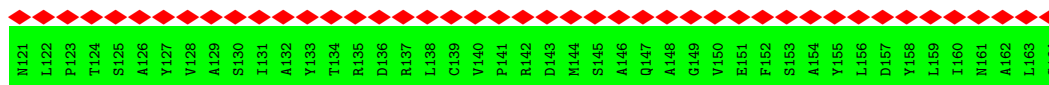
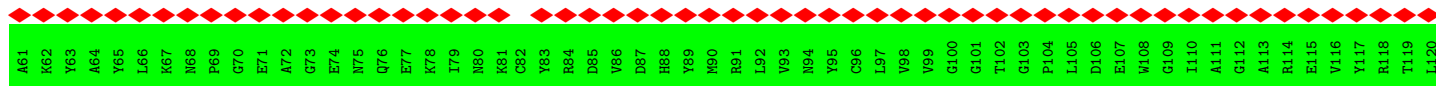
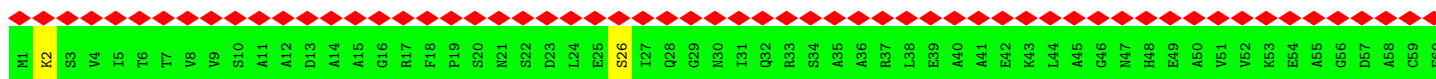




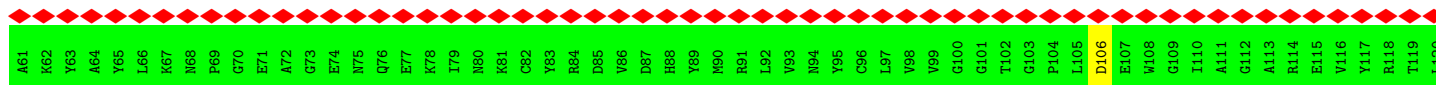
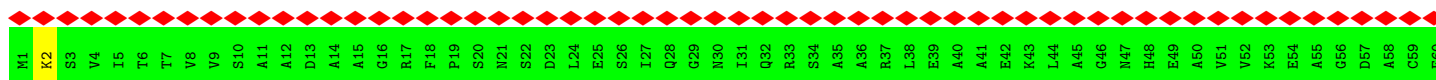
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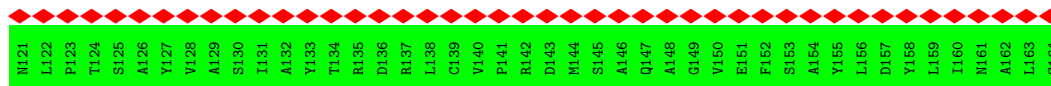
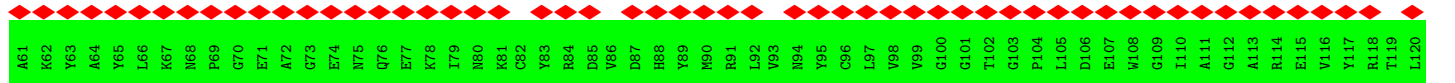
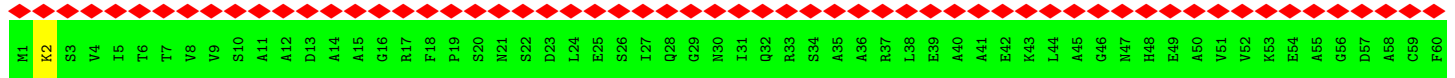


• Molecule 3: Phycoerythrin alpha subunit

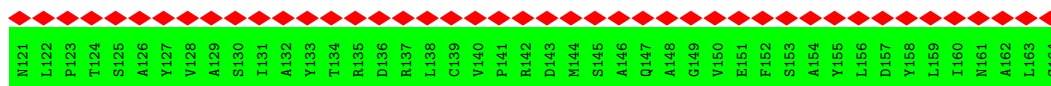
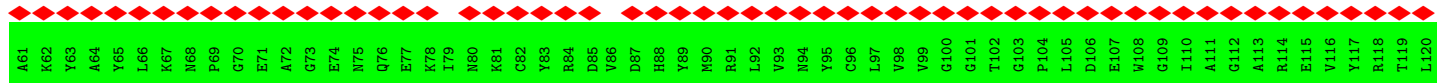
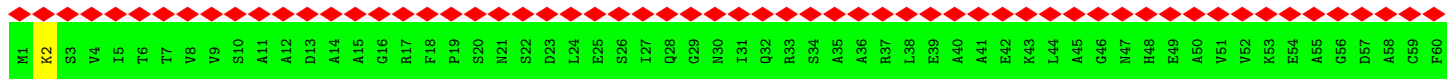




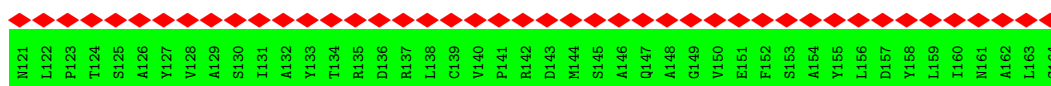
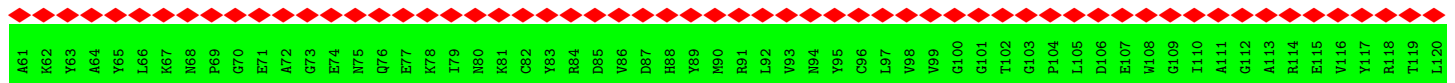
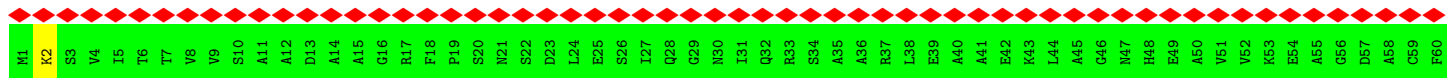
• Molecule 3: Phycoerythrin alpha subunit



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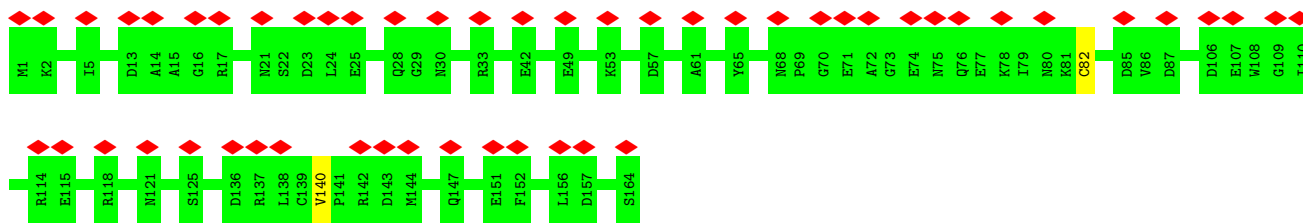


• Molecule 3: Phycoerythrin alpha subunit

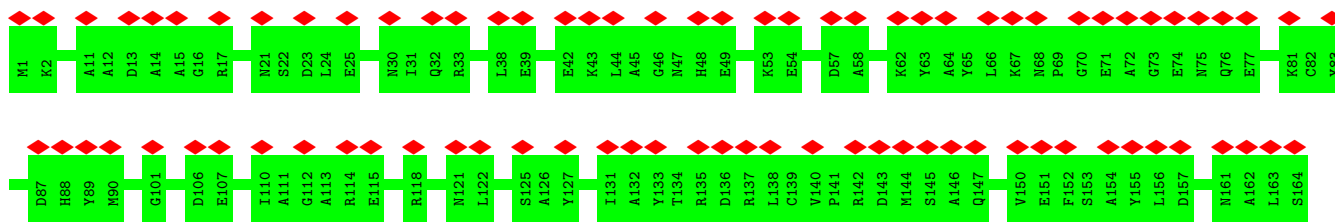


• Molecule 3: Phycoerythrin alpha subunit

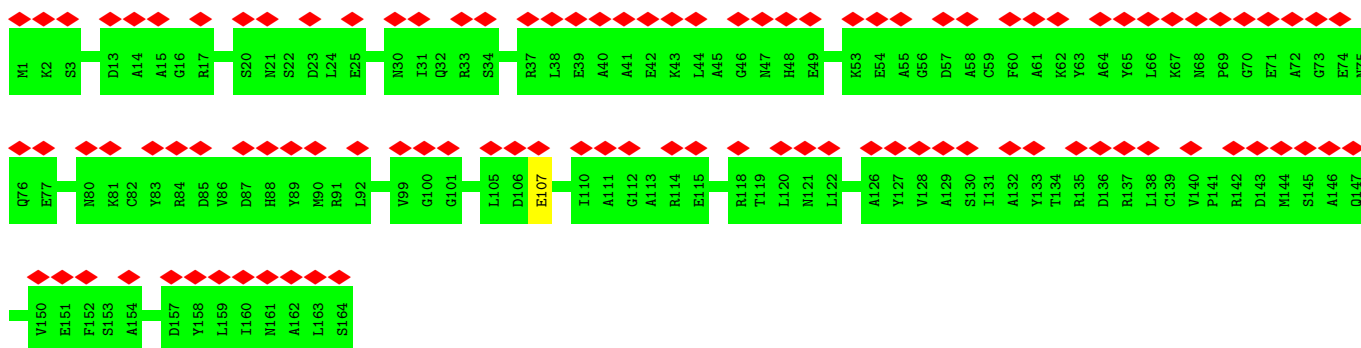




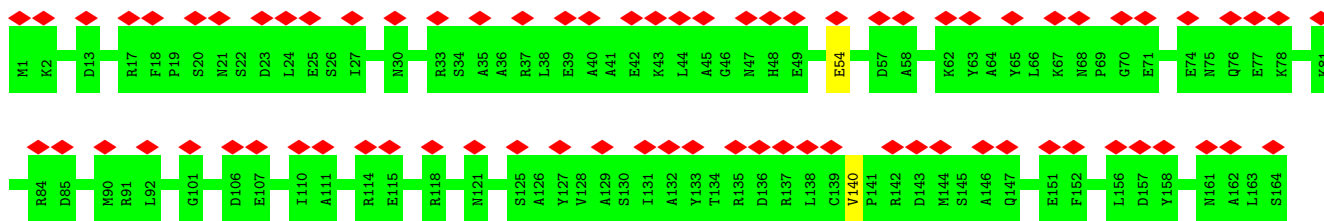
- Molecule 3: Phycoerythrin alpha subunit



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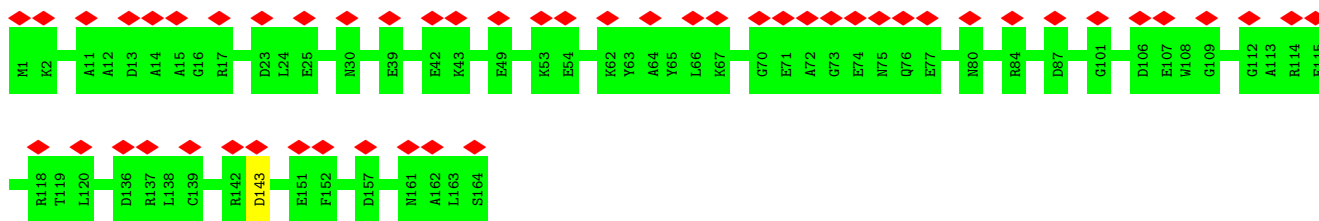


- Molecule 3: Phycoerythrin alpha subunit

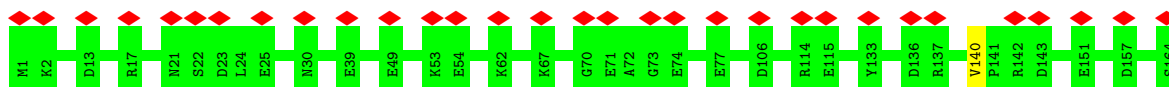


- Molecule 3: Phycoerythrin alpha subunit





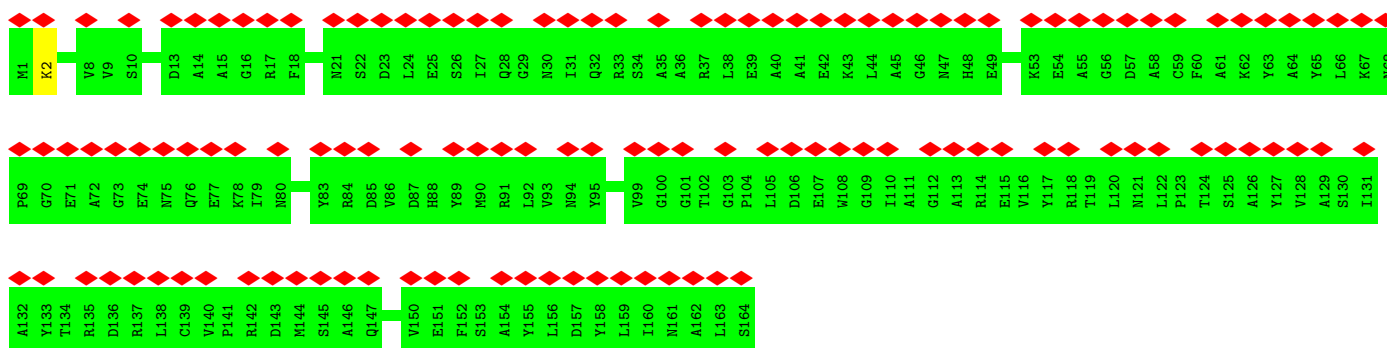
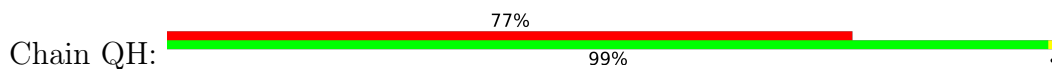
- Molecule 3: Phycoerythrin alpha subunit



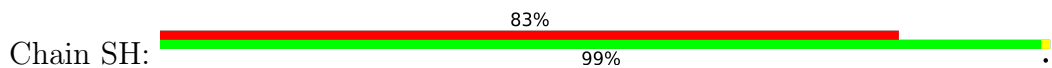
- Molecule 3: Phycoerythrin alpha subunit

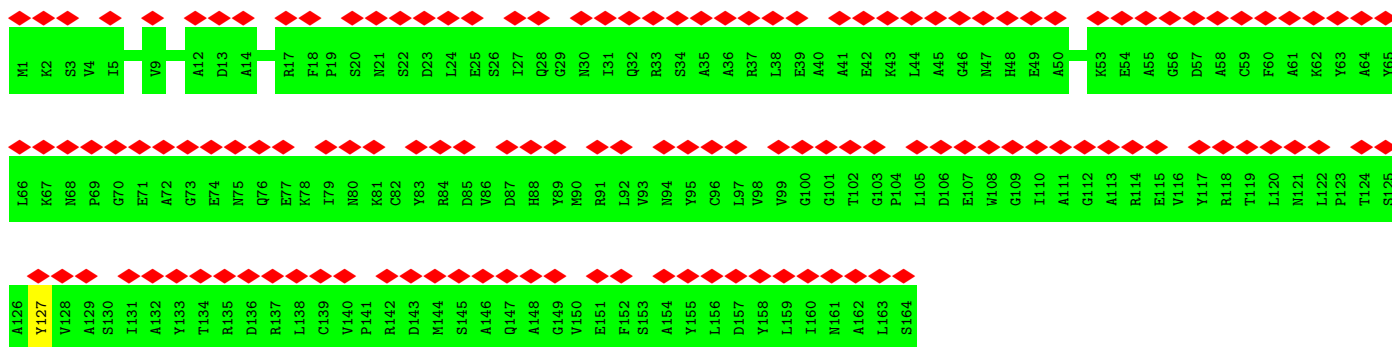


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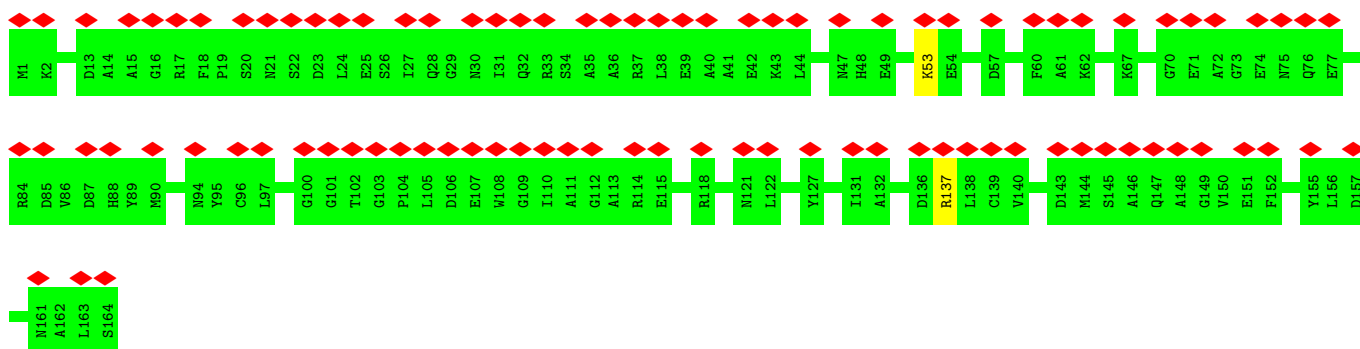


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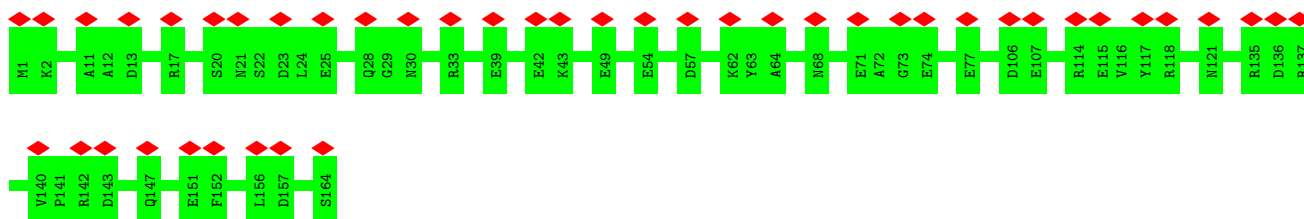




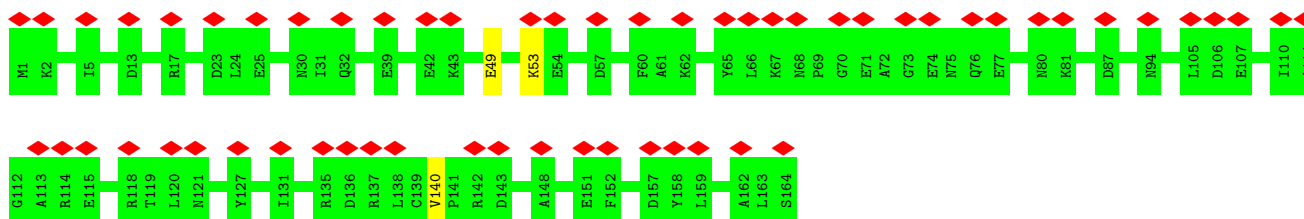
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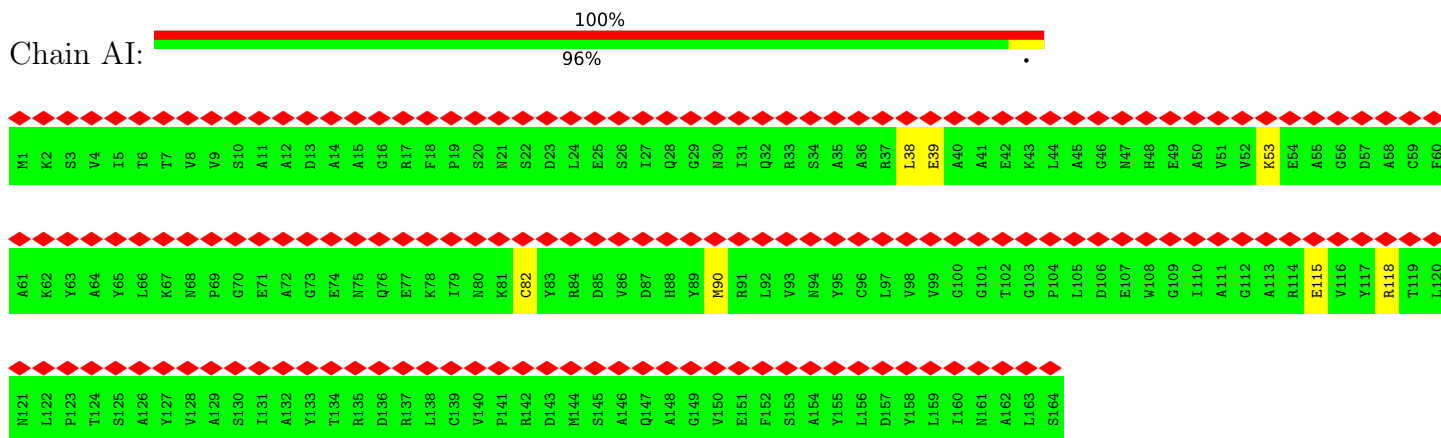
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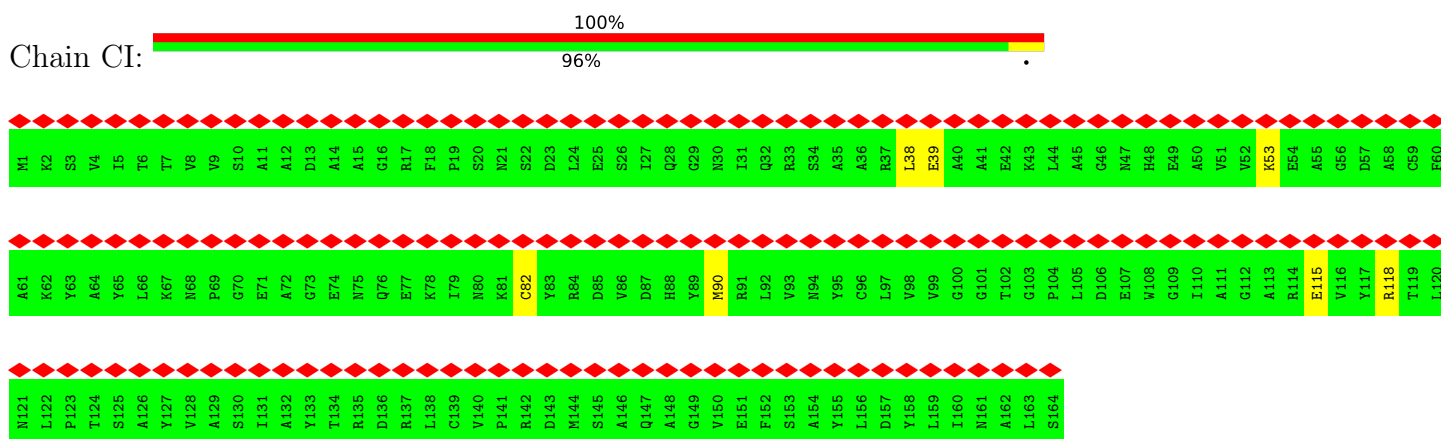
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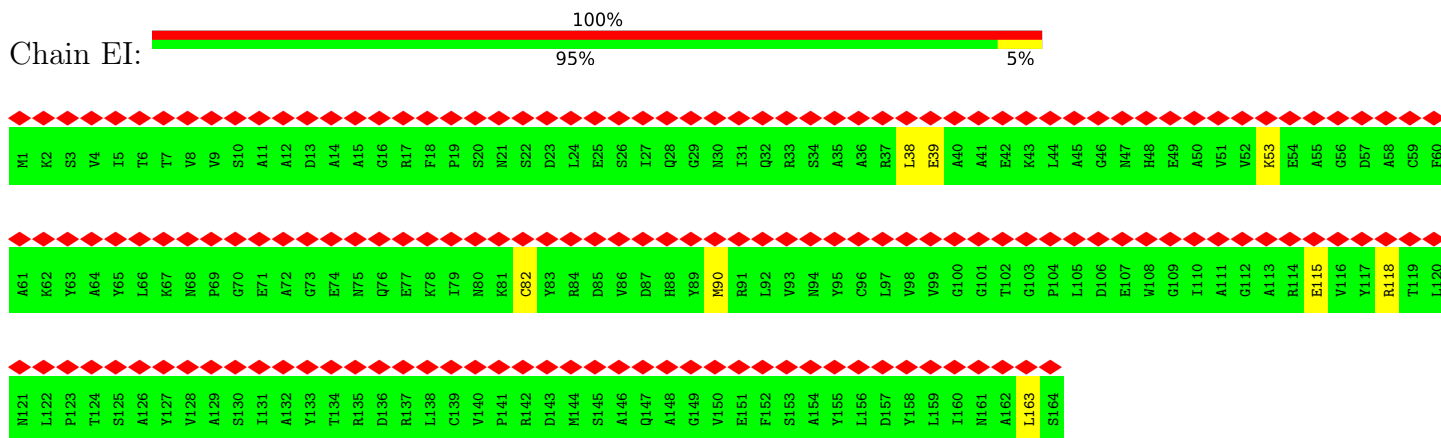
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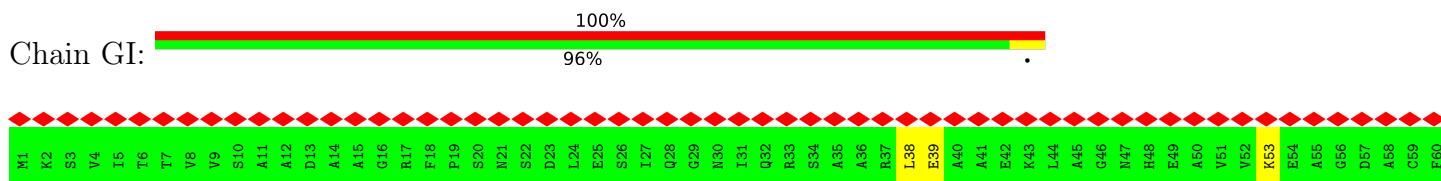
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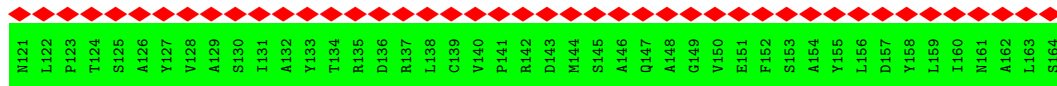
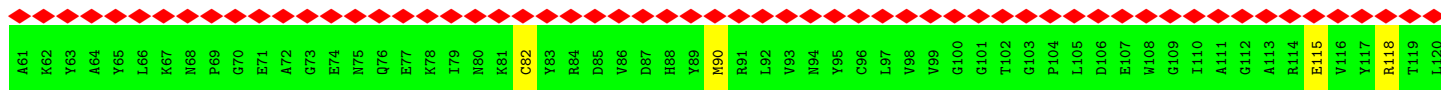


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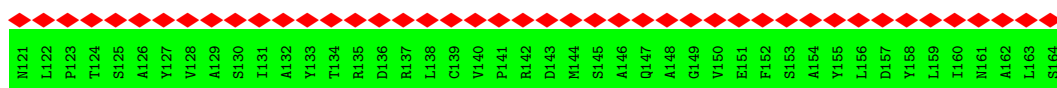
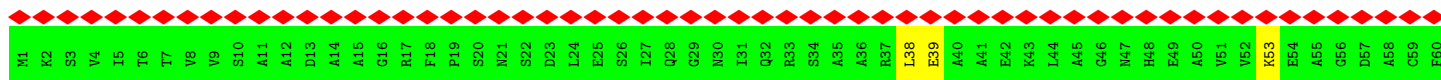


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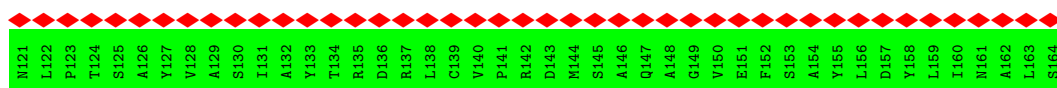
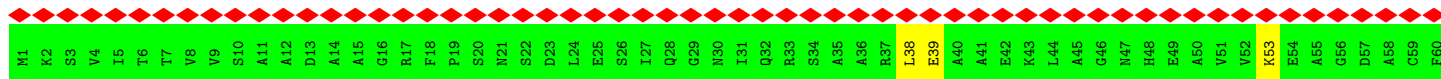




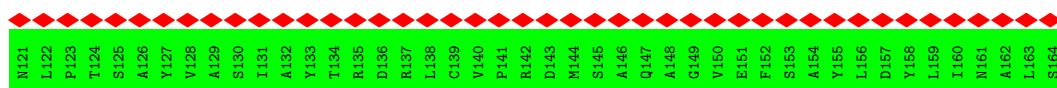
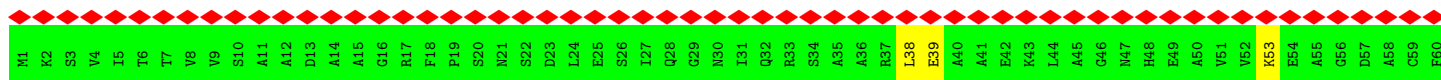
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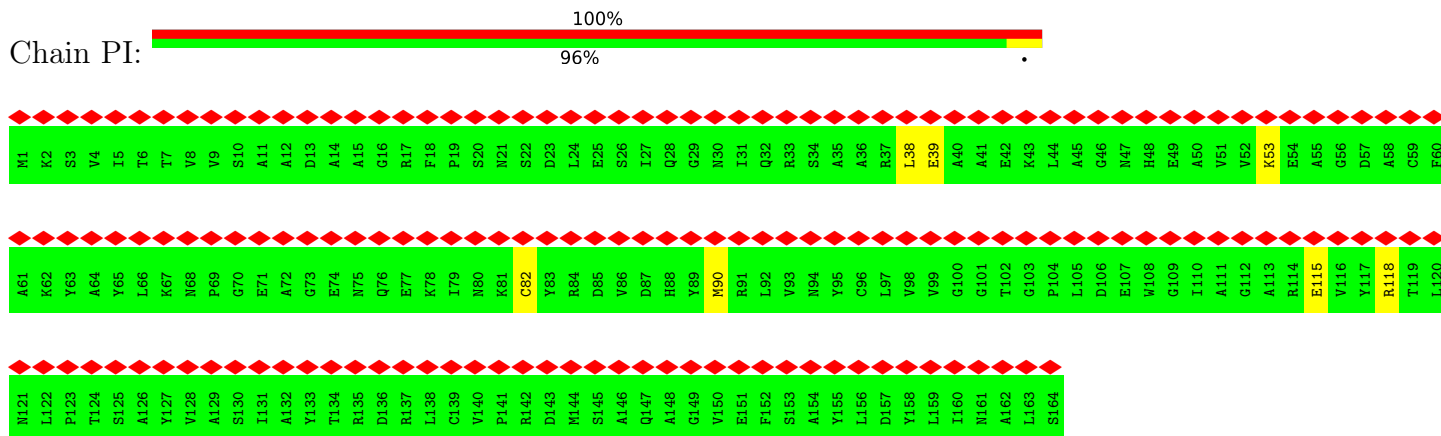
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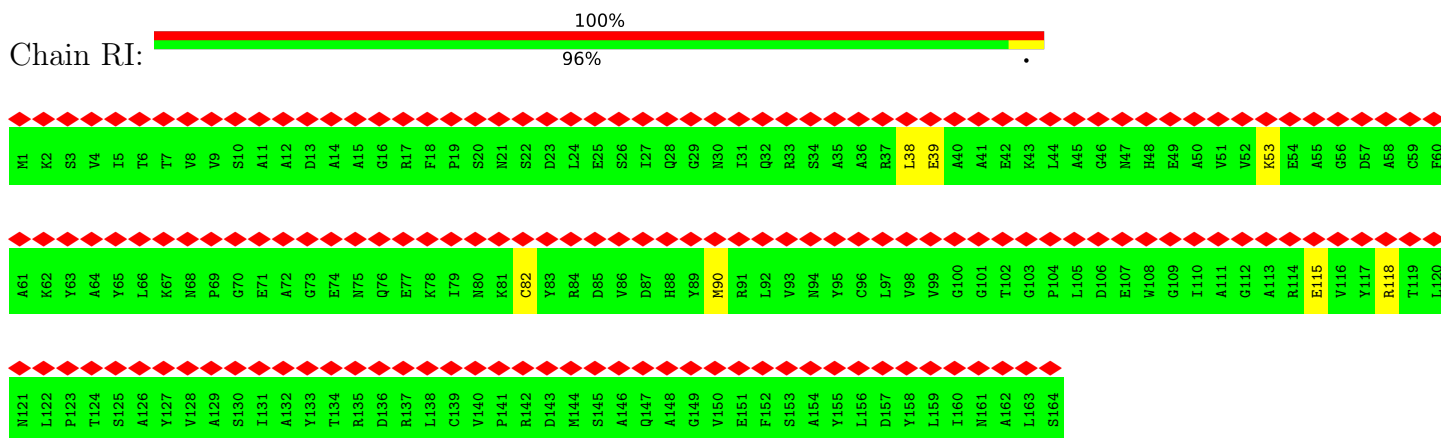
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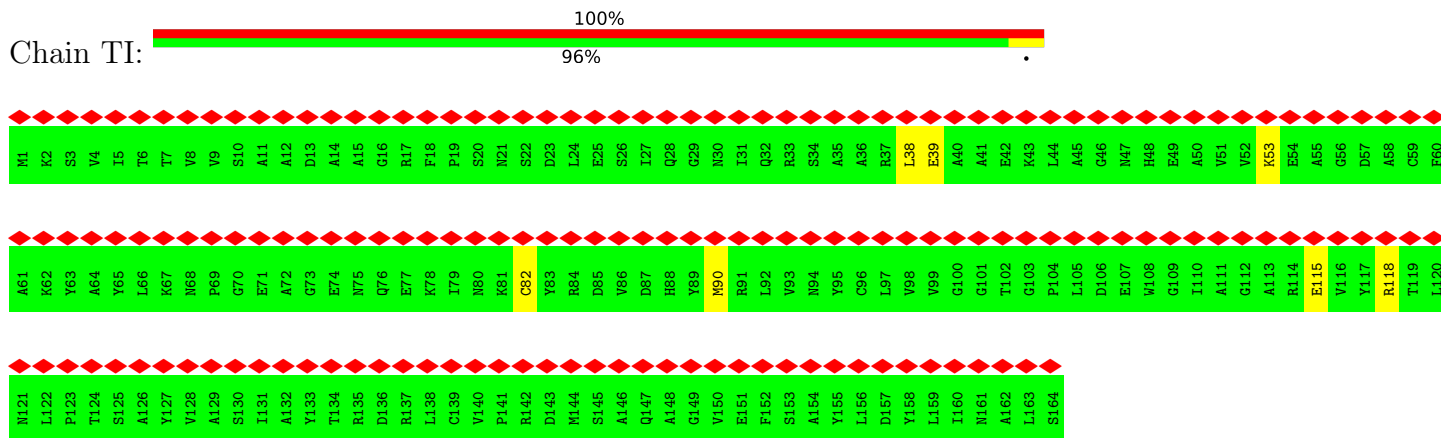
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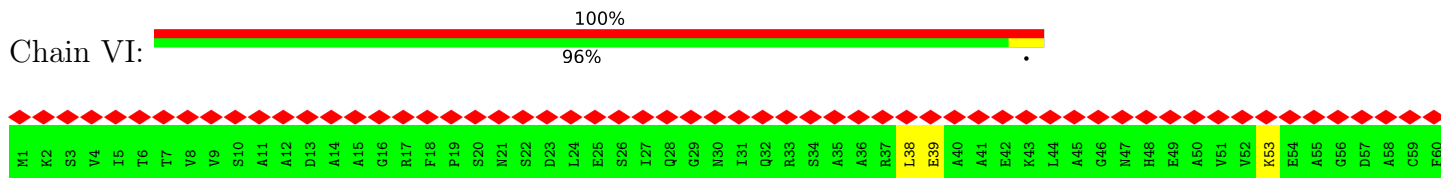
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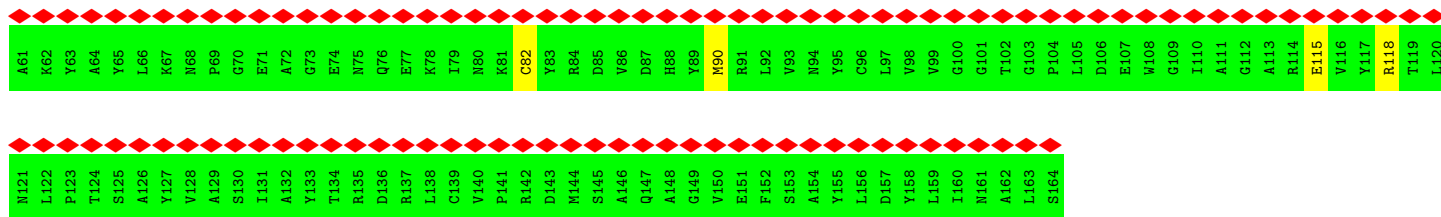


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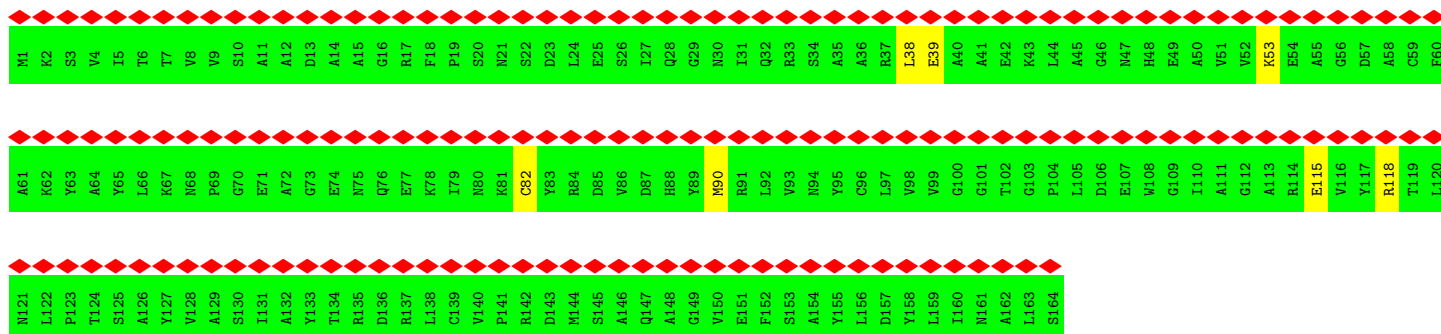


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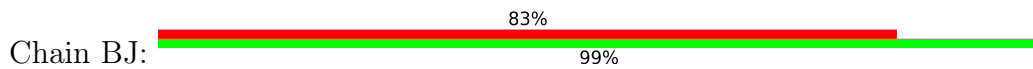




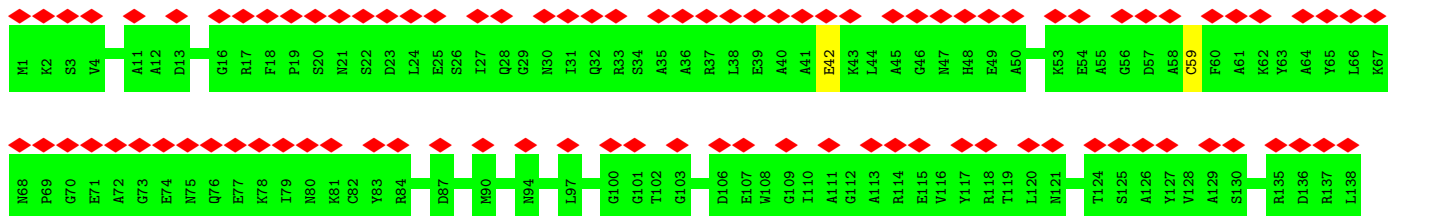
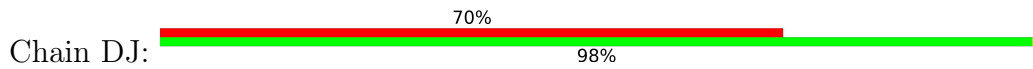
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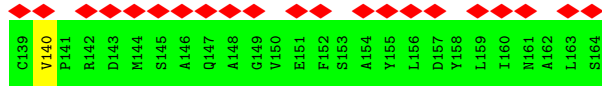


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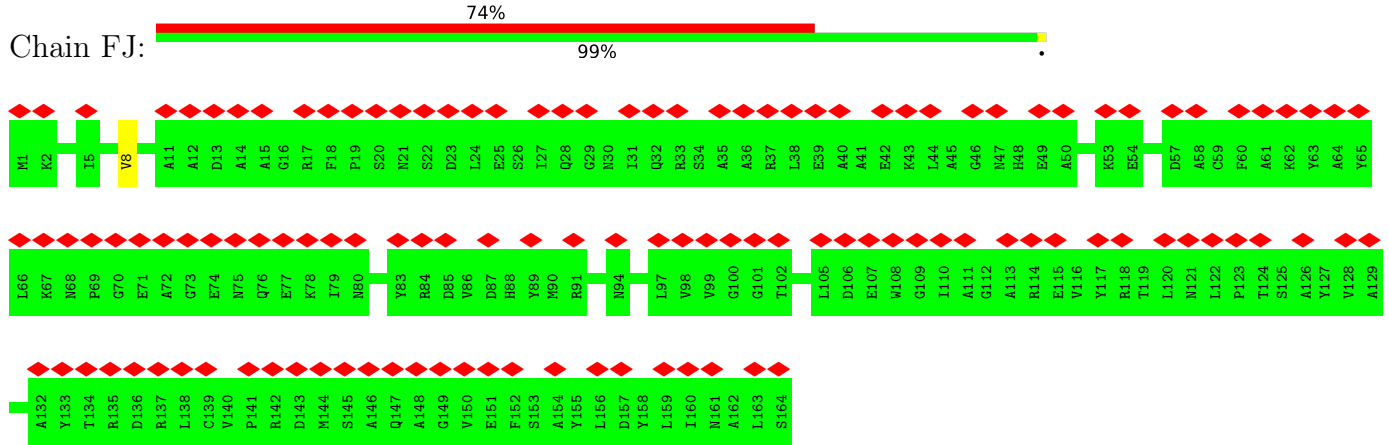


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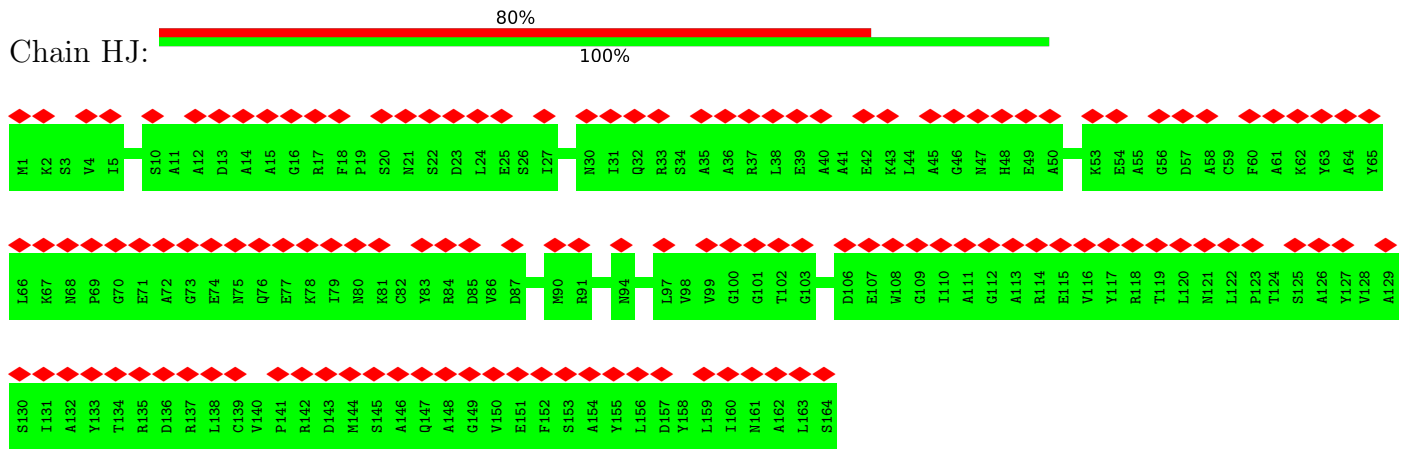




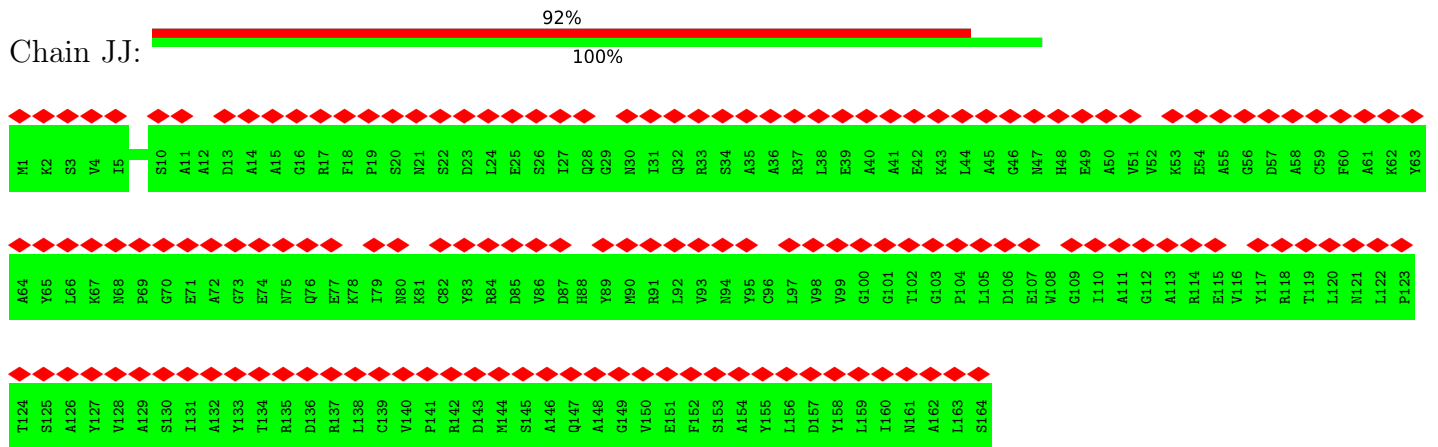
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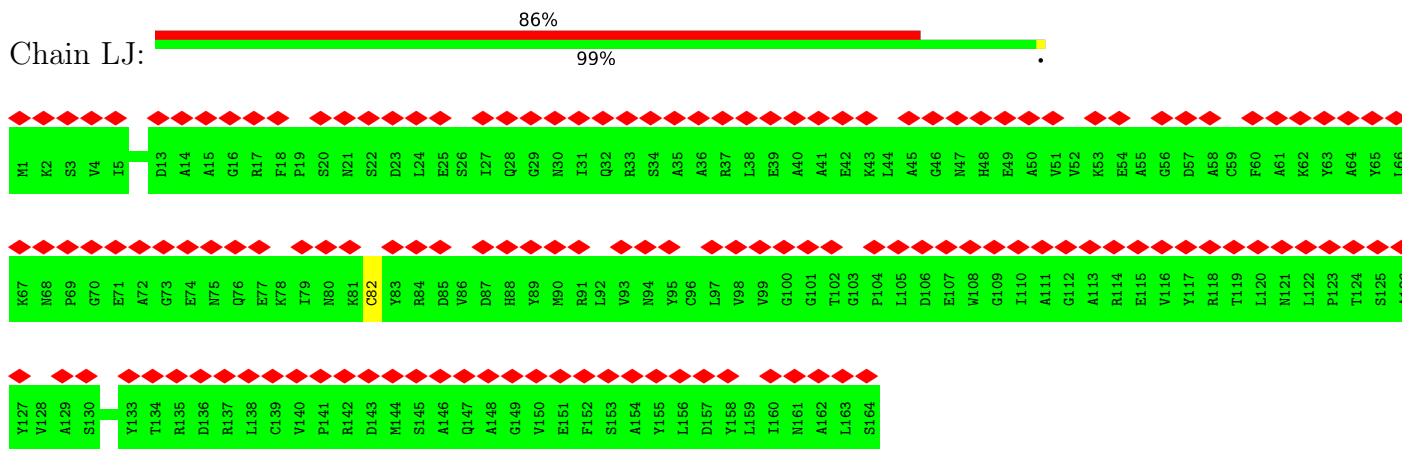
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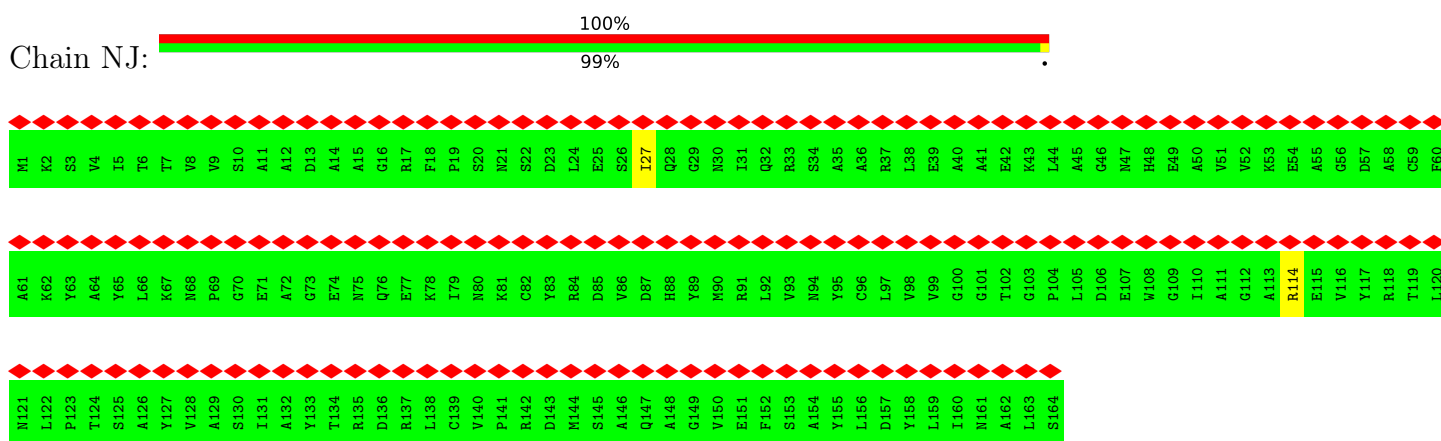
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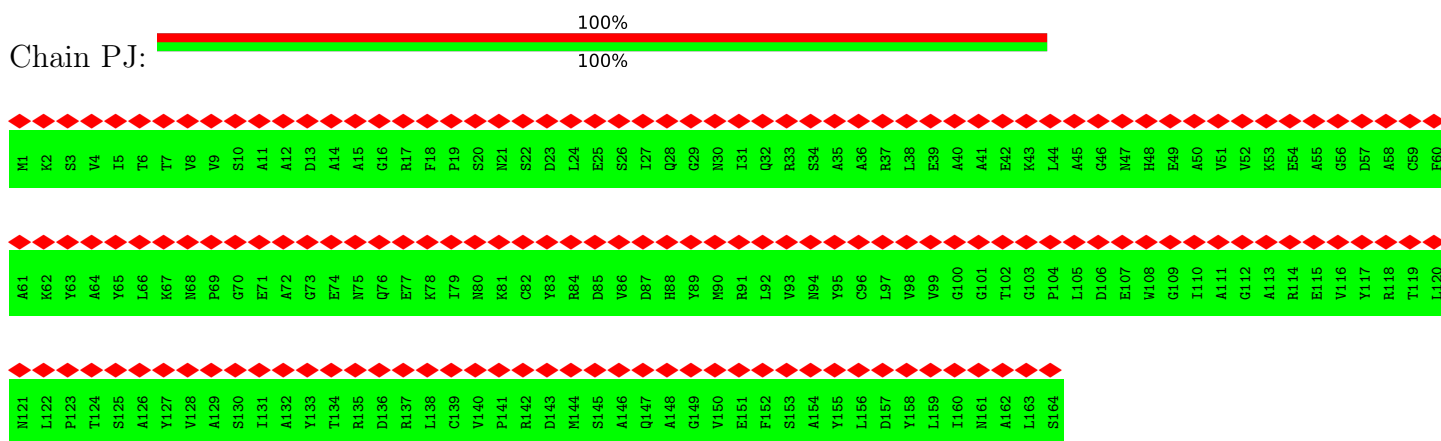
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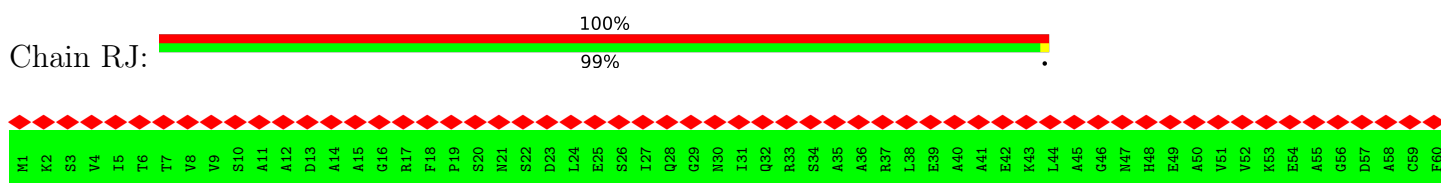
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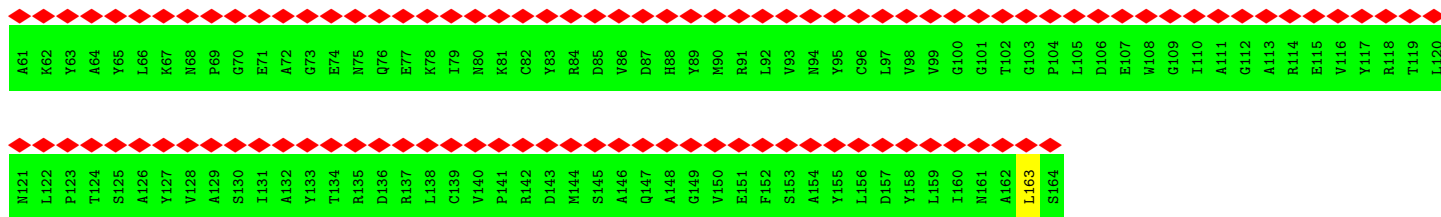


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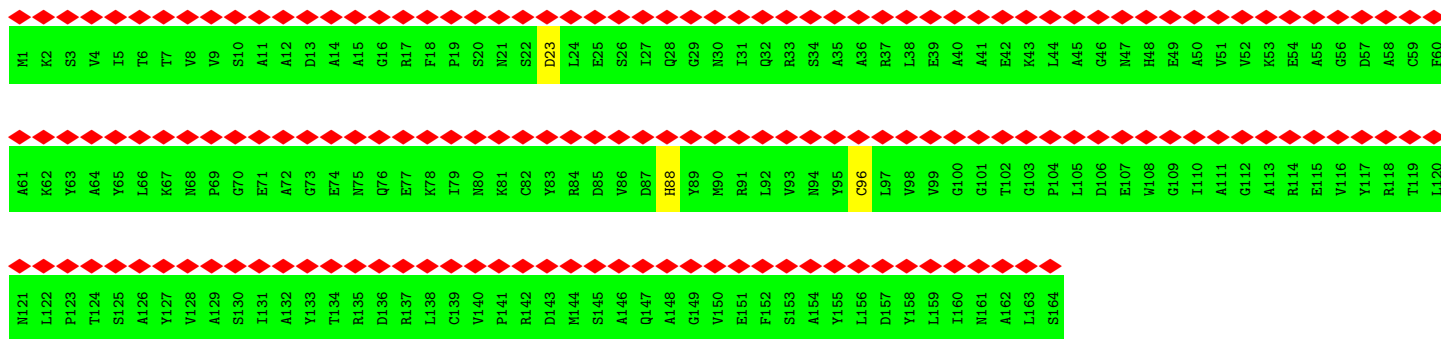


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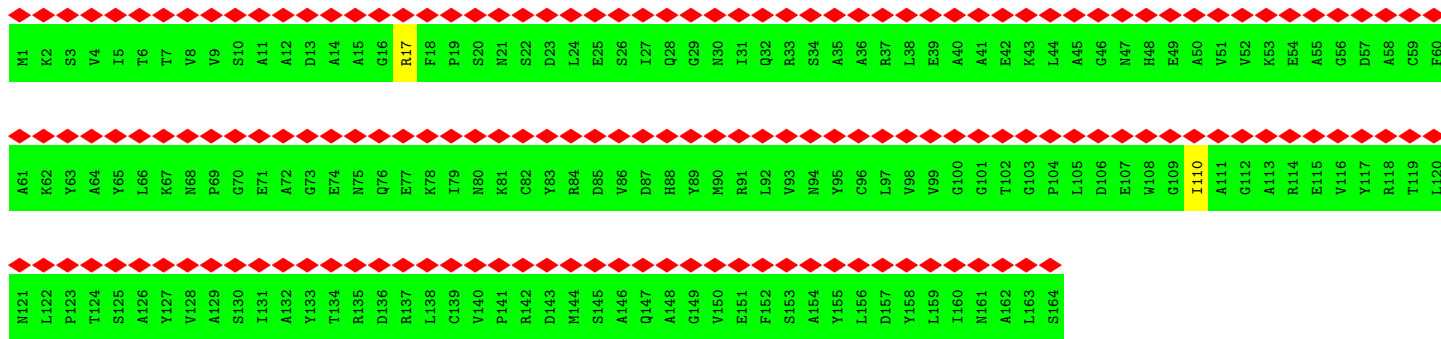




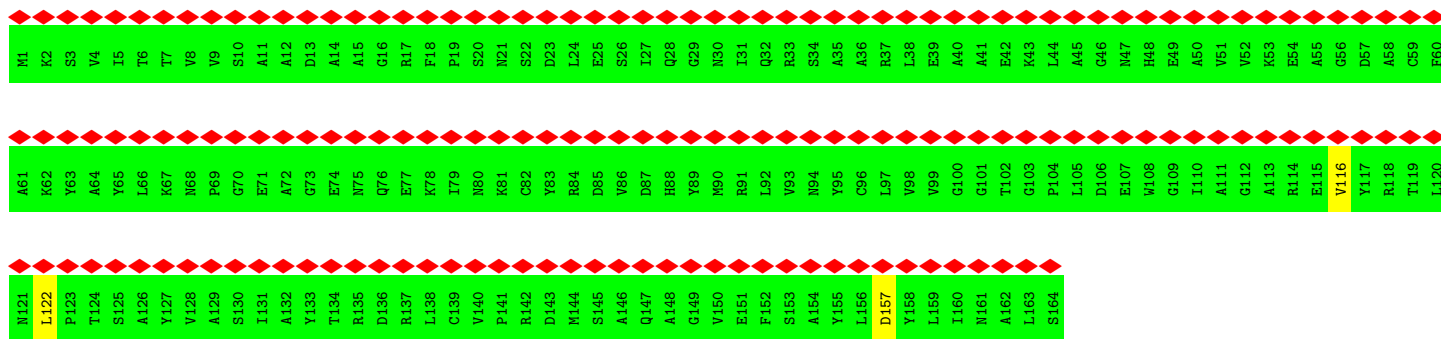
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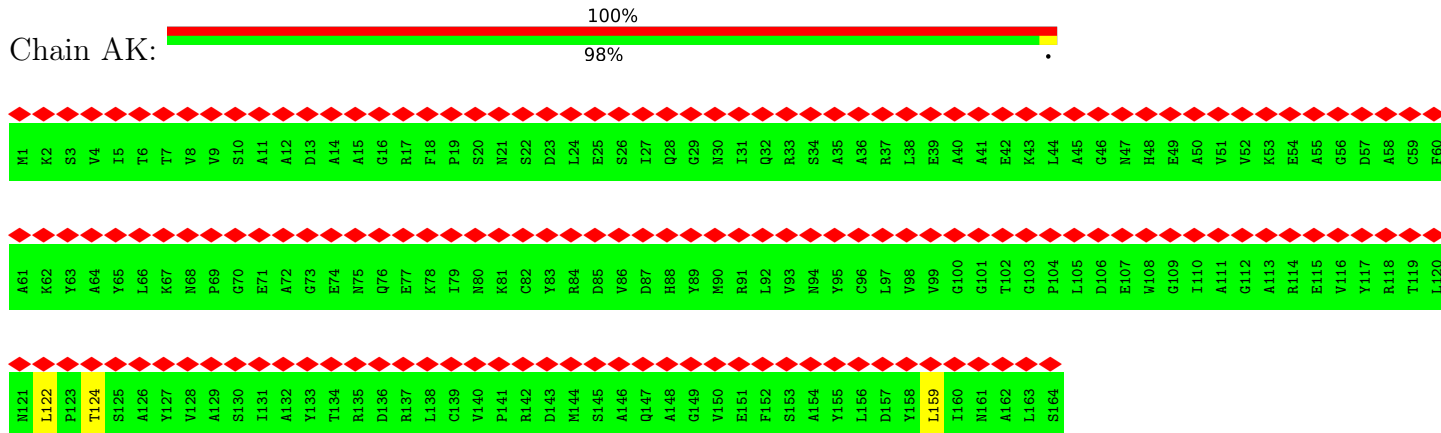
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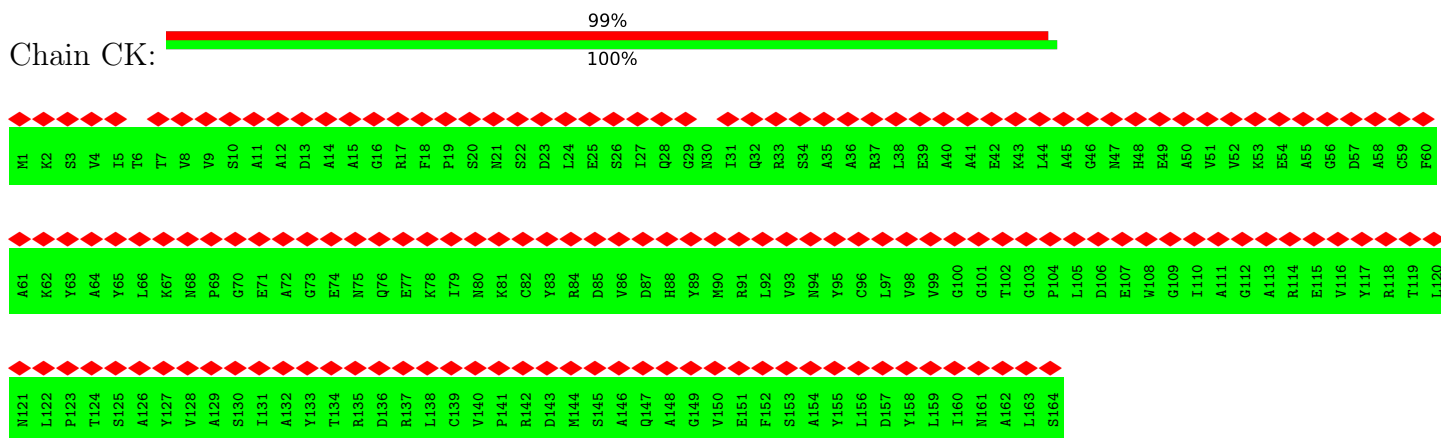
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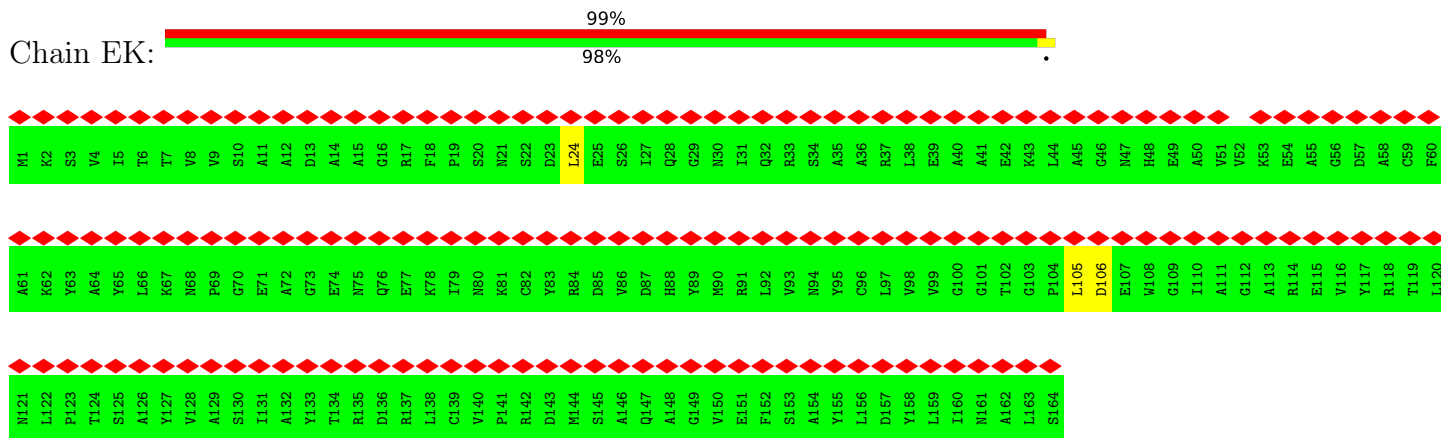
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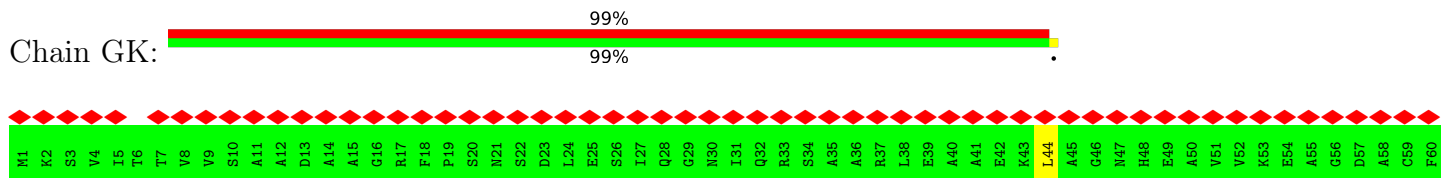
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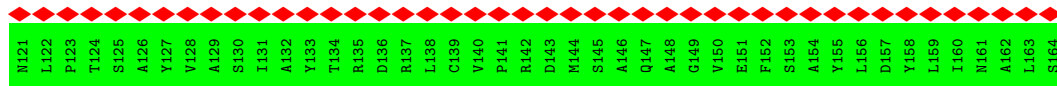
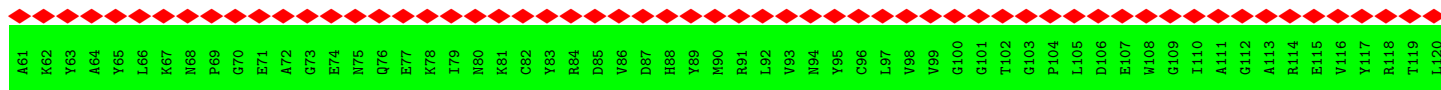


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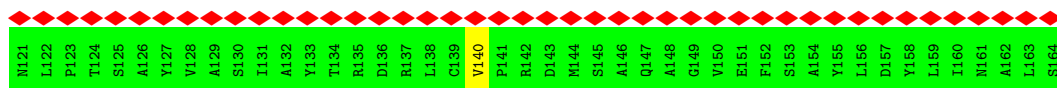
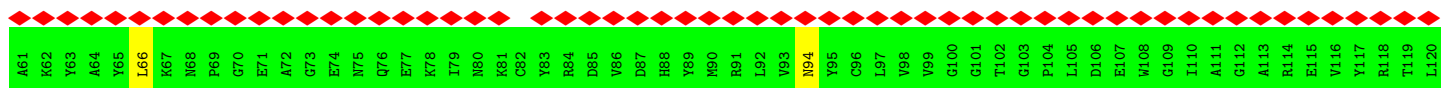
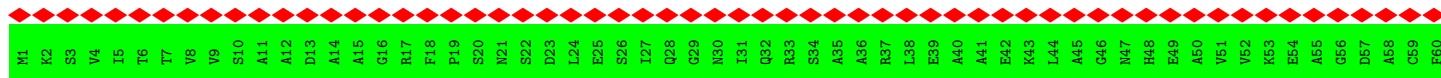


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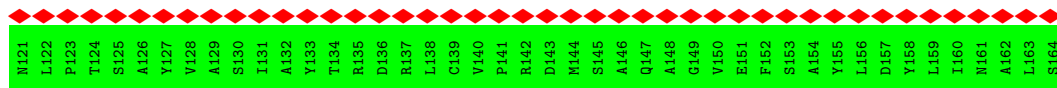
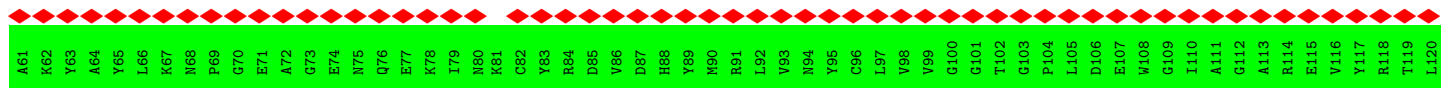
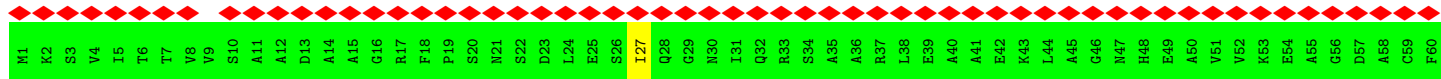




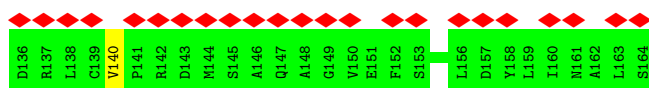
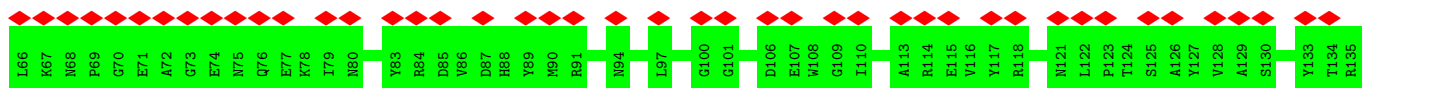
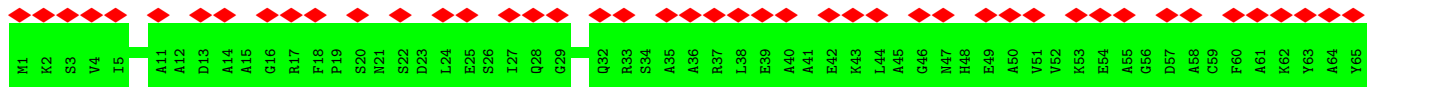
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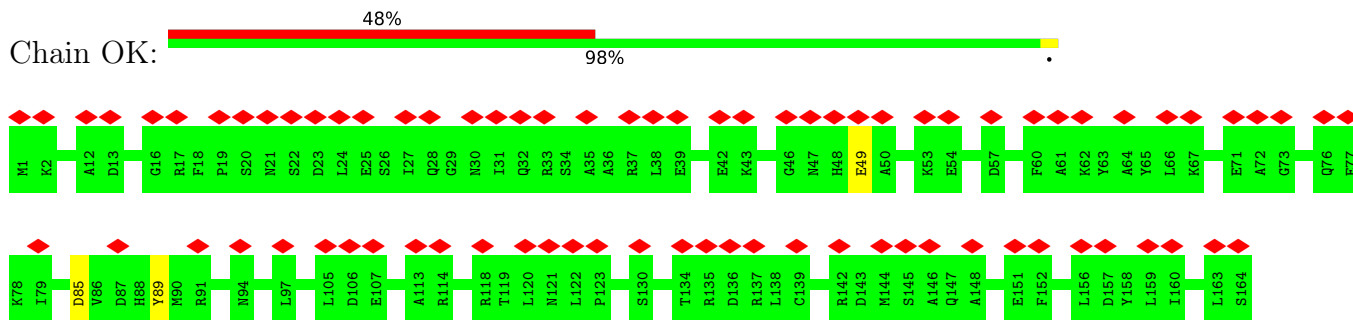
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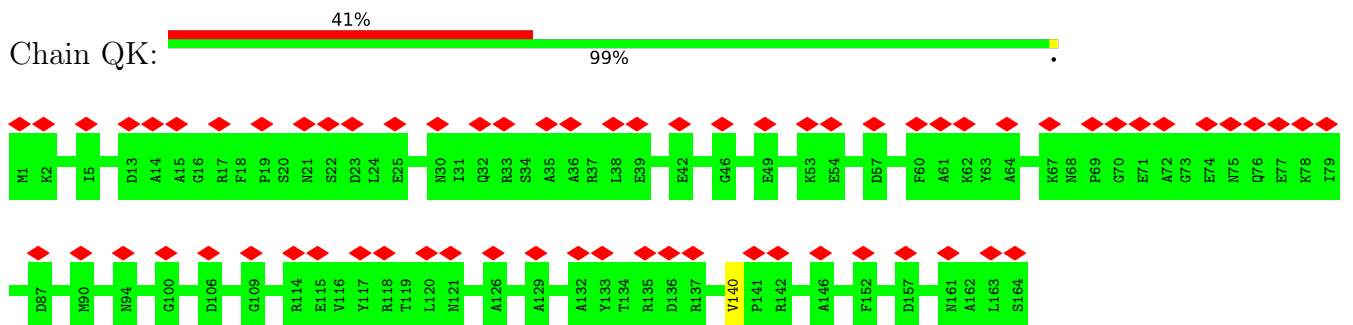
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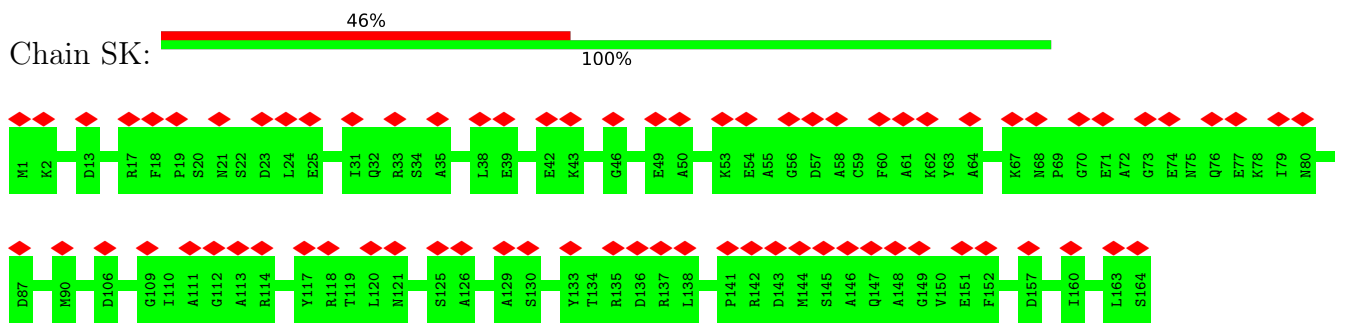
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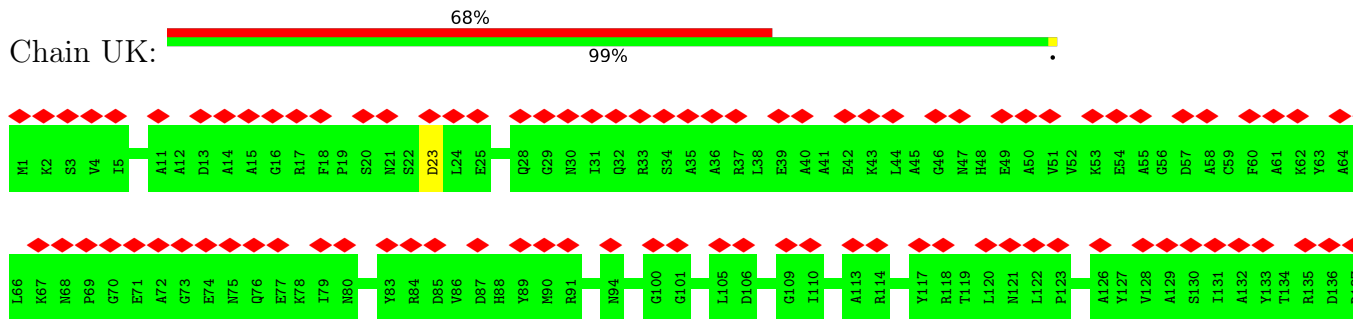
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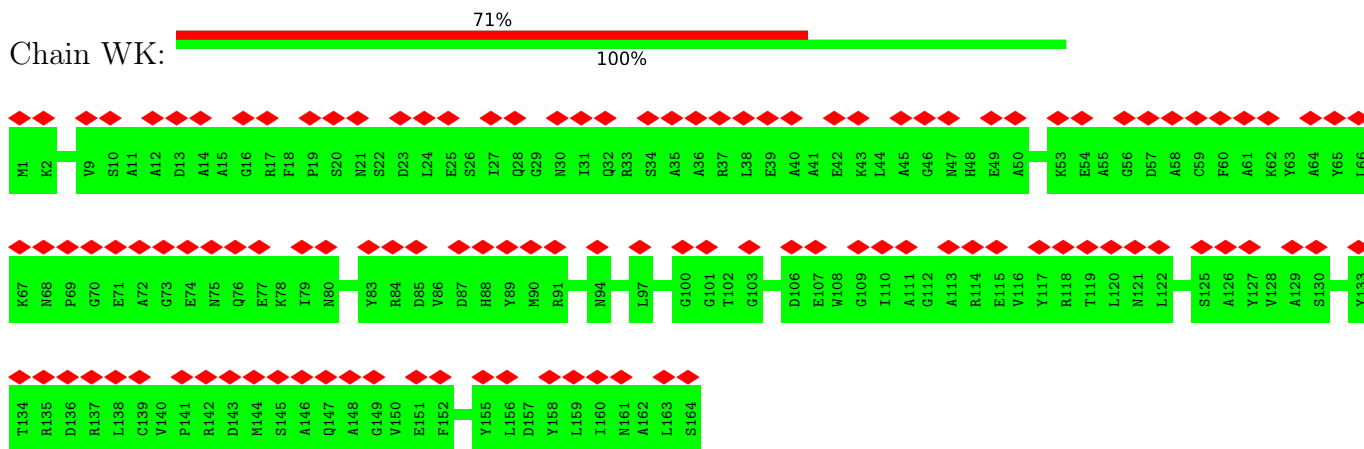
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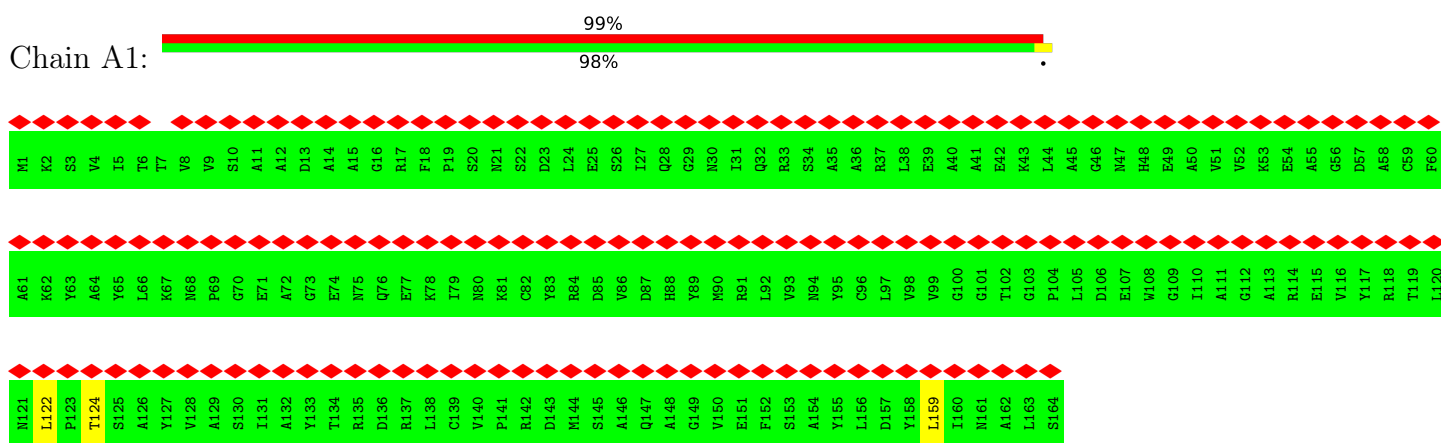
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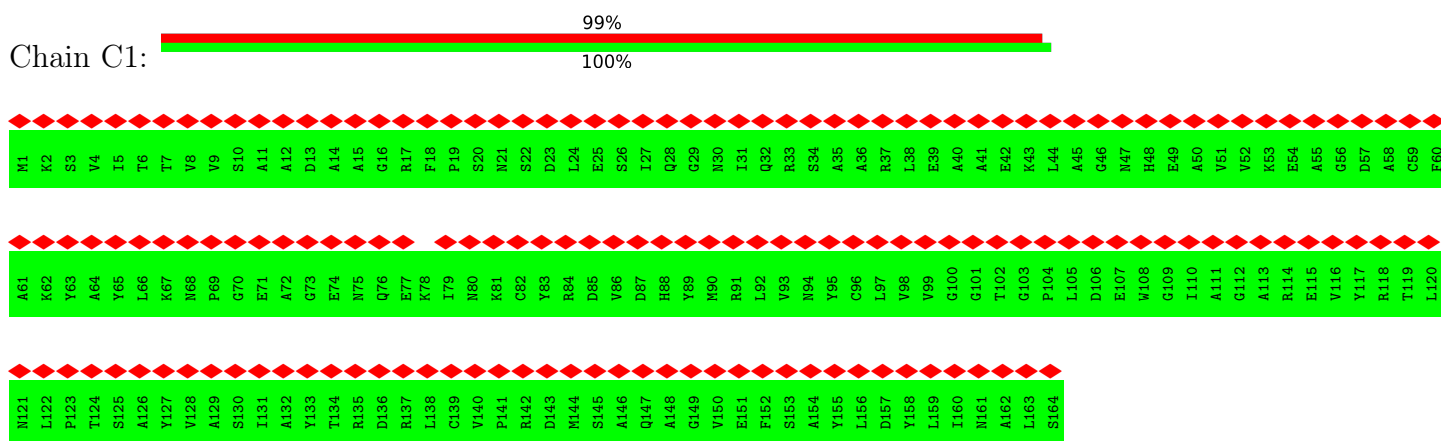
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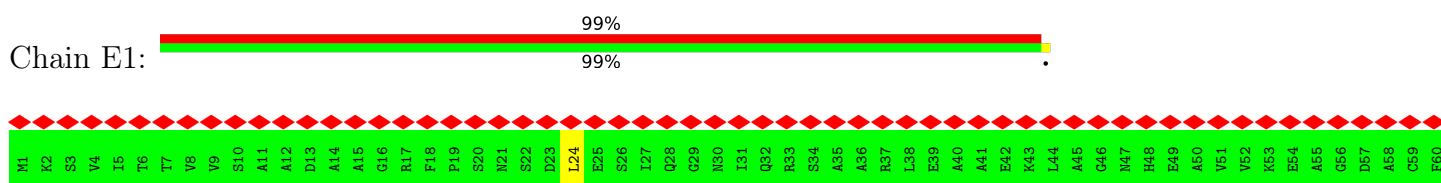
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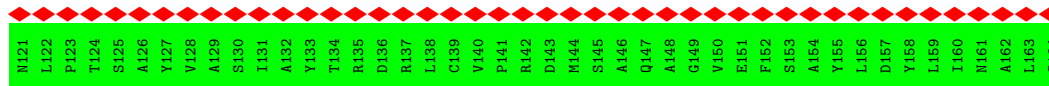
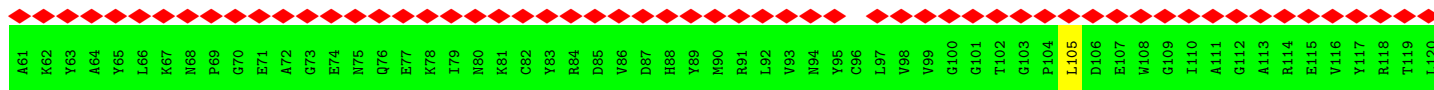


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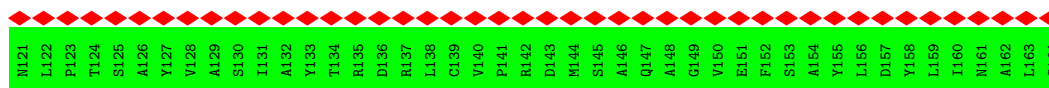
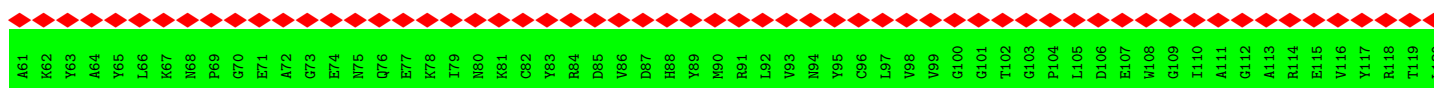
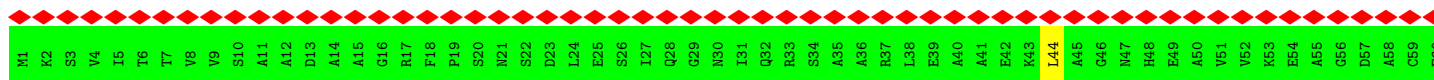


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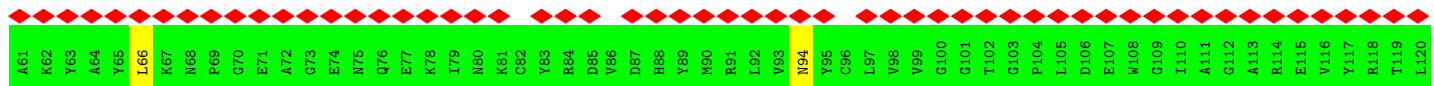
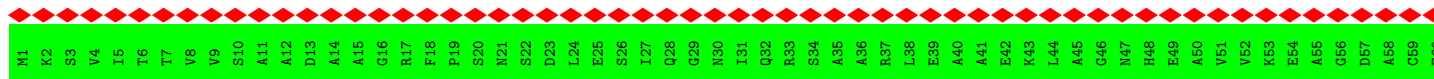




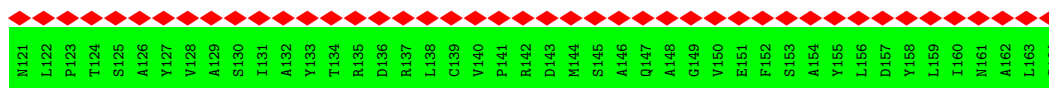
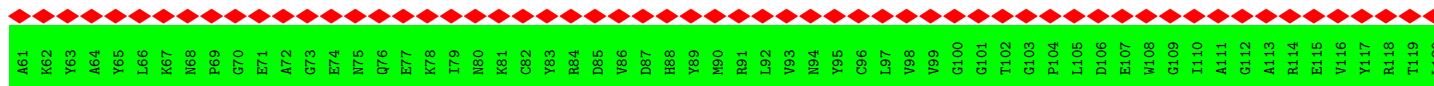
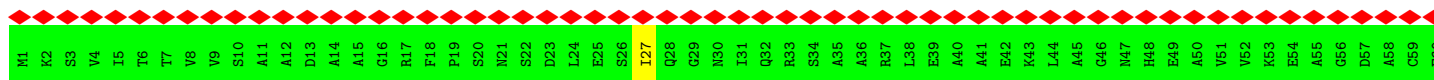
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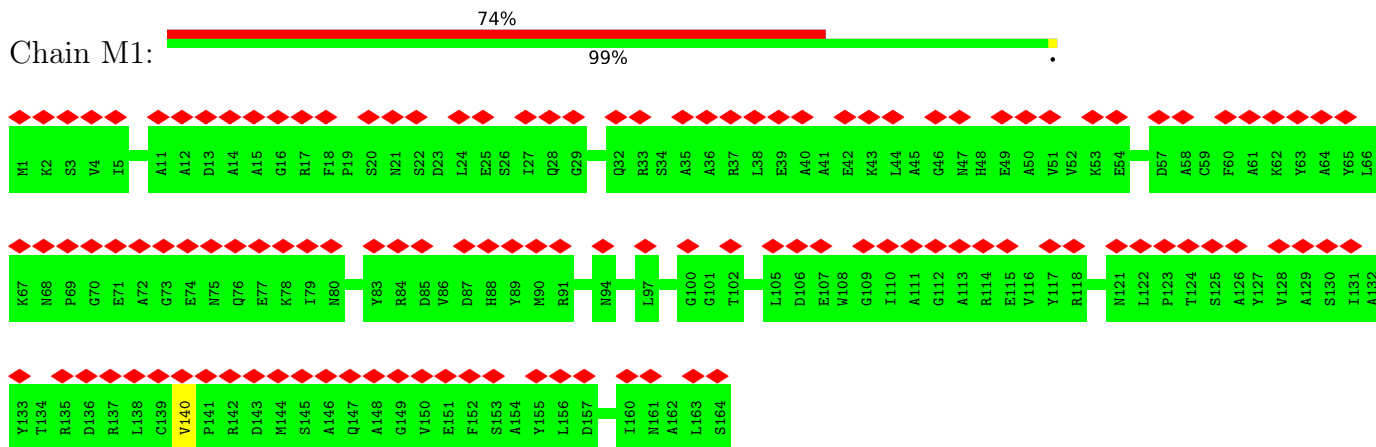
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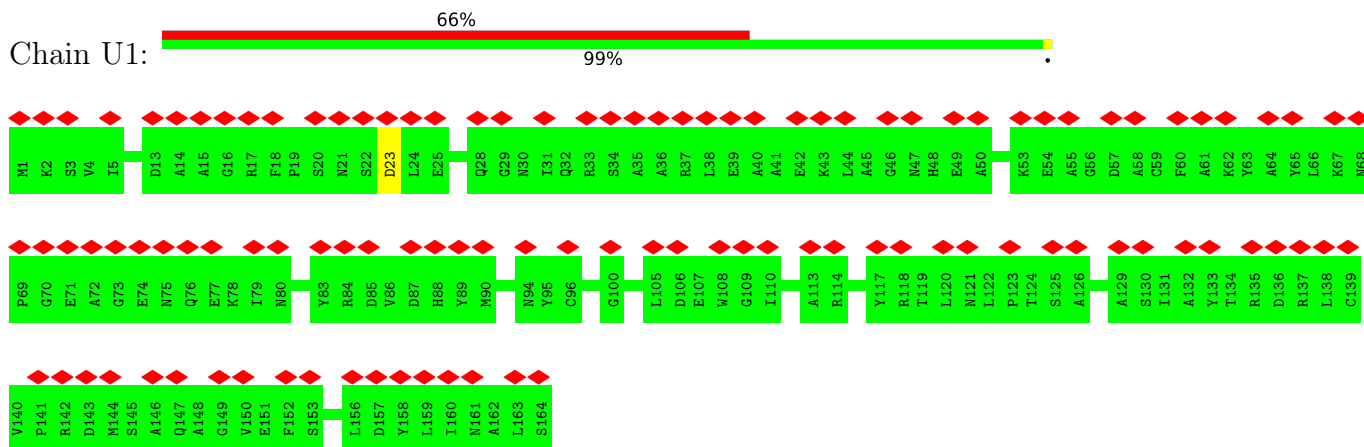


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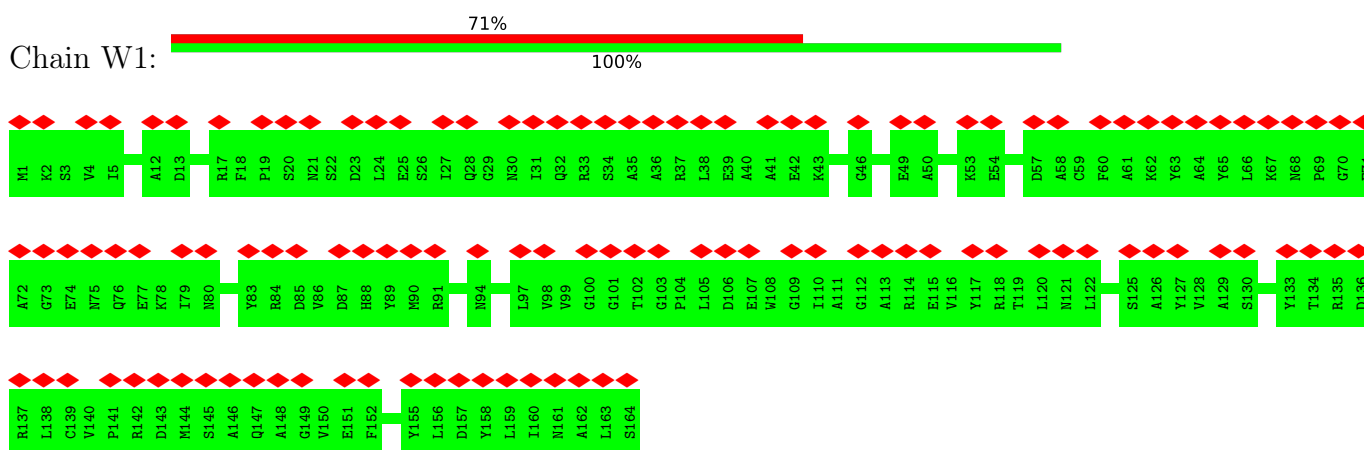


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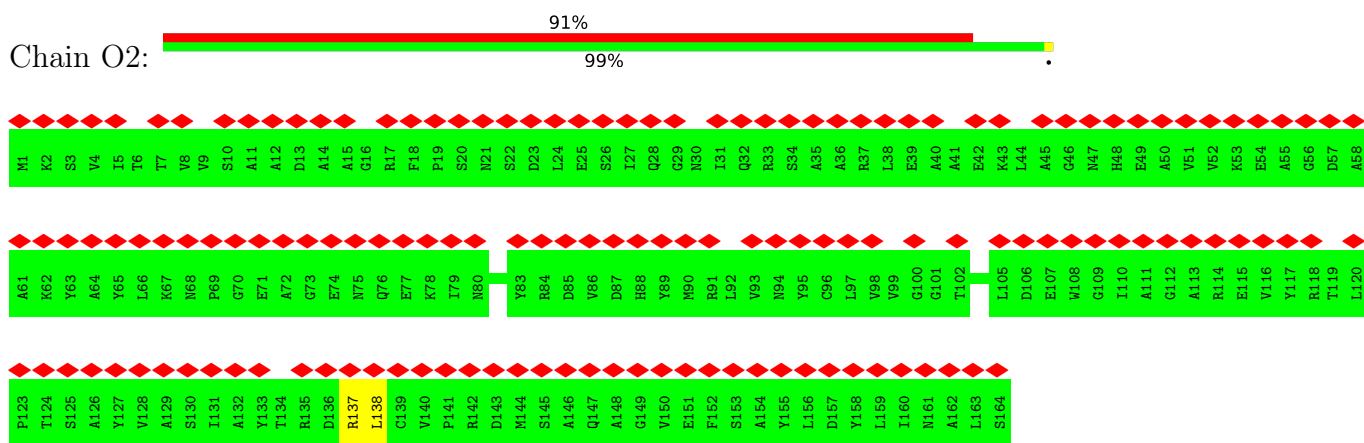




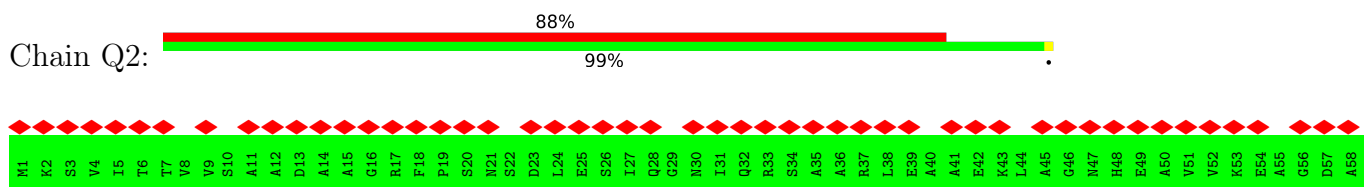
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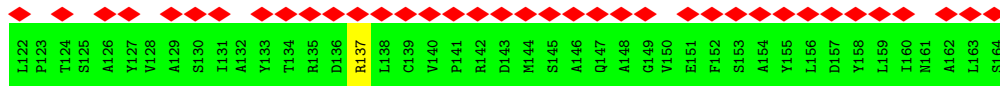
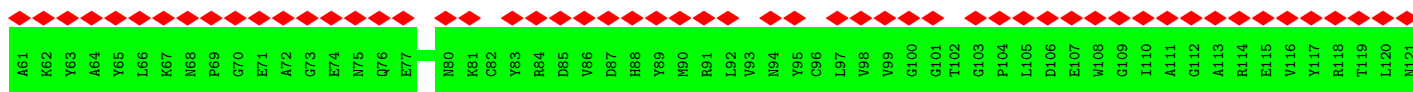


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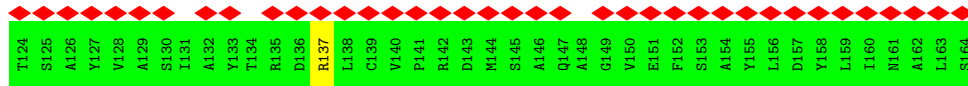
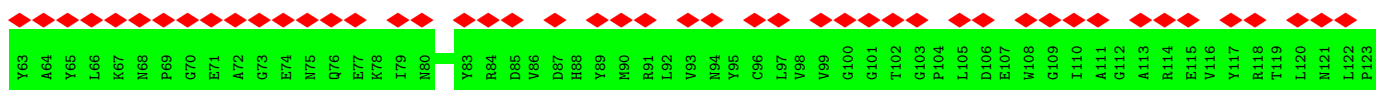
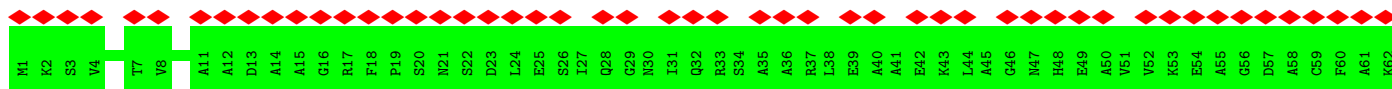


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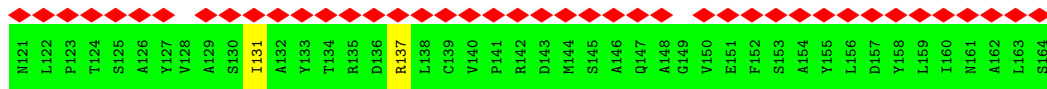
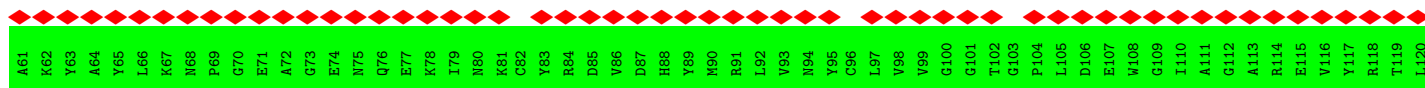
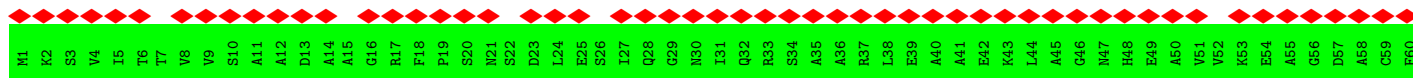




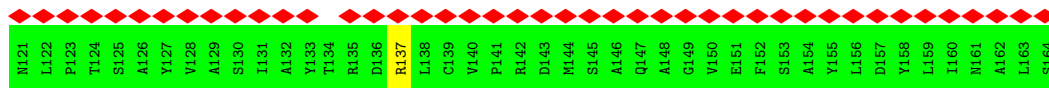
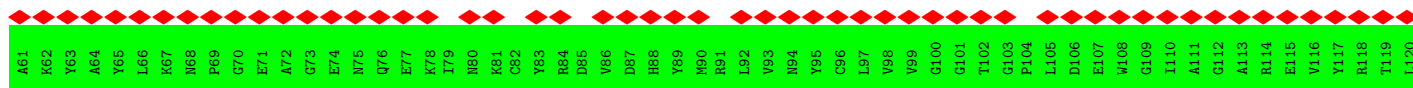
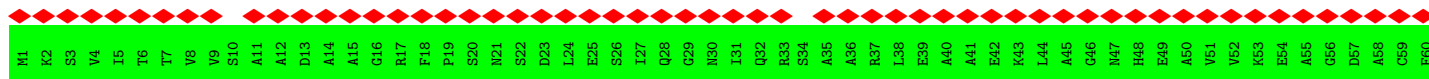
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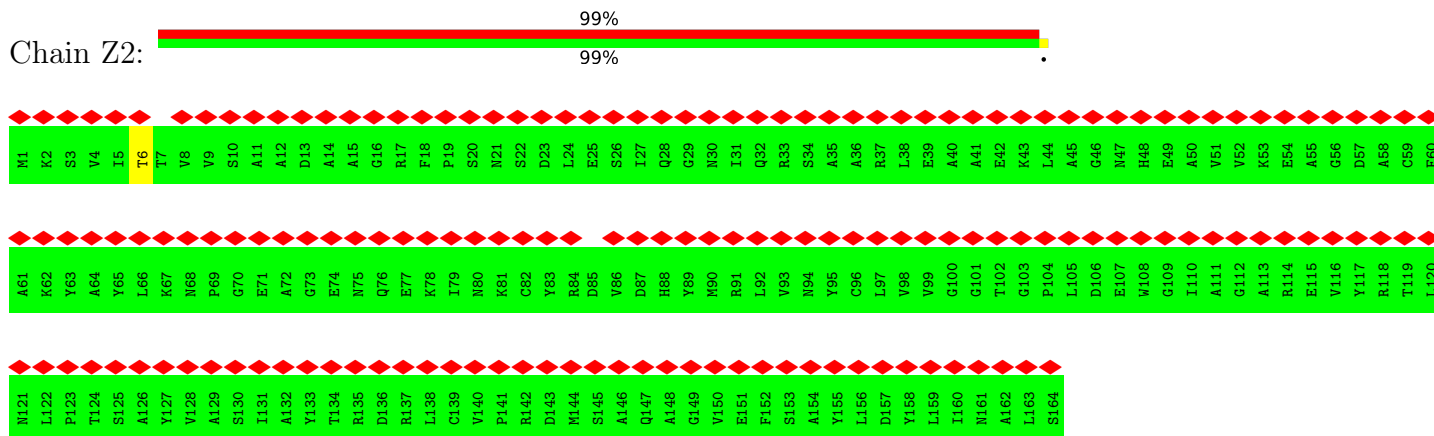
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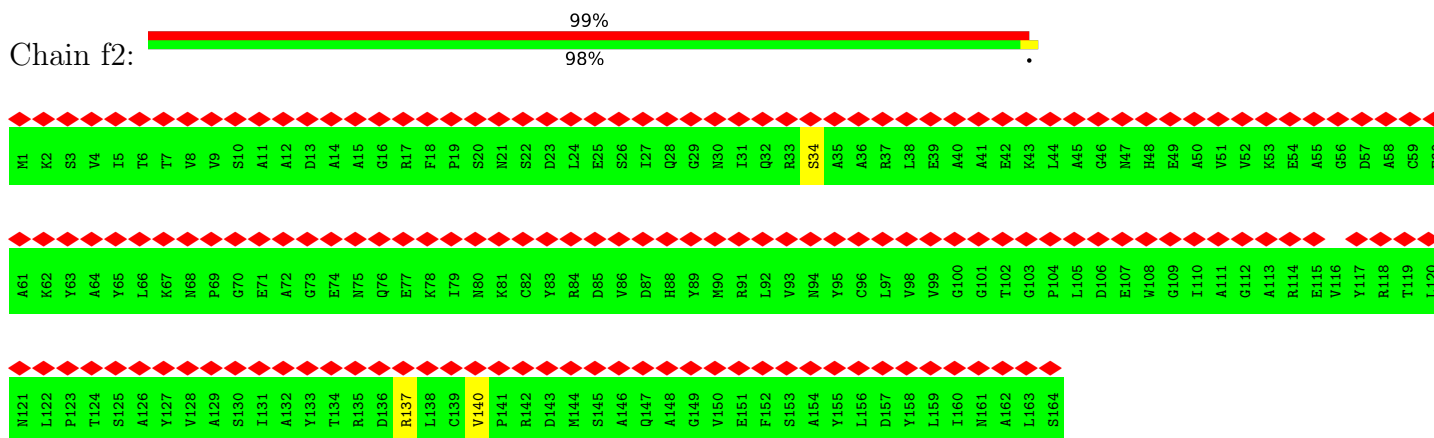
• Molecule 3: Phycoerythrin alpha subunit



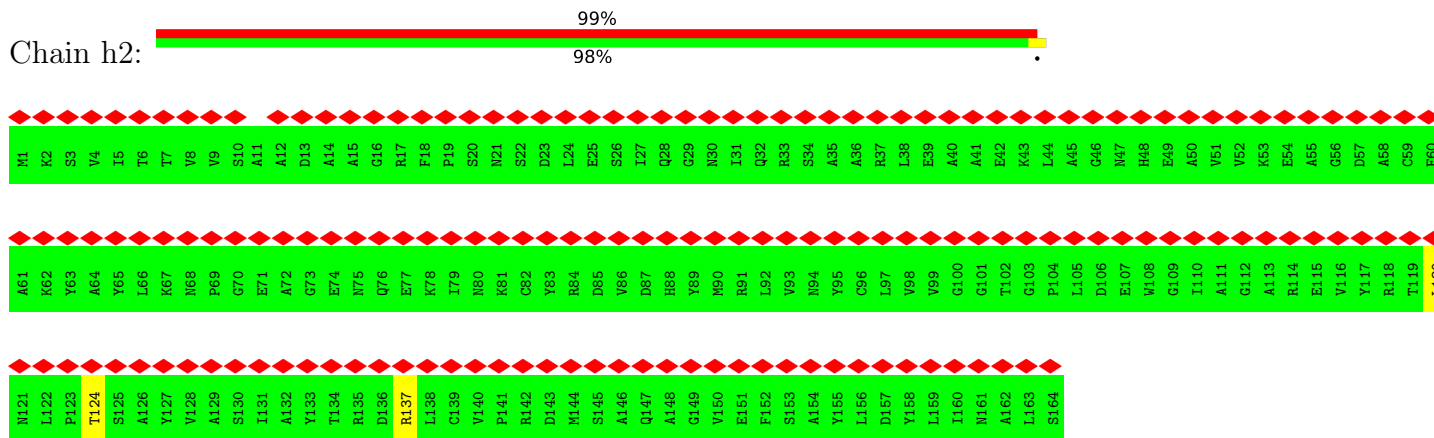
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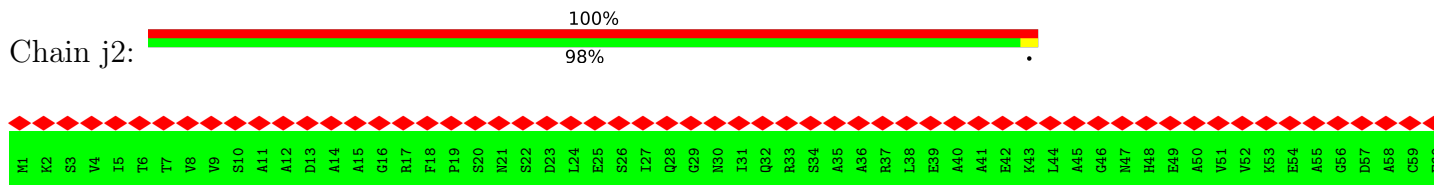
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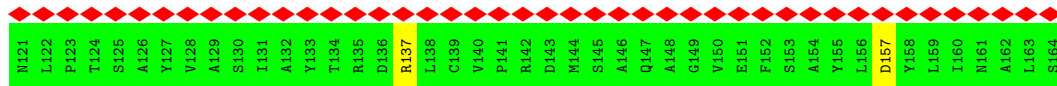
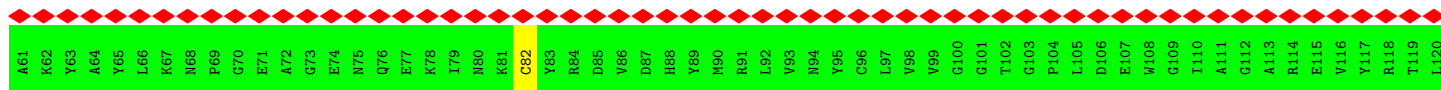


• Molecule 3: Phycoerythrin alpha subunit

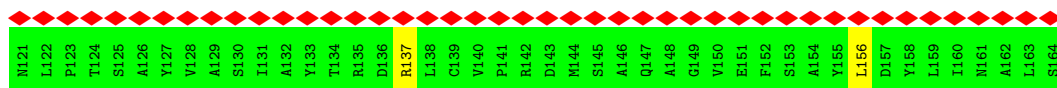
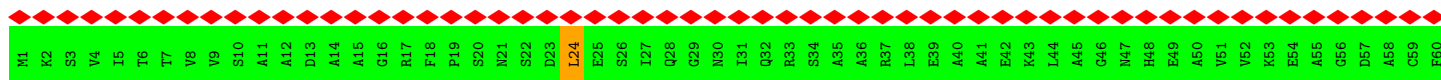


• Molecule 3: Phycoerythrin alpha subunit

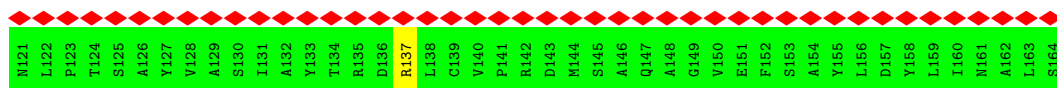
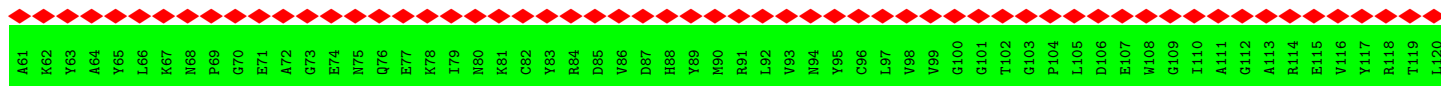
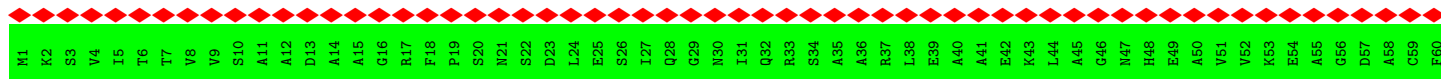




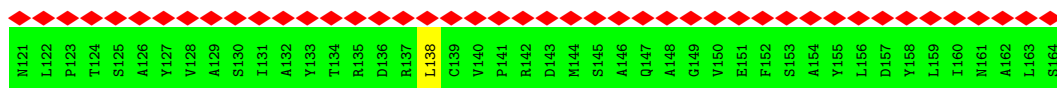
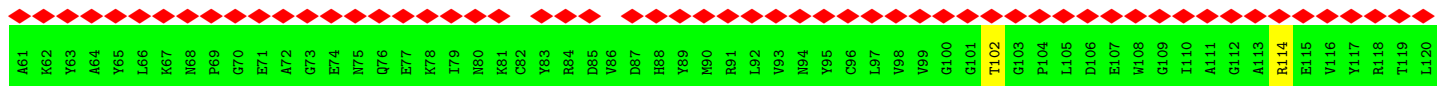
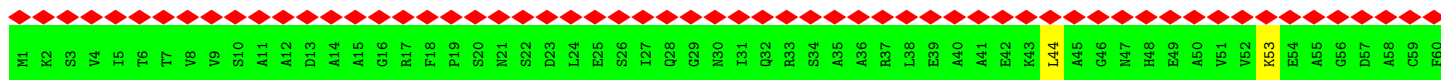
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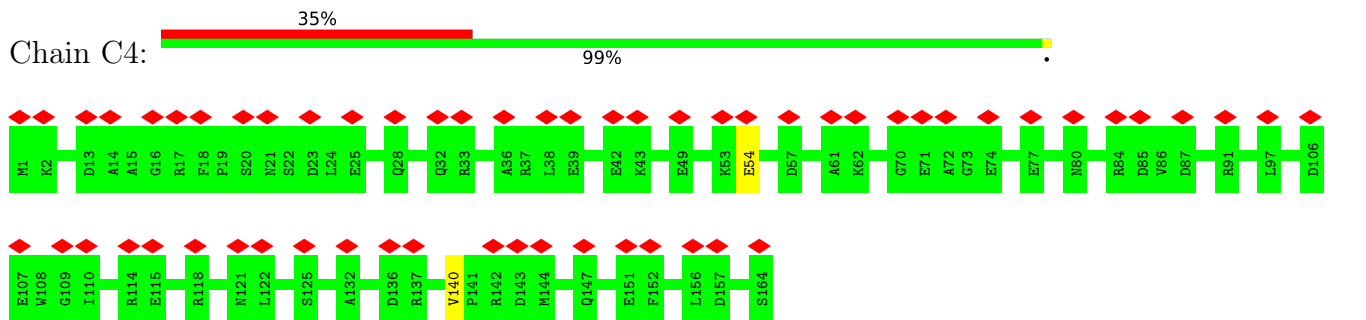
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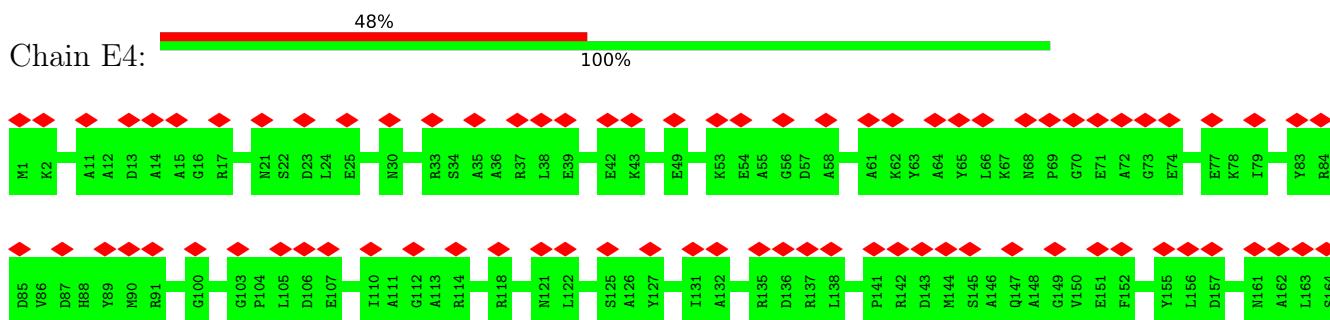
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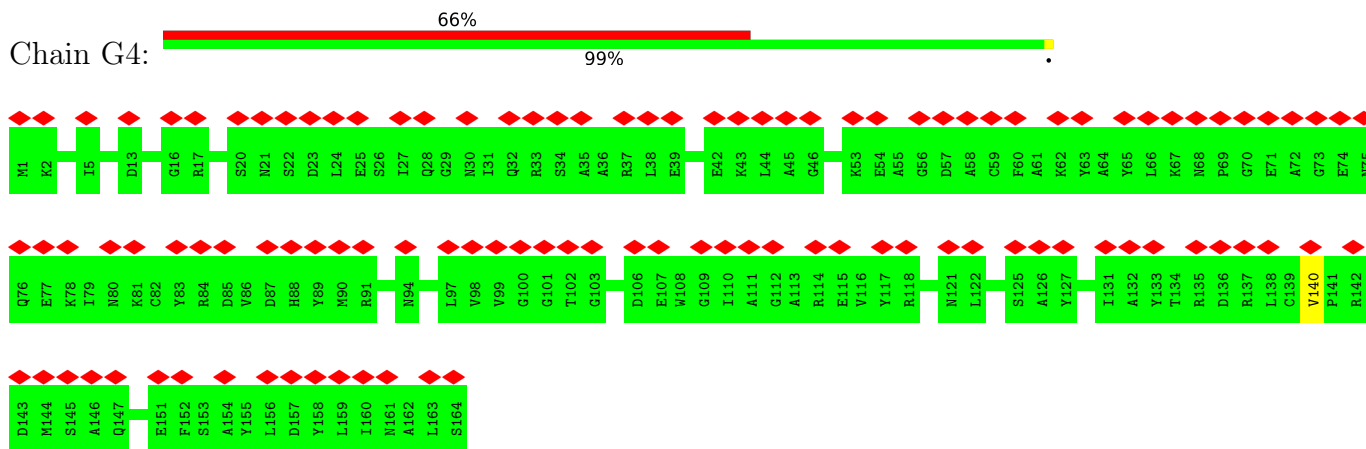
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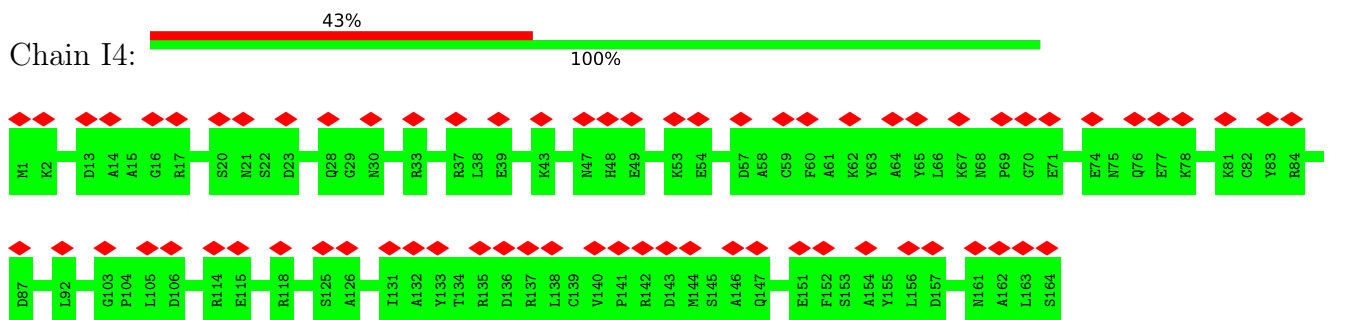
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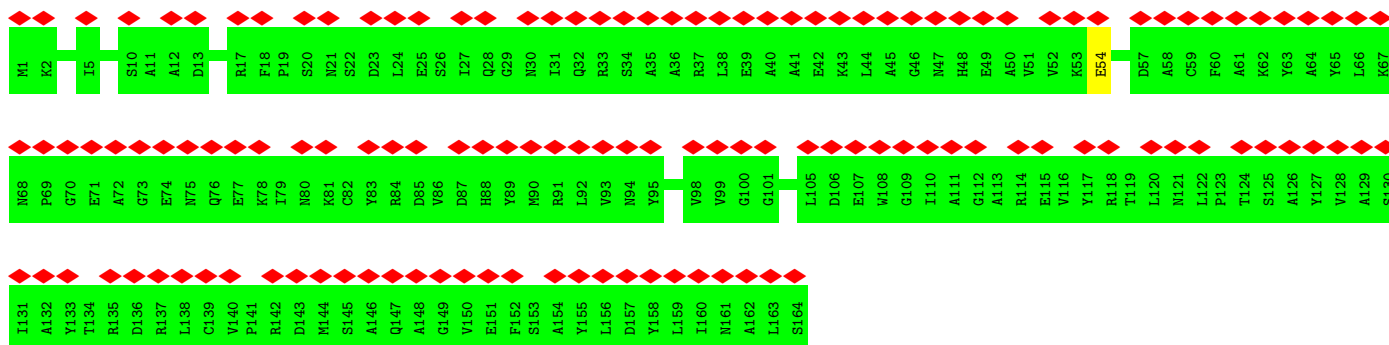
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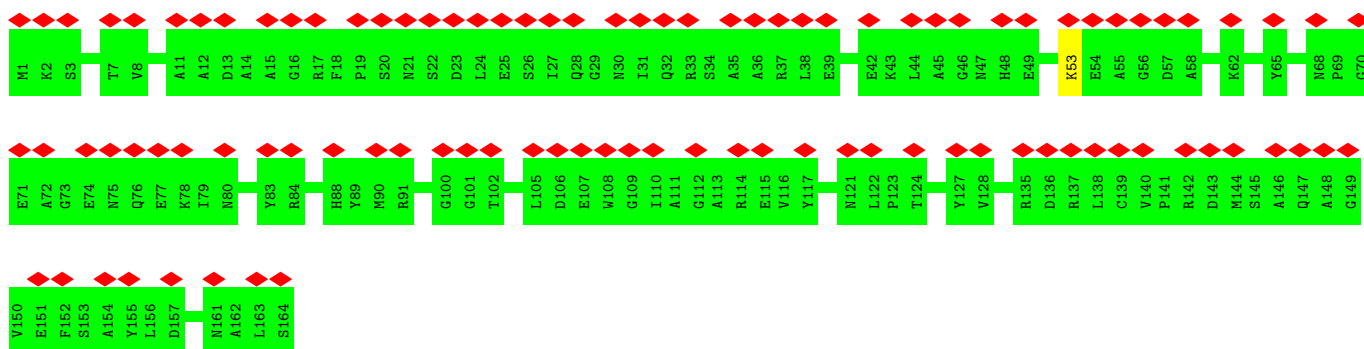
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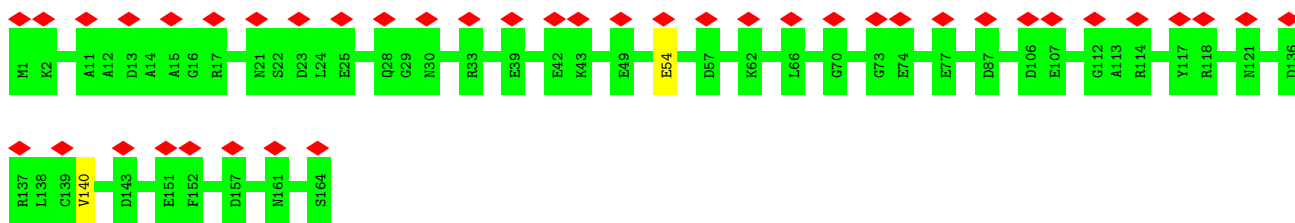
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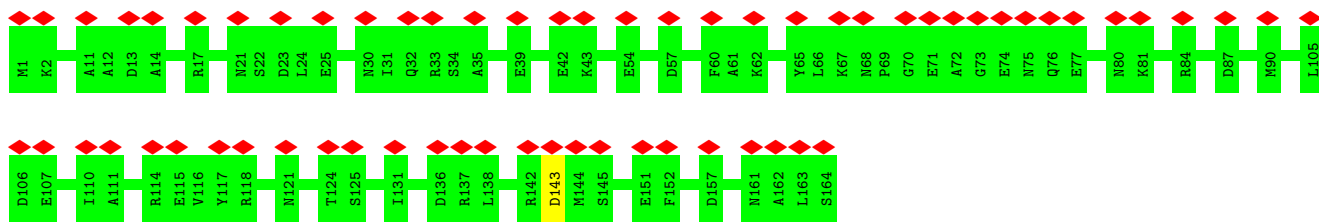
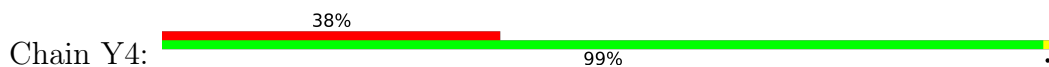
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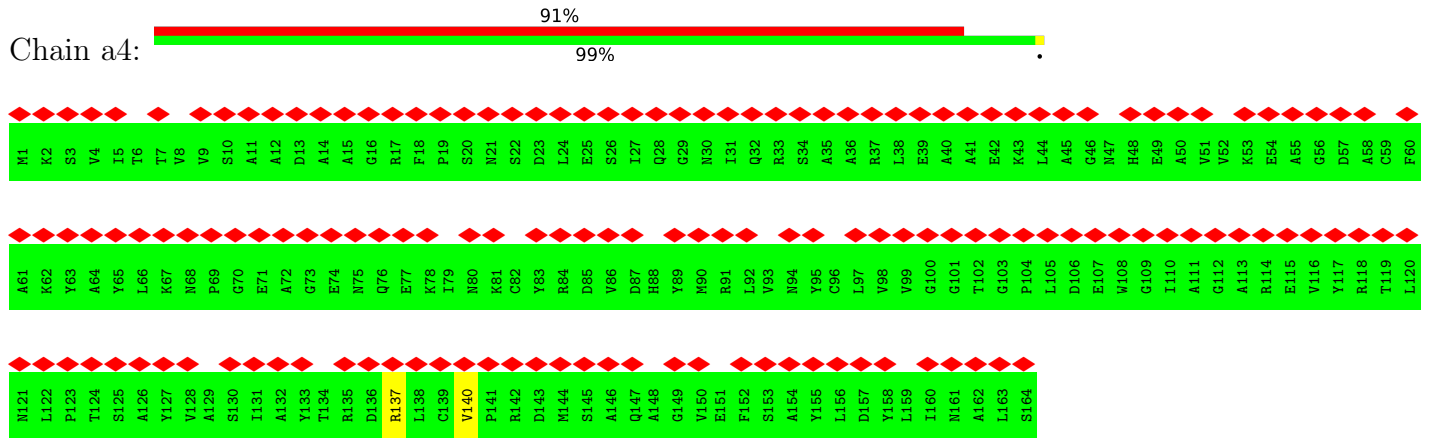
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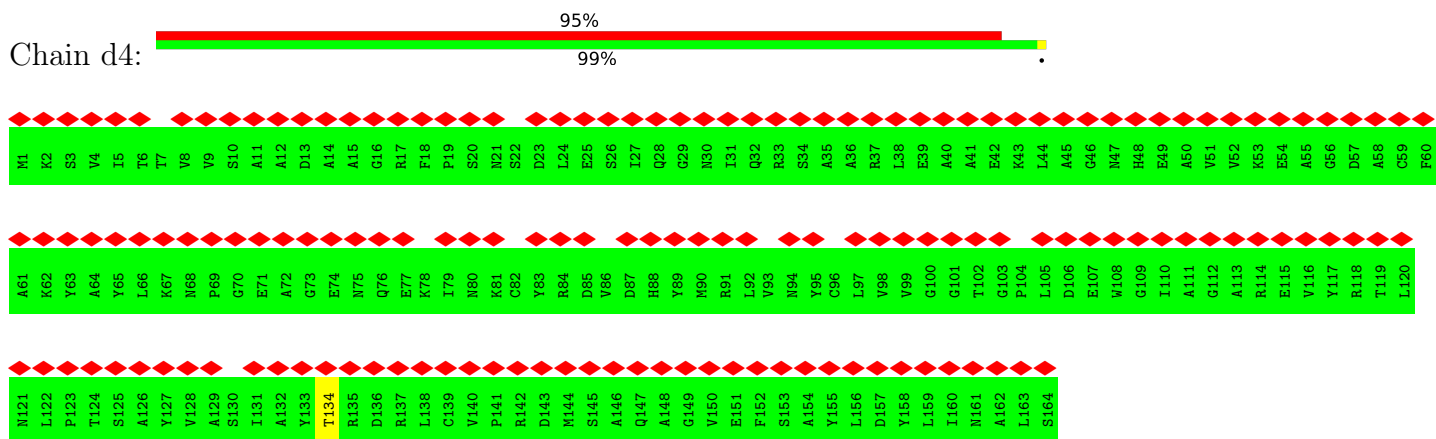
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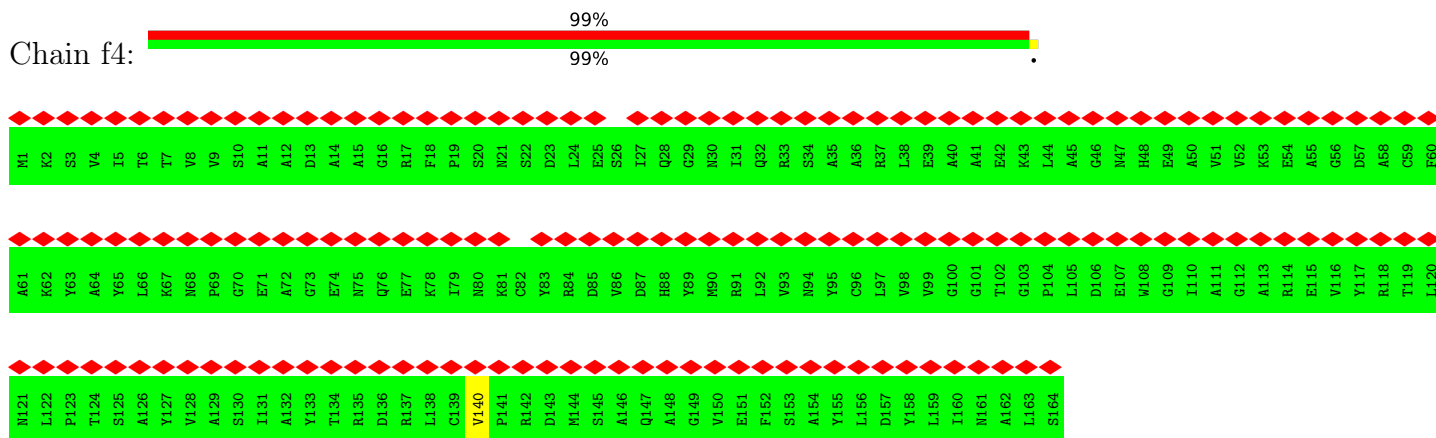
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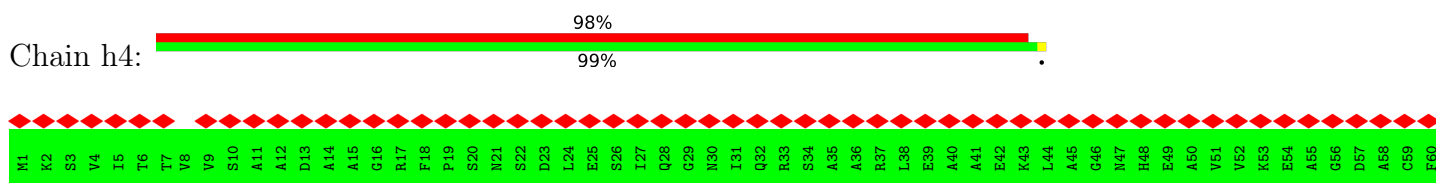
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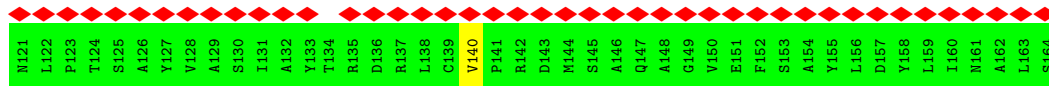
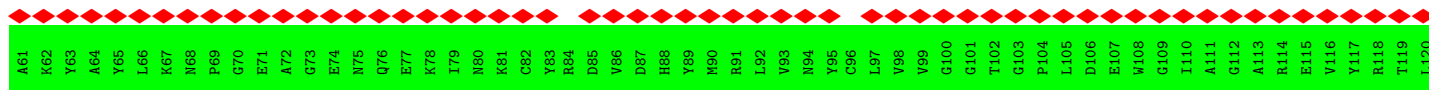


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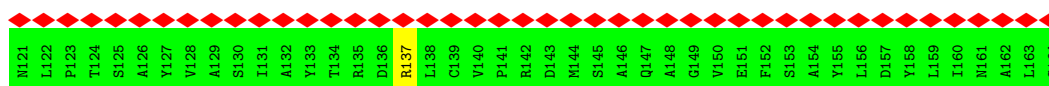
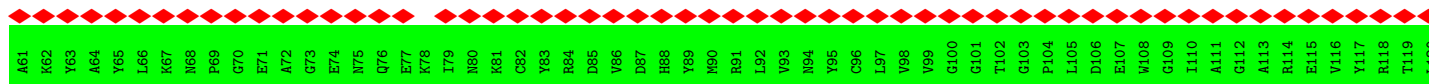
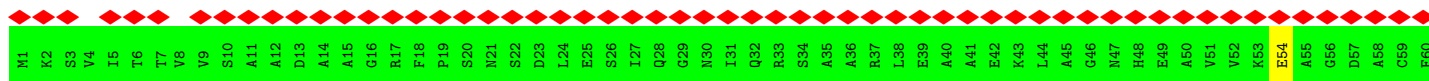


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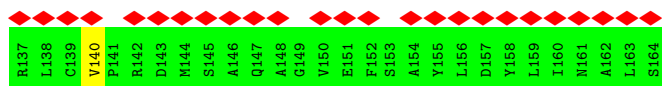
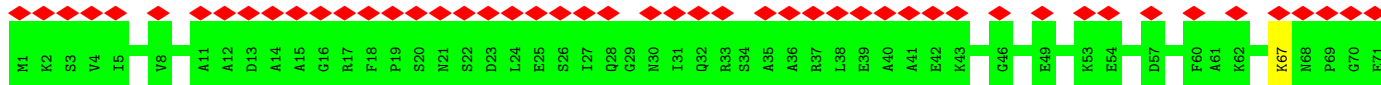
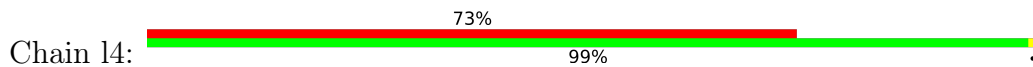




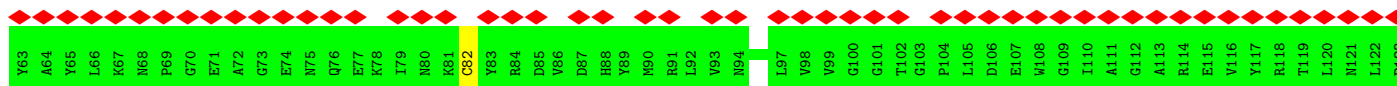
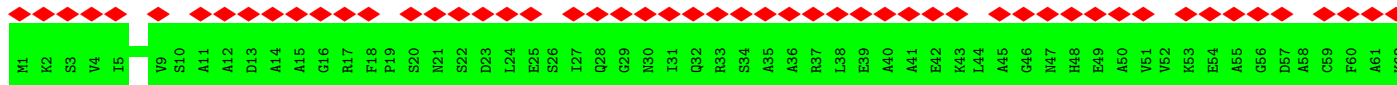
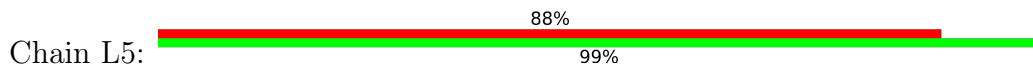
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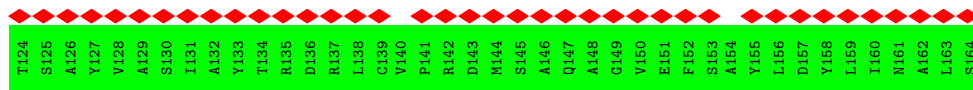


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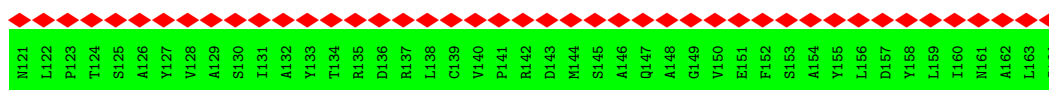
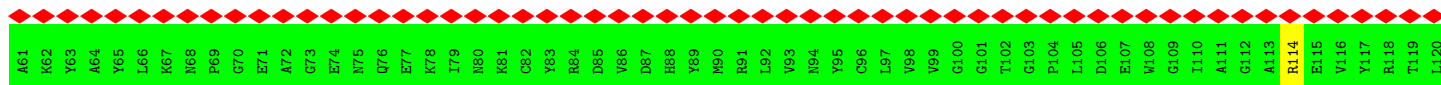
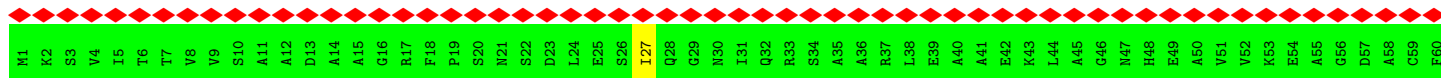


• Molecule 3: Phycoerythrin alpha subunit

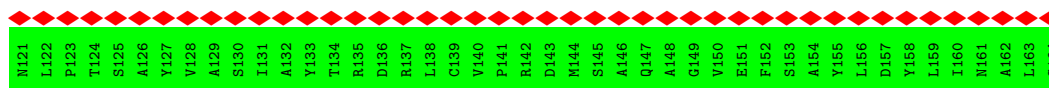
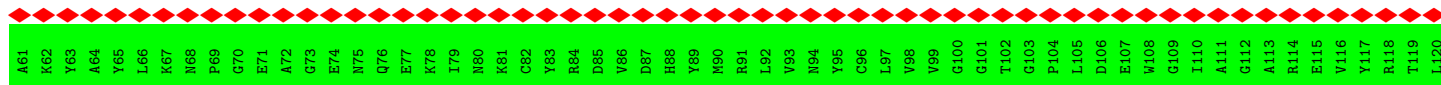
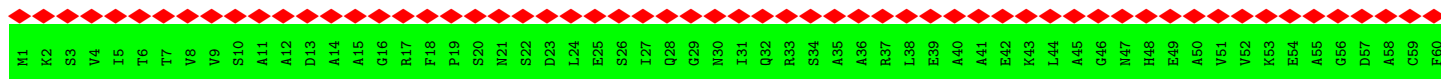




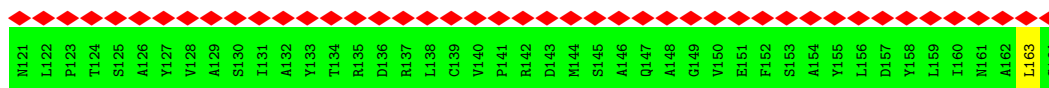
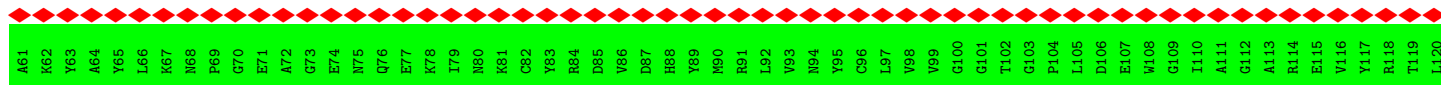
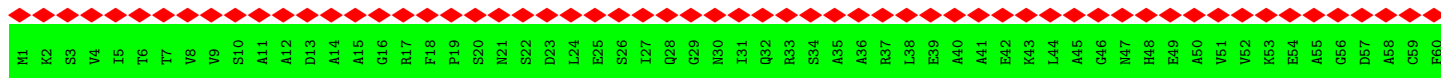
• Molecule 3: Phycoerythrin alpha subunit



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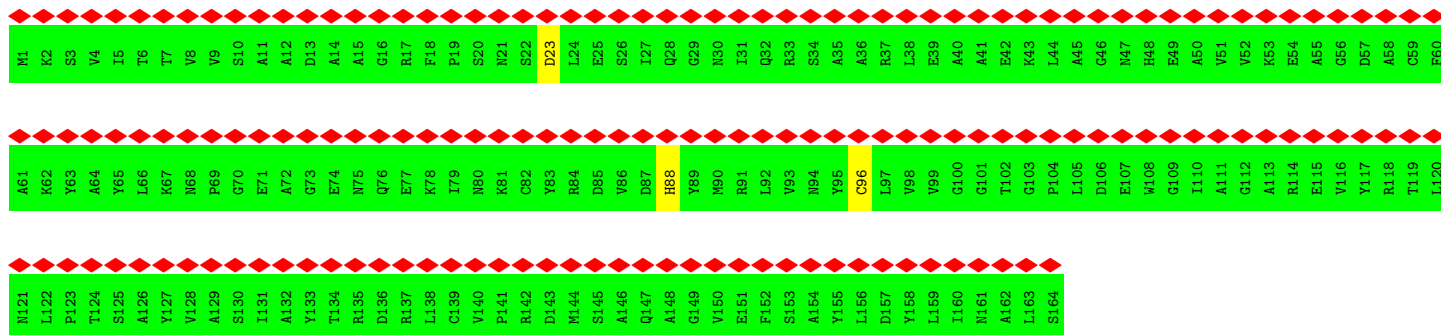


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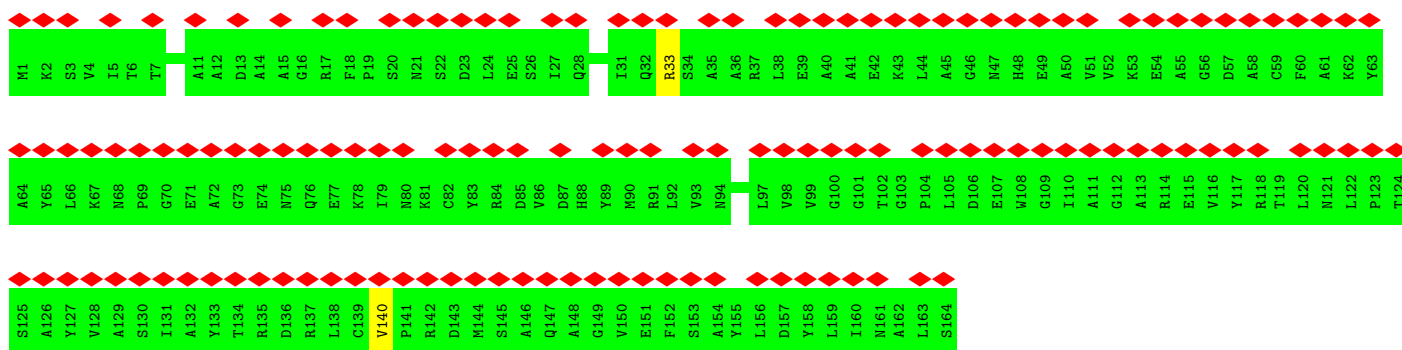


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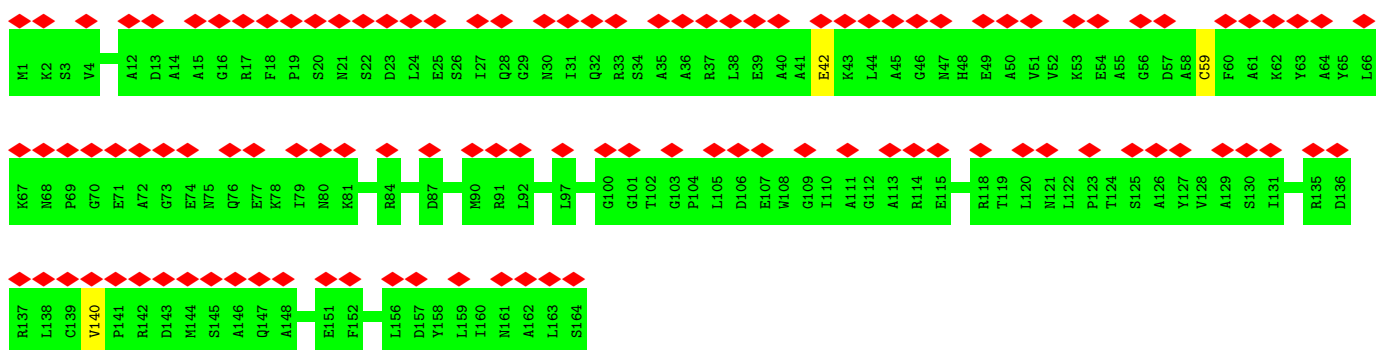




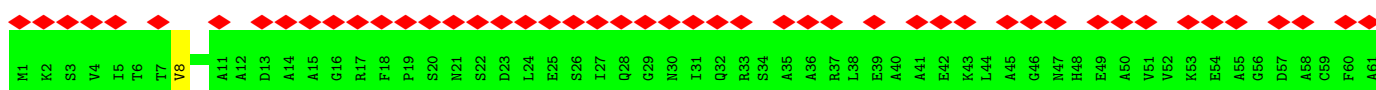
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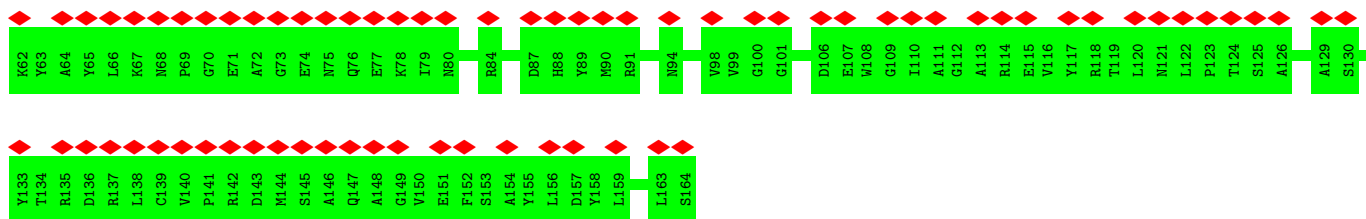


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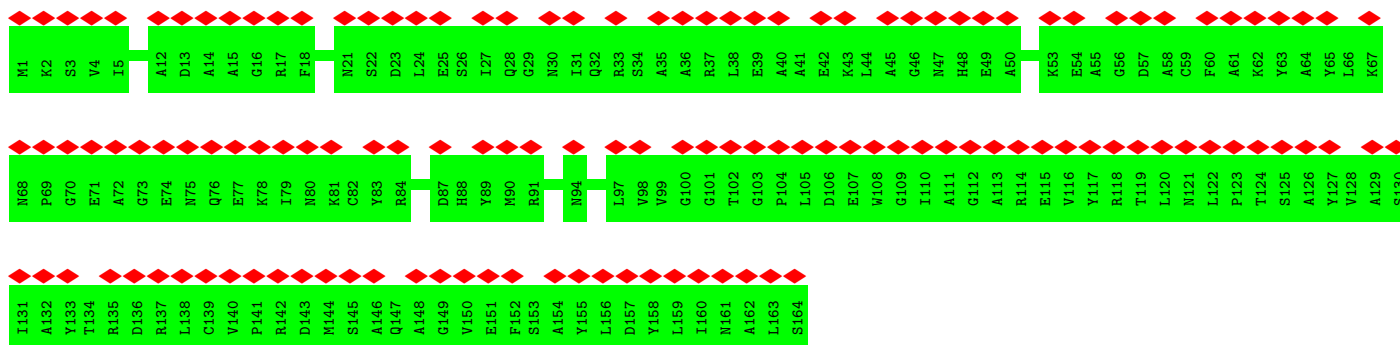
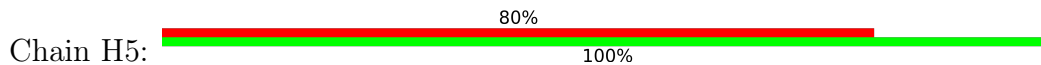


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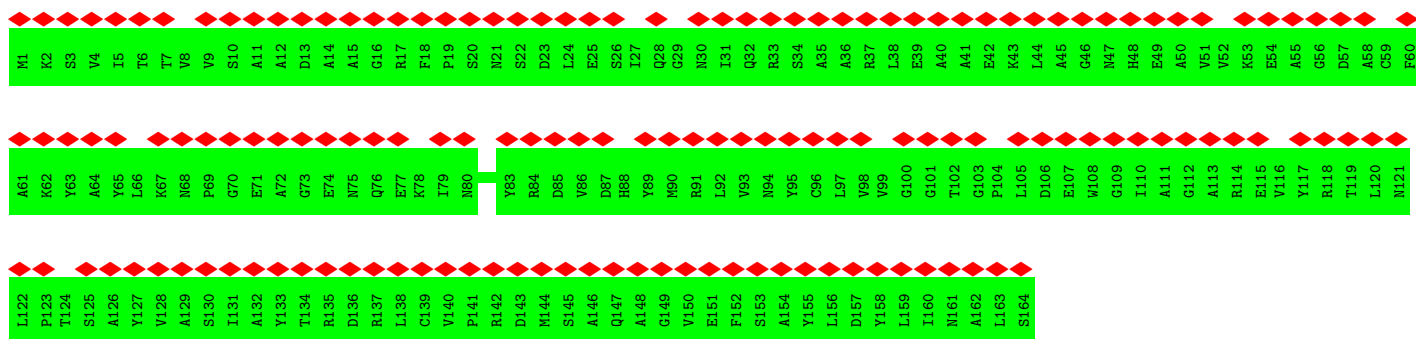




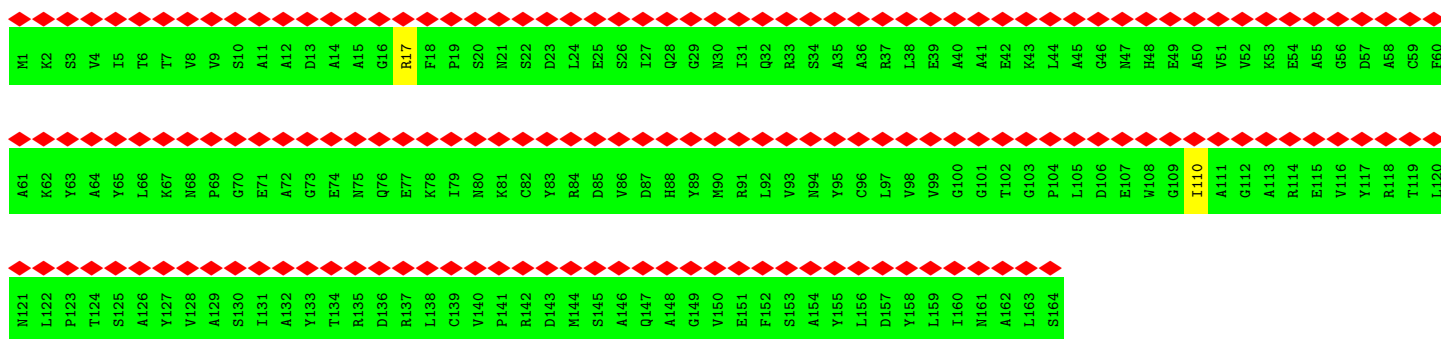
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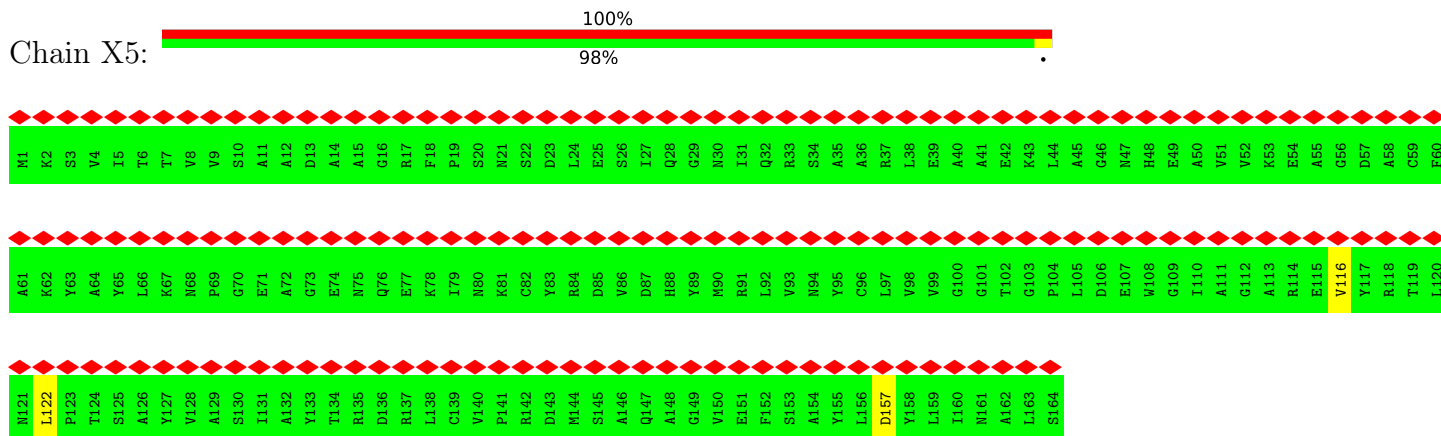
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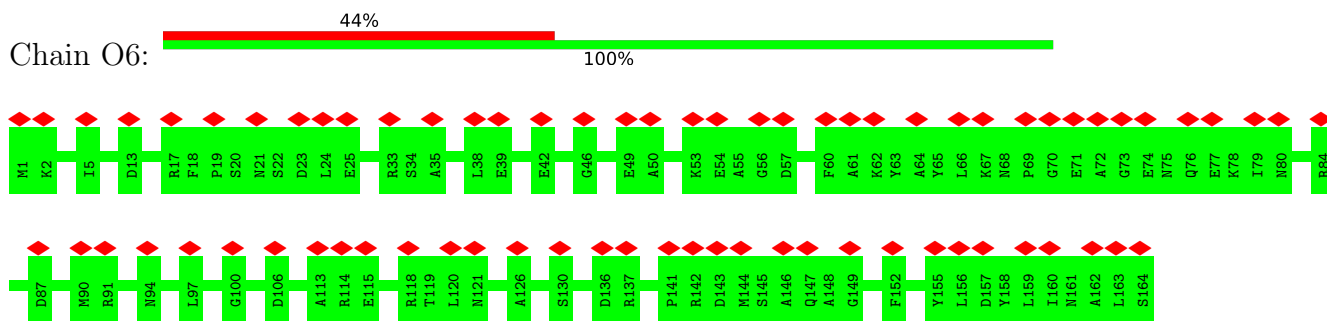
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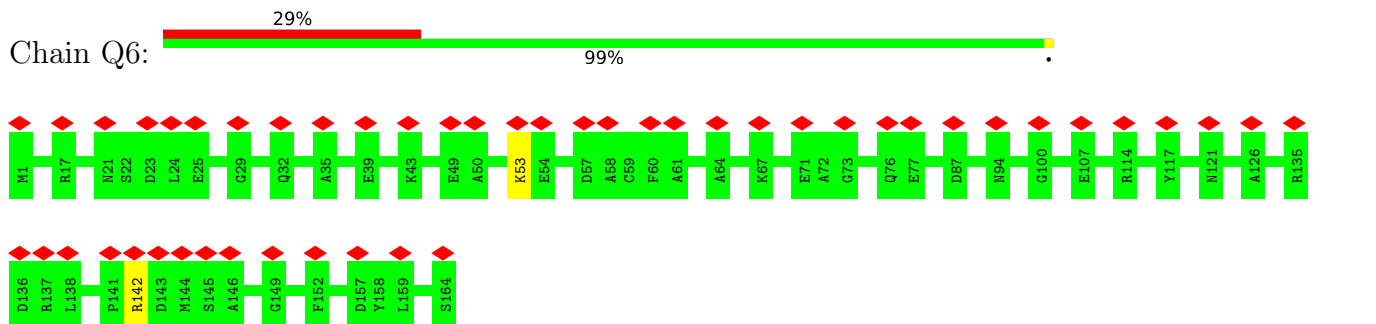
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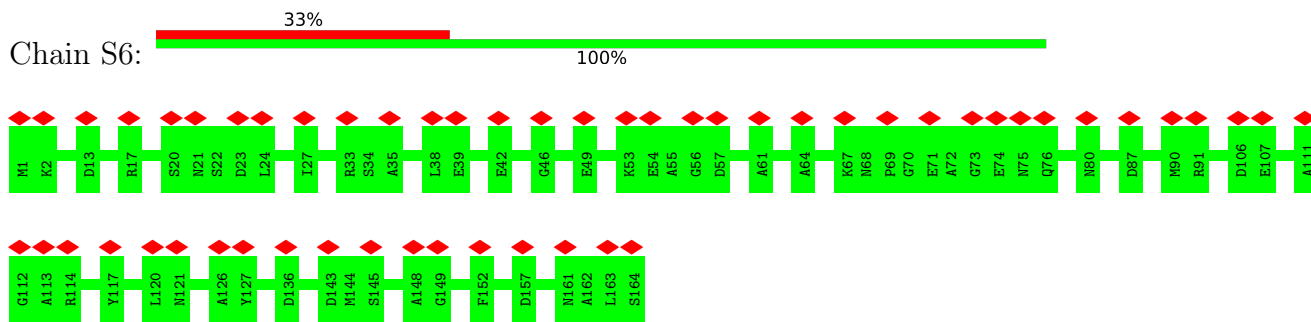
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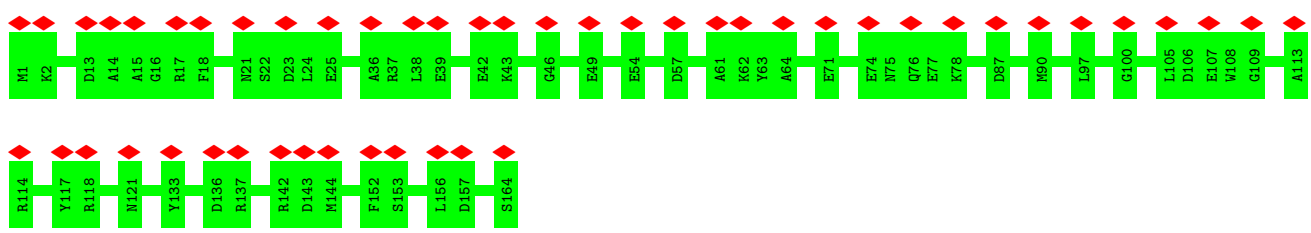
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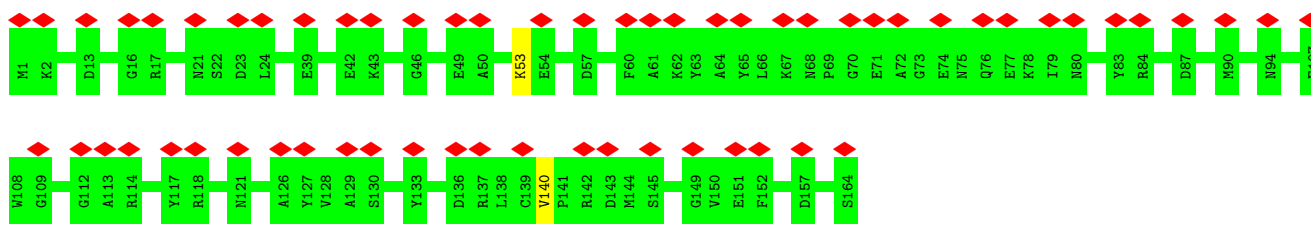
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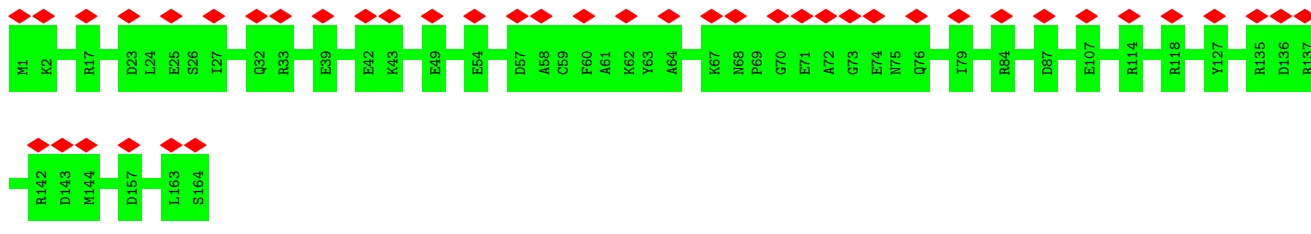
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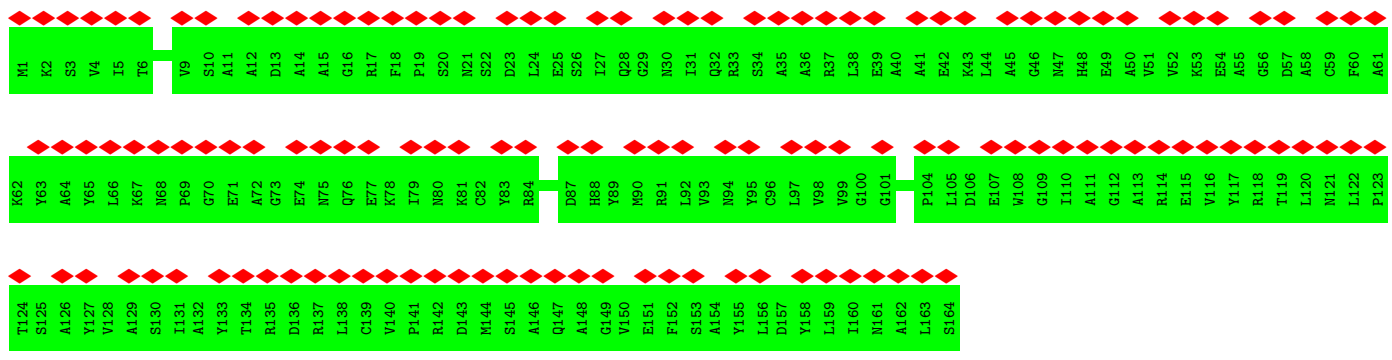
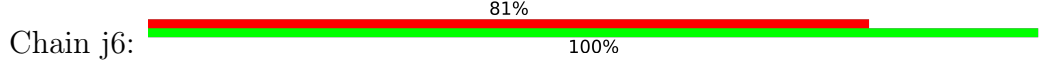
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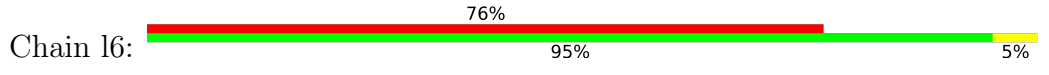
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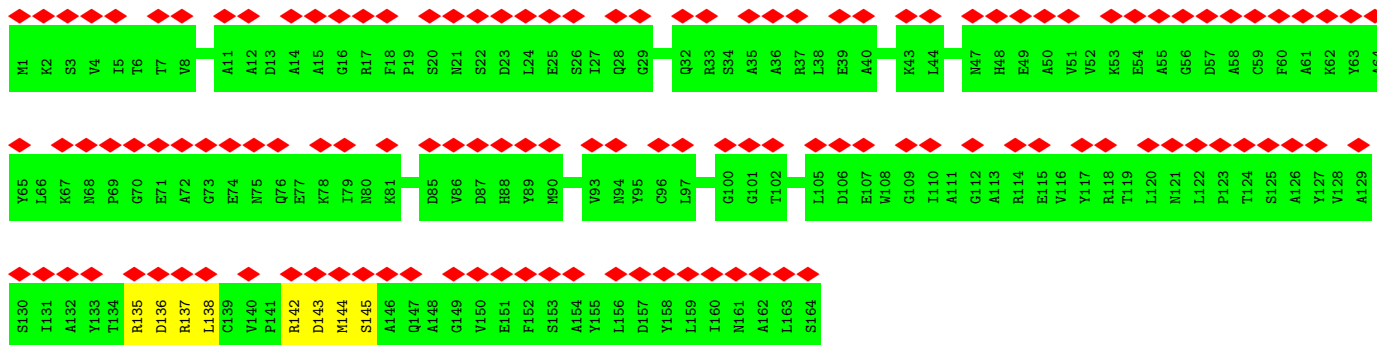


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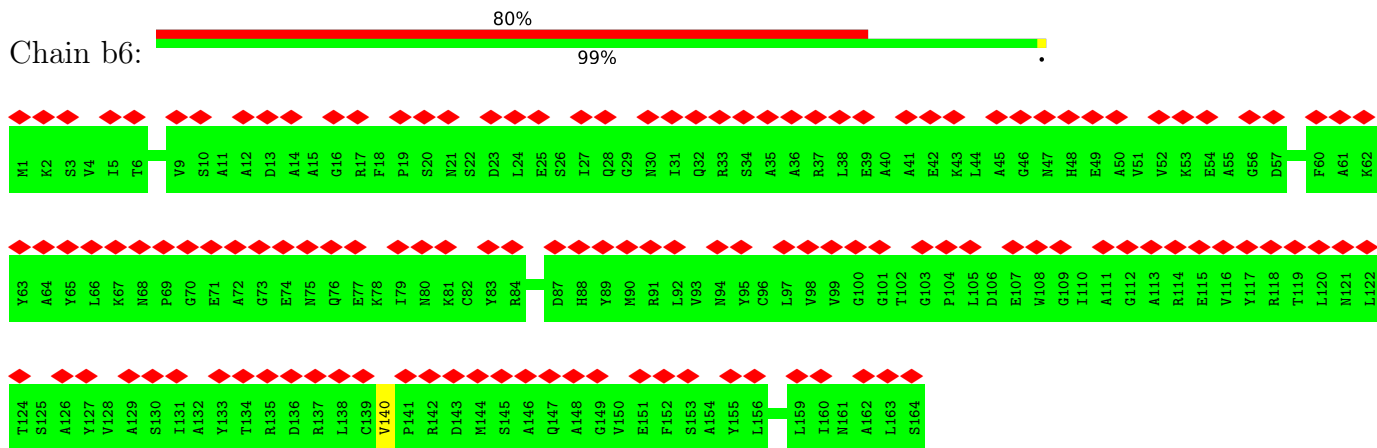


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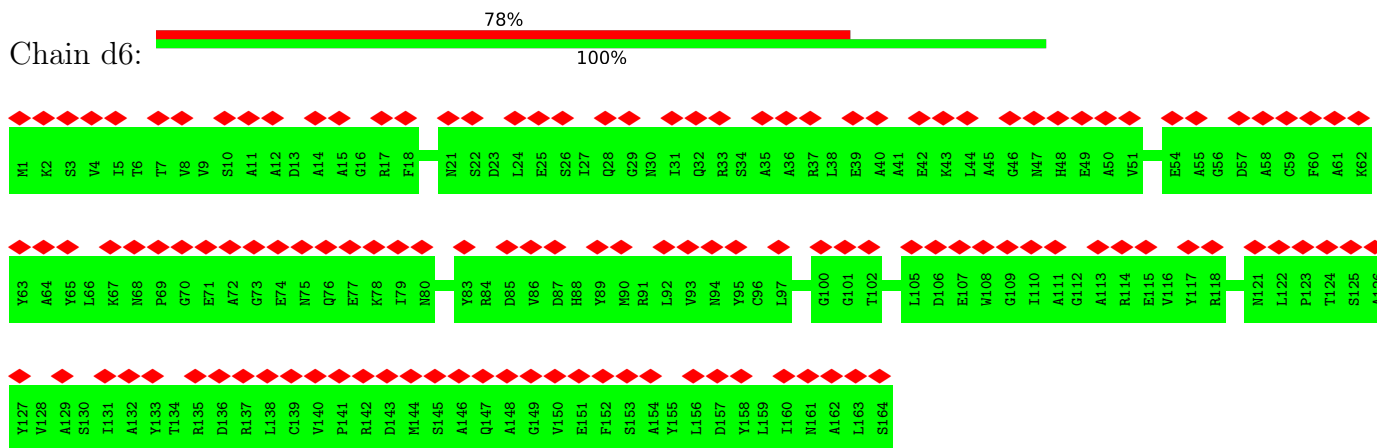




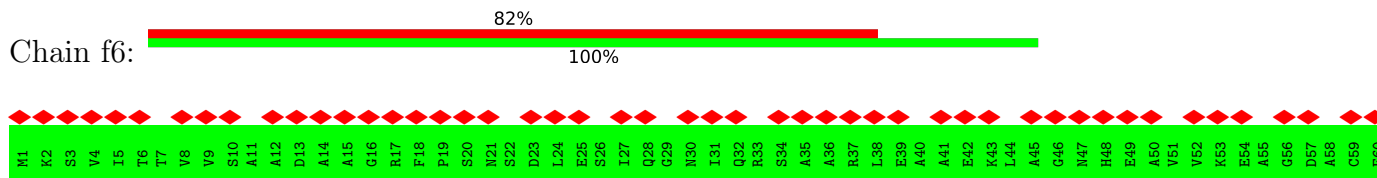
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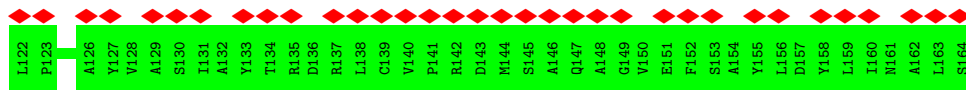
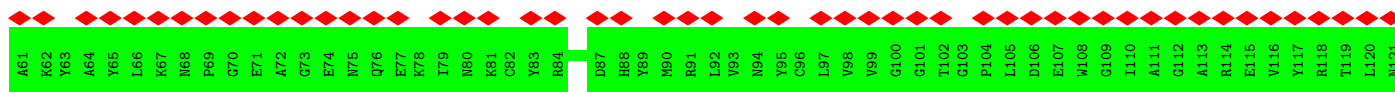


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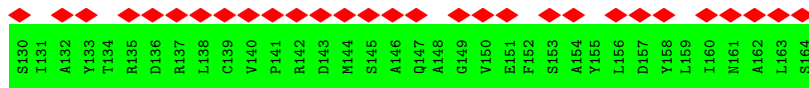
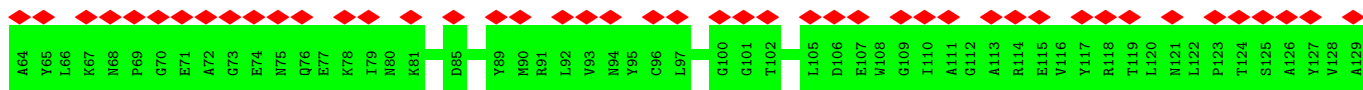
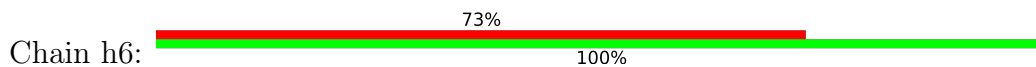


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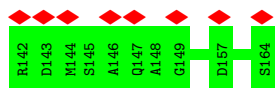
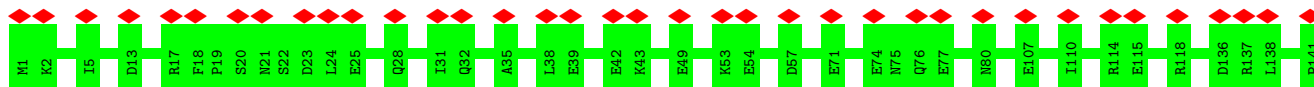




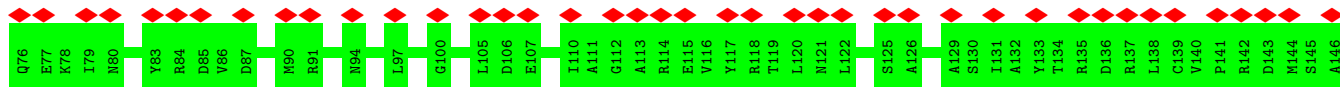
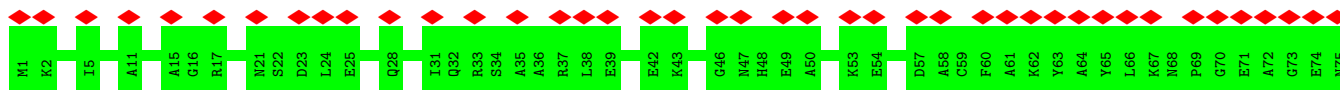
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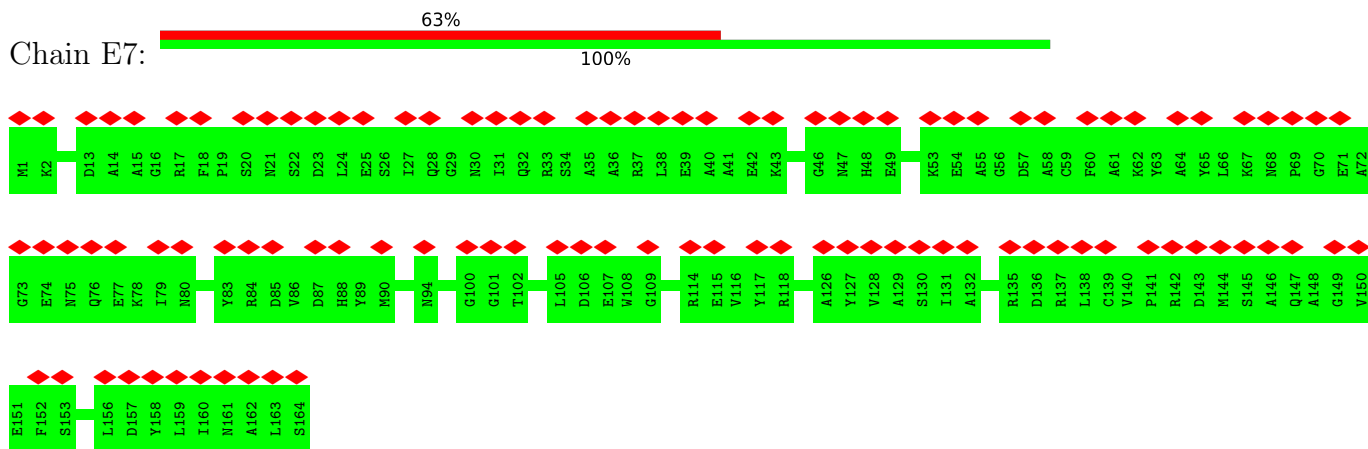
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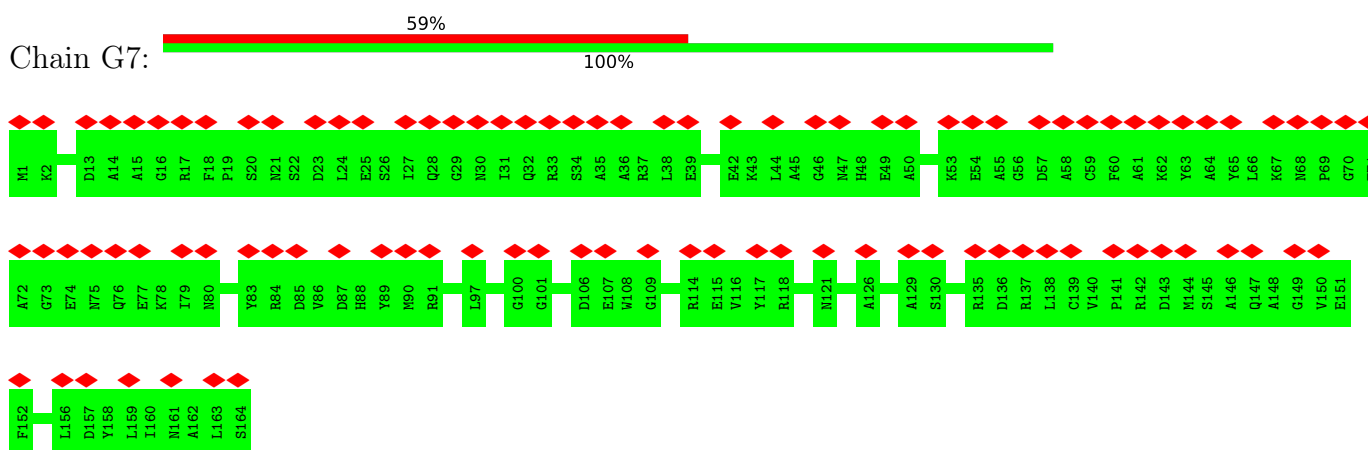
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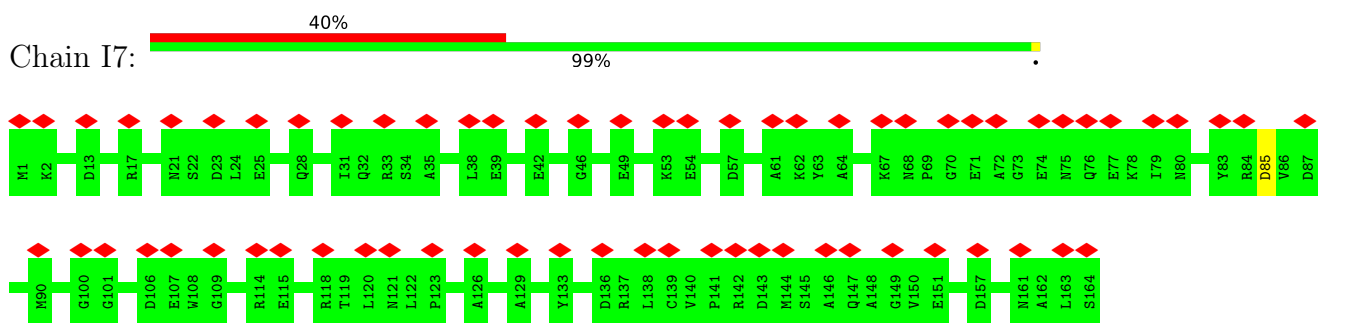
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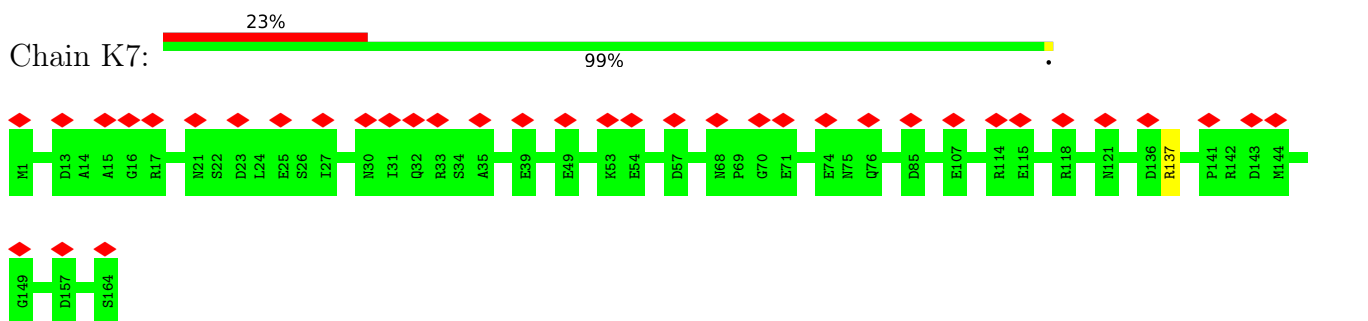
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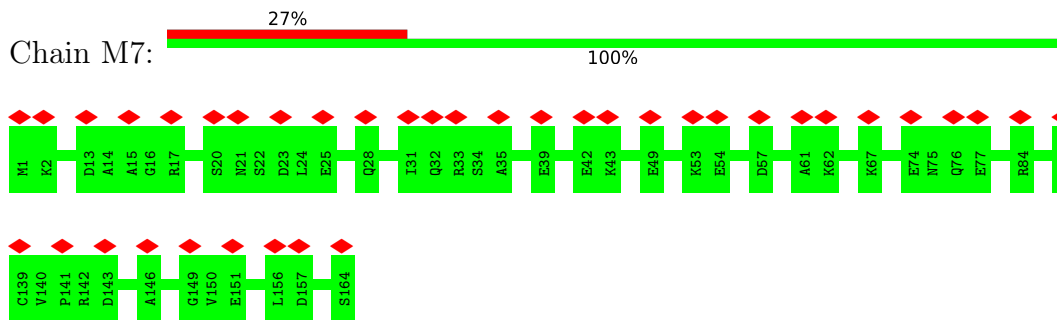
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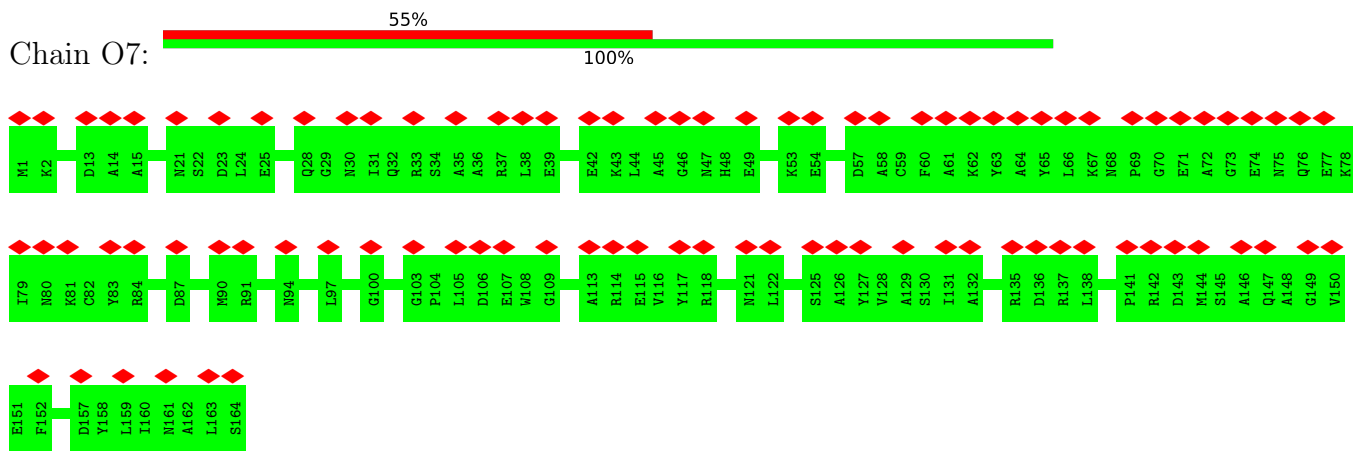
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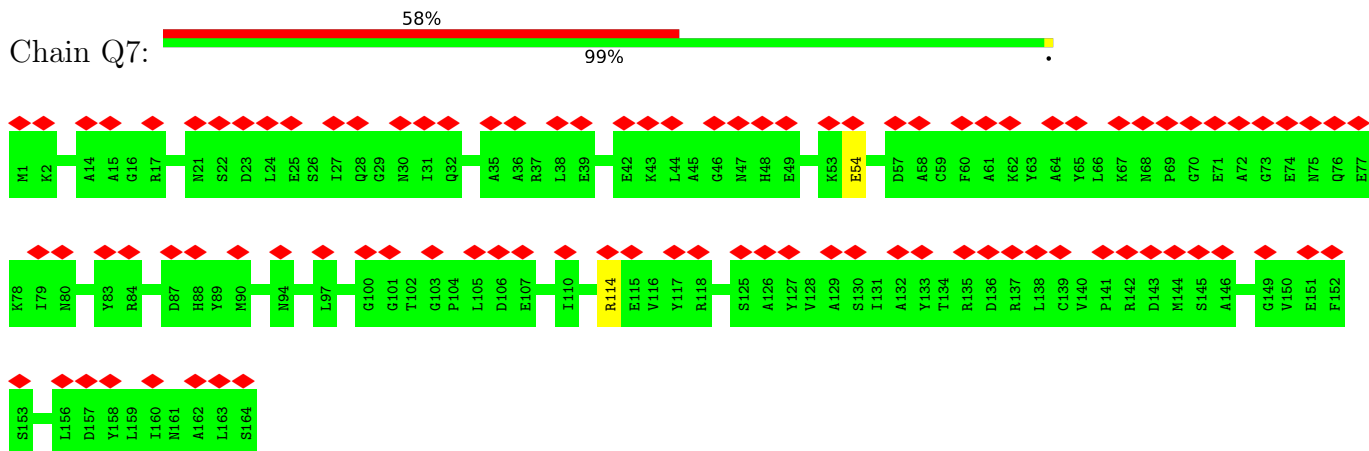
• Molecule 3: Phycoerythrin alpha subunit



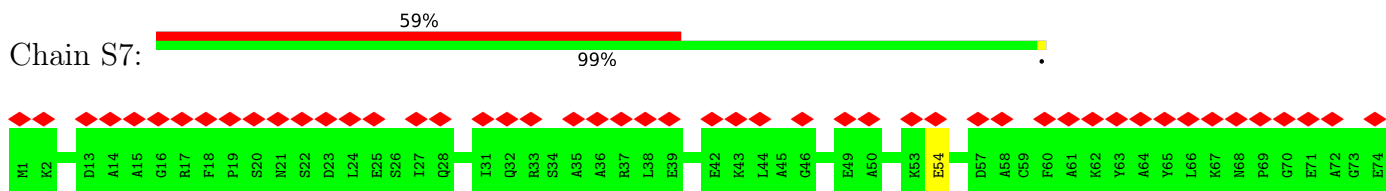
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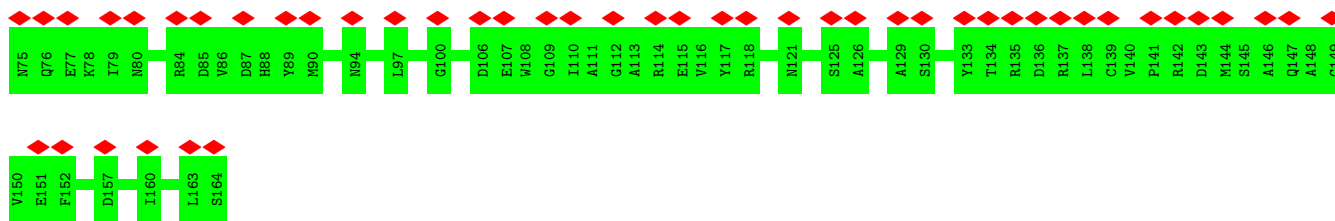


• Molecule 3: Phycoerythrin alpha subunit

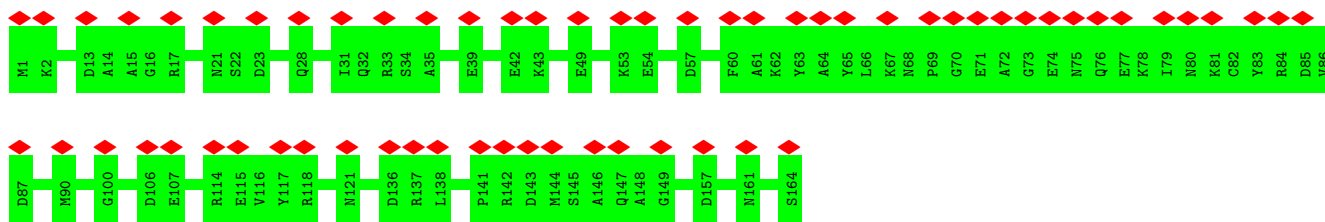
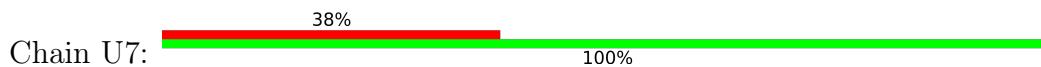


• Molecule 3: Phycoerythrin alpha subunit

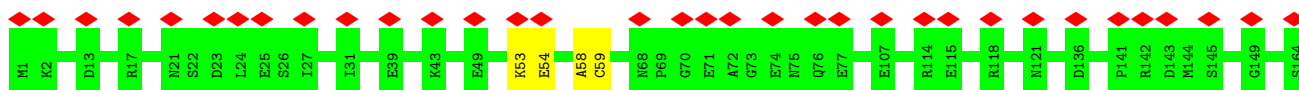




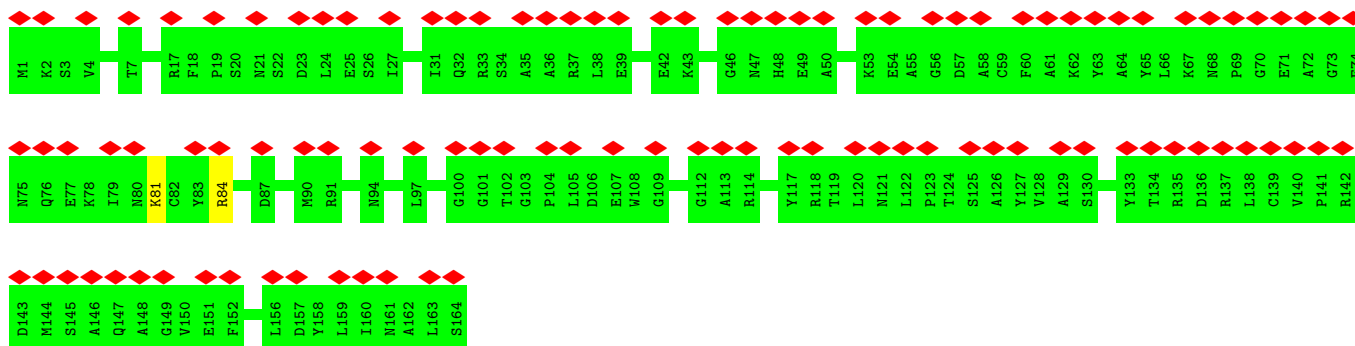
- Molecule 3: Phycoerythrin alpha subunit



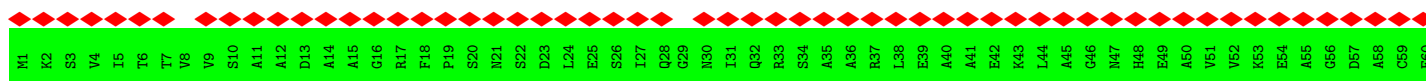
- Molecule 3: Phycoerythrin alpha subunit

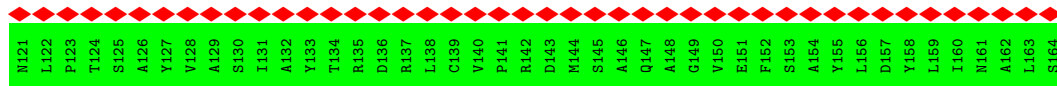
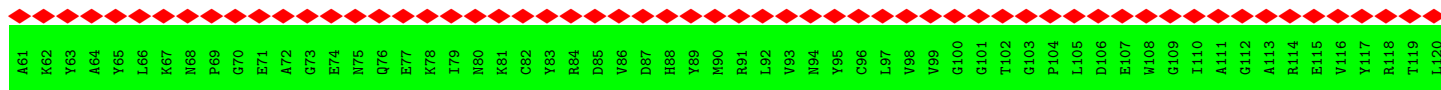


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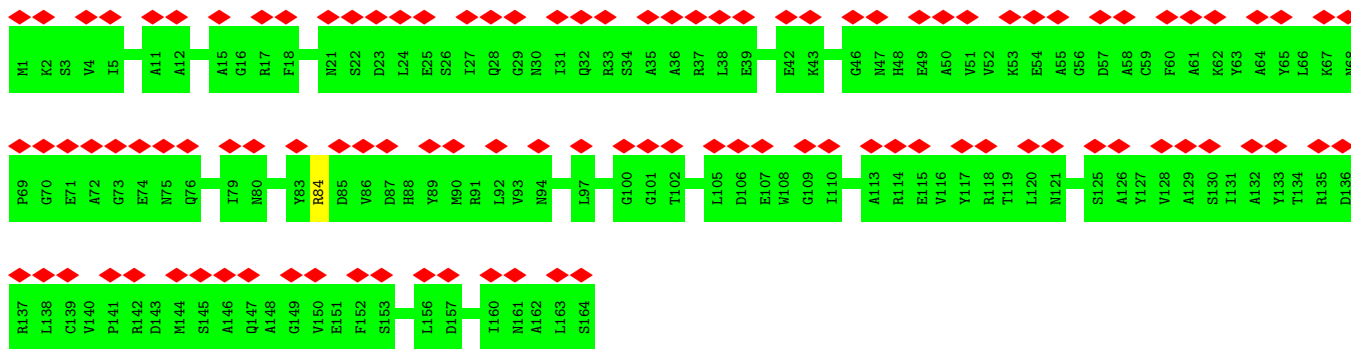


- Molecule 3: Phycoerythrin alpha subunit

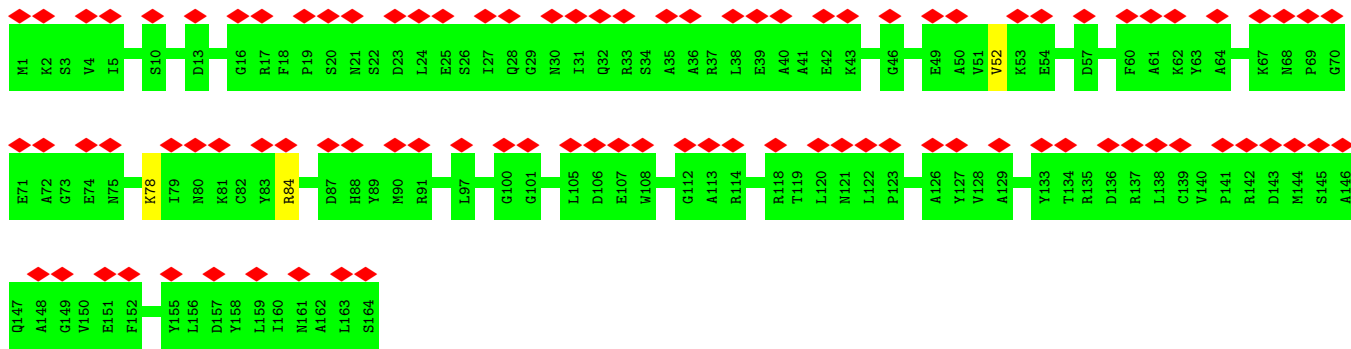




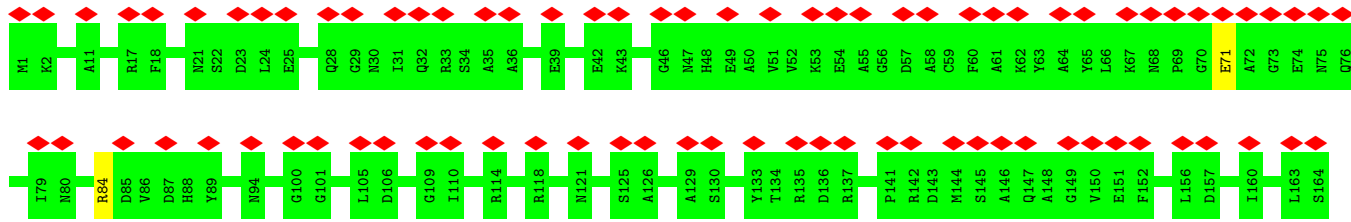
• Molecule 3: Phycoerythrin alpha subunit



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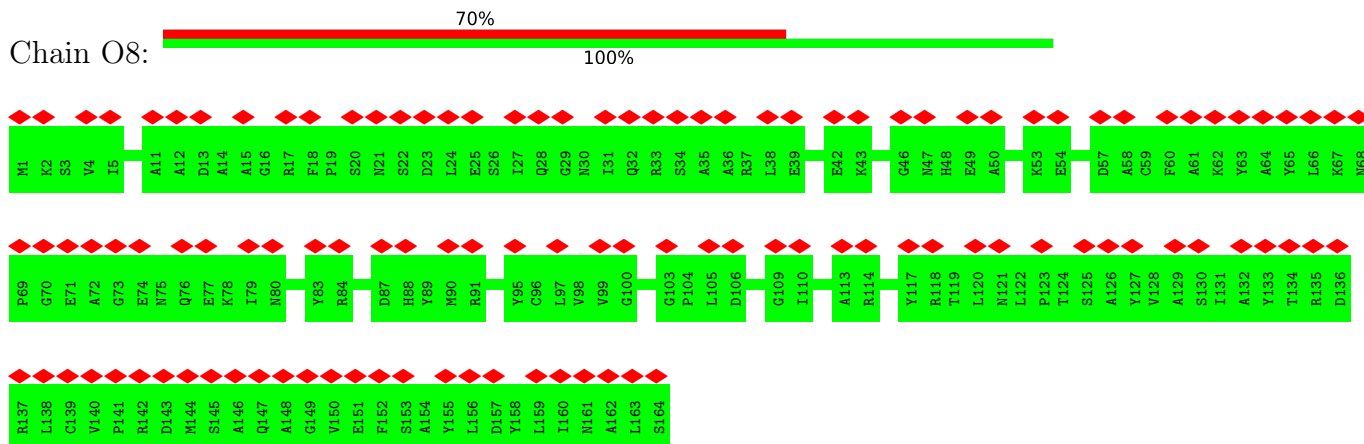


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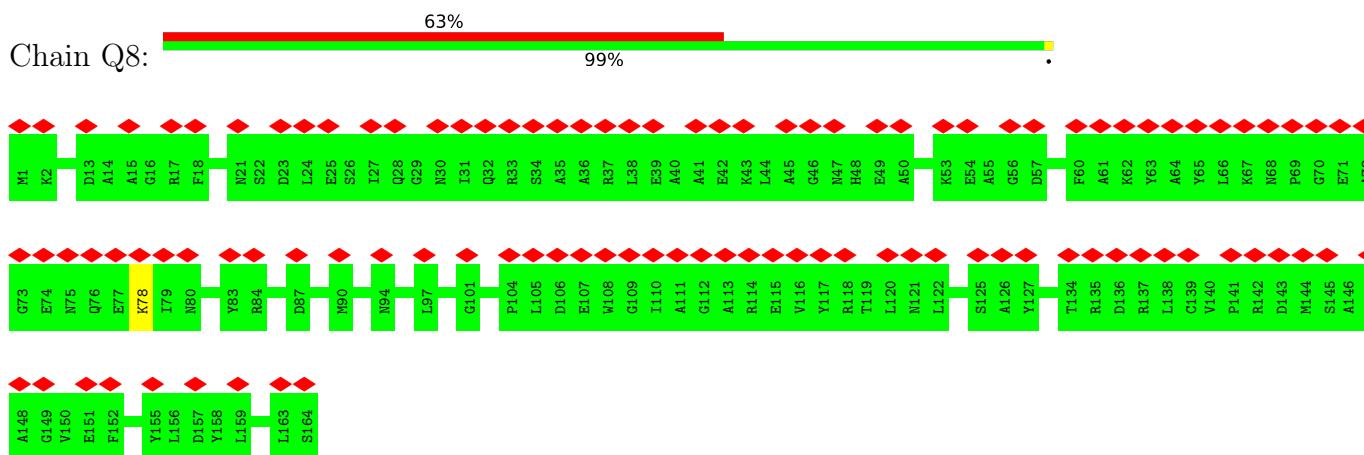


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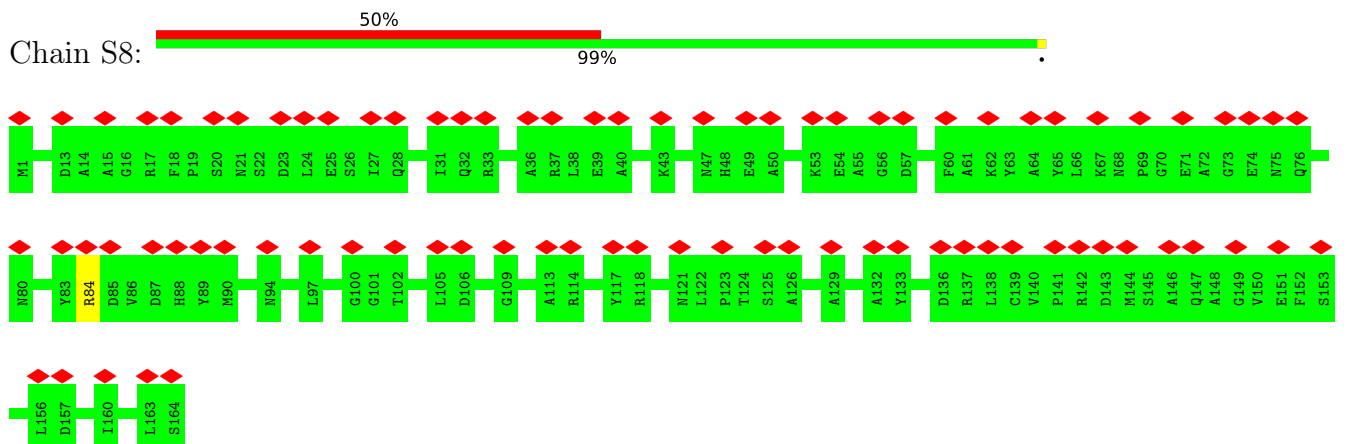
• Molecule 3: Phycoerythrin alpha subunit



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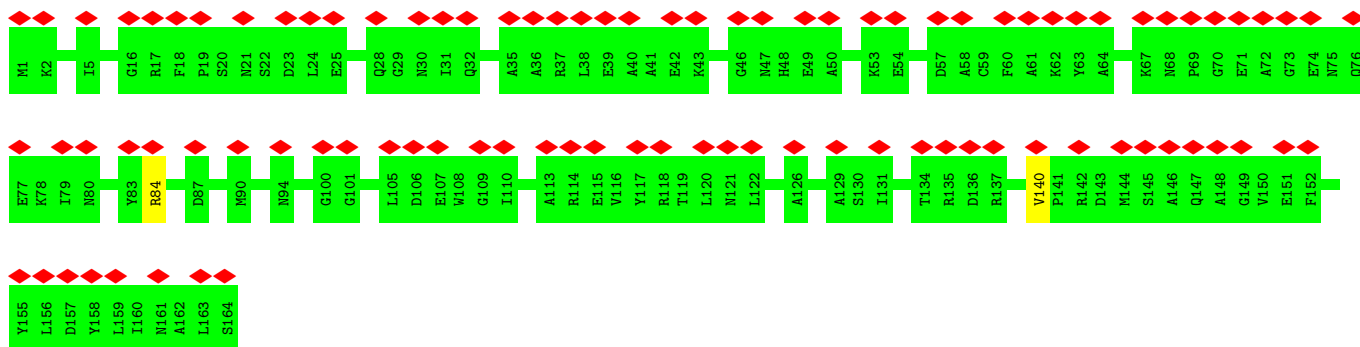


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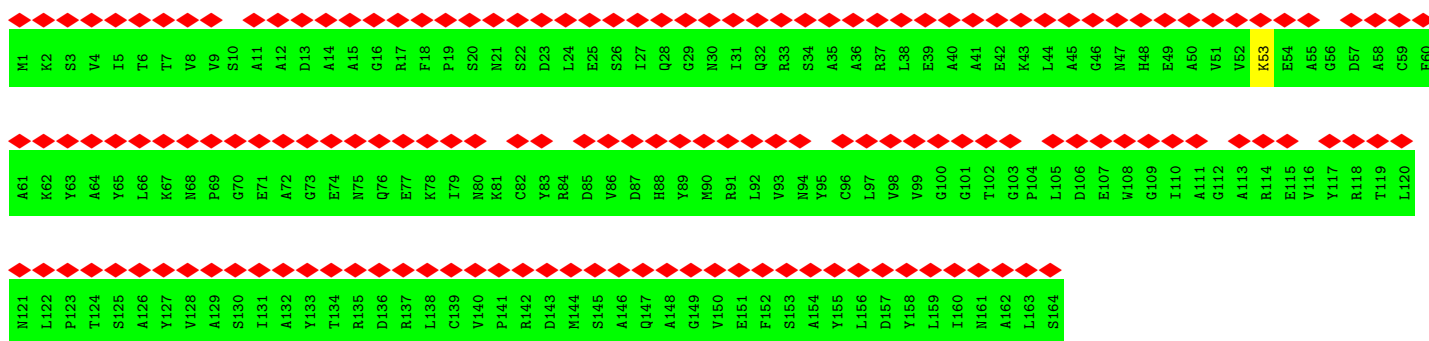


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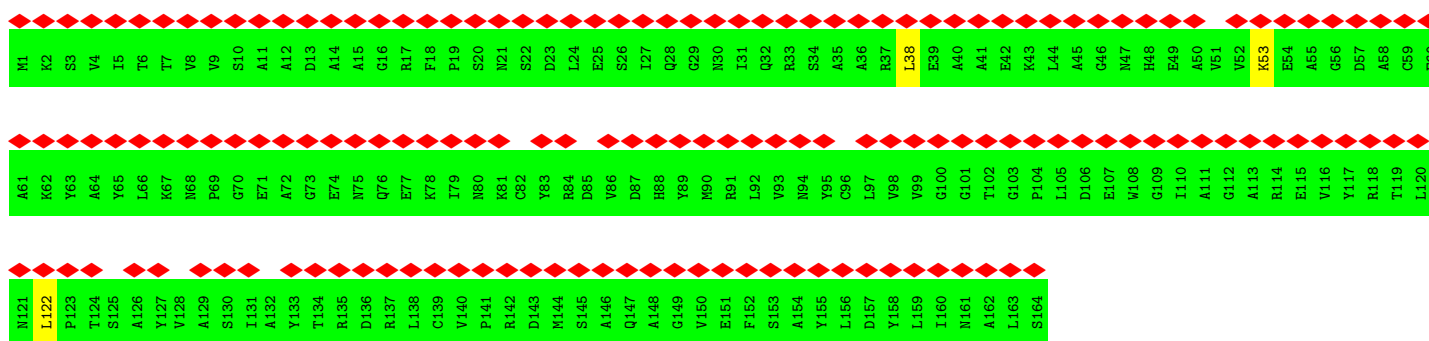




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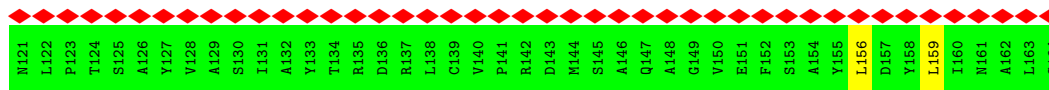


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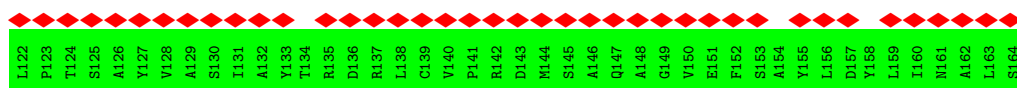
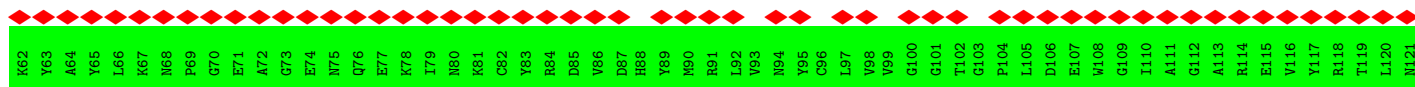
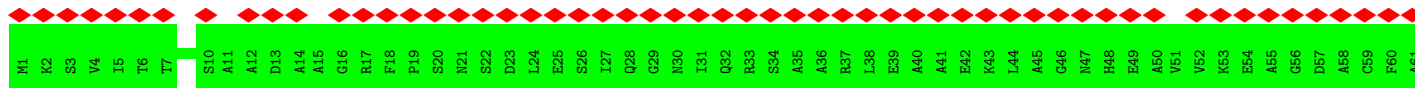
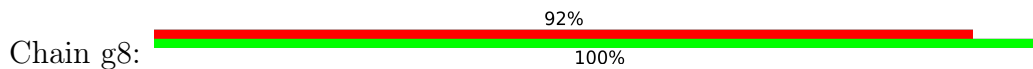


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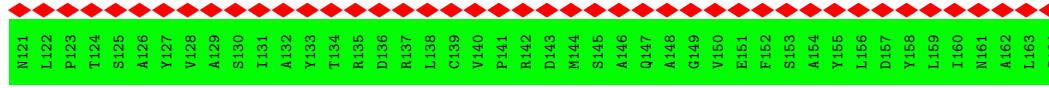
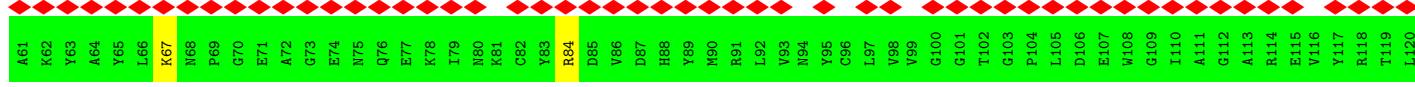
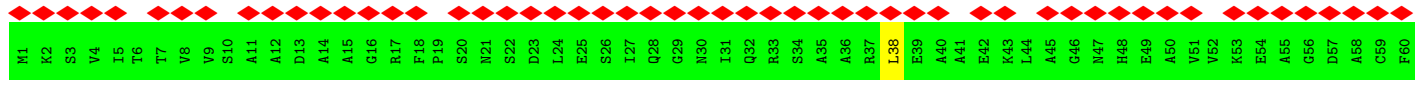




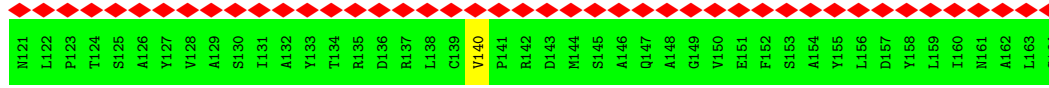
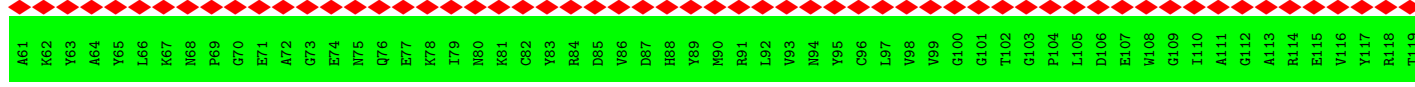
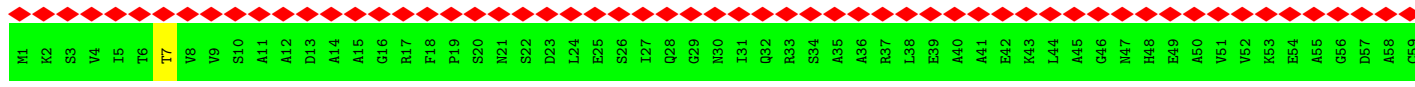
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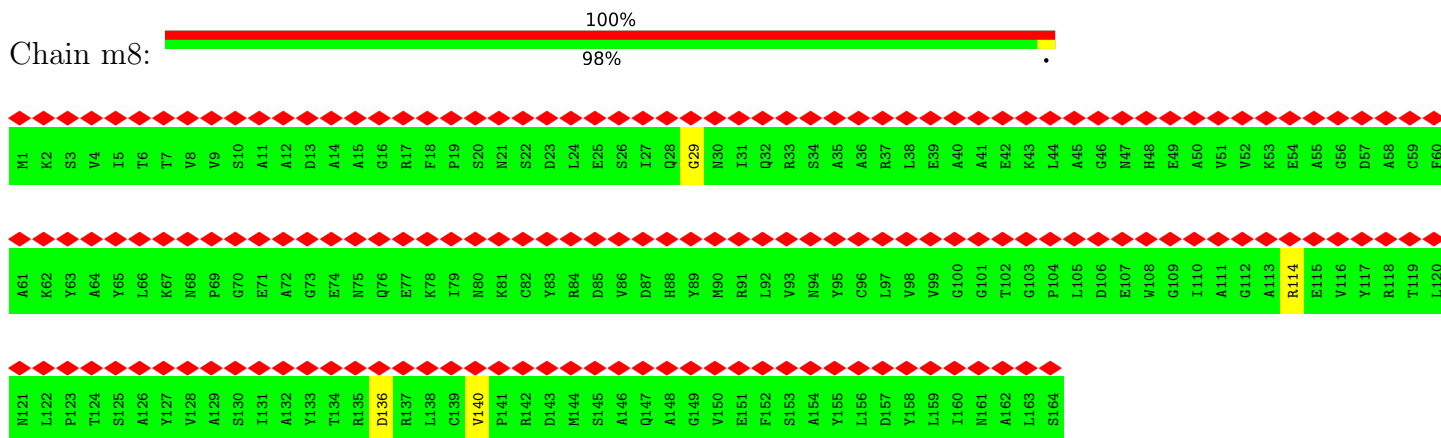
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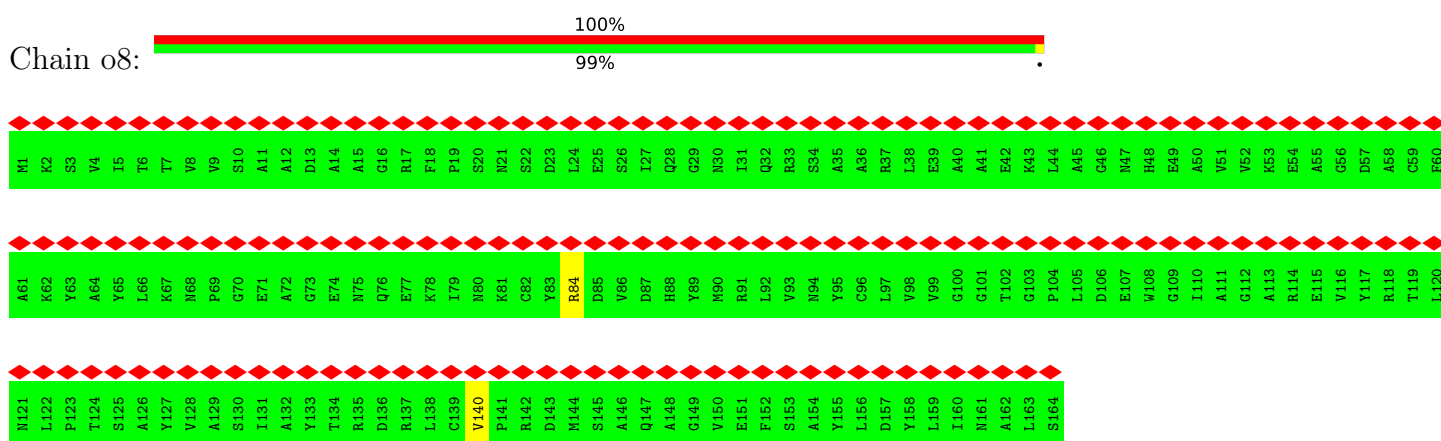
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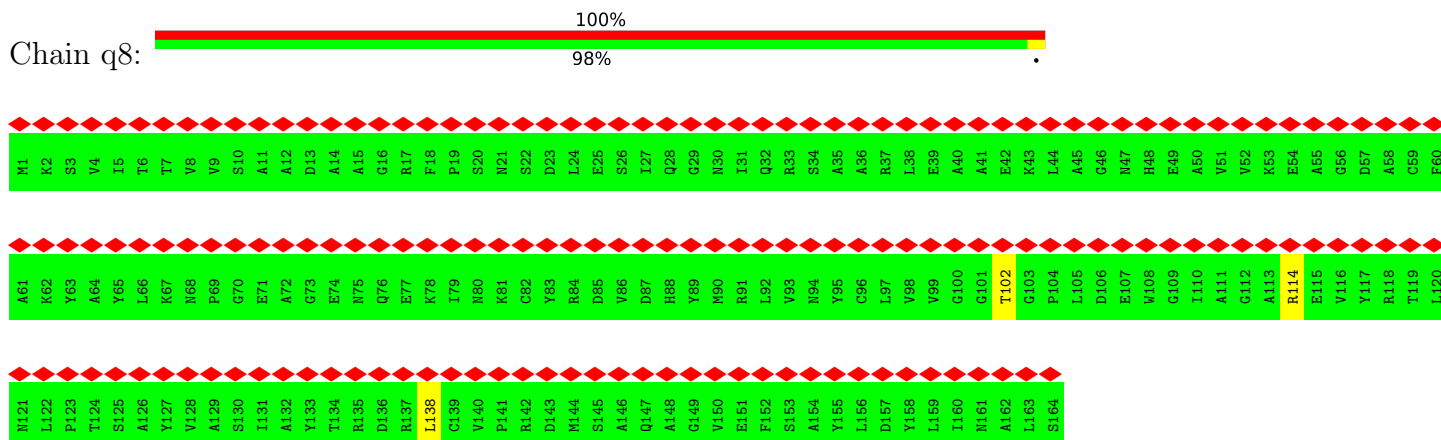
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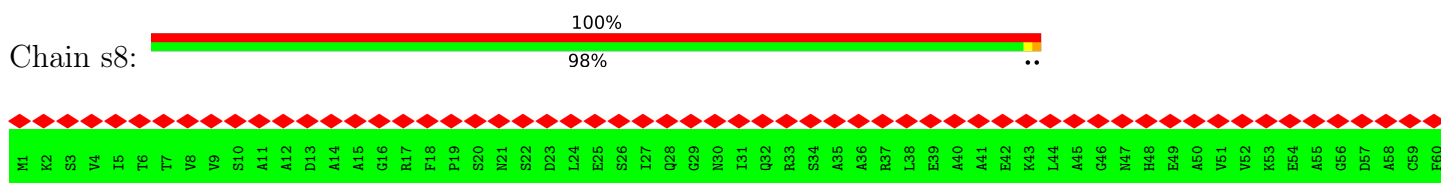
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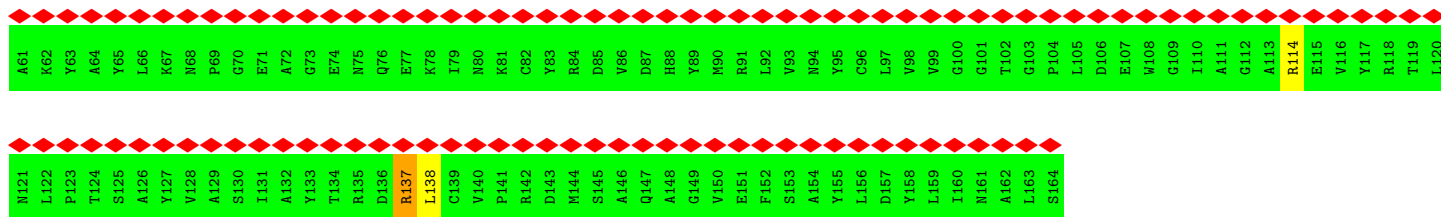


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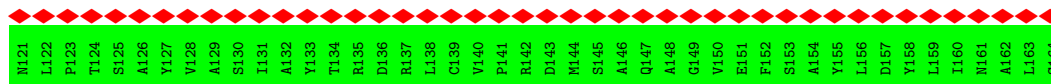
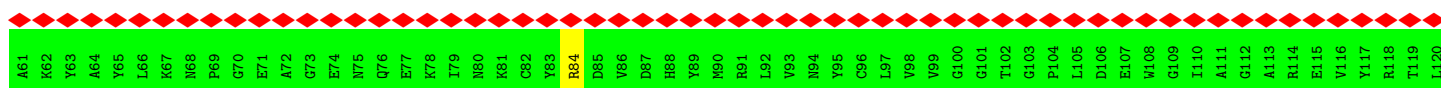
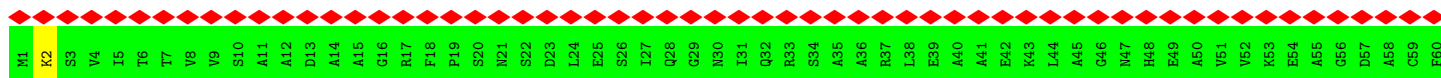


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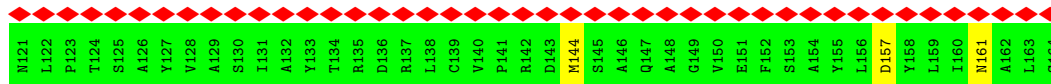
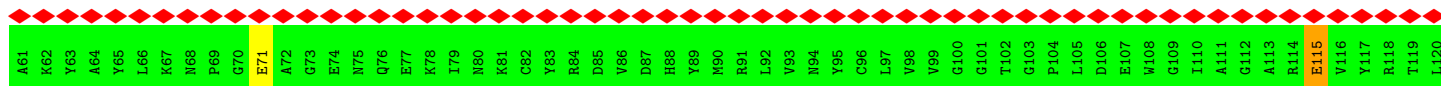
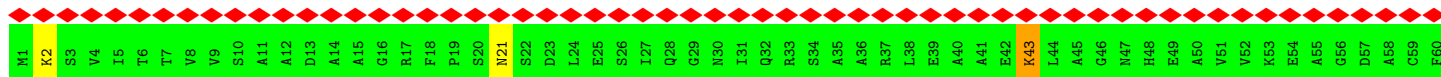




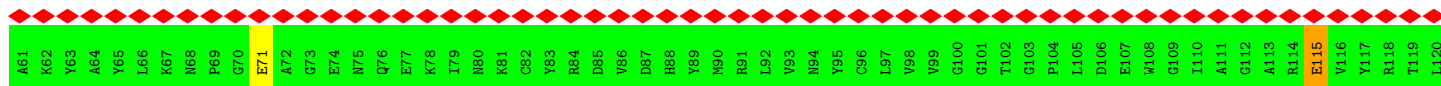
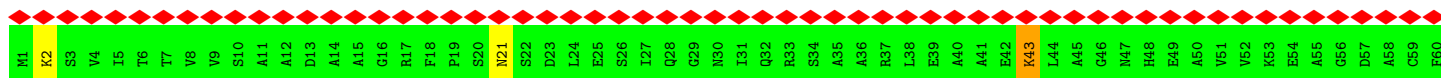
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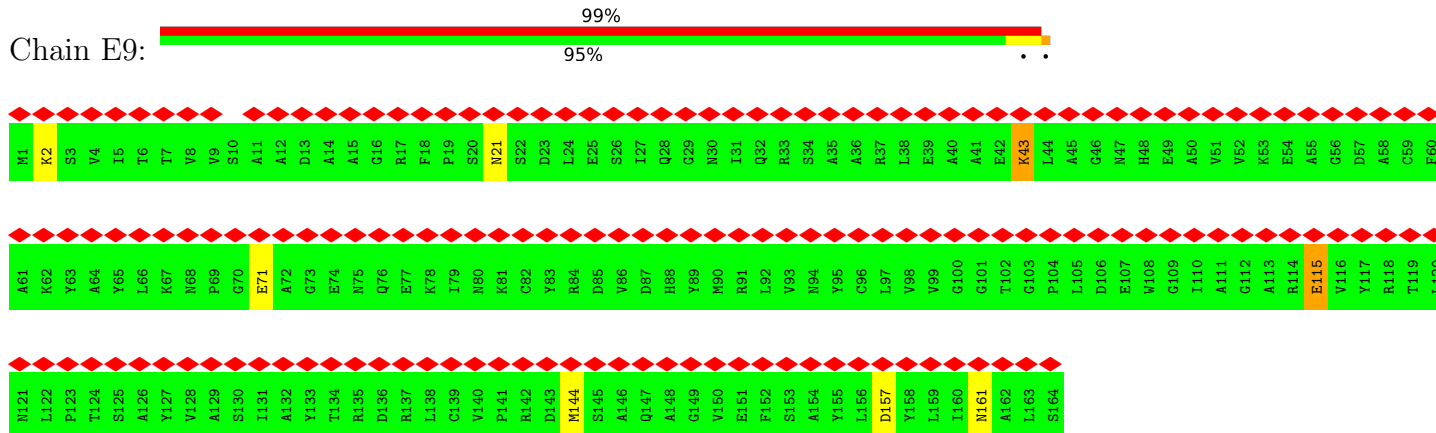
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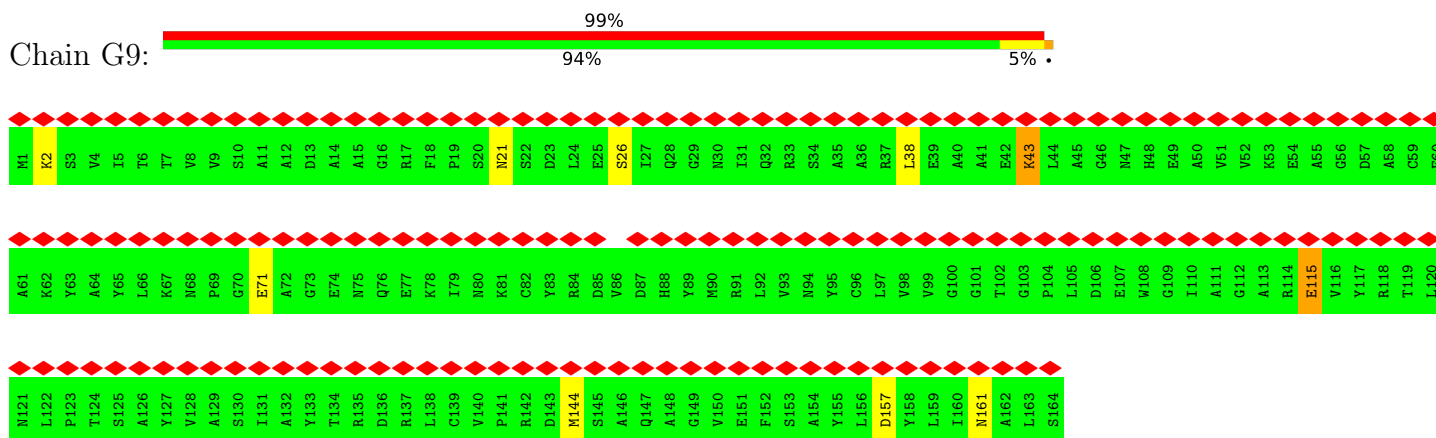
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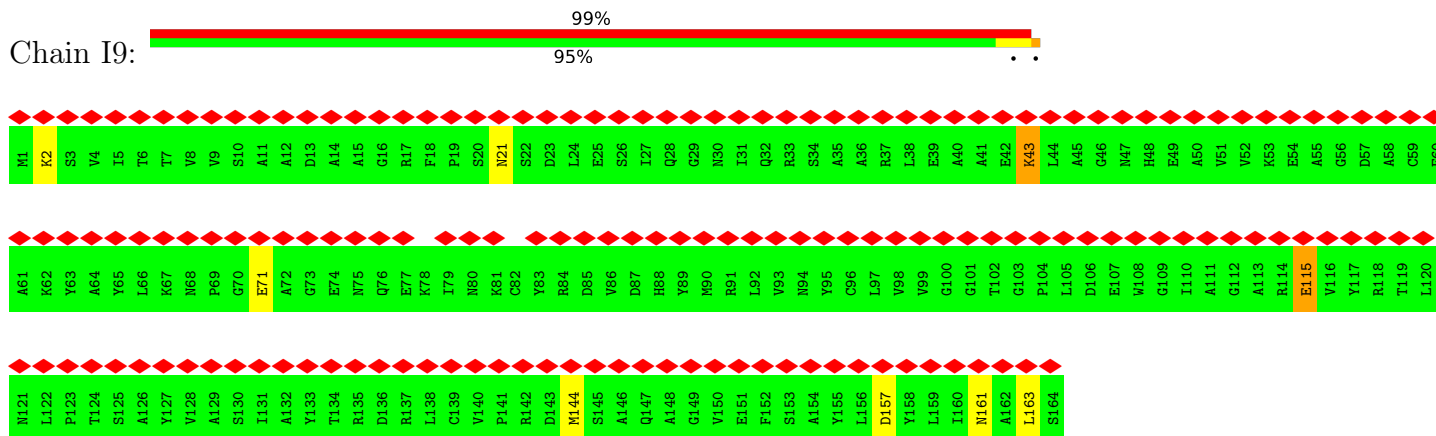
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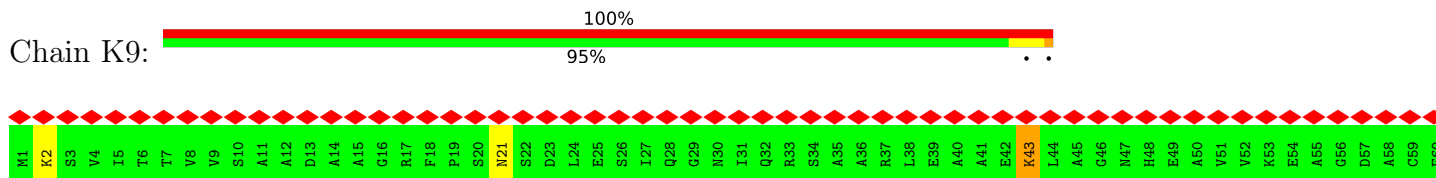
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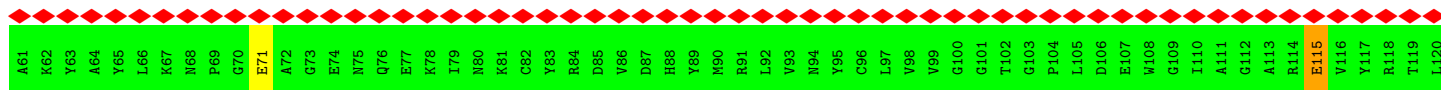


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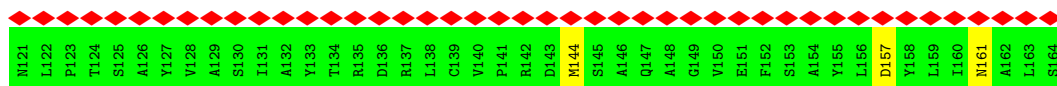
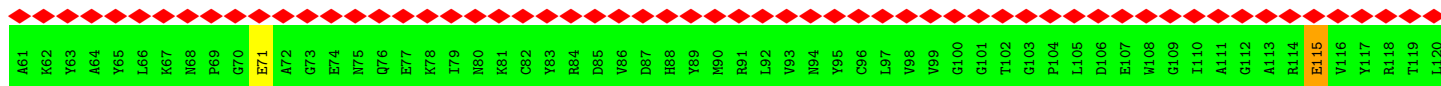
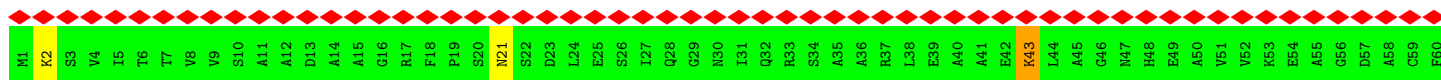


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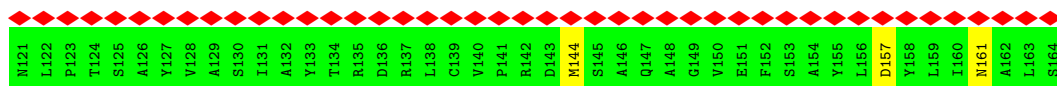
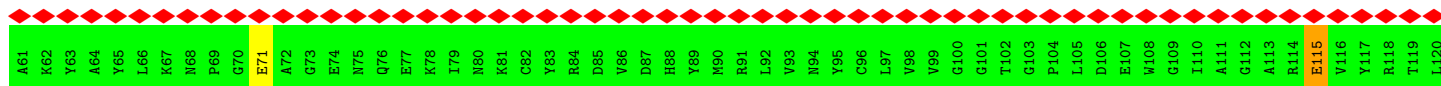
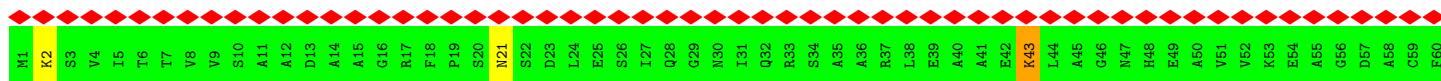




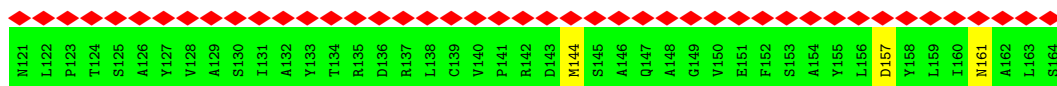
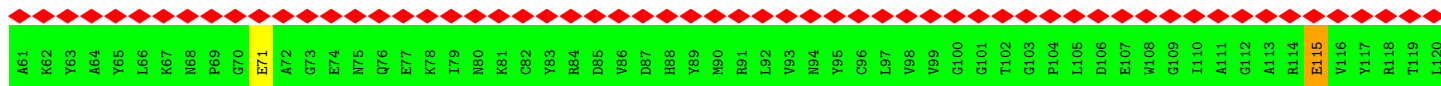
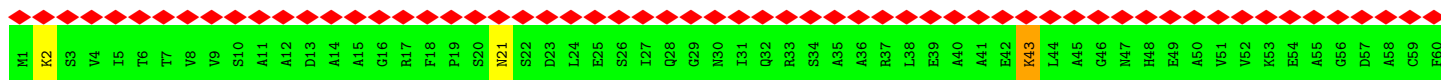
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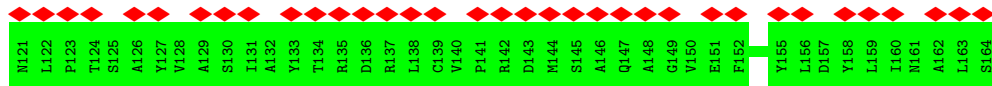
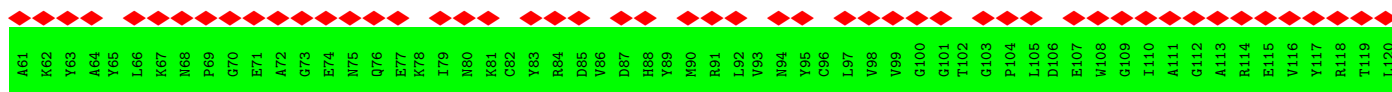


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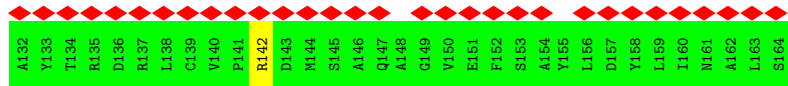
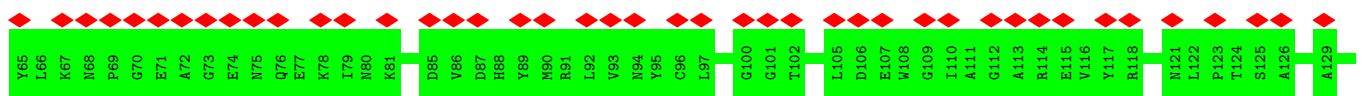
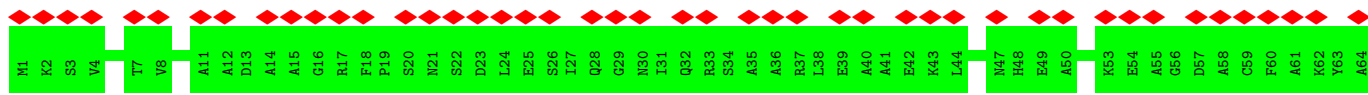
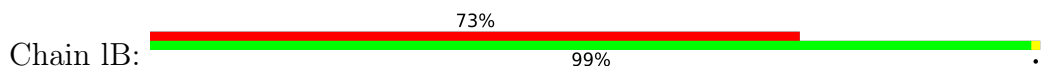


• Molecule 3: Phycoerythrin alpha subunit

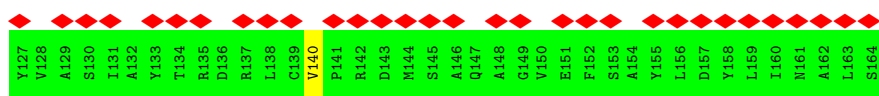
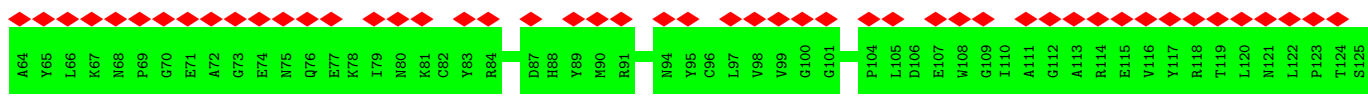
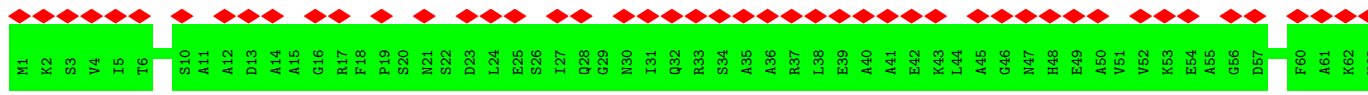
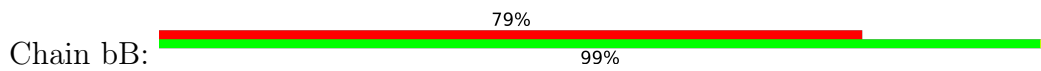




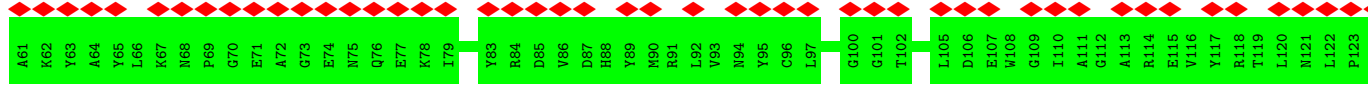
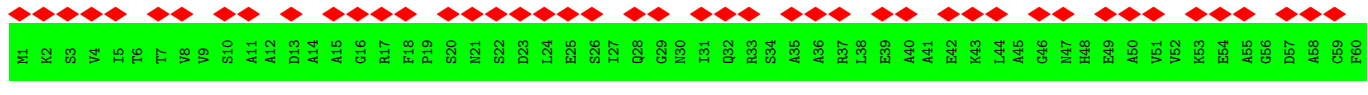
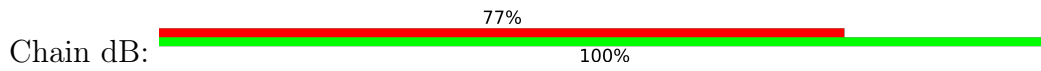
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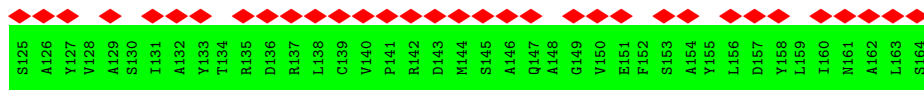


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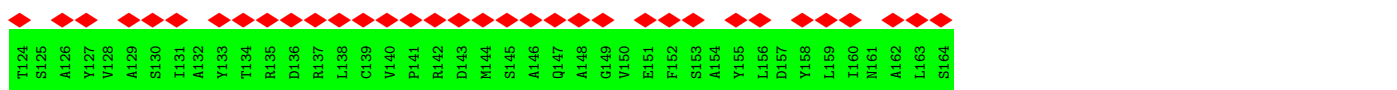
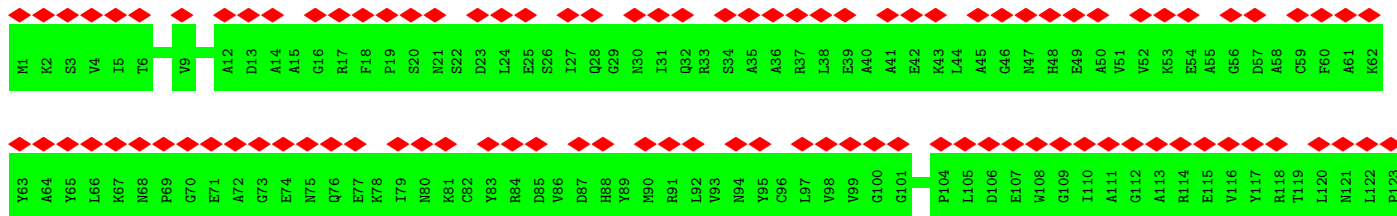
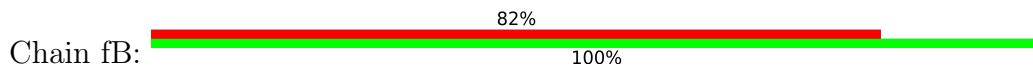


• Molecule 3: Phycoerythrin alpha subunit

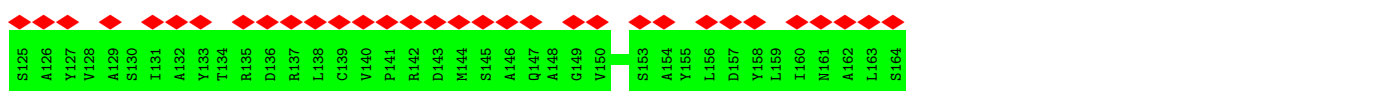
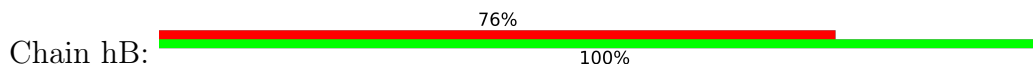




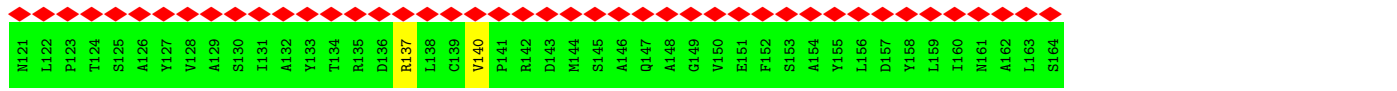
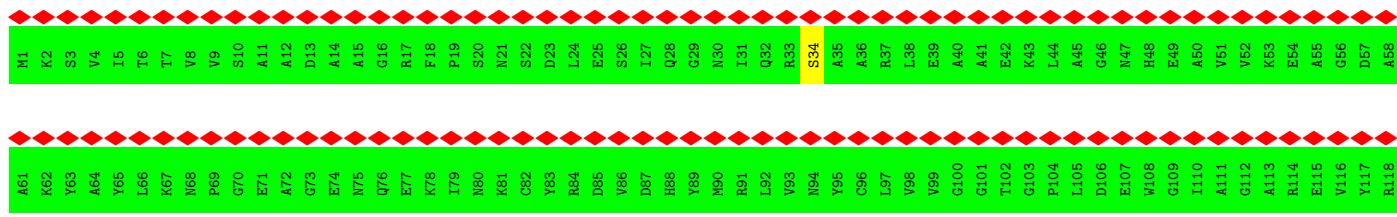
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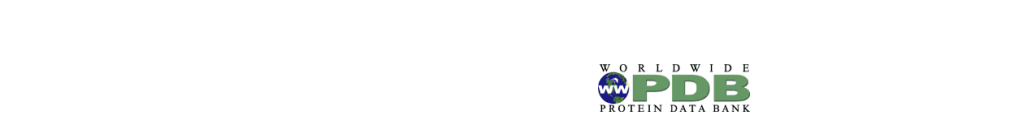
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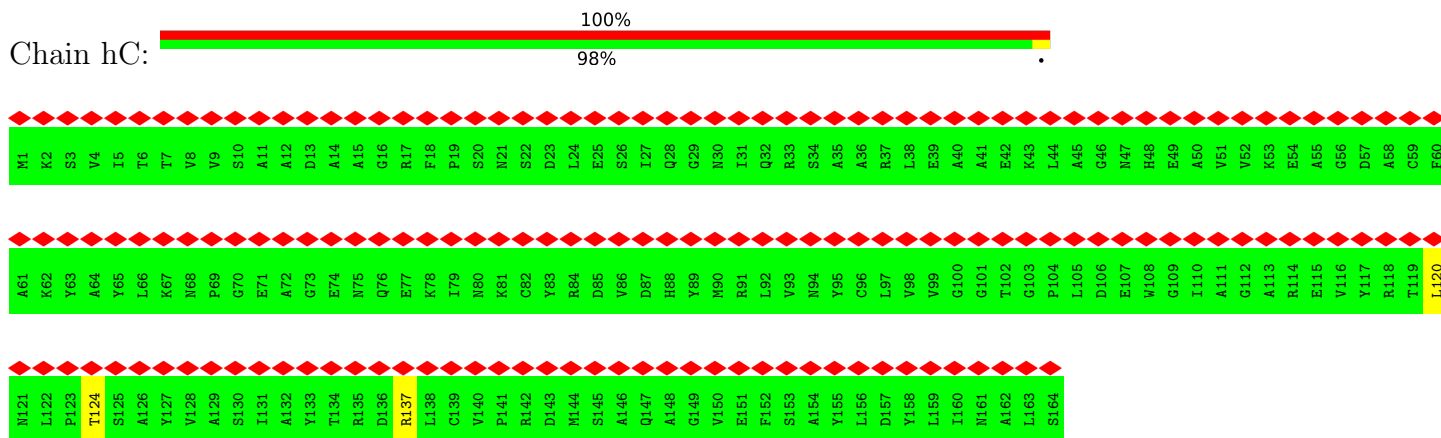


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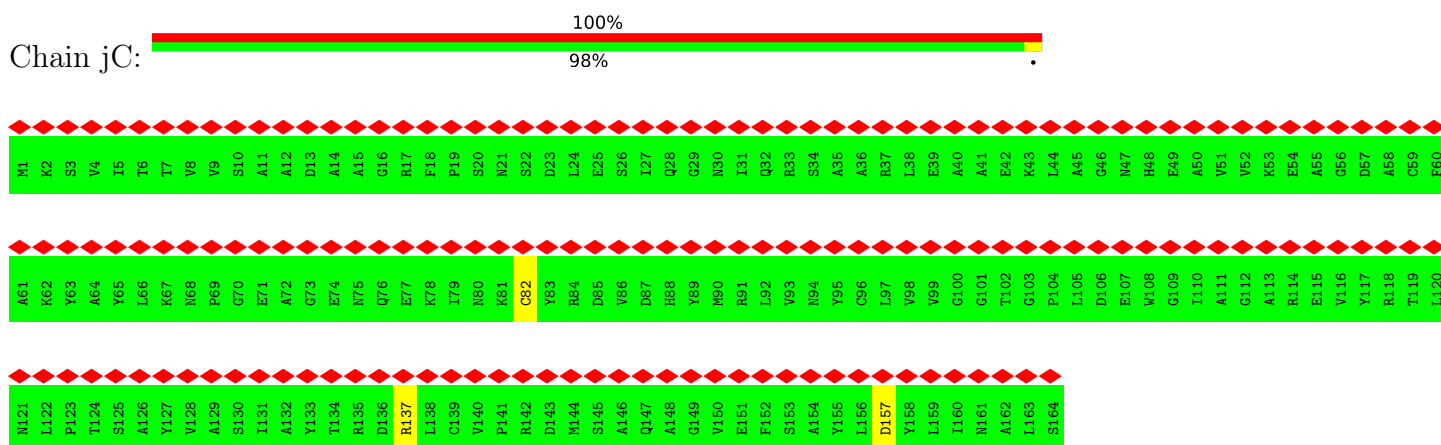


• Molecule 3: Phycoerythrin alpha subunit

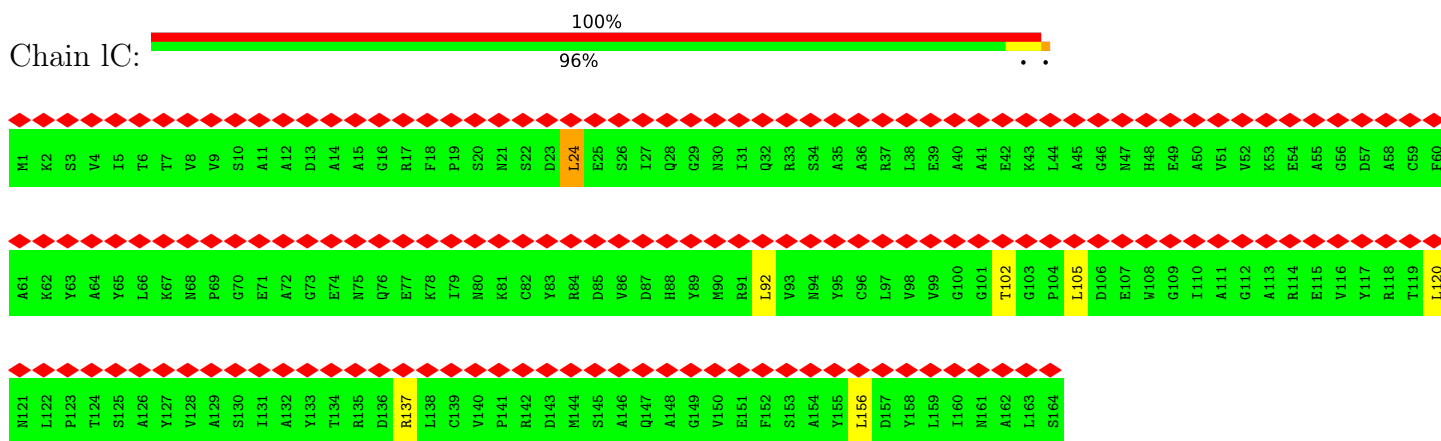




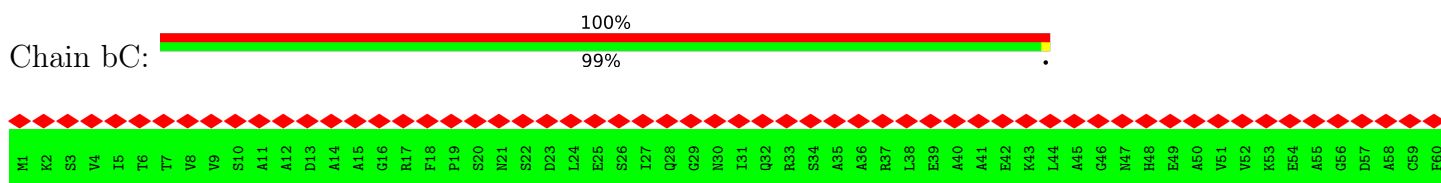
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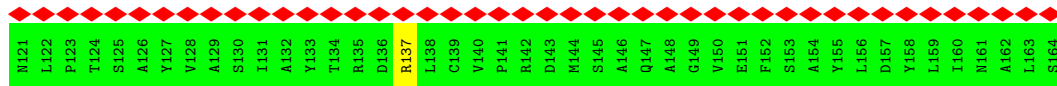
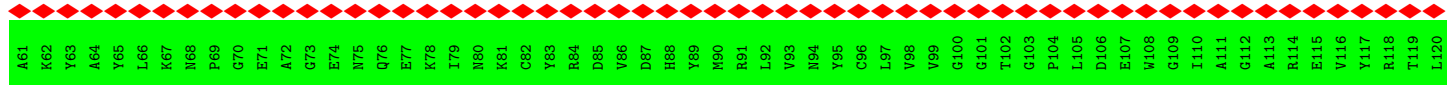


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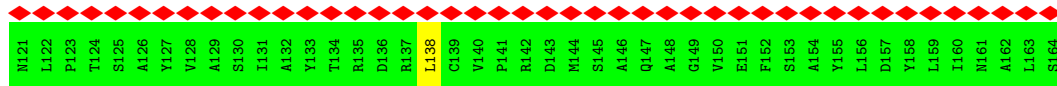
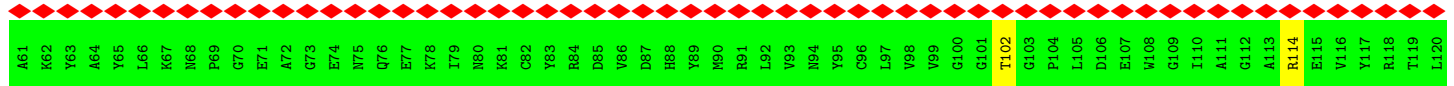
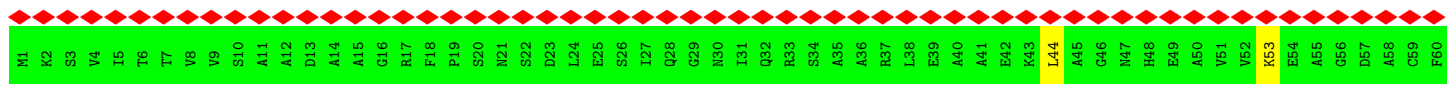


• Molecule 3: Phycoerythrin alpha subunit

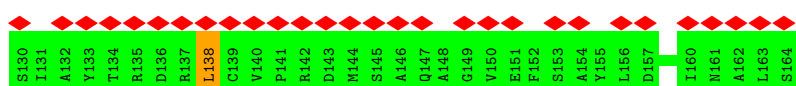
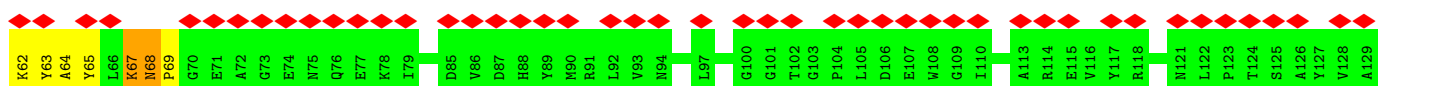
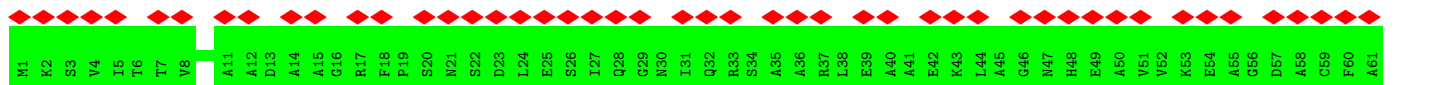
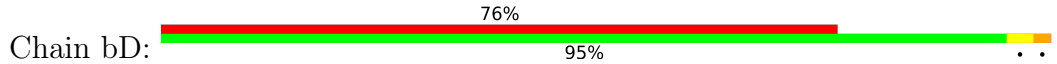




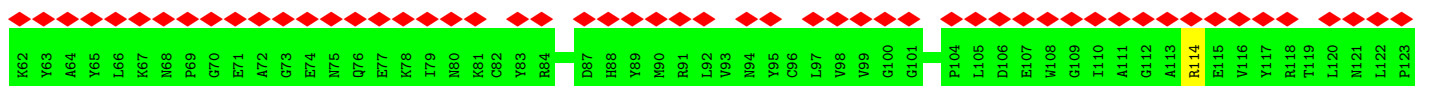
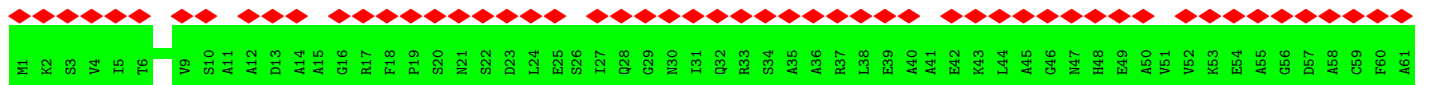
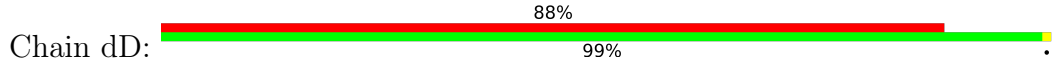
• Molecule 3: Phycoerythrin alpha subunit

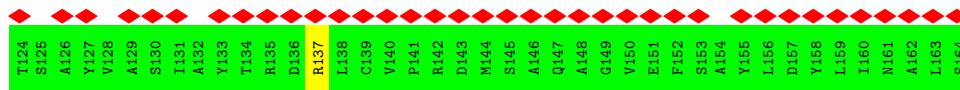


• Molecule 3: Phycoerythrin alpha subunit

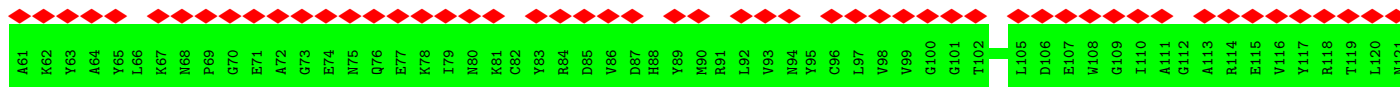
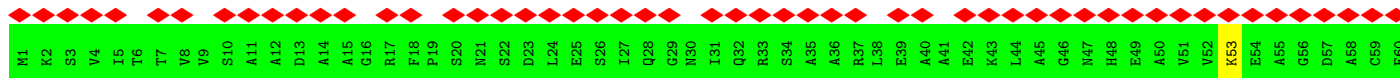
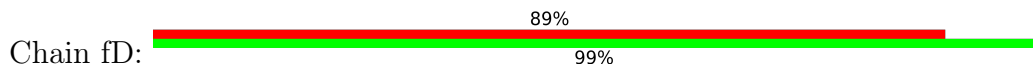


• Molecule 3: Phycoerythrin alpha subunit

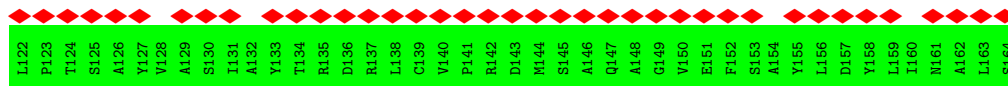
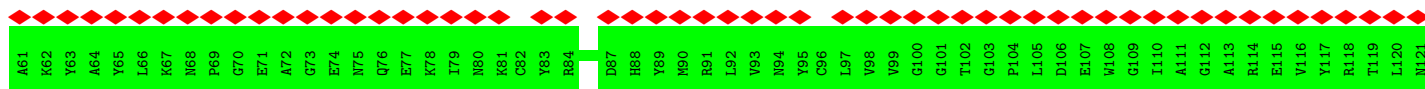
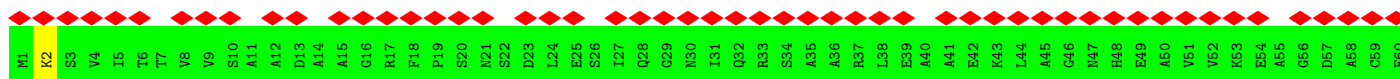




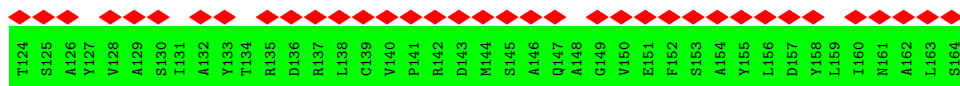
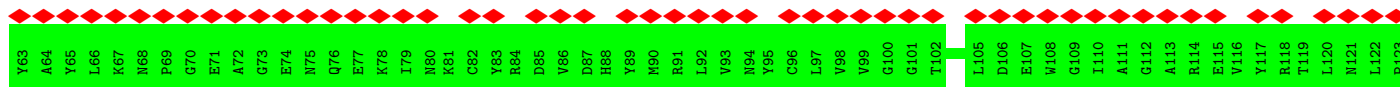
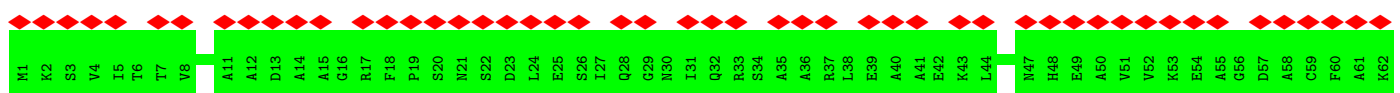
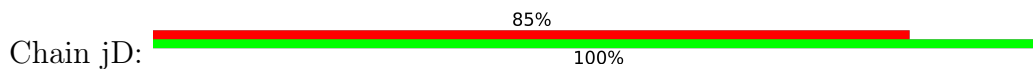
• Molecule 3: Phycoerythrin alpha subunit



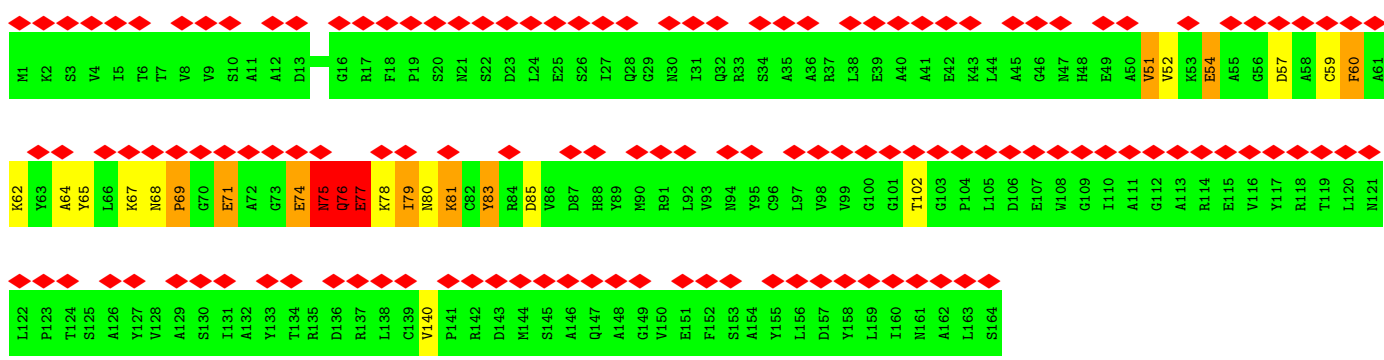
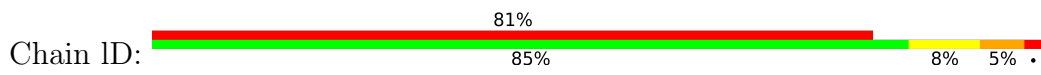
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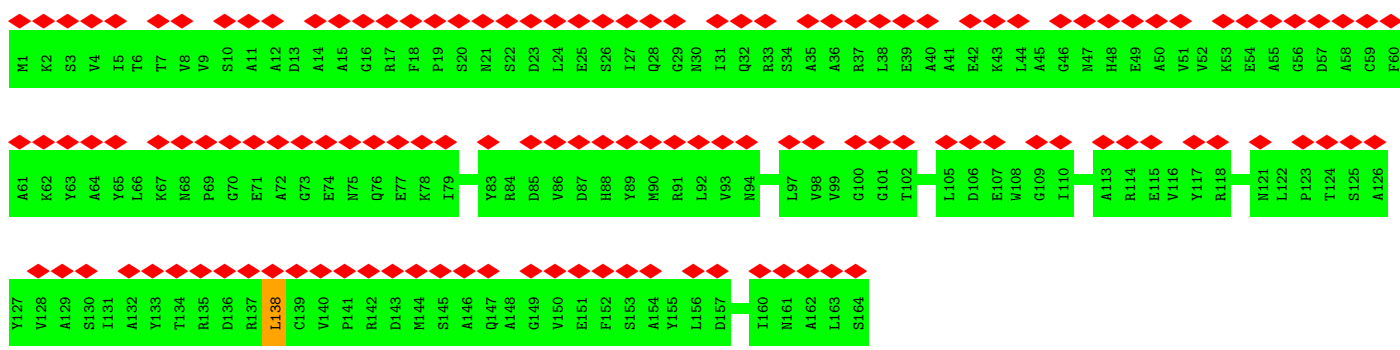
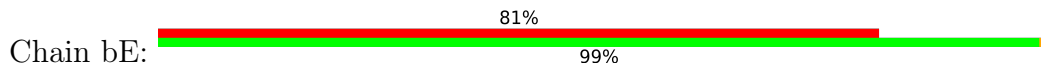
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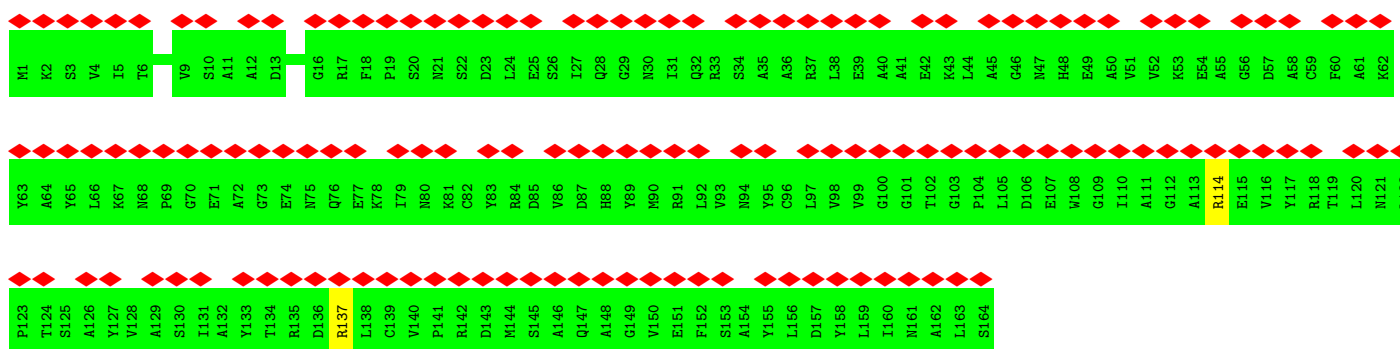
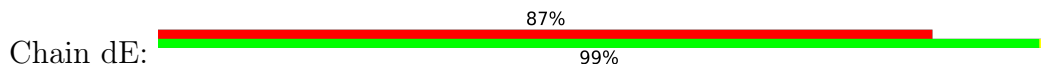
• Molecule 3: Phycoerythrin alpha subunit



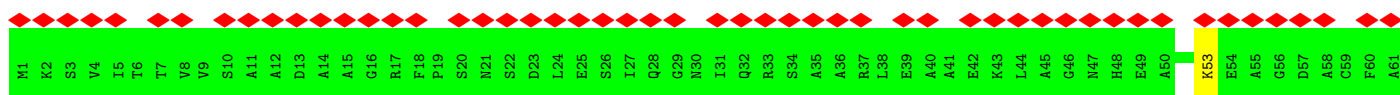
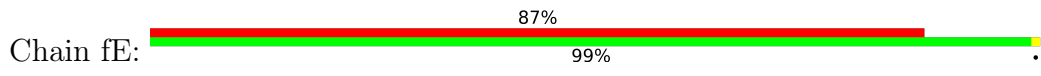
• Molecule 3: Phycoerythrin alpha subunit

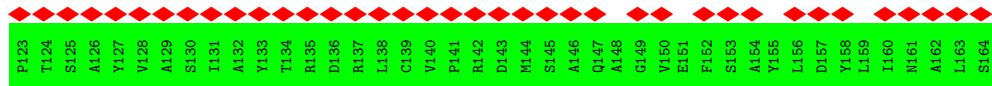
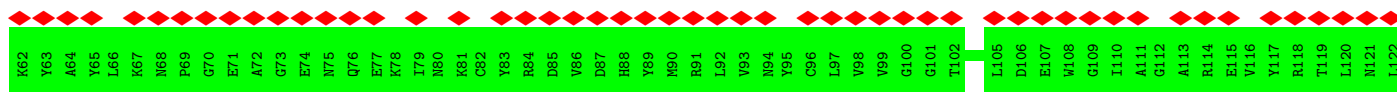


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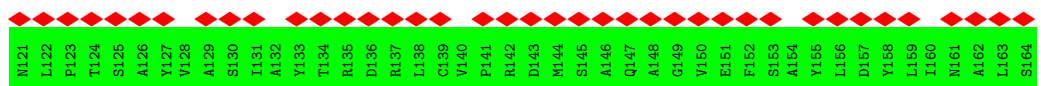
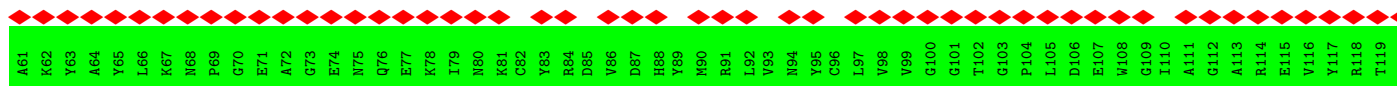
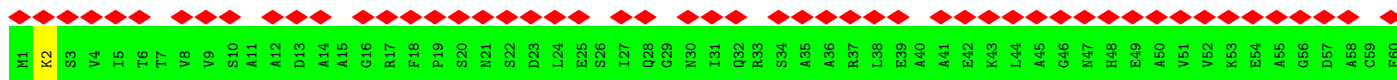
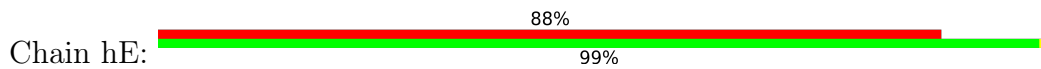


• Molecule 3: Phycoerythrin alpha subunit

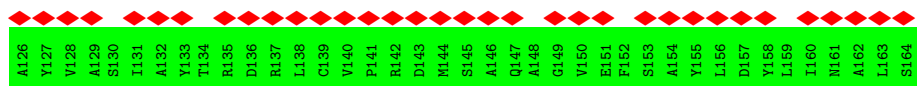
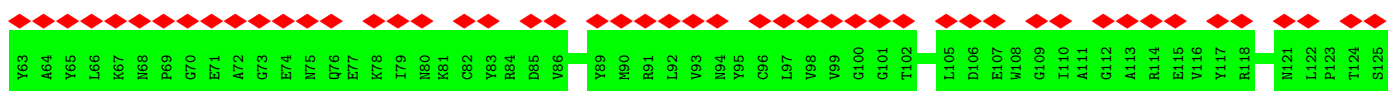
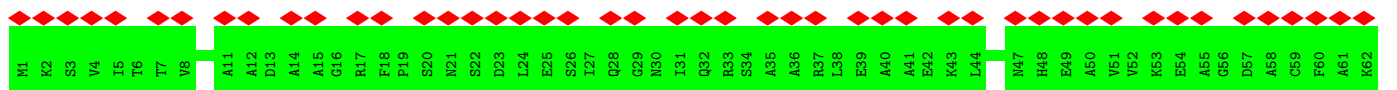
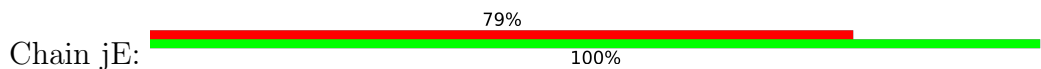




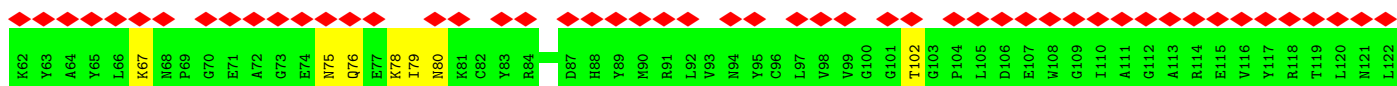
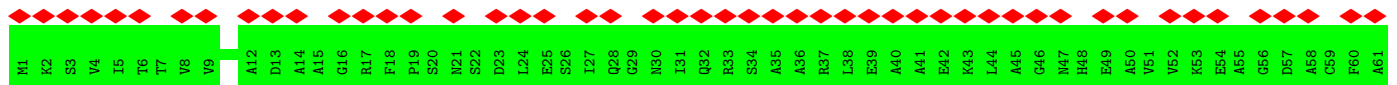
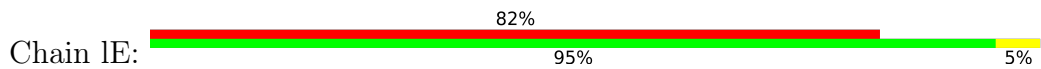
• Molecule 3: Phycoerythrin alpha subunit



• Molecule 3: Phycoerythrin alpha subunit

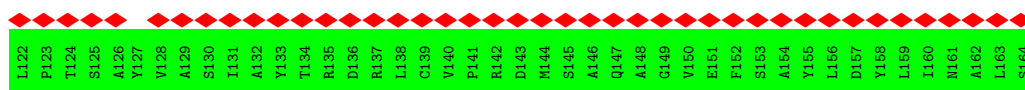
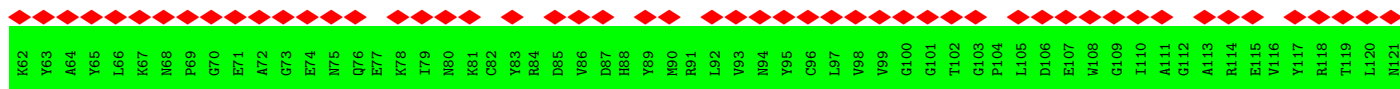
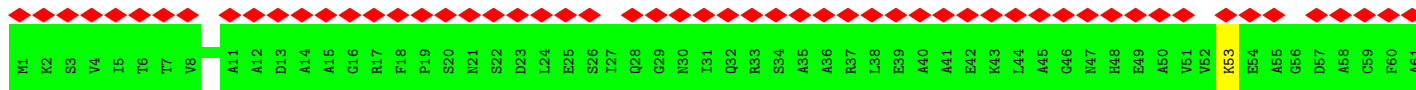


• Molecule 3: Phycoerythrin alpha subunit

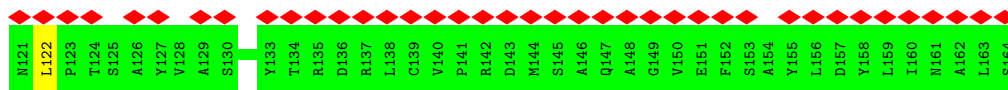
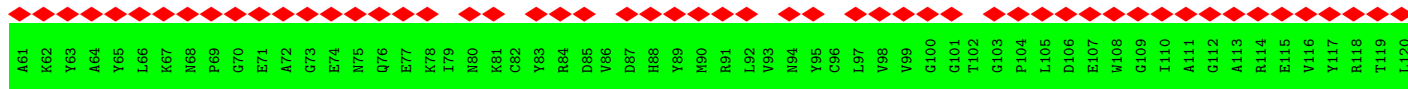
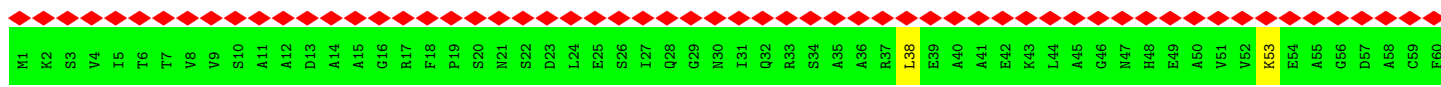




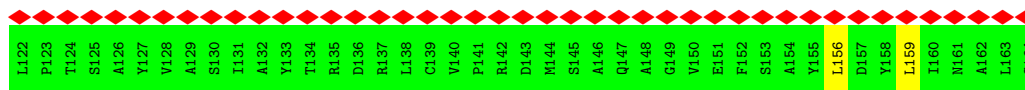
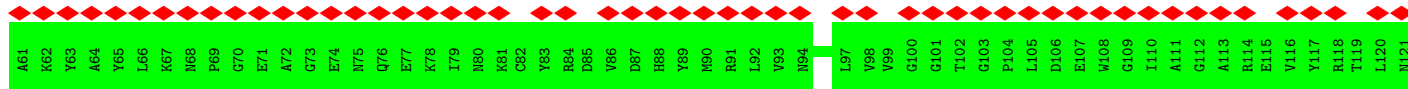
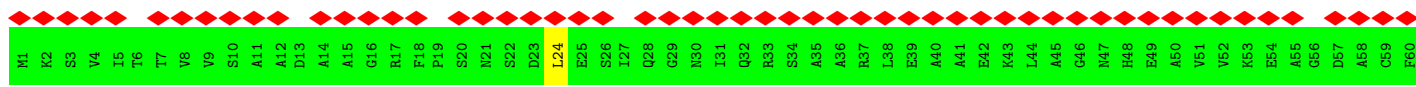
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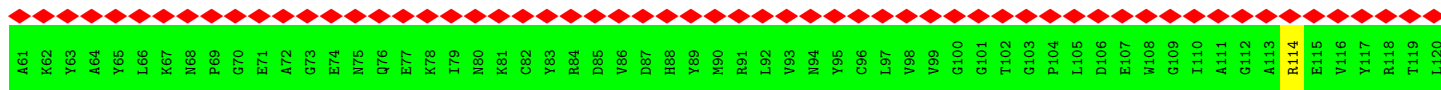
• Molecule 3: Phycoerythrin alpha subunit



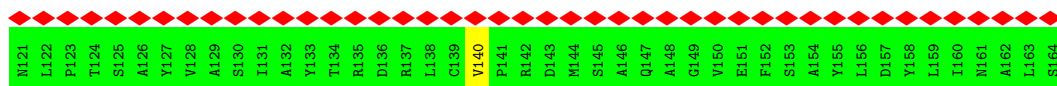
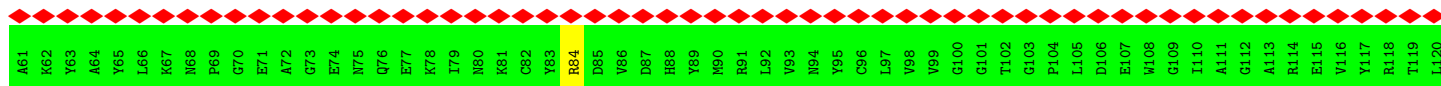
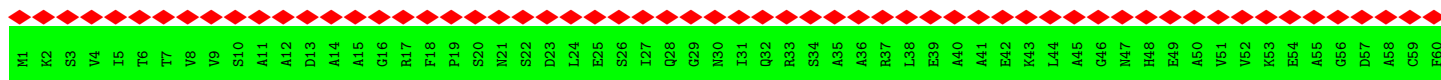
• Molecule 3: Phycoerythrin alpha subunit



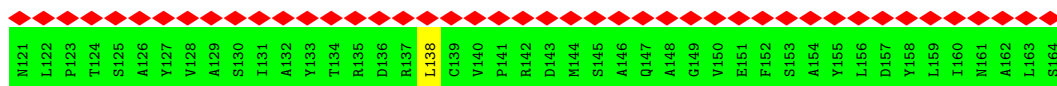
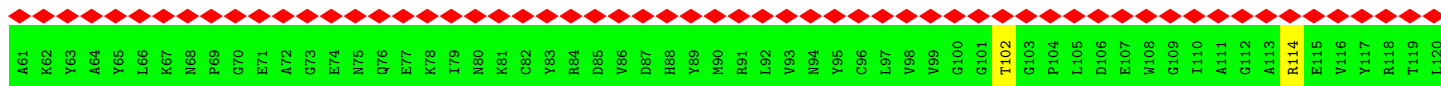
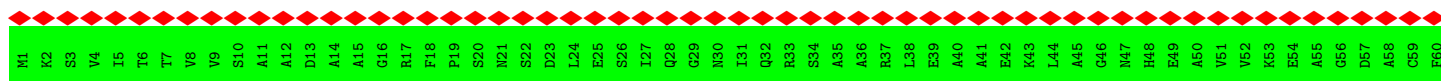
• Molecule 3: Phycoerythrin alpha subunit



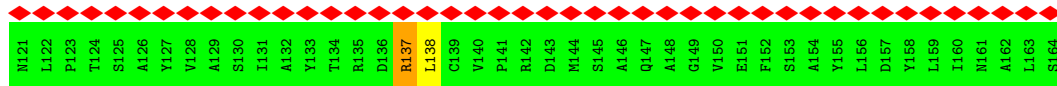
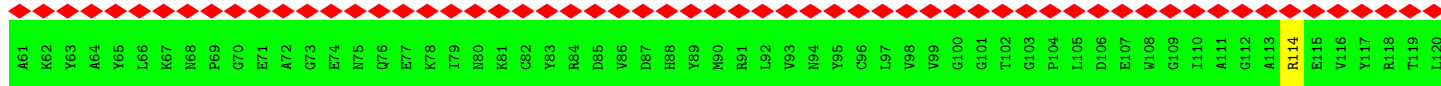
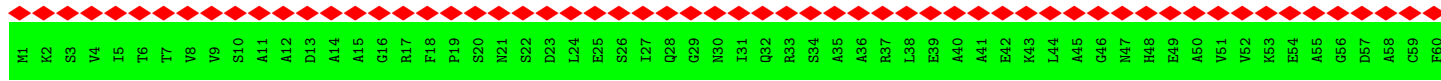
• Molecule 3: Phycoerythrin alpha subunit



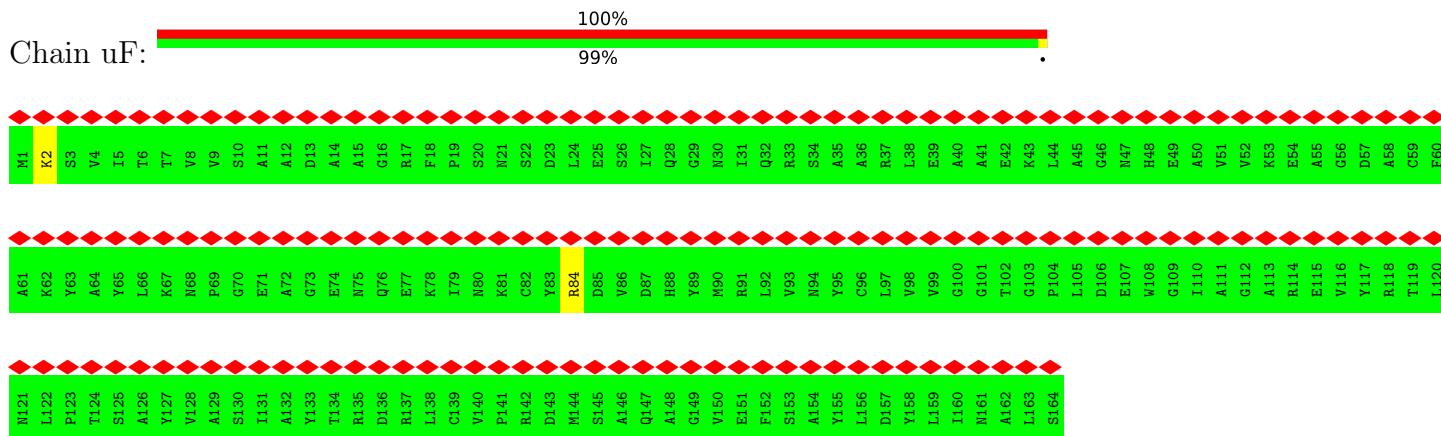
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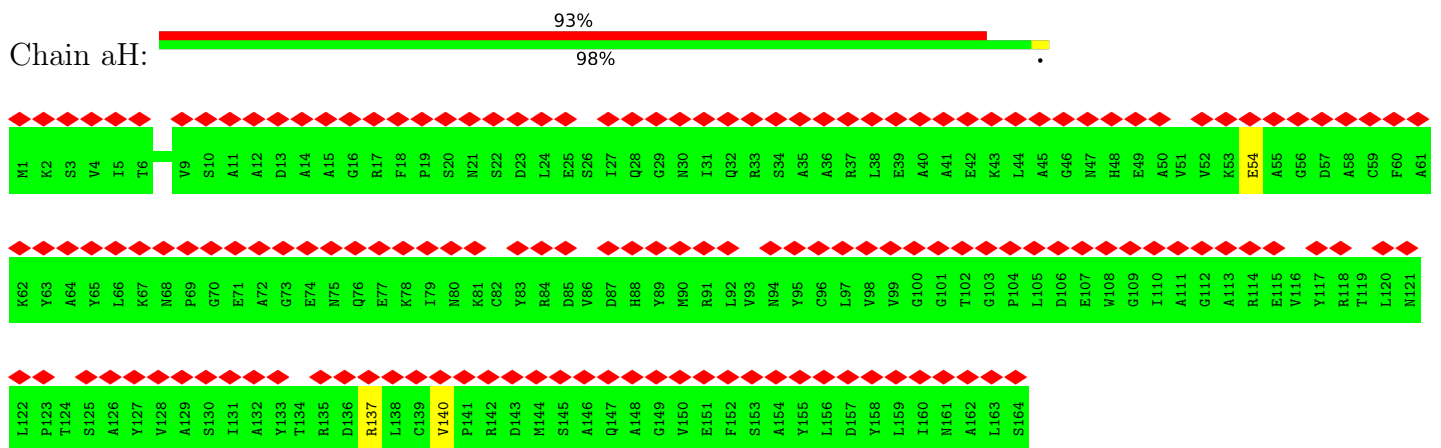
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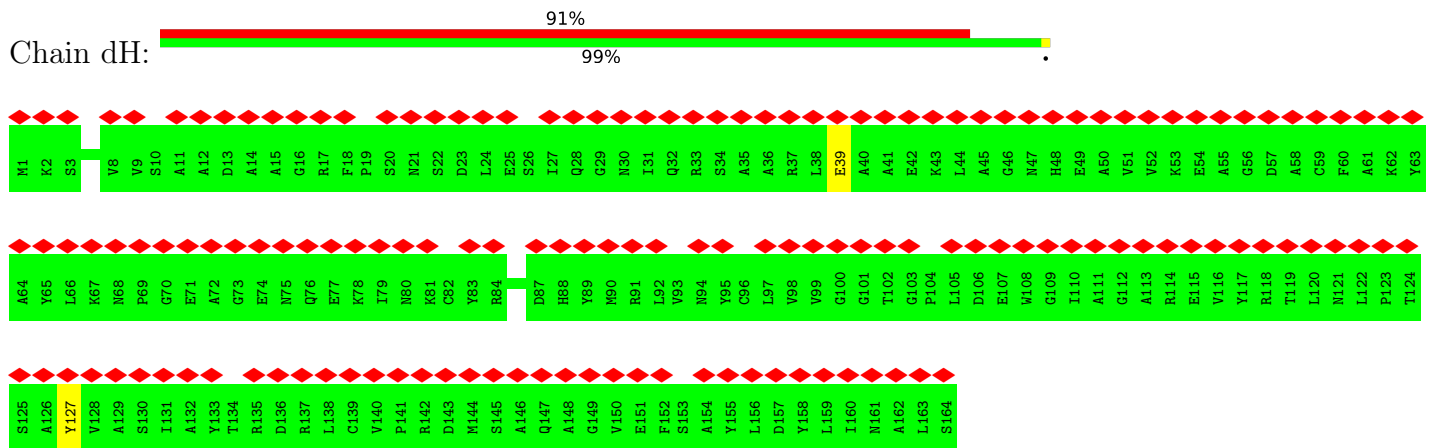
• Molecule 3: Phycoerythrin alpha subunit



• Molecule 3: Phycoerythrin alpha subunit

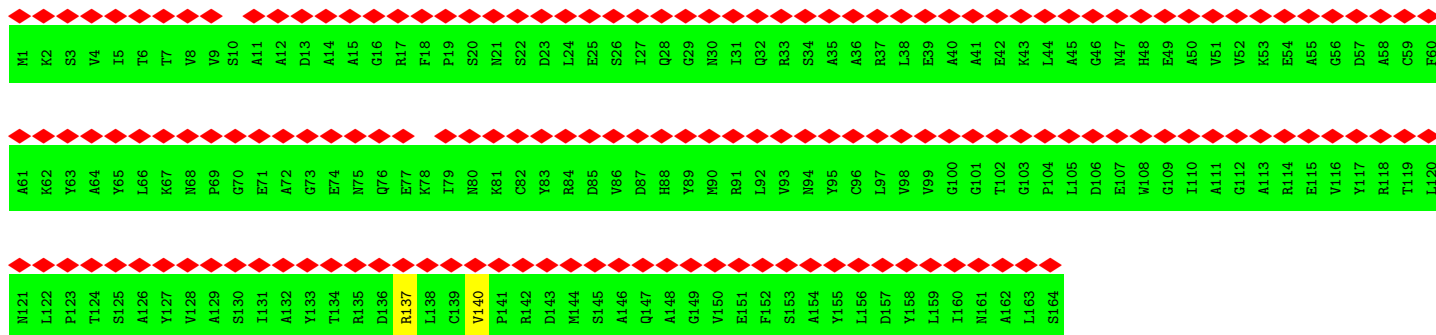


• Molecule 3: Phycoerythrin alpha subunit

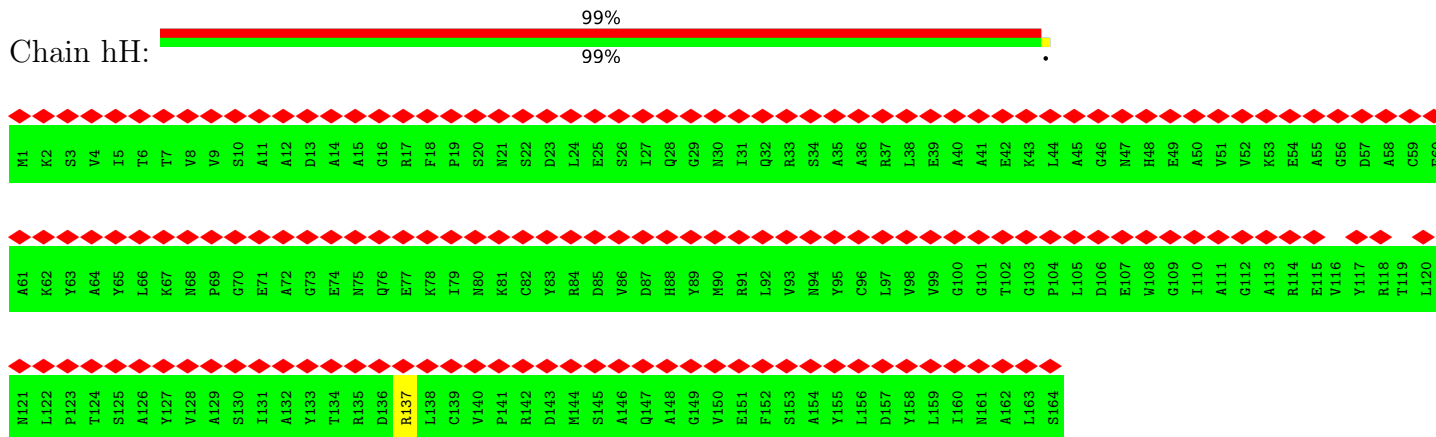


• Molecule 3: Phycoerythrin alpha subunit

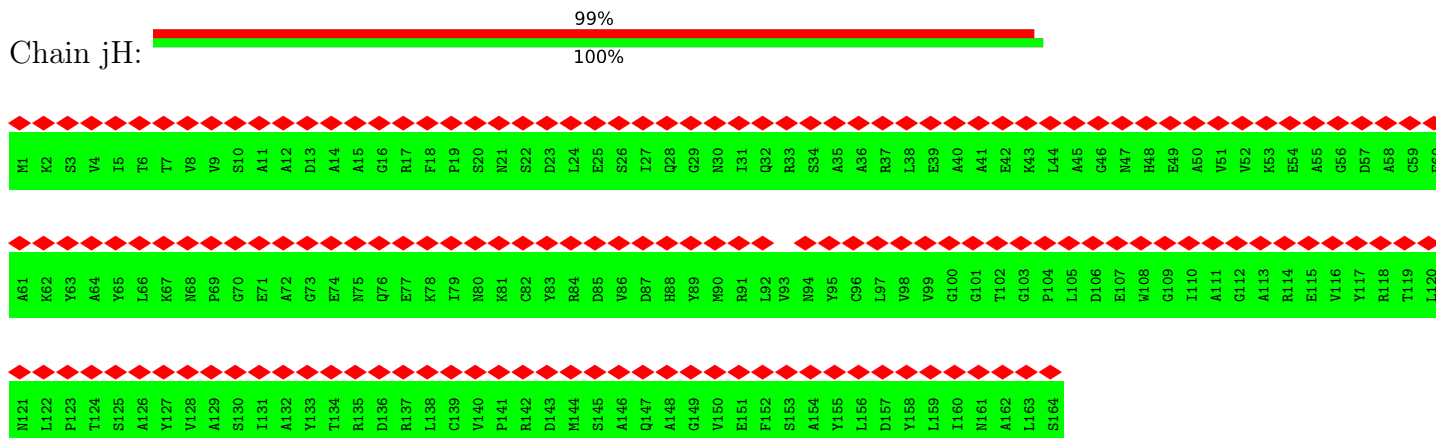




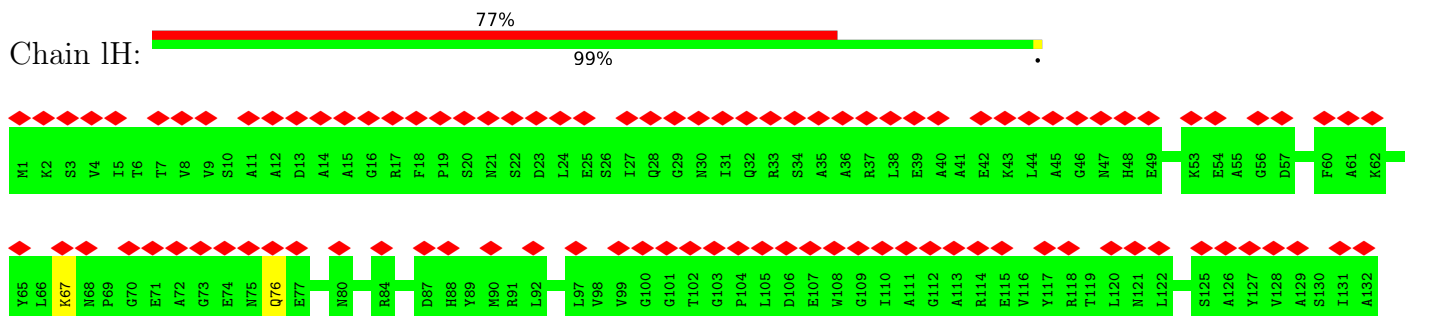
• Molecule 3: Phycoerythrin alpha subunit

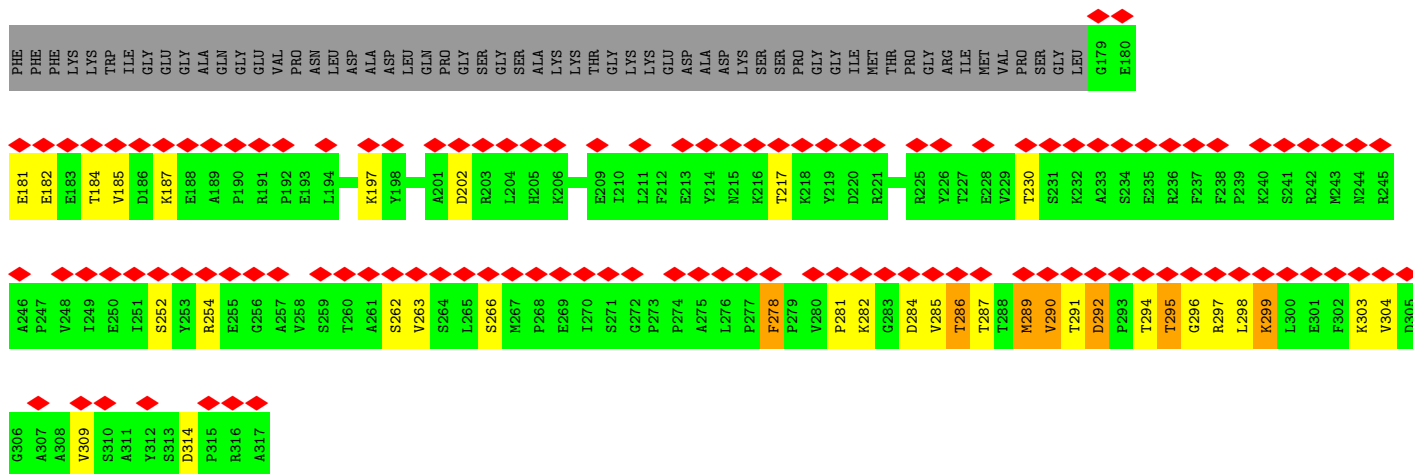


• Molecule 3: Phycoerythrin alpha subunit

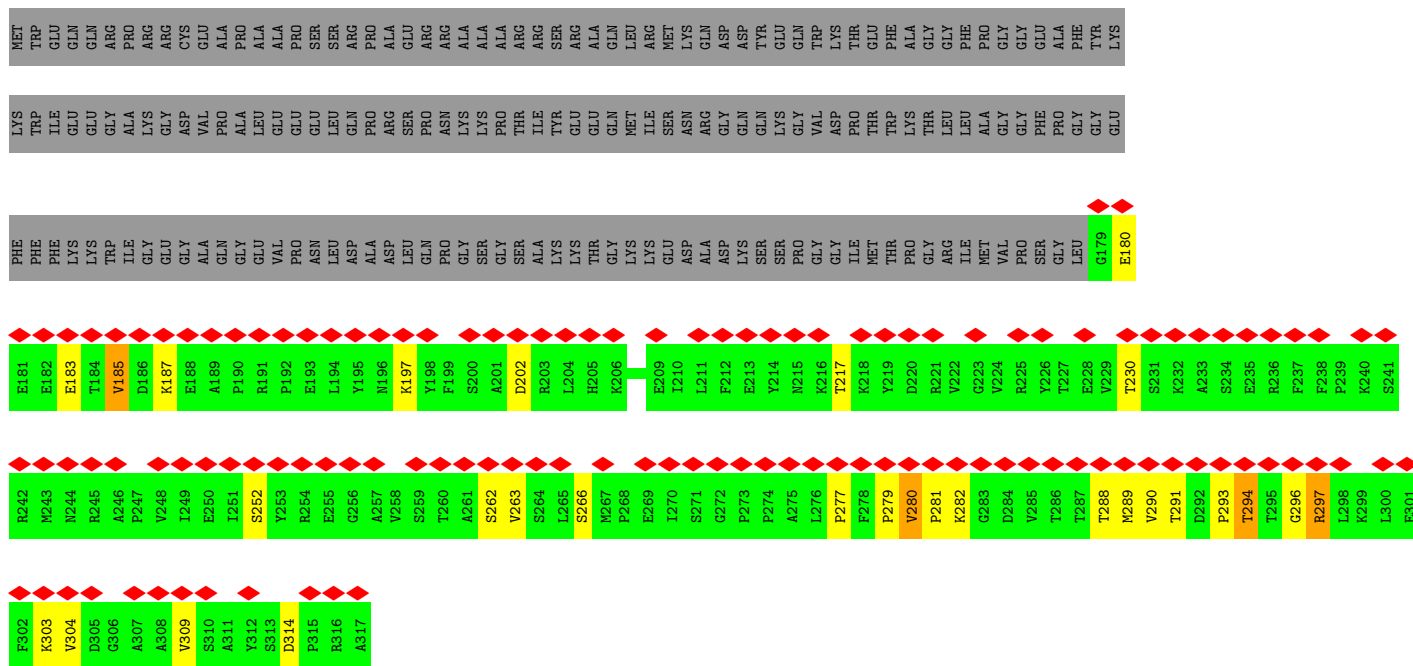
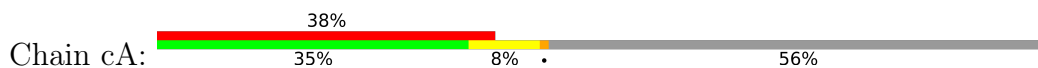


• Molecule 3: Phycoerythrin alpha subunit

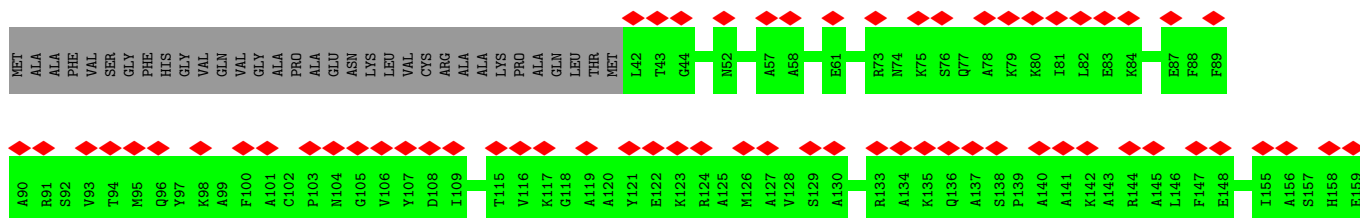
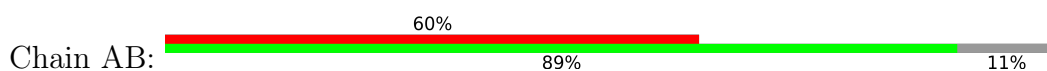


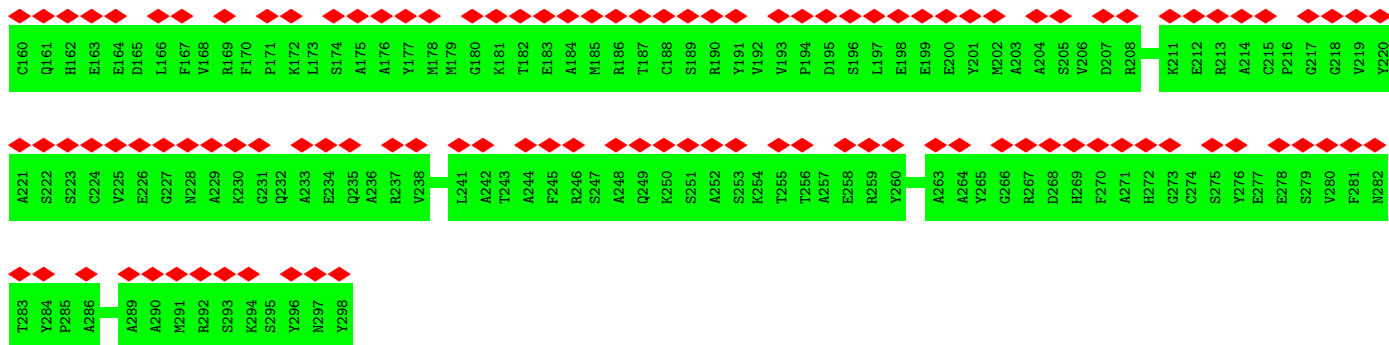


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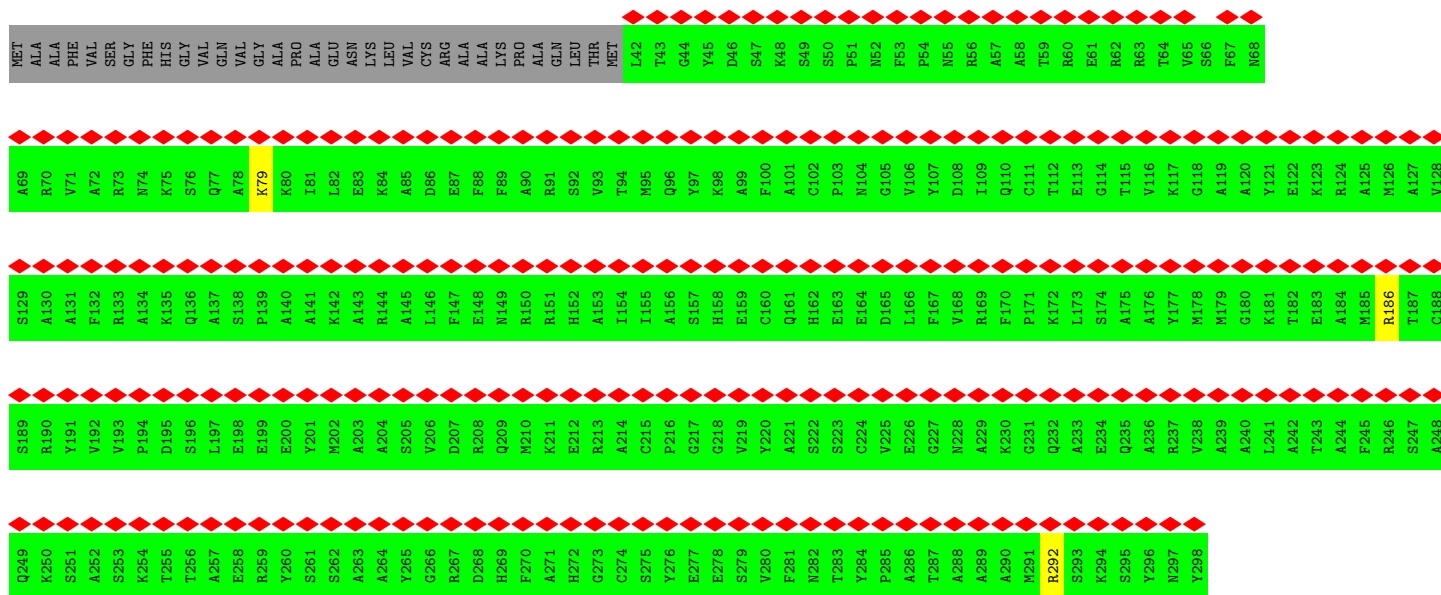
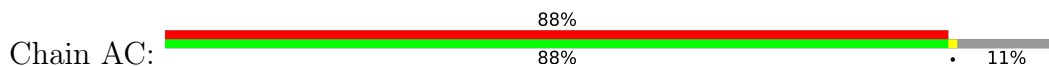


• Molecule 6: R-phycoerythrin gamma chain, chloroplastic

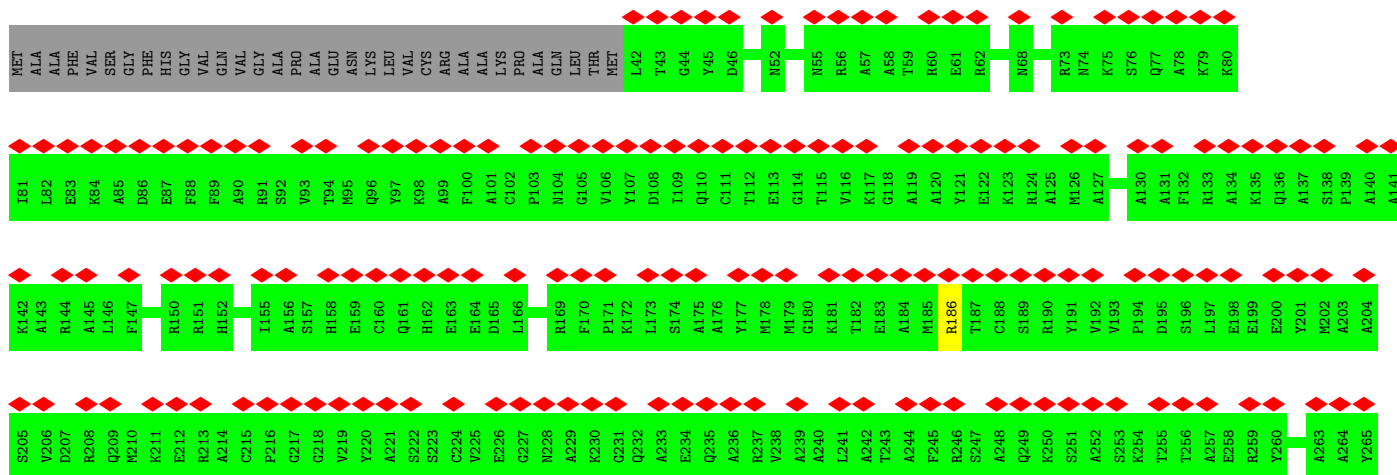
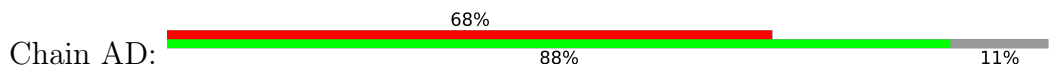


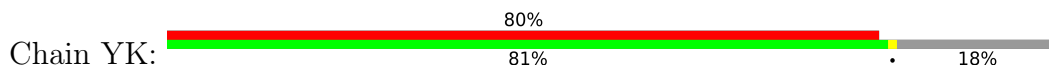


• Molecule 6: R-phycoerythrin gamma chain, chloroplastic



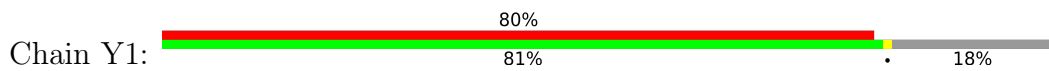
• Molecule 6: R-phycoerythrin gamma chain, chloroplastic





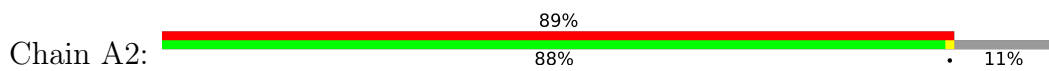
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A69	R70	V71	A72	R73	N74	K75	S76	Q77	A78	K79	K80	I81	L82	E83	K84	A85	D86	E87	F88	F89	A90	R91	S92	V93	T94	M95	Q96	Y97	K98	A99	F100	A101	C102	P103	N104	G105	V106	Y107	D108	I109	Q110	C111	T112	E113	G114	T115	V116	K117	G118	A119	A120	Y121	E122	K123	R124	A125	M126	A127	V128	
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• Molecule 6: R-phycoerythrin gamma chain, chloroplastic

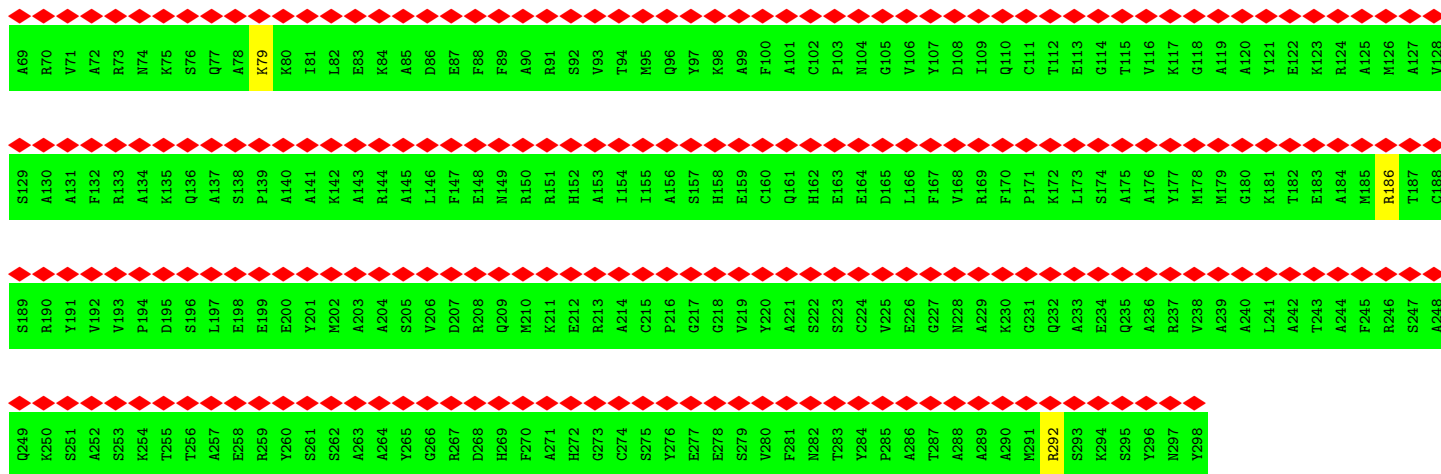


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A69	R70	V71	A72	R73	N74	K75	S76	Q77	A78	K79	K80	I81	L82	E83	K84	A85	D86	E87	F88	F89	A90	R91	S92	V93	T94	M95	Q96	Y97	K98	A99	F100	A101	C102	P103	N104	G105	V106	Y107	D108	I109	Q110	C111	T112	E113	G114	T115	V116	K117	G118	A119	A120	Y121	E122	K123	R124	A125	M126	A127	V128	
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Q249	K250	S251	A252	S253	K254	T255	T256	A257	E258	R259	Y260	S261	S262	A263	A264	Y265	G266	R267	D268	H269	F270	A271	H272	G273	C274	S275	Y276	E277	E278	S279	V280	F281	N282	T283	Y284	P285	A286	T287	A288	A289	A290	M291	R292	S293	K294	S295	Y296	M297	Y298											

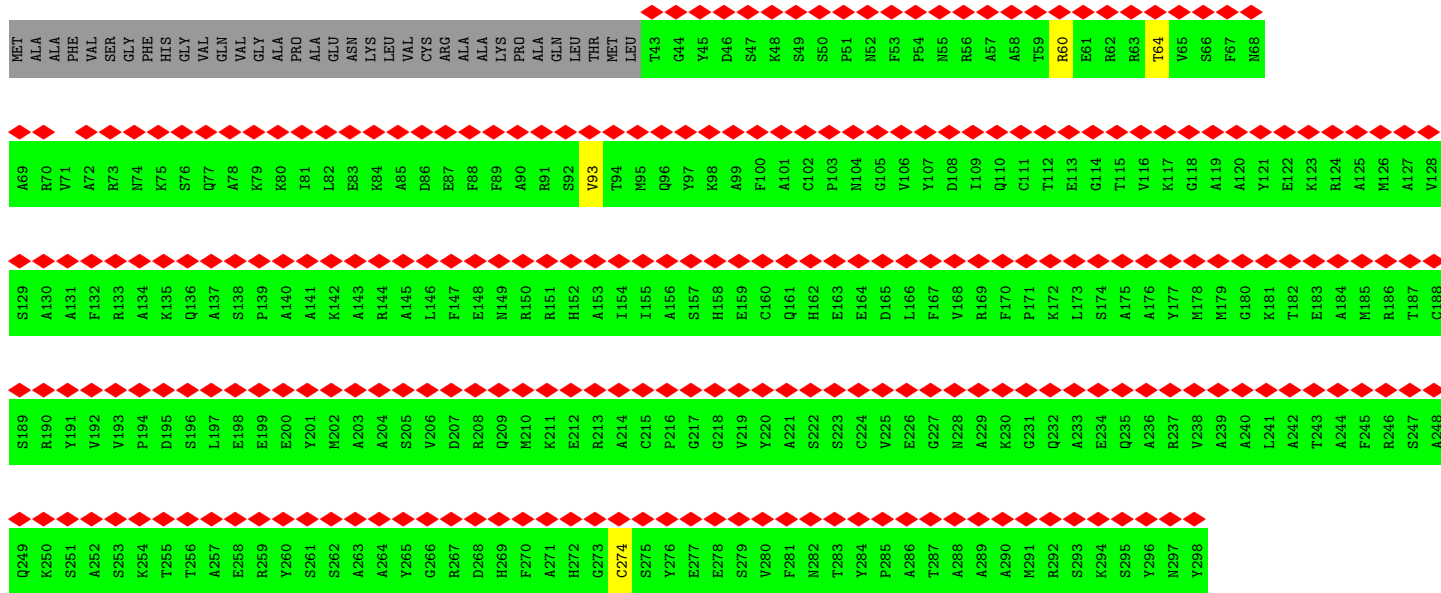
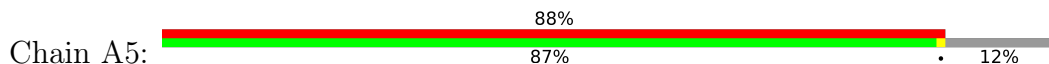
• Molecule 6: R-phycoerythrin gamma chain, chloroplastic



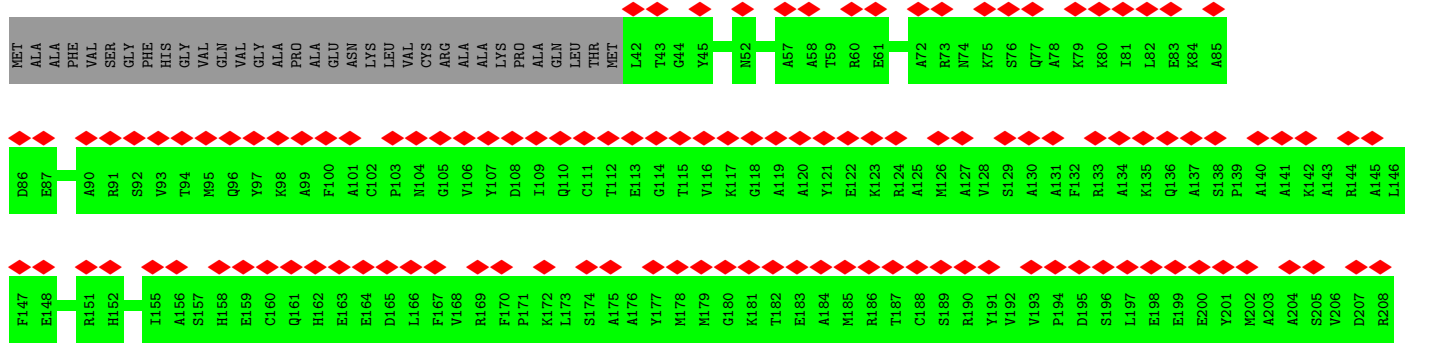
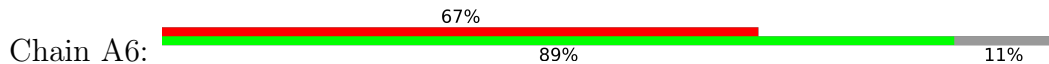
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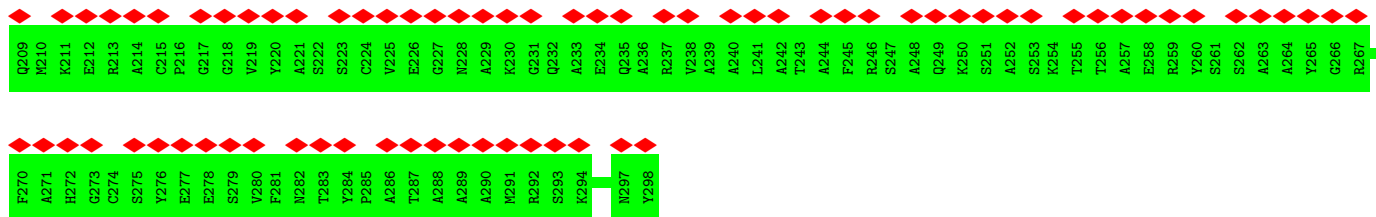


• Molecule 6: R-phycoerythrin gamma chain, chloroplastic

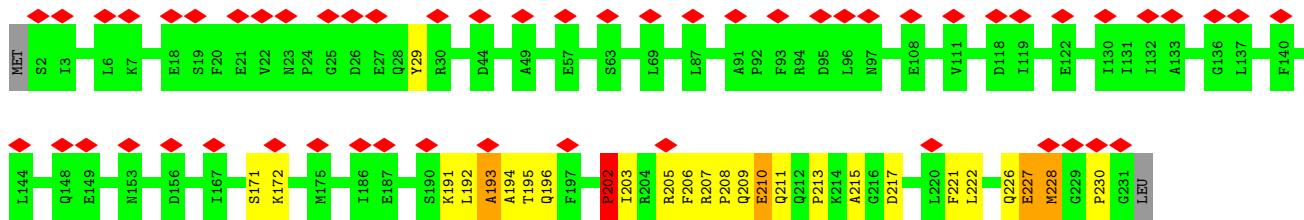
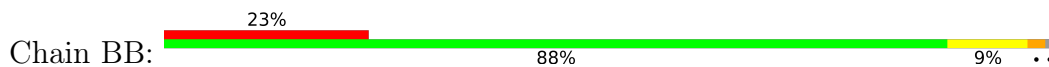


• Molecule 6: R-phycoerythrin gamma chain, chloroplastic

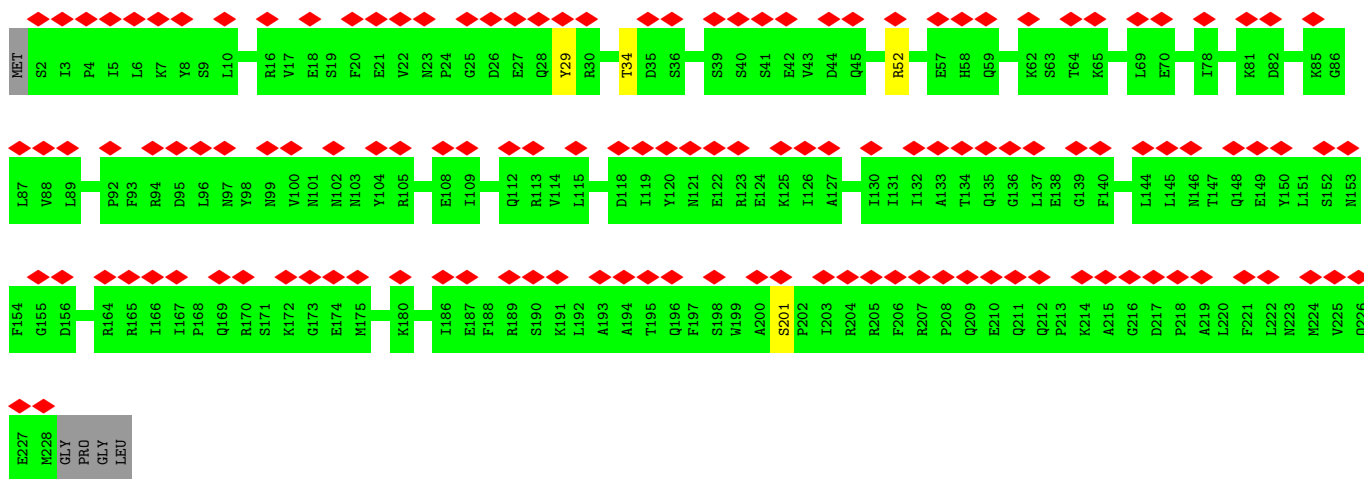




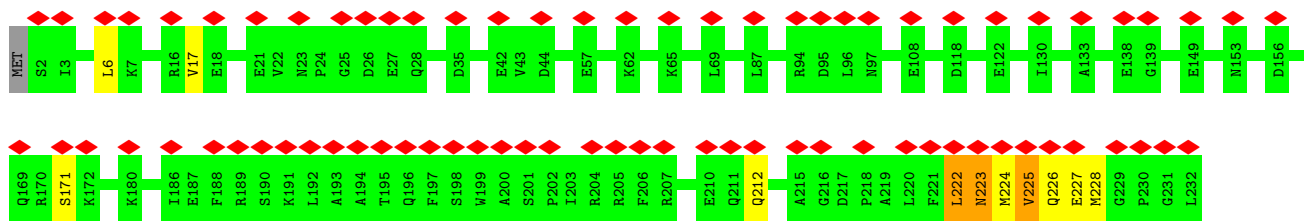
• Molecule 7: Phycobilisome rod-core linker polypeptide



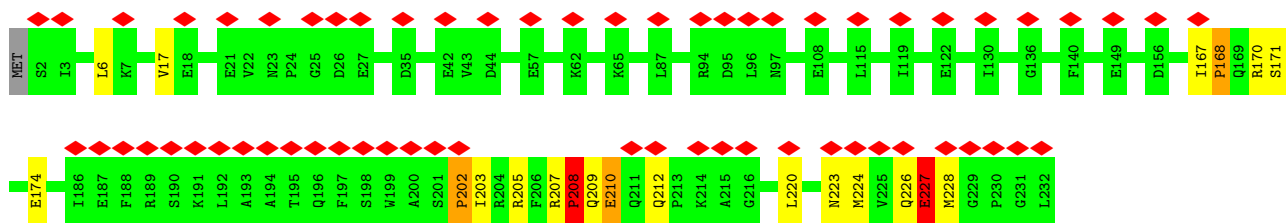
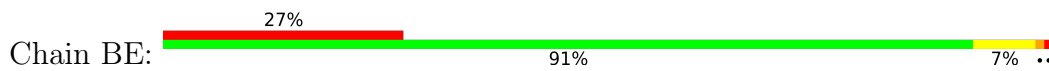
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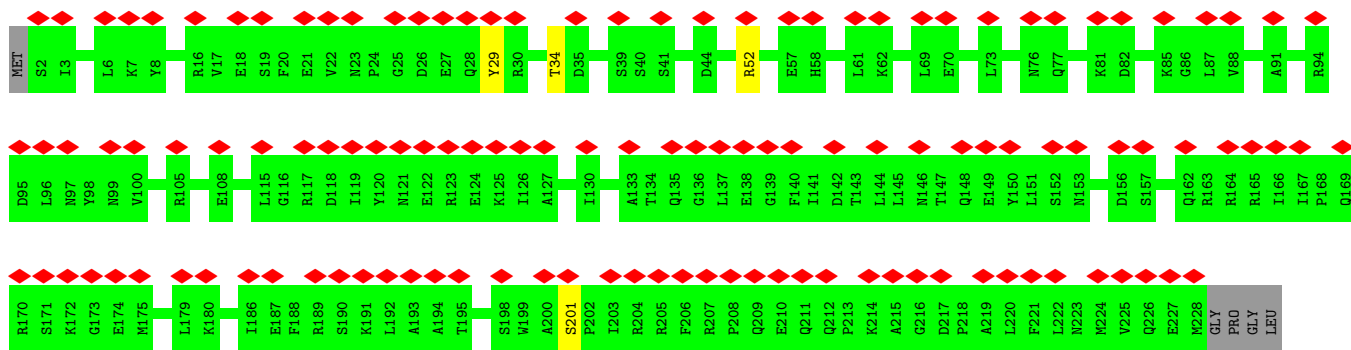
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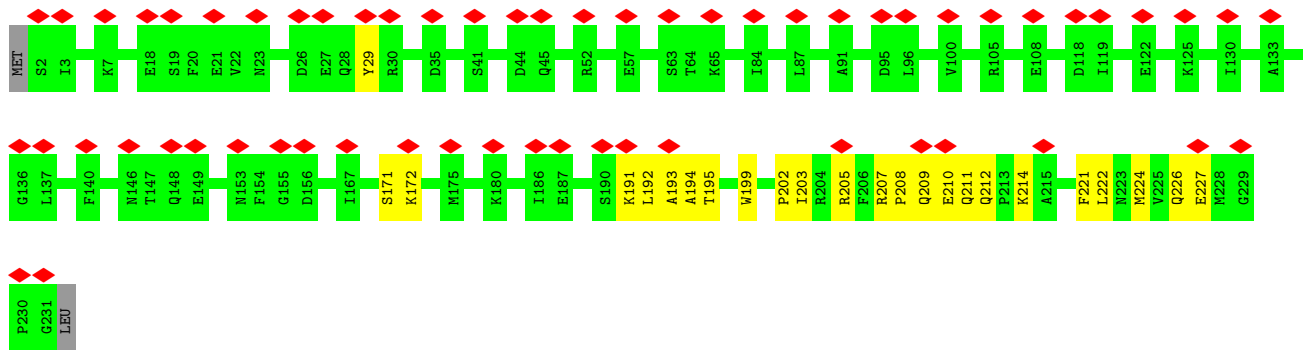
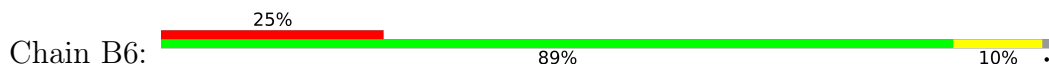
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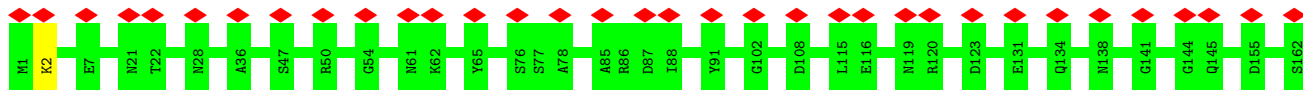
• Molecule 7: Phycobilisome rod-core linker polypeptide



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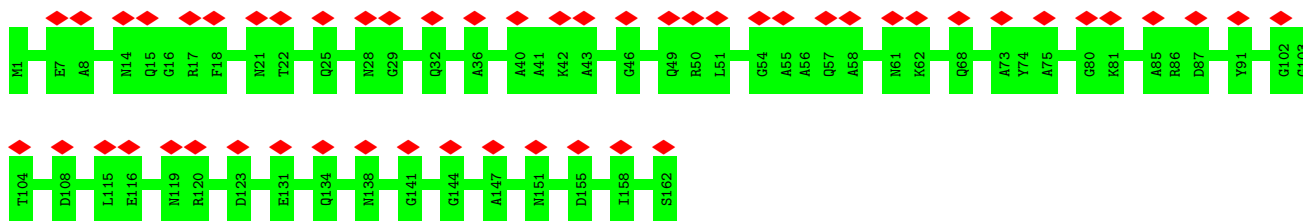


• Molecule 8: C-phycoyanin alpha subunit

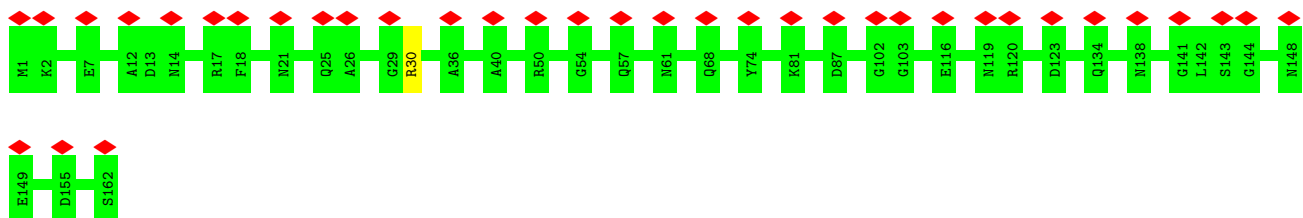


• Molecule 8: C-phycoyanin alpha subunit

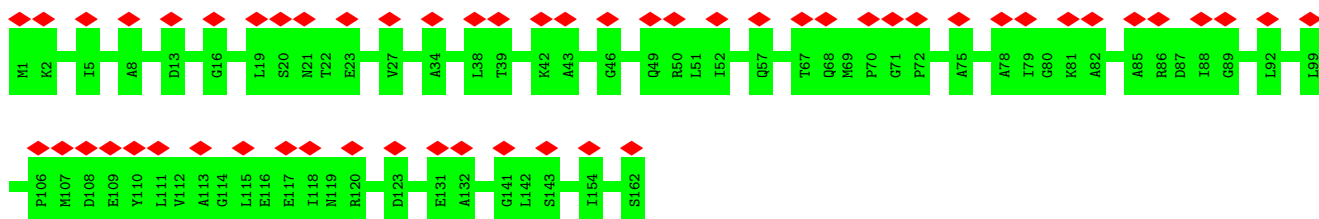




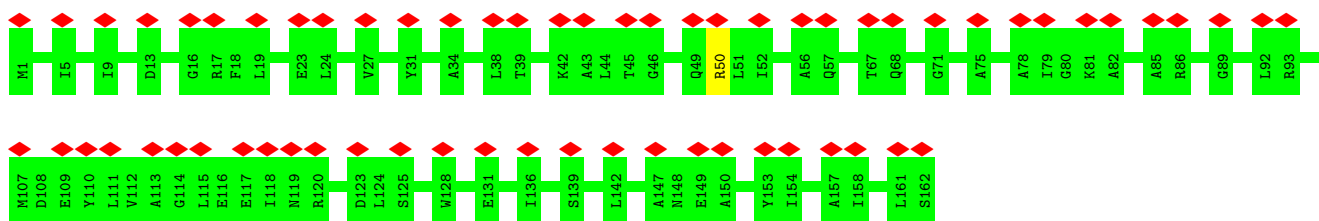
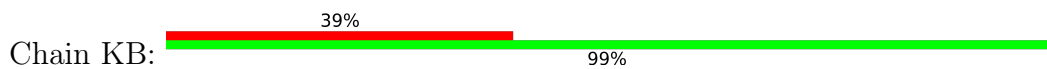
- Molecule 8: C-phycoerythrin alpha subunit



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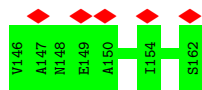


- Molecule 8: C-phycoerythrin alpha subunit

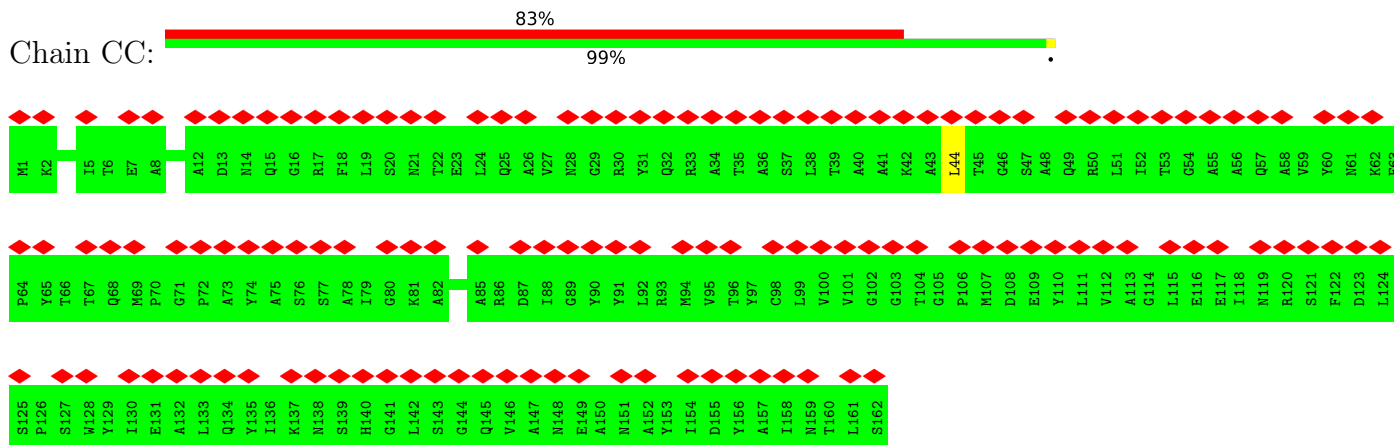


- Molecule 8: C-phycoerythrin alpha subunit

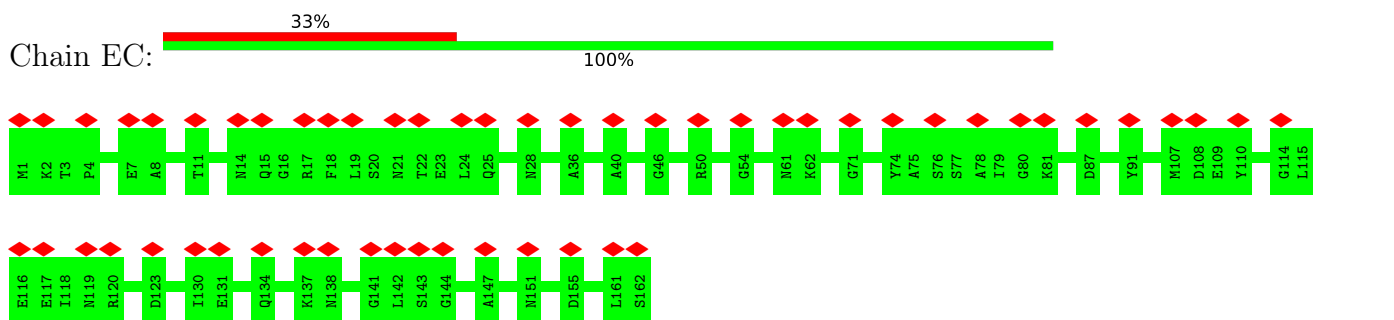




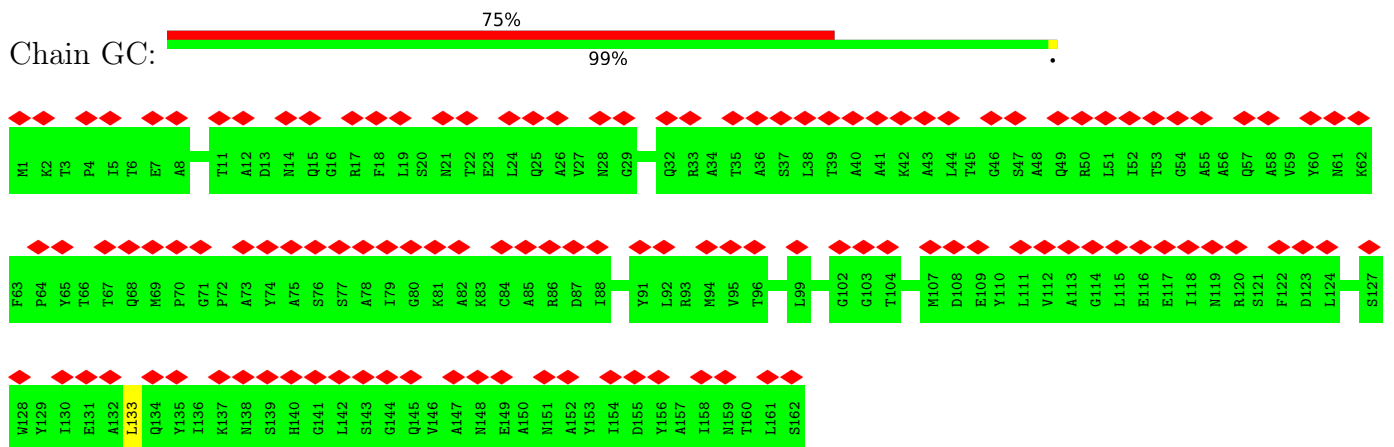
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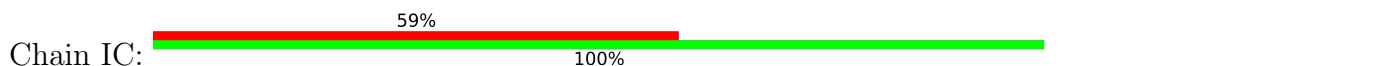
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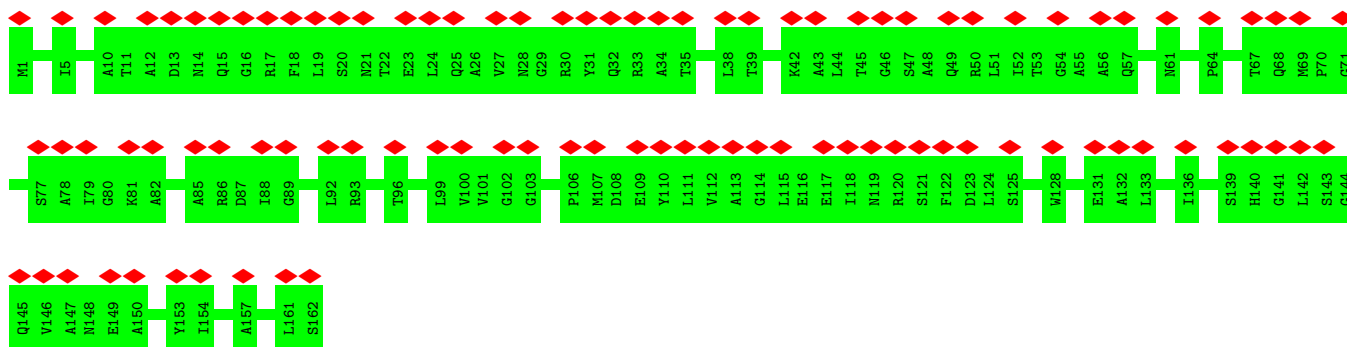


• Molecule 8: C-phycoerythrin alpha subunit

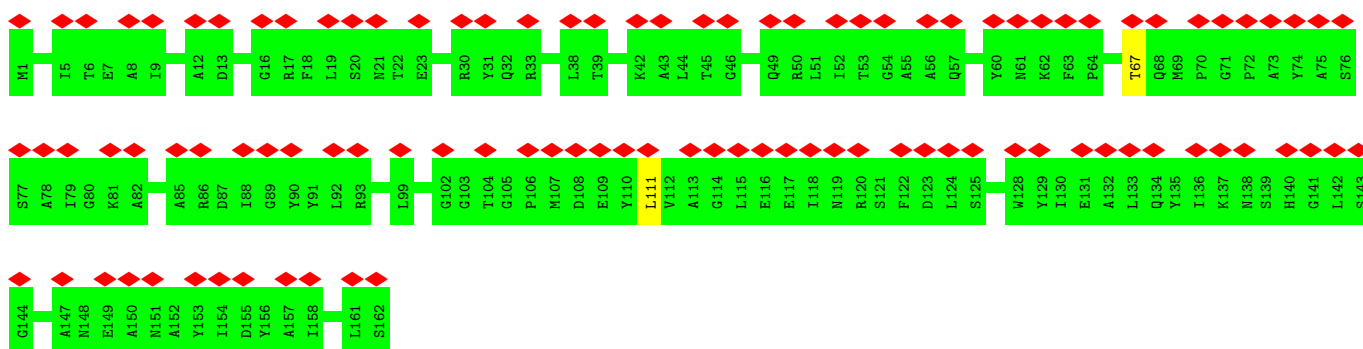


• Molecule 8: C-phycoerythrin alpha subunit

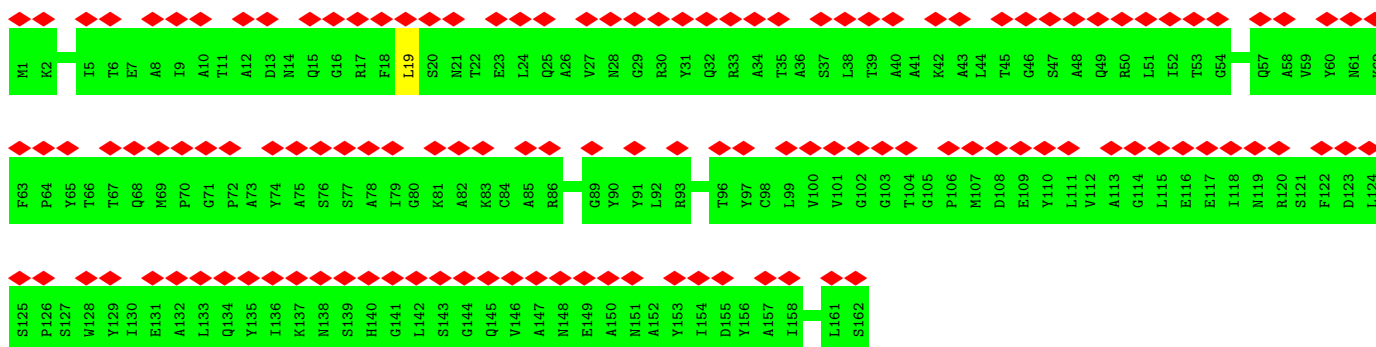
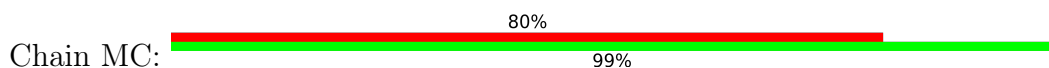




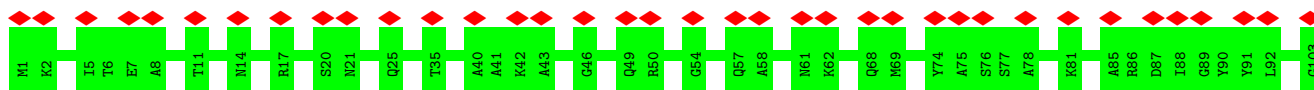
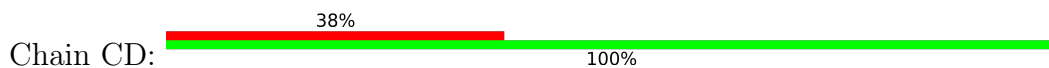
- Molecule 8: C-phycoerythrin alpha subunit

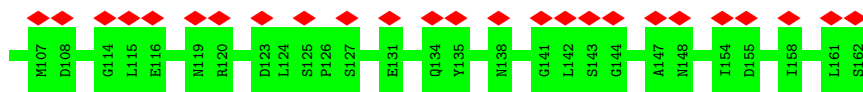


- Molecule 8: C-phycoerythrin alpha subunit

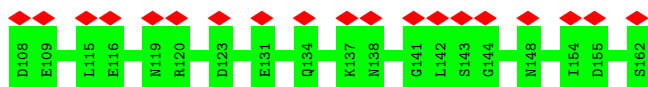
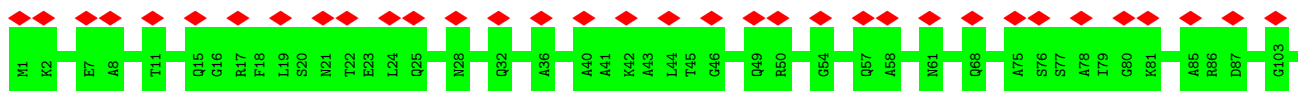


- Molecule 8: C-phycoerythrin alpha subunit

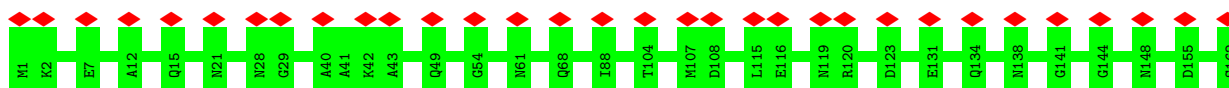




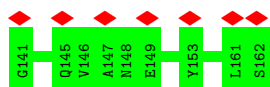
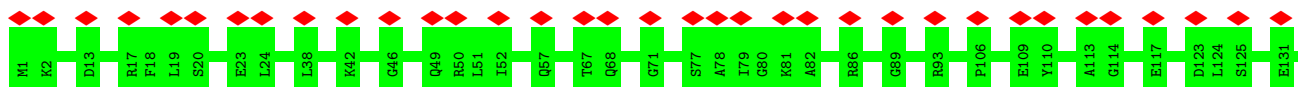
- Molecule 8: C-phycoerythrin alpha subunit



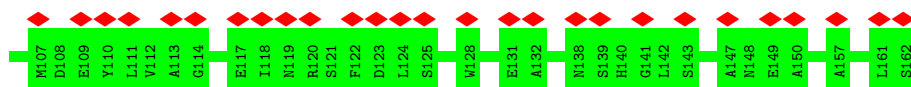
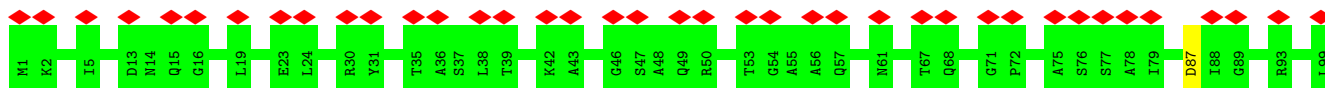
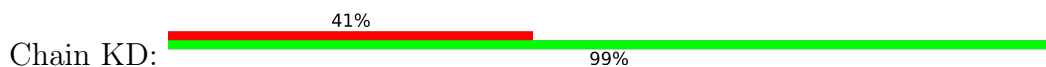
- Molecule 8: C-phycoerythrin alpha subunit



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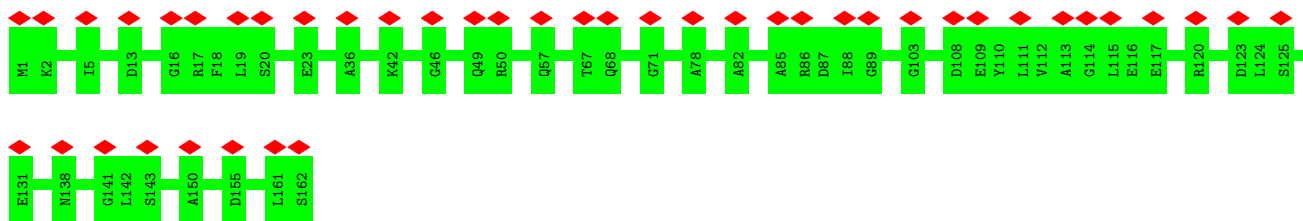


- Molecule 8: C-phycoerythrin alpha subunit

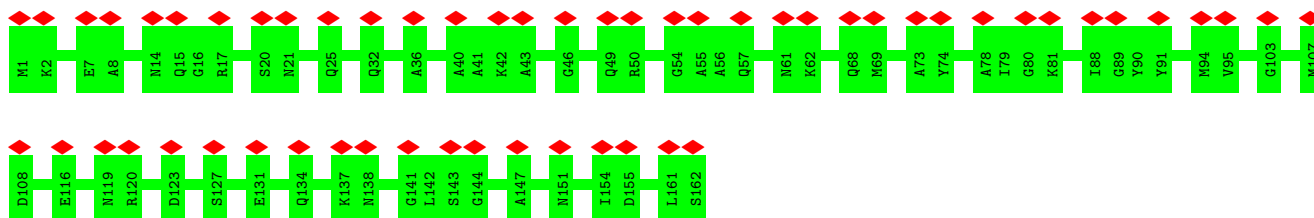


- Molecule 8: C-phycoerythrin alpha subunit

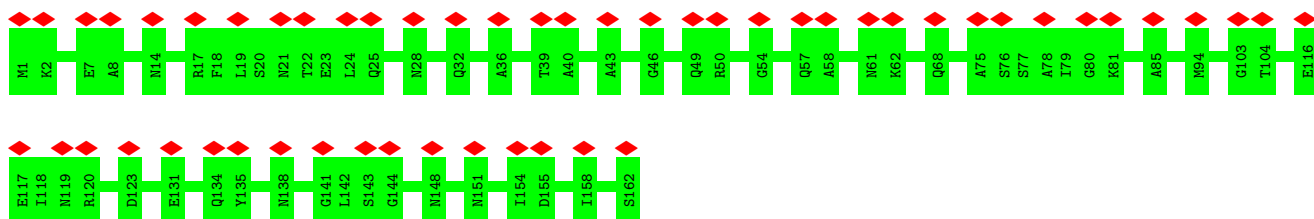




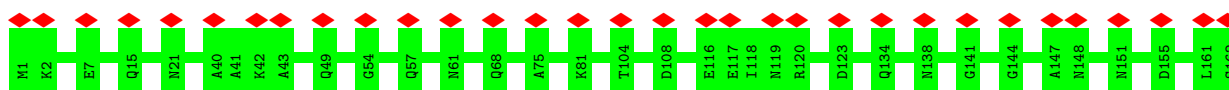
- Molecule 8: C-phycoerythrin alpha subunit



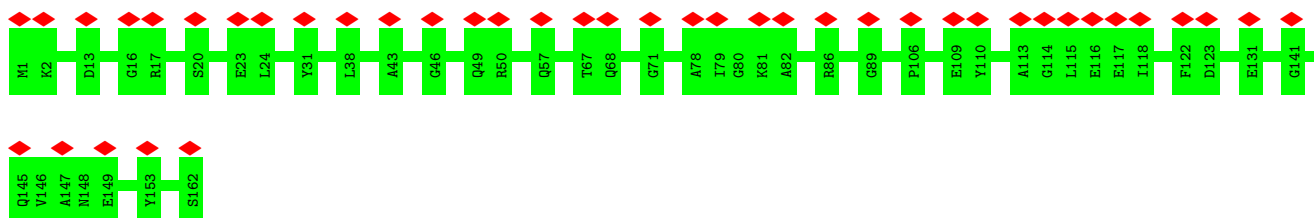
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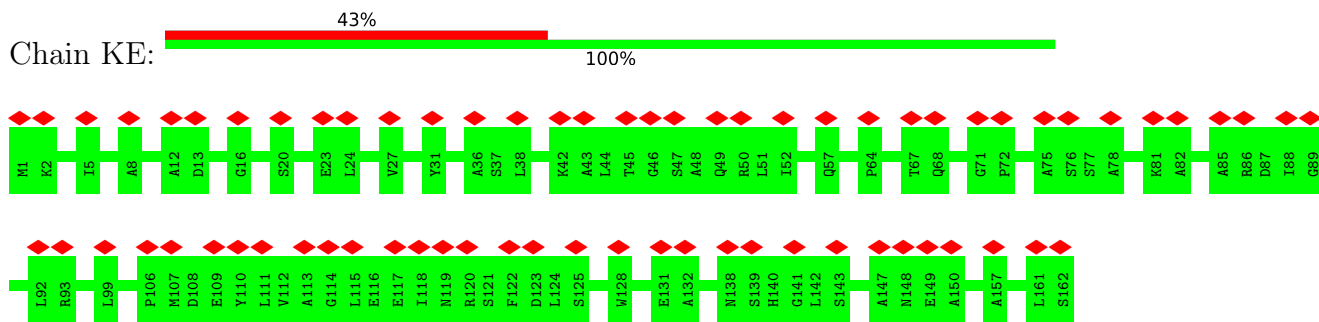
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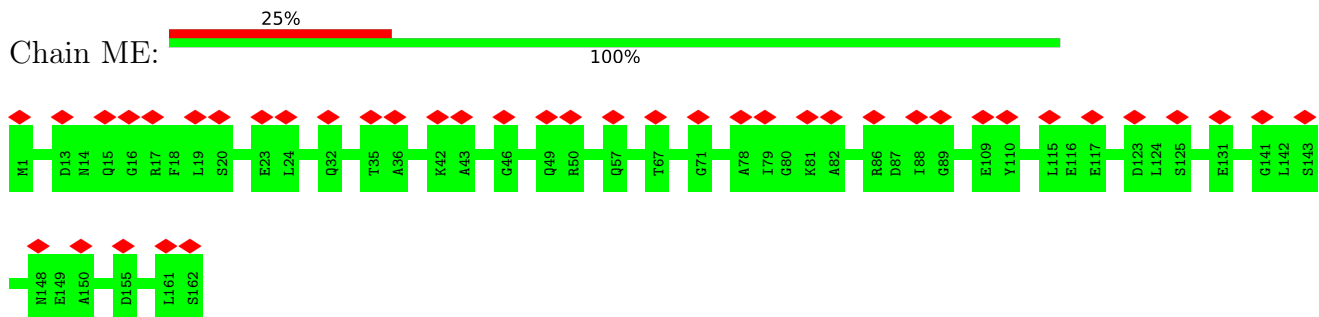
- Molecule 8: C-phycoerythrin alpha subunit



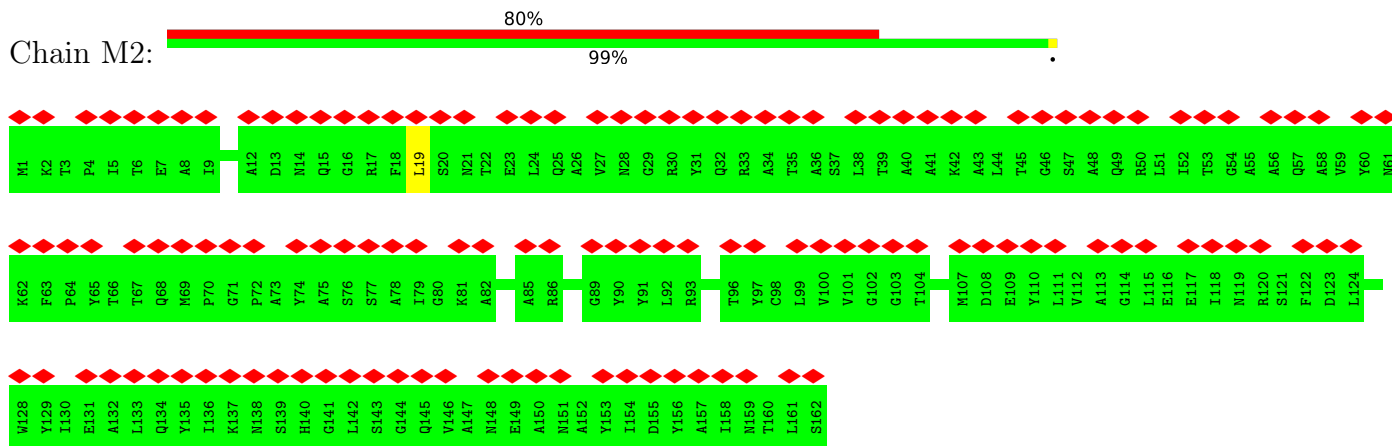
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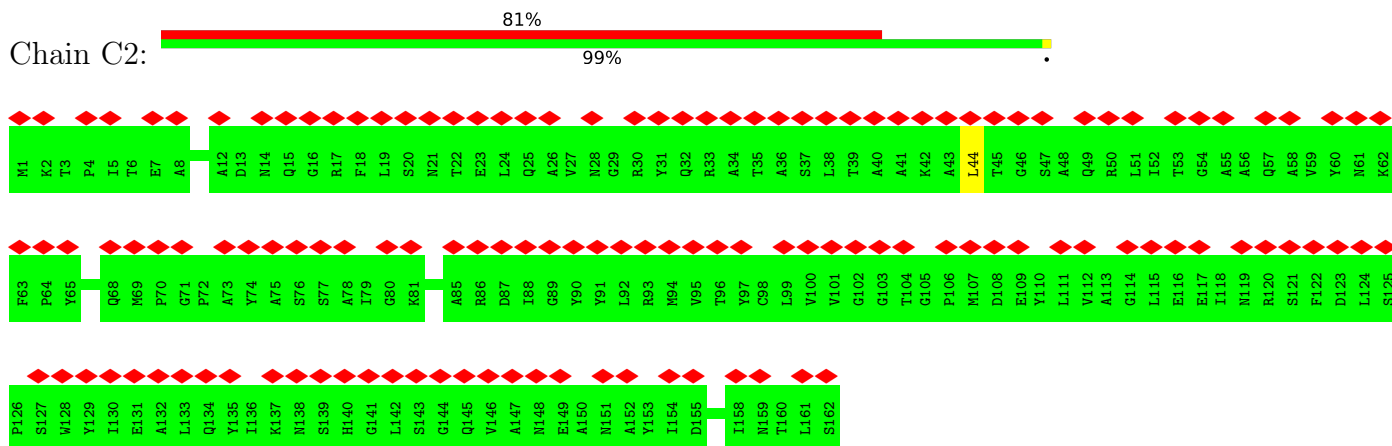
• Molecule 8: C-phycoerythrin alpha subunit



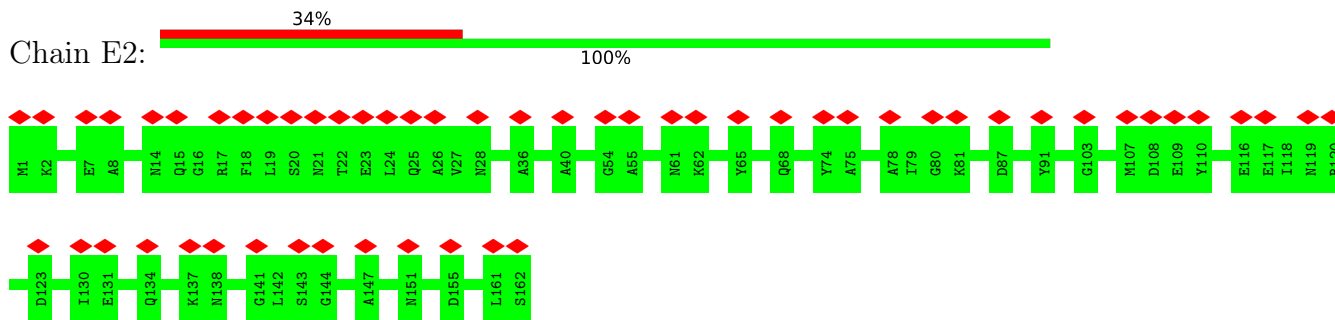
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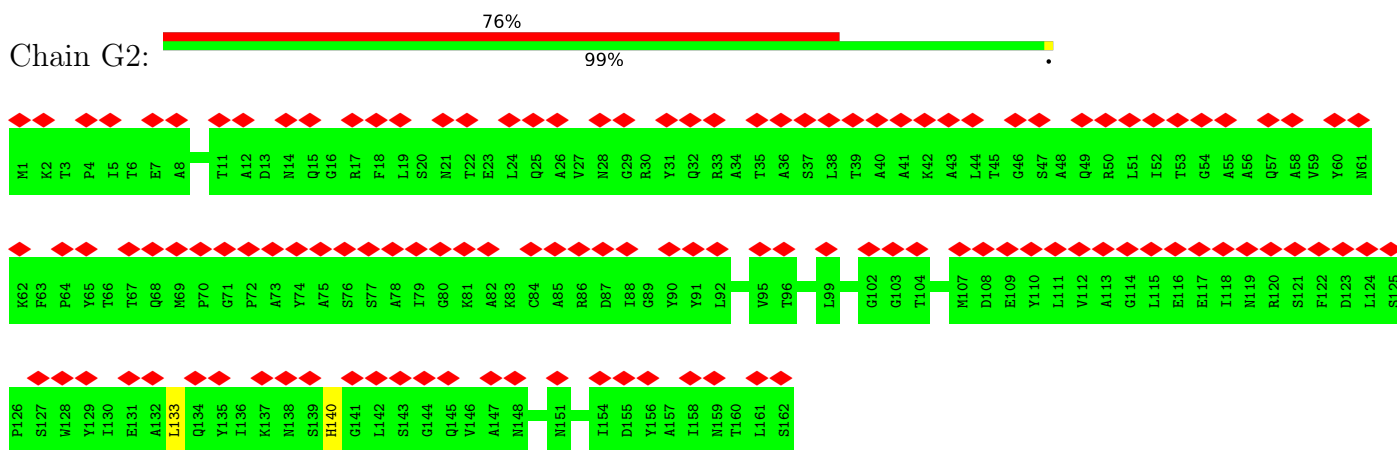
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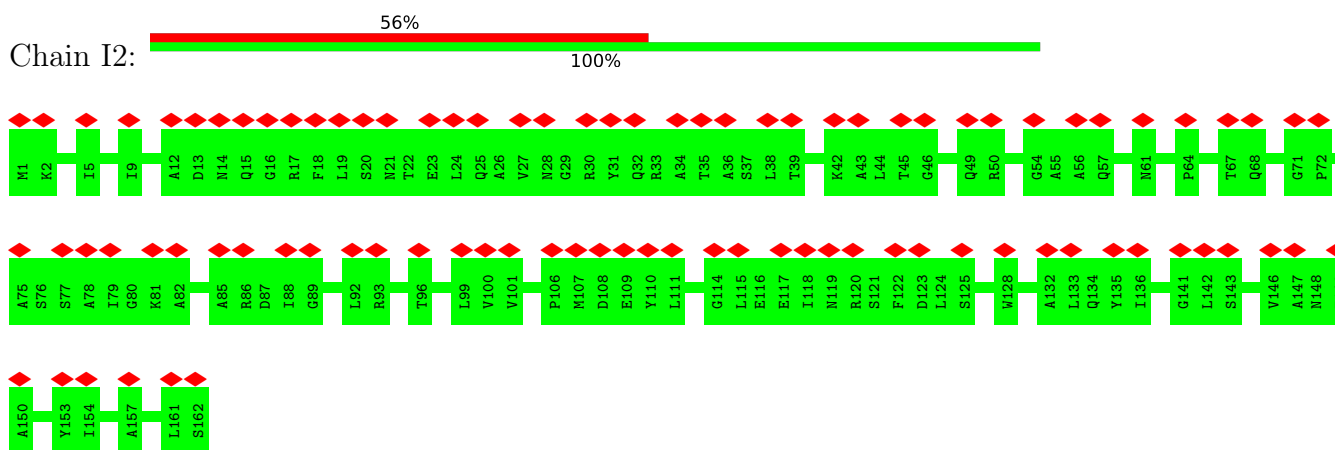
- Molecule 8: C-phycoerythrin alpha subunit



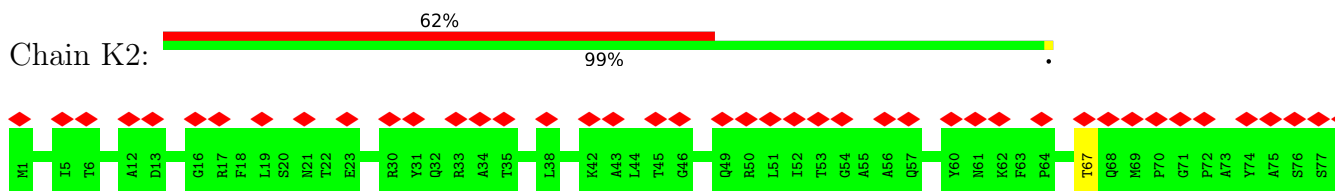
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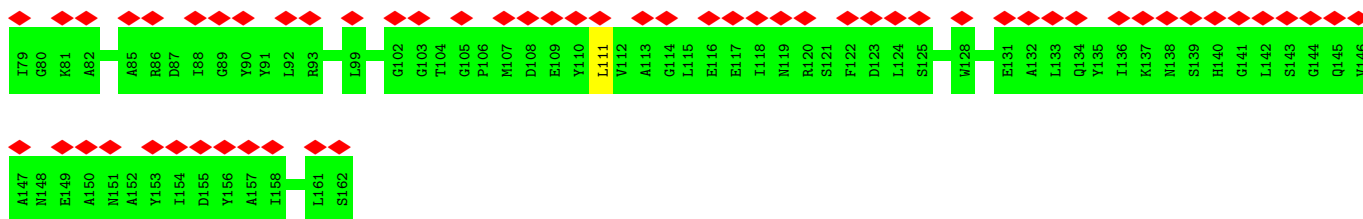


- Molecule 8: C-phycoerythrin alpha subunit

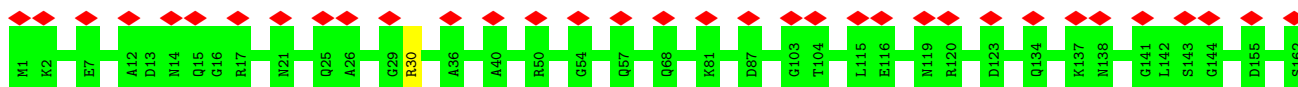


- Molecule 8: C-phycoerythrin alpha subunit

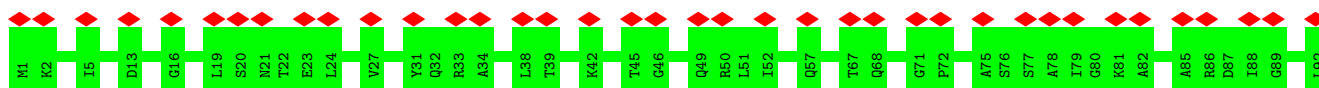
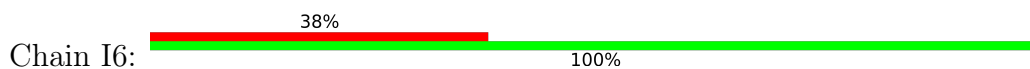




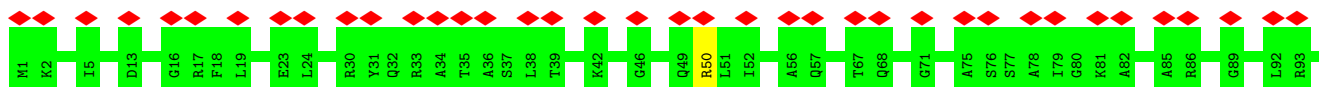
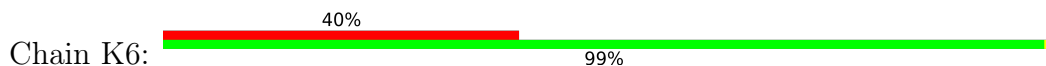
- Molecule 8: C-phycoerythrin alpha subunit



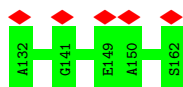
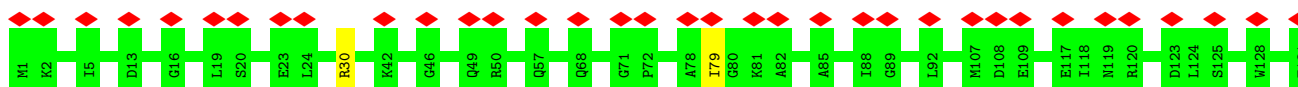
- Molecule 8: C-phycoerythrin alpha subunit



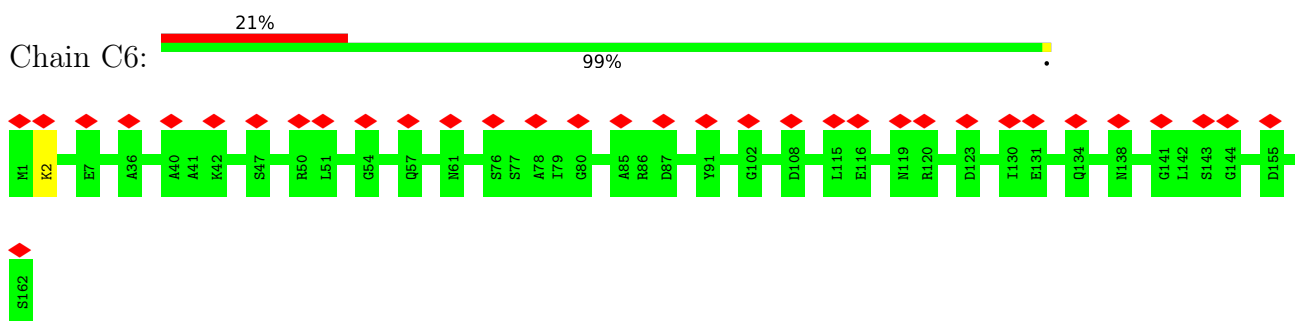
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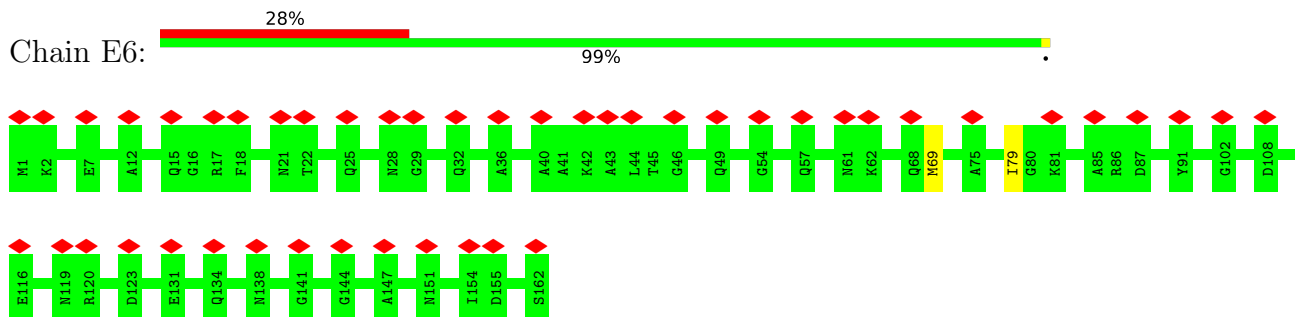
- Molecule 8: C-phycoerythrin alpha subunit



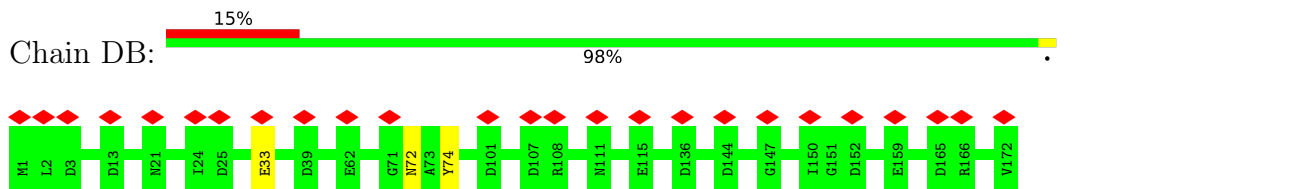
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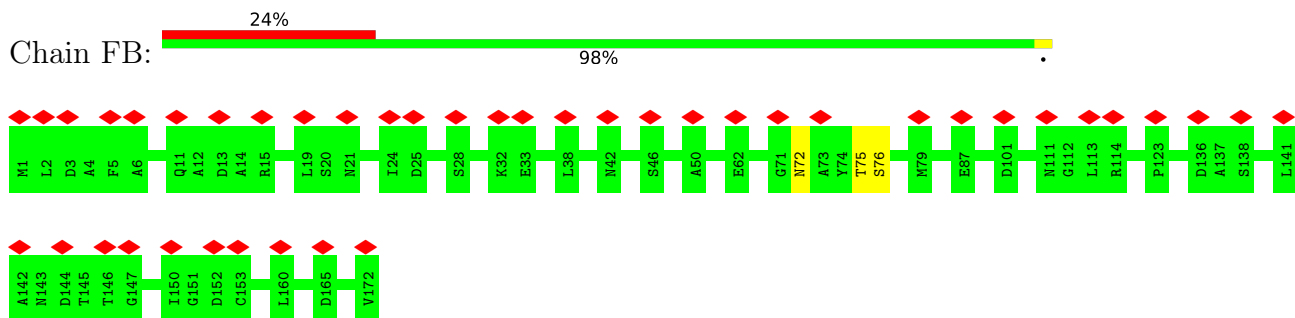
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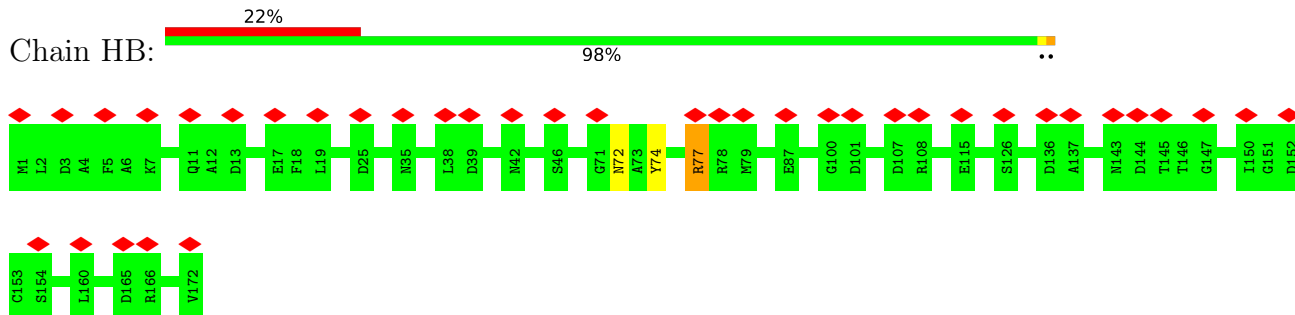
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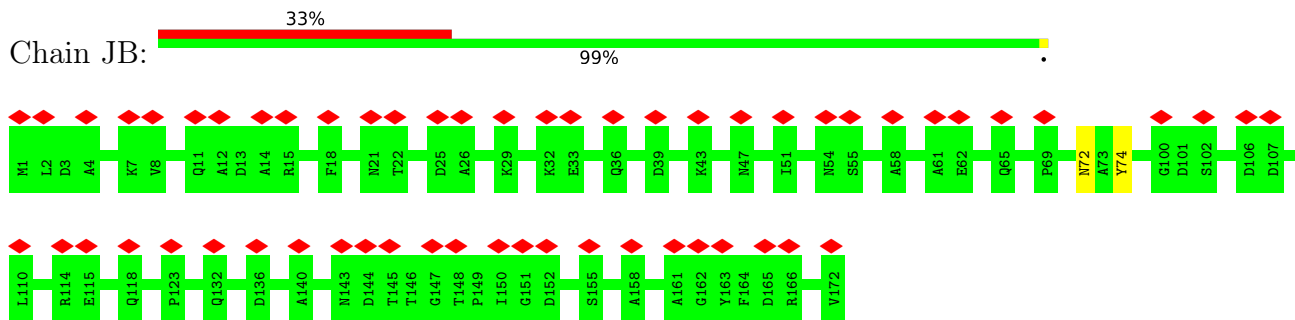
- Molecule 9: C-phycoerythrin beta subunit



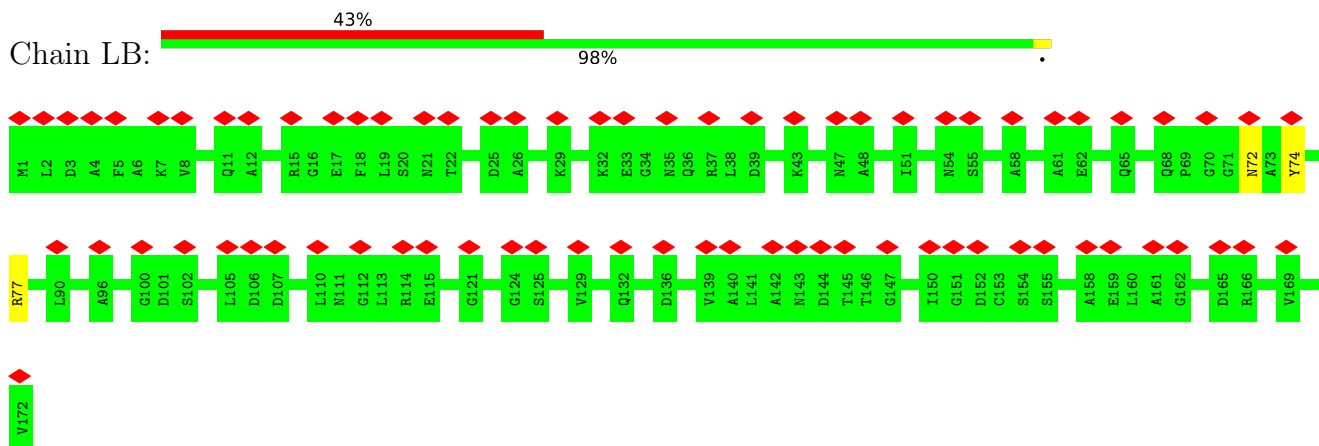
- Molecule 9: C-phycoerythrin beta subunit



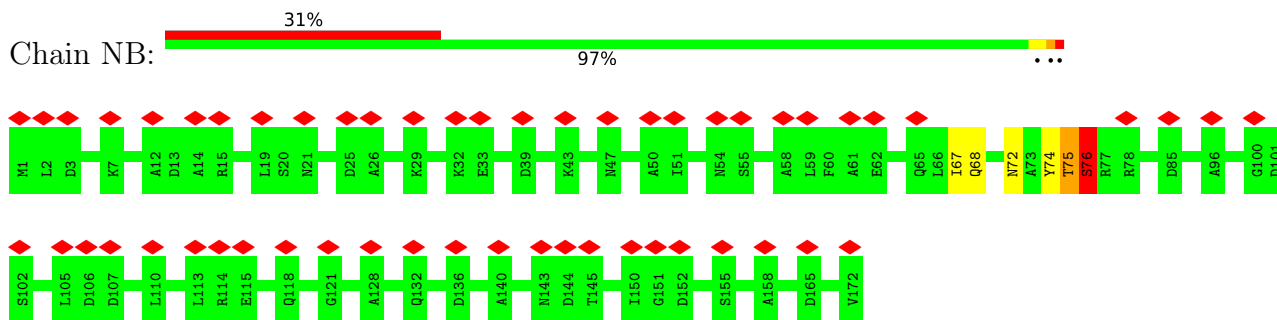
• Molecule 9: C-phycoerythrin beta subunit



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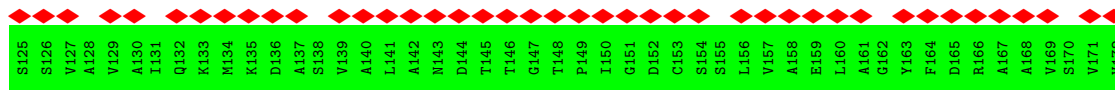


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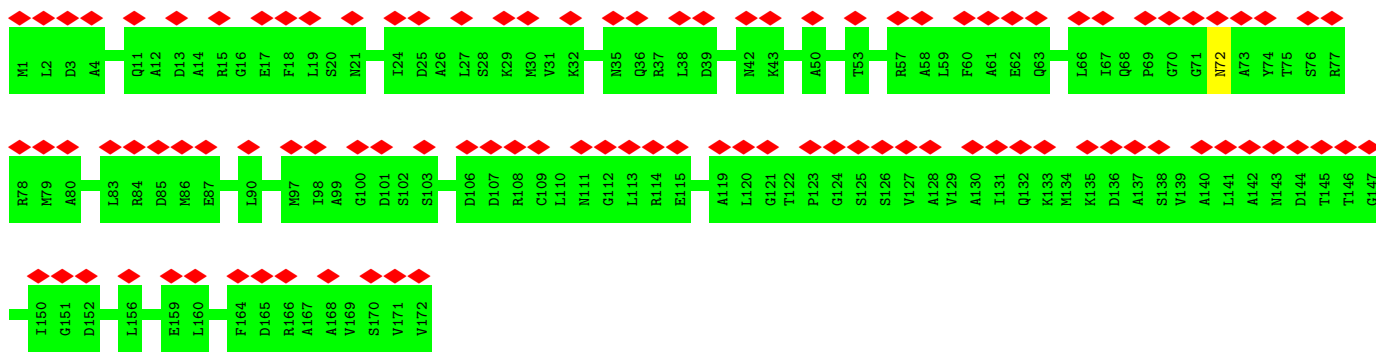


• Molecule 9: C-phycoerythrin beta subunit





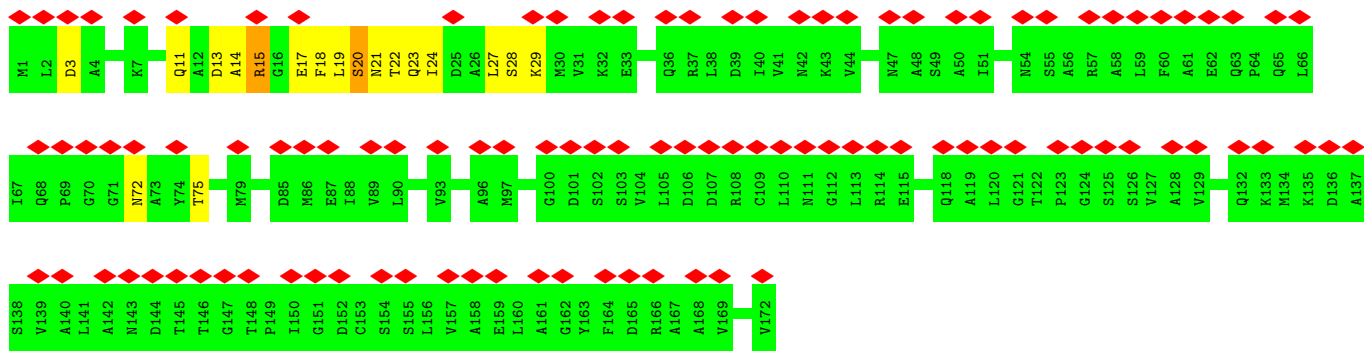
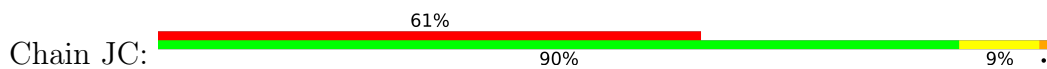
- Molecule 9: C-phycoerythrin beta subunit



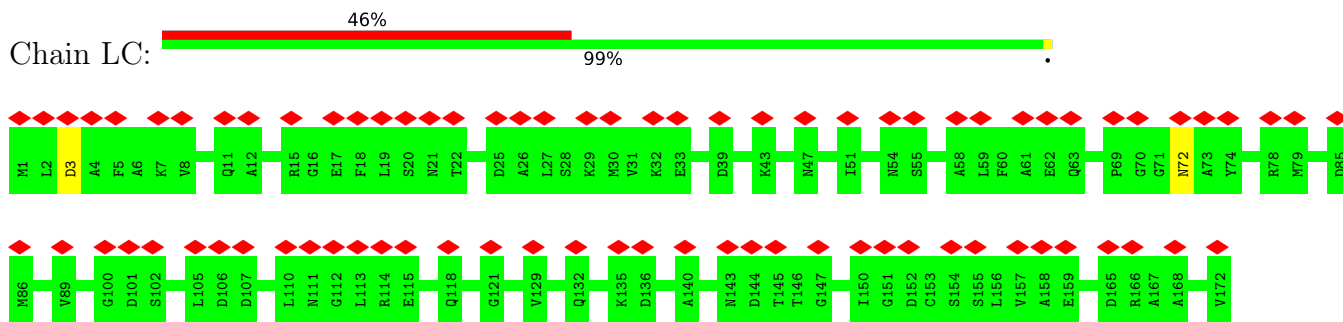
- Molecule 9: C-phycoerythrin beta subunit



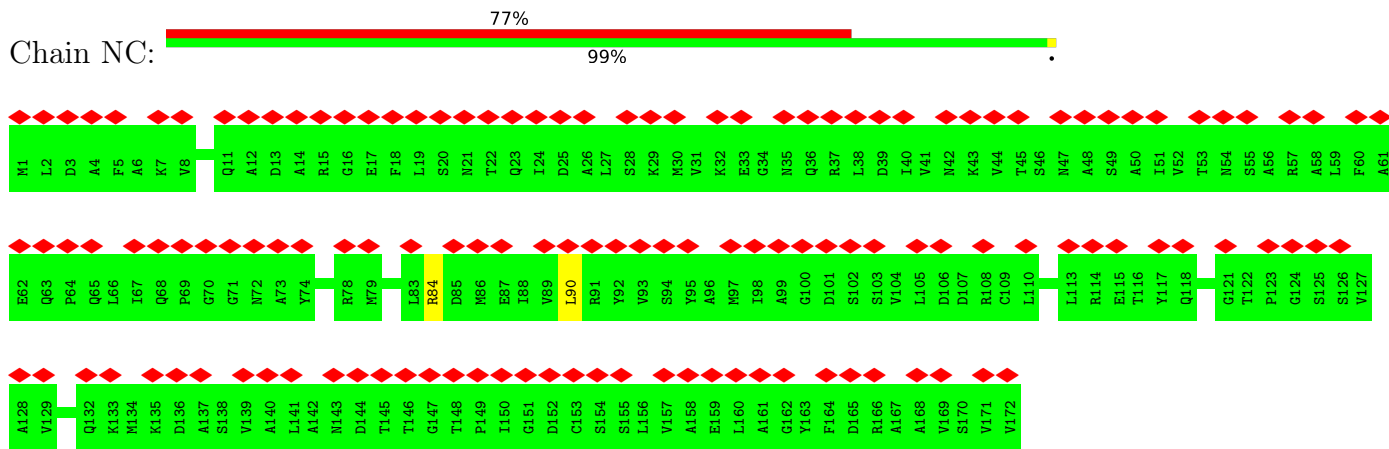
- Molecule 9: C-phycoerythrin beta subunit



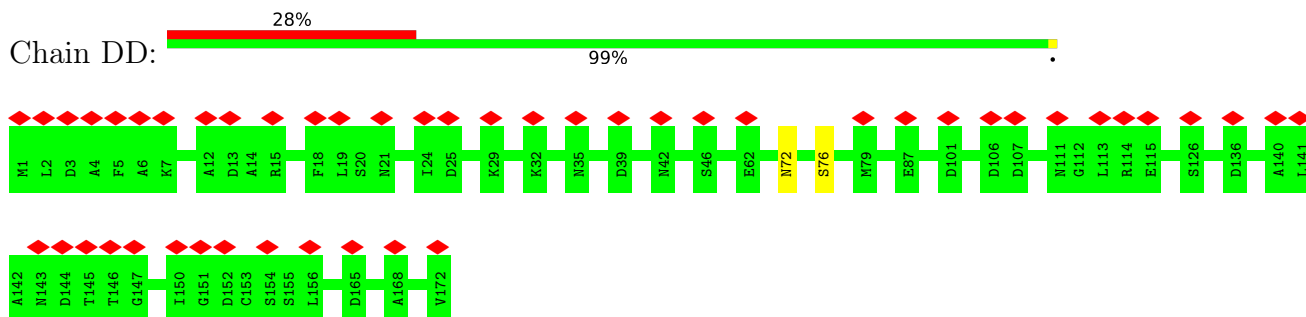
- Molecule 9: C-phycoerythrin beta subunit



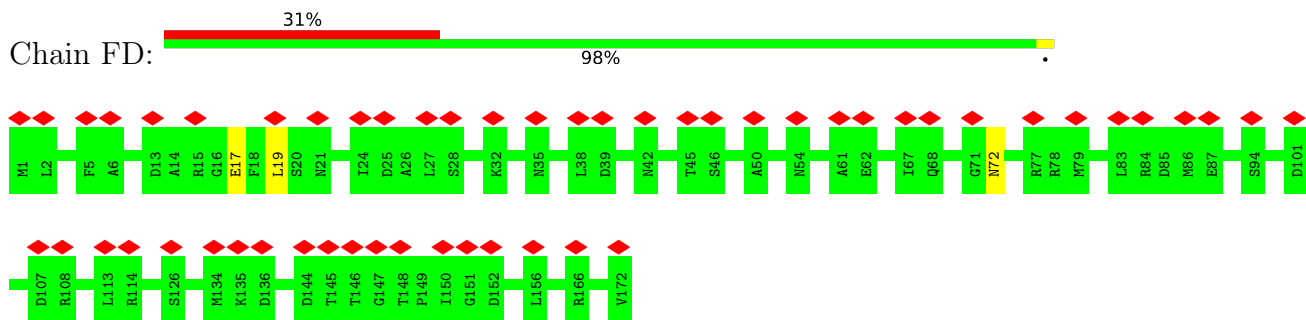
• Molecule 9: C-phycoerythrin beta subunit



• Molecule 9: C-phycoerythrin beta subunit

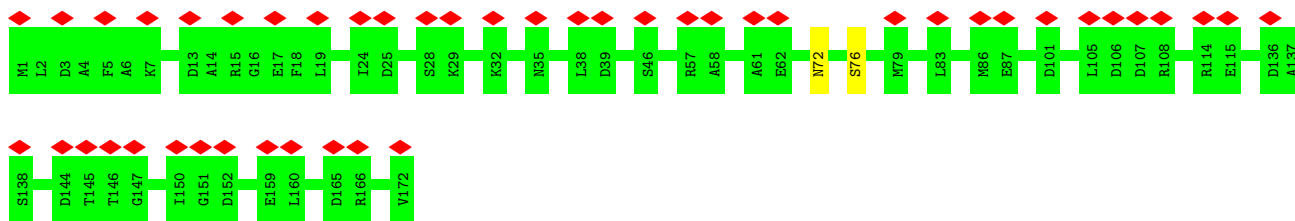


• Molecule 9: C-phycoerythrin beta subunit

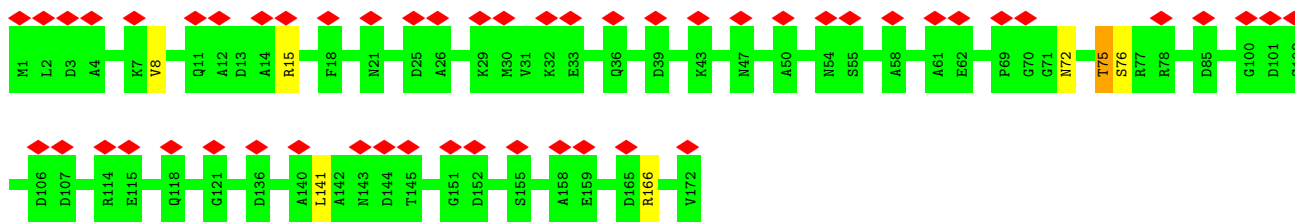


• Molecule 9: C-phycoerythrin beta subunit

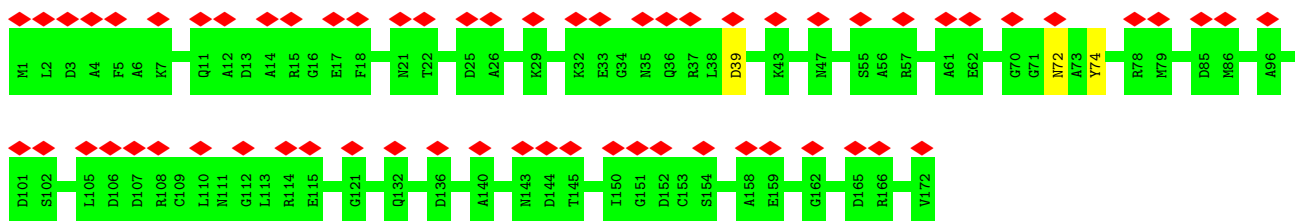
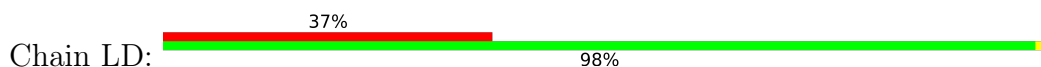




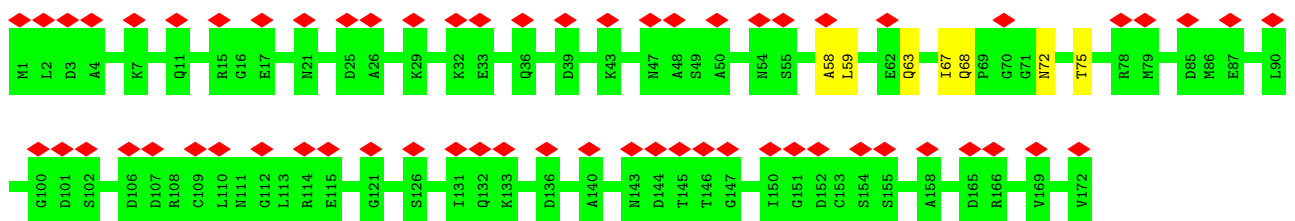
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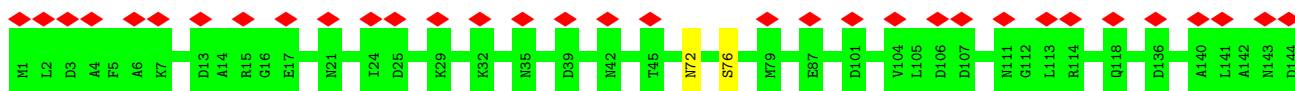
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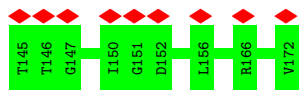


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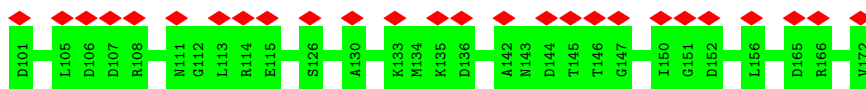


- Molecule 9: C-phycoerythrin beta subunit

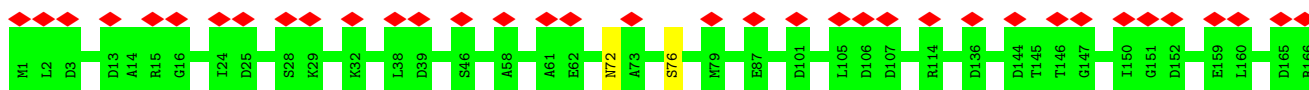




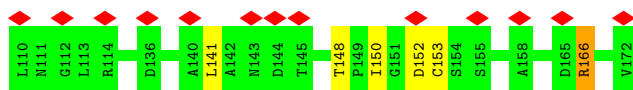
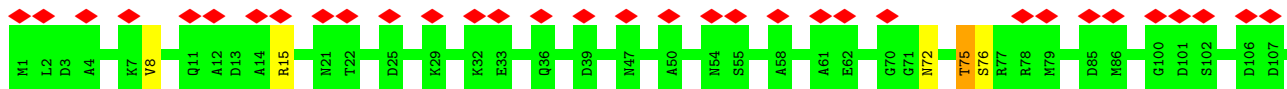
- Molecule 9: C-phycoerythrin beta subunit



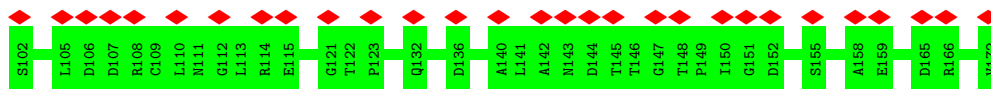
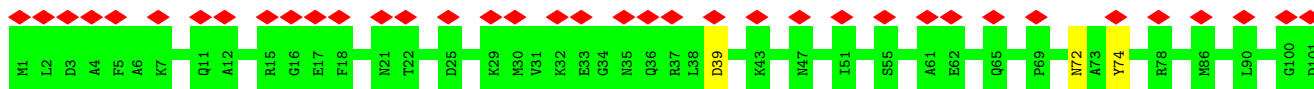
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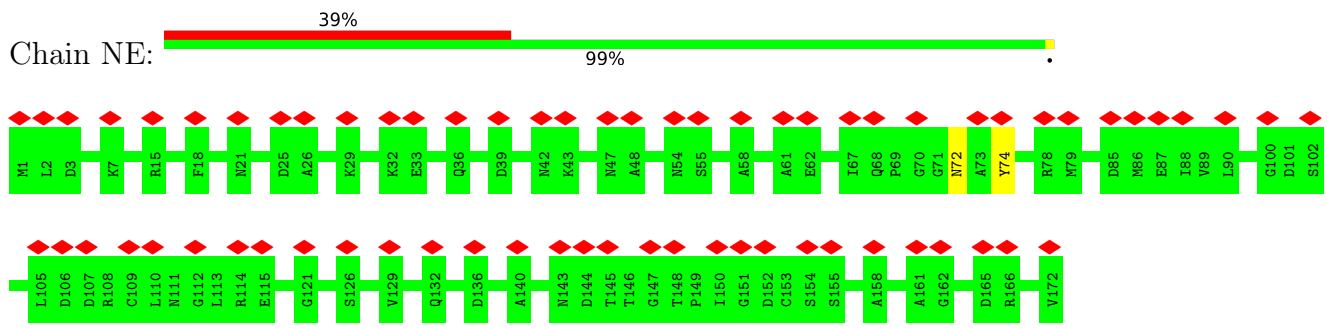
- Molecule 9: C-phycoerythrin beta subunit



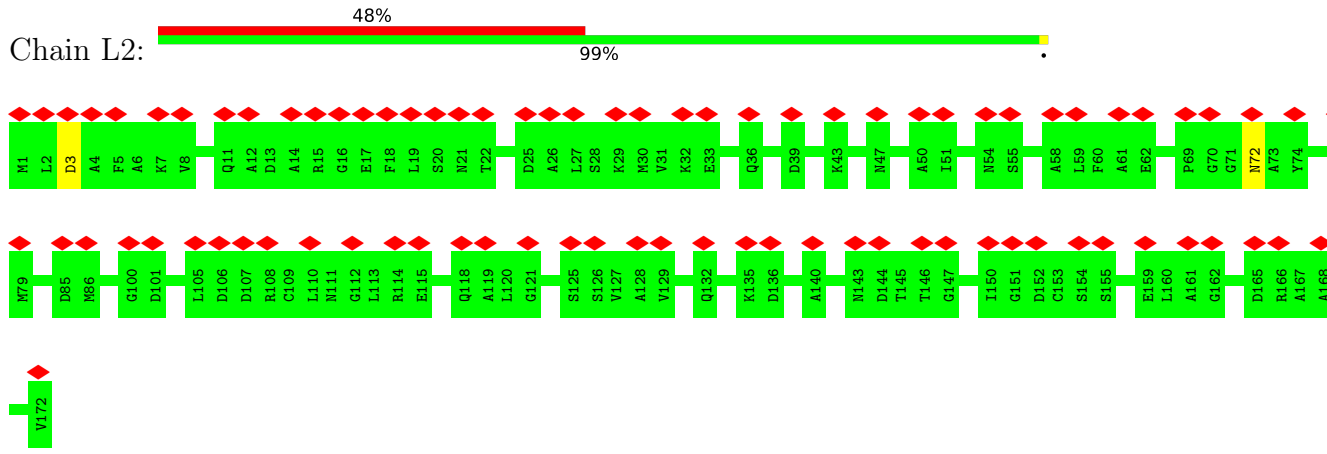
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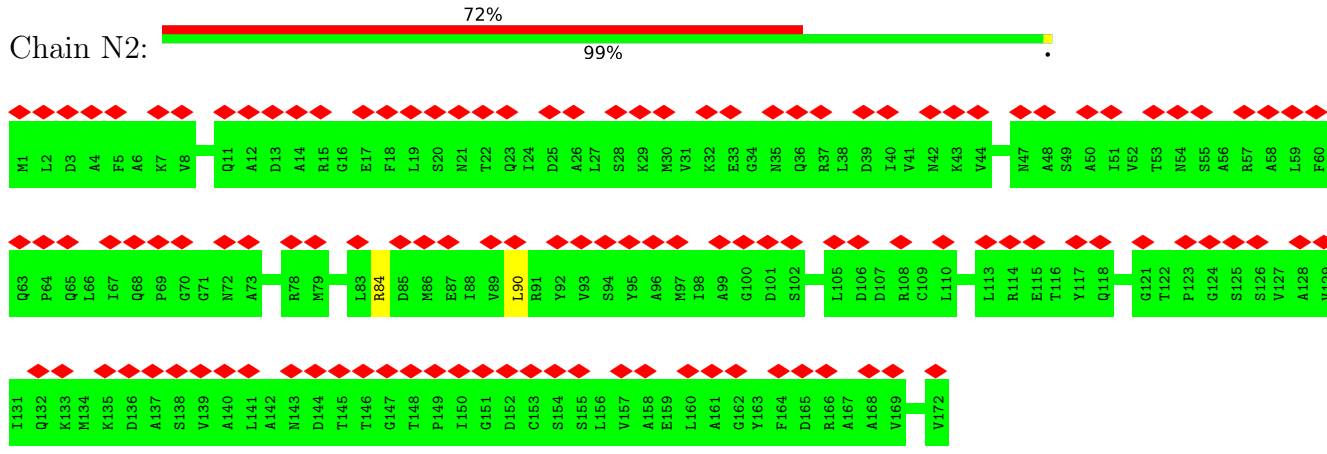
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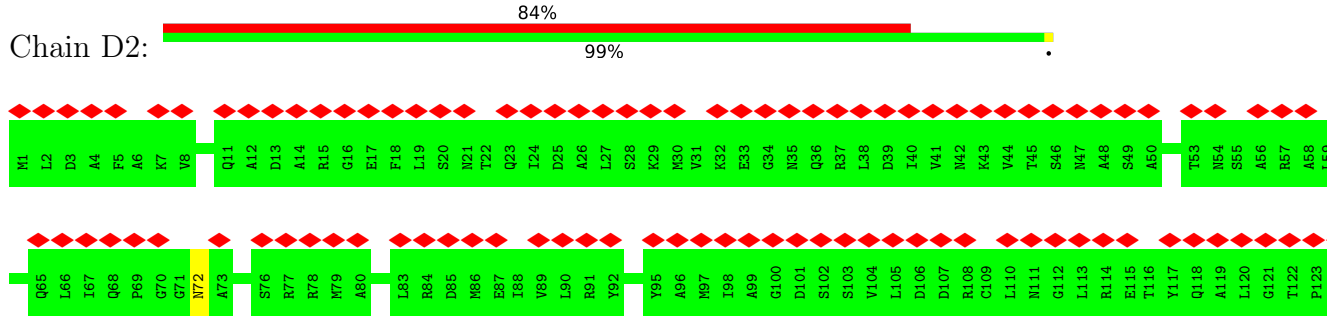
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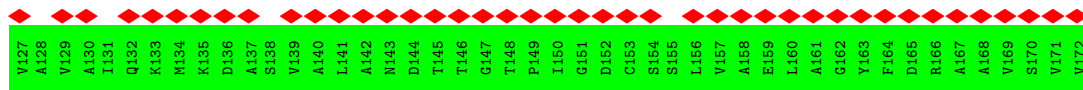


• Molecule 9: C-phycoyanin beta subunit

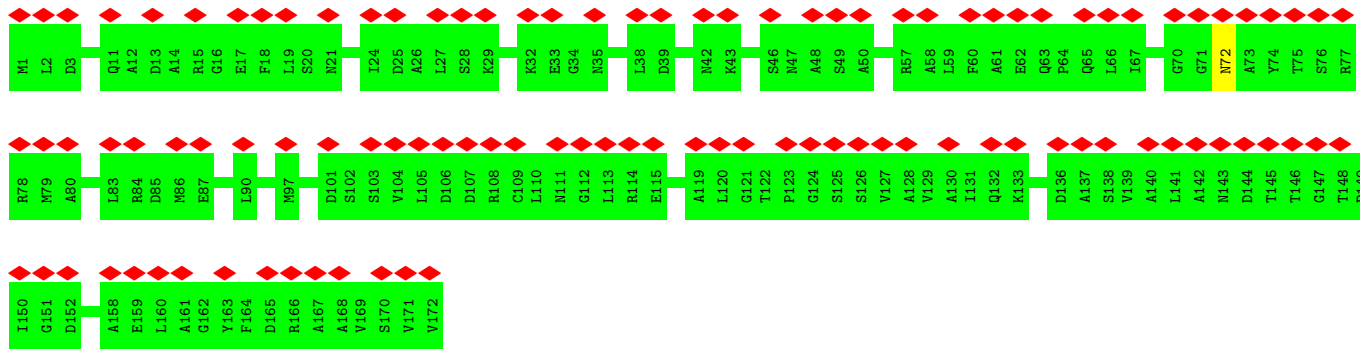


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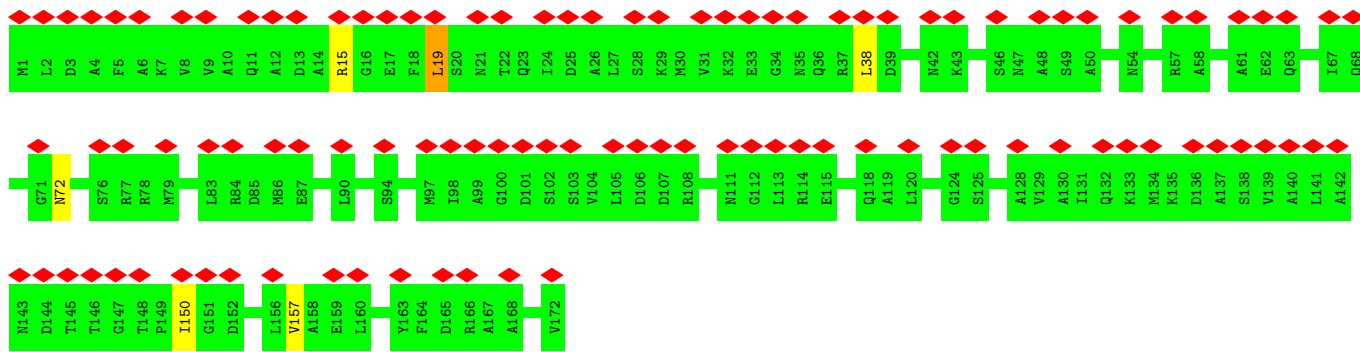




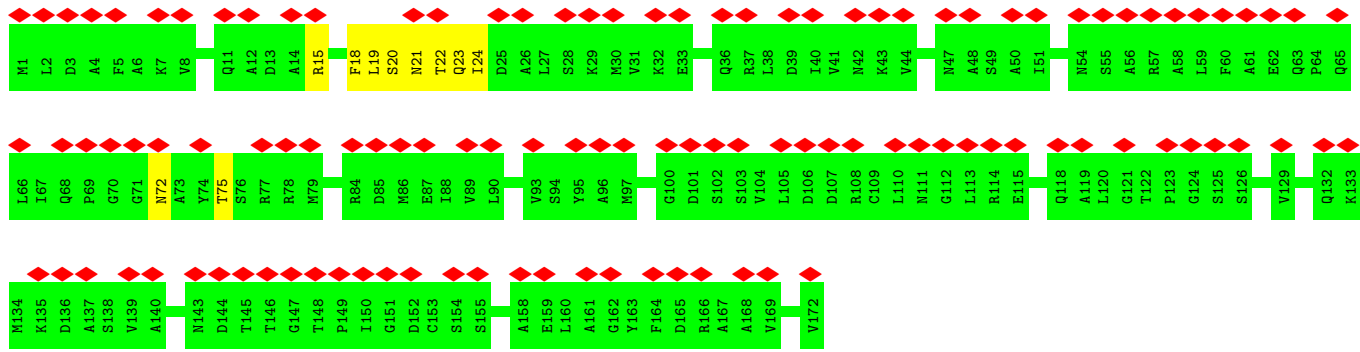
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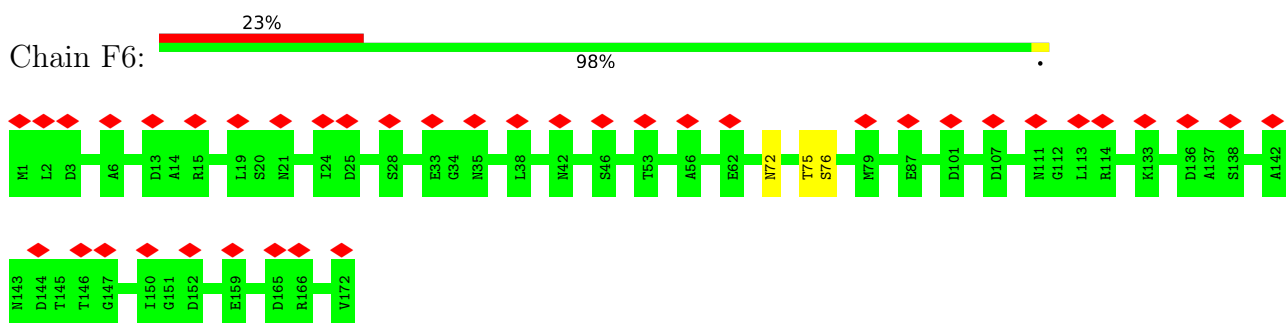
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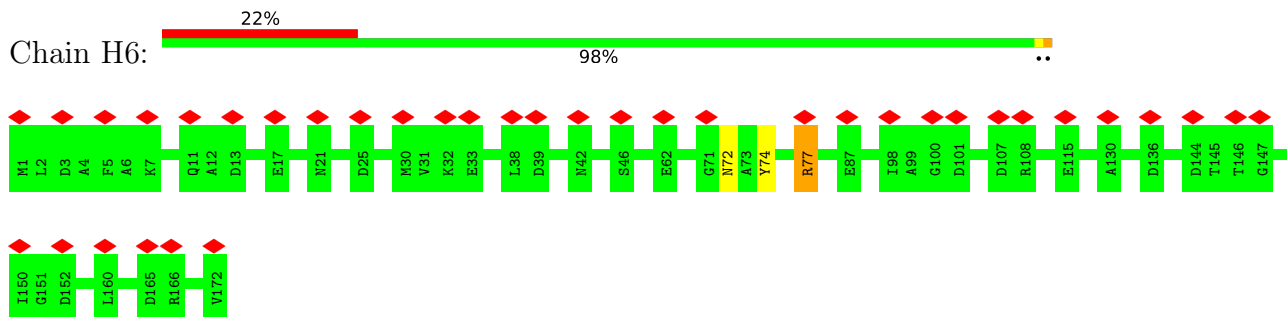
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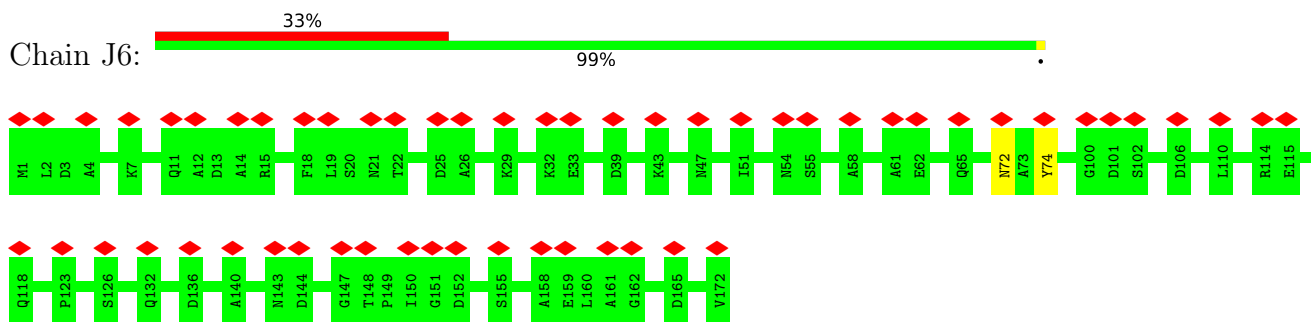
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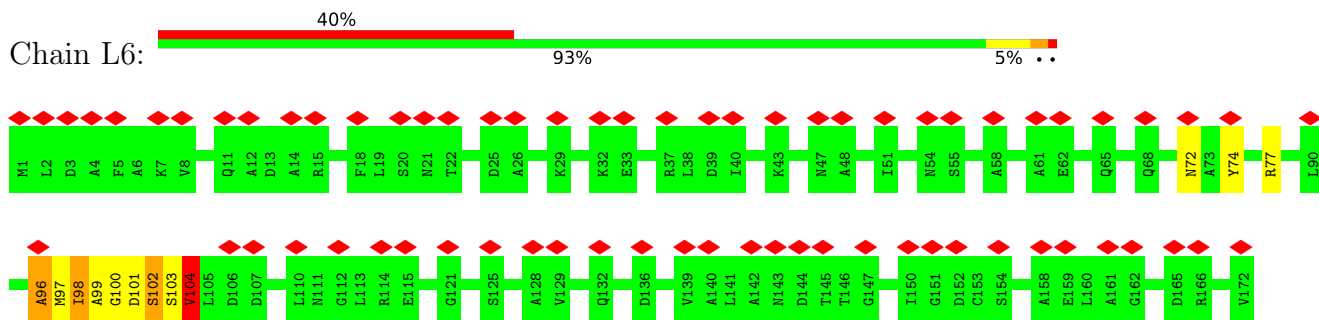
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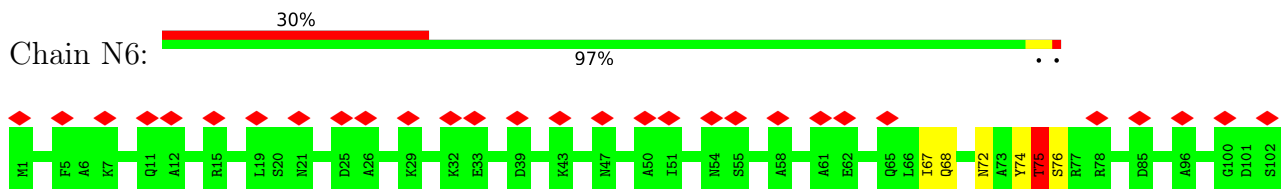
- Molecule 9: C-phycoerythrin beta subunit

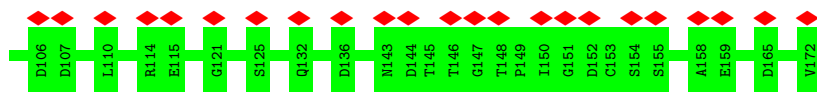


- Molecule 9: C-phycoerythrin beta subunit

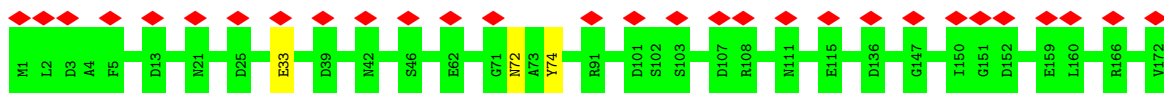


- Molecule 9: C-phycoerythrin beta subunit

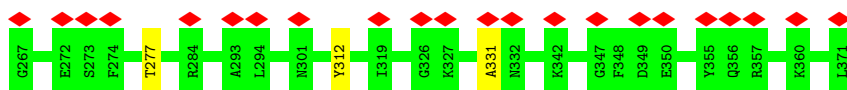
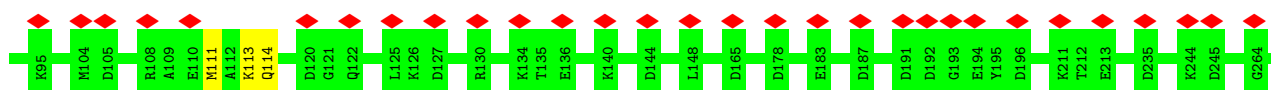
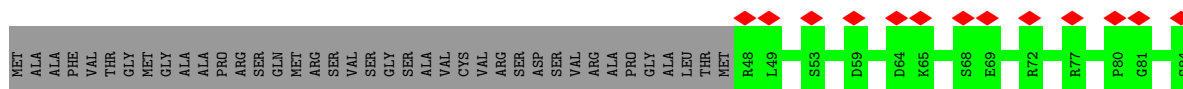
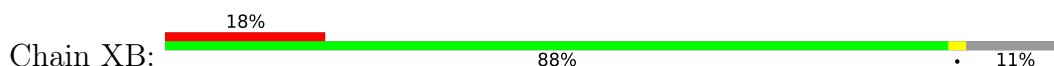




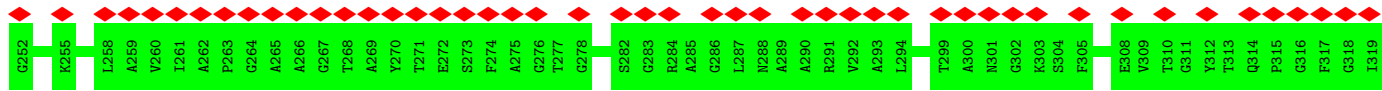
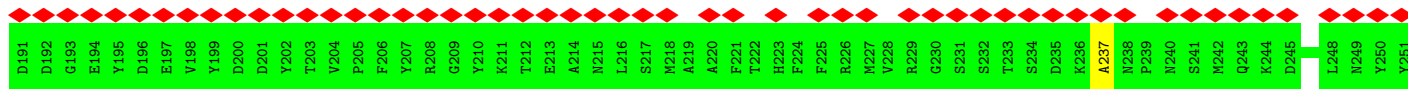
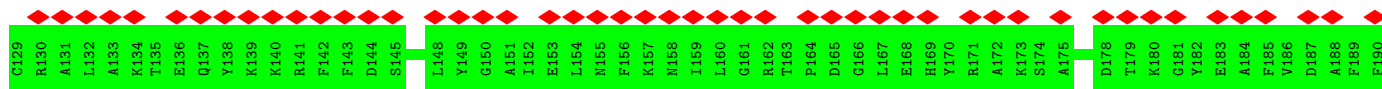
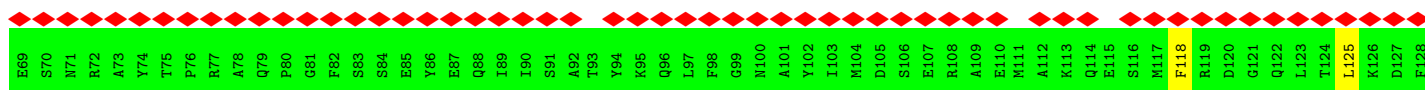
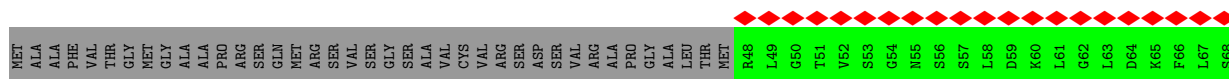
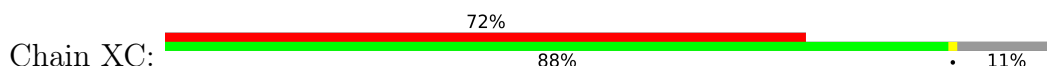
• Molecule 9: C-phycoerythrin beta subunit

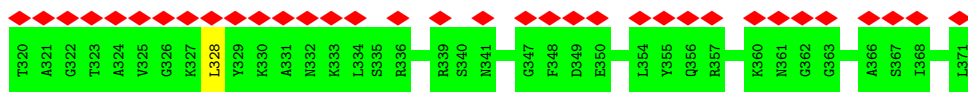


• Molecule 10: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

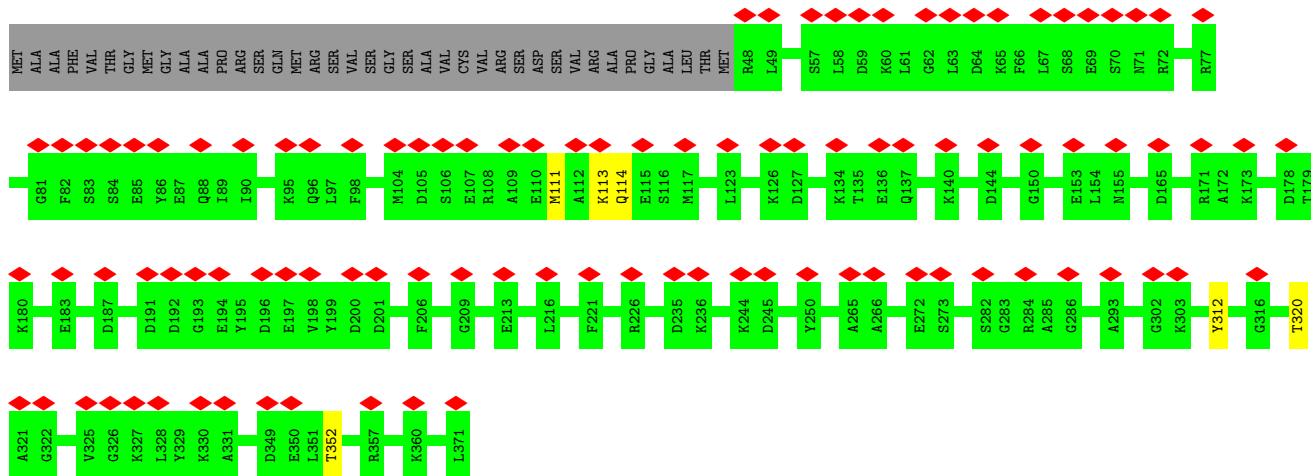
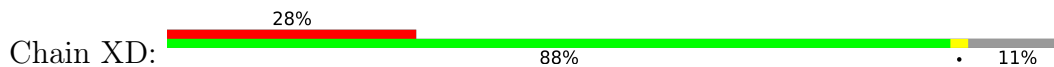


• Molecule 10: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

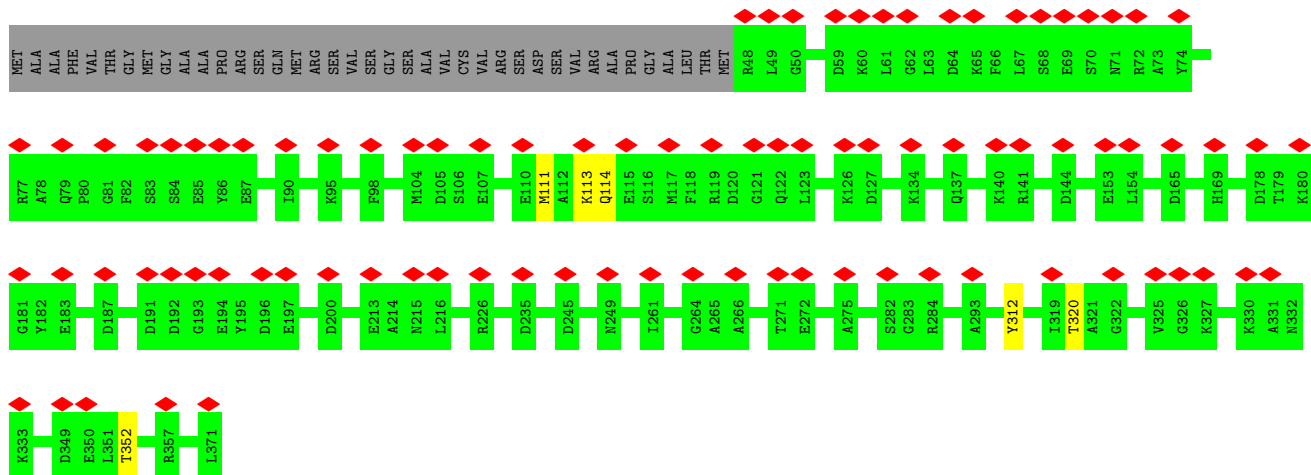
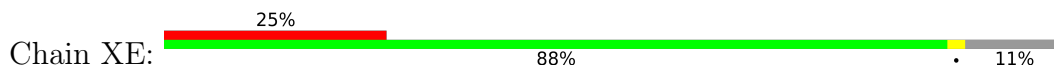




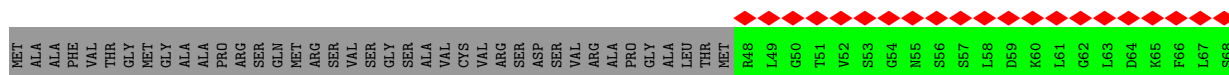
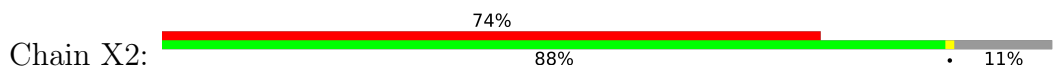
• Molecule 10: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



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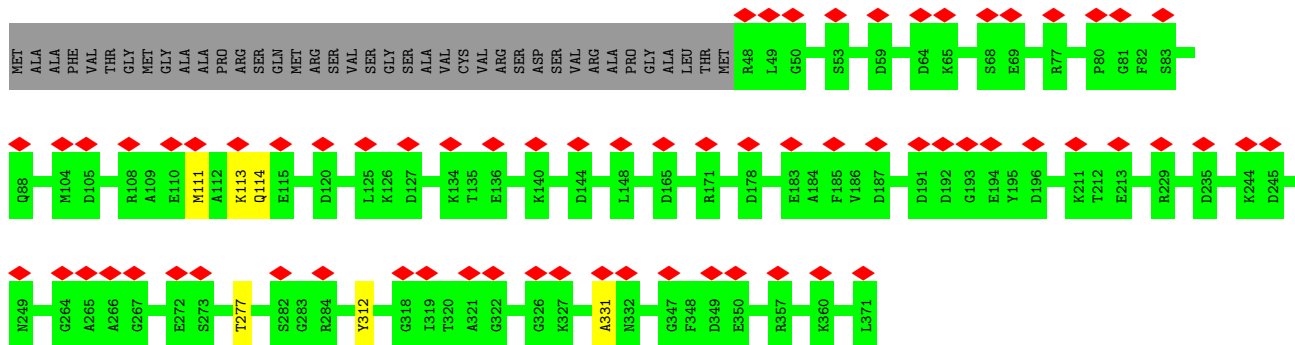
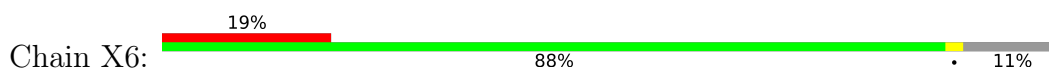


• Molecule 10: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

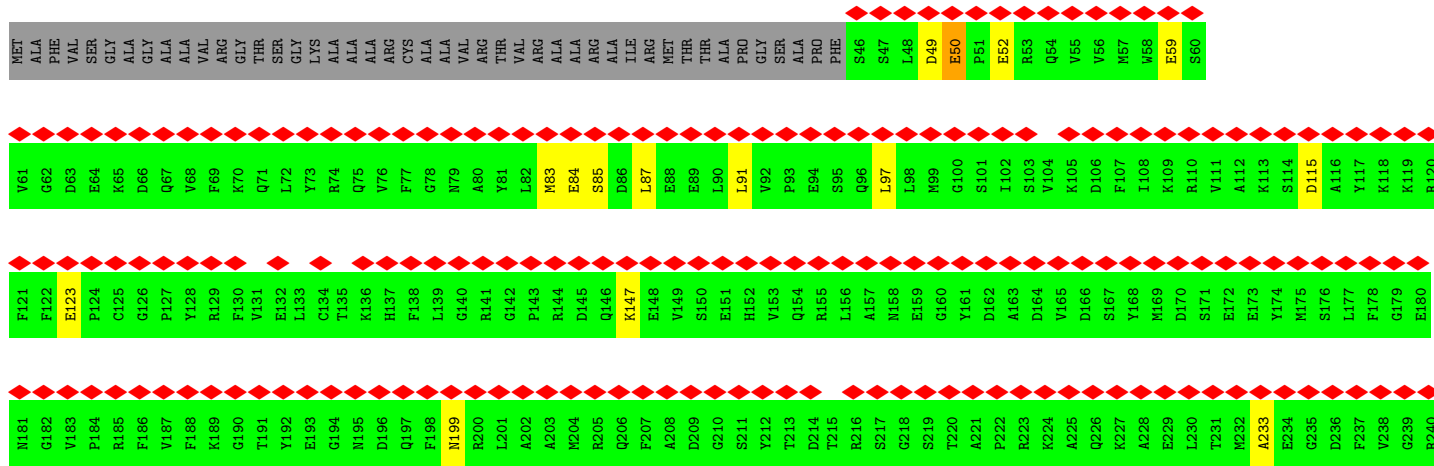
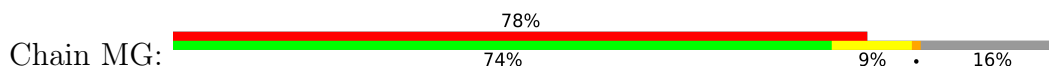


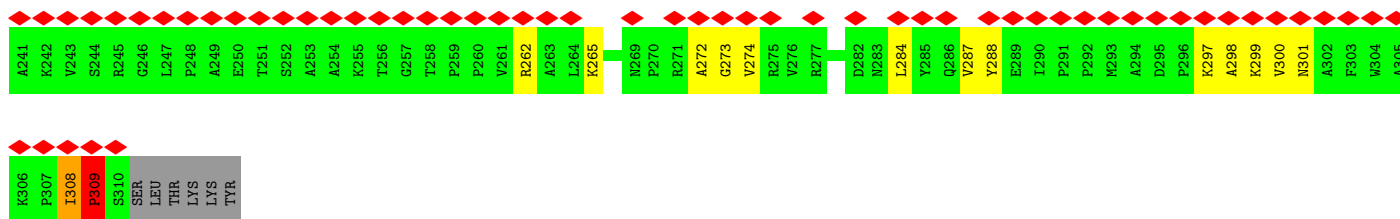


• Molecule 10: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

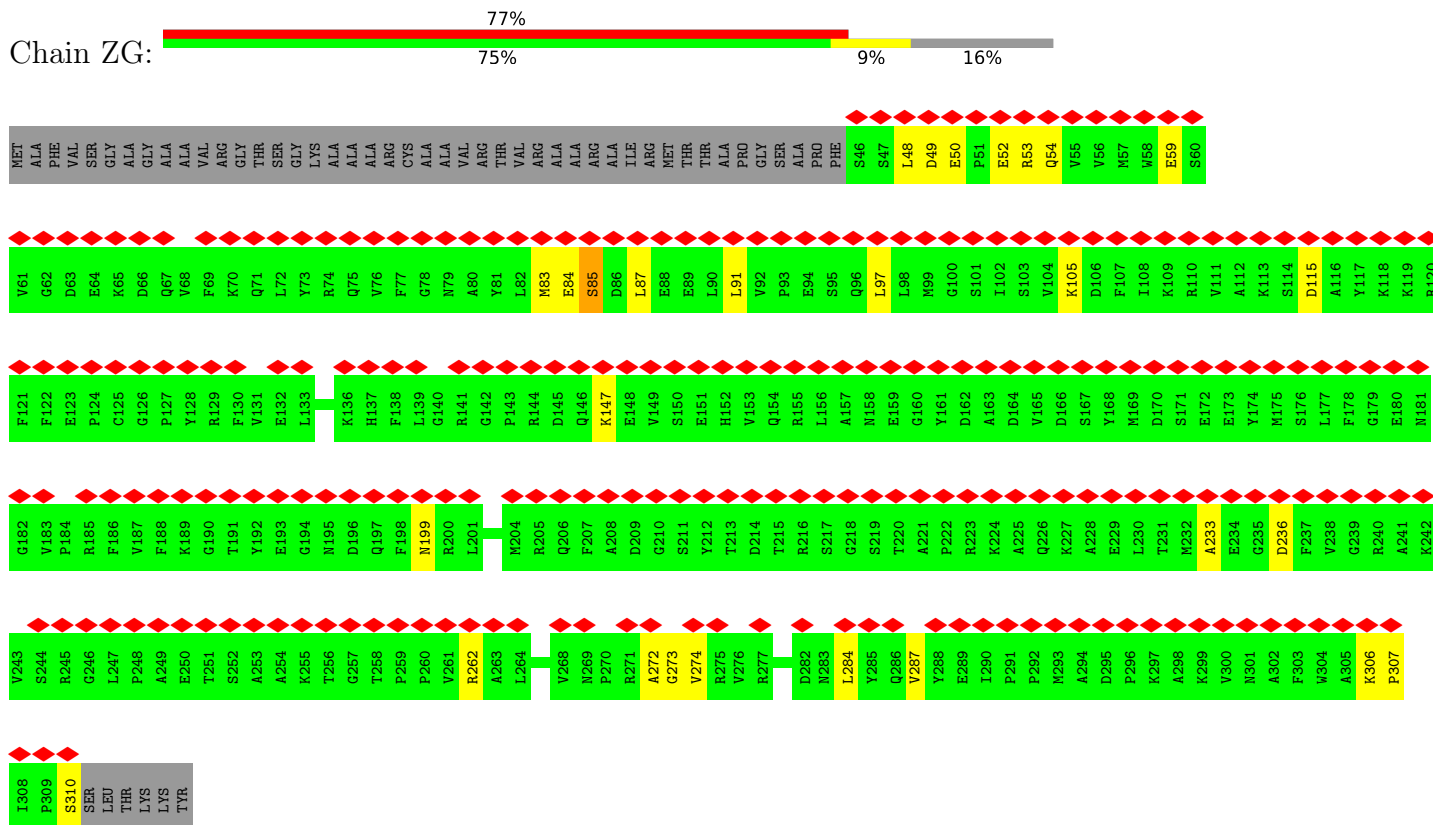


• Molecule 11: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

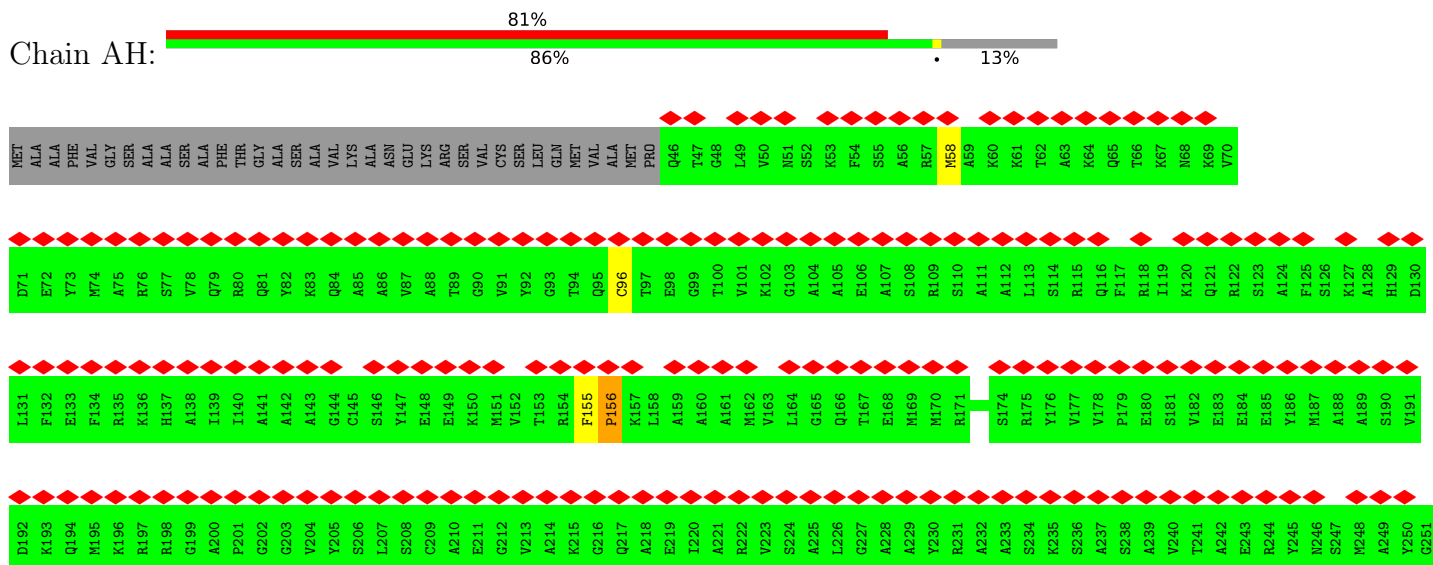


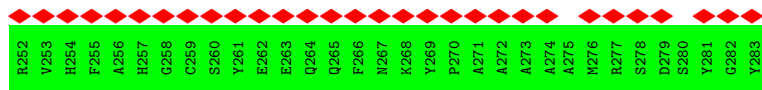


• Molecule 11: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

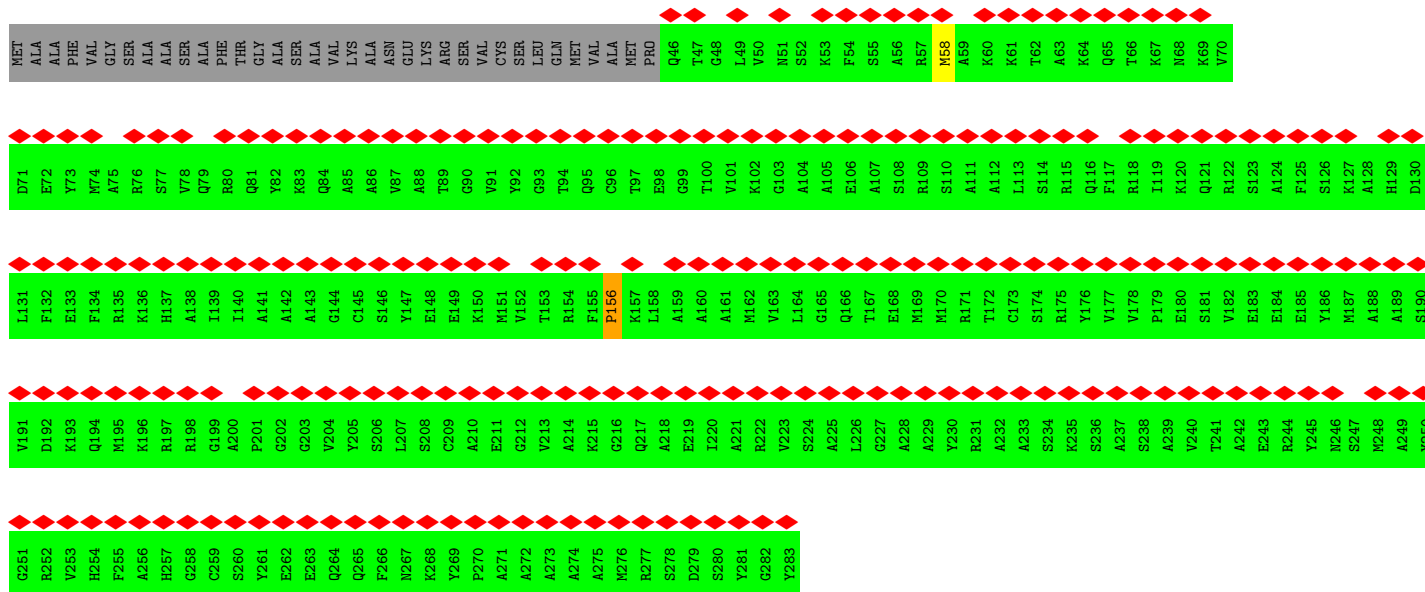
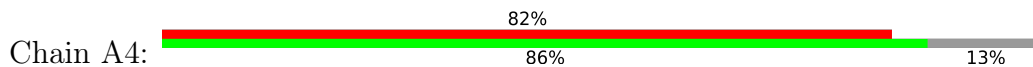


• Molecule 12: R-phycoerythrin gamma chain, chloroplastic

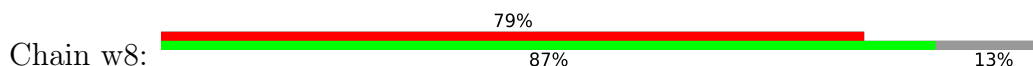




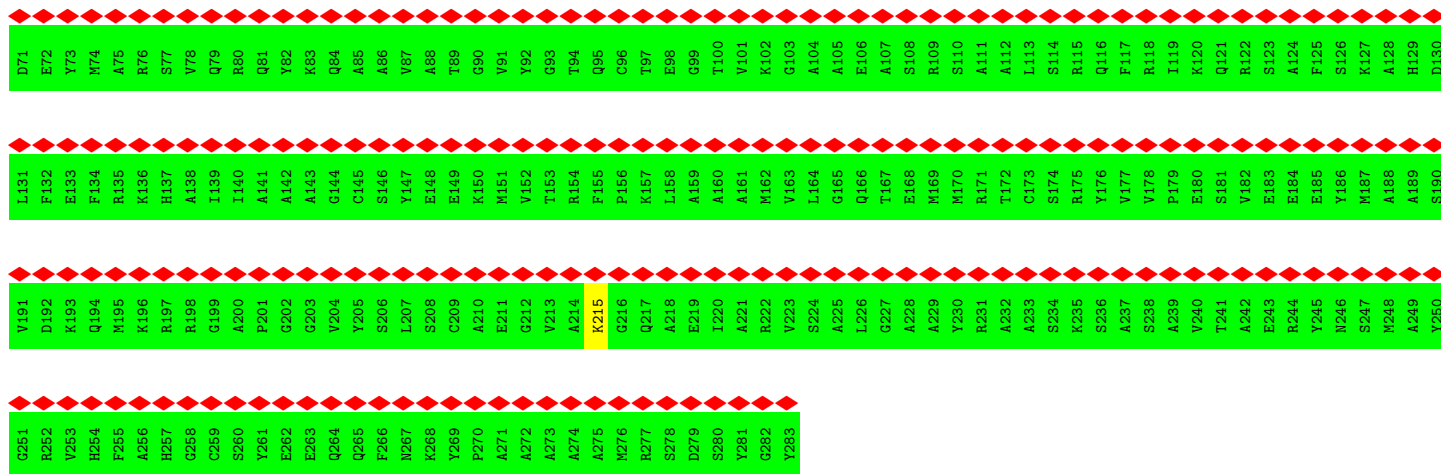
• Molecule 12: R-phycoerythrin gamma chain, chloroplastic



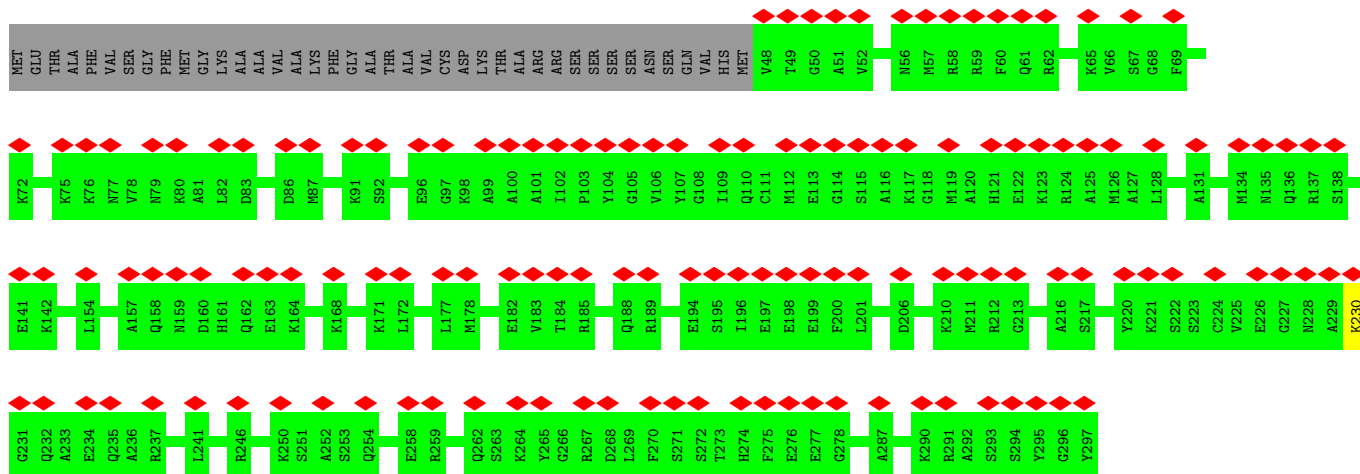
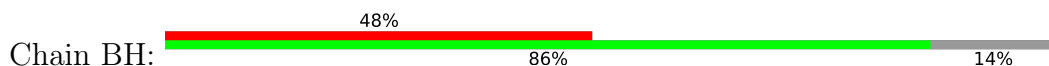
• Molecule 12: R-phycoerythrin gamma chain, chloroplastic



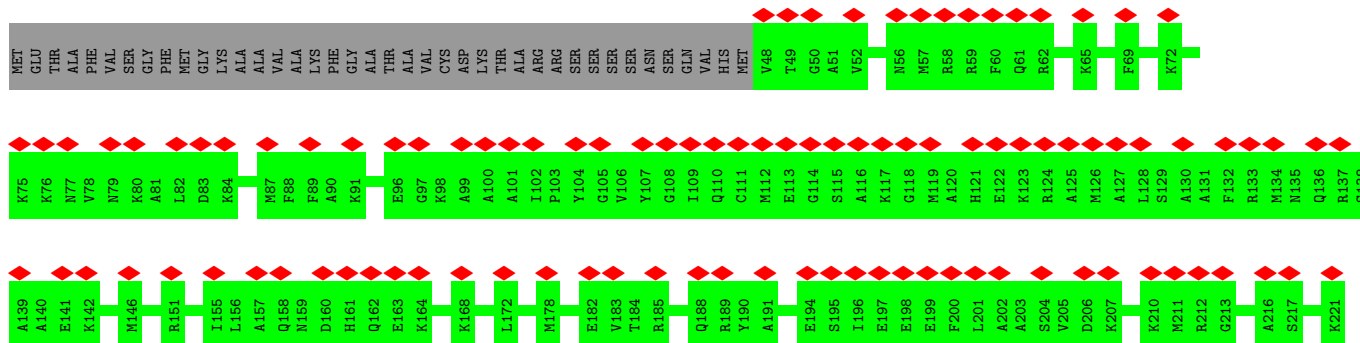
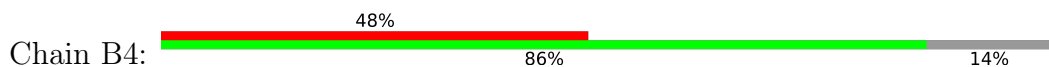
• Molecule 12: R-phycoerythrin gamma chain, chloroplastic

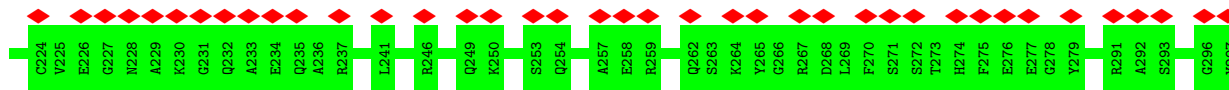


• Molecule 13: R-phycoerythrin gamma chain, chloroplastic

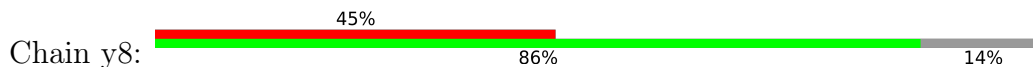


• Molecule 13: R-phycoerythrin gamma chain, chloroplastic

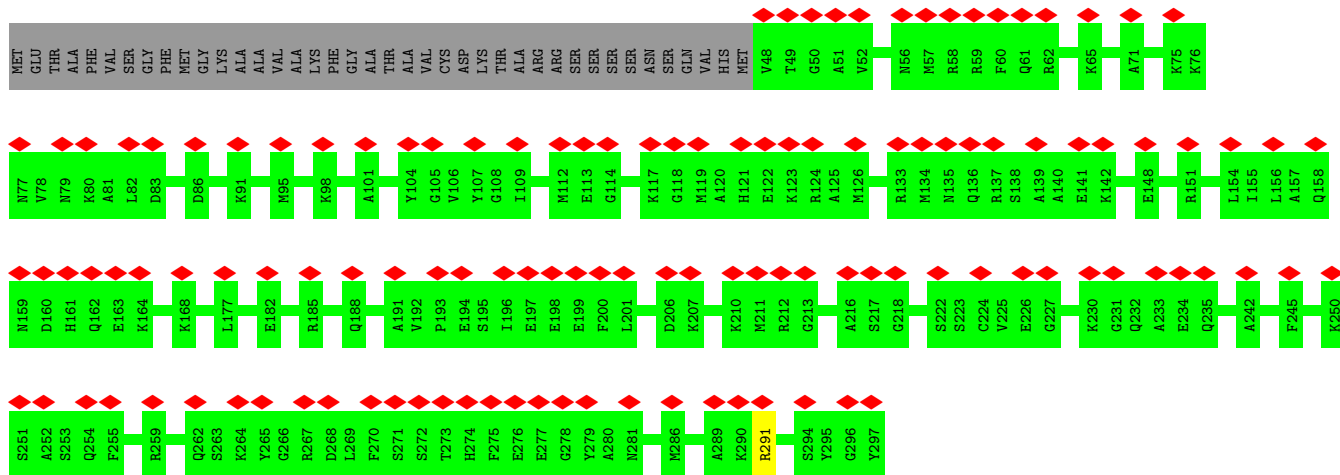
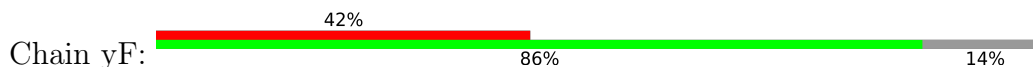




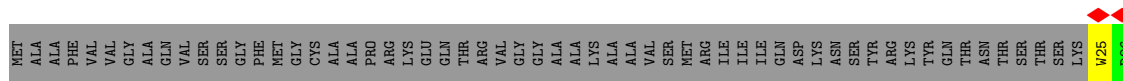
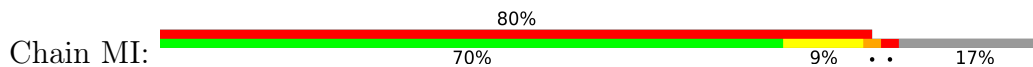
• Molecule 13: R-phycoerythrin gamma chain, chloroplastic

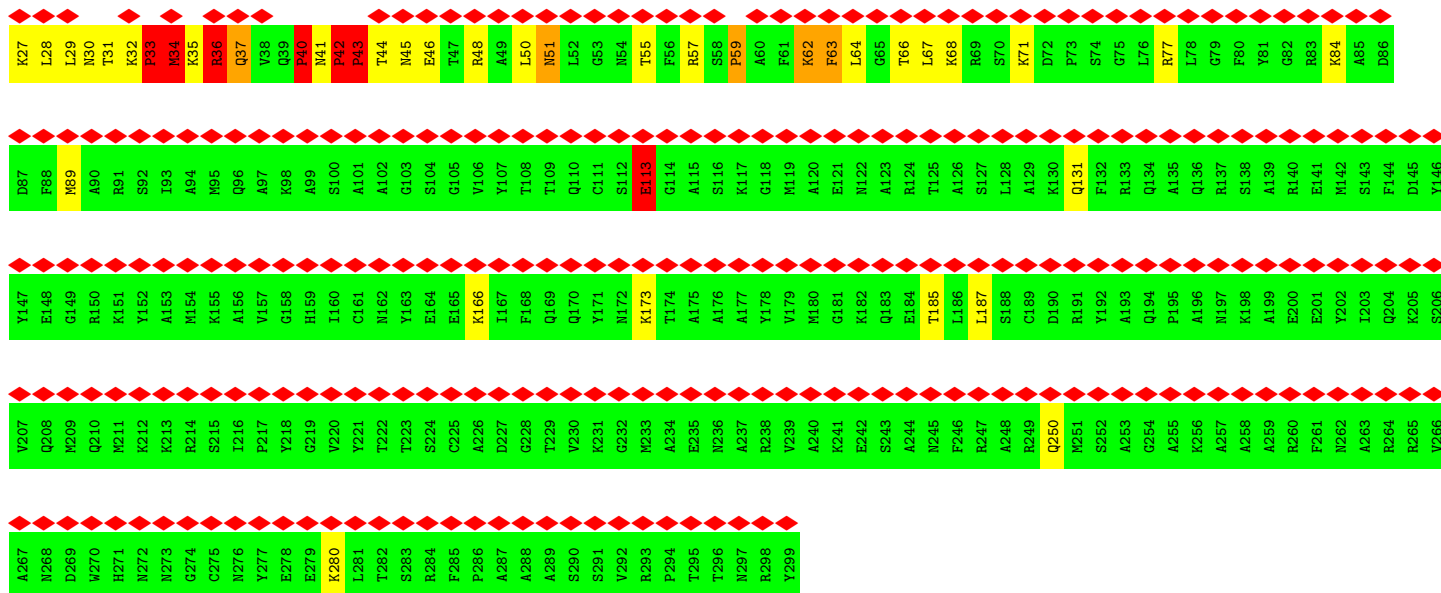


• Molecule 13: R-phycoerythrin gamma chain, chloroplastic



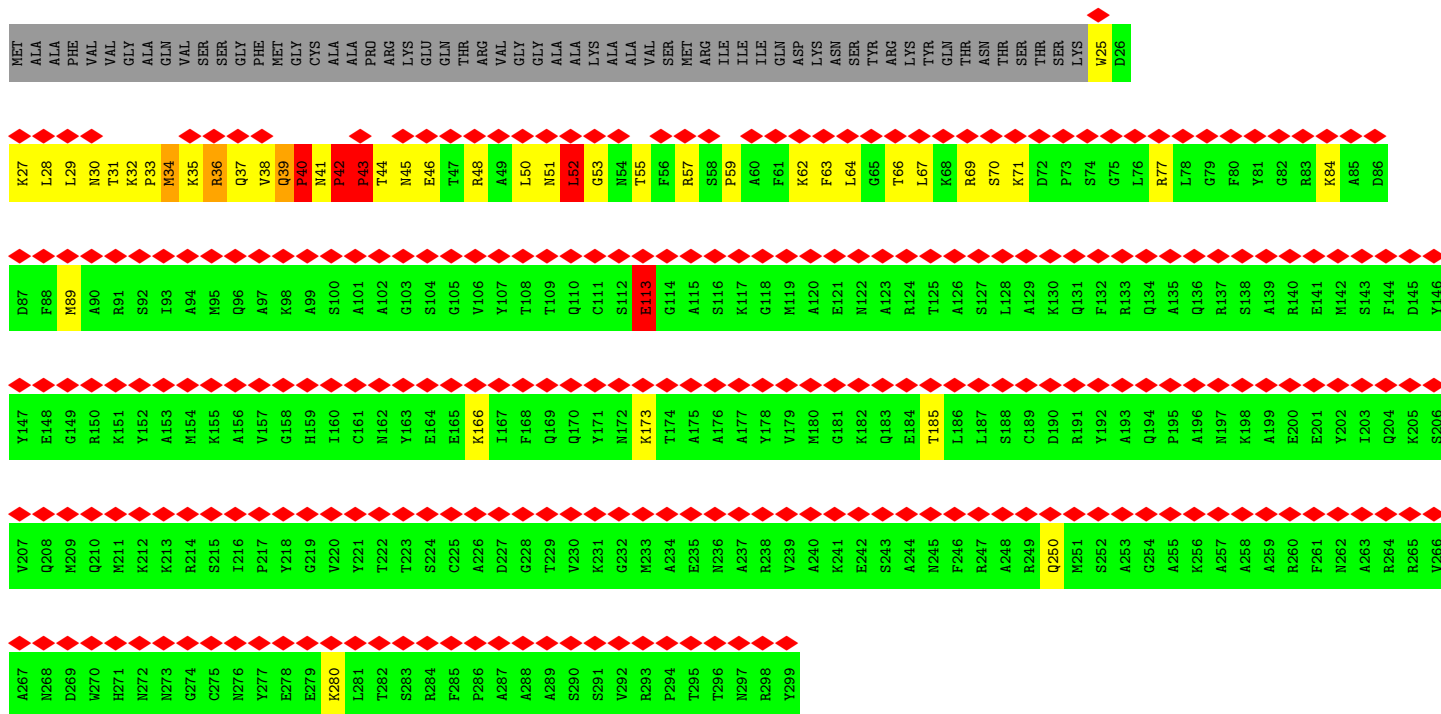
• Molecule 14: R-phycoerythrin gamma chain, chloroplastic





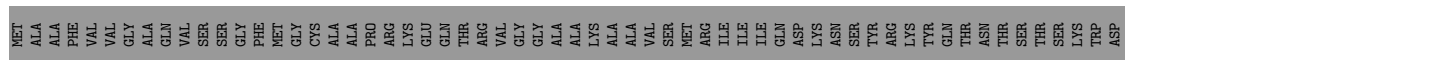
• Molecule 14: R-phycoerythrin gamma chain, chloroplactic

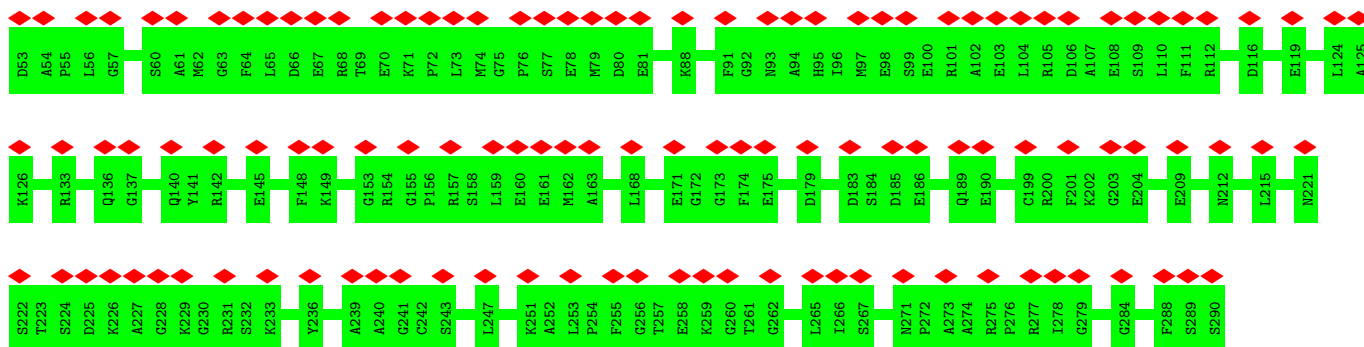
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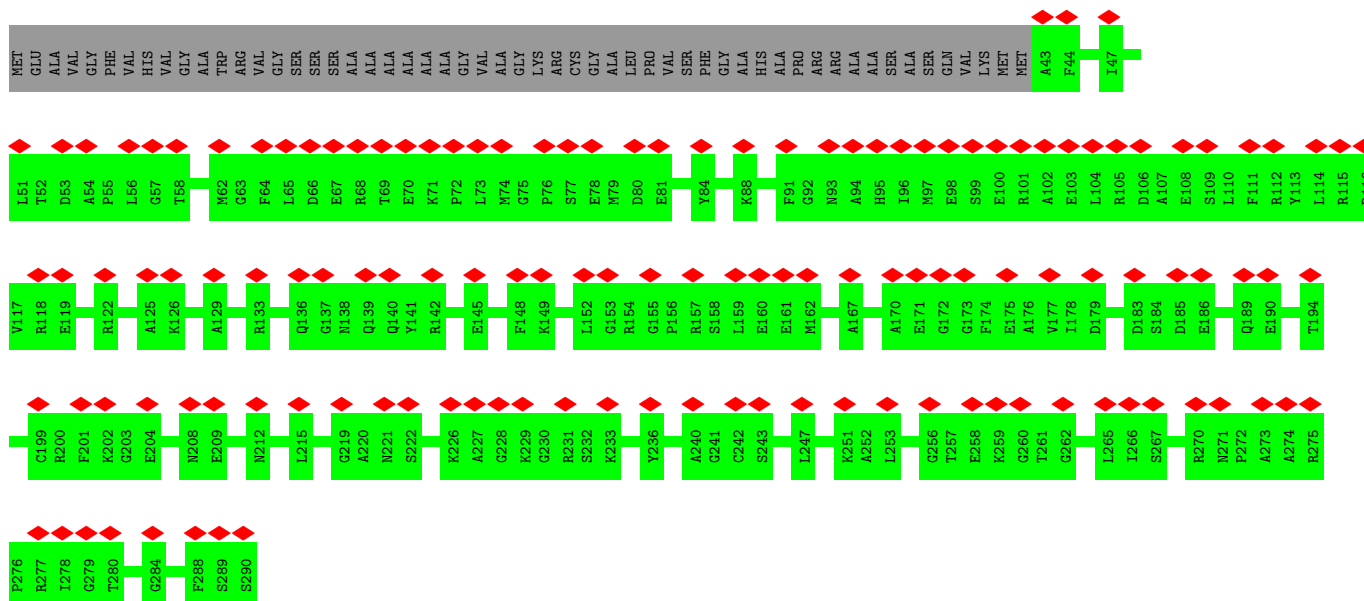
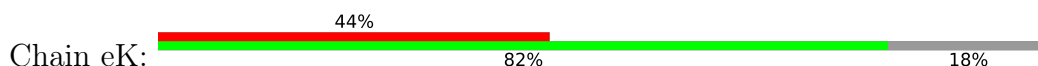
• Molecule 14: R-phycoerythrin gamma chain, chloroplactic

Chain M9:

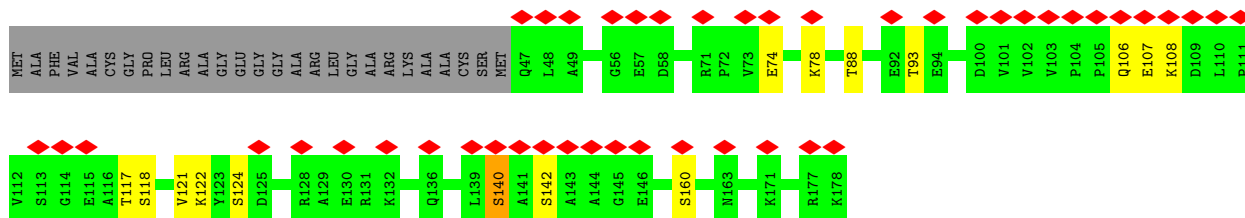
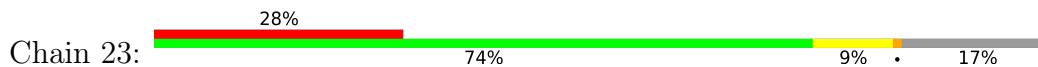




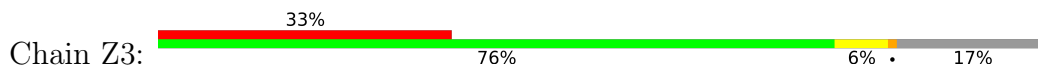
• Molecule 15: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

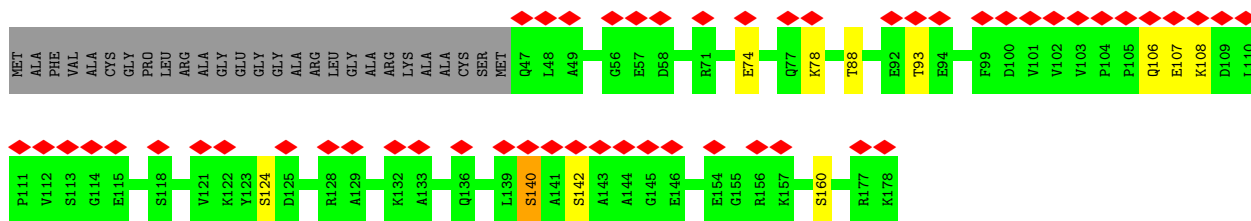


• Molecule 16: Lrc4

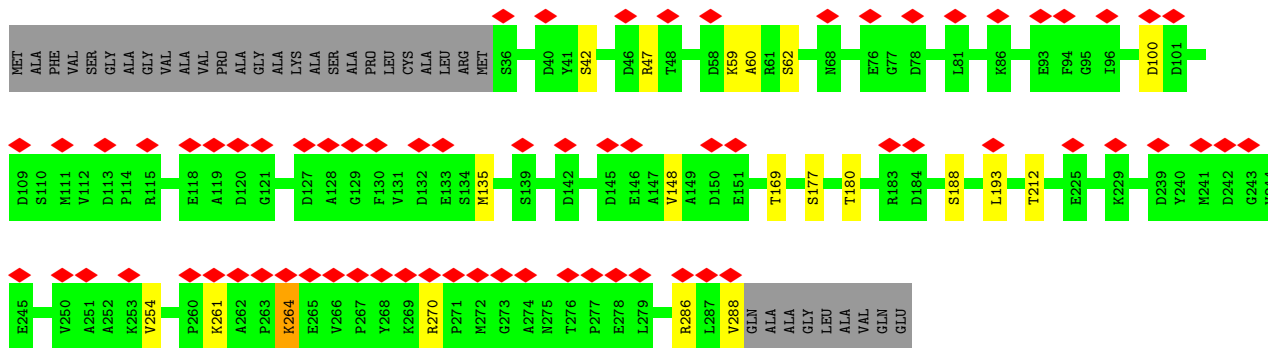
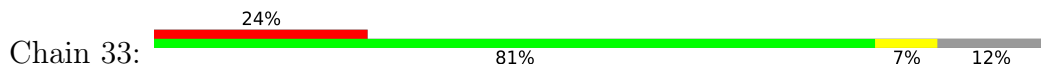


• Molecule 16: Lrc4

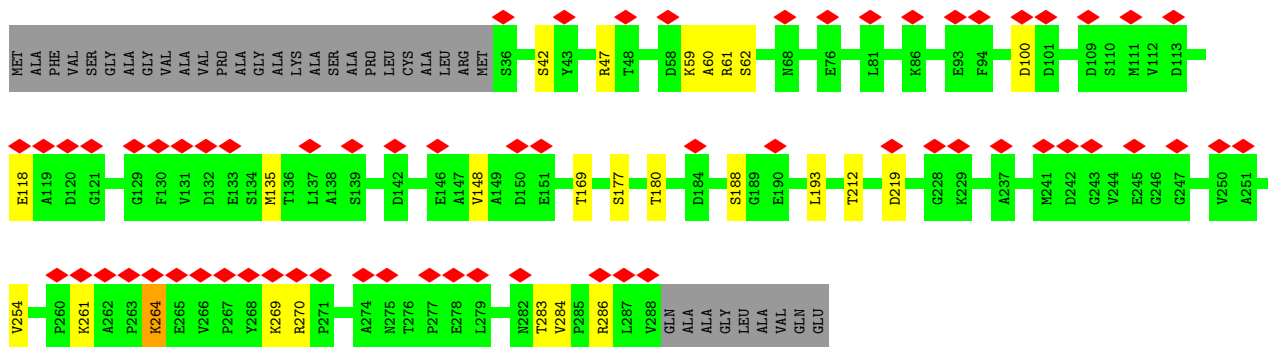
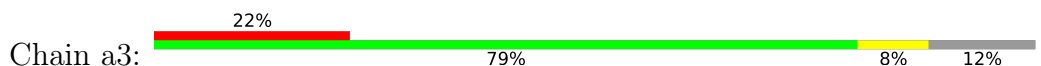




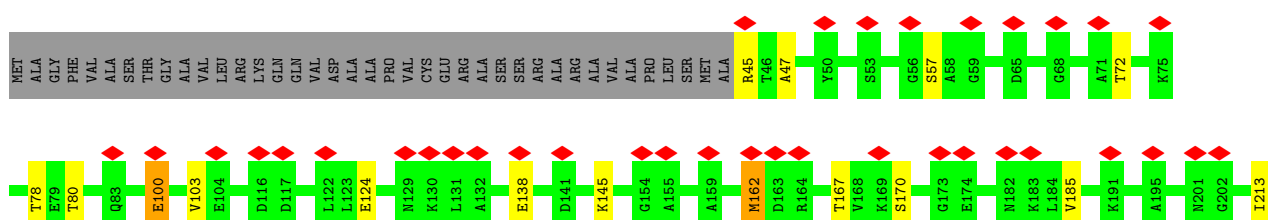
• Molecule 17: LRC5

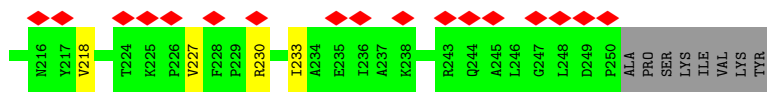


• Molecule 17: LRC5

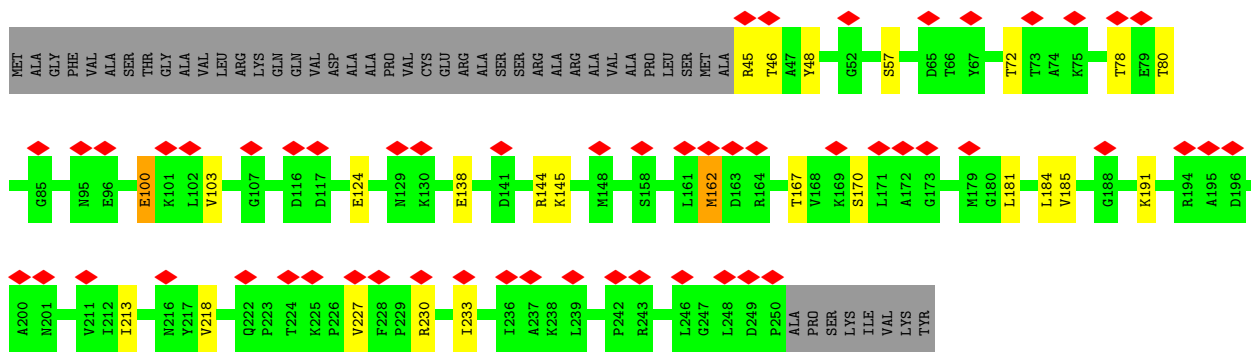


• Molecule 18: FAS1 domain-containing protein

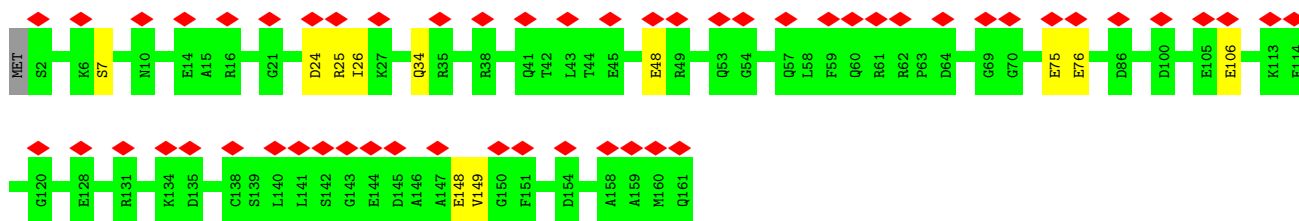
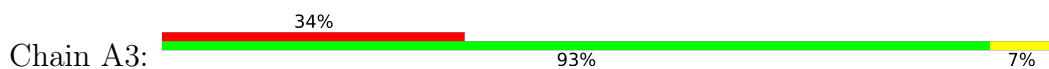




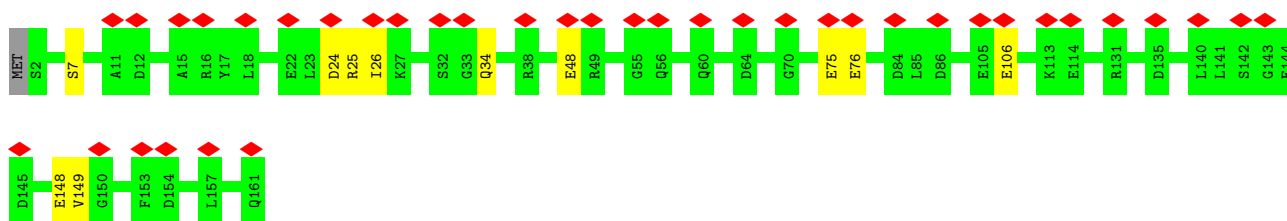
• Molecule 18: FAS1 domain-containing protein



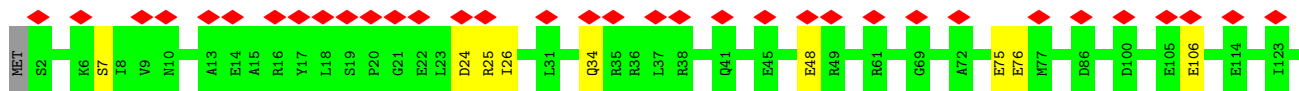
• Molecule 19: Allophycocyanin alpha subunit

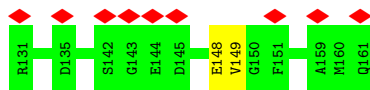


• Molecule 19: Allophycocyanin alpha subunit

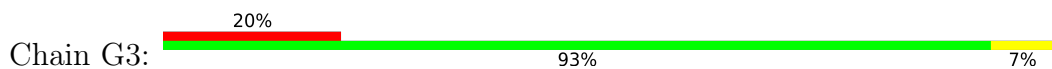


• Molecule 19: Allophycocyanin alpha subunit

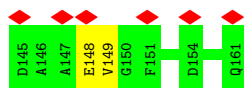
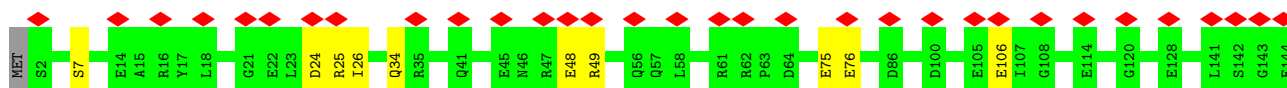




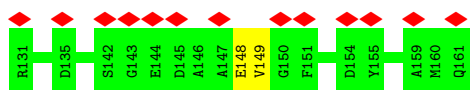
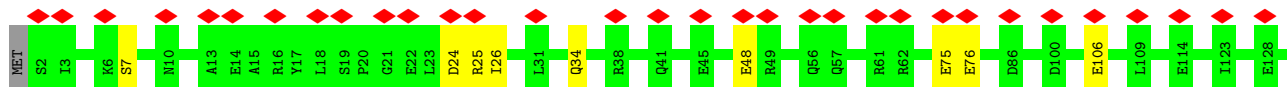
- Molecule 19: Allophycocyanin alpha subunit



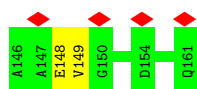
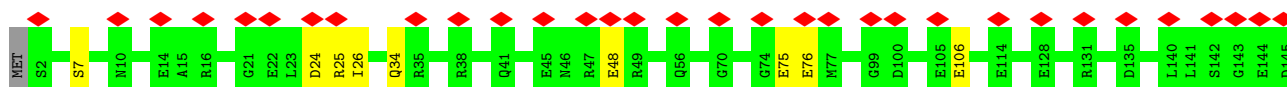
- Molecule 19: Allophycocyanin alpha subunit



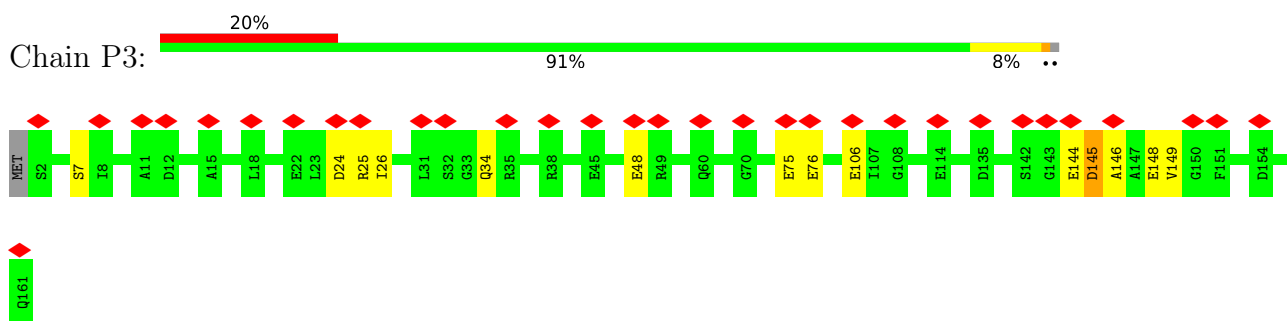
- Molecule 19: Allophycocyanin alpha subunit



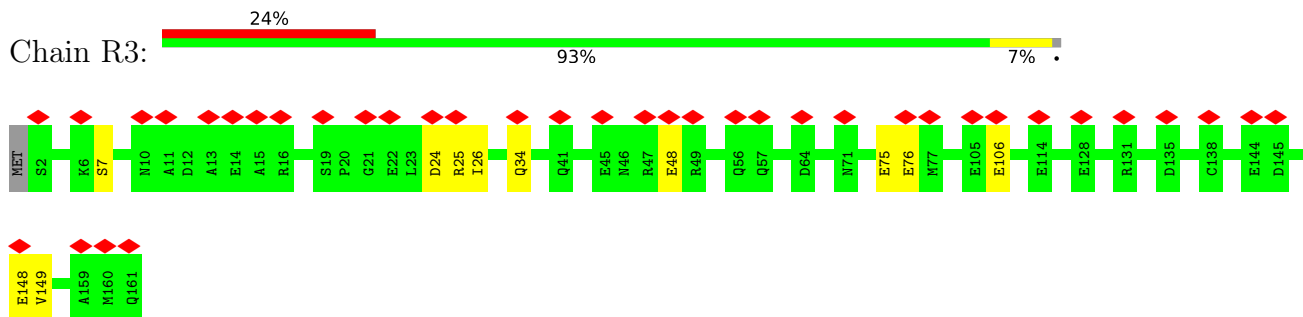
- Molecule 19: Allophycocyanin alpha subunit



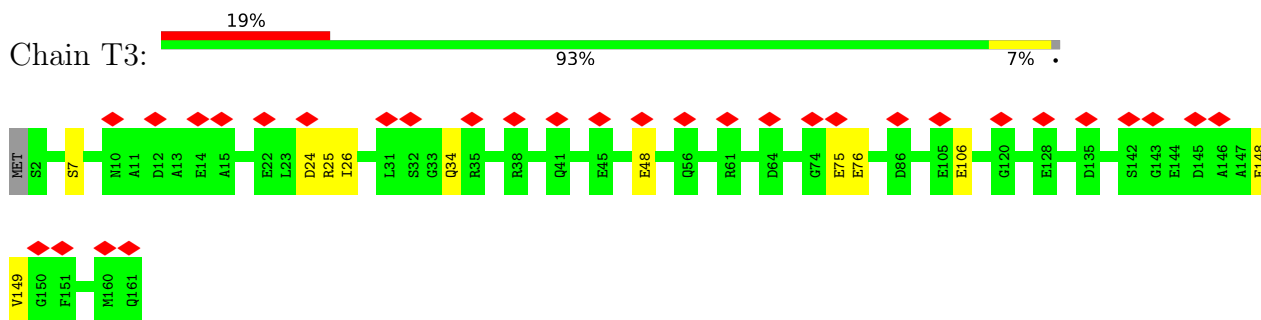
- Molecule 19: Allophycocyanin alpha subunit



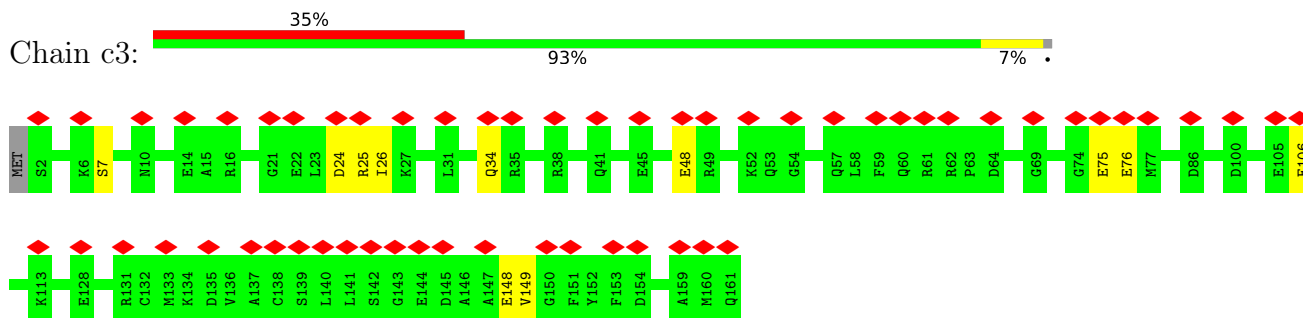
- Molecule 19: Allophycocyanin alpha subunit



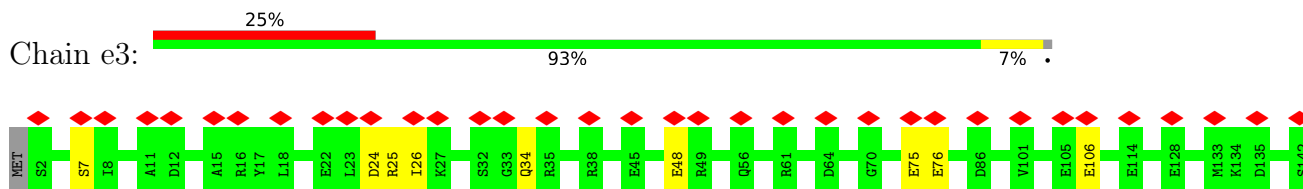
- Molecule 19: Allophycocyanin alpha subunit

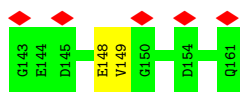


- Molecule 19: Allophycocyanin alpha subunit

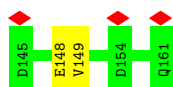
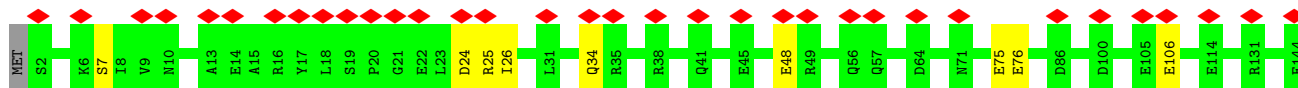
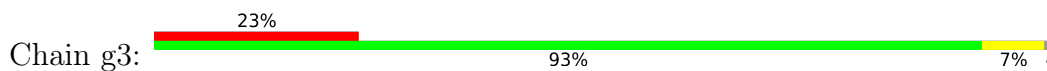


- Molecule 19: Allophycocyanin alpha subunit

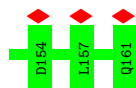
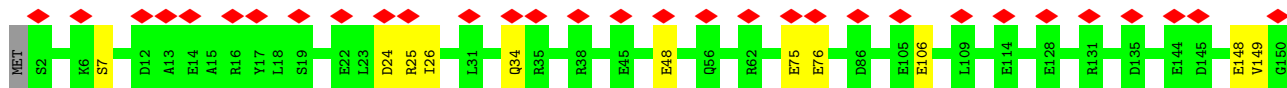
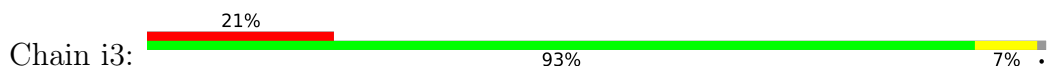




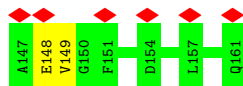
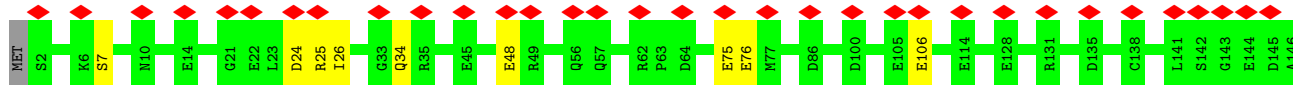
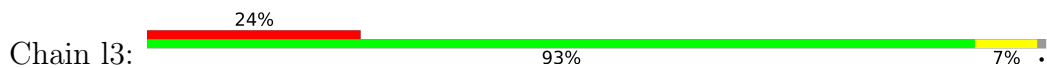
- Molecule 19: Allophycocyanin alpha subunit



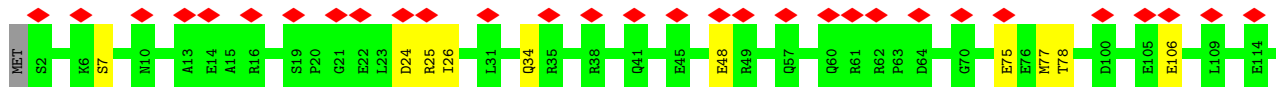
- Molecule 19: Allophycocyanin alpha subunit



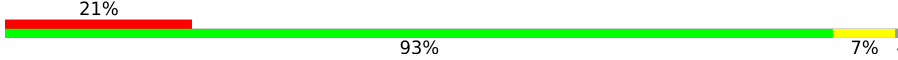
- Molecule 19: Allophycocyanin alpha subunit

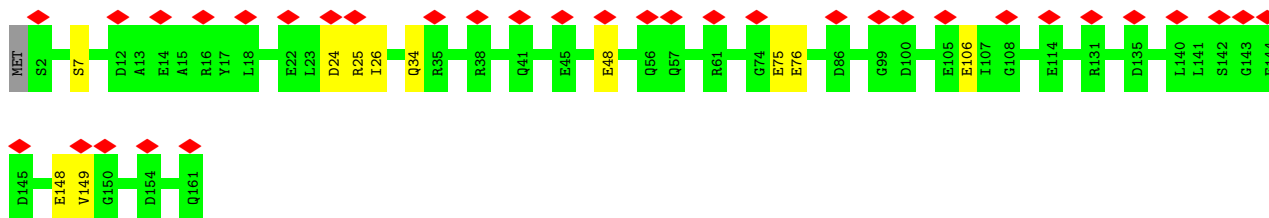


- Molecule 19: Allophycocyanin alpha subunit




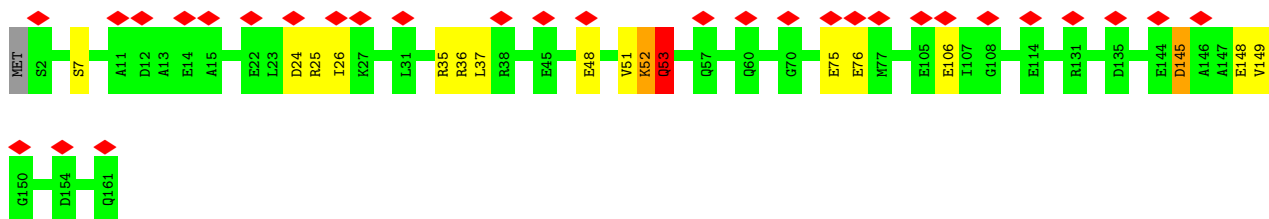
- Molecule 19: Allophycocyanin alpha subunit

Chain p3: 

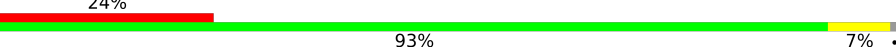


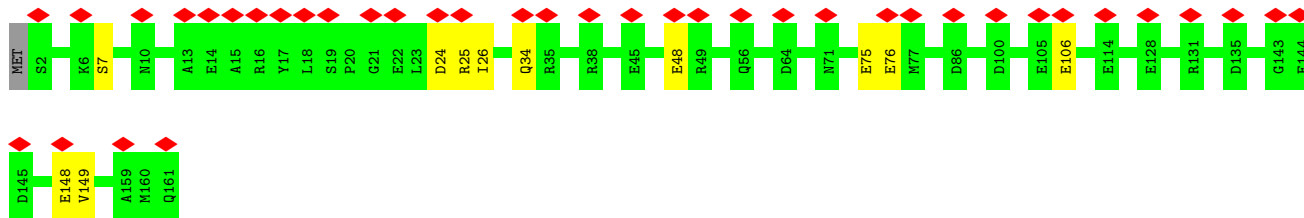
- Molecule 19: Allophycocyanin alpha subunit

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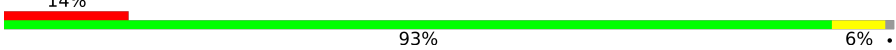


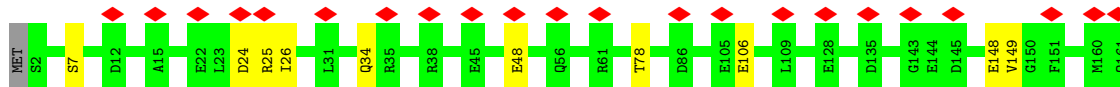
- Molecule 19: Allophycocyanin alpha subunit

Chain t3: 



- Molecule 19: Allophycocyanin alpha subunit

Chain v3: 



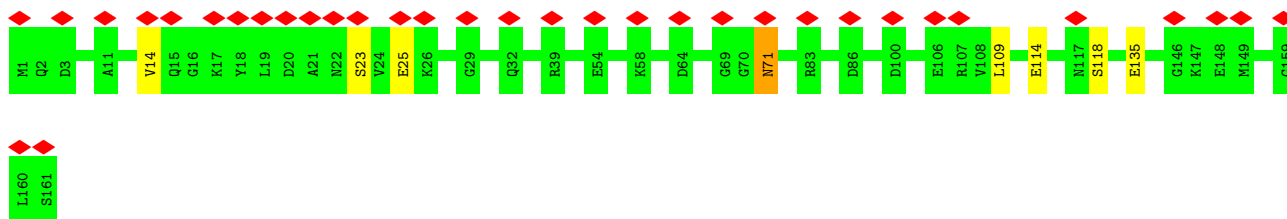
- Molecule 20: Allophycocyanin beta subunit

Chain B3: 

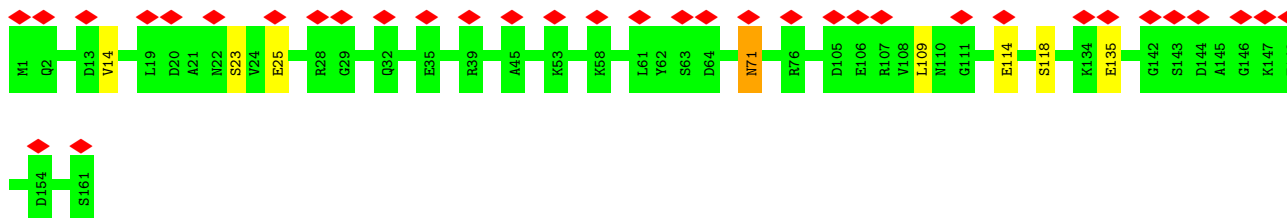


- Molecule 20: Allophycocyanin beta subunit

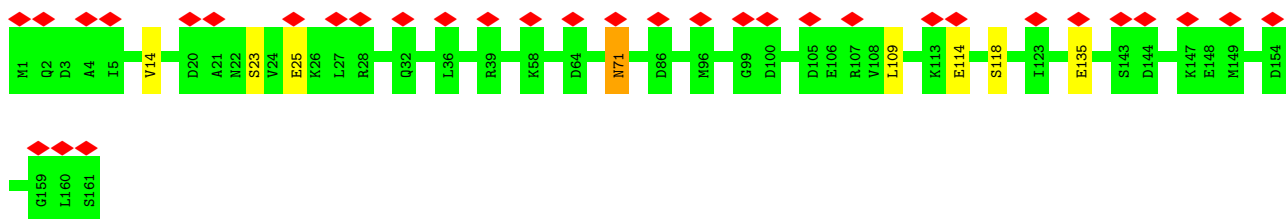
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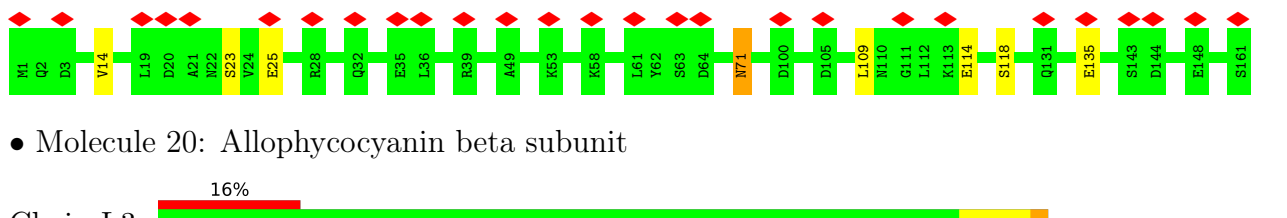
• Molecule 20: Allophycocyanin beta subunit



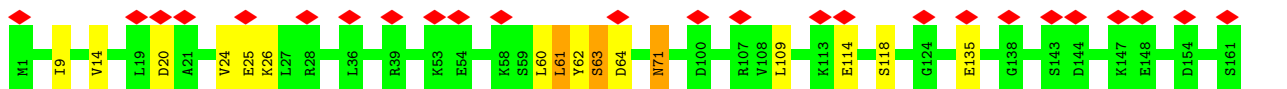
• Molecule 20: Allophycocyanin beta subunit



• Molecule 20: Allophycocyanin beta subunit

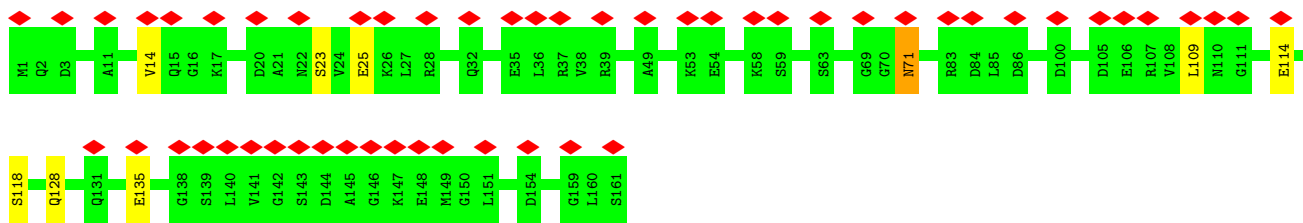


• Molecule 20: Allophycocyanin beta subunit

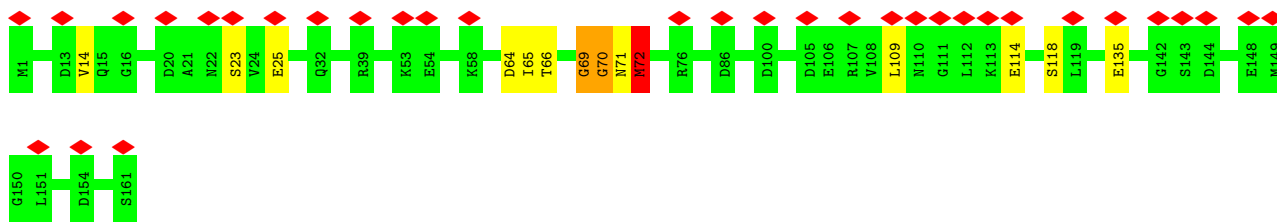
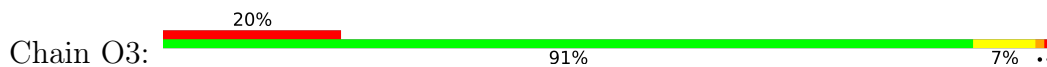


• Molecule 20: Allophycocyanin beta subunit

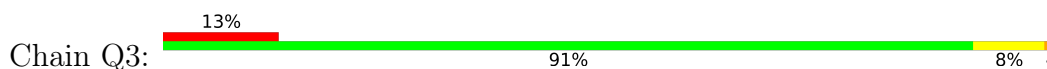




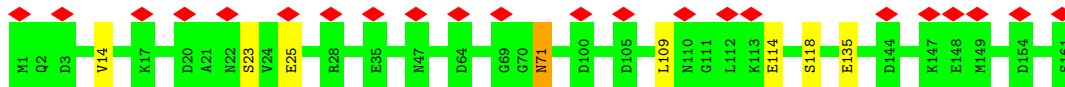
- Molecule 20: Allophycocyanin beta subunit



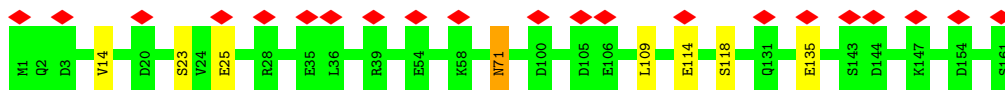
- Molecule 20: Allophycocyanin beta subunit



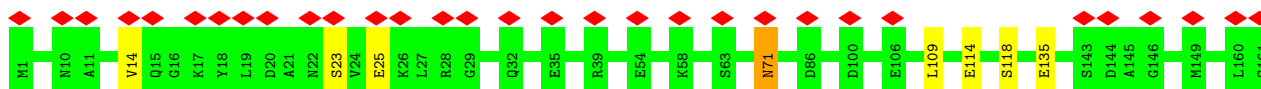
- Molecule 20: Allophycocyanin beta subunit



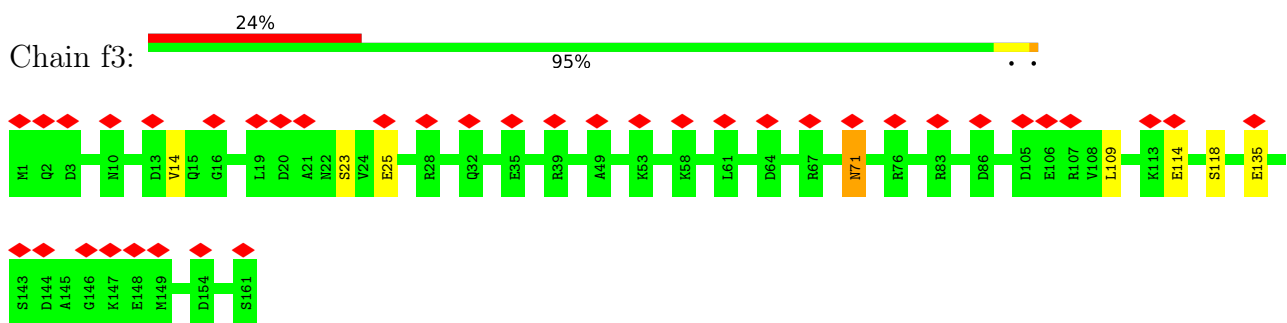
- Molecule 20: Allophycocyanin beta subunit



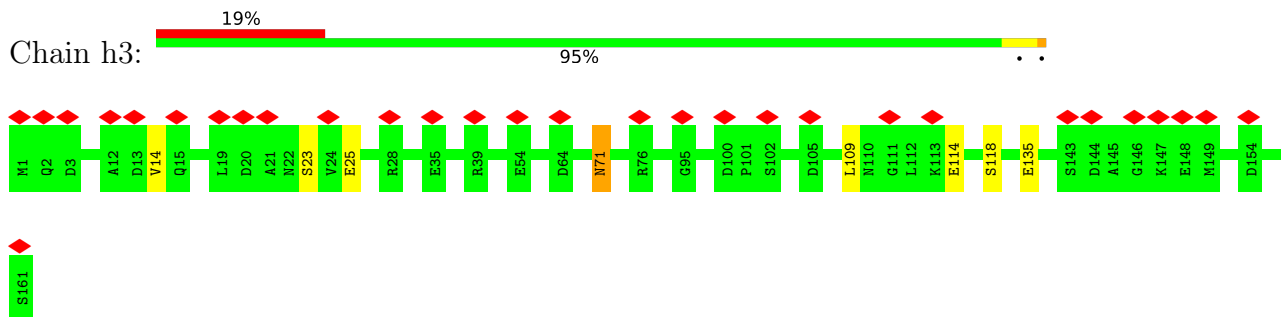
- Molecule 20: Allophycocyanin beta subunit



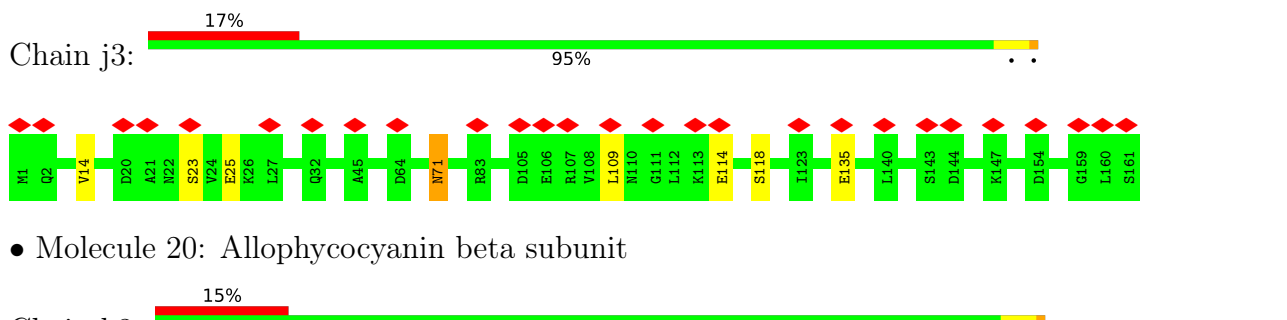
- Molecule 20: Allophycocyanin beta subunit



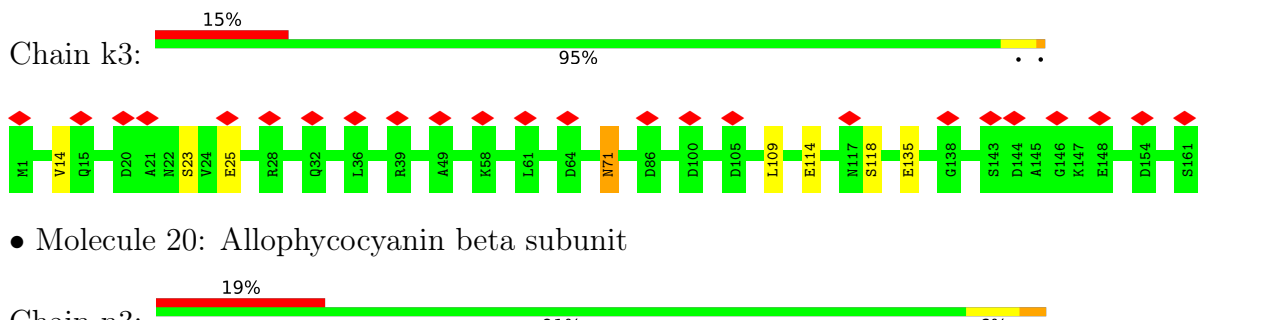
- Molecule 20: Allophycocyanin beta subunit



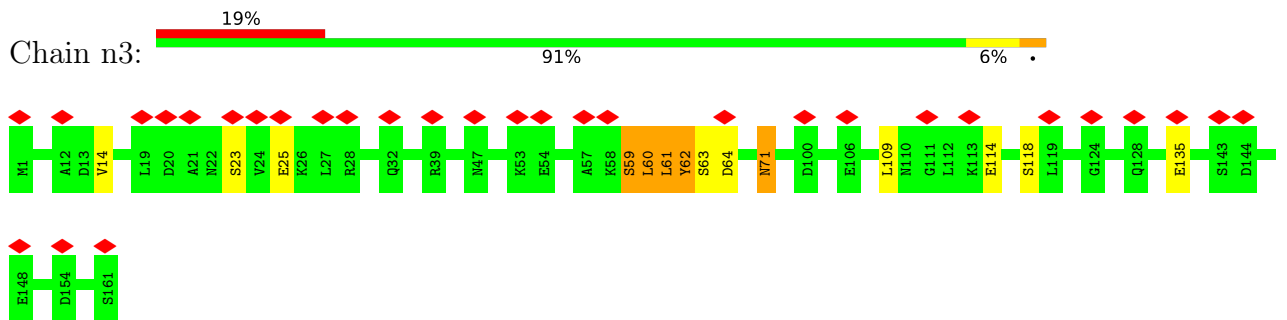
- Molecule 20: Allophycocyanin beta subunit



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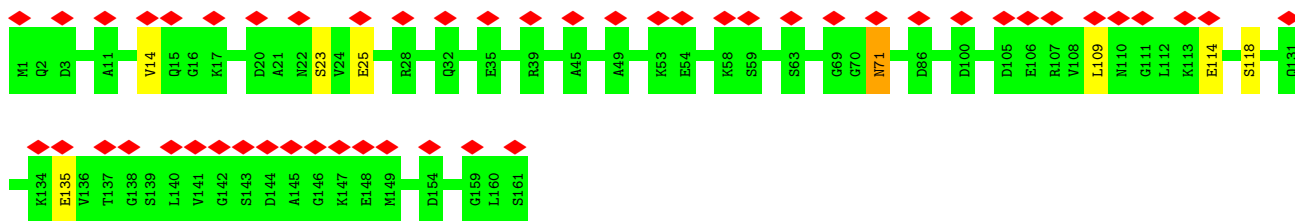


- Molecule 20: Allophycocyanin beta subunit

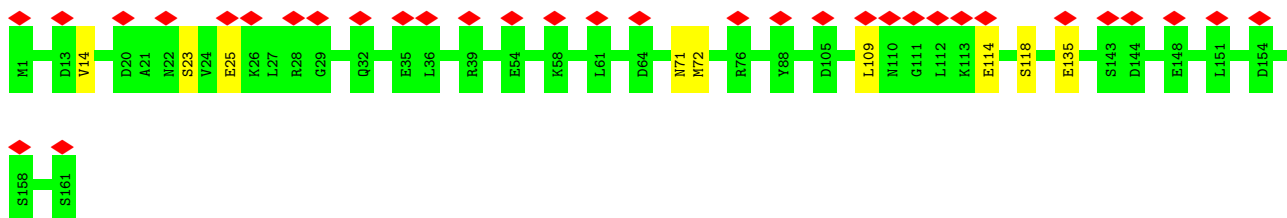


- Molecule 20: Allophycocyanin beta subunit

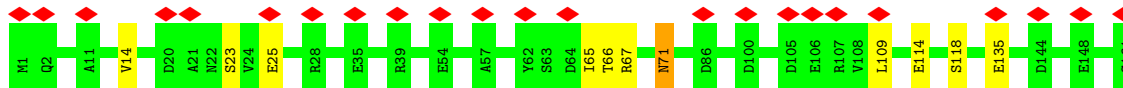
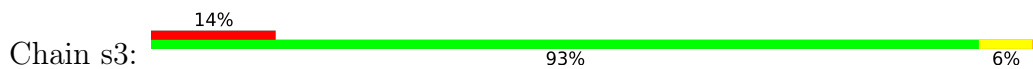




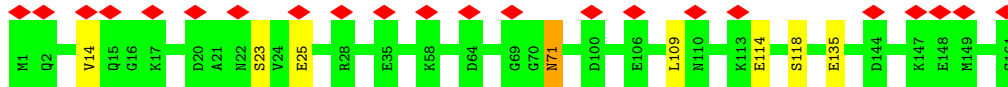
• Molecule 20: Allophycocyanin beta subunit



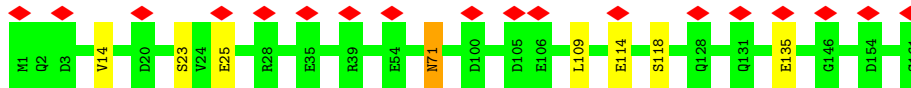
• Molecule 20: Allophycocyanin beta subunit



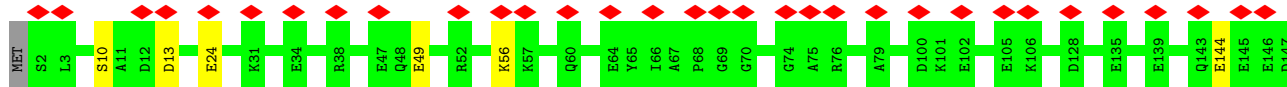
• Molecule 20: Allophycocyanin beta subunit

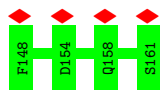


• Molecule 20: Allophycocyanin beta subunit

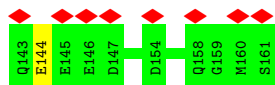
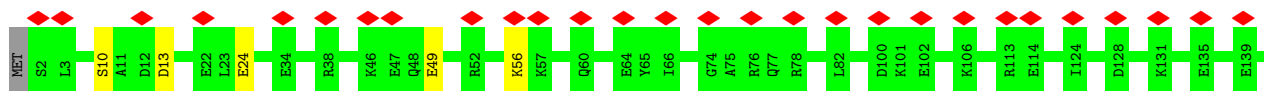


• Molecule 21: Allophycocyanin gamma subunit





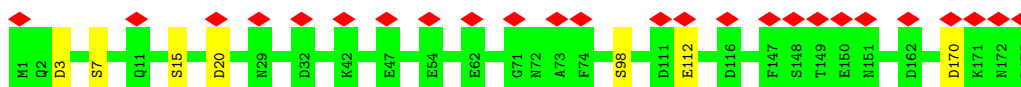
- Molecule 21: Allophycocyanin gamma subunit



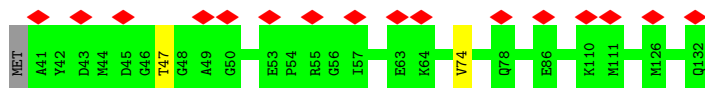
- Molecule 22: Allophycocyanin beta 18 subunit



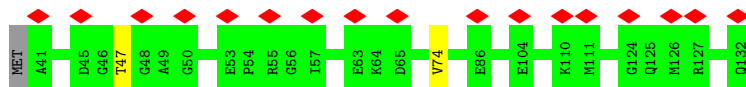
- Molecule 22: Allophycocyanin beta 18 subunit



- Molecule 23: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core



- Molecule 23: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

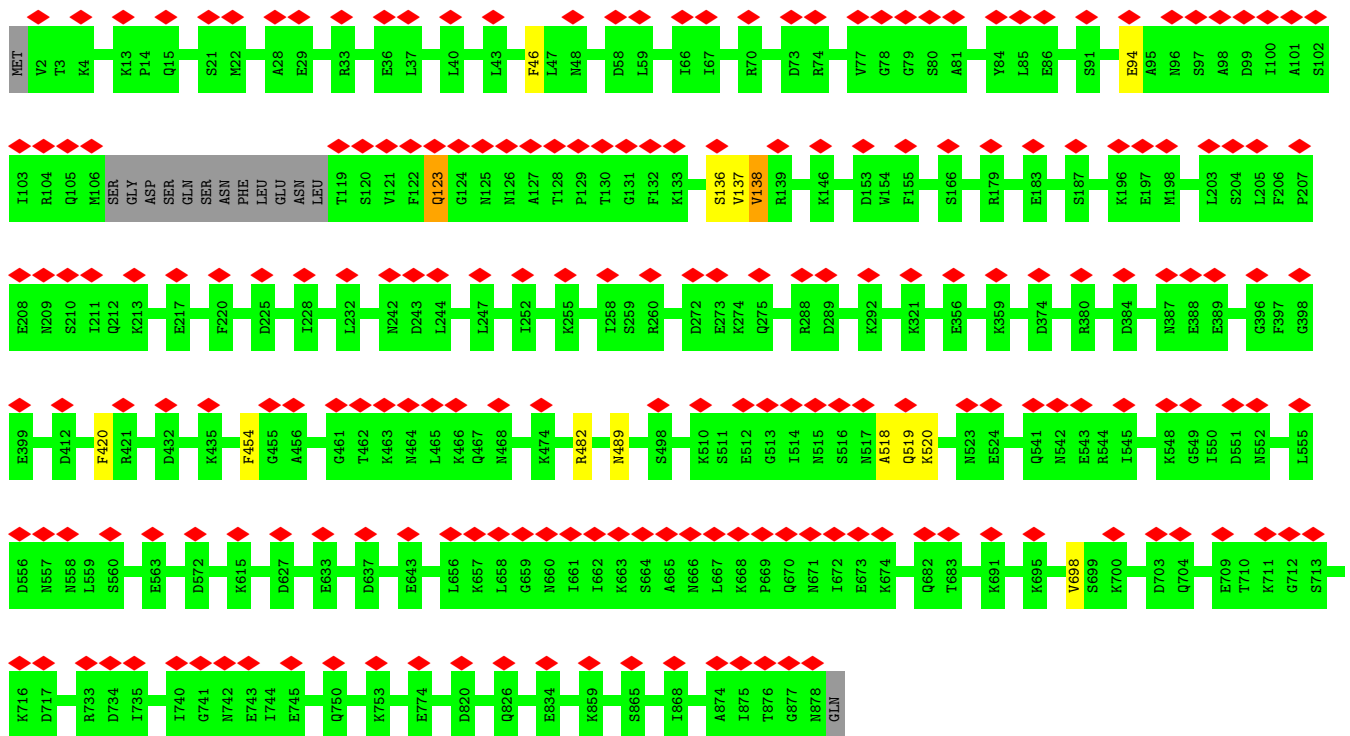


- Molecule 24: Phycobiliprotein ApcE

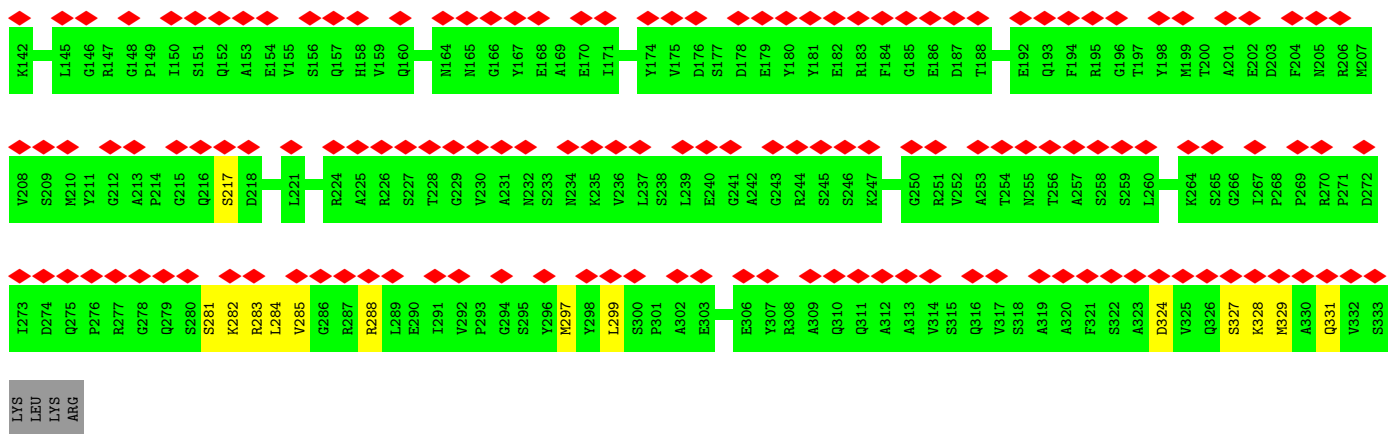




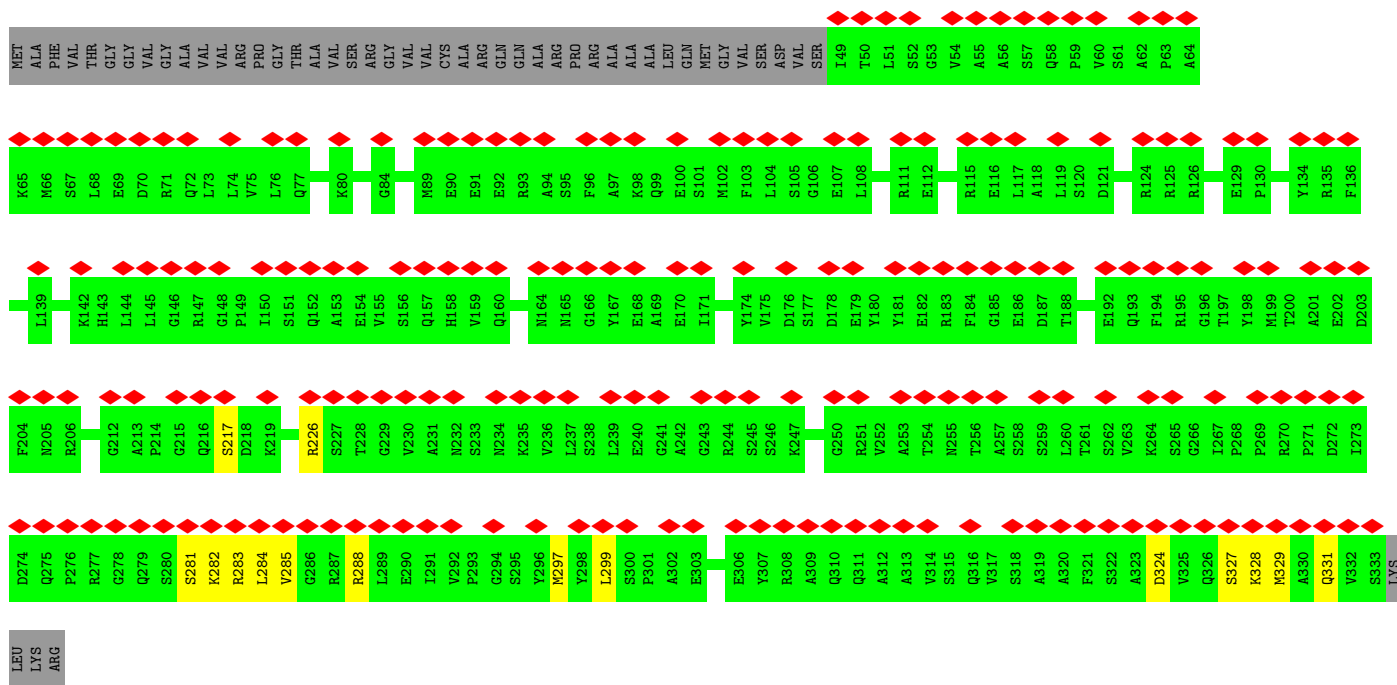
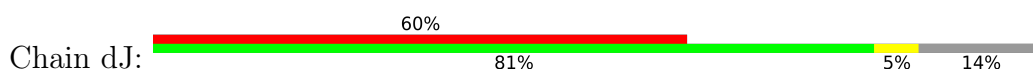
• Molecule 24: Phycobiliprotein ApcE



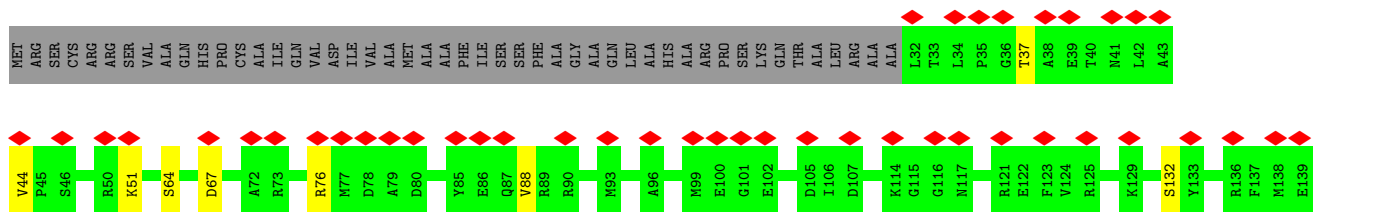
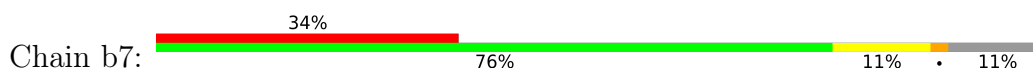
• Molecule 25: Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod

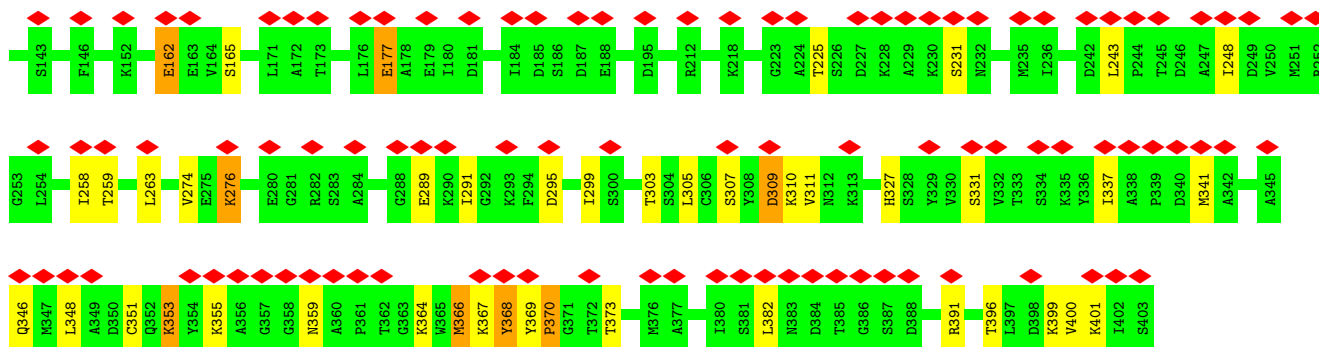


• Molecule 26: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

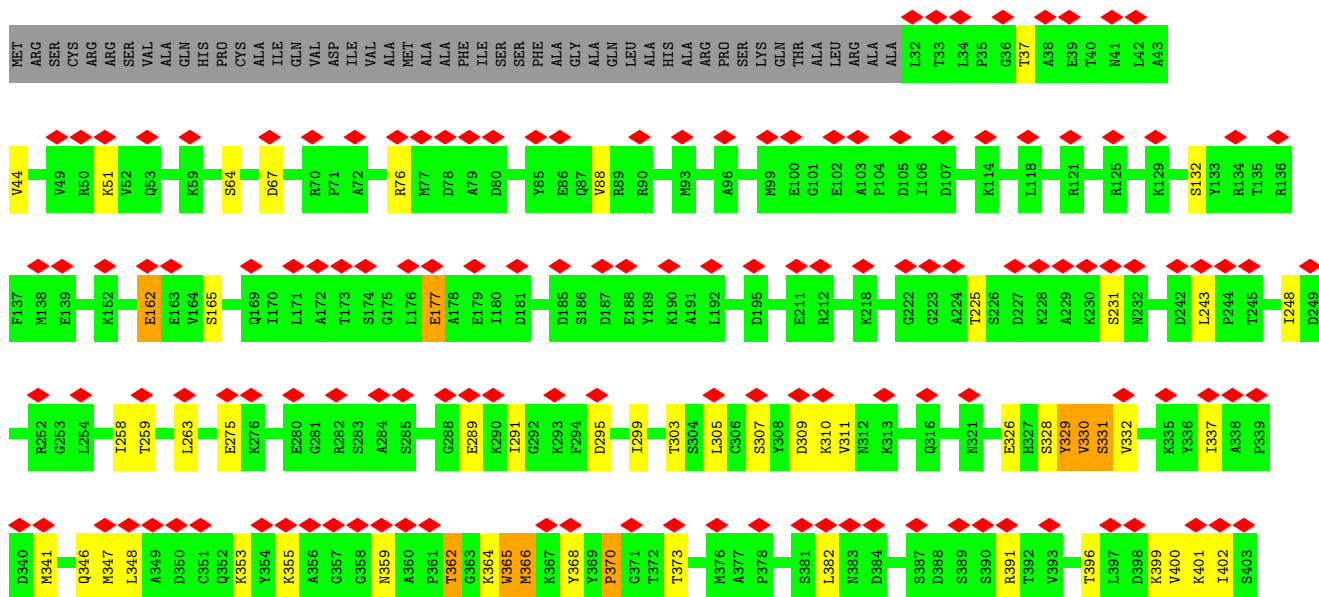
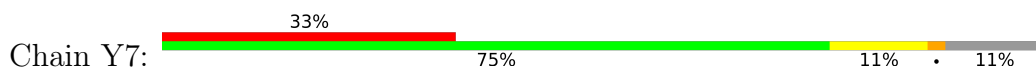


• Molecule 27: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

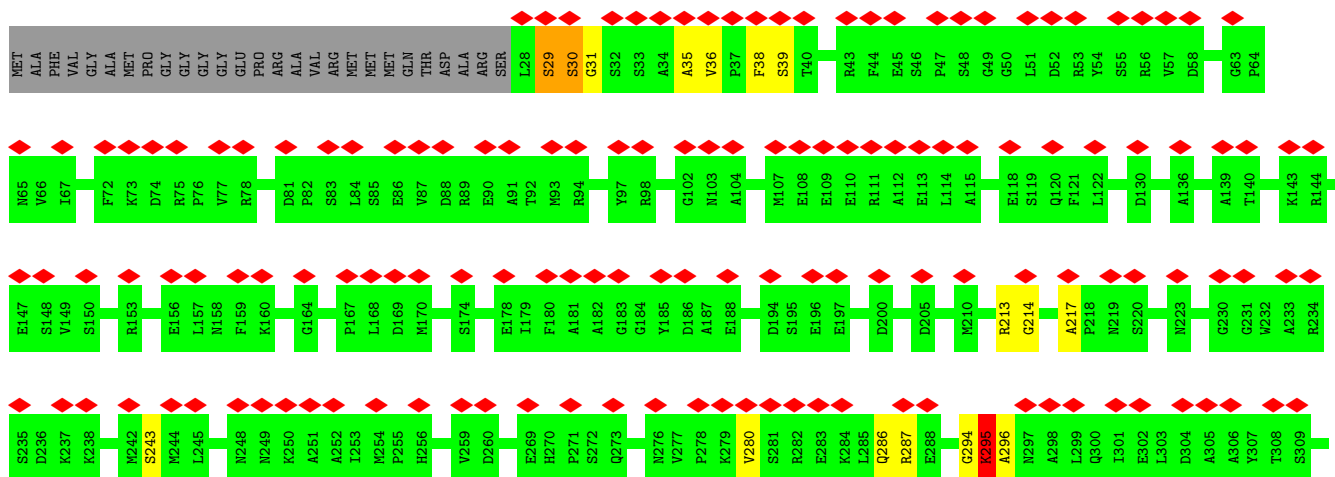
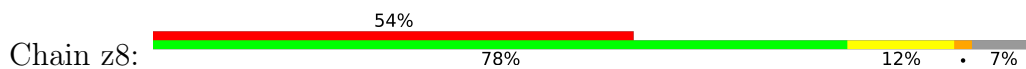


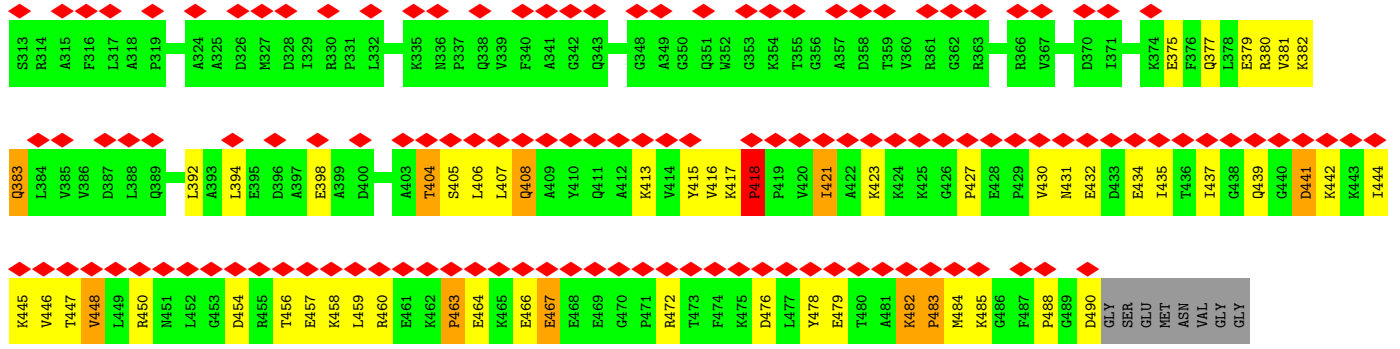


- Molecule 27: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

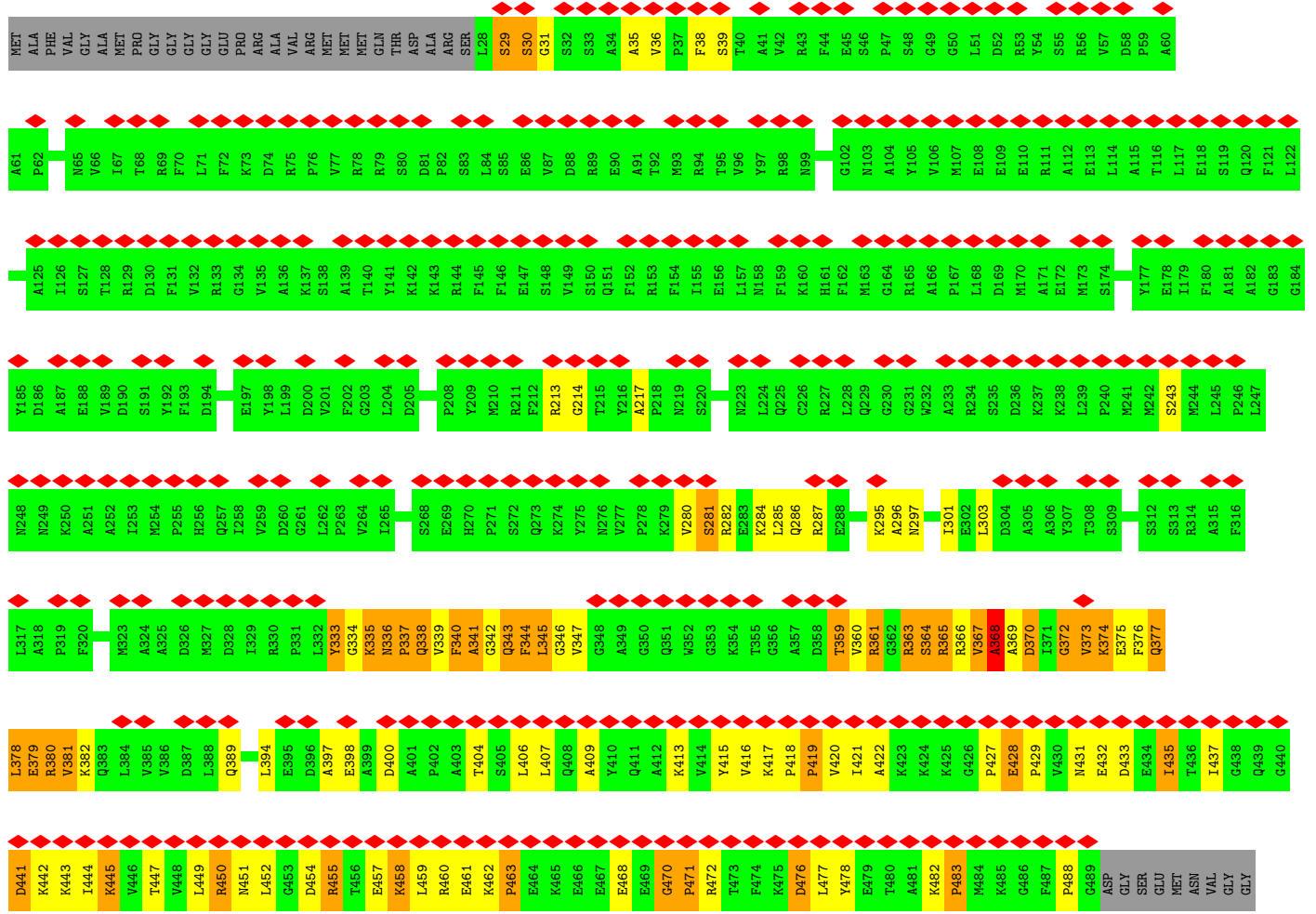


- Molecule 28: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

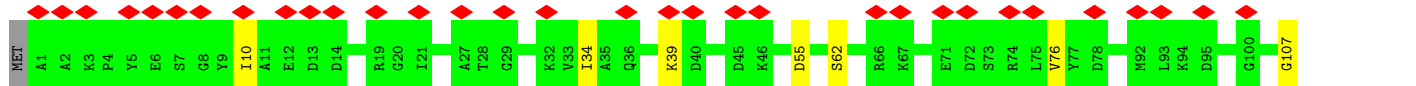
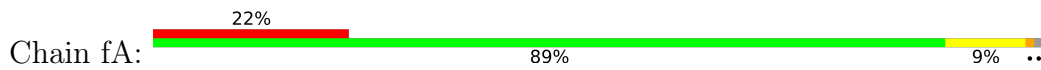




• Molecule 28: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



• Molecule 29: FAS1 domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	215000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	6000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.353	Depositor
Minimum map value	-0.833	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.081	Depositor
Recommended contour level	0.36	Depositor
Map size (Å)	626.688, 626.688, 626.688	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.632, 1.632, 1.632	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: MEN, PUB, 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	AA	1.16	9/793 (1.1%)	1.60	14/1069 (1.3%)
1	EA	0.54	0/797	0.97	2/1073 (0.2%)
2	B1	0.33	0/1297	0.66	0/1750
2	B7	0.31	0/1297	0.59	1/1750 (0.1%)
2	B8	0.32	0/1303	0.57	1/1758 (0.1%)
2	B9	0.43	1/1297 (0.1%)	0.70	3/1750 (0.2%)
2	BA	0.39	0/1297	0.60	0/1750
2	BF	0.32	0/1303	0.56	1/1758 (0.1%)
2	BG	0.37	0/1297	0.73	5/1750 (0.3%)
2	BI	0.32	0/1294	0.60	1/1746 (0.1%)
2	BK	0.33	0/1297	0.66	0/1750
2	C5	0.37	0/1297	0.61	0/1750
2	CA	0.38	0/1297	0.61	1/1750 (0.1%)
2	CJ	0.37	0/1297	0.61	0/1750
2	D1	0.33	0/1297	0.62	0/1750
2	D4	0.30	0/1315	0.54	1/1774 (0.1%)
2	D7	0.31	0/1297	0.59	1/1750 (0.1%)
2	D8	0.36	0/1315	0.60	0/1774
2	D9	0.38	1/1297 (0.1%)	0.58	0/1750
2	DA	0.43	0/1065	0.66	1/1437 (0.1%)
2	DF	0.35	0/1315	0.58	0/1774
2	DG	0.36	0/1297	0.62	3/1750 (0.2%)
2	DH	0.35	0/1315	0.55	0/1774
2	DI	0.40	0/1297	0.75	4/1750 (0.2%)
2	DK	0.33	0/1297	0.62	0/1750
2	E5	0.37	0/1297	0.63	1/1750 (0.1%)
2	EJ	0.37	0/1297	0.63	1/1750 (0.1%)
2	F1	0.33	0/1297	0.63	1/1750 (0.1%)
2	F4	0.32	0/1315	0.62	4/1774 (0.2%)
2	F7	0.33	0/1297	0.61	1/1750 (0.1%)
2	F8	0.44	0/1315	0.62	0/1774
2	F9	0.43	0/1297	0.63	1/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	FA	0.43	0/1297	0.64	2/1750 (0.1%)
2	FF	0.44	0/1315	0.62	0/1774
2	FG	0.36	0/1297	0.72	3/1750 (0.2%)
2	FH	0.41	0/1315	0.68	3/1774 (0.2%)
2	FI	0.36	0/1297	0.63	2/1750 (0.1%)
2	FK	0.34	0/1297	0.63	1/1750 (0.1%)
2	G5	0.32	0/1297	0.61	1/1750 (0.1%)
2	GA	0.39	0/1297	0.56	0/1750
2	GJ	0.32	0/1297	0.61	1/1750 (0.1%)
2	H1	0.34	0/1309	0.64	0/1766
2	H4	0.30	0/1315	0.59	2/1774 (0.1%)
2	H7	0.31	0/1309	0.66	1/1766 (0.1%)
2	H8	0.37	0/1315	0.56	1/1774 (0.1%)
2	H9	0.38	0/1309	0.59	0/1766
2	HA	0.40	0/1273	0.69	0/1718
2	HF	0.37	0/1315	0.56	1/1774 (0.1%)
2	HG	0.39	0/1303	0.71	3/1758 (0.2%)
2	HH	0.37	0/1315	0.57	1/1774 (0.1%)
2	HI	0.32	0/1309	0.59	1/1766 (0.1%)
2	HK	0.34	0/1309	0.64	0/1766
2	I5	0.42	0/1309	0.71	3/1766 (0.2%)
2	IA	0.45	0/1297	0.71	3/1750 (0.2%)
2	IJ	0.41	0/1309	0.72	3/1766 (0.2%)
2	J1	0.34	0/1297	0.65	0/1750
2	J4	0.30	0/1309	0.52	0/1766
2	J7	0.41	0/1297	0.66	3/1750 (0.2%)
2	J8	0.39	0/1315	0.60	2/1774 (0.1%)
2	J9	0.40	0/1297	0.59	0/1750
2	JF	0.39	0/1315	0.60	2/1774 (0.1%)
2	JG	0.38	0/1297	0.67	2/1750 (0.1%)
2	JH	0.36	0/1309	0.56	0/1766
2	JI	0.36	0/1297	0.64	2/1750 (0.1%)
2	JK	0.34	0/1297	0.65	0/1750
2	K5	0.33	0/1297	0.57	0/1750
2	KJ	0.33	0/1297	0.57	0/1750
2	L1	0.34	0/1297	0.65	0/1750
2	L4	0.32	0/1315	0.53	0/1774
2	L7	0.31	0/1297	0.60	1/1750 (0.1%)
2	L8	0.49	0/1315	0.67	2/1774 (0.1%)
2	L9	0.41	0/1297	0.59	0/1750
2	LA	0.36	0/1293	0.85	6/1746 (0.3%)
2	LF	0.49	0/1315	0.67	2/1774 (0.1%)
2	LG	0.40	0/1297	0.64	1/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	LH	0.42	0/1315	0.63	3/1774 (0.2%)
2	LI	0.30	0/1297	0.54	1/1750 (0.1%)
2	LK	0.34	0/1297	0.65	0/1750
2	M5	0.34	0/1297	0.61	0/1750
2	MA	0.41	0/1297	0.66	1/1750 (0.1%)
2	MJ	0.34	0/1297	0.61	0/1750
2	N1	0.35	0/1315	0.56	0/1774
2	N4	0.37	0/1315	0.64	1/1774 (0.1%)
2	N7	0.31	0/1297	0.61	2/1750 (0.1%)
2	N8	0.34	0/1315	0.62	0/1774
2	NA	0.43	0/1056	0.65	0/1426
2	NF	0.33	0/1315	0.62	0/1774
2	NH	0.45	0/1315	0.65	1/1774 (0.1%)
2	NK	0.35	0/1315	0.56	0/1774
2	O5	0.33	0/1297	0.62	1/1750 (0.1%)
2	O9	0.38	0/1297	0.60	0/1750
2	OA	0.41	0/1297	0.67	1/1750 (0.1%)
2	OG	0.38	0/1297	0.75	6/1750 (0.3%)
2	OI	0.34	0/1297	0.61	0/1750
2	OJ	0.33	0/1297	0.62	1/1750 (0.1%)
2	P1	0.41	0/1315	0.59	0/1774
2	P2	0.35	0/1297	0.63	2/1750 (0.1%)
2	P4	0.28	0/1297	0.50	0/1750
2	P6	0.30	0/1297	0.47	0/1750
2	P7	0.31	0/1297	0.61	2/1750 (0.1%)
2	P8	0.33	0/1315	0.59	0/1774
2	PA	0.39	0/1297	0.61	1/1750 (0.1%)
2	PB	0.30	0/1297	0.47	0/1750
2	PC	0.35	0/1297	0.62	1/1750 (0.1%)
2	PD	0.37	0/1297	0.47	0/1750
2	PE	0.36	0/1297	0.47	0/1750
2	PF	0.33	0/1315	0.60	0/1774
2	PH	0.31	0/1297	0.50	0/1750
2	PK	0.41	0/1315	0.59	0/1774
2	Q5	0.33	0/1297	0.67	4/1750 (0.2%)
2	Q9	0.38	0/1297	0.59	0/1750
2	QA	0.40	0/1273	0.66	0/1718
2	QG	0.41	0/1297	0.73	7/1750 (0.4%)
2	QI	0.39	0/1297	0.75	3/1750 (0.2%)
2	QJ	0.33	0/1297	0.67	4/1750 (0.2%)
2	R1	0.42	0/1315	0.58	0/1774
2	R2	0.34	0/1297	0.62	1/1750 (0.1%)
2	R4	0.32	0/1303	0.51	0/1758

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	R6	0.35	0/1297	0.49	0/1750
2	R7	0.32	0/1297	0.63	2/1750 (0.1%)
2	R8	0.36	0/1309	0.58	0/1766
2	RA	0.35	0/1297	0.63	2/1750 (0.1%)
2	RB	0.35	0/1297	0.49	0/1750
2	RC	0.34	0/1297	0.62	1/1750 (0.1%)
2	RD	0.32	0/1297	0.49	0/1750
2	RE	0.33	0/1297	0.49	0/1750
2	RF	0.36	0/1309	0.58	0/1766
2	RH	0.36	0/1303	0.65	2/1758 (0.1%)
2	RK	0.41	0/1315	0.58	0/1774
2	S5	0.34	0/1297	0.60	0/1750
2	S9	0.44	0/1297	0.66	2/1750 (0.1%)
2	SA	0.43	0/1297	0.64	1/1750 (0.1%)
2	SG	0.39	1/1297 (0.1%)	0.70	3/1750 (0.2%)
2	SI	0.36	0/1297	0.57	0/1750
2	SJ	0.34	0/1297	0.60	0/1750
2	T1	0.54	0/1315	0.62	0/1774
2	T2	0.33	0/1297	0.62	0/1750
2	T4	0.31	0/1315	0.55	0/1774
2	T6	0.33	0/1297	0.47	0/1750
2	T7	0.33	0/1309	0.67	3/1766 (0.2%)
2	T8	0.37	0/1309	0.61	1/1766 (0.1%)
2	TB	0.33	0/1297	0.47	0/1750
2	TC	0.34	0/1297	0.62	0/1750
2	TD	0.36	0/1297	0.49	0/1750
2	TE	0.36	0/1297	0.49	0/1750
2	TF	0.38	0/1309	0.61	1/1766 (0.1%)
2	TH	0.37	0/1315	0.63	1/1774 (0.1%)
2	TK	0.54	0/1315	0.62	0/1774
2	U5	0.35	0/1309	0.66	0/1766
2	U9	0.35	0/1309	0.59	0/1766
2	UG	0.38	0/1303	0.65	3/1758 (0.2%)
2	UI	0.36	0/1309	0.64	0/1766
2	UJ	0.35	0/1309	0.66	0/1766
2	V1	0.34	0/1315	0.57	0/1774
2	V2	0.37	0/1305	0.69	2/1762 (0.1%)
2	V4	0.31	0/1315	0.61	2/1774 (0.1%)
2	V6	0.38	0/1297	0.49	0/1750
2	V7	0.35	0/1297	0.63	1/1750 (0.1%)
2	V8	0.35	0/1309	0.61	2/1766 (0.1%)
2	VA	0.38	0/1297	0.70	3/1750 (0.2%)
2	VB	0.38	0/1297	0.49	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	VC	0.39	0/1303	0.70	1/1758 (0.1%)
2	VD	0.31	0/1309	0.54	2/1766 (0.1%)
2	VE	0.31	0/1309	0.53	2/1766 (0.1%)
2	VF	0.35	0/1309	0.61	2/1766 (0.1%)
2	VH	0.36	0/1315	0.65	3/1774 (0.2%)
2	VK	0.34	0/1315	0.57	0/1774
2	W5	0.33	0/1297	0.70	4/1750 (0.2%)
2	W9	0.47	0/1297	0.65	2/1750 (0.1%)
2	WG	0.37	0/1297	0.75	4/1750 (0.2%)
2	WI	0.35	0/1297	0.66	3/1750 (0.2%)
2	WJ	0.33	0/1297	0.70	4/1750 (0.2%)
2	X1	0.41	0/1315	0.59	0/1774
2	X4	0.31	0/1309	0.57	2/1766 (0.1%)
2	X7	0.32	0/1297	0.62	2/1750 (0.1%)
2	X8	0.38	0/1315	0.62	0/1774
2	XA	0.35	0/1297	0.61	1/1750 (0.1%)
2	XF	0.37	0/1315	0.62	0/1774
2	XH	0.37	0/1309	0.58	1/1766 (0.1%)
2	XK	0.41	0/1315	0.59	0/1774
2	Y2	0.32	0/1297	0.61	0/1750
2	Y5	0.33	0/1297	0.62	0/1750
2	Y6	0.32	0/1297	0.47	0/1750
2	Y9	0.41	0/1297	0.66	1/1750 (0.1%)
2	YA	0.36	0/1297	0.60	1/1750 (0.1%)
2	YB	0.32	0/1297	0.53	1/1750 (0.1%)
2	YC	0.32	0/1297	0.61	0/1750
2	YD	0.40	0/1297	0.50	0/1750
2	YE	0.40	0/1297	0.50	0/1750
2	YG	0.41	0/1297	0.64	0/1750
2	YI	0.32	0/1297	0.53	0/1750
2	YJ	0.33	0/1297	0.62	0/1750
2	Z4	0.32	0/1315	0.54	1/1774 (0.1%)
2	Z8	0.33	0/1315	0.69	2/1774 (0.1%)
2	ZA	0.35	0/1112	0.65	0/1500
2	ZF	0.33	0/1315	0.69	2/1774 (0.1%)
2	ZH	0.40	0/1315	0.58	1/1774 (0.1%)
2	a2	0.33	0/1297	0.63	0/1750
2	a6	0.38	0/1297	0.53	0/1750
2	aA	0.38	0/1297	0.58	0/1750
2	aB	0.38	0/1297	0.53	0/1750
2	aC	0.33	0/1297	0.63	0/1750
2	aD	0.32	0/1297	0.48	0/1750
2	aE	0.32	0/1297	0.48	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	b8	0.33	0/1315	0.58	0/1774
2	bA	0.33	0/1297	0.59	1/1750 (0.1%)
2	bF	0.33	0/1315	0.58	1/1774 (0.1%)
2	c2	0.33	0/1297	0.60	1/1750 (0.1%)
2	c4	0.30	0/1309	0.59	1/1766 (0.1%)
2	c6	0.27	0/1297	0.46	0/1750
2	cB	0.27	0/1297	0.46	0/1750
2	cC	0.33	0/1297	0.60	1/1750 (0.1%)
2	cD	0.30	0/1297	0.53	0/1750
2	cE	0.30	0/1297	0.53	0/1750
2	cH	0.32	0/1309	0.60	1/1766 (0.1%)
2	d8	0.34	0/1309	0.64	2/1766 (0.1%)
2	dA	0.33	0/1297	0.55	0/1750
2	dF	0.33	0/1309	0.64	2/1766 (0.1%)
2	e2	0.35	0/1297	0.63	0/1750
2	e4	0.29	0/1315	0.55	0/1774
2	e6	0.28	0/1297	0.48	0/1750
2	eA	0.37	0/1297	0.55	0/1750
2	eB	0.29	0/1297	0.48	0/1750
2	eC	0.35	0/1297	0.63	0/1750
2	eD	0.29	0/1297	0.53	0/1750
2	eE	0.29	0/1297	0.52	0/1750
2	eH	0.35	0/1315	0.59	0/1774
2	f8	0.33	0/1309	0.61	0/1766
2	fF	0.33	0/1309	0.61	0/1766
2	g2	0.35	0/1297	0.62	0/1750
2	g4	0.28	0/1315	0.56	0/1774
2	g6	0.27	0/1297	0.50	0/1750
2	gA	0.42	0/1102	0.73	2/1488 (0.1%)
2	gB	0.27	0/1297	0.50	0/1750
2	gC	0.34	0/1297	0.62	0/1750
2	gD	0.29	0/1297	0.51	0/1750
2	gE	0.29	0/1297	0.50	0/1750
2	gH	0.29	0/1315	0.56	0/1774
2	h8	0.32	0/1315	0.61	0/1774
2	hF	0.32	0/1315	0.61	0/1774
2	i2	0.34	0/1309	0.68	1/1766 (0.1%)
2	i4	0.29	0/1315	0.55	0/1774
2	i6	0.28	0/1303	0.51	0/1758
2	iB	0.28	0/1303	0.51	0/1758
2	iC	0.34	0/1309	0.68	1/1766 (0.1%)
2	iD	0.29	0/1309	0.57	0/1766
2	iE	0.29	0/1309	0.57	0/1766

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	iH	0.32	0/1315	0.59	0/1774
2	j8	0.32	0/1315	0.58	0/1774
2	jF	0.32	0/1315	0.58	0/1774
2	k2	0.32	0/1297	0.64	1/1750 (0.1%)
2	k4	0.29	0/1315	0.55	0/1774
2	k6	0.34	0/1297	0.60	1/1750 (0.1%)
2	kB	0.43	0/1297	0.88	10/1750 (0.6%)
2	kC	0.32	0/1297	0.64	1/1750 (0.1%)
2	kD	0.35	0/1297	0.65	3/1750 (0.2%)
2	kE	0.30	0/1297	0.50	0/1750
2	kH	0.32	0/1315	0.60	0/1774
2	l8	0.33	0/1315	0.64	2/1774 (0.1%)
2	lF	0.33	0/1315	0.64	2/1774 (0.1%)
2	m2	0.35	0/1297	0.68	2/1750 (0.1%)
2	m4	0.29	0/1315	0.59	1/1774 (0.1%)
2	m6	0.28	0/1297	0.46	0/1750
2	mB	0.28	0/1297	0.46	0/1750
2	mC	0.35	0/1297	0.68	2/1750 (0.1%)
2	mD	0.28	0/1297	0.56	0/1750
2	mE	0.28	0/1297	0.56	0/1750
2	mH	0.32	0/1315	0.60	0/1774
2	n8	0.35	0/1315	0.62	2/1774 (0.1%)
2	nF	0.34	0/1315	0.62	2/1774 (0.1%)
2	p8	0.31	0/1315	0.66	2/1774 (0.1%)
2	pF	0.31	0/1315	0.67	2/1774 (0.1%)
2	r8	0.32	0/1315	0.66	2/1774 (0.1%)
2	rF	0.32	0/1315	0.66	2/1774 (0.1%)
2	t8	0.34	0/1309	0.65	0/1766
2	tF	0.33	0/1309	0.65	0/1766
2	v8	0.34	0/1315	0.67	2/1774 (0.1%)
2	vF	0.33	0/1315	0.67	2/1774 (0.1%)
3	A1	0.34	0/1271	0.64	1/1721 (0.1%)
3	A7	0.36	0/1271	0.55	0/1721
3	A8	0.32	0/1271	0.60	1/1721 (0.1%)
3	A9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	AF	0.32	0/1271	0.60	1/1721 (0.1%)
3	AG	0.39	0/1271	0.60	0/1721
3	AI	0.33	0/1271	0.61	0/1721
3	AK	0.34	0/1271	0.64	1/1721 (0.1%)
3	B5	0.35	0/1271	0.60	0/1721
3	BJ	0.35	0/1271	0.60	0/1721
3	C1	0.34	0/1271	0.58	0/1721
3	C4	0.32	0/1271	0.54	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	C7	0.33	0/1271	0.54	0/1721
3	C8	0.33	0/1271	0.71	3/1721 (0.2%)
3	C9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	CF	0.34	0/1271	0.71	3/1721 (0.2%)
3	CG	0.39	0/1271	0.60	0/1721
3	CH	0.38	0/1271	0.56	0/1721
3	CI	0.33	0/1271	0.61	0/1721
3	CK	0.33	0/1271	0.58	0/1721
3	D5	0.38	0/1271	0.63	0/1721
3	DJ	0.38	0/1271	0.63	0/1721
3	E1	0.33	0/1271	0.61	1/1721 (0.1%)
3	E4	0.29	0/1271	0.53	0/1721
3	E7	0.31	0/1271	0.53	0/1721
3	E8	0.38	0/1271	0.64	1/1721 (0.1%)
3	E9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	EF	0.38	0/1271	0.64	2/1721 (0.1%)
3	EG	0.39	0/1271	0.60	0/1721
3	EH	0.34	0/1271	0.53	0/1721
3	EI	0.33	0/1271	0.61	0/1721
3	EK	0.33	0/1271	0.61	2/1721 (0.1%)
3	F5	0.38	0/1271	0.60	0/1721
3	FJ	0.38	0/1271	0.60	0/1721
3	G1	0.34	0/1271	0.61	1/1721 (0.1%)
3	G4	0.29	0/1271	0.48	0/1721
3	G7	0.32	0/1271	0.52	0/1721
3	G8	0.50	0/1271	0.83	5/1721 (0.3%)
3	G9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	GF	0.50	0/1271	0.83	5/1721 (0.3%)
3	GG	0.39	0/1271	0.60	0/1721
3	GH	0.33	0/1271	0.55	0/1721
3	GI	0.33	0/1271	0.61	0/1721
3	GK	0.34	0/1271	0.61	1/1721 (0.1%)
3	H5	0.34	0/1271	0.60	0/1721
3	HJ	0.34	0/1271	0.60	0/1721
3	I1	0.33	0/1271	0.63	1/1721 (0.1%)
3	I4	0.31	0/1271	0.53	0/1721
3	I7	0.34	0/1271	0.54	0/1721
3	I8	0.48	0/1271	0.77	4/1721 (0.2%)
3	I9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	IF	0.49	0/1271	0.77	4/1721 (0.2%)
3	IG	0.39	0/1271	0.60	0/1721
3	IH	0.37	0/1271	0.54	0/1721
3	II	0.33	0/1271	0.61	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	IK	0.32	0/1271	0.63	1/1721 (0.1%)
3	J5	0.34	0/1271	0.58	0/1721
3	JA	0.45	0/1271	0.60	0/1721
3	JJ	0.33	0/1271	0.58	0/1721
3	K1	0.35	0/1271	0.64	1/1721 (0.1%)
3	K4	0.34	0/1271	0.54	0/1721
3	K7	0.38	0/1267	0.55	0/1716
3	K8	0.38	0/1271	0.60	0/1721
3	K9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	KF	0.38	0/1271	0.60	0/1721
3	KG	0.39	0/1271	0.60	0/1721
3	KH	0.43	0/1271	0.59	0/1721
3	KI	0.33	0/1271	0.61	0/1721
3	KK	0.35	0/1271	0.64	1/1721 (0.1%)
3	L5	0.35	0/1271	0.59	0/1721
3	LJ	0.35	0/1271	0.59	0/1721
3	M1	0.36	0/1271	0.57	0/1721
3	M4	0.36	0/1271	0.56	0/1721
3	M7	0.36	0/1271	0.54	0/1721
3	M8	0.31	0/1271	0.61	0/1721
3	MF	0.31	0/1271	0.61	0/1721
3	MH	0.47	0/1271	0.60	0/1721
3	MK	0.36	0/1271	0.58	0/1721
3	N5	0.33	0/1271	0.60	1/1721 (0.1%)
3	N9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	NG	0.39	0/1271	0.60	0/1721
3	NI	0.33	0/1271	0.61	0/1721
3	NJ	0.33	0/1271	0.60	1/1721 (0.1%)
3	O1	0.48	0/1271	0.63	1/1721 (0.1%)
3	O2	0.33	0/1271	0.59	0/1721
3	O4	0.31	0/1271	0.52	1/1721 (0.1%)
3	O6	0.34	0/1271	0.47	0/1721
3	O7	0.33	0/1271	0.60	0/1721
3	O8	0.35	0/1271	0.60	0/1721
3	OB	0.34	0/1271	0.47	0/1721
3	OC	0.33	0/1271	0.59	0/1721
3	OD	0.37	0/1271	0.49	0/1721
3	OE	0.37	0/1271	0.49	0/1721
3	OF	0.35	0/1271	0.60	1/1721 (0.1%)
3	OH	0.34	0/1271	0.54	0/1721
3	OK	0.47	0/1271	0.63	1/1721 (0.1%)
3	P5	0.34	0/1271	0.63	0/1721
3	P9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	PG	0.39	0/1271	0.60	0/1721
3	PI	0.33	0/1271	0.61	0/1721
3	PJ	0.34	0/1271	0.63	0/1721
3	Q1	0.44	0/1271	0.60	0/1721
3	Q2	0.34	0/1271	0.60	2/1721 (0.1%)
3	Q4	0.29	0/1271	0.52	0/1721
3	Q6	0.39	0/1271	0.48	0/1721
3	Q7	0.32	0/1271	0.55	0/1721
3	Q8	0.36	0/1271	0.66	1/1721 (0.1%)
3	QB	0.39	0/1271	0.48	0/1721
3	QC	0.34	0/1271	0.61	2/1721 (0.1%)
3	QD	0.33	0/1271	0.50	0/1721
3	QE	0.33	0/1271	0.50	0/1721
3	QF	0.36	0/1271	0.66	1/1721 (0.1%)
3	QH	0.34	0/1271	0.54	0/1721
3	QK	0.44	0/1271	0.60	0/1721
3	R5	0.35	0/1271	0.63	1/1721 (0.1%)
3	R9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	RG	0.39	0/1271	0.60	0/1721
3	RI	0.33	0/1271	0.61	0/1721
3	RJ	0.35	0/1271	0.63	1/1721 (0.1%)
3	S1	0.46	0/1271	0.63	0/1721
3	S2	0.35	0/1271	0.65	2/1721 (0.1%)
3	S4	0.30	0/1271	0.50	0/1721
3	S6	0.36	0/1271	0.49	0/1721
3	S7	0.34	0/1271	0.55	0/1721
3	S8	0.40	0/1271	0.69	2/1721 (0.1%)
3	SB	0.36	0/1271	0.49	0/1721
3	SC	0.35	0/1271	0.64	2/1721 (0.1%)
3	SD	0.35	0/1271	0.49	0/1721
3	SE	0.34	0/1271	0.49	0/1721
3	SF	0.40	0/1271	0.67	2/1721 (0.1%)
3	SH	0.33	0/1271	0.53	0/1721
3	SK	0.45	0/1271	0.63	0/1721
3	T5	0.35	0/1271	0.62	0/1721
3	T9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	TA	0.44	0/1271	0.60	0/1721
3	TG	0.39	0/1271	0.60	0/1721
3	TI	0.33	0/1271	0.61	0/1721
3	TJ	0.35	0/1271	0.62	0/1721
3	U1	0.38	0/1271	0.58	0/1721
3	U2	0.33	0/1271	0.69	3/1721 (0.2%)
3	U4	0.32	0/1267	0.55	0/1717

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	U6	0.39	0/1271	0.48	0/1721
3	U7	0.36	0/1271	0.56	0/1721
3	U8	0.41	0/1271	0.68	2/1721 (0.1%)
3	UB	0.39	0/1271	0.48	0/1721
3	UC	0.33	0/1271	0.69	3/1721 (0.2%)
3	UD	0.32	0/1271	0.50	0/1721
3	UE	0.32	0/1271	0.50	0/1721
3	UF	0.41	0/1271	0.68	2/1721 (0.1%)
3	UH	0.40	0/1271	0.59	0/1721
3	UK	0.38	0/1271	0.58	0/1721
3	V5	0.34	0/1271	0.62	1/1721 (0.1%)
3	V9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	VG	0.39	0/1271	0.60	0/1721
3	VI	0.33	0/1271	0.61	0/1721
3	VJ	0.34	0/1271	0.62	1/1721 (0.1%)
3	W1	0.38	0/1271	0.56	0/1721
3	W2	0.33	0/1271	0.64	1/1721 (0.1%)
3	W4	0.34	0/1271	0.59	1/1721 (0.1%)
3	W6	0.37	0/1271	0.49	0/1721
3	W7	0.38	0/1271	0.59	0/1721
3	W8	0.35	0/1271	0.62	2/1721 (0.1%)
3	WB	0.37	0/1271	0.50	0/1721
3	WC	0.33	0/1271	0.64	2/1721 (0.1%)
3	WD	0.38	0/1271	0.50	0/1721
3	WE	0.38	0/1271	0.50	0/1721
3	WF	0.34	0/1271	0.62	2/1721 (0.1%)
3	WH	0.45	0/1271	0.59	0/1721
3	WK	0.38	0/1271	0.56	0/1721
3	X5	0.34	0/1271	0.65	1/1721 (0.1%)
3	X9	0.45	1/1271 (0.1%)	0.71	1/1721 (0.1%)
3	XG	0.39	0/1271	0.60	0/1721
3	XI	0.33	0/1271	0.61	0/1721
3	XJ	0.34	0/1271	0.65	1/1721 (0.1%)
3	Y4	0.34	0/1267	0.57	1/1717 (0.1%)
3	Y8	0.34	0/1271	0.57	0/1721
3	YF	0.34	0/1271	0.57	0/1721
3	YH	0.40	0/1271	0.58	0/1721
3	Z2	0.33	0/1271	0.59	0/1721
3	Z6	0.39	0/1271	0.48	0/1721
3	ZB	0.39	0/1271	0.48	0/1721
3	ZC	0.33	0/1271	0.59	0/1721
3	ZD	0.37	0/1271	0.53	0/1721
3	ZE	0.36	0/1271	0.50	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	a4	0.29	0/1271	0.53	0/1721
3	a8	0.34	0/1271	0.62	0/1721
3	aF	0.34	0/1271	0.62	0/1721
3	aH	0.33	0/1271	0.56	0/1721
3	b2	0.32	0/1271	0.71	2/1721 (0.1%)
3	b6	0.30	0/1271	0.52	0/1721
3	bB	0.30	0/1271	0.52	0/1721
3	bC	0.32	0/1271	0.71	2/1721 (0.1%)
3	bD	0.52	0/1271	0.84	10/1721 (0.6%)
3	bE	0.31	0/1271	0.53	1/1721 (0.1%)
3	c8	0.33	0/1271	0.62	1/1721 (0.1%)
3	cF	0.33	0/1271	0.61	1/1721 (0.1%)
3	d2	0.34	0/1271	0.70	2/1721 (0.1%)
3	d4	0.30	0/1271	0.57	0/1721
3	d6	0.31	0/1271	0.52	0/1721
3	dB	0.31	0/1271	0.51	0/1721
3	dC	0.35	0/1271	0.70	2/1721 (0.1%)
3	dD	0.29	0/1271	0.50	0/1721
3	dE	0.29	0/1271	0.50	0/1721
3	dH	0.31	0/1271	0.59	0/1721
3	e8	0.34	0/1271	0.65	1/1721 (0.1%)
3	eF	0.34	0/1271	0.65	1/1721 (0.1%)
3	f2	0.34	0/1271	0.69	2/1721 (0.1%)
3	f4	0.28	0/1271	0.56	0/1721
3	f6	0.30	0/1271	0.53	0/1721
3	fB	0.29	0/1271	0.53	0/1721
3	fC	0.34	0/1271	0.69	2/1721 (0.1%)
3	fD	0.29	0/1271	0.51	0/1721
3	fE	0.28	0/1271	0.51	0/1721
3	fH	0.31	0/1271	0.56	0/1721
3	g8	0.31	0/1271	0.58	0/1721
3	gF	0.31	0/1271	0.59	0/1721
3	h2	0.32	0/1271	0.69	3/1721 (0.2%)
3	h4	0.27	0/1271	0.51	0/1721
3	h6	0.31	0/1271	0.49	0/1721
3	hB	0.32	0/1271	0.49	0/1721
3	hC	0.32	0/1271	0.69	3/1721 (0.2%)
3	hD	0.30	0/1271	0.51	0/1721
3	hE	0.30	0/1271	0.51	0/1721
3	hH	0.30	0/1271	0.54	0/1721
3	i8	0.35	0/1271	0.62	2/1721 (0.1%)
3	iF	0.35	0/1271	0.62	2/1721 (0.1%)
3	j2	0.35	0/1271	0.72	3/1721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
3	j4	0.29	0/1271	0.52	0/1721
3	j6	0.31	0/1271	0.50	0/1721
3	jB	0.31	0/1271	0.50	0/1721
3	jC	0.35	0/1271	0.72	3/1721 (0.2%)
3	jD	0.29	0/1271	0.47	0/1721
3	jE	0.29	0/1271	0.47	0/1721
3	jH	0.30	0/1271	0.55	0/1721
3	k8	0.33	0/1271	0.63	0/1721
3	kF	0.33	0/1271	0.63	0/1721
3	l2	0.37	0/1271	0.76	7/1721 (0.4%)
3	l4	0.30	0/1271	0.59	0/1721
3	l6	0.34	0/1271	0.52	0/1721
3	lB	0.32	0/1271	0.48	0/1721
3	lC	0.37	0/1271	0.76	7/1721 (0.4%)
3	lD	0.70	1/1259 (0.1%)	1.27	23/1706 (1.3%)
3	lE	0.32	0/1271	0.55	0/1721
3	lH	0.35	0/1271	0.61	0/1721
3	m8	0.35	0/1271	0.65	0/1721
3	mF	0.35	0/1271	0.65	0/1721
3	o8	0.33	0/1271	0.64	0/1721
3	oF	0.33	0/1271	0.64	0/1721
3	q8	0.32	0/1271	0.65	1/1721 (0.1%)
3	qF	0.32	0/1271	0.65	1/1721 (0.1%)
3	s8	0.36	0/1271	0.60	2/1721 (0.1%)
3	sF	0.36	0/1271	0.60	2/1721 (0.1%)
3	u8	0.33	0/1271	0.62	1/1721 (0.1%)
3	uF	0.33	0/1271	0.62	1/1721 (0.1%)
4	KA	0.55	2/1754 (0.1%)	0.88	7/2373 (0.3%)
4	UA	0.49	1/1763 (0.1%)	0.87	8/2386 (0.3%)
5	WA	0.62	0/1105	1.04	4/1499 (0.3%)
5	cA	0.57	0/1111	0.94	5/1508 (0.3%)
6	A2	0.35	0/2025	0.59	0/2722
6	A5	0.36	0/2017	0.60	0/2711
6	A6	0.30	0/2025	0.49	0/2722
6	AB	0.30	0/2025	0.49	0/2722
6	AC	0.36	0/2025	0.59	0/2722
6	AD	0.30	0/2025	0.50	0/2722
6	AE	0.30	0/2025	0.50	0/2722
6	AJ	0.36	0/2017	0.59	0/2711
6	Y1	0.35	0/1866	0.58	0/2506
6	YK	0.35	0/1866	0.58	0/2506
7	B2	0.40	0/1917	0.64	0/2592
7	B6	0.55	0/1933	0.72	0/2614

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	BB	0.55	0/1933	0.75	3/2614 (0.1%)
7	BC	0.40	0/1917	0.64	0/2592
7	BD	0.54	0/1938	0.74	6/2621 (0.2%)
7	BE	0.54	0/1939	0.73	4/2622 (0.2%)
8	C2	0.32	0/1251	0.59	0/1699
8	C6	0.43	0/1251	0.52	1/1699 (0.1%)
8	CB	0.43	0/1251	0.52	1/1699 (0.1%)
8	CC	0.32	0/1251	0.59	0/1699
8	CD	0.37	0/1251	0.48	0/1699
8	CE	0.37	0/1251	0.48	0/1699
8	E2	0.41	0/1251	0.59	0/1699
8	E6	0.42	0/1251	0.51	0/1699
8	EB	0.42	0/1251	0.49	0/1699
8	EC	0.41	0/1251	0.59	0/1699
8	ED	0.43	0/1251	0.50	0/1699
8	EE	0.43	0/1251	0.50	0/1699
8	G2	0.34	0/1251	0.61	1/1699 (0.1%)
8	G6	0.40	0/1251	0.48	0/1699
8	GB	0.40	0/1251	0.48	0/1699
8	GC	0.32	0/1251	0.58	1/1699 (0.1%)
8	GD	0.51	0/1251	0.52	0/1699
8	GE	0.52	0/1251	0.52	0/1699
8	I2	0.42	0/1251	0.59	0/1699
8	I6	0.41	0/1251	0.48	0/1699
8	IB	0.41	0/1251	0.48	0/1699
8	IC	0.42	0/1251	0.59	0/1699
8	ID	0.50	0/1251	0.52	0/1699
8	IE	0.50	0/1251	0.52	0/1699
8	K2	0.36	0/1251	0.56	1/1699 (0.1%)
8	K6	0.45	0/1251	0.49	0/1699
8	KB	0.46	0/1251	0.49	0/1699
8	KC	0.36	0/1251	0.56	1/1699 (0.1%)
8	KD	0.42	0/1251	0.53	1/1699 (0.1%)
8	KE	0.40	0/1251	0.46	0/1699
8	M2	0.32	0/1251	0.55	1/1699 (0.1%)
8	M6	0.41	0/1251	0.49	0/1699
8	MB	0.41	0/1251	0.49	0/1699
8	MC	0.32	0/1251	0.55	1/1699 (0.1%)
8	MD	0.48	0/1251	0.50	0/1699
8	ME	0.48	0/1251	0.50	0/1699
9	D2	0.32	0/1274	0.61	0/1723
9	D6	0.39	0/1274	0.52	0/1723
9	DB	0.39	0/1274	0.52	0/1723

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
9	DC	0.32	0/1274	0.61	0/1723
9	DD	0.42	0/1274	0.50	0/1723
9	DE	0.42	0/1274	0.50	0/1723
9	F2	0.32	0/1274	0.52	0/1723
9	F6	0.41	0/1274	0.51	0/1723
9	FB	0.41	0/1274	0.51	0/1723
9	FC	0.32	0/1274	0.52	0/1723
9	FD	0.38	0/1274	0.49	0/1723
9	FE	0.38	0/1274	0.49	0/1723
9	H2	0.40	0/1274	0.69	0/1723
9	H6	0.40	0/1274	0.55	1/1723 (0.1%)
9	HB	0.40	0/1274	0.55	1/1723 (0.1%)
9	HC	0.45	0/1270	0.81	4/1718 (0.2%)
9	HD	0.44	0/1274	0.52	0/1723
9	HE	0.44	0/1274	0.52	0/1723
9	J2	0.43	0/1270	0.72	3/1718 (0.2%)
9	J6	0.41	0/1274	0.54	0/1723
9	JB	0.41	0/1274	0.54	0/1723
9	JC	0.40	0/1274	0.72	2/1723 (0.1%)
9	JD	0.59	0/1274	0.61	2/1723 (0.1%)
9	JE	0.59	0/1274	0.66	3/1723 (0.2%)
9	L2	0.46	0/1274	0.67	1/1723 (0.1%)
9	L6	1.00	10/1274 (0.8%)	0.98	13/1723 (0.8%)
9	LB	0.44	0/1274	0.57	0/1723
9	LC	0.46	0/1274	0.67	1/1723 (0.1%)
9	LD	0.47	0/1274	0.53	0/1723
9	LE	0.47	0/1274	0.53	0/1723
9	N2	0.32	0/1274	0.62	3/1723 (0.2%)
9	N6	0.47	0/1274	0.63	3/1723 (0.2%)
9	NB	0.48	0/1274	0.65	3/1723 (0.2%)
9	NC	0.32	0/1274	0.62	3/1723 (0.2%)
9	ND	0.49	0/1274	0.65	1/1723 (0.1%)
9	NE	0.44	0/1274	0.52	0/1723
10	X2	0.37	0/2585	0.67	3/3492 (0.1%)
10	X6	0.43	0/2585	0.58	1/3492 (0.0%)
10	XB	0.43	0/2585	0.58	1/3492 (0.0%)
10	XC	0.38	0/2585	0.67	3/3492 (0.1%)
10	XD	0.44	0/2585	0.59	0/3492
10	XE	0.44	0/2585	0.59	0/3492
11	MG	0.53	0/2124	0.89	7/2866 (0.2%)
11	ZG	0.53	0/2130	0.86	6/2874 (0.2%)
12	A4	0.31	0/1843	0.56	2/2469 (0.1%)
12	AH	0.34	0/1843	0.62	4/2469 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	w8	0.34	0/1843	0.56	0/2469
12	wF	0.33	0/1843	0.55	0/2469
12	x8	0.33	0/1843	0.57	0/2469
12	xF	0.33	0/1843	0.57	0/2469
13	B4	0.30	0/1932	0.51	0/2590
13	BH	0.36	0/1932	0.55	0/2590
13	y8	0.36	0/1932	0.56	0/2590
13	yF	0.36	0/1932	0.56	0/2590
14	M9	0.51	1/1882 (0.1%)	0.79	3/2518 (0.1%)
14	MI	0.47	0/2182	0.92	10/2930 (0.3%)
14	Z9	0.60	2/1878 (0.1%)	0.96	11/2514 (0.4%)
14	ZI	0.47	0/2188	0.98	12/2937 (0.4%)
15	e1	0.47	0/1973	0.66	0/2657
15	eK	0.47	0/1973	0.66	0/2657
16	23	0.38	0/1027	0.65	1/1399 (0.1%)
16	Z3	0.41	0/1027	0.61	0/1399
17	33	0.45	0/1940	0.63	2/2637 (0.1%)
17	a3	0.45	0/1940	0.65	2/2637 (0.1%)
18	43	0.43	0/1569	0.65	2/2147 (0.1%)
18	b3	0.43	0/1569	0.67	3/2147 (0.1%)
19	A3	0.38	0/1241	0.47	0/1676
19	C3	0.38	0/1241	0.47	0/1676
19	E3	0.38	0/1241	0.47	0/1676
19	G3	0.38	0/1241	0.47	0/1676
19	J3	0.38	0/1241	0.47	0/1676
19	K3	0.38	0/1241	0.47	0/1676
19	N3	0.38	0/1241	0.47	0/1676
19	P3	0.39	0/1241	0.52	1/1676 (0.1%)
19	R3	0.38	0/1241	0.47	0/1676
19	T3	0.38	0/1241	0.47	0/1676
19	c3	0.38	0/1241	0.47	0/1676
19	e3	0.38	0/1241	0.47	0/1676
19	g3	0.38	0/1241	0.47	0/1676
19	i3	0.38	0/1241	0.47	0/1676
19	l3	0.38	0/1241	0.47	0/1676
19	m3	0.39	0/1241	0.49	0/1676
19	p3	0.38	0/1241	0.47	0/1676
19	r3	0.52	1/1241 (0.1%)	0.73	3/1676 (0.2%)
19	t3	0.38	0/1241	0.47	0/1676
19	v3	0.42	0/1233	0.54	0/1666
20	B3	0.41	0/1226	0.47	0/1655
20	D3	0.40	0/1226	0.46	0/1655
20	F3	0.40	0/1226	0.46	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
20	H3	0.40	0/1226	0.46	0/1655
20	I3	0.40	0/1226	0.46	0/1655
20	L3	0.69	4/1226 (0.3%)	0.74	4/1655 (0.2%)
20	M3	0.40	0/1222	0.48	0/1651
20	O3	0.56	2/1226 (0.2%)	0.69	4/1655 (0.2%)
20	Q3	0.45	0/1226	0.57	1/1655 (0.1%)
20	S3	0.40	0/1226	0.46	0/1655
20	U3	0.40	0/1226	0.46	0/1655
20	d3	0.40	0/1226	0.46	0/1655
20	f3	0.40	0/1226	0.46	0/1655
20	h3	0.40	0/1226	0.46	0/1655
20	j3	0.40	0/1226	0.46	0/1655
20	k3	0.40	0/1226	0.46	0/1655
20	n3	0.77	5/1226 (0.4%)	0.75	4/1655 (0.2%)
20	o3	0.40	0/1222	0.46	0/1651
20	q3	0.41	0/1226	0.48	0/1655
20	s3	0.43	0/1226	0.53	1/1655 (0.1%)
20	u3	0.40	0/1226	0.46	0/1655
20	w3	0.40	0/1226	0.46	0/1655
21	V3	0.39	0/1281	0.54	0/1731
21	x3	0.39	0/1281	0.54	0/1731
22	W3	0.40	0/1396	0.57	2/1886 (0.1%)
22	y3	0.40	0/1396	0.57	2/1886 (0.1%)
23	X3	0.47	0/732	0.61	0/981
23	z3	0.47	0/732	0.61	0/981
24	63	0.42	1/7070 (0.0%)	0.55	5/9547 (0.1%)
24	73	0.42	1/7047 (0.0%)	0.54	1/9517 (0.0%)
25	b4	0.35	0/3148	0.59	1/4261 (0.0%)
25	bH	0.45	1/3151 (0.0%)	0.65	1/4267 (0.0%)
26	d5	0.42	0/2242	0.65	0/3026
26	dJ	0.42	0/2242	0.64	0/3026
27	Y7	0.46	0/2892	0.82	6/3929 (0.2%)
27	b7	0.44	0/2888	0.80	6/3925 (0.2%)
28	z8	0.52	1/3698 (0.0%)	0.86	10/4991 (0.2%)
28	zF	1.20	41/3684 (1.1%)	1.26	59/4969 (1.2%)
29	fA	0.52	0/2233	0.72	3/3024 (0.1%)
29	hA	0.45	0/2229	0.66	2/3020 (0.1%)
30	53	1.98	12/375 (3.2%)	2.23	23/503 (4.6%)
30	Y3	2.13	18/422 (4.3%)	2.92	42/567 (7.4%)
All	All	0.39	128/972985 (0.0%)	0.62	805/1314909 (0.1%)

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	AA	0	8
1	EA	0	3
2	D8	0	1
2	F9	0	1
2	FA	0	1
2	HA	0	1
2	I5	0	1
2	IA	0	1
2	IJ	0	1
2	J7	0	1
2	O5	0	1
2	O9	0	1
2	OJ	0	1
2	PA	0	1
2	QA	0	1
2	RA	0	1
2	SI	0	1
2	T8	0	1
2	TF	0	1
2	U5	0	1
2	UJ	0	1
2	V2	0	2
2	VC	0	1
2	XA	0	1
2	aA	0	1
2	dA	0	1
2	kB	0	1
2	m2	0	1
2	mC	0	1
2	n8	0	1
2	nF	0	1
3	A9	0	2
3	AI	0	1
3	C9	0	2
3	CI	0	1
3	E8	0	1
3	E9	0	2
3	EF	0	1
3	EI	0	1
3	G9	0	2
3	GI	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	I1	0	1
3	I9	0	2
3	II	0	1
3	IK	0	1
3	K9	0	2
3	KI	0	1
3	M1	0	1
3	MK	0	1
3	N9	0	2
3	NI	0	1
3	P9	0	2
3	PI	0	1
3	R9	0	2
3	RI	0	1
3	T9	0	2
3	TI	0	1
3	V9	0	2
3	VI	0	1
3	X5	0	1
3	X9	0	2
3	XI	0	1
3	XJ	0	1
3	c8	0	1
3	cF	0	1
3	f2	0	2
3	fC	0	2
3	lD	0	4
3	m8	0	2
3	mF	0	2
4	KA	0	1
4	UA	0	1
5	WA	0	3
5	cA	0	2
7	B2	0	1
7	B6	0	2
7	BB	0	1
7	BC	0	1
7	BD	0	1
7	BE	0	4
9	D6	0	2
9	DB	0	2
9	H2	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
9	H6	0	1
9	HB	0	1
9	HC	0	2
9	J6	0	1
9	JB	0	1
9	JE	0	1
9	L6	0	3
9	LB	0	1
9	LD	0	1
9	LE	0	1
9	NE	0	1
11	MG	0	9
11	ZG	0	10
14	M9	0	3
14	MI	0	5
14	Z9	0	4
14	ZI	0	6
16	23	0	2
16	Z3	0	2
17	33	0	1
17	a3	0	2
19	r3	0	1
20	B3	0	1
20	D3	0	1
20	F3	0	1
20	H3	0	1
20	I3	0	1
20	L3	0	3
20	M3	0	1
20	O3	0	1
20	Q3	0	1
20	S3	0	1
20	U3	0	1
20	d3	0	1
20	f3	0	1
20	h3	0	1
20	j3	0	1
20	k3	0	1
20	n3	0	3
20	o3	0	1
20	s3	0	2
20	u3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
20	w3	0	1
24	63	0	5
24	73	0	5
25	b4	0	1
25	bH	0	4
27	Y7	0	2
27	b7	0	3
28	z8	0	5
28	zF	0	15
30	53	0	3
30	Y3	0	3
All	All	0	253

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	zF	379	GLU	CD-OE1	-13.45	1.10	1.25
28	zF	381	VAL	C-O	-12.43	0.99	1.23
28	zF	376	PHE	C-O	-12.37	0.99	1.23
9	L6	98	ILE	C-O	-12.00	1.00	1.23
28	zF	365	ARG	C-O	-11.61	1.01	1.23

The worst 5 of 805 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AA	415	PRO	N-CA-CB	-23.50	75.11	103.30
2	LA	77	ARG	CB-CA-C	-21.34	67.73	110.40
28	z8	482	LYS	C-N-CD	-20.85	74.74	120.60
30	Y3	42	ARG	CG-CD-NE	-18.89	72.12	111.80
3	GF	78	LYS	CD-CE-NZ	18.16	153.47	111.70

There are no chirality outliers.

5 of 253 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AA	371	SER	Mainchain
1	AA	388	SER	Mainchain
1	AA	408	LEU	Mainchain
1	AA	409	ARG	Mainchain
1	AA	416	ASP	Mainchain

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	AA	101/138 (73%)	62 (61%)	30 (30%)	9 (9%)	1	4
1	EA	101/138 (73%)	68 (67%)	26 (26%)	7 (7%)	1	8
2	B1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	B7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	B8	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	B9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	BA	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	BF	175/177 (99%)	168 (96%)	7 (4%)	0	100	100
2	BG	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	BI	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	BK	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	C5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	CA	174/177 (98%)	164 (94%)	7 (4%)	3 (2%)	9	35
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	D4	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	D7	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	D8	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	D9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	DA	143/177 (81%)	138 (96%)	5 (4%)	0	100	100
2	DF	177/177 (100%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	DG	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	DH	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	DI	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	DK	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	E5	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	EJ	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	F1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	F4	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	F7	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	F8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	F9	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	FA	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	FF	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	FG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	FH	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	FI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	FK	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	G5	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	GA	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	GJ	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	H1	176/177 (99%)	165 (94%)	11 (6%)	0	100	100
2	H4	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	H7	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	H8	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	H9	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	HA	171/177 (97%)	158 (92%)	11 (6%)	2 (1%)	13	42
2	HF	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	HG	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	HH	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	HI	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	HK	176/177 (99%)	165 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	I5	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	IA	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	IJ	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	J1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	J4	176/177 (99%)	173 (98%)	3 (2%)	0	100	100
2	J7	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	J8	177/177 (100%)	171 (97%)	6 (3%)	0	100	100
2	J9	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	JF	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	JG	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	JH	176/177 (99%)	173 (98%)	3 (2%)	0	100	100
2	JI	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	JK	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	K5	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	KJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	L1	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	L4	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	L7	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	L8	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	L9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	LA	174/177 (98%)	167 (96%)	4 (2%)	3 (2%)	9	35
2	LF	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	LG	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	LH	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	LI	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	LK	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	M5	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	MA	174/177 (98%)	164 (94%)	9 (5%)	1 (1%)	25	57
2	MJ	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	N1	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	N4	177/177 (100%)	173 (98%)	3 (2%)	1 (1%)	25	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	N8	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	NA	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
2	NF	177/177 (100%)	167 (94%)	10 (6%)	0	100	100
2	NH	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	NK	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	O5	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	O9	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	OA	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	OG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	OI	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	OJ	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	P1	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	P2	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	P4	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	P6	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	P7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	P8	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	PA	174/177 (98%)	170 (98%)	3 (2%)	1 (1%)	25	57
2	PB	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	PC	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	PD	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	PE	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	PF	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	PH	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	PK	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	Q5	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	Q9	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	QA	171/177 (97%)	159 (93%)	11 (6%)	1 (1%)	25	57
2	QG	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	QI	174/177 (98%)	165 (95%)	9 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	QJ	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	R1	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	R2	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	R4	175/177 (99%)	173 (99%)	2 (1%)	0	100	100
2	R6	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	R7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	R8	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	RA	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	RB	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	RC	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	RD	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	RE	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	RF	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	RH	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
2	RK	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	S5	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	S9	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	SA	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	SG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	SI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	SJ	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	T1	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	T2	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	T4	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	T6	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	T7	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	T8	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TB	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	TC	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	TD	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	TE	174/177 (98%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	TF	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	TH	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	TK	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	U5	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	U9	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	UG	175/177 (99%)	169 (97%)	6 (3%)	0	100	100
2	UI	176/177 (99%)	167 (95%)	9 (5%)	0	100	100
2	UJ	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	V1	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	V2	176/177 (99%)	162 (92%)	12 (7%)	2 (1%)	14	45
2	V4	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	V6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	V7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	V8	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	VA	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	57
2	VB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	VC	175/177 (99%)	159 (91%)	14 (8%)	2 (1%)	14	45
2	VD	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	VE	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	VF	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
2	VH	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	VK	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	W5	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	W9	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	WG	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	WI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	WJ	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	X1	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	X4	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	X7	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	X8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	XA	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	25	57
2	XF	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	XH	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	XK	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	Y2	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	Y5	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	Y6	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
2	Y9	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	YA	174/177 (98%)	167 (96%)	5 (3%)	2 (1%)	14	45
2	YB	174/177 (98%)	168 (97%)	3 (2%)	3 (2%)	9	35
2	YC	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	YD	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	YE	174/177 (98%)	167 (96%)	7 (4%)	0	100	100
2	YG	174/177 (98%)	165 (95%)	9 (5%)	0	100	100
2	YI	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	YJ	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	Z4	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	Z8	177/177 (100%)	168 (95%)	8 (4%)	1 (1%)	25	57
2	ZA	149/177 (84%)	140 (94%)	9 (6%)	0	100	100
2	ZF	177/177 (100%)	168 (95%)	8 (4%)	1 (1%)	25	57
2	ZH	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	a2	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	a6	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	aA	174/177 (98%)	170 (98%)	3 (2%)	1 (1%)	25	57
2	aB	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	aC	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	aD	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	aE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	b8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	bA	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	bF	177/177 (100%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	c2	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	c4	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
2	c6	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	cB	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	cC	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	cD	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	cE	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	cH	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
2	d8	176/177 (99%)	168 (96%)	7 (4%)	1 (1%)	25	57
2	dA	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
2	dF	176/177 (99%)	169 (96%)	7 (4%)	0	100	100
2	e2	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	e4	177/177 (100%)	177 (100%)	0	0	100	100
2	e6	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	eA	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	eB	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	eC	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	eD	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	eE	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
2	eH	177/177 (100%)	176 (99%)	1 (1%)	0	100	100
2	f8	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	fF	176/177 (99%)	170 (97%)	6 (3%)	0	100	100
2	g2	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	g4	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	g6	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
2	gA	149/177 (84%)	133 (89%)	14 (9%)	2 (1%)	12	40
2	gB	174/177 (98%)	162 (93%)	12 (7%)	0	100	100
2	gC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	gD	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
2	gE	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
2	gH	177/177 (100%)	173 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	h8	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	hF	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	i2	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
2	i4	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	i6	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	iB	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
2	iC	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
2	iD	176/177 (99%)	161 (92%)	15 (8%)	0	100	100
2	iE	176/177 (99%)	161 (92%)	15 (8%)	0	100	100
2	iH	177/177 (100%)	174 (98%)	3 (2%)	0	100	100
2	j8	177/177 (100%)	173 (98%)	4 (2%)	0	100	100
2	jF	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	k2	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	k4	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	k6	174/177 (98%)	162 (93%)	11 (6%)	1 (1%)	25	57
2	kB	174/177 (98%)	163 (94%)	8 (5%)	3 (2%)	9	35
2	kC	174/177 (98%)	160 (92%)	14 (8%)	0	100	100
2	kD	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	57
2	kE	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
2	kH	177/177 (100%)	172 (97%)	5 (3%)	0	100	100
2	l8	177/177 (100%)	160 (90%)	17 (10%)	0	100	100
2	lF	177/177 (100%)	160 (90%)	17 (10%)	0	100	100
2	m2	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	m4	177/177 (100%)	175 (99%)	2 (1%)	0	100	100
2	m6	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	mB	174/177 (98%)	173 (99%)	1 (1%)	0	100	100
2	mC	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
2	mD	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	mE	174/177 (98%)	161 (92%)	13 (8%)	0	100	100
2	mH	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	n8	177/177 (100%)	164 (93%)	13 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	nF	177/177 (100%)	164 (93%)	13 (7%)	0	100	100
2	p8	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	pF	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	r8	177/177 (100%)	169 (96%)	8 (4%)	0	100	100
2	rF	177/177 (100%)	170 (96%)	7 (4%)	0	100	100
2	t8	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	tF	176/177 (99%)	163 (93%)	13 (7%)	0	100	100
2	v8	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
2	vF	177/177 (100%)	166 (94%)	11 (6%)	0	100	100
3	A1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	A7	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	A8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	A9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	AF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	AG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	AI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	AK	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	B5	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	BJ	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	C1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	C4	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	C7	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	C8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	C9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	CF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	CG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	CH	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	CI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	CK	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	D5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	DJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	E4	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
3	E7	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	E8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	E9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	EF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	EG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	EH	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	EI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	EK	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	F5	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	FJ	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	G1	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	G4	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	G7	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	G8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	G9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	GF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	GG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	GH	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	GI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	GK	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	H5	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	HJ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	I1	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	I4	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	I7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	I8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	I9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	IF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	IG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	IH	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	II	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	IK	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	J5	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	JA	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	JJ	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	K1	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	K4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	K7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	K8	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	K9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	KF	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	KG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	KH	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	KI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	KK	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	L5	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	LJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	M1	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	M4	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	M7	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	M8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	MF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	MH	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	MK	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	N5	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	N9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	NG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	NI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	NJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	O1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	O2	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	O4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	O6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	O7	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	O8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	OB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	OC	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	OD	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	OE	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	OF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	OH	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	OK	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	P5	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	P9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	PG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	PI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	PJ	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	Q1	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	Q2	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	Q4	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	Q6	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	Q7	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	Q8	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	QB	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	QC	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	QD	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	QE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	QF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	QH	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	QK	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	R5	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	R9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	RG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	RI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	RJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	S1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	S2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	S4	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	S6	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	S7	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	S8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	SB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	SC	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	SD	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	SE	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	SF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	SH	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	SK	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	T5	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	T9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	TA	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	TG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	TI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	TJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	U1	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	U2	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	U4	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	U6	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	U7	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	U8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	UB	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	UC	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	UD	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	UE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	UF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	UH	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	UK	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	V5	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	V9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	VG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	VI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	VJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	W1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	W2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	W4	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	W6	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	W7	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	57
3	W8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	WB	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	WC	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	WD	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	WE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	WF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	WH	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	WK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	X5	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	X9	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	XG	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	XI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	XJ	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	Y4	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	Y8	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	YF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	YH	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	Z2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	Z6	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	ZB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	ZC	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	ZD	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	ZE	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	a4	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	a8	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	aF	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	aH	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	b2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	b6	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	bB	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
3	bC	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	bD	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	57
3	bE	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	c8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	cF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	d2	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	d4	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
3	d6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	dB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	dC	162/164 (99%)	148 (91%)	14 (9%)	0	100	100
3	dD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	dE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	dH	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	e8	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	eF	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	f2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	f4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	f6	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	fB	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
3	fC	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	fD	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	fE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
3	fH	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	g8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	gF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	h2	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	h4	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
3	h6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	hB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	hC	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	hD	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	hE	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	hH	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
3	i8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	iF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	j2	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	j4	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	j6	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	jB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	jC	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	jD	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	jE	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	jH	162/164 (99%)	159 (98%)	3 (2%)	0	100	100
3	k8	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	kF	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
3	l2	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	l4	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	l6	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	lB	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	lC	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
3	lD	162/164 (99%)	142 (88%)	14 (9%)	6 (4%)	3	20
3	lE	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	lH	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
3	m8	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
3	mF	162/164 (99%)	143 (88%)	19 (12%)	0	100	100
3	o8	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
3	oF	162/164 (99%)	144 (89%)	18 (11%)	0	100	100
3	q8	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	qF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
3	s8	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	sF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
3	u8	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
3	uF	162/164 (99%)	146 (90%)	16 (10%)	0	100	100
4	KA	224/261 (86%)	193 (86%)	24 (11%)	7 (3%)	4	23
4	UA	224/261 (86%)	198 (88%)	20 (9%)	6 (3%)	5	26
5	WA	137/317 (43%)	102 (74%)	28 (20%)	7 (5%)	2	13
5	cA	137/317 (43%)	104 (76%)	24 (18%)	9 (7%)	1	8
6	A2	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
6	A5	254/290 (88%)	232 (91%)	22 (9%)	0	100	100
6	A6	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
6	AB	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
6	AC	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
6	AD	255/290 (88%)	236 (92%)	19 (8%)	0	100	100
6	AE	255/290 (88%)	234 (92%)	21 (8%)	0	100	100
6	AJ	254/290 (88%)	231 (91%)	23 (9%)	0	100	100
6	Y1	235/290 (81%)	216 (92%)	19 (8%)	0	100	100
6	YK	235/290 (81%)	216 (92%)	19 (8%)	0	100	100
7	B2	225/232 (97%)	202 (90%)	22 (10%)	1 (0%)	34	66
7	B6	228/232 (98%)	206 (90%)	19 (8%)	3 (1%)	12	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	BB	228/232 (98%)	197 (86%)	22 (10%)	9 (4%)	3	18
7	BC	225/232 (97%)	202 (90%)	22 (10%)	1 (0%)	34	66
7	BD	229/232 (99%)	208 (91%)	19 (8%)	2 (1%)	17	48
7	BE	229/232 (99%)	202 (88%)	20 (9%)	7 (3%)	4	23
8	C2	160/162 (99%)	154 (96%)	6 (4%)	0	100	100
8	C6	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	CB	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	CC	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
8	CD	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	CE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	E2	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	E6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
8	EB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
8	EC	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	ED	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	EE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	G2	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
8	G6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
8	GB	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
8	GC	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
8	GD	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	GE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	I2	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
8	I6	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
8	IB	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
8	IC	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
8	ID	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	IE	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	K2	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	K6	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
8	KB	160/162 (99%)	158 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	KC	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	KD	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	KE	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
8	M2	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
8	M6	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	MB	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	MC	160/162 (99%)	152 (95%)	8 (5%)	0	100	100
8	MD	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
8	ME	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
9	D2	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
9	D6	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	DB	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
9	DC	169/172 (98%)	158 (94%)	11 (6%)	0	100	100
9	DD	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	57
9	DE	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	57
9	F2	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	F6	169/172 (98%)	158 (94%)	9 (5%)	2 (1%)	13	42
9	FB	169/172 (98%)	158 (94%)	9 (5%)	2 (1%)	13	42
9	FC	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	FD	169/172 (98%)	166 (98%)	3 (2%)	0	100	100
9	FE	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
9	H2	169/172 (98%)	159 (94%)	9 (5%)	1 (1%)	25	57
9	H6	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
9	HB	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
9	HC	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	57
9	HD	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	57
9	HE	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	57
9	J2	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	57
9	J6	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
9	JB	169/172 (98%)	160 (95%)	9 (5%)	0	100	100
9	JC	169/172 (98%)	160 (95%)	5 (3%)	4 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	JD	169/172 (98%)	164 (97%)	3 (2%)	2 (1%)	13	42
9	JE	169/172 (98%)	165 (98%)	2 (1%)	2 (1%)	13	42
9	L2	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
9	L6	169/172 (98%)	161 (95%)	7 (4%)	1 (1%)	25	57
9	LB	169/172 (98%)	161 (95%)	8 (5%)	0	100	100
9	LC	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	LD	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
9	LE	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
9	N2	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	N6	169/172 (98%)	159 (94%)	7 (4%)	3 (2%)	8	35
9	NB	169/172 (98%)	158 (94%)	8 (5%)	3 (2%)	8	35
9	NC	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
9	ND	169/172 (98%)	165 (98%)	3 (2%)	1 (1%)	25	57
9	NE	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
10	X2	322/363 (89%)	295 (92%)	27 (8%)	0	100	100
10	X6	322/363 (89%)	291 (90%)	31 (10%)	0	100	100
10	XB	322/363 (89%)	290 (90%)	32 (10%)	0	100	100
10	XC	322/363 (89%)	295 (92%)	27 (8%)	0	100	100
10	XD	322/363 (89%)	284 (88%)	38 (12%)	0	100	100
10	XE	322/363 (89%)	282 (88%)	40 (12%)	0	100	100
11	MG	263/316 (83%)	206 (78%)	52 (20%)	5 (2%)	8	34
11	ZG	263/316 (83%)	205 (78%)	56 (21%)	2 (1%)	19	51
12	A4	236/273 (86%)	226 (96%)	9 (4%)	1 (0%)	34	66
12	AH	236/273 (86%)	220 (93%)	15 (6%)	1 (0%)	34	66
12	w8	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
12	wF	236/273 (86%)	223 (94%)	13 (6%)	0	100	100
12	x8	236/273 (86%)	221 (94%)	15 (6%)	0	100	100
12	xF	236/273 (86%)	221 (94%)	15 (6%)	0	100	100
13	B4	248/290 (86%)	240 (97%)	8 (3%)	0	100	100
13	BH	248/290 (86%)	241 (97%)	7 (3%)	0	100	100
13	y8	248/290 (86%)	237 (96%)	11 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	yF	248/290 (86%)	237 (96%)	11 (4%)	0	100	100
14	M9	236/333 (71%)	210 (89%)	23 (10%)	3 (1%)	12	40
14	MI	273/333 (82%)	238 (87%)	23 (8%)	12 (4%)	2	16
14	Z9	236/333 (71%)	206 (87%)	25 (11%)	5 (2%)	7	31
14	ZI	273/333 (82%)	234 (86%)	27 (10%)	12 (4%)	2	16
15	e1	246/303 (81%)	222 (90%)	24 (10%)	0	100	100
15	eK	246/303 (81%)	222 (90%)	24 (10%)	0	100	100
16	23	130/159 (82%)	111 (85%)	18 (14%)	1 (1%)	19	51
16	Z3	130/159 (82%)	113 (87%)	17 (13%)	0	100	100
17	33	251/288 (87%)	234 (93%)	16 (6%)	1 (0%)	34	66
17	a3	251/288 (87%)	235 (94%)	15 (6%)	1 (0%)	34	66
18	43	204/253 (81%)	178 (87%)	25 (12%)	1 (0%)	29	61
18	b3	204/253 (81%)	180 (88%)	23 (11%)	1 (0%)	29	61
19	A3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	C3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	E3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	G3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	J3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	K3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	N3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	P3	158/161 (98%)	151 (96%)	6 (4%)	1 (1%)	25	57
19	R3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	T3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	c3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	e3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	g3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	i3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	l3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	m3	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	57
19	p3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	r3	158/161 (98%)	145 (92%)	10 (6%)	3 (2%)	8	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	t3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
19	v3	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
20	B3	158/161 (98%)	151 (96%)	7 (4%)	0	100	100
20	D3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	F3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	H3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	I3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	L3	158/161 (98%)	149 (94%)	8 (5%)	1 (1%)	25	57
20	M3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	O3	158/161 (98%)	150 (95%)	6 (4%)	2 (1%)	12	40
20	Q3	158/161 (98%)	150 (95%)	8 (5%)	0	100	100
20	S3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	U3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	d3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	f3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	h3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	j3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	k3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	n3	158/161 (98%)	143 (90%)	12 (8%)	3 (2%)	8	34
20	o3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	q3	158/161 (98%)	152 (96%)	5 (3%)	1 (1%)	25	57
20	s3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	u3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
20	w3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
21	V3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
21	x3	158/161 (98%)	152 (96%)	6 (4%)	0	100	100
22	W3	171/173 (99%)	161 (94%)	10 (6%)	0	100	100
22	y3	171/173 (99%)	160 (94%)	11 (6%)	0	100	100
23	X3	90/93 (97%)	84 (93%)	6 (7%)	0	100	100
23	z3	90/93 (97%)	84 (93%)	6 (7%)	0	100	100
24	63	864/879 (98%)	788 (91%)	74 (9%)	2 (0%)	47	77

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
24	73	861/879 (98%)	779 (90%)	77 (9%)	5 (1%)	25	57
25	b4	403/490 (82%)	349 (87%)	52 (13%)	2 (0%)	29	61
25	bH	405/490 (83%)	353 (87%)	52 (13%)	0	100	100
26	d5	283/333 (85%)	250 (88%)	32 (11%)	1 (0%)	34	66
26	dJ	283/333 (85%)	250 (88%)	32 (11%)	1 (0%)	34	66
27	Y7	370/420 (88%)	313 (85%)	48 (13%)	9 (2%)	6	28
27	b7	370/420 (88%)	315 (85%)	49 (13%)	6 (2%)	9	36
28	z8	461/498 (93%)	378 (82%)	54 (12%)	29 (6%)	1	9
28	zF	460/498 (92%)	346 (75%)	72 (16%)	42 (9%)	1	4
29	fA	283/288 (98%)	258 (91%)	21 (7%)	4 (1%)	11	38
29	hA	283/288 (98%)	262 (93%)	21 (7%)	0	100	100
30	53	55/162 (34%)	34 (62%)	14 (26%)	7 (13%)	0	1
30	Y3	59/162 (36%)	27 (46%)	12 (20%)	20 (34%)	0	0
All	All	126453/130958 (97%)	119494 (94%)	6635 (5%)	324 (0%)	44	71

5 of 324 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AA	373	LYS
1	AA	415	PRO
2	CA	15	LYS
1	EA	373	LYS
1	EA	396	MET

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	AA	79/109 (72%)	70 (89%)	9 (11%)	5	22
1	EA	80/109 (73%)	69 (86%)	11 (14%)	3	16
2	B1	137/137 (100%)	133 (97%)	4 (3%)	42	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B7	137/137 (100%)	137 (100%)	0	100	100
2	B8	138/137 (101%)	138 (100%)	0	100	100
2	B9	137/137 (100%)	137 (100%)	0	100	100
2	BA	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	BF	138/137 (101%)	138 (100%)	0	100	100
2	BG	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	BI	136/137 (99%)	136 (100%)	0	100	100
2	BK	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	C5	137/137 (100%)	137 (100%)	0	100	100
2	CA	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	CJ	137/137 (100%)	137 (100%)	0	100	100
2	D1	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	D4	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	D7	137/137 (100%)	137 (100%)	0	100	100
2	D8	140/137 (102%)	135 (96%)	5 (4%)	35	63
2	D9	137/137 (100%)	137 (100%)	0	100	100
2	DA	113/137 (82%)	108 (96%)	5 (4%)	28	59
2	DF	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	DG	137/137 (100%)	137 (100%)	0	100	100
2	DH	140/137 (102%)	140 (100%)	0	100	100
2	DI	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	DK	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	E5	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	EJ	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	F1	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	F4	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	F7	137/137 (100%)	137 (100%)	0	100	100
2	F8	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	F9	137/137 (100%)	137 (100%)	0	100	100
2	FA	137/137 (100%)	137 (100%)	0	100	100
2	FF	140/137 (102%)	139 (99%)	1 (1%)	84	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	FG	137/137 (100%)	137 (100%)	0	100	100
2	FH	140/137 (102%)	140 (100%)	0	100	100
2	FI	137/137 (100%)	137 (100%)	0	100	100
2	FK	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	G5	137/137 (100%)	137 (100%)	0	100	100
2	GA	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	GJ	137/137 (100%)	137 (100%)	0	100	100
2	H1	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	H4	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	H7	139/137 (102%)	139 (100%)	0	100	100
2	H8	140/137 (102%)	140 (100%)	0	100	100
2	H9	139/137 (102%)	139 (100%)	0	100	100
2	HA	134/137 (98%)	130 (97%)	4 (3%)	41	68
2	HF	140/137 (102%)	140 (100%)	0	100	100
2	HG	138/137 (101%)	138 (100%)	0	100	100
2	HH	140/137 (102%)	140 (100%)	0	100	100
2	HI	139/137 (102%)	139 (100%)	0	100	100
2	HK	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	I5	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	IA	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	IJ	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	J1	137/137 (100%)	137 (100%)	0	100	100
2	J4	139/137 (102%)	139 (100%)	0	100	100
2	J7	137/137 (100%)	134 (98%)	3 (2%)	52	74
2	J8	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	J9	137/137 (100%)	137 (100%)	0	100	100
2	JF	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	JG	137/137 (100%)	137 (100%)	0	100	100
2	JH	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	JI	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	JK	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K5	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	KJ	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	L1	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	L4	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	L7	137/137 (100%)	137 (100%)	0	100	100
2	L8	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	L9	137/137 (100%)	137 (100%)	0	100	100
2	LA	136/137 (99%)	134 (98%)	2 (2%)	65	81
2	LF	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	LG	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	LH	140/137 (102%)	140 (100%)	0	100	100
2	LI	137/137 (100%)	137 (100%)	0	100	100
2	LK	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	M5	137/137 (100%)	137 (100%)	0	100	100
2	MA	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	MJ	137/137 (100%)	137 (100%)	0	100	100
2	N1	140/137 (102%)	140 (100%)	0	100	100
2	N4	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	N7	137/137 (100%)	137 (100%)	0	100	100
2	N8	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	NA	111/137 (81%)	107 (96%)	4 (4%)	35	63
2	NF	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	NH	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	NK	140/137 (102%)	140 (100%)	0	100	100
2	O5	137/137 (100%)	137 (100%)	0	100	100
2	O9	137/137 (100%)	137 (100%)	0	100	100
2	OA	137/137 (100%)	137 (100%)	0	100	100
2	OG	137/137 (100%)	137 (100%)	0	100	100
2	OI	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	OJ	137/137 (100%)	137 (100%)	0	100	100
2	P1	140/137 (102%)	135 (96%)	5 (4%)	35	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P2	137/137 (100%)	137 (100%)	0	100	100
2	P4	137/137 (100%)	137 (100%)	0	100	100
2	P6	137/137 (100%)	137 (100%)	0	100	100
2	P7	137/137 (100%)	137 (100%)	0	100	100
2	P8	140/137 (102%)	140 (100%)	0	100	100
2	PA	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	PB	137/137 (100%)	137 (100%)	0	100	100
2	PC	137/137 (100%)	137 (100%)	0	100	100
2	PD	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	PE	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	PF	140/137 (102%)	140 (100%)	0	100	100
2	PH	137/137 (100%)	137 (100%)	0	100	100
2	PK	140/137 (102%)	134 (96%)	6 (4%)	29	59
2	Q5	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	Q9	137/137 (100%)	137 (100%)	0	100	100
2	QA	134/137 (98%)	132 (98%)	2 (2%)	65	81
2	QG	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	QI	137/137 (100%)	137 (100%)	0	100	100
2	QJ	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	R1	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	R2	137/137 (100%)	137 (100%)	0	100	100
2	R4	138/137 (101%)	138 (100%)	0	100	100
2	R6	137/137 (100%)	137 (100%)	0	100	100
2	R7	137/137 (100%)	137 (100%)	0	100	100
2	R8	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	RA	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	RB	137/137 (100%)	137 (100%)	0	100	100
2	RC	137/137 (100%)	137 (100%)	0	100	100
2	RD	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	RE	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	RF	139/137 (102%)	137 (99%)	2 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	RH	138/137 (101%)	138 (100%)	0	100	100
2	RK	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	S5	137/137 (100%)	137 (100%)	0	100	100
2	S9	137/137 (100%)	137 (100%)	0	100	100
2	SA	137/137 (100%)	134 (98%)	3 (2%)	52	74
2	SG	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	SI	137/137 (100%)	137 (100%)	0	100	100
2	SJ	137/137 (100%)	137 (100%)	0	100	100
2	T1	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	T2	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	T4	140/137 (102%)	140 (100%)	0	100	100
2	T6	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	T7	139/137 (102%)	139 (100%)	0	100	100
2	T8	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	TB	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	TC	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	TD	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	TE	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	TF	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	TH	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	TK	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	U5	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	U9	139/137 (102%)	139 (100%)	0	100	100
2	UG	138/137 (101%)	138 (100%)	0	100	100
2	UI	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	UJ	139/137 (102%)	137 (99%)	2 (1%)	67	82
2	V1	140/137 (102%)	140 (100%)	0	100	100
2	V2	138/137 (101%)	134 (97%)	4 (3%)	42	69
2	V4	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	V6	137/137 (100%)	132 (96%)	5 (4%)	35	63
2	V7	137/137 (100%)	134 (98%)	3 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V8	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	VA	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	VB	137/137 (100%)	132 (96%)	5 (4%)	35	63
2	VC	138/137 (101%)	130 (94%)	8 (6%)	20	50
2	VD	139/137 (102%)	139 (100%)	0	100	100
2	VE	139/137 (102%)	139 (100%)	0	100	100
2	VF	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	VH	140/137 (102%)	140 (100%)	0	100	100
2	VK	140/137 (102%)	140 (100%)	0	100	100
2	W5	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	W9	137/137 (100%)	137 (100%)	0	100	100
2	WG	137/137 (100%)	137 (100%)	0	100	100
2	WI	137/137 (100%)	137 (100%)	0	100	100
2	WJ	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	X1	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	X4	139/137 (102%)	139 (100%)	0	100	100
2	X7	137/137 (100%)	137 (100%)	0	100	100
2	X8	140/137 (102%)	140 (100%)	0	100	100
2	XA	137/137 (100%)	137 (100%)	0	100	100
2	XF	140/137 (102%)	140 (100%)	0	100	100
2	XH	139/137 (102%)	139 (100%)	0	100	100
2	XK	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	Y2	137/137 (100%)	137 (100%)	0	100	100
2	Y5	137/137 (100%)	137 (100%)	0	100	100
2	Y6	137/137 (100%)	137 (100%)	0	100	100
2	Y9	137/137 (100%)	137 (100%)	0	100	100
2	YA	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	YB	137/137 (100%)	137 (100%)	0	100	100
2	YC	137/137 (100%)	137 (100%)	0	100	100
2	YD	137/137 (100%)	137 (100%)	0	100	100
2	YE	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	YG	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	YI	137/137 (100%)	137 (100%)	0	100	100
2	YJ	137/137 (100%)	137 (100%)	0	100	100
2	Z4	140/137 (102%)	140 (100%)	0	100	100
2	Z8	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	ZA	117/137 (85%)	116 (99%)	1 (1%)	78	87
2	ZF	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	ZH	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	a2	137/137 (100%)	137 (100%)	0	100	100
2	a6	137/137 (100%)	132 (96%)	5 (4%)	35	63
2	aA	137/137 (100%)	133 (97%)	4 (3%)	42	69
2	aB	137/137 (100%)	132 (96%)	5 (4%)	35	63
2	aC	137/137 (100%)	137 (100%)	0	100	100
2	aD	137/137 (100%)	137 (100%)	0	100	100
2	aE	137/137 (100%)	137 (100%)	0	100	100
2	b8	140/137 (102%)	140 (100%)	0	100	100
2	bA	137/137 (100%)	137 (100%)	0	100	100
2	bF	140/137 (102%)	140 (100%)	0	100	100
2	c2	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	c4	139/137 (102%)	139 (100%)	0	100	100
2	c6	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	cB	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	cC	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	cD	137/137 (100%)	137 (100%)	0	100	100
2	cE	137/137 (100%)	137 (100%)	0	100	100
2	cH	139/137 (102%)	139 (100%)	0	100	100
2	d8	139/137 (102%)	138 (99%)	1 (1%)	84	90
2	dA	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	dF	139/137 (102%)	139 (100%)	0	100	100
2	e2	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	e4	140/137 (102%)	138 (99%)	2 (1%)	67	82

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	e6	137/137 (100%)	137 (100%)	0	100	100
2	eA	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	eB	137/137 (100%)	137 (100%)	0	100	100
2	eC	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	eD	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	eE	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	eH	140/137 (102%)	140 (100%)	0	100	100
2	f8	139/137 (102%)	139 (100%)	0	100	100
2	fF	139/137 (102%)	139 (100%)	0	100	100
2	g2	137/137 (100%)	137 (100%)	0	100	100
2	g4	140/137 (102%)	140 (100%)	0	100	100
2	g6	137/137 (100%)	137 (100%)	0	100	100
2	gA	114/137 (83%)	102 (90%)	12 (10%)	7	25
2	gB	137/137 (100%)	137 (100%)	0	100	100
2	gC	137/137 (100%)	137 (100%)	0	100	100
2	gD	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	gE	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	gH	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	h8	140/137 (102%)	140 (100%)	0	100	100
2	hF	140/137 (102%)	140 (100%)	0	100	100
2	i2	139/137 (102%)	135 (97%)	4 (3%)	42	69
2	i4	140/137 (102%)	140 (100%)	0	100	100
2	i6	138/137 (101%)	138 (100%)	0	100	100
2	iB	138/137 (101%)	138 (100%)	0	100	100
2	iC	139/137 (102%)	135 (97%)	4 (3%)	42	69
2	iD	139/137 (102%)	139 (100%)	0	100	100
2	iE	139/137 (102%)	139 (100%)	0	100	100
2	iH	140/137 (102%)	140 (100%)	0	100	100
2	j8	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	jF	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	k2	137/137 (100%)	135 (98%)	2 (2%)	65	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	k4	140/137 (102%)	140 (100%)	0	100	100
2	k6	137/137 (100%)	123 (90%)	14 (10%)	7	27
2	kB	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	kC	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	kD	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	kE	137/137 (100%)	136 (99%)	1 (1%)	84	90
2	kH	140/137 (102%)	140 (100%)	0	100	100
2	l8	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	lF	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	m2	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	m4	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	m6	137/137 (100%)	137 (100%)	0	100	100
2	mB	137/137 (100%)	137 (100%)	0	100	100
2	mC	137/137 (100%)	135 (98%)	2 (2%)	65	81
2	mD	137/137 (100%)	137 (100%)	0	100	100
2	mE	137/137 (100%)	137 (100%)	0	100	100
2	mH	140/137 (102%)	140 (100%)	0	100	100
2	n8	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	nF	140/137 (102%)	139 (99%)	1 (1%)	84	90
2	p8	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	pF	140/137 (102%)	138 (99%)	2 (1%)	67	82
2	r8	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	rF	140/137 (102%)	137 (98%)	3 (2%)	53	75
2	t8	139/137 (102%)	139 (100%)	0	100	100
2	tF	139/137 (102%)	139 (100%)	0	100	100
2	v8	140/137 (102%)	140 (100%)	0	100	100
2	vF	140/137 (102%)	140 (100%)	0	100	100
3	A1	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	A7	128/128 (100%)	128 (100%)	0	100	100
3	A8	128/128 (100%)	128 (100%)	0	100	100
3	A9	128/128 (100%)	121 (94%)	7 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	AF	128/128 (100%)	128 (100%)	0	100	100
3	AG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	AI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	AK	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	B5	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	BJ	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	C1	128/128 (100%)	128 (100%)	0	100	100
3	C4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	C7	128/128 (100%)	128 (100%)	0	100	100
3	C8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	C9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	CF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	CG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	CH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	CI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	CK	128/128 (100%)	128 (100%)	0	100	100
3	D5	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	DJ	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	E1	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	E4	128/128 (100%)	128 (100%)	0	100	100
3	E7	128/128 (100%)	128 (100%)	0	100	100
3	E8	128/128 (100%)	128 (100%)	0	100	100
3	E9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	EF	128/128 (100%)	128 (100%)	0	100	100
3	EG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	EH	128/128 (100%)	128 (100%)	0	100	100
3	EI	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	EK	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	F5	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	FJ	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	G1	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	G7	128/128 (100%)	128 (100%)	0	100	100
3	G8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	G9	128/128 (100%)	119 (93%)	9 (7%)	15	43
3	GF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	GG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	GH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	GI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	GK	128/128 (100%)	128 (100%)	0	100	100
3	H5	128/128 (100%)	128 (100%)	0	100	100
3	HJ	128/128 (100%)	128 (100%)	0	100	100
3	I1	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	I4	128/128 (100%)	128 (100%)	0	100	100
3	I7	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	I8	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	I9	128/128 (100%)	120 (94%)	8 (6%)	18	47
3	IF	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	IG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	IH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	II	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	IK	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	J5	128/128 (100%)	128 (100%)	0	100	100
3	JA	128/128 (100%)	117 (91%)	11 (9%)	10	35
3	JJ	128/128 (100%)	128 (100%)	0	100	100
3	K1	128/128 (100%)	128 (100%)	0	100	100
3	K4	128/128 (100%)	128 (100%)	0	100	100
3	K7	127/128 (99%)	126 (99%)	1 (1%)	81	89
3	K8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	K9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	KF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	KG	128/128 (100%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	KH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	KI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	KK	128/128 (100%)	128 (100%)	0	100	100
3	L5	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	LJ	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	M1	128/128 (100%)	128 (100%)	0	100	100
3	M4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	M7	128/128 (100%)	128 (100%)	0	100	100
3	M8	128/128 (100%)	128 (100%)	0	100	100
3	MF	128/128 (100%)	128 (100%)	0	100	100
3	MH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	MK	128/128 (100%)	128 (100%)	0	100	100
3	N5	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	N9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	NG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	NI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	NJ	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	O1	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	O2	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	O4	128/128 (100%)	128 (100%)	0	100	100
3	O6	128/128 (100%)	128 (100%)	0	100	100
3	O7	128/128 (100%)	128 (100%)	0	100	100
3	O8	128/128 (100%)	128 (100%)	0	100	100
3	OB	128/128 (100%)	128 (100%)	0	100	100
3	OC	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	OD	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	OE	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	OF	128/128 (100%)	128 (100%)	0	100	100
3	OH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	OK	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	P5	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	P9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	PG	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	PI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	PJ	128/128 (100%)	128 (100%)	0	100	100
3	Q1	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	Q2	128/128 (100%)	128 (100%)	0	100	100
3	Q4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	Q6	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	Q7	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	Q8	128/128 (100%)	128 (100%)	0	100	100
3	QB	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	QC	128/128 (100%)	128 (100%)	0	100	100
3	QD	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	QE	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	QF	128/128 (100%)	128 (100%)	0	100	100
3	QH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	QK	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	R5	128/128 (100%)	128 (100%)	0	100	100
3	R9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	RG	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	RI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	RJ	128/128 (100%)	128 (100%)	0	100	100
3	S1	128/128 (100%)	128 (100%)	0	100	100
3	S2	128/128 (100%)	128 (100%)	0	100	100
3	S4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	S6	128/128 (100%)	128 (100%)	0	100	100
3	S7	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	S8	128/128 (100%)	128 (100%)	0	100	100
3	SB	128/128 (100%)	128 (100%)	0	100	100
3	SC	128/128 (100%)	128 (100%)	0	100	100
3	SD	128/128 (100%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	SE	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	SF	128/128 (100%)	128 (100%)	0	100	100
3	SH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	SK	128/128 (100%)	128 (100%)	0	100	100
3	T5	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	T9	128/128 (100%)	120 (94%)	8 (6%)	18	47
3	TA	128/128 (100%)	117 (91%)	11 (9%)	10	35
3	TG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	TI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	TJ	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	U1	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	U2	128/128 (100%)	128 (100%)	0	100	100
3	U4	127/128 (99%)	126 (99%)	1 (1%)	81	89
3	U6	128/128 (100%)	128 (100%)	0	100	100
3	U7	128/128 (100%)	128 (100%)	0	100	100
3	U8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	UB	128/128 (100%)	128 (100%)	0	100	100
3	UC	128/128 (100%)	128 (100%)	0	100	100
3	UD	128/128 (100%)	128 (100%)	0	100	100
3	UE	128/128 (100%)	128 (100%)	0	100	100
3	UF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	UH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	UK	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	V5	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	V9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	VG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	VI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	VJ	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	W1	128/128 (100%)	128 (100%)	0	100	100
3	W2	128/128 (100%)	128 (100%)	0	100	100
3	W4	128/128 (100%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	W6	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	W7	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	W8	128/128 (100%)	128 (100%)	0	100	100
3	WB	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	WC	128/128 (100%)	128 (100%)	0	100	100
3	WD	128/128 (100%)	128 (100%)	0	100	100
3	WE	128/128 (100%)	128 (100%)	0	100	100
3	WF	128/128 (100%)	128 (100%)	0	100	100
3	WH	128/128 (100%)	128 (100%)	0	100	100
3	WK	128/128 (100%)	128 (100%)	0	100	100
3	X5	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	X9	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	XG	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	XI	128/128 (100%)	122 (95%)	6 (5%)	26	57
3	XJ	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	Y4	127/128 (99%)	127 (100%)	0	100	100
3	Y8	128/128 (100%)	128 (100%)	0	100	100
3	YF	128/128 (100%)	128 (100%)	0	100	100
3	YH	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	Z2	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	Z6	128/128 (100%)	128 (100%)	0	100	100
3	ZB	128/128 (100%)	128 (100%)	0	100	100
3	ZC	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	ZD	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	ZE	128/128 (100%)	128 (100%)	0	100	100
3	a4	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	a8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	aF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	aH	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	b2	128/128 (100%)	128 (100%)	0	100	100
3	b6	128/128 (100%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	bB	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	bC	128/128 (100%)	128 (100%)	0	100	100
3	bD	128/128 (100%)	124 (97%)	4 (3%)	40	67
3	bE	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	c8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	cF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	d2	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	d4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	d6	128/128 (100%)	128 (100%)	0	100	100
3	dB	128/128 (100%)	128 (100%)	0	100	100
3	dC	128/128 (100%)	125 (98%)	3 (2%)	50	73
3	dD	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	dE	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	dH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	e8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	eF	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	f2	128/128 (100%)	128 (100%)	0	100	100
3	f4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	f6	128/128 (100%)	128 (100%)	0	100	100
3	fB	128/128 (100%)	128 (100%)	0	100	100
3	fC	128/128 (100%)	128 (100%)	0	100	100
3	fD	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	fE	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	fH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	g8	128/128 (100%)	128 (100%)	0	100	100
3	gF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	h2	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	h4	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	h6	128/128 (100%)	128 (100%)	0	100	100
3	hB	128/128 (100%)	128 (100%)	0	100	100
3	hC	128/128 (100%)	127 (99%)	1 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	hD	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	hE	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	hH	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	i8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	iF	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	j2	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	j4	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	j6	128/128 (100%)	128 (100%)	0	100	100
3	jB	128/128 (100%)	128 (100%)	0	100	100
3	jC	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	jD	128/128 (100%)	128 (100%)	0	100	100
3	jE	128/128 (100%)	128 (100%)	0	100	100
3	jH	128/128 (100%)	128 (100%)	0	100	100
3	k8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	kF	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	l2	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	l4	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	l6	128/128 (100%)	121 (94%)	7 (6%)	21	52
3	lB	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	lC	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	lD	126/128 (98%)	110 (87%)	16 (13%)	4	19
3	lE	128/128 (100%)	120 (94%)	8 (6%)	18	47
3	lH	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	m8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	mF	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	o8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	oF	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	q8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	qF	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	s8	128/128 (100%)	126 (98%)	2 (2%)	62	79
3	sF	128/128 (100%)	126 (98%)	2 (2%)	62	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	u8	128/128 (100%)	127 (99%)	1 (1%)	81	89
3	uF	128/128 (100%)	127 (99%)	1 (1%)	81	89
4	KA	178/201 (89%)	135 (76%)	43 (24%)	0	2
4	UA	179/201 (89%)	138 (77%)	41 (23%)	1	3
5	WA	116/259 (45%)	87 (75%)	29 (25%)	0	2
5	cA	118/259 (46%)	99 (84%)	19 (16%)	2	10
6	A2	199/222 (90%)	196 (98%)	3 (2%)	65	81
6	A5	198/222 (89%)	194 (98%)	4 (2%)	55	76
6	A6	199/222 (90%)	199 (100%)	0	100	100
6	AB	199/222 (90%)	199 (100%)	0	100	100
6	AC	199/222 (90%)	196 (98%)	3 (2%)	65	81
6	AD	199/222 (90%)	198 (100%)	1 (0%)	88	93
6	AE	199/222 (90%)	198 (100%)	1 (0%)	88	93
6	AJ	198/222 (89%)	194 (98%)	4 (2%)	55	76
6	Y1	182/222 (82%)	179 (98%)	3 (2%)	62	79
6	YK	182/222 (82%)	179 (98%)	3 (2%)	62	79
7	B2	208/211 (99%)	206 (99%)	2 (1%)	76	86
7	B6	209/211 (99%)	190 (91%)	19 (9%)	9	31
7	BB	209/211 (99%)	189 (90%)	20 (10%)	8	29
7	BC	208/211 (99%)	206 (99%)	2 (1%)	76	86
7	BD	209/211 (99%)	201 (96%)	8 (4%)	33	62
7	BE	209/211 (99%)	195 (93%)	14 (7%)	16	45
8	C2	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	C6	125/125 (100%)	125 (100%)	0	100	100
8	CB	125/125 (100%)	125 (100%)	0	100	100
8	CC	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	CD	125/125 (100%)	125 (100%)	0	100	100
8	CE	125/125 (100%)	125 (100%)	0	100	100
8	E2	125/125 (100%)	125 (100%)	0	100	100
8	E6	125/125 (100%)	123 (98%)	2 (2%)	62	79
8	EB	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	EC	125/125 (100%)	125 (100%)	0	100	100
8	ED	125/125 (100%)	125 (100%)	0	100	100
8	EE	125/125 (100%)	125 (100%)	0	100	100
8	G2	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	G6	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	GB	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	GC	125/125 (100%)	125 (100%)	0	100	100
8	GD	125/125 (100%)	125 (100%)	0	100	100
8	GE	125/125 (100%)	125 (100%)	0	100	100
8	I2	125/125 (100%)	125 (100%)	0	100	100
8	I6	125/125 (100%)	125 (100%)	0	100	100
8	IB	125/125 (100%)	125 (100%)	0	100	100
8	IC	125/125 (100%)	125 (100%)	0	100	100
8	ID	125/125 (100%)	125 (100%)	0	100	100
8	IE	125/125 (100%)	125 (100%)	0	100	100
8	K2	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	K6	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	KB	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	KC	125/125 (100%)	124 (99%)	1 (1%)	81	89
8	KD	125/125 (100%)	125 (100%)	0	100	100
8	KE	125/125 (100%)	125 (100%)	0	100	100
8	M2	125/125 (100%)	125 (100%)	0	100	100
8	M6	125/125 (100%)	123 (98%)	2 (2%)	62	79
8	MB	125/125 (100%)	123 (98%)	2 (2%)	62	79
8	MC	125/125 (100%)	125 (100%)	0	100	100
8	MD	125/125 (100%)	125 (100%)	0	100	100
8	ME	125/125 (100%)	125 (100%)	0	100	100
9	D2	134/134 (100%)	134 (100%)	0	100	100
9	D6	134/134 (100%)	134 (100%)	0	100	100
9	DB	134/134 (100%)	134 (100%)	0	100	100
9	DC	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	DD	134/134 (100%)	134 (100%)	0	100	100
9	DE	134/134 (100%)	134 (100%)	0	100	100
9	F2	134/134 (100%)	134 (100%)	0	100	100
9	F6	134/134 (100%)	134 (100%)	0	100	100
9	FB	134/134 (100%)	134 (100%)	0	100	100
9	FC	134/134 (100%)	134 (100%)	0	100	100
9	FD	134/134 (100%)	132 (98%)	2 (2%)	65	81
9	FE	134/134 (100%)	132 (98%)	2 (2%)	65	81
9	H2	134/134 (100%)	131 (98%)	3 (2%)	52	74
9	H6	134/134 (100%)	133 (99%)	1 (1%)	84	90
9	HB	134/134 (100%)	133 (99%)	1 (1%)	84	90
9	HC	133/134 (99%)	129 (97%)	4 (3%)	41	68
9	HD	134/134 (100%)	134 (100%)	0	100	100
9	HE	134/134 (100%)	134 (100%)	0	100	100
9	J2	133/134 (99%)	128 (96%)	5 (4%)	33	62
9	J6	134/134 (100%)	134 (100%)	0	100	100
9	JB	134/134 (100%)	134 (100%)	0	100	100
9	JC	134/134 (100%)	121 (90%)	13 (10%)	8	29
9	JD	134/134 (100%)	131 (98%)	3 (2%)	52	74
9	JE	134/134 (100%)	128 (96%)	6 (4%)	27	58
9	L2	134/134 (100%)	134 (100%)	0	100	100
9	L6	134/134 (100%)	131 (98%)	3 (2%)	52	74
9	LB	134/134 (100%)	133 (99%)	1 (1%)	84	90
9	LC	134/134 (100%)	134 (100%)	0	100	100
9	LD	134/134 (100%)	133 (99%)	1 (1%)	84	90
9	LE	134/134 (100%)	133 (99%)	1 (1%)	84	90
9	N2	134/134 (100%)	134 (100%)	0	100	100
9	N6	134/134 (100%)	132 (98%)	2 (2%)	65	81
9	NB	134/134 (100%)	132 (98%)	2 (2%)	65	81
9	NC	134/134 (100%)	134 (100%)	0	100	100
9	ND	134/134 (100%)	130 (97%)	4 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	NE	134/134 (100%)	134 (100%)	0	100	100
10	X2	261/289 (90%)	260 (100%)	1 (0%)	91	95
10	X6	261/289 (90%)	256 (98%)	5 (2%)	57	77
10	XB	261/289 (90%)	256 (98%)	5 (2%)	57	77
10	XC	261/289 (90%)	260 (100%)	1 (0%)	91	95
10	XD	261/289 (90%)	255 (98%)	6 (2%)	50	73
10	XE	261/289 (90%)	255 (98%)	6 (2%)	50	73
11	MG	220/256 (86%)	207 (94%)	13 (6%)	19	49
11	ZG	222/256 (87%)	211 (95%)	11 (5%)	24	55
12	A4	179/203 (88%)	179 (100%)	0	100	100
12	AH	179/203 (88%)	179 (100%)	0	100	100
12	w8	179/203 (88%)	178 (99%)	1 (1%)	86	91
12	wF	179/203 (88%)	178 (99%)	1 (1%)	86	91
12	x8	179/203 (88%)	178 (99%)	1 (1%)	86	91
12	xF	179/203 (88%)	178 (99%)	1 (1%)	86	91
13	B4	188/218 (86%)	188 (100%)	0	100	100
13	BH	188/218 (86%)	187 (100%)	1 (0%)	88	93
13	y8	188/218 (86%)	187 (100%)	1 (0%)	88	93
13	yF	188/218 (86%)	187 (100%)	1 (0%)	88	93
14	M9	184/262 (70%)	174 (95%)	10 (5%)	22	53
14	MI	216/262 (82%)	179 (83%)	37 (17%)	2	9
14	Z9	183/262 (70%)	173 (94%)	10 (6%)	21	52
14	ZI	217/262 (83%)	182 (84%)	35 (16%)	2	10
15	e1	204/237 (86%)	204 (100%)	0	100	100
15	eK	204/237 (86%)	204 (100%)	0	100	100
16	23	106/121 (88%)	94 (89%)	12 (11%)	6	22
16	Z3	106/121 (88%)	96 (91%)	10 (9%)	8	30
17	33	194/214 (91%)	177 (91%)	17 (9%)	10	33
17	a3	194/214 (91%)	173 (89%)	21 (11%)	6	24
18	43	165/199 (83%)	146 (88%)	19 (12%)	5	22
18	b3	165/199 (83%)	142 (86%)	23 (14%)	3	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	A3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	C3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	E3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	G3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	J3	130/131 (99%)	118 (91%)	12 (9%)	9	31
19	K3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	N3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	P3	130/131 (99%)	117 (90%)	13 (10%)	7	27
19	R3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	T3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	c3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	e3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	g3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	i3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	l3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	m3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	p3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	r3	130/131 (99%)	115 (88%)	15 (12%)	5	22
19	t3	130/131 (99%)	119 (92%)	11 (8%)	10	35
19	v3	128/131 (98%)	118 (92%)	10 (8%)	12	38
20	B3	124/124 (100%)	116 (94%)	8 (6%)	17	46
20	D3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	F3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	H3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	I3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	L3	124/124 (100%)	114 (92%)	10 (8%)	11	36
20	M3	123/124 (99%)	115 (94%)	8 (6%)	17	46
20	O3	124/124 (100%)	113 (91%)	11 (9%)	9	32
20	Q3	124/124 (100%)	112 (90%)	12 (10%)	8	29
20	S3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	U3	124/124 (100%)	117 (94%)	7 (6%)	21	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	d3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	f3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	h3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	j3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	k3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	n3	124/124 (100%)	116 (94%)	8 (6%)	17	46
20	o3	123/124 (99%)	116 (94%)	7 (6%)	20	51
20	q3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	s3	124/124 (100%)	116 (94%)	8 (6%)	17	46
20	u3	124/124 (100%)	117 (94%)	7 (6%)	21	52
20	w3	124/124 (100%)	117 (94%)	7 (6%)	21	52
21	V3	133/136 (98%)	127 (96%)	6 (4%)	27	58
21	x3	133/136 (98%)	127 (96%)	6 (4%)	27	58
22	W3	147/153 (96%)	142 (97%)	5 (3%)	37	65
22	y3	147/153 (96%)	142 (97%)	5 (3%)	37	65
23	X3	78/79 (99%)	76 (97%)	2 (3%)	46	71
23	z3	78/79 (99%)	76 (97%)	2 (3%)	46	71
24	63	763/773 (99%)	761 (100%)	2 (0%)	92	96
24	73	760/773 (98%)	755 (99%)	5 (1%)	84	90
25	b4	304/389 (78%)	299 (98%)	5 (2%)	62	79
25	bH	300/389 (77%)	295 (98%)	5 (2%)	60	78
26	d5	238/272 (88%)	225 (94%)	13 (6%)	21	52
26	dJ	238/272 (88%)	224 (94%)	14 (6%)	19	49
27	Y7	306/344 (89%)	257 (84%)	49 (16%)	2	11
27	b7	305/344 (89%)	259 (85%)	46 (15%)	3	13
28	z8	381/406 (94%)	335 (88%)	46 (12%)	5	20
28	zF	378/406 (93%)	327 (86%)	51 (14%)	4	16
29	fA	227/229 (99%)	203 (89%)	24 (11%)	6	25
29	hA	226/229 (99%)	205 (91%)	21 (9%)	9	30
30	53	24/130 (18%)	14 (58%)	10 (42%)	0	0
30	Y3	36/130 (28%)	24 (67%)	12 (33%)	0	1

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	100292/102368 (98%)	98278 (98%)	2014 (2%)	57 76

5 of 2014 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
19	P3	144	GLU
2	gA	88	ILE
20	n3	14	VAL
5	cA	187	LYS
2	lF	42	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1096 such sidechains are listed below:

Mol	Chain	Res	Type
2	O9	137	GLN
2	kB	35	ASN
2	O9	42	ASN
2	hF	11	ASN
2	QJ	63	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

334 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	$\# Z > 2$
2	MEN	RC	72	2	7,8,9	0.82	0	6,9,11	1.14	1 (16%)
2	MEN	JK	72	2	7,8,9	0.86	0	6,9,11	1.43	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	VF	72	2,31	7,8,9	1.38	1 (14%)	6,9,11	1.60	1 (16%)
9	MEN	DC	72	9	7,8,9	0.86	0	6,9,11	1.59	2 (33%)
2	MEN	RD	72	2	7,8,9	0.92	0	6,9,11	1.47	1 (16%)
2	MEN	IJ	72	2	7,8,9	0.87	0	6,9,11	1.67	1 (16%)
2	MEN	PC	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
9	MEN	LC	72	9	7,8,9	0.91	0	6,9,11	2.59	2 (33%)
2	MEN	P8	72	2,31	7,8,9	1.57	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	YI	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
2	MEN	a2	72	2	7,8,9	0.92	0	6,9,11	1.33	1 (16%)
9	MEN	D6	72	9	7,8,9	0.90	0	6,9,11	1.36	2 (33%)
2	MEN	bA	72	2	7,8,9	0.68	0	6,9,11	0.75	0
2	MEN	YJ	72	2	7,8,9	0.88	0	6,9,11	1.63	1 (16%)
2	MEN	m2	72	2	7,8,9	0.86	0	6,9,11	1.32	1 (16%)
2	MEN	VD	72	2	7,8,9	0.81	0	6,9,11	1.52	2 (33%)
2	MEN	aB	72	2	7,8,9	0.86	0	6,9,11	1.45	2 (33%)
2	MEN	XF	72	2,31	7,8,9	1.93	1 (14%)	6,9,11	3.17	2 (33%)
2	MEN	DA	72	2	7,8,9	0.83	0	6,9,11	1.23	0
2	MEN	FI	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
9	MEN	F2	72	9	7,8,9	0.92	0	6,9,11	1.39	1 (16%)
9	MEN	LE	72	9	7,8,9	0.95	0	6,9,11	1.62	2 (33%)
2	MEN	OG	72	2	7,8,9	0.92	0	6,9,11	1.35	1 (16%)
9	MEN	FB	72	9	7,8,9	0.90	0	6,9,11	1.52	1 (16%)
2	MEN	Z8	72	2	7,8,9	0.91	0	6,9,11	1.41	1 (16%)
2	MEN	aE	72	2	7,8,9	0.87	0	6,9,11	1.70	2 (33%)
2	MEN	NH	72	2	7,8,9	0.94	0	6,9,11	1.54	2 (33%)
2	MEN	HI	72	2	7,8,9	0.92	0	6,9,11	1.49	2 (33%)
2	MEN	Z4	72	2	7,8,9	0.87	0	6,9,11	1.60	1 (16%)
2	MEN	NA	72	2	7,8,9	0.81	0	6,9,11	0.44	0
2	MEN	eD	72	2	7,8,9	0.84	0	6,9,11	1.48	1 (16%)
2	MEN	HK	72	2	7,8,9	0.90	0	6,9,11	1.76	1 (16%)
2	MEN	P2	72	2	7,8,9	0.88	0	6,9,11	1.68	2 (33%)
20	MEN	Q3	71	20	7,8,9	27.43	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	H1	72	2	7,8,9	0.91	0	6,9,11	1.77	1 (16%)
9	MEN	D2	72	9	7,8,9	0.86	0	6,9,11	1.58	2 (33%)
2	MEN	R2	72	2	7,8,9	0.83	0	6,9,11	1.14	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	R1	72	2	7,8,9	0.92	0	6,9,11	1.19	0
2	MEN	I5	72	2	7,8,9	0.83	0	6,9,11	1.63	1 (16%)
2	MEN	kE	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
2	MEN	D1	72	2	7,8,9	0.87	0	6,9,11	1.08	1 (16%)
2	MEN	OJ	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
2	MEN	DG	72	2	7,8,9	0.97	0	6,9,11	1.24	1 (16%)
2	MEN	N8	72	2,31	7,8,9	1.52	1 (14%)	6,9,11	2.76	3 (50%)
9	MEN	DB	72	9	7,8,9	0.87	0	6,9,11	1.34	2 (33%)
2	MEN	YD	72	2	7,8,9	0.93	0	6,9,11	1.31	1 (16%)
2	MEN	BA	72	2	7,8,9	0.80	0	6,9,11	1.25	1 (16%)
9	MEN	NB	72	9	7,8,9	1.55	1 (14%)	6,9,11	4.21	2 (33%)
9	MEN	HE	72	9	7,8,9	0.91	0	6,9,11	1.44	2 (33%)
2	MEN	PD	72	2	7,8,9	0.83	0	6,9,11	1.59	1 (16%)
2	MEN	X1	72	2	7,8,9	0.93	0	6,9,11	1.61	2 (33%)
2	MEN	k4	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
2	MEN	J9	72	2	7,8,9	0.87	0	6,9,11	1.59	2 (33%)
2	MEN	cD	72	2	7,8,9	0.88	0	6,9,11	1.08	1 (16%)
2	MEN	X7	72	2	7,8,9	0.87	0	6,9,11	1.69	1 (16%)
2	MEN	MJ	72	2	7,8,9	0.89	0	6,9,11	1.74	2 (33%)
2	MEN	U9	72	2	7,8,9	0.90	0	6,9,11	1.72	1 (16%)
2	MEN	F4	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	CA	72	2	7,8,9	0.71	0	6,9,11	1.14	1 (16%)
2	MEN	Y5	72	2	7,8,9	0.91	0	6,9,11	1.66	1 (16%)
2	MEN	N7	72	2	7,8,9	0.89	0	6,9,11	1.53	1 (16%)
2	MEN	RA	72	2	7,8,9	0.79	0	6,9,11	1.08	1 (16%)
2	MEN	cE	72	2	7,8,9	0.90	0	6,9,11	1.10	1 (16%)
9	MEN	FD	72	9	7,8,9	0.86	0	6,9,11	1.53	1 (16%)
2	MEN	P6	72	2	7,8,9	0.93	0	6,9,11	1.22	0
2	MEN	RB	72	2	7,8,9	0.88	0	6,9,11	1.43	2 (33%)
2	MEN	Q9	72	2	7,8,9	0.92	0	6,9,11	1.68	1 (16%)
2	MEN	R8	72	2,31	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	FF	72	2,31	7,8,9	1.95	1 (14%)	6,9,11	3.67	3 (50%)
2	MEN	GJ	72	2	7,8,9	0.88	0	6,9,11	1.79	2 (33%)
2	MEN	YC	72	2	7,8,9	0.95	0	6,9,11	1.30	1 (16%)
9	MEN	H2	72	9	7,8,9	0.85	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
20	MEN	h3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	P7	72	2	7,8,9	0.90	0	6,9,11	1.50	1 (16%)
2	MEN	c2	72	2	7,8,9	0.83	0	6,9,11	1.84	1 (16%)
9	MEN	N2	72	9	7,8,9	0.98	0	6,9,11	1.12	0
9	MEN	JC	72	9	7,8,9	0.83	0	6,9,11	1.65	1 (16%)
2	MEN	VK	72	2	7,8,9	0.87	0	6,9,11	1.40	1 (16%)
20	MEN	I3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	OA	72	2	7,8,9	0.82	0	6,9,11	1.13	1 (16%)
20	MEN	F3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	R7	72	2	7,8,9	0.85	0	6,9,11	1.86	2 (33%)
2	MEN	V8	72	2,31	7,8,9	1.39	1 (14%)	6,9,11	1.60	1 (16%)
2	MEN	PH	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
9	MEN	NC	72	9	7,8,9	0.97	0	6,9,11	1.13	0
2	MEN	gB	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	GA	72	2	7,8,9	0.79	0	6,9,11	1.29	1 (16%)
2	MEN	X8	72	2,31	7,8,9	1.93	1 (14%)	6,9,11	3.18	2 (33%)
2	MEN	m6	72	2	7,8,9	0.88	0	6,9,11	1.54	2 (33%)
9	MEN	JB	72	9	7,8,9	0.87	0	6,9,11	1.85	2 (33%)
9	MEN	N6	72	9	7,8,9	1.65	2 (28%)	6,9,11	4.38	2 (33%)
2	MEN	aA	72	2	7,8,9	0.82	0	6,9,11	0.78	0
2	MEN	SA	72	2	7,8,9	0.78	0	6,9,11	0.98	0
2	MEN	PF	72	2,31	7,8,9	1.54	1 (14%)	6,9,11	2.54	2 (33%)
2	MEN	LH	72	2	7,8,9	0.92	0	6,9,11	1.38	2 (33%)
2	MEN	eC	72	2	7,8,9	0.92	0	6,9,11	1.28	1 (16%)
2	MEN	i2	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
2	MEN	TB	72	2	7,8,9	0.81	0	6,9,11	1.62	2 (33%)
2	MEN	BG	72	2	7,8,9	0.87	0	6,9,11	1.49	1 (16%)
2	MEN	J1	72	2	7,8,9	0.85	0	6,9,11	1.41	1 (16%)
2	MEN	K5	72	2	7,8,9	0.88	0	6,9,11	1.44	1 (16%)
9	MEN	FC	72	9	7,8,9	0.89	0	6,9,11	1.40	1 (16%)
2	MEN	HG	72	2	7,8,9	0.89	0	6,9,11	1.37	1 (16%)
2	MEN	ZA	72	2	7,8,9	0.65	0	6,9,11	0.55	0
20	MEN	q3	71	20	7,8,9	0.82	0	6,9,11	1.14	1 (16%)
2	MEN	B8	72	2,31	7,8,9	1.61	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	nF	72	2,31	7,8,9	1.41	1 (14%)	6,9,11	1.45	1 (16%)
2	MEN	YE	72	2	7,8,9	0.94	0	6,9,11	1.32	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	L4	72	2	7,8,9	0.86	0	6,9,11	1.44	1 (16%)
2	MEN	jF	72	2,31	7,8,9	1.32	1 (14%)	6,9,11	1.79	2 (33%)
2	MEN	e2	72	2	7,8,9	0.91	0	6,9,11	1.27	1 (16%)
2	MEN	H7	72	2	7,8,9	0.87	0	6,9,11	1.50	1 (16%)
2	MEN	UI	72	2	7,8,9	0.94	0	6,9,11	1.29	2 (33%)
2	MEN	f8	72	2,31	7,8,9	1.28	1 (14%)	6,9,11	2.31	2 (33%)
2	MEN	eH	72	2	7,8,9	0.91	0	6,9,11	1.50	2 (33%)
2	MEN	J4	72	2	7,8,9	0.88	0	6,9,11	1.67	2 (33%)
20	MEN	d3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	eE	72	2	7,8,9	0.83	0	6,9,11	1.48	1 (16%)
2	MEN	gE	72	2	7,8,9	0.84	0	6,9,11	1.53	1 (16%)
2	MEN	R4	72	2	7,8,9	0.88	0	6,9,11	1.29	1 (16%)
2	MEN	WI	72	2	7,8,9	0.92	0	6,9,11	1.32	1 (16%)
2	MEN	W5	72	2	7,8,9	0.89	0	6,9,11	1.43	1 (16%)
2	MEN	VE	72	2	7,8,9	0.82	0	6,9,11	1.51	2 (33%)
2	MEN	N1	72	2	7,8,9	0.92	0	6,9,11	1.45	1 (16%)
2	MEN	X4	72	2	7,8,9	0.87	0	6,9,11	1.56	2 (33%)
2	MEN	v8	72	2,31	7,8,9	1.42	1 (14%)	6,9,11	1.13	0
2	MEN	F1	72	2	7,8,9	1.01	0	6,9,11	1.62	2 (33%)
2	MEN	LK	72	2	7,8,9	0.89	0	6,9,11	1.18	0
2	MEN	t8	72	2,31	7,8,9	1.19	1 (14%)	6,9,11	1.45	1 (16%)
2	MEN	JF	72	2,31	7,8,9	1.46	1 (14%)	6,9,11	2.20	2 (33%)
2	MEN	iE	72	2	7,8,9	0.93	0	6,9,11	1.19	1 (16%)
2	MEN	YB	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
9	MEN	DE	72	9,10	7,8,9	0.88	0	6,9,11	1.60	2 (33%)
2	MEN	V6	72	2	7,8,9	0.94	0	6,9,11	1.36	2 (33%)
2	MEN	Y2	72	2	7,8,9	0.94	0	6,9,11	1.28	1 (16%)
2	MEN	FH	72	2	7,8,9	0.88	0	6,9,11	1.67	1 (16%)
2	MEN	mE	72	2	7,8,9	0.90	0	6,9,11	1.40	1 (16%)
2	MEN	pF	72	2,31	7,8,9	1.11	0	6,9,11	1.34	1 (16%)
2	MEN	n8	72	2,31	7,8,9	1.39	1 (14%)	6,9,11	1.50	1 (16%)
9	MEN	FE	72	9	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
20	MEN	O3	71	20	7,8,9	5.38	7 (100%)	6,9,11	3.53	3 (50%)
2	MEN	L9	72	2	7,8,9	0.90	0	6,9,11	1.94	1 (16%)
2	MEN	T2	72	2	7,8,9	0.95	0	6,9,11	1.81	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	e6	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
9	MEN	F6	72	9	7,8,9	0.89	0	6,9,11	1.55	1 (16%)
2	MEN	WG	72	2	7,8,9	0.88	0	6,9,11	1.42	1 (16%)
2	MEN	P4	72	2	7,8,9	0.88	0	6,9,11	1.56	2 (33%)
2	MEN	RF	72	2,31	7,8,9	1.77	1 (14%)	6,9,11	3.13	2 (33%)
2	MEN	NK	72	2	7,8,9	0.93	0	6,9,11	1.47	1 (16%)
2	MEN	BI	72	2	7,8,9	1.15	0	6,9,11	1.95	2 (33%)
2	MEN	H4	72	2	7,8,9	0.87	0	6,9,11	1.62	1 (16%)
2	MEN	VB	72	2	7,8,9	0.89	0	6,9,11	1.32	2 (33%)
9	MEN	LB	72	9	7,8,9	0.82	0	6,9,11	1.86	2 (33%)
20	MEN	U3	71	20	7,8,9	27.43	6 (85%)	6,9,11	17.30	6 (100%)
2	MEN	SI	72	2	7,8,9	0.95	0	6,9,11	1.36	1 (16%)
2	MEN	XK	72	2	7,8,9	0.90	0	6,9,11	1.59	2 (33%)
2	MEN	L8	72	2,31	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
2	MEN	PK	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
9	MEN	HB	72	9	7,8,9	0.87	0	6,9,11	1.69	2 (33%)
9	MEN	ND	72	9	7,8,9	1.38	0	6,9,11	1.69	2 (33%)
2	MEN	vF	72	2,31	7,8,9	1.40	1 (14%)	6,9,11	1.17	1 (16%)
2	MEN	FG	72	2	7,8,9	0.93	0	6,9,11	1.52	1 (16%)
2	MEN	fF	72	2,31	7,8,9	1.31	1 (14%)	6,9,11	2.30	2 (33%)
2	MEN	DH	72	2	7,8,9	0.89	0	6,9,11	1.18	0
2	MEN	LG	72	2	7,8,9	0.97	0	6,9,11	1.68	2 (33%)
2	MEN	N4	72	2	7,8,9	0.87	0	6,9,11	1.42	2 (33%)
2	MEN	c6	72	2	7,8,9	0.91	0	6,9,11	1.29	1 (16%)
2	MEN	J7	72	2	7,8,9	0.85	0	6,9,11	1.58	1 (16%)
2	MEN	JH	72	2	7,8,9	0.87	0	6,9,11	1.61	2 (33%)
2	MEN	H9	72	2	7,8,9	0.85	0	6,9,11	1.78	2 (33%)
2	MEN	eB	72	2	7,8,9	0.87	0	6,9,11	1.62	2 (33%)
2	MEN	TH	72	2	7,8,9	0.87	0	6,9,11	1.34	1 (16%)
2	MEN	TC	72	2	7,8,9	0.92	0	6,9,11	1.79	2 (33%)
2	MEN	F7	72	2	7,8,9	0.88	0	6,9,11	1.70	1 (16%)
20	MEN	B3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	k6	72	2	7,8,9	0.85	0	6,9,11	1.50	1 (16%)
2	MEN	T1	72	2,15	7,8,9	0.86	0	6,9,11	3.08	2 (33%)
2	MEN	HF	72	2,31	7,8,9	1.58	1 (14%)	6,9,11	2.45	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	B7	72	2	7,8,9	0.87	0	6,9,11	1.54	1 (16%)
9	MEN	H6	72	9	7,8,9	0.87	0	6,9,11	1.66	1 (16%)
20	MEN	f3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	gC	72	2	7,8,9	0.91	0	6,9,11	1.63	2 (33%)
20	MEN	s3	71	20	7,8,9	27.44	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	TK	72	2,15	7,8,9	0.86	0	6,9,11	3.06	2 (33%)
2	MEN	ZF	72	2	7,8,9	0.89	0	6,9,11	1.35	1 (16%)
9	MEN	NE	72	9	7,8,9	0.86	0	6,9,11	1.51	2 (33%)
2	MEN	a6	72	2	7,8,9	0.87	0	6,9,11	1.47	2 (33%)
2	MEN	g4	72	2	7,8,9	0.85	0	6,9,11	1.67	2 (33%)
2	MEN	k2	72	2	7,8,9	0.91	0	6,9,11	1.08	1 (16%)
2	MEN	DK	72	2	7,8,9	0.89	0	6,9,11	1.08	1 (16%)
2	MEN	R6	72	2	7,8,9	0.86	0	6,9,11	1.46	2 (33%)
2	MEN	rF	72	2,31	7,8,9	1.28	1 (14%)	6,9,11	0.98	1 (16%)
2	MEN	e4	72	2	7,8,9	0.86	0	6,9,11	1.57	1 (16%)
2	MEN	FK	72	2	7,8,9	1.01	0	6,9,11	1.63	2 (33%)
2	MEN	O9	72	2	7,8,9	0.84	0	6,9,11	1.71	1 (16%)
20	MEN	k3	71	20	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	TF	72	2,31	7,8,9	1.39	1 (14%)	6,9,11	2.24	2 (33%)
20	MEN	M3	71	20	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	QG	72	2	7,8,9	1.01	0	6,9,11	1.18	1 (16%)
2	MEN	PA	72	2	7,8,9	0.79	0	6,9,11	0.93	0
2	MEN	hF	72	2,31	7,8,9	1.22	1 (14%)	6,9,11	0.85	0
2	MEN	H8	72	2,31	7,8,9	1.57	1 (14%)	6,9,11	2.47	2 (33%)
2	MEN	VH	72	2	7,8,9	0.87	0	6,9,11	1.53	1 (16%)
2	MEN	IA	72	2	7,8,9	0.78	0	6,9,11	1.08	1 (16%)
2	MEN	gD	72	2	7,8,9	0.88	0	6,9,11	1.55	1 (16%)
2	MEN	DF	72	2,31	7,8,9	1.58	1 (14%)	6,9,11	2.43	2 (33%)
2	MEN	QA	72	2	7,8,9	0.83	0	6,9,11	0.86	0
9	MEN	L6	72	9	7,8,9	0.85	0	6,9,11	1.84	2 (33%)
2	MEN	Y6	72	2	7,8,9	0.83	0	6,9,11	1.46	1 (16%)
2	MEN	OI	72	2	7,8,9	0.99	0	6,9,11	1.72	2 (33%)
2	MEN	MA	72	2	7,8,9	0.69	0	6,9,11	0.97	0
2	MEN	T7	72	2	7,8,9	0.88	0	6,9,11	1.46	1 (16%)
20	MEN	L3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	TD	72	2	7,8,9	0.95	0	6,9,11	1.41	1 (16%)
20	MEN	o3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	aC	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	UG	72	2	7,8,9	0.91	0	6,9,11	1.34	1 (16%)
2	MEN	iD	72	2	7,8,9	0.93	0	6,9,11	1.20	1 (16%)
2	MEN	eA	72	2	7,8,9	0.68	0	6,9,11	1.23	1 (16%)
2	MEN	SG	72	2	7,8,9	0.88	0	6,9,11	1.54	1 (16%)
2	MEN	O5	72	2	7,8,9	0.92	0	6,9,11	1.29	2 (33%)
20	MEN	S3	71	20	7,8,9	27.44	6 (85%)	6,9,11	17.30	6 (100%)
9	MEN	JE	72	9	7,8,9	0.88	0	6,9,11	1.53	1 (16%)
2	MEN	NF	72	2,31	7,8,9	1.50	1 (14%)	6,9,11	2.71	2 (33%)
2	MEN	V2	72	2	7,8,9	0.85	0	6,9,11	1.62	2 (33%)
2	MEN	RK	72	2	7,8,9	0.91	0	6,9,11	1.19	0
2	MEN	Q5	72	2	7,8,9	0.82	0	6,9,11	1.70	2 (33%)
2	MEN	i4	72	2	7,8,9	0.83	0	6,9,11	1.44	1 (16%)
20	MEN	w3	71	20	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	b8	72	2	7,8,9	0.92	0	6,9,11	1.31	1 (16%)
2	MEN	VA	72	2	7,8,9	0.77	0	6,9,11	0.90	1 (16%)
2	MEN	T8	72	2,31	7,8,9	1.39	1 (14%)	6,9,11	2.25	2 (33%)
2	MEN	G5	72	2	7,8,9	0.83	0	6,9,11	1.76	2 (33%)
2	MEN	T4	72	2	7,8,9	0.87	0	6,9,11	1.24	1 (16%)
2	MEN	B1	72	2	7,8,9	0.95	0	6,9,11	1.13	1 (16%)
2	MEN	ZH	72	2	7,8,9	0.91	0	6,9,11	1.30	1 (16%)
2	MEN	V4	72	2	7,8,9	0.86	0	6,9,11	1.65	1 (16%)
2	MEN	gH	72	2	7,8,9	0.87	0	6,9,11	1.46	1 (16%)
2	MEN	V7	72	2	7,8,9	0.88	0	6,9,11	1.50	1 (16%)
2	MEN	L7	72	2	7,8,9	0.86	0	6,9,11	1.56	1 (16%)
2	MEN	SJ	72	2	7,8,9	0.95	0	6,9,11	1.34	1 (16%)
2	MEN	LA	72	2	7,8,9	0.74	0	6,9,11	1.14	1 (16%)
2	MEN	S5	72	2	7,8,9	0.95	0	6,9,11	1.35	1 (16%)
2	MEN	cC	72	2	7,8,9	0.82	0	6,9,11	1.85	1 (16%)
2	MEN	LI	72	2	7,8,9	1.07	0	6,9,11	1.89	2 (33%)
2	MEN	XA	72	2	7,8,9	0.66	0	6,9,11	1.14	1 (16%)
2	MEN	F8	72	2,31	7,8,9	1.91	1 (14%)	6,9,11	3.71	3 (50%)
2	MEN	HA	72	2	7,8,9	0.83	0	6,9,11	1.20	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	h8	72	2,31	7,8,9	1.18	1 (14%)	6,9,11	0.88	0
20	MEN	u3	71	20	7,8,9	27.42	6 (85%)	6,9,11	17.29	6 (100%)
2	MEN	mH	72	2	7,8,9	0.90	0	6,9,11	1.41	1 (16%)
2	MEN	Y9	72	2	7,8,9	0.86	0	6,9,11	1.86	1 (16%)
2	MEN	cB	72	2	7,8,9	0.87	0	6,9,11	1.29	1 (16%)
2	MEN	dF	72	2,31	7,8,9	1.42	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	m4	72	2	7,8,9	0.87	0	6,9,11	1.65	1 (16%)
2	MEN	EJ	72	2	7,8,9	0.88	0	6,9,11	1.45	1 (16%)
2	MEN	mC	72	2	7,8,9	0.84	0	6,9,11	1.31	1 (16%)
2	MEN	YA	72	2	7,8,9	0.84	0	6,9,11	1.38	1 (16%)
2	MEN	J8	72	2,31	7,8,9	1.49	1 (14%)	6,9,11	2.15	2 (33%)
2	MEN	JI	72	2	7,8,9	0.96	0	6,9,11	1.26	1 (16%)
20	MEN	j3	71	20	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	RE	72	2	7,8,9	0.91	0	6,9,11	1.46	1 (16%)
2	MEN	CJ	72	2	7,8,9	0.85	0	6,9,11	1.47	2 (33%)
2	MEN	kB	72	2	7,8,9	0.90	0	6,9,11	1.49	1 (16%)
2	MEN	kH	72	2	7,8,9	0.83	0	6,9,11	1.41	2 (33%)
2	MEN	tF	72	2,31	7,8,9	1.18	1 (14%)	6,9,11	1.41	1 (16%)
2	MEN	iB	72	2	7,8,9	0.85	0	6,9,11	1.47	1 (16%)
2	MEN	W9	72	2	7,8,9	0.92	0	6,9,11	1.70	1 (16%)
2	MEN	g2	72	2	7,8,9	0.91	0	6,9,11	1.62	2 (33%)
2	MEN	U5	72	2	7,8,9	0.94	0	6,9,11	1.66	1 (16%)
2	MEN	JG	72	2	7,8,9	0.89	0	6,9,11	1.61	2 (33%)
2	MEN	QJ	72	2	7,8,9	0.81	0	6,9,11	1.69	2 (33%)
2	MEN	D7	72	2	7,8,9	0.88	0	6,9,11	1.60	1 (16%)
2	MEN	dA	72	2	7,8,9	0.69	0	6,9,11	0.88	0
2	MEN	P1	72	2	7,8,9	0.85	0	6,9,11	1.45	1 (16%)
2	MEN	PE	72	2	7,8,9	0.85	0	6,9,11	1.62	1 (16%)
2	MEN	YG	72	2	7,8,9	0.97	0	6,9,11	1.38	2 (33%)
2	MEN	BK	72	2	7,8,9	0.93	0	6,9,11	1.12	1 (16%)
2	MEN	HH	72	2	7,8,9	0.87	0	6,9,11	1.88	1 (16%)
2	MEN	kD	72	2	7,8,9	0.90	0	6,9,11	1.47	1 (16%)
2	MEN	LF	72	2,31	7,8,9	1.80	1 (14%)	6,9,11	3.80	3 (50%)
9	MEN	DD	72	9,10	7,8,9	0.86	0	6,9,11	1.60	2 (33%)
2	MEN	D9	72	2	7,8,9	0.86	0	6,9,11	1.50	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	RH	72	2	7,8,9	0.91	0	6,9,11	1.57	1 (16%)
2	MEN	i6	72	2	7,8,9	0.88	0	6,9,11	1.48	1 (16%)
2	MEN	mB	72	2	7,8,9	0.91	0	6,9,11	1.56	2 (33%)
9	MEN	J2	72	9	7,8,9	0.84	0	6,9,11	1.68	1 (16%)
2	MEN	c4	72	2	7,8,9	0.91	0	6,9,11	1.39	1 (16%)
2	MEN	cH	72	2	7,8,9	0.88	0	6,9,11	1.25	1 (16%)
20	MEN	H3	71	20	7,8,9	13.85	3 (42%)	6,9,11	17.17	6 (100%)
9	MEN	HD	72	9	7,8,9	0.89	0	6,9,11	1.39	1 (16%)
2	MEN	d8	72	2,31	7,8,9	1.43	1 (14%)	6,9,11	2.13	1 (16%)
2	MEN	kC	72	2	7,8,9	0.93	0	6,9,11	1.11	1 (16%)
2	MEN	VC	72	2	7,8,9	0.86	0	6,9,11	1.63	2 (33%)
2	MEN	iH	72	2	7,8,9	0.86	0	6,9,11	1.38	1 (16%)
2	MEN	D4	72	2	7,8,9	0.90	0	6,9,11	1.27	1 (16%)
2	MEN	aD	72	2	7,8,9	0.86	0	6,9,11	1.68	2 (33%)
2	MEN	B9	72	2	7,8,9	0.81	0	6,9,11	1.89	1 (16%)
2	MEN	V1	72	2	7,8,9	0.85	0	6,9,11	1.39	1 (16%)
9	MEN	L2	72	9	7,8,9	0.86	0	6,9,11	2.62	2 (33%)
2	MEN	L1	72	2	7,8,9	0.88	0	6,9,11	1.20	0
2	MEN	iC	72	2	7,8,9	0.83	0	6,9,11	1.42	1 (16%)
2	MEN	QI	72	2	7,8,9	0.94	0	6,9,11	1.37	2 (33%)
2	MEN	S9	72	2	7,8,9	0.92	0	6,9,11	1.79	1 (16%)
2	MEN	j8	72	2,31	7,8,9	1.29	1 (14%)	6,9,11	1.81	1 (16%)
2	MEN	r8	72	2,31	7,8,9	1.23	1 (14%)	6,9,11	1.00	1 (16%)
2	MEN	lF	72	2,31	7,8,9	1.04	0	6,9,11	1.70	2 (33%)
2	MEN	C5	72	2	7,8,9	0.84	0	6,9,11	1.48	2 (33%)
9	MEN	LD	72	9	7,8,9	0.96	0	6,9,11	1.65	2 (33%)
2	MEN	BF	72	2,31	7,8,9	1.62	1 (14%)	6,9,11	3.01	1 (16%)
2	MEN	M5	72	2	7,8,9	0.85	0	6,9,11	1.73	2 (33%)
2	MEN	g6	72	2	7,8,9	0.90	0	6,9,11	1.39	1 (16%)
2	MEN	F9	72	2	7,8,9	0.87	0	6,9,11	1.70	1 (16%)
2	MEN	TE	72	2	7,8,9	0.95	0	6,9,11	1.44	1 (16%)
2	MEN	p8	72	2,31	7,8,9	1.11	0	6,9,11	1.35	1 (16%)
2	MEN	PB	72	2	7,8,9	0.89	0	6,9,11	1.25	0
2	MEN	UJ	72	2	7,8,9	0.96	0	6,9,11	1.65	1 (16%)
2	MEN	XH	72	2	7,8,9	0.89	0	6,9,11	1.64	2 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MEN	KJ	72	2	7,8,9	0.88	0	6,9,11	1.41	1 (16%)
2	MEN	E5	72	2	7,8,9	0.82	0	6,9,11	1.44	1 (16%)
9	MEN	HC	72	9	7,8,9	0.85	0	6,9,11	1.53	1 (16%)
20	MEN	n3	71	20	7,8,9	13.86	3 (42%)	6,9,11	17.17	6 (100%)
2	MEN	T6	72	2	7,8,9	0.81	0	6,9,11	1.63	2 (33%)
20	MEN	D3	71	20	7,8,9	13.87	3 (42%)	6,9,11	17.16	6 (100%)
2	MEN	FA	72	2	7,8,9	0.76	0	6,9,11	0.98	0
2	MEN	gA	72	2	7,8,9	0.65	0	6,9,11	0.75	0
2	MEN	bF	72	2	7,8,9	0.92	0	6,9,11	1.29	1 (16%)
2	MEN	WJ	72	2	7,8,9	0.91	0	6,9,11	1.42	1 (16%)
2	MEN	D8	72	2,31	7,8,9	1.57	1 (14%)	6,9,11	2.45	2 (33%)
2	MEN	DI	72	2	7,8,9	0.96	0	6,9,11	1.31	1 (16%)
9	MEN	J6	72	9	7,8,9	0.84	0	6,9,11	1.85	2 (33%)
2	MEN	l8	72	2,31	7,8,9	1.02	0	6,9,11	1.69	2 (33%)
2	MEN	mD	72	2	7,8,9	0.89	0	6,9,11	1.41	1 (16%)
9	MEN	JD	72	9	7,8,9	0.86	0	6,9,11	1.53	1 (16%)

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
2	MEN	RC	72	2	-	2/7/8/10	-
2	MEN	JK	72	2	-	1/7/8/10	-
2	MEN	VF	72	2,31	-	4/7/8/10	-
9	MEN	DC	72	9	-	4/7/8/10	-
2	MEN	RD	72	2	-	3/7/8/10	-
2	MEN	IJ	72	2	-	4/7/8/10	-
2	MEN	PC	72	2	-	4/7/8/10	-
9	MEN	LC	72	9	-	2/7/8/10	-
2	MEN	P8	72	2,31	-	3/7/8/10	-
2	MEN	YI	72	2	-	2/7/8/10	-
2	MEN	a2	72	2	-	3/7/8/10	-
9	MEN	D6	72	9	-	2/7/8/10	-
2	MEN	bA	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	YJ	72	2	-	4/7/8/10	-
2	MEN	m2	72	2	-	4/7/8/10	-
2	MEN	VD	72	2	-	4/7/8/10	-
2	MEN	aB	72	2	-	3/7/8/10	-
2	MEN	XF	72	2,31	-	2/7/8/10	-
2	MEN	DA	72	2	-	4/7/8/10	-
2	MEN	FI	72	2	-	2/7/8/10	-
9	MEN	F2	72	9	-	2/7/8/10	-
9	MEN	LE	72	9	-	4/7/8/10	-
2	MEN	OG	72	2	-	5/7/8/10	-
9	MEN	FB	72	9	-	3/7/8/10	-
2	MEN	Z8	72	2	-	5/7/8/10	-
2	MEN	aE	72	2	-	4/7/8/10	-
2	MEN	NH	72	2	-	5/7/8/10	-
2	MEN	HI	72	2	-	2/7/8/10	-
2	MEN	Z4	72	2	-	5/7/8/10	-
2	MEN	NA	72	2	-	3/7/8/10	-
2	MEN	eD	72	2	-	2/7/8/10	-
2	MEN	HK	72	2	-	4/7/8/10	-
2	MEN	P2	72	2	-	4/7/8/10	-
20	MEN	Q3	71	20	-	6/7/8/10	-
2	MEN	H1	72	2	-	4/7/8/10	-
9	MEN	D2	72	9	-	4/7/8/10	-
2	MEN	R2	72	2	-	2/7/8/10	-
2	MEN	R1	72	2	-	4/7/8/10	-
2	MEN	I5	72	2	-	4/7/8/10	-
2	MEN	kE	72	2	-	4/7/8/10	-
2	MEN	D1	72	2	-	3/7/8/10	-
2	MEN	OJ	72	2	-	2/7/8/10	-
2	MEN	DG	72	2	-	4/7/8/10	-
2	MEN	N8	72	2,31	-	2/7/8/10	-
9	MEN	DB	72	9	-	2/7/8/10	-
2	MEN	YD	72	2	-	5/7/8/10	-
2	MEN	BA	72	2	-	5/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	MEN	NB	72	9	-	4/7/8/10	-
9	MEN	HE	72	9	-	4/7/8/10	-
2	MEN	PD	72	2	-	3/7/8/10	-
2	MEN	X1	72	2	-	4/7/8/10	-
2	MEN	k4	72	2	-	4/7/8/10	-
2	MEN	J9	72	2	-	5/7/8/10	-
2	MEN	cD	72	2	-	3/7/8/10	-
2	MEN	X7	72	2	-	4/7/8/10	-
2	MEN	MJ	72	2	-	2/7/8/10	-
2	MEN	U9	72	2	-	4/7/8/10	-
2	MEN	F4	72	2	-	4/7/8/10	-
2	MEN	CA	72	2	-	2/7/8/10	-
2	MEN	Y5	72	2	-	4/7/8/10	-
2	MEN	N7	72	2	-	4/7/8/10	-
2	MEN	RA	72	2	-	7/7/8/10	-
2	MEN	cE	72	2	-	3/7/8/10	-
9	MEN	FD	72	9	-	3/7/8/10	-
2	MEN	P6	72	2	-	4/7/8/10	-
2	MEN	RB	72	2	-	4/7/8/10	-
2	MEN	Q9	72	2	-	4/7/8/10	-
2	MEN	R8	72	2,31	-	2/7/8/10	-
2	MEN	FF	72	2,31	-	2/7/8/10	-
2	MEN	GJ	72	2	-	4/7/8/10	-
2	MEN	YC	72	2	-	4/7/8/10	-
9	MEN	H2	72	9	-	4/7/8/10	-
20	MEN	h3	71	20	-	5/7/8/10	-
2	MEN	P7	72	2	-	4/7/8/10	-
2	MEN	c2	72	2	-	4/7/8/10	-
9	MEN	N2	72	9	-	2/7/8/10	-
9	MEN	JC	72	9	-	1/7/8/10	-
2	MEN	VK	72	2	-	4/7/8/10	-
20	MEN	I3	71	20	-	5/7/8/10	-
2	MEN	OA	72	2	-	4/7/8/10	-
20	MEN	F3	71	20	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	R7	72	2	-	4/7/8/10	-
2	MEN	V8	72	2,31	-	4/7/8/10	-
2	MEN	PH	72	2	-	4/7/8/10	-
9	MEN	NC	72	9	-	2/7/8/10	-
2	MEN	gB	72	2	-	4/7/8/10	-
2	MEN	GA	72	2	-	6/7/8/10	-
2	MEN	X8	72	2,31	-	2/7/8/10	-
2	MEN	m6	72	2	-	4/7/8/10	-
9	MEN	JB	72	9	-	2/7/8/10	-
9	MEN	N6	72	9	-	4/7/8/10	-
2	MEN	aA	72	2	-	4/7/8/10	-
2	MEN	SA	72	2	-	3/7/8/10	-
2	MEN	PF	72	2,31	-	3/7/8/10	-
2	MEN	LH	72	2	-	5/7/8/10	-
2	MEN	eC	72	2	-	3/7/8/10	-
2	MEN	i2	72	2	-	4/7/8/10	-
2	MEN	TB	72	2	-	3/7/8/10	-
2	MEN	BG	72	2	-	5/7/8/10	-
2	MEN	J1	72	2	-	1/7/8/10	-
2	MEN	K5	72	2	-	4/7/8/10	-
9	MEN	FC	72	9	-	2/7/8/10	-
2	MEN	HG	72	2	-	4/7/8/10	-
2	MEN	ZA	72	2	-	6/7/8/10	-
20	MEN	q3	71	20	-	2/7/8/10	-
2	MEN	B8	72	2,31	-	2/7/8/10	-
2	MEN	nF	72	2,31	-	3/7/8/10	-
2	MEN	YE	72	2	-	5/7/8/10	-
2	MEN	L4	72	2	-	4/7/8/10	-
2	MEN	jF	72	2,31	-	4/7/8/10	-
2	MEN	e2	72	2	-	3/7/8/10	-
2	MEN	H7	72	2	-	4/7/8/10	-
2	MEN	UI	72	2	-	2/7/8/10	-
2	MEN	f8	72	2,31	-	2/7/8/10	-
2	MEN	eH	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	J4	72	2	-	4/7/8/10	-
20	MEN	d3	71	20	-	5/7/8/10	-
2	MEN	eE	72	2	-	2/7/8/10	-
2	MEN	gE	72	2	-	4/7/8/10	-
2	MEN	R4	72	2	-	4/7/8/10	-
2	MEN	WI	72	2	-	2/7/8/10	-
2	MEN	W5	72	2	-	4/7/8/10	-
2	MEN	VE	72	2	-	4/7/8/10	-
2	MEN	N1	72	2	-	4/7/8/10	-
2	MEN	X4	72	2	-	4/7/8/10	-
2	MEN	v8	72	2,31	-	1/7/8/10	-
2	MEN	F1	72	2	-	4/7/8/10	-
2	MEN	LK	72	2	-	5/7/8/10	-
2	MEN	t8	72	2,31	-	4/7/8/10	-
2	MEN	JF	72	2,31	-	2/7/8/10	-
2	MEN	iE	72	2	-	3/7/8/10	-
2	MEN	YB	72	2	-	4/7/8/10	-
9	MEN	DE	72	9,10	-	4/7/8/10	-
2	MEN	V6	72	2	-	2/7/8/10	-
2	MEN	Y2	72	2	-	4/7/8/10	-
2	MEN	FH	72	2	-	4/7/8/10	-
2	MEN	mE	72	2	-	3/7/8/10	-
2	MEN	pF	72	2,31	-	3/7/8/10	-
2	MEN	n8	72	2,31	-	3/7/8/10	-
9	MEN	FE	72	9	-	3/7/8/10	-
20	MEN	O3	71	20	-	3/7/8/10	-
2	MEN	L9	72	2	-	4/7/8/10	-
2	MEN	T2	72	2	-	5/7/8/10	-
2	MEN	e6	72	2	-	5/7/8/10	-
9	MEN	F6	72	9	-	3/7/8/10	-
2	MEN	WG	72	2	-	5/7/8/10	-
2	MEN	P4	72	2	-	5/7/8/10	-
2	MEN	RF	72	2,31	-	2/7/8/10	-
2	MEN	NK	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	BI	72	2	-	4/7/8/10	-
2	MEN	H4	72	2	-	4/7/8/10	-
2	MEN	VB	72	2	-	2/7/8/10	-
9	MEN	LB	72	9	-	4/7/8/10	-
20	MEN	U3	71	20	-	6/7/8/10	-
2	MEN	SI	72	2	-	2/7/8/10	-
2	MEN	XK	72	2	-	4/7/8/10	-
2	MEN	L8	72	2,31	-	3/7/8/10	-
2	MEN	PK	72	2	-	4/7/8/10	-
9	MEN	HB	72	9	-	2/7/8/10	-
9	MEN	ND	72	9	-	1/7/8/10	-
2	MEN	vF	72	2,31	-	1/7/8/10	-
2	MEN	FG	72	2	-	5/7/8/10	-
2	MEN	fF	72	2,31	-	2/7/8/10	-
2	MEN	DH	72	2	-	3/7/8/10	-
2	MEN	LG	72	2	-	4/7/8/10	-
2	MEN	N4	72	2	-	4/7/8/10	-
2	MEN	c6	72	2	-	2/7/8/10	-
2	MEN	J7	72	2	-	4/7/8/10	-
2	MEN	JH	72	2	-	3/7/8/10	-
2	MEN	H9	72	2	-	4/7/8/10	-
2	MEN	eB	72	2	-	5/7/8/10	-
2	MEN	TH	72	2	-	5/7/8/10	-
2	MEN	TC	72	2	-	5/7/8/10	-
2	MEN	F7	72	2	-	5/7/8/10	-
20	MEN	B3	71	20	-	5/7/8/10	-
2	MEN	k6	72	2	-	5/7/8/10	-
2	MEN	T1	72	2,15	-	6/7/8/10	-
2	MEN	HF	72	2,31	-	2/7/8/10	-
2	MEN	B7	72	2	-	4/7/8/10	-
9	MEN	H6	72	9	-	2/7/8/10	-
20	MEN	f3	71	20	-	4/7/8/10	-
2	MEN	gC	72	2	-	3/7/8/10	-
20	MEN	s3	71	20	-	6/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	TK	72	2,15	-	6/7/8/10	-
2	MEN	ZF	72	2	-	5/7/8/10	-
9	MEN	NE	72	9	-	4/7/8/10	-
2	MEN	a6	72	2	-	3/7/8/10	-
2	MEN	g4	72	2	-	5/7/8/10	-
2	MEN	k2	72	2	-	4/7/8/10	-
2	MEN	DK	72	2	-	3/7/8/10	-
2	MEN	R6	72	2	-	4/7/8/10	-
2	MEN	rF	72	2,31	-	3/7/8/10	-
2	MEN	e4	72	2	-	4/7/8/10	-
2	MEN	FK	72	2	-	4/7/8/10	-
2	MEN	O9	72	2	-	4/7/8/10	-
20	MEN	k3	71	20	-	4/7/8/10	-
2	MEN	TF	72	2,31	-	2/7/8/10	-
20	MEN	M3	71	20	-	4/7/8/10	-
2	MEN	QG	72	2	-	4/7/8/10	-
2	MEN	PA	72	2	-	4/7/8/10	-
2	MEN	hF	72	2,31	-	2/7/8/10	-
2	MEN	H8	72	2,31	-	2/7/8/10	-
2	MEN	VH	72	2	-	4/7/8/10	-
2	MEN	IA	72	2	-	4/7/8/10	-
2	MEN	gD	72	2	-	4/7/8/10	-
2	MEN	DF	72	2,31	-	2/7/8/10	-
2	MEN	QA	72	2	-	6/7/8/10	-
9	MEN	L6	72	9	-	4/7/8/10	-
2	MEN	Y6	72	2	-	4/7/8/10	-
2	MEN	OI	72	2	-	4/7/8/10	-
2	MEN	MA	72	2	-	2/7/8/10	-
2	MEN	T7	72	2	-	4/7/8/10	-
20	MEN	L3	71	20	-	4/7/8/10	-
2	MEN	TD	72	2	-	3/7/8/10	-
20	MEN	o3	71	20	-	5/7/8/10	-
2	MEN	aC	72	2	-	3/7/8/10	-
2	MEN	UG	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	iD	72	2	-	3/7/8/10	-
2	MEN	eA	72	2	-	3/7/8/10	-
2	MEN	SG	72	2	-	4/7/8/10	-
2	MEN	O5	72	2	-	2/7/8/10	-
20	MEN	S3	71	20	-	6/7/8/10	-
9	MEN	JE	72	9	-	2/7/8/10	-
2	MEN	NF	72	2,31	-	2/7/8/10	-
2	MEN	V2	72	2	-	4/7/8/10	-
2	MEN	RK	72	2	-	4/7/8/10	-
2	MEN	Q5	72	2	-	4/7/8/10	-
2	MEN	i4	72	2	-	4/7/8/10	-
20	MEN	w3	71	20	-	6/7/8/10	-
2	MEN	b8	72	2	-	4/7/8/10	-
2	MEN	VA	72	2	-	4/7/8/10	-
2	MEN	T8	72	2,31	-	2/7/8/10	-
2	MEN	G5	72	2	-	4/7/8/10	-
2	MEN	T4	72	2	-	3/7/8/10	-
2	MEN	B1	72	2	-	4/7/8/10	-
2	MEN	ZH	72	2	-	4/7/8/10	-
2	MEN	V4	72	2	-	4/7/8/10	-
2	MEN	gH	72	2	-	2/7/8/10	-
2	MEN	V7	72	2	-	4/7/8/10	-
2	MEN	L7	72	2	-	4/7/8/10	-
2	MEN	SJ	72	2	-	4/7/8/10	-
2	MEN	LA	72	2	-	4/7/8/10	-
2	MEN	S5	72	2	-	4/7/8/10	-
2	MEN	cC	72	2	-	4/7/8/10	-
2	MEN	LI	72	2	-	2/7/8/10	-
2	MEN	XA	72	2	-	5/7/8/10	-
2	MEN	F8	72	2,31	-	2/7/8/10	-
2	MEN	HA	72	2	-	2/7/8/10	-
2	MEN	h8	72	2,31	-	2/7/8/10	-
20	MEN	u3	71	20	-	6/7/8/10	-
2	MEN	mH	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	Y9	72	2	-	4/7/8/10	-
2	MEN	cB	72	2	-	2/7/8/10	-
2	MEN	dF	72	2,31	-	3/7/8/10	-
2	MEN	m4	72	2	-	4/7/8/10	-
2	MEN	EJ	72	2	-	3/7/8/10	-
2	MEN	mC	72	2	-	4/7/8/10	-
2	MEN	YA	72	2	-	4/7/8/10	-
2	MEN	J8	72	2,31	-	2/7/8/10	-
2	MEN	JI	72	2	-	2/7/8/10	-
20	MEN	j3	71	20	-	4/7/8/10	-
2	MEN	RE	72	2	-	3/7/8/10	-
2	MEN	CJ	72	2	-	4/7/8/10	-
2	MEN	kB	72	2	-	5/7/8/10	-
2	MEN	kH	72	2	-	4/7/8/10	-
2	MEN	tF	72	2,31	-	4/7/8/10	-
2	MEN	iB	72	2	-	4/7/8/10	-
2	MEN	W9	72	2	-	4/7/8/10	-
2	MEN	g2	72	2	-	3/7/8/10	-
2	MEN	U5	72	2	-	3/7/8/10	-
2	MEN	JG	72	2	-	5/7/8/10	-
2	MEN	QJ	72	2	-	4/7/8/10	-
2	MEN	D7	72	2	-	4/7/8/10	-
2	MEN	dA	72	2	-	5/7/8/10	-
2	MEN	P1	72	2	-	4/7/8/10	-
2	MEN	PE	72	2	-	3/7/8/10	-
2	MEN	YG	72	2	-	3/7/8/10	-
2	MEN	BK	72	2	-	4/7/8/10	-
2	MEN	HH	72	2	-	4/7/8/10	-
2	MEN	kD	72	2	-	4/7/8/10	-
2	MEN	LF	72	2,31	-	3/7/8/10	-
9	MEN	DD	72	9,10	-	4/7/8/10	-
2	MEN	D9	72	2	-	4/7/8/10	-
2	MEN	RH	72	2	-	4/7/8/10	-
2	MEN	i6	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	mB	72	2	-	4/7/8/10	-
9	MEN	J2	72	9	-	1/7/8/10	-
2	MEN	c4	72	2	-	4/7/8/10	-
2	MEN	cH	72	2	-	4/7/8/10	-
20	MEN	H3	71	20	-	4/7/8/10	-
9	MEN	HD	72	9	-	4/7/8/10	-
2	MEN	d8	72	2,31	-	3/7/8/10	-
2	MEN	kC	72	2	-	4/7/8/10	-
2	MEN	VC	72	2	-	4/7/8/10	-
2	MEN	iH	72	2	-	4/7/8/10	-
2	MEN	D4	72	2	-	5/7/8/10	-
2	MEN	aD	72	2	-	4/7/8/10	-
2	MEN	B9	72	2	-	4/7/8/10	-
2	MEN	V1	72	2	-	4/7/8/10	-
9	MEN	L2	72	9	-	2/7/8/10	-
2	MEN	L1	72	2	-	5/7/8/10	-
2	MEN	iC	72	2	-	4/7/8/10	-
2	MEN	QI	72	2	-	2/7/8/10	-
2	MEN	S9	72	2	-	4/7/8/10	-
2	MEN	j8	72	2,31	-	4/7/8/10	-
2	MEN	r8	72	2,31	-	3/7/8/10	-
2	MEN	lF	72	2,31	-	4/7/8/10	-
2	MEN	C5	72	2	-	4/7/8/10	-
9	MEN	LD	72	9	-	4/7/8/10	-
2	MEN	BF	72	2,31	-	2/7/8/10	-
2	MEN	M5	72	2	-	2/7/8/10	-
2	MEN	g6	72	2	-	4/7/8/10	-
2	MEN	F9	72	2	-	4/7/8/10	-
2	MEN	TE	72	2	-	3/7/8/10	-
2	MEN	p8	72	2,31	-	3/7/8/10	-
2	MEN	PB	72	2	-	4/7/8/10	-
2	MEN	UJ	72	2	-	3/7/8/10	-
2	MEN	XH	72	2	-	5/7/8/10	-
2	MEN	KJ	72	2	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MEN	E5	72	2	-	3/7/8/10	-
9	MEN	HC	72	9	-	4/7/8/10	-
20	MEN	n3	71	20	-	4/7/8/10	-
2	MEN	T6	72	2	-	3/7/8/10	-
20	MEN	D3	71	20	-	5/7/8/10	-
2	MEN	FA	72	2	-	3/7/8/10	-
2	MEN	gA	72	2	-	5/7/8/10	-
2	MEN	bF	72	2	-	4/7/8/10	-
2	MEN	WJ	72	2	-	4/7/8/10	-
2	MEN	D8	72	2,31	-	2/7/8/10	-
2	MEN	DI	72	2	-	2/7/8/10	-
9	MEN	J6	72	9	-	2/7/8/10	-
2	MEN	l8	72	2,31	-	4/7/8/10	-
2	MEN	mD	72	2	-	3/7/8/10	-
9	MEN	JD	72	9	-	2/7/8/10	-

The worst 5 of 128 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	S3	71	MEN	CE2-ND2	67.26	2.65	1.45
20	Q3	71	MEN	CE2-ND2	67.24	2.65	1.45
20	s3	71	MEN	CE2-ND2	67.24	2.65	1.45
20	U3	71	MEN	CE2-ND2	67.22	2.65	1.45
20	w3	71	MEN	CE2-ND2	67.21	2.65	1.45

The worst 5 of 526 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	U3	71	MEN	OD1-CG-CB	-38.81	64.66	121.50
20	S3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
20	s3	71	MEN	OD1-CG-CB	-38.79	64.69	121.50
20	Q3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50
20	w3	71	MEN	OD1-CG-CB	-38.78	64.69	121.50

There are no chirality outliers.

5 of 1198 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BA	72	MEN	N-CA-CB-CG
2	BA	72	MEN	C-CA-CB-CG
2	BA	72	MEN	CB-CG-ND2-CE2
2	CA	72	MEN	C-CA-CB-CG
2	DA	72	MEN	CB-CG-ND2-CE2

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](#)

1602 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	$\# Z > 2$
31	PEB	OE	202	3	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
33	CYC	DC	1001	9	42,46,46	3.36	15 (35%)	50,67,67	2.85	18 (36%)
31	PEB	Y1	303	6	43,46,46	3.39	10 (23%)	45,67,67	2.74	18 (40%)
31	PEB	c2	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.33	16 (35%)
31	PEB	A5	301	31,6	43,46,46	3.49	10 (23%)	45,67,67	2.66	15 (33%)
31	PEB	Q1	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.65	16 (35%)
31	PEB	k4	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.50	15 (33%)
31	PEB	H1	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.14	14 (31%)
31	PEB	U4	201	2,3	43,46,46	3.27	11 (25%)	45,67,67	2.49	14 (31%)
31	PEB	q8	201	2,3	43,46,46	3.41	12 (27%)	45,67,67	2.68	17 (37%)
31	PEB	C5	202	2,6	43,46,46	3.15	11 (25%)	45,67,67	2.23	18 (40%)
31	PEB	XJ	202	3	43,46,46	3.57	12 (27%)	45,67,67	1.92	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	K7	201	2,3	43,46,46	3.36	11 (25%)	45,67,67	2.49	15 (33%)
31	PEB	Y7	501	2	43,46,46	3.32	10 (23%)	45,67,67	2.15	15 (33%)
31	PEB	V1	201	2,15	43,46,46	3.37	10 (23%)	45,67,67	2.12	13 (28%)
31	PEB	B5	203	2,3	43,46,46	2.94	9 (20%)	45,67,67	2.38	14 (31%)
31	PEB	GF	202	3	43,46,46	2.64	11 (25%)	45,67,67	3.01	20 (44%)
31	PEB	R6	203	2	43,46,46	3.44	10 (23%)	45,67,67	1.98	11 (24%)
31	PEB	JA	201	3	43,46,46	3.37	11 (25%)	45,67,67	2.76	16 (35%)
31	PEB	QK	202	3	43,46,46	3.20	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	Y7	503	2,27	43,46,46	3.20	10 (23%)	45,67,67	2.00	14 (31%)
31	PEB	kF	201	3	43,46,46	3.40	10 (23%)	45,67,67	2.06	12 (26%)
31	PEB	AF	202	3	43,46,46	3.52	12 (27%)	45,67,67	1.91	12 (26%)
31	PEB	RI	202	3	43,46,46	3.59	11 (25%)	45,67,67	2.66	17 (37%)
31	PEB	HG	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.10	13 (28%)
31	PEB	YK	303	6	43,46,46	3.41	10 (23%)	45,67,67	2.74	18 (40%)
31	PEB	M1	201	3	43,46,46	3.27	11 (25%)	45,67,67	2.42	14 (31%)
31	PEB	YD	201	2	43,46,46	3.10	11 (25%)	45,67,67	2.60	20 (44%)
33	CYC	k3	1001	20	42,46,46	3.43	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	GJ	202	2	43,46,46	3.42	9 (20%)	45,67,67	2.10	17 (37%)
31	PEB	TA	202	3	43,46,46	3.22	10 (23%)	45,67,67	2.33	16 (35%)
31	PEB	fD	203	2,3	43,46,46	3.41	11 (25%)	45,67,67	2.18	13 (28%)
31	PEB	JK	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.75	16 (35%)
31	PEB	dC	201	2,3	43,46,46	3.26	10 (23%)	45,67,67	2.35	15 (33%)
31	PEB	lC	202	3	43,46,46	3.50	11 (25%)	45,67,67	2.76	15 (33%)
31	PEB	l8	202	2	43,46,46	3.43	11 (25%)	45,67,67	2.11	16 (35%)
31	PEB	J1	201	2,6	43,46,46	3.29	9 (20%)	45,67,67	2.44	13 (28%)
31	PEB	WH	203	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.69	19 (42%)
31	PEB	b2	201	3	43,46,46	3.36	11 (25%)	45,67,67	2.04	15 (33%)
31	PEB	RC	202	2	43,46,46	3.52	11 (25%)	45,67,67	1.74	11 (24%)
31	PEB	QB	201	3	43,46,46	3.31	11 (25%)	45,67,67	2.70	20 (44%)
31	PEB	VF	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.65	18 (40%)
31	PEB	l1	202	3	43,46,46	3.44	11 (25%)	45,67,67	1.87	12 (26%)
31	PEB	C8	201	3	43,46,46	3.36	10 (23%)	45,67,67	2.27	14 (31%)
31	PEB	Z9	302	14	43,46,46	3.12	11 (25%)	45,67,67	2.41	14 (31%)
31	PEB	KJ	202	2	43,46,46	3.35	9 (20%)	45,67,67	2.16	15 (33%)
31	PEB	HA	203	2	43,46,46	3.18	10 (23%)	45,67,67	2.11	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	fD	201	3	43,46,46	3.36	10 (23%)	45,67,67	2.12	17 (37%)
31	PEB	T4	201	2	43,46,46	3.30	11 (25%)	45,67,67	2.39	12 (26%)
31	PEB	HI	202	2	43,46,46	3.20	10 (23%)	45,67,67	2.30	13 (28%)
31	PEB	H8	201	2	43,46,46	3.14	13 (30%)	45,67,67	2.92	21 (46%)
31	PEB	bA	201	2	43,46,46	3.22	10 (23%)	45,67,67	2.16	15 (33%)
33	CYC	K3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	CG	202	3	43,46,46	3.21	10 (23%)	45,67,67	2.31	14 (31%)
32	PUB	KK	203	6,3	42,46,46	3.37	7 (16%)	37,67,67	3.58	17 (45%)
31	PEB	ZC	201	2,3	43,46,46	3.26	9 (20%)	45,67,67	3.15	17 (37%)
31	PEB	f8	202	2	43,46,46	3.62	12 (27%)	45,67,67	2.01	18 (40%)
31	PEB	iB	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.32	14 (31%)
31	PEB	aE	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.34	15 (33%)
31	PEB	PJ	203	3	43,46,46	3.39	9 (20%)	45,67,67	2.10	12 (26%)
31	PEB	GK	202	3	43,46,46	3.36	11 (25%)	45,67,67	1.98	15 (33%)
31	PEB	u8	202	3	43,46,46	3.43	11 (25%)	45,67,67	1.97	15 (33%)
31	PEB	wF	301	12	43,46,46	3.24	9 (20%)	45,67,67	2.30	15 (33%)
31	PEB	kH	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.40	16 (35%)
31	PEB	S1	202	3	43,46,46	3.20	10 (23%)	45,67,67	1.95	12 (26%)
31	PEB	M8	201	3	43,46,46	3.27	10 (23%)	45,67,67	1.87	14 (31%)
31	PEB	VJ	202	3	43,46,46	3.53	11 (25%)	45,67,67	2.07	12 (26%)
32	PUB	y8	303	13	42,46,46	3.32	7 (16%)	37,67,67	3.10	13 (35%)
31	PEB	oF	202	3	43,46,46	3.51	9 (20%)	45,67,67	1.96	12 (26%)
31	PEB	YH	202	3	43,46,46	3.17	10 (23%)	45,67,67	2.20	15 (33%)
31	PEB	ZD	201	3	43,46,46	3.33	11 (25%)	45,67,67	2.15	16 (35%)
31	PEB	i2	201	2	43,46,46	3.34	12 (27%)	45,67,67	2.04	16 (35%)
31	PEB	VF	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.55	15 (33%)
31	PEB	GA	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.10	15 (33%)
31	PEB	M4	203	3	43,46,46	3.27	11 (25%)	45,67,67	2.22	16 (35%)
31	PEB	YF	202	3	43,46,46	3.42	11 (25%)	45,67,67	1.90	13 (28%)
31	PEB	QF	202	3	43,46,46	3.41	11 (25%)	45,67,67	1.94	13 (28%)
31	PEB	UH	201	2,3	43,46,46	3.17	10 (23%)	45,67,67	2.53	19 (42%)
31	PEB	FH	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.44	16 (35%)
31	PEB	DG	202	2	43,46,46	3.27	9 (20%)	45,67,67	2.06	14 (31%)
31	PEB	Y2	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.03	12 (26%)
33	CYC	r3	1001	19	42,46,46	3.69	14 (33%)	50,67,67	2.93	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	P1	202	2	43,46,46	3.15	10 (23%)	45,67,67	2.63	16 (35%)
31	PEB	TJ	202	3	43,46,46	3.46	10 (23%)	45,67,67	2.04	15 (33%)
31	PEB	KF	201	2,3	43,46,46	3.12	10 (23%)	45,67,67	2.52	14 (31%)
31	PEB	Q2	203	3	43,46,46	3.28	11 (25%)	45,67,67	2.07	14 (31%)
31	PEB	YF	203	2,3	43,46,46	3.43	11 (25%)	45,67,67	2.69	17 (37%)
31	PEB	P8	202	2	43,46,46	3.60	11 (25%)	45,67,67	2.08	14 (31%)
31	PEB	R6	201	2,10	43,46,46	3.32	10 (23%)	45,67,67	2.38	14 (31%)
31	PEB	AE	304	6	43,46,46	3.30	9 (20%)	45,67,67	2.16	16 (35%)
31	PEB	jE	201	3	43,46,46	3.43	12 (27%)	45,67,67	2.10	15 (33%)
31	PEB	DK	203	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	16 (35%)
31	PEB	IJ	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.32	15 (33%)
33	CYC	DD	1001	9	42,46,46	3.16	14 (33%)	50,67,67	3.00	21 (42%)
33	CYC	x3	1001	-	42,46,46	3.51	12 (28%)	50,67,67	2.97	23 (46%)
31	PEB	Y1	302	31,6	43,46,46	3.33	10 (23%)	45,67,67	3.21	18 (40%)
31	PEB	UB	202	3	43,46,46	3.30	10 (23%)	45,67,67	1.89	12 (26%)
31	PEB	E1	201	3	43,46,46	3.56	12 (27%)	45,67,67	2.31	14 (31%)
31	PEB	s8	202	3	43,46,46	3.45	10 (23%)	45,67,67	2.05	15 (33%)
31	PEB	kC	203	2,3	43,46,46	3.35	10 (23%)	45,67,67	2.26	16 (35%)
31	PEB	K4	202	3	43,46,46	3.28	11 (25%)	45,67,67	2.15	15 (33%)
31	PEB	KA	304	2,4	43,46,46	3.27	10 (23%)	45,67,67	2.12	14 (31%)
31	PEB	EI	201	3	43,46,46	3.38	9 (20%)	45,67,67	1.95	14 (31%)
31	PEB	eF	202	3	43,46,46	3.12	10 (23%)	45,67,67	2.25	20 (44%)
31	PEB	GI	201	3	43,46,46	3.37	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	M7	201	3	43,46,46	3.39	10 (23%)	45,67,67	2.30	17 (37%)
31	PEB	cF	203	2,3	43,46,46	3.33	12 (27%)	45,67,67	2.78	17 (37%)
31	PEB	FA	201	2,4	43,46,46	3.27	11 (25%)	45,67,67	2.19	13 (28%)
31	PEB	LI	203	2	43,46,46	3.40	11 (25%)	45,67,67	2.32	15 (33%)
31	PEB	cD	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.11	16 (35%)
31	PEB	CG	201	3	43,46,46	3.34	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	IG	202	3	43,46,46	3.22	9 (20%)	45,67,67	2.31	14 (31%)
31	PEB	VA	202	2,3	43,46,46	3.32	10 (23%)	45,67,67	2.09	15 (33%)
31	PEB	AC	301	6	43,46,46	3.40	8 (18%)	45,67,67	2.12	14 (31%)
31	PEB	K4	203	2,3	43,46,46	3.19	10 (23%)	45,67,67	2.64	18 (40%)
31	PEB	QC	203	3	43,46,46	3.30	9 (20%)	45,67,67	2.08	14 (31%)
31	PEB	T5	202	3	43,46,46	3.44	10 (23%)	45,67,67	2.05	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	T9	202	3	43,46,46	3.36	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	QE	202	3	43,46,46	3.43	10 (23%)	45,67,67	2.06	15 (33%)
31	PEB	Q8	201	3	43,46,46	3.12	9 (20%)	45,67,67	2.26	14 (31%)
31	PEB	DG	201	2,11	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
31	PEB	XG	202	3	43,46,46	3.22	9 (20%)	45,67,67	2.32	14 (31%)
31	PEB	P7	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.09	17 (37%)
31	PEB	A7	203	2,3	43,46,46	3.42	11 (25%)	45,67,67	2.58	15 (33%)
31	PEB	JF	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.34	16 (35%)
31	PEB	iE	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.02	14 (31%)
31	PEB	GG	203	3	43,46,46	3.22	10 (23%)	45,67,67	2.32	14 (31%)
31	PEB	eB	203	2	43,46,46	3.33	9 (20%)	45,67,67	1.98	12 (26%)
31	PEB	DA	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.09	16 (35%)
31	PEB	h4	203	3	43,46,46	3.34	9 (20%)	45,67,67	2.64	13 (28%)
31	PEB	D2	1002	9	43,46,46	3.31	11 (25%)	45,67,67	2.13	15 (33%)
31	PEB	V5	201	3	43,46,46	3.17	10 (23%)	45,67,67	2.29	12 (26%)
31	PEB	L5	202	3	43,46,46	3.36	11 (25%)	45,67,67	2.25	14 (31%)
31	PEB	v8	201	2	43,46,46	3.48	10 (23%)	45,67,67	2.85	18 (40%)
32	PUB	NJ	201	6,3	42,46,46	3.77	9 (21%)	37,67,67	3.15	12 (32%)
31	PEB	VH	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.46	18 (40%)
31	PEB	KK	202	3	43,46,46	3.45	10 (23%)	45,67,67	1.80	11 (24%)
31	PEB	WH	201	3	43,46,46	3.28	11 (25%)	45,67,67	2.40	17 (37%)
31	PEB	U9	203	2	43,46,46	3.32	10 (23%)	45,67,67	1.96	16 (35%)
31	PEB	AE	301	6	43,46,46	3.33	11 (25%)	45,67,67	2.33	16 (35%)
31	PEB	R7	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.09	15 (33%)
31	PEB	R5	202	3	43,46,46	3.35	11 (25%)	45,67,67	1.99	13 (28%)
31	PEB	MI	301	2,14	43,46,46	3.33	10 (23%)	45,67,67	1.86	13 (28%)
31	PEB	WG	202	2,3	43,46,46	3.04	12 (27%)	45,67,67	2.88	16 (35%)
31	PEB	bD	201	3	43,46,46	3.32	10 (23%)	45,67,67	2.09	16 (35%)
31	PEB	R4	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.59	17 (37%)
31	PEB	UE	201	2,3	43,46,46	3.29	10 (23%)	45,67,67	2.39	16 (35%)
31	PEB	NG	203	2,3	43,46,46	3.06	12 (27%)	45,67,67	2.67	14 (31%)
31	PEB	A7	201	3	43,46,46	3.23	10 (23%)	45,67,67	2.20	15 (33%)
33	CYC	H3	1001	24,20	42,46,46	3.45	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	MA	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.25	17 (37%)
33	CYC	v3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.93	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	GH	202	3	43,46,46	3.40	10 (23%)	45,67,67	2.02	14 (31%)
31	PEB	KG	203	3	43,46,46	3.22	10 (23%)	45,67,67	2.31	14 (31%)
31	PEB	VB	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.20	16 (35%)
31	PEB	YE	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.28	17 (37%)
31	PEB	U9	201	2,14	43,46,46	3.59	14 (32%)	45,67,67	2.21	14 (31%)
31	PEB	HH	201	2	43,46,46	3.18	10 (23%)	45,67,67	2.39	15 (33%)
31	PEB	E7	201	3	43,46,46	3.30	11 (25%)	45,67,67	2.02	14 (31%)
31	PEB	l4	202	3	43,46,46	3.28	10 (23%)	45,67,67	2.21	15 (33%)
31	PEB	N9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	fF	201	2,12	43,46,46	3.39	9 (20%)	45,67,67	3.06	16 (35%)
31	PEB	G7	202	3	43,46,46	3.25	10 (23%)	45,67,67	2.24	15 (33%)
31	PEB	OD	201	3	43,46,46	3.37	10 (23%)	45,67,67	2.22	14 (31%)
31	PEB	Z4	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.57	14 (31%)
31	PEB	g2	202	2	43,46,46	3.50	11 (25%)	45,67,67	2.22	14 (31%)
31	PEB	gE	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.50	13 (28%)
31	PEB	f8	201	2,12	43,46,46	3.42	10 (23%)	45,67,67	3.07	16 (35%)
33	CYC	K6	1001	8	42,46,46	3.27	14 (33%)	50,67,67	2.89	19 (38%)
31	PEB	YG	201	2,11	43,46,46	3.36	11 (25%)	45,67,67	2.06	16 (35%)
31	PEB	YC	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.03	12 (26%)
33	CYC	MD	1001	8,9	42,46,46	3.15	14 (33%)	50,67,67	2.88	19 (38%)
31	PEB	P4	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.24	14 (31%)
31	PEB	b6	202	3	43,46,46	3.44	10 (23%)	45,67,67	2.00	13 (28%)
31	PEB	GK	201	3	43,46,46	3.11	9 (20%)	45,67,67	2.23	13 (28%)
33	CYC	IE	1001	8,9	42,46,46	3.18	13 (30%)	50,67,67	2.85	18 (36%)
31	PEB	T8	202	2	43,46,46	3.44	12 (27%)	45,67,67	2.22	17 (37%)
31	PEB	i8	201	2,3	43,46,46	3.41	10 (23%)	45,67,67	2.38	14 (31%)
31	PEB	h6	202	3	43,46,46	3.40	10 (23%)	45,67,67	2.00	13 (28%)
31	PEB	CK	201	3	43,46,46	3.30	12 (27%)	45,67,67	2.55	17 (37%)
31	PEB	X4	202	2	43,46,46	3.33	12 (27%)	45,67,67	2.53	16 (35%)
31	PEB	VK	203	2	43,46,46	3.54	12 (27%)	45,67,67	1.97	16 (35%)
33	CYC	F2	1001	9	42,46,46	3.32	14 (33%)	50,67,67	2.89	18 (36%)
31	PEB	KG	201	2,3	43,46,46	3.16	13 (30%)	45,67,67	2.83	14 (31%)
31	PEB	P4	201	2	43,46,46	3.38	12 (27%)	45,67,67	2.57	15 (33%)
31	PEB	l4	203	3	43,46,46	3.34	11 (25%)	45,67,67	2.37	15 (33%)
31	PEB	P2	201	2,10	43,46,46	3.37	10 (23%)	45,67,67	2.25	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	M4	201	2,3	43,46,46	3.18	10 (23%)	45,67,67	2.51	17 (37%)
31	PEB	m8	202	3	43,46,46	3.42	10 (23%)	45,67,67	2.20	14 (31%)
31	PEB	SK	201	3	43,46,46	3.19	10 (23%)	45,67,67	2.76	16 (35%)
31	PEB	q8	202	3	43,46,46	3.39	11 (25%)	45,67,67	3.43	18 (40%)
31	PEB	nF	202	2	43,46,46	3.61	12 (27%)	45,67,67	1.94	13 (28%)
31	PEB	OF	202	3	43,46,46	3.09	9 (20%)	45,67,67	2.20	15 (33%)
31	PEB	QF	201	3	43,46,46	3.13	9 (20%)	45,67,67	2.28	14 (31%)
31	PEB	I5	202	2,26	43,46,46	3.68	13 (30%)	45,67,67	2.36	18 (40%)
31	PEB	EF	201	3	43,46,46	3.07	9 (20%)	45,67,67	2.32	14 (31%)
31	PEB	T2	202	2	43,46,46	3.32	9 (20%)	45,67,67	1.81	12 (26%)
31	PEB	Y2	201	2	43,46,46	3.51	11 (25%)	45,67,67	2.31	18 (40%)
31	PEB	VK	201	2,15	43,46,46	3.35	10 (23%)	45,67,67	2.10	13 (28%)
31	PEB	DF	203	2,3	43,46,46	3.15	10 (23%)	45,67,67	2.69	16 (35%)
31	PEB	a4	202	3	43,46,46	3.35	10 (23%)	45,67,67	2.09	13 (28%)
31	PEB	o8	202	3	43,46,46	3.52	9 (20%)	45,67,67	1.95	14 (31%)
31	PEB	TJ	201	2,3	43,46,46	3.36	13 (30%)	45,67,67	2.31	13 (28%)
31	PEB	C4	203	2,3	43,46,46	3.18	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	l4	201	2,3	43,46,46	3.31	11 (25%)	45,67,67	2.46	16 (35%)
33	CYC	CE	1001	8,9	42,46,46	3.26	15 (35%)	50,67,67	2.70	18 (36%)
31	PEB	iC	202	2	43,46,46	3.54	11 (25%)	45,67,67	1.85	12 (26%)
31	PEB	l2	201	2,3	43,46,46	3.40	10 (23%)	45,67,67	2.27	15 (33%)
31	PEB	DI	203	2	43,46,46	3.48	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	P8	201	2	43,46,46	3.31	8 (18%)	45,67,67	3.21	18 (40%)
31	PEB	YJ	201	2	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
31	PEB	DF	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.02	15 (33%)
31	PEB	QA	202	2,4	43,46,46	3.40	10 (23%)	45,67,67	1.98	15 (33%)
31	PEB	L8	202	2	43,46,46	3.65	11 (25%)	45,67,67	2.71	15 (33%)
31	PEB	KA	301	2,4	43,46,46	3.28	10 (23%)	45,67,67	2.21	18 (40%)
31	PEB	c8	201	3	43,46,46	3.22	10 (23%)	45,67,67	2.30	15 (33%)
32	PUB	AE	302	6	42,46,46	3.41	9 (21%)	37,67,67	3.31	16 (43%)
31	PEB	N4	202	2	43,46,46	3.32	11 (25%)	45,67,67	2.52	15 (33%)
33	CYC	73	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	YE	201	2	43,46,46	3.09	10 (23%)	45,67,67	2.59	20 (44%)
31	PEB	RG	203	2,3	43,46,46	2.94	10 (23%)	45,67,67	2.96	15 (33%)
31	PEB	TK	202	2	43,46,46	2.76	9 (20%)	45,67,67	3.00	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	TI	201	3	43,46,46	3.37	11 (25%)	45,67,67	1.94	14 (31%)
31	PEB	B9	201	2,14,31	43,46,46	3.35	11 (25%)	45,67,67	2.10	15 (33%)
33	CYC	j3	1001	24,20	42,46,46	3.42	14 (33%)	50,67,67	3.16	21 (42%)
33	CYC	y3	1001	22	42,46,46	3.43	13 (30%)	50,67,67	3.01	23 (46%)
31	PEB	UA	302	2,4	43,46,46	3.46	11 (25%)	45,67,67	2.16	16 (35%)
31	PEB	ND	201	8,9	43,46,46	3.37	11 (25%)	45,67,67	2.23	15 (33%)
31	PEB	BI	201	2	43,46,46	3.51	11 (25%)	45,67,67	2.20	14 (31%)
32	PUB	N5	201	6,3	42,46,46	3.77	9 (21%)	37,67,67	3.13	12 (32%)
31	PEB	eF	201	2,3	43,46,46	3.42	13 (30%)	45,67,67	2.23	17 (37%)
31	PEB	O8	202	3	43,46,46	3.10	9 (20%)	45,67,67	2.20	15 (33%)
31	PEB	Y9	202	2	43,46,46	3.25	11 (25%)	45,67,67	2.24	15 (33%)
31	PEB	eD	203	2	43,46,46	3.58	12 (27%)	45,67,67	2.70	18 (40%)
31	PEB	HJ	202	3	43,46,46	3.42	12 (27%)	45,67,67	2.44	16 (35%)
31	PEB	R1	202	2	43,46,46	3.09	11 (25%)	45,67,67	2.93	15 (33%)
31	PEB	QA	204	2	43,46,46	3.25	10 (23%)	45,67,67	2.04	12 (26%)
31	PEB	OE	203	2,3	43,46,46	3.20	11 (25%)	45,67,67	2.24	16 (35%)
31	PEB	e6	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.25	16 (35%)
33	CYC	i3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	HC	1002	9	43,46,46	3.45	11 (25%)	45,67,67	2.30	14 (31%)
31	PEB	iF	203	3	43,46,46	3.46	12 (27%)	45,67,67	2.04	14 (31%)
33	CYC	BD	1001	9,7	42,46,46	3.34	14 (33%)	50,67,67	2.84	22 (44%)
31	PEB	LJ	201	2,3	43,46,46	3.35	11 (25%)	45,67,67	2.43	16 (35%)
31	PEB	hD	202	3	43,46,46	3.36	11 (25%)	45,67,67	2.00	14 (31%)
31	PEB	U2	202	3	43,46,46	3.30	12 (27%)	45,67,67	2.13	17 (37%)
33	CYC	NC	1001	9,7	42,46,46	3.37	16 (38%)	50,67,67	2.85	23 (46%)
33	CYC	JC	1001	9	42,46,46	3.21	15 (35%)	50,67,67	2.86	23 (46%)
31	PEB	RE	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.18	17 (37%)
31	PEB	A1	202	3	43,46,46	3.43	11 (25%)	45,67,67	1.98	12 (26%)
31	PEB	D9	202	2	43,46,46	3.27	12 (27%)	45,67,67	2.20	15 (33%)
31	PEB	XJ	203	3	43,46,46	3.41	10 (23%)	45,67,67	1.97	13 (28%)
31	PEB	BJ	201	3	43,46,46	3.22	10 (23%)	45,67,67	2.33	16 (35%)
31	PEB	hD	203	3	43,46,46	3.32	9 (20%)	45,67,67	2.01	13 (28%)
31	PEB	j2	201	3	43,46,46	3.17	10 (23%)	45,67,67	2.19	16 (35%)
31	PEB	eE	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.31	13 (28%)
31	PEB	UD	202	3	43,46,46	3.49	10 (23%)	45,67,67	2.05	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	bB	202	3	43,46,46	3.43	10 (23%)	45,67,67	2.00	13 (28%)
33	CYC	D2	1001	9	42,46,46	3.35	13 (30%)	50,67,67	2.86	18 (36%)
31	PEB	DJ	203	3	43,46,46	3.27	10 (23%)	45,67,67	2.24	15 (33%)
31	PEB	k2	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.08	16 (35%)
31	PEB	SC	201	3	43,46,46	3.31	12 (27%)	45,67,67	2.38	14 (31%)
31	PEB	C7	203	3	43,46,46	3.39	10 (23%)	45,67,67	1.95	14 (31%)
31	PEB	V5	203	2,3	43,46,46	3.26	13 (30%)	45,67,67	2.37	14 (31%)
33	CYC	DE	1001	9	42,46,46	3.17	14 (33%)	50,67,67	3.01	21 (42%)
31	PEB	UA	301	2,4	43,46,46	3.30	10 (23%)	45,67,67	2.28	16 (35%)
31	PEB	dB	201	3	43,46,46	3.28	10 (23%)	45,67,67	2.20	16 (35%)
31	PEB	mB	202	2	43,46,46	3.30	12 (27%)	45,67,67	2.37	16 (35%)
31	PEB	N6	1002	9	43,46,46	3.30	10 (23%)	45,67,67	2.14	16 (35%)
31	PEB	IF	202	3	43,46,46	1.07	2 (4%)	45,67,67	0.98	2 (4%)
31	PEB	S7	201	2,3	43,46,46	3.46	11 (25%)	45,67,67	2.54	15 (33%)
31	PEB	gH	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.75	15 (33%)
31	PEB	LI	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.03	12 (26%)
31	PEB	E7	203	2,3	43,46,46	3.46	11 (25%)	45,67,67	2.48	15 (33%)
31	PEB	a2	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.11	16 (35%)
31	PEB	JJ	202	3	43,46,46	3.45	10 (23%)	45,67,67	2.20	15 (33%)
31	PEB	H9	203	2	43,46,46	3.35	9 (20%)	45,67,67	1.91	14 (31%)
31	PEB	K4	201	3	43,46,46	3.35	11 (25%)	45,67,67	2.12	13 (28%)
31	PEB	DH	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.45	16 (35%)
31	PEB	J5	203	3	43,46,46	3.19	10 (23%)	45,67,67	2.06	13 (28%)
31	PEB	K1	201	3	43,46,46	3.26	11 (25%)	45,67,67	2.47	16 (35%)
31	PEB	D8	202	2	43,46,46	3.46	10 (23%)	45,67,67	2.03	14 (31%)
31	PEB	E4	203	3	43,46,46	3.29	10 (23%)	45,67,67	2.08	14 (31%)
31	PEB	W4	203	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.46	15 (33%)
31	PEB	I8	202	3	43,46,46	1.10	2 (4%)	45,67,67	1.00	2 (4%)
33	CYC	L3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	MK	202	3	43,46,46	3.33	10 (23%)	45,67,67	2.00	13 (28%)
33	CYC	F3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	F5	203	2,3	43,46,46	3.42	13 (30%)	45,67,67	3.08	13 (28%)
31	PEB	j8	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.84	18 (40%)
31	PEB	O4	203	2,3	43,46,46	3.33	11 (25%)	45,67,67	2.30	15 (33%)
31	PEB	AI	202	3	43,46,46	3.59	10 (23%)	45,67,67	2.66	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	JI	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.37	17 (37%)
31	PEB	Q9	201	2,14	43,46,46	3.25	11 (25%)	45,67,67	2.11	17 (37%)
31	PEB	Y4	202	3	43,46,46	3.35	10 (23%)	45,67,67	2.17	13 (28%)
31	PEB	H9	201	2,14	43,46,46	3.66	15 (34%)	45,67,67	2.48	15 (33%)
31	PEB	XF	201	2	43,46,46	3.37	10 (23%)	45,67,67	3.73	17 (37%)
31	PEB	E5	202	2,26	43,46,46	3.30	11 (25%)	45,67,67	2.18	16 (35%)
31	PEB	Y6	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.15	16 (35%)
32	PUB	yF	303	13	42,46,46	3.30	7 (16%)	37,67,67	3.12	13 (35%)
31	PEB	JF	201	2	43,46,46	3.40	11 (25%)	45,67,67	3.08	17 (37%)
31	PEB	SI	202	2	43,46,46	3.28	12 (27%)	45,67,67	2.21	15 (33%)
31	PEB	mE	203	2	43,46,46	3.46	11 (25%)	45,67,67	1.97	14 (31%)
33	CYC	Q3	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	II	202	3	43,46,46	3.58	11 (25%)	45,67,67	2.66	17 (37%)
31	PEB	FG	202	2	43,46,46	3.26	9 (20%)	45,67,67	2.19	15 (33%)
31	PEB	hE	203	3	43,46,46	3.32	10 (23%)	45,67,67	2.00	13 (28%)
31	PEB	f4	202	3	43,46,46	3.33	10 (23%)	45,67,67	2.30	15 (33%)
31	PEB	AB	304	6	43,46,46	3.36	10 (23%)	45,67,67	2.06	13 (28%)
31	PEB	GF	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.65	23 (51%)
31	PEB	Q5	201	2,6	43,46,46	3.48	10 (23%)	45,67,67	2.26	19 (42%)
33	CYC	U3	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	VC	201	2	43,46,46	3.37	12 (27%)	45,67,67	2.40	18 (40%)
31	PEB	WJ	202	2,6	43,46,46	3.44	10 (23%)	45,67,67	2.10	15 (33%)
31	PEB	UG	201	2	43,46,46	3.43	12 (27%)	45,67,67	2.18	15 (33%)
31	PEB	KH	202	3	43,46,46	3.15	10 (23%)	45,67,67	2.67	18 (40%)
31	PEB	b7	501	2	43,46,46	3.33	10 (23%)	45,67,67	2.23	15 (33%)
31	PEB	kE	201	2	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
31	PEB	L8	201	2	43,46,46	3.36	11 (25%)	45,67,67	3.49	19 (42%)
31	PEB	R6	202	2	43,46,46	3.23	11 (25%)	45,67,67	2.49	16 (35%)
31	PEB	T6	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.02	13 (28%)
31	PEB	rF	201	2,12	43,46,46	3.46	11 (25%)	45,67,67	2.23	13 (28%)
31	PEB	QD	201	2,3	43,46,46	3.16	11 (25%)	45,67,67	2.65	17 (37%)
31	PEB	hH	202	3	43,46,46	3.33	11 (25%)	45,67,67	2.08	15 (33%)
31	PEB	TG	203	3	43,46,46	3.22	9 (20%)	45,67,67	2.31	14 (31%)
31	PEB	hE	201	2,3	43,46,46	3.60	12 (27%)	45,67,67	2.56	10 (22%)
31	PEB	eF	203	3	43,46,46	3.38	10 (23%)	45,67,67	2.15	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	FF	201	2	43,46,46	3.51	10 (23%)	45,67,67	3.87	16 (35%)
33	CYC	C2	1001	8,9	42,46,46	3.27	13 (30%)	50,67,67	2.73	20 (40%)
31	PEB	UE	202	3	43,46,46	3.48	10 (23%)	45,67,67	2.05	15 (33%)
31	PEB	IF	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.10	15 (33%)
31	PEB	NJ	202	3	43,46,46	3.44	12 (27%)	45,67,67	1.85	12 (26%)
31	PEB	X9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	NH	201	2	43,46,46	3.17	10 (23%)	45,67,67	2.82	17 (37%)
33	CYC	p3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.93	18 (36%)
31	PEB	d8	201	2	43,46,46	3.48	10 (23%)	45,67,67	2.46	17 (37%)
31	PEB	Z4	201	2	43,46,46	3.37	11 (25%)	45,67,67	2.41	14 (31%)
31	PEB	T6	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.17	17 (37%)
31	PEB	P6	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.23	17 (37%)
31	PEB	RI	201	3	43,46,46	3.38	10 (23%)	45,67,67	1.95	14 (31%)
31	PEB	cC	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.31	16 (35%)
31	PEB	W7	202	3	43,46,46	3.26	10 (23%)	45,67,67	2.16	17 (37%)
31	PEB	UI	204	2,3	43,46,46	3.57	11 (25%)	45,67,67	2.64	16 (35%)
31	PEB	d2	203	3	43,46,46	3.40	10 (23%)	45,67,67	2.83	15 (33%)
31	PEB	EI	202	3	43,46,46	3.58	11 (25%)	45,67,67	2.66	17 (37%)
32	PUB	wF	304	12	42,46,46	3.43	7 (16%)	37,67,67	3.12	17 (45%)
31	PEB	yF	301	13	43,46,46	3.36	10 (23%)	45,67,67	2.10	15 (33%)
31	PEB	X4	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.28	14 (31%)
31	PEB	ZI	303	14	43,46,46	3.38	10 (23%)	45,67,67	2.38	17 (37%)
31	PEB	TH	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.22	16 (35%)
31	PEB	AB	301	6	43,46,46	3.39	11 (25%)	45,67,67	2.00	14 (31%)
31	PEB	Z9	301	14,31	43,46,46	3.24	11 (25%)	45,67,67	2.71	19 (42%)
31	PEB	RE	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.26	17 (37%)
31	PEB	Q4	201	2,3	43,46,46	3.30	9 (20%)	45,67,67	2.40	15 (33%)
31	PEB	DJ	201	2,3	43,46,46	3.18	11 (25%)	45,67,67	2.39	14 (31%)
31	PEB	DA	202	2	43,46,46	3.22	10 (23%)	45,67,67	2.12	13 (28%)
31	PEB	L1	202	2	43,46,46	3.18	10 (23%)	45,67,67	2.75	17 (37%)
31	PEB	S2	201	3	43,46,46	3.31	12 (27%)	45,67,67	2.37	14 (31%)
33	CYC	E3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.92	18 (36%)
31	PEB	U1	202	3	43,46,46	3.34	10 (23%)	45,67,67	1.94	13 (28%)
31	PEB	QD	203	3	43,46,46	3.38	10 (23%)	45,67,67	2.00	15 (33%)
31	PEB	K8	203	3	43,46,46	3.32	9 (20%)	45,67,67	2.05	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	Y9	203	2	43,46,46	3.21	9 (20%)	45,67,67	2.03	14 (31%)
31	PEB	e2	202	2	43,46,46	3.45	11 (25%)	45,67,67	1.96	14 (31%)
31	PEB	UA	304	2,4	43,46,46	3.57	13 (30%)	45,67,67	2.69	18 (40%)
31	PEB	fB	202	3	43,46,46	3.41	10 (23%)	45,67,67	1.97	14 (31%)
31	PEB	O2	202	3	43,46,46	3.31	10 (23%)	45,67,67	2.46	15 (33%)
31	PEB	gA	201	2	43,46,46	3.38	11 (25%)	45,67,67	2.17	14 (31%)
33	CYC	t3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	kB	202	2	43,46,46	3.34	11 (25%)	45,67,67	2.35	14 (31%)
31	PEB	JG	202	2	43,46,46	3.39	10 (23%)	45,67,67	1.82	13 (28%)
31	PEB	I4	202	3	43,46,46	3.27	11 (25%)	45,67,67	2.26	14 (31%)
33	CYC	I6	1001	8	42,46,46	3.19	13 (30%)	50,67,67	2.82	20 (40%)
31	PEB	GA	203	2	43,46,46	3.31	10 (23%)	45,67,67	2.17	16 (35%)
31	PEB	D1	202	2	43,46,46	3.23	11 (25%)	45,67,67	2.50	16 (35%)
31	PEB	SK	202	3	43,46,46	3.20	10 (23%)	45,67,67	1.96	12 (26%)
31	PEB	BK	201	2,31	43,46,46	3.32	11 (25%)	45,67,67	2.18	17 (37%)
31	PEB	RC	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.17	18 (40%)
31	PEB	EH	202	3	43,46,46	3.20	10 (23%)	45,67,67	2.13	12 (26%)
31	PEB	A4	301	12	43,46,46	3.28	11 (25%)	45,67,67	2.22	14 (31%)
31	PEB	OH	202	3	43,46,46	3.39	10 (23%)	45,67,67	2.87	16 (35%)
31	PEB	IF	201	3	43,46,46	2.70	11 (25%)	45,67,67	2.79	16 (35%)
31	PEB	fC	202	3	43,46,46	3.47	9 (20%)	45,67,67	2.59	15 (33%)
31	PEB	b8	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
31	PEB	R9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	SD	201	2,3	43,46,46	3.23	9 (20%)	45,67,67	2.46	14 (31%)
31	PEB	dD	201	2,3	43,46,46	3.39	10 (23%)	45,67,67	2.42	16 (35%)
31	PEB	SF	201	2,3	43,46,46	3.22	11 (25%)	45,67,67	2.59	15 (33%)
33	CYC	N6	1001	9	42,46,46	3.37	15 (35%)	50,67,67	2.85	21 (42%)
31	PEB	TF	201	2	43,46,46	3.28	8 (18%)	45,67,67	2.93	15 (33%)
31	PEB	P1	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.06	13 (28%)
31	PEB	TJ	203	3	43,46,46	3.38	8 (18%)	45,67,67	2.13	12 (26%)
33	CYC	GB	1001	8	42,46,46	3.32	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	AJ	302	6	43,46,46	3.31	9 (20%)	45,67,67	2.00	16 (35%)
33	CYC	g3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.92	19 (38%)
31	PEB	EG	201	3	43,46,46	3.33	9 (20%)	45,67,67	1.98	13 (28%)
31	PEB	E9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.22	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	Q8	203	2,3	43,46,46	3.43	13 (30%)	45,67,67	3.27	16 (35%)
31	PEB	BG	203	2	43,46,46	3.46	10 (23%)	45,67,67	2.36	15 (33%)
33	CYC	S3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	g4	202	2	43,46,46	3.43	9 (20%)	45,67,67	2.32	16 (35%)
31	PEB	aH	204	2,3	43,46,46	3.25	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	OE	201	3	43,46,46	3.39	10 (23%)	45,67,67	2.24	15 (33%)
31	PEB	eB	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.15	15 (33%)
33	CYC	NB	1001	9	42,46,46	3.36	15 (35%)	50,67,67	2.84	21 (42%)
31	PEB	XH	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.47	15 (33%)
31	PEB	XA	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.18	15 (33%)
31	PEB	c8	202	3	43,46,46	3.39	8 (18%)	45,67,67	2.01	13 (28%)
31	PEB	I8	201	3	43,46,46	2.70	11 (25%)	45,67,67	2.79	16 (35%)
33	CYC	d3	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	S9	201	2,14	43,46,46	3.48	11 (25%)	45,67,67	2.22	17 (37%)
31	PEB	O6	202	3	43,46,46	3.35	11 (25%)	45,67,67	1.85	11 (24%)
31	PEB	A2	302	6	43,46,46	3.39	11 (25%)	45,67,67	1.95	12 (26%)
31	PEB	JH	202	2	43,46,46	3.35	10 (23%)	45,67,67	2.35	18 (40%)
31	PEB	R1	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.16	16 (35%)
31	PEB	OB	201	3	43,46,46	3.36	10 (23%)	45,67,67	2.49	17 (37%)
31	PEB	X8	202	2	43,46,46	3.26	12 (27%)	45,67,67	2.64	16 (35%)
31	PEB	C5	201	2	43,46,46	3.46	10 (23%)	45,67,67	1.99	15 (33%)
31	PEB	G7	203	3	43,46,46	3.37	11 (25%)	45,67,67	1.98	13 (28%)
33	CYC	ID	1001	8,9	42,46,46	3.19	13 (30%)	50,67,67	2.84	18 (36%)
31	PEB	AI	201	3	43,46,46	3.38	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	iH	202	2,12	43,46,46	3.35	10 (23%)	45,67,67	2.29	15 (33%)
33	CYC	J2	1001	9	42,46,46	3.21	15 (35%)	50,67,67	2.86	22 (44%)
31	PEB	hD	201	2,3	43,46,46	3.60	13 (30%)	45,67,67	2.56	10 (22%)
31	PEB	M5	201	2	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
31	PEB	TK	203	2	43,46,46	3.29	10 (23%)	45,67,67	2.26	17 (37%)
31	PEB	kC	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.10	16 (35%)
31	PEB	FJ	201	3	43,46,46	3.25	11 (25%)	45,67,67	2.63	17 (37%)
31	PEB	T5	203	3	43,46,46	3.40	8 (18%)	45,67,67	2.13	12 (26%)
31	PEB	O1	202	3	43,46,46	3.27	10 (23%)	45,67,67	1.97	15 (33%)
33	CYC	FD	202	8,9	42,46,46	3.24	15 (35%)	50,67,67	2.71	17 (34%)
31	PEB	QE	203	3	43,46,46	3.40	9 (20%)	45,67,67	1.99	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CYC	FC	1001	9	42,46,46	3.32	14 (33%)	50,67,67	2.90	18 (36%)
31	PEB	iD	201	2	43,46,46	3.48	11 (25%)	45,67,67	1.97	14 (31%)
31	PEB	WB	201	3	43,46,46	3.26	11 (25%)	45,67,67	2.59	17 (37%)
31	PEB	N5	202	3	43,46,46	3.43	11 (25%)	45,67,67	1.82	12 (26%)
31	PEB	O9	203	2	43,46,46	3.15	10 (23%)	45,67,67	2.02	16 (35%)
31	PEB	RH	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.40	15 (33%)
31	PEB	J9	203	2	43,46,46	3.21	10 (23%)	45,67,67	2.02	15 (33%)
31	PEB	h2	202	3	43,46,46	3.38	12 (27%)	45,67,67	2.15	14 (31%)
31	PEB	b7	503	2,27	43,46,46	3.29	10 (23%)	45,67,67	2.06	14 (31%)
31	PEB	JC	1002	9	43,46,46	3.18	10 (23%)	45,67,67	2.15	14 (31%)
31	PEB	OC	202	3	43,46,46	3.31	10 (23%)	45,67,67	2.47	15 (33%)
31	PEB	WJ	201	2	43,46,46	3.48	13 (30%)	45,67,67	1.96	15 (33%)
33	CYC	EE	1001	8,9	42,46,46	3.21	15 (35%)	50,67,67	2.76	21 (42%)
31	PEB	M4	202	3	43,46,46	3.18	11 (25%)	45,67,67	2.16	13 (28%)
31	PEB	YK	302	31,6	43,46,46	3.35	10 (23%)	45,67,67	3.21	18 (40%)
31	PEB	Z9	303	14	43,46,46	3.17	11 (25%)	45,67,67	2.87	19 (42%)
31	PEB	o8	203	3	43,46,46	3.38	11 (25%)	45,67,67	2.29	13 (28%)
31	PEB	f2	202	3	43,46,46	3.47	9 (20%)	45,67,67	2.59	15 (33%)
31	PEB	N5	204	2,3	43,46,46	3.49	9 (20%)	45,67,67	2.23	15 (33%)
31	PEB	VD	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.18	15 (33%)
31	PEB	fE	201	3	43,46,46	3.34	10 (23%)	45,67,67	2.12	17 (37%)
31	PEB	A5	302	6	43,46,46	3.32	9 (20%)	45,67,67	1.99	16 (35%)
31	PEB	H5	203	3	43,46,46	3.45	10 (23%)	45,67,67	2.13	12 (26%)
32	PUB	Y1	304	6	42,46,46	3.53	8 (19%)	37,67,67	3.04	16 (43%)
31	PEB	O9	201	2,14,31	43,46,46	3.28	11 (25%)	45,67,67	2.06	17 (37%)
31	PEB	lF	201	2	43,46,46	3.42	11 (25%)	45,67,67	2.59	15 (33%)
31	PEB	SE	201	2,3	43,46,46	3.22	9 (20%)	45,67,67	2.46	14 (31%)
31	PEB	YB	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.15	16 (35%)
31	PEB	WI	202	2	43,46,46	3.58	11 (25%)	45,67,67	2.49	17 (37%)
31	PEB	YB	202	2	43,46,46	3.20	11 (25%)	45,67,67	2.33	15 (33%)
31	PEB	GH	203	2,3	43,46,46	3.16	10 (23%)	45,67,67	2.60	18 (40%)
32	PUB	MI	303	14	42,46,46	3.38	9 (21%)	37,67,67	4.03	18 (48%)
31	PEB	i6	201	2	43,46,46	3.41	10 (23%)	45,67,67	1.99	15 (33%)
31	PEB	YH	203	3	43,46,46	3.18	10 (23%)	45,67,67	2.25	17 (37%)
31	PEB	S4	202	3	43,46,46	3.42	12 (27%)	45,67,67	1.99	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	HF	201	2	43,46,46	3.13	13 (30%)	45,67,67	2.92	21 (46%)
31	PEB	HG	203	2,3	43,46,46	2.90	12 (27%)	45,67,67	2.88	16 (35%)
31	PEB	WE	201	3	43,46,46	3.34	10 (23%)	45,67,67	2.33	18 (40%)
31	PEB	X5	202	3	43,46,46	3.53	11 (25%)	45,67,67	1.94	14 (31%)
33	CYC	KD	202	-	42,46,46	1.09	1 (2%)	50,67,67	0.95	2 (4%)
31	PEB	V2	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.16	16 (35%)
31	PEB	Y9	201	2,14	43,46,46	3.20	10 (23%)	45,67,67	2.16	17 (37%)
31	PEB	z8	501	2,28	43,46,46	3.08	9 (20%)	45,67,67	2.07	15 (33%)
31	PEB	E5	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.08	14 (31%)
31	PEB	MA	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.18	16 (35%)
31	PEB	d5	401	2,26	43,46,46	3.30	10 (23%)	45,67,67	2.30	18 (40%)
31	PEB	YA	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.03	15 (33%)
31	PEB	kD	201	2	43,46,46	3.34	9 (20%)	45,67,67	2.15	16 (35%)
31	PEB	VJ	201	3	43,46,46	3.20	10 (23%)	45,67,67	2.30	12 (26%)
31	PEB	D4	202	2,13	43,46,46	3.45	10 (23%)	45,67,67	2.30	13 (28%)
31	PEB	LJ	203	3	43,46,46	3.37	9 (20%)	45,67,67	2.04	14 (31%)
31	PEB	SE	203	-	43,46,46	1.08	2 (4%)	45,67,67	1.01	2 (4%)
31	PEB	Q4	203	3	43,46,46	3.36	10 (23%)	45,67,67	2.15	14 (31%)
31	PEB	N8	201	2	43,46,46	3.33	10 (23%)	45,67,67	3.07	16 (35%)
31	PEB	n8	202	2	43,46,46	3.59	13 (30%)	45,67,67	1.94	13 (28%)
33	CYC	E2	1001	8,9	42,46,46	3.05	14 (33%)	50,67,67	3.18	20 (40%)
31	PEB	SG	201	2	43,46,46	3.23	11 (25%)	45,67,67	2.25	14 (31%)
31	PEB	eD	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.31	13 (28%)
31	PEB	IH	201	2,3	43,46,46	3.21	11 (25%)	45,67,67	2.53	16 (35%)
31	PEB	OC	201	3	43,46,46	3.33	13 (30%)	45,67,67	2.34	16 (35%)
31	PEB	ZA	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.10	13 (28%)
31	PEB	MH	202	3	43,46,46	3.07	9 (20%)	45,67,67	2.32	16 (35%)
31	PEB	LJ	202	3	43,46,46	3.37	11 (25%)	45,67,67	2.25	14 (31%)
31	PEB	IC	201	3	43,46,46	3.44	12 (27%)	45,67,67	2.04	13 (28%)
31	PEB	q8	203	3	43,46,46	3.51	12 (27%)	45,67,67	2.31	16 (35%)
31	PEB	X1	201	2,15	43,46,46	3.63	11 (25%)	45,67,67	2.34	19 (42%)
31	PEB	H1	202	2	43,46,46	3.37	11 (25%)	45,67,67	2.58	17 (37%)
31	PEB	BG	201	2	43,46,46	3.43	12 (27%)	45,67,67	2.44	19 (42%)
31	PEB	OF	203	3	43,46,46	3.26	8 (18%)	45,67,67	2.01	16 (35%)
33	CYC	c3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.92	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	RK	202	2	43,46,46	3.09	10 (23%)	45,67,67	2.94	15 (33%)
31	PEB	VD	201	2	43,46,46	3.38	11 (25%)	45,67,67	2.04	16 (35%)
32	PUB	AD	302	6	42,46,46	3.40	9 (21%)	37,67,67	3.31	16 (43%)
31	PEB	a4	203	3	43,46,46	3.32	11 (25%)	45,67,67	2.36	15 (33%)
31	PEB	F2	1002	9	43,46,46	3.30	10 (23%)	45,67,67	2.15	12 (26%)
33	CYC	IB	1001	8	42,46,46	3.19	13 (30%)	50,67,67	2.82	20 (40%)
31	PEB	H7	201	2,27	43,46,46	3.49	11 (25%)	45,67,67	2.03	15 (33%)
31	PEB	E1	202	3	43,46,46	3.41	12 (27%)	45,67,67	1.99	13 (28%)
31	PEB	L1	203	2	43,46,46	3.46	10 (23%)	45,67,67	1.81	13 (28%)
32	PUB	K1	203	6,3	42,46,46	3.36	7 (16%)	37,67,67	3.59	17 (45%)
31	PEB	OJ	202	2	43,46,46	3.49	13 (30%)	45,67,67	1.97	15 (33%)
31	PEB	B7	201	2	43,46,46	3.45	12 (27%)	45,67,67	2.17	18 (40%)
31	PEB	UG	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.12	15 (33%)
31	PEB	IF	203	2,3	43,46,46	3.08	11 (25%)	45,67,67	2.73	17 (37%)
32	PUB	M9	304	14,3	42,46,46	3.65	9 (21%)	37,67,67	3.54	16 (43%)
31	PEB	V8	202	2	43,46,46	3.44	11 (25%)	45,67,67	2.65	18 (40%)
31	PEB	W5	202	2,6	43,46,46	3.42	11 (25%)	45,67,67	2.09	15 (33%)
31	PEB	cH	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.24	14 (31%)
31	PEB	hH	201	2,3	43,46,46	3.33	12 (27%)	45,67,67	2.44	16 (35%)
31	PEB	M9	303	14	43,46,46	3.18	11 (25%)	45,67,67	2.87	19 (42%)
32	PUB	AB	303	6	42,46,46	3.41	7 (16%)	37,67,67	3.02	14 (37%)
31	PEB	a8	203	3	43,46,46	3.34	9 (20%)	45,67,67	2.33	16 (35%)
31	PEB	X8	201	2	43,46,46	3.39	10 (23%)	45,67,67	3.73	17 (37%)
31	PEB	wF	302	12	43,46,46	3.33	9 (20%)	45,67,67	2.23	15 (33%)
31	PEB	ZB	202	3	43,46,46	3.30	10 (23%)	45,67,67	1.93	12 (26%)
31	PEB	V9	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	g8	201	3	43,46,46	3.12	11 (25%)	45,67,67	2.38	15 (33%)
31	PEB	CI	202	3	43,46,46	3.58	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	T1	203	2	43,46,46	3.30	10 (23%)	45,67,67	2.26	17 (37%)
31	PEB	gD	202	2	43,46,46	3.37	9 (20%)	45,67,67	2.49	13 (28%)
31	PEB	DF	201	2	43,46,46	3.26	8 (18%)	45,67,67	3.08	18 (40%)
31	PEB	H1	203	2	43,46,46	3.55	12 (27%)	45,67,67	2.47	16 (35%)
31	PEB	RA	201	2,5	43,46,46	3.47	10 (23%)	45,67,67	2.11	14 (31%)
31	PEB	v8	202	2	43,46,46	3.50	11 (25%)	45,67,67	1.97	16 (35%)
31	PEB	PJ	202	3	43,46,46	3.48	11 (25%)	45,67,67	2.21	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	RG	202	3	43,46,46	3.21	10 (23%)	45,67,67	2.31	14 (31%)
33	CYC	H2	1001	9	42,46,46	3.30	13 (30%)	50,67,67	2.89	22 (44%)
31	PEB	kB	201	2	43,46,46	3.42	12 (27%)	45,67,67	1.97	12 (26%)
31	PEB	JG	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.16	17 (37%)
31	PEB	b7	502	2	43,46,46	3.29	10 (23%)	45,67,67	2.04	16 (35%)
31	PEB	hB	201	3	43,46,46	3.40	11 (25%)	45,67,67	2.34	19 (42%)
31	PEB	SI	201	2,14	43,46,46	3.31	11 (25%)	45,67,67	2.43	14 (31%)
31	PEB	OI	202	2	43,46,46	3.08	10 (23%)	45,67,67	2.56	19 (42%)
33	CYC	GD	201	8,9	42,46,46	3.19	14 (33%)	50,67,67	2.88	18 (36%)
32	PUB	AH	304	12	42,46,46	3.42	7 (16%)	37,67,67	3.51	18 (48%)
31	PEB	U5	201	2,6	43,46,46	3.51	12 (27%)	45,67,67	2.13	17 (37%)
31	PEB	FG	201	2	43,46,46	3.30	13 (30%)	45,67,67	2.23	16 (35%)
31	PEB	W8	202	3	43,46,46	3.31	11 (25%)	45,67,67	2.28	18 (40%)
31	PEB	fH	203	2,3	43,46,46	3.35	12 (27%)	45,67,67	2.38	14 (31%)
31	PEB	C7	202	3	43,46,46	3.34	11 (25%)	45,67,67	2.12	14 (31%)
31	PEB	KH	201	3	43,46,46	3.21	10 (23%)	45,67,67	2.26	16 (35%)
31	PEB	O5	202	2	43,46,46	3.47	13 (30%)	45,67,67	1.98	15 (33%)
31	PEB	P5	203	3	43,46,46	3.39	9 (20%)	45,67,67	2.12	12 (26%)
31	PEB	GF	201	2,3	43,46,46	3.17	12 (27%)	45,67,67	3.04	20 (44%)
31	PEB	G7	201	2,3	43,46,46	3.45	11 (25%)	45,67,67	2.60	16 (35%)
31	PEB	BK	202	2	43,46,46	3.48	11 (25%)	45,67,67	3.05	18 (40%)
31	PEB	fE	203	2,3	43,46,46	3.39	11 (25%)	45,67,67	2.19	13 (28%)
31	PEB	CA	202	2,1	43,46,46	3.26	10 (23%)	45,67,67	2.16	16 (35%)
31	PEB	k8	203	2,3	43,46,46	3.46	12 (27%)	45,67,67	2.31	11 (24%)
31	PEB	JJ	203	3	43,46,46	3.22	9 (20%)	45,67,67	2.08	13 (28%)
31	PEB	lF	203	2,3	43,46,46	3.40	14 (32%)	45,67,67	2.53	16 (35%)
31	PEB	O7	202	3	43,46,46	3.35	10 (23%)	45,67,67	2.10	14 (31%)
31	PEB	R2	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.16	18 (40%)
31	PEB	VE	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.06	16 (35%)
31	PEB	fH	201	3	43,46,46	3.28	9 (20%)	45,67,67	2.10	14 (31%)
31	PEB	UI	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.27	15 (33%)
31	PEB	iE	201	2	43,46,46	3.45	11 (25%)	45,67,67	1.97	14 (31%)
31	PEB	R1	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.24	19 (42%)
31	PEB	VI	202	3	43,46,46	3.57	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	S5	202	2	43,46,46	3.36	10 (23%)	45,67,67	1.98	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	MF	203	2,3	43,46,46	3.33	13 (30%)	45,67,67	2.57	16 (35%)
31	PEB	L5	201	2,3	43,46,46	3.33	11 (25%)	45,67,67	2.42	16 (35%)
31	PEB	BH	301	13	43,46,46	3.28	10 (23%)	45,67,67	2.22	16 (35%)
31	PEB	IK	202	3	43,46,46	3.42	11 (25%)	45,67,67	1.87	12 (26%)
31	PEB	m8	201	3	43,46,46	3.40	10 (23%)	45,67,67	2.11	15 (33%)
31	PEB	lE	202	3	43,46,46	3.34	11 (25%)	45,67,67	2.01	14 (31%)
33	CYC	J6	1001	9	42,46,46	3.11	16 (38%)	50,67,67	2.96	21 (42%)
31	PEB	J5	201	2,3	43,46,46	3.20	11 (25%)	45,67,67	2.24	12 (26%)
31	PEB	A5	304	6,31	43,46,46	3.44	11 (25%)	45,67,67	2.27	16 (35%)
31	PEB	MF	202	3	43,46,46	3.45	12 (27%)	45,67,67	1.96	15 (33%)
31	PEB	I7	203	2,3	43,46,46	3.37	11 (25%)	45,67,67	2.62	15 (33%)
31	PEB	E4	201	2,3	43,46,46	3.30	12 (27%)	45,67,67	2.42	16 (35%)
31	PEB	j8	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.17	13 (28%)
31	PEB	U6	201	3	43,46,46	3.20	10 (23%)	45,67,67	2.80	19 (42%)
31	PEB	eE	201	2	43,46,46	3.40	11 (25%)	45,67,67	1.96	14 (31%)
31	PEB	FI	203	2	43,46,46	3.24	9 (20%)	45,67,67	2.21	17 (37%)
31	PEB	AJ	304	6,31	43,46,46	3.45	11 (25%)	45,67,67	2.27	17 (37%)
31	PEB	a4	201	3,12	43,46,46	3.33	11 (25%)	45,67,67	2.20	15 (33%)
32	PUB	w8	304	12	42,46,46	3.40	8 (19%)	37,67,67	3.12	17 (45%)
31	PEB	g6	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	VG	201	3	43,46,46	3.34	9 (20%)	45,67,67	1.97	13 (28%)
32	PUB	AE	303	6	42,46,46	3.45	7 (16%)	37,67,67	3.00	14 (37%)
31	PEB	VJ	203	2,3	43,46,46	3.26	13 (30%)	45,67,67	2.37	13 (28%)
31	PEB	XI	202	3	43,46,46	3.59	11 (25%)	45,67,67	2.66	17 (37%)
31	PEB	c6	202	2	43,46,46	3.46	12 (27%)	45,67,67	2.38	14 (31%)
32	PUB	xF	306	12	42,46,46	3.60	7 (16%)	37,67,67	2.90	15 (40%)
31	PEB	jB	202	3	43,46,46	3.32	11 (25%)	45,67,67	1.95	12 (26%)
31	PEB	B8	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.35	14 (31%)
31	PEB	f4	203	2,3	43,46,46	3.31	11 (25%)	45,67,67	2.48	16 (35%)
31	PEB	C4	201	3	43,46,46	3.24	10 (23%)	45,67,67	2.10	13 (28%)
31	PEB	gF	201	3	43,46,46	3.12	11 (25%)	45,67,67	2.39	15 (33%)
31	PEB	P6	203	2	43,46,46	3.33	9 (20%)	45,67,67	1.85	13 (28%)
31	PEB	oF	201	3	43,46,46	3.35	11 (25%)	45,67,67	2.25	15 (33%)
31	PEB	iD	202	2	43,46,46	3.49	10 (23%)	45,67,67	2.02	15 (33%)
33	CYC	W3	1001	22	42,46,46	3.44	13 (30%)	50,67,67	3.01	23 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	tF	202	2	43,46,46	3.64	12 (27%)	45,67,67	2.63	15 (33%)
31	PEB	OJ	201	2,6,31	43,46,46	3.40	10 (23%)	45,67,67	1.99	15 (33%)
33	CYC	w3	1001	24,20	42,46,46	3.43	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	F7	202	2	43,46,46	3.27	10 (23%)	45,67,67	2.18	16 (35%)
31	PEB	O4	202	3	43,46,46	3.36	12 (27%)	45,67,67	2.46	16 (35%)
31	PEB	a8	201	2,3	43,46,46	3.42	12 (27%)	45,67,67	2.42	15 (33%)
31	PEB	W9	202	2	43,46,46	3.48	12 (27%)	45,67,67	2.33	17 (37%)
31	PEB	K8	202	3	43,46,46	3.36	11 (25%)	45,67,67	2.36	16 (35%)
31	PEB	M9	302	14	43,46,46	3.14	10 (23%)	45,67,67	2.42	14 (31%)
31	PEB	vF	202	2	43,46,46	3.49	10 (23%)	45,67,67	1.96	16 (35%)
31	PEB	mE	201	2	43,46,46	3.49	13 (30%)	45,67,67	1.94	13 (28%)
33	CYC	JC	1003	8,9	42,46,46	3.21	12 (28%)	50,67,67	2.65	19 (38%)
31	PEB	S1	201	3	43,46,46	3.18	10 (23%)	45,67,67	2.76	16 (35%)
31	PEB	EK	201	3	43,46,46	3.57	12 (27%)	45,67,67	2.32	14 (31%)
31	PEB	dE	203	3	43,46,46	3.48	12 (27%)	45,67,67	2.08	15 (33%)
31	PEB	RJ	203	2,3	43,46,46	3.37	12 (27%)	45,67,67	2.32	16 (35%)
32	PUB	xF	305	12	42,46,46	3.38	7 (16%)	37,67,67	3.26	15 (40%)
31	PEB	VI	201	3	43,46,46	3.38	10 (23%)	45,67,67	1.95	14 (31%)
31	PEB	C9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	G9	202	3	43,46,46	3.36	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	R8	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.31	15 (33%)
31	PEB	J7	201	2	43,46,46	3.49	12 (27%)	45,67,67	2.07	16 (35%)
31	PEB	cA	403	5,2	43,46,46	3.30	10 (23%)	45,67,67	2.21	18 (40%)
31	PEB	cB	203	2	43,46,46	3.46	12 (27%)	45,67,67	1.99	11 (24%)
31	PEB	S4	201	3	43,46,46	3.38	11 (25%)	45,67,67	2.00	13 (28%)
31	PEB	L9	203	2	43,46,46	3.16	10 (23%)	45,67,67	2.18	17 (37%)
31	PEB	KI	202	3	43,46,46	3.59	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	F1	203	2	43,46,46	3.60	12 (27%)	45,67,67	1.98	16 (35%)
31	PEB	CA	201	2	43,46,46	3.38	11 (25%)	45,67,67	2.49	15 (33%)
31	PEB	mD	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.56	14 (31%)
31	PEB	C8	202	3	43,46,46	3.08	8 (18%)	45,67,67	2.07	15 (33%)
31	PEB	G8	201	2,3	43,46,46	3.17	12 (27%)	45,67,67	3.03	21 (46%)
31	PEB	UE	203	3	43,46,46	3.41	10 (23%)	45,67,67	2.04	15 (33%)
31	PEB	h6	201	3	43,46,46	3.42	11 (25%)	45,67,67	2.36	18 (40%)
31	PEB	LE	1002	8,9	43,46,46	3.32	10 (23%)	45,67,67	1.90	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	B4	301	13	43,46,46	3.36	10 (23%)	45,67,67	2.19	16 (35%)
31	PEB	j4	202	3	43,46,46	3.29	10 (23%)	45,67,67	2.84	13 (28%)
31	PEB	UF	201	3	43,46,46	2.77	10 (23%)	45,67,67	3.00	17 (37%)
31	PEB	RD	202	2	43,46,46	3.40	10 (23%)	45,67,67	2.17	17 (37%)
31	PEB	d4	203	3	43,46,46	3.41	10 (23%)	45,67,67	2.37	12 (26%)
31	PEB	YI	202	2	43,46,46	3.44	12 (27%)	45,67,67	2.28	14 (31%)
31	PEB	IH	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.31	14 (31%)
31	PEB	I8	203	2,3	43,46,46	3.06	11 (25%)	45,67,67	2.74	18 (40%)
31	PEB	LD	1002	8,9	43,46,46	3.32	10 (23%)	45,67,67	1.89	13 (28%)
32	PUB	x8	305	12	42,46,46	3.41	7 (16%)	37,67,67	3.26	15 (40%)
31	PEB	dE	204	3	43,46,46	3.43	13 (30%)	45,67,67	2.12	13 (28%)
31	PEB	l6	201	3	43,46,46	3.34	10 (23%)	45,67,67	2.26	17 (37%)
31	PEB	W1	202	3	43,46,46	3.41	12 (27%)	45,67,67	2.04	13 (28%)
33	CYC	KB	1001	8	42,46,46	3.26	14 (33%)	50,67,67	2.89	19 (38%)
31	PEB	A1	201	3	43,46,46	3.45	12 (27%)	45,67,67	2.30	17 (37%)
31	PEB	JH	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.38	14 (31%)
31	PEB	d4	202	3	43,46,46	3.38	11 (25%)	45,67,67	2.00	13 (28%)
33	CYC	J3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.94	19 (38%)
31	PEB	j2	202	3	43,46,46	3.42	13 (30%)	45,67,67	2.63	16 (35%)
31	PEB	jC	203	2,3	43,46,46	3.48	14 (32%)	45,67,67	2.50	15 (33%)
31	PEB	WD	203	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.28	17 (37%)
31	PEB	Y8	201	3	43,46,46	3.28	9 (20%)	45,67,67	2.04	15 (33%)
31	PEB	IA	202	2	43,46,46	3.23	11 (25%)	45,67,67	2.28	15 (33%)
31	PEB	B9	202	2	43,46,46	3.45	12 (27%)	45,67,67	2.29	13 (28%)
33	CYC	KE	202	8,9	42,46,46	3.19	14 (33%)	50,67,67	2.74	19 (38%)
31	PEB	OB	202	3	43,46,46	3.37	11 (25%)	45,67,67	1.85	11 (24%)
31	PEB	NJ	204	2,3	43,46,46	3.50	11 (25%)	45,67,67	2.23	16 (35%)
31	PEB	mF	202	3	43,46,46	3.43	10 (23%)	45,67,67	2.19	14 (31%)
31	PEB	W2	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	T2	201	2,10	43,46,46	3.38	12 (27%)	45,67,67	2.21	20 (44%)
32	PUB	xF	301	12	42,46,46	3.24	8 (19%)	37,67,67	3.35	19 (51%)
31	PEB	JB	1002	9	43,46,46	3.30	11 (25%)	45,67,67	2.11	14 (31%)
31	PEB	ZA	201	2	43,46,46	3.38	10 (23%)	45,67,67	1.96	14 (31%)
31	PEB	MH	201	2,3	43,46,46	3.11	10 (23%)	45,67,67	2.60	18 (40%)
31	PEB	aB	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.00	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	HJ	203	3	43,46,46	3.44	10 (23%)	45,67,67	2.13	12 (26%)
31	PEB	j6	202	3	43,46,46	3.37	11 (25%)	45,67,67	1.95	12 (26%)
31	PEB	FC	1002	9	43,46,46	3.31	10 (23%)	45,67,67	2.15	12 (26%)
31	PEB	C8	203	3	43,46,46	3.46	12 (27%)	45,67,67	1.99	16 (35%)
31	PEB	S7	202	3	43,46,46	3.40	11 (25%)	45,67,67	2.16	16 (35%)
31	PEB	kB	203	2	43,46,46	1.08	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	F7	201	2,27	43,46,46	3.49	12 (27%)	45,67,67	2.11	16 (35%)
31	PEB	jC	201	3	43,46,46	3.18	10 (23%)	45,67,67	2.18	16 (35%)
31	PEB	f2	203	2,3	43,46,46	3.48	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	D1	203	2	43,46,46	3.38	10 (23%)	45,67,67	1.98	16 (35%)
31	PEB	A2	305	6	43,46,46	3.44	11 (25%)	45,67,67	2.42	15 (33%)
31	PEB	JE	201	8	43,46,46	3.24	10 (23%)	45,67,67	2.32	17 (37%)
31	PEB	G1	201	3	43,46,46	3.11	8 (18%)	45,67,67	2.22	13 (28%)
31	PEB	V6	202	2	43,46,46	3.13	10 (23%)	45,67,67	2.43	18 (40%)
31	PEB	S6	201	3	43,46,46	3.43	11 (25%)	45,67,67	2.67	18 (40%)
31	PEB	UJ	201	2,6	43,46,46	3.49	12 (27%)	45,67,67	2.13	17 (37%)
31	PEB	WC	202	3	43,46,46	3.37	10 (23%)	45,67,67	2.53	16 (35%)
31	PEB	RJ	202	3	43,46,46	3.36	11 (25%)	45,67,67	1.98	13 (28%)
31	PEB	O7	201	2,3	43,46,46	3.41	11 (25%)	45,67,67	2.48	15 (33%)
31	PEB	k6	202	2	43,46,46	3.34	12 (27%)	45,67,67	2.36	14 (31%)
31	PEB	MI	304	14	43,46,46	3.38	10 (23%)	45,67,67	2.38	17 (37%)
31	PEB	BA	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.16	14 (31%)
33	CYC	M6	1001	8	42,46,46	3.17	12 (28%)	50,67,67	2.89	17 (34%)
31	PEB	TC	202	2	43,46,46	3.32	9 (20%)	45,67,67	1.82	13 (28%)
32	PUB	A4	303	12	42,46,46	3.36	8 (19%)	37,67,67	3.53	16 (43%)
33	CYC	GE	201	8,9	42,46,46	3.17	13 (30%)	50,67,67	2.89	19 (38%)
31	PEB	KE	201	8,9	43,46,46	3.30	11 (25%)	45,67,67	2.09	15 (33%)
31	PEB	fA	301	2,29	43,46,46	3.49	12 (27%)	45,67,67	2.00	15 (33%)
31	PEB	hH	203	3	43,46,46	3.48	11 (25%)	45,67,67	2.24	15 (33%)
31	PEB	UI	201	2,14	43,46,46	3.46	10 (23%)	45,67,67	2.09	13 (28%)
31	PEB	B1	202	2	43,46,46	3.47	11 (25%)	45,67,67	3.07	17 (37%)
31	PEB	Y4	201	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.55	17 (37%)
33	CYC	BE	1001	9,7	42,46,46	3.35	14 (33%)	50,67,67	2.81	22 (44%)
31	PEB	pF	202	2	43,46,46	3.59	11 (25%)	45,67,67	2.72	18 (40%)
31	PEB	D5	203	3	43,46,46	3.28	10 (23%)	45,67,67	2.27	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	F9	203	2	43,46,46	3.25	10 (23%)	45,67,67	2.10	17 (37%)
31	PEB	X8	203	2	43,46,46	3.47	11 (25%)	45,67,67	2.26	17 (37%)
31	PEB	UK	201	3	43,46,46	3.23	10 (23%)	45,67,67	2.61	13 (28%)
31	PEB	m2	202	2	43,46,46	3.70	11 (25%)	45,67,67	1.85	11 (24%)
31	PEB	bC	202	3	43,46,46	3.54	11 (25%)	45,67,67	2.60	17 (37%)
31	PEB	C4	202	3	43,46,46	3.32	11 (25%)	45,67,67	2.24	16 (35%)
31	PEB	fC	203	2,3	43,46,46	3.44	11 (25%)	45,67,67	2.19	15 (33%)
31	PEB	NK	203	2	43,46,46	3.34	10 (23%)	45,67,67	2.36	17 (37%)
31	PEB	NG	202	3	43,46,46	3.22	9 (20%)	45,67,67	2.32	14 (31%)
31	PEB	UD	201	2,3	43,46,46	3.28	10 (23%)	45,67,67	2.38	16 (35%)
31	PEB	BI	203	2	43,46,46	3.39	9 (20%)	45,67,67	2.03	12 (26%)
32	PUB	B4	302	13	42,46,46	3.36	7 (16%)	37,67,67	3.28	15 (40%)
31	PEB	M7	203	2,3	43,46,46	3.35	11 (25%)	45,67,67	2.69	15 (33%)
31	PEB	CH	202	3	43,46,46	3.25	10 (23%)	45,67,67	2.11	14 (31%)
31	PEB	gA	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.19	14 (31%)
31	PEB	f4	201	3	43,46,46	3.37	10 (23%)	45,67,67	2.05	12 (26%)
31	PEB	DK	202	2	43,46,46	3.22	11 (25%)	45,67,67	2.50	16 (35%)
31	PEB	Q5	202	2	43,46,46	3.47	12 (27%)	45,67,67	1.83	13 (28%)
31	PEB	SH	203	2,3	43,46,46	3.29	10 (23%)	45,67,67	2.47	16 (35%)
31	PEB	Q8	202	3	43,46,46	3.39	10 (23%)	45,67,67	1.94	13 (28%)
31	PEB	hF	202	2	43,46,46	3.45	10 (23%)	45,67,67	1.98	15 (33%)
31	PEB	Q7	202	3	43,46,46	3.29	12 (27%)	45,67,67	1.96	14 (31%)
31	PEB	D8	203	2,3	43,46,46	3.13	10 (23%)	45,67,67	2.68	16 (35%)
31	PEB	WE	203	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.29	17 (37%)
32	PUB	A6	303	6	42,46,46	3.41	7 (16%)	37,67,67	3.01	14 (37%)
31	PEB	CH	203	2,3	43,46,46	3.14	10 (23%)	45,67,67	2.57	18 (40%)
31	PEB	N5	203	3	43,46,46	3.36	8 (18%)	45,67,67	2.03	13 (28%)
31	PEB	RA	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.10	16 (35%)
31	PEB	AH	302	12	43,46,46	3.24	9 (20%)	45,67,67	2.18	13 (28%)
31	PEB	hA	301	2,29	43,46,46	3.49	11 (25%)	45,67,67	2.01	15 (33%)
31	PEB	UI	203	2	43,46,46	3.44	10 (23%)	45,67,67	2.17	16 (35%)
31	PEB	Q7	203	2,3	43,46,46	3.47	12 (27%)	45,67,67	2.54	17 (37%)
31	PEB	QI	202	2	43,46,46	3.51	12 (27%)	45,67,67	2.31	17 (37%)
31	PEB	fC	201	3	43,46,46	3.48	13 (30%)	45,67,67	2.00	14 (31%)
31	PEB	g6	203	2	43,46,46	3.45	11 (25%)	45,67,67	2.18	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	OC	203	2,3	43,46,46	3.24	10 (23%)	45,67,67	2.42	14 (31%)
31	PEB	LI	202	2	43,46,46	3.49	11 (25%)	45,67,67	2.34	14 (31%)
31	PEB	kD	202	2,6	43,46,46	3.45	12 (27%)	45,67,67	2.24	17 (37%)
31	PEB	T8	201	2	43,46,46	3.26	8 (18%)	45,67,67	2.94	15 (33%)
31	PEB	cB	201	2	43,46,46	3.39	10 (23%)	45,67,67	1.99	14 (31%)
32	PUB	y8	302	13	42,46,46	3.36	7 (16%)	37,67,67	3.16	19 (51%)
31	PEB	JJ	201	2,3	43,46,46	3.21	13 (30%)	45,67,67	2.23	13 (28%)
31	PEB	NK	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.31	18 (40%)
31	PEB	WF	202	3	43,46,46	3.30	11 (25%)	45,67,67	2.29	18 (40%)
31	PEB	Y6	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.33	15 (33%)
31	PEB	NI	202	3	43,46,46	3.58	10 (23%)	45,67,67	2.65	17 (37%)
33	CYC	f3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	G9	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	d6	202	3	43,46,46	3.34	11 (25%)	45,67,67	1.88	12 (26%)
31	PEB	D8	201	2	43,46,46	3.25	8 (18%)	45,67,67	3.07	17 (37%)
31	PEB	m6	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
31	PEB	SI	203	2	43,46,46	3.32	10 (23%)	45,67,67	2.25	16 (35%)
31	PEB	TB	203	2	43,46,46	3.42	10 (23%)	45,67,67	2.02	13 (28%)
33	CYC	N3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.92	19 (38%)
33	CYC	BD	1002	9,7	42,46,46	3.23	14 (33%)	50,67,67	2.91	23 (46%)
31	PEB	IH	201	2,3	43,46,46	3.20	10 (23%)	45,67,67	2.43	15 (33%)
31	PEB	a6	203	2	43,46,46	3.47	13 (30%)	45,67,67	2.00	14 (31%)
33	CYC	D2	1003	8,9	42,46,46	3.15	12 (28%)	50,67,67	2.94	20 (40%)
31	PEB	cC	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.07	15 (33%)
31	PEB	AG	202	3	43,46,46	3.22	11 (25%)	45,67,67	2.31	14 (31%)
31	PEB	J9	202	2	43,46,46	3.26	11 (25%)	45,67,67	2.20	14 (31%)
31	PEB	b2	202	3	43,46,46	3.52	10 (23%)	45,67,67	2.61	17 (37%)
31	PEB	MJ	202	2	43,46,46	3.31	9 (20%)	45,67,67	1.99	13 (28%)
31	PEB	DJ	202	3	43,46,46	3.16	12 (27%)	45,67,67	2.76	20 (44%)
31	PEB	jH	203	2,3	43,46,46	3.27	12 (27%)	45,67,67	2.52	18 (40%)
31	PEB	dF	201	2	43,46,46	3.45	10 (23%)	45,67,67	2.45	16 (35%)
31	PEB	H5	201	2,3	43,46,46	3.19	11 (25%)	45,67,67	2.43	16 (35%)
31	PEB	rF	202	2	43,46,46	3.44	12 (27%)	45,67,67	2.05	13 (28%)
31	PEB	m2	201	2	43,46,46	3.49	11 (25%)	45,67,67	1.91	15 (33%)
33	CYC	EB	1001	8	42,46,46	3.17	15 (35%)	50,67,67	2.96	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	YG	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.13	15 (33%)
31	PEB	ZB	201	3	43,46,46	3.35	12 (27%)	45,67,67	2.78	18 (40%)
31	PEB	cH	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.73	15 (33%)
31	PEB	XJ	201	2,3	43,46,46	3.34	11 (25%)	45,67,67	2.47	15 (33%)
31	PEB	D5	202	3	43,46,46	3.16	12 (27%)	45,67,67	2.76	19 (42%)
31	PEB	OG	202	2,3	43,46,46	2.87	11 (25%)	45,67,67	2.88	16 (35%)
33	CYC	LB	1001	9	42,46,46	3.14	16 (38%)	50,67,67	2.96	22 (44%)
31	PEB	YF	201	3	43,46,46	3.25	9 (20%)	45,67,67	2.03	15 (33%)
31	PEB	U8	201	3	43,46,46	2.78	10 (23%)	45,67,67	2.99	17 (37%)
31	PEB	iF	201	2,3	43,46,46	3.41	10 (23%)	45,67,67	2.39	14 (31%)
31	PEB	iF	202	3	43,46,46	3.27	10 (23%)	45,67,67	2.31	18 (40%)
31	PEB	OK	202	3	43,46,46	3.25	10 (23%)	45,67,67	1.98	15 (33%)
31	PEB	dC	202	3	43,46,46	3.41	12 (27%)	45,67,67	2.11	15 (33%)
33	CYC	HB	1001	9	42,46,46	3.23	15 (35%)	50,67,67	3.08	23 (46%)
31	PEB	Y6	203	2	43,46,46	3.40	11 (25%)	45,67,67	2.05	13 (28%)
31	PEB	t8	201	2	43,46,46	3.53	10 (23%)	45,67,67	2.85	16 (35%)
31	PEB	OG	203	2	43,46,46	3.38	9 (20%)	45,67,67	2.00	14 (31%)
31	PEB	PD	202	2,10	43,46,46	3.37	10 (23%)	45,67,67	2.23	18 (40%)
31	PEB	V1	202	2	43,46,46	3.21	10 (23%)	45,67,67	2.57	18 (40%)
31	PEB	B5	202	3	43,46,46	3.33	9 (20%)	45,67,67	2.02	15 (33%)
33	CYC	DB	1001	9	42,46,46	3.12	13 (30%)	50,67,67	2.79	20 (40%)
31	PEB	mH	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.09	15 (33%)
31	PEB	L6	1002	9	43,46,46	3.36	10 (23%)	45,67,67	2.68	18 (40%)
31	PEB	AH	301	12	43,46,46	3.17	10 (23%)	45,67,67	2.30	15 (33%)
31	PEB	LH	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.27	16 (35%)
33	CYC	A3	1001	19	42,46,46	3.66	14 (33%)	50,67,67	2.92	20 (40%)
32	PUB	AC	303	6	42,46,46	3.60	8 (19%)	37,67,67	3.19	15 (40%)
31	PEB	VG	202	3	43,46,46	3.23	10 (23%)	45,67,67	2.31	14 (31%)
31	PEB	F4	201	2,25	43,46,46	3.29	10 (23%)	45,67,67	2.60	16 (35%)
33	CYC	I2	201	8,9	42,46,46	3.18	12 (28%)	50,67,67	2.97	22 (44%)
31	PEB	KF	202	3	43,46,46	3.34	11 (25%)	45,67,67	2.36	16 (35%)
31	PEB	RK	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.24	19 (42%)
31	PEB	HK	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.14	14 (31%)
31	PEB	eC	202	2	43,46,46	3.44	11 (25%)	45,67,67	1.95	13 (28%)
31	PEB	D9	201	2,14	43,46,46	3.16	10 (23%)	45,67,67	2.09	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	HE	1002	8,9	43,46,46	3.31	12 (27%)	45,67,67	2.13	12 (26%)
31	PEB	D1	201	2,6	43,46,46	3.41	13 (30%)	45,67,67	2.40	14 (31%)
32	PUB	CI	203	14,3	42,46,46	3.33	10 (23%)	37,67,67	4.36	16 (43%)
31	PEB	WC	201	3	43,46,46	3.23	10 (23%)	45,67,67	2.23	15 (33%)
33	CYC	R3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.92	18 (36%)
31	PEB	XK	201	2,15	43,46,46	3.63	11 (25%)	45,67,67	2.35	19 (42%)
31	PEB	PG	202	3	43,46,46	3.22	11 (25%)	45,67,67	2.31	14 (31%)
33	CYC	C6	1001	8	42,46,46	3.24	15 (35%)	50,67,67	2.92	20 (40%)
33	CYC	CB	1001	8	42,46,46	3.25	14 (33%)	50,67,67	2.93	21 (42%)
31	PEB	U7	201	3	43,46,46	3.33	11 (25%)	45,67,67	2.20	16 (35%)
31	PEB	Q4	204	3	43,46,46	3.37	11 (25%)	45,67,67	1.89	10 (22%)
33	CYC	FB	1001	9	42,46,46	3.26	14 (33%)	50,67,67	2.99	20 (40%)
31	PEB	y8	301	13	43,46,46	3.34	10 (23%)	45,67,67	2.08	15 (33%)
31	PEB	iH	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.53	16 (35%)
31	PEB	OF	201	2,3	43,46,46	3.31	12 (27%)	45,67,67	2.57	18 (40%)
31	PEB	SA	203	2	43,46,46	3.24	10 (23%)	45,67,67	2.35	15 (33%)
31	PEB	M5	202	2	43,46,46	3.33	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	O7	203	3	43,46,46	3.02	10 (23%)	45,67,67	2.23	14 (31%)
31	PEB	F5	201	3	43,46,46	3.26	12 (27%)	45,67,67	2.62	17 (37%)
31	PEB	pF	201	2	43,46,46	3.31	9 (20%)	45,67,67	2.73	17 (37%)
31	PEB	Q6	202	3	43,46,46	1.10	2 (4%)	45,67,67	1.01	2 (4%)
31	PEB	k4	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.38	14 (31%)
31	PEB	iC	201	2	43,46,46	3.34	12 (27%)	45,67,67	2.04	16 (35%)
31	PEB	SH	201	3	43,46,46	3.21	10 (23%)	45,67,67	2.43	15 (33%)
31	PEB	ZD	202	2,3	43,46,46	3.13	10 (23%)	45,67,67	2.46	17 (37%)
31	PEB	f6	202	3	43,46,46	3.43	12 (27%)	45,67,67	1.97	14 (31%)
31	PEB	jF	201	2	43,46,46	3.34	11 (25%)	45,67,67	2.83	18 (40%)
31	PEB	ZH	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.43	14 (31%)
31	PEB	KH	203	2,3	43,46,46	3.06	11 (25%)	45,67,67	2.81	17 (37%)
31	PEB	QF	203	2,3	43,46,46	3.45	13 (30%)	45,67,67	3.26	16 (35%)
31	PEB	OA	201	2,4	43,46,46	3.33	11 (25%)	45,67,67	2.10	13 (28%)
31	PEB	M1	202	3	43,46,46	3.33	10 (23%)	45,67,67	2.01	13 (28%)
32	PUB	A6	302	6	42,46,46	3.44	7 (16%)	37,67,67	3.14	16 (43%)
31	PEB	fB	201	3	43,46,46	3.35	11 (25%)	45,67,67	2.23	16 (35%)
31	PEB	m4	202	2,12	43,46,46	3.37	11 (25%)	45,67,67	2.32	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	AA	501	2,1	43,46,46	3.22	10 (23%)	45,67,67	2.23	16 (35%)
31	PEB	a2	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.11	13 (28%)
31	PEB	UH	202	3	43,46,46	3.17	10 (23%)	45,67,67	2.33	15 (33%)
31	PEB	QH	204	3	43,46,46	3.38	10 (23%)	45,67,67	1.97	11 (24%)
31	PEB	RB	202	2	43,46,46	3.21	11 (25%)	45,67,67	2.49	16 (35%)
32	PUB	AB	302	6	42,46,46	3.45	7 (16%)	37,67,67	3.14	16 (43%)
33	CYC	JB	1001	9	42,46,46	3.14	16 (38%)	50,67,67	2.96	22 (44%)
33	CYC	F6	1001	9	42,46,46	3.25	13 (30%)	50,67,67	2.98	20 (40%)
32	PUB	M9	305	14,3	42,46,46	3.60	9 (21%)	37,67,67	3.50	16 (43%)
31	PEB	TG	202	3	43,46,46	3.35	9 (20%)	45,67,67	1.98	13 (28%)
31	PEB	V8	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.57	15 (33%)
31	PEB	IJ	202	2,26	43,46,46	3.67	13 (30%)	45,67,67	2.35	18 (40%)
31	PEB	E8	202	3	43,46,46	3.37	11 (25%)	45,67,67	2.02	16 (35%)
31	PEB	S8	201	2,3	43,46,46	3.19	12 (27%)	45,67,67	2.58	15 (33%)
31	PEB	U4	203	3	43,46,46	3.42	12 (27%)	45,67,67	2.33	14 (31%)
31	PEB	k2	202	2	43,46,46	3.46	11 (25%)	45,67,67	2.04	14 (31%)
31	PEB	MH	203	3	43,46,46	3.23	10 (23%)	45,67,67	2.25	13 (28%)
33	CYC	ED	1001	8,9	42,46,46	3.22	15 (35%)	50,67,67	2.76	21 (42%)
31	PEB	GJ	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.33	15 (33%)
31	PEB	TA	201	3	43,46,46	3.38	11 (25%)	45,67,67	2.77	16 (35%)
31	PEB	ZE	202	2,3	43,46,46	3.15	10 (23%)	45,67,67	2.45	16 (35%)
31	PEB	k8	202	3	43,46,46	3.56	11 (25%)	45,67,67	1.89	12 (26%)
31	PEB	eC	201	2	43,46,46	3.45	11 (25%)	45,67,67	2.09	16 (35%)
31	PEB	l8	201	2	43,46,46	3.39	12 (27%)	45,67,67	2.59	15 (33%)
31	PEB	h8	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.43	17 (37%)
31	PEB	sF	201	3	43,46,46	3.21	11 (25%)	45,67,67	2.07	13 (28%)
33	CYC	HE	1001	9	42,46,46	3.12	13 (30%)	50,67,67	3.07	21 (42%)
31	PEB	YJ	202	2,31	43,46,46	3.51	11 (25%)	45,67,67	1.98	12 (26%)
31	PEB	W8	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.15	12 (26%)
31	PEB	RF	202	2	43,46,46	3.39	11 (25%)	45,67,67	2.32	15 (33%)
31	PEB	l1	201	3	43,46,46	3.35	12 (27%)	45,67,67	2.19	13 (28%)
31	PEB	jD	202	3	43,46,46	3.42	11 (25%)	45,67,67	1.96	13 (28%)
31	PEB	F1	201	2,6	43,46,46	3.43	9 (20%)	45,67,67	2.07	15 (33%)
31	PEB	G4	203	2,3	43,46,46	3.24	11 (25%)	45,67,67	2.44	14 (31%)
31	PEB	Y1	301	31,6	43,46,46	3.31	11 (25%)	45,67,67	2.59	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PUB	ZI	305	14,3	42,46,46	3.33	10 (23%)	37,67,67	4.36	16 (43%)
31	PEB	K7	202	3	43,46,46	3.19	10 (23%)	45,67,67	2.14	16 (35%)
31	PEB	uF	202	3	43,46,46	3.49	10 (23%)	45,67,67	2.02	14 (31%)
31	PEB	PK	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.18	17 (37%)
31	PEB	QJ	202	2	43,46,46	3.48	12 (27%)	45,67,67	1.83	13 (28%)
31	PEB	jB	201	3	43,46,46	3.40	11 (25%)	45,67,67	2.30	17 (37%)
31	PEB	bE	201	3	43,46,46	3.39	10 (23%)	45,67,67	2.13	13 (28%)
31	PEB	V5	202	3	43,46,46	3.53	10 (23%)	45,67,67	2.06	12 (26%)
31	PEB	G5	202	2	43,46,46	3.44	9 (20%)	45,67,67	2.10	17 (37%)
31	PEB	PC	201	2,10	43,46,46	3.39	10 (23%)	45,67,67	2.26	17 (37%)
31	PEB	T9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	OG	201	2	43,46,46	3.50	13 (30%)	45,67,67	2.31	15 (33%)
31	PEB	DI	201	2	43,46,46	3.28	11 (25%)	45,67,67	2.06	16 (35%)
31	PEB	EJ	202	2,26	43,46,46	3.29	11 (25%)	45,67,67	2.16	17 (37%)
31	PEB	d2	201	2,3	43,46,46	3.26	9 (20%)	45,67,67	2.34	14 (31%)
31	PEB	UF	202	3	43,46,46	3.23	9 (20%)	45,67,67	2.15	12 (26%)
31	PEB	k8	201	3	43,46,46	3.41	10 (23%)	45,67,67	2.05	11 (24%)
31	PEB	WI	203	2	43,46,46	3.42	11 (25%)	45,67,67	2.15	16 (35%)
31	PEB	e6	203	2	43,46,46	3.30	9 (20%)	45,67,67	1.98	12 (26%)
31	PEB	PD	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.30	18 (40%)
31	PEB	A7	202	3	43,46,46	3.32	11 (25%)	45,67,67	2.01	14 (31%)
31	PEB	l6	202	-	43,46,46	3.47	12 (27%)	45,67,67	1.91	16 (35%)
31	PEB	eB	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.24	16 (35%)
31	PEB	W2	203	2,3	43,46,46	3.41	12 (27%)	45,67,67	2.33	16 (35%)
31	PEB	WG	203	2	43,46,46	3.39	10 (23%)	45,67,67	1.74	12 (26%)
31	PEB	Y5	201	2	43,46,46	3.46	11 (25%)	45,67,67	2.00	12 (26%)
31	PEB	r8	201	2,12	43,46,46	3.46	11 (25%)	45,67,67	2.23	13 (28%)
31	PEB	VB	202	2	43,46,46	3.14	10 (23%)	45,67,67	2.43	17 (37%)
31	PEB	KA	303	2,4	43,46,46	3.66	12 (27%)	45,67,67	2.19	16 (35%)
33	CYC	e3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	mF	201	3	43,46,46	3.40	10 (23%)	45,67,67	2.11	15 (33%)
31	PEB	N7	201	2	43,46,46	3.41	11 (25%)	45,67,67	2.07	16 (35%)
31	PEB	A6	301	6	43,46,46	3.37	9 (20%)	45,67,67	2.00	14 (31%)
31	PEB	e4	202	2,12	43,46,46	3.30	11 (25%)	45,67,67	2.30	17 (37%)
31	PEB	FI	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.37	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CYC	G6	1001	8	42,46,46	3.33	14 (33%)	50,67,67	2.93	18 (36%)
31	PEB	B7	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.21	16 (35%)
31	PEB	P1	201	2	43,46,46	3.40	10 (23%)	45,67,67	2.19	16 (35%)
31	PEB	N9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	G1	202	3	43,46,46	3.38	10 (23%)	45,67,67	1.99	15 (33%)
31	PEB	TE	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.29	19 (42%)
31	PEB	wF	303	12	43,46,46	3.47	11 (25%)	45,67,67	2.08	15 (33%)
31	PEB	cA	401	2,5	43,46,46	3.36	10 (23%)	45,67,67	1.99	15 (33%)
31	PEB	OD	202	3	43,46,46	3.36	10 (23%)	45,67,67	2.06	15 (33%)
33	CYC	LD	1001	9	42,46,46	3.22	15 (35%)	50,67,67	3.05	21 (42%)
33	CYC	n3	1001	20	42,46,46	3.43	14 (33%)	50,67,67	3.15	21 (42%)
33	CYC	M2	201	8,9	42,46,46	3.21	12 (28%)	50,67,67	2.66	19 (38%)
31	PEB	dC	203	3	43,46,46	3.39	12 (27%)	45,67,67	2.81	15 (33%)
31	PEB	N8	202	2	43,46,46	3.50	10 (23%)	45,67,67	1.93	13 (28%)
33	CYC	V3	1001	-	42,46,46	3.50	11 (26%)	50,67,67	2.97	23 (46%)
31	PEB	II	201	3	43,46,46	3.38	12 (27%)	45,67,67	1.94	14 (31%)
33	CYC	HC	1001	9	42,46,46	3.30	15 (35%)	50,67,67	2.88	22 (44%)
31	PEB	IG	203	2,3	43,46,46	2.90	13 (30%)	45,67,67	3.05	16 (35%)
31	PEB	PH	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.32	15 (33%)
31	PEB	P2	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.00	17 (37%)
31	PEB	QJ	201	2,6	43,46,46	3.47	11 (25%)	45,67,67	2.25	18 (40%)
31	PEB	x8	303	12	43,46,46	3.45	11 (25%)	45,67,67	1.98	12 (26%)
31	PEB	mD	203	2	43,46,46	3.46	11 (25%)	45,67,67	1.96	15 (33%)
31	PEB	M9	301	14,31	43,46,46	3.25	11 (25%)	45,67,67	2.71	19 (42%)
31	PEB	T6	202	2	43,46,46	3.34	11 (25%)	45,67,67	2.24	14 (31%)
31	PEB	f6	201	3	43,46,46	3.33	10 (23%)	45,67,67	2.23	16 (35%)
31	PEB	S6	202	3,29	43,46,46	3.34	11 (25%)	45,67,67	1.97	13 (28%)
31	PEB	OH	201	3	43,46,46	3.21	10 (23%)	45,67,67	2.06	15 (33%)
31	PEB	dA	201	2	43,46,46	3.31	11 (25%)	45,67,67	2.07	15 (33%)
31	PEB	aC	202	2	43,46,46	3.47	10 (23%)	45,67,67	2.10	16 (35%)
31	PEB	P6	202	2	43,46,46	3.29	11 (25%)	45,67,67	2.47	16 (35%)
31	PEB	xF	302	12	43,46,46	3.38	12 (27%)	45,67,67	2.91	13 (28%)
33	CYC	N2	1001	9,7	42,46,46	3.36	16 (38%)	50,67,67	2.84	22 (44%)
31	PEB	LB	1002	9	43,46,46	3.35	10 (23%)	45,67,67	2.66	18 (40%)
31	PEB	YI	203	2	43,46,46	3.32	9 (20%)	45,67,67	2.11	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	R5	203	2,3	43,46,46	3.40	12 (27%)	45,67,67	2.33	16 (35%)
31	PEB	QC	202	3	43,46,46	3.39	11 (25%)	45,67,67	2.50	17 (37%)
31	PEB	ZC	203	3	43,46,46	3.40	12 (27%)	45,67,67	2.51	16 (35%)
31	PEB	K5	201	2	43,46,46	3.37	11 (25%)	45,67,67	1.97	14 (31%)
31	PEB	L9	201	2,14	43,46,46	3.31	10 (23%)	45,67,67	2.03	16 (35%)
31	PEB	XG	201	3	43,46,46	3.35	10 (23%)	45,67,67	1.98	14 (31%)
31	PEB	LG	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.04	14 (31%)
31	PEB	qF	203	3	43,46,46	3.50	12 (27%)	45,67,67	2.29	16 (35%)
31	PEB	LC	1002	9	43,46,46	3.11	10 (23%)	45,67,67	2.37	14 (31%)
31	PEB	C1	201	3	43,46,46	3.28	12 (27%)	45,67,67	2.54	17 (37%)
31	PEB	H5	202	3	43,46,46	3.40	12 (27%)	45,67,67	2.45	16 (35%)
31	PEB	nF	201	2	43,46,46	3.46	10 (23%)	45,67,67	3.21	17 (37%)
31	PEB	IA	203	2	43,46,46	3.25	10 (23%)	45,67,67	2.26	16 (35%)
31	PEB	UA	303	2,4	43,46,46	3.28	10 (23%)	45,67,67	2.05	14 (31%)
32	PUB	AH	303	12	42,46,46	3.26	8 (19%)	37,67,67	3.64	18 (48%)
31	PEB	hB	202	3	43,46,46	3.41	9 (20%)	45,67,67	1.99	13 (28%)
31	PEB	N2	1002	9	43,46,46	3.28	12 (27%)	45,67,67	2.09	11 (24%)
33	CYC	L6	1001	9	42,46,46	3.13	16 (38%)	50,67,67	2.97	22 (44%)
32	PUB	QH	202	3,13	42,46,46	3.37	7 (16%)	37,67,67	3.52	18 (48%)
31	PEB	c4	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.39	12 (26%)
31	PEB	ZD	203	3	43,46,46	3.34	11 (25%)	45,67,67	2.16	16 (35%)
32	PUB	x8	301	12	42,46,46	3.25	8 (19%)	37,67,67	3.36	19 (51%)
31	PEB	A4	302	12	43,46,46	3.36	8 (18%)	45,67,67	2.09	14 (31%)
31	PEB	c2	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.08	16 (35%)
31	PEB	WD	201	26,3	43,46,46	3.32	10 (23%)	45,67,67	2.02	13 (28%)
31	PEB	t8	202	2	43,46,46	3.65	11 (25%)	45,67,67	2.62	16 (35%)
31	PEB	CJ	202	2,6	43,46,46	3.13	11 (25%)	45,67,67	2.25	18 (40%)
33	CYC	C3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	P9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	EA	501	2,1	43,46,46	3.26	10 (23%)	45,67,67	2.23	16 (35%)
31	PEB	V2	203	2,3	43,46,46	3.39	11 (25%)	45,67,67	2.53	16 (35%)
31	PEB	PG	201	3	43,46,46	3.35	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	TK	201	2	43,46,46	3.56	11 (25%)	45,67,67	2.32	17 (37%)
31	PEB	FB	1002	9	43,46,46	3.26	10 (23%)	45,67,67	2.22	17 (37%)
31	PEB	EG	202	3	43,46,46	3.22	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
31	PEB	HD	1002	8,9	43,46,46	3.29	12 (27%)	45,67,67	2.11	12 (26%)
31	PEB	WF	201	2,3	43,46,46	3.26	12 (27%)	45,67,67	2.63	21 (46%)
31	PEB	X7	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.13	16 (35%)
31	PEB	ZG	401	2,11	43,46,46	3.59	14 (32%)	45,67,67	3.02	19 (42%)
31	PEB	LK	201	2,31	43,46,46	3.42	11 (25%)	45,67,67	2.23	15 (33%)
31	PEB	HA	201	2	43,46,46	3.26	10 (23%)	45,67,67	2.04	14 (31%)
31	PEB	cD	202	2	43,46,46	3.48	10 (23%)	45,67,67	1.99	13 (28%)
31	PEB	OI	203	2	43,46,46	3.42	11 (25%)	45,67,67	2.06	16 (35%)
32	PUB	x8	306	12	42,46,46	3.61	7 (16%)	37,67,67	2.91	15 (40%)
31	PEB	BA	203	2	43,46,46	3.32	10 (23%)	45,67,67	2.22	16 (35%)
31	PEB	T7	201	2,27	43,46,46	3.57	12 (27%)	45,67,67	2.02	15 (33%)
31	PEB	XK	202	2	43,46,46	3.02	9 (20%)	45,67,67	2.62	19 (42%)
31	PEB	YH	201	2,3	43,46,46	3.26	11 (25%)	45,67,67	2.52	18 (40%)
31	PEB	e6	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.15	15 (33%)
31	PEB	aA	202	2	43,46,46	3.35	10 (23%)	45,67,67	1.99	16 (35%)
31	PEB	b6	201	3	43,46,46	3.37	10 (23%)	45,67,67	2.38	16 (35%)
31	PEB	B1	203	2	43,46,46	3.34	9 (20%)	45,67,67	1.99	14 (31%)
31	PEB	SC	202	3	43,46,46	3.32	9 (20%)	45,67,67	2.40	13 (28%)
31	PEB	lE	201	2,3	43,46,46	3.36	12 (27%)	45,67,67	2.25	13 (28%)
32	PUB	Z9	305	14,3	42,46,46	3.60	9 (21%)	37,67,67	3.50	16 (43%)
31	PEB	EF	202	3	43,46,46	3.36	11 (25%)	45,67,67	2.02	16 (35%)
31	PEB	dB	202	3	43,46,46	3.35	11 (25%)	45,67,67	1.88	12 (26%)
31	PEB	BK	203	2	43,46,46	3.34	9 (20%)	45,67,67	1.99	13 (28%)
31	PEB	CJ	201	2	43,46,46	3.46	10 (23%)	45,67,67	1.98	15 (33%)
31	PEB	i4	201	2	43,46,46	3.42	12 (27%)	45,67,67	2.41	17 (37%)
31	PEB	O6	201	3	43,46,46	3.35	11 (25%)	45,67,67	2.49	18 (40%)
31	PEB	k6	201	2	43,46,46	3.43	11 (25%)	45,67,67	1.98	12 (26%)
31	PEB	DA	203	2	43,46,46	3.12	10 (23%)	45,67,67	2.15	15 (33%)
31	PEB	A2	301	6	43,46,46	3.40	8 (18%)	45,67,67	2.12	14 (31%)
31	PEB	R7	201	2,27	43,46,46	3.42	12 (27%)	45,67,67	2.11	16 (35%)
31	PEB	WF	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.16	12 (26%)
31	PEB	kF	203	2,3	43,46,46	3.41	11 (25%)	45,67,67	2.30	11 (24%)
31	PEB	J8	202	2	43,46,46	3.49	11 (25%)	45,67,67	2.33	16 (35%)
31	PEB	HH	202	2	43,46,46	3.29	10 (23%)	45,67,67	2.52	15 (33%)
31	PEB	DH	202	2,13	43,46,46	3.39	10 (23%)	45,67,67	2.57	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CYC	KC	201	8,9	42,46,46	3.18	11 (26%)	50,67,67	2.92	22 (44%)
33	CYC	MB	1001	8	42,46,46	3.16	12 (28%)	50,67,67	2.88	17 (34%)
31	PEB	a6	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.56	15 (33%)
31	PEB	R8	201	2	43,46,46	3.27	9 (20%)	45,67,67	3.71	21 (46%)
31	PEB	fF	202	2	43,46,46	3.58	12 (27%)	45,67,67	2.00	18 (40%)
31	PEB	ZF	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.42	17 (37%)
31	PEB	AD	304	6	43,46,46	3.30	10 (23%)	45,67,67	2.15	16 (35%)
31	PEB	aD	202	2	43,46,46	3.35	11 (25%)	45,67,67	2.34	15 (33%)
33	CYC	CC	1001	8,9	42,46,46	3.25	13 (30%)	50,67,67	2.72	20 (40%)
31	PEB	j2	203	2,3	43,46,46	3.51	14 (32%)	45,67,67	2.50	15 (33%)
31	PEB	F8	201	2	43,46,46	3.48	10 (23%)	45,67,67	3.85	17 (37%)
31	PEB	KF	203	3	43,46,46	3.30	10 (23%)	45,67,67	2.05	17 (37%)
31	PEB	A6	305	6	43,46,46	3.38	10 (23%)	45,67,67	2.00	13 (28%)
33	CYC	K2	201	8,9	42,46,46	3.18	11 (26%)	50,67,67	2.95	22 (44%)
31	PEB	D4	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.30	16 (35%)
31	PEB	dD	202	6,3	43,46,46	3.37	10 (23%)	45,67,67	2.15	14 (31%)
31	PEB	LH	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.55	13 (28%)
31	PEB	CH	201	3	43,46,46	3.22	10 (23%)	45,67,67	2.34	16 (35%)
31	PEB	E7	202	3	43,46,46	3.31	10 (23%)	45,67,67	2.01	13 (28%)
31	PEB	kH	201	2	43,46,46	3.35	12 (27%)	45,67,67	2.33	14 (31%)
31	PEB	XF	202	2	43,46,46	3.25	12 (27%)	45,67,67	2.62	16 (35%)
31	PEB	cE	202	2	43,46,46	3.46	11 (25%)	45,67,67	1.98	13 (28%)
31	PEB	A9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.93	14 (31%)
31	PEB	F5	202	3	43,46,46	3.42	11 (25%)	45,67,67	1.99	15 (33%)
31	PEB	AC	305	6	43,46,46	3.45	9 (20%)	45,67,67	2.43	15 (33%)
31	PEB	Y7	502	2	43,46,46	3.31	11 (25%)	45,67,67	2.17	15 (33%)
31	PEB	O8	201	2,3	43,46,46	3.30	12 (27%)	45,67,67	2.58	18 (40%)
31	PEB	XA	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.08	16 (35%)
31	PEB	xF	303	12	43,46,46	3.42	10 (23%)	45,67,67	1.98	12 (26%)
31	PEB	AG	203	2,3	43,46,46	3.01	13 (30%)	45,67,67	2.72	15 (33%)
31	PEB	IK	201	3	43,46,46	3.33	12 (27%)	45,67,67	2.19	13 (28%)
31	PEB	S9	202	2	43,46,46	3.25	11 (25%)	45,67,67	2.30	13 (28%)
31	PEB	aC	201	2	43,46,46	3.39	9 (20%)	45,67,67	2.13	13 (28%)
31	PEB	HJ	201	2,3	43,46,46	3.20	11 (25%)	45,67,67	2.42	16 (35%)
31	PEB	d4	201	2,3	43,46,46	3.32	12 (27%)	45,67,67	2.57	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	mC	201	2	43,46,46	3.49	12 (27%)	45,67,67	1.89	14 (31%)
31	PEB	LA	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.11	14 (31%)
31	PEB	NA	202	2	43,46,46	3.24	10 (23%)	45,67,67	2.13	13 (28%)
31	PEB	QC	201	2,3	43,46,46	3.32	11 (25%)	45,67,67	2.51	17 (37%)
31	PEB	EJ	201	2	43,46,46	3.30	10 (23%)	45,67,67	2.09	14 (31%)
31	PEB	D9	203	2	43,46,46	3.22	9 (20%)	45,67,67	2.05	16 (35%)
31	PEB	PB	202	2	43,46,46	3.30	11 (25%)	45,67,67	2.49	16 (35%)
31	PEB	R5	201	3	43,46,46	3.50	12 (27%)	45,67,67	2.09	13 (28%)
31	PEB	FH	201	2,25	43,46,46	3.31	9 (20%)	45,67,67	2.69	19 (42%)
31	PEB	w8	302	12	43,46,46	3.31	9 (20%)	45,67,67	2.22	15 (33%)
31	PEB	VC	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.14	16 (35%)
31	PEB	U2	201	2,3	43,46,46	3.39	11 (25%)	45,67,67	2.54	15 (33%)
31	PEB	mB	203	2	43,46,46	3.46	12 (27%)	45,67,67	2.17	15 (33%)
31	PEB	NE	201	8,9	43,46,46	3.36	11 (25%)	45,67,67	2.23	15 (33%)
33	CYC	LC	1001	9	42,46,46	3.52	16 (38%)	50,67,67	3.08	24 (48%)
31	PEB	F9	201	2,14	43,46,46	3.27	10 (23%)	45,67,67	2.31	21 (46%)
31	PEB	TB	202	2	43,46,46	3.36	12 (27%)	45,67,67	2.25	14 (31%)
31	PEB	H8	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.38	16 (35%)
31	PEB	W9	203	2	43,46,46	3.21	9 (20%)	45,67,67	2.11	16 (35%)
31	PEB	P5	202	3	43,46,46	3.48	11 (25%)	45,67,67	2.20	16 (35%)
31	PEB	TD	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.28	19 (42%)
31	PEB	hC	202	3	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	V1	203	2	43,46,46	3.55	12 (27%)	45,67,67	1.96	15 (33%)
31	PEB	FF	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.52	17 (37%)
31	PEB	gD	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.01	16 (35%)
31	PEB	QH	201	2,3	43,46,46	3.26	11 (25%)	45,67,67	2.41	16 (35%)
31	PEB	L2	1002	9	43,46,46	3.11	10 (23%)	45,67,67	2.37	14 (31%)
31	PEB	xF	304	12	43,46,46	3.46	10 (23%)	45,67,67	2.27	16 (35%)
31	PEB	VA	201	2	43,46,46	3.32	11 (25%)	45,67,67	1.99	13 (28%)
31	PEB	T5	201	2,3	43,46,46	3.35	13 (30%)	45,67,67	2.29	13 (28%)
31	PEB	VG	203	2,3	43,46,46	2.71	10 (23%)	45,67,67	3.05	18 (40%)
31	PEB	l8	203	2,3	43,46,46	3.39	14 (32%)	45,67,67	2.54	16 (35%)
33	CYC	u3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	L7	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.14	16 (35%)
31	PEB	A8	201	3	43,46,46	3.24	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
31	PEB	SB	201	3,29	43,46,46	3.31	11 (25%)	45,67,67	1.95	13 (28%)
31	PEB	A9	201	3	43,46,46	3.21	11 (25%)	45,67,67	2.21	15 (33%)
31	PEB	B1	201	2,31	43,46,46	3.33	11 (25%)	45,67,67	2.18	17 (37%)
31	PEB	L4	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.50	17 (37%)
31	PEB	aF	202	3	43,46,46	3.29	11 (25%)	45,67,67	2.17	16 (35%)
31	PEB	PI	201	3	43,46,46	3.37	11 (25%)	45,67,67	1.95	14 (31%)
31	PEB	J5	202	3	43,46,46	3.39	12 (27%)	45,67,67	2.19	15 (33%)
31	PEB	h8	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.00	16 (35%)
31	PEB	dD	204	3	43,46,46	3.41	13 (30%)	45,67,67	2.11	13 (28%)
31	PEB	SJ	201	2,6	43,46,46	3.38	10 (23%)	45,67,67	2.09	13 (28%)
31	PEB	W7	201	2,3	43,46,46	3.38	11 (25%)	45,67,67	2.63	15 (33%)
31	PEB	RK	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
31	PEB	Z8	202	2	43,46,46	3.57	12 (27%)	45,67,67	2.06	14 (31%)
31	PEB	c6	203	2	43,46,46	3.47	11 (25%)	45,67,67	1.99	11 (24%)
31	PEB	MK	201	3	43,46,46	3.28	10 (23%)	45,67,67	2.42	14 (31%)
31	PEB	dH	202	3	43,46,46	3.28	11 (25%)	45,67,67	2.08	13 (28%)
31	PEB	TH	201	2	43,46,46	3.23	10 (23%)	45,67,67	2.45	16 (35%)
31	PEB	PB	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.23	17 (37%)
33	CYC	M3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	JI	201	2	43,46,46	3.48	11 (25%)	45,67,67	2.43	15 (33%)
31	PEB	o8	201	3	43,46,46	3.31	10 (23%)	45,67,67	2.25	15 (33%)
33	CYC	B3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	lD	202	3	43,46,46	3.35	10 (23%)	45,67,67	2.02	14 (31%)
31	PEB	V7	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.20	17 (37%)
31	PEB	kE	202	2,6	43,46,46	3.46	12 (27%)	45,67,67	2.24	17 (37%)
31	PEB	k6	203	2	43,46,46	1.09	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	Z2	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.50	16 (35%)
31	PEB	b8	202	2	43,46,46	3.62	9 (20%)	45,67,67	2.36	14 (31%)
31	PEB	i8	202	3	43,46,46	3.25	10 (23%)	45,67,67	2.31	18 (40%)
31	PEB	SD	202	3	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
31	PEB	hC	201	3	43,46,46	3.38	11 (25%)	45,67,67	2.16	14 (31%)
31	PEB	QK	201	3	43,46,46	3.24	11 (25%)	45,67,67	2.65	16 (35%)
31	PEB	GH	201	3	43,46,46	3.20	10 (23%)	45,67,67	2.30	17 (37%)
31	PEB	PE	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.30	18 (40%)
31	PEB	cB	202	2	43,46,46	3.49	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
31	PEB	AF	201	3	43,46,46	3.24	10 (23%)	45,67,67	2.30	17 (37%)
31	PEB	UC	203	3	43,46,46	3.33	10 (23%)	45,67,67	2.34	15 (33%)
31	PEB	HG	201	2	43,46,46	3.43	12 (27%)	45,67,67	2.23	14 (31%)
31	PEB	J8	201	2	43,46,46	3.38	10 (23%)	45,67,67	3.05	17 (37%)
31	PEB	NJ	203	3	43,46,46	3.36	8 (18%)	45,67,67	2.02	13 (28%)
31	PEB	ID	203	3	43,46,46	3.46	11 (25%)	45,67,67	1.98	14 (31%)
31	PEB	C1	202	3	43,46,46	1.06	2 (4%)	45,67,67	1.00	2 (4%)
33	CYC	H6	1001	9	42,46,46	3.26	14 (33%)	50,67,67	3.08	23 (46%)
31	PEB	J1	202	2	43,46,46	3.27	10 (23%)	45,67,67	2.75	16 (35%)
31	PEB	Q6	201	3	43,46,46	3.32	11 (25%)	45,67,67	2.70	20 (44%)
31	PEB	X1	202	2	43,46,46	3.02	9 (20%)	45,67,67	2.63	18 (40%)
31	PEB	R4	201	2	43,46,46	3.28	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	XH	202	2	43,46,46	3.19	11 (25%)	45,67,67	2.40	17 (37%)
31	PEB	H4	202	2	43,46,46	3.42	12 (27%)	45,67,67	2.70	21 (46%)
31	PEB	D6	1002	9	43,46,46	3.31	10 (23%)	45,67,67	2.19	17 (37%)
31	PEB	BG	202	2,3	43,46,46	3.02	11 (25%)	45,67,67	2.81	16 (35%)
31	PEB	dE	201	2,3	43,46,46	3.35	9 (20%)	45,67,67	2.43	16 (35%)
31	PEB	RJ	201	3	43,46,46	3.51	12 (27%)	45,67,67	2.09	13 (28%)
31	PEB	ZE	203	3	43,46,46	3.35	10 (23%)	45,67,67	2.16	17 (37%)
31	PEB	g2	201	2	43,46,46	3.57	10 (23%)	45,67,67	1.92	15 (33%)
31	PEB	P9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.21	15 (33%)
31	PEB	r8	202	2	43,46,46	3.43	12 (27%)	45,67,67	2.05	13 (28%)
31	PEB	X5	201	2,3	43,46,46	3.35	10 (23%)	45,67,67	2.46	15 (33%)
31	PEB	KD	201	8,9	43,46,46	3.31	11 (25%)	45,67,67	2.10	15 (33%)
31	PEB	L7	201	2	43,46,46	3.32	10 (23%)	45,67,67	2.03	15 (33%)
31	PEB	PJ	201	2,3	43,46,46	3.48	13 (30%)	45,67,67	2.12	13 (28%)
31	PEB	Z6	202	3	43,46,46	3.29	10 (23%)	45,67,67	1.93	12 (26%)
31	PEB	MJ	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.07	15 (33%)
31	PEB	PH	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.31	17 (37%)
31	PEB	LF	201	2	43,46,46	3.37	11 (25%)	45,67,67	3.50	19 (42%)
31	PEB	ID	201	2,3	43,46,46	3.38	13 (30%)	45,67,67	2.22	13 (28%)
31	PEB	X9	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	s8	203	2,3	43,46,46	3.49	13 (30%)	45,67,67	2.76	16 (35%)
31	PEB	FJ	202	3	43,46,46	3.42	12 (27%)	45,67,67	1.99	15 (33%)
31	PEB	bB	201	3	43,46,46	3.40	10 (23%)	45,67,67	2.39	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	aB	202	2	43,46,46	3.31	12 (27%)	45,67,67	2.58	15 (33%)
33	CYC	q3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	eK	301	15,3	43,46,46	1.08	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	uF	203	3	43,46,46	3.46	11 (25%)	45,67,67	1.98	15 (33%)
31	PEB	RH	202	2	43,46,46	3.26	10 (23%)	45,67,67	2.50	15 (33%)
31	PEB	O2	203	2,3	43,46,46	3.28	10 (23%)	45,67,67	2.40	15 (33%)
31	PEB	U8	202	3	43,46,46	3.26	9 (20%)	45,67,67	2.17	13 (28%)
31	PEB	iB	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.00	15 (33%)
31	PEB	ZE	201	2,3	43,46,46	3.33	11 (25%)	45,67,67	2.13	16 (35%)
31	PEB	O4	201	3	43,46,46	3.34	11 (25%)	45,67,67	2.27	14 (31%)
31	PEB	W9	201	2	43,46,46	3.19	10 (23%)	45,67,67	2.24	18 (40%)
31	PEB	FK	201	2,6	43,46,46	3.42	10 (23%)	45,67,67	2.06	15 (33%)
31	PEB	g8	202	3	43,46,46	3.37	10 (23%)	45,67,67	2.05	15 (33%)
31	PEB	HA	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.10	15 (33%)
31	PEB	hF	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.43	17 (37%)
33	CYC	63	901	24	42,46,46	3.25	15 (35%)	50,67,67	3.08	24 (48%)
33	CYC	l3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.92	20 (40%)
31	PEB	X1	203	2	43,46,46	3.51	11 (25%)	45,67,67	2.30	18 (40%)
31	PEB	T7	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.15	17 (37%)
32	PUB	A2	303	6	42,46,46	3.60	8 (19%)	37,67,67	3.19	15 (40%)
31	PEB	L1	201	2,31	43,46,46	3.44	11 (25%)	45,67,67	2.24	15 (33%)
31	PEB	i2	202	2	43,46,46	3.51	10 (23%)	45,67,67	1.86	12 (26%)
31	PEB	aH	202	3	43,46,46	3.26	10 (23%)	45,67,67	2.29	18 (40%)
31	PEB	U2	203	3	43,46,46	3.32	9 (20%)	45,67,67	2.34	15 (33%)
31	PEB	x8	302	12	43,46,46	3.39	11 (25%)	45,67,67	2.91	13 (28%)
31	PEB	D7	202	2	43,46,46	3.37	10 (23%)	45,67,67	2.17	17 (37%)
31	PEB	fE	202	3	43,46,46	3.44	12 (27%)	45,67,67	1.97	14 (31%)
31	PEB	G4	202	3	43,46,46	3.38	11 (25%)	45,67,67	2.04	13 (28%)
33	CYC	h3	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	O2	201	3	43,46,46	3.36	13 (30%)	45,67,67	2.34	16 (35%)
31	PEB	BF	201	2	43,46,46	3.40	11 (25%)	45,67,67	3.48	16 (35%)
31	PEB	D7	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
31	PEB	BJ	202	3	43,46,46	3.33	10 (23%)	45,67,67	2.01	15 (33%)
31	PEB	H4	201	2	43,46,46	3.21	10 (23%)	45,67,67	2.53	15 (33%)
31	PEB	gF	202	3	43,46,46	3.34	10 (23%)	45,67,67	2.04	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	FJ	203	2,3	43,46,46	3.41	13 (30%)	45,67,67	3.07	13 (28%)
31	PEB	VC	203	2,3	43,46,46	3.39	11 (25%)	45,67,67	2.54	17 (37%)
31	PEB	YK	301	31,6	43,46,46	3.30	11 (25%)	45,67,67	2.58	13 (28%)
31	PEB	IH	202	3	43,46,46	3.16	12 (27%)	45,67,67	2.48	17 (37%)
33	CYC	L2	1001	9	42,46,46	3.51	16 (38%)	50,67,67	3.09	25 (50%)
31	PEB	H7	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.21	14 (31%)
31	PEB	U7	202	3	43,46,46	3.47	12 (27%)	45,67,67	2.11	15 (33%)
31	PEB	KJ	201	2	43,46,46	3.36	10 (23%)	45,67,67	1.98	14 (31%)
31	PEB	J9	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.13	16 (35%)
31	PEB	MF	201	3	43,46,46	3.32	10 (23%)	45,67,67	1.88	13 (28%)
31	PEB	V4	201	2	43,46,46	3.35	10 (23%)	45,67,67	2.14	13 (28%)
31	PEB	OD	203	2,3	43,46,46	3.23	11 (25%)	45,67,67	2.24	16 (35%)
31	PEB	L4	201	2	43,46,46	3.41	10 (23%)	45,67,67	2.23	13 (28%)
31	PEB	T4	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.21	16 (35%)
31	PEB	PF	202	2	43,46,46	3.59	11 (25%)	45,67,67	2.07	14 (31%)
31	PEB	M7	202	3	43,46,46	3.32	10 (23%)	45,67,67	2.08	15 (33%)
31	PEB	WD	202	3	43,46,46	3.34	11 (25%)	45,67,67	2.32	17 (37%)
31	PEB	aD	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.16	19 (42%)
31	PEB	qF	202	3	43,46,46	3.37	11 (25%)	45,67,67	3.42	18 (40%)
31	PEB	j6	201	3	43,46,46	3.40	11 (25%)	45,67,67	2.31	17 (37%)
31	PEB	m6	203	2	43,46,46	3.46	13 (30%)	45,67,67	2.17	15 (33%)
31	PEB	SH	202	3	43,46,46	3.36	10 (23%)	45,67,67	2.06	13 (28%)
33	CYC	O3	1001	20	42,46,46	3.43	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	Z8	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.41	17 (37%)
31	PEB	SF	203	3	43,46,46	3.24	10 (23%)	45,67,67	2.14	14 (31%)
31	PEB	ZI	301	14	43,46,46	3.11	10 (23%)	45,67,67	2.26	15 (33%)
31	PEB	R2	202	2	43,46,46	3.51	11 (25%)	45,67,67	1.72	10 (22%)
31	PEB	jF	202	2	43,46,46	3.45	10 (23%)	45,67,67	2.17	13 (28%)
31	PEB	SG	202	2	43,46,46	3.31	10 (23%)	45,67,67	2.00	13 (28%)
31	PEB	VE	202	2	43,46,46	3.48	10 (23%)	45,67,67	2.20	15 (33%)
32	PUB	Z9	304	14,3	42,46,46	3.65	9 (21%)	37,67,67	3.55	16 (43%)
31	PEB	cA	402	2,5	43,46,46	3.24	10 (23%)	45,67,67	2.50	15 (33%)
31	PEB	QG	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.08	15 (33%)
31	PEB	FI	201	2,14	43,46,46	3.39	10 (23%)	45,67,67	2.29	16 (35%)
32	PUB	AD	303	6	42,46,46	3.43	7 (16%)	37,67,67	3.00	14 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	LK	202	2	43,46,46	3.17	10 (23%)	45,67,67	2.77	17 (37%)
31	PEB	RB	201	2,10	43,46,46	3.33	11 (25%)	45,67,67	2.37	15 (33%)
31	PEB	J4	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.37	15 (33%)
31	PEB	WA	402	5,2	43,46,46	3.32	10 (23%)	45,67,67	2.27	19 (42%)
31	PEB	JI	203	2	43,46,46	3.38	11 (25%)	45,67,67	2.10	14 (31%)
31	PEB	IG	201	3	43,46,46	3.35	9 (20%)	45,67,67	1.98	13 (28%)
31	PEB	GA	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.18	15 (33%)
33	CYC	FD	201	9	42,46,46	3.25	15 (35%)	50,67,67	2.90	18 (36%)
31	PEB	LK	203	2	43,46,46	3.49	9 (20%)	45,67,67	1.81	13 (28%)
31	PEB	NK	202	2	43,46,46	3.01	9 (20%)	45,67,67	3.12	17 (37%)
31	PEB	P5	201	2,3	43,46,46	3.45	13 (30%)	45,67,67	2.12	13 (28%)
31	PEB	mD	201	2	43,46,46	3.48	13 (30%)	45,67,67	1.95	13 (28%)
31	PEB	JA	202	3	43,46,46	3.21	10 (23%)	45,67,67	2.32	16 (35%)
33	CYC	ME	1001	8,9	42,46,46	3.17	14 (33%)	50,67,67	2.89	19 (38%)
31	PEB	S4	203	2,3	43,46,46	3.32	11 (25%)	45,67,67	2.31	15 (33%)
32	PUB	AC	304	6	42,46,46	3.72	8 (19%)	37,67,67	3.97	17 (45%)
31	PEB	lB	202	-	43,46,46	3.48	11 (25%)	45,67,67	1.92	16 (35%)
31	PEB	i4	202	2,12	43,46,46	3.38	12 (27%)	45,67,67	2.32	14 (31%)
31	PEB	F8	202	2	43,46,46	3.43	10 (23%)	45,67,67	2.52	17 (37%)
31	PEB	A6	304	6	43,46,46	3.38	9 (20%)	45,67,67	2.08	13 (28%)
31	PEB	VH	201	2	43,46,46	3.38	10 (23%)	45,67,67	2.26	14 (31%)
31	PEB	t8	203	2,3	43,46,46	3.51	12 (27%)	45,67,67	2.18	12 (26%)
31	PEB	O5	201	2,6,31	43,46,46	3.41	10 (23%)	45,67,67	1.99	15 (33%)
31	PEB	U9	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.31	15 (33%)
31	PEB	QA	203	2	43,46,46	3.31	10 (23%)	45,67,67	2.10	15 (33%)
31	PEB	Z6	201	3	43,46,46	3.34	12 (27%)	45,67,67	2.77	18 (40%)
31	PEB	JK	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.30	15 (33%)
33	CYC	LE	1001	9	42,46,46	3.24	14 (33%)	50,67,67	3.05	20 (40%)
31	PEB	GI	202	3	43,46,46	3.58	11 (25%)	45,67,67	2.66	17 (37%)
31	PEB	NB	1002	9	43,46,46	3.32	10 (23%)	45,67,67	2.14	17 (37%)
31	PEB	PK	202	2	43,46,46	3.12	10 (23%)	45,67,67	2.64	16 (35%)
31	PEB	uF	201	2,3	43,46,46	3.46	12 (27%)	45,67,67	2.19	11 (24%)
31	PEB	X5	203	3	43,46,46	3.41	10 (23%)	45,67,67	1.98	13 (28%)
32	PUB	Q4	202	3,13	42,46,46	3.45	7 (16%)	37,67,67	3.33	16 (43%)
31	PEB	ZF	202	2	43,46,46	3.55	12 (27%)	45,67,67	2.05	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	QI	201	2	43,46,46	3.57	11 (25%)	45,67,67	2.15	15 (33%)
33	CYC	D3	1001	24,20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	U1	201	3	43,46,46	3.23	10 (23%)	45,67,67	2.61	13 (28%)
31	PEB	aB	201	2	43,46,46	3.30	11 (25%)	45,67,67	2.30	17 (37%)
31	PEB	ZH	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.48	15 (33%)
33	CYC	E6	1001	8	42,46,46	3.19	15 (35%)	50,67,67	2.95	19 (38%)
31	PEB	WA	401	2,5	43,46,46	3.14	10 (23%)	45,67,67	2.39	15 (33%)
31	PEB	hE	202	3	43,46,46	3.37	11 (25%)	45,67,67	2.00	14 (31%)
31	PEB	N1	201	2	43,46,46	3.29	10 (23%)	45,67,67	2.31	17 (37%)
31	PEB	O8	203	3	43,46,46	3.30	9 (20%)	45,67,67	2.03	16 (35%)
31	PEB	p8	202	2	43,46,46	3.59	11 (25%)	45,67,67	2.74	18 (40%)
31	PEB	AB	305	6	43,46,46	3.39	10 (23%)	45,67,67	2.01	13 (28%)
33	CYC	o3	1001	20	42,46,46	3.44	14 (33%)	50,67,67	3.15	21 (42%)
31	PEB	Z2	201	2,3	43,46,46	3.26	9 (20%)	45,67,67	3.16	17 (37%)
31	PEB	ZA	203	2	43,46,46	3.38	10 (23%)	45,67,67	2.07	14 (31%)
31	PEB	gC	202	2	43,46,46	3.50	11 (25%)	45,67,67	2.22	14 (31%)
31	PEB	cE	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.13	16 (35%)
31	PEB	SB	202	3	43,46,46	3.40	11 (25%)	45,67,67	2.66	18 (40%)
31	PEB	XK	203	2	43,46,46	3.48	11 (25%)	45,67,67	2.30	18 (40%)
31	PEB	PI	202	3	43,46,46	3.58	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	HI	203	2	43,46,46	3.41	11 (25%)	45,67,67	2.28	13 (28%)
31	PEB	TG	201	2,3	43,46,46	2.88	12 (27%)	45,67,67	2.80	16 (35%)
31	PEB	U7	203	2,3	43,46,46	3.39	11 (25%)	45,67,67	2.53	16 (35%)
31	PEB	jH	201	3	43,46,46	3.30	10 (23%)	45,67,67	2.20	14 (31%)
31	PEB	T1	202	2	43,46,46	2.77	9 (20%)	45,67,67	2.99	19 (42%)
32	PUB	ZI	302	14	42,46,46	3.39	9 (21%)	37,67,67	4.03	18 (48%)
31	PEB	iB	203	2	43,46,46	3.52	12 (27%)	45,67,67	1.90	14 (31%)
31	PEB	f2	201	3	43,46,46	3.48	13 (30%)	45,67,67	2.00	13 (28%)
31	PEB	WH	202	3	43,46,46	3.26	10 (23%)	45,67,67	2.63	17 (37%)
31	PEB	Y8	202	3	43,46,46	3.38	11 (25%)	45,67,67	1.87	13 (28%)
31	PEB	MI	302	14	43,46,46	3.11	10 (23%)	45,67,67	2.26	15 (33%)
31	PEB	WG	201	2	43,46,46	3.43	12 (27%)	45,67,67	2.42	16 (35%)
31	PEB	CF	201	3	43,46,46	3.38	9 (20%)	45,67,67	2.29	14 (31%)
31	PEB	VK	202	2	43,46,46	3.20	9 (20%)	45,67,67	2.58	18 (40%)
31	PEB	zF	501	2,28	43,46,46	3.09	8 (18%)	45,67,67	2.08	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	gB	202	2	43,46,46	3.34	10 (23%)	45,67,67	2.32	14 (31%)
31	PEB	UD	203	3	43,46,46	3.40	11 (25%)	45,67,67	2.04	15 (33%)
31	PEB	C9	202	3	43,46,46	3.34	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	SE	202	3	43,46,46	3.30	10 (23%)	45,67,67	2.09	17 (37%)
31	PEB	l2	202	3	43,46,46	3.45	11 (25%)	45,67,67	2.04	13 (28%)
31	PEB	DB	1002	9	43,46,46	3.32	11 (25%)	45,67,67	2.18	17 (37%)
31	PEB	HI	201	2,14	43,46,46	3.45	10 (23%)	45,67,67	1.96	13 (28%)
31	PEB	oF	203	3	43,46,46	3.38	11 (25%)	45,67,67	2.28	13 (28%)
31	PEB	jE	202	3	43,46,46	3.42	11 (25%)	45,67,67	1.95	13 (28%)
32	PUB	BH	302	13	42,46,46	3.23	7 (16%)	37,67,67	3.28	13 (35%)
31	PEB	i6	202	2	43,46,46	3.25	10 (23%)	45,67,67	2.32	14 (31%)
31	PEB	U4	202	3	43,46,46	3.24	11 (25%)	45,67,67	2.25	14 (31%)
31	PEB	SA	202	2	43,46,46	3.33	11 (25%)	45,67,67	2.22	17 (37%)
32	PUB	AJ	303	6,3	42,46,46	3.48	8 (19%)	37,67,67	3.17	15 (40%)
31	PEB	jD	201	3	43,46,46	3.40	12 (27%)	45,67,67	2.08	15 (33%)
31	PEB	RB	203	2	43,46,46	3.45	10 (23%)	45,67,67	1.98	11 (24%)
31	PEB	a4	204	2,3	43,46,46	3.38	11 (25%)	45,67,67	2.39	14 (31%)
31	PEB	WK	201	3	43,46,46	3.17	10 (23%)	45,67,67	2.29	15 (33%)
31	PEB	CK	202	3	43,46,46	1.08	2 (4%)	45,67,67	0.99	2 (4%)
31	PEB	OK	201	3	43,46,46	3.09	10 (23%)	45,67,67	2.81	20 (44%)
31	PEB	fH	202	3	43,46,46	3.46	11 (25%)	45,67,67	2.15	17 (37%)
31	PEB	EH	203	3	43,46,46	3.25	10 (23%)	45,67,67	2.15	16 (35%)
31	PEB	BI	202	2	43,46,46	3.22	12 (27%)	45,67,67	2.69	19 (42%)
31	PEB	PC	202	2	43,46,46	3.47	10 (23%)	45,67,67	1.99	17 (37%)
31	PEB	PF	201	2	43,46,46	3.34	9 (20%)	45,67,67	3.23	18 (40%)
32	PUB	YK	304	6	42,46,46	3.53	8 (19%)	37,67,67	3.04	16 (43%)
31	PEB	W5	201	2	43,46,46	3.48	13 (30%)	45,67,67	1.95	15 (33%)
31	PEB	AK	201	3	43,46,46	3.49	12 (27%)	45,67,67	2.31	18 (40%)
31	PEB	ZI	304	14	43,46,46	3.11	12 (27%)	45,67,67	2.71	16 (35%)
31	PEB	AK	202	3	43,46,46	3.43	11 (25%)	45,67,67	1.98	12 (26%)
33	CYC	73	1002	24	42,46,46	3.42	15 (35%)	50,67,67	3.15	23 (46%)
31	PEB	NC	1002	9	43,46,46	3.26	11 (25%)	45,67,67	2.09	12 (26%)
31	PEB	QD	202	3	43,46,46	3.44	10 (23%)	45,67,67	2.07	15 (33%)
31	PEB	j4	201	3	43,46,46	3.32	10 (23%)	45,67,67	2.49	16 (35%)
31	PEB	h4	202	3	43,46,46	3.41	12 (27%)	45,67,67	2.27	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	XF	203	2	43,46,46	3.49	11 (25%)	45,67,67	2.26	17 (37%)
31	PEB	J2	1002	9	43,46,46	3.17	10 (23%)	45,67,67	2.13	14 (31%)
31	PEB	p8	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.73	17 (37%)
31	PEB	E9	202	3	43,46,46	3.36	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	UC	202	3	43,46,46	3.29	13 (30%)	45,67,67	2.13	16 (35%)
31	PEB	JK	201	2,6	43,46,46	3.30	10 (23%)	45,67,67	2.44	13 (28%)
31	PEB	e2	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.09	16 (35%)
31	PEB	S5	201	2,6	43,46,46	3.39	10 (23%)	45,67,67	2.09	13 (28%)
31	PEB	S9	203	2	43,46,46	3.21	10 (23%)	45,67,67	2.00	16 (35%)
31	PEB	CI	201	3	43,46,46	3.38	12 (27%)	45,67,67	1.94	14 (31%)
31	PEB	bF	202	2	43,46,46	3.63	10 (23%)	45,67,67	2.38	15 (33%)
31	PEB	d6	201	3	43,46,46	3.27	10 (23%)	45,67,67	2.19	16 (35%)
31	PEB	J4	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.29	15 (33%)
31	PEB	NA	203	2	43,46,46	3.27	11 (25%)	45,67,67	2.15	15 (33%)
31	PEB	WI	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.34	16 (35%)
31	PEB	QH	203	3	43,46,46	3.29	10 (23%)	45,67,67	2.17	13 (28%)
31	PEB	N7	202	2	43,46,46	3.38	11 (25%)	45,67,67	2.26	17 (37%)
31	PEB	Q2	202	3	43,46,46	3.40	12 (27%)	45,67,67	2.50	17 (37%)
33	CYC	FE	1001	9	42,46,46	3.26	13 (30%)	50,67,67	2.90	18 (36%)
31	PEB	FK	203	2	43,46,46	3.58	12 (27%)	45,67,67	1.97	17 (37%)
32	PUB	A2	304	6	42,46,46	3.72	8 (19%)	37,67,67	3.97	17 (45%)
31	PEB	I9	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	PA	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.26	15 (33%)
31	PEB	eA	201	2	43,46,46	3.31	10 (23%)	45,67,67	2.14	15 (33%)
31	PEB	I7	202	3	43,46,46	3.26	9 (20%)	45,67,67	2.06	14 (31%)
31	PEB	eH	202	2,12	43,46,46	3.26	10 (23%)	45,67,67	2.26	14 (31%)
31	PEB	AG	201	3	43,46,46	3.34	9 (20%)	45,67,67	1.97	13 (28%)
31	PEB	e1	301	15,3	43,46,46	3.37	10 (23%)	45,67,67	1.95	13 (28%)
31	PEB	XI	201	3	43,46,46	3.37	10 (23%)	45,67,67	1.95	14 (31%)
31	PEB	EK	202	3	43,46,46	3.41	12 (27%)	45,67,67	1.98	13 (28%)
31	PEB	w8	301	12	43,46,46	3.21	9 (20%)	45,67,67	2.28	15 (33%)
31	PEB	mH	202	2,12	43,46,46	3.35	10 (23%)	45,67,67	2.63	16 (35%)
31	PEB	a6	201	2	43,46,46	3.33	10 (23%)	45,67,67	2.29	17 (37%)
32	PUB	A4	304	12	42,46,46	3.36	7 (16%)	37,67,67	3.18	16 (43%)
31	PEB	J7	202	2	43,46,46	3.32	10 (23%)	45,67,67	2.14	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	B8	201	2	43,46,46	3.40	12 (27%)	45,67,67	3.50	16 (35%)
31	PEB	g4	201	2	43,46,46	3.42	10 (23%)	45,67,67	2.32	14 (31%)
31	PEB	Y7	504	2,27	43,46,46	3.33	10 (23%)	45,67,67	2.19	15 (33%)
31	PEB	QA	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.02	15 (33%)
31	PEB	IH	203	3	43,46,46	3.32	10 (23%)	45,67,67	2.37	15 (33%)
31	PEB	S2	202	3	43,46,46	3.32	10 (23%)	45,67,67	2.41	13 (28%)
31	PEB	L5	203	3	43,46,46	3.37	9 (20%)	45,67,67	2.04	14 (31%)
31	PEB	h2	203	2,3	43,46,46	1.08	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	SA	201	2	43,46,46	3.18	10 (23%)	45,67,67	2.14	15 (33%)
31	PEB	GD	202	8,9	43,46,46	3.23	10 (23%)	45,67,67	2.31	17 (37%)
31	PEB	dE	202	6,3	43,46,46	3.35	9 (20%)	45,67,67	2.14	14 (31%)
31	PEB	cF	202	9,3	43,46,46	1.07	2 (4%)	45,67,67	1.00	2 (4%)
32	PUB	A5	303	6,3	42,46,46	3.47	8 (19%)	37,67,67	3.17	15 (40%)
31	PEB	G8	202	3	43,46,46	2.65	11 (25%)	45,67,67	3.02	20 (44%)
31	PEB	MI	305	14	43,46,46	3.11	11 (25%)	45,67,67	2.72	16 (35%)
31	PEB	NA	201	2	43,46,46	3.24	10 (23%)	45,67,67	2.21	17 (37%)
31	PEB	gH	202	2	43,46,46	3.41	12 (27%)	45,67,67	2.52	17 (37%)
31	PEB	TI	202	3	43,46,46	3.59	10 (23%)	45,67,67	2.66	17 (37%)
31	PEB	E8	201	3	43,46,46	3.08	9 (20%)	45,67,67	2.33	14 (31%)
31	PEB	D5	201	2,3	43,46,46	3.19	11 (25%)	45,67,67	2.39	14 (31%)
31	PEB	mE	202	2	43,46,46	3.42	11 (25%)	45,67,67	2.55	14 (31%)
31	PEB	V9	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	LF	202	2	43,46,46	3.66	11 (25%)	45,67,67	2.71	15 (33%)
31	PEB	K1	202	3	43,46,46	3.44	10 (23%)	45,67,67	1.80	11 (24%)
31	PEB	M8	202	3	43,46,46	3.48	11 (25%)	45,67,67	1.96	15 (33%)
31	PEB	O1	201	3	43,46,46	3.09	10 (23%)	45,67,67	2.81	20 (44%)
31	PEB	IE	203	3	43,46,46	3.46	11 (25%)	45,67,67	1.97	14 (31%)
31	PEB	L9	202	2	43,46,46	3.32	11 (25%)	45,67,67	2.15	14 (31%)
31	PEB	GG	202	3	43,46,46	3.35	9 (20%)	45,67,67	1.98	13 (28%)
31	PEB	Q9	203	2	43,46,46	3.13	11 (25%)	45,67,67	2.07	15 (33%)
31	PEB	YB	203	2	43,46,46	3.38	11 (25%)	45,67,67	2.04	13 (28%)
31	PEB	aF	203	3	43,46,46	3.37	10 (23%)	45,67,67	2.32	17 (37%)
31	PEB	W2	202	3	43,46,46	3.36	9 (20%)	45,67,67	2.52	16 (35%)
31	PEB	V4	202	2	43,46,46	3.33	10 (23%)	45,67,67	2.22	15 (33%)
31	PEB	u8	201	3	43,46,46	3.53	11 (25%)	45,67,67	2.04	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
33	CYC	HD	1001	9	42,46,46	3.12	14 (33%)	50,67,67	3.07	21 (42%)
31	PEB	gC	201	2	43,46,46	3.58	10 (23%)	45,67,67	1.93	15 (33%)
31	PEB	I4	203	3	43,46,46	3.28	9 (20%)	45,67,67	2.23	14 (31%)
31	PEB	U6	202	3	43,46,46	3.31	9 (20%)	45,67,67	1.90	12 (26%)
31	PEB	LG	201	2,11	43,46,46	3.38	10 (23%)	45,67,67	2.00	15 (33%)
31	PEB	Z2	202	3	43,46,46	3.31	10 (23%)	45,67,67	2.19	17 (37%)
31	PEB	K9	202	3	43,46,46	3.34	10 (23%)	45,67,67	1.93	14 (31%)
31	PEB	Q9	202	2	43,46,46	3.38	10 (23%)	45,67,67	2.62	15 (33%)
31	PEB	H9	202	2	43,46,46	3.30	10 (23%)	45,67,67	2.28	14 (31%)
31	PEB	Q7	201	3	43,46,46	3.29	11 (25%)	45,67,67	2.10	15 (33%)
31	PEB	dJ	401	2,26	43,46,46	3.32	10 (23%)	45,67,67	2.32	18 (40%)
33	CYC	LC	1003	8,9	42,46,46	3.17	12 (28%)	50,67,67	2.96	22 (44%)
31	PEB	HF	202	2	43,46,46	3.42	10 (23%)	45,67,67	2.38	16 (35%)
31	PEB	T1	201	2	43,46,46	3.54	11 (25%)	45,67,67	2.32	18 (40%)
31	PEB	DE	1002	8,9	43,46,46	3.31	12 (27%)	45,67,67	2.26	14 (31%)
31	PEB	OH	203	2,3	43,46,46	3.16	11 (25%)	45,67,67	2.62	18 (40%)
31	PEB	HB	1002	9	43,46,46	3.22	10 (23%)	45,67,67	2.07	16 (35%)
31	PEB	qF	201	2,3	43,46,46	3.42	12 (27%)	45,67,67	2.70	17 (37%)
31	PEB	g8	203	2,3	43,46,46	3.29	11 (25%)	45,67,67	2.56	16 (35%)
33	CYC	P3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.93	19 (38%)
31	PEB	Q2	201	2,3	43,46,46	3.31	11 (25%)	45,67,67	2.49	17 (37%)
31	PEB	RF	201	2	43,46,46	3.27	10 (23%)	45,67,67	3.72	21 (46%)
31	PEB	UB	201	3	43,46,46	3.19	10 (23%)	45,67,67	2.80	19 (42%)
33	CYC	G3	1001	19	42,46,46	3.68	14 (33%)	50,67,67	2.93	19 (38%)
33	CYC	D6	1001	9	42,46,46	3.12	13 (30%)	50,67,67	2.81	20 (40%)
31	PEB	W4	202	3	43,46,46	3.29	11 (25%)	45,67,67	2.18	14 (31%)
31	PEB	AD	301	6	43,46,46	3.35	11 (25%)	45,67,67	2.35	17 (37%)
31	PEB	jC	202	3	43,46,46	3.40	12 (27%)	45,67,67	2.62	16 (35%)
33	CYC	EC	1001	8,9	42,46,46	3.04	14 (33%)	50,67,67	3.17	20 (40%)
31	PEB	U5	202	2	43,46,46	3.52	9 (20%)	45,67,67	1.89	15 (33%)
31	PEB	KG	202	3	43,46,46	3.35	10 (23%)	45,67,67	1.97	13 (28%)
31	PEB	vF	201	2	43,46,46	3.47	10 (23%)	45,67,67	2.88	18 (40%)
31	PEB	BF	202	2	43,46,46	3.44	10 (23%)	45,67,67	2.35	14 (31%)
31	PEB	F6	1002	9	43,46,46	3.24	10 (23%)	45,67,67	2.22	17 (37%)
31	PEB	FK	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.72	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	NI	201	3	43,46,46	3.37	11 (25%)	45,67,67	1.94	14 (31%)
31	PEB	a8	202	3	43,46,46	3.25	11 (25%)	45,67,67	2.17	16 (35%)
31	PEB	mB	201	2	43,46,46	3.39	11 (25%)	45,67,67	2.11	15 (33%)
31	PEB	fD	202	3	43,46,46	3.42	13 (30%)	45,67,67	1.97	14 (31%)
31	PEB	aF	201	2,3	43,46,46	3.43	11 (25%)	45,67,67	2.40	15 (33%)
31	PEB	AC	302	6	43,46,46	3.41	10 (23%)	45,67,67	1.95	12 (26%)
31	PEB	i8	203	3	43,46,46	3.47	12 (27%)	45,67,67	2.03	14 (31%)
31	PEB	c6	201	2	43,46,46	3.37	10 (23%)	45,67,67	1.98	15 (33%)
31	PEB	UJ	202	2	43,46,46	3.51	9 (20%)	45,67,67	1.88	14 (31%)
31	PEB	S8	202	3	43,46,46	3.25	12 (27%)	45,67,67	2.40	16 (35%)
31	PEB	EH	201	2,3	43,46,46	3.10	11 (25%)	45,67,67	2.62	17 (37%)
31	PEB	I4	201	2,3	43,46,46	3.27	11 (25%)	45,67,67	2.48	15 (33%)
31	PEB	e8	203	3	43,46,46	3.35	10 (23%)	45,67,67	2.15	13 (28%)
31	PEB	G5	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.34	15 (33%)
31	PEB	cF	201	3	43,46,46	3.20	10 (23%)	45,67,67	2.31	15 (33%)
31	PEB	lB	201	3	43,46,46	3.31	11 (25%)	45,67,67	2.26	17 (37%)
31	PEB	G4	201	3	43,46,46	3.32	10 (23%)	45,67,67	2.16	15 (33%)
31	PEB	b2	203	2,3	43,46,46	3.34	12 (27%)	45,67,67	2.58	16 (35%)
31	PEB	j4	203	2,3	43,46,46	3.36	12 (27%)	45,67,67	2.46	14 (31%)
31	PEB	aE	201	2	43,46,46	3.28	10 (23%)	45,67,67	2.16	19 (42%)
31	PEB	e8	202	3	43,46,46	3.16	10 (23%)	45,67,67	2.26	19 (42%)
31	PEB	J1	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.31	14 (31%)
31	PEB	K8	201	2,3	43,46,46	3.12	10 (23%)	45,67,67	2.52	14 (31%)
31	PEB	sF	202	3	43,46,46	3.44	11 (25%)	45,67,67	2.05	15 (33%)
31	PEB	W6	201	3	43,46,46	3.29	11 (25%)	45,67,67	2.59	16 (35%)
31	PEB	V6	201	2	43,46,46	3.34	10 (23%)	45,67,67	2.20	16 (35%)
31	PEB	d8	202	2	43,46,46	3.68	11 (25%)	45,67,67	1.84	15 (33%)
31	PEB	ZC	202	3	43,46,46	3.29	10 (23%)	45,67,67	2.18	17 (37%)
31	PEB	UK	202	3	43,46,46	3.32	10 (23%)	45,67,67	1.95	13 (28%)
31	PEB	w8	303	12	43,46,46	3.47	11 (25%)	45,67,67	2.07	15 (33%)
31	PEB	GG	201	2,3	43,46,46	2.86	12 (27%)	45,67,67	2.76	15 (33%)
31	PEB	gB	203	2	43,46,46	3.44	11 (25%)	45,67,67	2.19	13 (28%)
31	PEB	F1	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.72	19 (42%)
31	PEB	aA	201	2	43,46,46	3.24	10 (23%)	45,67,67	2.34	16 (35%)
31	PEB	h4	201	2,3	43,46,46	3.33	12 (27%)	45,67,67	2.34	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	n8	201	2	43,46,46	3.47	10 (23%)	45,67,67	3.23	17 (37%)
31	PEB	x8	304	12	43,46,46	3.48	10 (23%)	45,67,67	2.28	17 (37%)
31	PEB	l2	203	3	43,46,46	3.47	12 (27%)	45,67,67	2.75	15 (33%)
31	PEB	K5	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.15	15 (33%)
31	PEB	i6	203	2	43,46,46	3.54	11 (25%)	45,67,67	1.90	13 (28%)
31	PEB	RD	201	2	43,46,46	3.43	10 (23%)	45,67,67	2.24	17 (37%)
31	PEB	c8	203	2,3	43,46,46	3.30	13 (30%)	45,67,67	2.77	17 (37%)
31	PEB	NF	202	2	43,46,46	3.51	10 (23%)	45,67,67	1.93	13 (28%)
31	PEB	e4	201	2	43,46,46	3.35	11 (25%)	45,67,67	2.43	15 (33%)
31	PEB	H6	1002	9	43,46,46	3.28	10 (23%)	45,67,67	2.07	15 (33%)
31	PEB	YI	201	2	43,46,46	3.52	11 (25%)	45,67,67	2.21	14 (31%)
31	PEB	bD	202	3	43,46,46	3.37	10 (23%)	45,67,67	2.14	14 (31%)
31	PEB	KA	302	2,4	43,46,46	3.34	10 (23%)	45,67,67	2.20	15 (33%)
31	PEB	W1	201	3	43,46,46	3.17	10 (23%)	45,67,67	2.31	15 (33%)
31	PEB	bC	201	3	43,46,46	3.37	11 (25%)	45,67,67	2.03	15 (33%)
31	PEB	N1	203	2	43,46,46	3.35	10 (23%)	45,67,67	2.36	17 (37%)
31	PEB	S8	203	3	43,46,46	3.25	9 (20%)	45,67,67	2.14	14 (31%)
31	PEB	B9	203	2	43,46,46	3.22	10 (23%)	45,67,67	2.04	16 (35%)
31	PEB	F9	202	2	43,46,46	3.17	10 (23%)	45,67,67	2.43	17 (37%)
31	PEB	dD	203	3	43,46,46	3.49	12 (27%)	45,67,67	2.07	15 (33%)
31	PEB	QI	203	2	43,46,46	3.44	10 (23%)	45,67,67	2.21	16 (35%)
31	PEB	WE	202	26,3	43,46,46	3.35	10 (23%)	45,67,67	2.01	13 (28%)
31	PEB	DI	202	2	43,46,46	3.47	12 (27%)	45,67,67	2.32	16 (35%)
31	PEB	W4	201	3	43,46,46	3.37	10 (23%)	45,67,67	2.20	16 (35%)
31	PEB	S7	203	3	43,46,46	3.54	11 (25%)	45,67,67	2.05	13 (28%)
32	PUB	yF	302	13	42,46,46	3.40	7 (16%)	37,67,67	3.16	19 (51%)
31	PEB	N1	202	2	43,46,46	3.04	9 (20%)	45,67,67	3.12	17 (37%)
31	PEB	H2	1002	9	43,46,46	3.46	12 (27%)	45,67,67	2.31	14 (31%)
31	PEB	DK	201	2,6	43,46,46	3.39	13 (30%)	45,67,67	2.40	14 (31%)
31	PEB	W8	201	2,3	43,46,46	3.24	11 (25%)	45,67,67	2.63	21 (46%)
31	PEB	I7	201	3	43,46,46	3.32	10 (23%)	45,67,67	2.17	16 (35%)
31	PEB	h2	201	2,14,3	43,46,46	3.38	11 (25%)	45,67,67	2.44	16 (35%)
31	PEB	s8	201	3	43,46,46	3.20	11 (25%)	45,67,67	2.07	13 (28%)
31	PEB	eH	201	2	43,46,46	3.24	10 (23%)	45,67,67	2.65	18 (40%)
31	PEB	M8	203	2,3	43,46,46	3.34	13 (30%)	45,67,67	2.56	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	d2	202	3	43,46,46	3.39	12 (27%)	45,67,67	2.11	15 (33%)
31	PEB	eC	203	2,3	43,46,46	3.33	12 (27%)	45,67,67	2.58	16 (35%)
31	PEB	g6	202	2	43,46,46	3.31	9 (20%)	45,67,67	2.32	14 (31%)
31	PEB	sF	203	2,3	43,46,46	3.50	13 (30%)	45,67,67	2.75	16 (35%)
31	PEB	aH	203	3	43,46,46	3.36	11 (25%)	45,67,67	2.13	15 (33%)
31	PEB	DD	1002	8,9	43,46,46	3.30	12 (27%)	45,67,67	2.25	14 (31%)
31	PEB	WC	203	2,3	43,46,46	3.41	12 (27%)	45,67,67	2.32	16 (35%)
31	PEB	UH	203	3	43,46,46	3.42	10 (23%)	45,67,67	2.16	14 (31%)
31	PEB	QB	202	3	43,46,46	1.06	2 (4%)	45,67,67	1.00	2 (4%)
31	PEB	CF	203	3	43,46,46	3.42	12 (27%)	45,67,67	1.98	16 (35%)
31	PEB	TF	202	2	43,46,46	3.43	12 (27%)	45,67,67	2.22	18 (40%)
31	PEB	PK	203	2	43,46,46	3.40	10 (23%)	45,67,67	2.06	13 (28%)
31	PEB	BJ	203	2,3	43,46,46	2.93	9 (20%)	45,67,67	2.38	14 (31%)
31	PEB	CF	202	3	43,46,46	3.07	8 (18%)	45,67,67	2.08	15 (33%)
31	PEB	QE	201	2,3	43,46,46	3.17	11 (25%)	45,67,67	2.64	17 (37%)
31	PEB	gF	203	2,3	43,46,46	3.26	11 (25%)	45,67,67	2.57	16 (35%)
31	PEB	R9	201	3	43,46,46	3.23	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	DC	1002	9	43,46,46	3.32	11 (25%)	45,67,67	2.14	14 (31%)
31	PEB	HK	202	2	43,46,46	3.34	11 (25%)	45,67,67	2.59	17 (37%)
31	PEB	NH	202	2	43,46,46	3.27	10 (23%)	45,67,67	2.57	18 (40%)
31	PEB	AJ	301	6,31	43,46,46	3.49	10 (23%)	45,67,67	2.66	15 (33%)
31	PEB	mC	202	2	43,46,46	3.70	10 (23%)	45,67,67	1.86	12 (26%)
31	PEB	Q1	202	3	43,46,46	3.18	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	dA	202	2	43,46,46	3.25	10 (23%)	45,67,67	1.97	13 (28%)
31	PEB	dF	202	2	43,46,46	3.70	11 (25%)	45,67,67	1.85	15 (33%)
33	CYC	m3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.92	19 (38%)
31	PEB	aH	201	3,12	43,46,46	3.26	11 (25%)	45,67,67	2.20	14 (31%)
31	PEB	YC	201	2	43,46,46	3.51	11 (25%)	45,67,67	2.31	18 (40%)
31	PEB	BA	201	2	43,46,46	3.36	11 (25%)	45,67,67	2.17	14 (31%)
31	PEB	KK	201	3	43,46,46	3.26	12 (27%)	45,67,67	2.48	17 (37%)
31	PEB	RG	201	3	43,46,46	3.35	9 (20%)	45,67,67	1.97	13 (28%)
31	PEB	IA	201	2	43,46,46	3.25	10 (23%)	45,67,67	2.12	13 (28%)
31	PEB	I5	201	2	43,46,46	3.43	11 (25%)	45,67,67	2.33	15 (33%)
31	PEB	TC	201	2,10	43,46,46	3.35	12 (27%)	45,67,67	2.20	19 (42%)
31	PEB	dH	201	2,3	43,46,46	3.31	12 (27%)	45,67,67	2.34	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	NF	201	2	43,46,46	3.34	10 (23%)	45,67,67	3.08	17 (37%)
31	PEB	m4	201	2	43,46,46	3.45	12 (27%)	45,67,67	2.43	16 (35%)
33	CYC	BE	1002	9,7	42,46,46	3.23	15 (35%)	50,67,67	2.91	23 (46%)
31	PEB	K9	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.22	15 (33%)
31	PEB	P7	202	2	43,46,46	3.36	10 (23%)	45,67,67	2.22	17 (37%)
31	PEB	UC	201	2,3	43,46,46	3.41	11 (25%)	45,67,67	2.54	15 (33%)
31	PEB	G8	203	3	43,46,46	3.39	11 (25%)	45,67,67	2.64	22 (48%)
33	CYC	I3	1001	20	42,46,46	3.43	14 (33%)	50,67,67	3.16	21 (42%)
31	PEB	MG	401	3,11	43,46,46	1.09	2 (4%)	45,67,67	0.99	2 (4%)
31	PEB	TB	201	2	43,46,46	3.36	10 (23%)	45,67,67	2.16	17 (37%)
31	PEB	bF	201	2	43,46,46	3.39	10 (23%)	45,67,67	2.08	15 (33%)
31	PEB	V7	201	2	43,46,46	3.45	11 (25%)	45,67,67	2.09	17 (37%)
31	PEB	kC	202	2	43,46,46	3.45	11 (25%)	45,67,67	2.06	14 (31%)
31	PEB	jH	202	3	43,46,46	3.46	8 (18%)	45,67,67	2.04	14 (31%)
31	PEB	gC	203	2,14,3	43,46,46	3.38	11 (25%)	45,67,67	2.44	16 (35%)
31	PEB	kF	202	3	43,46,46	3.59	12 (27%)	45,67,67	1.91	12 (26%)
31	PEB	WK	202	3	43,46,46	3.44	11 (25%)	45,67,67	2.05	13 (28%)
33	CYC	T3	1001	19	42,46,46	3.67	14 (33%)	50,67,67	2.94	19 (38%)
31	PEB	gA	203	2	43,46,46	3.24	11 (25%)	45,67,67	2.34	15 (33%)
31	PEB	N4	201	2	43,46,46	3.27	10 (23%)	45,67,67	2.78	18 (40%)
31	PEB	NG	201	3	43,46,46	3.34	10 (23%)	45,67,67	1.98	13 (28%)
31	PEB	YD	202	2	43,46,46	3.41	10 (23%)	45,67,67	2.29	17 (37%)
31	PEB	PE	202	2,10	43,46,46	3.35	10 (23%)	45,67,67	2.22	18 (40%)
31	PEB	X7	201	2	43,46,46	3.29	11 (25%)	45,67,67	2.09	16 (35%)
31	PEB	tF	201	2	43,46,46	3.52	10 (23%)	45,67,67	2.86	15 (33%)
31	PEB	C7	201	2,3	43,46,46	3.39	12 (27%)	45,67,67	2.49	17 (37%)
31	PEB	V2	201	2	43,46,46	3.40	12 (27%)	45,67,67	2.42	18 (40%)
31	PEB	Y4	203	3	43,46,46	3.33	13 (30%)	45,67,67	2.14	12 (26%)
31	PEB	F4	202	2	43,46,46	3.30	11 (25%)	45,67,67	2.29	16 (35%)
31	PEB	Y8	203	2,3	43,46,46	3.41	13 (30%)	45,67,67	2.68	17 (37%)
31	PEB	B5	201	3	43,46,46	3.22	11 (25%)	45,67,67	2.32	16 (35%)
31	PEB	HK	203	2	43,46,46	3.58	11 (25%)	45,67,67	2.48	16 (35%)
31	PEB	J6	1002	9	43,46,46	3.30	11 (25%)	45,67,67	2.12	14 (31%)
33	CYC	DC	1003	8,9	42,46,46	3.14	12 (28%)	50,67,67	2.96	20 (40%)
31	PEB	SJ	202	2	43,46,46	3.36	10 (23%)	45,67,67	1.98	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	PEB	m6	202	2	43,46,46	3.32	12 (27%)	45,67,67	2.38	16 (35%)
31	PEB	gE	201	2	43,46,46	3.37	10 (23%)	45,67,67	2.01	16 (35%)
31	PEB	Y5	202	2,31	43,46,46	3.51	11 (25%)	45,67,67	1.98	12 (26%)
31	PEB	KI	201	3	43,46,46	3.37	11 (25%)	45,67,67	1.94	14 (31%)
31	PEB	c4	202	2	43,46,46	3.39	10 (23%)	45,67,67	2.24	18 (40%)
31	PEB	A8	202	3	43,46,46	3.52	12 (27%)	45,67,67	1.91	12 (26%)
31	PEB	SF	202	3	43,46,46	3.25	12 (27%)	45,67,67	2.41	16 (35%)
31	PEB	OI	201	2	43,46,46	3.40	11 (25%)	45,67,67	2.30	16 (35%)
31	PEB	E4	202	3	43,46,46	3.30	10 (23%)	45,67,67	2.17	17 (37%)
31	PEB	IH	202	3	43,46,46	3.16	11 (25%)	45,67,67	2.38	14 (31%)
31	PEB	I9	202	3	43,46,46	3.34	10 (23%)	45,67,67	1.94	14 (31%)
31	PEB	eD	201	2	43,46,46	3.37	11 (25%)	45,67,67	1.95	13 (28%)
31	PEB	e8	201	2,3	43,46,46	3.42	13 (30%)	45,67,67	2.22	17 (37%)
31	PEB	O9	202	2	43,46,46	3.28	11 (25%)	45,67,67	2.27	16 (35%)
31	PEB	gB	201	2	43,46,46	3.39	11 (25%)	45,67,67	1.98	13 (28%)

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
31	PEB	OE	202	3	-	10/24/74/74	0/4/4/4
33	CYC	DC	1001	9	-	6/25/74/74	0/4/4/4
31	PEB	Y1	303	6	-	16/24/74/74	0/4/4/4
31	PEB	c2	202	2	-	11/24/74/74	0/4/4/4
31	PEB	A5	301	31,6	-	9/24/74/74	0/4/4/4
31	PEB	Q1	201	3	-	6/24/74/74	0/4/4/4
31	PEB	k4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	H1	201	2	-	4/24/74/74	0/4/4/4
31	PEB	U4	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	q8	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	C5	202	2,6	-	4/24/74/74	0/4/4/4
31	PEB	XJ	202	3	-	11/24/74/74	0/4/4/4
31	PEB	K7	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	Y7	501	2	-	3/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	V1	201	2,15	-	11/24/74/74	0/4/4/4
31	PEB	B5	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	GF	202	3	-	7/24/74/74	0/4/4/4
31	PEB	R6	203	2	-	9/24/74/74	0/4/4/4
31	PEB	JA	201	3	-	9/24/74/74	0/4/4/4
31	PEB	QK	202	3	-	9/24/74/74	0/4/4/4
31	PEB	Y7	503	2,27	-	11/24/74/74	0/4/4/4
31	PEB	kF	201	3	-	12/24/74/74	0/4/4/4
31	PEB	AF	202	3	-	11/24/74/74	0/4/4/4
31	PEB	RI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	HG	202	2	-	7/24/74/74	0/4/4/4
31	PEB	YK	303	6	-	16/24/74/74	0/4/4/4
31	PEB	M1	201	3	-	10/24/74/74	0/4/4/4
31	PEB	YD	201	2	-	10/24/74/74	0/4/4/4
33	CYC	k3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	GJ	202	2	-	13/24/74/74	0/4/4/4
31	PEB	TA	202	3	-	9/24/74/74	0/4/4/4
31	PEB	fD	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	JK	202	2	-	10/24/74/74	0/4/4/4
31	PEB	dC	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	lC	202	3	-	13/24/74/74	0/4/4/4
31	PEB	l8	202	2	-	13/24/74/74	0/4/4/4
31	PEB	J1	201	2,6	-	3/24/74/74	0/4/4/4
31	PEB	WH	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	b2	201	3	-	10/24/74/74	0/4/4/4
31	PEB	RC	202	2	-	12/24/74/74	0/4/4/4
31	PEB	QB	201	3	-	8/24/74/74	0/4/4/4
31	PEB	VF	202	2	-	13/24/74/74	0/4/4/4
31	PEB	I1	202	3	-	12/24/74/74	0/4/4/4
31	PEB	C8	201	3	-	6/24/74/74	0/4/4/4
31	PEB	Z9	302	14	-	9/24/74/74	0/4/4/4
31	PEB	KJ	202	2	-	13/24/74/74	0/4/4/4
31	PEB	HA	203	2	-	12/24/74/74	0/4/4/4
31	PEB	fD	201	3	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	T4	201	2	-	6/24/74/74	0/4/4/4
31	PEB	HI	202	2	-	8/24/74/74	0/4/4/4
31	PEB	H8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	bA	201	2	-	10/24/74/74	0/4/4/4
33	CYC	K3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	CG	202	3	-	10/24/74/74	0/4/4/4
32	PUB	KK	203	6,3	-	6/24/74/74	0/4/4/4
31	PEB	ZC	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	f8	202	2	-	11/24/74/74	0/4/4/4
31	PEB	iB	202	2	-	8/24/74/74	0/4/4/4
31	PEB	aE	202	2	-	13/24/74/74	0/4/4/4
31	PEB	PJ	203	3	-	12/24/74/74	0/4/4/4
31	PEB	GK	202	3	-	13/24/74/74	0/4/4/4
31	PEB	u8	202	3	-	8/24/74/74	0/4/4/4
31	PEB	wF	301	12	-	11/24/74/74	0/4/4/4
31	PEB	kH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	S1	202	3	-	8/24/74/74	0/4/4/4
31	PEB	M8	201	3	-	6/24/74/74	0/4/4/4
31	PEB	VJ	202	3	-	12/24/74/74	0/4/4/4
32	PUB	y8	303	13	-	5/24/74/74	0/4/4/4
31	PEB	oF	202	3	-	9/24/74/74	0/4/4/4
31	PEB	YH	202	3	-	5/24/74/74	0/4/4/4
31	PEB	ZD	201	3	-	9/24/74/74	0/4/4/4
31	PEB	i2	201	2	-	8/24/74/74	0/4/4/4
31	PEB	VF	201	2	-	10/24/74/74	0/4/4/4
31	PEB	GA	202	2	-	9/24/74/74	0/4/4/4
31	PEB	M4	203	3	-	10/24/74/74	0/4/4/4
31	PEB	YF	202	3	-	10/24/74/74	0/4/4/4
31	PEB	QF	202	3	-	7/24/74/74	0/4/4/4
31	PEB	UH	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	FH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	DG	202	2	-	7/24/74/74	0/4/4/4
31	PEB	Y2	202	2	-	8/24/74/74	0/4/4/4
33	CYC	r3	1001	19	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	P1	202	2	-	7/24/74/74	0/4/4/4
31	PEB	TJ	202	3	-	9/24/74/74	0/4/4/4
31	PEB	KF	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	Q2	203	3	-	9/24/74/74	0/4/4/4
31	PEB	YF	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	P8	202	2	-	12/24/74/74	0/4/4/4
31	PEB	R6	201	2,10	-	2/24/74/74	0/4/4/4
31	PEB	AE	304	6	-	4/24/74/74	0/4/4/4
31	PEB	jE	201	3	-	9/24/74/74	0/4/4/4
31	PEB	DK	203	2	-	11/24/74/74	0/4/4/4
31	PEB	IJ	201	2	-	7/24/74/74	0/4/4/4
33	CYC	DD	1001	9	-	11/25/74/74	0/4/4/4
33	CYC	x3	1001	-	-	10/25/74/74	0/4/4/4
31	PEB	Y1	302	31,6	-	13/24/74/74	0/4/4/4
31	PEB	UB	202	3	-	10/24/74/74	0/4/4/4
31	PEB	E1	201	3	-	7/24/74/74	0/4/4/4
31	PEB	s8	202	3	-	9/24/74/74	0/4/4/4
31	PEB	kC	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	K4	202	3	-	14/24/74/74	0/4/4/4
31	PEB	KA	304	2,4	-	8/24/74/74	0/4/4/4
31	PEB	EI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	eF	202	3	-	8/24/74/74	0/4/4/4
31	PEB	GI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	M7	201	3	-	4/24/74/74	0/4/4/4
31	PEB	cF	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	FA	201	2,4	-	12/24/74/74	0/4/4/4
31	PEB	LI	203	2	-	7/24/74/74	0/4/4/4
31	PEB	cD	201	2	-	5/24/74/74	0/4/4/4
31	PEB	CG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	IG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	VA	202	2,3	-	10/24/74/74	0/4/4/4
31	PEB	AC	301	6	-	7/24/74/74	0/4/4/4
31	PEB	K4	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	QC	203	3	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	T5	202	3	-	9/24/74/74	0/4/4/4
31	PEB	T9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	QE	202	3	-	9/24/74/74	0/4/4/4
31	PEB	Q8	201	3	-	8/24/74/74	0/4/4/4
31	PEB	DG	201	2,11	-	11/24/74/74	0/4/4/4
31	PEB	XG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	P7	201	2	-	6/24/74/74	0/4/4/4
31	PEB	A7	203	2,3	-	11/24/74/74	0/4/4/4
31	PEB	JF	202	2	-	13/24/74/74	0/4/4/4
31	PEB	iE	202	2	-	10/24/74/74	0/4/4/4
31	PEB	GG	203	3	-	10/24/74/74	0/4/4/4
31	PEB	eB	203	2	-	8/24/74/74	0/4/4/4
31	PEB	DA	201	2	-	7/24/74/74	0/4/4/4
31	PEB	h4	203	3	-	13/24/74/74	0/4/4/4
31	PEB	D2	1002	9	-	11/24/74/74	0/4/4/4
31	PEB	V5	201	3	-	12/24/74/74	0/4/4/4
31	PEB	L5	202	3	-	9/24/74/74	0/4/4/4
31	PEB	v8	201	2	-	9/24/74/74	0/4/4/4
32	PUB	NJ	201	6,3	-	3/24/74/74	0/4/4/4
31	PEB	VH	202	2	-	8/24/74/74	0/4/4/4
31	PEB	KK	202	3	-	10/24/74/74	0/4/4/4
31	PEB	WH	201	3	-	5/24/74/74	0/4/4/4
31	PEB	U9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	AE	301	6	-	10/24/74/74	0/4/4/4
31	PEB	R7	202	2	-	7/24/74/74	0/4/4/4
31	PEB	R5	202	3	-	10/24/74/74	0/4/4/4
31	PEB	MI	301	2,14	-	6/24/74/74	0/4/4/4
31	PEB	WG	202	2,3	-	9/24/74/74	0/4/4/4
31	PEB	bD	201	3	-	10/24/74/74	0/4/4/4
31	PEB	R4	202	2	-	11/24/74/74	0/4/4/4
31	PEB	UE	201	2,3	-	5/24/74/74	0/4/4/4
31	PEB	NG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	A7	201	3	-	4/24/74/74	0/4/4/4
33	CYC	H3	1001	24,20	-	4/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	MA	202	2	-	9/24/74/74	0/4/4/4
33	CYC	v3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	GH	202	3	-	7/24/74/74	0/4/4/4
31	PEB	KG	203	3	-	10/24/74/74	0/4/4/4
31	PEB	VB	201	2	-	4/24/74/74	0/4/4/4
31	PEB	YE	202	2	-	12/24/74/74	0/4/4/4
31	PEB	U9	201	2,14	-	11/24/74/74	0/4/4/4
31	PEB	HH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	E7	201	3	-	7/24/74/74	0/4/4/4
31	PEB	l4	202	3	-	6/24/74/74	0/4/4/4
31	PEB	N9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	fF	201	2,12	-	11/24/74/74	0/4/4/4
31	PEB	G7	202	3	-	4/24/74/74	0/4/4/4
31	PEB	OD	201	3	-	9/24/74/74	0/4/4/4
31	PEB	Z4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	g2	202	2	-	6/24/74/74	0/4/4/4
31	PEB	gE	202	2	-	11/24/74/74	0/4/4/4
31	PEB	f8	201	2,12	-	11/24/74/74	0/4/4/4
33	CYC	K6	1001	8	-	7/25/74/74	0/4/4/4
31	PEB	YG	201	2,11	-	10/24/74/74	0/4/4/4
31	PEB	YC	202	2	-	8/24/74/74	0/4/4/4
33	CYC	MD	1001	8,9	-	7/25/74/74	0/4/4/4
31	PEB	P4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	b6	202	3	-	8/24/74/74	0/4/4/4
31	PEB	GK	201	3	-	6/24/74/74	0/4/4/4
33	CYC	IE	1001	8,9	-	8/25/74/74	0/4/4/4
31	PEB	T8	202	2	-	15/24/74/74	0/4/4/4
31	PEB	i8	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	h6	202	3	-	9/24/74/74	0/4/4/4
31	PEB	CK	201	3	-	9/24/74/74	0/4/4/4
31	PEB	X4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	VK	203	2	-	7/24/74/74	0/4/4/4
33	CYC	F2	1001	9	-	6/25/74/74	0/4/4/4
31	PEB	KG	201	2,3	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	P4	201	2	-	12/24/74/74	0/4/4/4
31	PEB	l4	203	3	-	12/24/74/74	0/4/4/4
31	PEB	P2	201	2,10	-	5/24/74/74	0/4/4/4
31	PEB	M4	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	m8	202	3	-	11/24/74/74	0/4/4/4
31	PEB	SK	201	3	-	6/24/74/74	0/4/4/4
31	PEB	q8	202	3	-	15/24/74/74	0/4/4/4
31	PEB	nF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	OF	202	3	-	9/24/74/74	0/4/4/4
31	PEB	QF	201	3	-	8/24/74/74	0/4/4/4
31	PEB	I5	202	2,26	-	7/24/74/74	0/4/4/4
31	PEB	EF	201	3	-	9/24/74/74	0/4/4/4
31	PEB	T2	202	2	-	15/24/74/74	0/4/4/4
31	PEB	Y2	201	2	-	7/24/74/74	0/4/4/4
31	PEB	VK	201	2,15	-	11/24/74/74	0/4/4/4
31	PEB	DF	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	a4	202	3	-	7/24/74/74	0/4/4/4
31	PEB	o8	202	3	-	9/24/74/74	0/4/4/4
31	PEB	TJ	201	2,3	-	13/24/74/74	0/4/4/4
31	PEB	C4	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	l4	201	2,3	-	8/24/74/74	0/4/4/4
33	CYC	CE	1001	8,9	-	8/25/74/74	0/4/4/4
31	PEB	iC	202	2	-	9/24/74/74	0/4/4/4
31	PEB	l2	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	DI	203	2	-	9/24/74/74	0/4/4/4
31	PEB	P8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	YJ	201	2	-	8/24/74/74	0/4/4/4
31	PEB	DF	202	2	-	12/24/74/74	0/4/4/4
31	PEB	QA	202	2,4	-	9/24/74/74	0/4/4/4
31	PEB	L8	202	2	-	14/24/74/74	0/4/4/4
31	PEB	KA	301	2,4	-	9/24/74/74	0/4/4/4
31	PEB	c8	201	3	-	11/24/74/74	0/4/4/4
32	PUB	AE	302	6	-	9/24/74/74	0/4/4/4
31	PEB	N4	202	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	73	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	YE	201	2	-	10/24/74/74	0/4/4/4
31	PEB	RG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	TK	202	2	-	9/24/74/74	0/4/4/4
31	PEB	TI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	B9	201	2,14,31	-	11/24/74/74	0/4/4/4
33	CYC	j3	1001	24,20	-	4/25/74/74	0/4/4/4
33	CYC	y3	1001	22	-	10/25/74/74	0/4/4/4
31	PEB	UA	302	2,4	-	9/24/74/74	0/4/4/4
31	PEB	ND	201	8,9	-	10/24/74/74	0/4/4/4
31	PEB	BI	201	2	-	12/24/74/74	0/4/4/4
32	PUB	N5	201	6,3	-	3/24/74/74	0/4/4/4
31	PEB	eF	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	O8	202	3	-	9/24/74/74	0/4/4/4
31	PEB	Y9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	eD	203	2	-	13/24/74/74	0/4/4/4
31	PEB	HJ	202	3	-	12/24/74/74	0/4/4/4
31	PEB	R1	202	2	-	10/24/74/74	0/4/4/4
31	PEB	QA	204	2	-	10/24/74/74	0/4/4/4
31	PEB	OE	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	e6	202	2	-	10/24/74/74	0/4/4/4
33	CYC	i3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	HC	1002	9	-	8/24/74/74	0/4/4/4
31	PEB	iF	203	3	-	12/24/74/74	0/4/4/4
33	CYC	BD	1001	9,7	-	12/25/74/74	0/4/4/4
31	PEB	LJ	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	hD	202	3	-	11/24/74/74	0/4/4/4
31	PEB	U2	202	3	-	6/24/74/74	0/4/4/4
33	CYC	NC	1001	9,7	-	8/25/74/74	0/4/4/4
33	CYC	JC	1001	9	-	5/25/74/74	0/4/4/4
31	PEB	RE	202	2	-	11/24/74/74	0/4/4/4
31	PEB	A1	202	3	-	12/24/74/74	0/4/4/4
31	PEB	D9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	XJ	203	3	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	BJ	201	3	-	11/24/74/74	0/4/4/4
31	PEB	hD	203	3	-	7/24/74/74	0/4/4/4
31	PEB	j2	201	3	-	9/24/74/74	0/4/4/4
31	PEB	eE	202	2	-	6/24/74/74	0/4/4/4
31	PEB	UD	202	3	-	9/24/74/74	0/4/4/4
31	PEB	bB	202	3	-	8/24/74/74	0/4/4/4
33	CYC	D2	1001	9	-	6/25/74/74	0/4/4/4
31	PEB	DJ	203	3	-	10/24/74/74	0/4/4/4
31	PEB	k2	201	2	-	8/24/74/74	0/4/4/4
31	PEB	SC	201	3	-	5/24/74/74	0/4/4/4
31	PEB	C7	203	3	-	9/24/74/74	0/4/4/4
31	PEB	V5	203	2,3	-	14/24/74/74	0/4/4/4
33	CYC	DE	1001	9	-	11/25/74/74	0/4/4/4
31	PEB	UA	301	2,4	-	9/24/74/74	0/4/4/4
31	PEB	dB	201	3	-	8/24/74/74	0/4/4/4
31	PEB	mB	202	2	-	8/24/74/74	0/4/4/4
31	PEB	N6	1002	9	-	8/24/74/74	0/4/4/4
31	PEB	IF	202	3	-	14/24/74/74	0/4/4/4
31	PEB	S7	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	gH	201	2	-	9/24/74/74	0/4/4/4
31	PEB	LI	201	2	-	10/24/74/74	0/4/4/4
31	PEB	E7	203	2,3	-	11/24/74/74	0/4/4/4
31	PEB	a2	202	2	-	10/24/74/74	0/4/4/4
31	PEB	JJ	202	3	-	14/24/74/74	0/4/4/4
31	PEB	H9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	K4	201	3	-	8/24/74/74	0/4/4/4
31	PEB	DH	201	2	-	11/24/74/74	0/4/4/4
31	PEB	J5	203	3	-	12/24/74/74	0/4/4/4
31	PEB	K1	201	3	-	7/24/74/74	0/4/4/4
31	PEB	D8	202	2	-	12/24/74/74	0/4/4/4
31	PEB	E4	203	3	-	11/24/74/74	0/4/4/4
31	PEB	W4	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	I8	202	3	-	14/24/74/74	0/4/4/4
33	CYC	L3	1001	20	-	4/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	MK	202	3	-	13/24/74/74	0/4/4/4
33	CYC	F3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	F5	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	j8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	O4	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	AI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	JI	202	2	-	8/24/74/74	0/4/4/4
31	PEB	Q9	201	2,14	-	8/24/74/74	0/4/4/4
31	PEB	Y4	202	3	-	8/24/74/74	0/4/4/4
31	PEB	H9	201	2,14	-	11/24/74/74	0/4/4/4
31	PEB	XF	201	2	-	10/24/74/74	0/4/4/4
31	PEB	E5	202	2,26	-	12/24/74/74	0/4/4/4
31	PEB	Y6	201	2	-	2/24/74/74	0/4/4/4
32	PUB	yF	303	13	-	5/24/74/74	0/4/4/4
31	PEB	JF	201	2	-	8/24/74/74	0/4/4/4
31	PEB	SI	202	2	-	7/24/74/74	0/4/4/4
31	PEB	mE	203	2	-	8/24/74/74	0/4/4/4
33	CYC	Q3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	II	202	3	-	15/24/74/74	0/4/4/4
31	PEB	FG	202	2	-	8/24/74/74	0/4/4/4
31	PEB	hE	203	3	-	7/24/74/74	0/4/4/4
31	PEB	f4	202	3	-	11/24/74/74	0/4/4/4
31	PEB	AB	304	6	-	9/24/74/74	0/4/4/4
31	PEB	GF	203	3	-	9/24/74/74	0/4/4/4
31	PEB	Q5	201	2,6	-	2/24/74/74	0/4/4/4
33	CYC	U3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	VC	201	2	-	2/24/74/74	0/4/4/4
31	PEB	WJ	202	2,6	-	4/24/74/74	0/4/4/4
31	PEB	UG	201	2	-	7/24/74/74	0/4/4/4
31	PEB	KH	202	3	-	15/24/74/74	0/4/4/4
31	PEB	b7	501	2	-	9/24/74/74	0/4/4/4
31	PEB	kE	201	2	-	13/24/74/74	0/4/4/4
31	PEB	L8	201	2	-	9/24/74/74	0/4/4/4
31	PEB	R6	202	2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	T6	203	2	-	11/24/74/74	0/4/4/4
31	PEB	rF	201	2,12	-	11/24/74/74	0/4/4/4
31	PEB	QD	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	hH	202	3	-	6/24/74/74	0/4/4/4
31	PEB	TG	203	3	-	10/24/74/74	0/4/4/4
31	PEB	hE	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	eF	203	3	-	9/24/74/74	0/4/4/4
31	PEB	FF	201	2	-	5/24/74/74	0/4/4/4
33	CYC	C2	1001	8,9	-	9/25/74/74	0/4/4/4
31	PEB	UE	202	3	-	9/24/74/74	0/4/4/4
31	PEB	lF	202	2	-	13/24/74/74	0/4/4/4
31	PEB	NJ	202	3	-	11/24/74/74	0/4/4/4
31	PEB	X9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	NH	201	2	-	9/24/74/74	0/4/4/4
33	CYC	p3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	d8	201	2	-	10/24/74/74	0/4/4/4
31	PEB	Z4	201	2	-	10/24/74/74	0/4/4/4
31	PEB	T6	201	2	-	5/24/74/74	0/4/4/4
31	PEB	P6	201	2	-	5/24/74/74	0/4/4/4
31	PEB	RI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	cC	202	2	-	11/24/74/74	0/4/4/4
31	PEB	W7	202	3	-	4/24/74/74	0/4/4/4
31	PEB	UI	204	2,3	-	9/24/74/74	0/4/4/4
31	PEB	d2	203	3	-	10/24/74/74	0/4/4/4
31	PEB	EI	202	3	-	15/24/74/74	0/4/4/4
32	PUB	wF	304	12	-	7/24/74/74	0/4/4/4
31	PEB	yF	301	13	-	8/24/74/74	0/4/4/4
31	PEB	X4	201	2	-	9/24/74/74	0/4/4/4
31	PEB	ZI	303	14	-	11/24/74/74	0/4/4/4
31	PEB	TH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	AB	301	6	-	7/24/74/74	0/4/4/4
31	PEB	Z9	301	14,31	-	8/24/74/74	0/4/4/4
31	PEB	RE	201	2	-	8/24/74/74	0/4/4/4
31	PEB	Q4	201	2,3	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	DJ	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	DA	202	2	-	9/24/74/74	0/4/4/4
31	PEB	L1	202	2	-	9/24/74/74	0/4/4/4
31	PEB	S2	201	3	-	5/24/74/74	0/4/4/4
33	CYC	E3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	U1	202	3	-	11/24/74/74	0/4/4/4
31	PEB	QD	203	3	-	10/24/74/74	0/4/4/4
31	PEB	K8	203	3	-	8/24/74/74	0/4/4/4
31	PEB	Y9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	e2	202	2	-	11/24/74/74	0/4/4/4
31	PEB	UA	304	2,4	-	13/24/74/74	0/4/4/4
31	PEB	fB	202	3	-	10/24/74/74	0/4/4/4
31	PEB	O2	202	3	-	7/24/74/74	0/4/4/4
31	PEB	gA	201	2	-	11/24/74/74	0/4/4/4
33	CYC	t3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	kB	202	2	-	13/24/74/74	0/4/4/4
31	PEB	JG	202	2	-	9/24/74/74	0/4/4/4
31	PEB	I4	202	3	-	7/24/74/74	0/4/4/4
33	CYC	I6	1001	8	-	9/25/74/74	0/4/4/4
31	PEB	GA	203	2	-	12/24/74/74	0/4/4/4
31	PEB	D1	202	2	-	14/24/74/74	0/4/4/4
31	PEB	SK	202	3	-	8/24/74/74	0/4/4/4
31	PEB	BK	201	2,31	-	8/24/74/74	0/4/4/4
31	PEB	RC	201	2	-	7/24/74/74	0/4/4/4
31	PEB	EH	202	3	-	5/24/74/74	0/4/4/4
31	PEB	A4	301	12	-	11/24/74/74	0/4/4/4
31	PEB	OH	202	3	-	15/24/74/74	0/4/4/4
31	PEB	IF	201	3	-	9/24/74/74	0/4/4/4
31	PEB	fC	202	3	-	9/24/74/74	0/4/4/4
31	PEB	b8	201	2	-	4/24/74/74	0/4/4/4
31	PEB	R9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	SD	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	dD	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	SF	201	2,3	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	N6	1001	9	-	11/25/74/74	0/4/4/4
31	PEB	TF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	P1	203	2	-	7/24/74/74	0/4/4/4
31	PEB	TJ	203	3	-	13/24/74/74	0/4/4/4
33	CYC	GB	1001	8	-	6/25/74/74	0/4/4/4
31	PEB	AJ	302	6	-	10/24/74/74	0/4/4/4
33	CYC	g3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	EG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	E9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	Q8	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	BG	203	2	-	8/24/74/74	0/4/4/4
33	CYC	S3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	g4	202	2	-	10/24/74/74	0/4/4/4
31	PEB	aH	204	2,3	-	5/24/74/74	0/4/4/4
31	PEB	OE	201	3	-	9/24/74/74	0/4/4/4
31	PEB	eB	201	2	-	5/24/74/74	0/4/4/4
33	CYC	NB	1001	9	-	11/25/74/74	0/4/4/4
31	PEB	XH	201	2	-	5/24/74/74	0/4/4/4
31	PEB	XA	201	2	-	8/24/74/74	0/4/4/4
31	PEB	c8	202	3	-	13/24/74/74	0/4/4/4
31	PEB	I8	201	3	-	9/24/74/74	0/4/4/4
33	CYC	d3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	S9	201	2,14	-	11/24/74/74	0/4/4/4
31	PEB	O6	202	3	-	6/24/74/74	0/4/4/4
31	PEB	A2	302	6	-	11/24/74/74	0/4/4/4
31	PEB	JH	202	2	-	8/24/74/74	0/4/4/4
31	PEB	R1	201	2	-	5/24/74/74	0/4/4/4
31	PEB	OB	201	3	-	9/24/74/74	0/4/4/4
31	PEB	X8	202	2	-	5/24/74/74	0/4/4/4
31	PEB	C5	201	2	-	7/24/74/74	0/4/4/4
31	PEB	G7	203	3	-	9/24/74/74	0/4/4/4
33	CYC	ID	1001	8,9	-	8/25/74/74	0/4/4/4
31	PEB	AI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	iH	202	2,12	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	J2	1001	9	-	4/25/74/74	0/4/4/4
31	PEB	hD	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	M5	201	2	-	7/24/74/74	0/4/4/4
31	PEB	TK	203	2	-	7/24/74/74	0/4/4/4
31	PEB	kC	201	2	-	8/24/74/74	0/4/4/4
31	PEB	FJ	201	3	-	13/24/74/74	0/4/4/4
31	PEB	T5	203	3	-	13/24/74/74	0/4/4/4
31	PEB	O1	202	3	-	11/24/74/74	0/4/4/4
33	CYC	FD	202	8,9	-	8/25/74/74	0/4/4/4
31	PEB	QE	203	3	-	10/24/74/74	0/4/4/4
33	CYC	FC	1001	9	-	6/25/74/74	0/4/4/4
31	PEB	iD	201	2	-	10/24/74/74	0/4/4/4
31	PEB	WB	201	3	-	7/24/74/74	0/4/4/4
31	PEB	N5	202	3	-	11/24/74/74	0/4/4/4
31	PEB	O9	203	2	-	14/24/74/74	0/4/4/4
31	PEB	RH	201	2	-	5/24/74/74	0/4/4/4
31	PEB	J9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	h2	202	3	-	11/24/74/74	0/4/4/4
31	PEB	b7	503	2,27	-	9/24/74/74	0/4/4/4
31	PEB	JC	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	OC	202	3	-	7/24/74/74	0/4/4/4
31	PEB	WJ	201	2	-	8/24/74/74	0/4/4/4
33	CYC	EE	1001	8,9	-	6/25/74/74	0/4/4/4
31	PEB	M4	202	3	-	7/24/74/74	0/4/4/4
31	PEB	YK	302	31,6	-	13/24/74/74	0/4/4/4
31	PEB	Z9	303	14	-	13/24/74/74	0/4/4/4
31	PEB	o8	203	3	-	17/24/74/74	0/4/4/4
31	PEB	f2	202	3	-	9/24/74/74	0/4/4/4
31	PEB	N5	204	2,3	-	12/24/74/74	0/4/4/4
31	PEB	VD	202	2	-	10/24/74/74	0/4/4/4
31	PEB	fE	201	3	-	10/24/74/74	0/4/4/4
31	PEB	A5	302	6	-	10/24/74/74	0/4/4/4
31	PEB	H5	203	3	-	12/24/74/74	0/4/4/4
32	PUB	Y1	304	6	-	3/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	O9	201	2,14,31	-	9/24/74/74	0/4/4/4
31	PEB	IF	201	2	-	11/24/74/74	0/4/4/4
31	PEB	SE	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	YB	201	2	-	2/24/74/74	0/4/4/4
31	PEB	WI	202	2	-	11/24/74/74	0/4/4/4
31	PEB	YB	202	2	-	6/24/74/74	0/4/4/4
31	PEB	GH	203	2,3	-	8/24/74/74	0/4/4/4
32	PUB	MI	303	14	-	7/24/74/74	0/4/4/4
31	PEB	i6	201	2	-	6/24/74/74	0/4/4/4
31	PEB	YH	203	3	-	9/24/74/74	0/4/4/4
31	PEB	S4	202	3	-	12/24/74/74	0/4/4/4
31	PEB	HF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	HG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	WE	201	3	-	7/24/74/74	0/4/4/4
31	PEB	X5	202	3	-	11/24/74/74	0/4/4/4
33	CYC	KD	202	-	-	13/25/74/74	0/4/4/4
31	PEB	V2	202	2	-	9/24/74/74	0/4/4/4
31	PEB	Y9	201	2,14	-	10/24/74/74	0/4/4/4
31	PEB	z8	501	2,28	-	6/24/74/74	0/4/4/4
31	PEB	E5	201	2	-	7/24/74/74	0/4/4/4
31	PEB	MA	201	2	-	3/24/74/74	0/4/4/4
31	PEB	d5	401	2,26	-	11/24/74/74	0/4/4/4
31	PEB	YA	201	2	-	8/24/74/74	0/4/4/4
31	PEB	kD	201	2	-	11/24/74/74	0/4/4/4
31	PEB	VJ	201	3	-	12/24/74/74	0/4/4/4
31	PEB	D4	202	2,13	-	10/24/74/74	0/4/4/4
31	PEB	LJ	203	3	-	11/24/74/74	0/4/4/4
31	PEB	SE	203	-	-	10/24/74/74	0/4/4/4
31	PEB	Q4	203	3	-	9/24/74/74	0/4/4/4
31	PEB	N8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	n8	202	2	-	11/24/74/74	0/4/4/4
33	CYC	E2	1001	8,9	-	7/25/74/74	0/4/4/4
31	PEB	SG	201	2	-	12/24/74/74	0/4/4/4
31	PEB	eD	202	2	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	IH	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	OC	201	3	-	11/24/74/74	0/4/4/4
31	PEB	ZA	202	2	-	10/24/74/74	0/4/4/4
31	PEB	MH	202	3	-	4/24/74/74	0/4/4/4
31	PEB	LJ	202	3	-	9/24/74/74	0/4/4/4
31	PEB	IC	201	3	-	10/24/74/74	0/4/4/4
31	PEB	q8	203	3	-	10/24/74/74	0/4/4/4
31	PEB	X1	201	2,15	-	5/24/74/74	0/4/4/4
31	PEB	H1	202	2	-	8/24/74/74	0/4/4/4
31	PEB	BG	201	2	-	9/24/74/74	0/4/4/4
31	PEB	OF	203	3	-	10/24/74/74	0/4/4/4
33	CYC	c3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	RK	202	2	-	10/24/74/74	0/4/4/4
31	PEB	VD	201	2	-	8/24/74/74	0/4/4/4
32	PUB	AD	302	6	-	9/24/74/74	0/4/4/4
31	PEB	a4	203	3	-	15/24/74/74	0/4/4/4
31	PEB	F2	1002	9	-	11/24/74/74	0/4/4/4
33	CYC	IB	1001	8	-	9/25/74/74	0/4/4/4
31	PEB	H7	201	2,27	-	6/24/74/74	0/4/4/4
31	PEB	E1	202	3	-	11/24/74/74	0/4/4/4
31	PEB	L1	203	2	-	9/24/74/74	0/4/4/4
32	PUB	K1	203	6,3	-	6/24/74/74	0/4/4/4
31	PEB	OJ	202	2	-	14/24/74/74	0/4/4/4
31	PEB	B7	201	2	-	8/24/74/74	0/4/4/4
31	PEB	UG	202	2	-	7/24/74/74	0/4/4/4
31	PEB	IF	203	2,3	-	4/24/74/74	0/4/4/4
32	PUB	M9	304	14,3	-	8/24/74/74	0/4/4/4
31	PEB	V8	202	2	-	13/24/74/74	0/4/4/4
31	PEB	W5	202	2,6	-	4/24/74/74	0/4/4/4
31	PEB	cH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	hH	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	M9	303	14	-	13/24/74/74	0/4/4/4
32	PUB	AB	303	6	-	7/24/74/74	0/4/4/4
31	PEB	a8	203	3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	X8	201	2	-	9/24/74/74	0/4/4/4
31	PEB	wF	302	12	-	9/24/74/74	0/4/4/4
31	PEB	ZB	202	3	-	9/24/74/74	0/4/4/4
31	PEB	V9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	g8	201	3	-	6/24/74/74	0/4/4/4
31	PEB	CI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	T1	203	2	-	7/24/74/74	0/4/4/4
31	PEB	gD	202	2	-	11/24/74/74	0/4/4/4
31	PEB	DF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	H1	203	2	-	12/24/74/74	0/4/4/4
31	PEB	RA	201	2,5	-	6/24/74/74	0/4/4/4
31	PEB	v8	202	2	-	9/24/74/74	0/4/4/4
31	PEB	PJ	202	3	-	10/24/74/74	0/4/4/4
31	PEB	RG	202	3	-	10/24/74/74	0/4/4/4
33	CYC	H2	1001	9	-	7/25/74/74	0/4/4/4
31	PEB	kB	201	2	-	8/24/74/74	0/4/4/4
31	PEB	JG	201	2	-	8/24/74/74	0/4/4/4
31	PEB	b7	502	2	-	4/24/74/74	0/4/4/4
31	PEB	hB	201	3	-	10/24/74/74	0/4/4/4
31	PEB	SI	201	2,14	-	13/24/74/74	0/4/4/4
31	PEB	OI	202	2	-	11/24/74/74	0/4/4/4
33	CYC	GD	201	8,9	-	7/25/74/74	0/4/4/4
32	PUB	AH	304	12	-	9/24/74/74	0/4/4/4
31	PEB	U5	201	2,6	-	9/24/74/74	0/4/4/4
31	PEB	FG	201	2	-	12/24/74/74	0/4/4/4
31	PEB	W8	202	3	-	8/24/74/74	0/4/4/4
31	PEB	fH	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	C7	202	3	-	6/24/74/74	0/4/4/4
31	PEB	KH	201	3	-	5/24/74/74	0/4/4/4
31	PEB	O5	202	2	-	14/24/74/74	0/4/4/4
31	PEB	P5	203	3	-	12/24/74/74	0/4/4/4
31	PEB	GF	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	G7	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	BK	202	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	fE	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	CA	202	2,1	-	3/24/74/74	0/4/4/4
31	PEB	k8	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	JJ	203	3	-	12/24/74/74	0/4/4/4
31	PEB	lF	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	O7	202	3	-	4/24/74/74	0/4/4/4
31	PEB	R2	201	2	-	7/24/74/74	0/4/4/4
31	PEB	VE	201	2	-	8/24/74/74	0/4/4/4
31	PEB	fH	201	3	-	5/24/74/74	0/4/4/4
31	PEB	UI	202	2	-	10/24/74/74	0/4/4/4
31	PEB	iE	201	2	-	10/24/74/74	0/4/4/4
31	PEB	R1	203	2	-	11/24/74/74	0/4/4/4
31	PEB	VI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	S5	202	2	-	9/24/74/74	0/4/4/4
31	PEB	MF	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	L5	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	BH	301	13	-	8/24/74/74	0/4/4/4
31	PEB	IK	202	3	-	12/24/74/74	0/4/4/4
31	PEB	m8	201	3	-	6/24/74/74	0/4/4/4
31	PEB	lE	202	3	-	14/24/74/74	0/4/4/4
33	CYC	J6	1001	9	-	9/25/74/74	0/4/4/4
31	PEB	J5	201	2,3	-	14/24/74/74	0/4/4/4
31	PEB	A5	304	6,31	-	11/24/74/74	0/4/4/4
31	PEB	MF	202	3	-	10/24/74/74	0/4/4/4
31	PEB	I7	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	E4	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	j8	202	2	-	12/24/74/74	0/4/4/4
31	PEB	U6	201	3	-	8/24/74/74	0/4/4/4
31	PEB	eE	201	2	-	9/24/74/74	0/4/4/4
31	PEB	FI	203	2	-	11/24/74/74	0/4/4/4
31	PEB	AJ	304	6,31	-	11/24/74/74	0/4/4/4
31	PEB	a4	201	3,12	-	10/24/74/74	0/4/4/4
32	PUB	w8	304	12	-	7/24/74/74	0/4/4/4
31	PEB	g6	201	2	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	VG	201	3	-	8/24/74/74	0/4/4/4
32	PUB	AE	303	6	-	8/24/74/74	0/4/4/4
31	PEB	VJ	203	2,3	-	14/24/74/74	0/4/4/4
31	PEB	XI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	c6	202	2	-	11/24/74/74	0/4/4/4
32	PUB	xF	306	12	-	6/24/74/74	0/4/4/4
31	PEB	jB	202	3	-	8/24/74/74	0/4/4/4
31	PEB	B8	202	2	-	13/24/74/74	0/4/4/4
31	PEB	f4	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	C4	201	3	-	7/24/74/74	0/4/4/4
31	PEB	gF	201	3	-	6/24/74/74	0/4/4/4
31	PEB	P6	203	2	-	6/24/74/74	0/4/4/4
31	PEB	oF	201	3	-	13/24/74/74	0/4/4/4
31	PEB	iD	202	2	-	10/24/74/74	0/4/4/4
33	CYC	W3	1001	22	-	10/25/74/74	0/4/4/4
31	PEB	tF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	OJ	201	2,6,31	-	8/24/74/74	0/4/4/4
33	CYC	w3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	F7	202	2	-	7/24/74/74	0/4/4/4
31	PEB	O4	202	3	-	7/24/74/74	0/4/4/4
31	PEB	a8	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	W9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	K8	202	3	-	4/24/74/74	0/4/4/4
31	PEB	M9	302	14	-	9/24/74/74	0/4/4/4
31	PEB	vF	202	2	-	9/24/74/74	0/4/4/4
31	PEB	mE	201	2	-	6/24/74/74	0/4/4/4
33	CYC	JC	1003	8,9	-	9/25/74/74	0/4/4/4
31	PEB	S1	201	3	-	6/24/74/74	0/4/4/4
31	PEB	EK	201	3	-	7/24/74/74	0/4/4/4
31	PEB	dE	203	3	-	8/24/74/74	0/4/4/4
31	PEB	RJ	203	2,3	-	10/24/74/74	0/4/4/4
32	PUB	xF	305	12	-	8/24/74/74	0/4/4/4
31	PEB	VI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	C9	201	3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	G9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	R8	202	2	-	13/24/74/74	0/4/4/4
31	PEB	J7	201	2	-	6/24/74/74	0/4/4/4
31	PEB	cA	403	5,2	-	6/24/74/74	0/4/4/4
31	PEB	cB	203	2	-	12/24/74/74	0/4/4/4
31	PEB	S4	201	3	-	10/24/74/74	0/4/4/4
31	PEB	L9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	KI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	F1	203	2	-	11/24/74/74	0/4/4/4
31	PEB	CA	201	2	-	9/24/74/74	0/4/4/4
31	PEB	mD	202	2	-	7/24/74/74	0/4/4/4
31	PEB	C8	202	3	-	6/24/74/74	0/4/4/4
31	PEB	G8	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	UE	203	3	-	13/24/74/74	0/4/4/4
31	PEB	h6	201	3	-	10/24/74/74	0/4/4/4
31	PEB	LE	1002	8,9	-	10/24/74/74	0/4/4/4
31	PEB	B4	301	13	-	12/24/74/74	0/4/4/4
31	PEB	j4	202	3	-	15/24/74/74	0/4/4/4
31	PEB	UF	201	3	-	8/24/74/74	0/4/4/4
31	PEB	RD	202	2	-	11/24/74/74	0/4/4/4
31	PEB	d4	203	3	-	13/24/74/74	0/4/4/4
31	PEB	YI	202	2	-	7/24/74/74	0/4/4/4
31	PEB	IH	203	3	-	9/24/74/74	0/4/4/4
31	PEB	I8	203	2,3	-	4/24/74/74	0/4/4/4
31	PEB	LD	1002	8,9	-	10/24/74/74	0/4/4/4
32	PUB	x8	305	12	-	8/24/74/74	0/4/4/4
31	PEB	dE	204	3	-	13/24/74/74	0/4/4/4
31	PEB	l6	201	3	-	8/24/74/74	0/4/4/4
31	PEB	W1	202	3	-	12/24/74/74	0/4/4/4
33	CYC	KB	1001	8	-	7/25/74/74	0/4/4/4
31	PEB	A1	201	3	-	11/24/74/74	0/4/4/4
31	PEB	JH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	d4	202	3	-	9/24/74/74	0/4/4/4
33	CYC	J3	1001	19	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	j2	202	3	-	8/24/74/74	0/4/4/4
31	PEB	jC	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	WD	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	Y8	201	3	-	7/24/74/74	0/4/4/4
31	PEB	IA	202	2	-	8/24/74/74	0/4/4/4
31	PEB	B9	202	2	-	9/24/74/74	0/4/4/4
33	CYC	KE	202	8,9	-	9/25/74/74	0/4/4/4
31	PEB	OB	202	3	-	6/24/74/74	0/4/4/4
31	PEB	NJ	204	2,3	-	12/24/74/74	0/4/4/4
31	PEB	mF	202	3	-	11/24/74/74	0/4/4/4
31	PEB	W2	201	3	-	8/24/74/74	0/4/4/4
31	PEB	T2	201	2,10	-	9/24/74/74	0/4/4/4
32	PUB	xF	301	12	-	7/24/74/74	0/4/4/4
31	PEB	JB	1002	9	-	12/24/74/74	0/4/4/4
31	PEB	ZA	201	2	-	10/24/74/74	0/4/4/4
31	PEB	MH	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	aB	203	2	-	12/24/74/74	0/4/4/4
31	PEB	HJ	203	3	-	12/24/74/74	0/4/4/4
31	PEB	j6	202	3	-	8/24/74/74	0/4/4/4
31	PEB	FC	1002	9	-	11/24/74/74	0/4/4/4
31	PEB	C8	203	3	-	11/24/74/74	0/4/4/4
31	PEB	S7	202	3	-	4/24/74/74	0/4/4/4
31	PEB	kB	203	2	-	12/24/74/74	0/4/4/4
31	PEB	F7	201	2,27	-	6/24/74/74	0/4/4/4
31	PEB	jC	201	3	-	9/24/74/74	0/4/4/4
31	PEB	f2	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	D1	203	2	-	11/24/74/74	0/4/4/4
31	PEB	A2	305	6	-	12/24/74/74	0/4/4/4
31	PEB	JE	201	8	-	9/24/74/74	0/4/4/4
31	PEB	G1	201	3	-	6/24/74/74	0/4/4/4
31	PEB	V6	202	2	-	12/24/74/74	0/4/4/4
31	PEB	S6	201	3	-	10/24/74/74	0/4/4/4
31	PEB	UJ	201	2,6	-	9/24/74/74	0/4/4/4
31	PEB	WC	202	3	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	RJ	202	3	-	10/24/74/74	0/4/4/4
31	PEB	O7	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	k6	202	2	-	13/24/74/74	0/4/4/4
31	PEB	MI	304	14	-	11/24/74/74	0/4/4/4
31	PEB	BA	202	2	-	7/24/74/74	0/4/4/4
33	CYC	M6	1001	8	-	8/25/74/74	0/4/4/4
31	PEB	TC	202	2	-	15/24/74/74	0/4/4/4
32	PUB	A4	303	12	-	11/24/74/74	0/4/4/4
33	CYC	GE	201	8,9	-	7/25/74/74	0/4/4/4
31	PEB	KE	201	8,9	-	6/24/74/74	0/4/4/4
31	PEB	fA	301	2,29	-	12/24/74/74	0/4/4/4
31	PEB	hH	203	3	-	13/24/74/74	0/4/4/4
31	PEB	UI	201	2,14	-	11/24/74/74	0/4/4/4
31	PEB	B1	202	2	-	8/24/74/74	0/4/4/4
31	PEB	Y4	201	2,3	-	7/24/74/74	0/4/4/4
33	CYC	BE	1001	9,7	-	12/25/74/74	0/4/4/4
31	PEB	pF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	D5	203	3	-	10/24/74/74	0/4/4/4
31	PEB	F9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	X8	203	2	-	11/24/74/74	0/4/4/4
31	PEB	UK	201	3	-	5/24/74/74	0/4/4/4
31	PEB	m2	202	2	-	10/24/74/74	0/4/4/4
31	PEB	bC	202	3	-	9/24/74/74	0/4/4/4
31	PEB	C4	202	3	-	11/24/74/74	0/4/4/4
31	PEB	fC	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	NK	203	2	-	8/24/74/74	0/4/4/4
31	PEB	NG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	UD	201	2,3	-	5/24/74/74	0/4/4/4
31	PEB	BI	203	2	-	9/24/74/74	0/4/4/4
32	PUB	B4	302	13	-	9/24/74/74	0/4/4/4
31	PEB	M7	203	2,3	-	11/24/74/74	0/4/4/4
31	PEB	CH	202	3	-	9/24/74/74	0/4/4/4
31	PEB	gA	202	2	-	8/24/74/74	0/4/4/4
31	PEB	f4	201	3	-	5/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	DK	202	2	-	14/24/74/74	0/4/4/4
31	PEB	Q5	202	2	-	12/24/74/74	0/4/4/4
31	PEB	SH	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	Q8	202	3	-	7/24/74/74	0/4/4/4
31	PEB	hF	202	2	-	9/24/74/74	0/4/4/4
31	PEB	Q7	202	3	-	11/24/74/74	0/4/4/4
31	PEB	D8	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	WE	203	2,3	-	7/24/74/74	0/4/4/4
32	PUB	A6	303	6	-	7/24/74/74	0/4/4/4
31	PEB	CH	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	N5	203	3	-	12/24/74/74	0/4/4/4
31	PEB	RA	202	2	-	10/24/74/74	0/4/4/4
31	PEB	AH	302	12	-	8/24/74/74	0/4/4/4
31	PEB	hA	301	2,29	-	12/24/74/74	0/4/4/4
31	PEB	UI	203	2	-	7/24/74/74	0/4/4/4
31	PEB	Q7	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	QI	202	2	-	7/24/74/74	0/4/4/4
31	PEB	fC	201	3	-	9/24/74/74	0/4/4/4
31	PEB	g6	203	2	-	10/24/74/74	0/4/4/4
31	PEB	OC	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	LI	202	2	-	8/24/74/74	0/4/4/4
31	PEB	kD	202	2,6	-	8/24/74/74	0/4/4/4
31	PEB	T8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	cB	201	2	-	7/24/74/74	0/4/4/4
32	PUB	y8	302	13	-	3/24/74/74	0/4/4/4
31	PEB	JJ	201	2,3	-	14/24/74/74	0/4/4/4
31	PEB	NK	201	2	-	3/24/74/74	0/4/4/4
31	PEB	WF	202	3	-	8/24/74/74	0/4/4/4
31	PEB	Y6	202	2	-	6/24/74/74	0/4/4/4
31	PEB	NI	202	3	-	15/24/74/74	0/4/4/4
33	CYC	f3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	G9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	d6	202	3	-	9/24/74/74	0/4/4/4
31	PEB	D8	201	2	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	m6	201	2	-	9/24/74/74	0/4/4/4
31	PEB	SI	203	2	-	13/24/74/74	0/4/4/4
31	PEB	TB	203	2	-	11/24/74/74	0/4/4/4
33	CYC	N3	1001	19	-	8/25/74/74	0/4/4/4
33	CYC	BD	1002	9,7	-	5/25/74/74	0/4/4/4
31	PEB	IH	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	a6	203	2	-	12/24/74/74	0/4/4/4
33	CYC	D2	1003	8,9	-	10/25/74/74	0/4/4/4
31	PEB	cC	201	2	-	6/24/74/74	0/4/4/4
31	PEB	AG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	J9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	b2	202	3	-	9/24/74/74	0/4/4/4
31	PEB	MJ	202	2	-	10/24/74/74	0/4/4/4
31	PEB	DJ	202	3	-	9/24/74/74	0/4/4/4
31	PEB	jH	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	dF	201	2	-	9/24/74/74	0/4/4/4
31	PEB	H5	201	2,3	-	12/24/74/74	0/4/4/4
31	PEB	rF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	m2	201	2	-	8/24/74/74	0/4/4/4
33	CYC	EB	1001	8	-	8/25/74/74	0/4/4/4
31	PEB	YG	202	2	-	6/24/74/74	0/4/4/4
31	PEB	ZB	201	3	-	7/24/74/74	0/4/4/4
31	PEB	cH	202	2	-	10/24/74/74	0/4/4/4
31	PEB	XJ	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	D5	202	3	-	9/24/74/74	0/4/4/4
31	PEB	OG	202	2,3	-	10/24/74/74	0/4/4/4
33	CYC	LB	1001	9	-	5/25/74/74	0/4/4/4
31	PEB	YF	201	3	-	7/24/74/74	0/4/4/4
31	PEB	U8	201	3	-	8/24/74/74	0/4/4/4
31	PEB	iF	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	iF	202	3	-	13/24/74/74	0/4/4/4
31	PEB	OK	202	3	-	11/24/74/74	0/4/4/4
31	PEB	dC	202	3	-	10/24/74/74	0/4/4/4
33	CYC	HB	1001	9	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	Y6	203	2	-	11/24/74/74	0/4/4/4
31	PEB	t8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	OG	203	2	-	7/24/74/74	0/4/4/4
31	PEB	PD	202	2,10	-	4/24/74/74	0/4/4/4
31	PEB	V1	202	2	-	10/24/74/74	0/4/4/4
31	PEB	B5	202	3	-	10/24/74/74	0/4/4/4
33	CYC	DB	1001	9	-	9/25/74/74	0/4/4/4
31	PEB	mH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	L6	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	AH	301	12	-	12/24/74/74	0/4/4/4
31	PEB	LH	202	2	-	9/24/74/74	0/4/4/4
33	CYC	A3	1001	19	-	8/25/74/74	0/4/4/4
32	PUB	AC	303	6	-	5/24/74/74	0/4/4/4
31	PEB	VG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	F4	201	2,25	-	8/24/74/74	0/4/4/4
33	CYC	I2	201	8,9	-	9/25/74/74	0/4/4/4
31	PEB	KF	202	3	-	4/24/74/74	0/4/4/4
31	PEB	RK	203	2	-	11/24/74/74	0/4/4/4
31	PEB	HK	201	2	-	4/24/74/74	0/4/4/4
31	PEB	eC	202	2	-	11/24/74/74	0/4/4/4
31	PEB	D9	201	2,14	-	6/24/74/74	0/4/4/4
31	PEB	HE	1002	8,9	-	8/24/74/74	0/4/4/4
31	PEB	D1	201	2,6	-	11/24/74/74	0/4/4/4
32	PUB	CI	203	14,3	-	14/24/74/74	0/4/4/4
31	PEB	WC	201	3	-	8/24/74/74	0/4/4/4
33	CYC	R3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	XK	201	2,15	-	5/24/74/74	0/4/4/4
31	PEB	PG	202	3	-	10/24/74/74	0/4/4/4
33	CYC	C6	1001	8	-	9/25/74/74	0/4/4/4
33	CYC	CB	1001	8	-	9/25/74/74	0/4/4/4
31	PEB	U7	201	3	-	4/24/74/74	0/4/4/4
31	PEB	Q4	204	3	-	10/24/74/74	0/4/4/4
33	CYC	FB	1001	9	-	9/25/74/74	0/4/4/4
31	PEB	y8	301	13	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	iH	201	2	-	9/24/74/74	0/4/4/4
31	PEB	OF	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	SA	203	2	-	8/24/74/74	0/4/4/4
31	PEB	M5	202	2	-	10/24/74/74	0/4/4/4
31	PEB	O7	203	3	-	11/24/74/74	0/4/4/4
31	PEB	F5	201	3	-	13/24/74/74	0/4/4/4
31	PEB	pF	201	2	-	10/24/74/74	0/4/4/4
31	PEB	Q6	202	3	-	9/24/74/74	0/4/4/4
31	PEB	k4	201	2	-	8/24/74/74	0/4/4/4
31	PEB	iC	201	2	-	8/24/74/74	0/4/4/4
31	PEB	SH	201	3	-	8/24/74/74	0/4/4/4
31	PEB	ZD	202	2,3	-	8/24/74/74	0/4/4/4
31	PEB	f6	202	3	-	10/24/74/74	0/4/4/4
31	PEB	jF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	ZH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	KH	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	QF	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	OA	201	2,4	-	11/24/74/74	0/4/4/4
31	PEB	M1	202	3	-	13/24/74/74	0/4/4/4
32	PUB	A6	302	6	-	2/24/74/74	0/4/4/4
31	PEB	fB	201	3	-	11/24/74/74	0/4/4/4
31	PEB	m4	202	2,12	-	8/24/74/74	0/4/4/4
31	PEB	AA	501	2,1	-	9/24/74/74	0/4/4/4
31	PEB	a2	201	2	-	7/24/74/74	0/4/4/4
31	PEB	UH	202	3	-	5/24/74/74	0/4/4/4
31	PEB	QH	204	3	-	9/24/74/74	0/4/4/4
31	PEB	RB	202	2	-	10/24/74/74	0/4/4/4
32	PUB	AB	302	6	-	2/24/74/74	0/4/4/4
33	CYC	JB	1001	9	-	9/25/74/74	0/4/4/4
33	CYC	F6	1001	9	-	9/25/74/74	0/4/4/4
32	PUB	M9	305	14,3	-	7/24/74/74	0/4/4/4
31	PEB	TG	202	3	-	8/24/74/74	0/4/4/4
31	PEB	V8	201	2	-	10/24/74/74	0/4/4/4
31	PEB	IJ	202	2,26	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	E8	202	3	-	10/24/74/74	0/4/4/4
31	PEB	S8	201	2,3	-	4/24/74/74	0/4/4/4
31	PEB	U4	203	3	-	9/24/74/74	0/4/4/4
31	PEB	k2	202	2	-	9/24/74/74	0/4/4/4
31	PEB	MH	203	3	-	9/24/74/74	0/4/4/4
33	CYC	ED	1001	8,9	-	6/25/74/74	0/4/4/4
31	PEB	GJ	201	2	-	4/24/74/74	0/4/4/4
31	PEB	TA	201	3	-	9/24/74/74	0/4/4/4
31	PEB	ZE	202	2,3	-	7/24/74/74	0/4/4/4
31	PEB	k8	202	3	-	10/24/74/74	0/4/4/4
31	PEB	eC	201	2	-	8/24/74/74	0/4/4/4
31	PEB	l8	201	2	-	11/24/74/74	0/4/4/4
31	PEB	h8	201	2	-	10/24/74/74	0/4/4/4
31	PEB	sF	201	3	-	12/24/74/74	0/4/4/4
33	CYC	HE	1001	9	-	8/25/74/74	0/4/4/4
31	PEB	YJ	202	2,31	-	7/24/74/74	0/4/4/4
31	PEB	W8	203	3	-	13/24/74/74	0/4/4/4
31	PEB	RF	202	2	-	13/24/74/74	0/4/4/4
31	PEB	I1	201	3	-	13/24/74/74	0/4/4/4
31	PEB	jD	202	3	-	6/24/74/74	0/4/4/4
31	PEB	F1	201	2,6	-	3/24/74/74	0/4/4/4
31	PEB	G4	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	Y1	301	31,6	-	13/24/74/74	0/4/4/4
32	PUB	ZI	305	14,3	-	14/24/74/74	0/4/4/4
31	PEB	K7	202	3	-	4/24/74/74	0/4/4/4
31	PEB	uF	202	3	-	10/24/74/74	0/4/4/4
31	PEB	PK	201	2	-	4/24/74/74	0/4/4/4
31	PEB	QJ	202	2	-	12/24/74/74	0/4/4/4
31	PEB	jB	201	3	-	11/24/74/74	0/4/4/4
31	PEB	bE	201	3	-	6/24/74/74	0/4/4/4
31	PEB	V5	202	3	-	12/24/74/74	0/4/4/4
31	PEB	G5	202	2	-	13/24/74/74	0/4/4/4
31	PEB	PC	201	2,10	-	5/24/74/74	0/4/4/4
31	PEB	T9	201	3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	OG	201	2	-	8/24/74/74	0/4/4/4
31	PEB	DI	201	2	-	10/24/74/74	0/4/4/4
31	PEB	EJ	202	2,26	-	12/24/74/74	0/4/4/4
31	PEB	d2	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	UF	202	3	-	9/24/74/74	0/4/4/4
31	PEB	k8	201	3	-	12/24/74/74	0/4/4/4
31	PEB	WI	203	2	-	8/24/74/74	0/4/4/4
31	PEB	e6	203	2	-	8/24/74/74	0/4/4/4
31	PEB	PD	201	2	-	14/24/74/74	0/4/4/4
31	PEB	A7	202	3	-	9/24/74/74	0/4/4/4
31	PEB	l6	202	-	-	10/24/74/74	0/4/4/4
31	PEB	eB	202	2	-	10/24/74/74	0/4/4/4
31	PEB	W2	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	WG	203	2	-	8/24/74/74	0/4/4/4
31	PEB	Y5	201	2	-	8/24/74/74	0/4/4/4
31	PEB	r8	201	2,12	-	11/24/74/74	0/4/4/4
31	PEB	VB	202	2	-	12/24/74/74	0/4/4/4
31	PEB	KA	303	2,4	-	11/24/74/74	0/4/4/4
33	CYC	e3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	mF	201	3	-	6/24/74/74	0/4/4/4
31	PEB	N7	201	2	-	8/24/74/74	0/4/4/4
31	PEB	A6	301	6	-	7/24/74/74	0/4/4/4
31	PEB	e4	202	2,12	-	6/24/74/74	0/4/4/4
31	PEB	FI	202	2	-	8/24/74/74	0/4/4/4
33	CYC	G6	1001	8	-	6/25/74/74	0/4/4/4
31	PEB	B7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	P1	201	2	-	4/24/74/74	0/4/4/4
31	PEB	N9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	G1	202	3	-	13/24/74/74	0/4/4/4
31	PEB	TE	201	2	-	3/24/74/74	0/4/4/4
31	PEB	wF	303	12	-	7/24/74/74	0/4/4/4
31	PEB	cA	401	2,5	-	6/24/74/74	0/4/4/4
31	PEB	OD	202	3	-	10/24/74/74	0/4/4/4
33	CYC	LD	1001	9	-	10/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	CYC	n3	1001	20	-	4/25/74/74	0/4/4/4
33	CYC	M2	201	8,9	-	9/25/74/74	0/4/4/4
31	PEB	dC	203	3	-	10/24/74/74	0/4/4/4
31	PEB	N8	202	2	-	10/24/74/74	0/4/4/4
33	CYC	V3	1001	-	-	10/25/74/74	0/4/4/4
31	PEB	II	201	3	-	8/24/74/74	0/4/4/4
33	CYC	HC	1001	9	-	7/25/74/74	0/4/4/4
31	PEB	IG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	PH	201	2	-	6/24/74/74	0/4/4/4
31	PEB	P2	202	2	-	8/24/74/74	0/4/4/4
31	PEB	QJ	201	2,6	-	2/24/74/74	0/4/4/4
31	PEB	x8	303	12	-	12/24/74/74	0/4/4/4
31	PEB	mD	203	2	-	8/24/74/74	0/4/4/4
31	PEB	M9	301	14,31	-	8/24/74/74	0/4/4/4
31	PEB	T6	202	2	-	5/24/74/74	0/4/4/4
31	PEB	f6	201	3	-	11/24/74/74	0/4/4/4
31	PEB	S6	202	3,29	-	10/24/74/74	0/4/4/4
31	PEB	OH	201	3	-	5/24/74/74	0/4/4/4
31	PEB	dA	201	2	-	8/24/74/74	0/4/4/4
31	PEB	aC	202	2	-	10/24/74/74	0/4/4/4
31	PEB	P6	202	2	-	6/24/74/74	0/4/4/4
31	PEB	xF	302	12	-	12/24/74/74	0/4/4/4
33	CYC	N2	1001	9,7	-	8/25/74/74	0/4/4/4
31	PEB	LB	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	YI	203	2	-	9/24/74/74	0/4/4/4
31	PEB	R5	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	QC	202	3	-	13/24/74/74	0/4/4/4
31	PEB	ZC	203	3	-	7/24/74/74	0/4/4/4
31	PEB	K5	201	2	-	9/24/74/74	0/4/4/4
31	PEB	L9	201	2,14	-	10/24/74/74	0/4/4/4
31	PEB	XG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	LG	202	2	-	7/24/74/74	0/4/4/4
31	PEB	qF	203	3	-	10/24/74/74	0/4/4/4
31	PEB	LC	1002	9	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	C1	201	3	-	9/24/74/74	0/4/4/4
31	PEB	H5	202	3	-	12/24/74/74	0/4/4/4
31	PEB	nF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	IA	203	2	-	8/24/74/74	0/4/4/4
31	PEB	UA	303	2,4	-	7/24/74/74	0/4/4/4
32	PUB	AH	303	12	-	13/24/74/74	0/4/4/4
31	PEB	hB	202	3	-	9/24/74/74	0/4/4/4
31	PEB	N2	1002	9	-	9/24/74/74	0/4/4/4
33	CYC	L6	1001	9	-	5/25/74/74	0/4/4/4
32	PUB	QH	202	3,13	-	5/24/74/74	0/4/4/4
31	PEB	c4	201	2	-	10/24/74/74	0/4/4/4
31	PEB	ZD	203	3	-	9/24/74/74	0/4/4/4
32	PUB	x8	301	12	-	7/24/74/74	0/4/4/4
31	PEB	A4	302	12	-	7/24/74/74	0/4/4/4
31	PEB	c2	201	2	-	6/24/74/74	0/4/4/4
31	PEB	WD	201	26,3	-	8/24/74/74	0/4/4/4
31	PEB	t8	202	2	-	11/24/74/74	0/4/4/4
31	PEB	CJ	202	2,6	-	4/24/74/74	0/4/4/4
33	CYC	C3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	P9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	EA	501	2,1	-	11/24/74/74	0/4/4/4
31	PEB	V2	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	PG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	TK	201	2	-	5/24/74/74	0/4/4/4
31	PEB	FB	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	EG	202	3	-	10/24/74/74	0/4/4/4
31	PEB	HD	1002	8,9	-	8/24/74/74	0/4/4/4
31	PEB	WF	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	X7	202	2	-	10/24/74/74	0/4/4/4
31	PEB	ZG	401	2,11	-	7/24/74/74	0/4/4/4
31	PEB	LK	201	2,31	-	5/24/74/74	0/4/4/4
31	PEB	HA	201	2	-	13/24/74/74	0/4/4/4
31	PEB	cD	202	2	-	10/24/74/74	0/4/4/4
31	PEB	OI	203	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	PUB	x8	306	12	-	6/24/74/74	0/4/4/4
31	PEB	BA	203	2	-	8/24/74/74	0/4/4/4
31	PEB	T7	201	2,27	-	6/24/74/74	0/4/4/4
31	PEB	XK	202	2	-	9/24/74/74	0/4/4/4
31	PEB	YH	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	e6	201	2	-	5/24/74/74	0/4/4/4
31	PEB	aA	202	2	-	8/24/74/74	0/4/4/4
31	PEB	b6	201	3	-	8/24/74/74	0/4/4/4
31	PEB	B1	203	2	-	12/24/74/74	0/4/4/4
31	PEB	SC	202	3	-	8/24/74/74	0/4/4/4
31	PEB	lE	201	2,3	-	9/24/74/74	0/4/4/4
32	PUB	Z9	305	14,3	-	7/24/74/74	0/4/4/4
31	PEB	EF	202	3	-	10/24/74/74	0/4/4/4
31	PEB	dB	202	3	-	9/24/74/74	0/4/4/4
31	PEB	BK	203	2	-	12/24/74/74	0/4/4/4
31	PEB	CJ	201	2	-	7/24/74/74	0/4/4/4
31	PEB	i4	201	2	-	10/24/74/74	0/4/4/4
31	PEB	O6	201	3	-	9/24/74/74	0/4/4/4
31	PEB	k6	201	2	-	8/24/74/74	0/4/4/4
31	PEB	DA	203	2	-	14/24/74/74	0/4/4/4
31	PEB	A2	301	6	-	7/24/74/74	0/4/4/4
31	PEB	R7	201	2,27	-	9/24/74/74	0/4/4/4
31	PEB	WF	203	3	-	13/24/74/74	0/4/4/4
31	PEB	kF	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	J8	202	2	-	13/24/74/74	0/4/4/4
31	PEB	HH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	DH	202	2,13	-	8/24/74/74	0/4/4/4
33	CYC	KC	201	8,9	-	9/25/74/74	0/4/4/4
33	CYC	MB	1001	8	-	8/25/74/74	0/4/4/4
31	PEB	a6	202	2	-	7/24/74/74	0/4/4/4
31	PEB	R8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	fF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	ZF	201	2	-	9/24/74/74	0/4/4/4
31	PEB	AD	304	6	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	aD	202	2	-	13/24/74/74	0/4/4/4
33	CYC	CC	1001	8,9	-	8/25/74/74	0/4/4/4
31	PEB	j2	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	F8	201	2	-	5/24/74/74	0/4/4/4
31	PEB	KF	203	3	-	8/24/74/74	0/4/4/4
31	PEB	A6	305	6	-	10/24/74/74	0/4/4/4
33	CYC	K2	201	8,9	-	9/25/74/74	0/4/4/4
31	PEB	D4	201	2	-	8/24/74/74	0/4/4/4
31	PEB	dD	202	6,3	-	11/24/74/74	0/4/4/4
31	PEB	LH	201	2	-	7/24/74/74	0/4/4/4
31	PEB	CH	201	3	-	4/24/74/74	0/4/4/4
31	PEB	E7	202	3	-	10/24/74/74	0/4/4/4
31	PEB	kH	201	2	-	11/24/74/74	0/4/4/4
31	PEB	XF	202	2	-	5/24/74/74	0/4/4/4
31	PEB	cE	202	2	-	10/24/74/74	0/4/4/4
31	PEB	A9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	F5	202	3	-	10/24/74/74	0/4/4/4
31	PEB	AC	305	6	-	12/24/74/74	0/4/4/4
31	PEB	Y7	502	2	-	5/24/74/74	0/4/4/4
31	PEB	O8	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	XA	202	2	-	10/24/74/74	0/4/4/4
31	PEB	xF	303	12	-	12/24/74/74	0/4/4/4
31	PEB	AG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	IK	201	3	-	13/24/74/74	0/4/4/4
31	PEB	S9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	aC	201	2	-	7/24/74/74	0/4/4/4
31	PEB	HJ	201	2,3	-	12/24/74/74	0/4/4/4
31	PEB	d4	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	mC	201	2	-	8/24/74/74	0/4/4/4
31	PEB	LA	201	2	-	10/24/74/74	0/4/4/4
31	PEB	NA	202	2	-	7/24/74/74	0/4/4/4
31	PEB	QC	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	EJ	201	2	-	7/24/74/74	0/4/4/4
31	PEB	D9	203	2	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	PB	202	2	-	6/24/74/74	0/4/4/4
31	PEB	R5	201	3	-	12/24/74/74	0/4/4/4
31	PEB	FH	201	2,25	-	8/24/74/74	0/4/4/4
31	PEB	w8	302	12	-	9/24/74/74	0/4/4/4
31	PEB	VC	202	2	-	9/24/74/74	0/4/4/4
31	PEB	U2	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	mB	203	2	-	9/24/74/74	0/4/4/4
31	PEB	NE	201	8,9	-	10/24/74/74	0/4/4/4
33	CYC	LC	1001	9	-	10/25/74/74	0/4/4/4
31	PEB	F9	201	2,14	-	11/24/74/74	0/4/4/4
31	PEB	TB	202	2	-	5/24/74/74	0/4/4/4
31	PEB	H8	202	2	-	12/24/74/74	0/4/4/4
31	PEB	W9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	P5	202	3	-	10/24/74/74	0/4/4/4
31	PEB	TD	201	2	-	3/24/74/74	0/4/4/4
31	PEB	hC	202	3	-	11/24/74/74	0/4/4/4
31	PEB	V1	203	2	-	7/24/74/74	0/4/4/4
31	PEB	FF	202	2	-	11/24/74/74	0/4/4/4
31	PEB	gD	201	2	-	6/24/74/74	0/4/4/4
31	PEB	QH	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	L2	1002	9	-	7/24/74/74	0/4/4/4
31	PEB	xF	304	12	-	9/24/74/74	0/4/4/4
31	PEB	VA	201	2	-	10/24/74/74	0/4/4/4
31	PEB	T5	201	2,3	-	13/24/74/74	0/4/4/4
31	PEB	VG	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	l8	203	2,3	-	10/24/74/74	0/4/4/4
33	CYC	u3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	L7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	A8	201	3	-	9/24/74/74	0/4/4/4
31	PEB	SB	201	3,29	-	10/24/74/74	0/4/4/4
31	PEB	A9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	B1	201	2,31	-	8/24/74/74	0/4/4/4
31	PEB	L4	202	2	-	10/24/74/74	0/4/4/4
31	PEB	aF	202	3	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	PI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	J5	202	3	-	14/24/74/74	0/4/4/4
31	PEB	h8	202	2	-	9/24/74/74	0/4/4/4
31	PEB	dD	204	3	-	13/24/74/74	0/4/4/4
31	PEB	SJ	201	2,6	-	6/24/74/74	0/4/4/4
31	PEB	W7	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	RK	201	2	-	5/24/74/74	0/4/4/4
31	PEB	Z8	202	2	-	10/24/74/74	0/4/4/4
31	PEB	c6	203	2	-	12/24/74/74	0/4/4/4
31	PEB	MK	201	3	-	10/24/74/74	0/4/4/4
31	PEB	dH	202	3	-	6/24/74/74	0/4/4/4
31	PEB	TH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	PB	201	2	-	5/24/74/74	0/4/4/4
33	CYC	M3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	JI	201	2	-	13/24/74/74	0/4/4/4
31	PEB	o8	201	3	-	13/24/74/74	0/4/4/4
33	CYC	B3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	lD	202	3	-	14/24/74/74	0/4/4/4
31	PEB	V7	202	2	-	7/24/74/74	0/4/4/4
31	PEB	kE	202	2,6	-	8/24/74/74	0/4/4/4
31	PEB	k6	203	2	-	12/24/74/74	0/4/4/4
31	PEB	Z2	203	3	-	7/24/74/74	0/4/4/4
31	PEB	b8	202	2	-	9/24/74/74	0/4/4/4
31	PEB	i8	202	3	-	13/24/74/74	0/4/4/4
31	PEB	SD	202	3	-	10/24/74/74	0/4/4/4
31	PEB	hC	201	3	-	11/24/74/74	0/4/4/4
31	PEB	QK	201	3	-	6/24/74/74	0/4/4/4
31	PEB	GH	201	3	-	6/24/74/74	0/4/4/4
31	PEB	PE	201	2	-	14/24/74/74	0/4/4/4
31	PEB	cB	202	2	-	11/24/74/74	0/4/4/4
31	PEB	AF	201	3	-	9/24/74/74	0/4/4/4
31	PEB	UC	203	3	-	9/24/74/74	0/4/4/4
31	PEB	HG	201	2	-	8/24/74/74	0/4/4/4
31	PEB	J8	201	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	NJ	203	3	-	12/24/74/74	0/4/4/4
31	PEB	ID	203	3	-	7/24/74/74	0/4/4/4
31	PEB	C1	202	3	-	13/24/74/74	0/4/4/4
33	CYC	H6	1001	9	-	7/25/74/74	0/4/4/4
31	PEB	J1	202	2	-	10/24/74/74	0/4/4/4
31	PEB	Q6	201	3	-	8/24/74/74	0/4/4/4
31	PEB	X1	202	2	-	9/24/74/74	0/4/4/4
31	PEB	R4	201	2	-	6/24/74/74	0/4/4/4
31	PEB	XH	202	2	-	8/24/74/74	0/4/4/4
31	PEB	H4	202	2	-	10/24/74/74	0/4/4/4
31	PEB	D6	1002	9	-	8/24/74/74	0/4/4/4
31	PEB	BG	202	2,3	-	10/24/74/74	0/4/4/4
31	PEB	dE	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	RJ	201	3	-	12/24/74/74	0/4/4/4
31	PEB	ZE	203	3	-	9/24/74/74	0/4/4/4
31	PEB	g2	201	2	-	10/24/74/74	0/4/4/4
31	PEB	P9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	r8	202	2	-	11/24/74/74	0/4/4/4
31	PEB	X5	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	KD	201	8,9	-	6/24/74/74	0/4/4/4
31	PEB	L7	201	2	-	7/24/74/74	0/4/4/4
31	PEB	PJ	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	Z6	202	3	-	9/24/74/74	0/4/4/4
31	PEB	MJ	201	2	-	7/24/74/74	0/4/4/4
31	PEB	PH	202	2	-	8/24/74/74	0/4/4/4
31	PEB	LF	201	2	-	9/24/74/74	0/4/4/4
31	PEB	ID	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	X9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	s8	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	FJ	202	3	-	10/24/74/74	0/4/4/4
31	PEB	bB	201	3	-	8/24/74/74	0/4/4/4
31	PEB	aB	202	2	-	7/24/74/74	0/4/4/4
33	CYC	q3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	eK	301	15,3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	uF	203	3	-	9/24/74/74	0/4/4/4
31	PEB	RH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	O2	203	2,3	-	10/24/74/74	0/4/4/4
31	PEB	U8	202	3	-	9/24/74/74	0/4/4/4
31	PEB	iB	201	2	-	6/24/74/74	0/4/4/4
31	PEB	ZE	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	O4	201	3	-	6/24/74/74	0/4/4/4
31	PEB	W9	201	2	-	7/24/74/74	0/4/4/4
31	PEB	FK	201	2,6	-	3/24/74/74	0/4/4/4
31	PEB	g8	202	3	-	11/24/74/74	0/4/4/4
31	PEB	HA	202	2	-	9/24/74/74	0/4/4/4
31	PEB	hF	201	2	-	10/24/74/74	0/4/4/4
33	CYC	63	901	24	-	8/25/74/74	0/4/4/4
33	CYC	l3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	X1	203	2	-	12/24/74/74	0/4/4/4
31	PEB	T7	202	2	-	11/24/74/74	0/4/4/4
32	PUB	A2	303	6	-	5/24/74/74	0/4/4/4
31	PEB	L1	201	2,31	-	6/24/74/74	0/4/4/4
31	PEB	i2	202	2	-	9/24/74/74	0/4/4/4
31	PEB	aH	202	3	-	6/24/74/74	0/4/4/4
31	PEB	U2	203	3	-	9/24/74/74	0/4/4/4
31	PEB	x8	302	12	-	12/24/74/74	0/4/4/4
31	PEB	D7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	fE	202	3	-	8/24/74/74	0/4/4/4
31	PEB	G4	202	3	-	12/24/74/74	0/4/4/4
33	CYC	h3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	O2	201	3	-	11/24/74/74	0/4/4/4
31	PEB	BF	201	2	-	11/24/74/74	0/4/4/4
31	PEB	D7	201	2	-	6/24/74/74	0/4/4/4
31	PEB	BJ	202	3	-	10/24/74/74	0/4/4/4
31	PEB	H4	201	2	-	9/24/74/74	0/4/4/4
31	PEB	gF	202	3	-	11/24/74/74	0/4/4/4
31	PEB	FJ	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	VC	203	2,3	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	YK	301	31,6	-	13/24/74/74	0/4/4/4
31	PEB	IH	202	3	-	7/24/74/74	0/4/4/4
33	CYC	L2	1001	9	-	10/25/74/74	0/4/4/4
31	PEB	H7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	U7	202	3	-	10/24/74/74	0/4/4/4
31	PEB	KJ	201	2	-	9/24/74/74	0/4/4/4
31	PEB	J9	201	2	-	9/24/74/74	0/4/4/4
31	PEB	MF	201	3	-	6/24/74/74	0/4/4/4
31	PEB	V4	201	2	-	8/24/74/74	0/4/4/4
31	PEB	OD	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	L4	201	2	-	4/24/74/74	0/4/4/4
31	PEB	T4	202	2	-	7/24/74/74	0/4/4/4
31	PEB	PF	202	2	-	12/24/74/74	0/4/4/4
31	PEB	M7	202	3	-	9/24/74/74	0/4/4/4
31	PEB	WD	202	3	-	7/24/74/74	0/4/4/4
31	PEB	aD	201	2	-	5/24/74/74	0/4/4/4
31	PEB	qF	202	3	-	15/24/74/74	0/4/4/4
31	PEB	j6	201	3	-	11/24/74/74	0/4/4/4
31	PEB	m6	203	2	-	9/24/74/74	0/4/4/4
31	PEB	SH	202	3	-	12/24/74/74	0/4/4/4
33	CYC	O3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	Z8	201	2	-	9/24/74/74	0/4/4/4
31	PEB	SF	203	3	-	9/24/74/74	0/4/4/4
31	PEB	ZI	301	14	-	16/24/74/74	0/4/4/4
31	PEB	R2	202	2	-	12/24/74/74	0/4/4/4
31	PEB	jF	202	2	-	12/24/74/74	0/4/4/4
31	PEB	SG	202	2	-	8/24/74/74	0/4/4/4
31	PEB	VE	202	2	-	10/24/74/74	0/4/4/4
32	PUB	Z9	304	14,3	-	8/24/74/74	0/4/4/4
31	PEB	cA	402	2,5	-	12/24/74/74	0/4/4/4
31	PEB	QG	201	2	-	8/24/74/74	0/4/4/4
31	PEB	FI	201	2,14	-	12/24/74/74	0/4/4/4
32	PUB	AD	303	6	-	8/24/74/74	0/4/4/4
31	PEB	LK	202	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	RB	201	2,10	-	2/24/74/74	0/4/4/4
31	PEB	J4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	WA	402	5,2	-	5/24/74/74	0/4/4/4
31	PEB	JI	203	2	-	9/24/74/74	0/4/4/4
31	PEB	IG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	GA	201	2	-	6/24/74/74	0/4/4/4
33	CYC	FD	201	9	-	5/25/74/74	0/4/4/4
31	PEB	LK	203	2	-	9/24/74/74	0/4/4/4
31	PEB	NK	202	2	-	8/24/74/74	0/4/4/4
31	PEB	P5	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	mD	201	2	-	6/24/74/74	0/4/4/4
31	PEB	JA	202	3	-	9/24/74/74	0/4/4/4
33	CYC	ME	1001	8,9	-	7/25/74/74	0/4/4/4
31	PEB	S4	203	2,3	-	8/24/74/74	0/4/4/4
32	PUB	AC	304	6	-	15/24/74/74	0/4/4/4
31	PEB	lB	202	-	-	10/24/74/74	0/4/4/4
31	PEB	i4	202	2,12	-	7/24/74/74	0/4/4/4
31	PEB	F8	202	2	-	11/24/74/74	0/4/4/4
31	PEB	A6	304	6	-	9/24/74/74	0/4/4/4
31	PEB	VH	201	2	-	8/24/74/74	0/4/4/4
31	PEB	t8	203	2,3	-	11/24/74/74	0/4/4/4
31	PEB	O5	201	2,6,31	-	8/24/74/74	0/4/4/4
31	PEB	U9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	QA	203	2	-	9/24/74/74	0/4/4/4
31	PEB	Z6	201	3	-	7/24/74/74	0/4/4/4
31	PEB	JK	203	2	-	16/24/74/74	0/4/4/4
33	CYC	LE	1001	9	-	10/25/74/74	0/4/4/4
31	PEB	GI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	NB	1002	9	-	8/24/74/74	0/4/4/4
31	PEB	PK	202	2	-	7/24/74/74	0/4/4/4
31	PEB	uF	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	X5	203	3	-	10/24/74/74	0/4/4/4
32	PUB	Q4	202	3,13	-	5/24/74/74	0/4/4/4
31	PEB	ZF	202	2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	QI	201	2	-	11/24/74/74	0/4/4/4
33	CYC	D3	1001	24,20	-	4/25/74/74	0/4/4/4
31	PEB	U1	201	3	-	5/24/74/74	0/4/4/4
31	PEB	aB	201	2	-	2/24/74/74	0/4/4/4
31	PEB	ZH	201	2	-	4/24/74/74	0/4/4/4
33	CYC	E6	1001	8	-	8/25/74/74	0/4/4/4
31	PEB	WA	401	2,5	-	11/24/74/74	0/4/4/4
31	PEB	hE	202	3	-	11/24/74/74	0/4/4/4
31	PEB	N1	201	2	-	3/24/74/74	0/4/4/4
31	PEB	O8	203	3	-	10/24/74/74	0/4/4/4
31	PEB	p8	202	2	-	11/24/74/74	0/4/4/4
31	PEB	AB	305	6	-	10/24/74/74	0/4/4/4
33	CYC	o3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	Z2	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	ZA	203	2	-	11/24/74/74	0/4/4/4
31	PEB	gC	202	2	-	6/24/74/74	0/4/4/4
31	PEB	cE	201	2	-	5/24/74/74	0/4/4/4
31	PEB	SB	202	3	-	10/24/74/74	0/4/4/4
31	PEB	XK	203	2	-	12/24/74/74	0/4/4/4
31	PEB	PI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	HI	203	2	-	10/24/74/74	0/4/4/4
31	PEB	TG	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	U7	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	jH	201	3	-	5/24/74/74	0/4/4/4
31	PEB	T1	202	2	-	9/24/74/74	0/4/4/4
32	PUB	ZI	302	14	-	7/24/74/74	0/4/4/4
31	PEB	iB	203	2	-	12/24/74/74	0/4/4/4
31	PEB	f2	201	3	-	9/24/74/74	0/4/4/4
31	PEB	WH	202	3	-	13/24/74/74	0/4/4/4
31	PEB	Y8	202	3	-	10/24/74/74	0/4/4/4
31	PEB	MI	302	14	-	16/24/74/74	0/4/4/4
31	PEB	WG	201	2	-	8/24/74/74	0/4/4/4
31	PEB	CF	201	3	-	6/24/74/74	0/4/4/4
31	PEB	VK	202	2	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	zF	501	2,28	-	6/24/74/74	0/4/4/4
31	PEB	gB	202	2	-	8/24/74/74	0/4/4/4
31	PEB	UD	203	3	-	13/24/74/74	0/4/4/4
31	PEB	C9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	SE	202	3	-	10/24/74/74	0/4/4/4
31	PEB	l2	202	3	-	10/24/74/74	0/4/4/4
31	PEB	DB	1002	9	-	8/24/74/74	0/4/4/4
31	PEB	HI	201	2,14	-	10/24/74/74	0/4/4/4
31	PEB	oF	203	3	-	17/24/74/74	0/4/4/4
31	PEB	jE	202	3	-	6/24/74/74	0/4/4/4
32	PUB	BH	302	13	-	7/24/74/74	0/4/4/4
31	PEB	i6	202	2	-	8/24/74/74	0/4/4/4
31	PEB	U4	202	3	-	4/24/74/74	0/4/4/4
31	PEB	SA	202	2	-	7/24/74/74	0/4/4/4
32	PUB	AJ	303	6,3	-	8/24/74/74	0/4/4/4
31	PEB	jD	201	3	-	9/24/74/74	0/4/4/4
31	PEB	RB	203	2	-	9/24/74/74	0/4/4/4
31	PEB	a4	204	2,3	-	9/24/74/74	0/4/4/4
31	PEB	WK	201	3	-	7/24/74/74	0/4/4/4
31	PEB	CK	202	3	-	13/24/74/74	0/4/4/4
31	PEB	OK	201	3	-	9/24/74/74	0/4/4/4
31	PEB	fH	202	3	-	10/24/74/74	0/4/4/4
31	PEB	EH	203	3	-	11/24/74/74	0/4/4/4
31	PEB	BI	202	2	-	8/24/74/74	0/4/4/4
31	PEB	PC	202	2	-	8/24/74/74	0/4/4/4
31	PEB	PF	201	2	-	7/24/74/74	0/4/4/4
32	PUB	YK	304	6	-	3/24/74/74	0/4/4/4
31	PEB	W5	201	2	-	8/24/74/74	0/4/4/4
31	PEB	AK	201	3	-	11/24/74/74	0/4/4/4
31	PEB	ZI	304	14	-	10/24/74/74	0/4/4/4
31	PEB	AK	202	3	-	12/24/74/74	0/4/4/4
33	CYC	73	1002	24	-	6/25/74/74	0/4/4/4
31	PEB	NC	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	QD	202	3	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	j4	201	3	-	10/24/74/74	0/4/4/4
31	PEB	h4	202	3	-	10/24/74/74	0/4/4/4
31	PEB	XF	203	2	-	11/24/74/74	0/4/4/4
31	PEB	J2	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	p8	201	2	-	10/24/74/74	0/4/4/4
31	PEB	E9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	UC	202	3	-	6/24/74/74	0/4/4/4
31	PEB	JK	201	2,6	-	3/24/74/74	0/4/4/4
31	PEB	e2	201	2	-	8/24/74/74	0/4/4/4
31	PEB	S5	201	2,6	-	6/24/74/74	0/4/4/4
31	PEB	S9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	CI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	bF	202	2	-	9/24/74/74	0/4/4/4
31	PEB	d6	201	3	-	8/24/74/74	0/4/4/4
31	PEB	J4	201	2	-	6/24/74/74	0/4/4/4
31	PEB	NA	203	2	-	13/24/74/74	0/4/4/4
31	PEB	WI	201	2	-	13/24/74/74	0/4/4/4
31	PEB	QH	203	3	-	7/24/74/74	0/4/4/4
31	PEB	N7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	Q2	202	3	-	13/24/74/74	0/4/4/4
33	CYC	FE	1001	9	-	5/25/74/74	0/4/4/4
31	PEB	FK	203	2	-	11/24/74/74	0/4/4/4
32	PUB	A2	304	6	-	15/24/74/74	0/4/4/4
31	PEB	I9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	PA	201	2	-	7/24/74/74	0/4/4/4
31	PEB	eA	201	2	-	5/24/74/74	0/4/4/4
31	PEB	I7	202	3	-	11/24/74/74	0/4/4/4
31	PEB	eH	202	2,12	-	6/24/74/74	0/4/4/4
31	PEB	AG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	e1	301	15,3	-	9/24/74/74	0/4/4/4
31	PEB	XI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	EK	202	3	-	11/24/74/74	0/4/4/4
31	PEB	w8	301	12	-	11/24/74/74	0/4/4/4
31	PEB	mH	202	2,12	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	a6	201	2	-	2/24/74/74	0/4/4/4
32	PUB	A4	304	12	-	8/24/74/74	0/4/4/4
31	PEB	J7	202	2	-	5/24/74/74	0/4/4/4
31	PEB	B8	201	2	-	11/24/74/74	0/4/4/4
31	PEB	g4	201	2	-	8/24/74/74	0/4/4/4
31	PEB	Y7	504	2,27	-	7/24/74/74	0/4/4/4
31	PEB	QA	201	2	-	13/24/74/74	0/4/4/4
31	PEB	IH	203	3	-	11/24/74/74	0/4/4/4
31	PEB	S2	202	3	-	8/24/74/74	0/4/4/4
31	PEB	L5	203	3	-	11/24/74/74	0/4/4/4
31	PEB	h2	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	SA	201	2	-	4/24/74/74	0/4/4/4
31	PEB	GD	202	8,9	-	9/24/74/74	0/4/4/4
31	PEB	dE	202	6,3	-	10/24/74/74	0/4/4/4
31	PEB	cF	202	9,3	-	17/24/74/74	0/4/4/4
32	PUB	A5	303	6,3	-	8/24/74/74	0/4/4/4
31	PEB	G8	202	3	-	7/24/74/74	0/4/4/4
31	PEB	MI	305	14	-	10/24/74/74	0/4/4/4
31	PEB	NA	201	2	-	6/24/74/74	0/4/4/4
31	PEB	gH	202	2	-	10/24/74/74	0/4/4/4
31	PEB	TI	202	3	-	15/24/74/74	0/4/4/4
31	PEB	E8	201	3	-	9/24/74/74	0/4/4/4
31	PEB	D5	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	mE	202	2	-	7/24/74/74	0/4/4/4
31	PEB	V9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	LF	202	2	-	14/24/74/74	0/4/4/4
31	PEB	K1	202	3	-	10/24/74/74	0/4/4/4
31	PEB	M8	202	3	-	10/24/74/74	0/4/4/4
31	PEB	O1	201	3	-	9/24/74/74	0/4/4/4
31	PEB	IE	203	3	-	7/24/74/74	0/4/4/4
31	PEB	L9	202	2	-	9/24/74/74	0/4/4/4
31	PEB	GG	202	3	-	8/24/74/74	0/4/4/4
31	PEB	Q9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	YB	203	2	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	aF	203	3	-	11/24/74/74	0/4/4/4
31	PEB	W2	202	3	-	9/24/74/74	0/4/4/4
31	PEB	V4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	u8	201	3	-	10/24/74/74	0/4/4/4
33	CYC	HD	1001	9	-	8/25/74/74	0/4/4/4
31	PEB	gC	201	2	-	10/24/74/74	0/4/4/4
31	PEB	I4	203	3	-	9/24/74/74	0/4/4/4
31	PEB	U6	202	3	-	10/24/74/74	0/4/4/4
31	PEB	LG	201	2,11	-	10/24/74/74	0/4/4/4
31	PEB	Z2	202	3	-	9/24/74/74	0/4/4/4
31	PEB	K9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	Q9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	H9	202	2	-	8/24/74/74	0/4/4/4
31	PEB	Q7	201	3	-	7/24/74/74	0/4/4/4
31	PEB	dJ	401	2,26	-	11/24/74/74	0/4/4/4
33	CYC	LC	1003	8,9	-	9/25/74/74	0/4/4/4
31	PEB	HF	202	2	-	12/24/74/74	0/4/4/4
31	PEB	T1	201	2	-	5/24/74/74	0/4/4/4
31	PEB	DE	1002	8,9	-	8/24/74/74	0/4/4/4
31	PEB	OH	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	HB	1002	9	-	7/24/74/74	0/4/4/4
31	PEB	qF	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	g8	203	2,3	-	9/24/74/74	0/4/4/4
33	CYC	P3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	Q2	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	RF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	UB	201	3	-	9/24/74/74	0/4/4/4
33	CYC	G3	1001	19	-	8/25/74/74	0/4/4/4
33	CYC	D6	1001	9	-	9/25/74/74	0/4/4/4
31	PEB	W4	202	3	-	13/24/74/74	0/4/4/4
31	PEB	AD	301	6	-	10/24/74/74	0/4/4/4
31	PEB	jC	202	3	-	8/24/74/74	0/4/4/4
33	CYC	EC	1001	8,9	-	7/25/74/74	0/4/4/4
31	PEB	U5	202	2	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	KG	202	3	-	8/24/74/74	0/4/4/4
31	PEB	vF	201	2	-	9/24/74/74	0/4/4/4
31	PEB	BF	202	2	-	13/24/74/74	0/4/4/4
31	PEB	F6	1002	9	-	9/24/74/74	0/4/4/4
31	PEB	FK	202	2	-	10/24/74/74	0/4/4/4
31	PEB	NI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	a8	202	3	-	9/24/74/74	0/4/4/4
31	PEB	mB	201	2	-	9/24/74/74	0/4/4/4
31	PEB	fD	202	3	-	8/24/74/74	0/4/4/4
31	PEB	aF	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	AC	302	6	-	11/24/74/74	0/4/4/4
31	PEB	i8	203	3	-	12/24/74/74	0/4/4/4
31	PEB	c6	201	2	-	7/24/74/74	0/4/4/4
31	PEB	UJ	202	2	-	8/24/74/74	0/4/4/4
31	PEB	S8	202	3	-	7/24/74/74	0/4/4/4
31	PEB	EH	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	I4	201	2,3	-	6/24/74/74	0/4/4/4
31	PEB	e8	203	3	-	9/24/74/74	0/4/4/4
31	PEB	G5	201	2	-	4/24/74/74	0/4/4/4
31	PEB	cF	201	3	-	11/24/74/74	0/4/4/4
31	PEB	lB	201	3	-	8/24/74/74	0/4/4/4
31	PEB	G4	201	3	-	8/24/74/74	0/4/4/4
31	PEB	b2	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	j4	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	aE	201	2	-	5/24/74/74	0/4/4/4
31	PEB	e8	202	3	-	8/24/74/74	0/4/4/4
31	PEB	J1	203	2	-	16/24/74/74	0/4/4/4
31	PEB	K8	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	sF	202	3	-	9/24/74/74	0/4/4/4
31	PEB	W6	201	3	-	7/24/74/74	0/4/4/4
31	PEB	V6	201	2	-	4/24/74/74	0/4/4/4
31	PEB	d8	202	2	-	12/24/74/74	0/4/4/4
31	PEB	ZC	202	3	-	9/24/74/74	0/4/4/4
31	PEB	UK	202	3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	w8	303	12	-	7/24/74/74	0/4/4/4
31	PEB	GG	201	2,3	-	10/24/74/74	0/4/4/4
31	PEB	gB	203	2	-	10/24/74/74	0/4/4/4
31	PEB	F1	202	2	-	10/24/74/74	0/4/4/4
31	PEB	aA	201	2	-	2/24/74/74	0/4/4/4
31	PEB	h4	201	2,3	-	8/24/74/74	0/4/4/4
31	PEB	n8	201	2	-	7/24/74/74	0/4/4/4
31	PEB	x8	304	12	-	9/24/74/74	0/4/4/4
31	PEB	l2	203	3	-	13/24/74/74	0/4/4/4
31	PEB	K5	202	2	-	13/24/74/74	0/4/4/4
31	PEB	i6	203	2	-	12/24/74/74	0/4/4/4
31	PEB	RD	201	2	-	8/24/74/74	0/4/4/4
31	PEB	c8	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	NF	202	2	-	10/24/74/74	0/4/4/4
31	PEB	e4	201	2	-	10/24/74/74	0/4/4/4
31	PEB	H6	1002	9	-	7/24/74/74	0/4/4/4
31	PEB	YI	201	2	-	11/24/74/74	0/4/4/4
31	PEB	bD	202	3	-	6/24/74/74	0/4/4/4
31	PEB	KA	302	2,4	-	9/24/74/74	0/4/4/4
31	PEB	W1	201	3	-	7/24/74/74	0/4/4/4
31	PEB	bC	201	3	-	10/24/74/74	0/4/4/4
31	PEB	N1	203	2	-	8/24/74/74	0/4/4/4
31	PEB	S8	203	3	-	9/24/74/74	0/4/4/4
31	PEB	B9	203	2	-	12/24/74/74	0/4/4/4
31	PEB	F9	202	2	-	11/24/74/74	0/4/4/4
31	PEB	dD	203	3	-	8/24/74/74	0/4/4/4
31	PEB	QI	203	2	-	9/24/74/74	0/4/4/4
31	PEB	WE	202	26,3	-	8/24/74/74	0/4/4/4
31	PEB	DI	202	2	-	7/24/74/74	0/4/4/4
31	PEB	W4	201	3	-	7/24/74/74	0/4/4/4
31	PEB	S7	203	3	-	11/24/74/74	0/4/4/4
32	PUB	yF	302	13	-	3/24/74/74	0/4/4/4
31	PEB	N1	202	2	-	8/24/74/74	0/4/4/4
31	PEB	H2	1002	9	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	DK	201	2,6	-	11/24/74/74	0/4/4/4
31	PEB	W8	201	2,3	-	7/24/74/74	0/4/4/4
31	PEB	I7	201	3	-	4/24/74/74	0/4/4/4
31	PEB	h2	201	2,14,3	-	9/24/74/74	0/4/4/4
31	PEB	s8	201	3	-	12/24/74/74	0/4/4/4
31	PEB	eH	201	2	-	11/24/74/74	0/4/4/4
31	PEB	M8	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	d2	202	3	-	10/24/74/74	0/4/4/4
31	PEB	eC	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	g6	202	2	-	8/24/74/74	0/4/4/4
31	PEB	sF	203	2,3	-	6/24/74/74	0/4/4/4
31	PEB	aH	203	3	-	10/24/74/74	0/4/4/4
31	PEB	DD	1002	8,9	-	8/24/74/74	0/4/4/4
31	PEB	WC	203	2,3	-	8/24/74/74	0/4/4/4
31	PEB	UH	203	3	-	9/24/74/74	0/4/4/4
31	PEB	QB	202	3	-	9/24/74/74	0/4/4/4
31	PEB	CF	203	3	-	11/24/74/74	0/4/4/4
31	PEB	TF	202	2	-	15/24/74/74	0/4/4/4
31	PEB	PK	203	2	-	7/24/74/74	0/4/4/4
31	PEB	BJ	203	2,3	-	12/24/74/74	0/4/4/4
31	PEB	CF	202	3	-	6/24/74/74	0/4/4/4
31	PEB	QE	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	gF	203	2,3	-	9/24/74/74	0/4/4/4
31	PEB	R9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	DC	1002	9	-	11/24/74/74	0/4/4/4
31	PEB	HK	202	2	-	8/24/74/74	0/4/4/4
31	PEB	NH	202	2	-	9/24/74/74	0/4/4/4
31	PEB	AJ	301	6,31	-	9/24/74/74	0/4/4/4
31	PEB	mC	202	2	-	10/24/74/74	0/4/4/4
31	PEB	Q1	202	3	-	9/24/74/74	0/4/4/4
31	PEB	dA	202	2	-	10/24/74/74	0/4/4/4
31	PEB	dF	202	2	-	12/24/74/74	0/4/4/4
33	CYC	m3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	aH	201	3,12	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	YC	201	2	-	7/24/74/74	0/4/4/4
31	PEB	BA	201	2	-	3/24/74/74	0/4/4/4
31	PEB	KK	201	3	-	7/24/74/74	0/4/4/4
31	PEB	RG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	IA	201	2	-	7/24/74/74	0/4/4/4
31	PEB	I5	201	2	-	7/24/74/74	0/4/4/4
31	PEB	TC	201	2,10	-	9/24/74/74	0/4/4/4
31	PEB	dH	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	NF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	m4	201	2	-	9/24/74/74	0/4/4/4
33	CYC	BE	1002	9,7	-	5/25/74/74	0/4/4/4
31	PEB	K9	201	3	-	11/24/74/74	0/4/4/4
31	PEB	P7	202	2	-	8/24/74/74	0/4/4/4
31	PEB	UC	201	2,3	-	9/24/74/74	0/4/4/4
31	PEB	G8	203	3	-	9/24/74/74	0/4/4/4
33	CYC	I3	1001	20	-	4/25/74/74	0/4/4/4
31	PEB	MG	401	3,11	-	10/24/74/74	0/4/4/4
31	PEB	TB	201	2	-	5/24/74/74	0/4/4/4
31	PEB	bF	201	2	-	4/24/74/74	0/4/4/4
31	PEB	V7	201	2	-	7/24/74/74	0/4/4/4
31	PEB	kC	202	2	-	9/24/74/74	0/4/4/4
31	PEB	jH	202	3	-	12/24/74/74	0/4/4/4
31	PEB	gC	203	2,14,3	-	9/24/74/74	0/4/4/4
31	PEB	kF	202	3	-	10/24/74/74	0/4/4/4
31	PEB	WK	202	3	-	12/24/74/74	0/4/4/4
33	CYC	T3	1001	19	-	8/25/74/74	0/4/4/4
31	PEB	gA	203	2	-	12/24/74/74	0/4/4/4
31	PEB	N4	201	2	-	10/24/74/74	0/4/4/4
31	PEB	NG	201	3	-	8/24/74/74	0/4/4/4
31	PEB	YD	202	2	-	11/24/74/74	0/4/4/4
31	PEB	PE	202	2,10	-	4/24/74/74	0/4/4/4
31	PEB	X7	201	2	-	5/24/74/74	0/4/4/4
31	PEB	tF	201	2	-	7/24/74/74	0/4/4/4
31	PEB	C7	201	2,3	-	11/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	PEB	V2	201	2	-	2/24/74/74	0/4/4/4
31	PEB	Y4	203	3	-	13/24/74/74	0/4/4/4
31	PEB	F4	202	2	-	9/24/74/74	0/4/4/4
31	PEB	Y8	203	2,3	-	7/24/74/74	0/4/4/4
31	PEB	B5	201	3	-	11/24/74/74	0/4/4/4
31	PEB	HK	203	2	-	12/24/74/74	0/4/4/4
31	PEB	J6	1002	9	-	12/24/74/74	0/4/4/4
33	CYC	DC	1003	8,9	-	10/25/74/74	0/4/4/4
31	PEB	SJ	202	2	-	9/24/74/74	0/4/4/4
31	PEB	m6	202	2	-	8/24/74/74	0/4/4/4
31	PEB	gE	201	2	-	6/24/74/74	0/4/4/4
31	PEB	Y5	202	2,31	-	7/24/74/74	0/4/4/4
31	PEB	KI	201	3	-	8/24/74/74	0/4/4/4
31	PEB	c4	202	2	-	10/24/74/74	0/4/4/4
31	PEB	A8	202	3	-	11/24/74/74	0/4/4/4
31	PEB	SF	202	3	-	7/24/74/74	0/4/4/4
31	PEB	OI	201	2	-	14/24/74/74	0/4/4/4
31	PEB	E4	202	3	-	7/24/74/74	0/4/4/4
31	PEB	IH	202	3	-	6/24/74/74	0/4/4/4
31	PEB	I9	202	3	-	11/24/74/74	0/4/4/4
31	PEB	eD	201	2	-	9/24/74/74	0/4/4/4
31	PEB	e8	201	2,3	-	11/24/74/74	0/4/4/4
31	PEB	O9	202	2	-	10/24/74/74	0/4/4/4
31	PEB	gB	201	2	-	4/24/74/74	0/4/4/4

The worst 5 of 17075 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	I5	202	PEB	CHB-C4B	18.87	1.50	1.35
31	IJ	202	PEB	CHB-C4B	18.85	1.50	1.35
32	NJ	201	PUB	CHB-C1C	18.64	1.50	1.35
32	N5	201	PUB	CHB-C1C	18.59	1.50	1.35
31	LF	202	PEB	CHB-C4B	18.51	1.50	1.35

The worst 5 of 24744 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	FF	201	PEB	OA-C1A-C2A	-17.66	112.13	126.17
31	F8	201	PEB	OA-C1A-C2A	-17.53	112.24	126.17
31	X8	201	PEB	OA-C1A-C2A	-16.33	113.19	126.17
31	RF	201	PEB	OA-C1A-C2A	-16.31	113.20	126.17
31	XF	201	PEB	OA-C1A-C2A	-16.28	113.23	126.17

There are no chirality outliers.

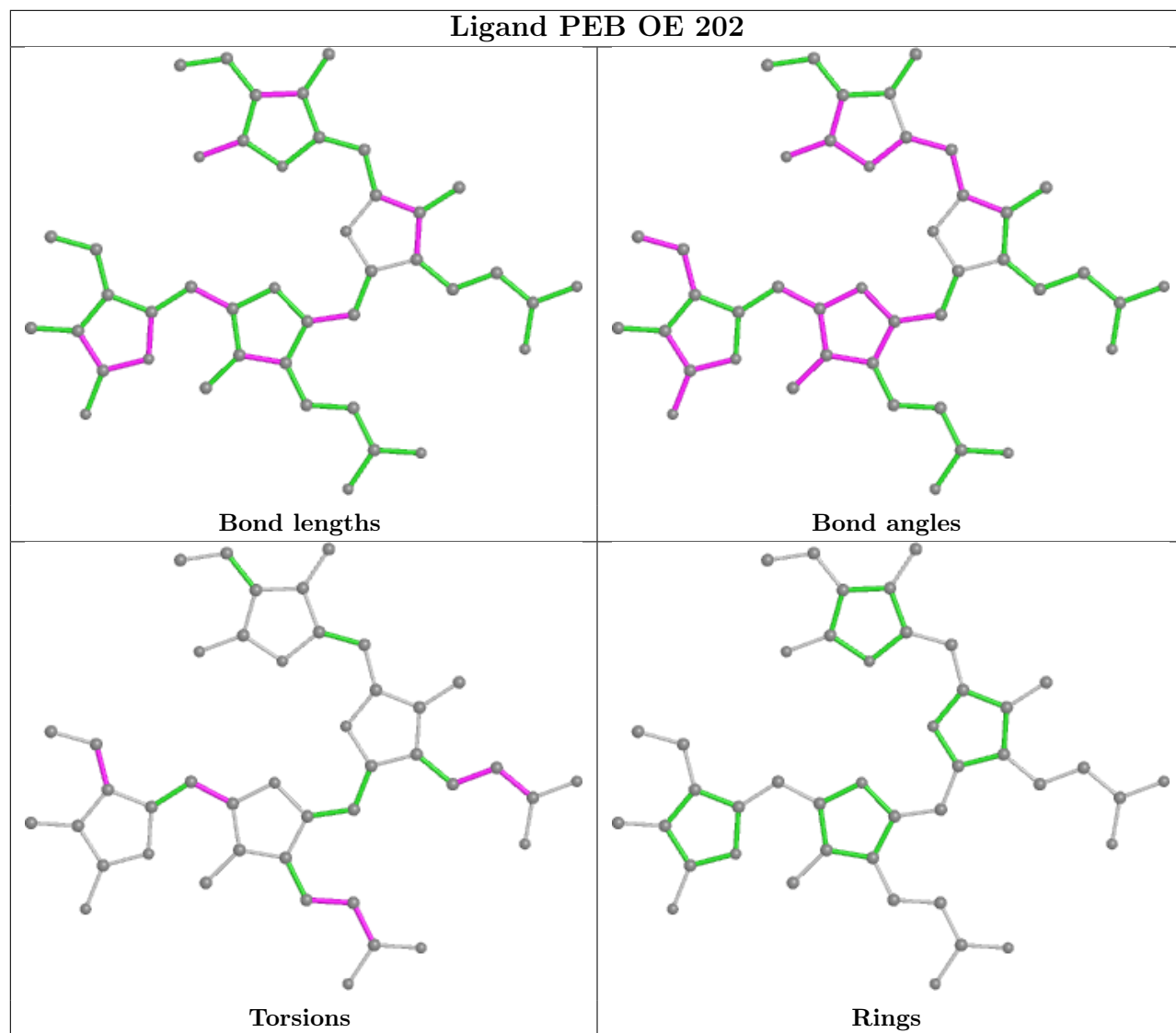
5 of 14212 torsion outliers are listed below:

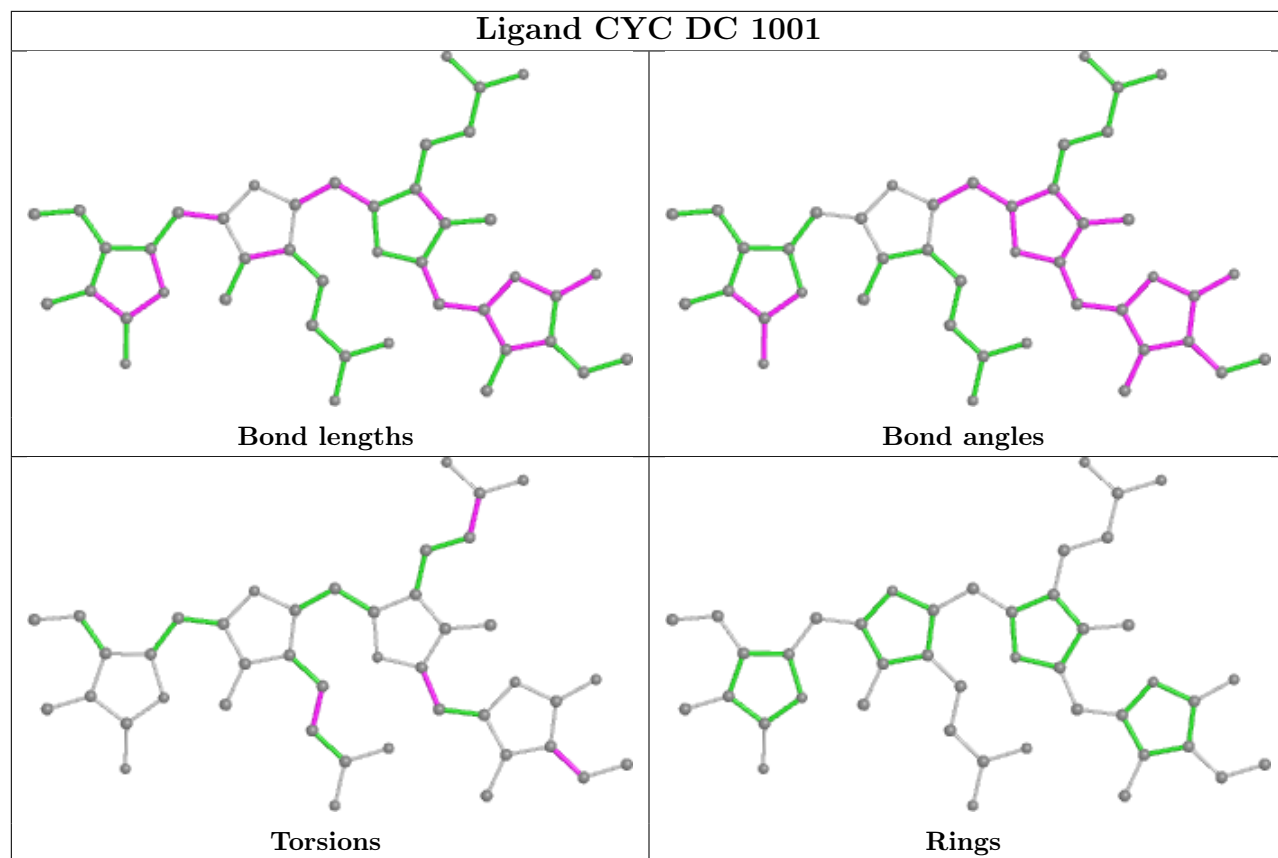
Mol	Chain	Res	Type	Atoms
31	AA	501	PEB	C2A-C3A-CAA-CBA
31	AA	501	PEB	C4A-C3A-CAA-CBA
31	AA	501	PEB	NB-C1B-CHA-C4A
31	AA	501	PEB	C2B-C1B-CHA-C4A
31	BA	201	PEB	NB-C1B-CHA-C4A

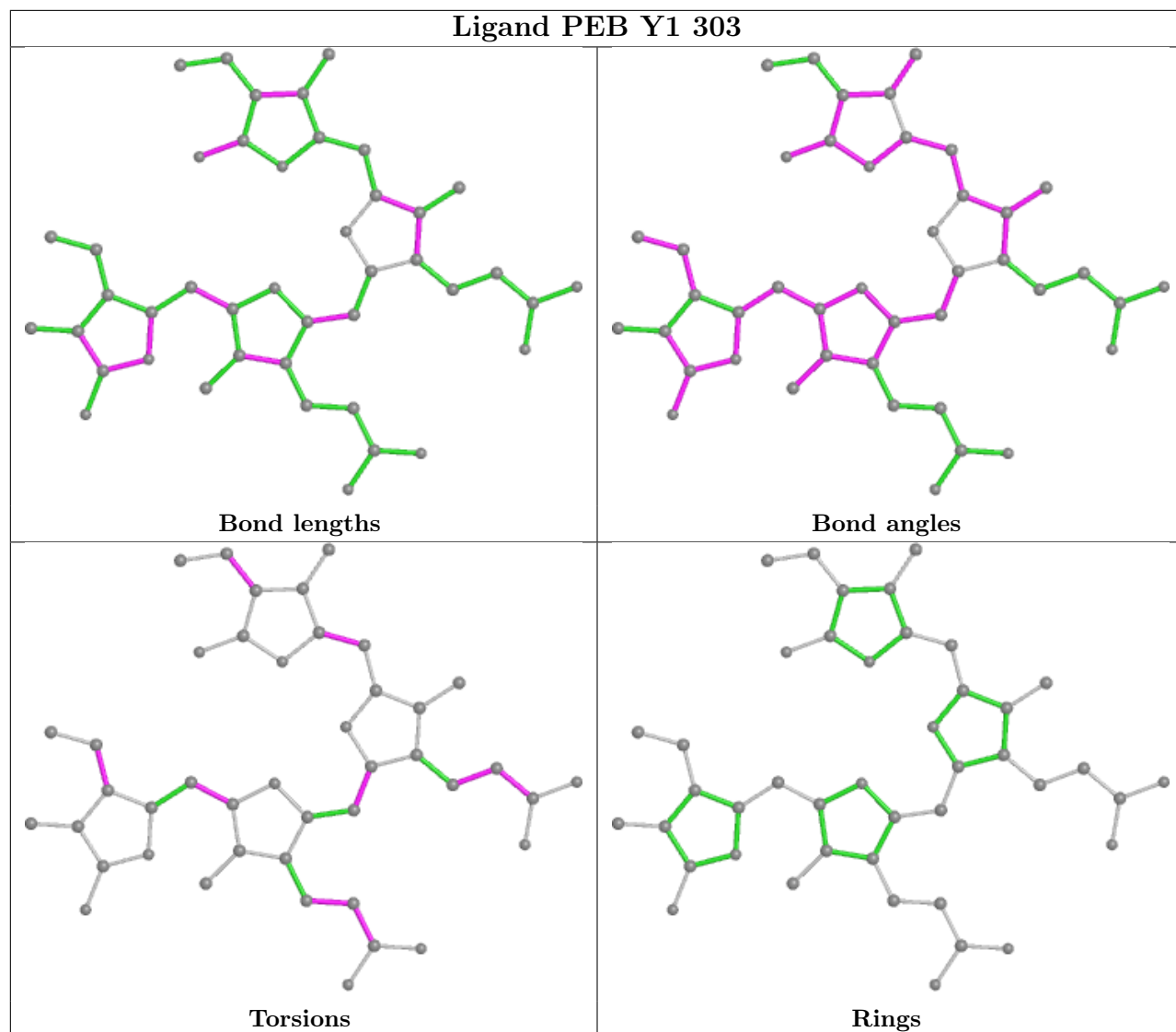
There are no ring outliers.

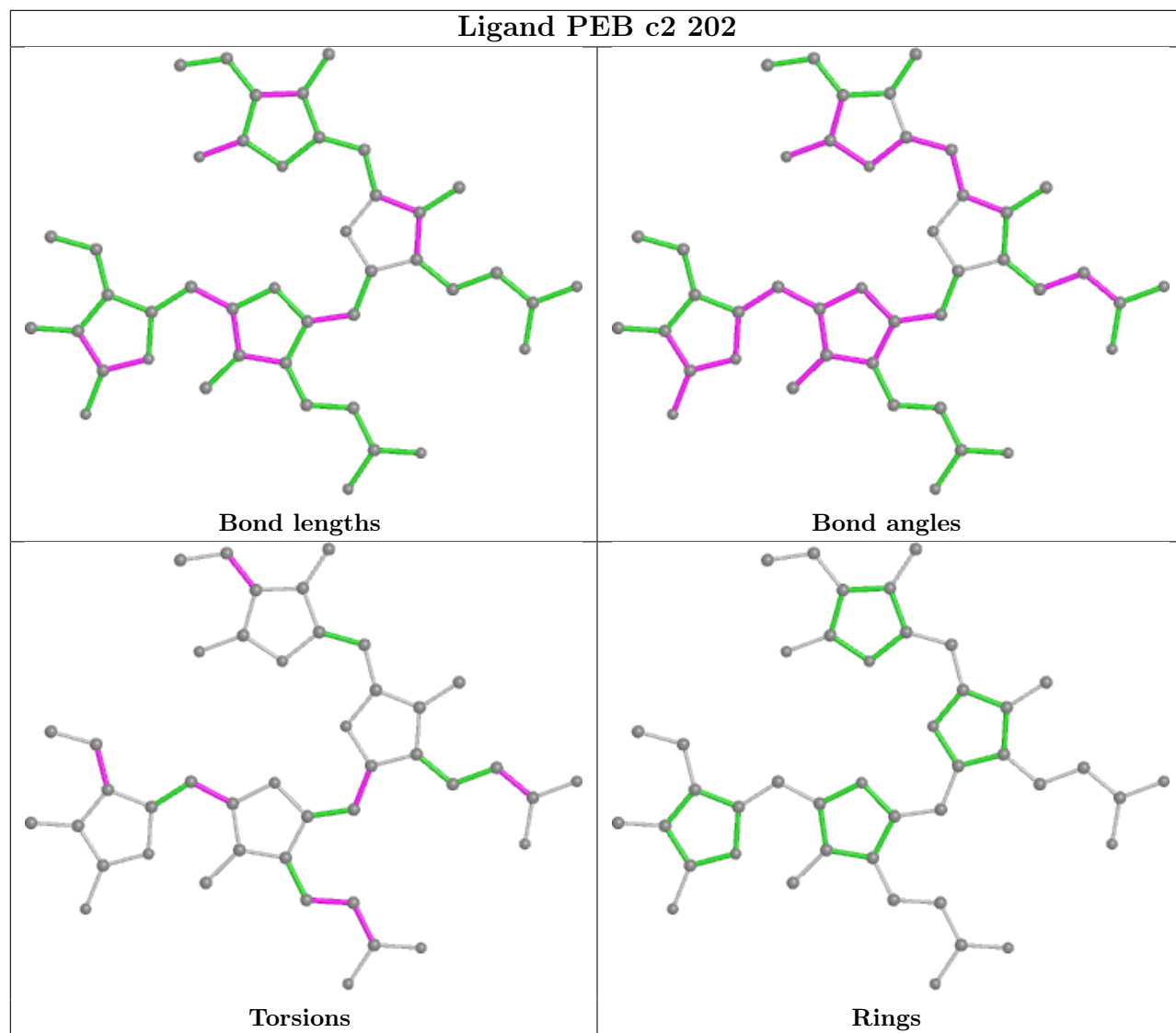
No monomer is involved in short contacts.

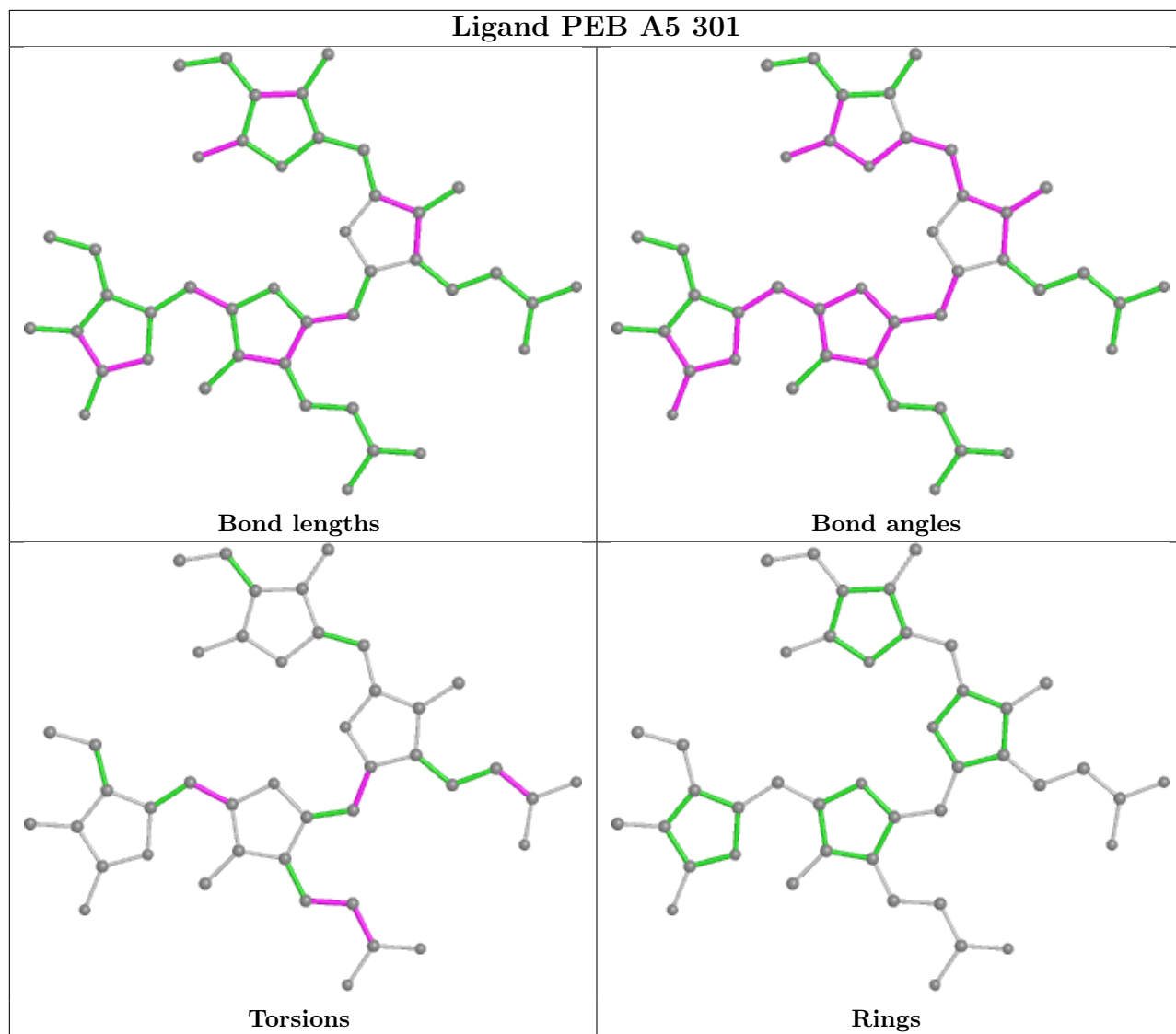
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

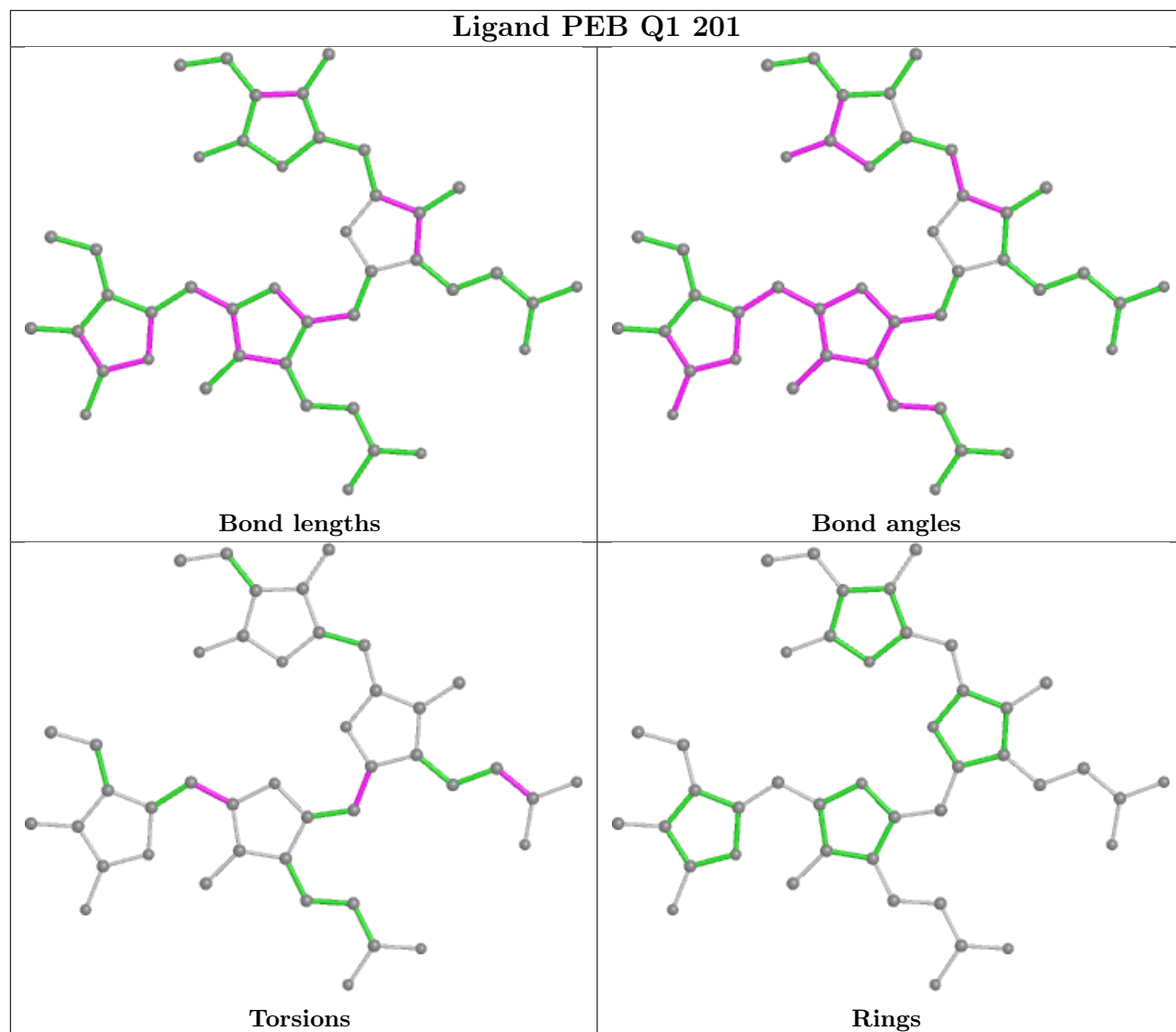


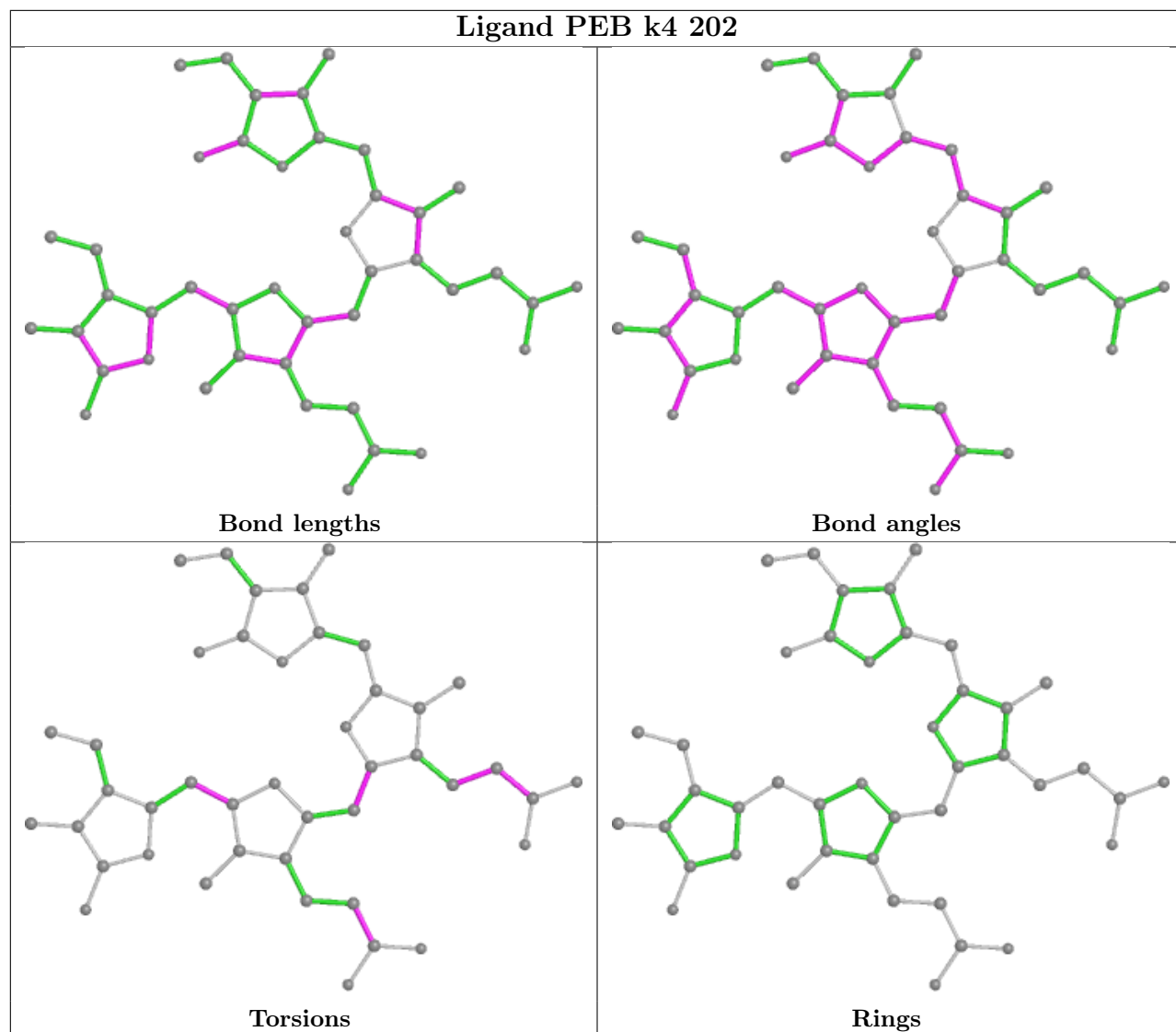


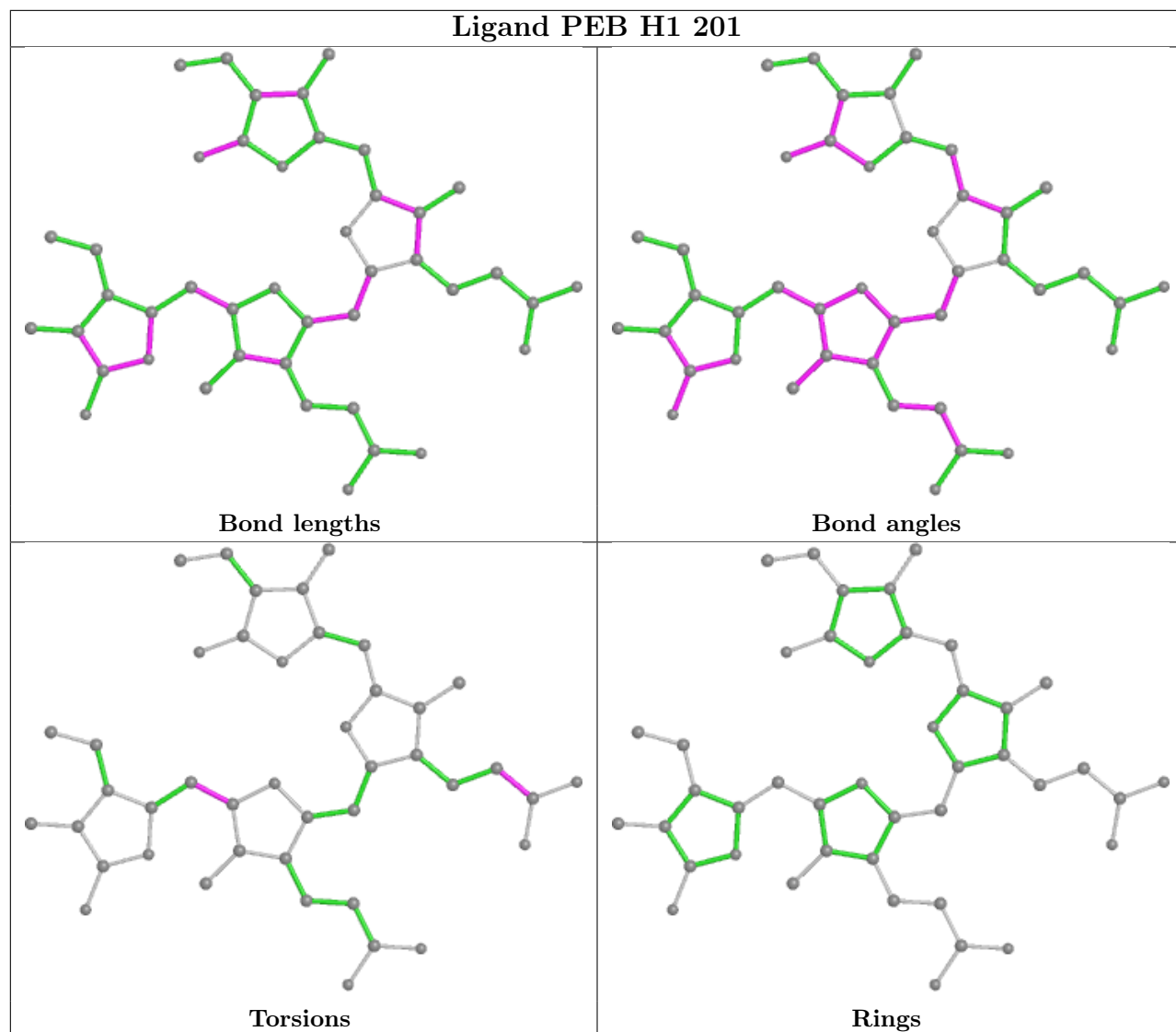


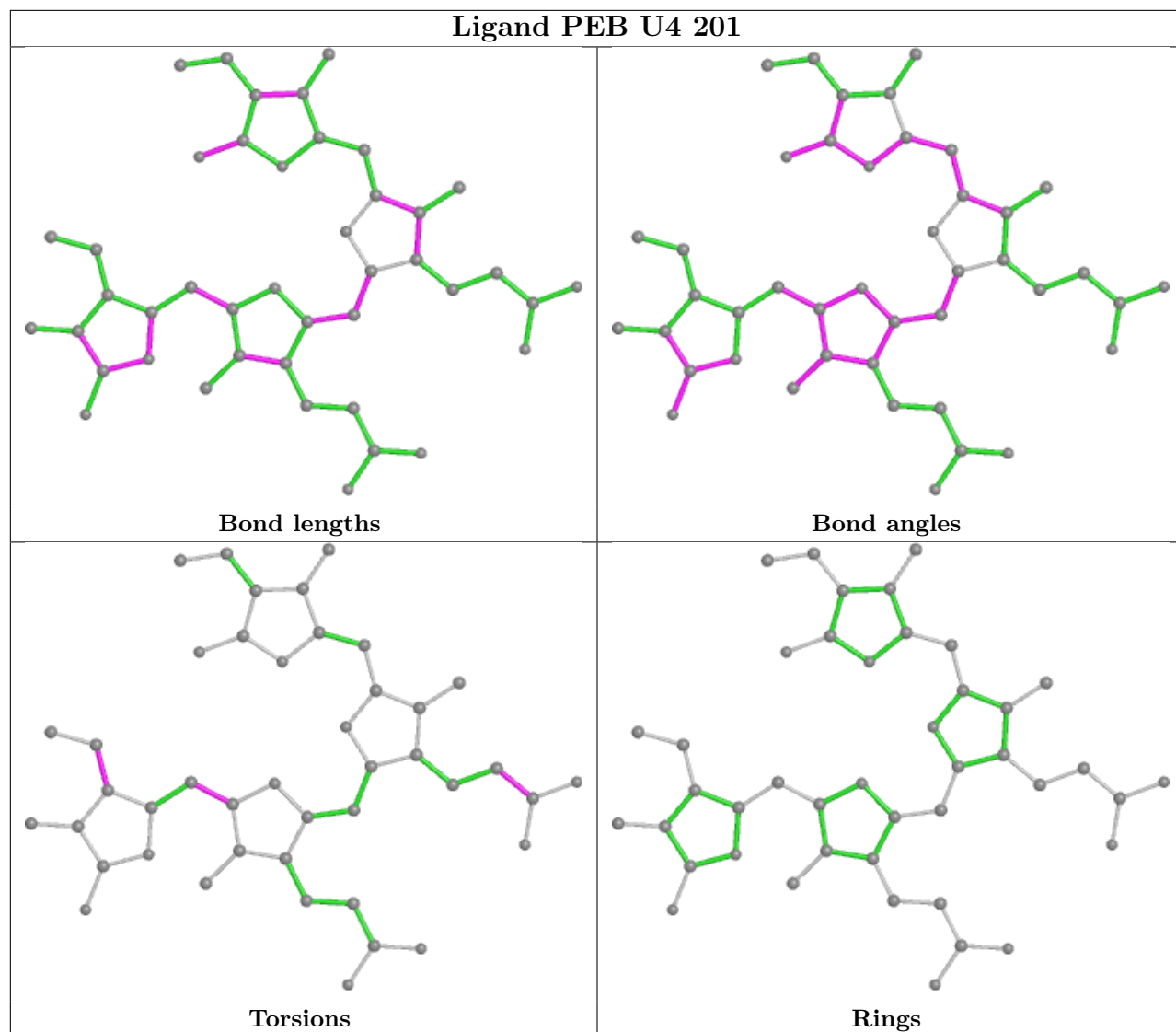


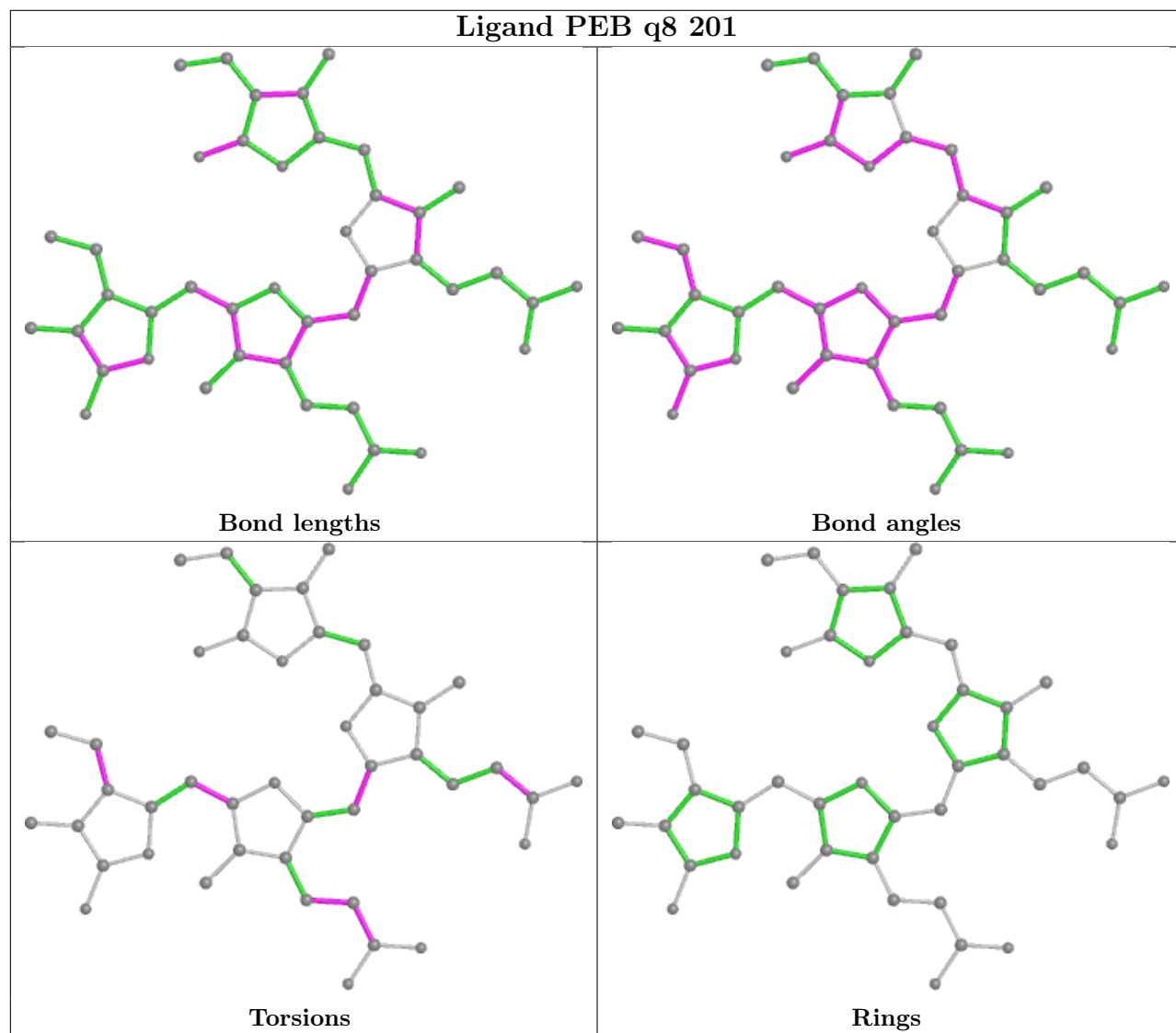


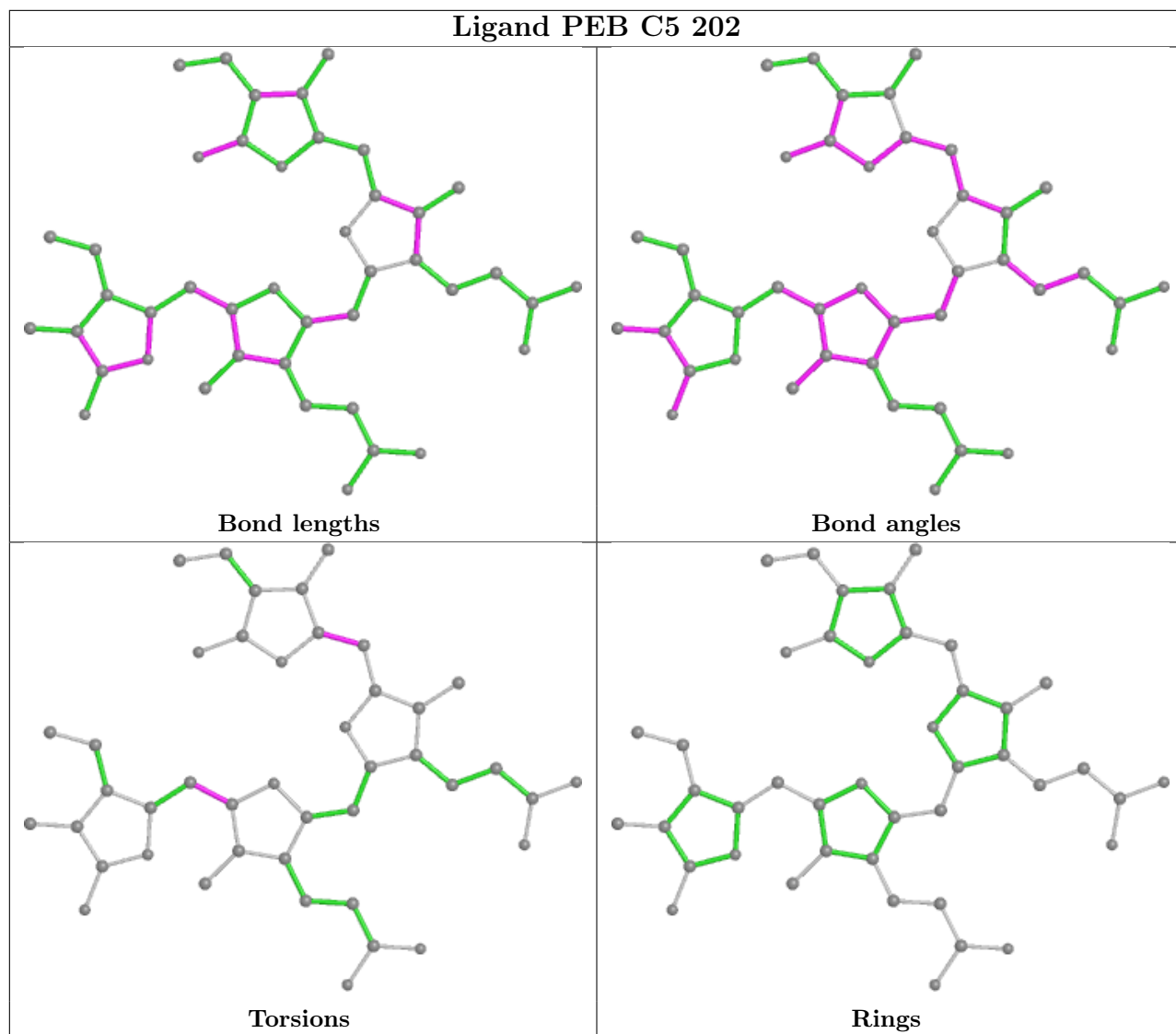


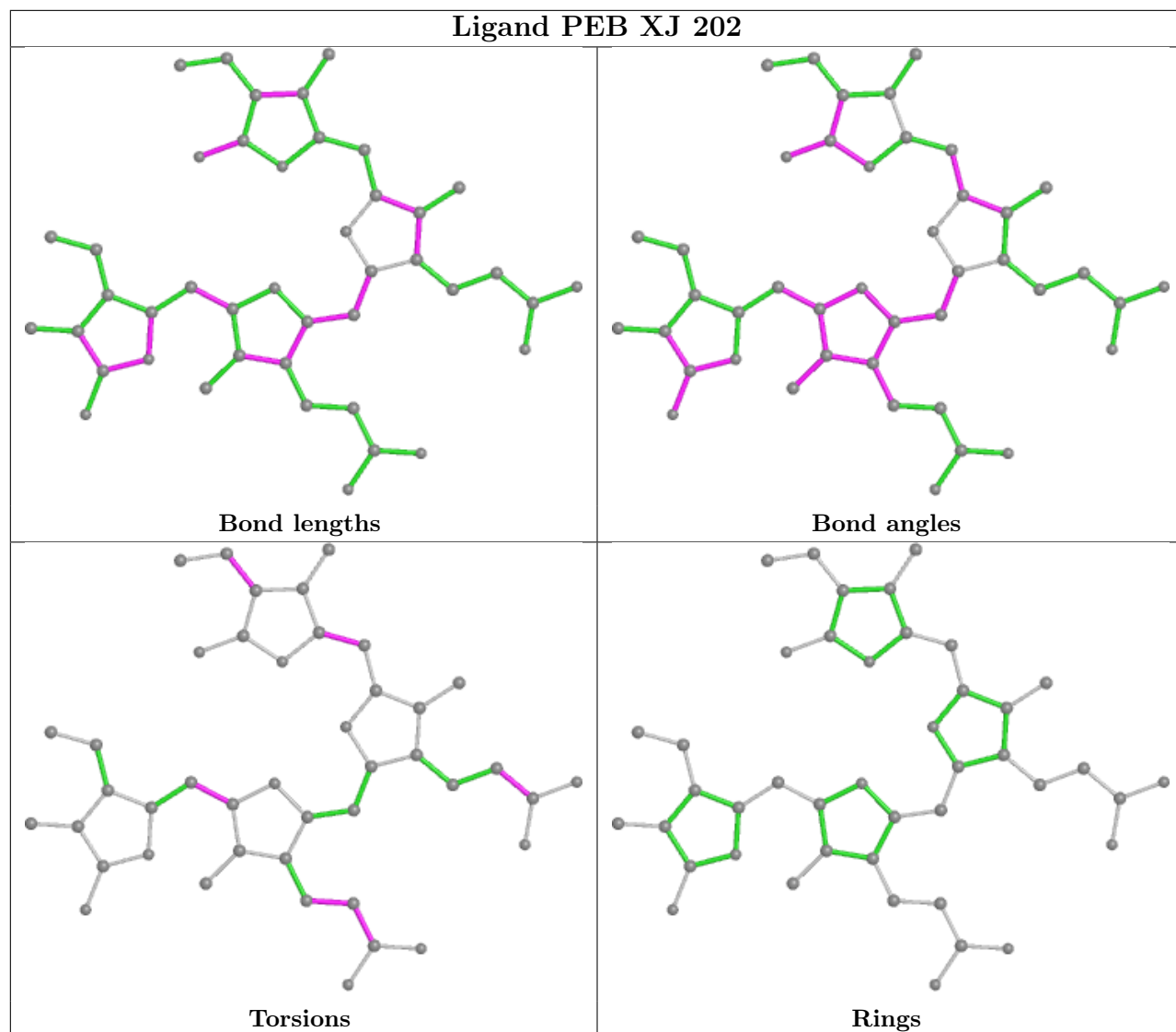


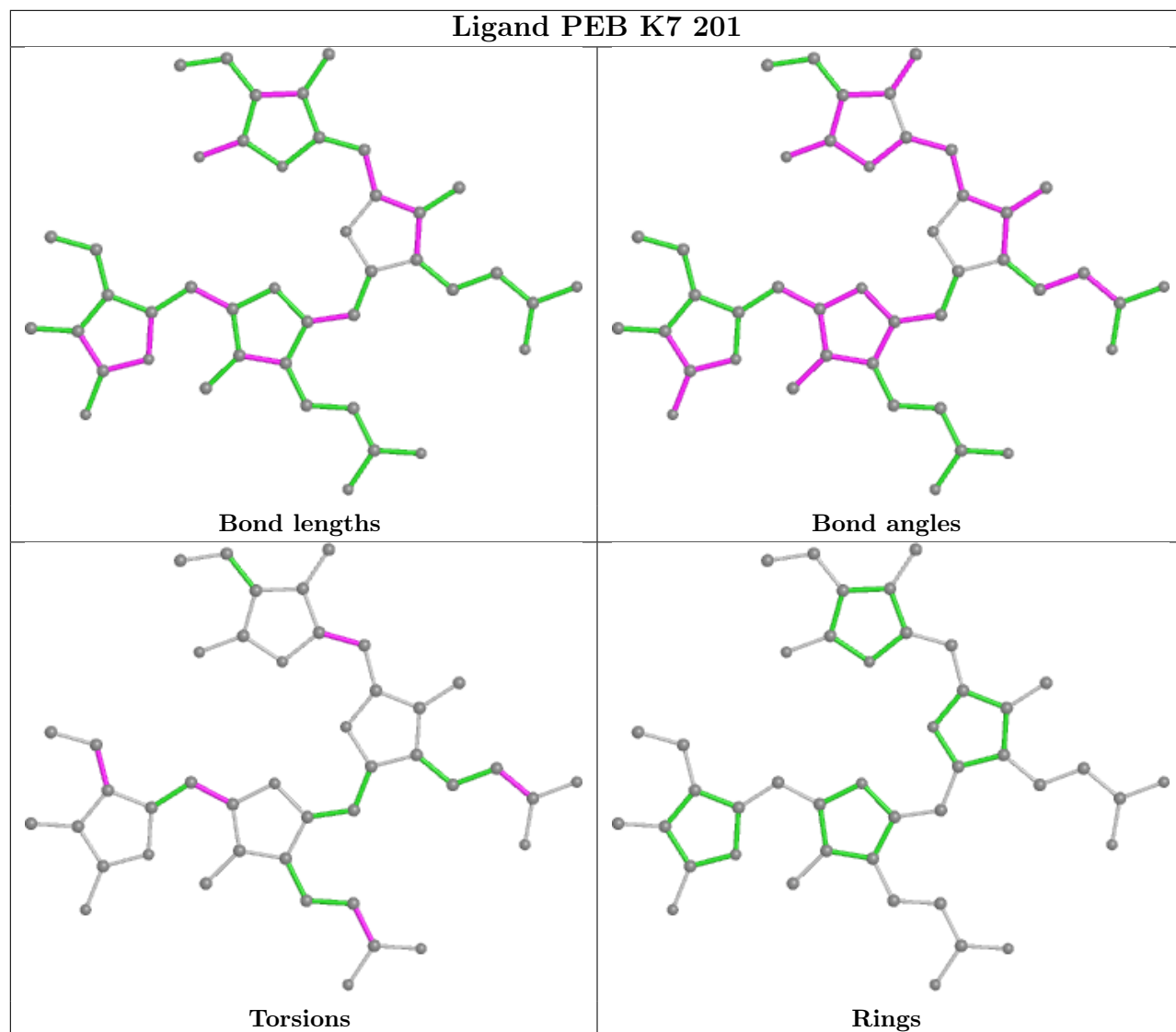


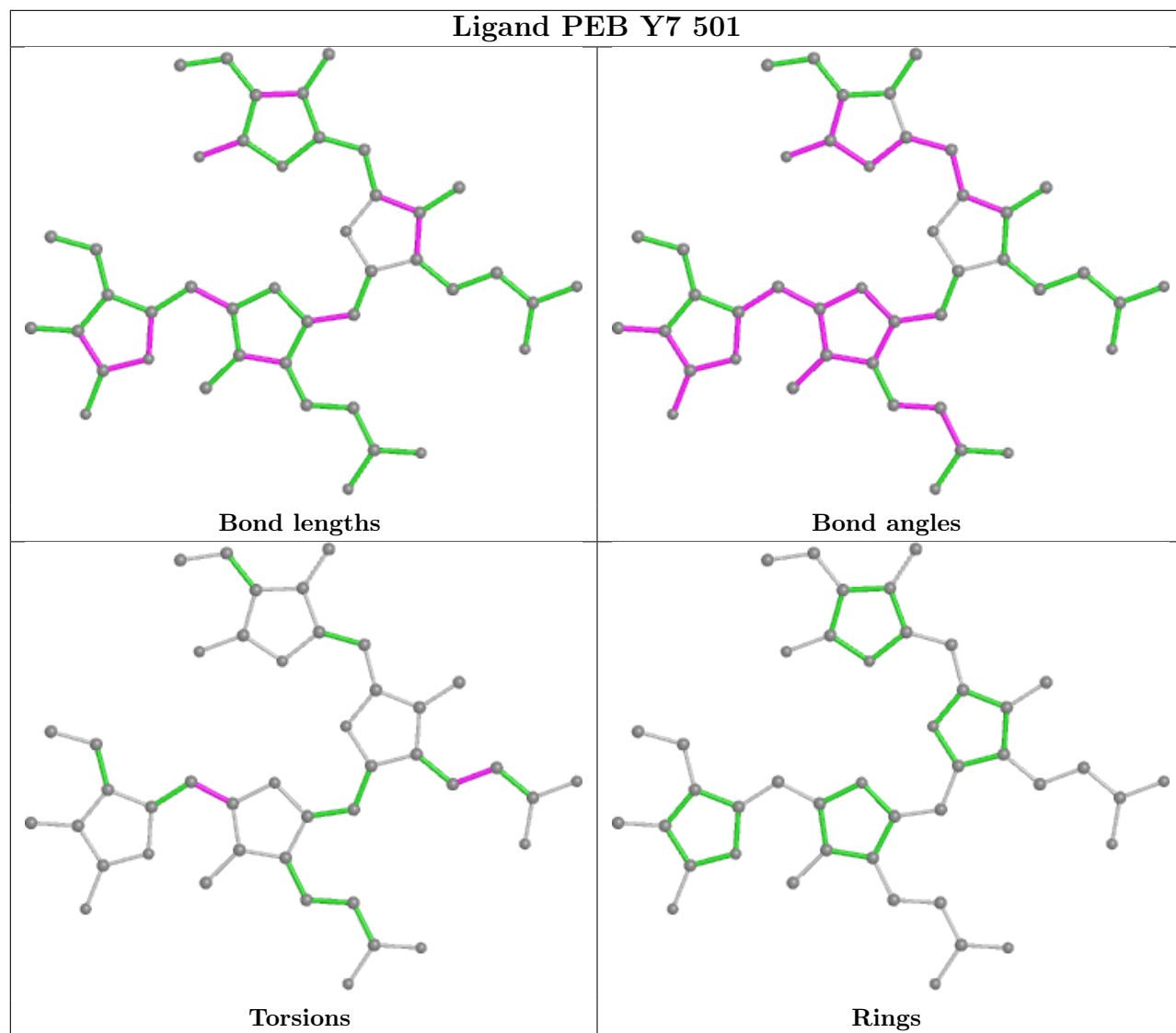


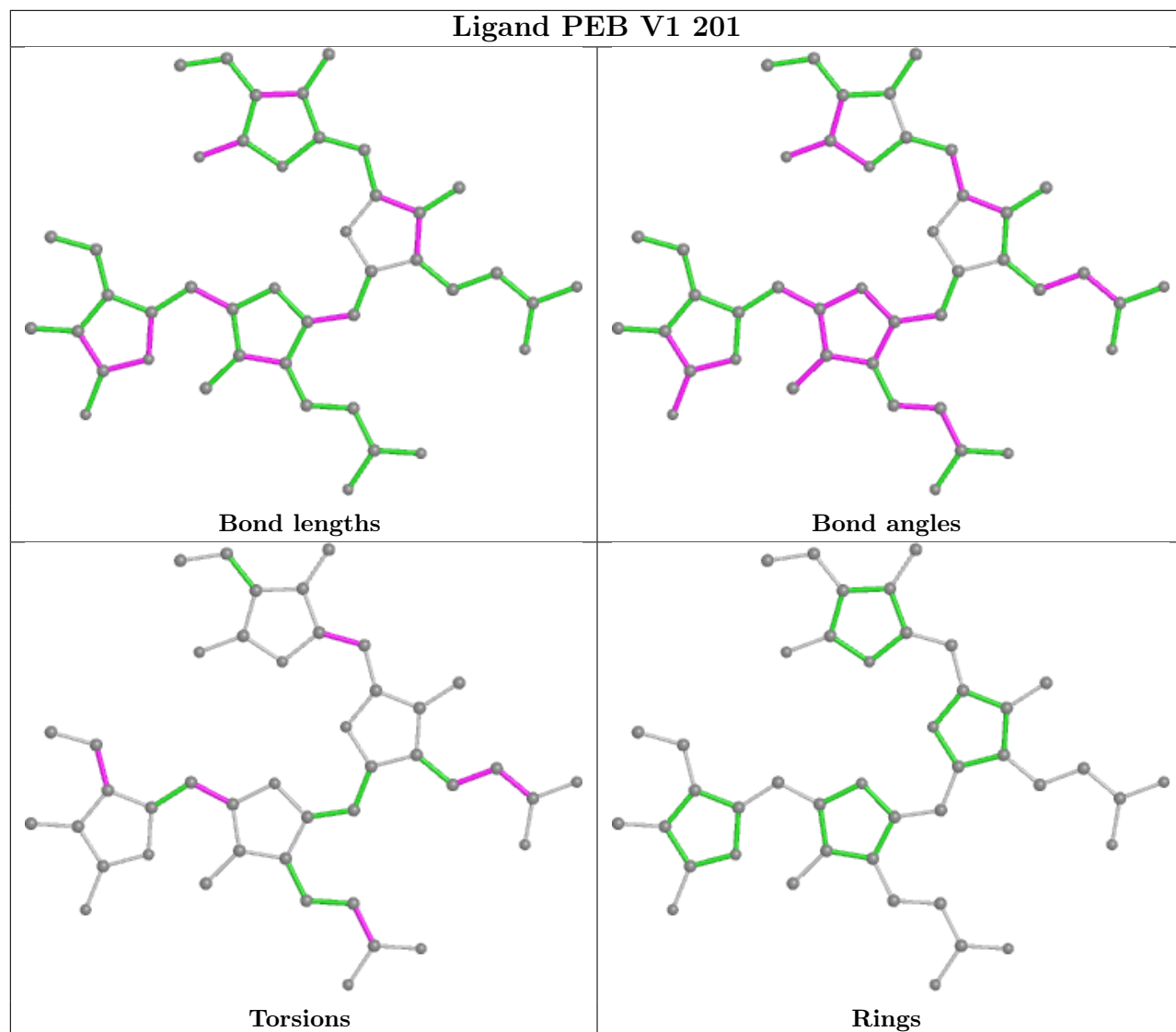


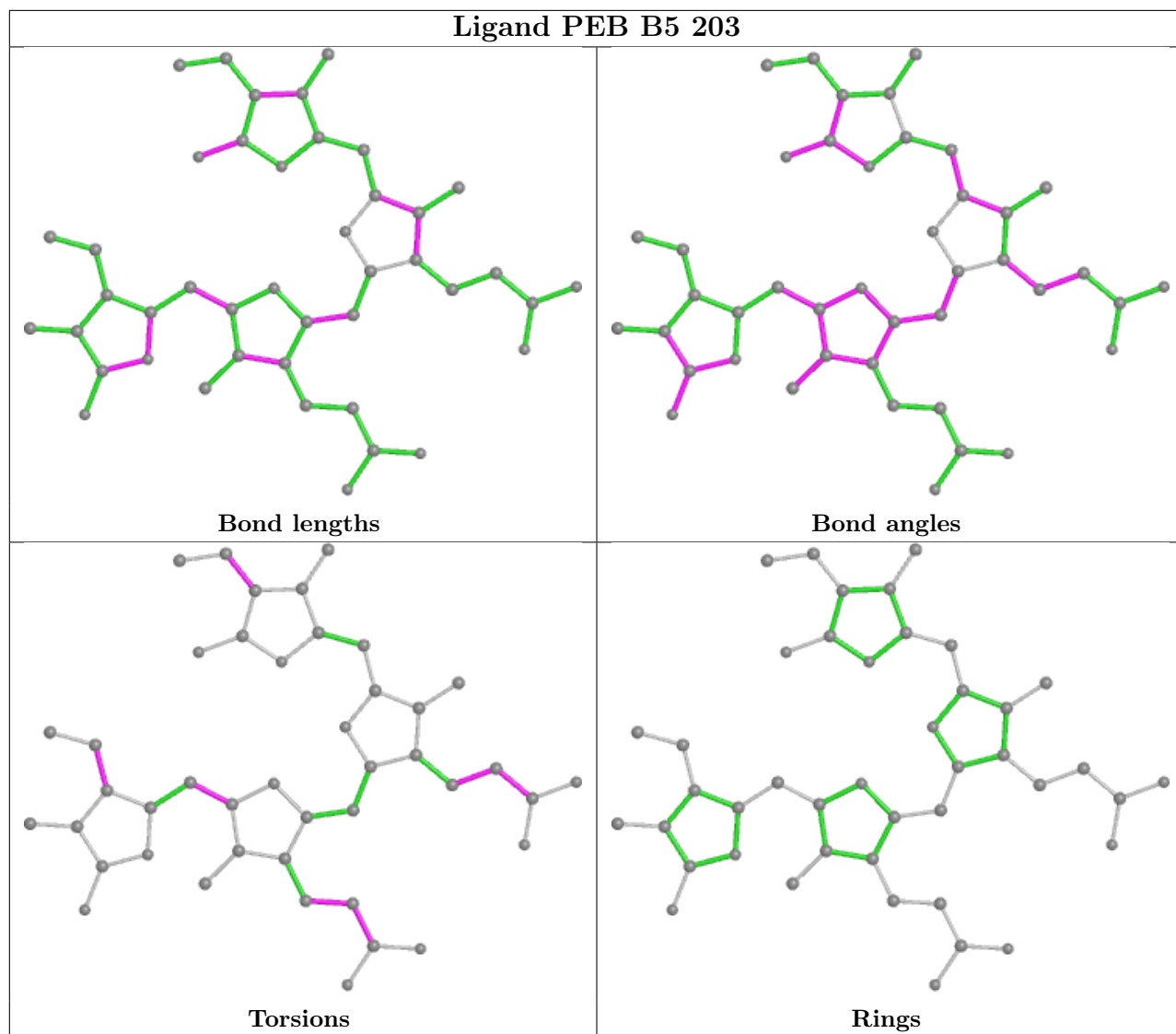


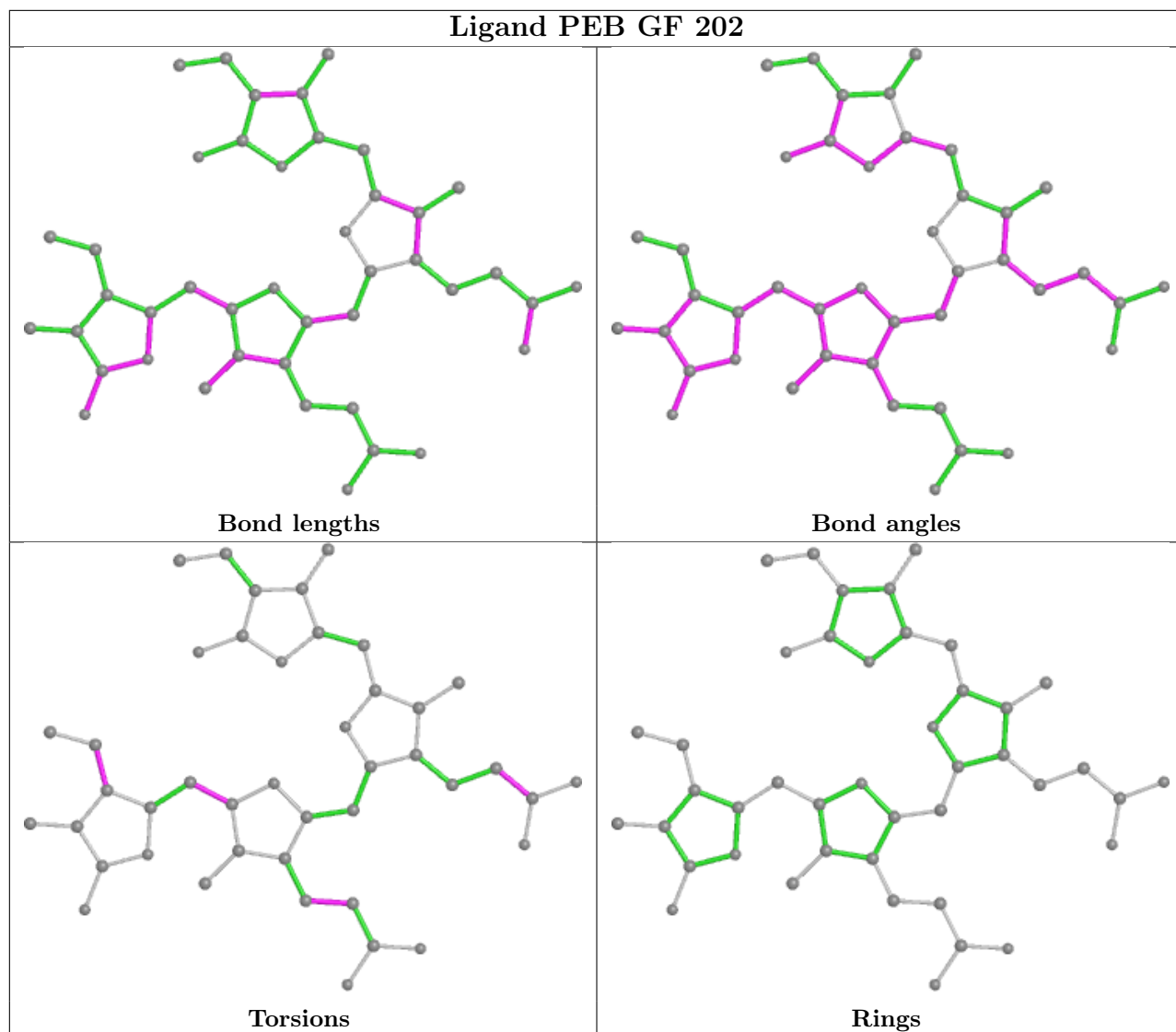


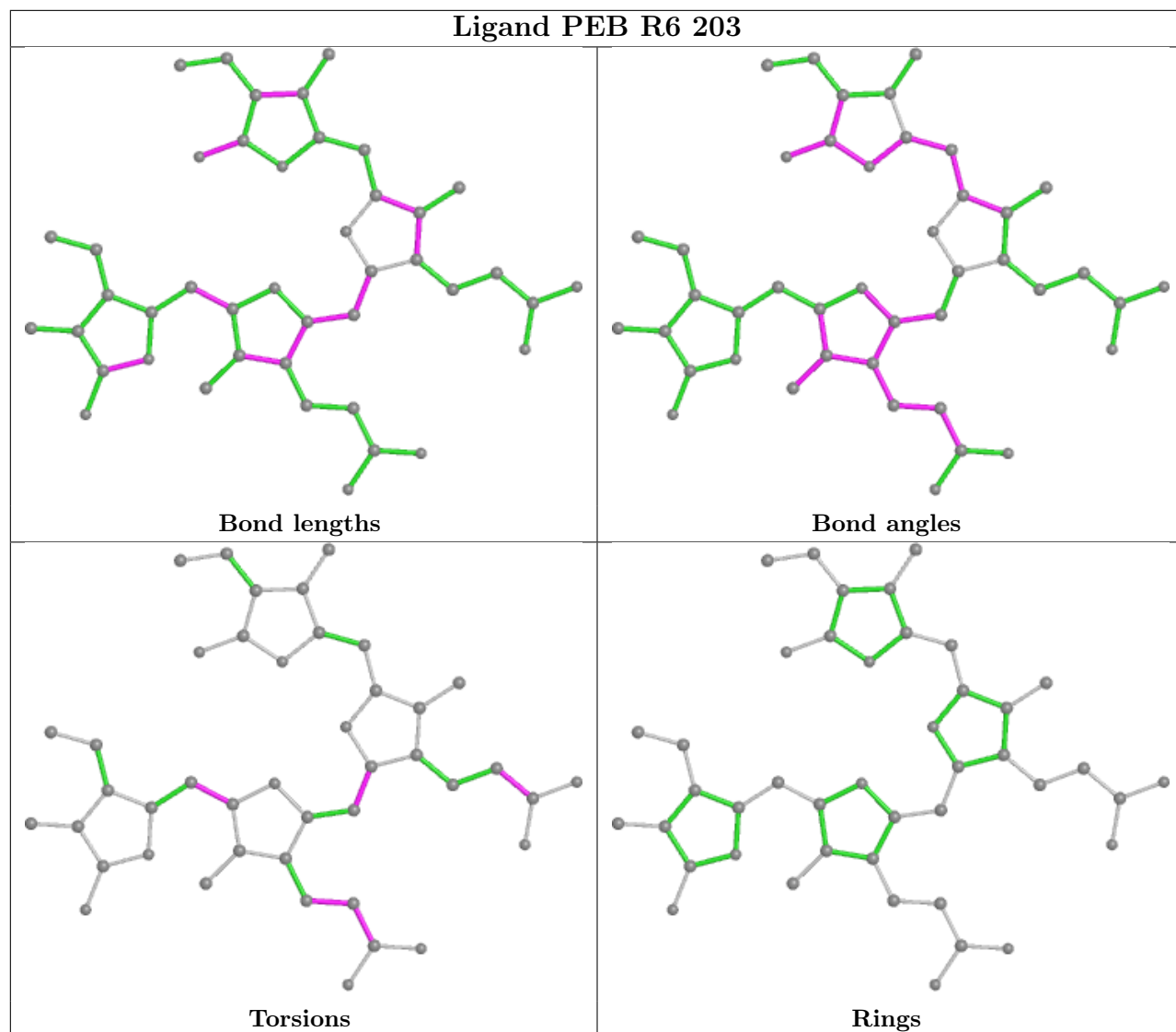


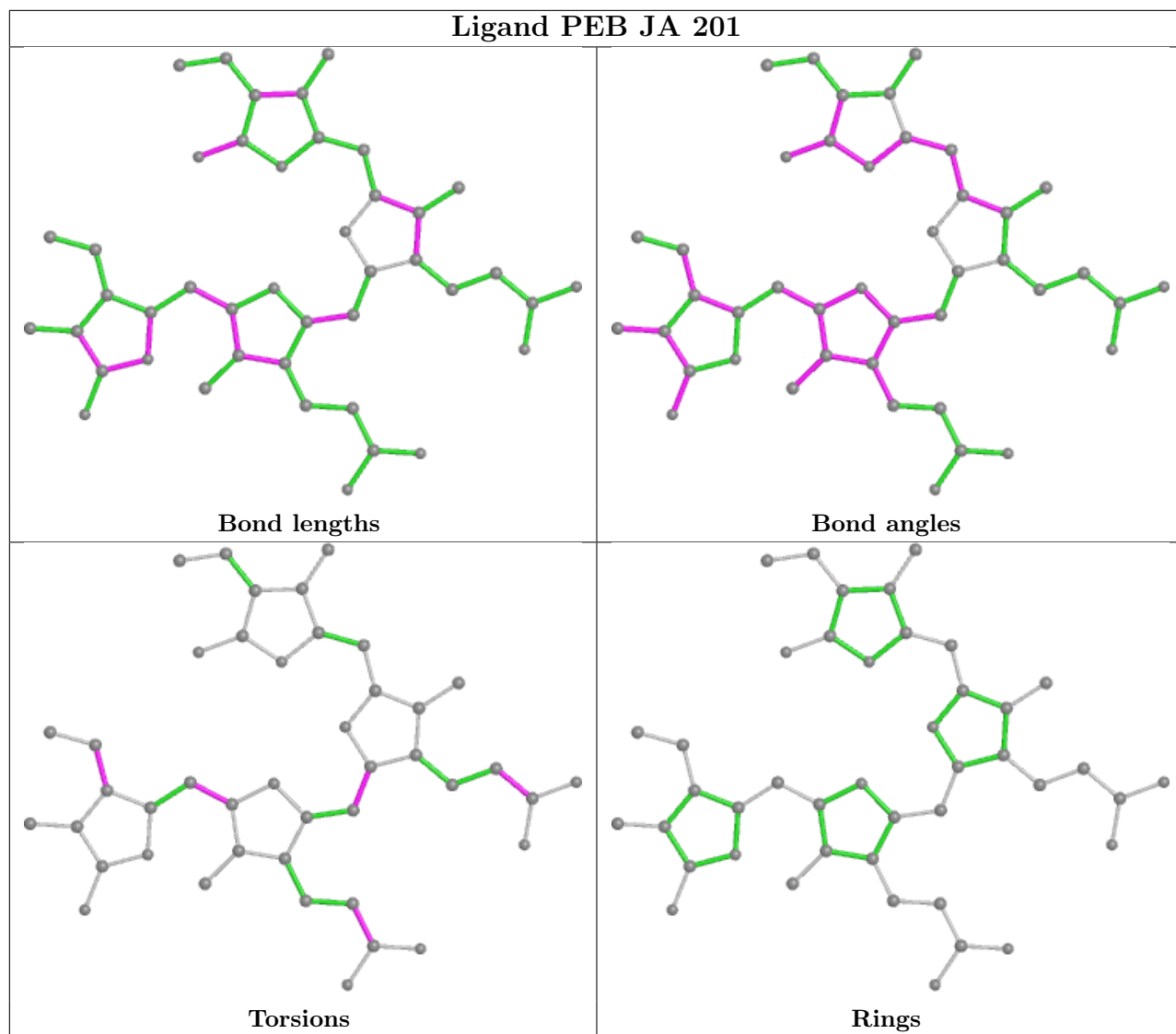


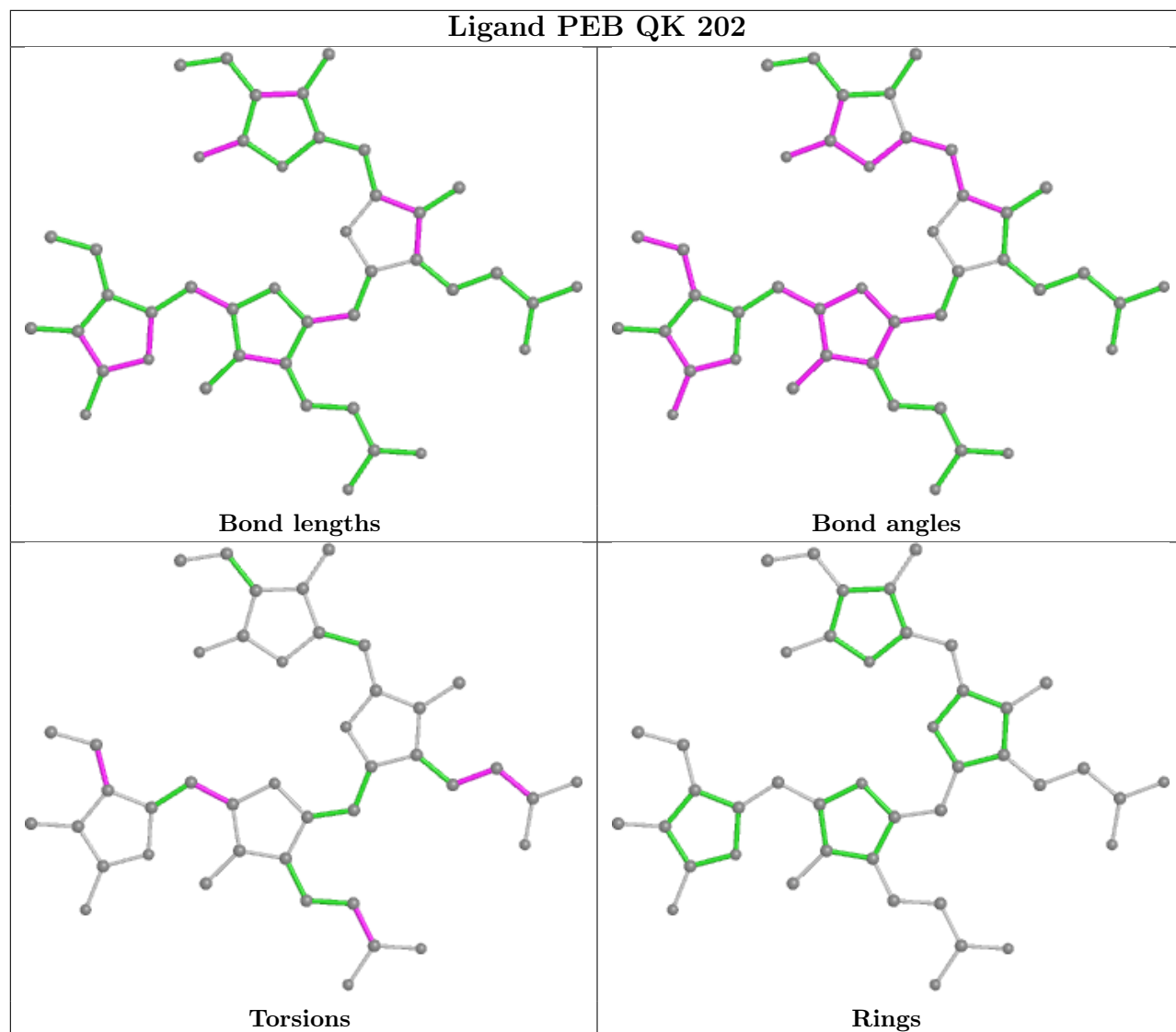


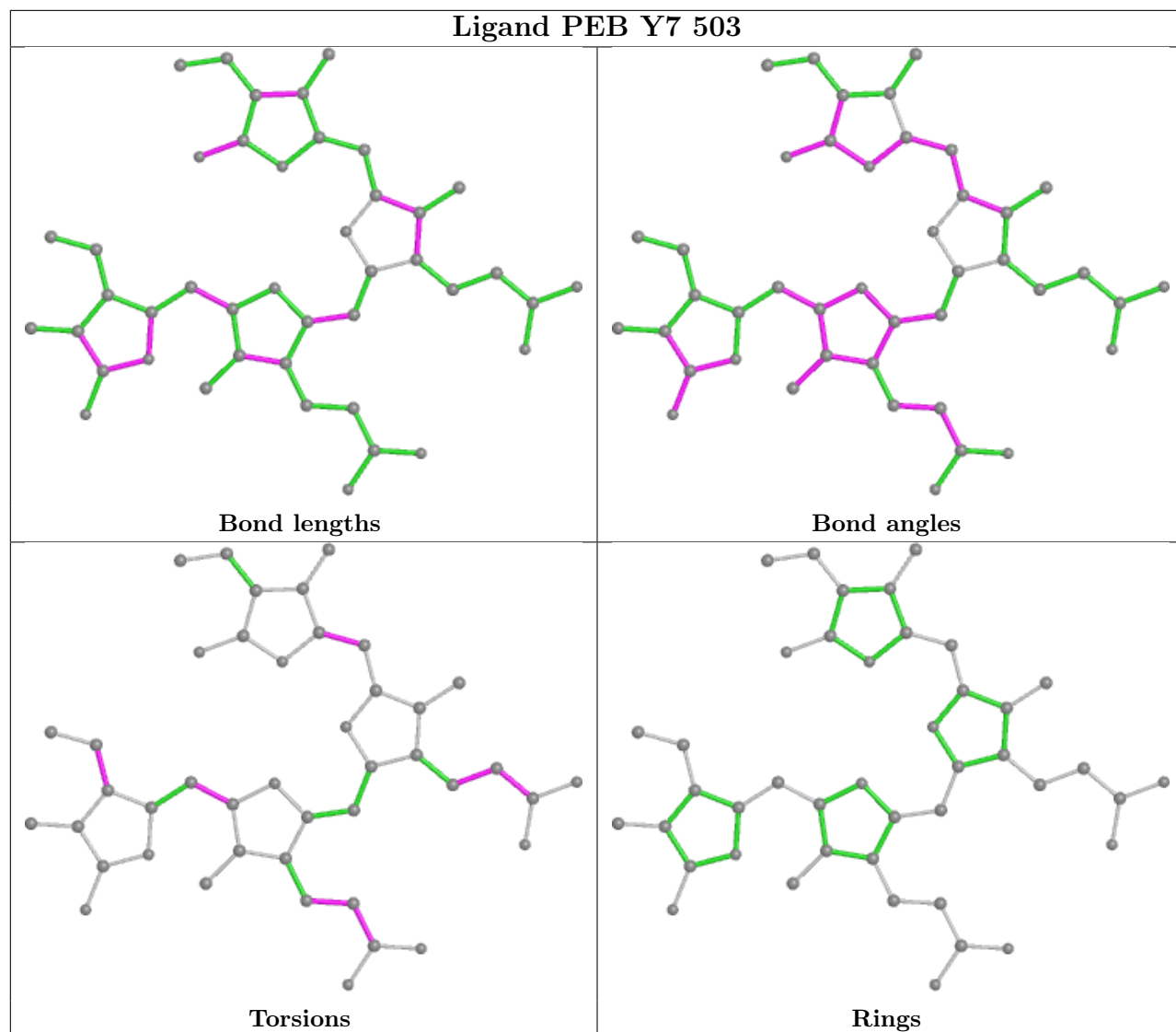


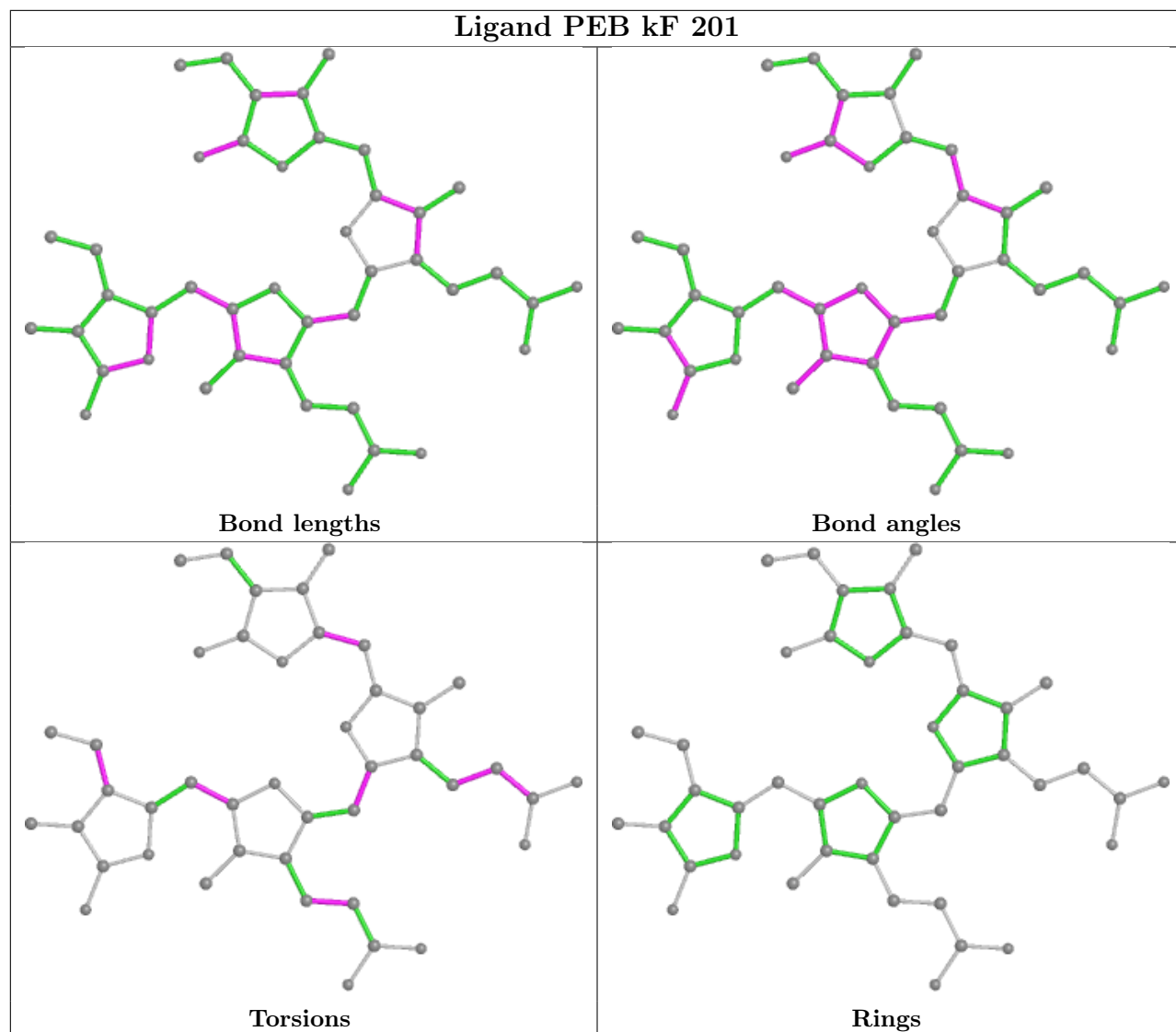


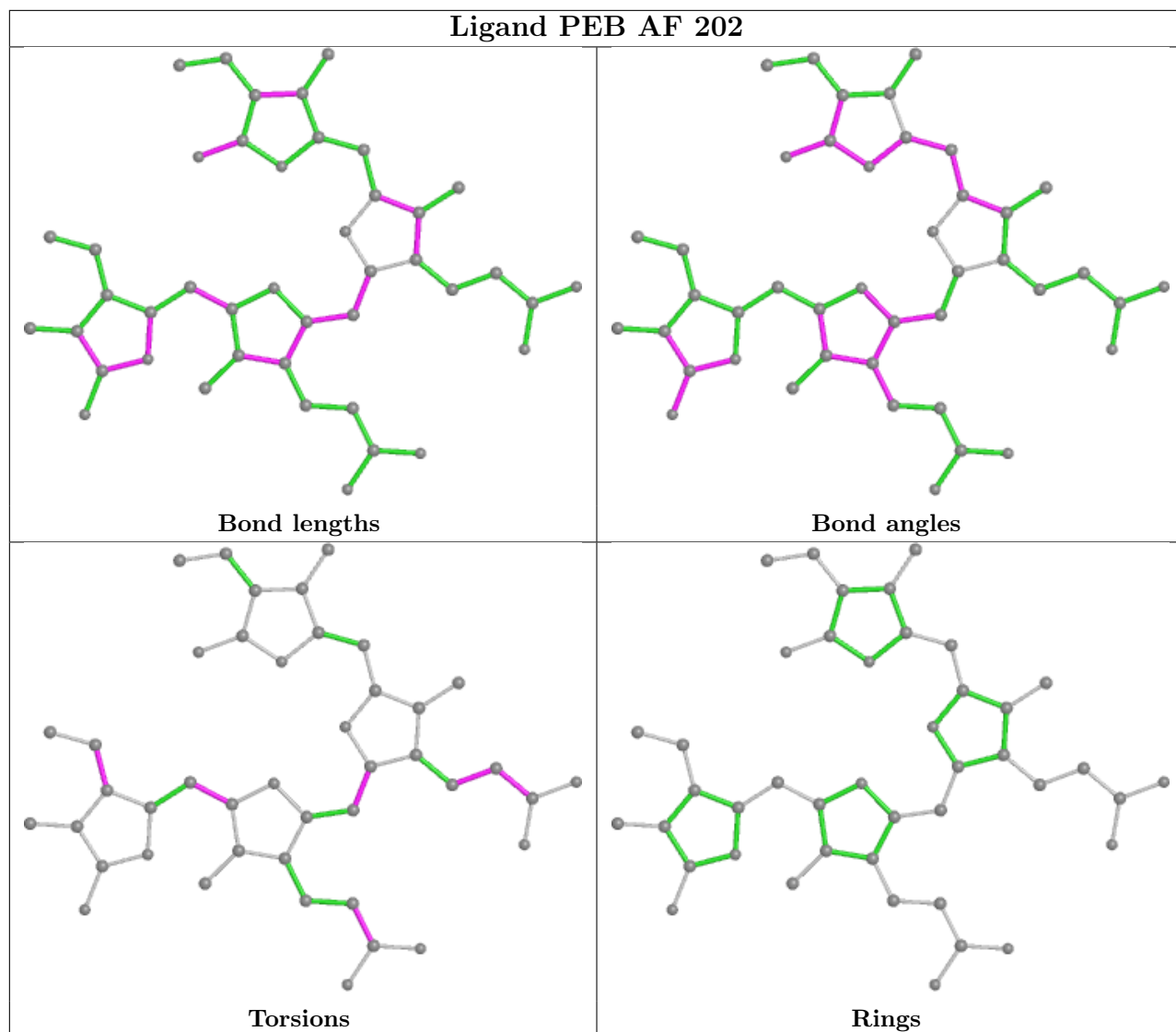


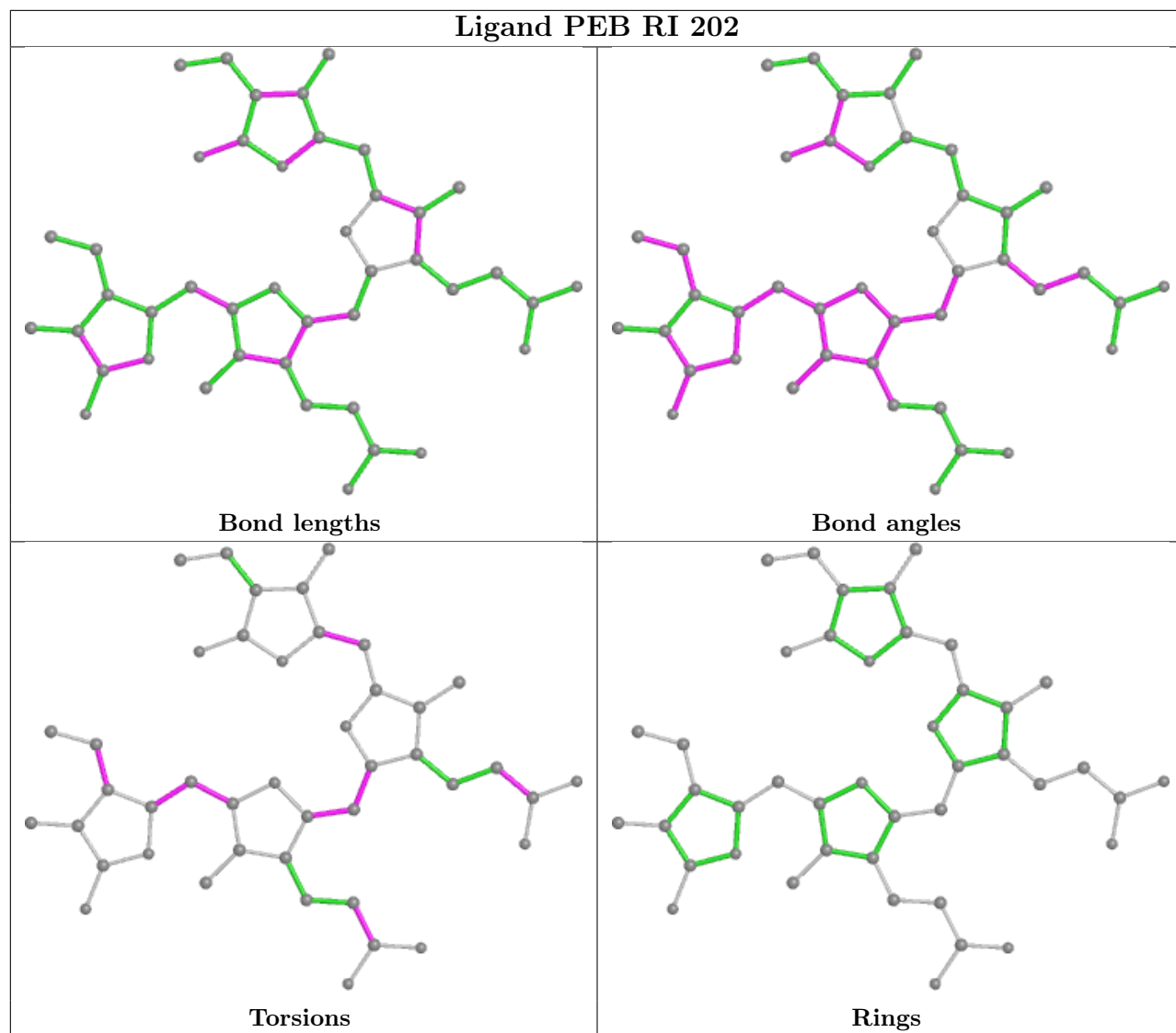


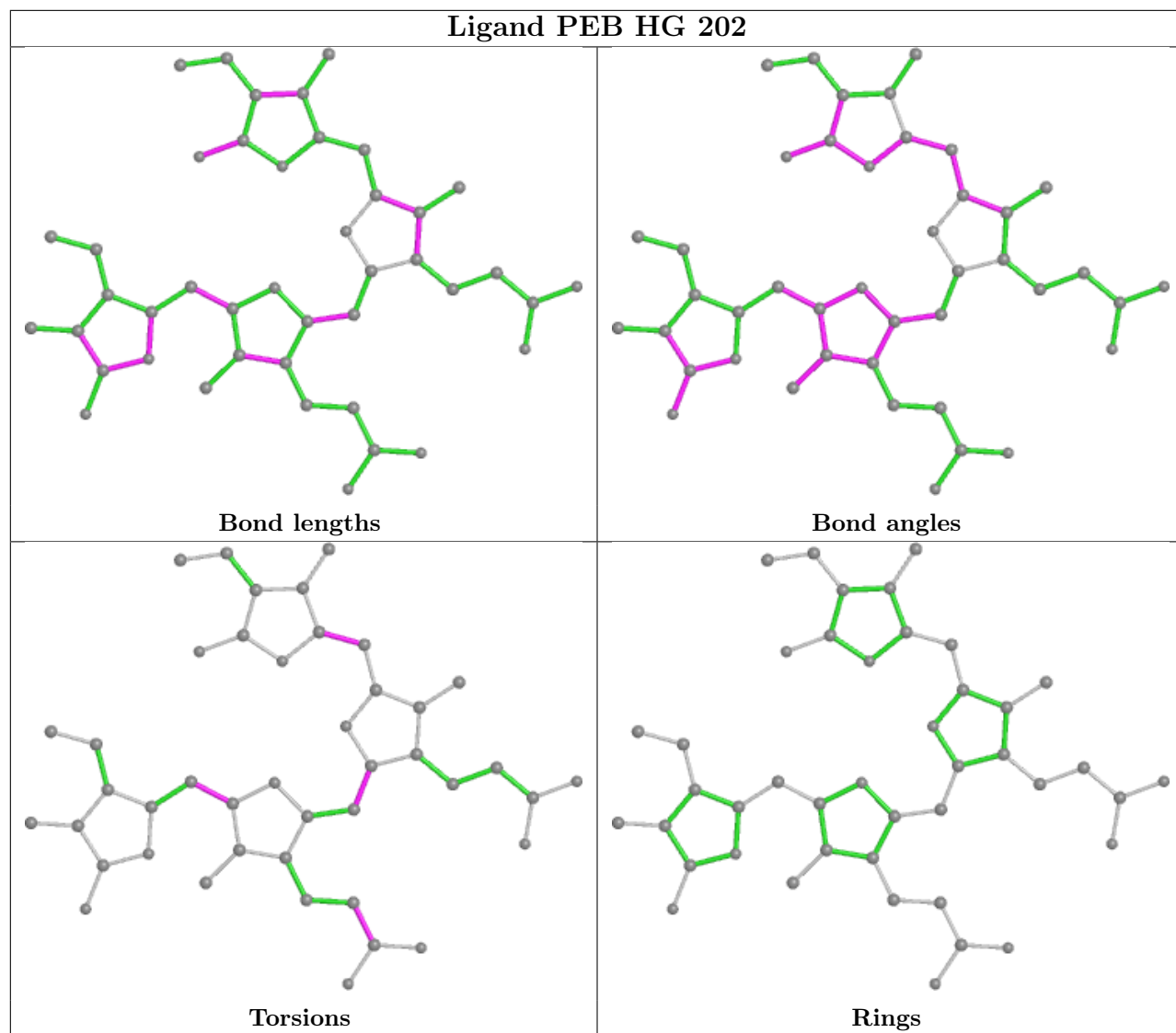


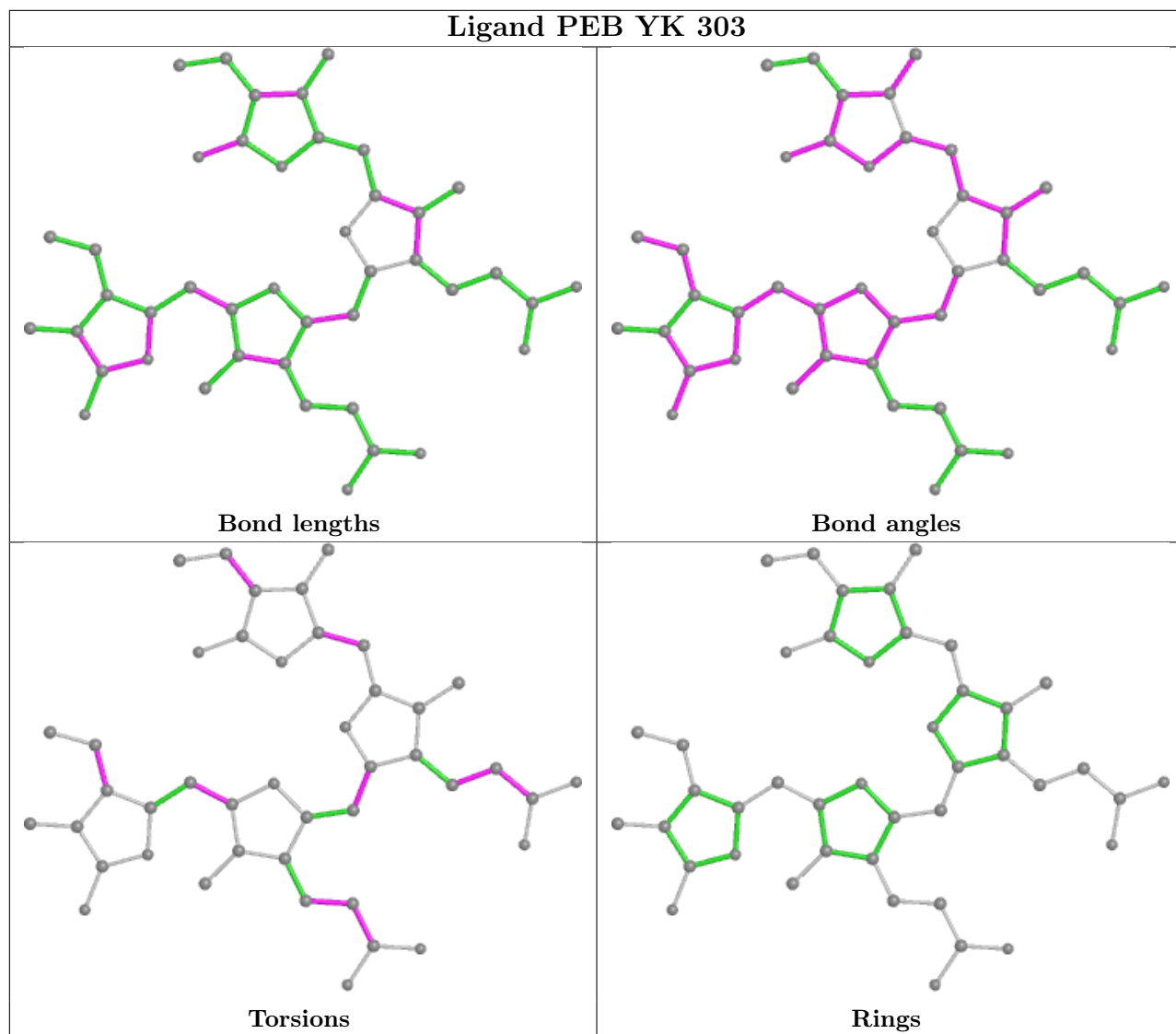


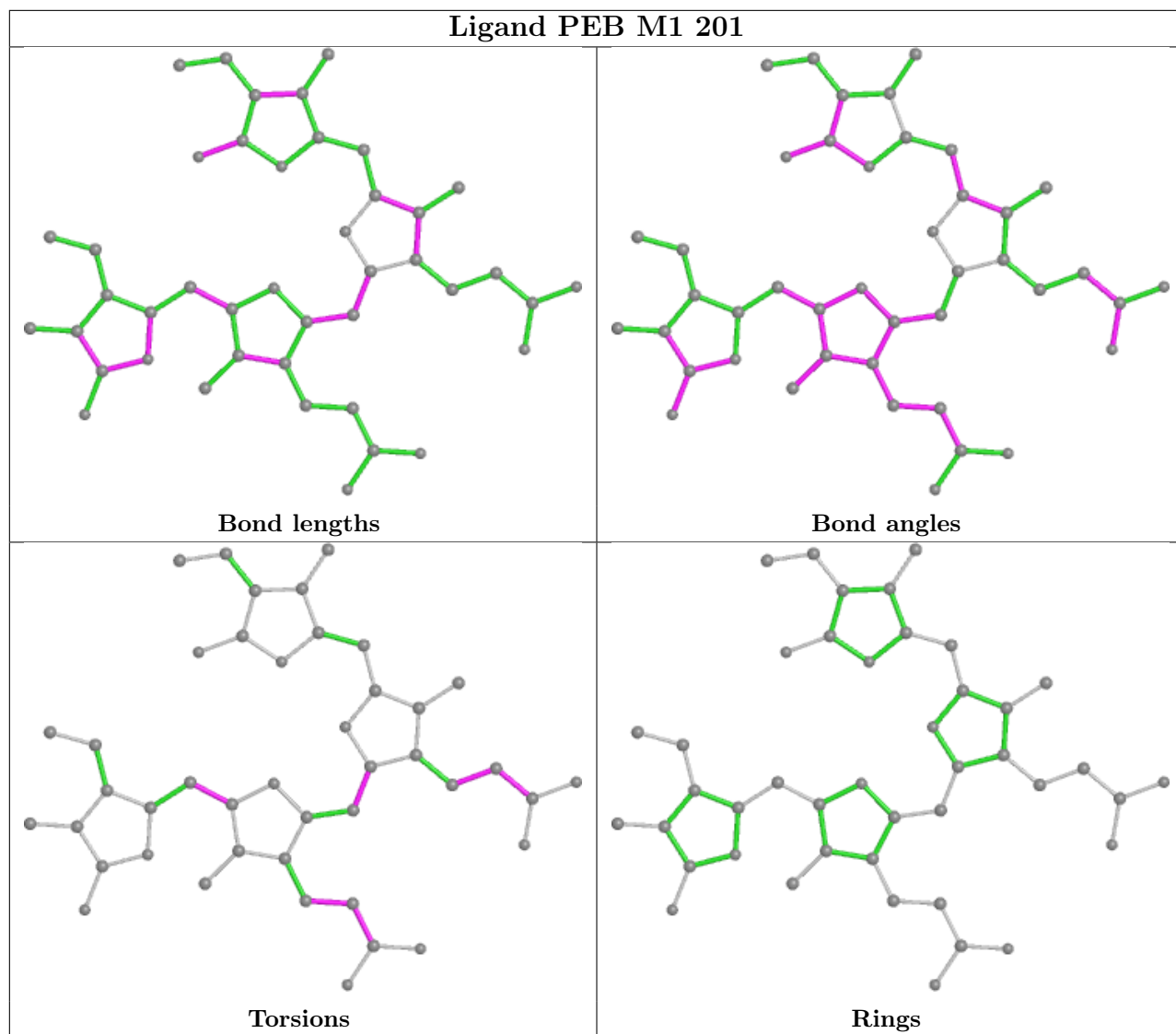


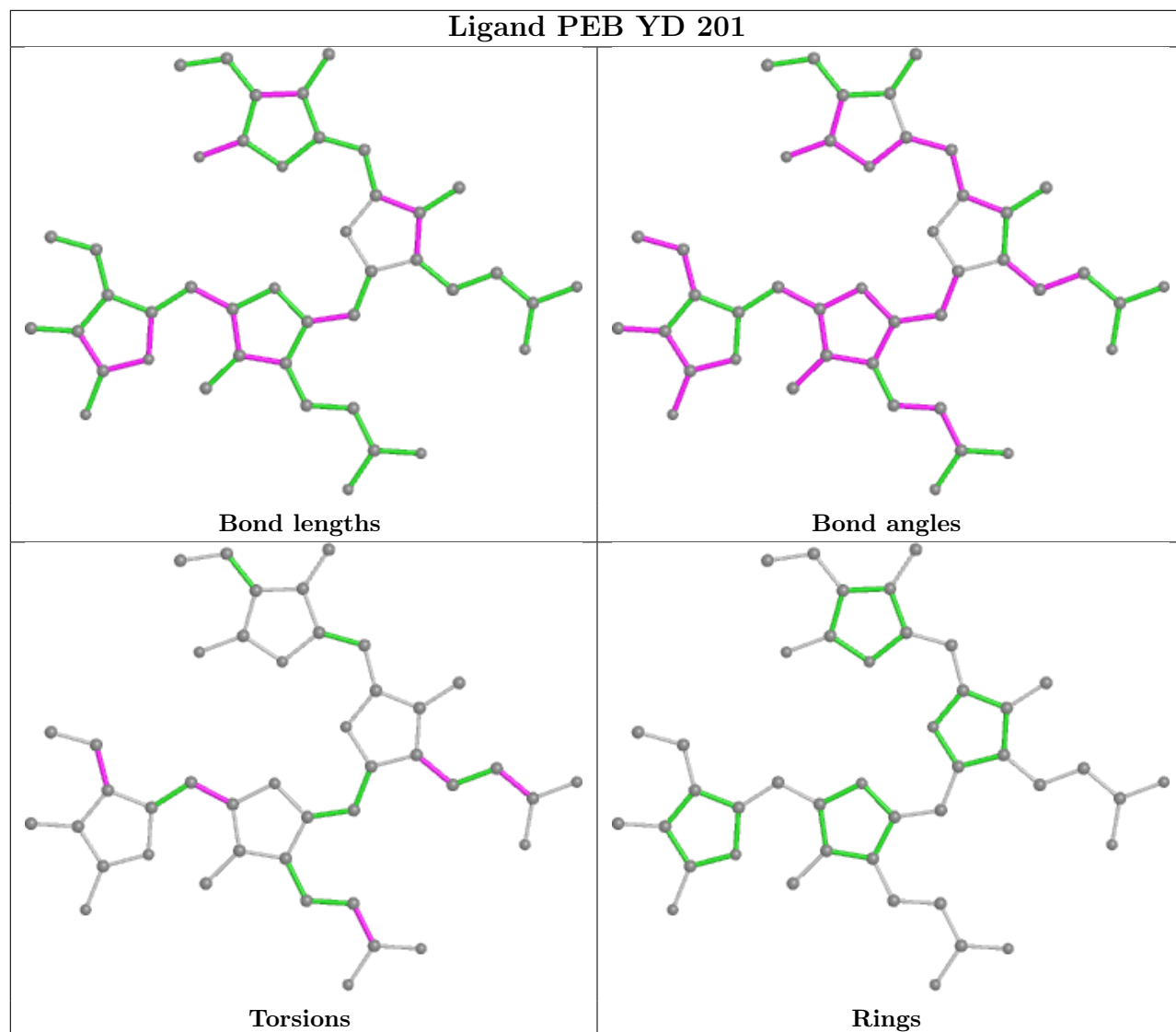


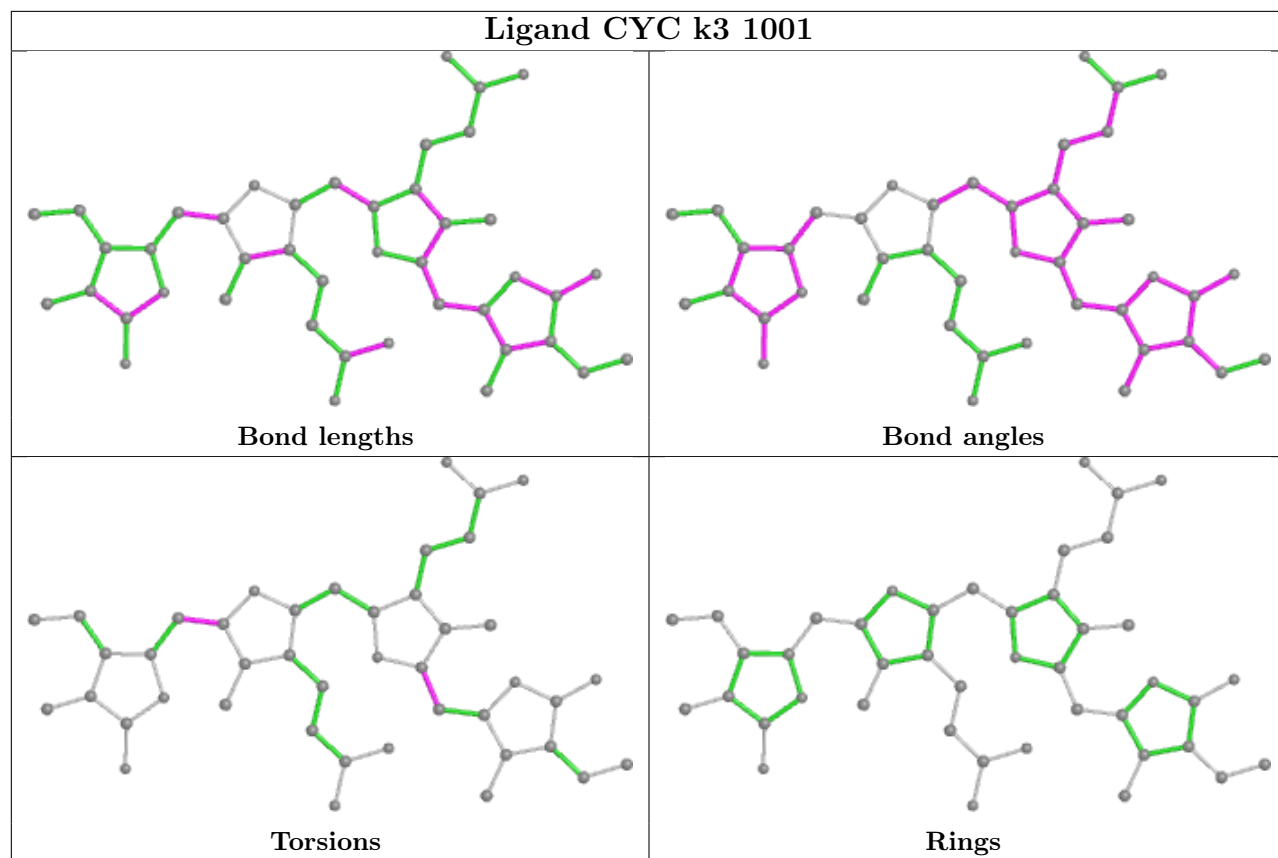


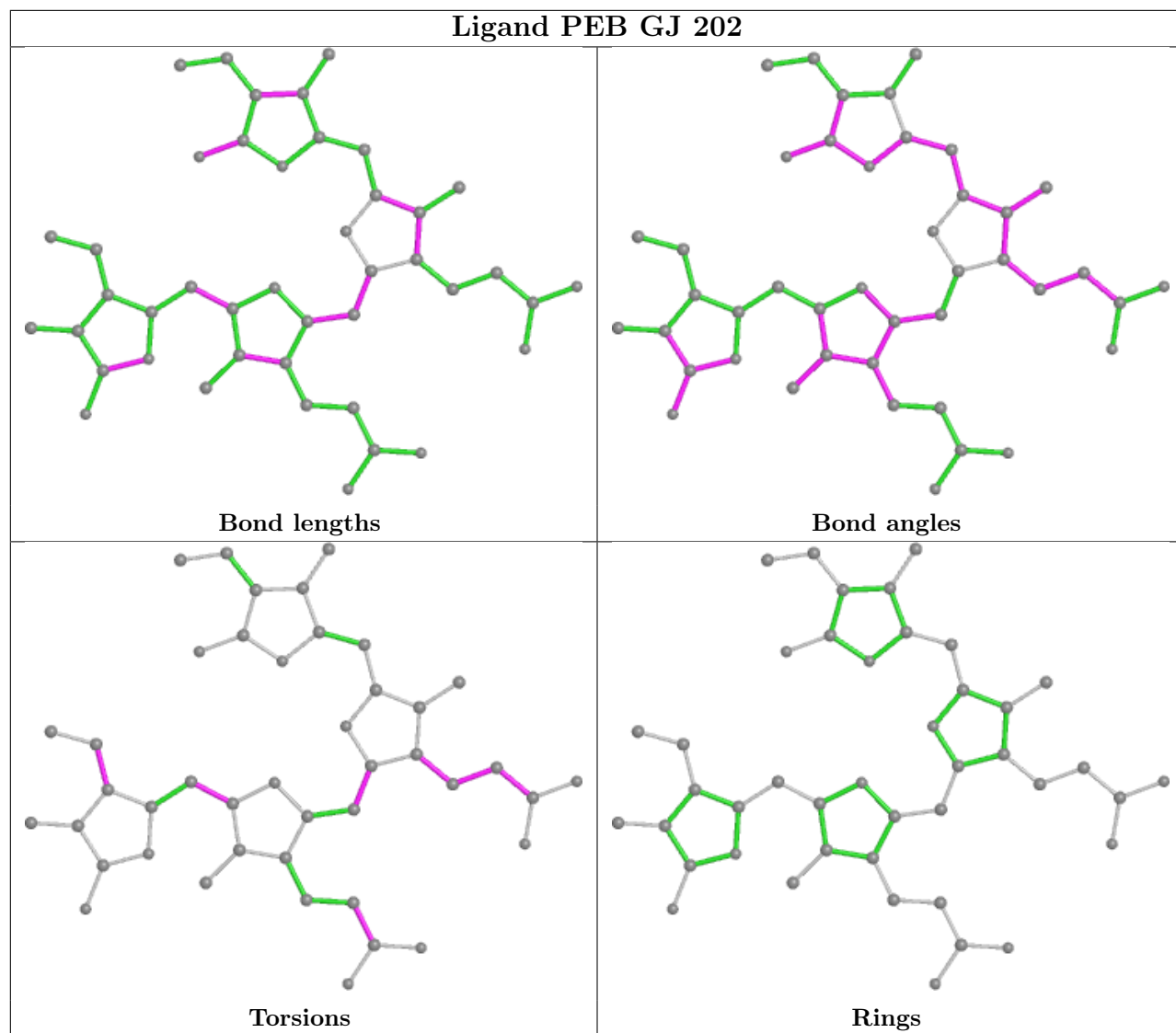


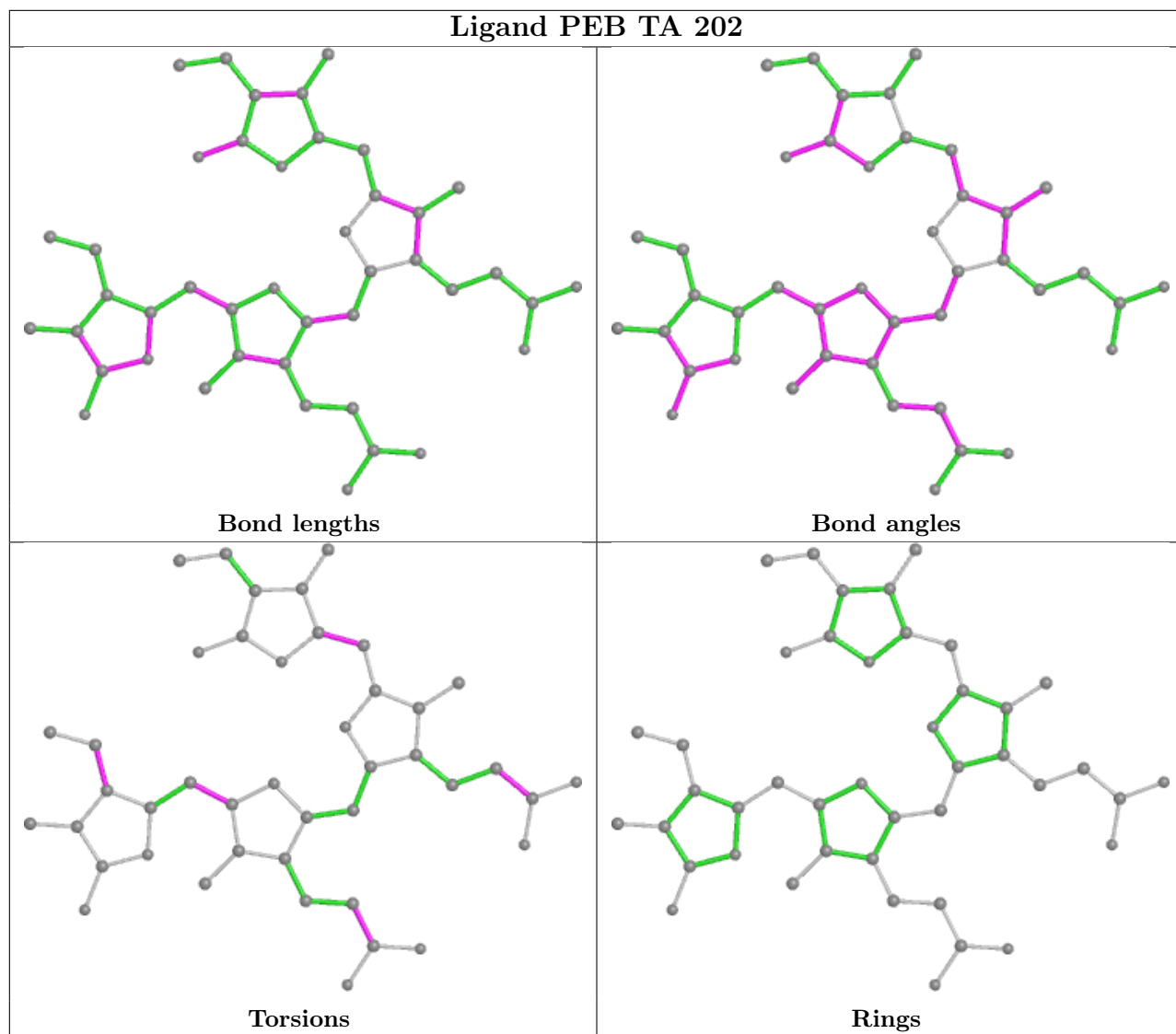


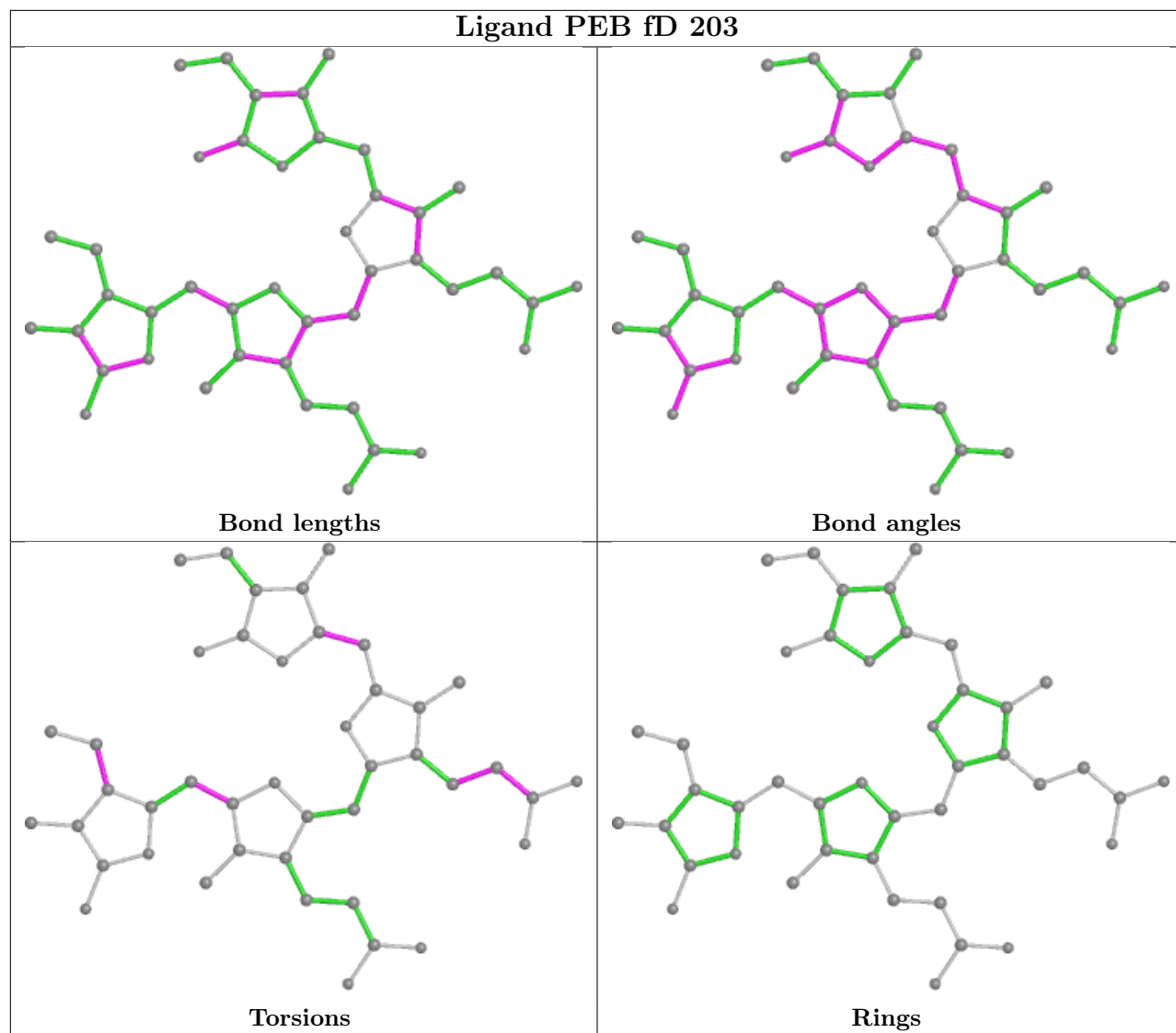


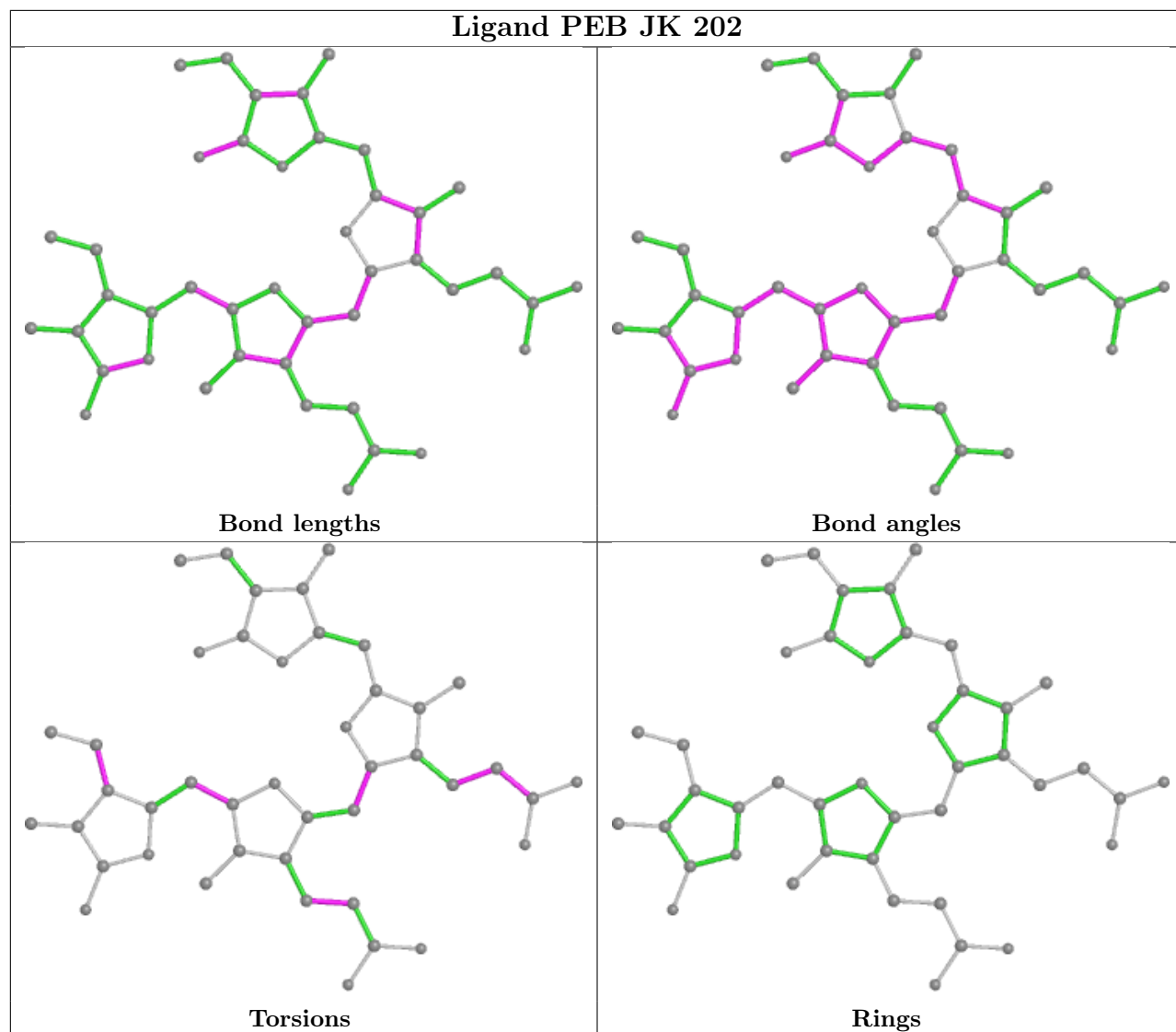


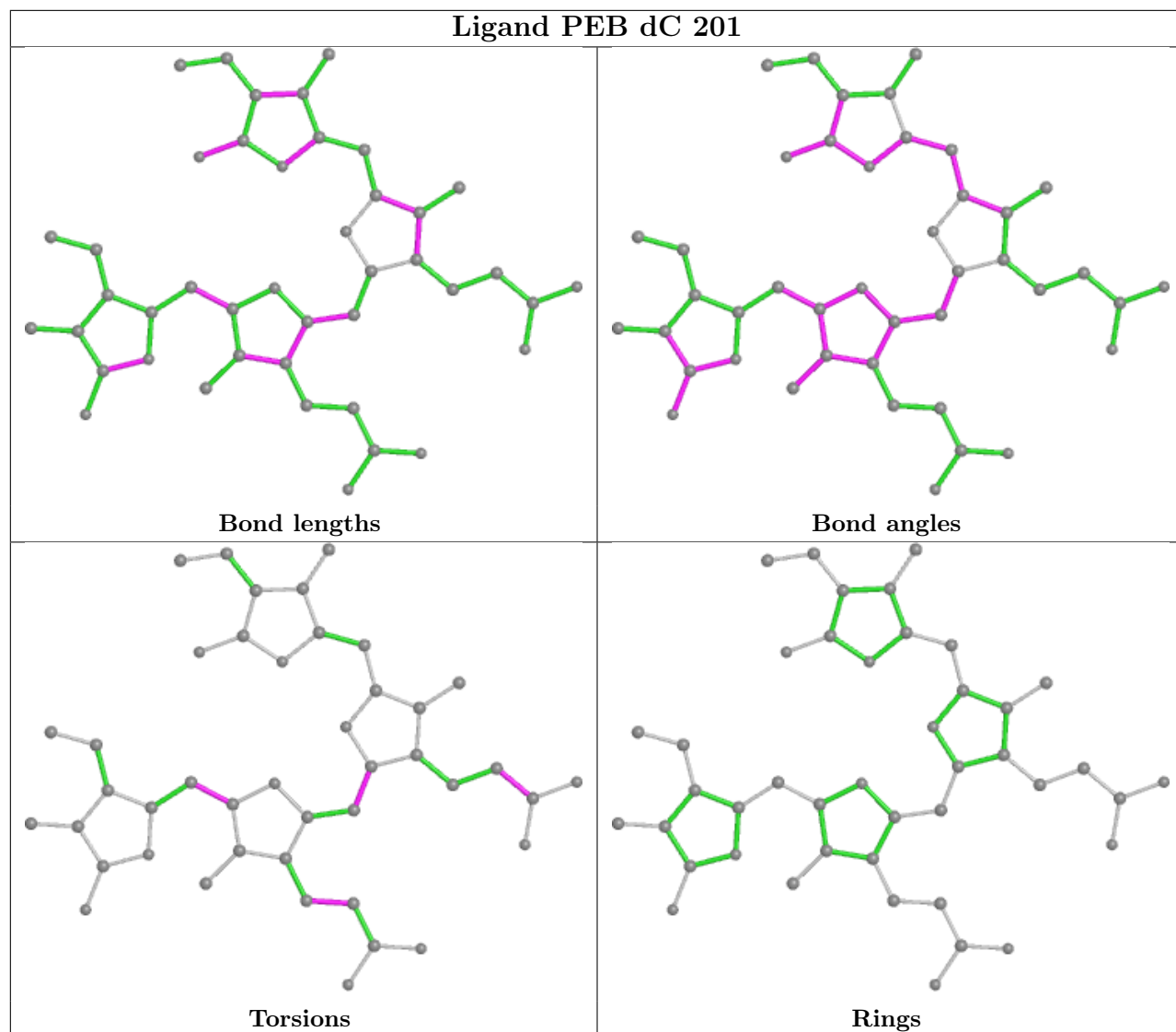


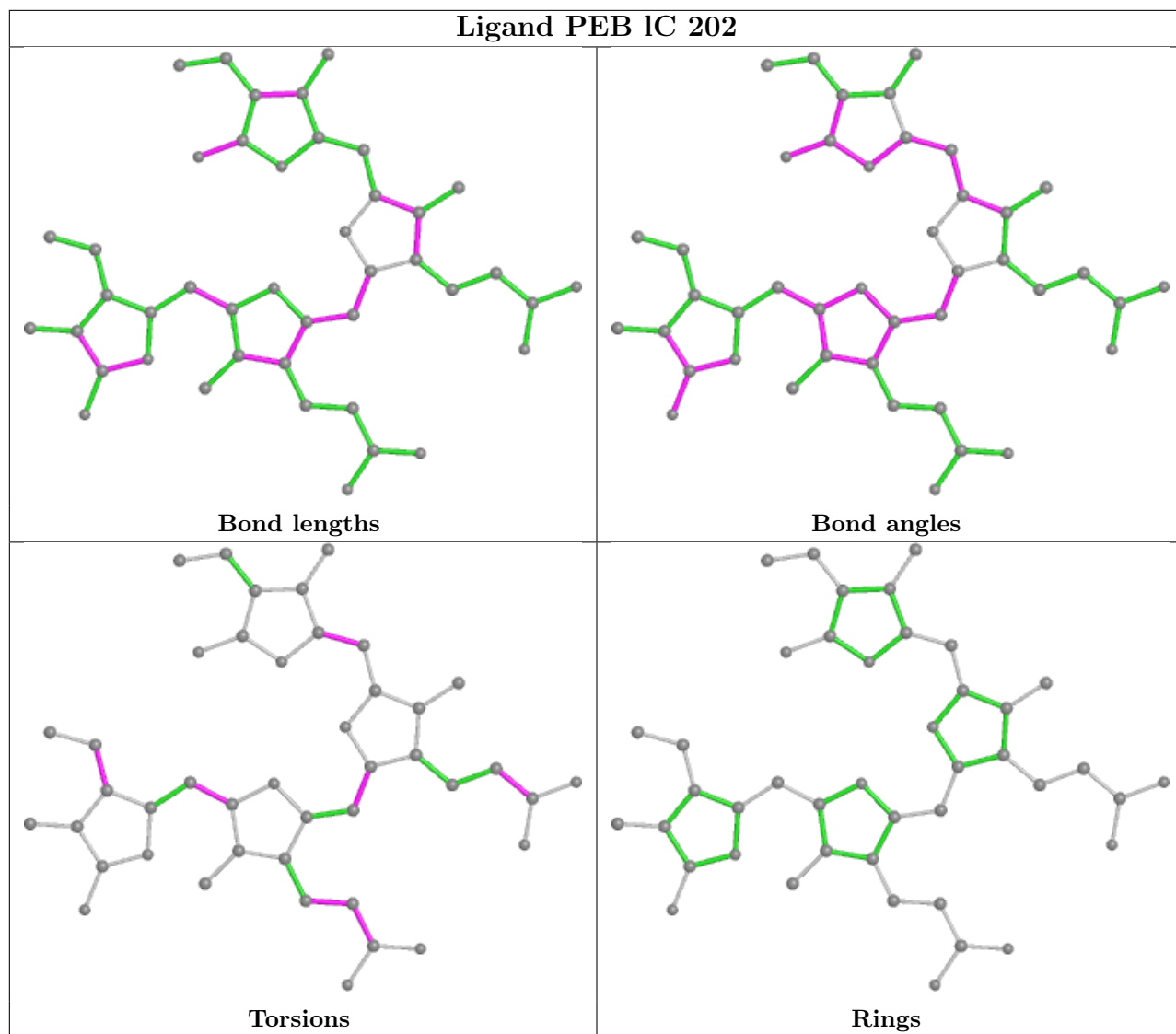


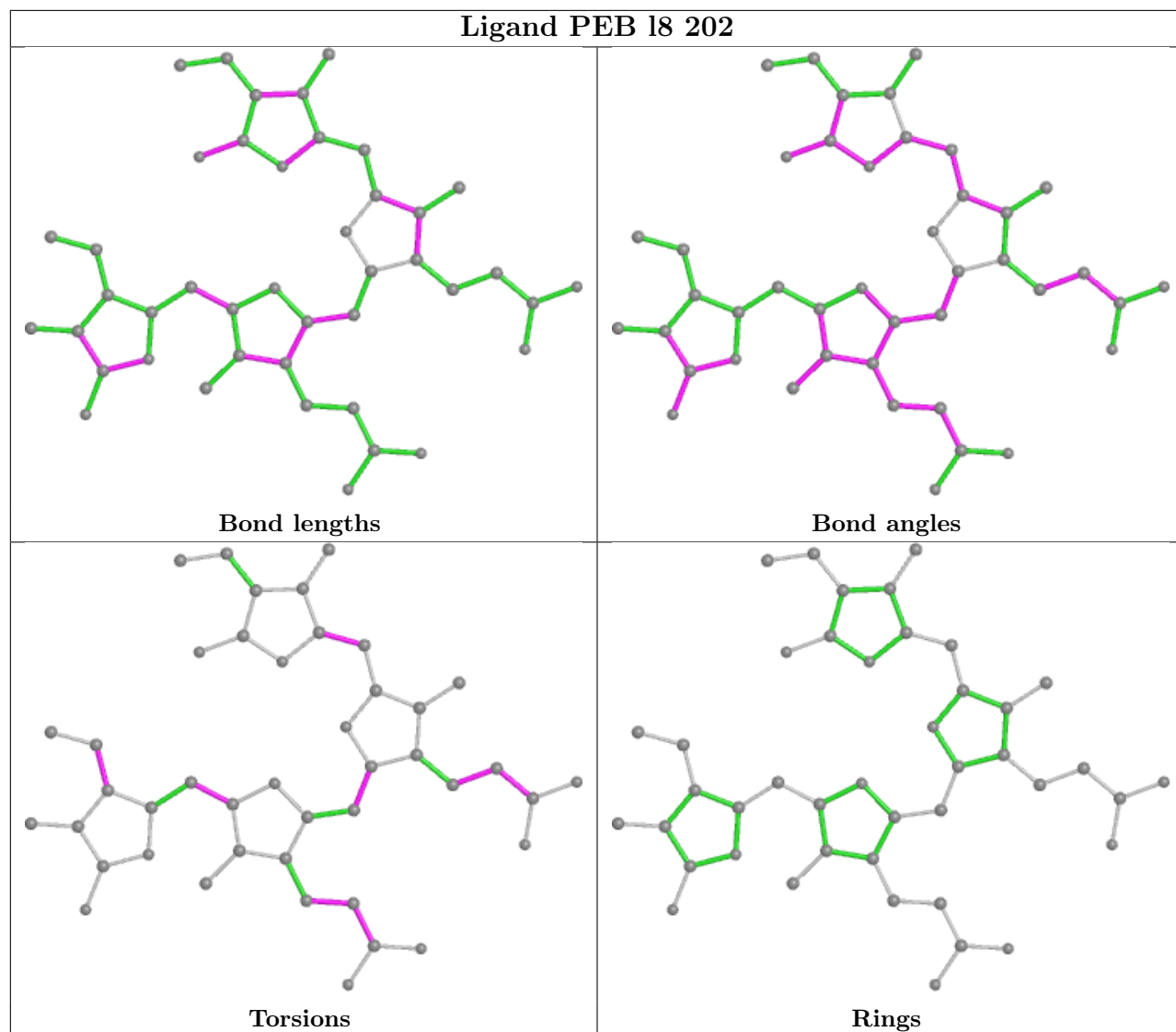


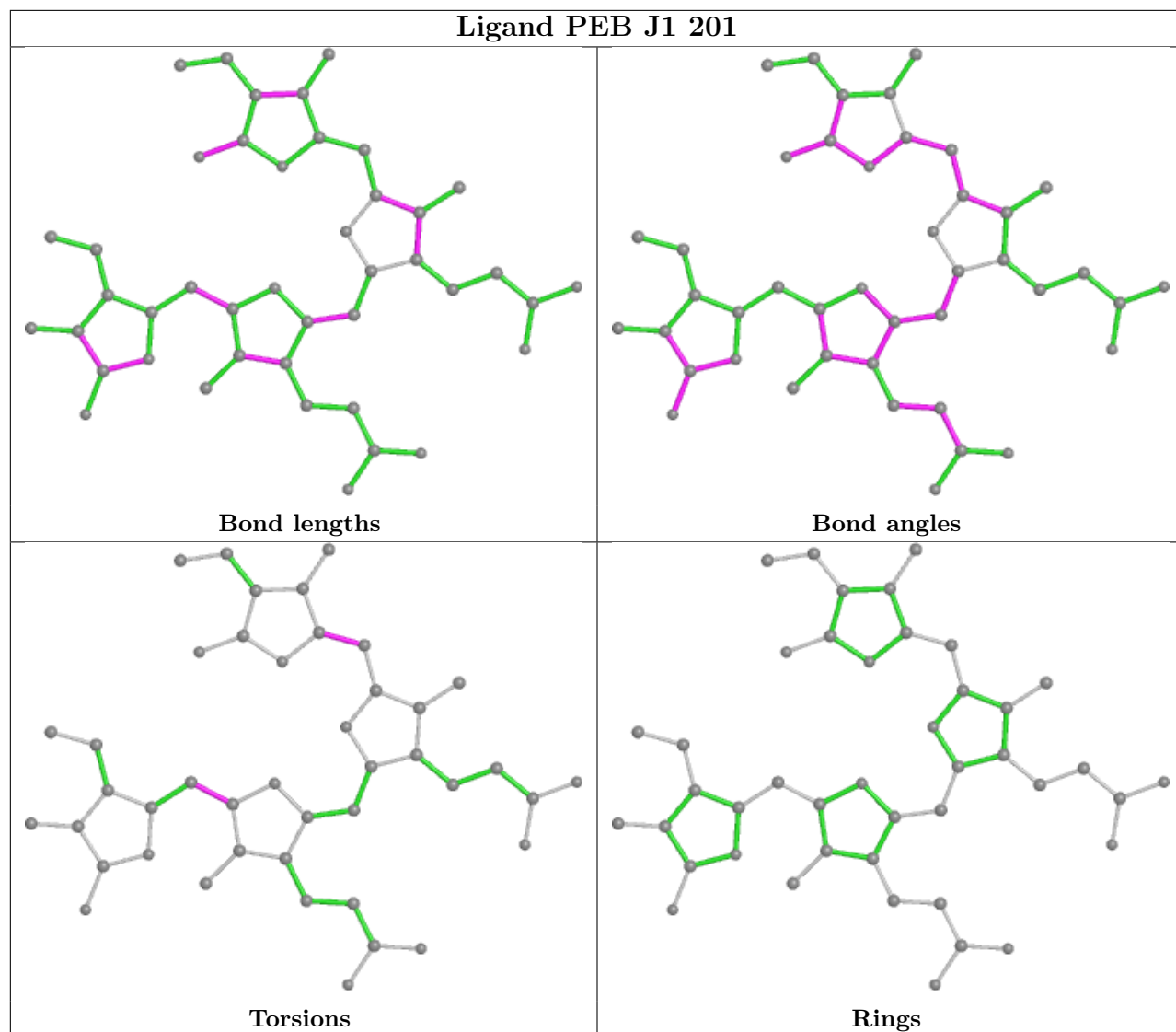


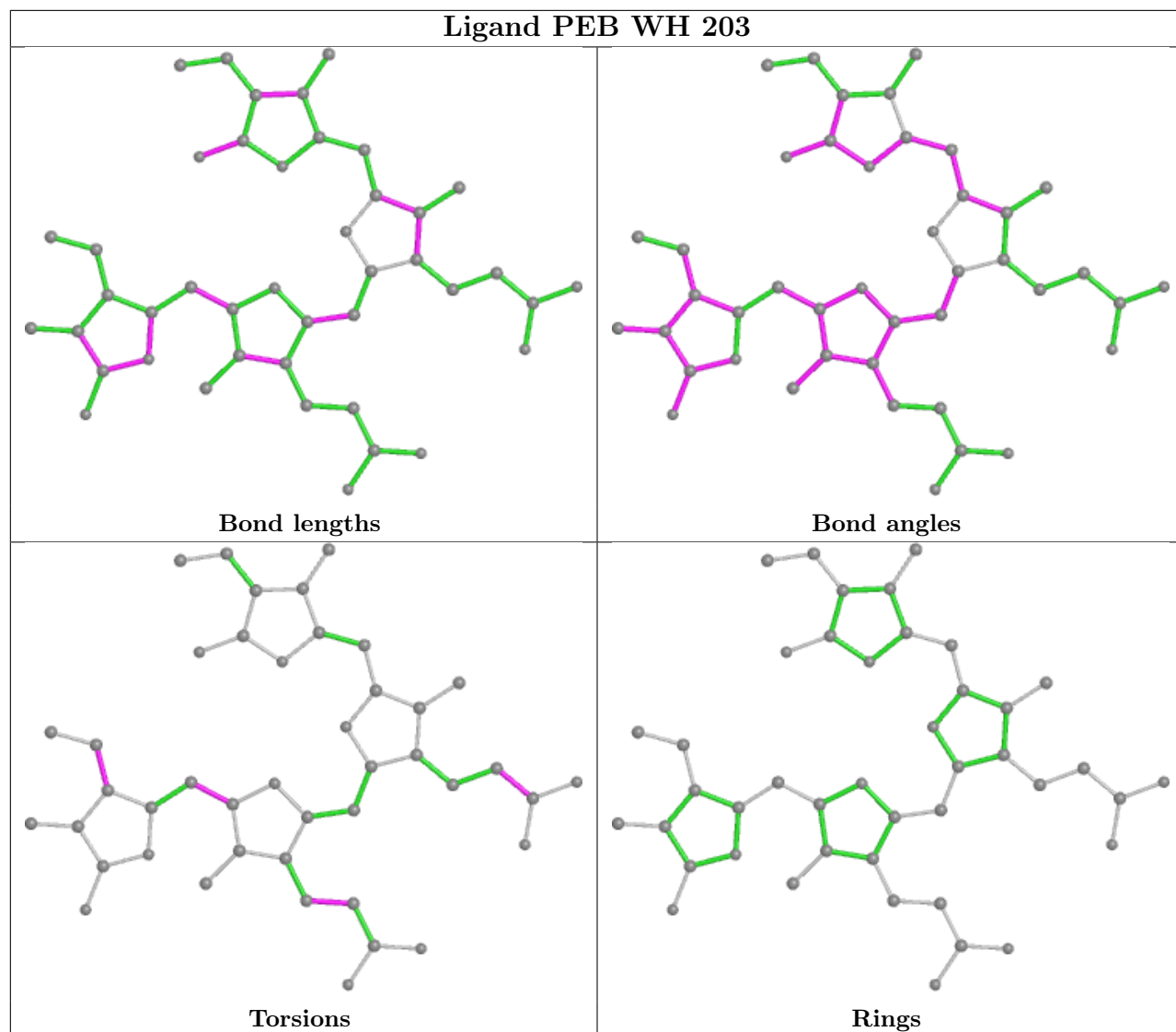


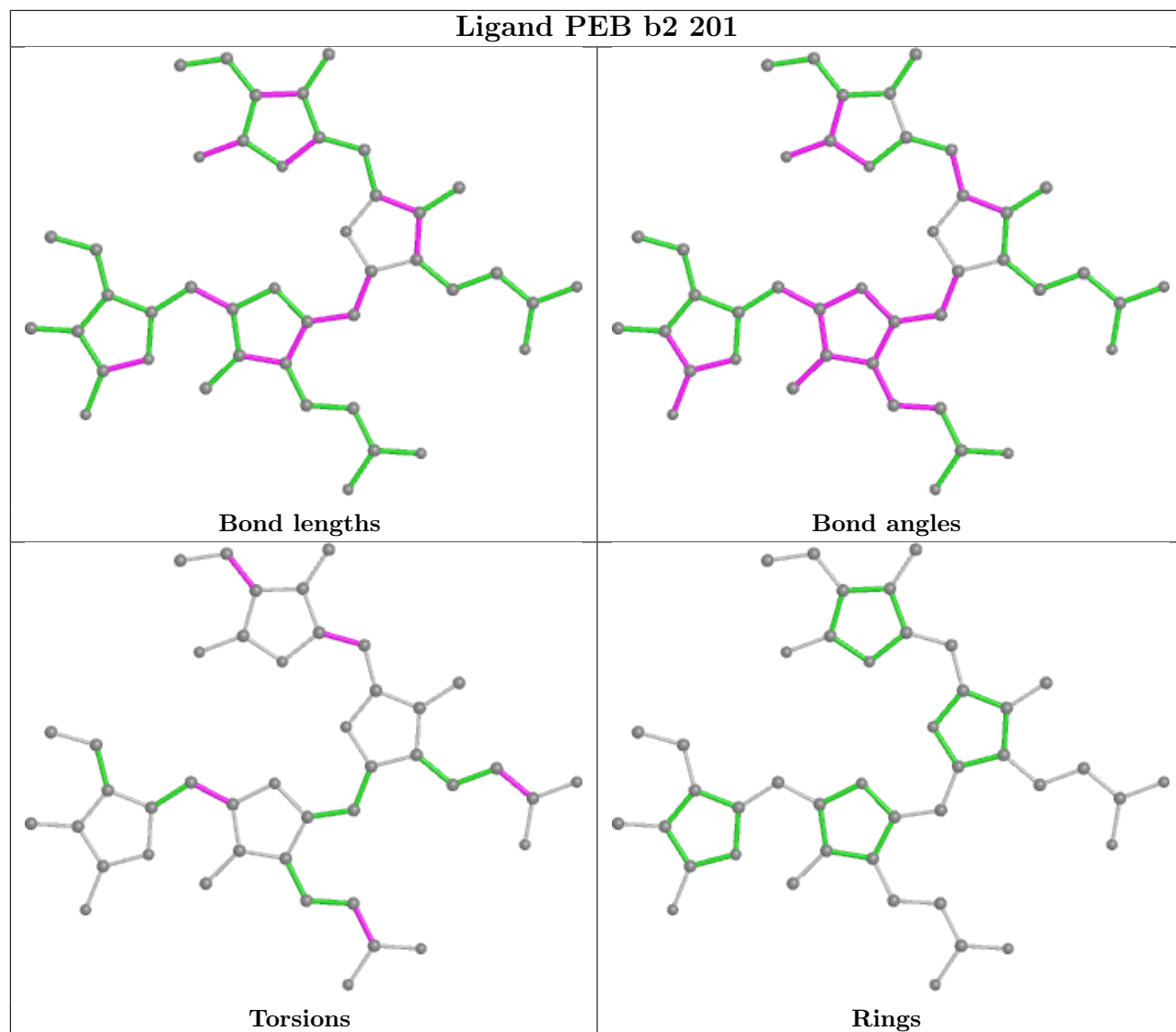


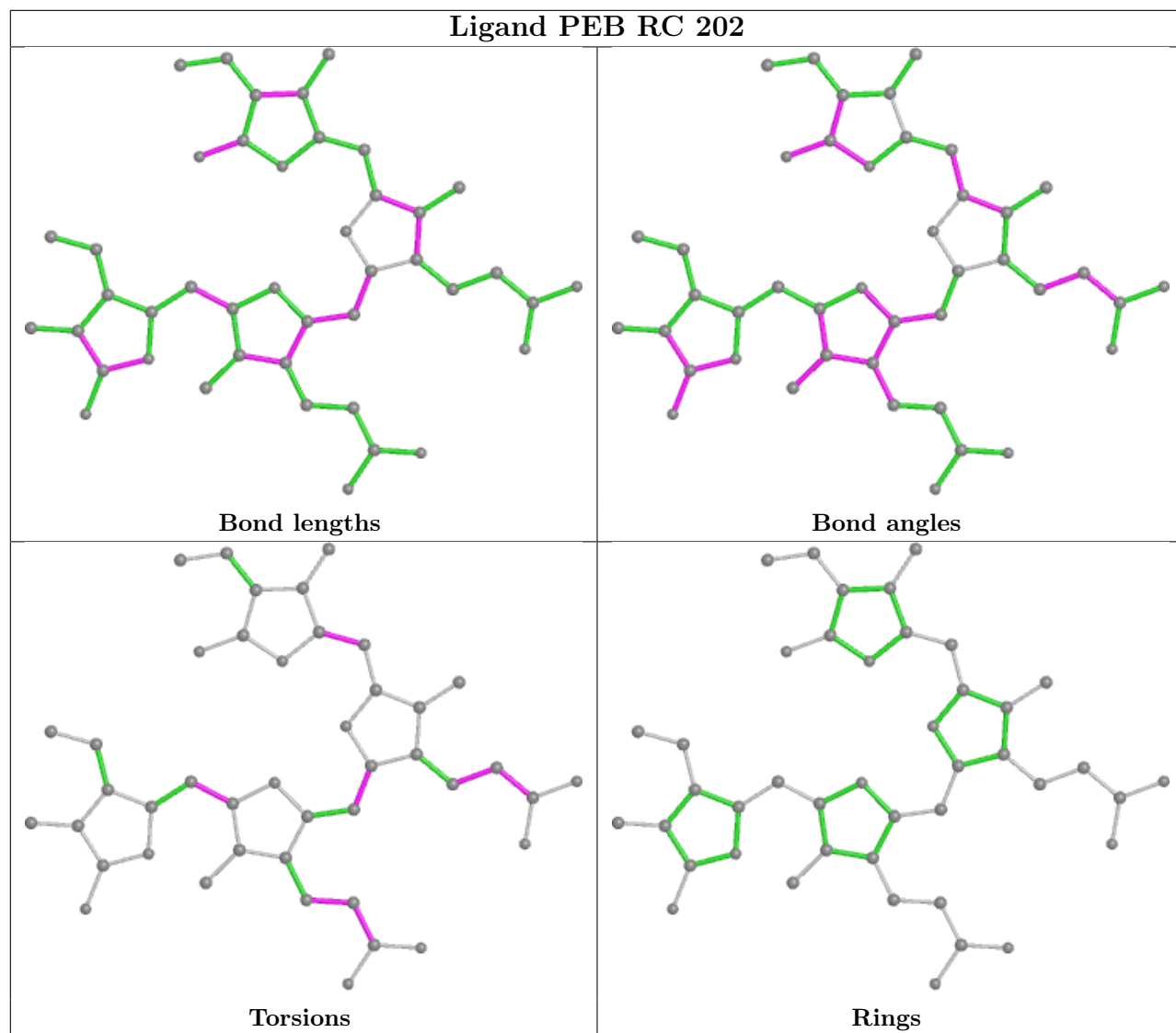


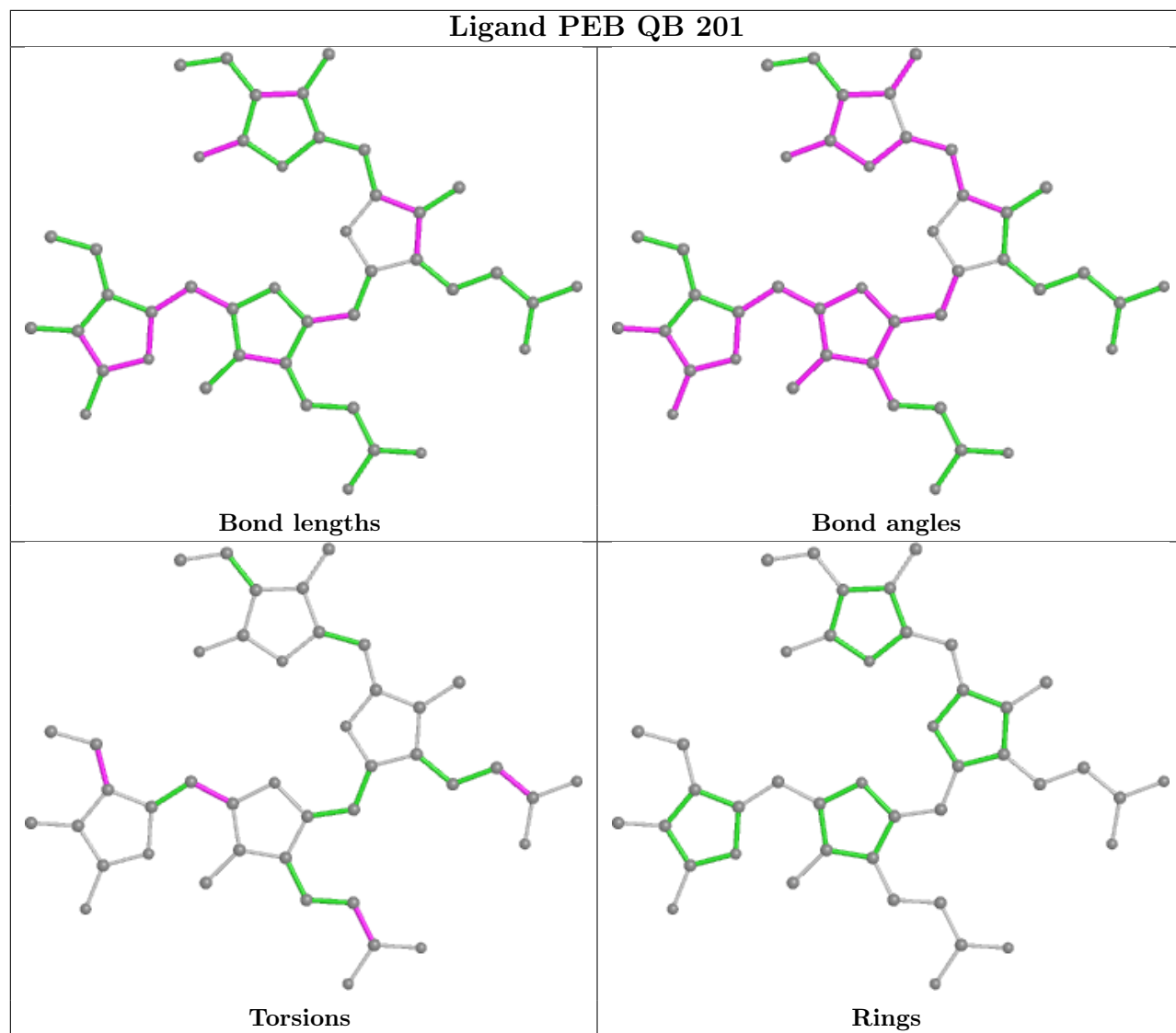


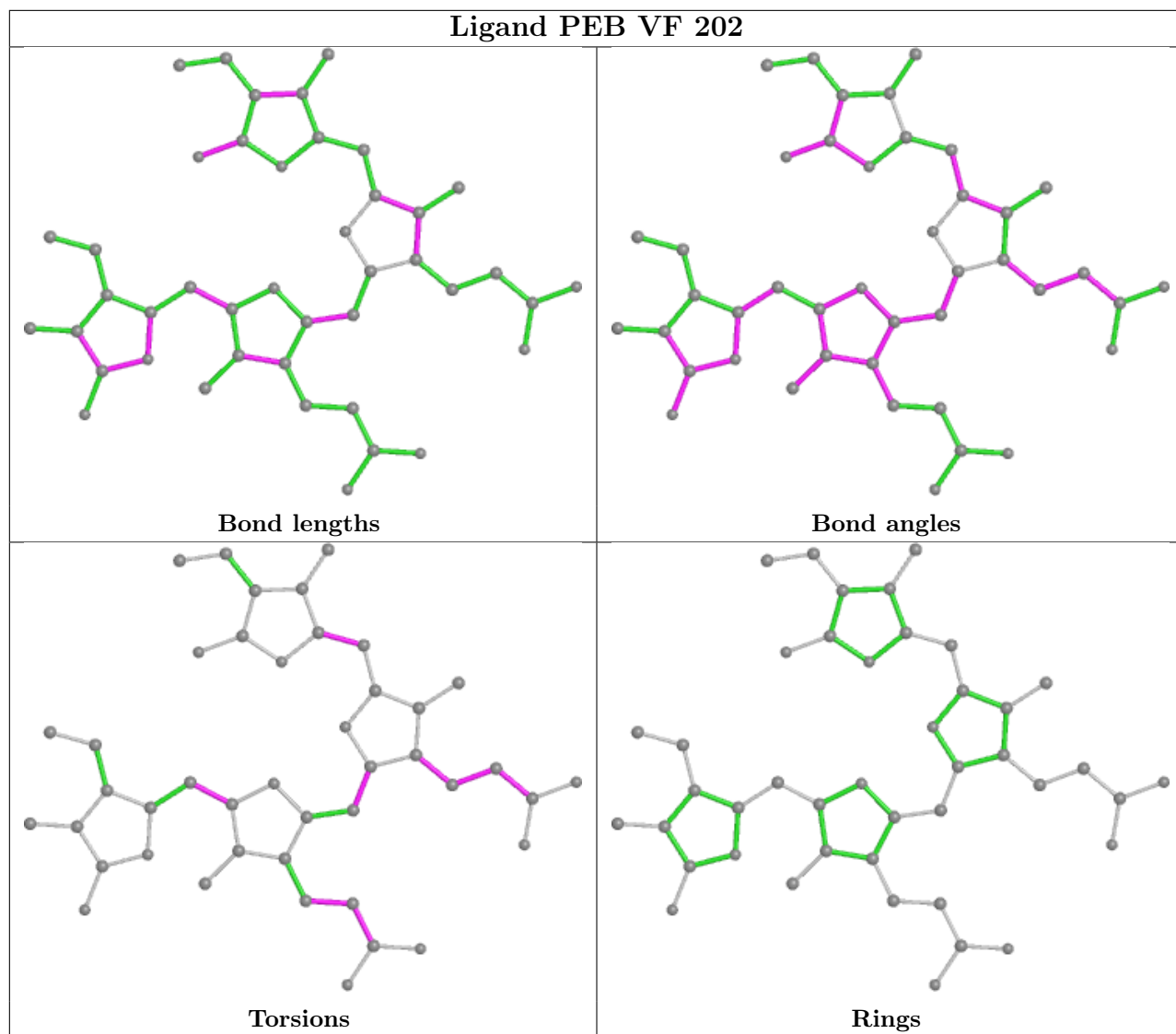


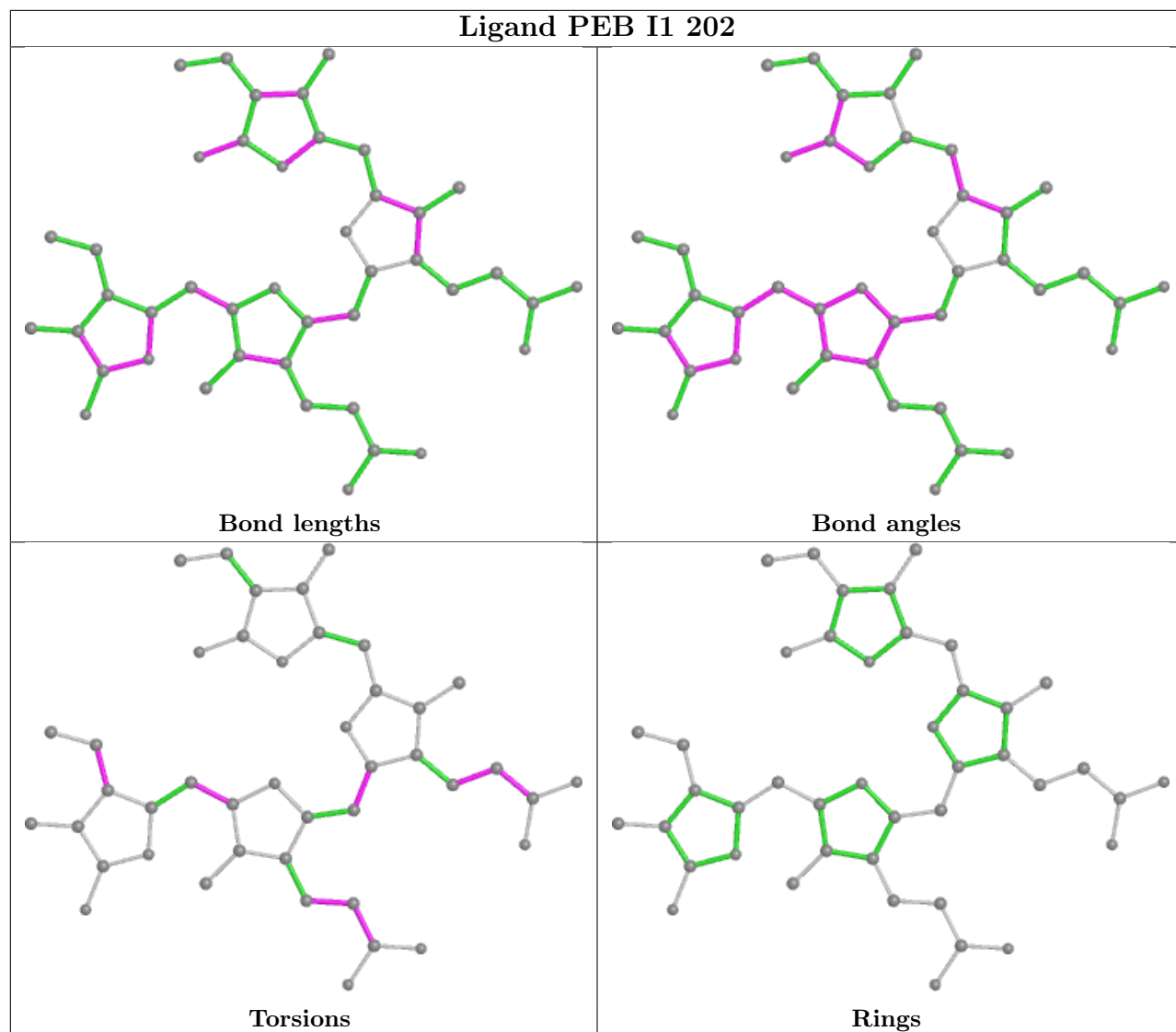


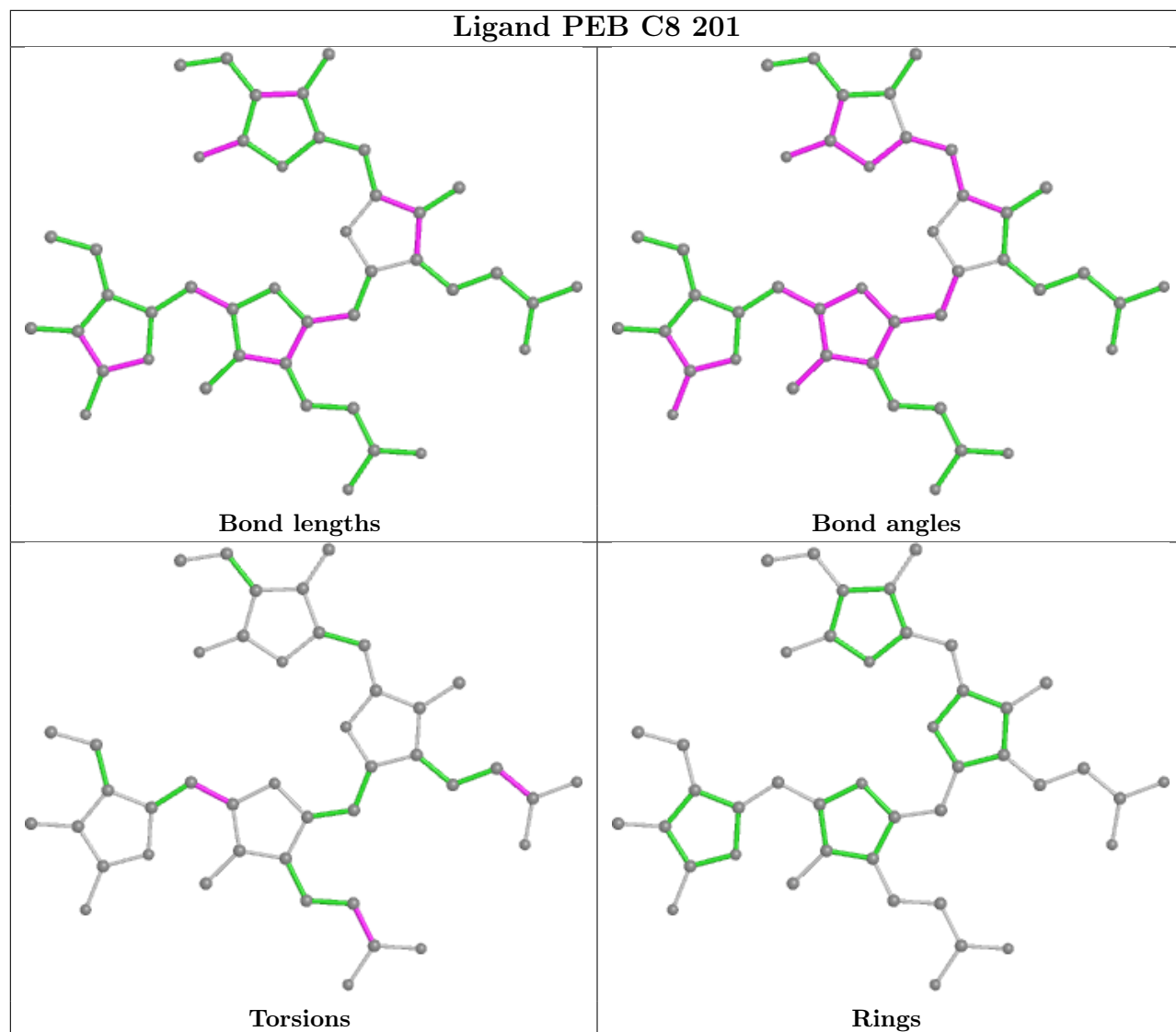


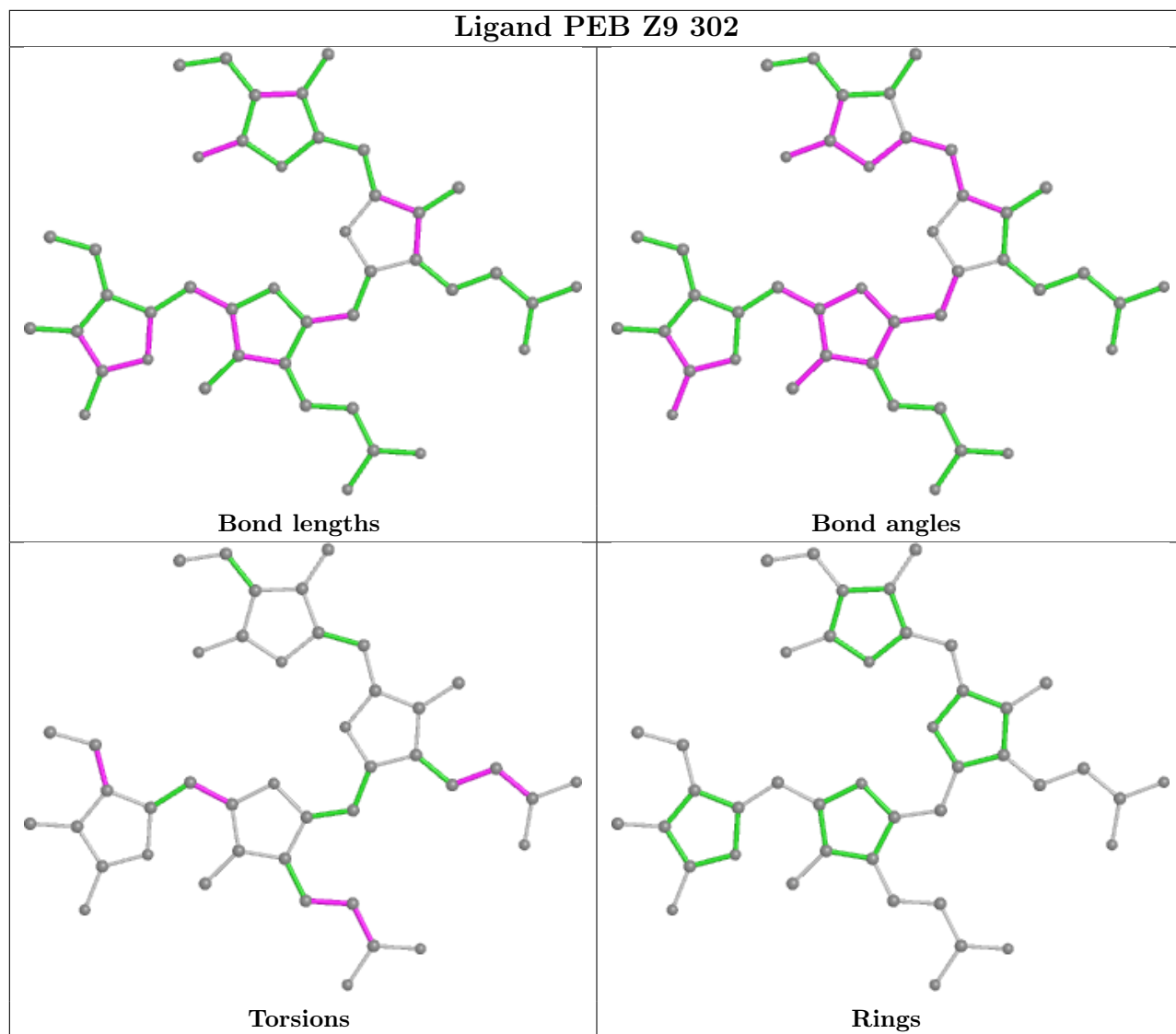


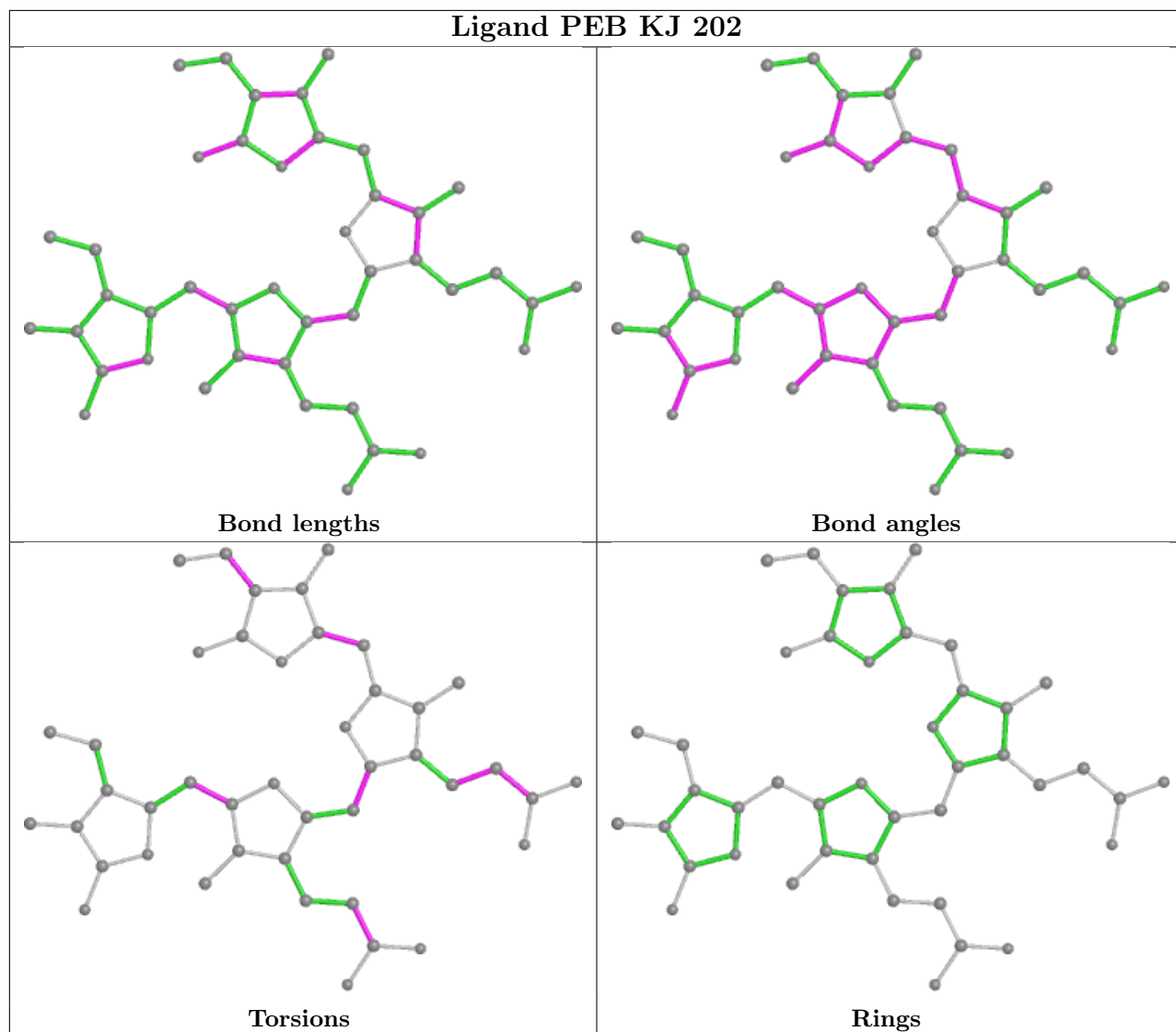


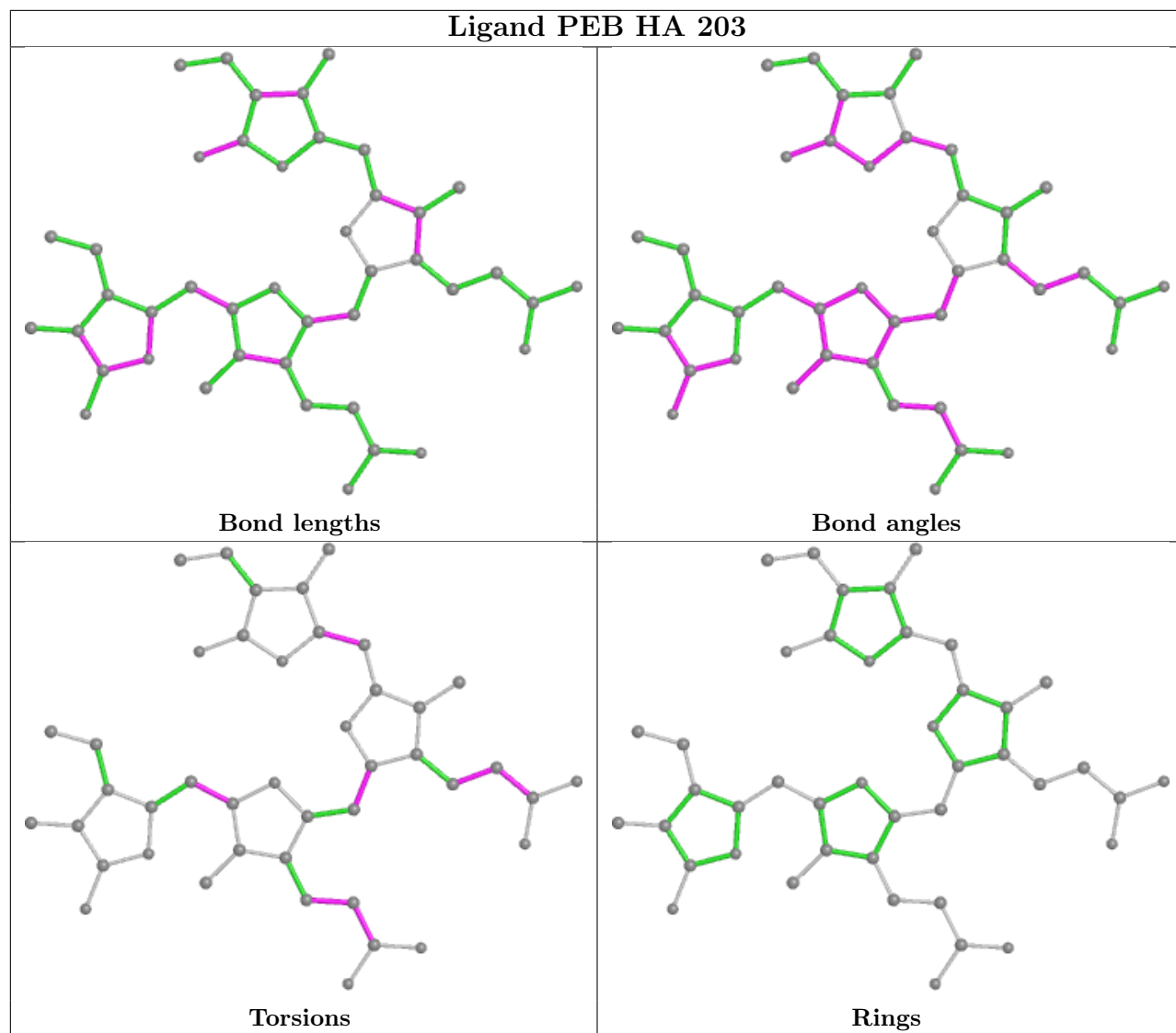


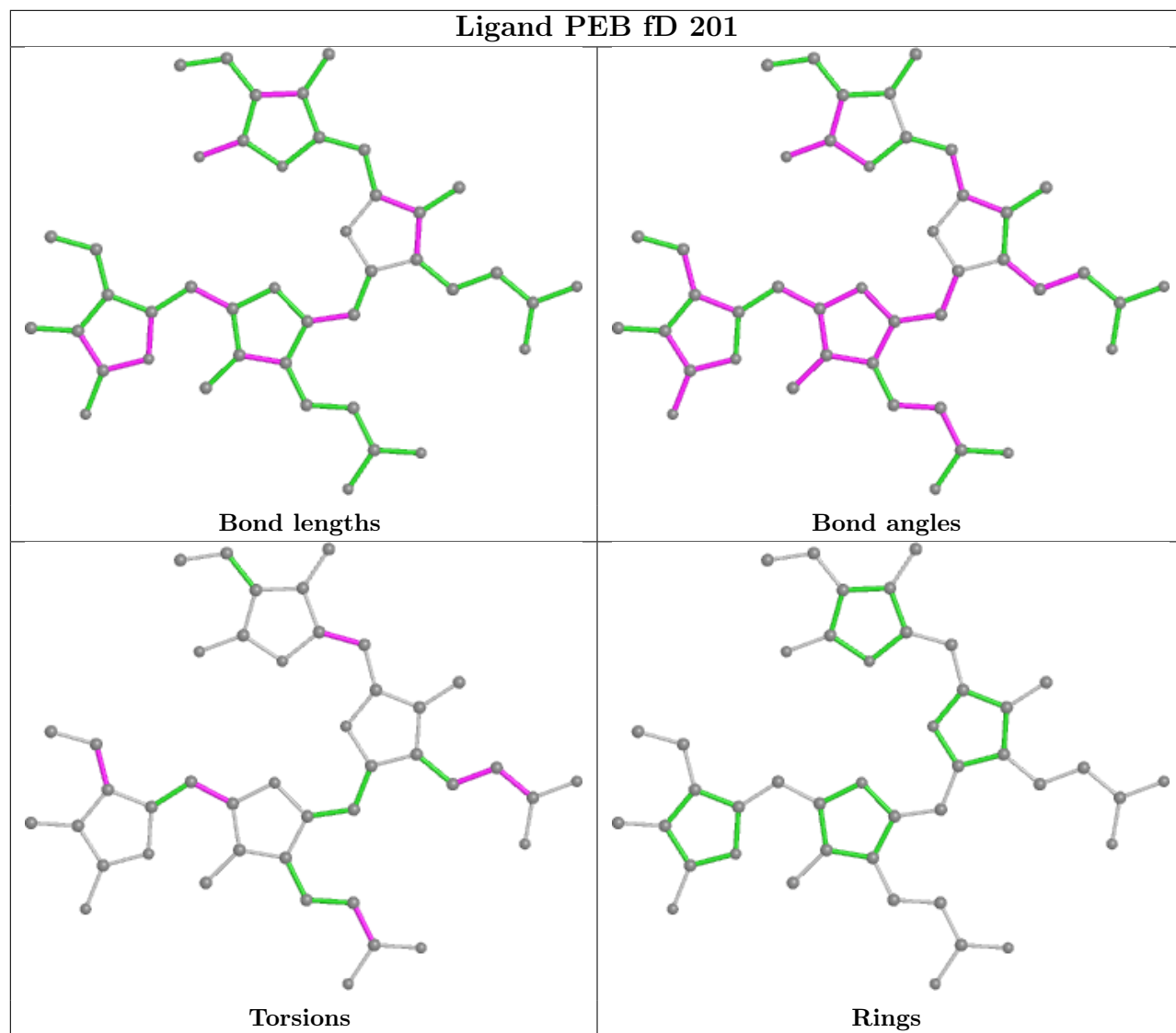


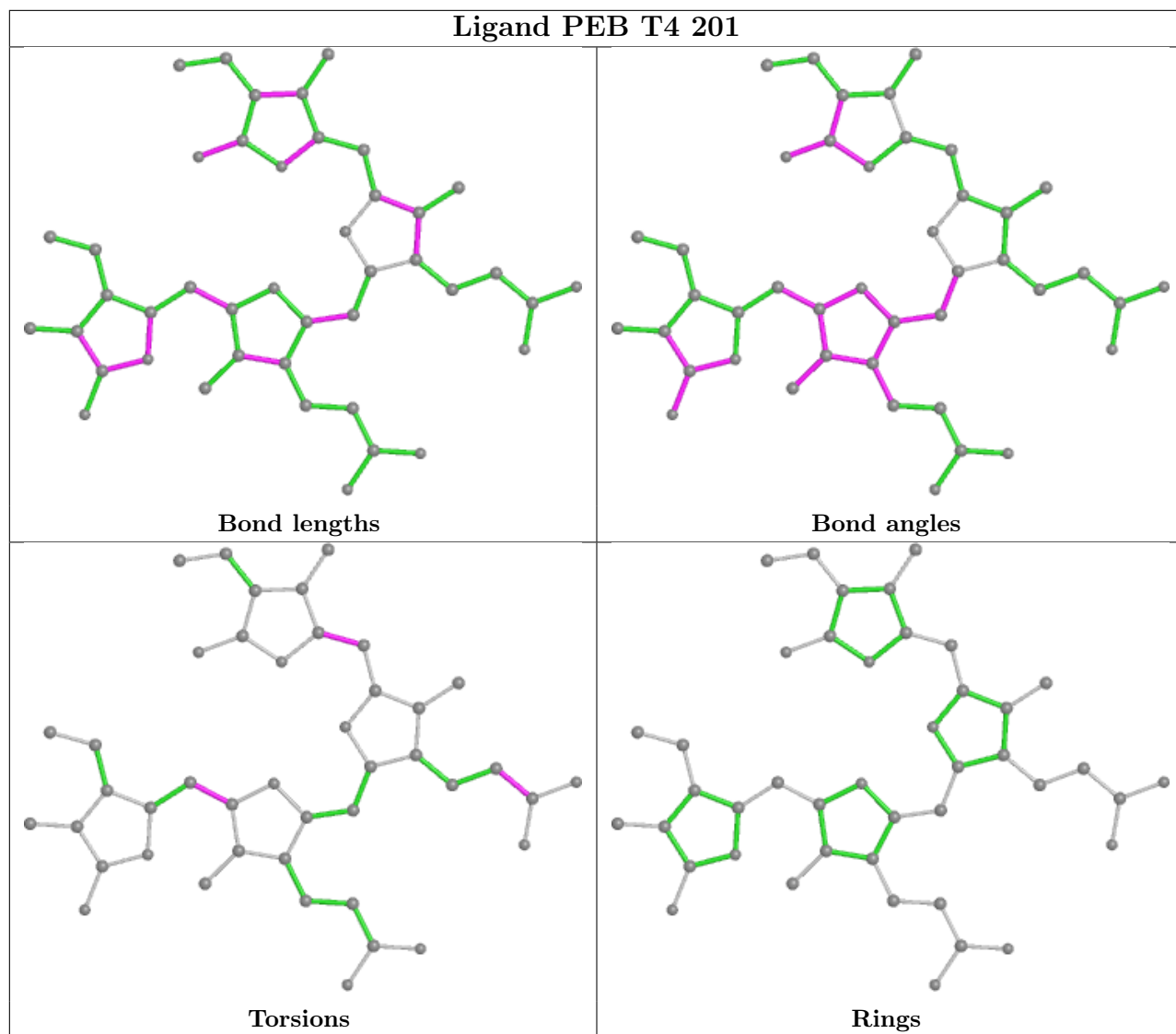


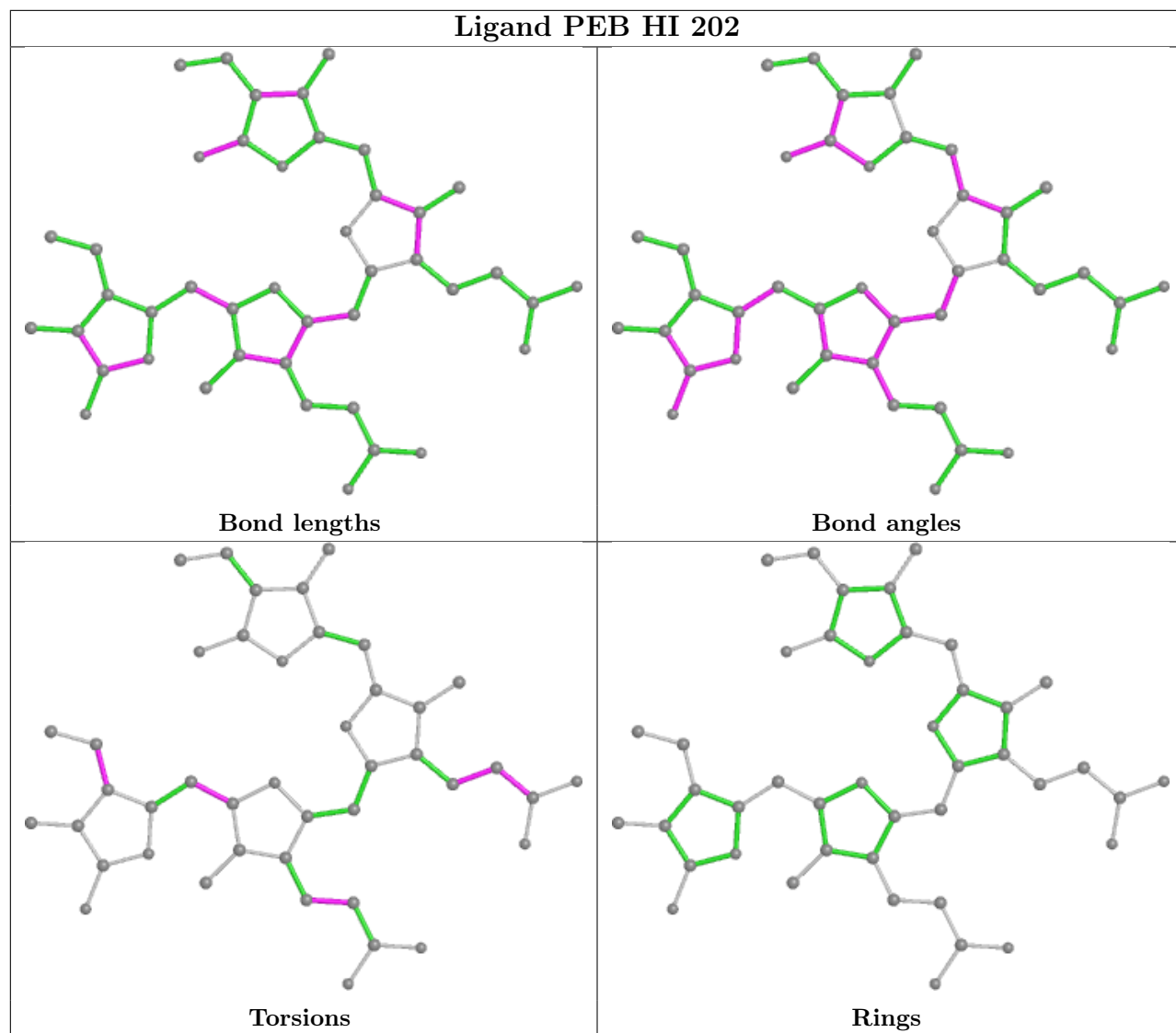


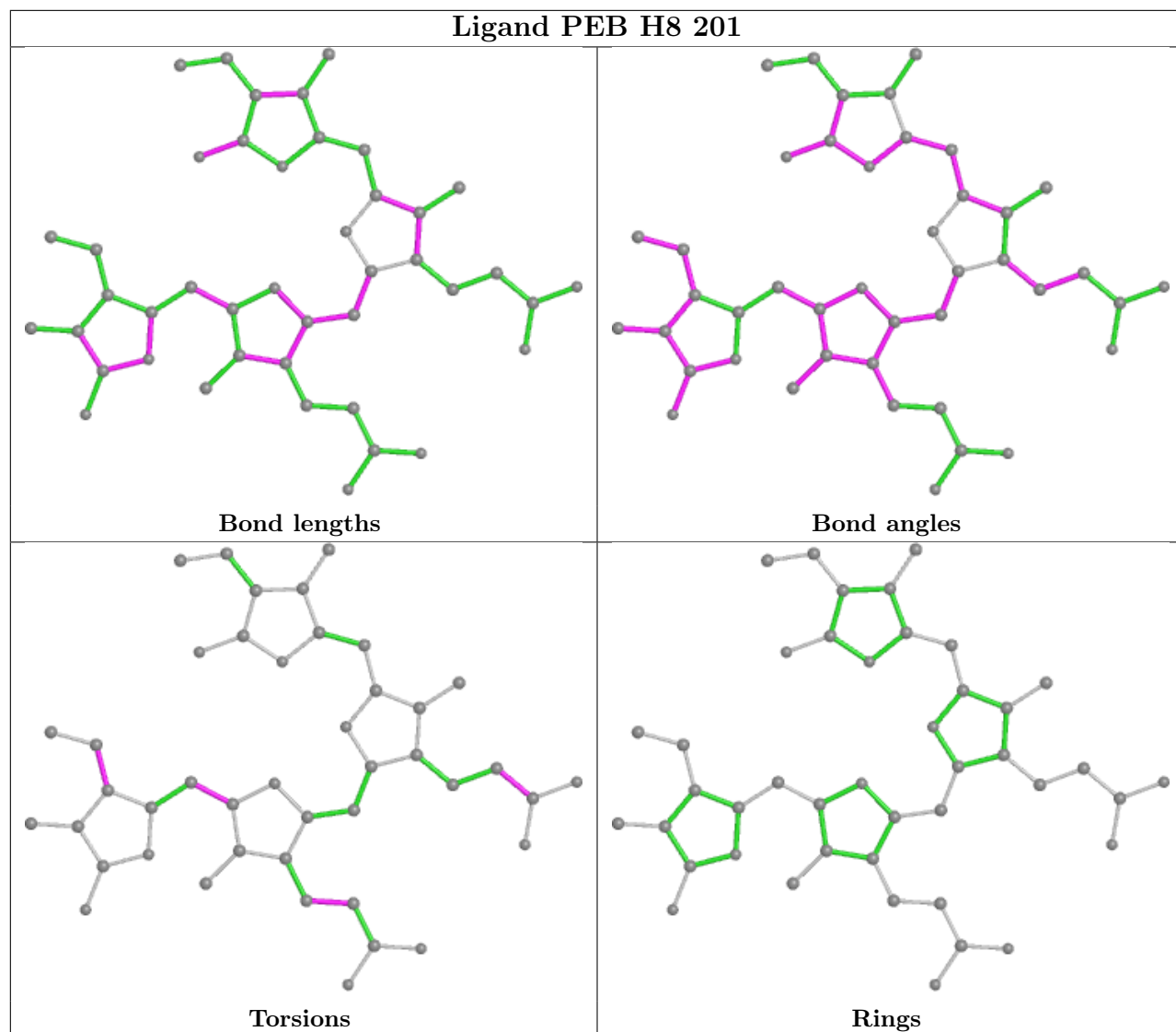


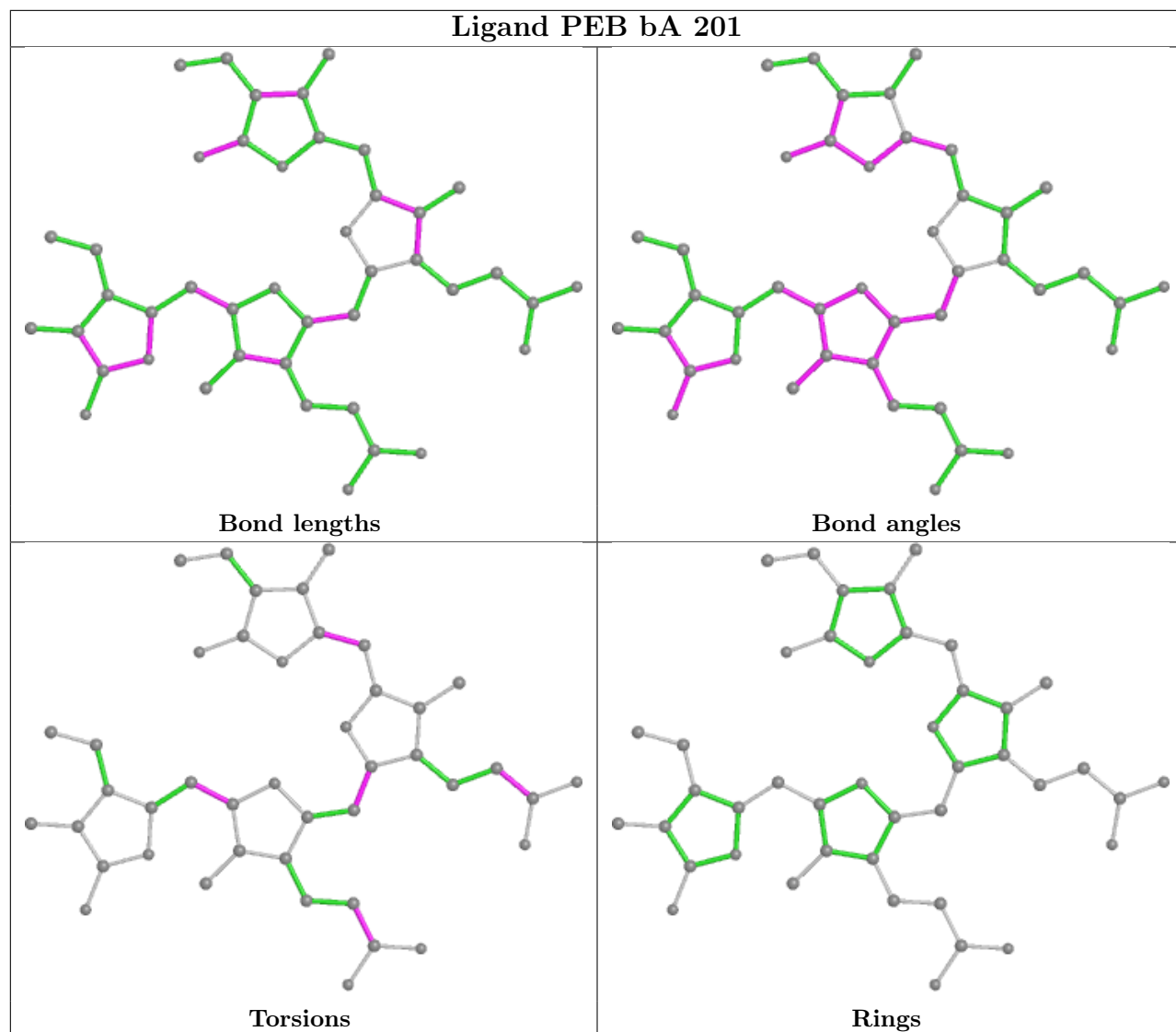


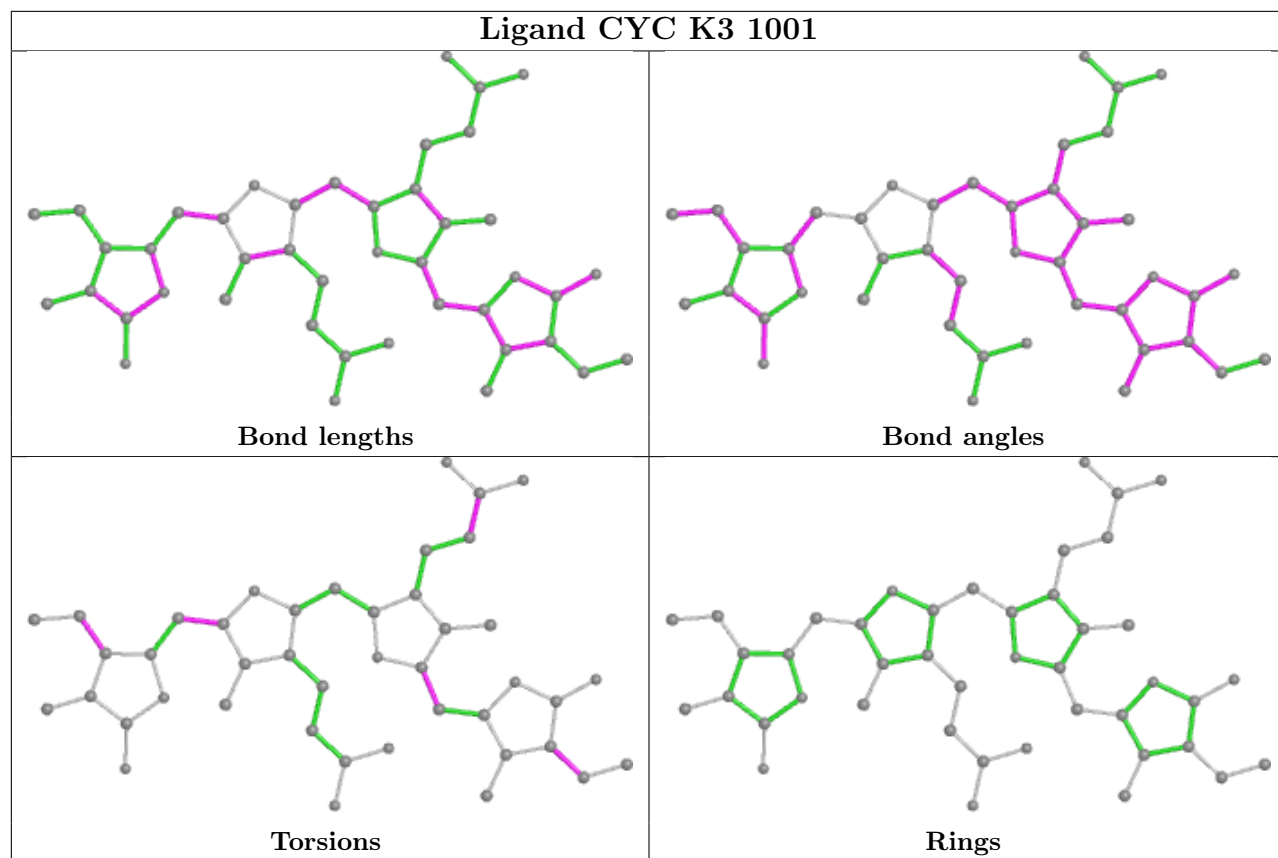


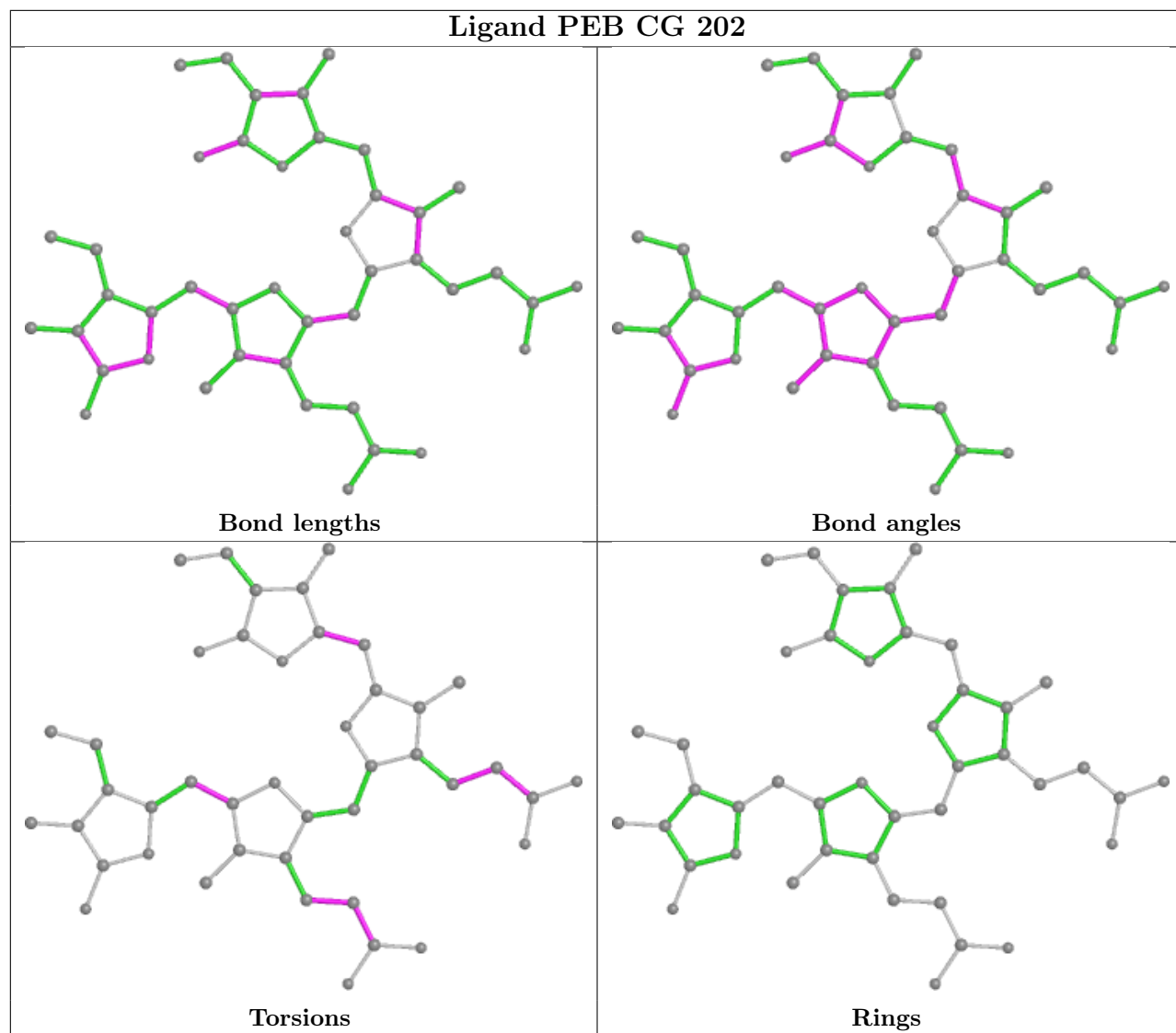


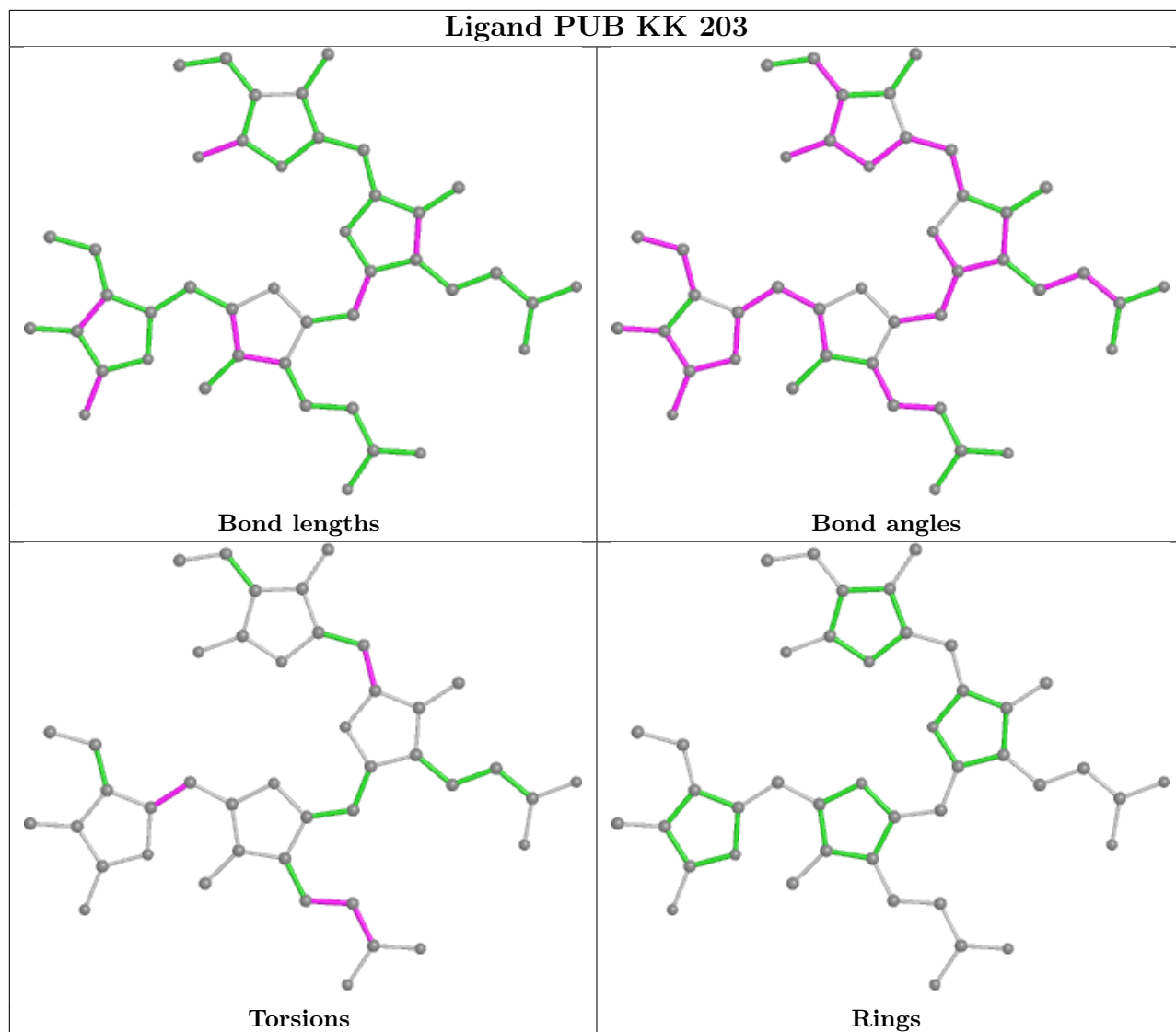


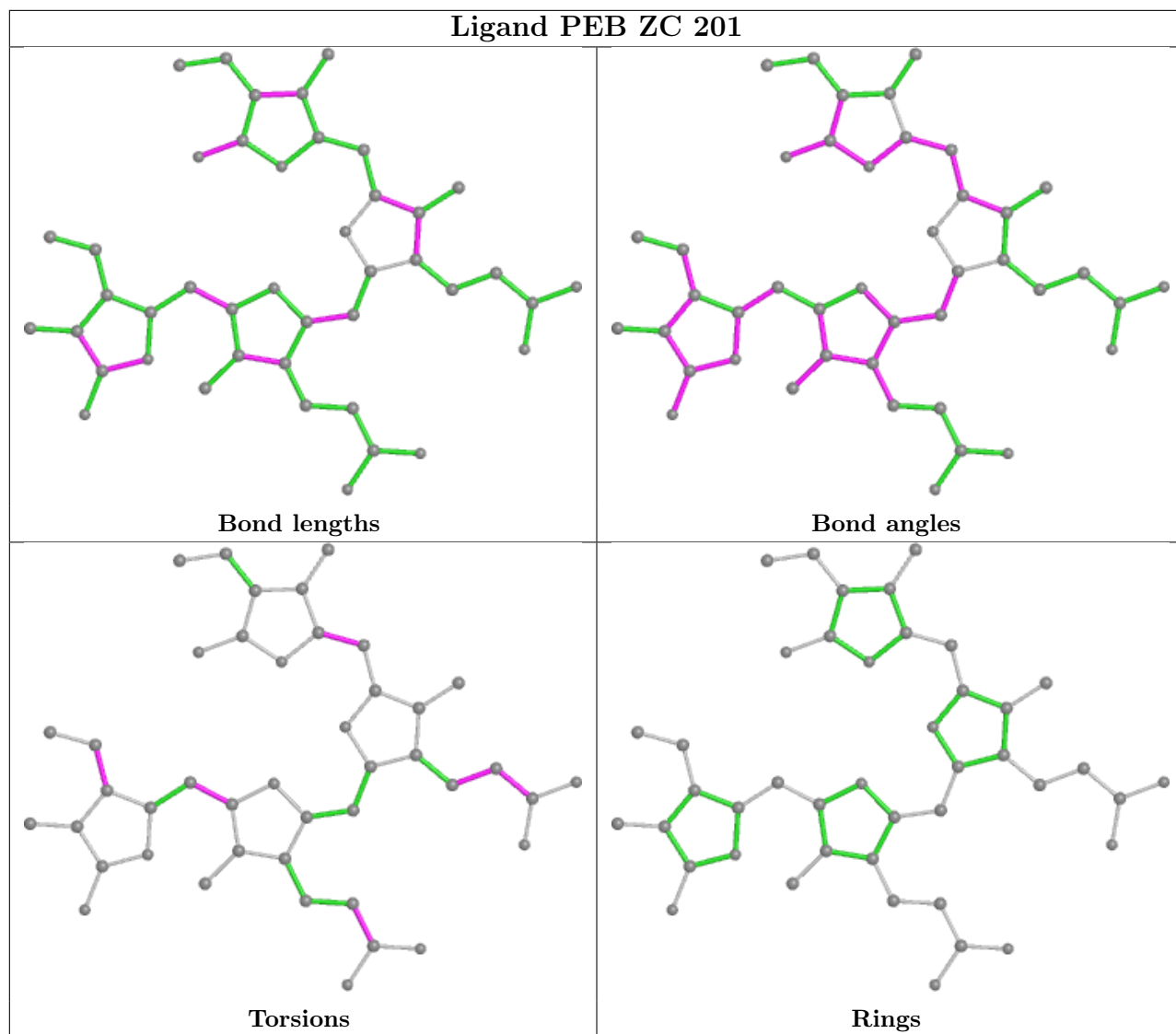


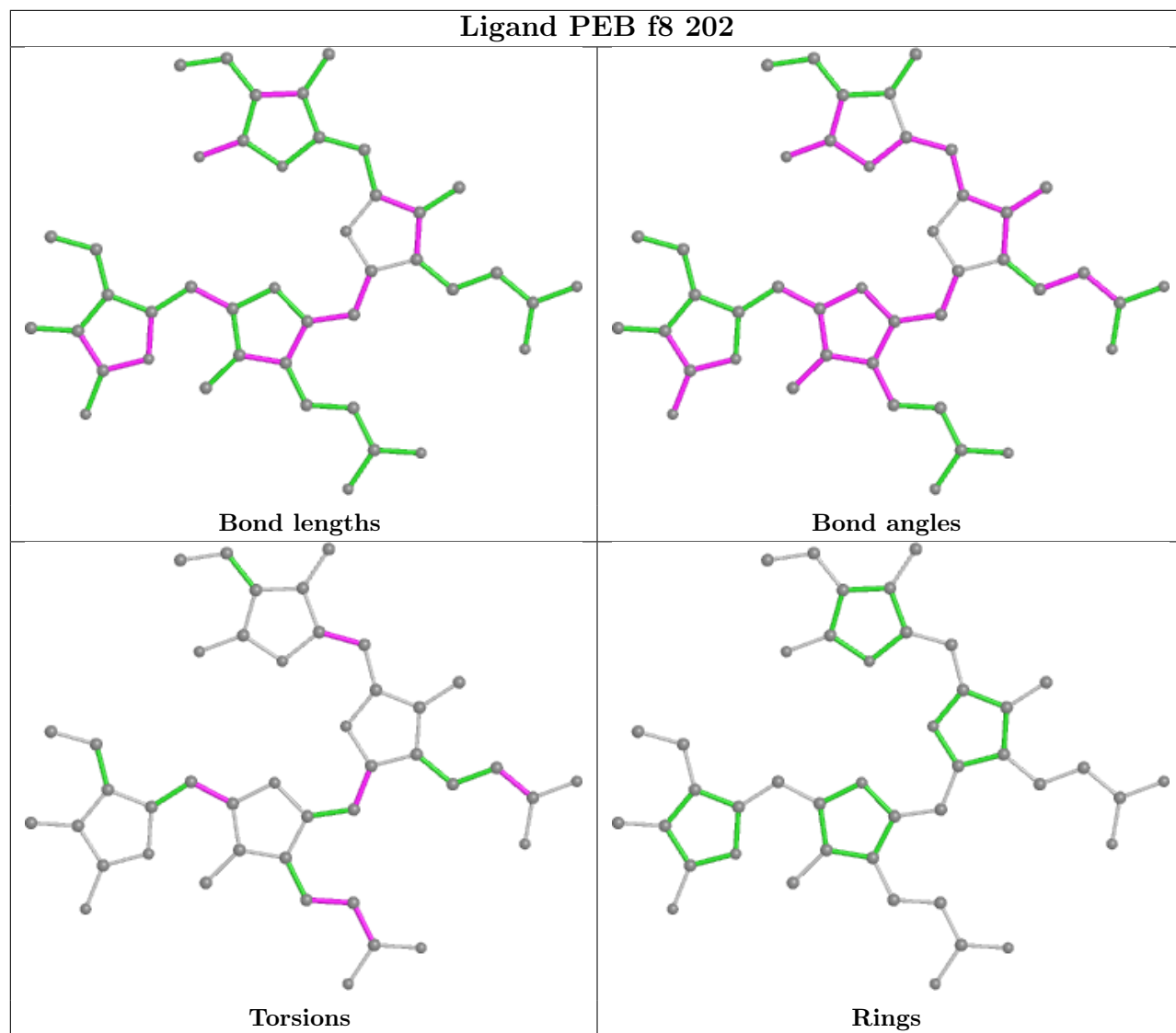


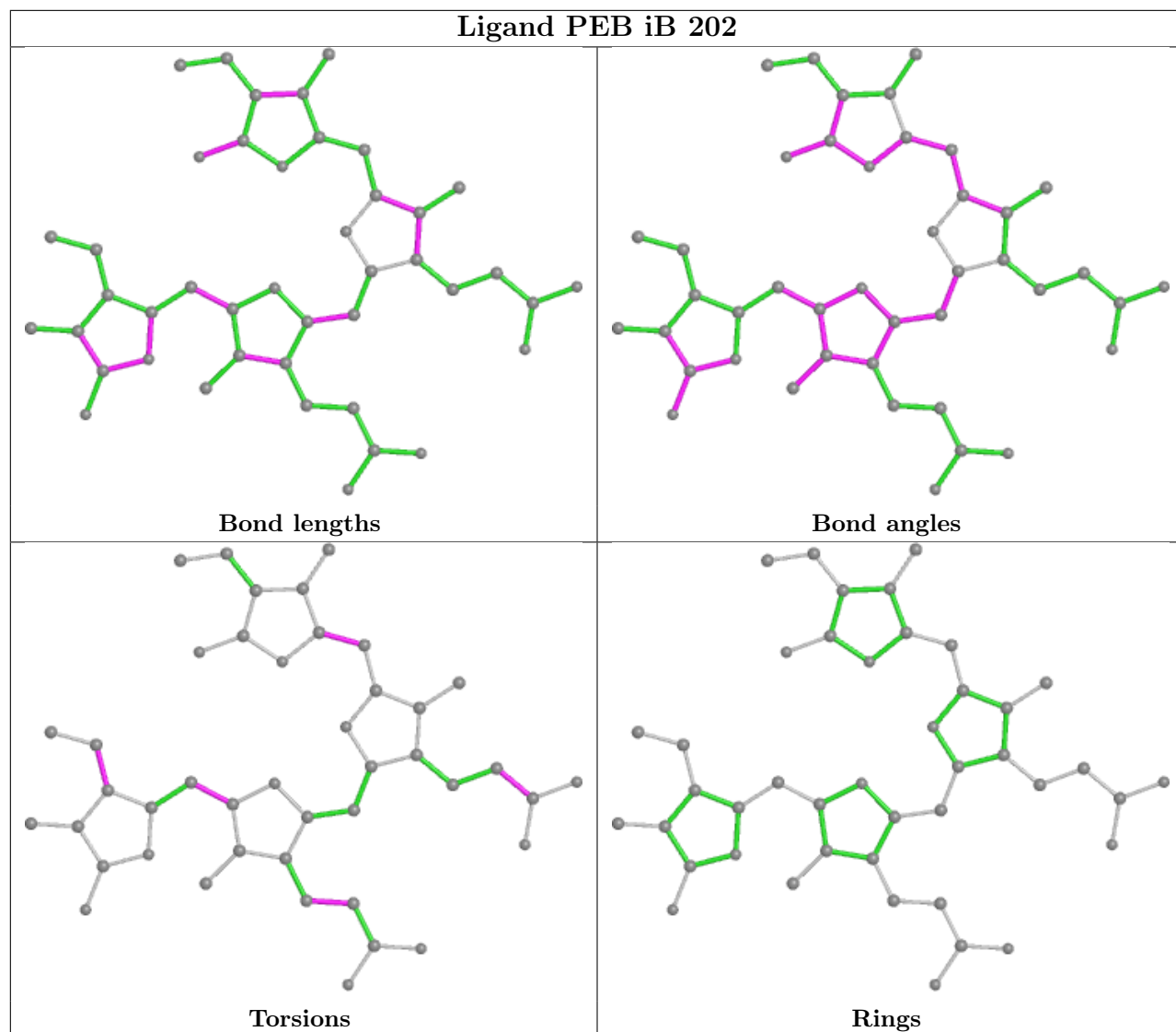


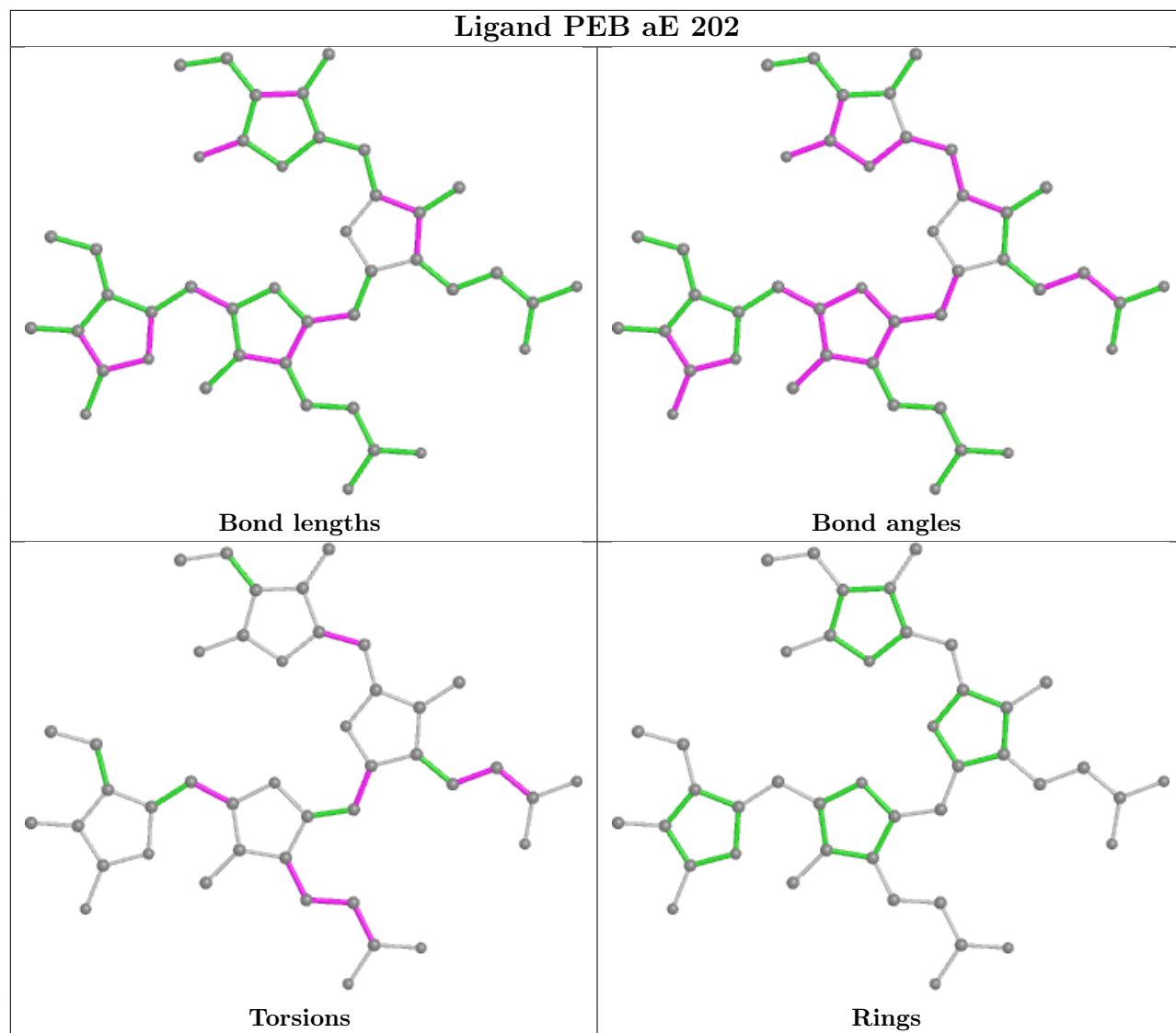


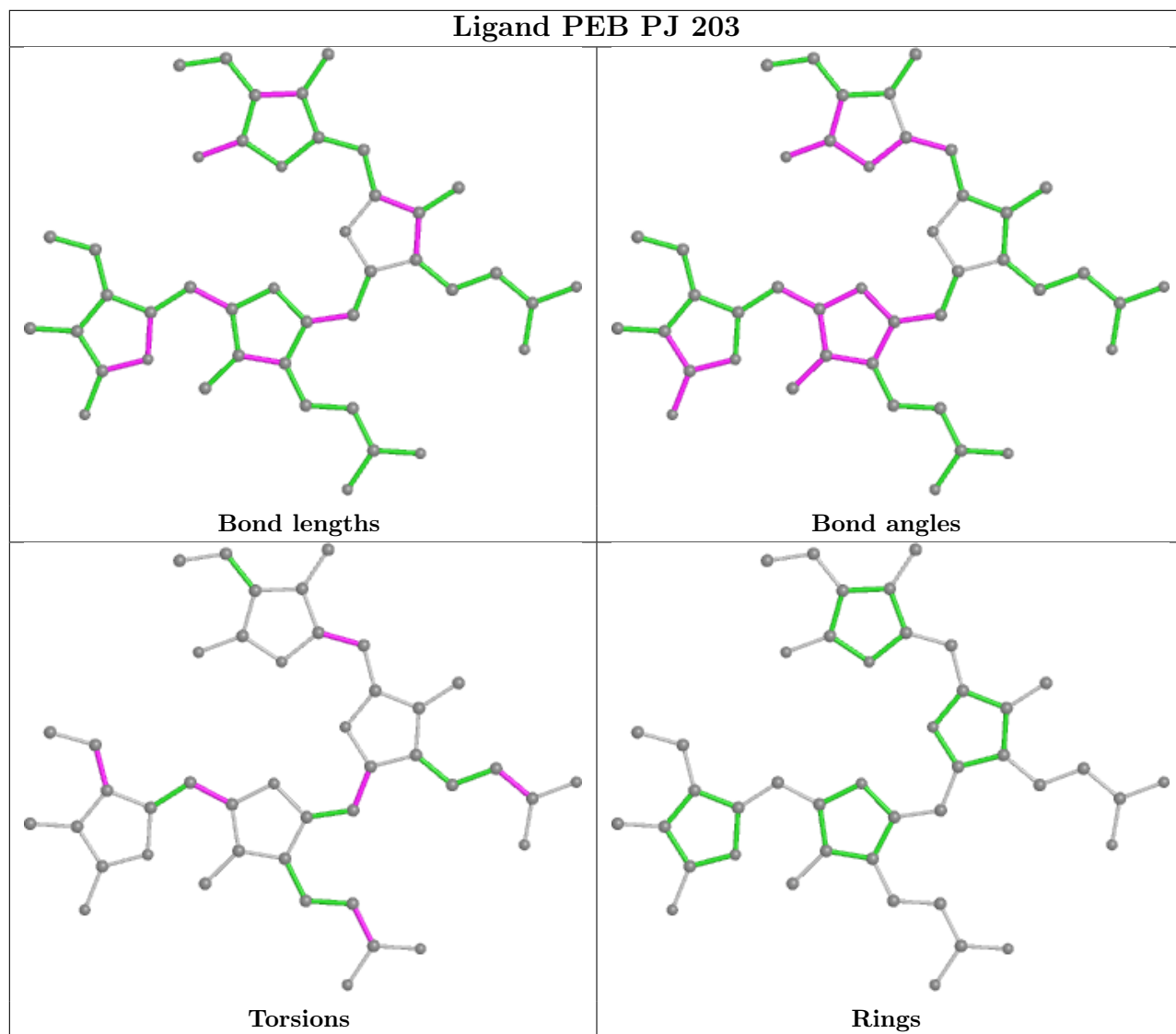


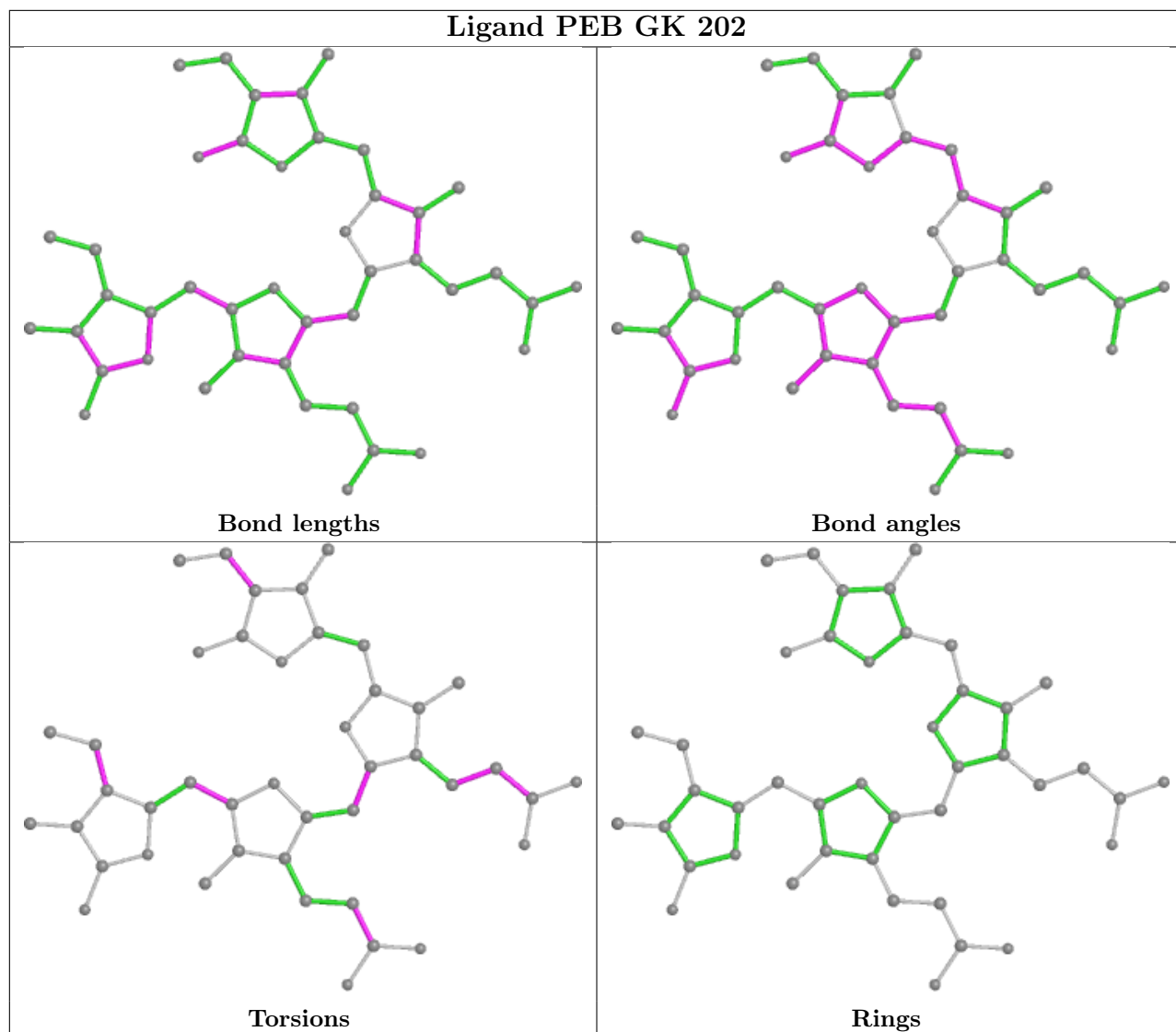


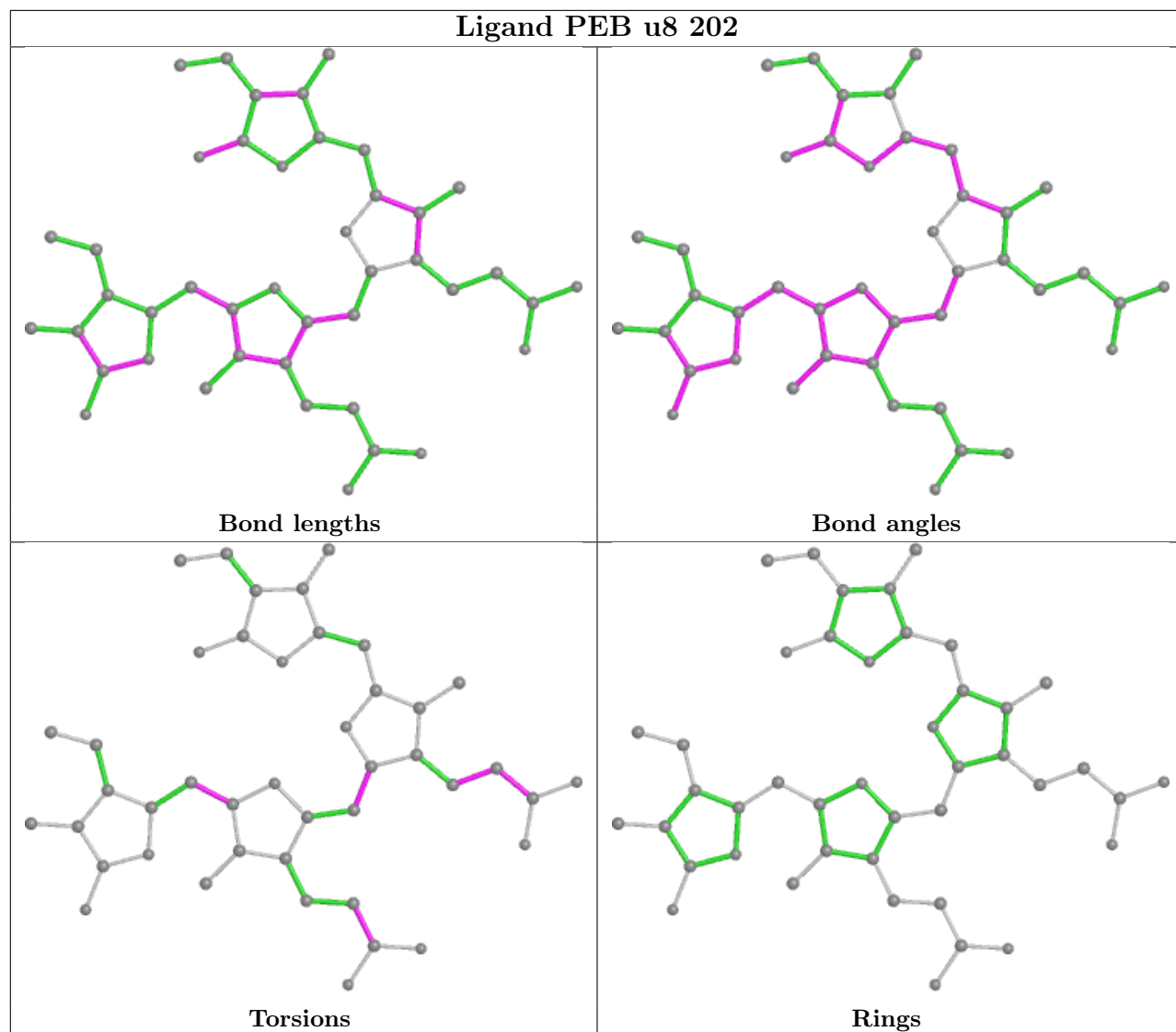


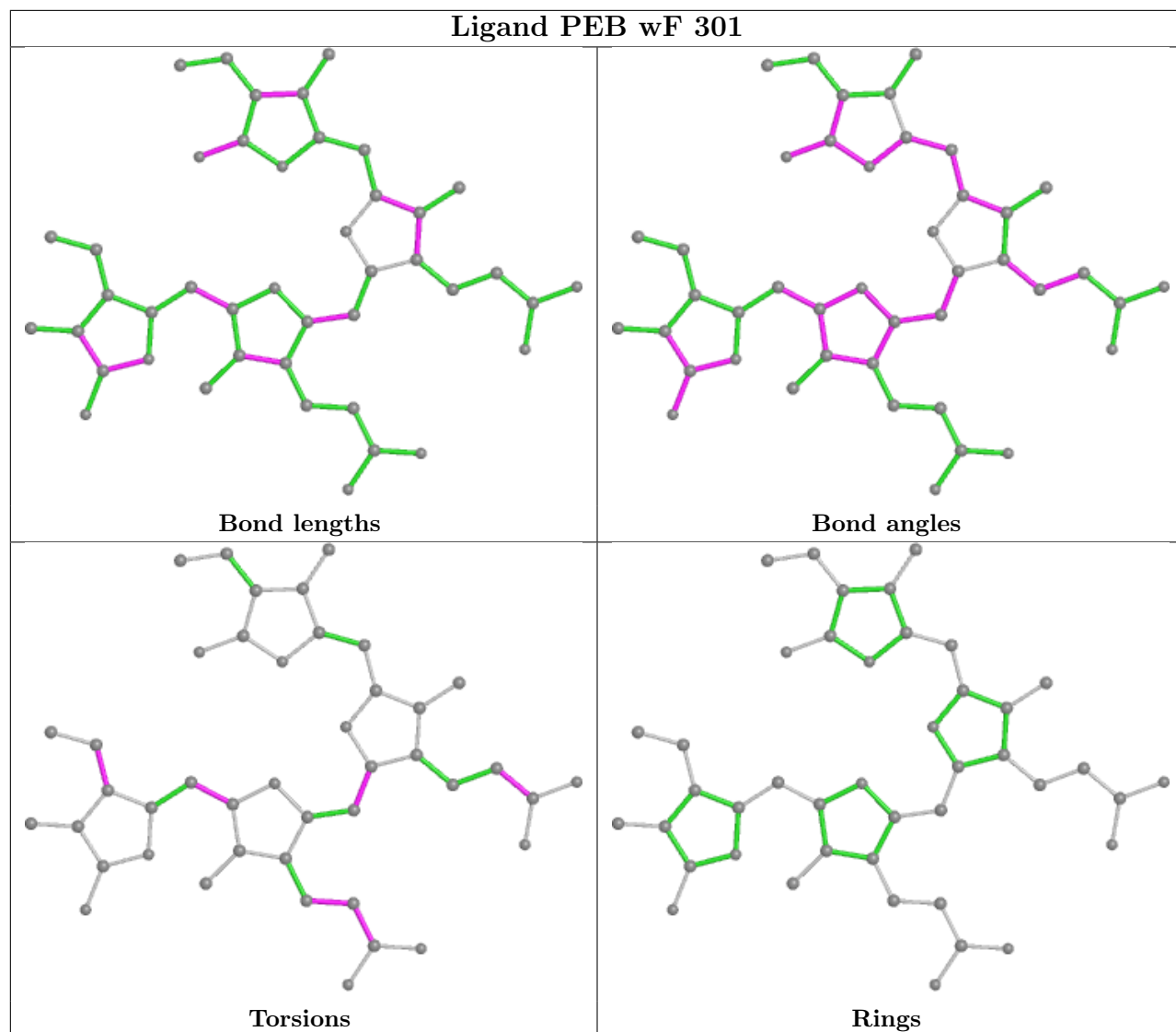


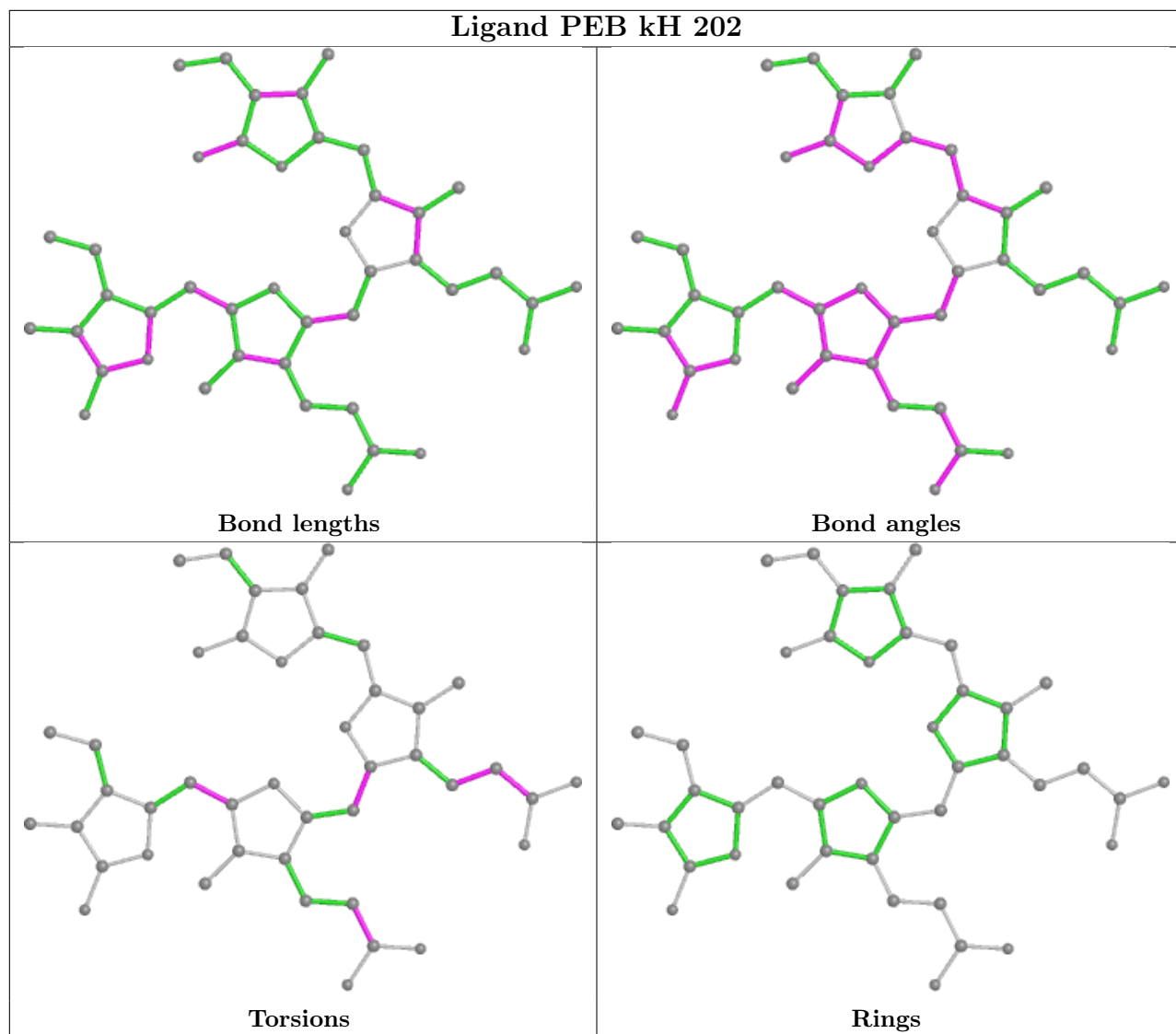


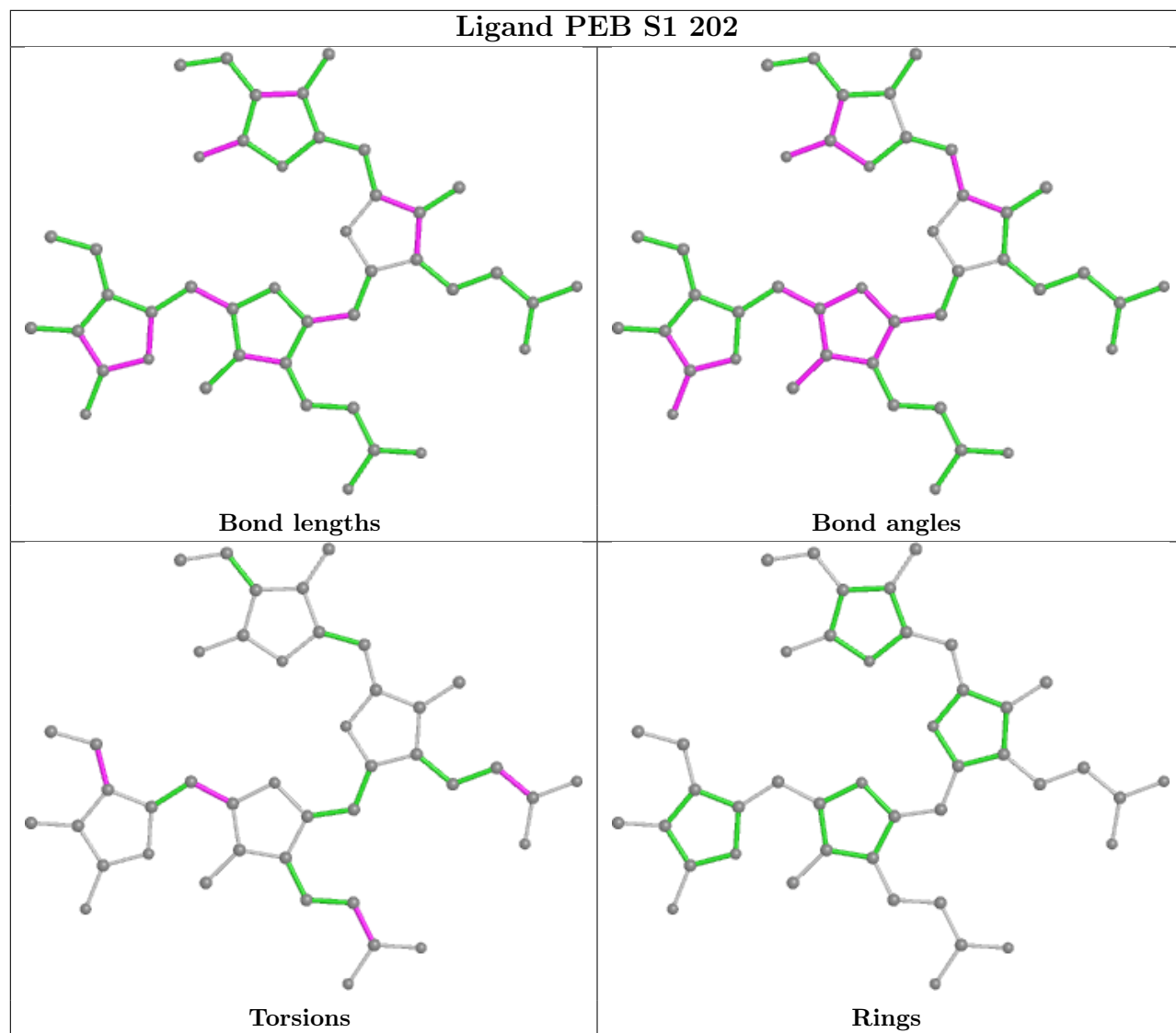


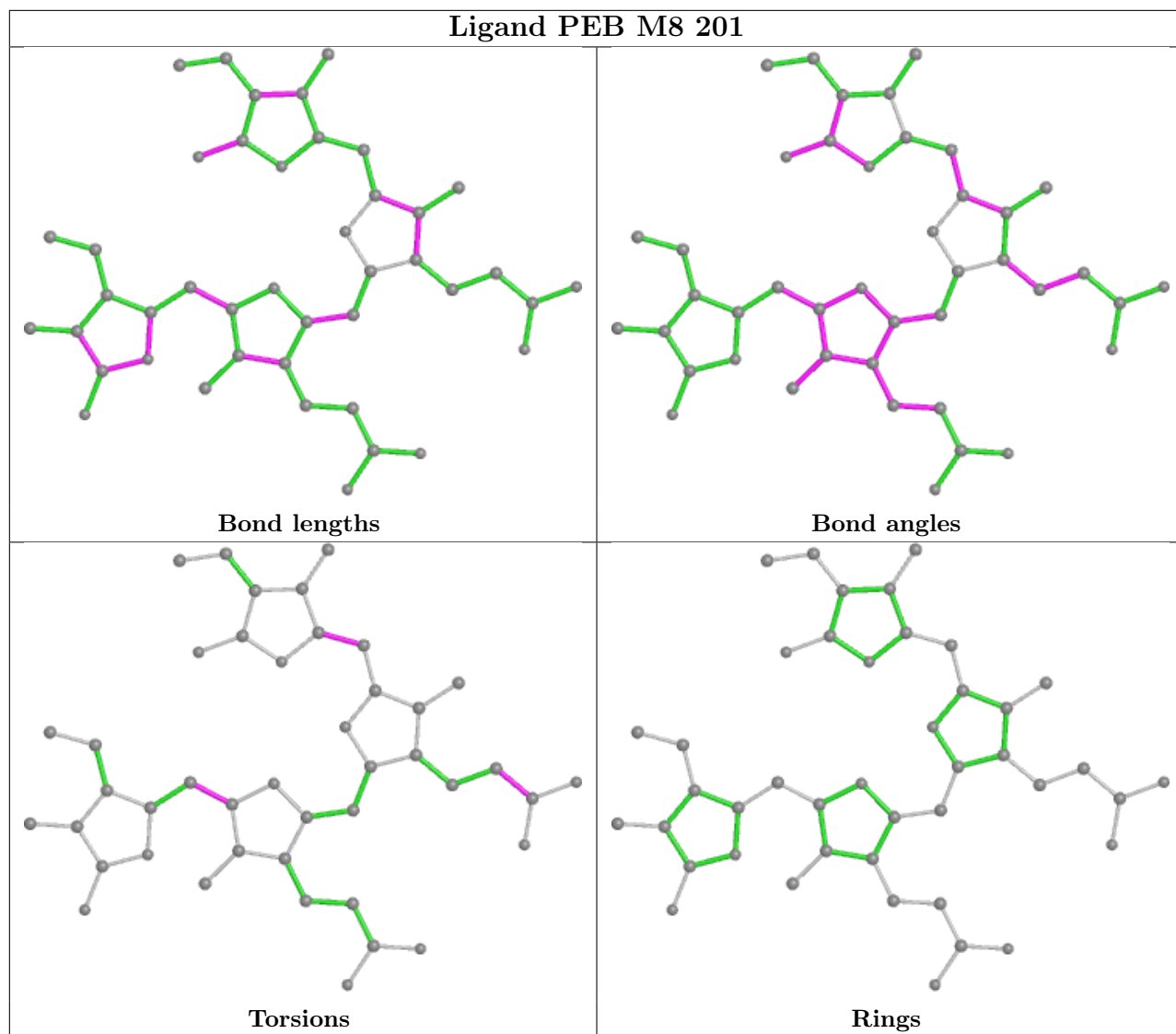


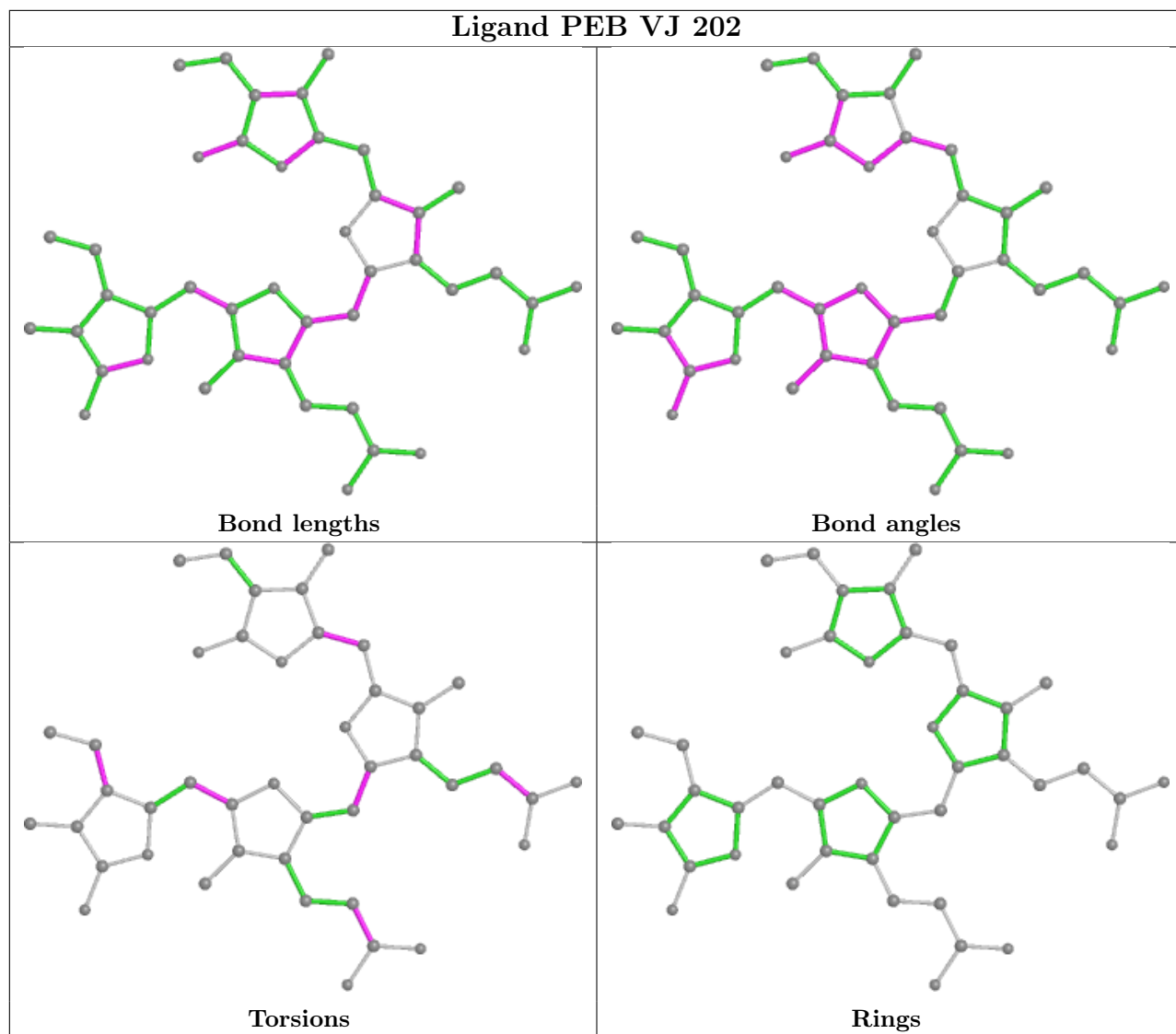


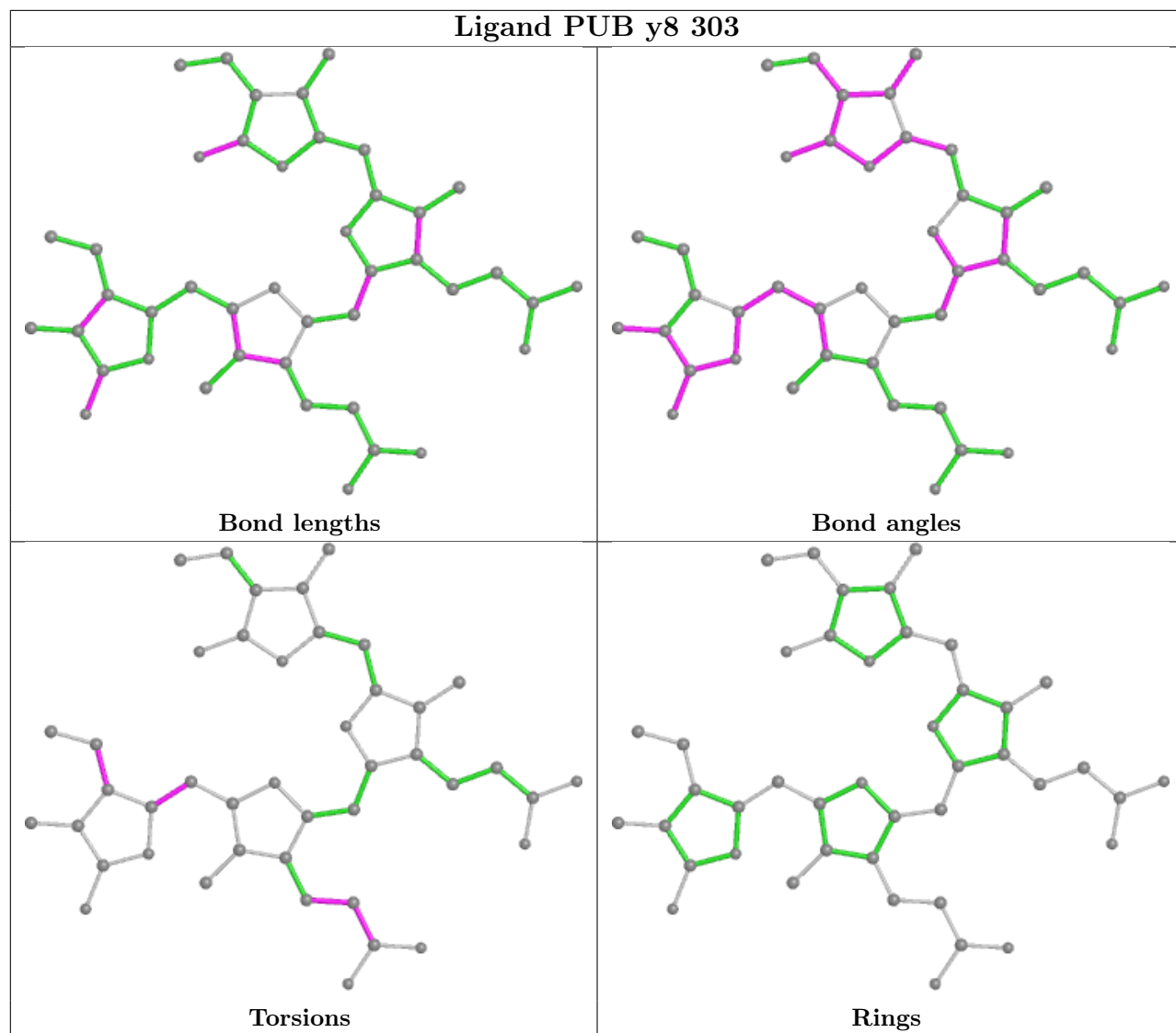


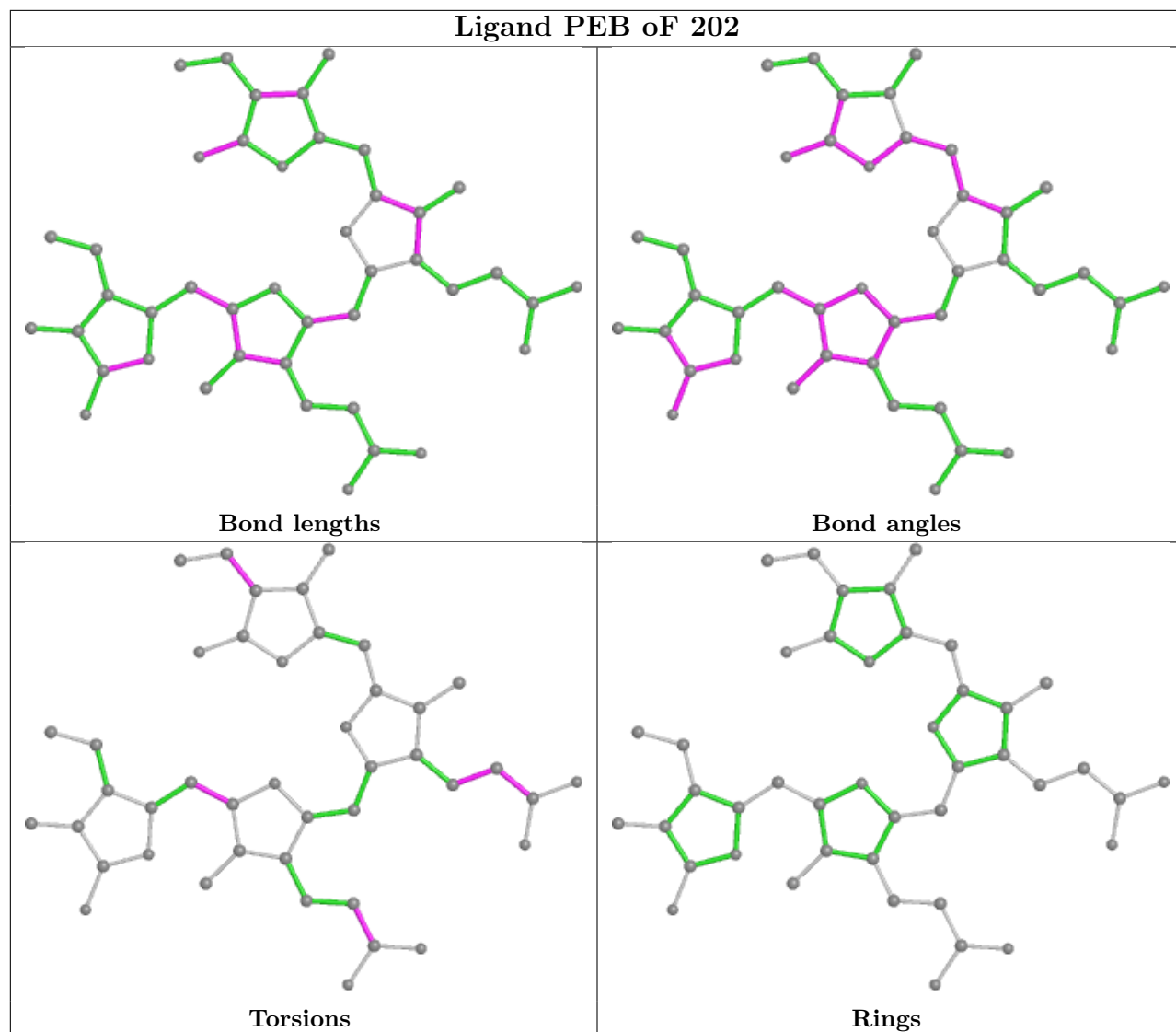


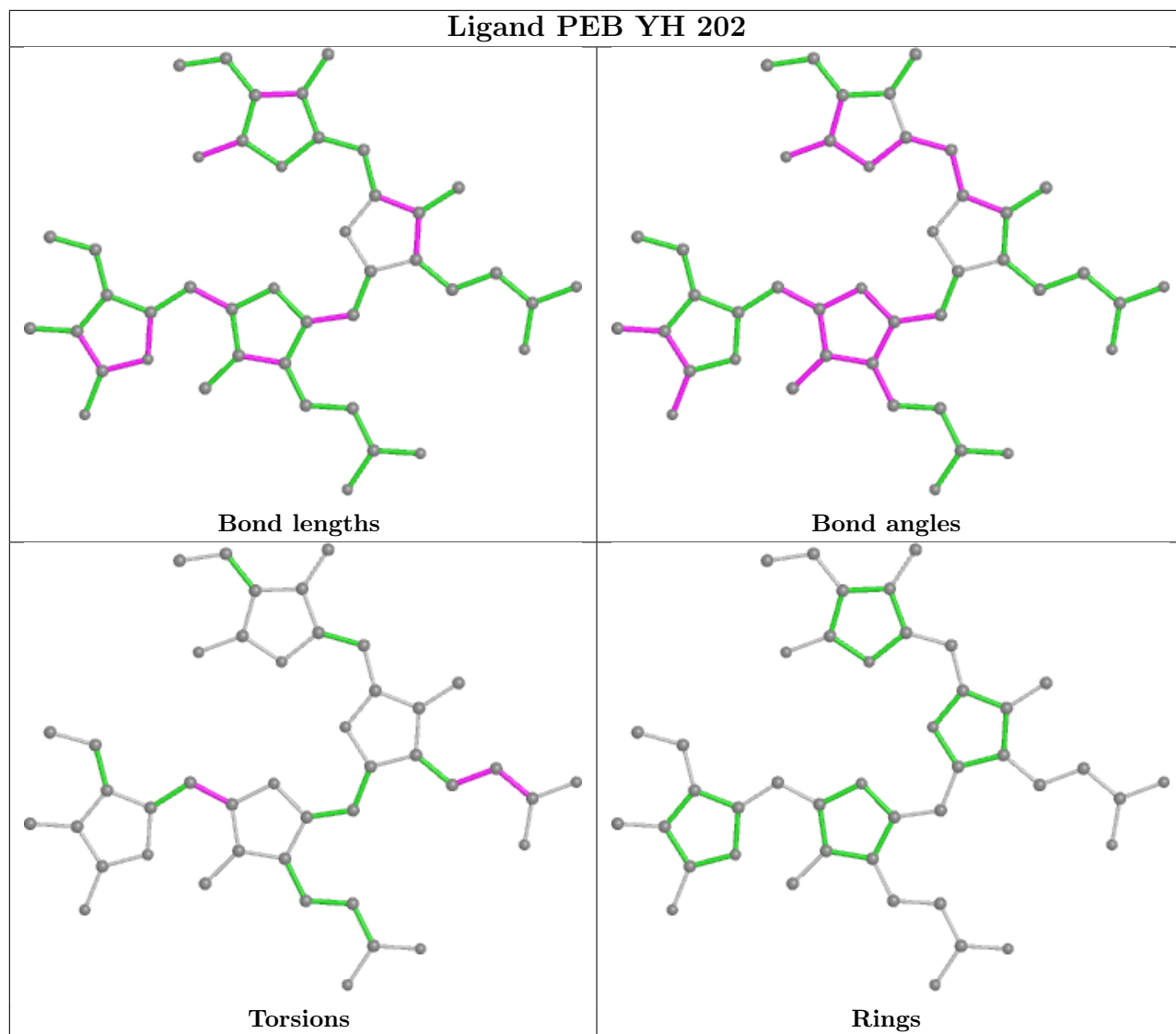


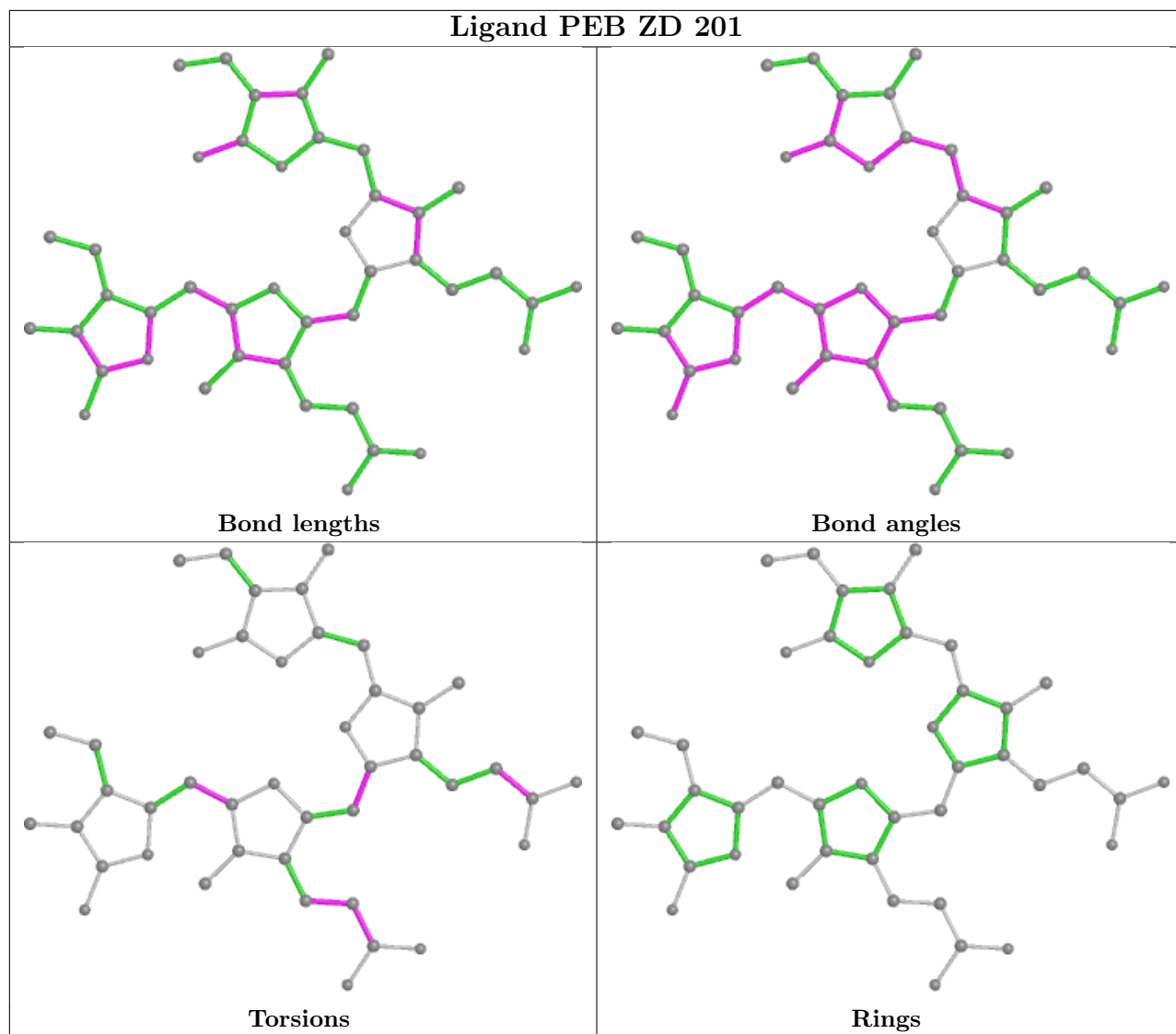


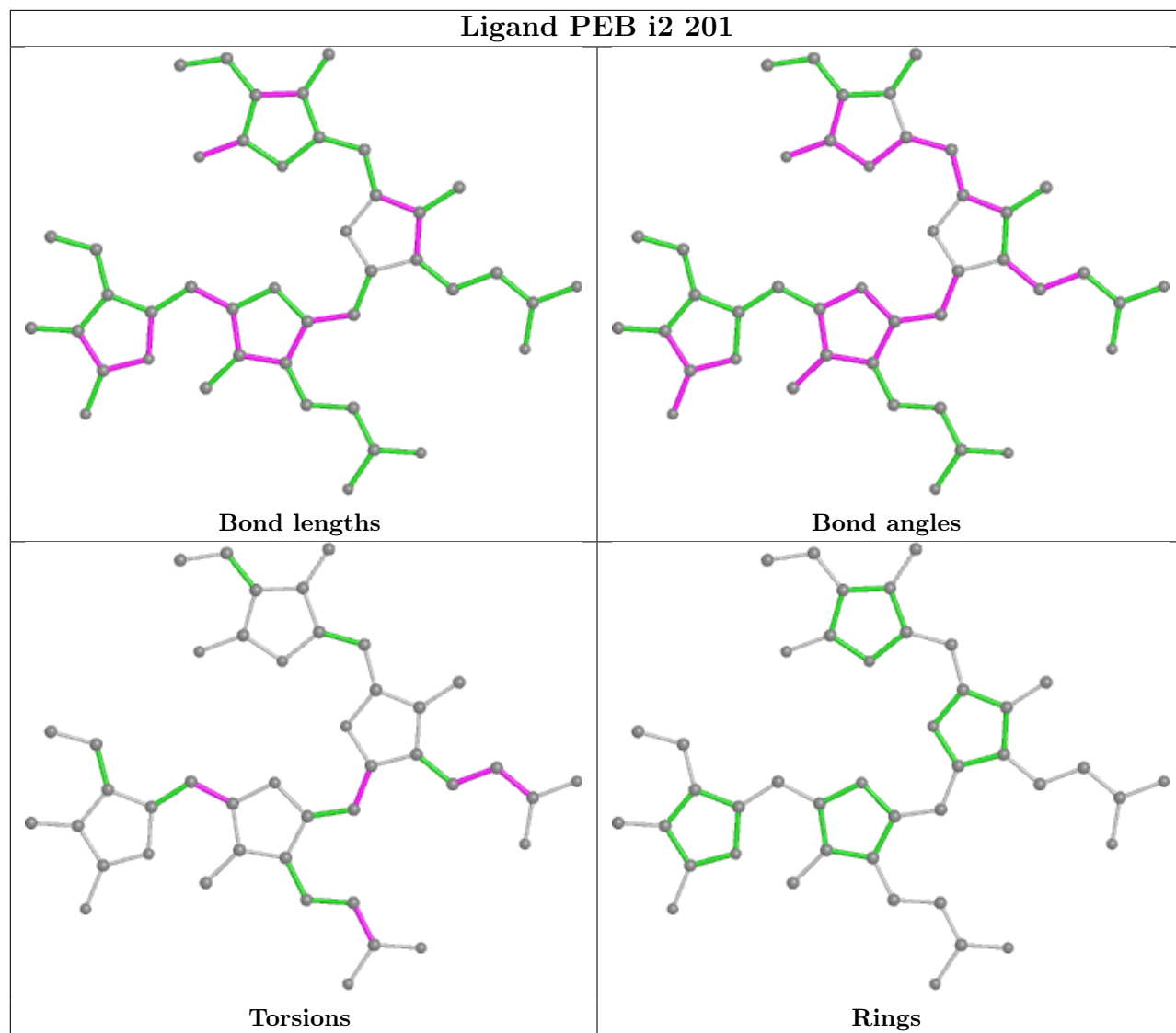


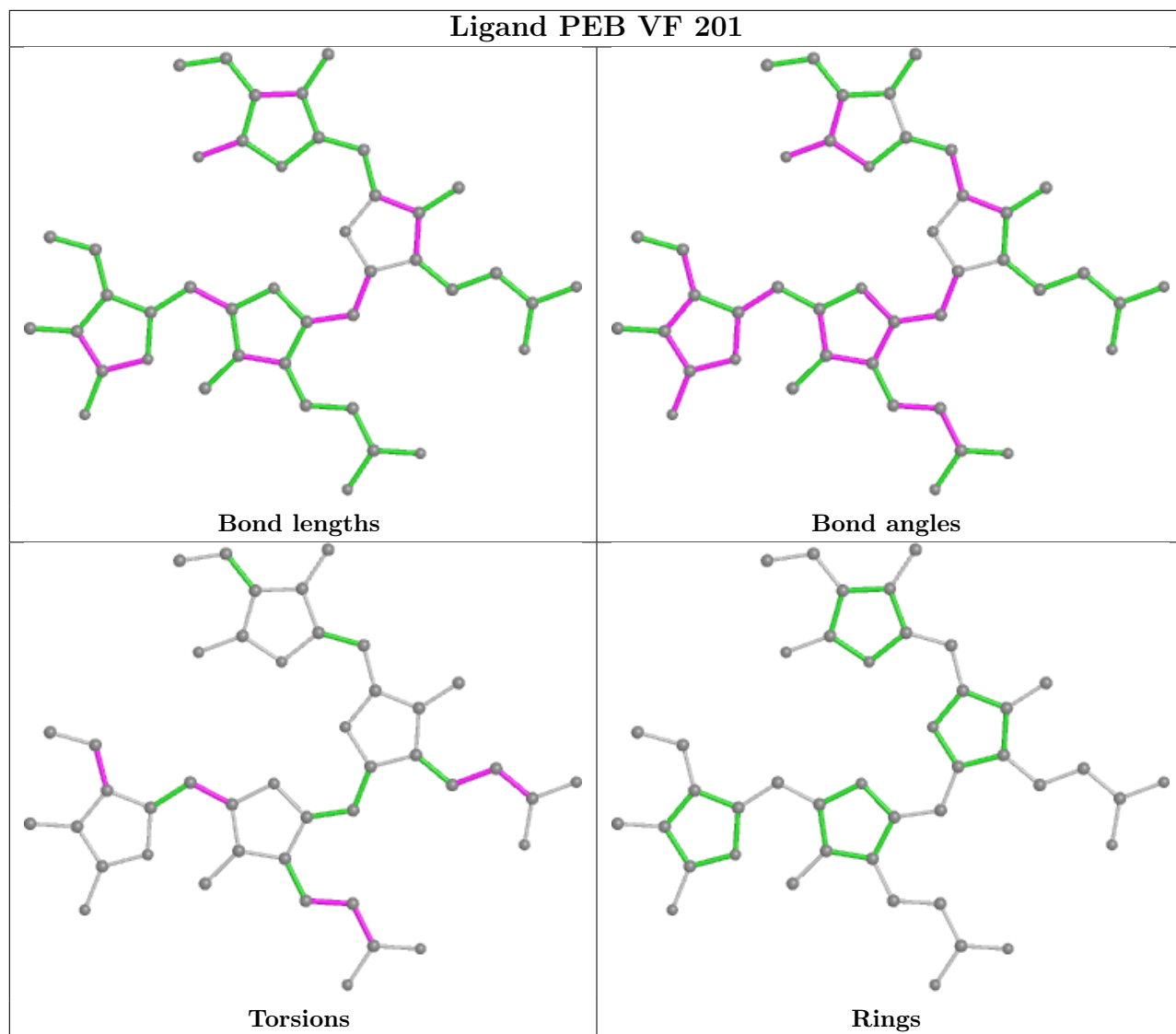


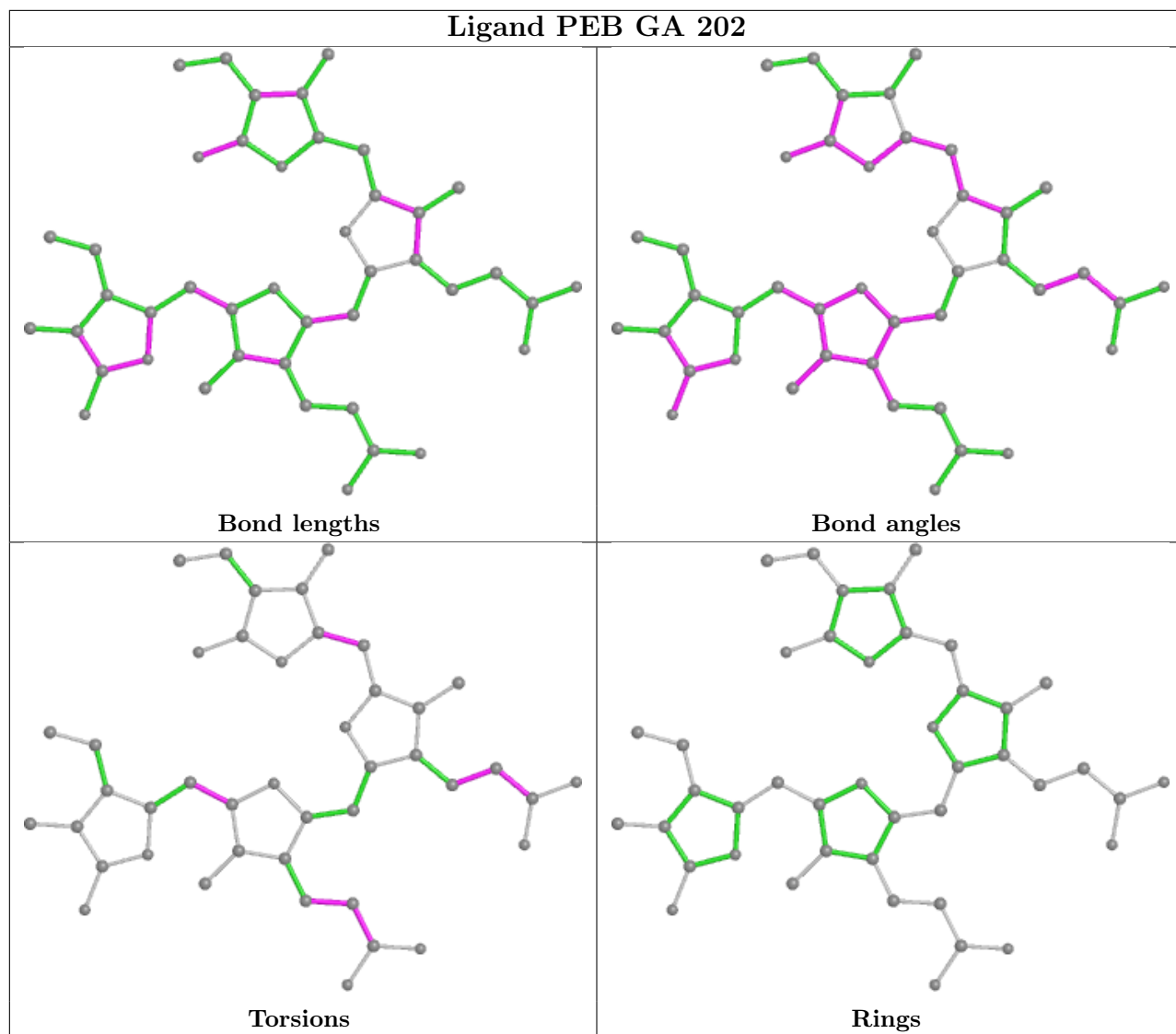


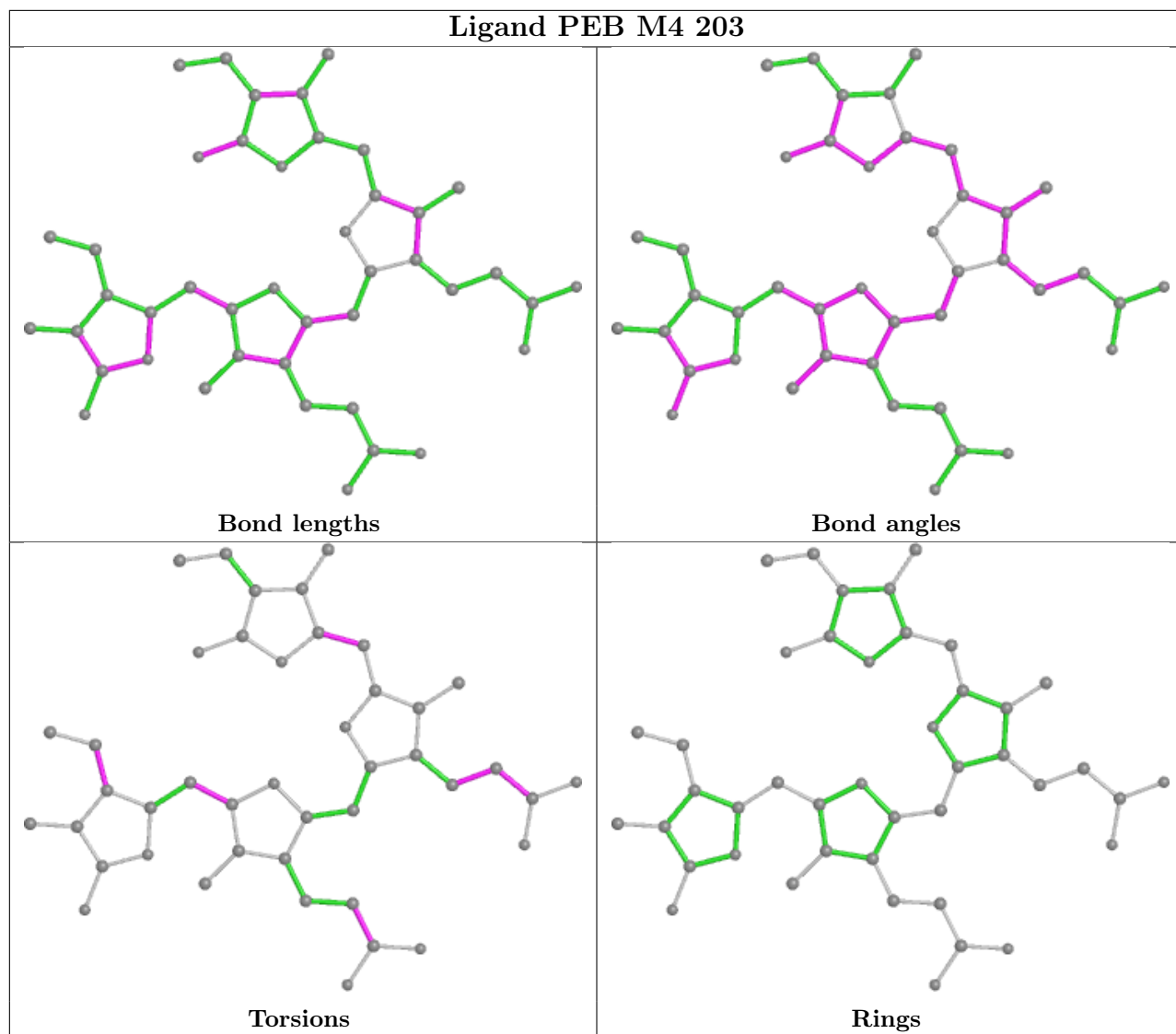


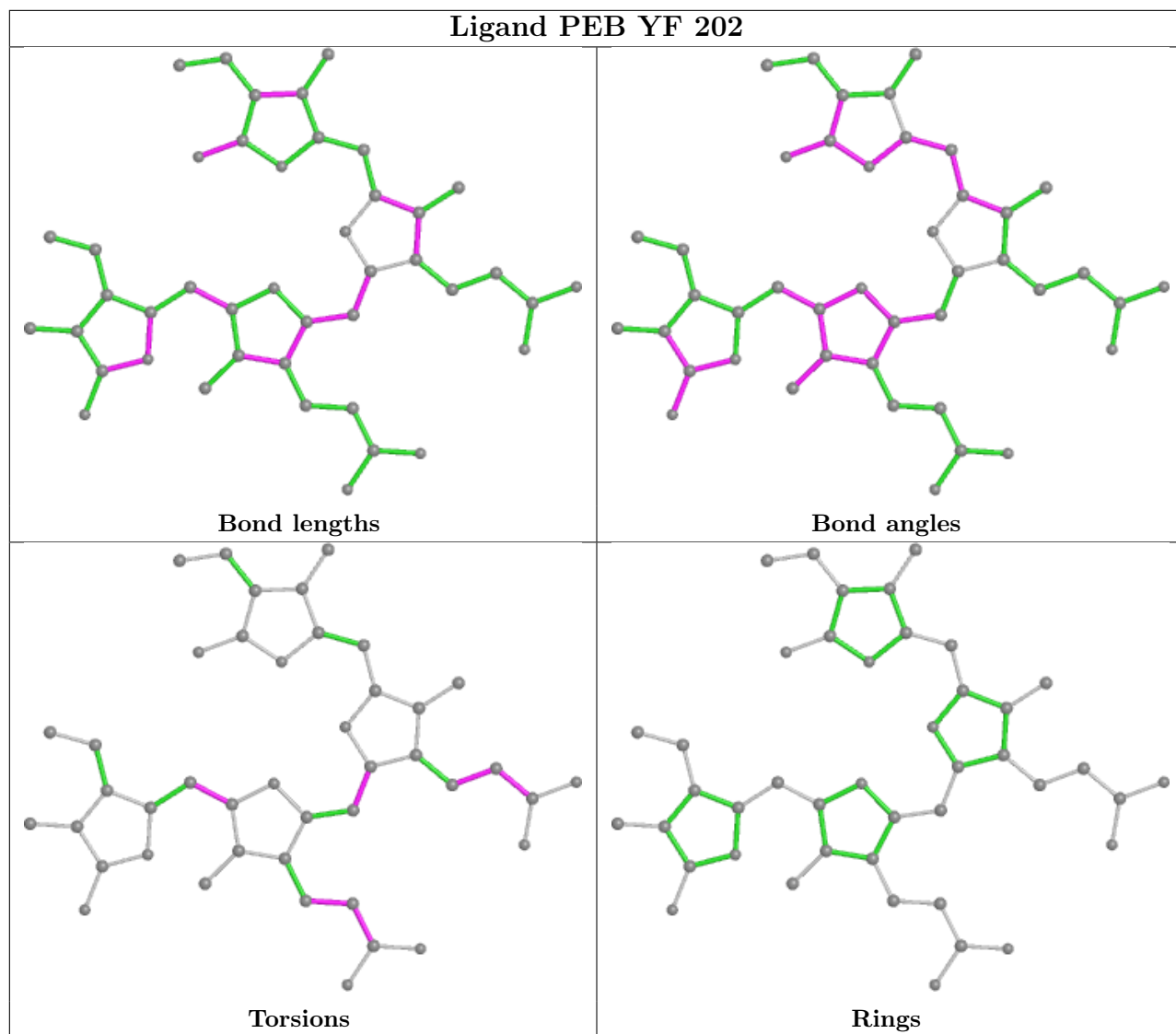


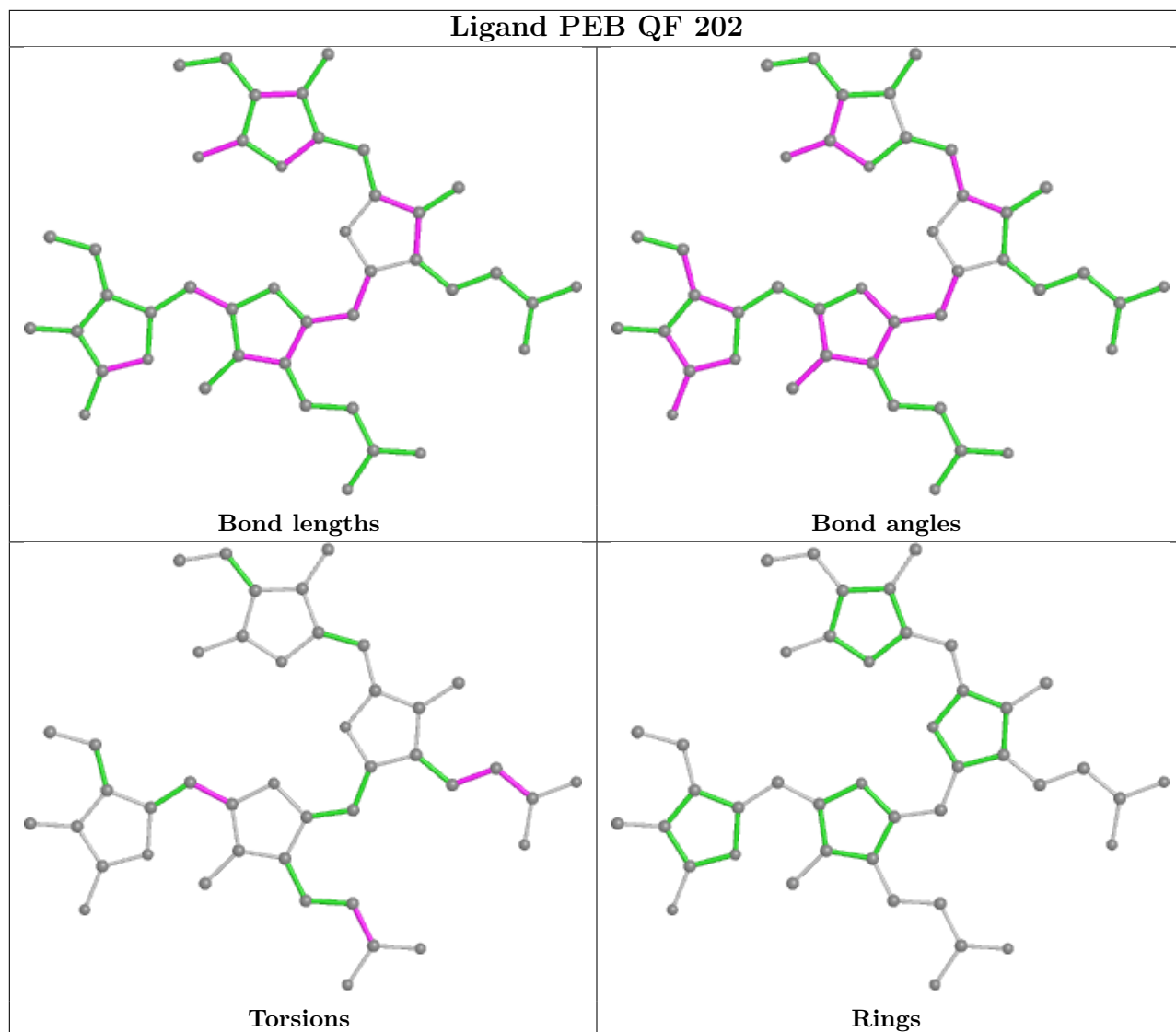


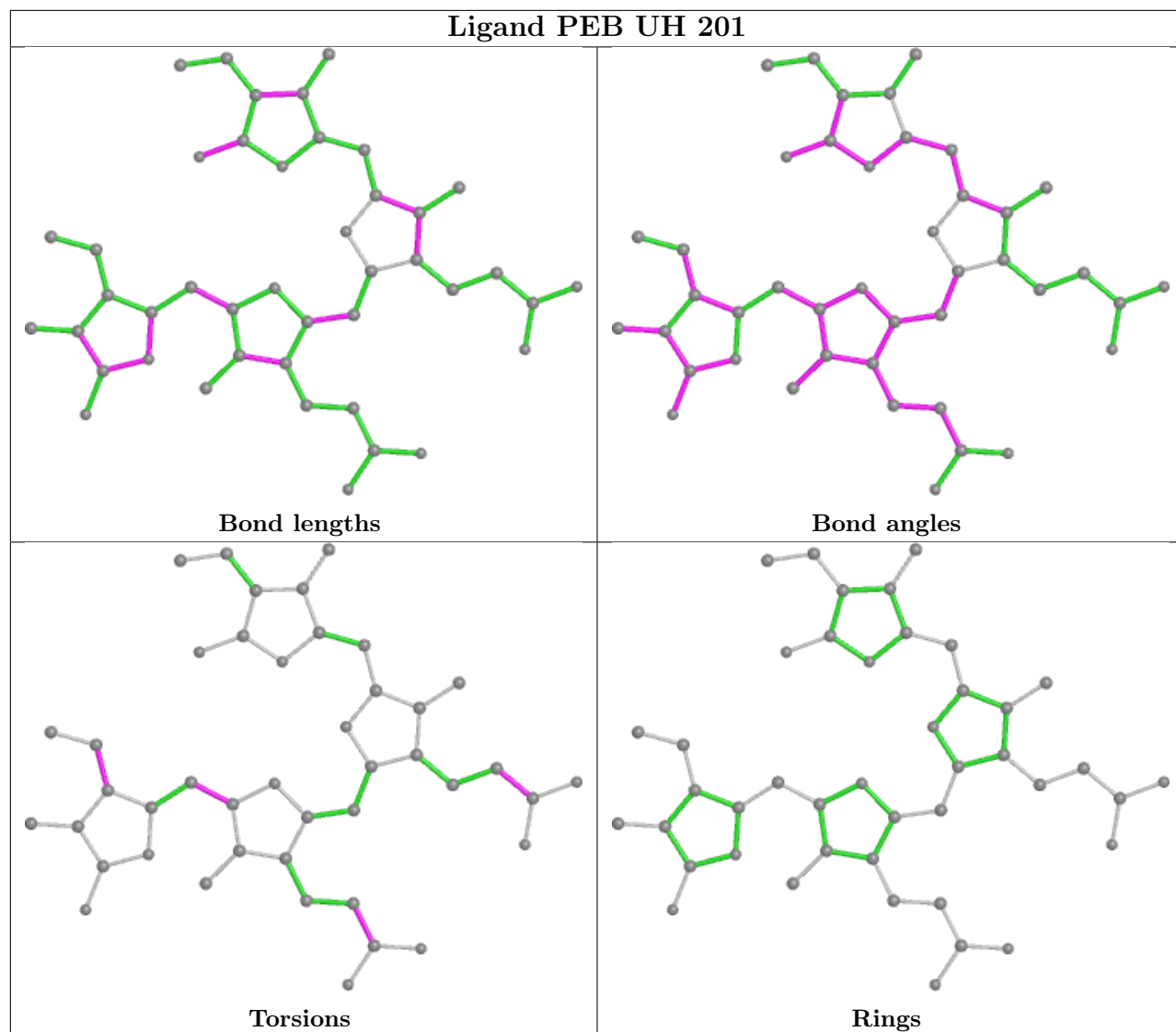


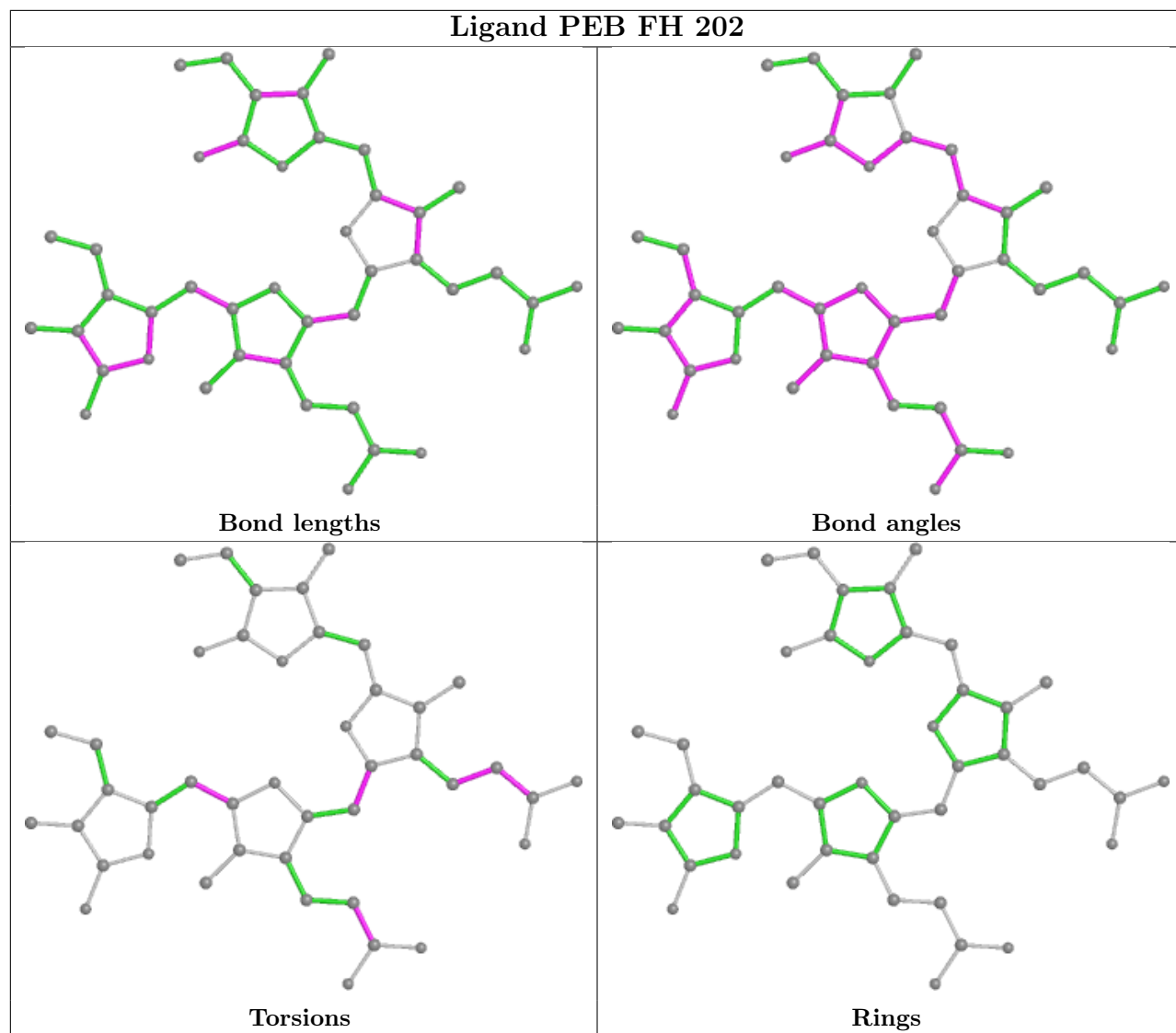


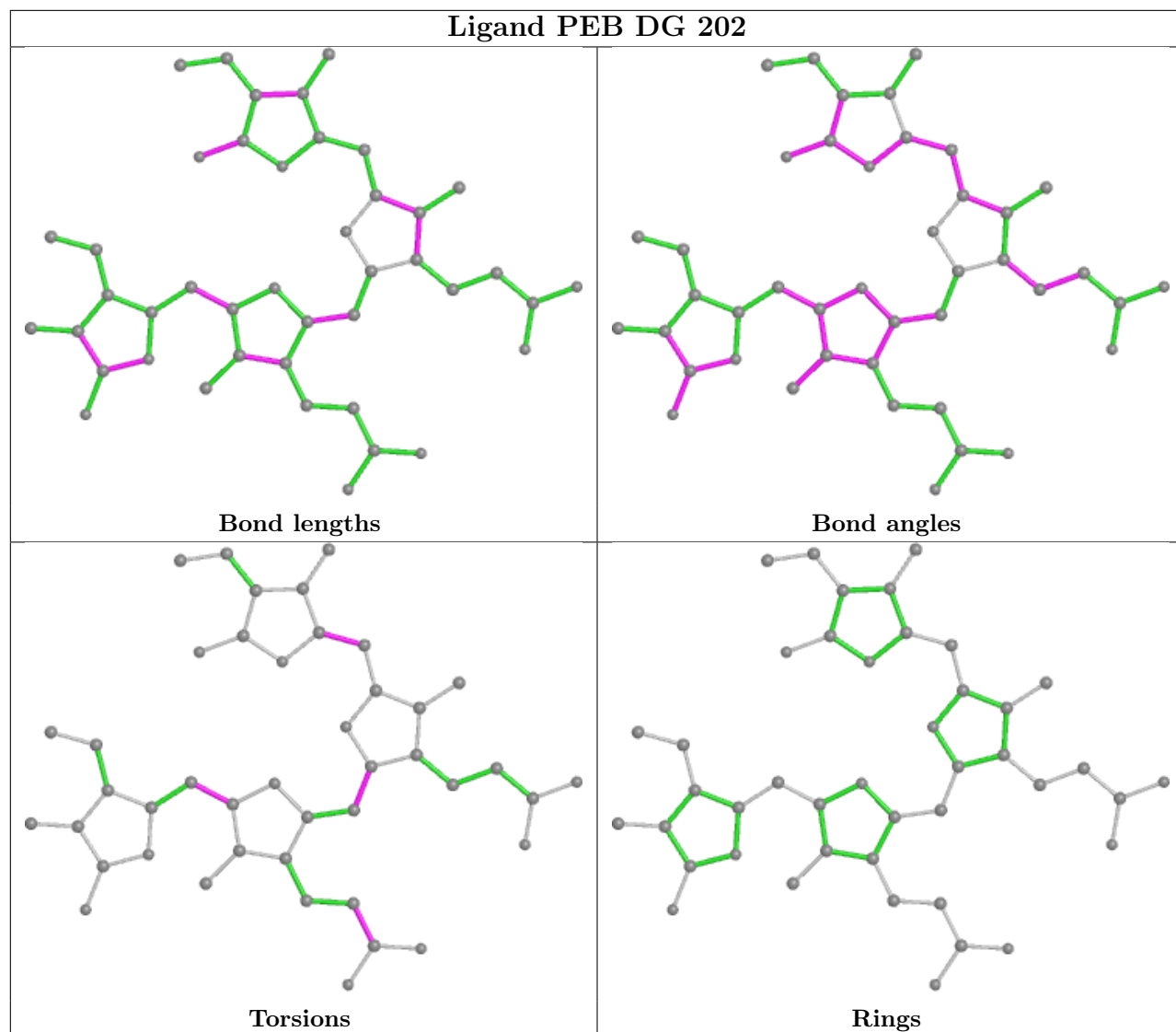


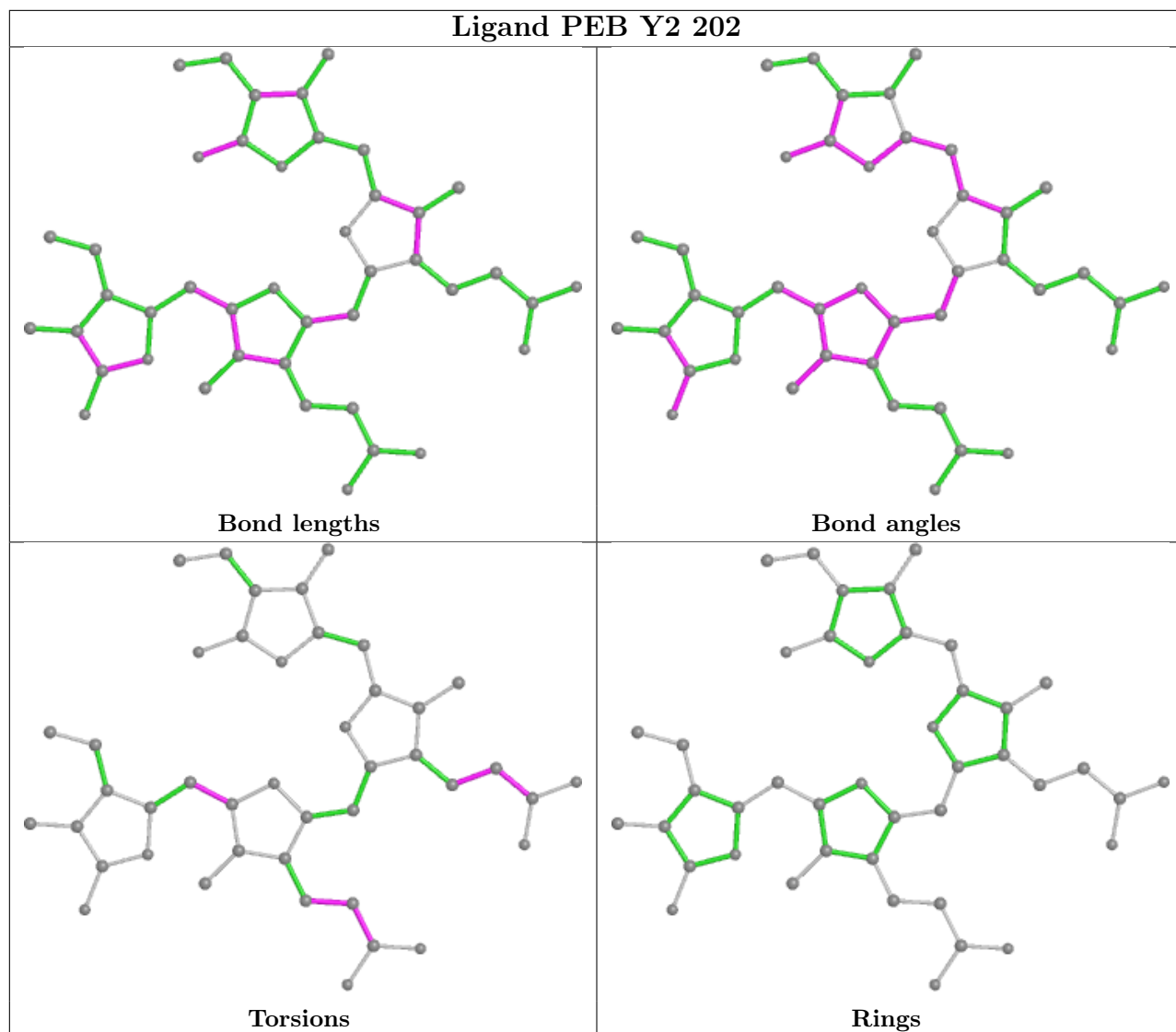


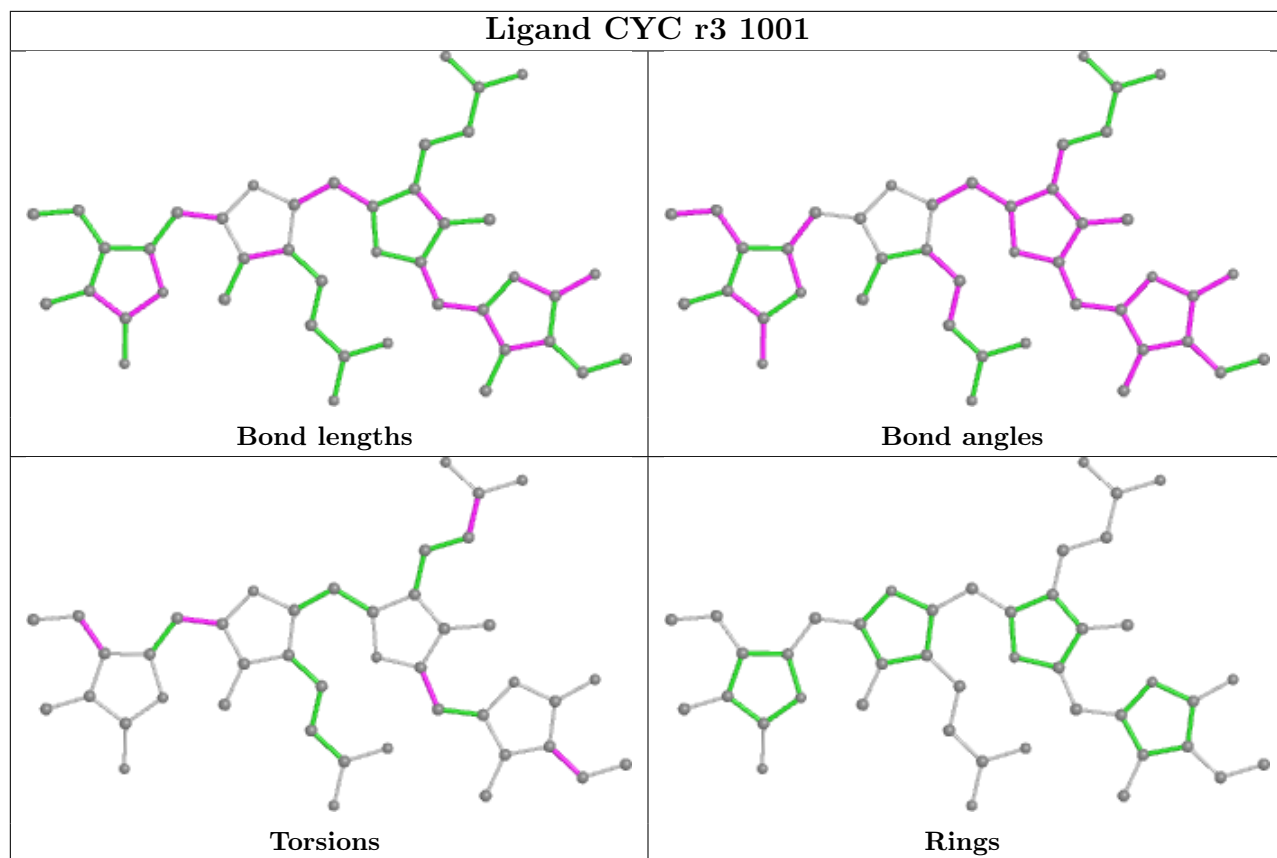


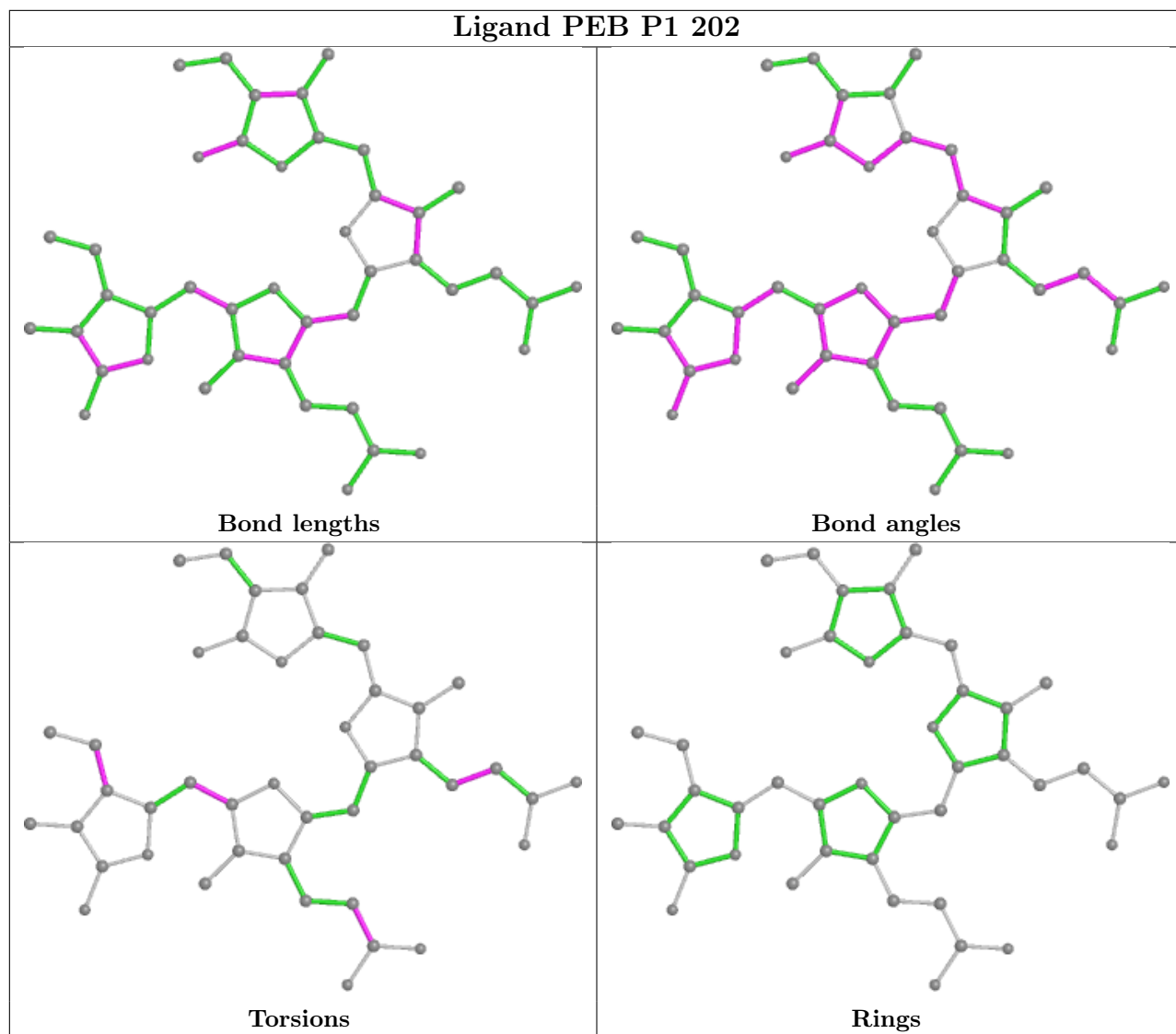


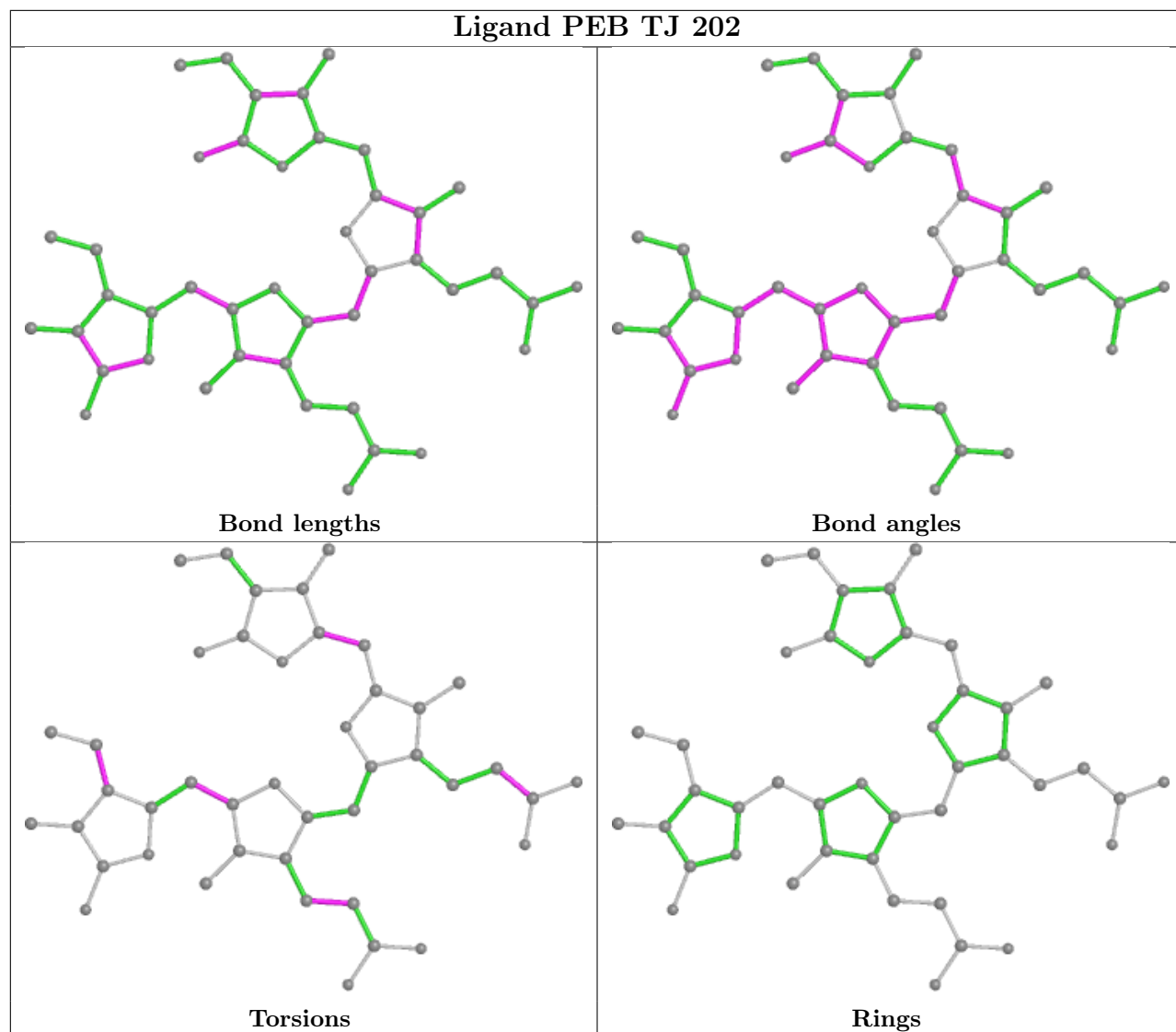


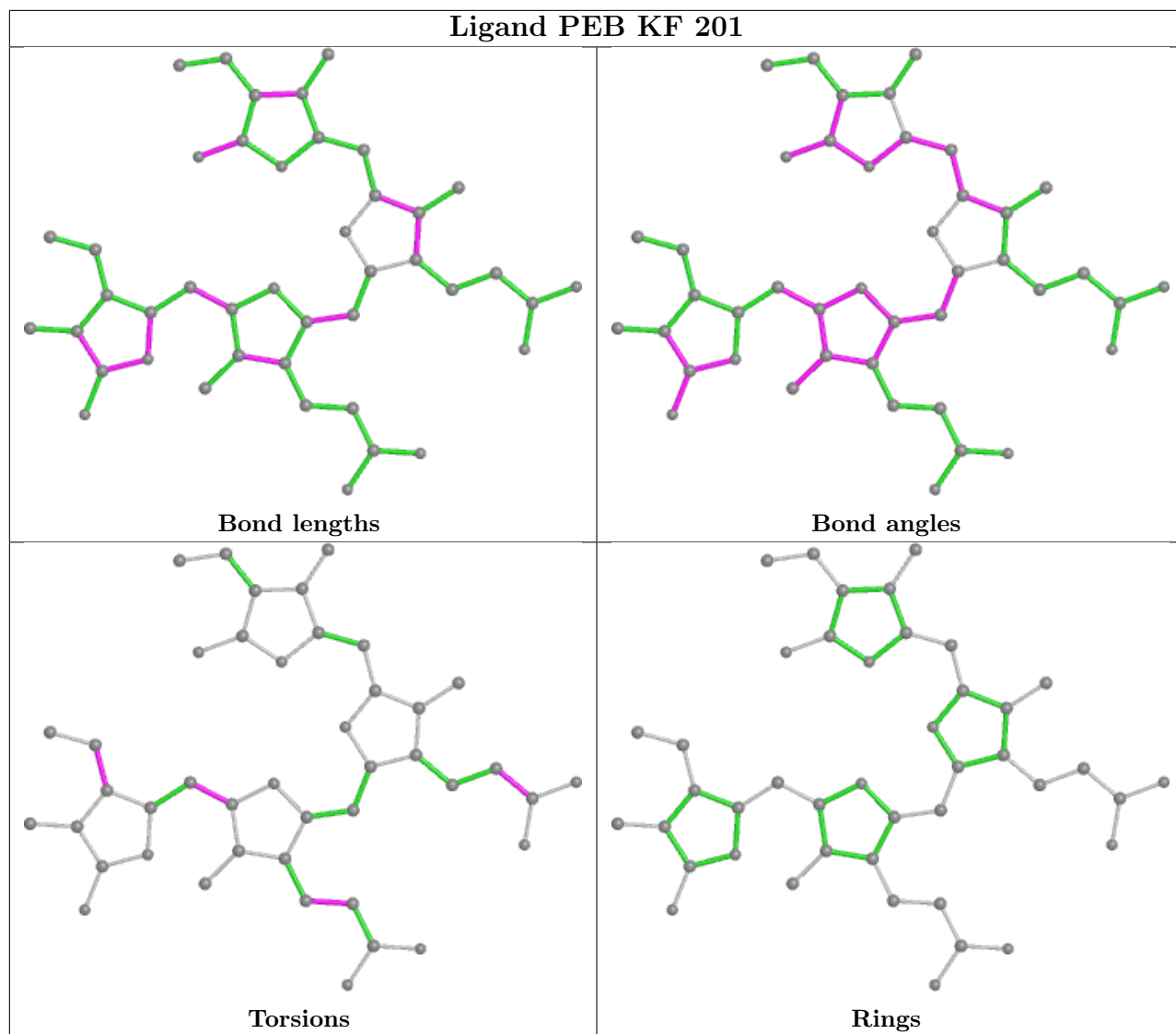


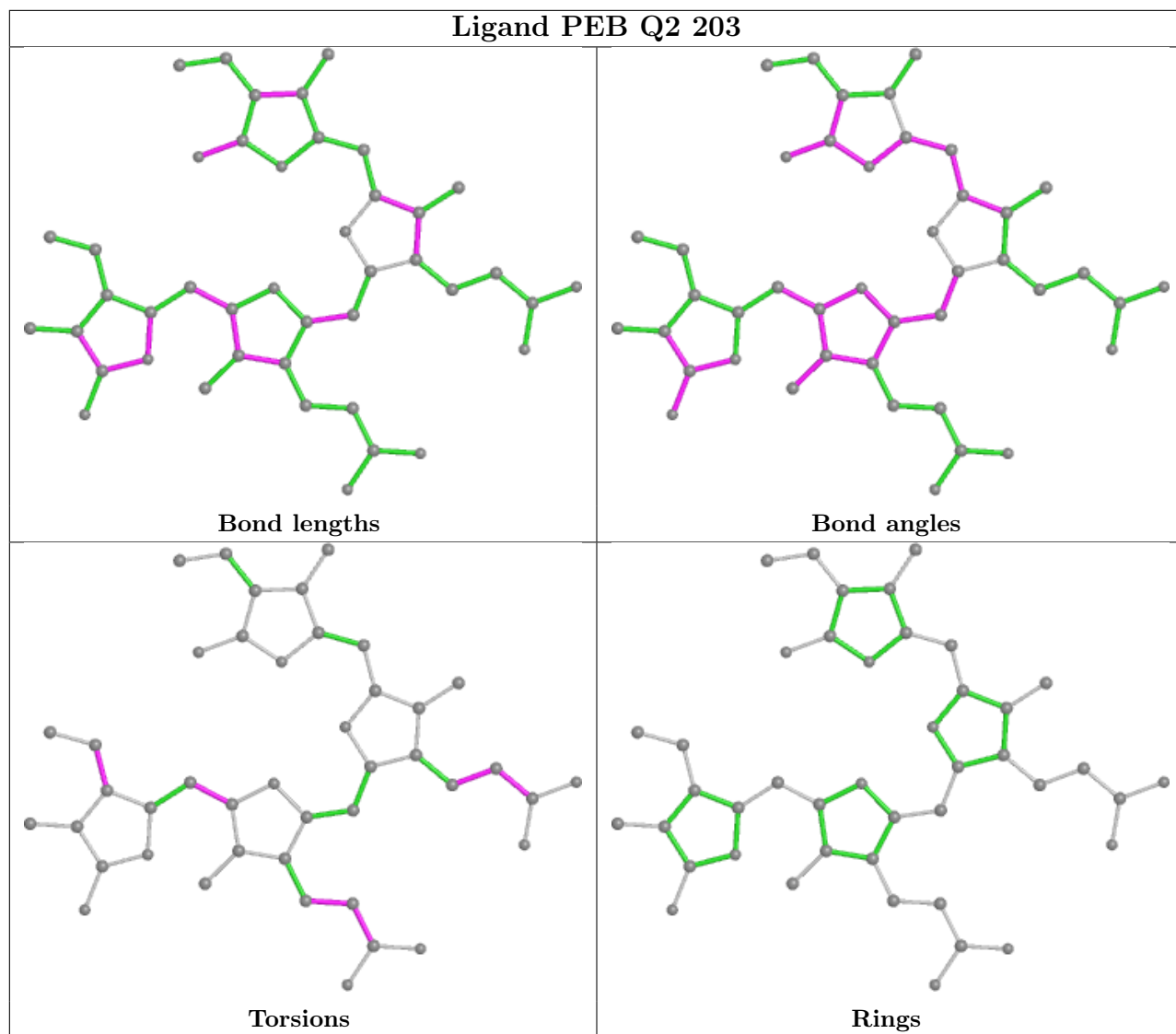


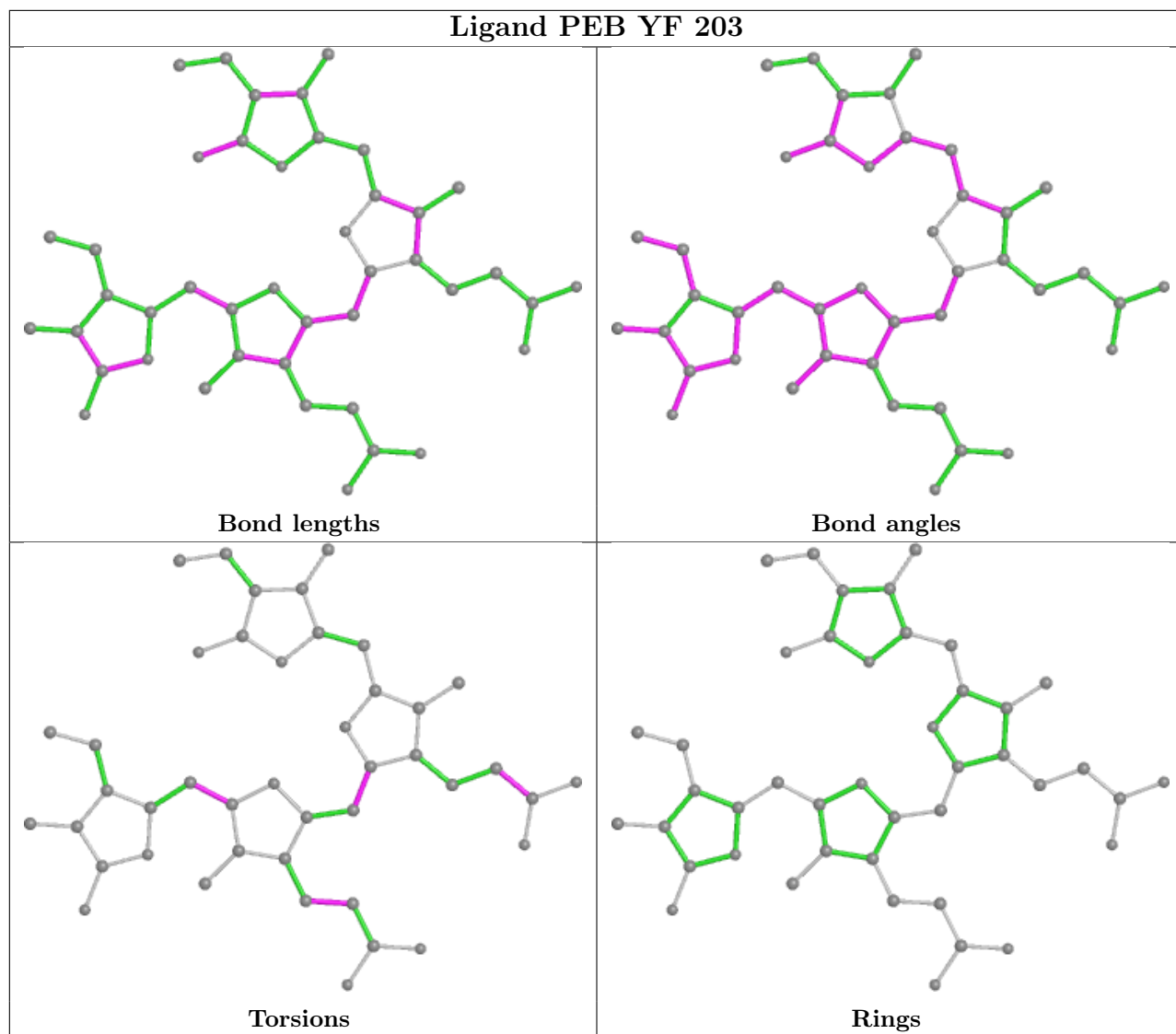


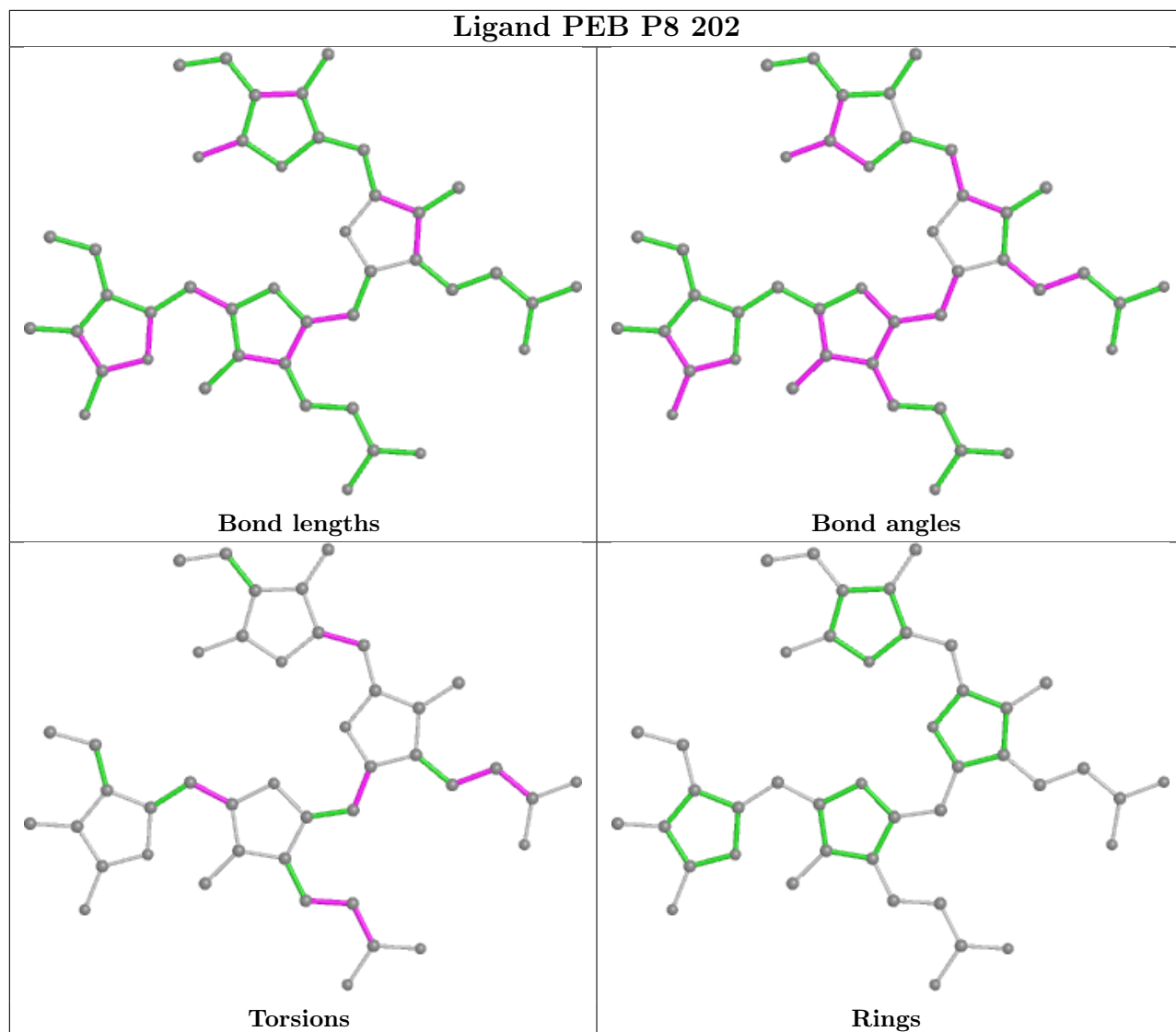


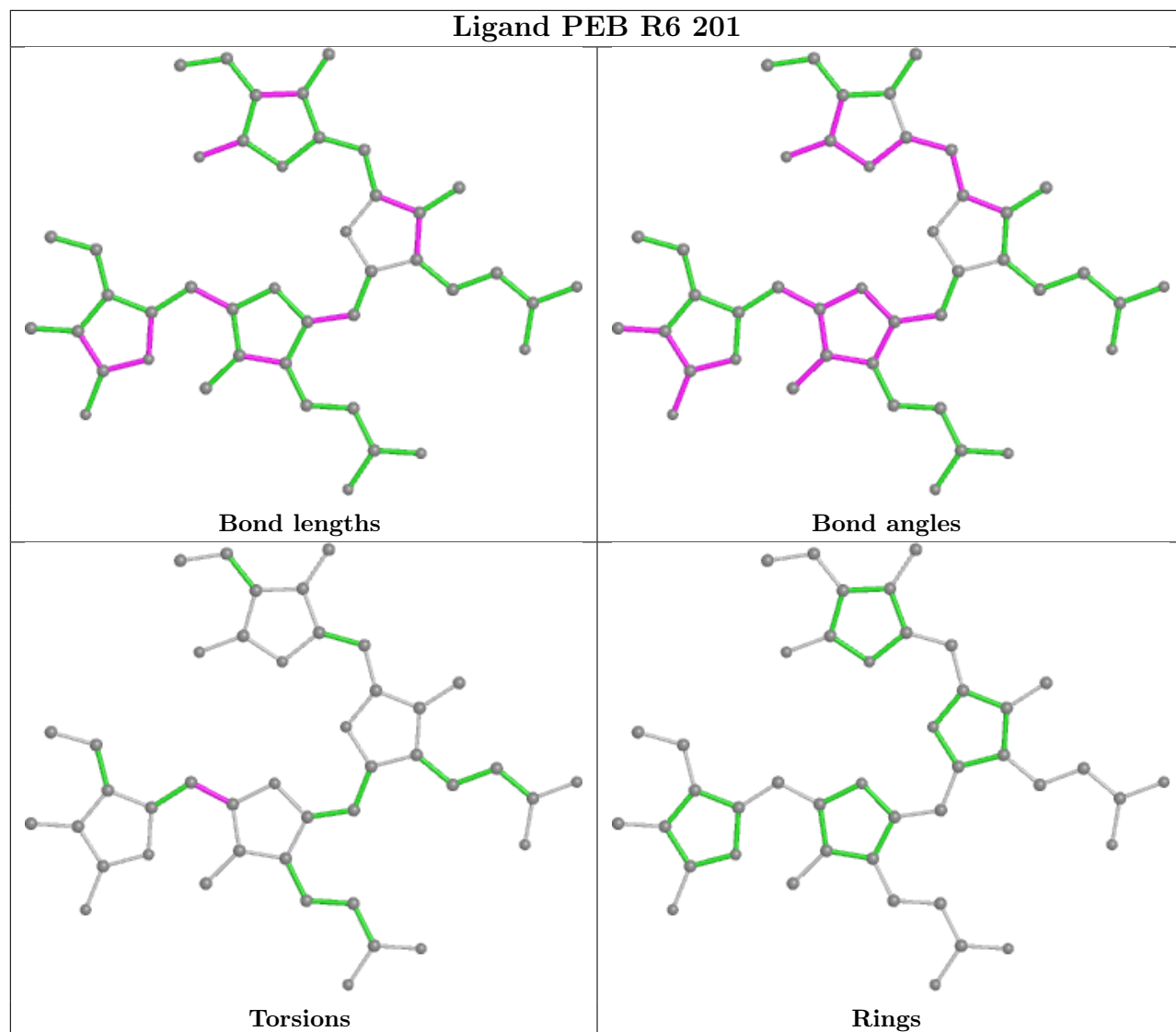


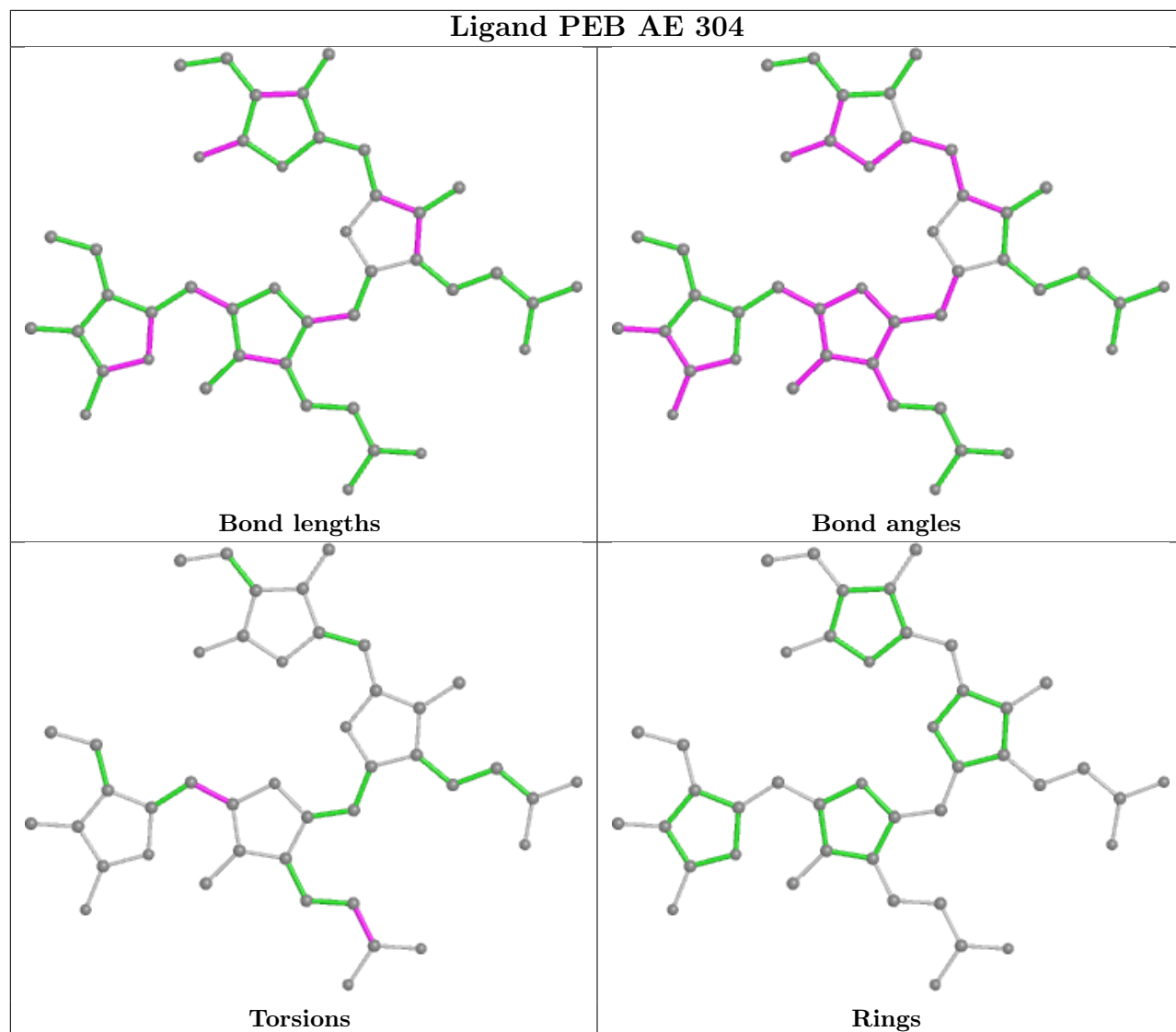


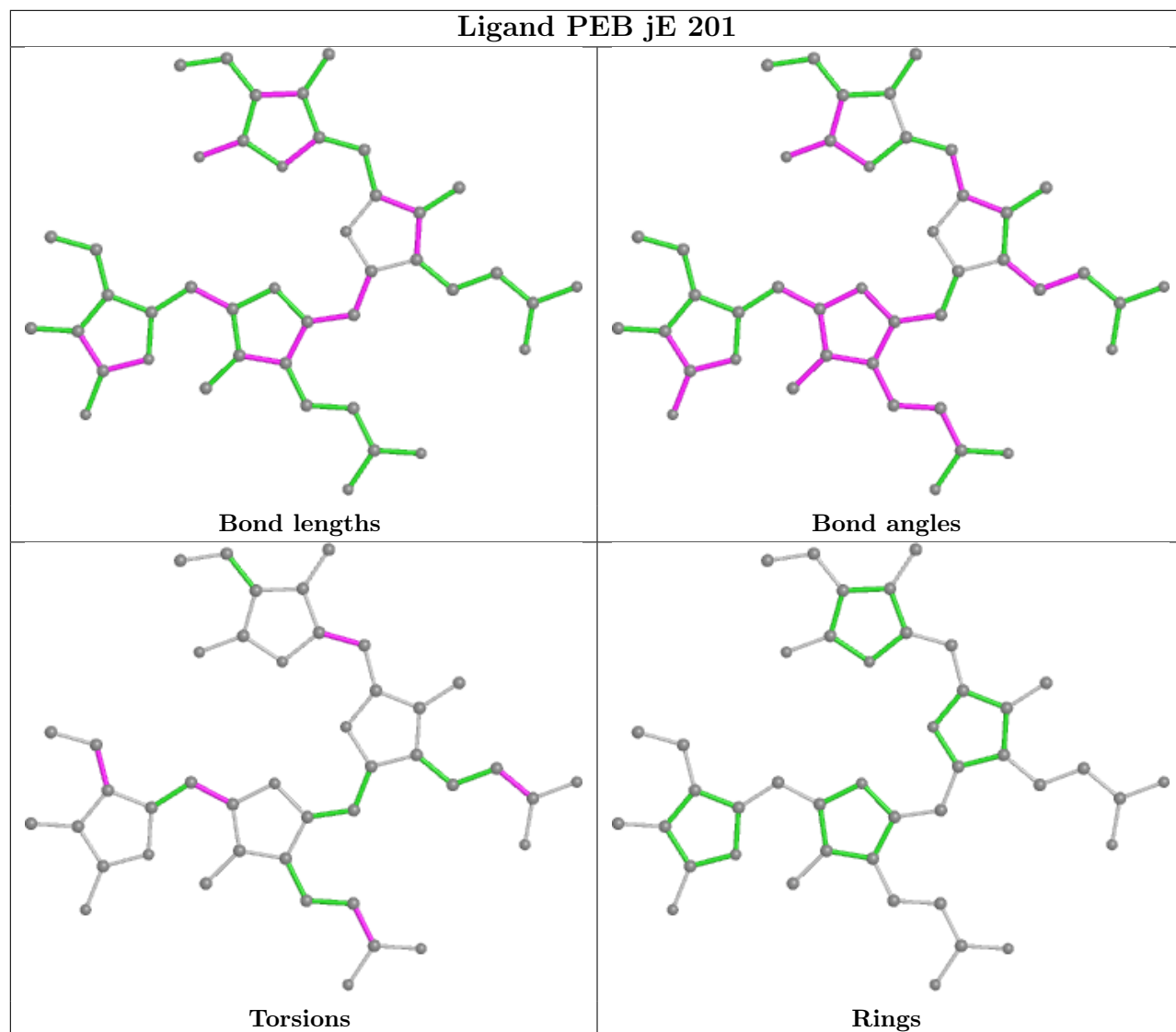


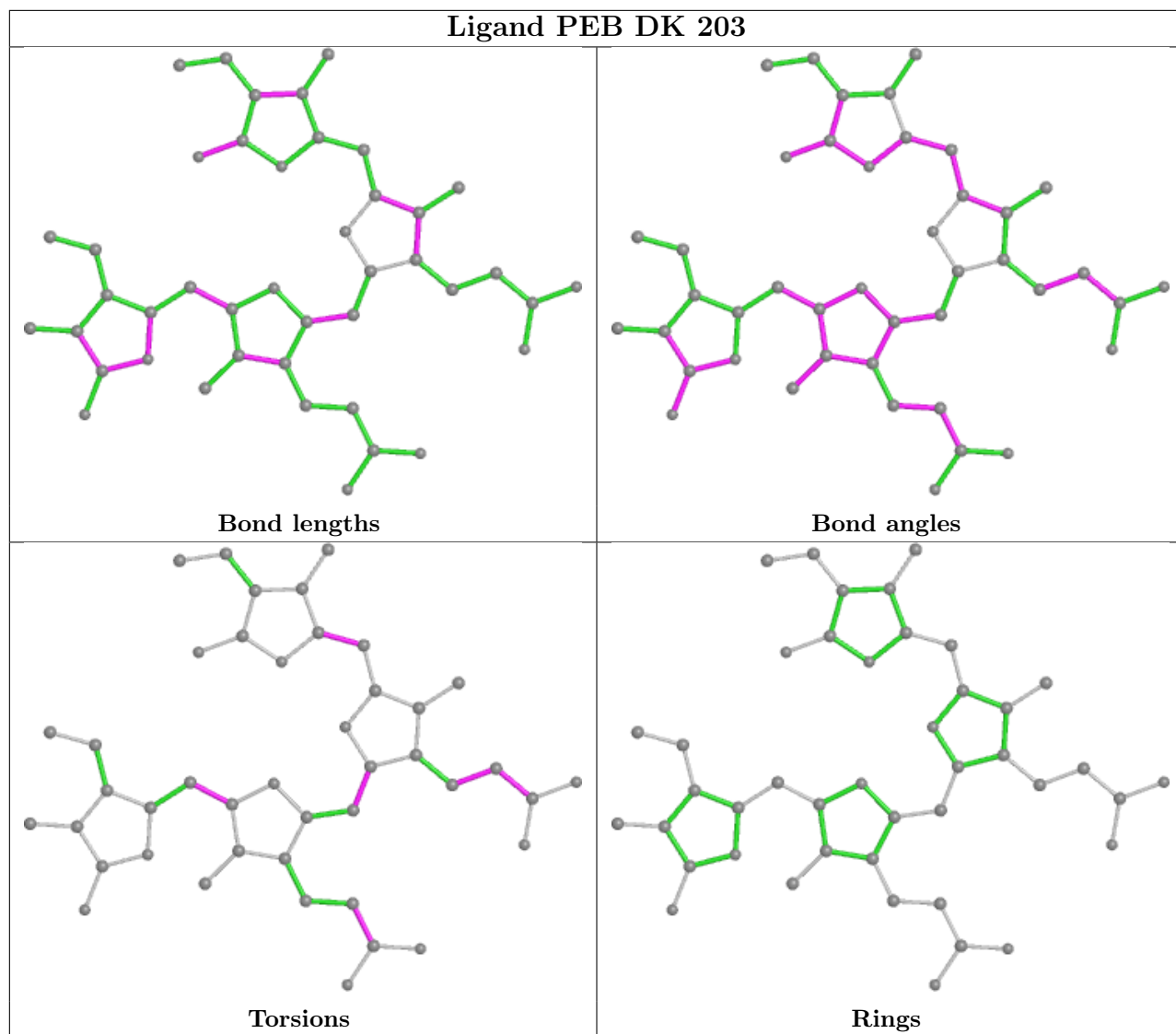


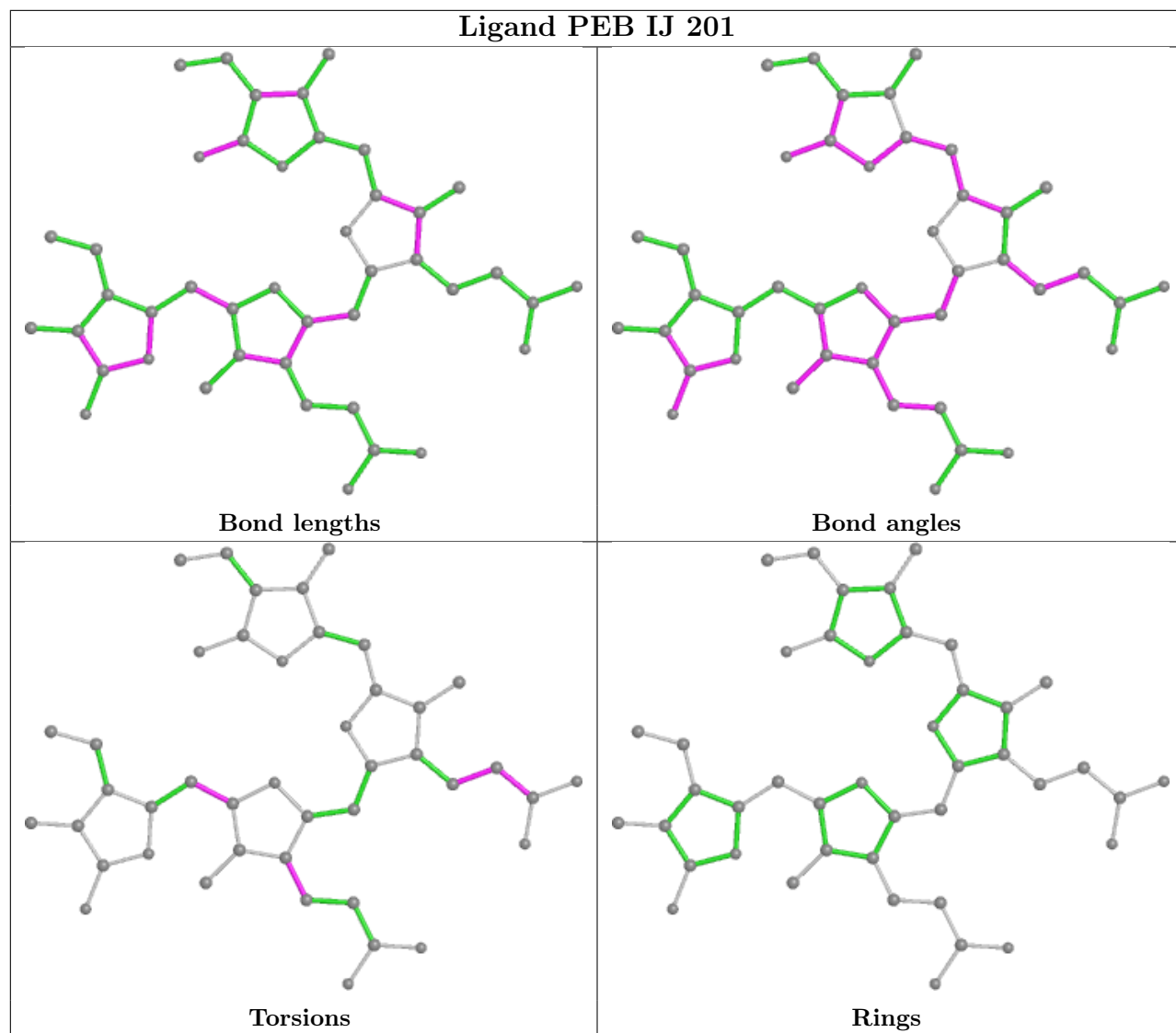


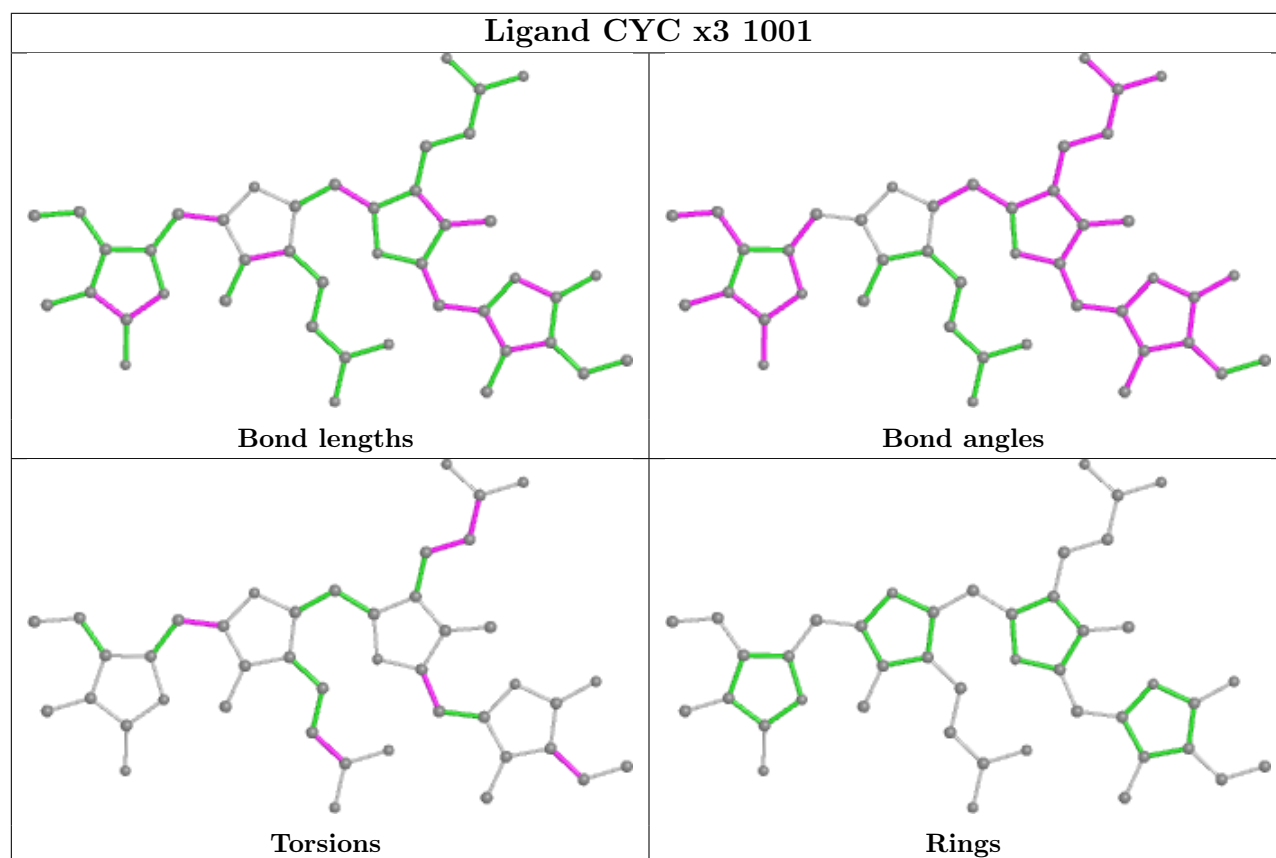
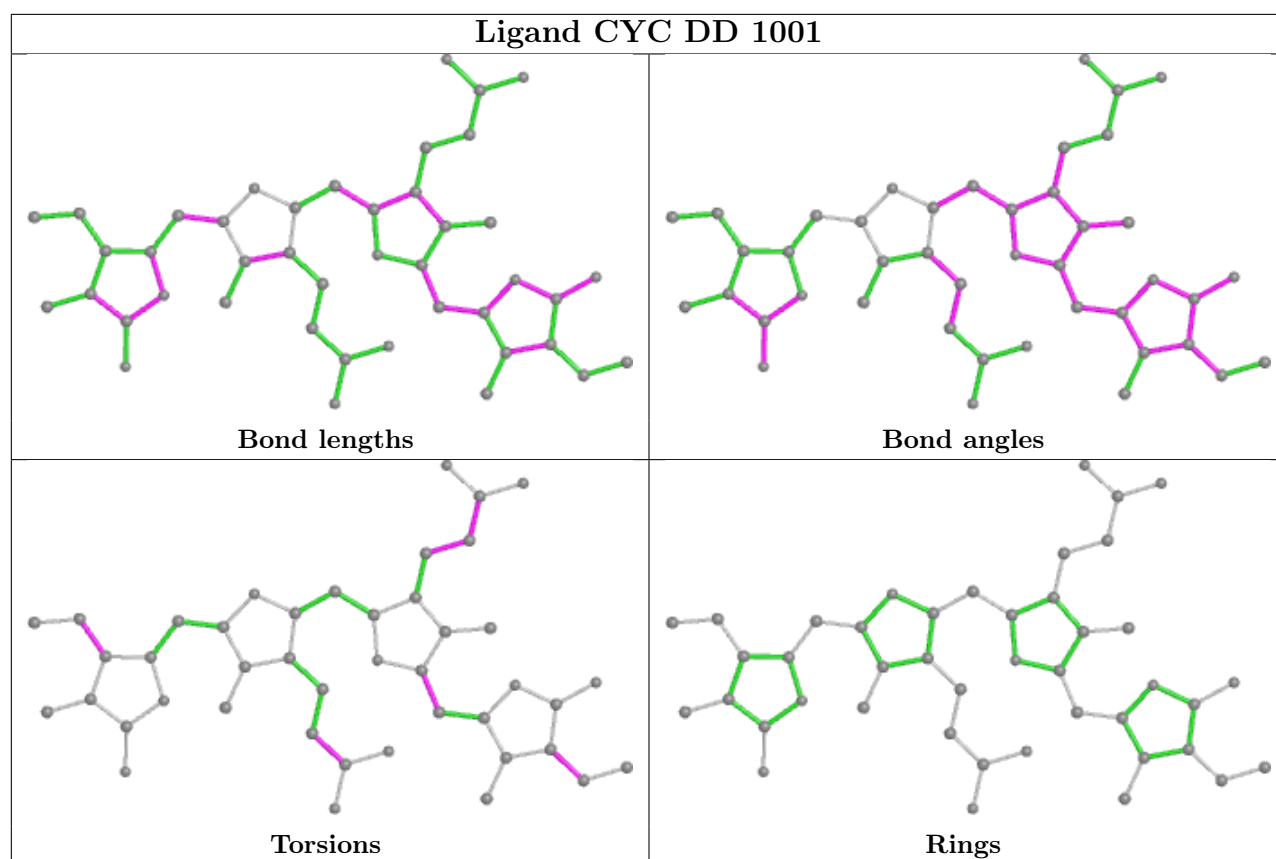


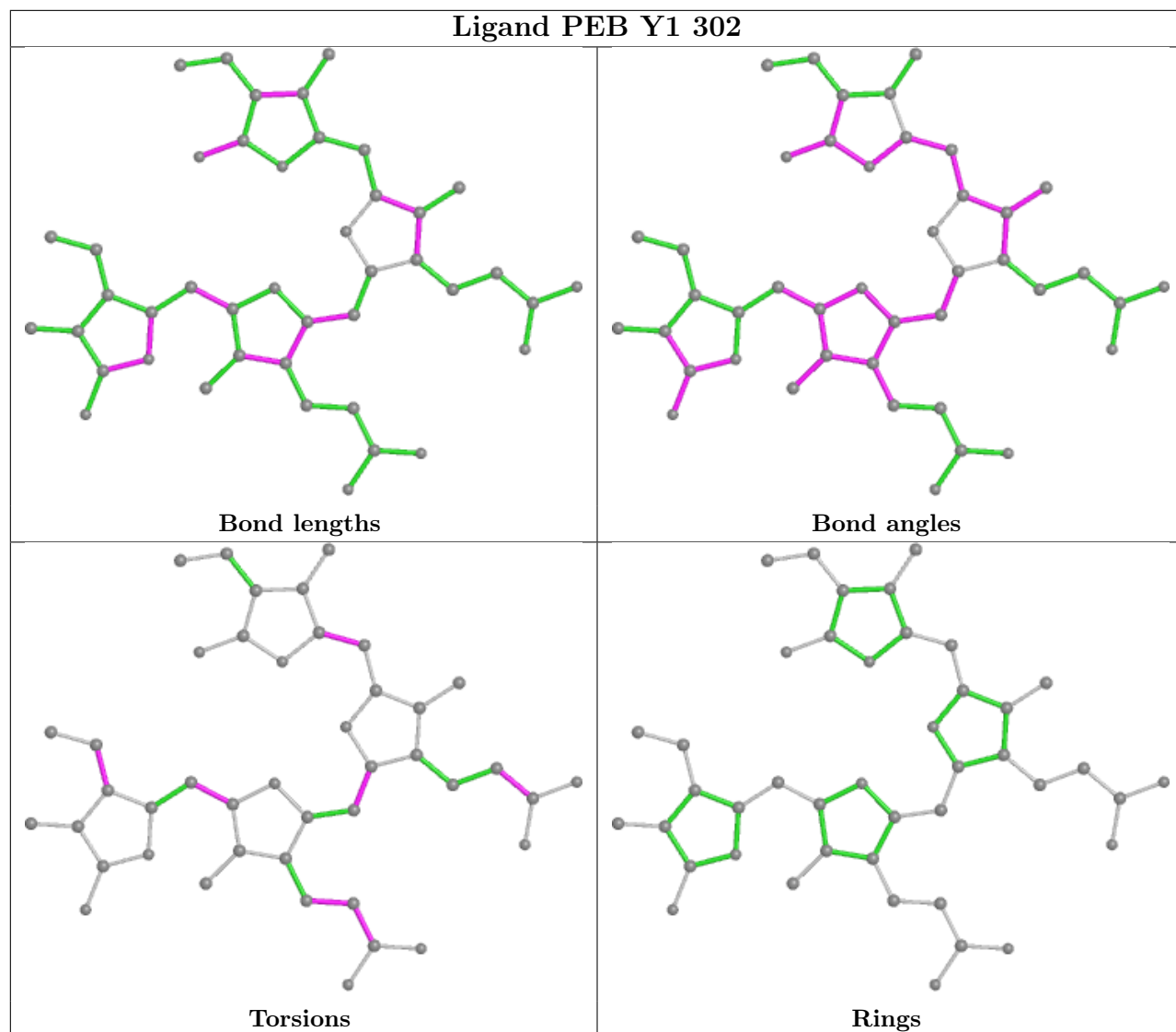


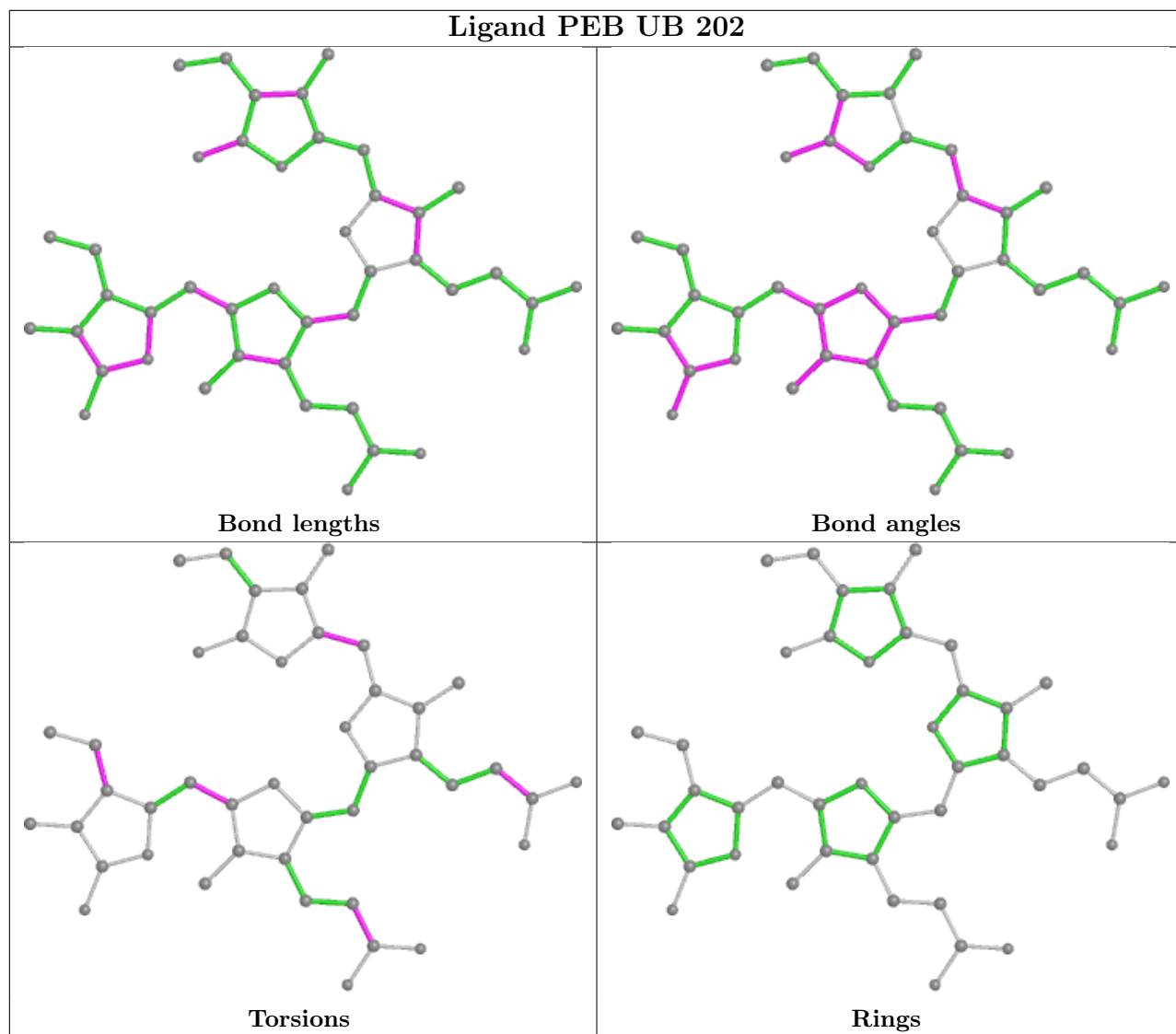


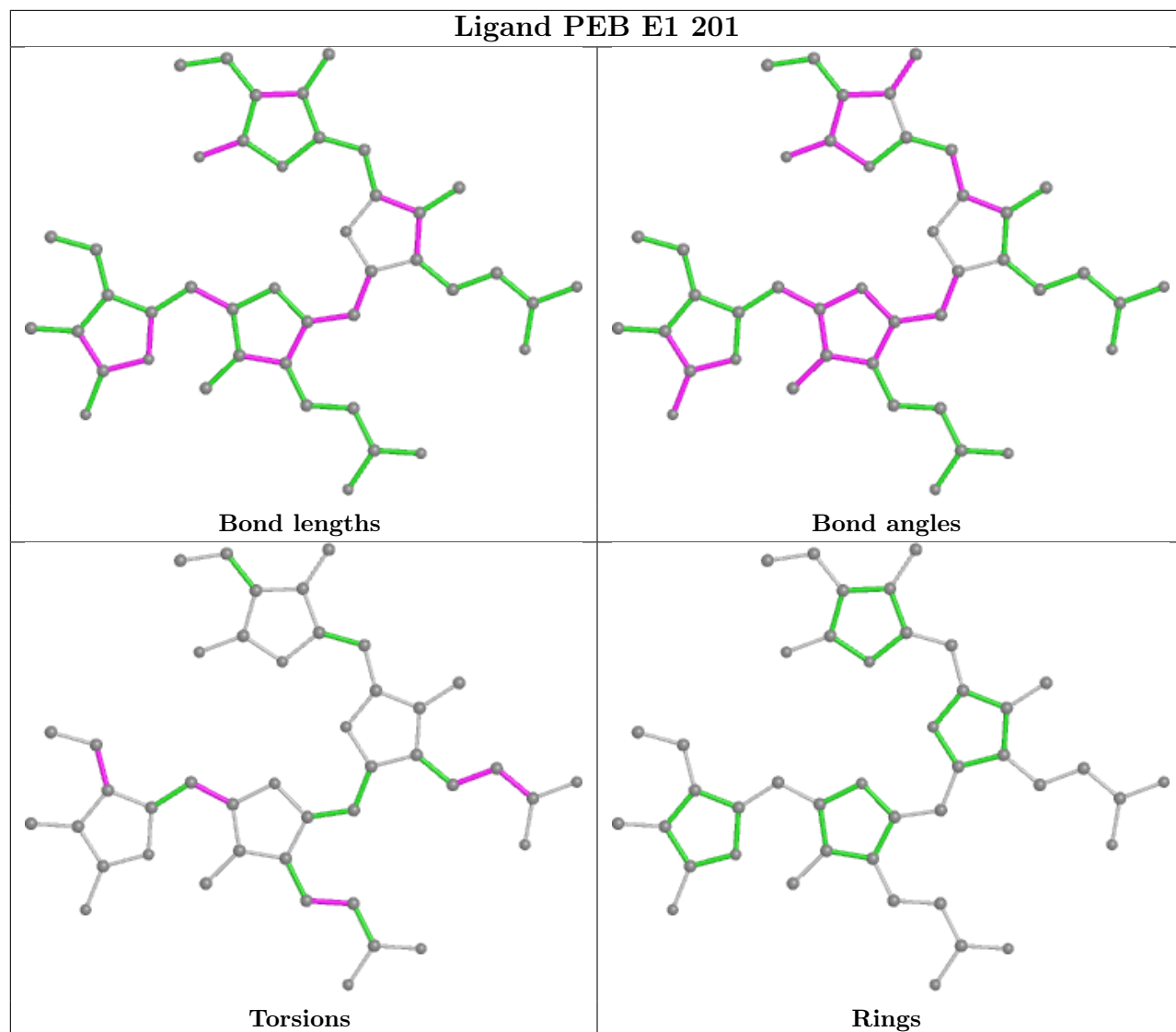


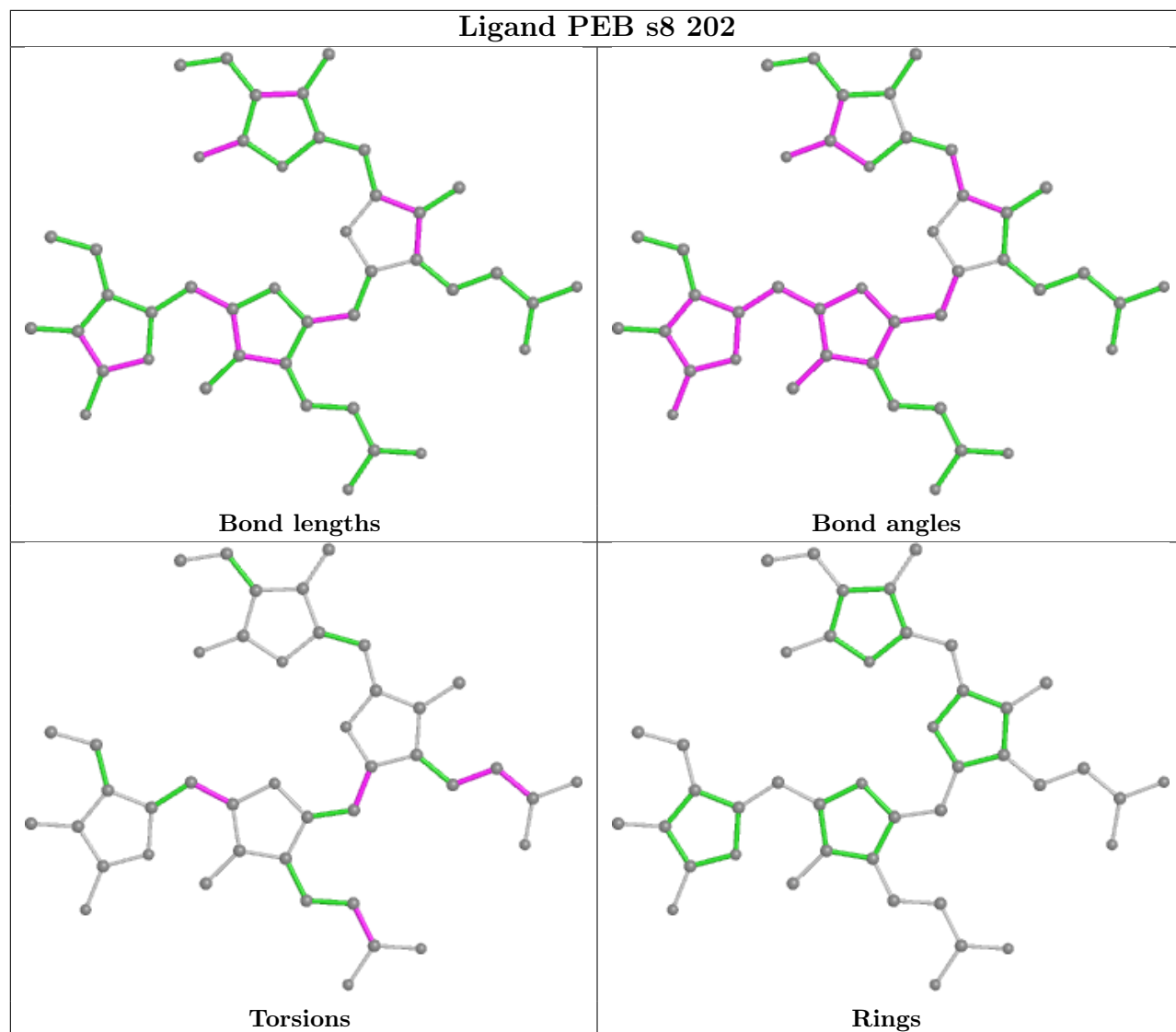


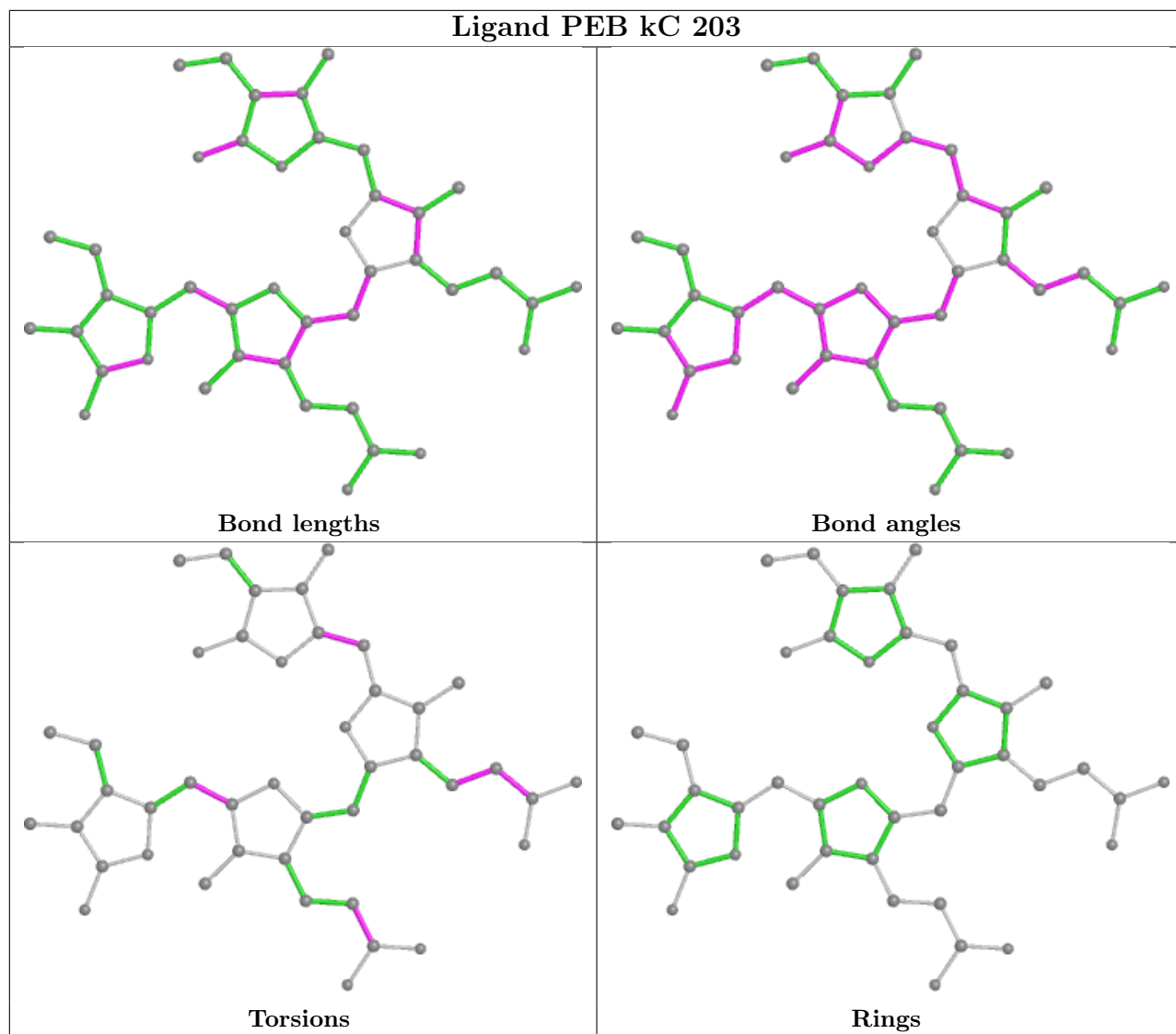


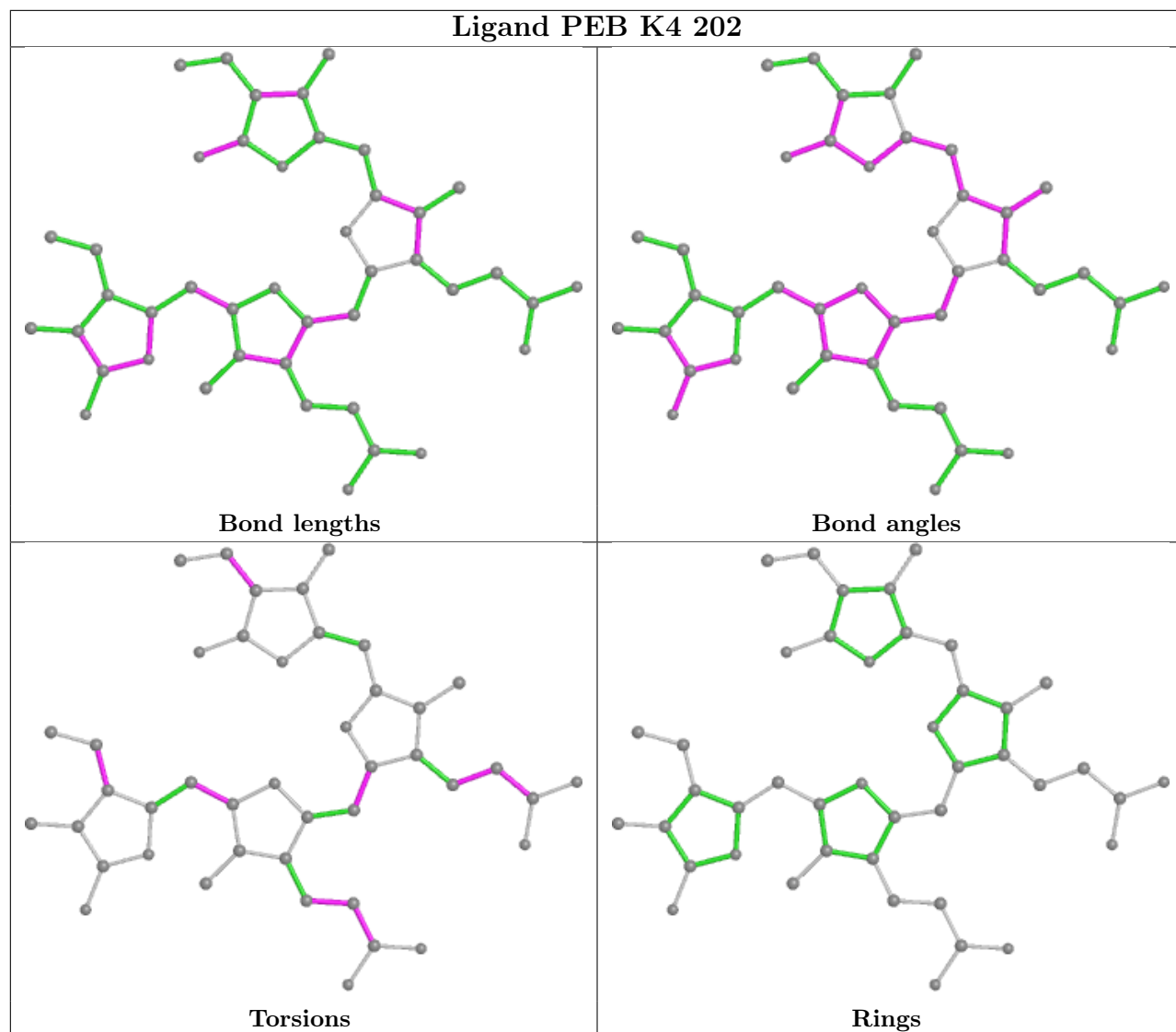


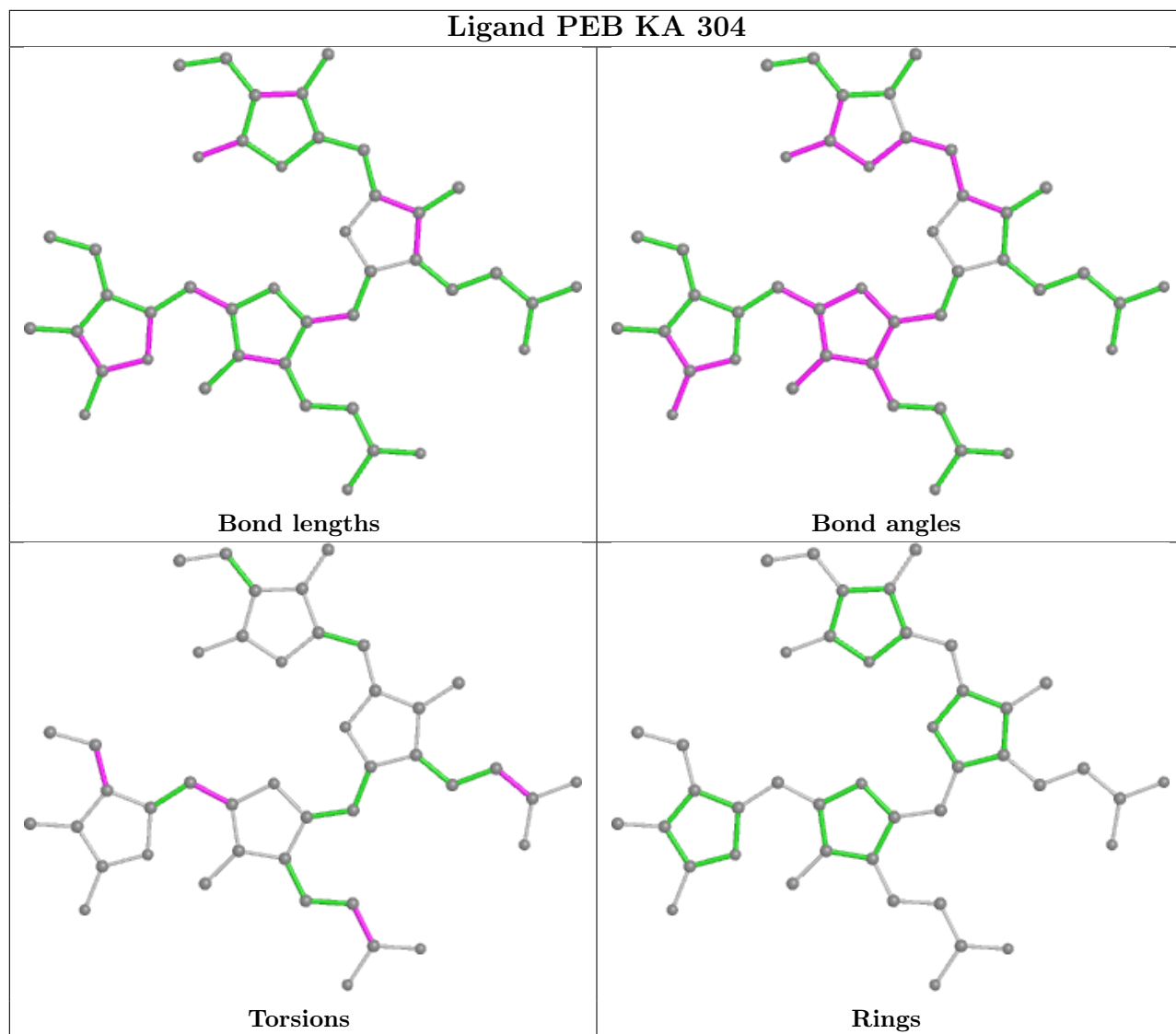


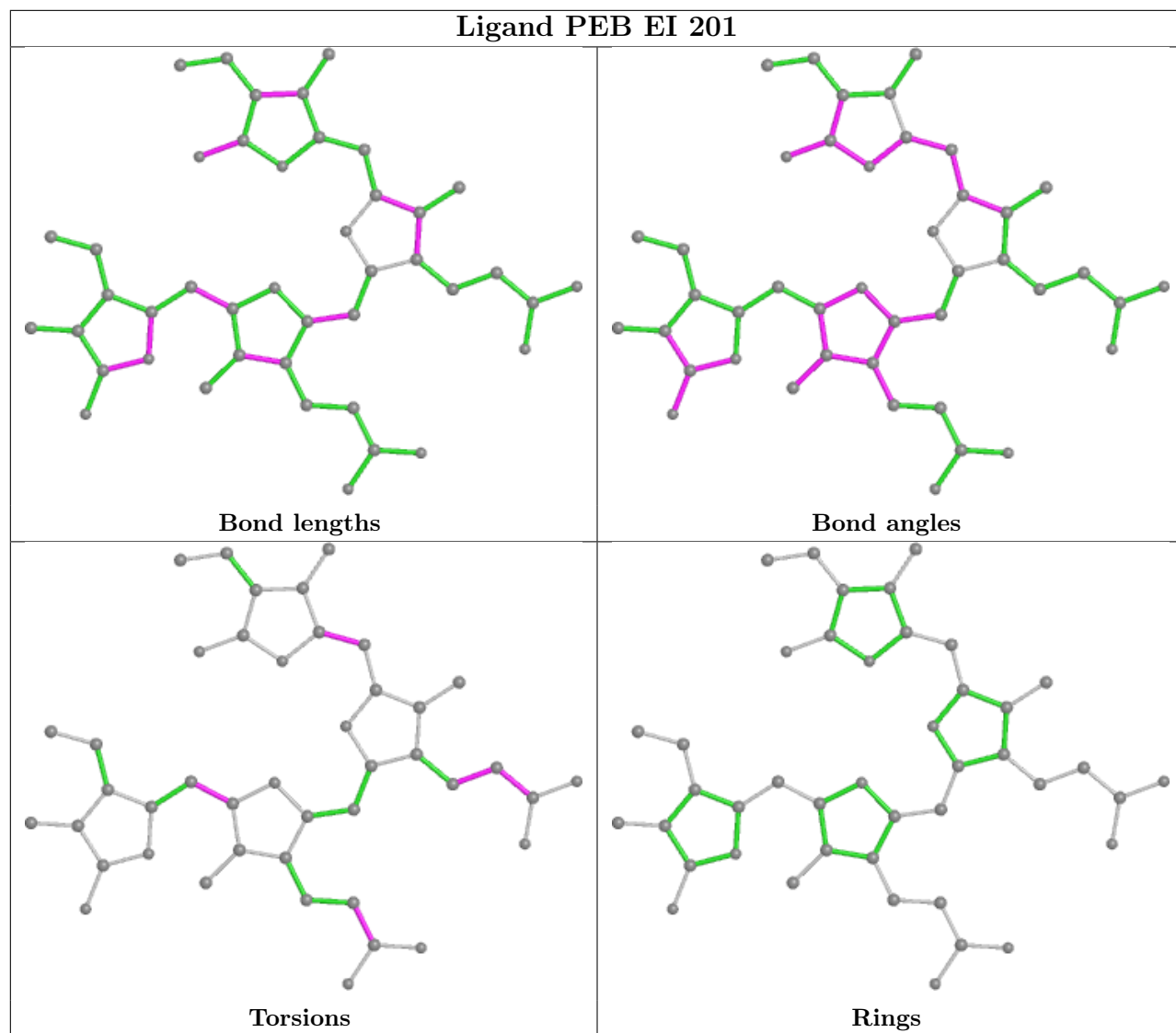


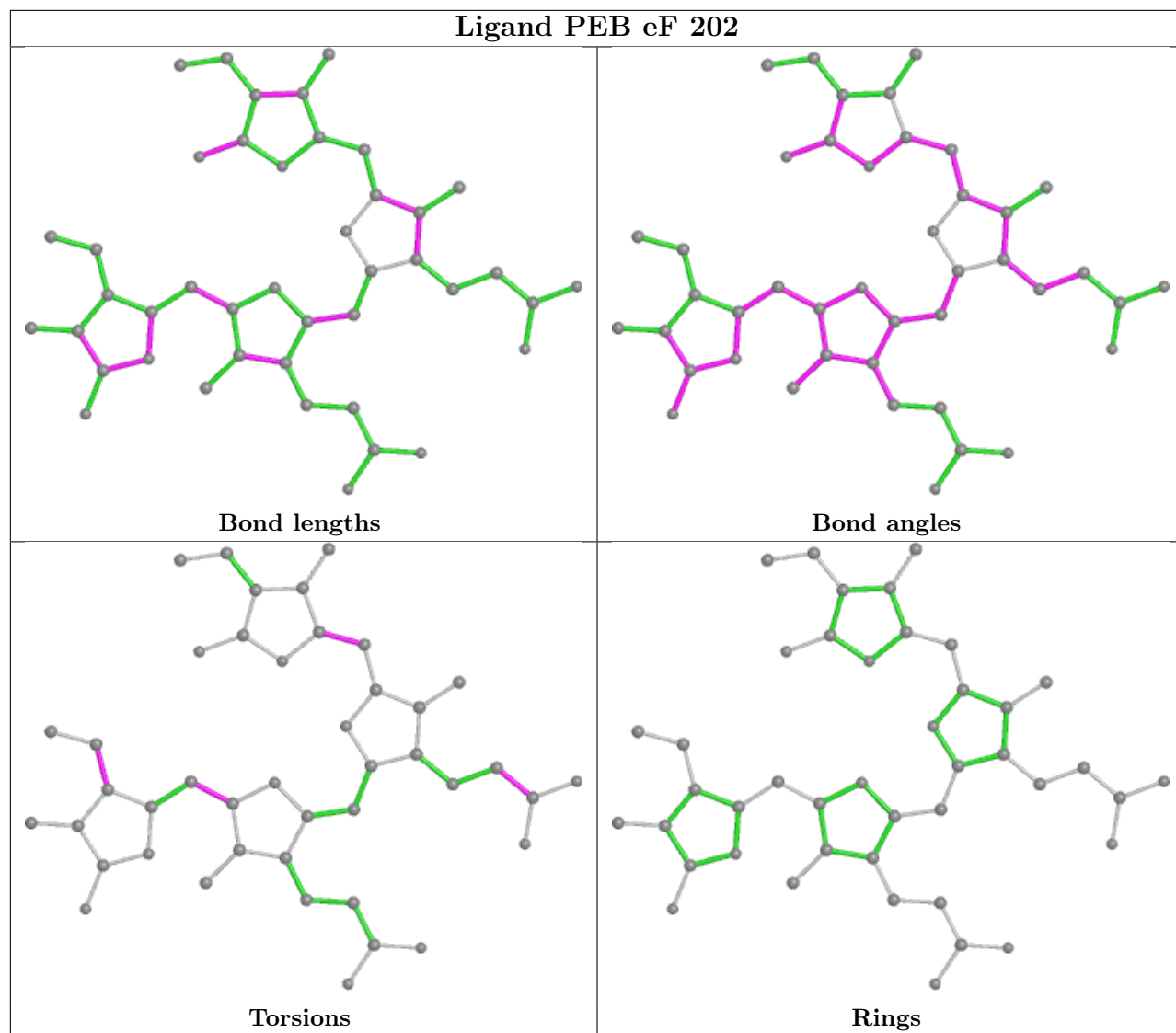


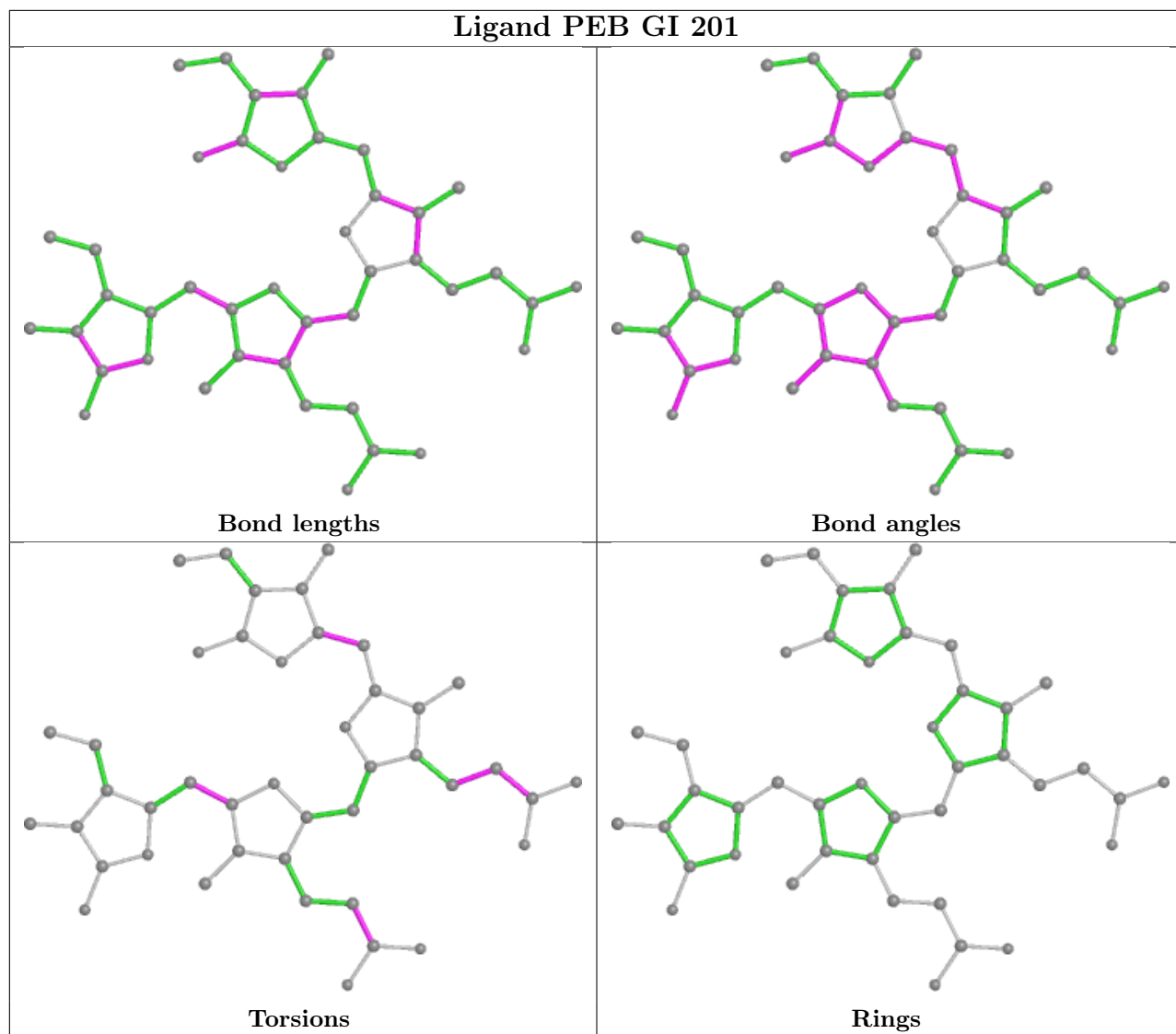


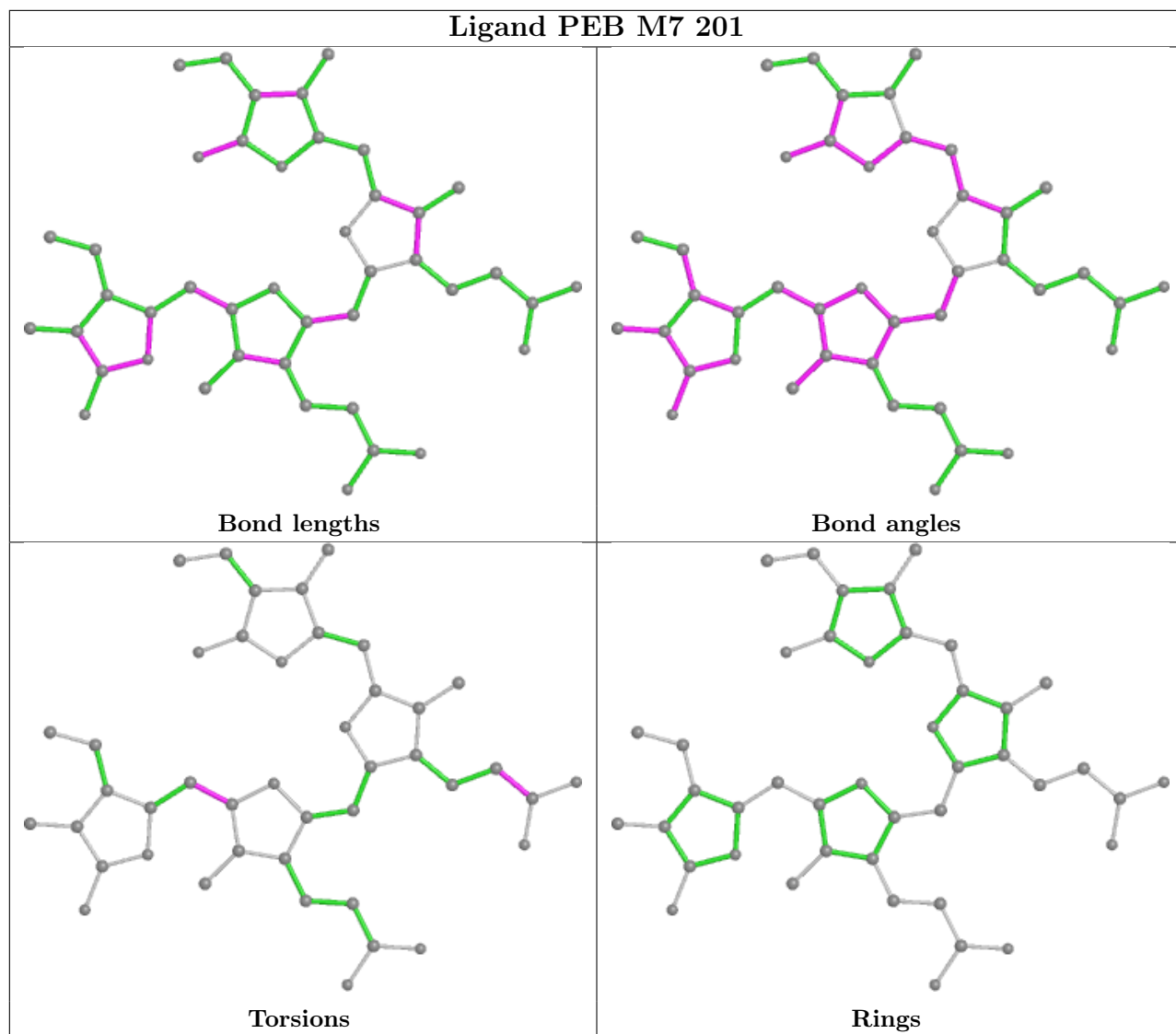


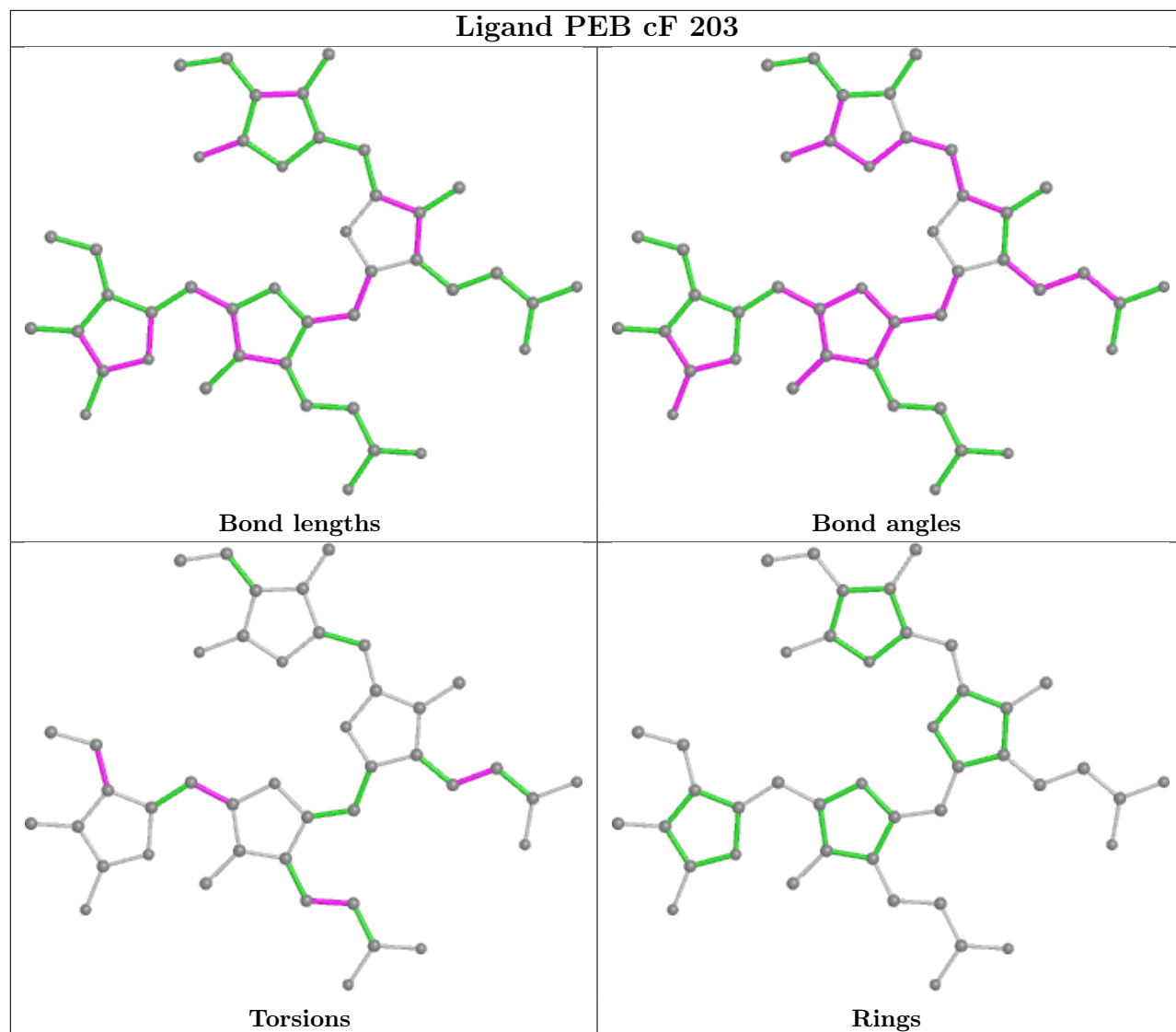


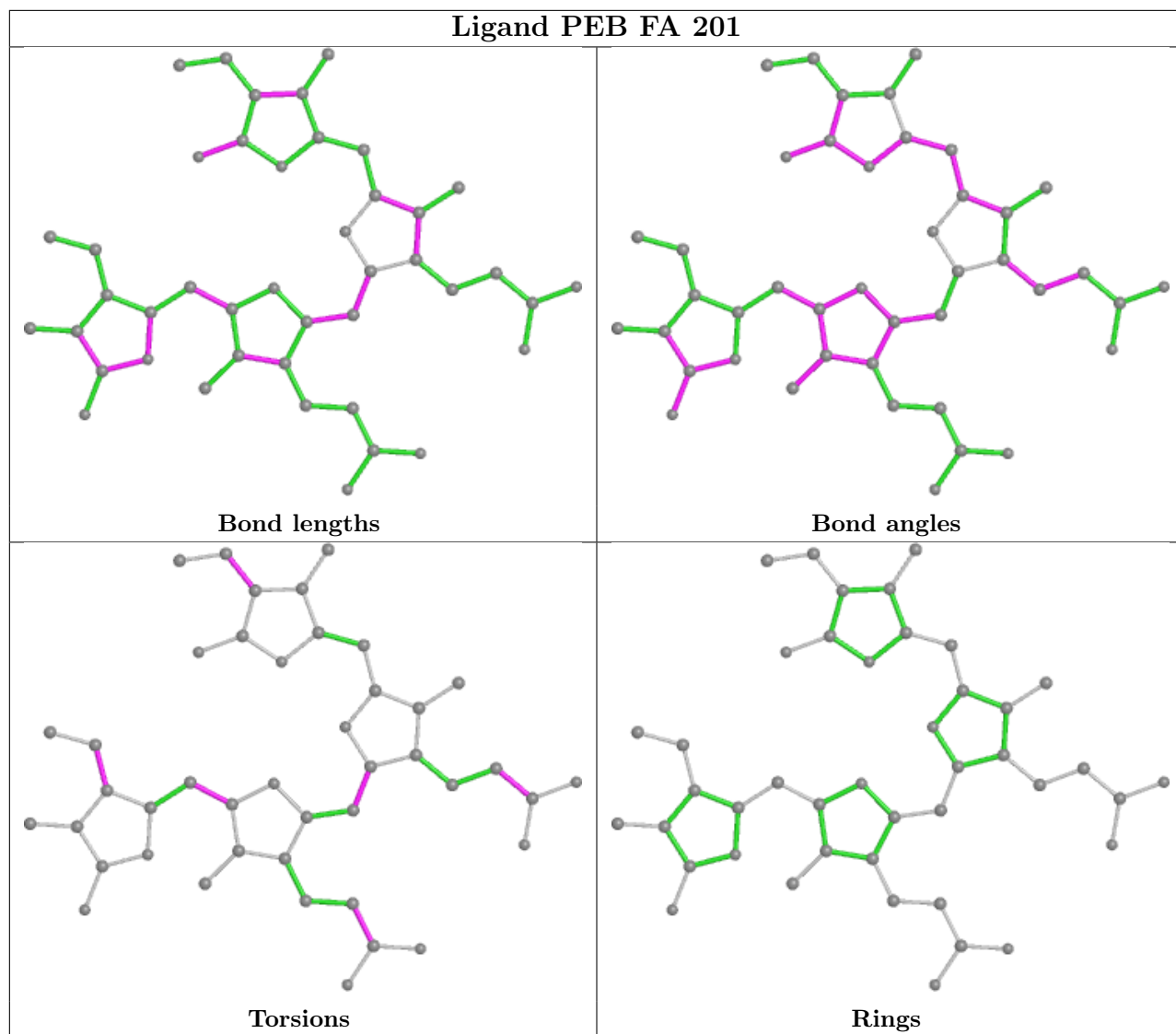


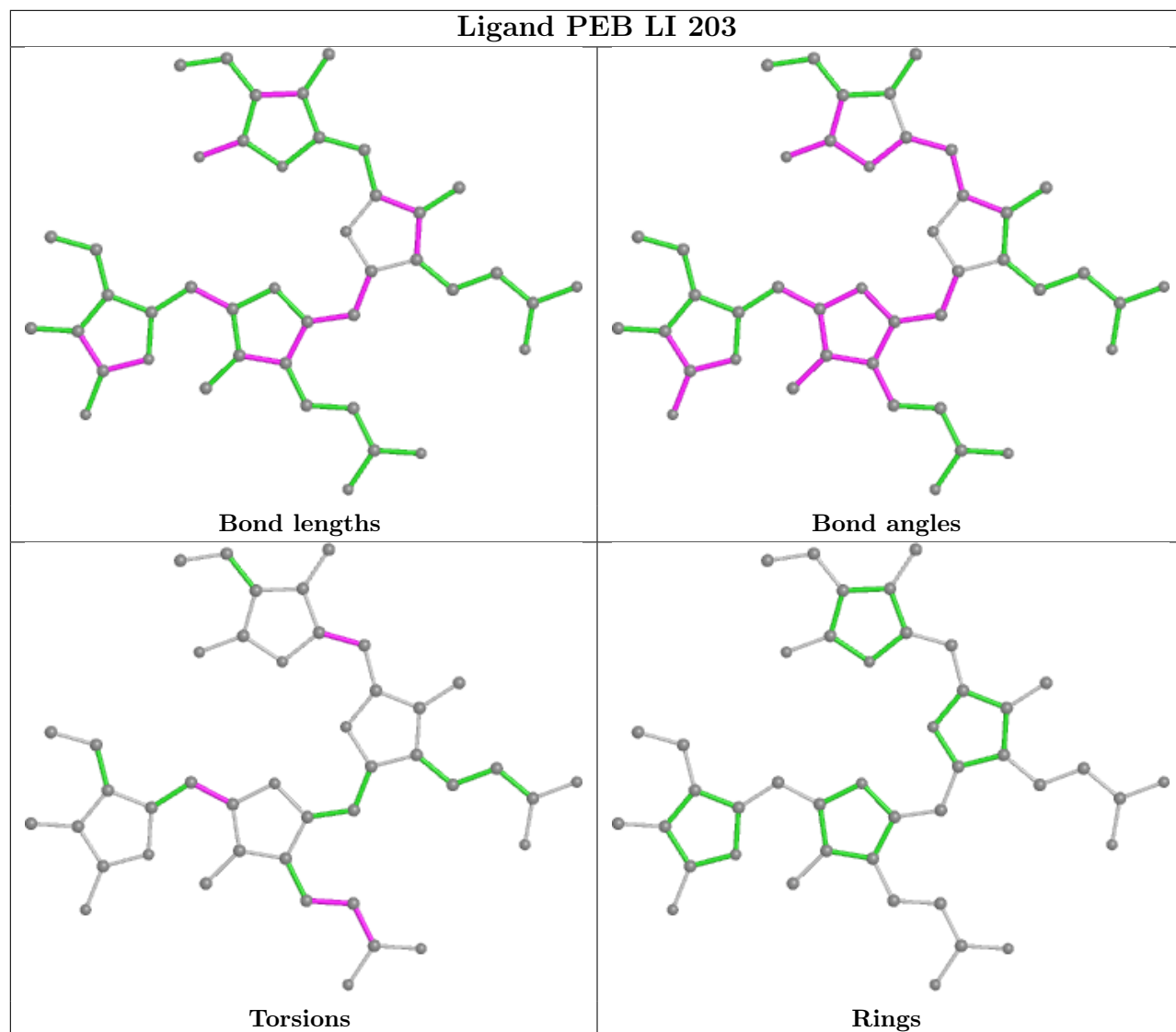


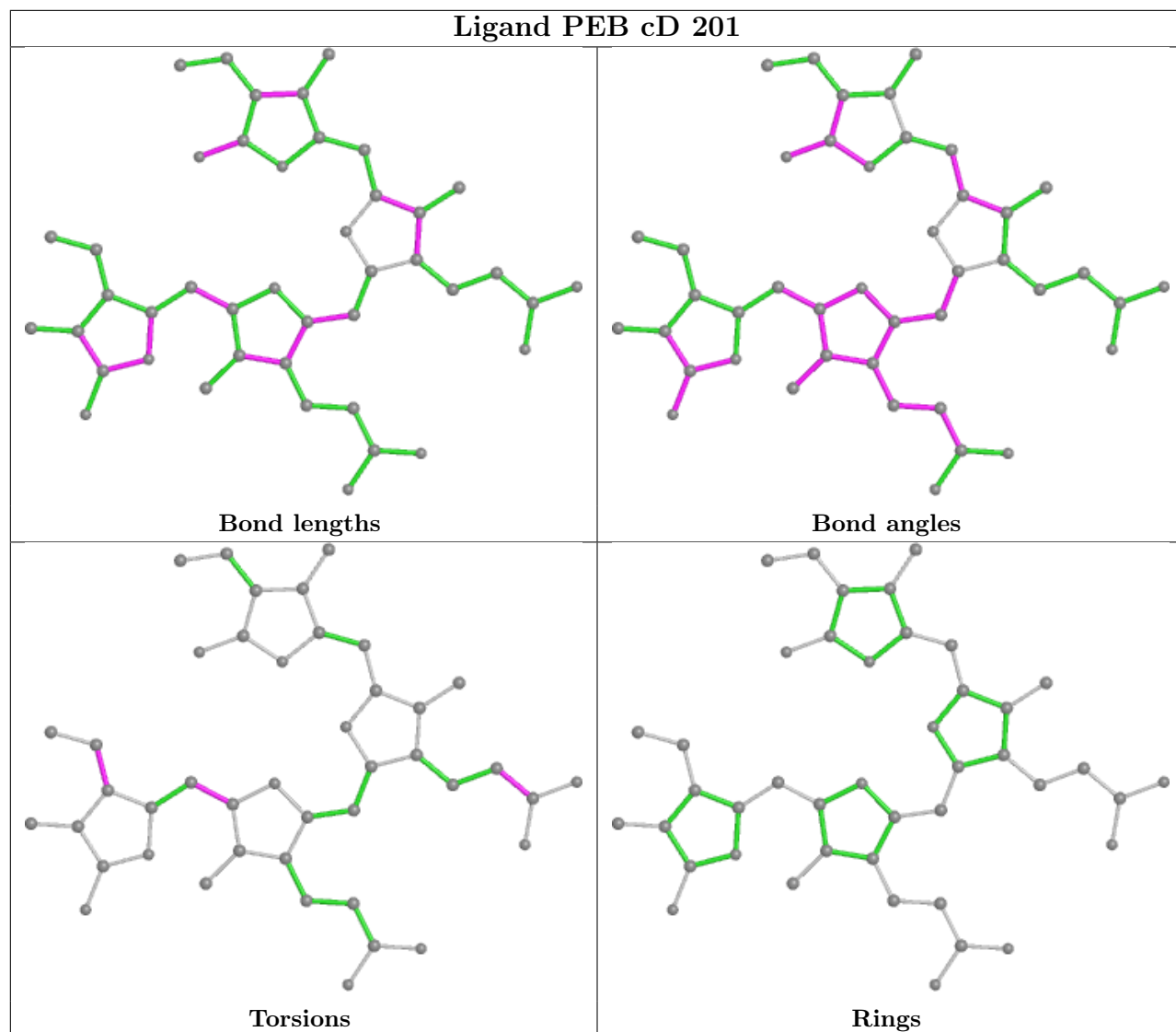


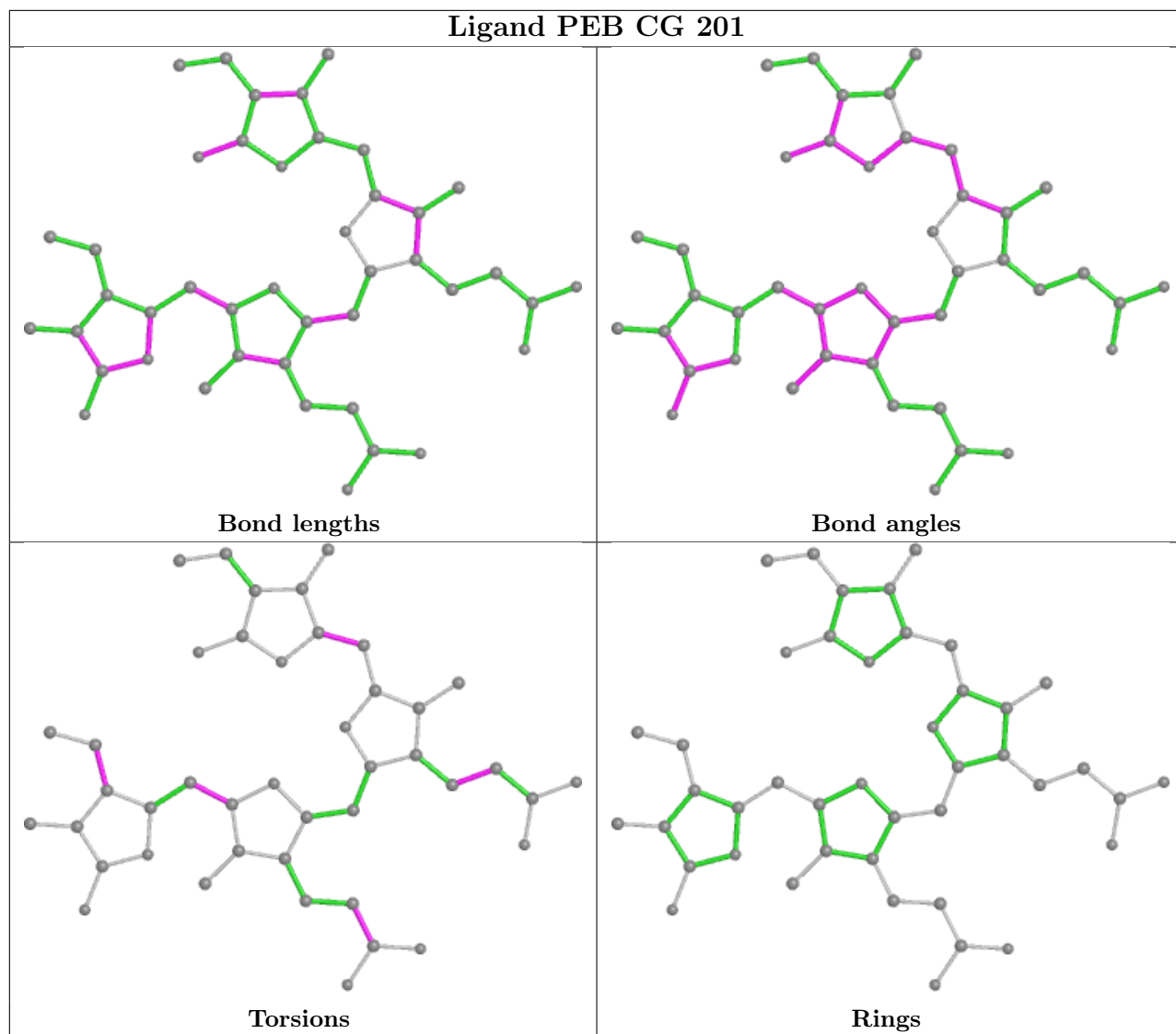


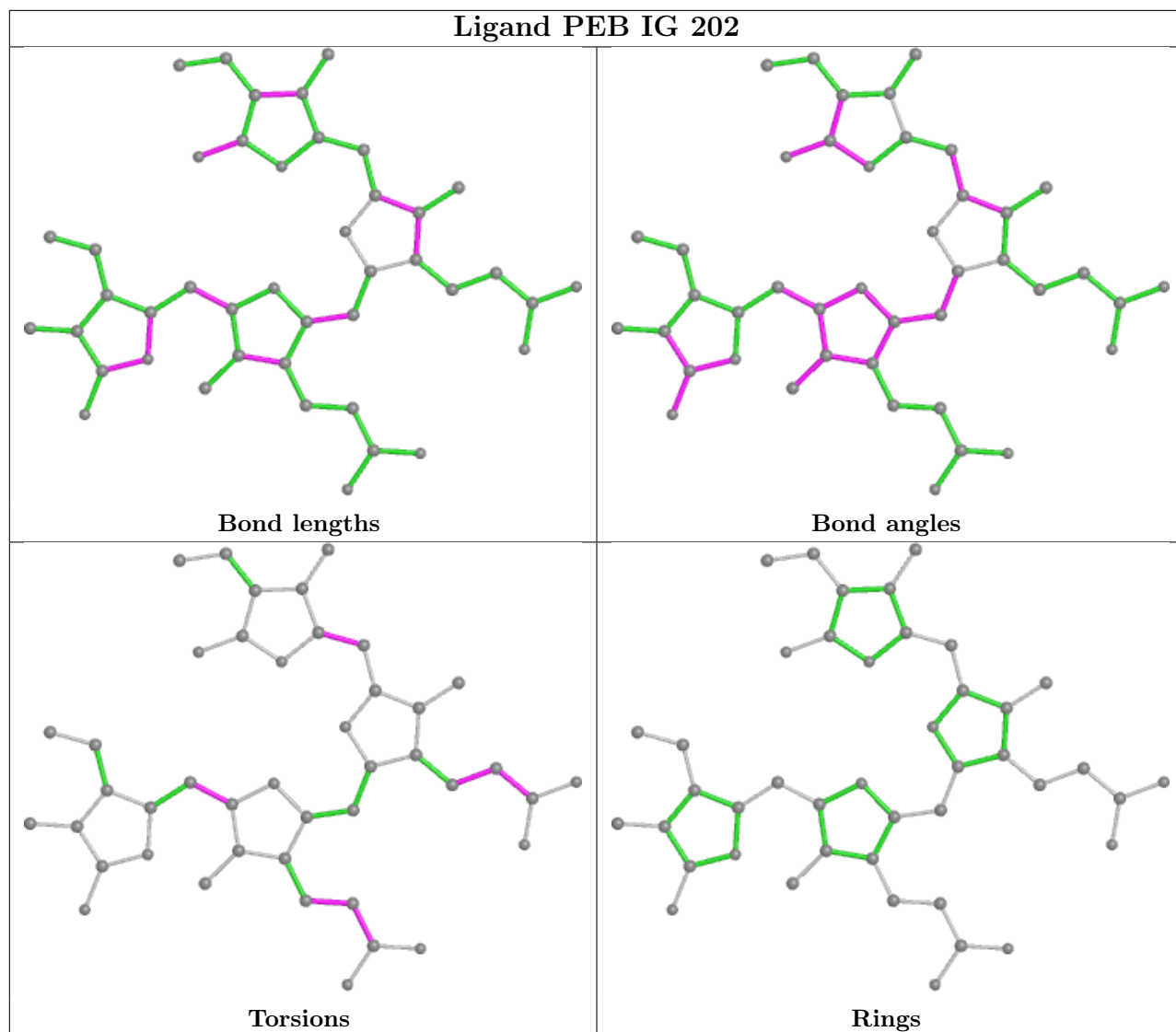


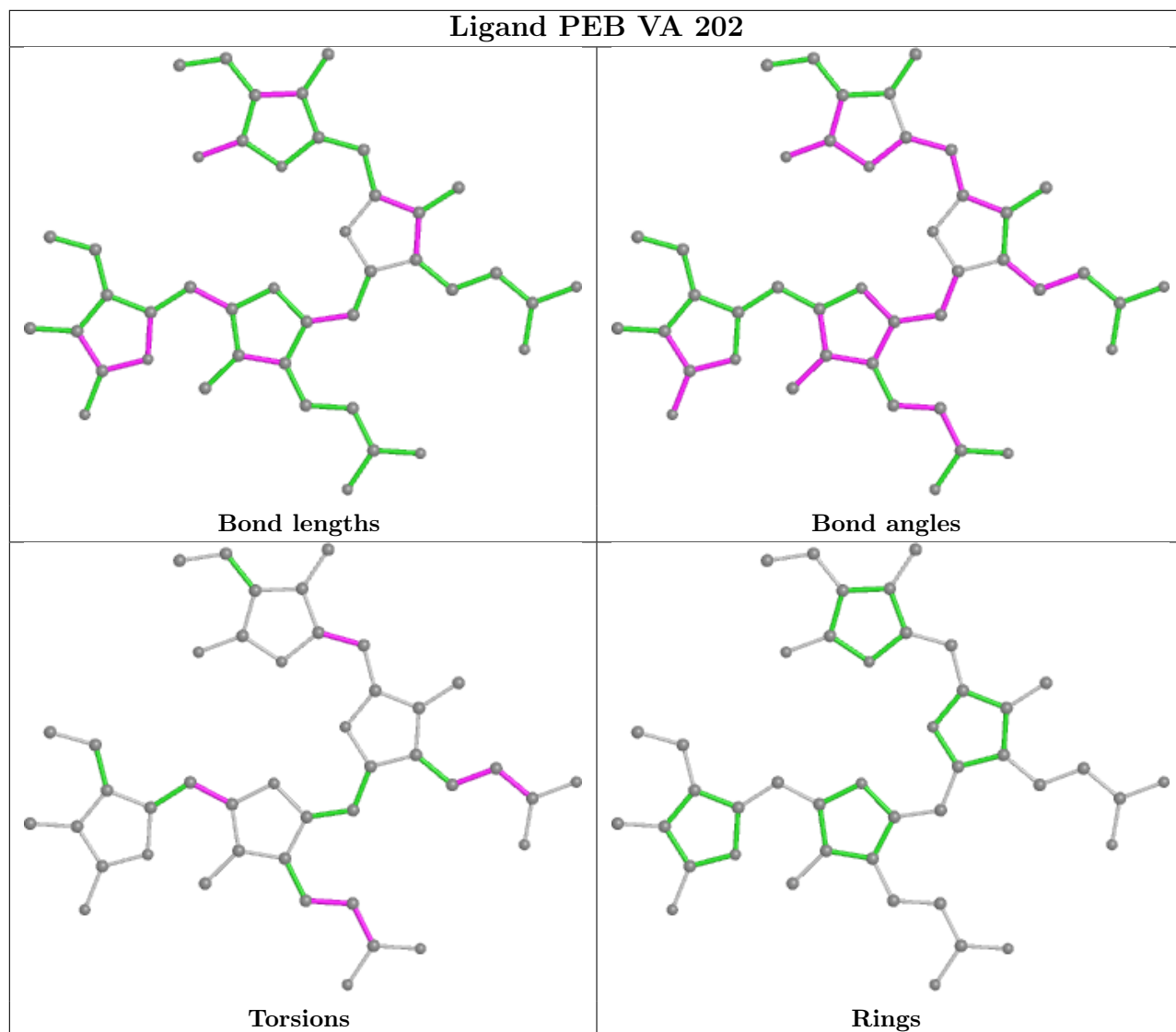


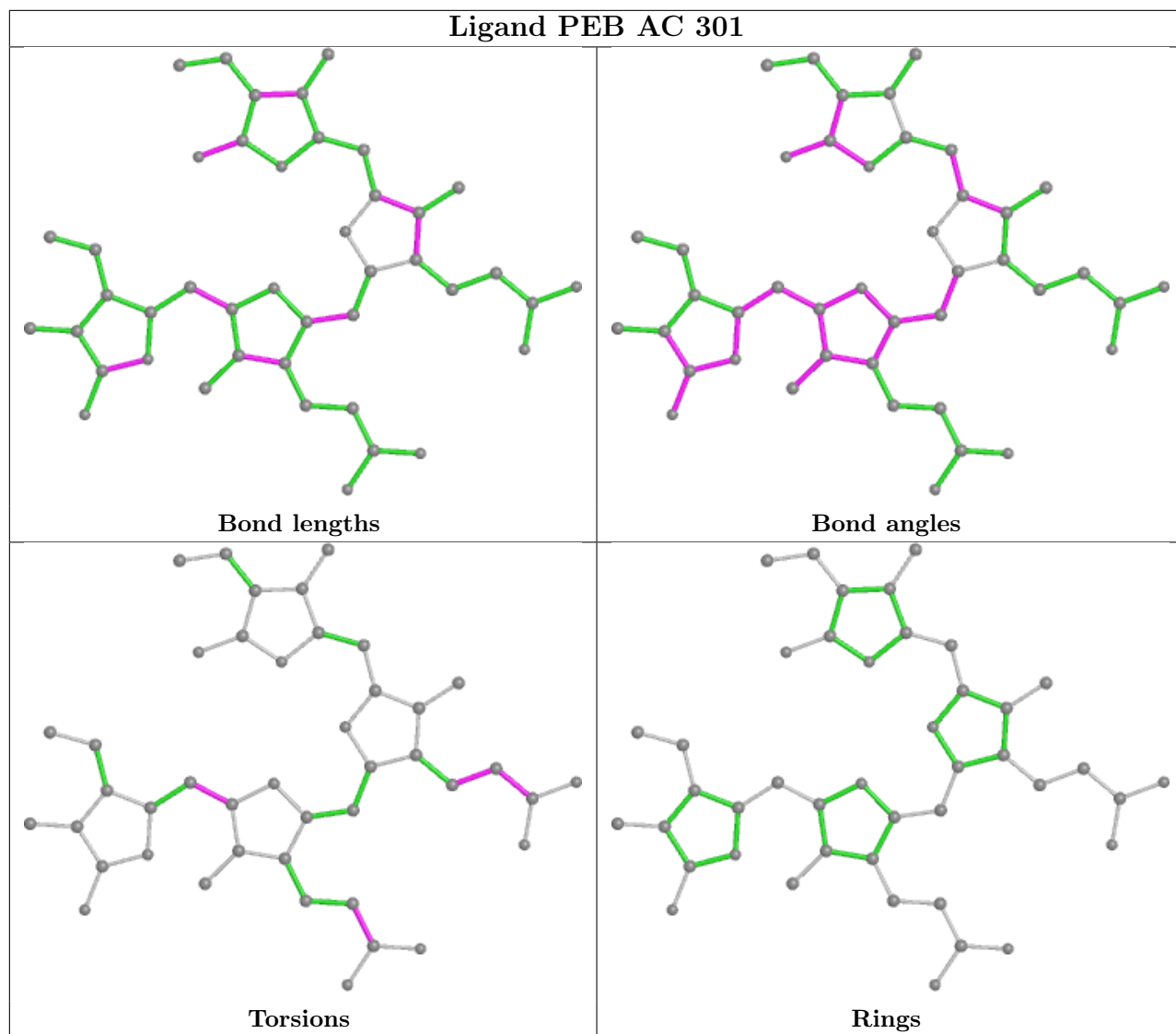


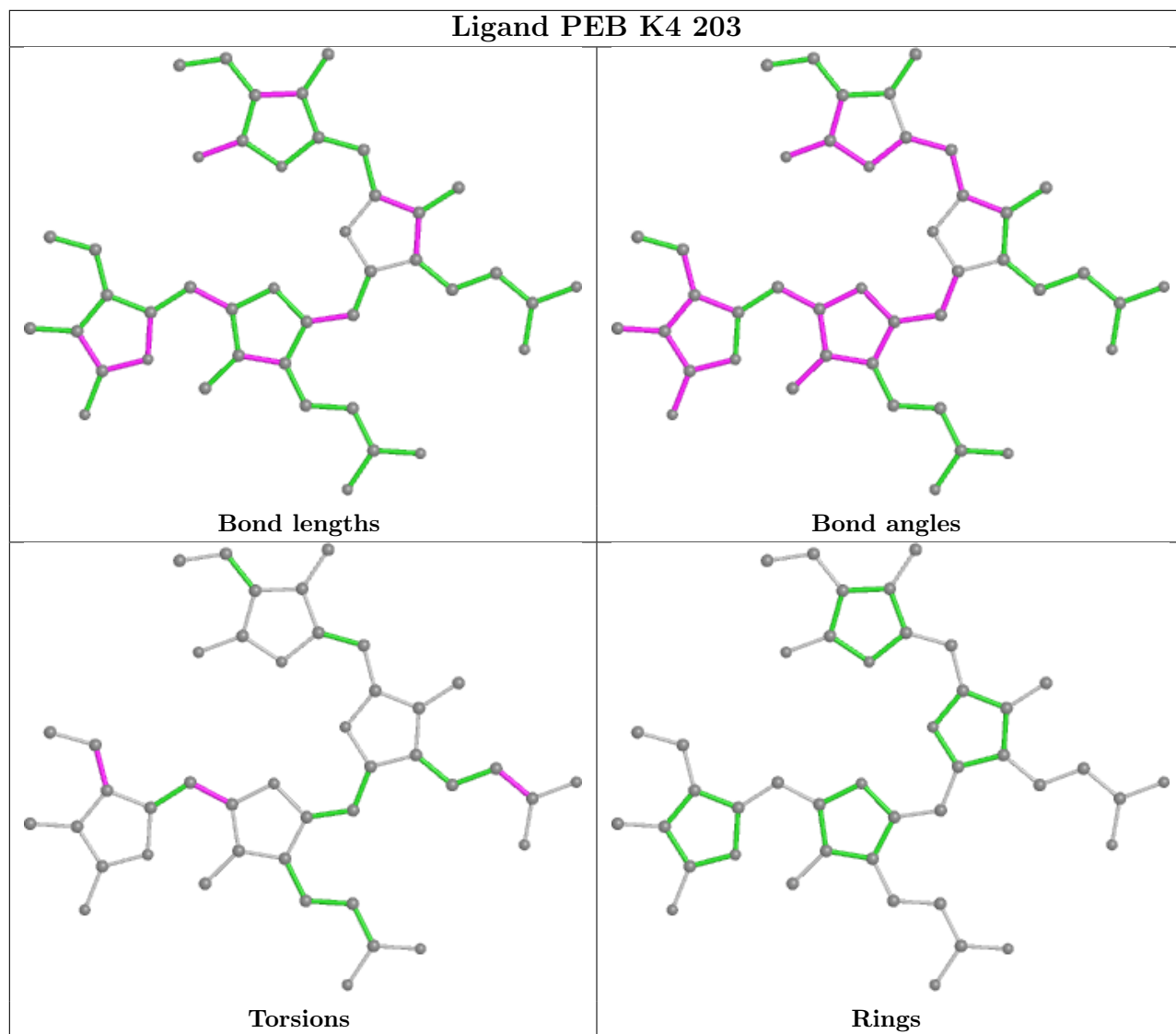


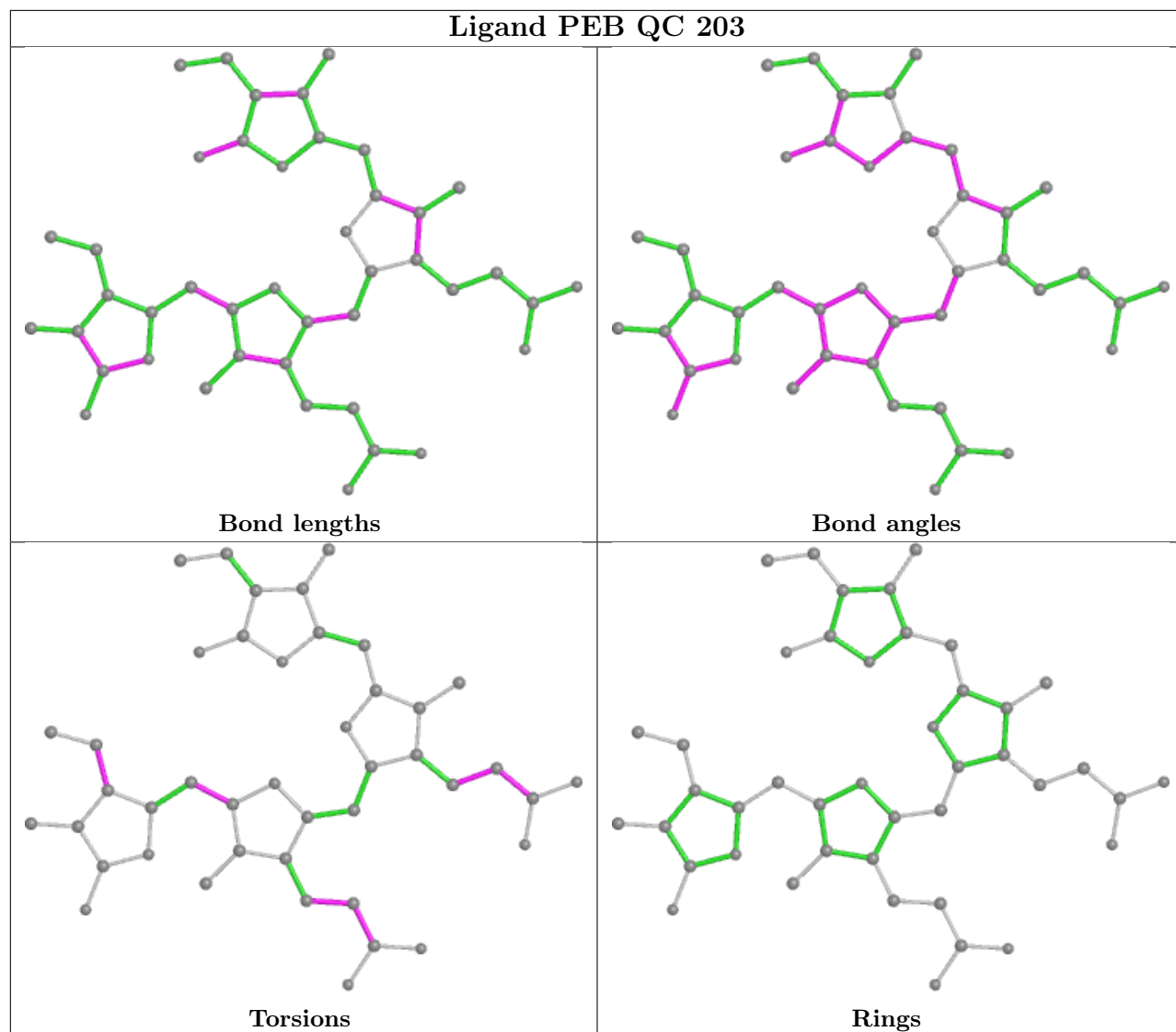


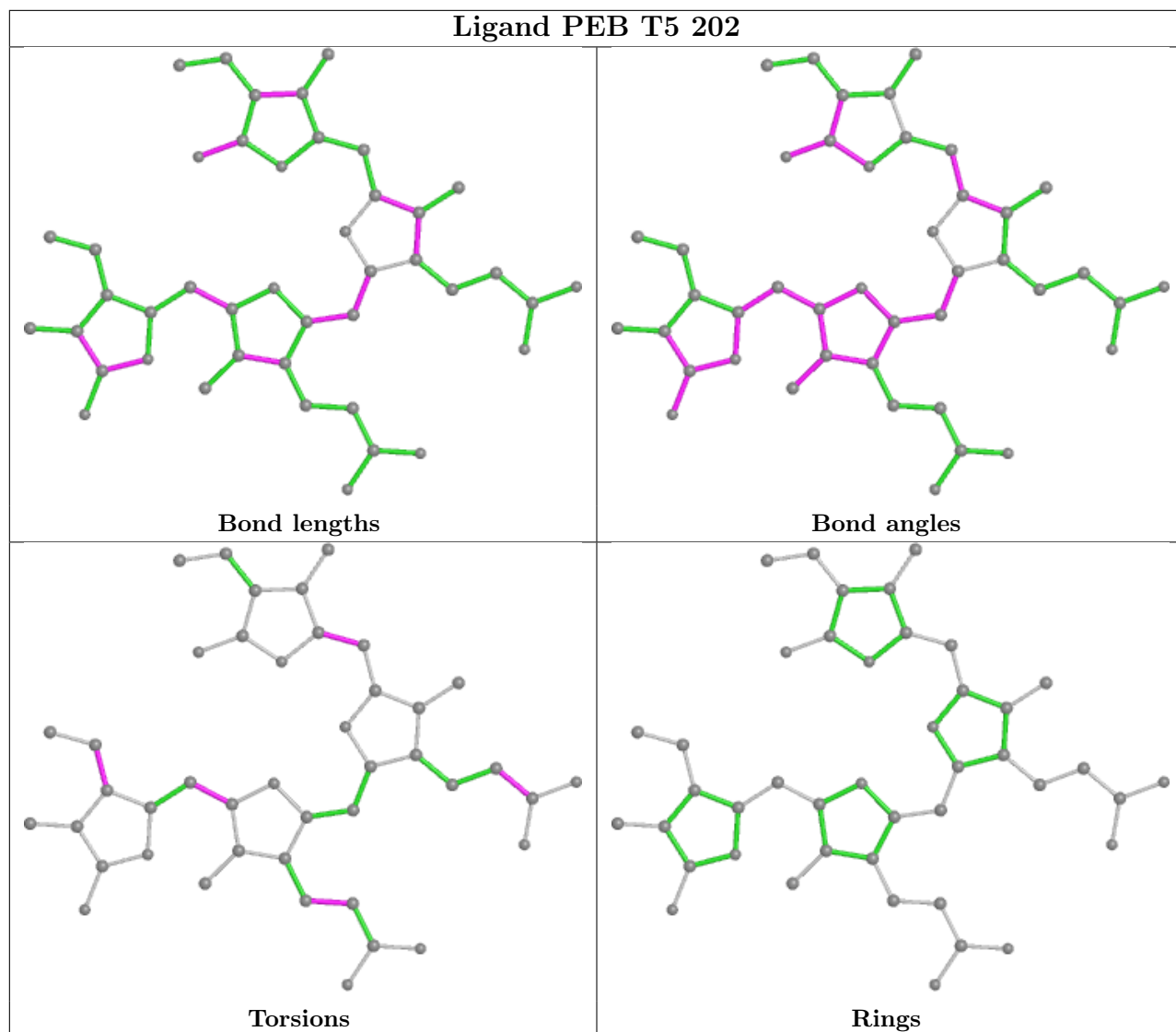


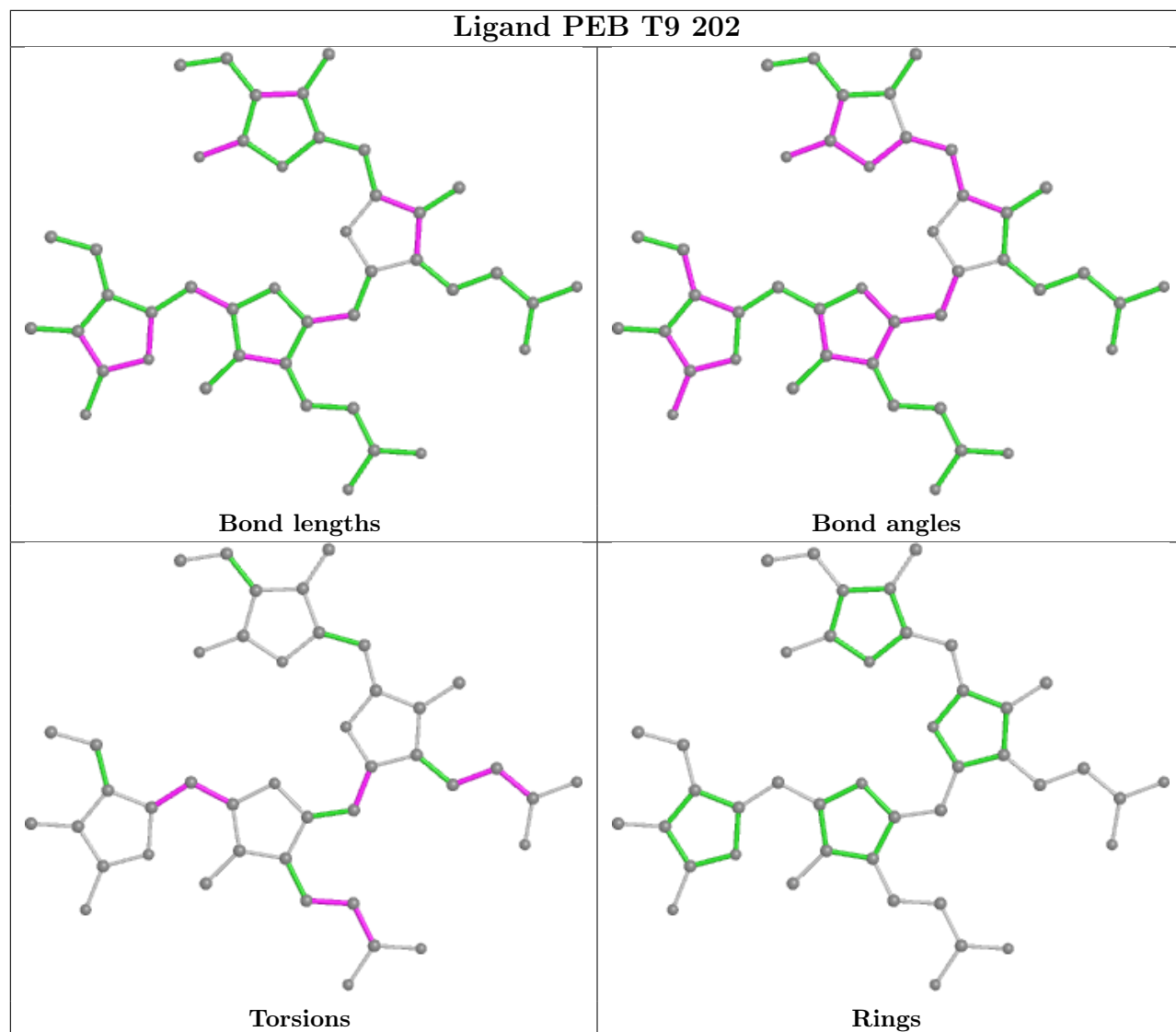


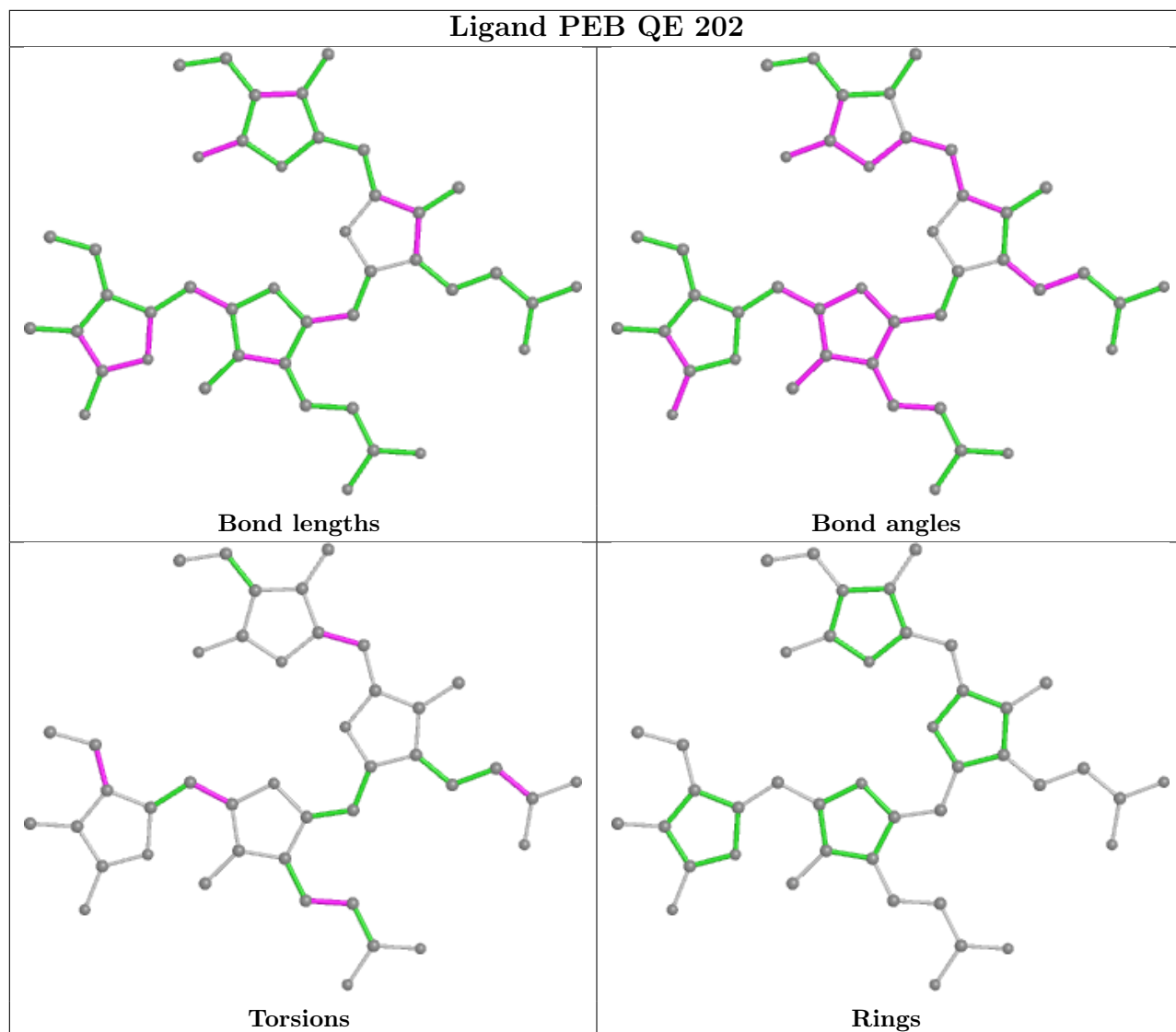


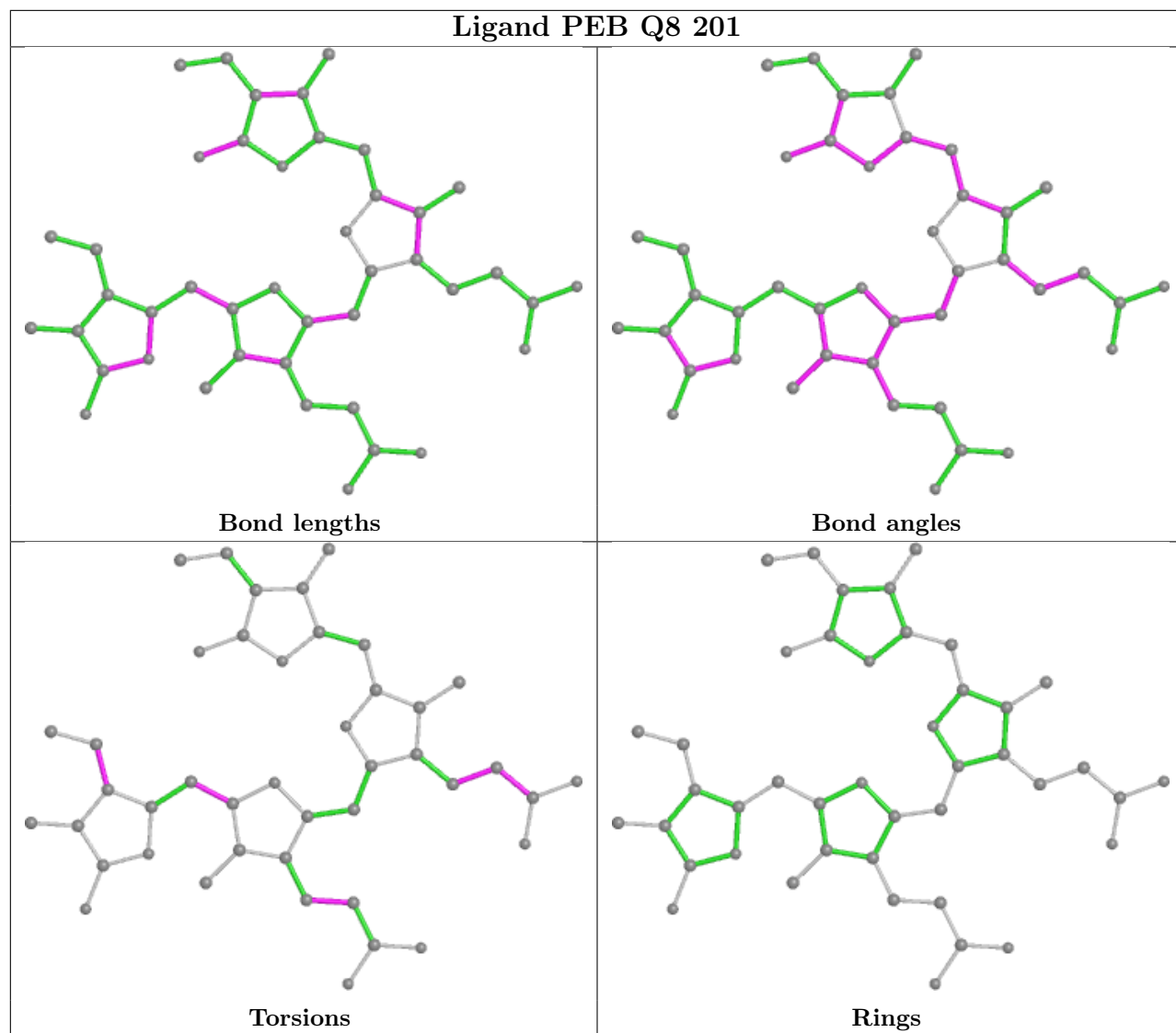


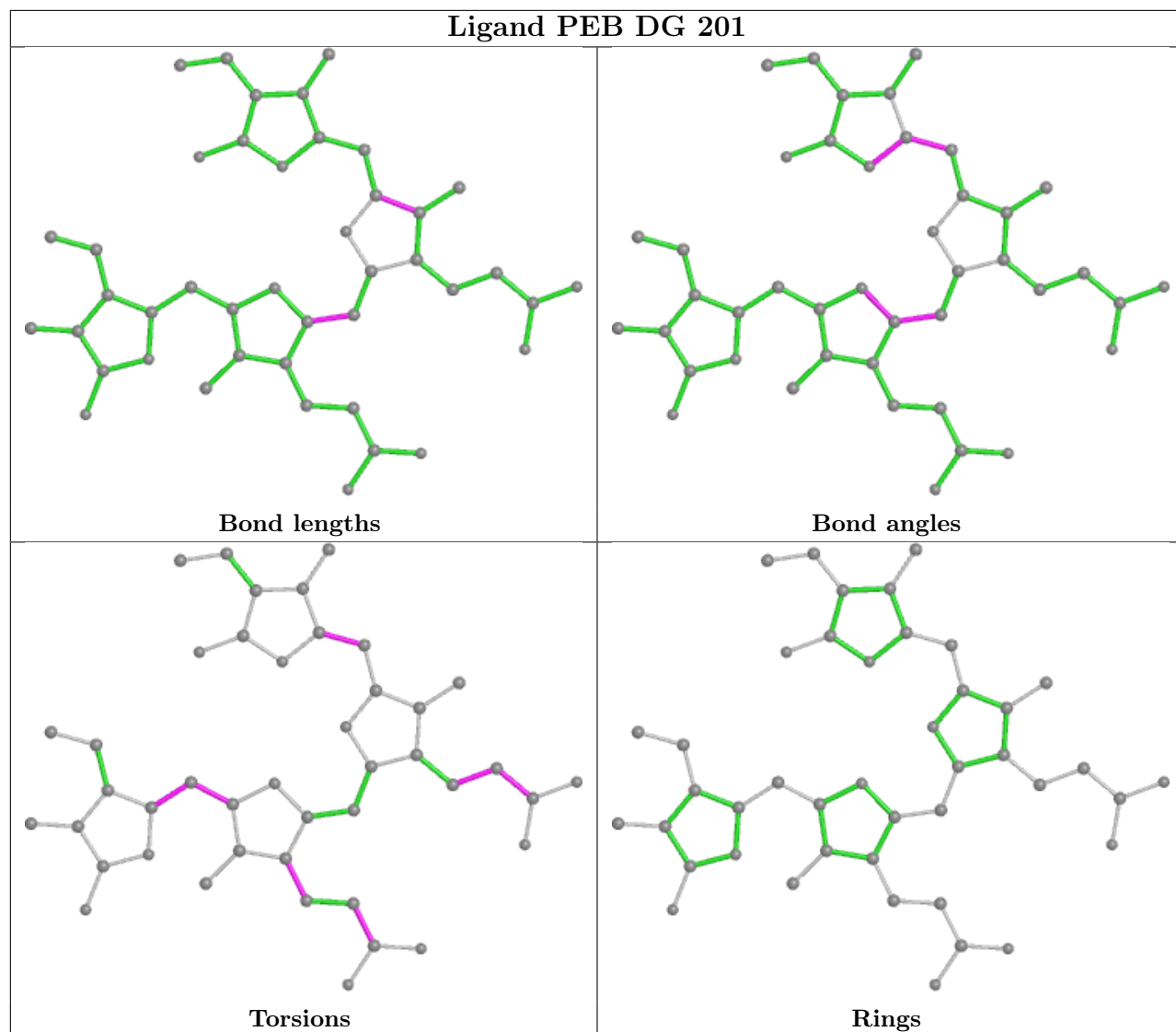


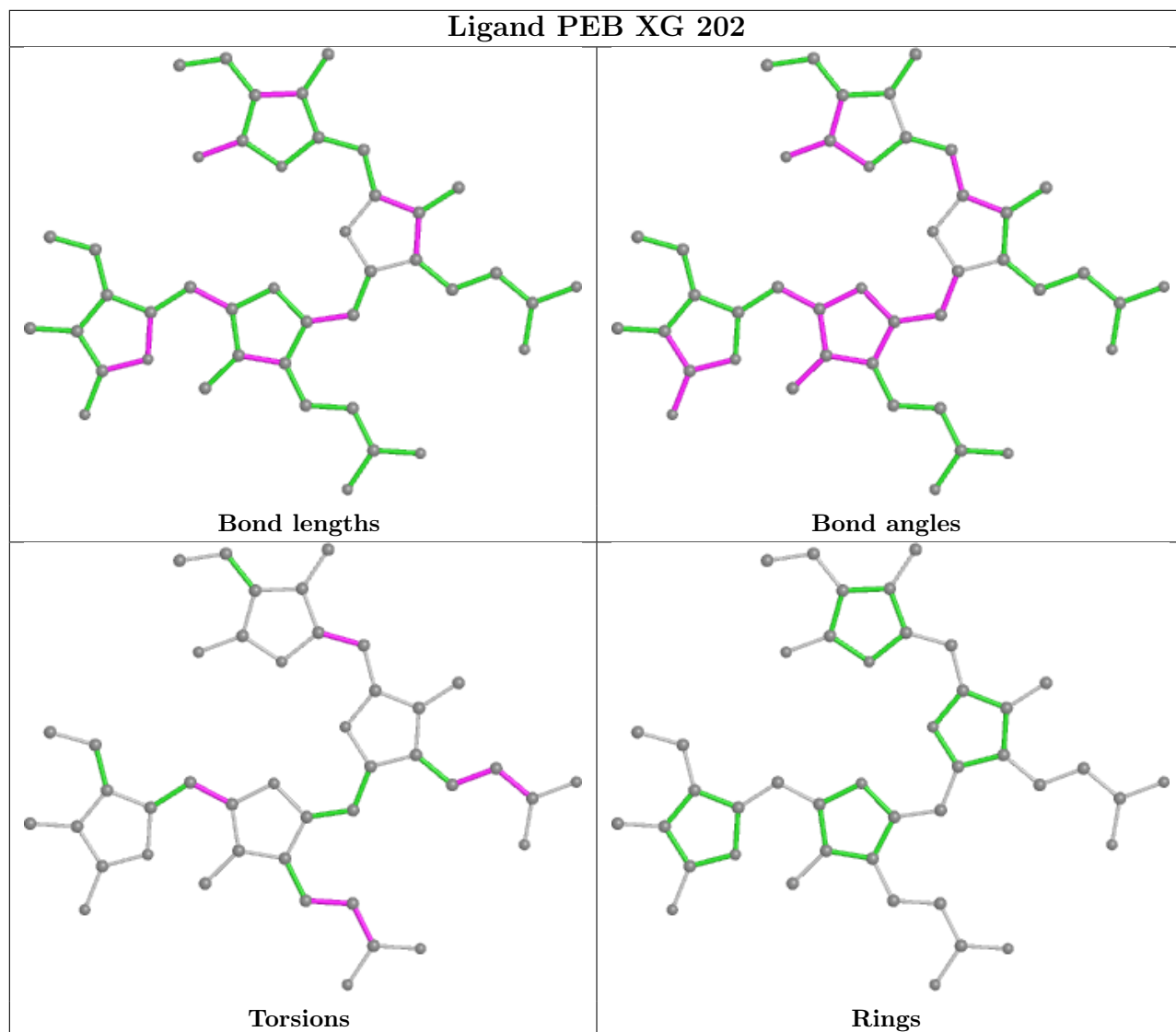


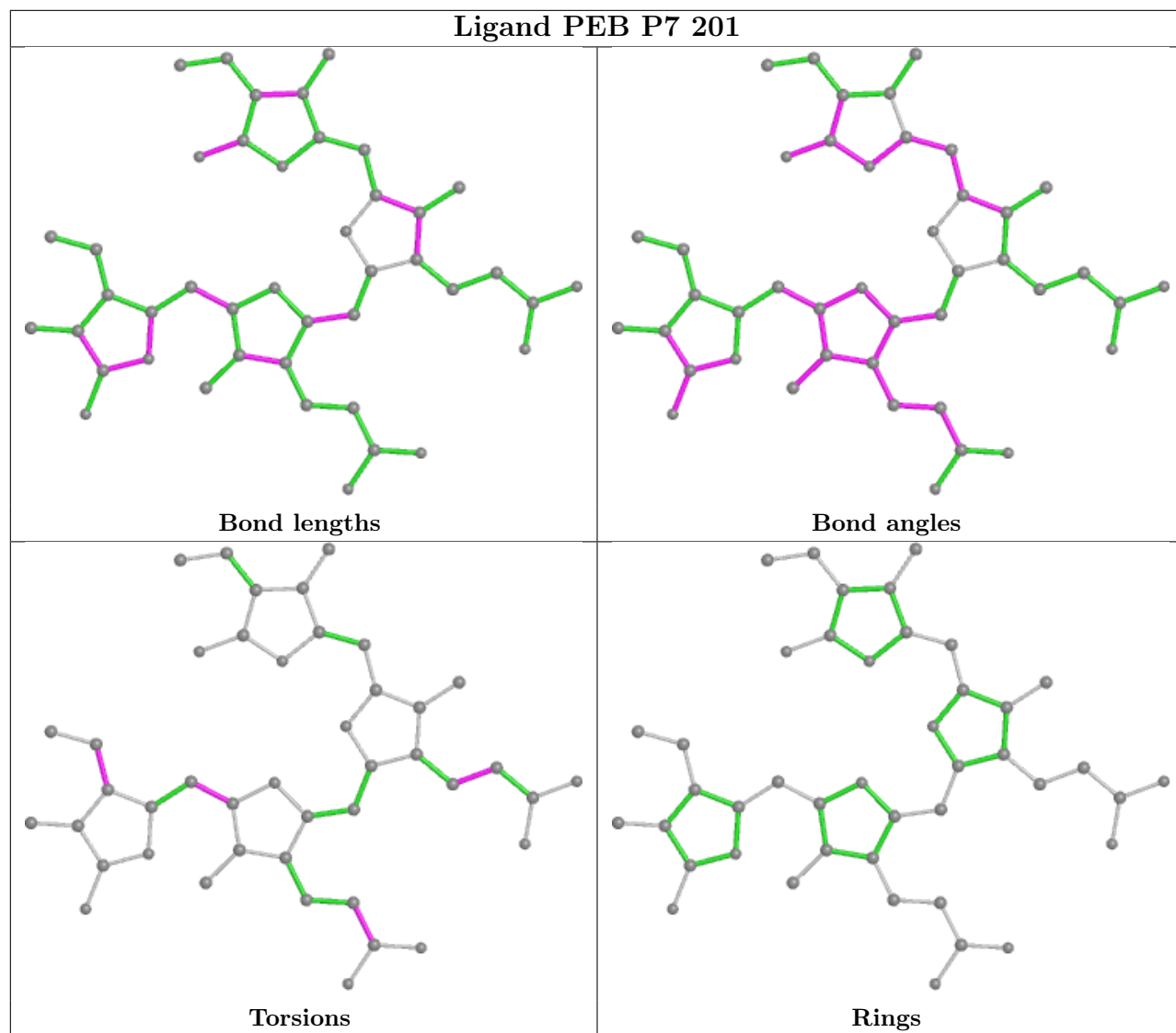


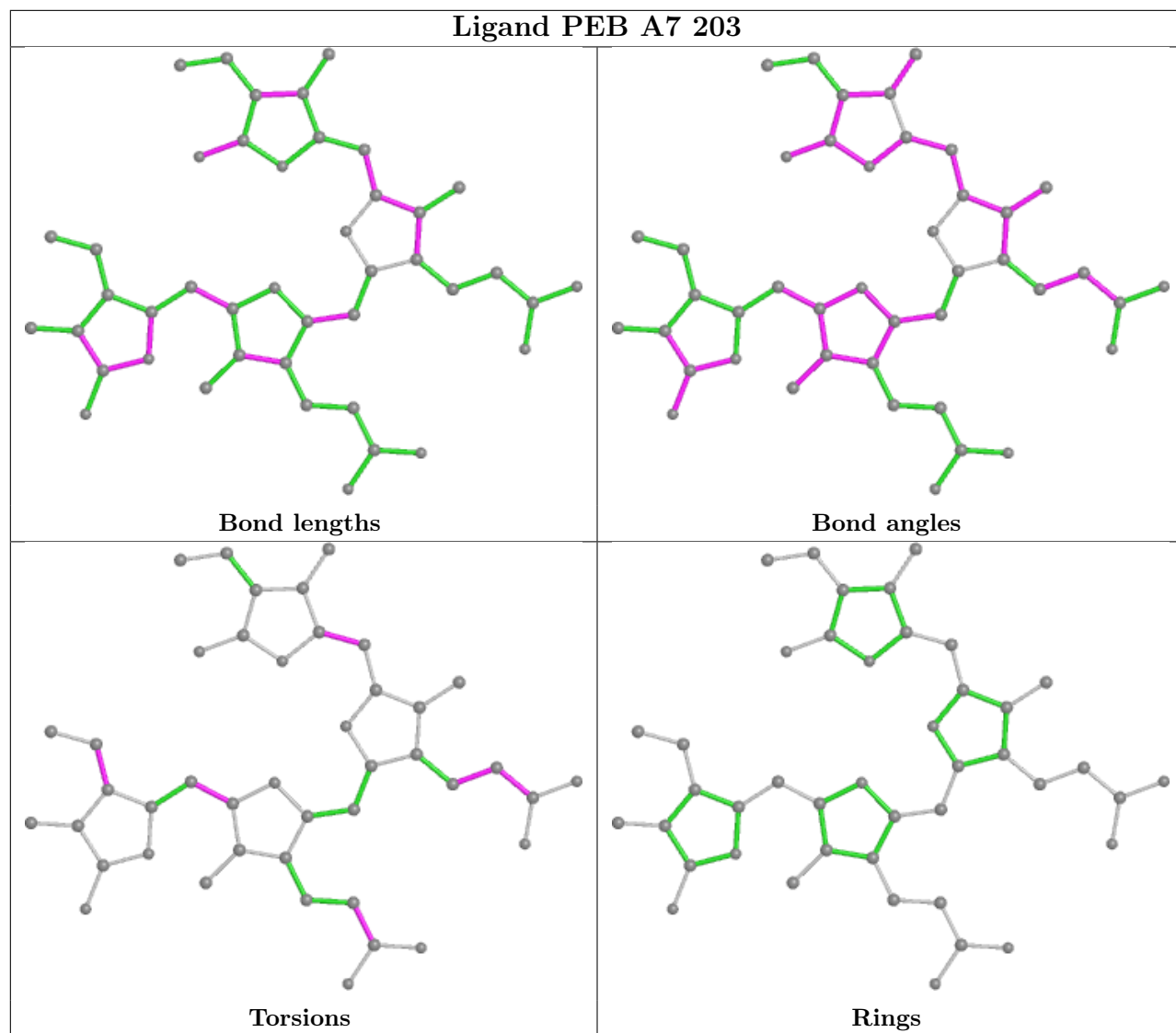


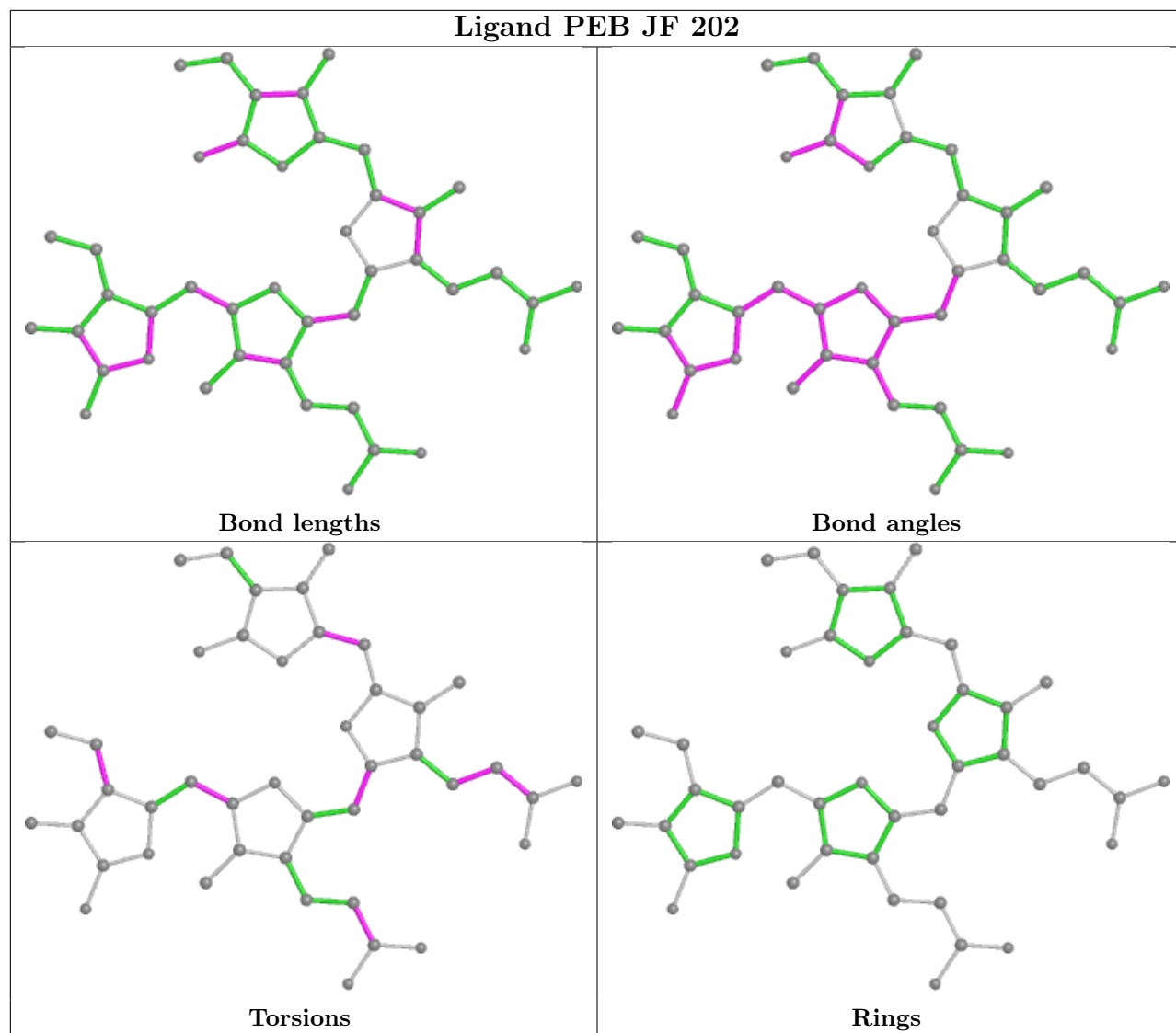


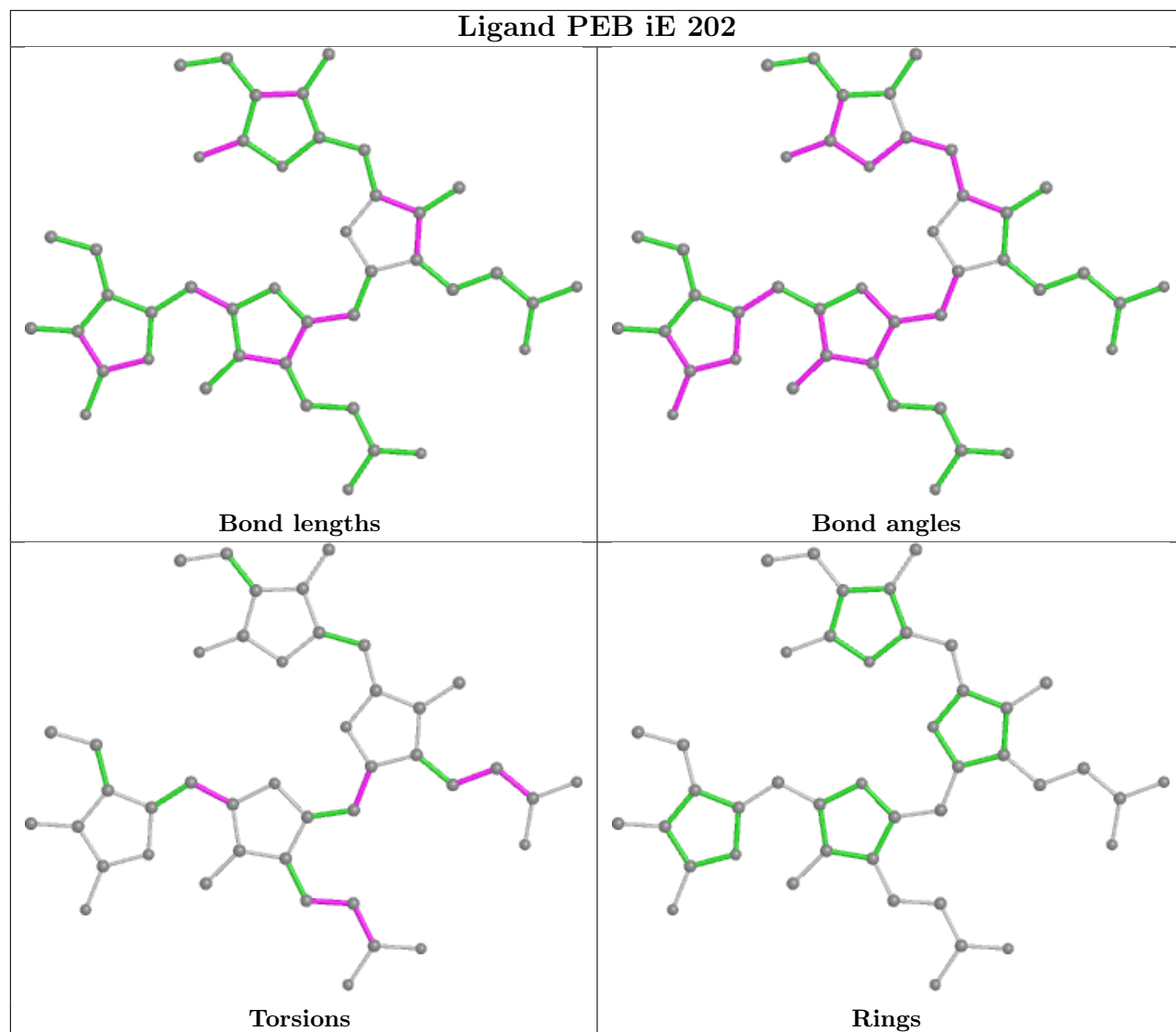


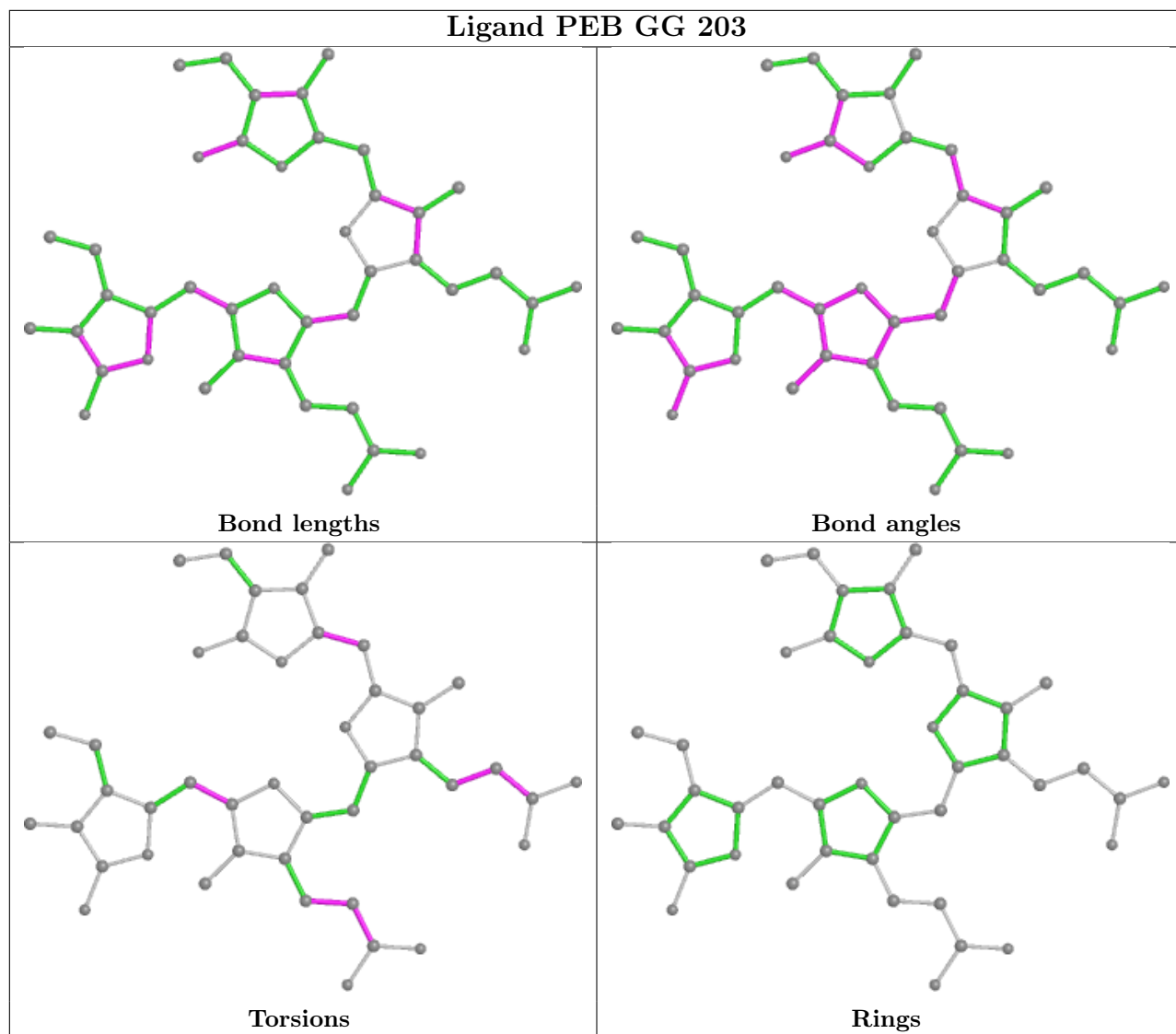


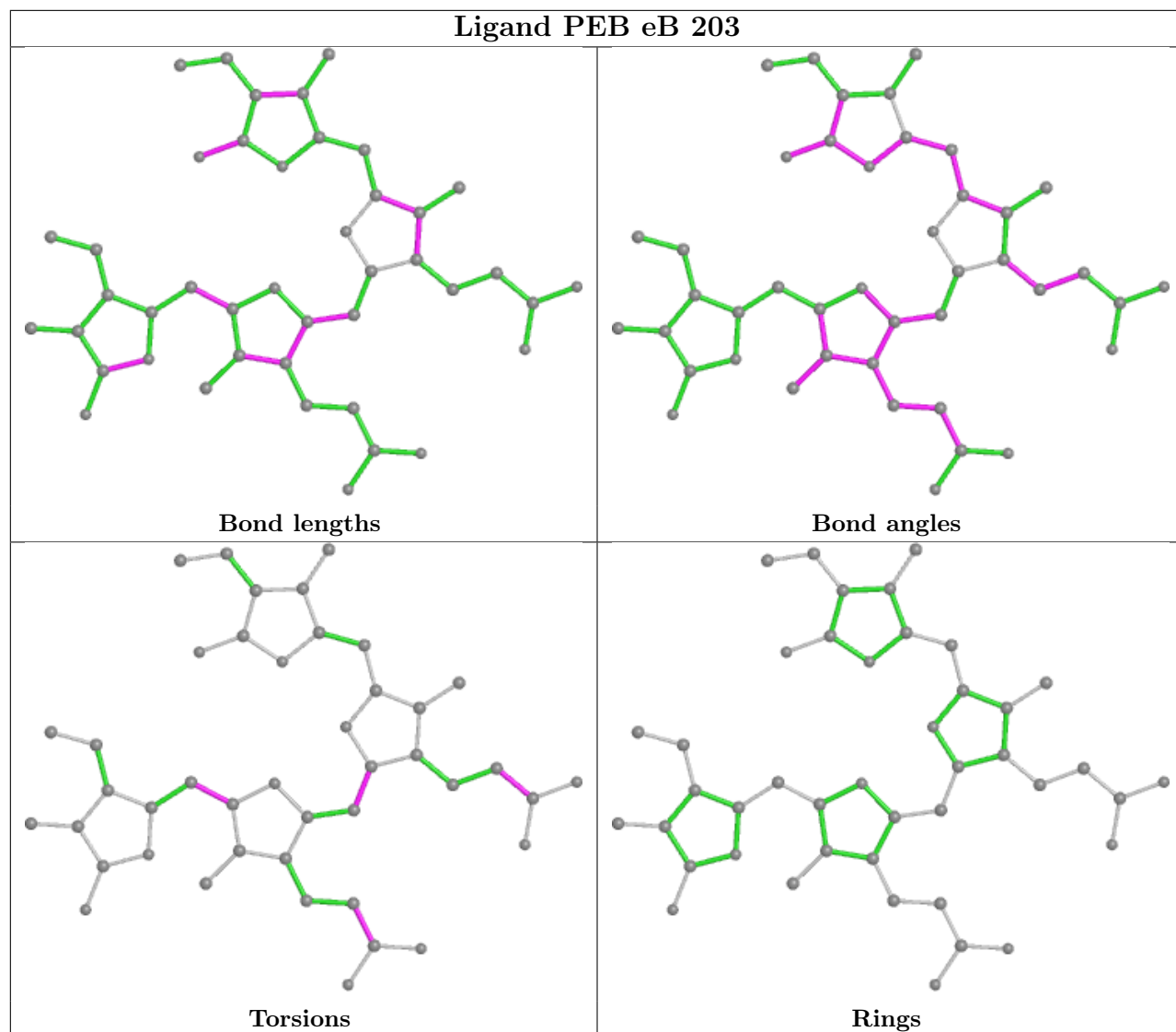


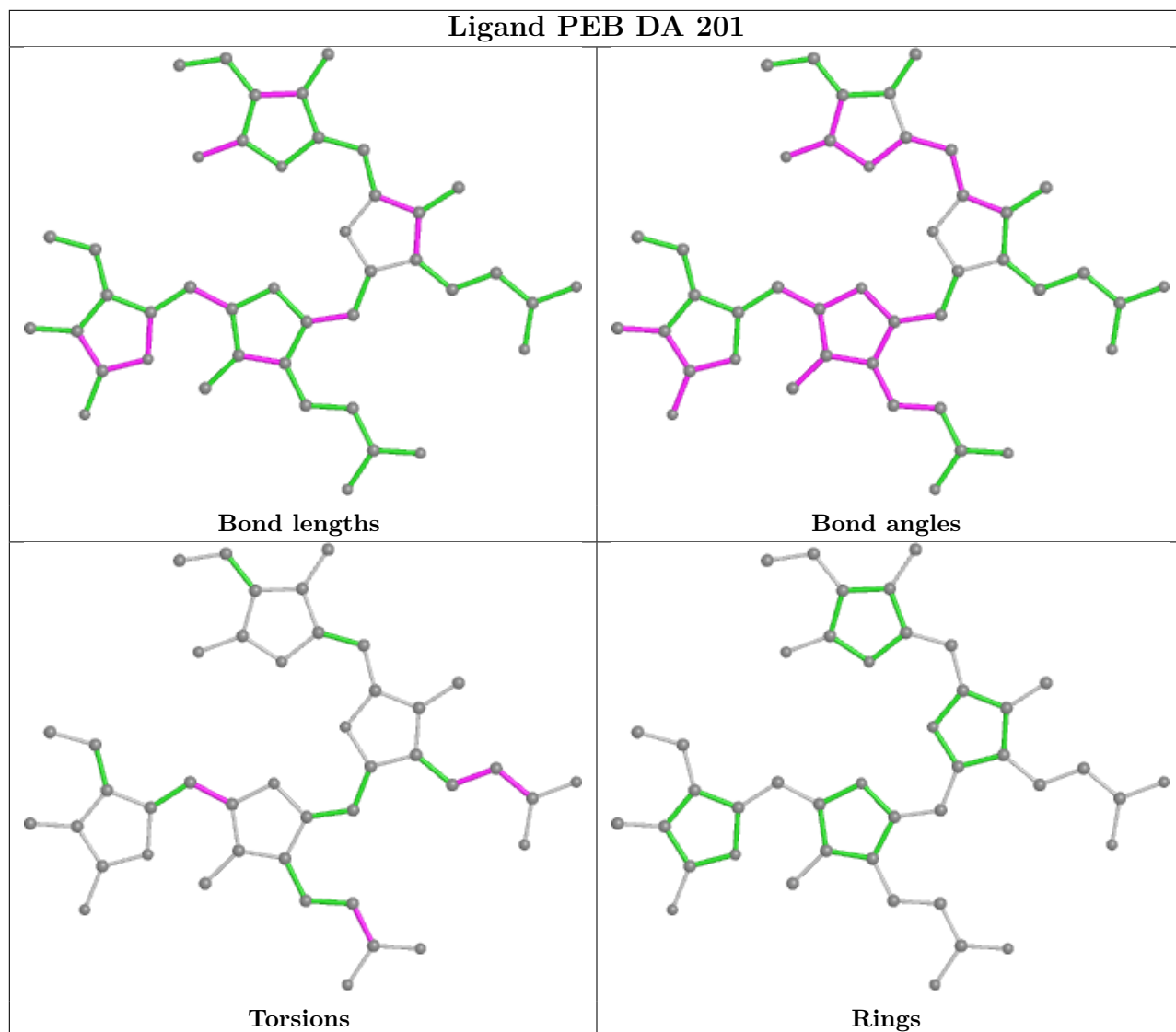


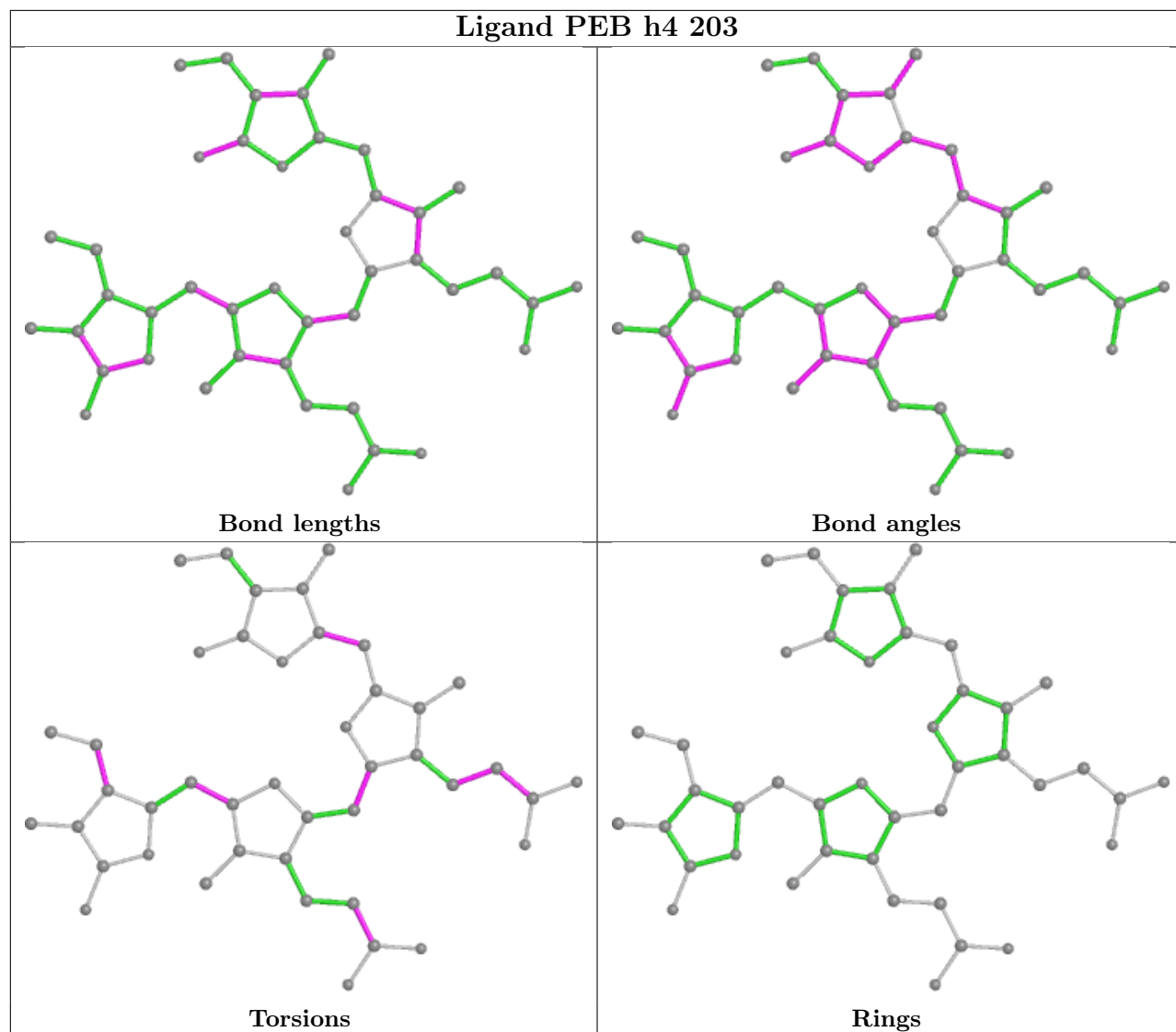


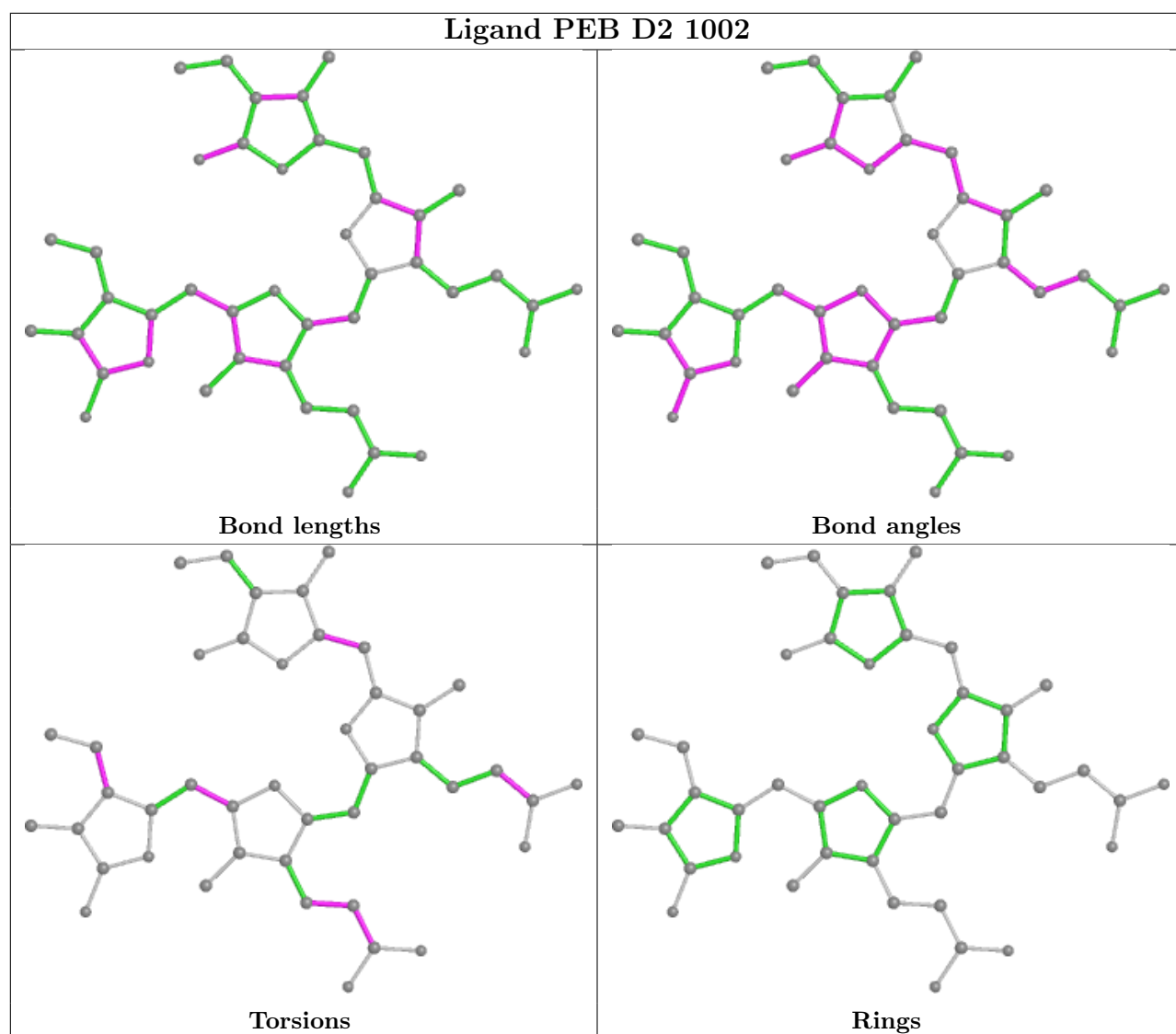


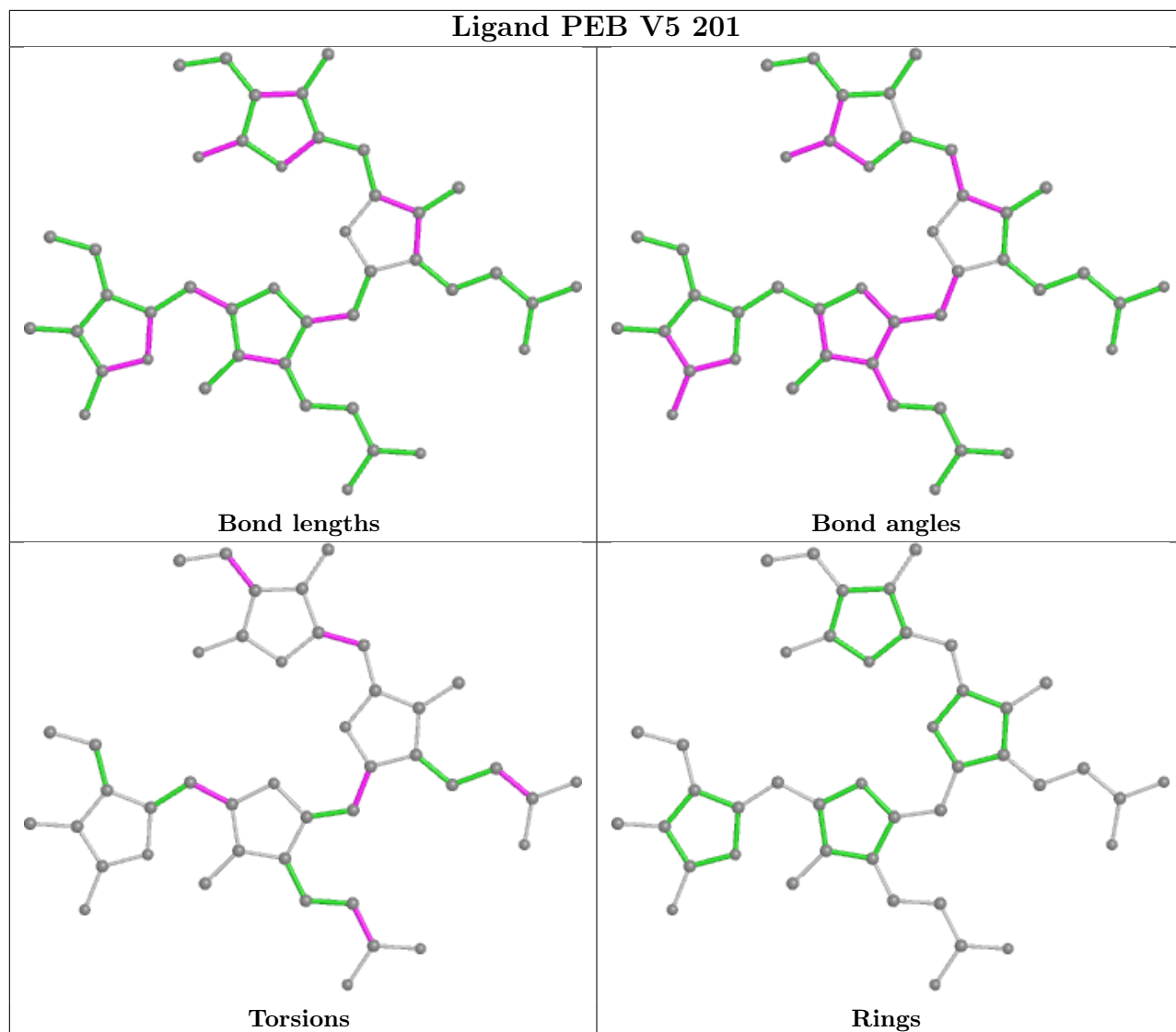


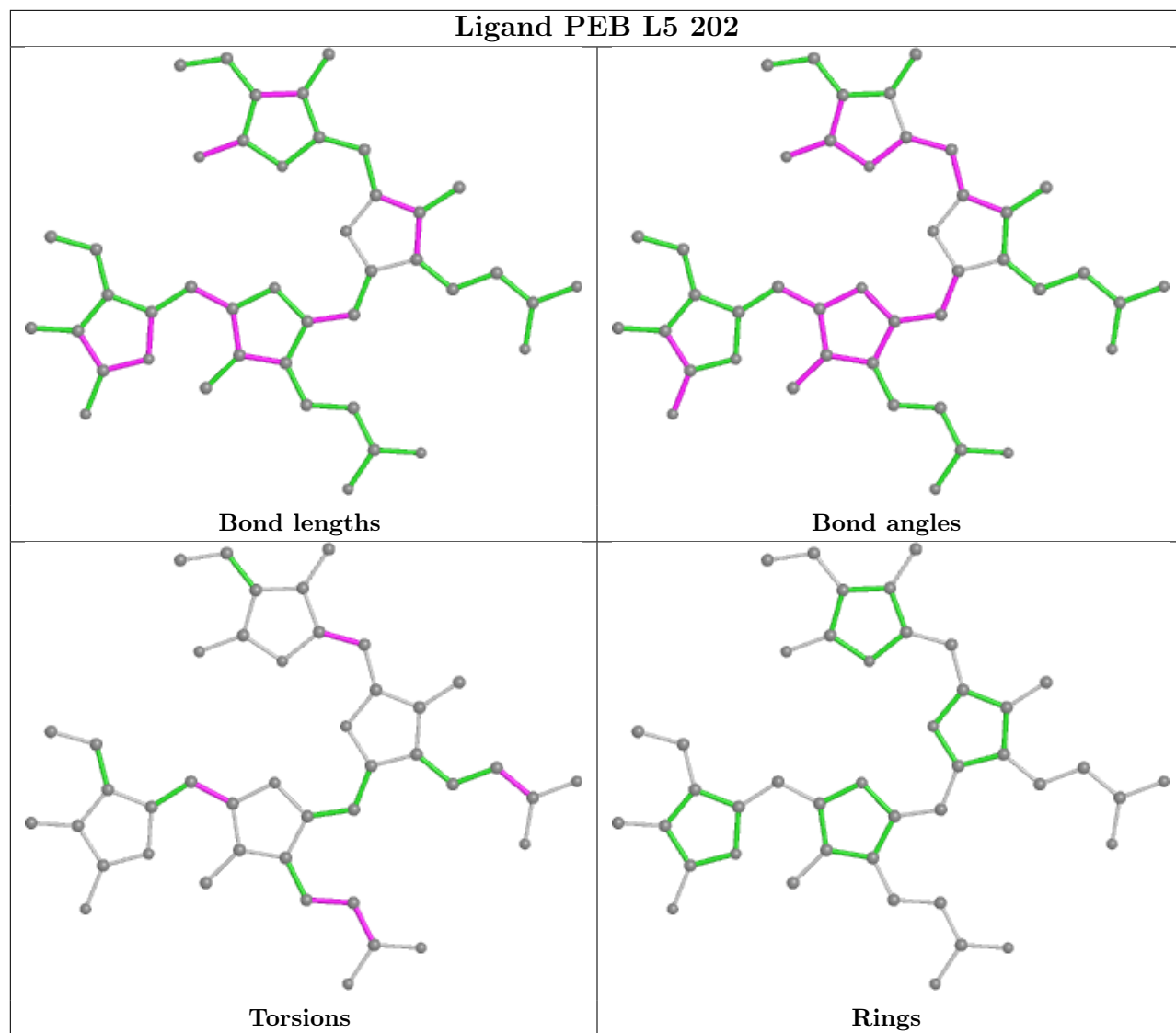


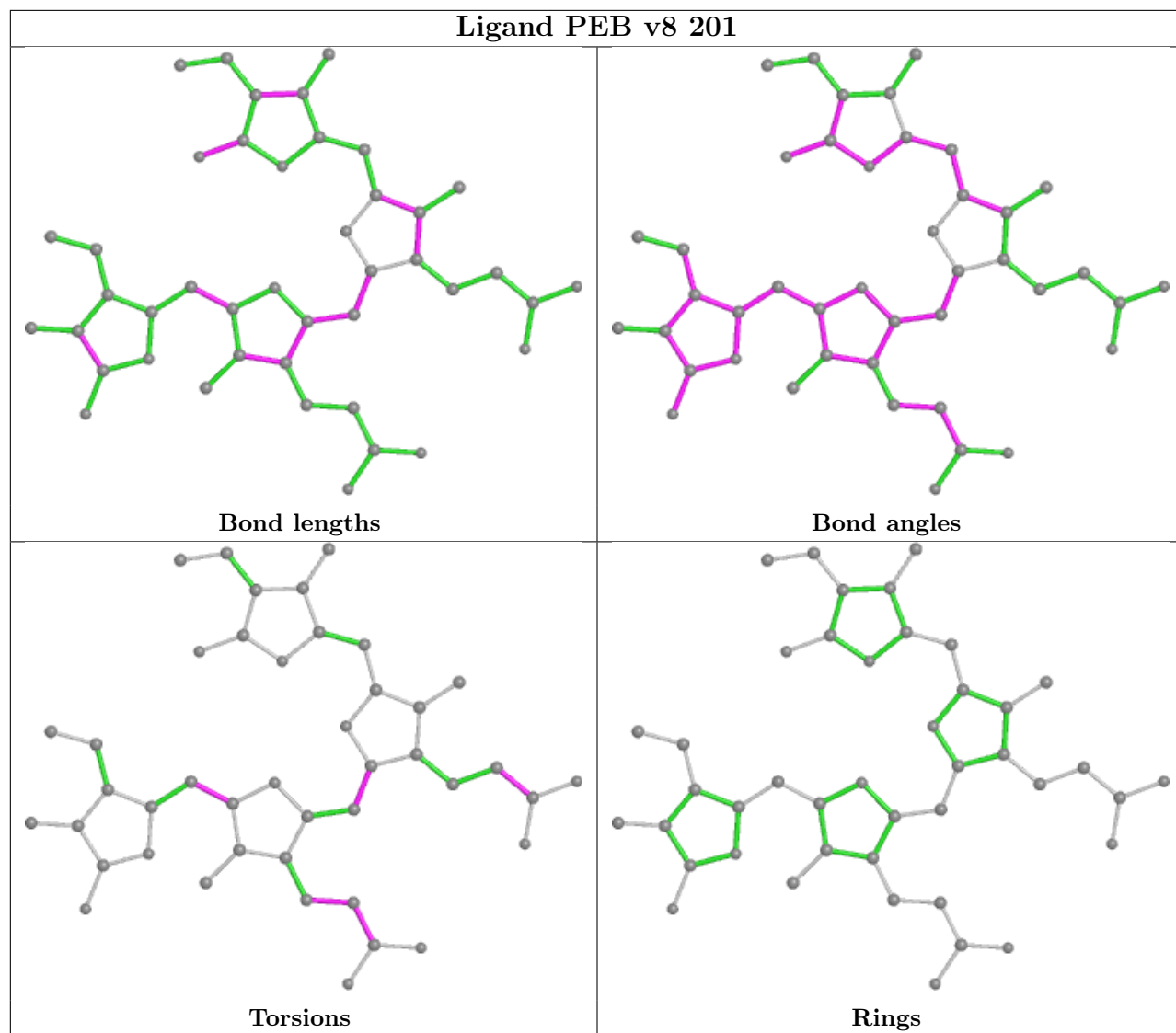


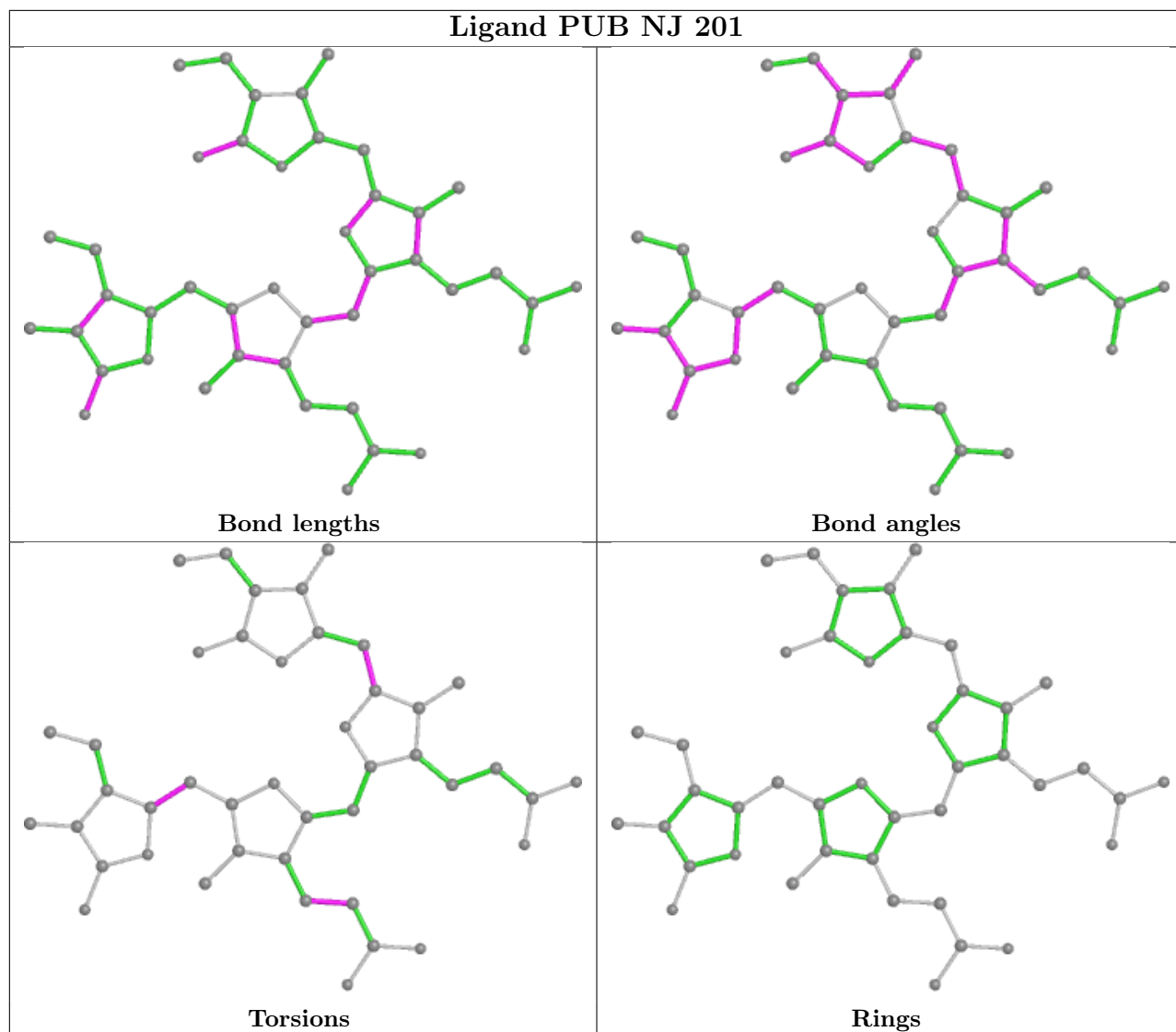


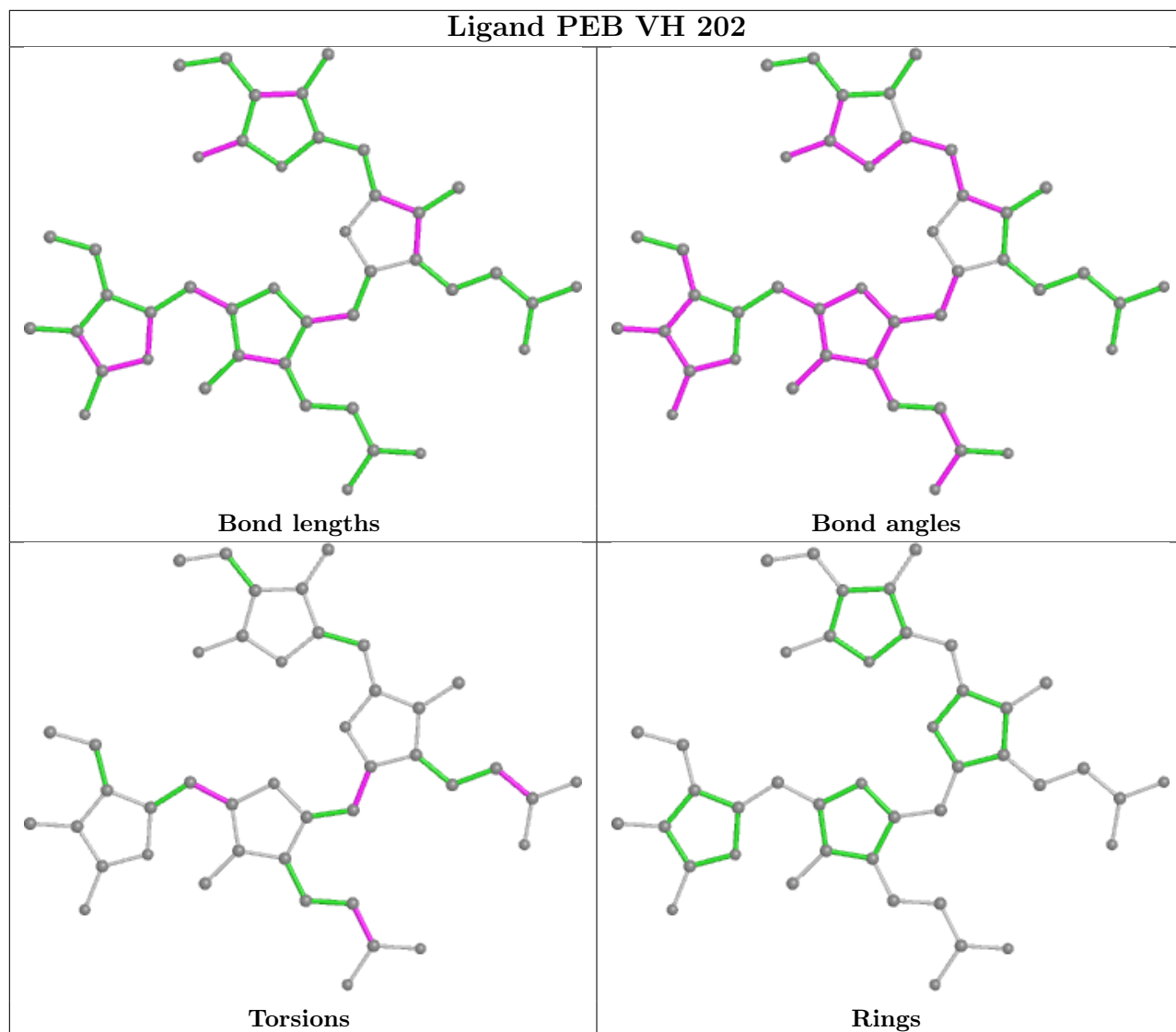


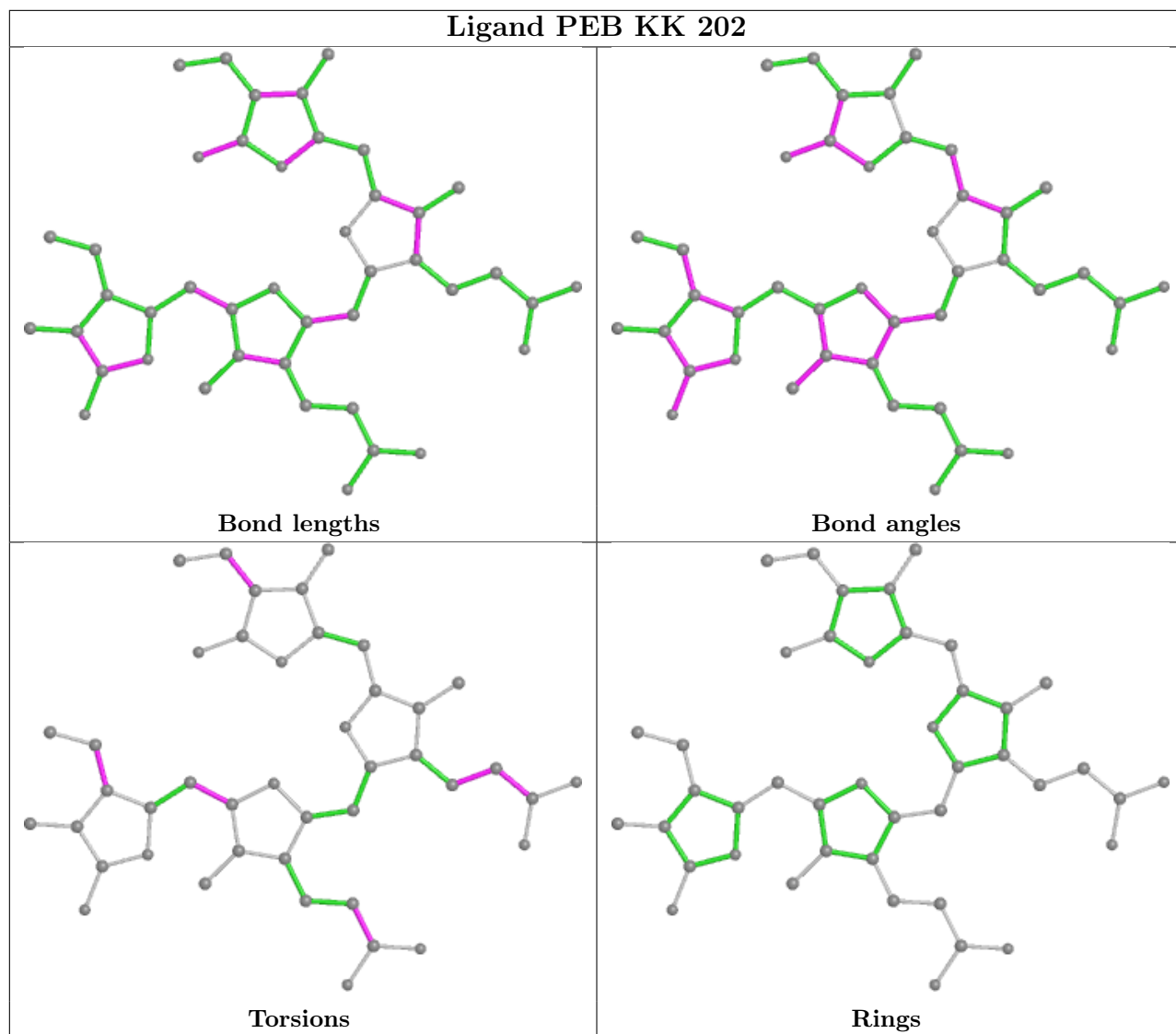


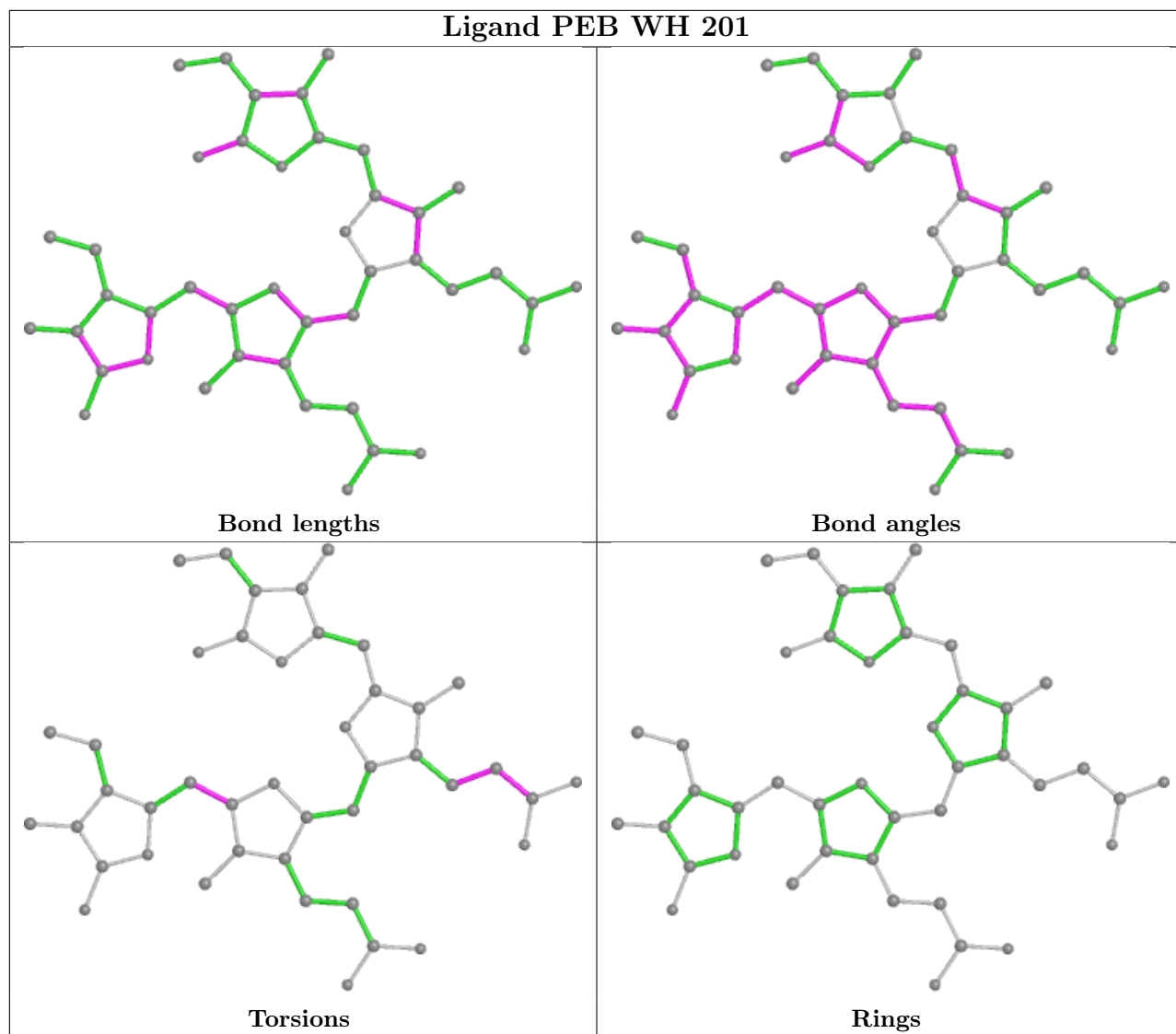


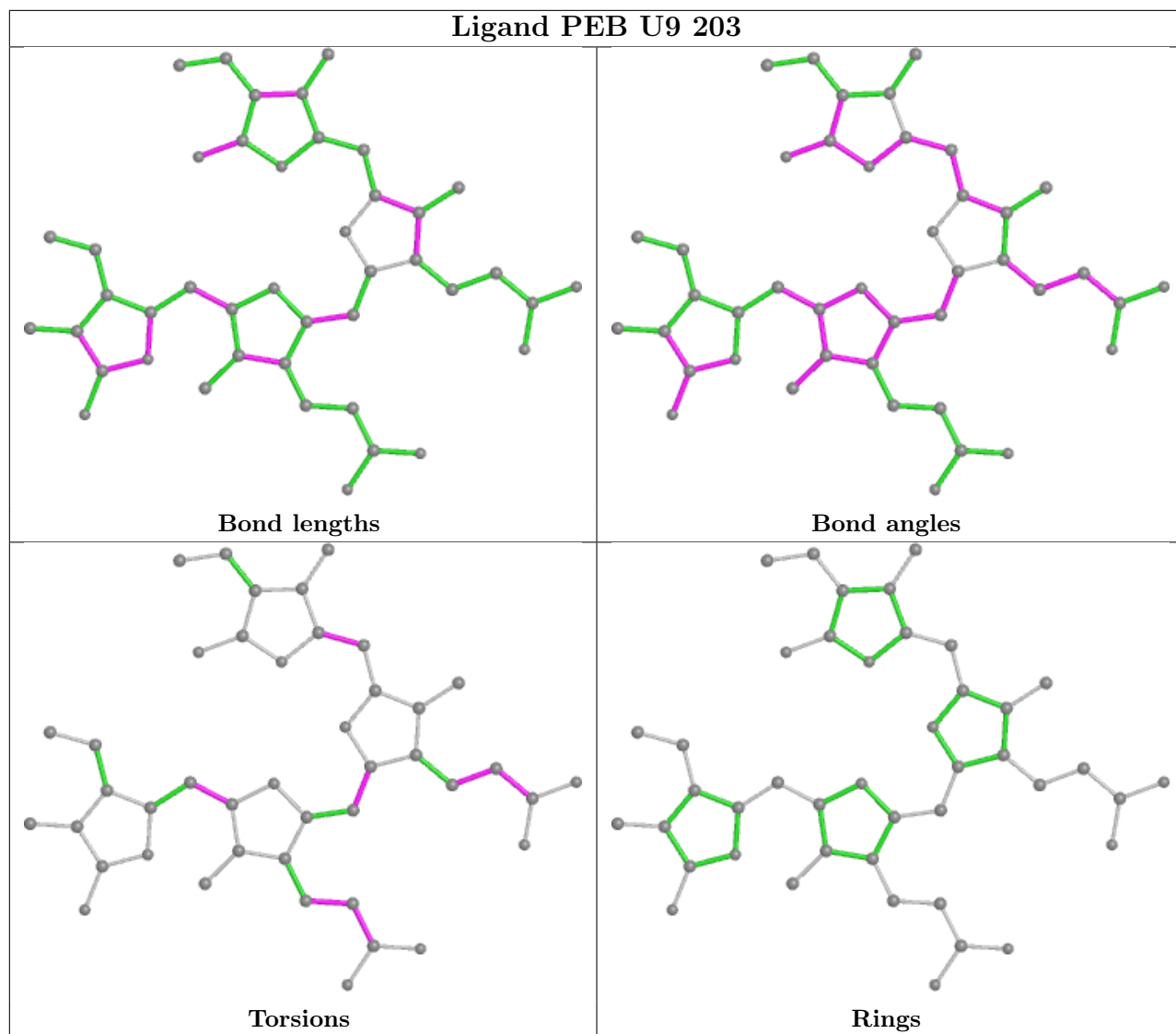


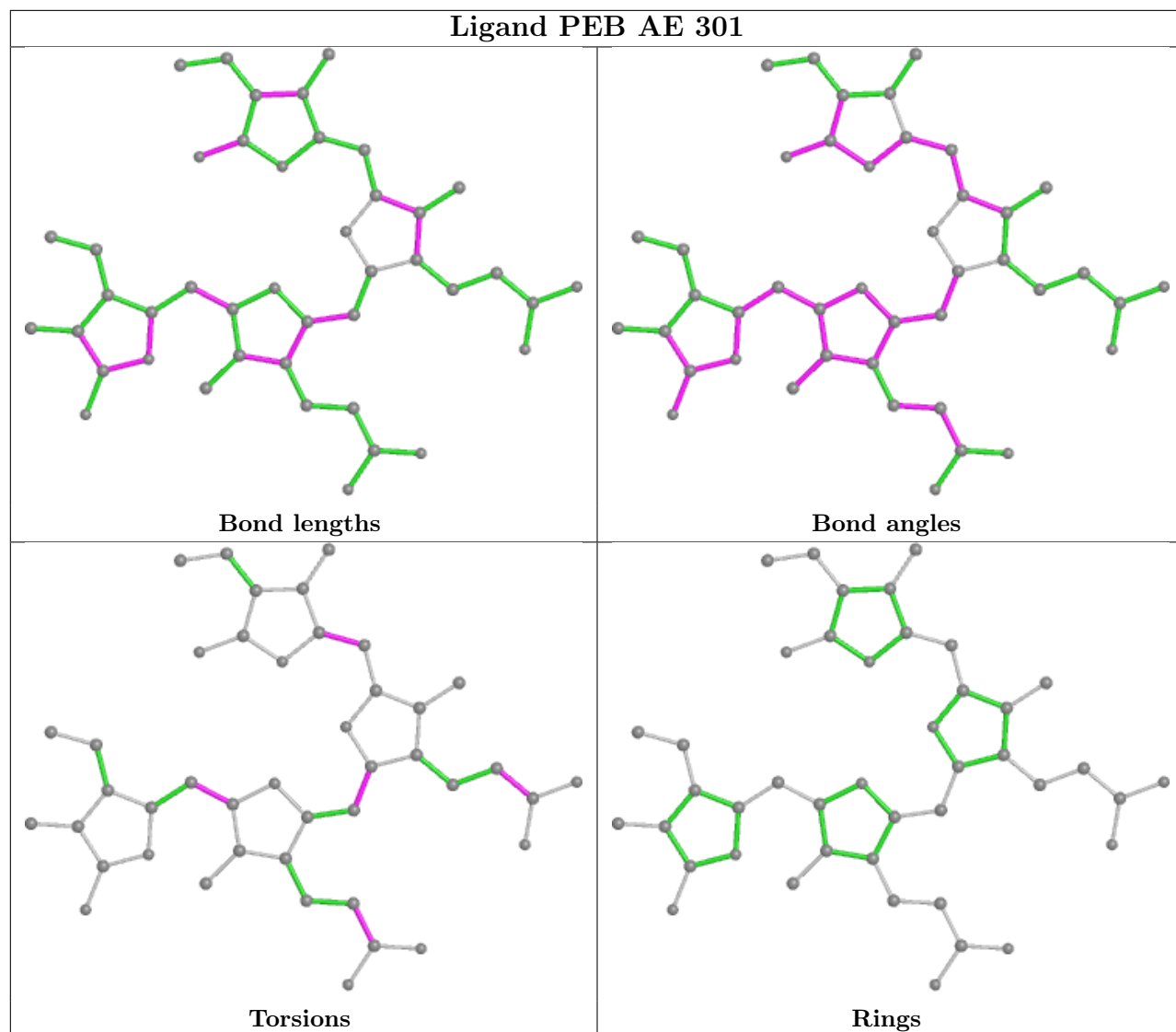


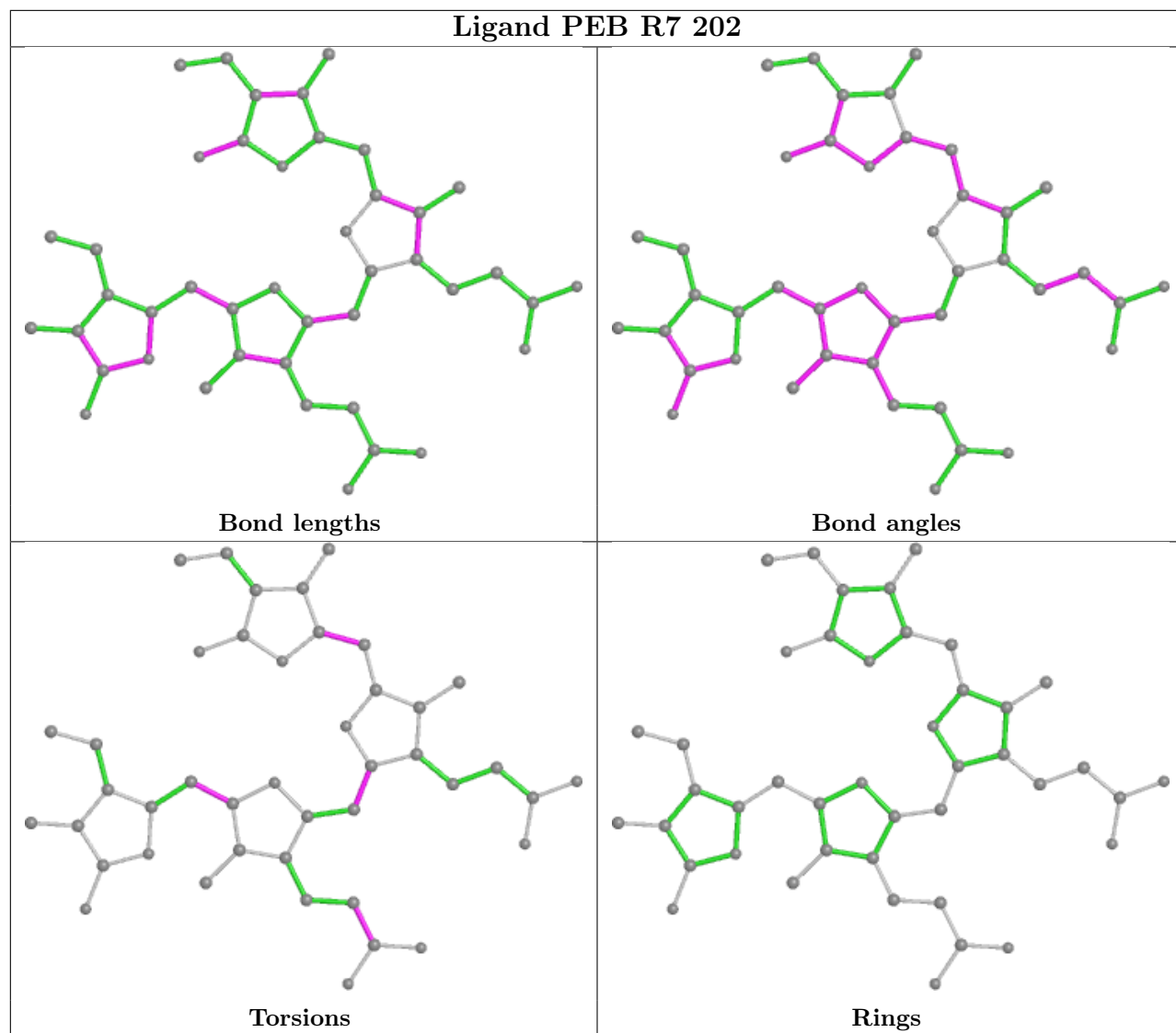


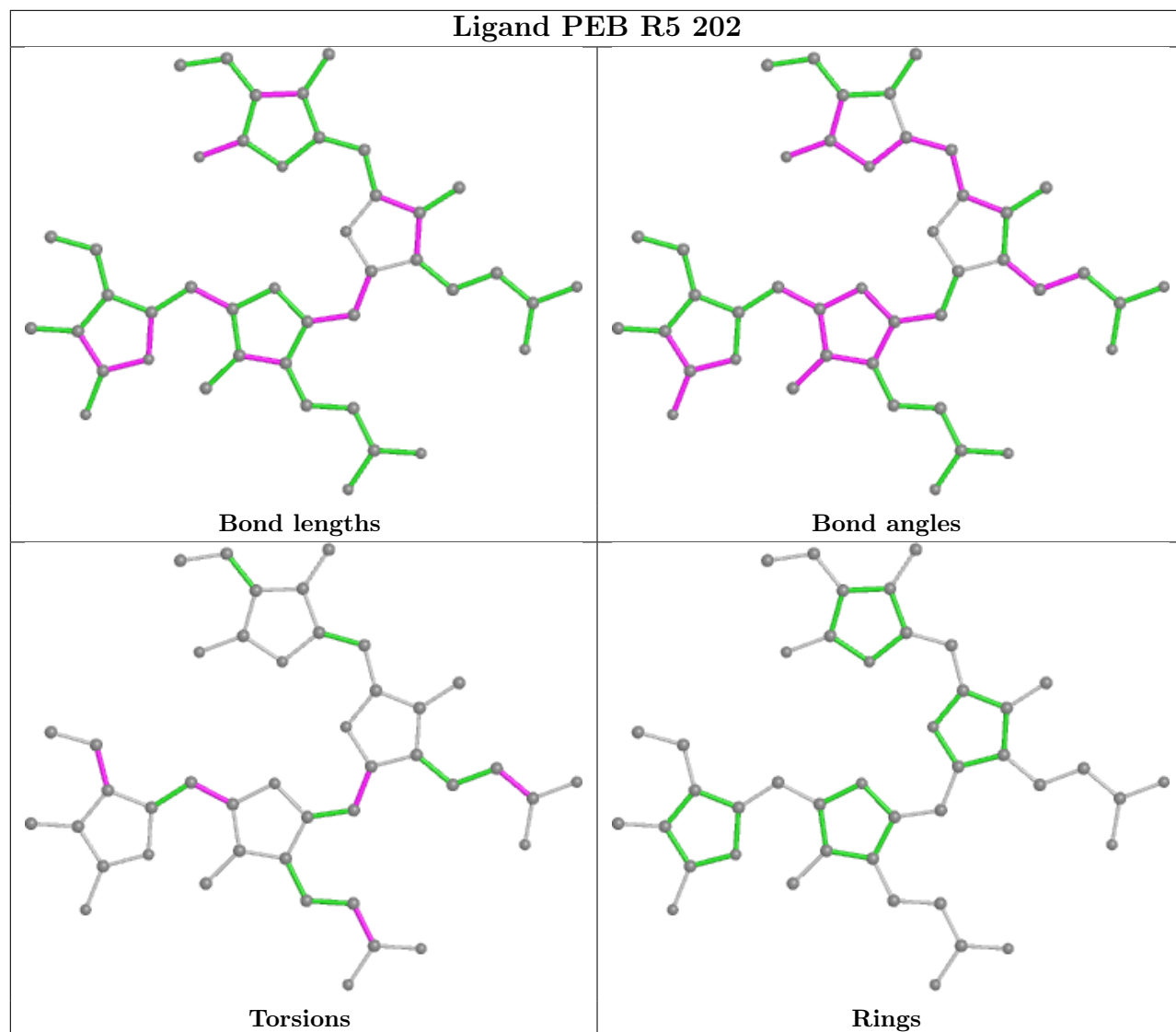


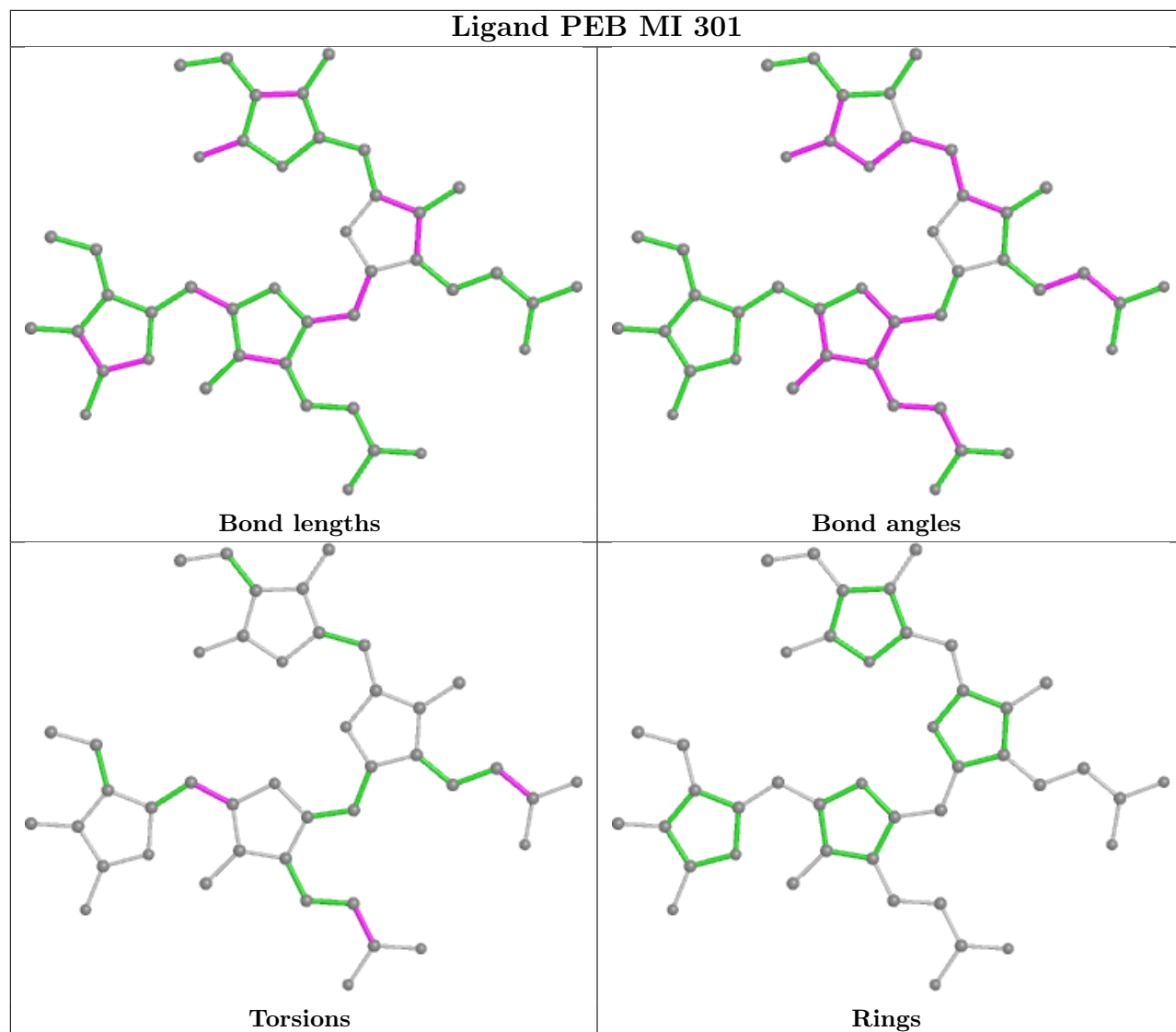


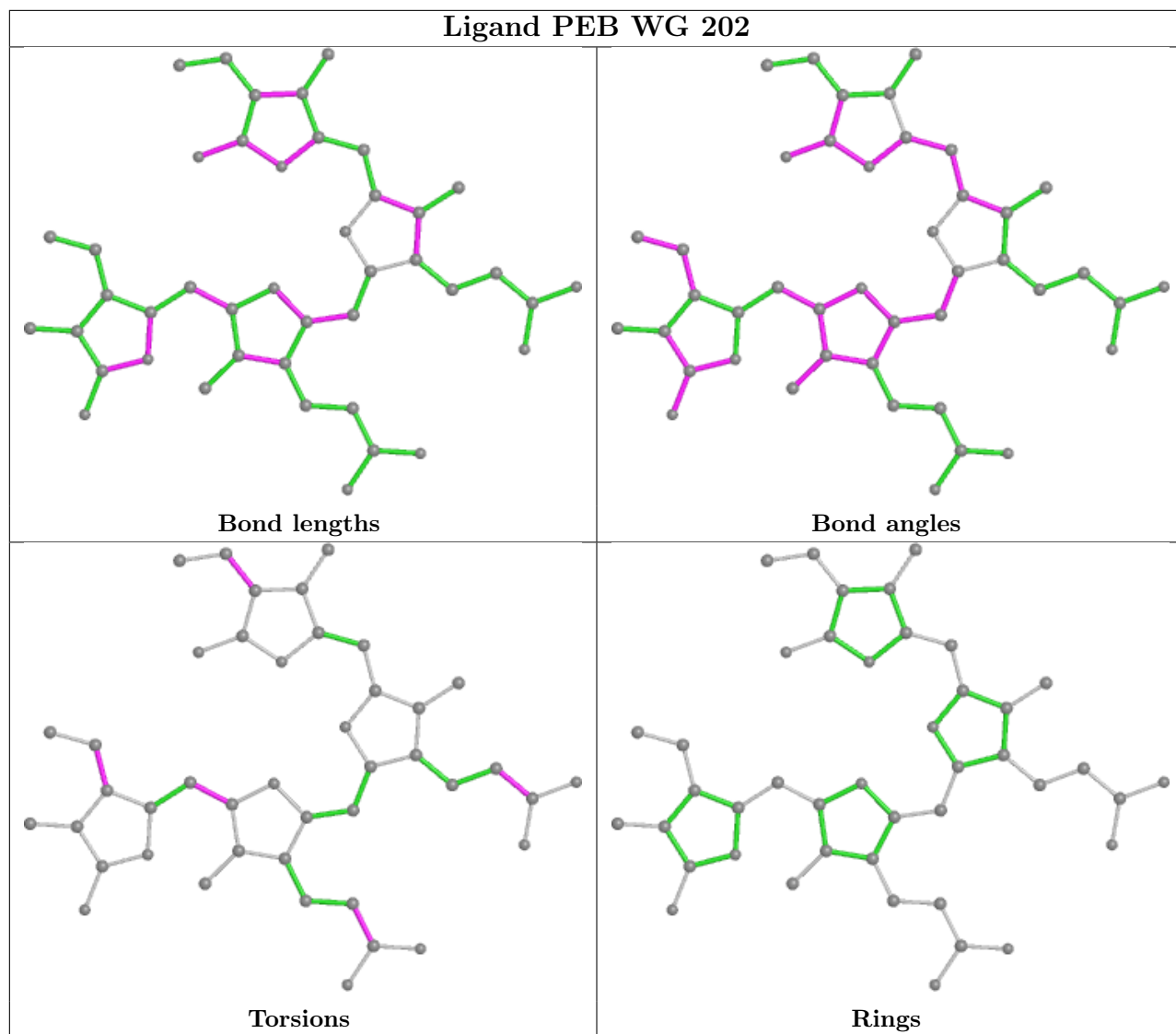


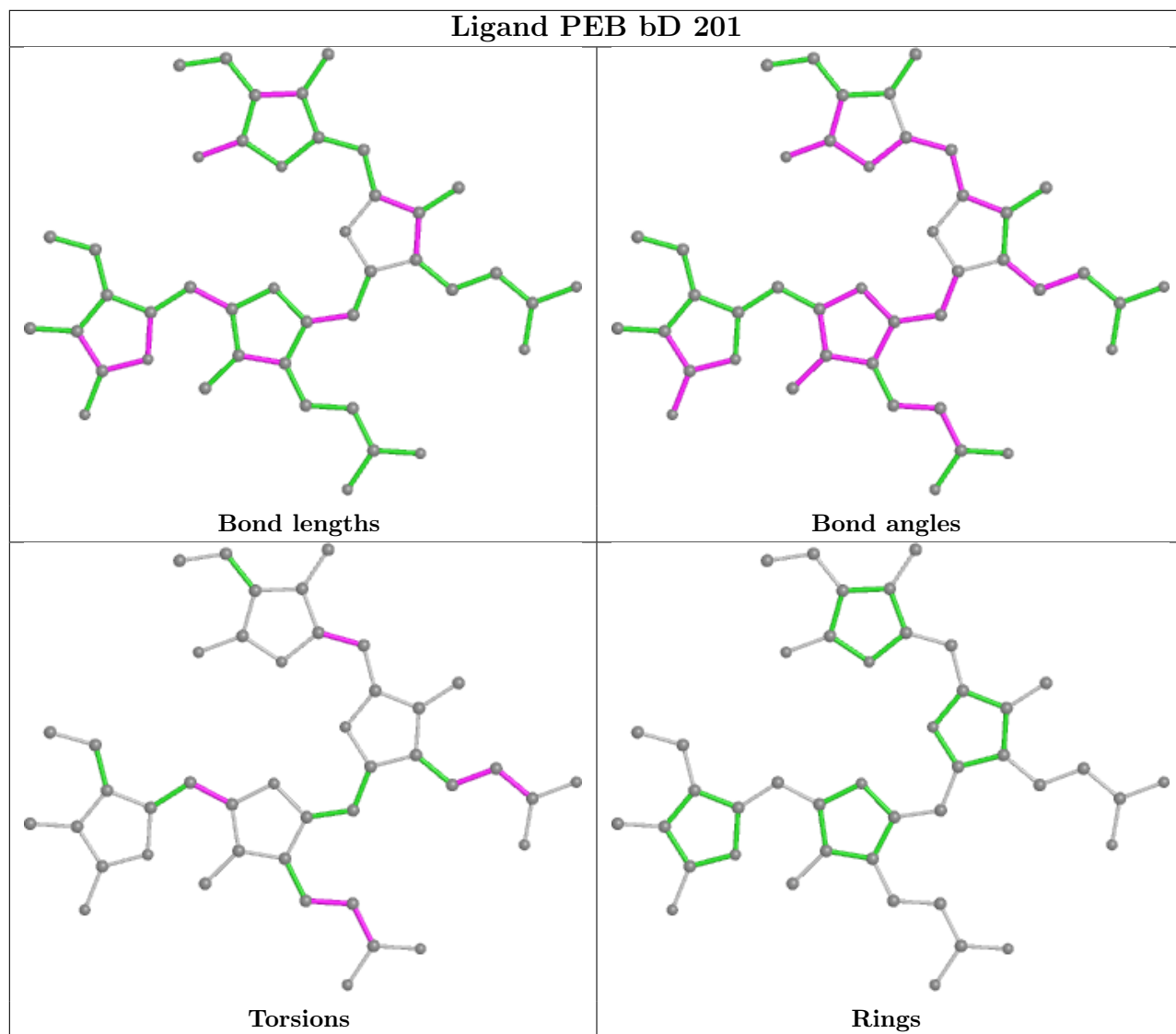


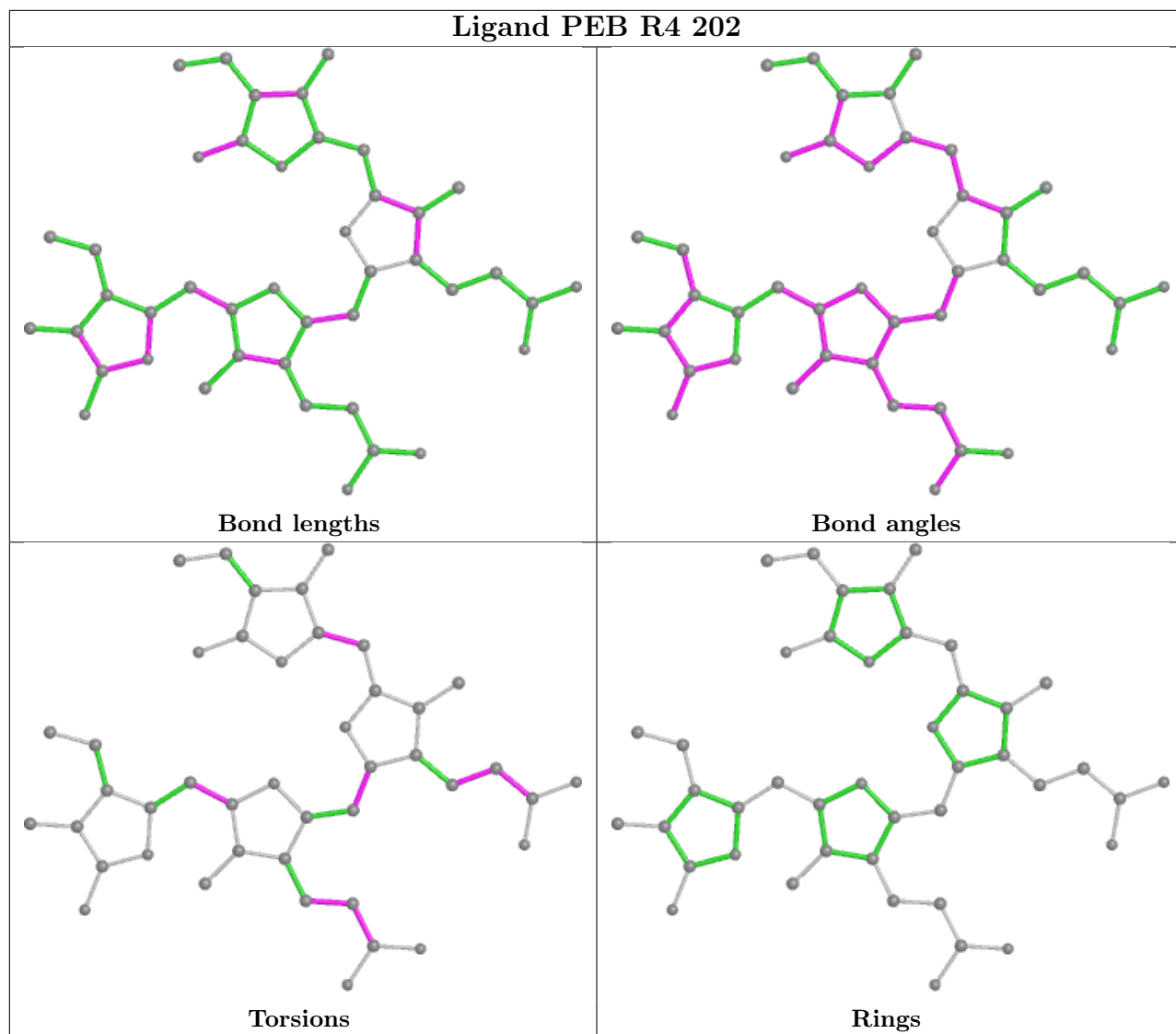


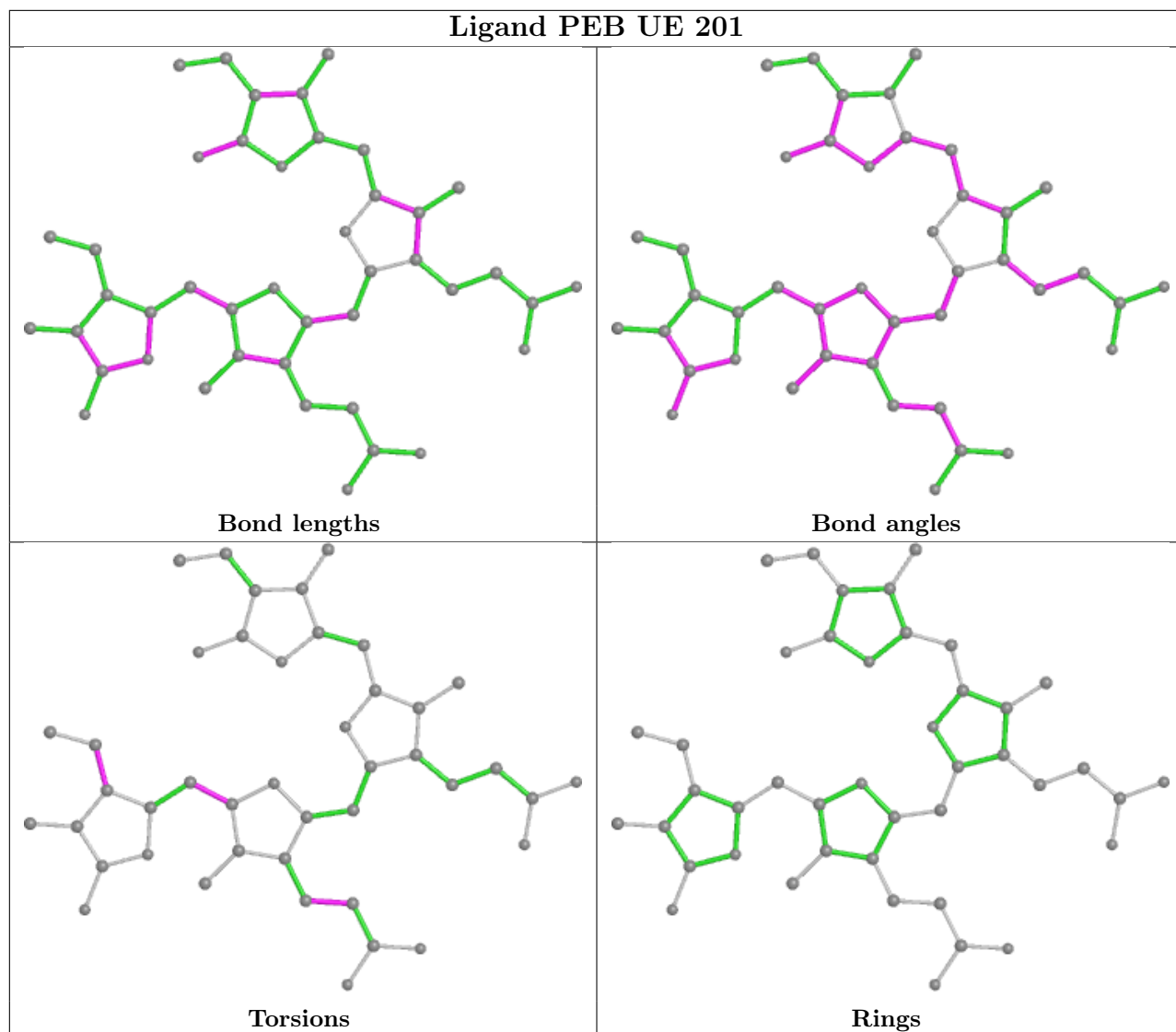


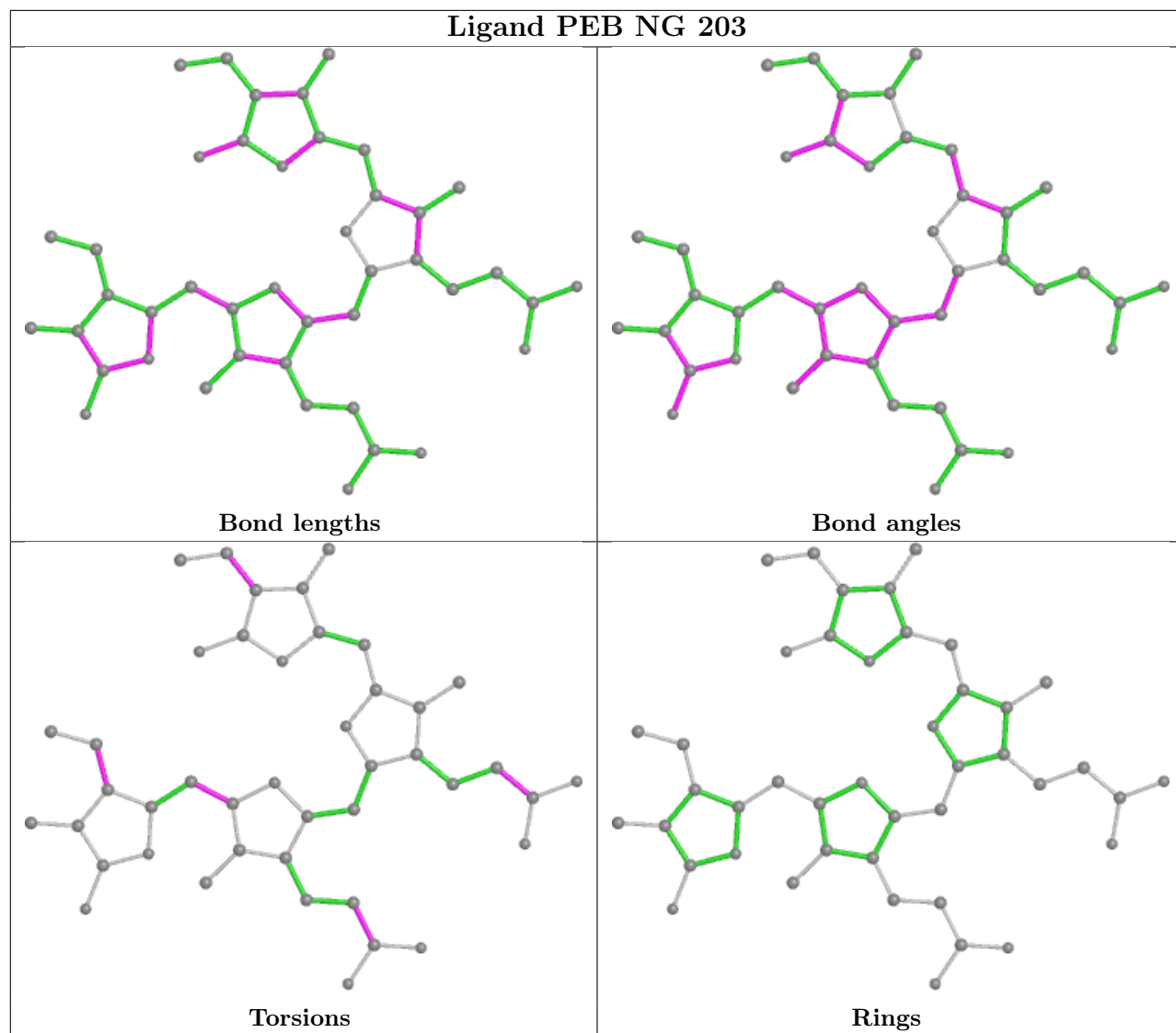


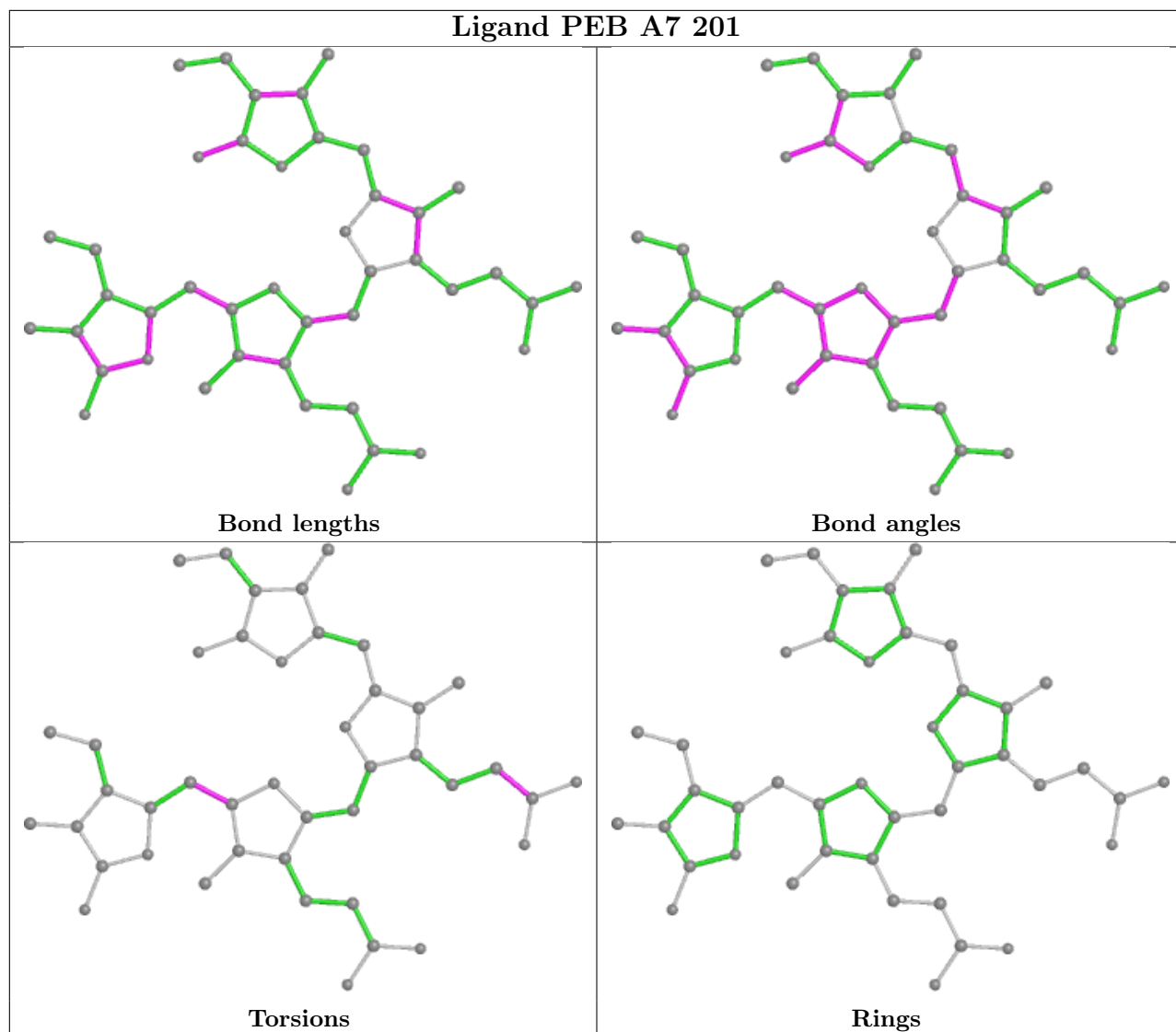


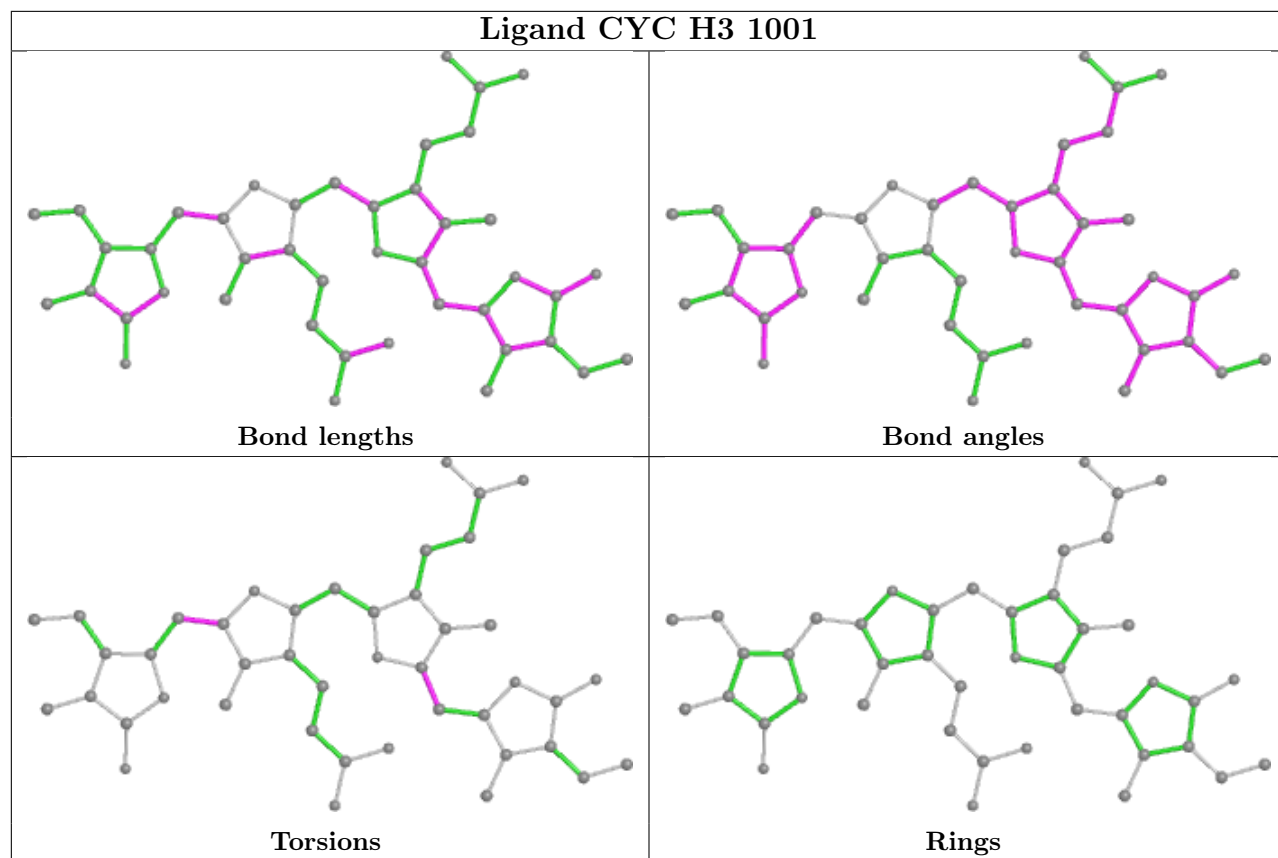


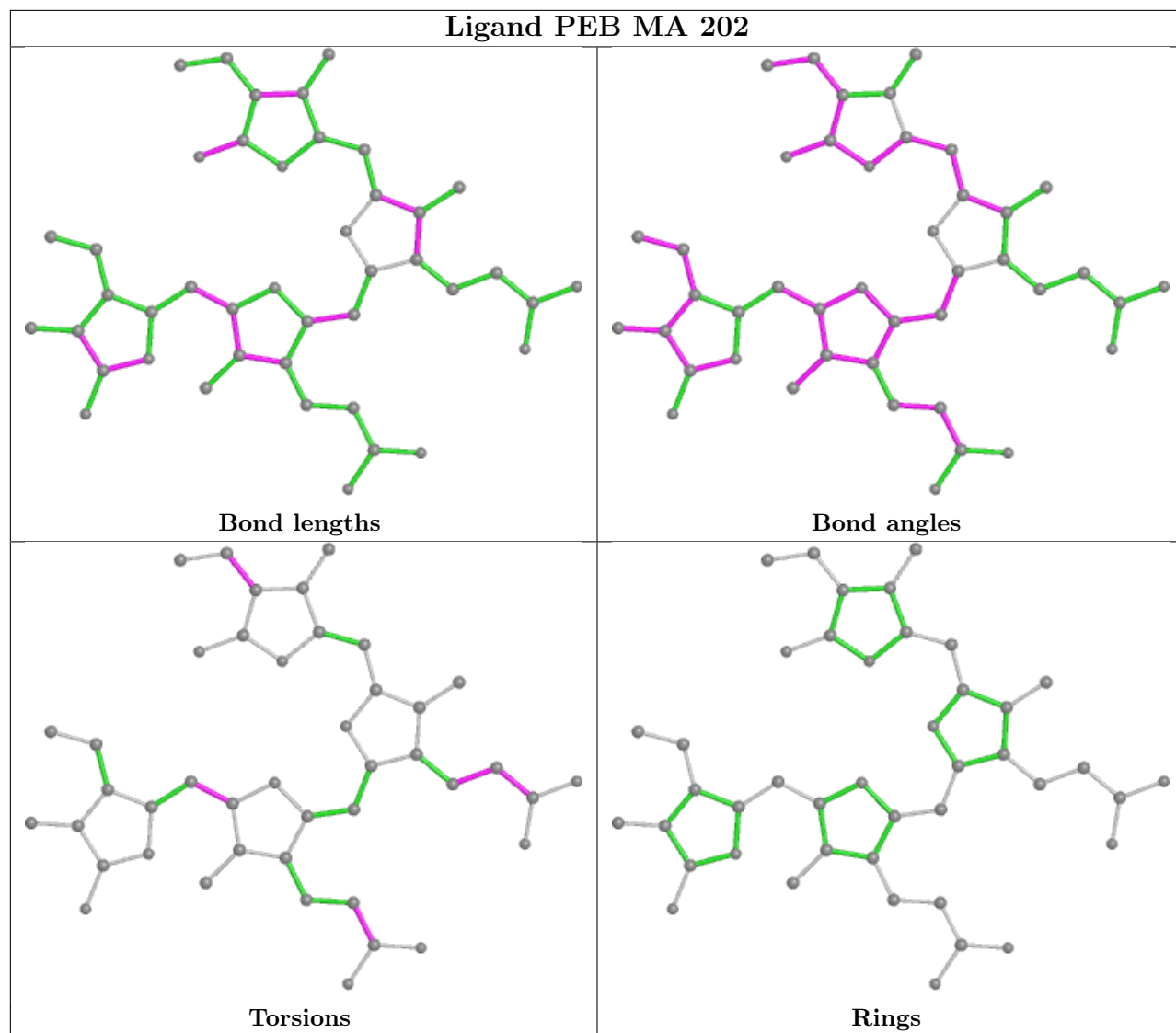


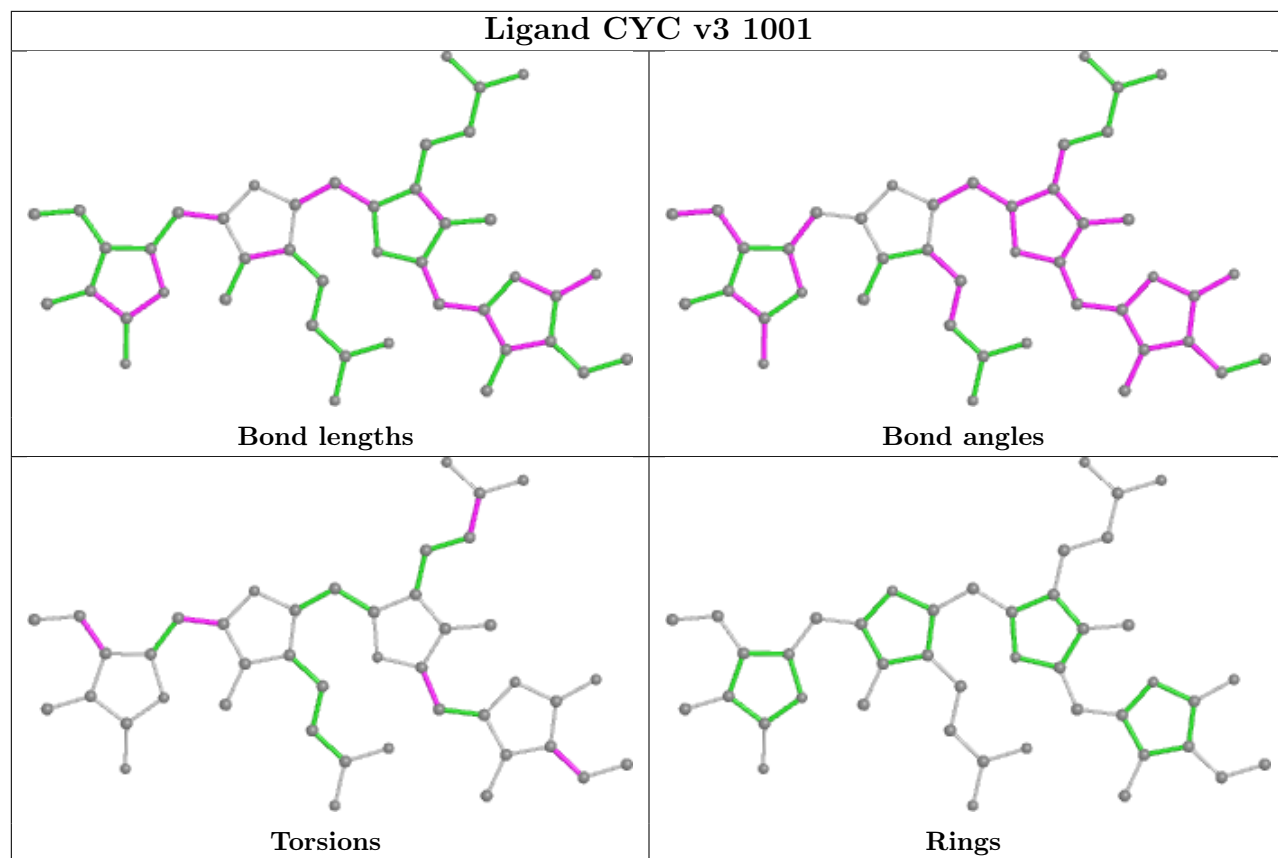


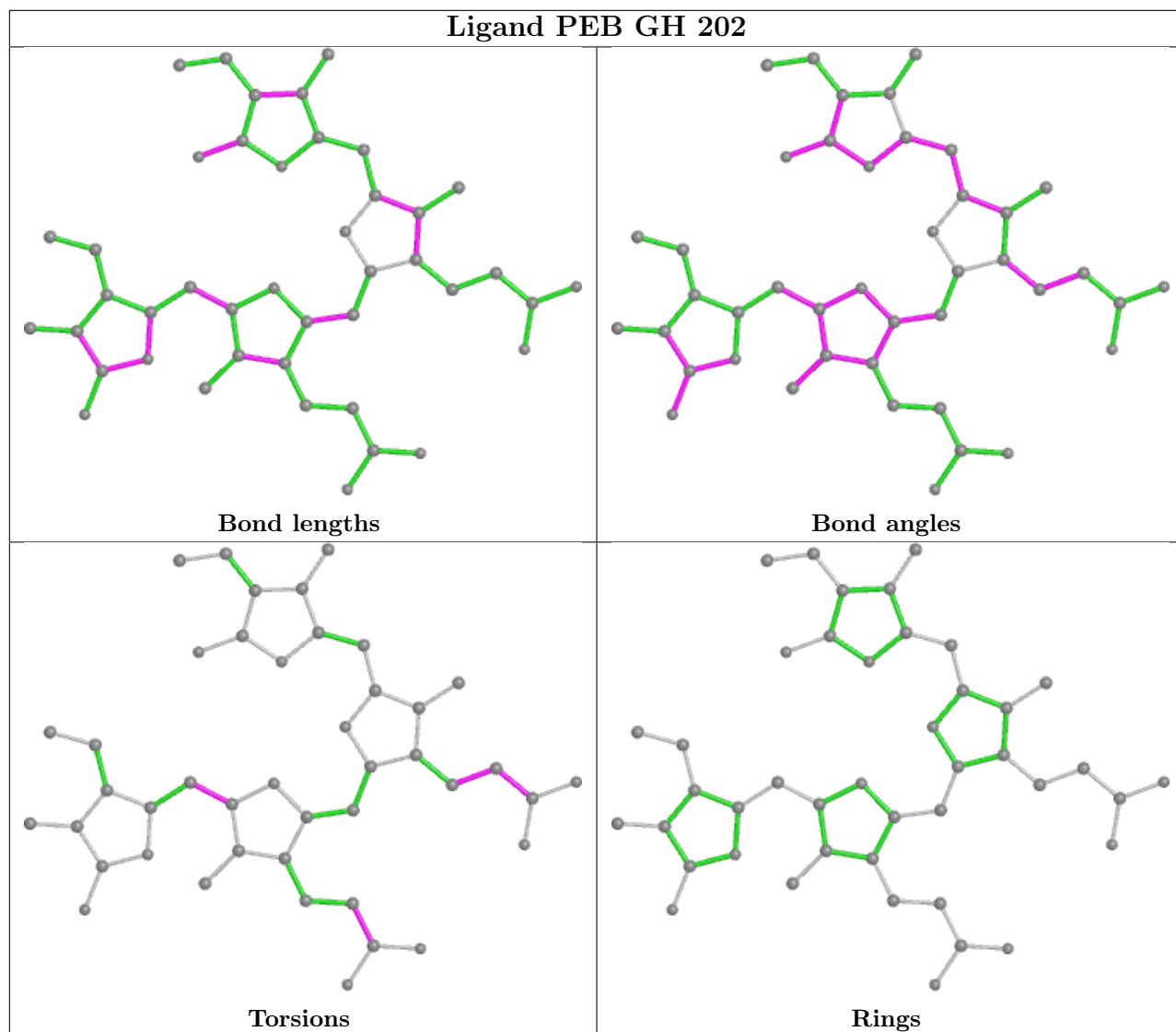


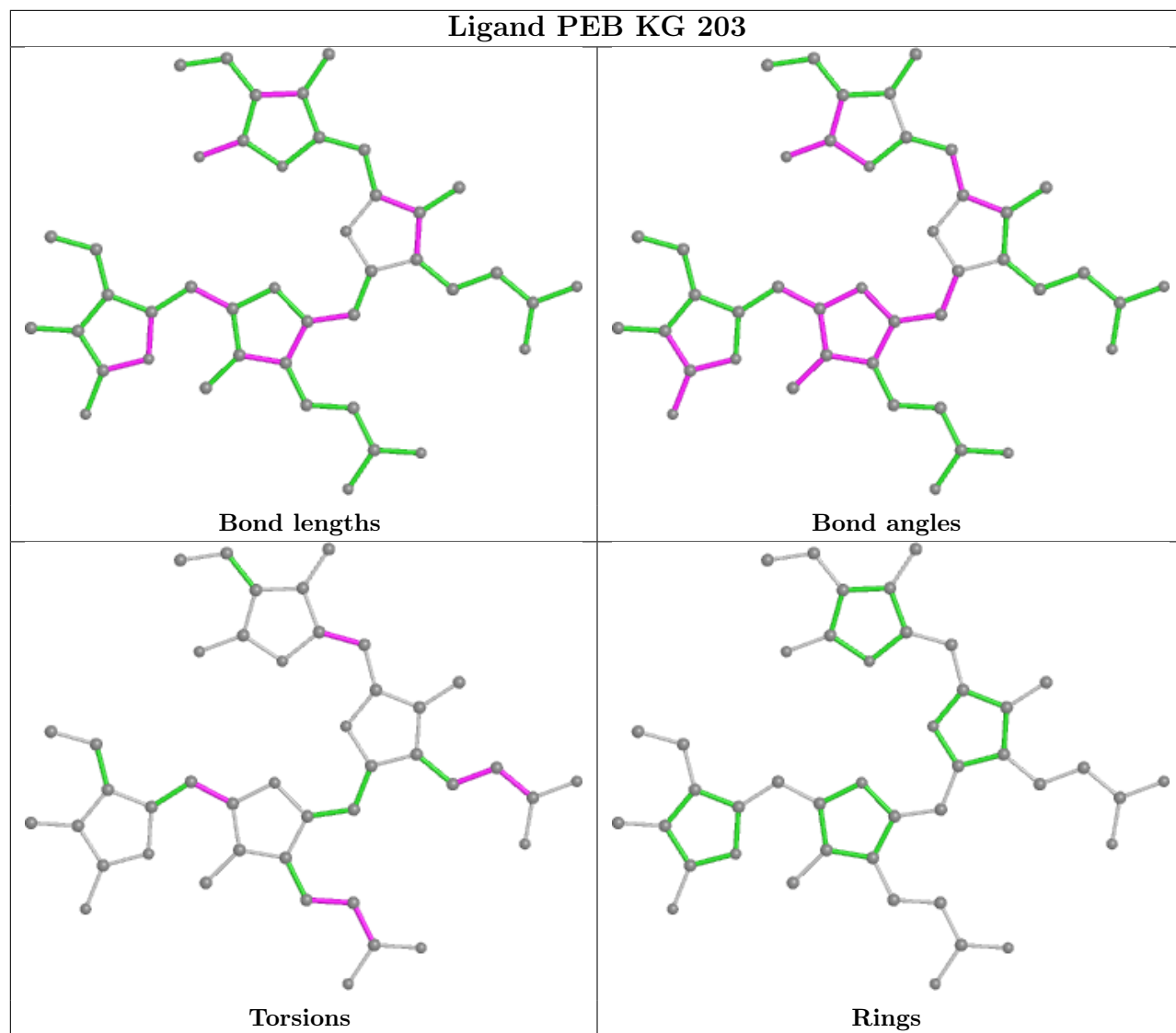


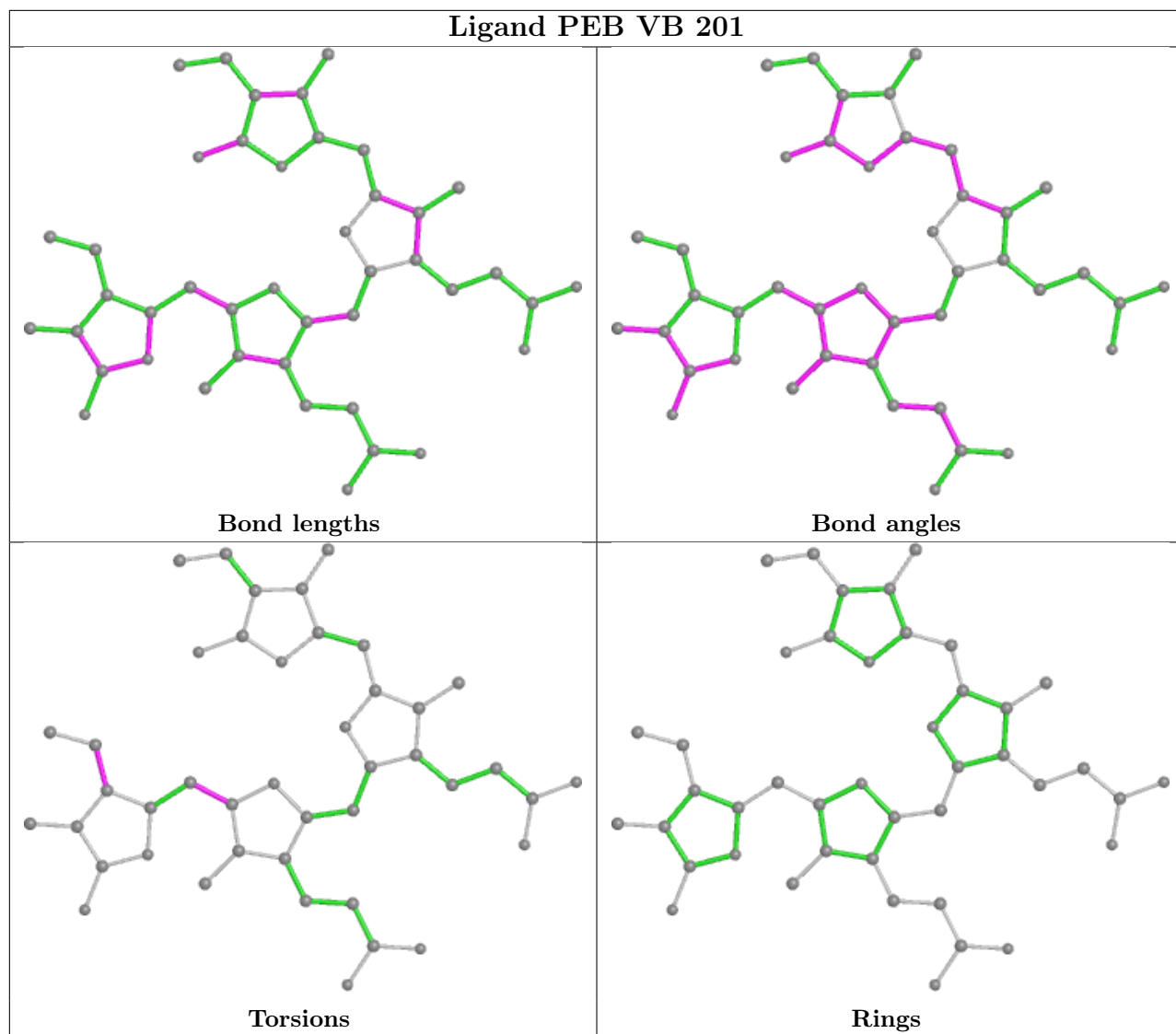


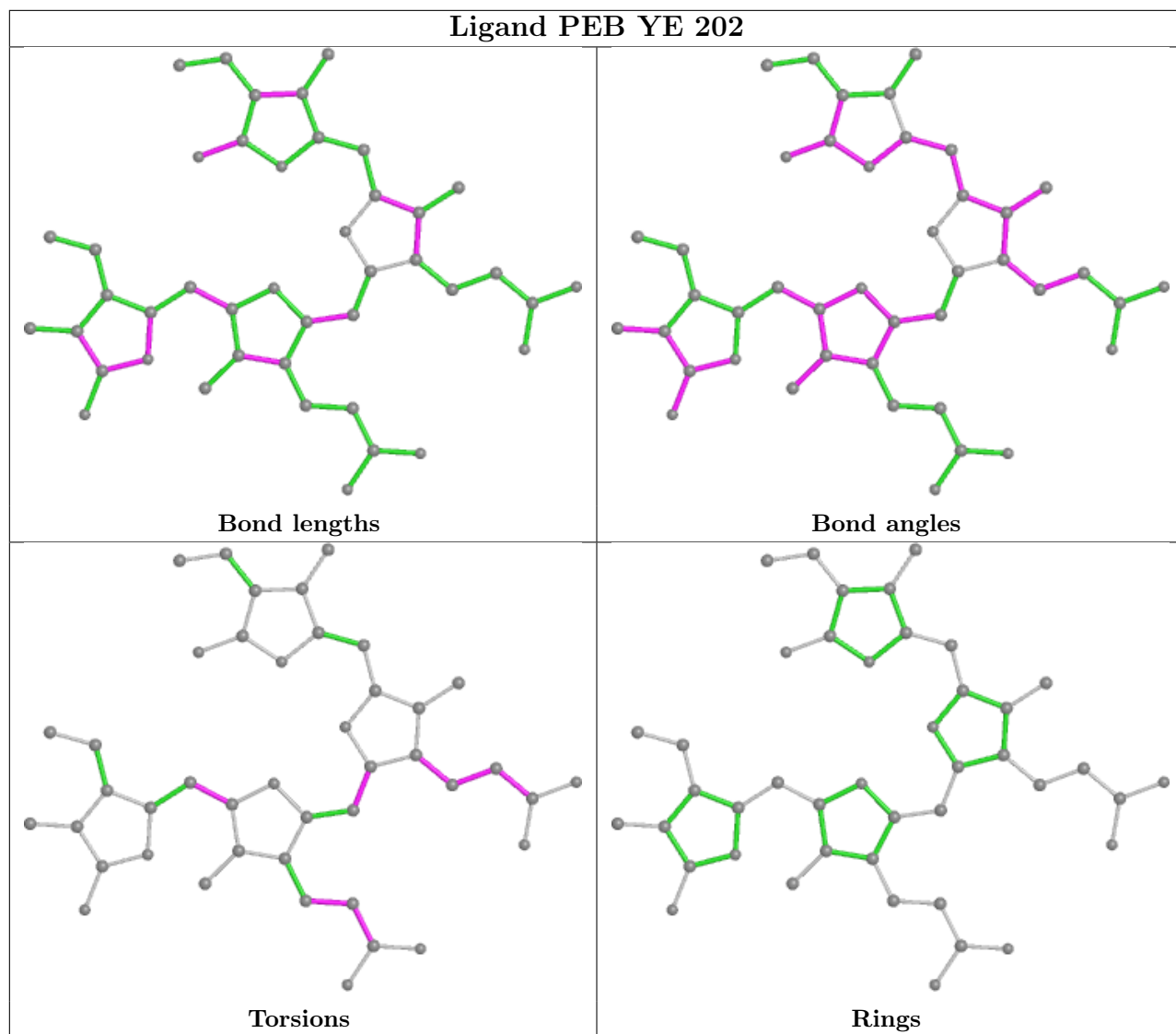


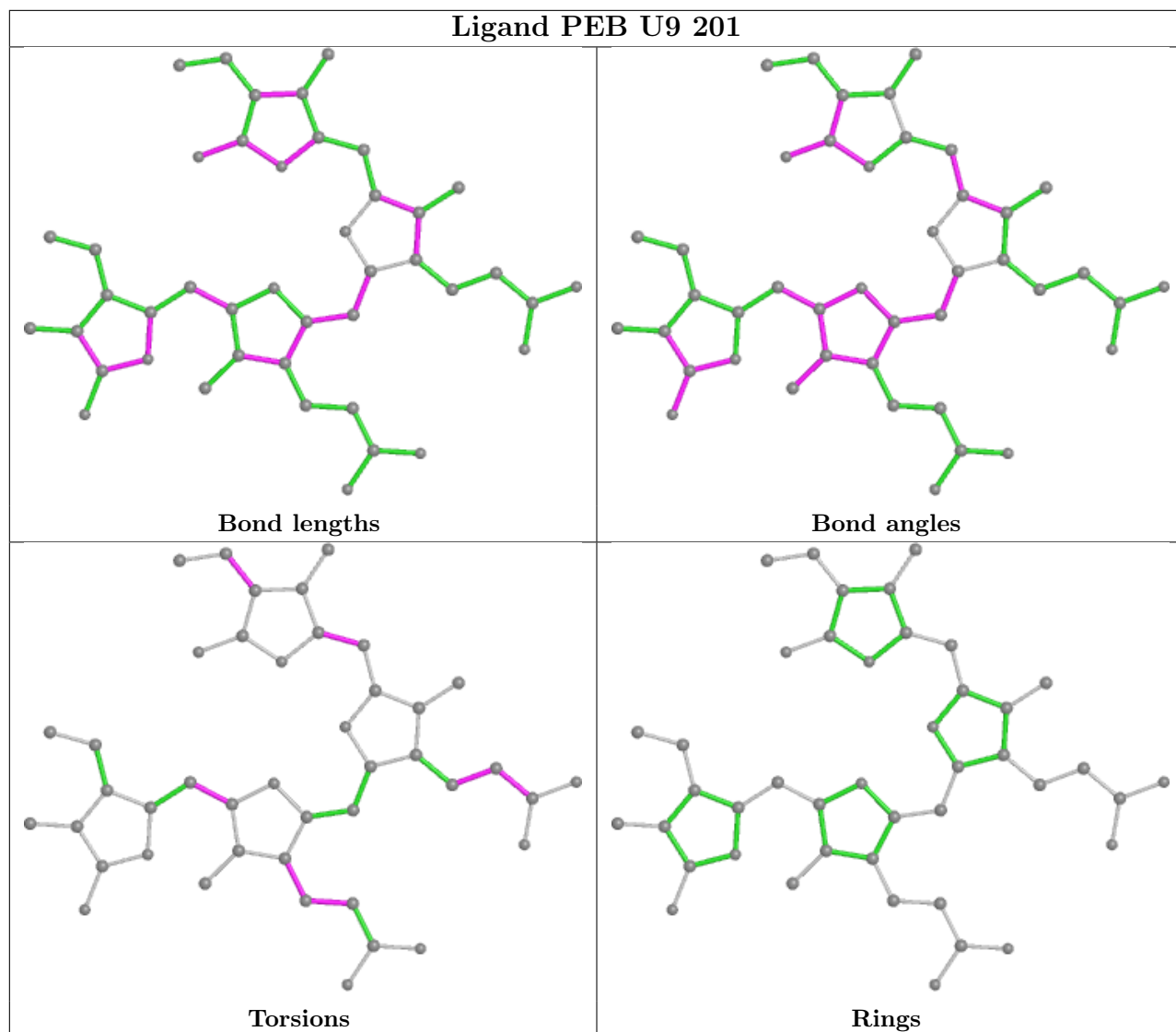


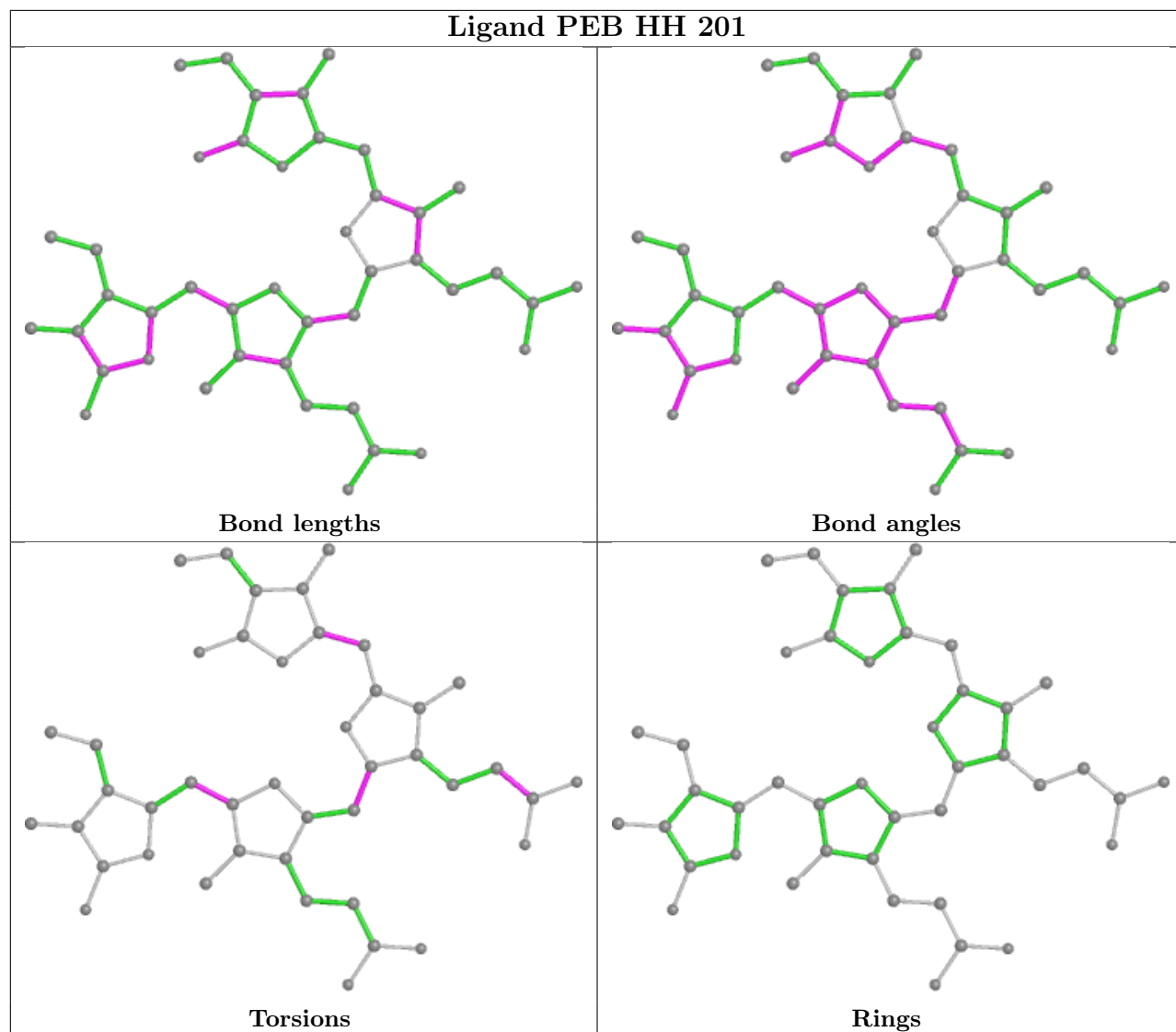


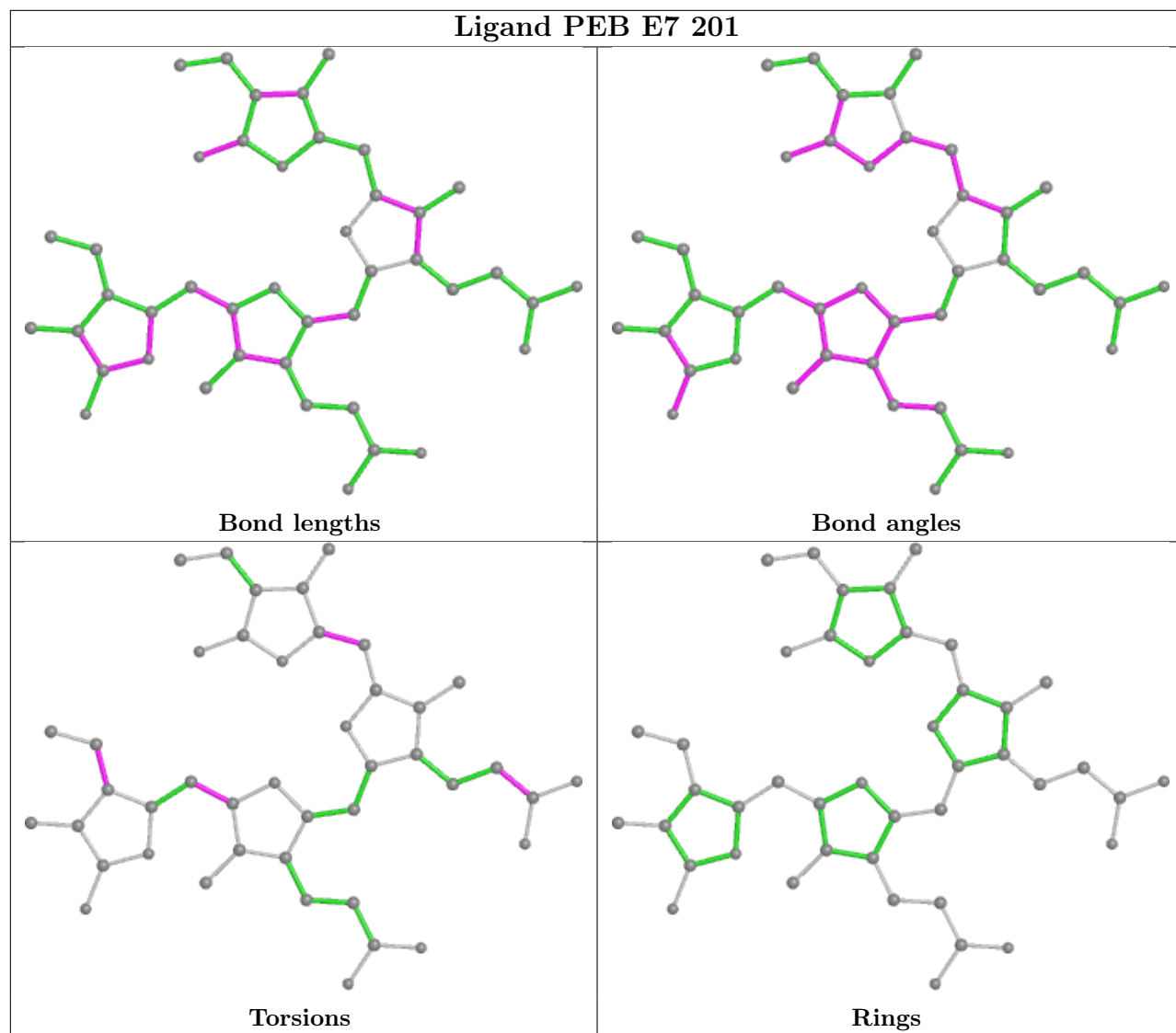


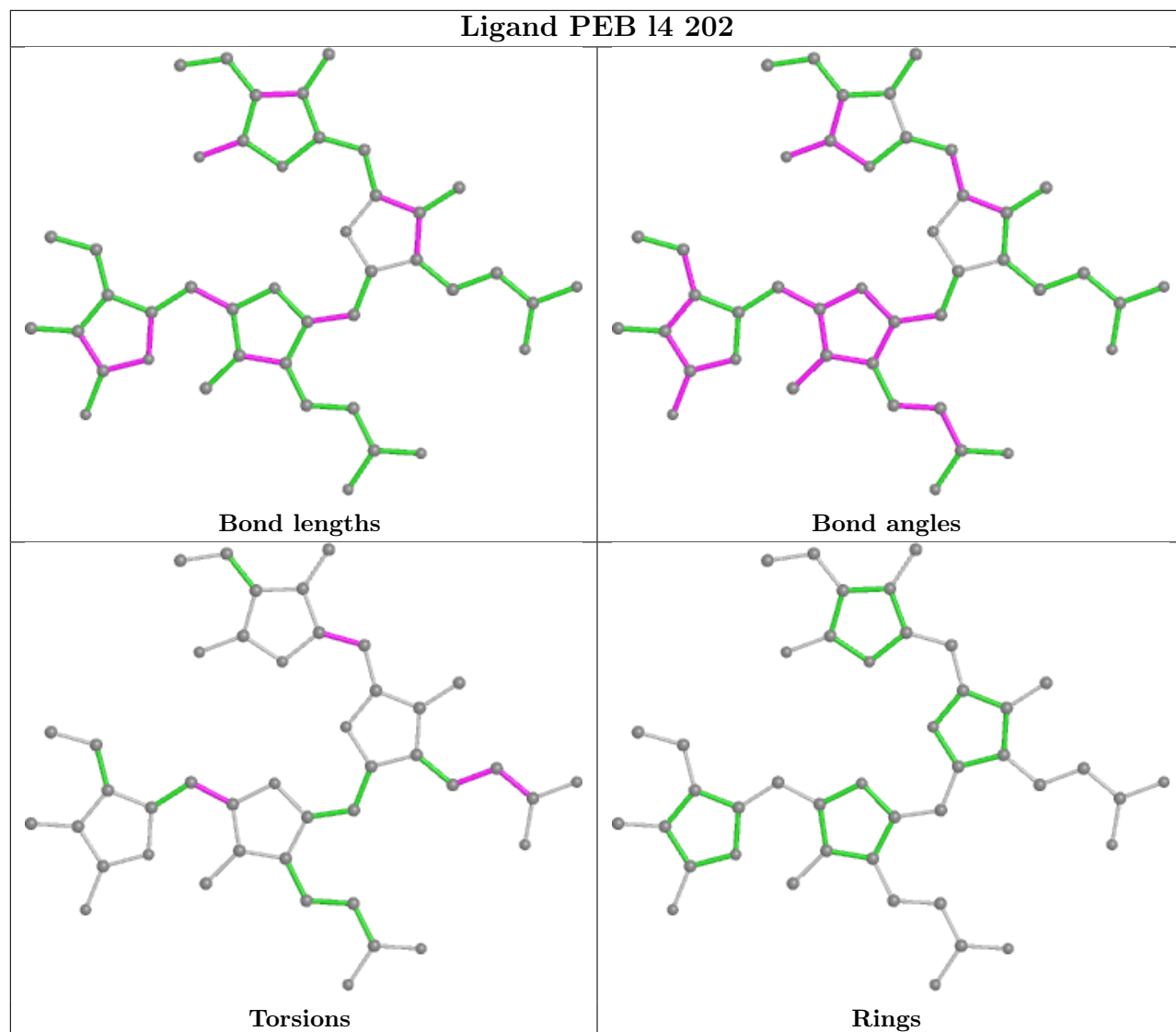


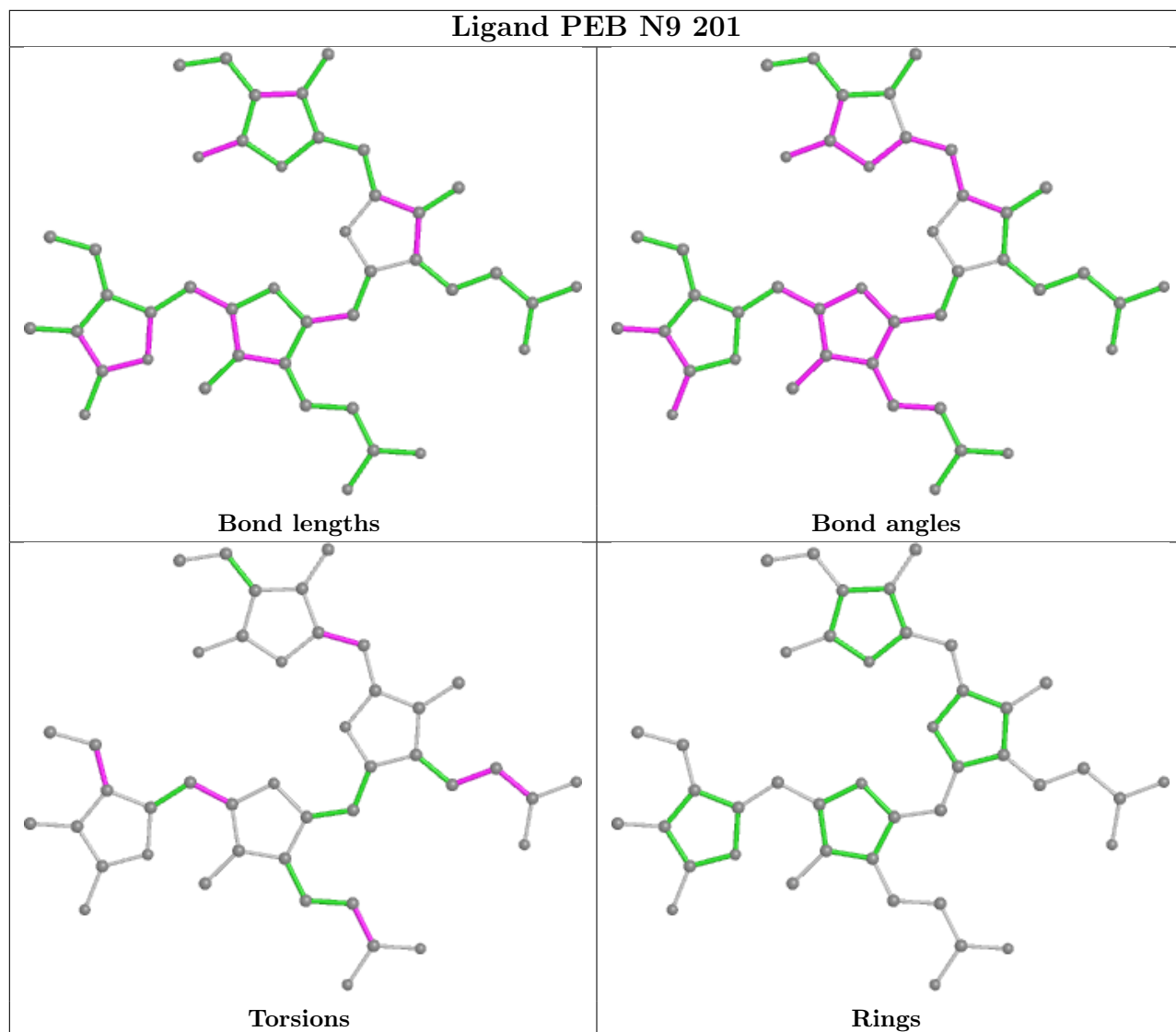


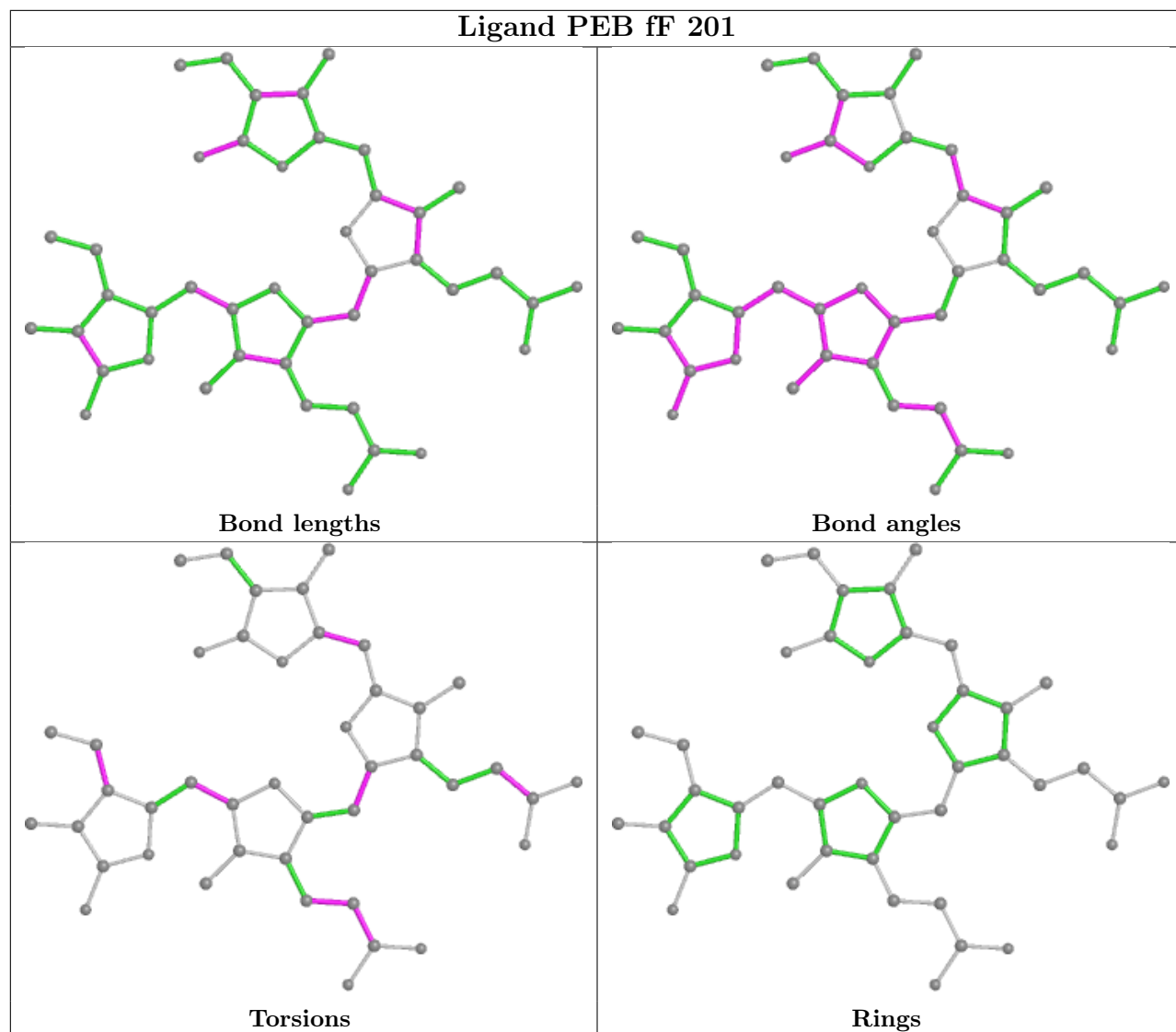


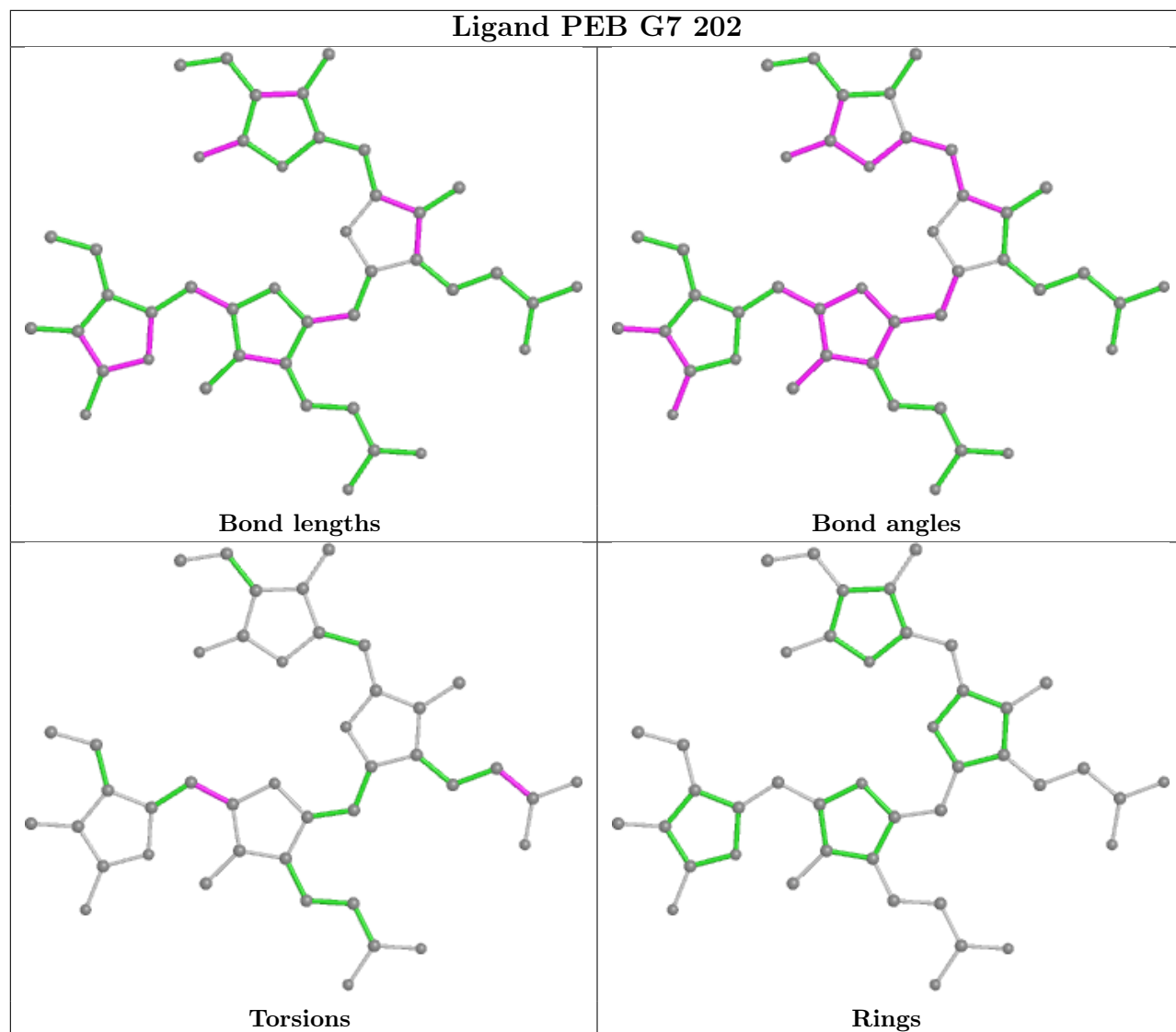


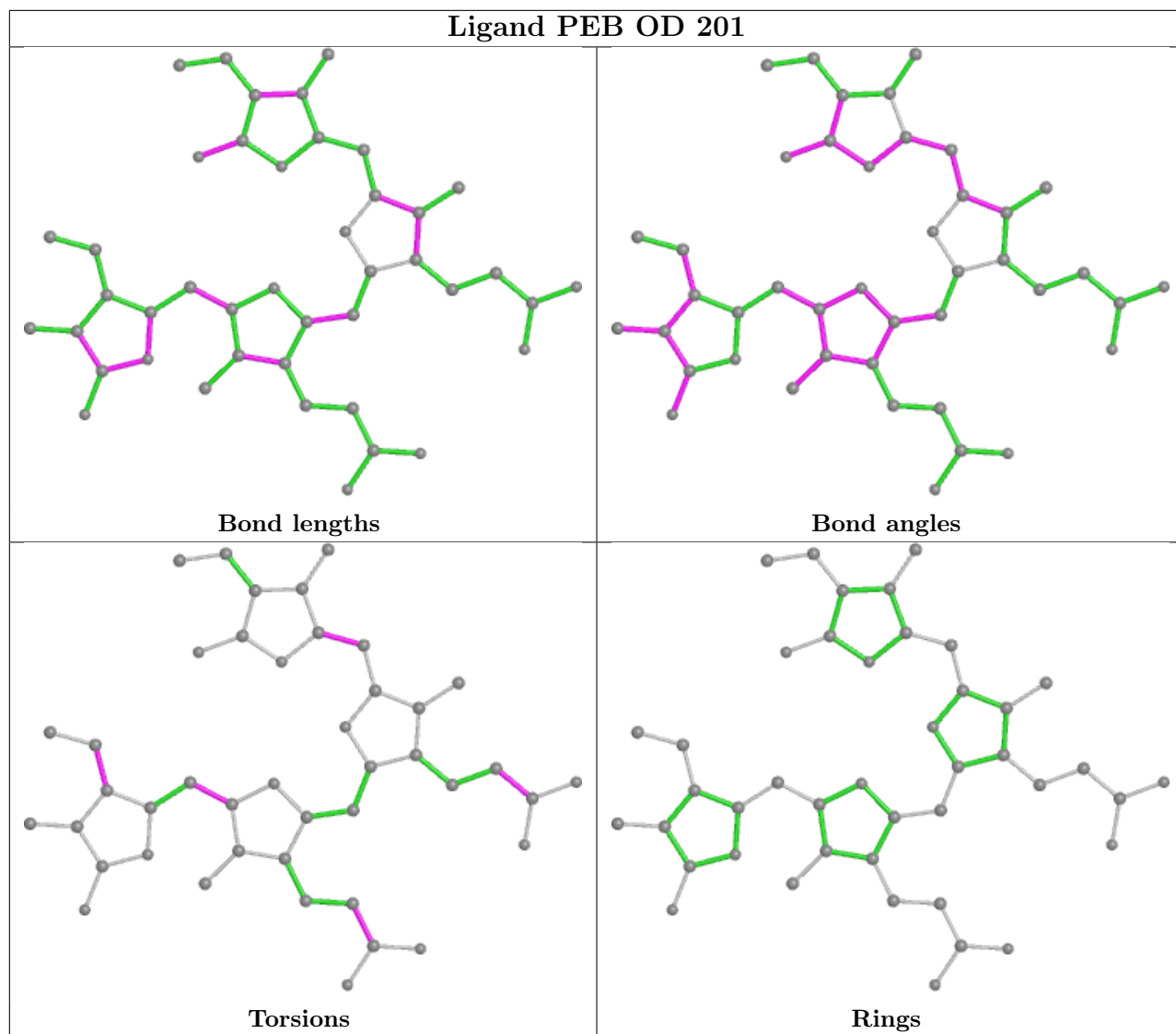


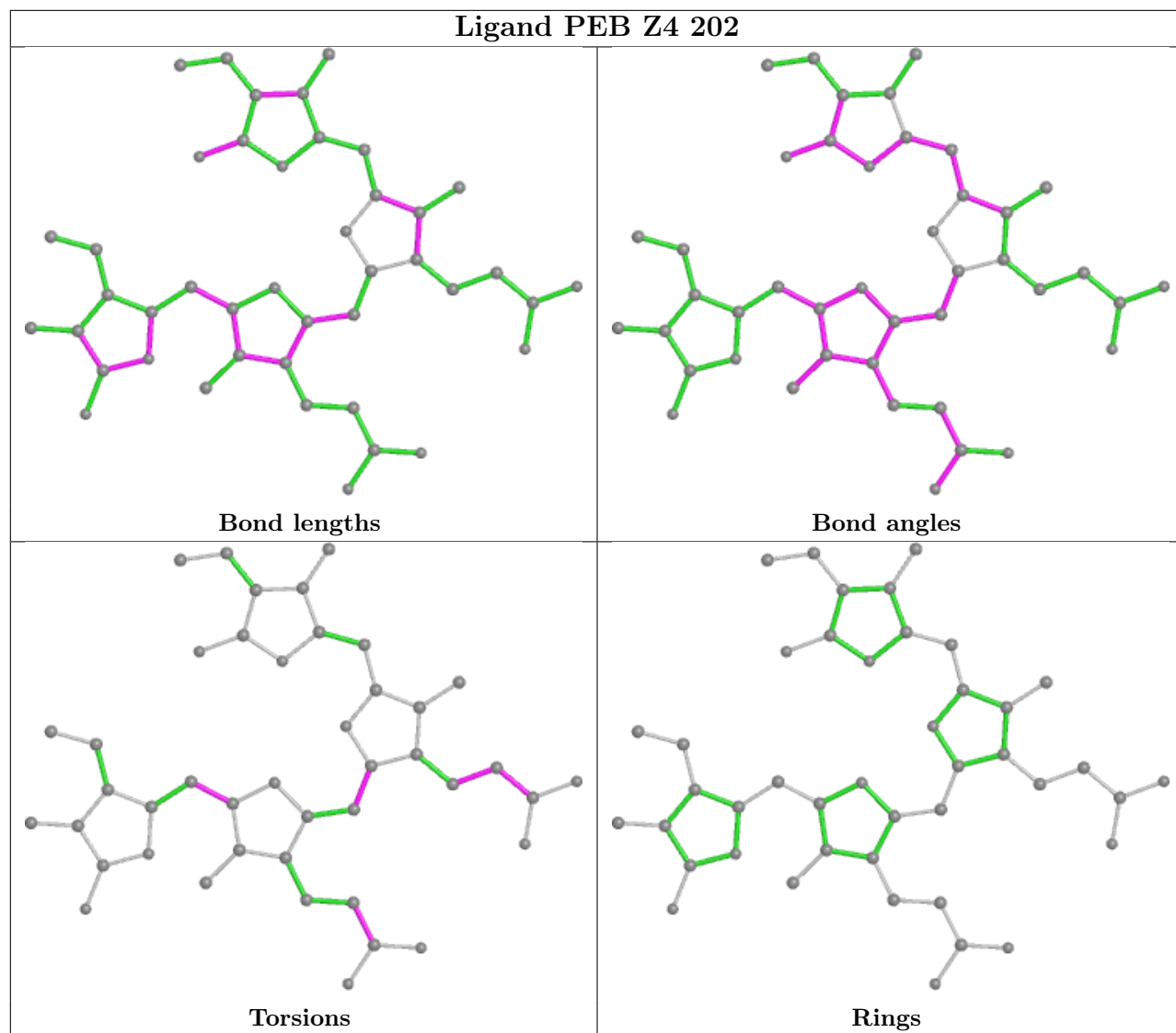


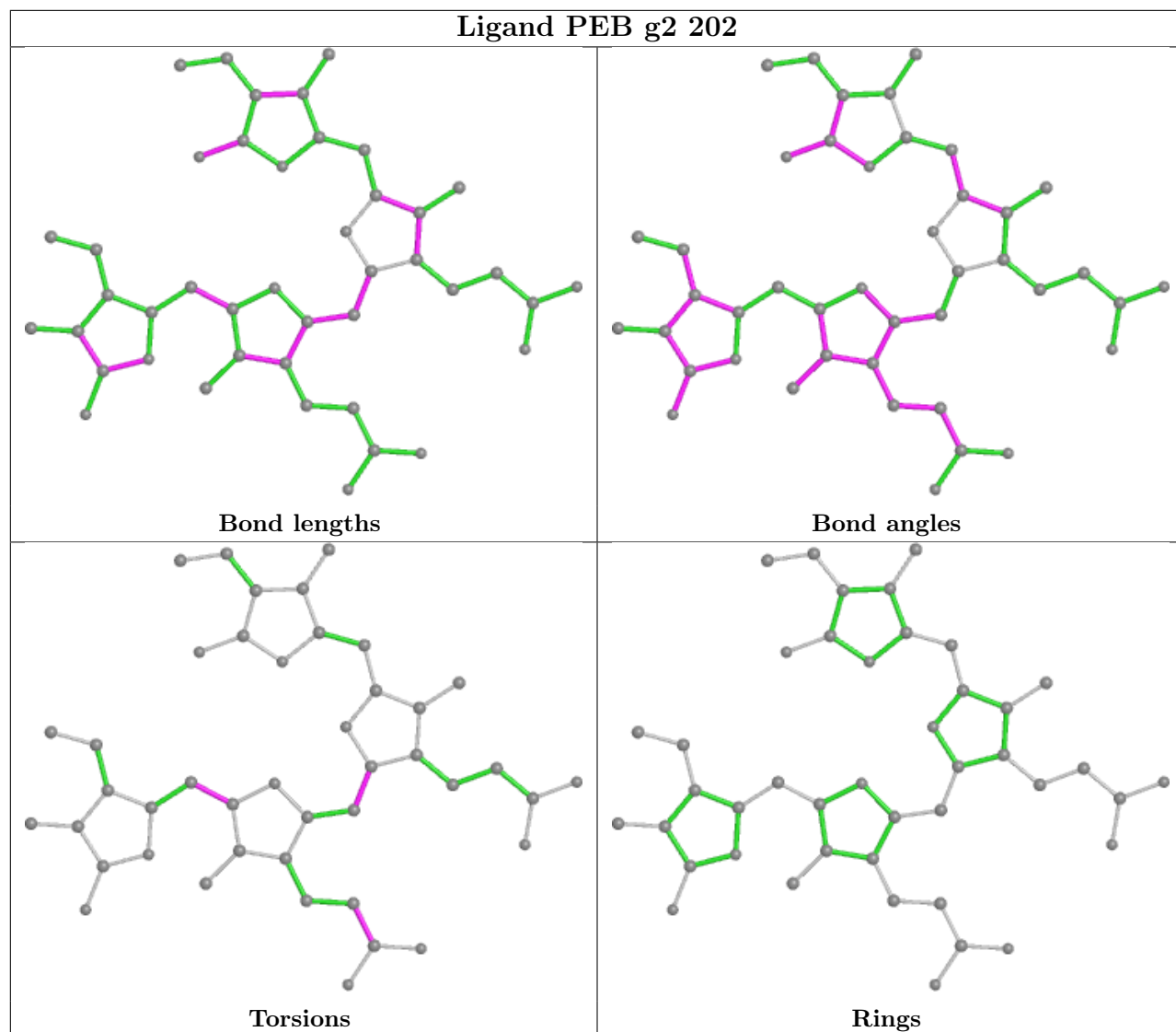


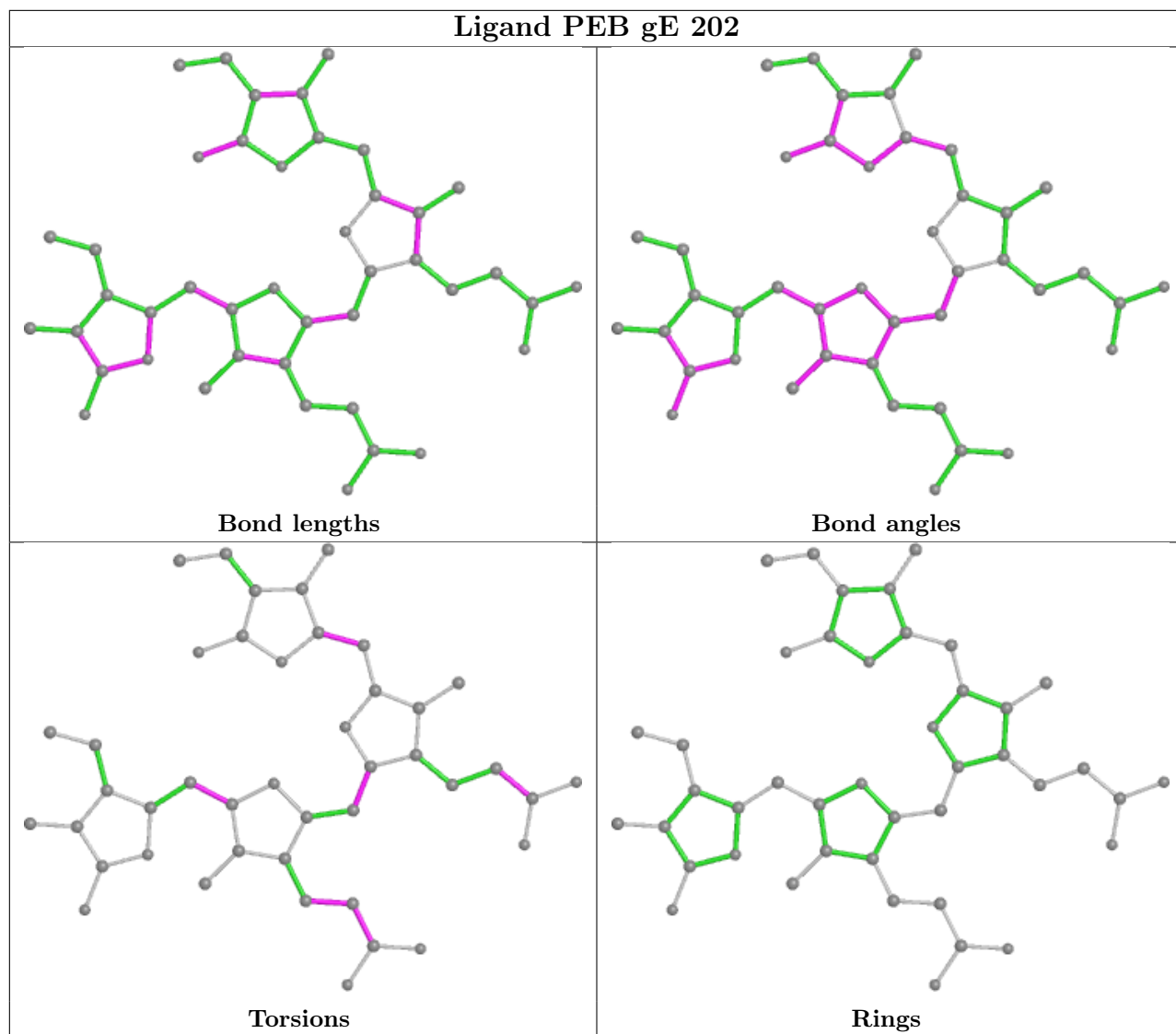


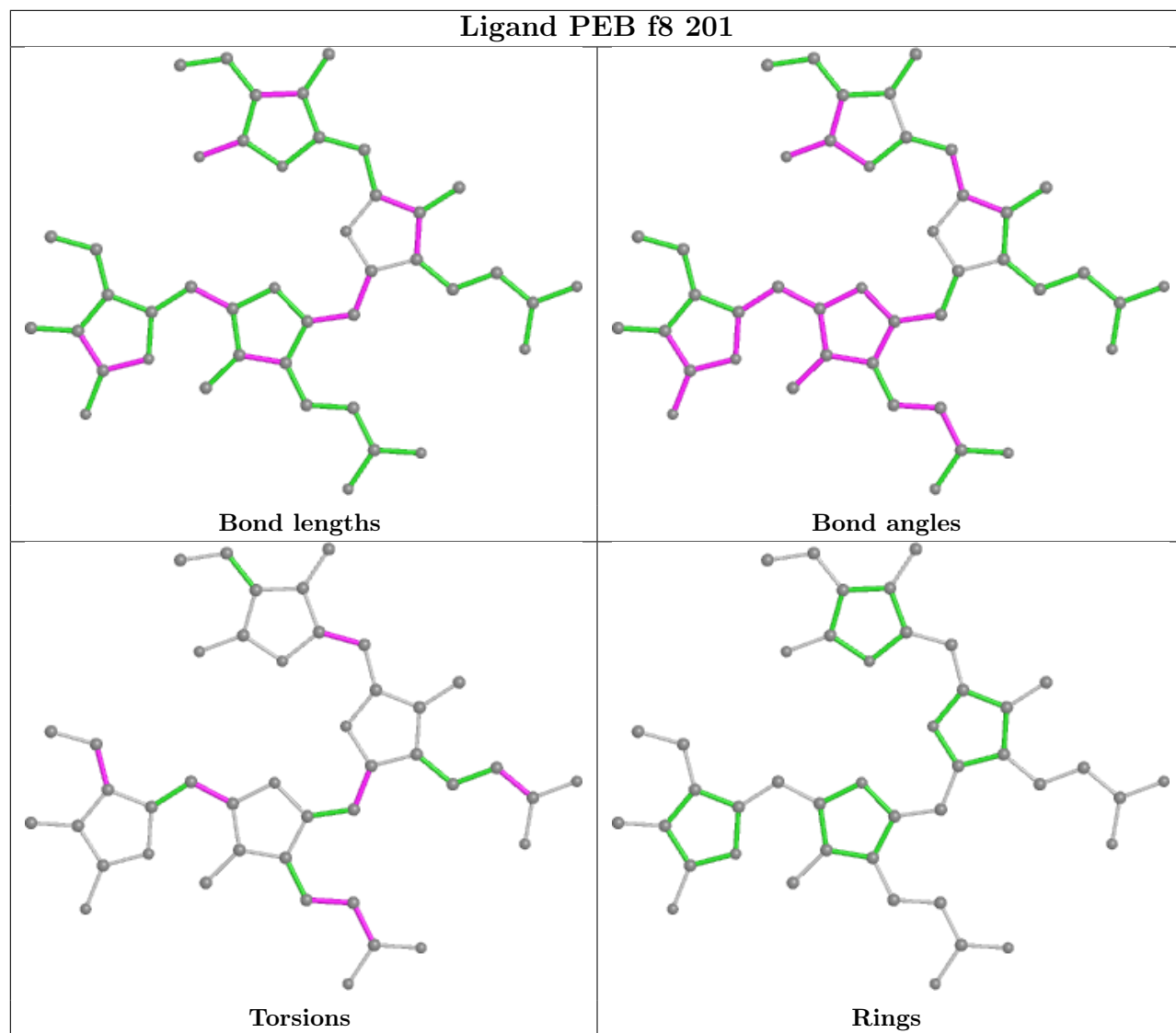


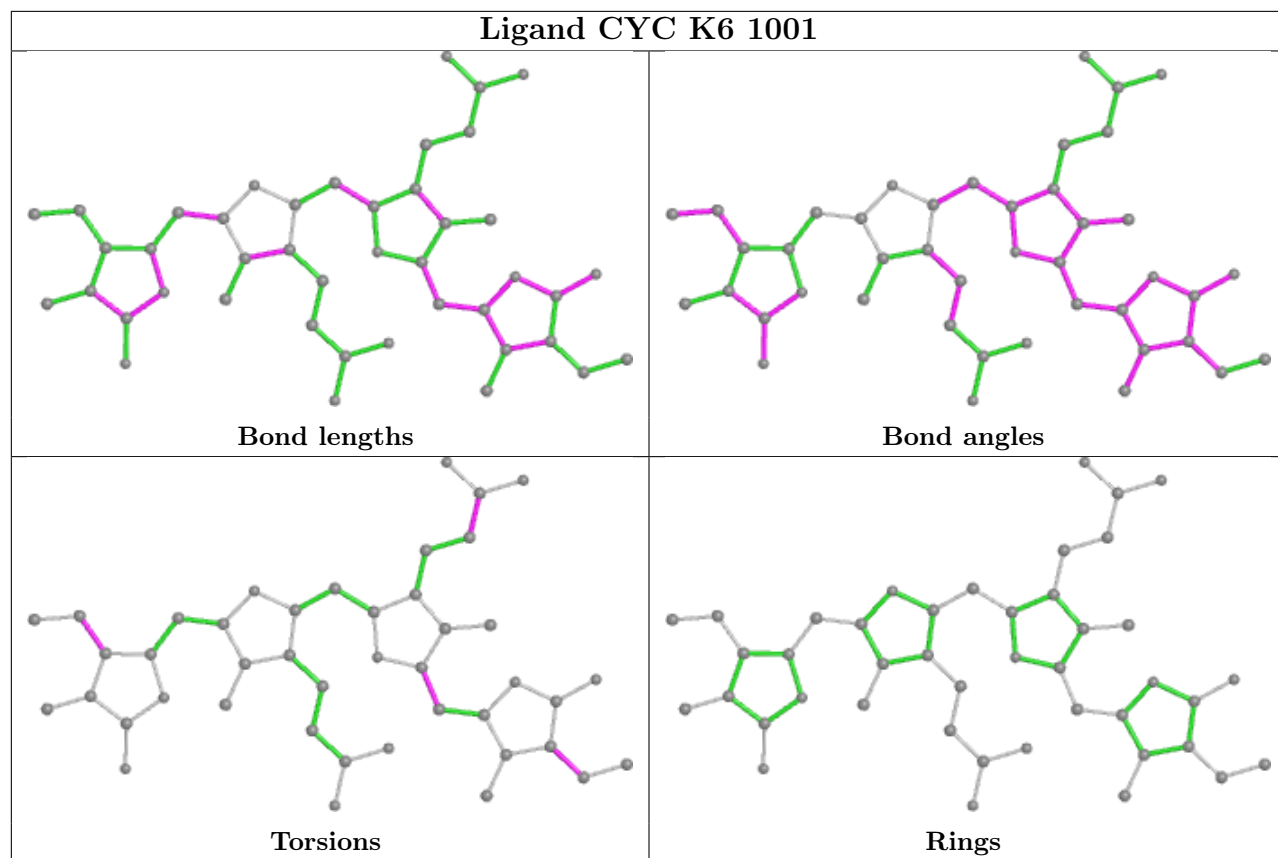


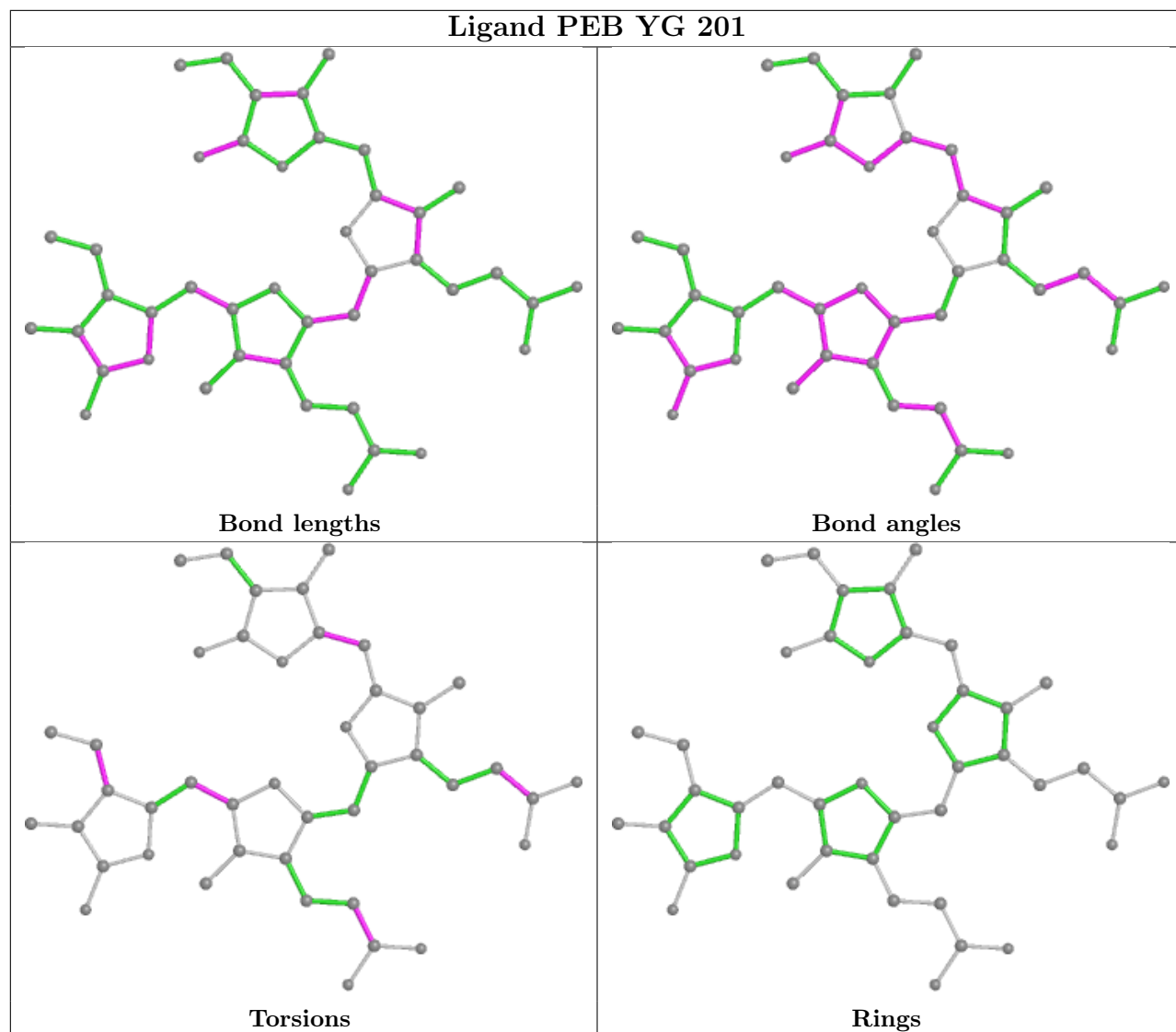


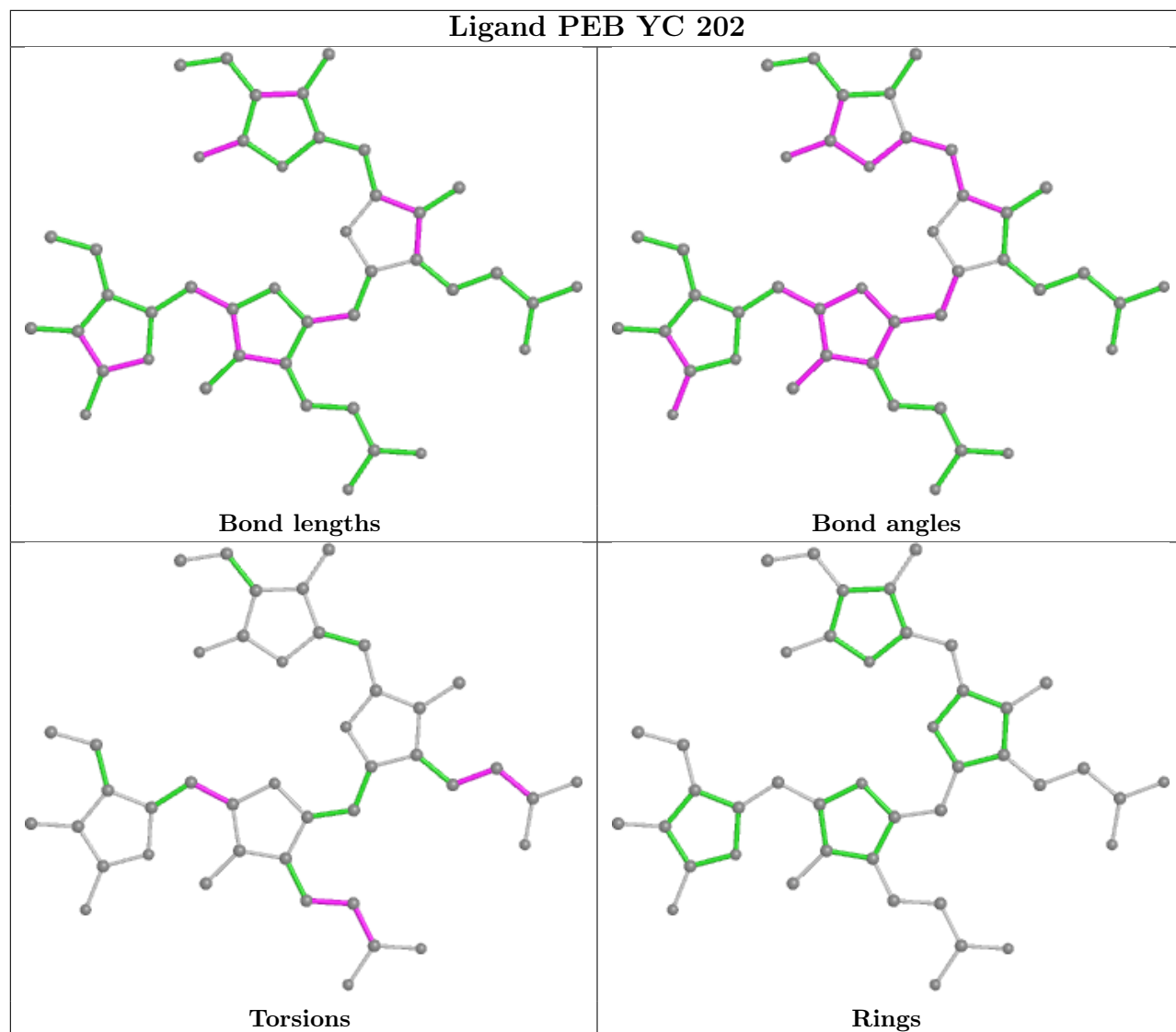


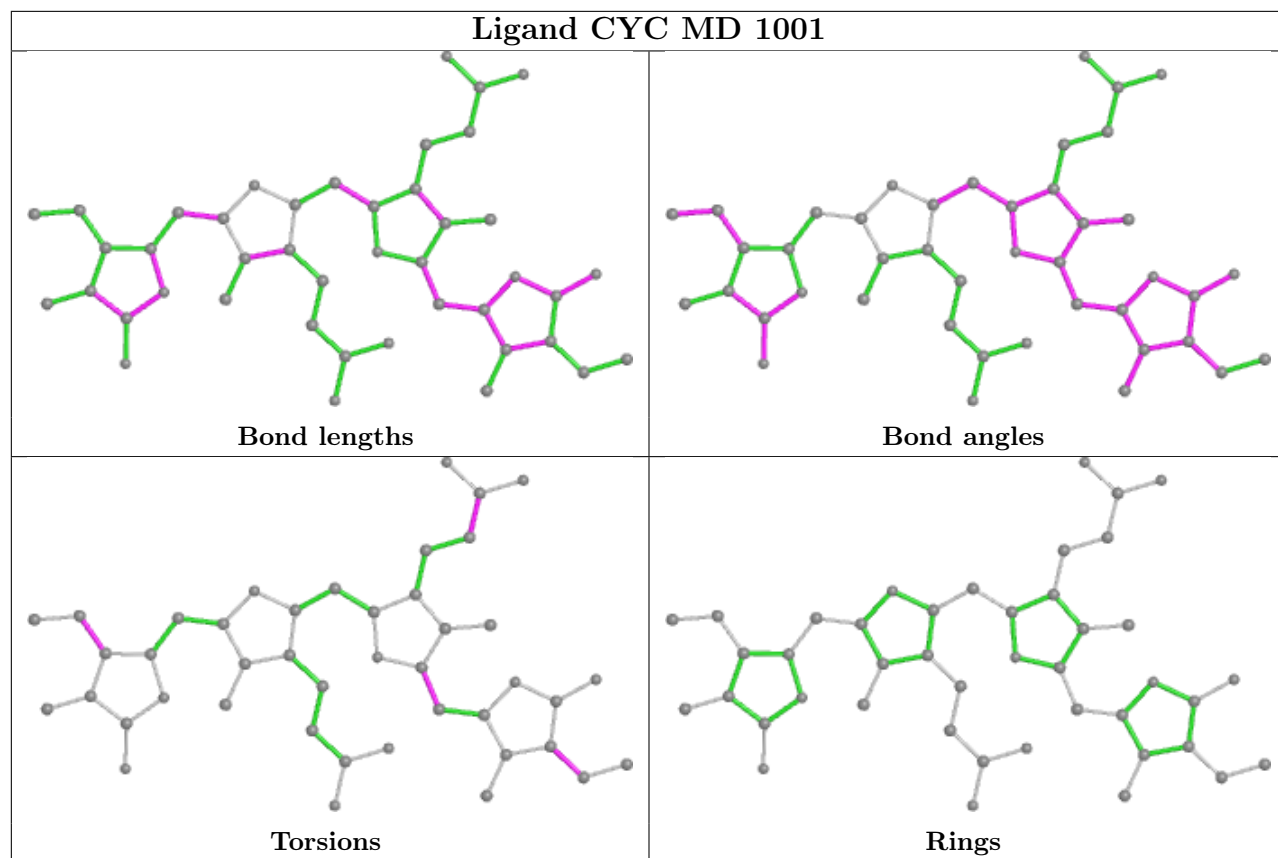


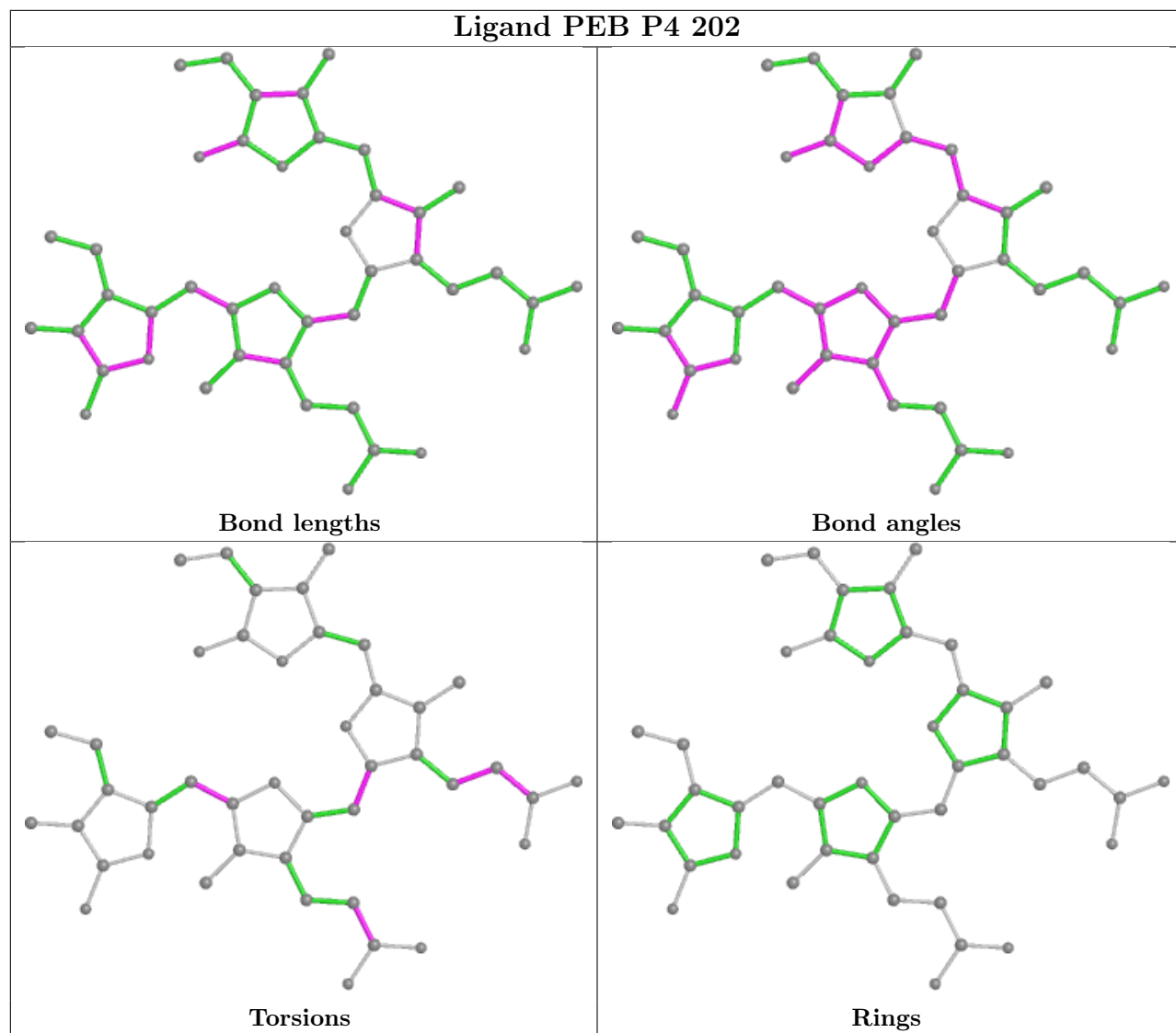


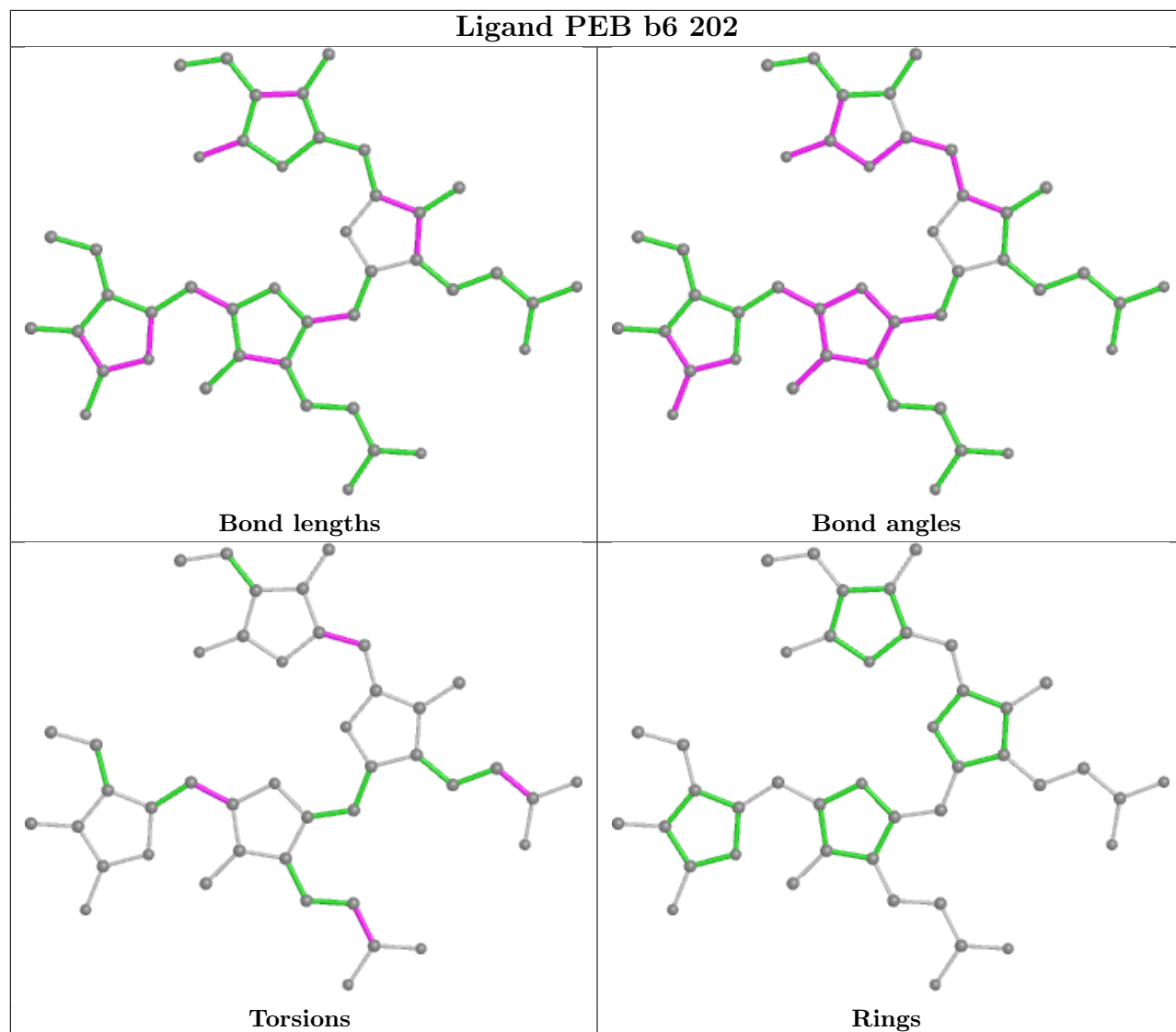


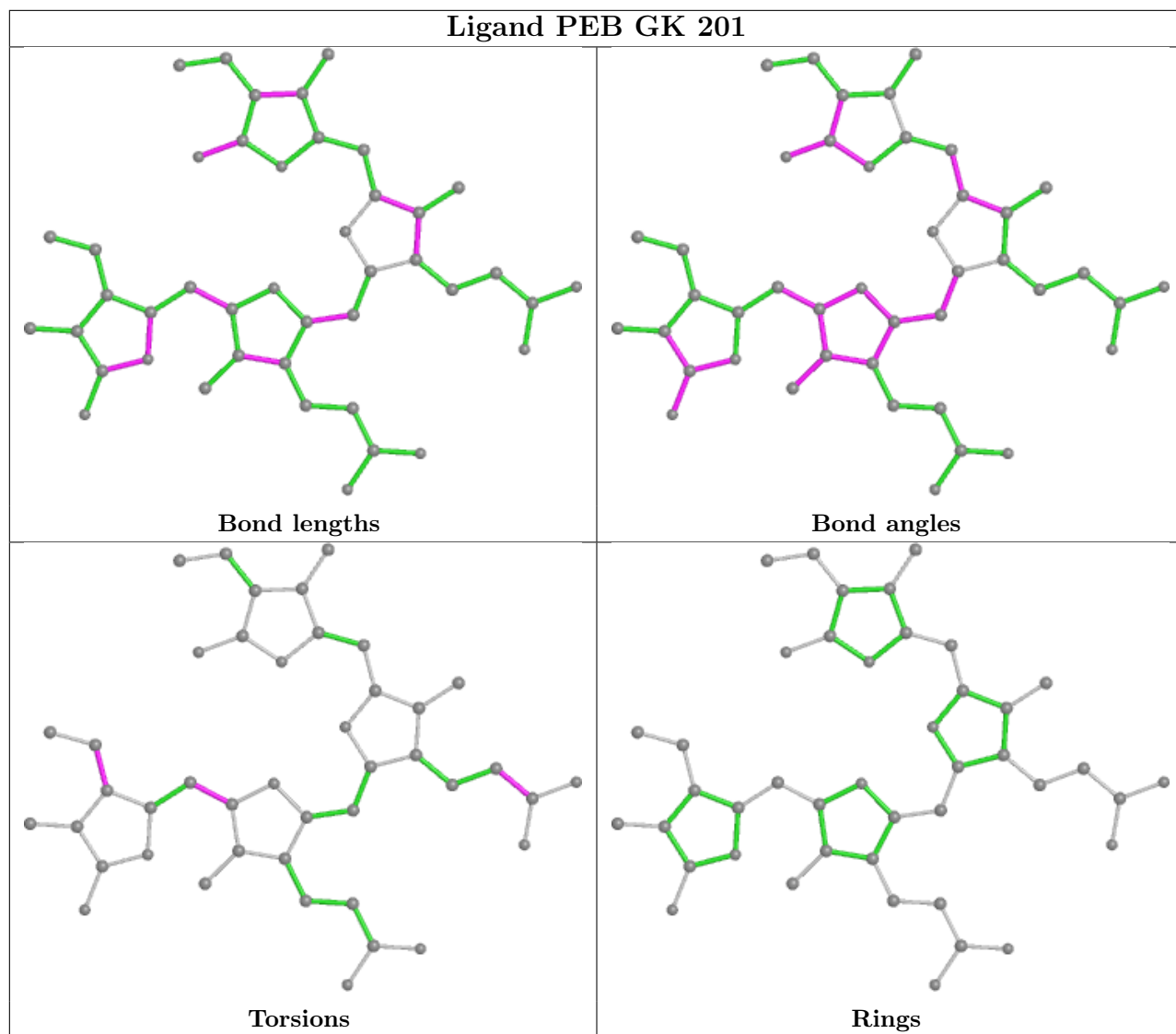


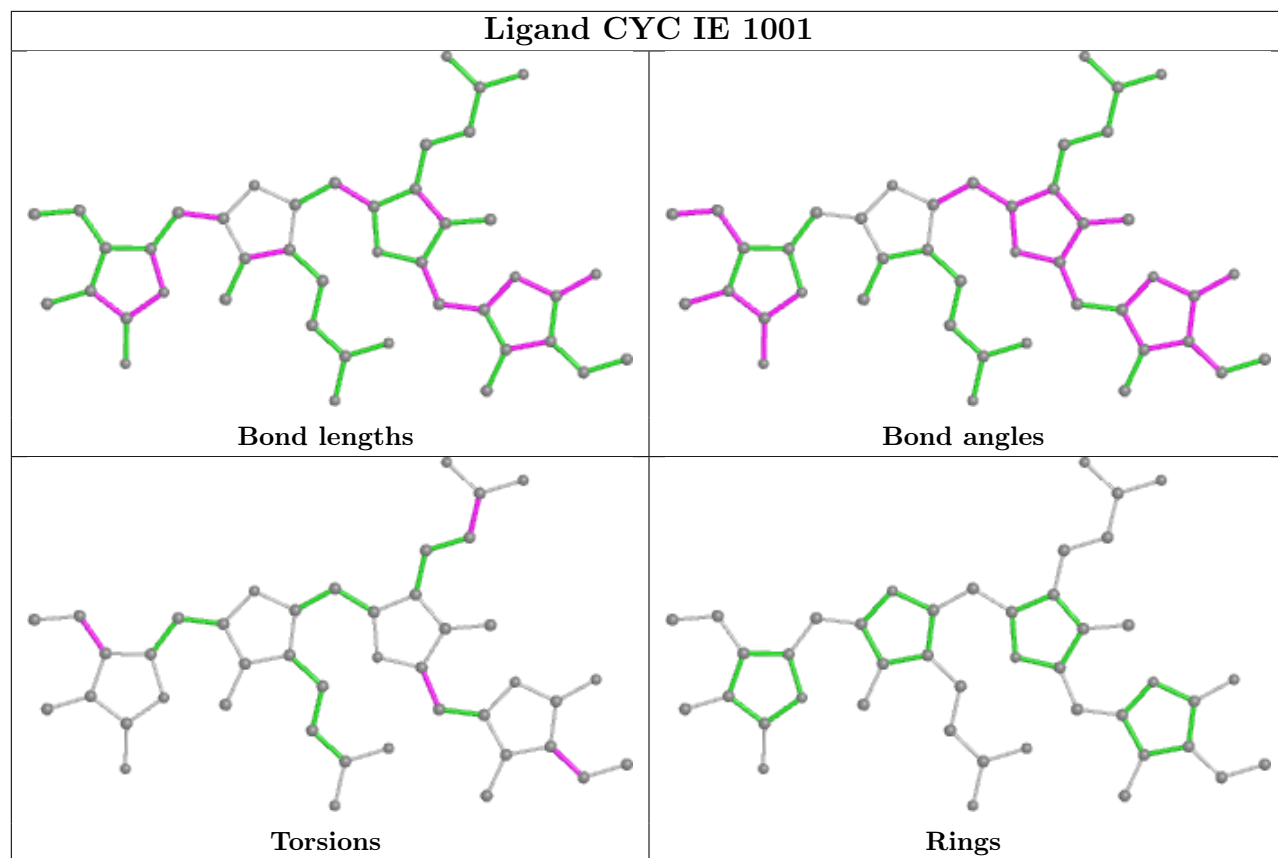


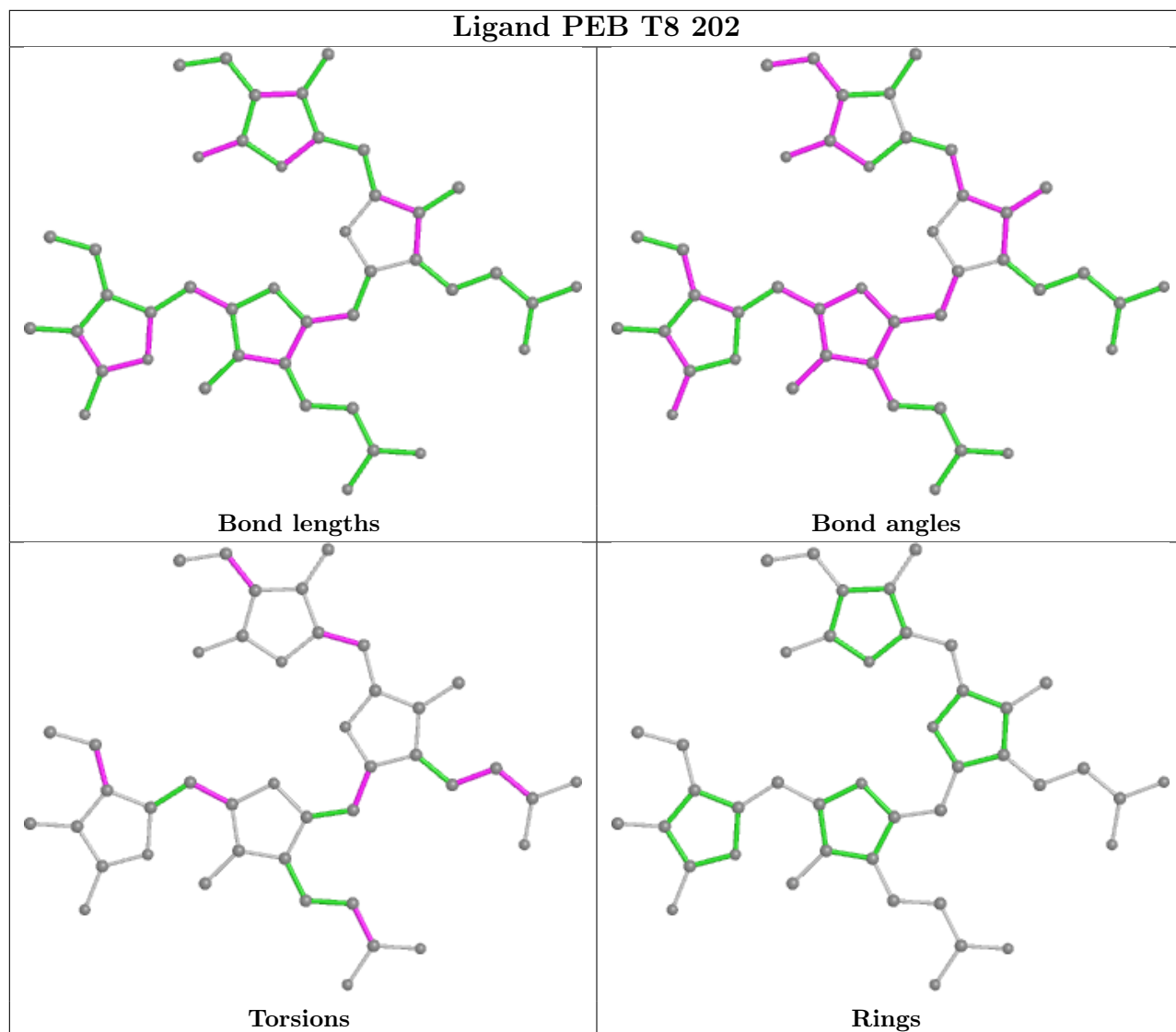


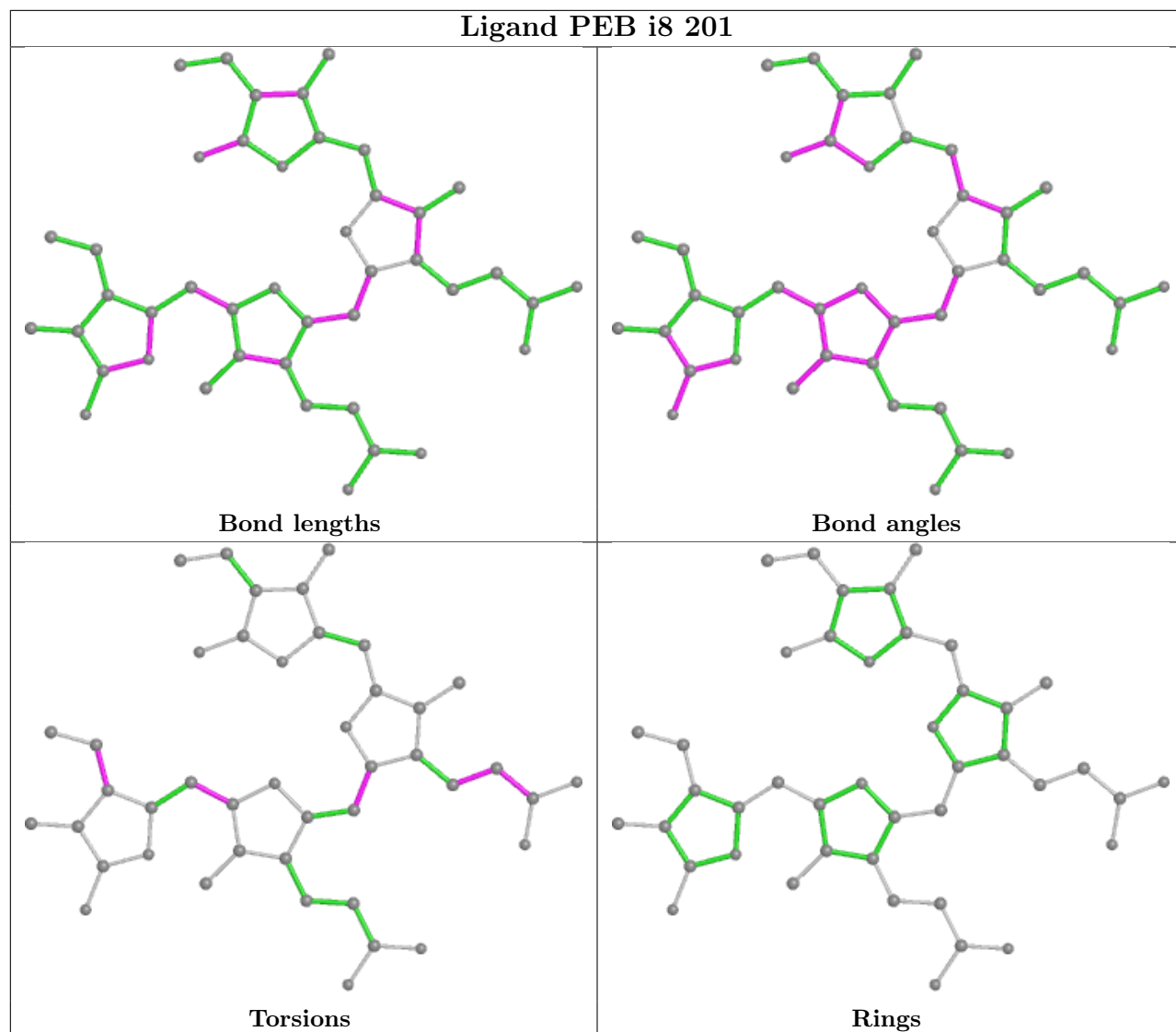


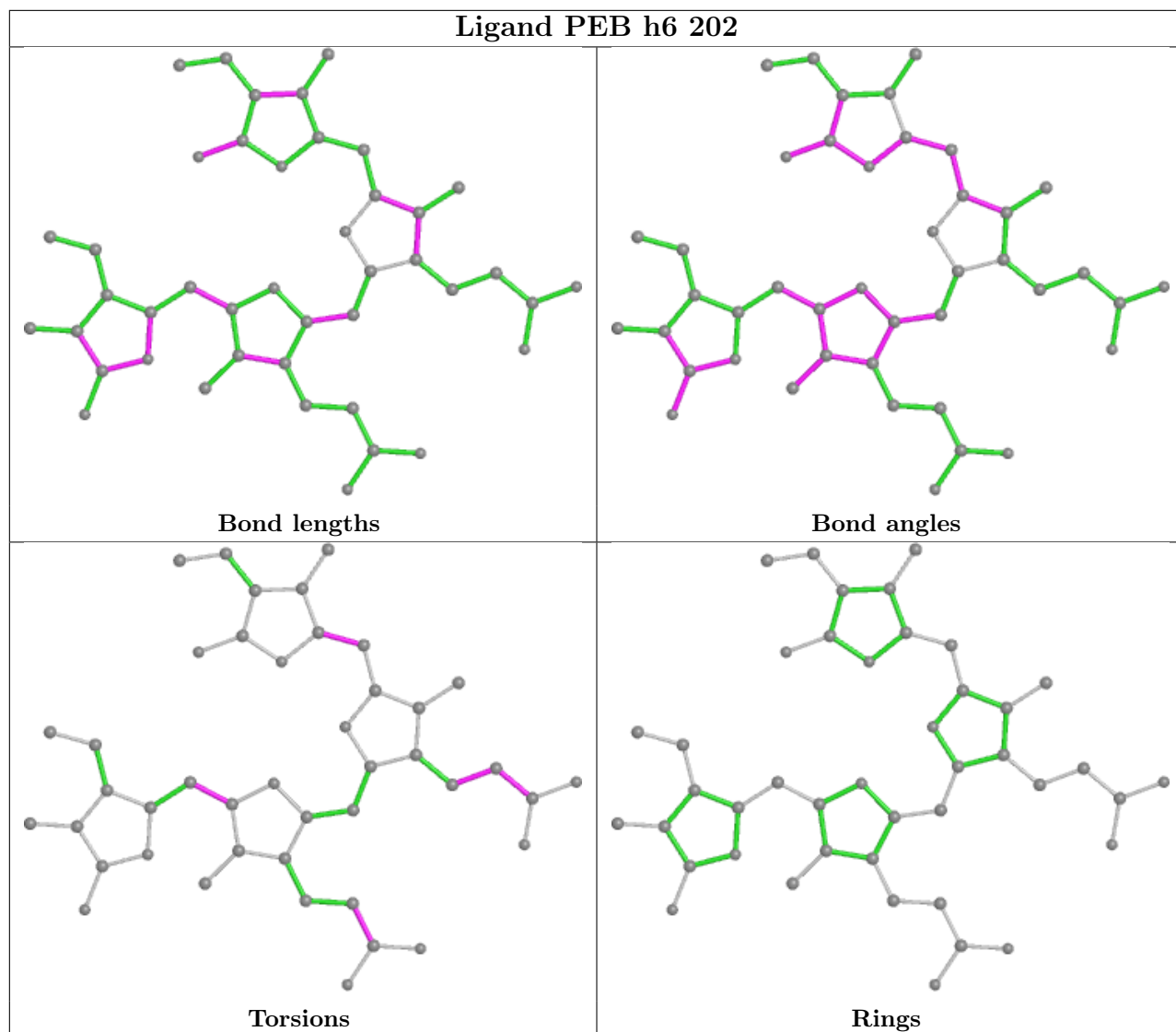


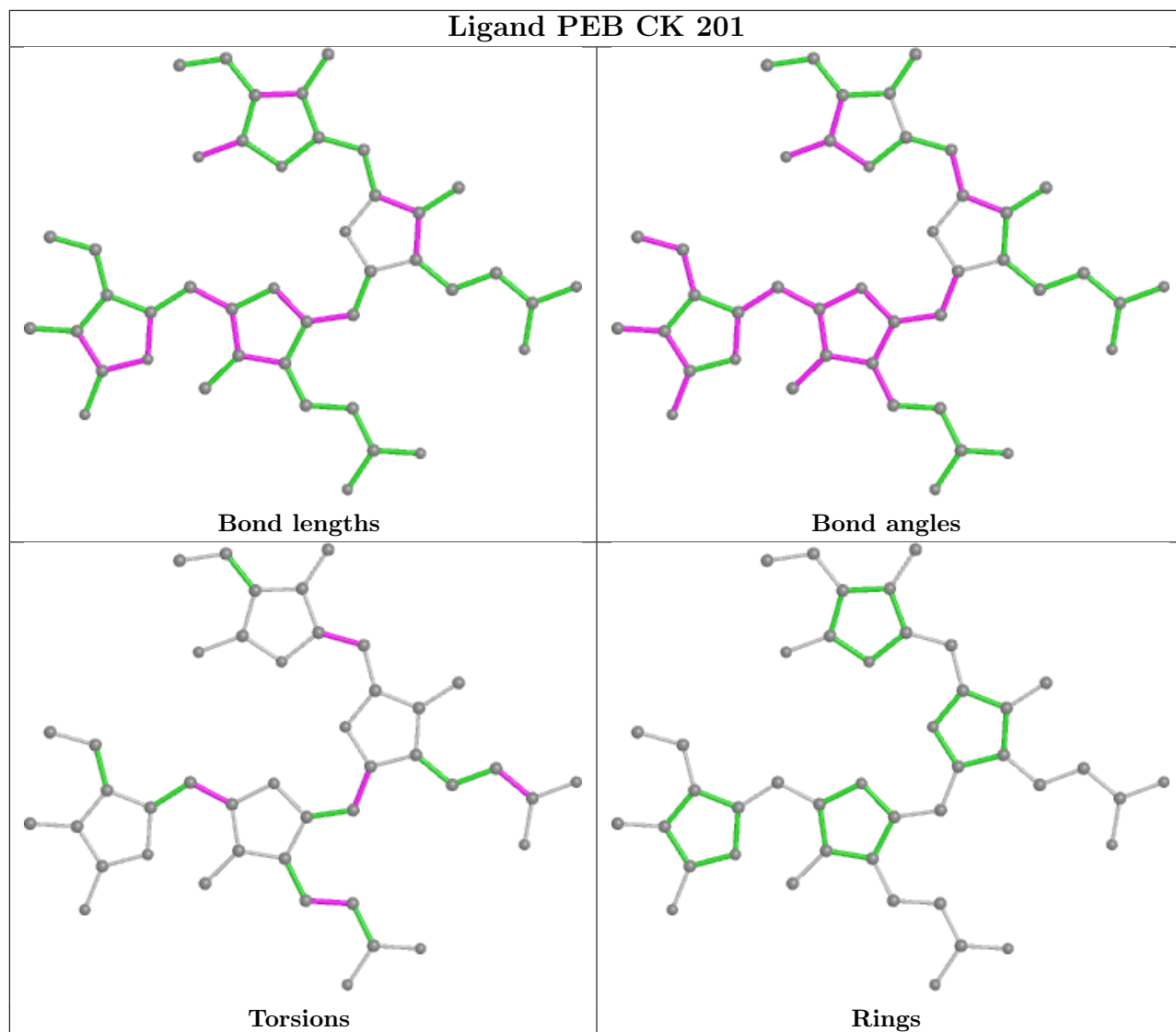


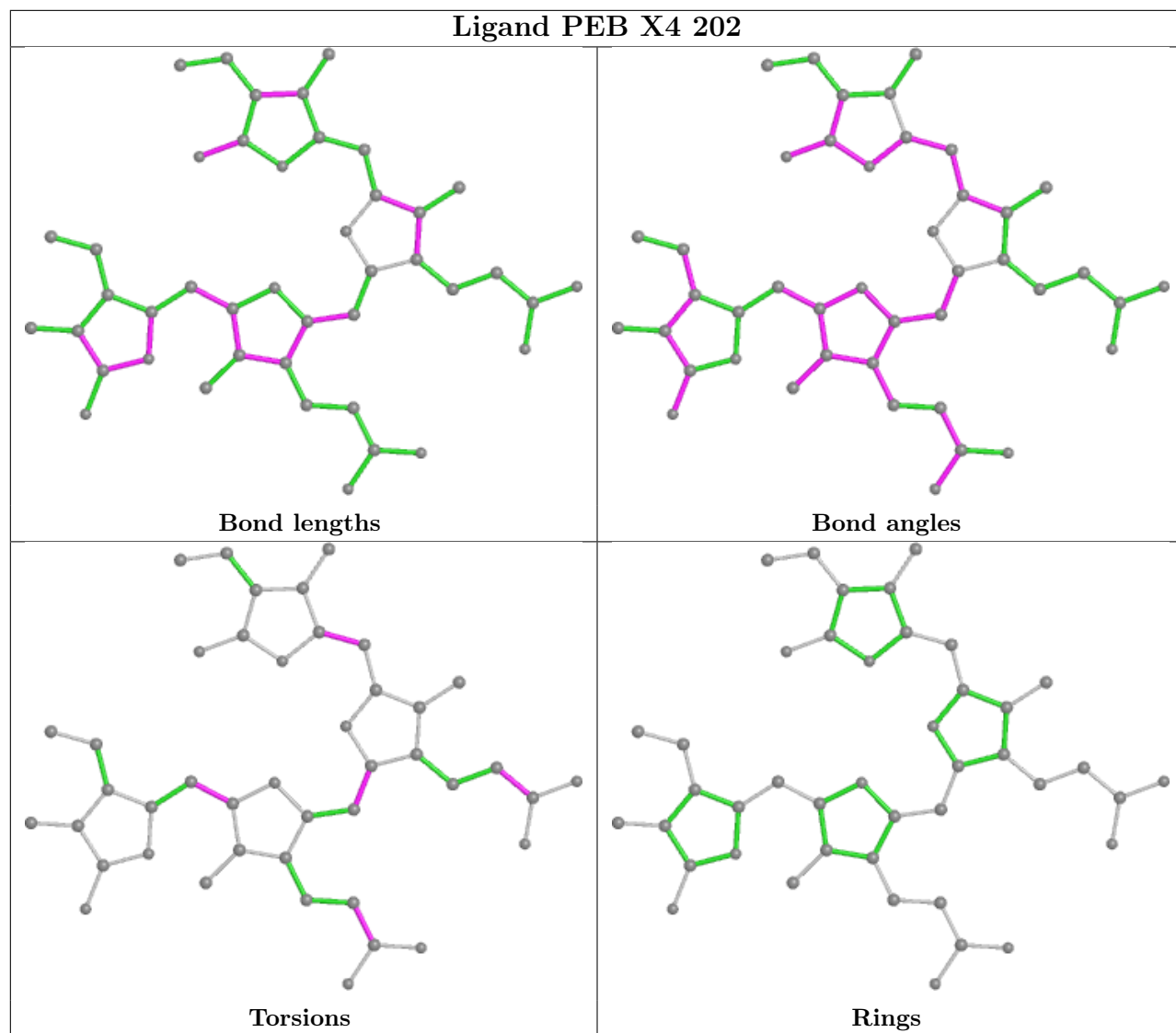


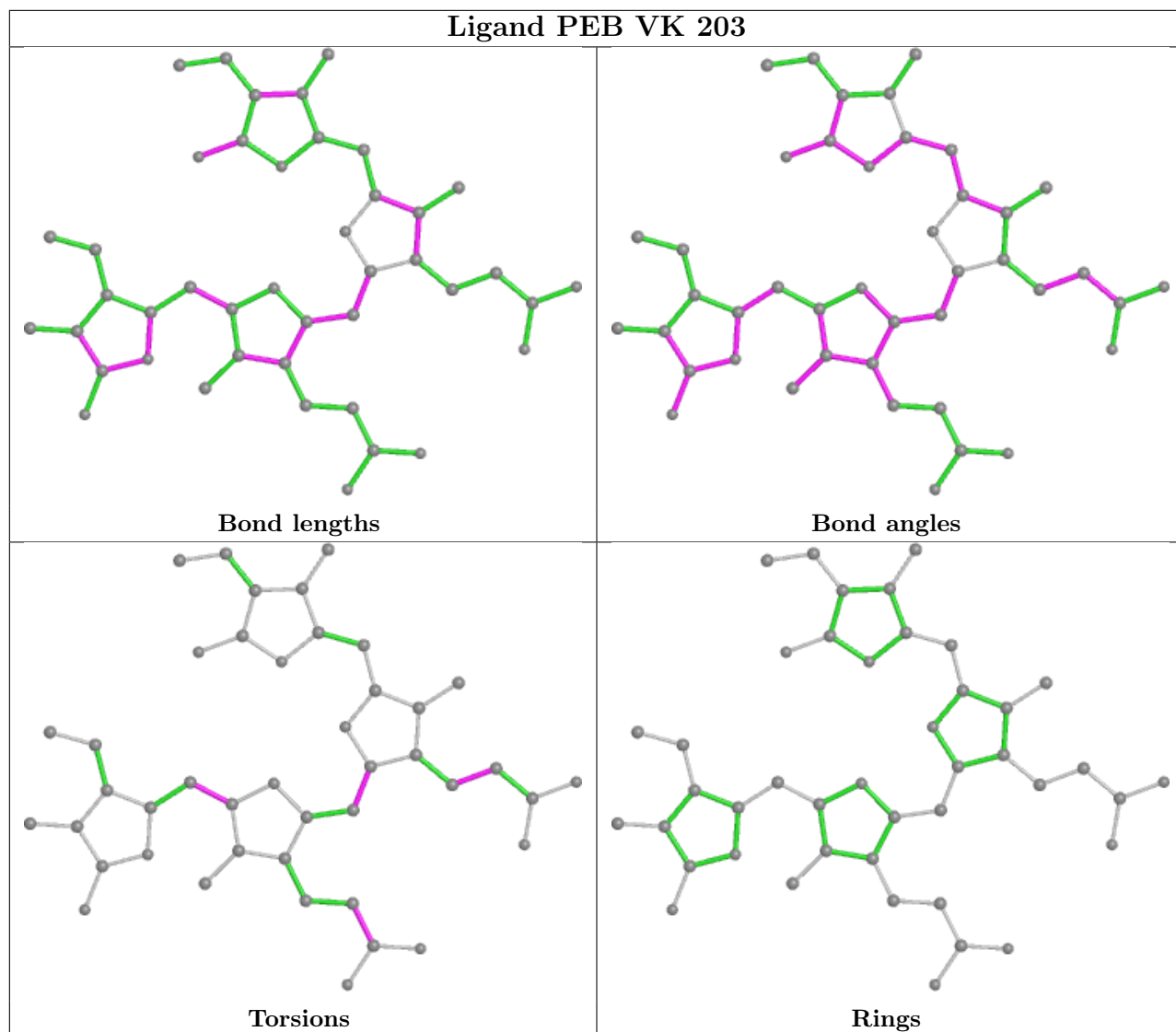


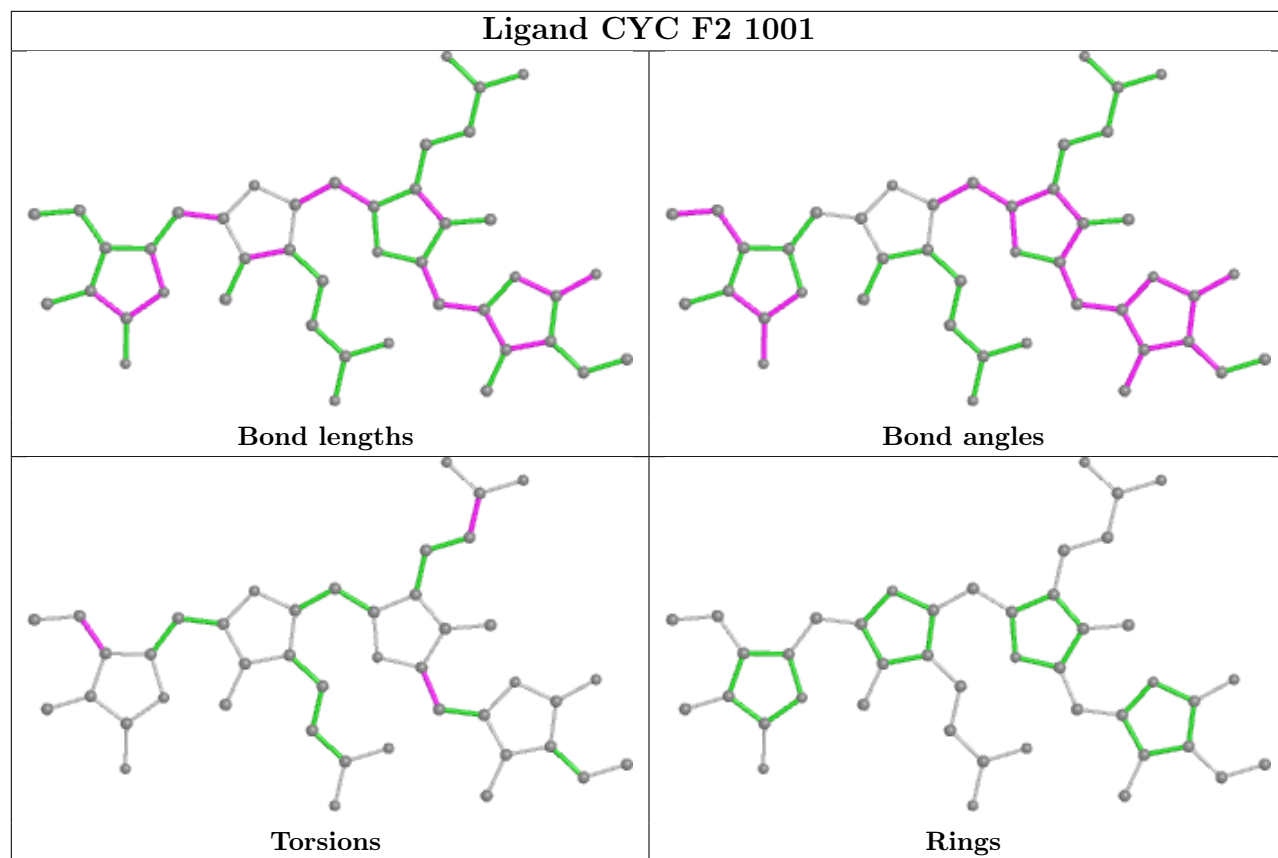


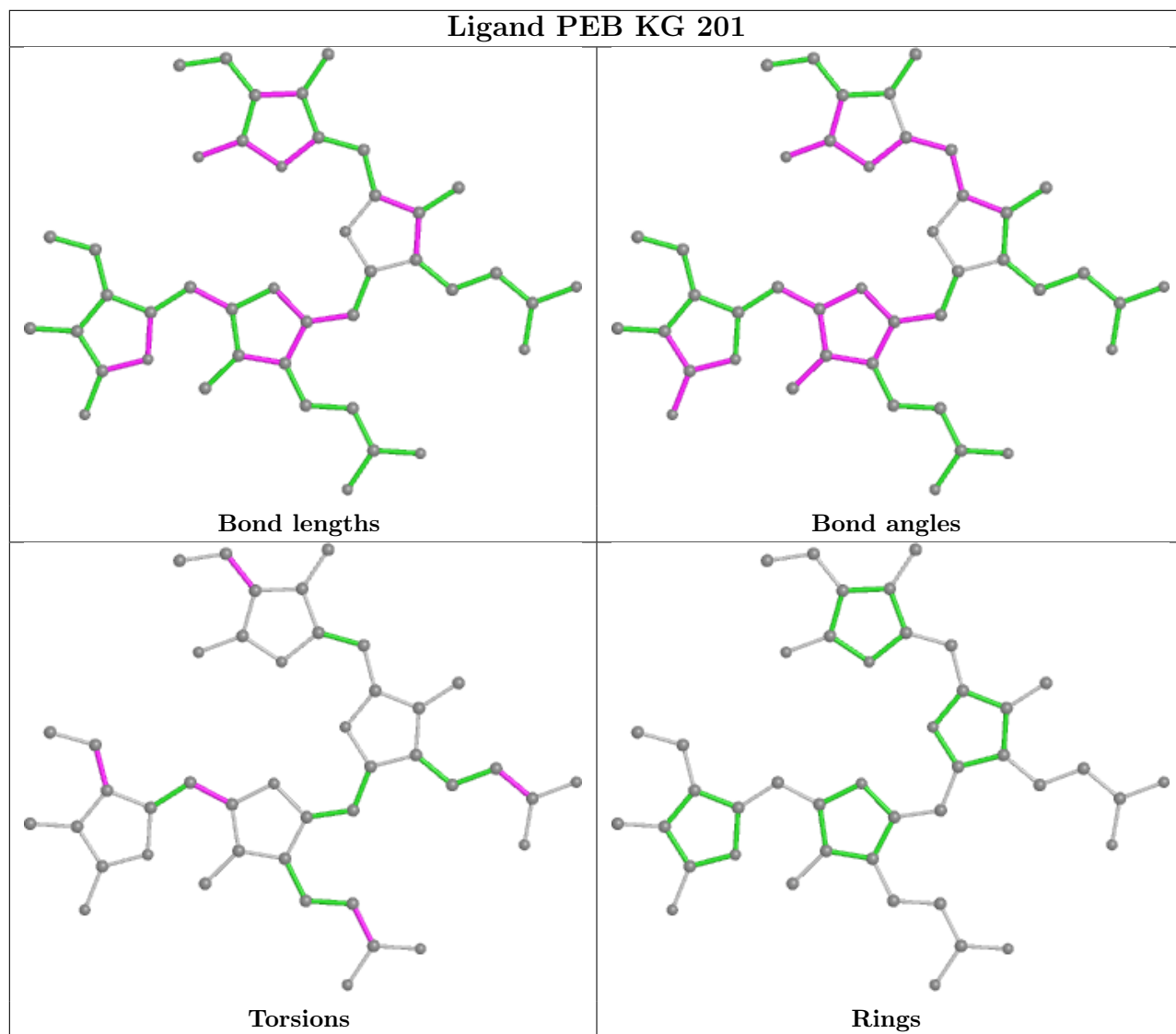


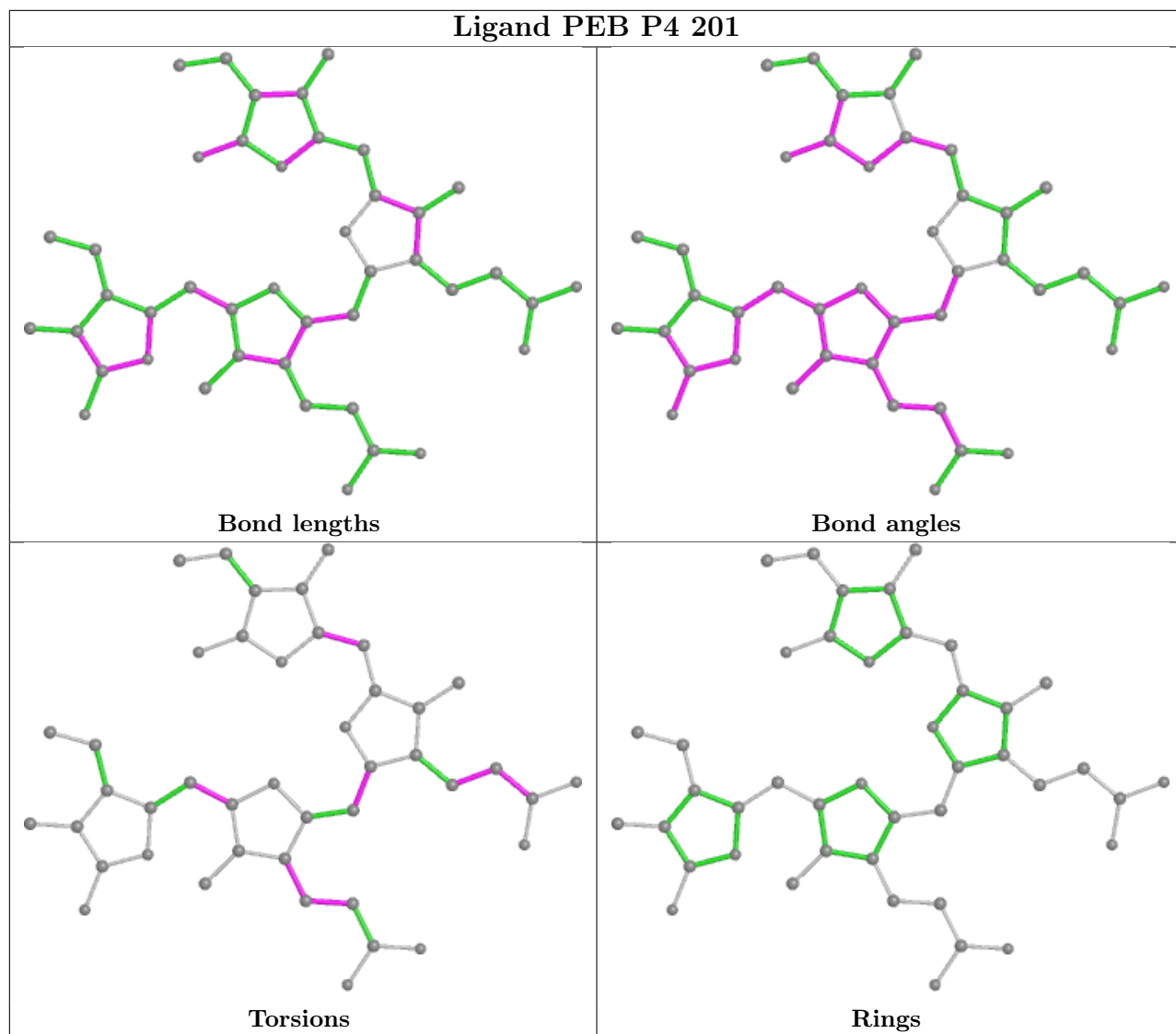


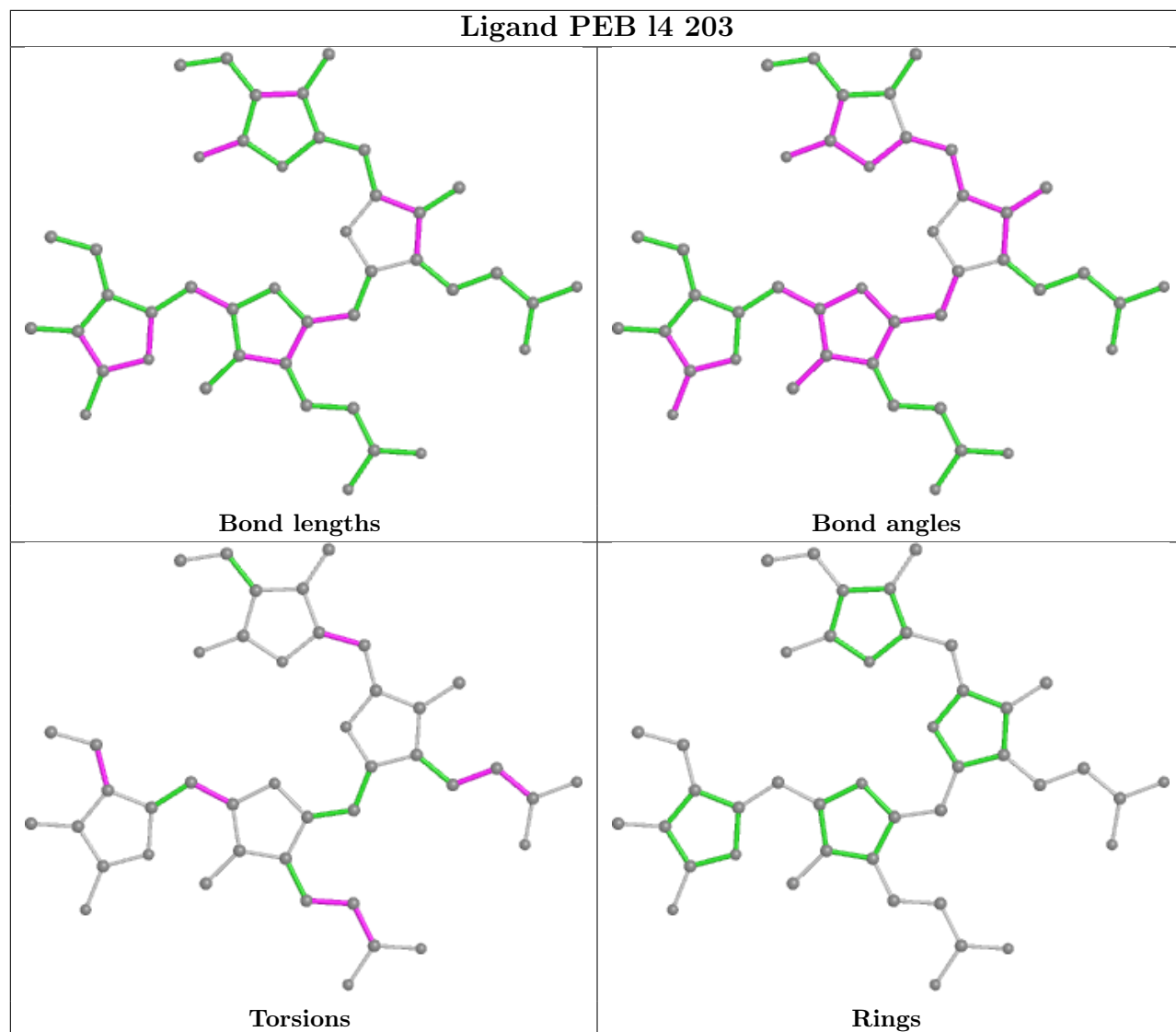


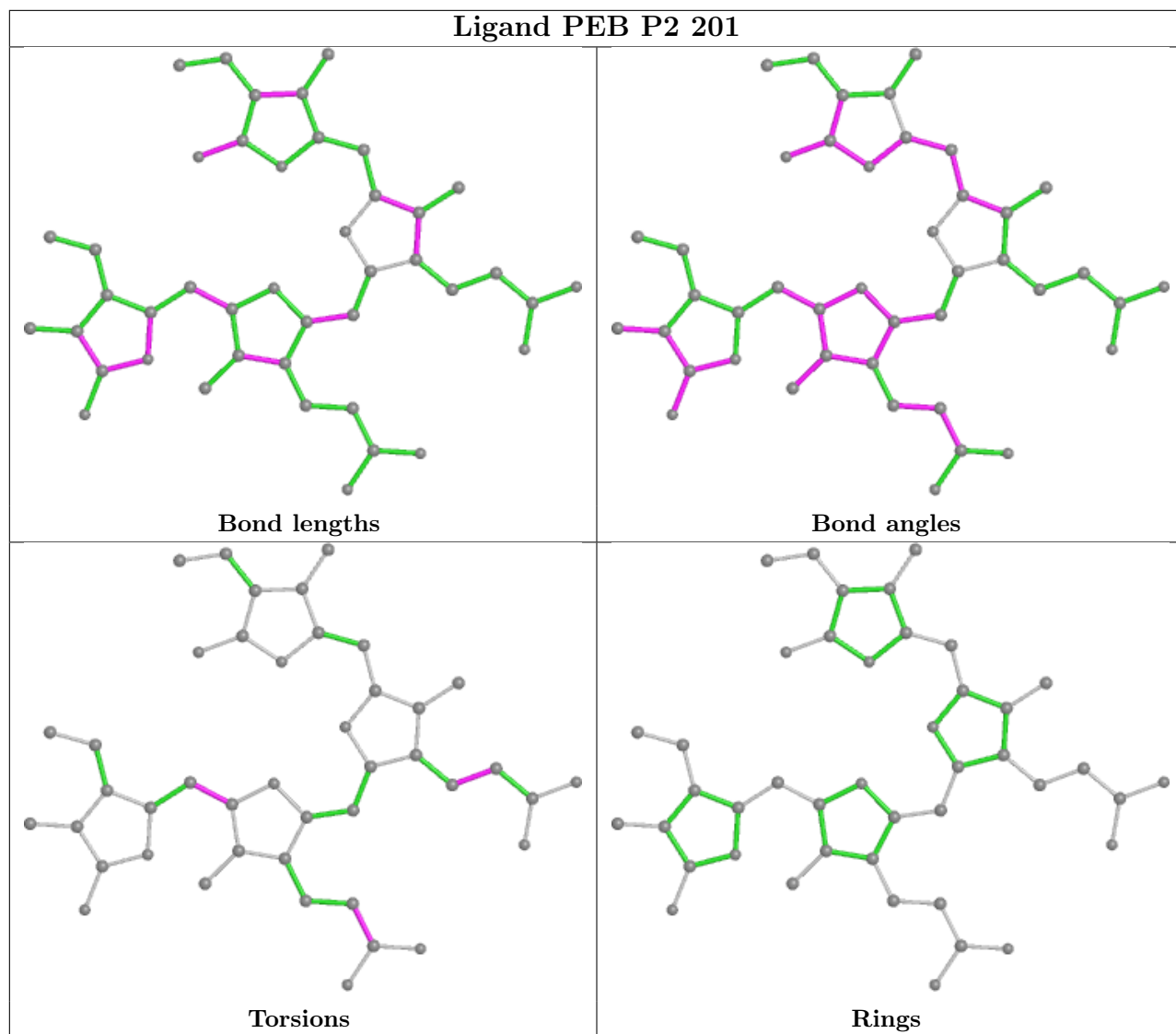


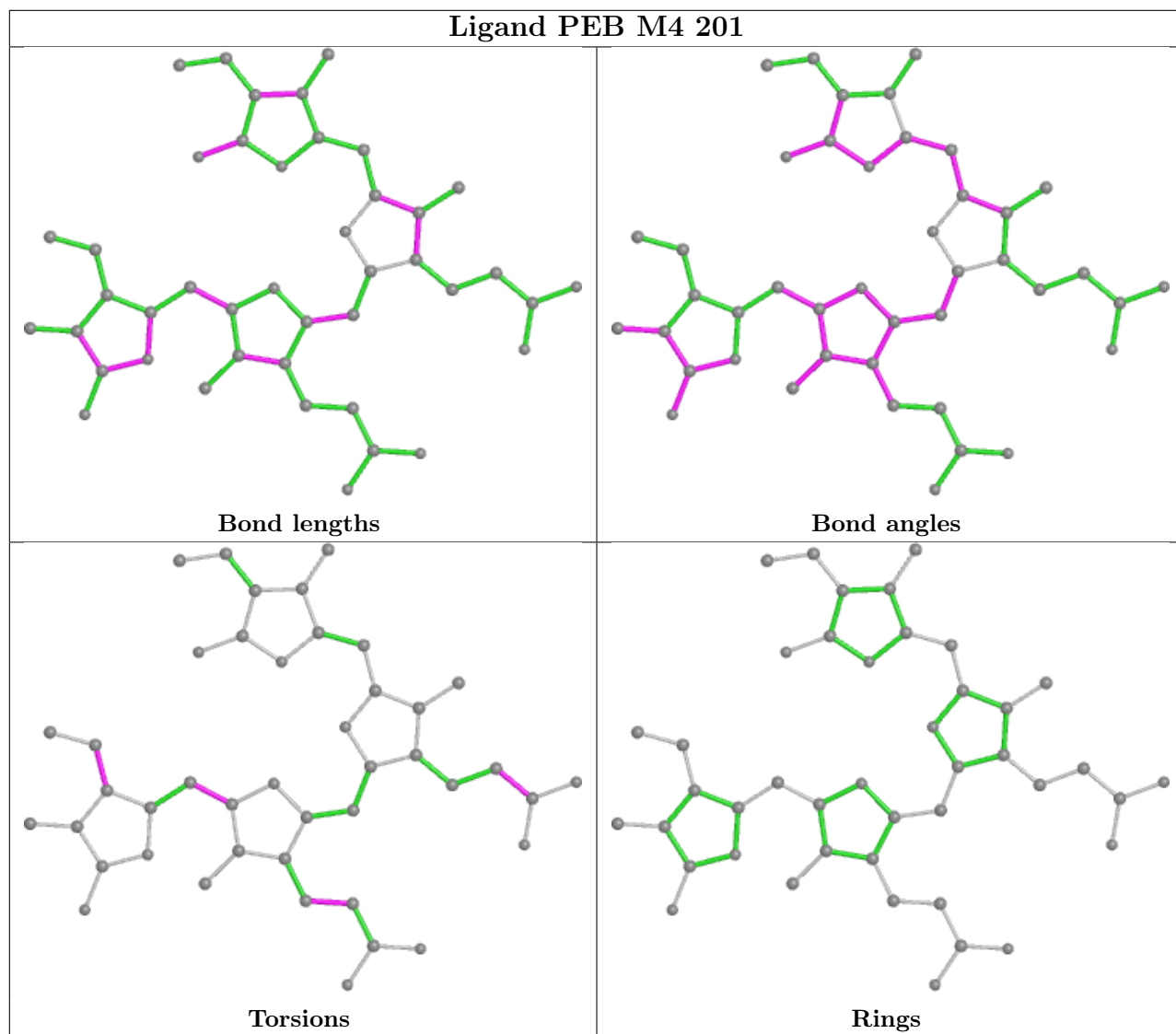


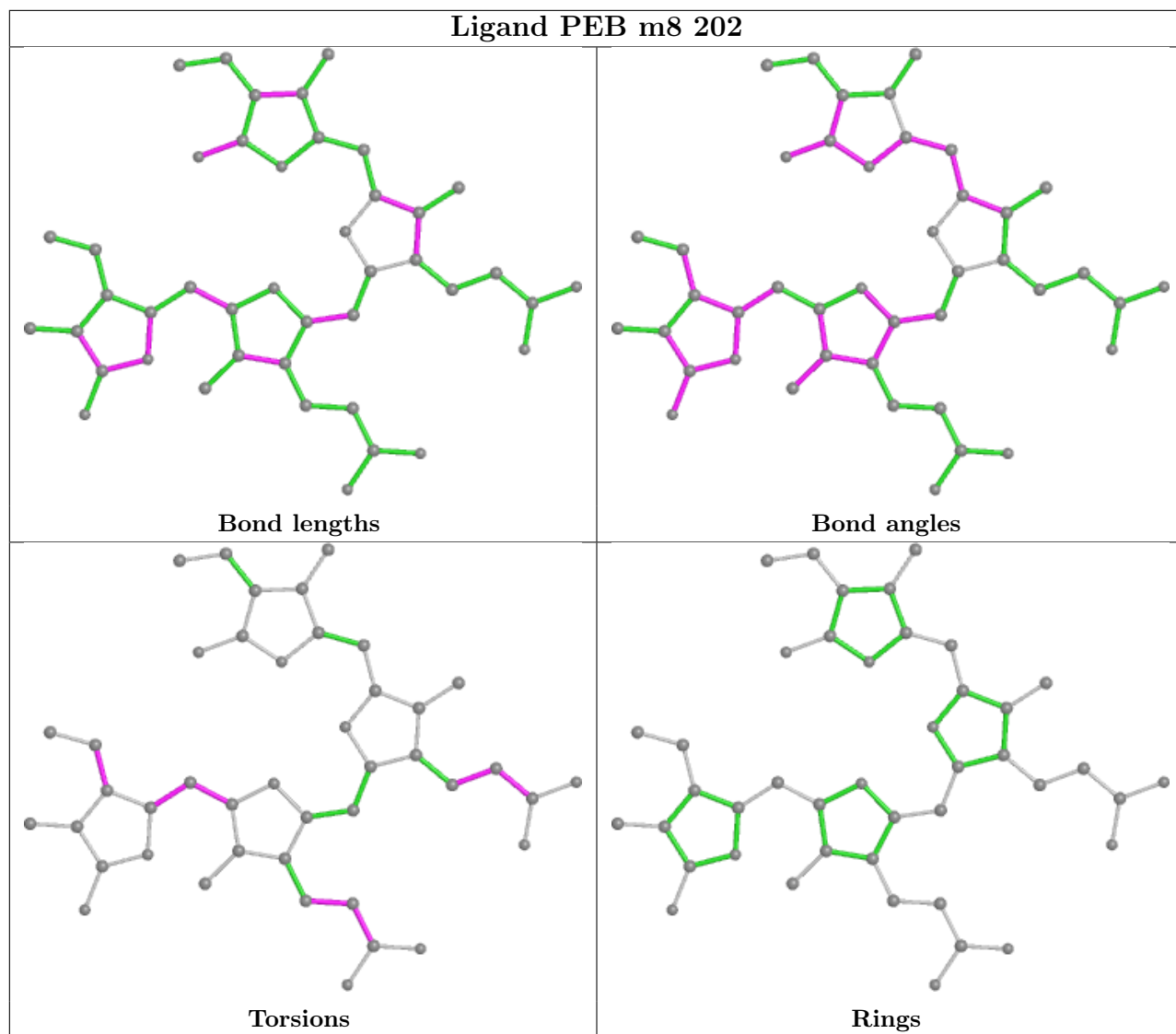


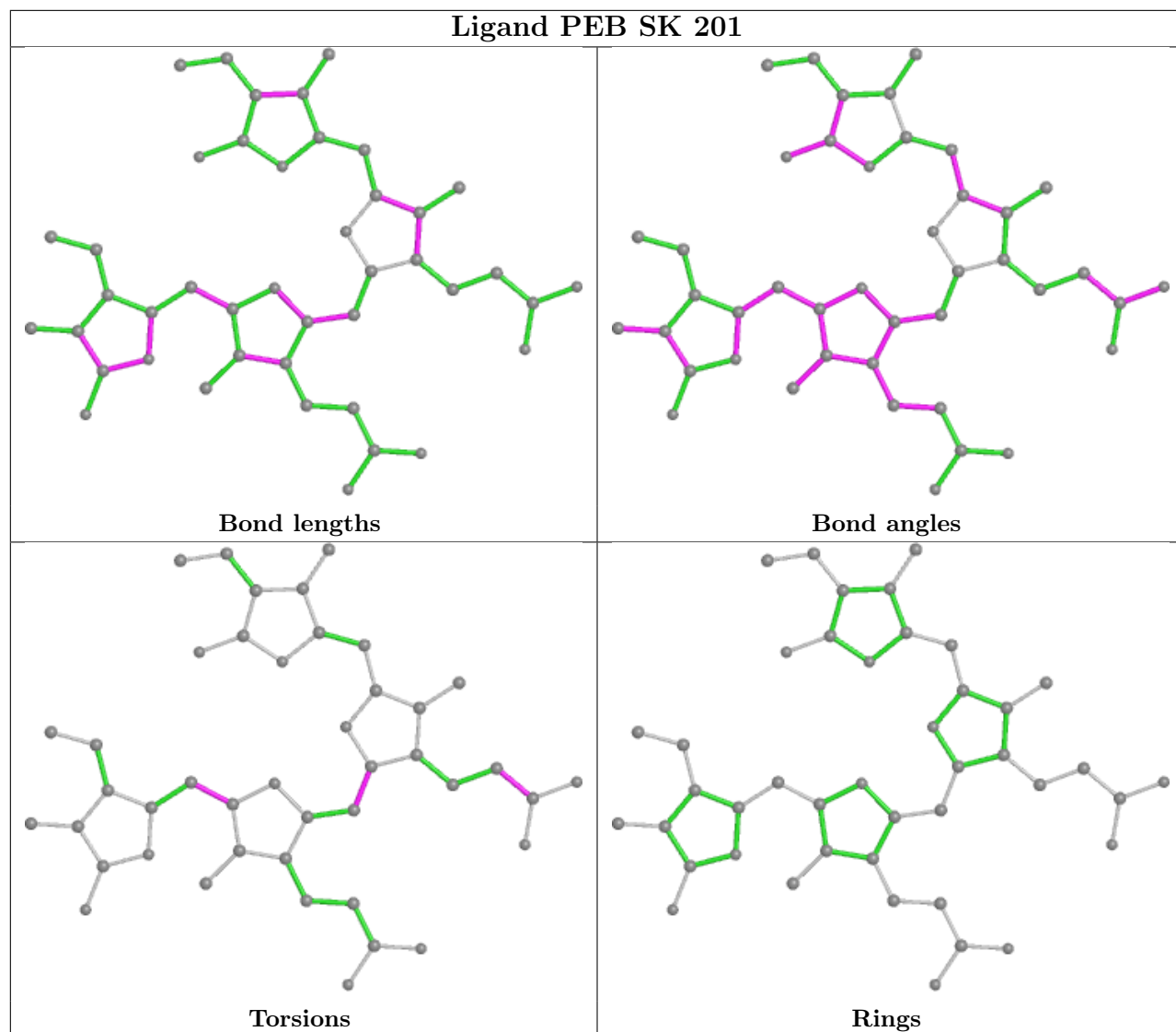


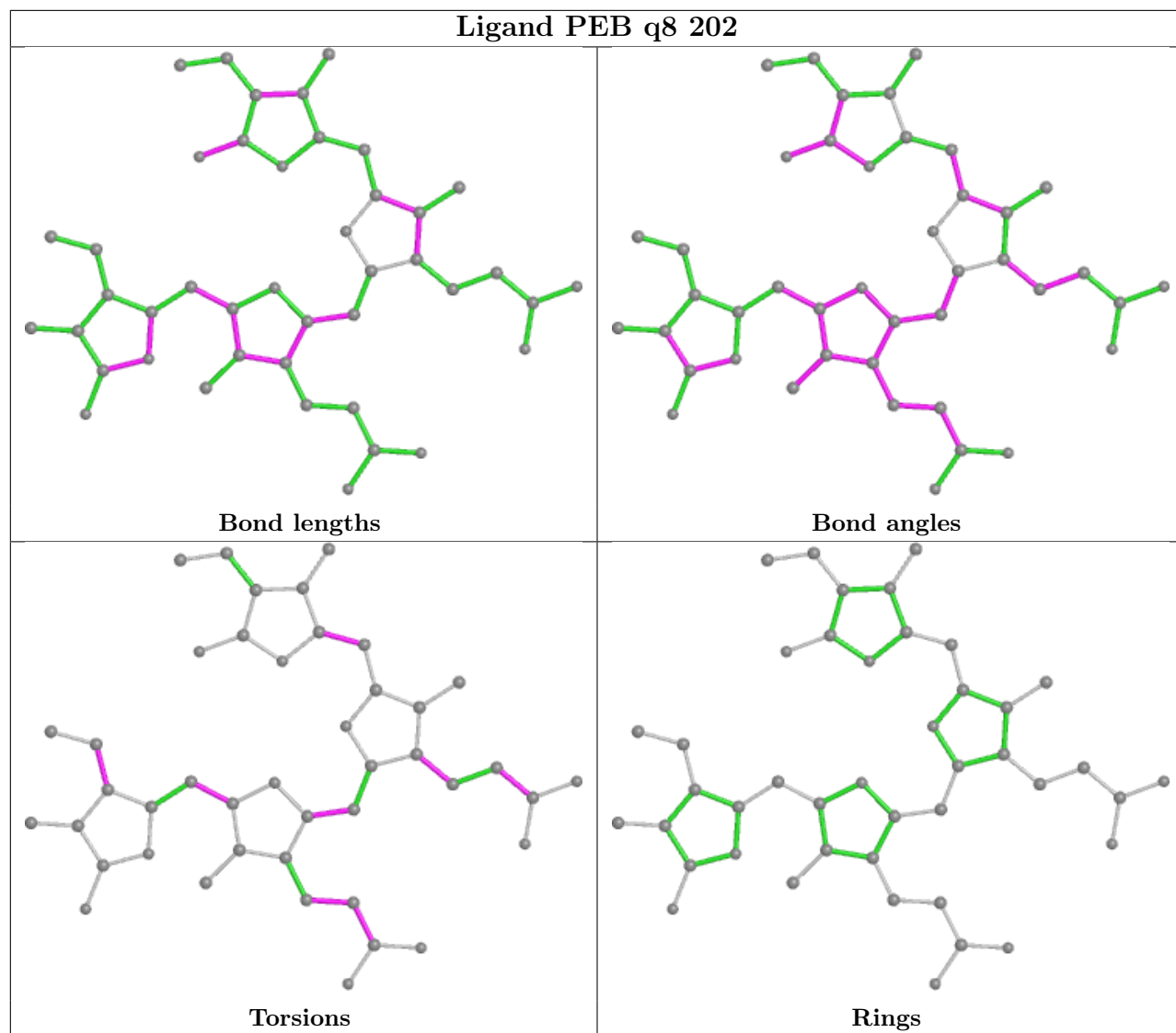


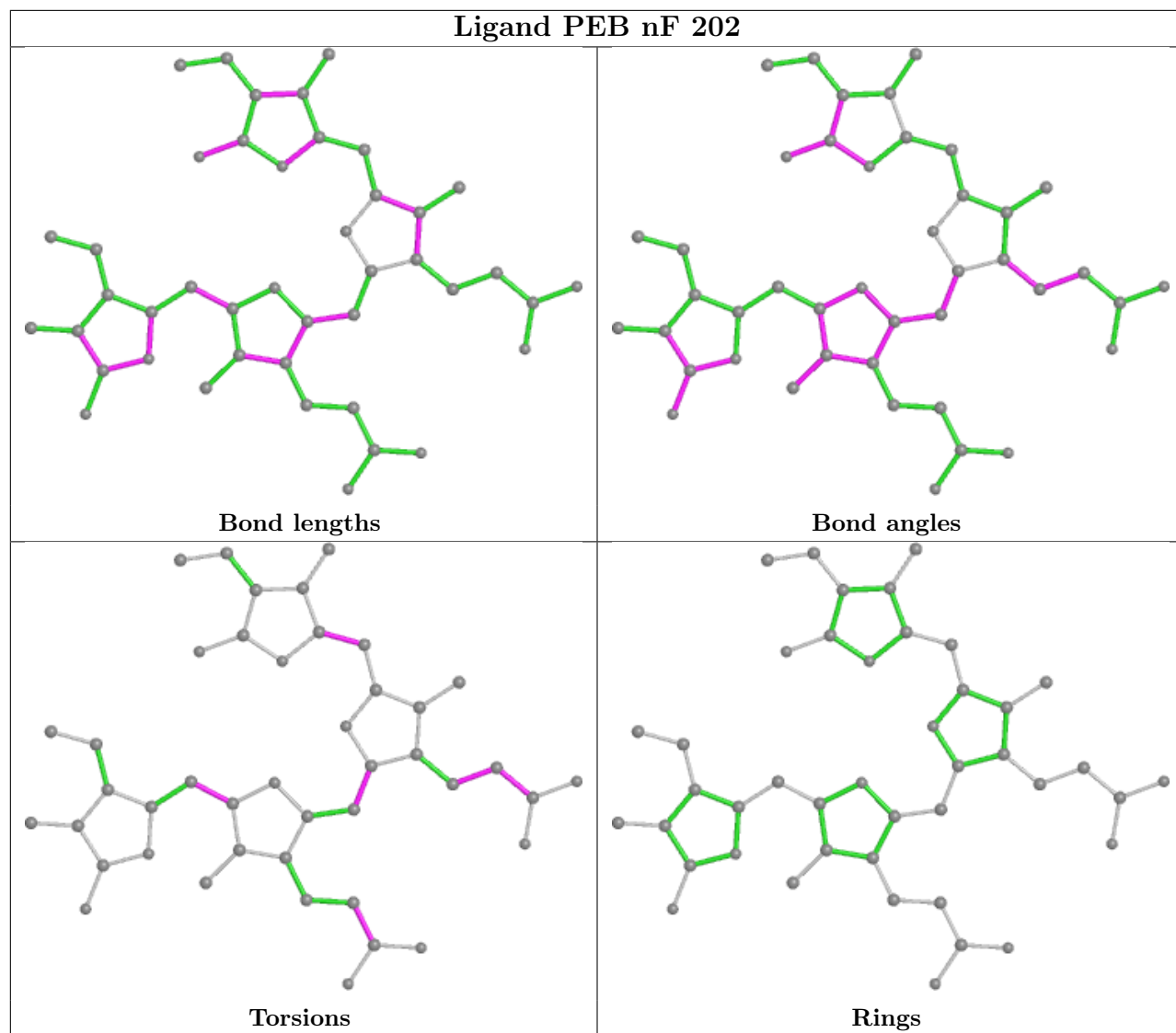


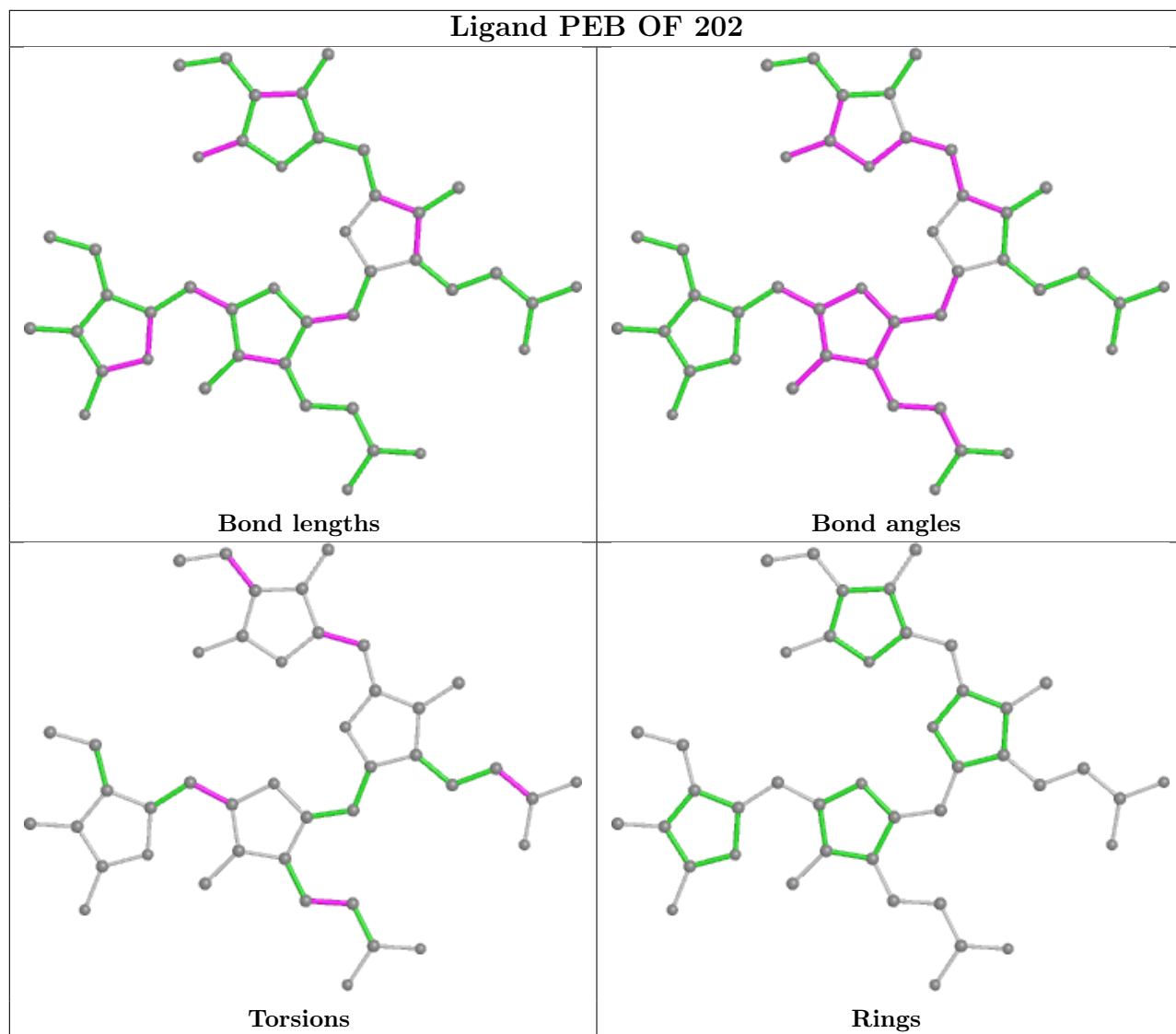


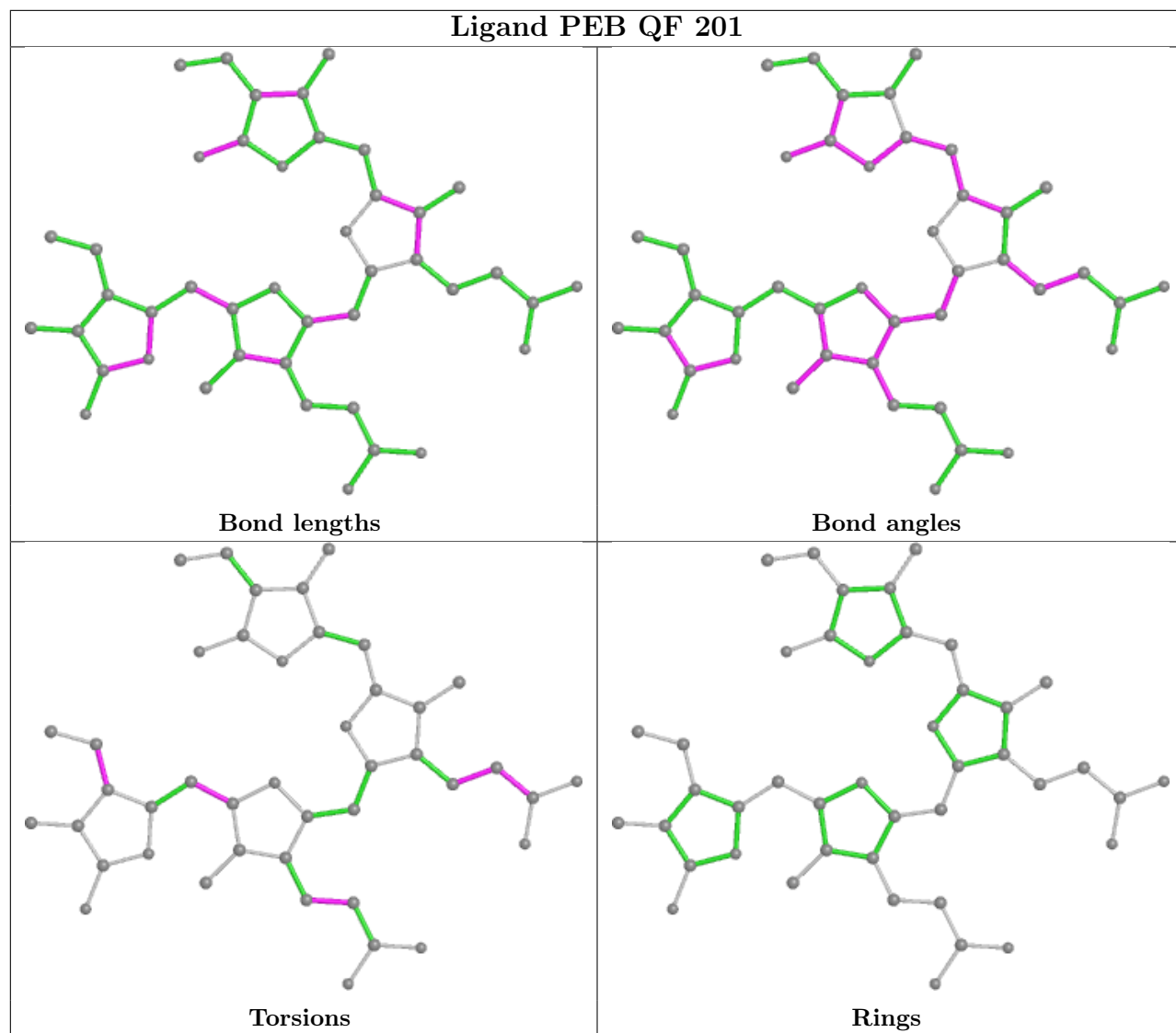


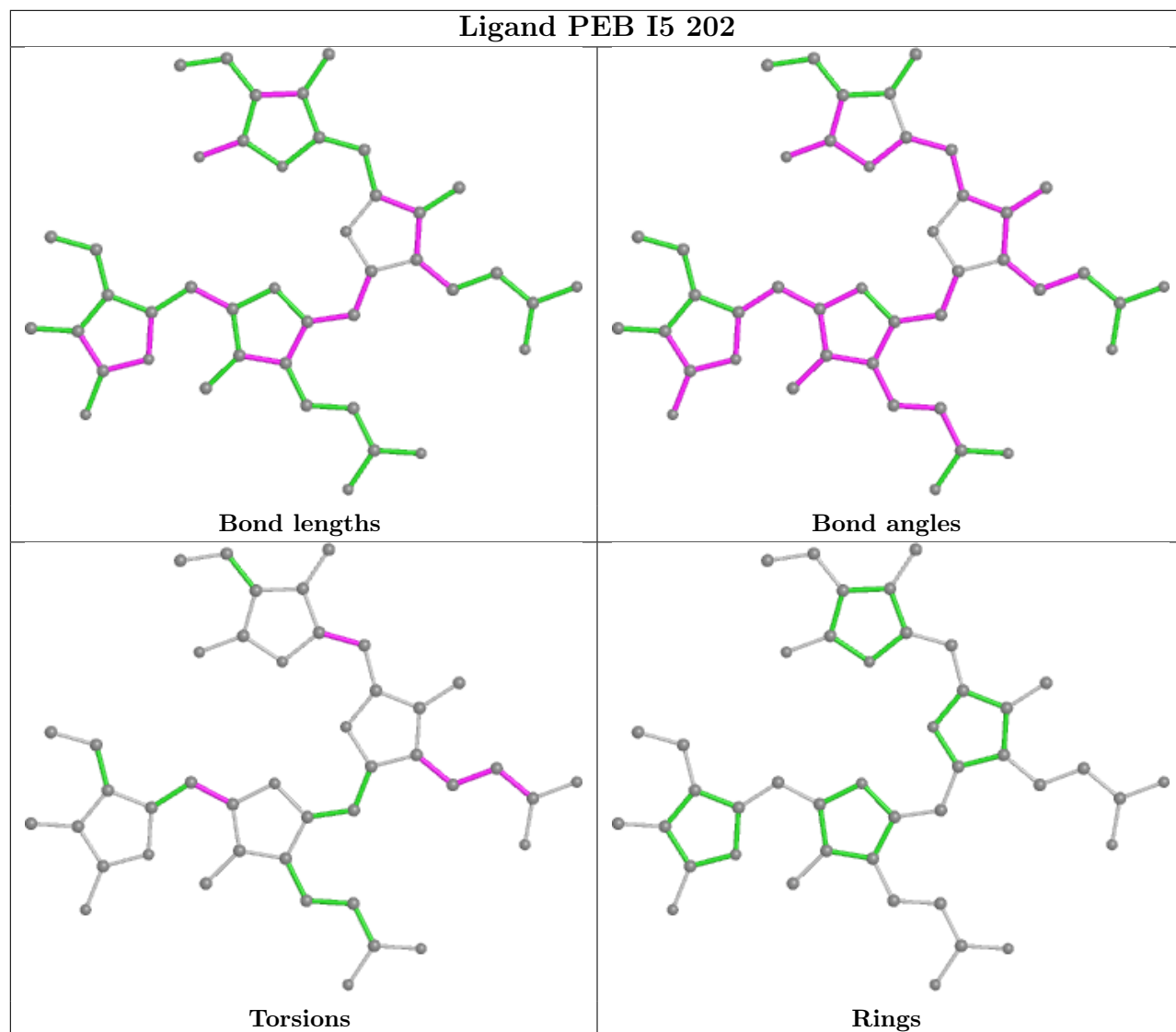


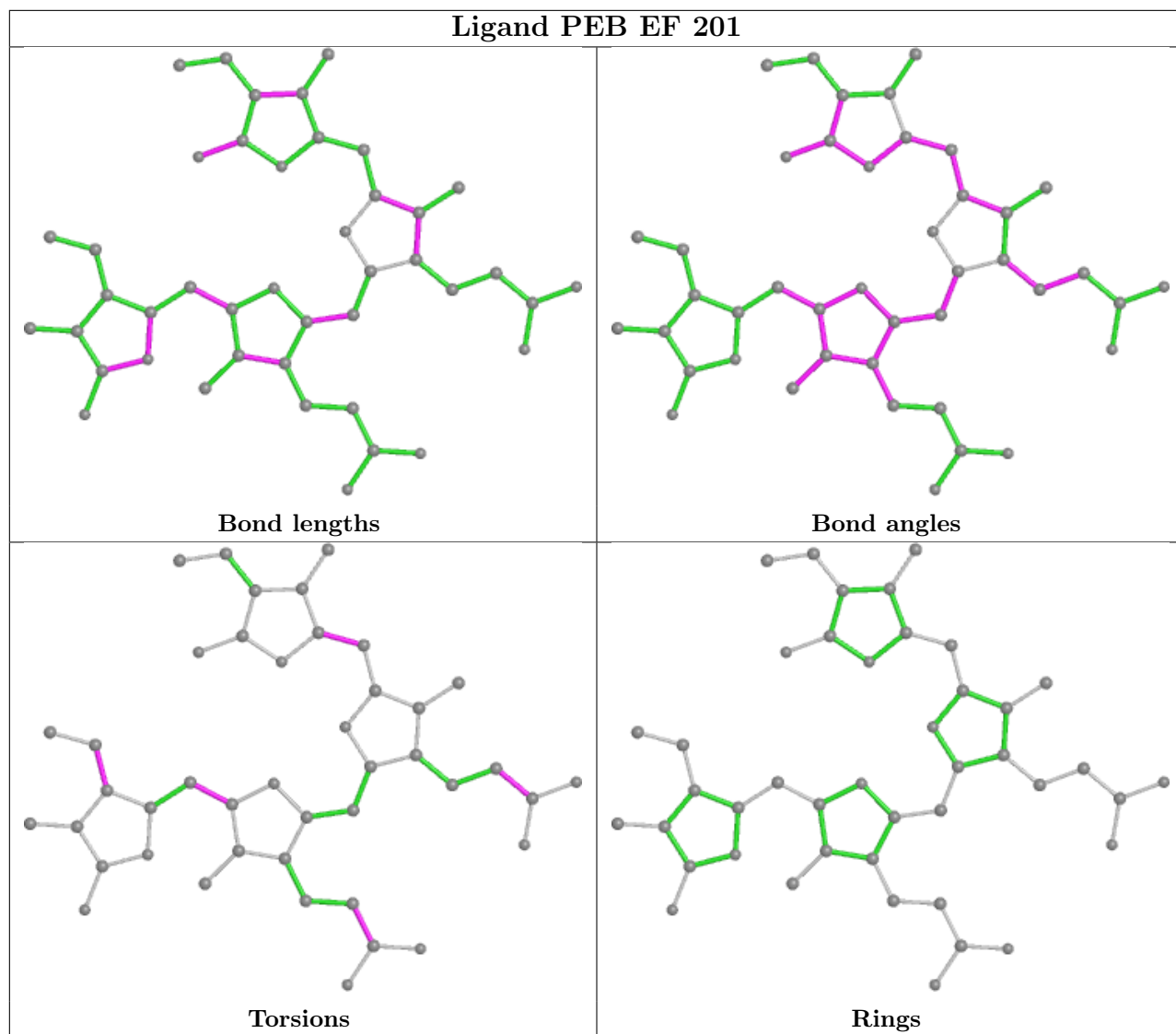


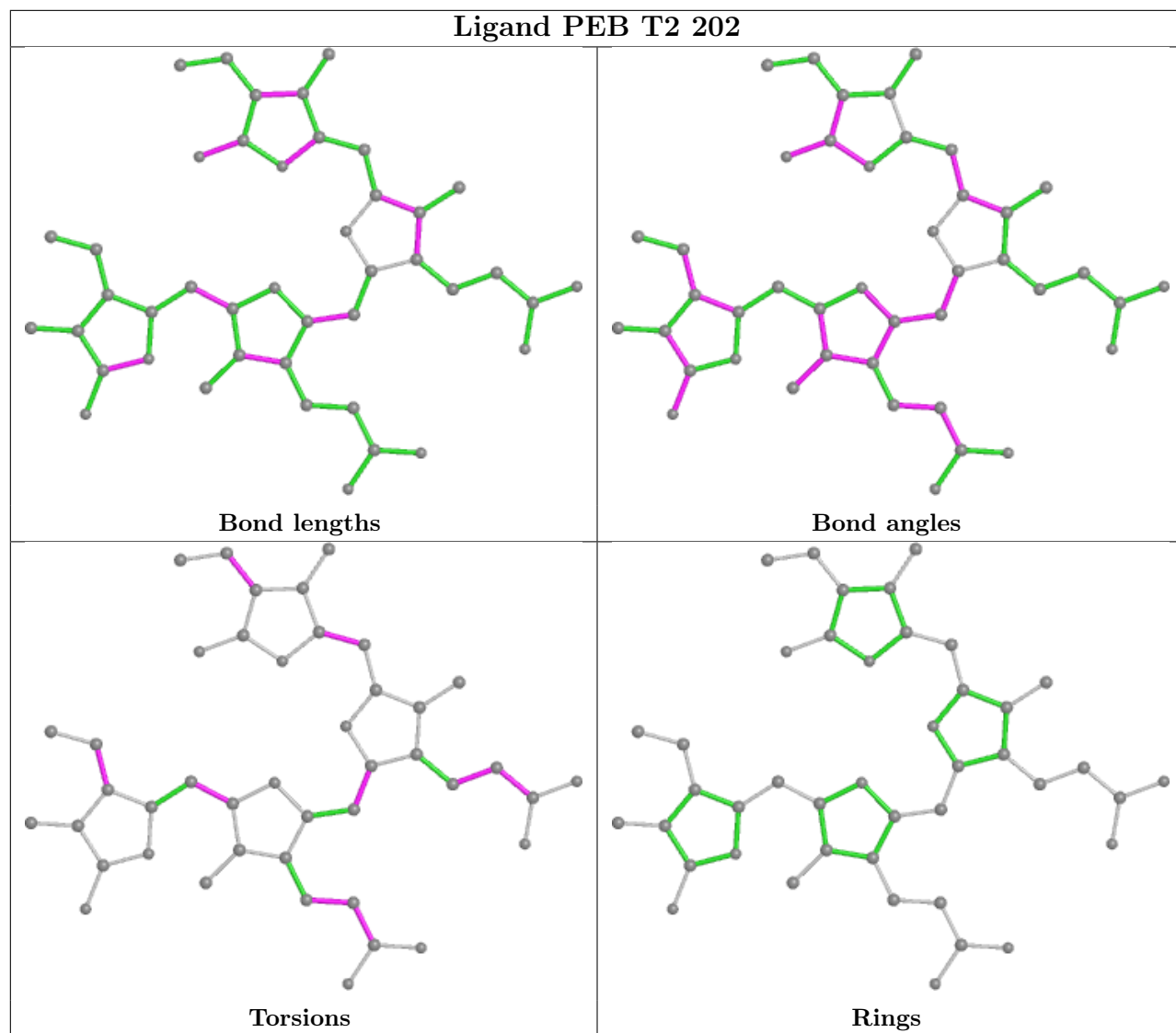


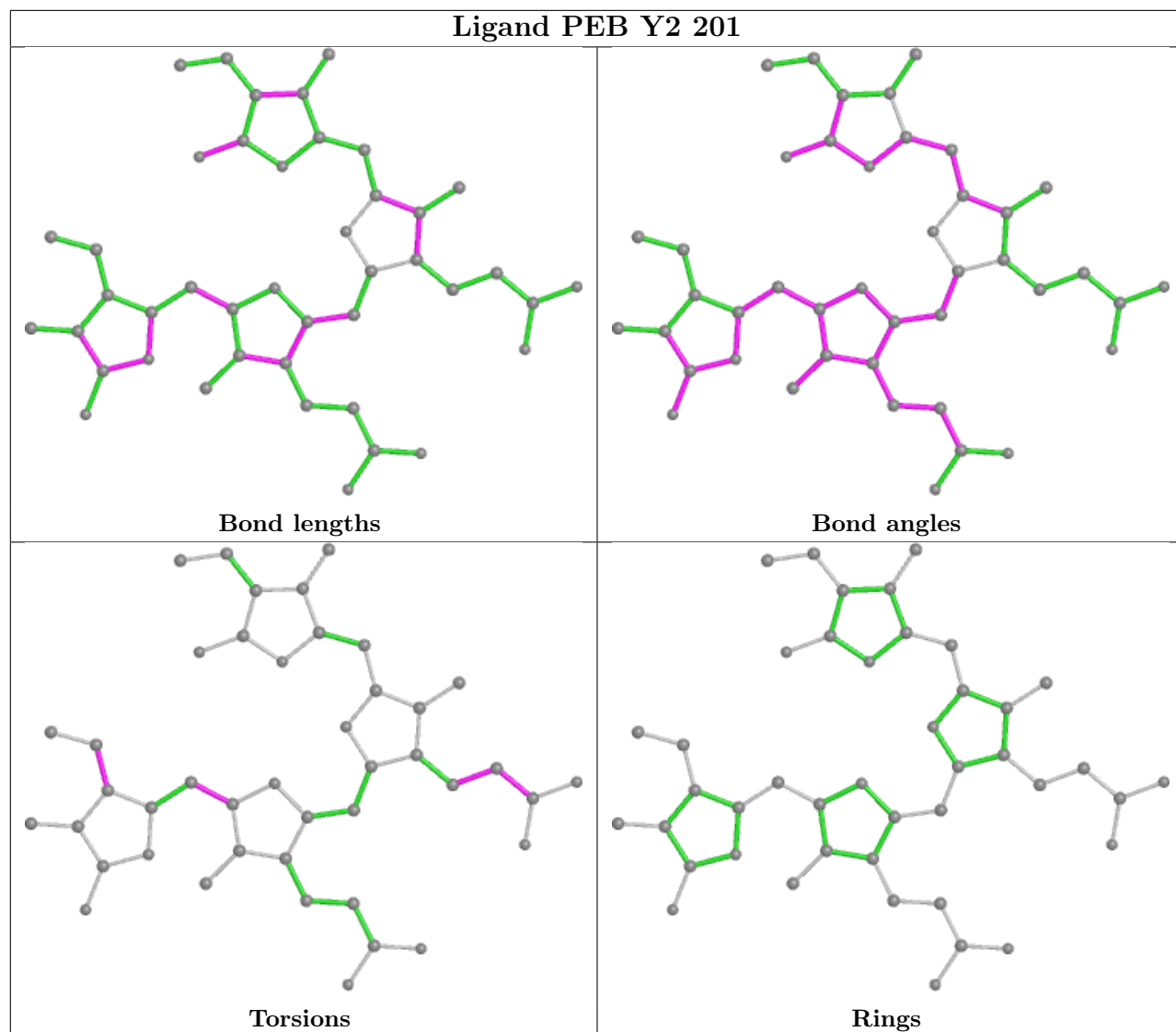


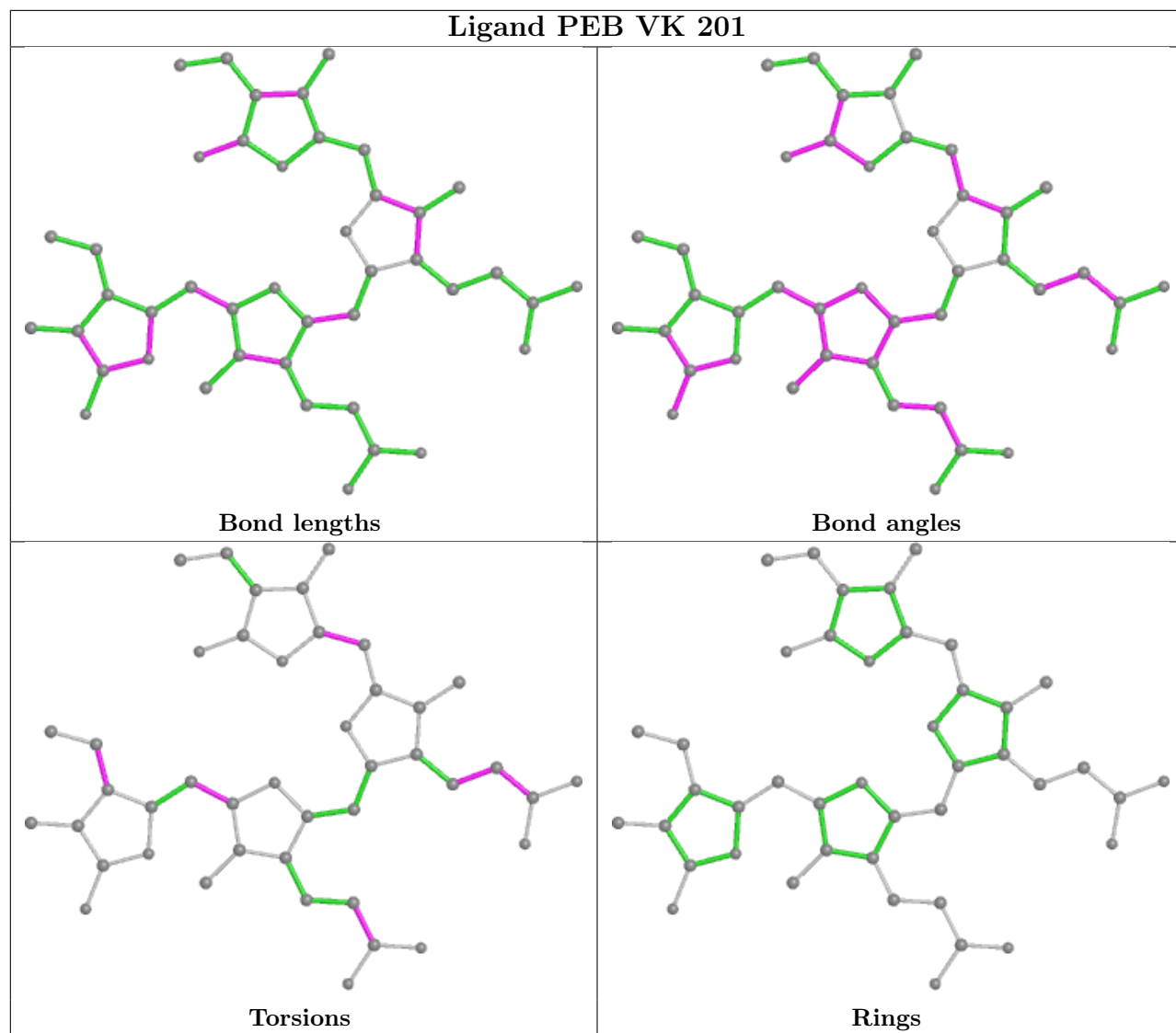


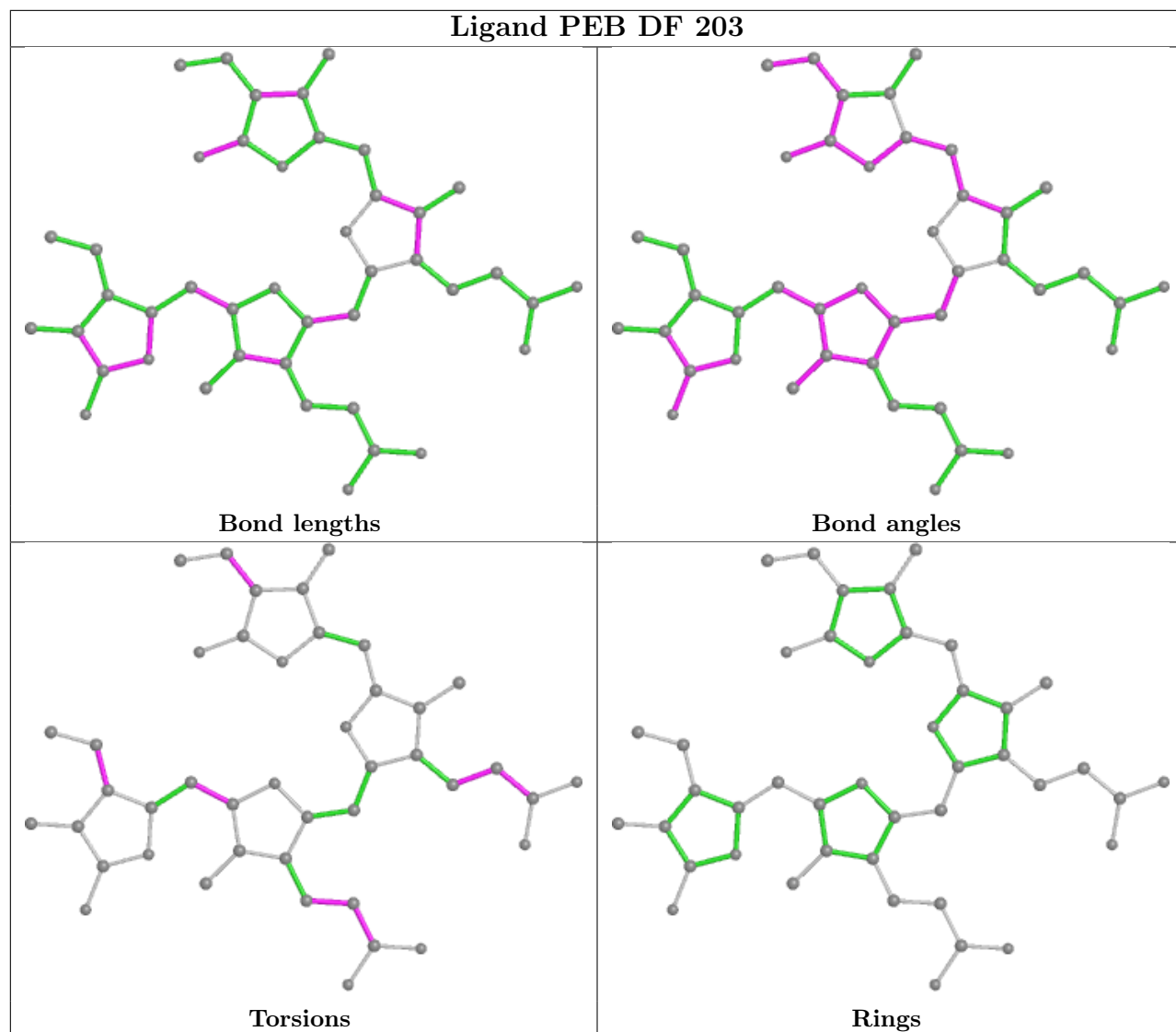


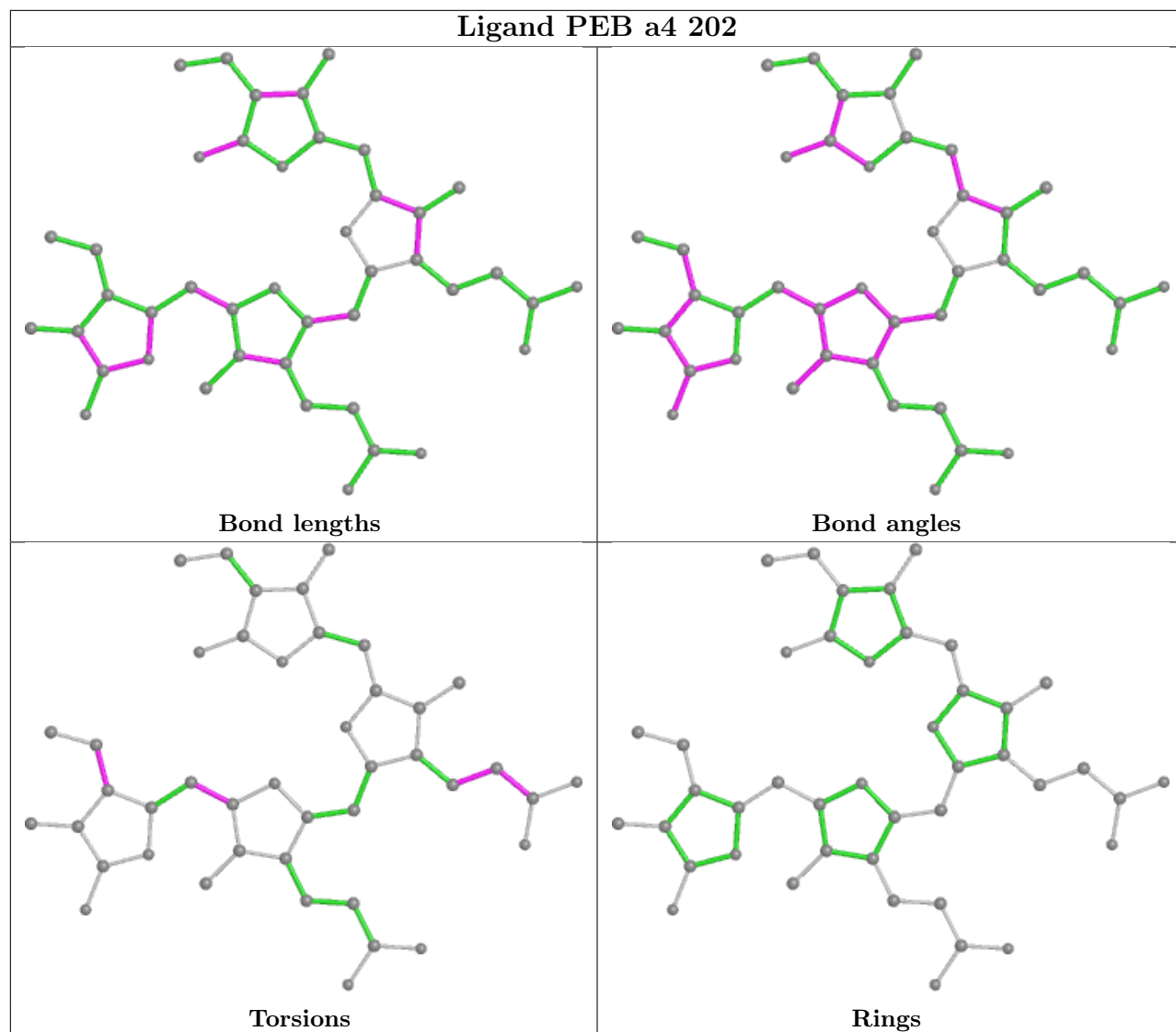


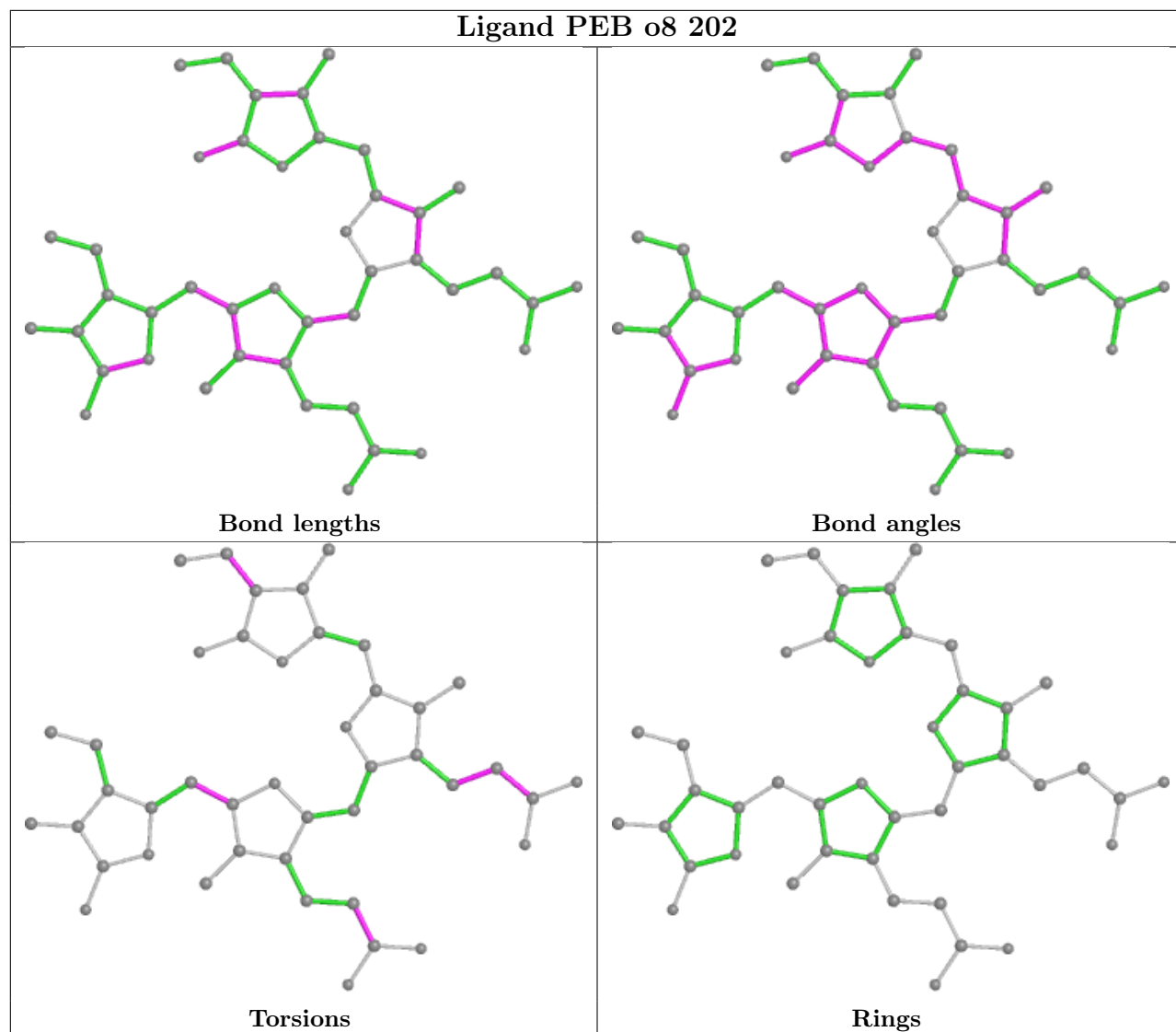


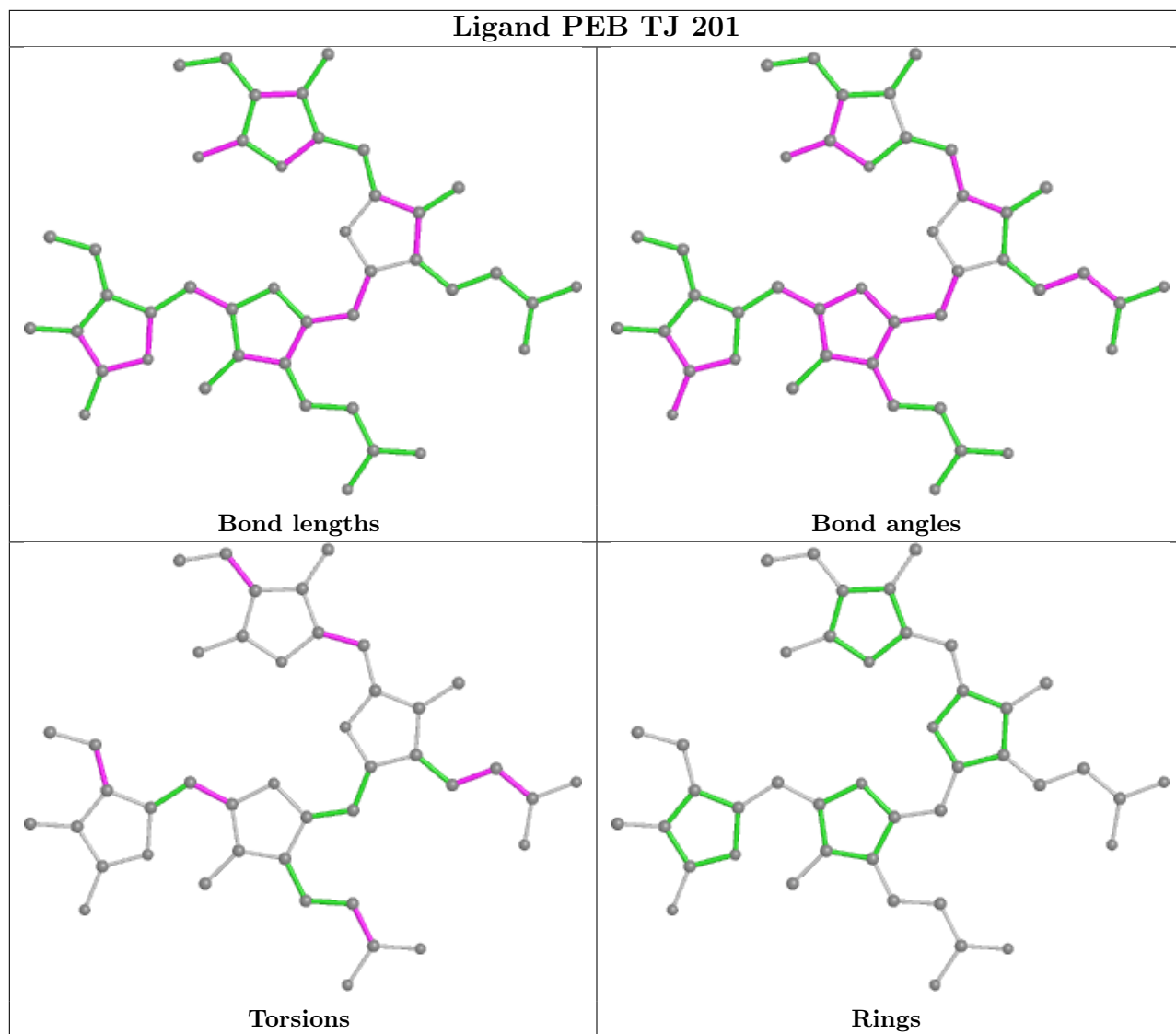


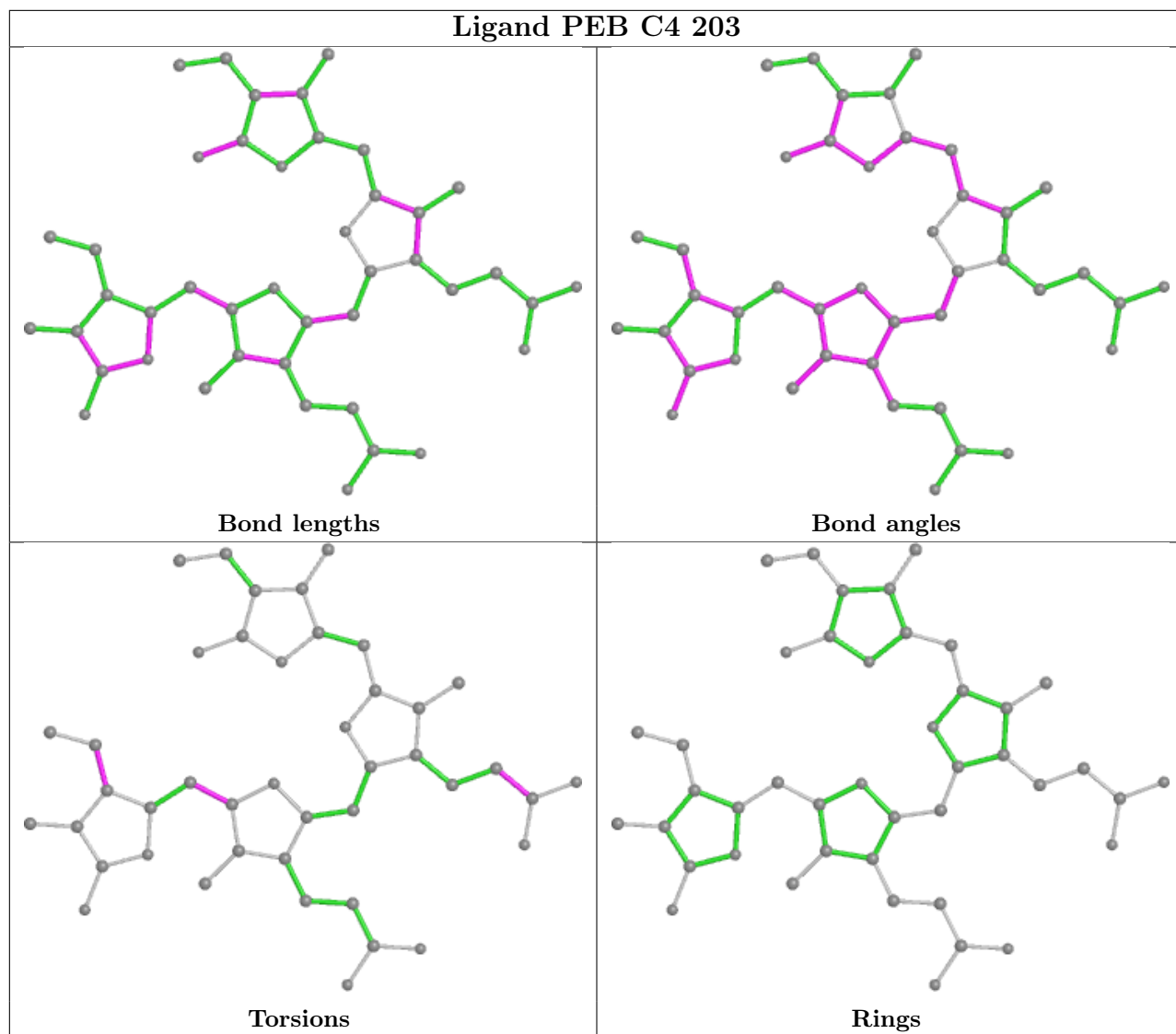


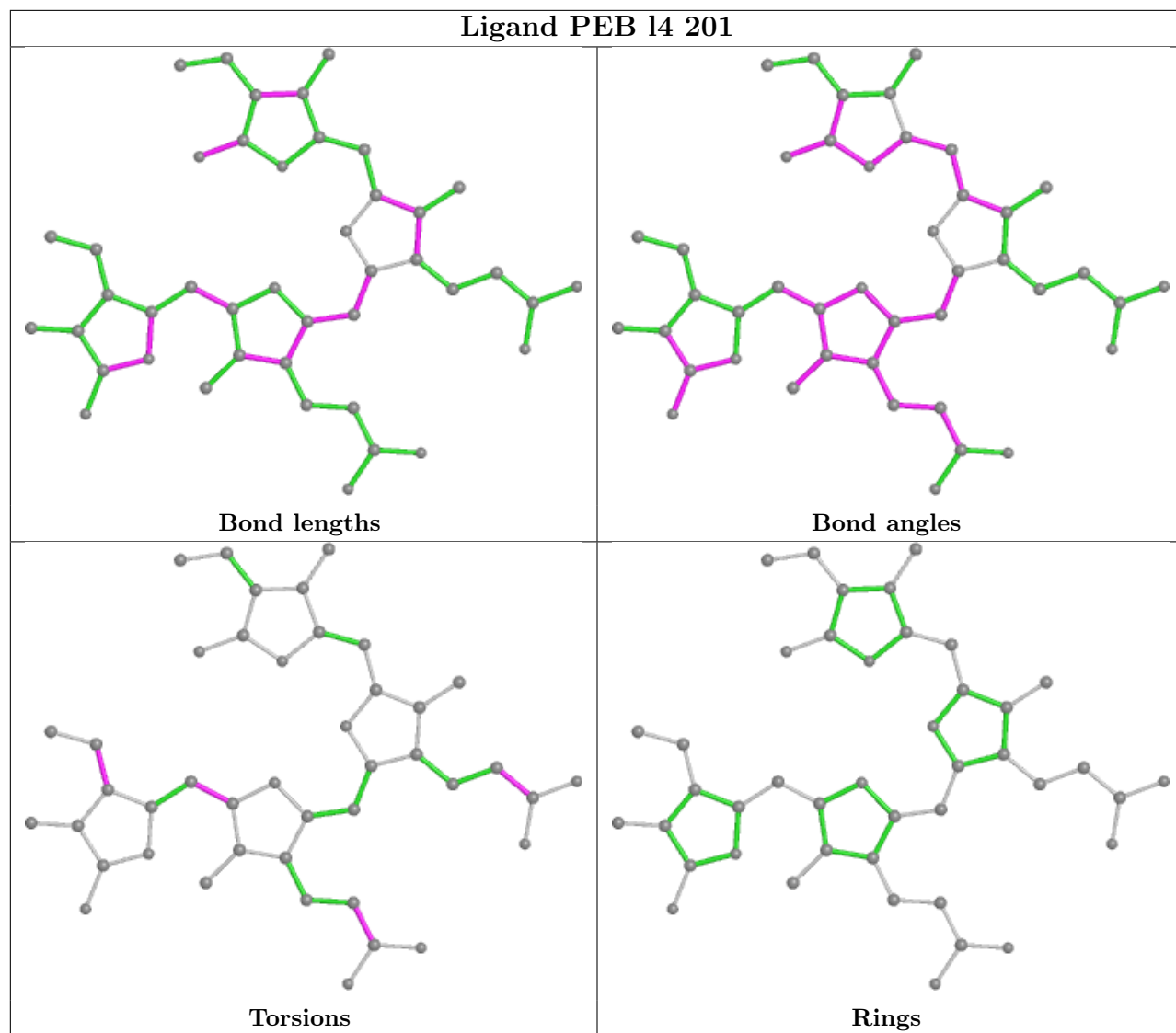


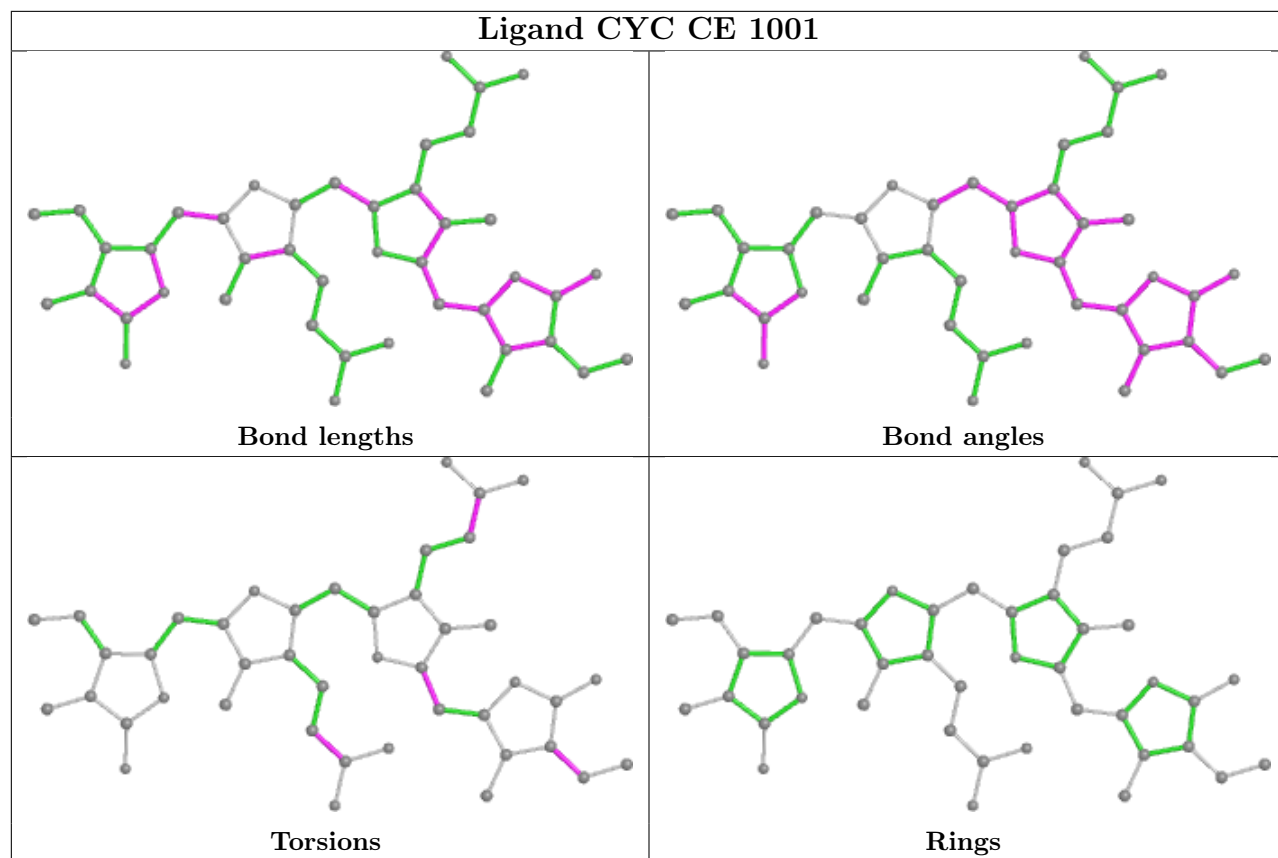


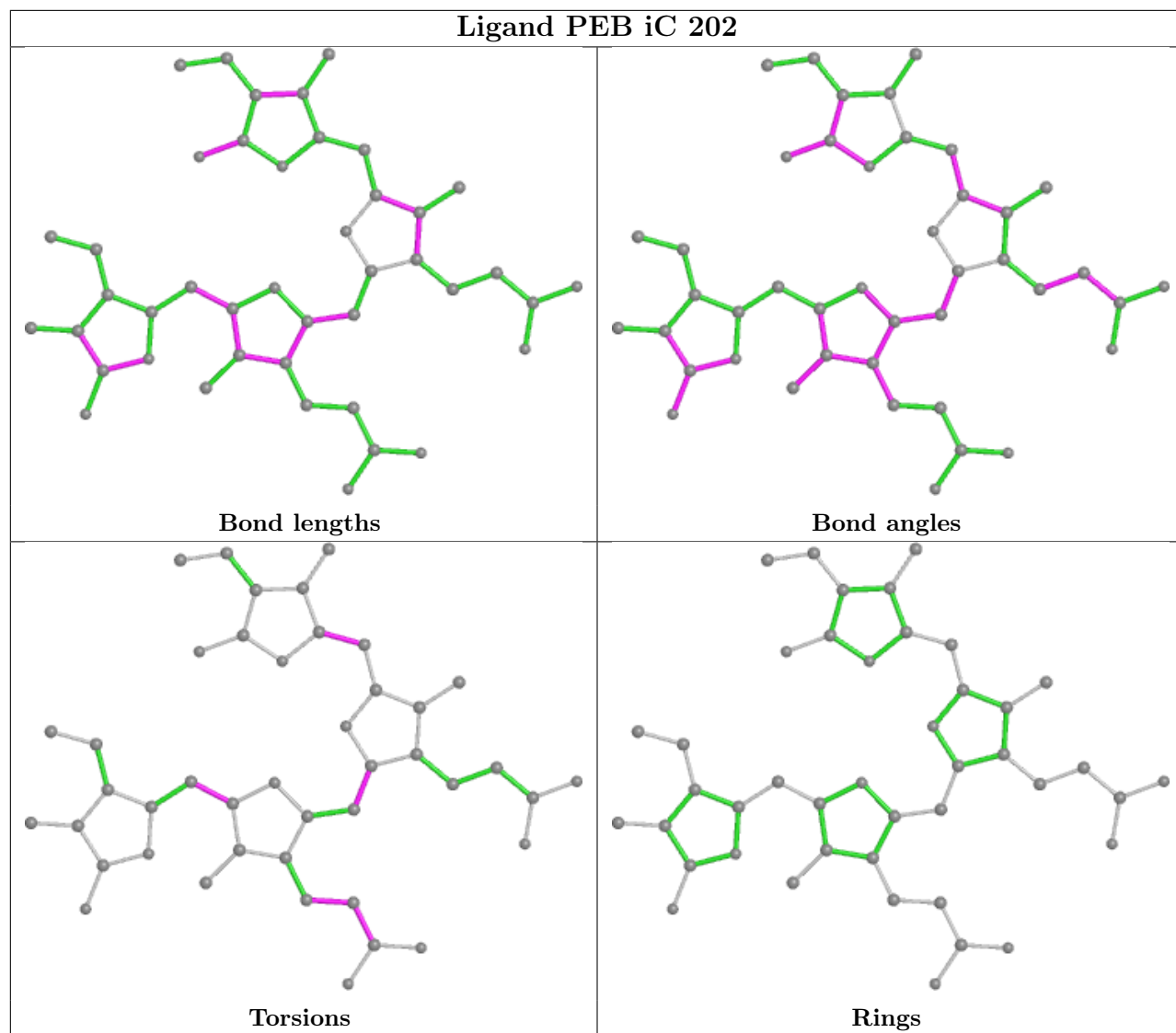


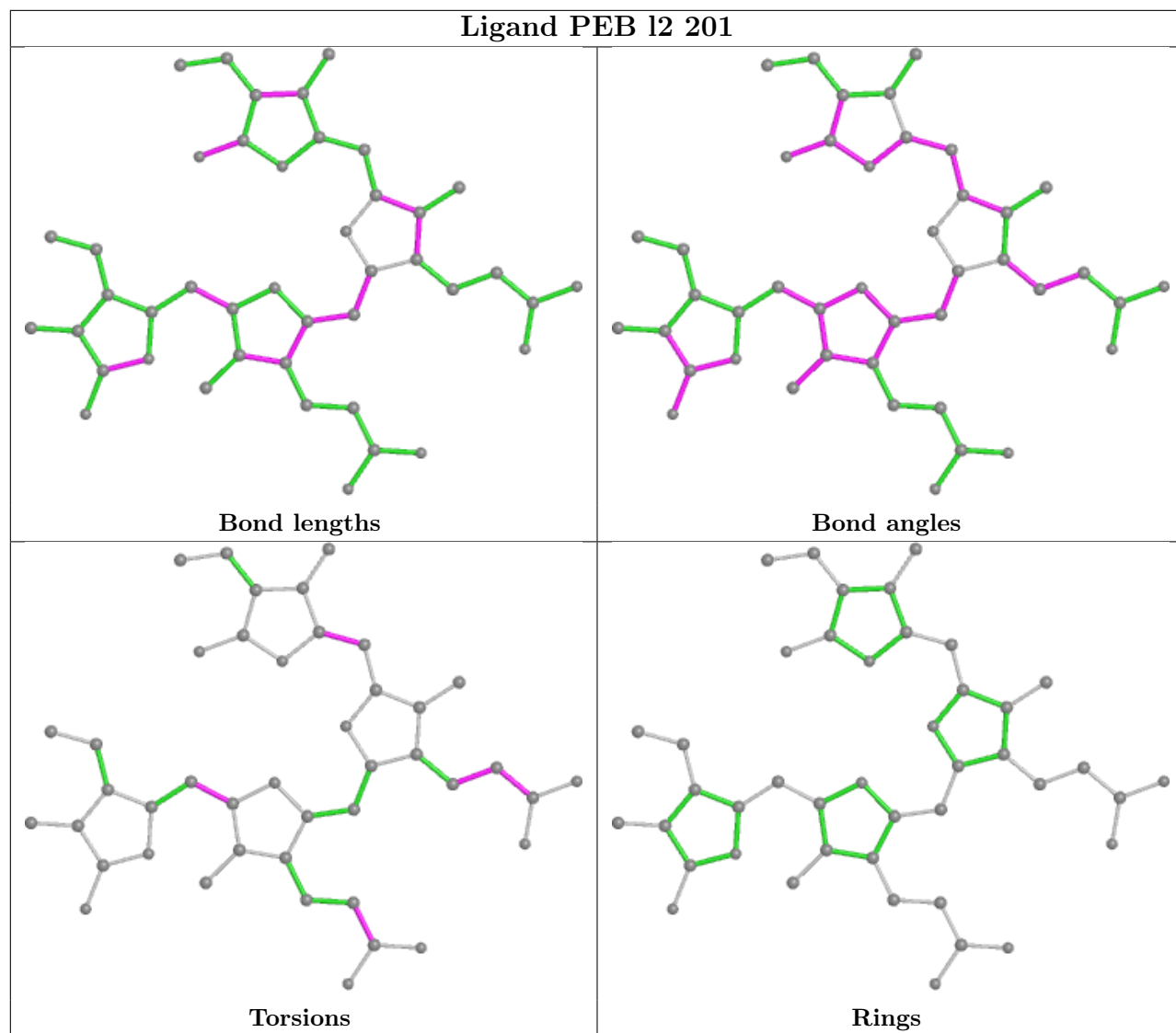


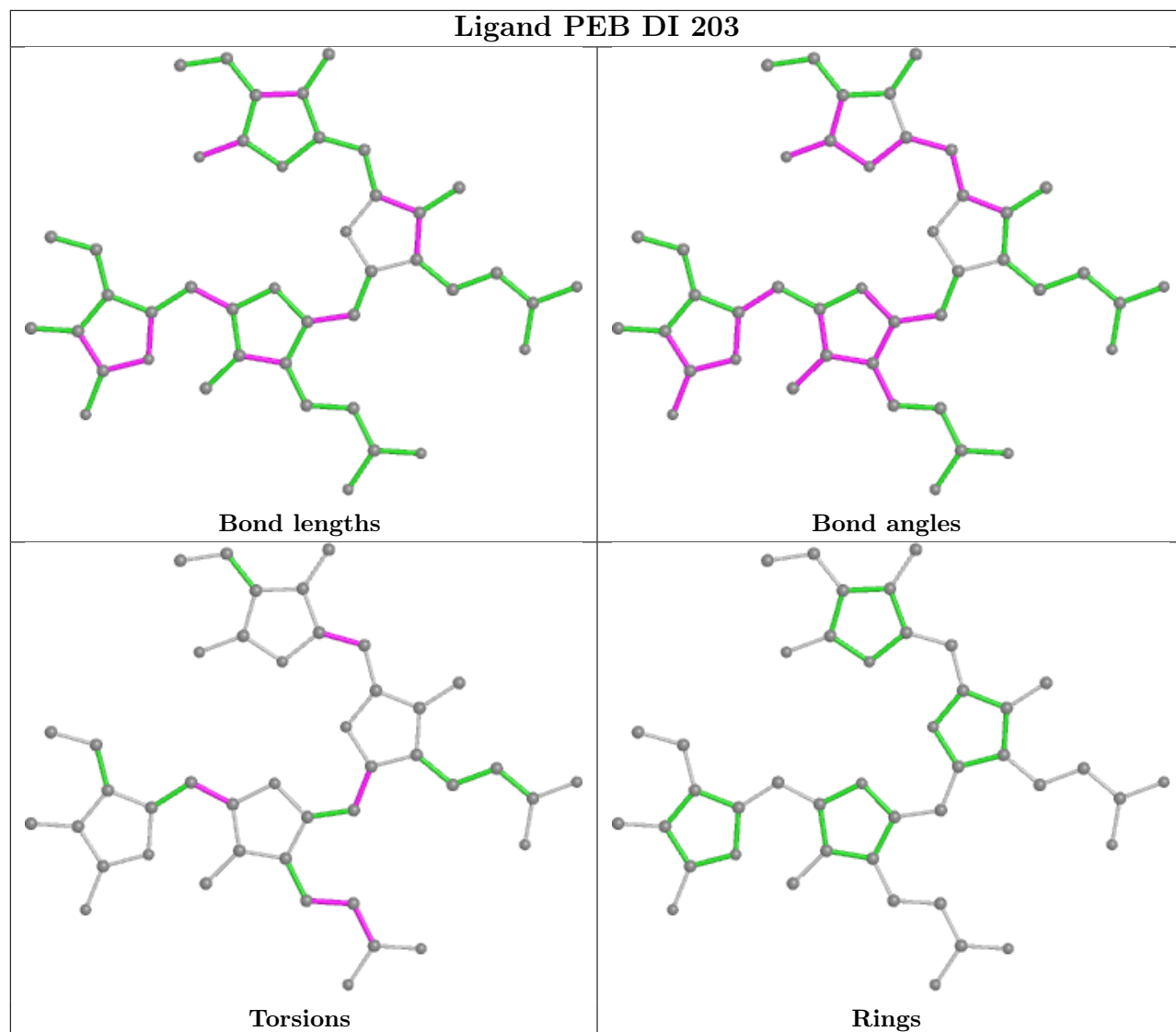


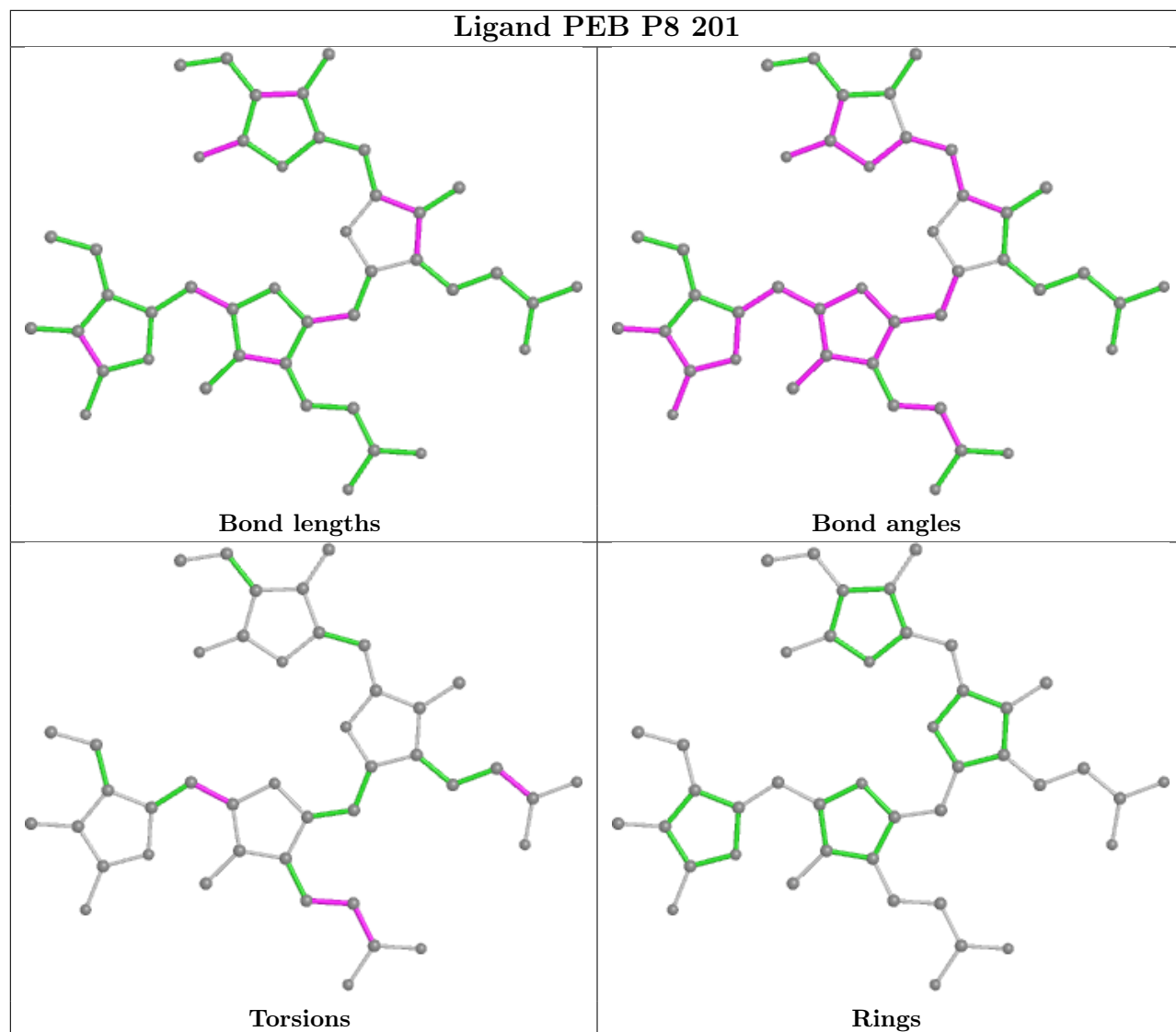


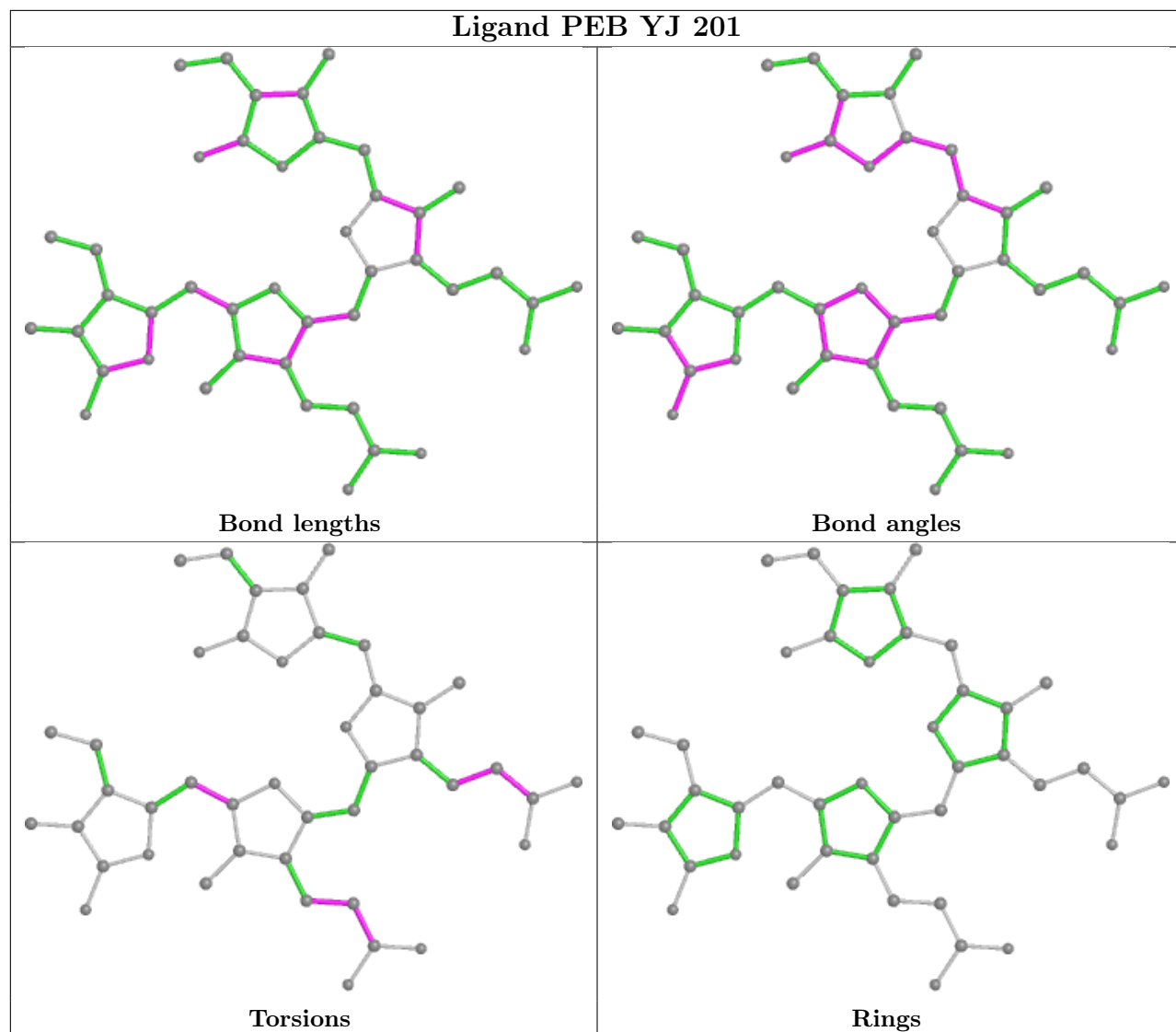


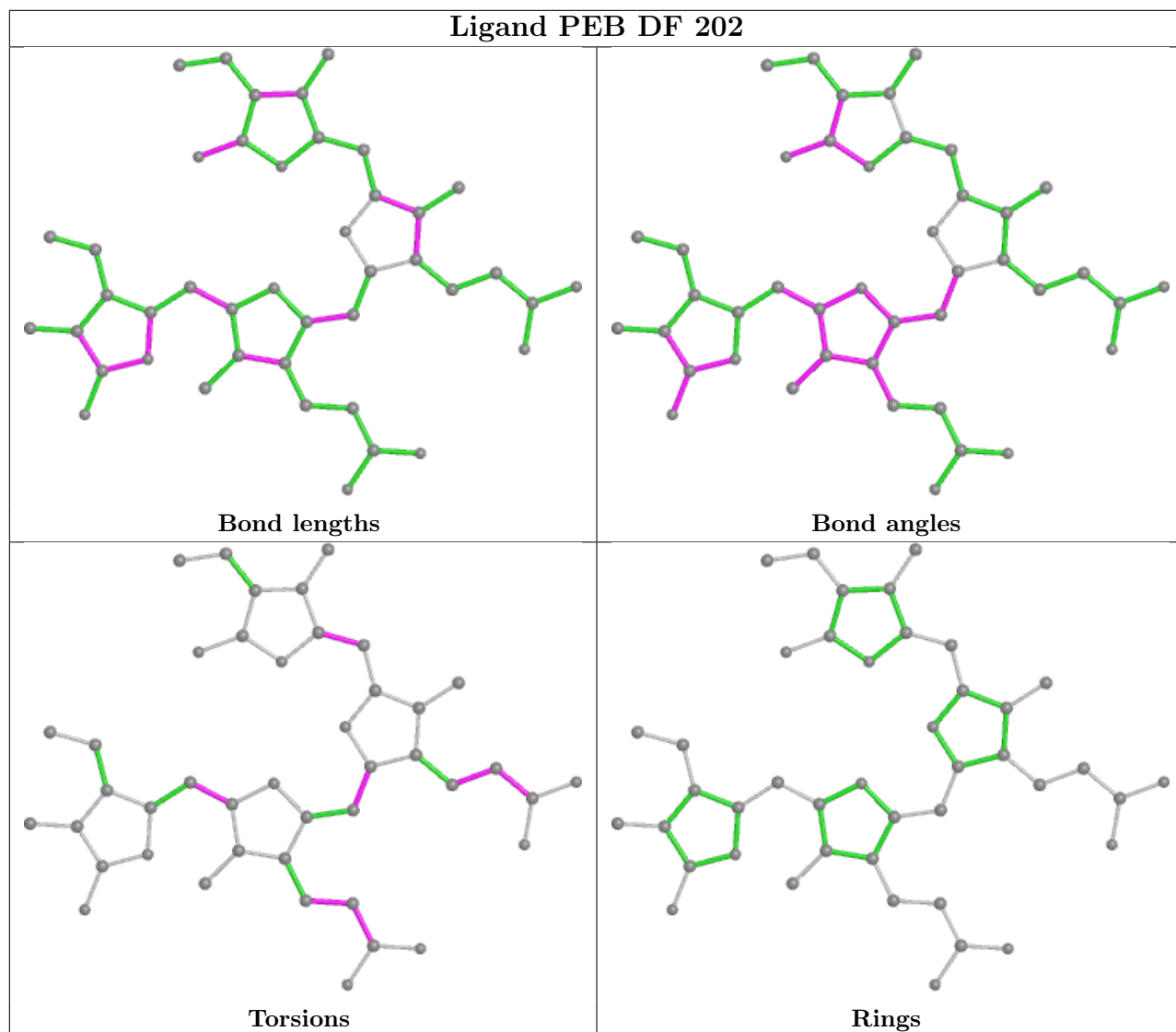


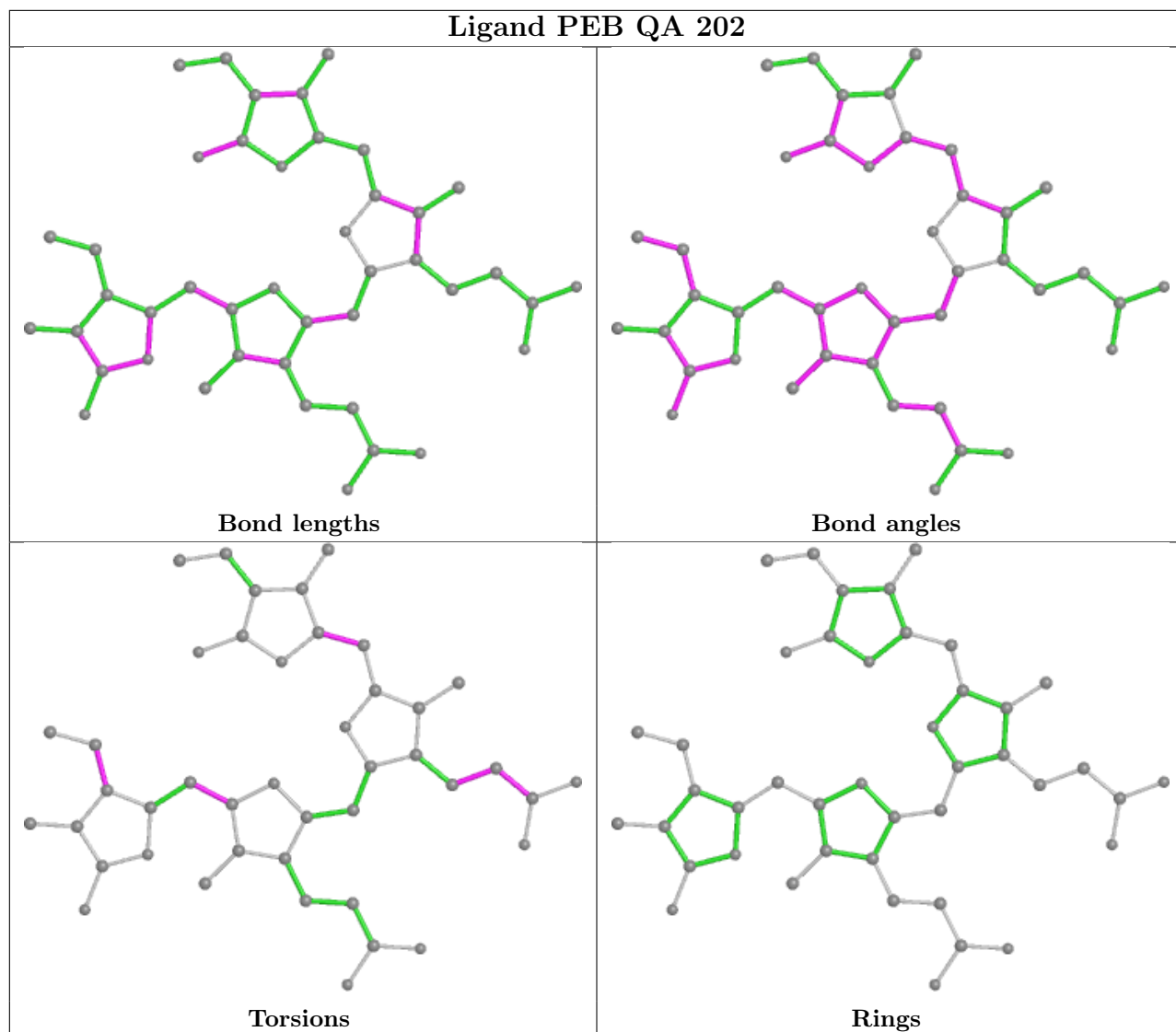


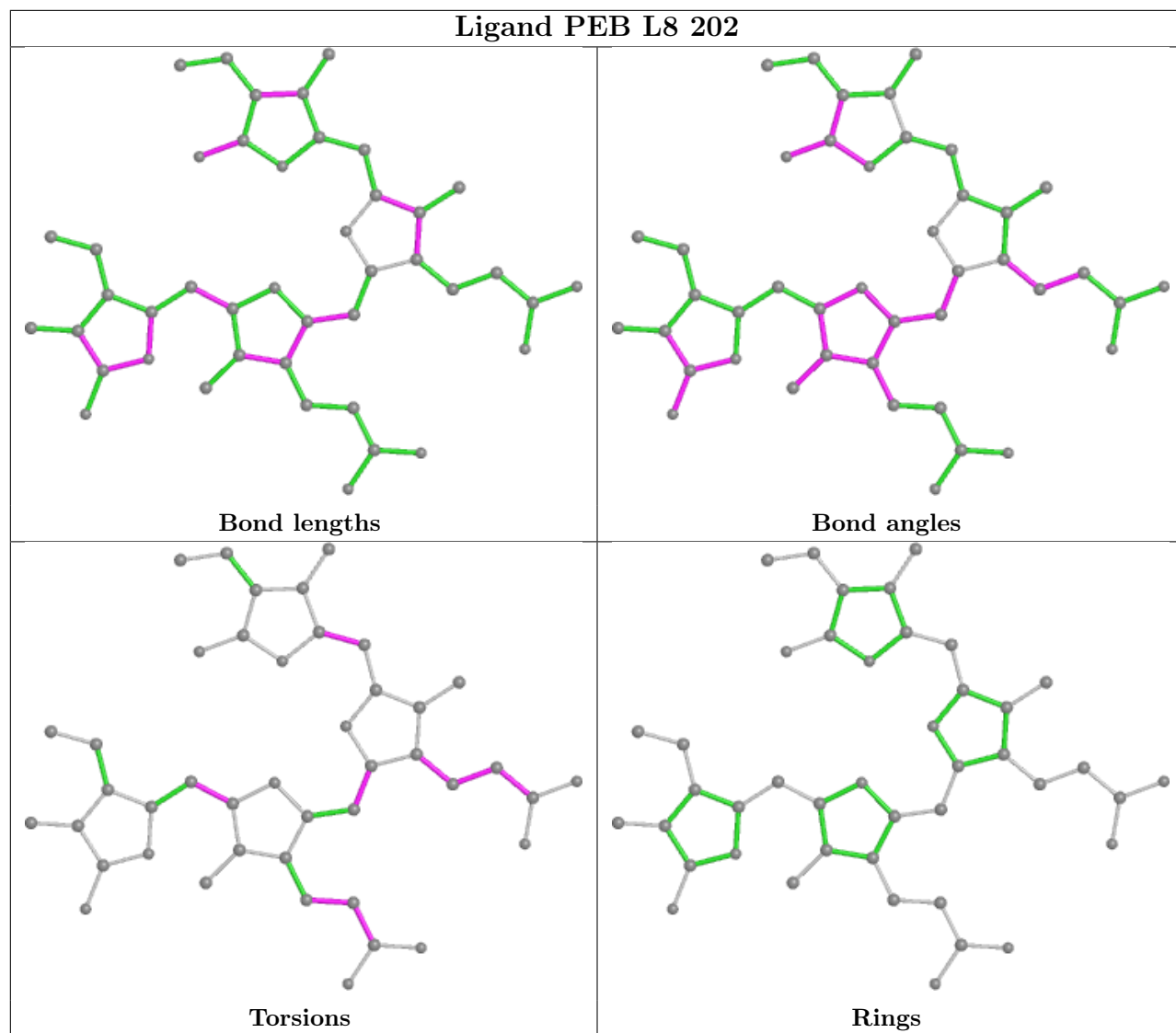


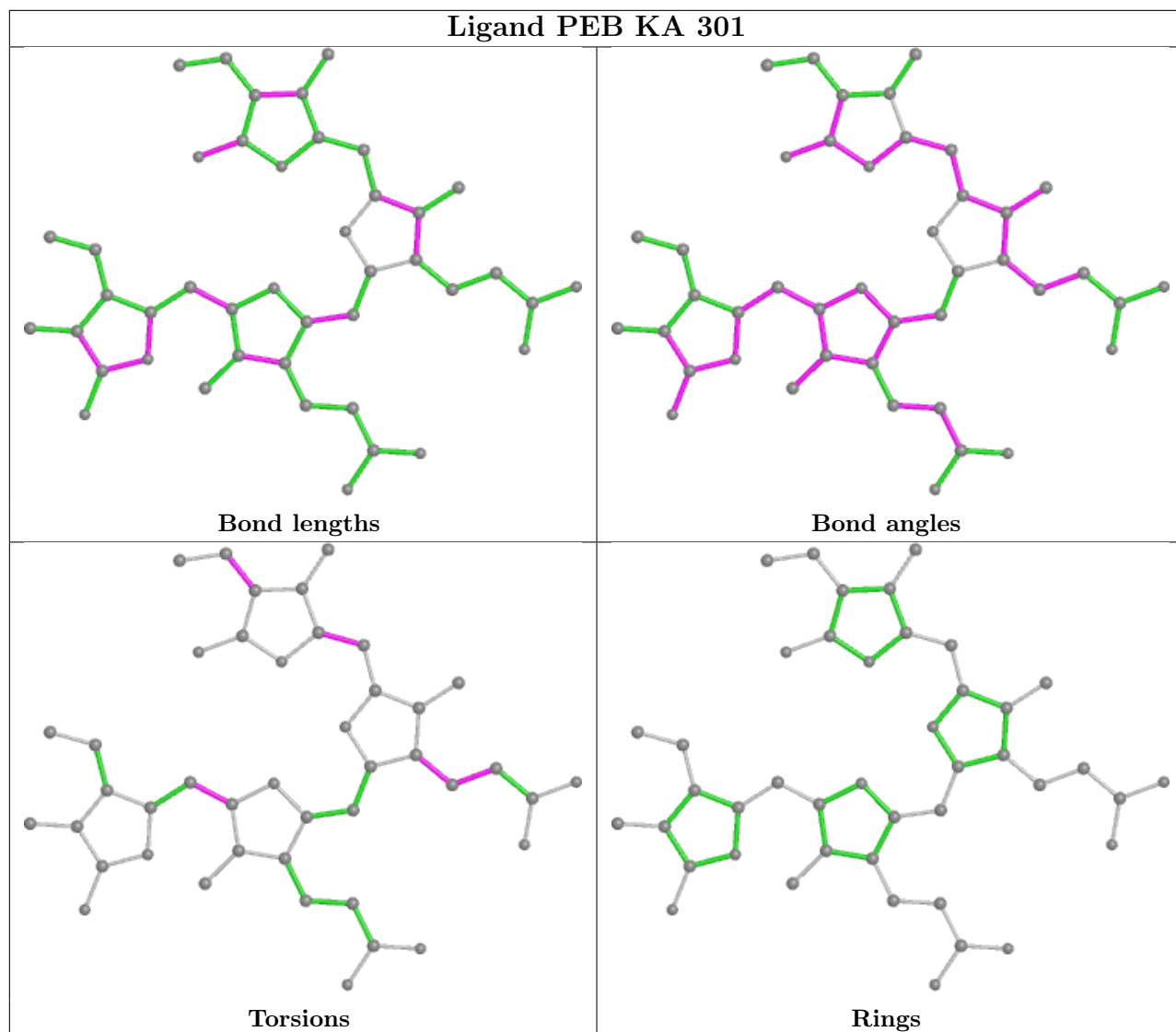


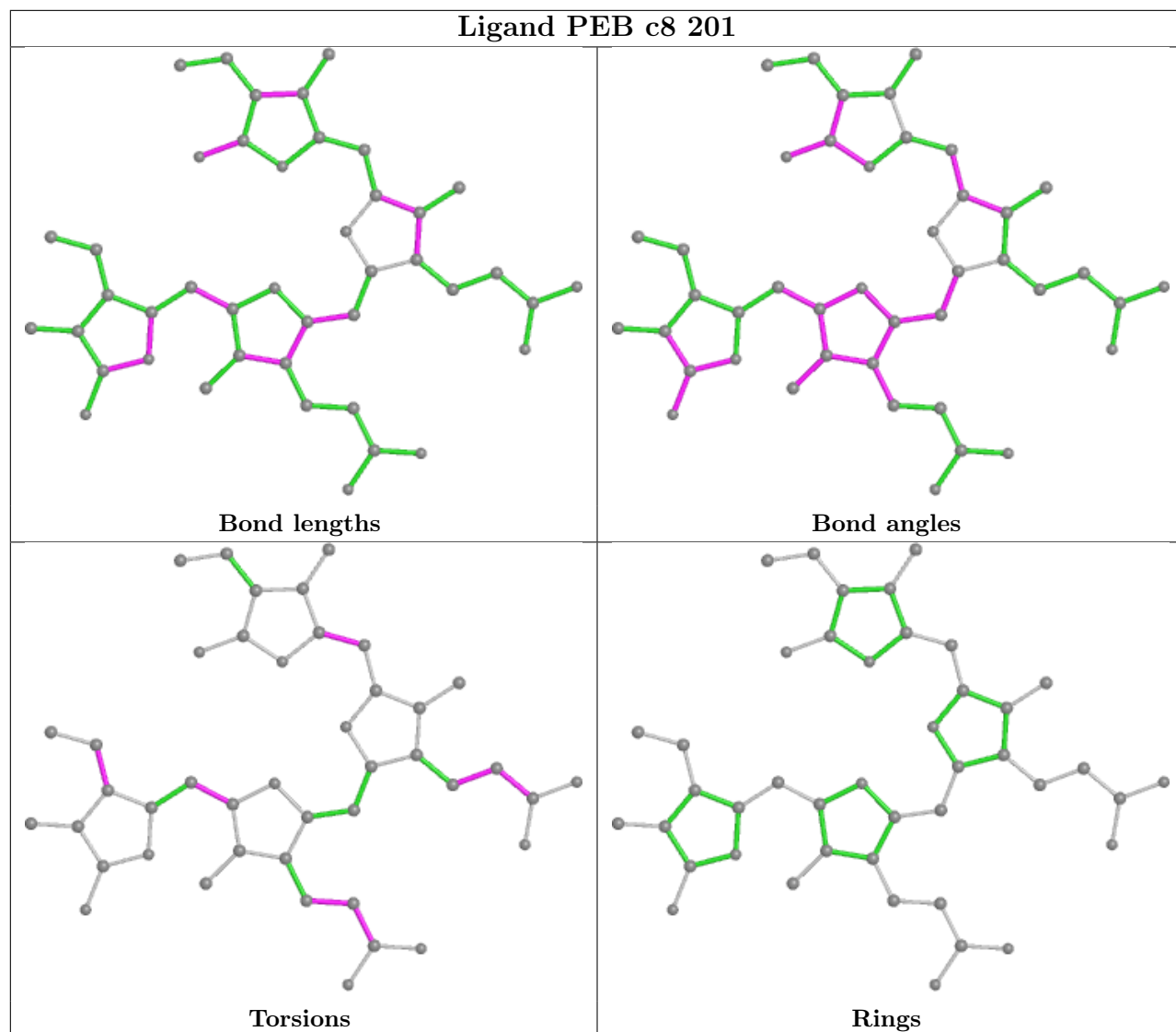


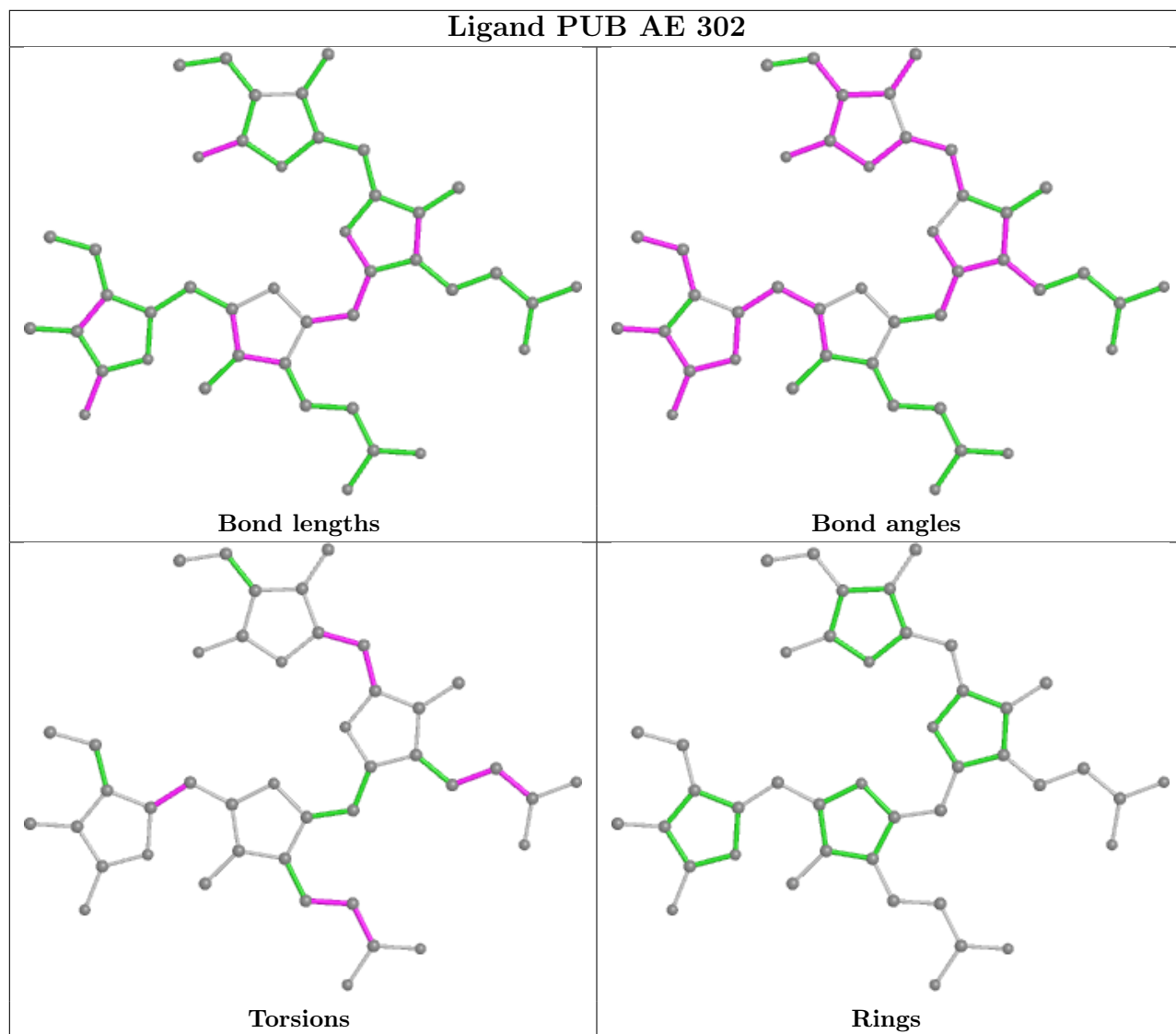


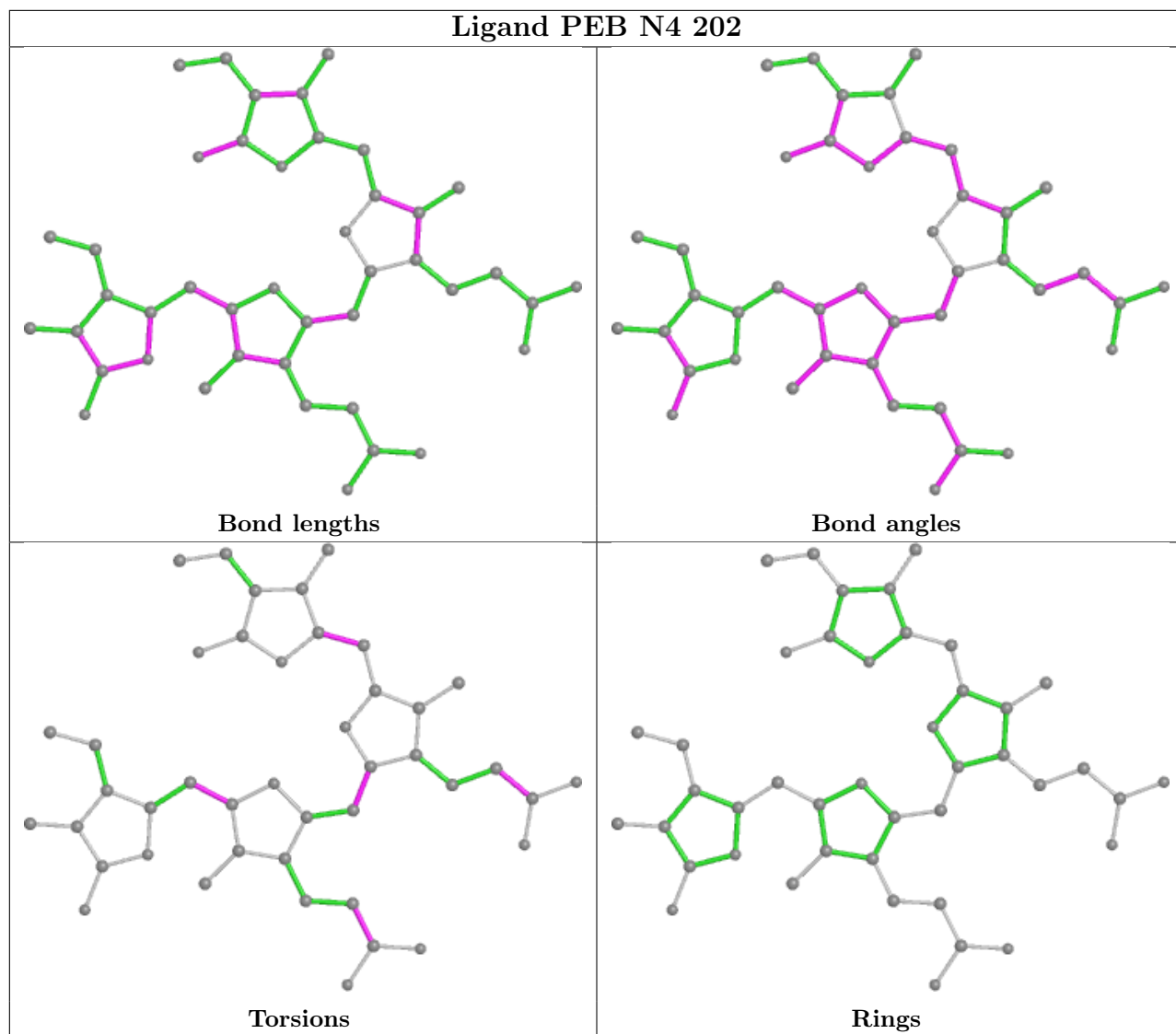


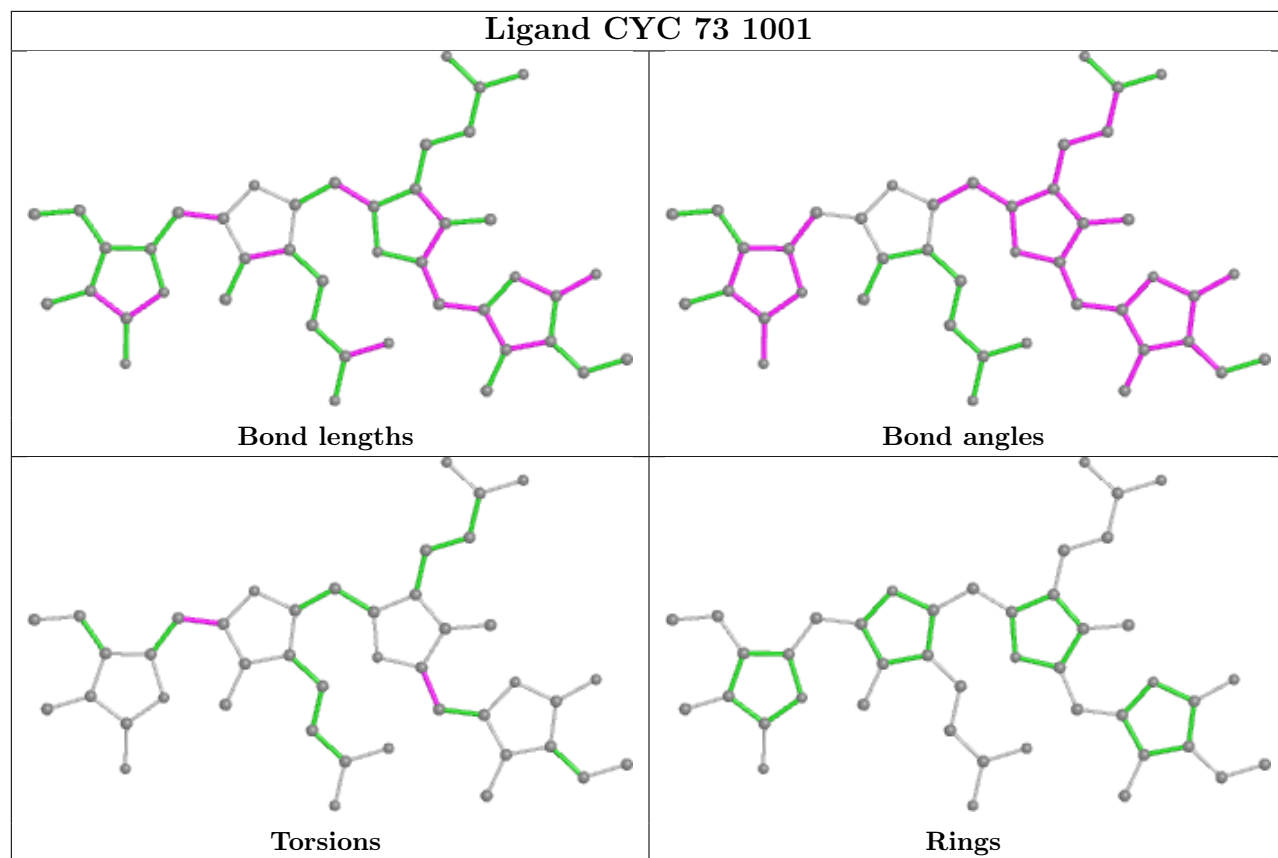


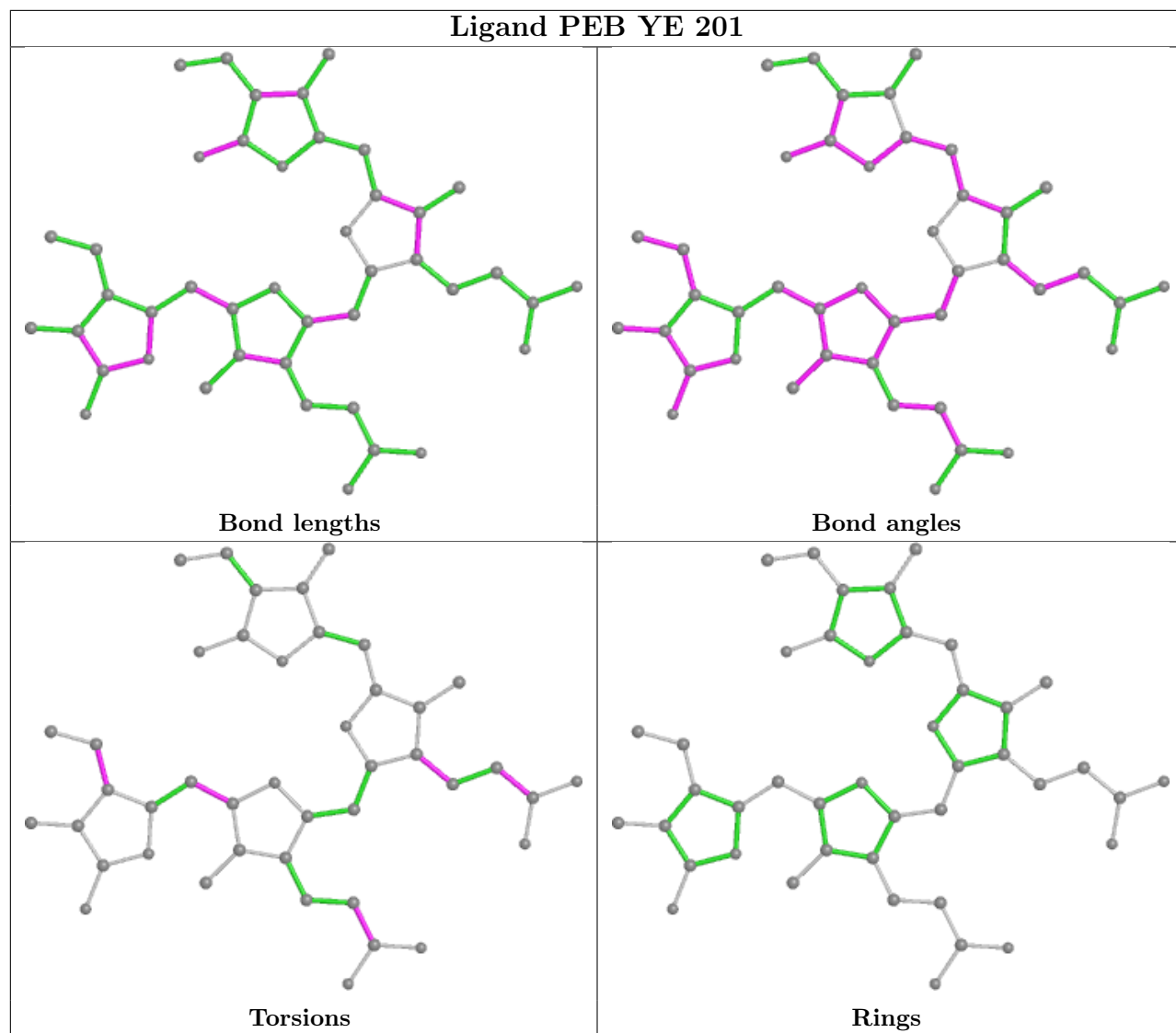


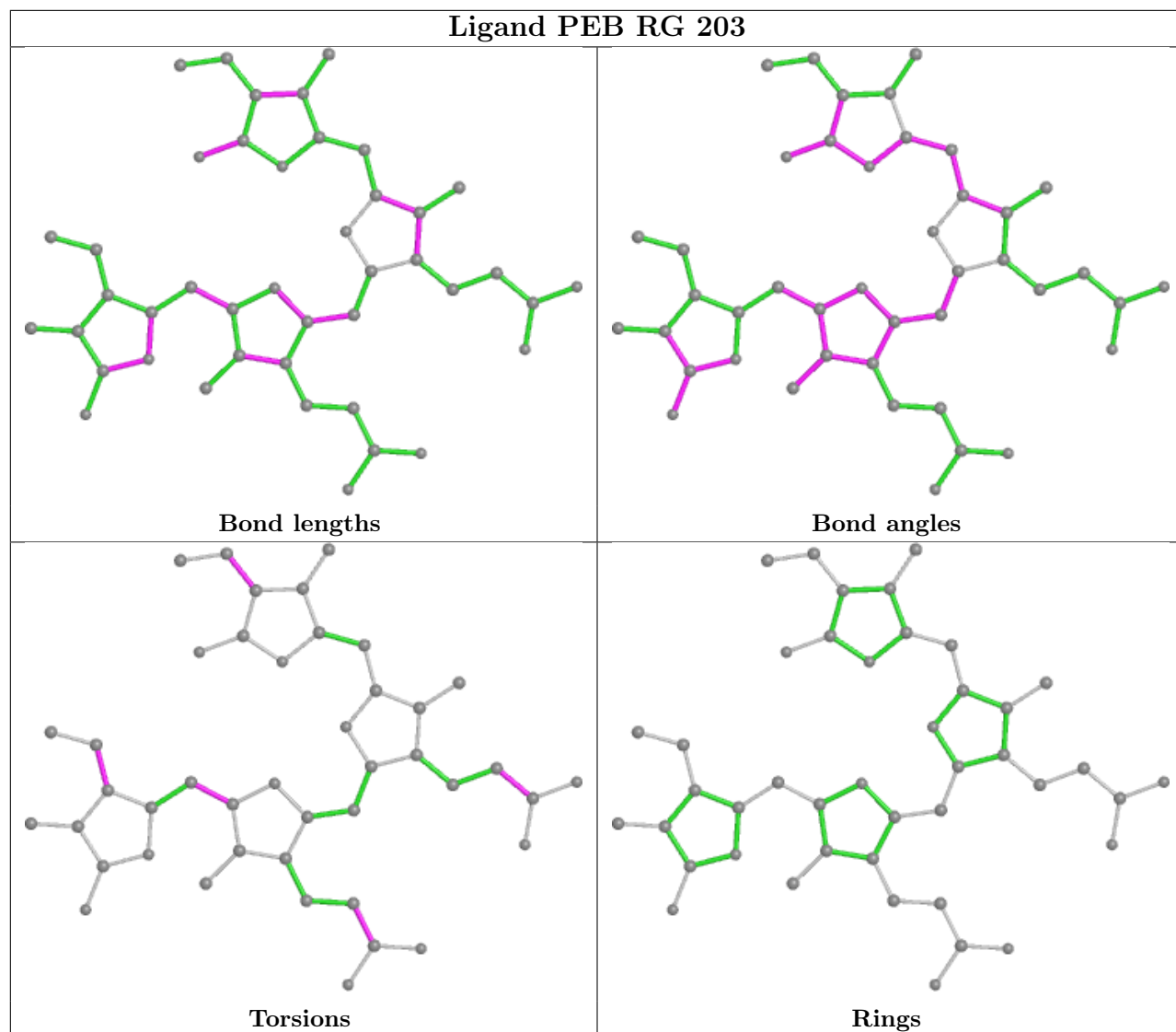


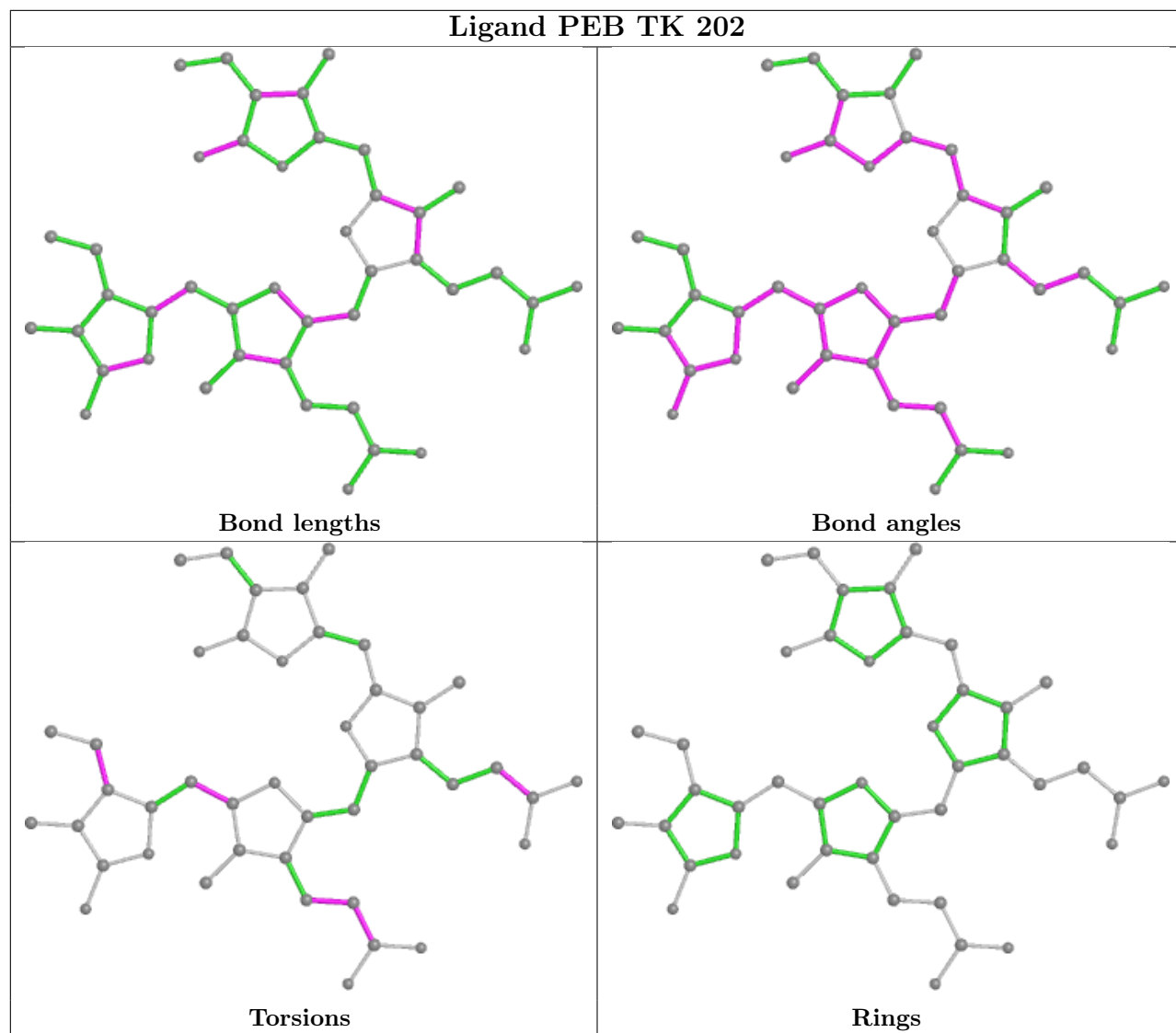


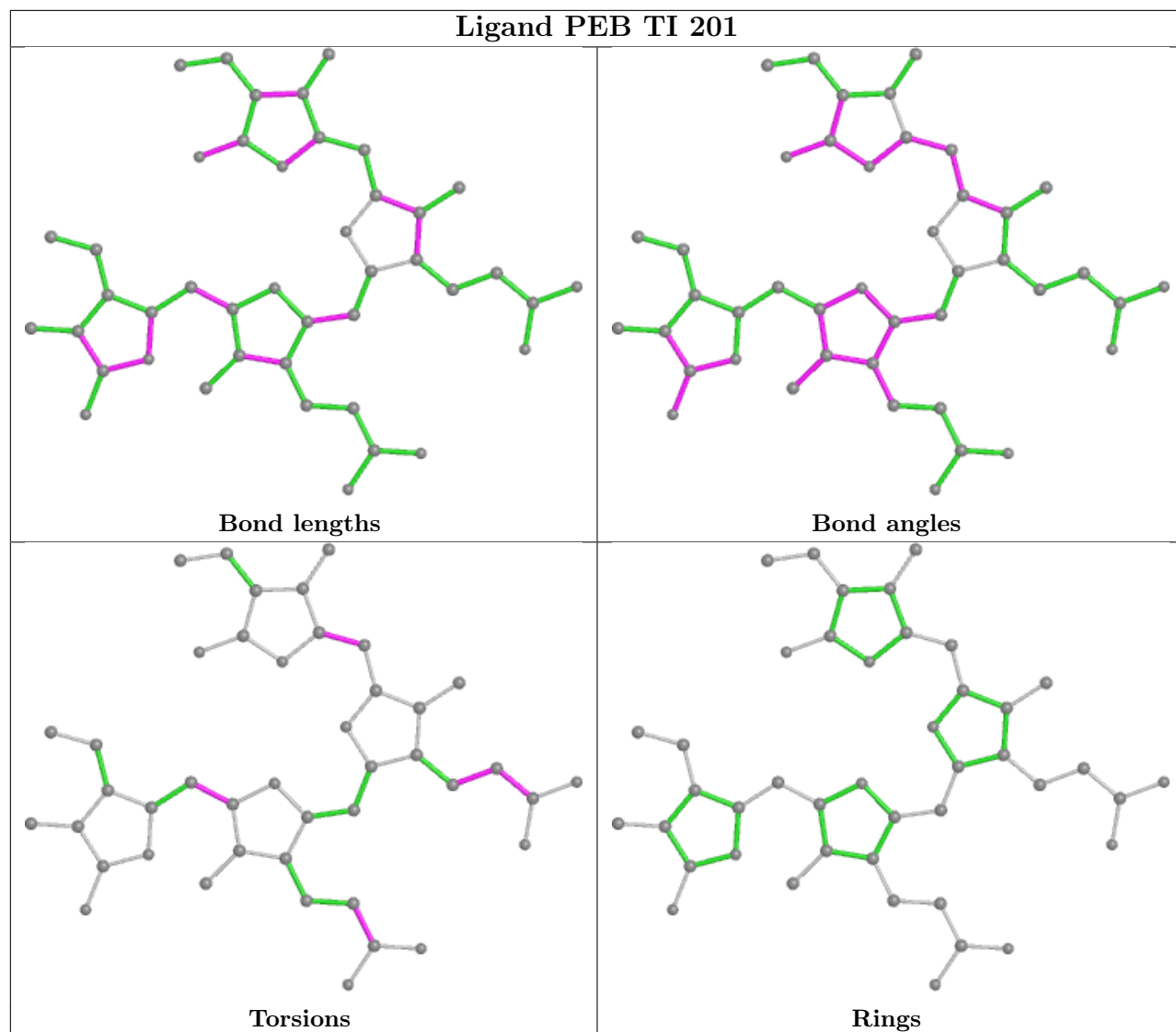


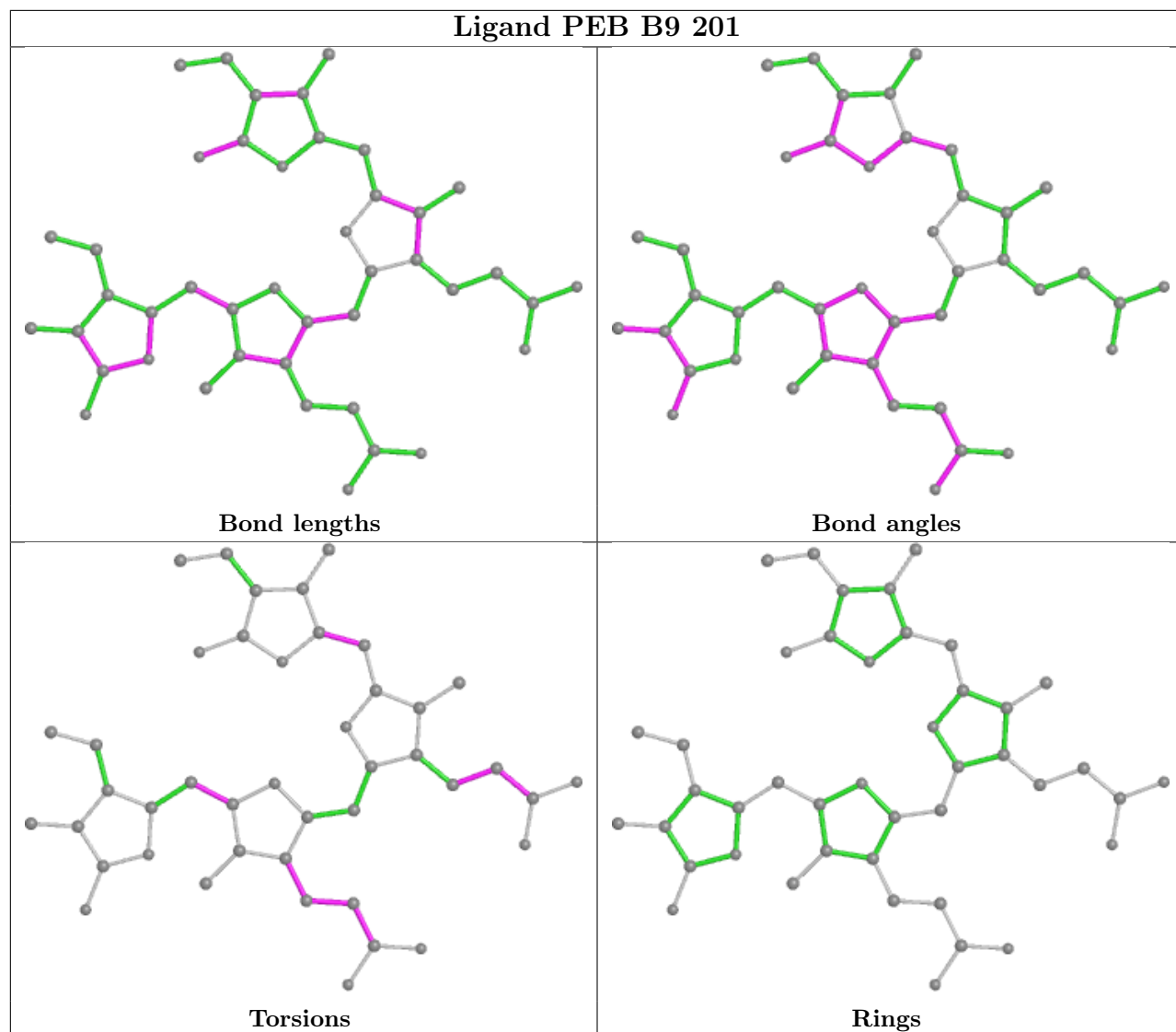


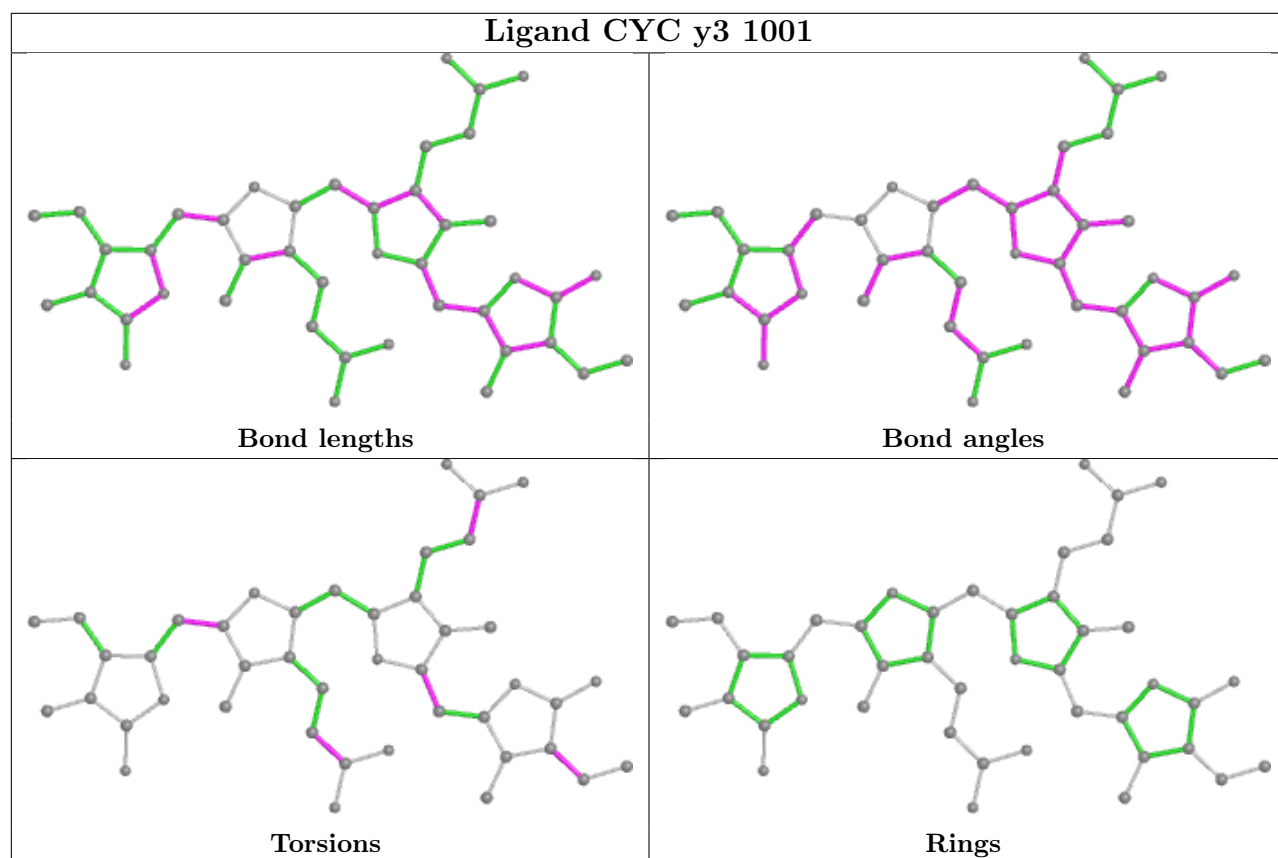
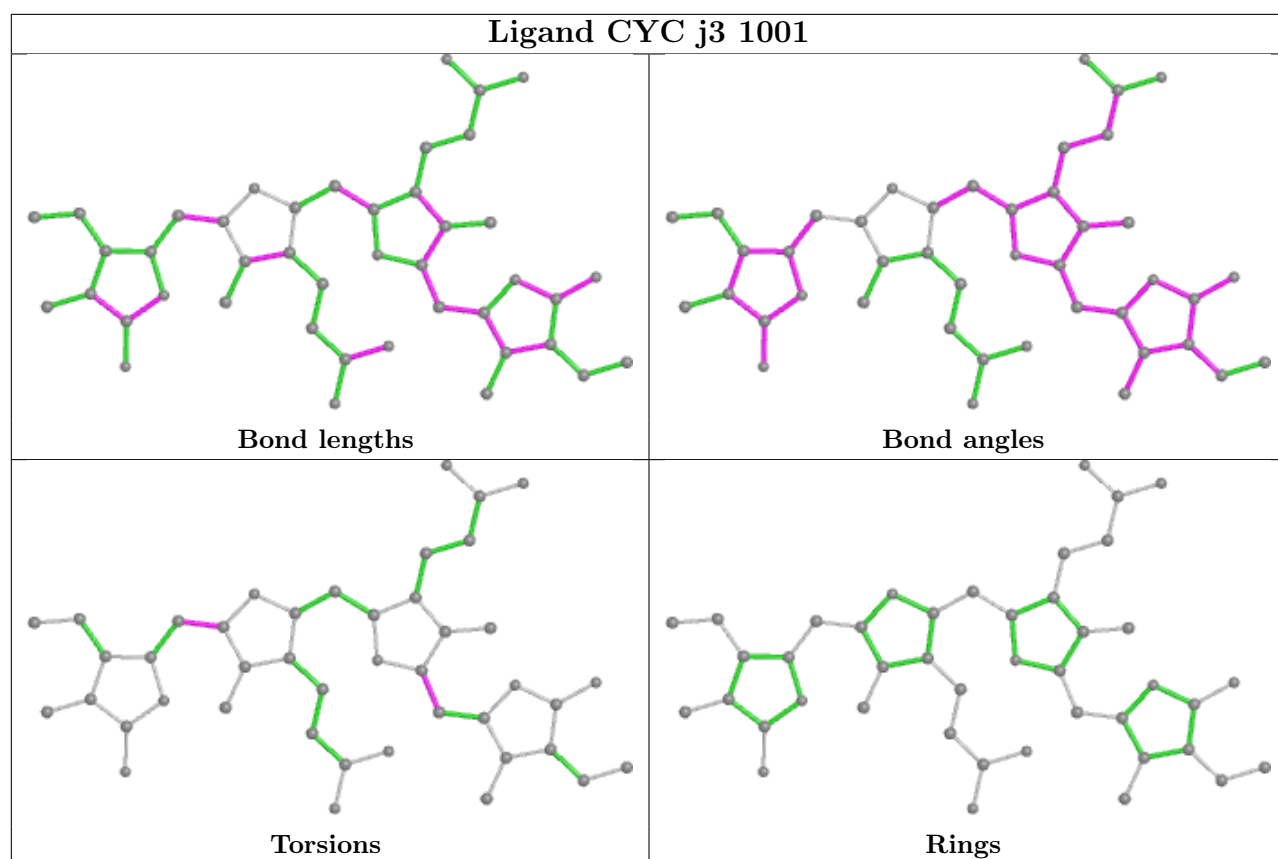


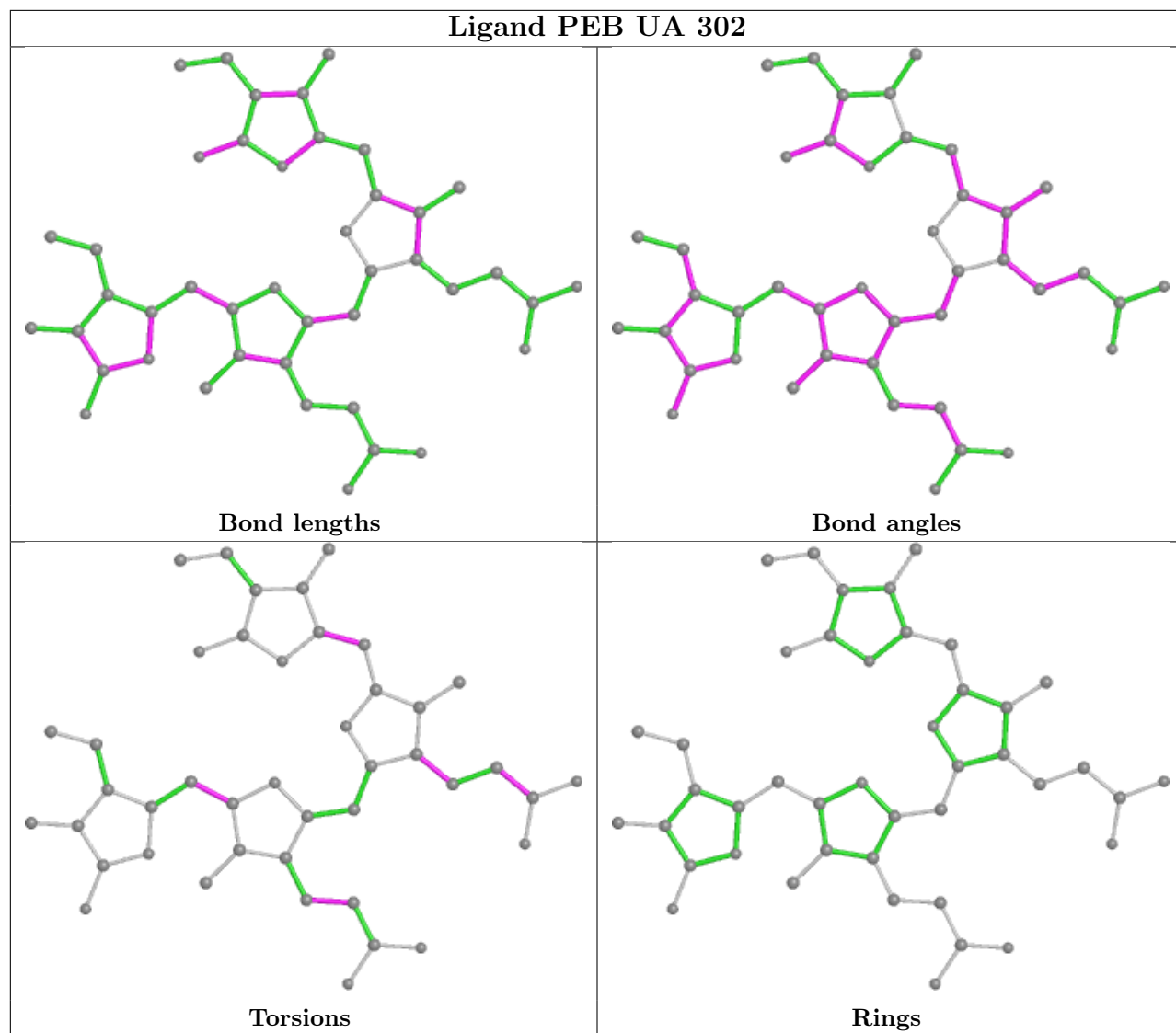


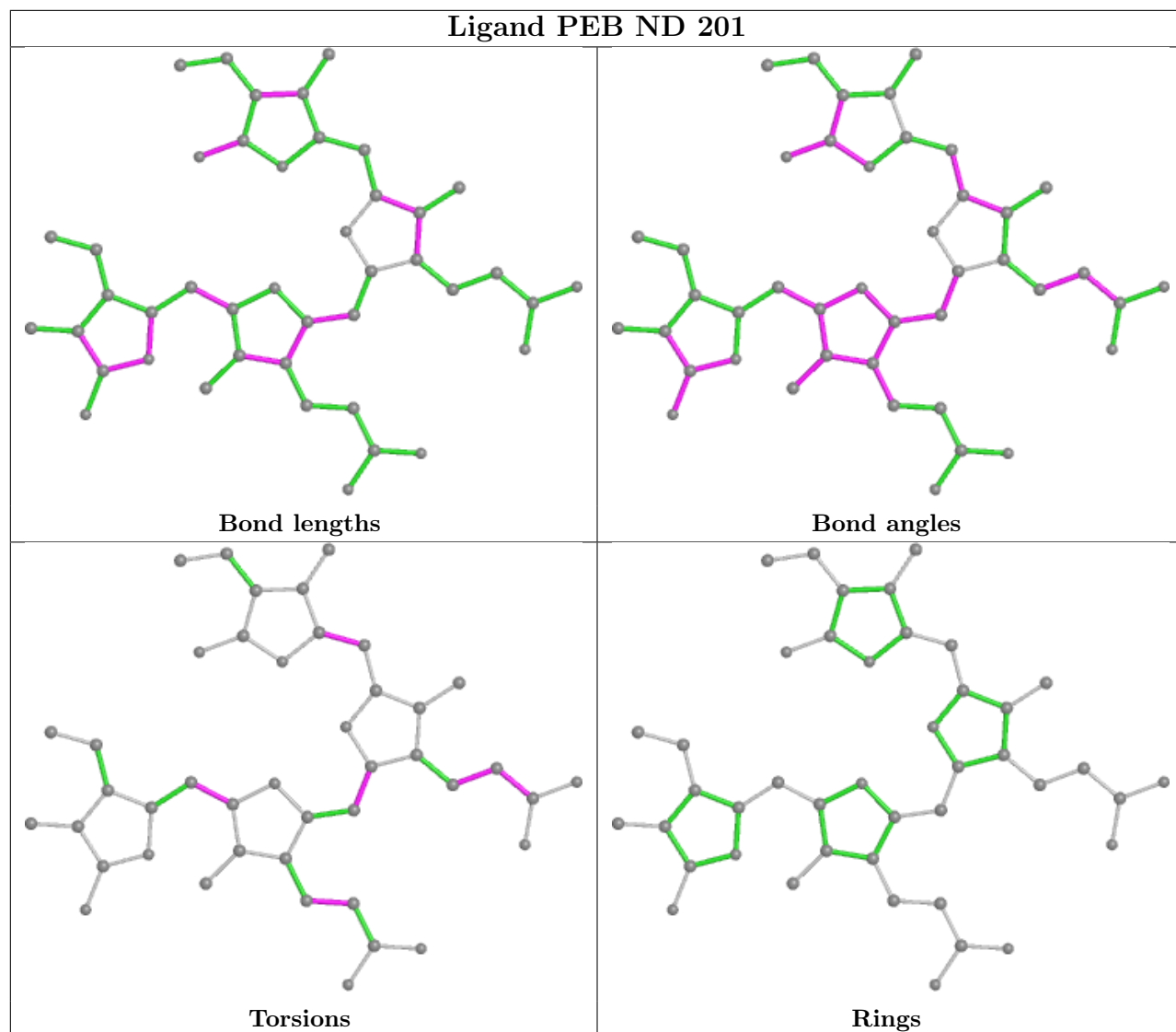


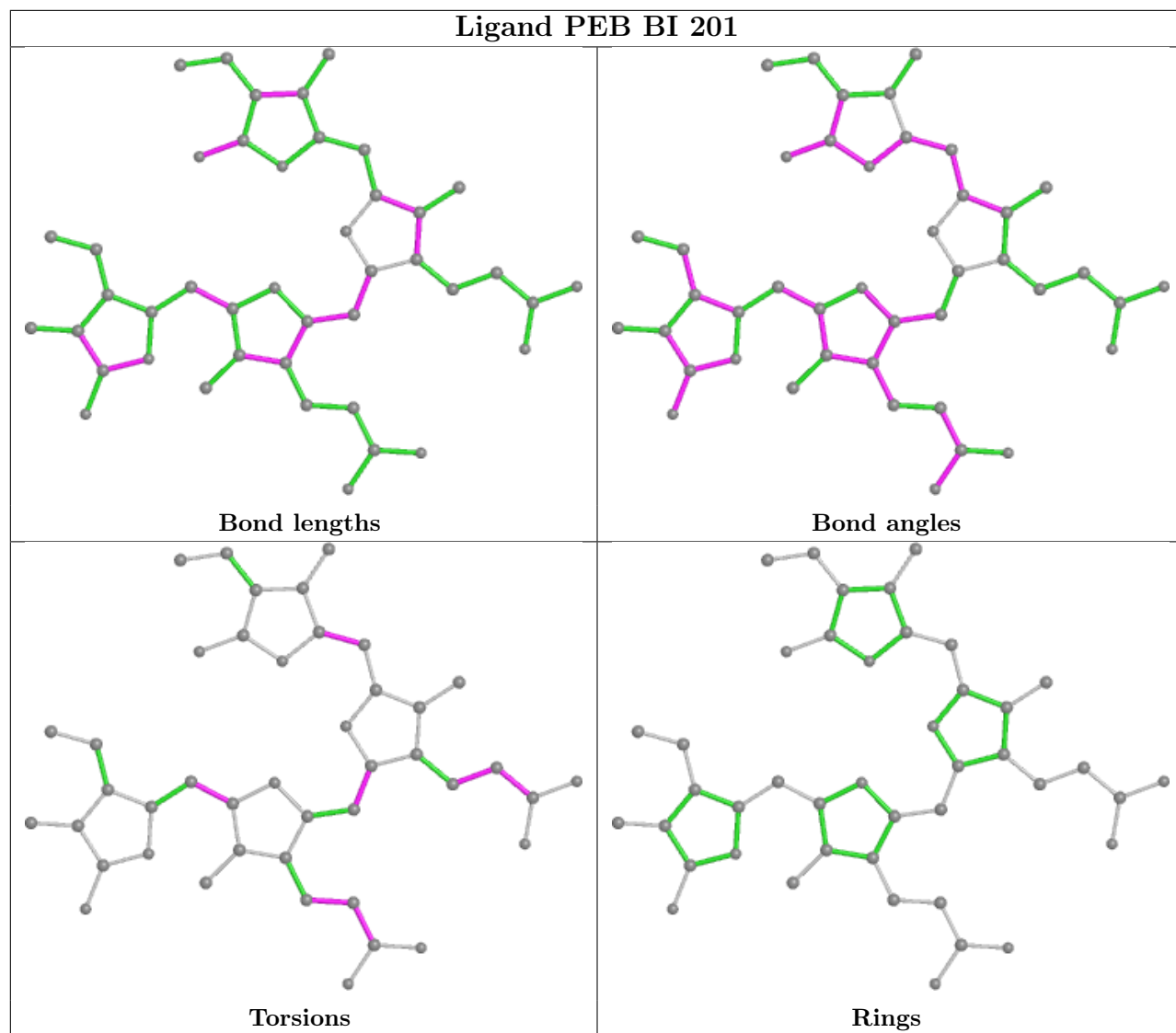


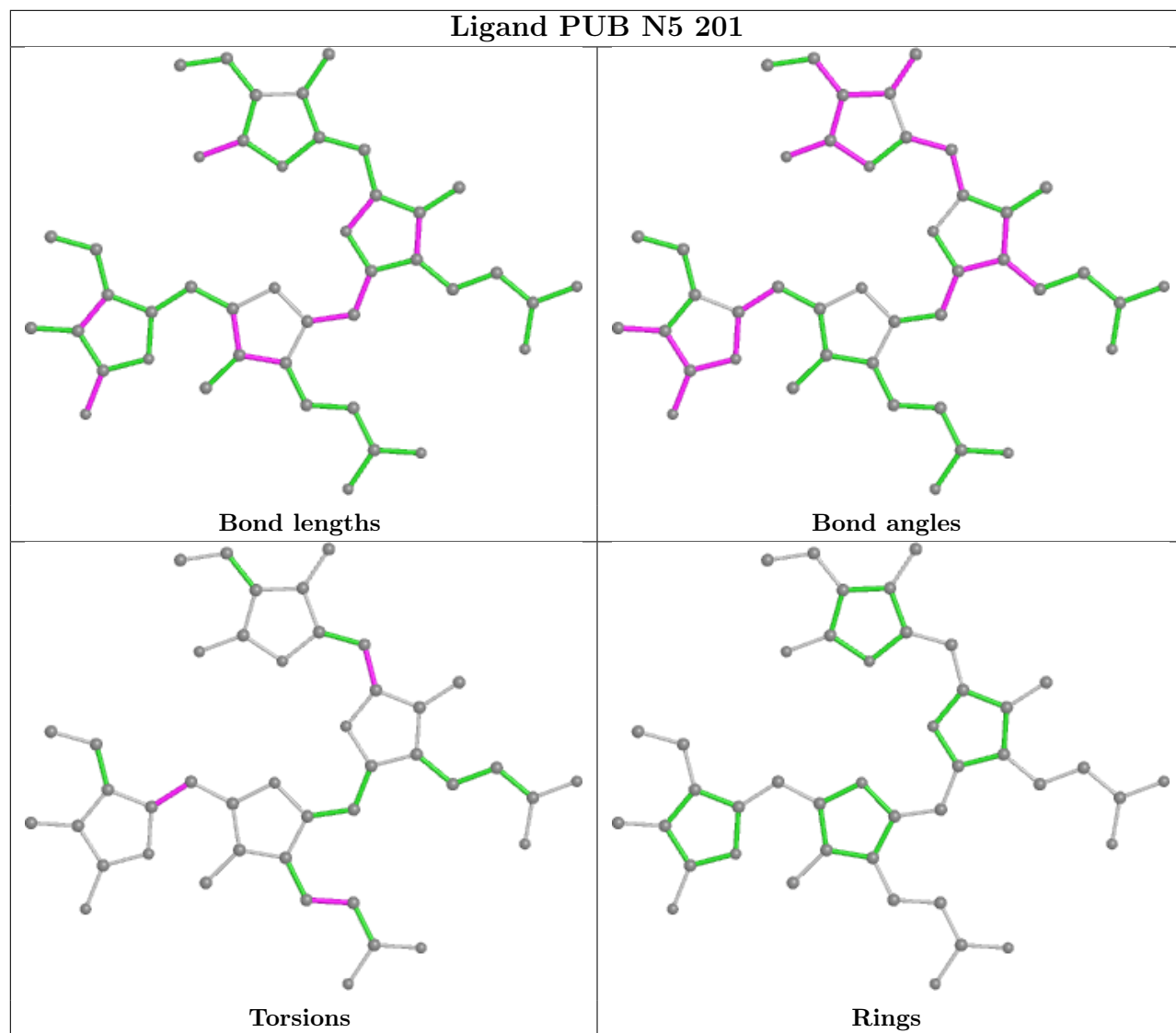


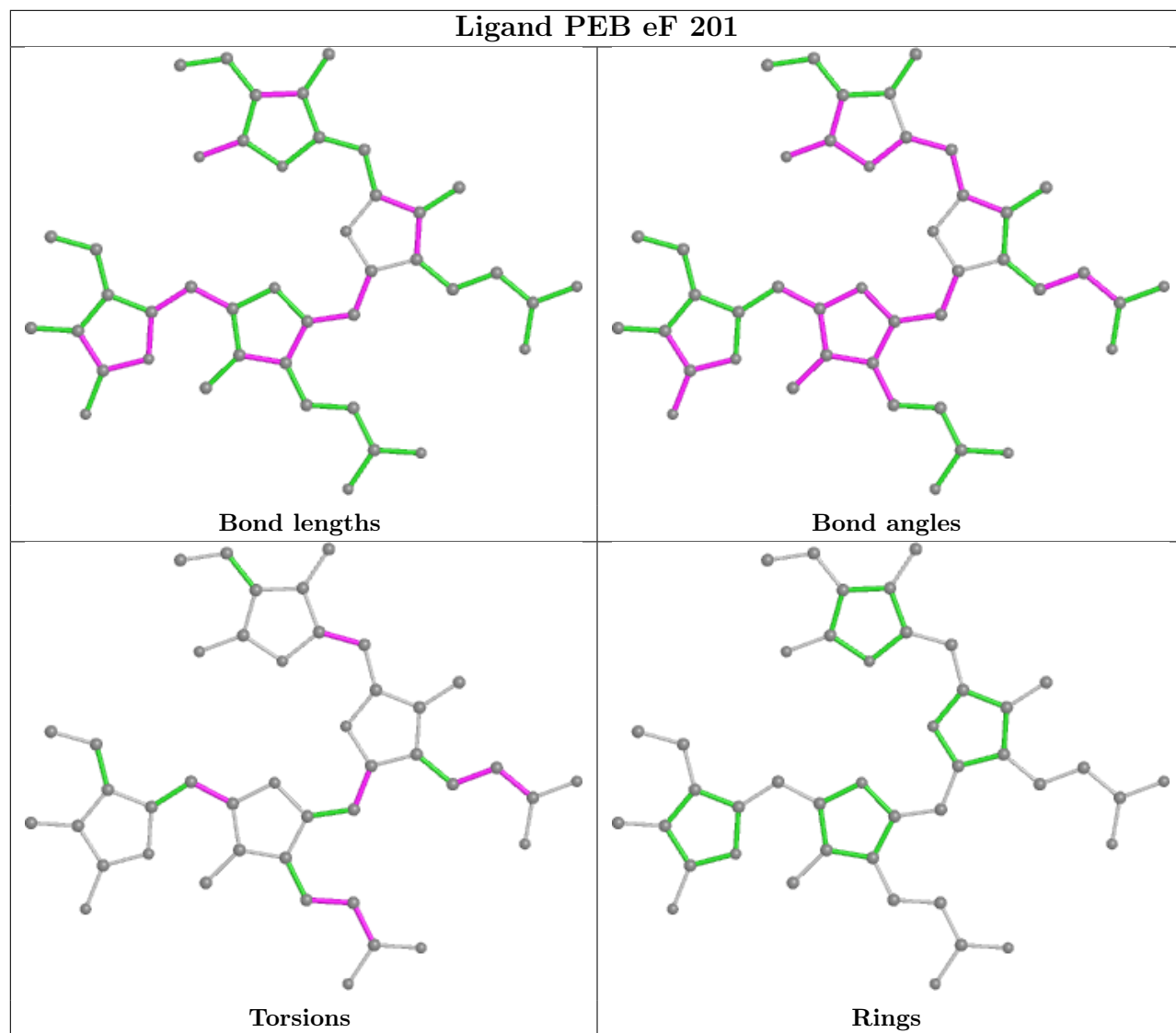


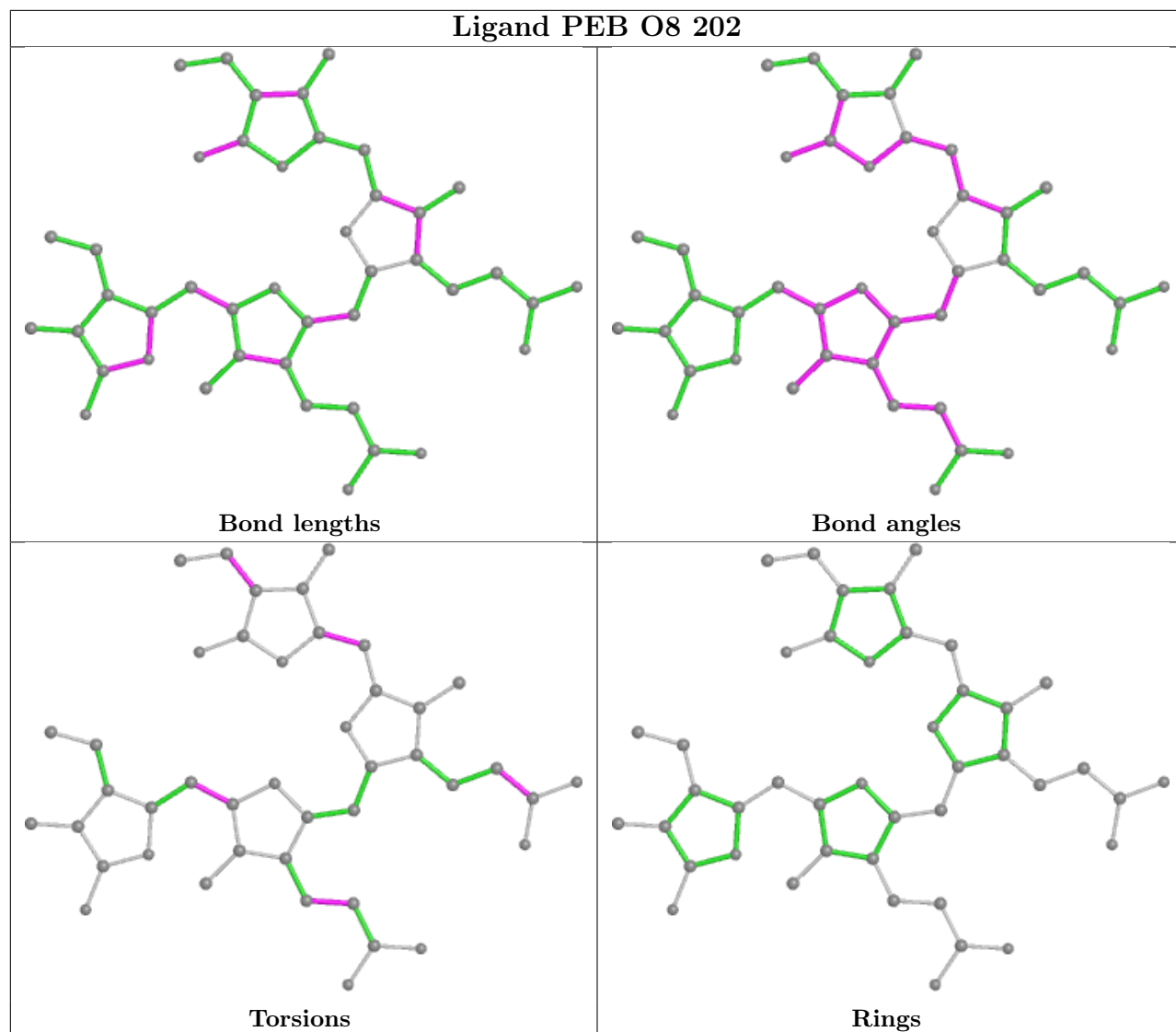


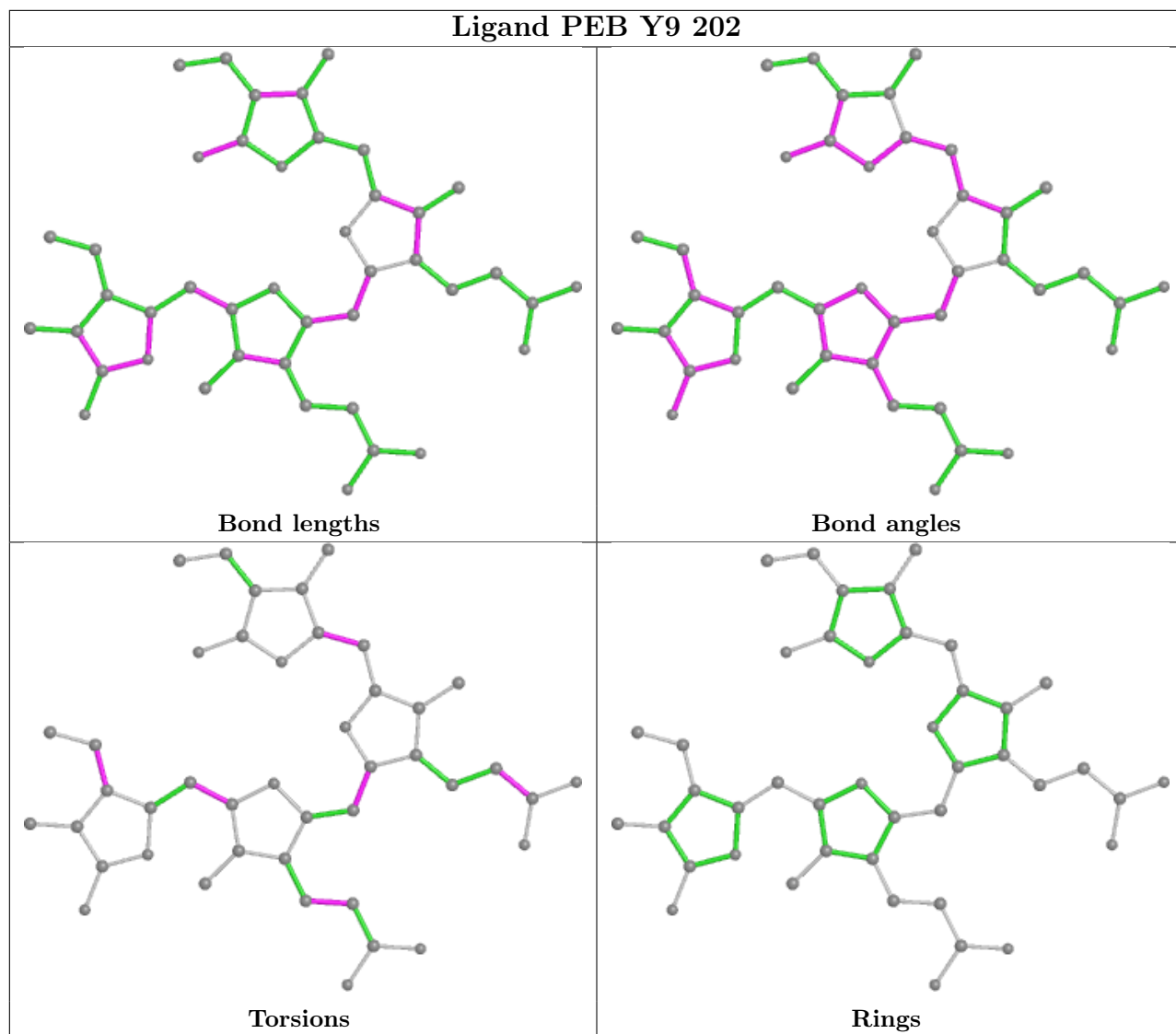


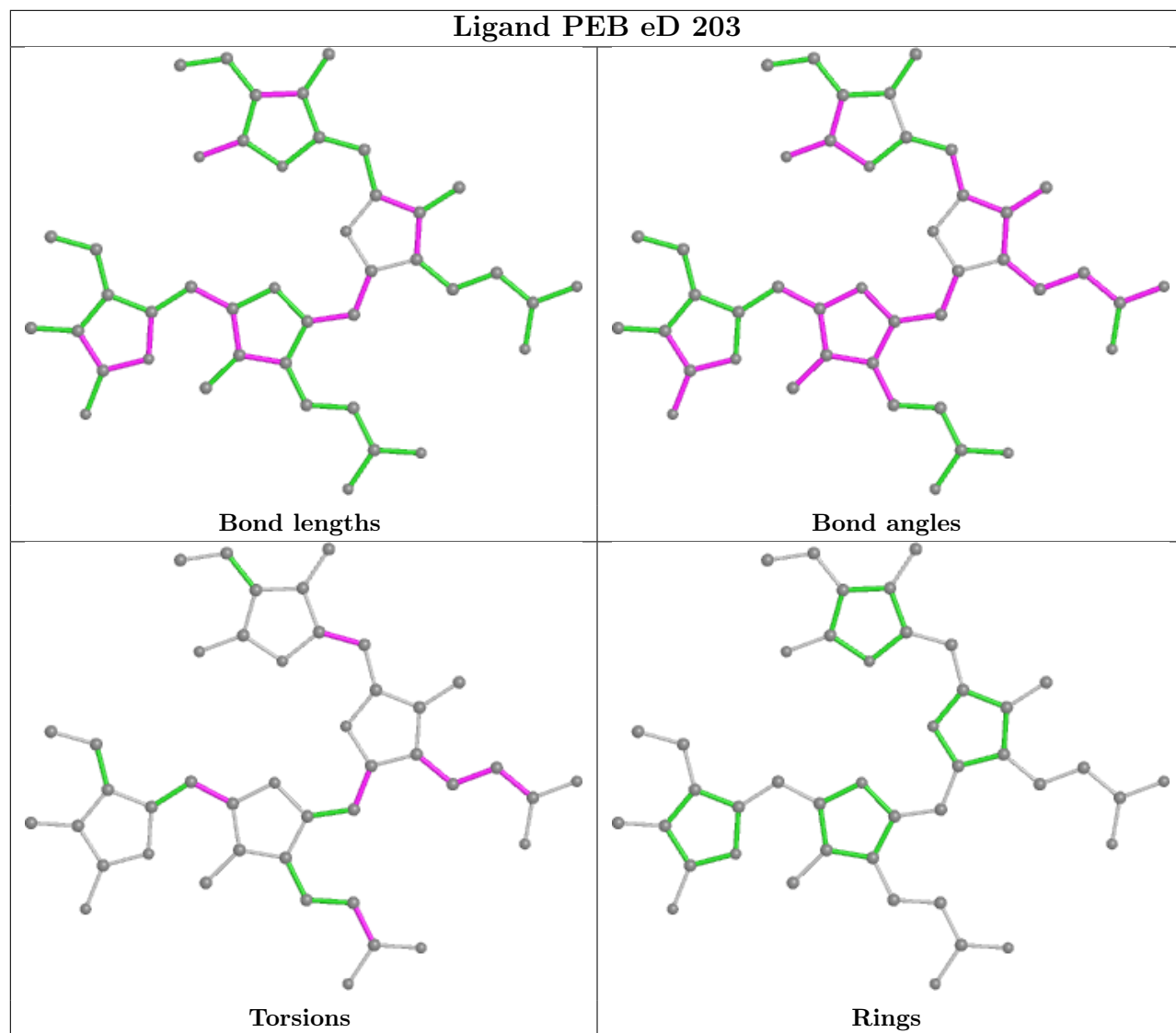


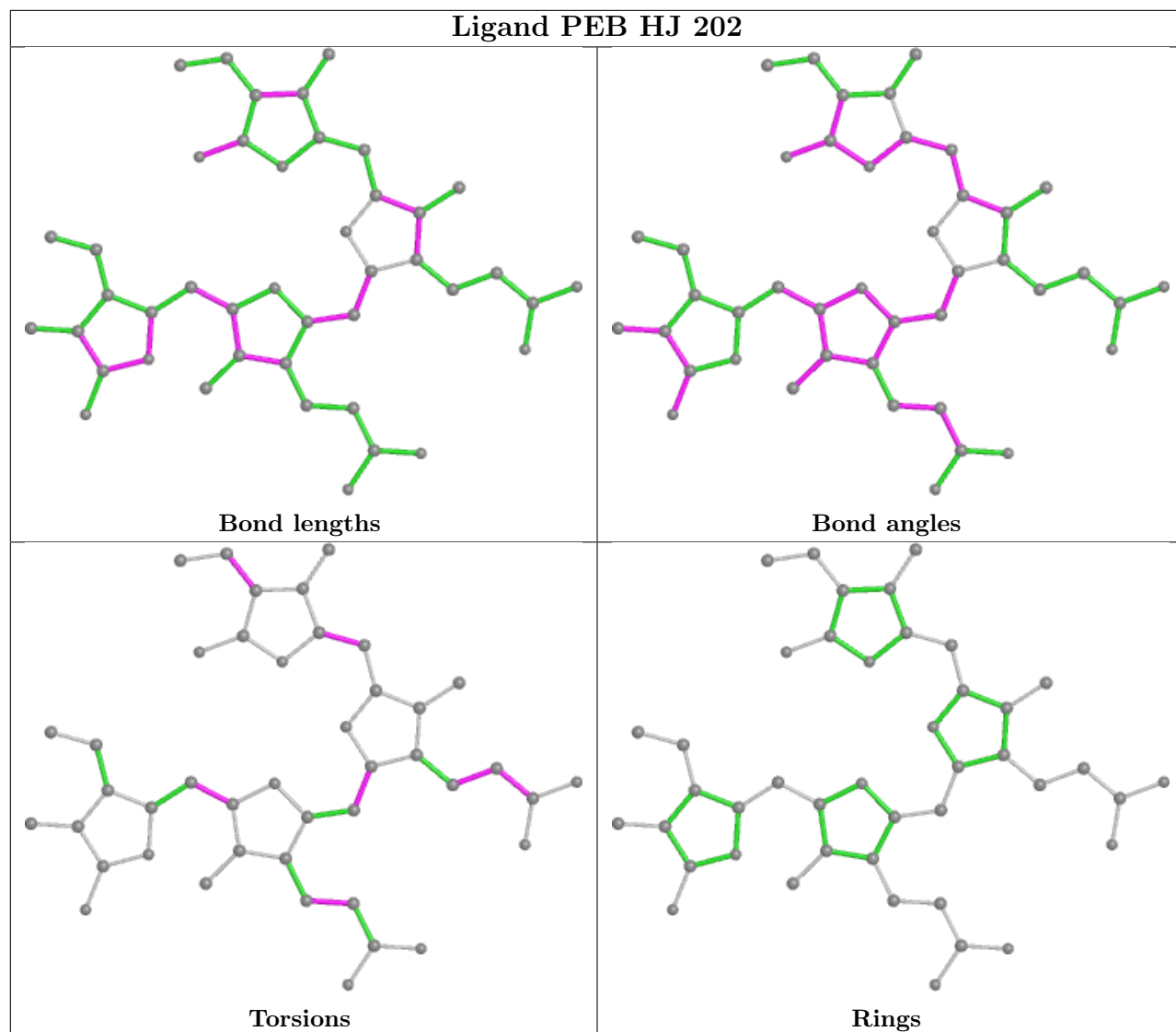


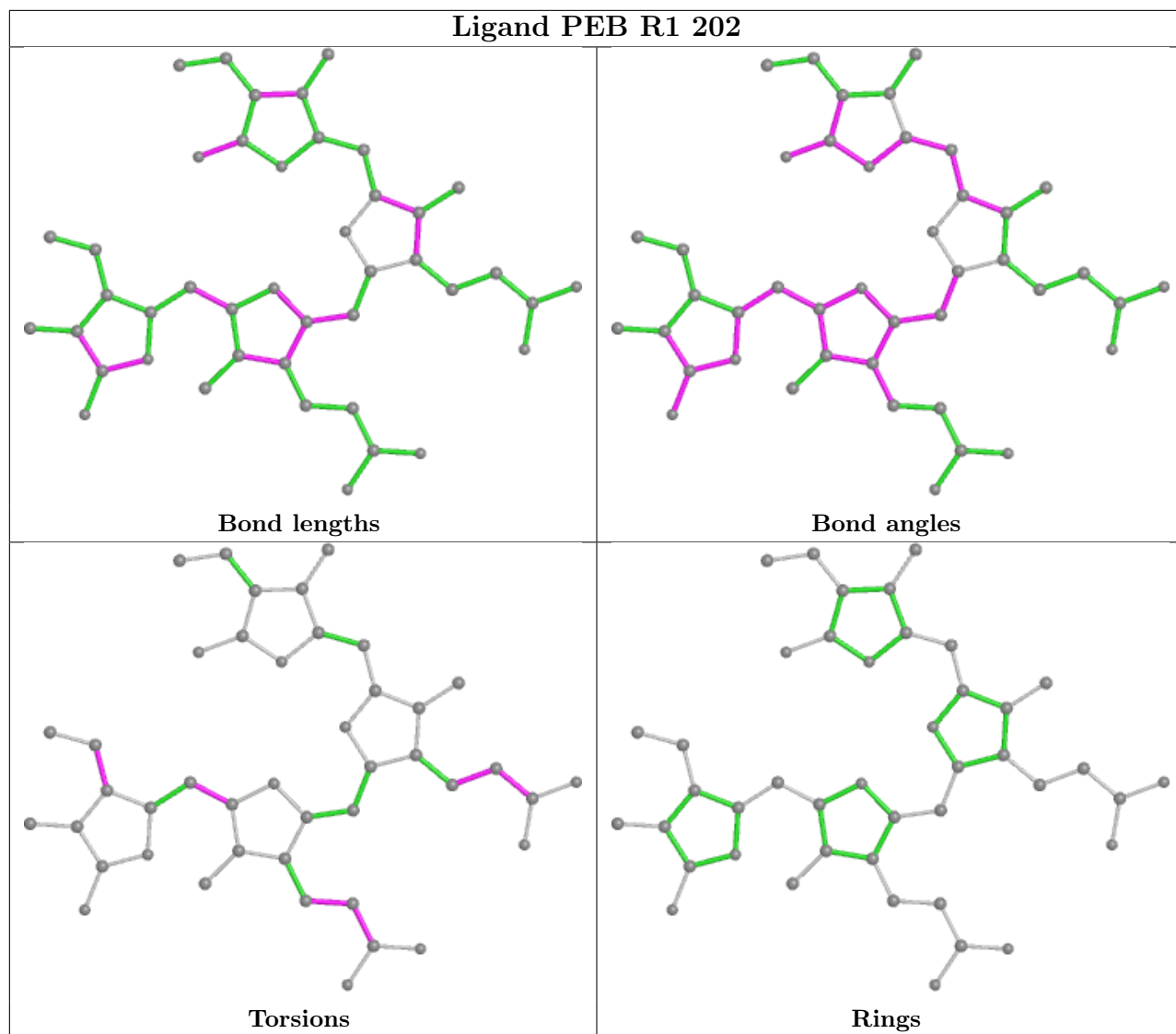


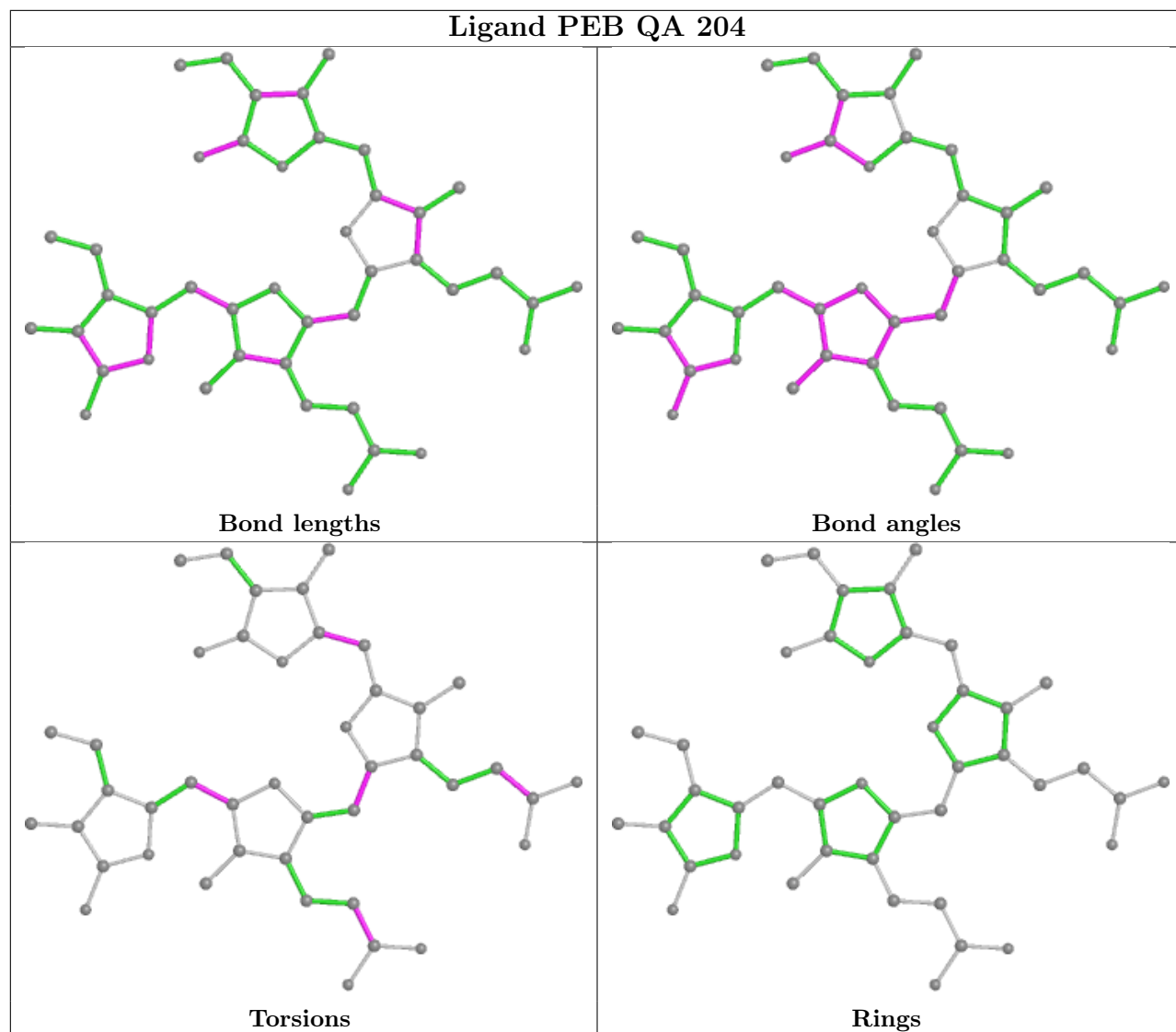


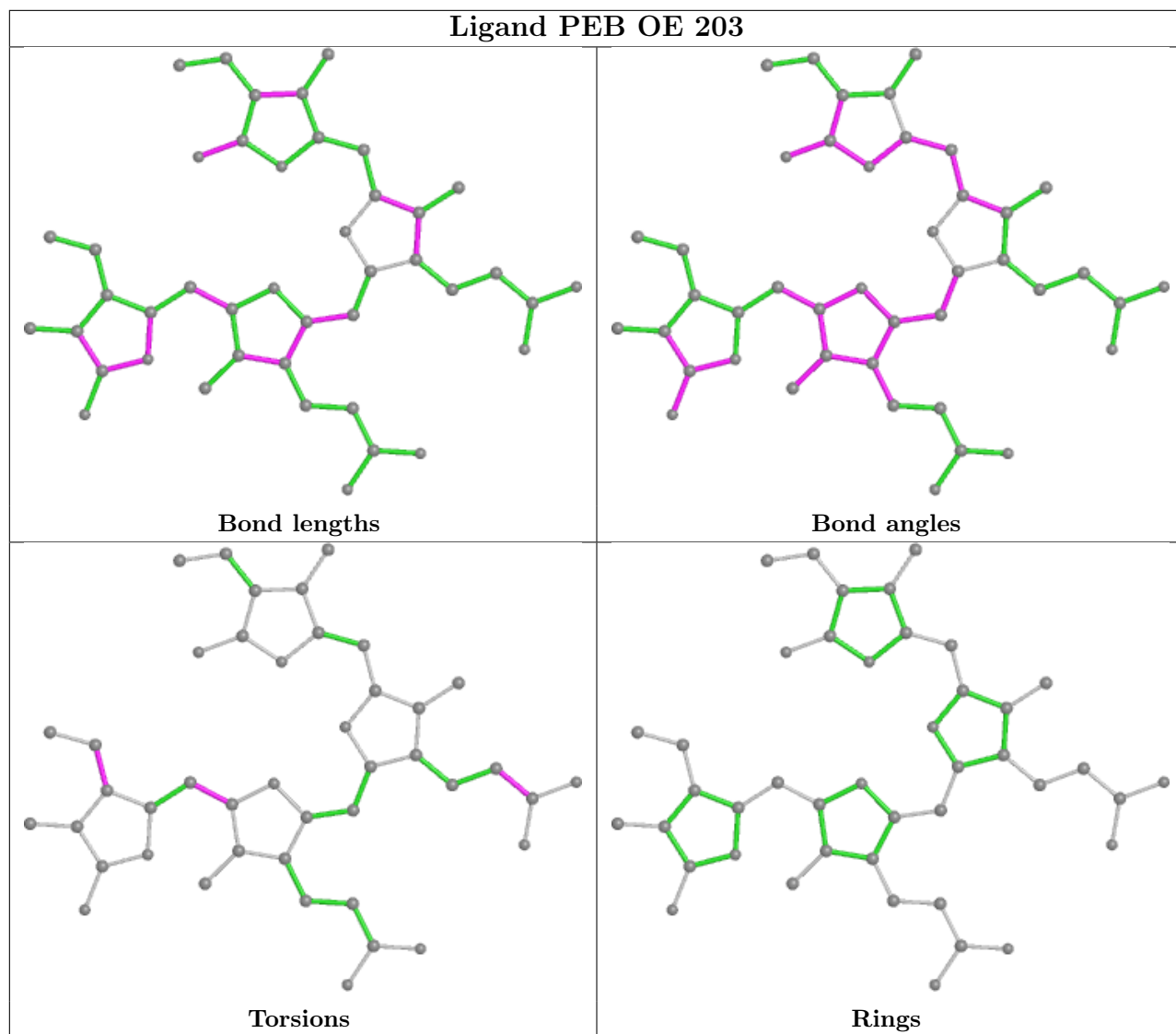


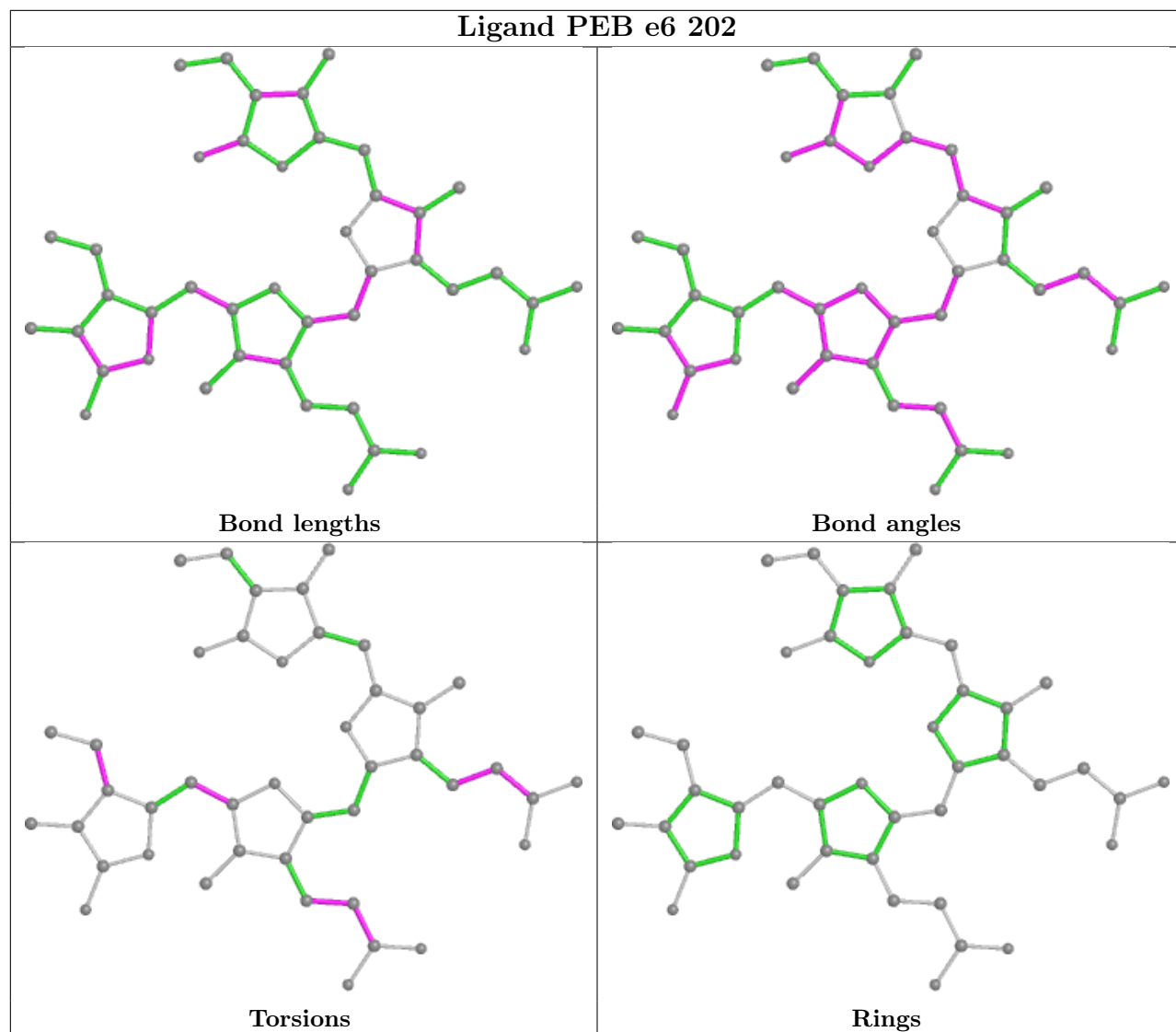


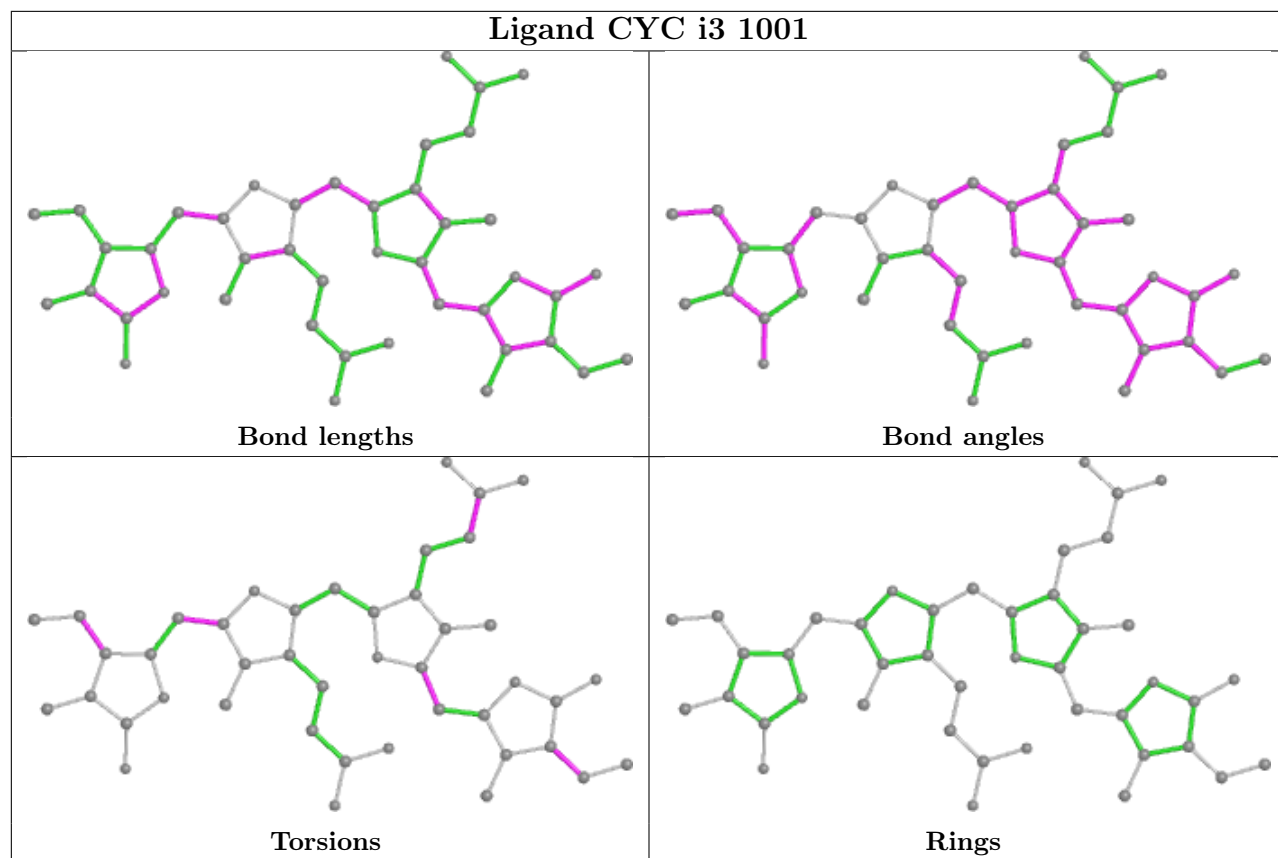


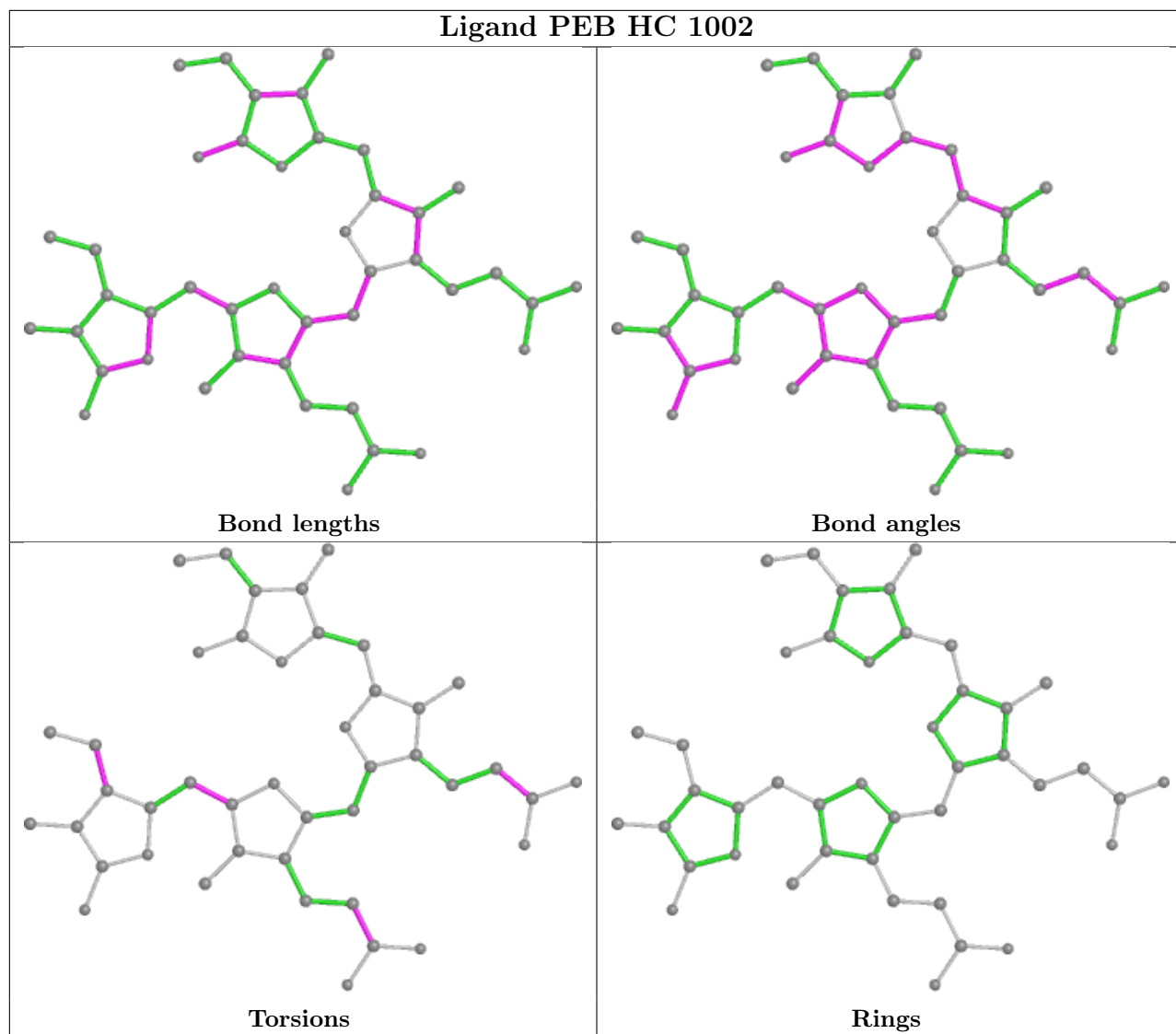


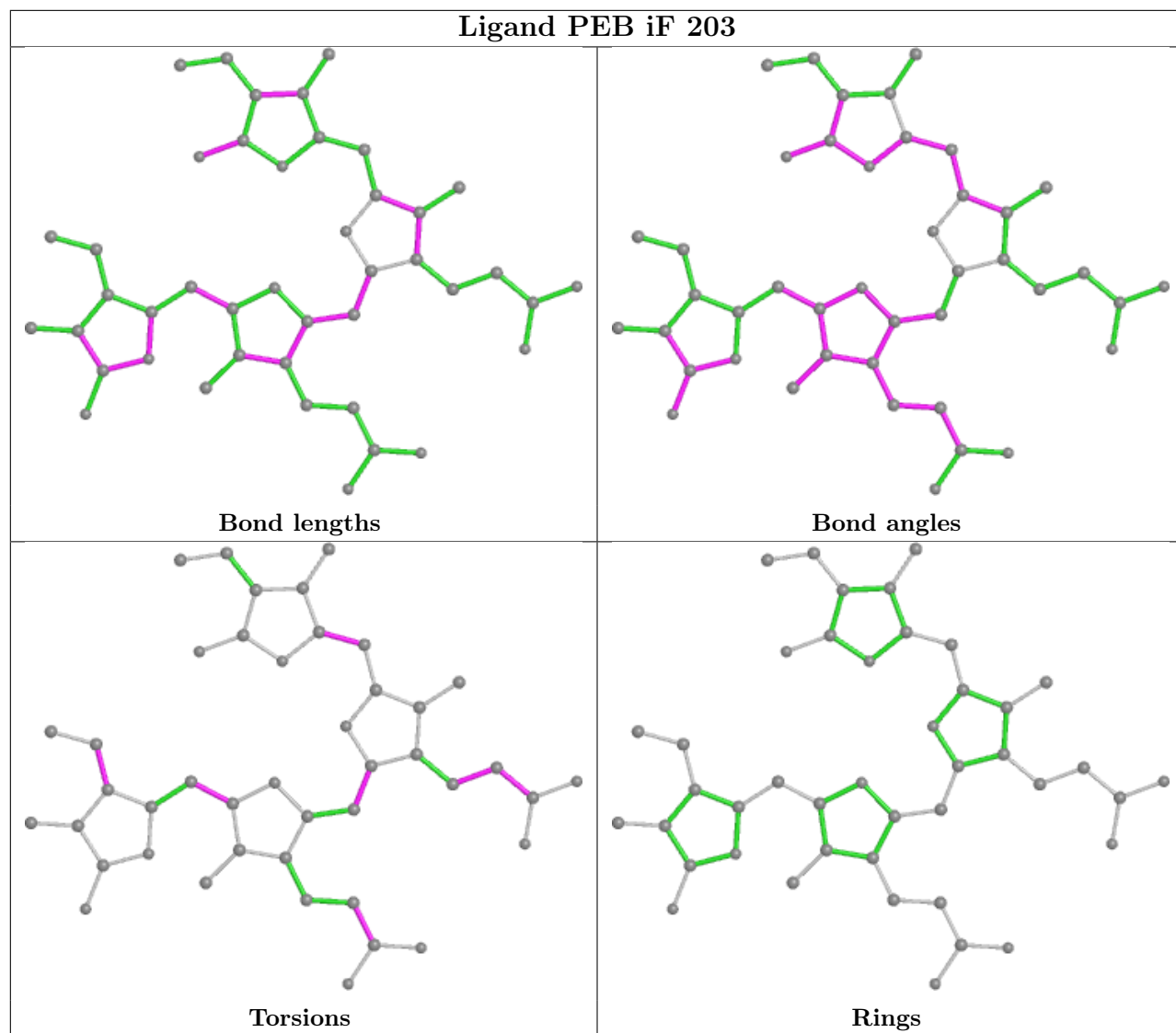


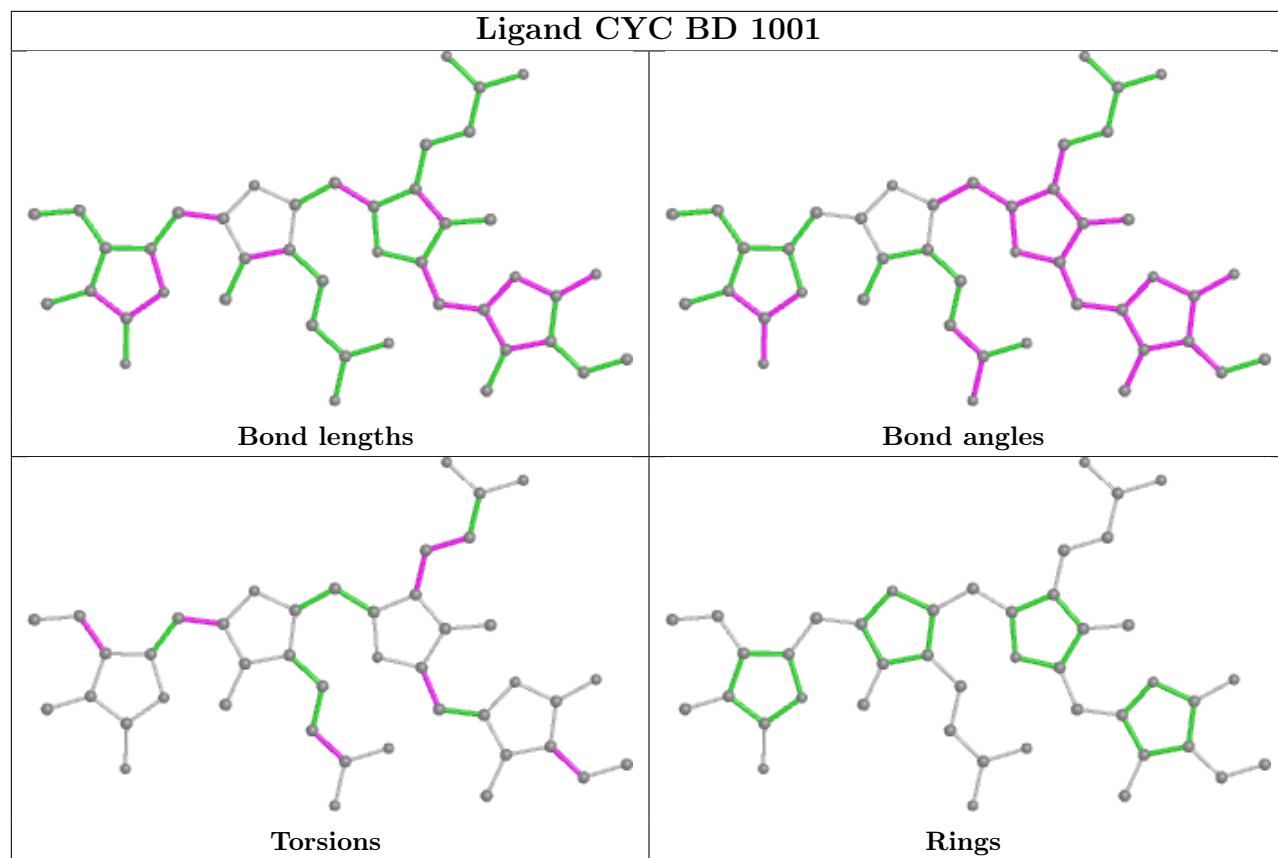


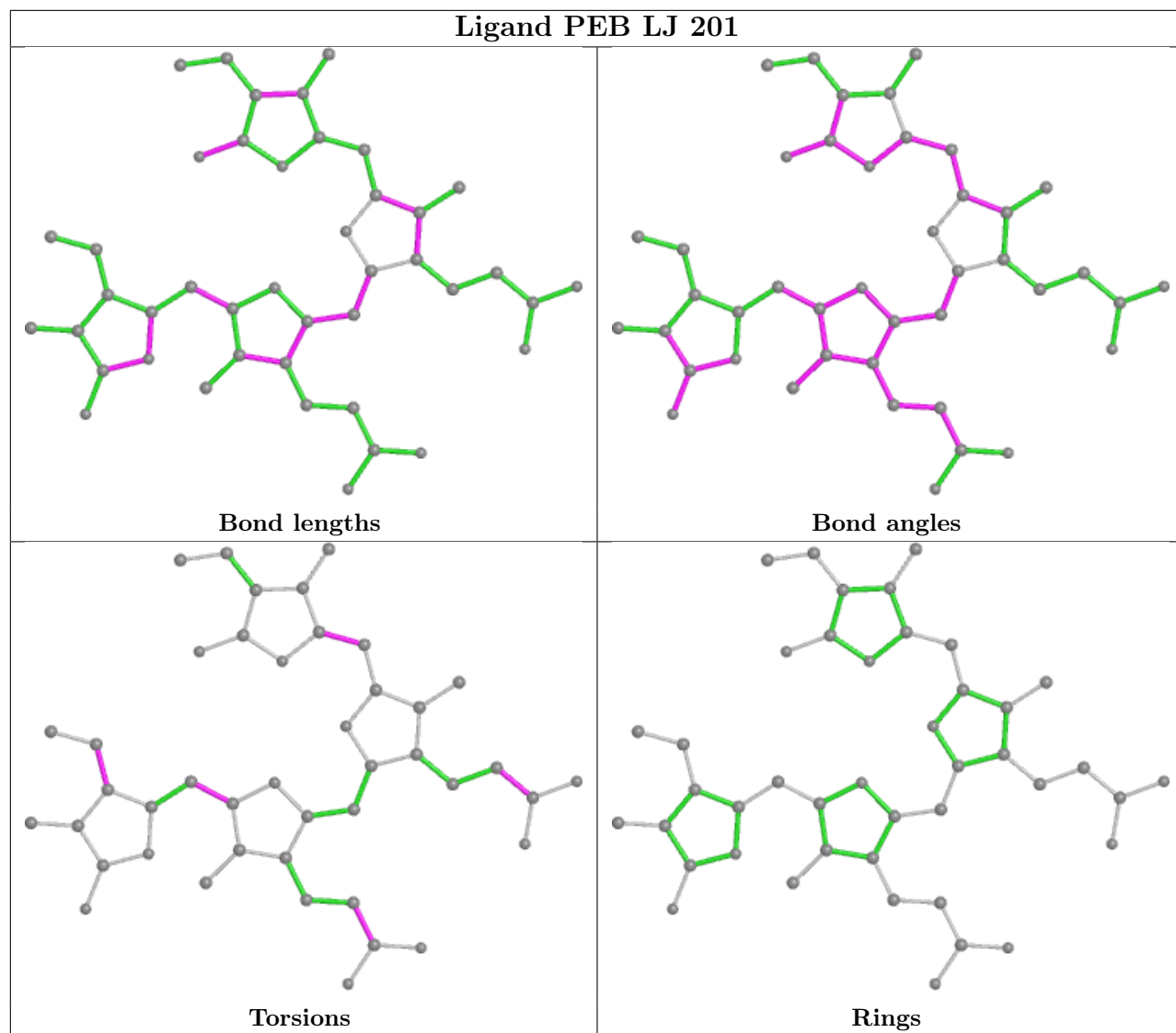


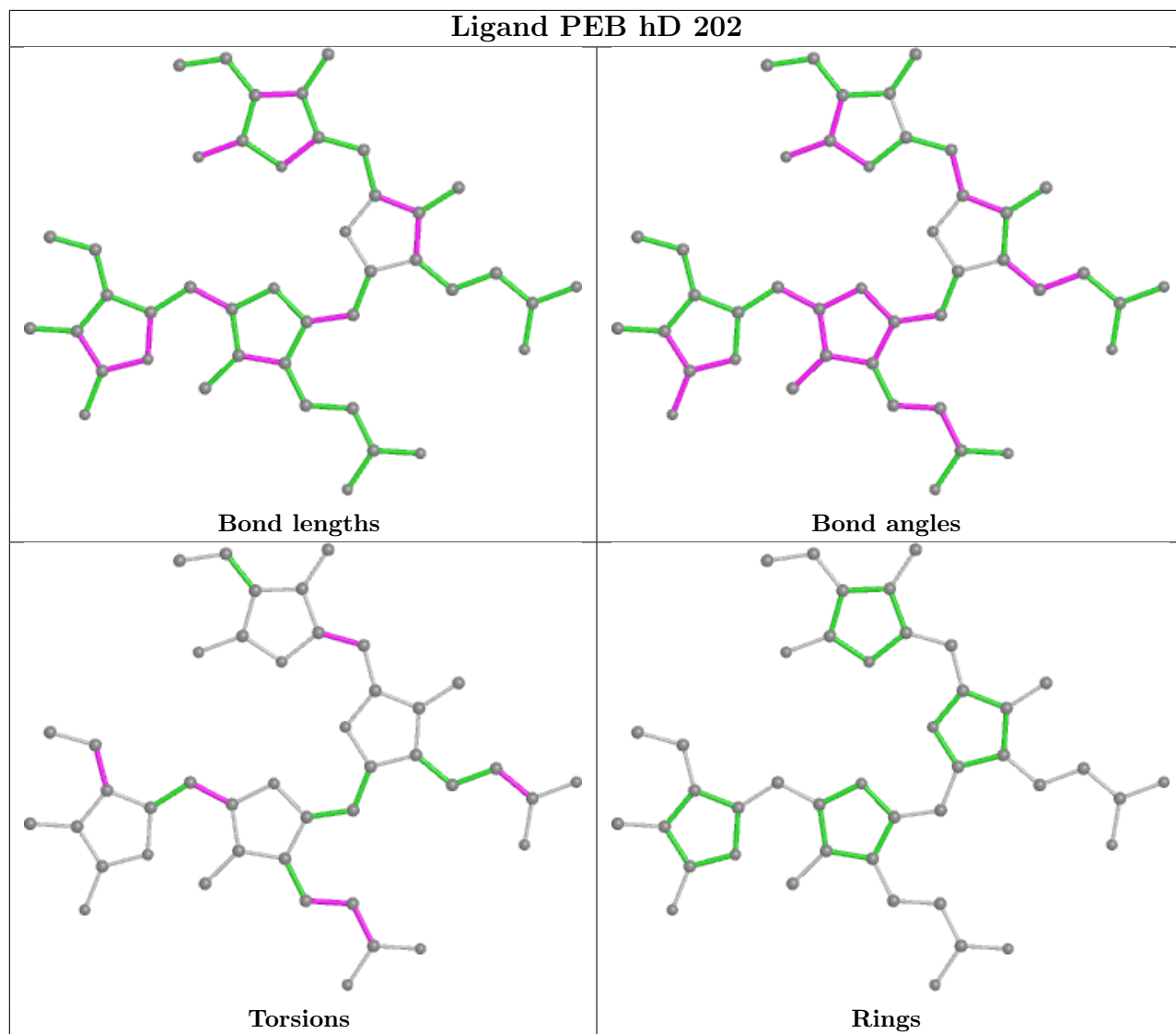


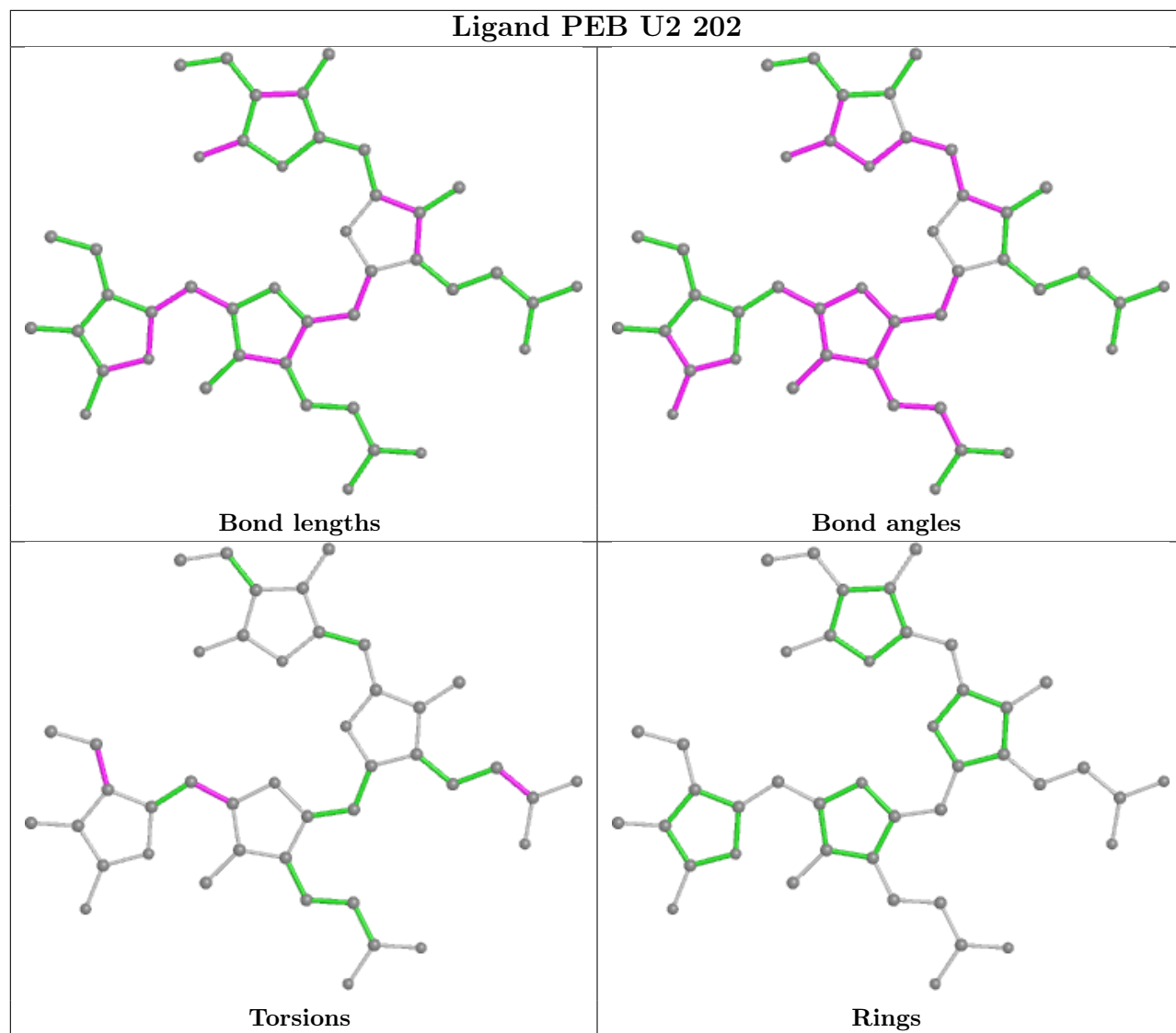


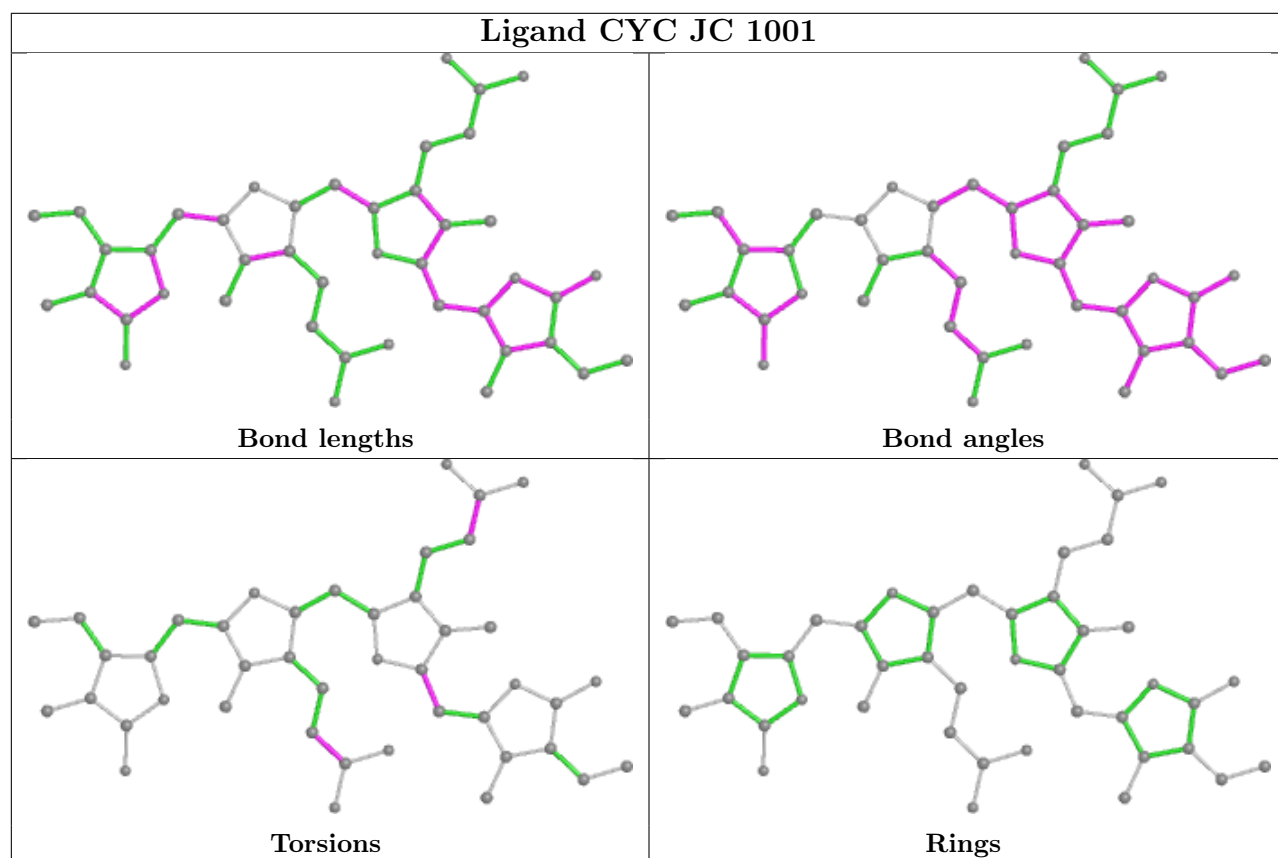
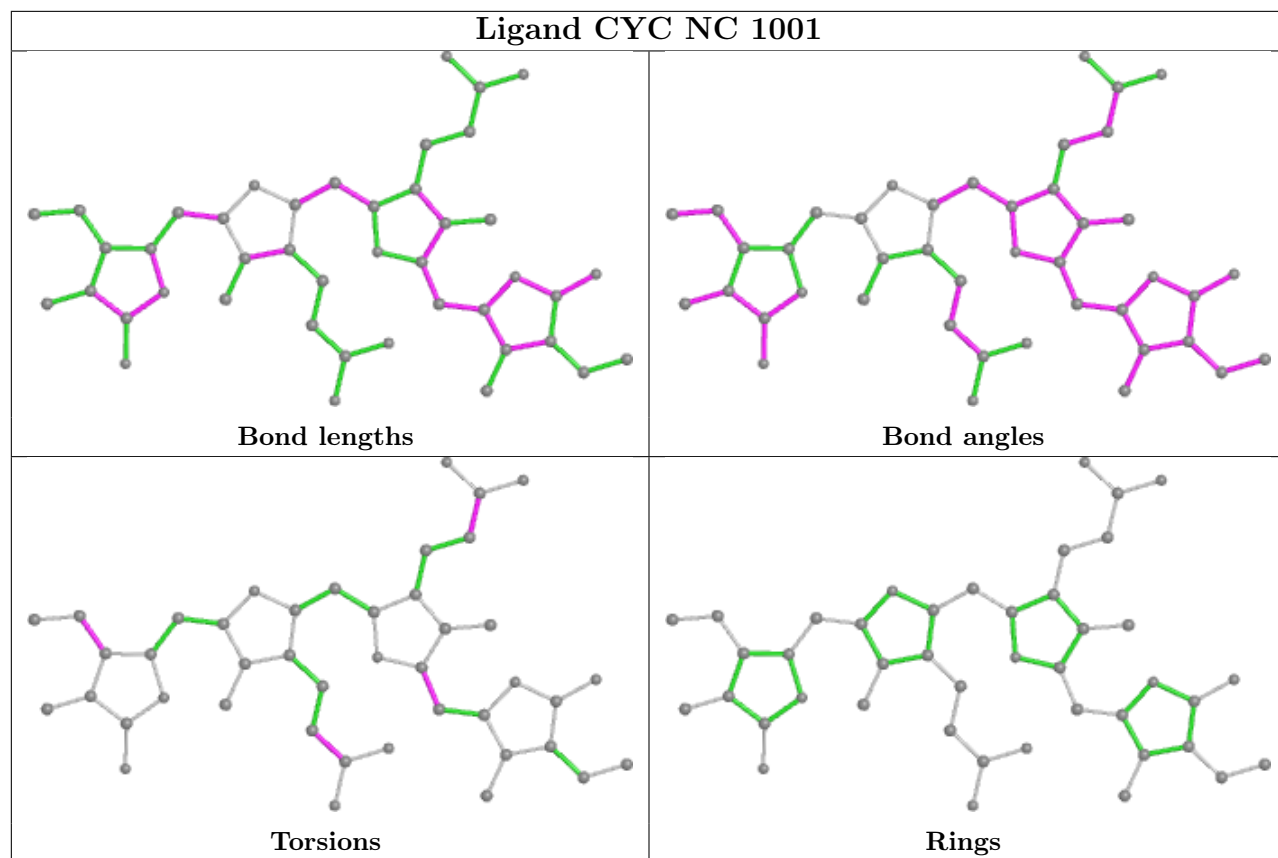


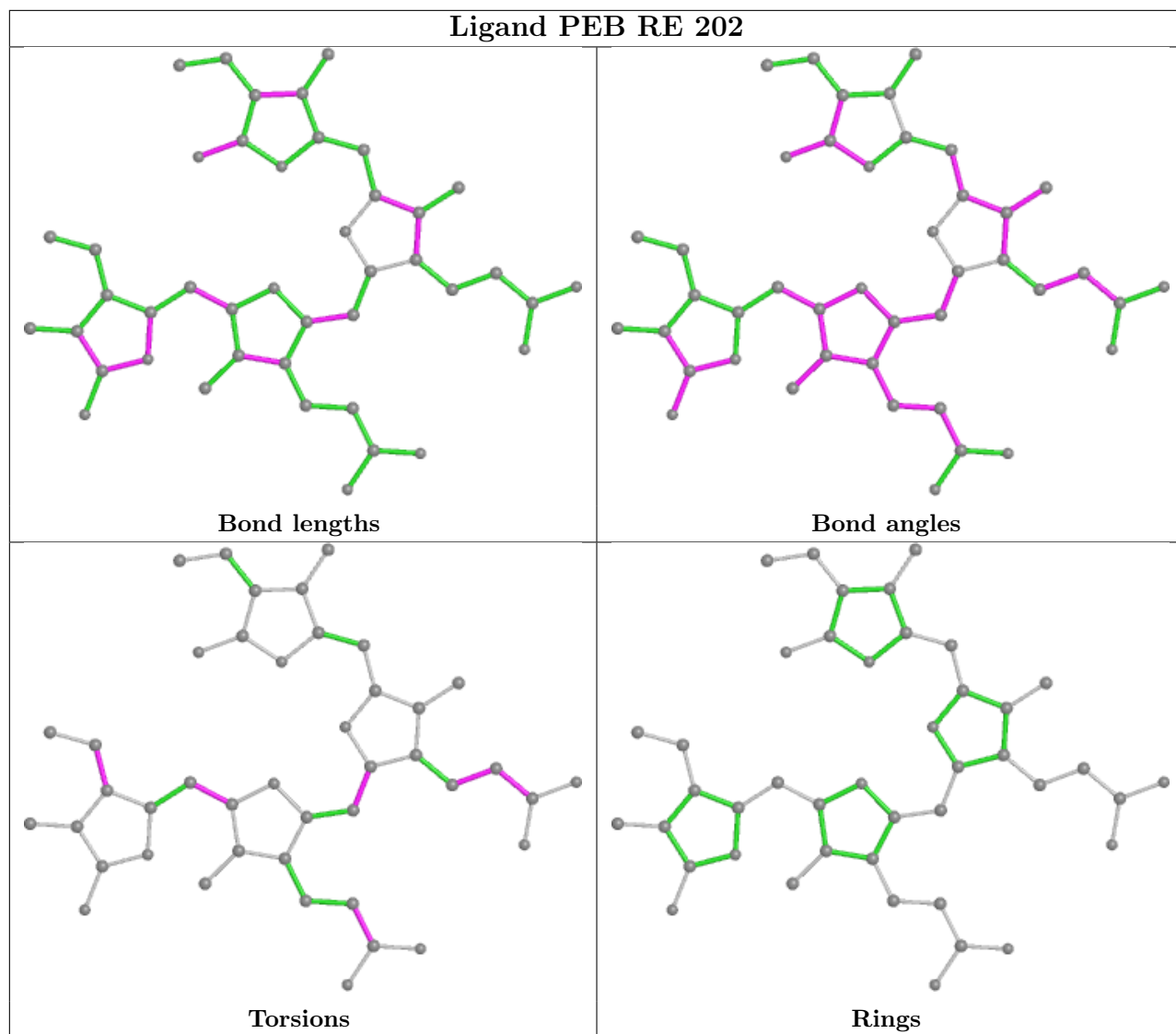


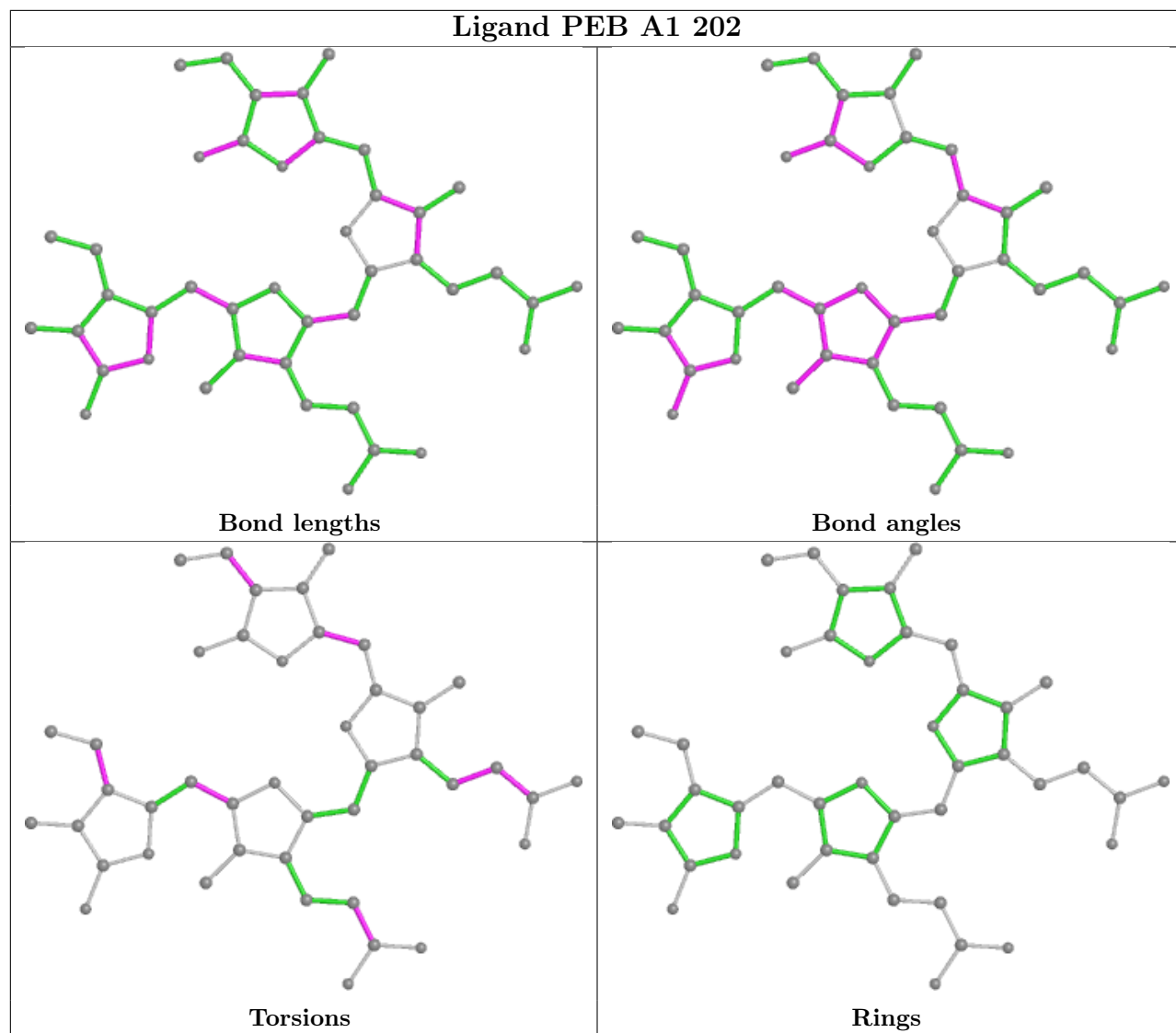


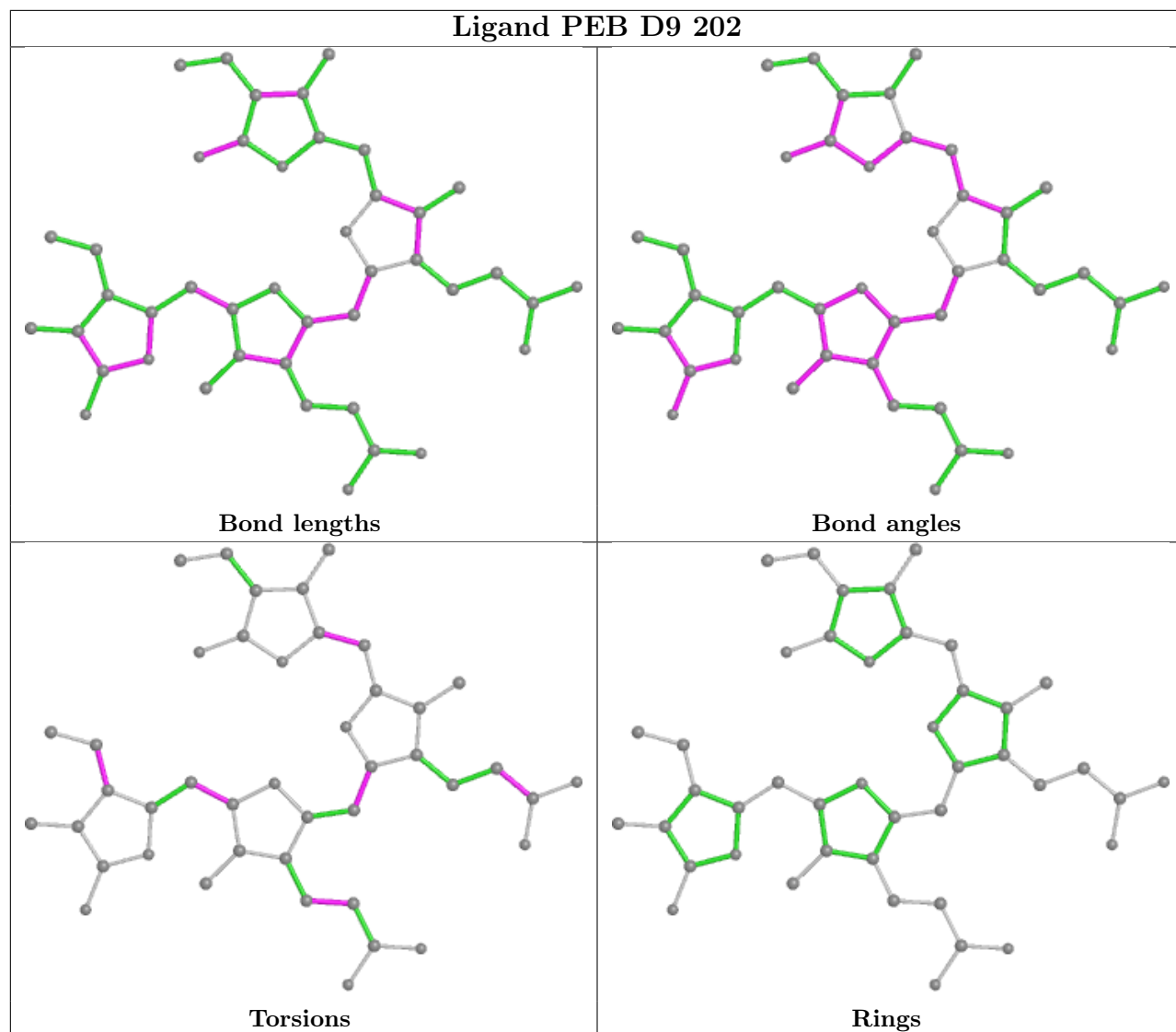


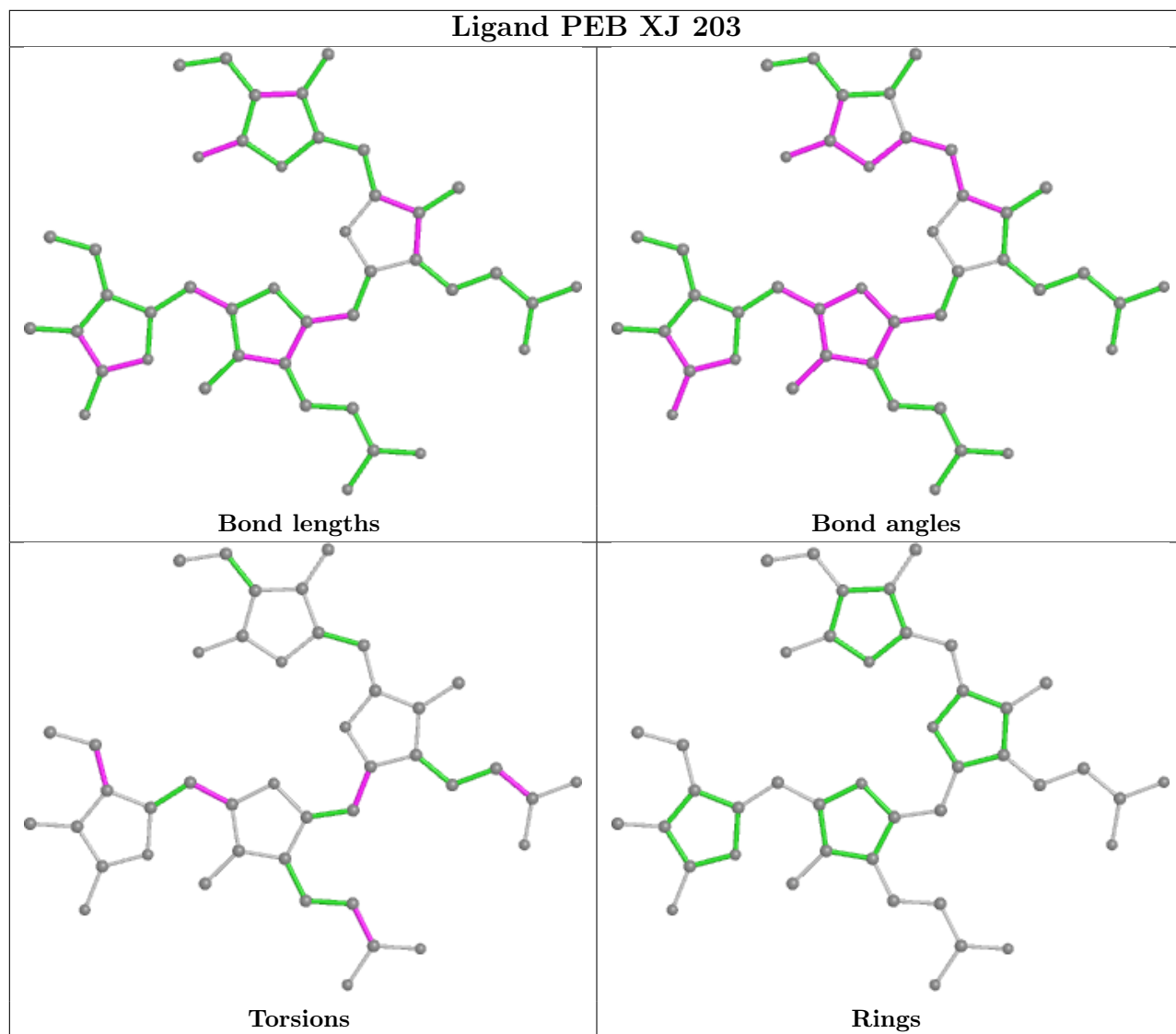


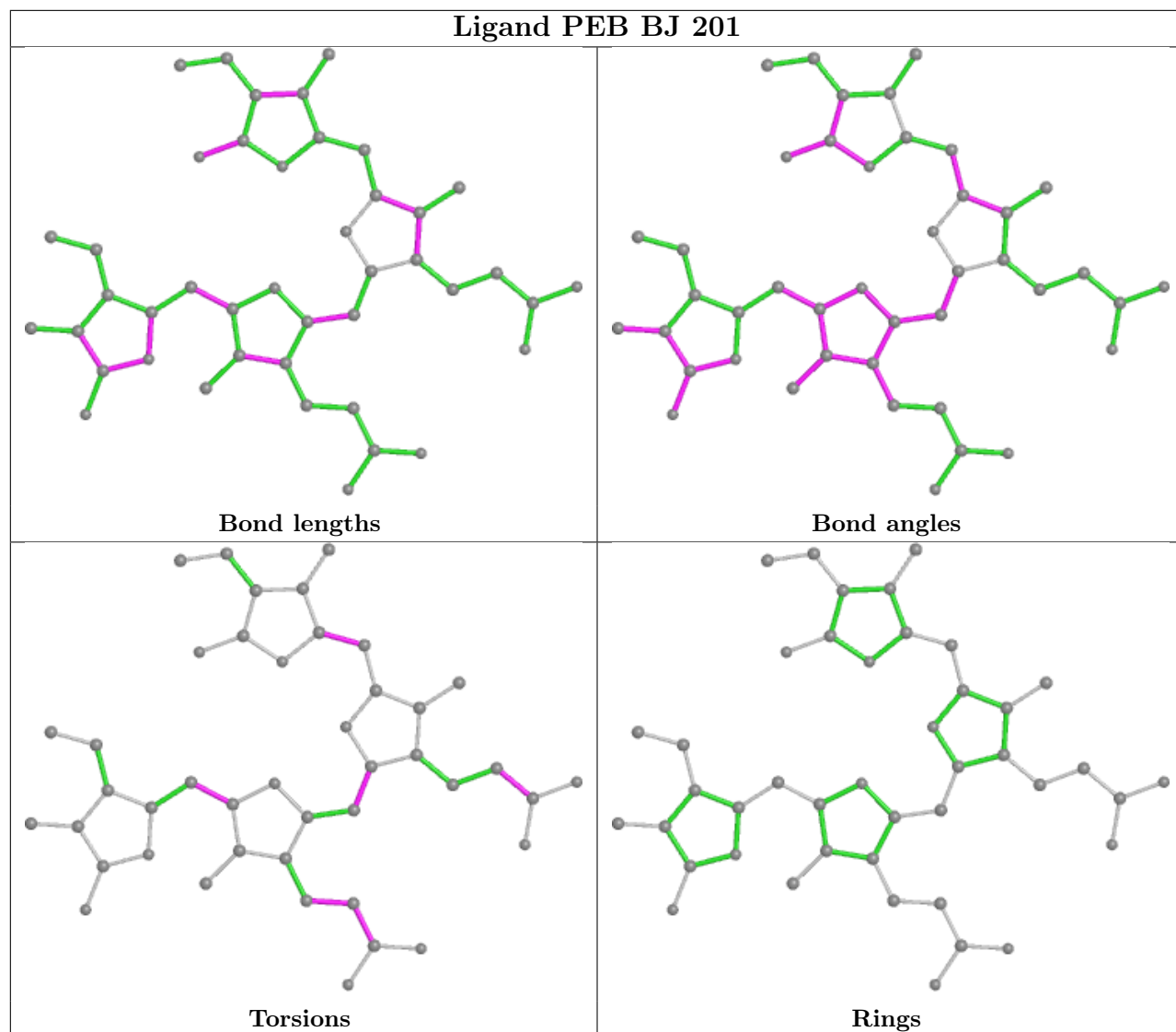


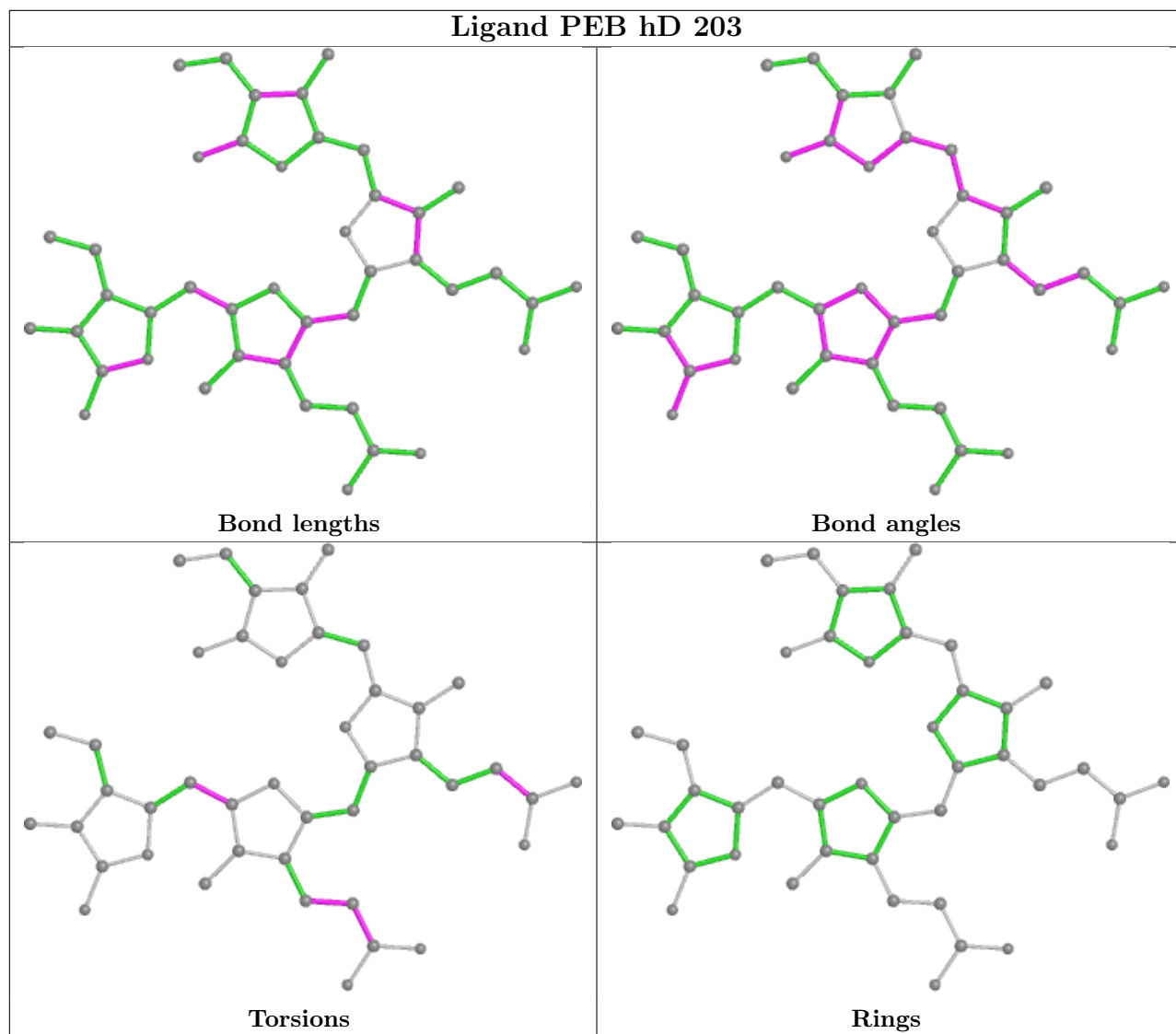


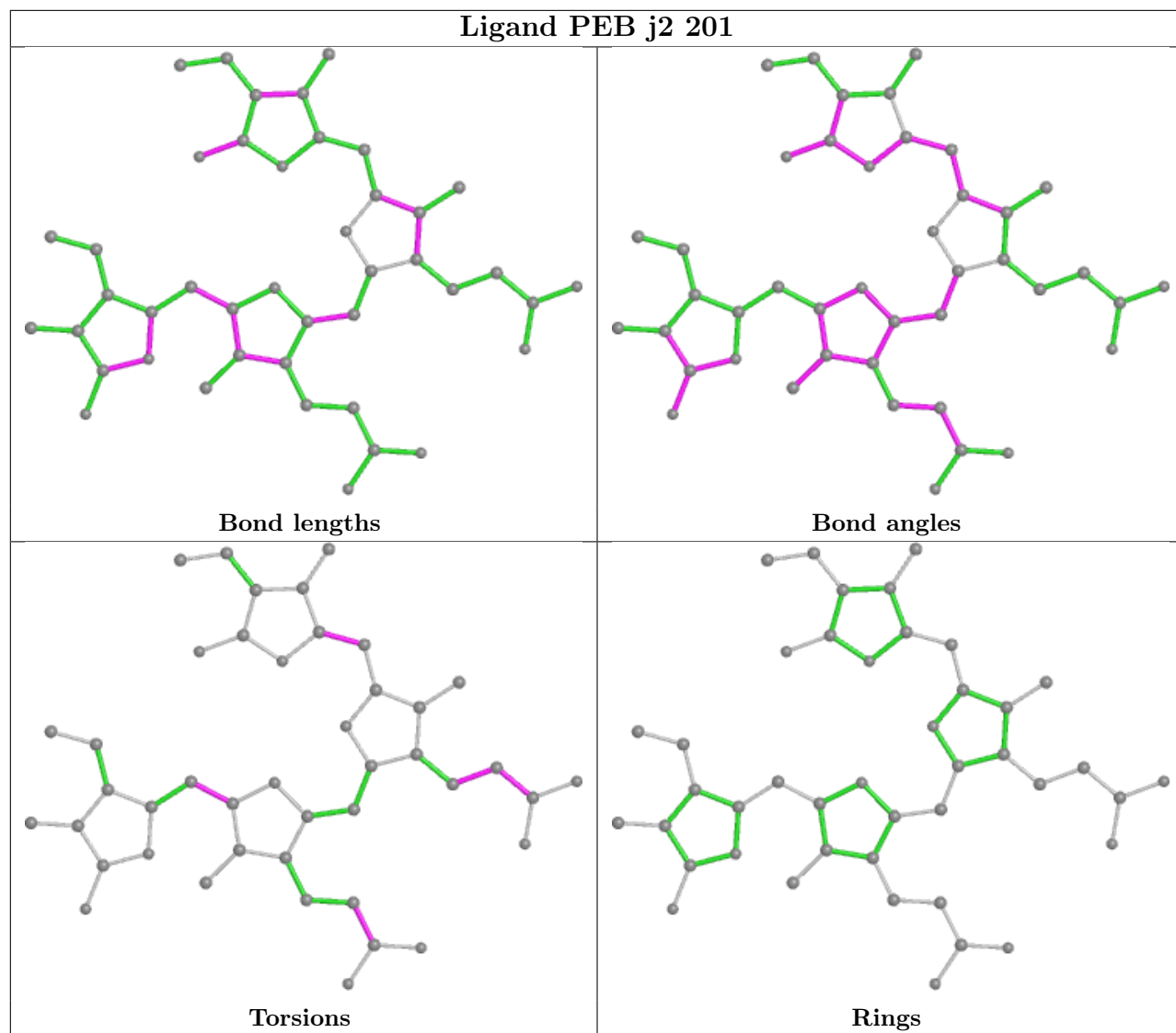


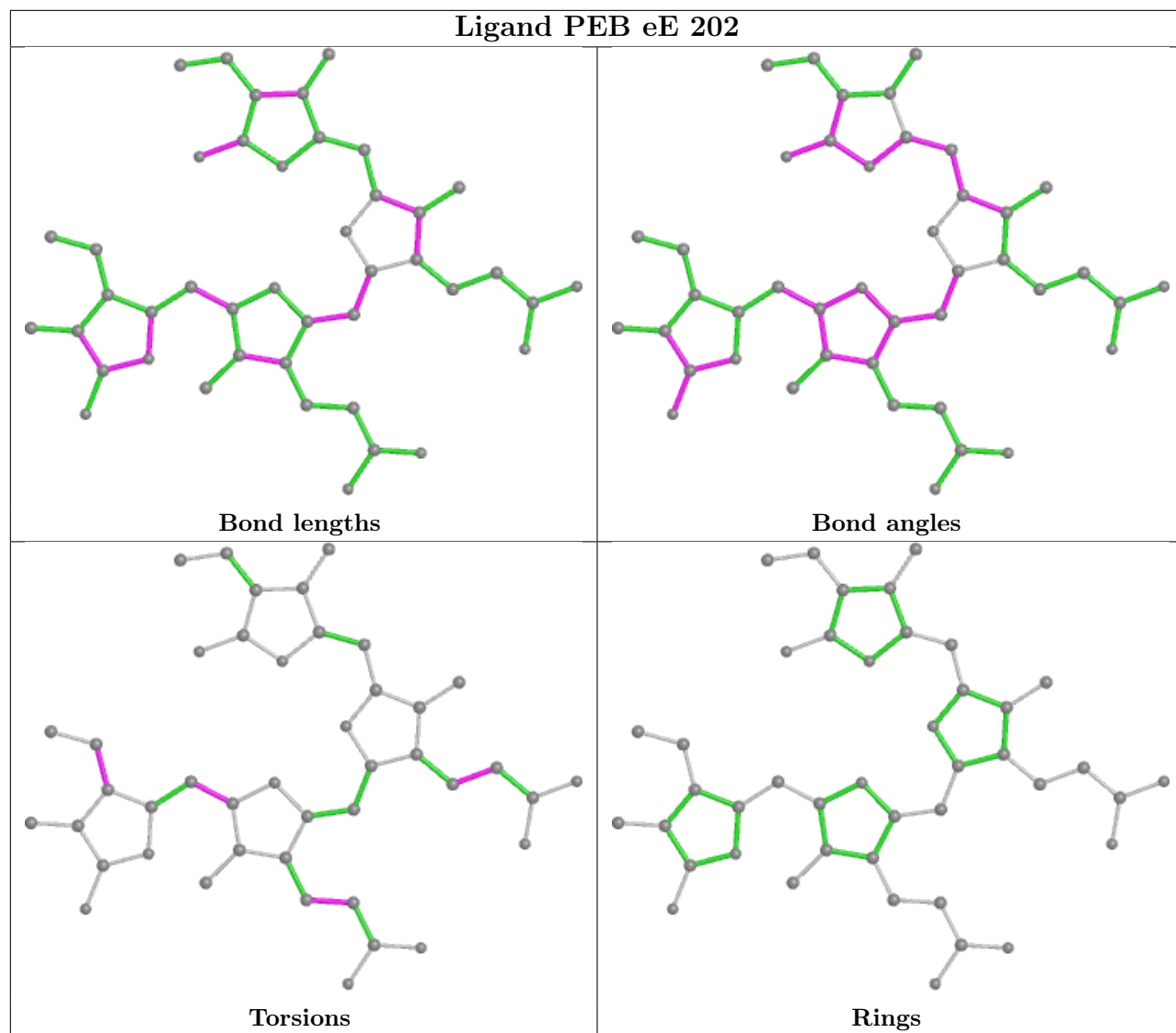


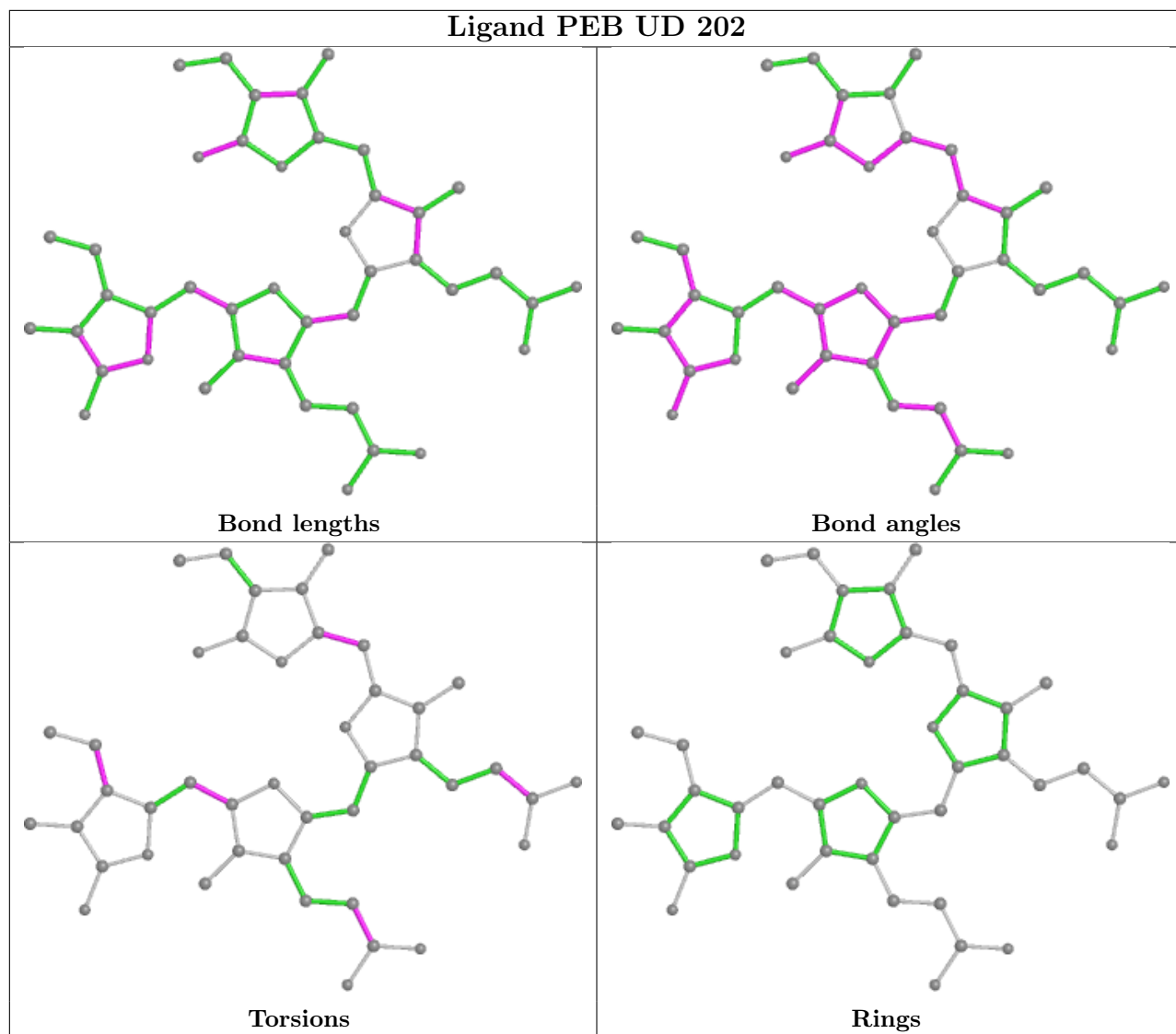


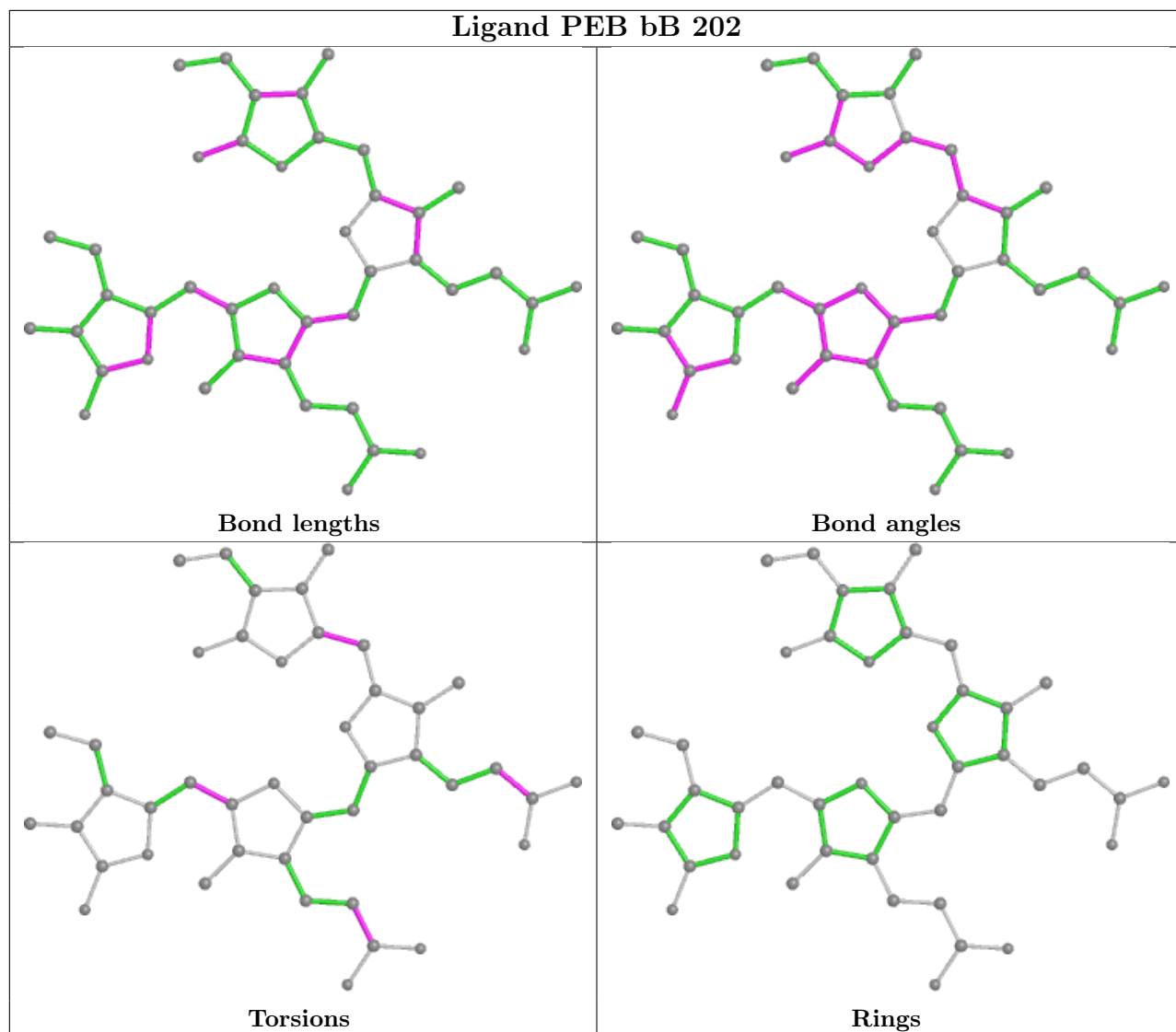


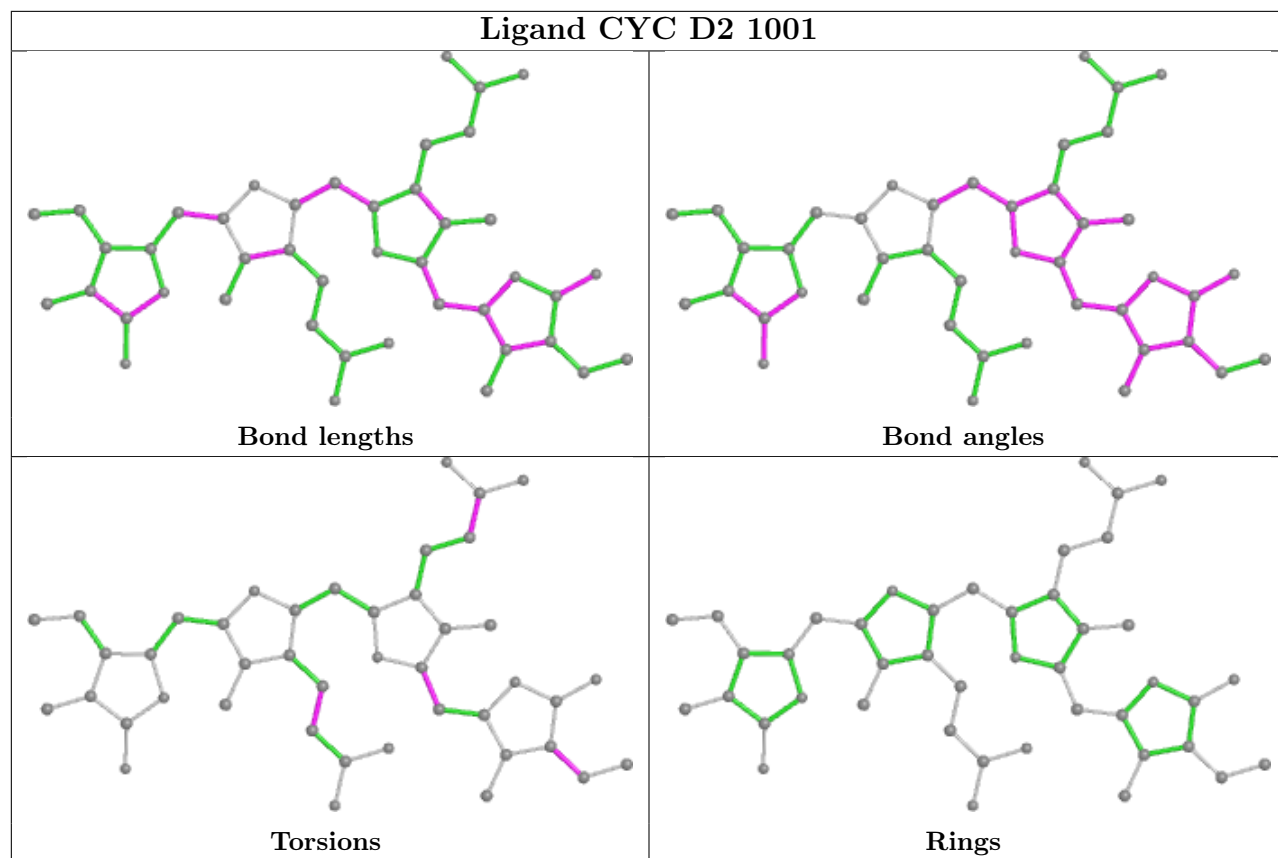


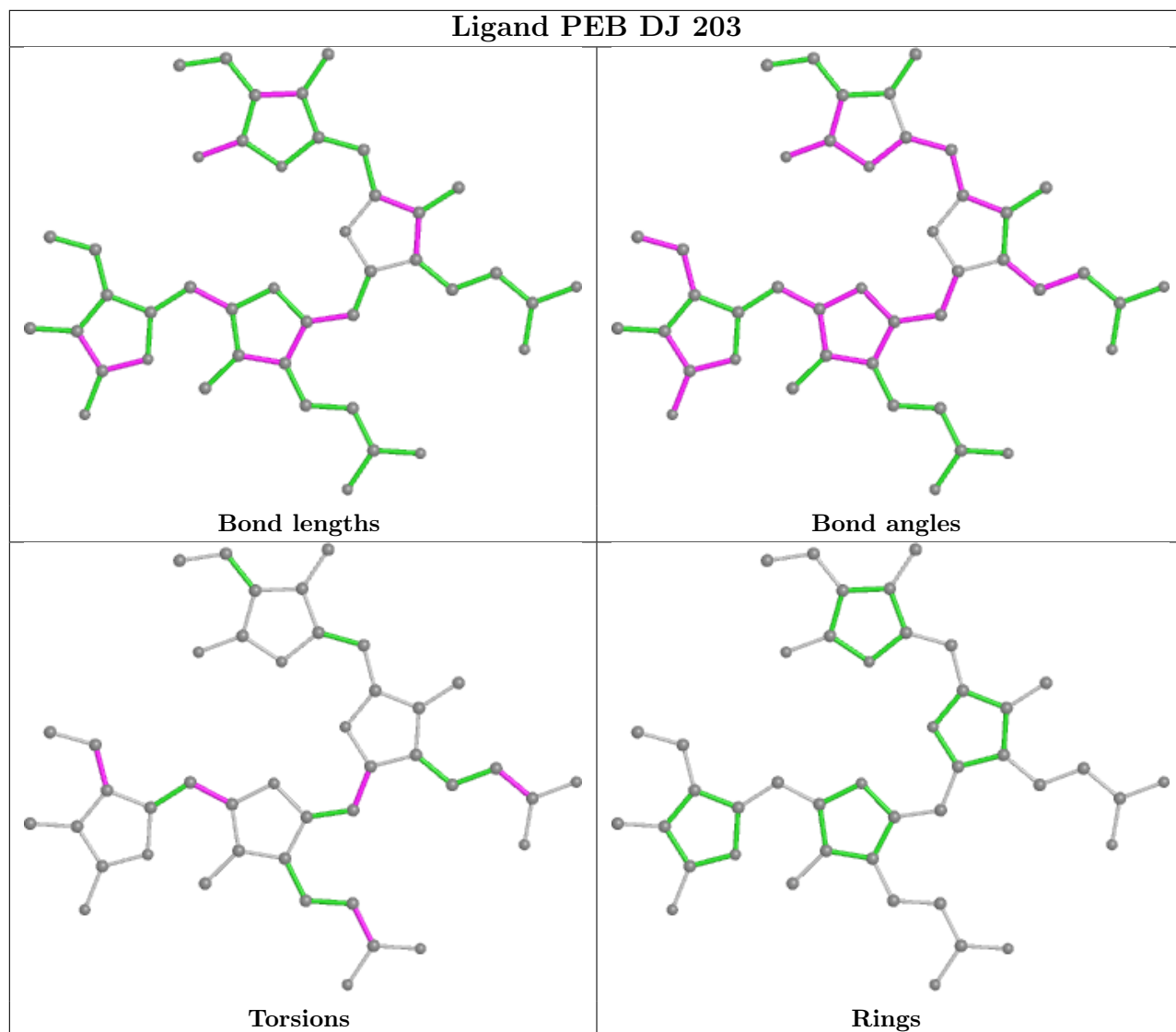


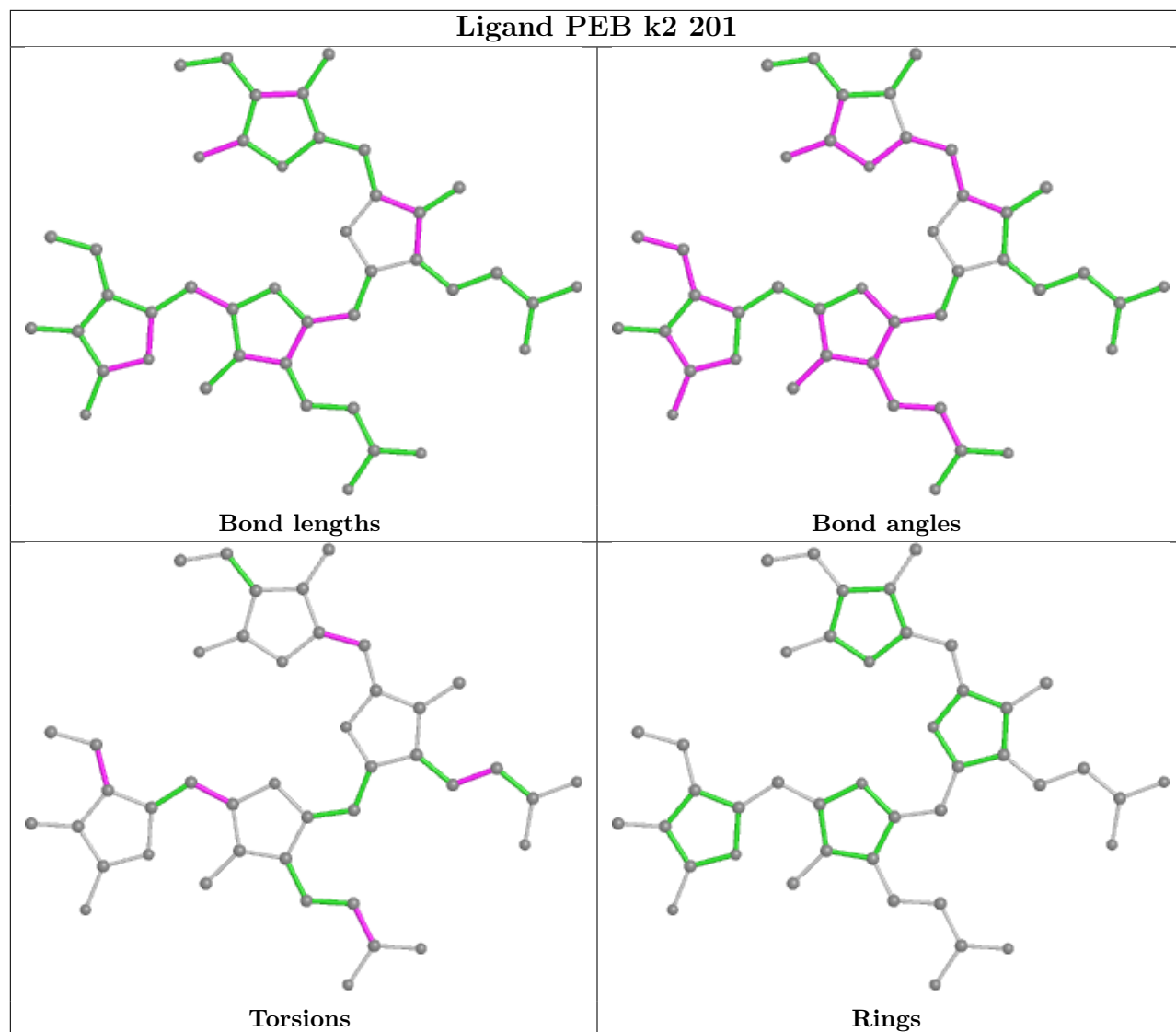


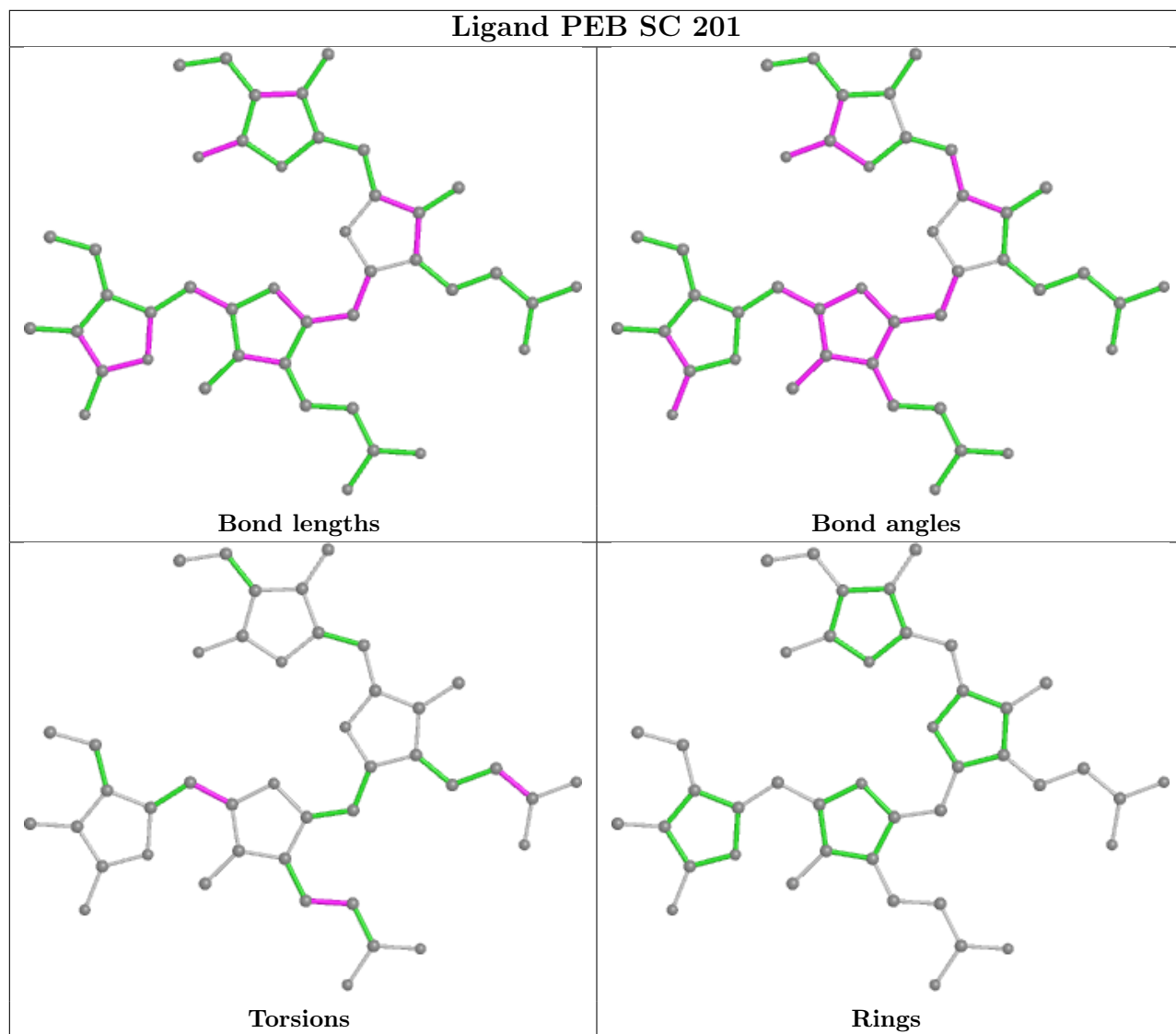


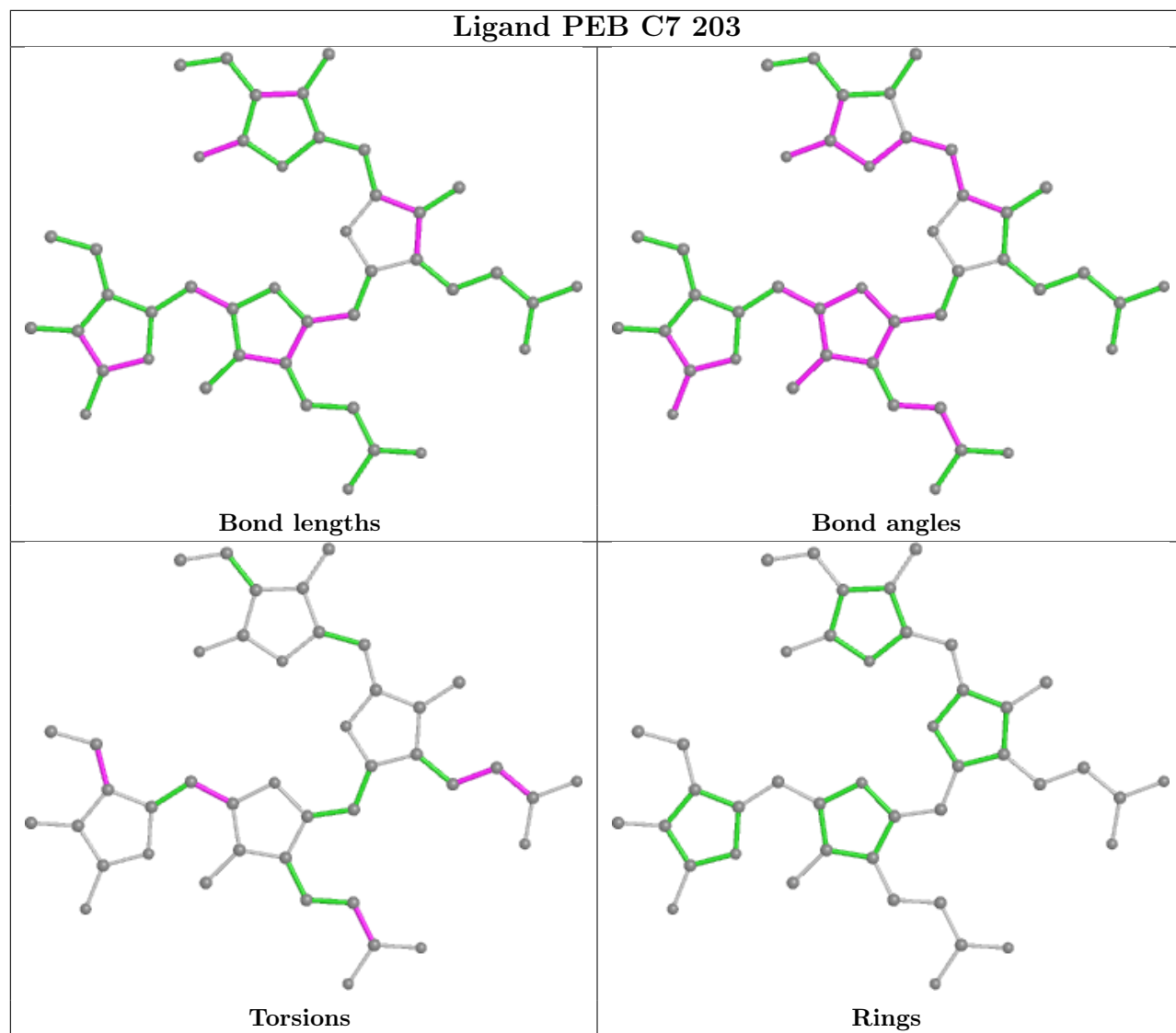


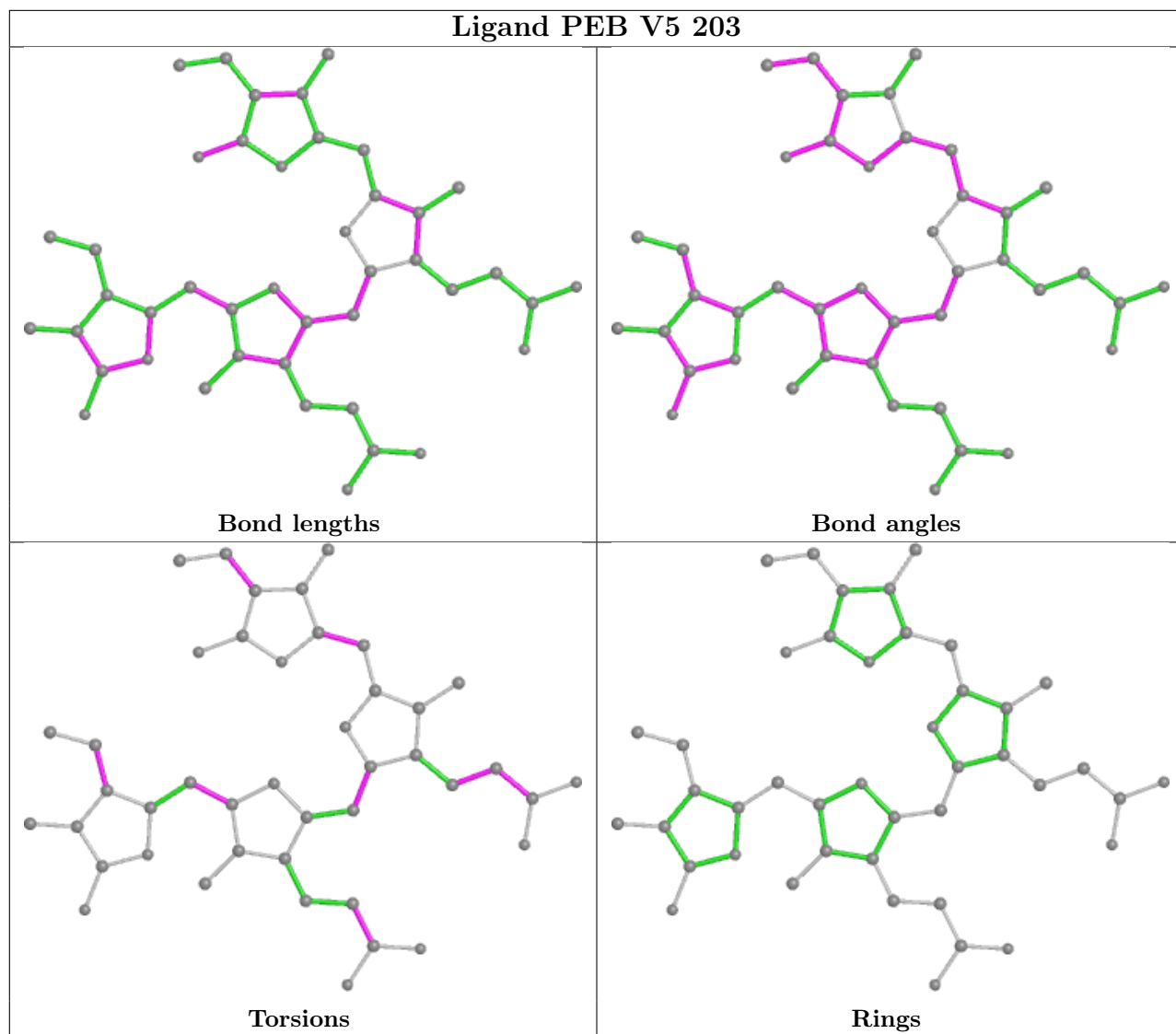


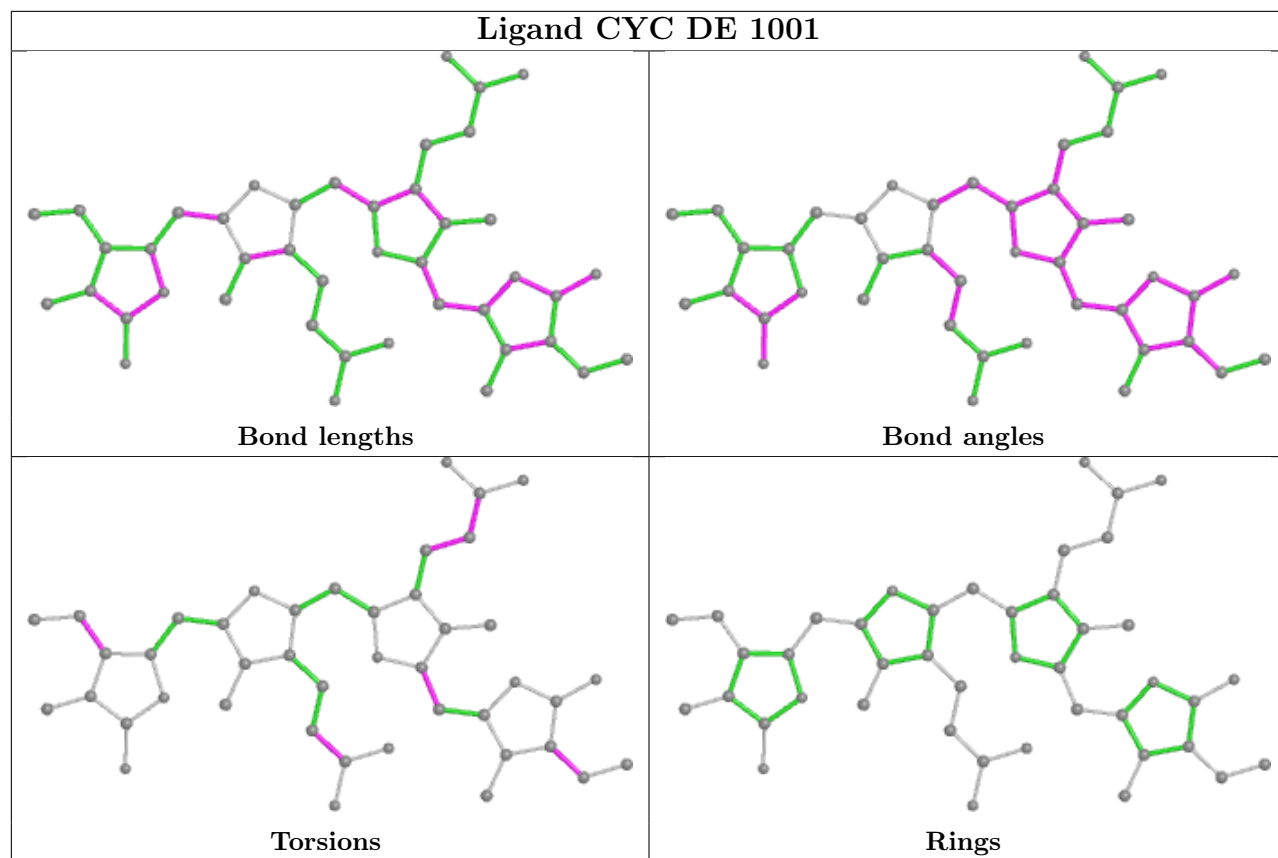


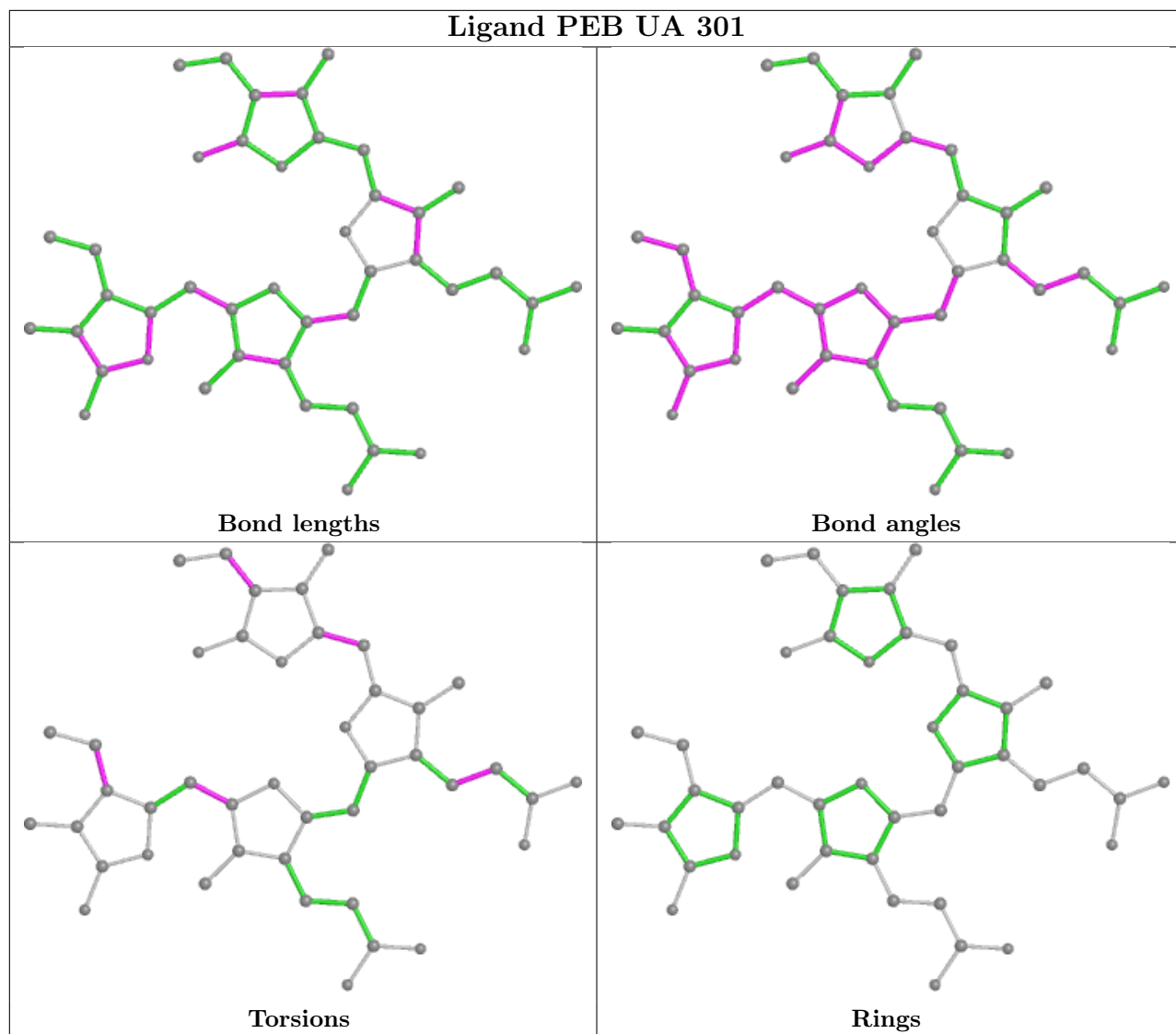


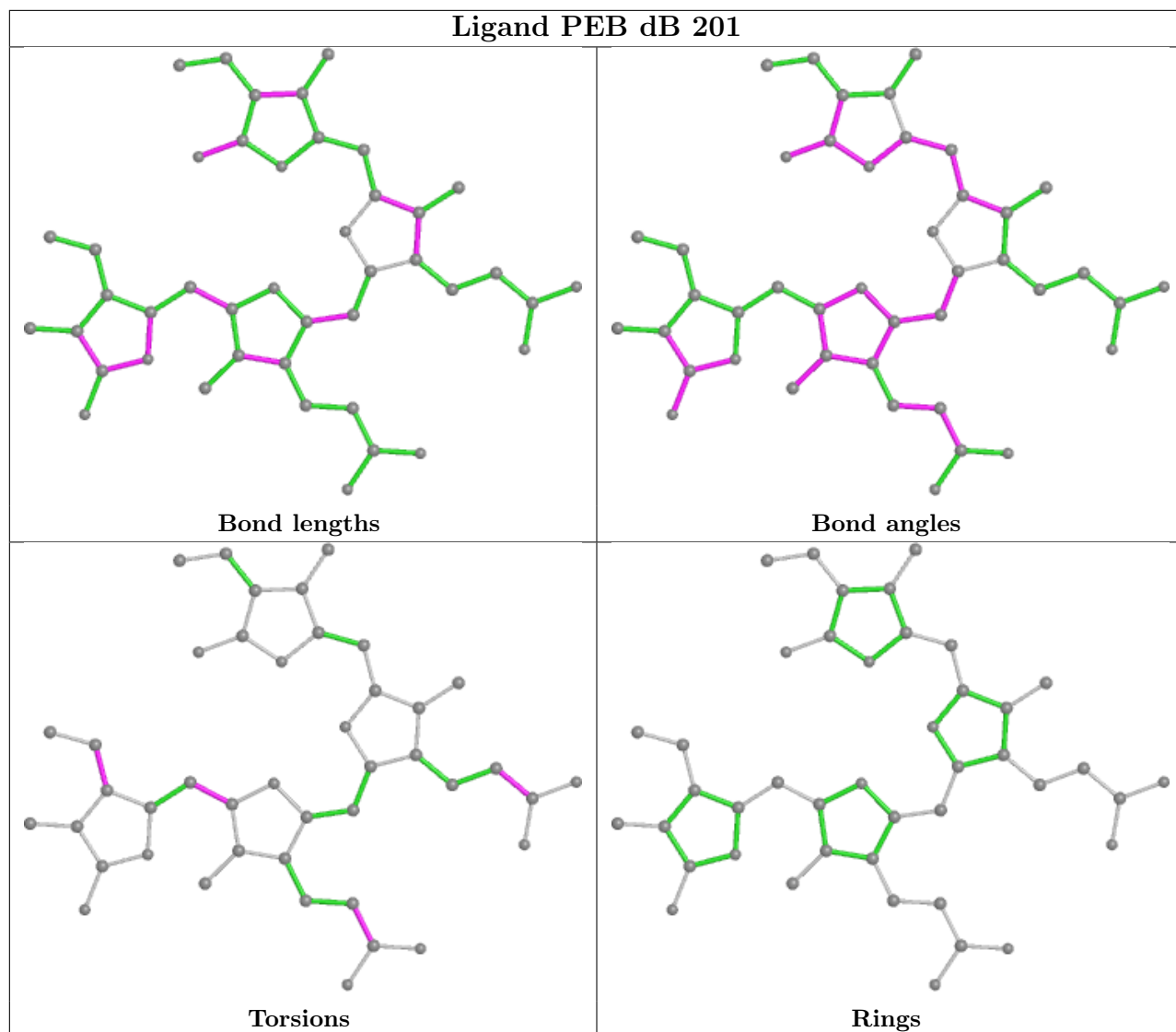


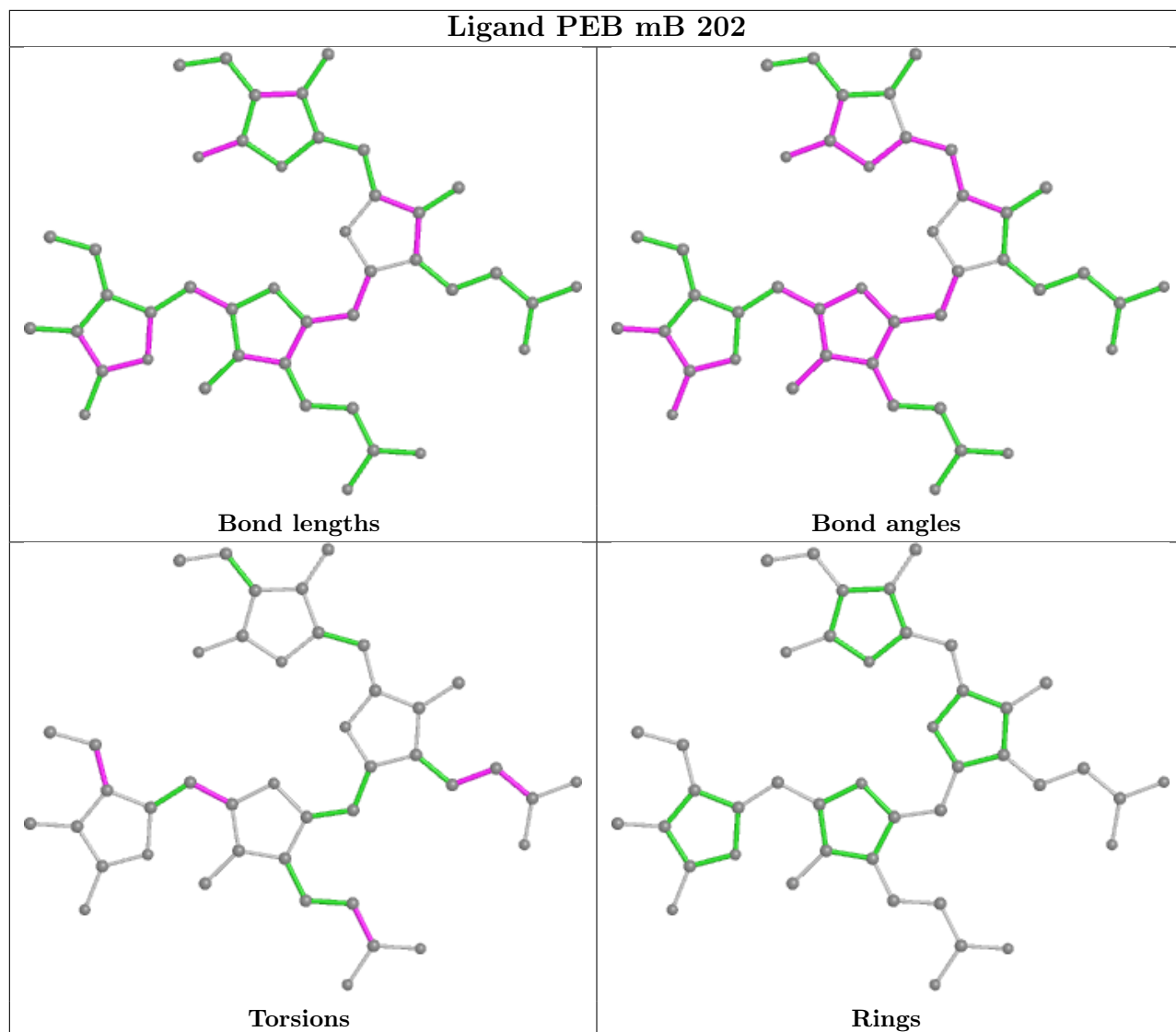


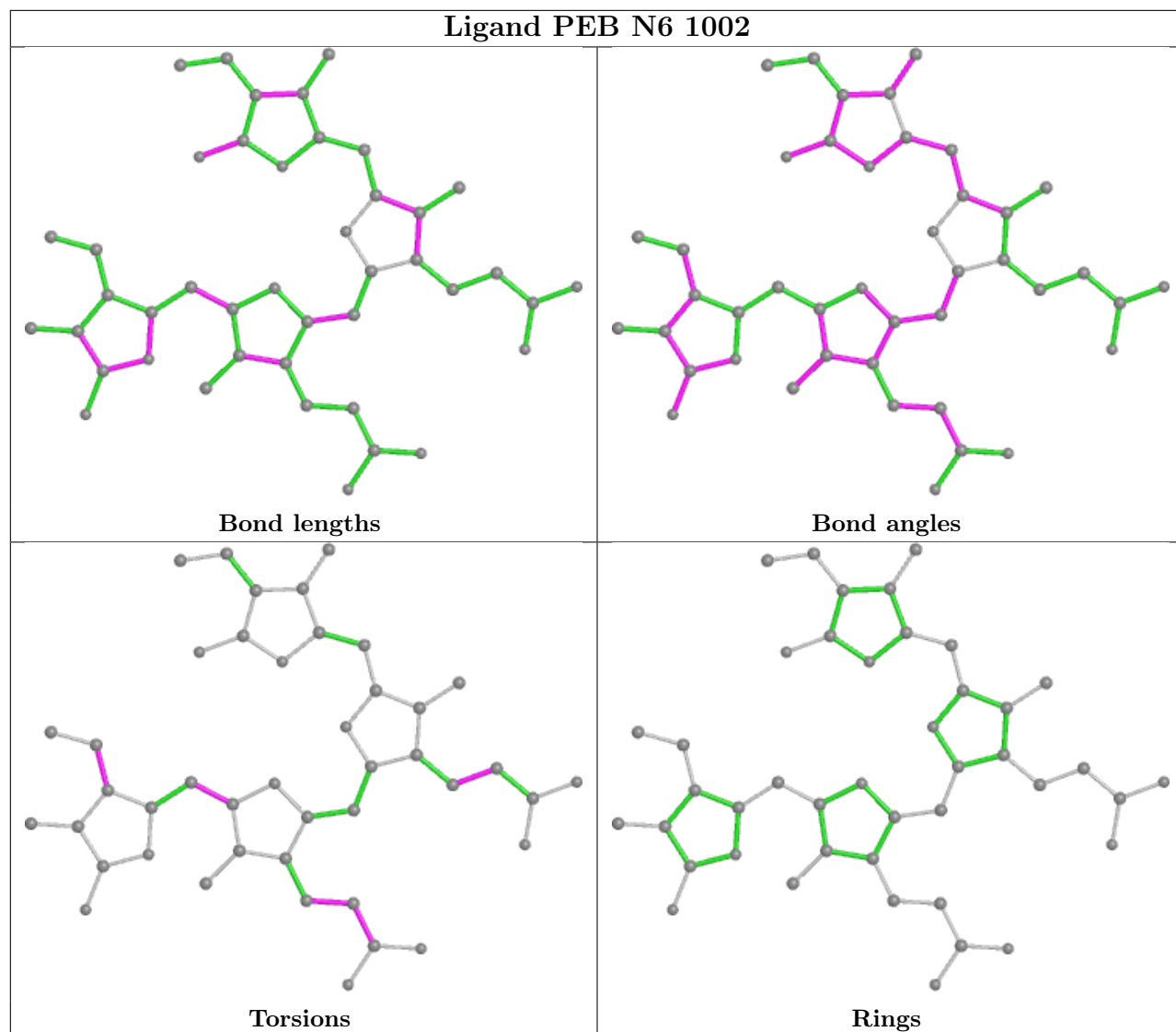


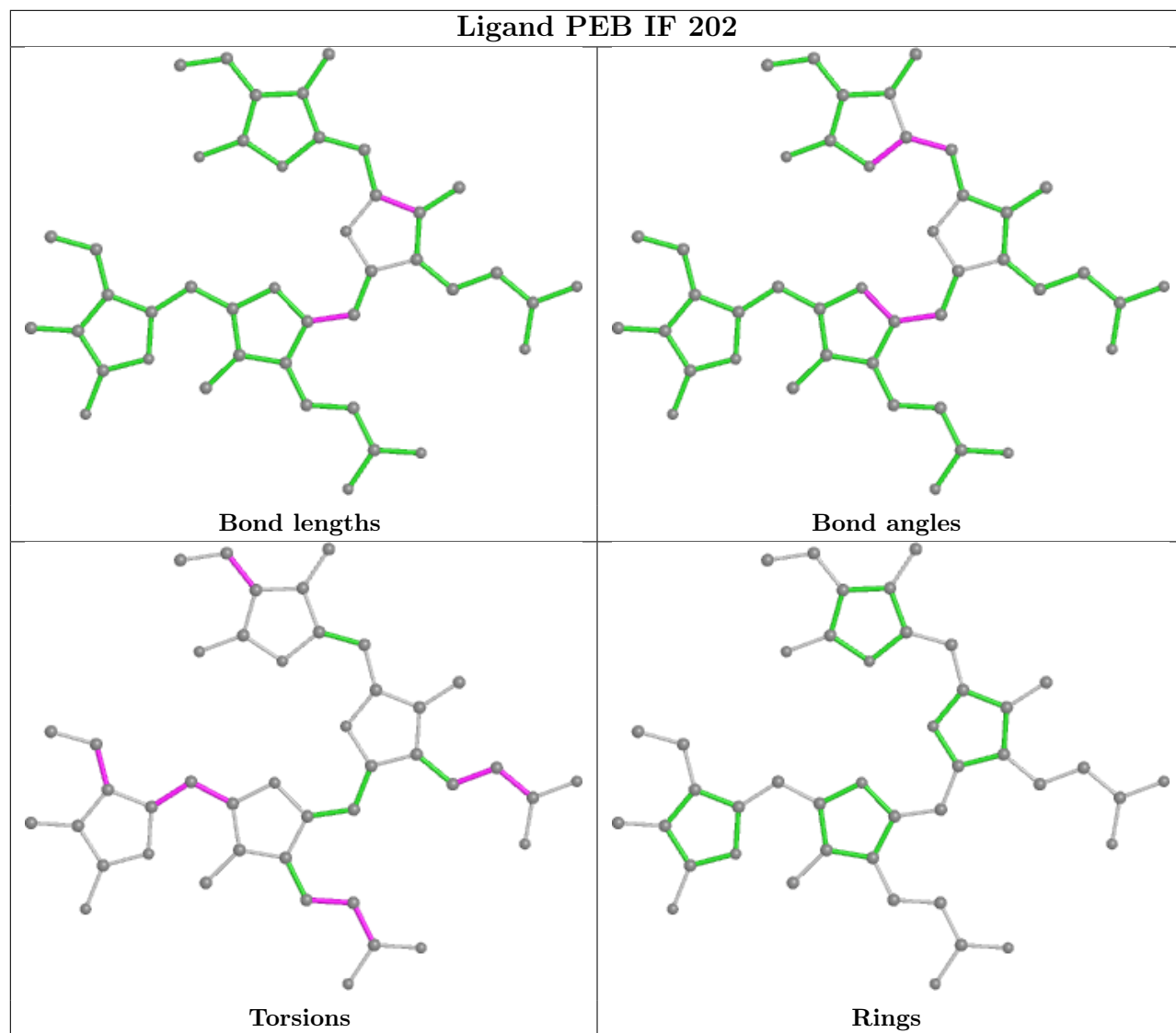


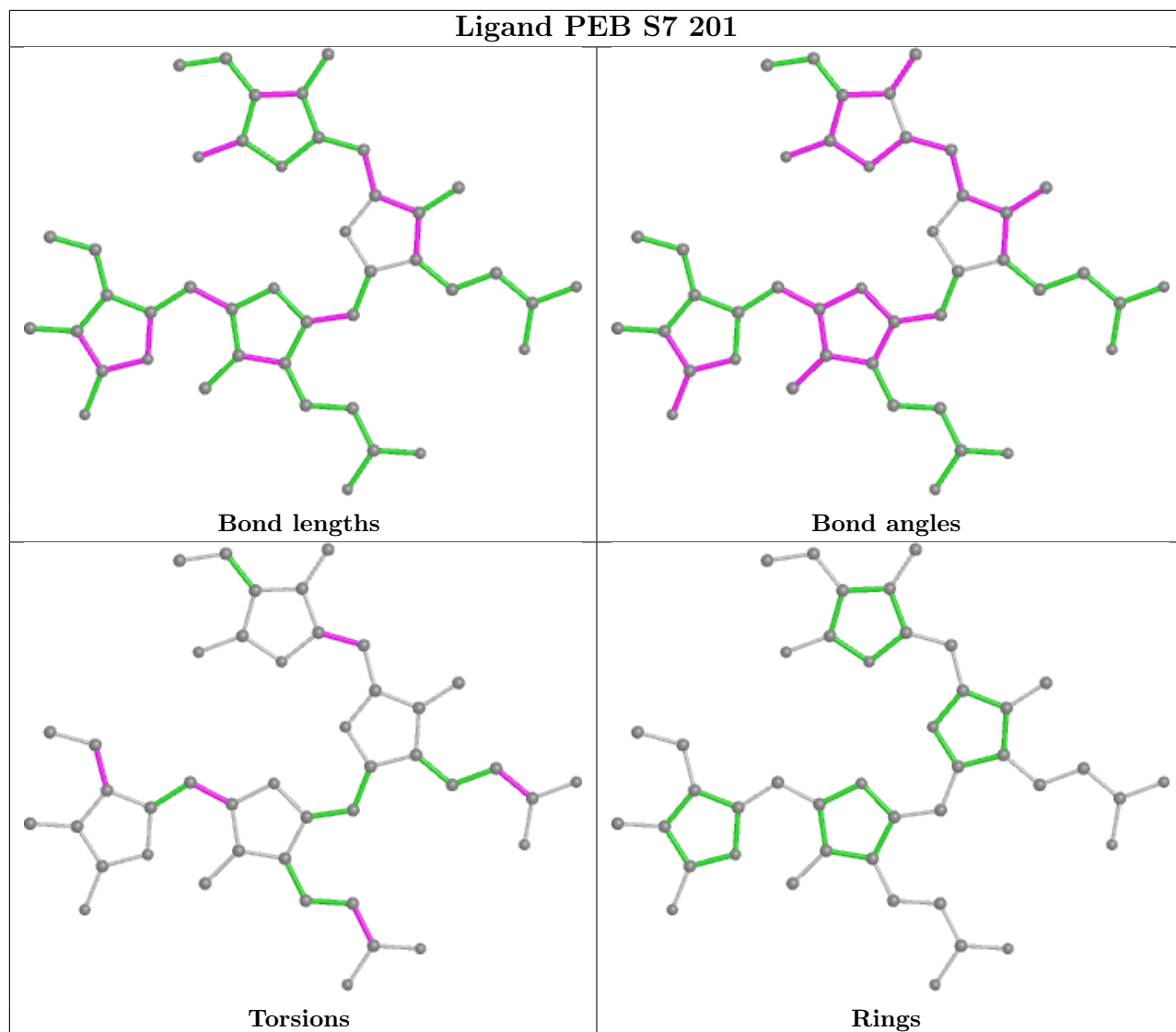


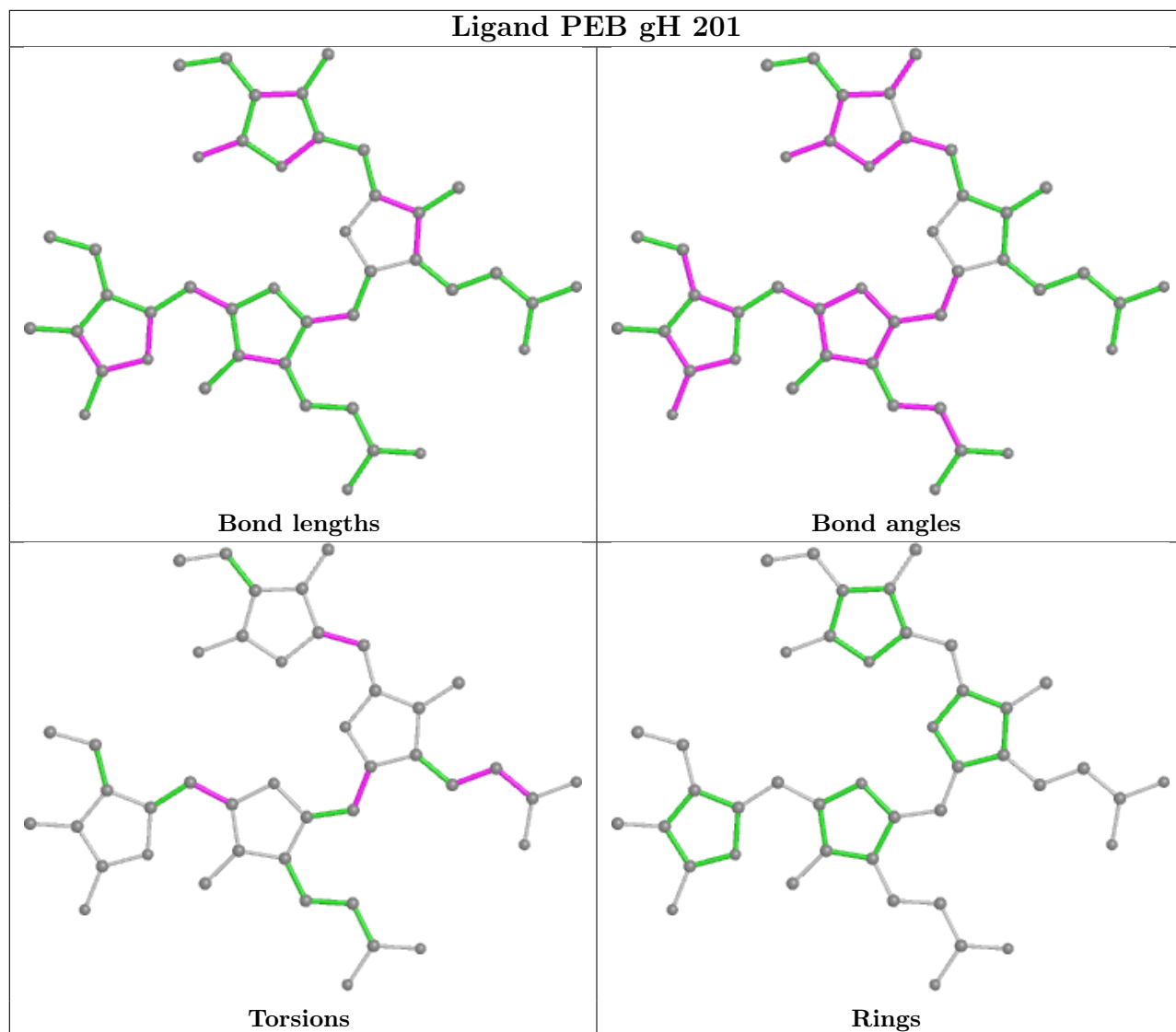


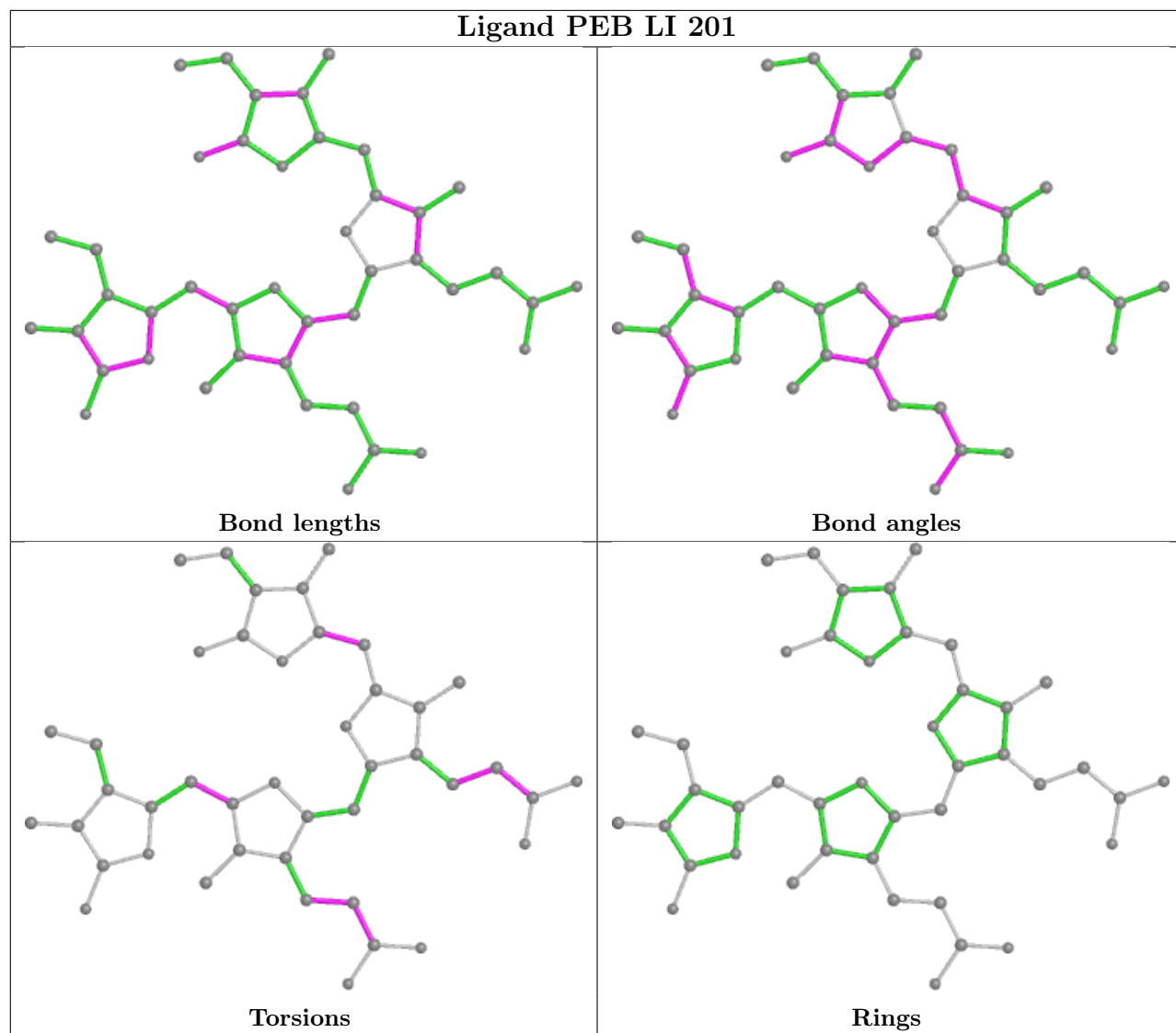


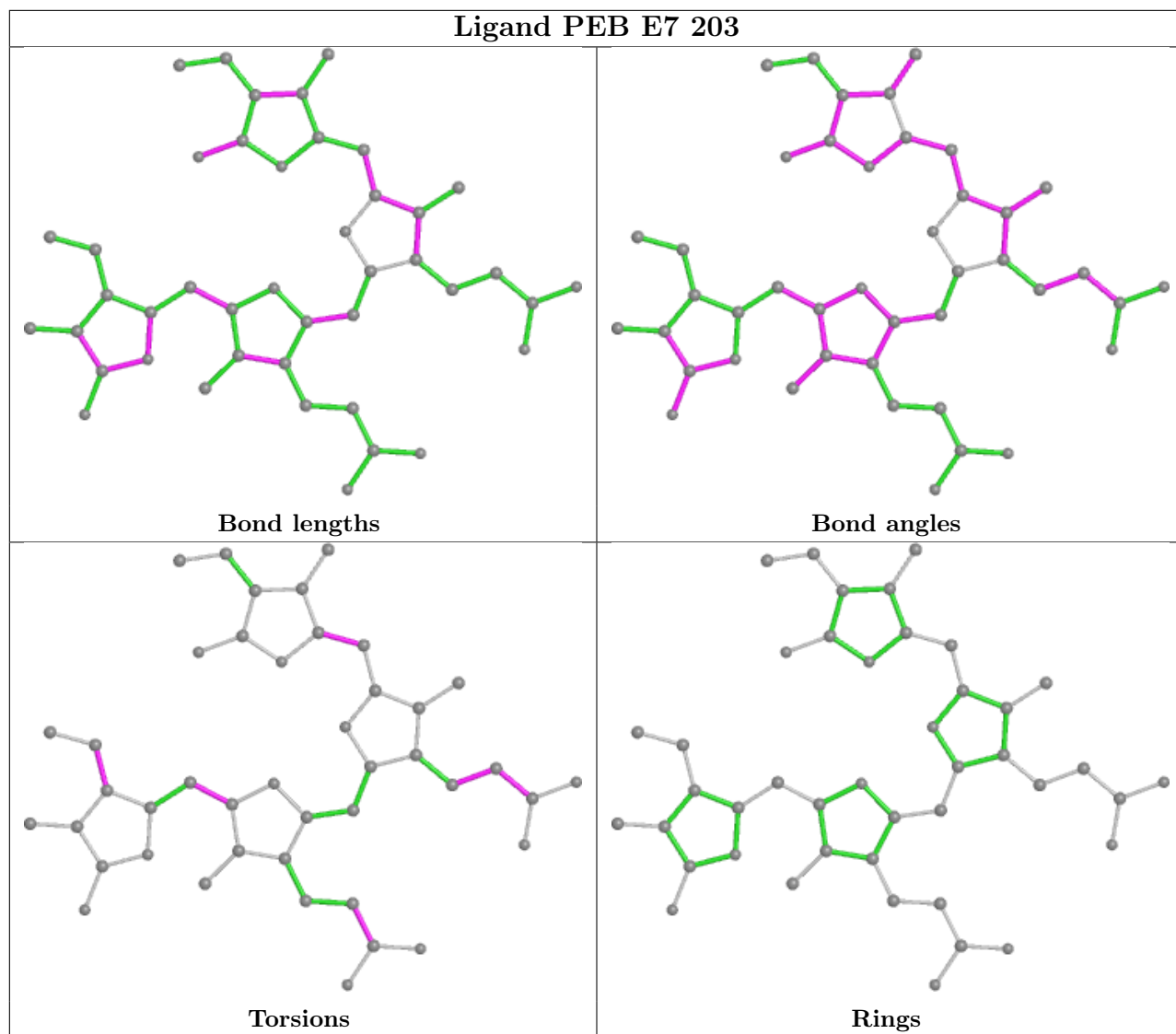


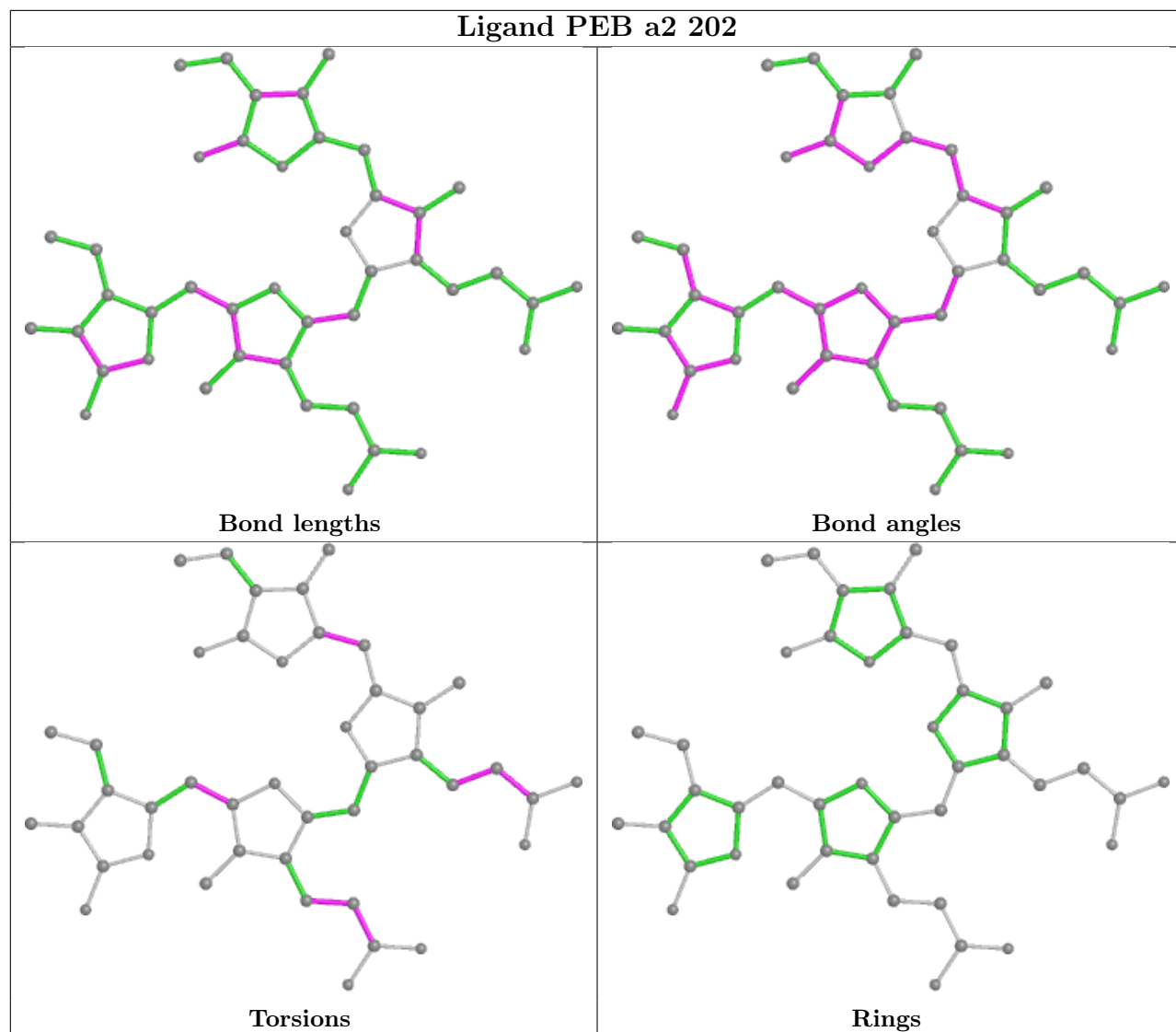


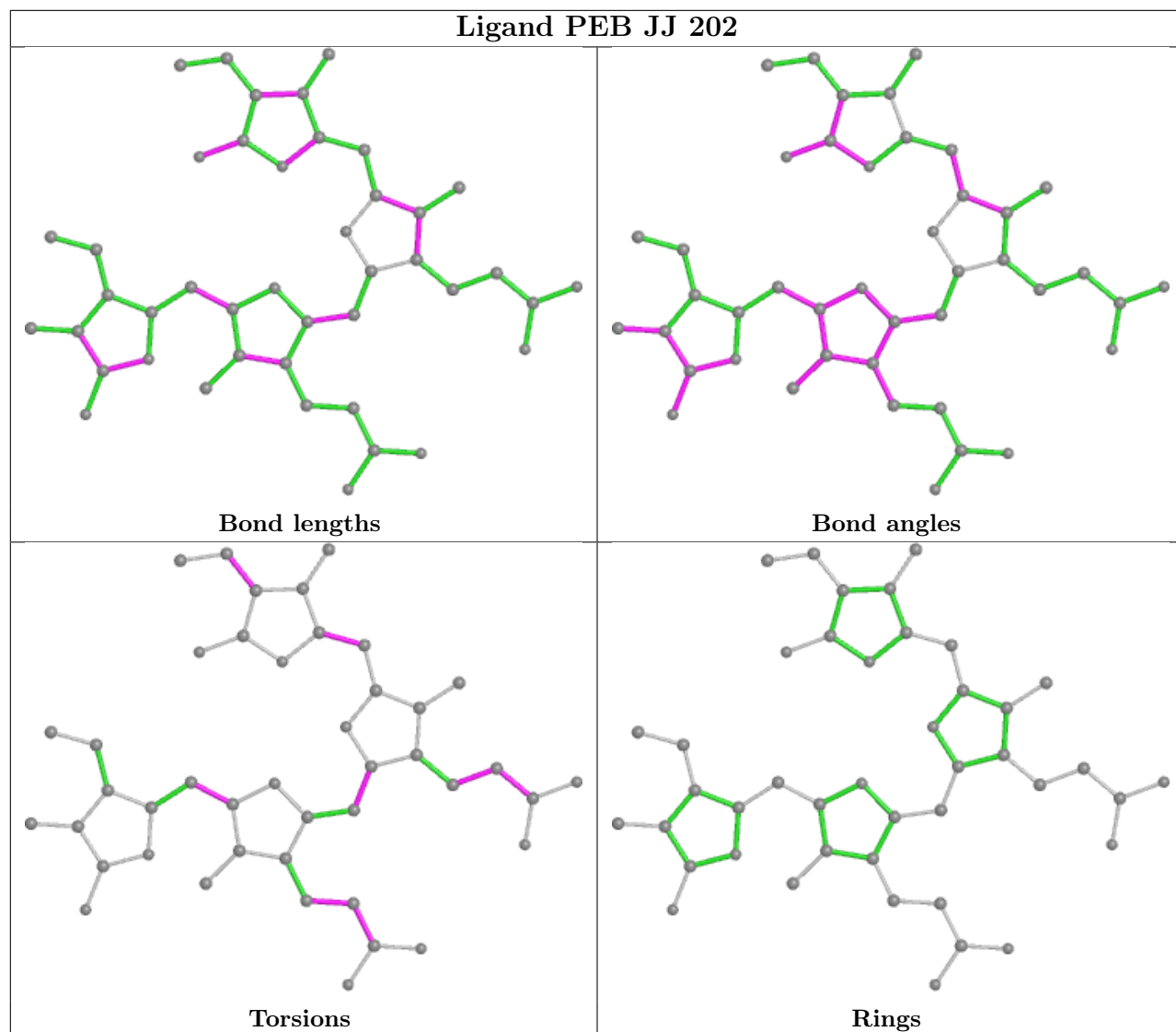


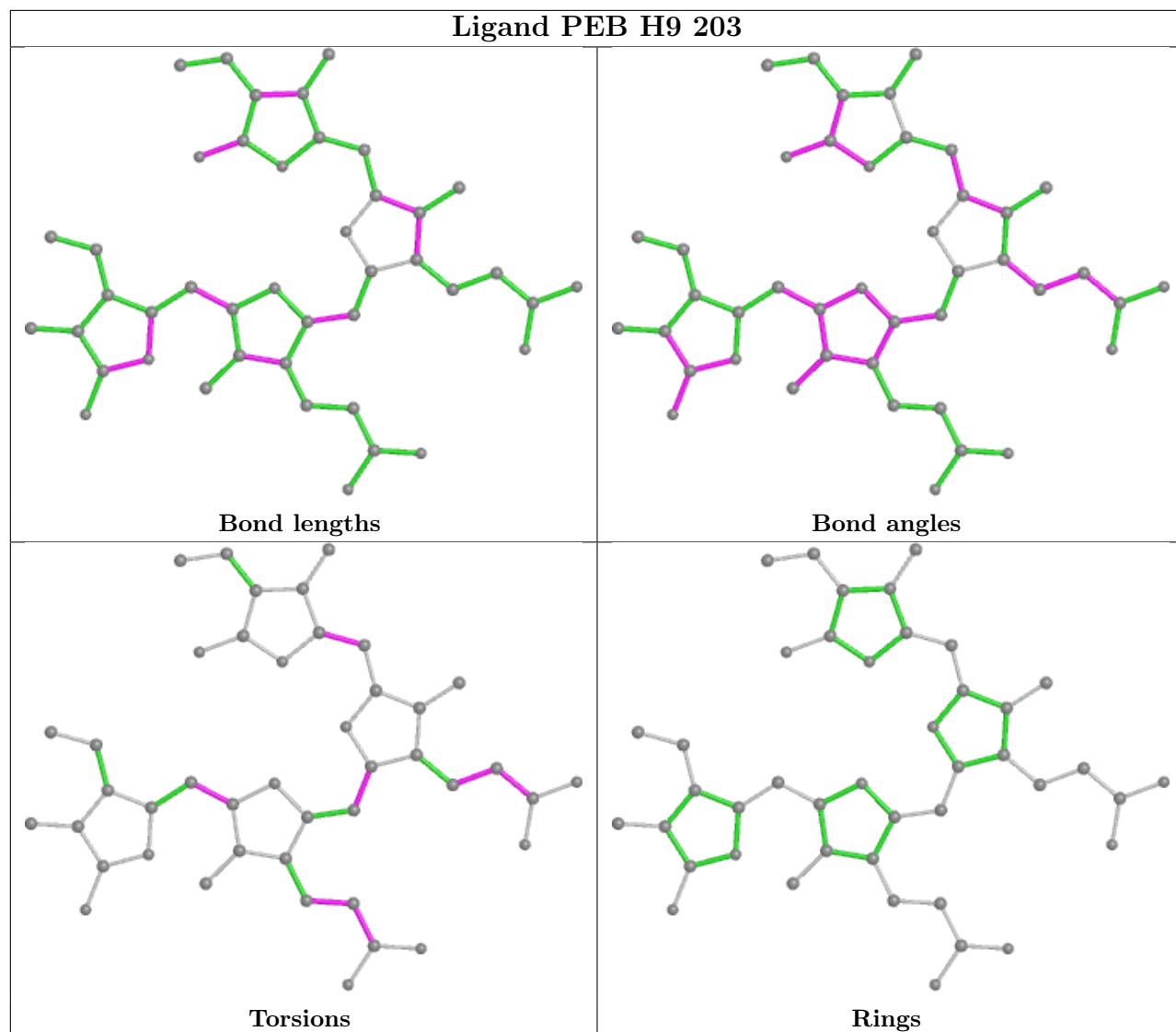


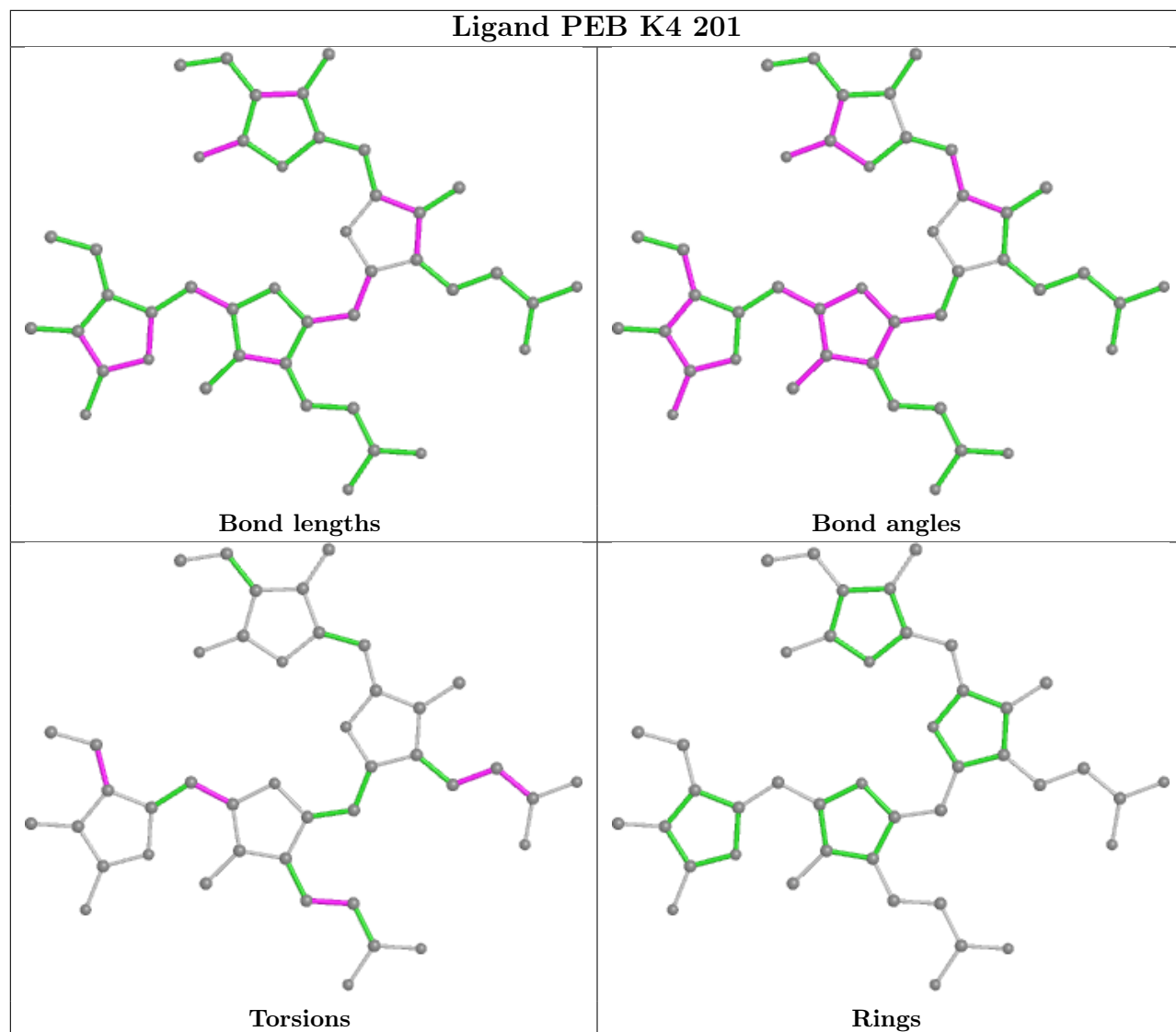


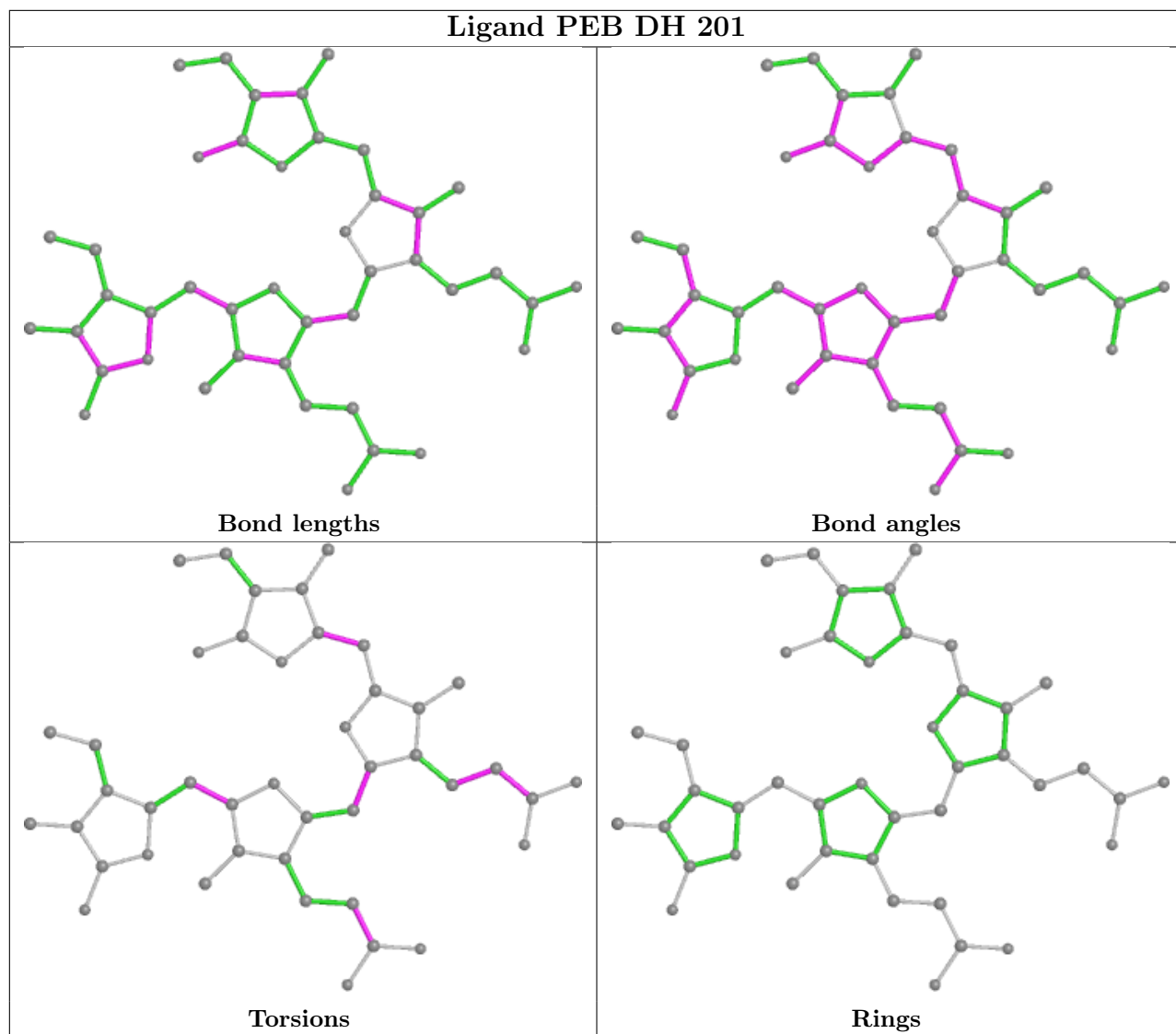


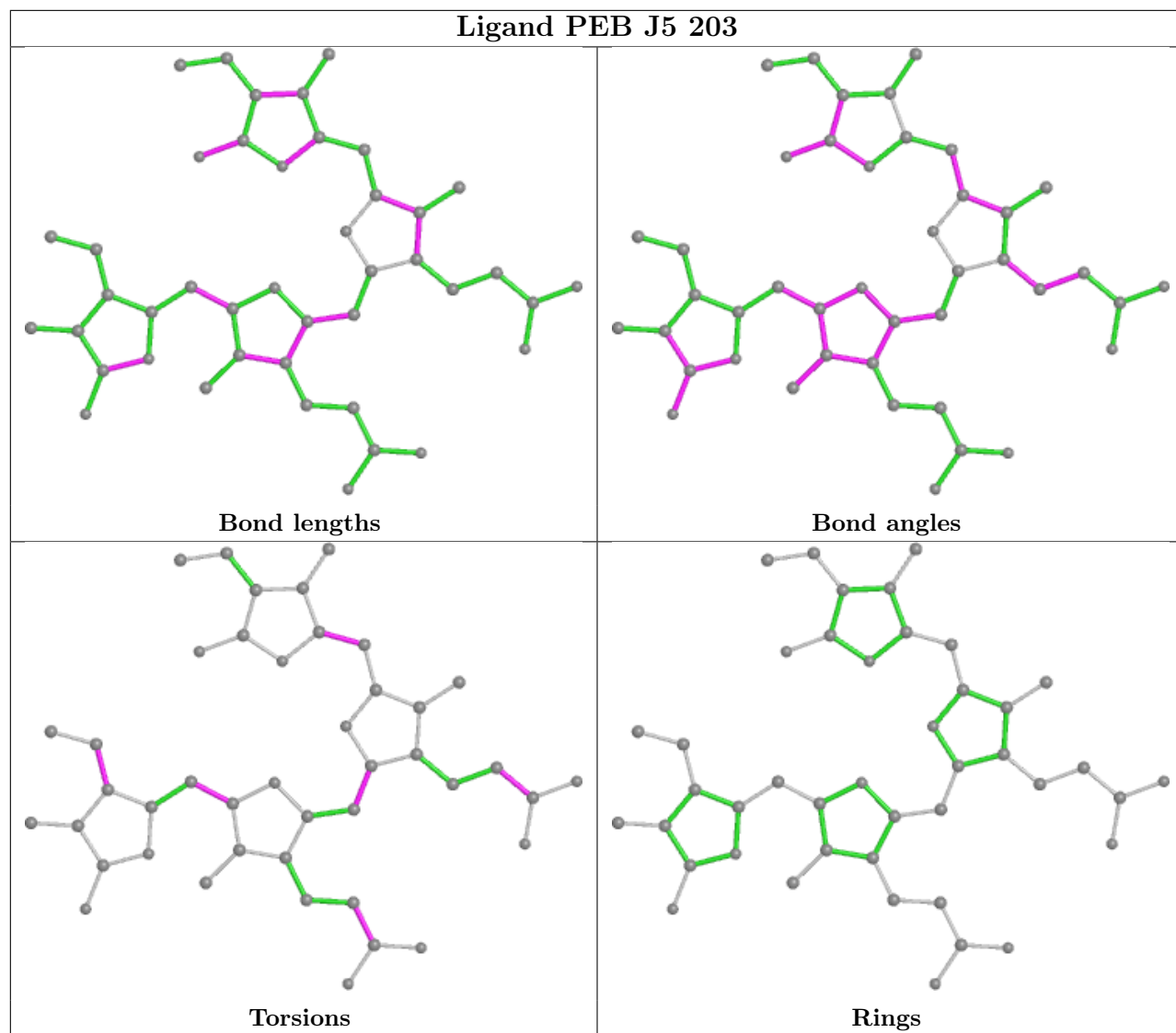


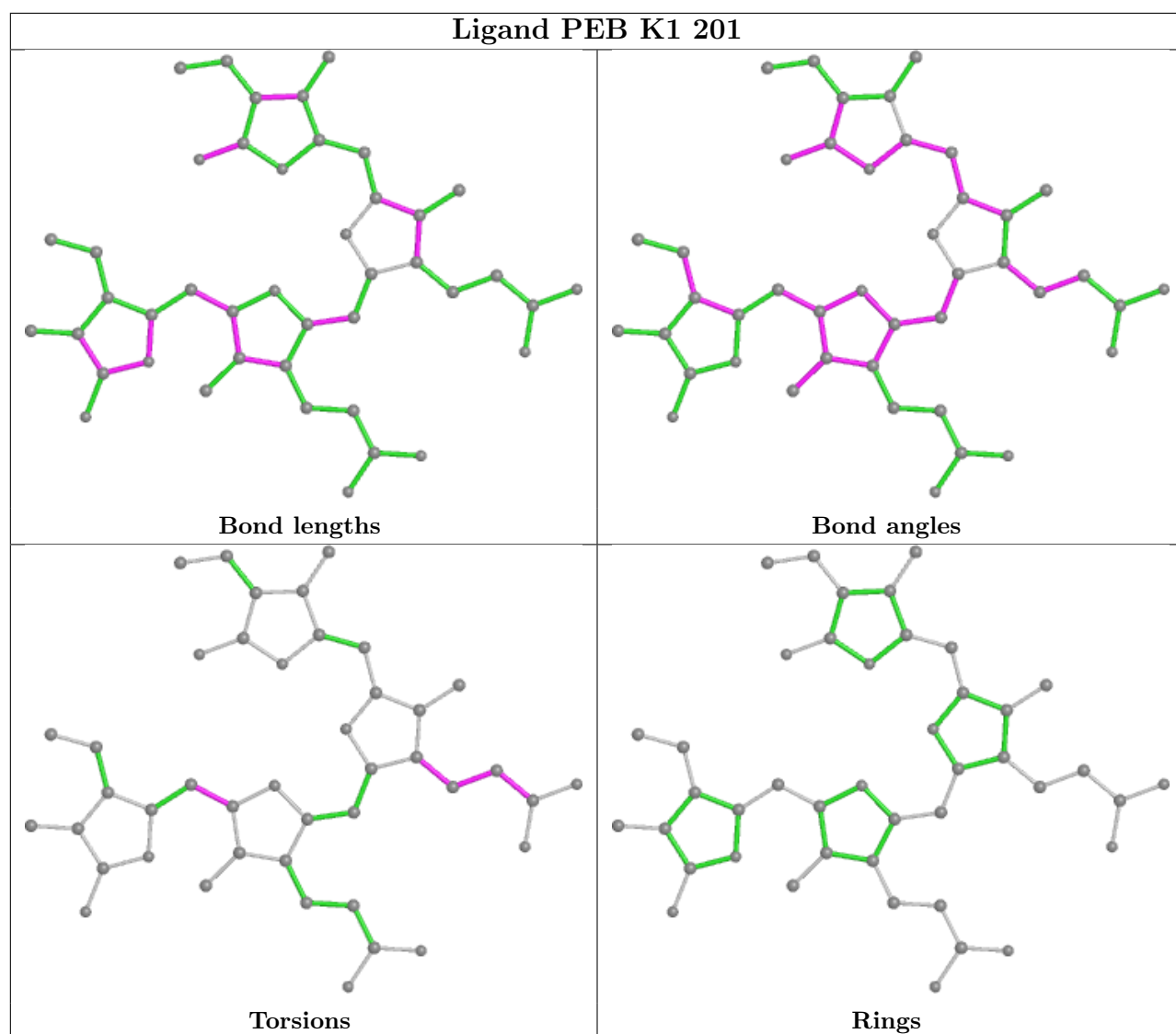


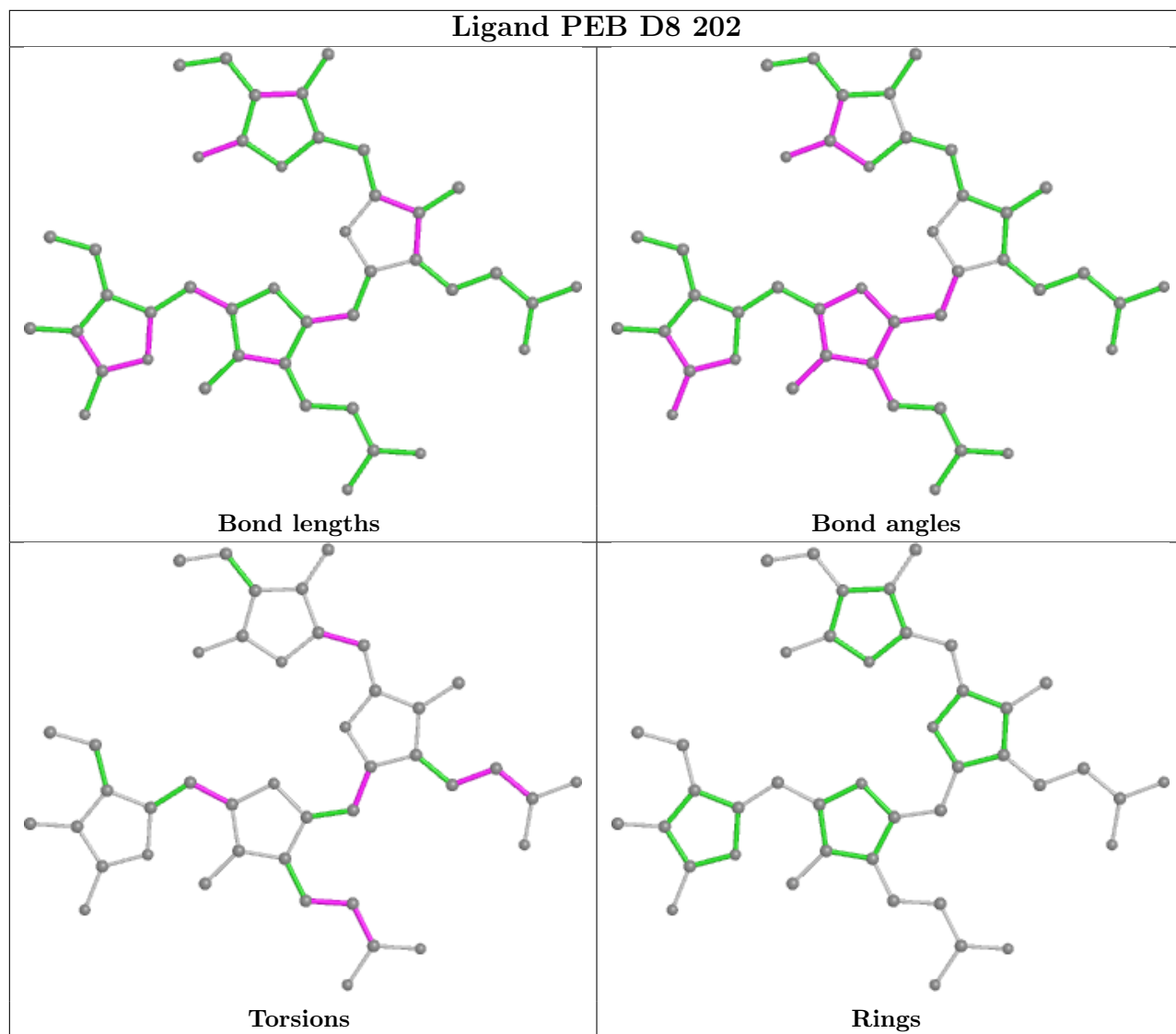


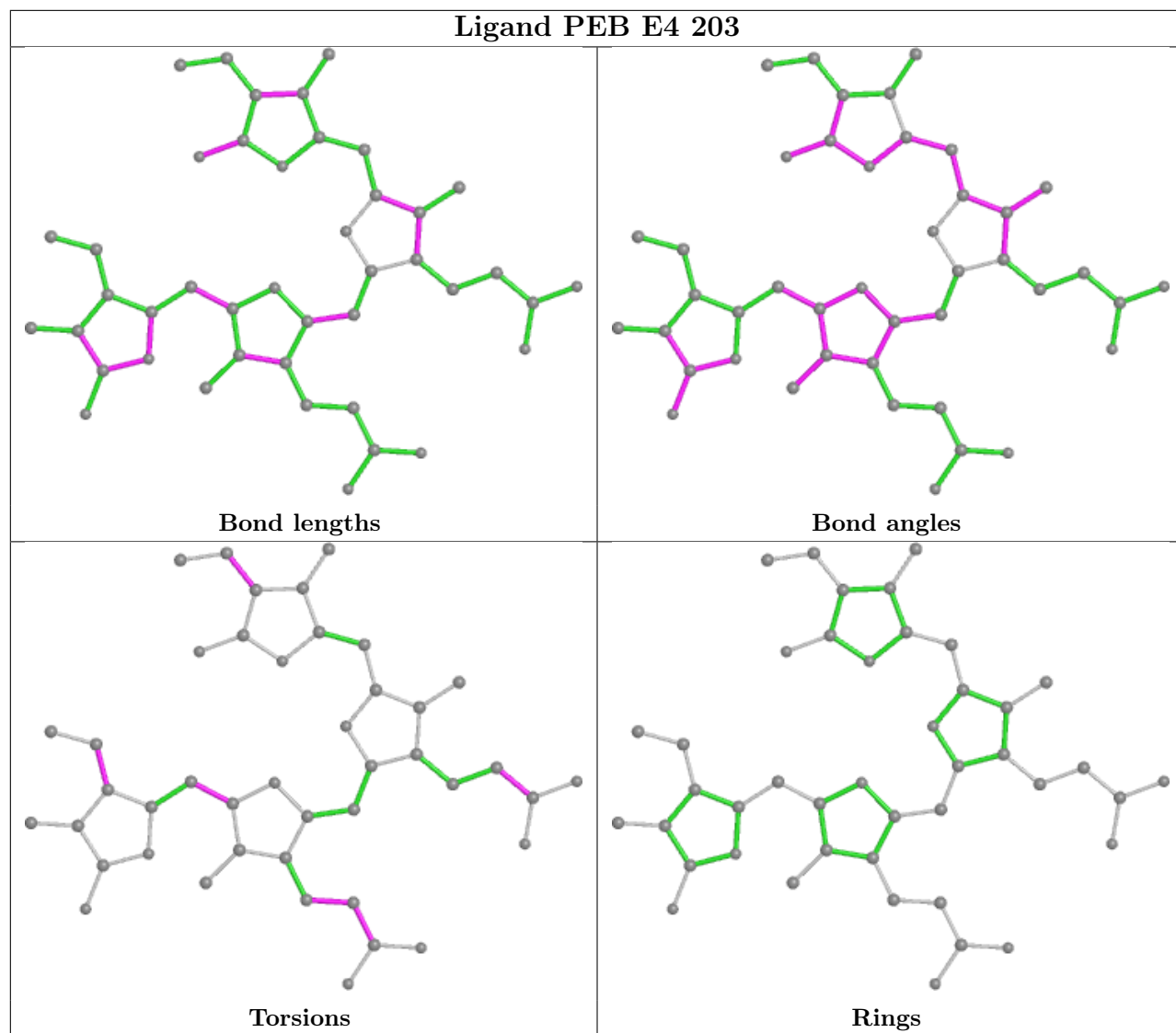


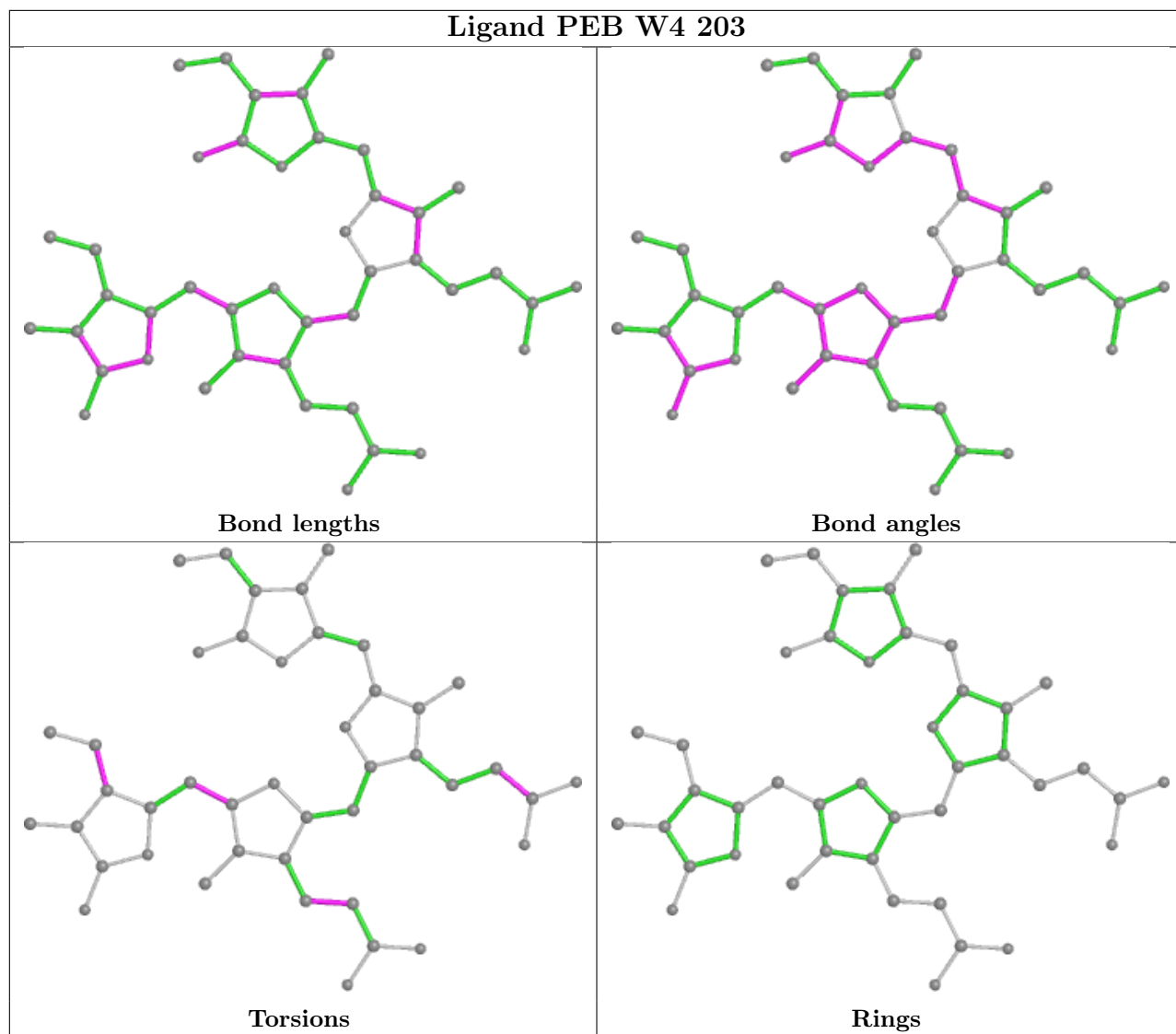


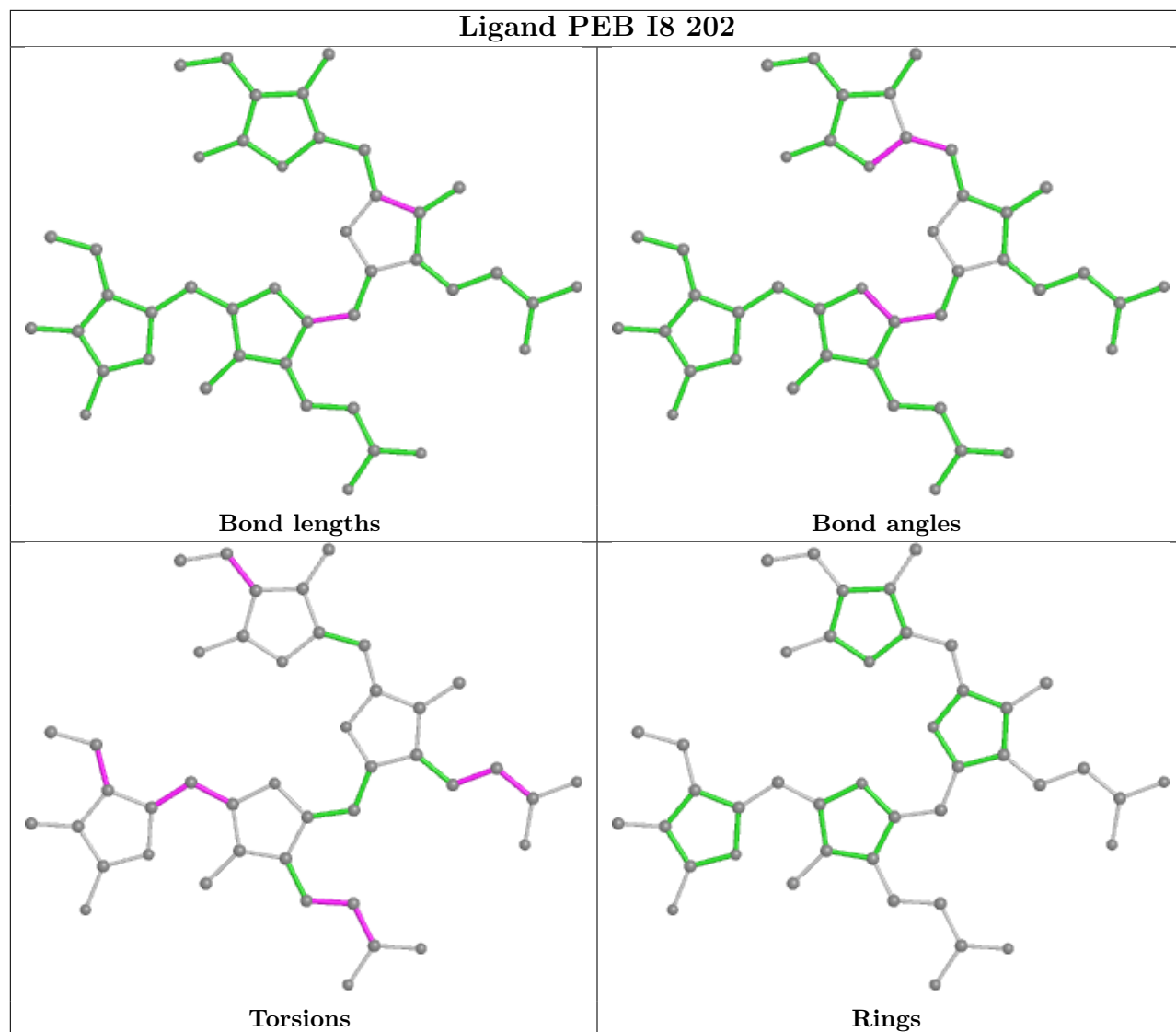


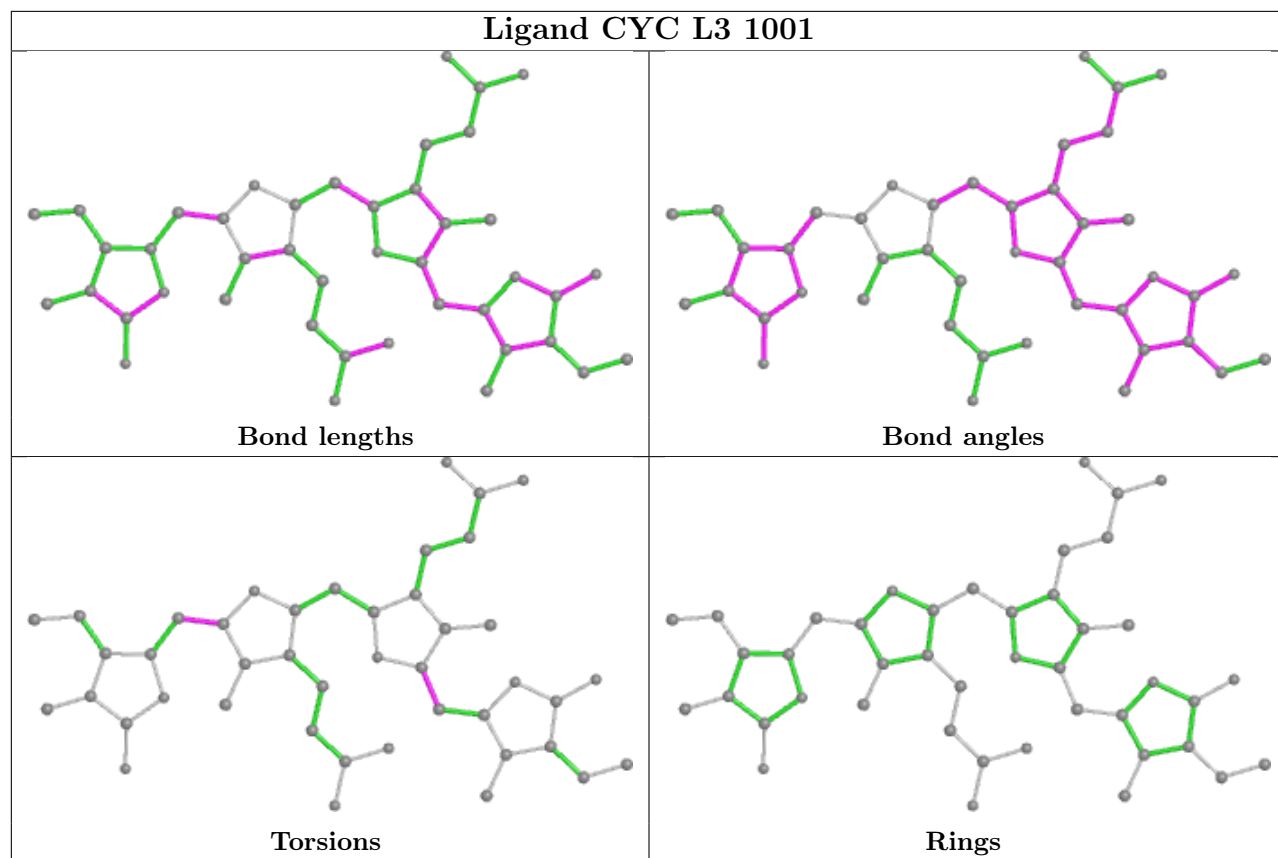


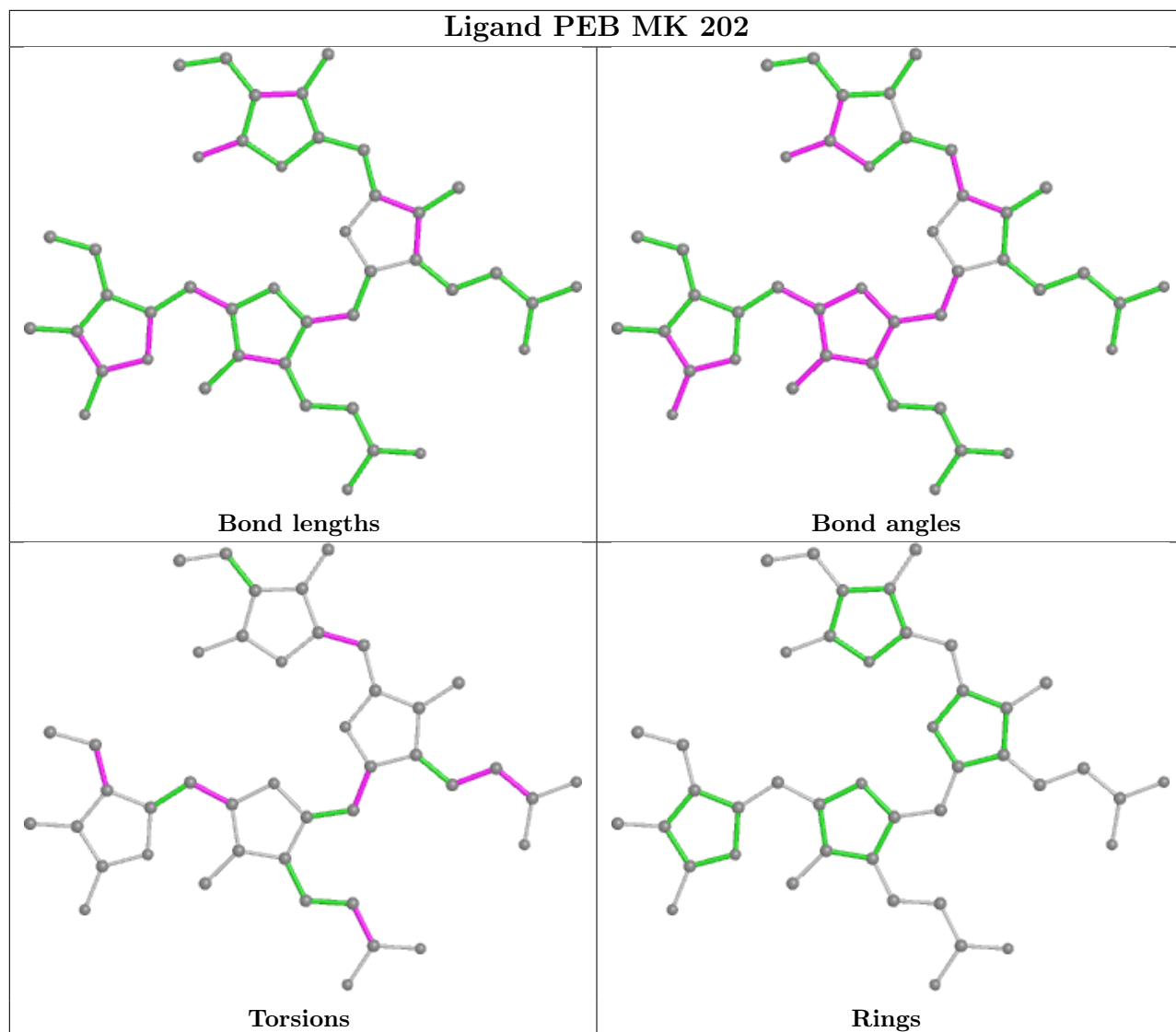


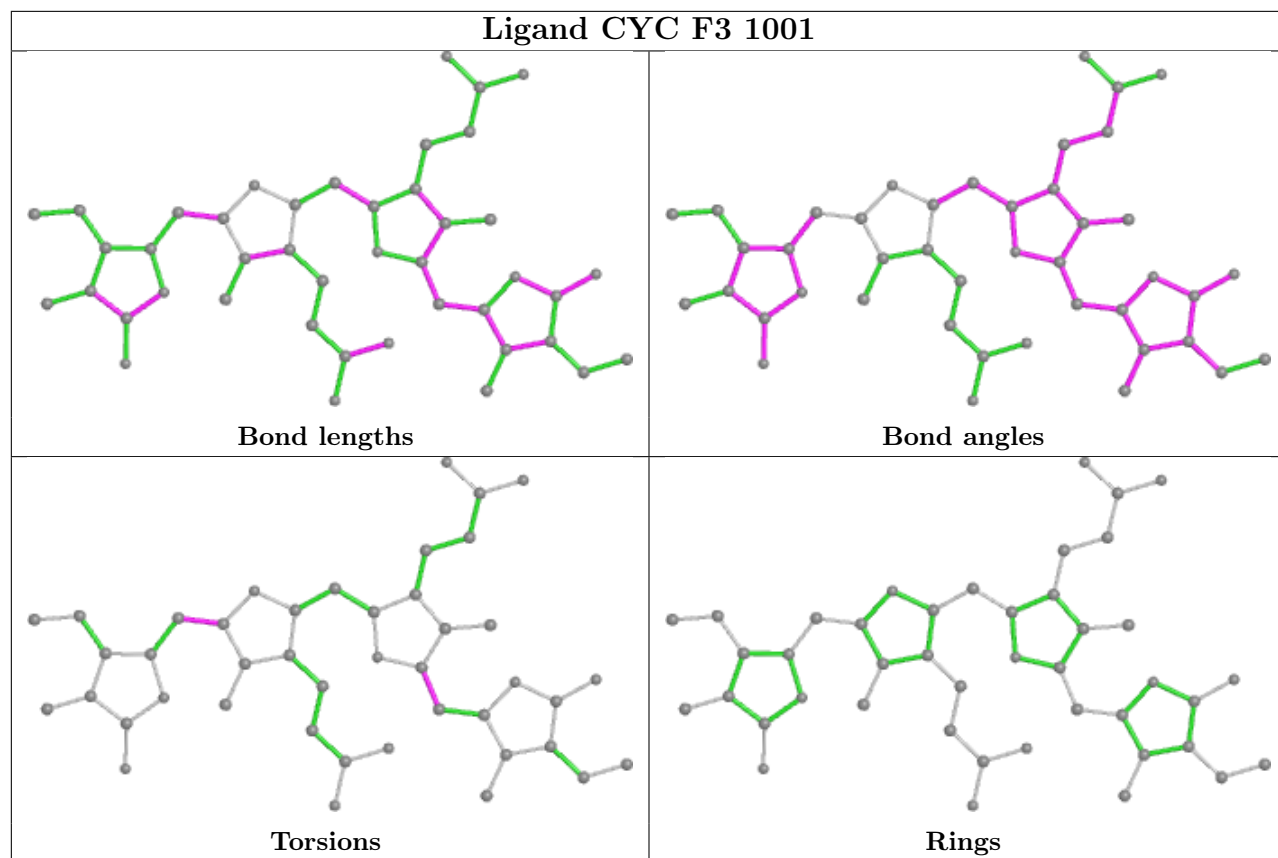


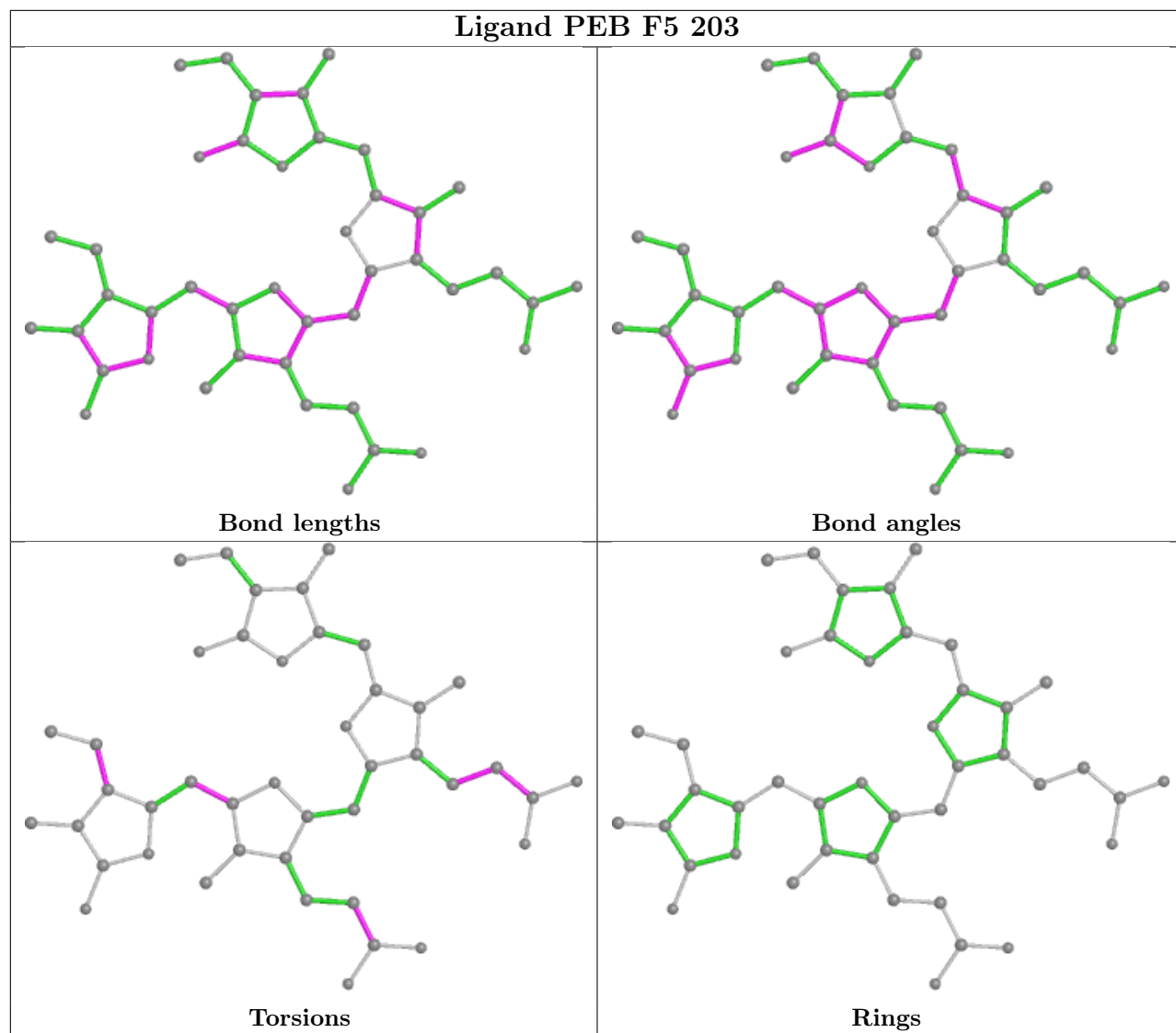


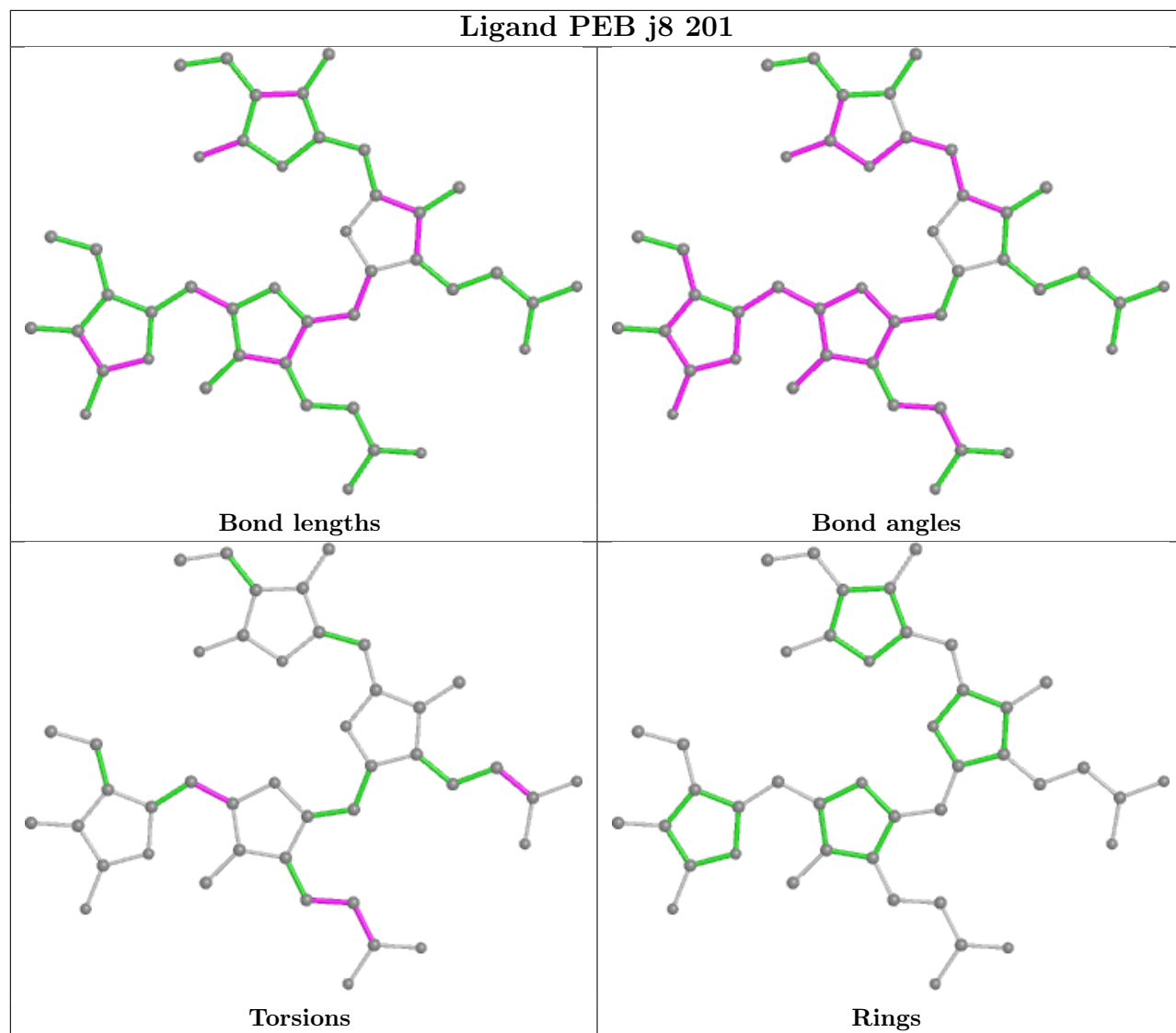


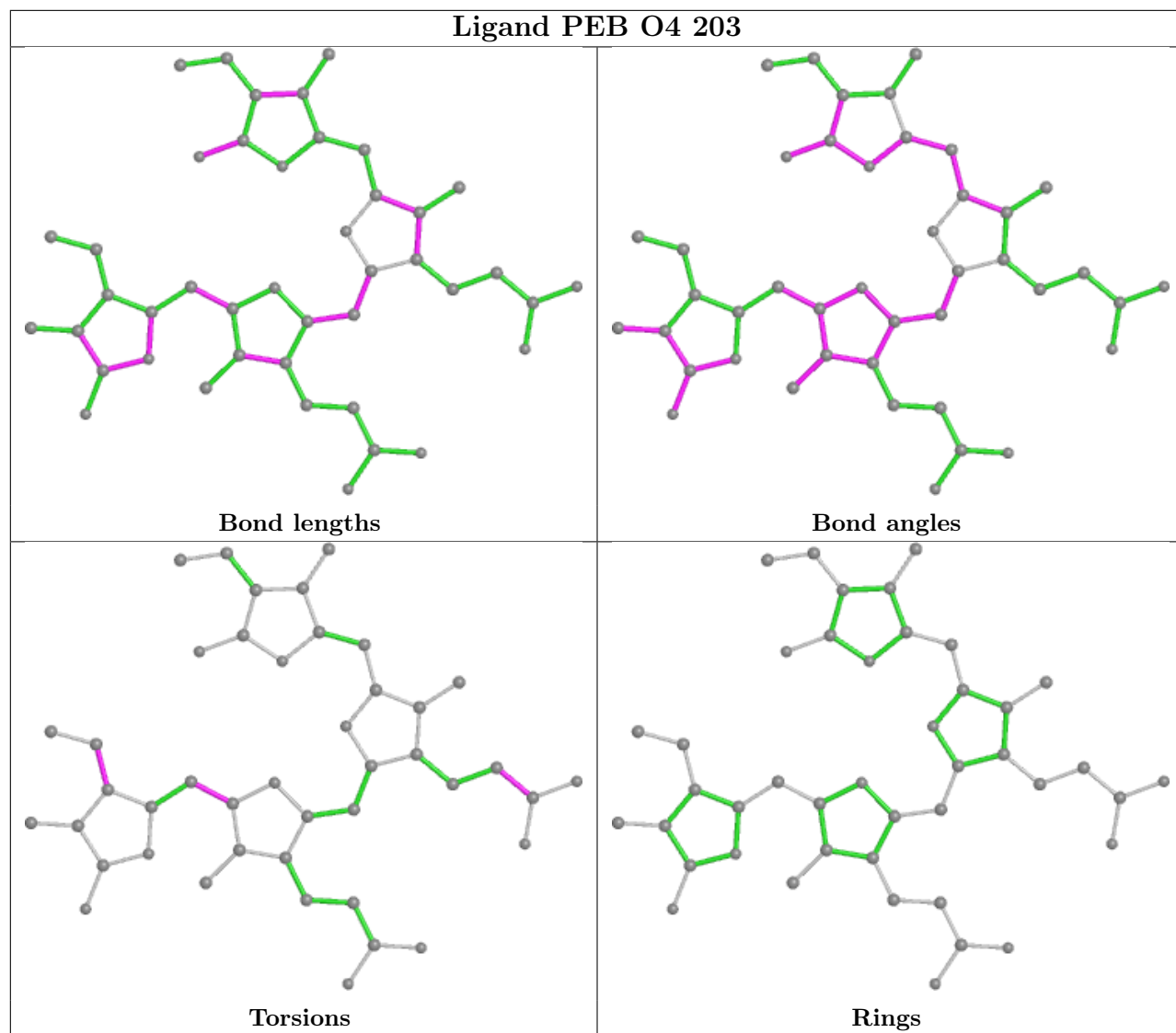


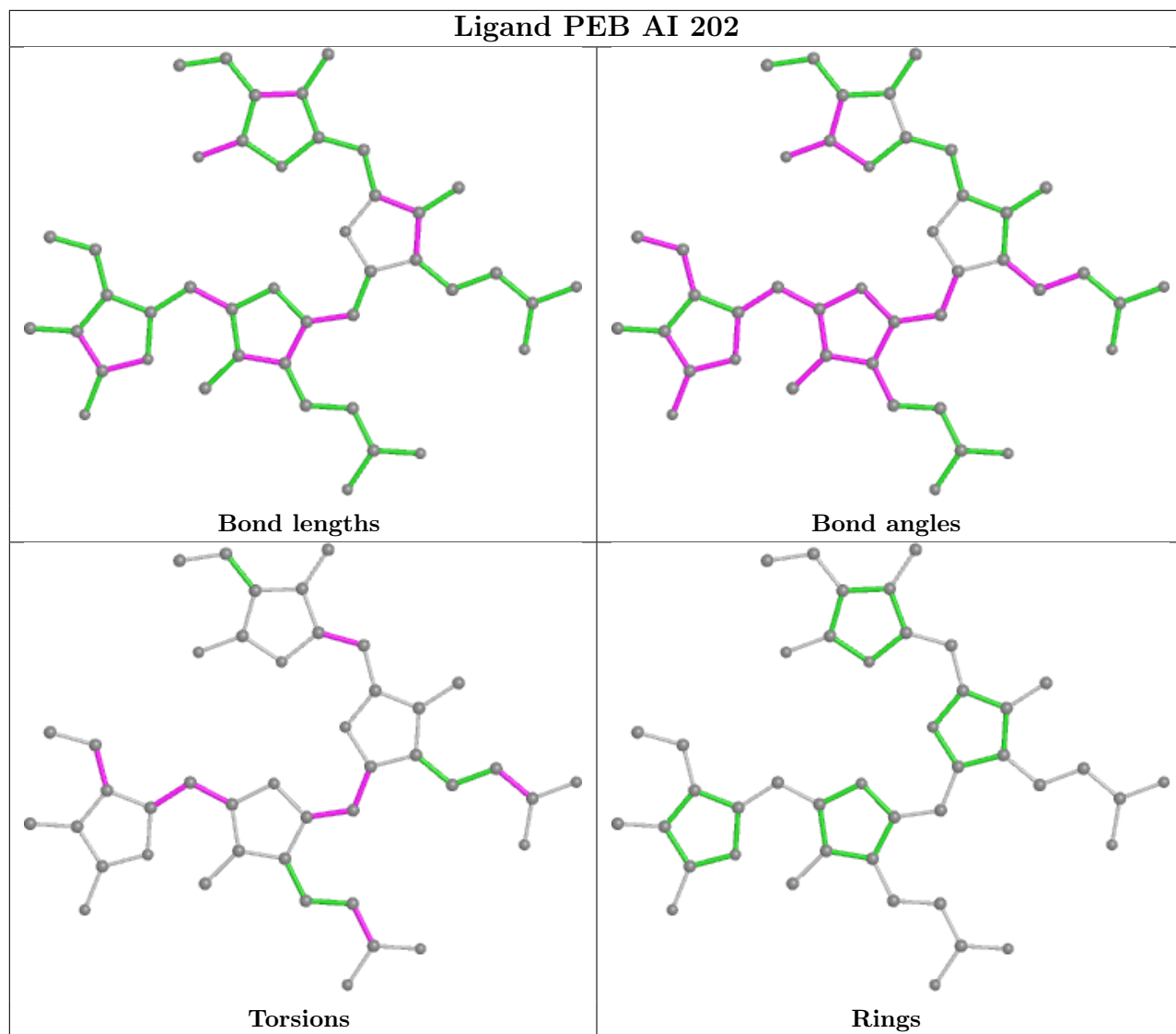


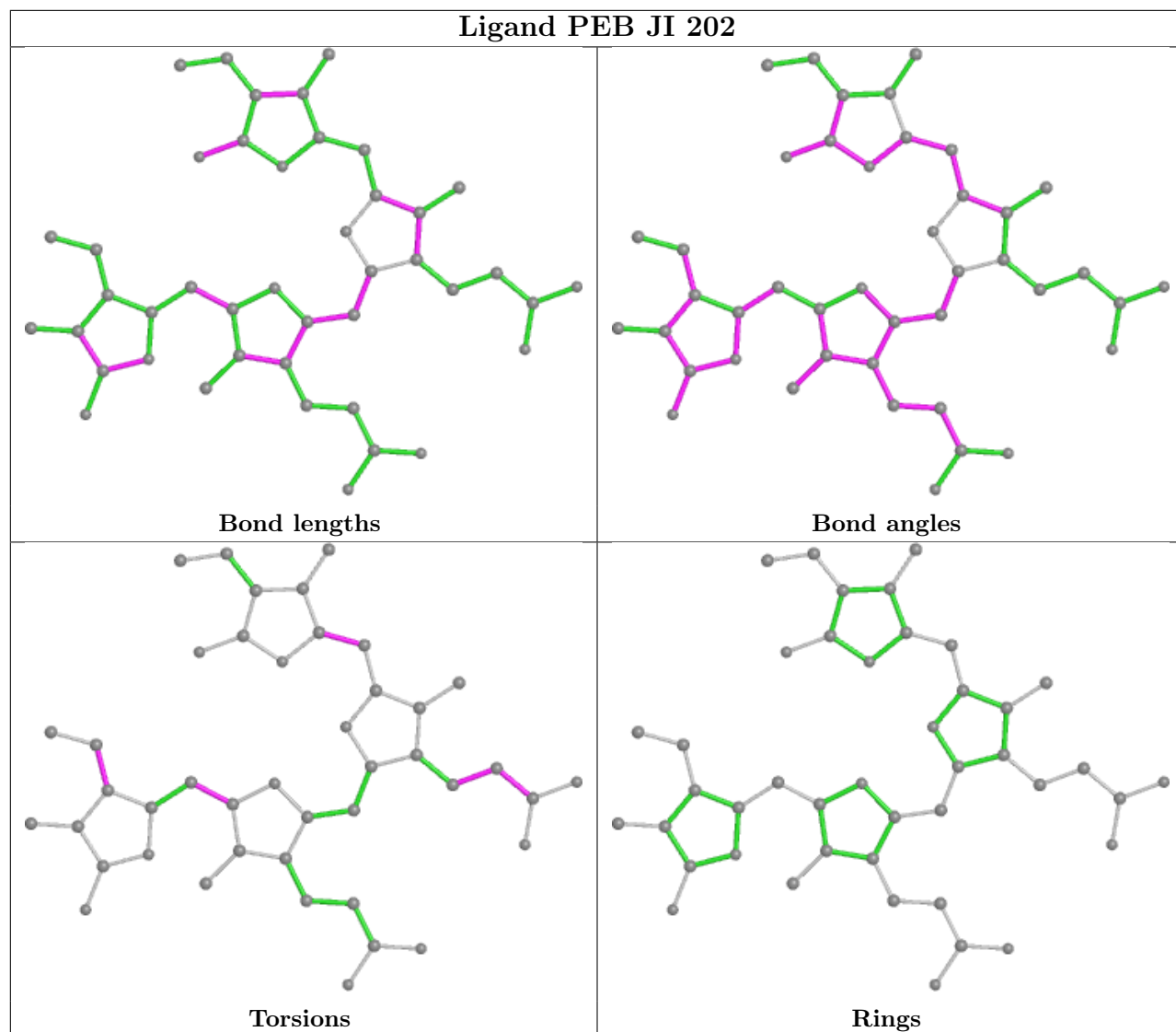


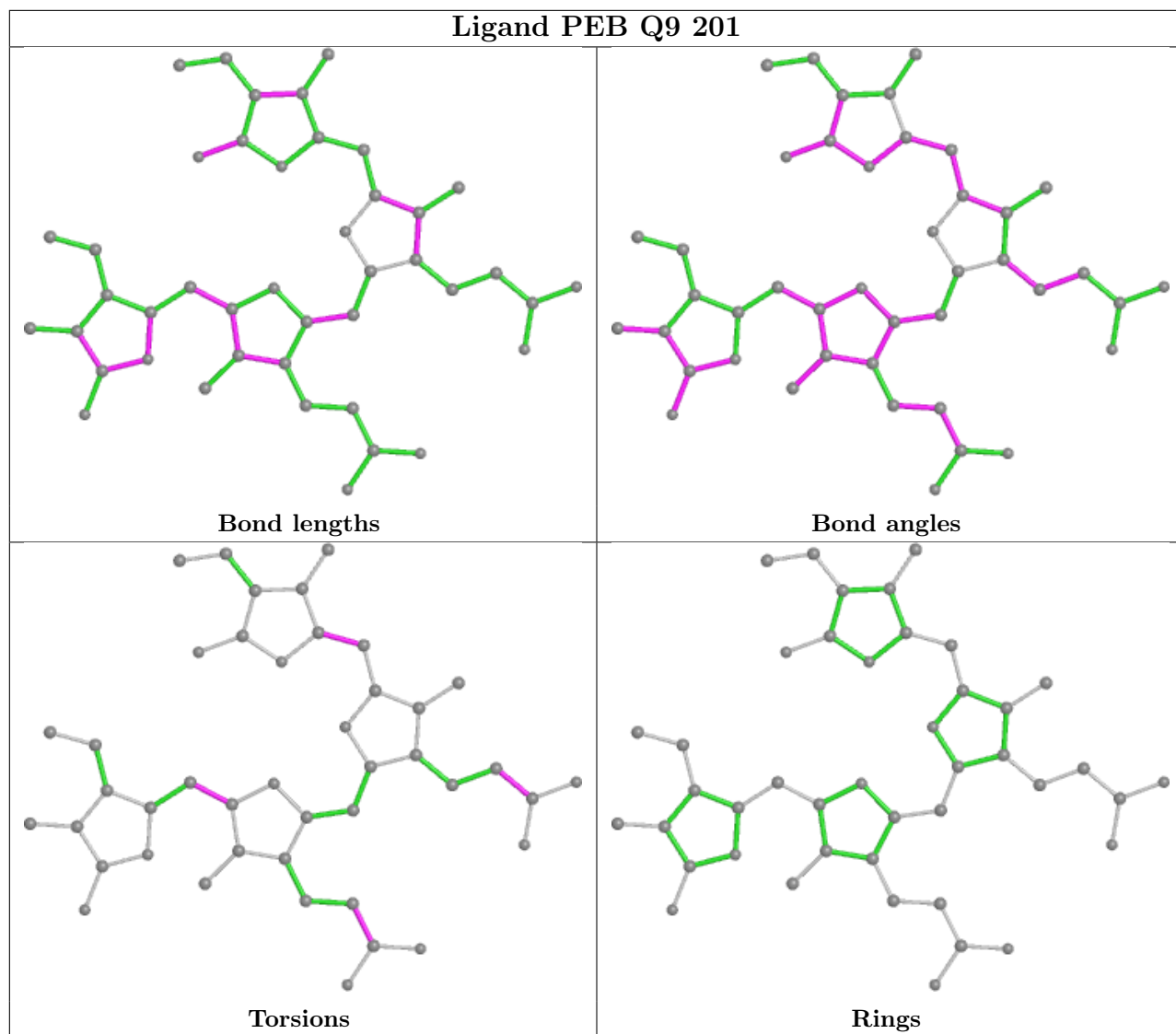


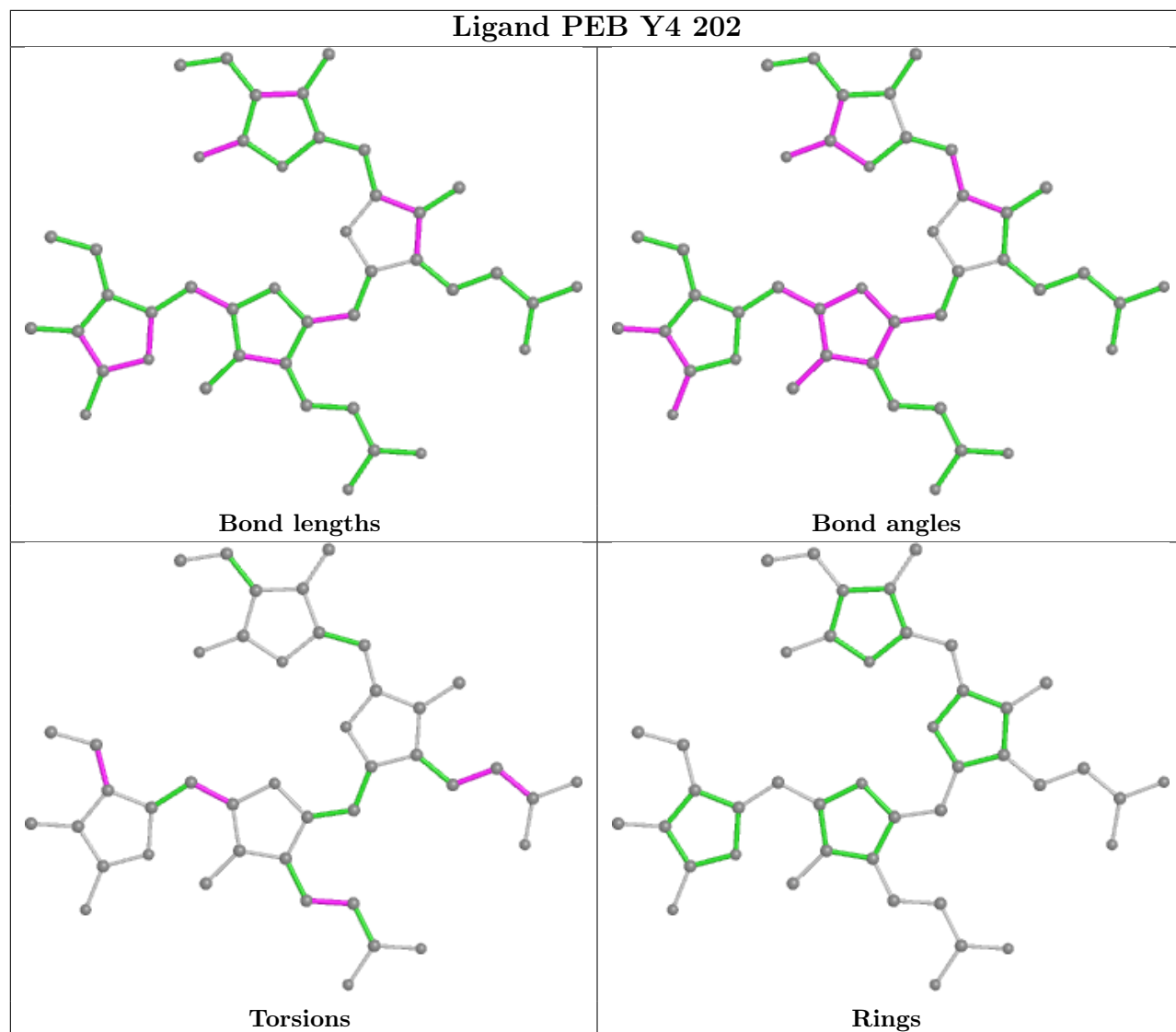


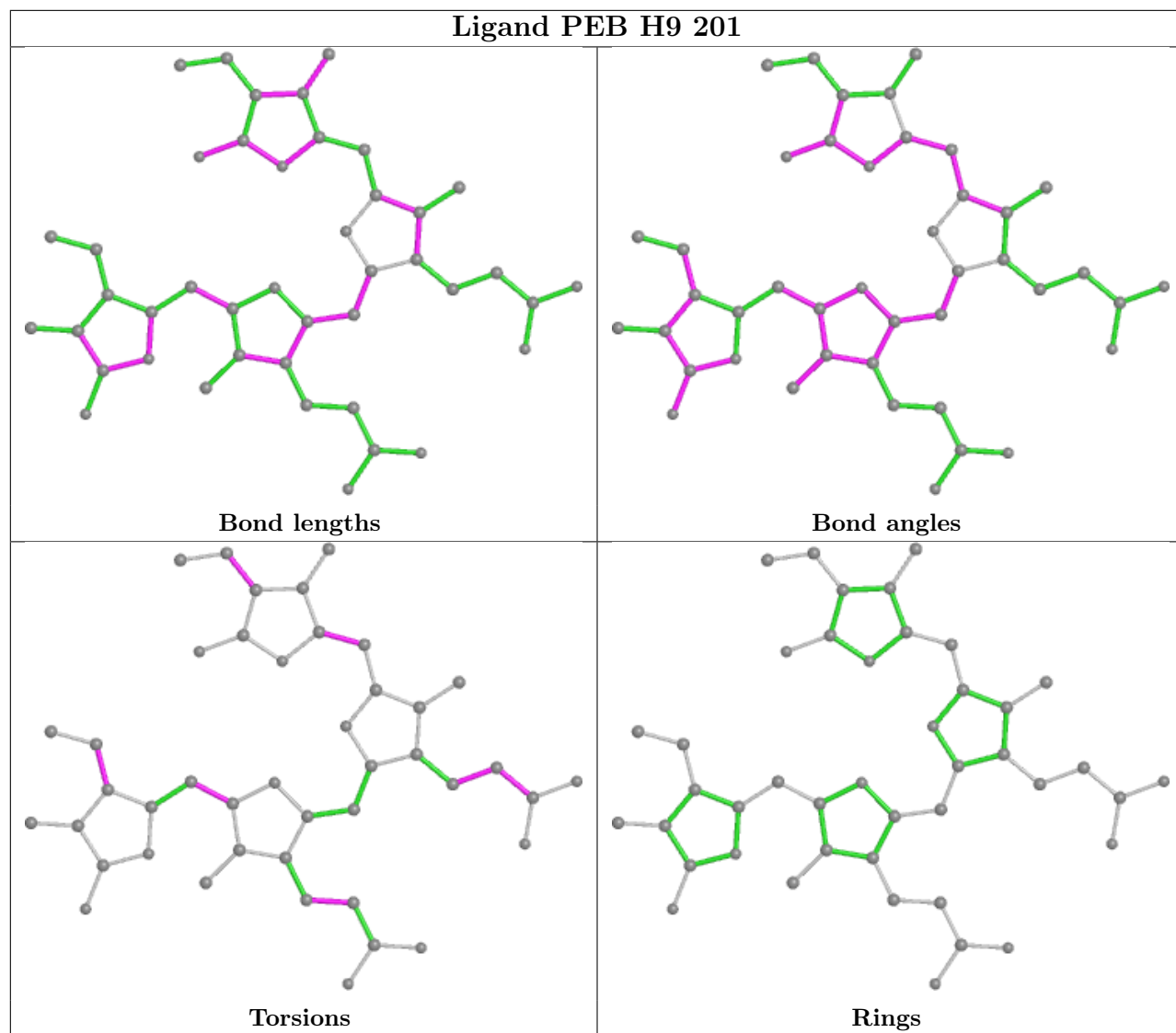


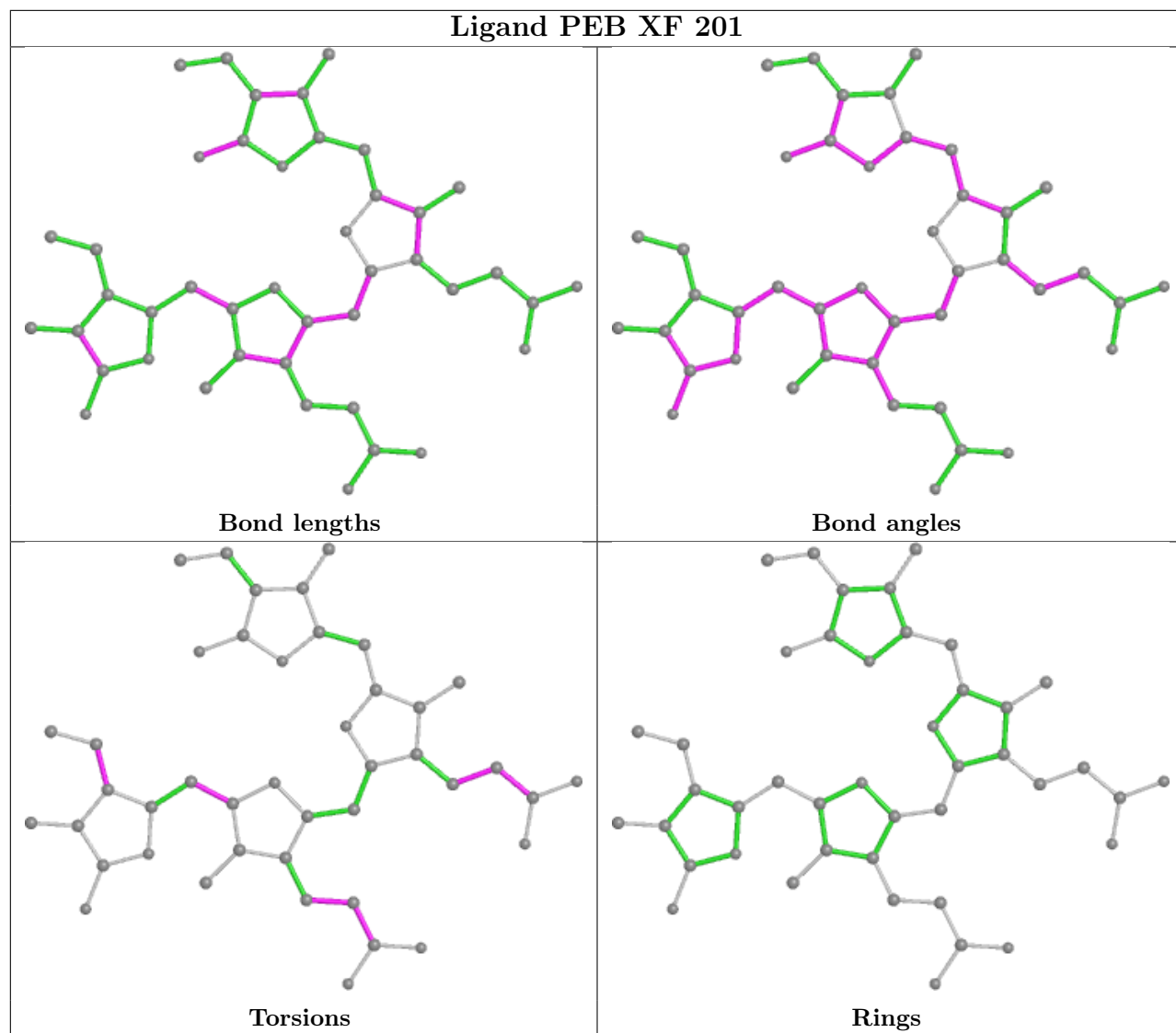


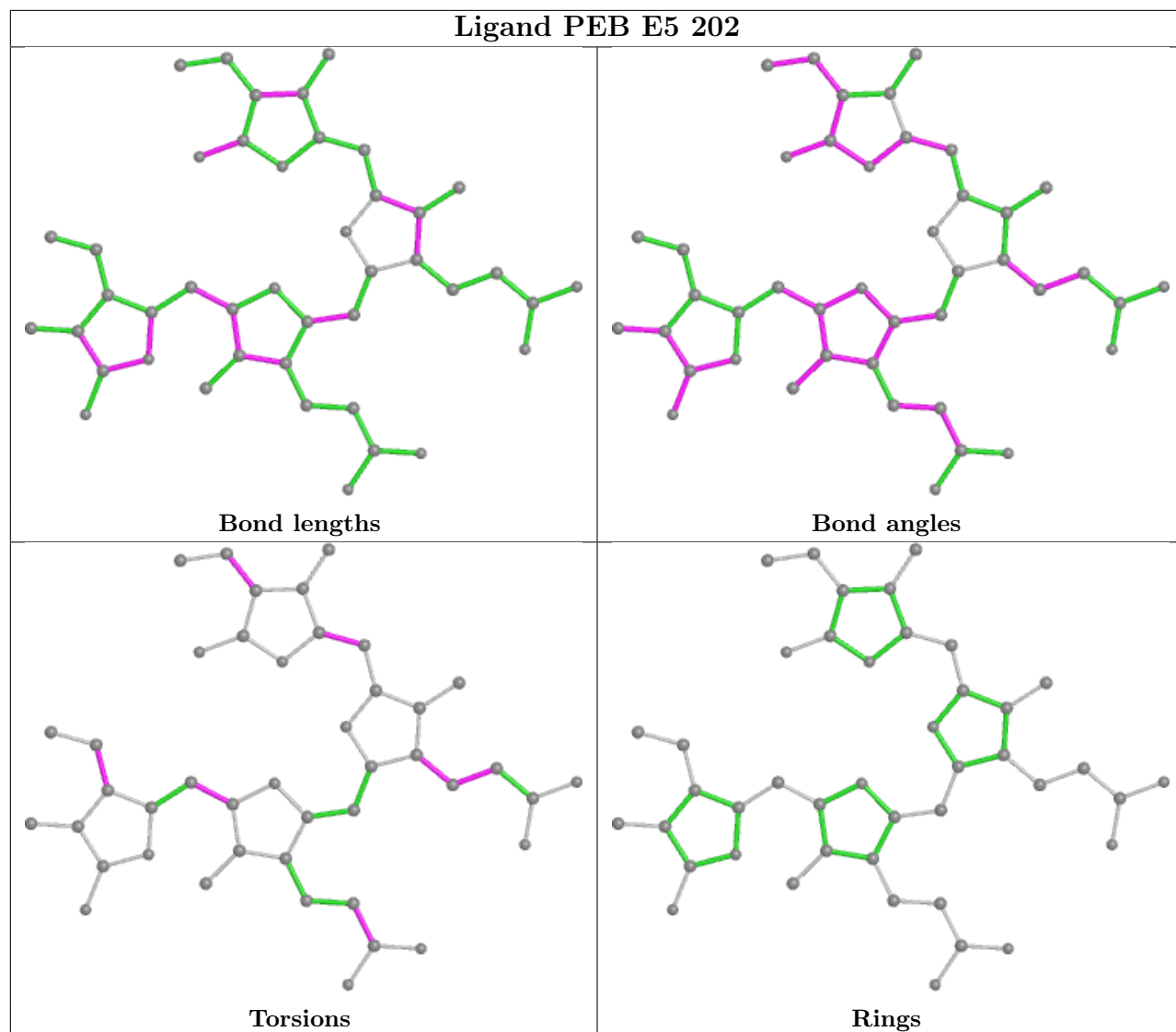


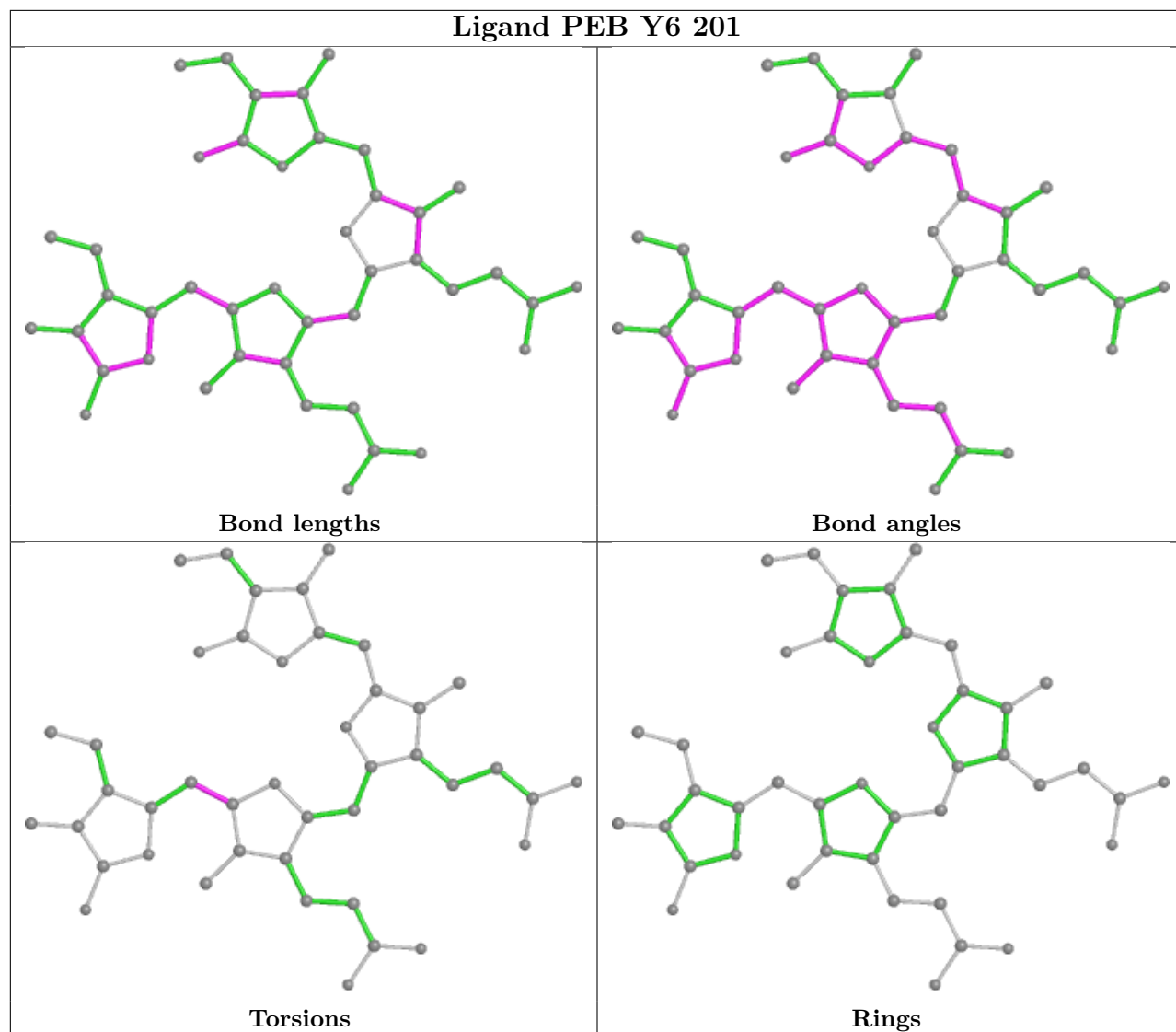


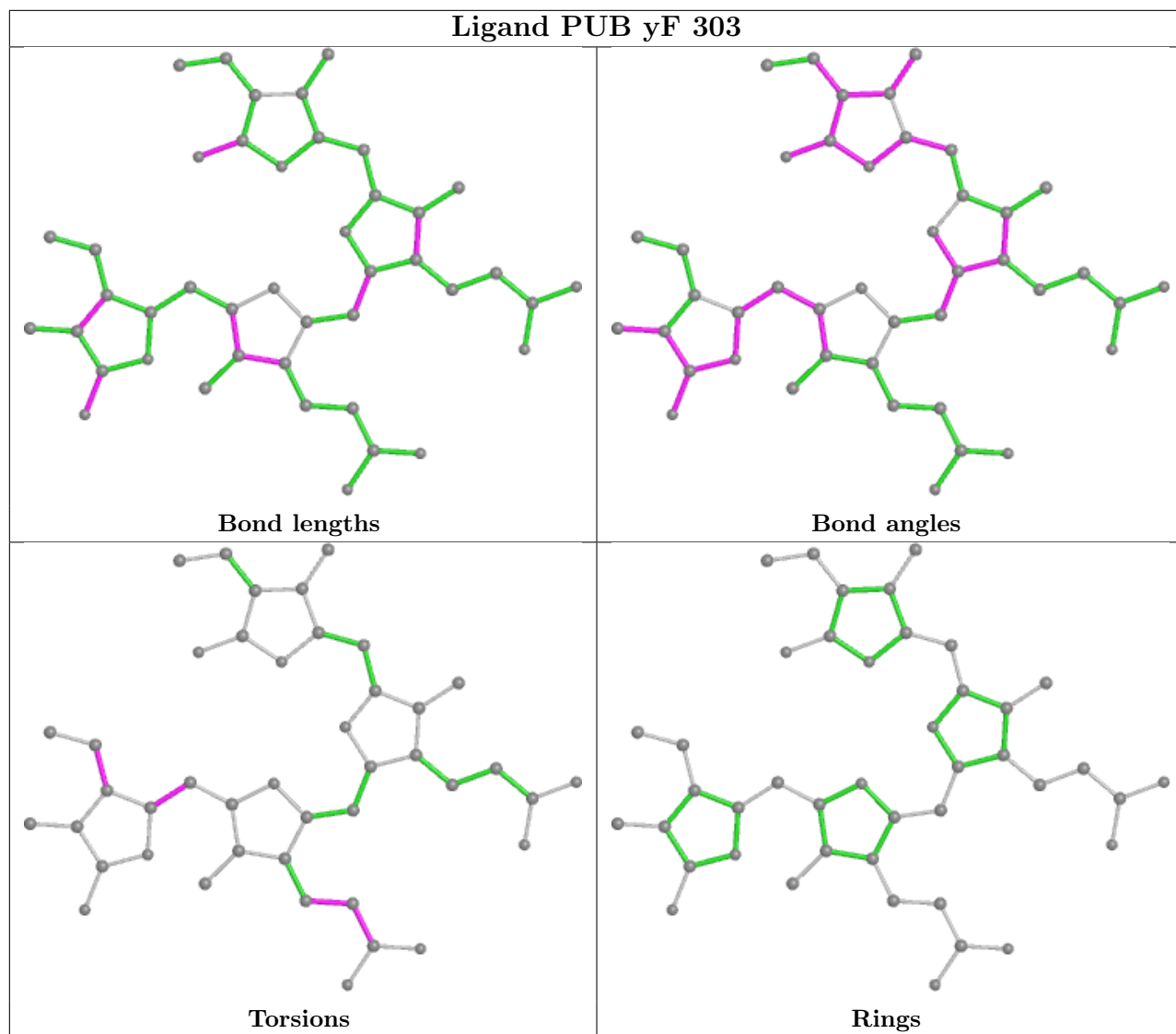


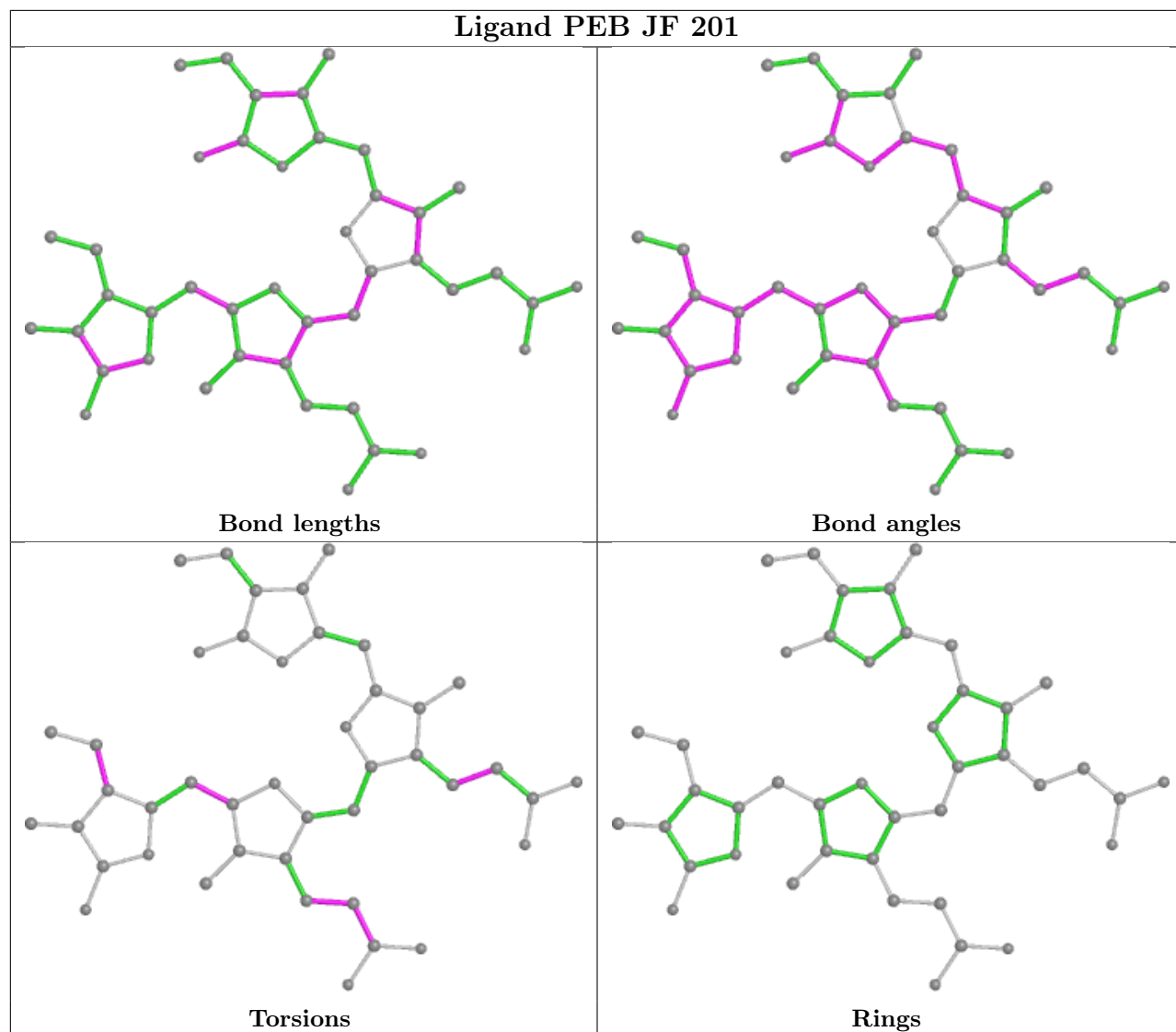


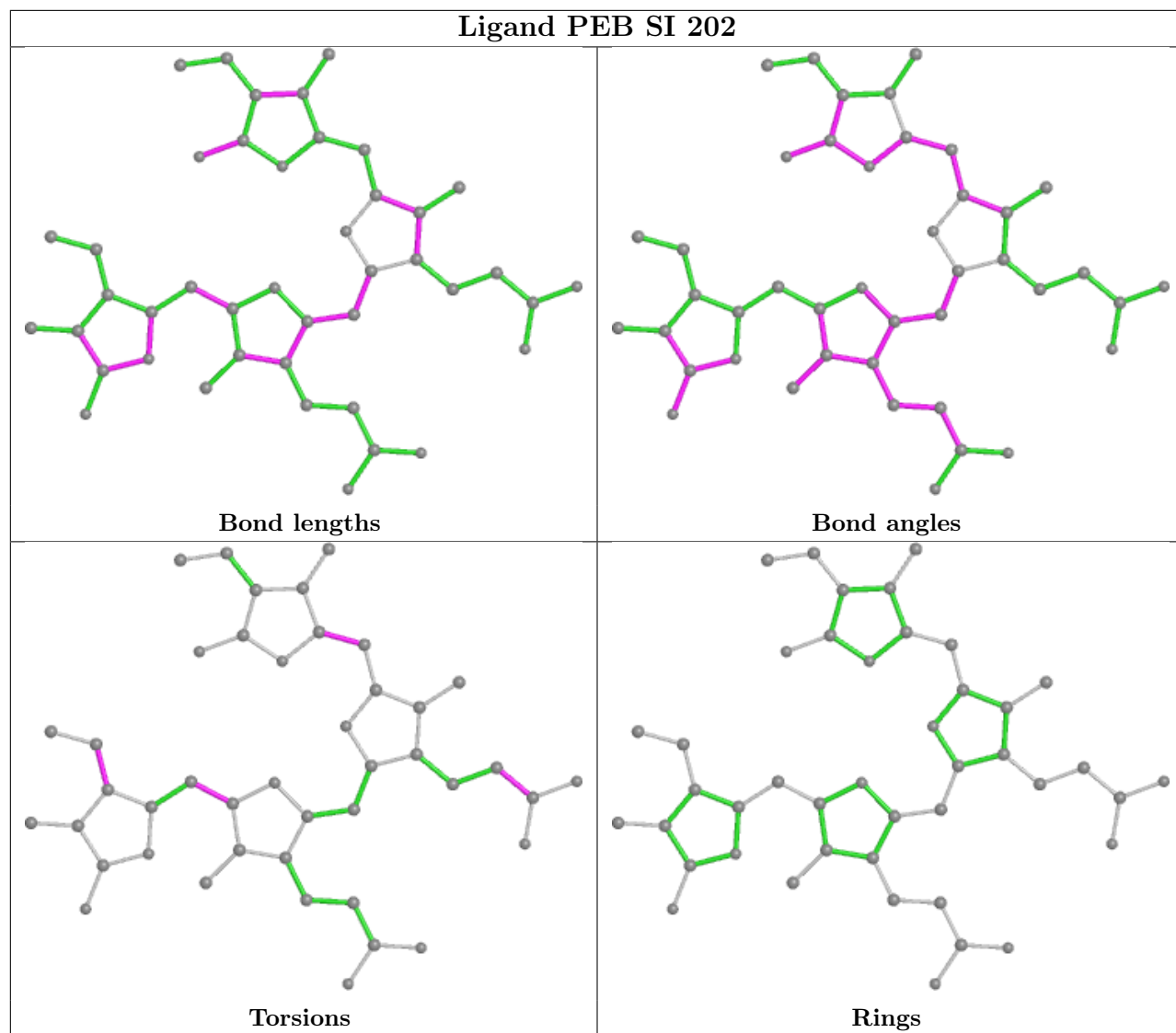


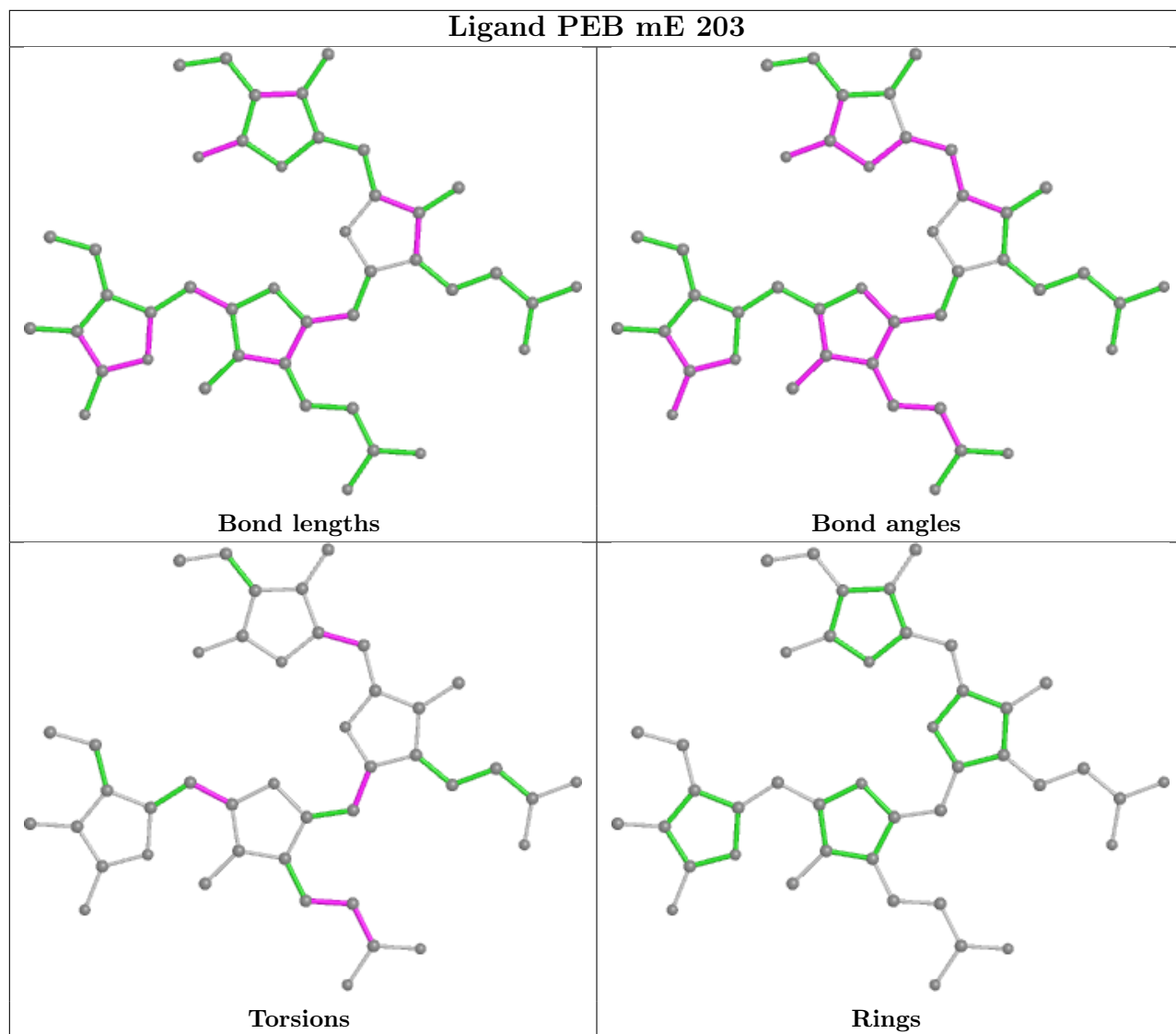


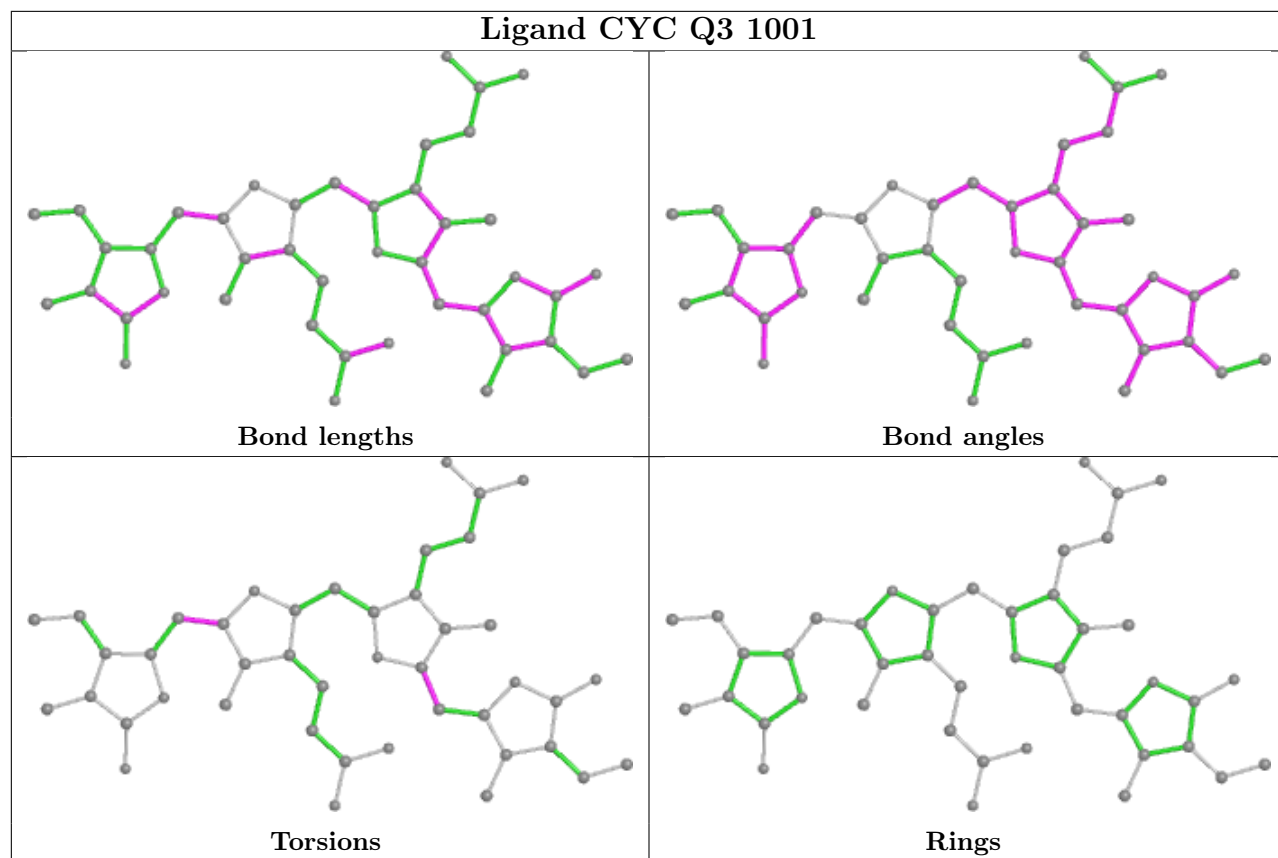


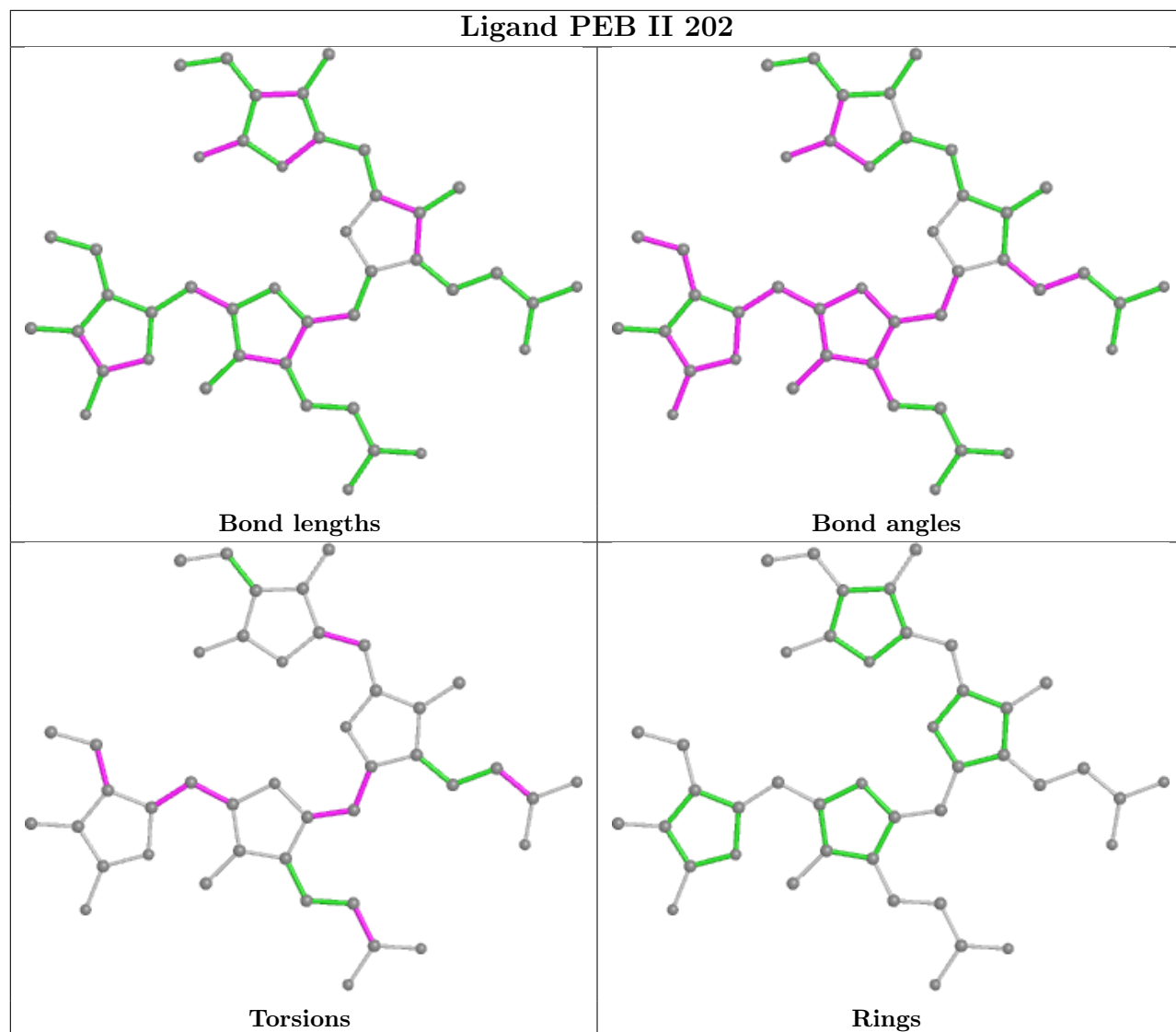


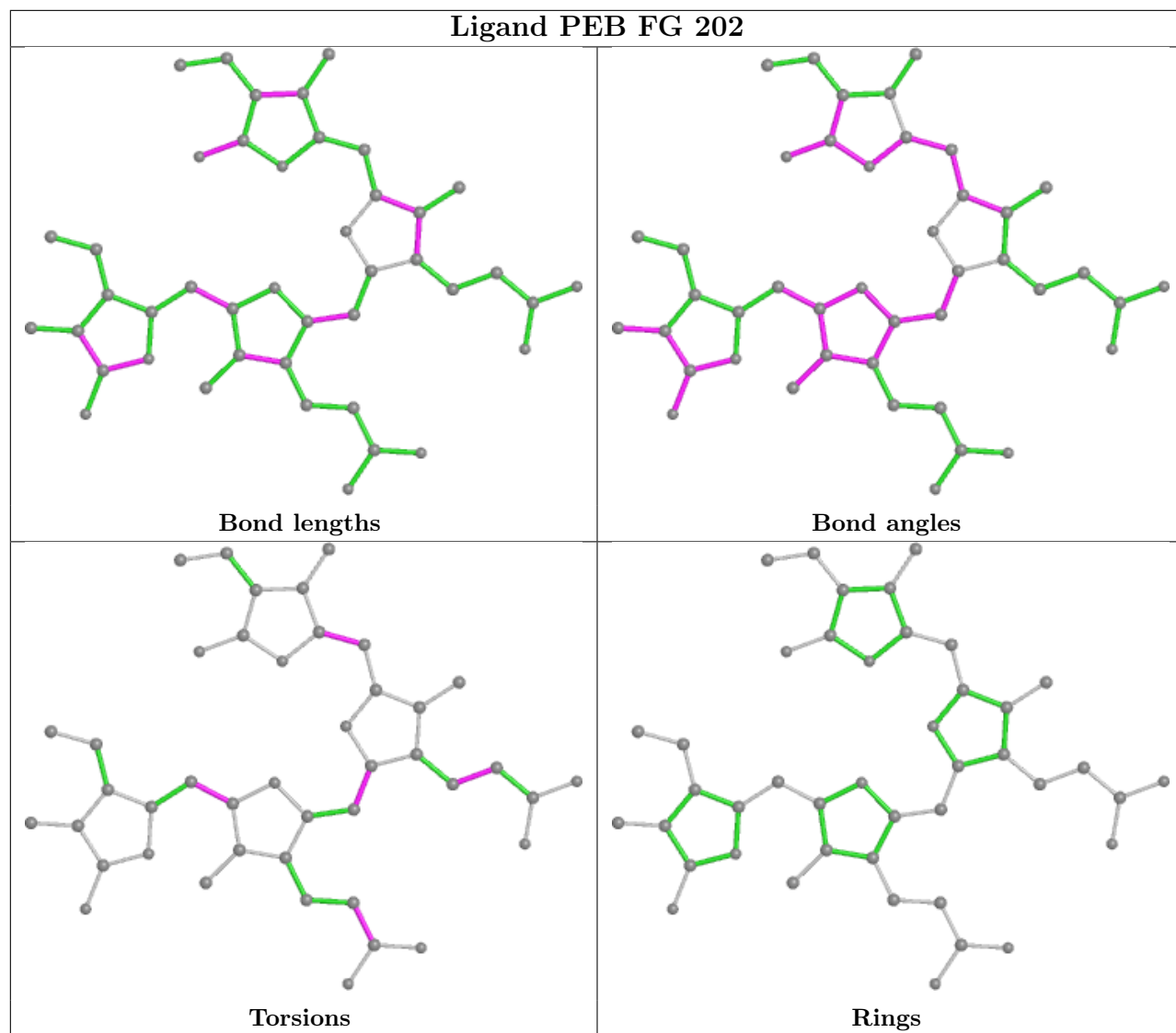


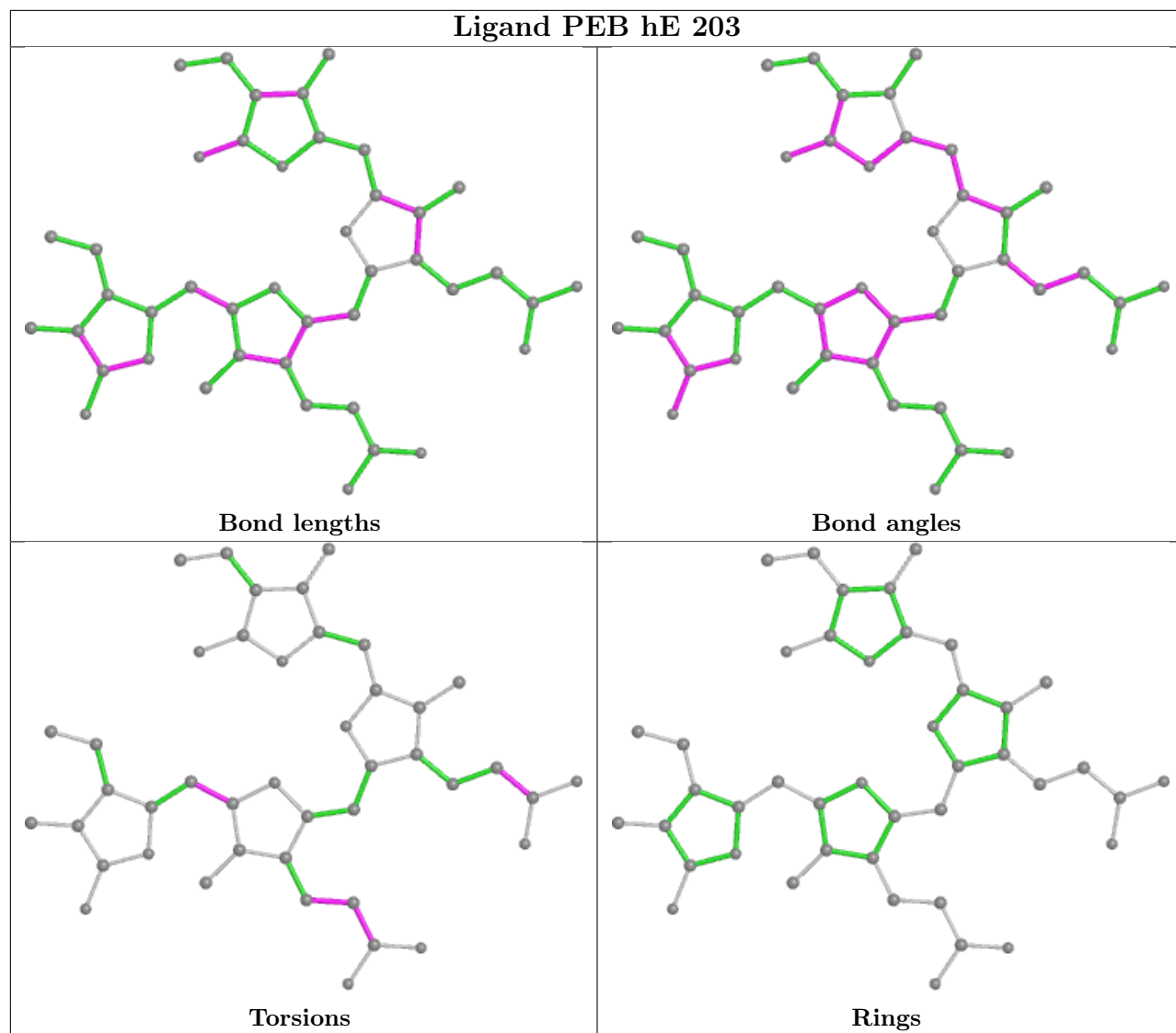


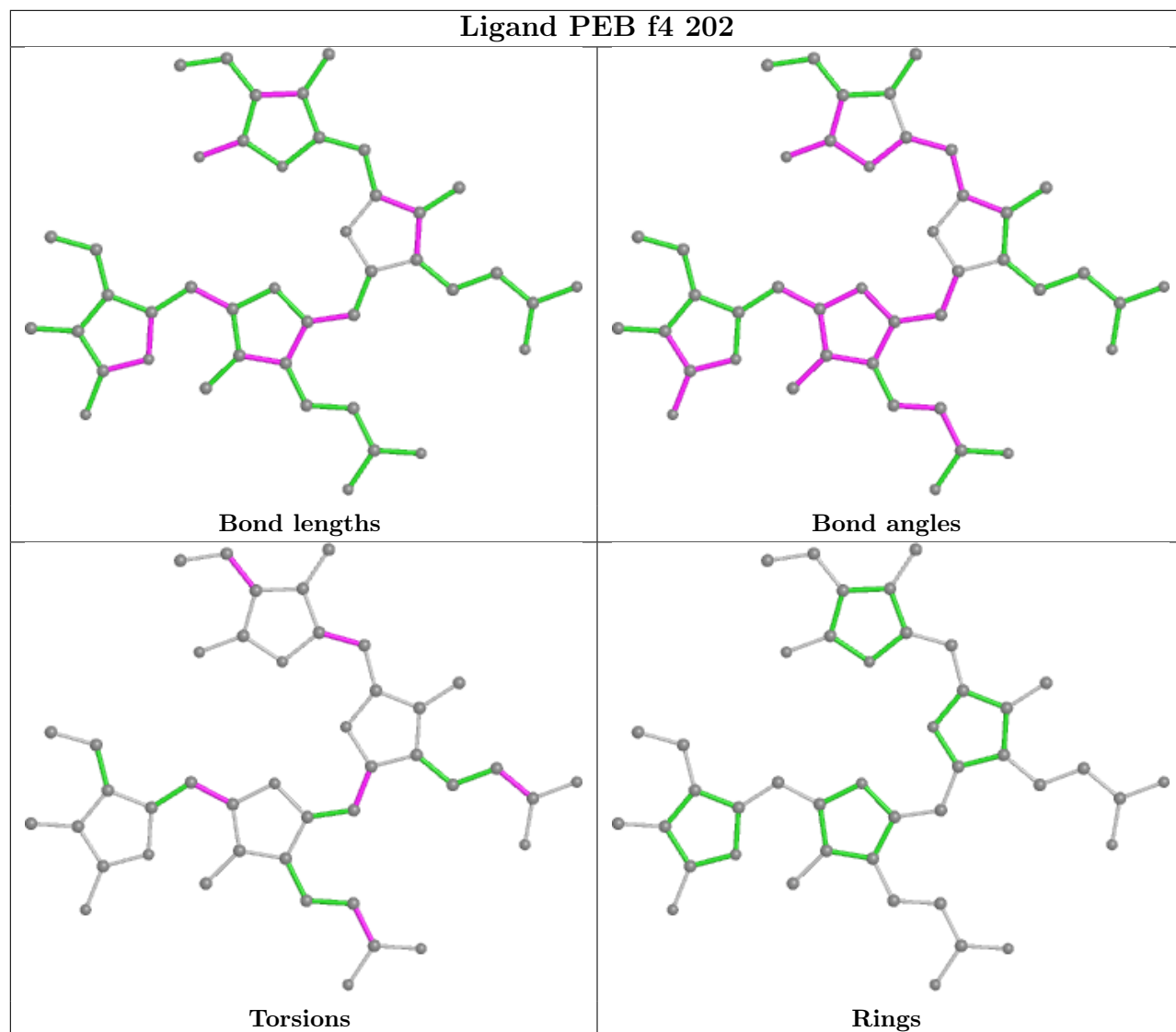


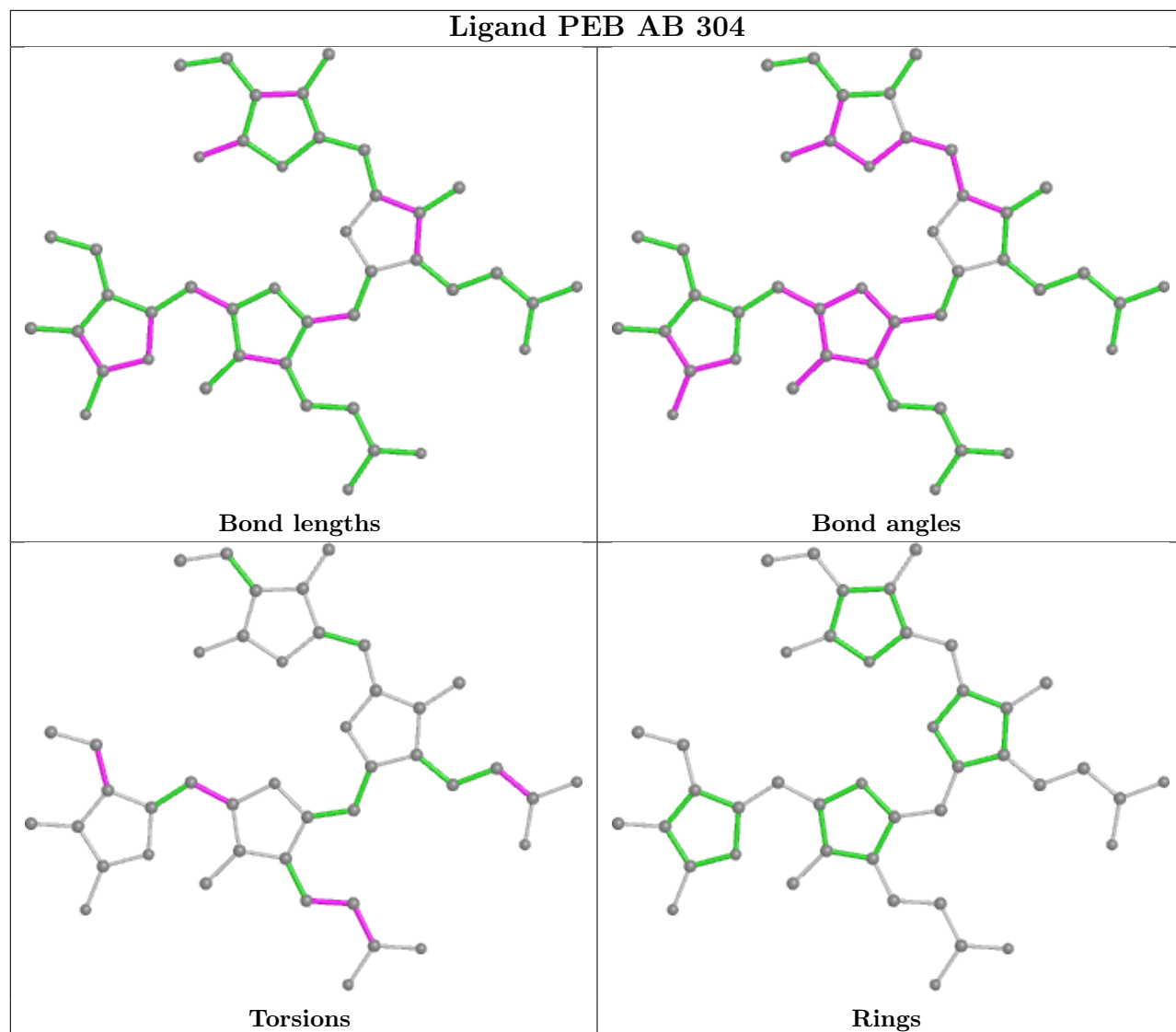


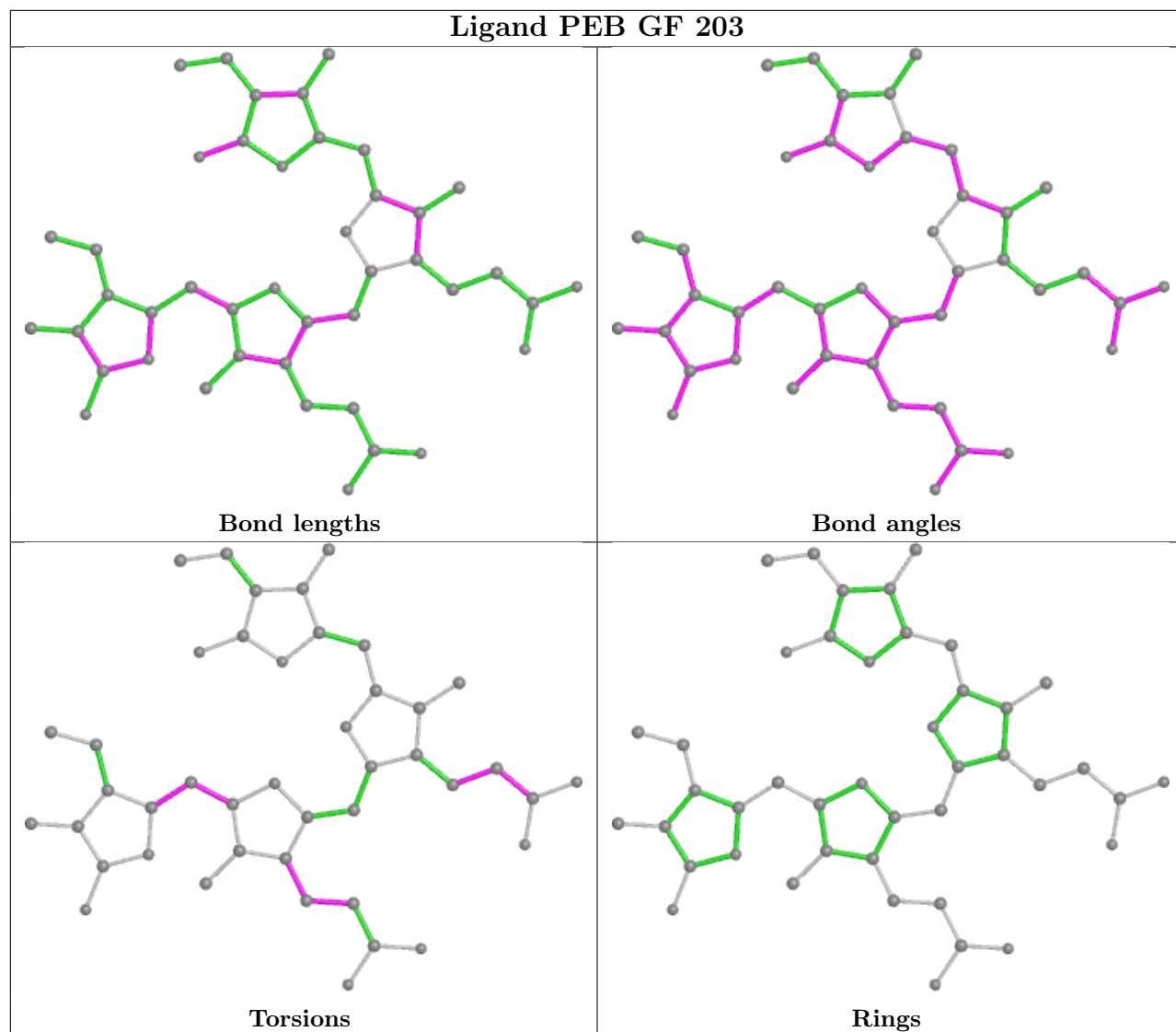


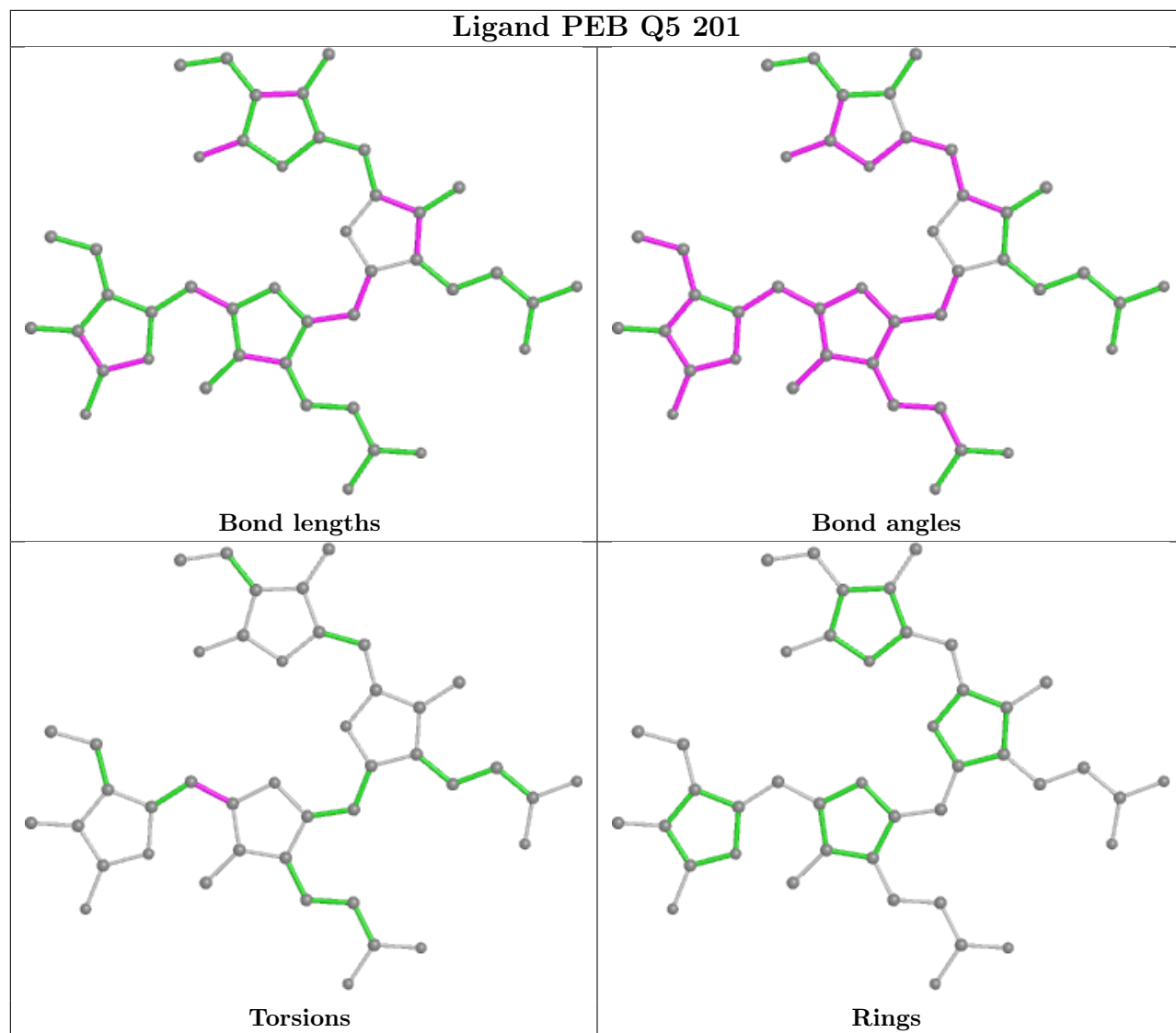


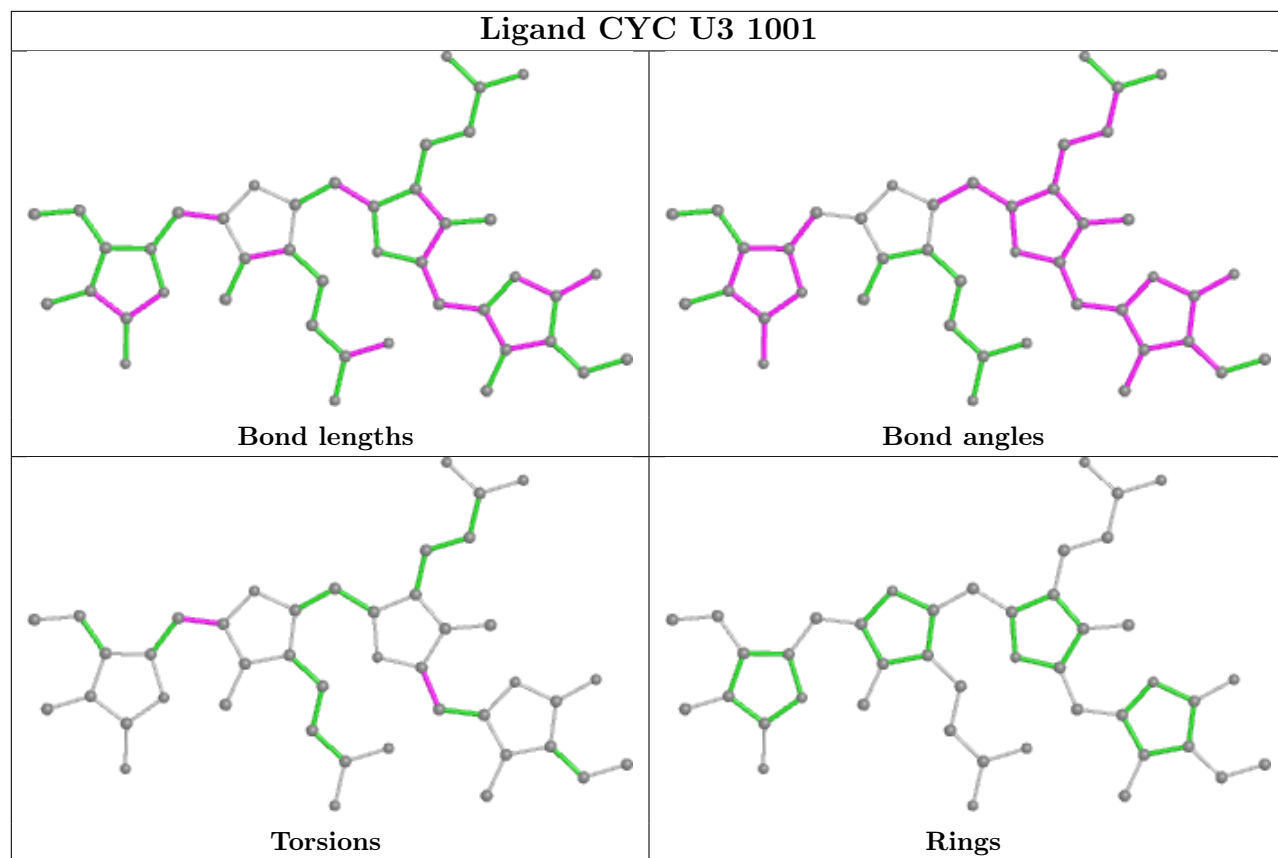


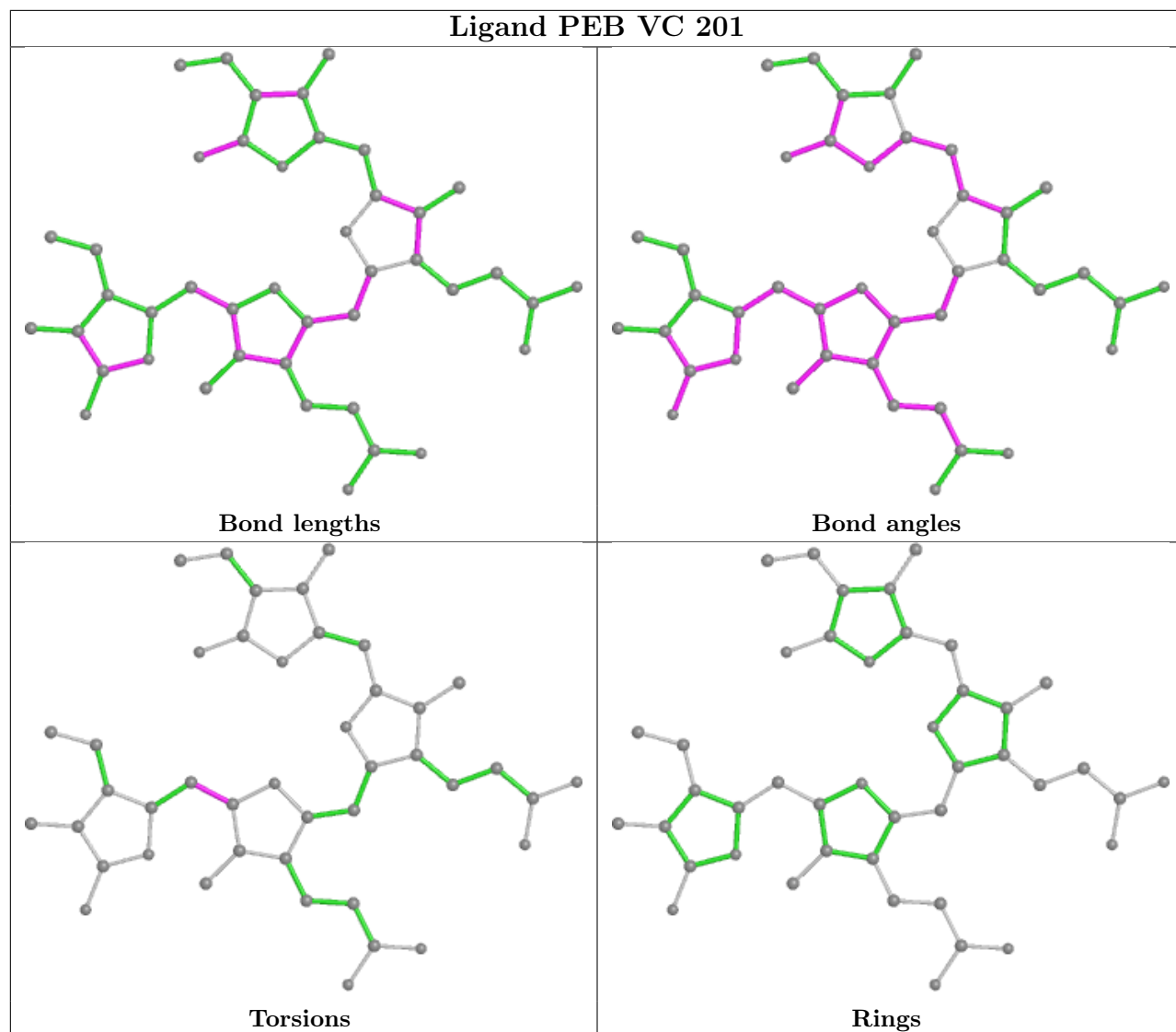


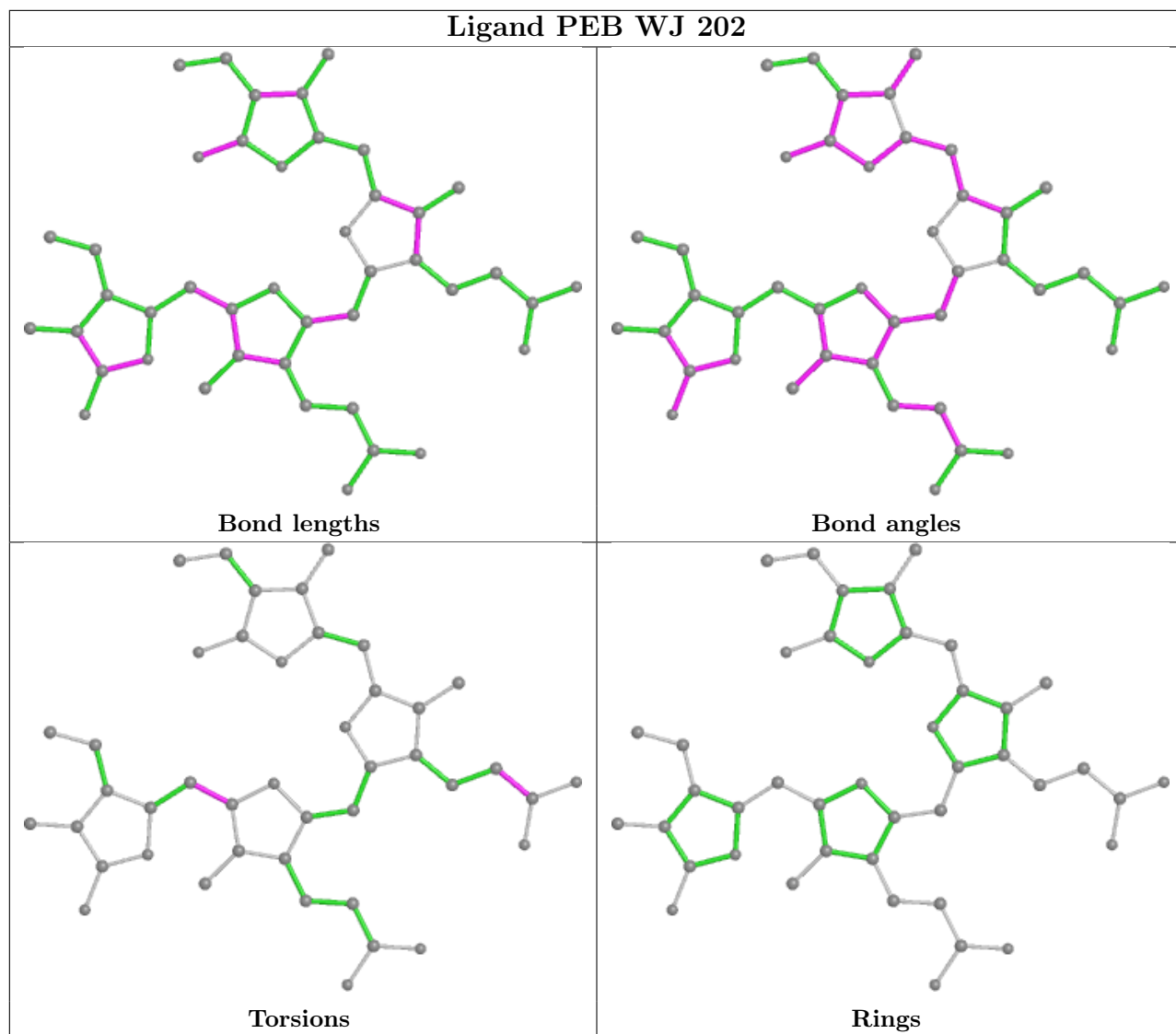


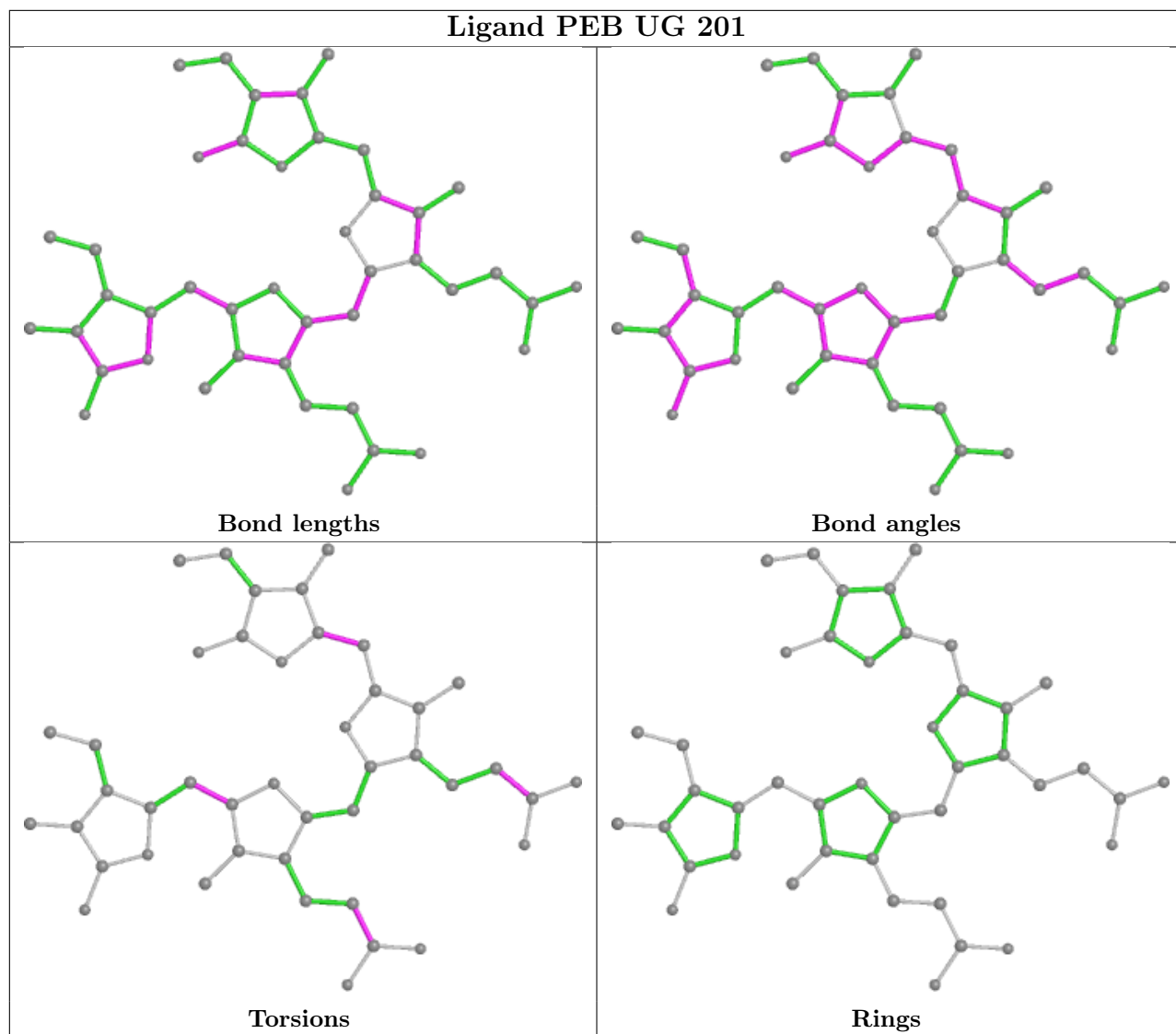


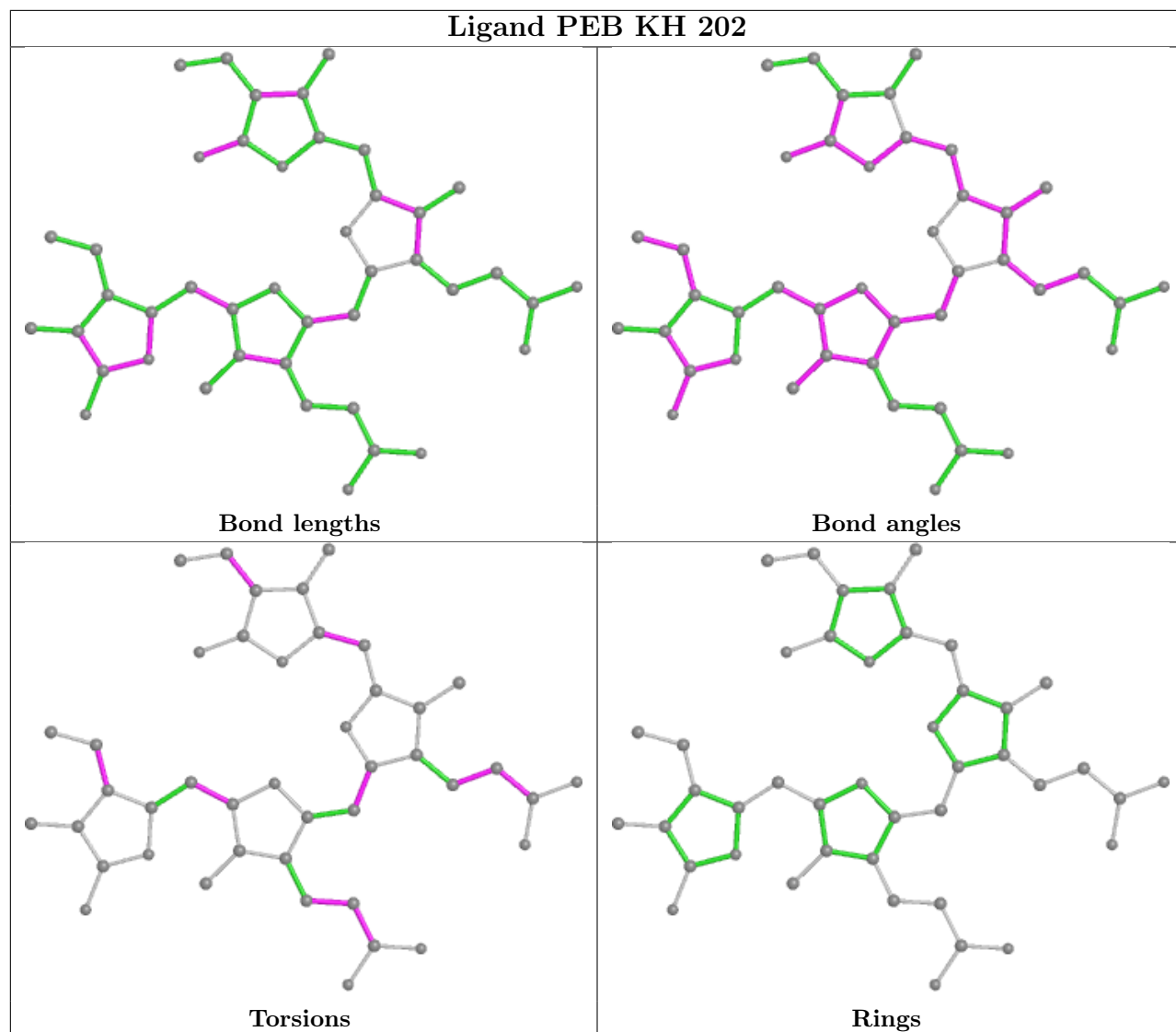


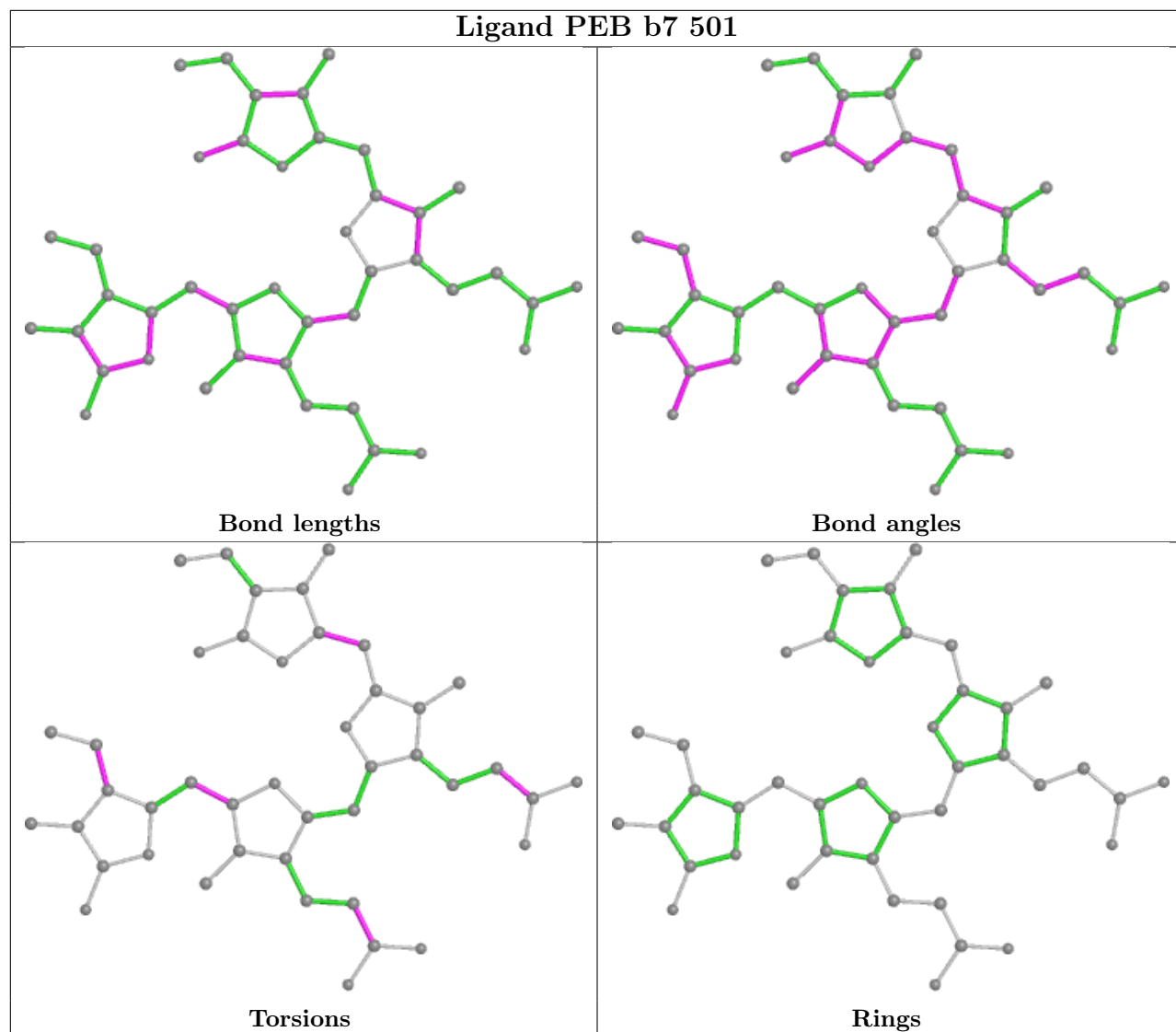


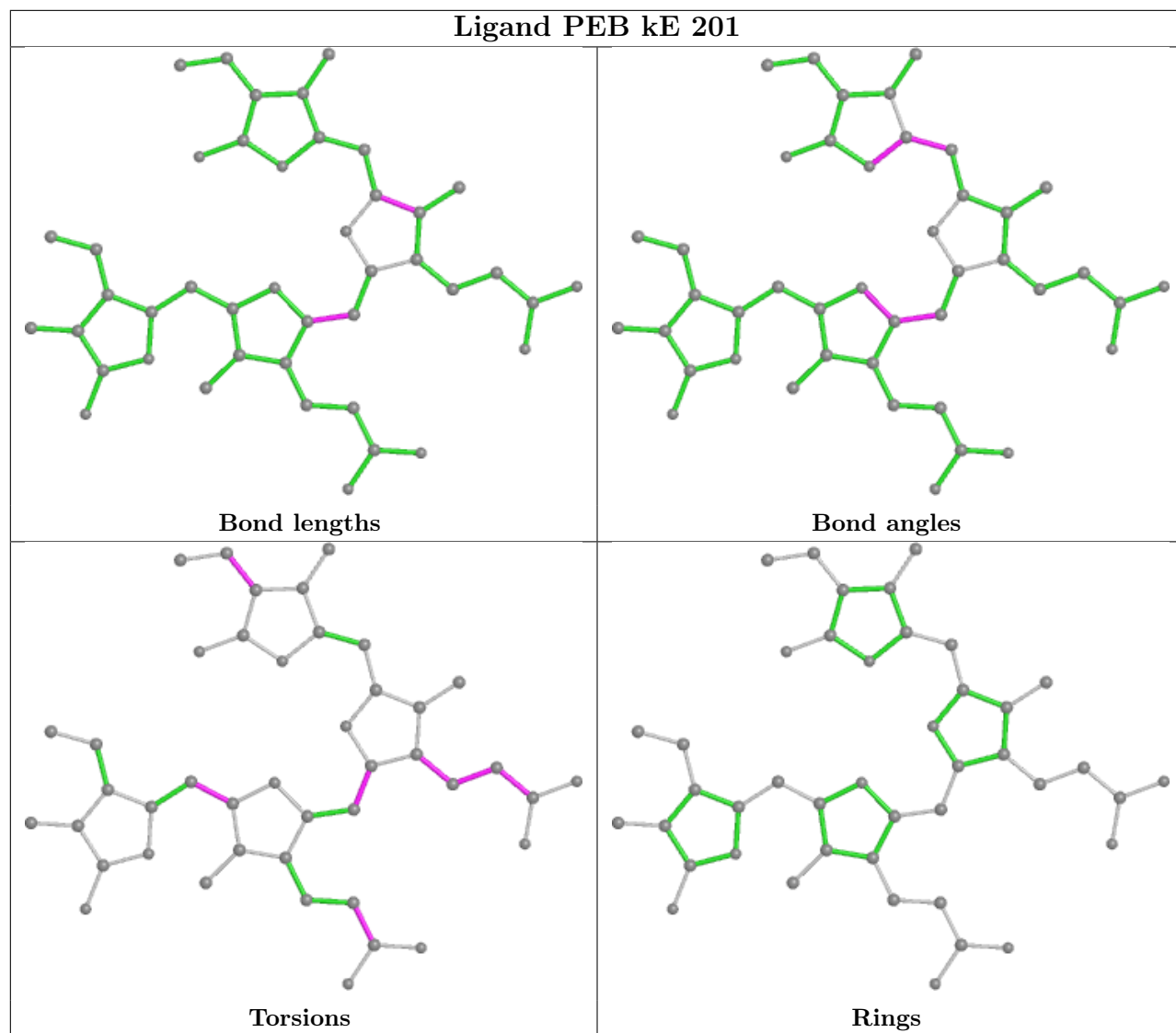


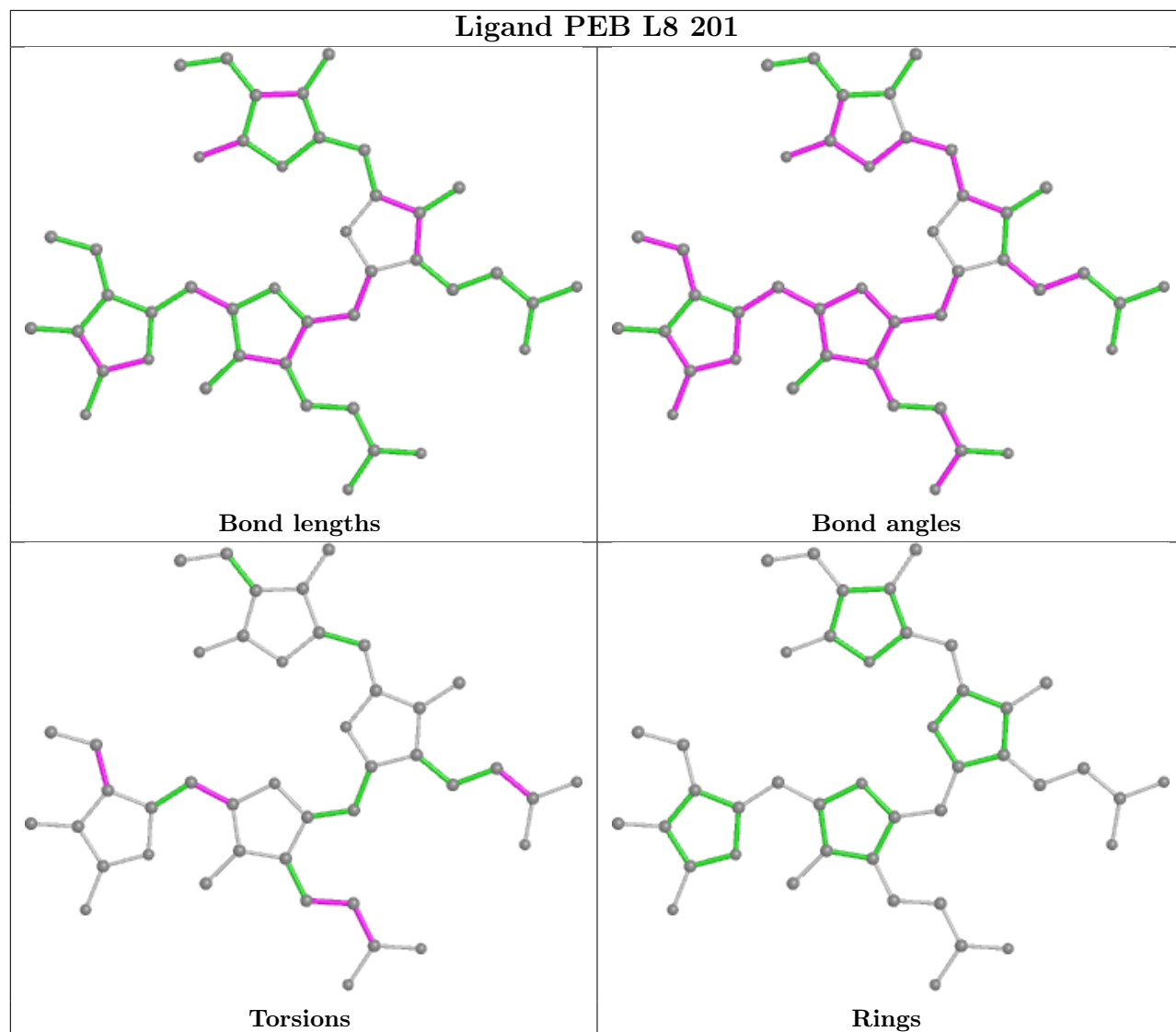


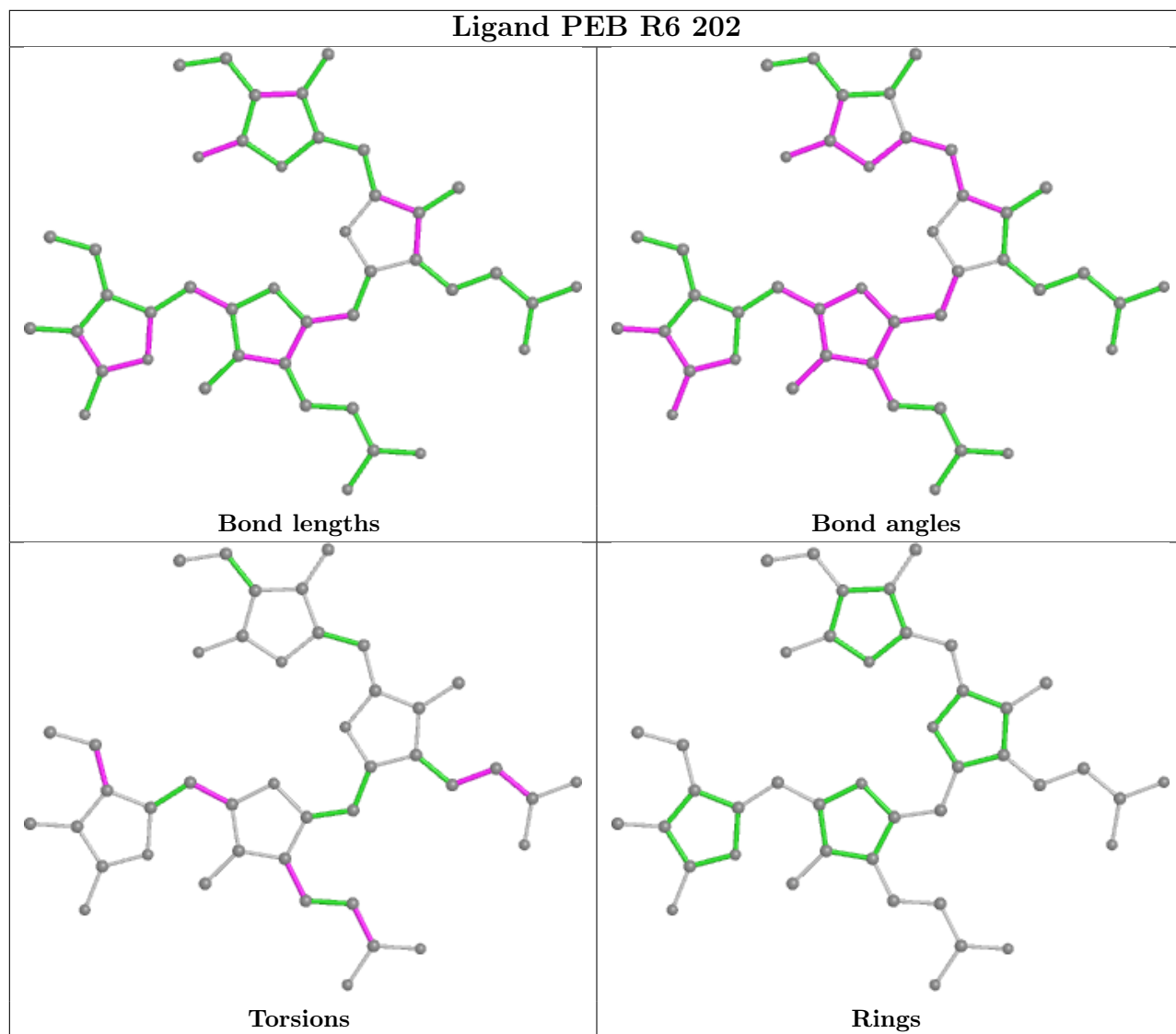


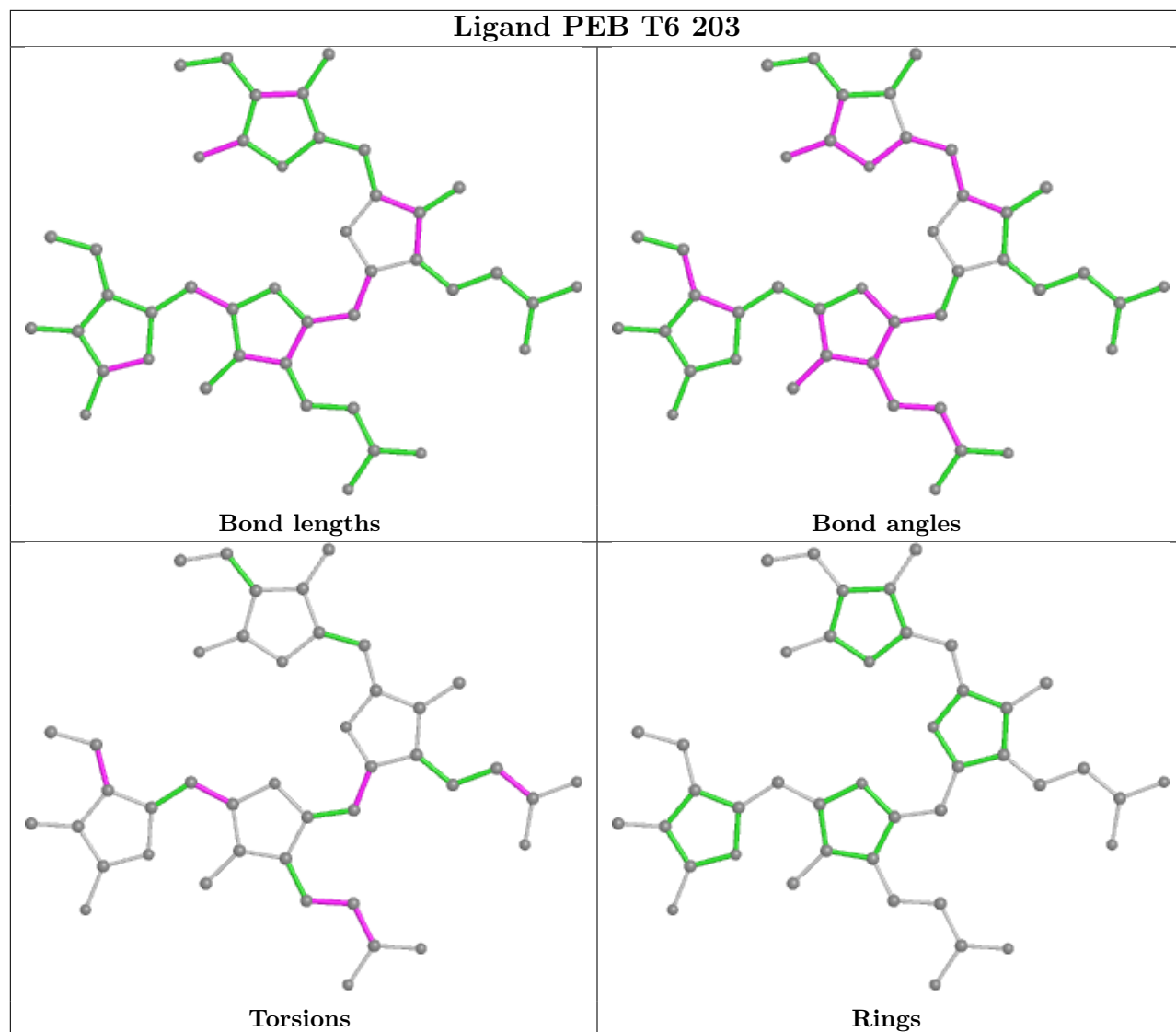


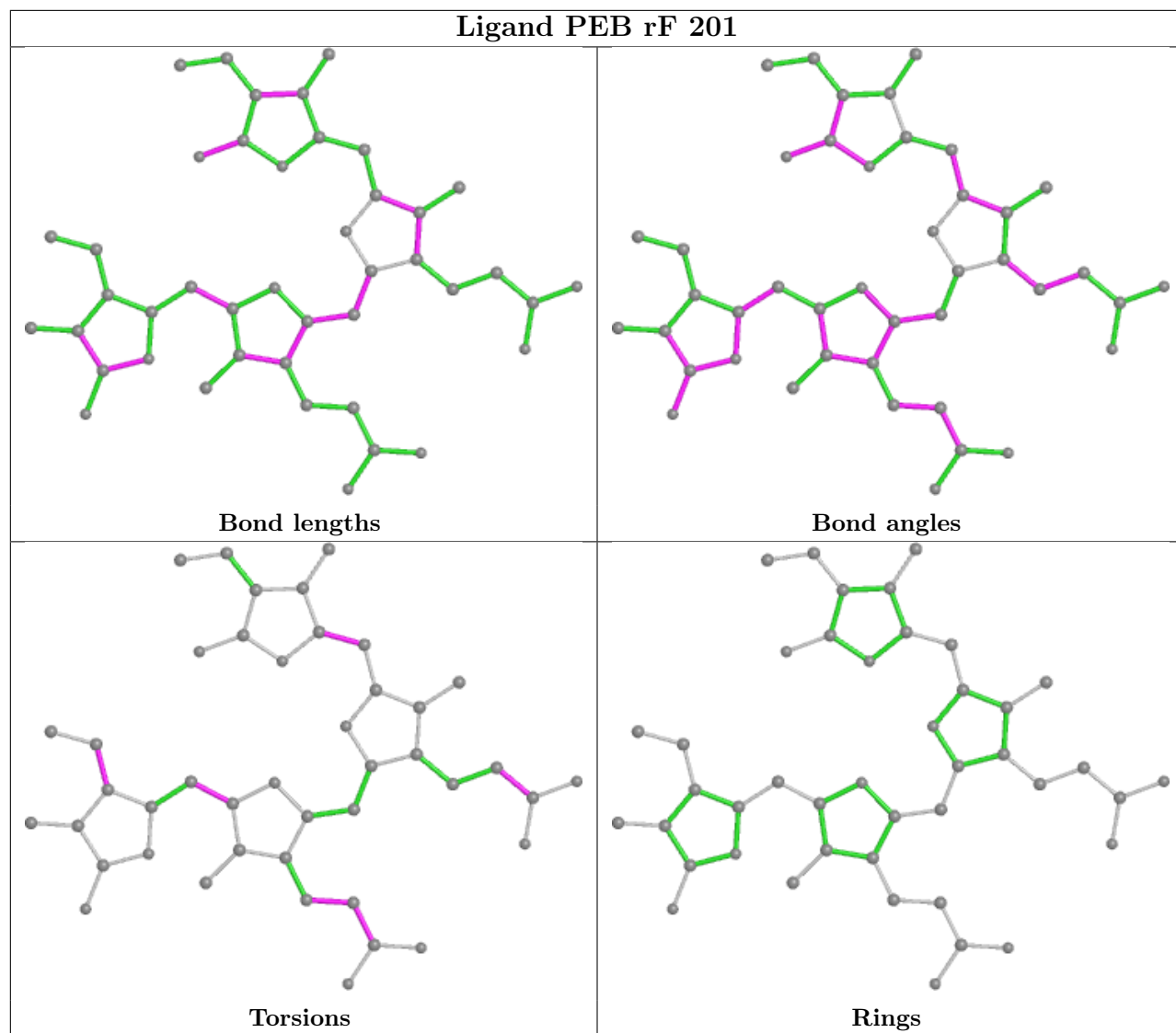


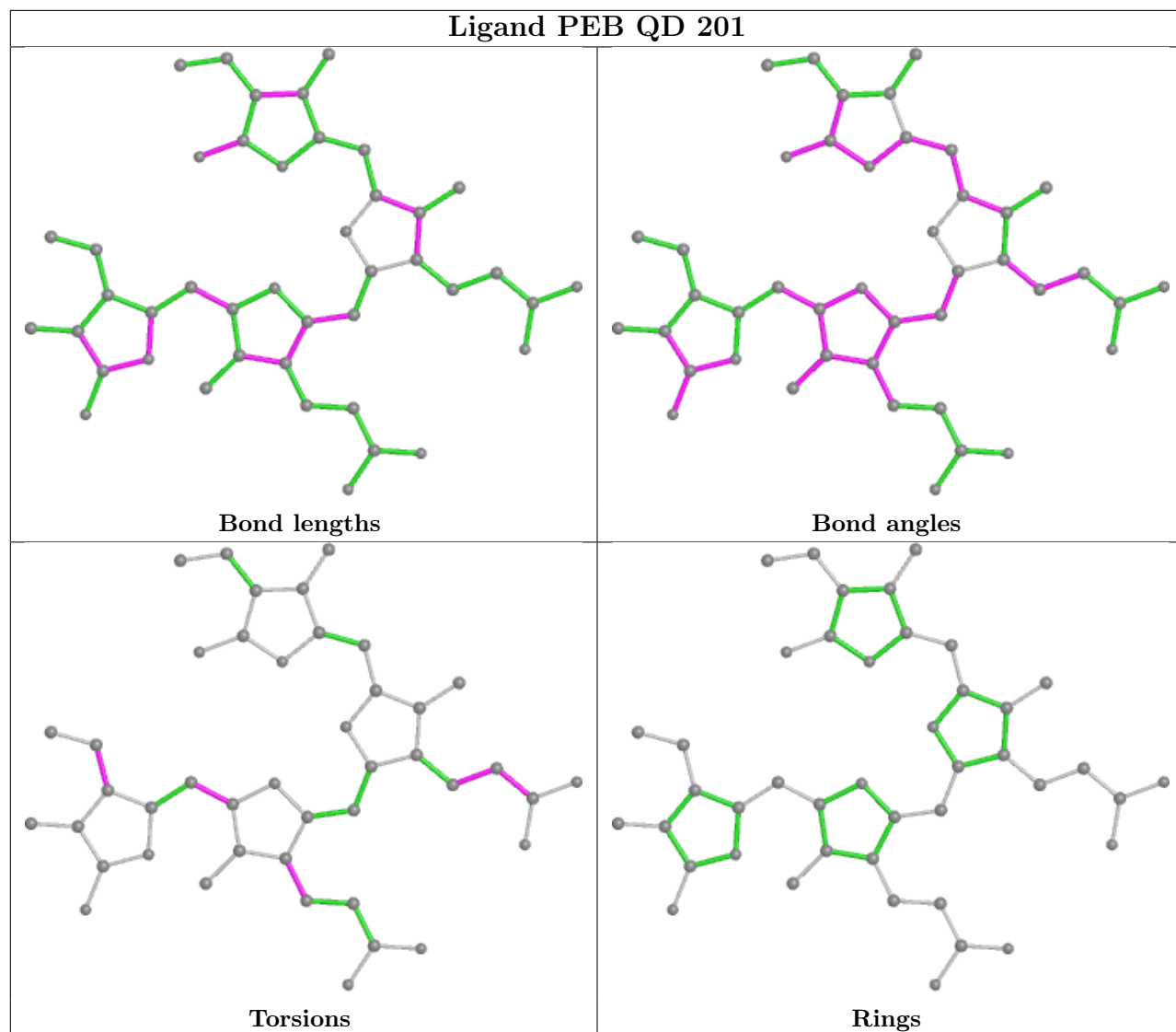


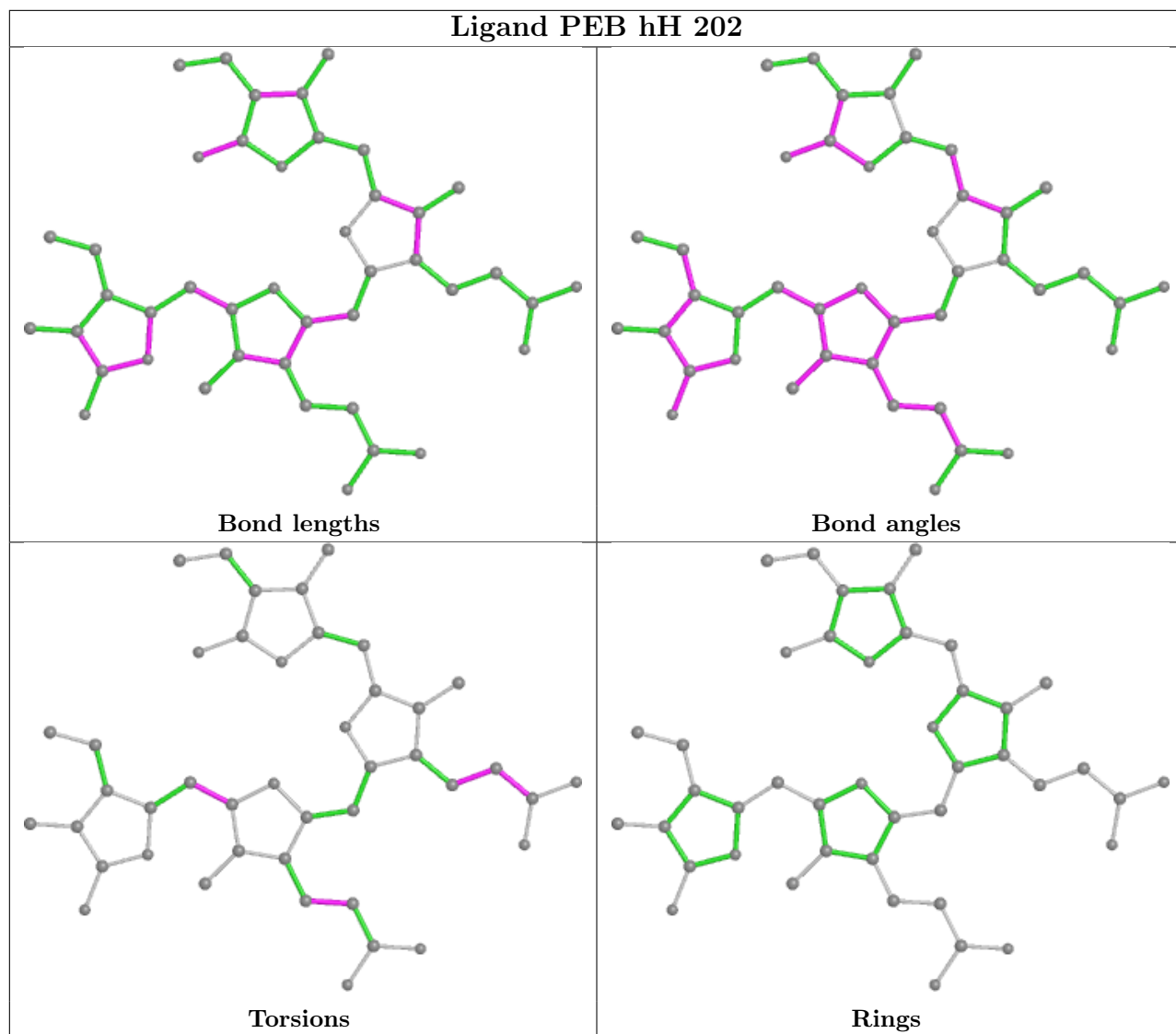


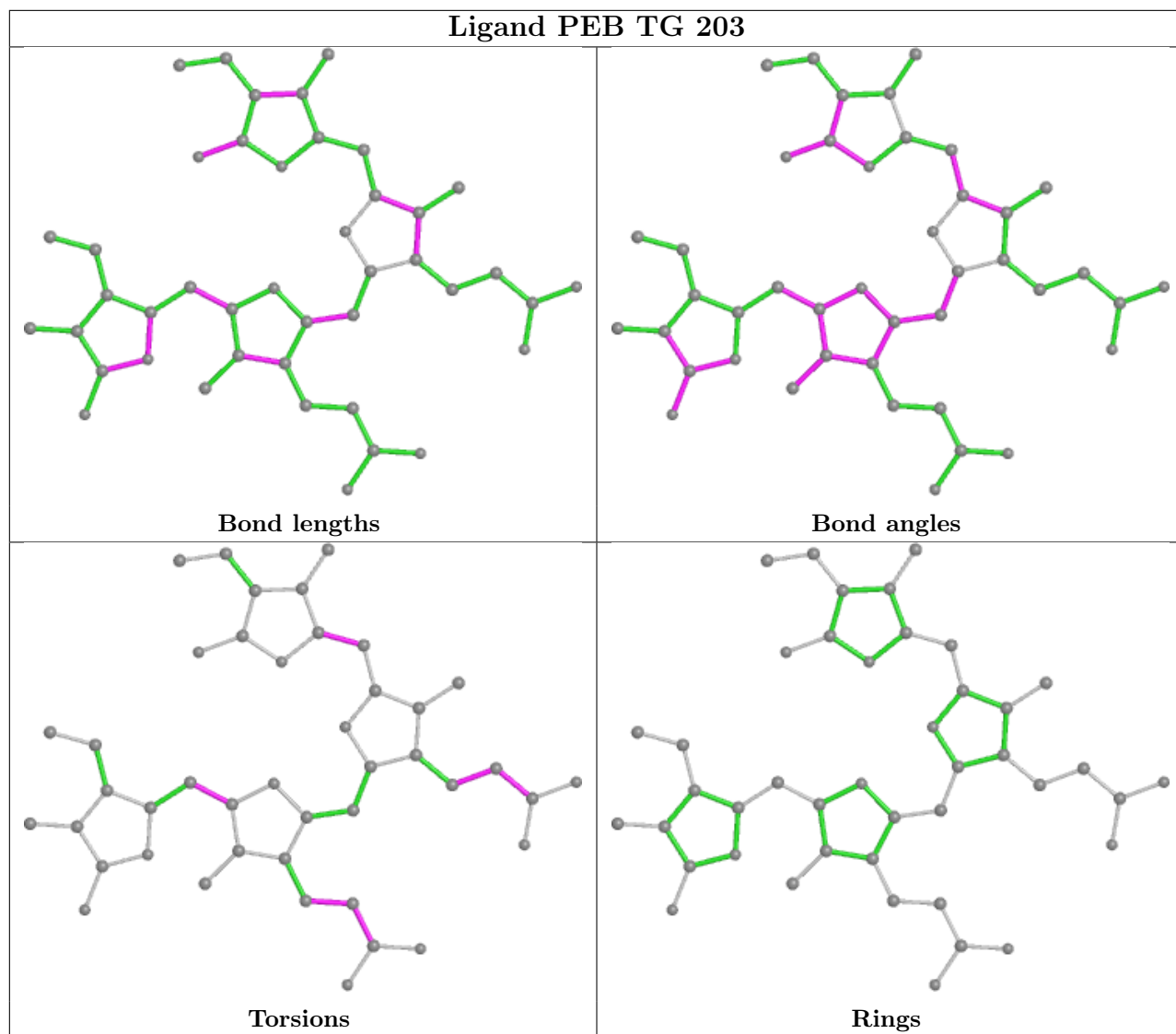


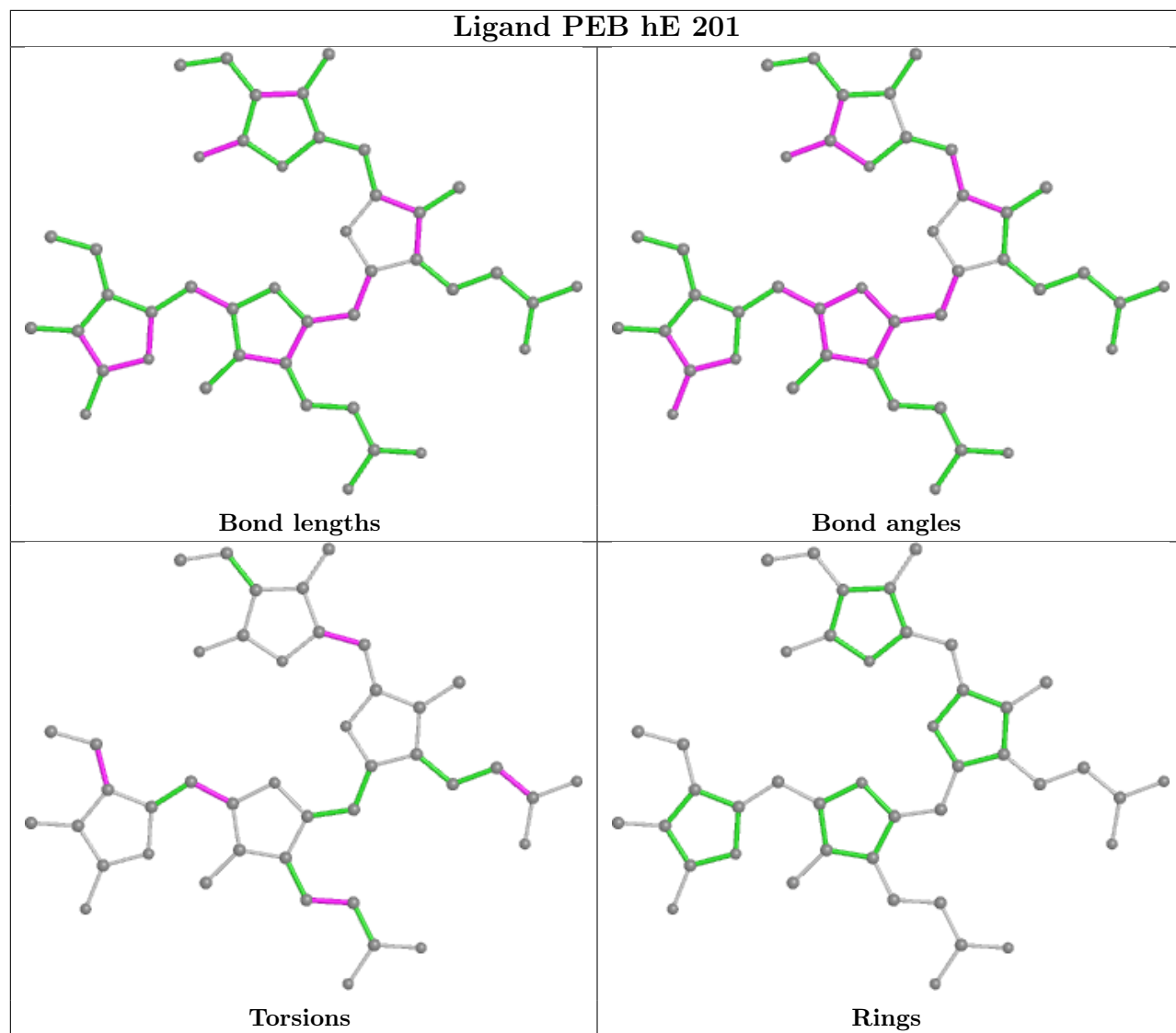


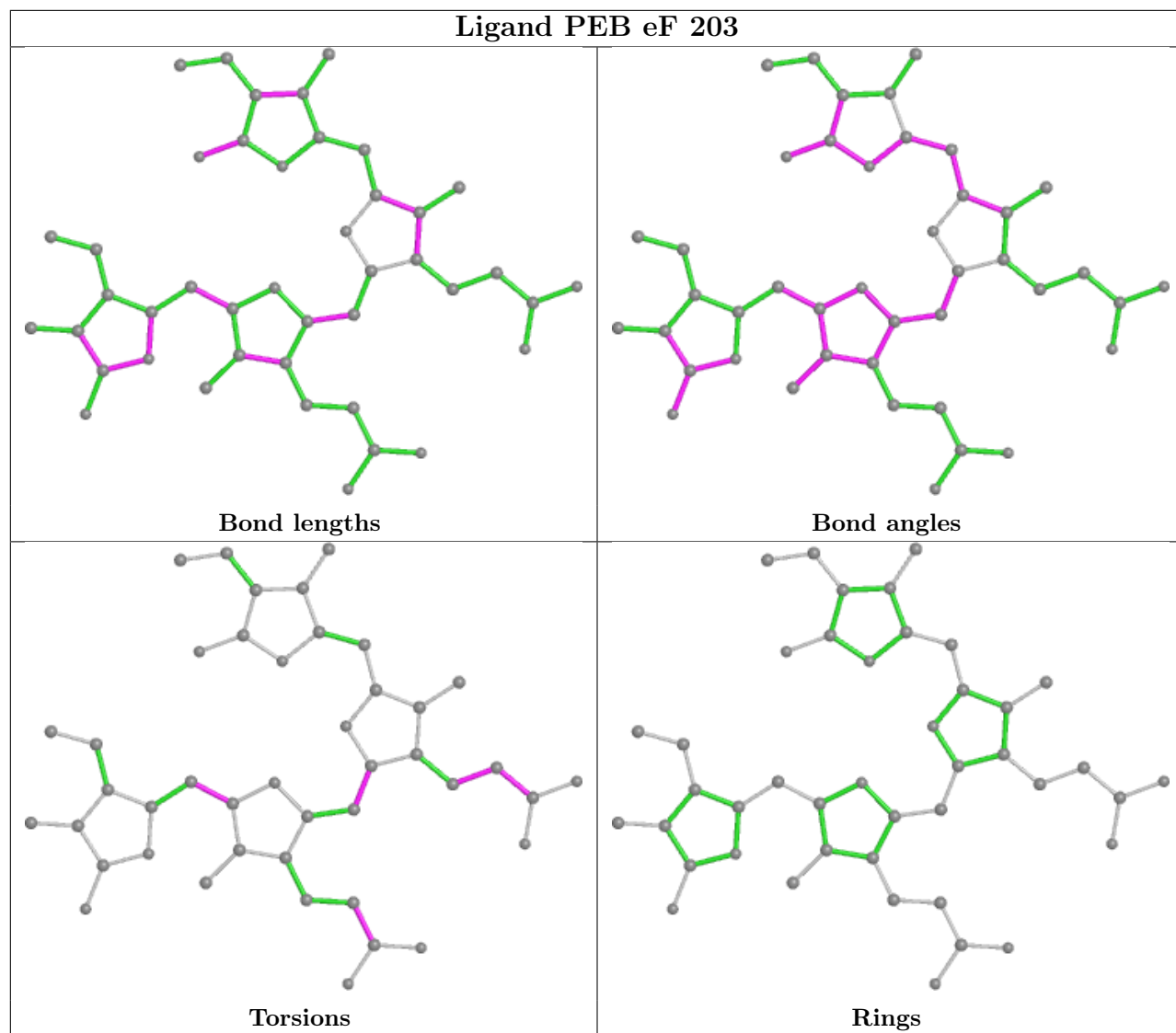


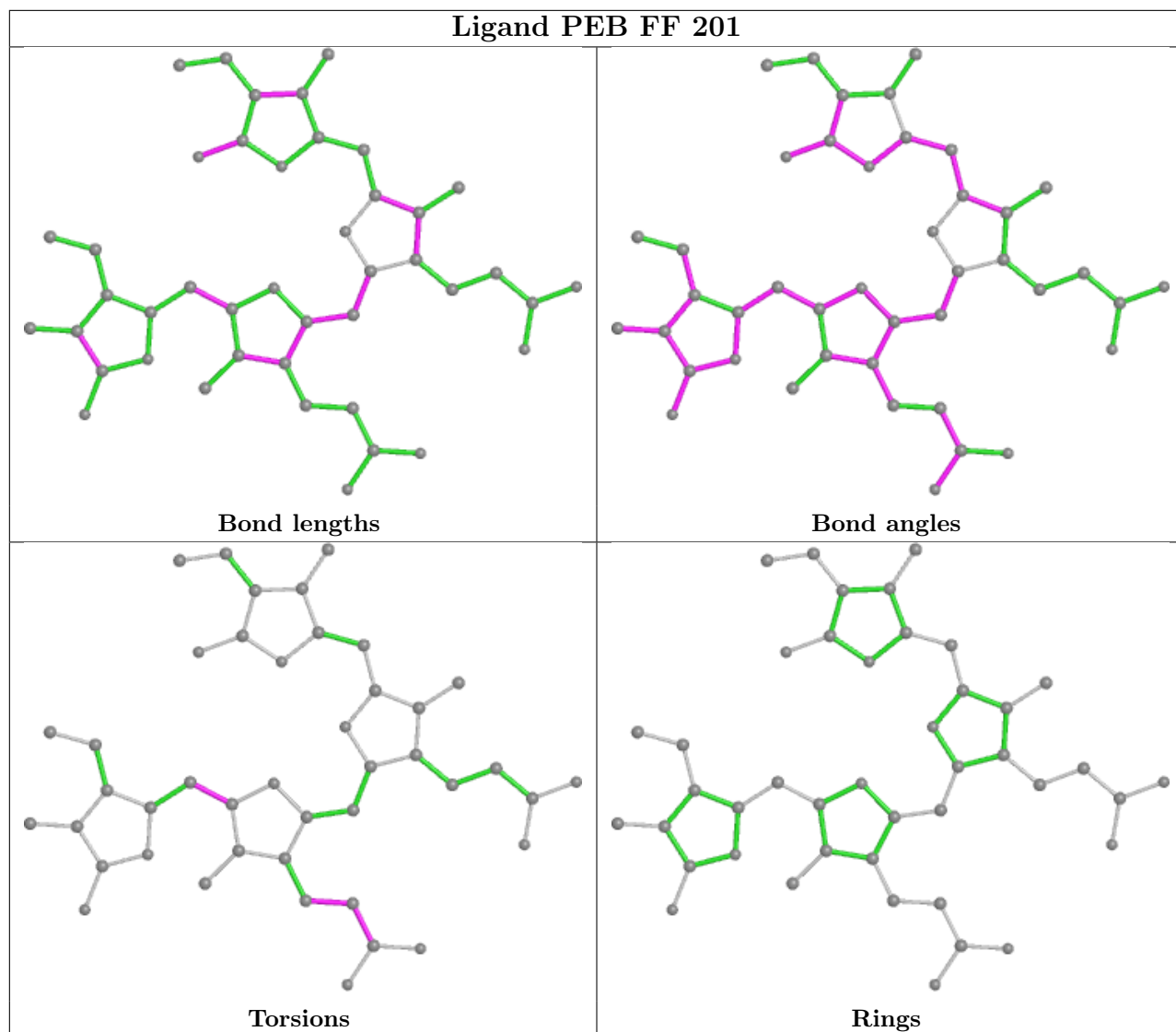


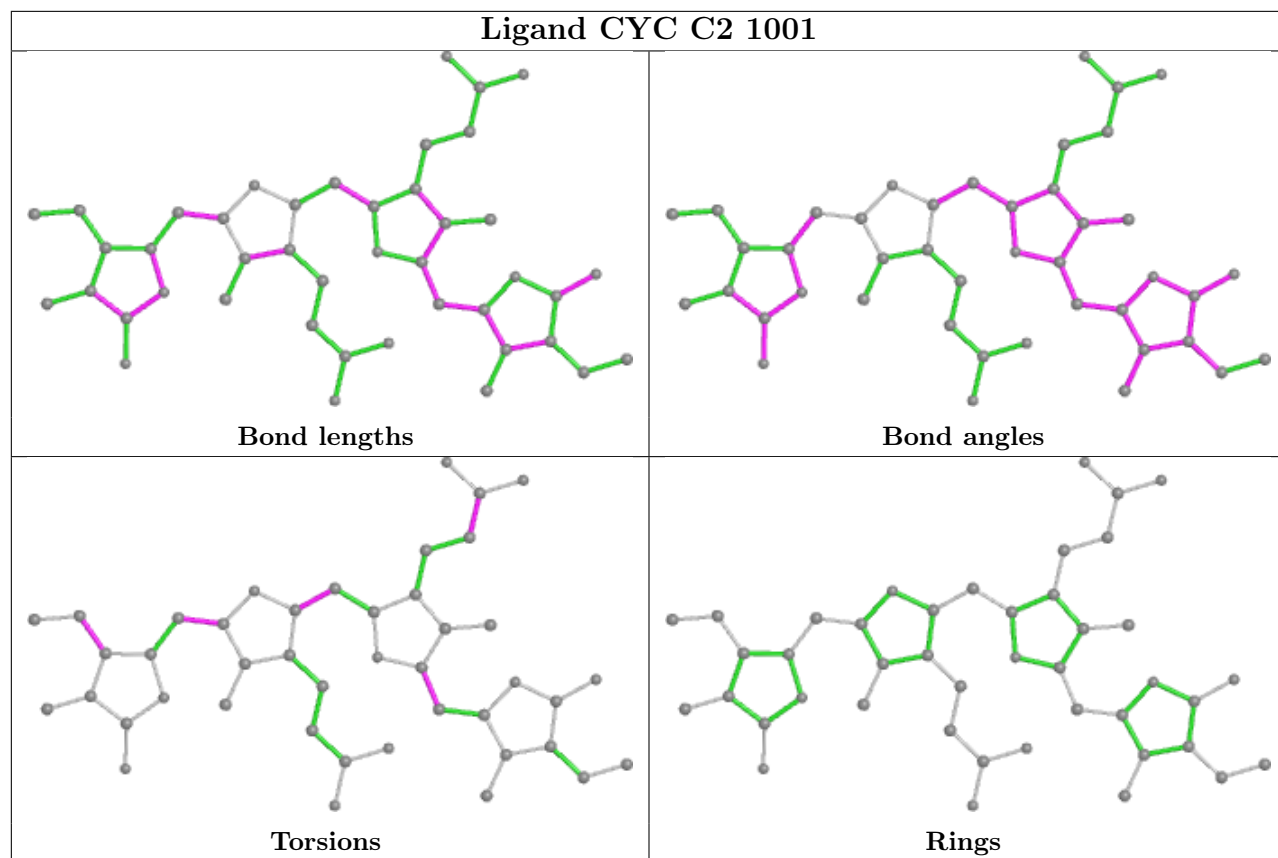


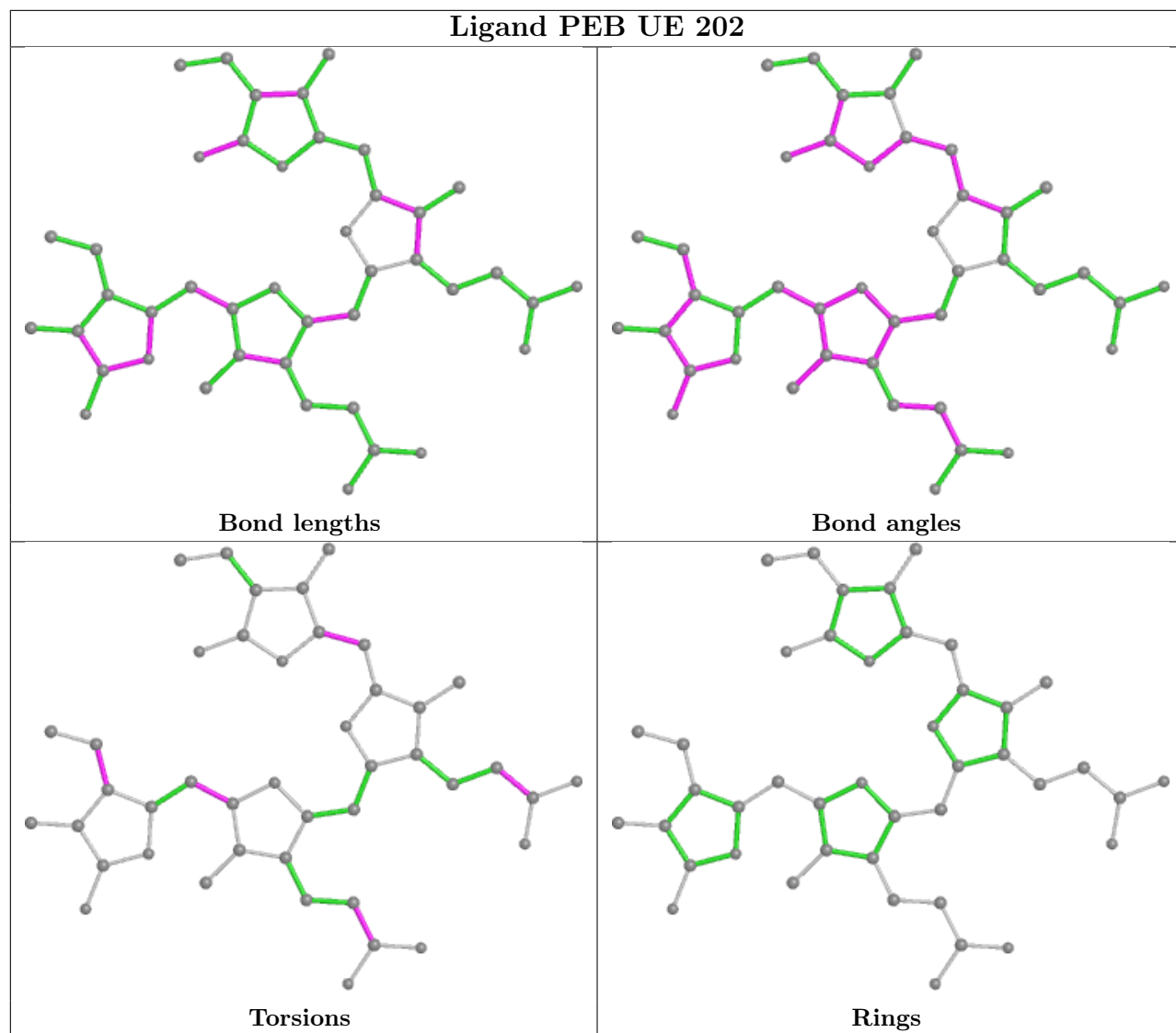


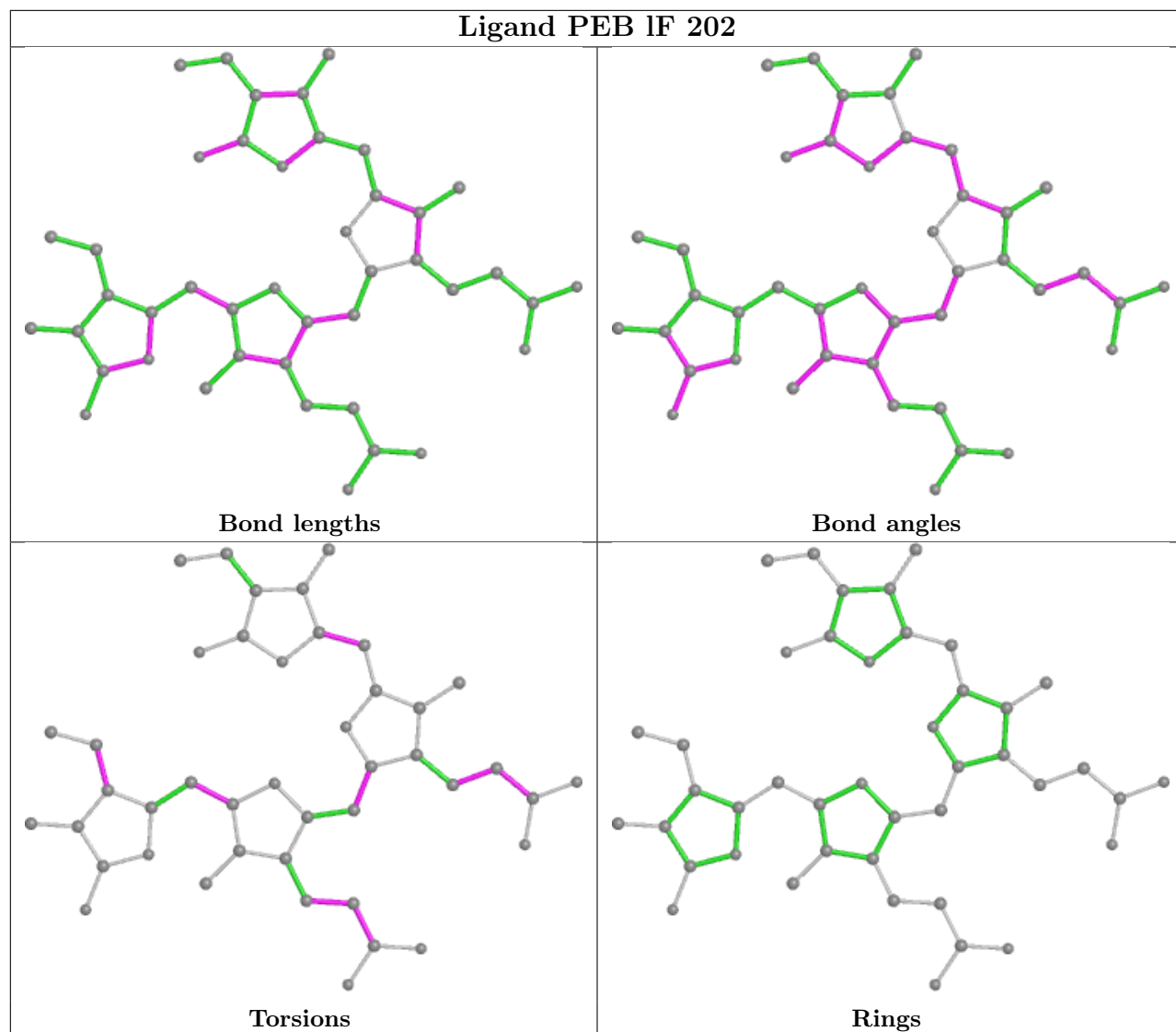


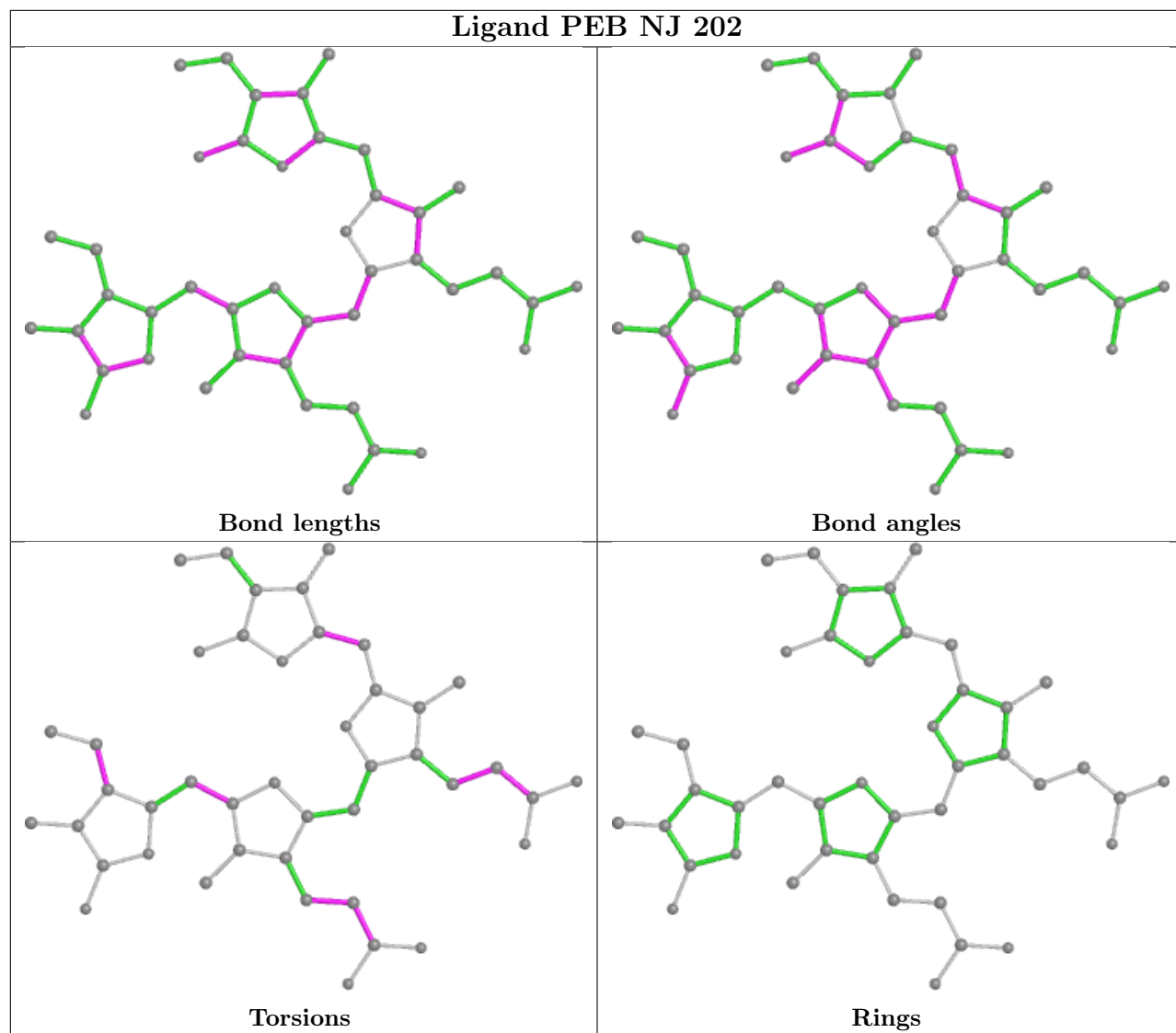


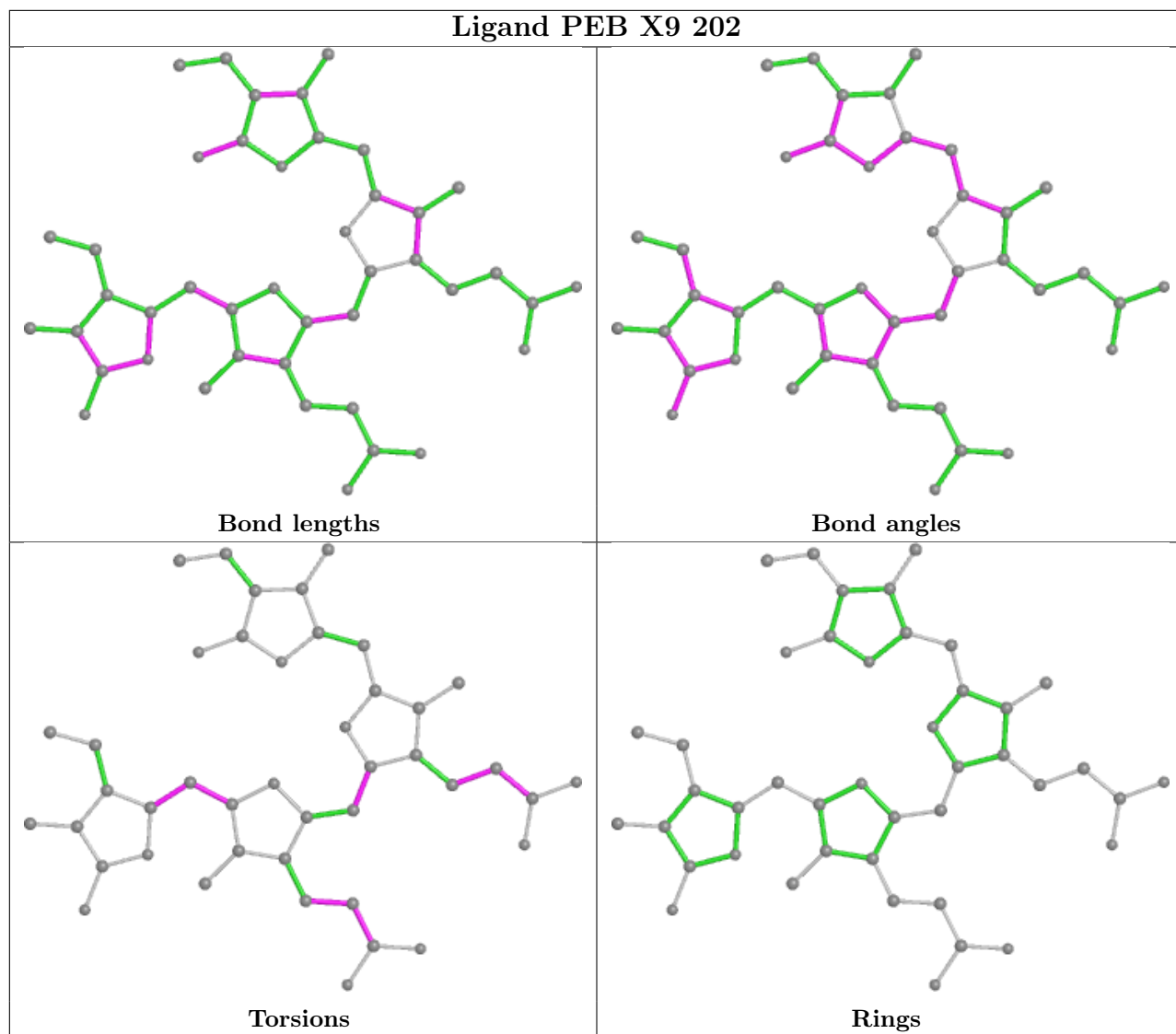


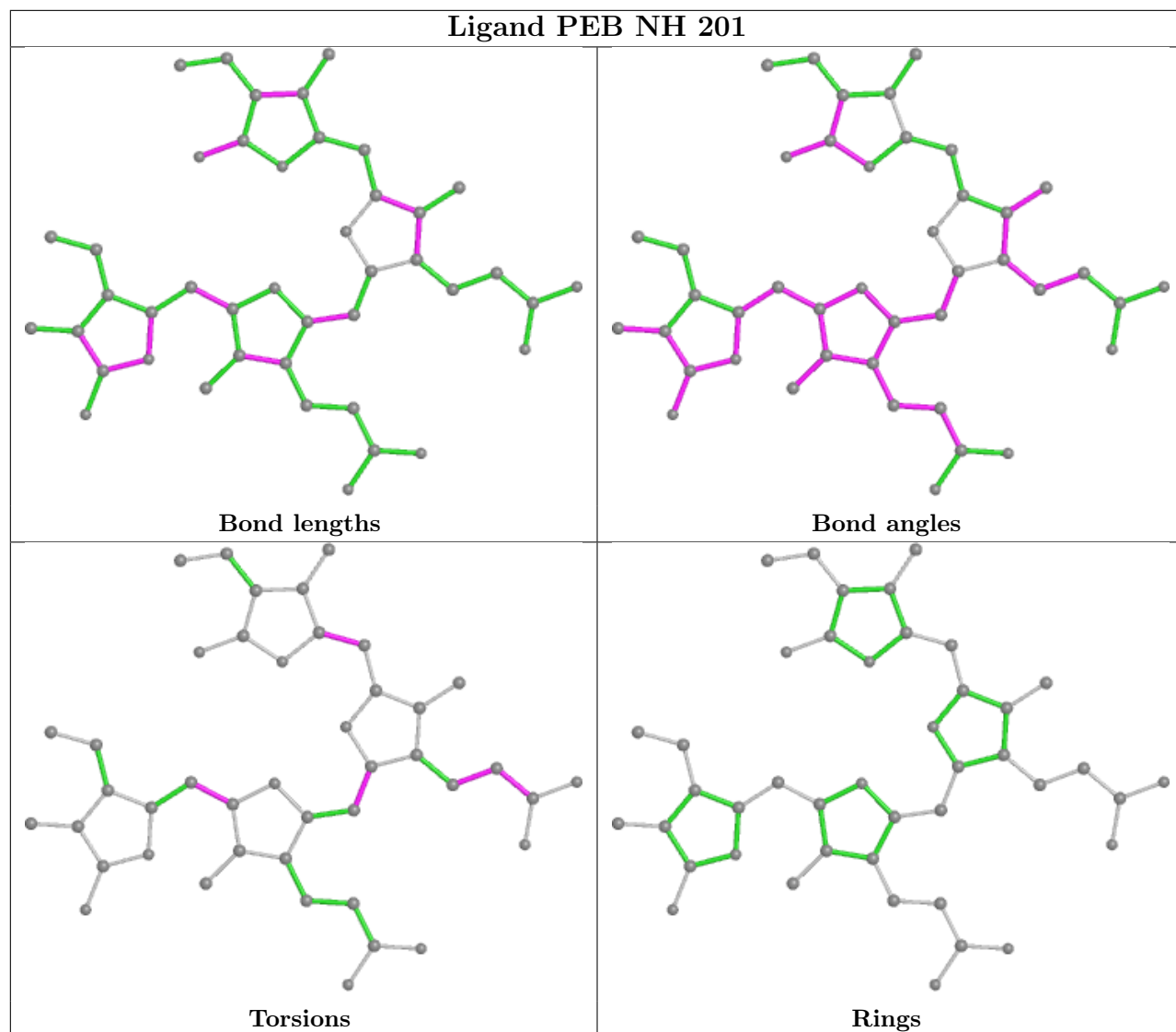


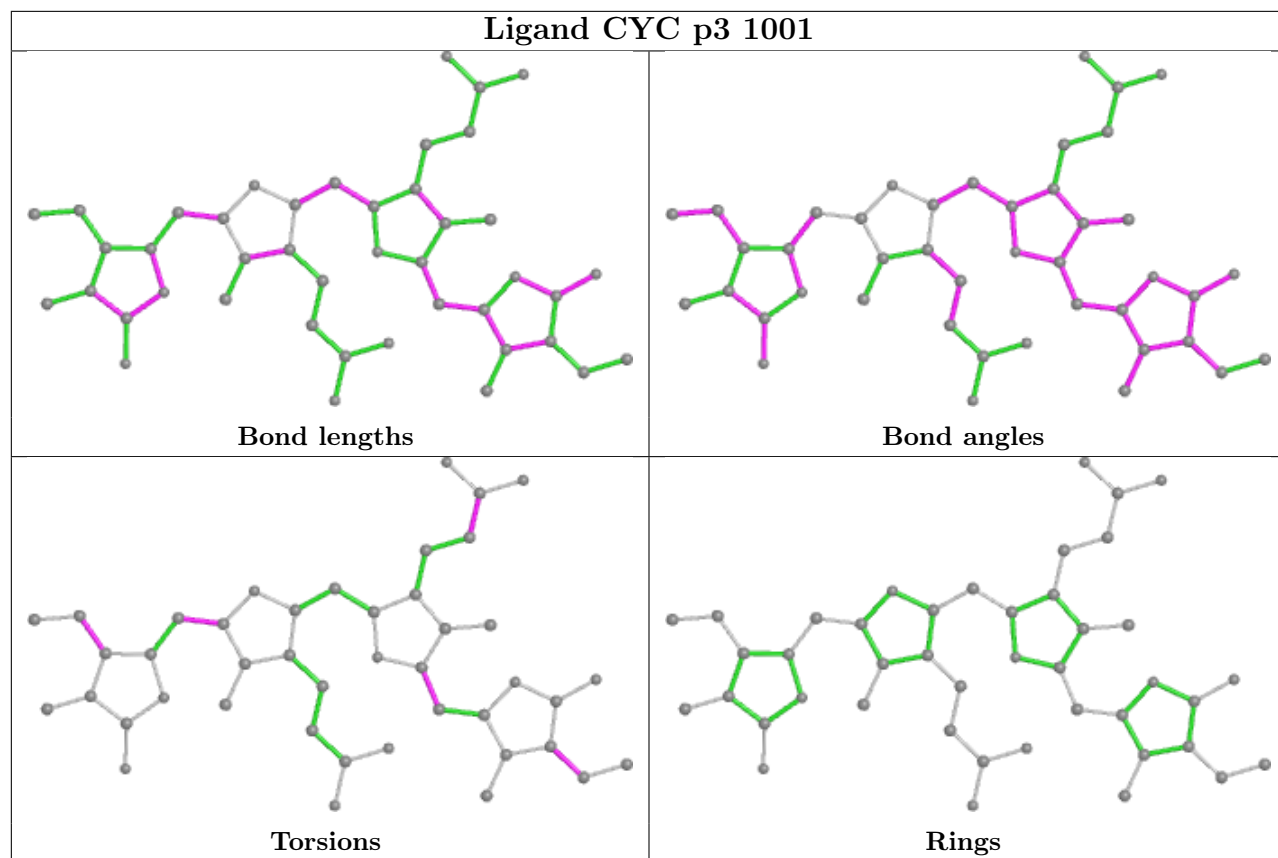


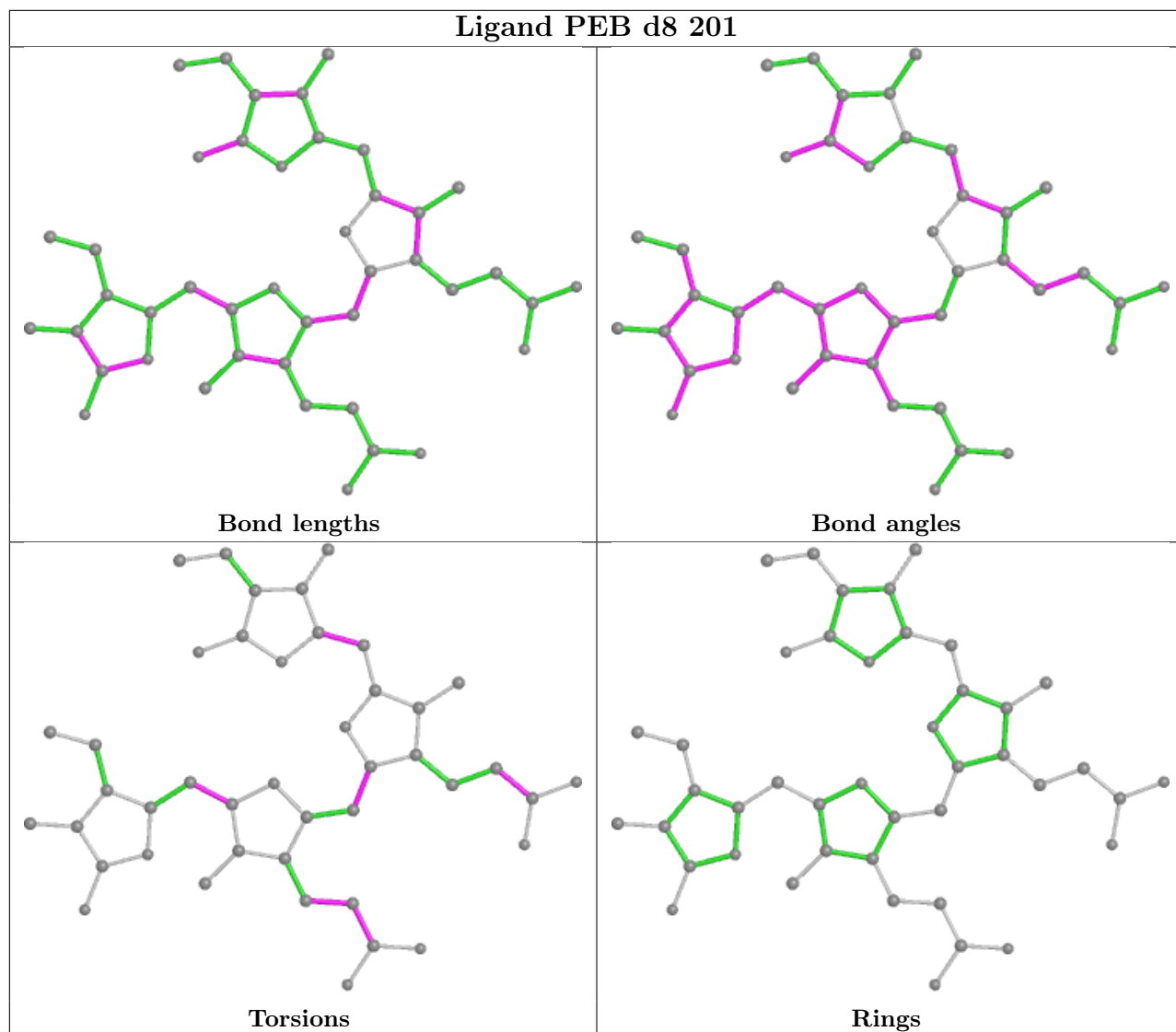


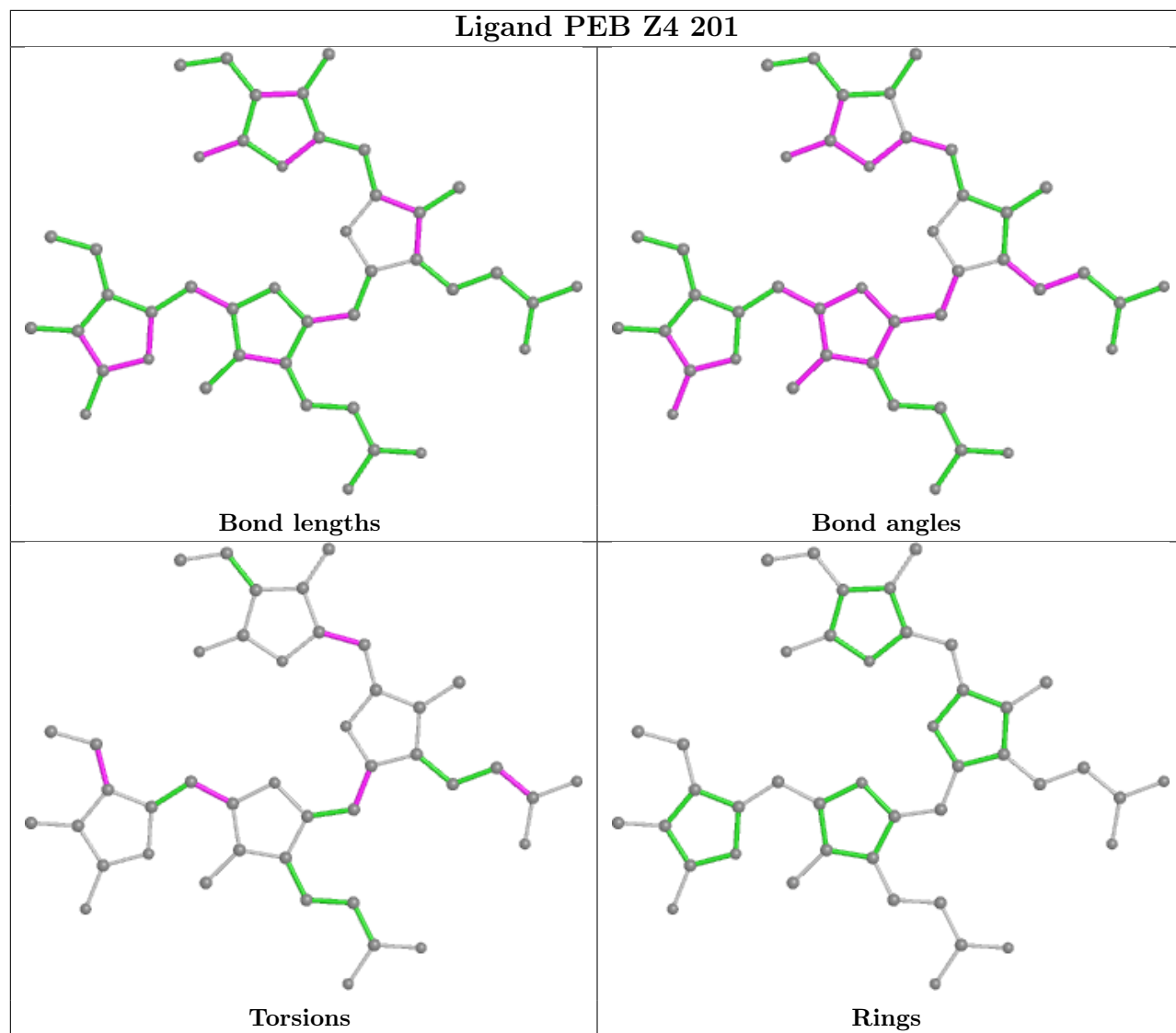


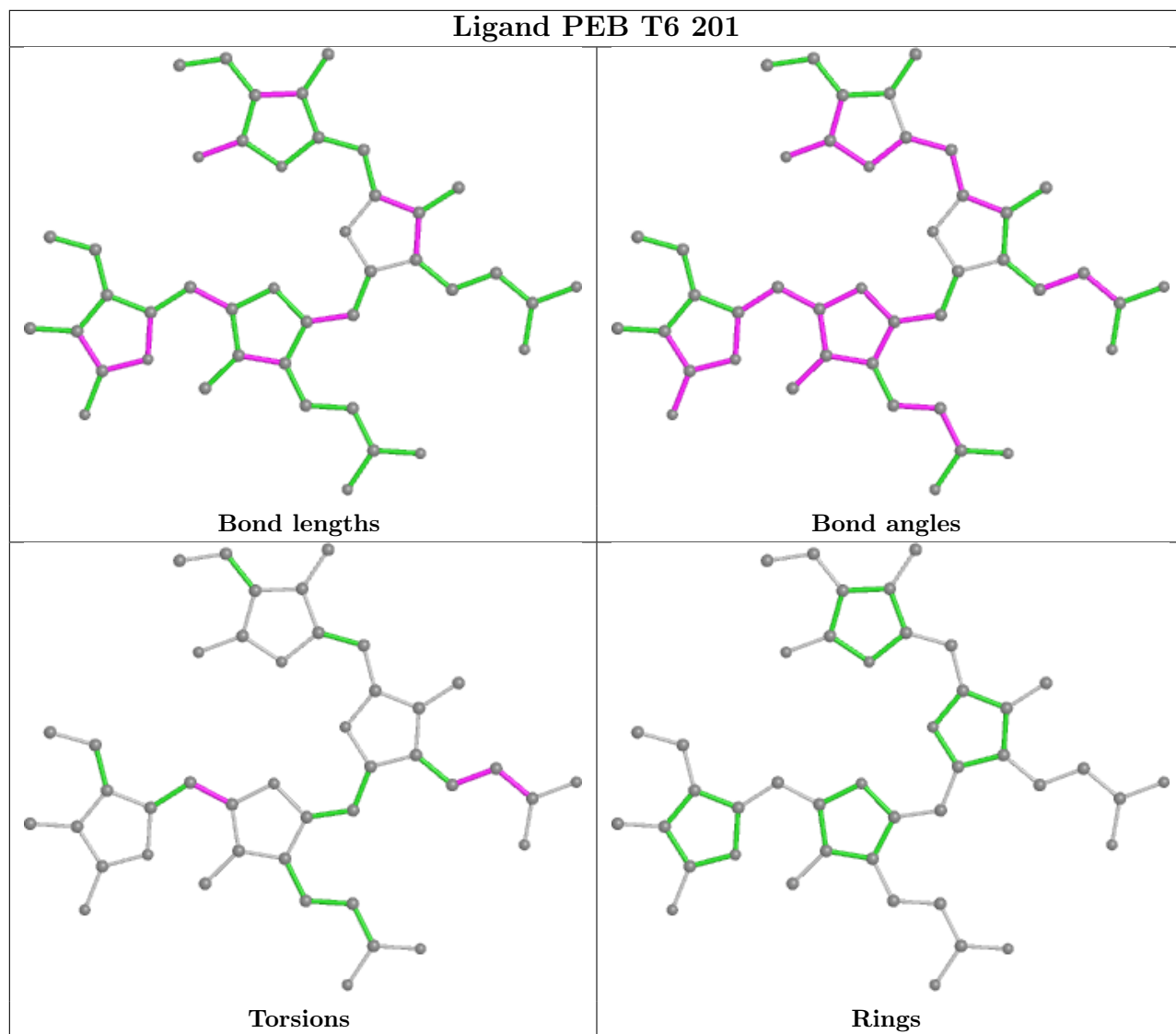


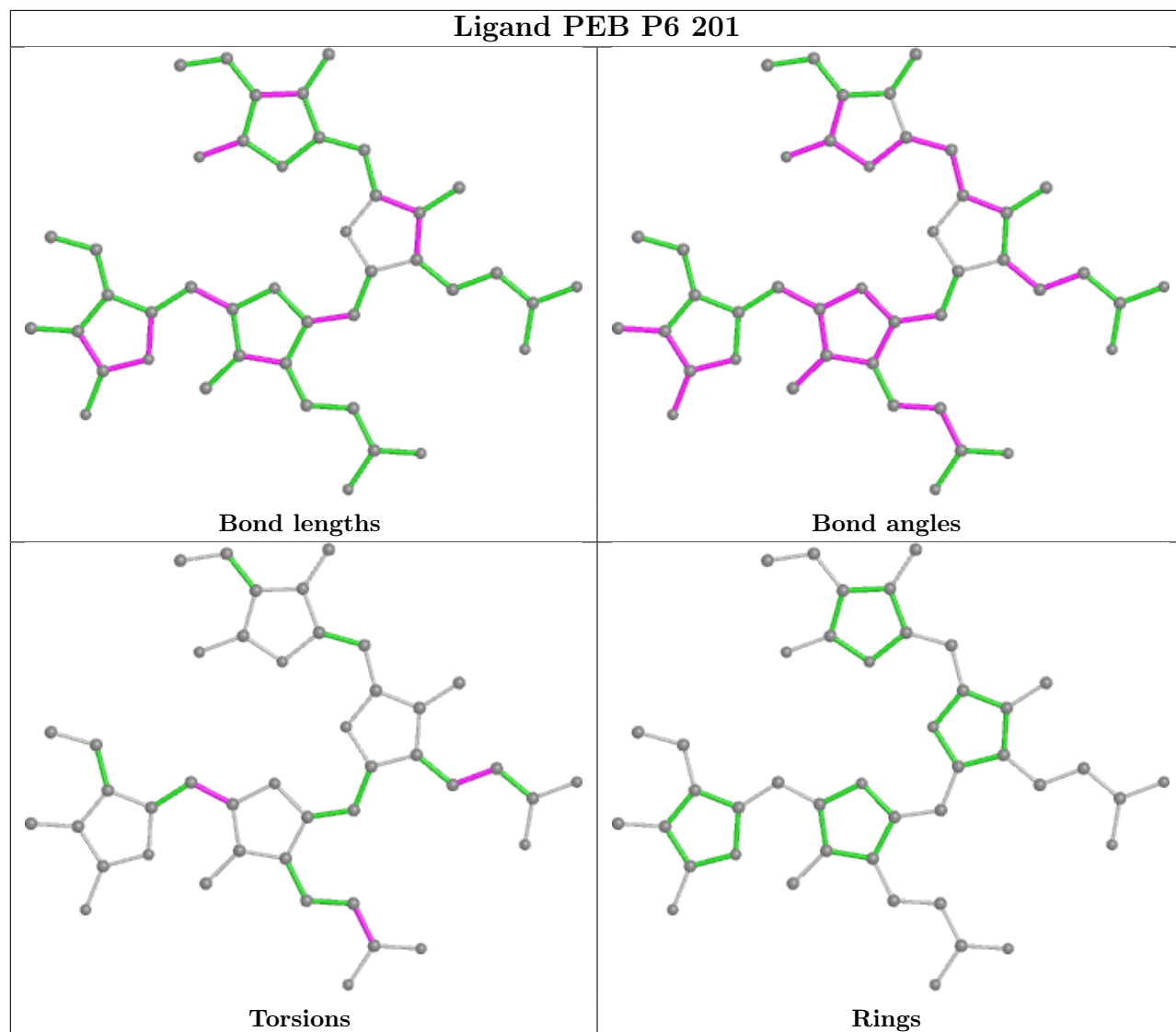


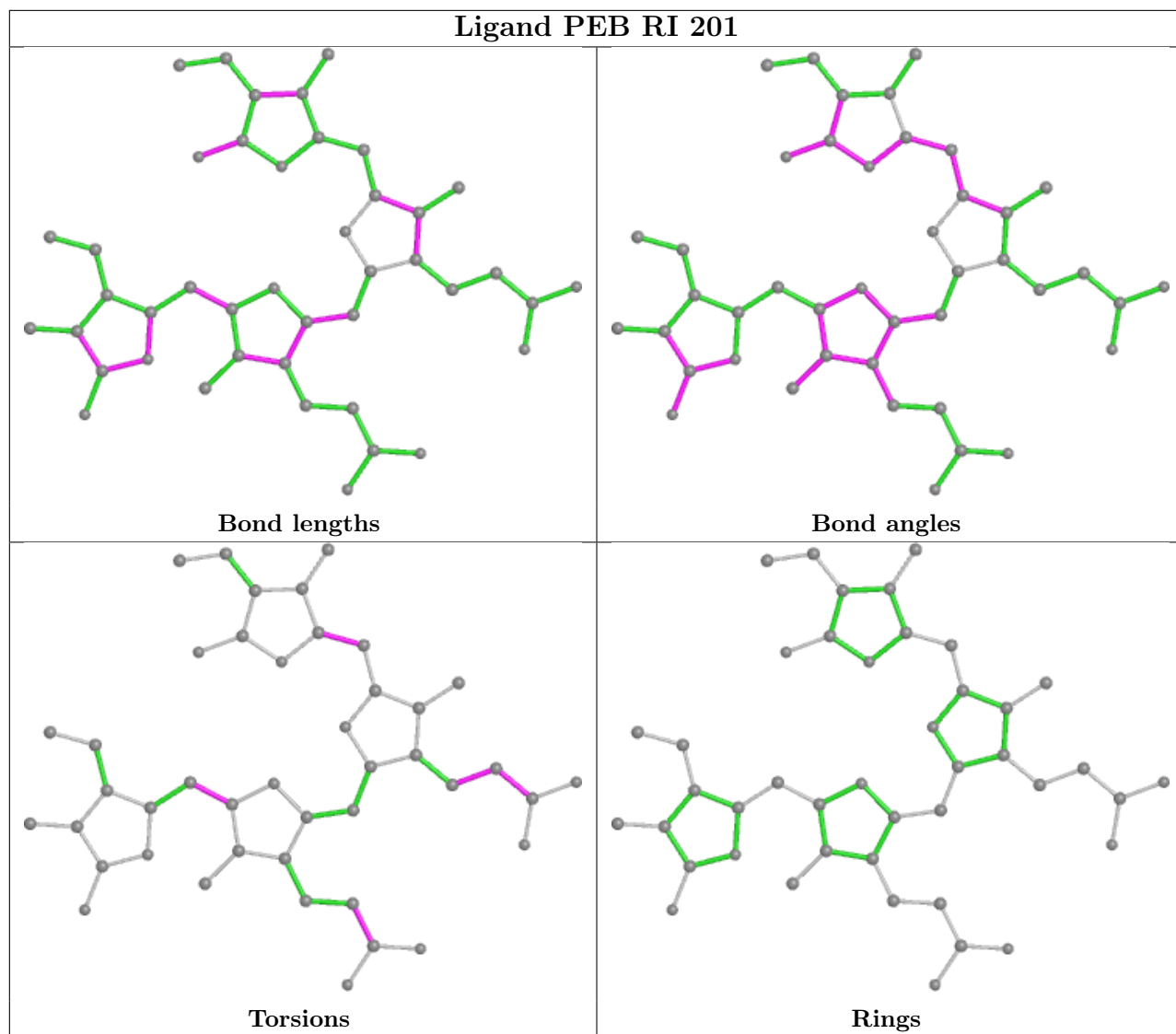


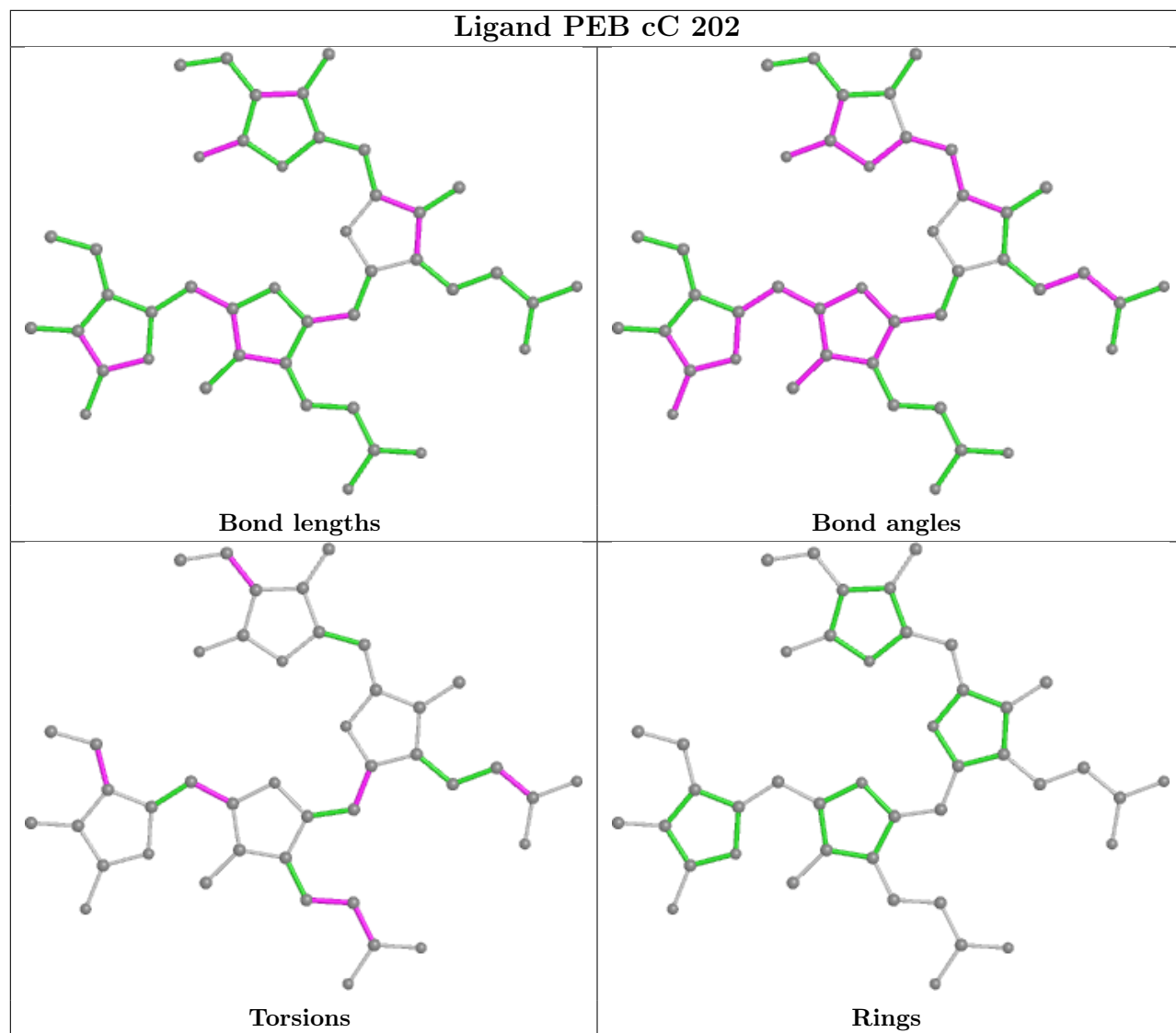


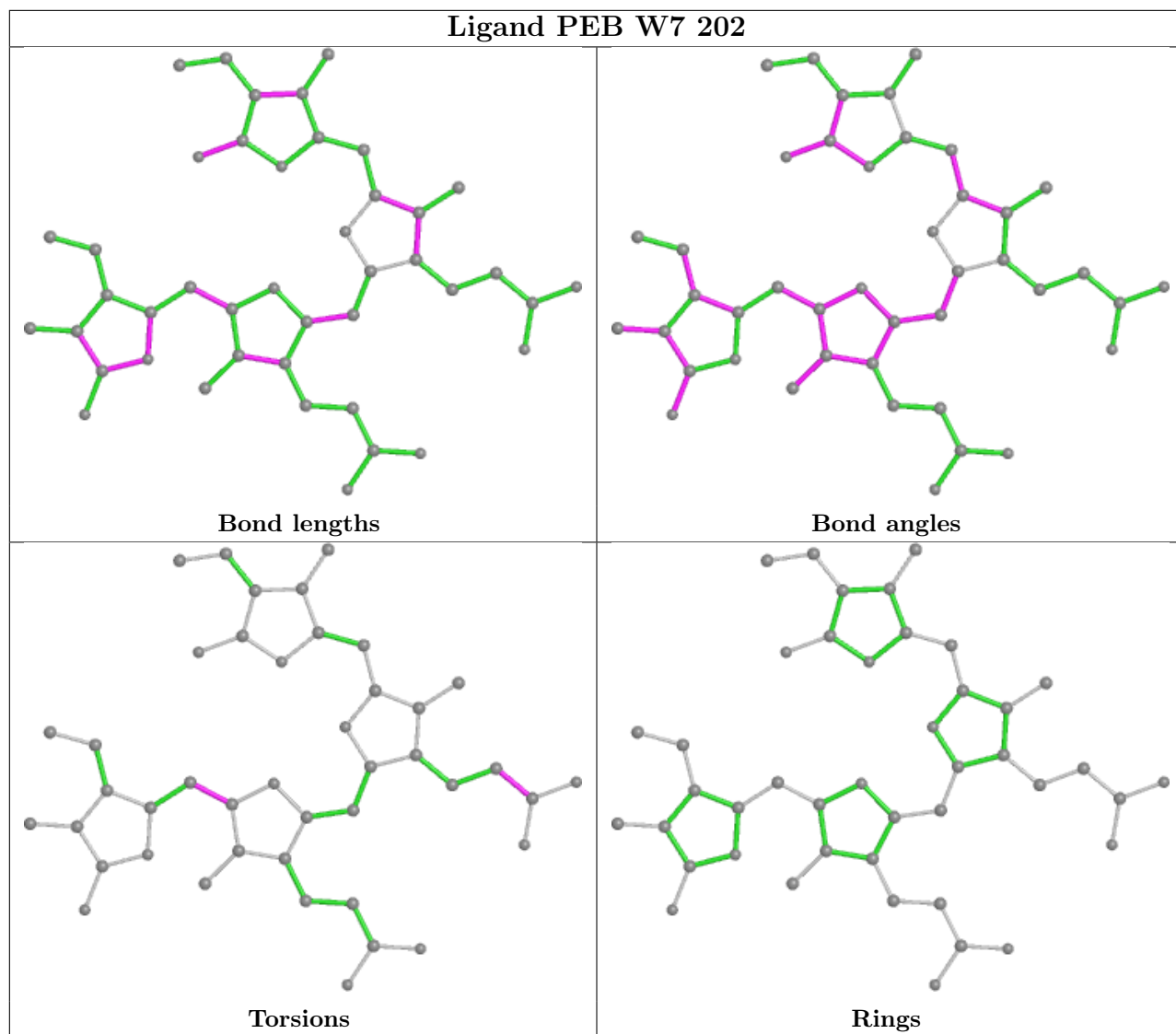


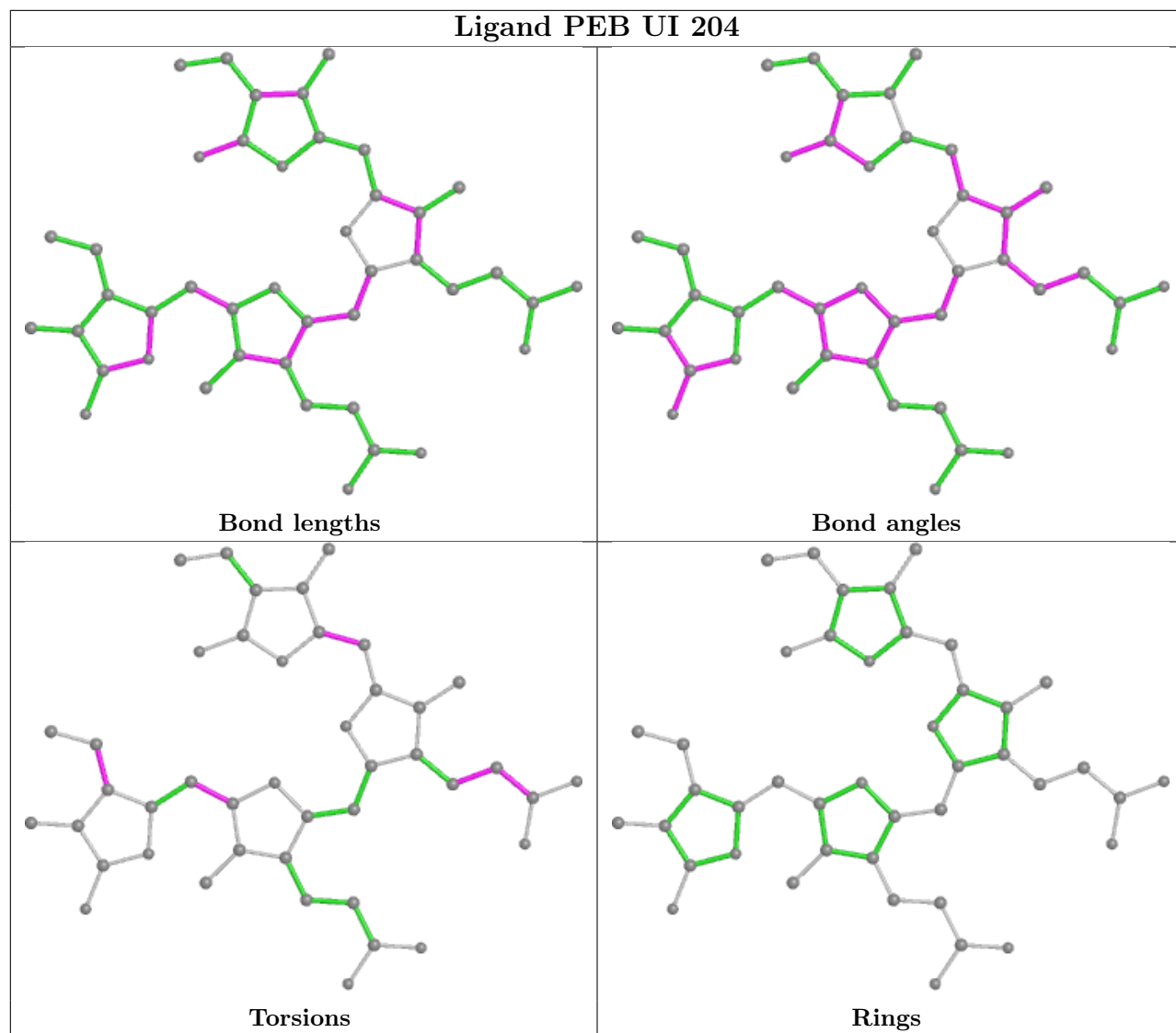


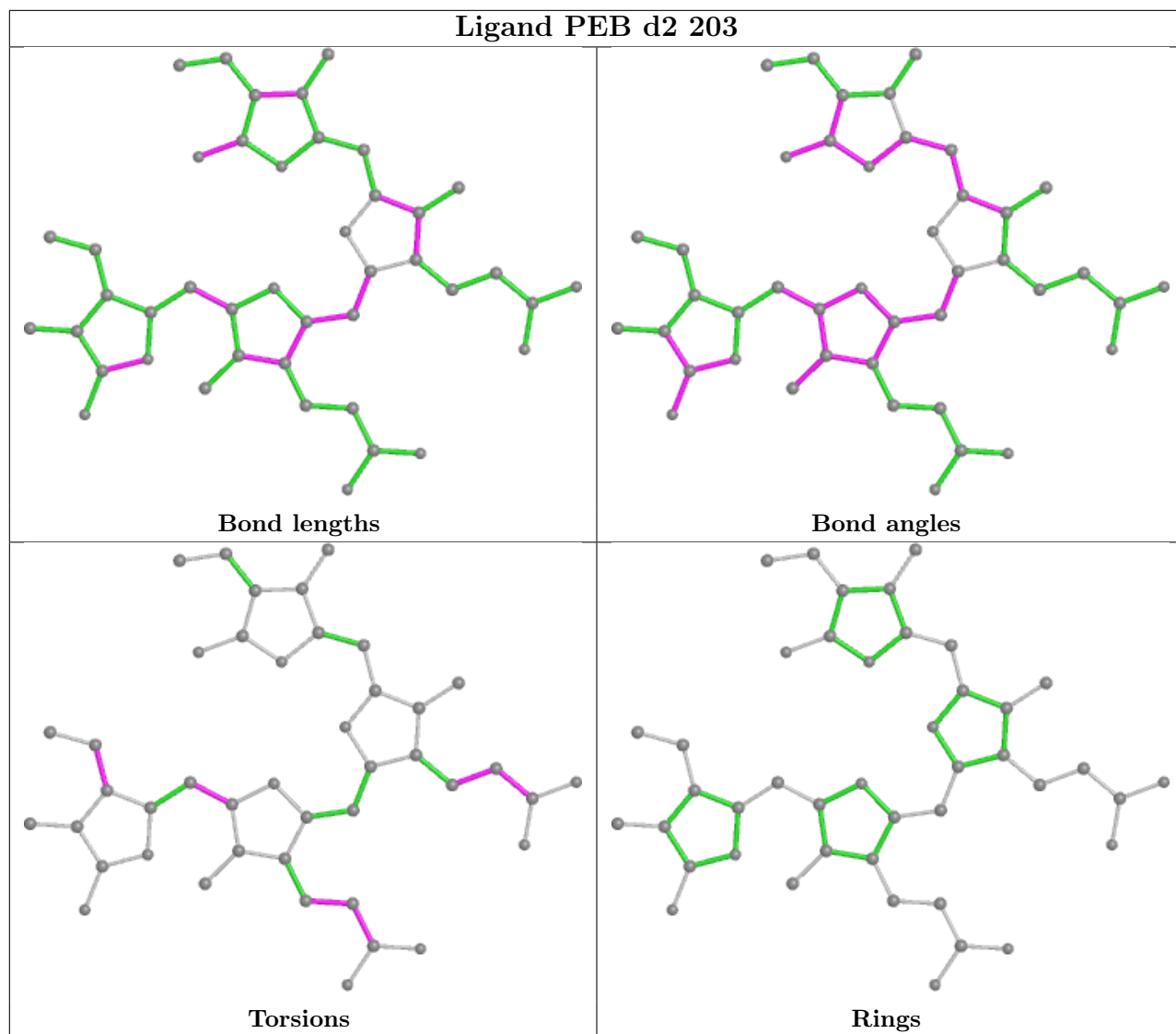


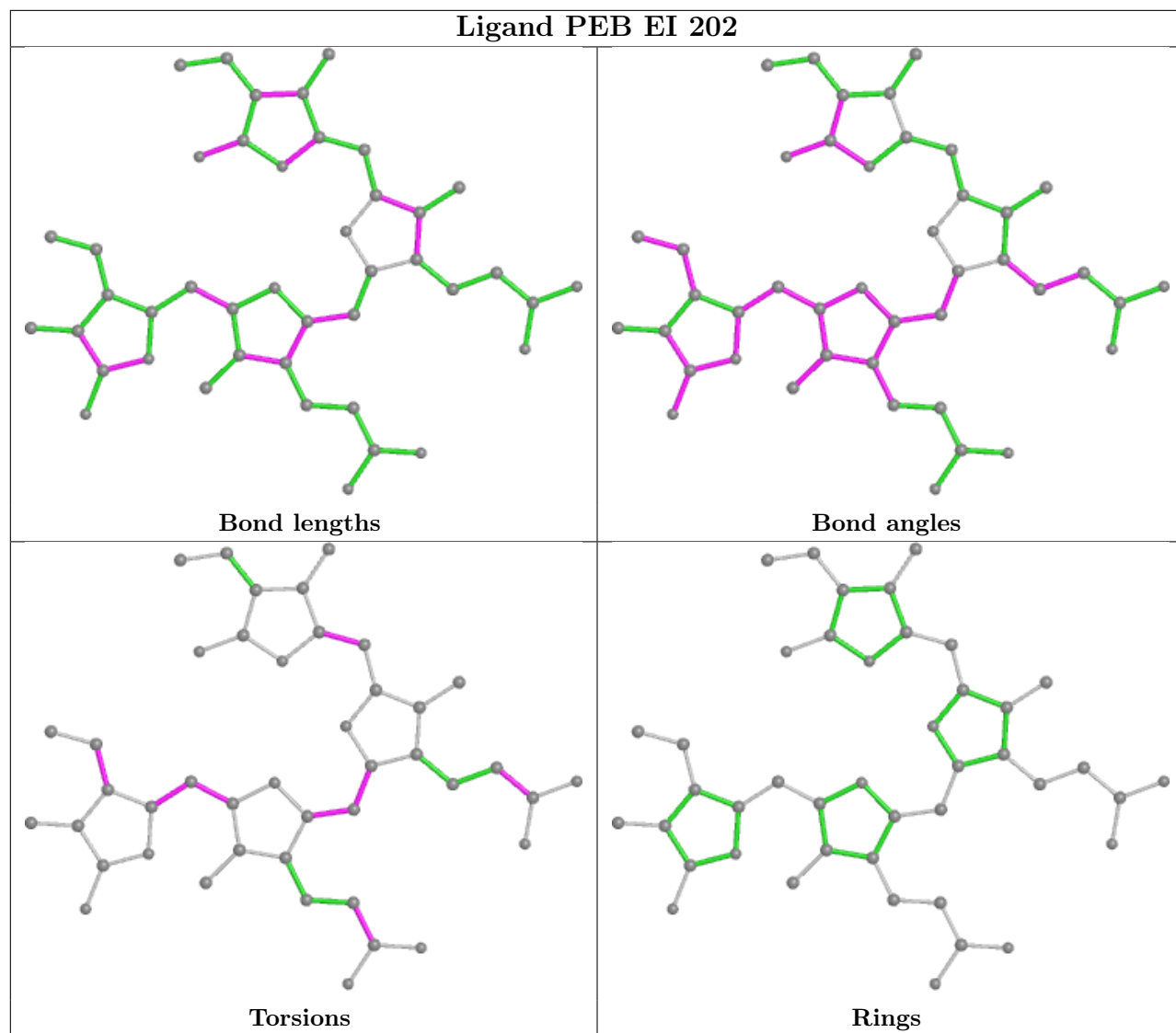


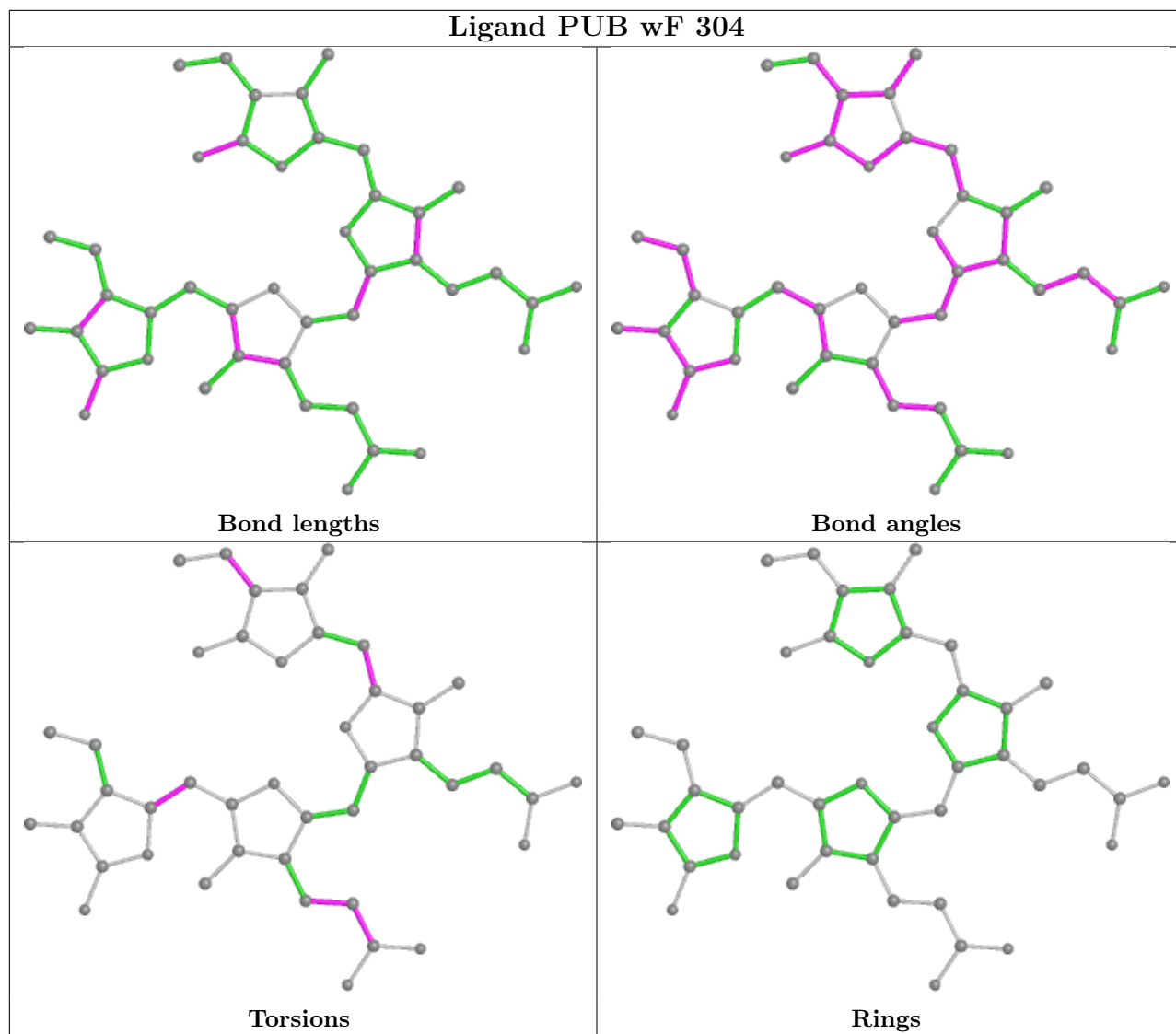


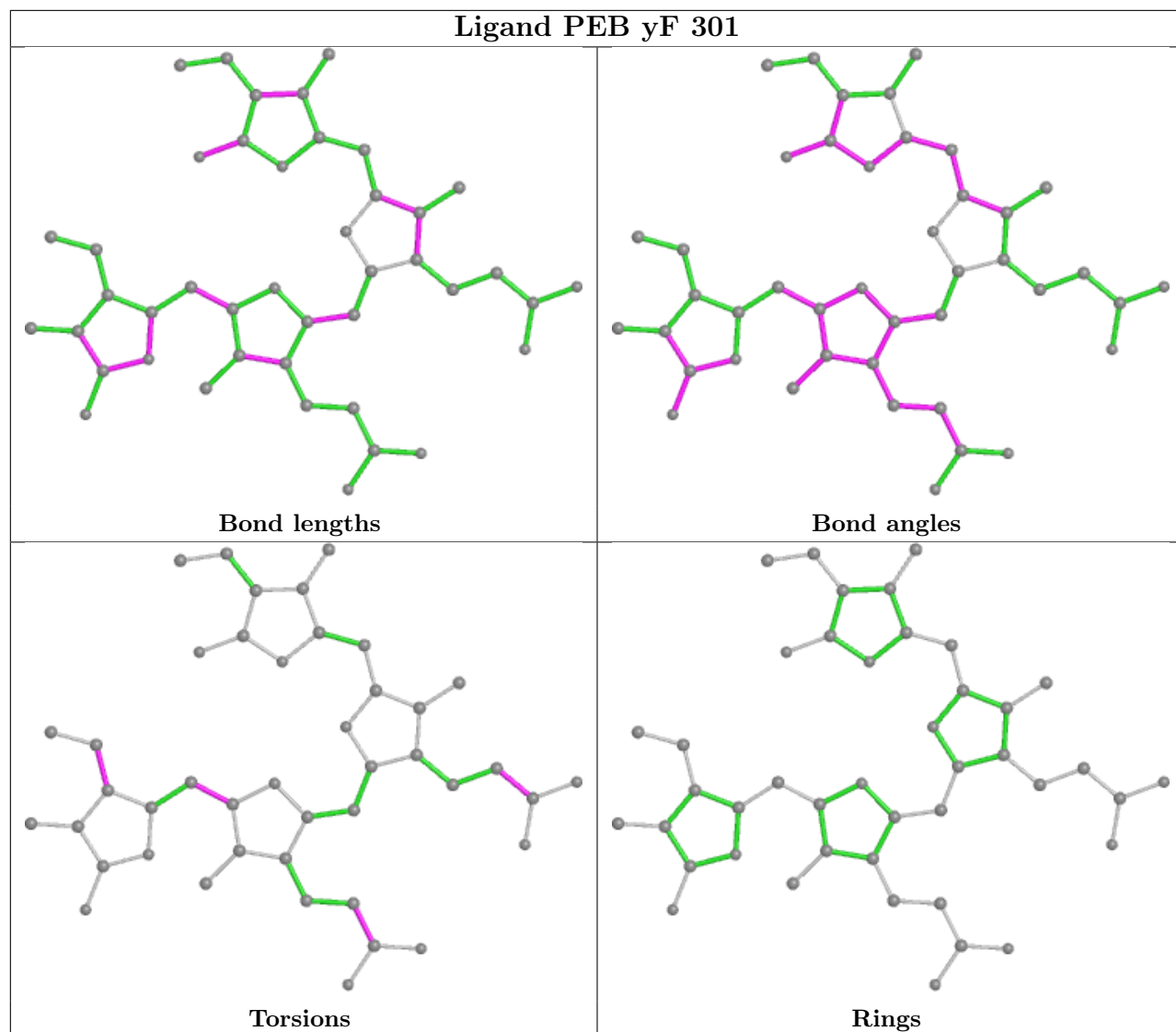


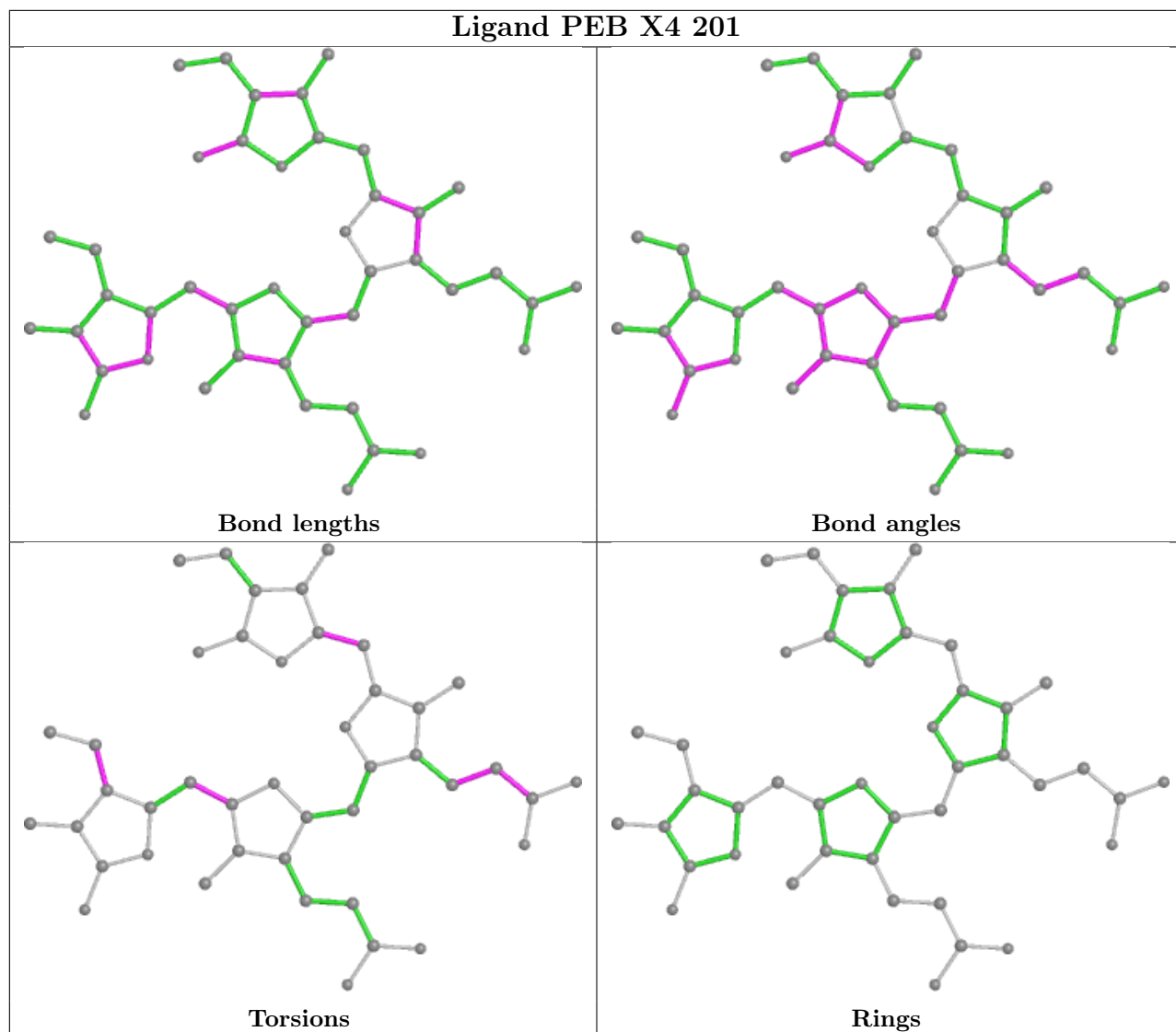


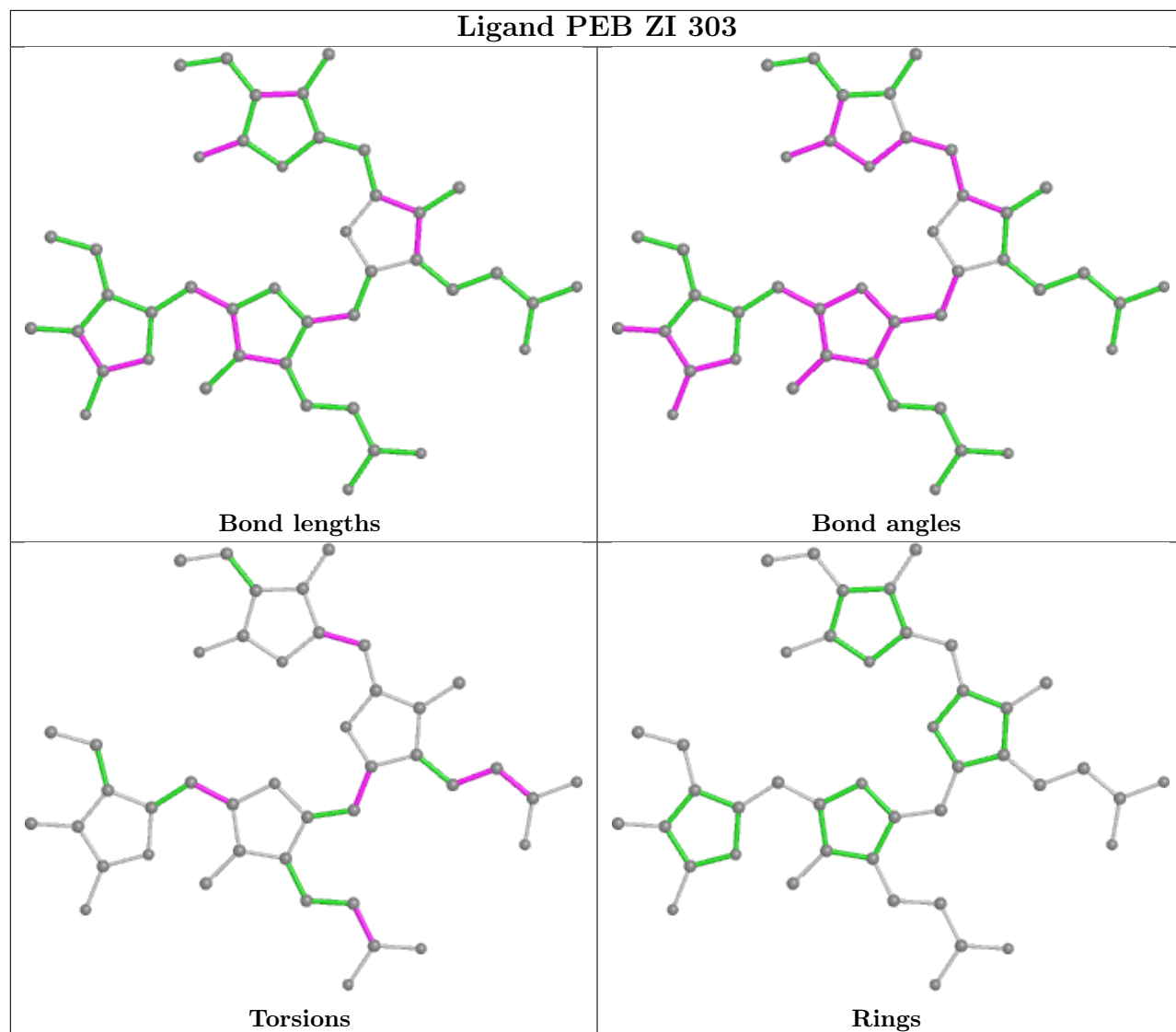


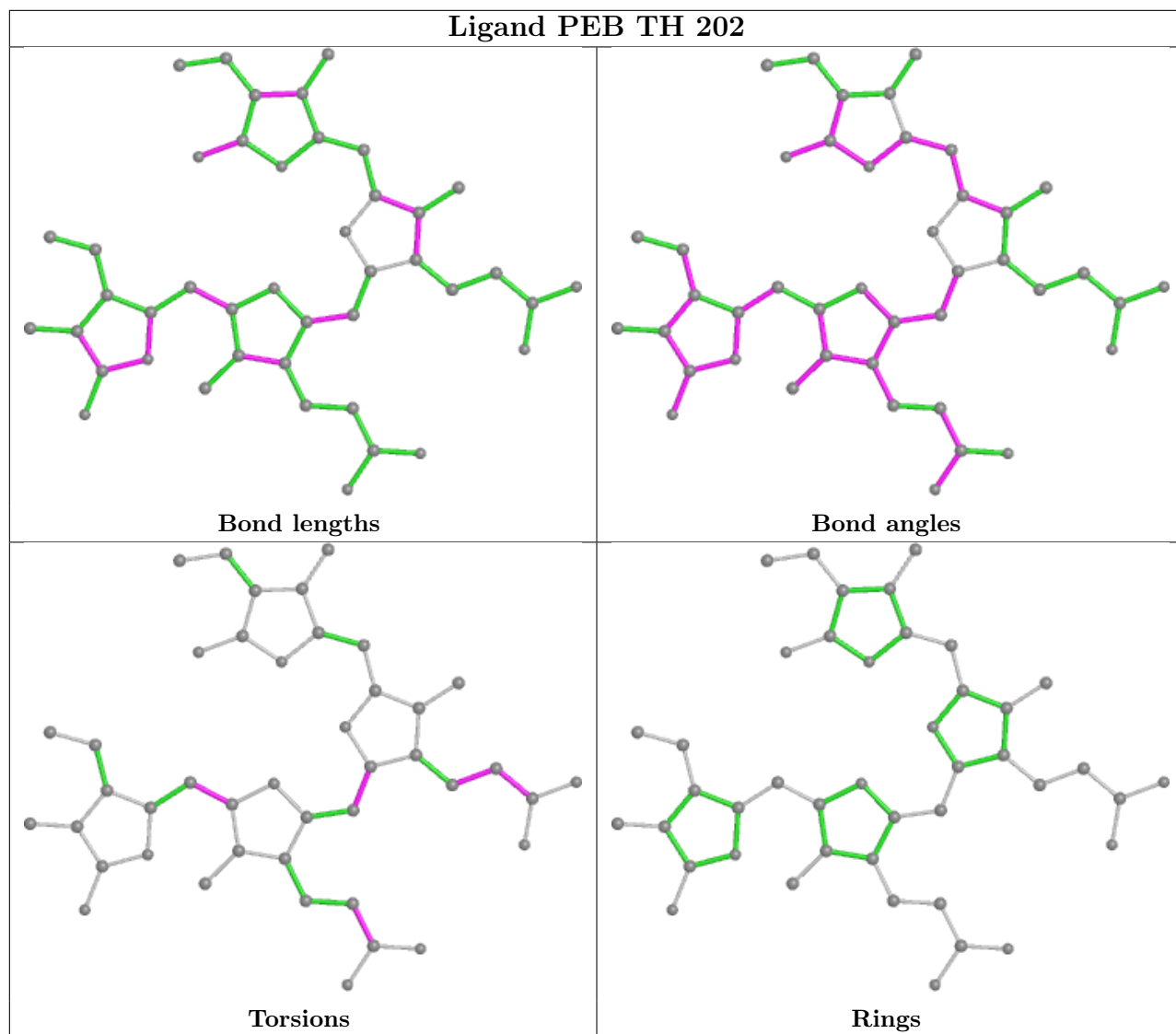


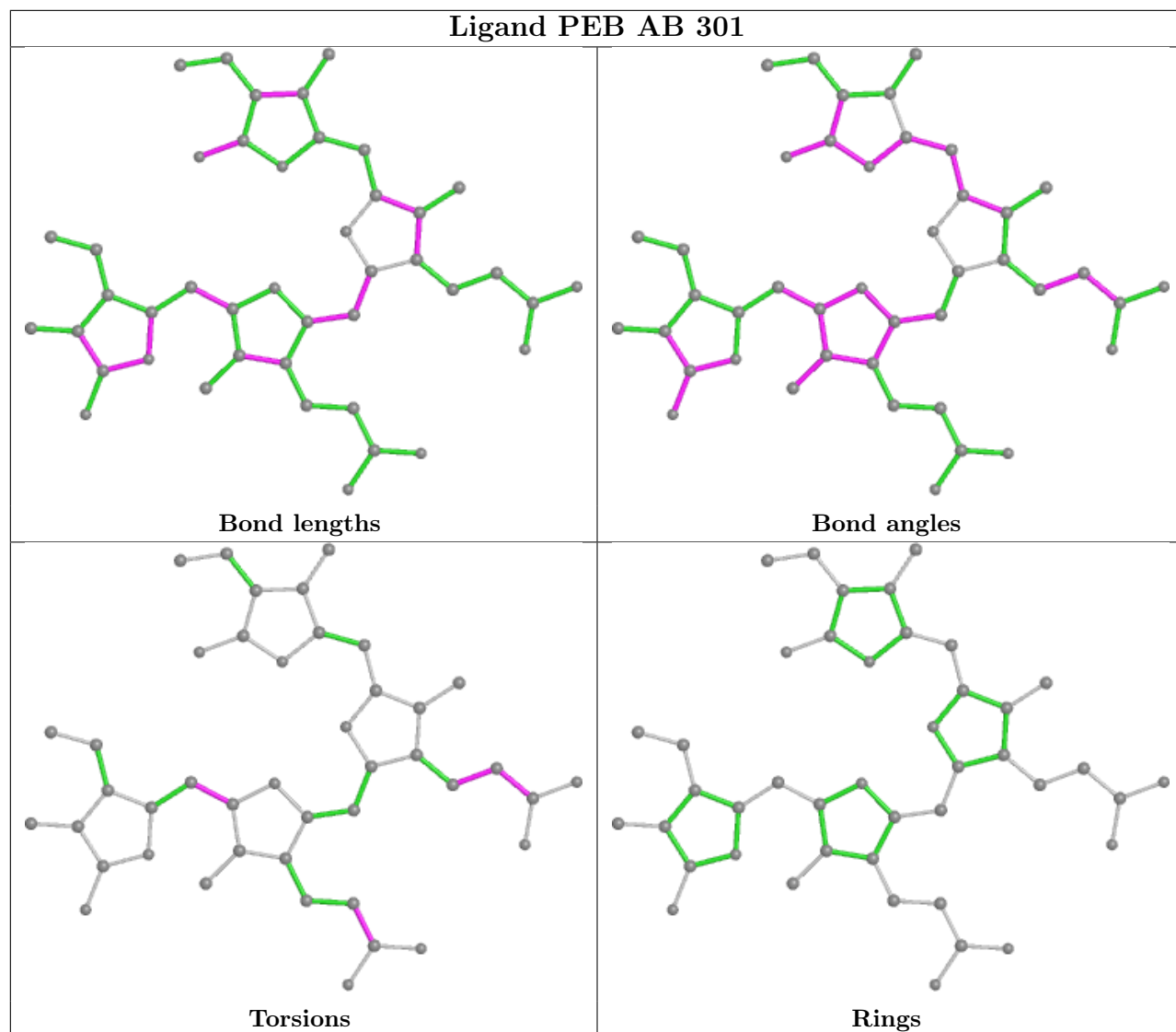


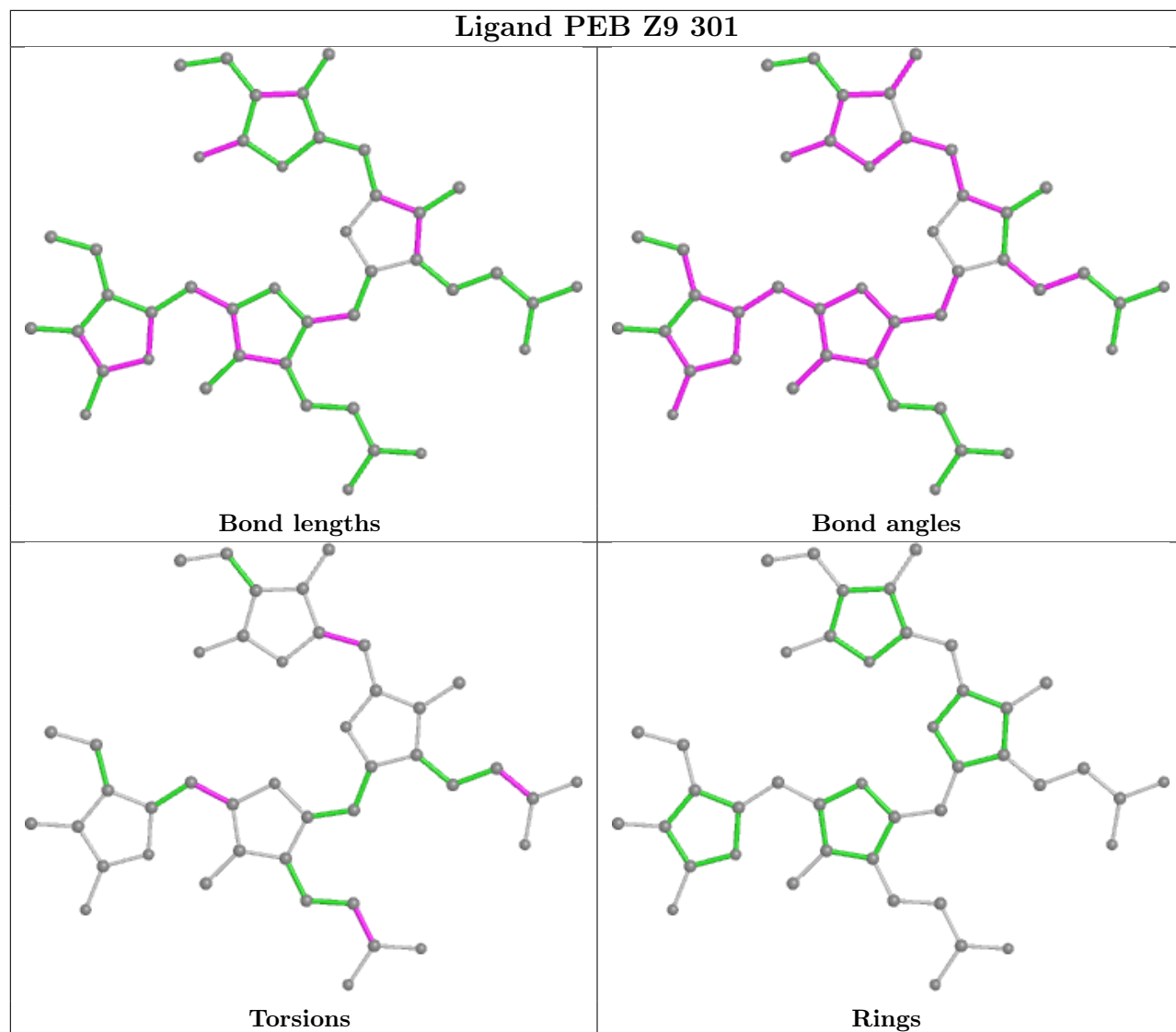


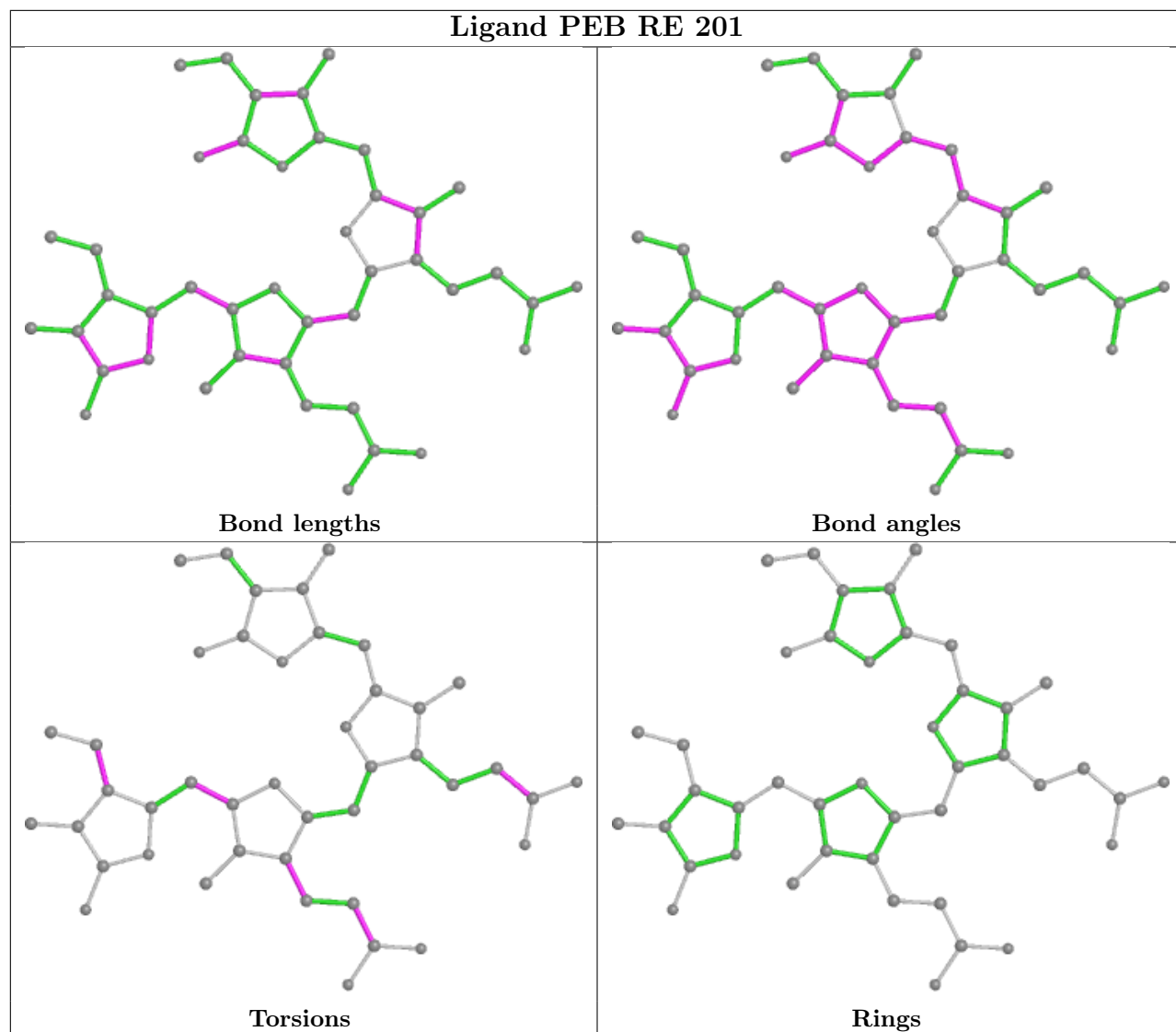


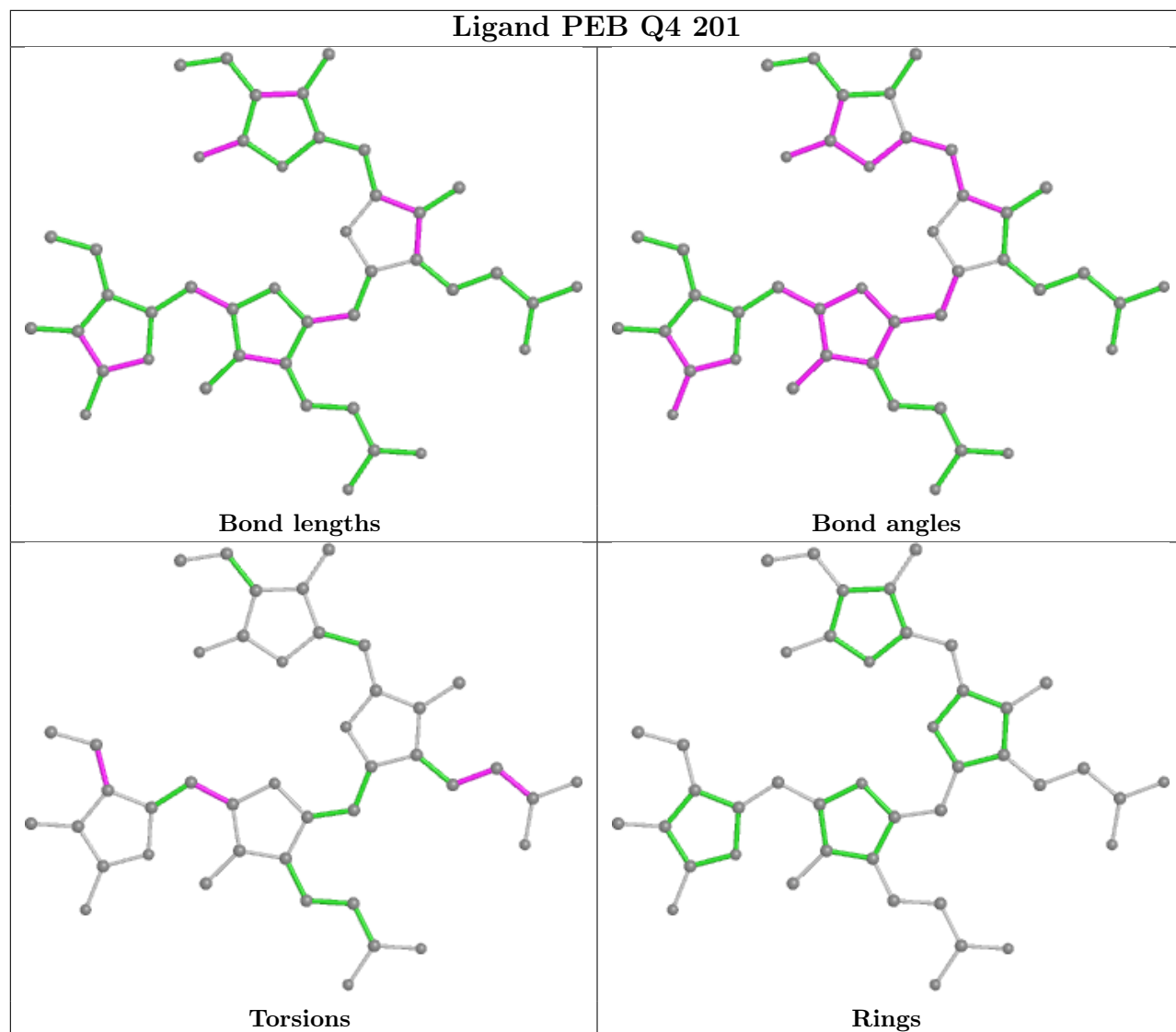


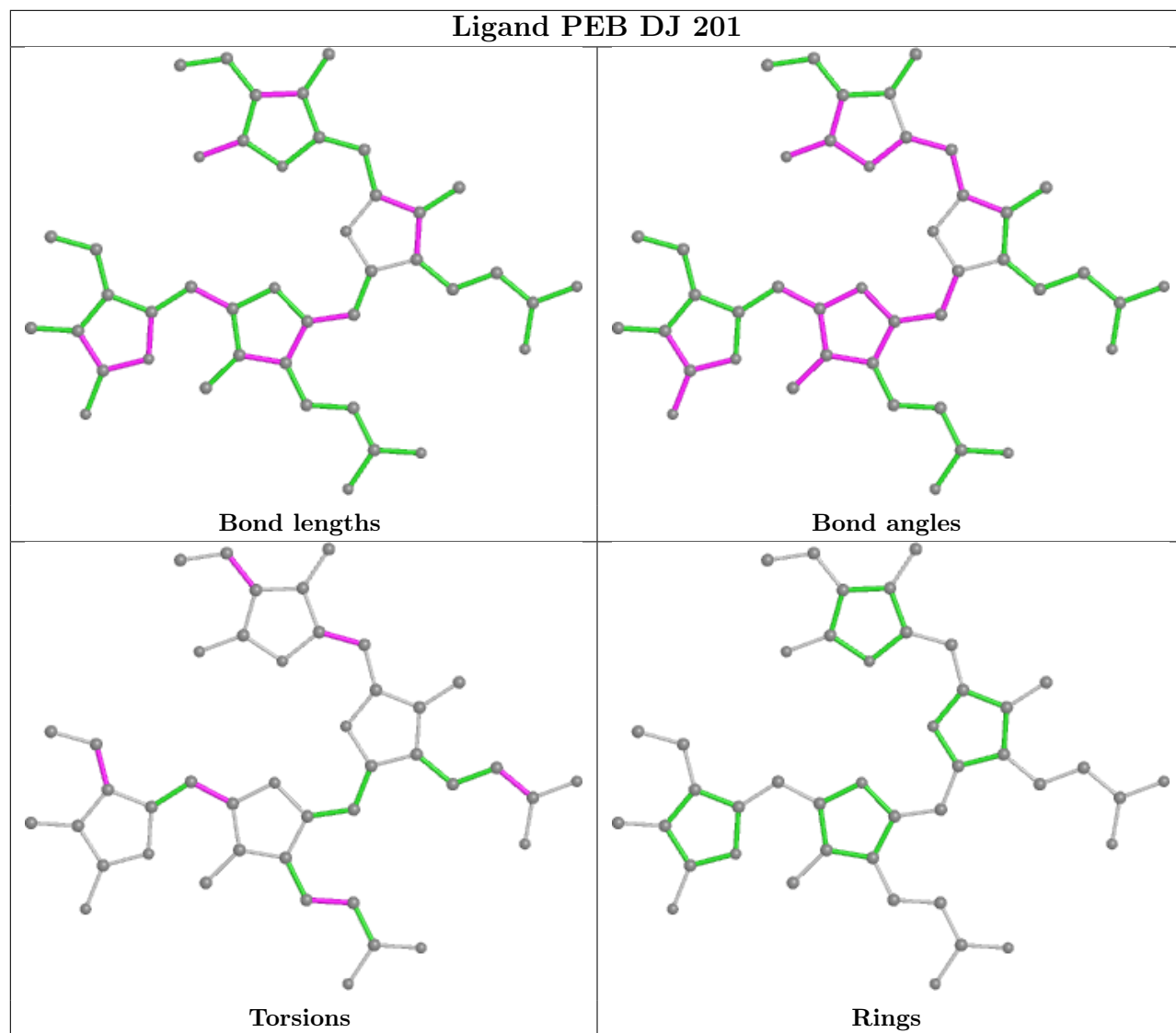


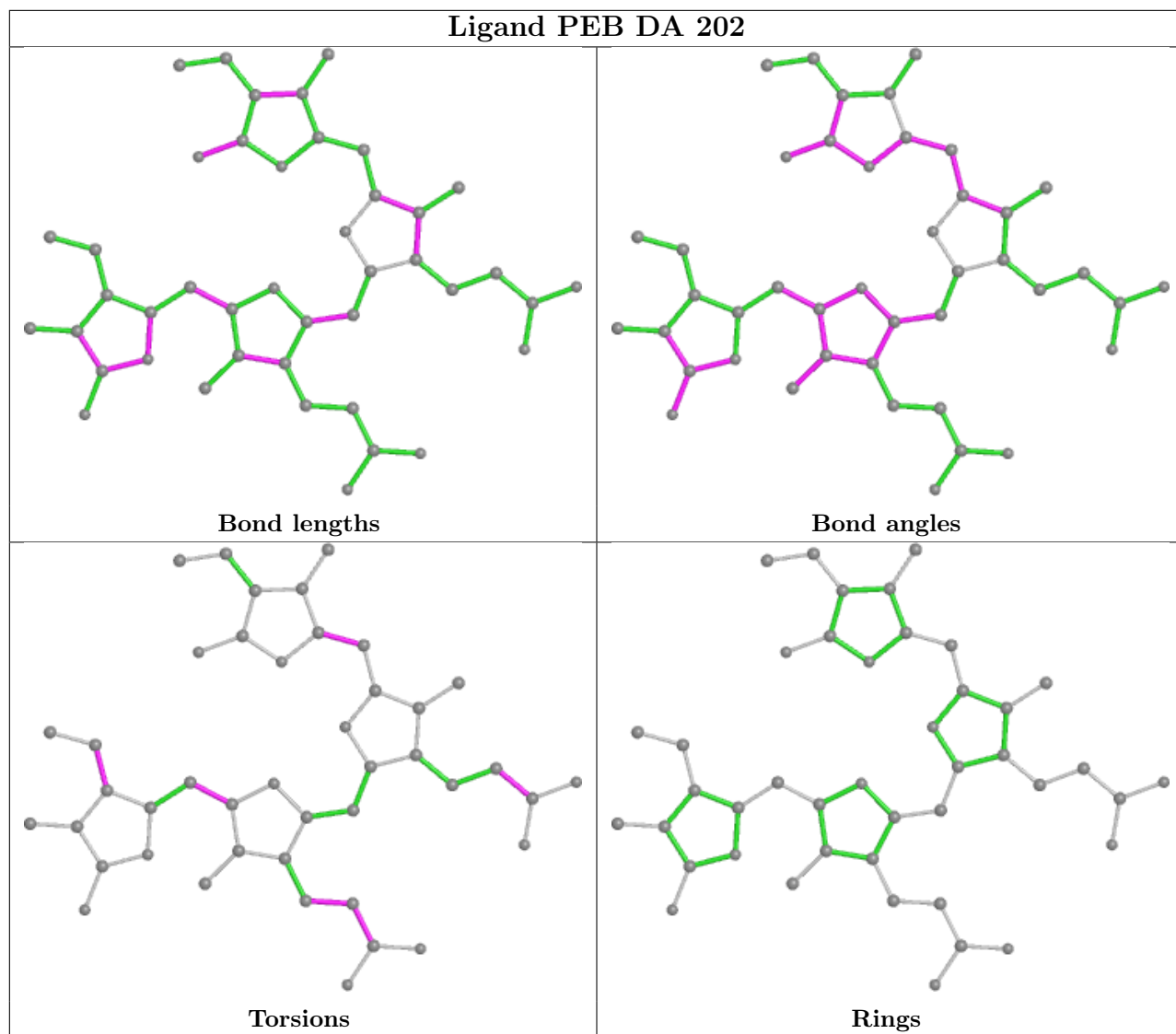


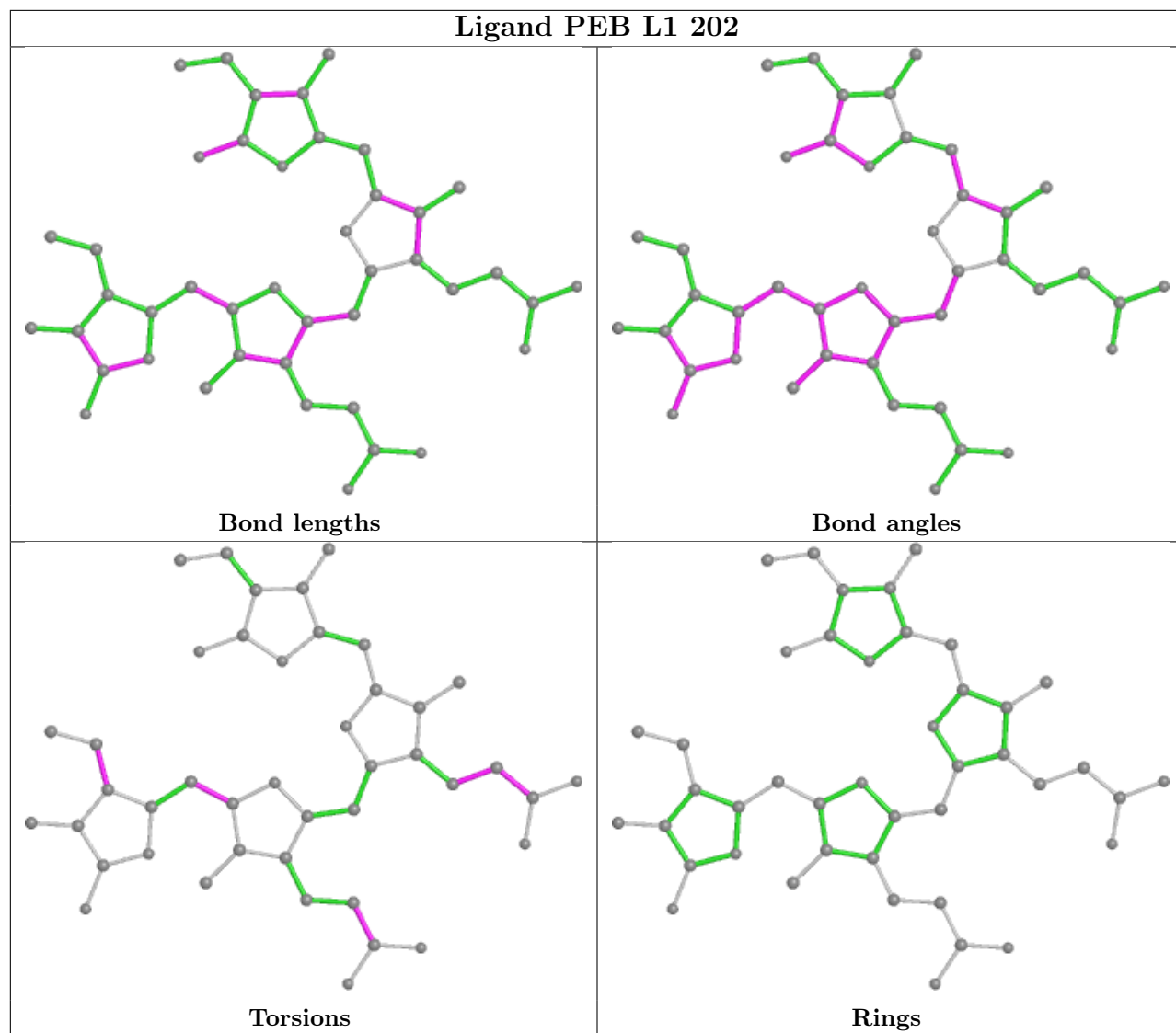


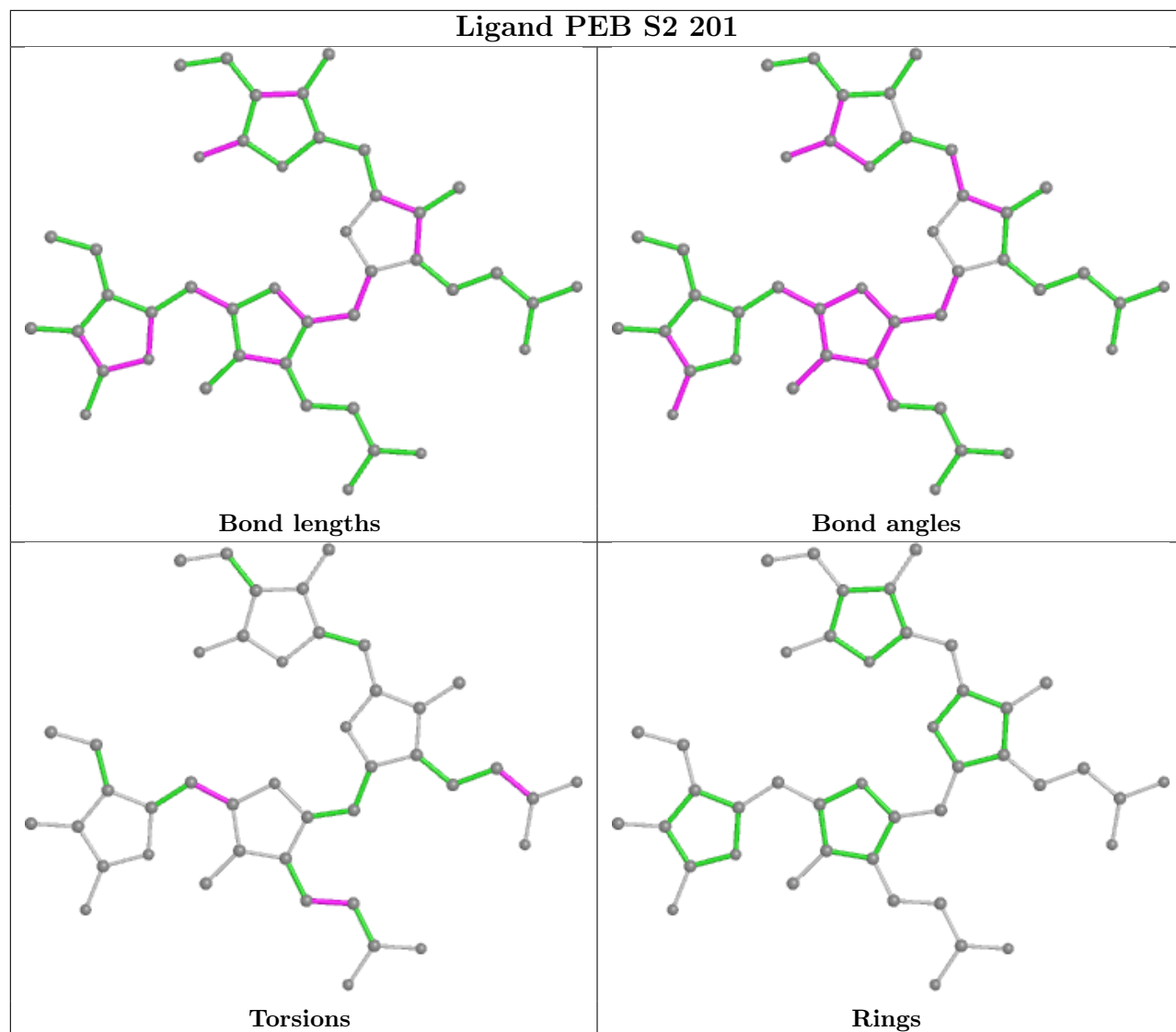


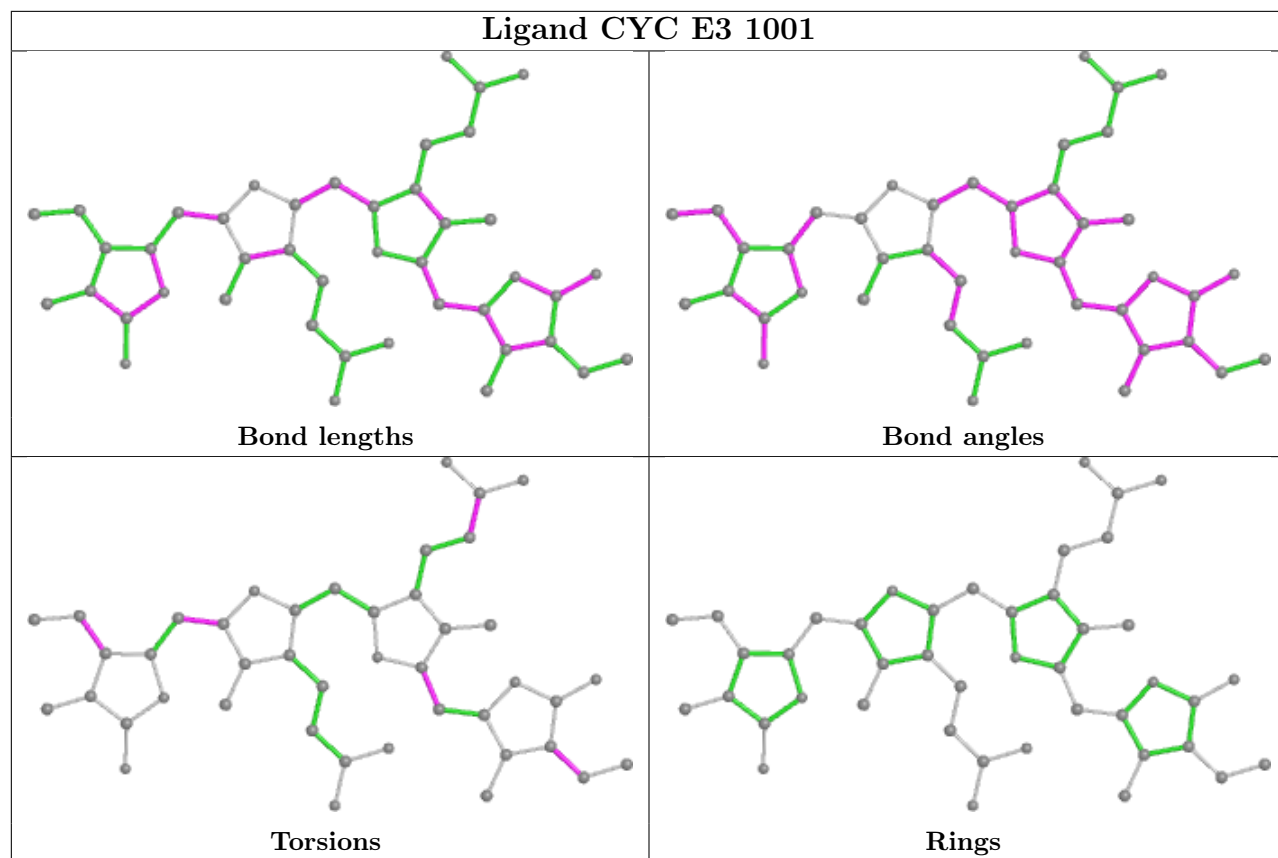


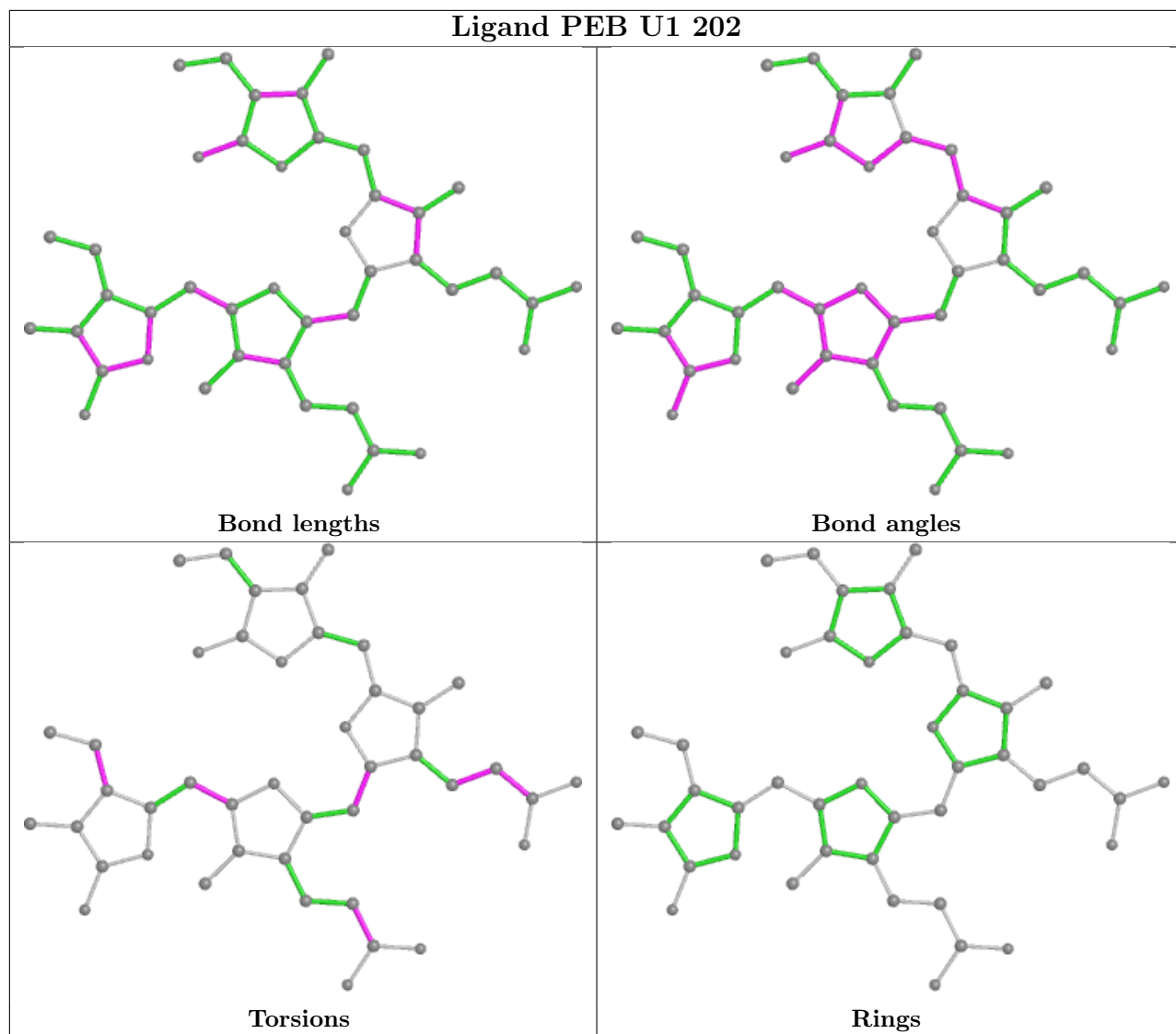


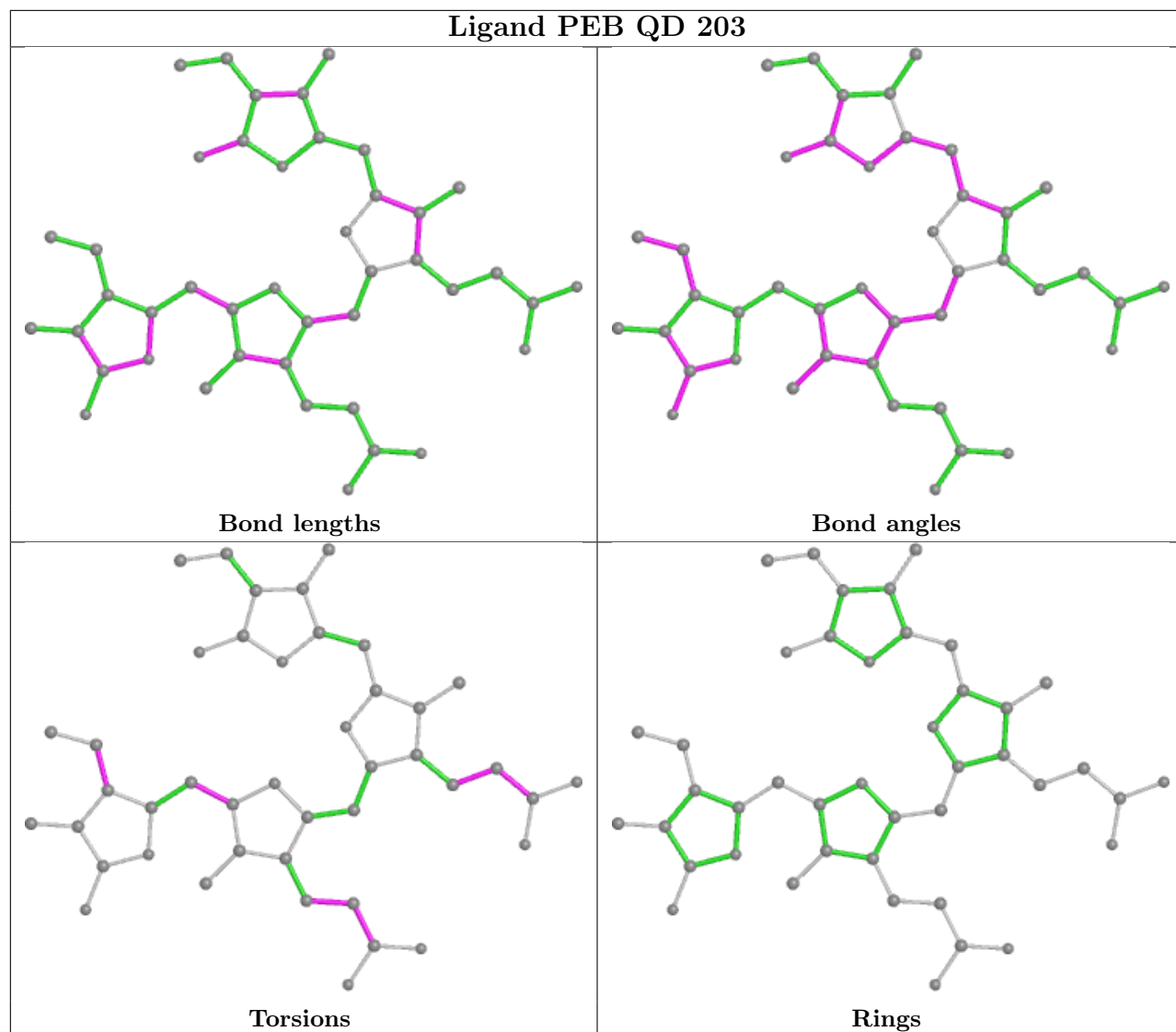


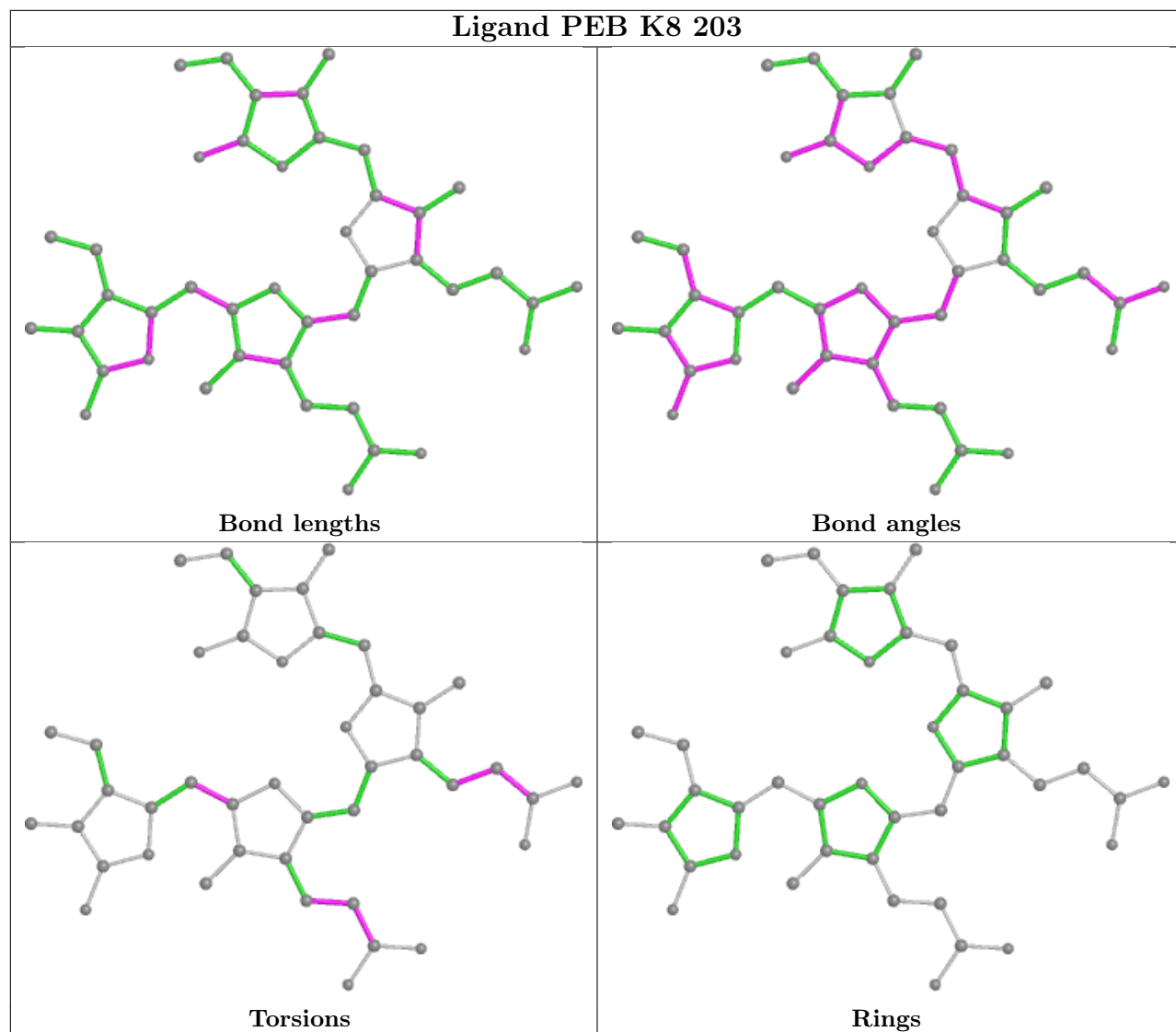


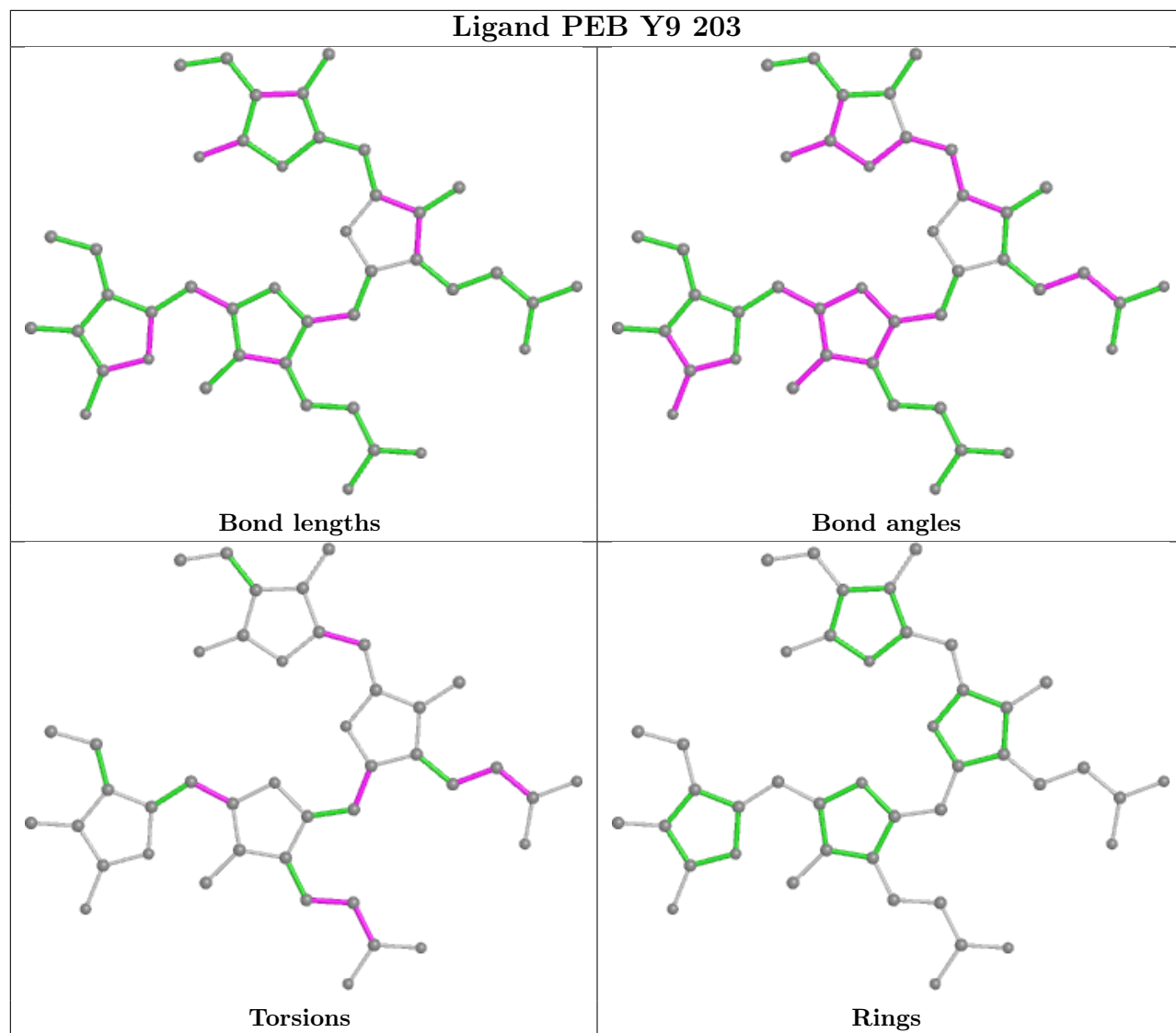


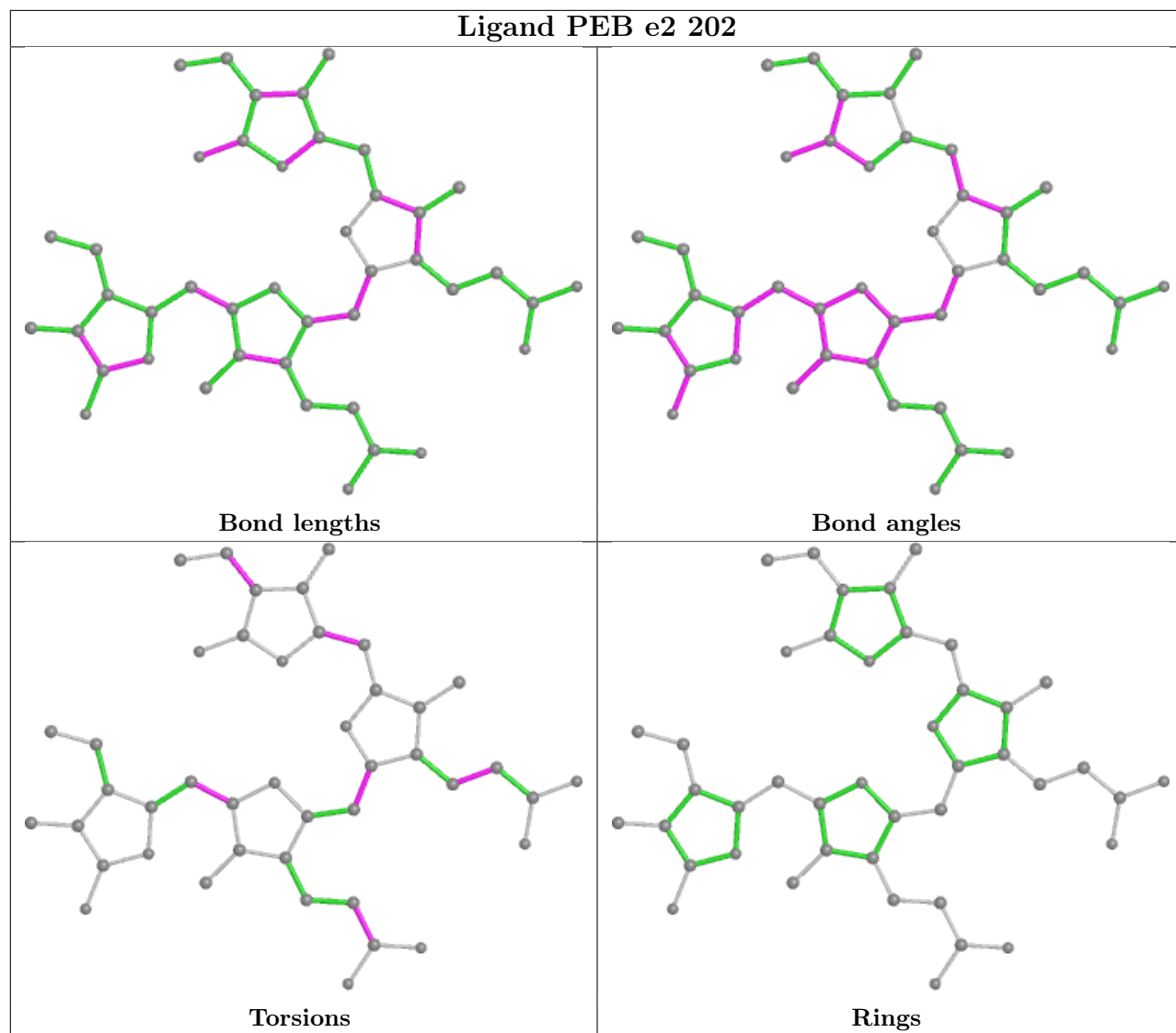


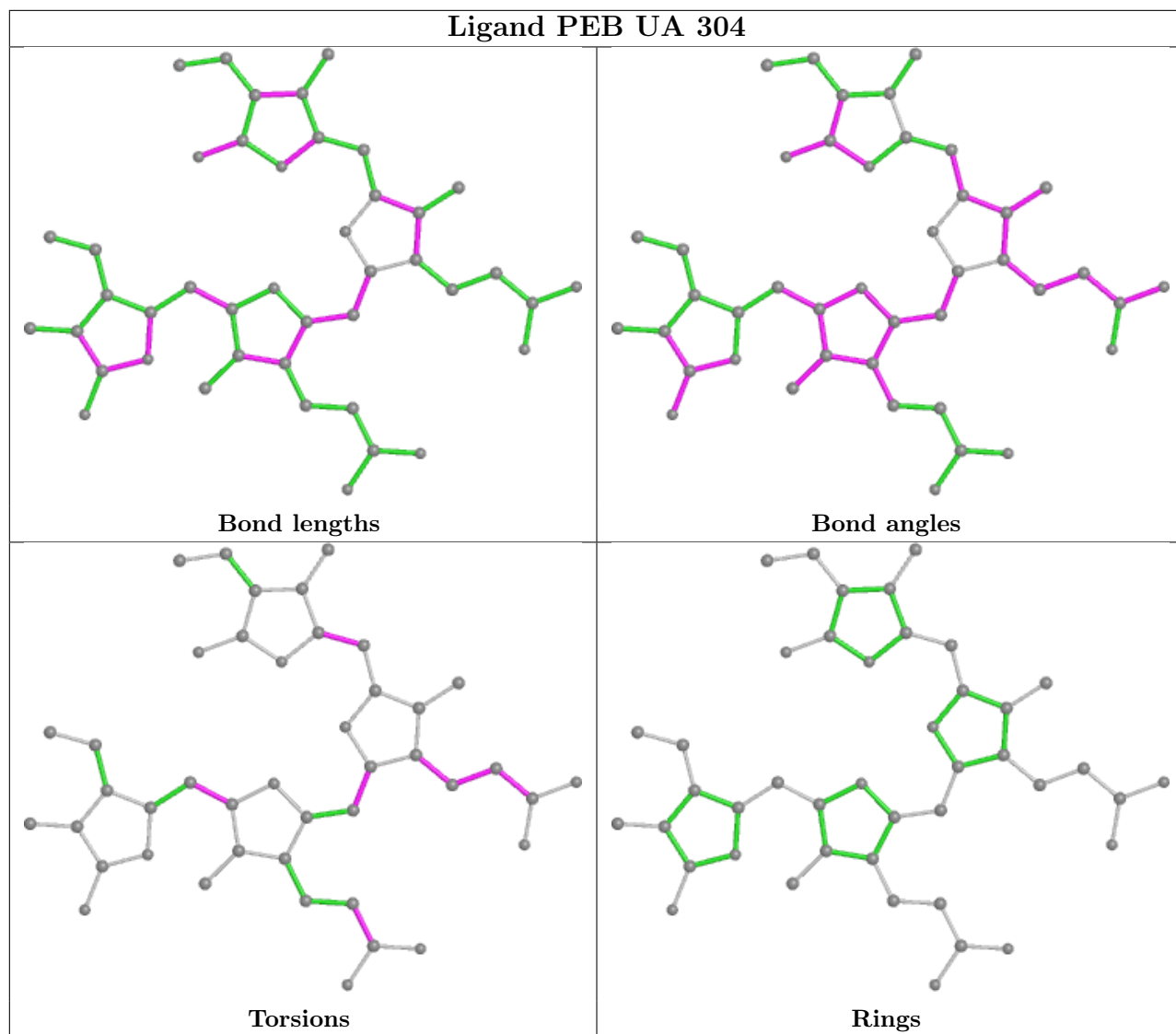


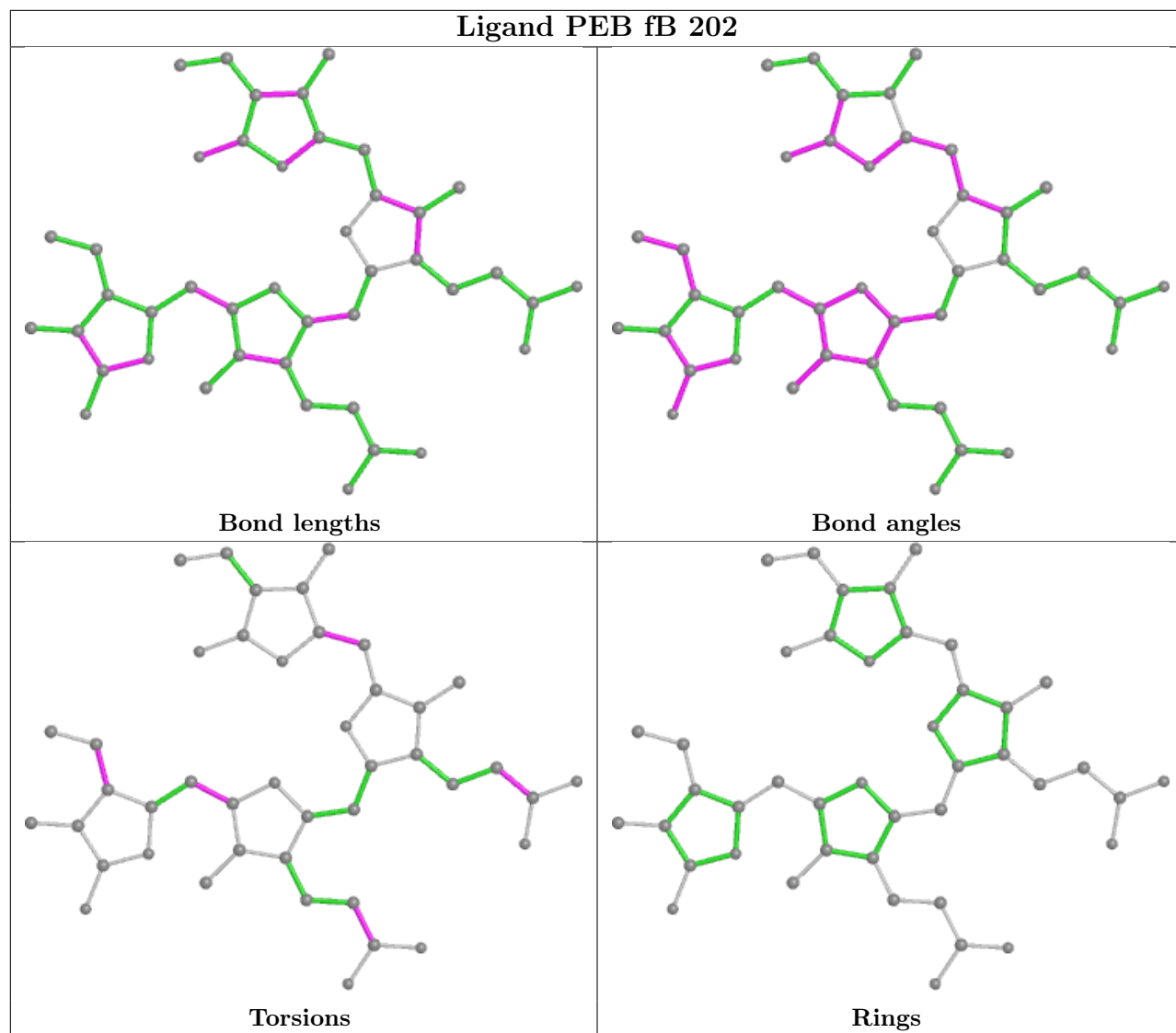


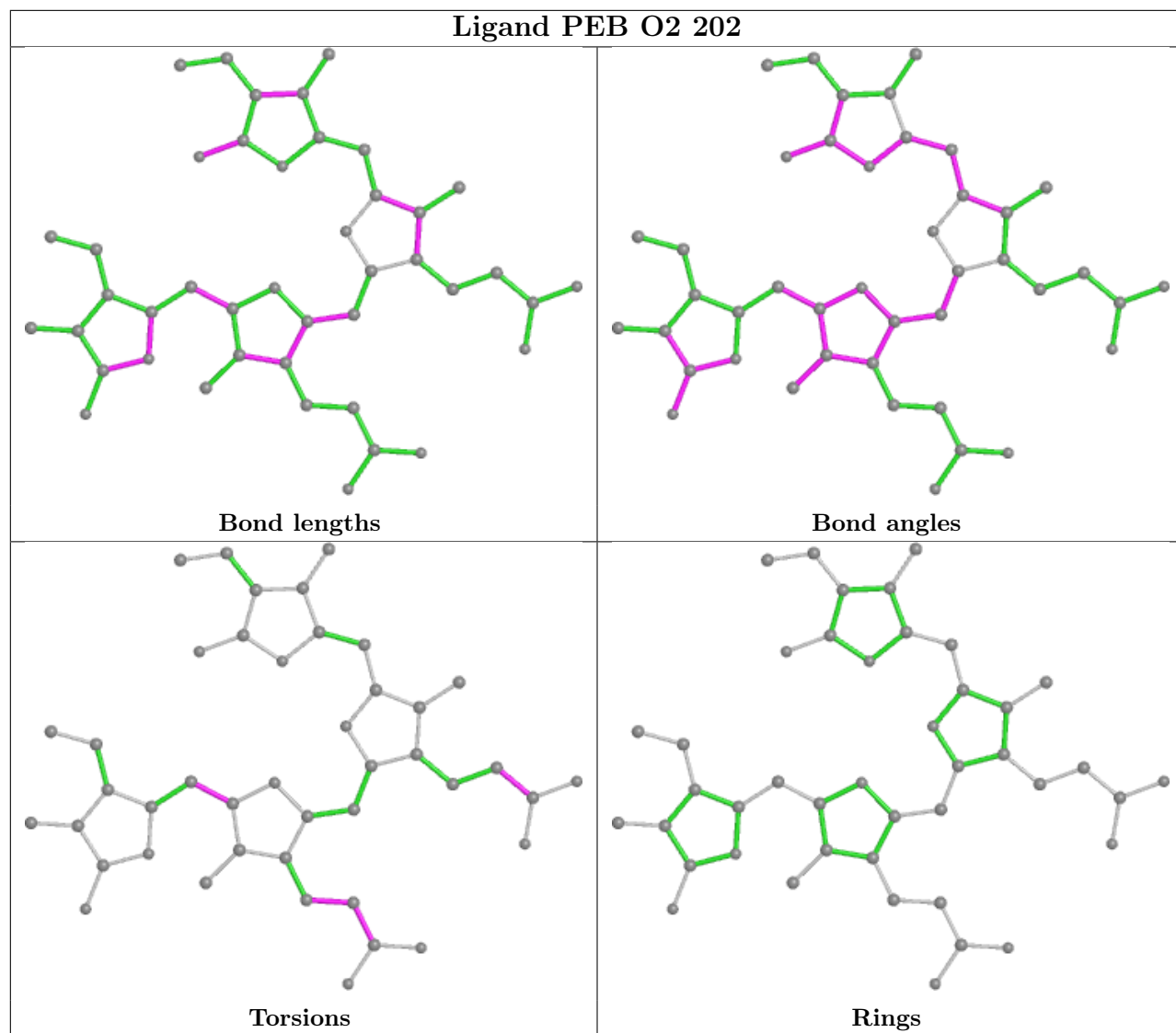


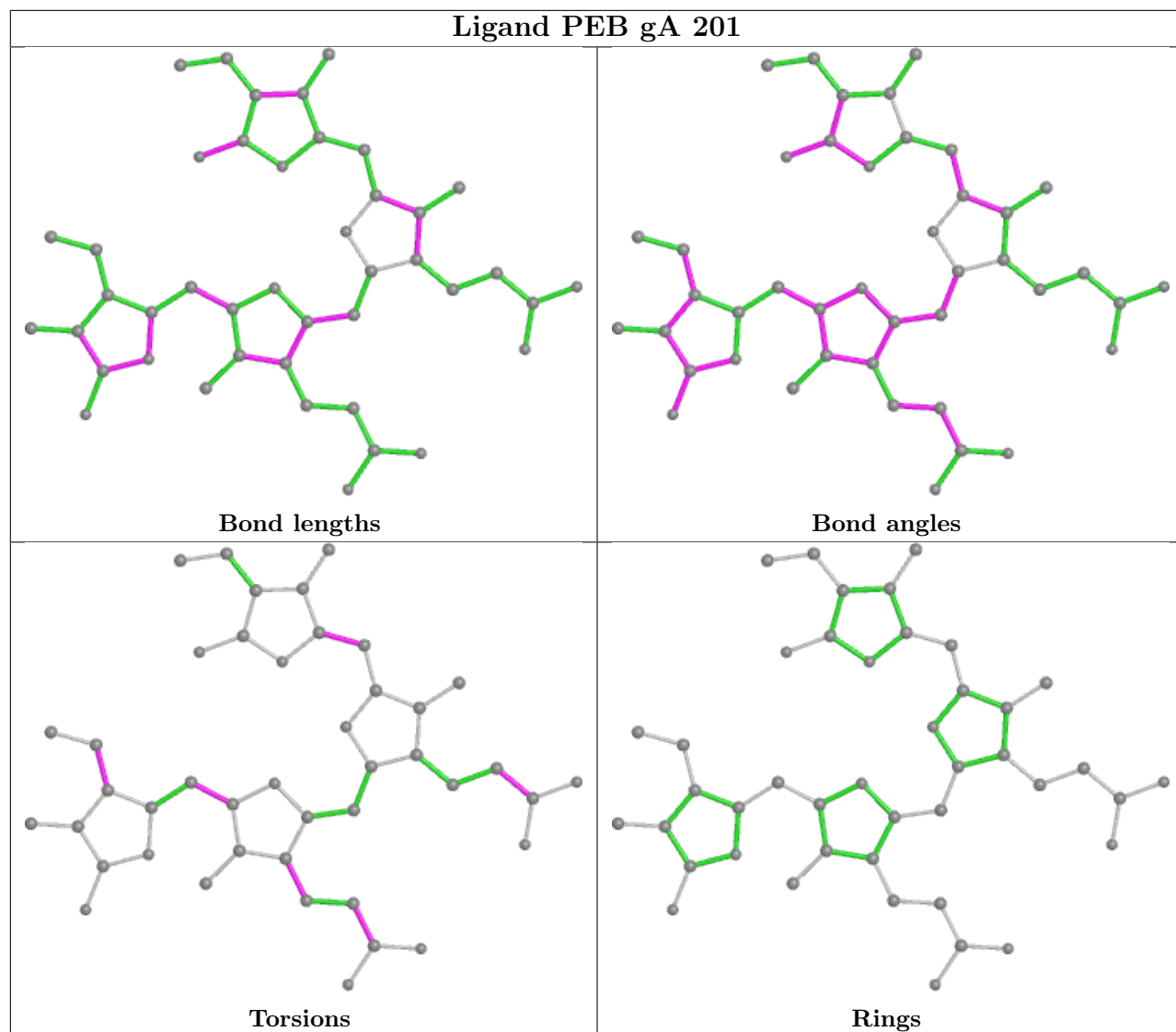


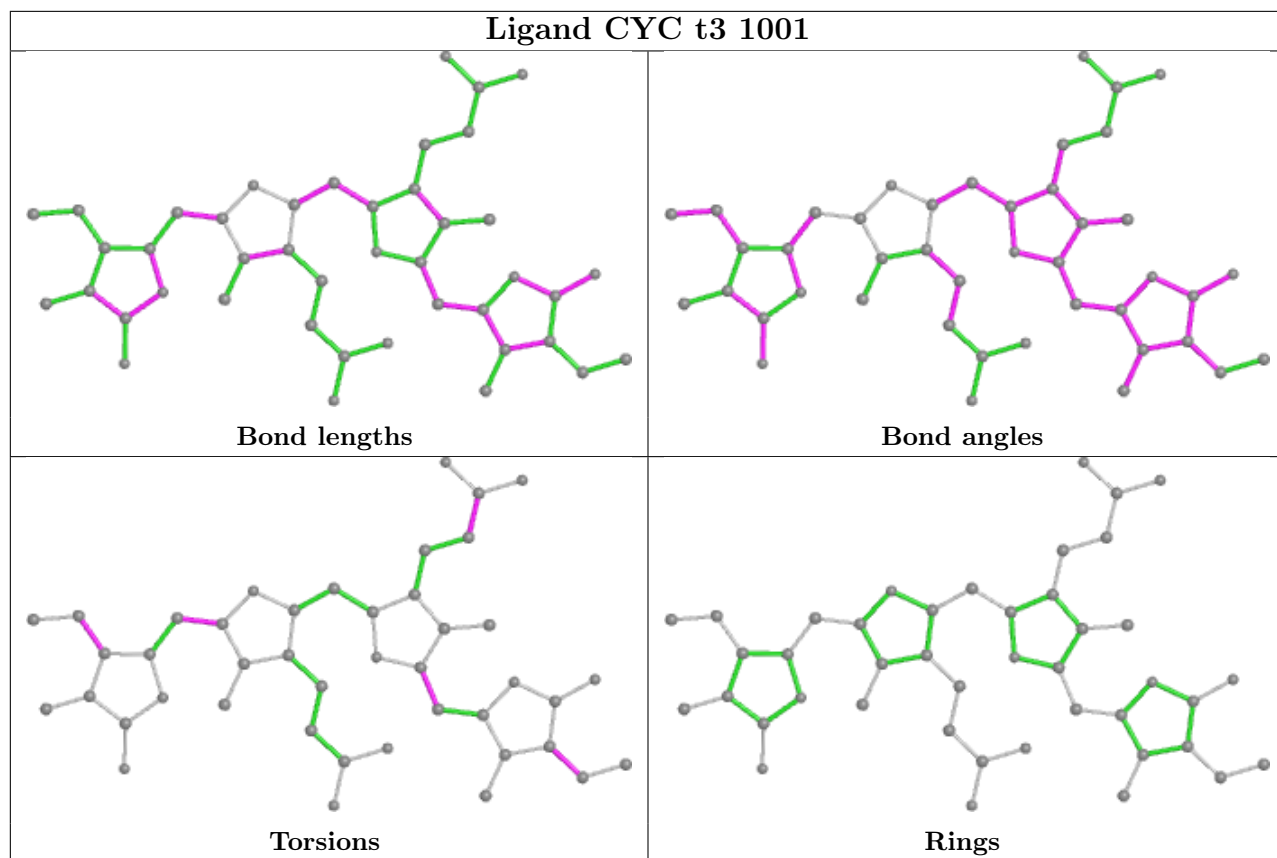


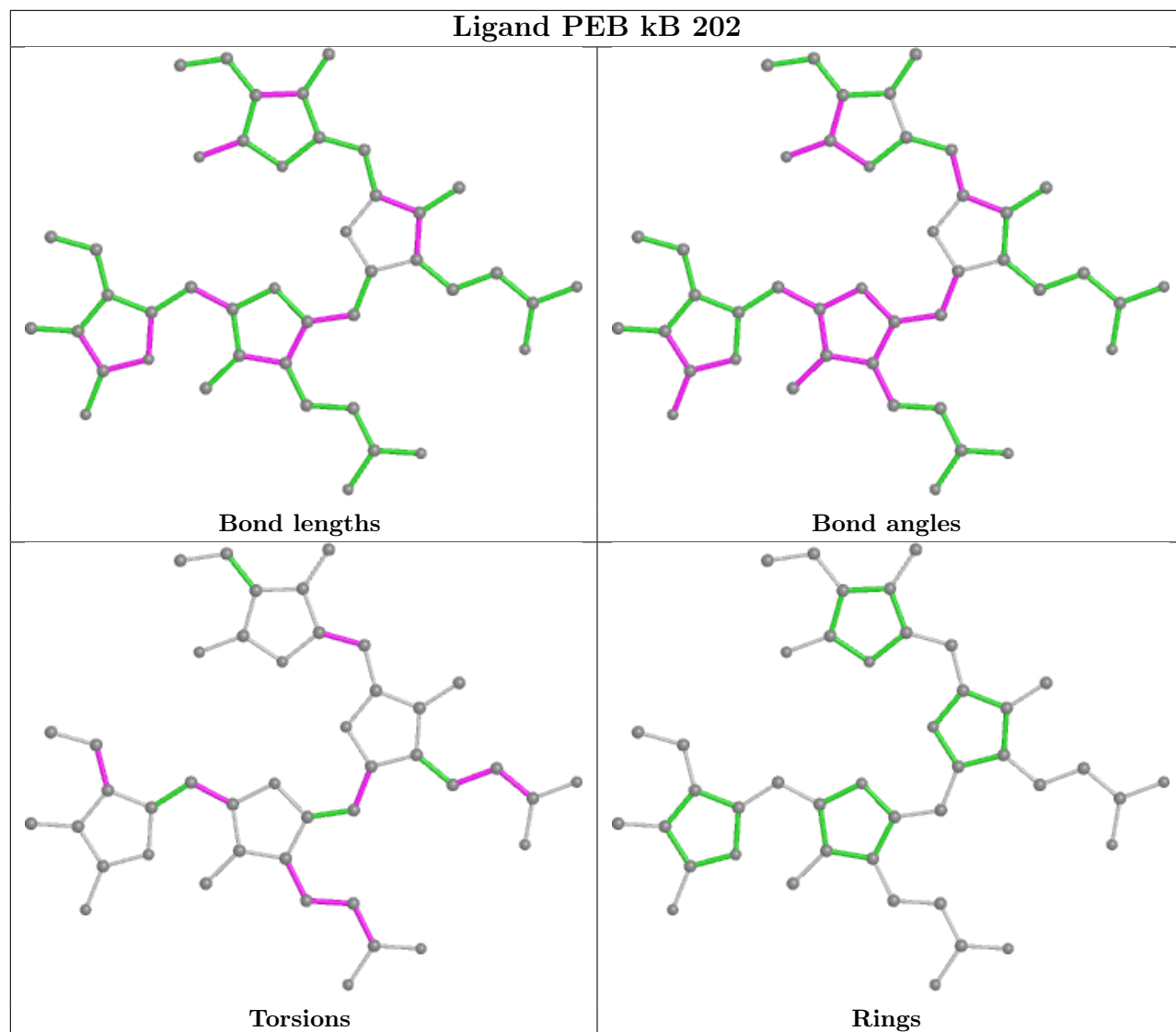


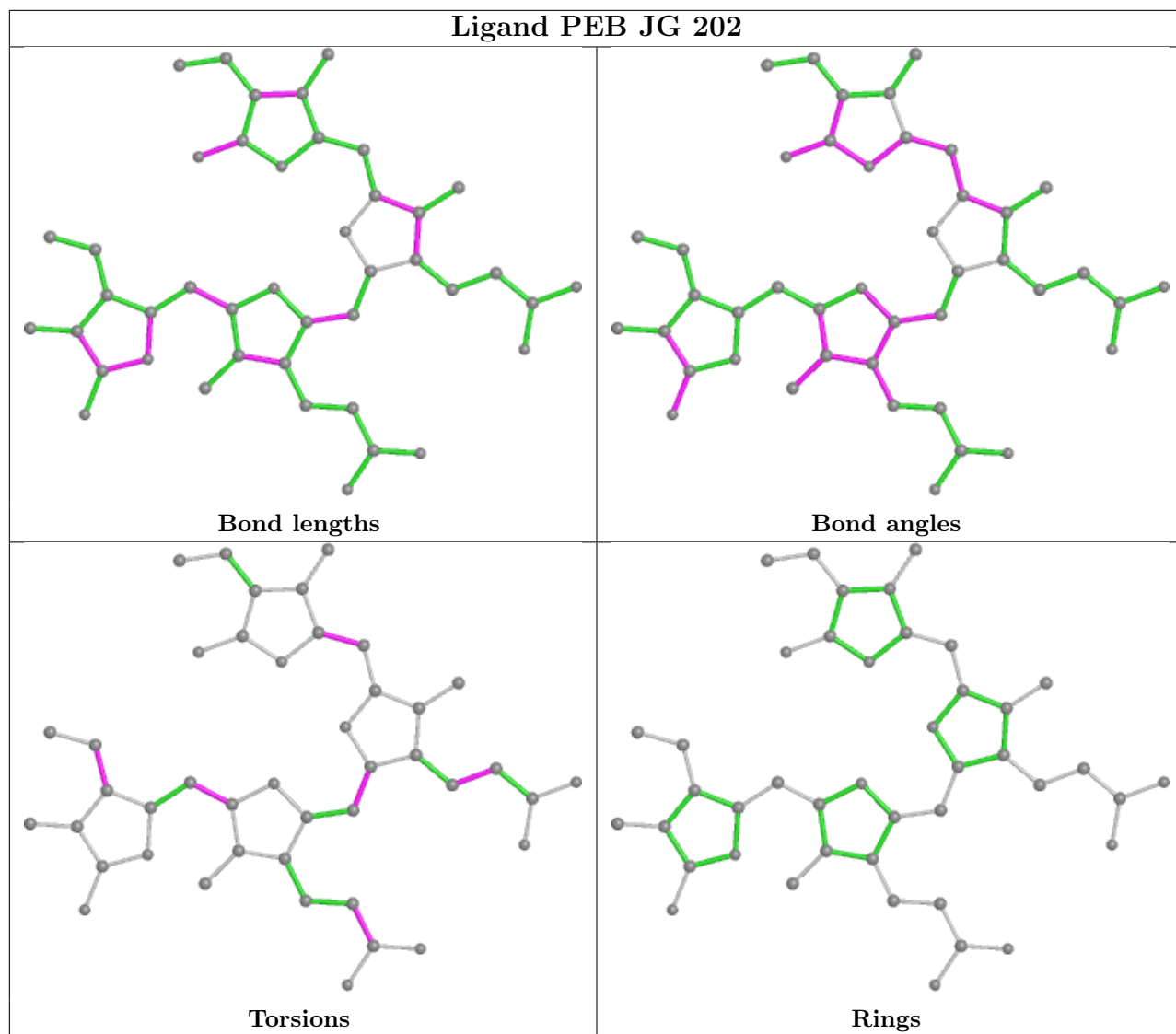


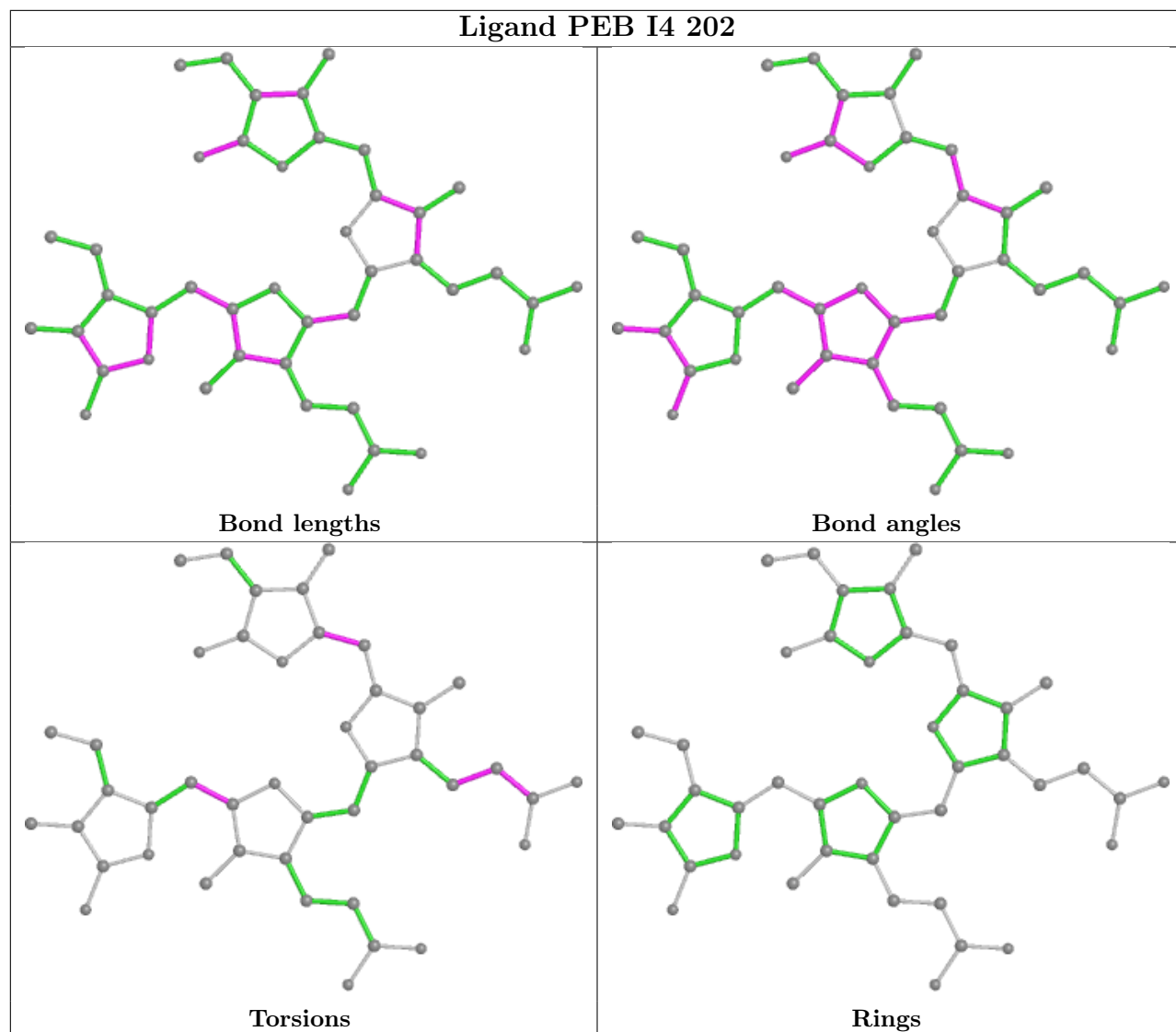


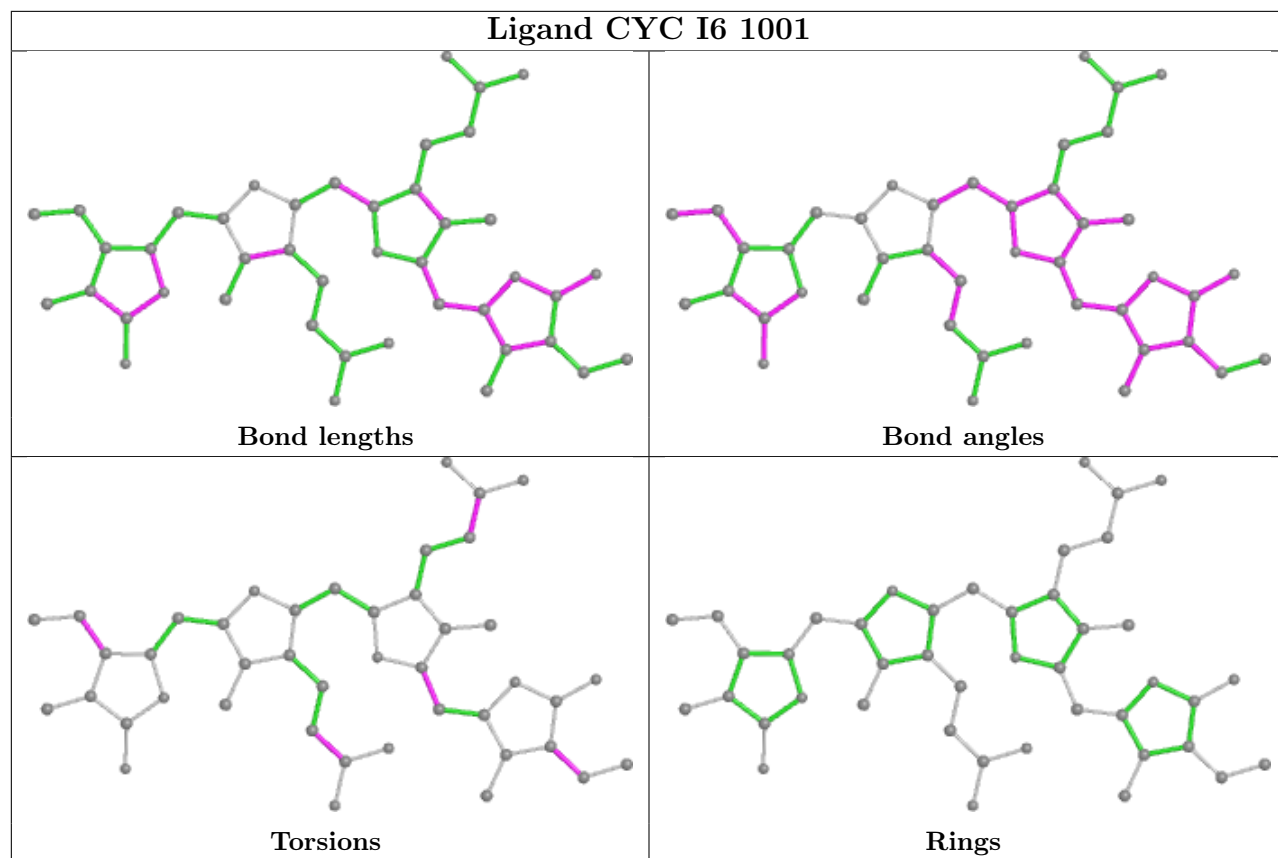


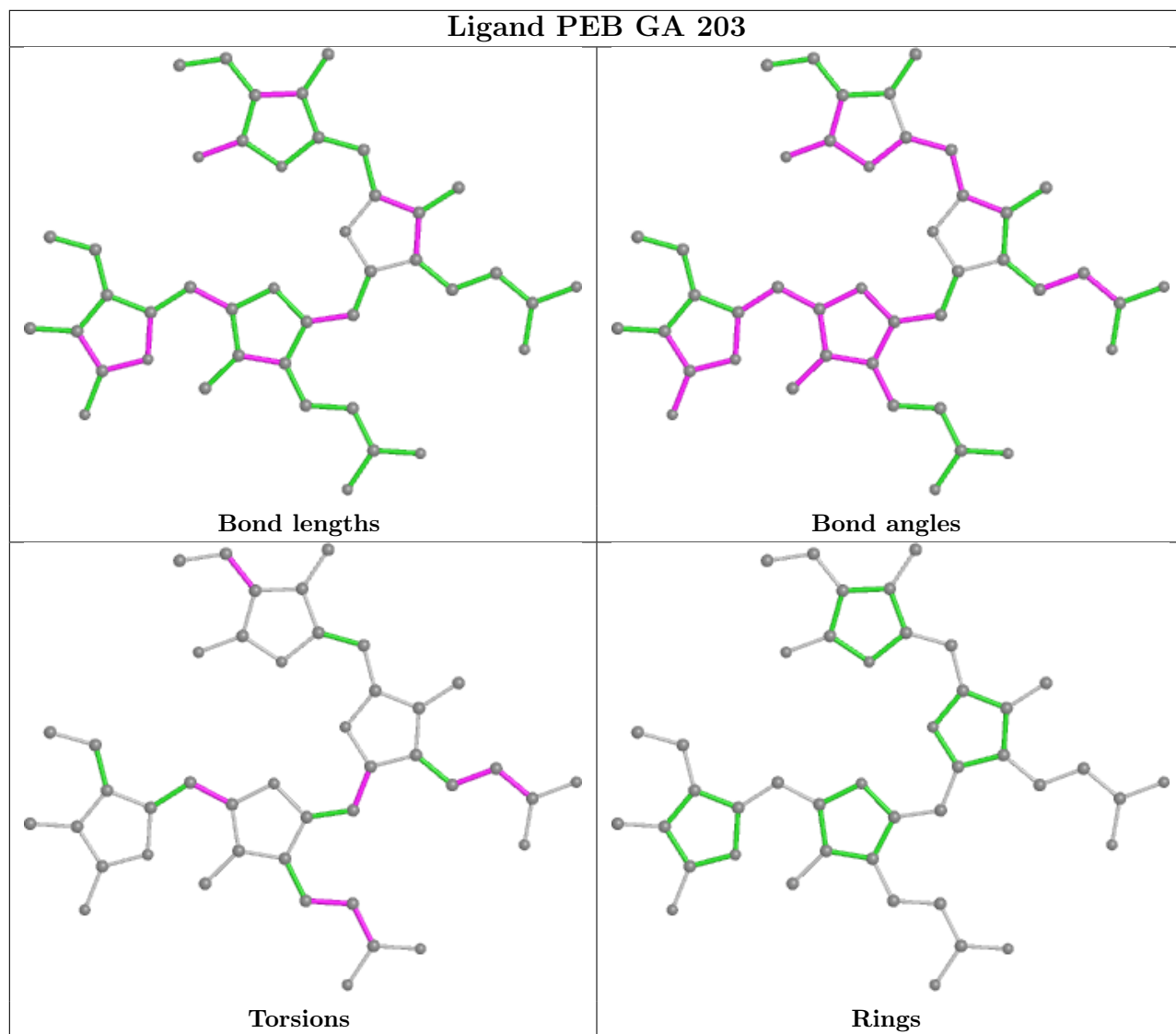


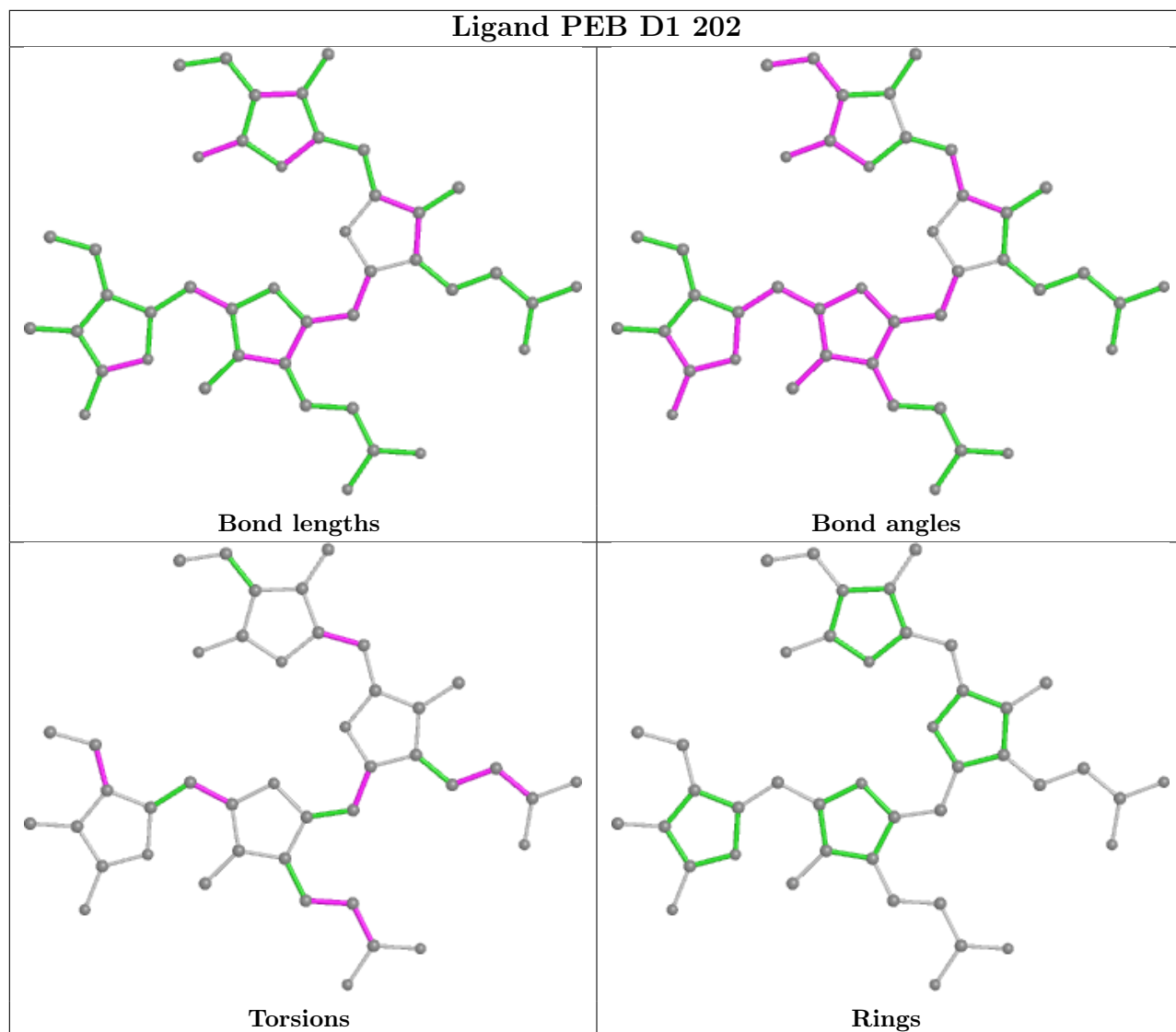


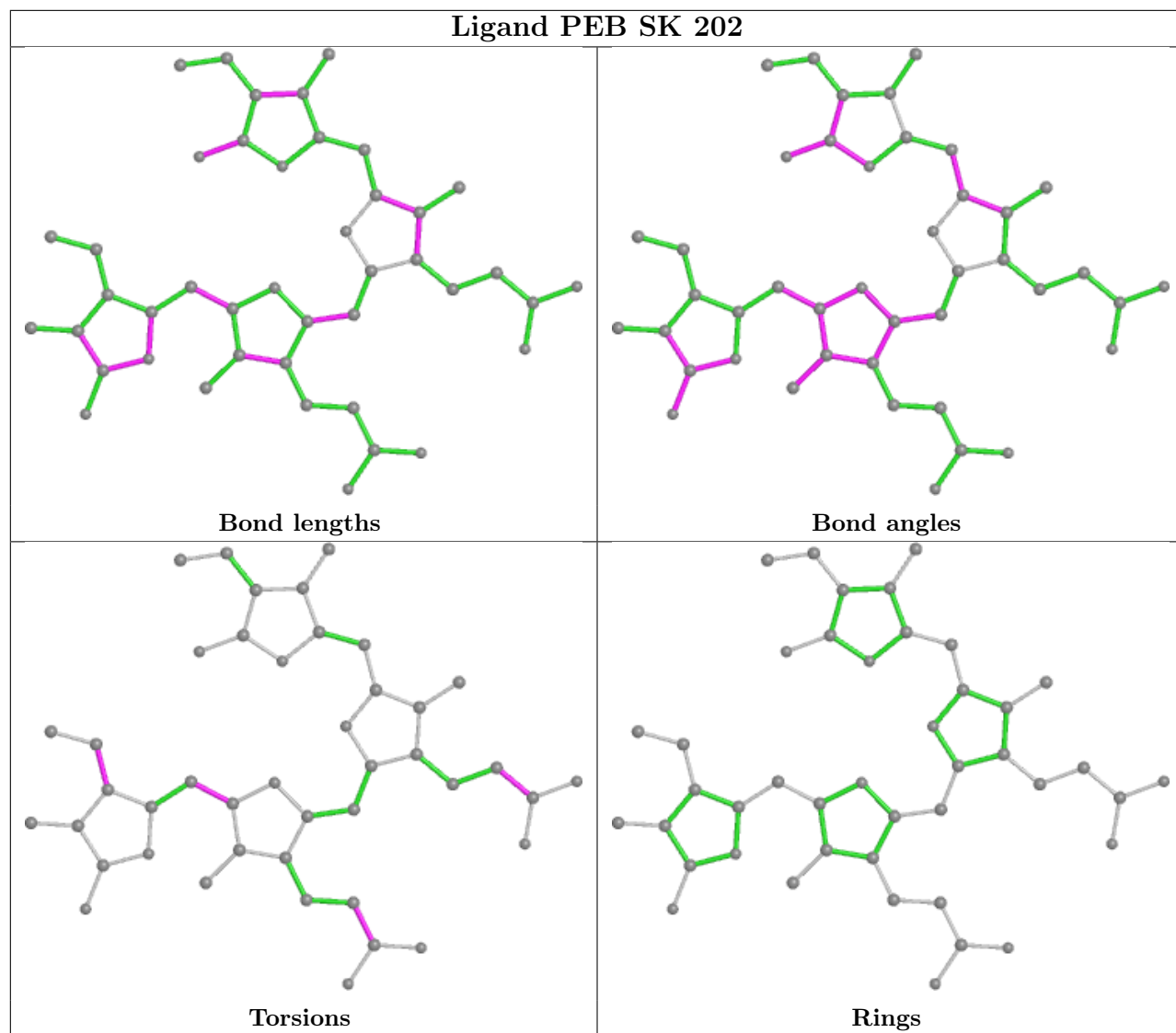


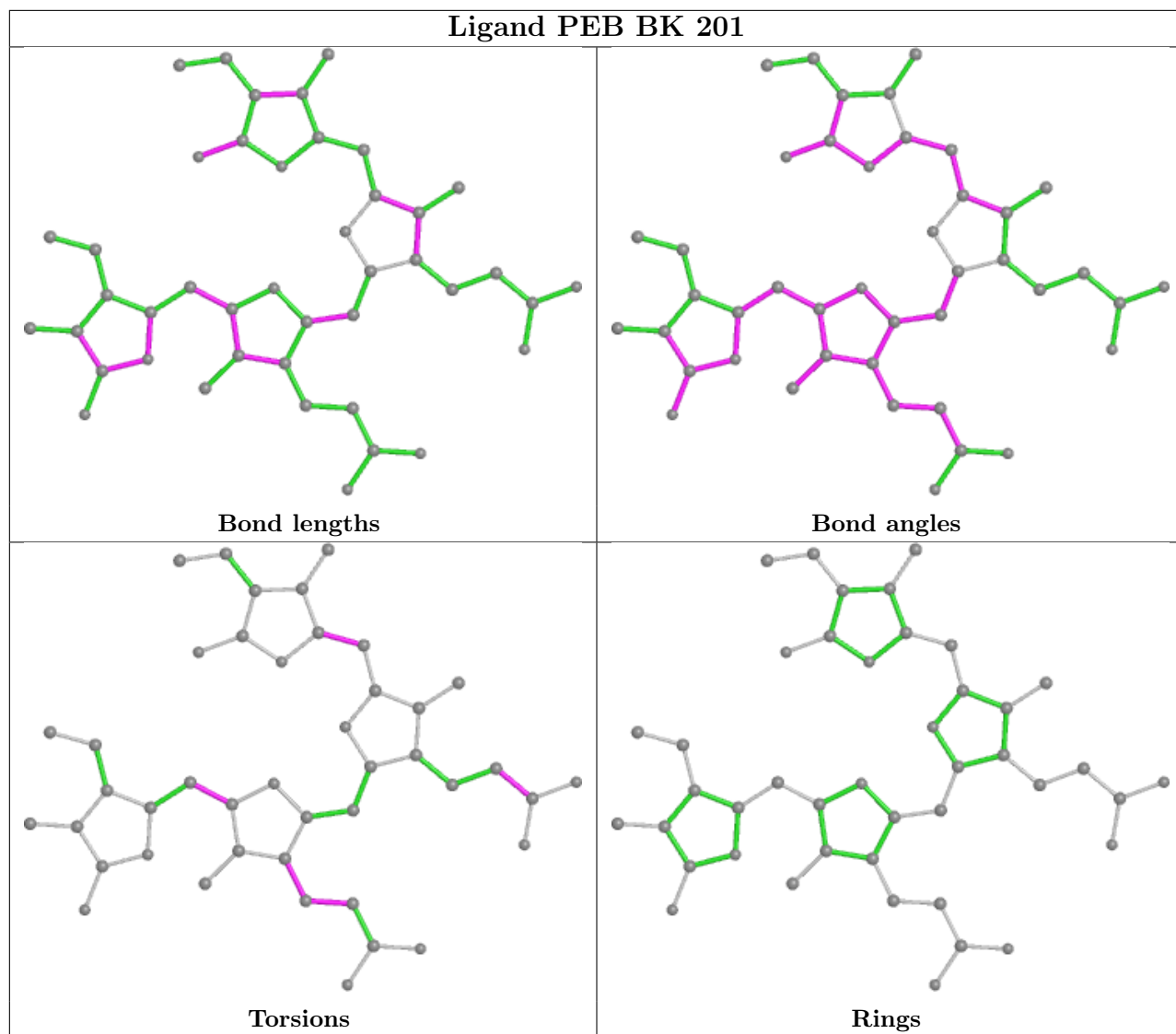


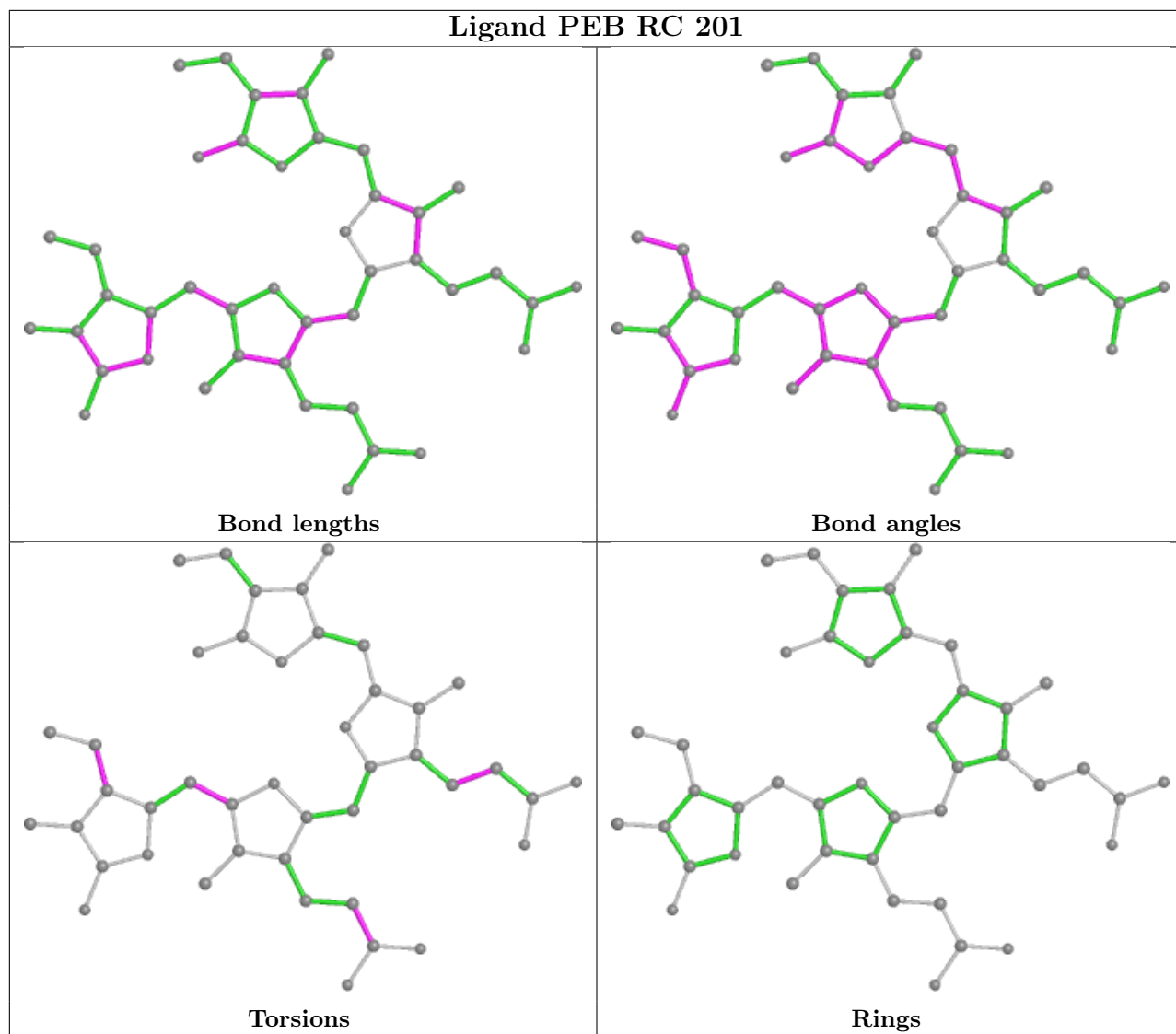


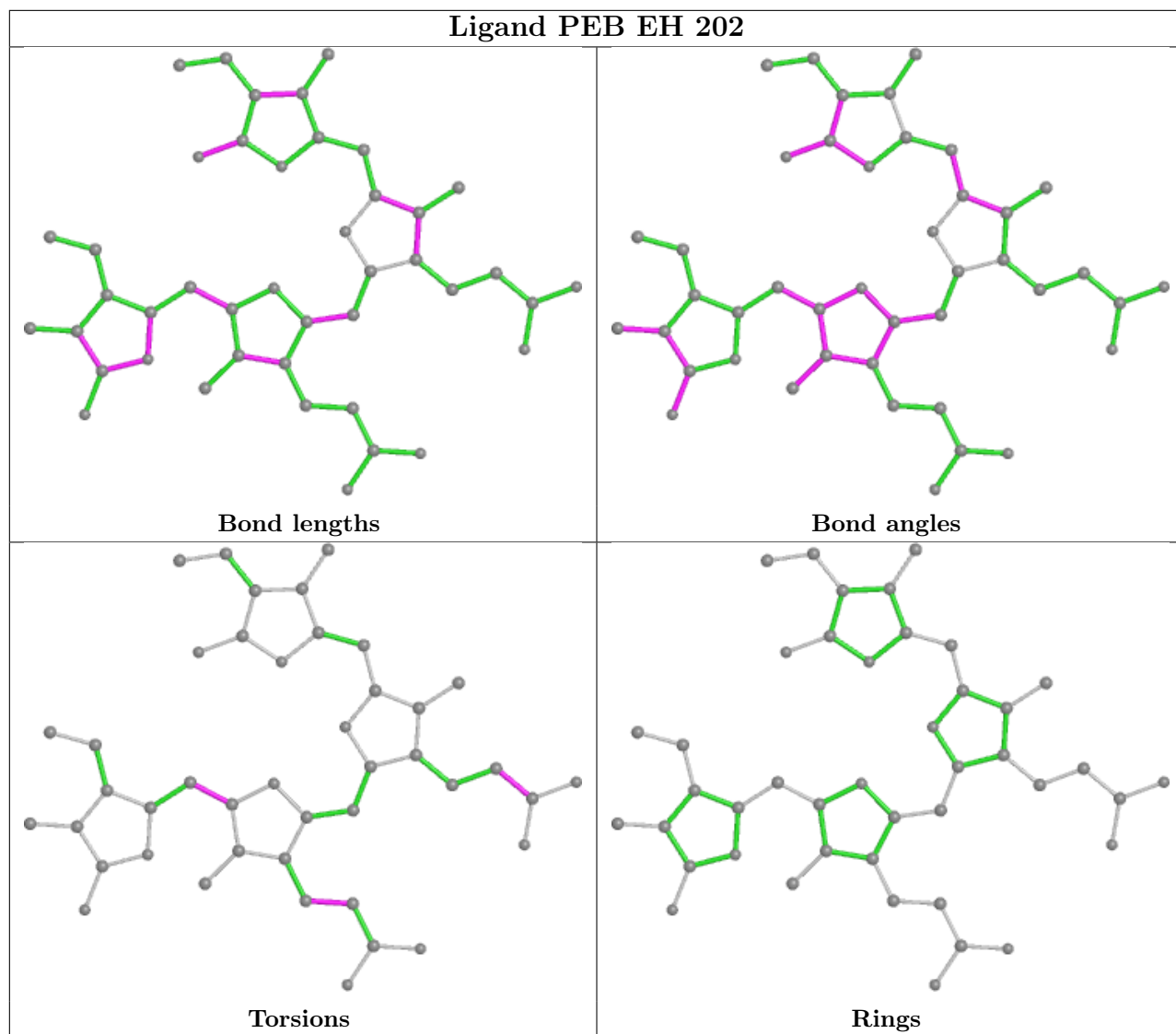


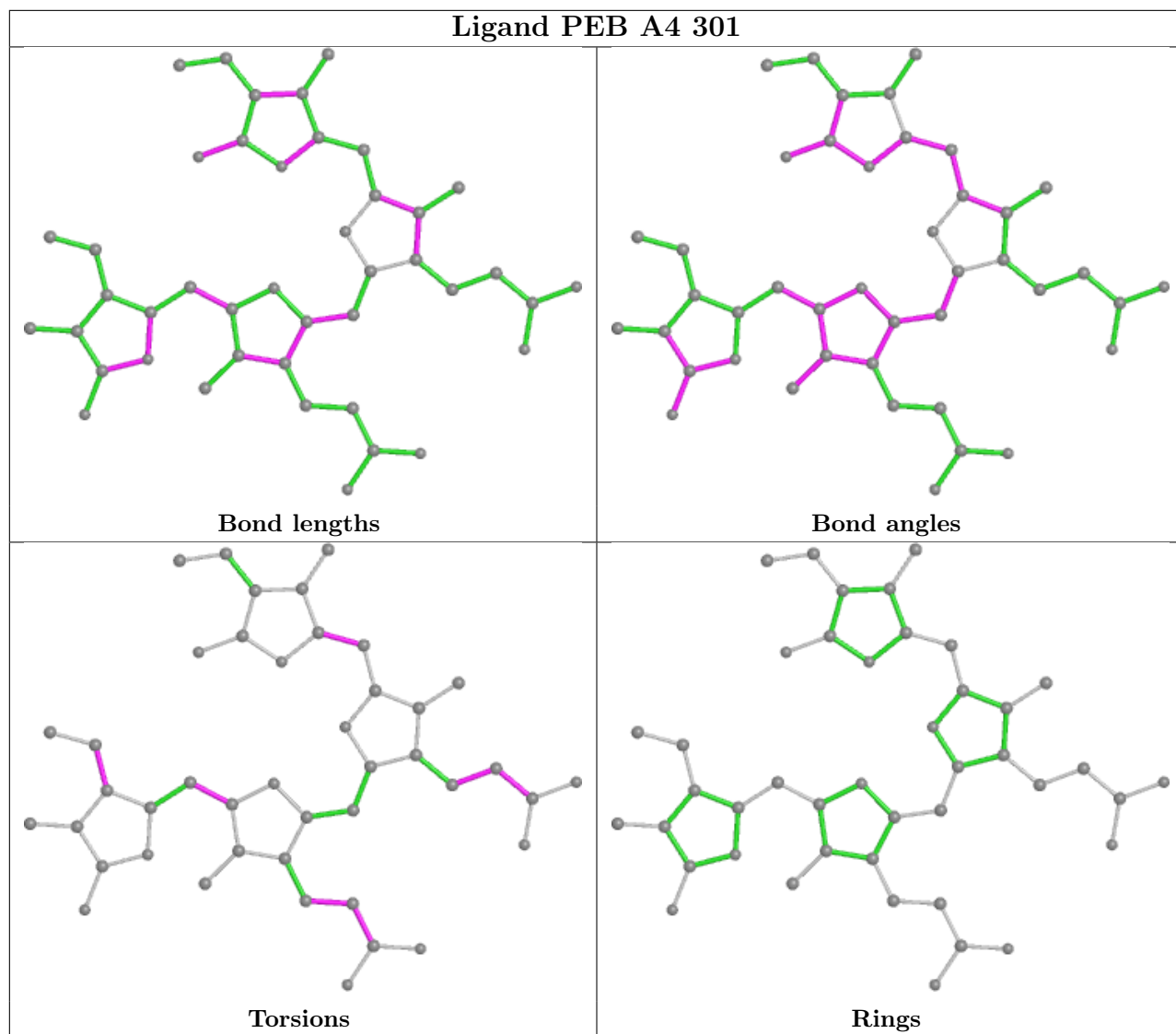


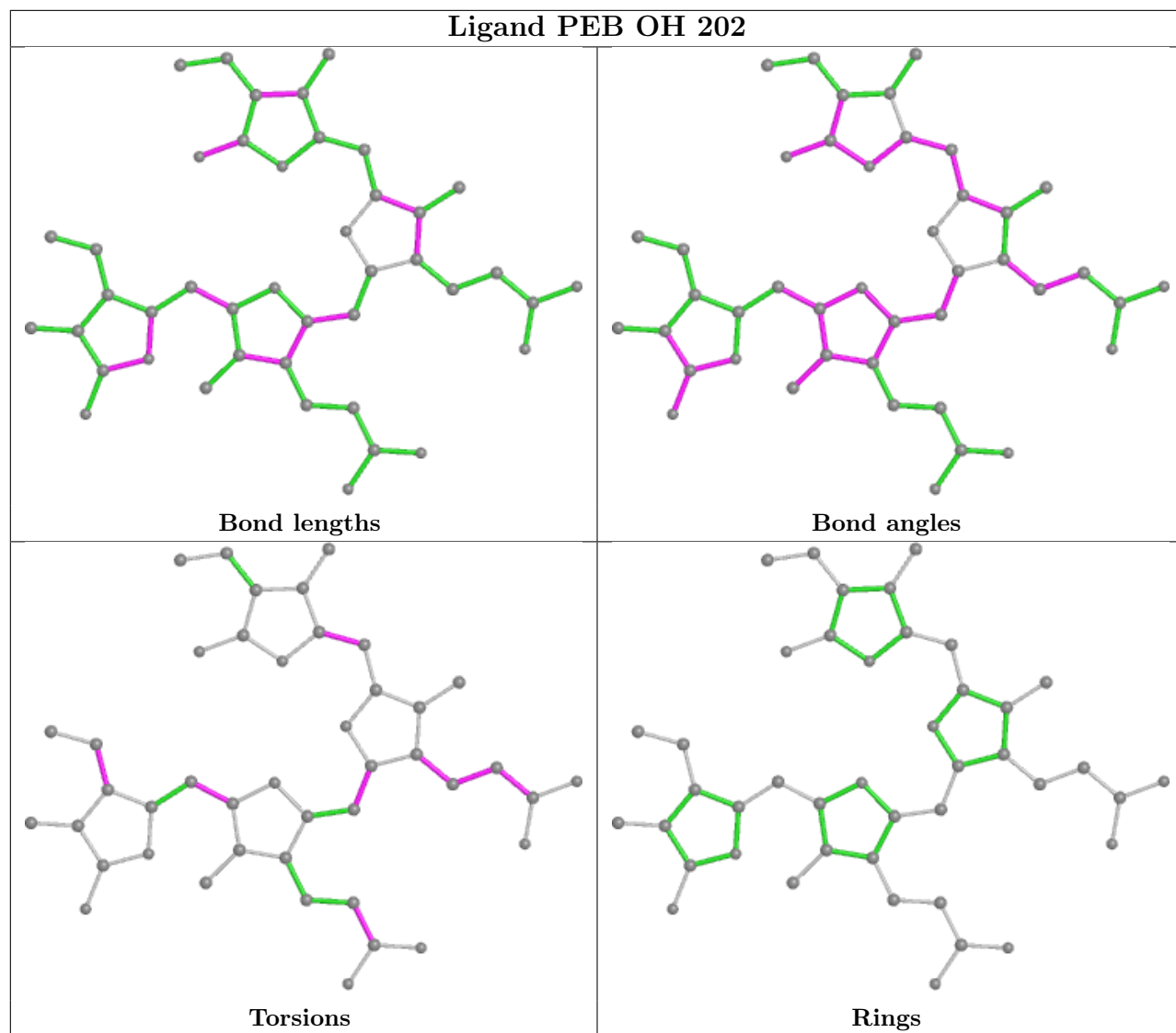


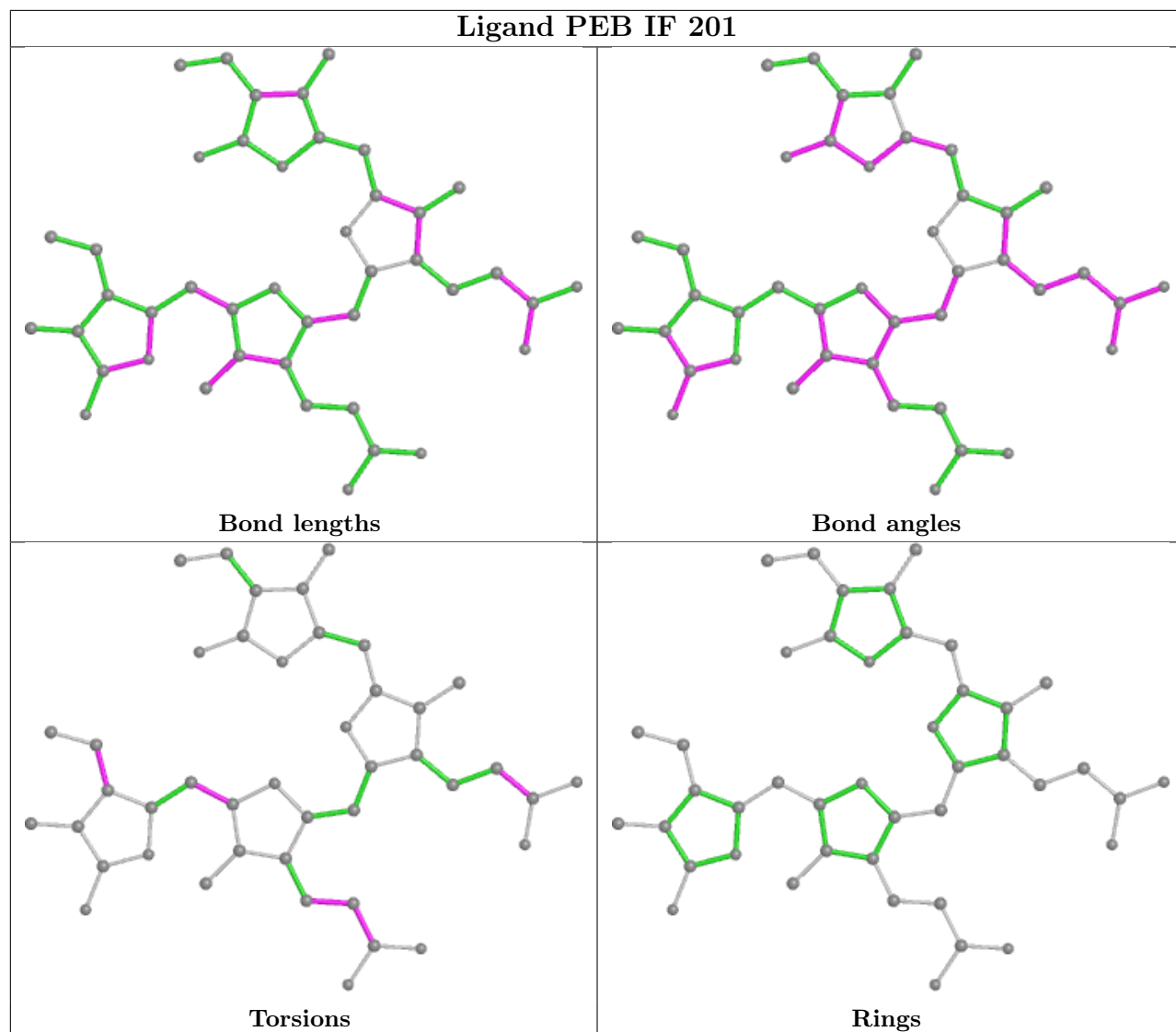


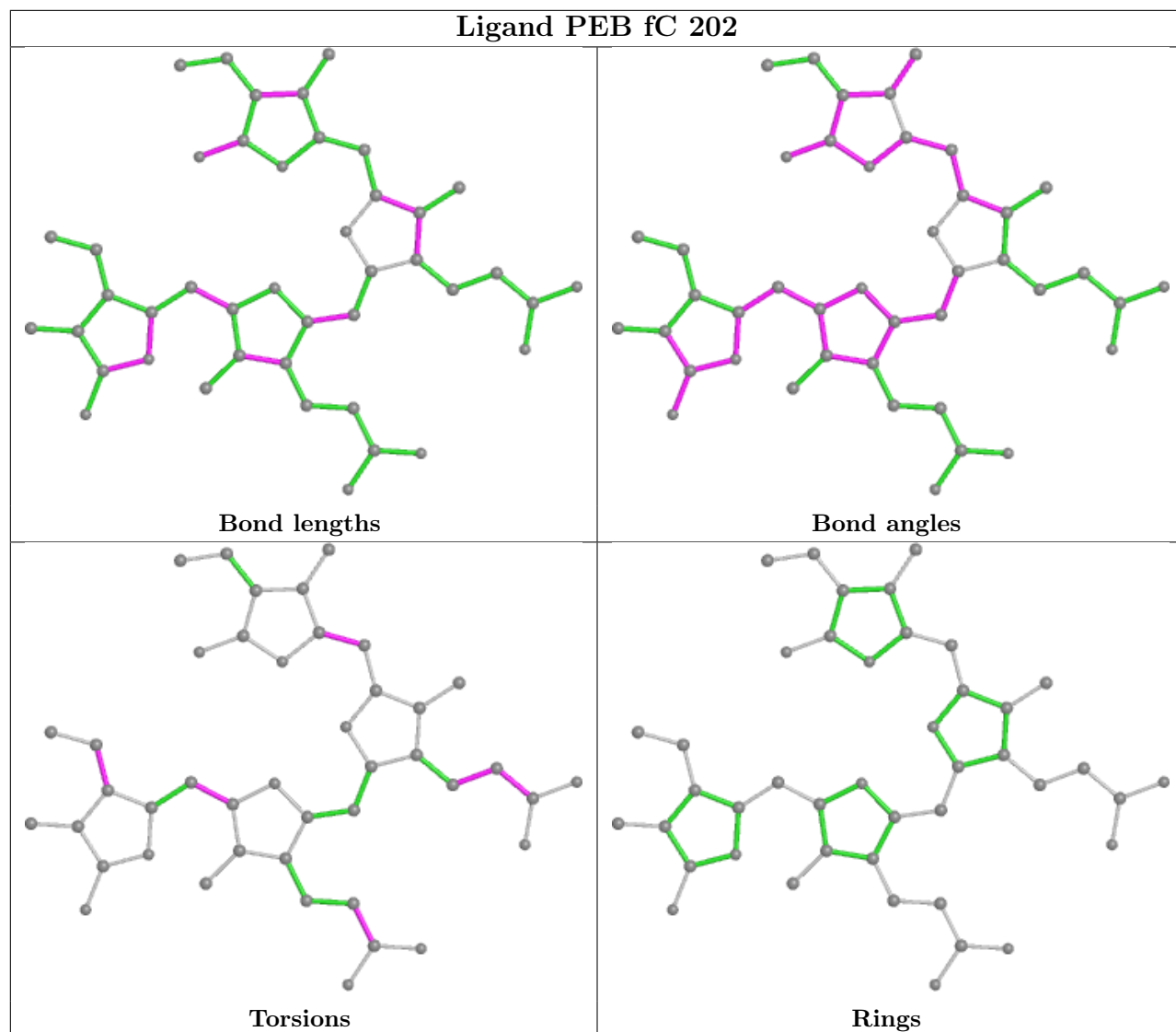


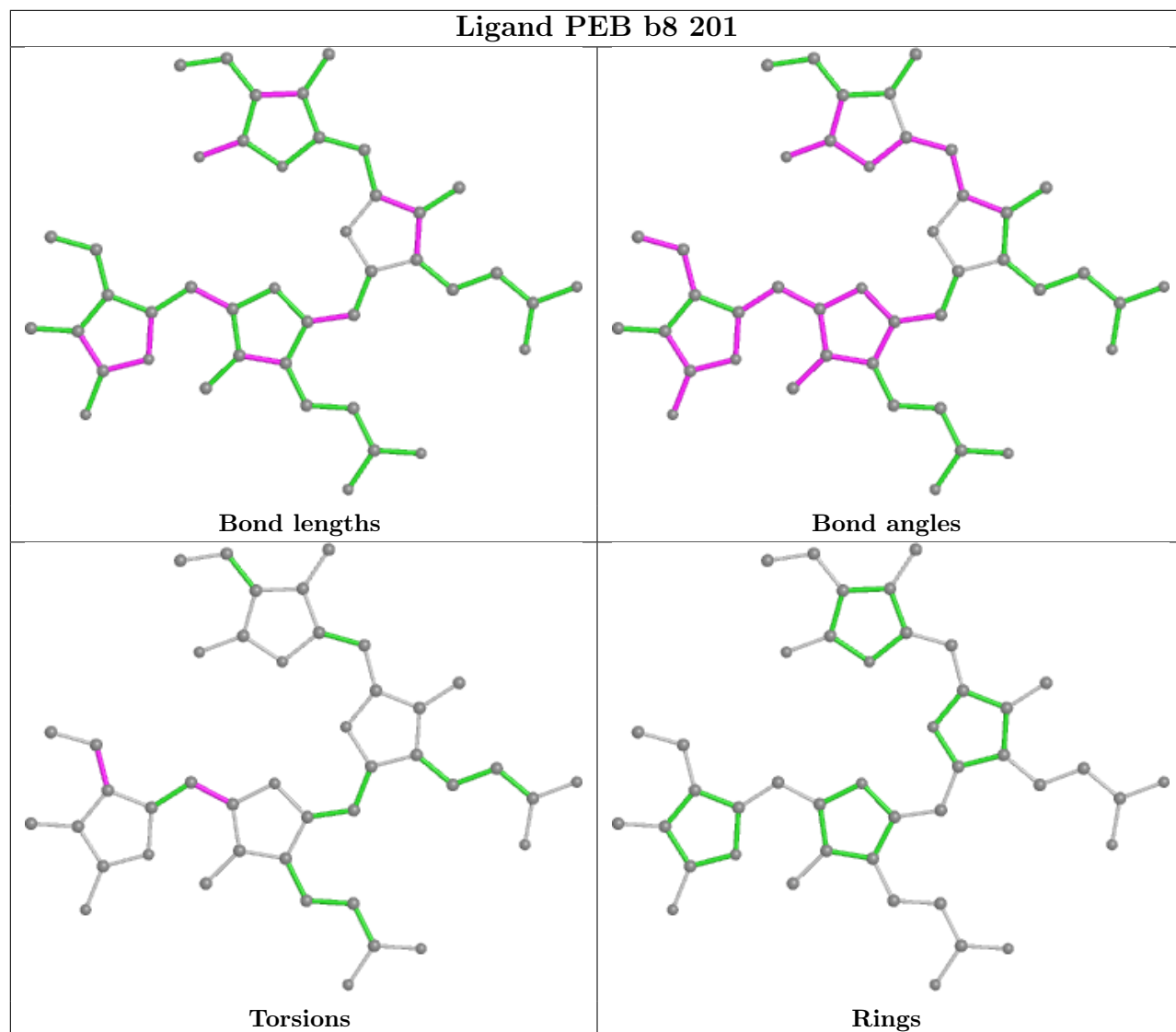


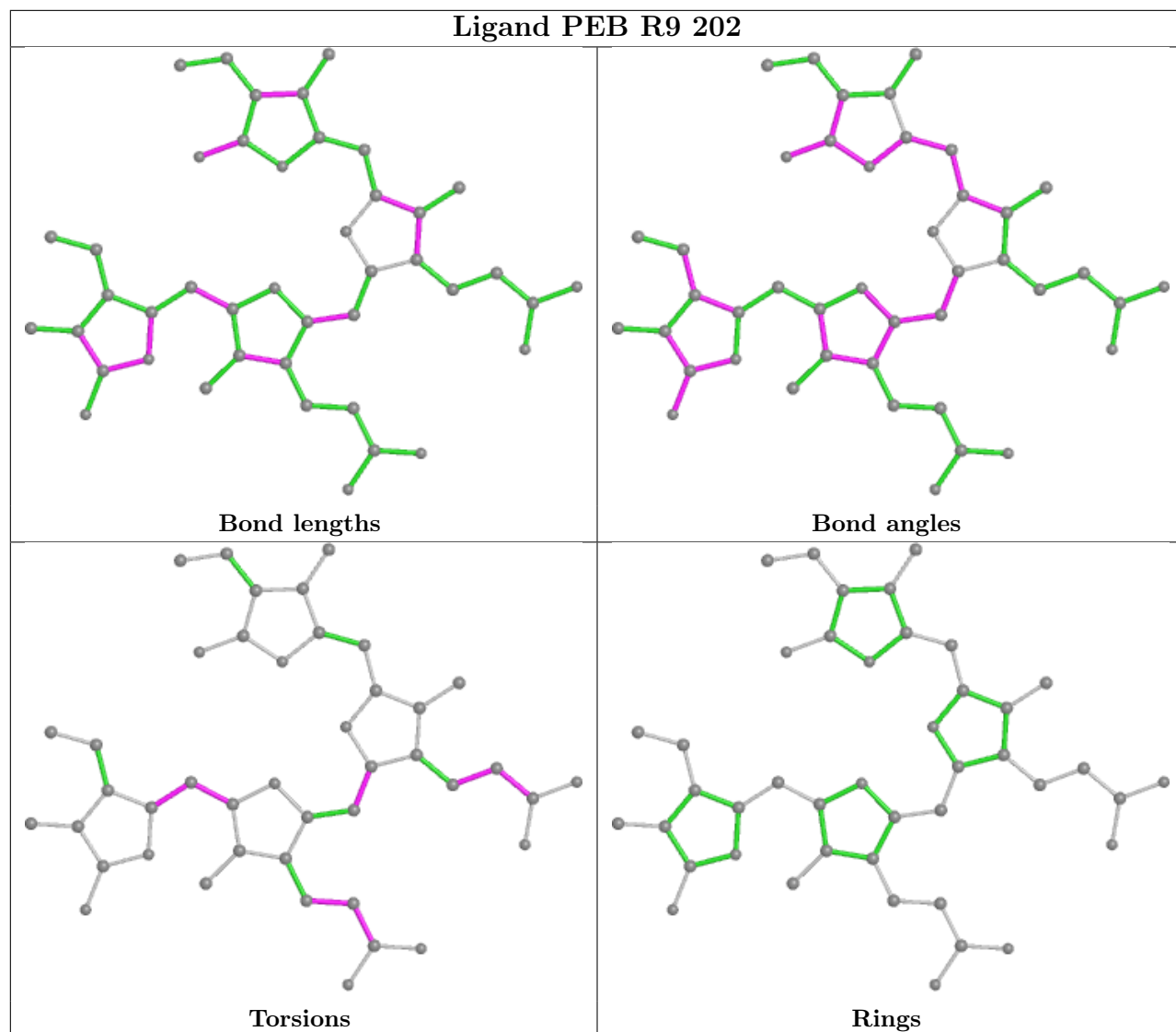


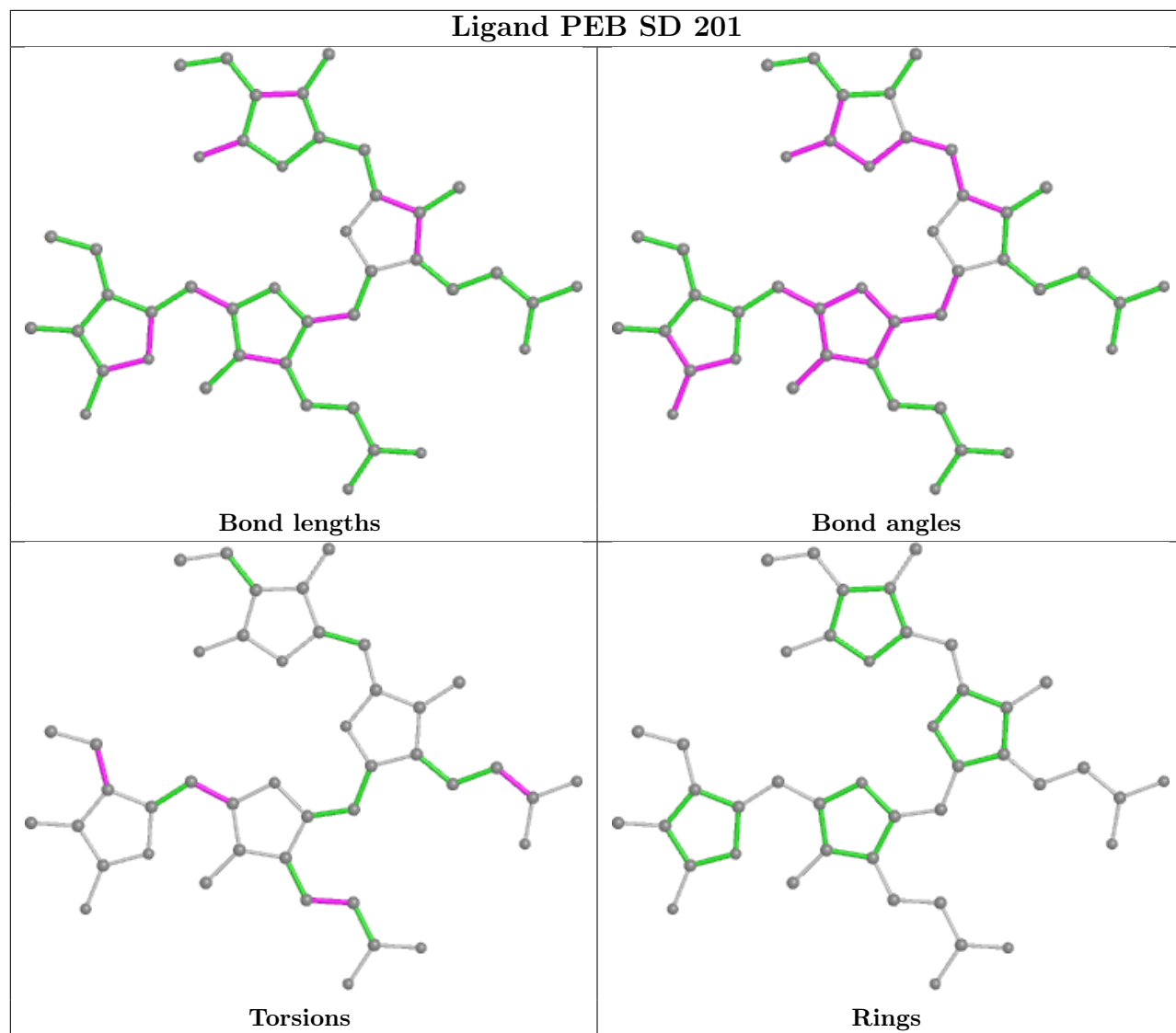


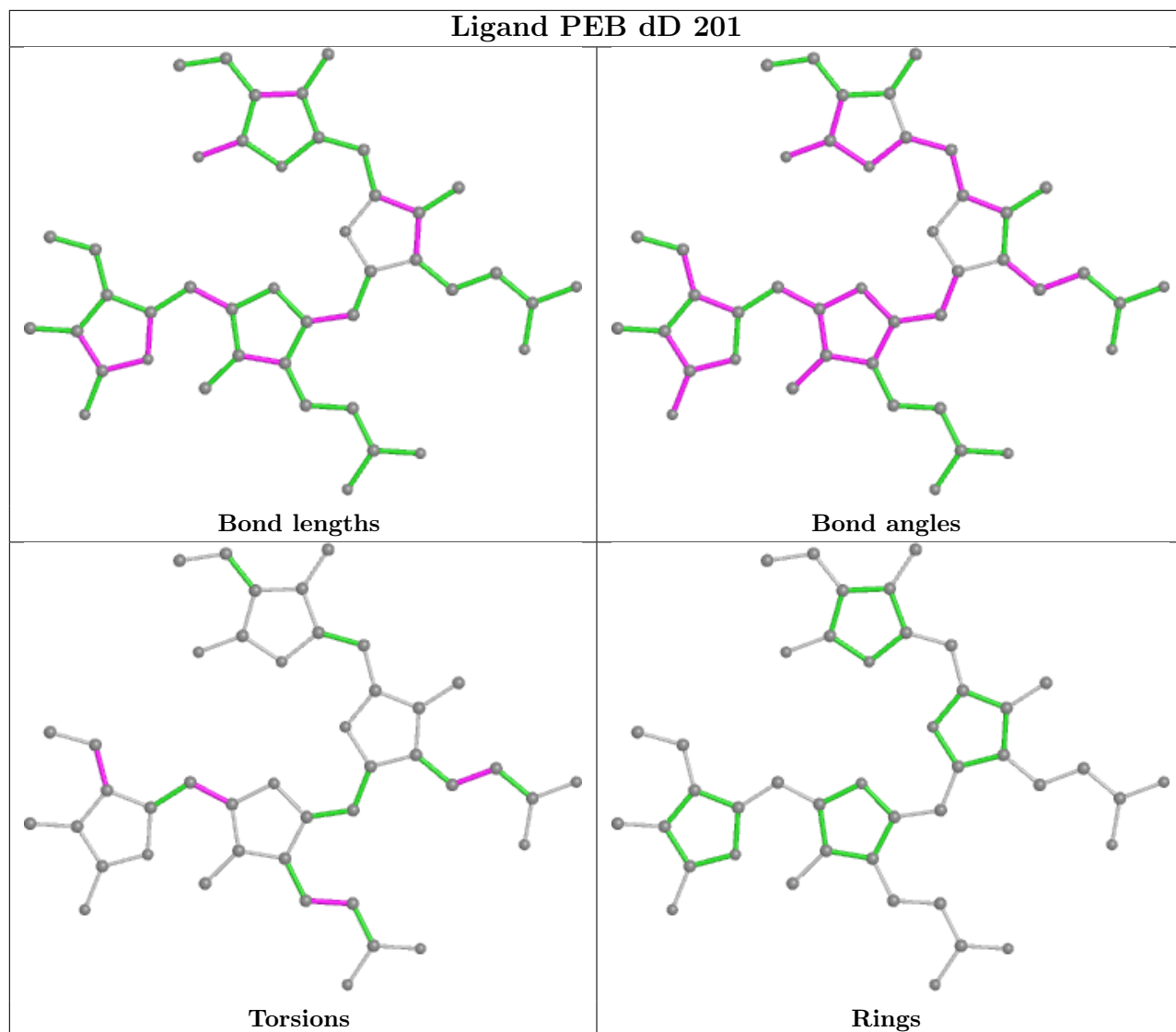


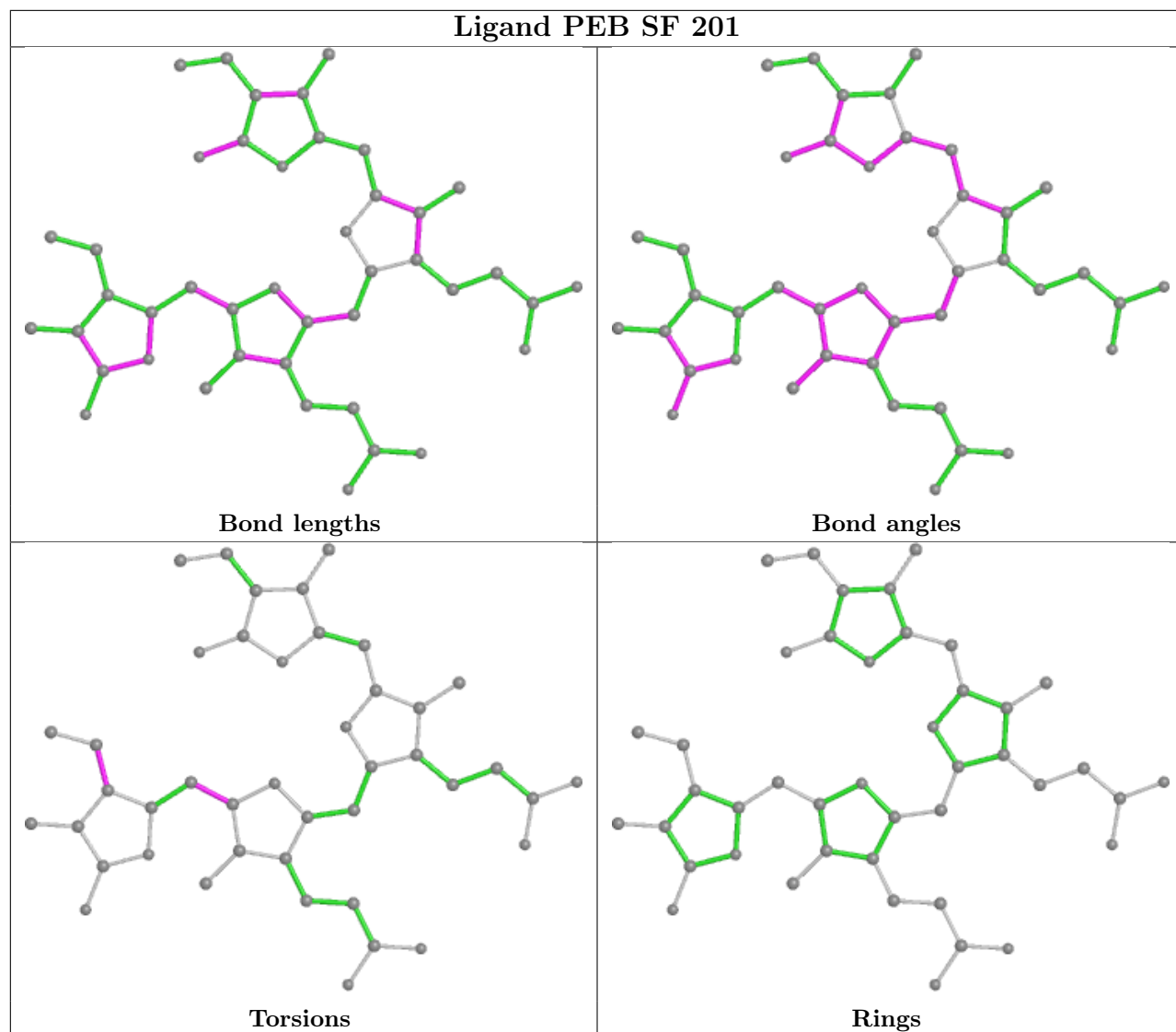


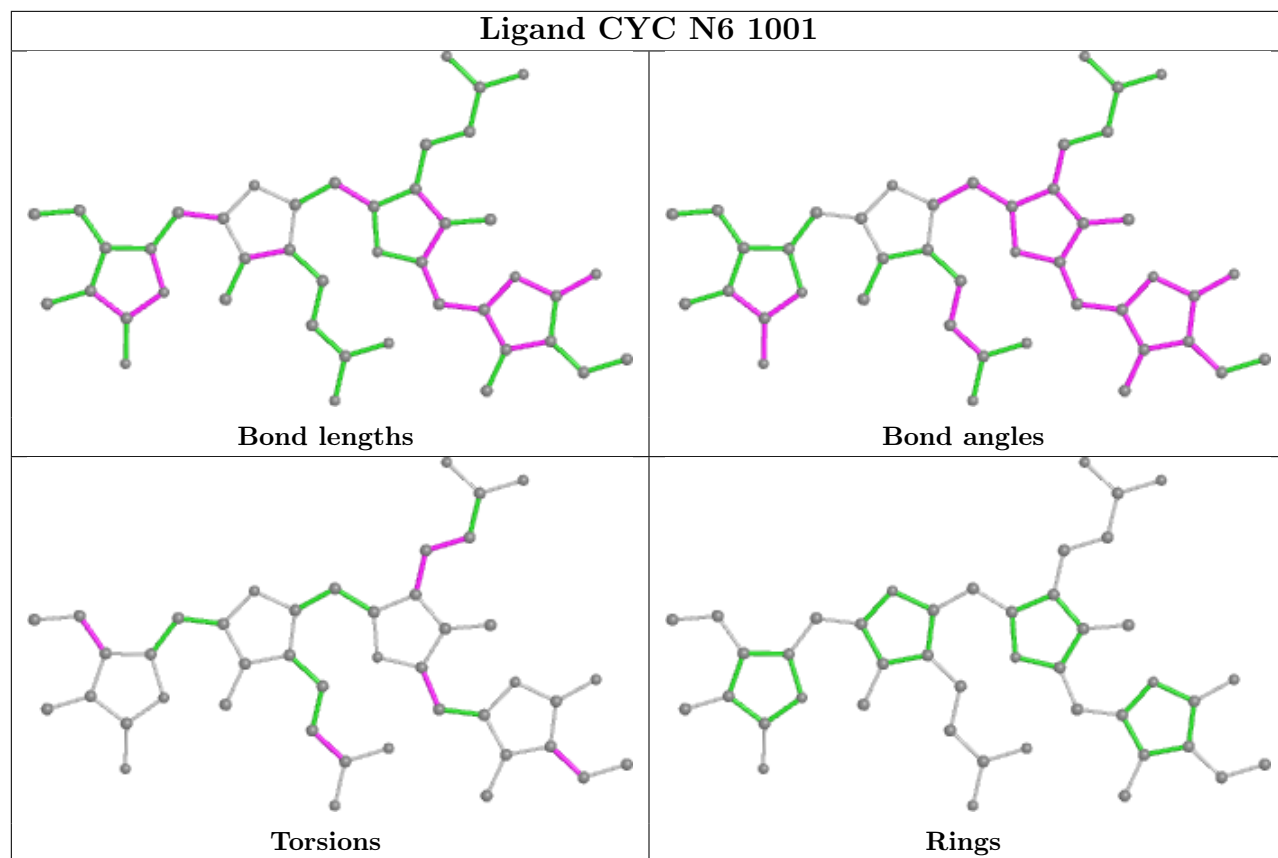


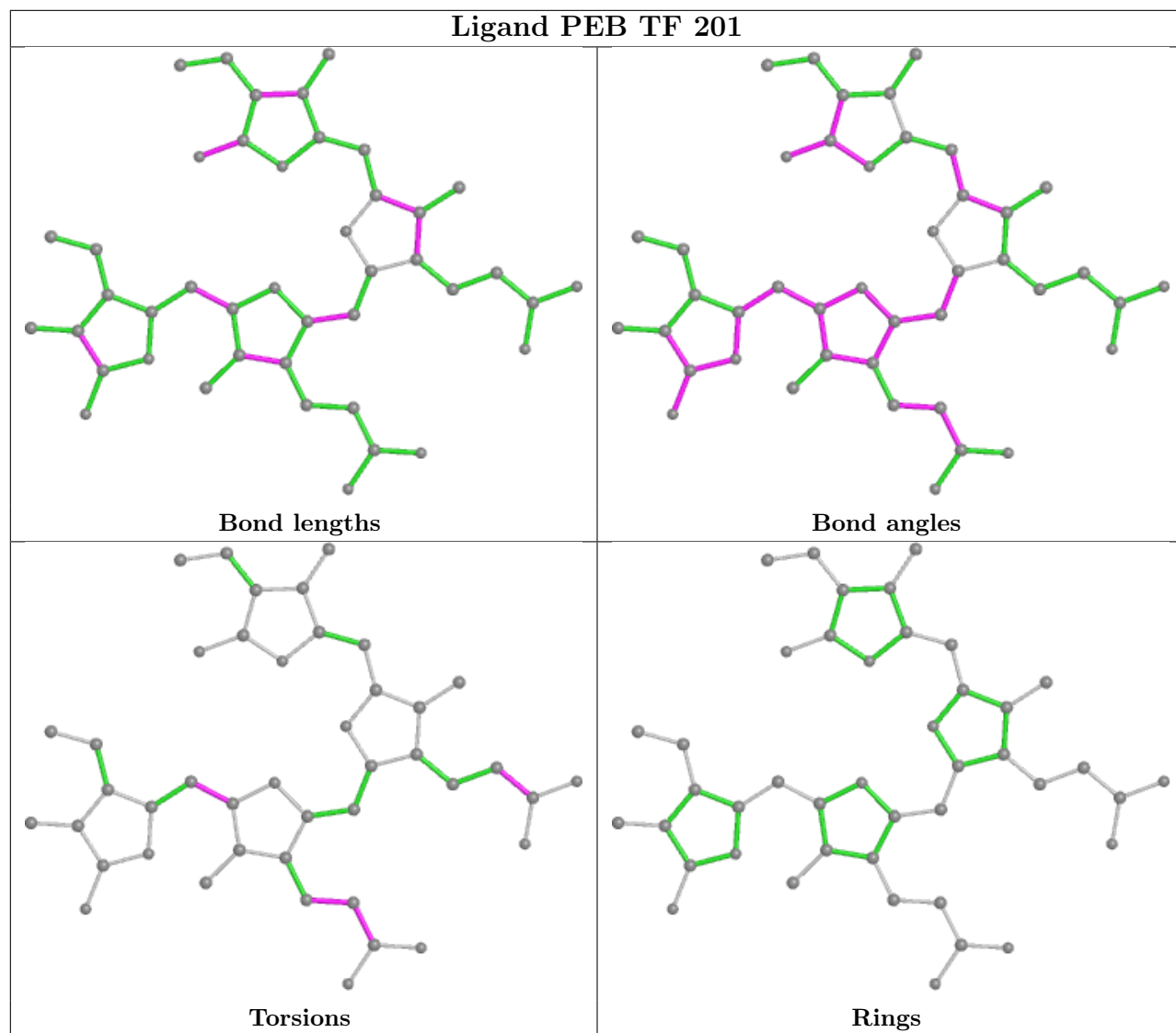


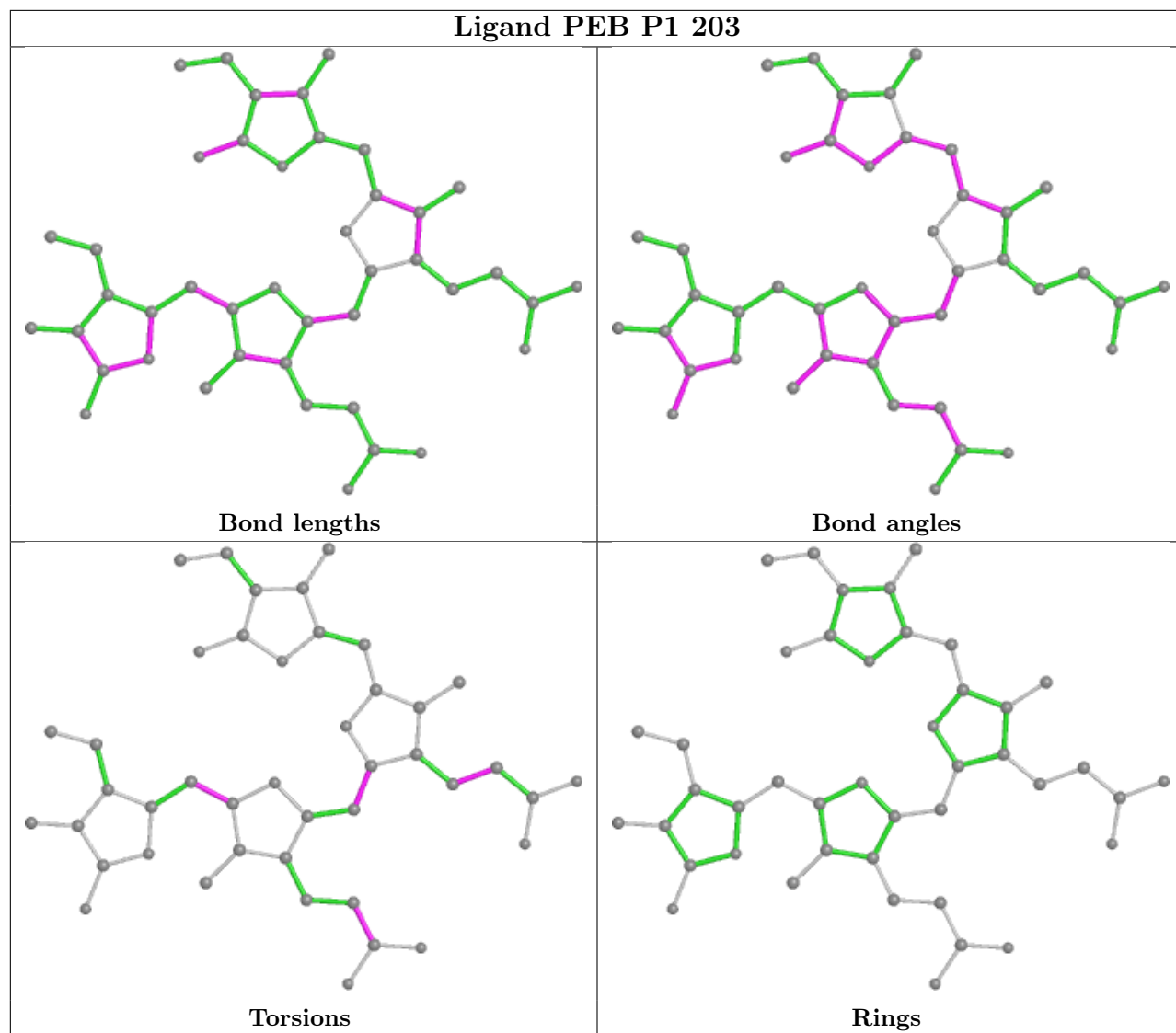


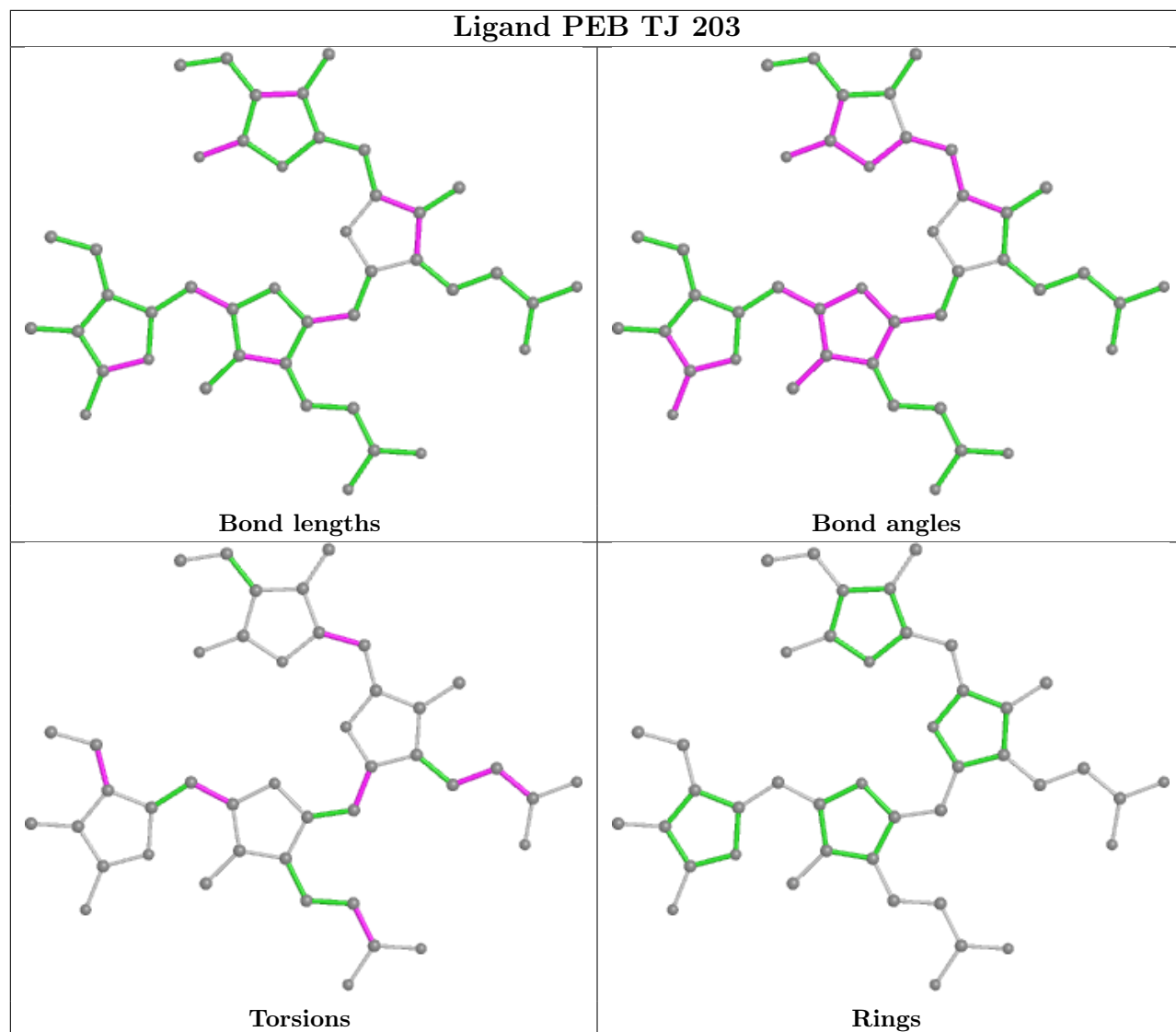


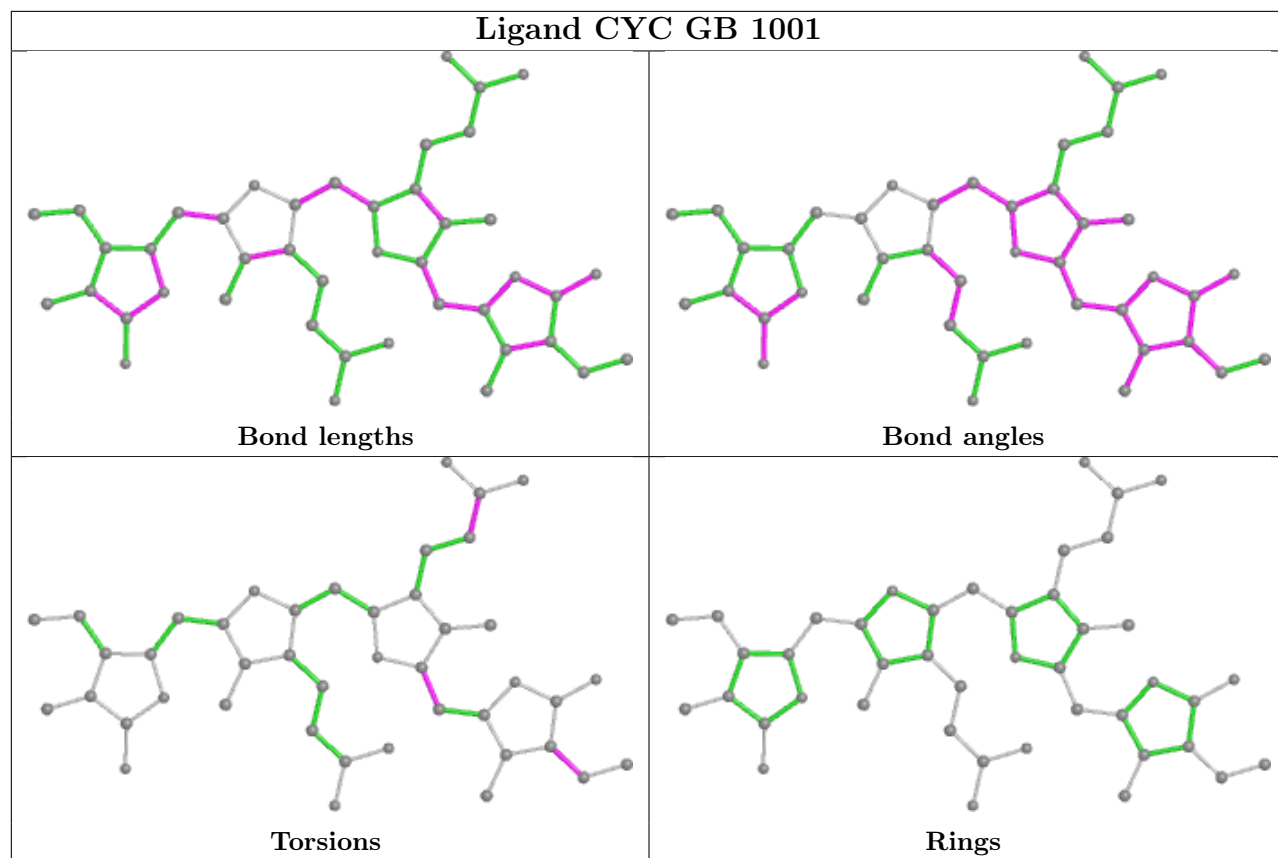


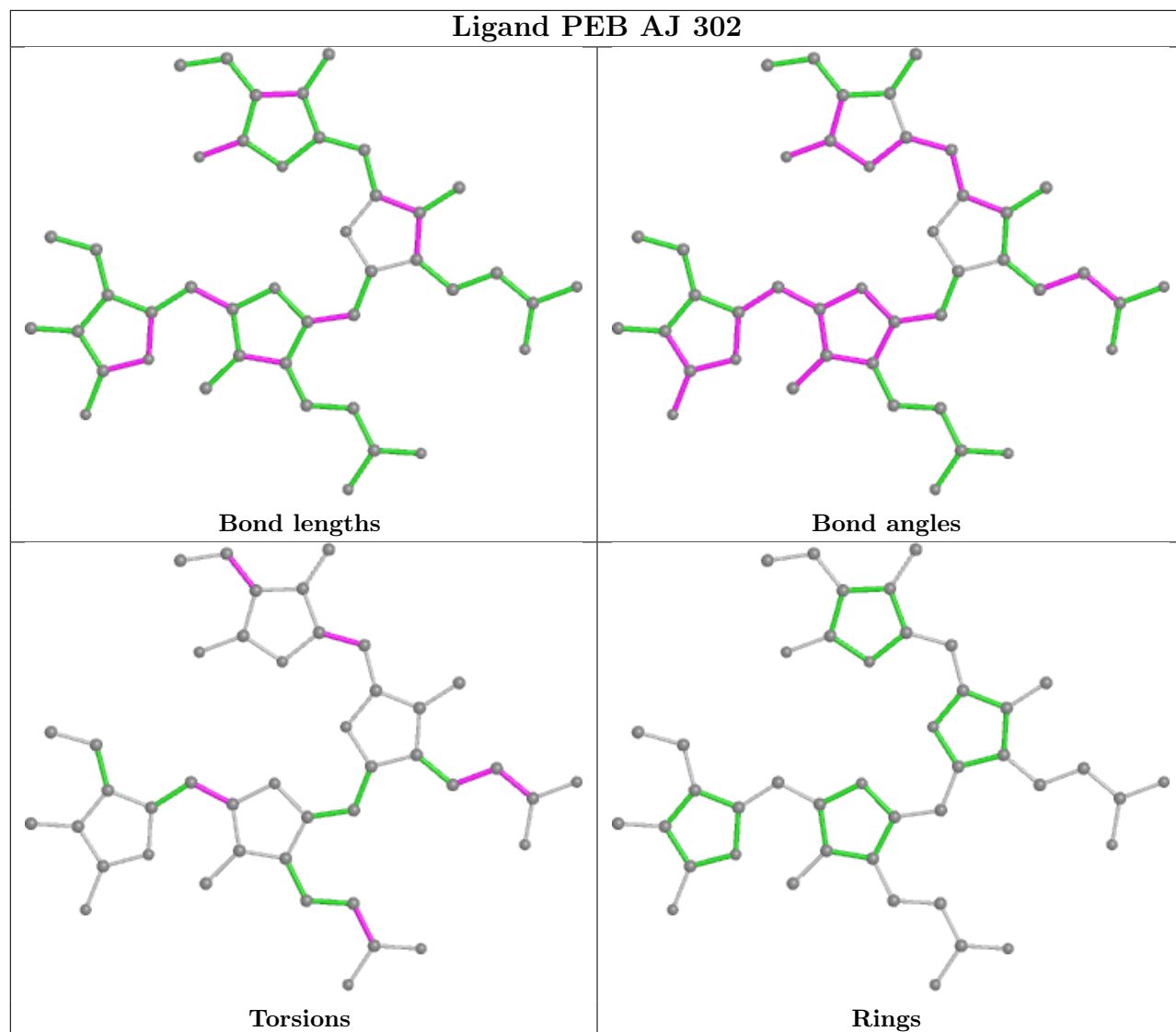


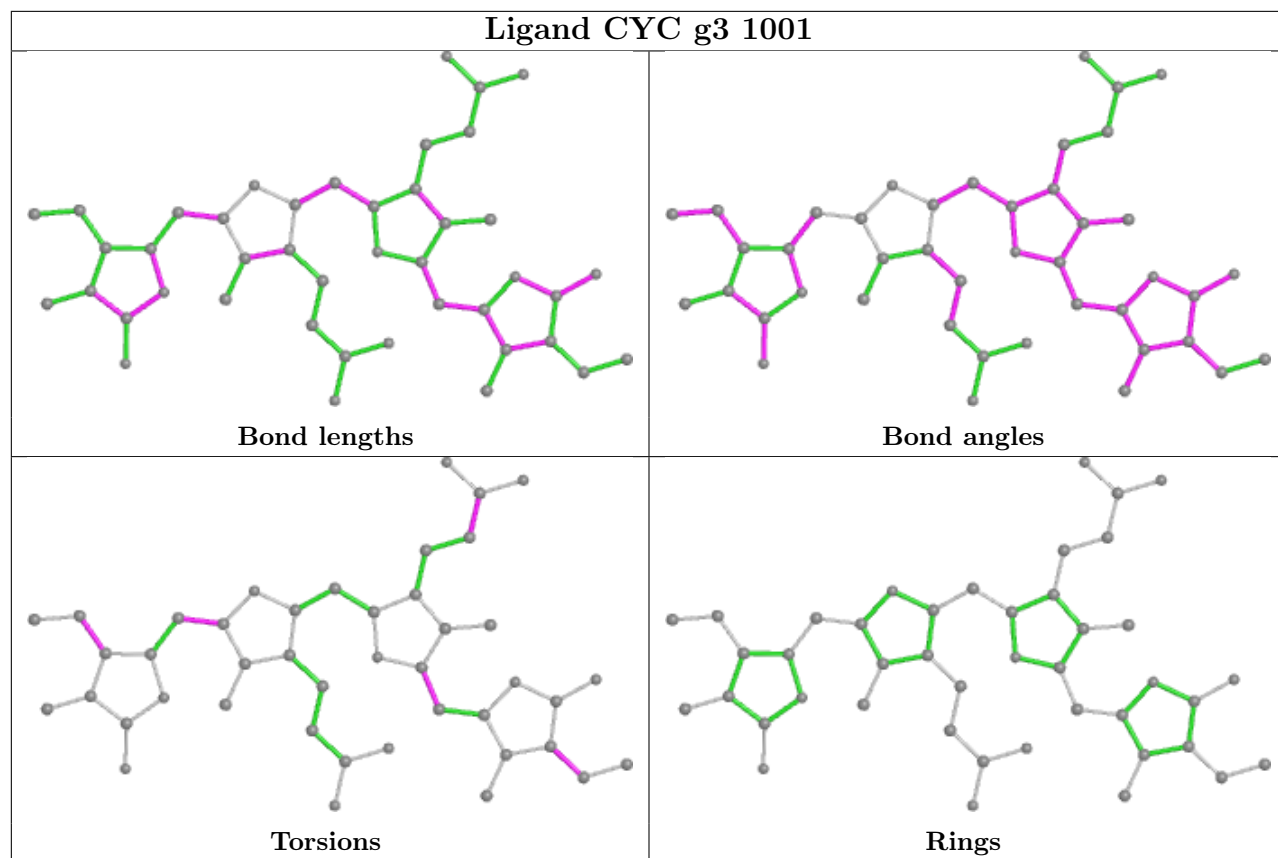


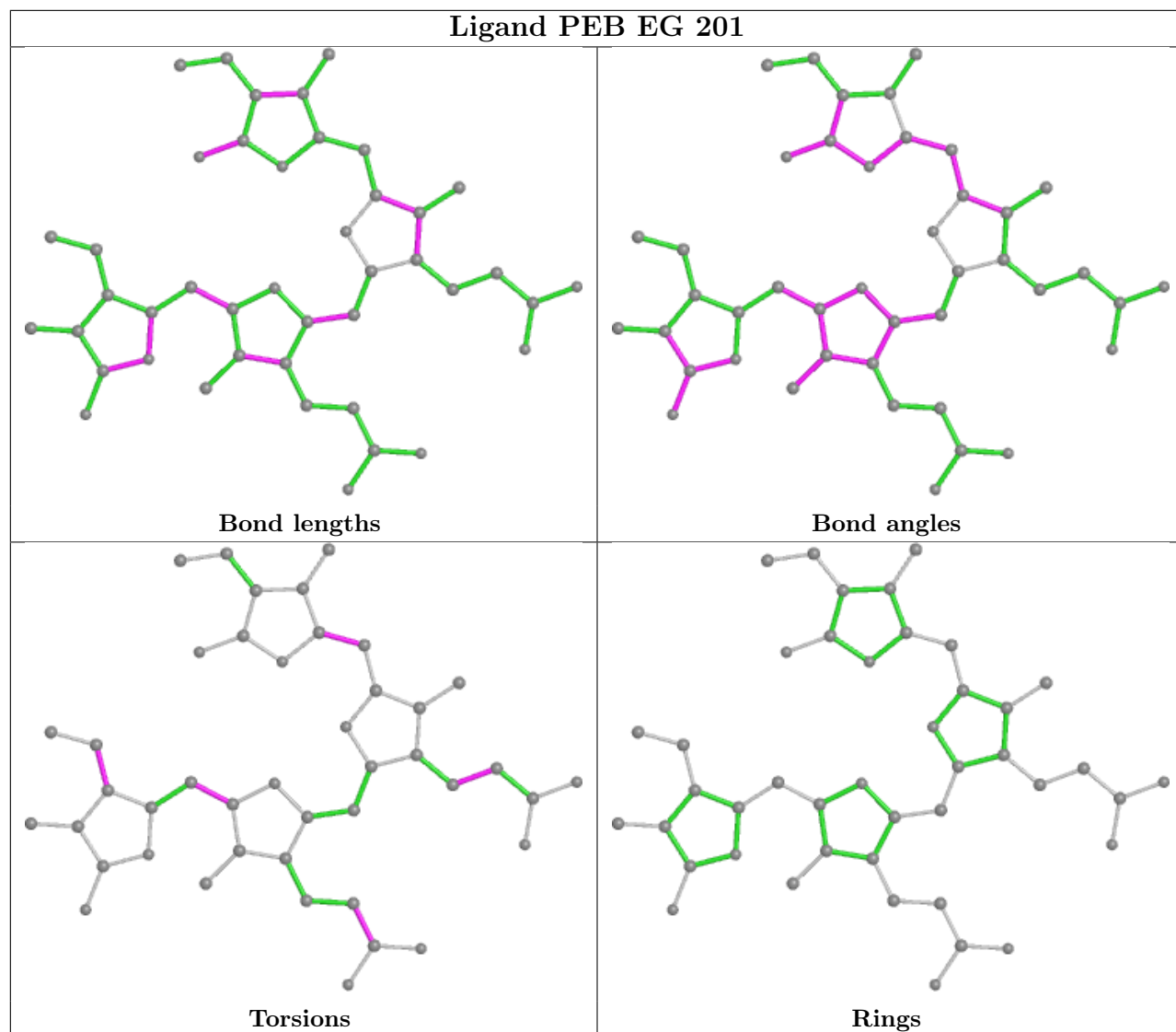


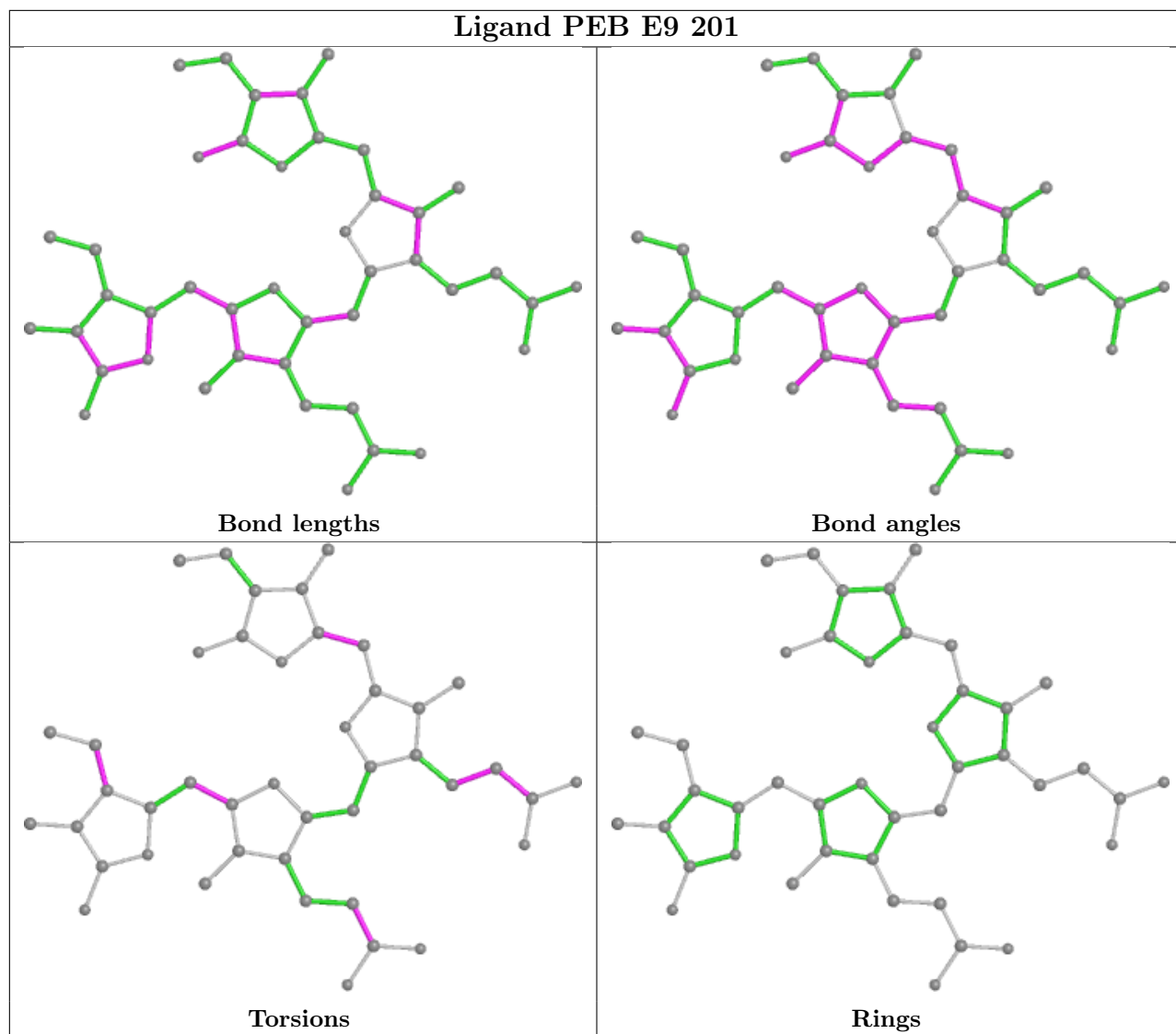


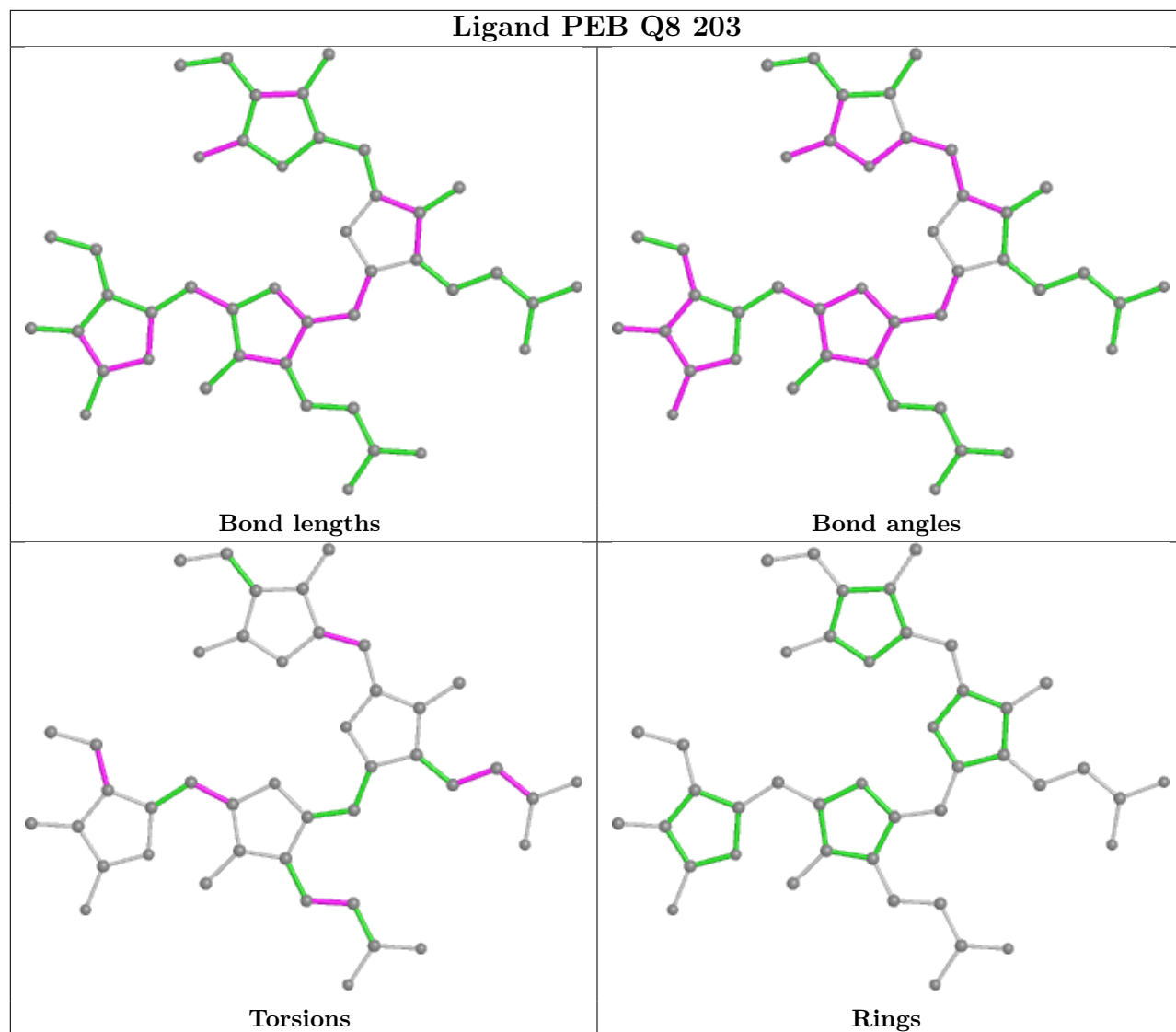


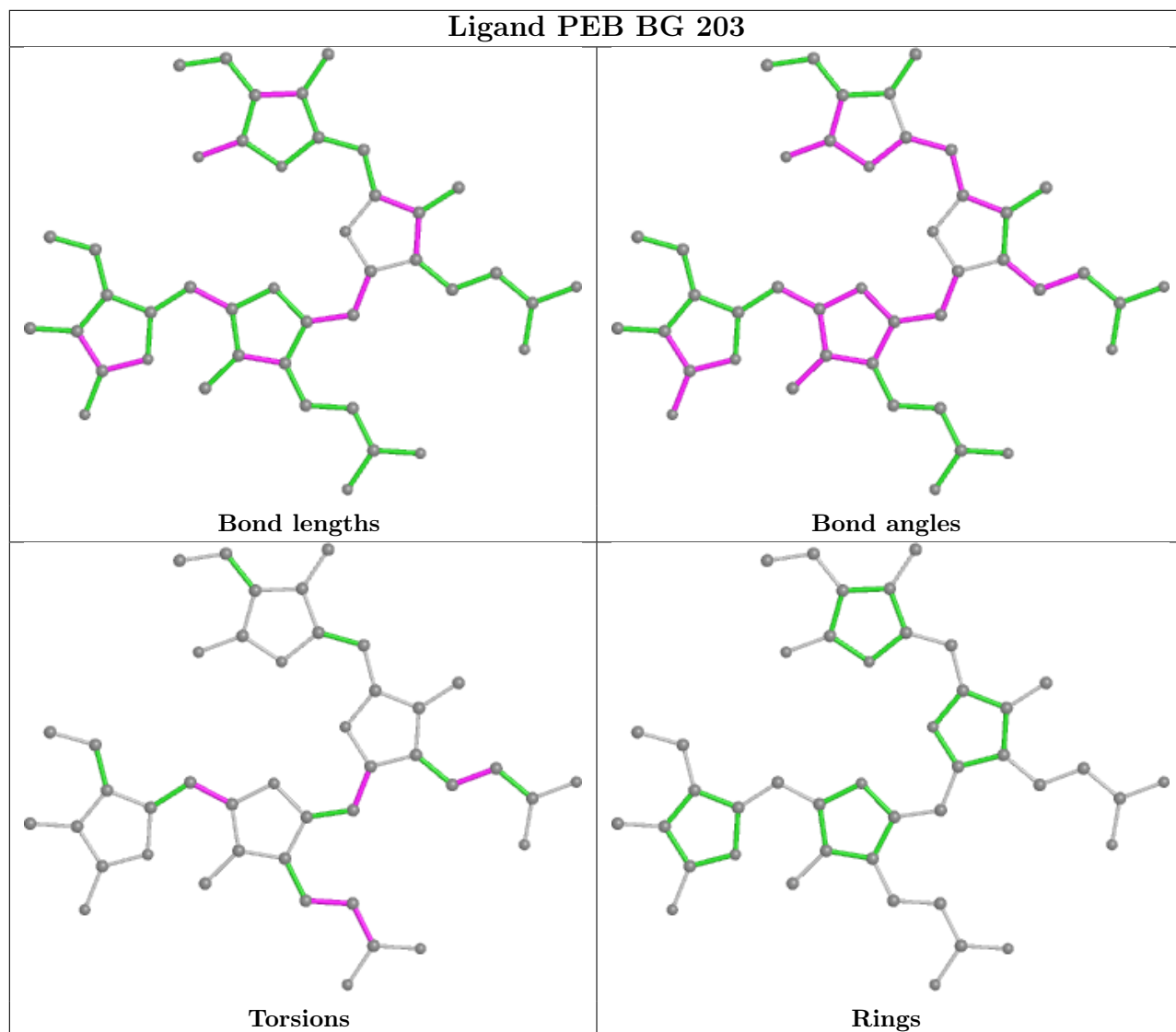


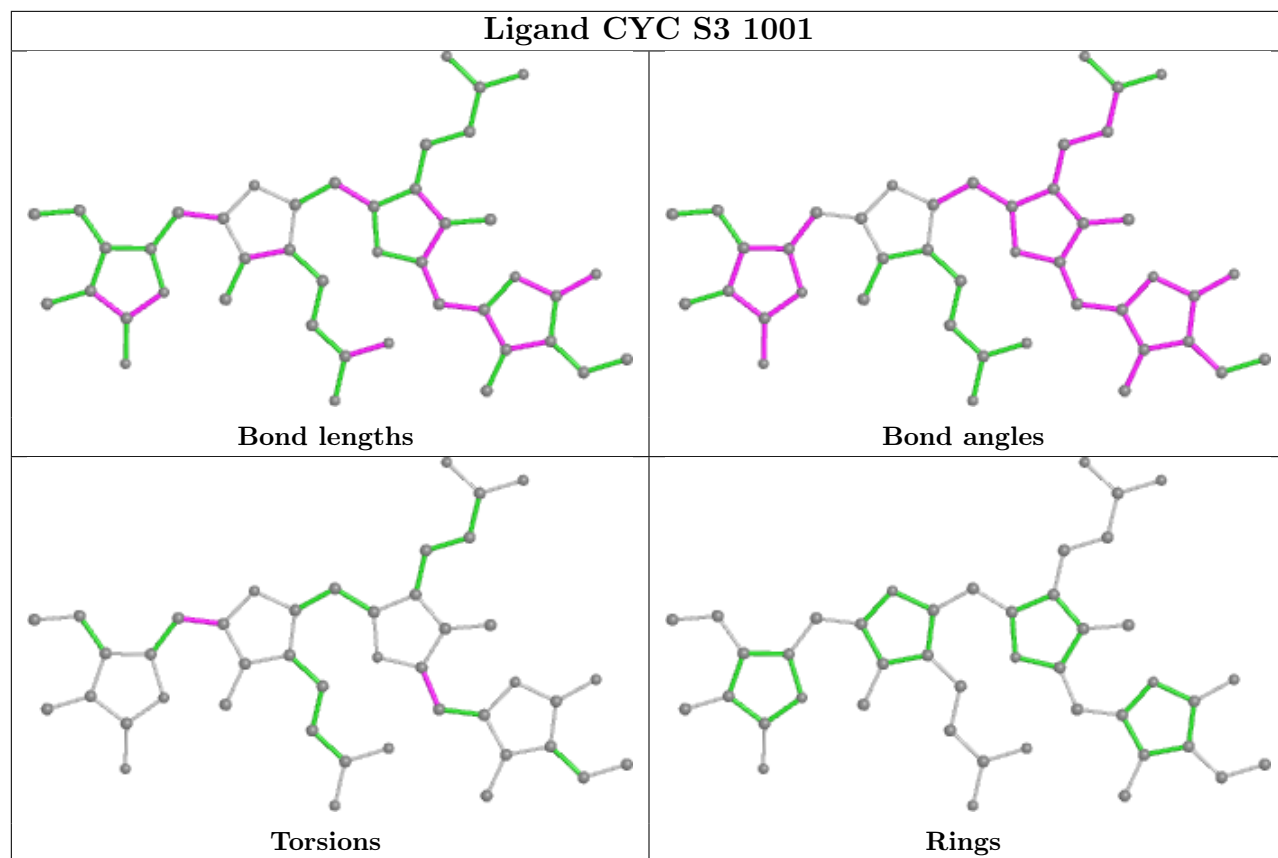


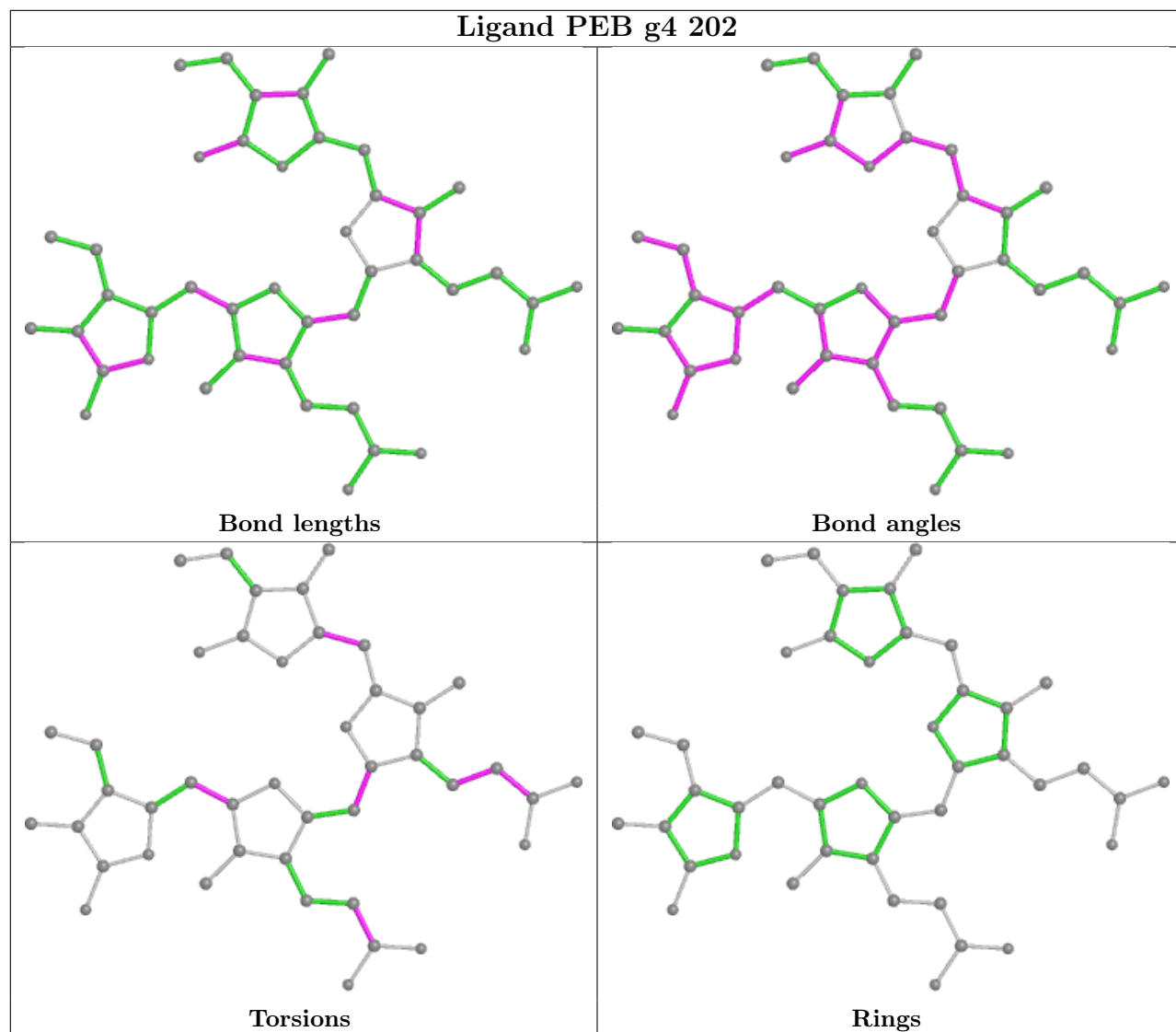


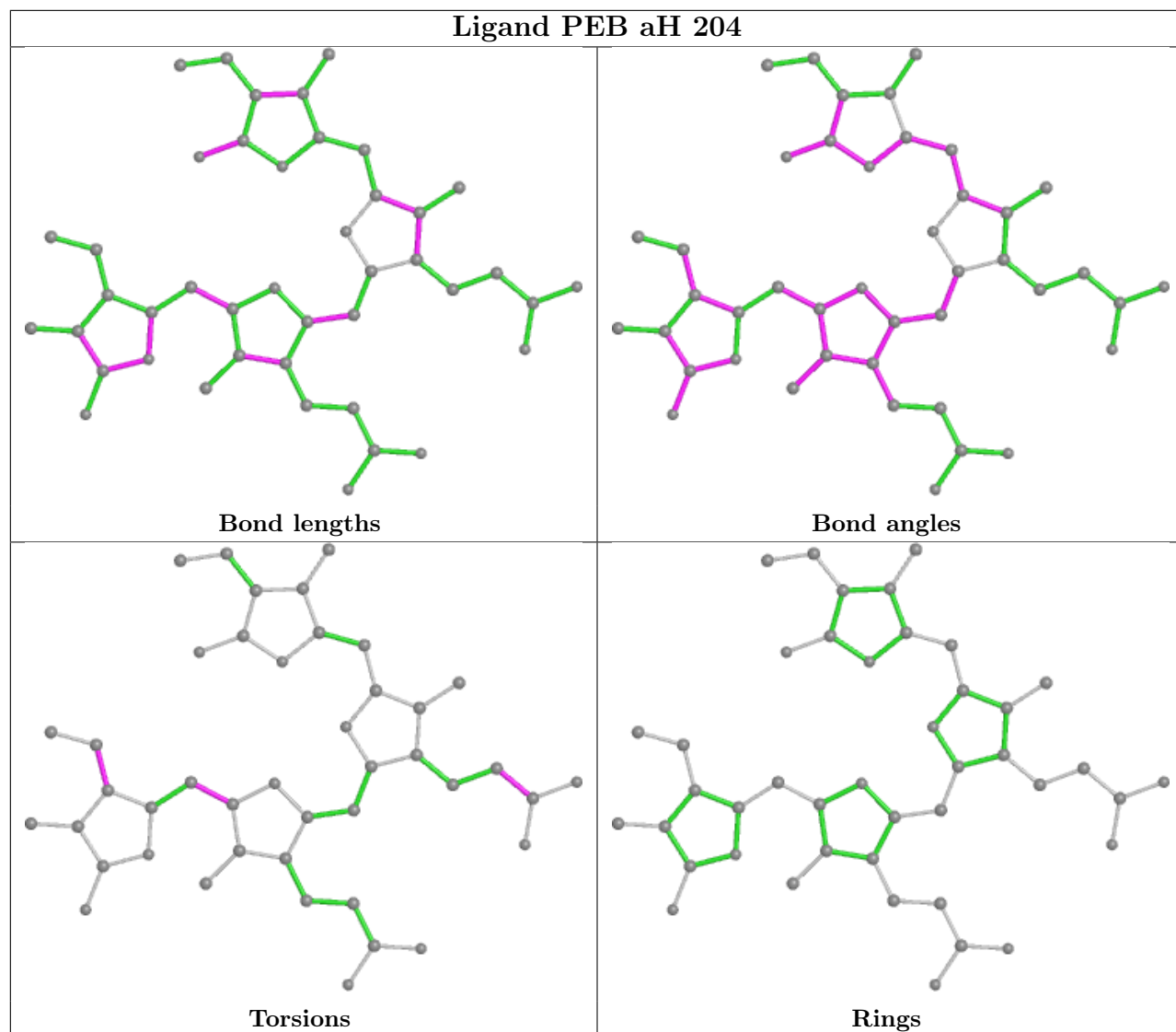


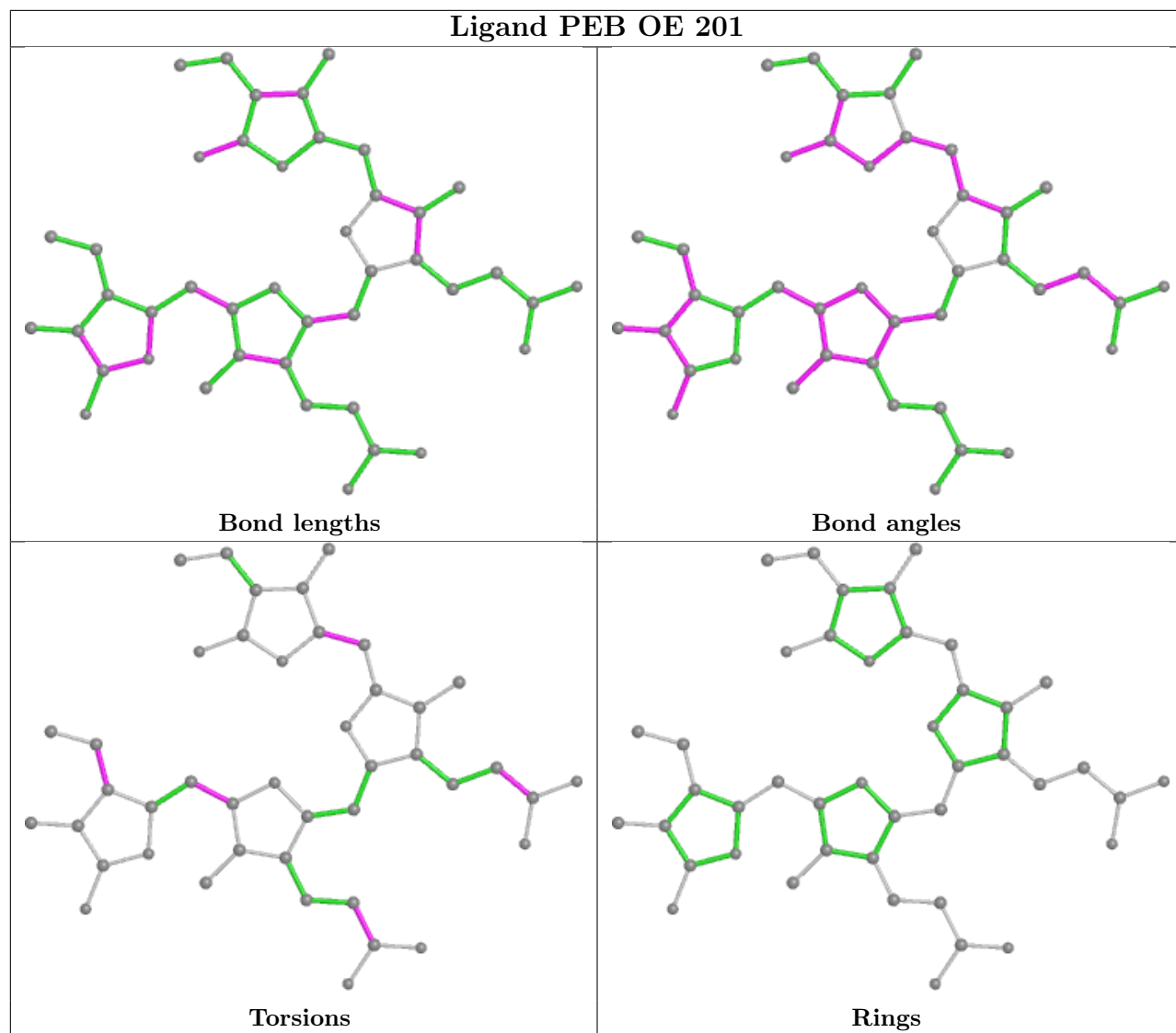


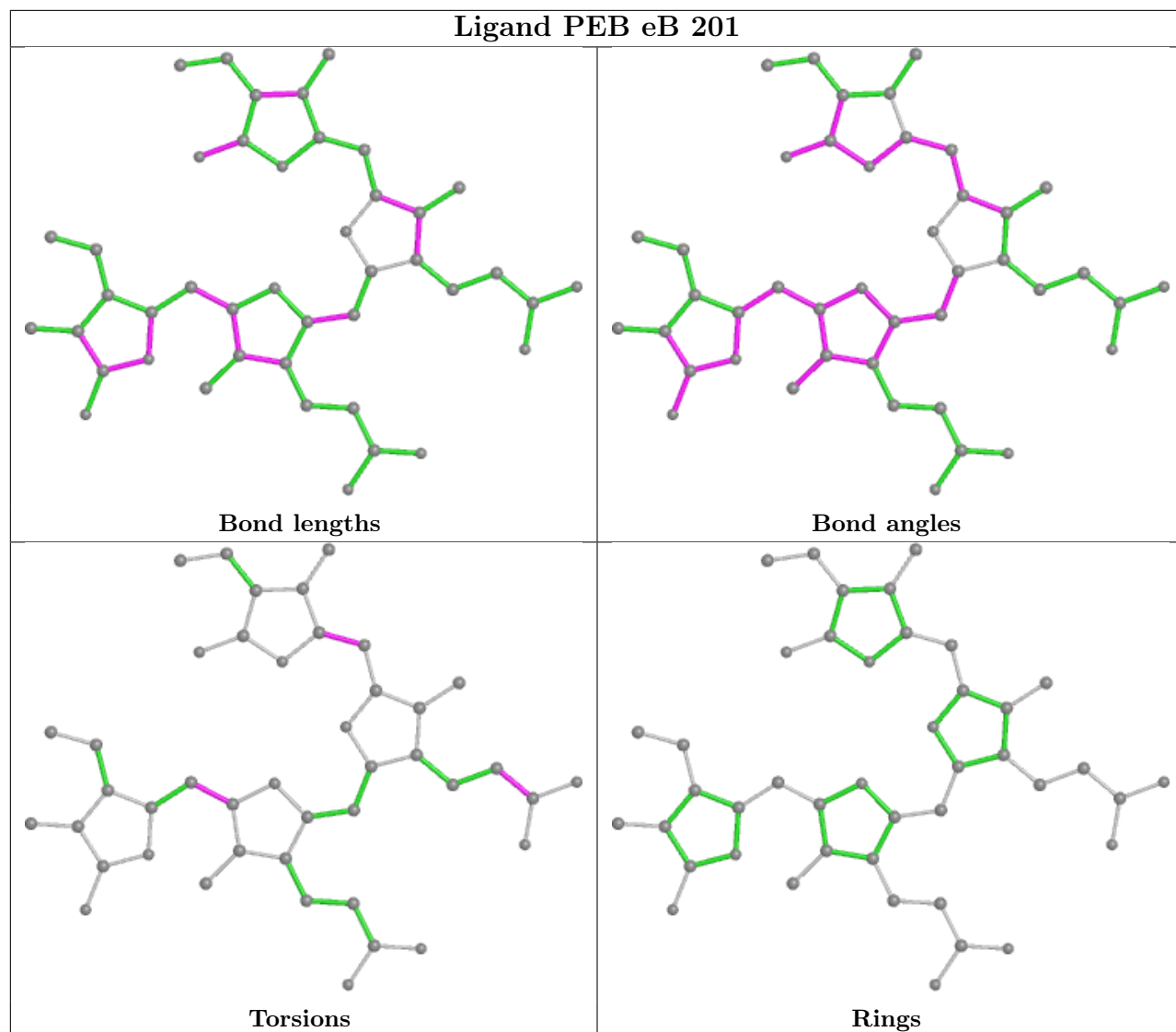


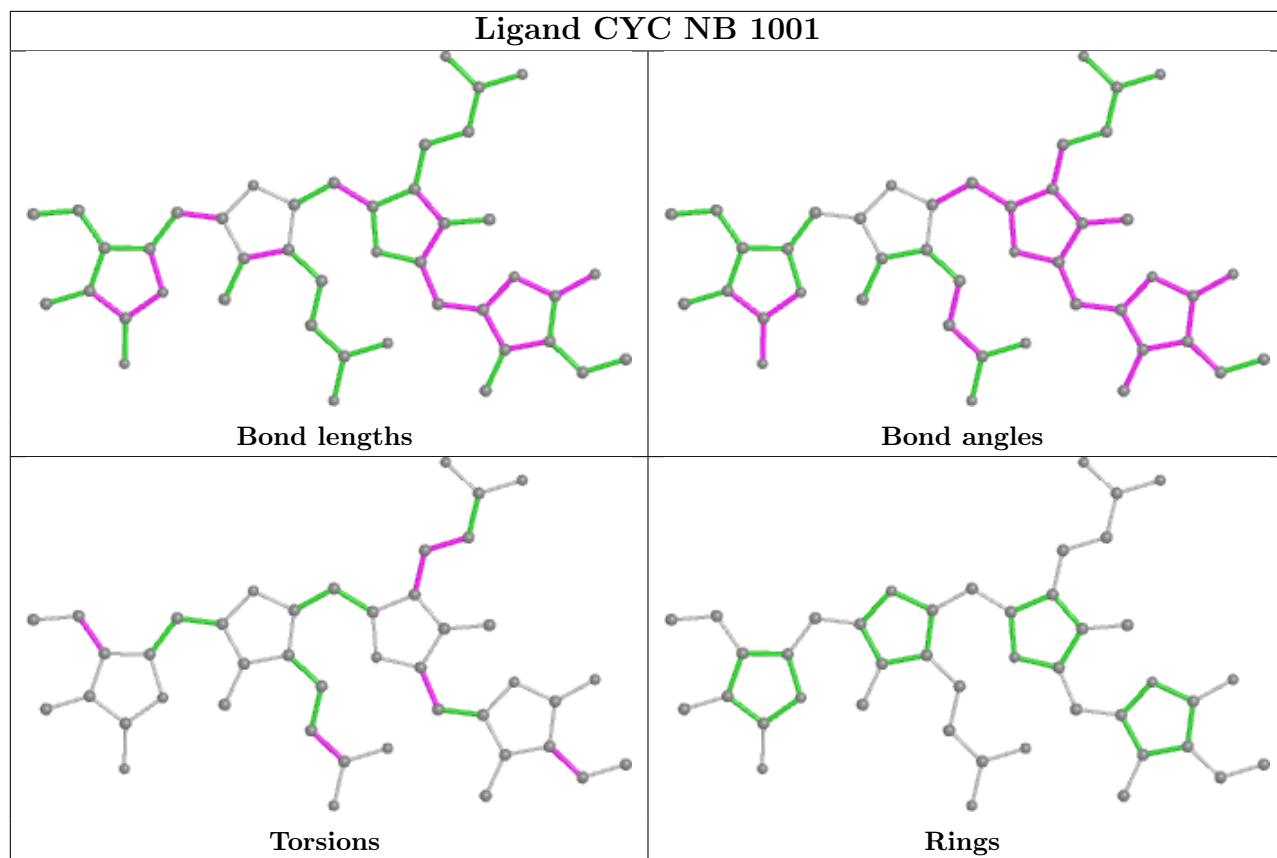


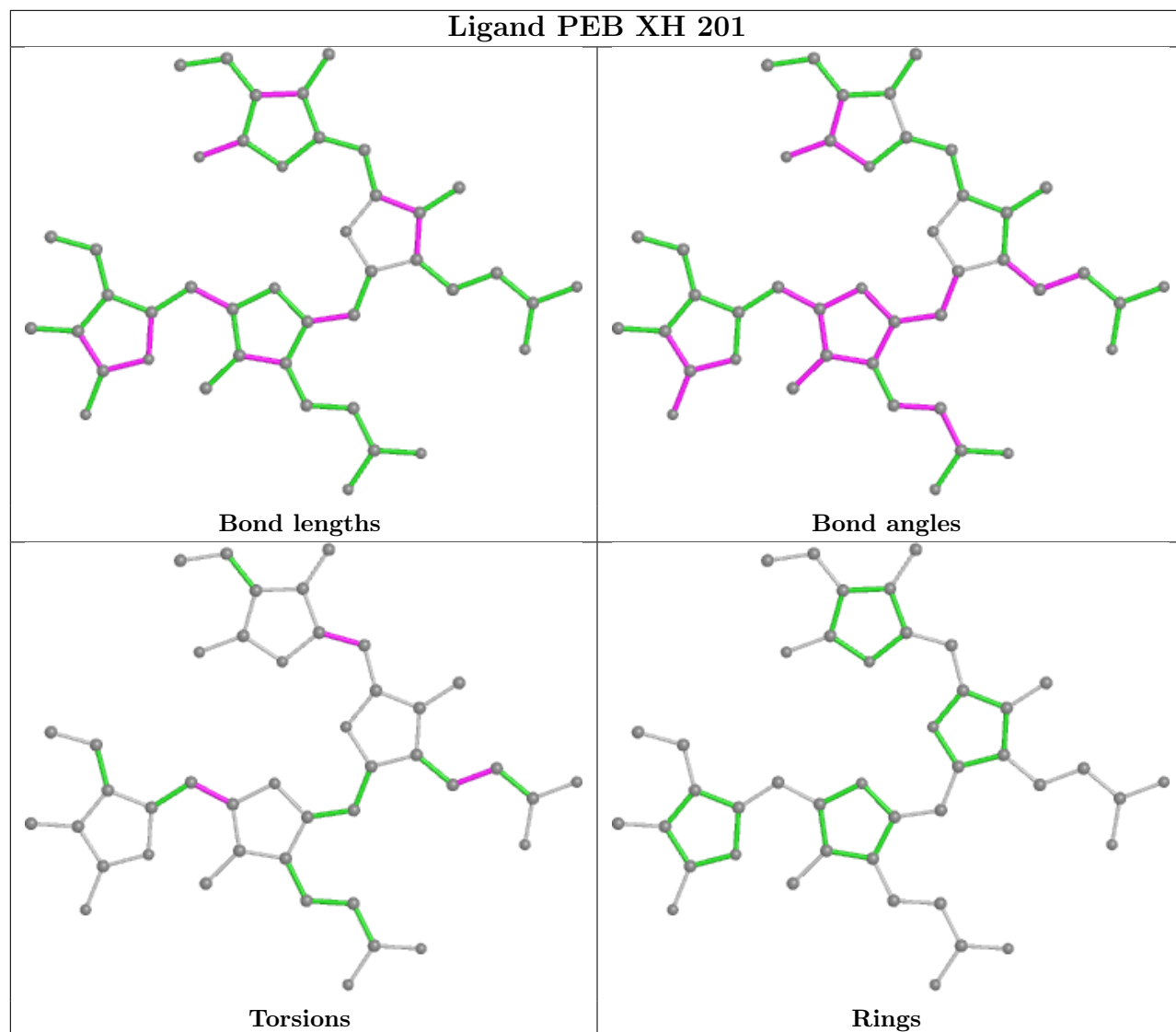


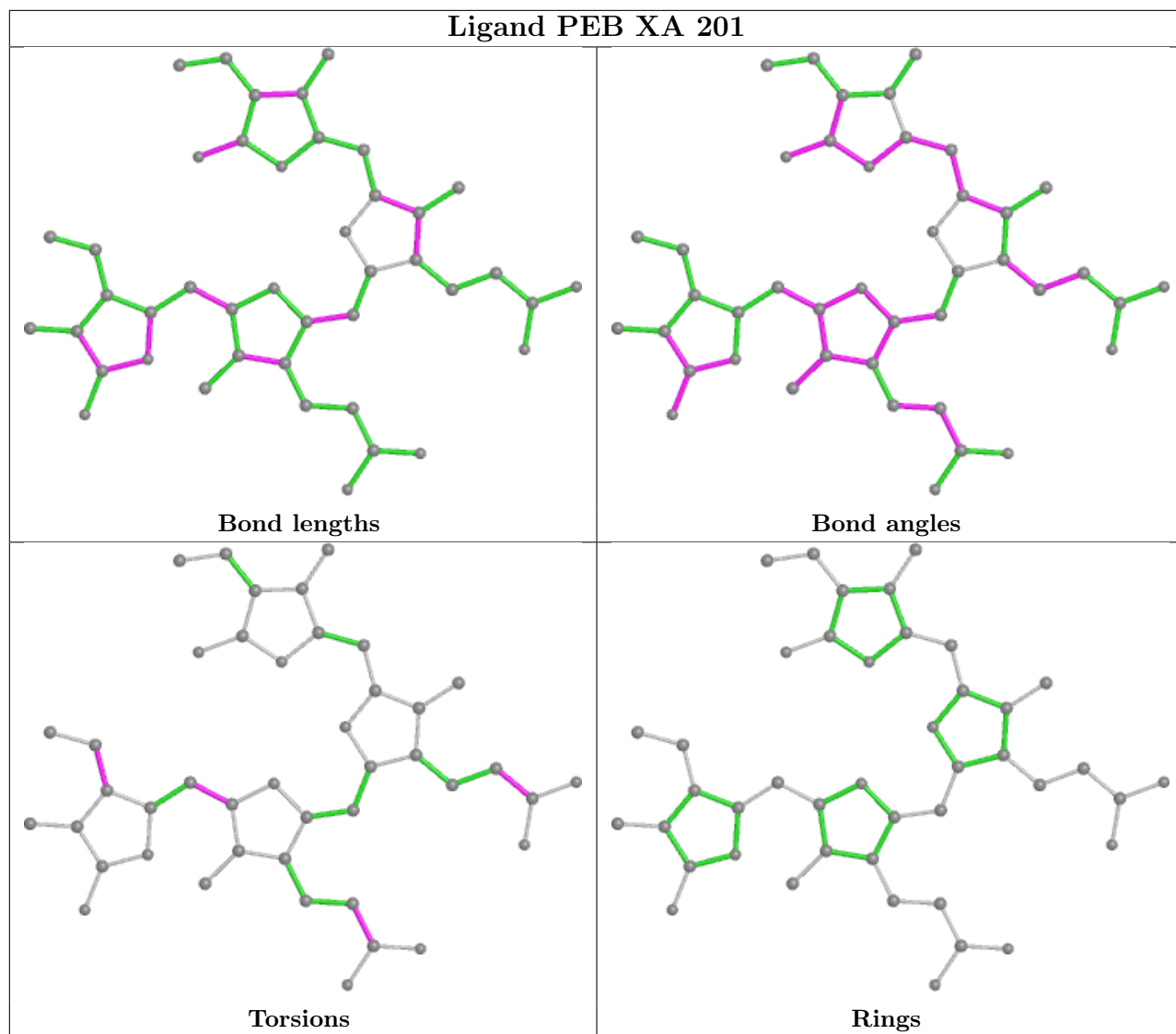


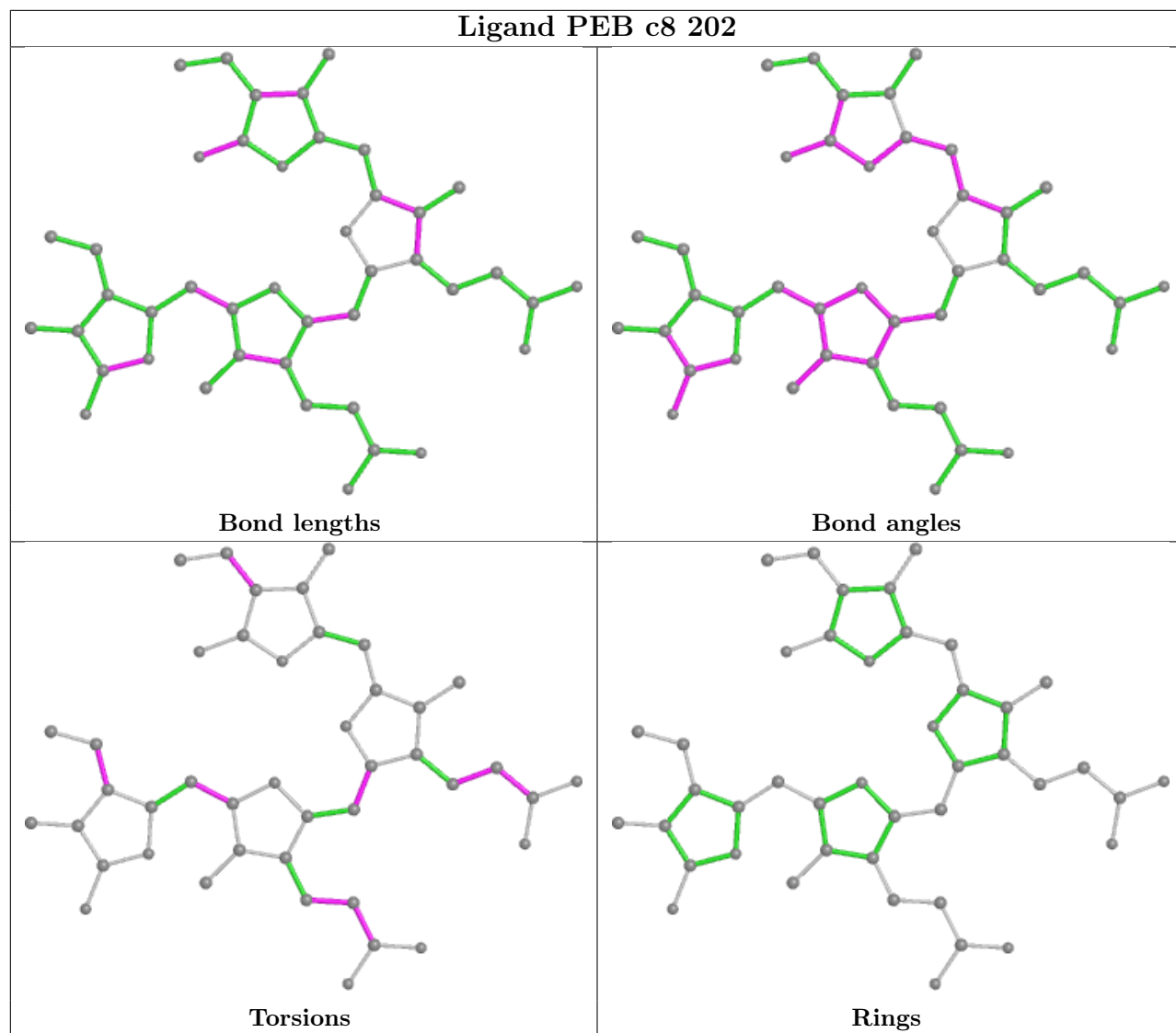


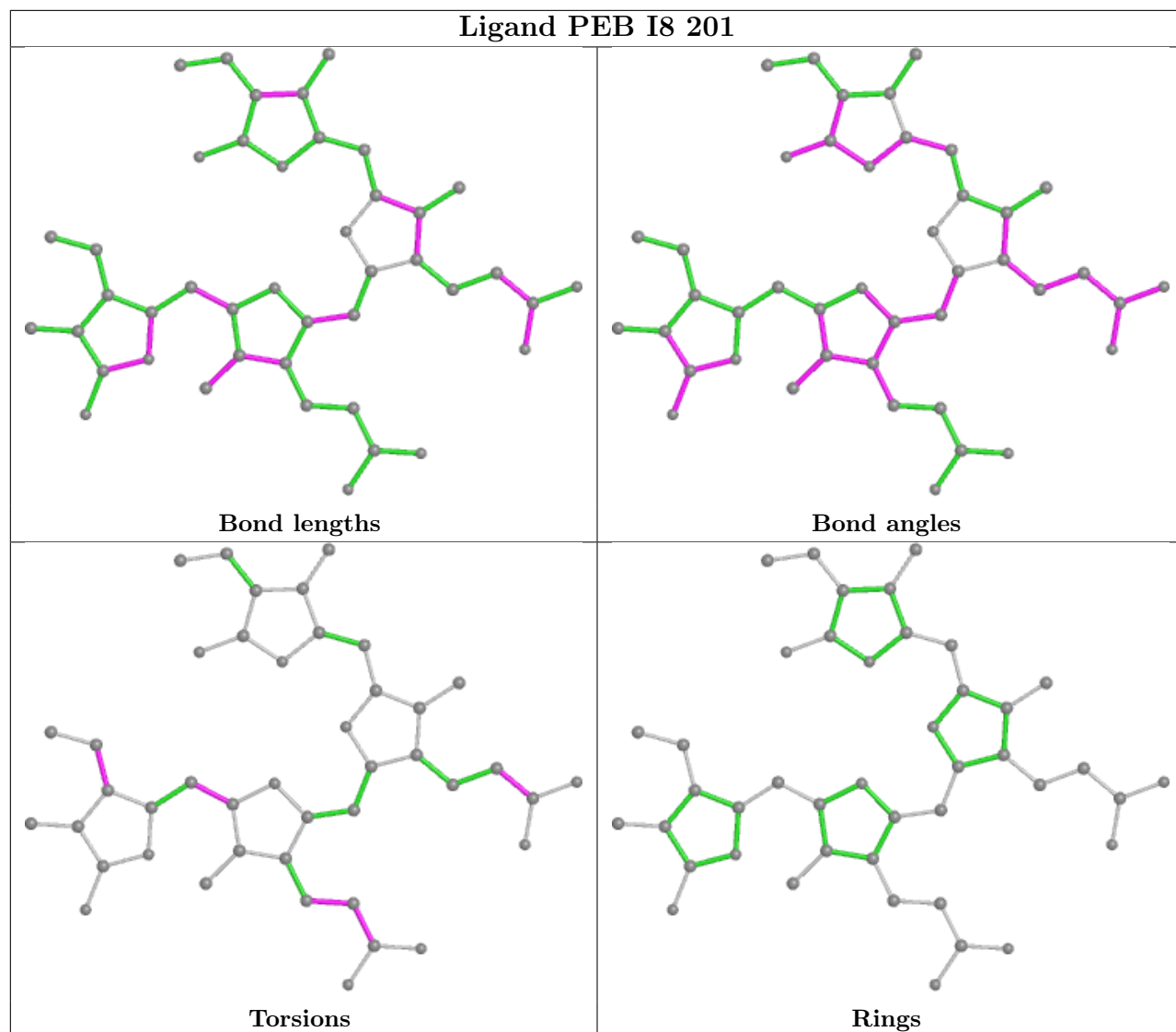


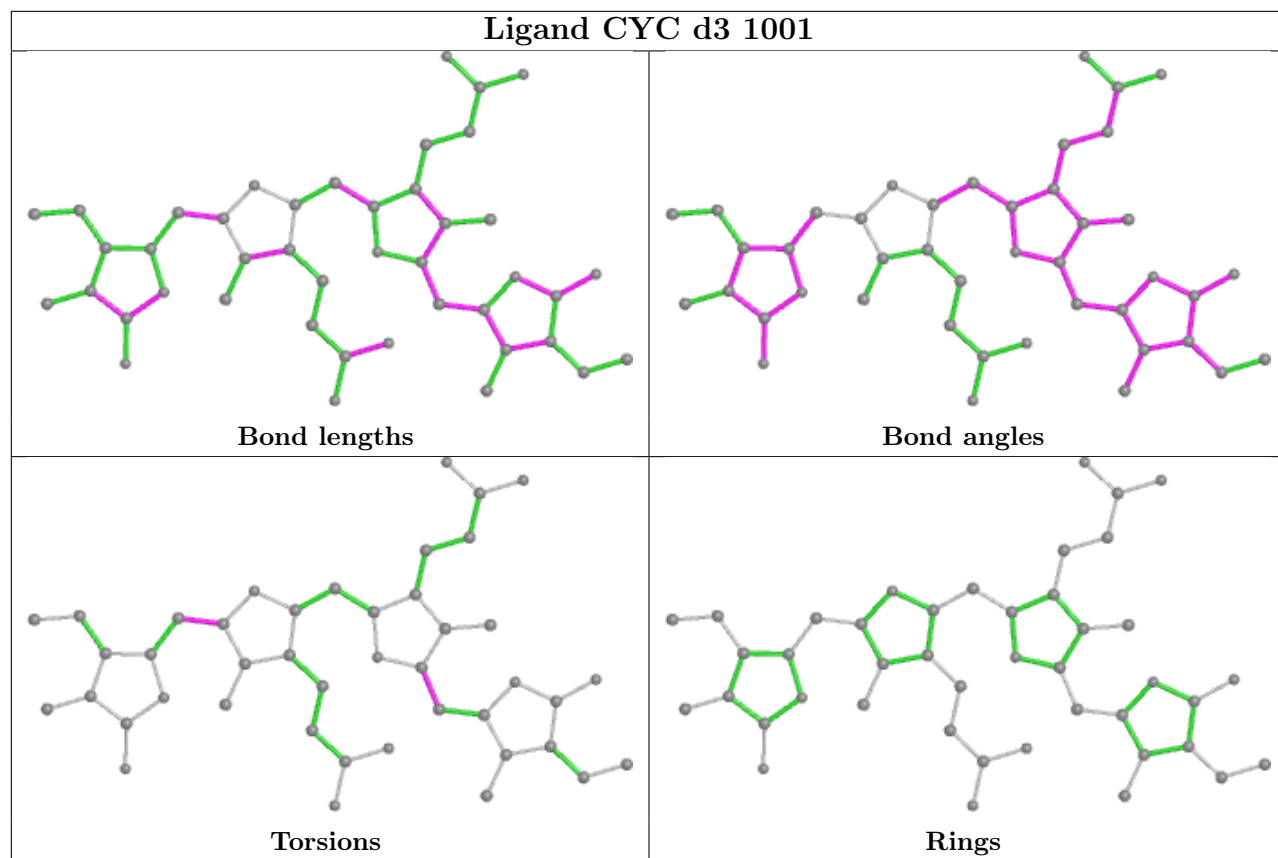


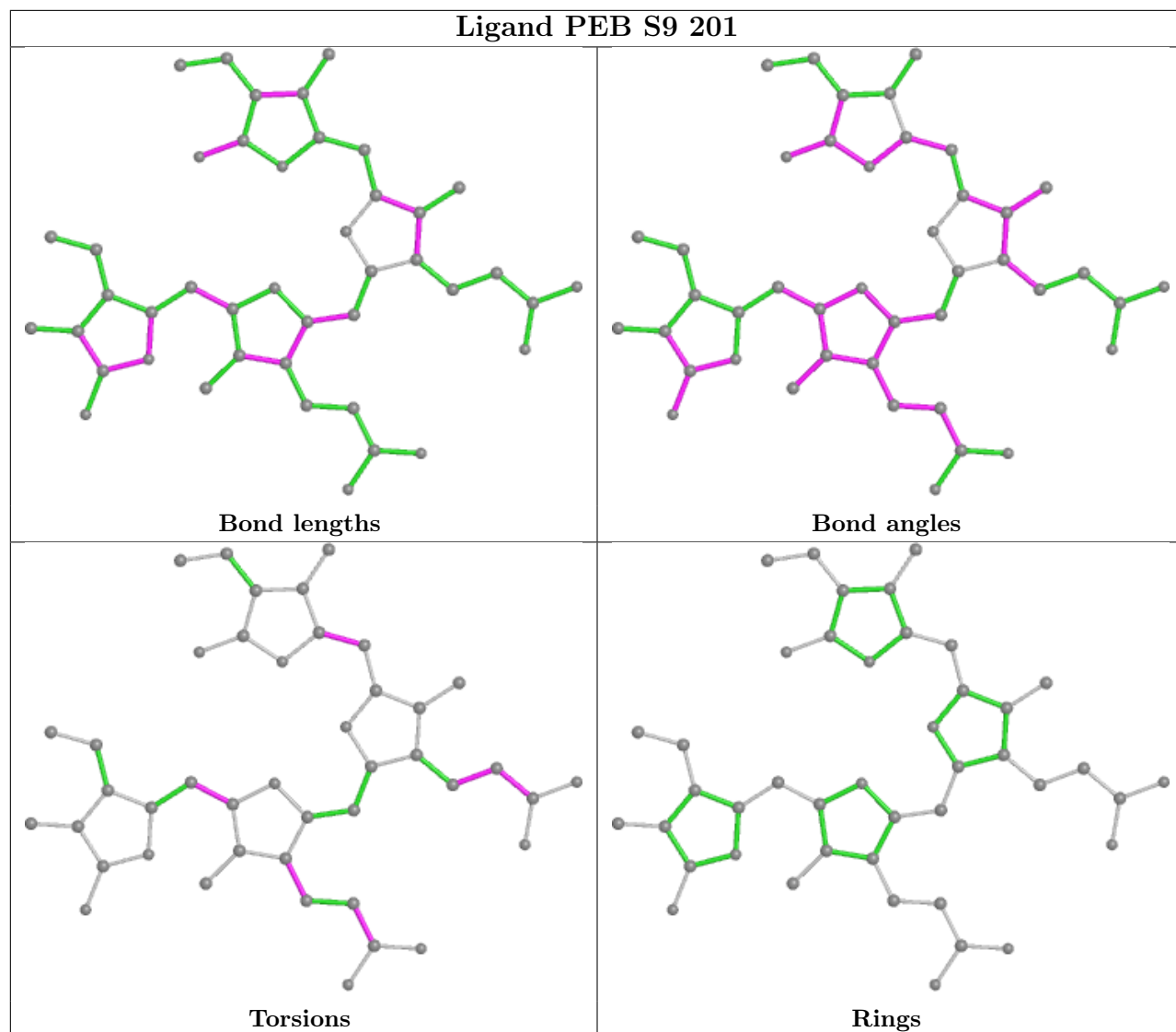


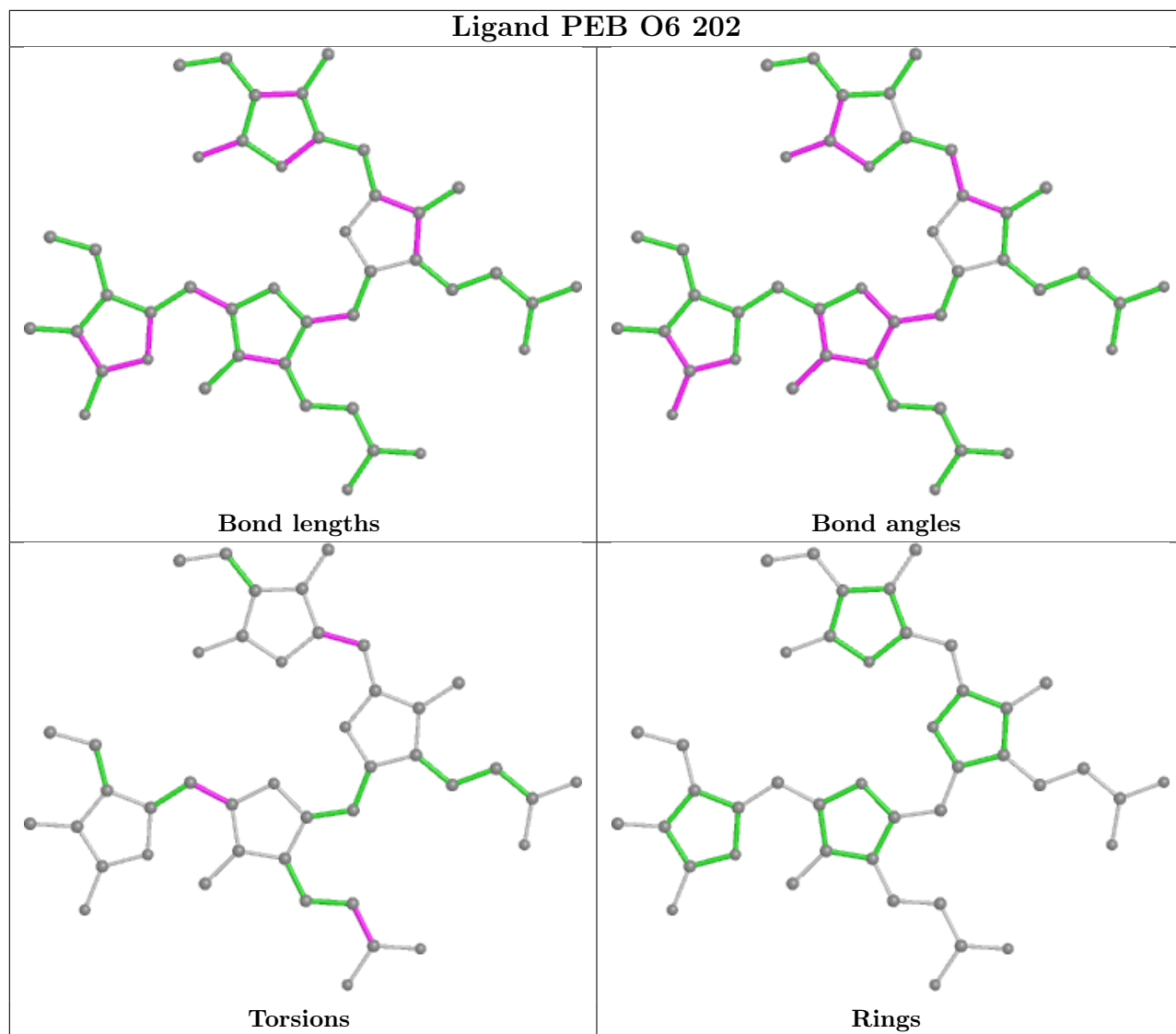


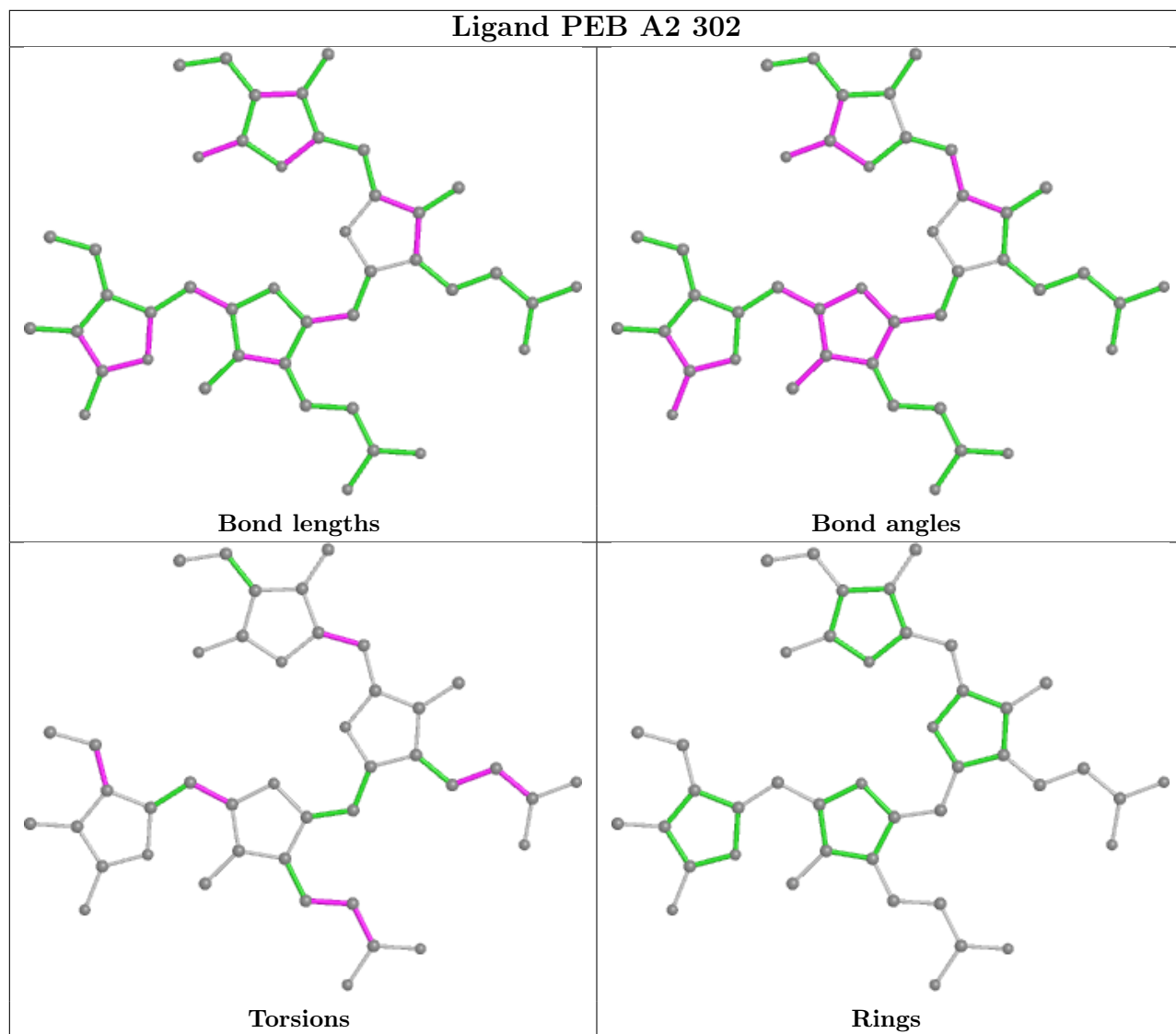


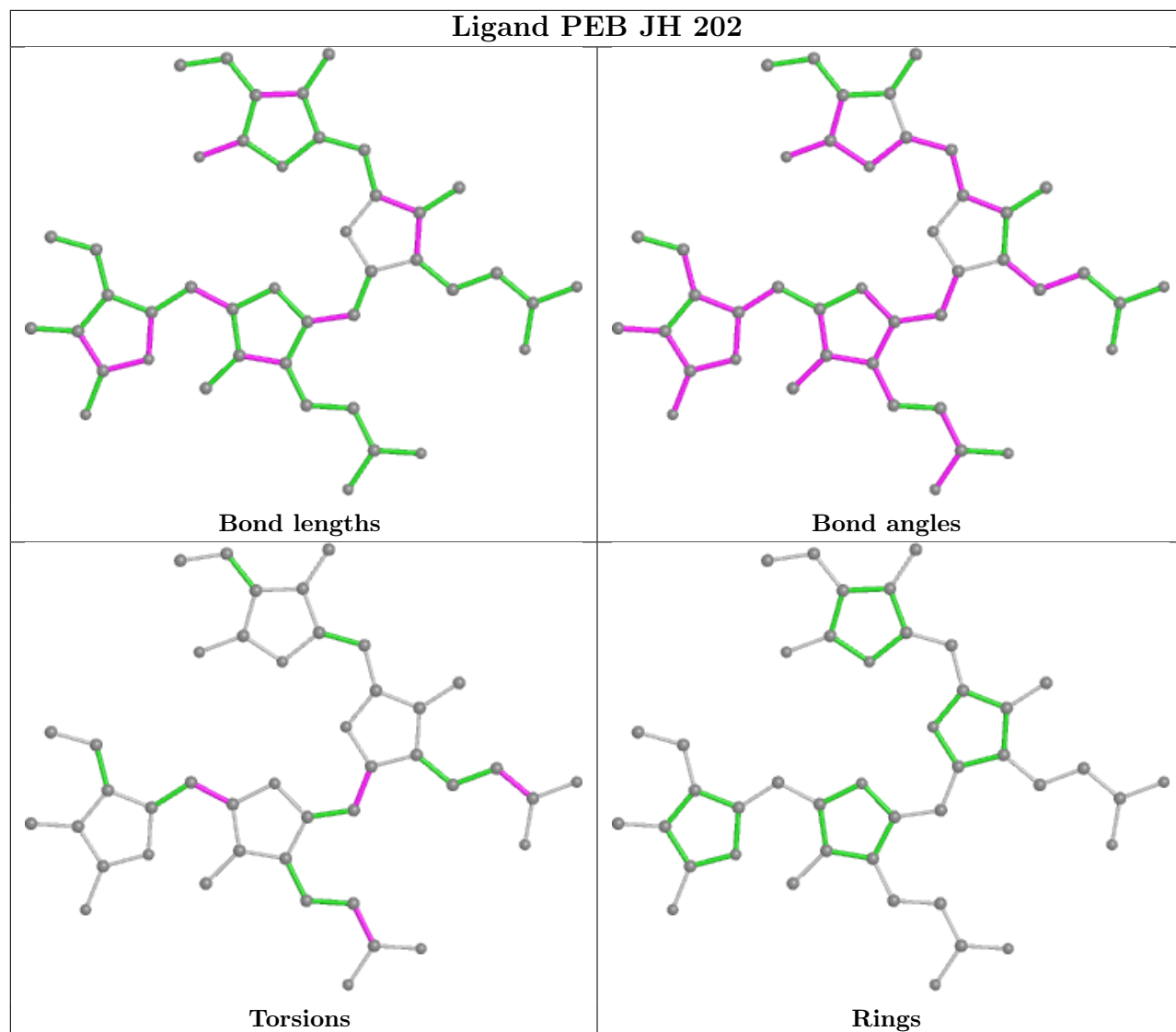


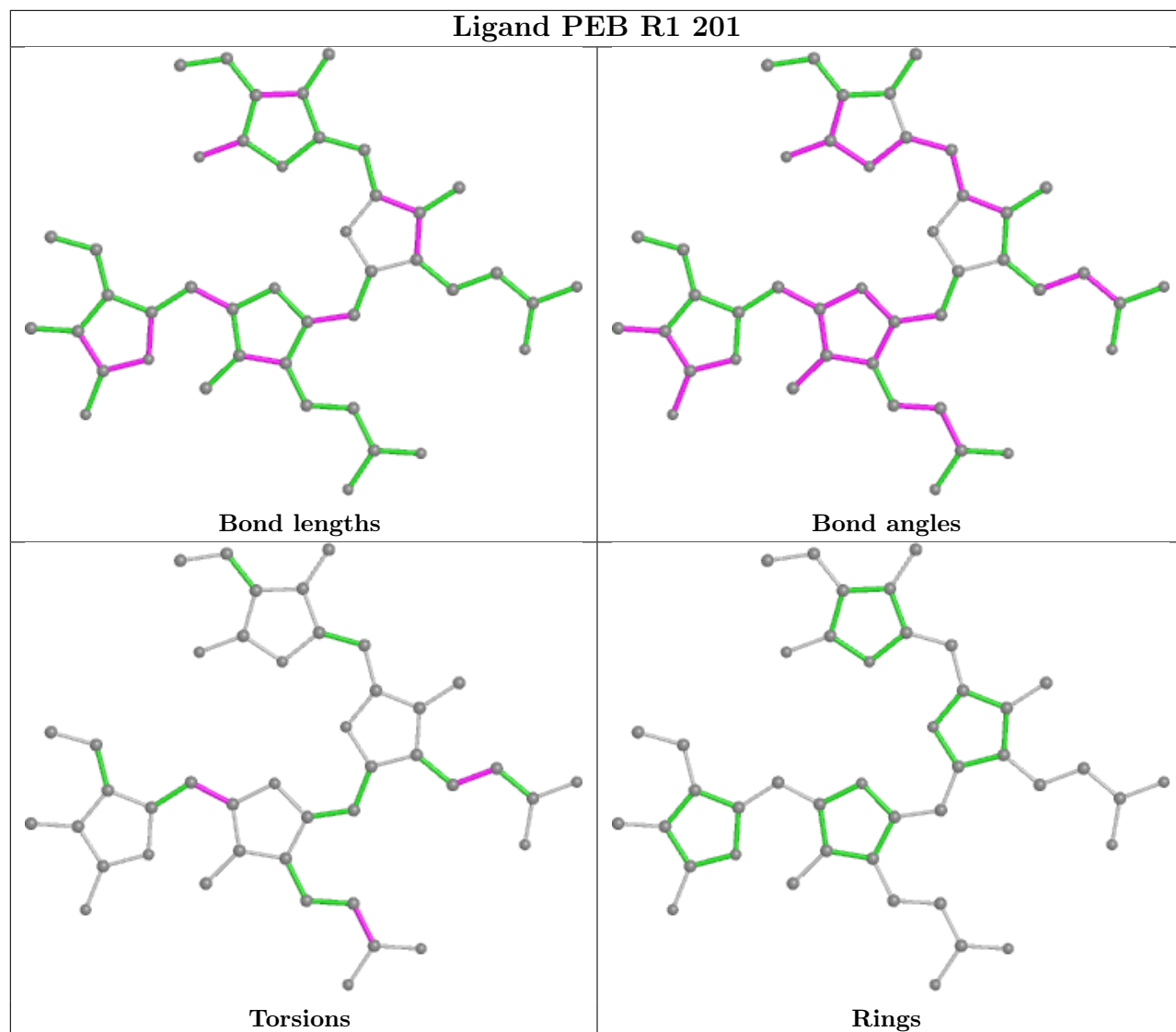


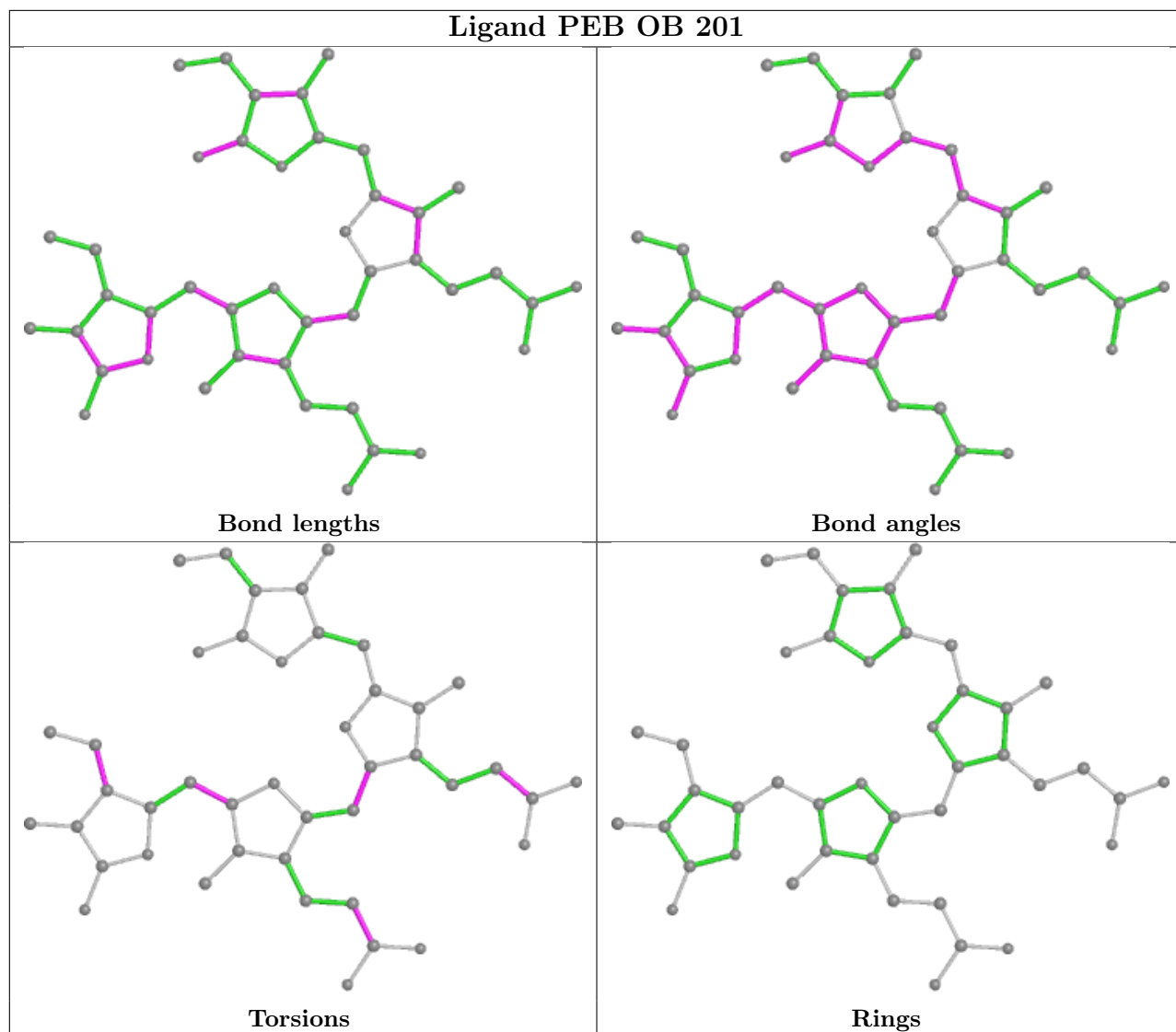


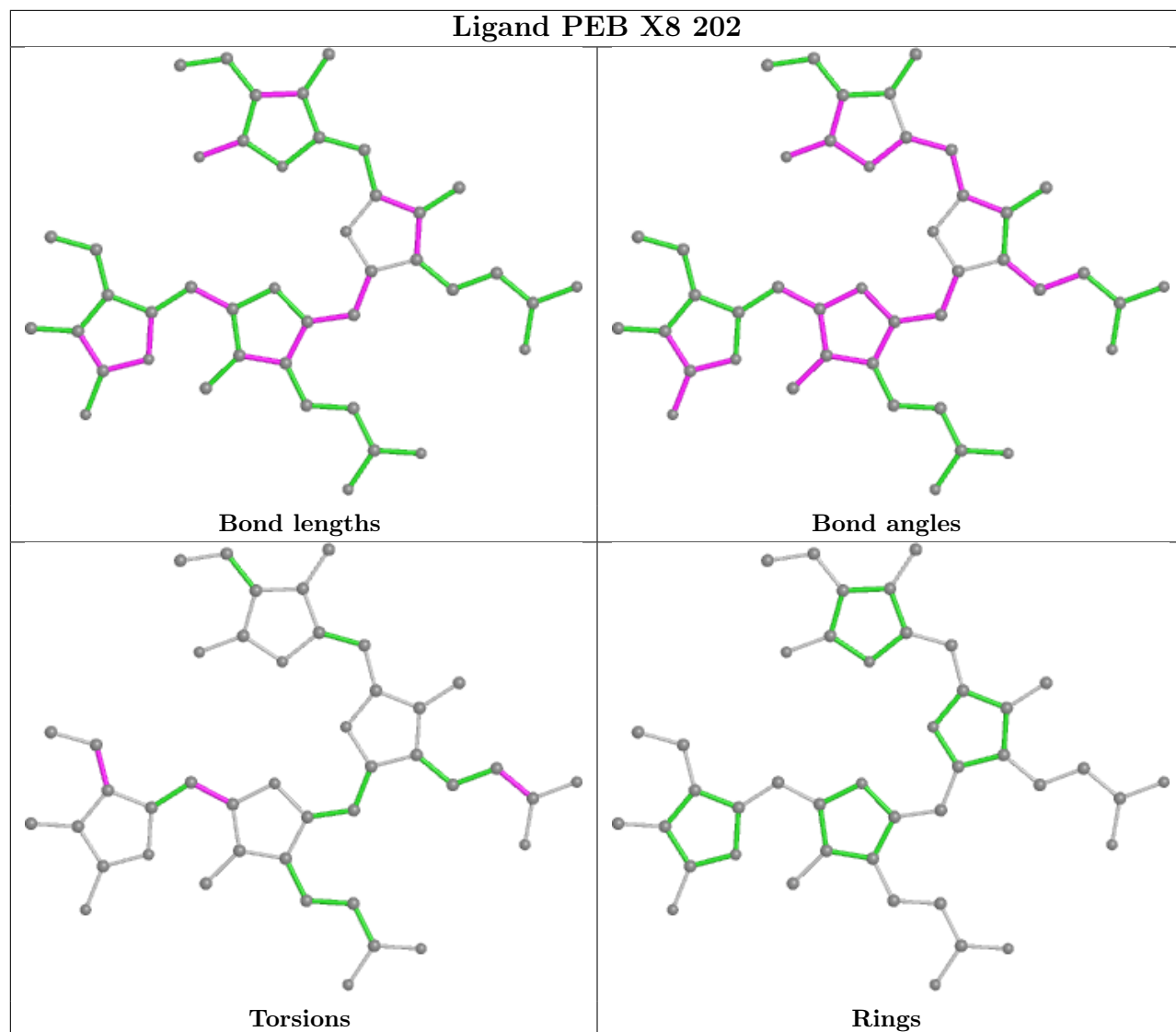


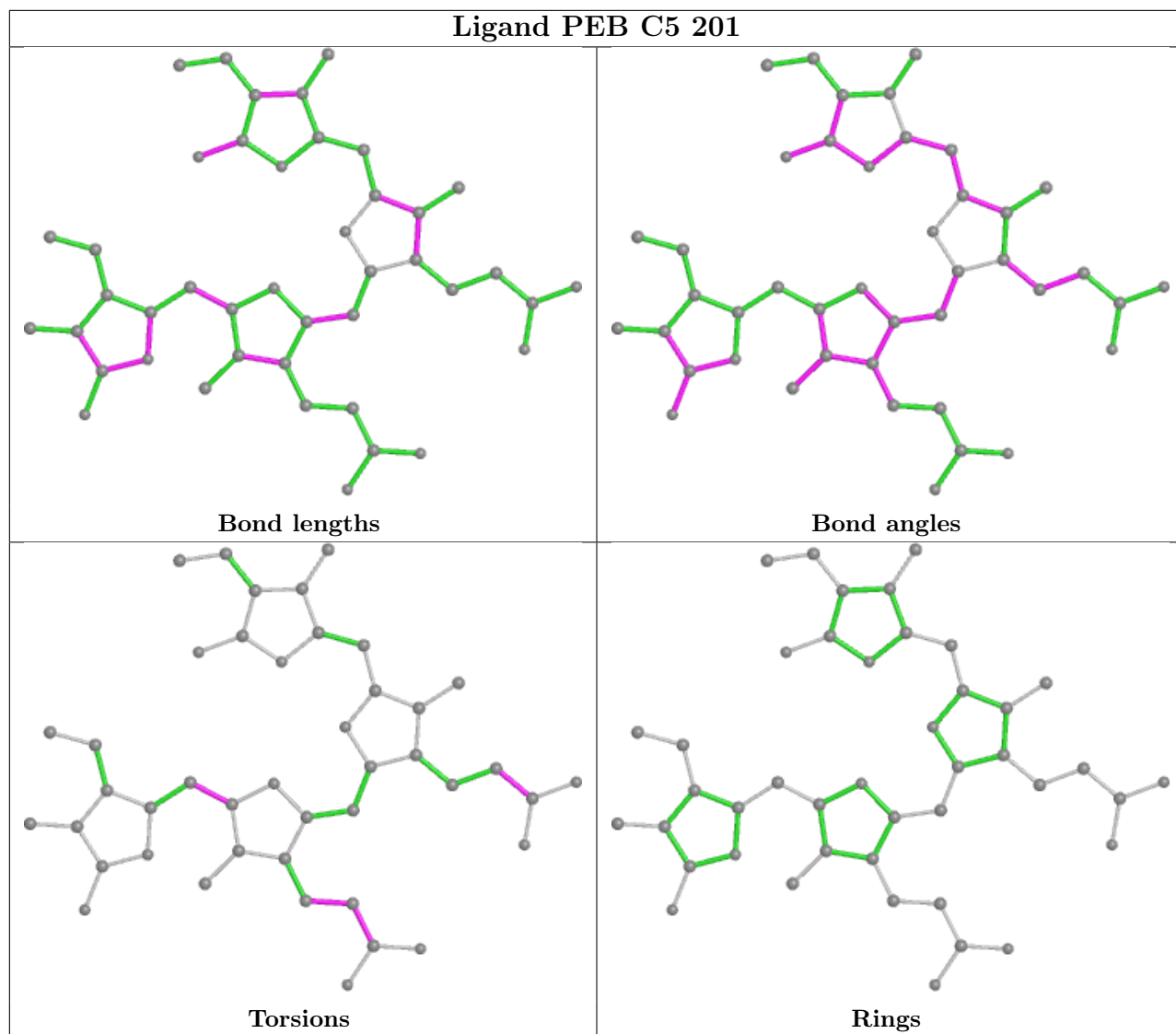


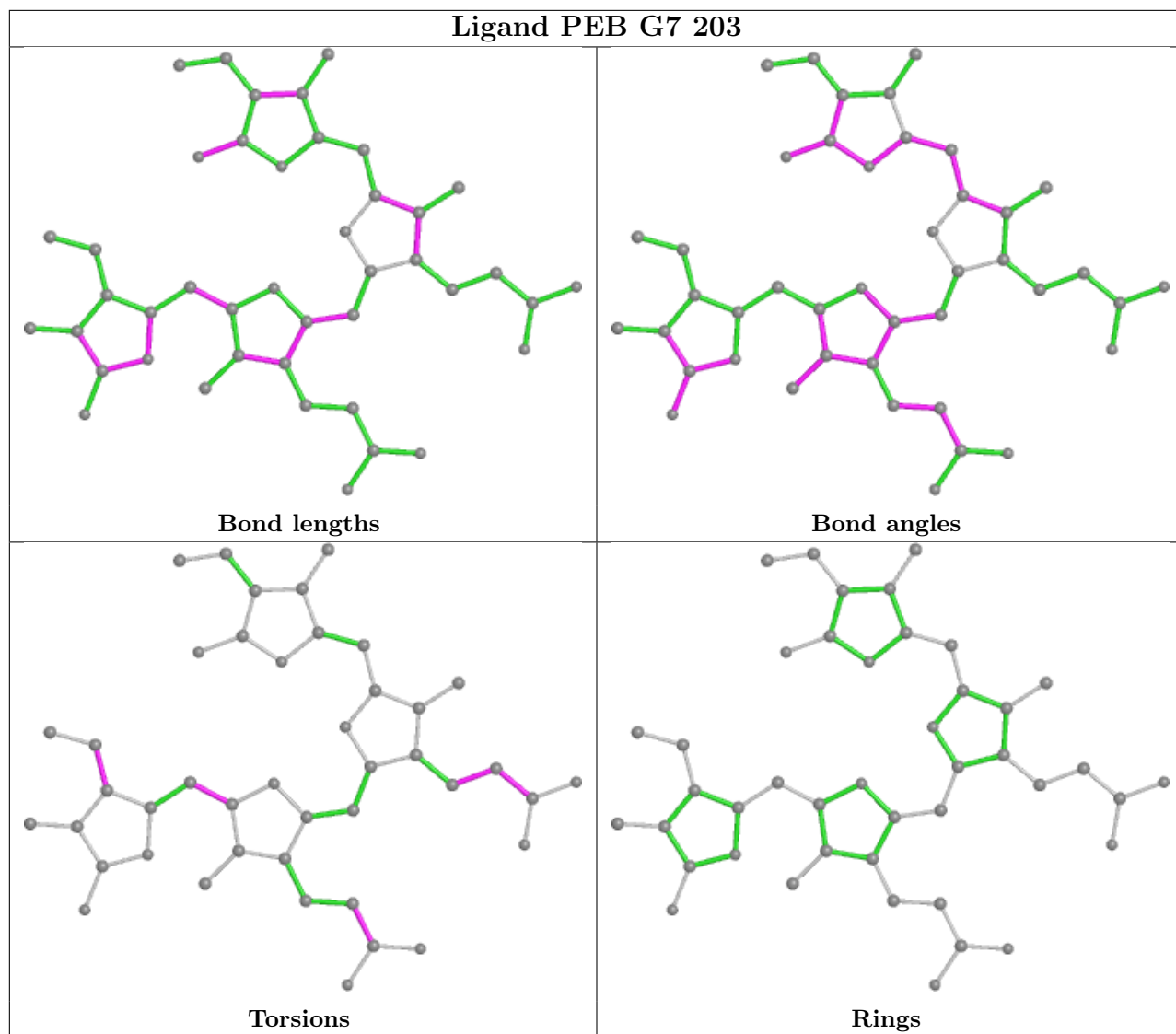


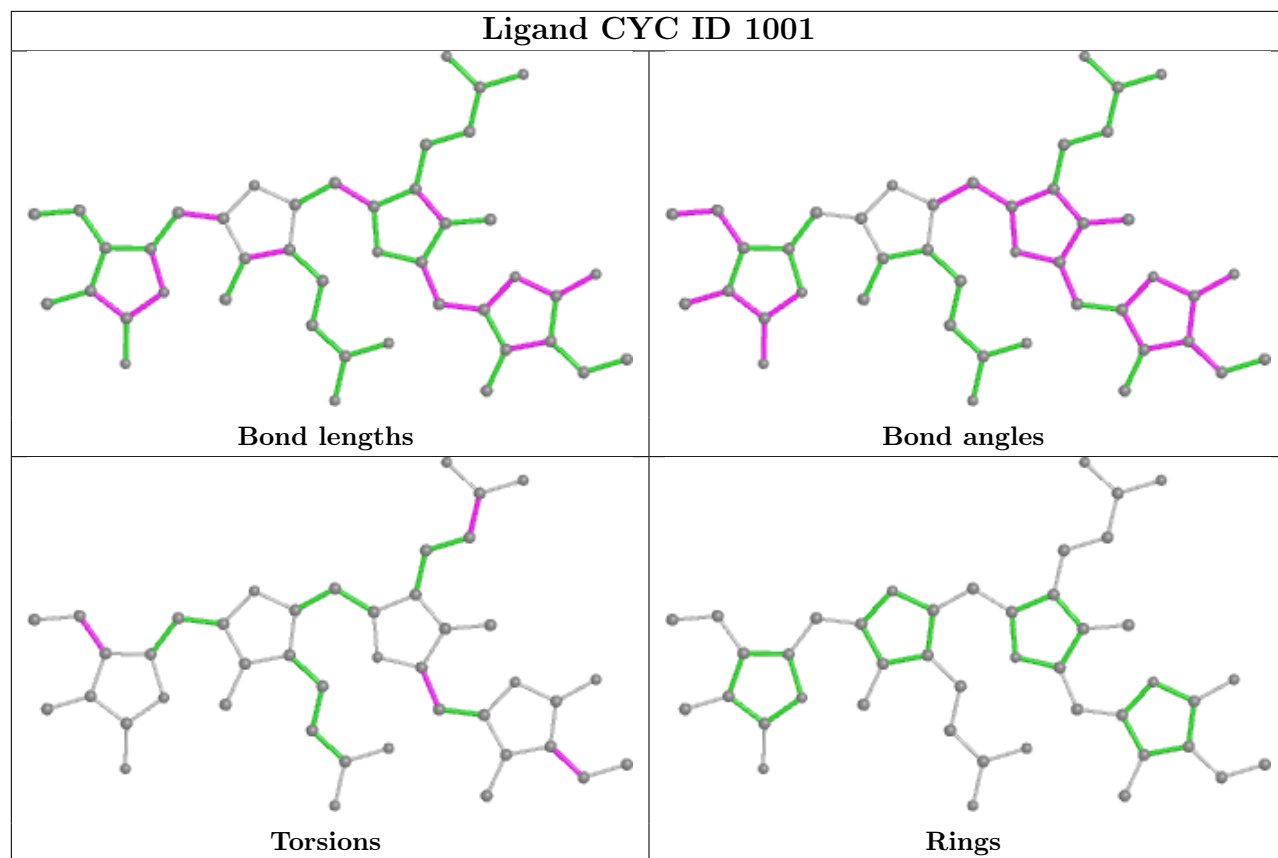


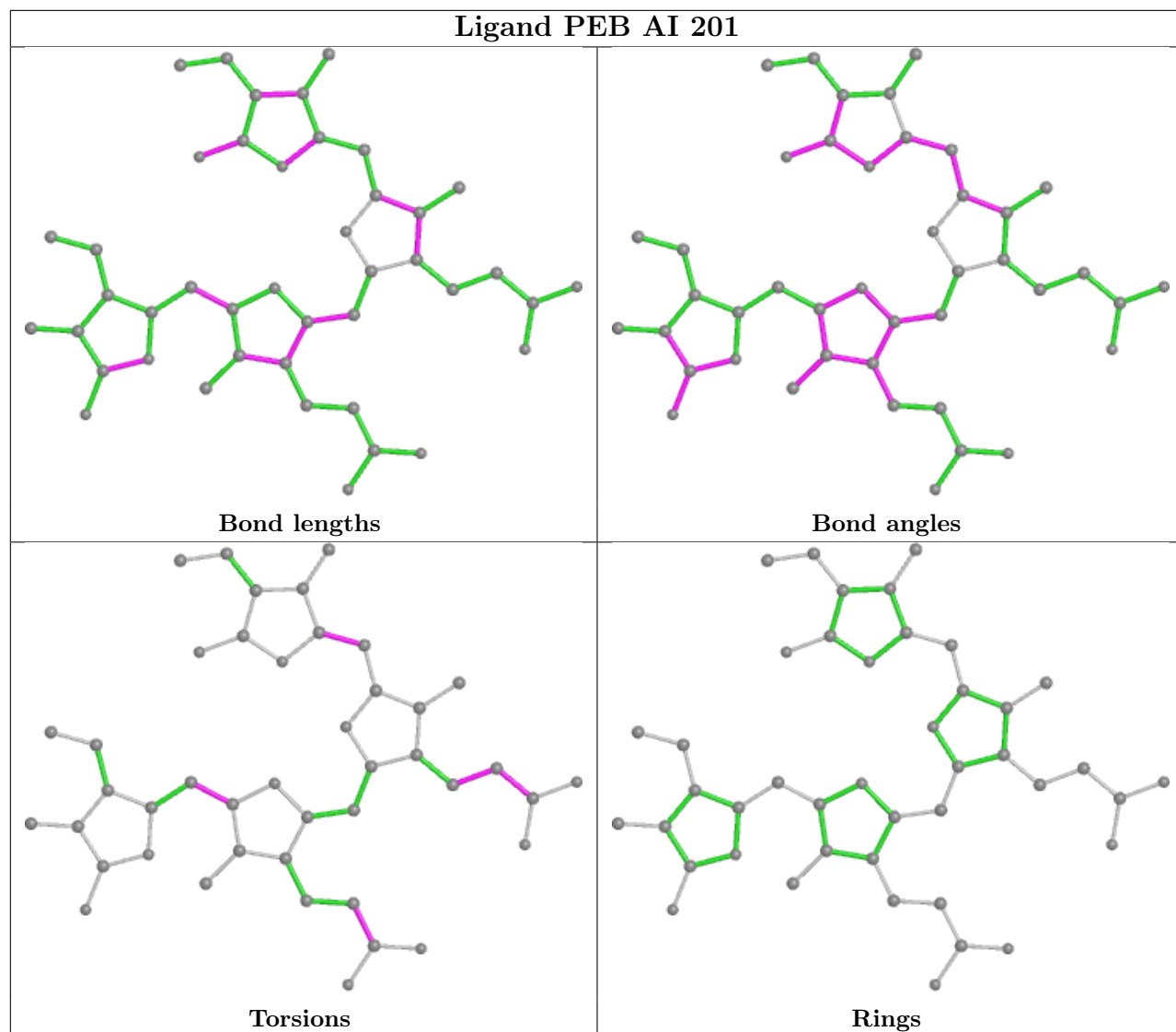


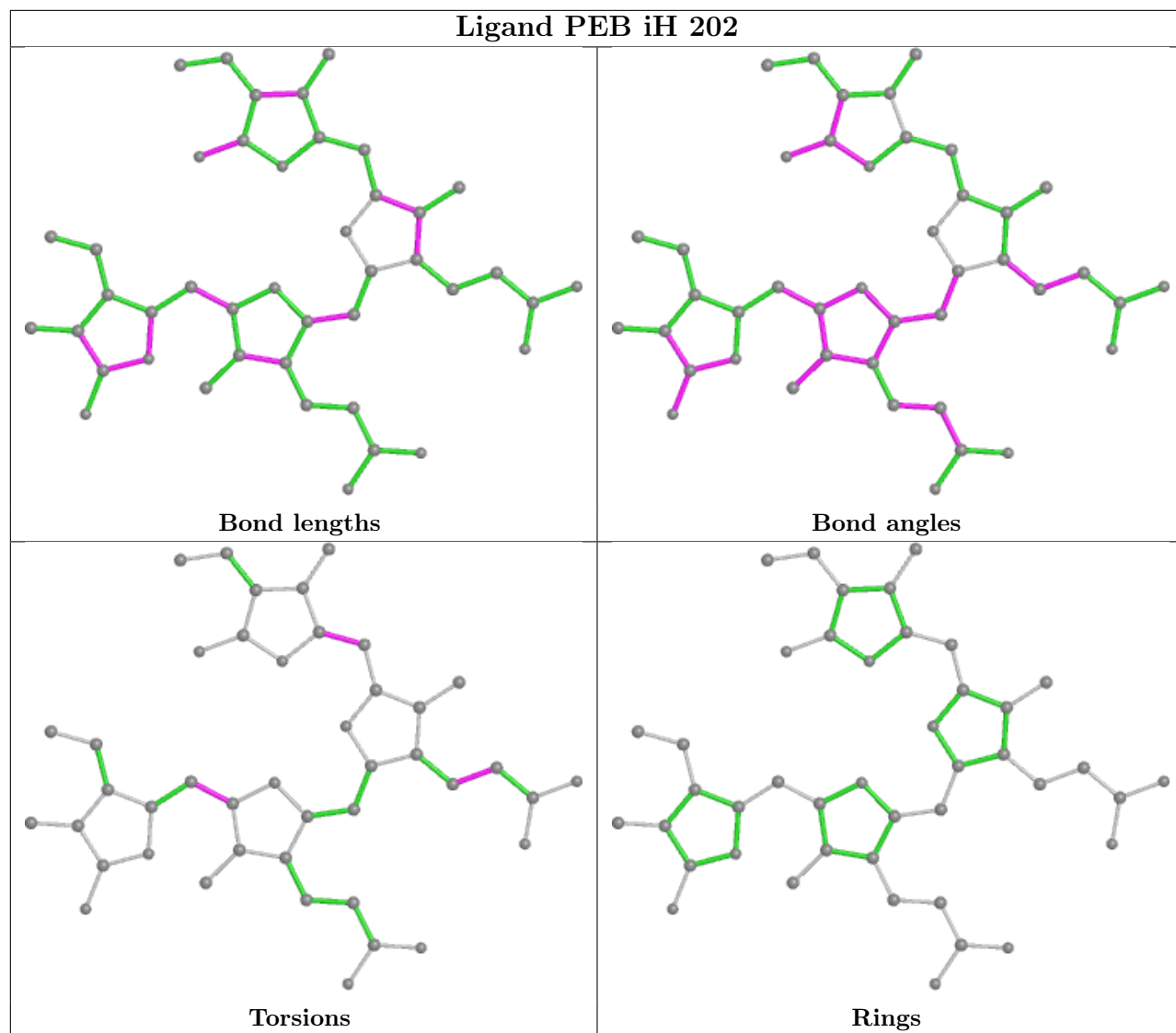


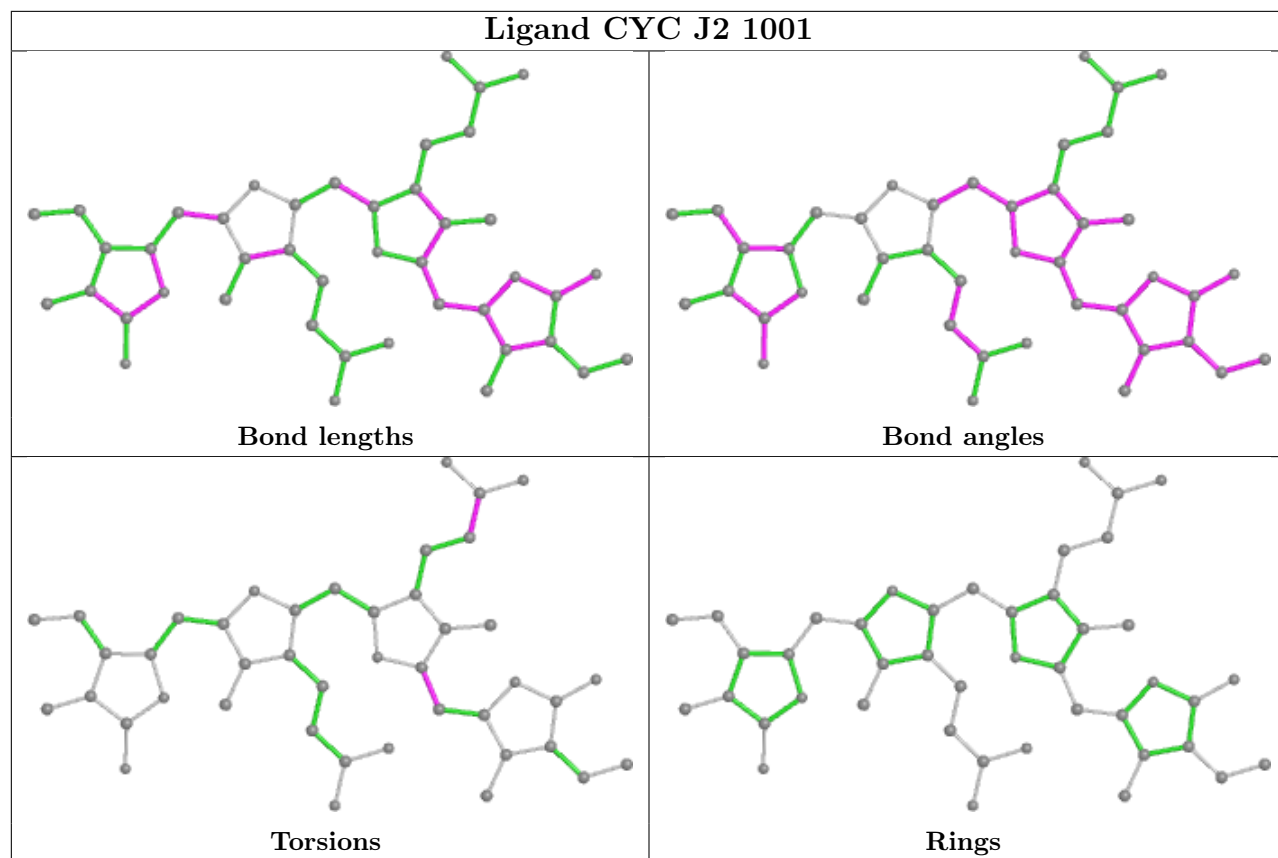


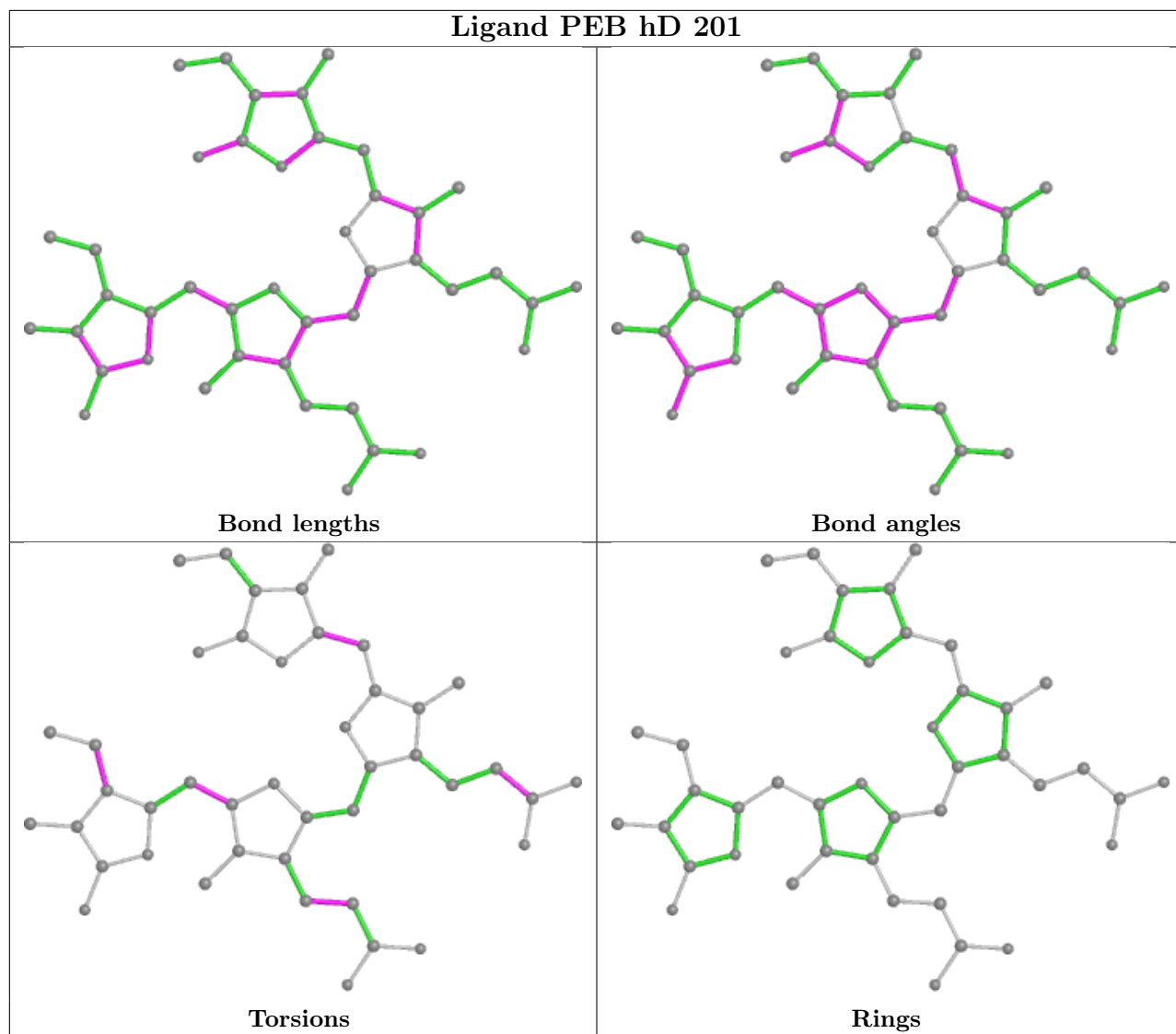


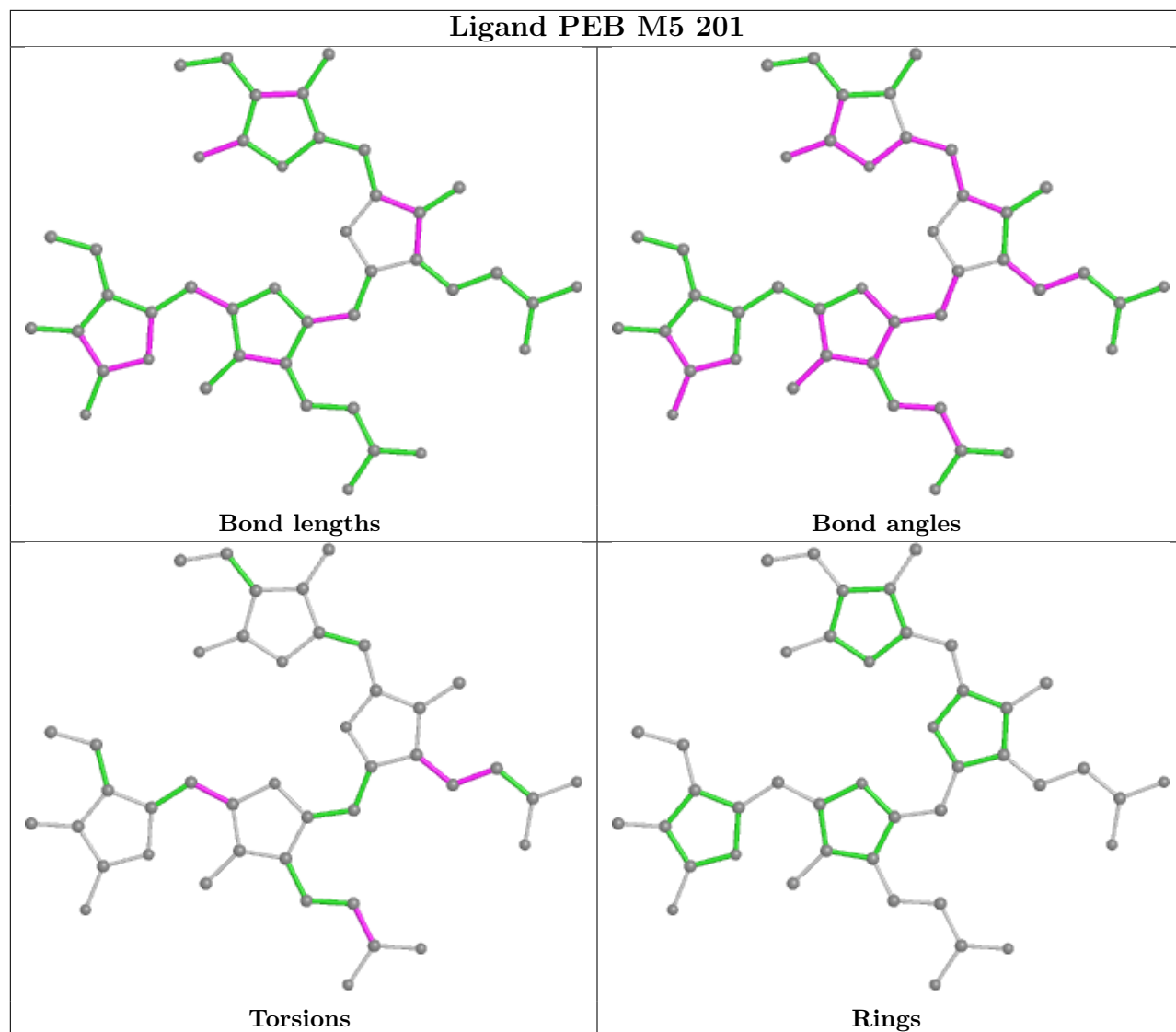


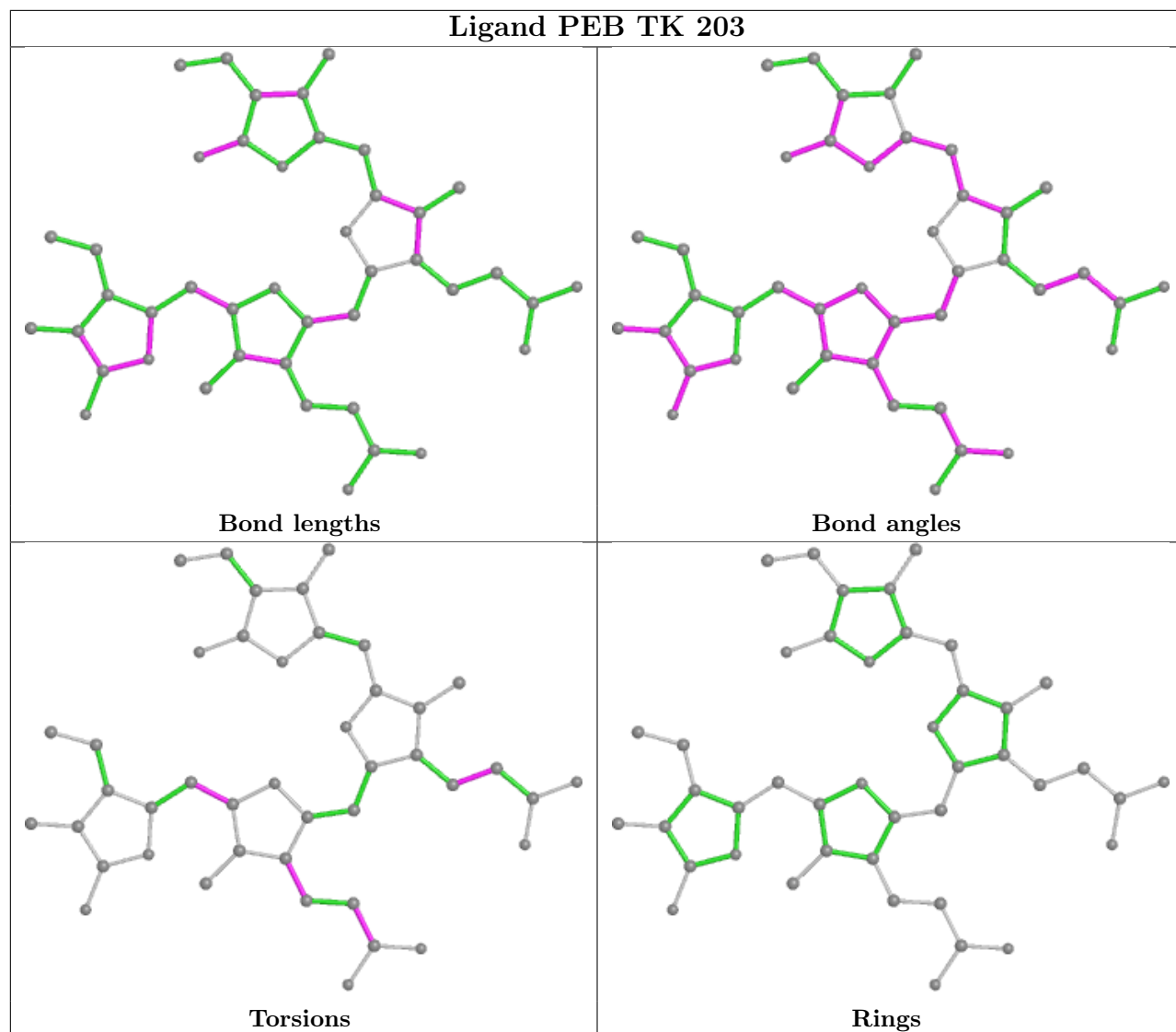


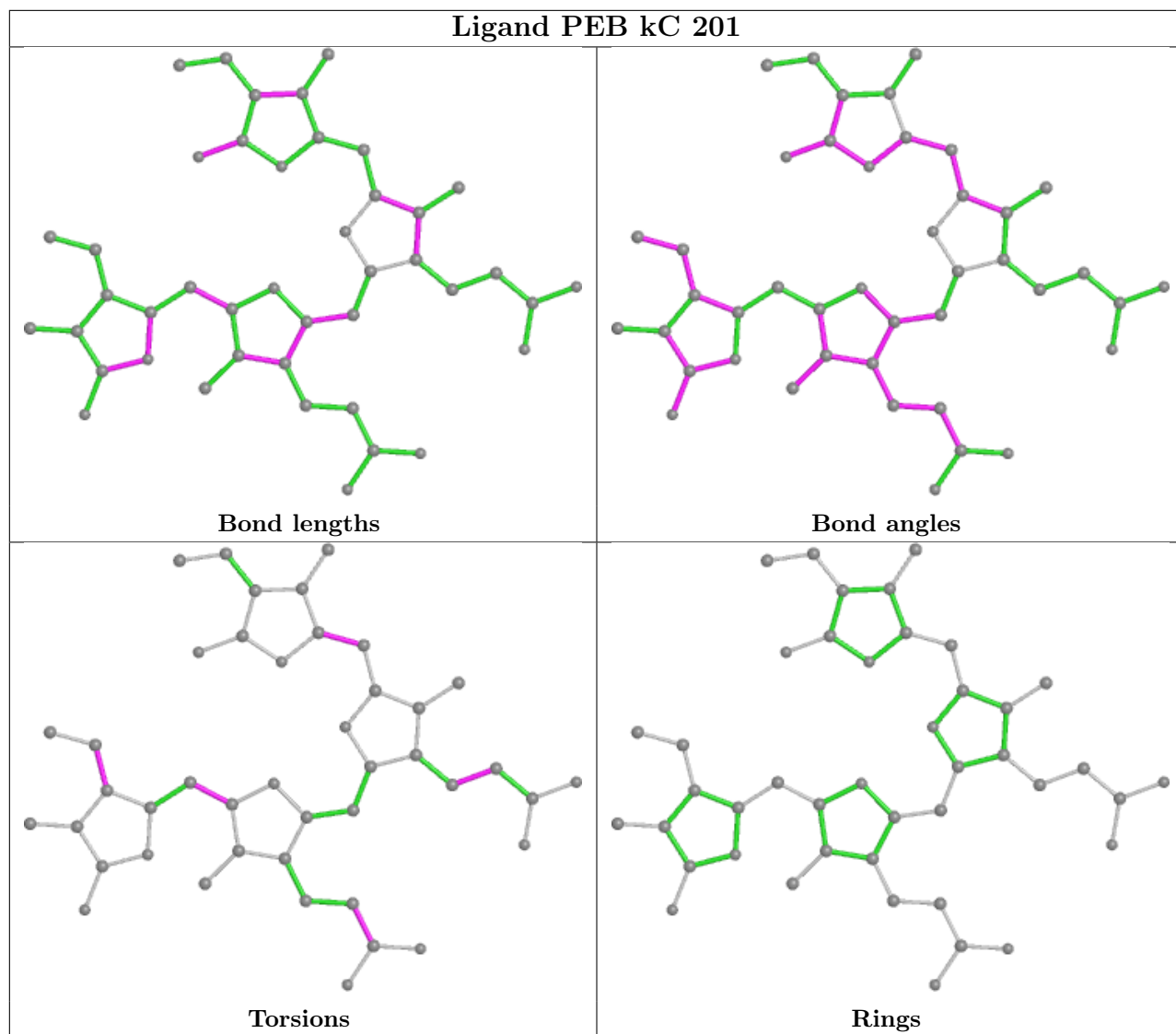


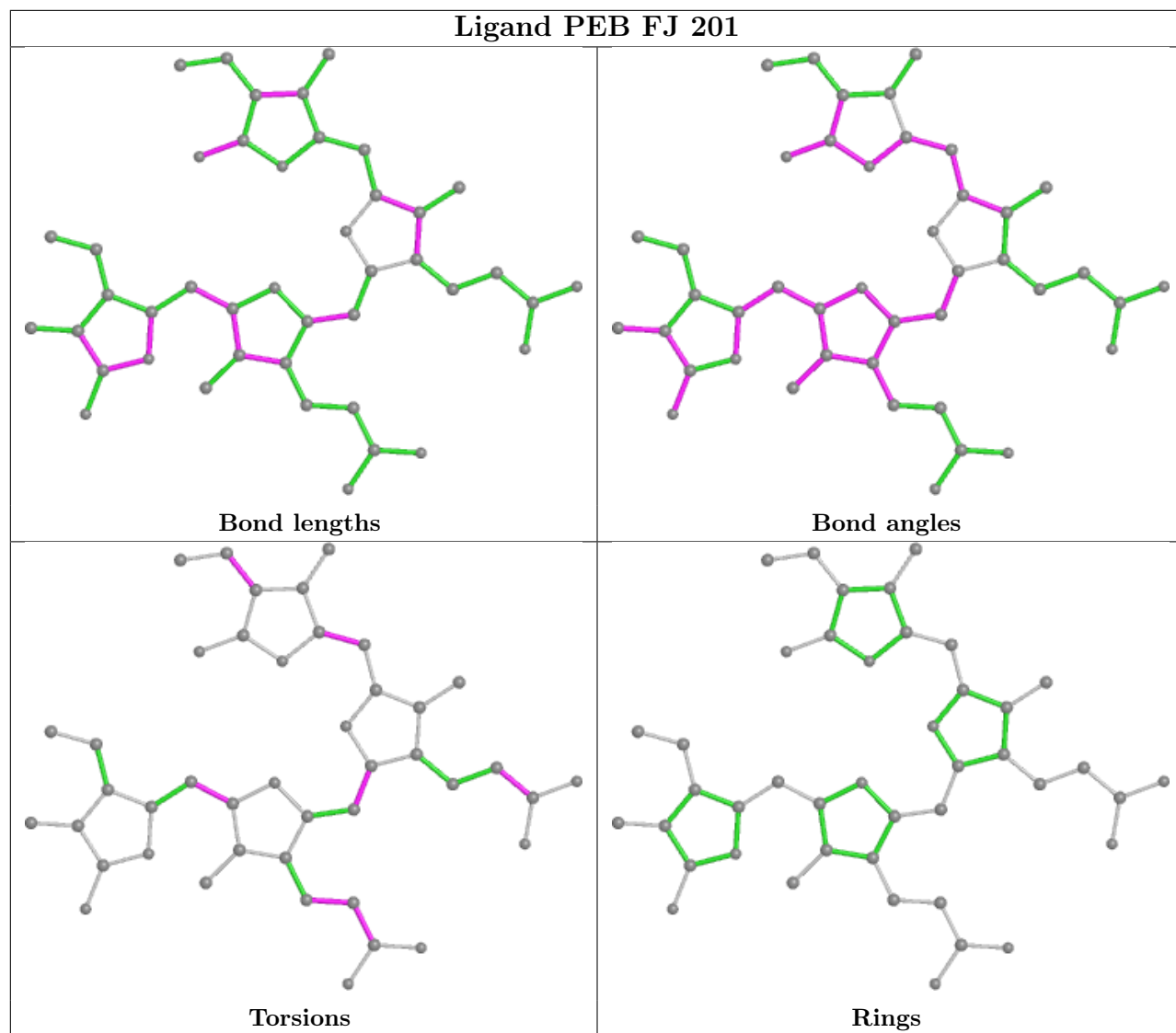


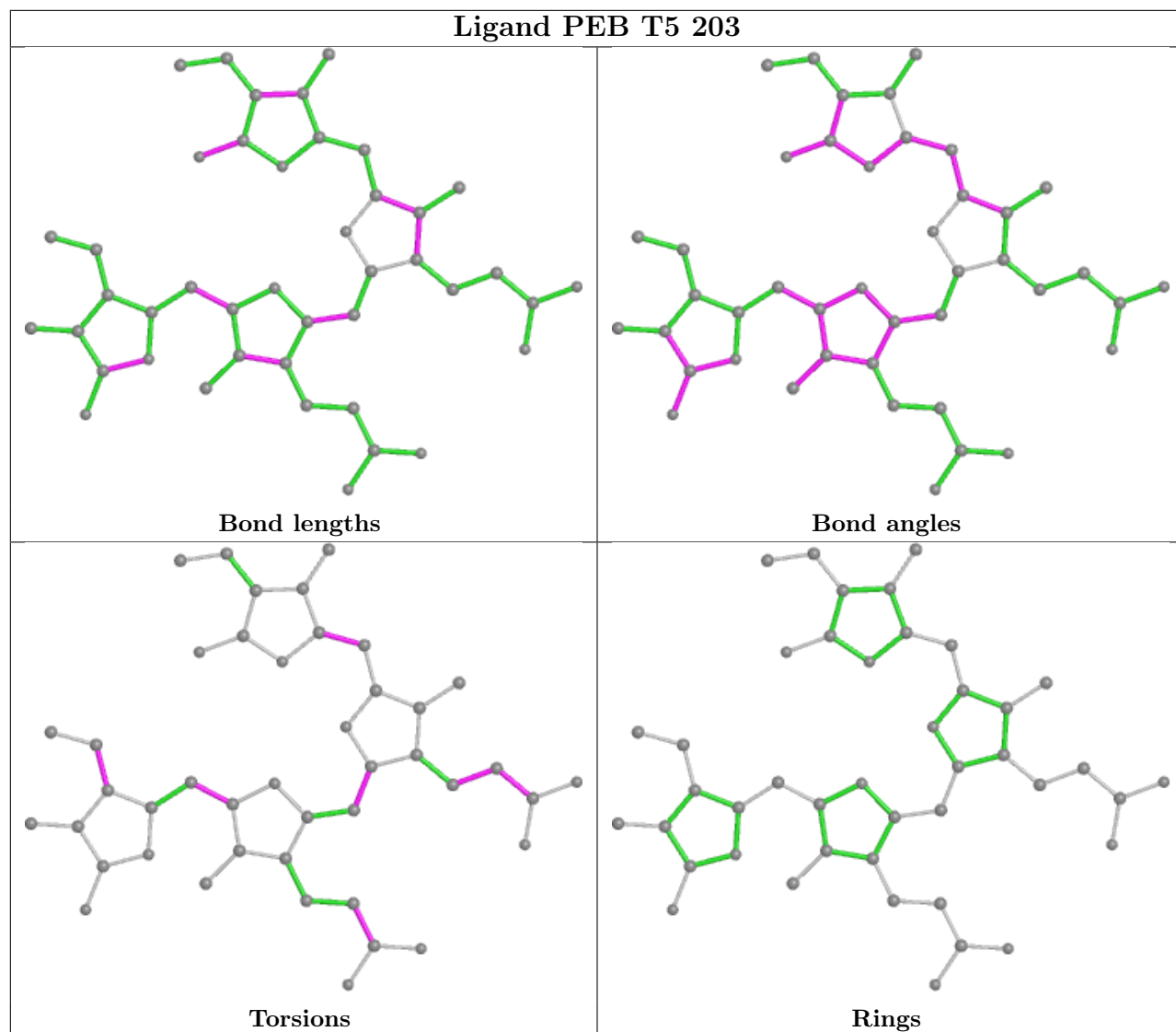


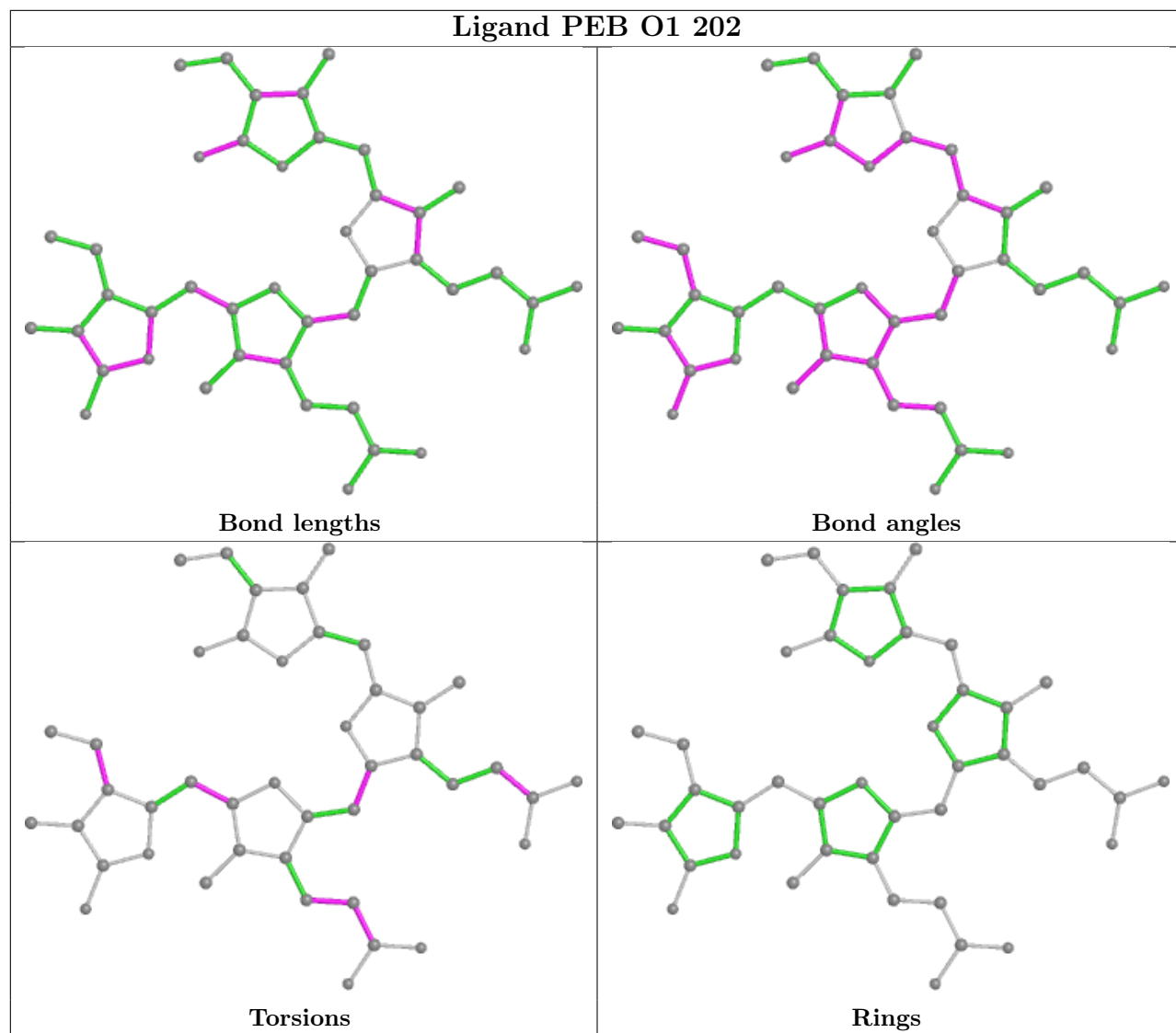


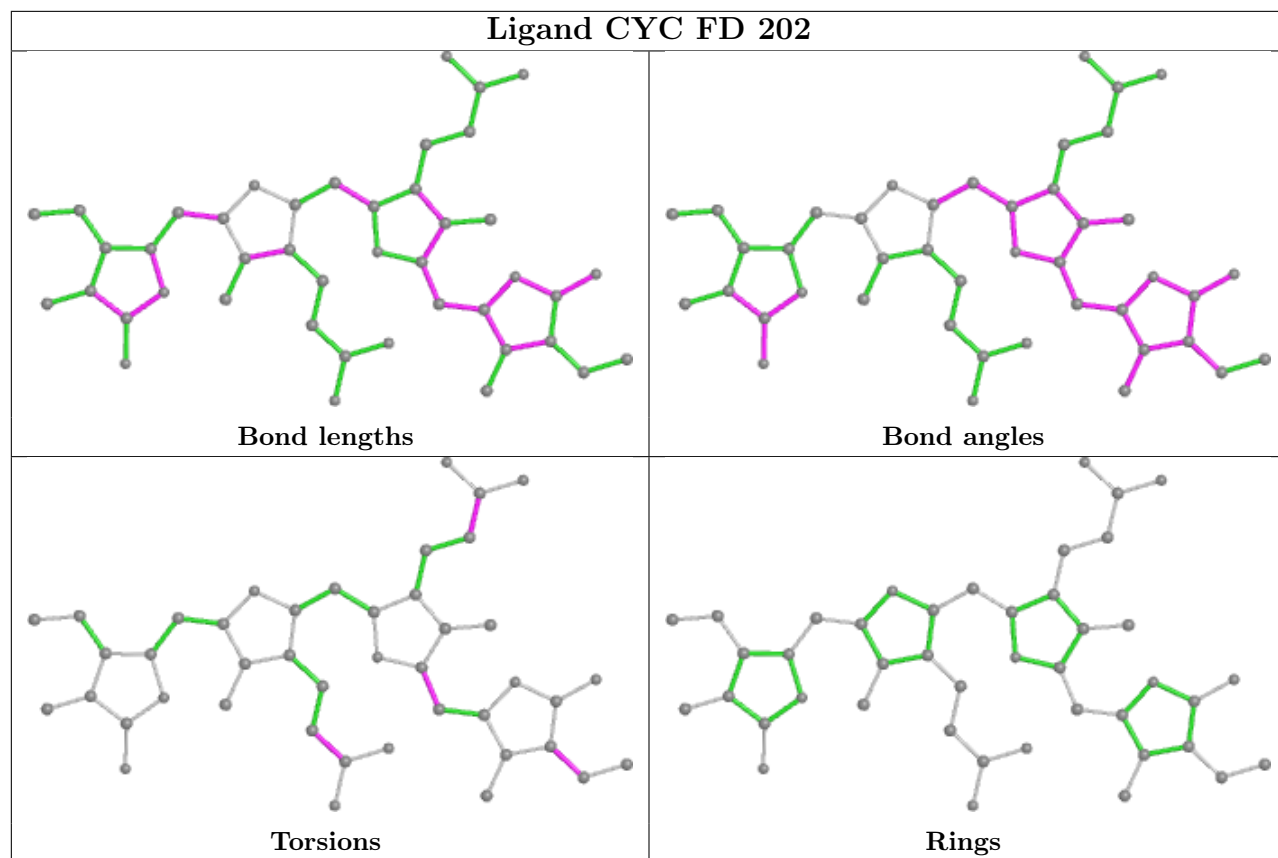


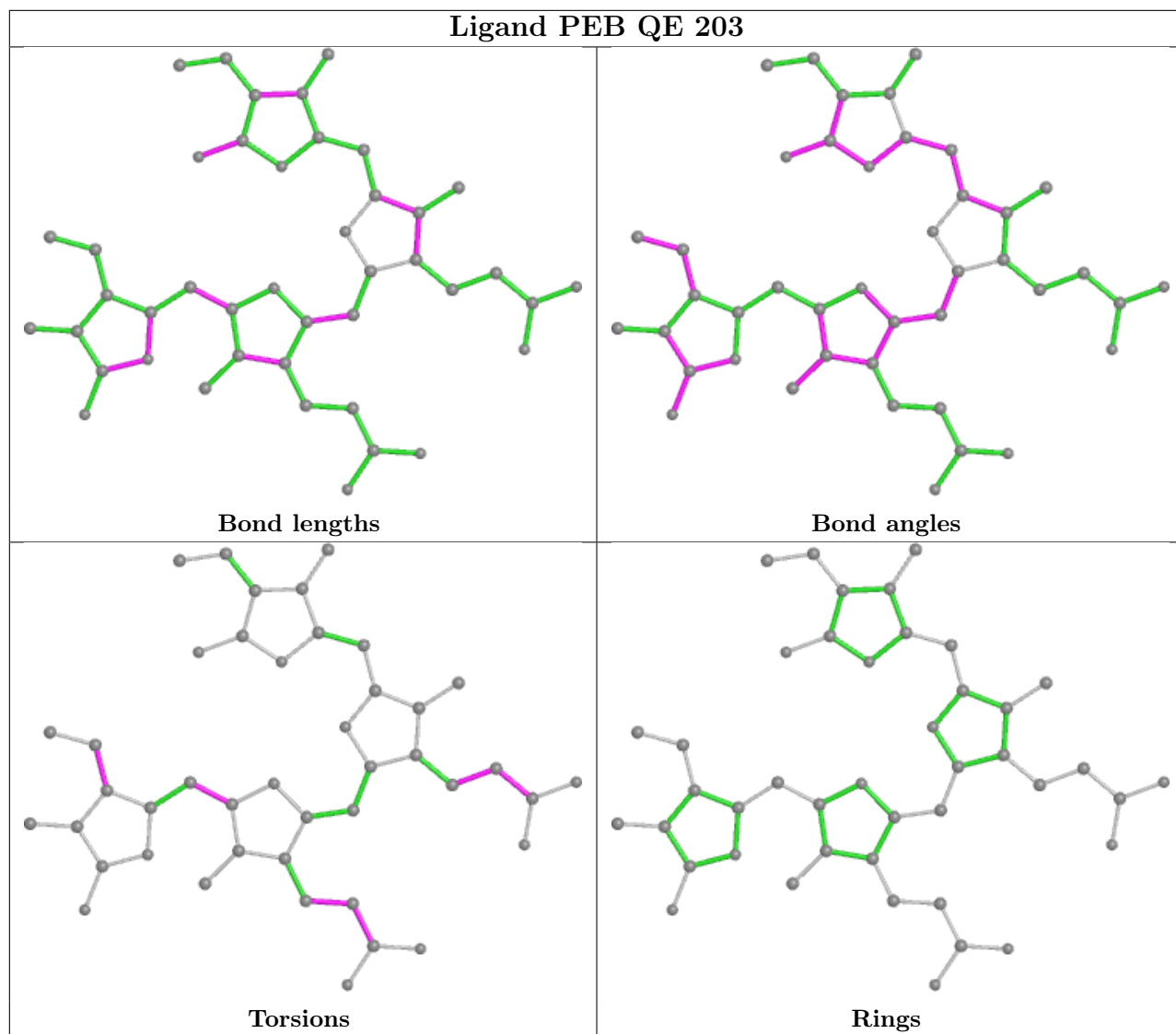


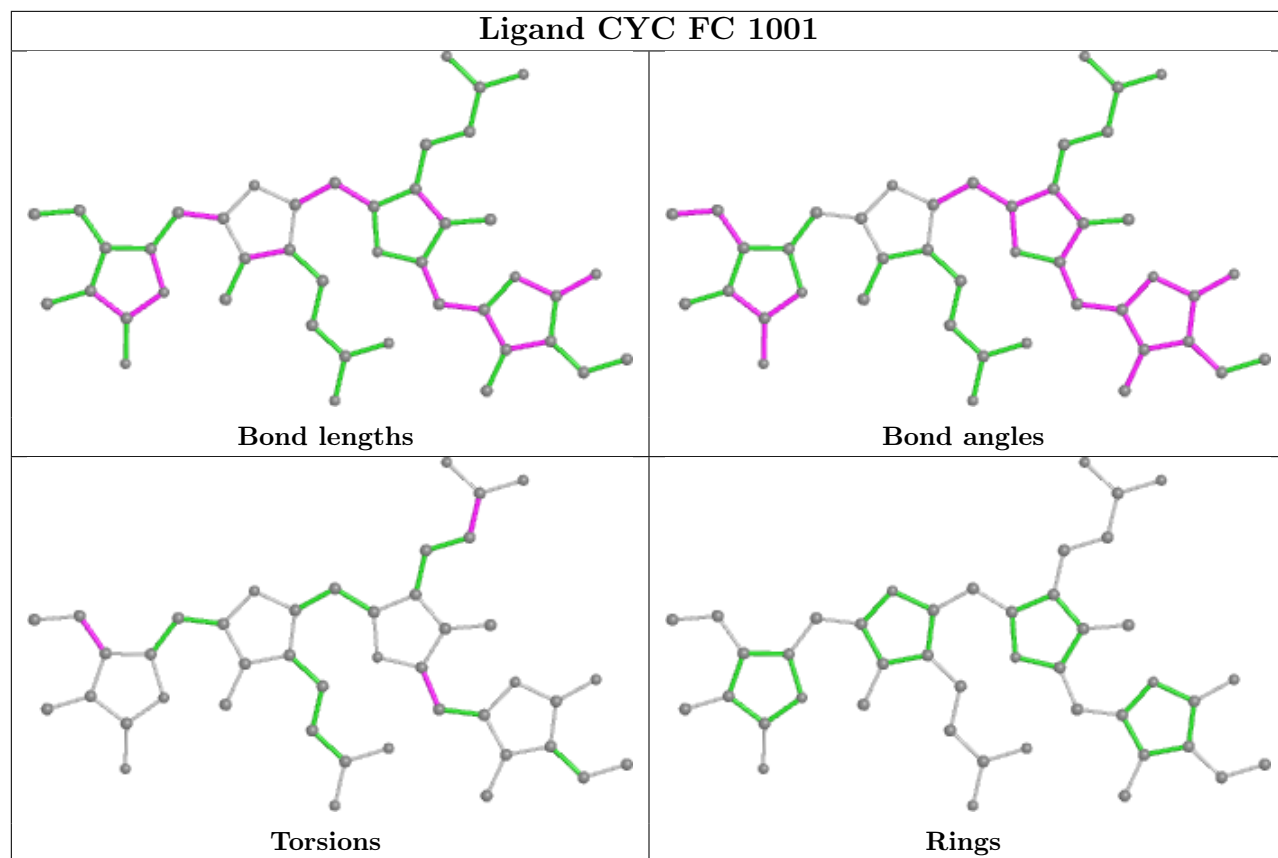


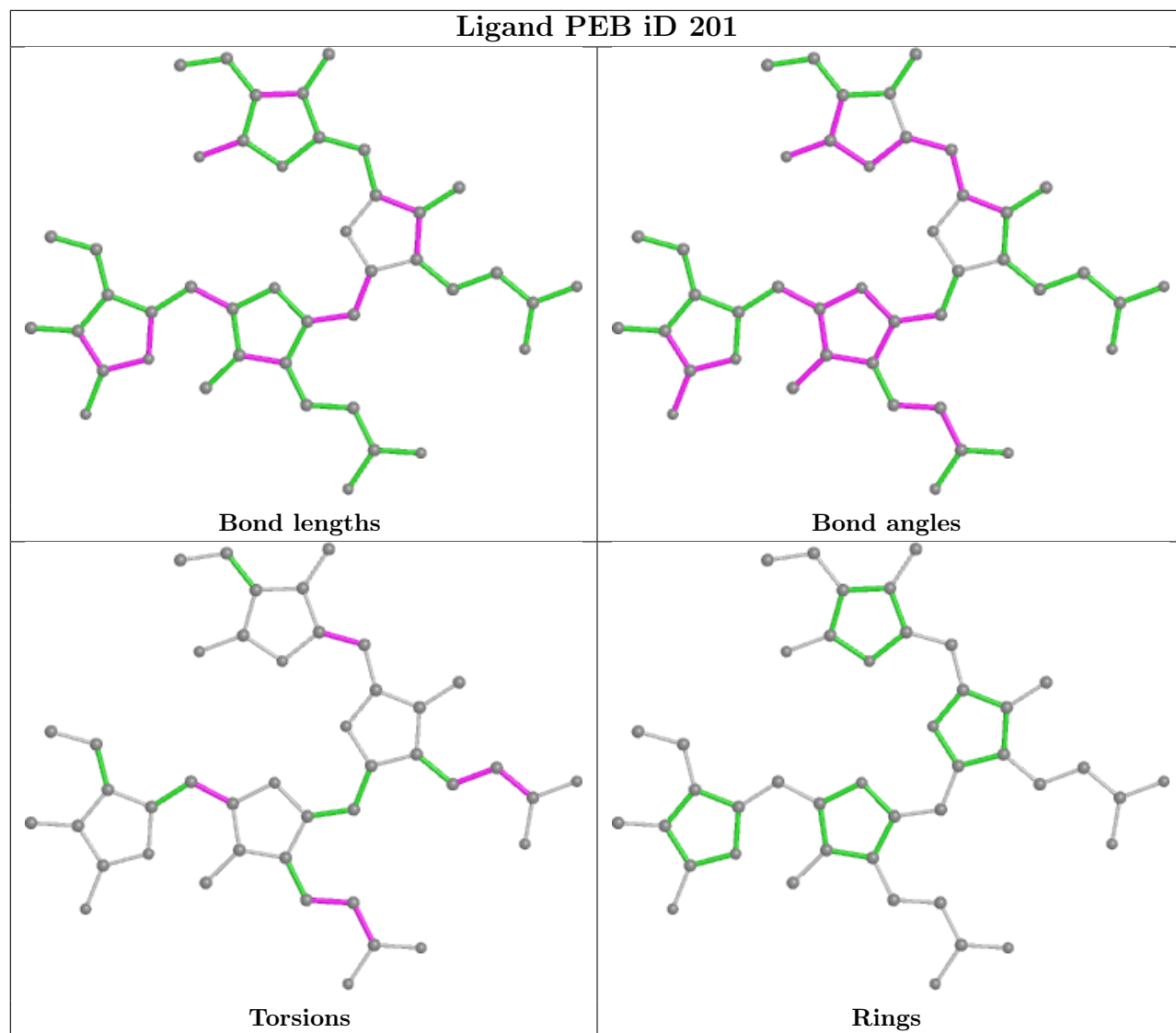


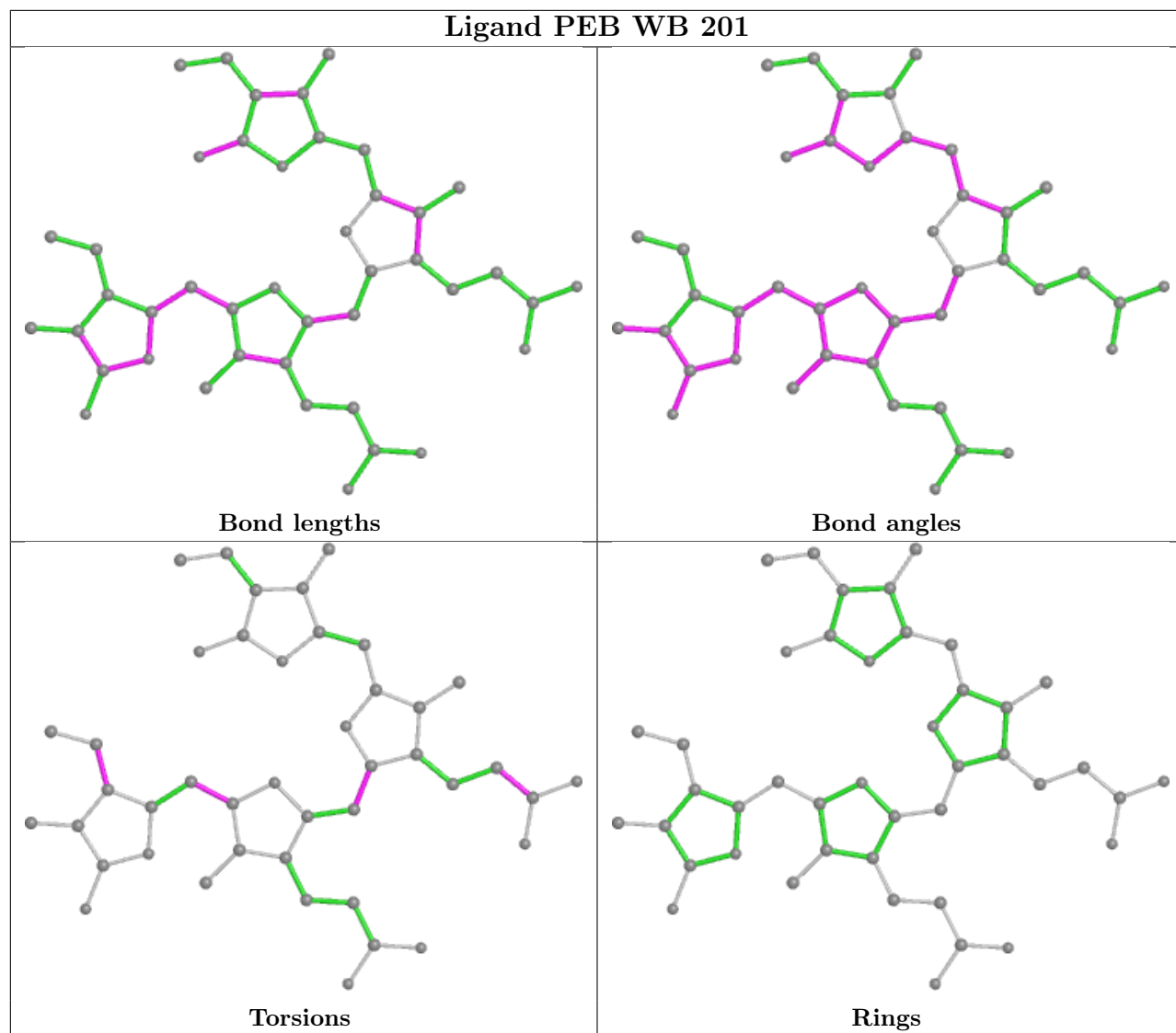


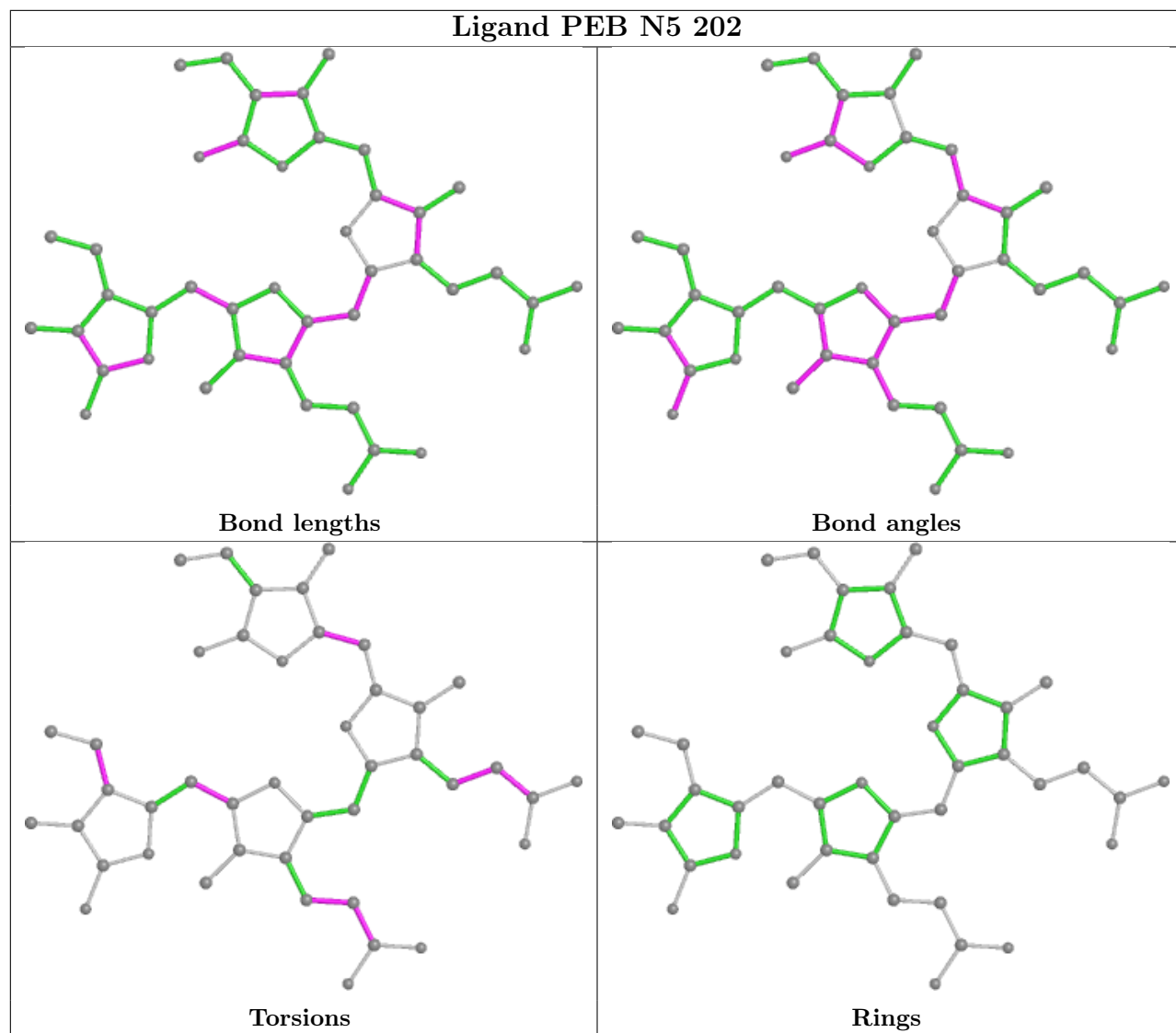


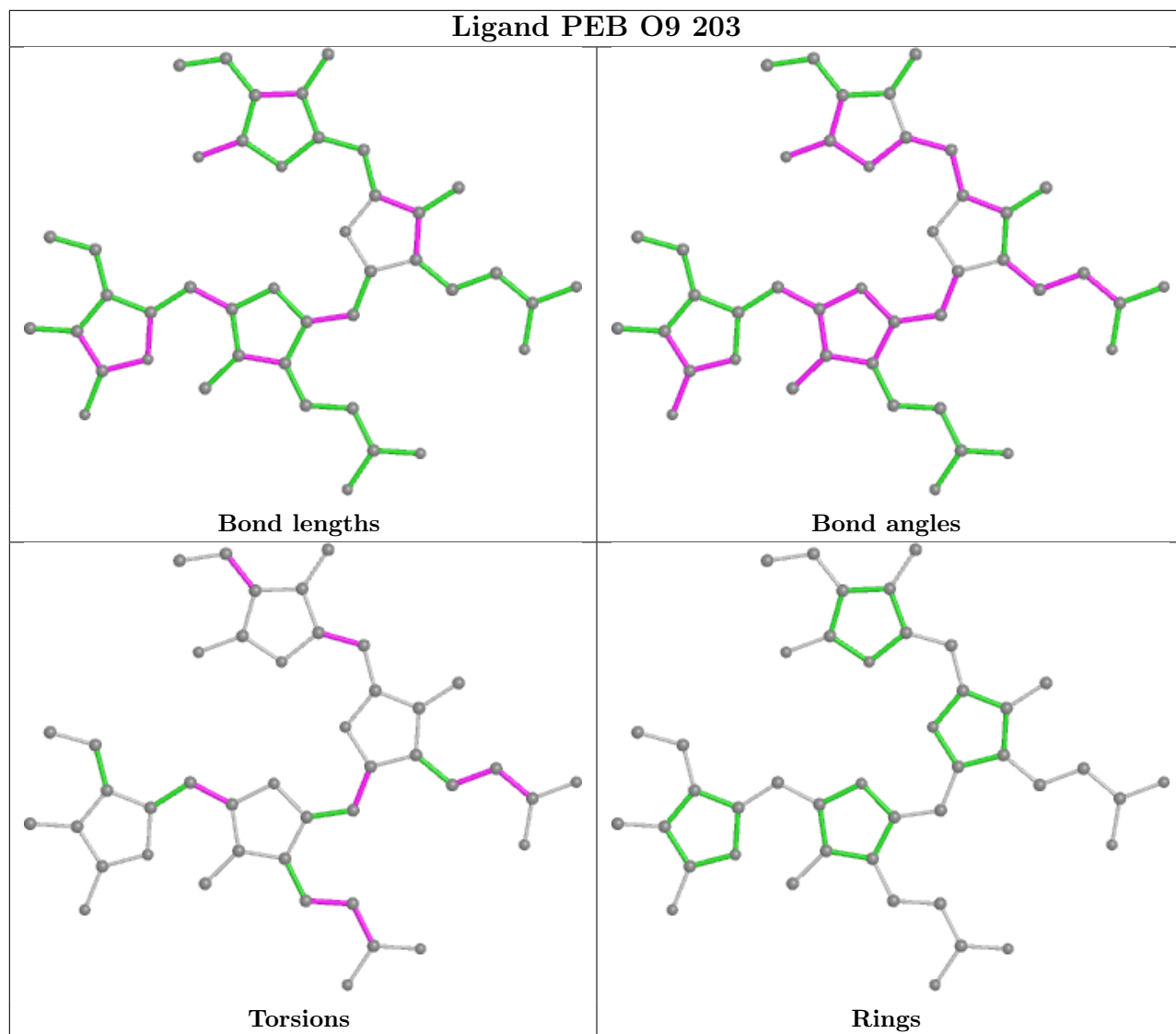


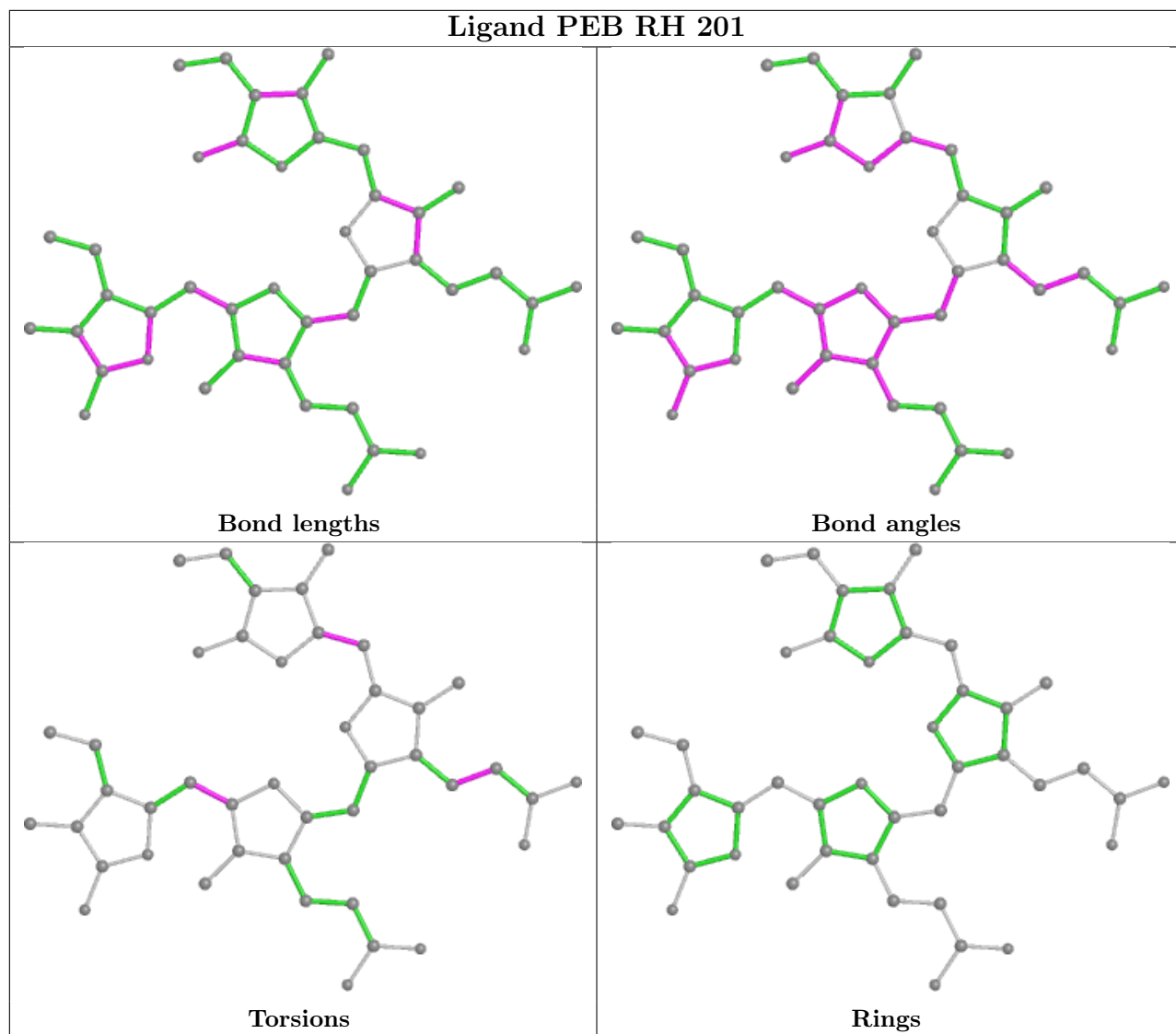


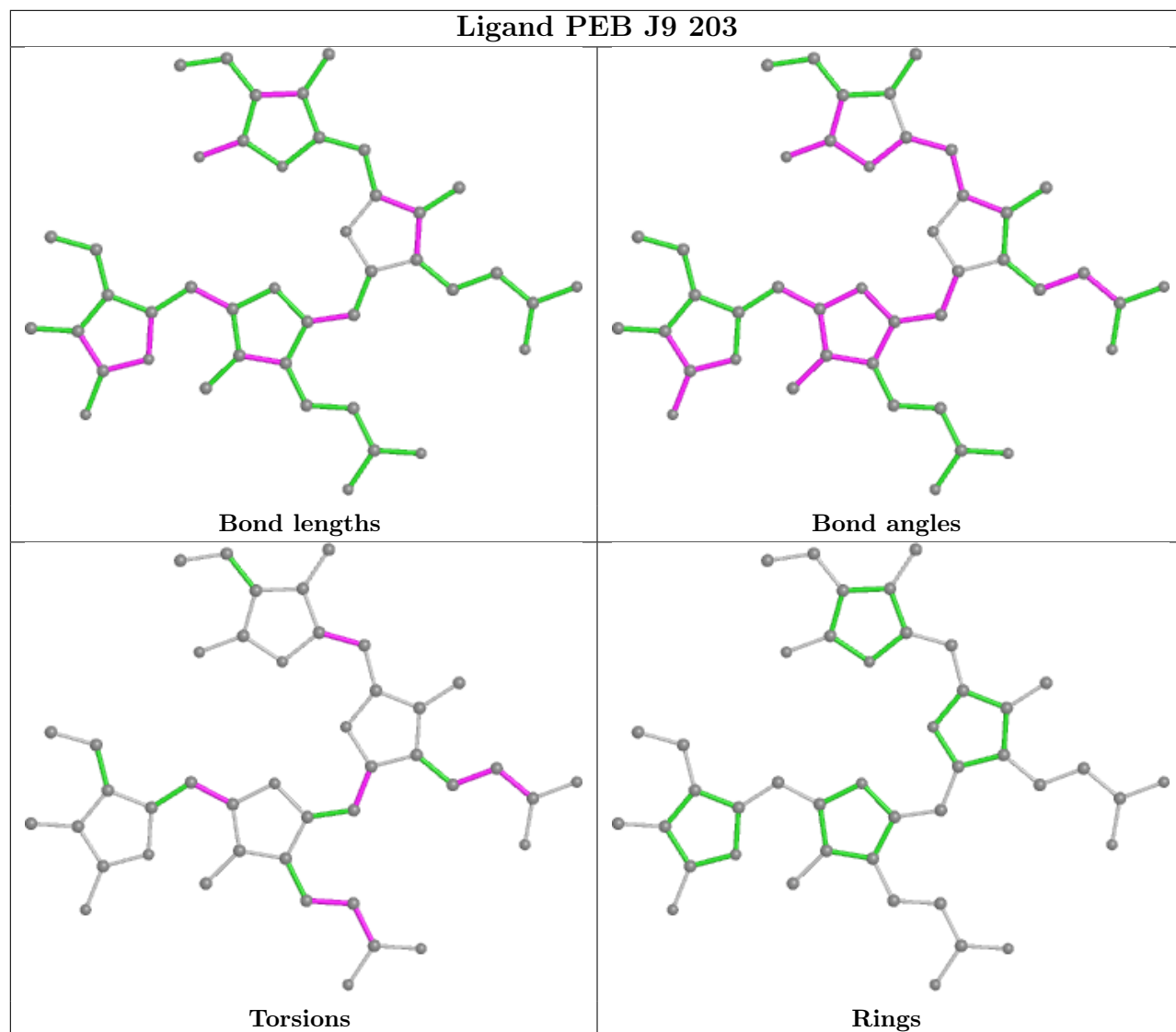


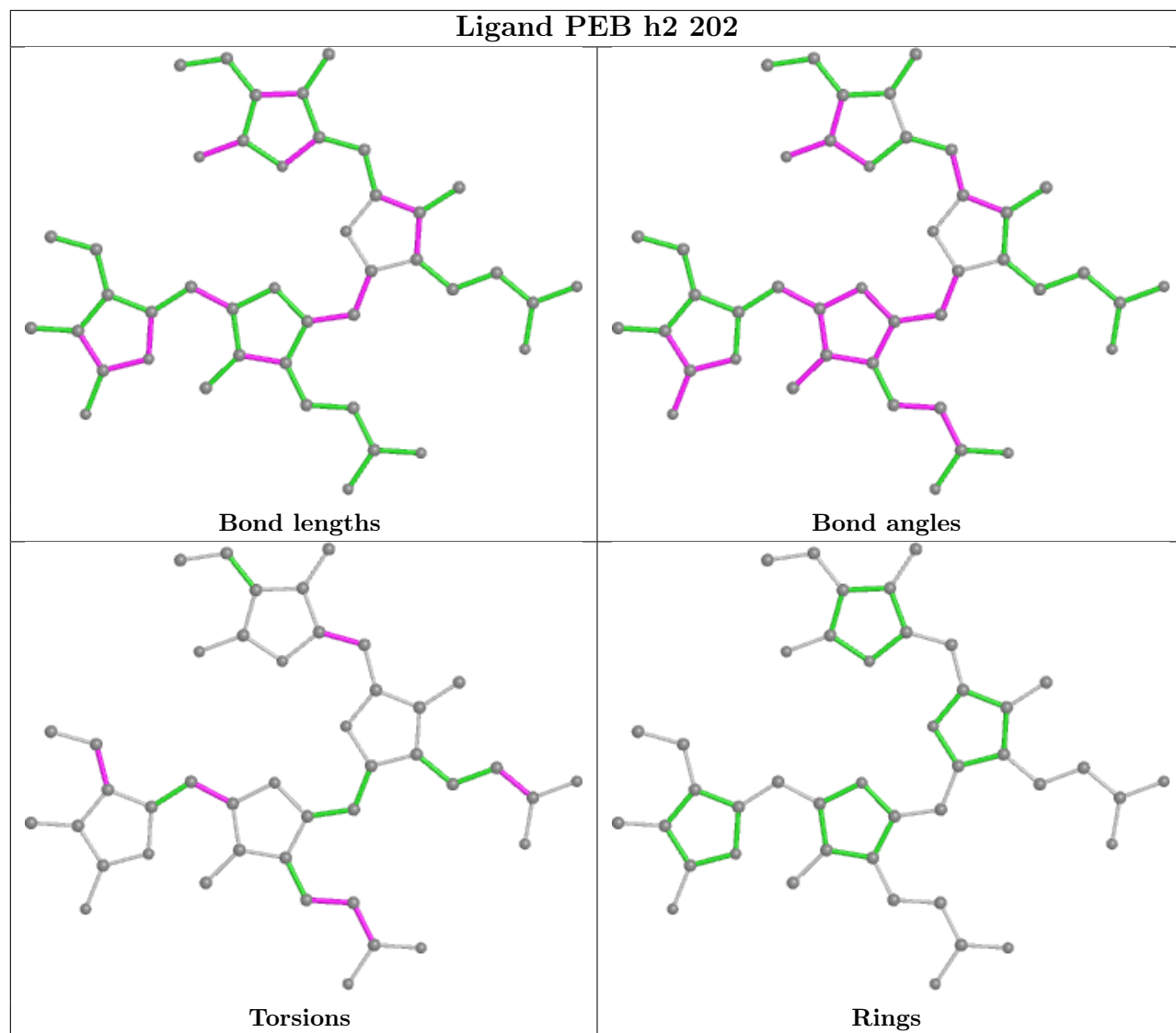


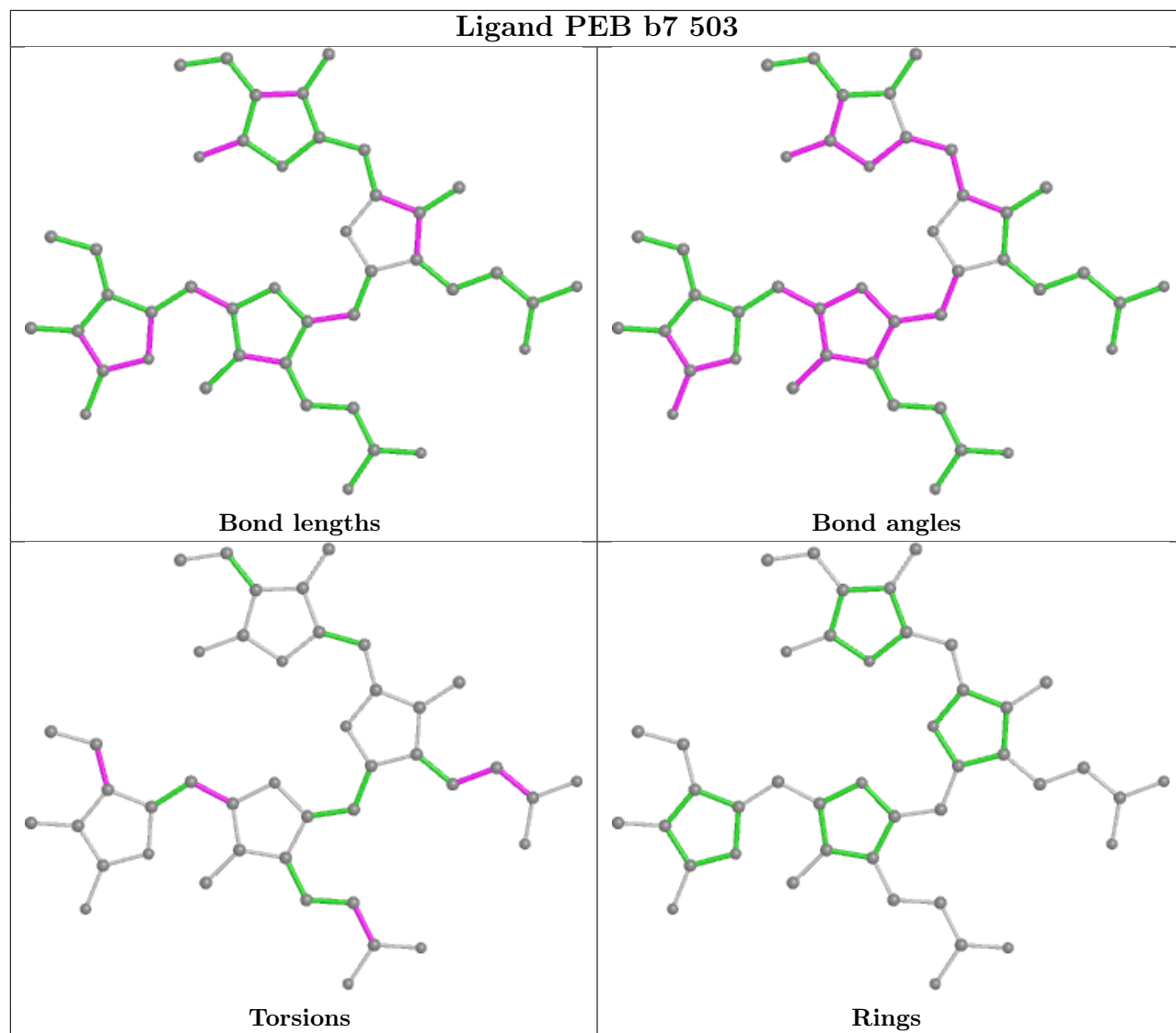


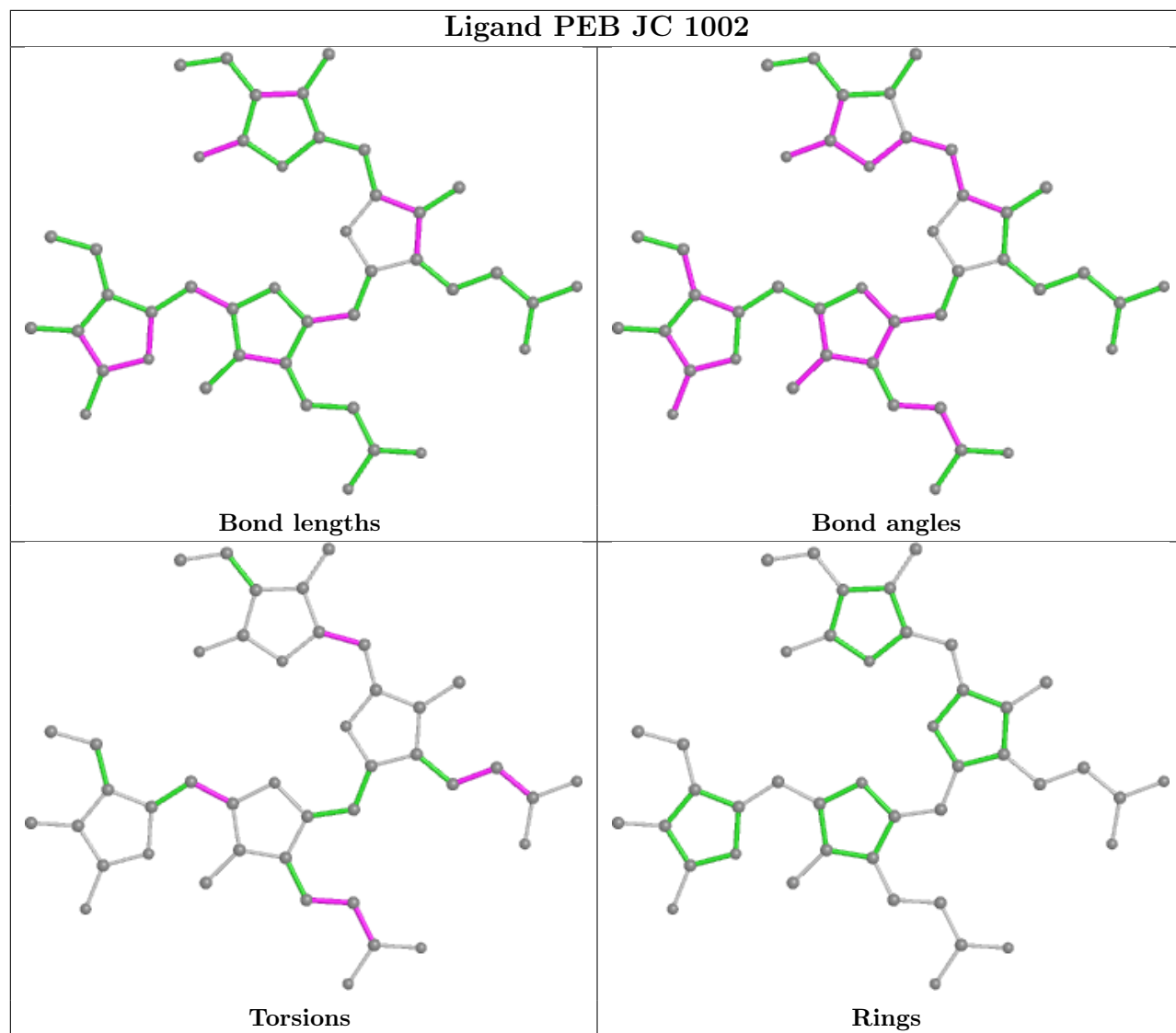


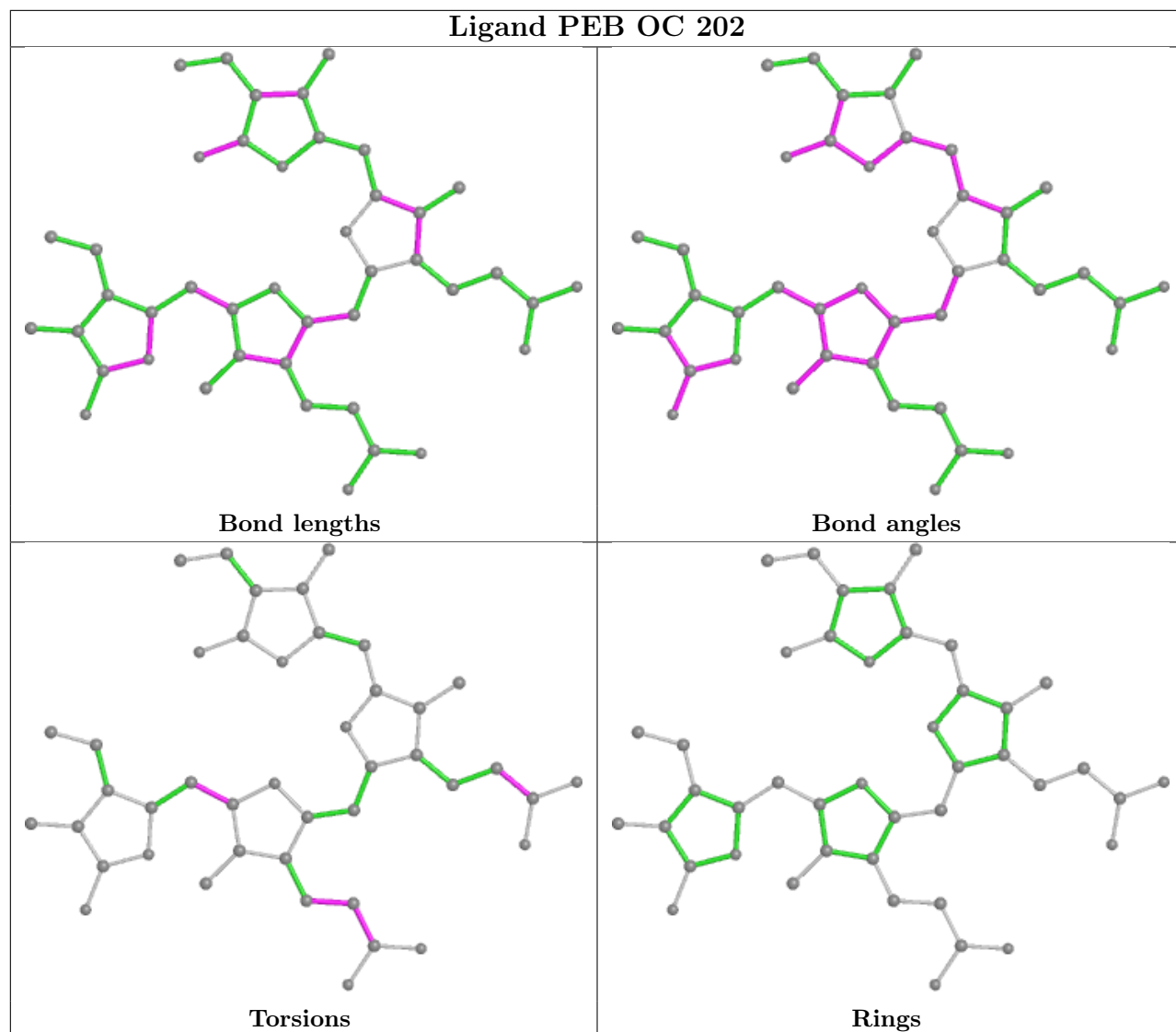


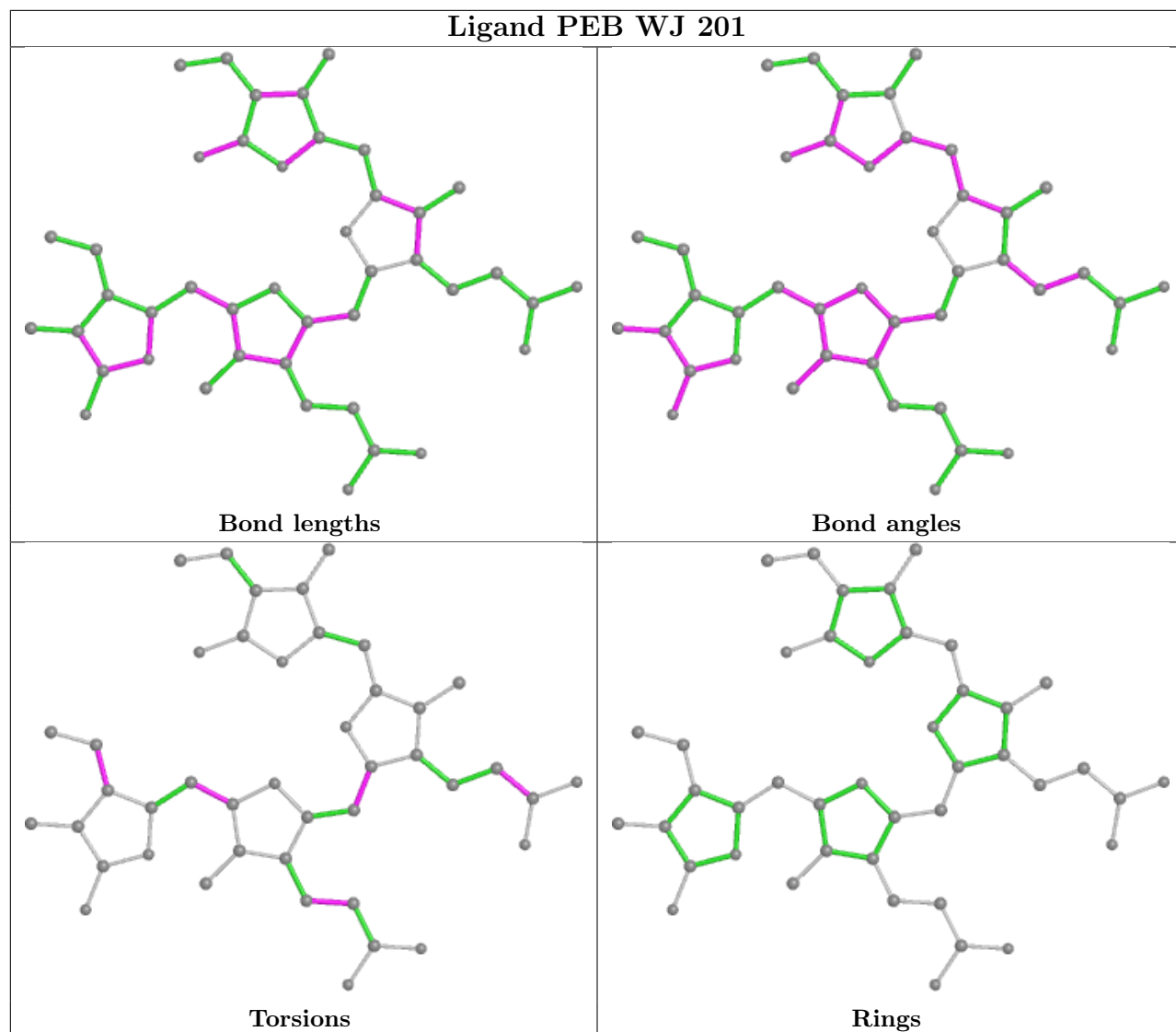


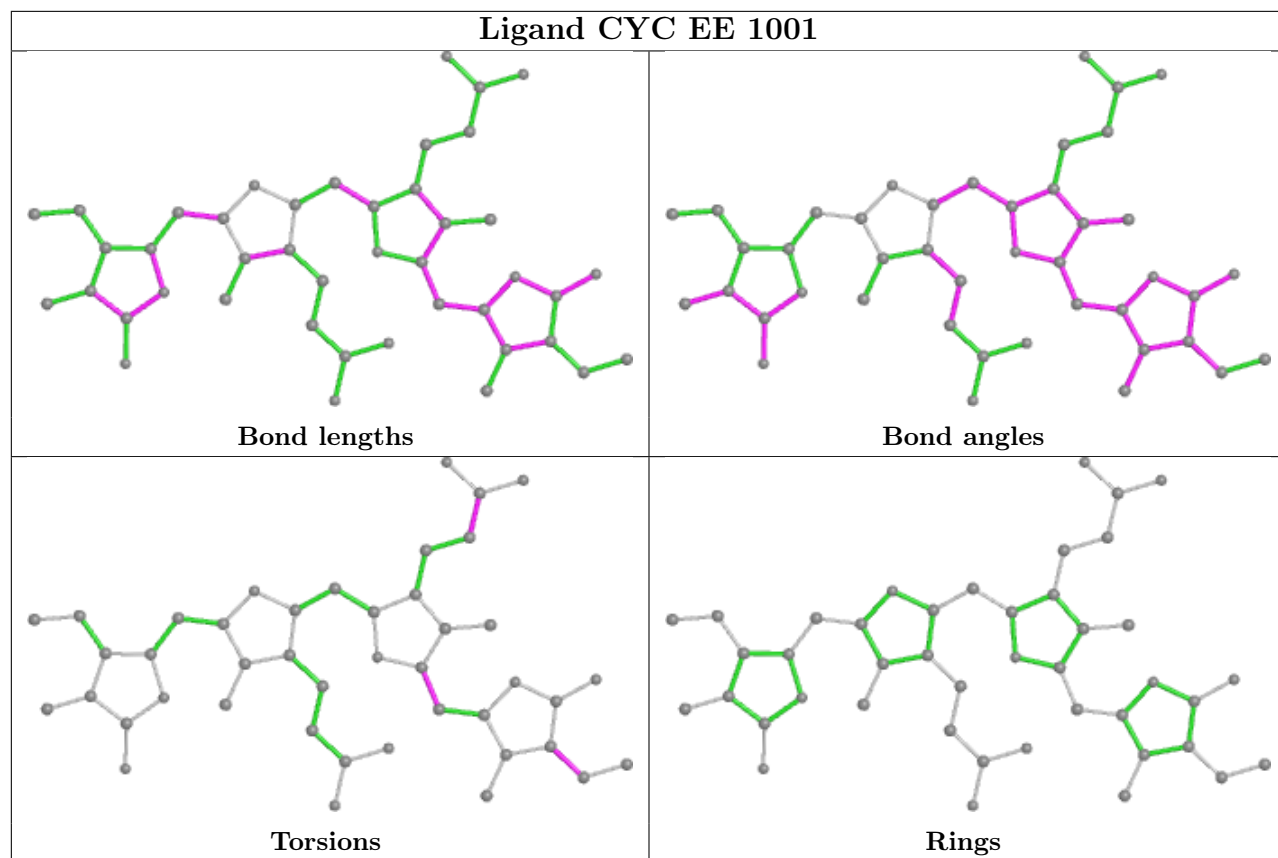


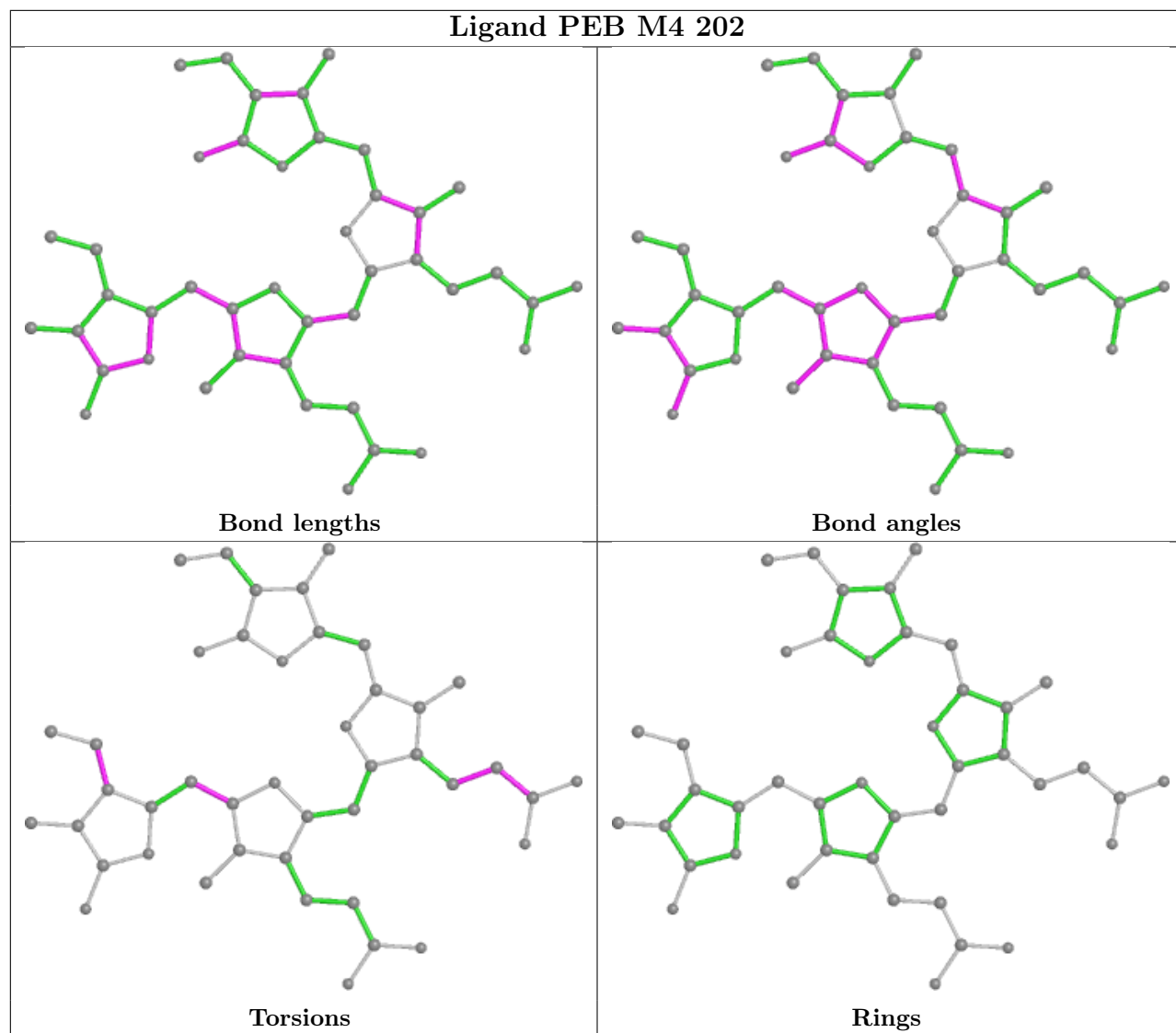


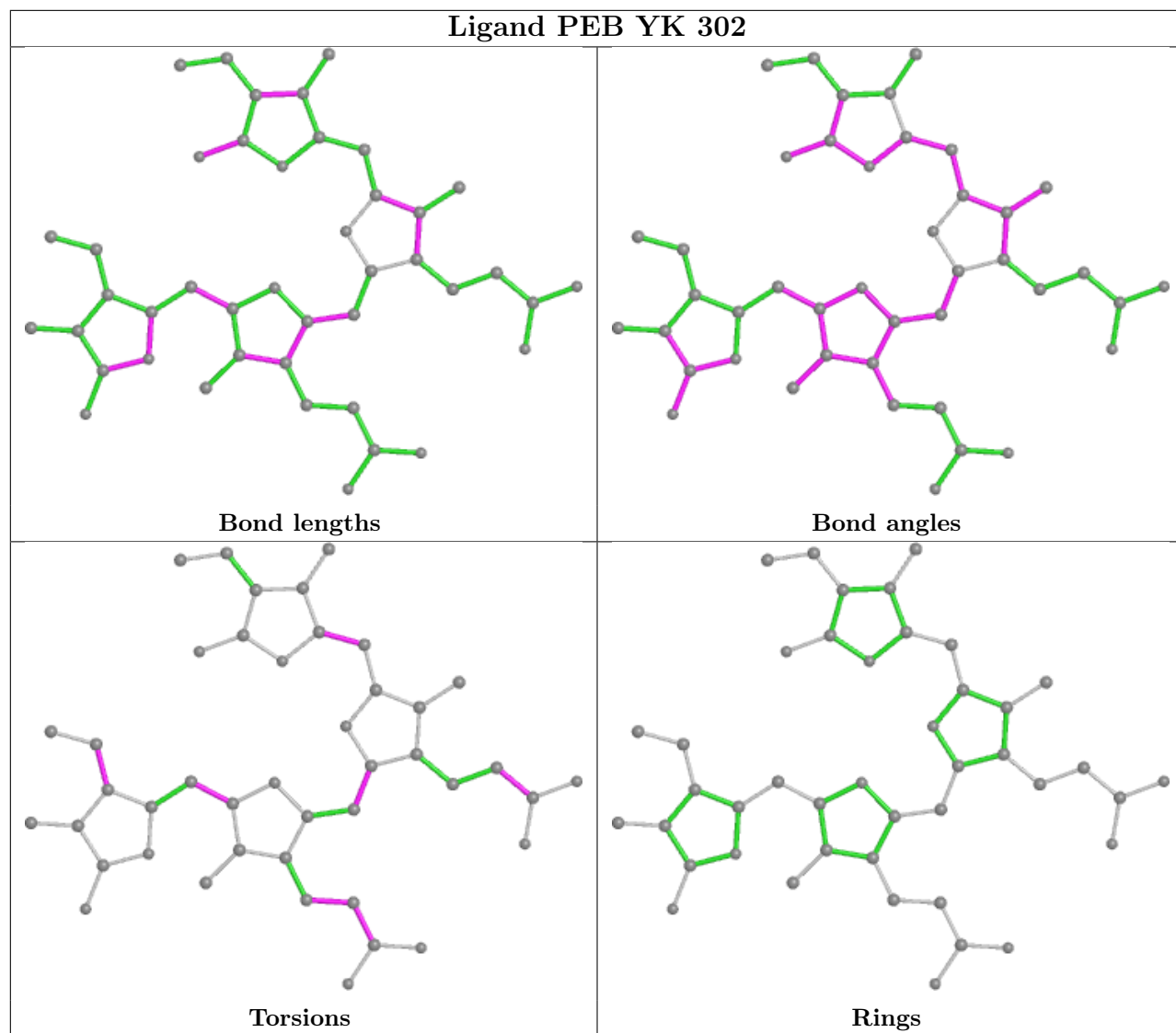


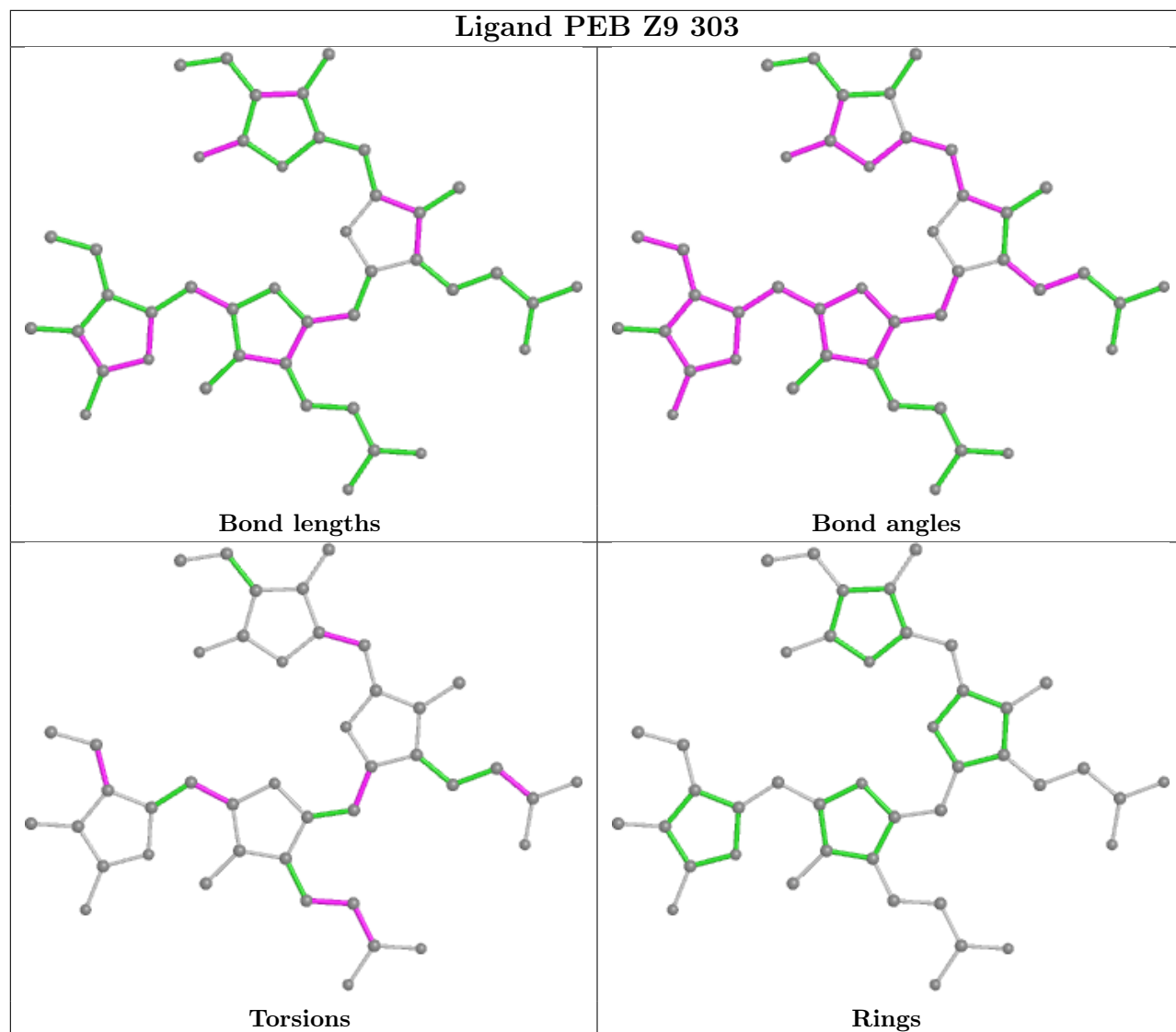


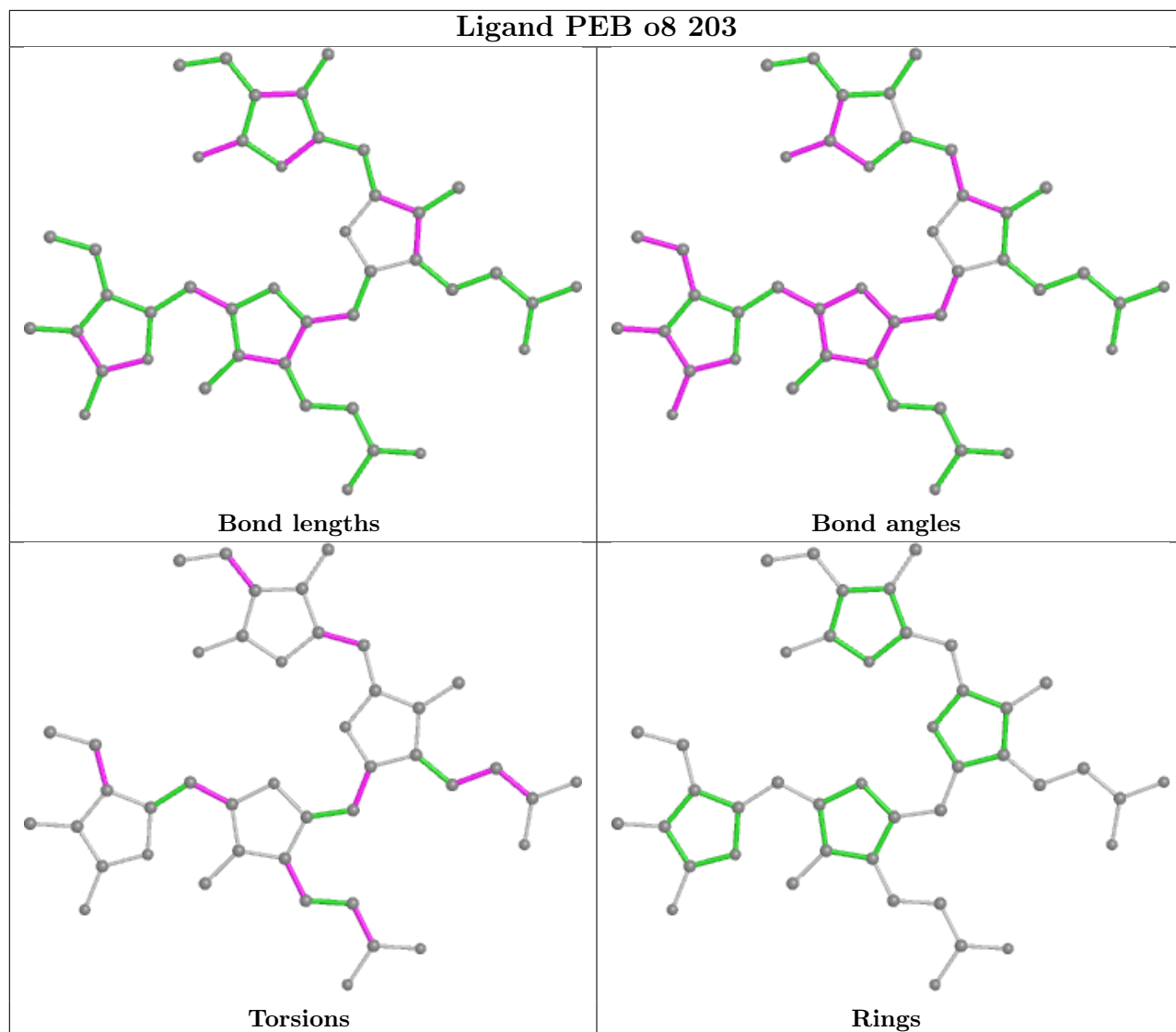


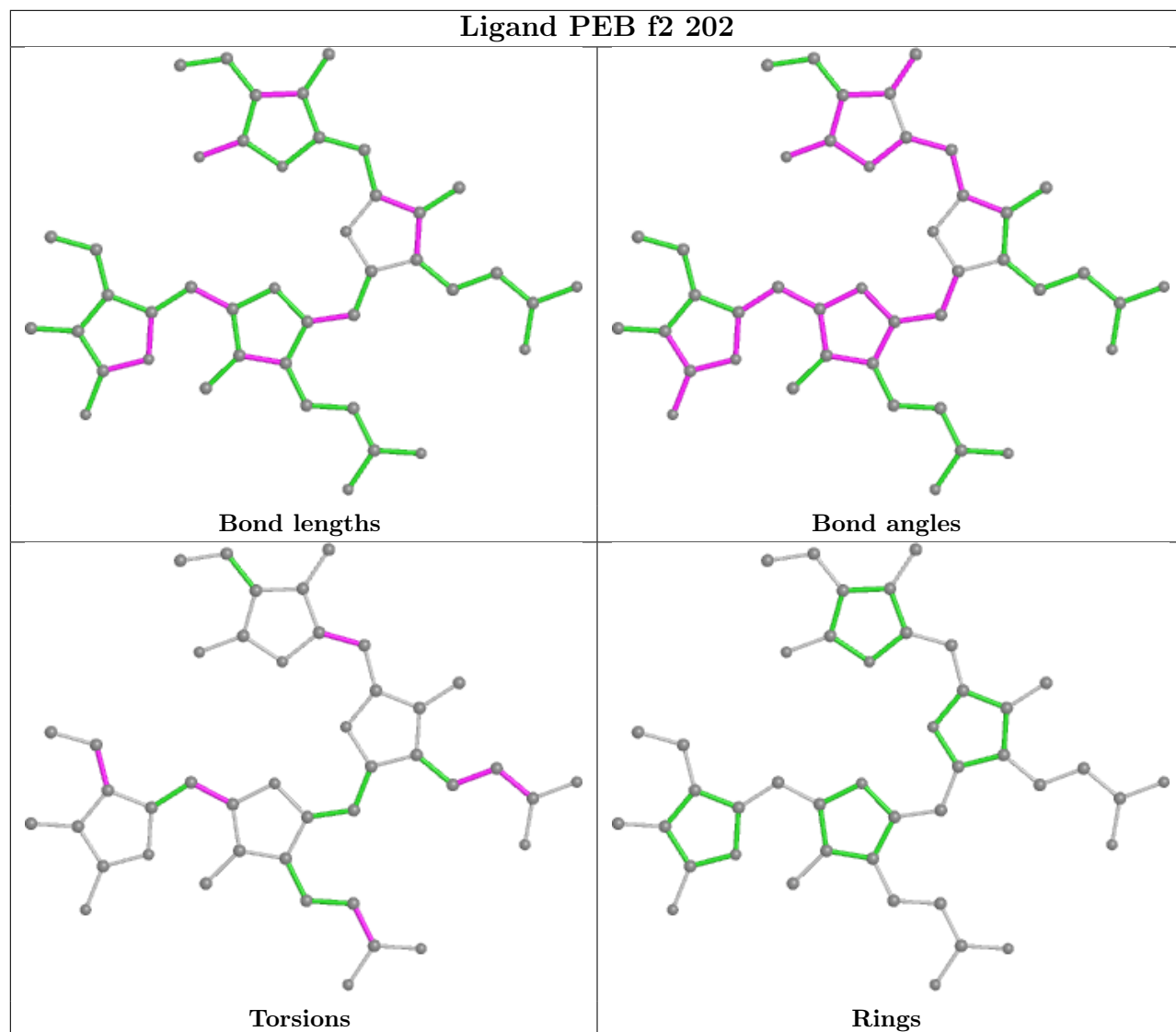


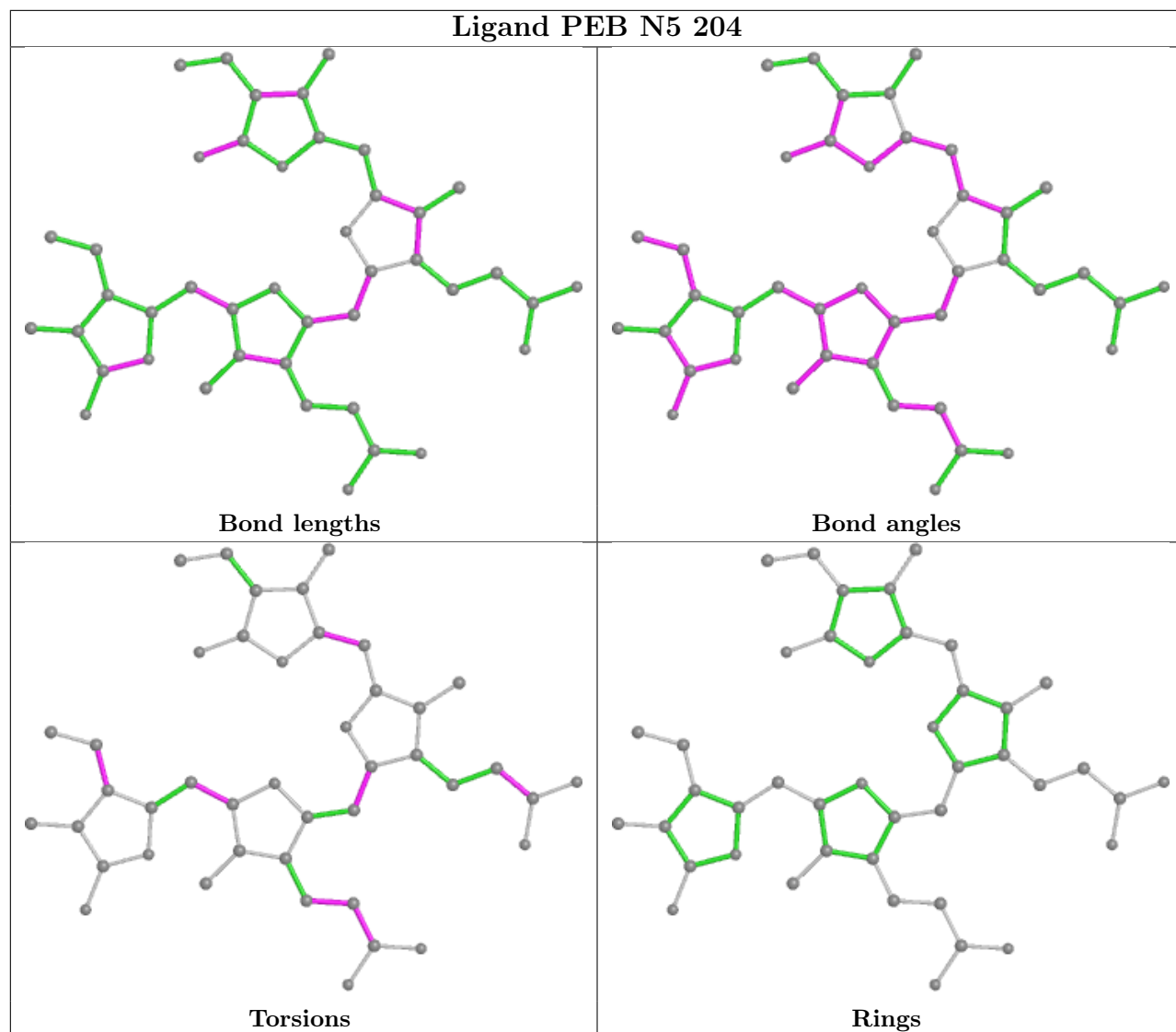


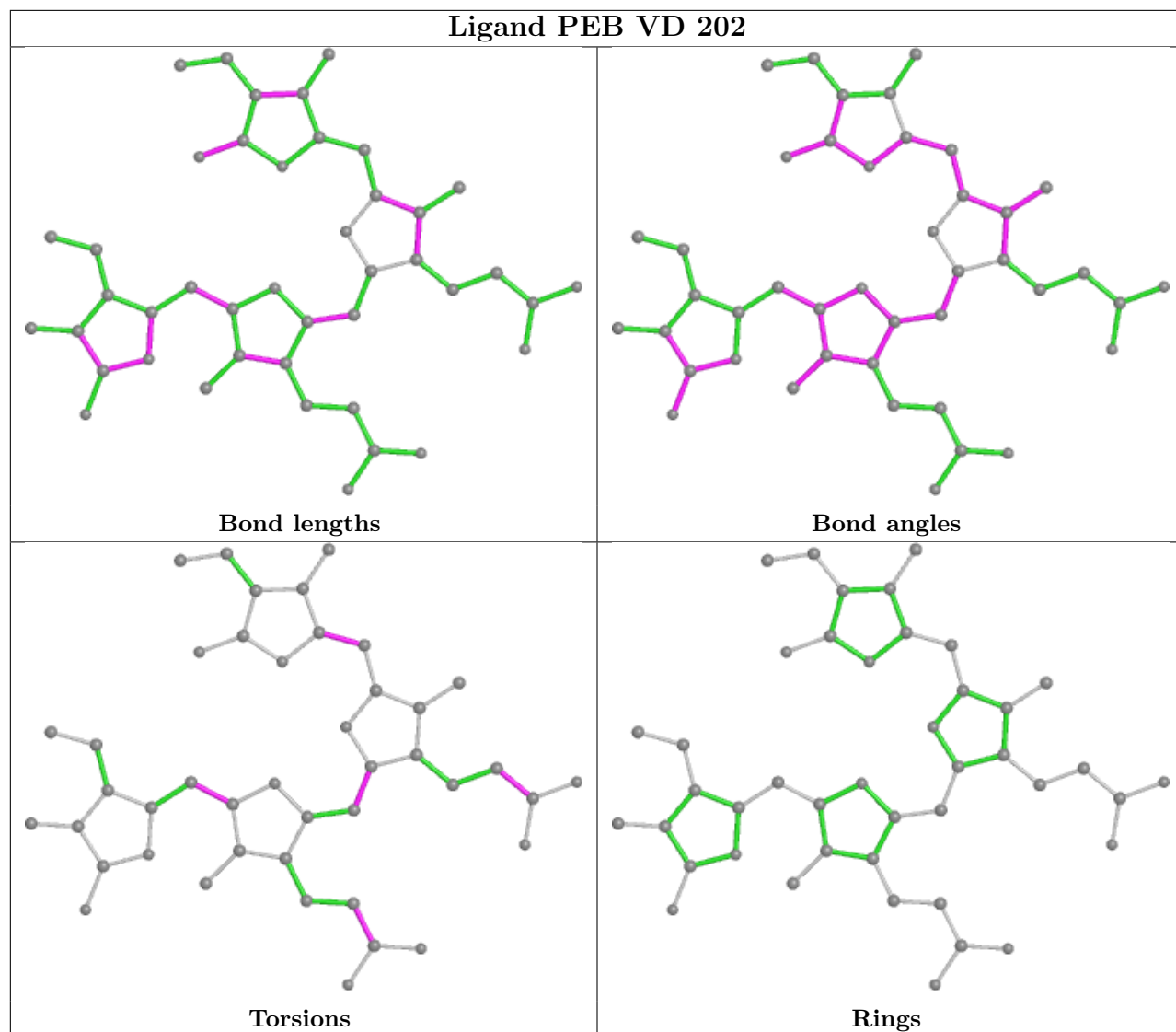


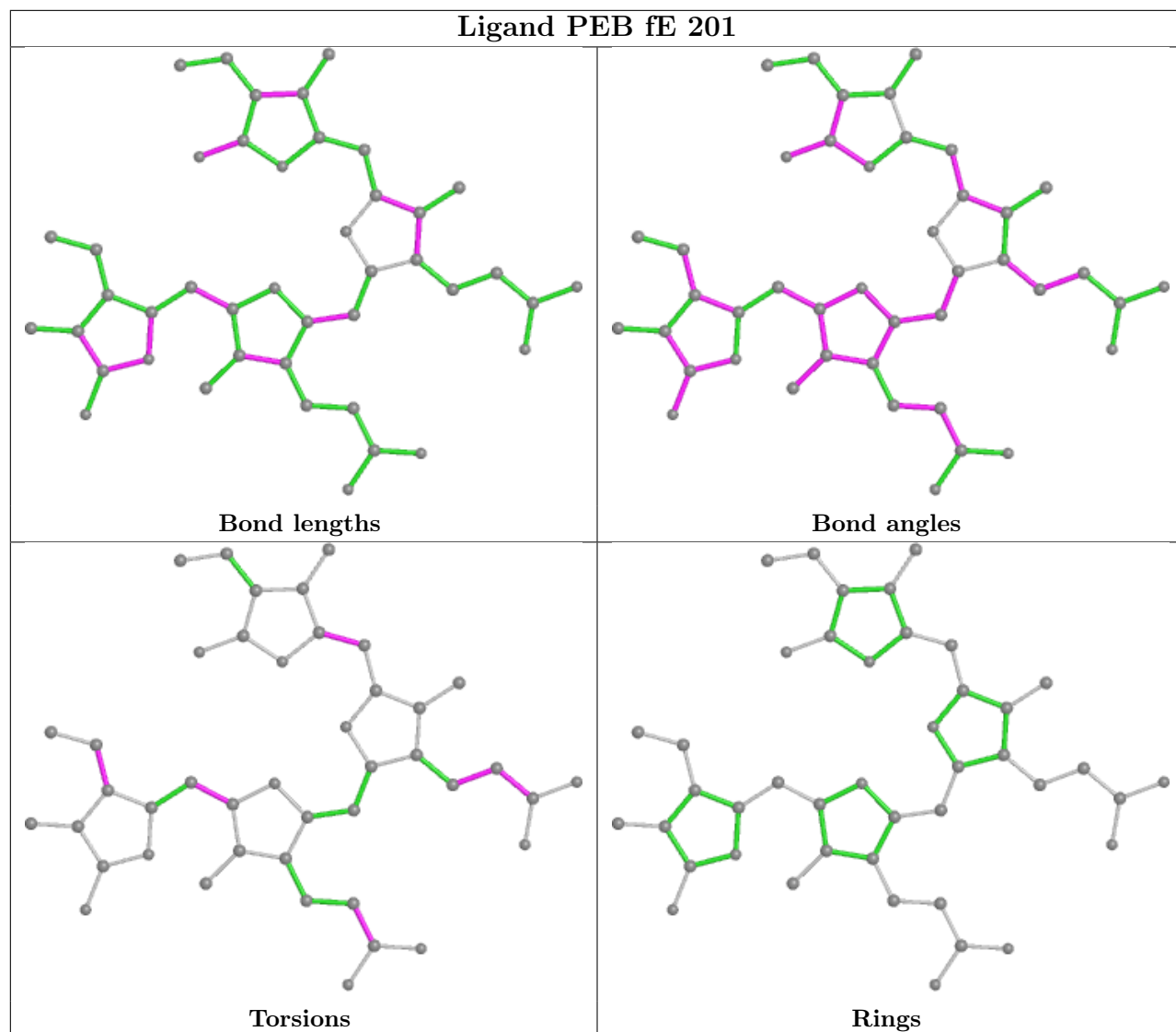


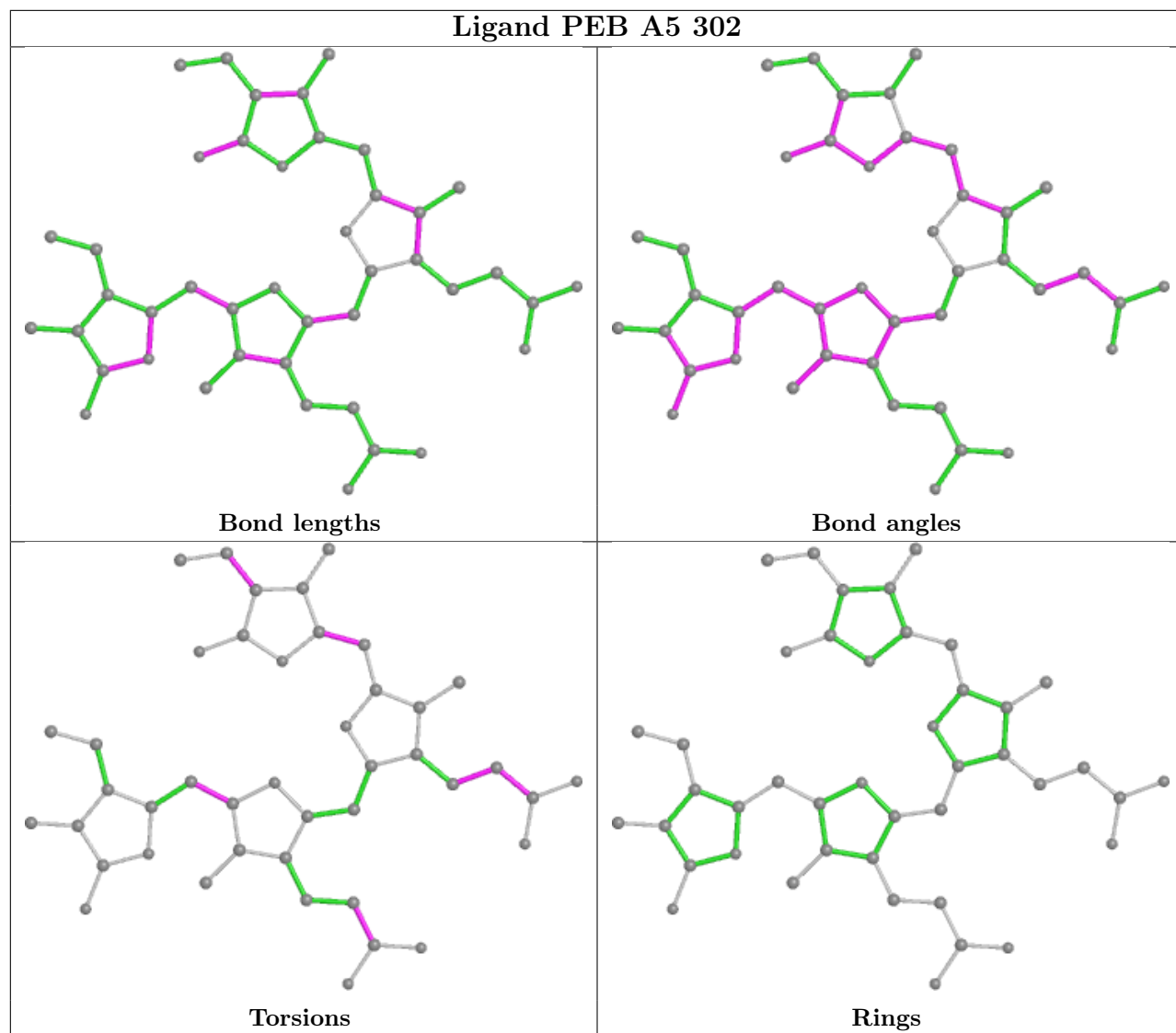


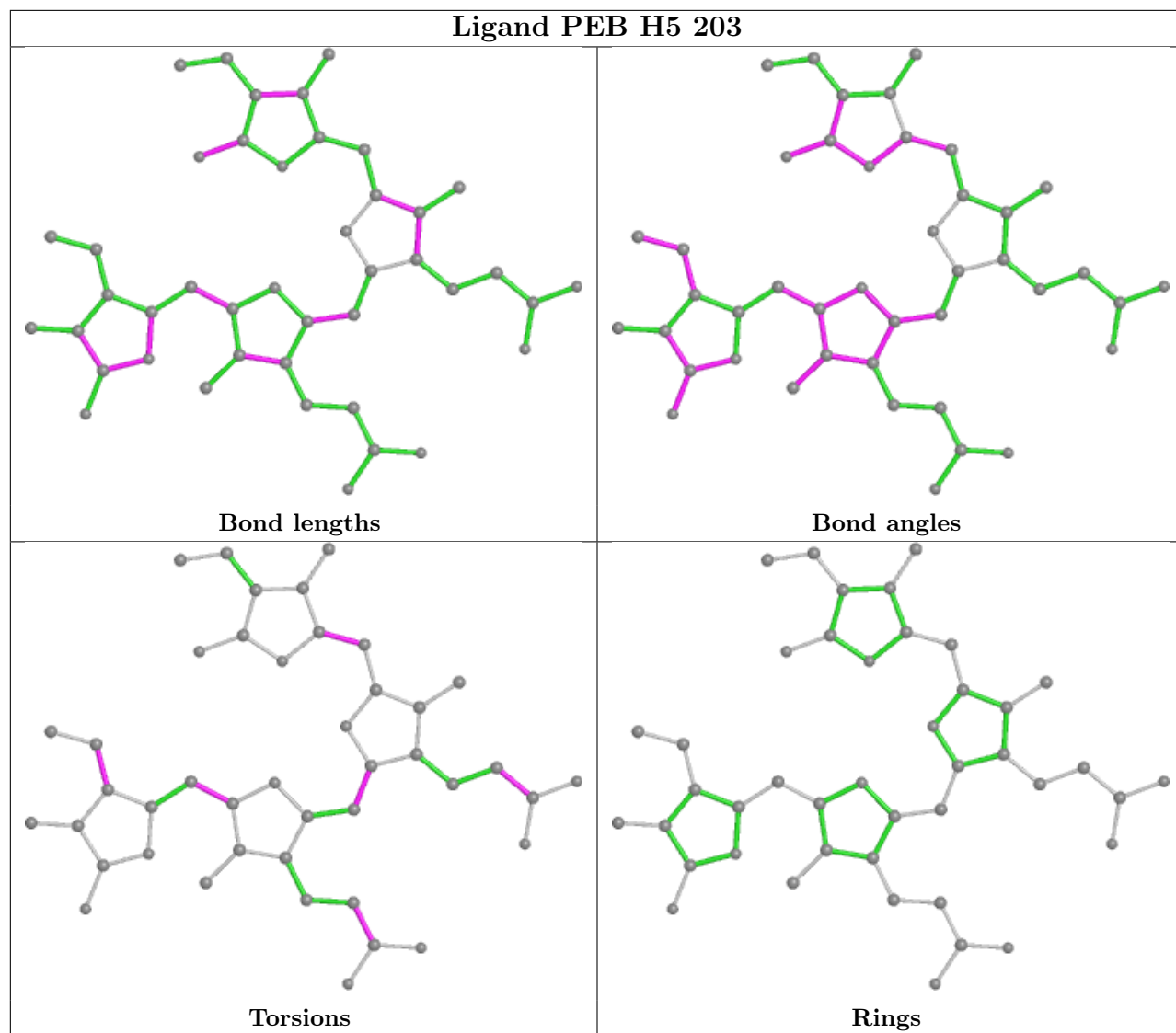


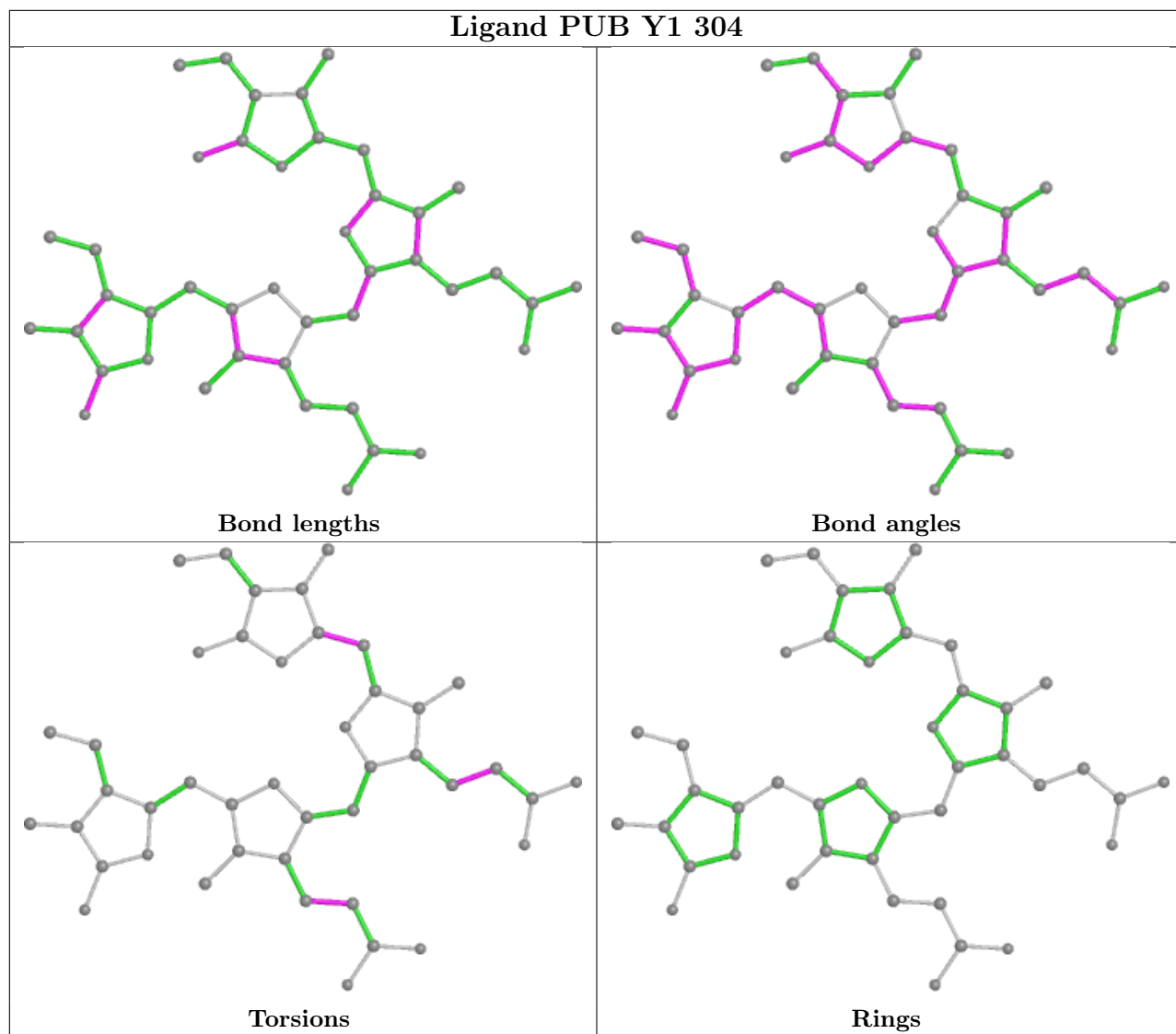


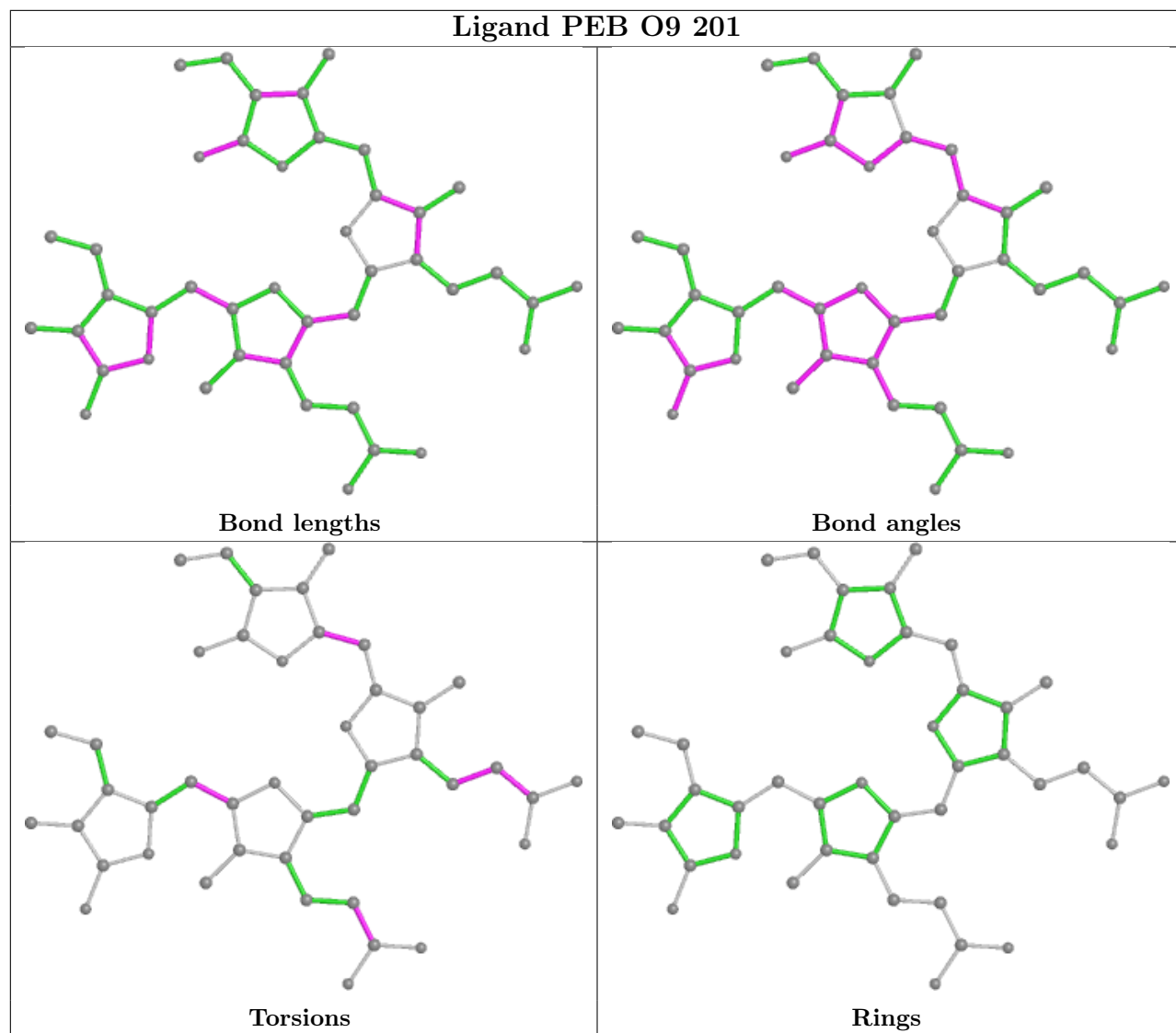


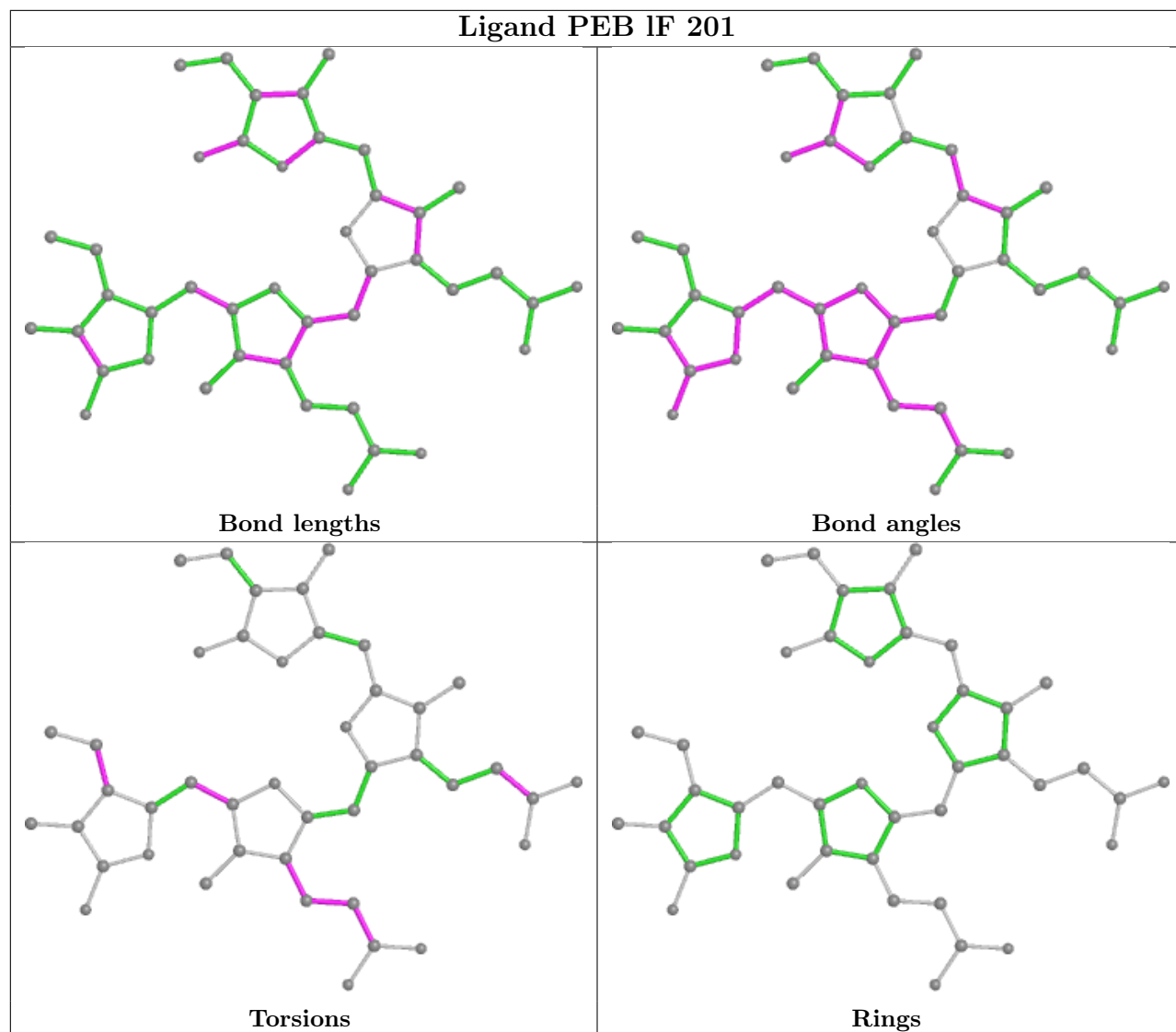


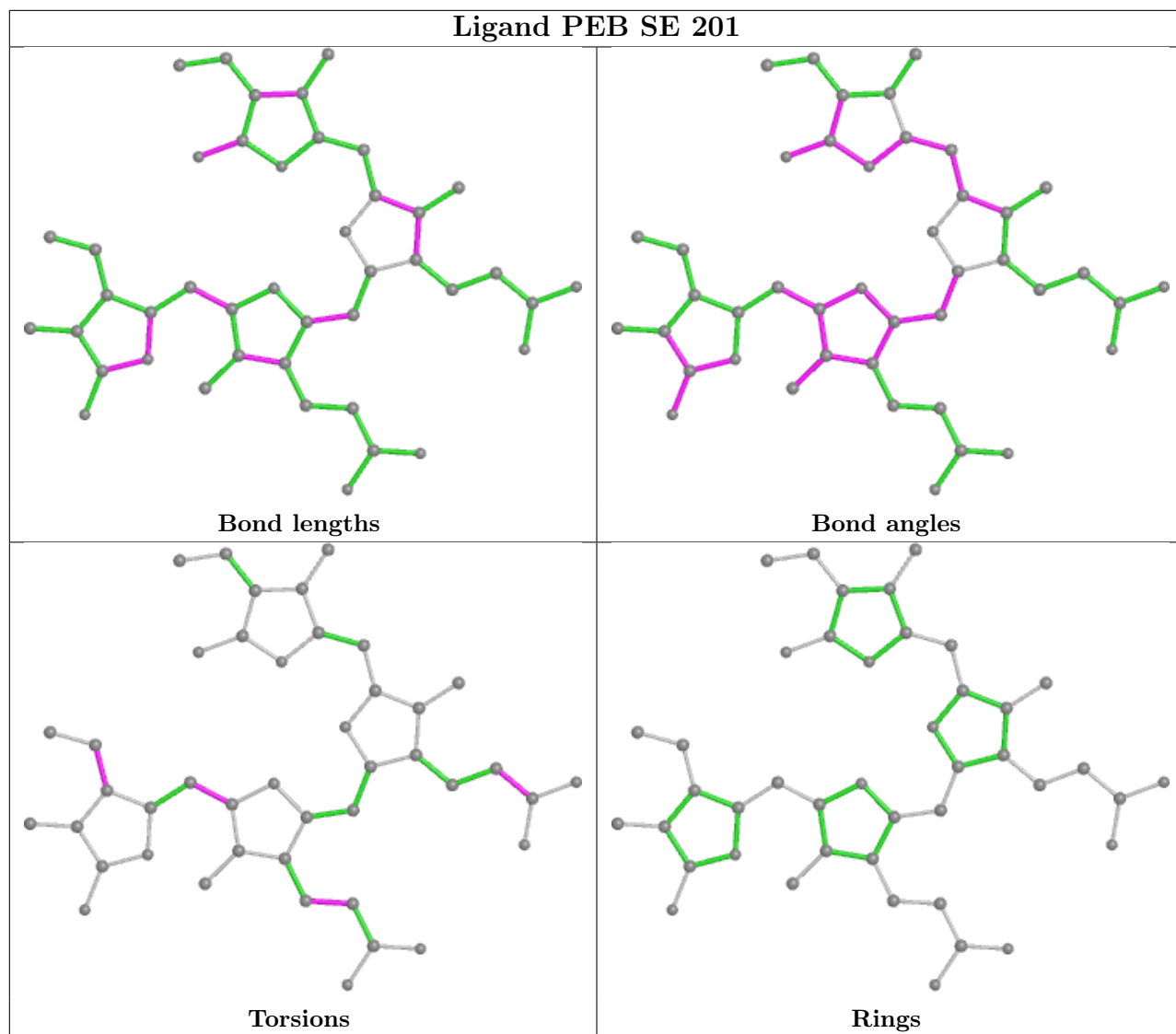


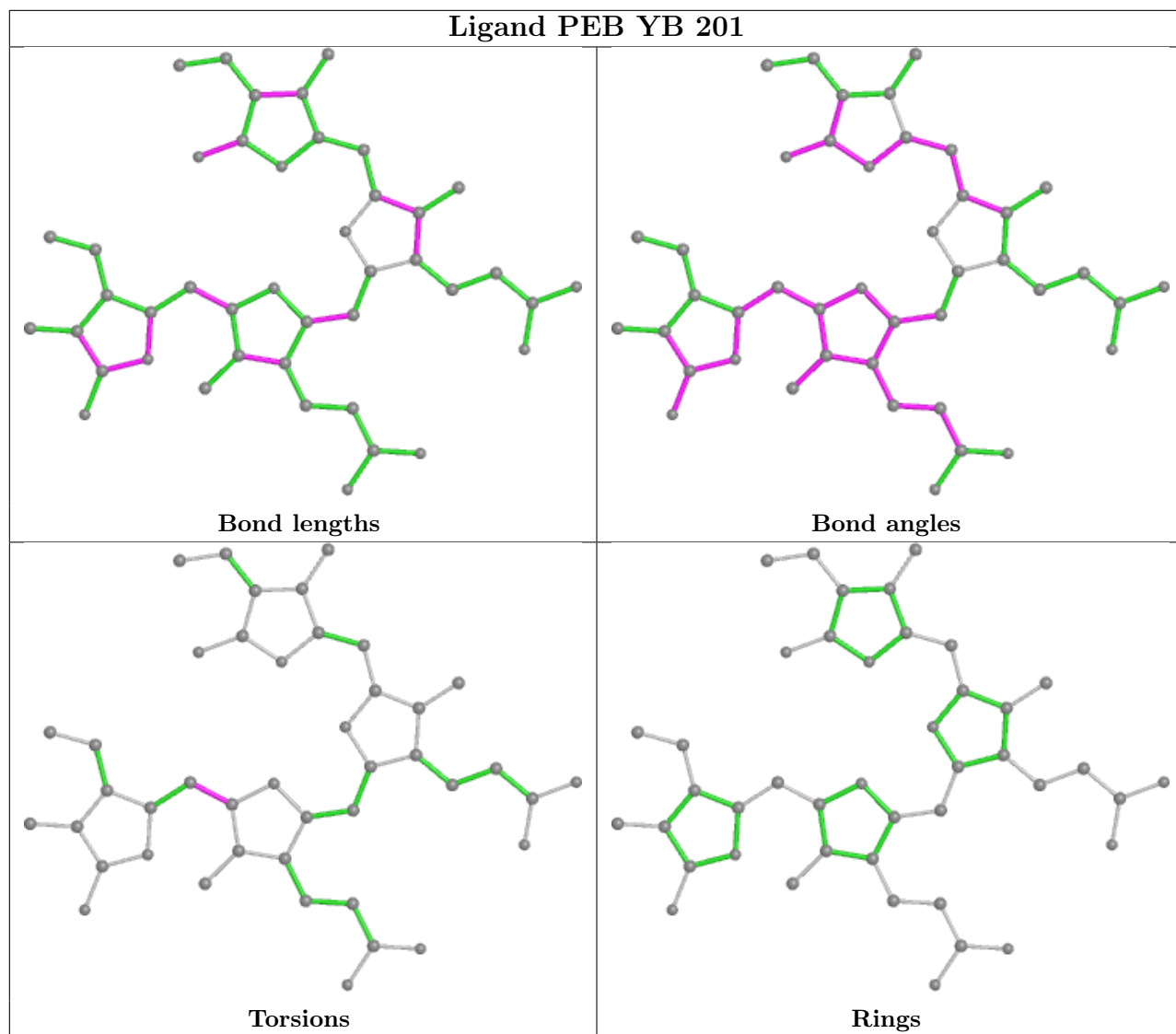


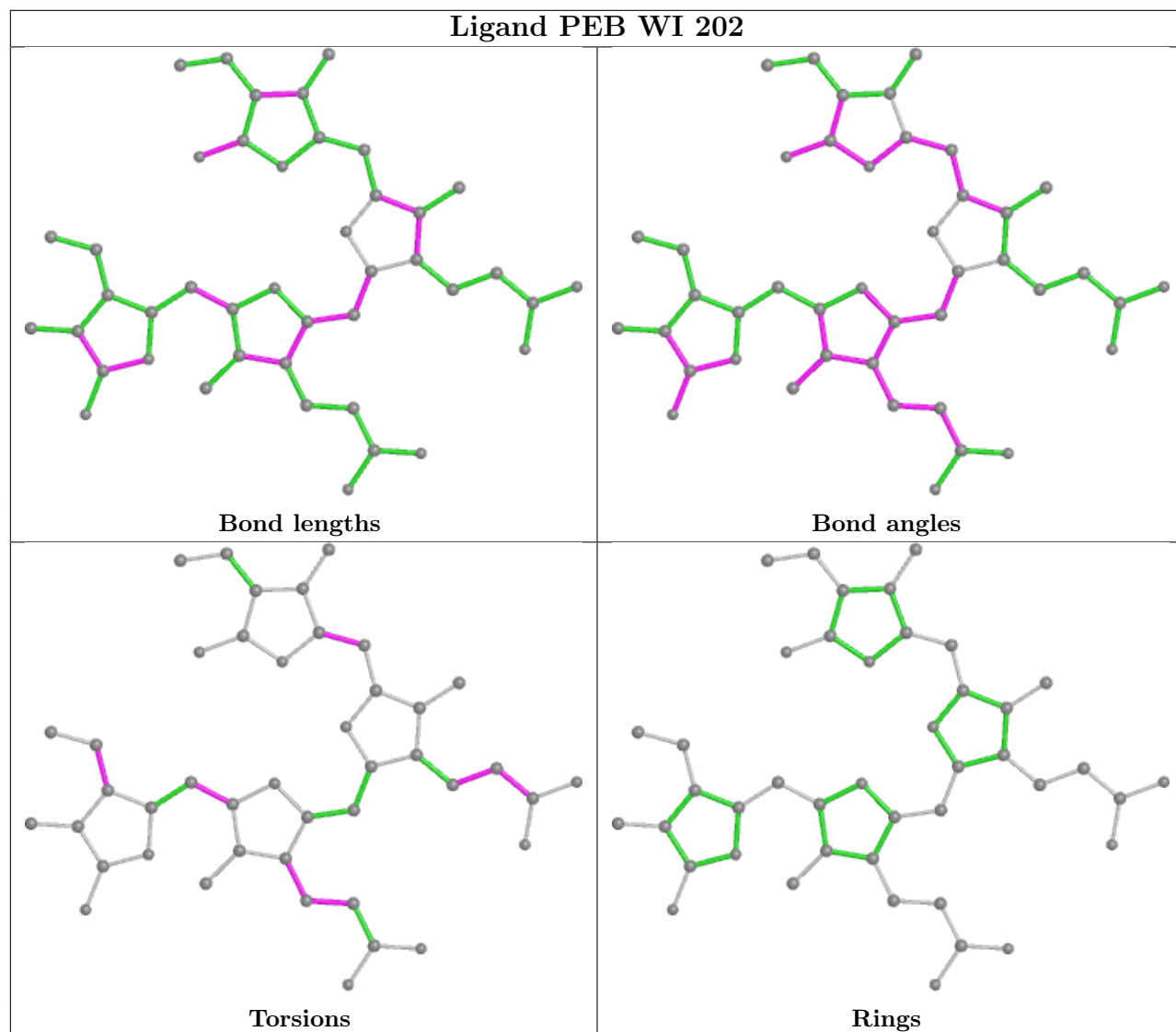


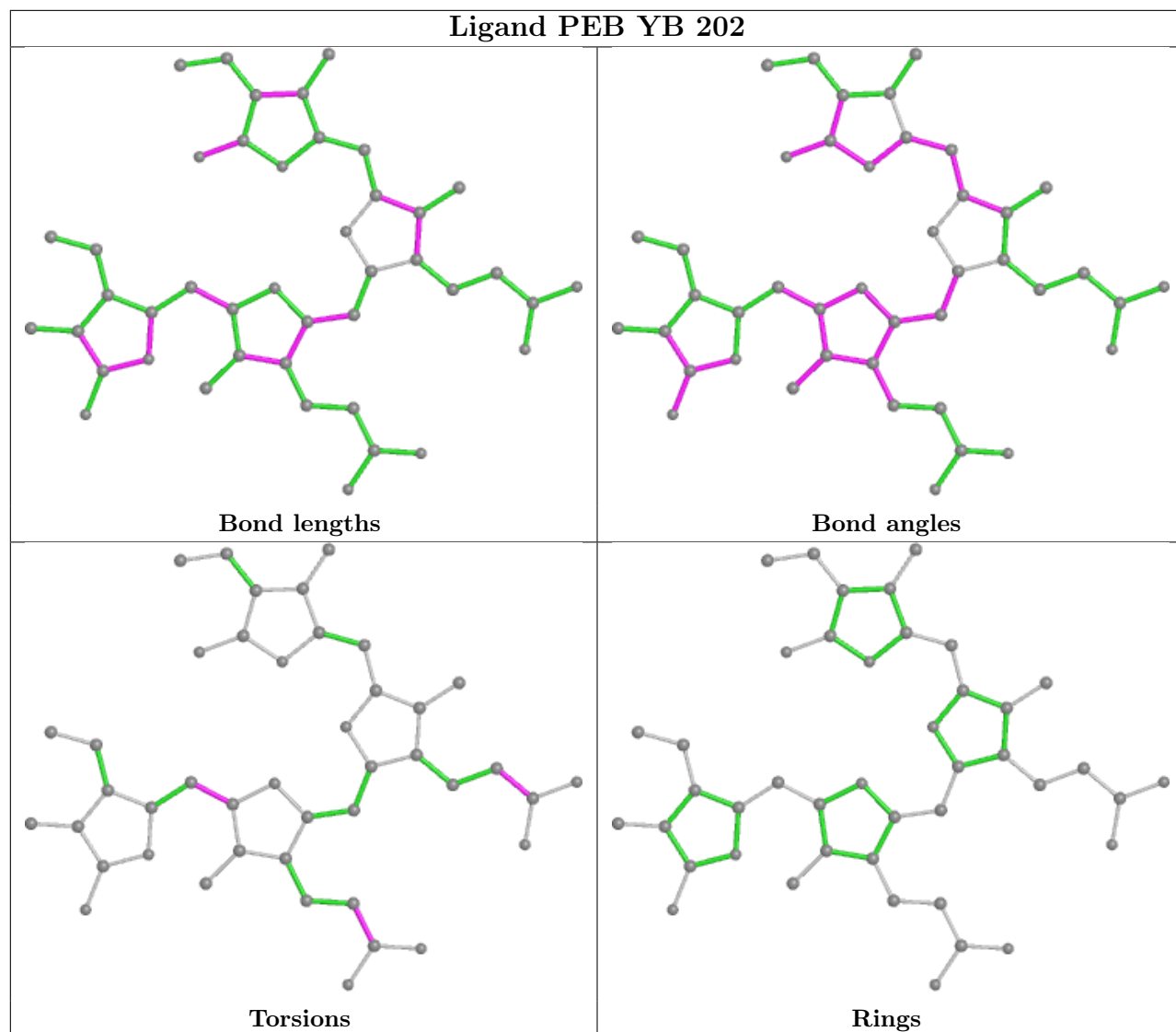


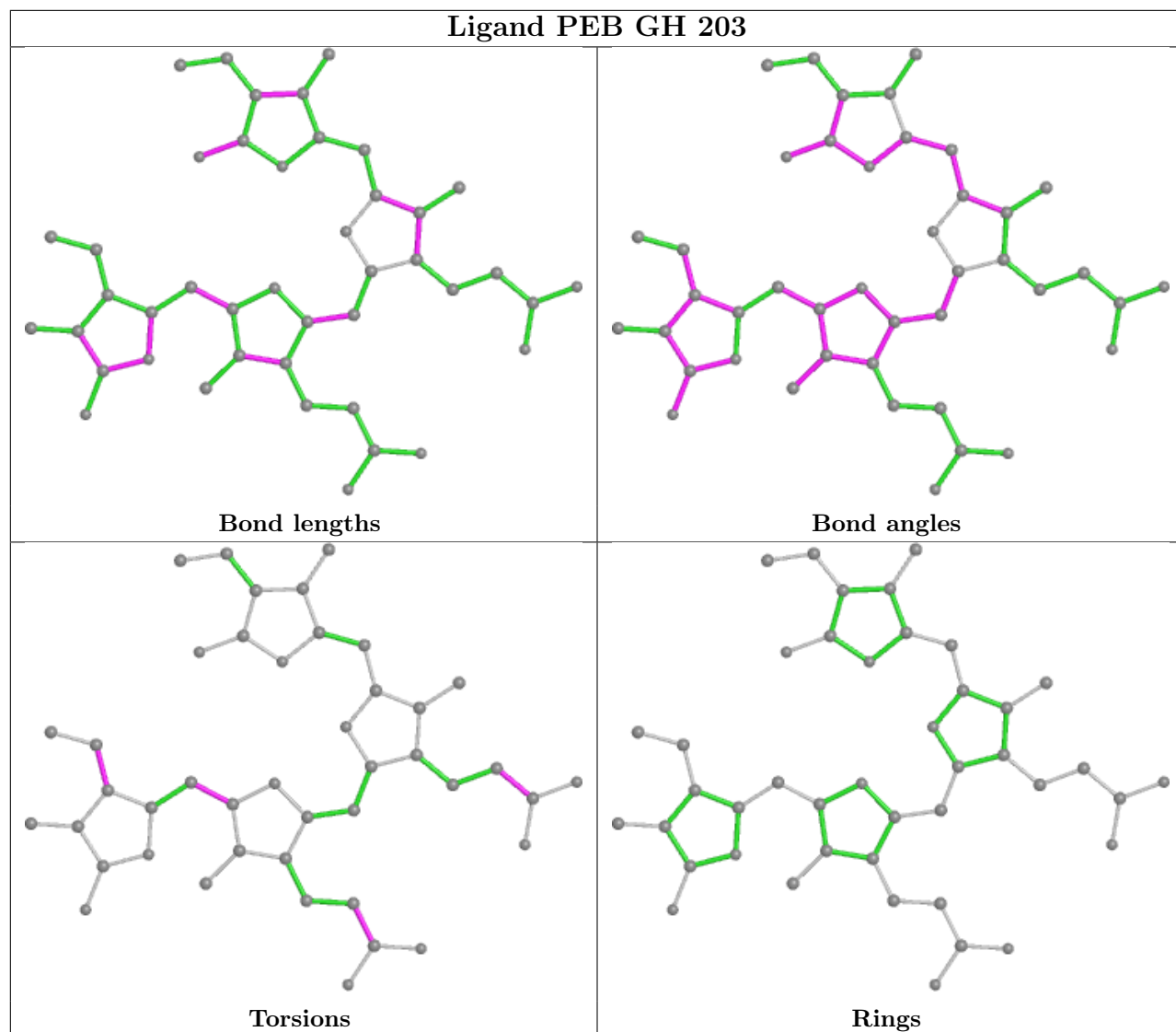


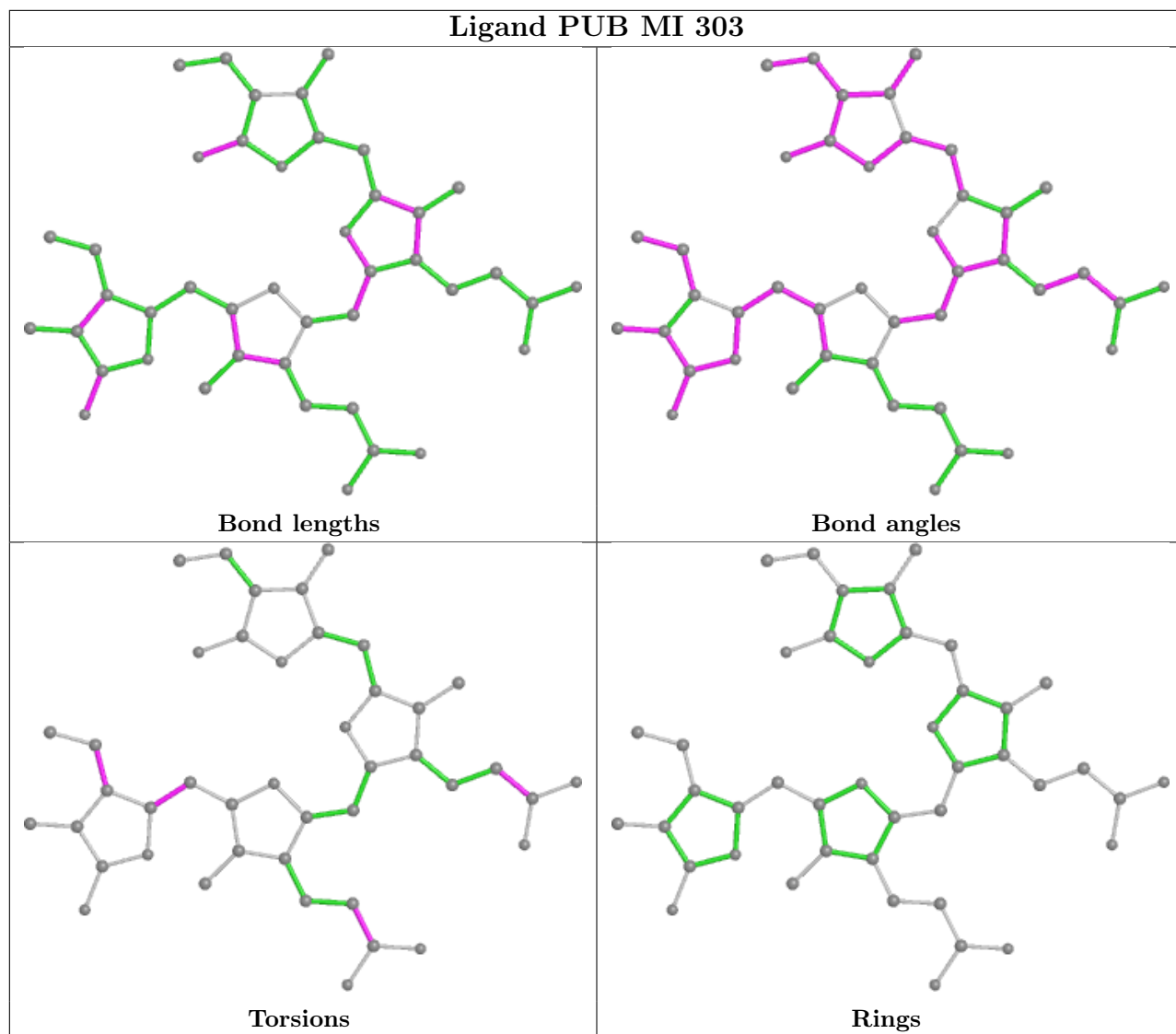


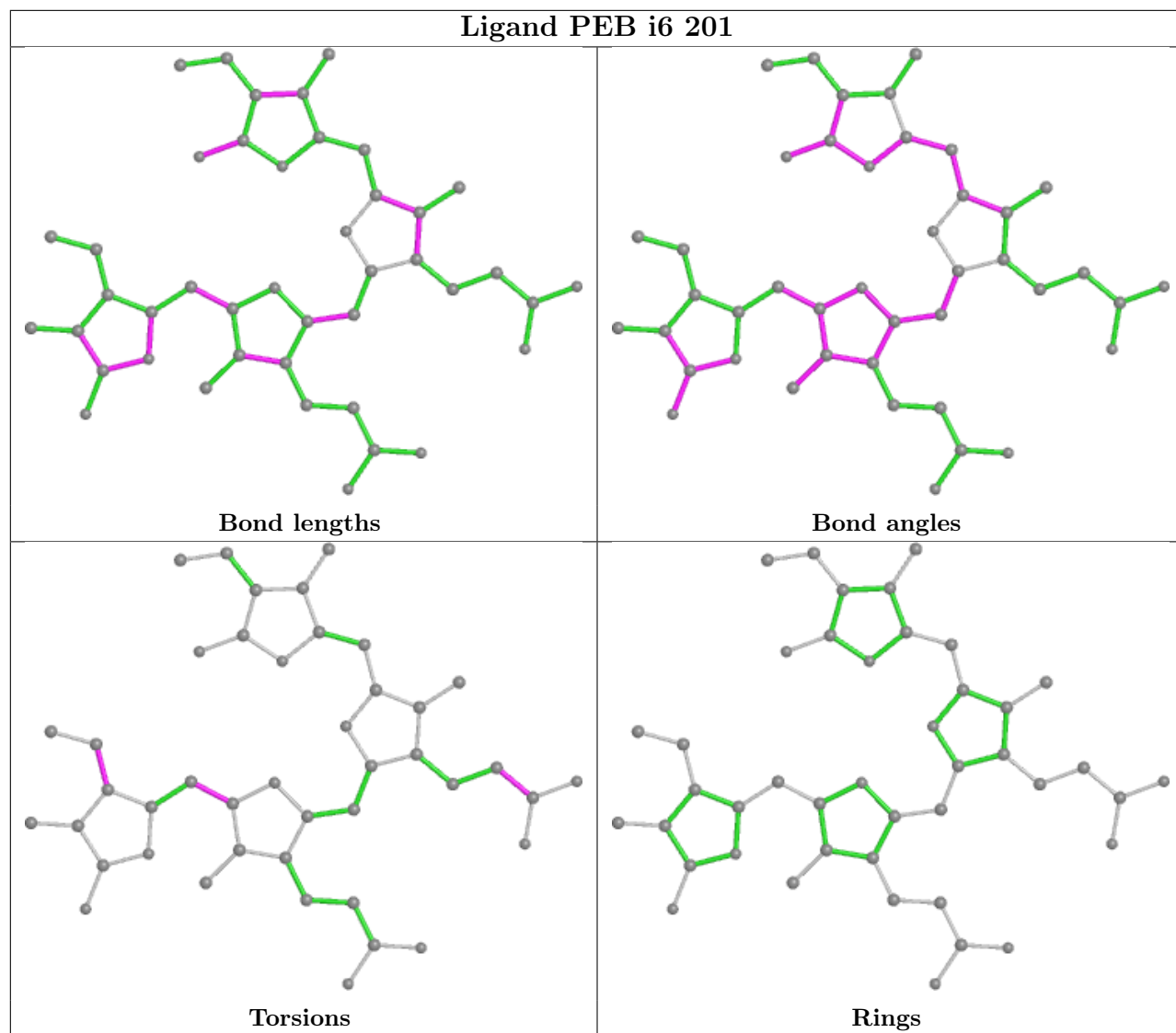


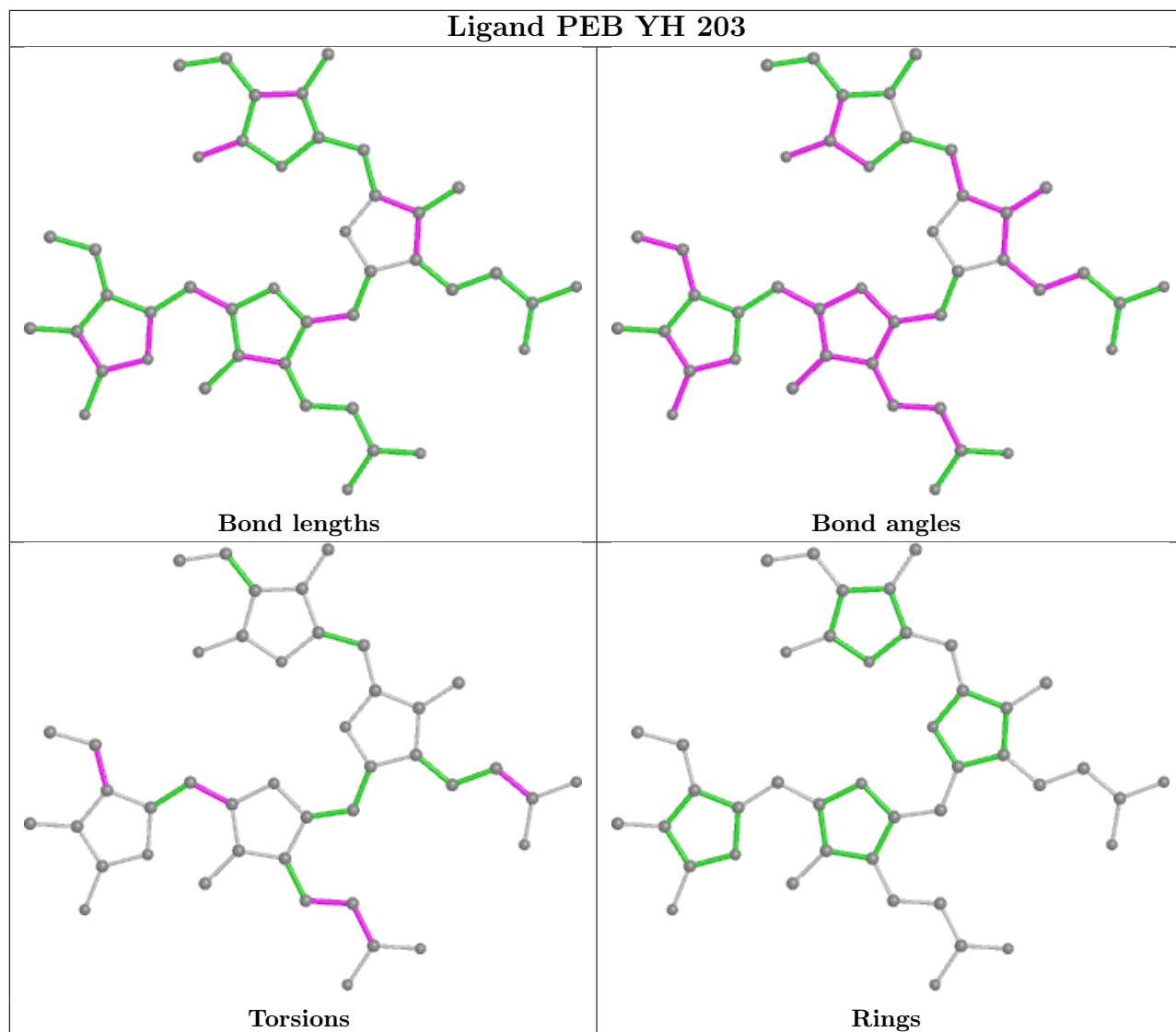


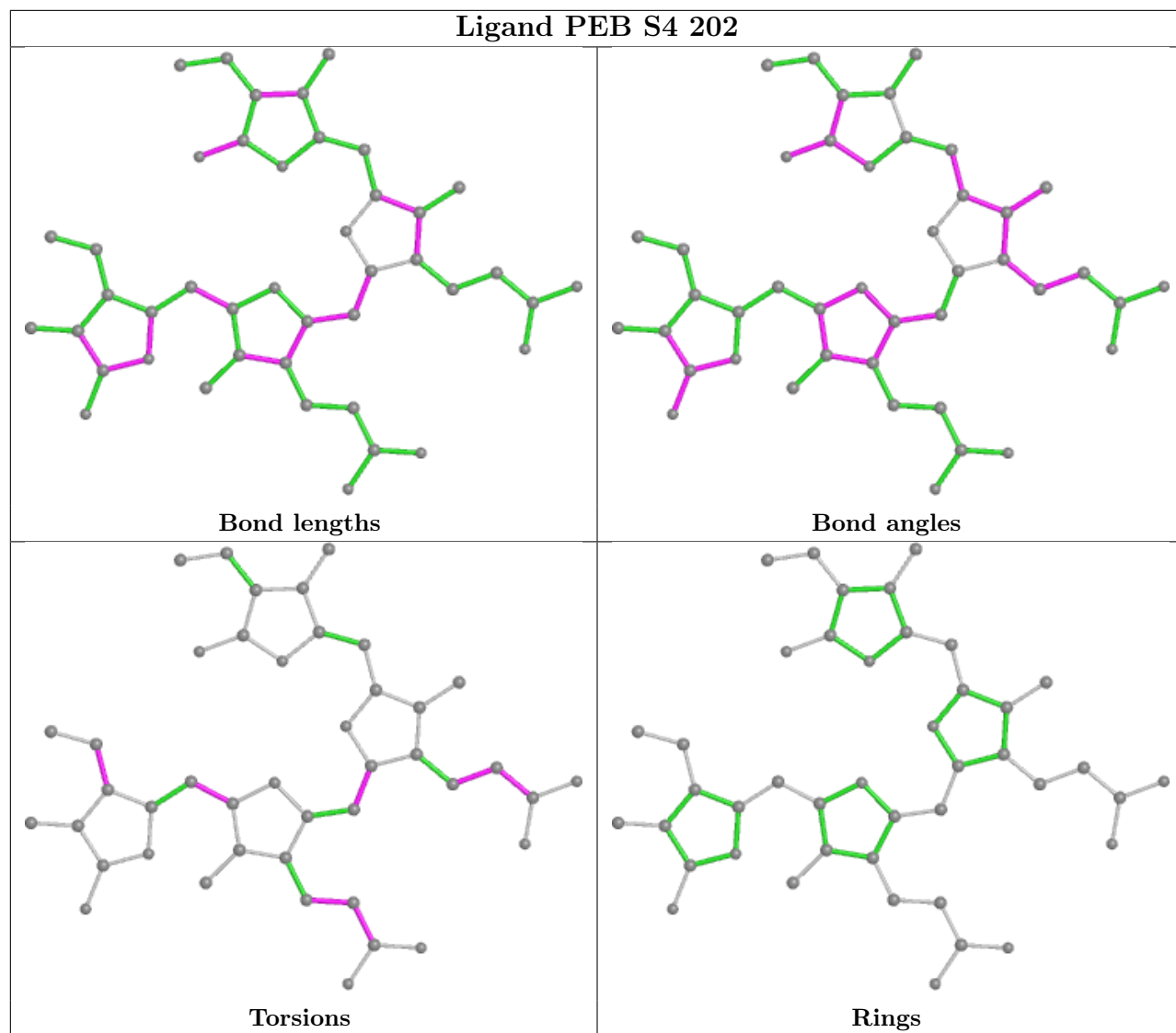


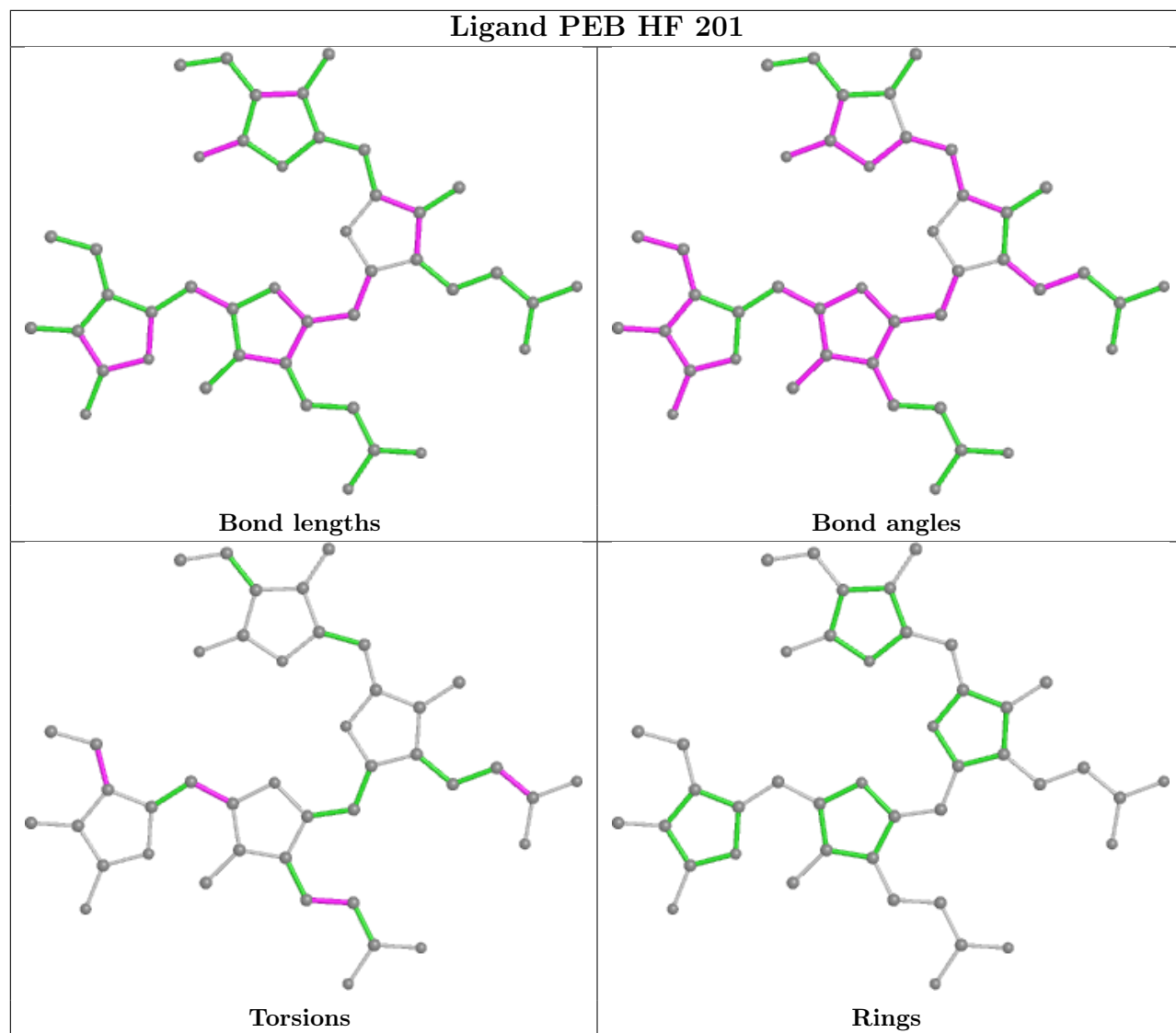


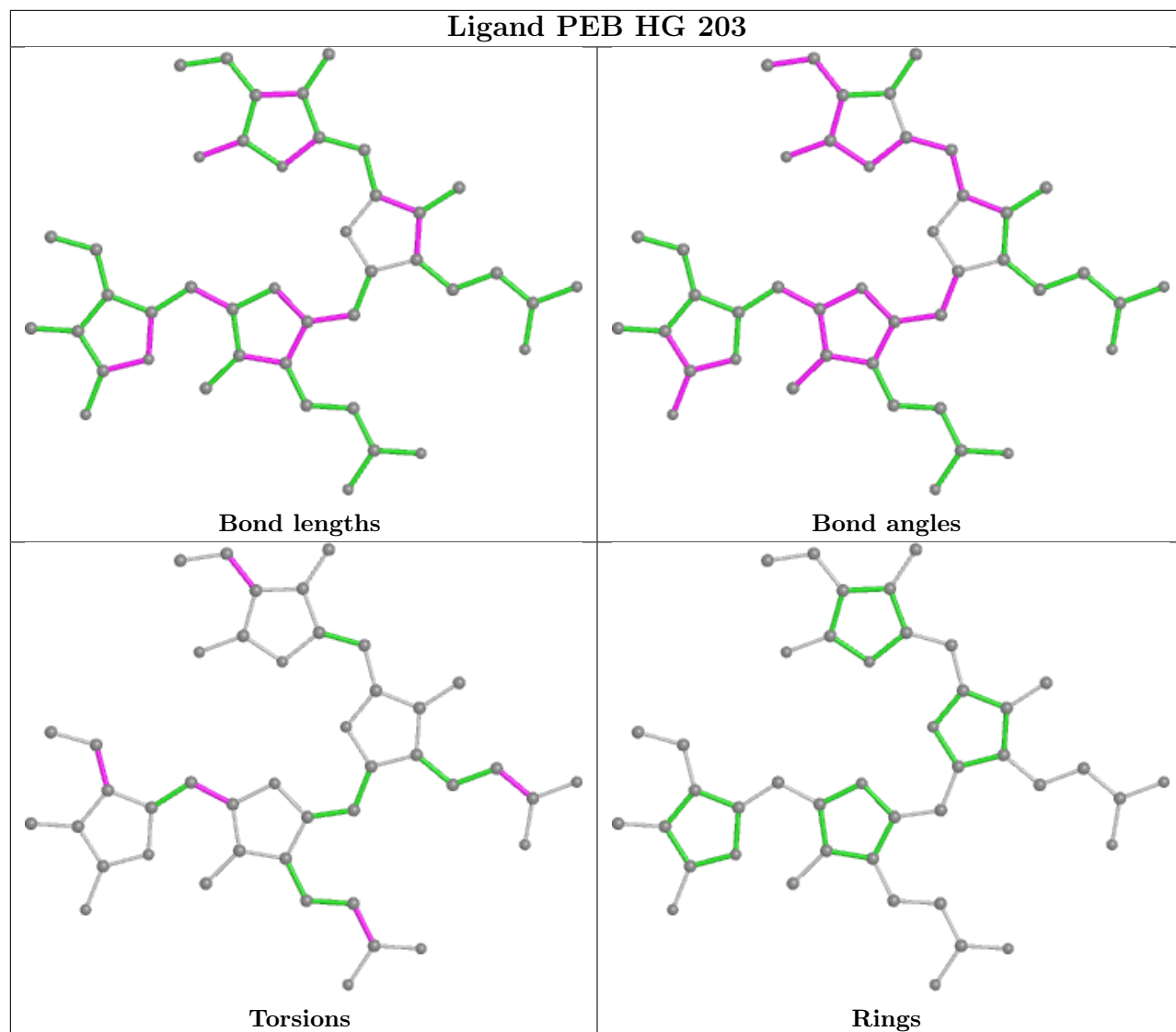


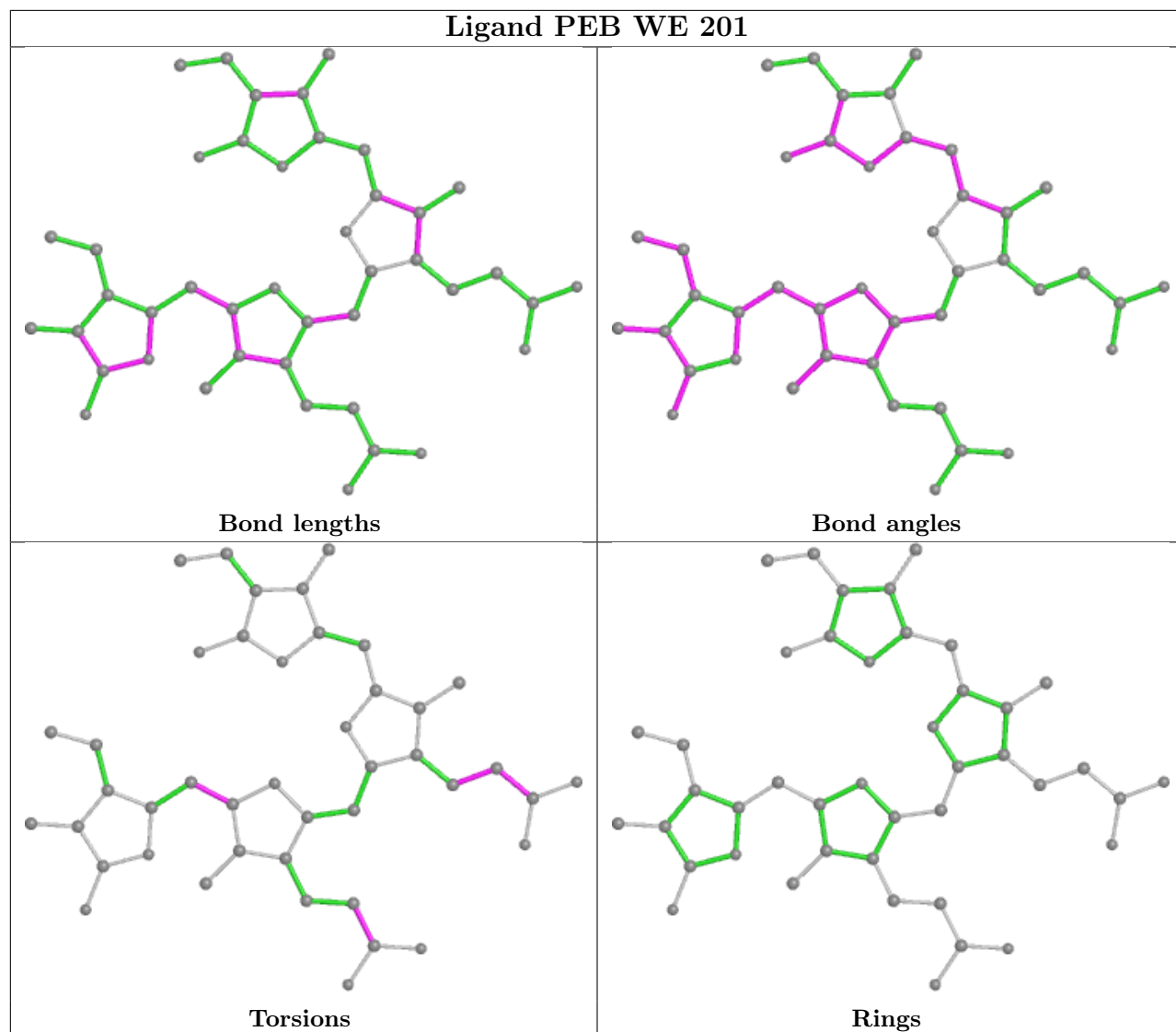


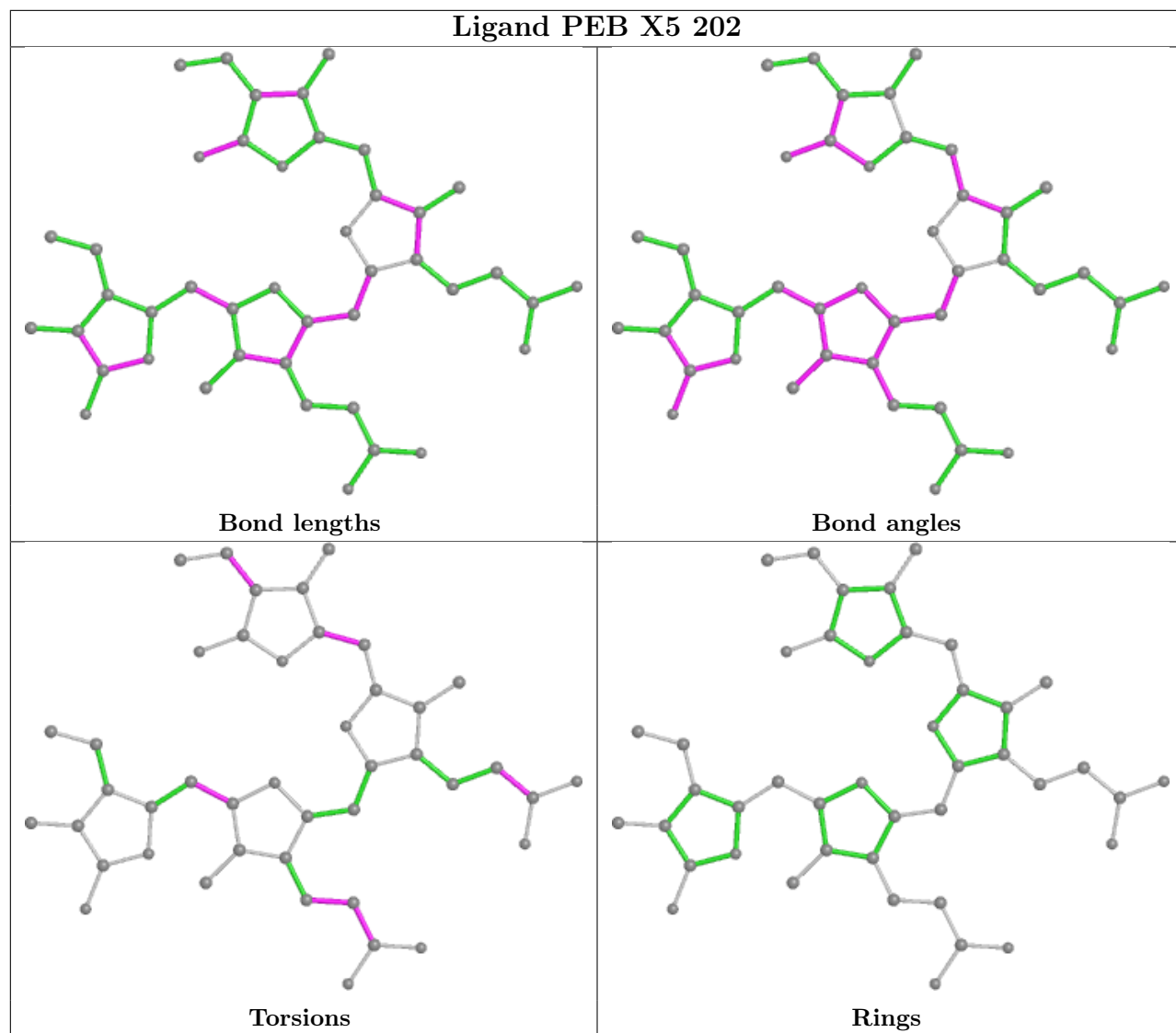


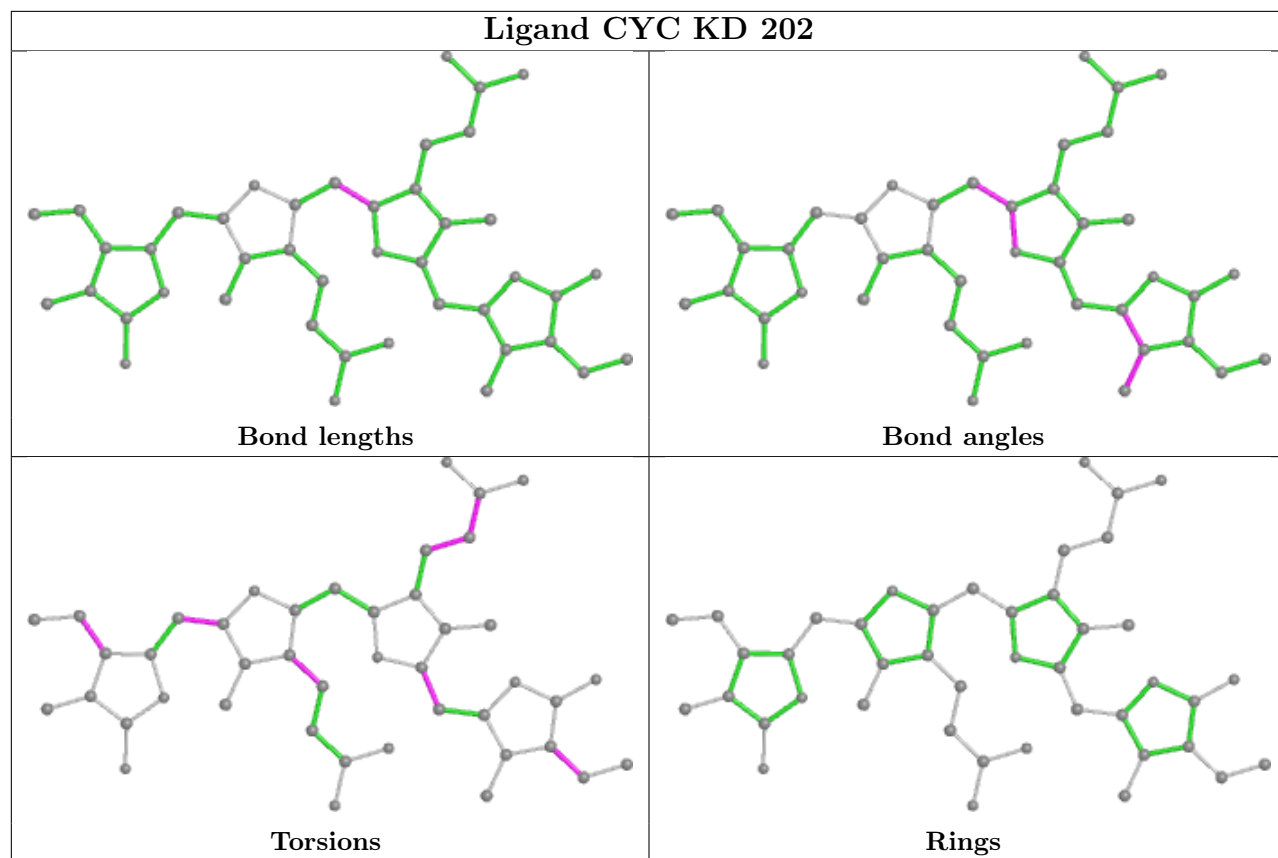


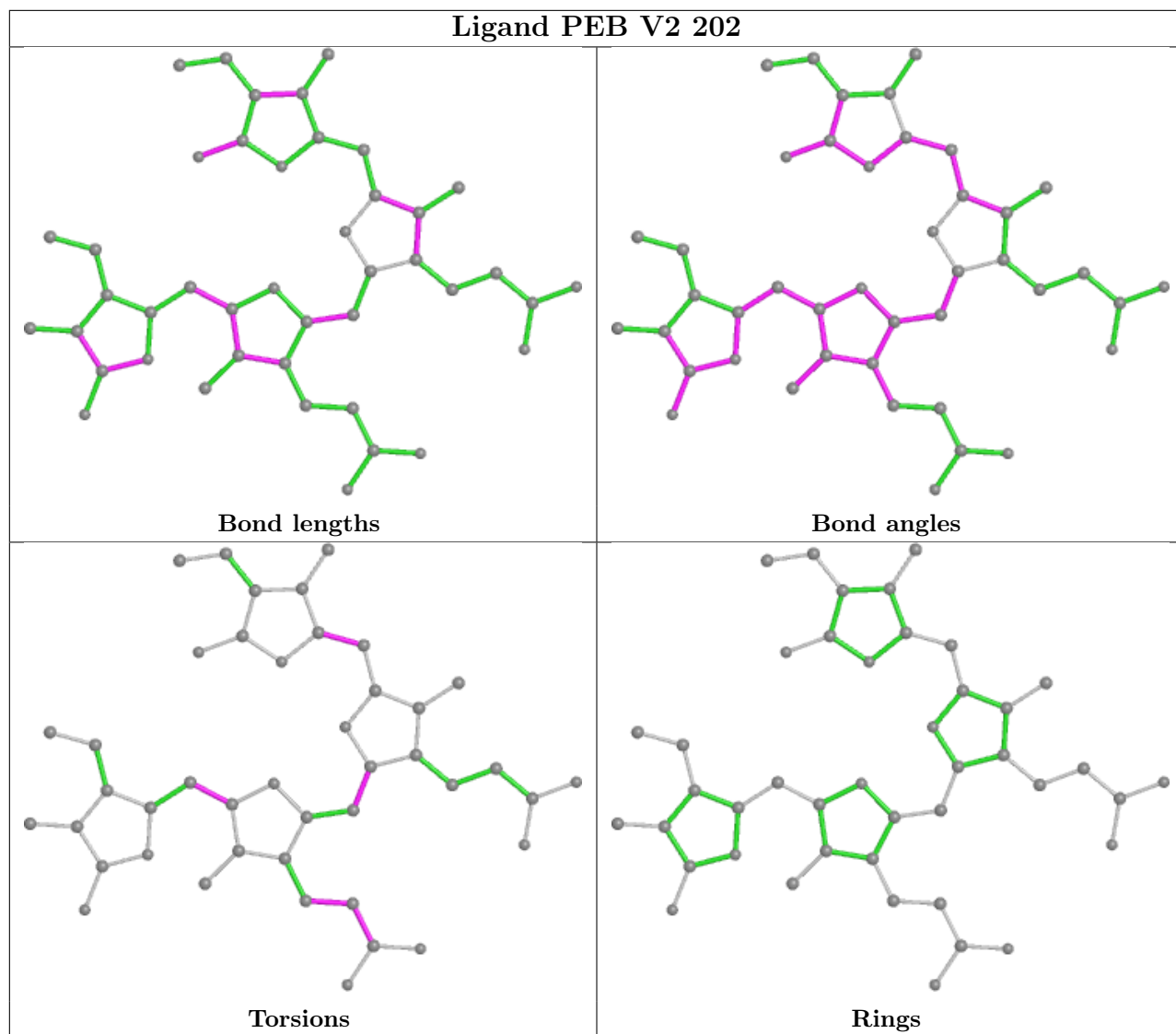


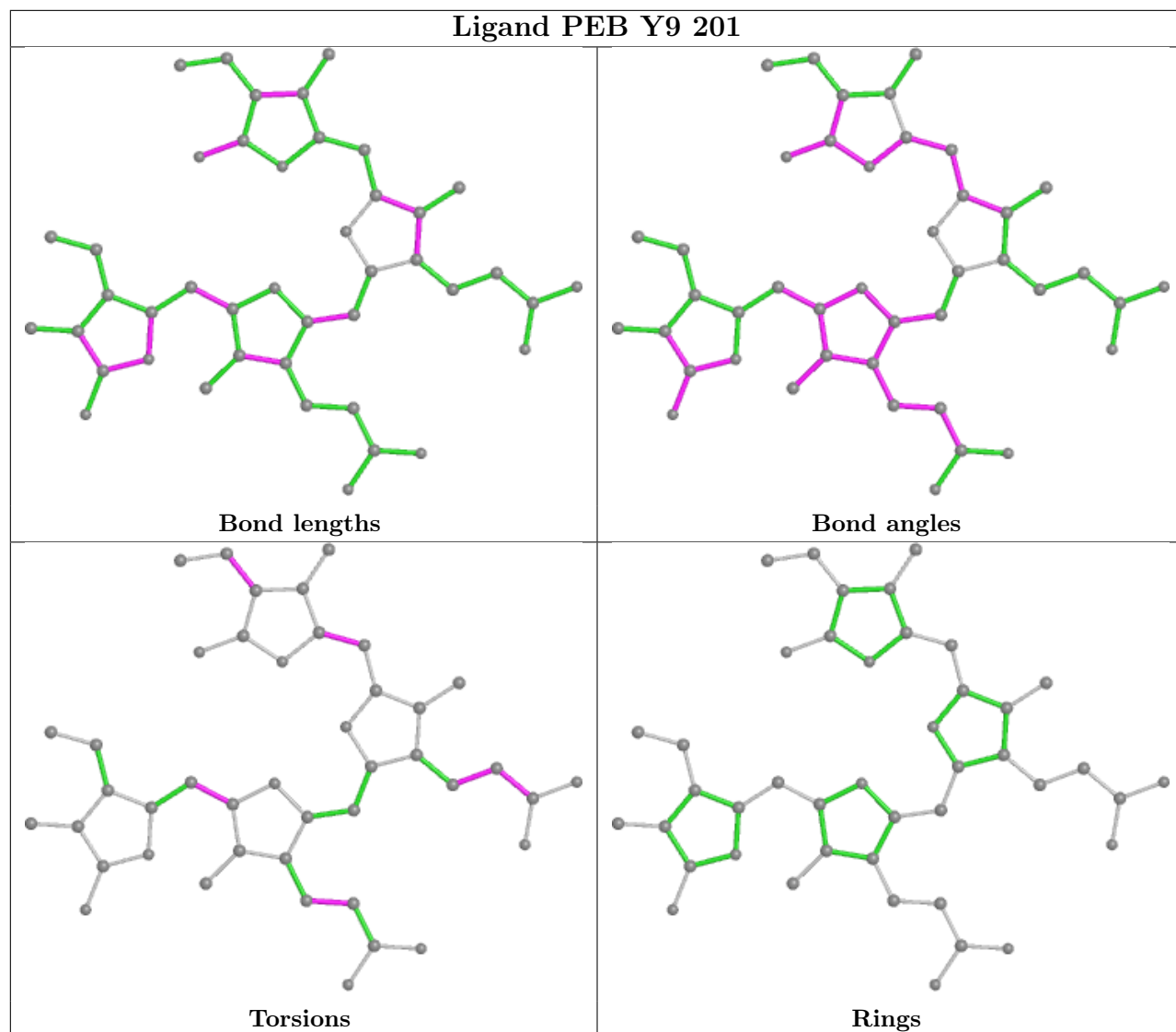


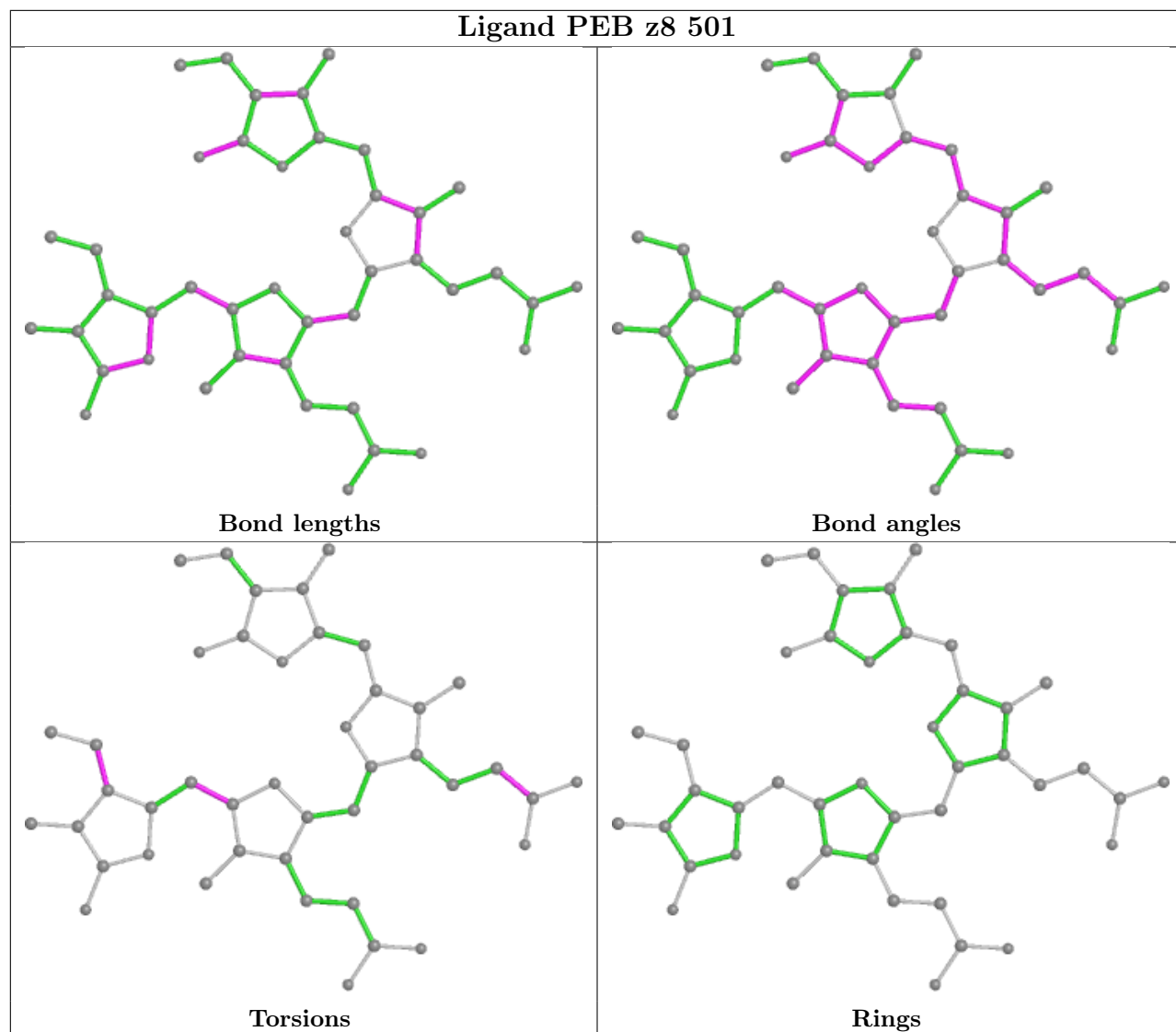


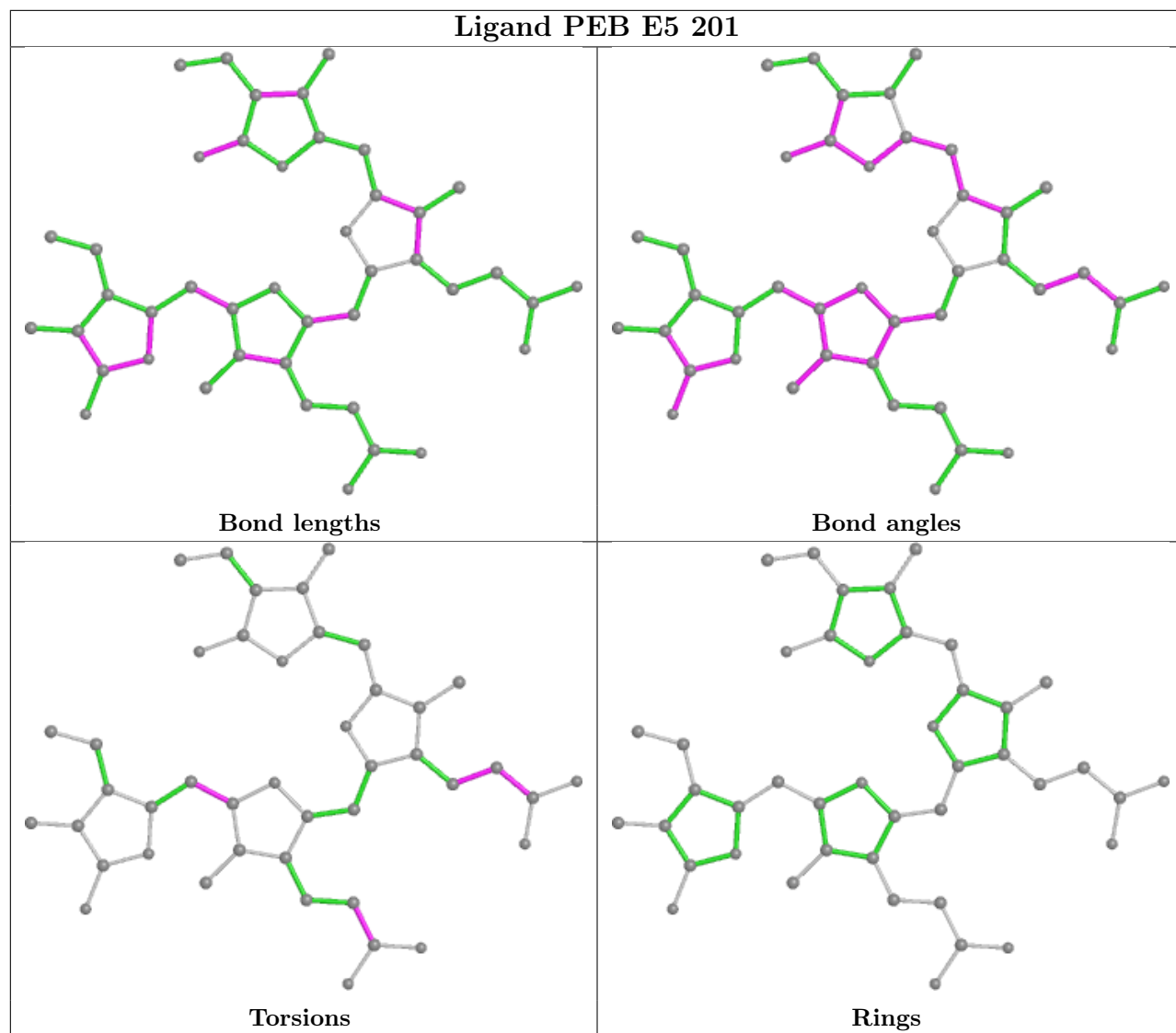


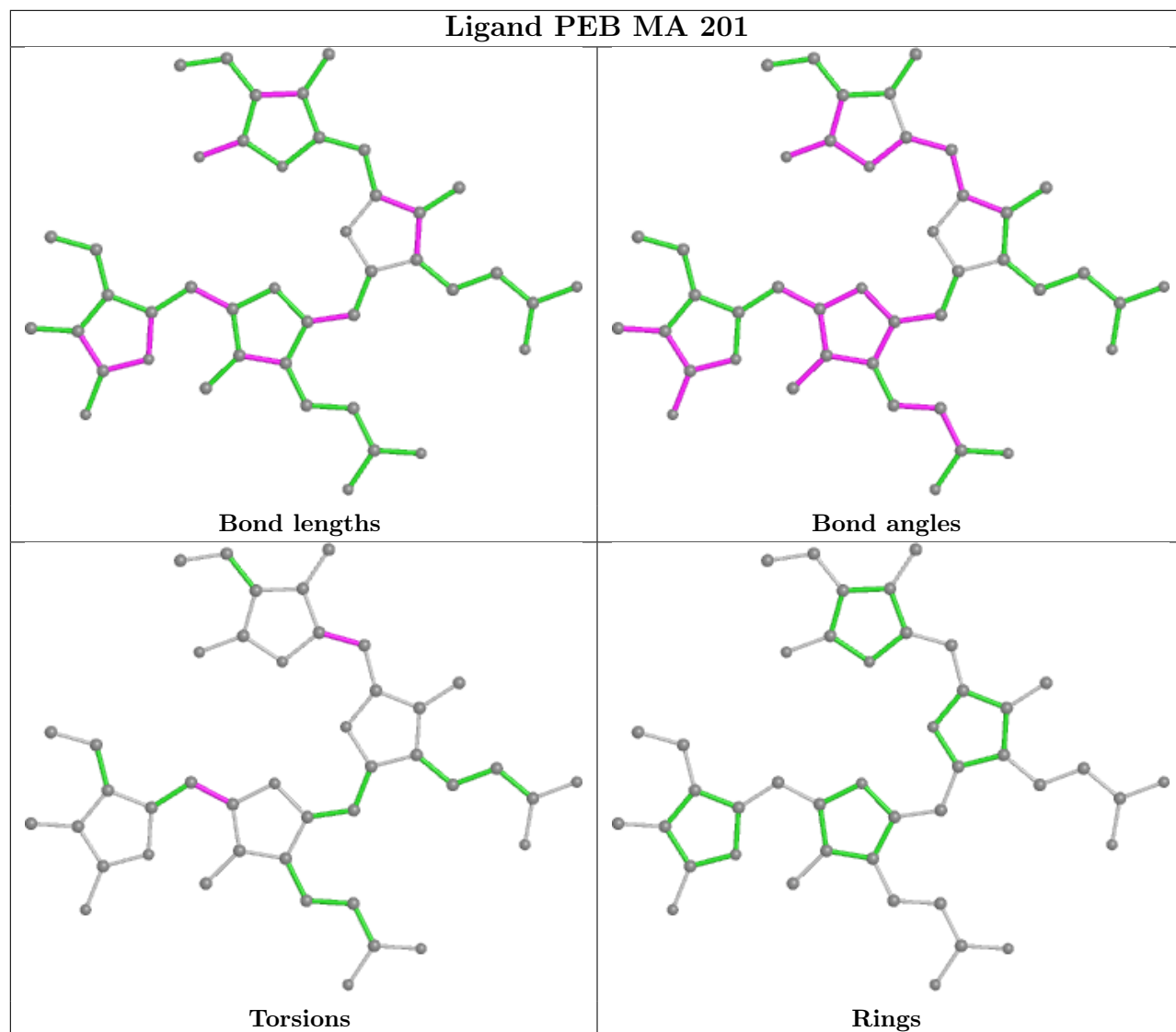


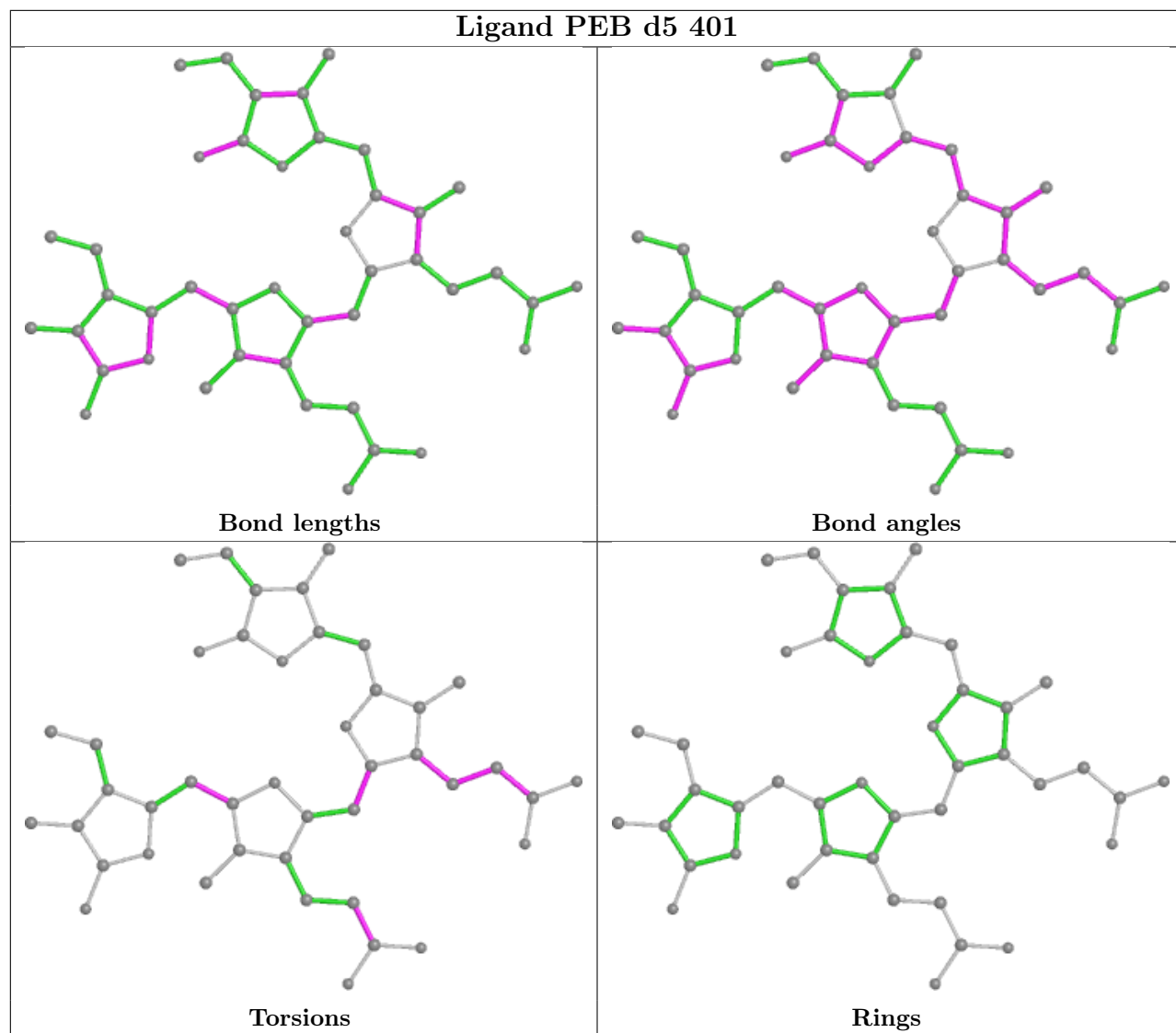


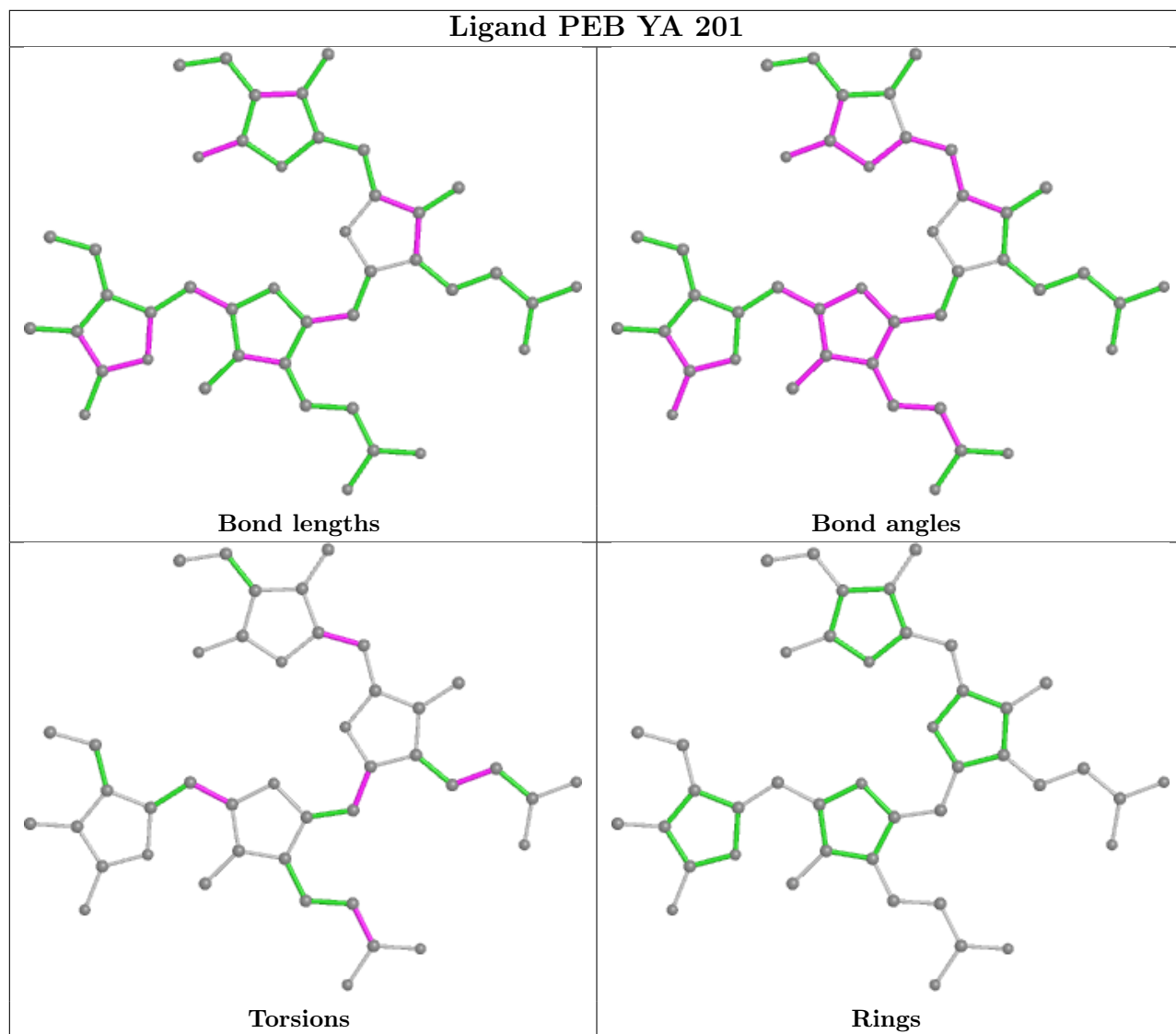


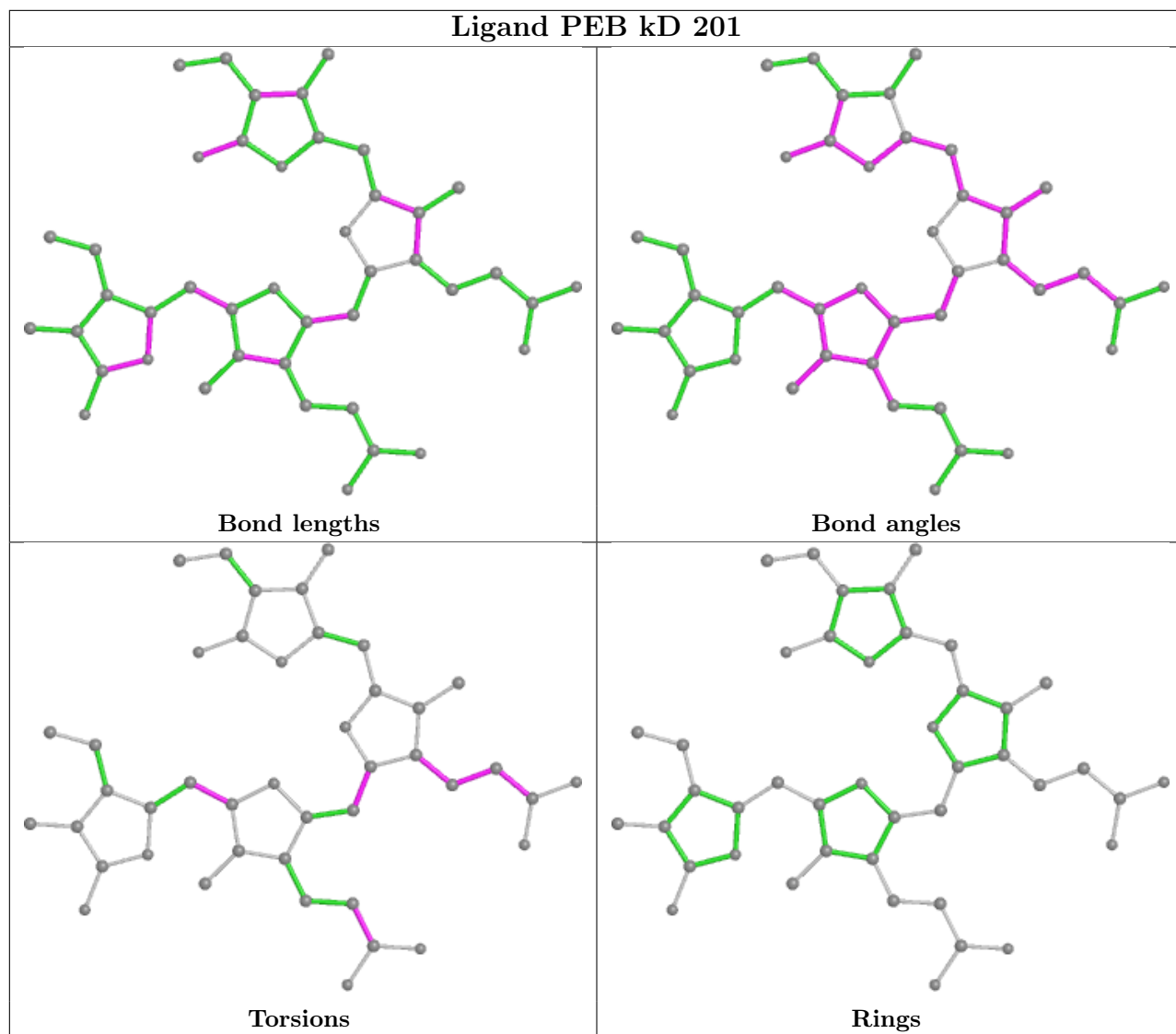


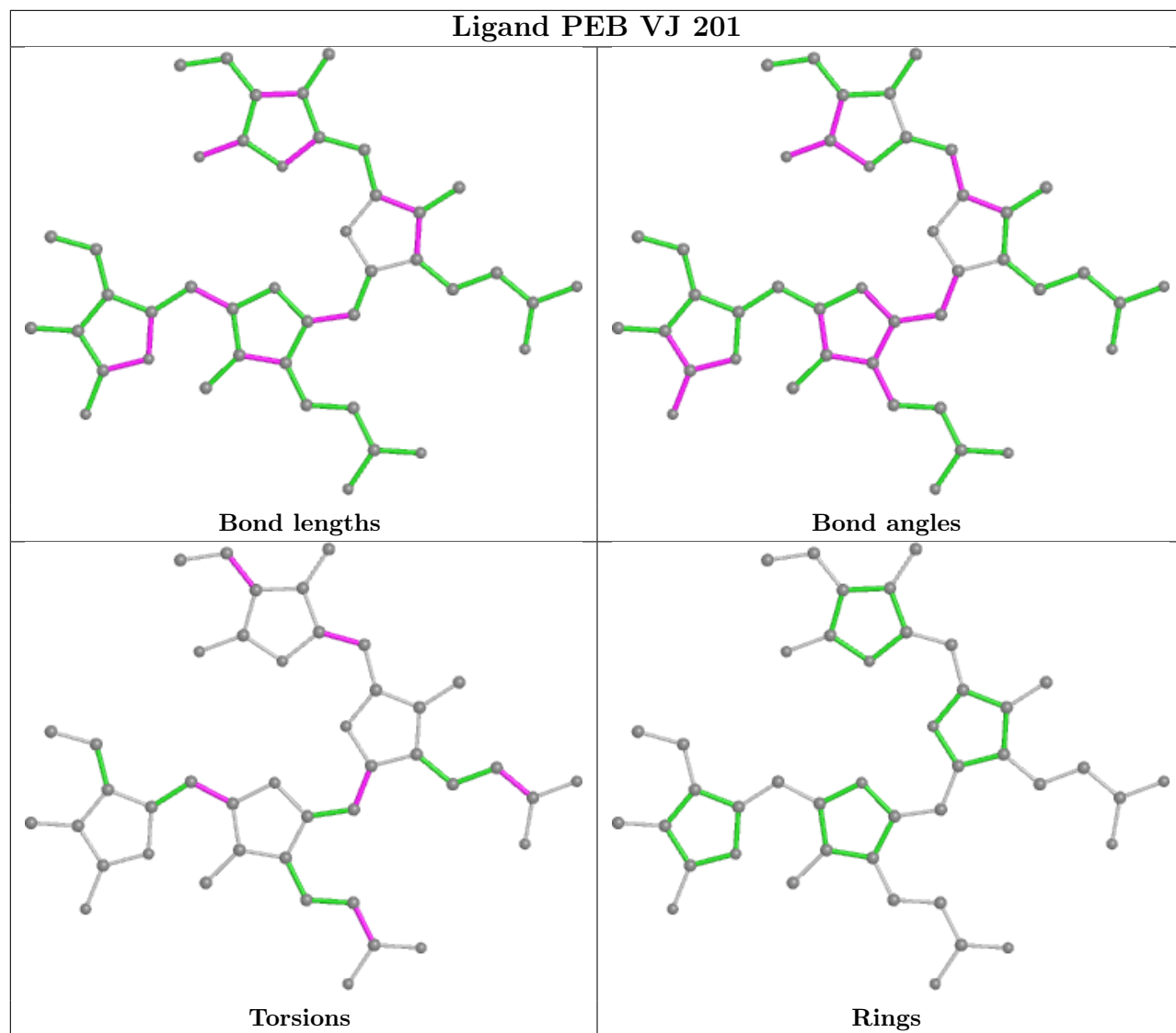


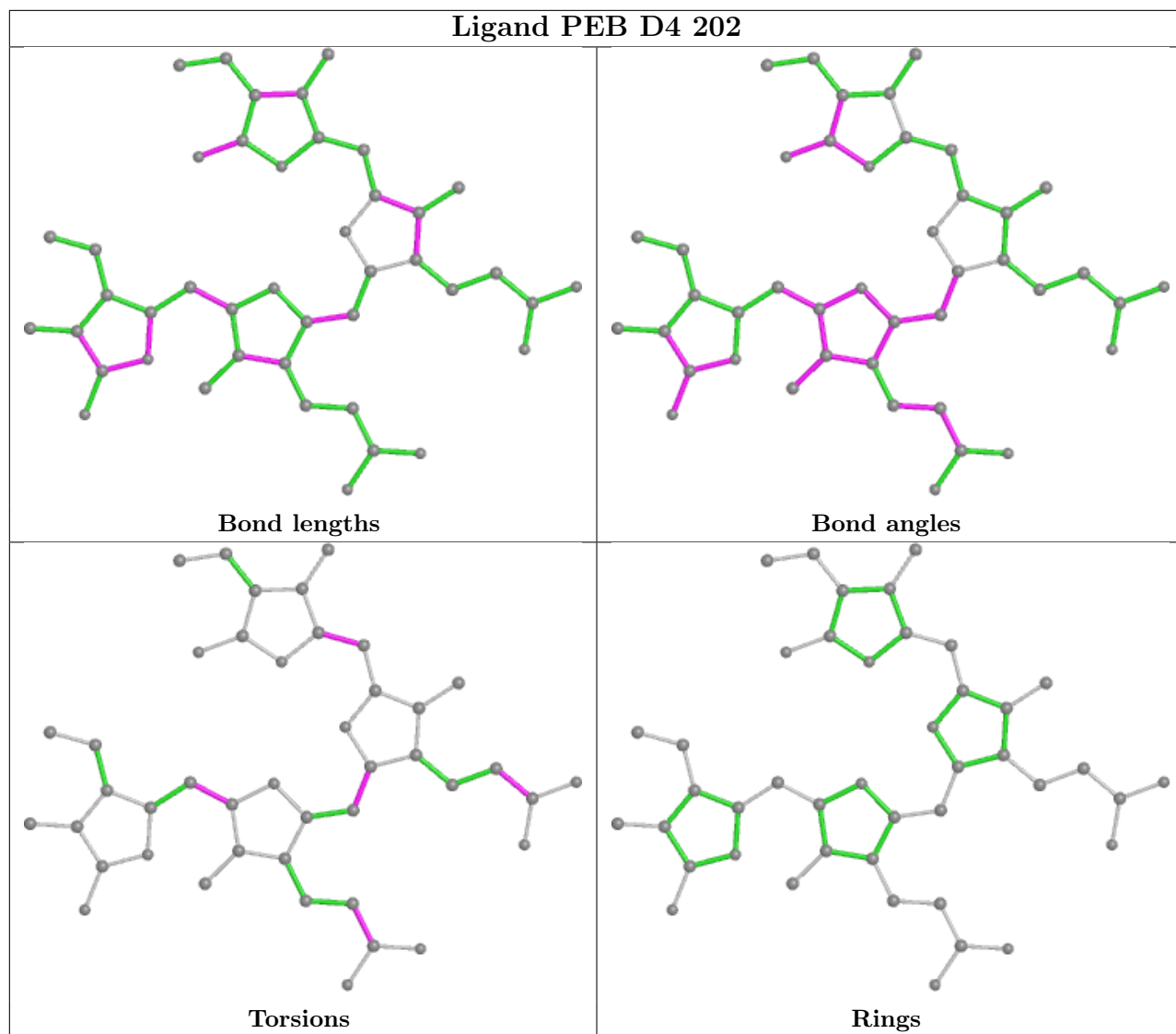


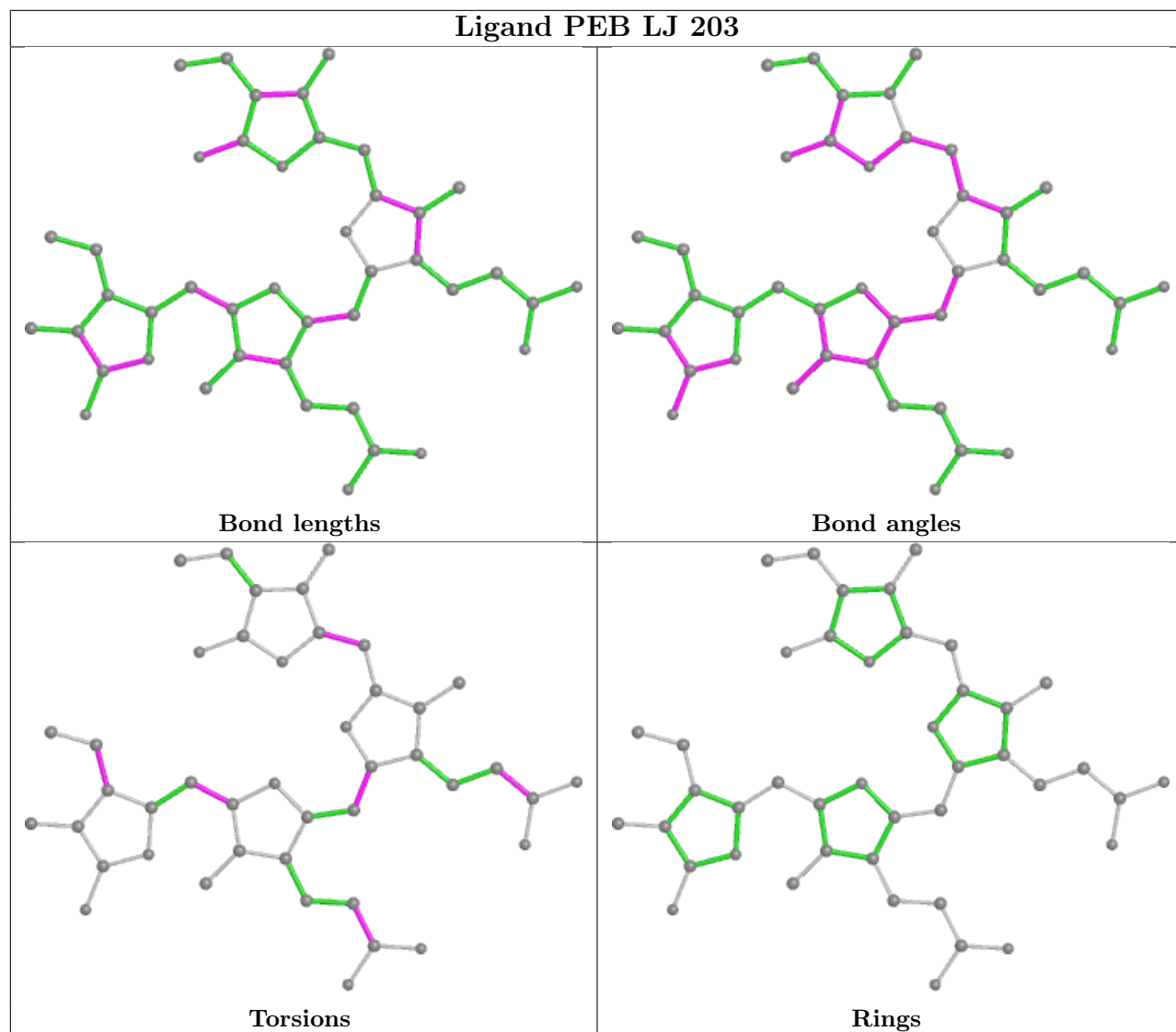


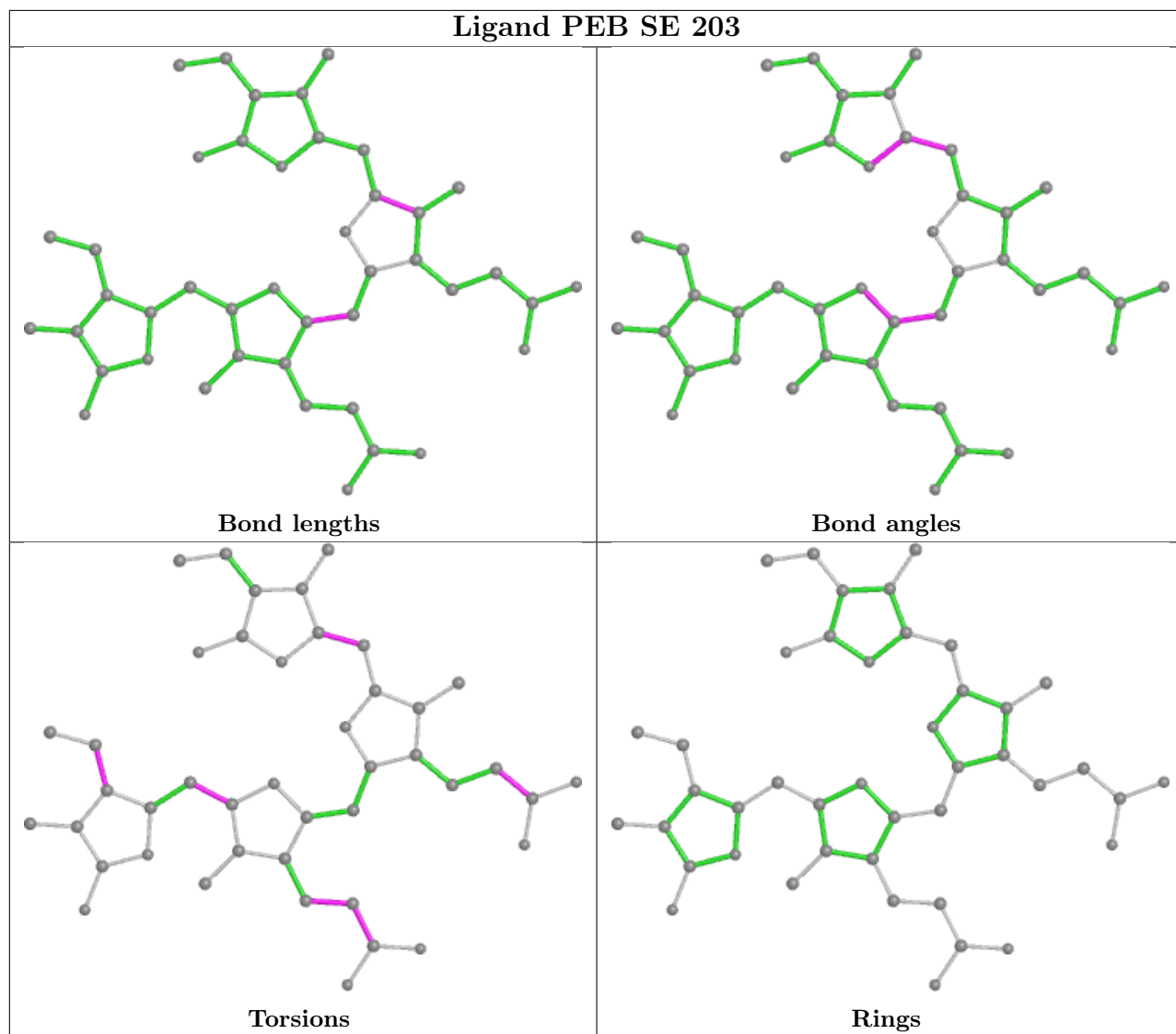


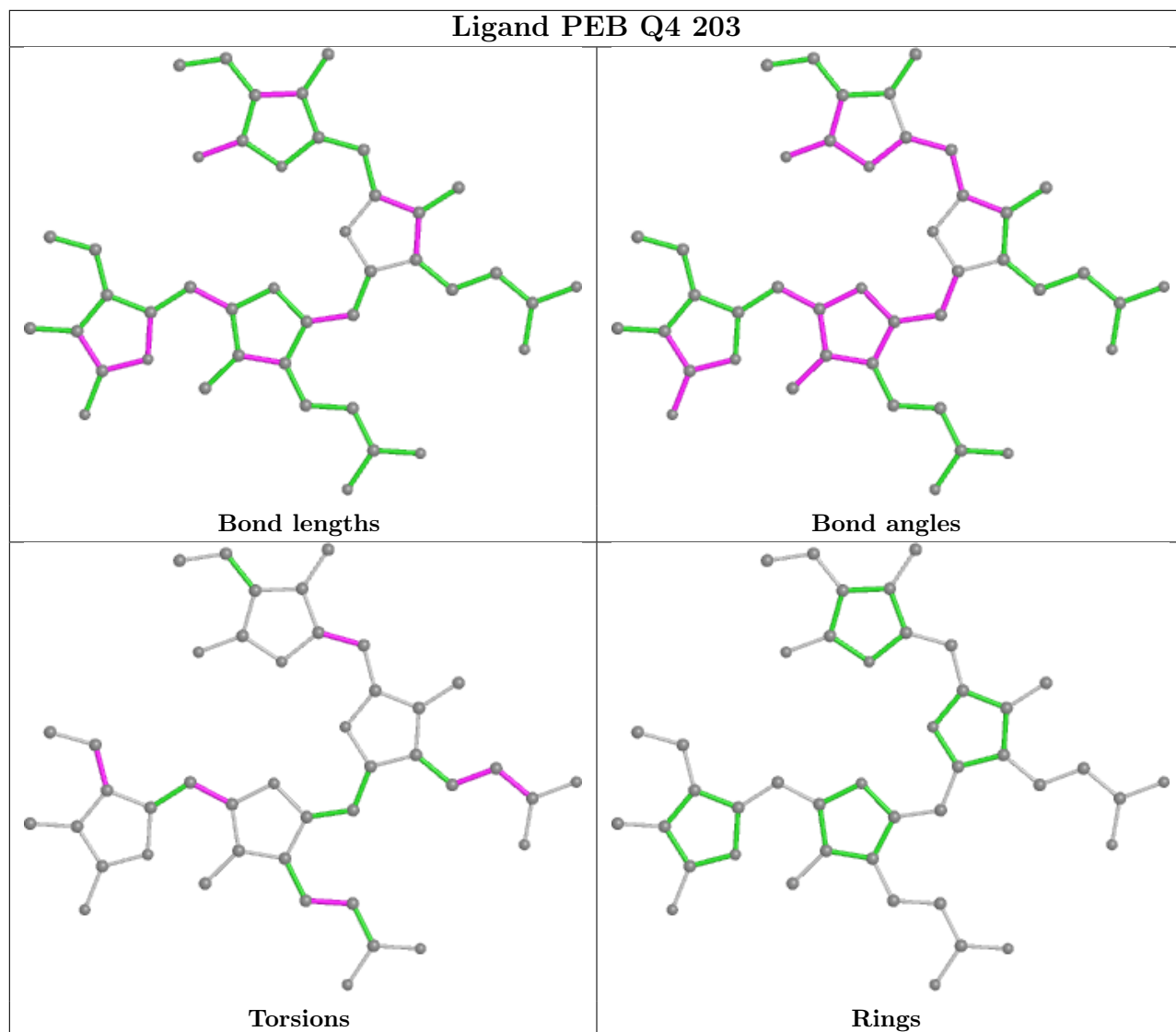


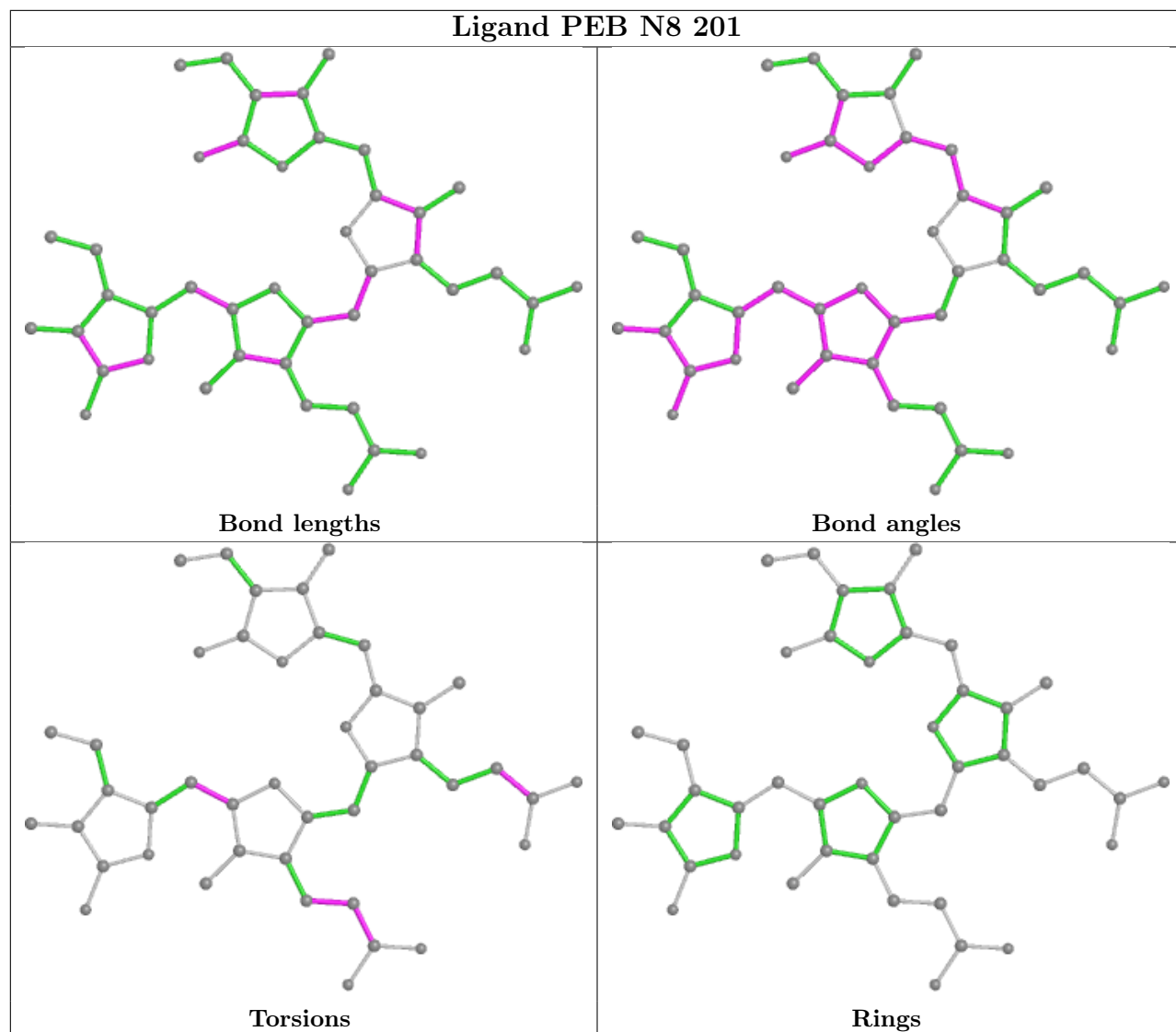


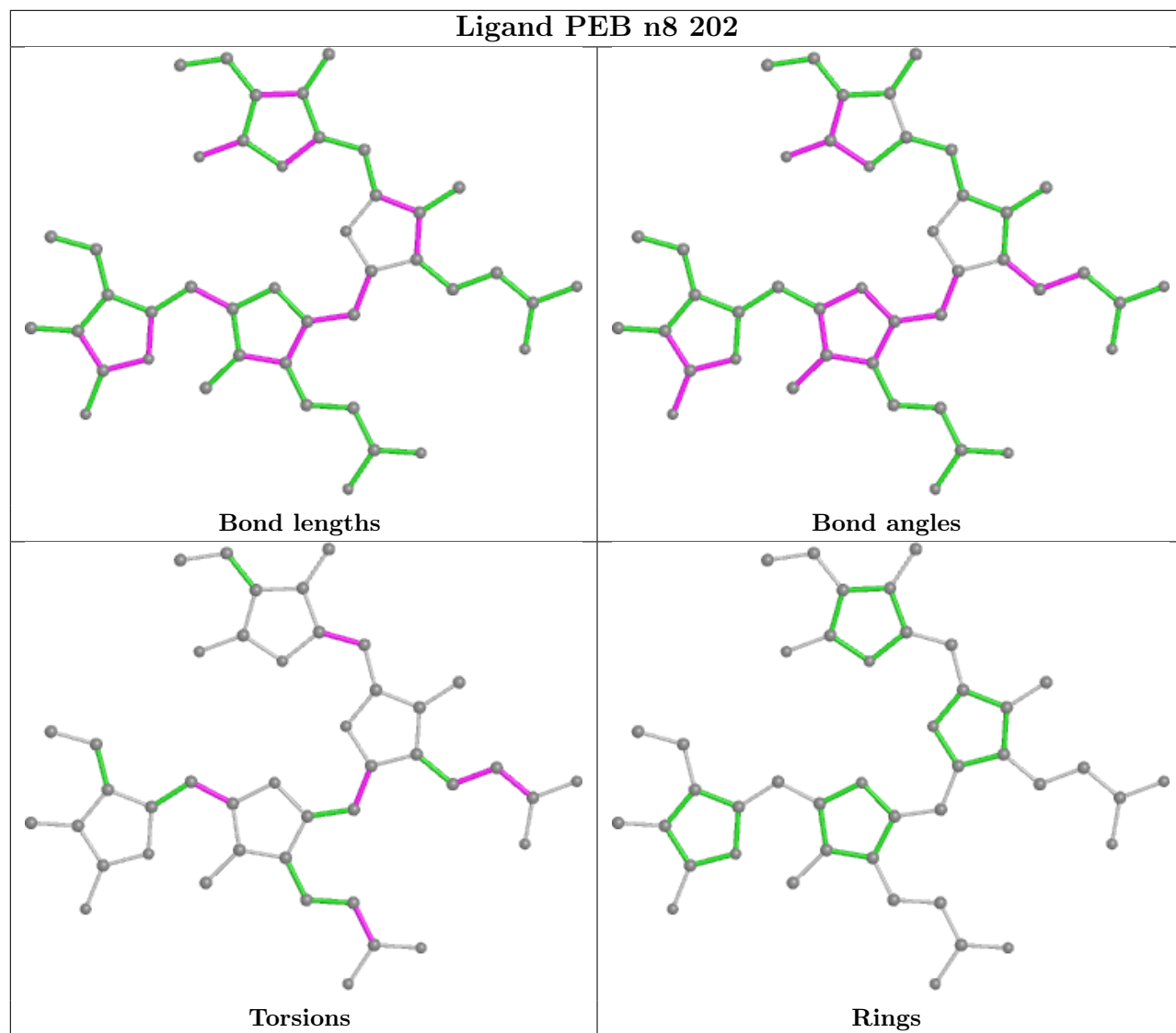


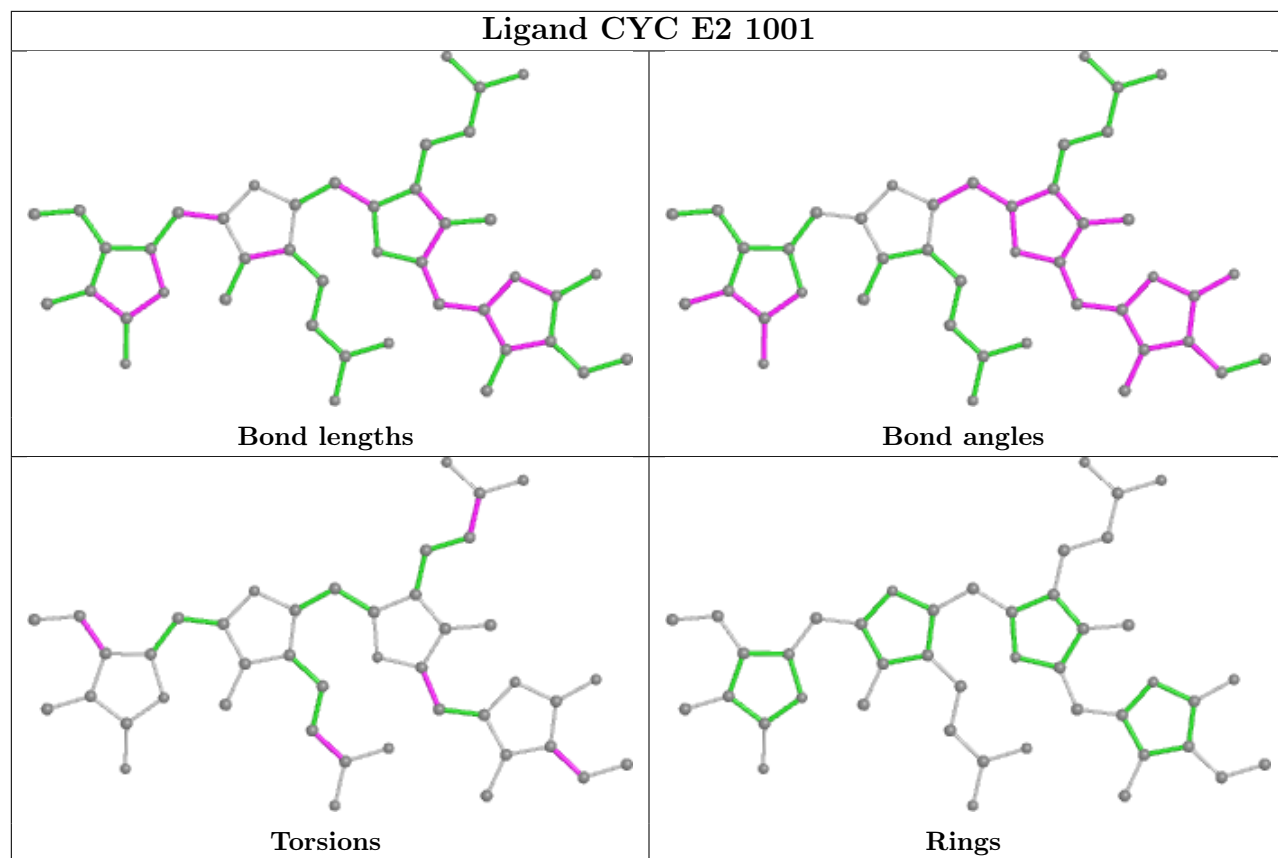


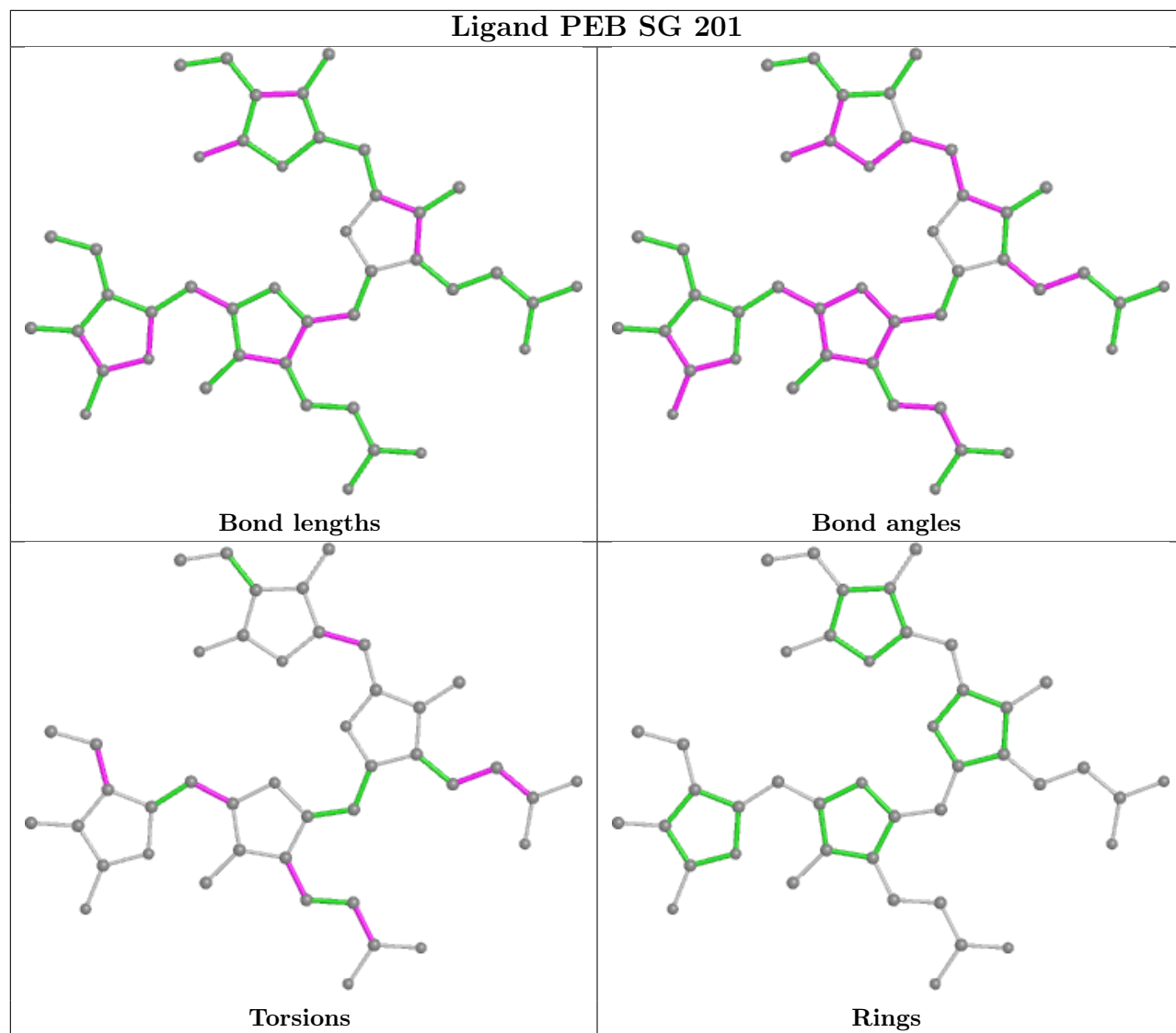


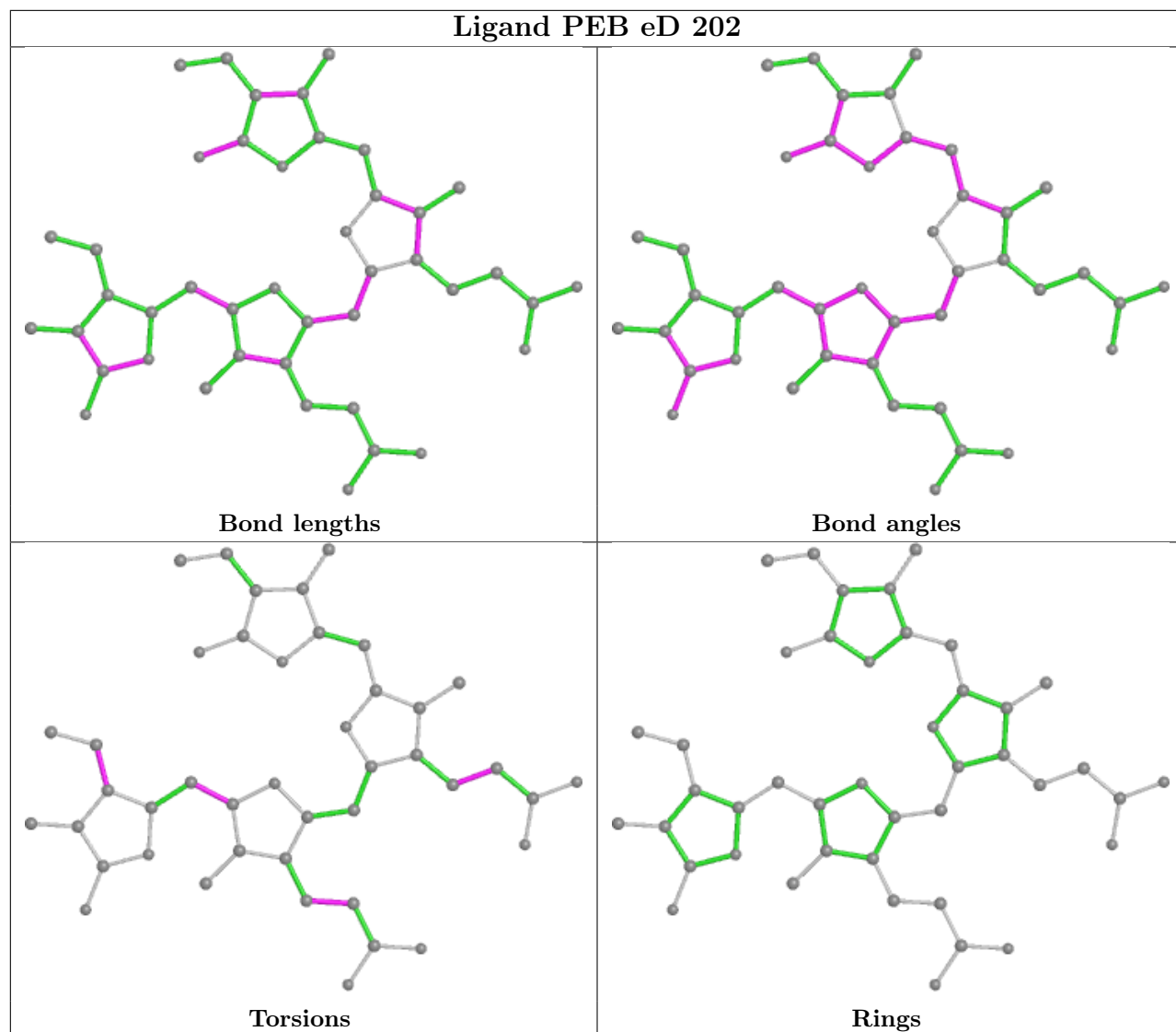


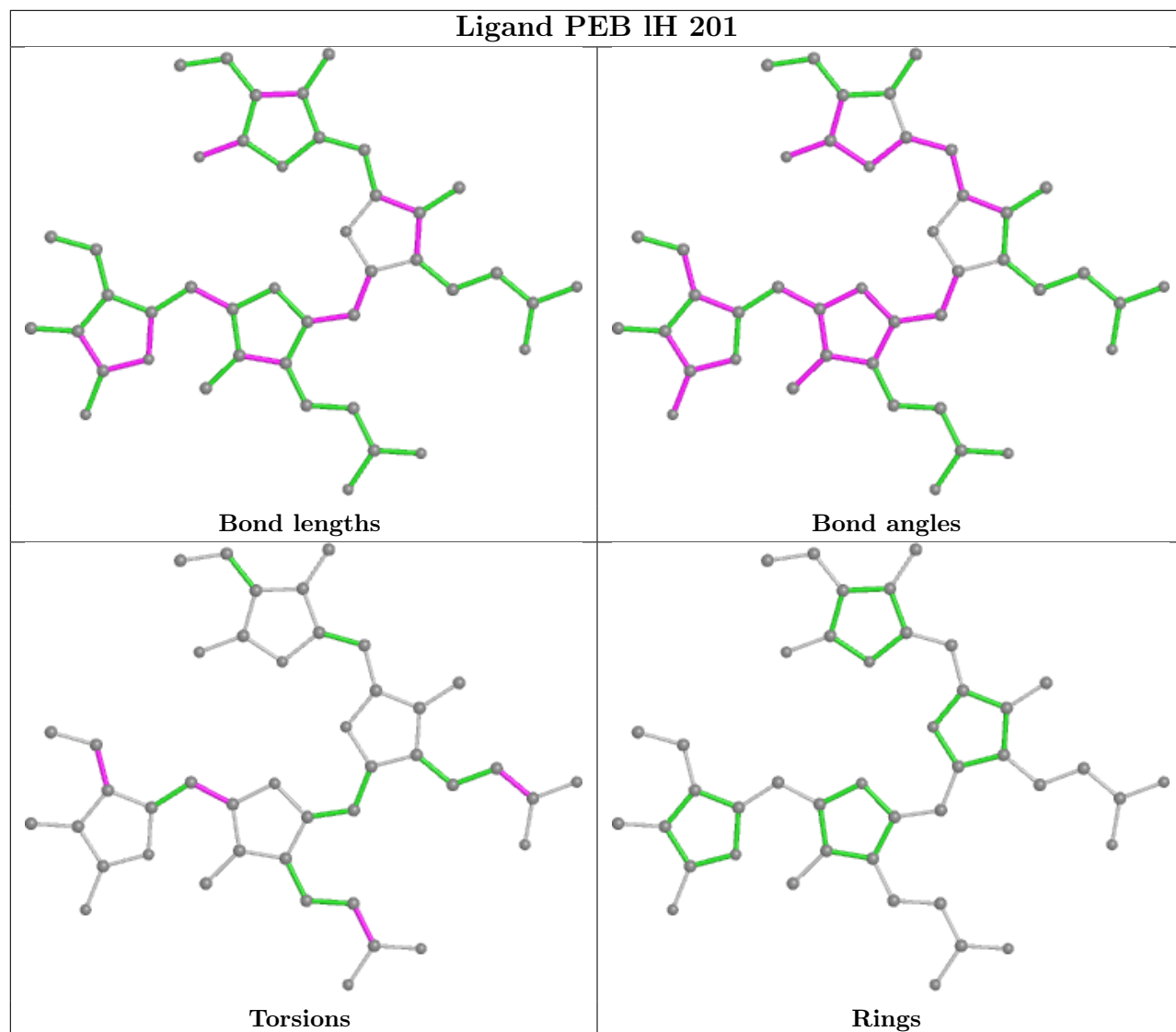


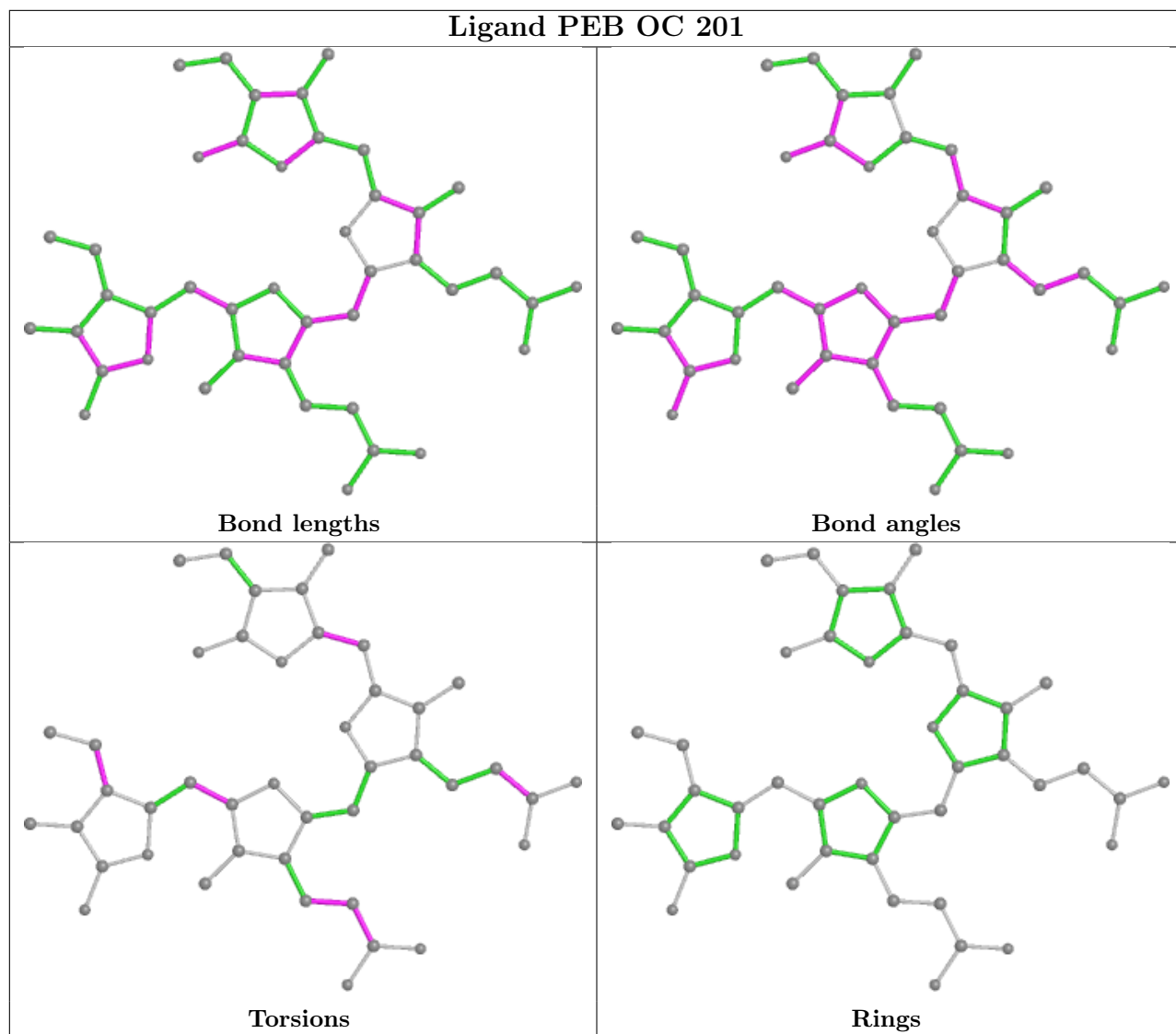


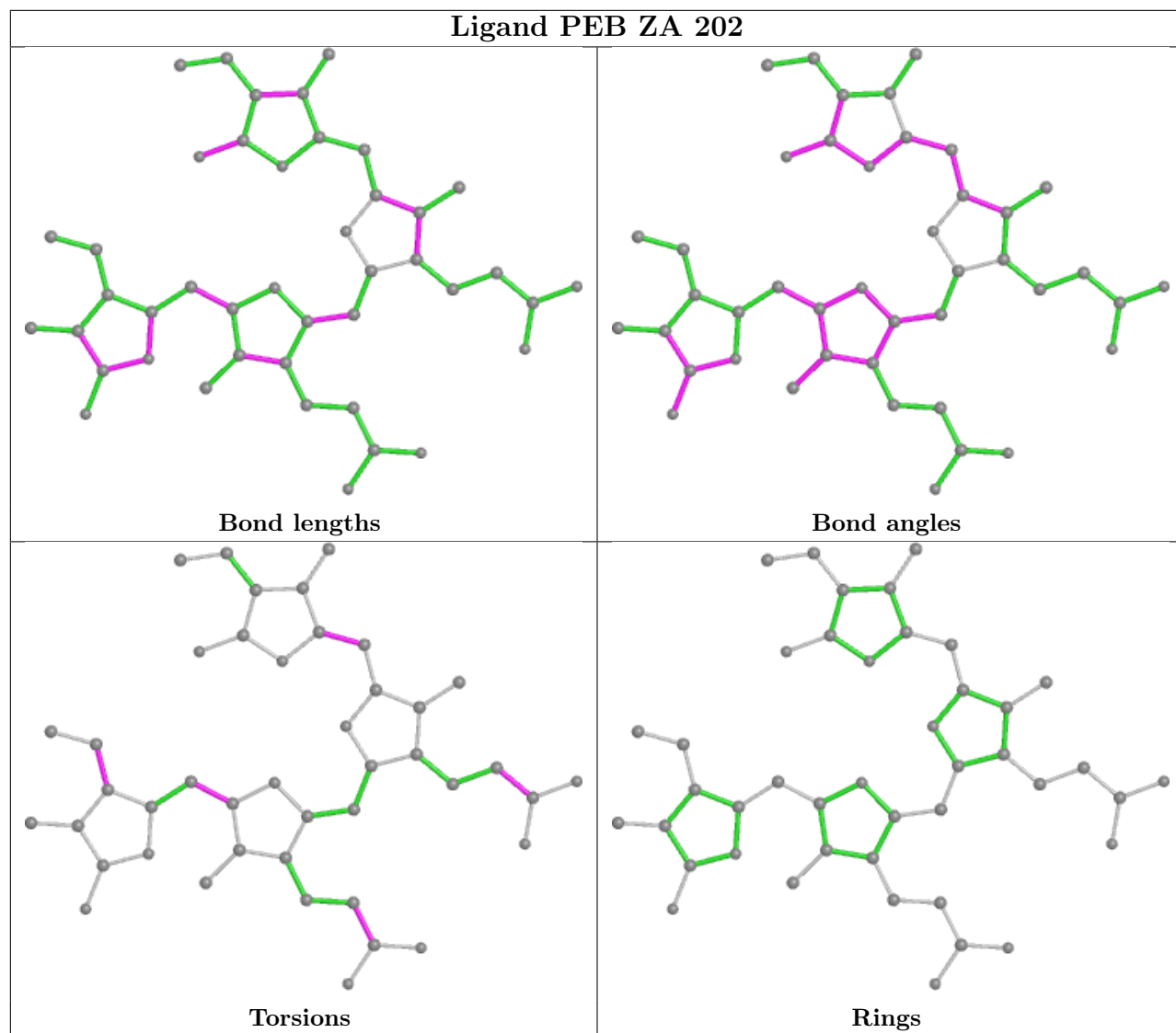


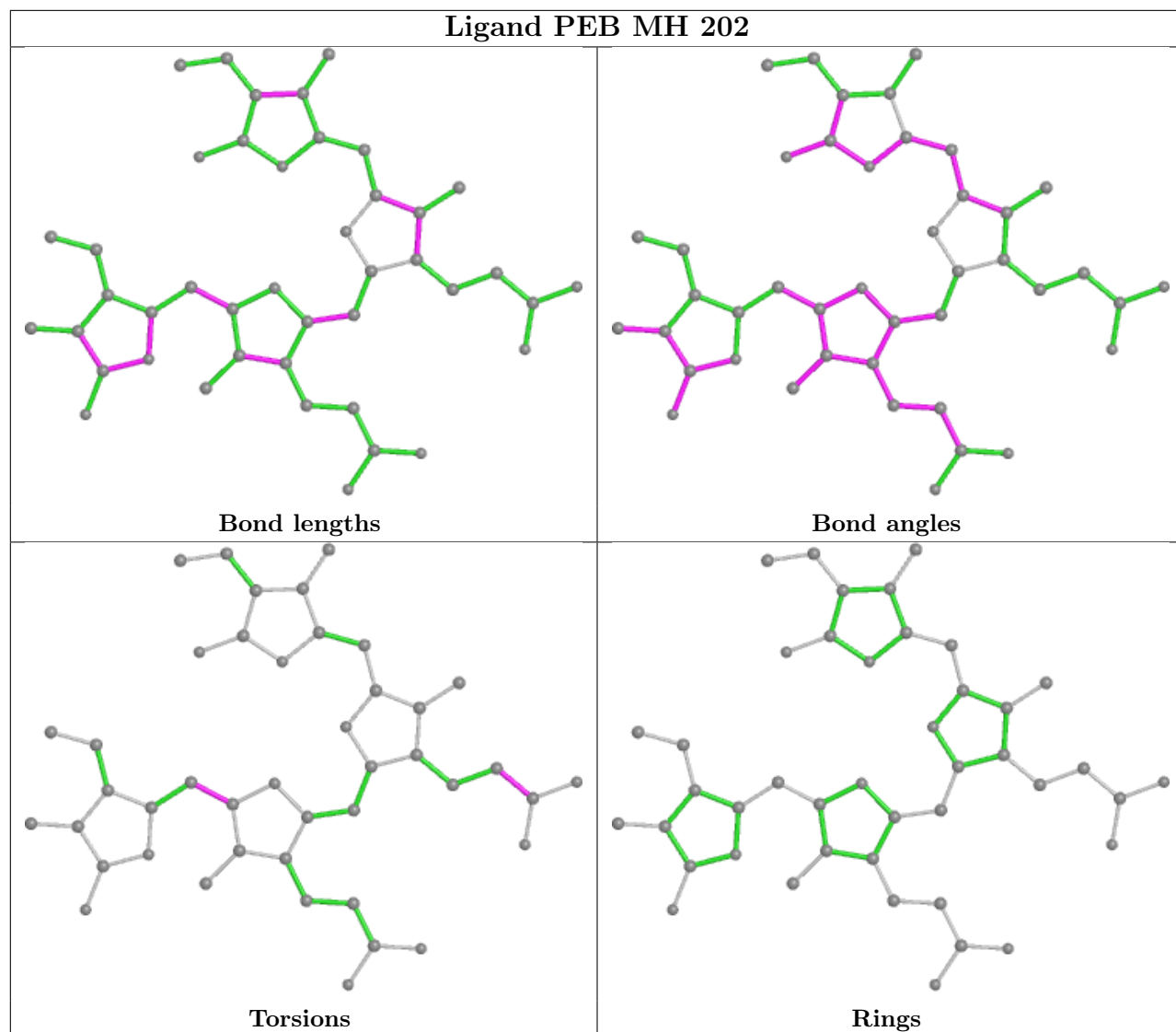


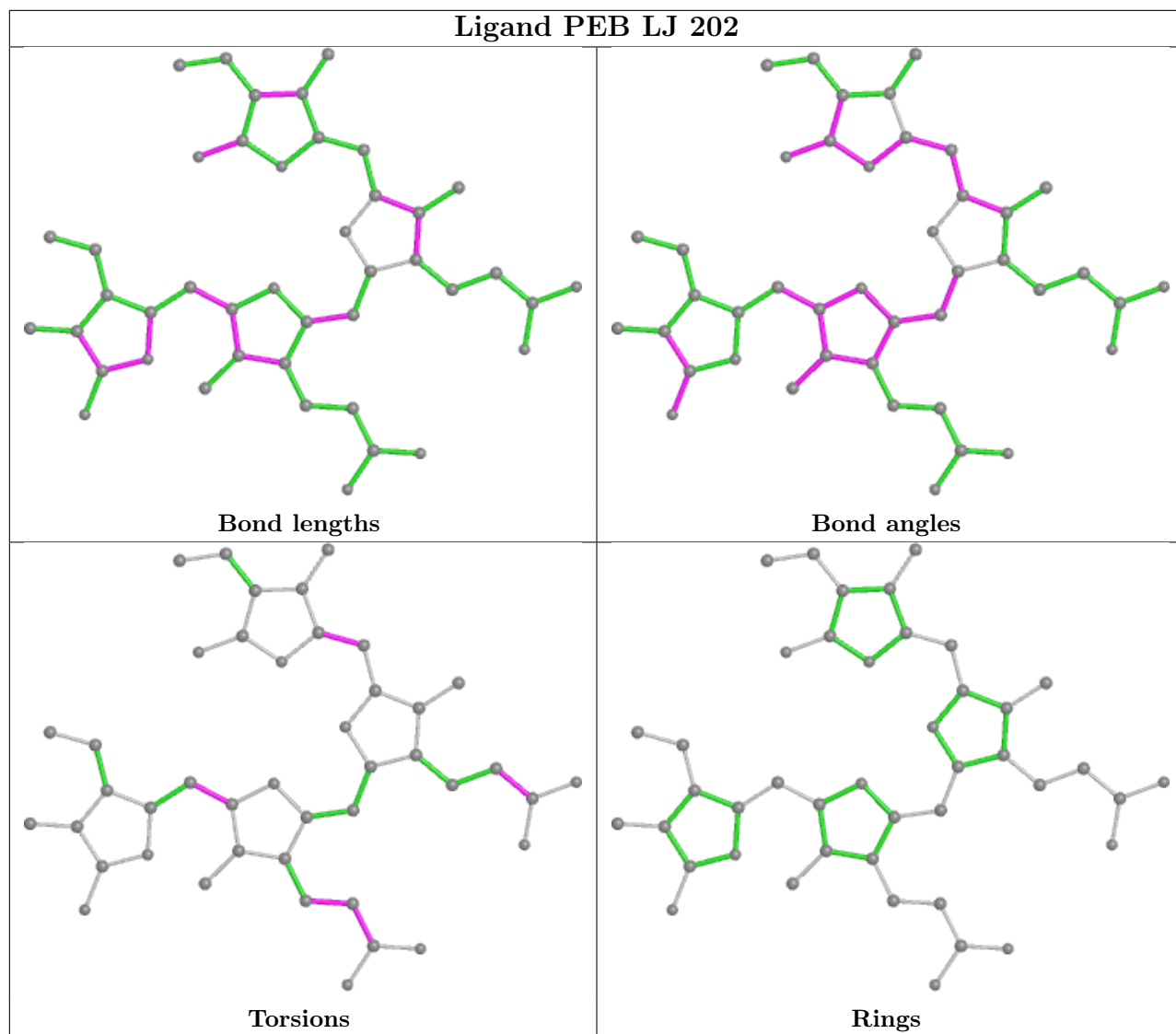


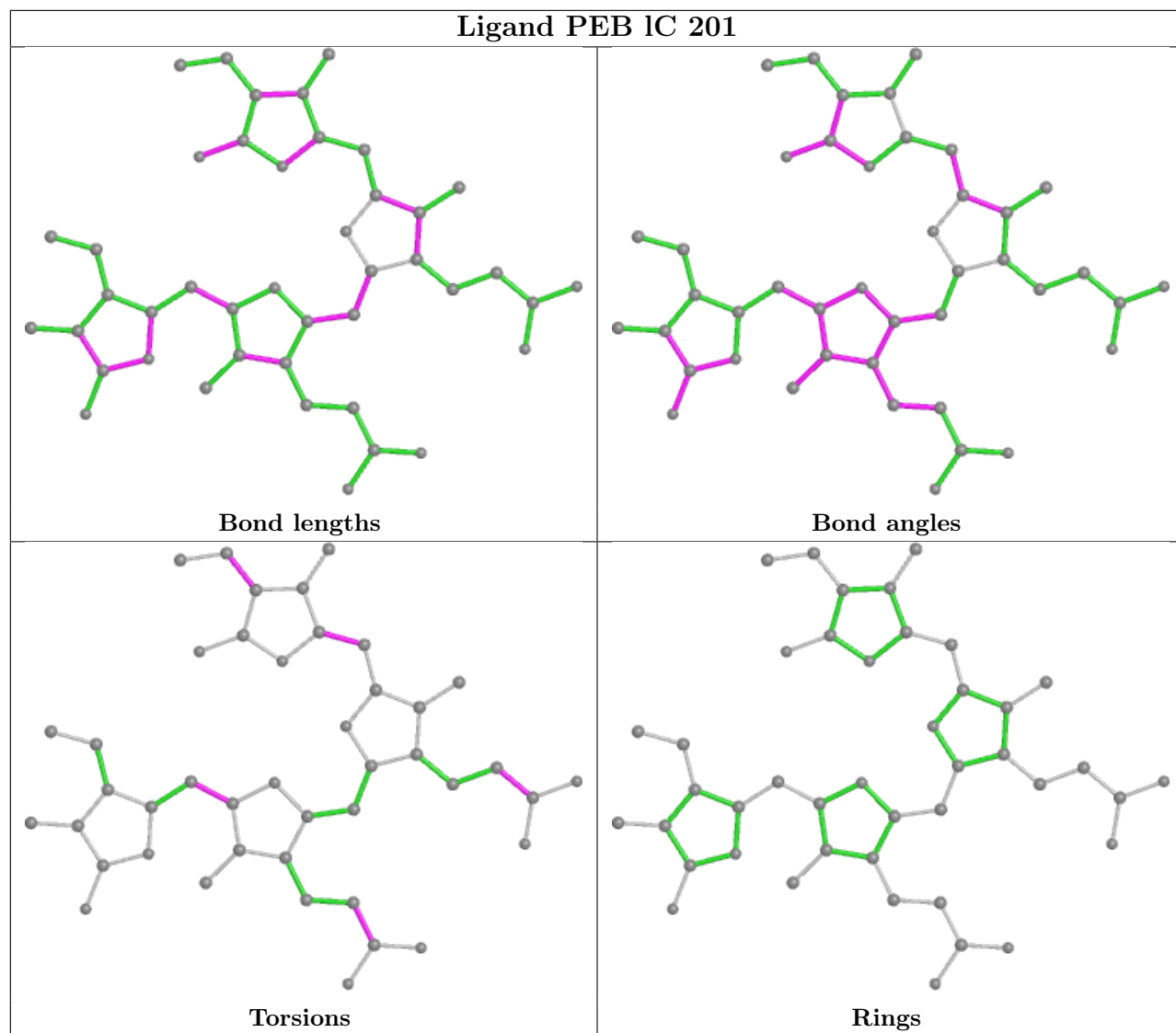


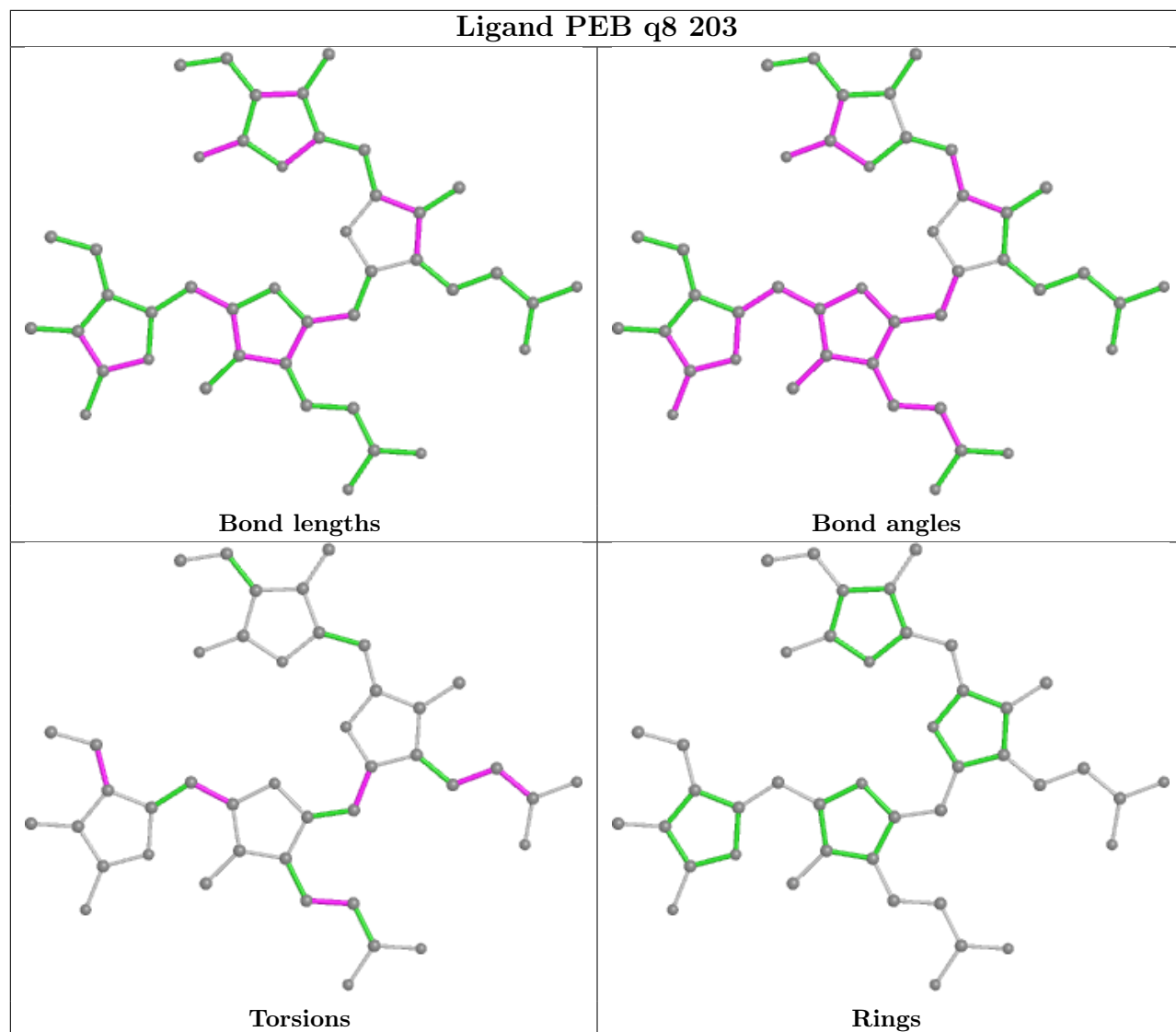


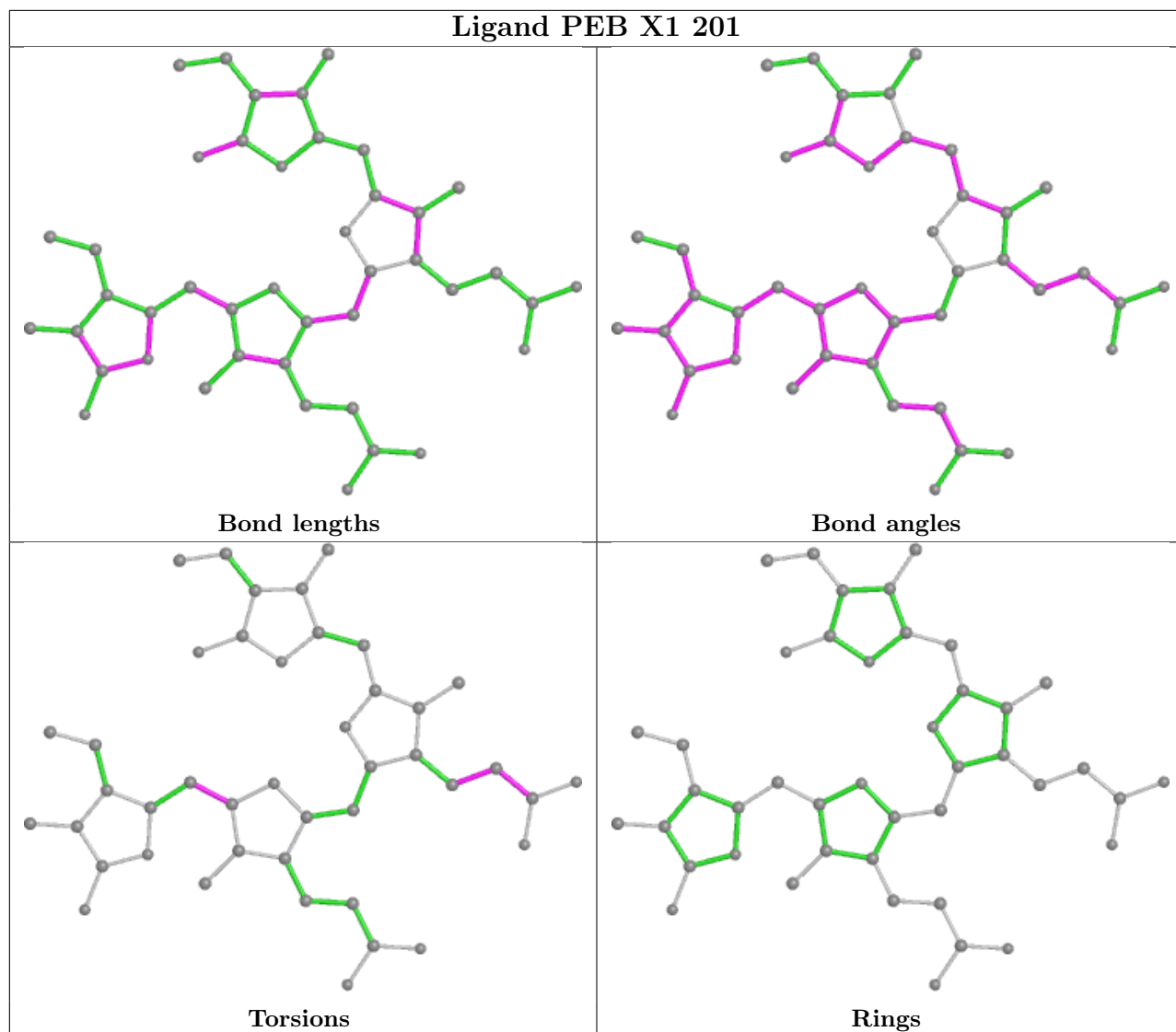


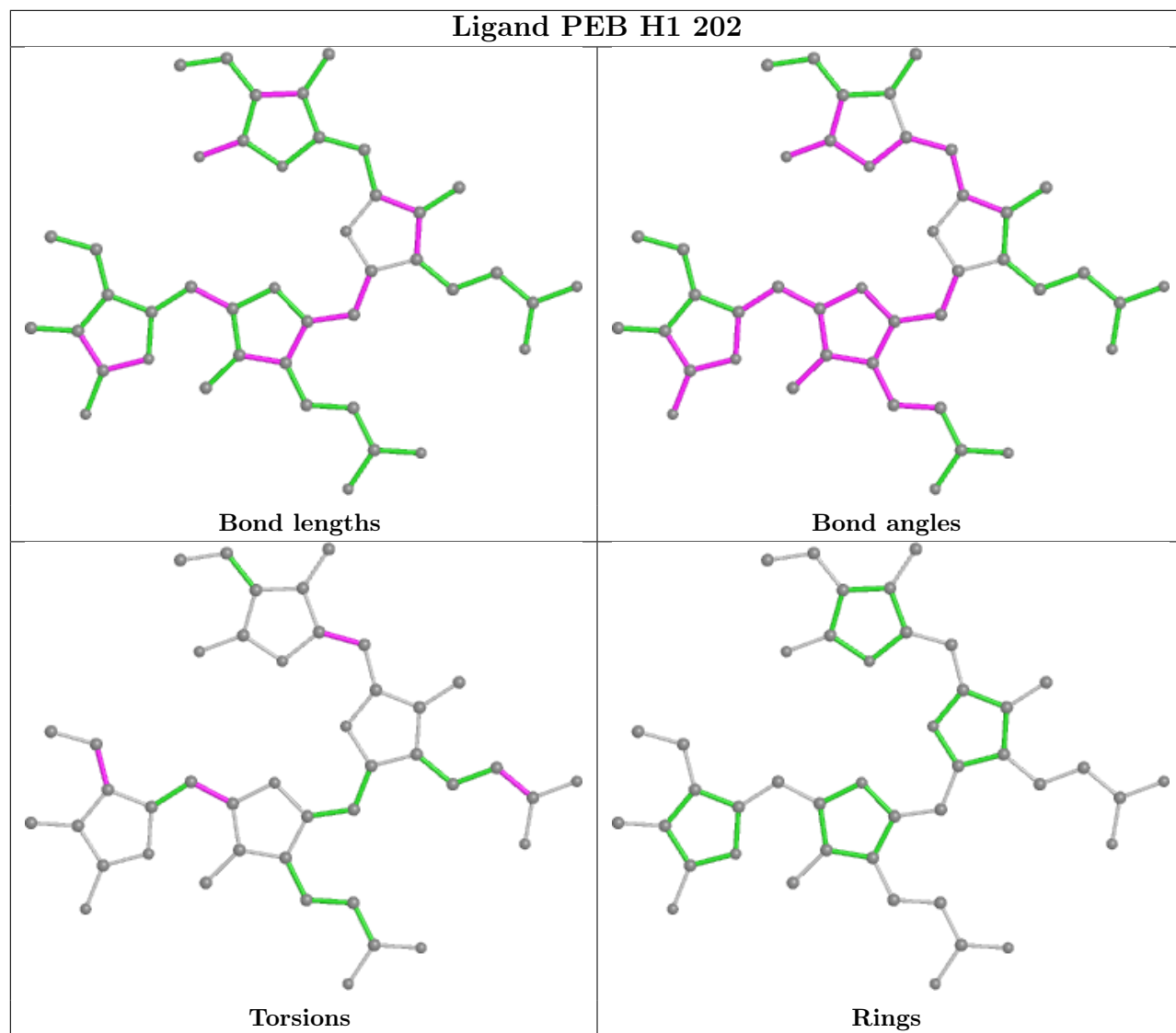


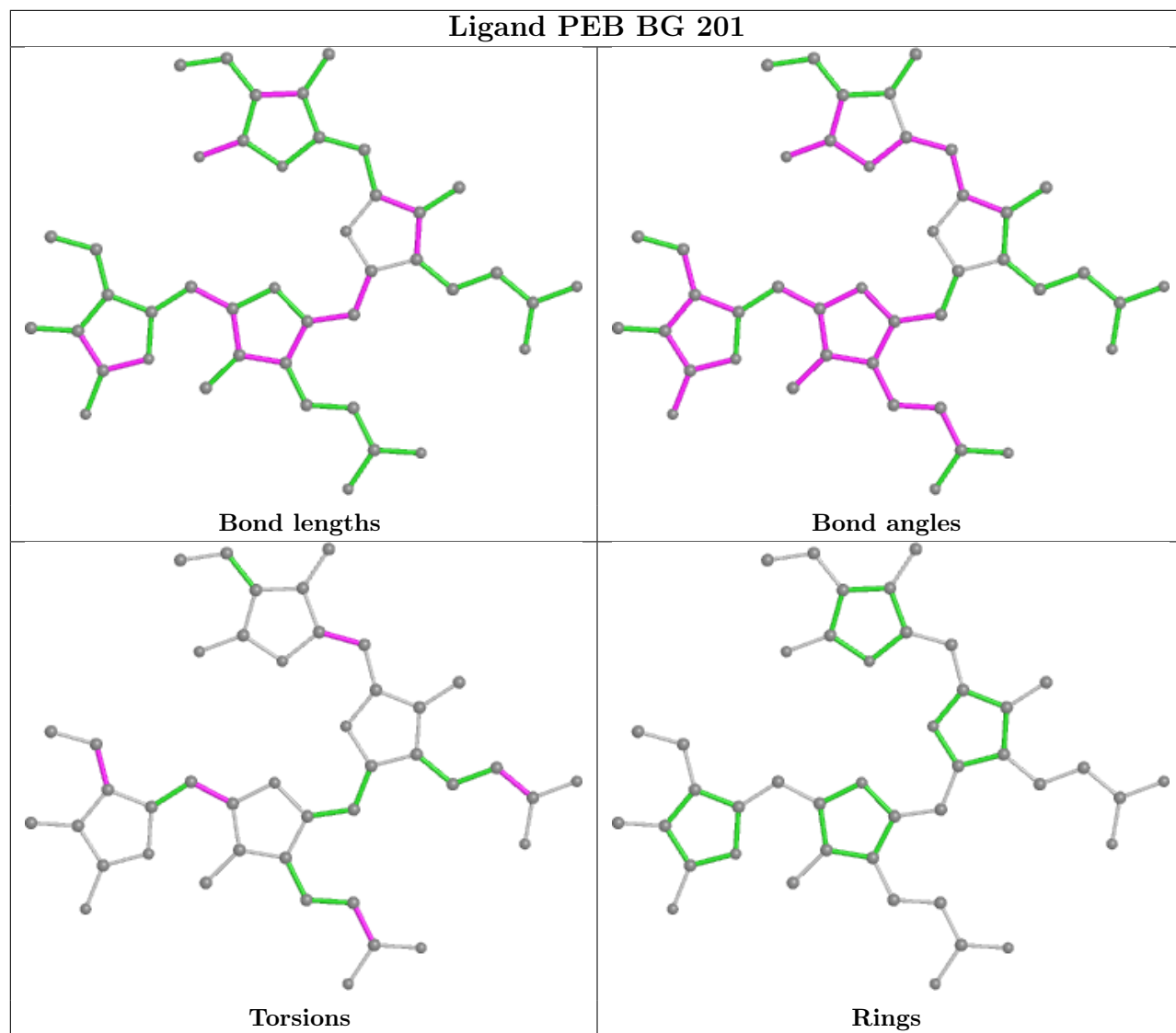


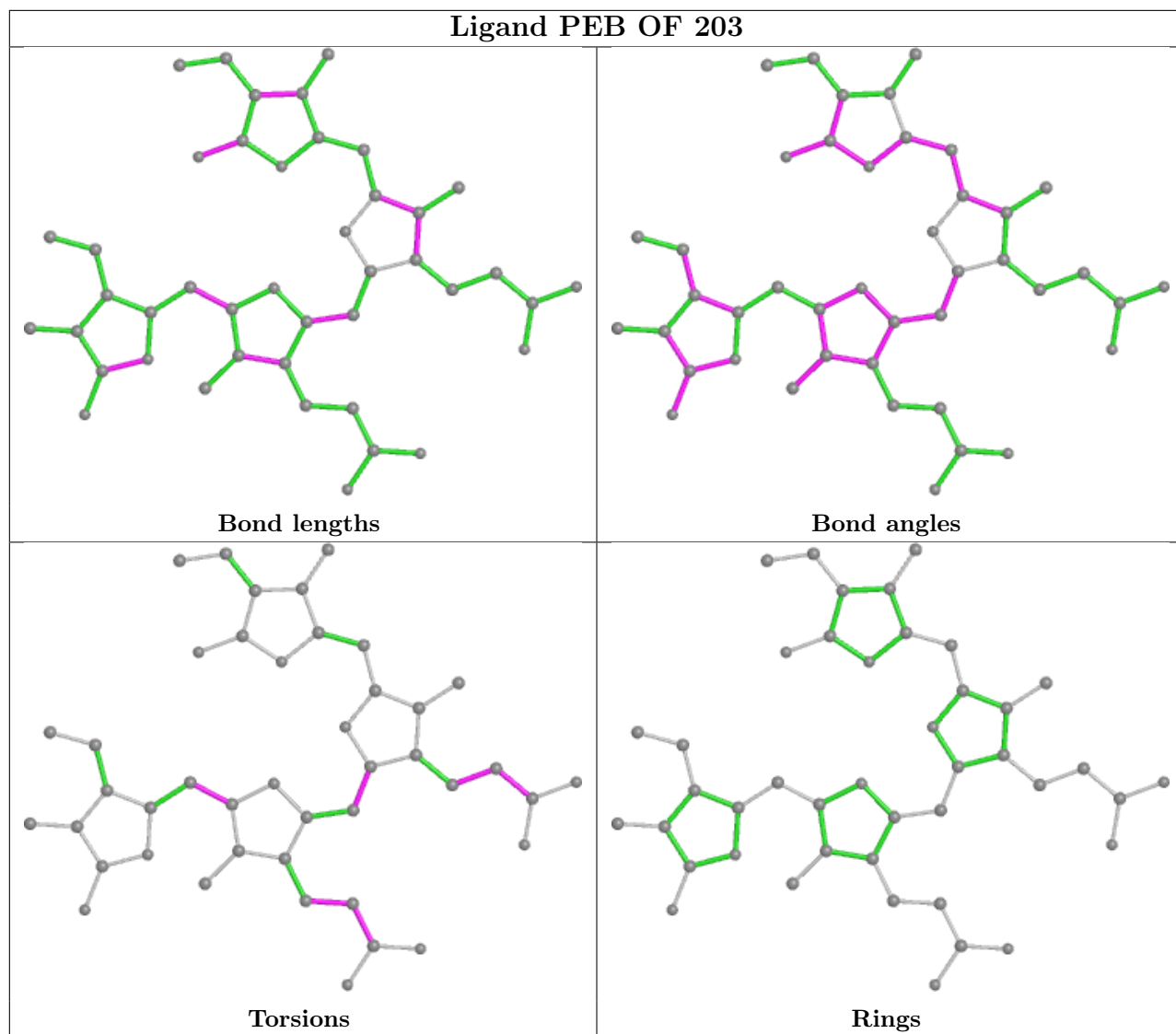


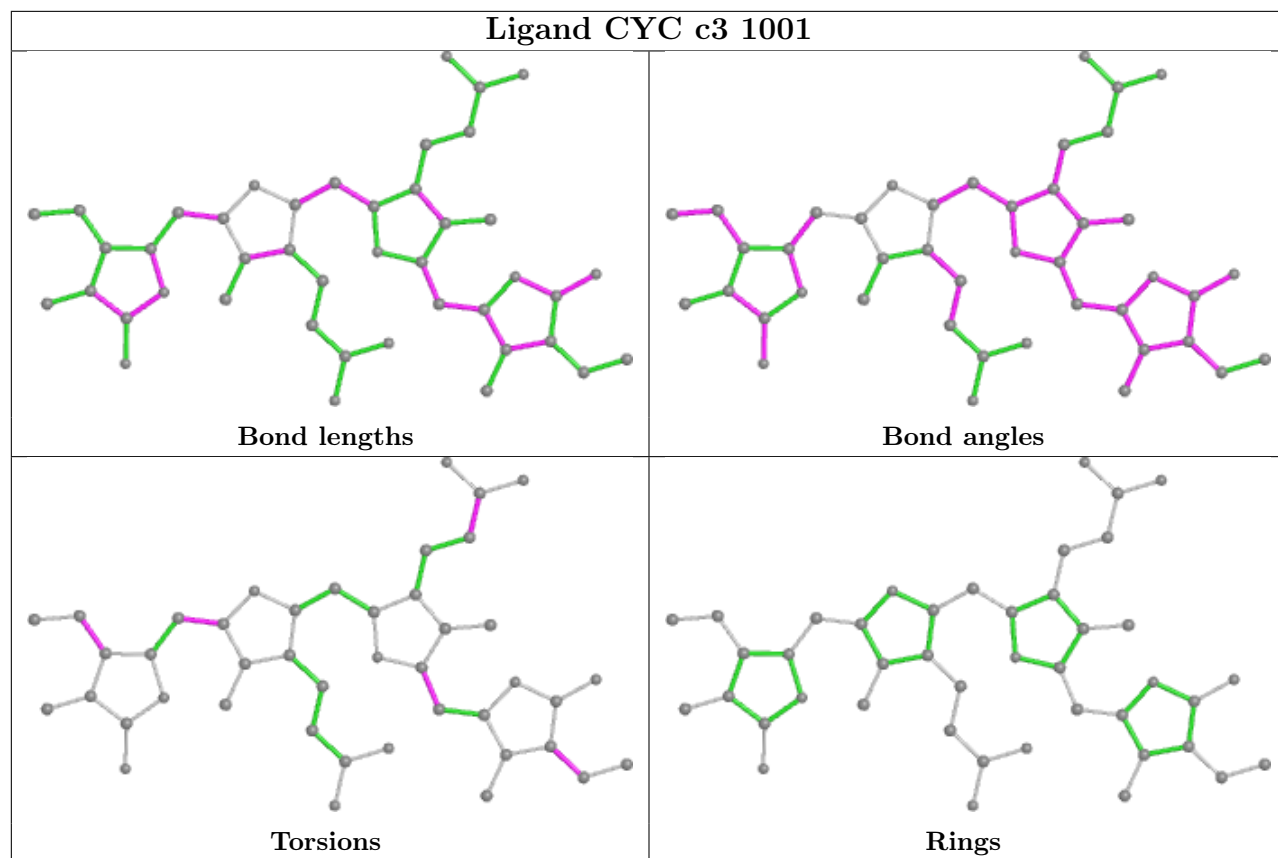


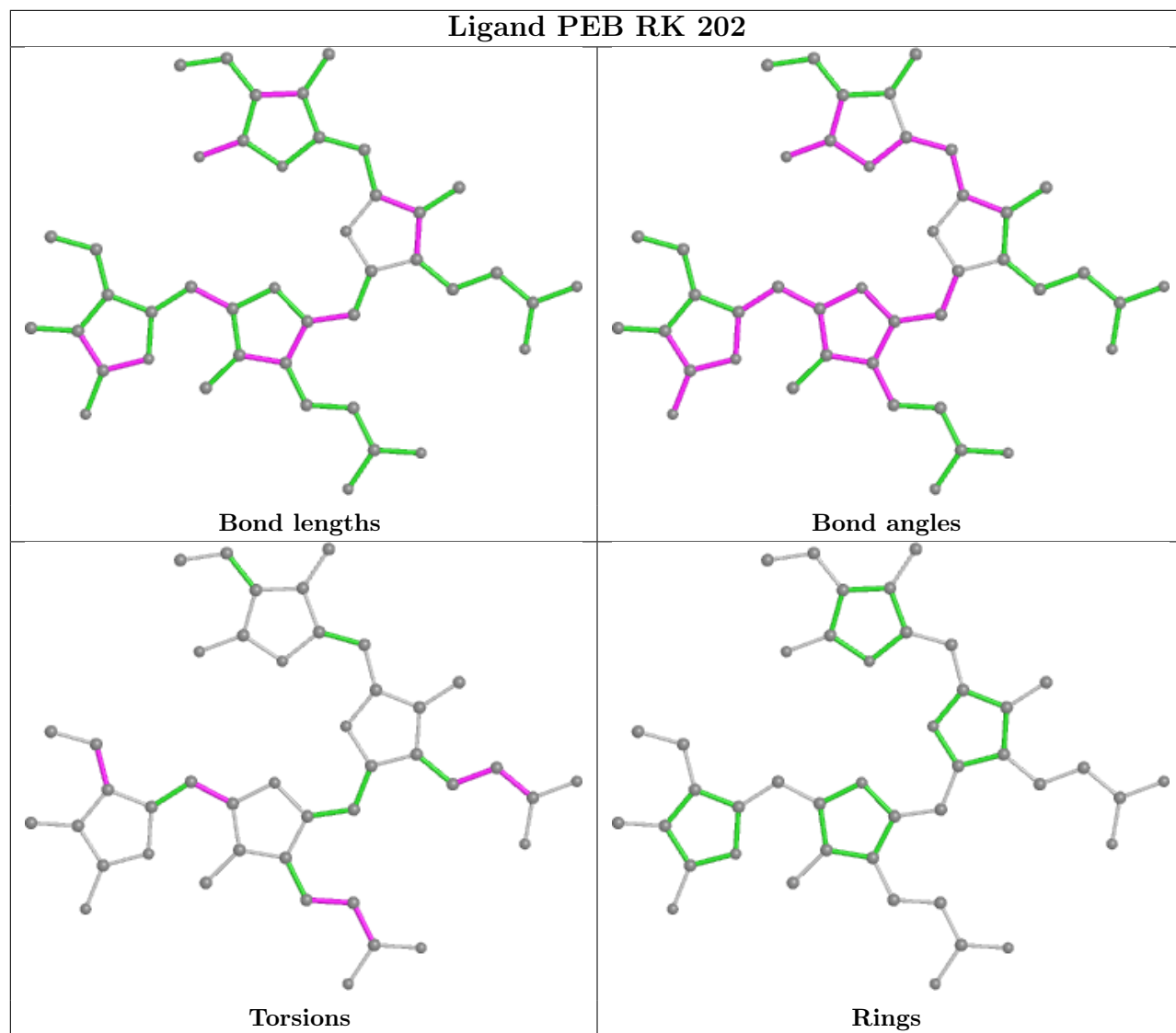


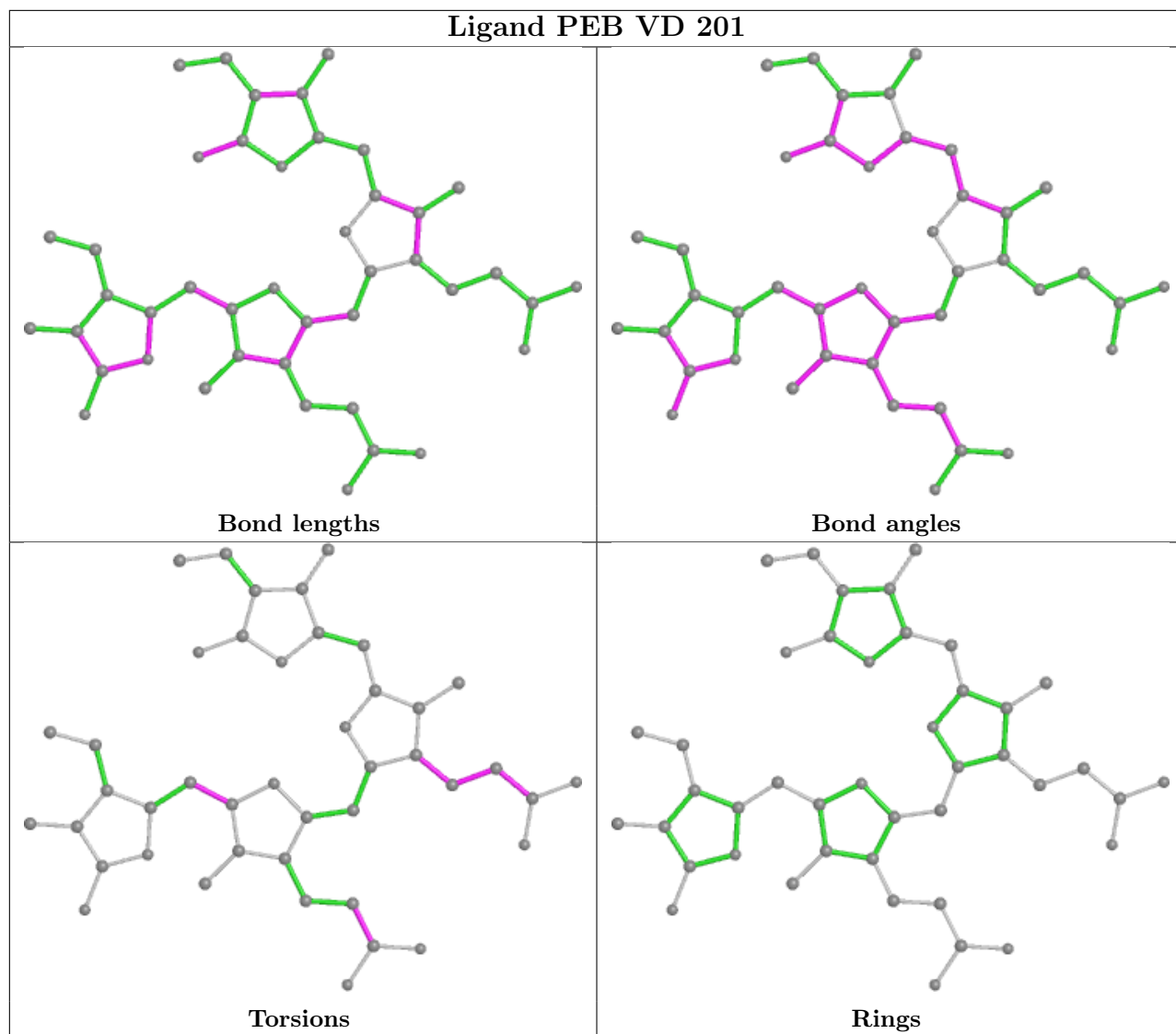


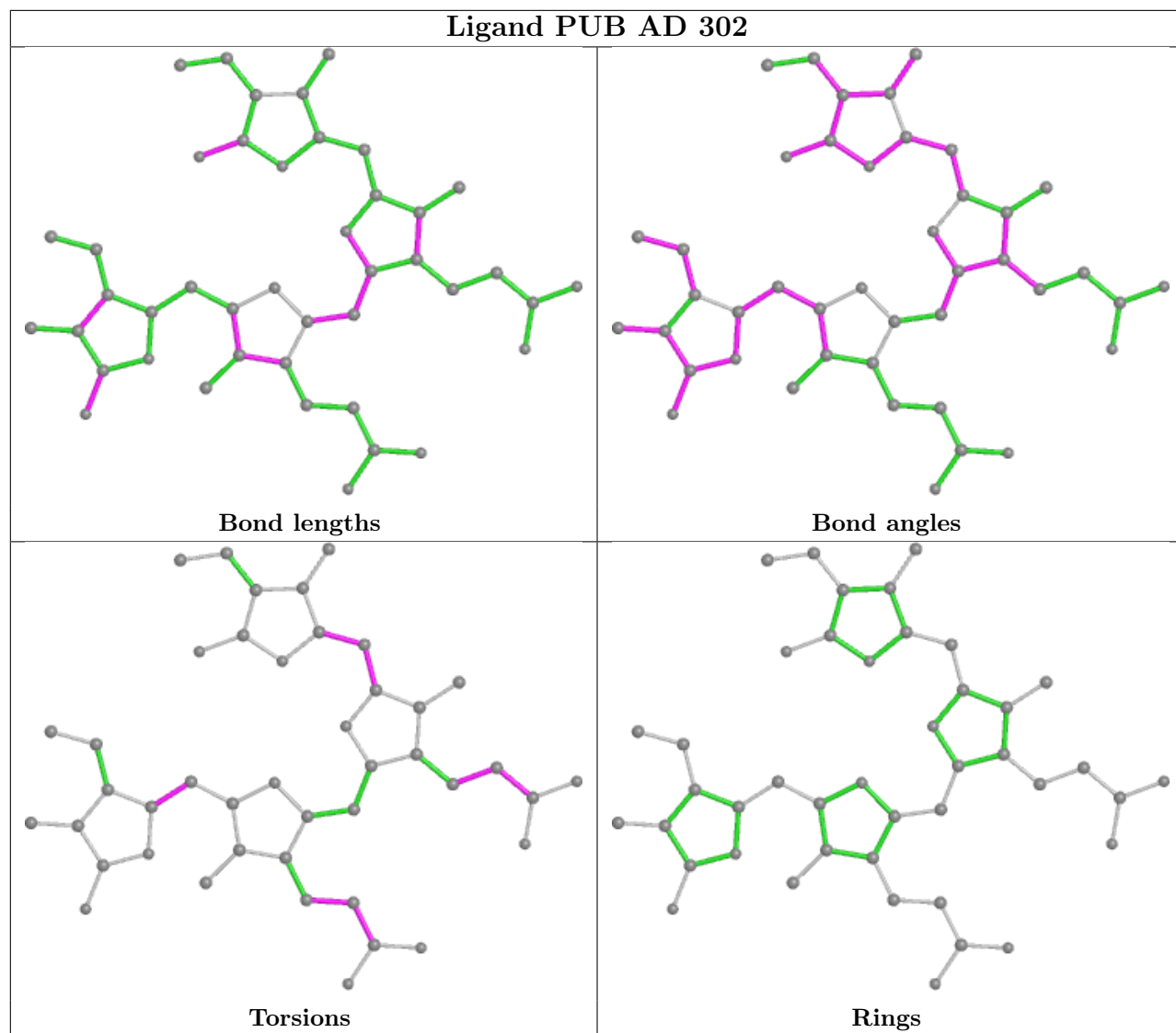


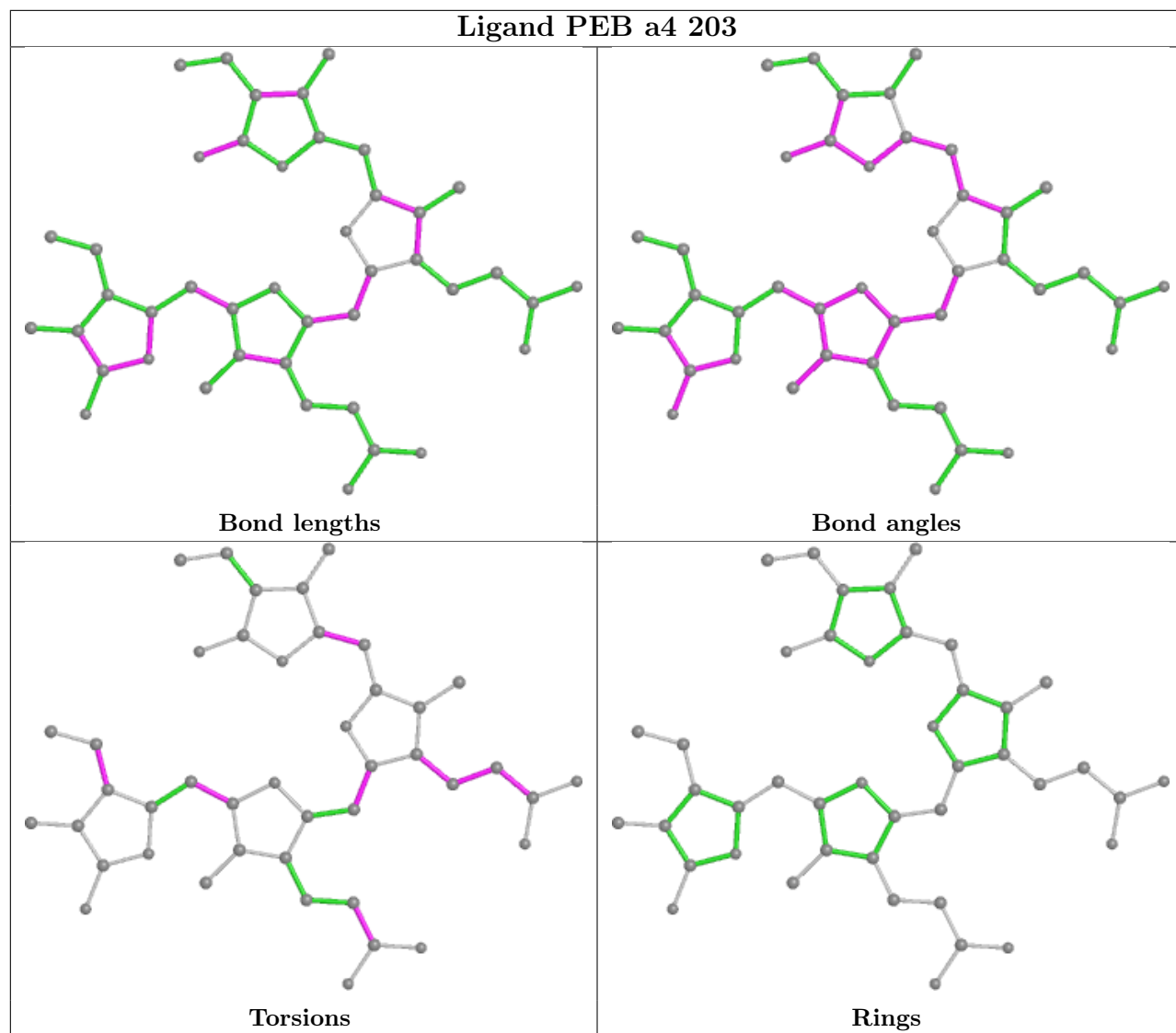


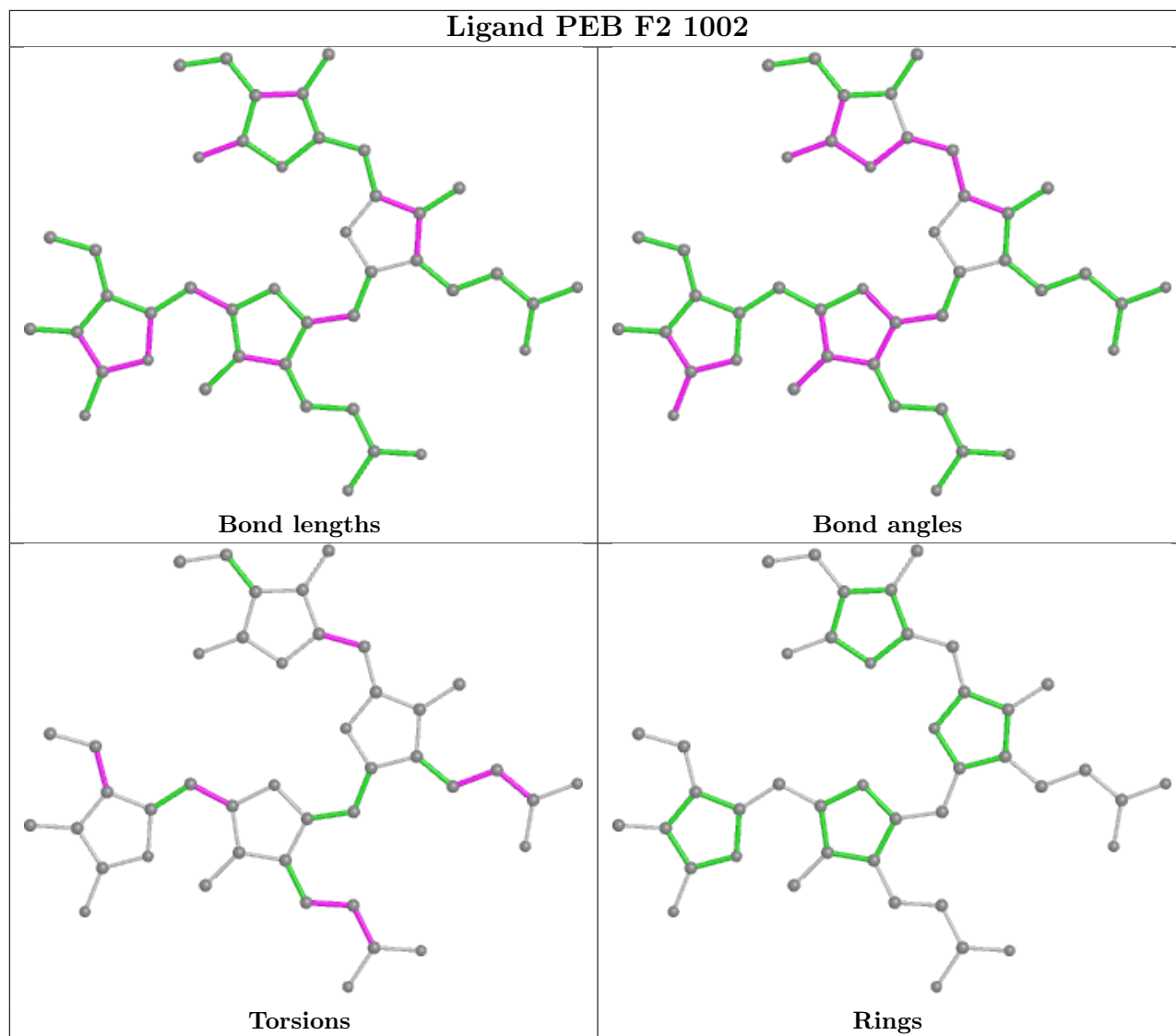


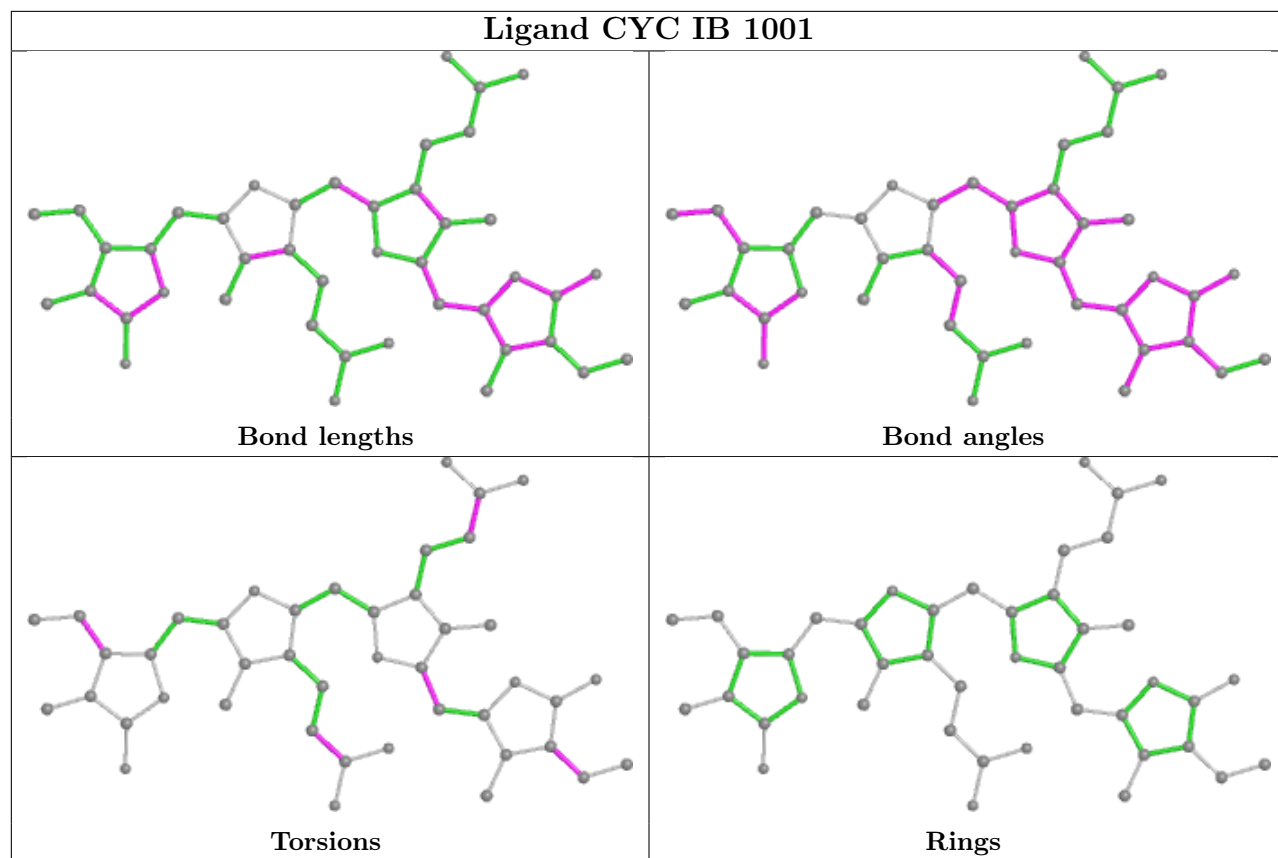


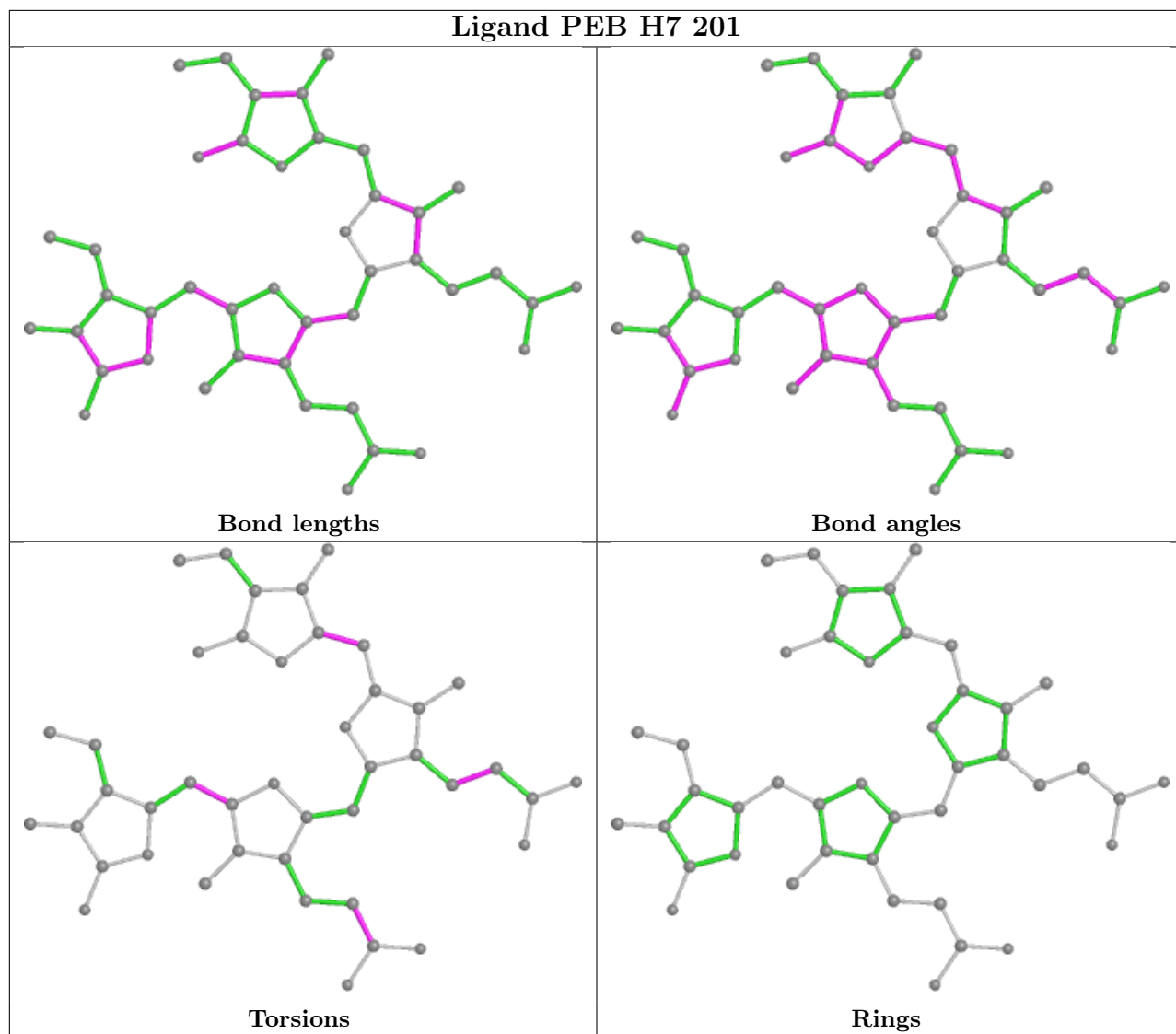


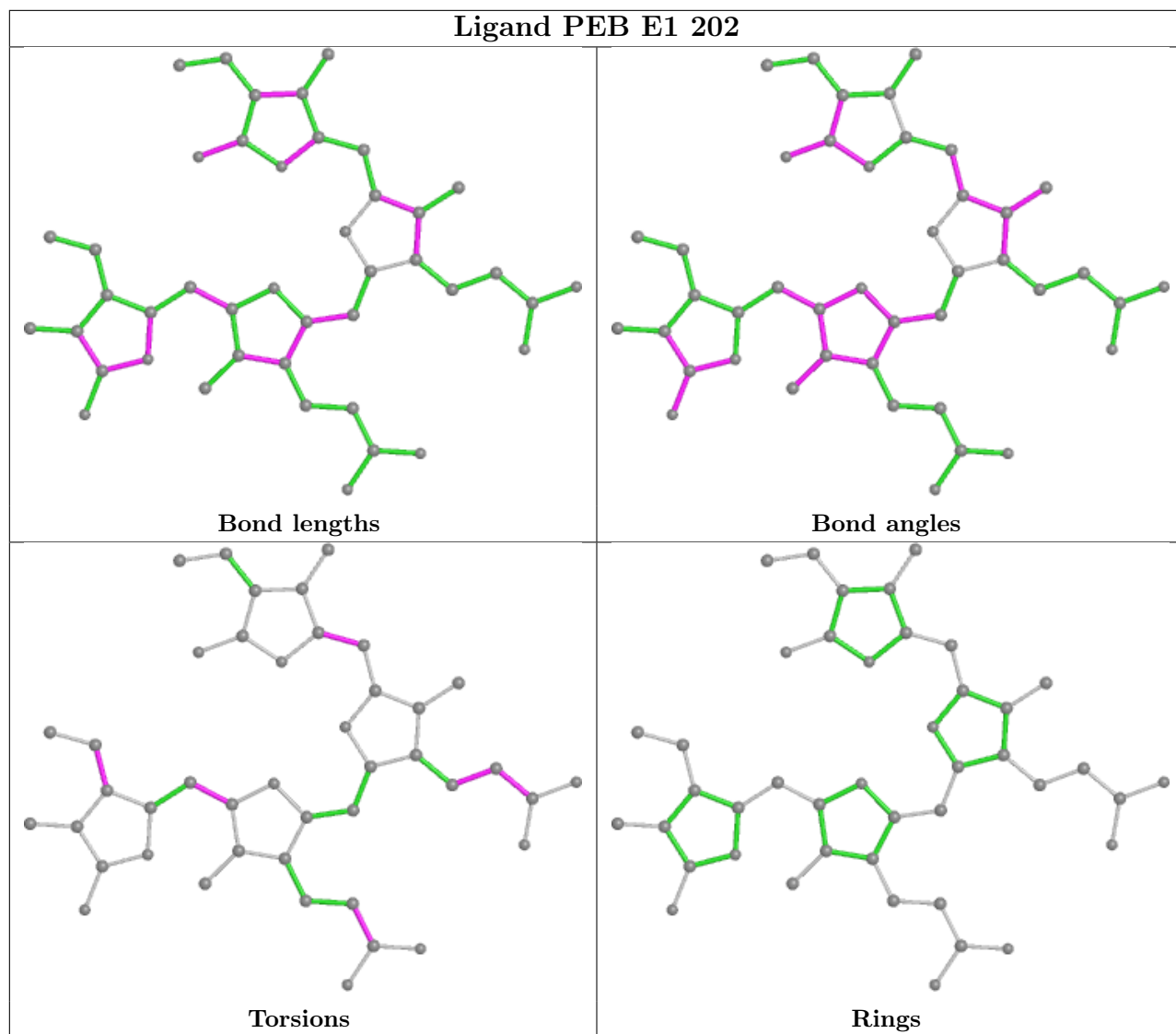


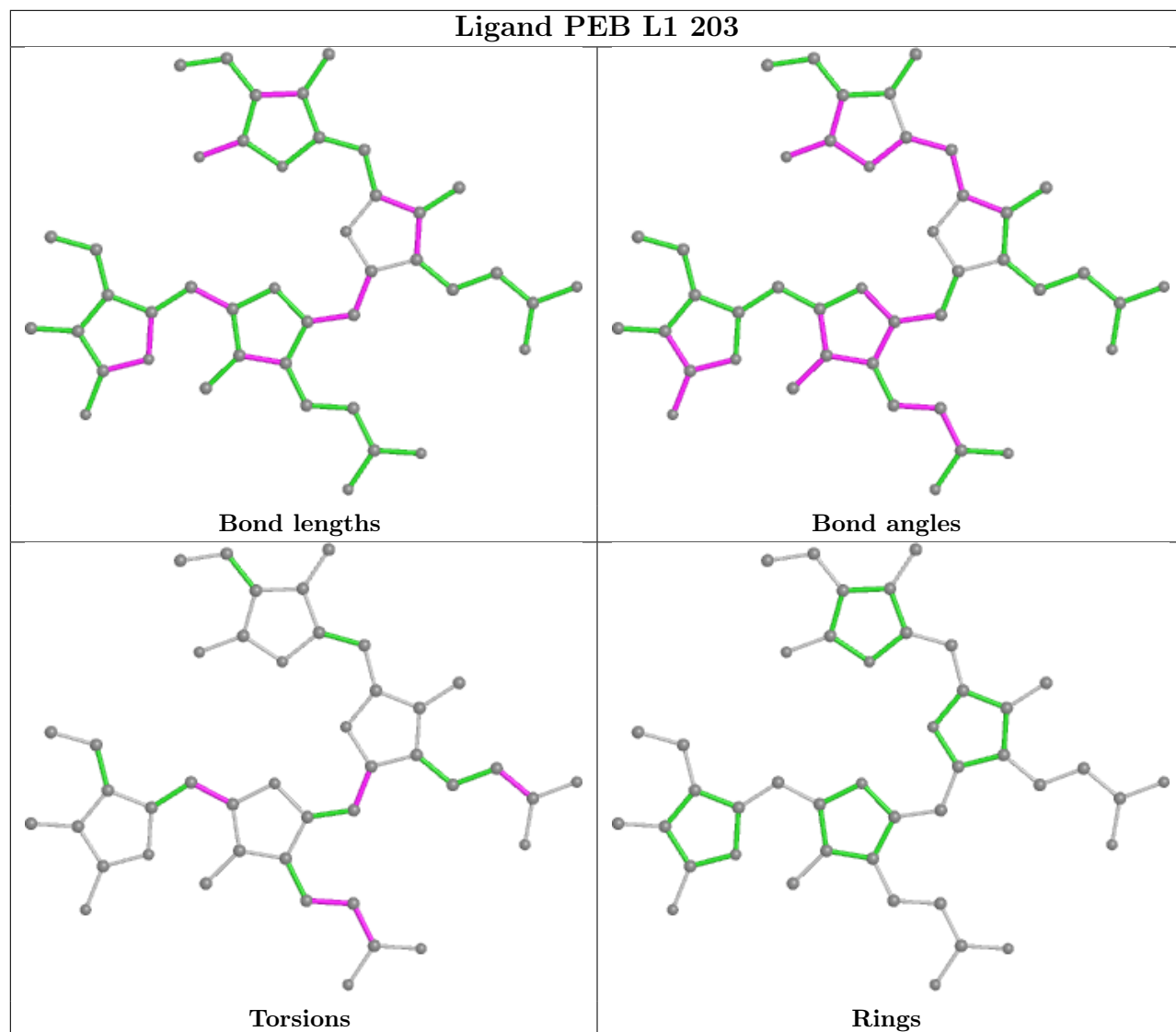


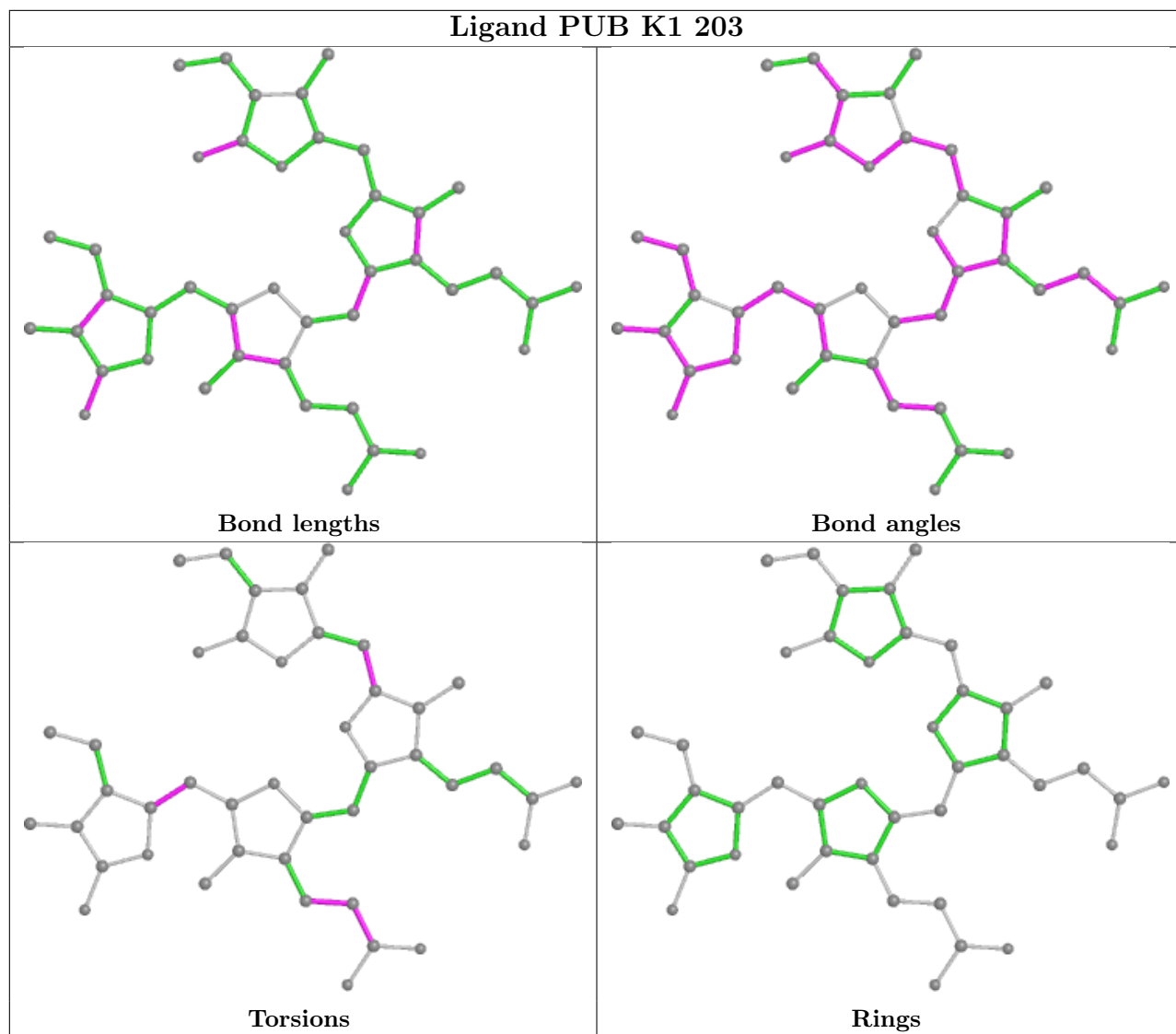


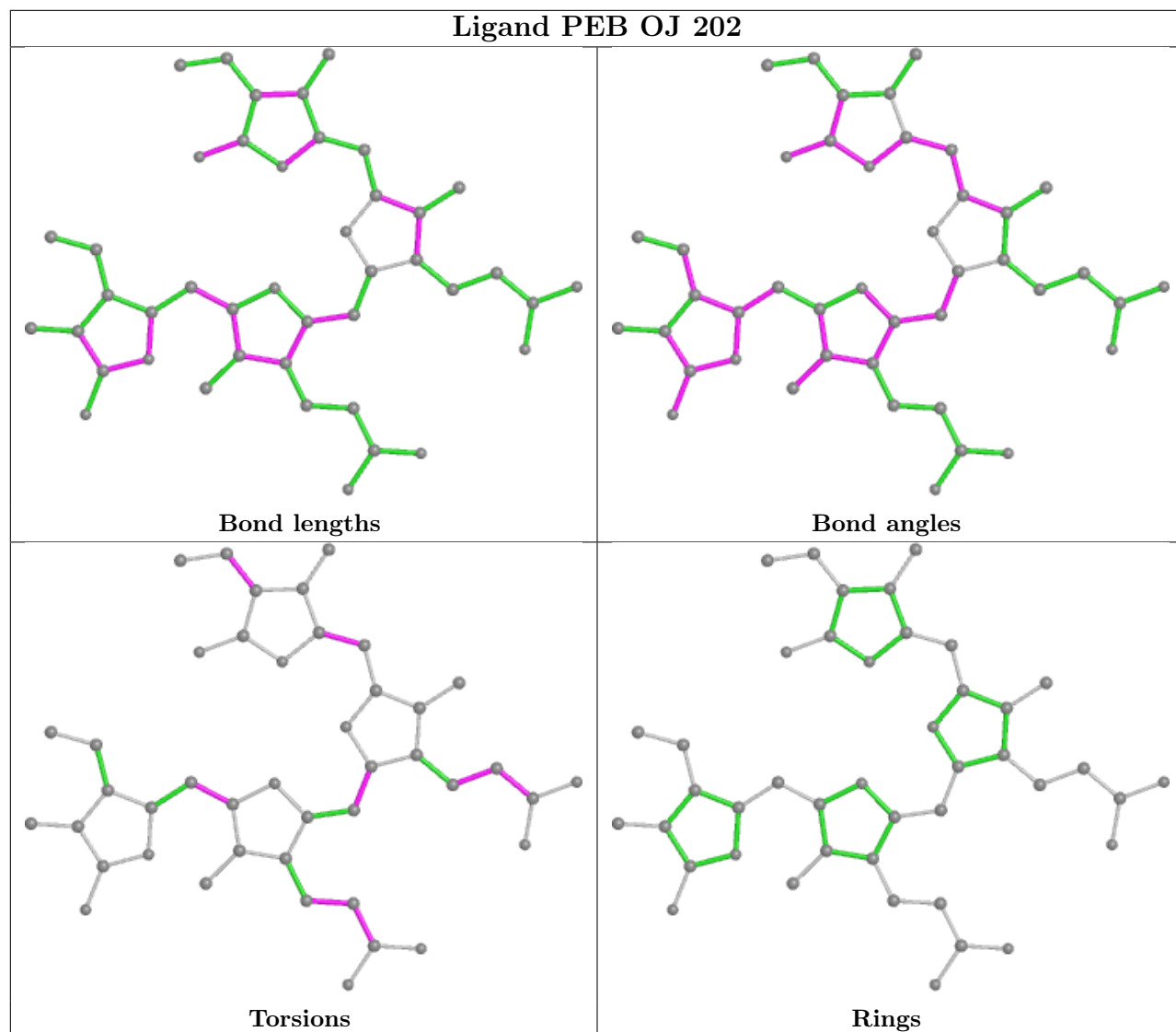


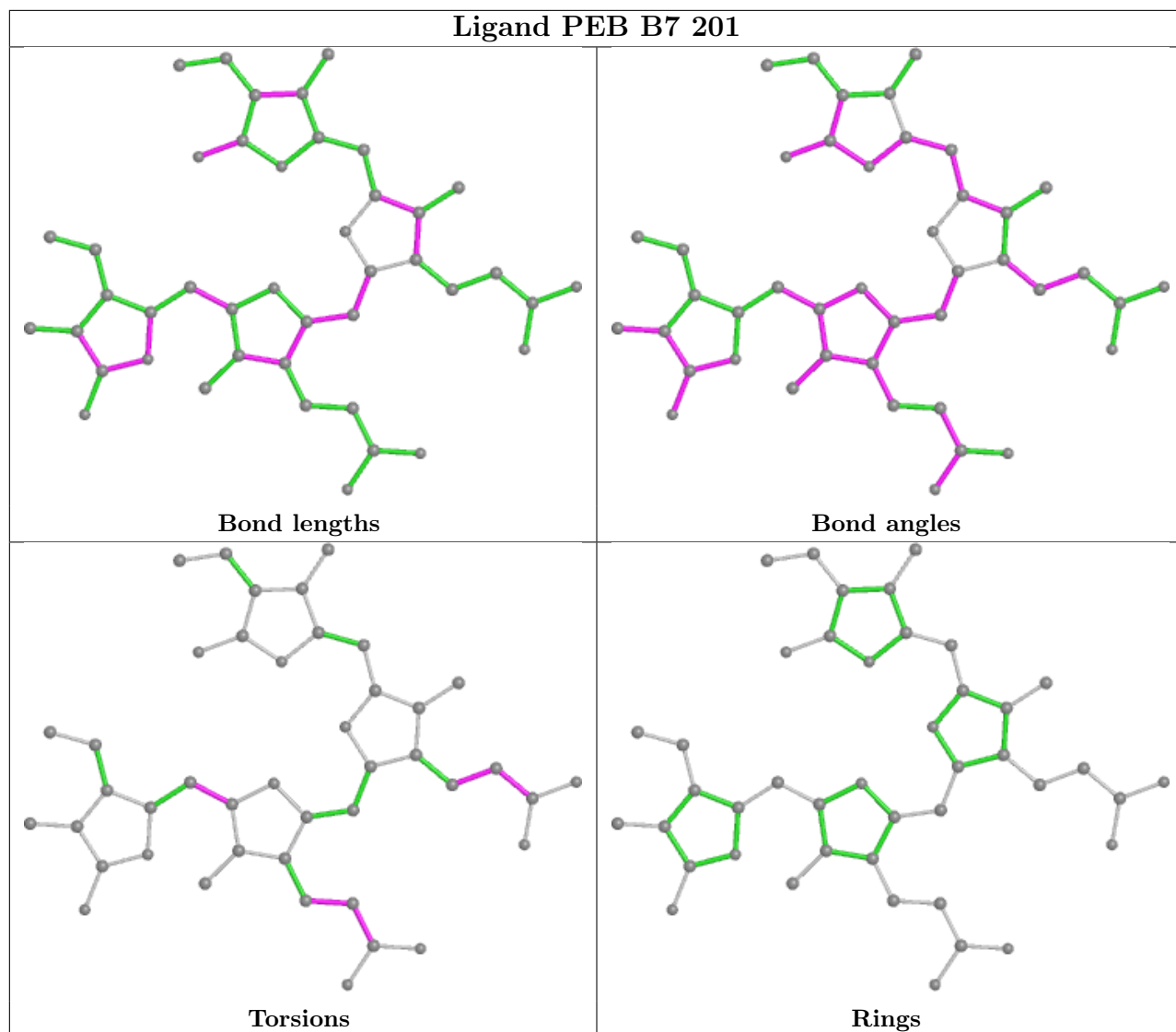


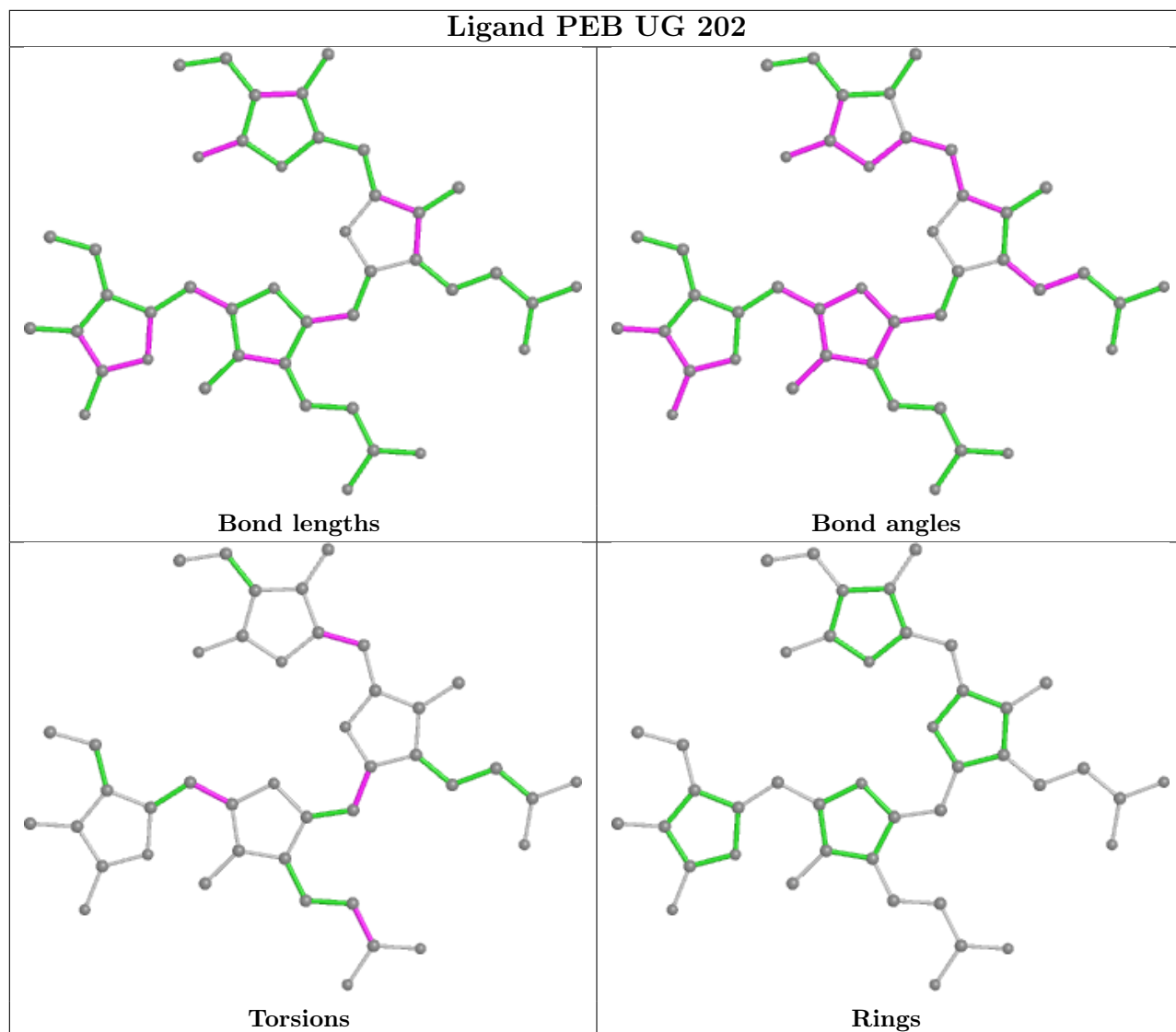


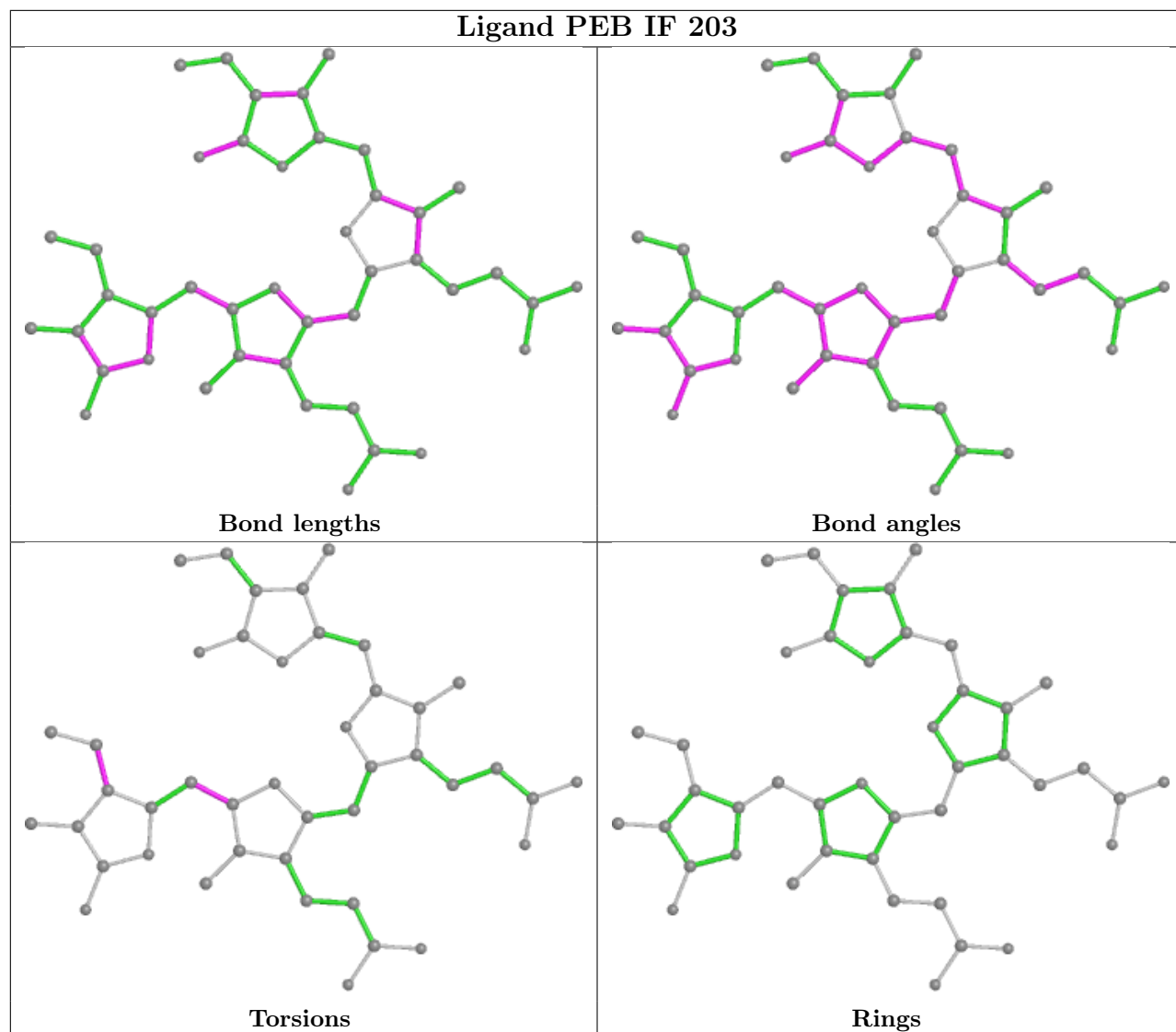


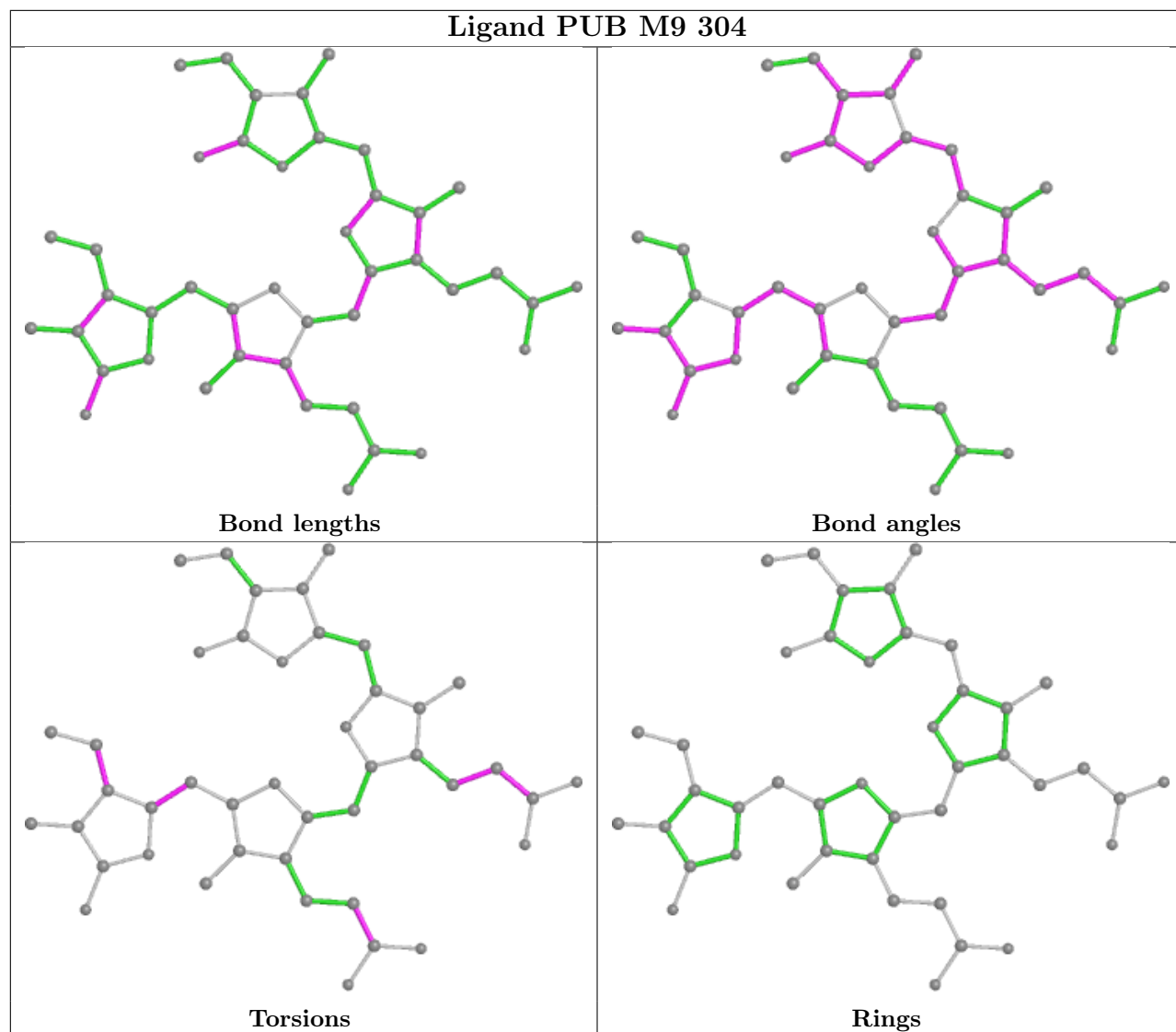


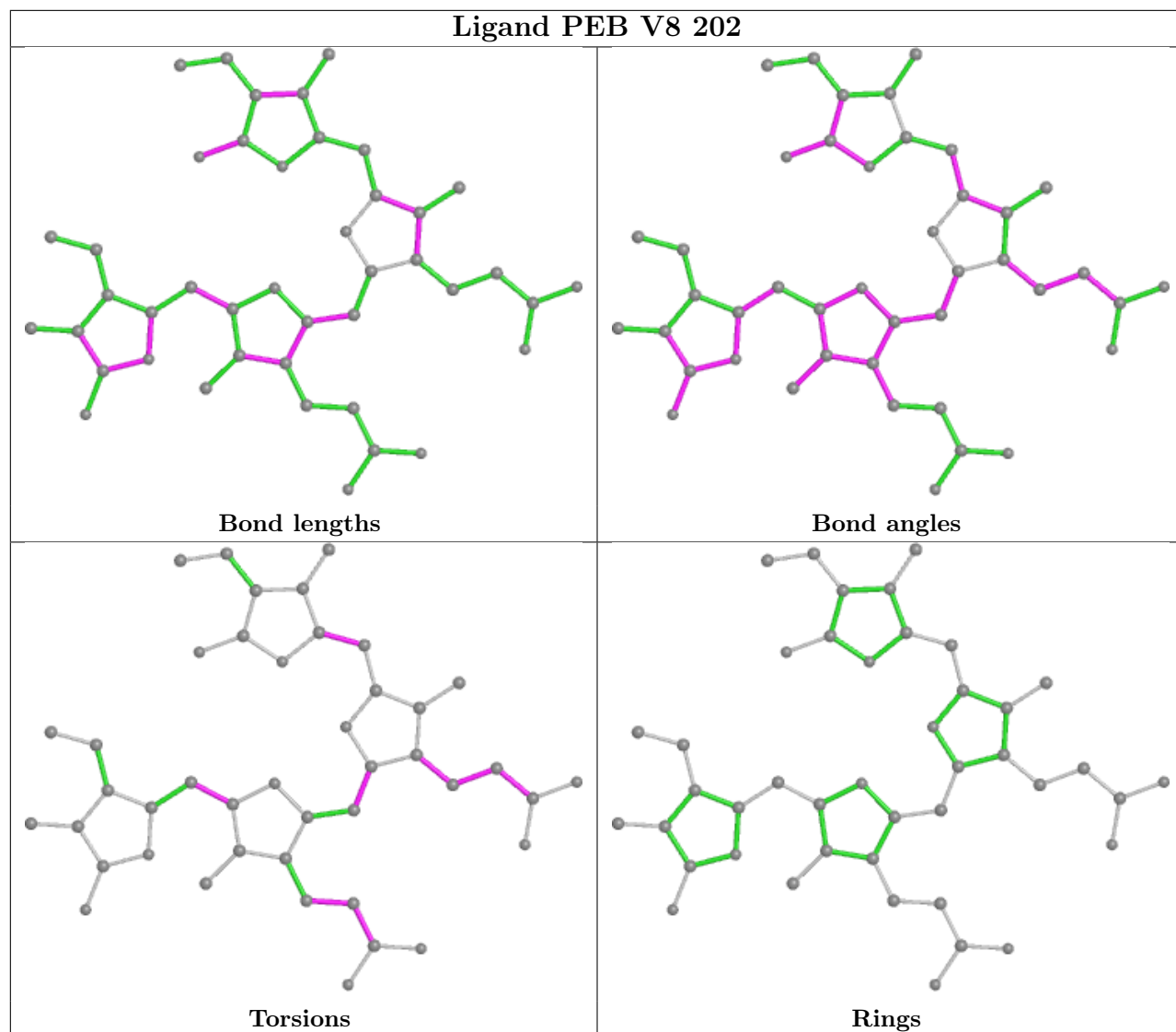


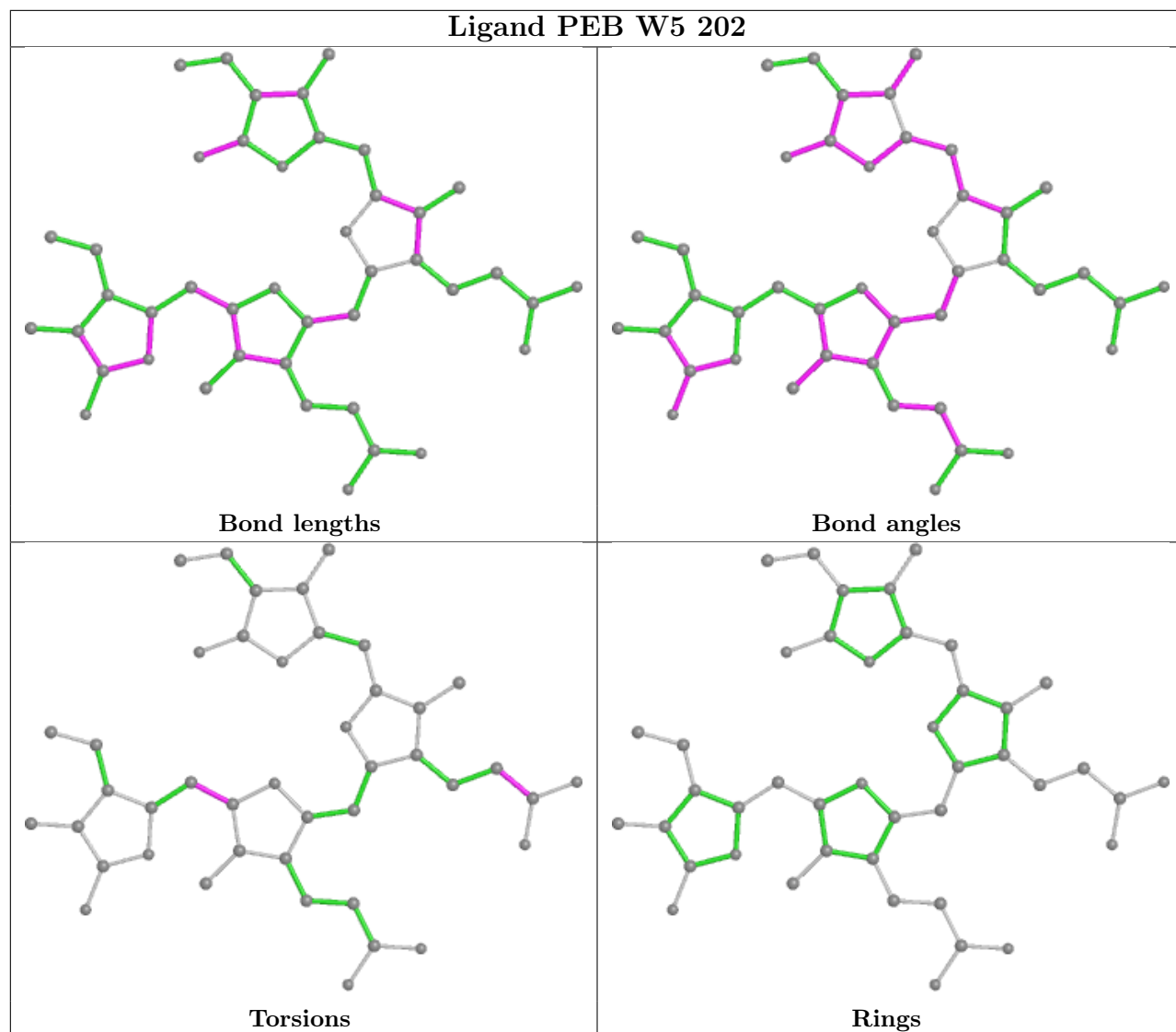


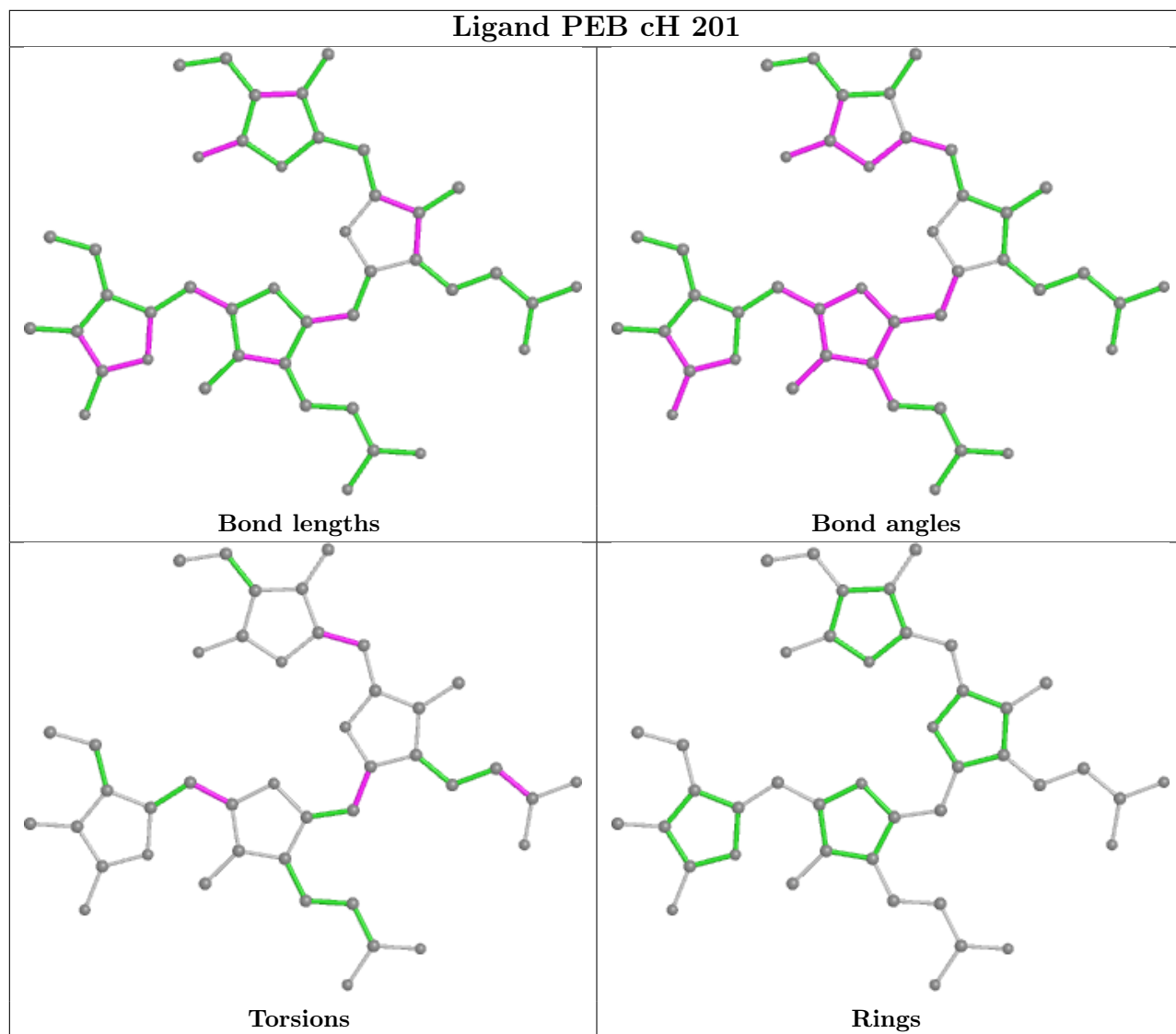


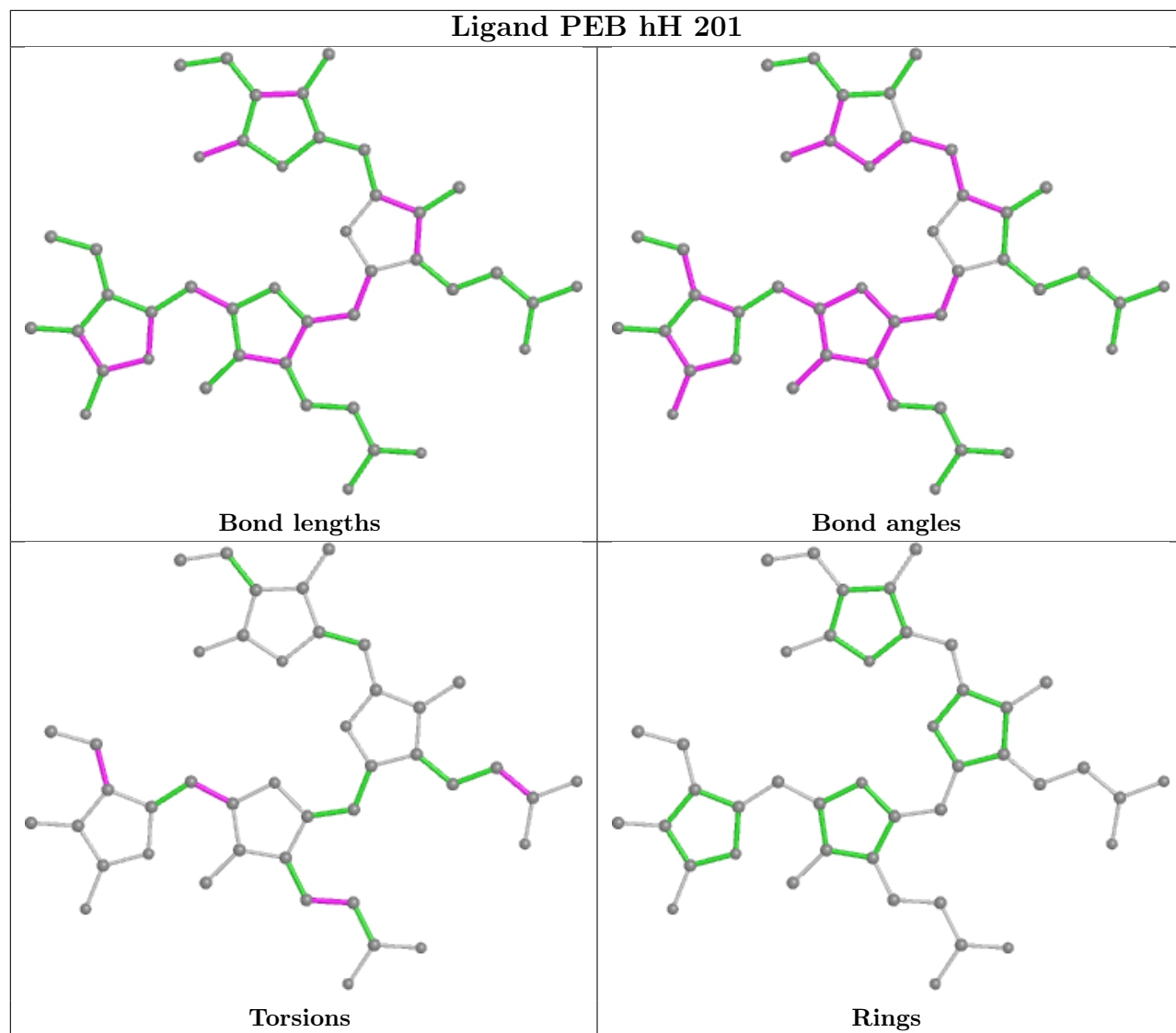


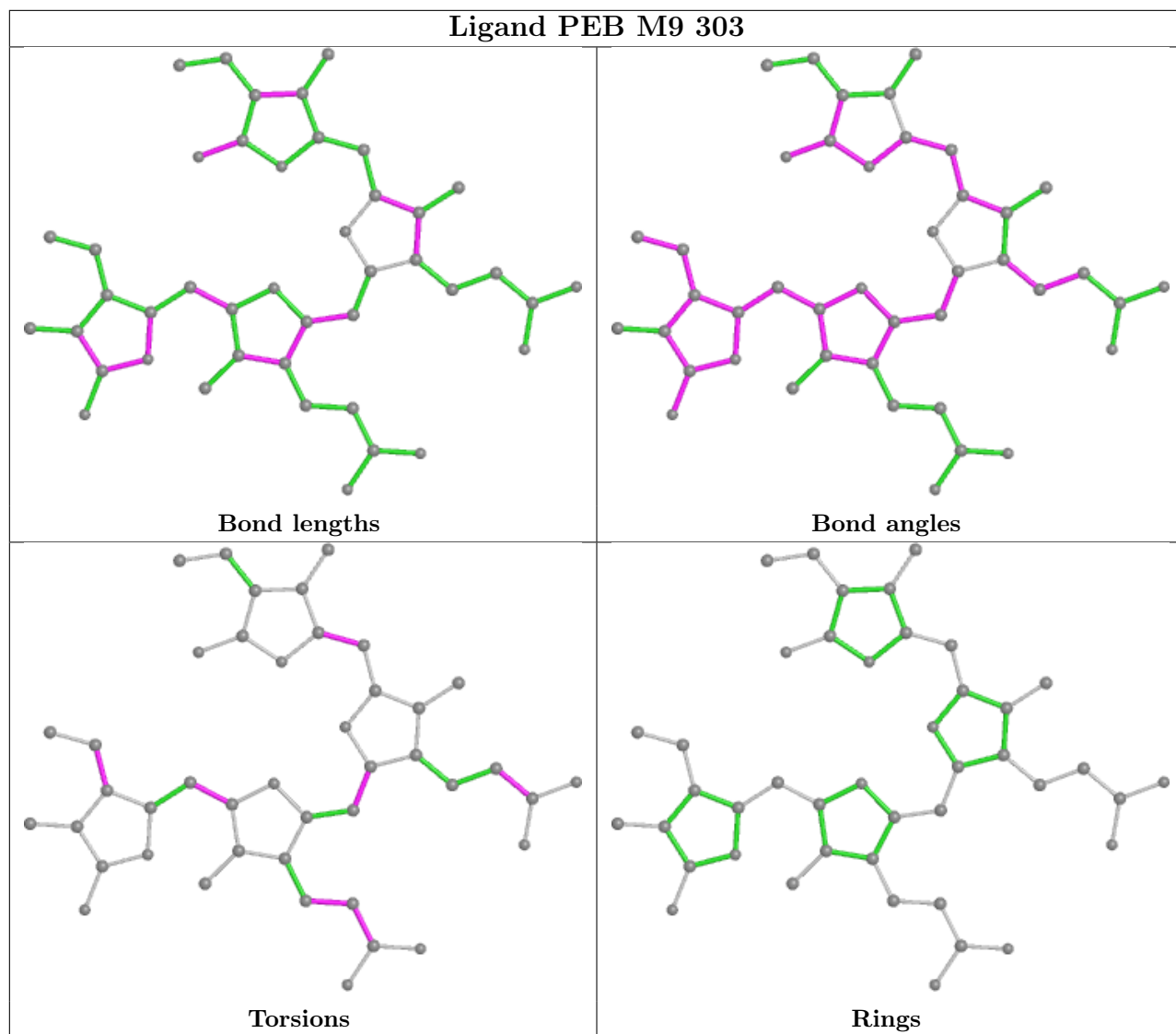


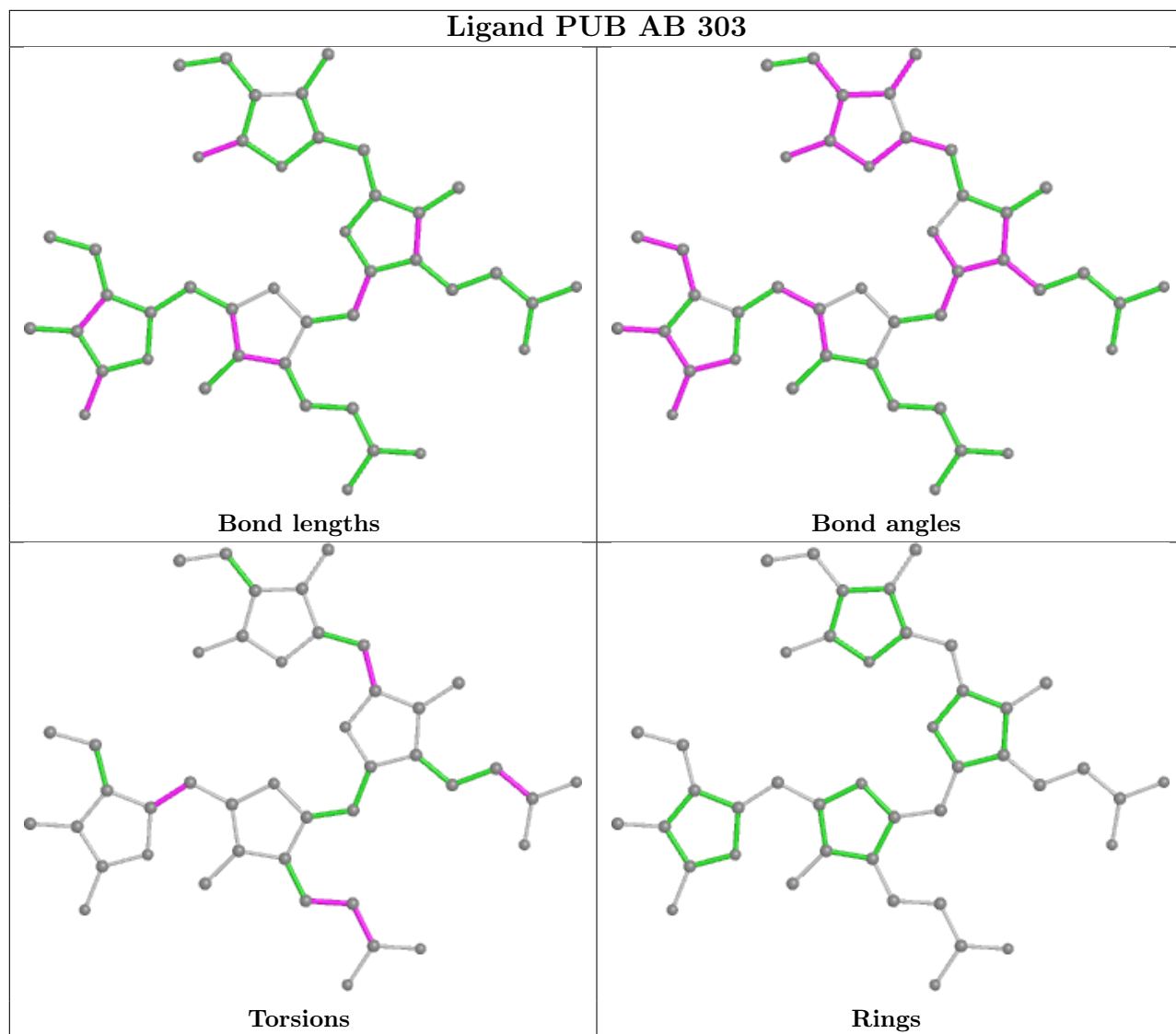


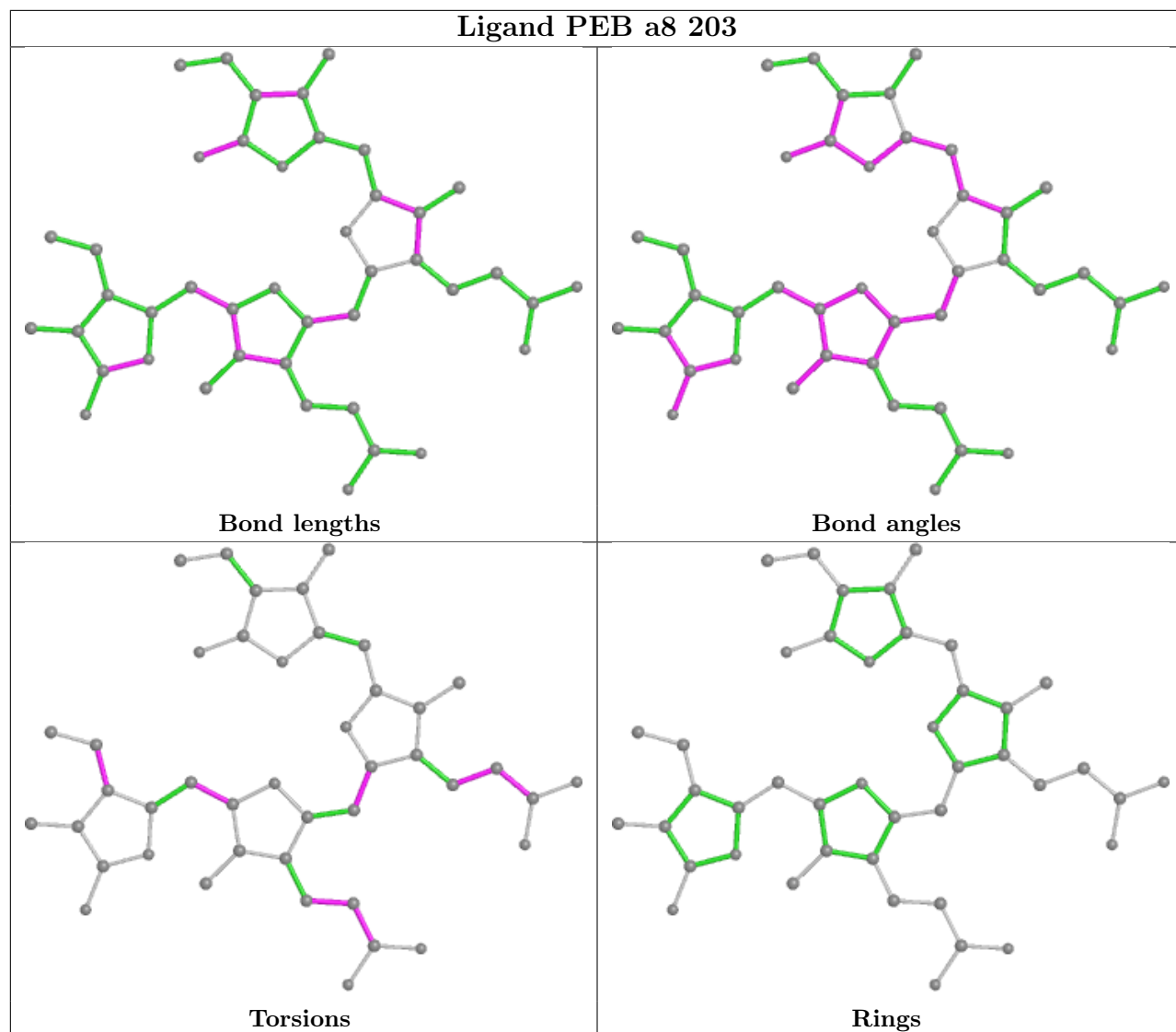


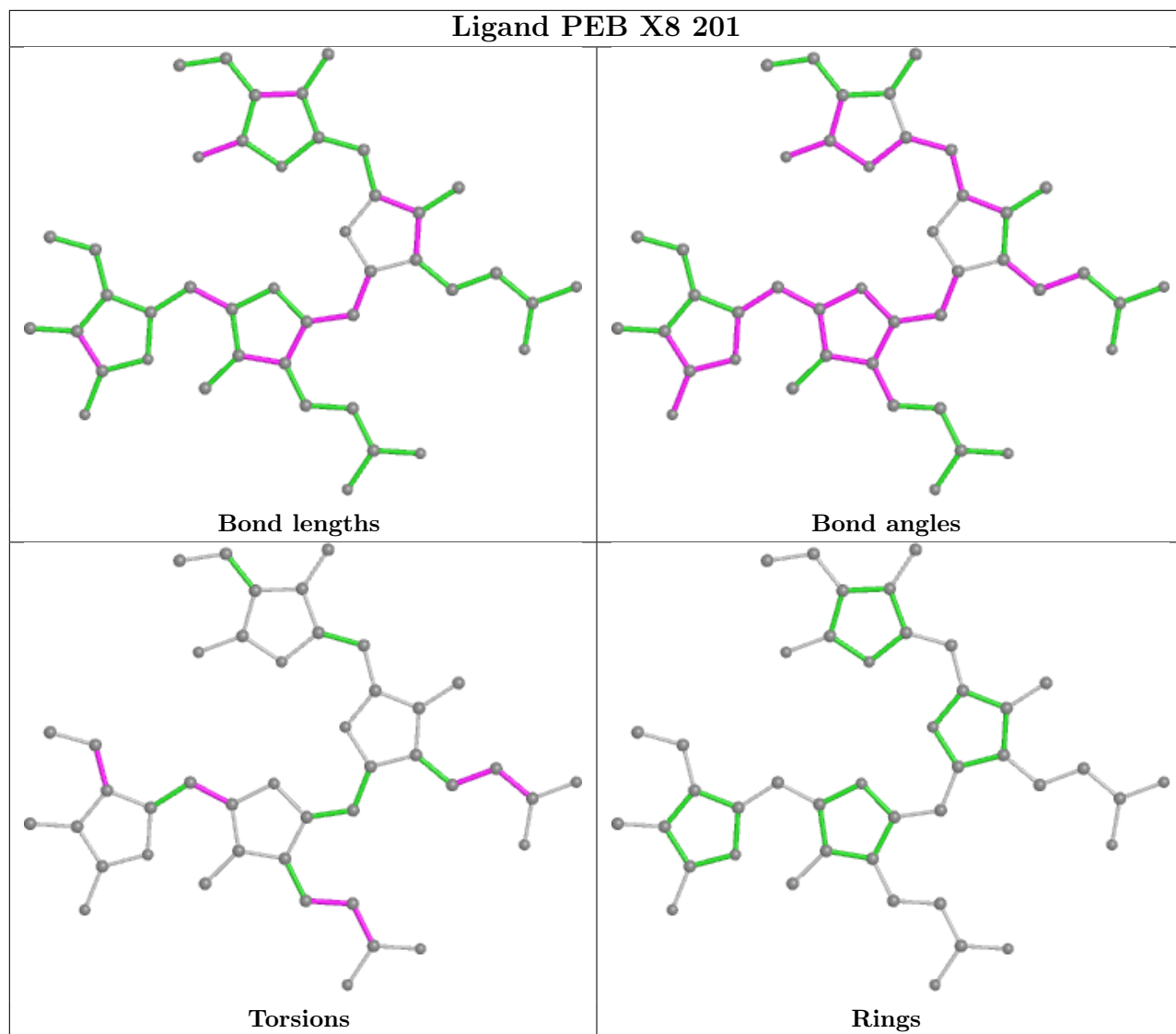


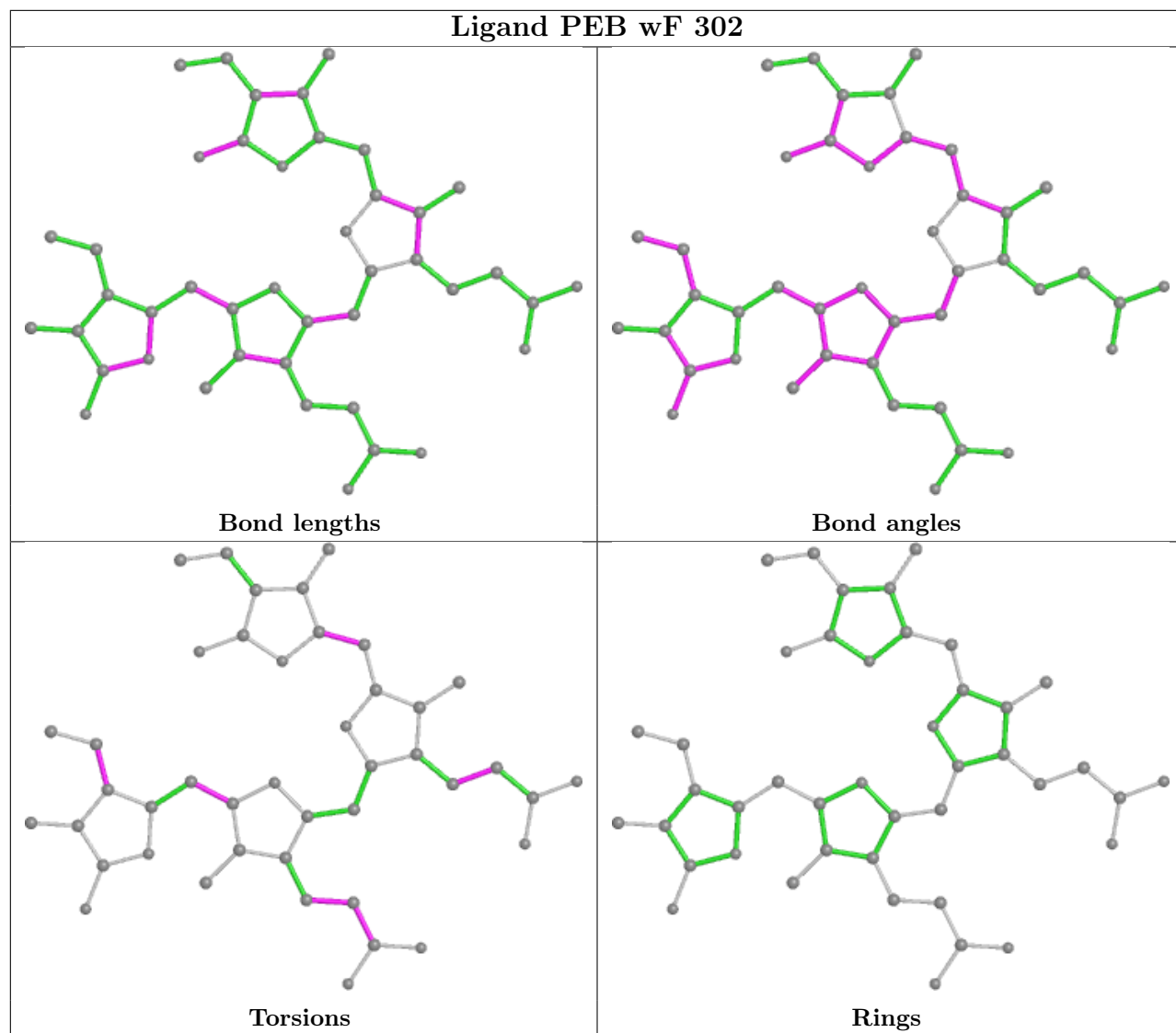


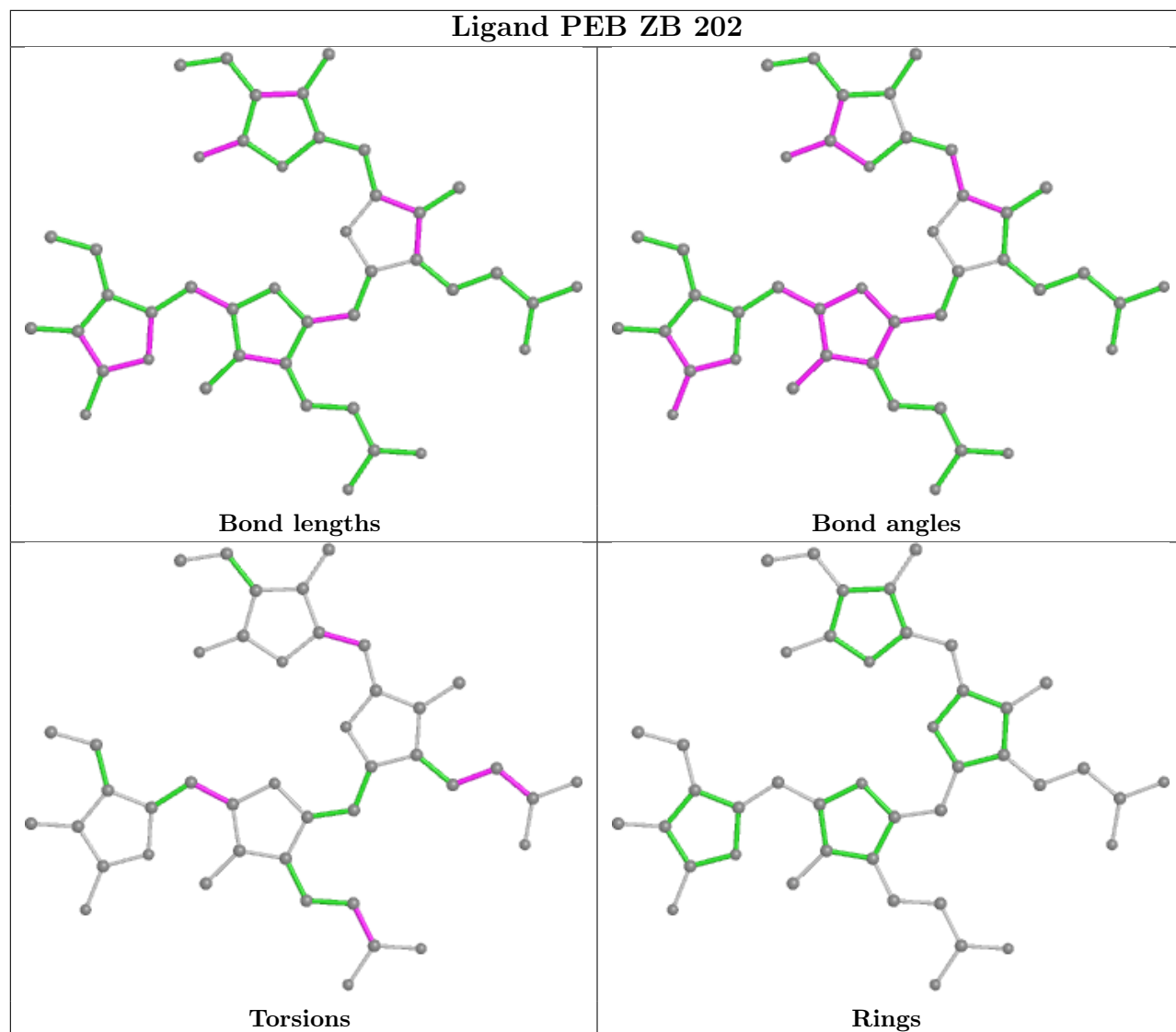


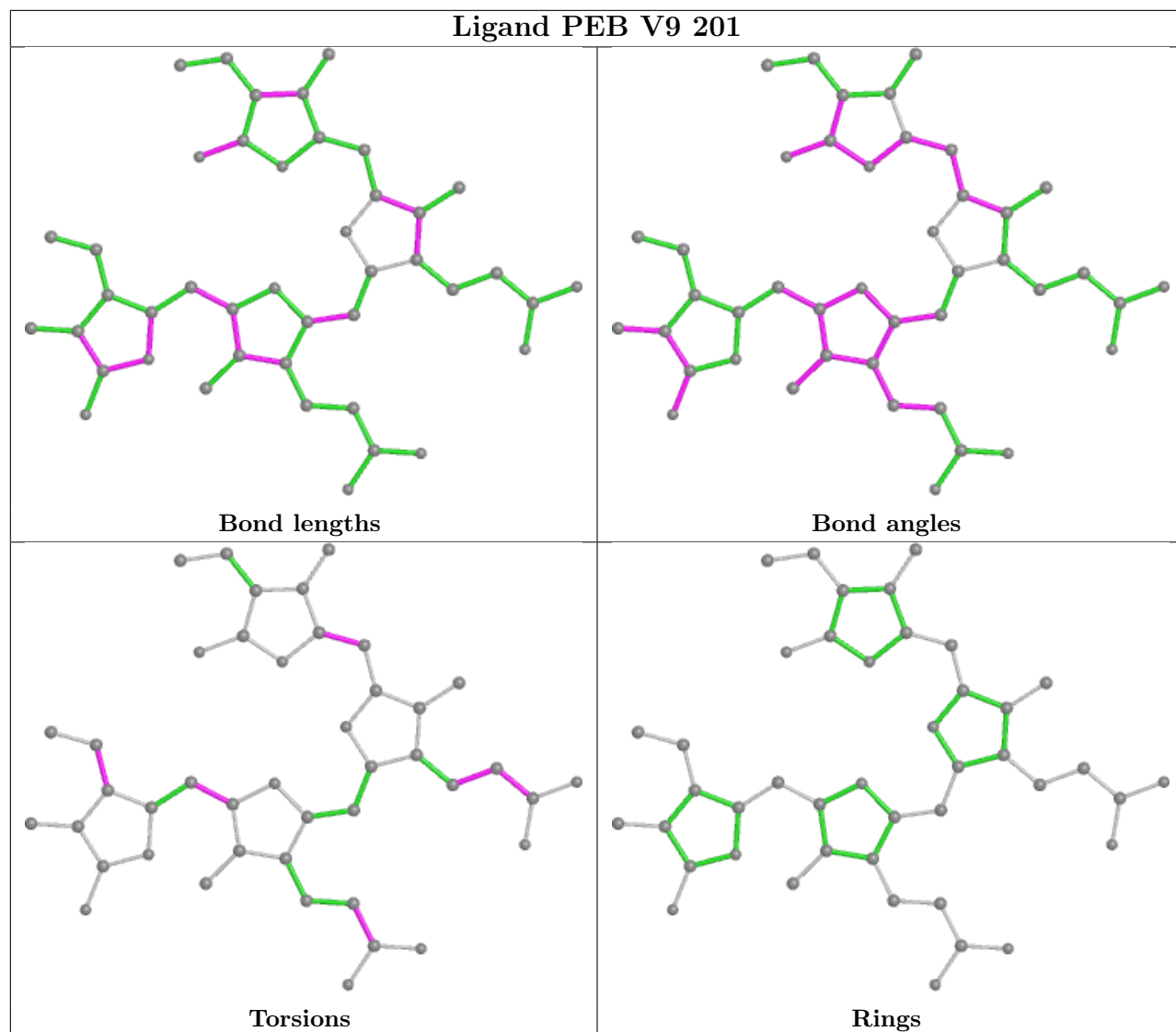


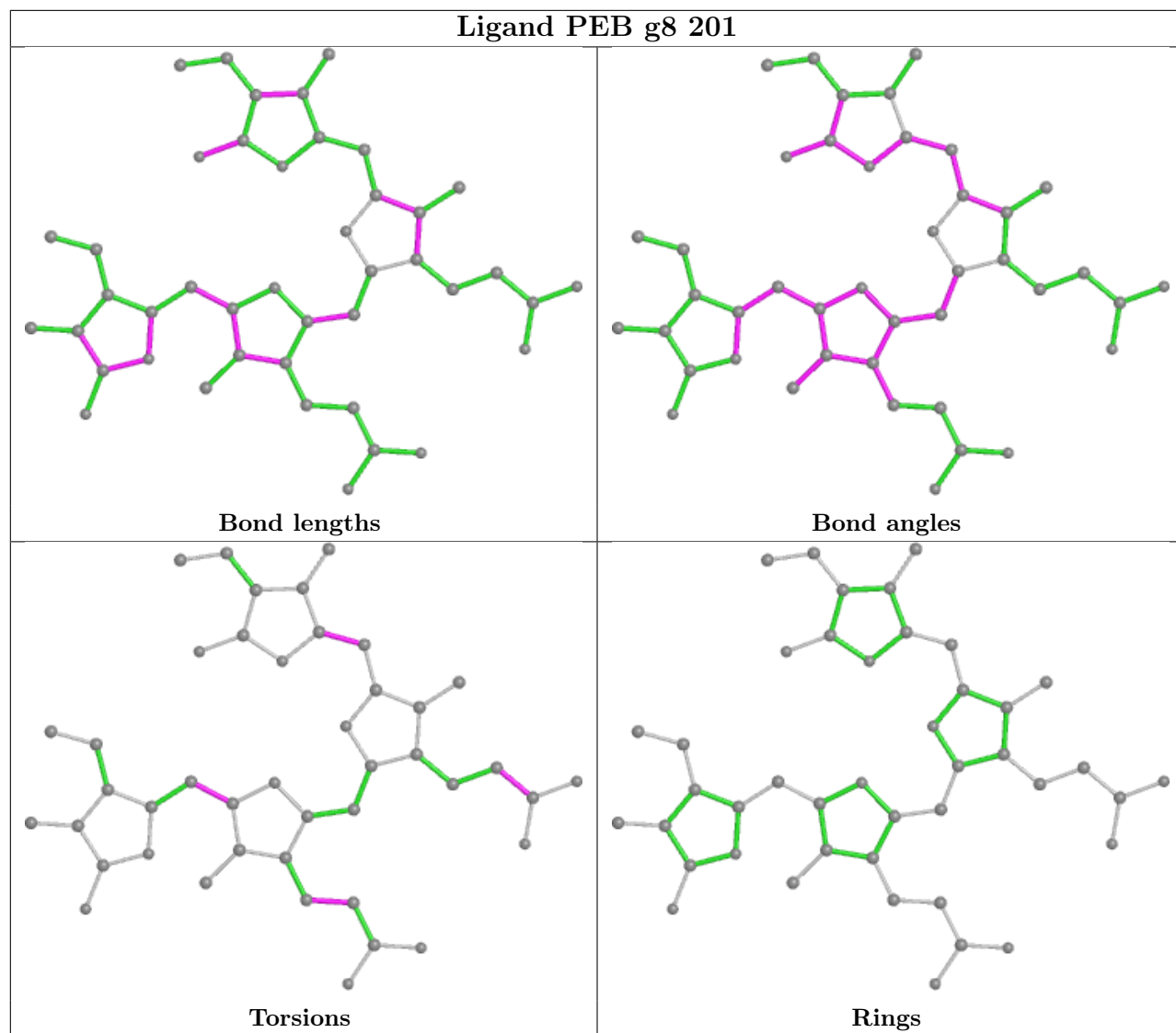


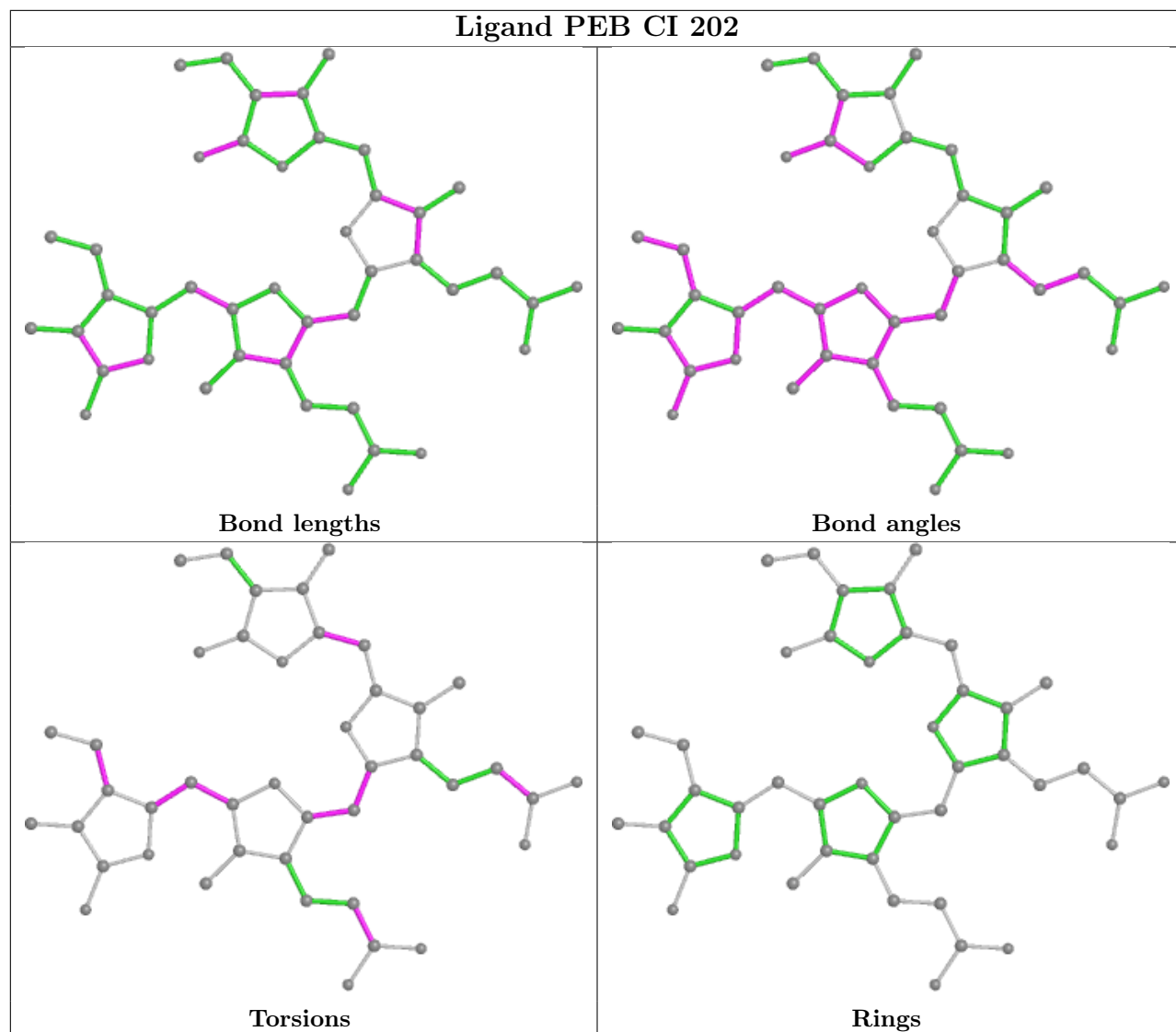


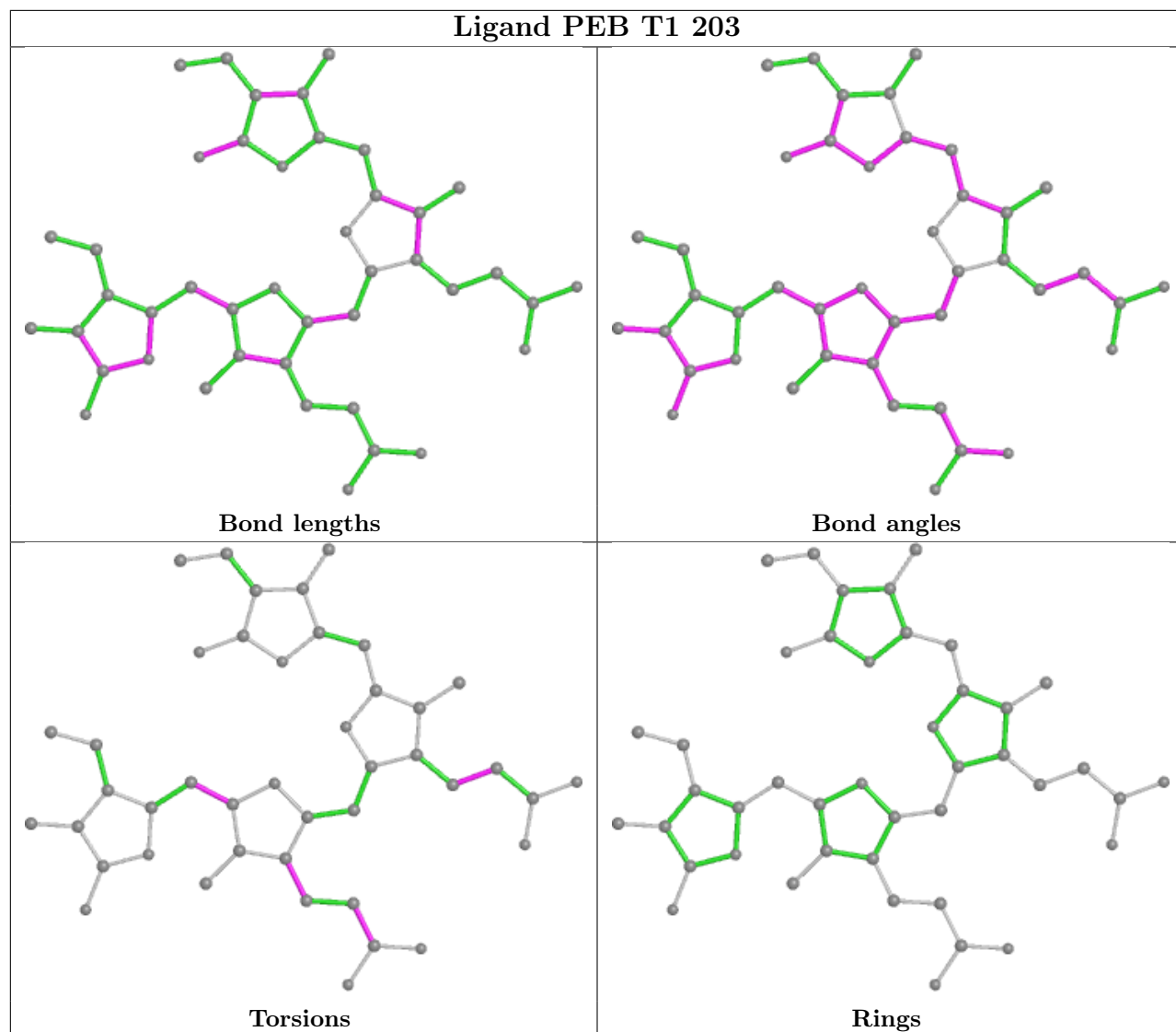


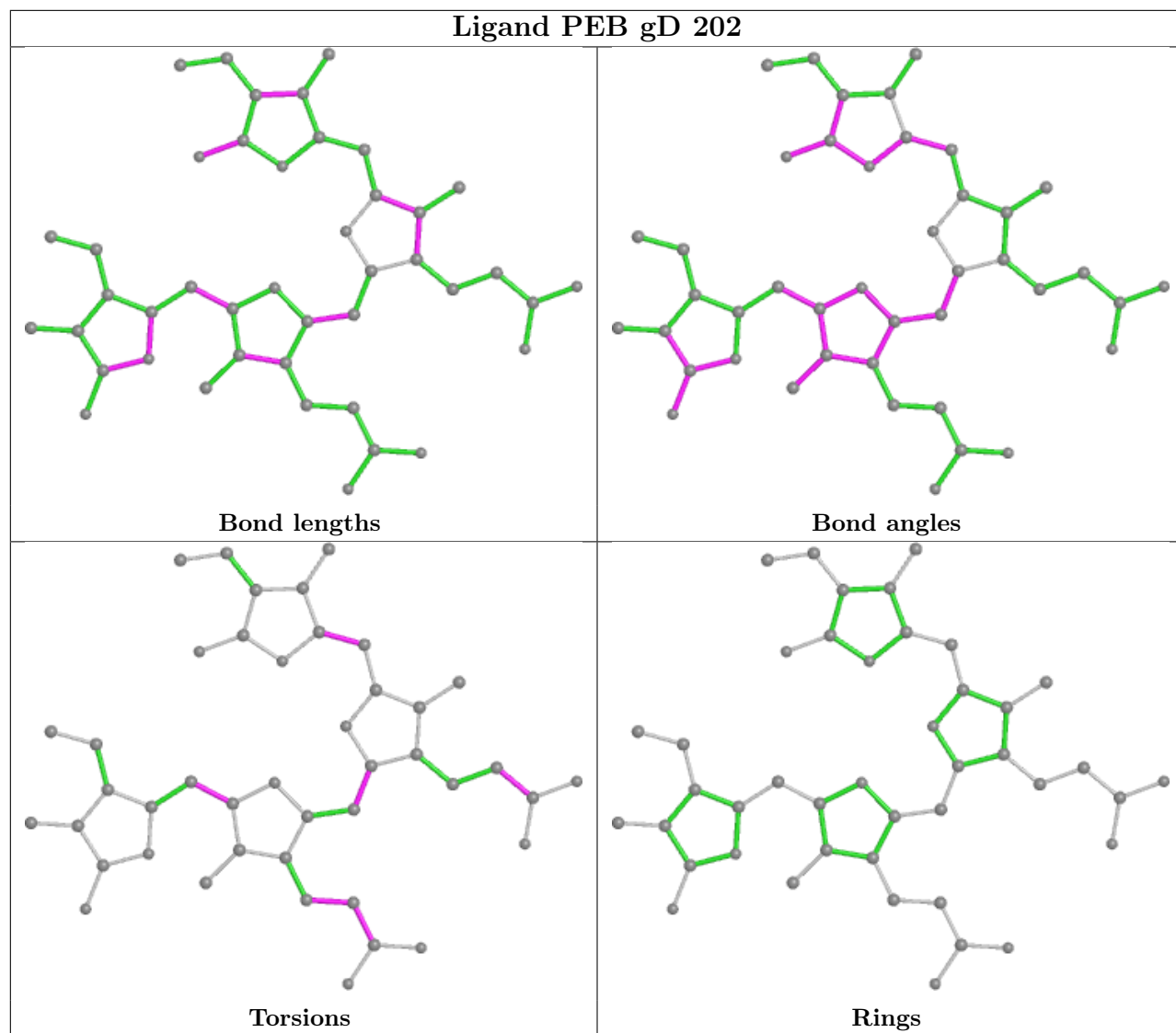


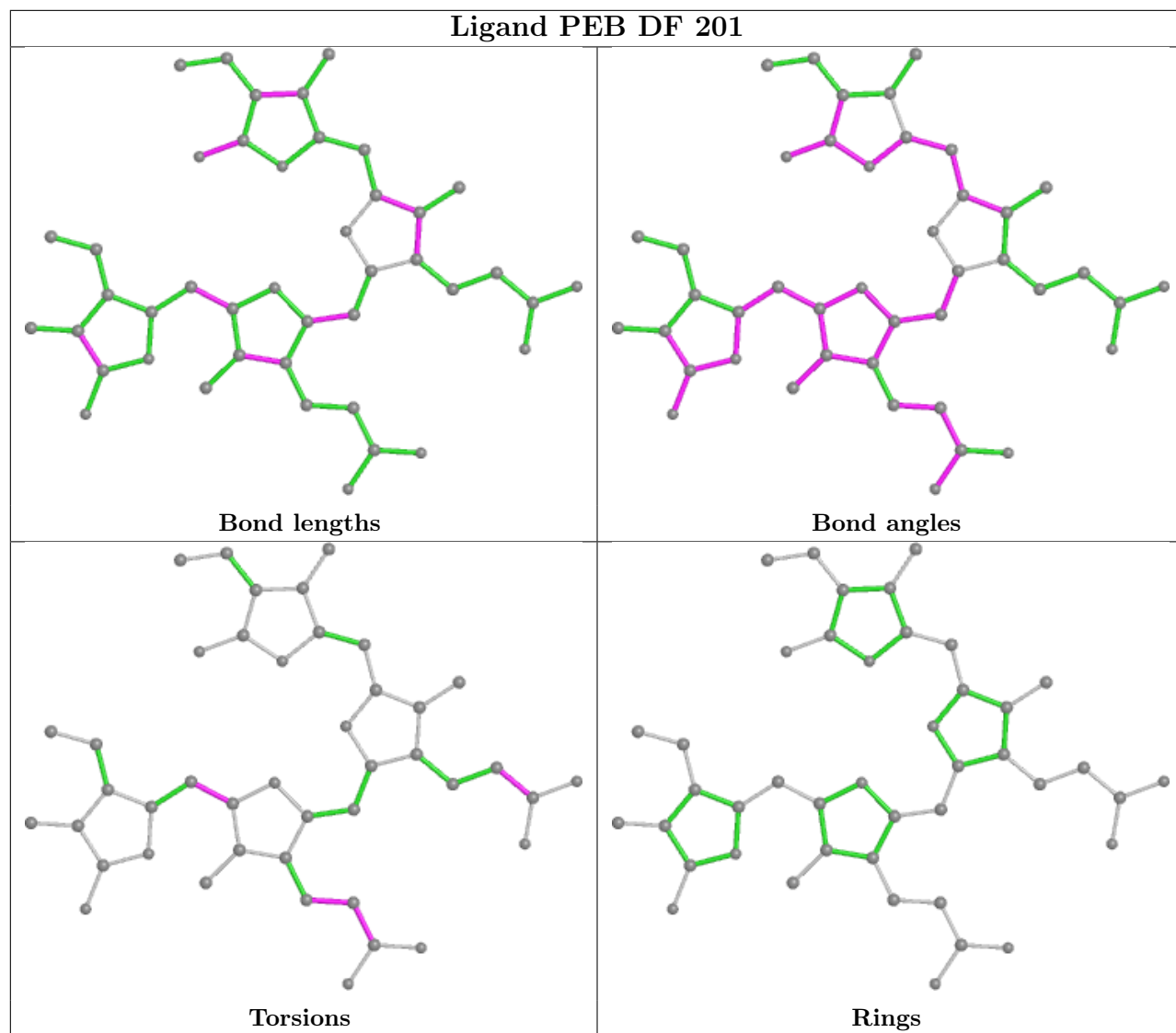


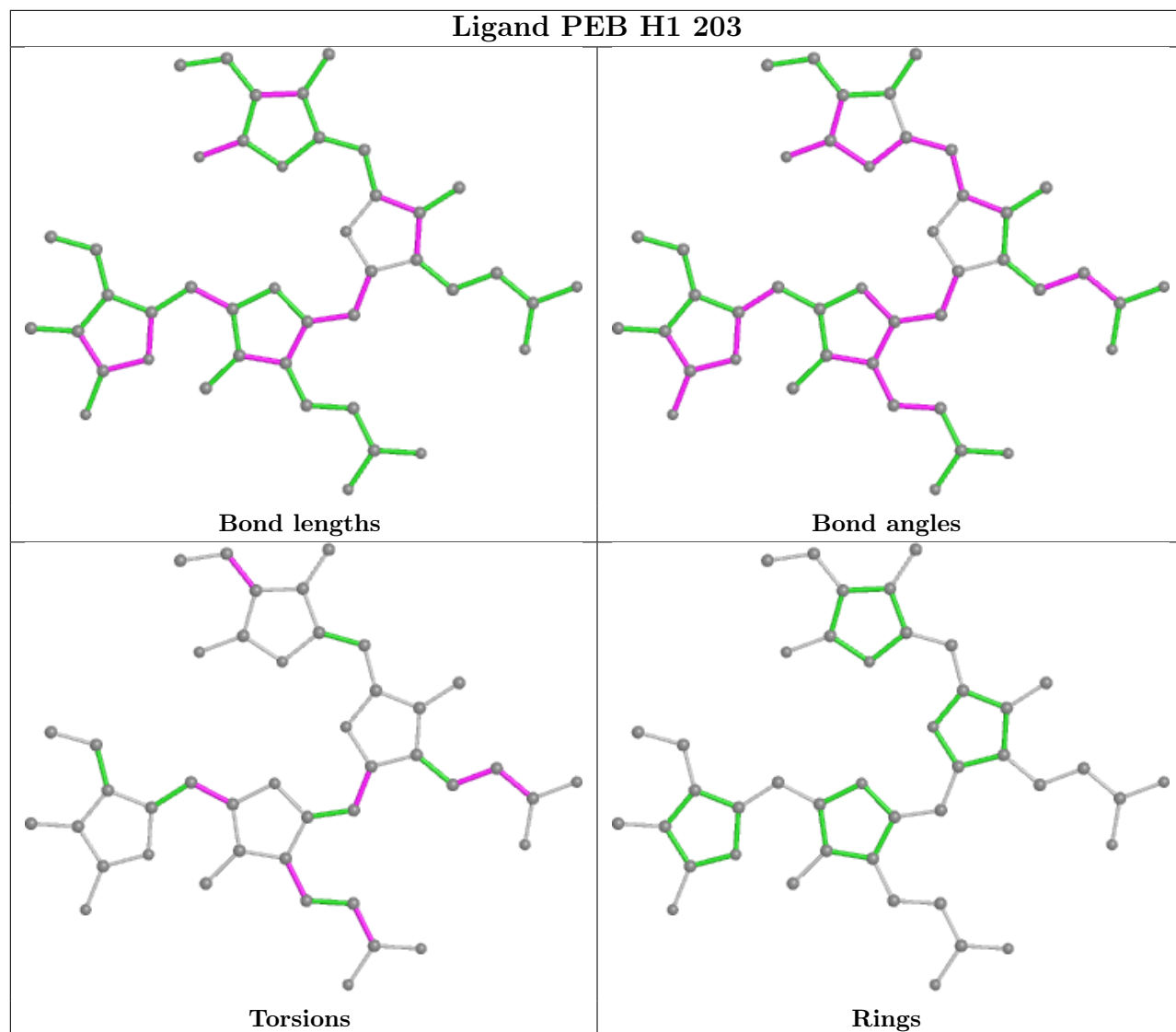


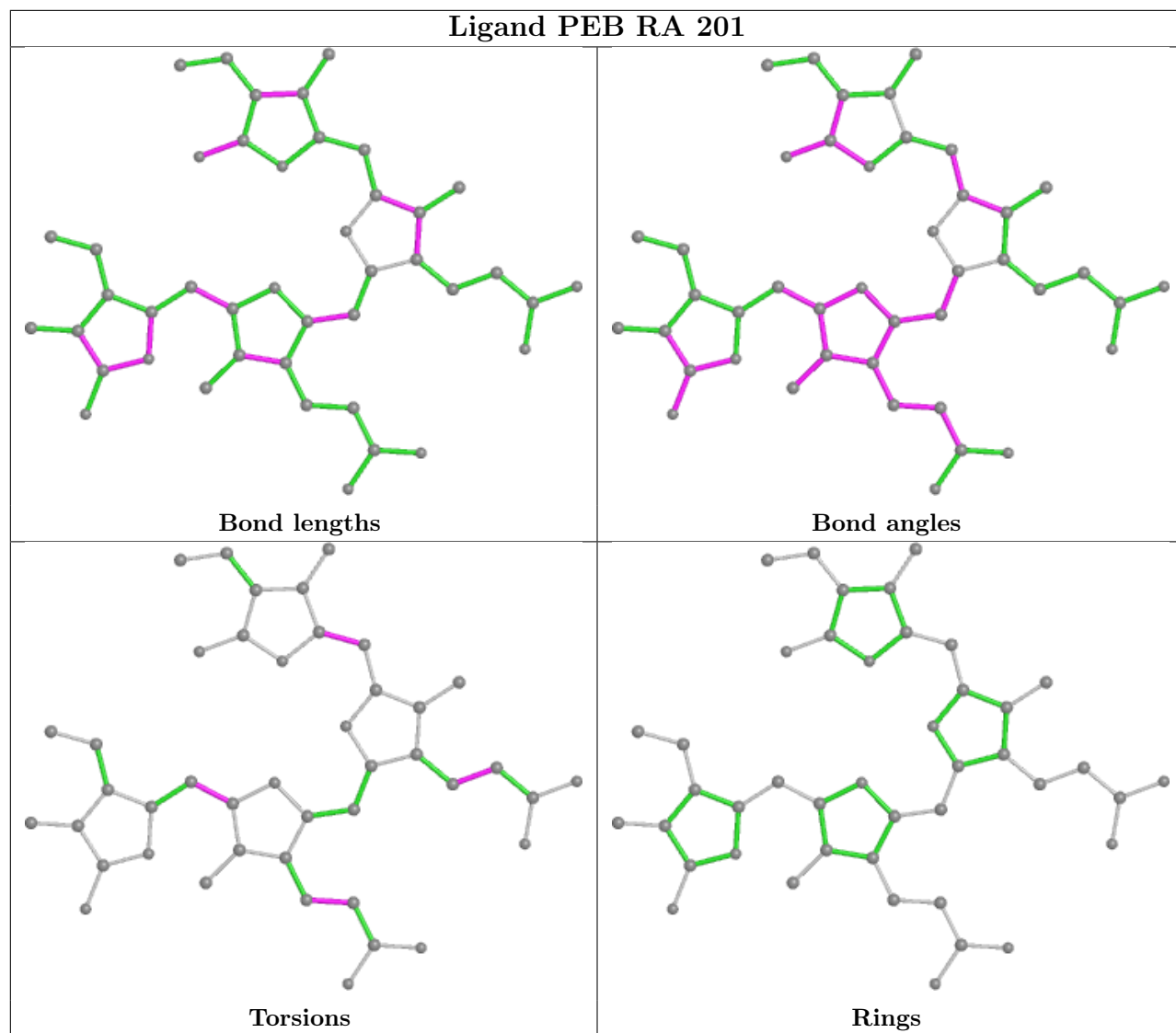


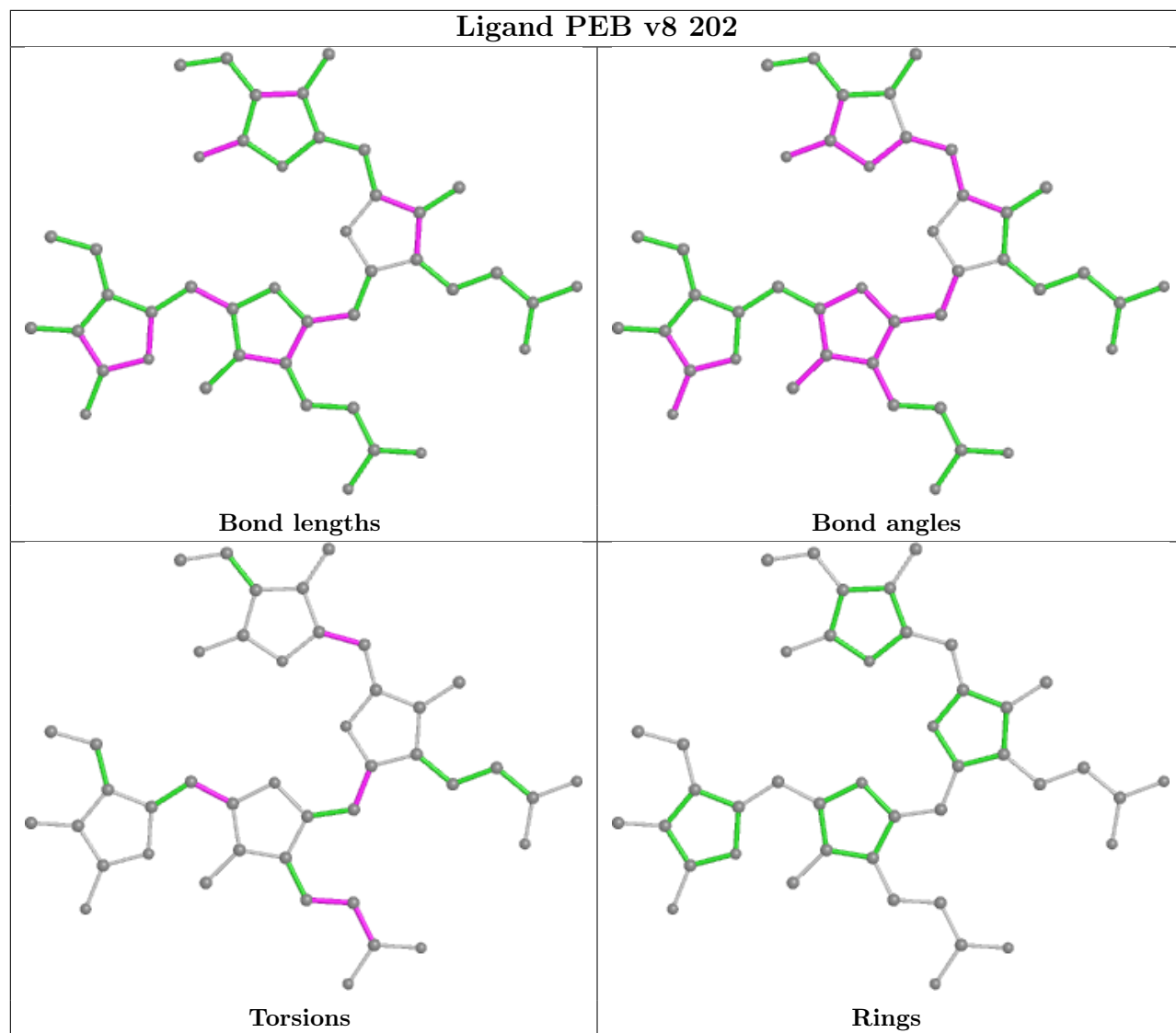


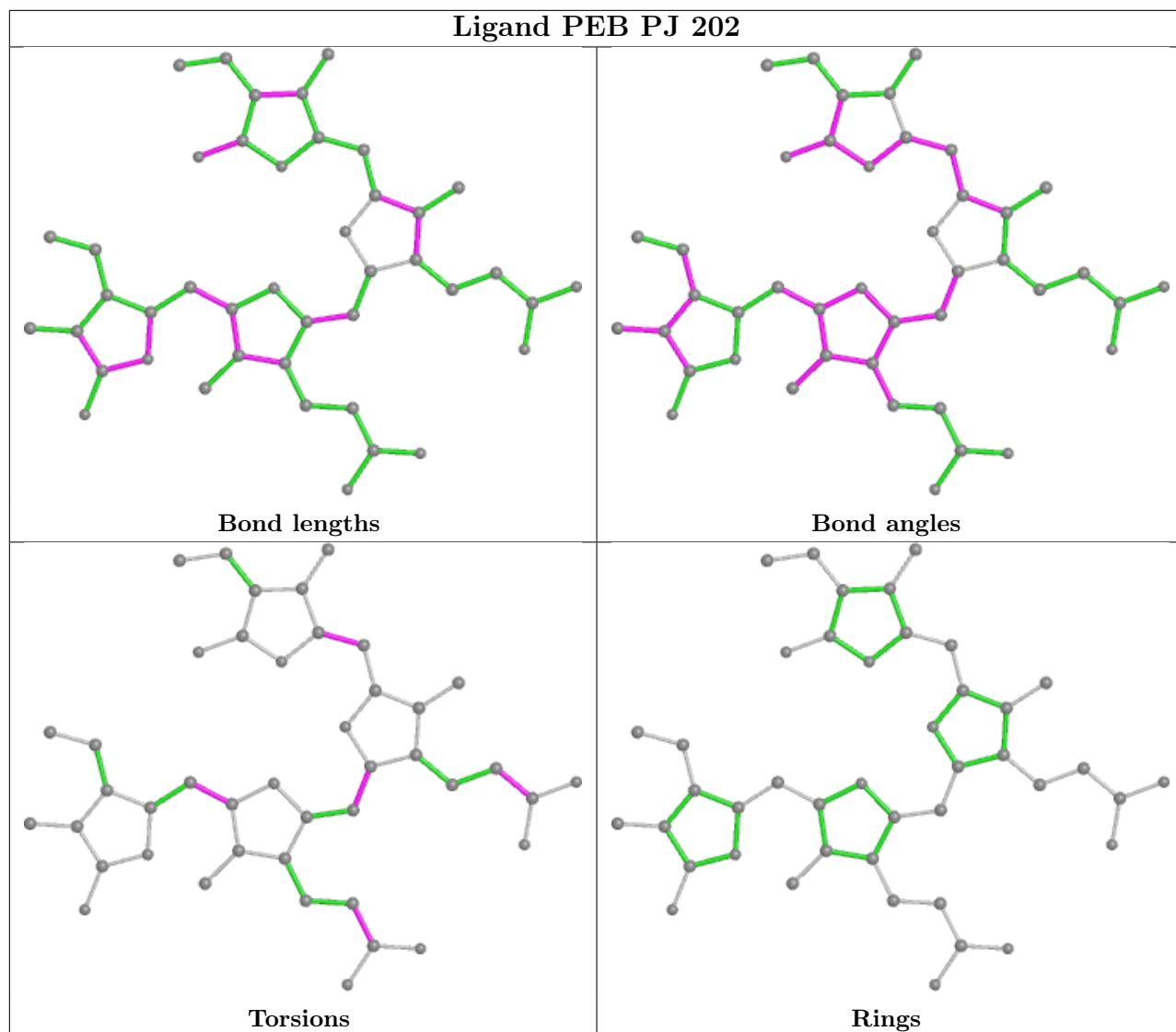


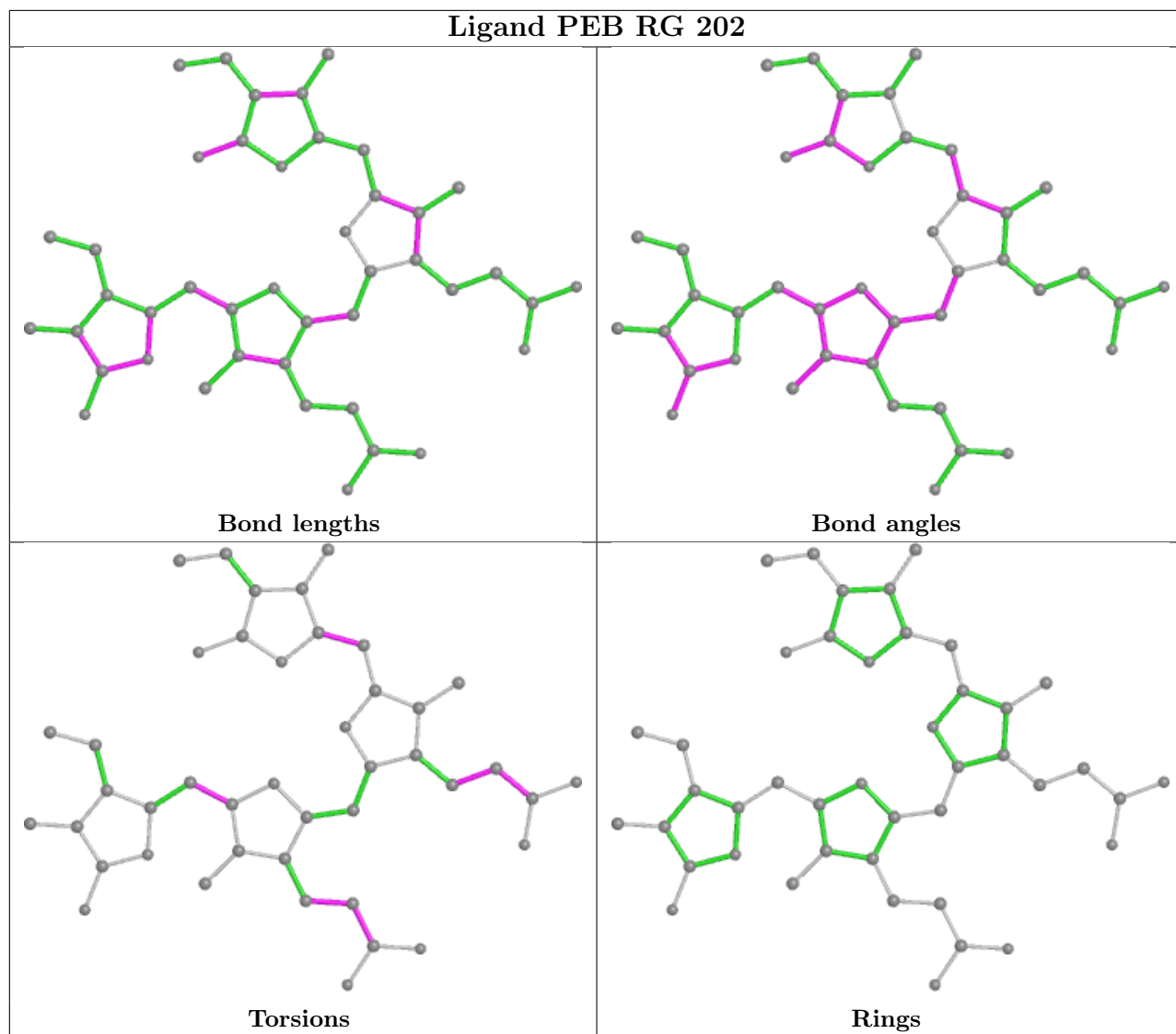


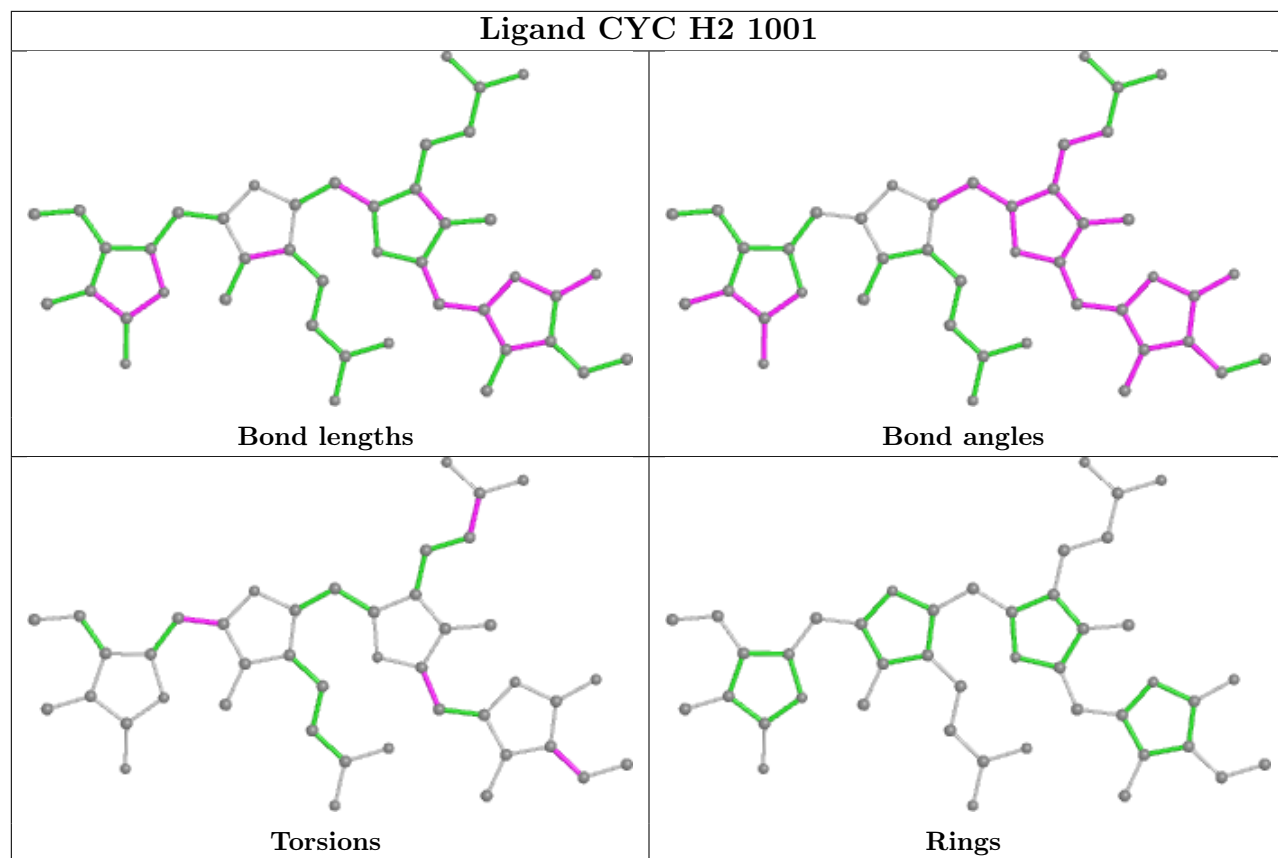


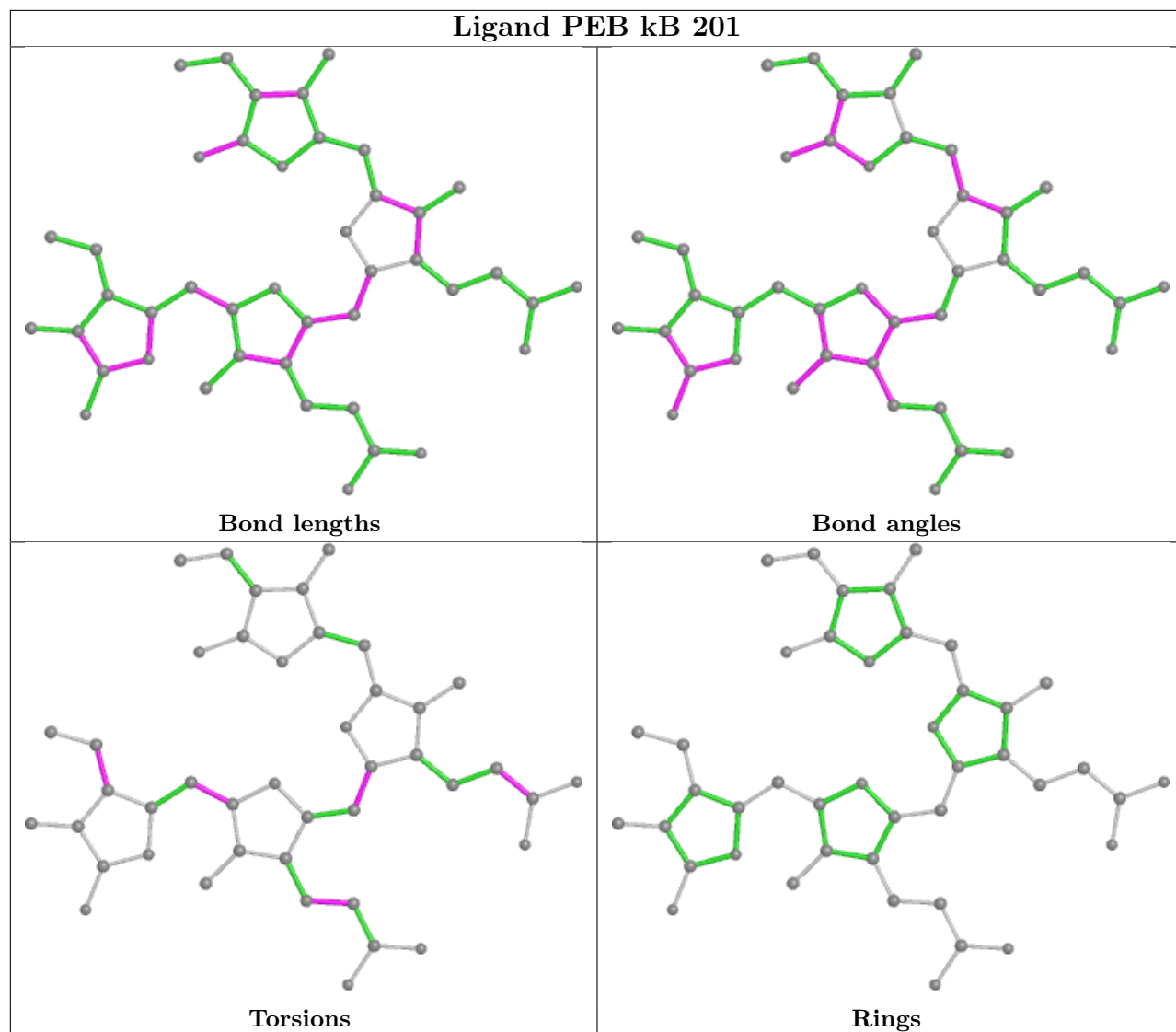


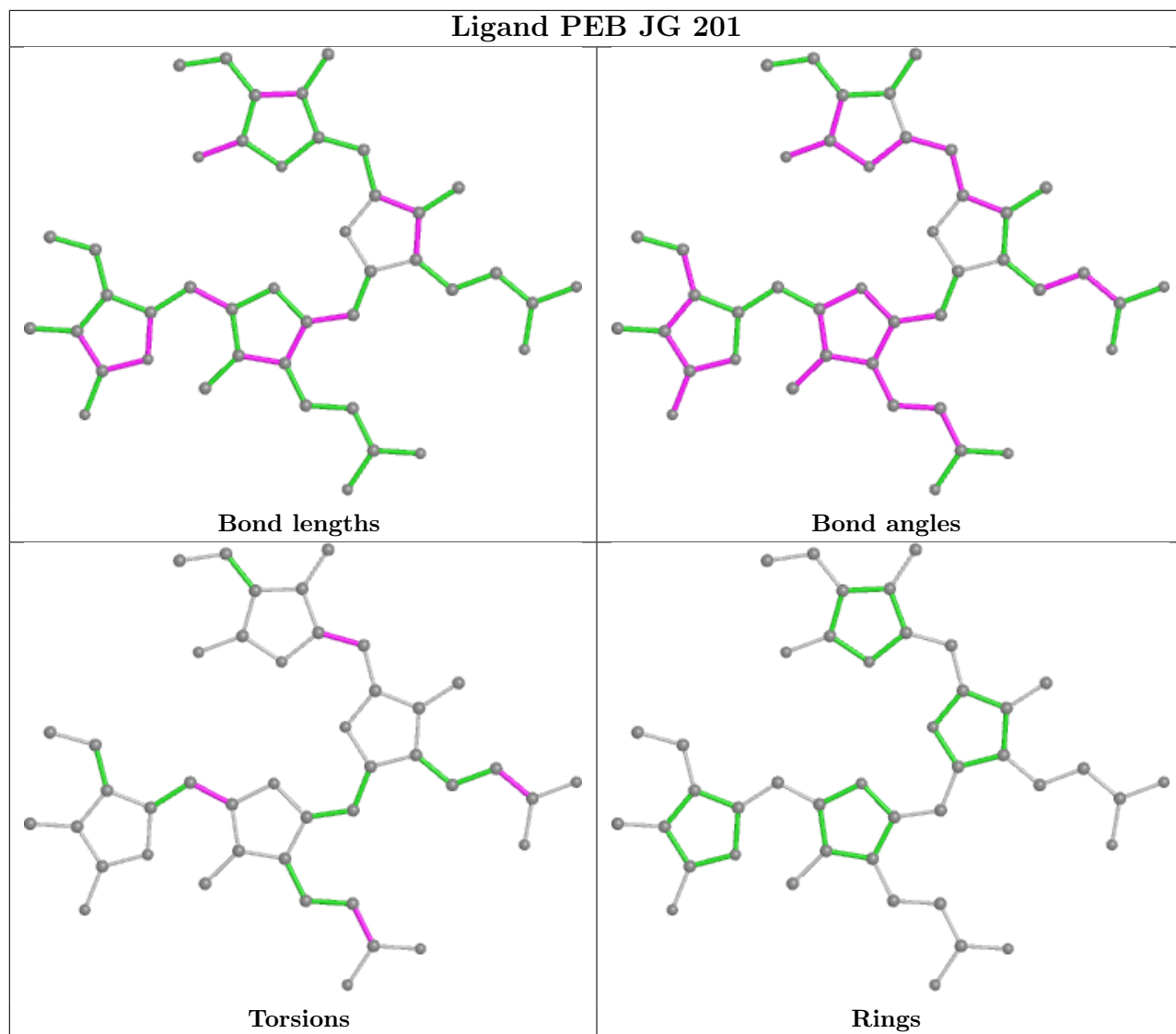


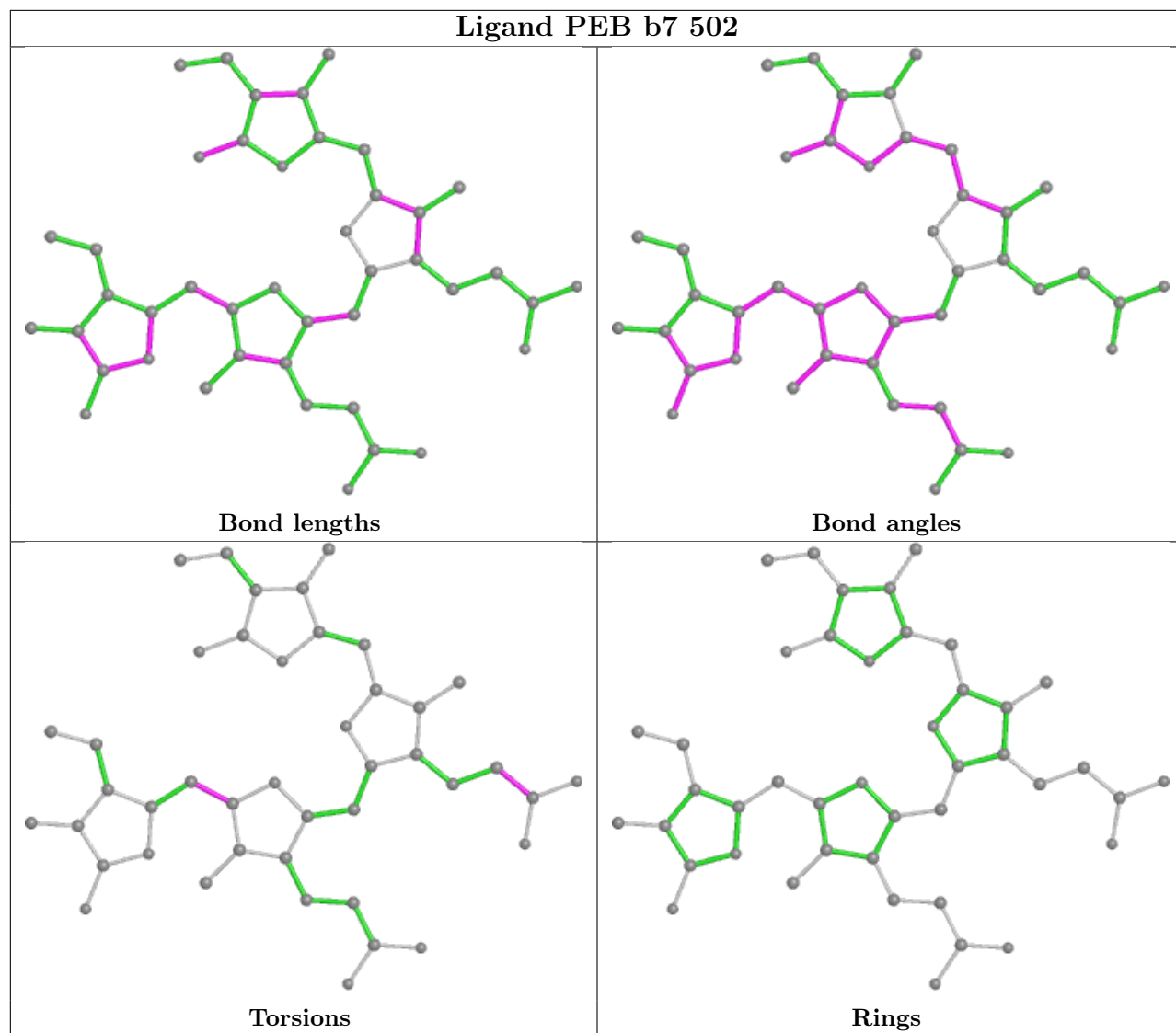


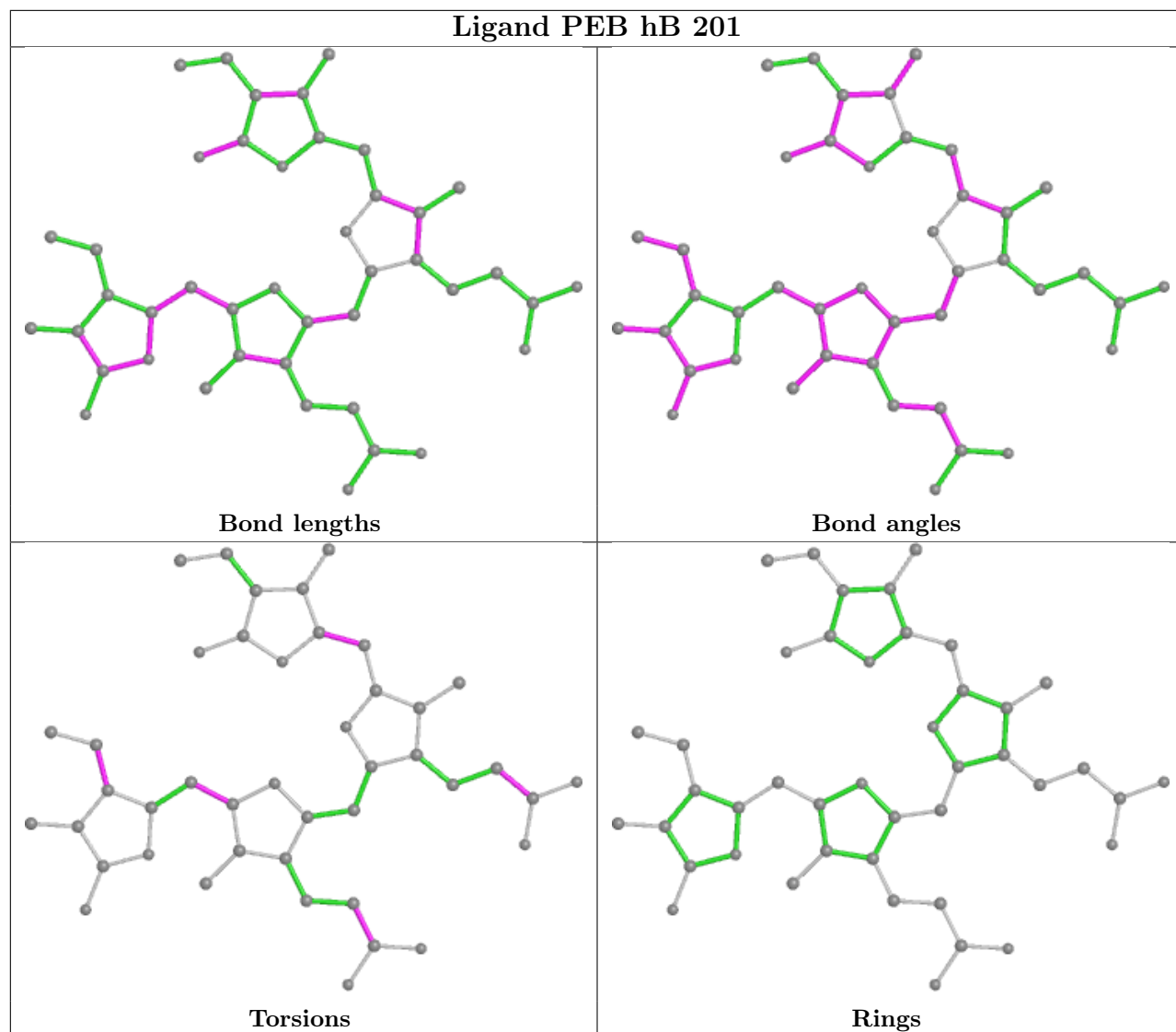


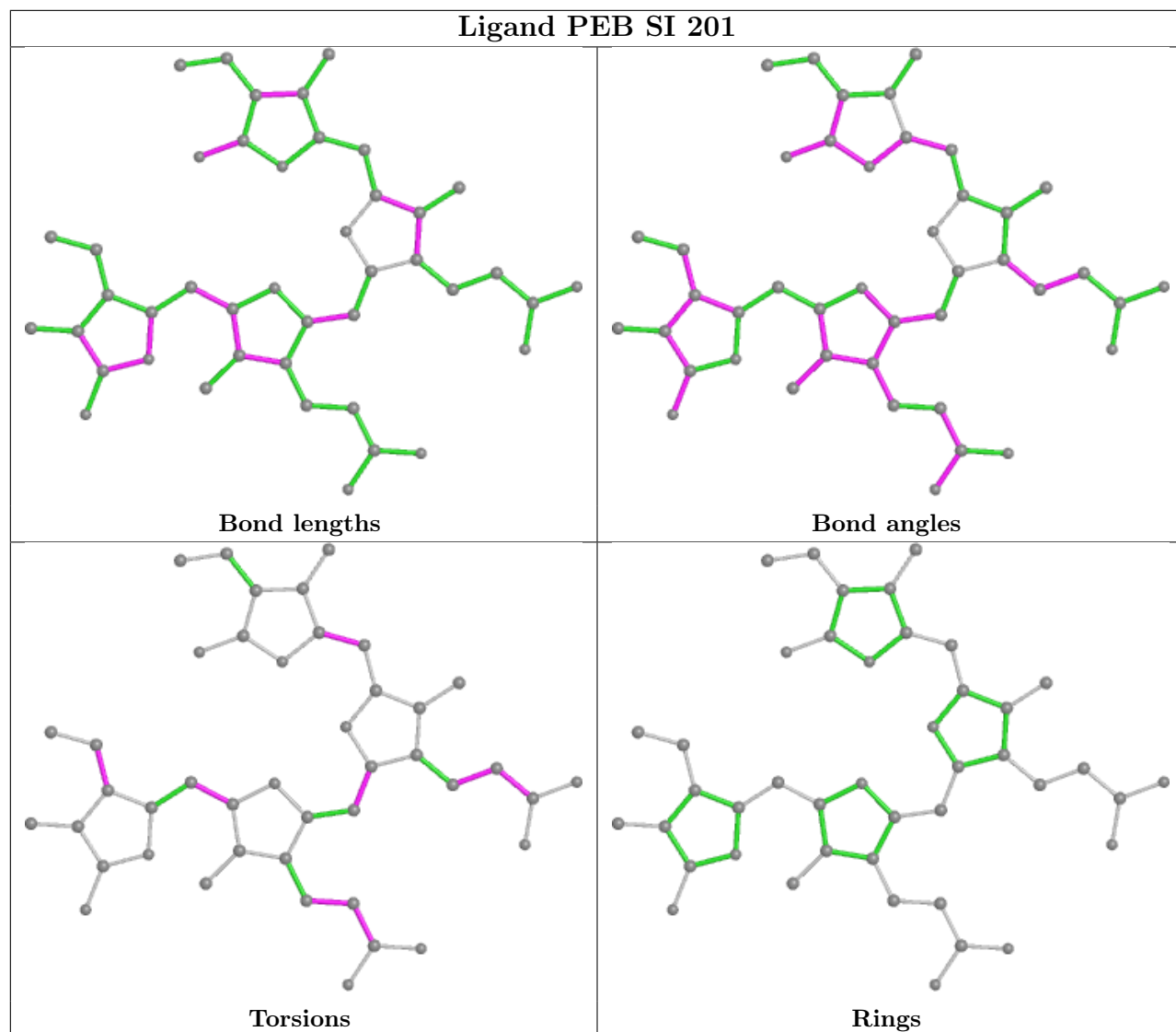


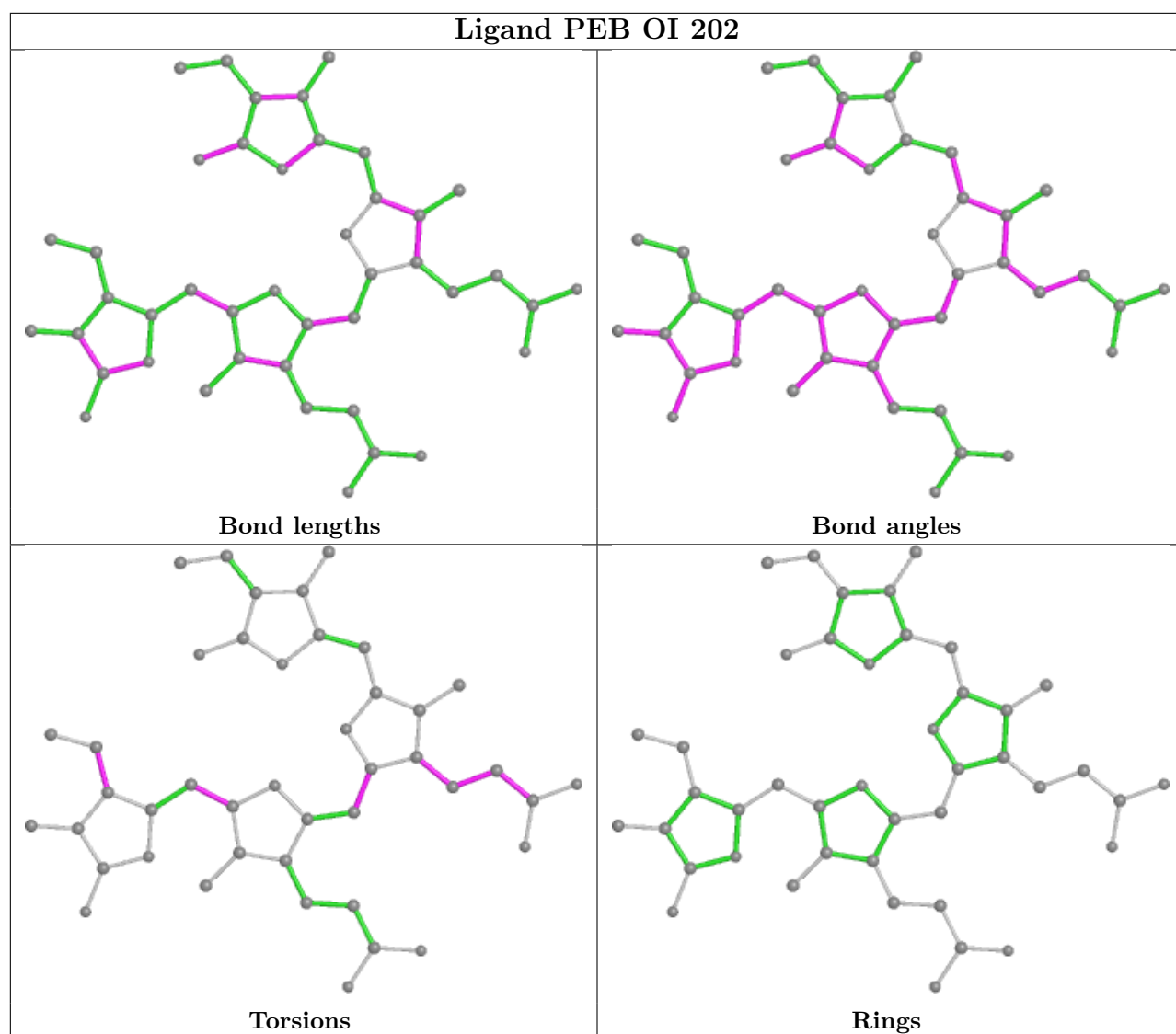


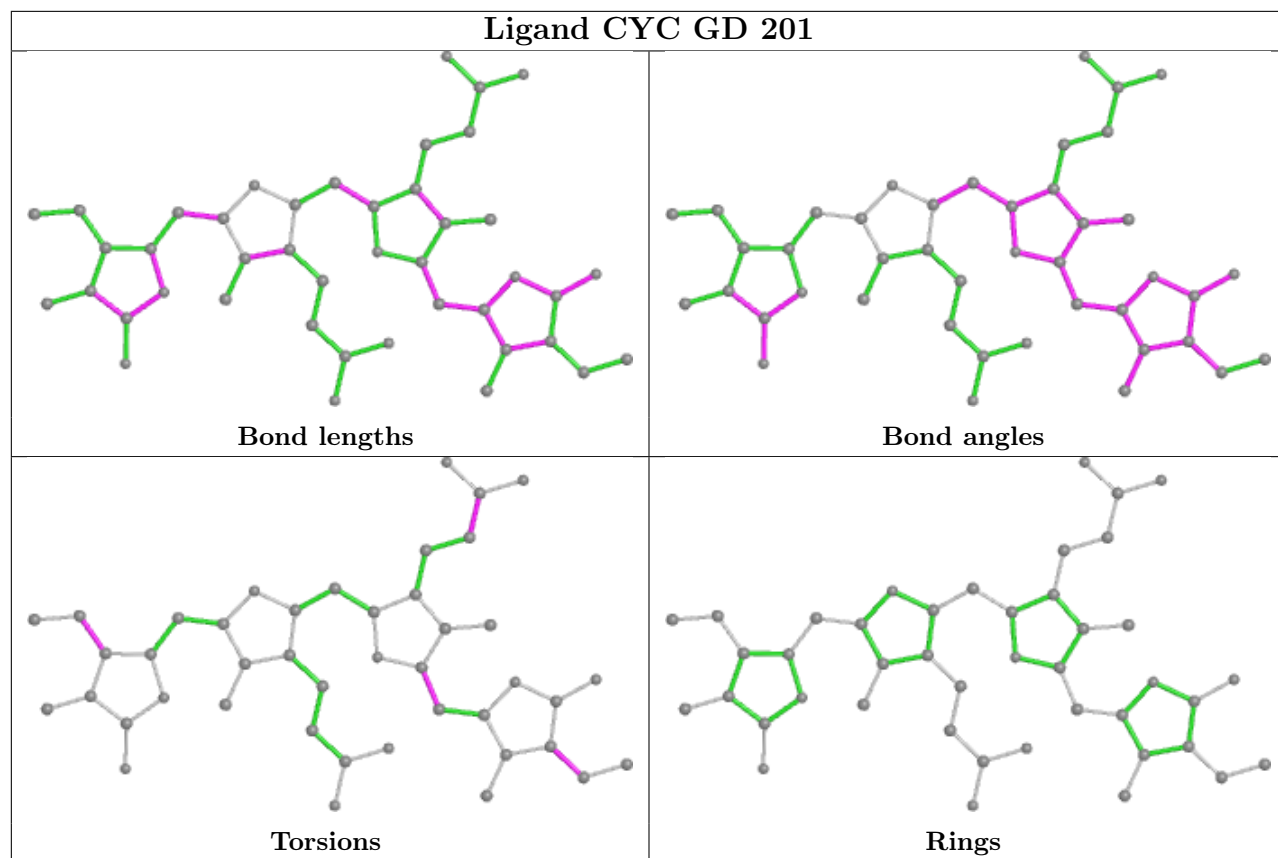


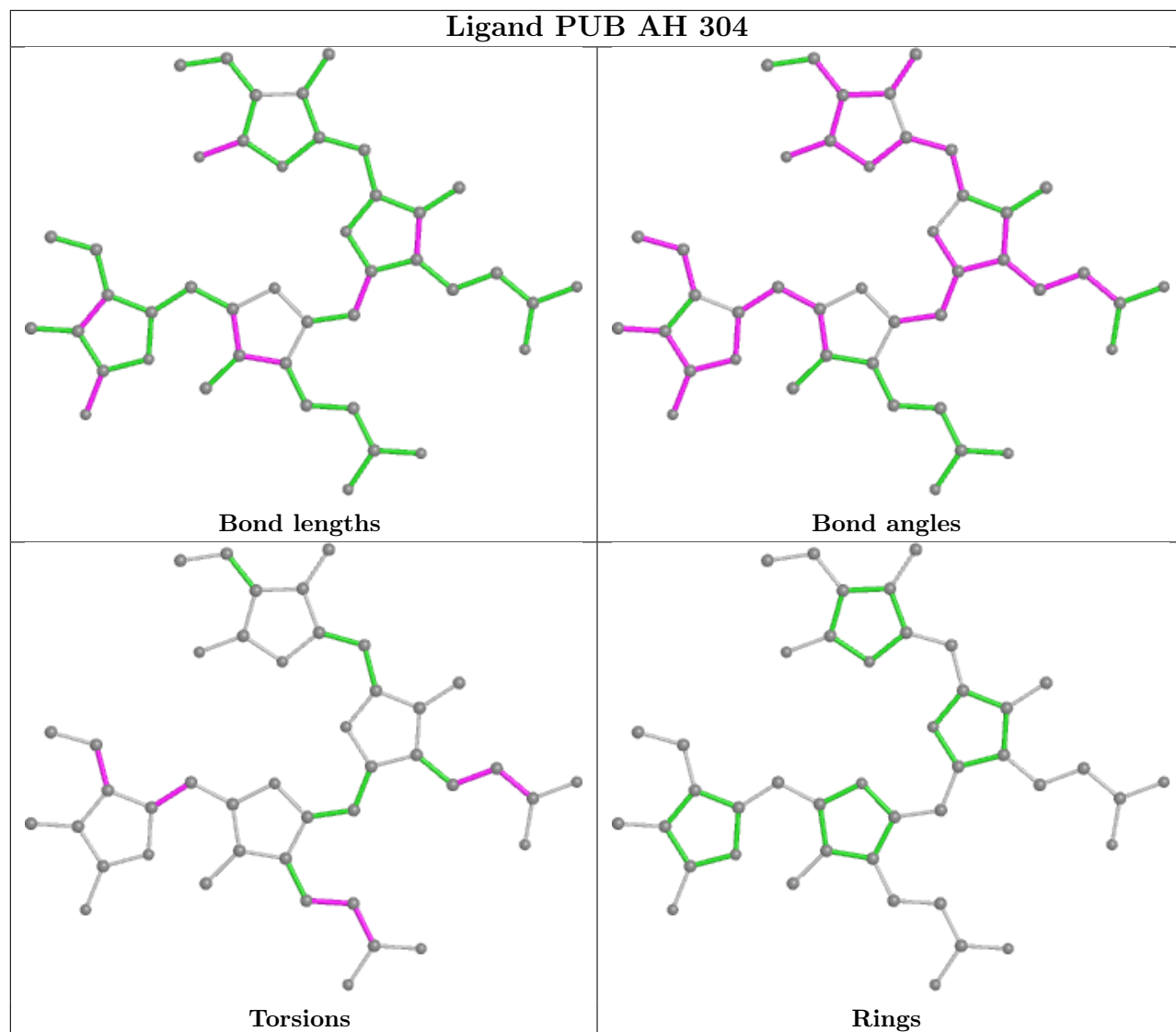


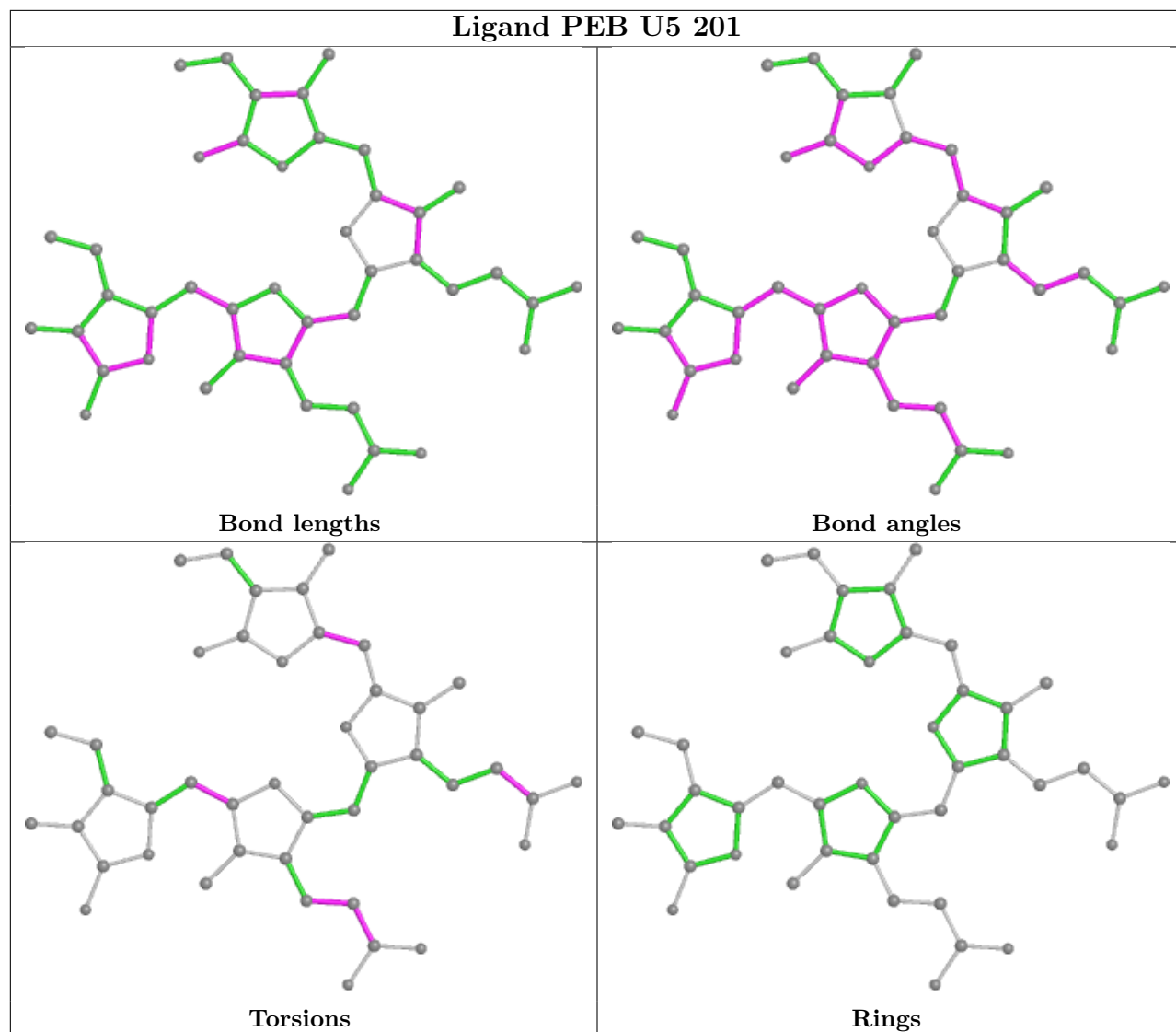


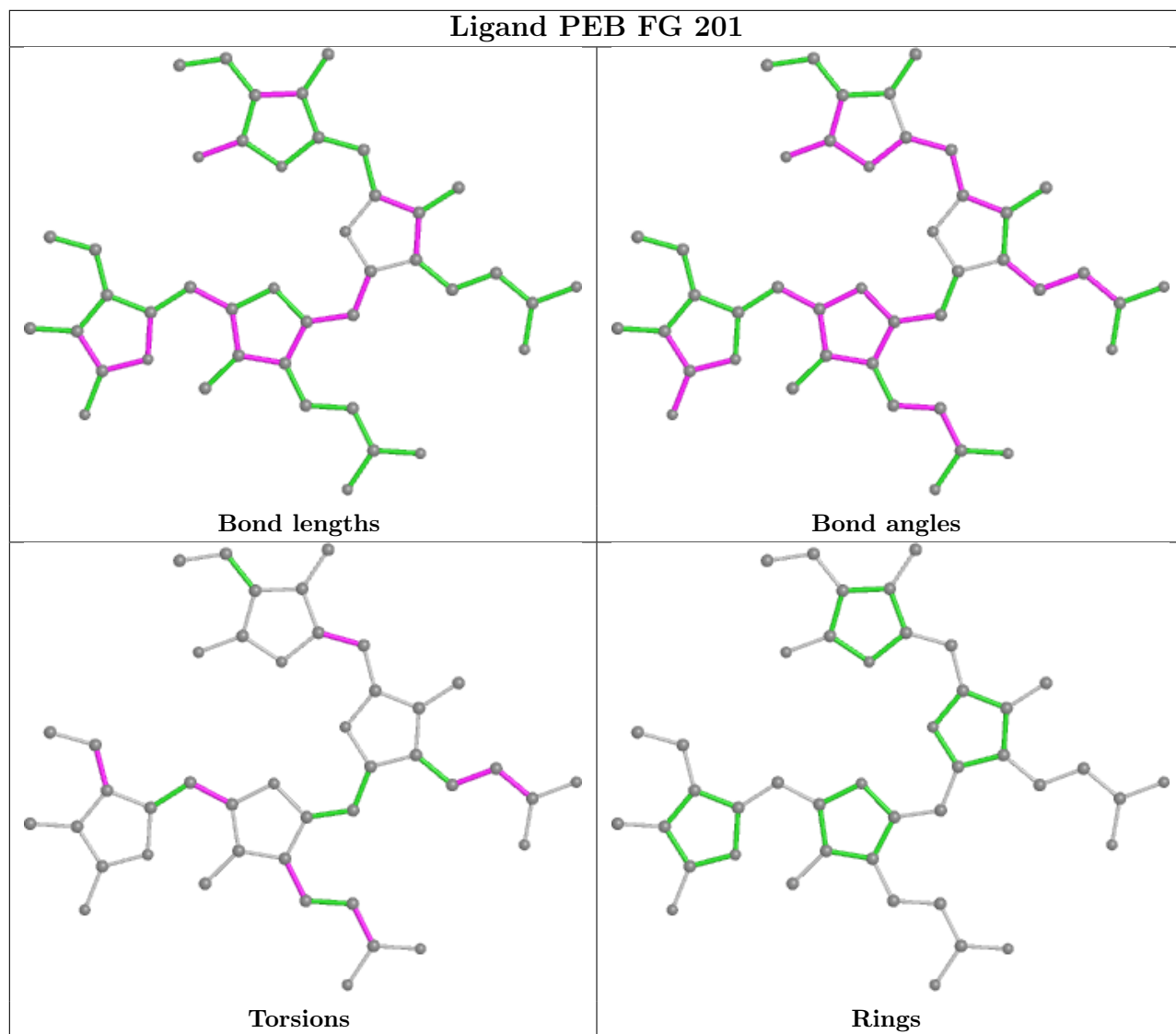


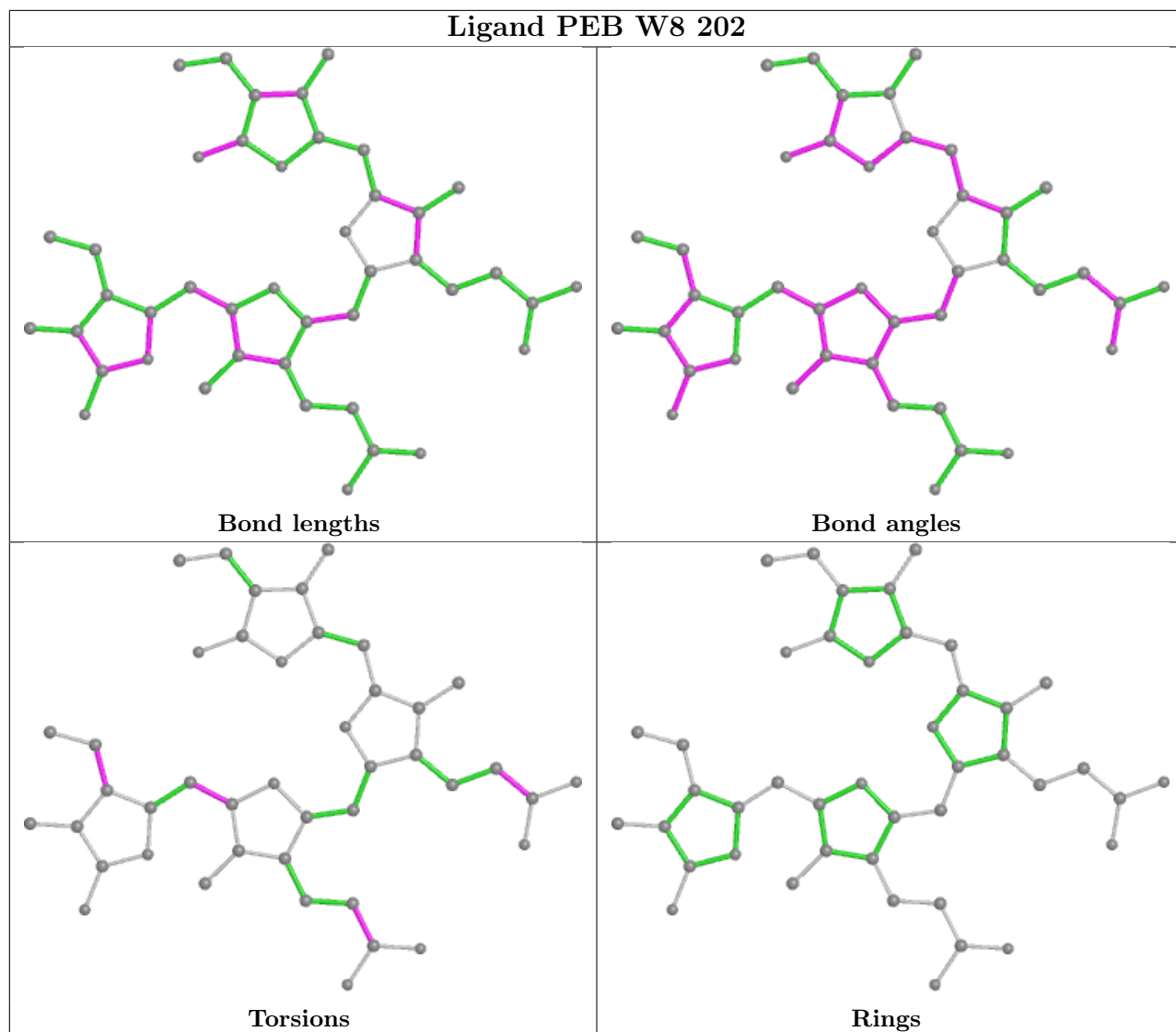


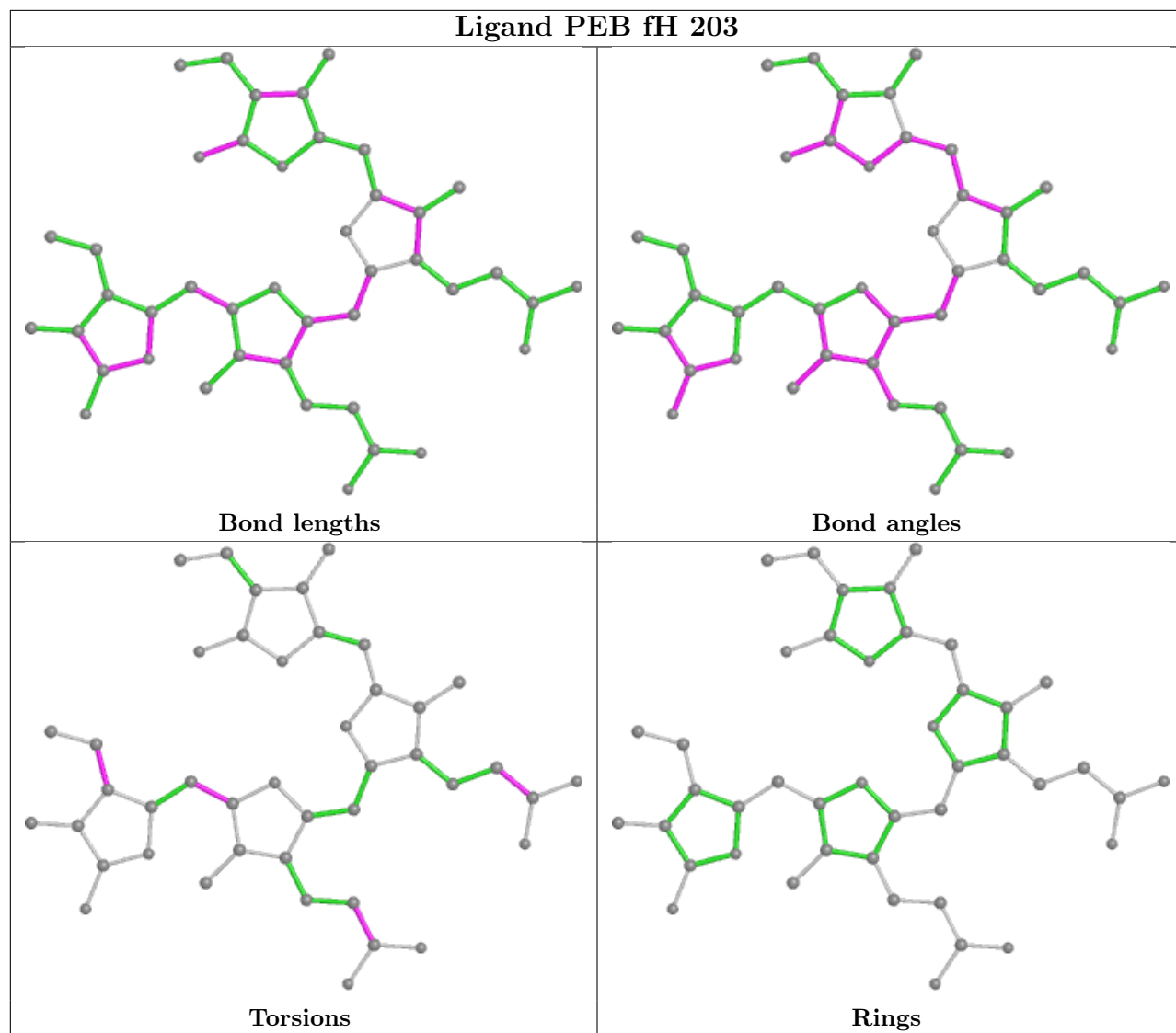


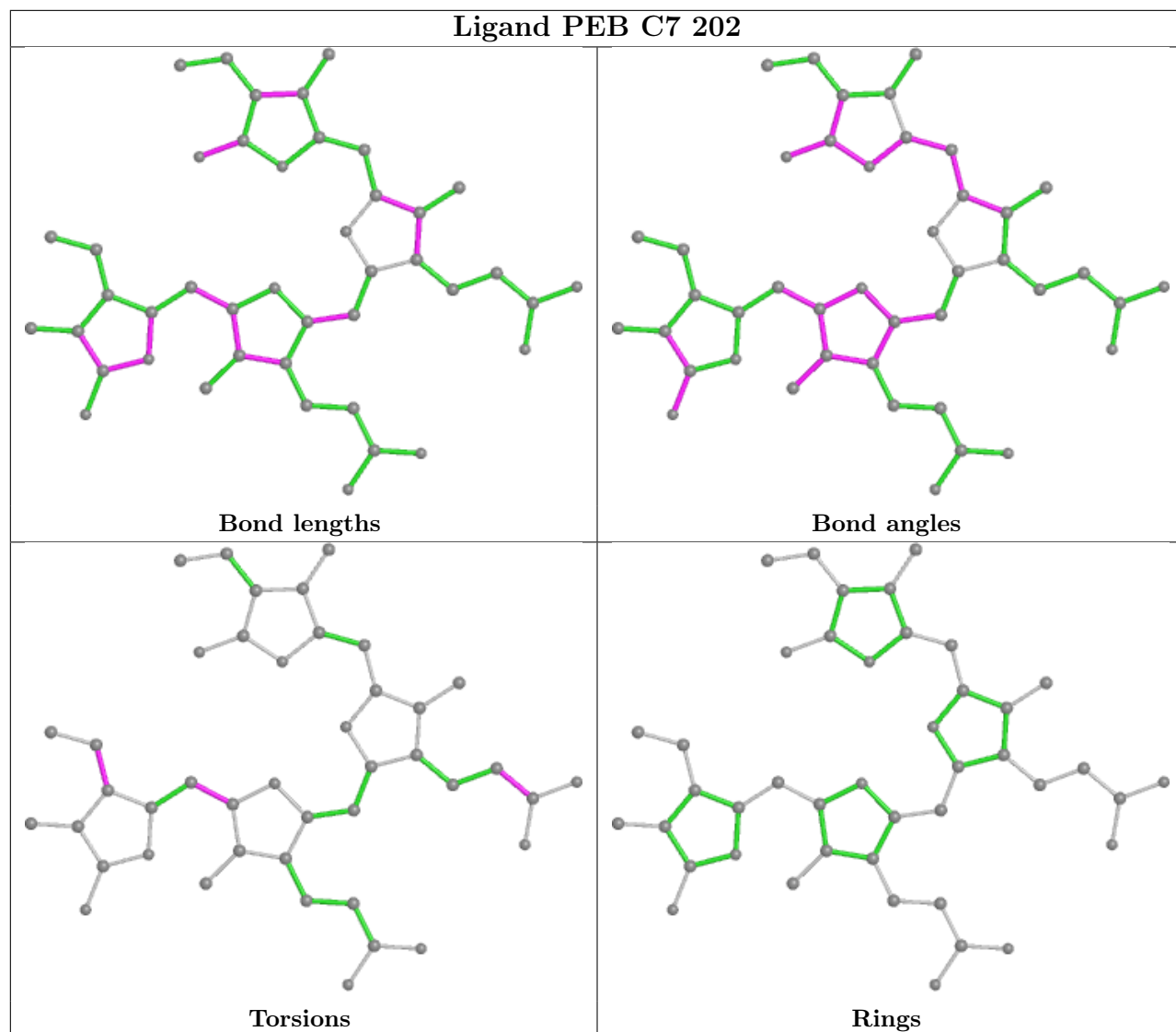


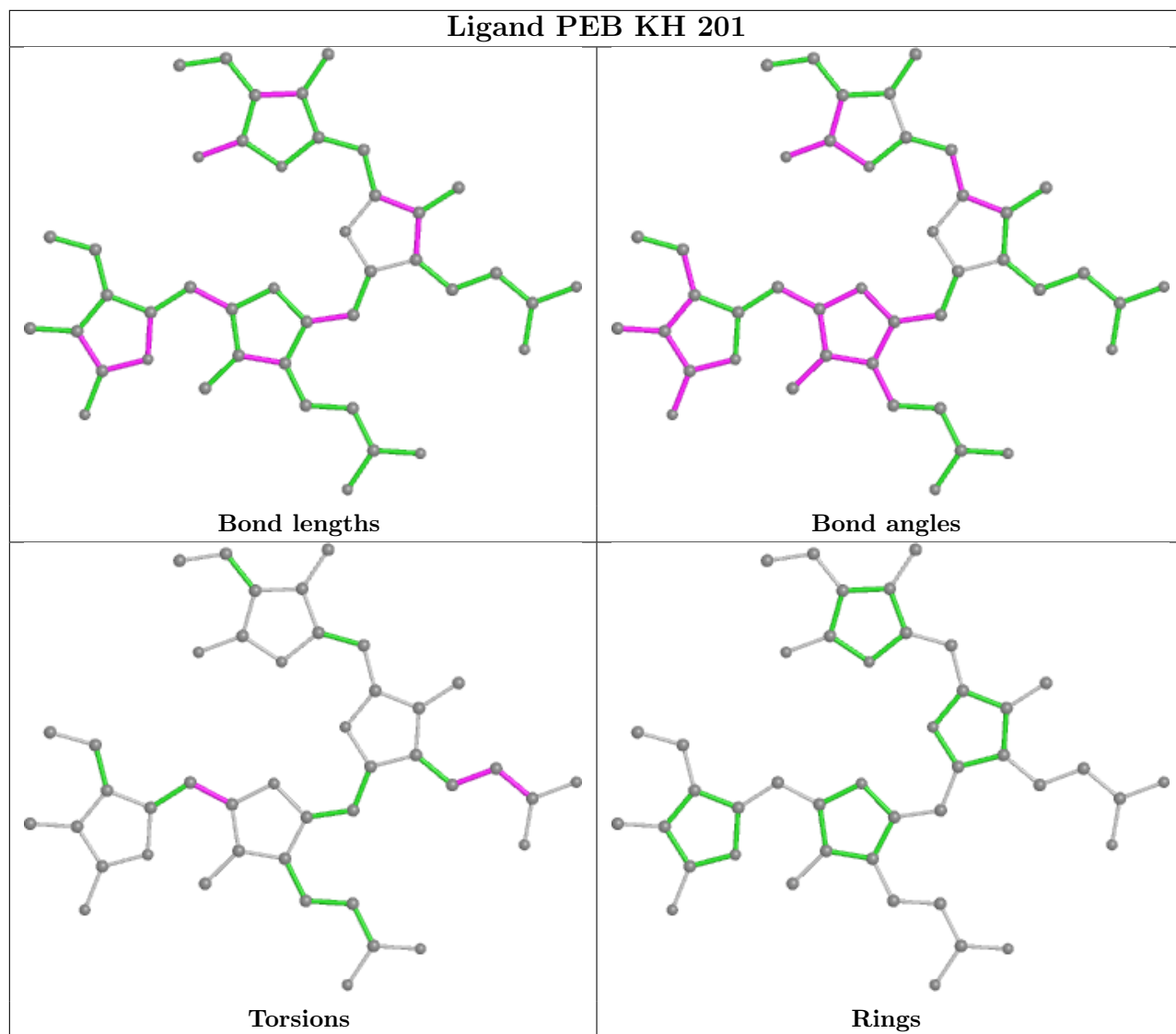


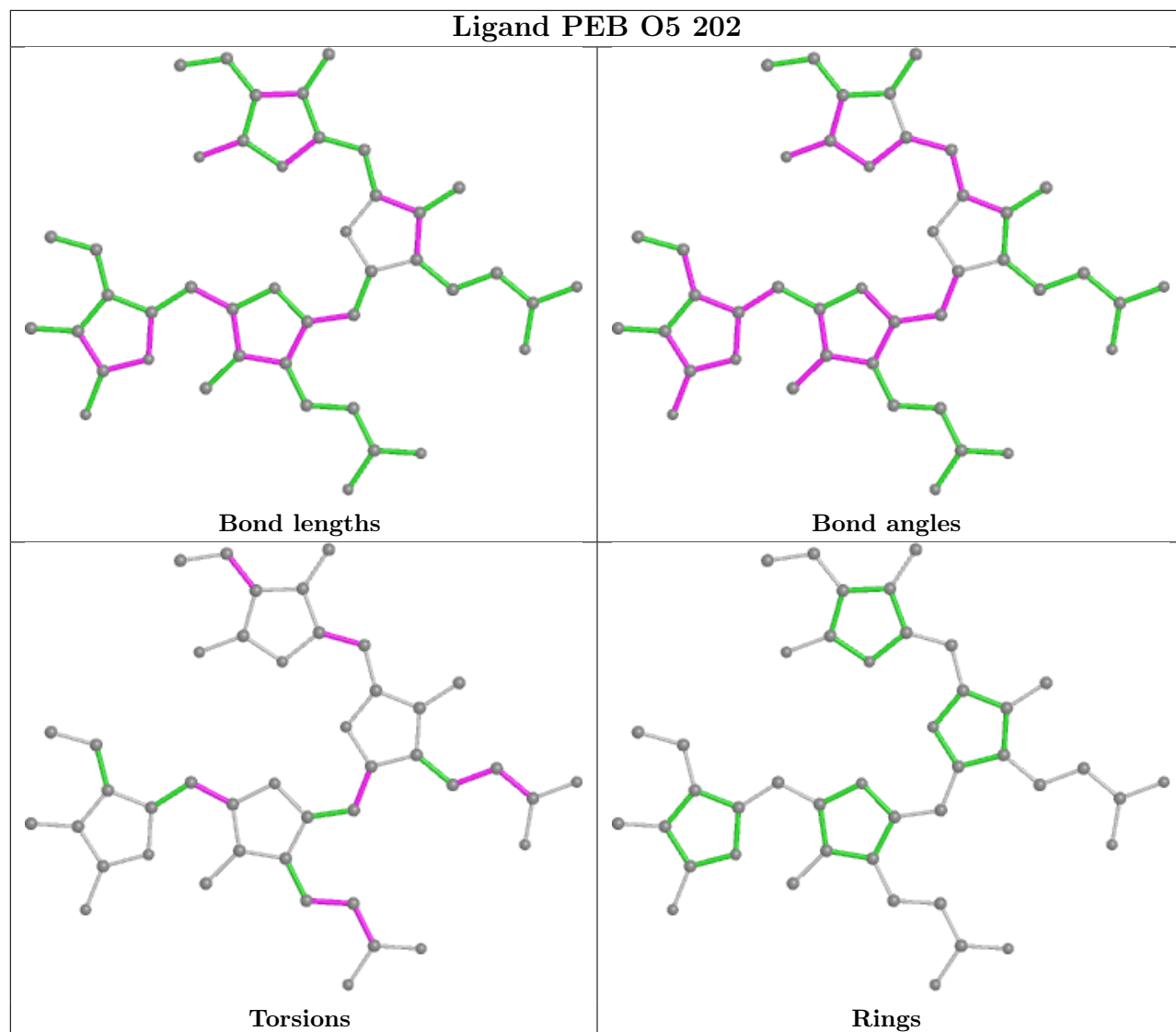


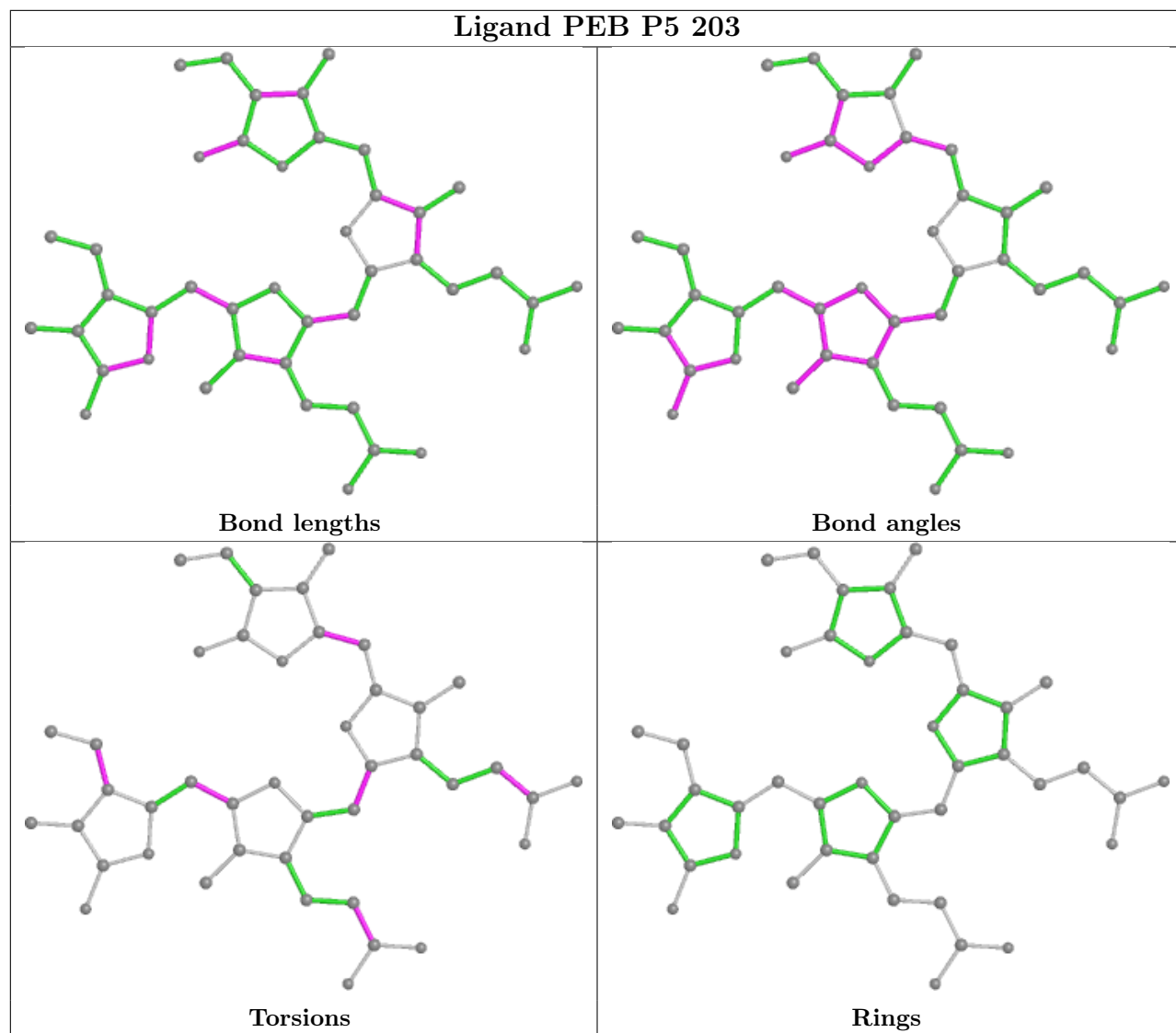


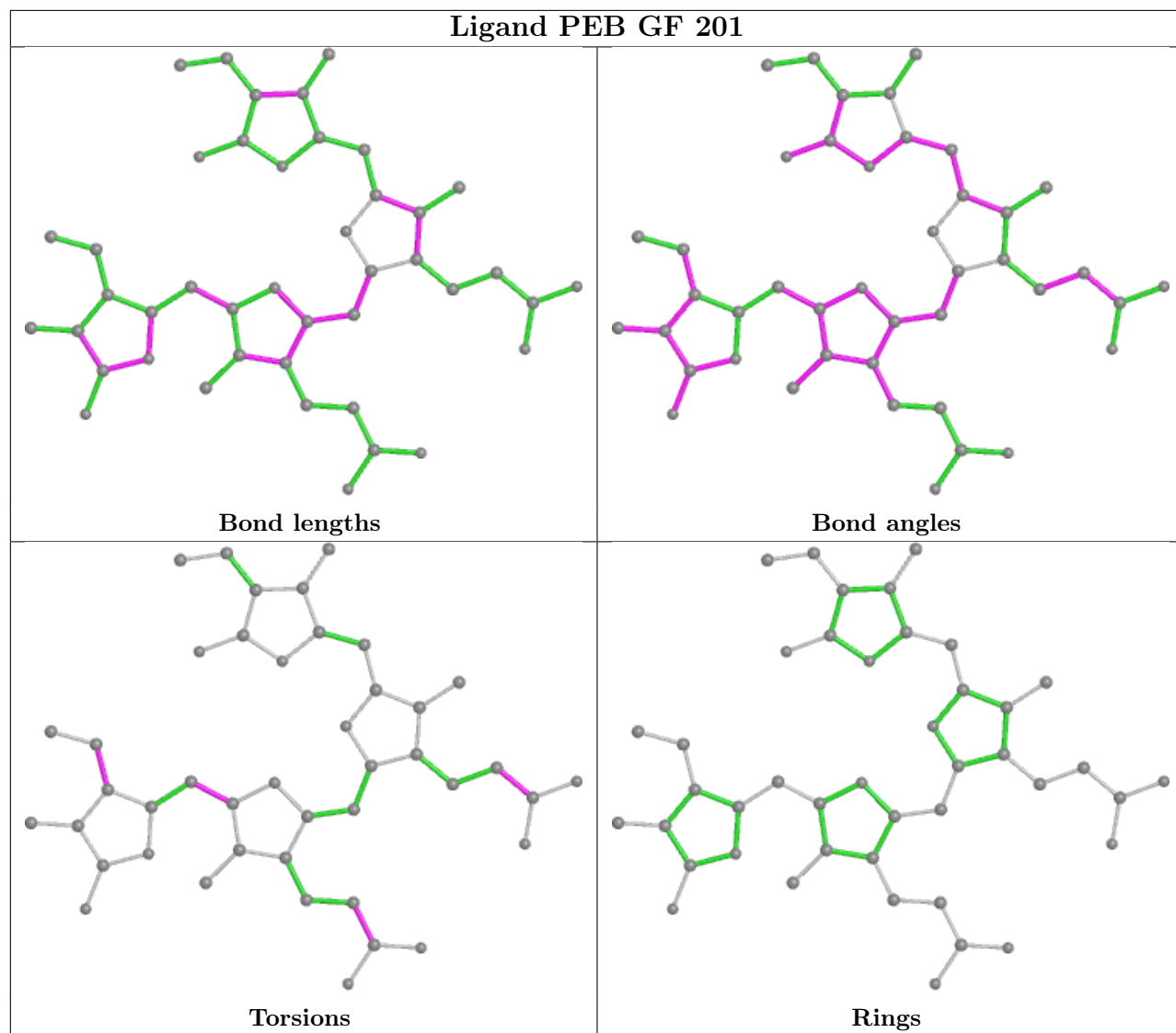


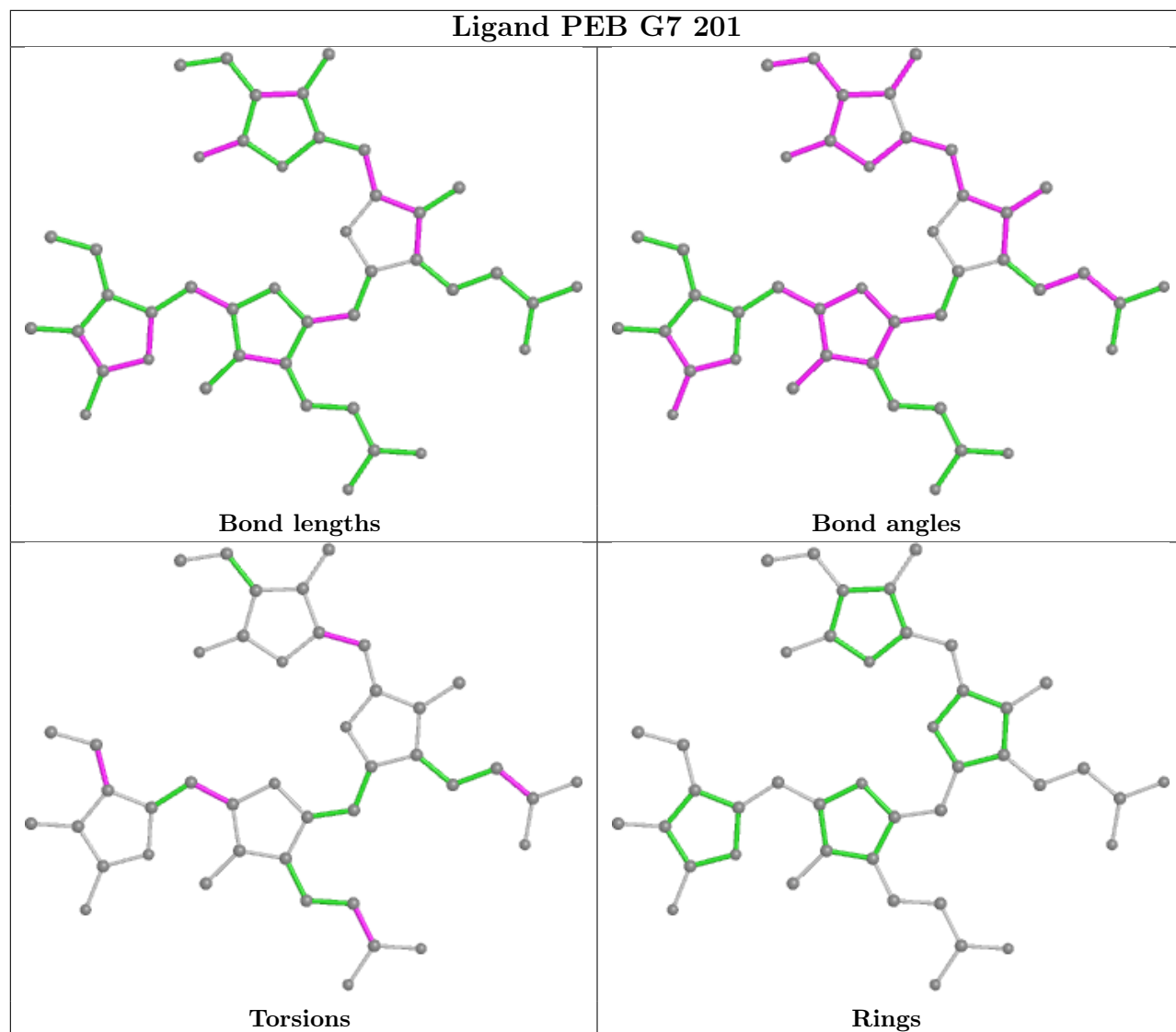


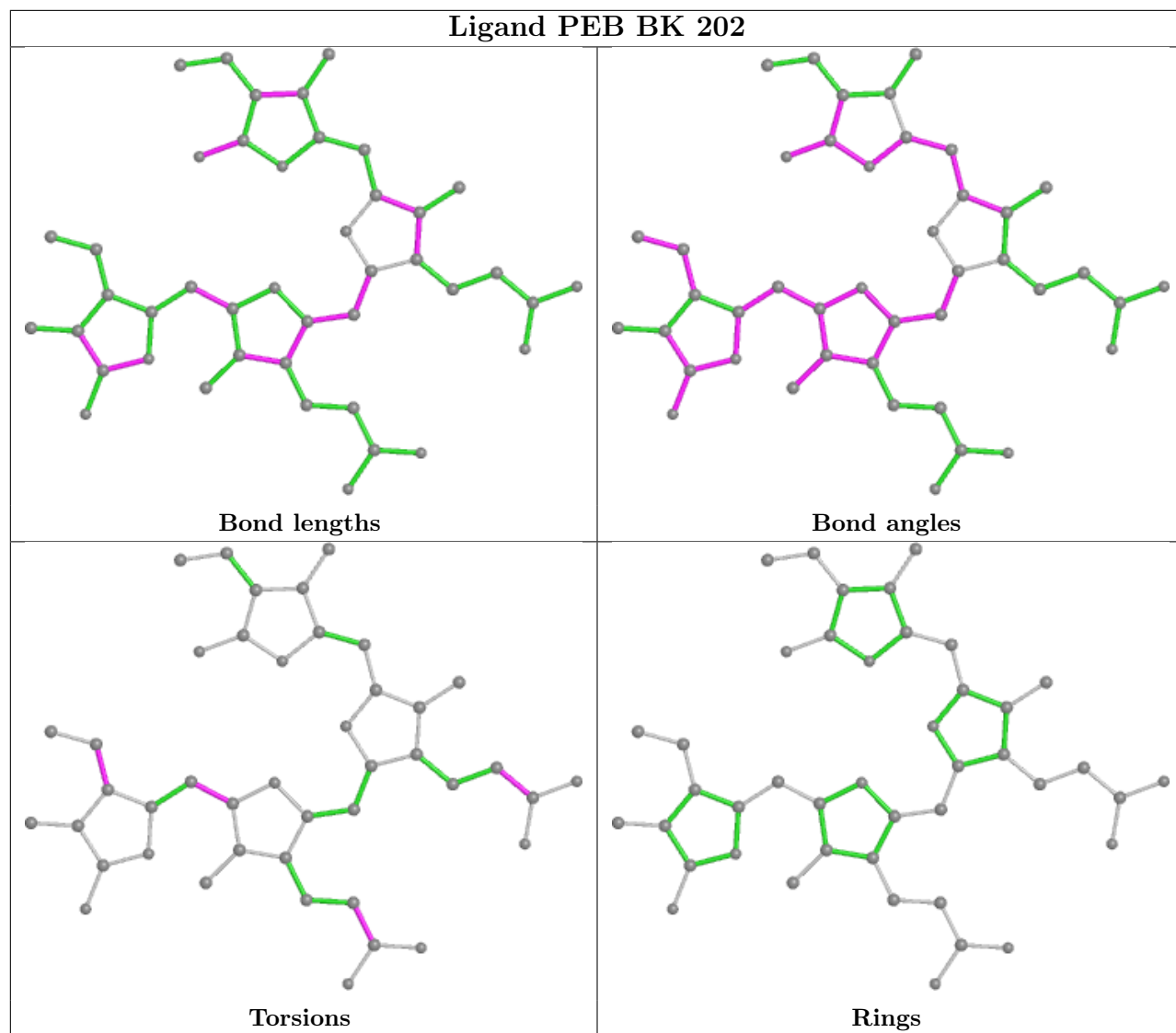


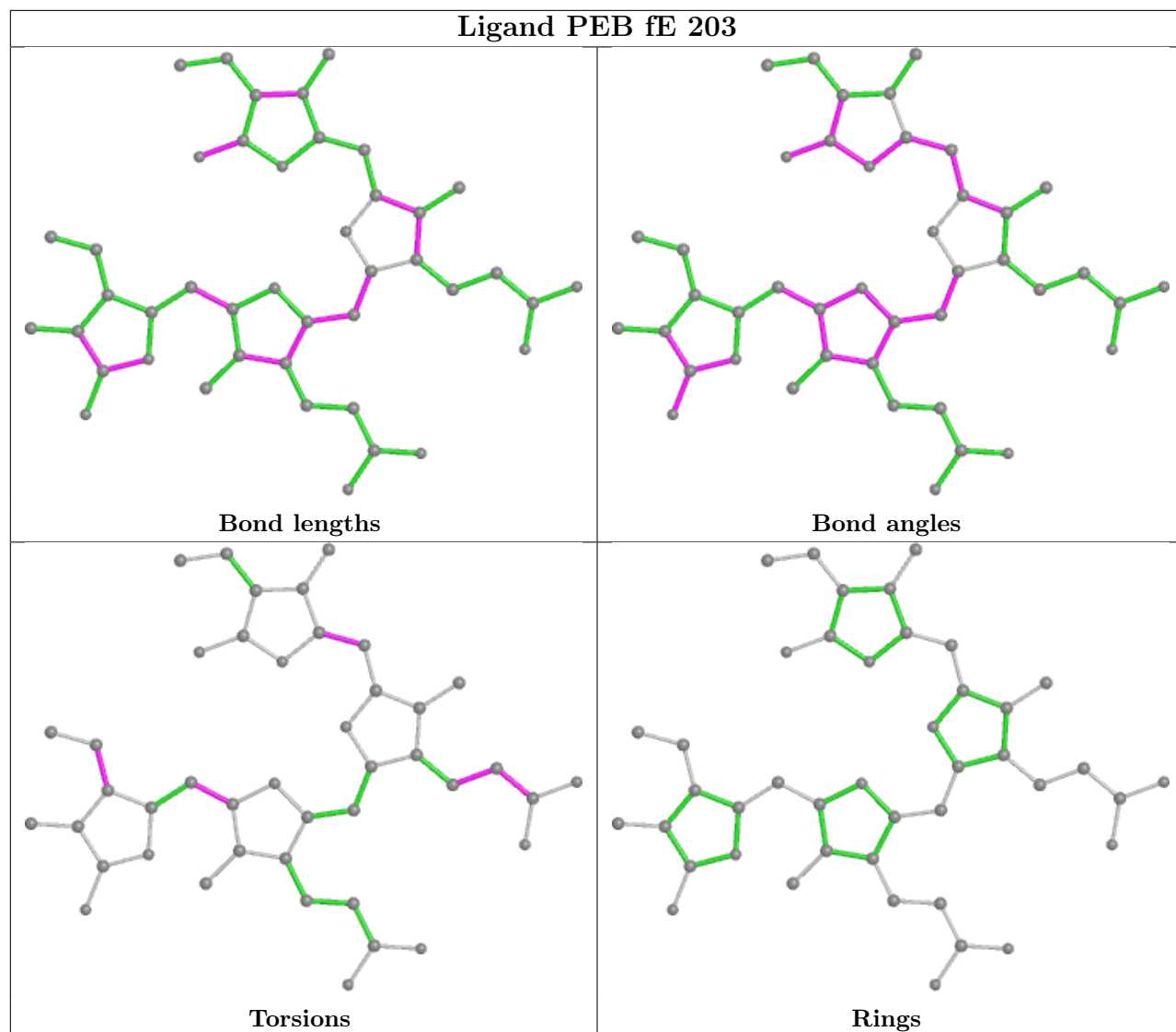


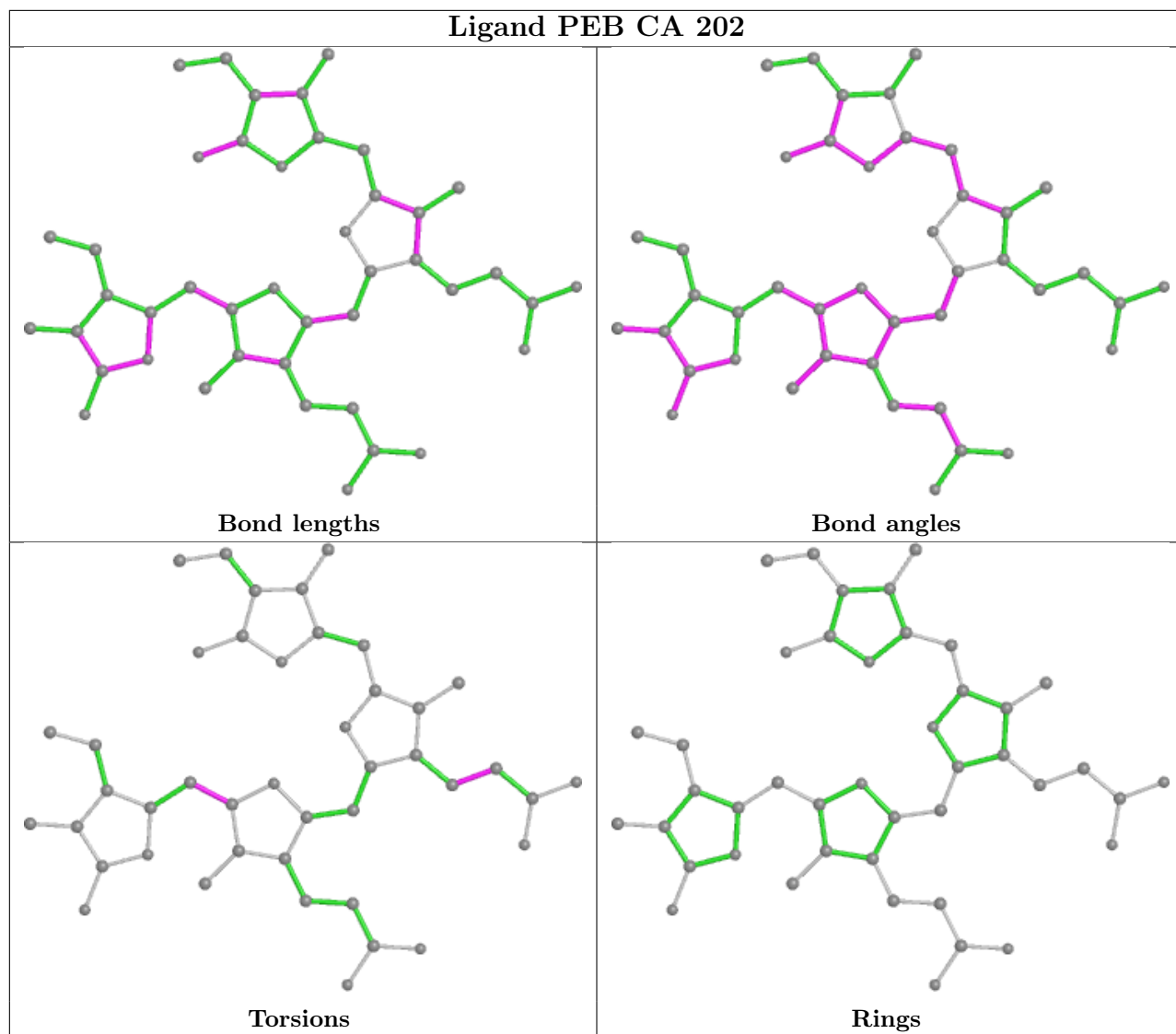


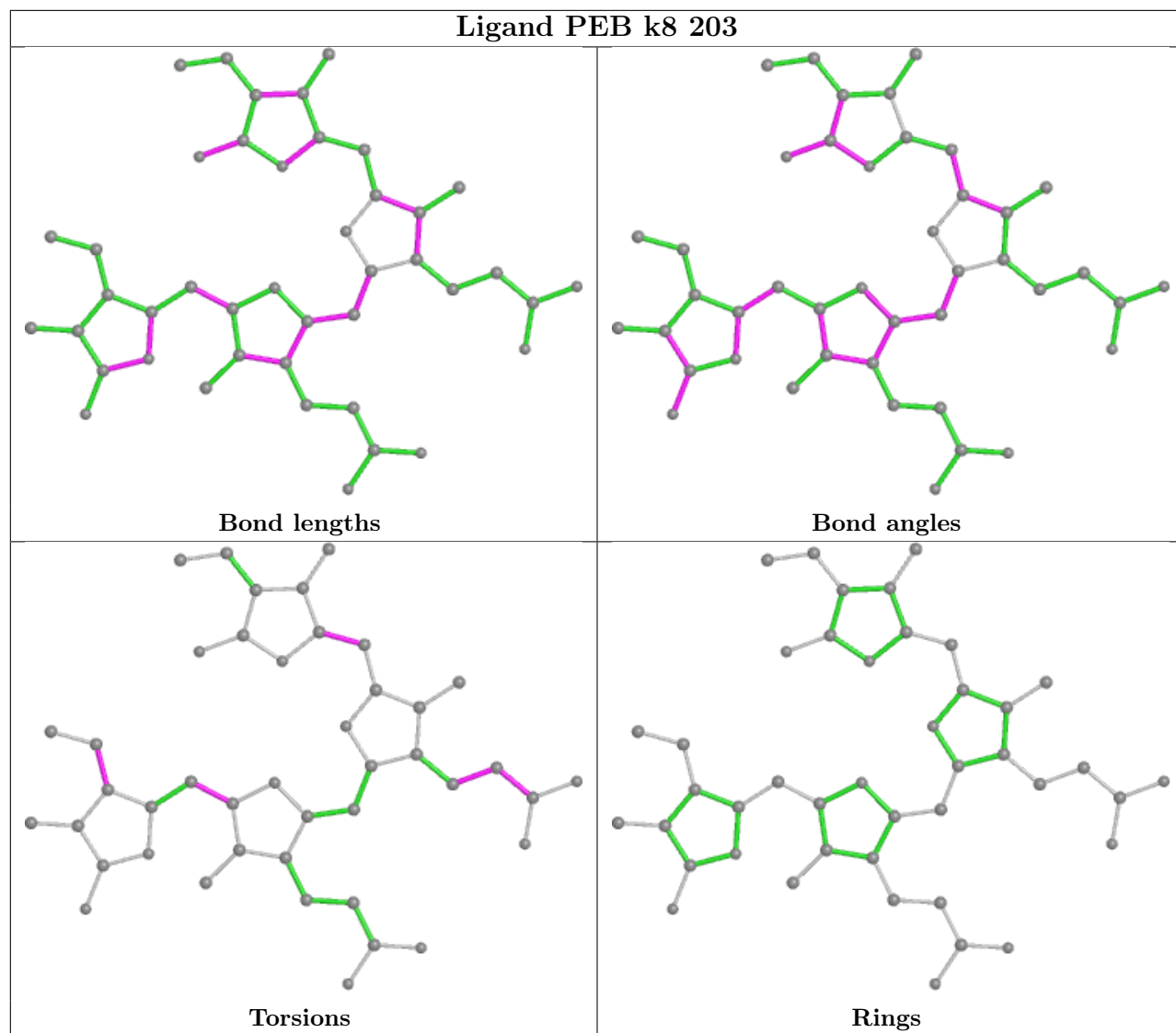


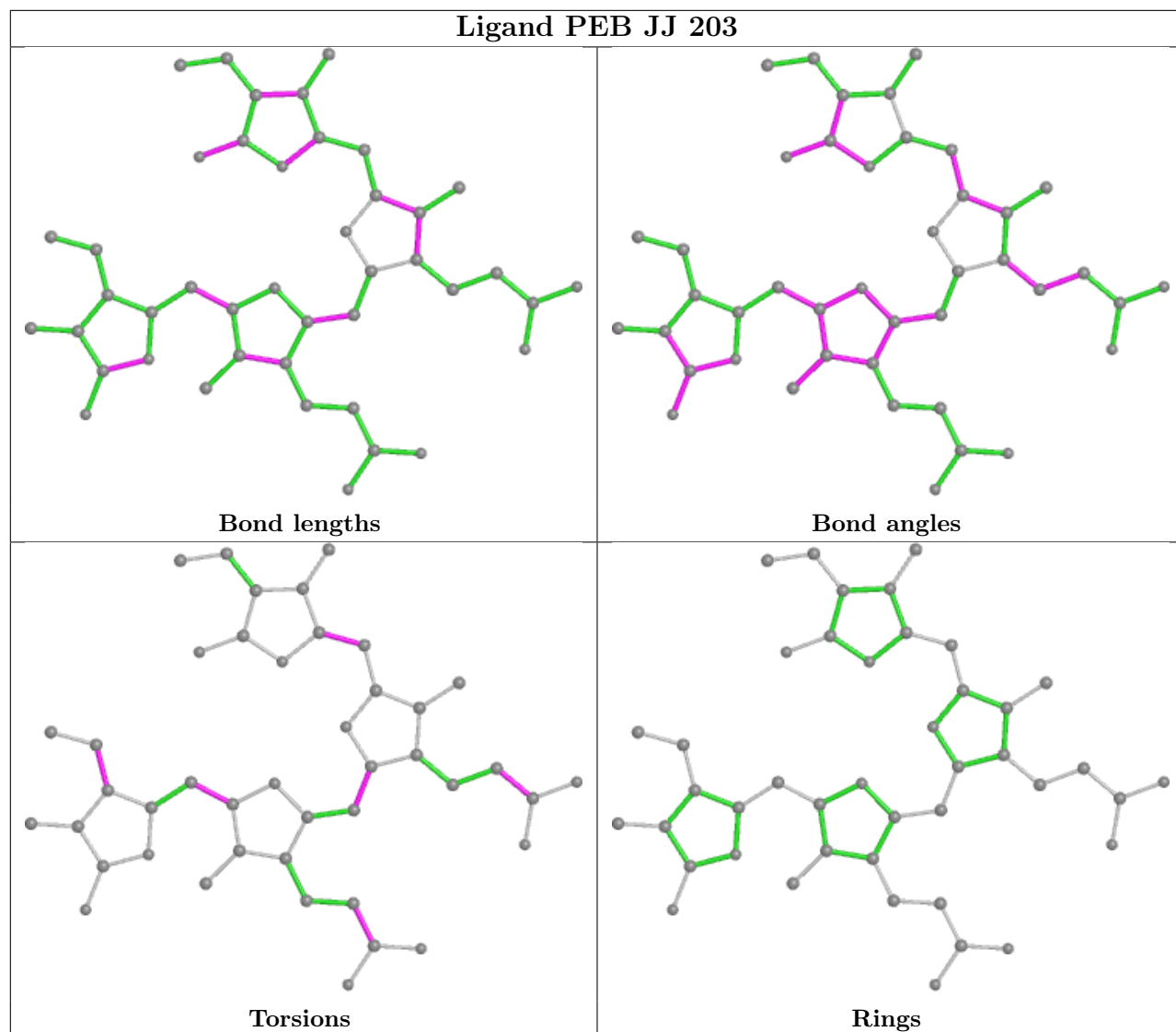


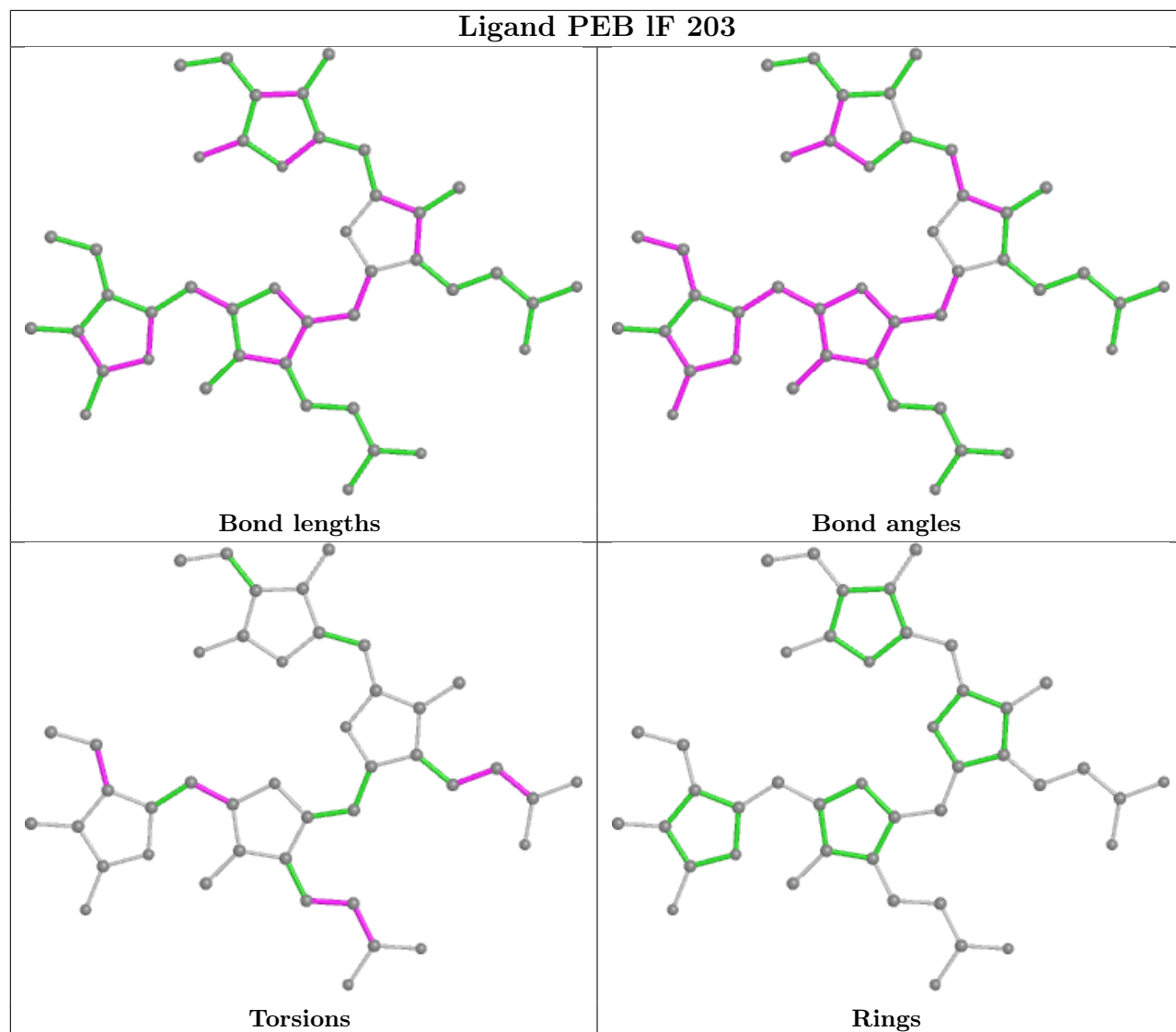


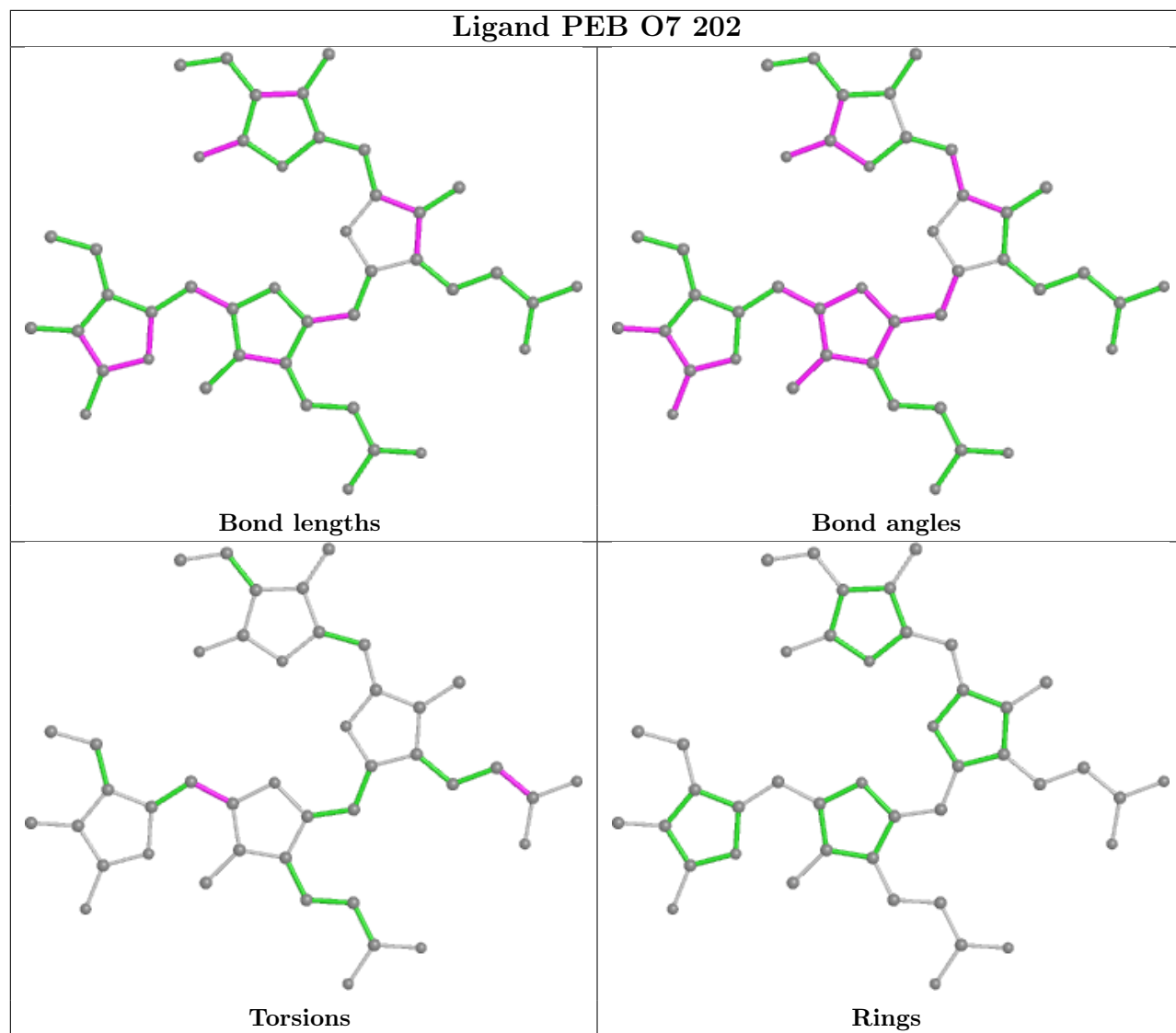


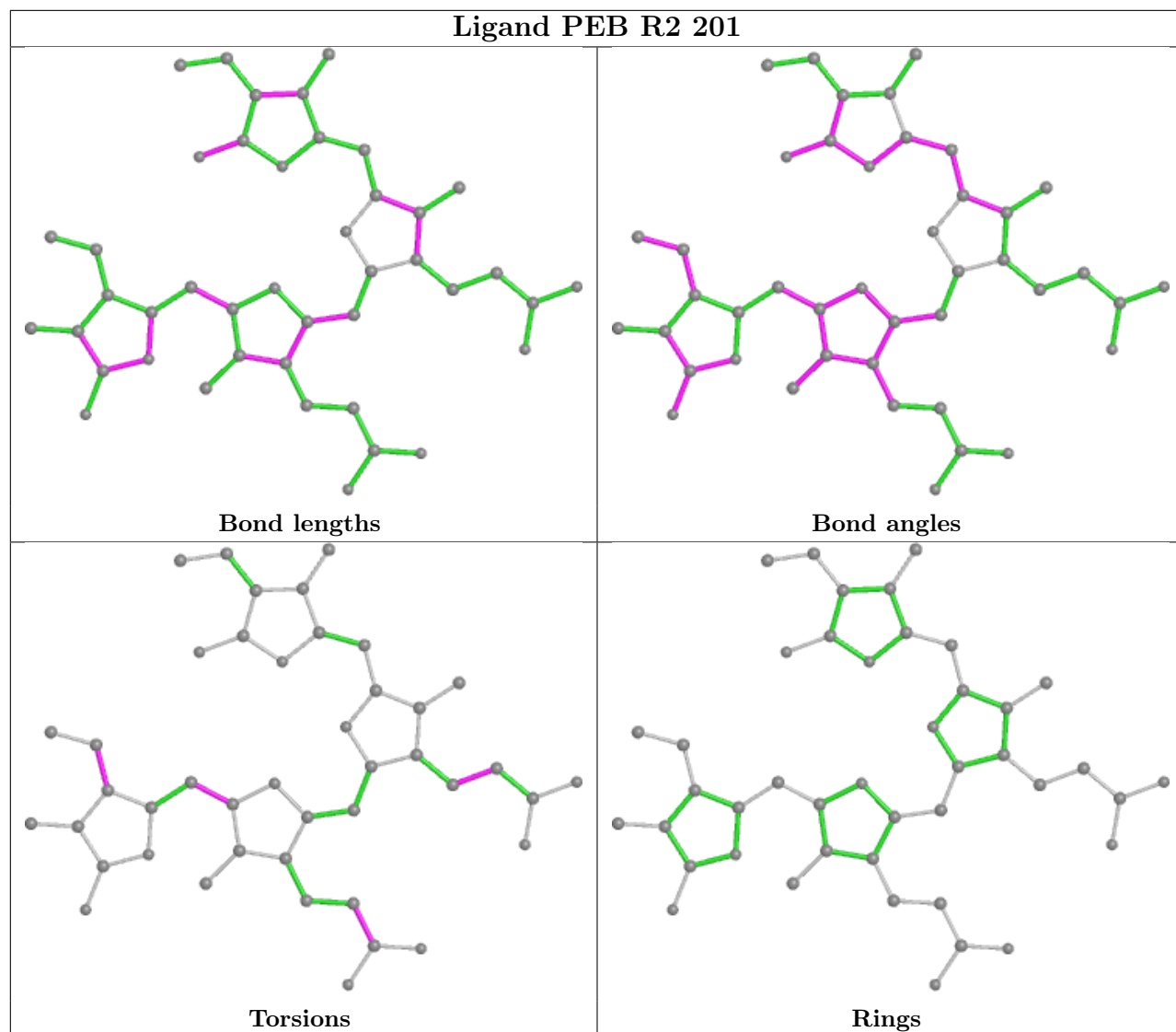


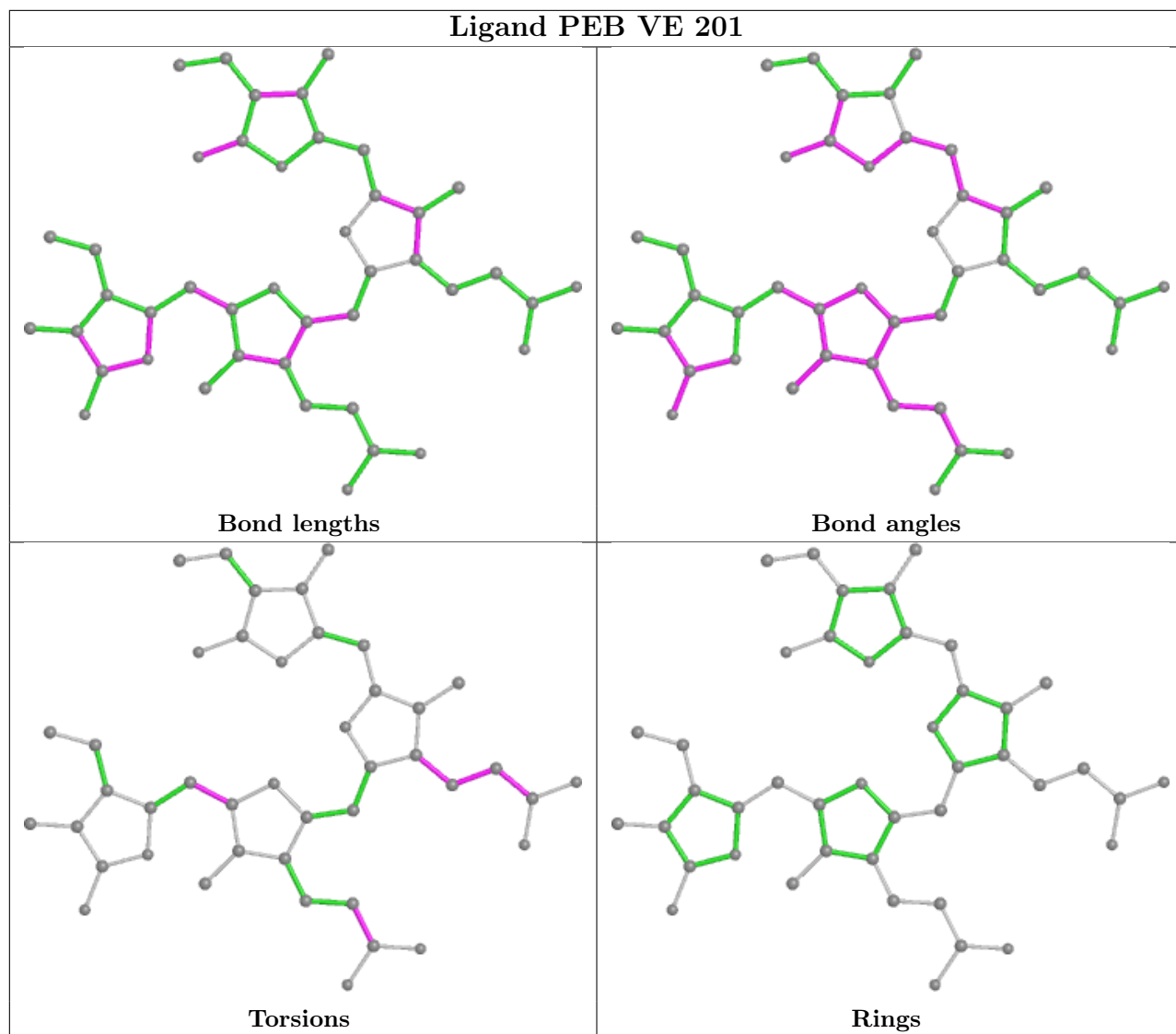


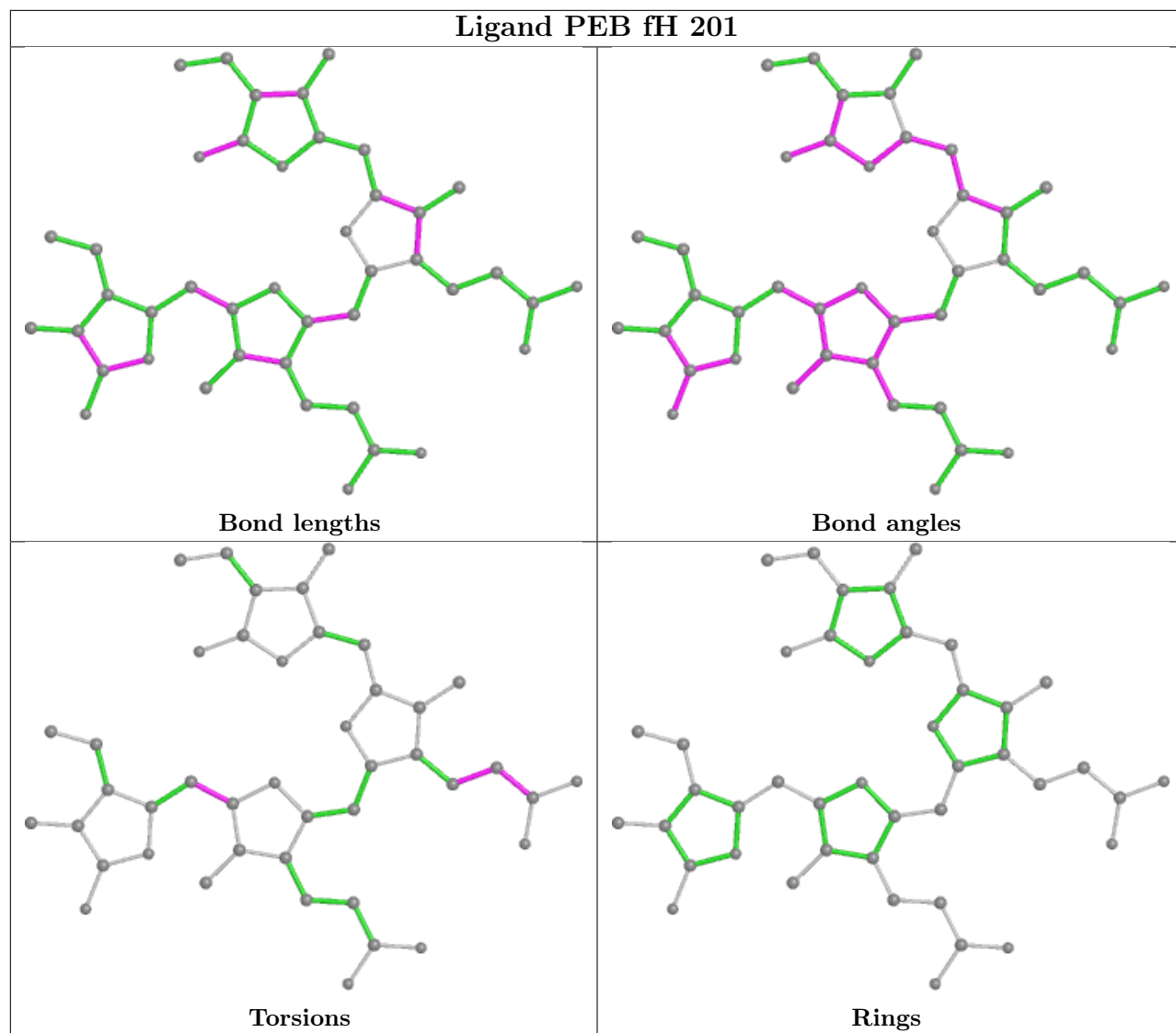


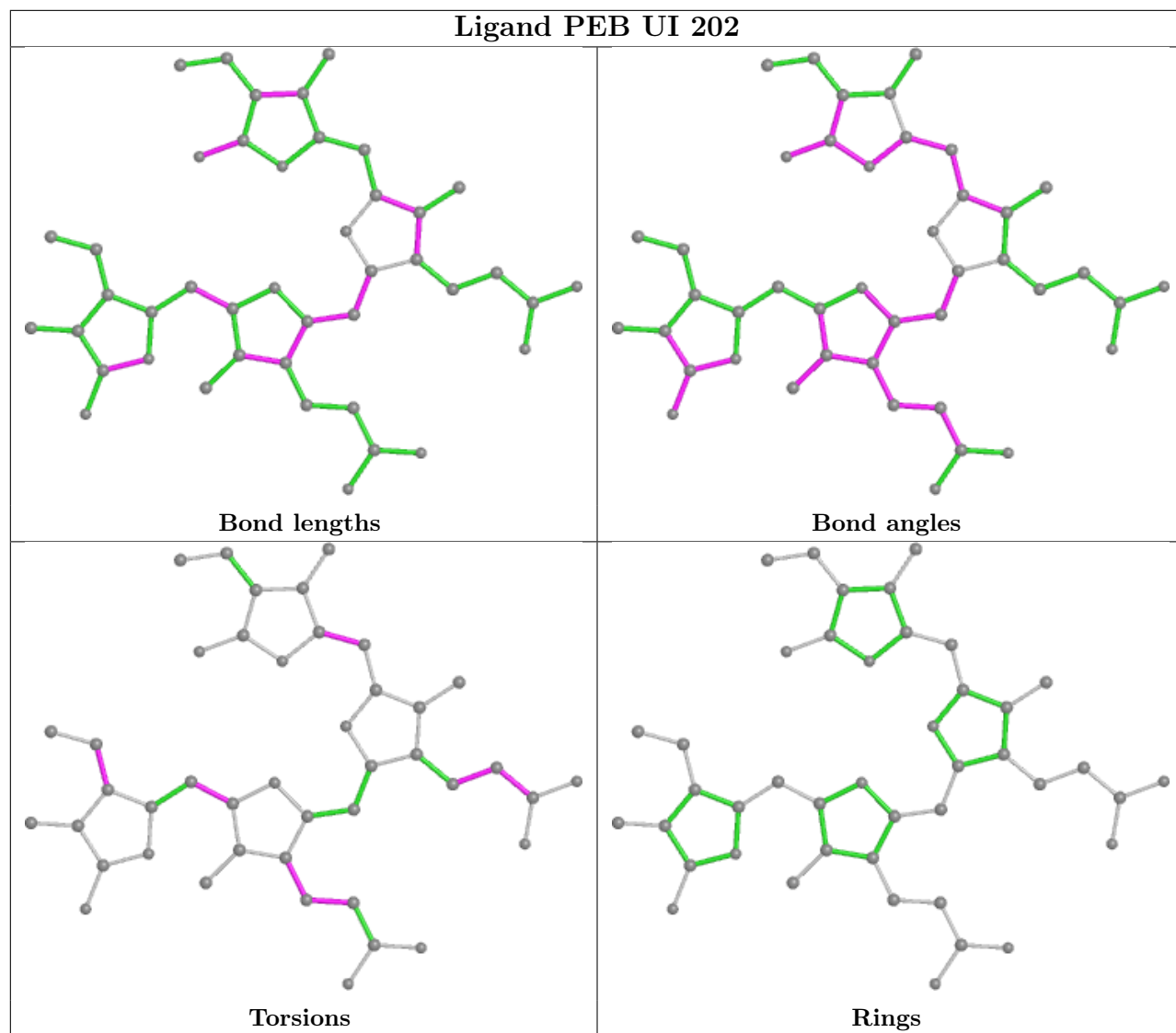


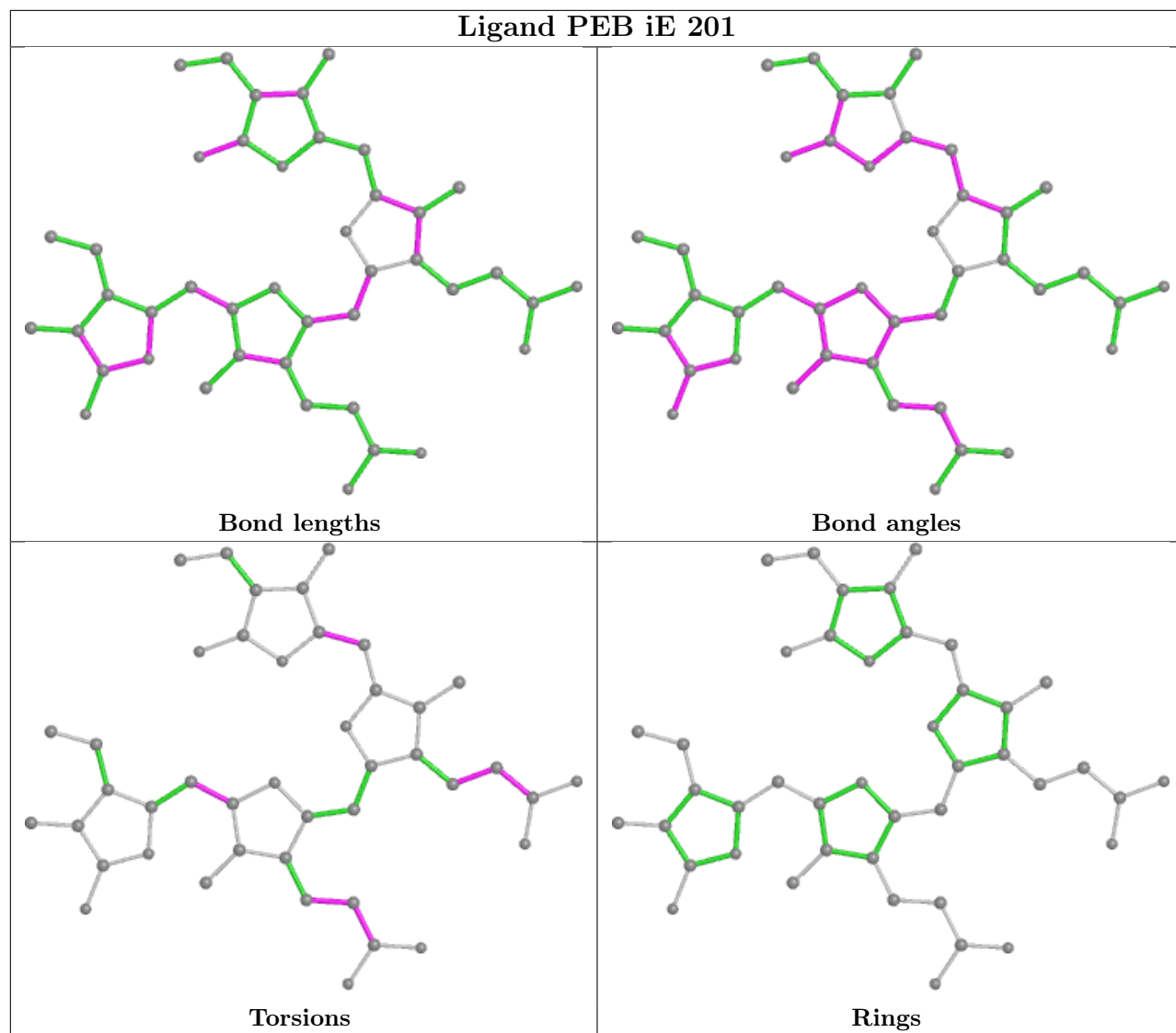


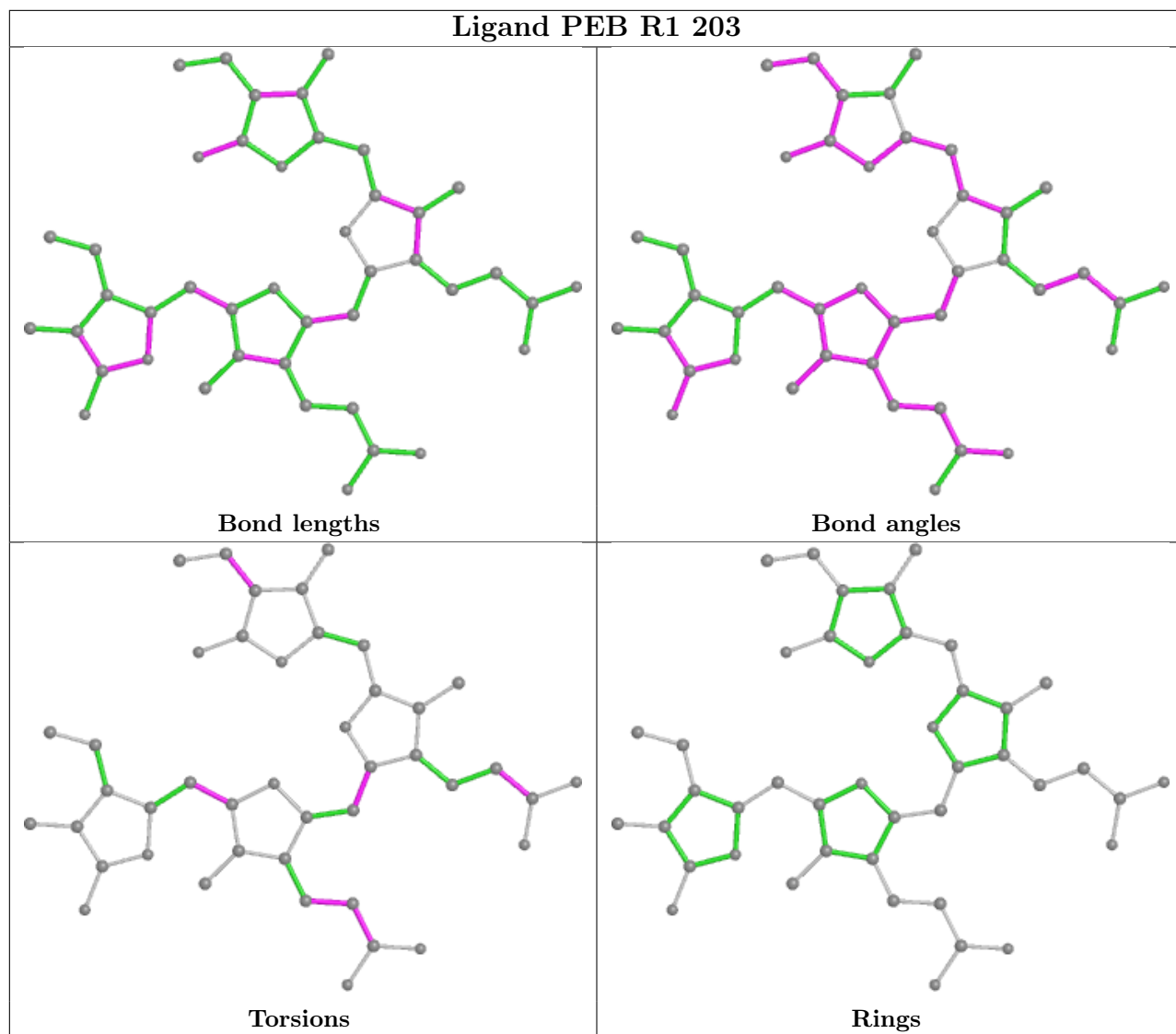


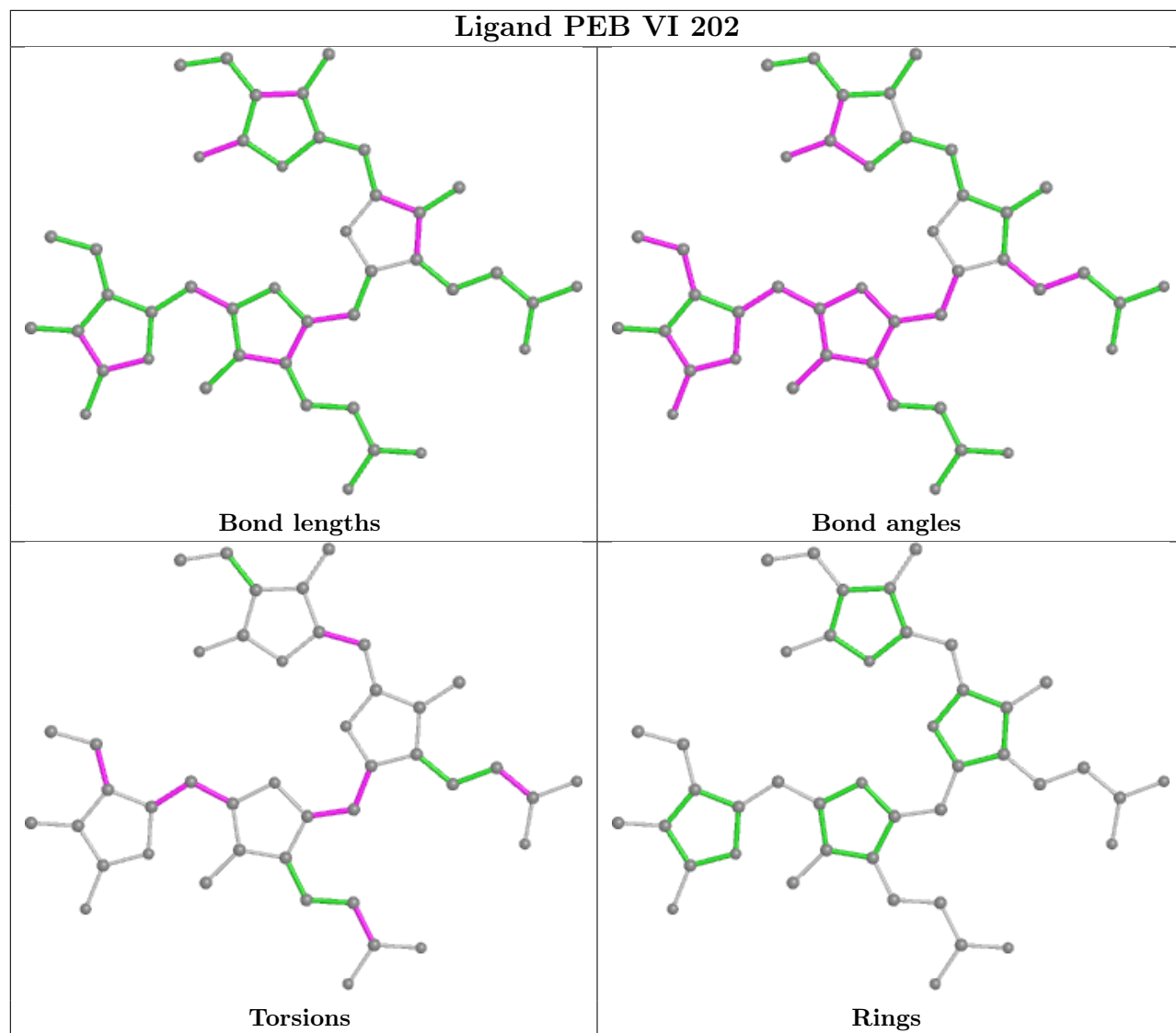


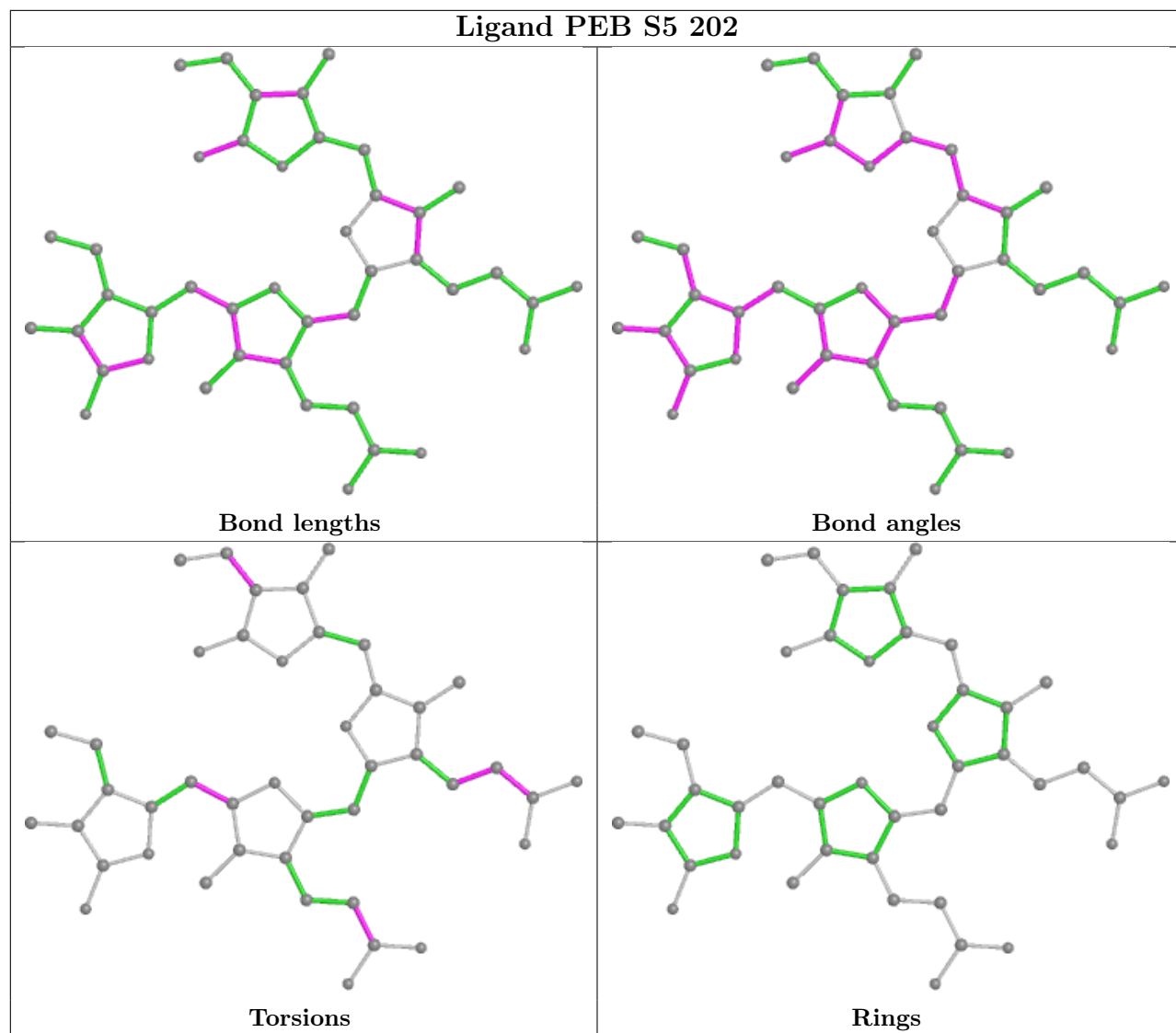


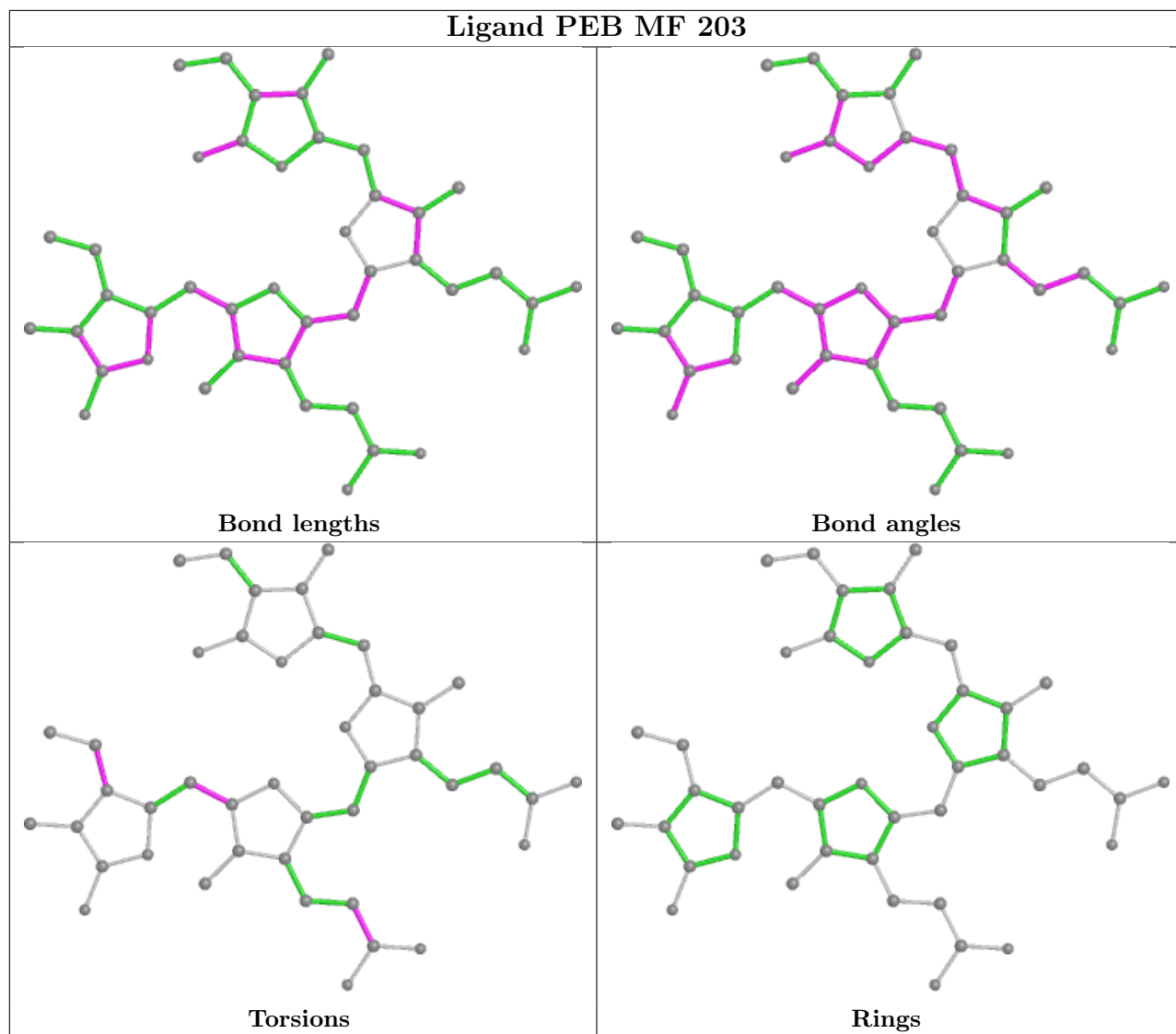


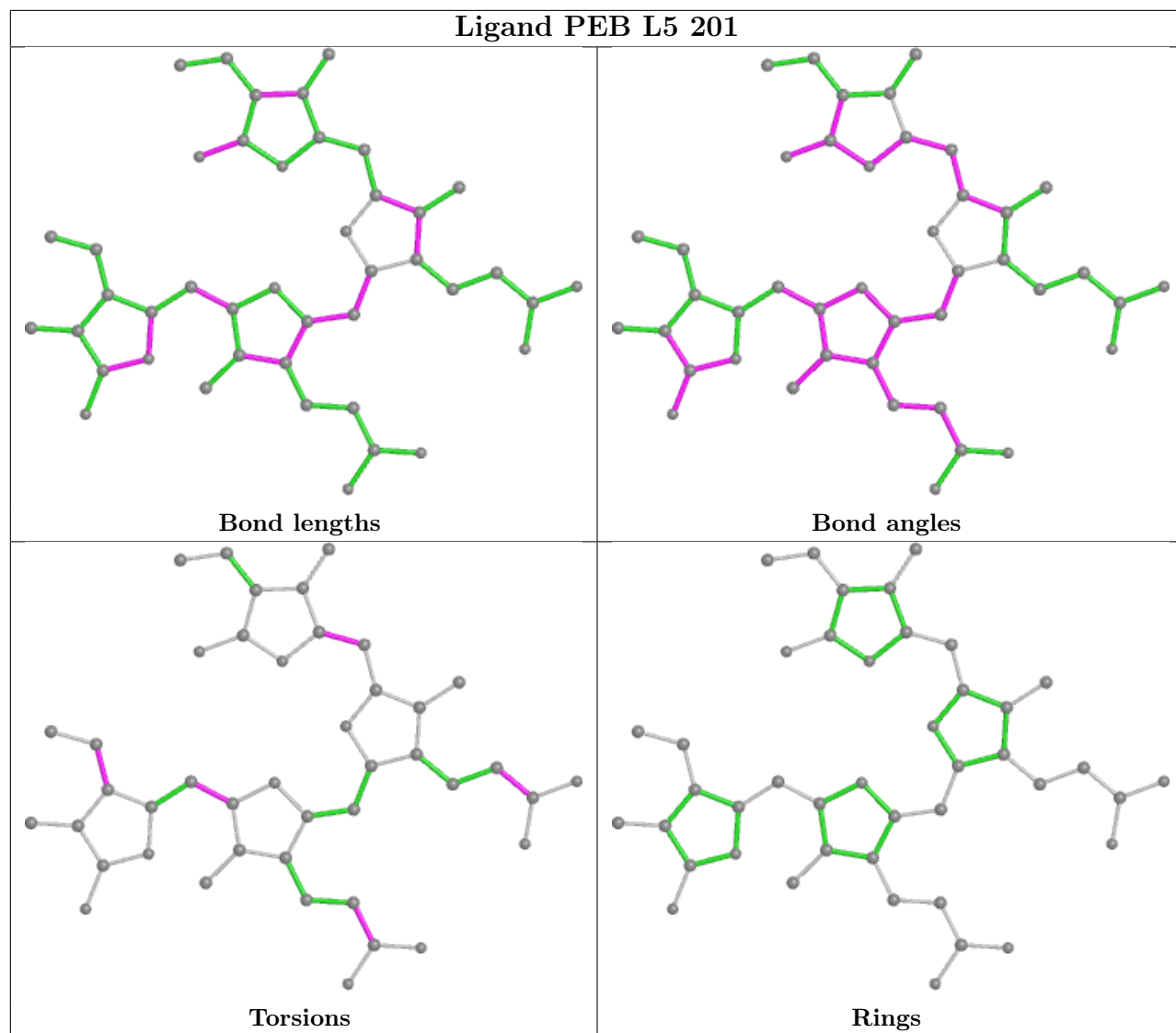


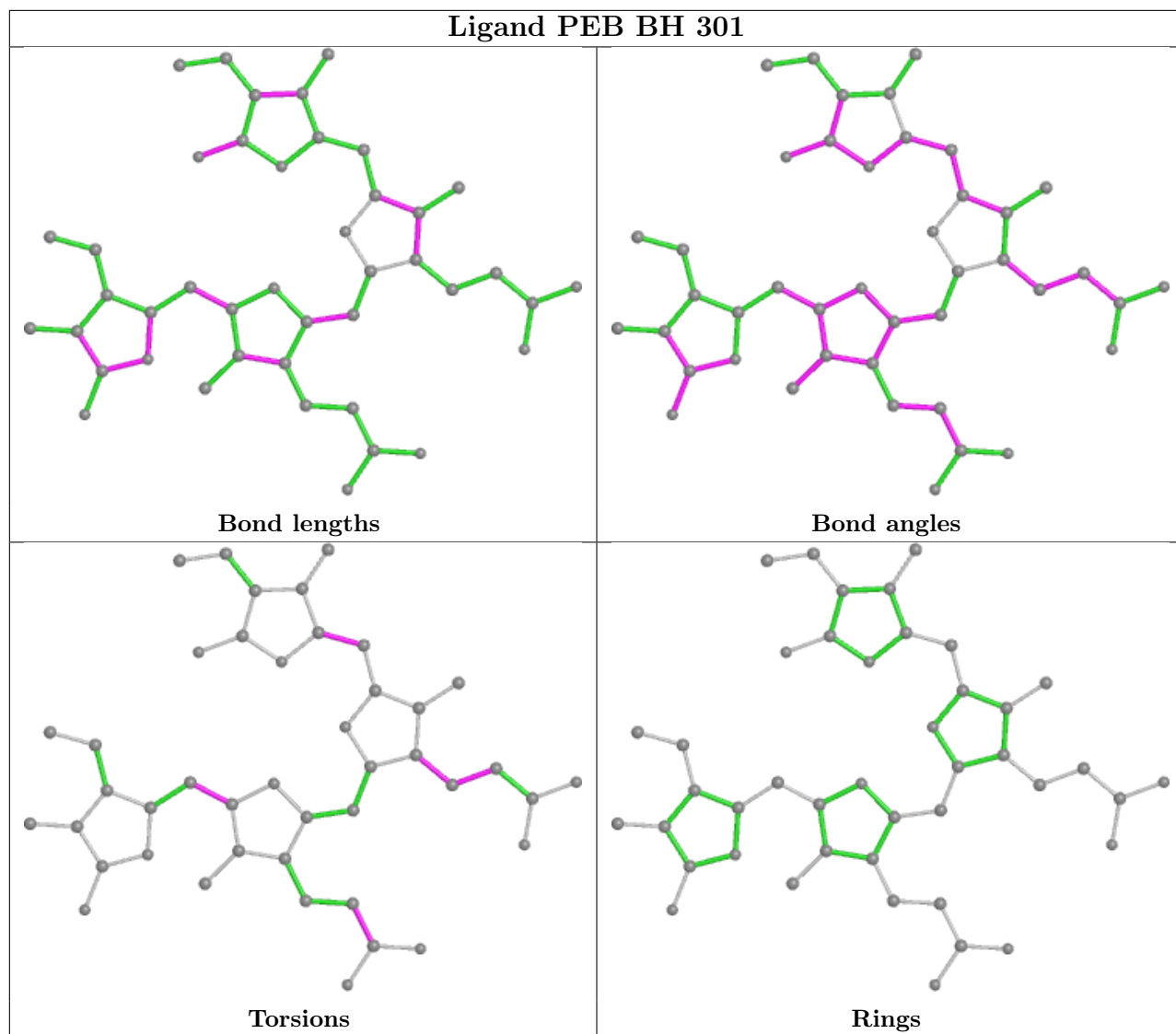


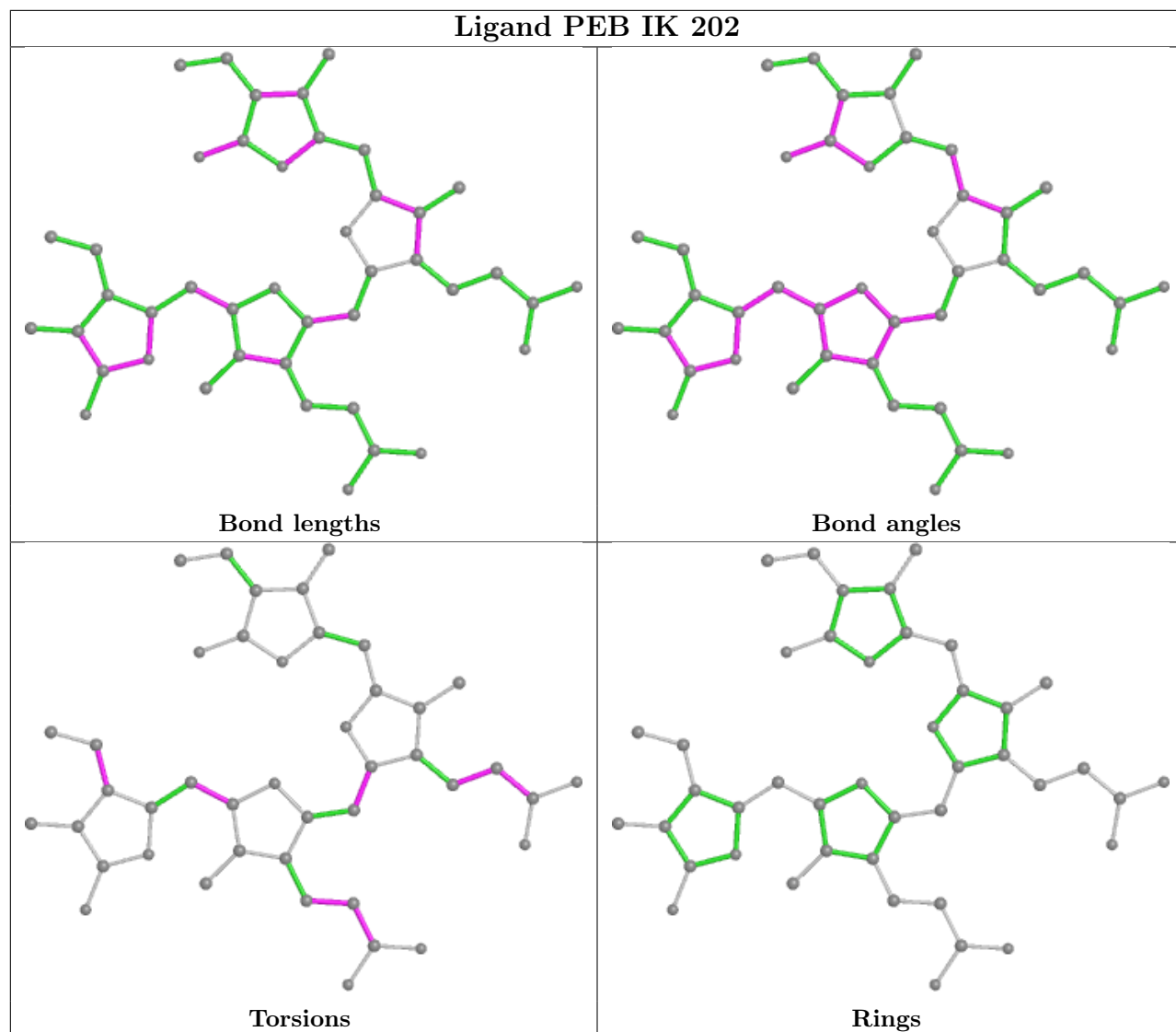


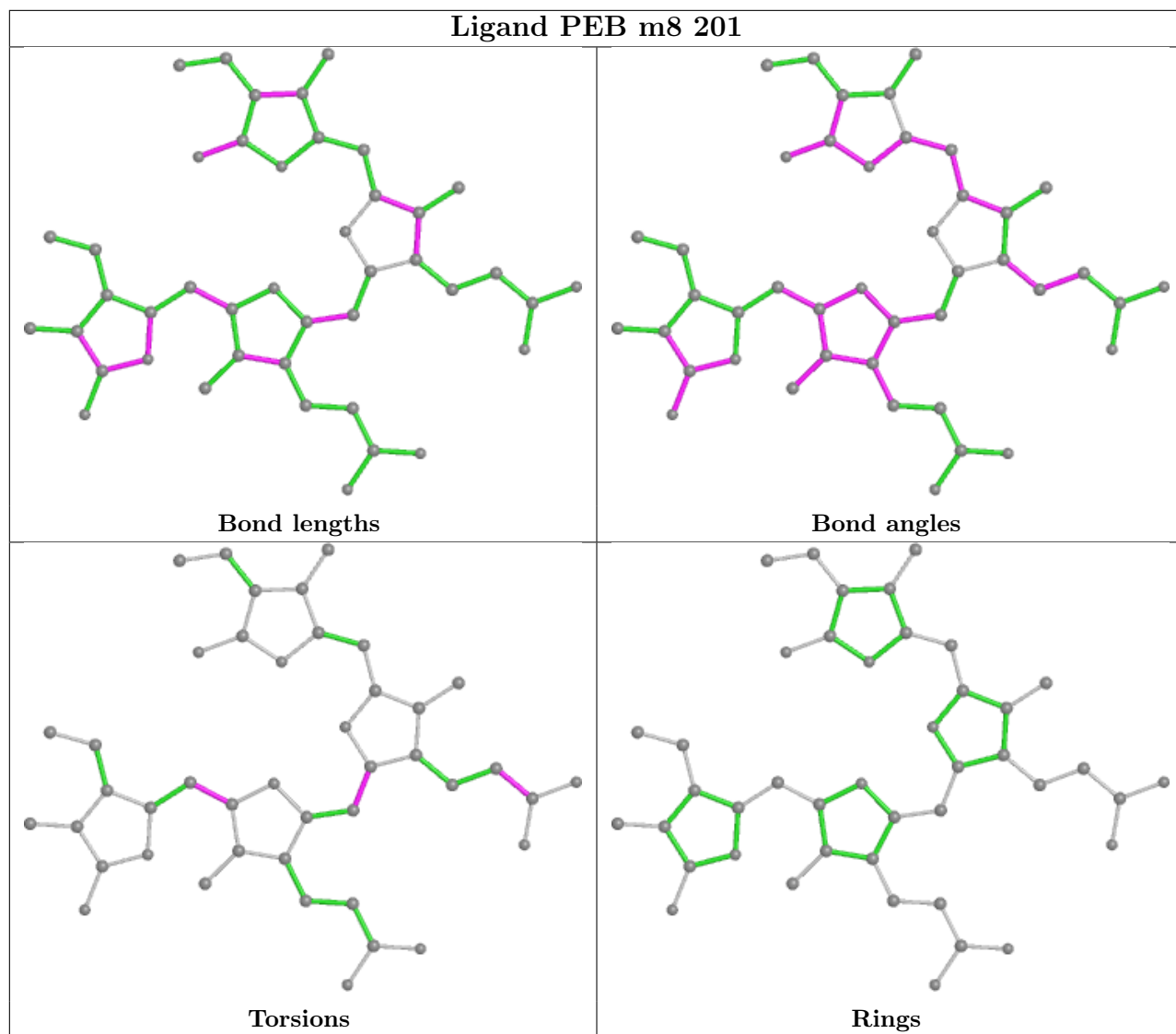


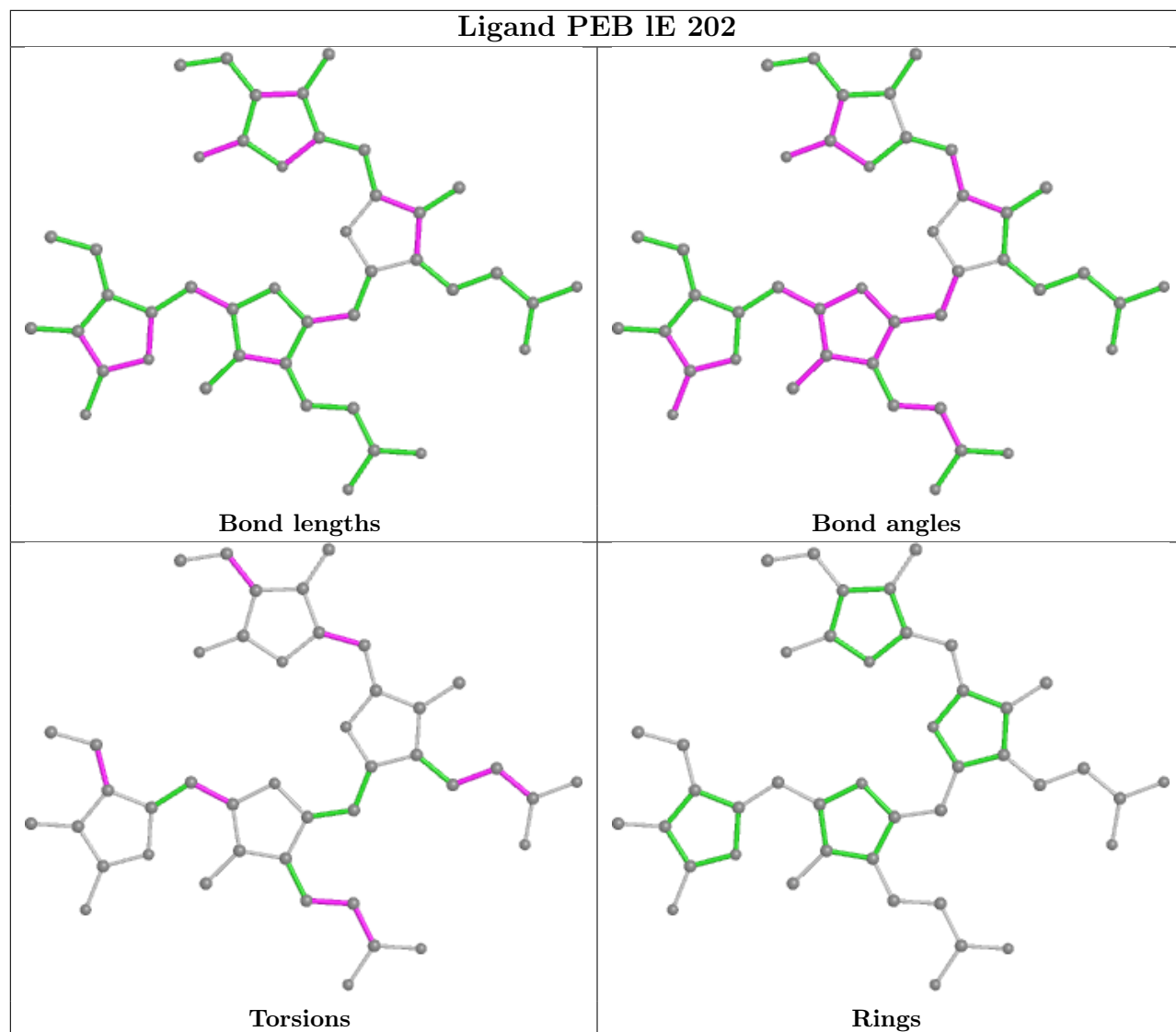


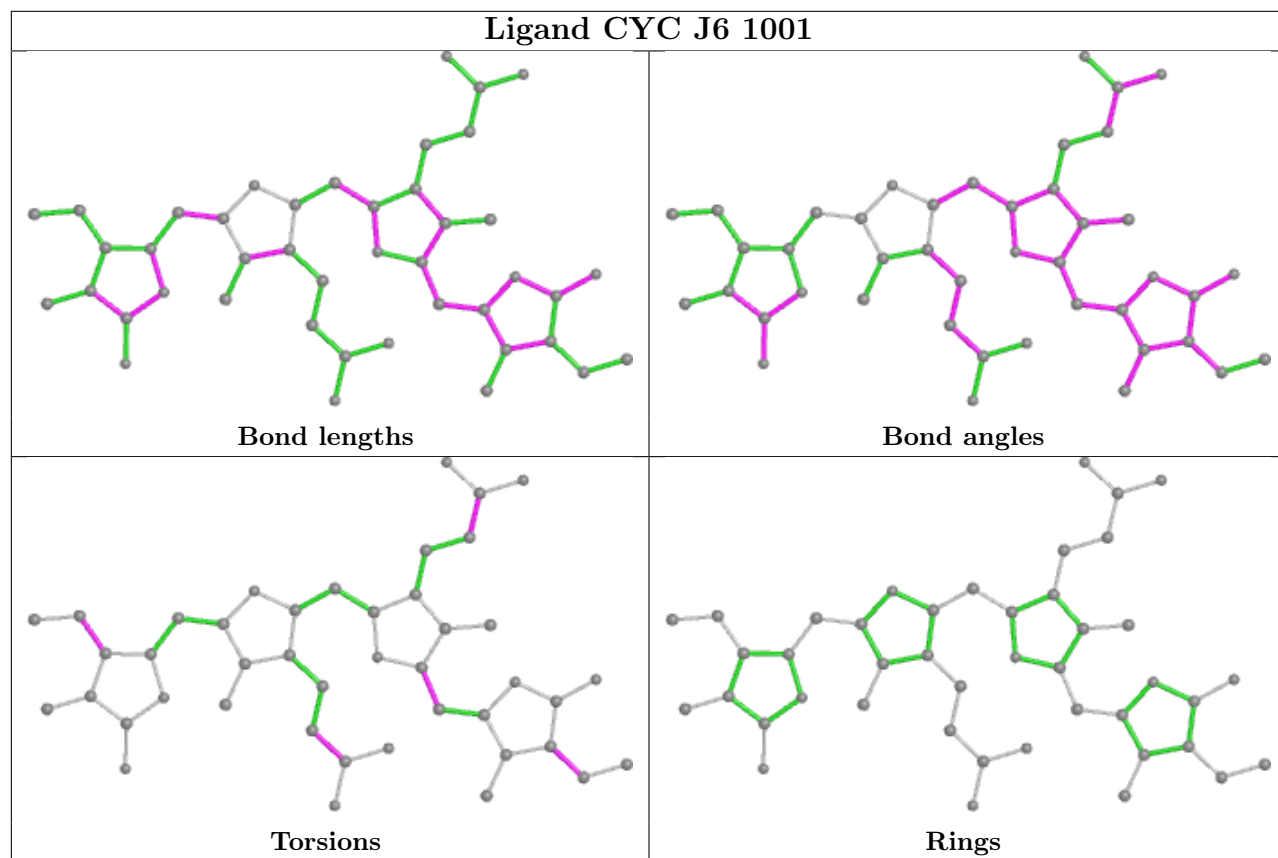


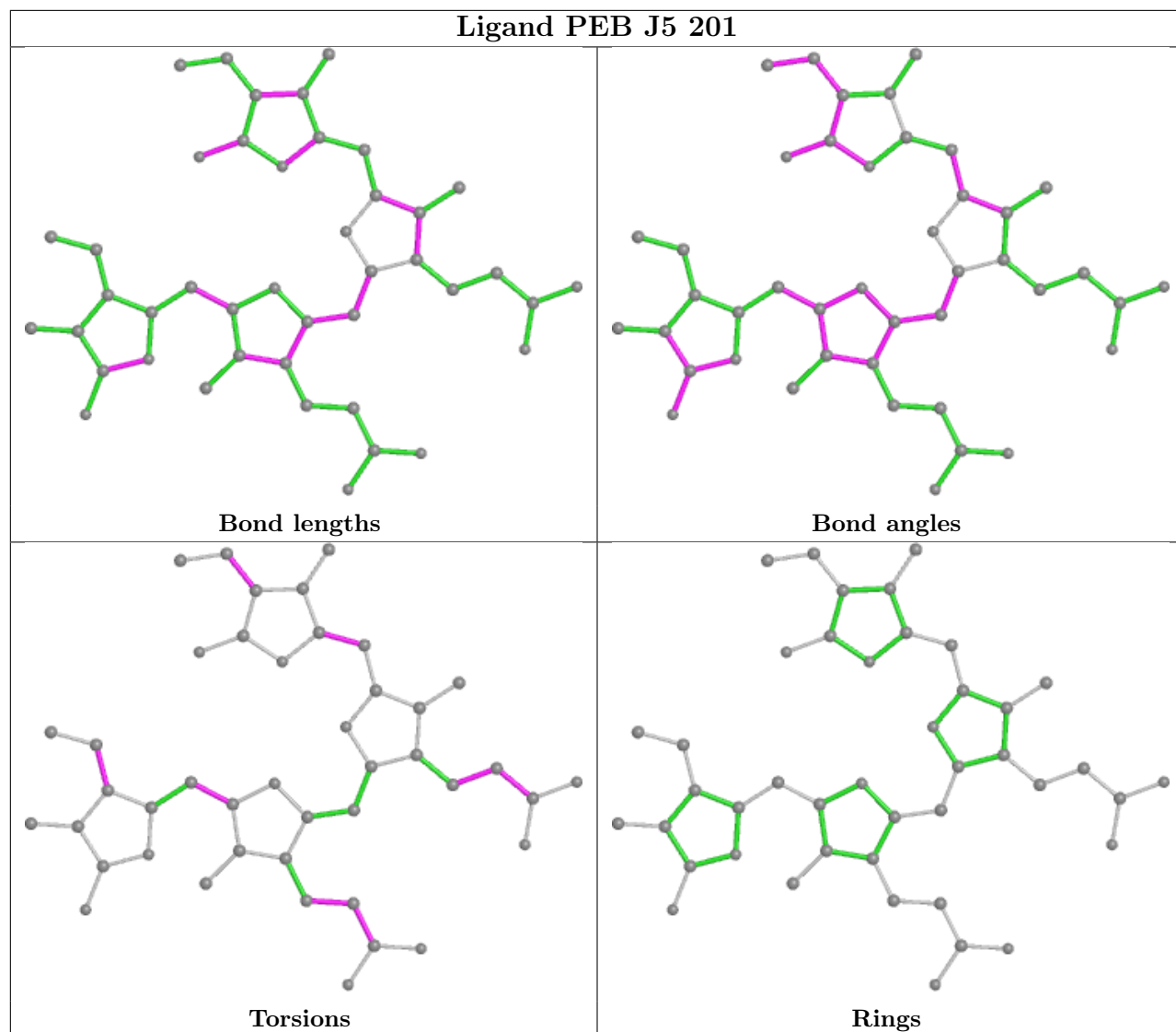


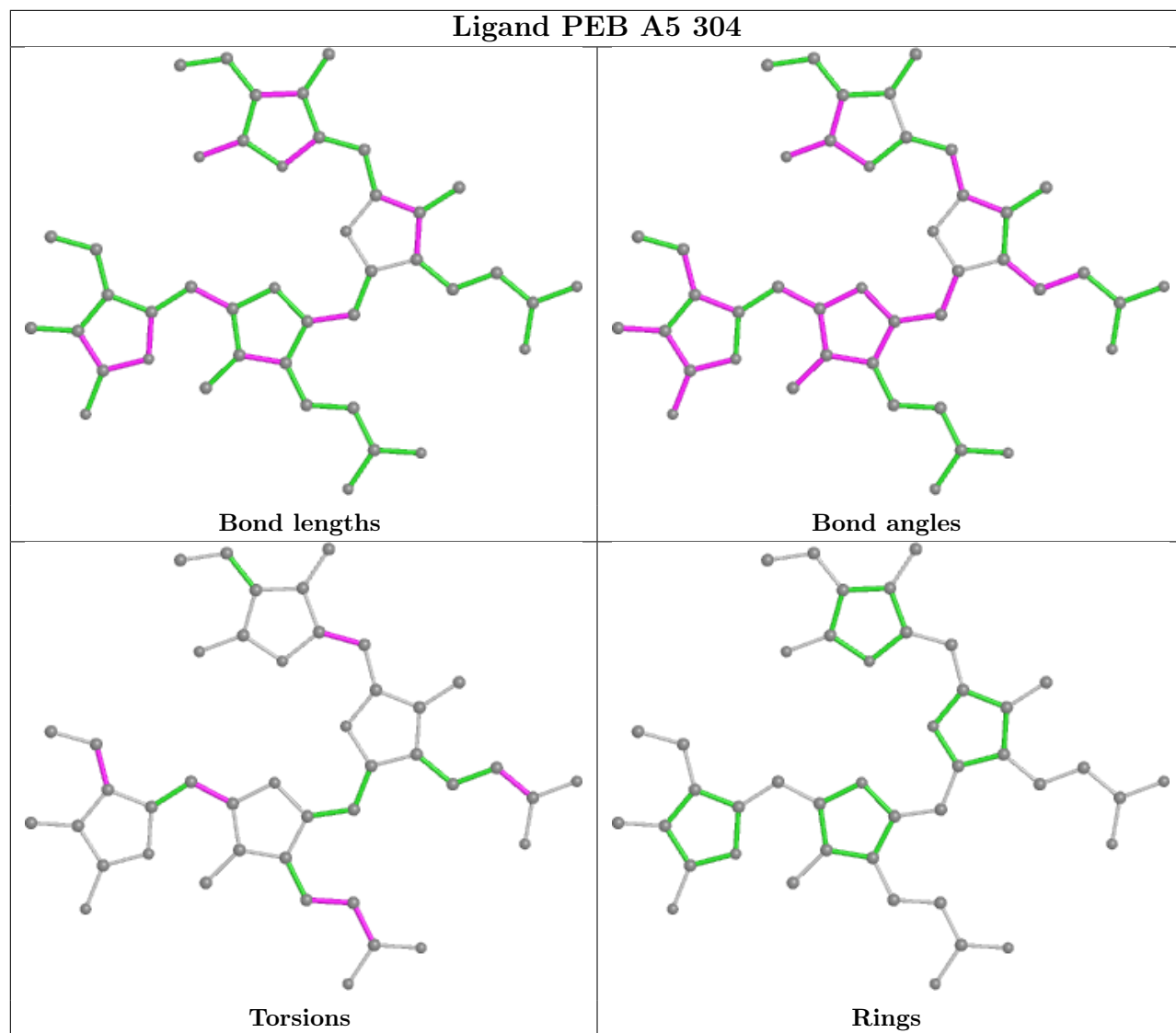


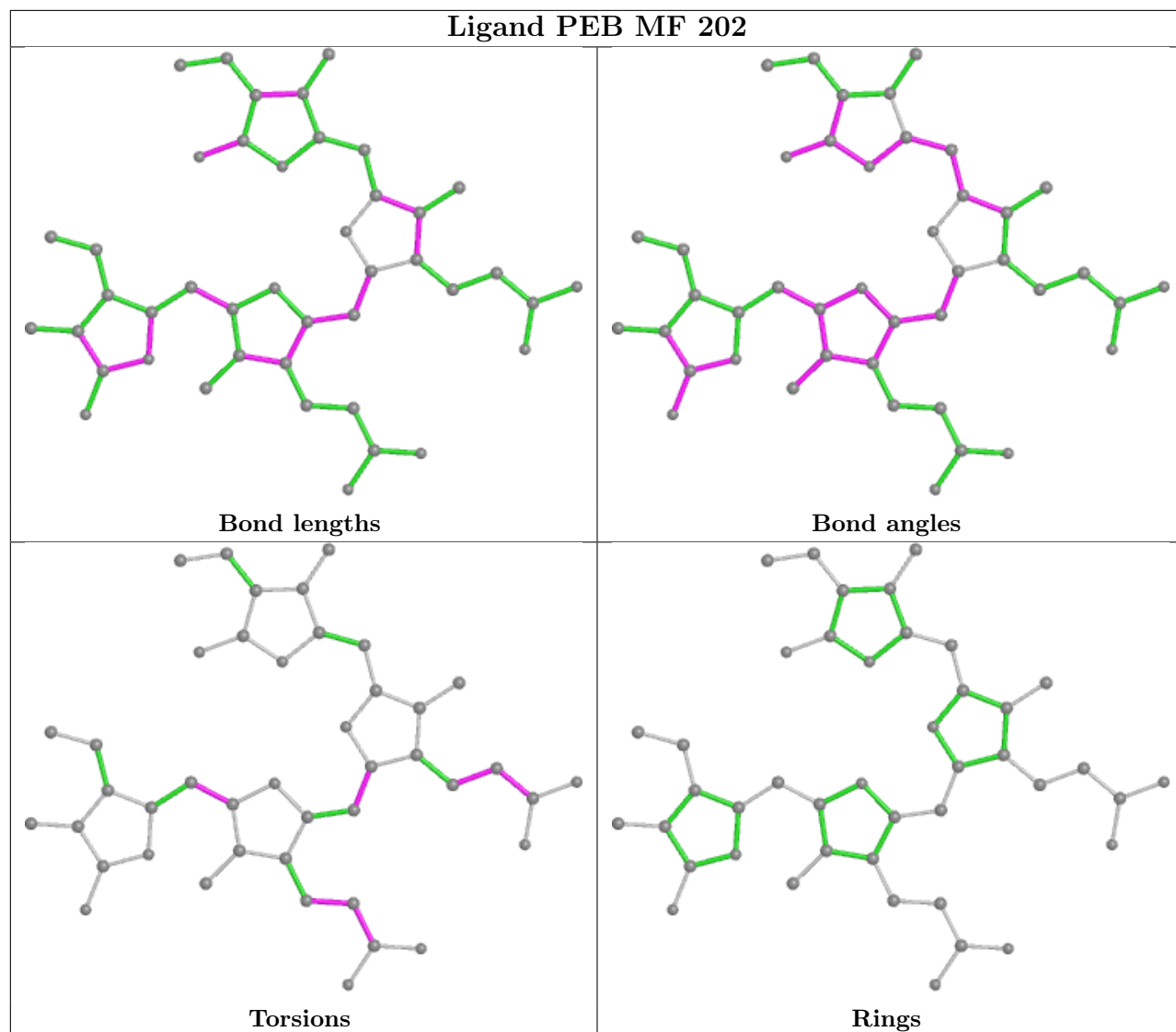


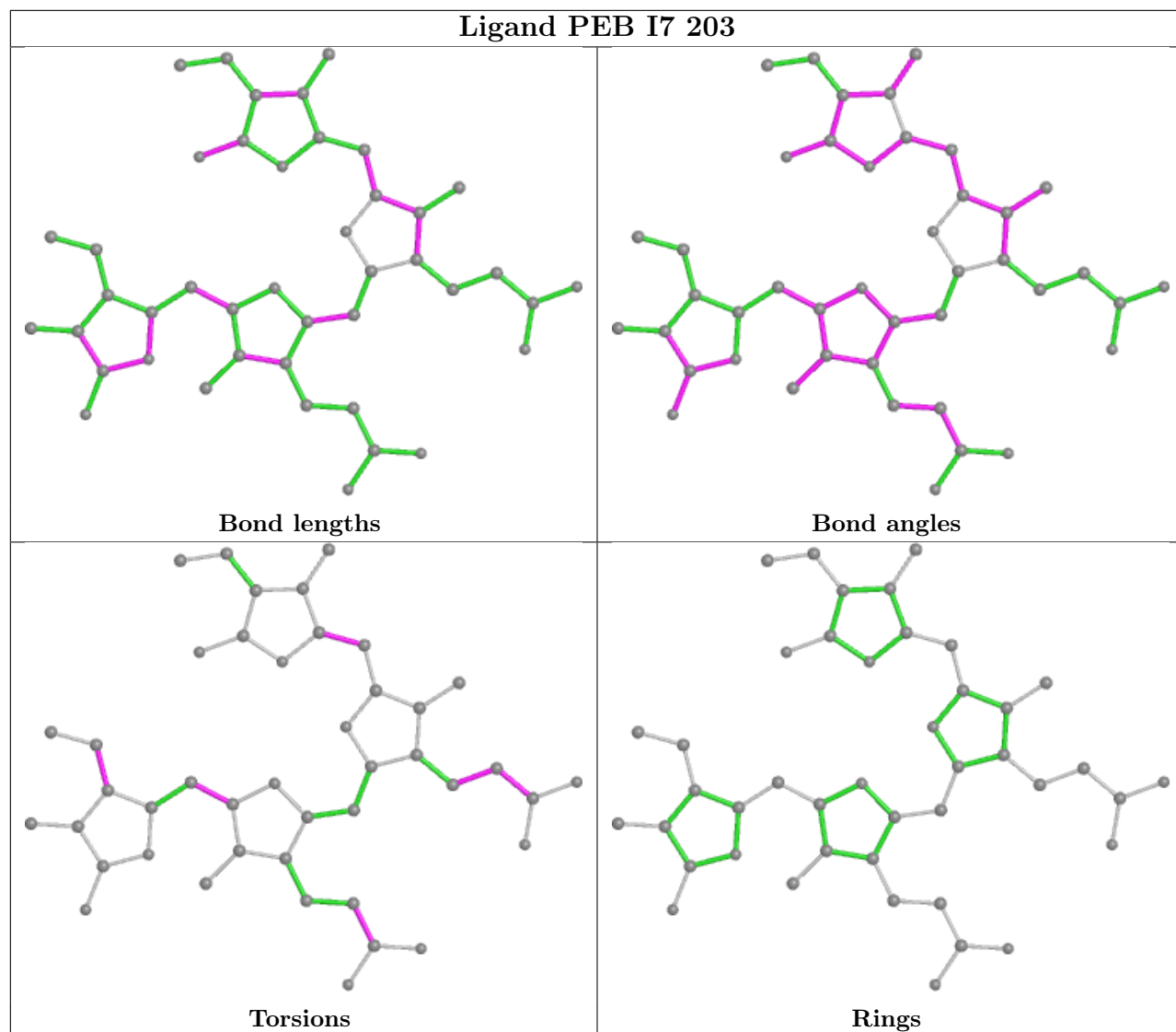


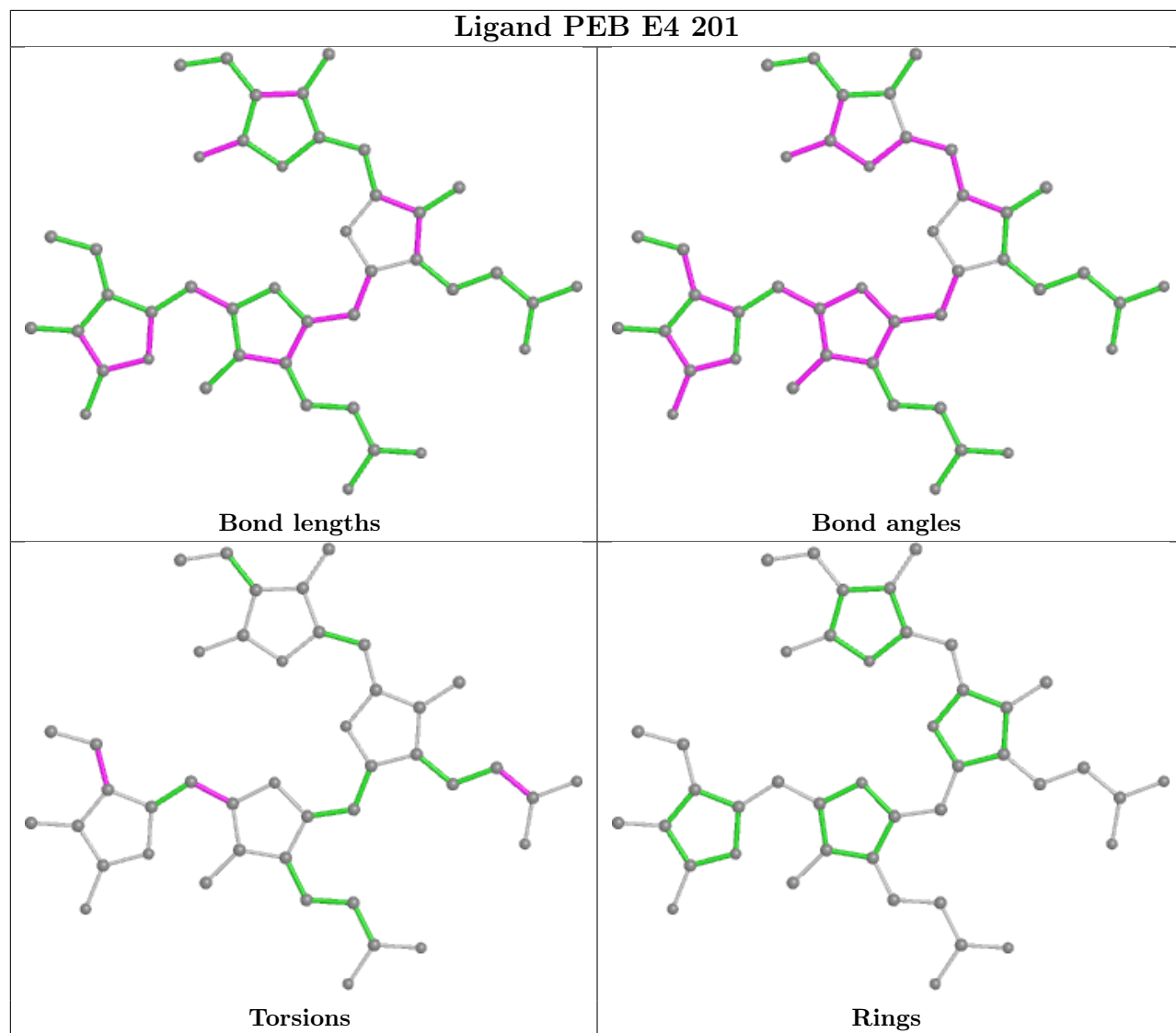


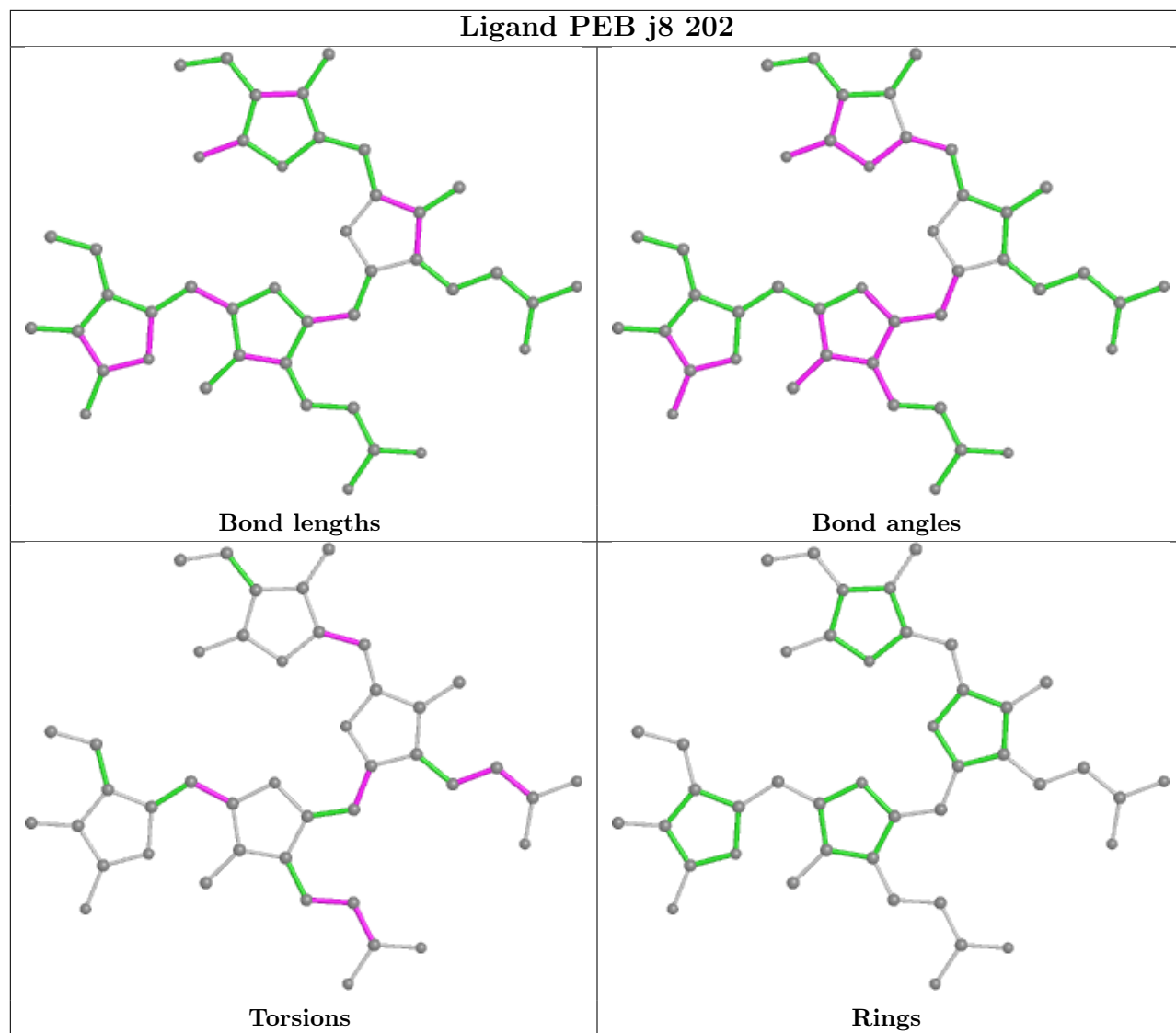


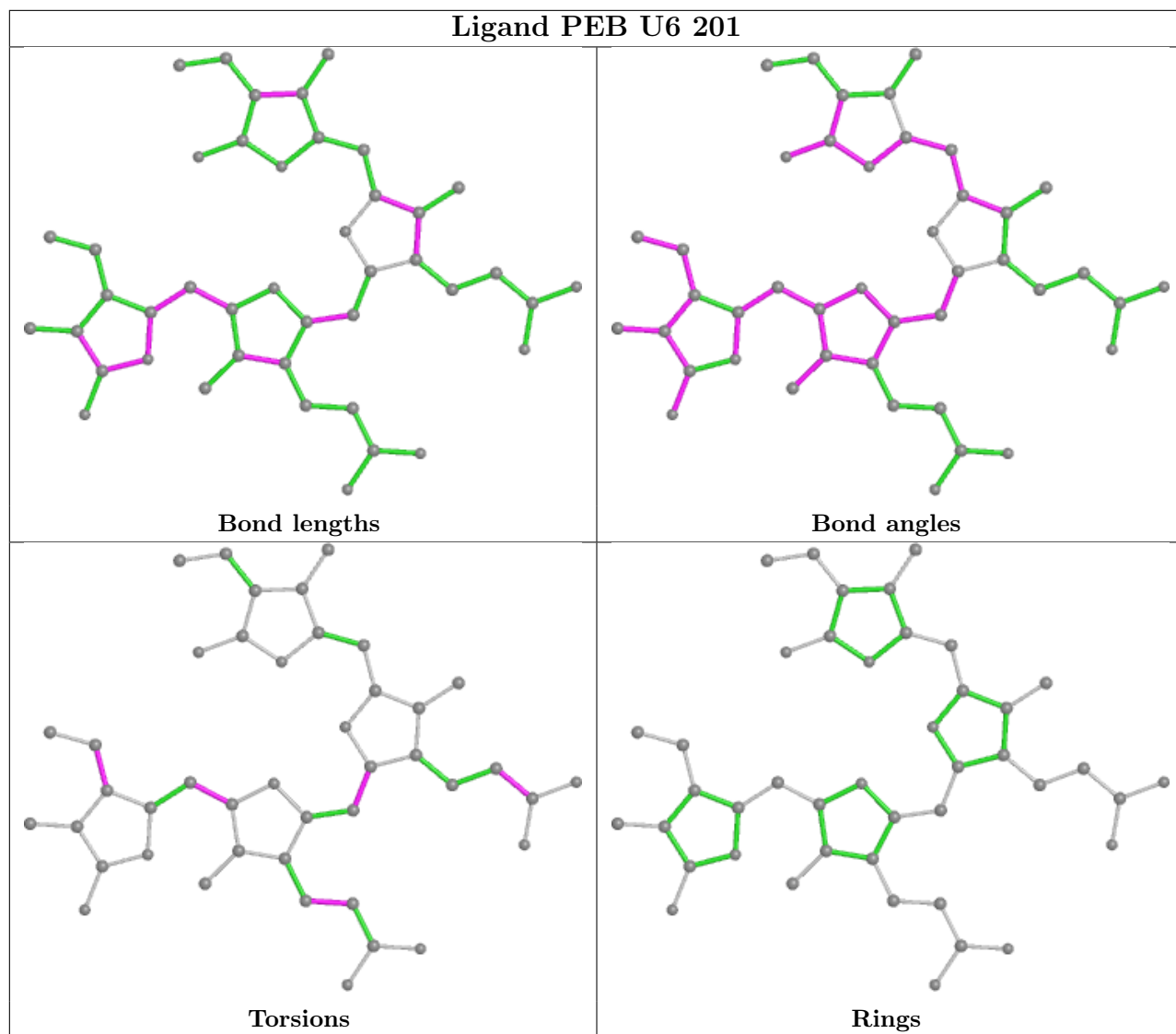


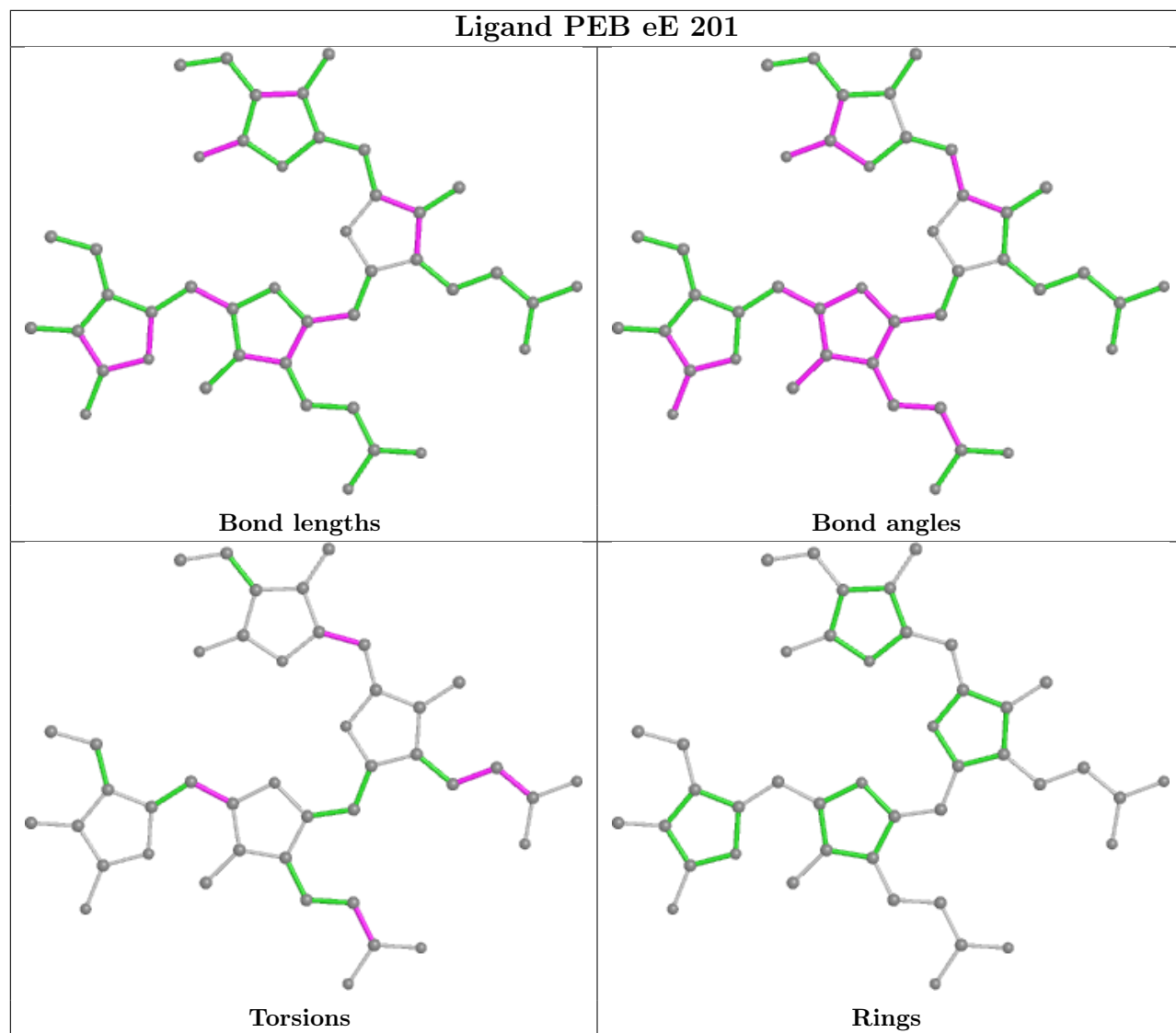


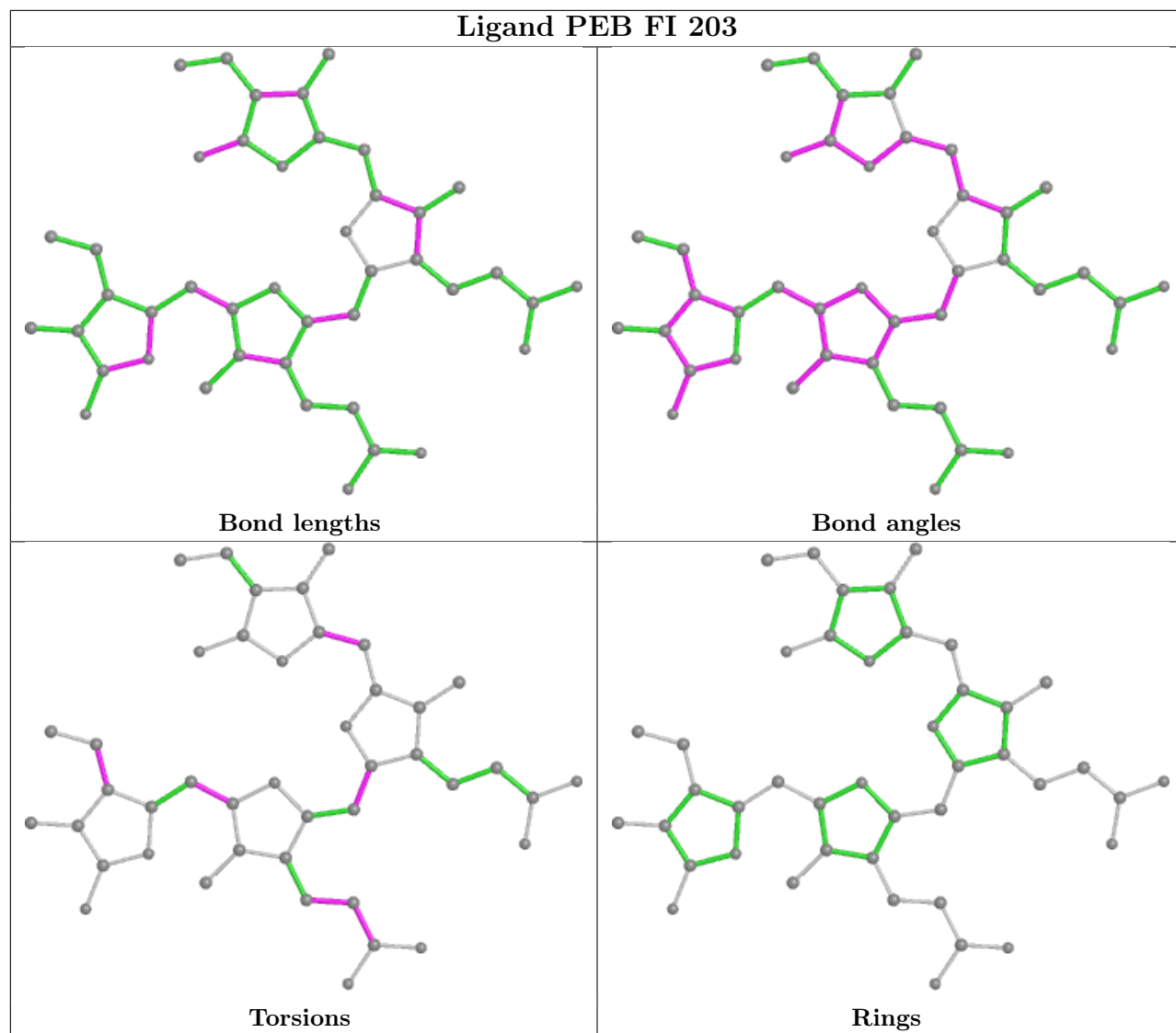


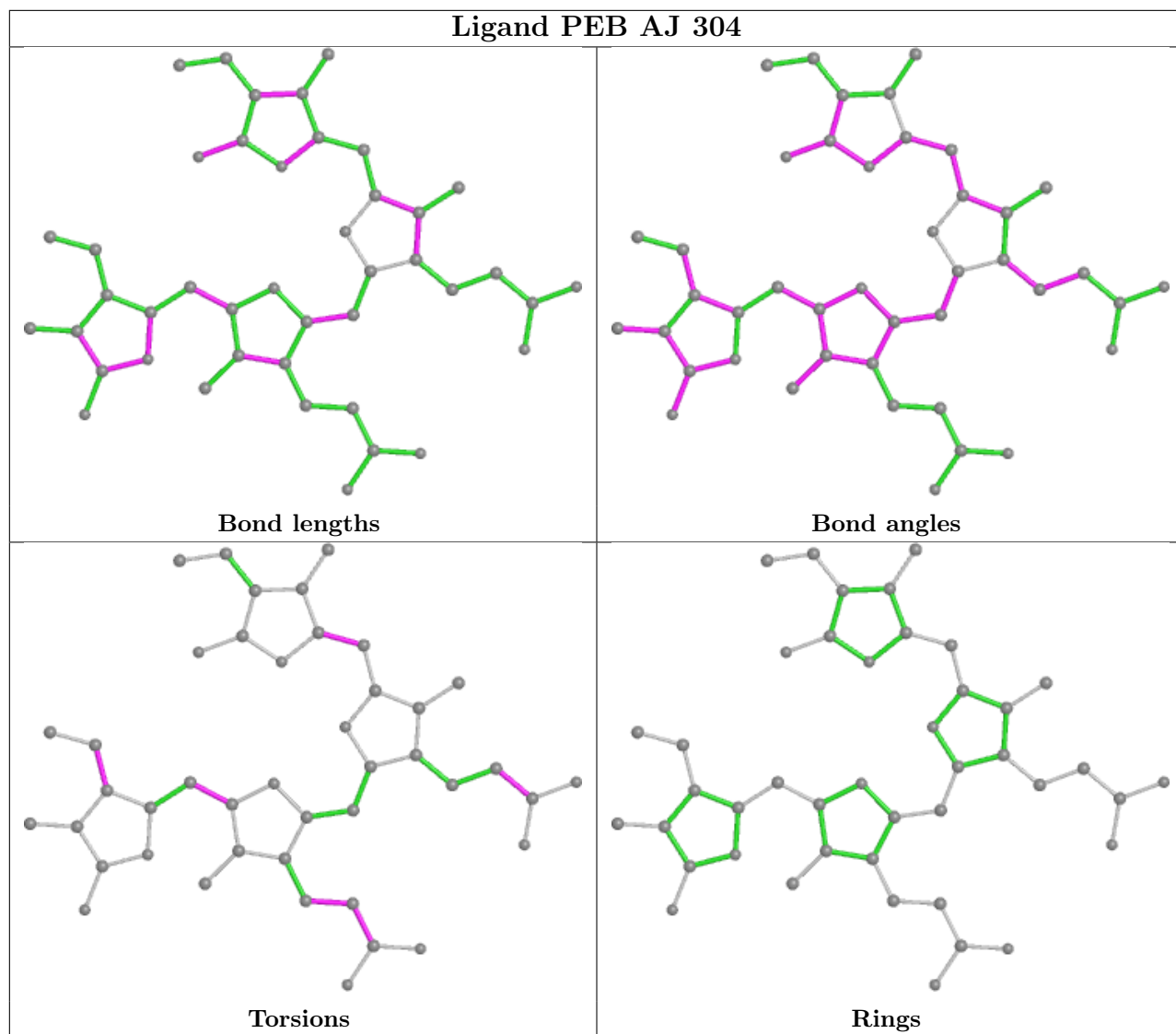


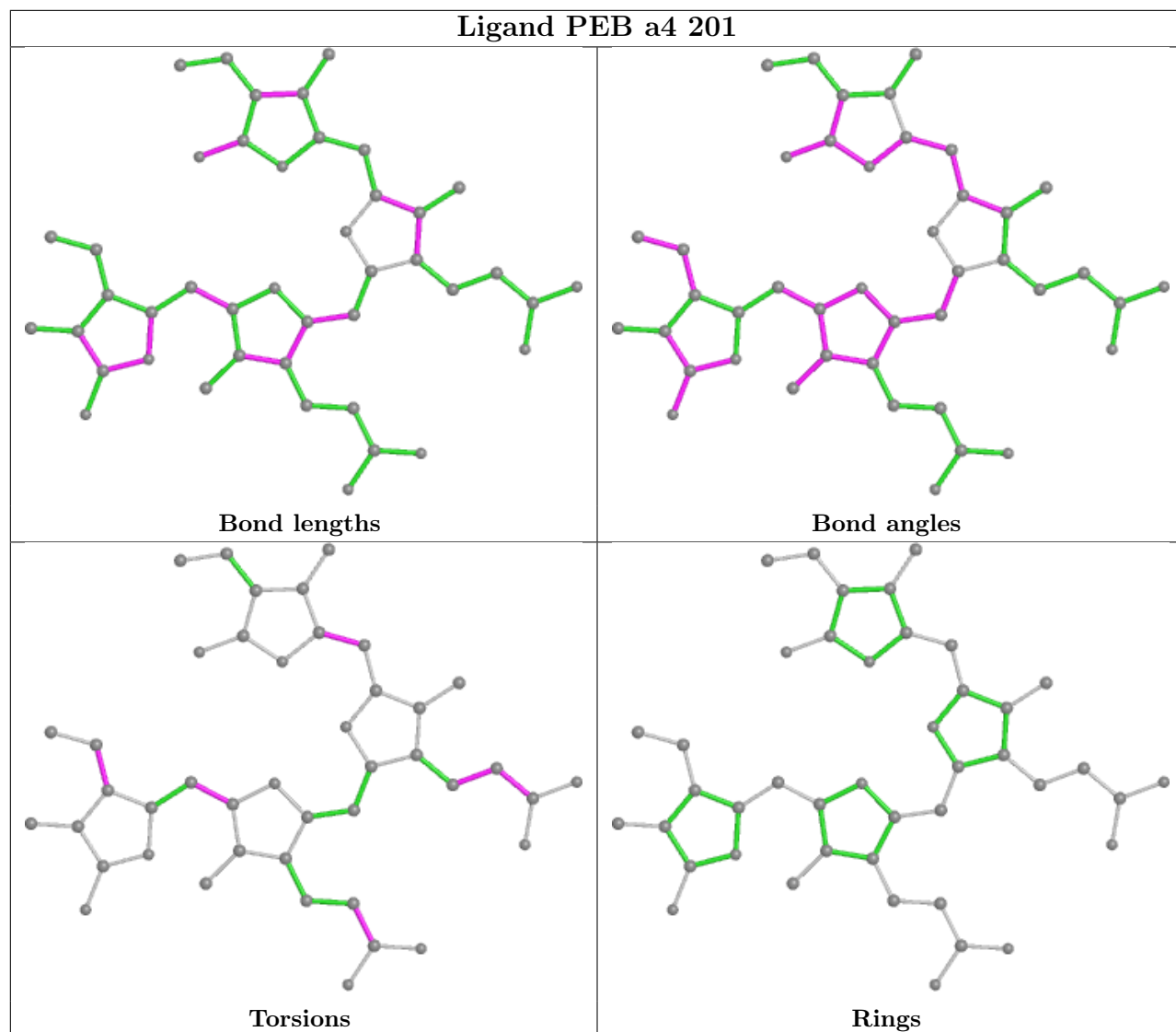


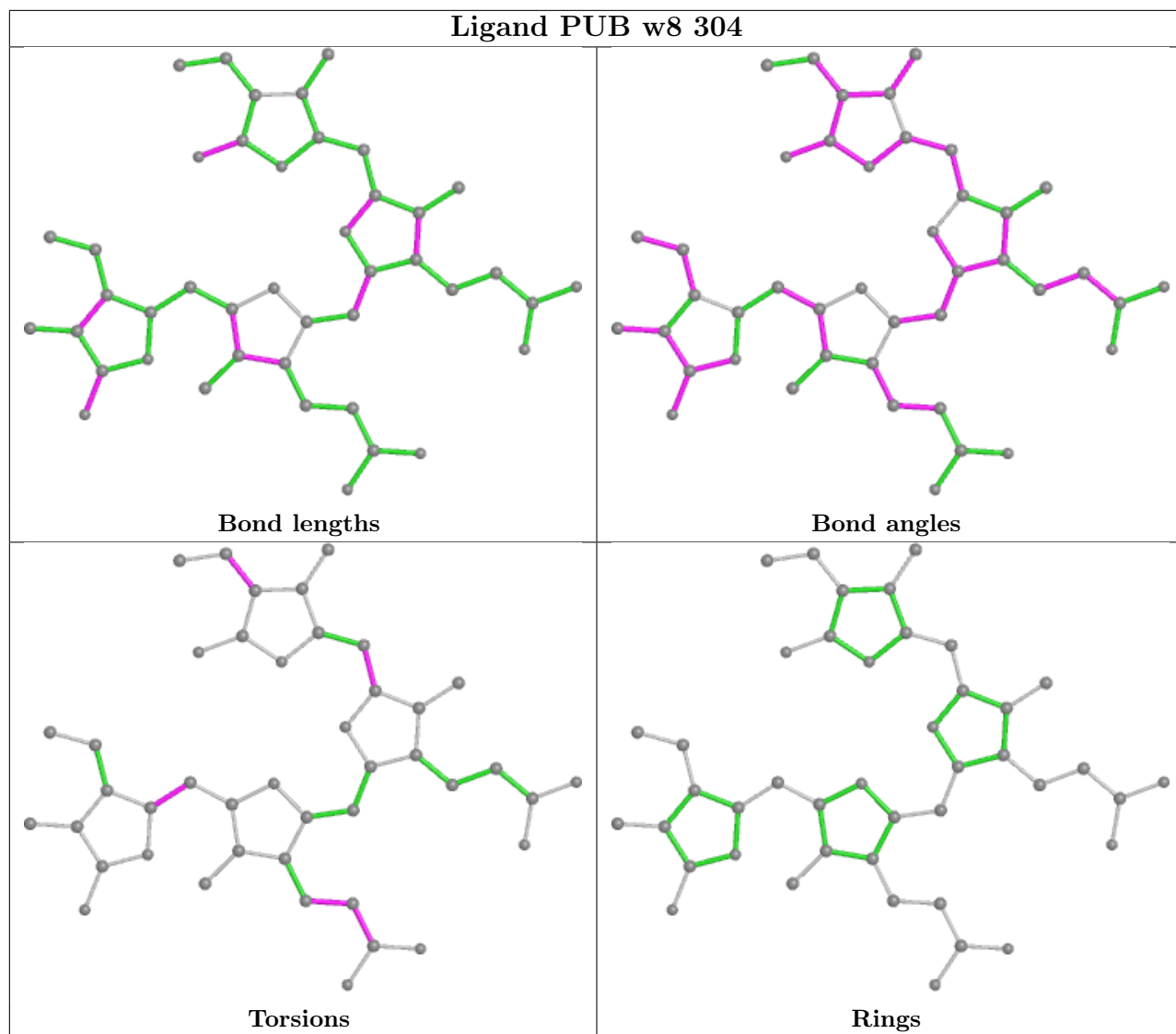


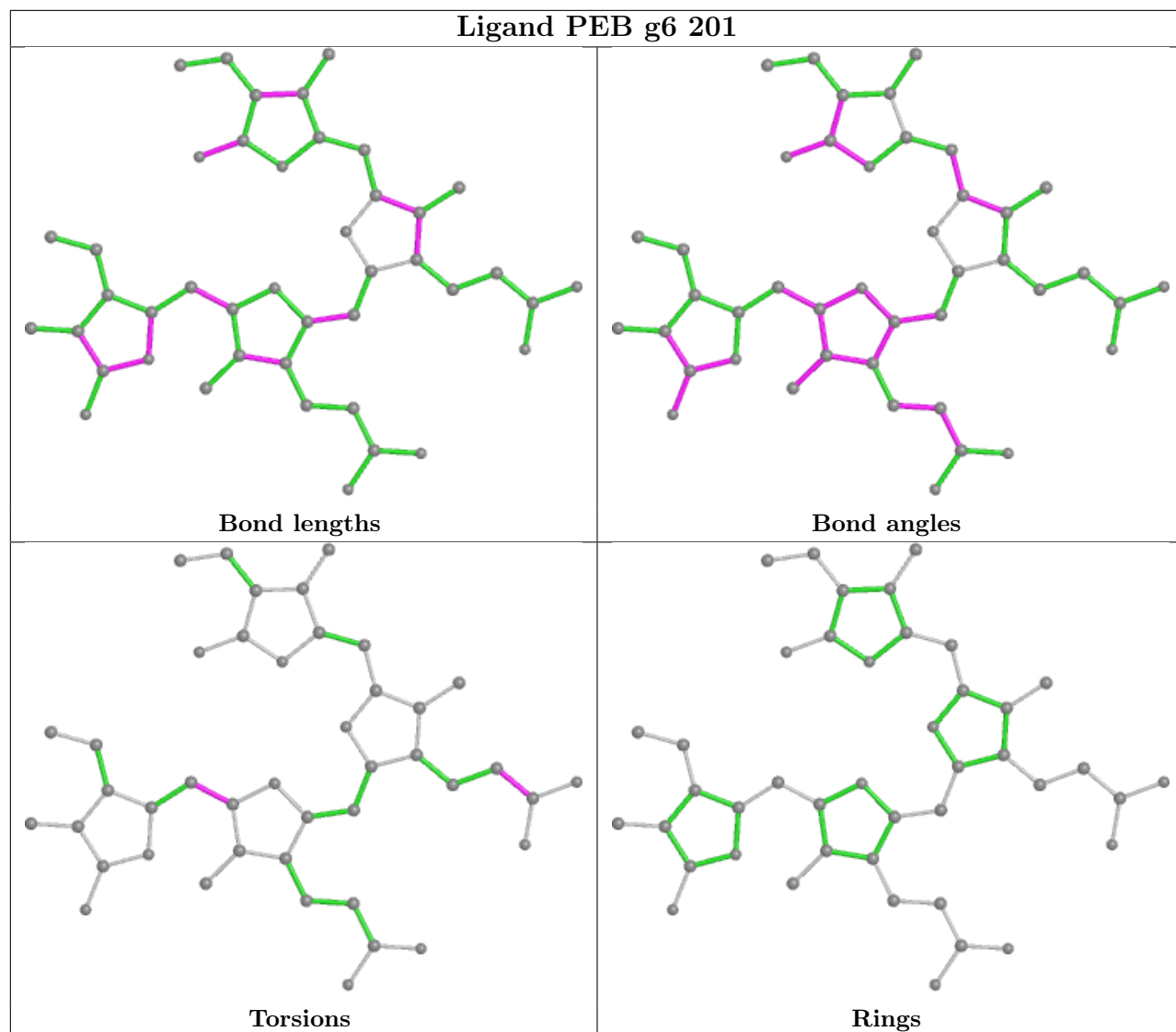


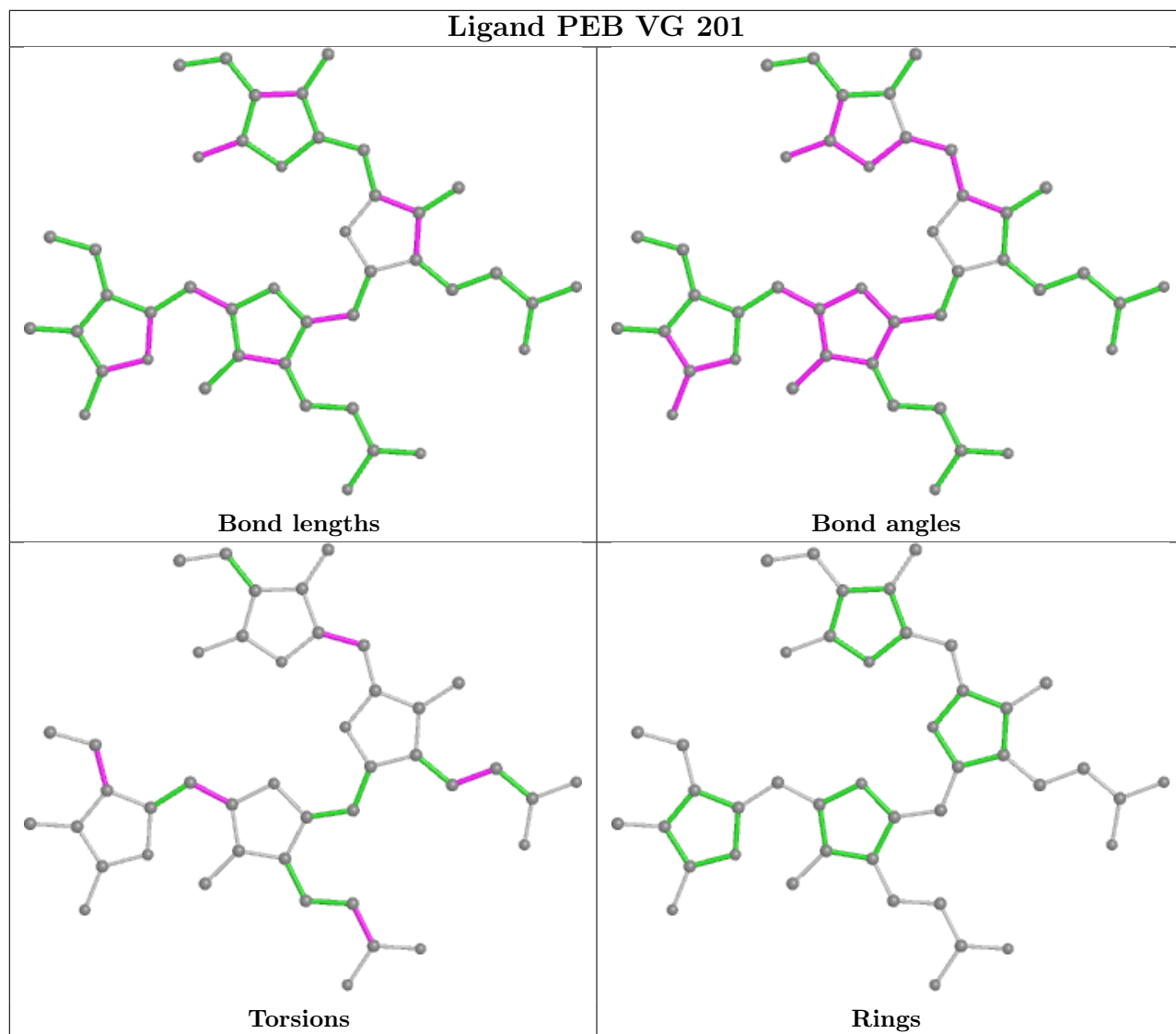


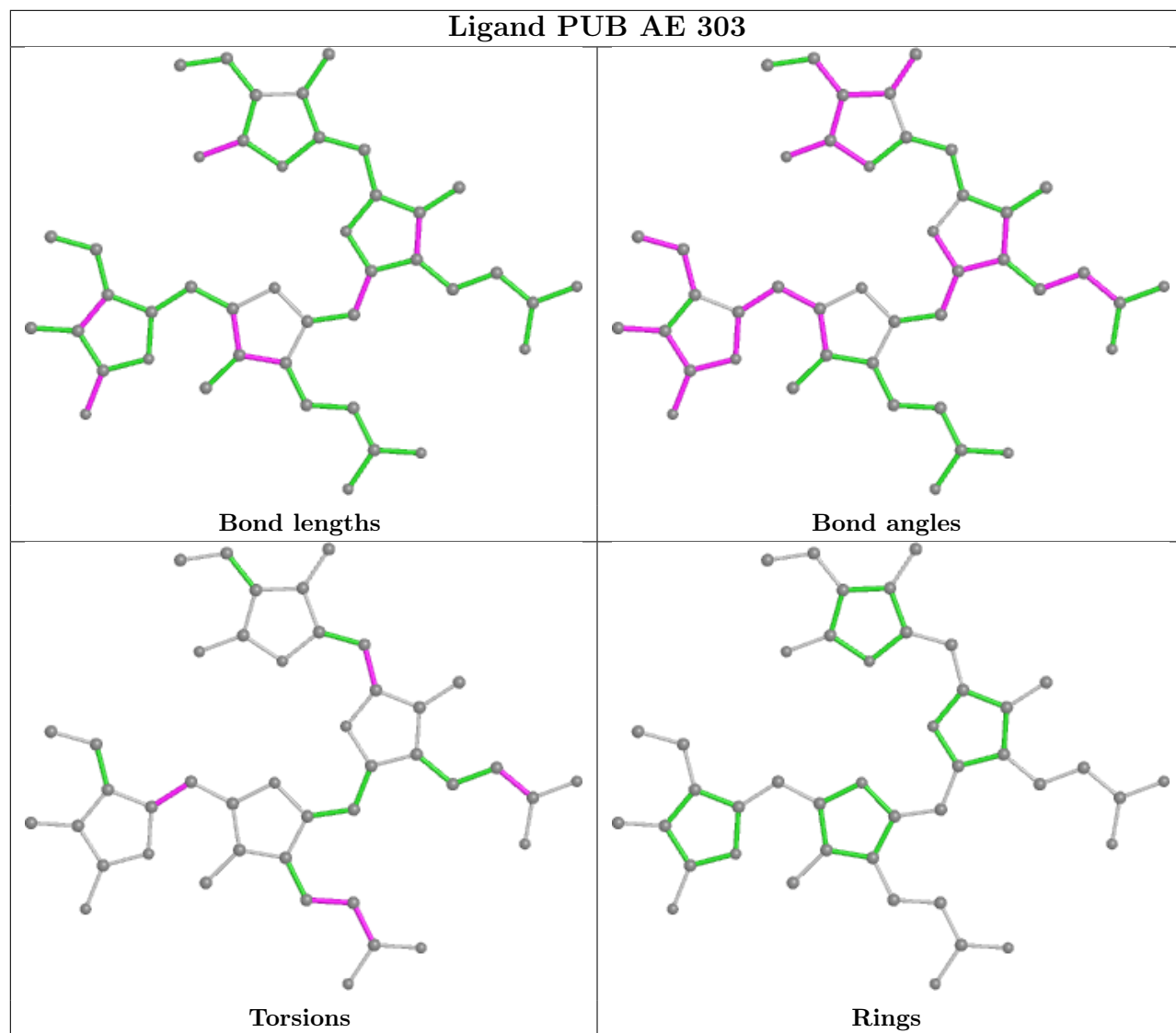


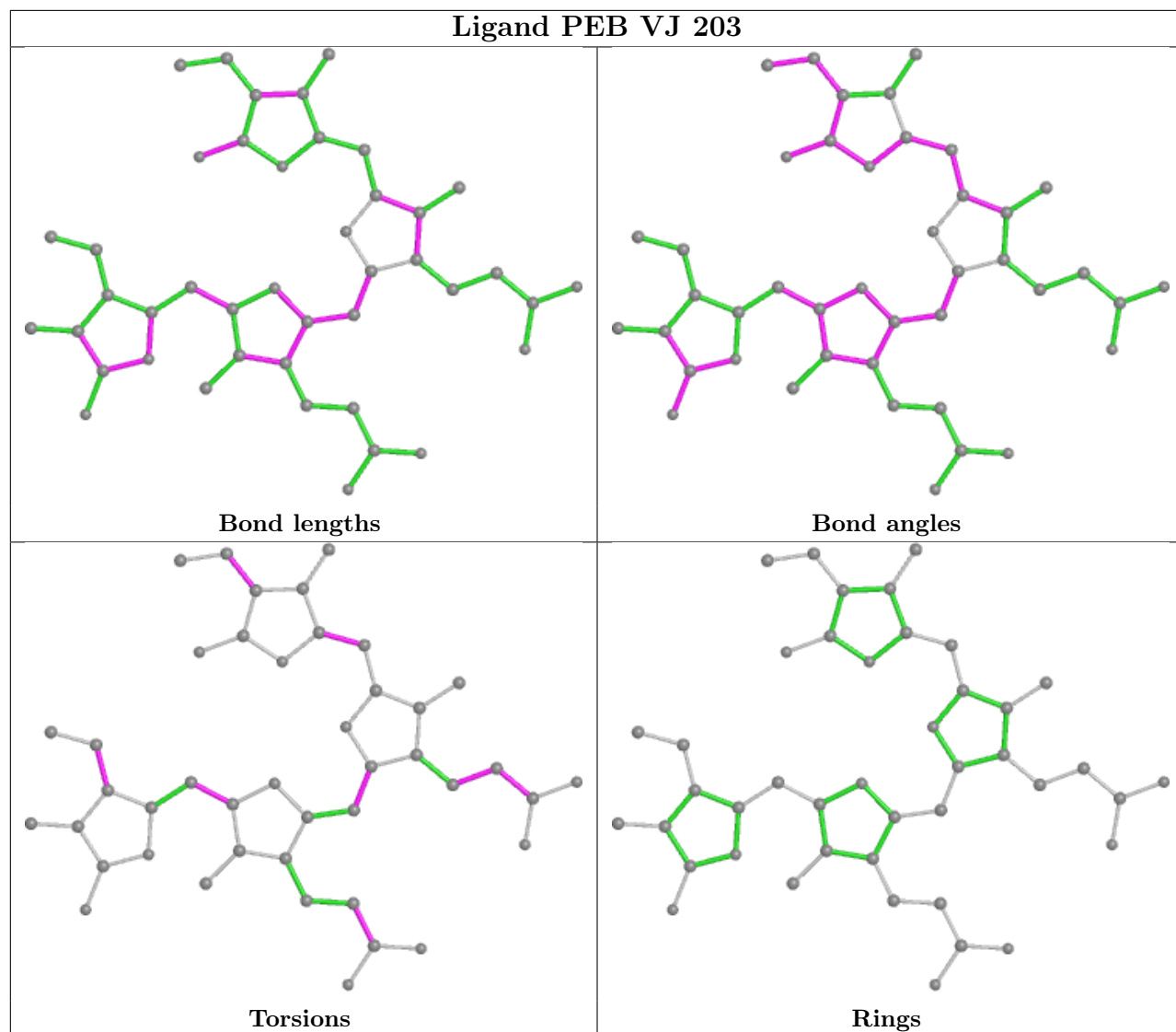


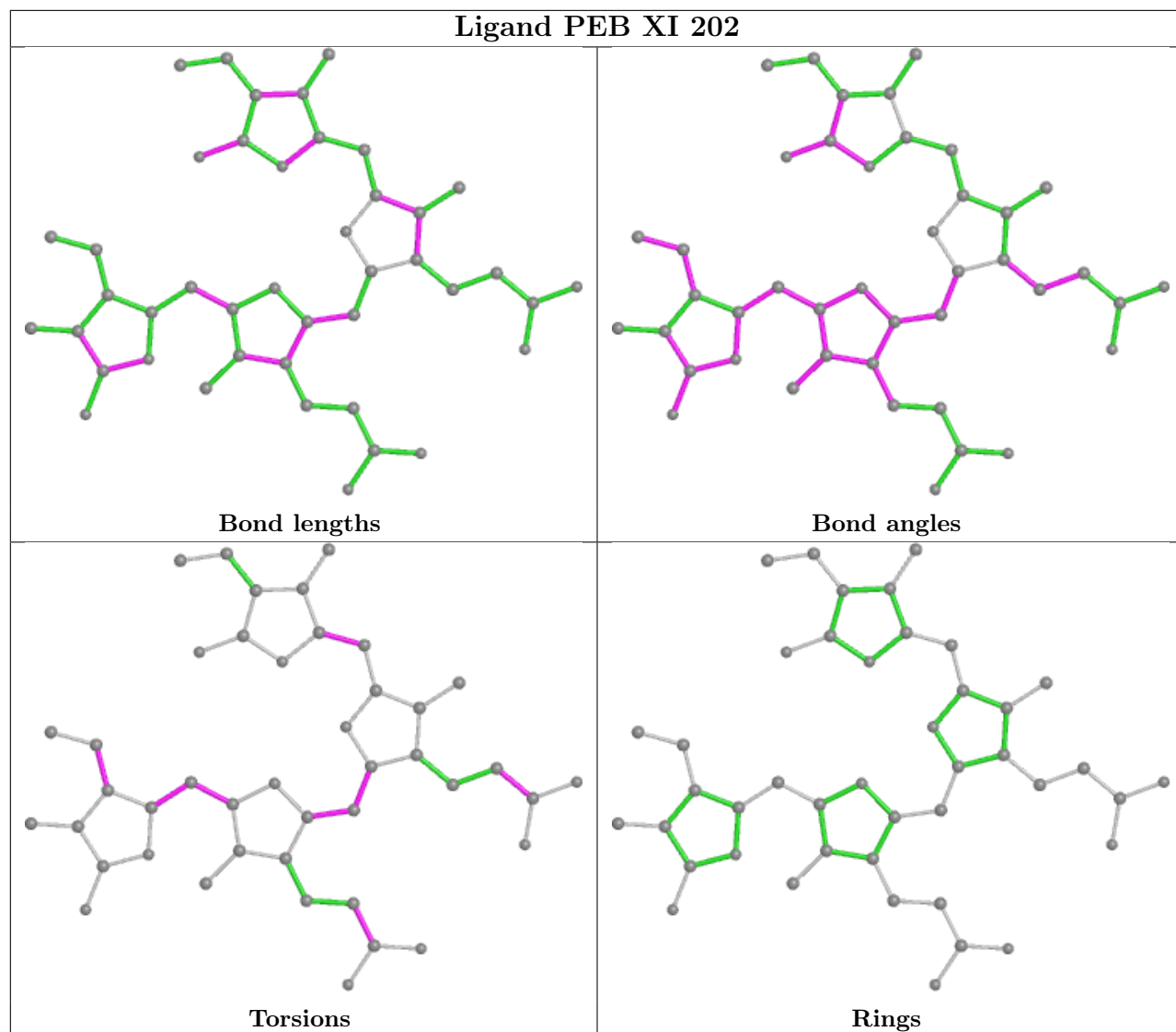


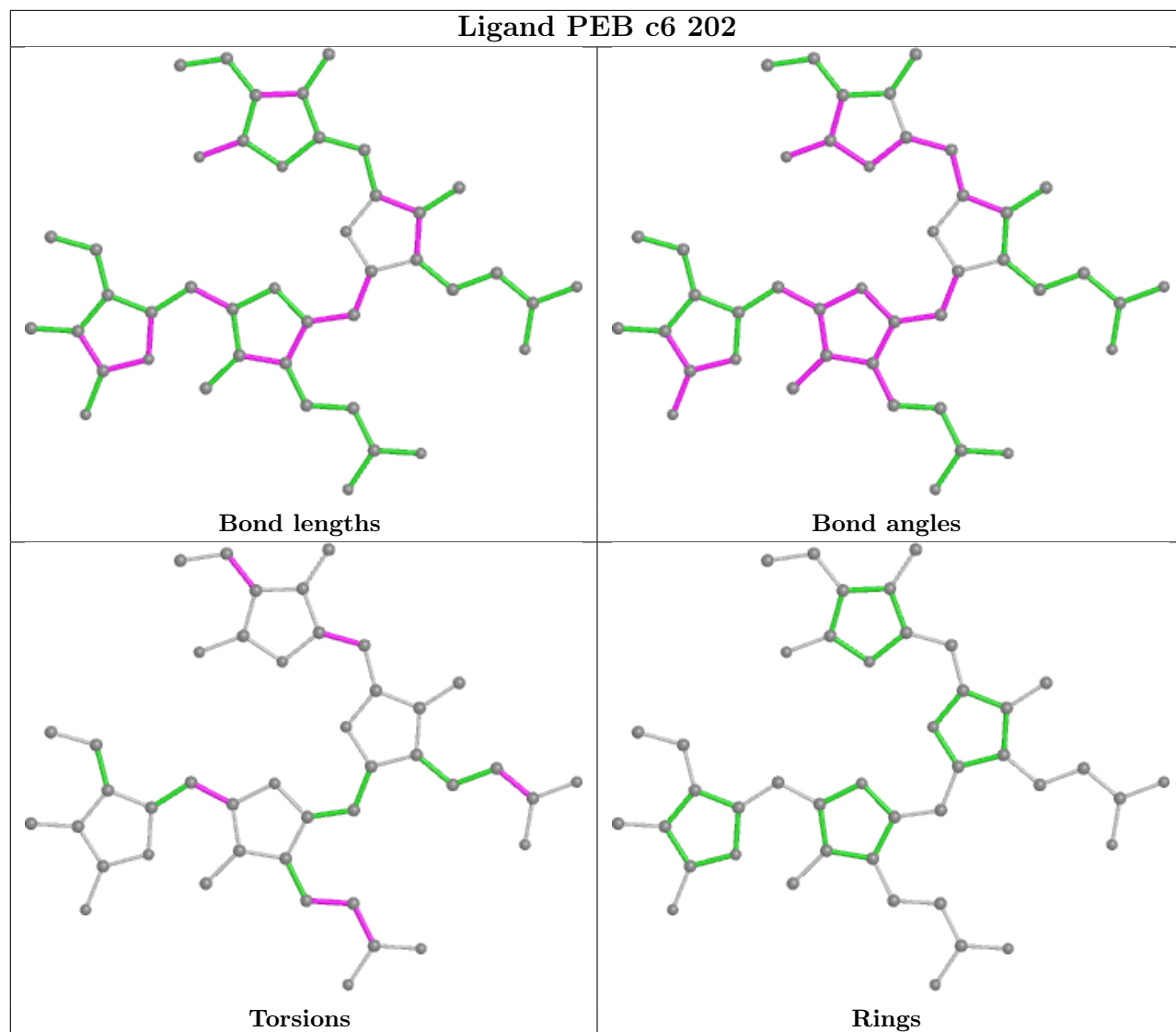


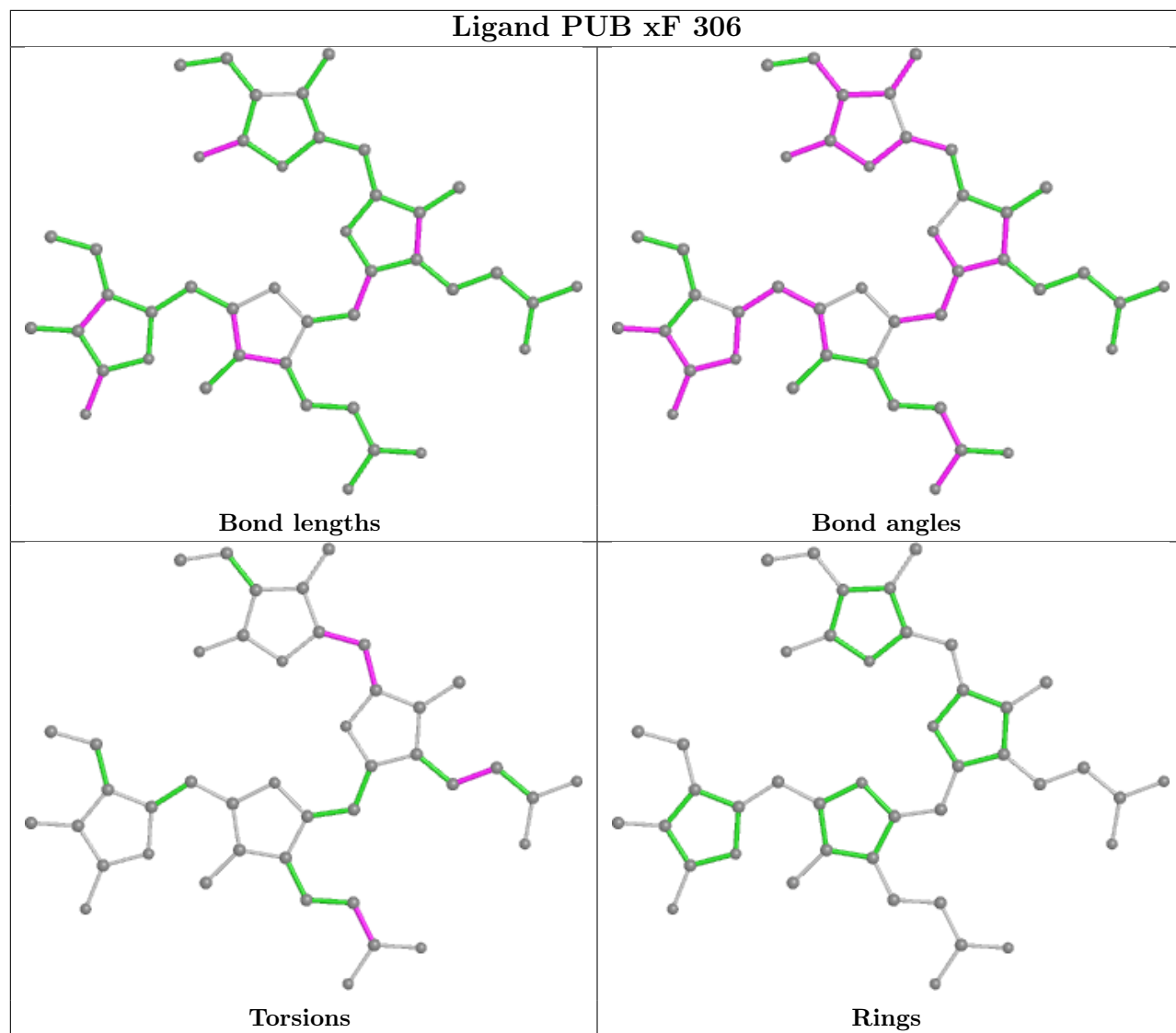


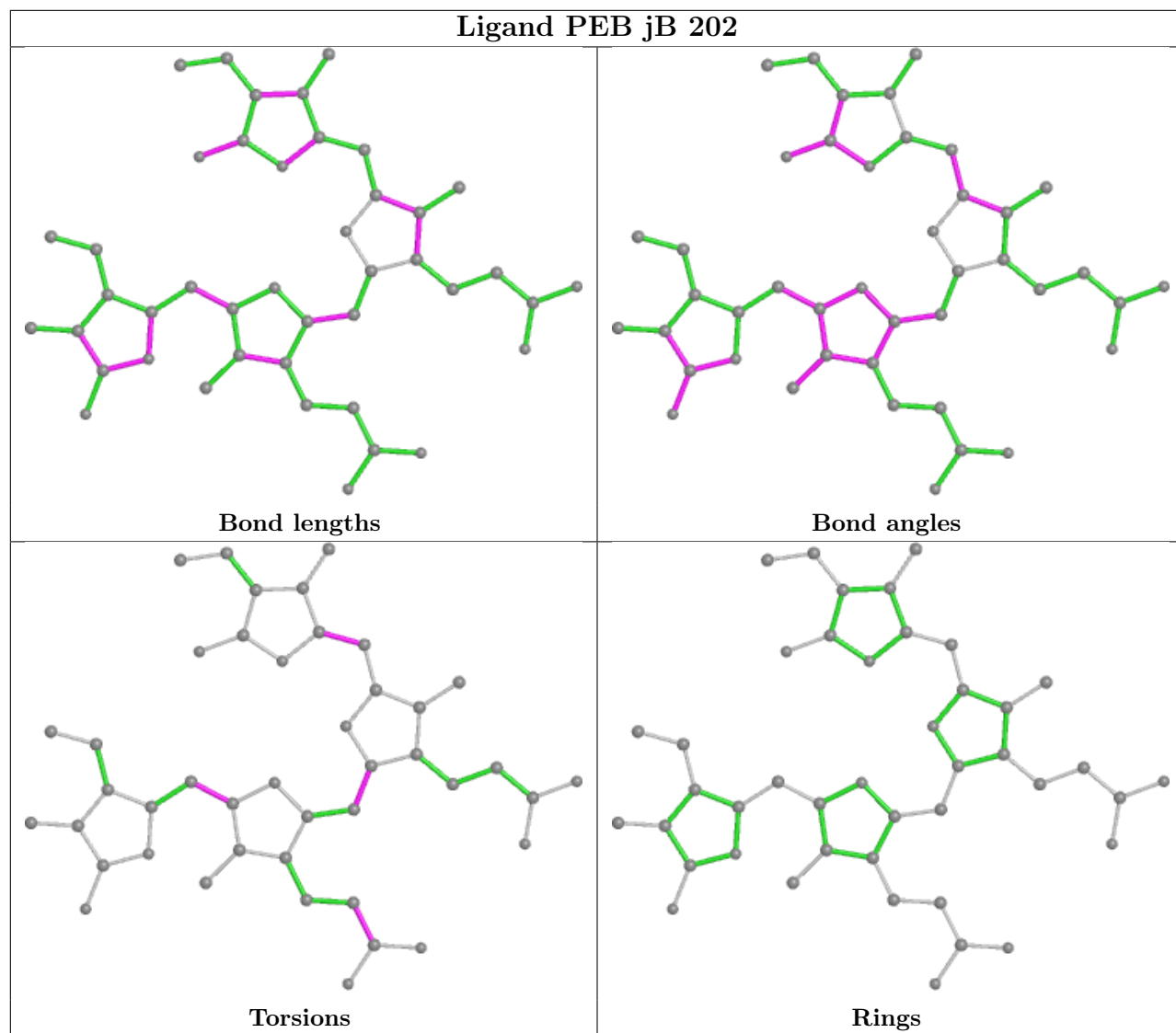


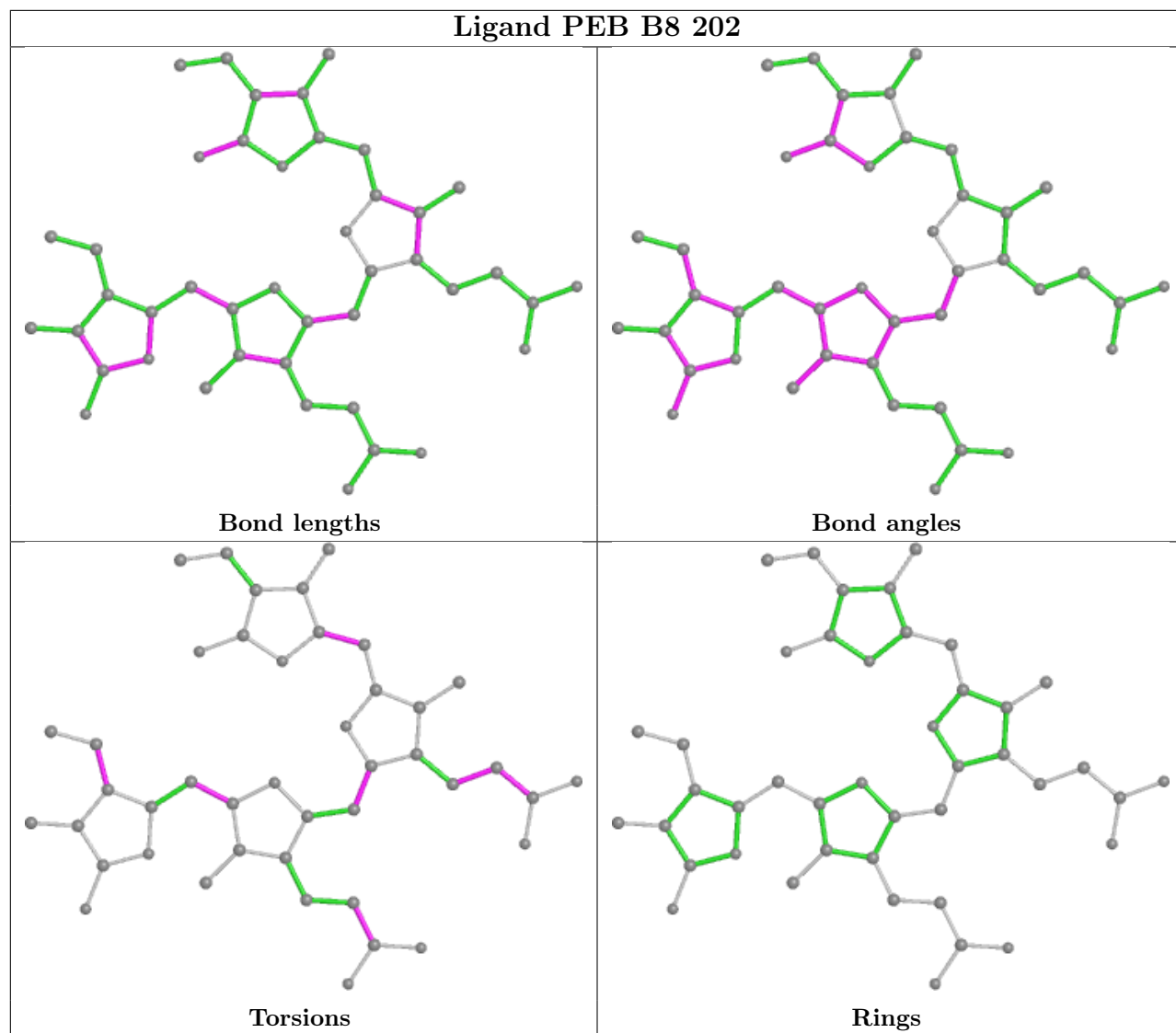


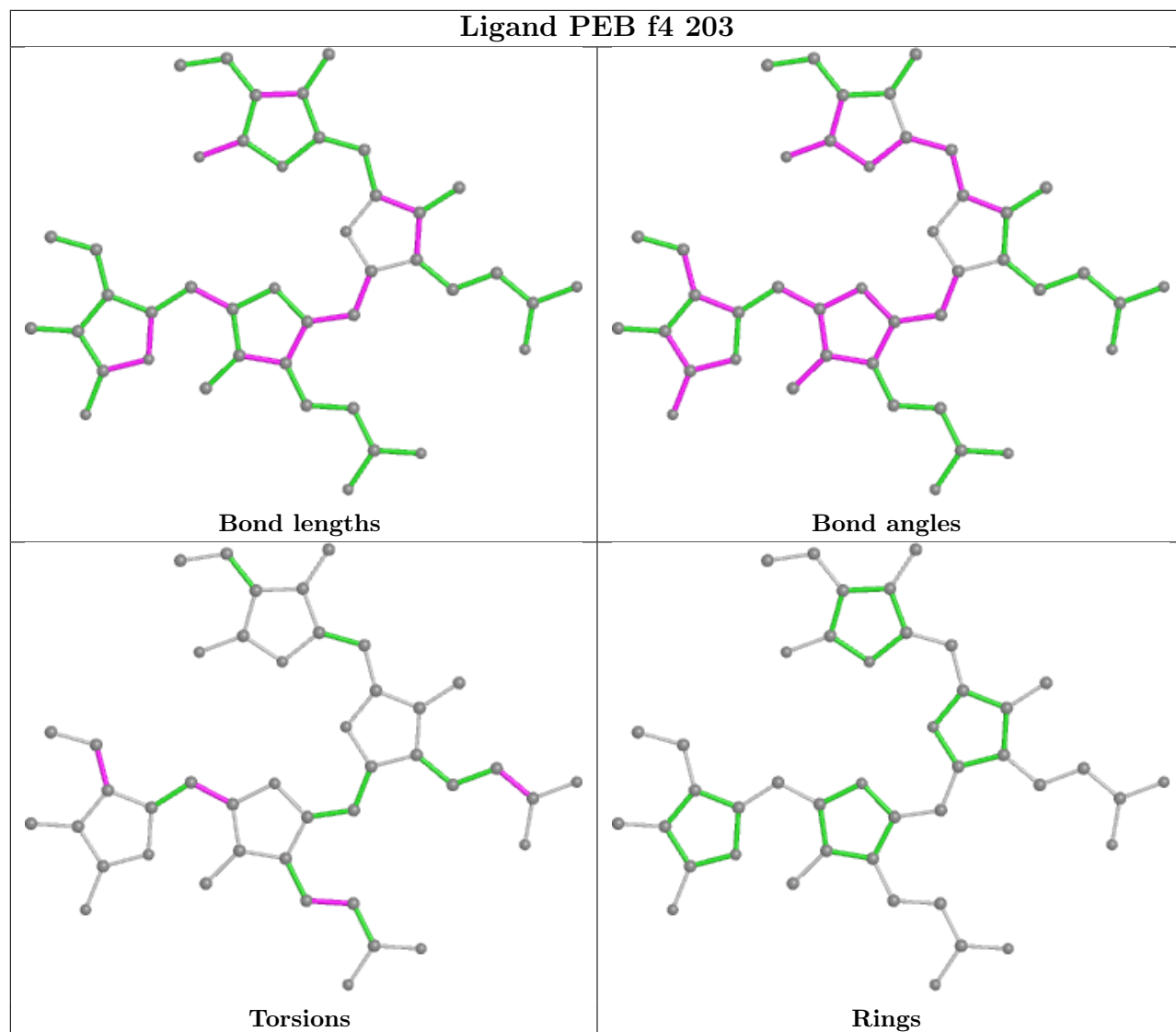


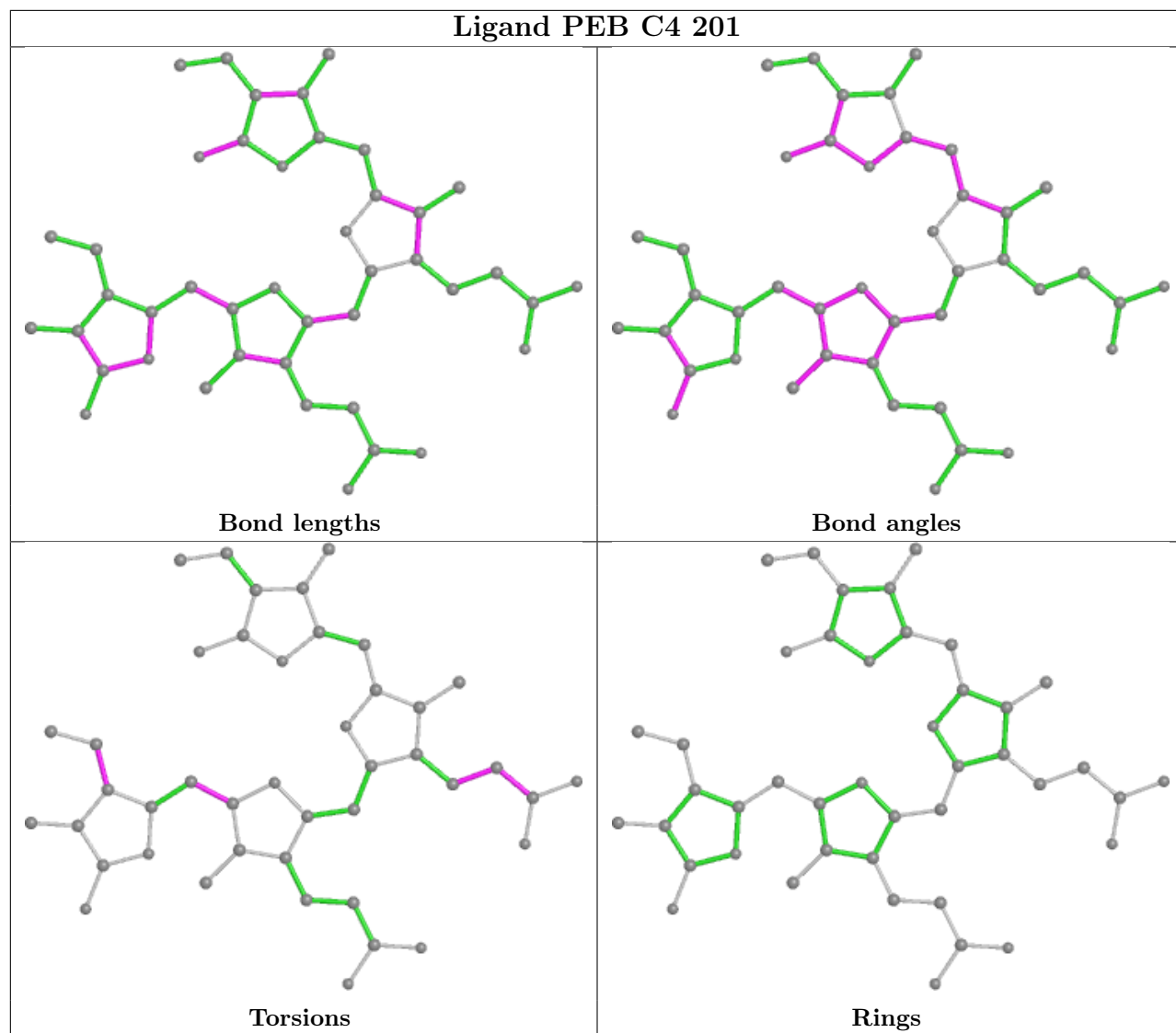


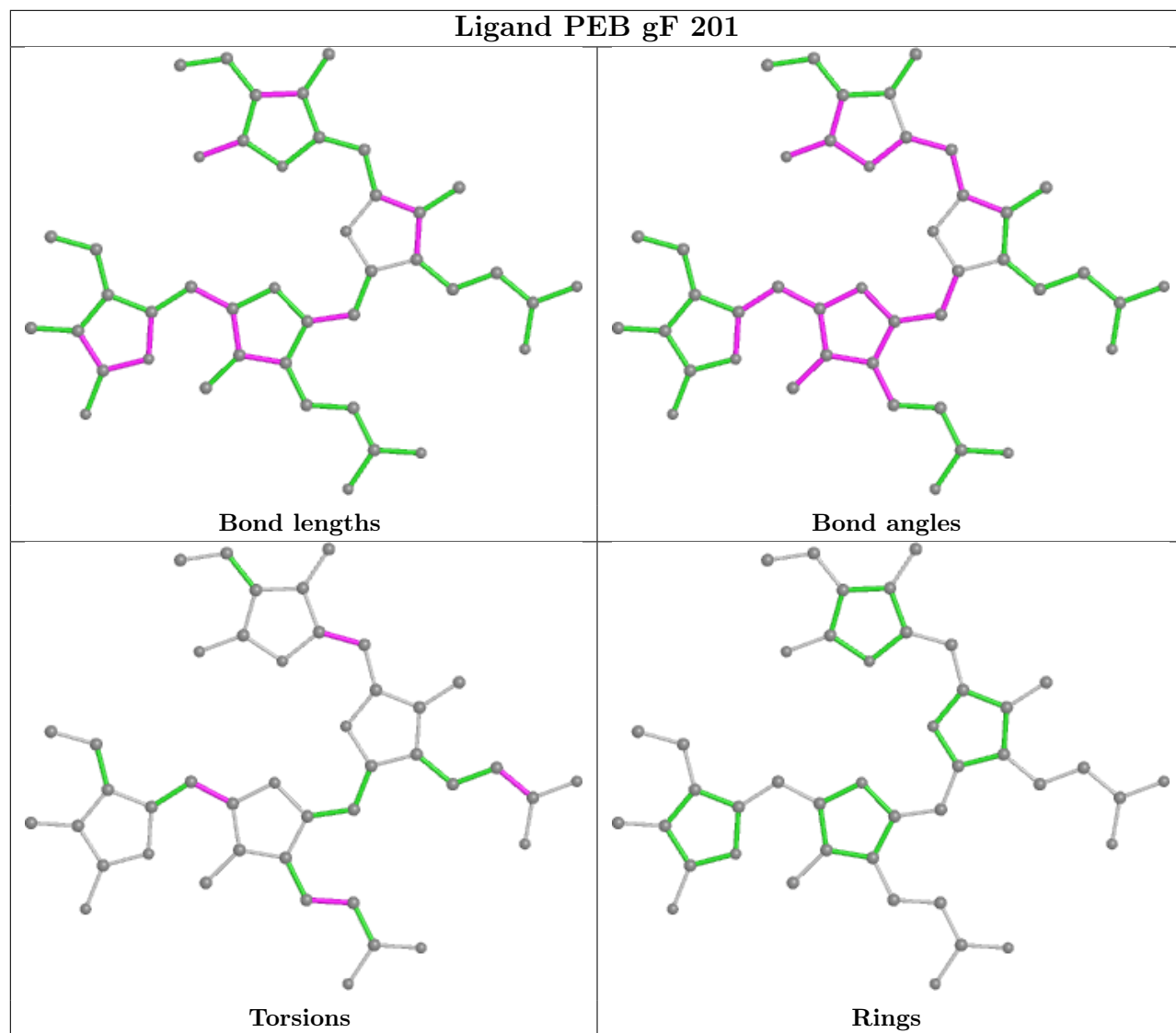


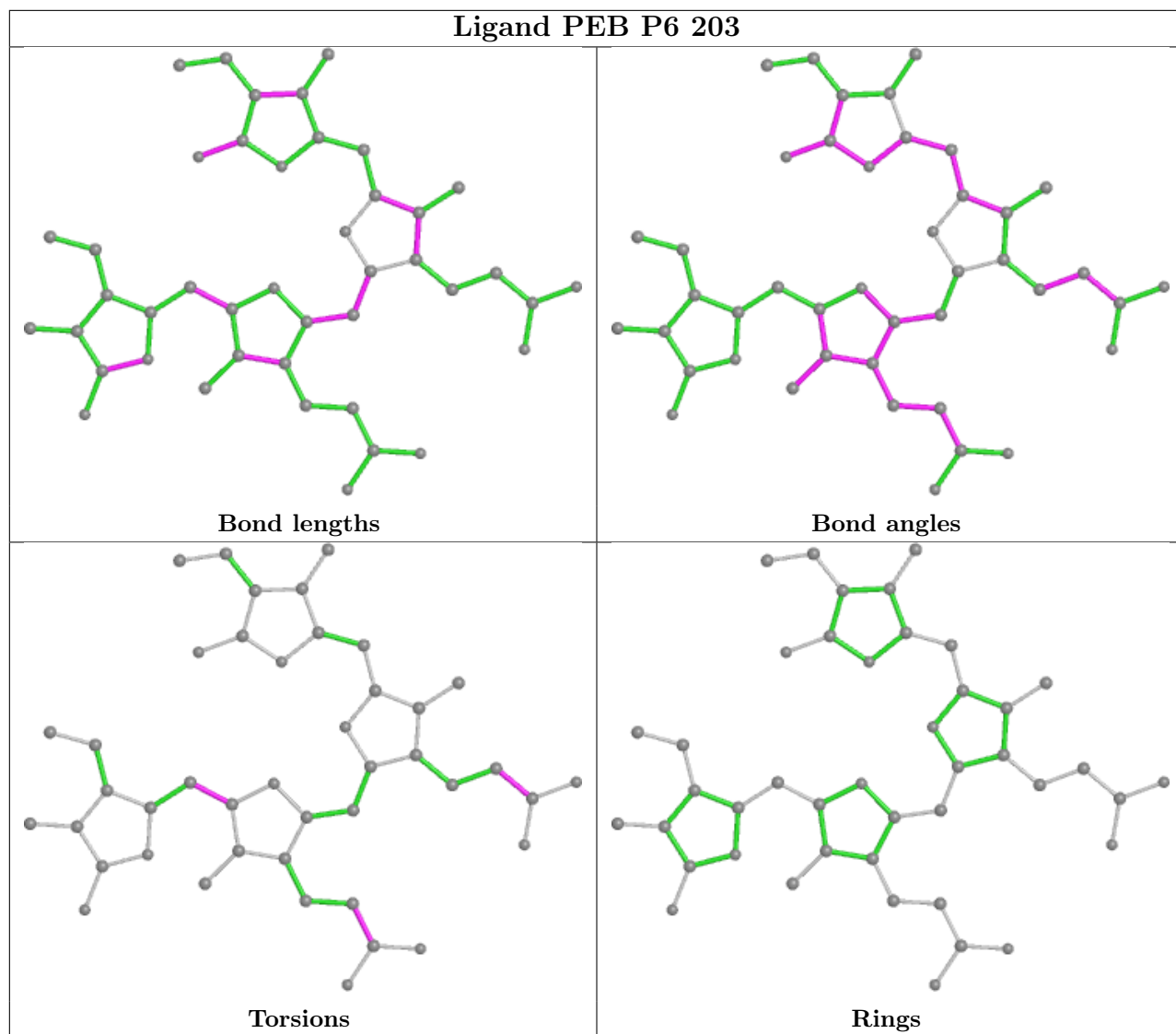


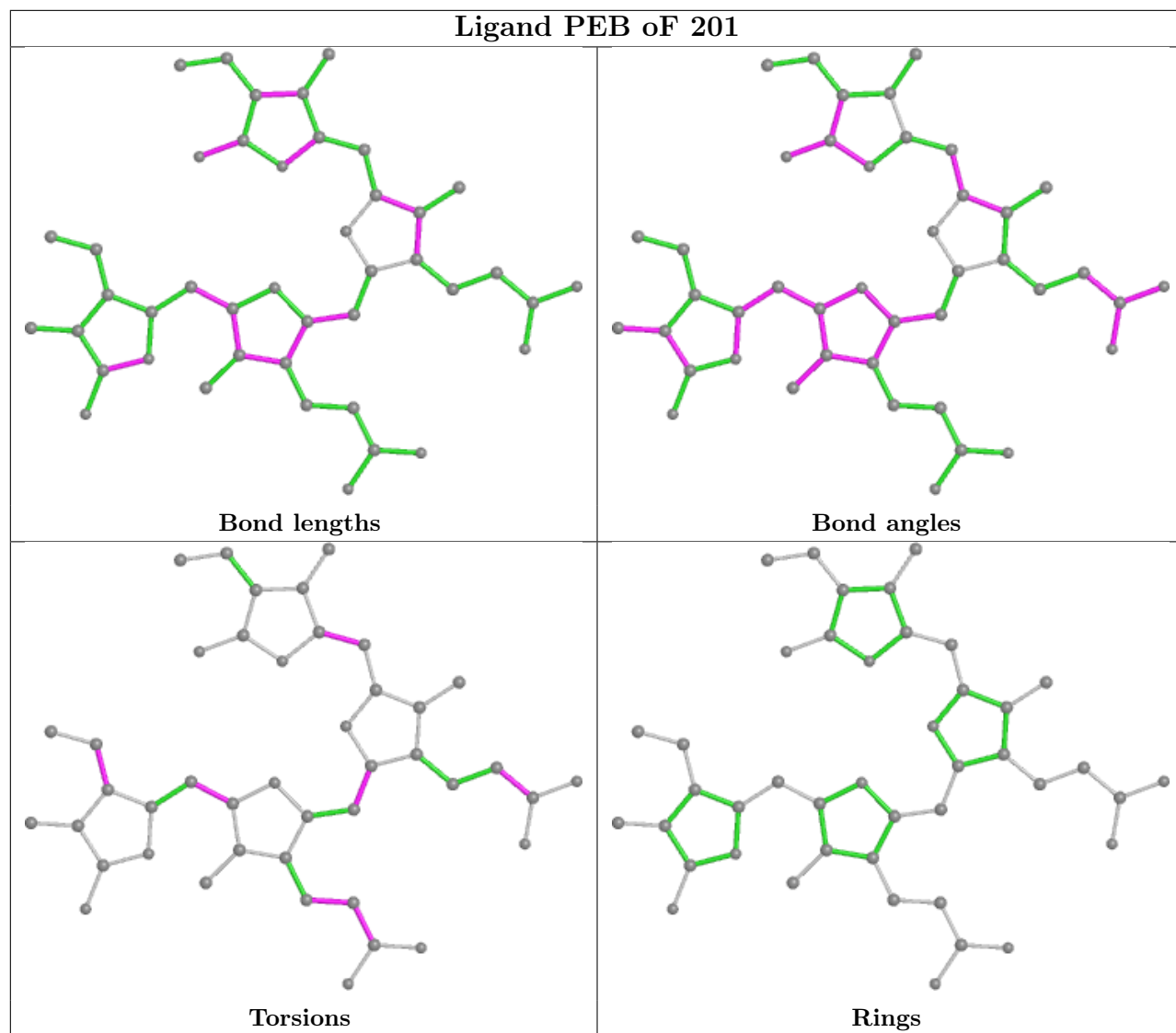


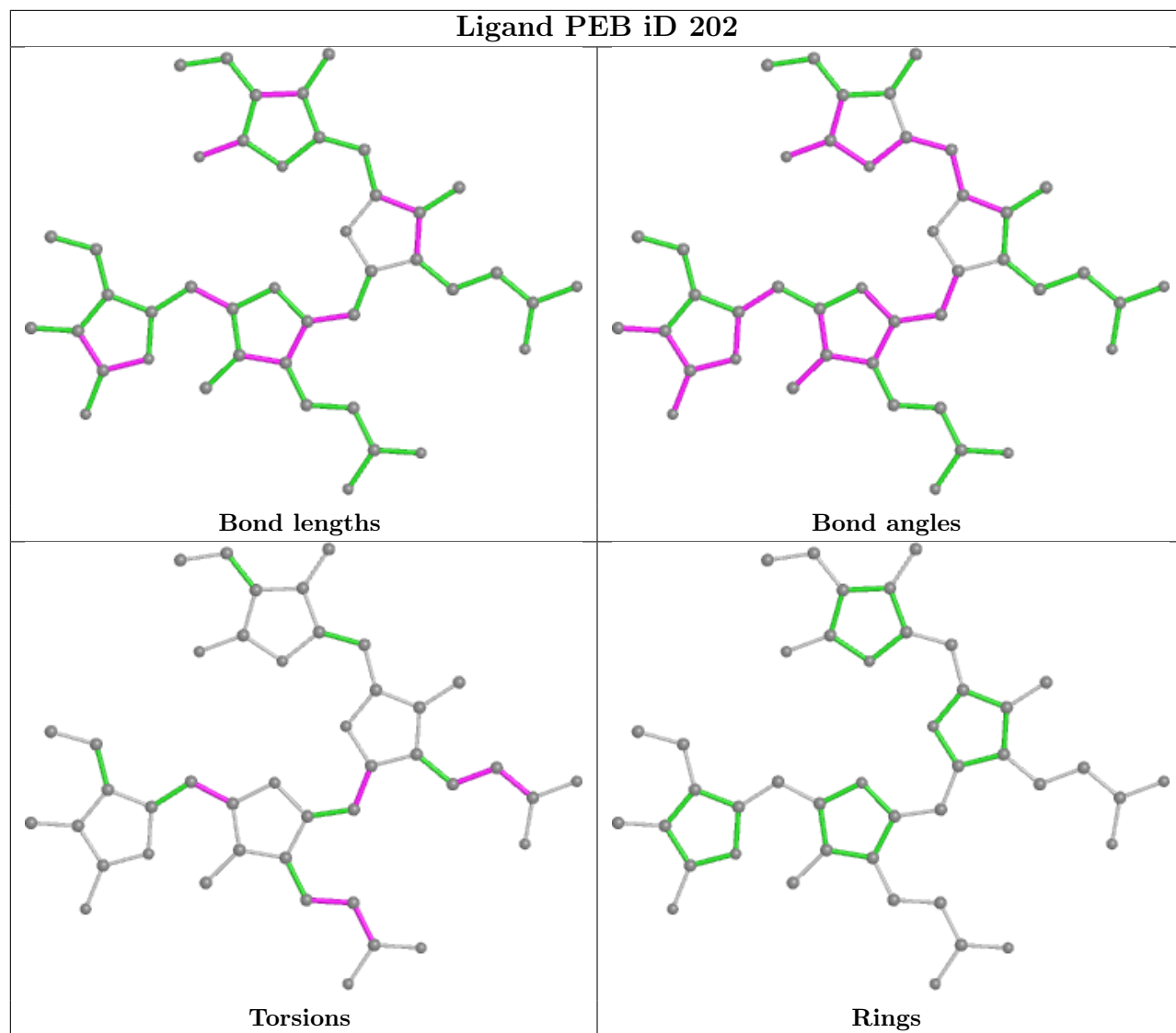


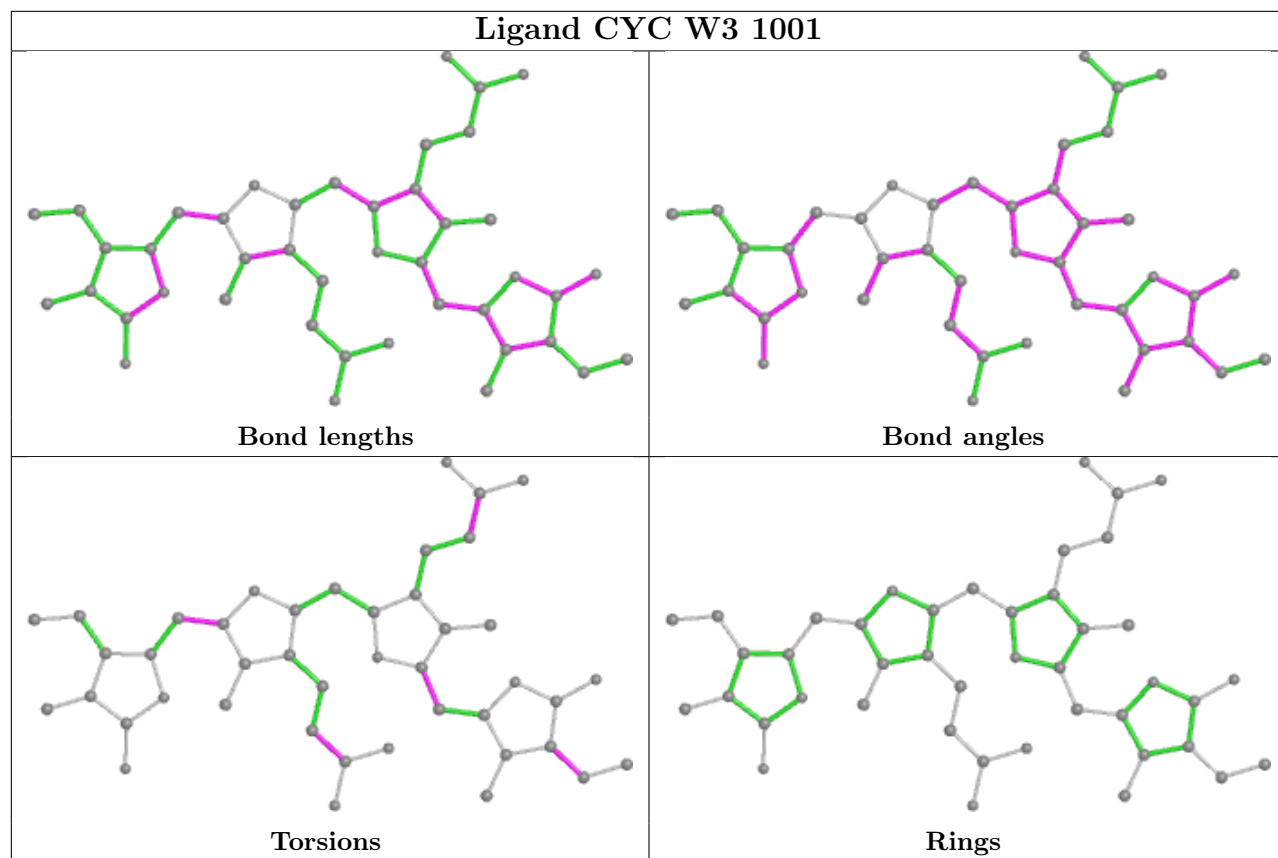


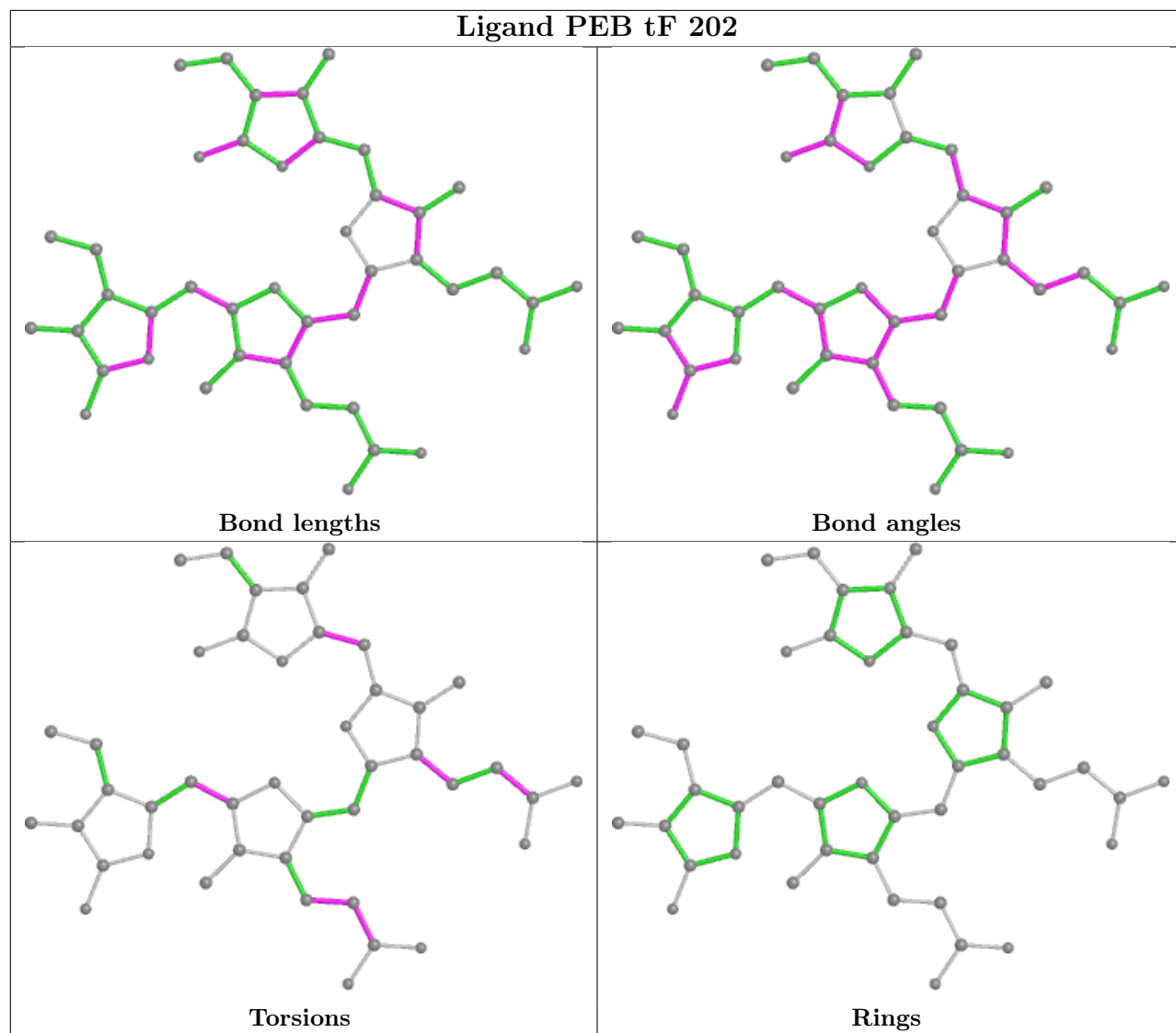


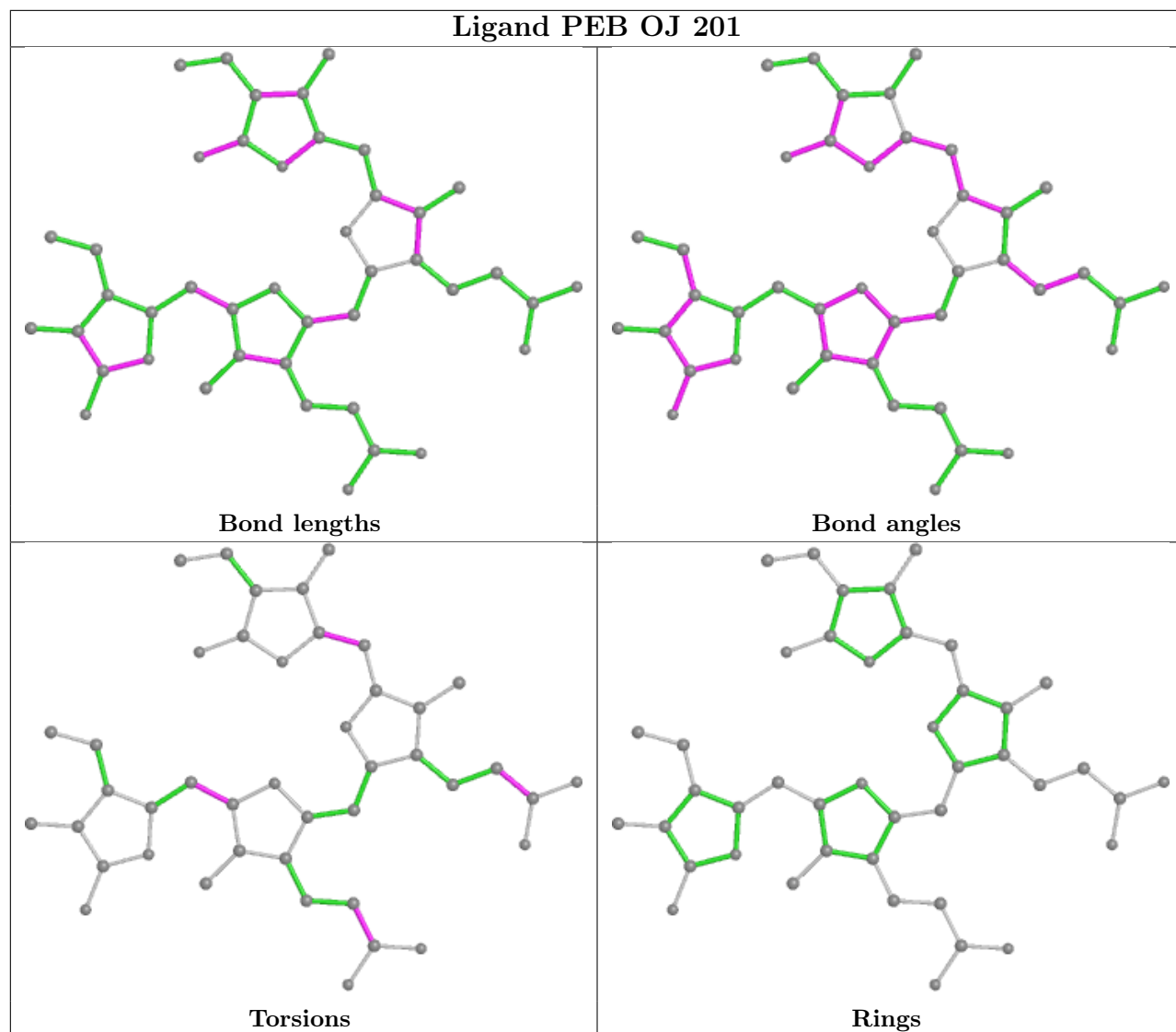


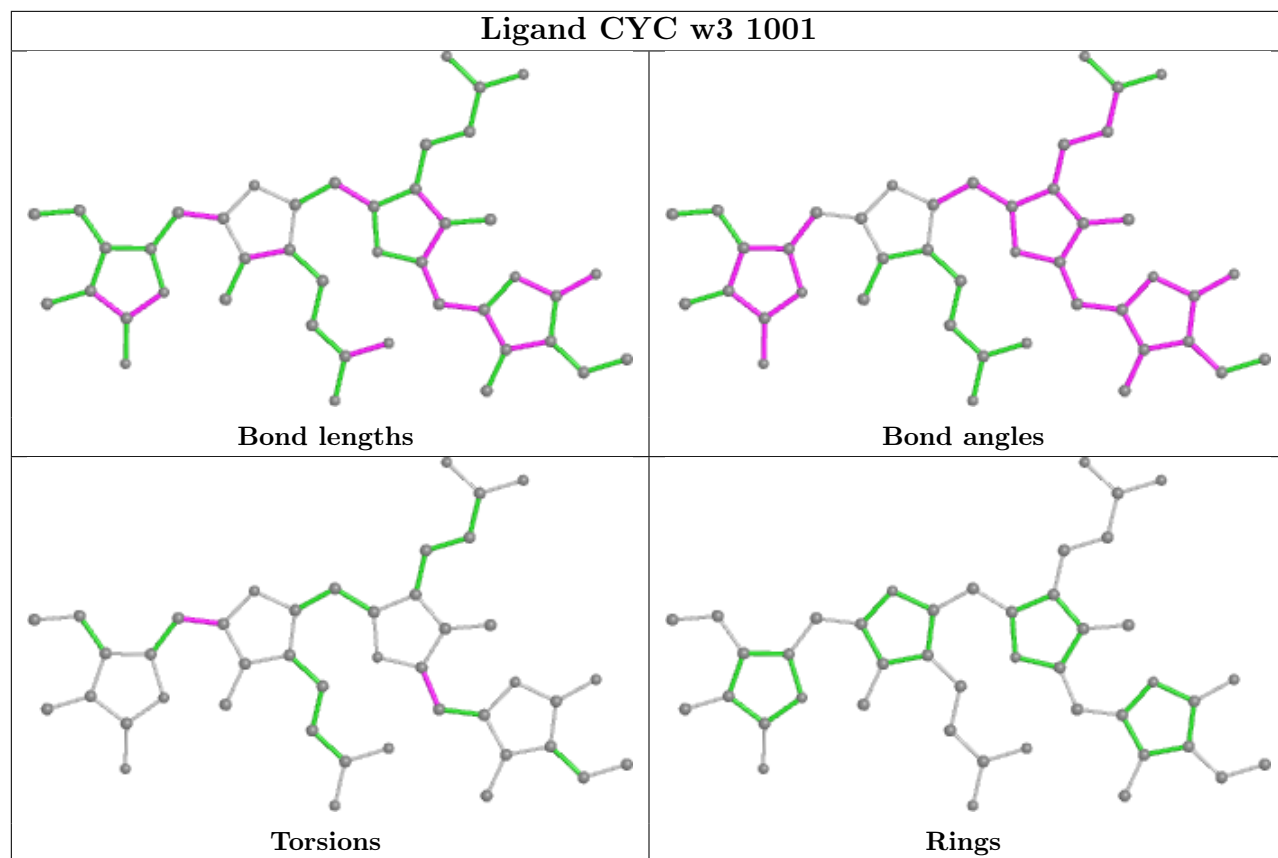


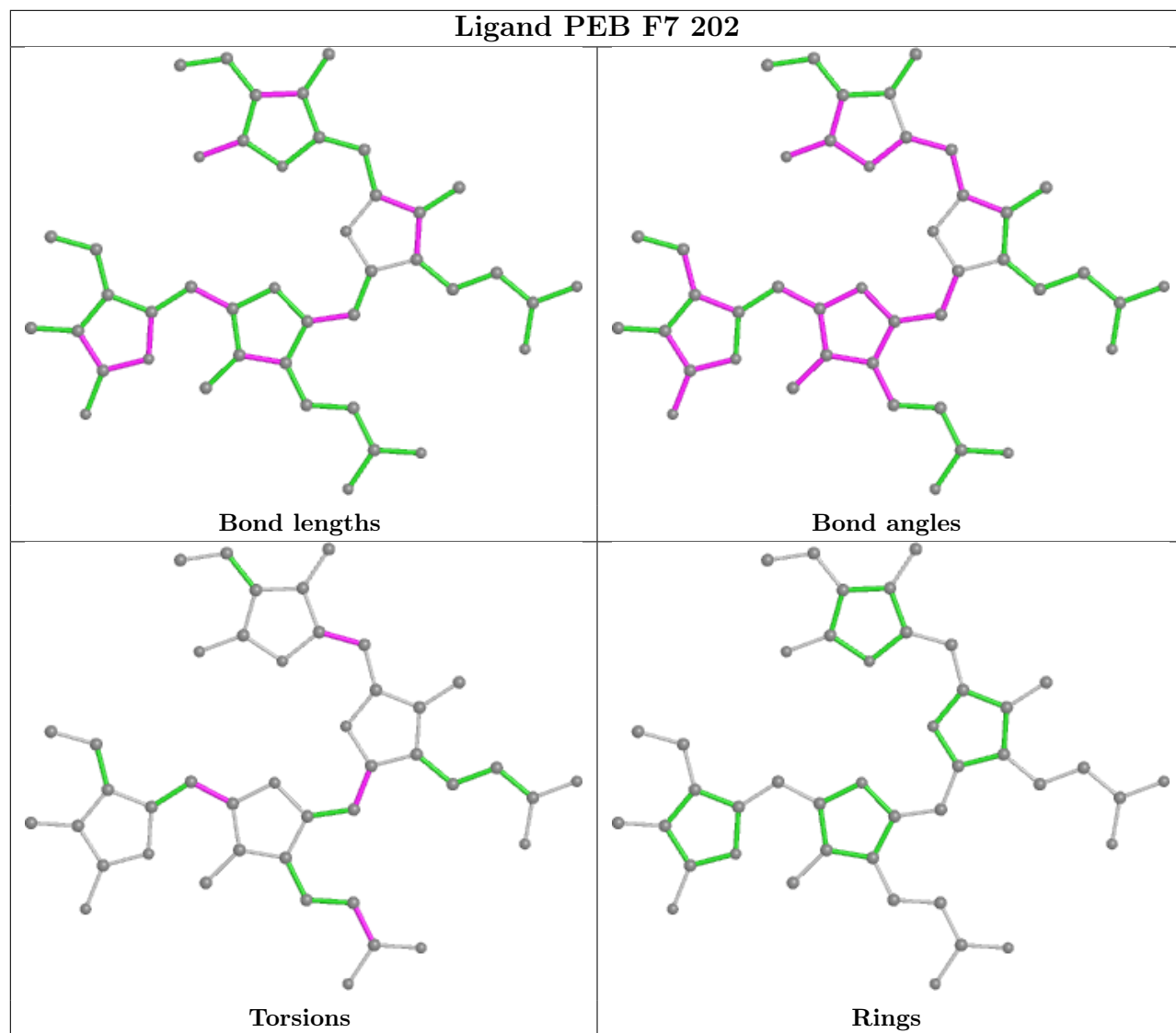


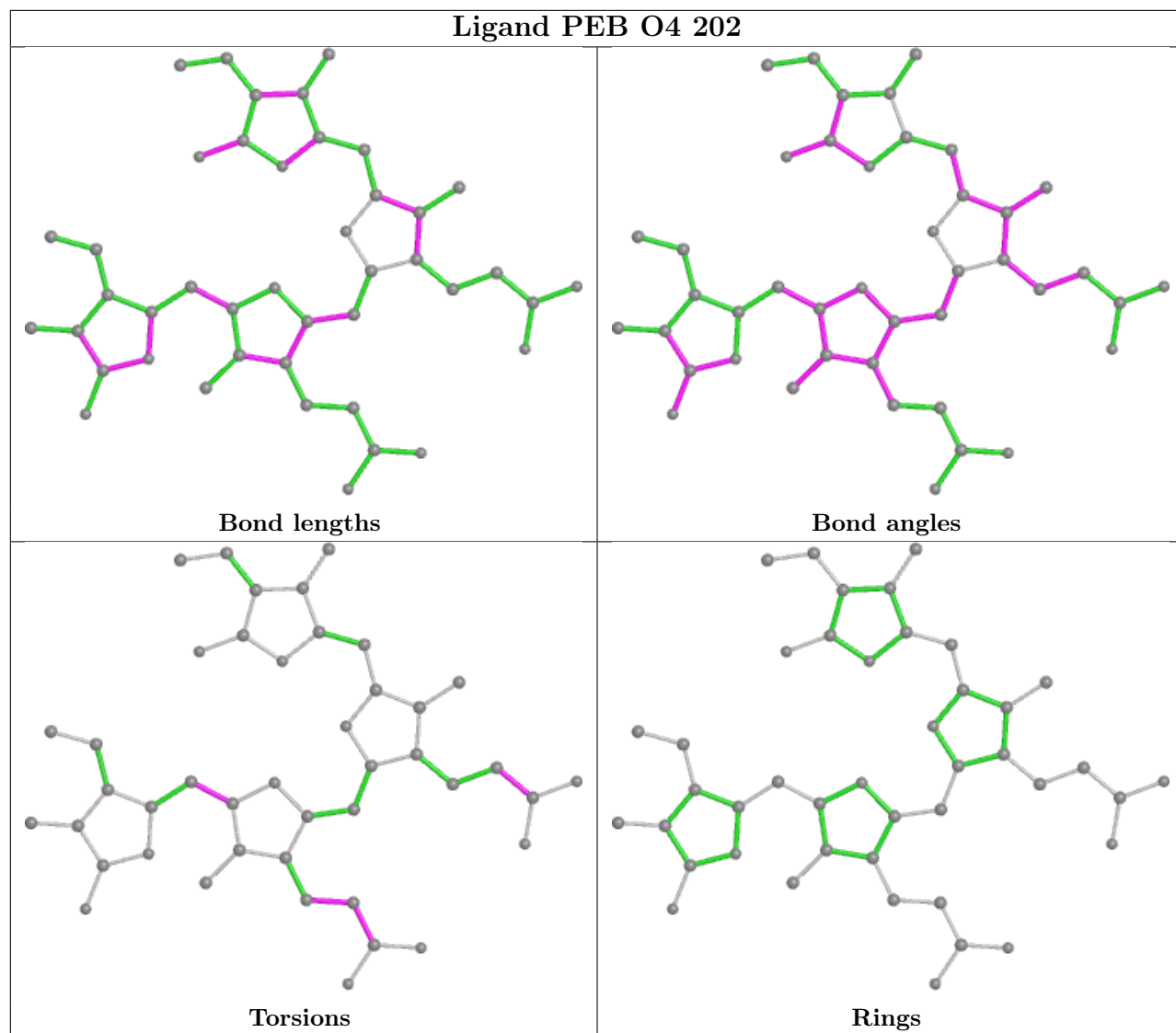


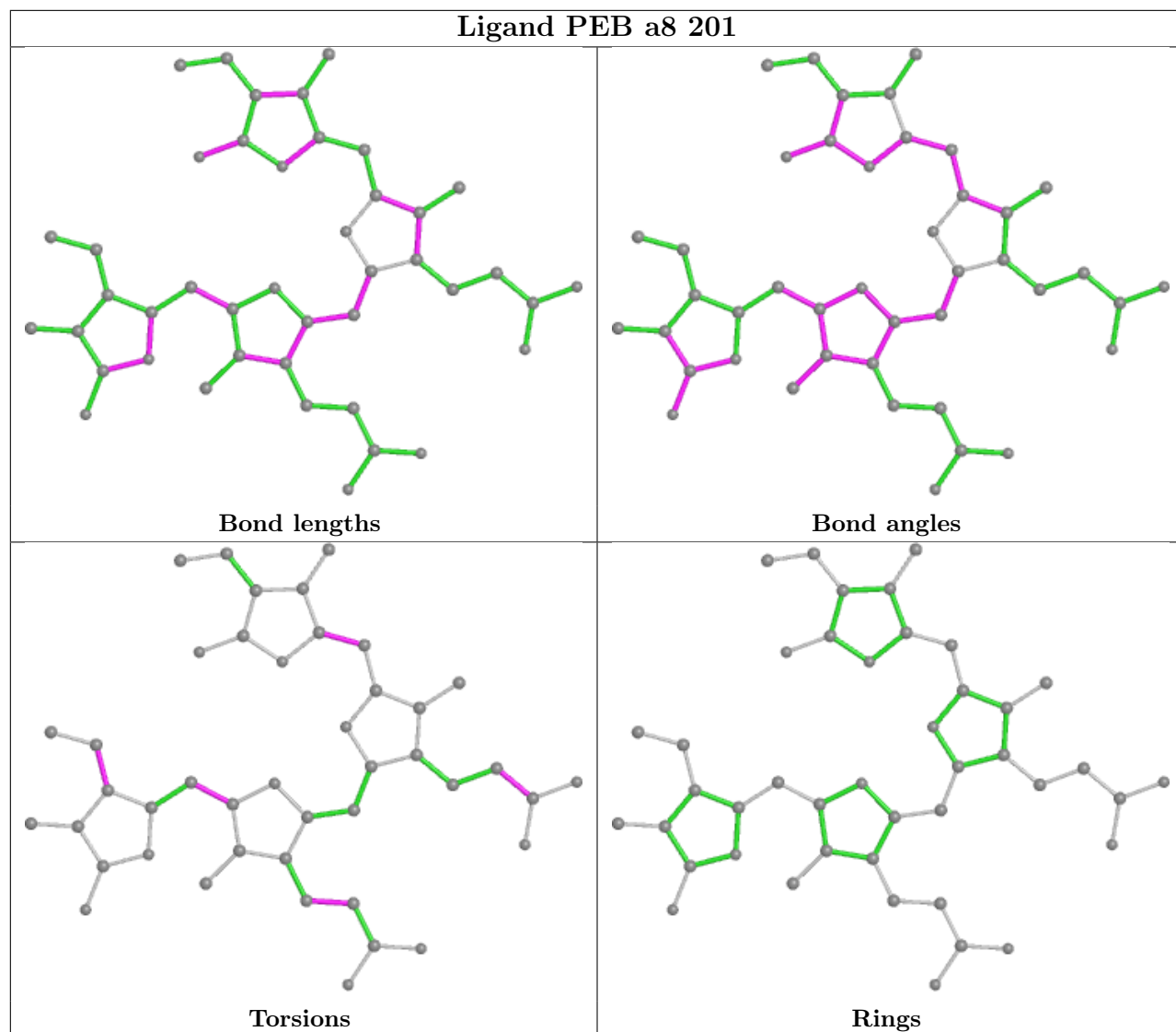


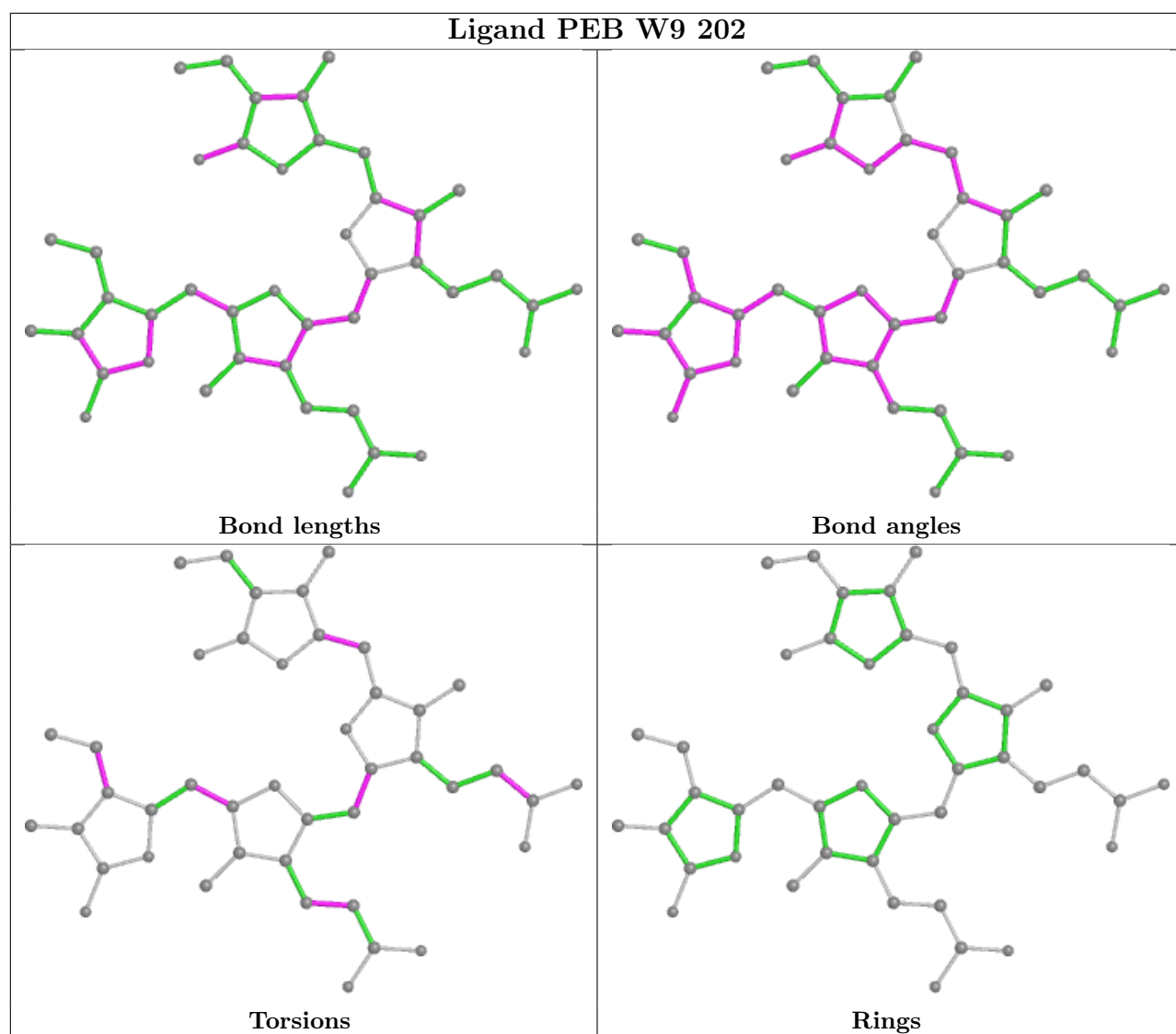


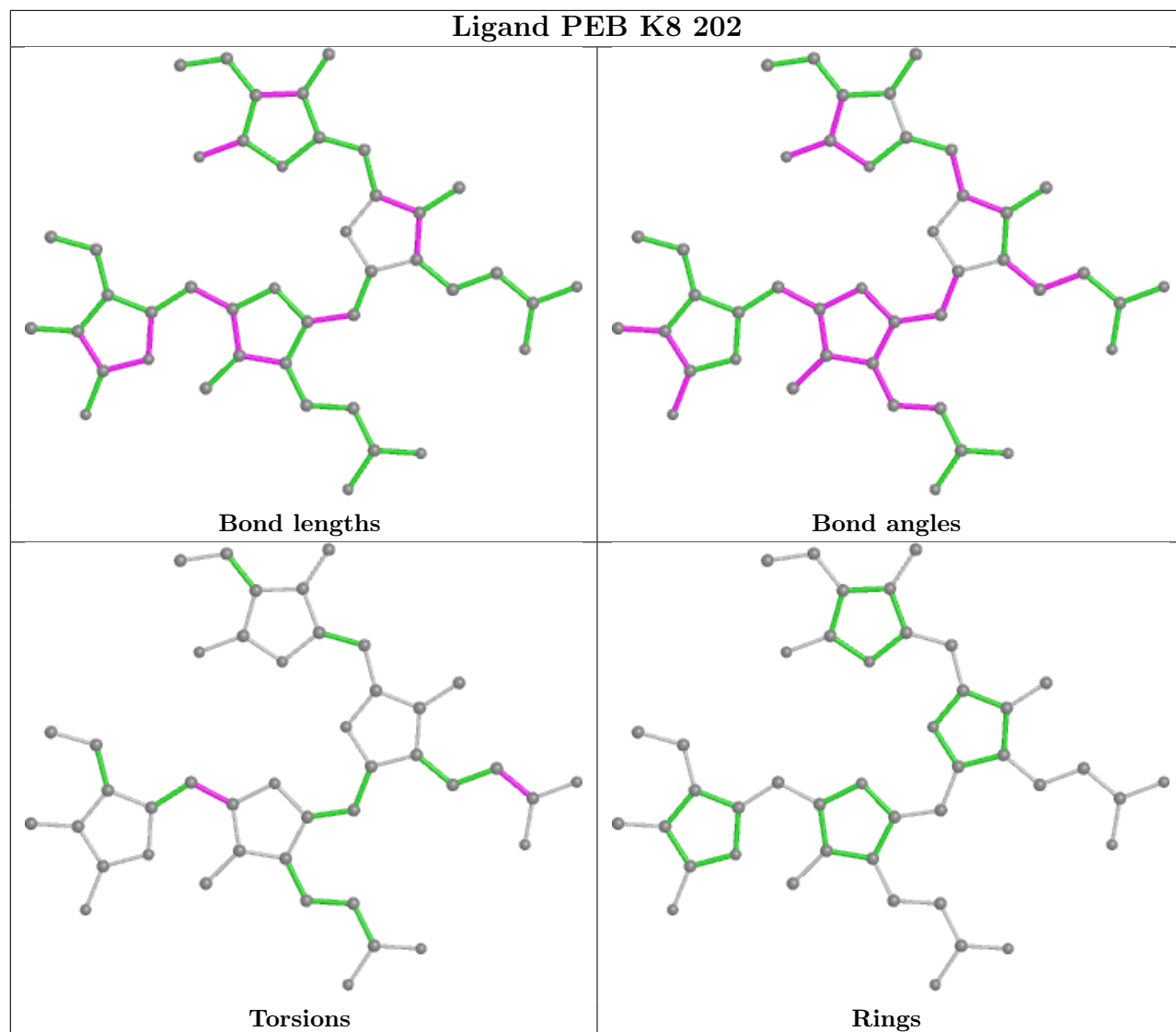


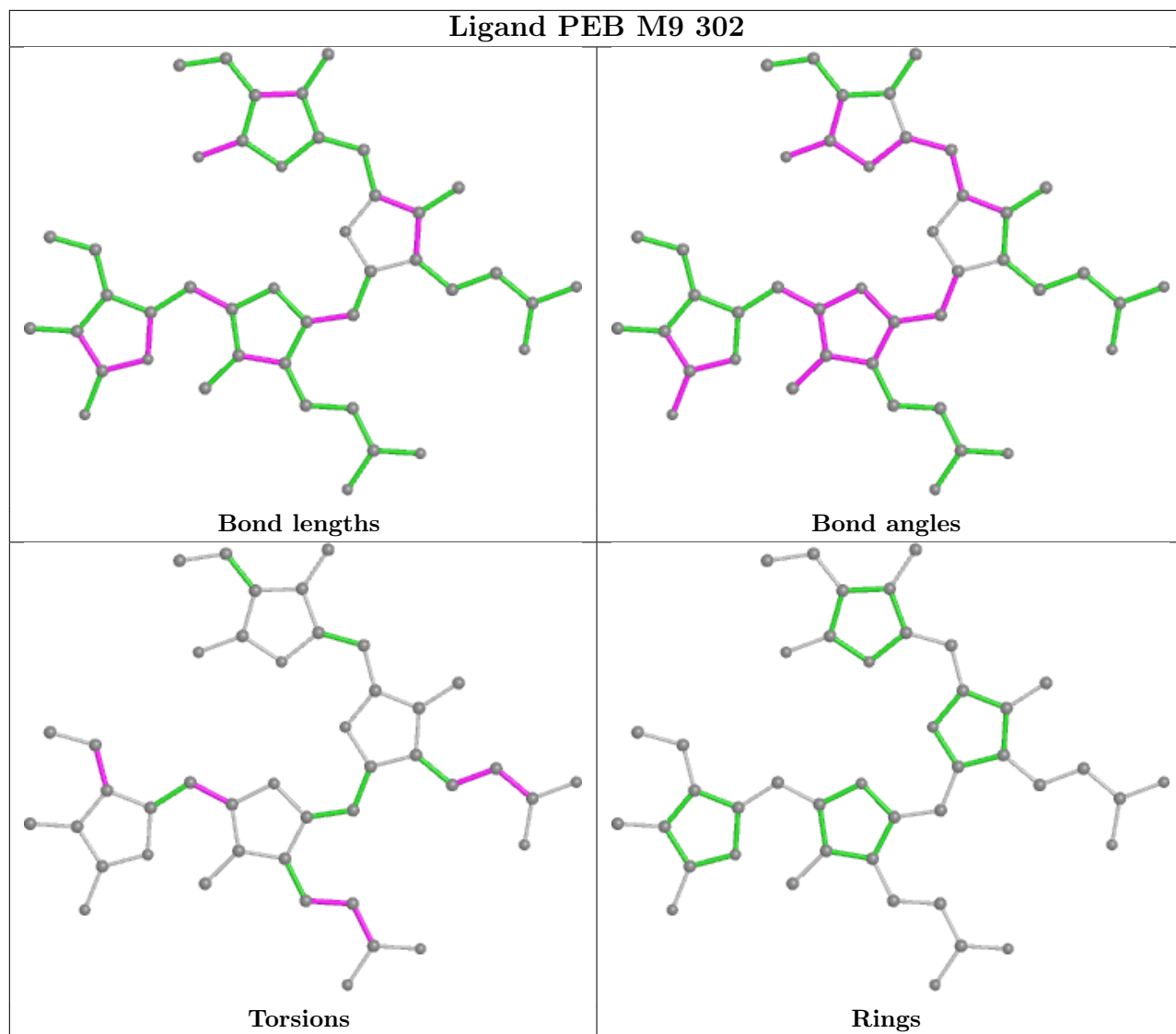


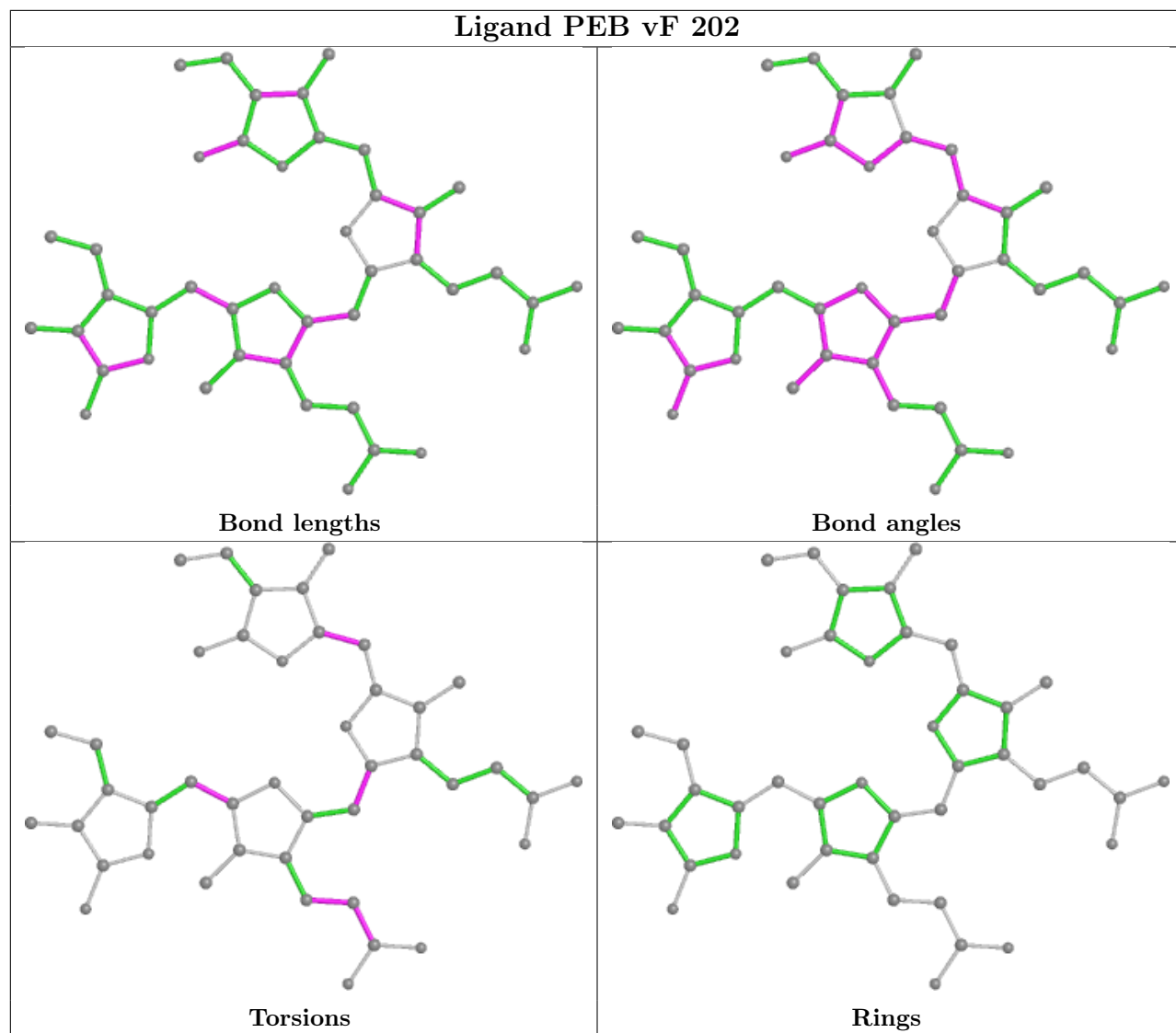


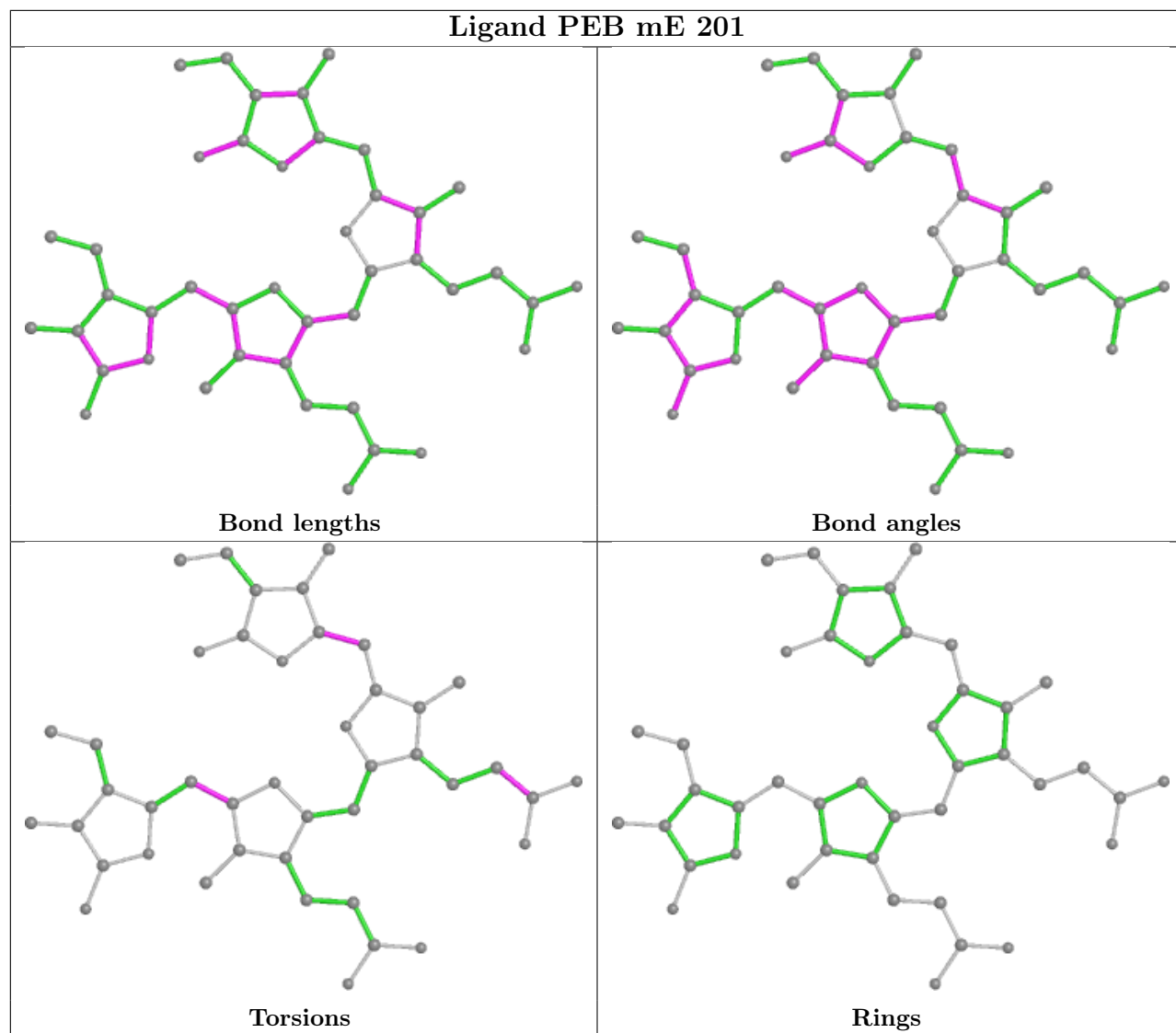


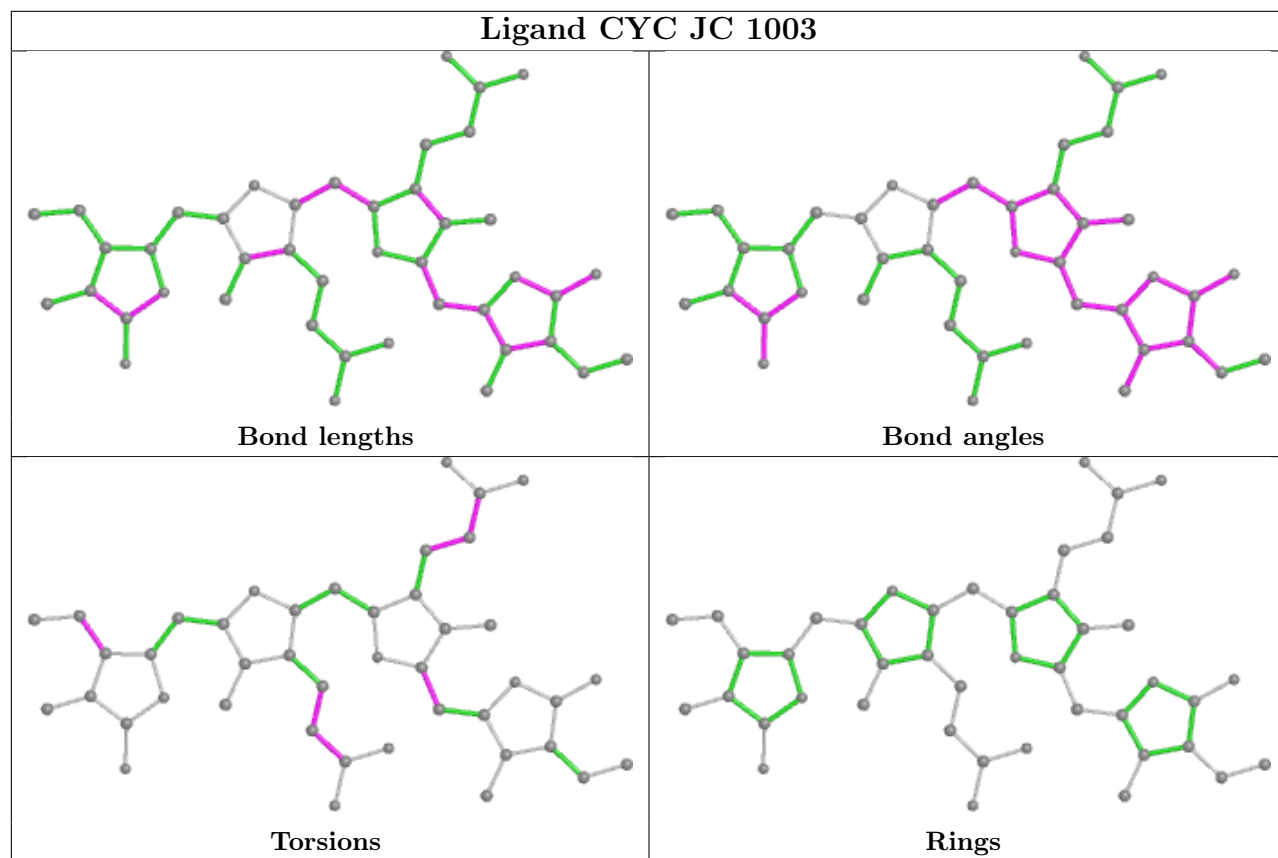


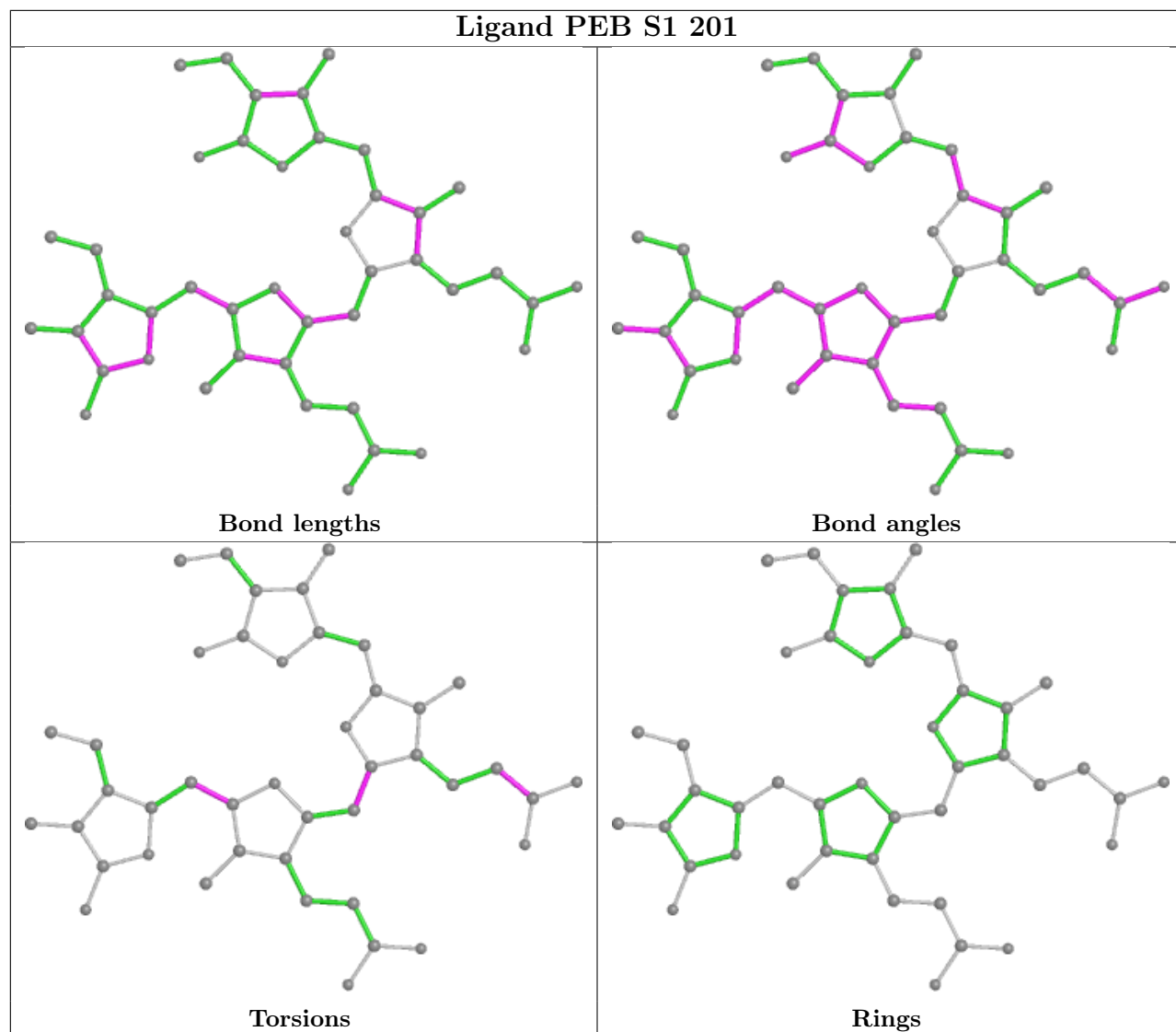


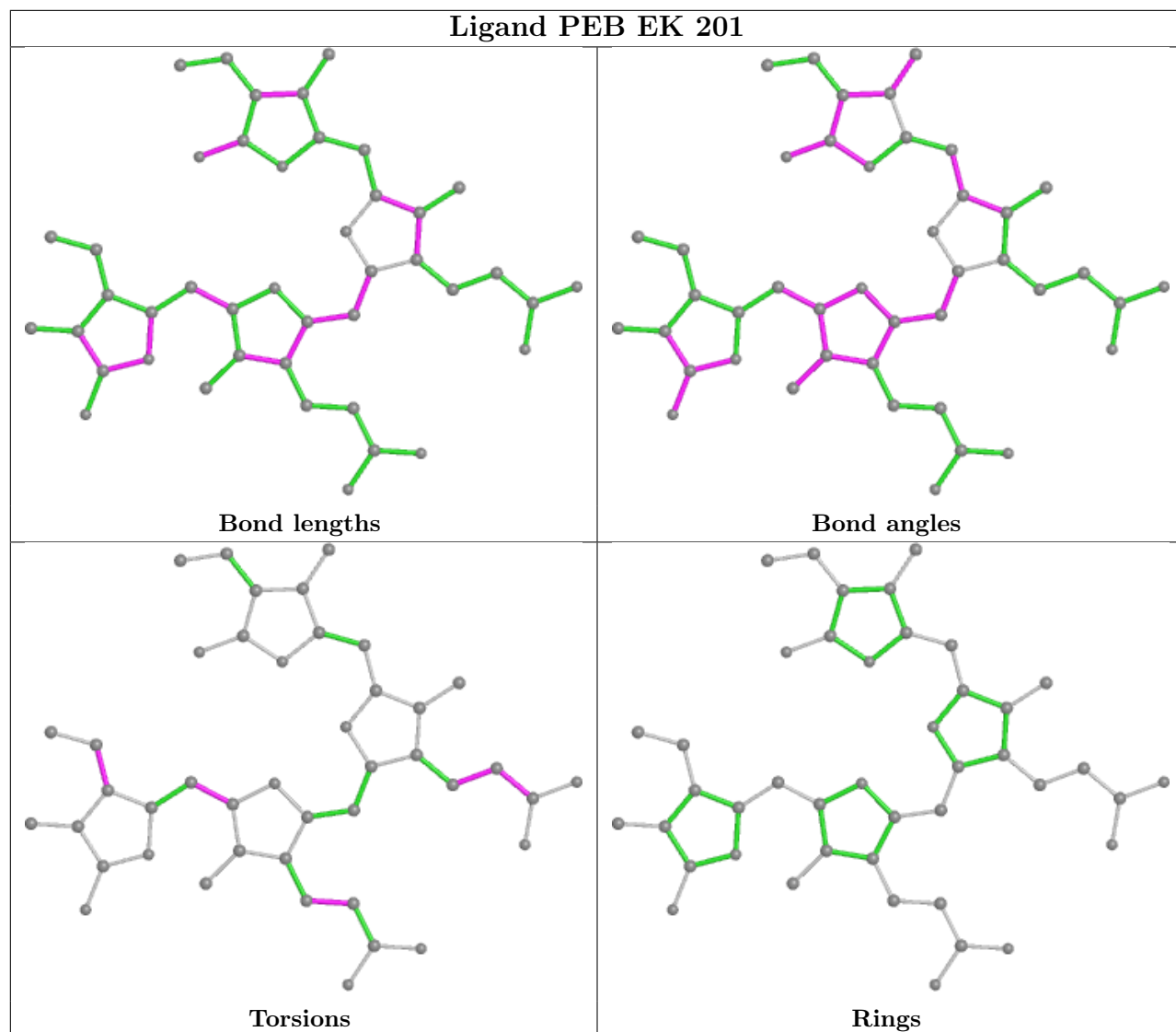


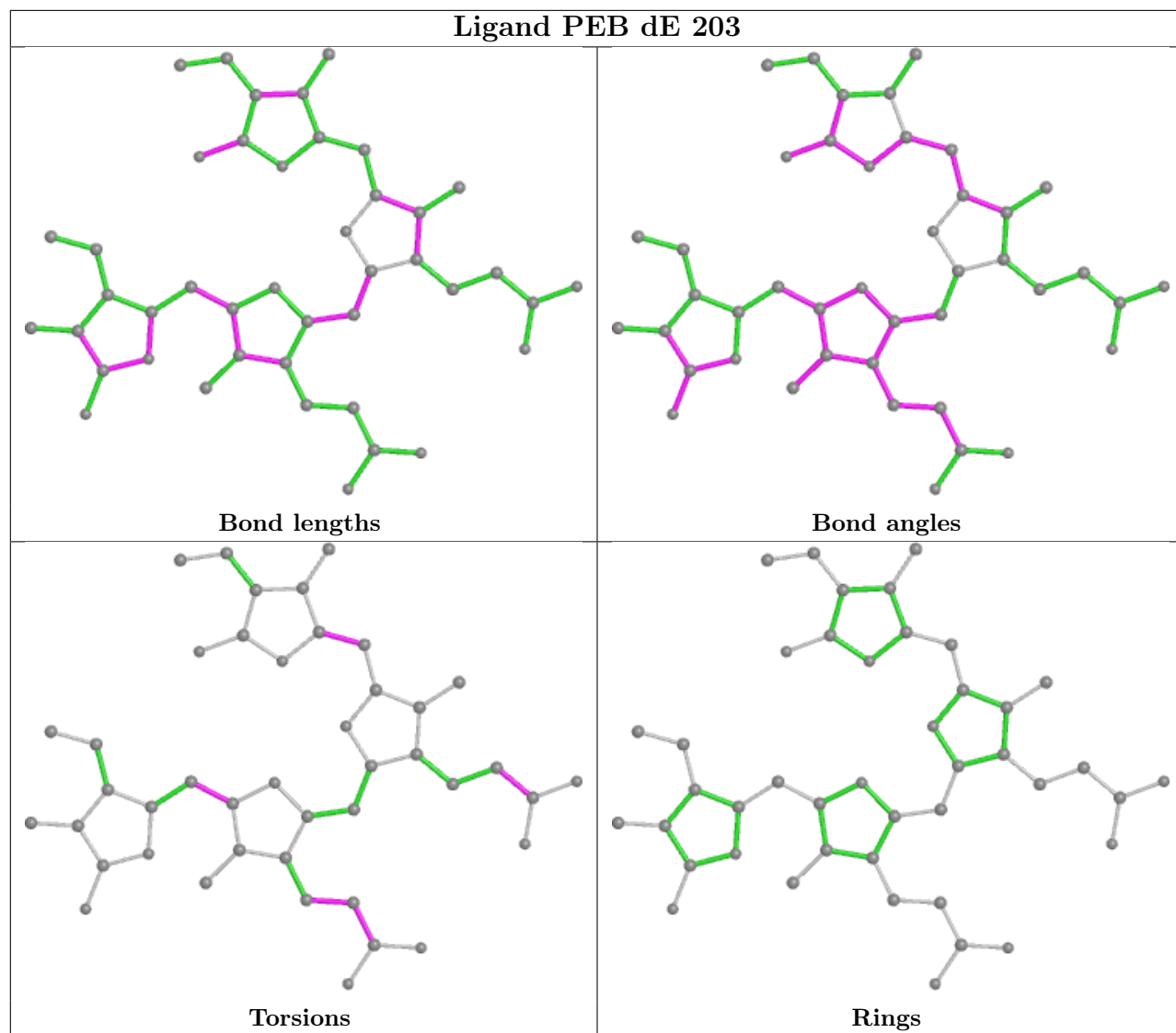


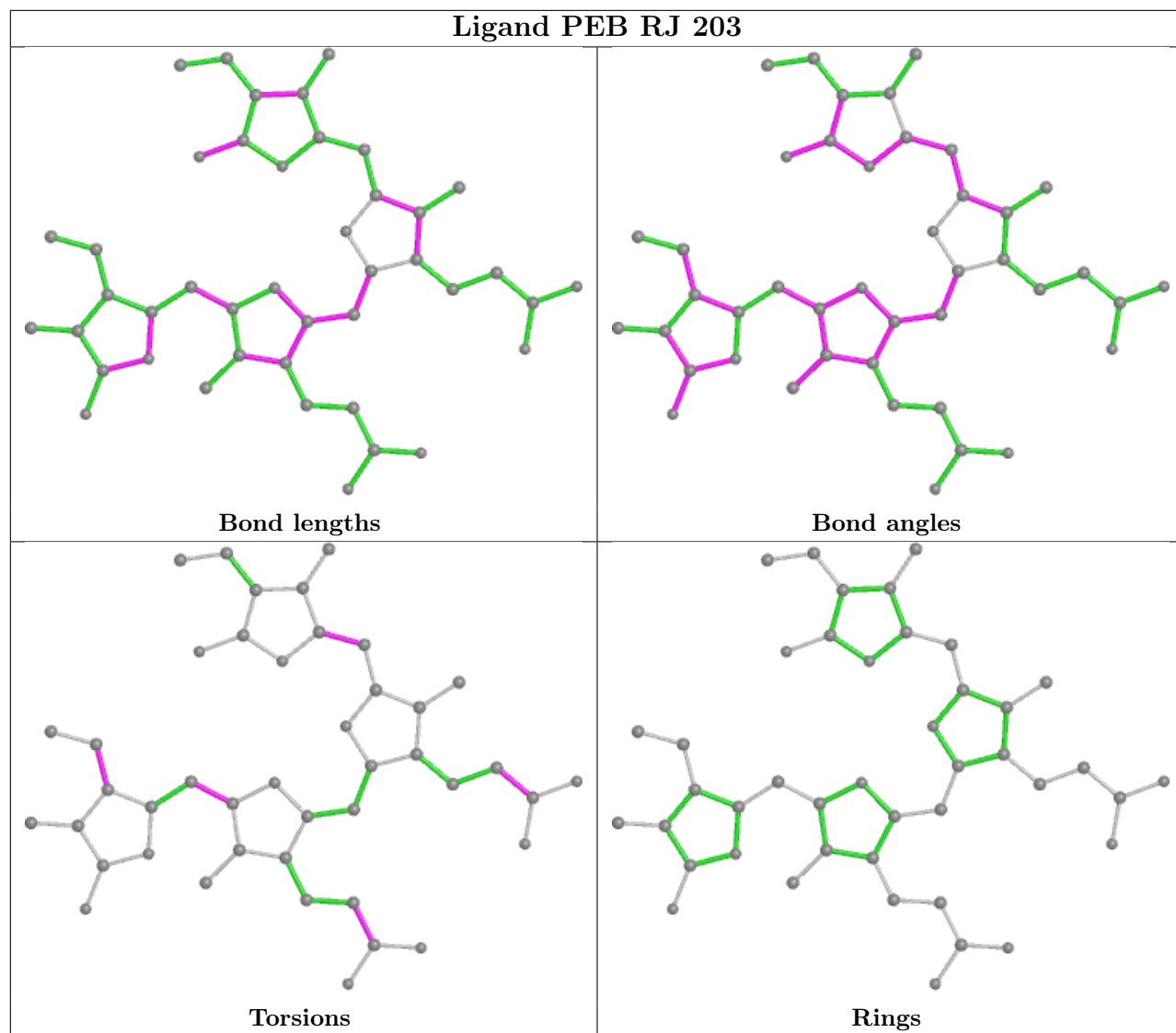


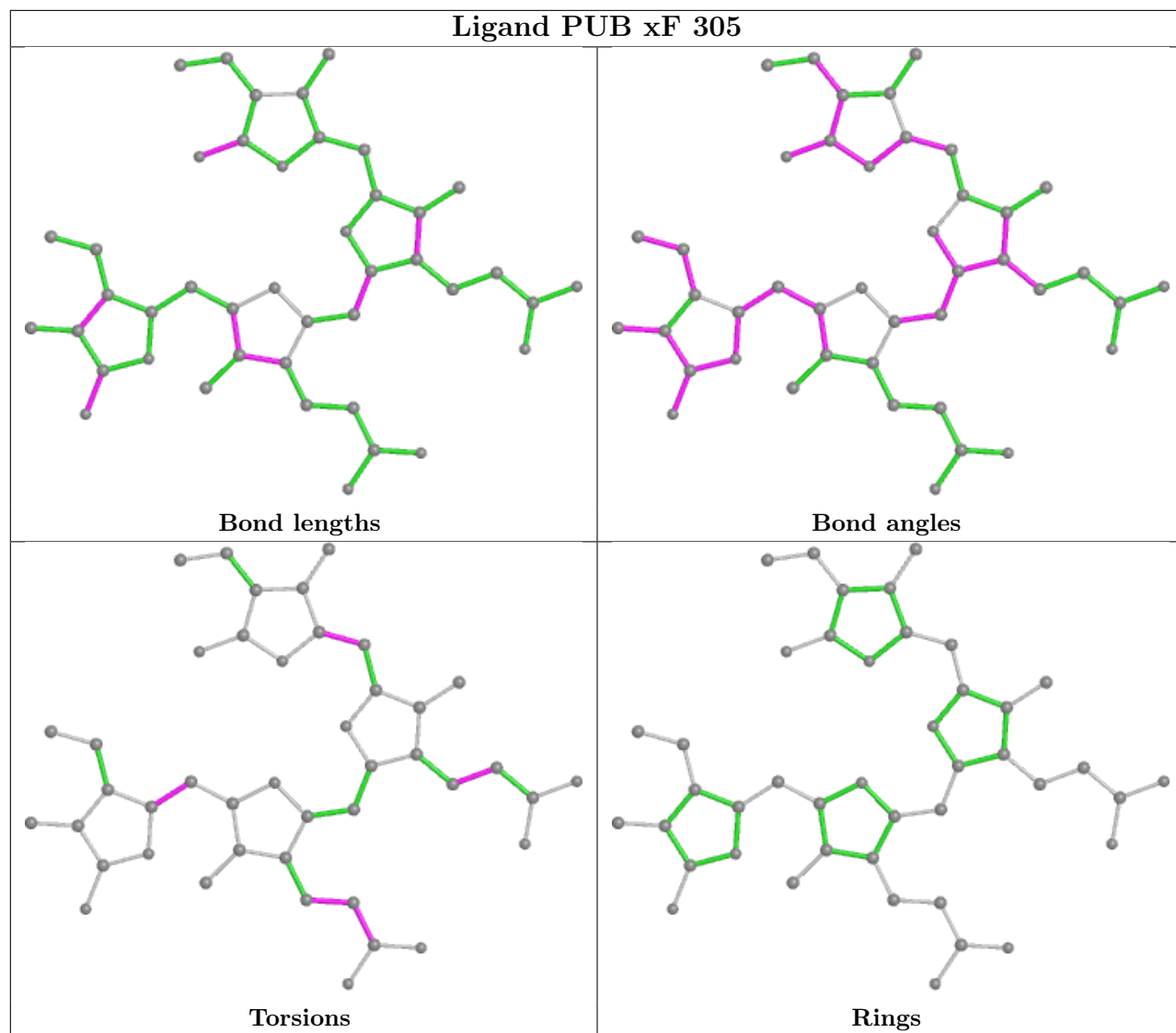


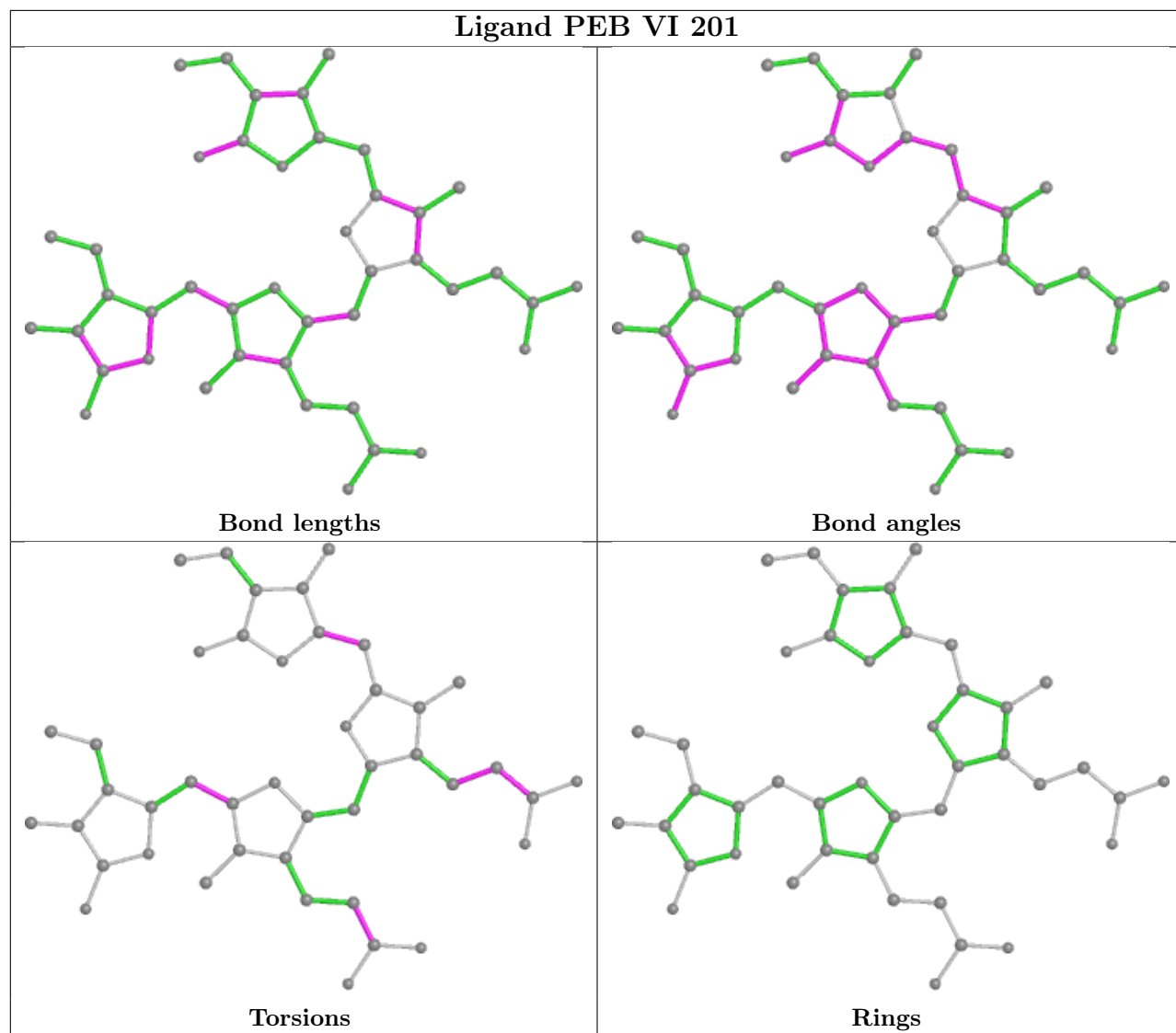


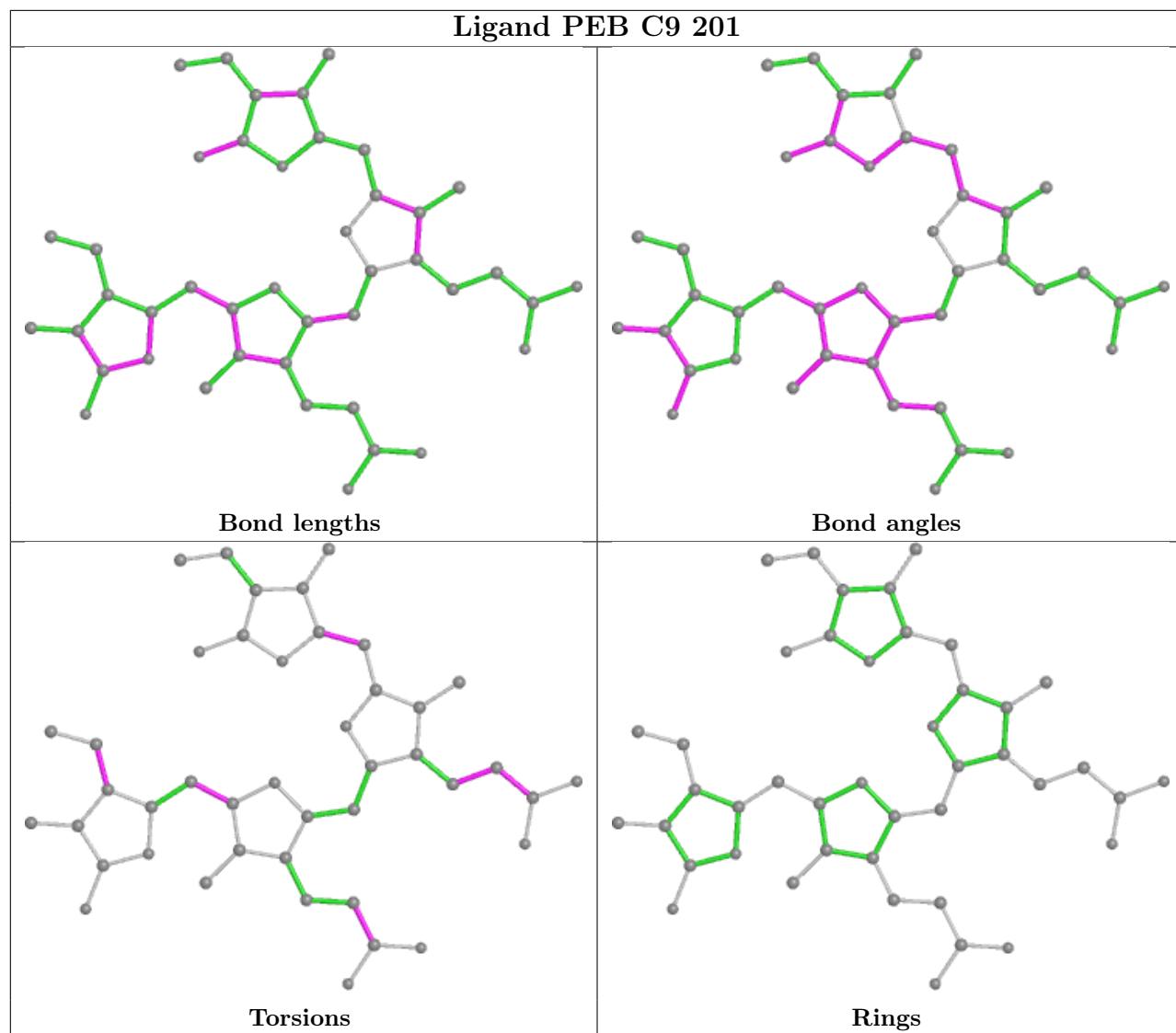


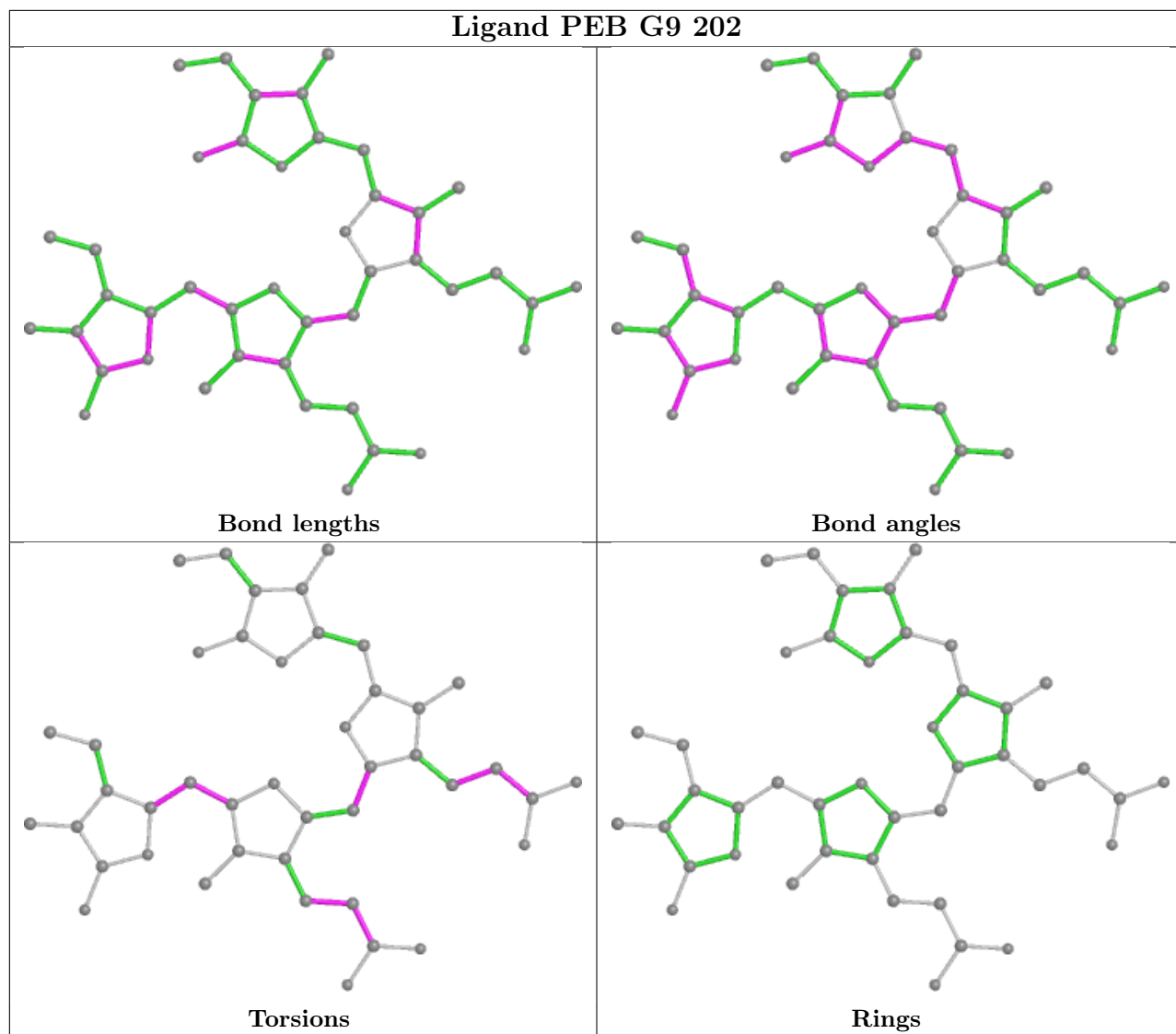


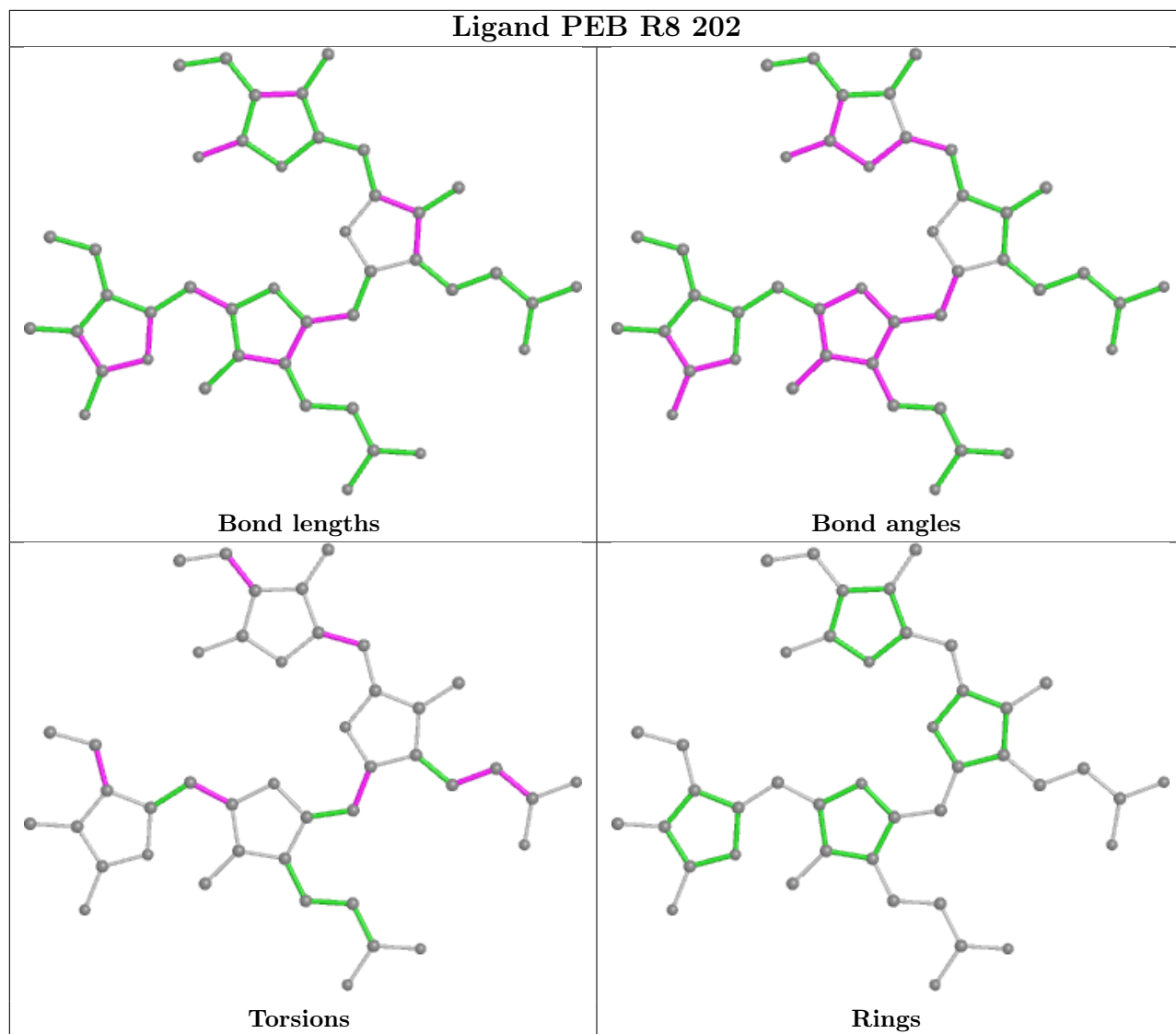


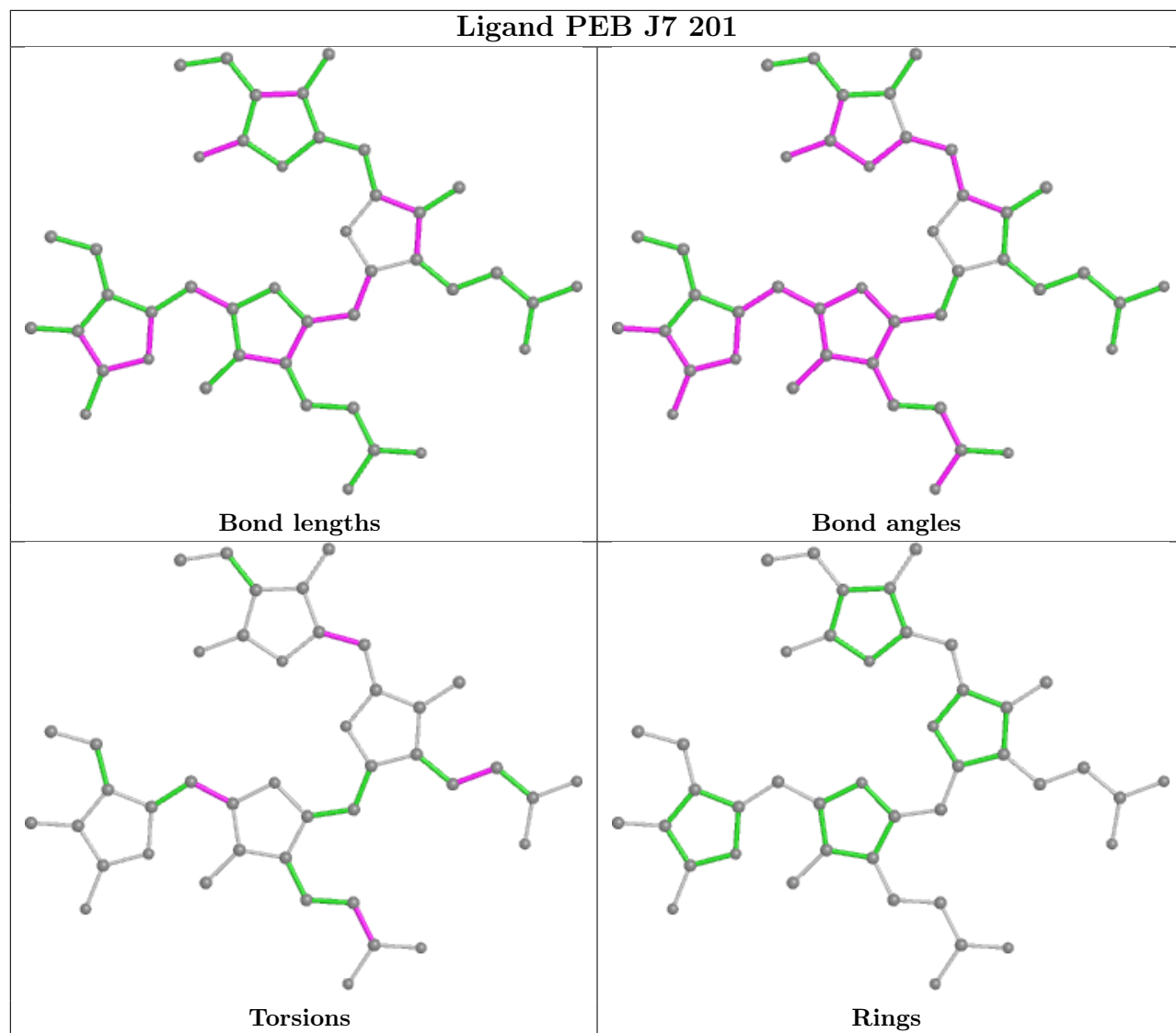


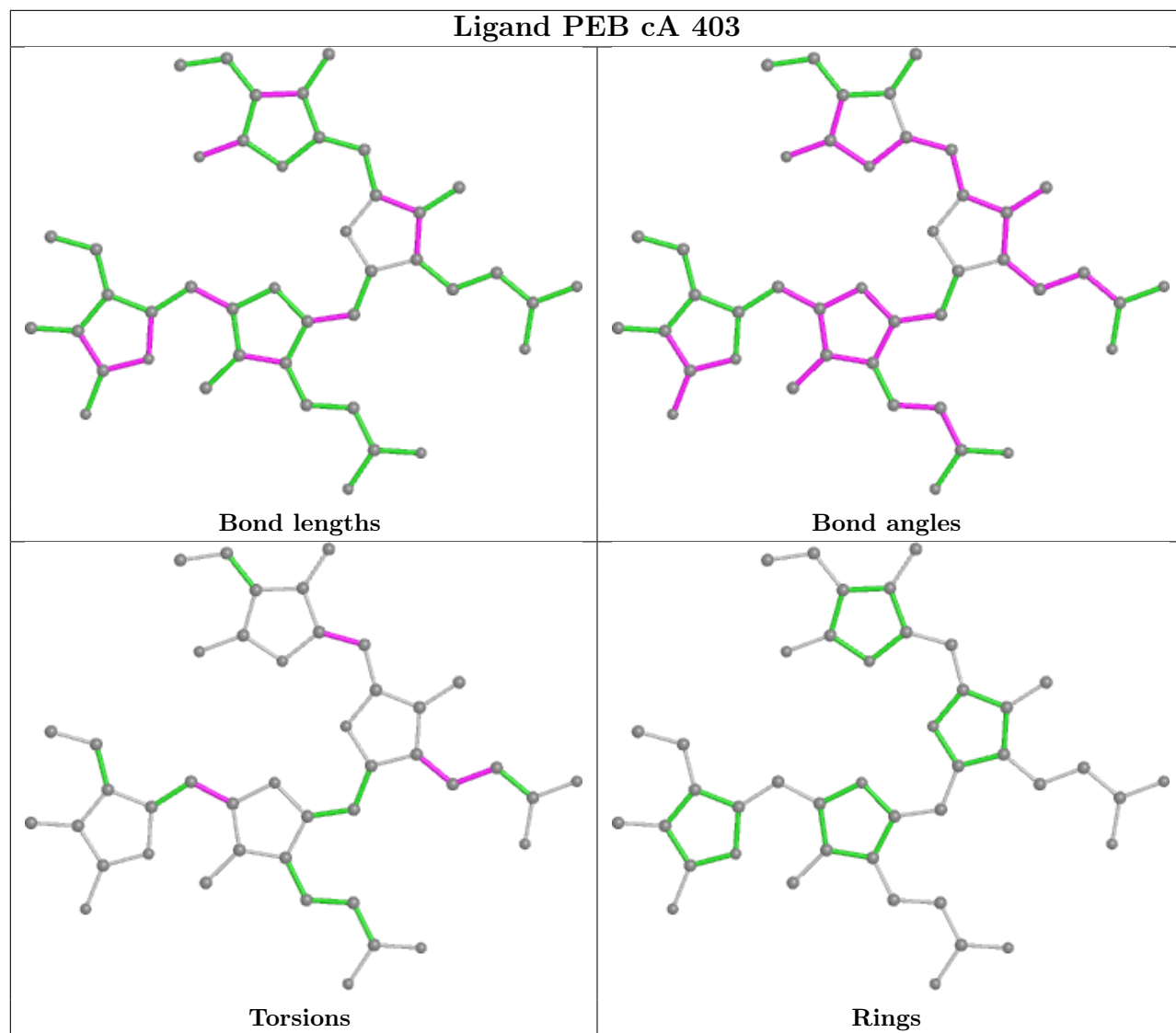


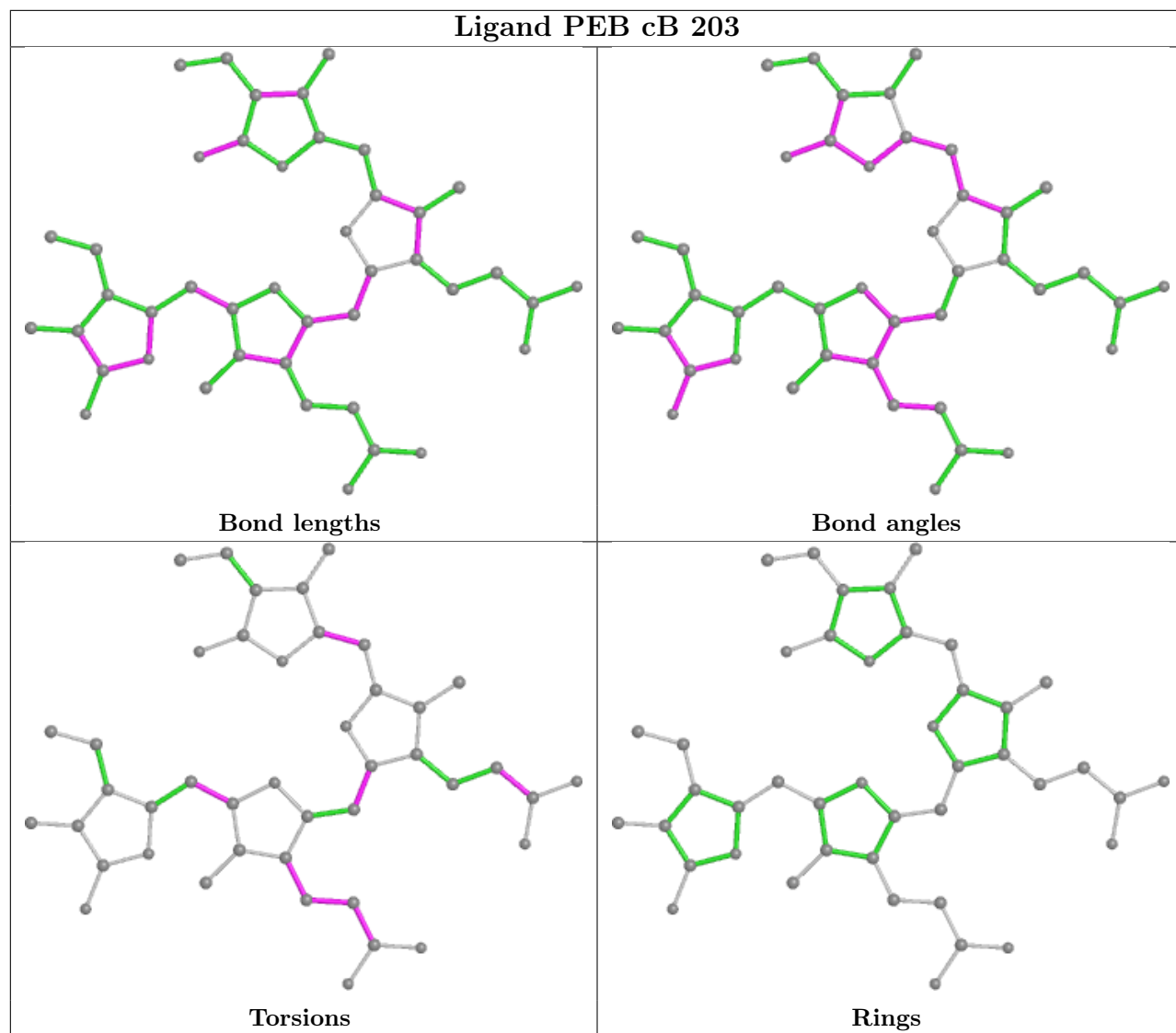


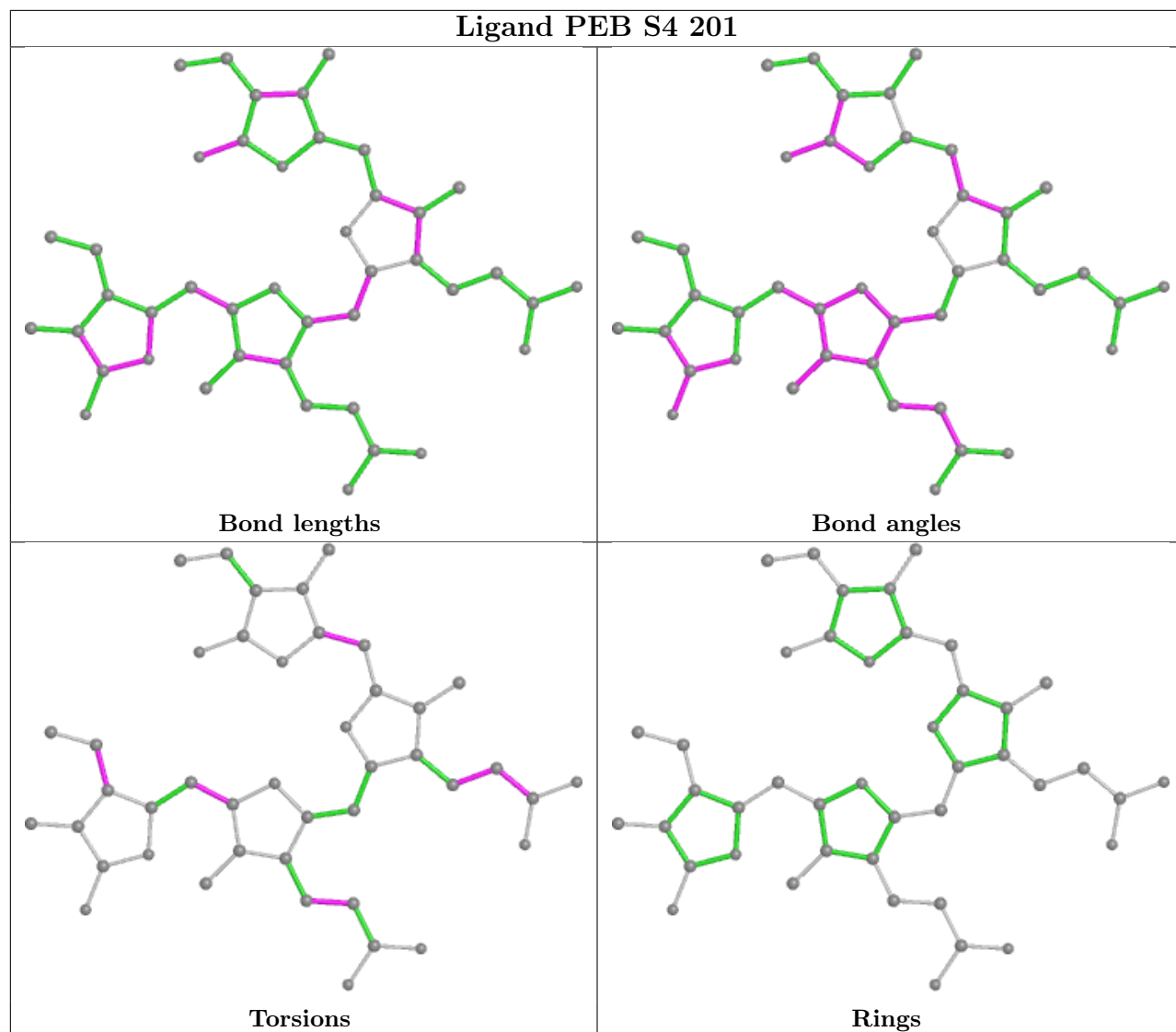


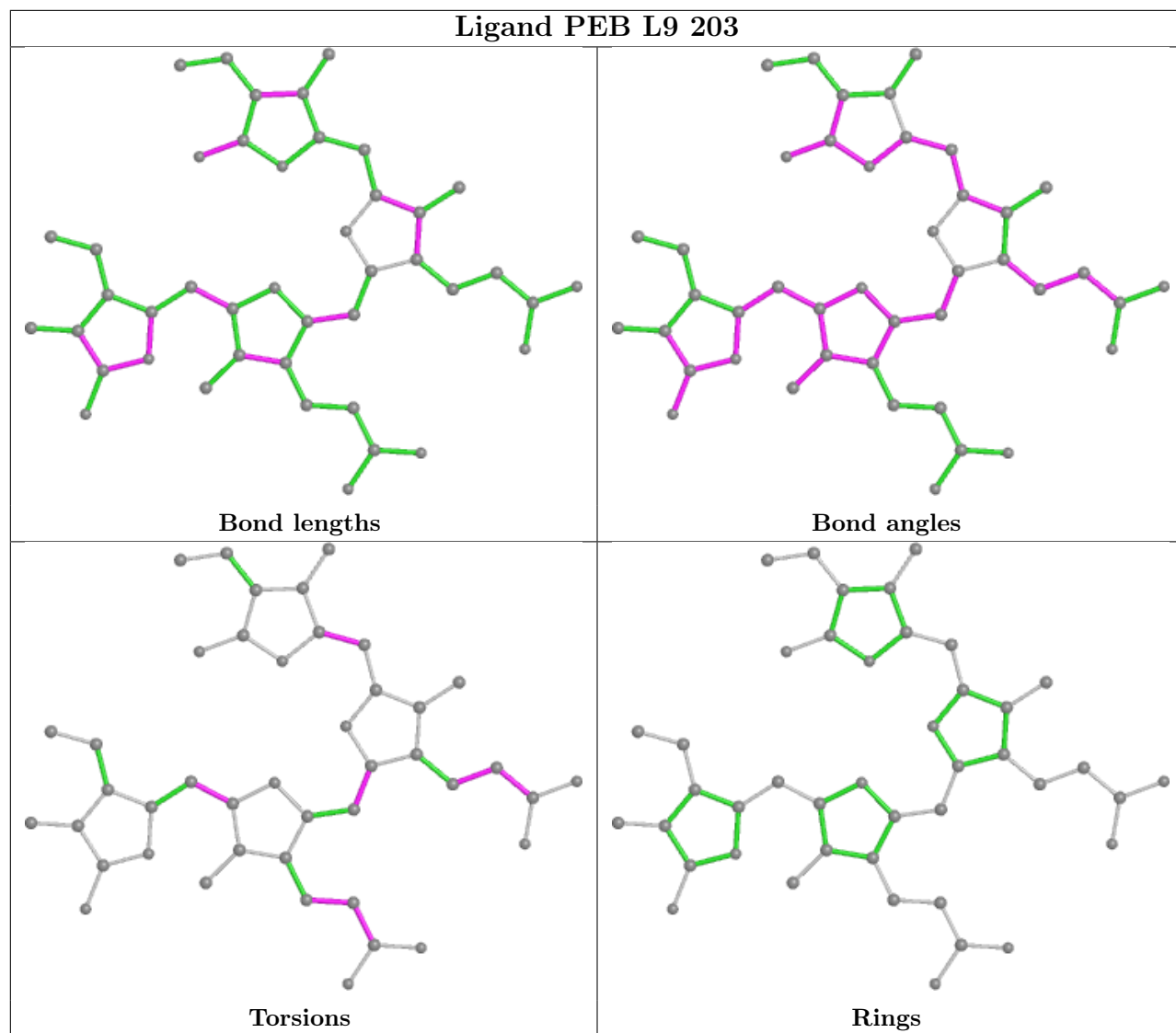


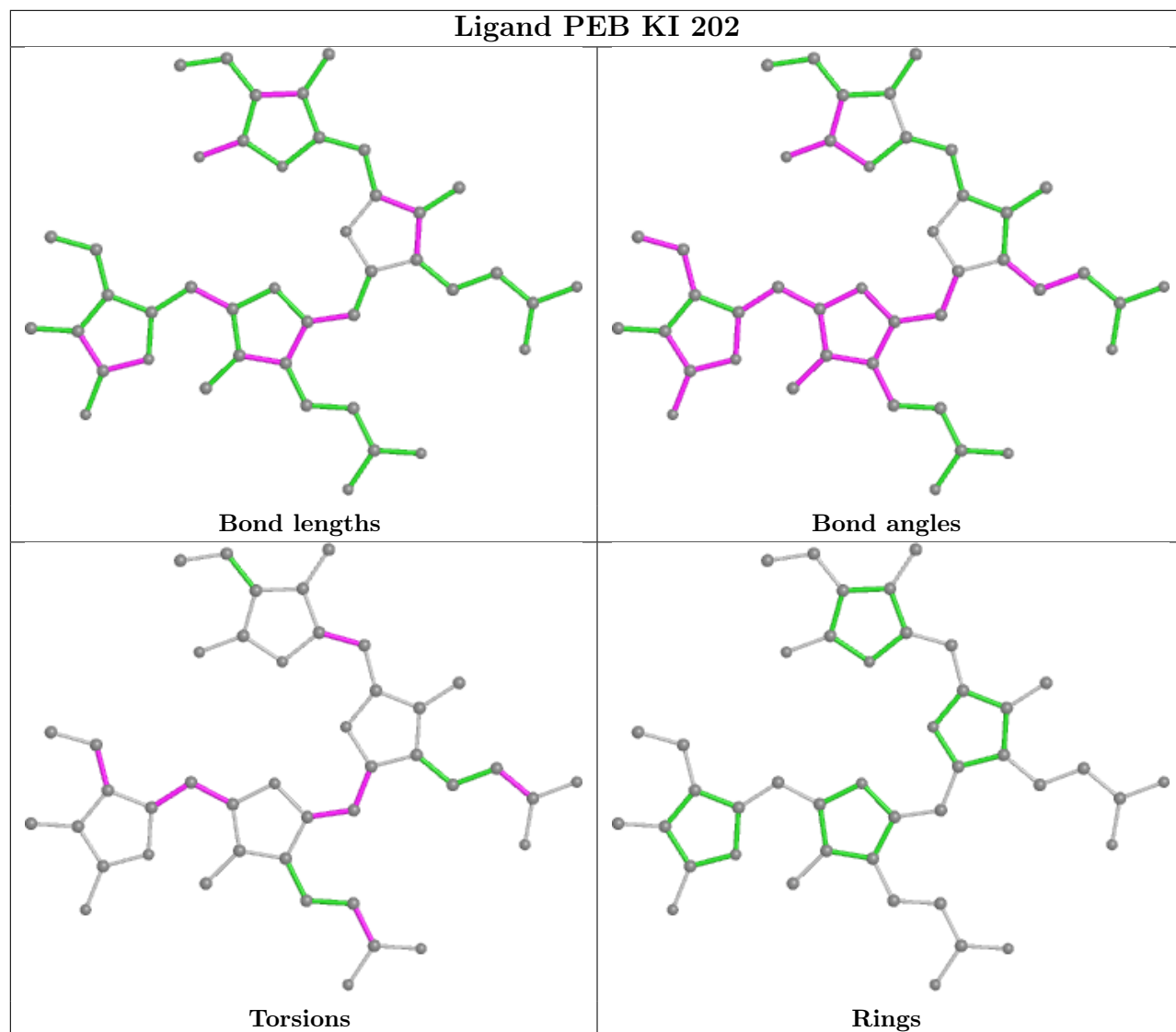


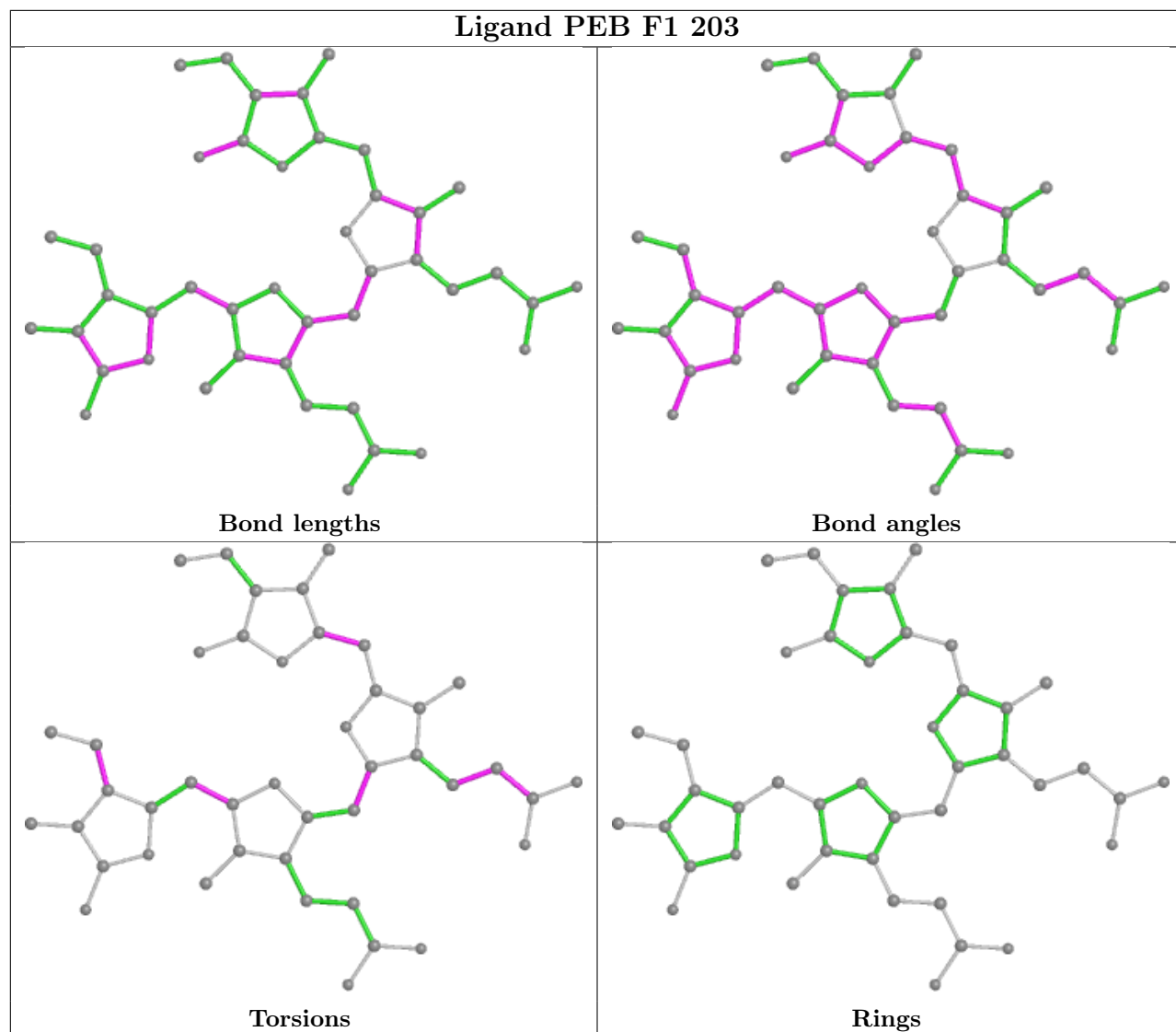


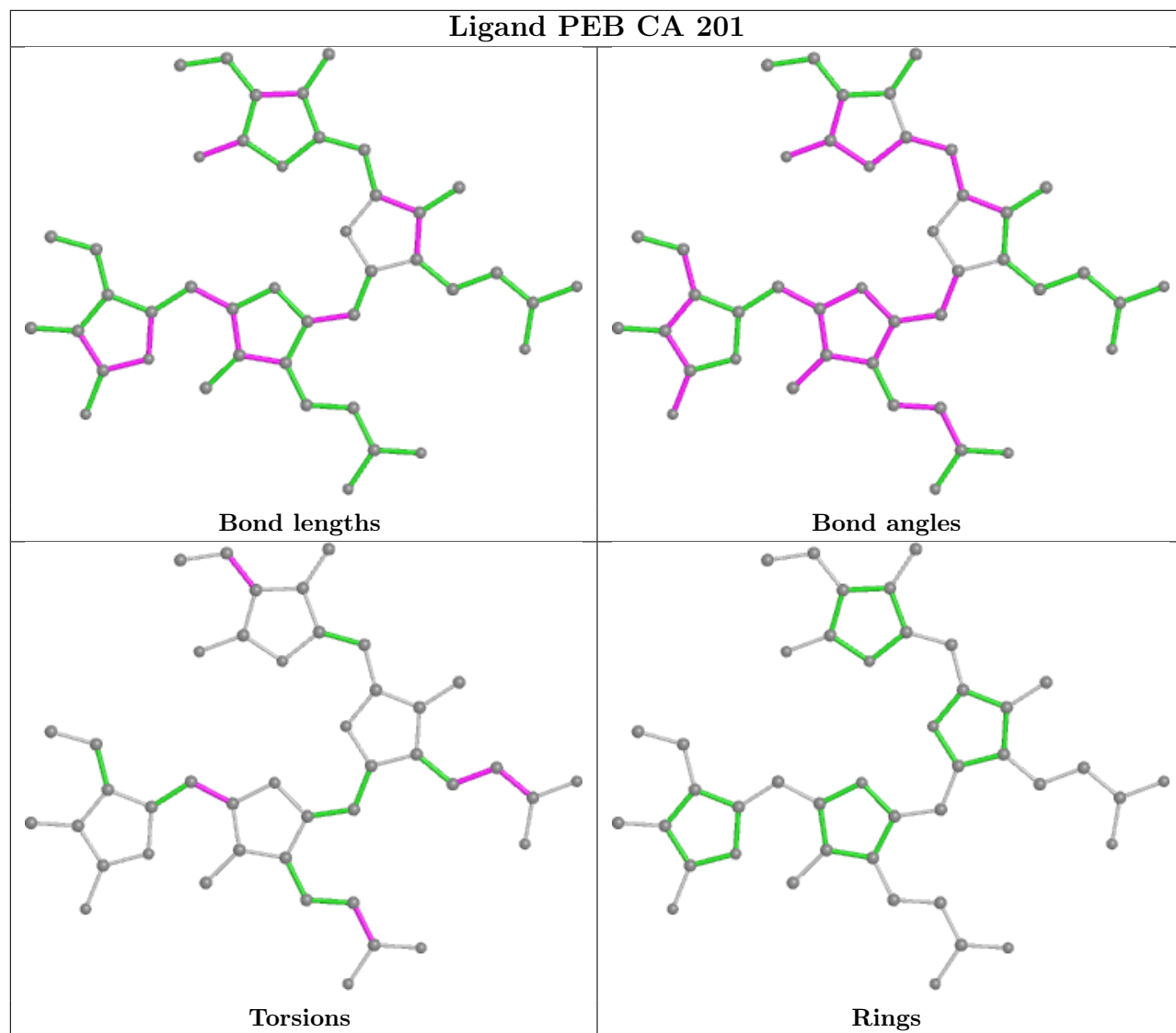


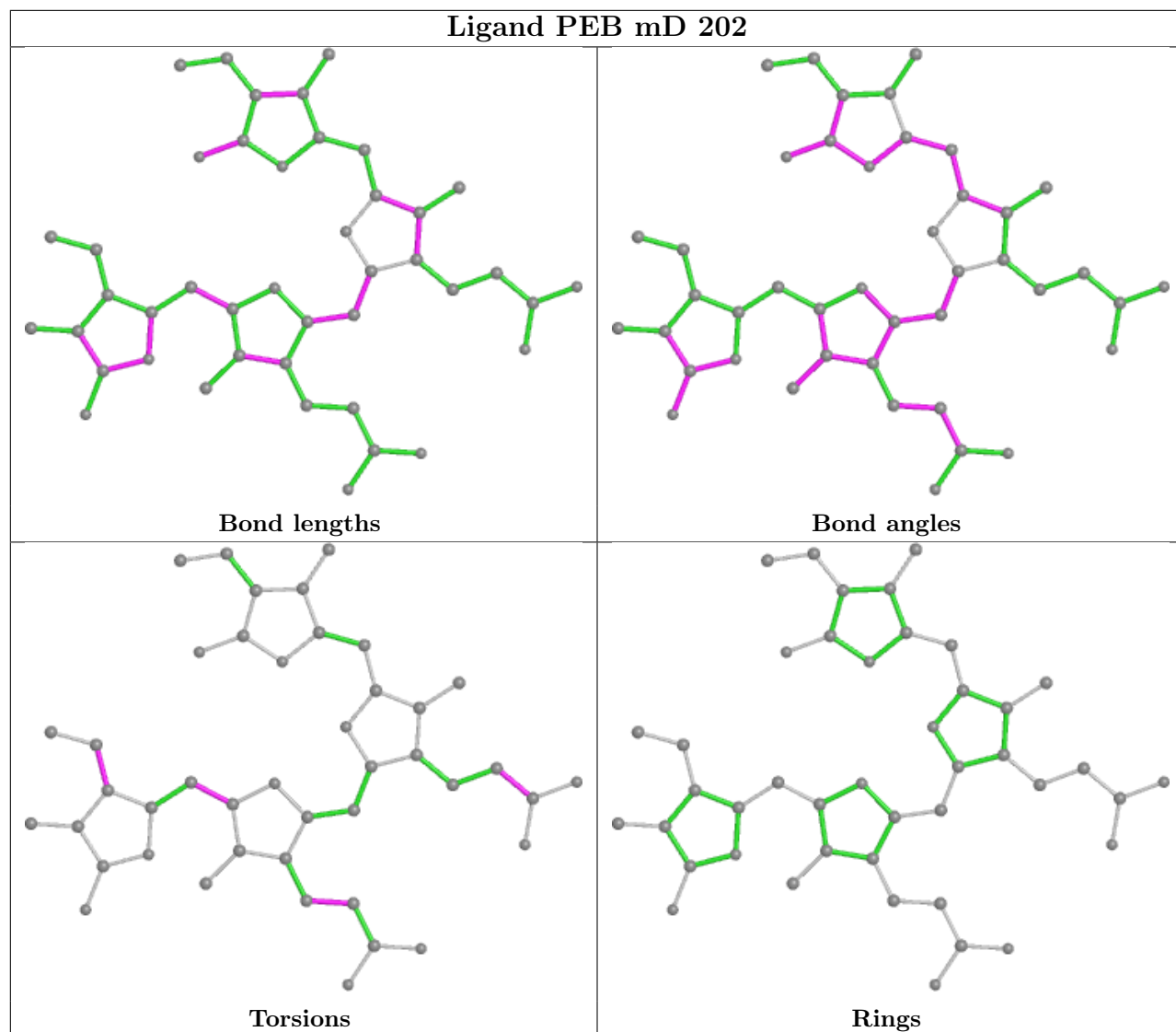


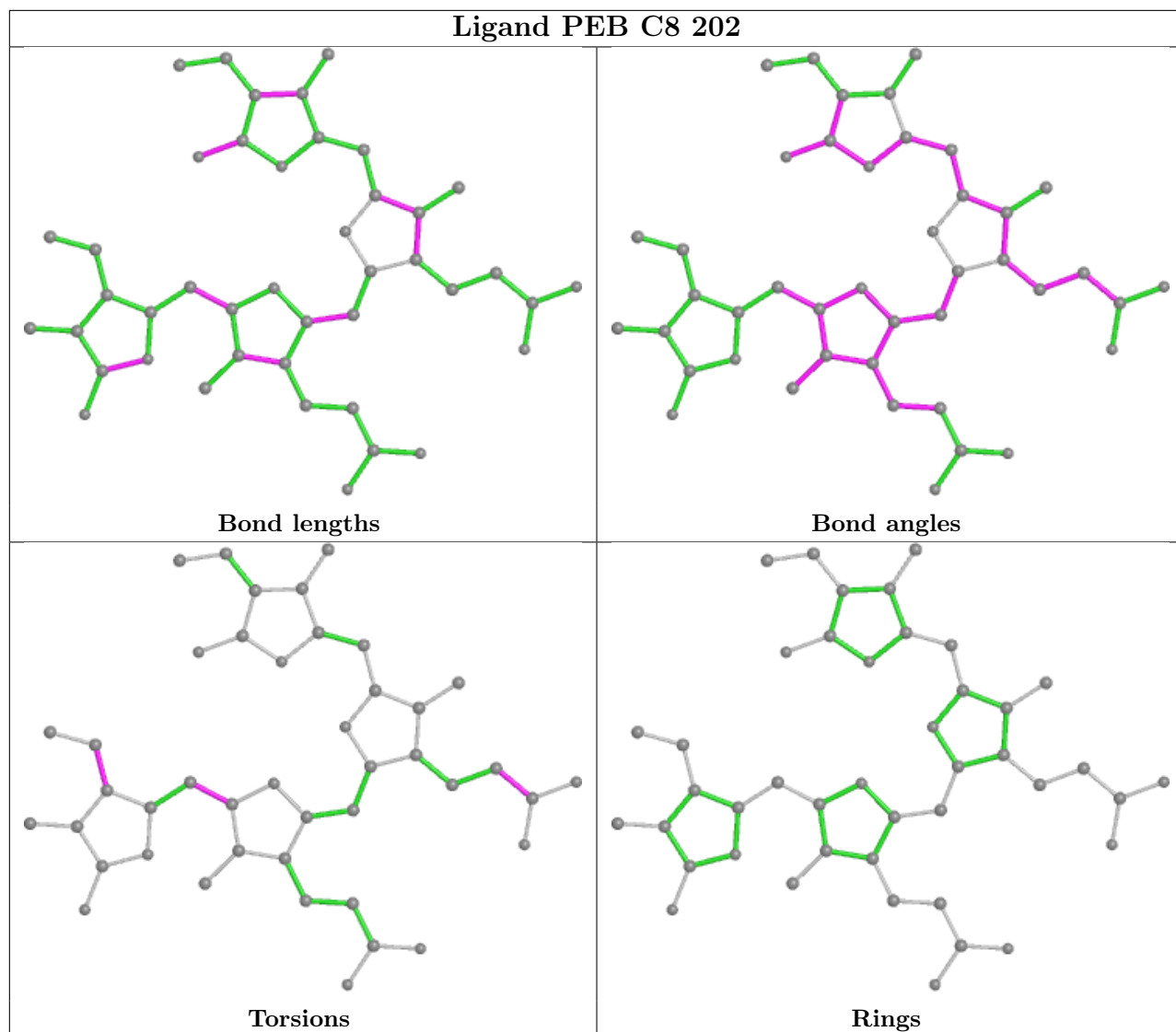


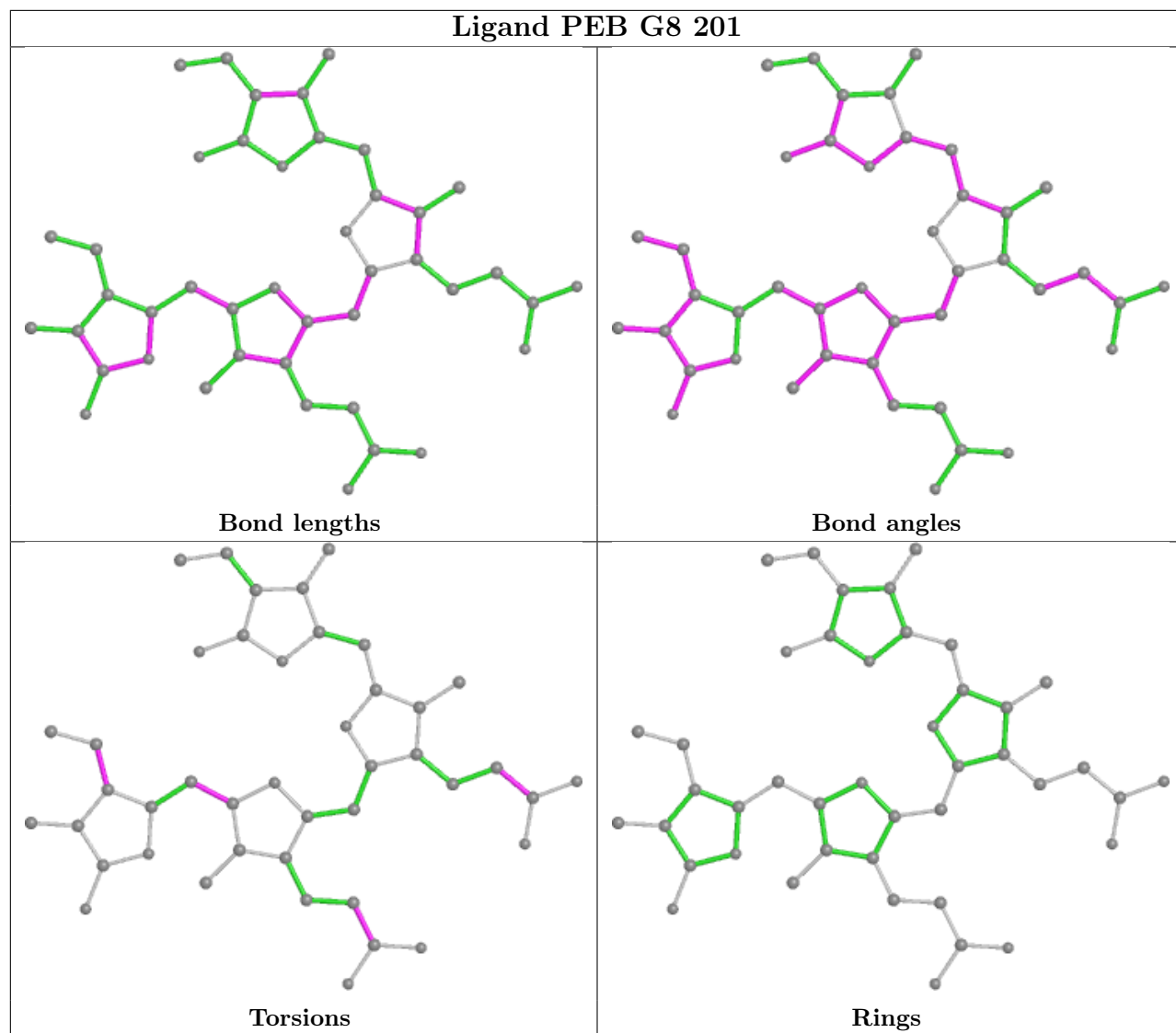


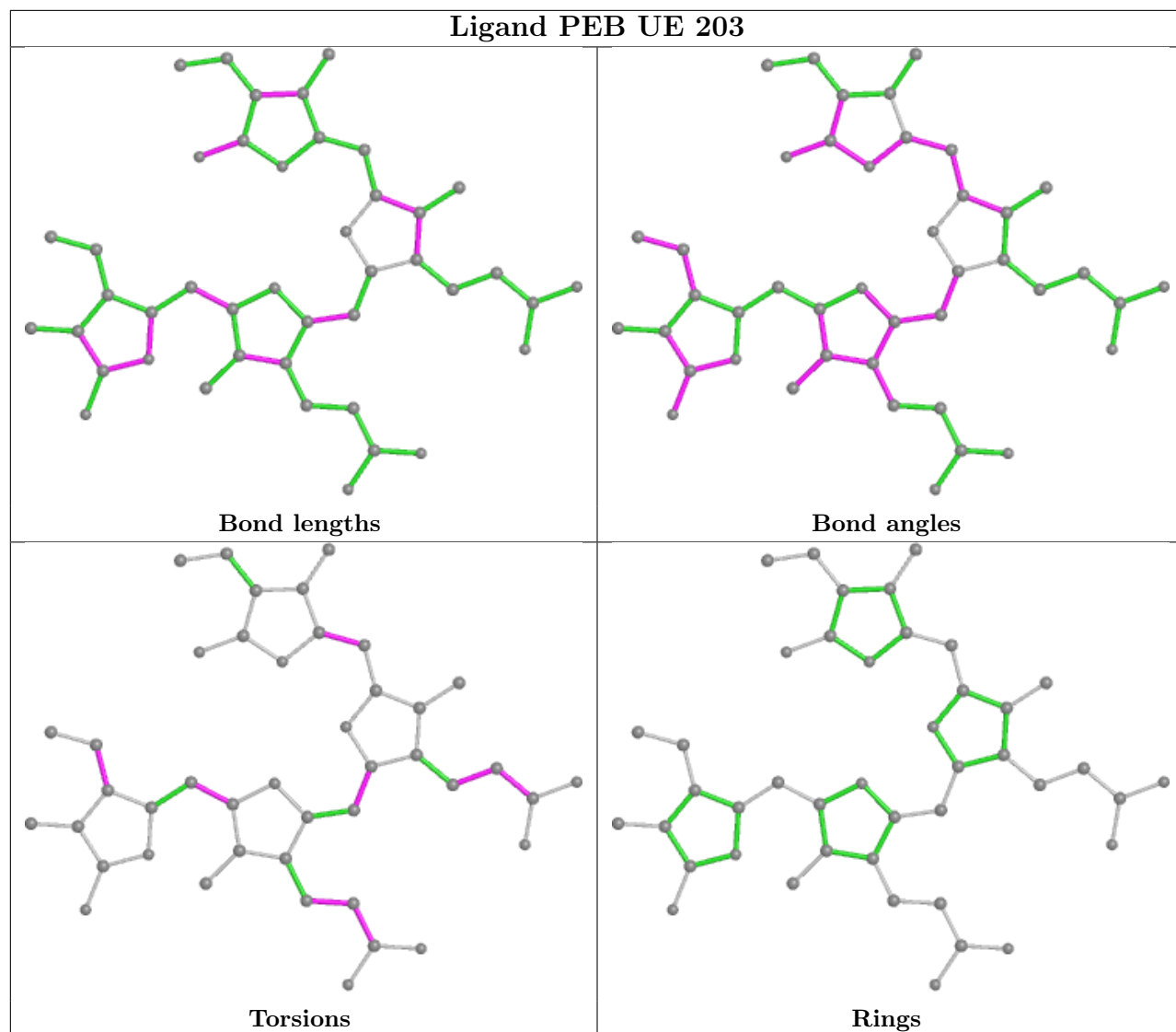


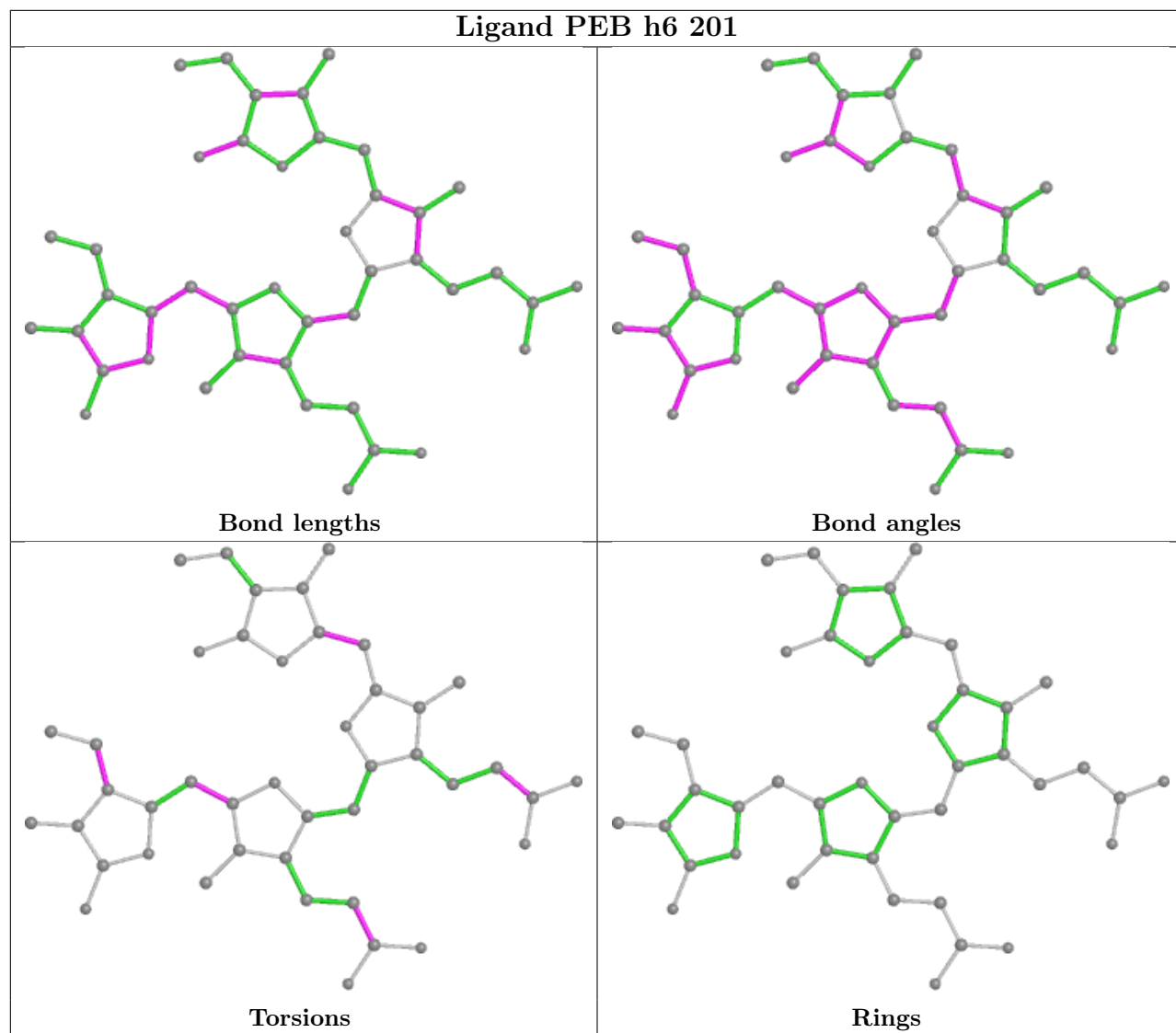


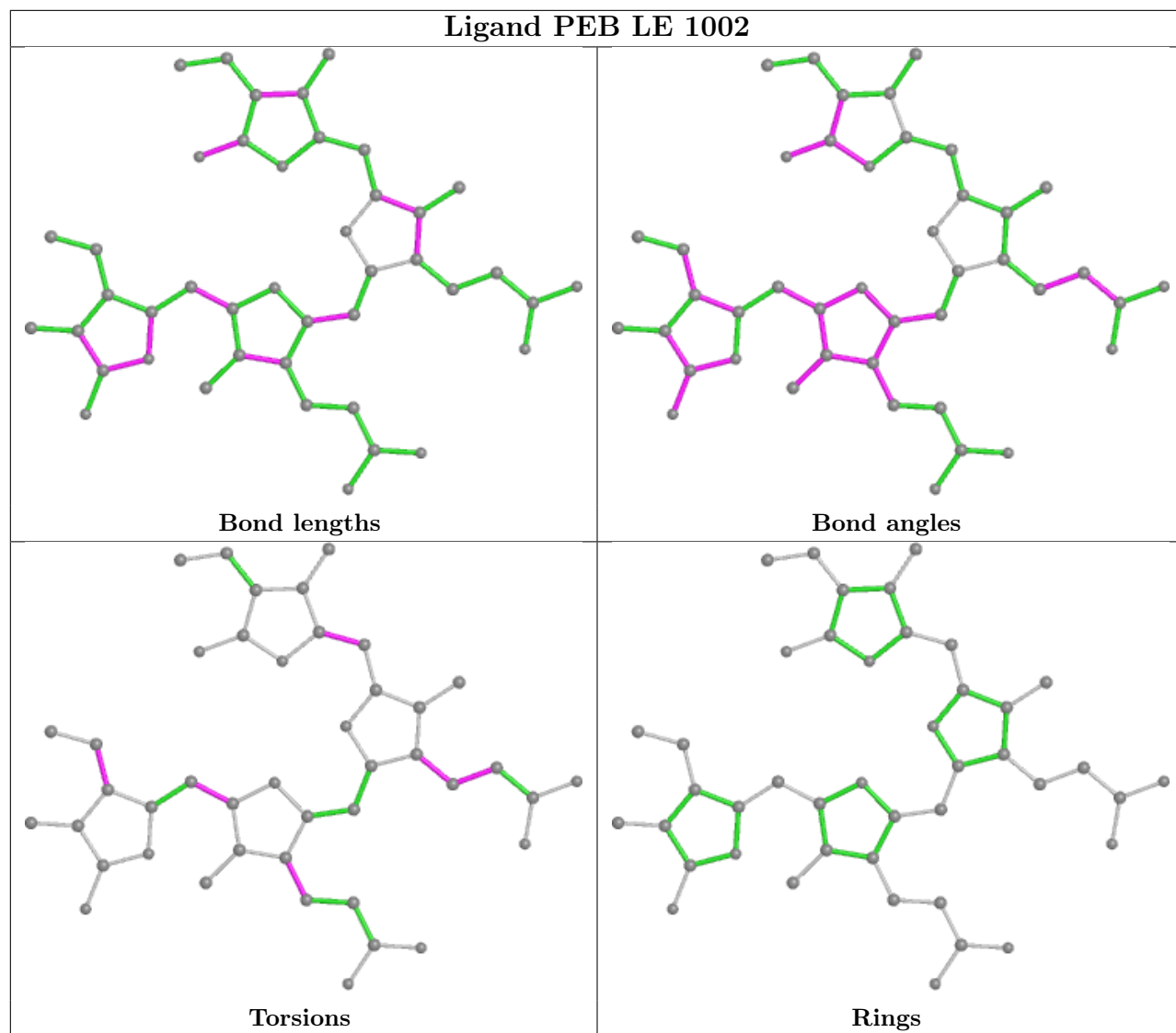


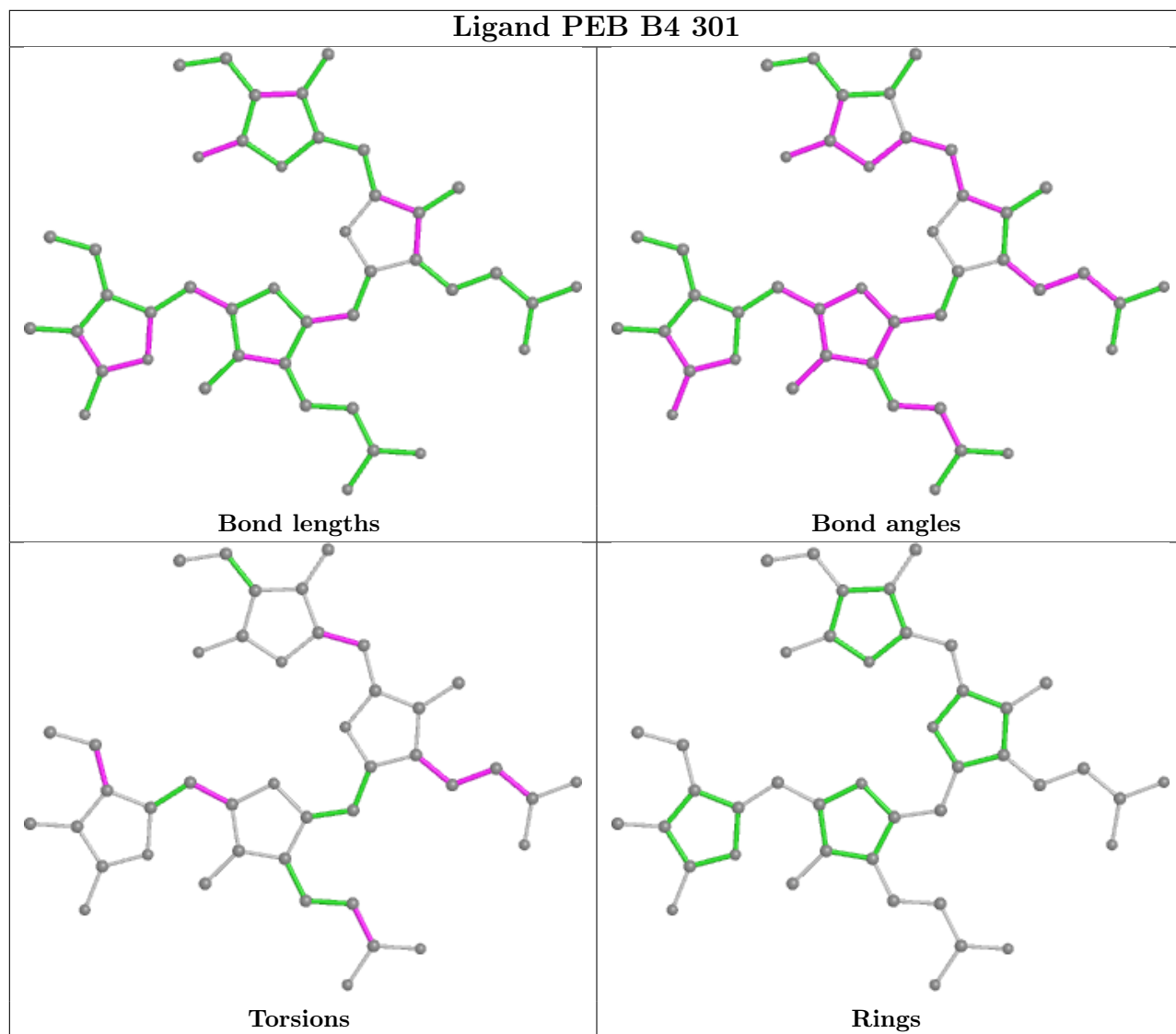


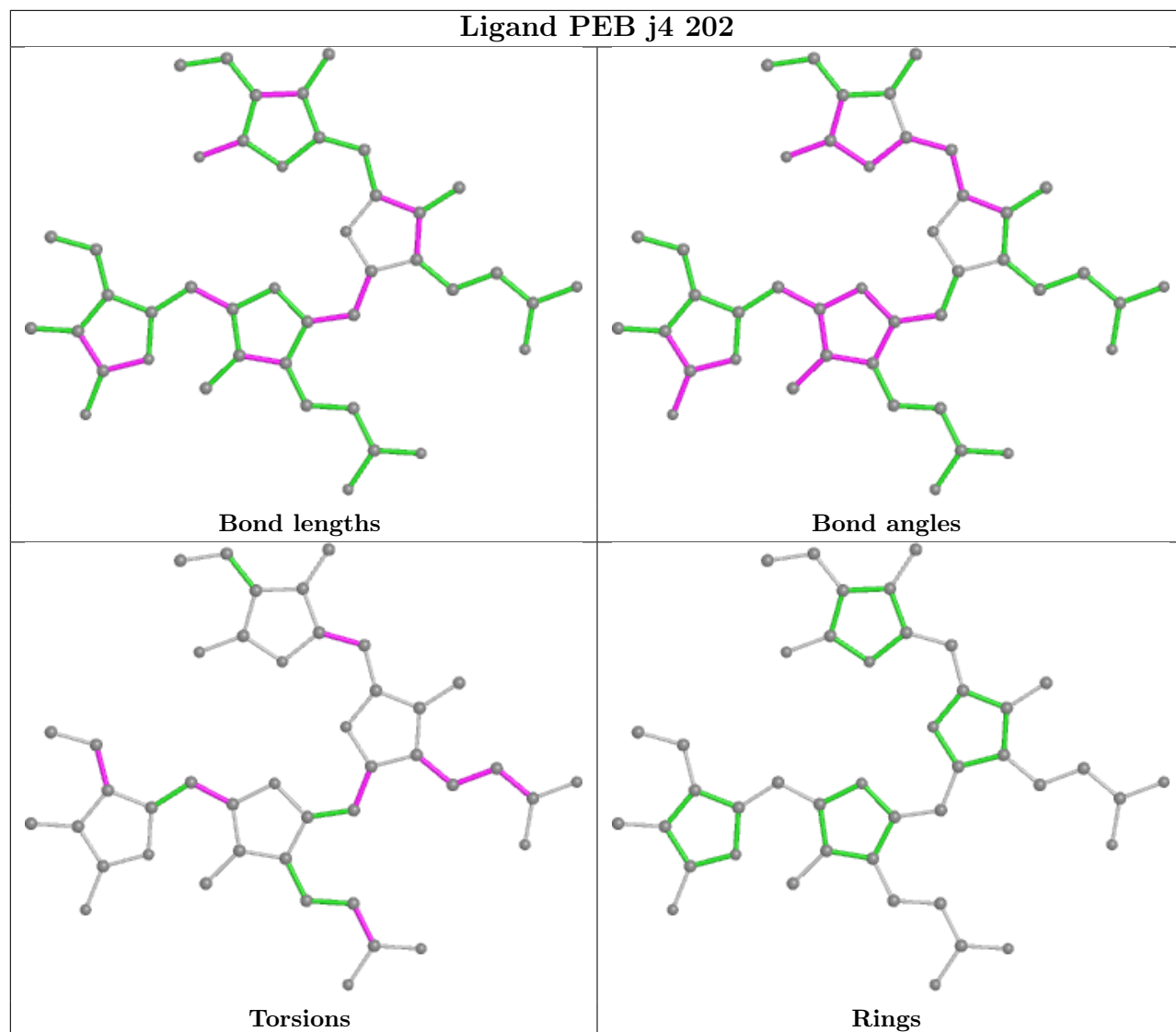


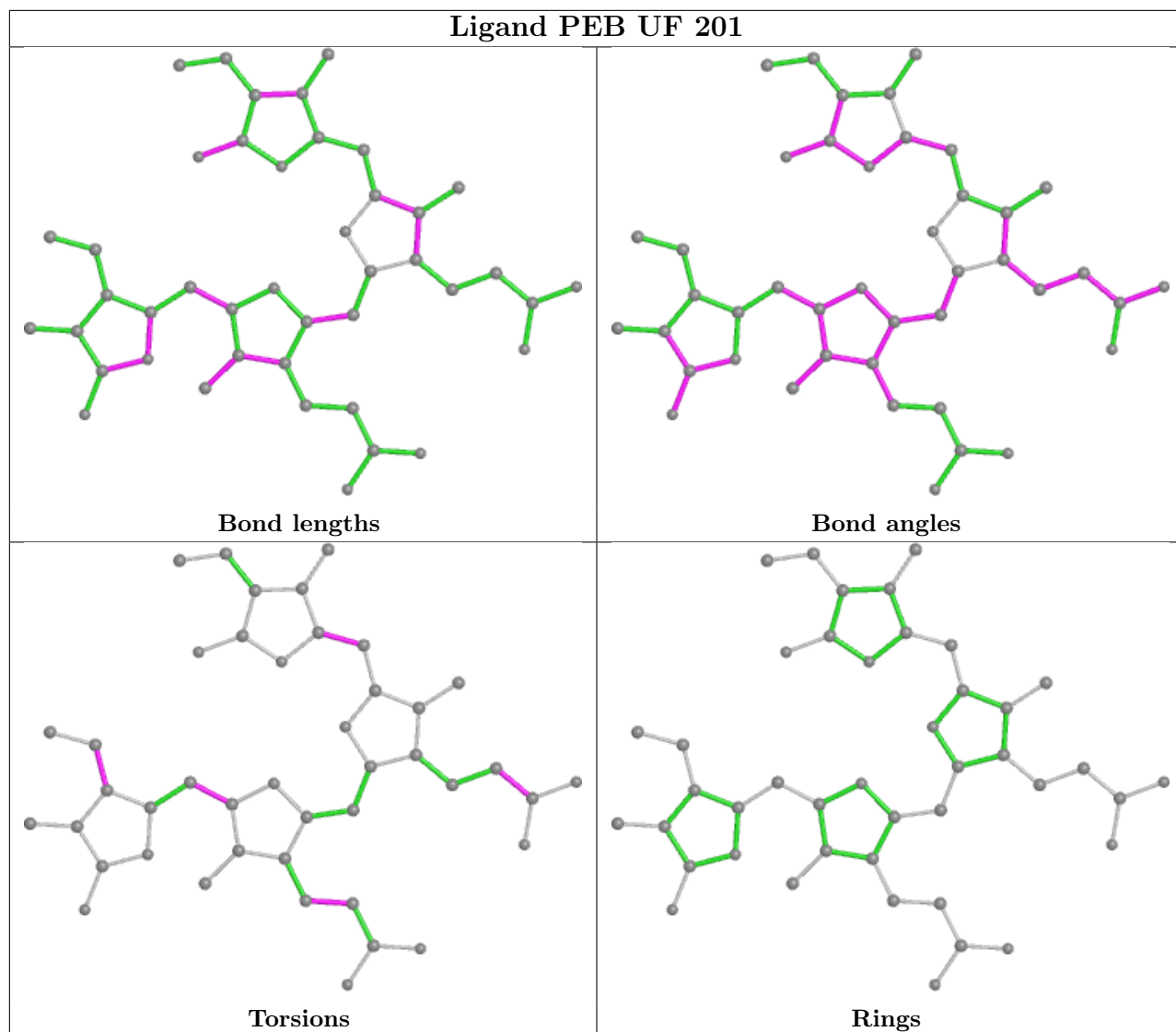


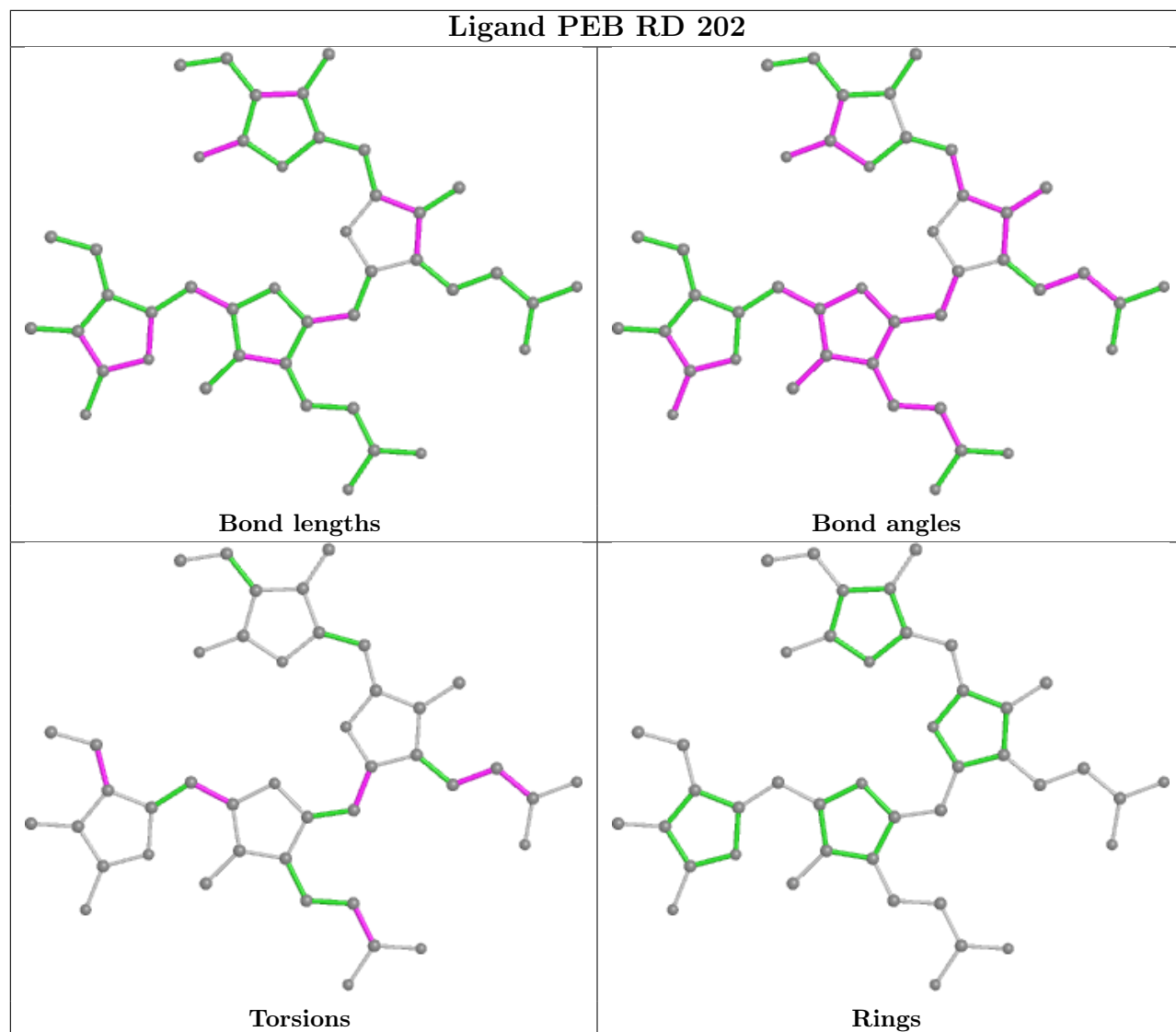


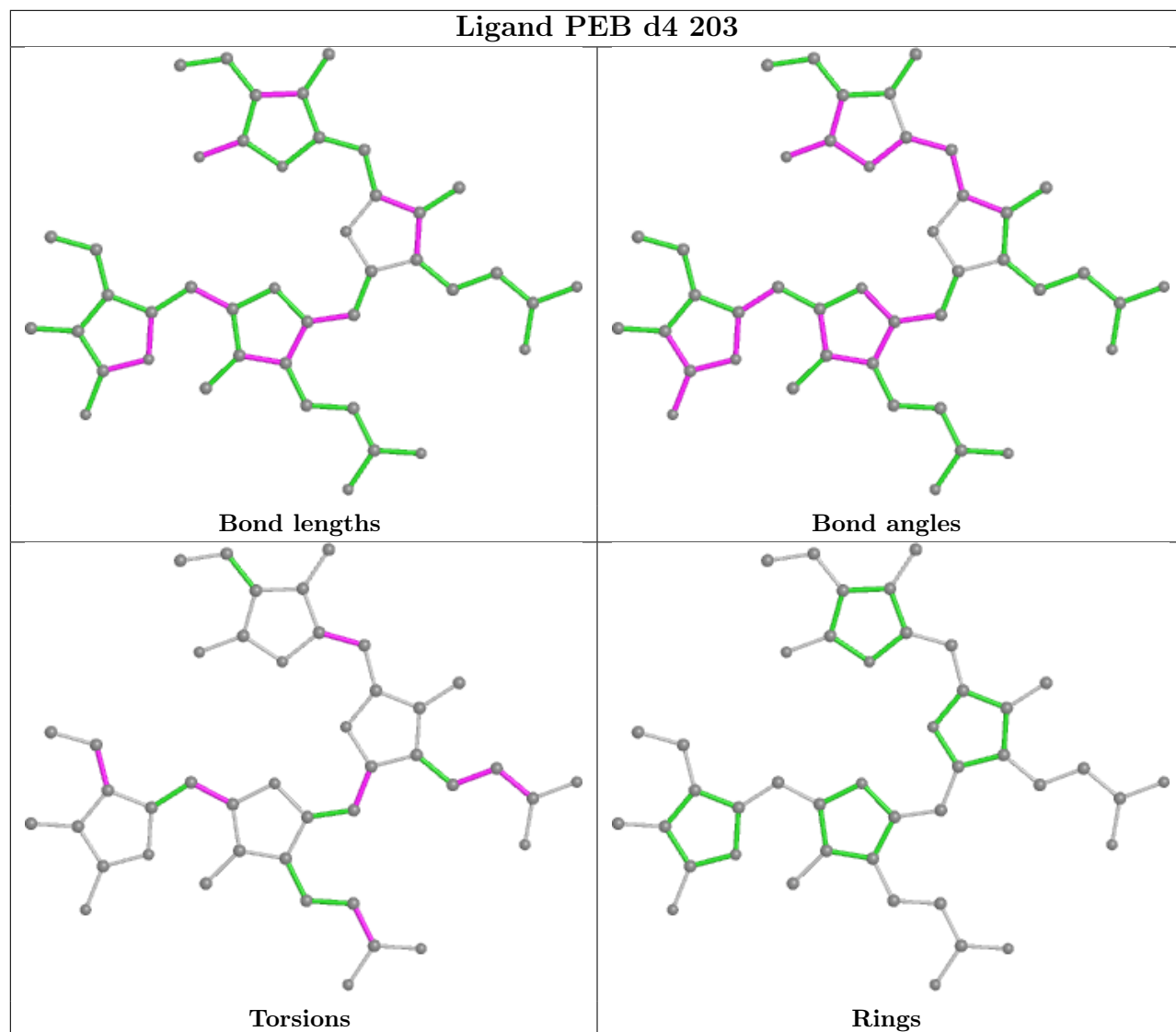


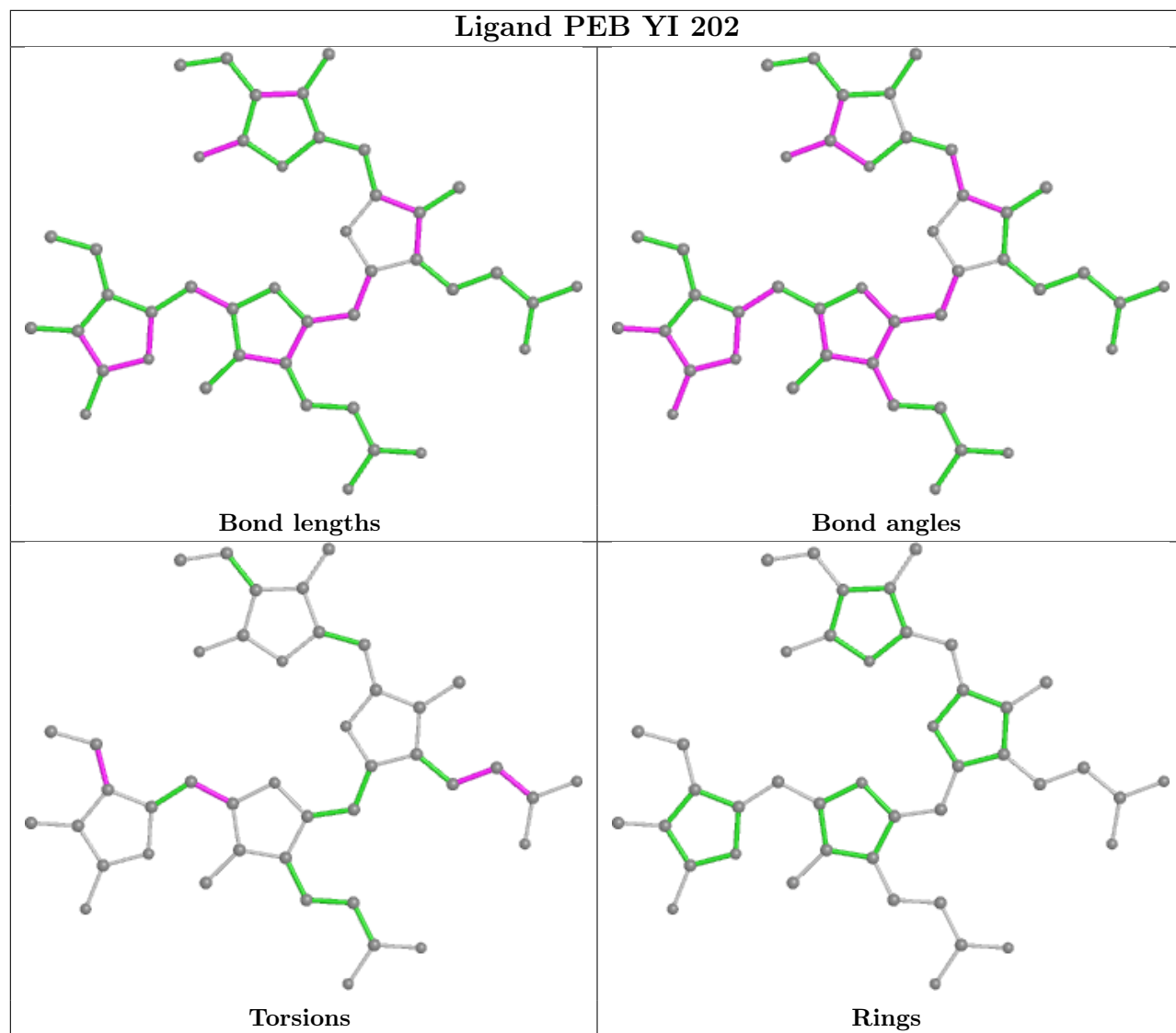


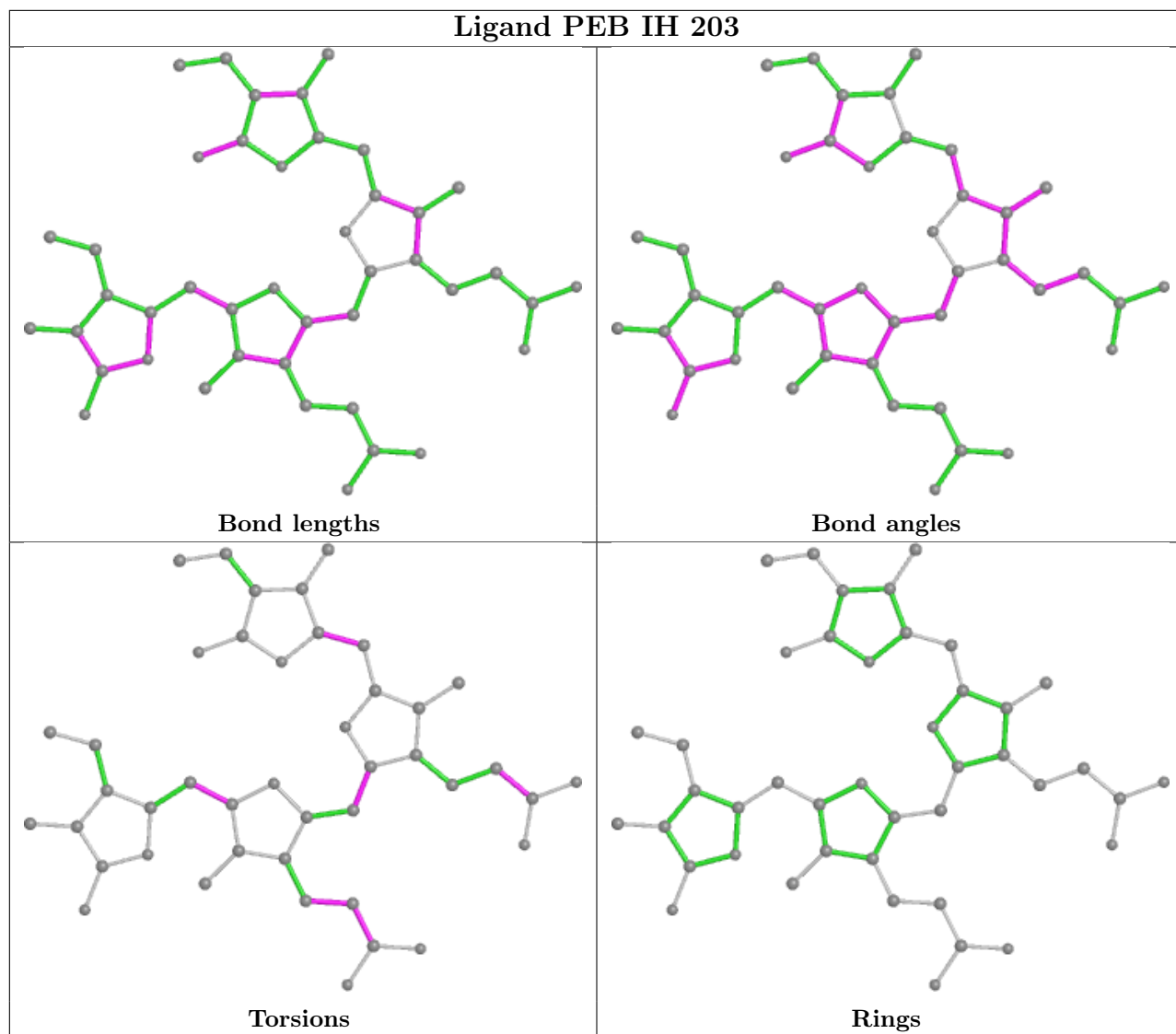


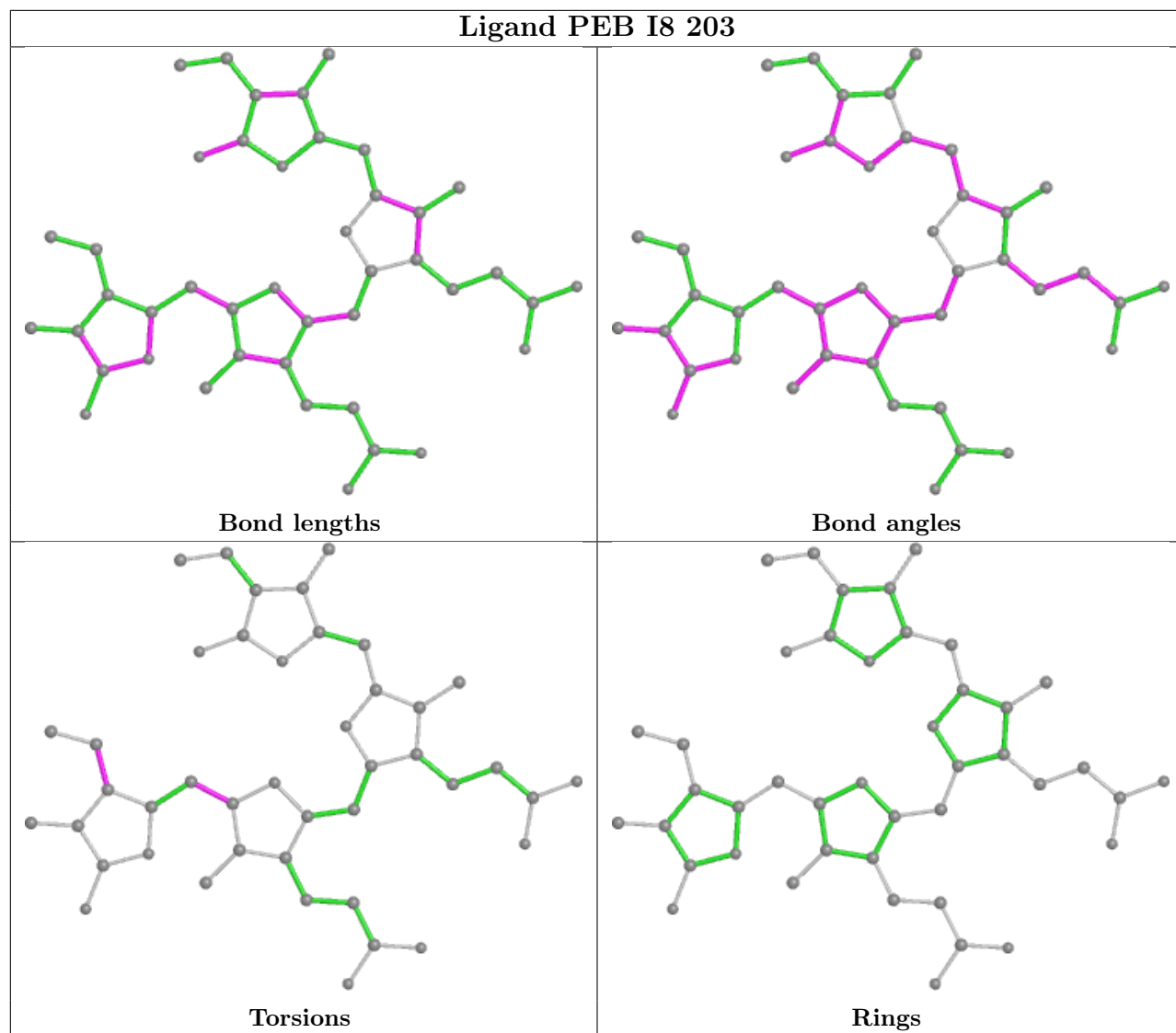


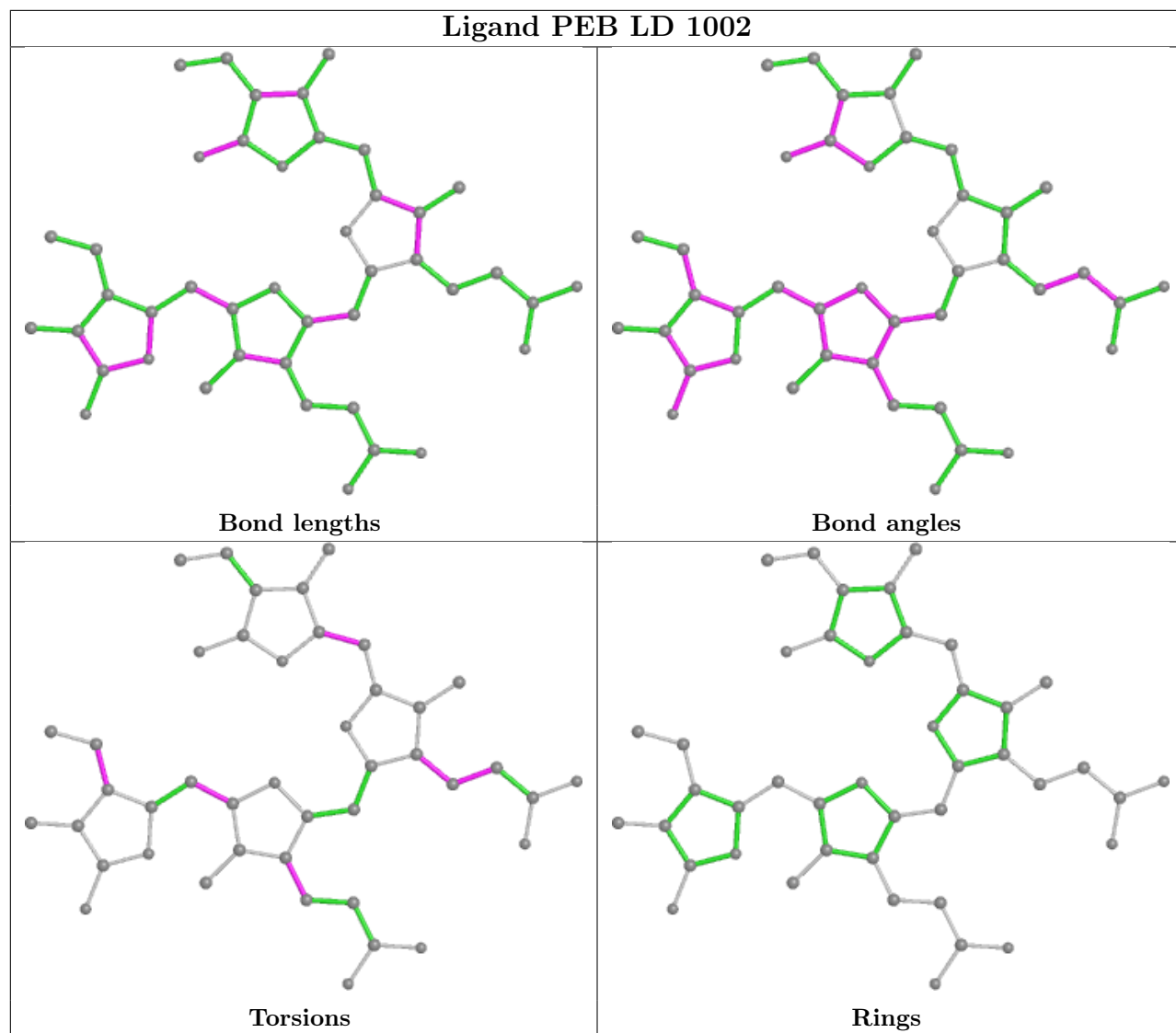


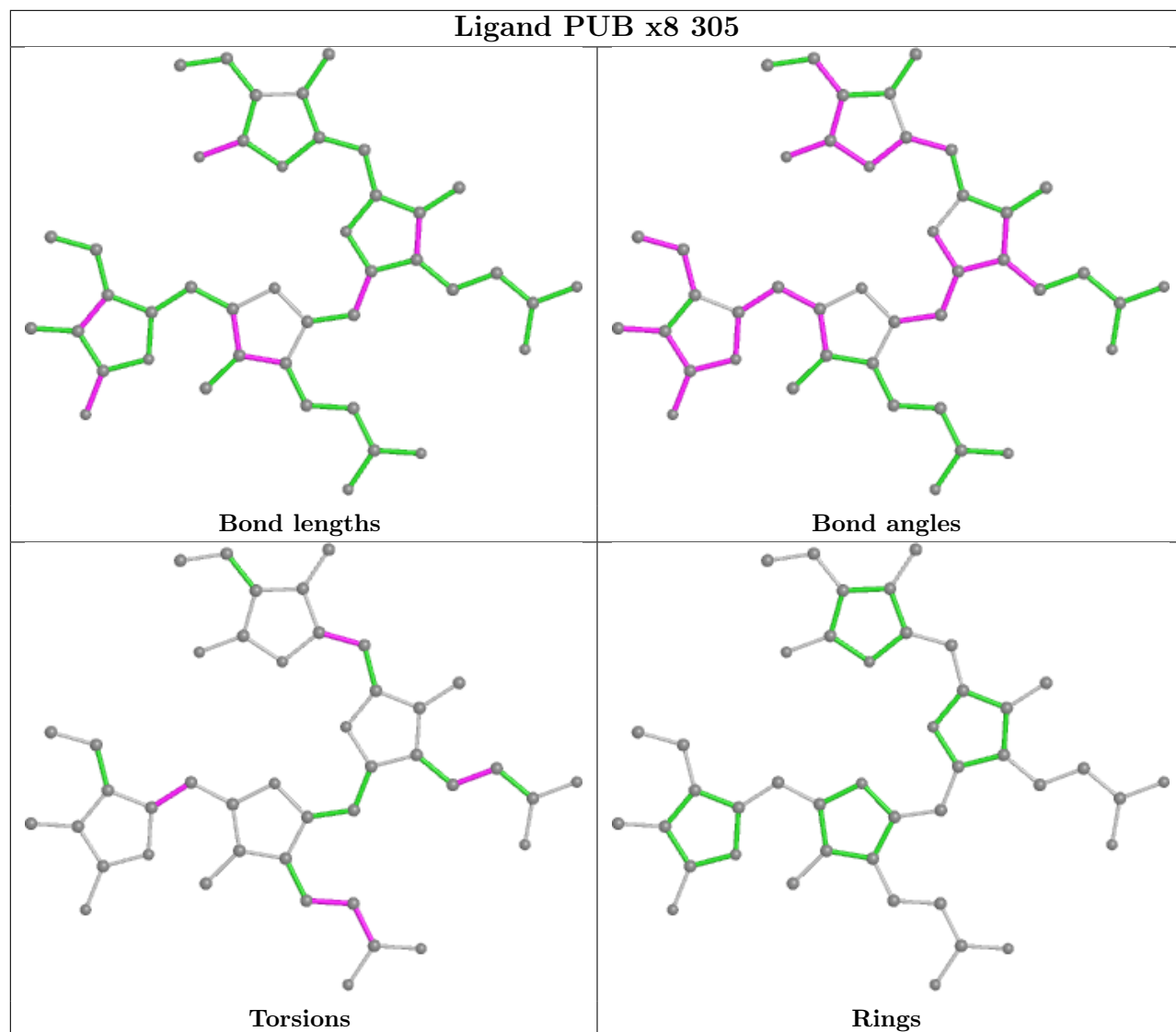


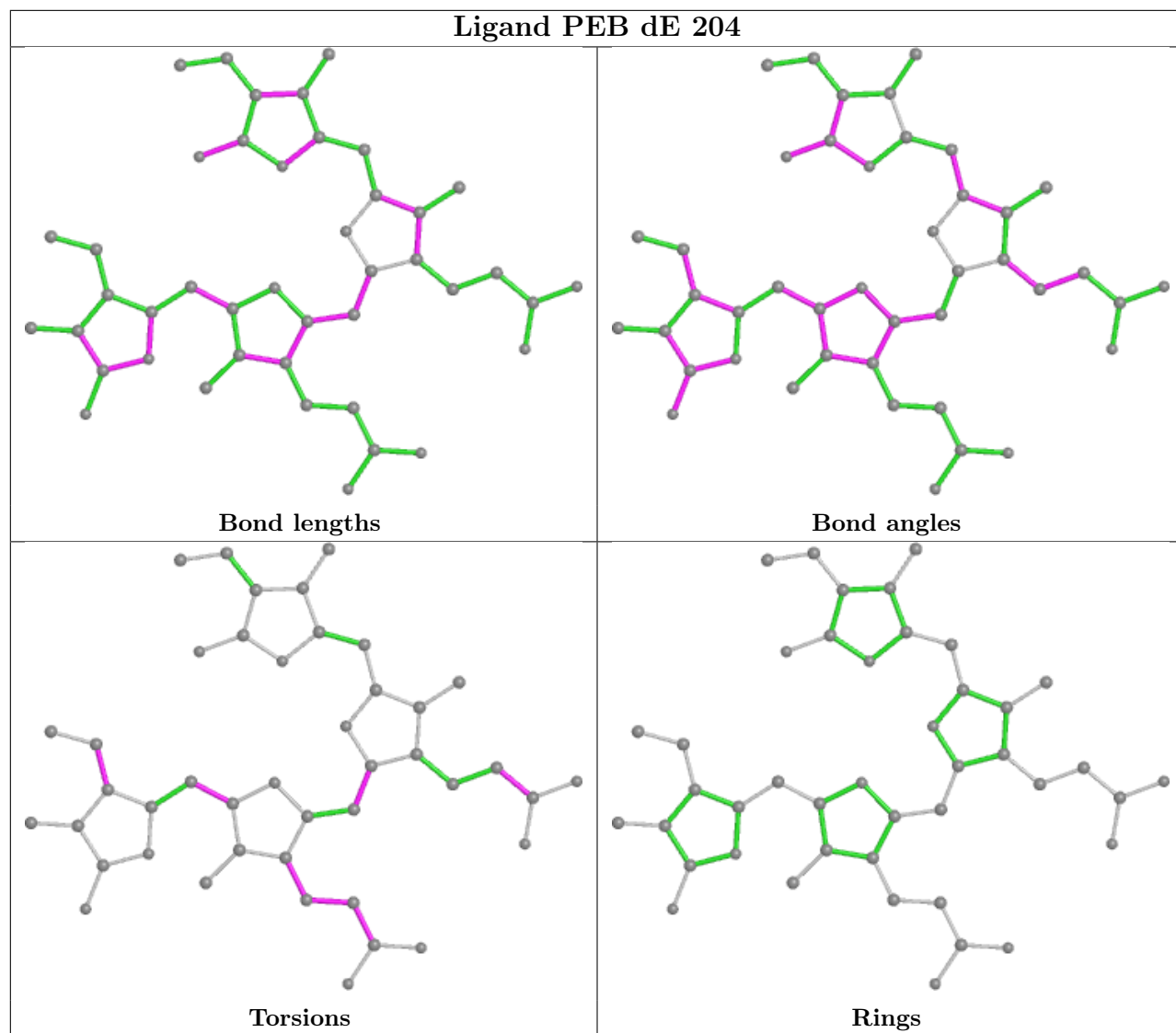


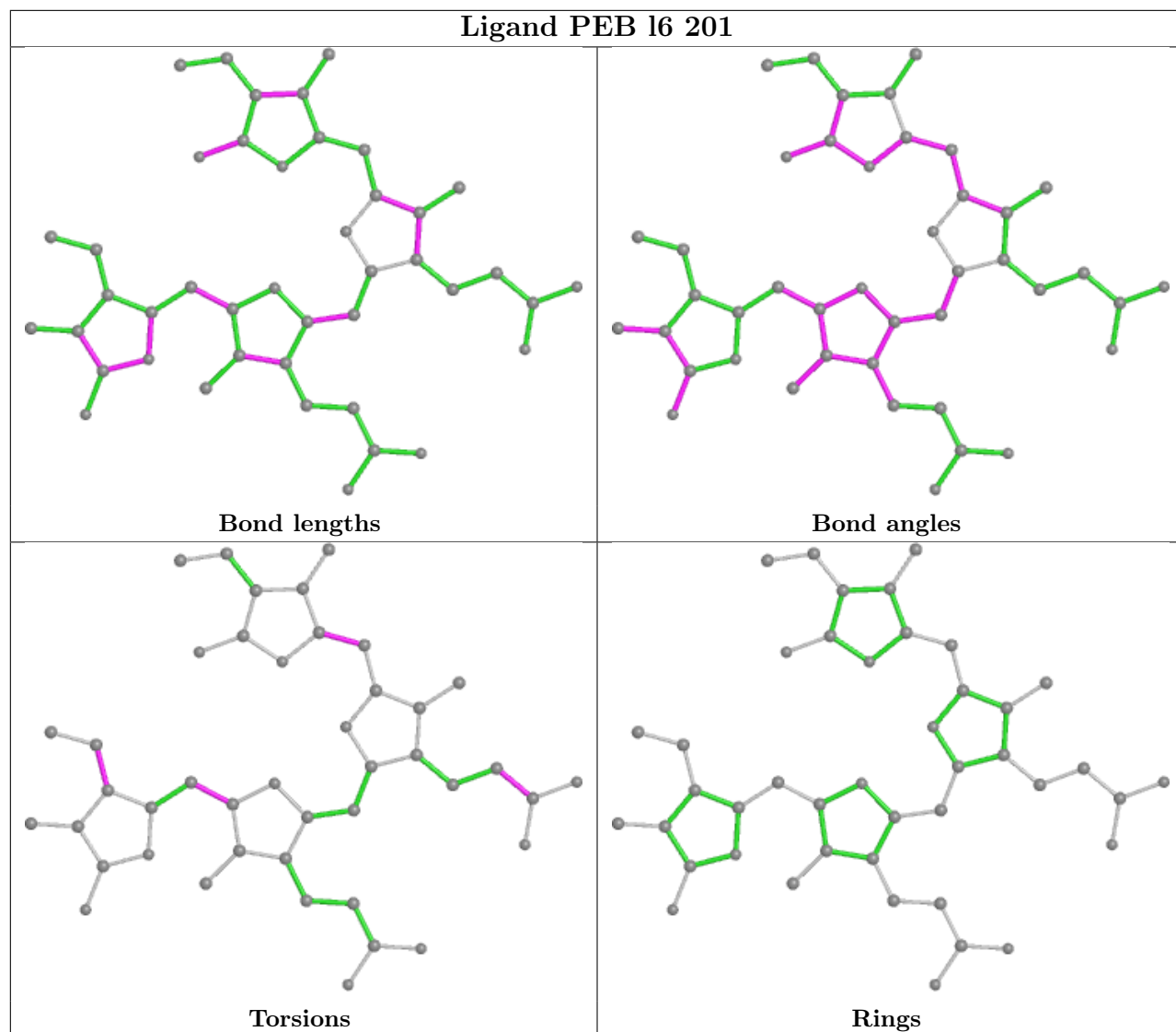


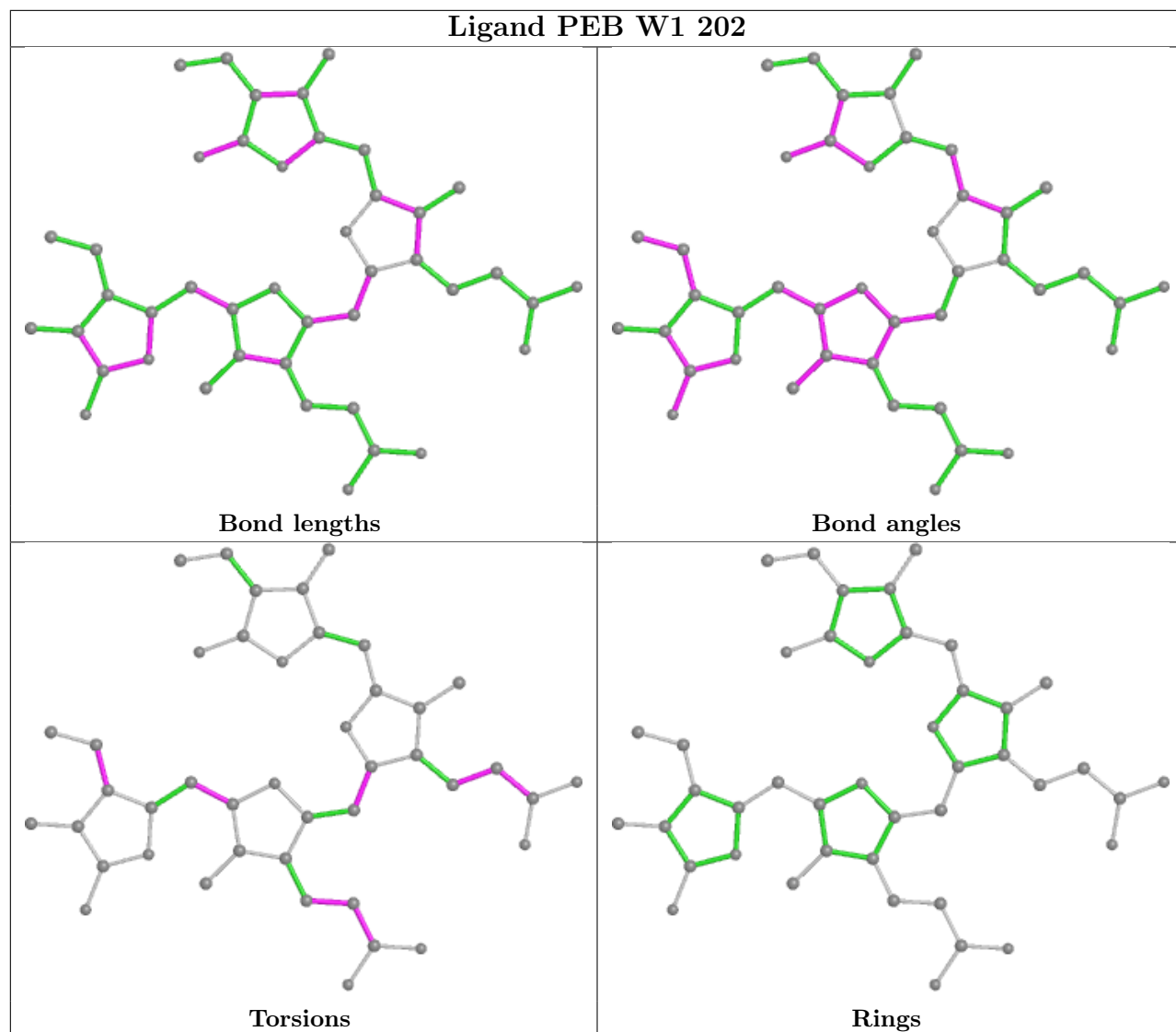


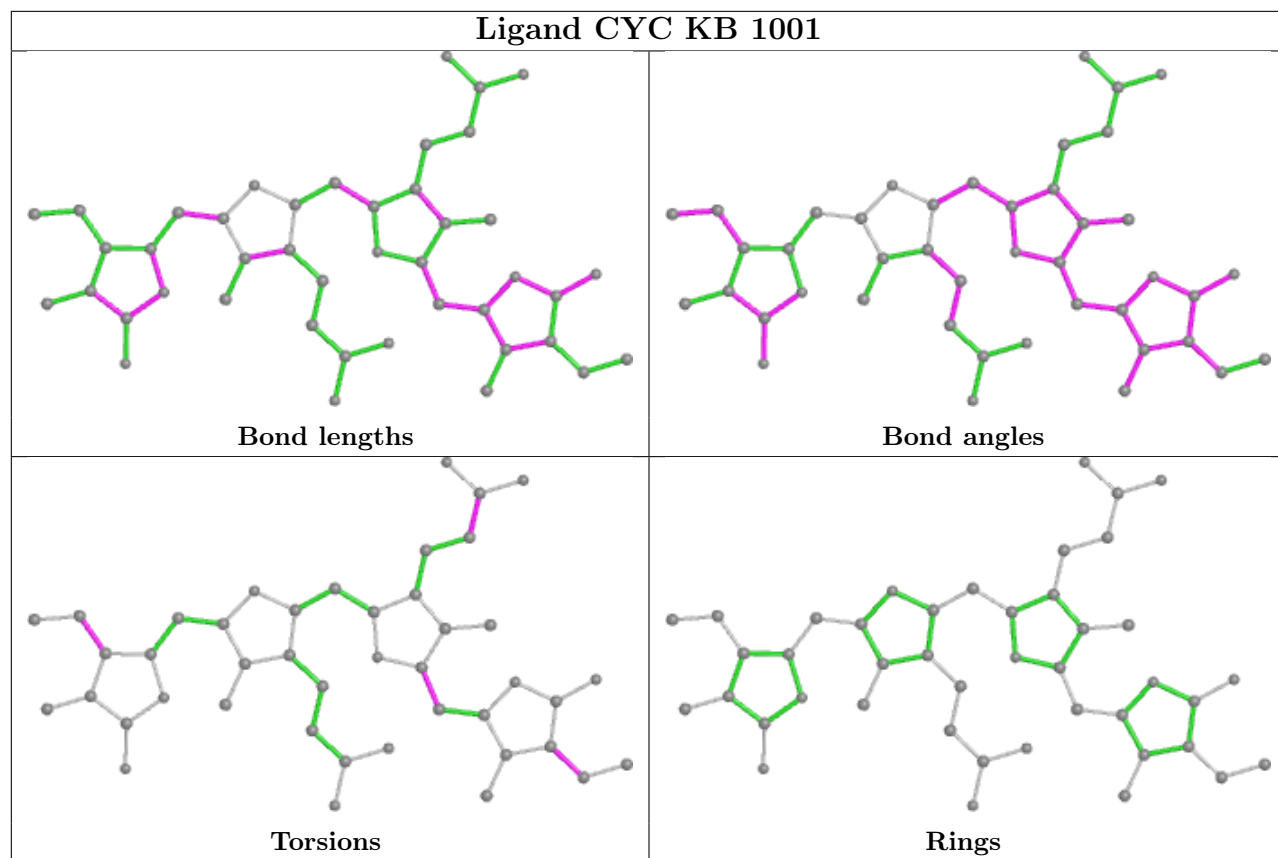


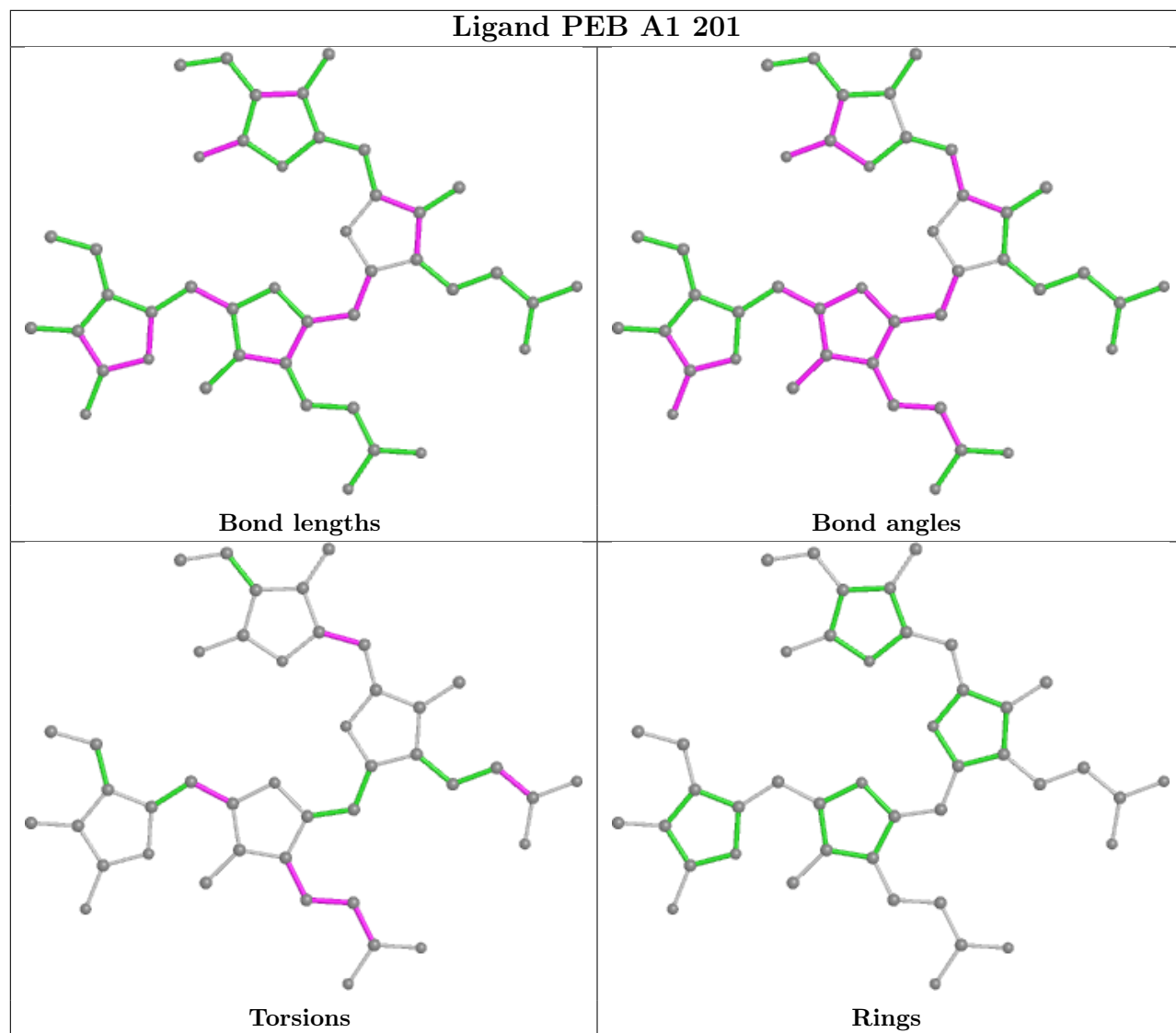


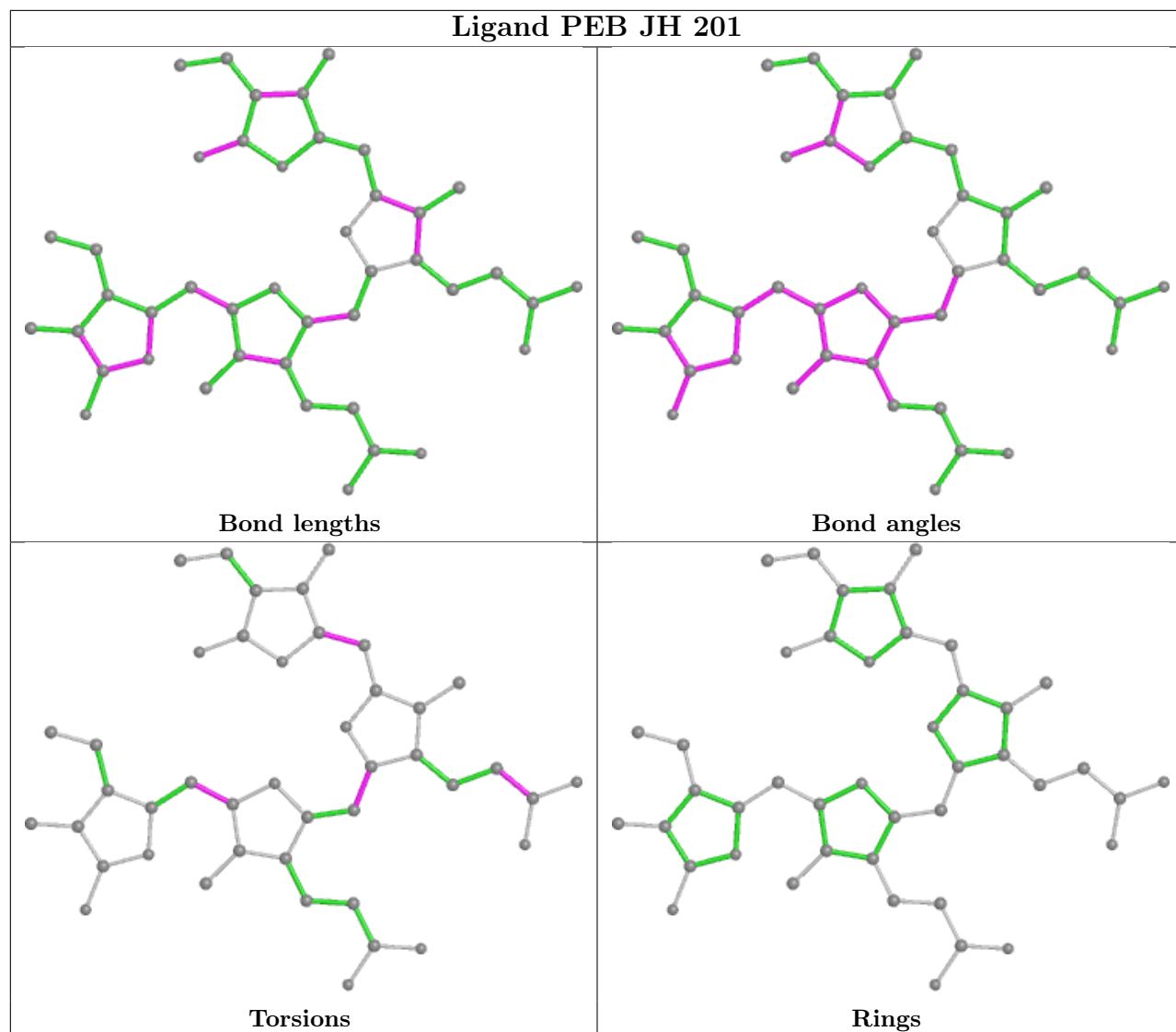


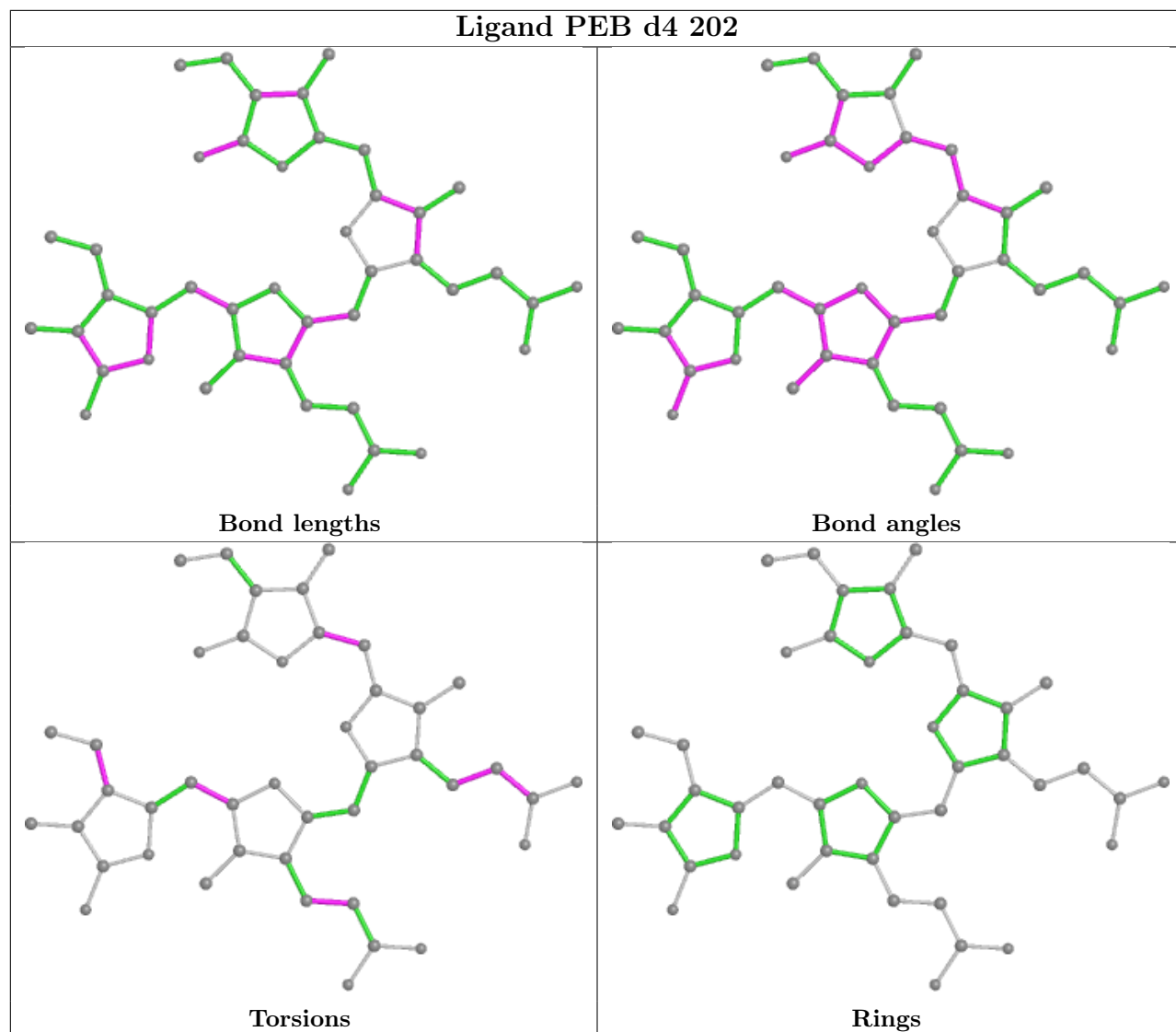


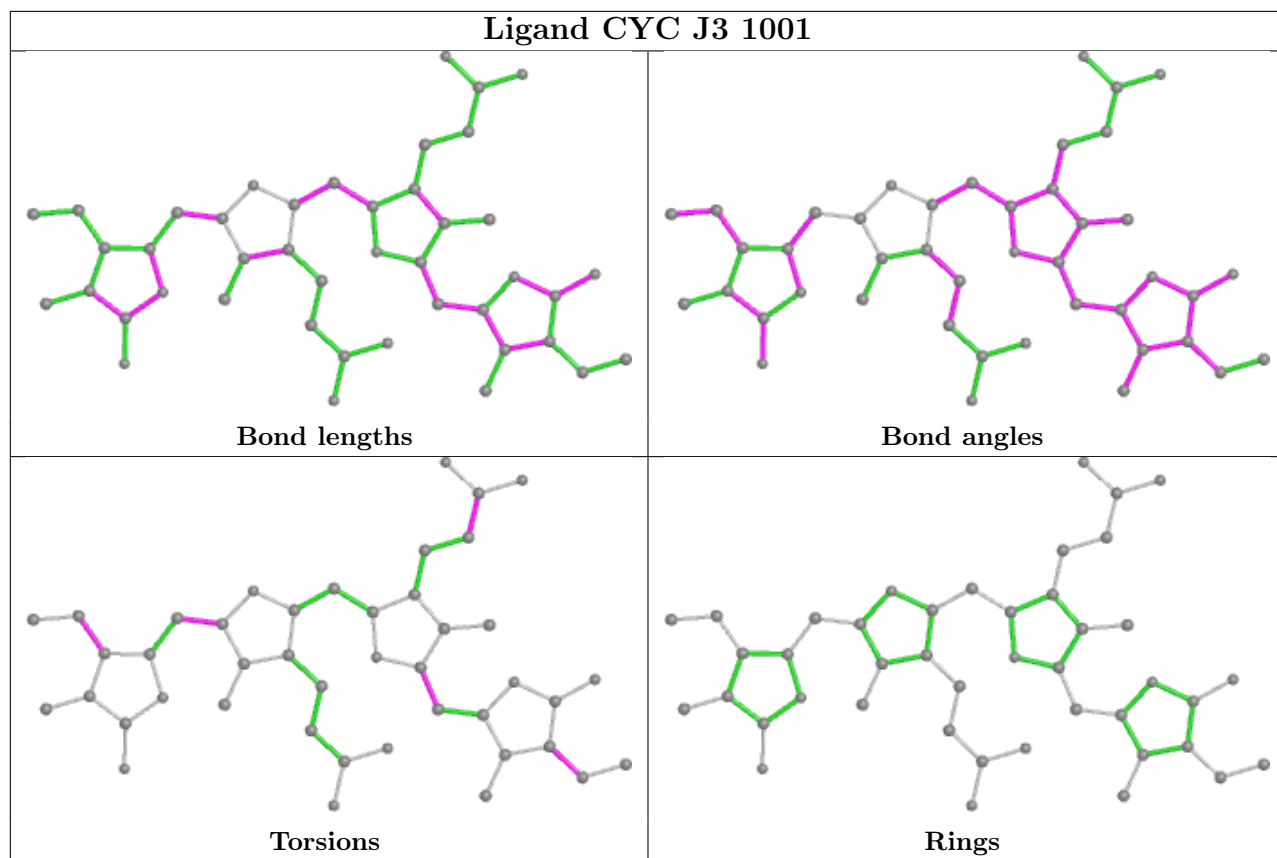


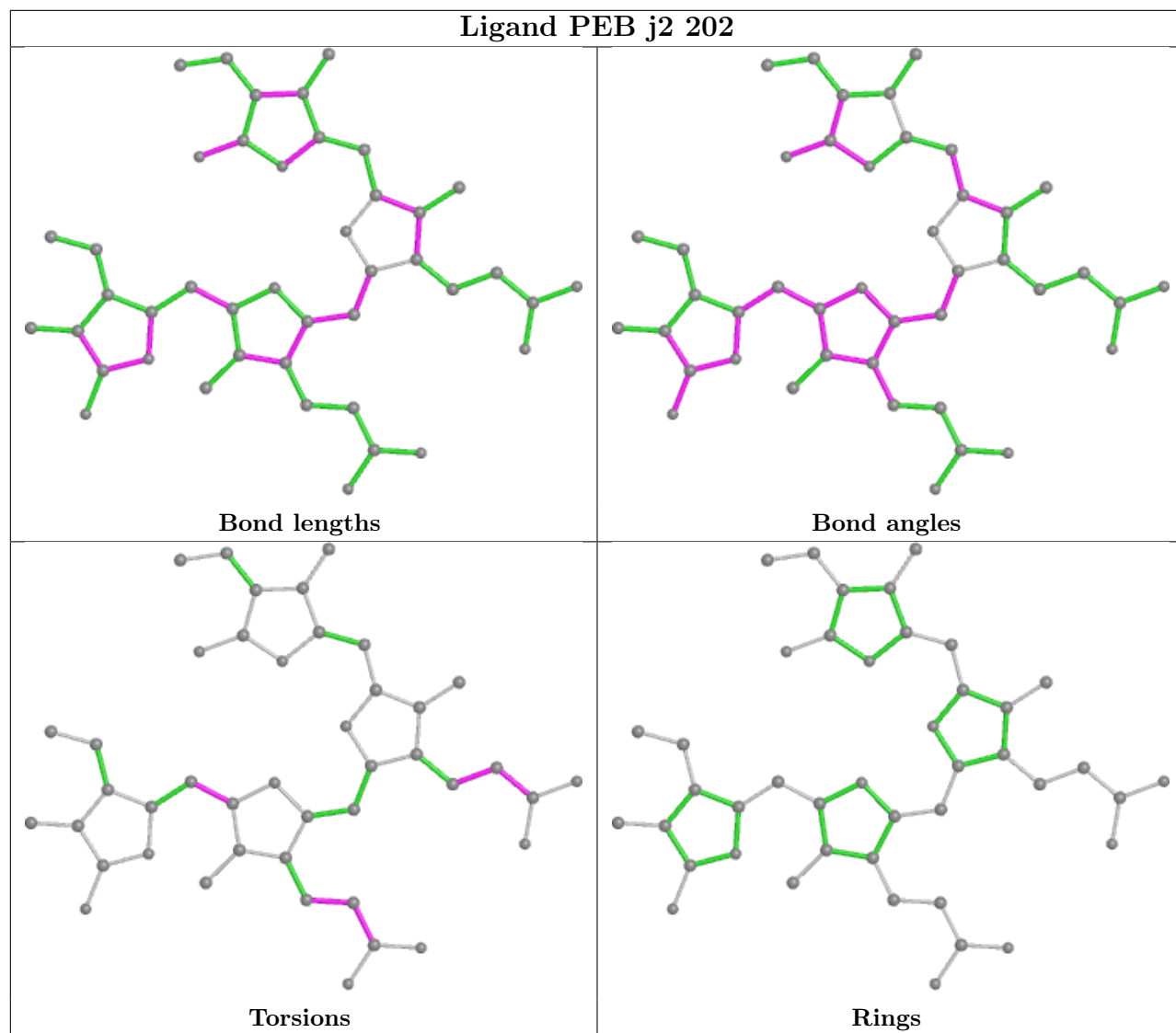


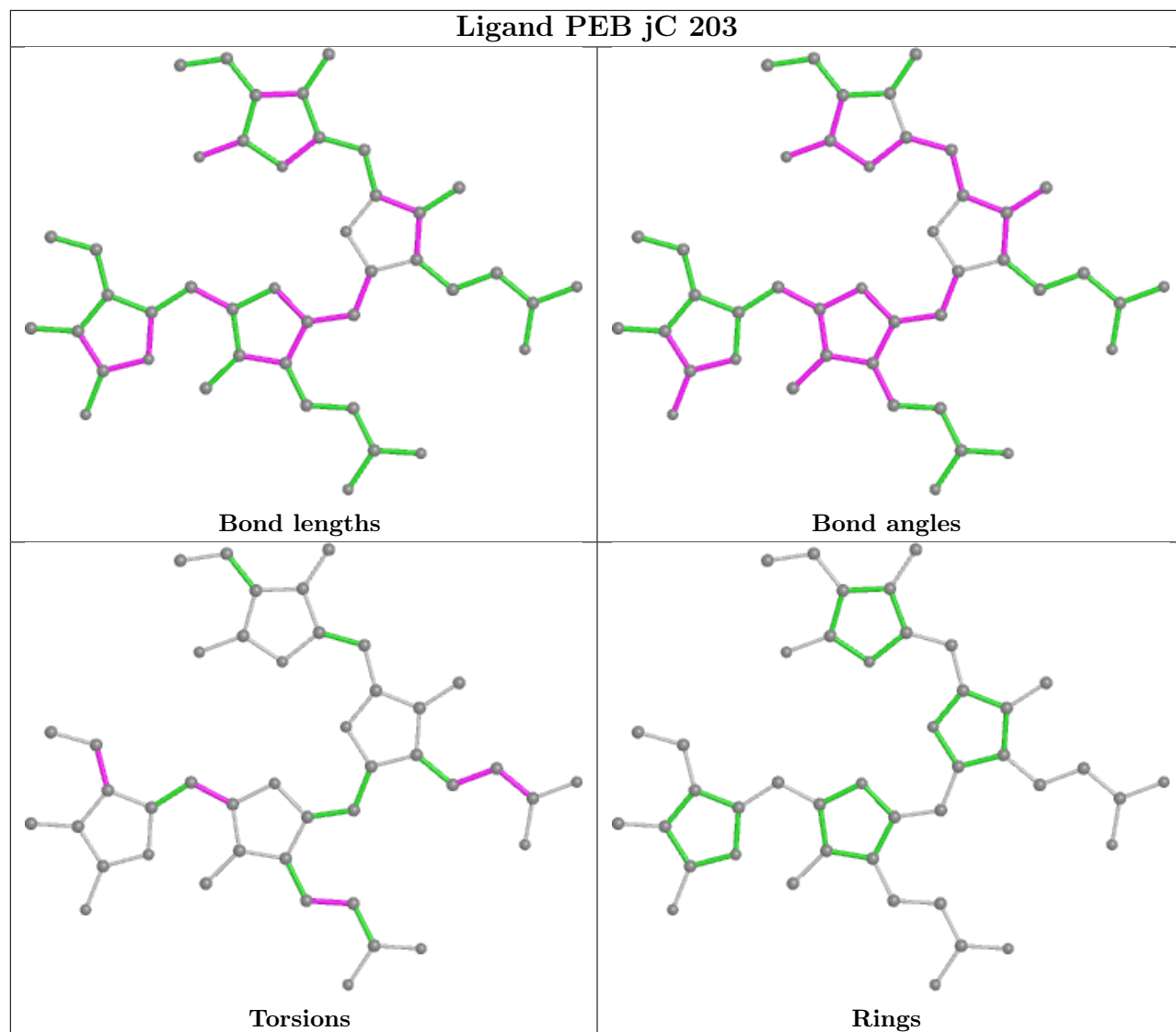


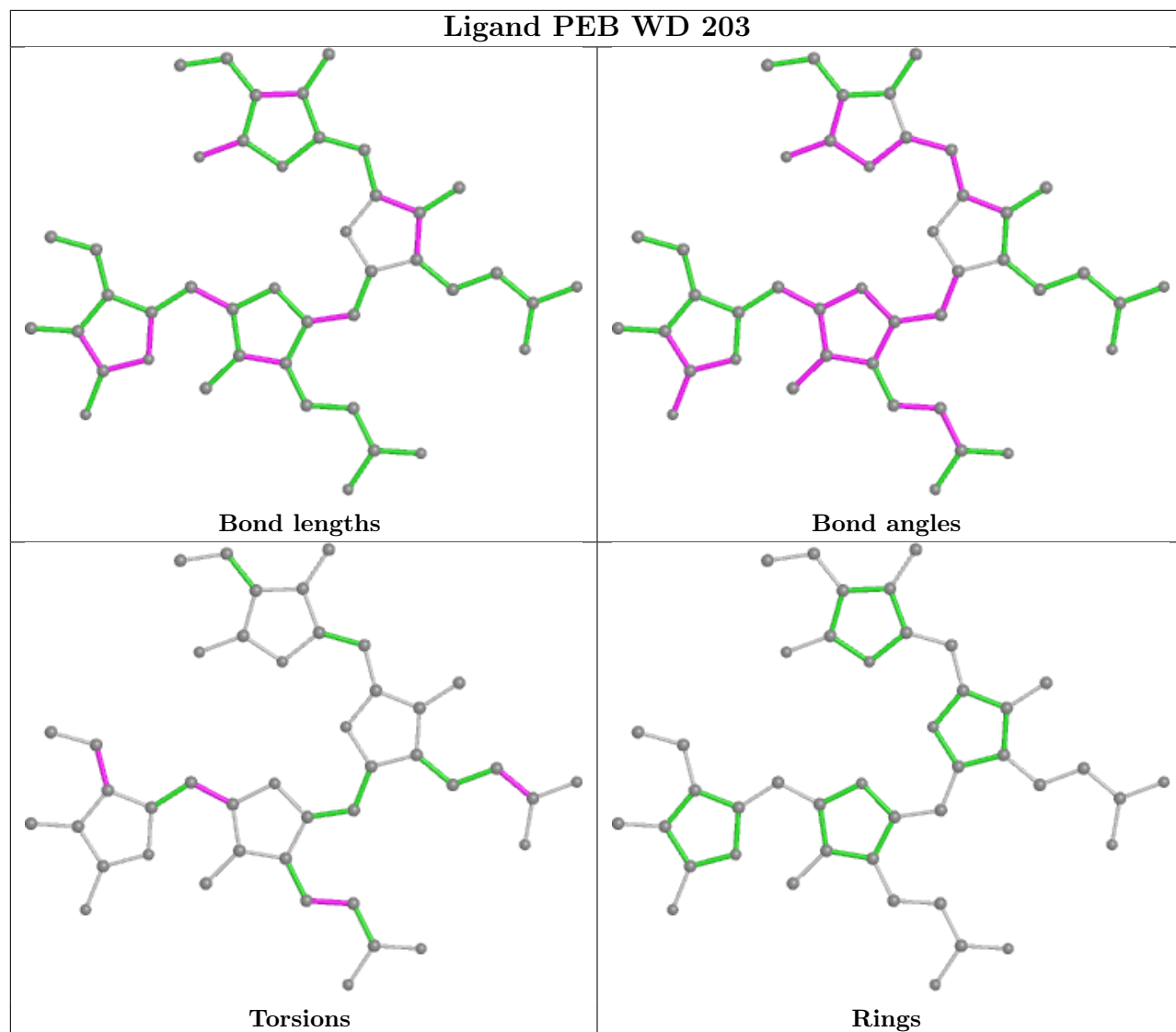


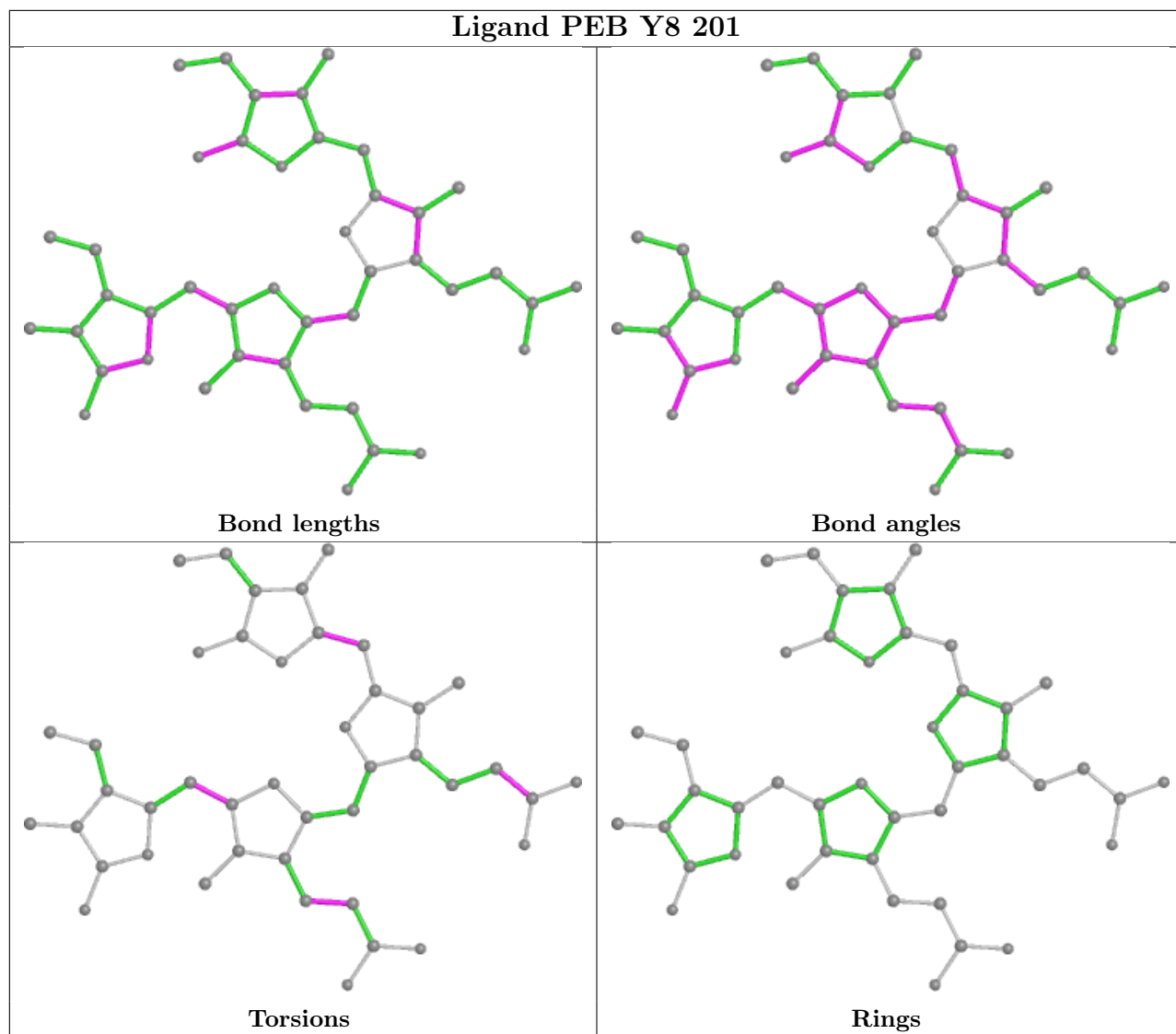


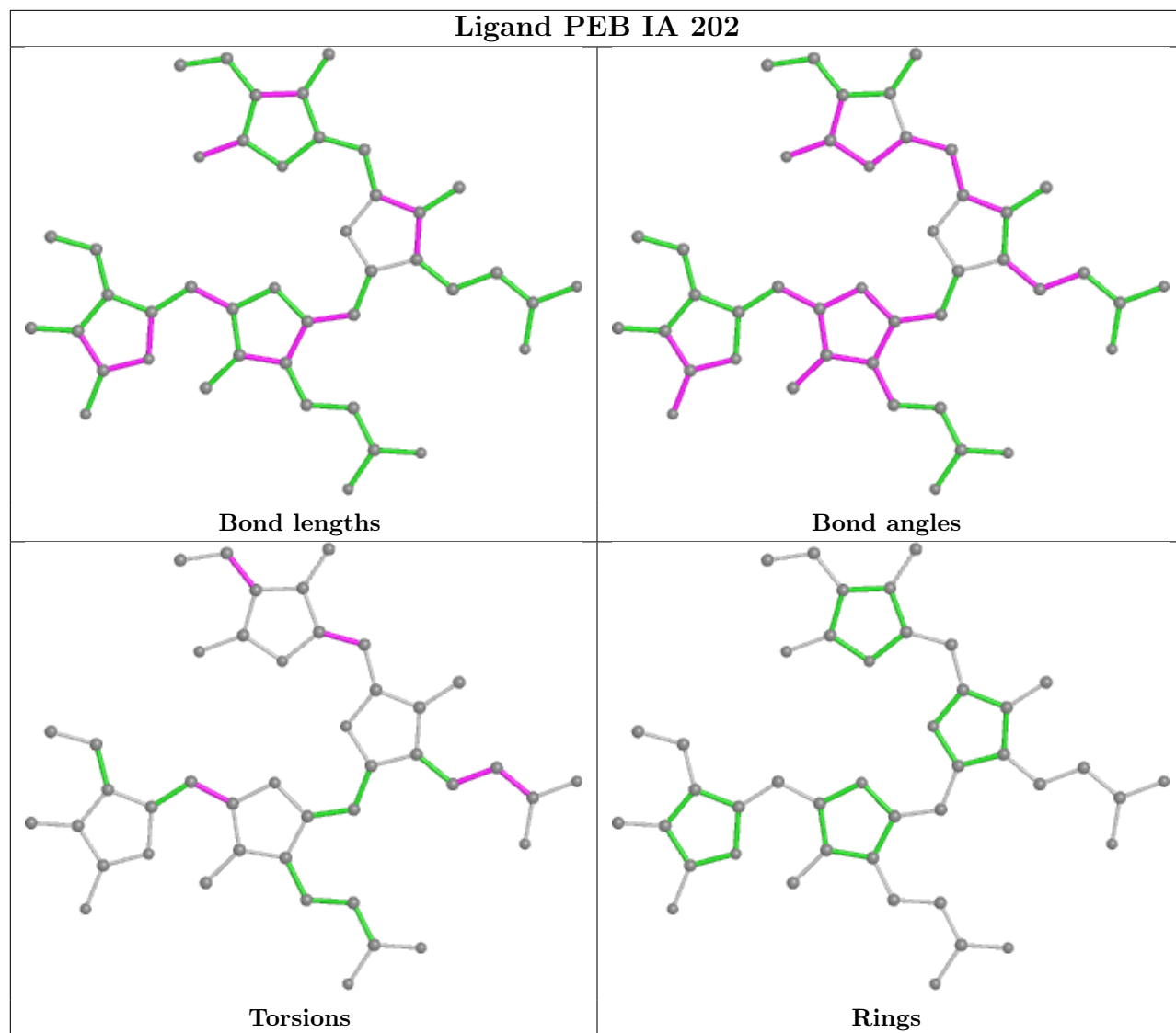


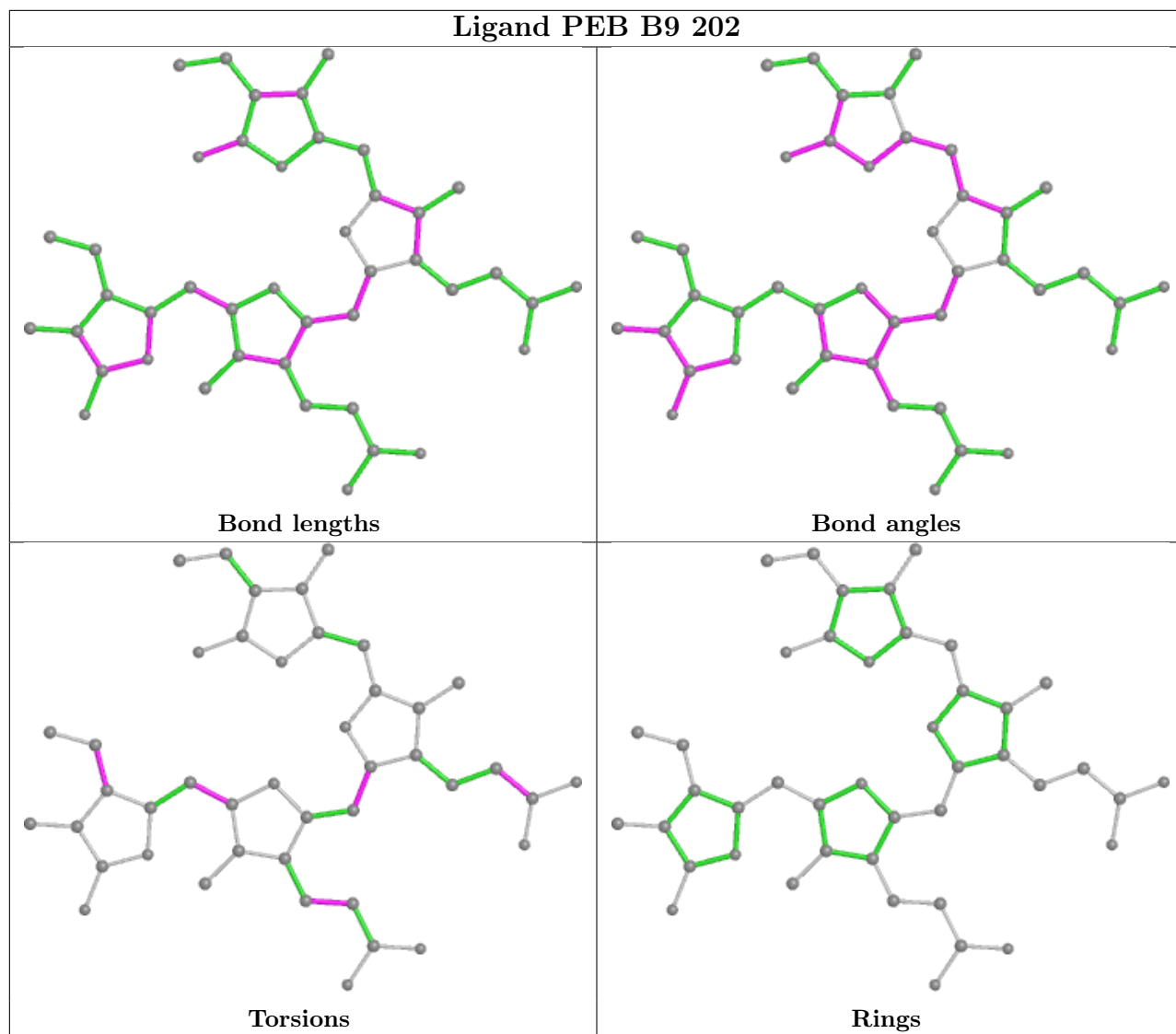


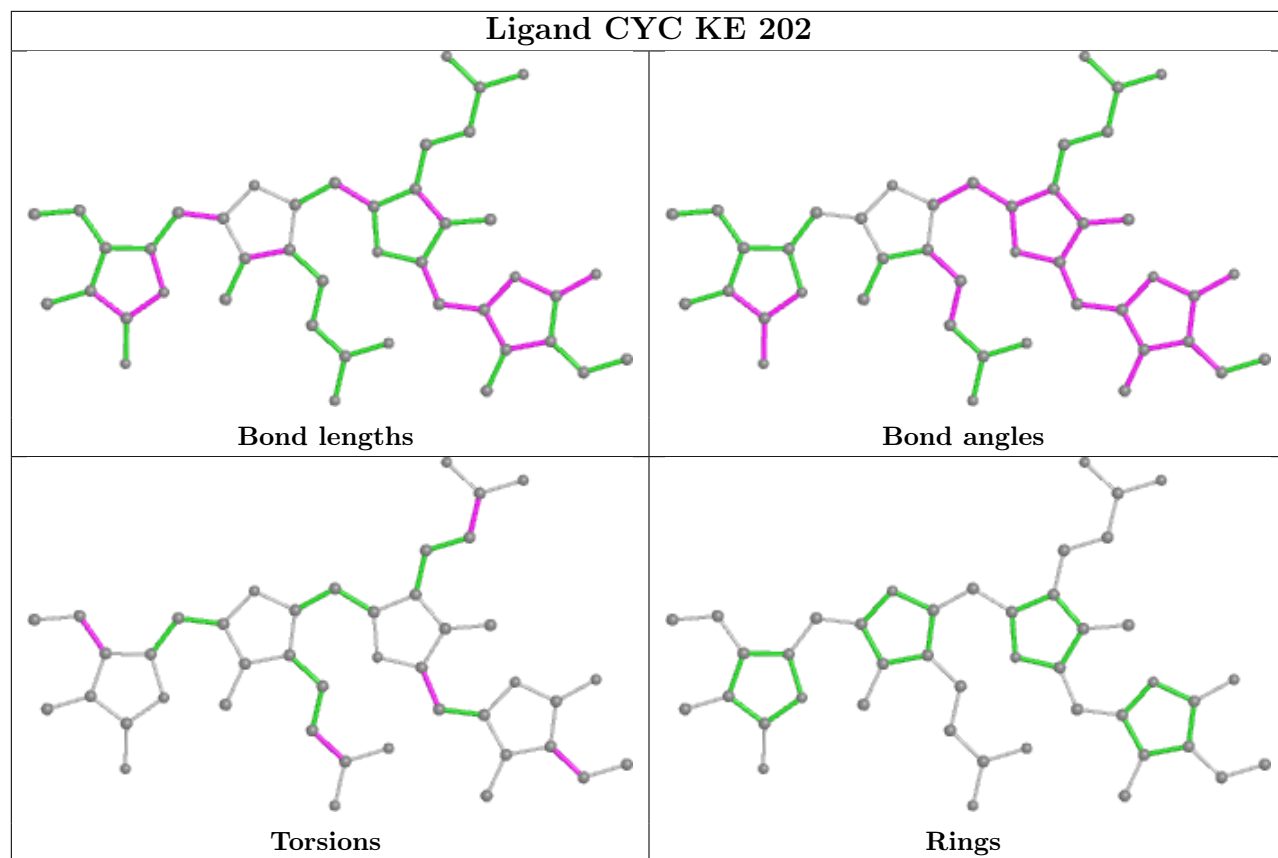


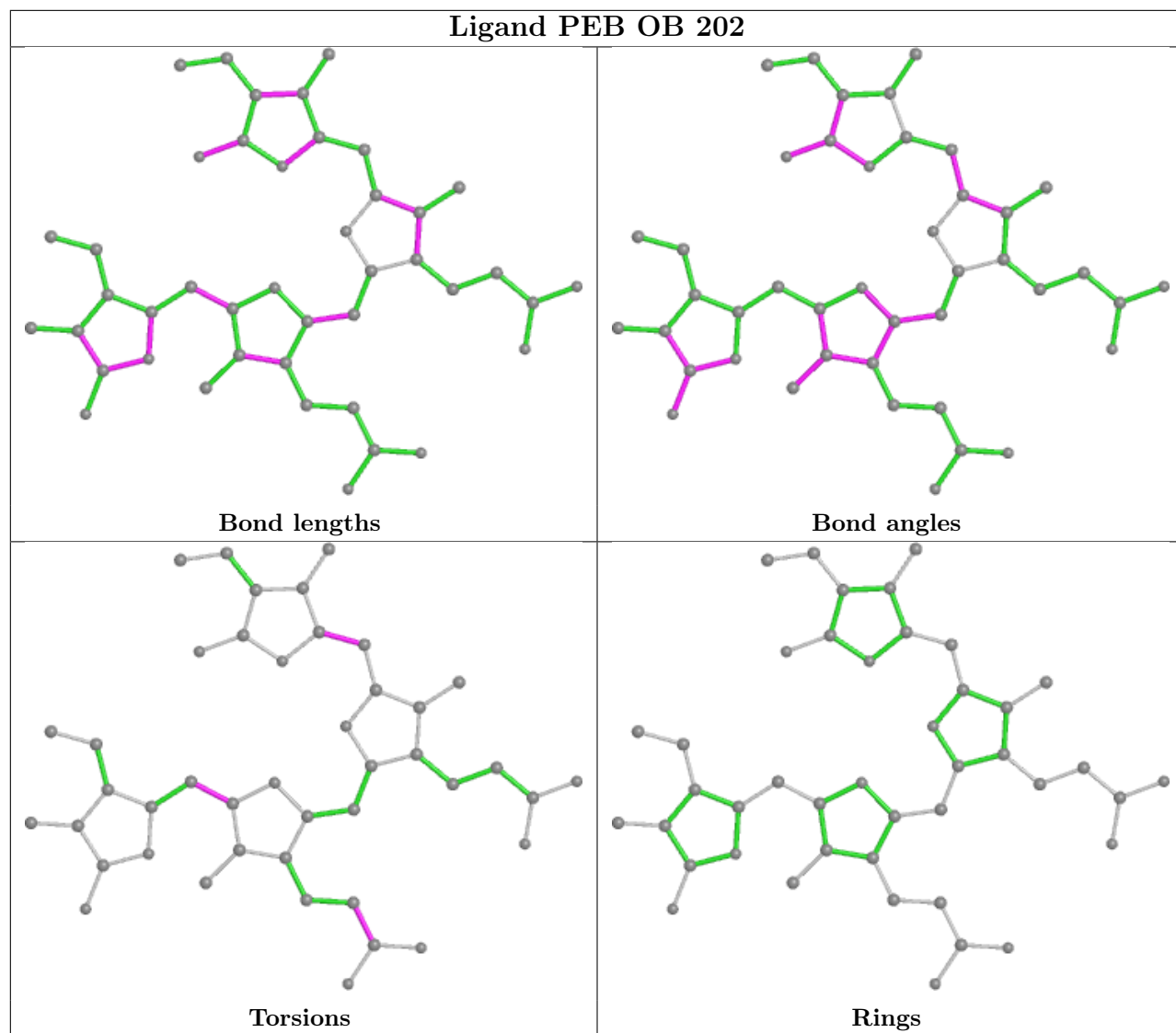


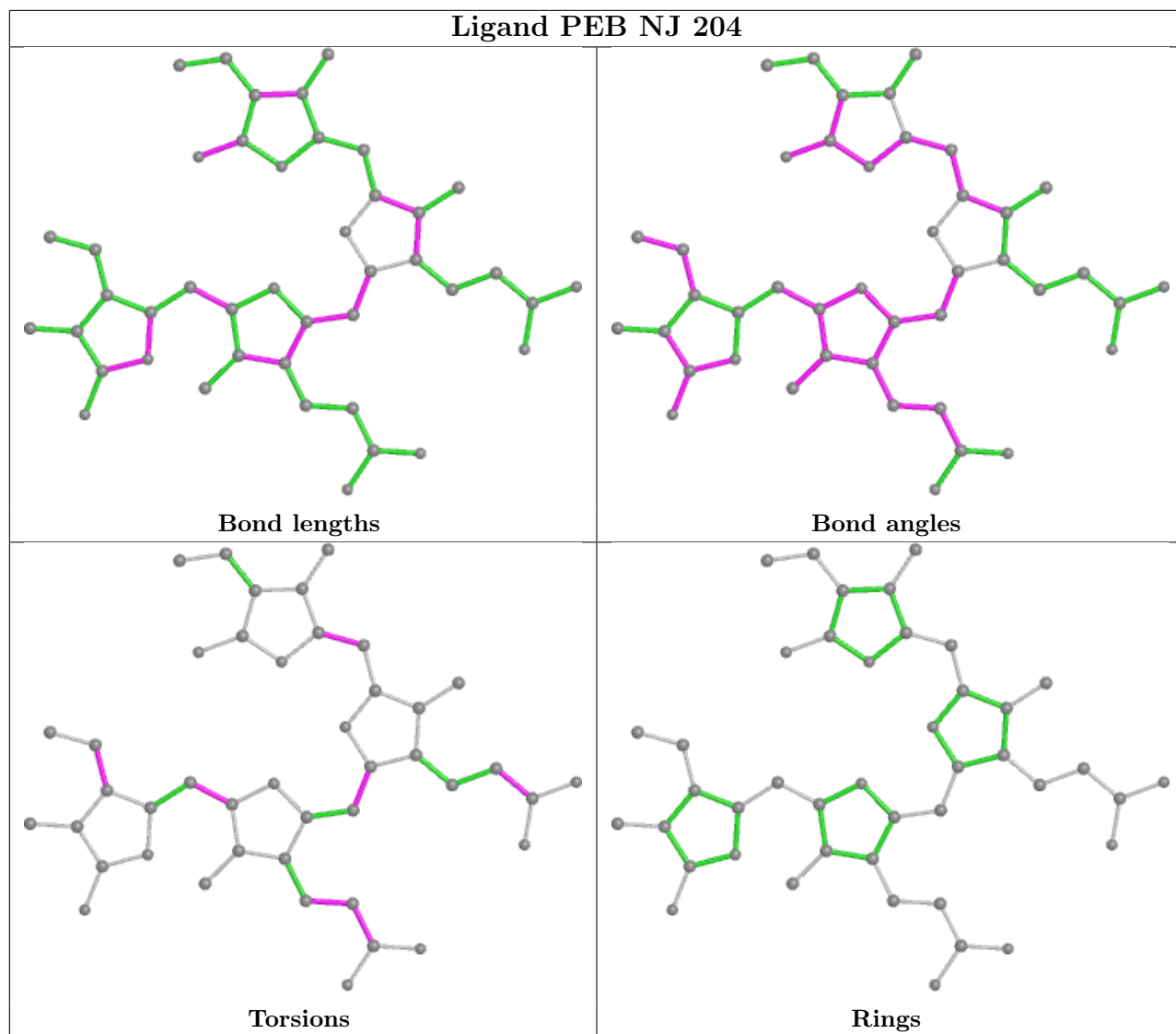


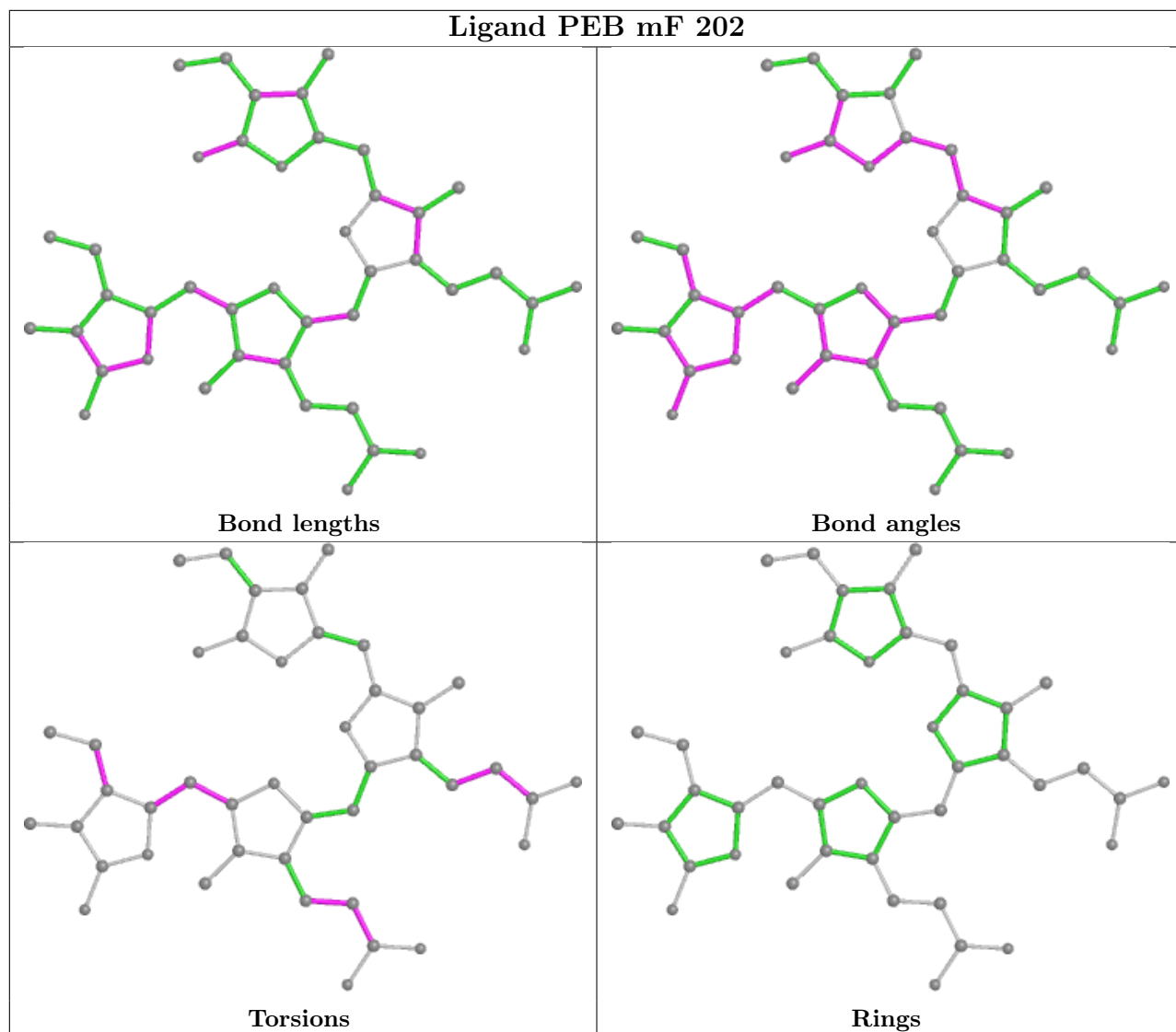


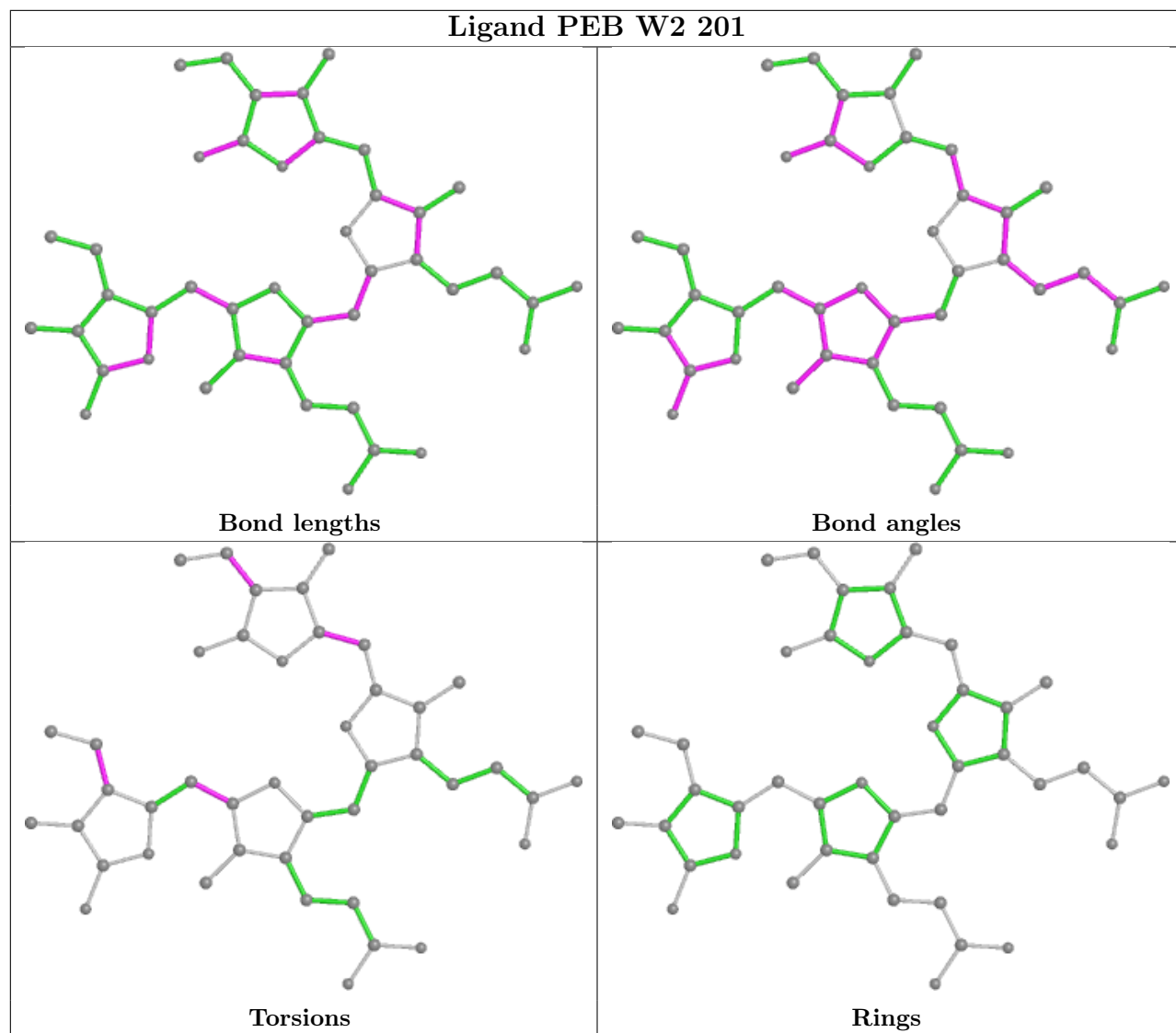


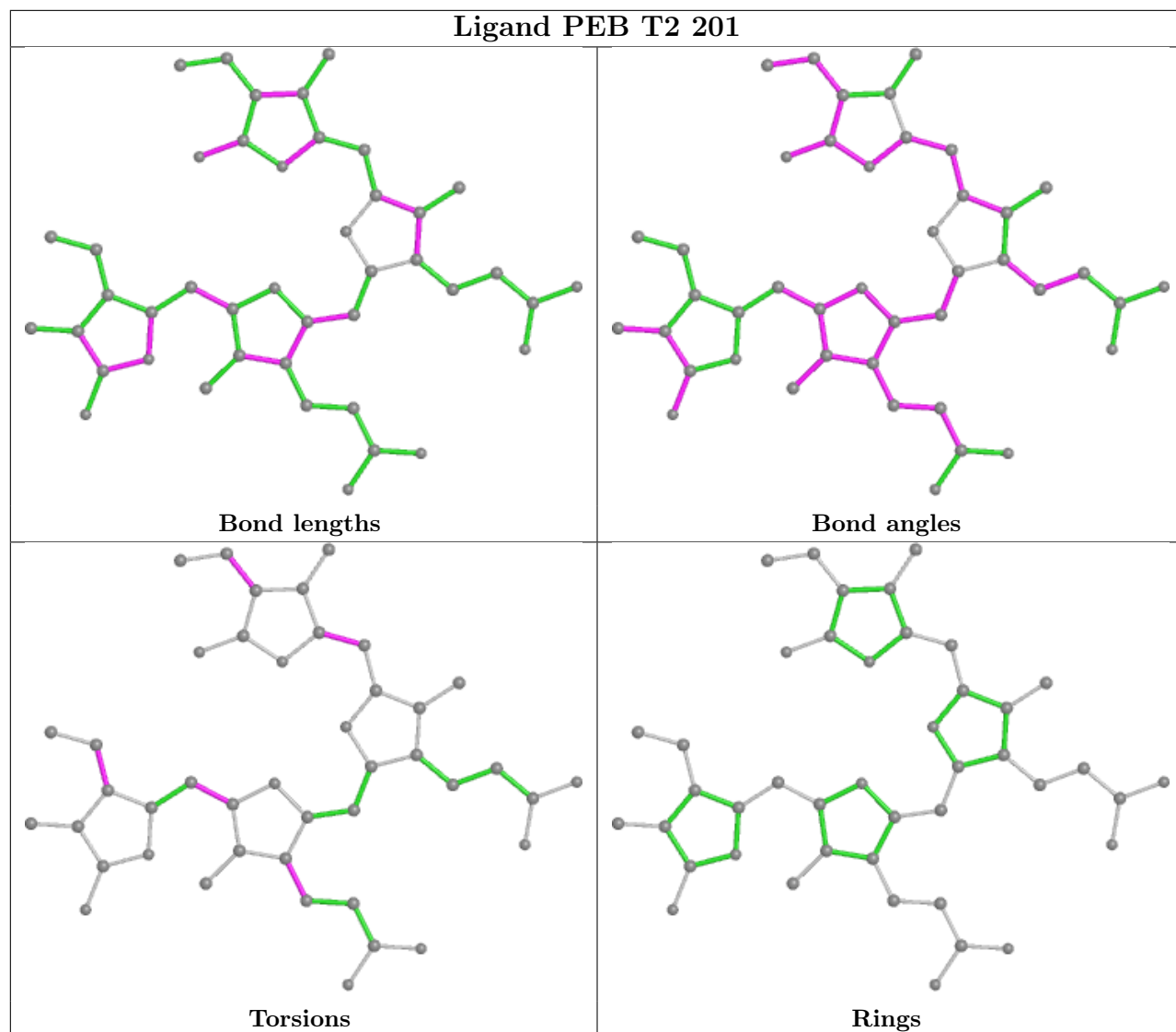


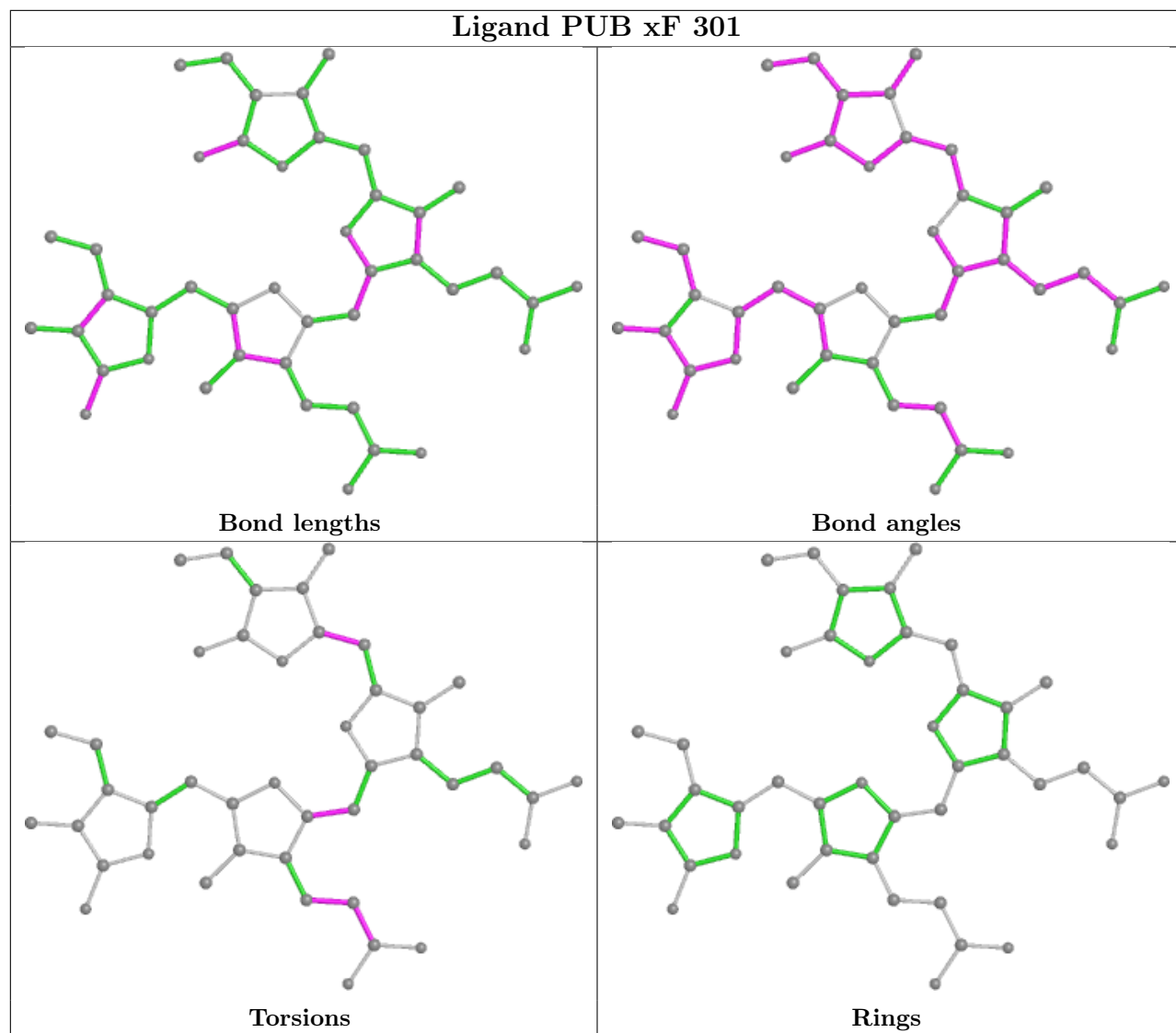


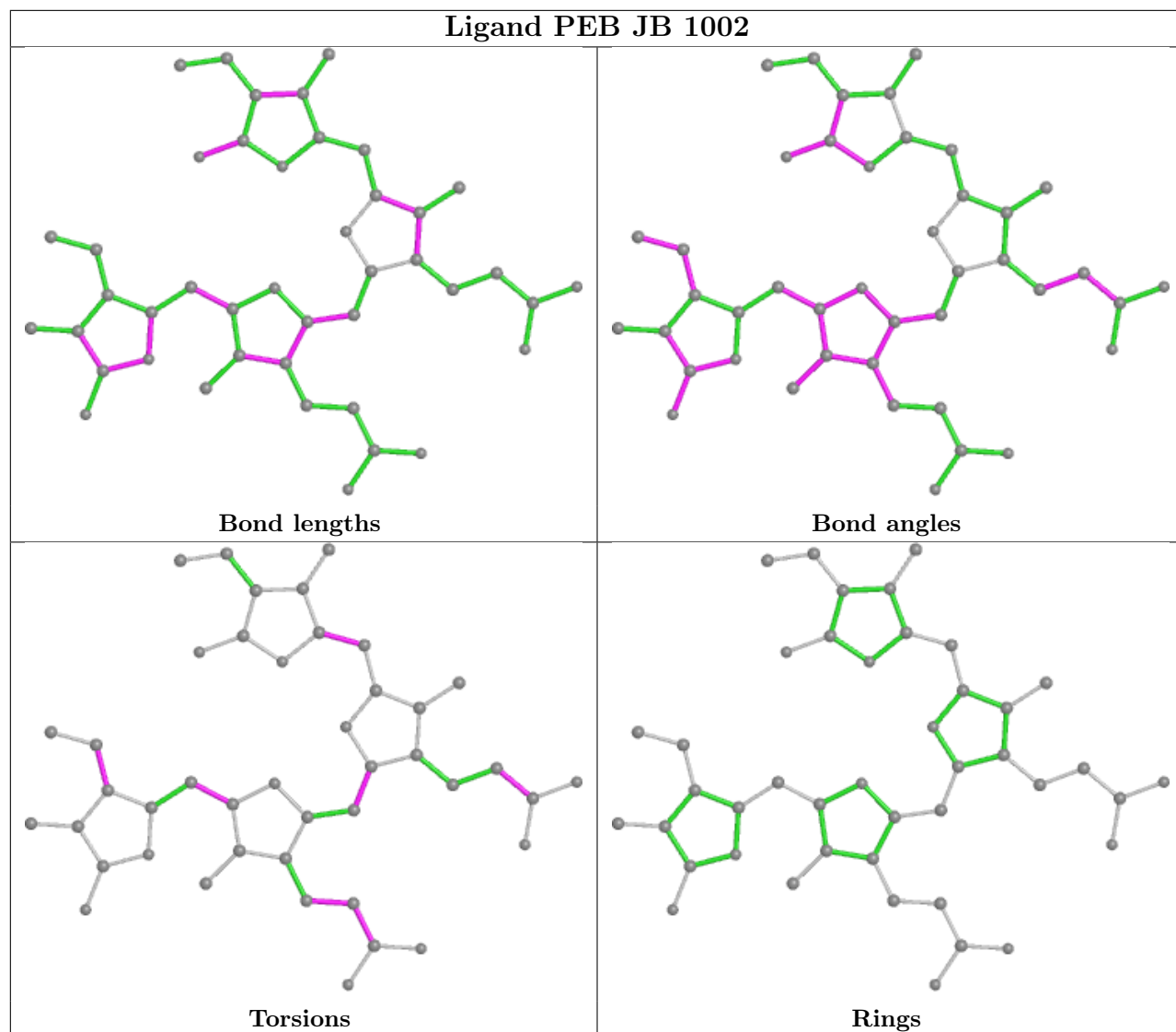


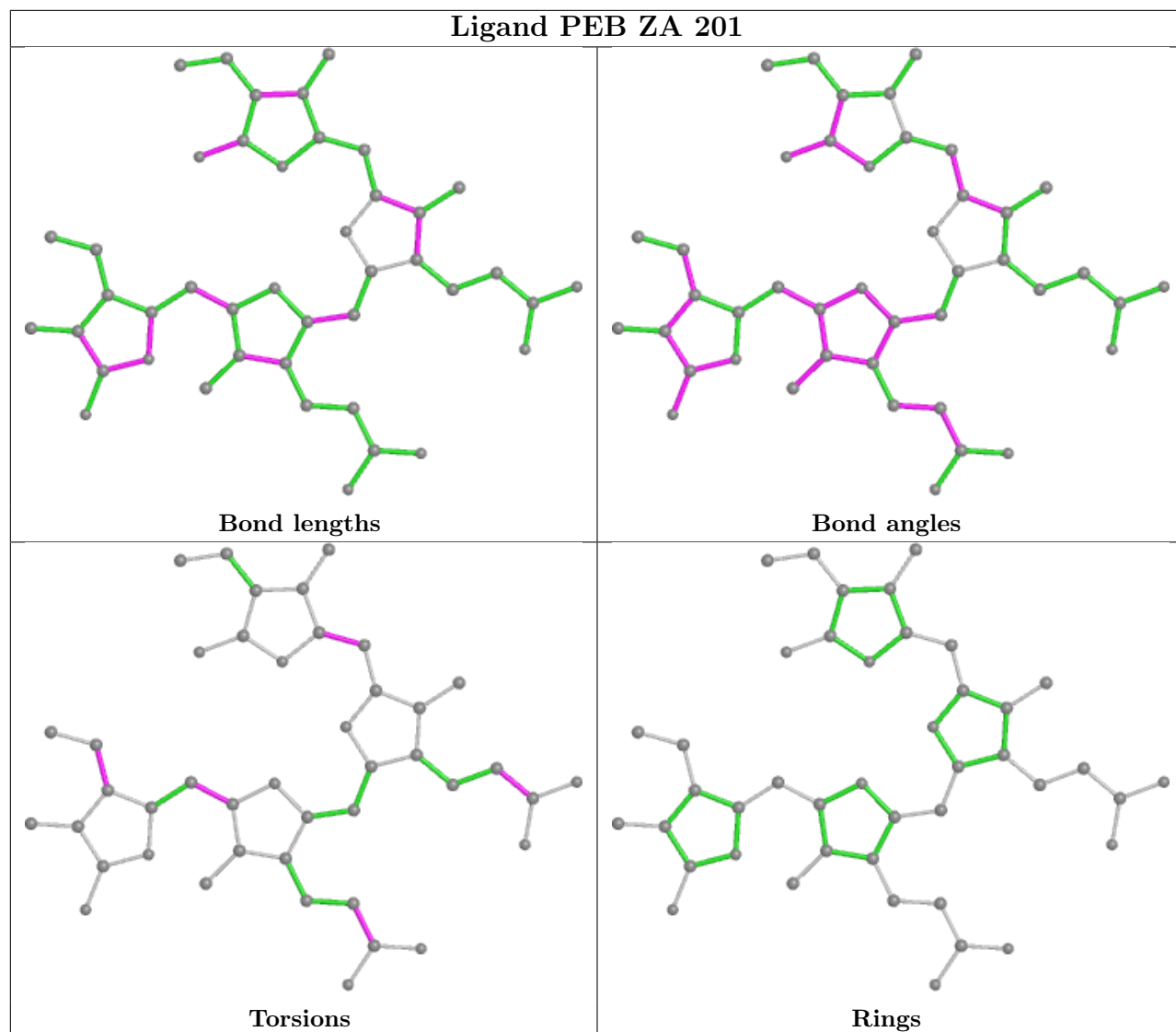


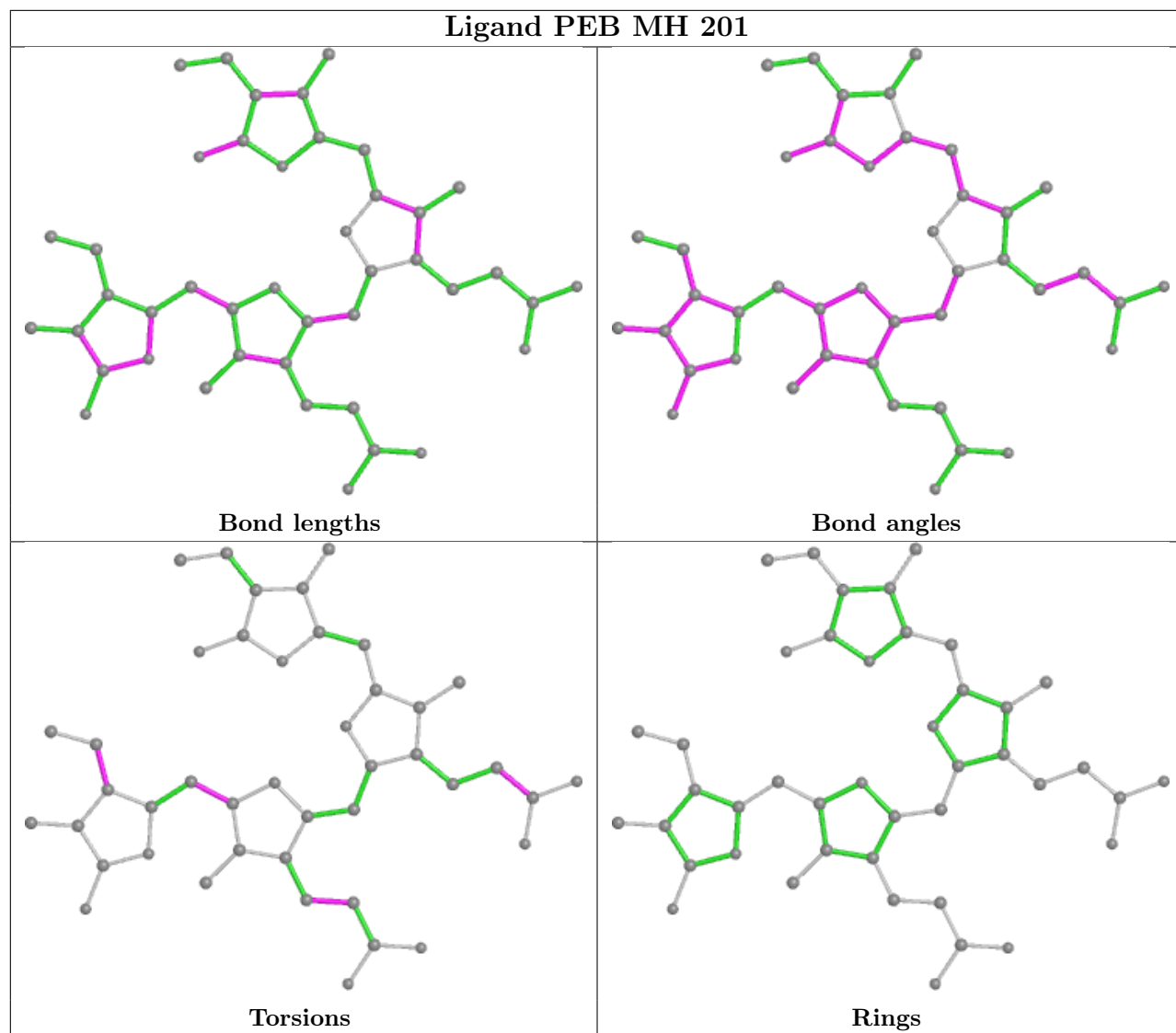


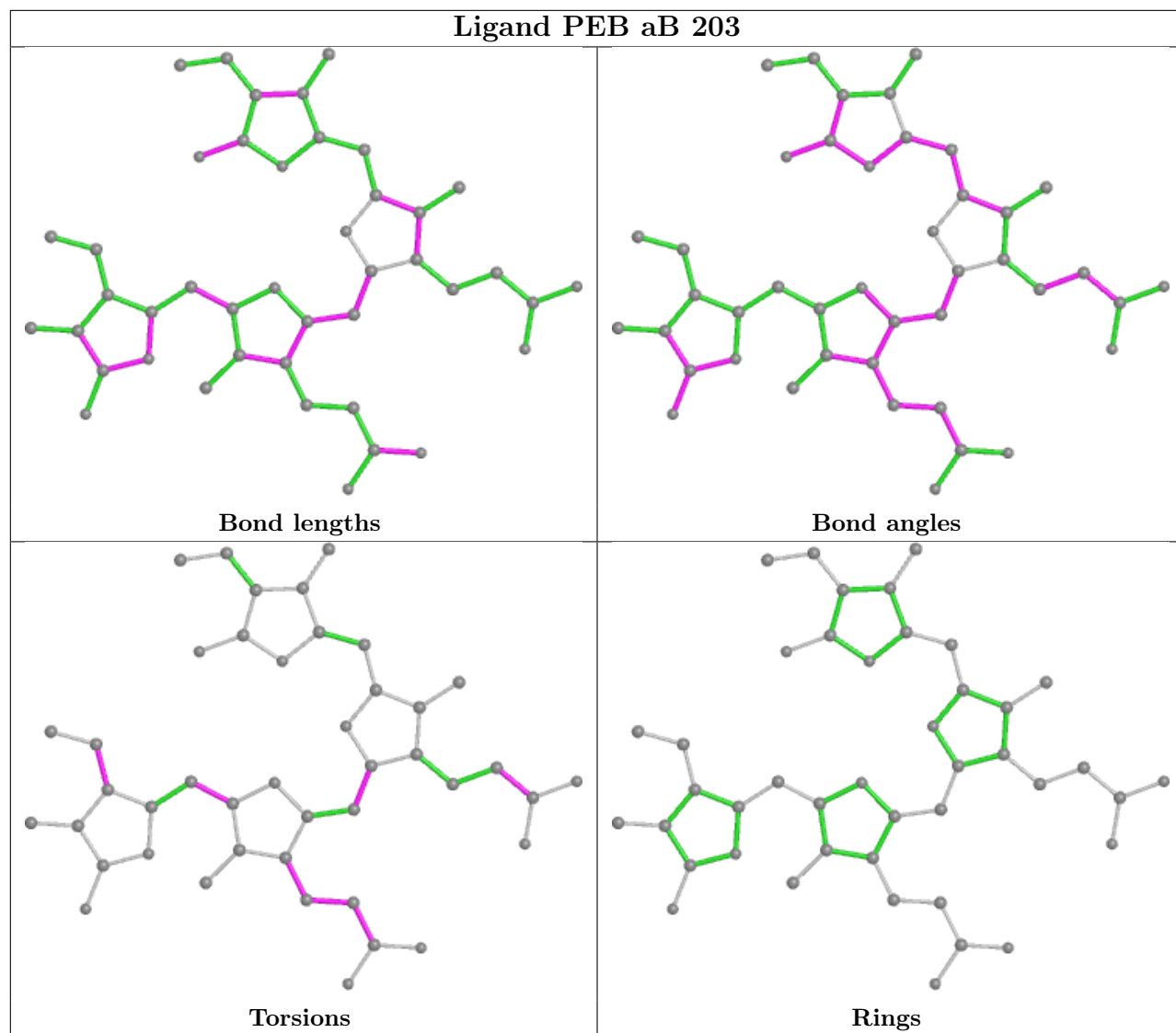


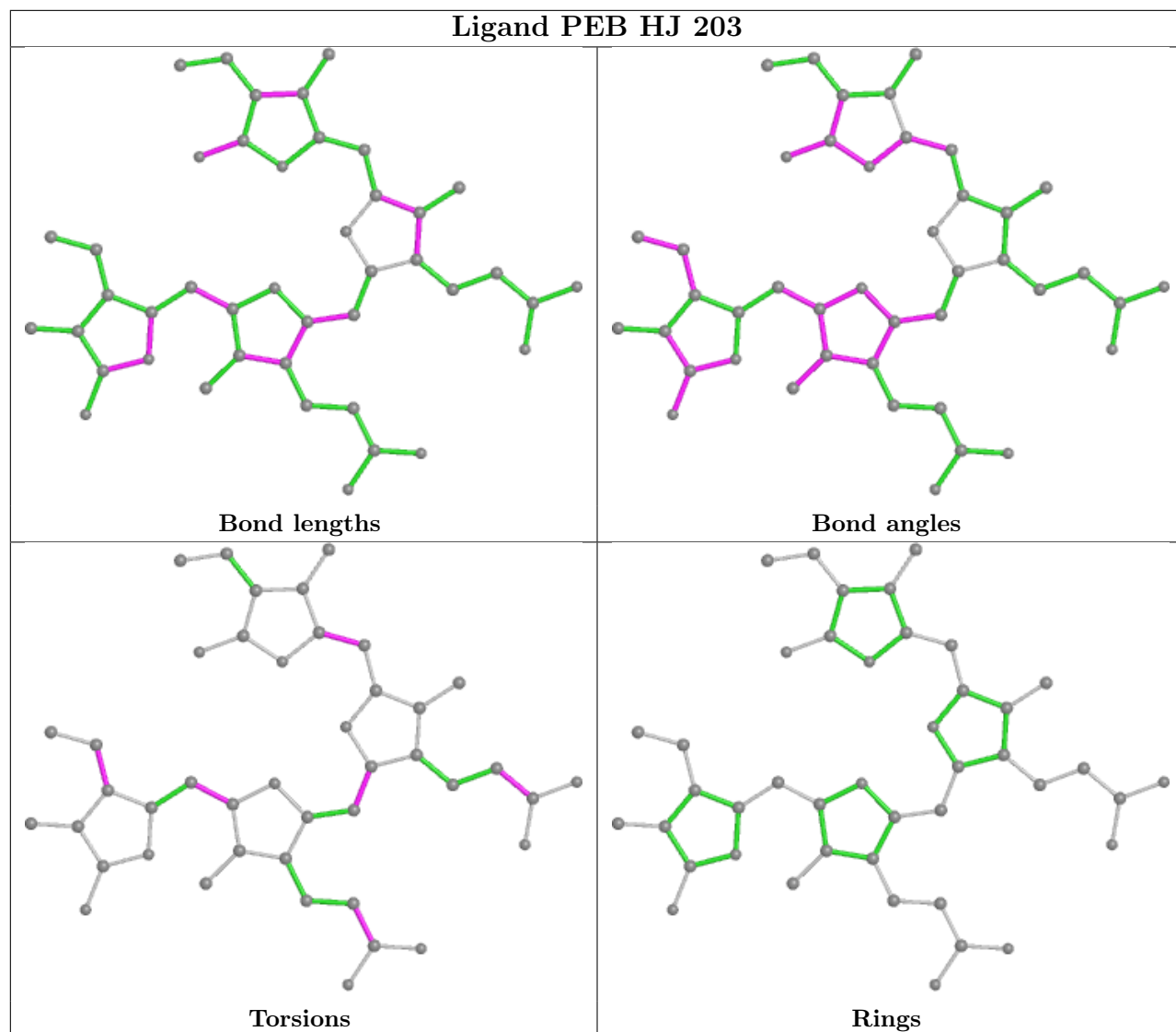


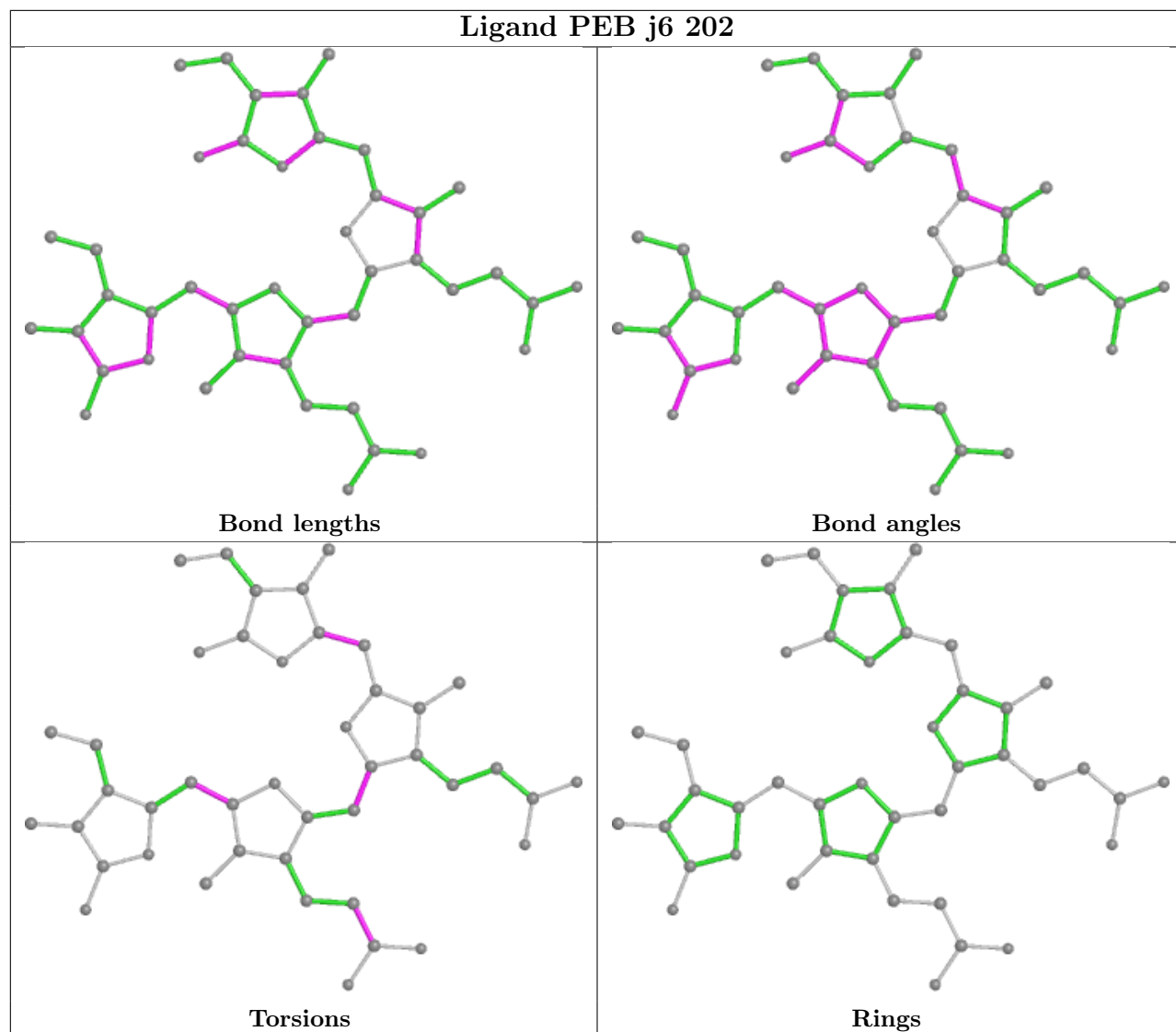


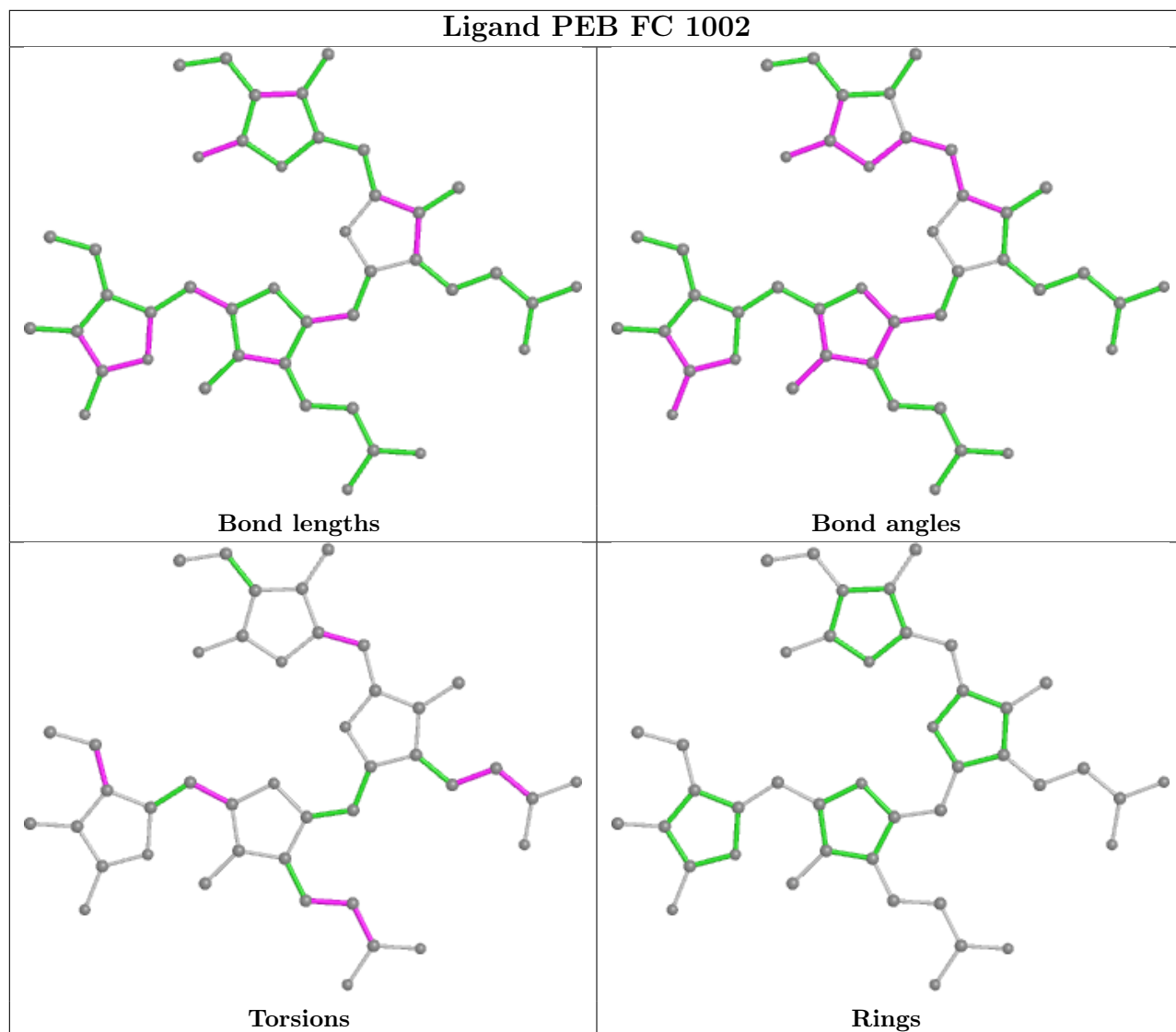


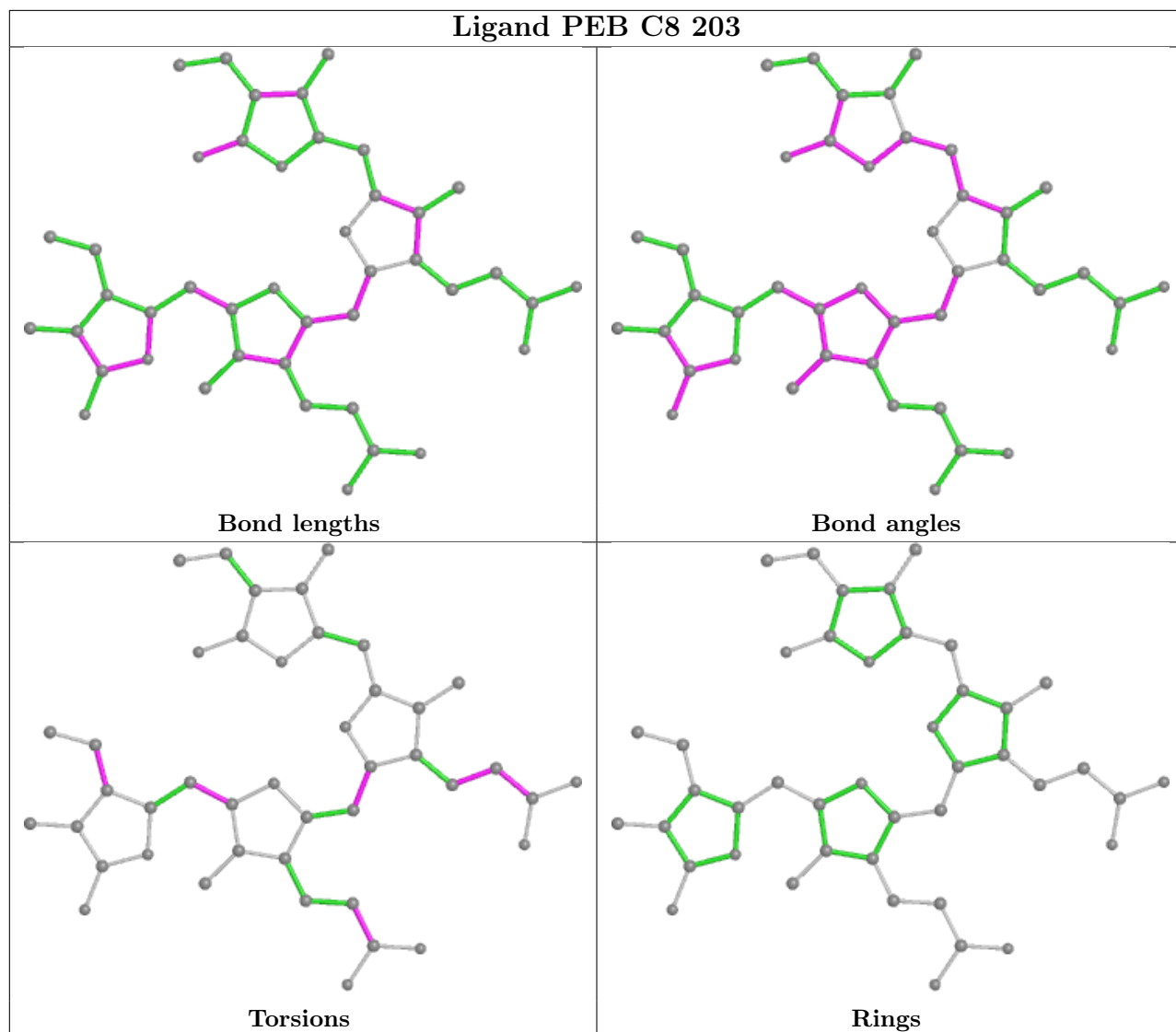


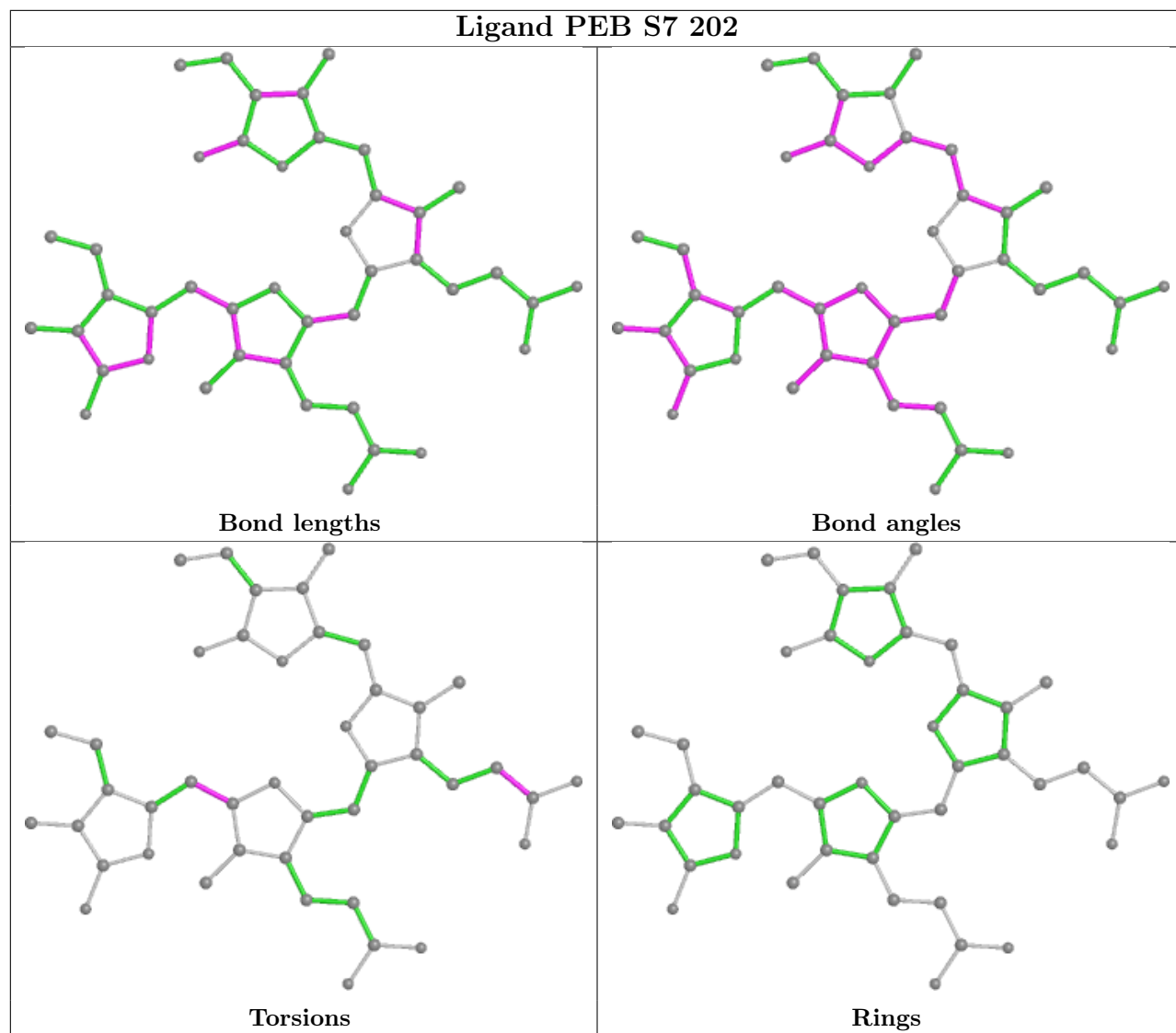


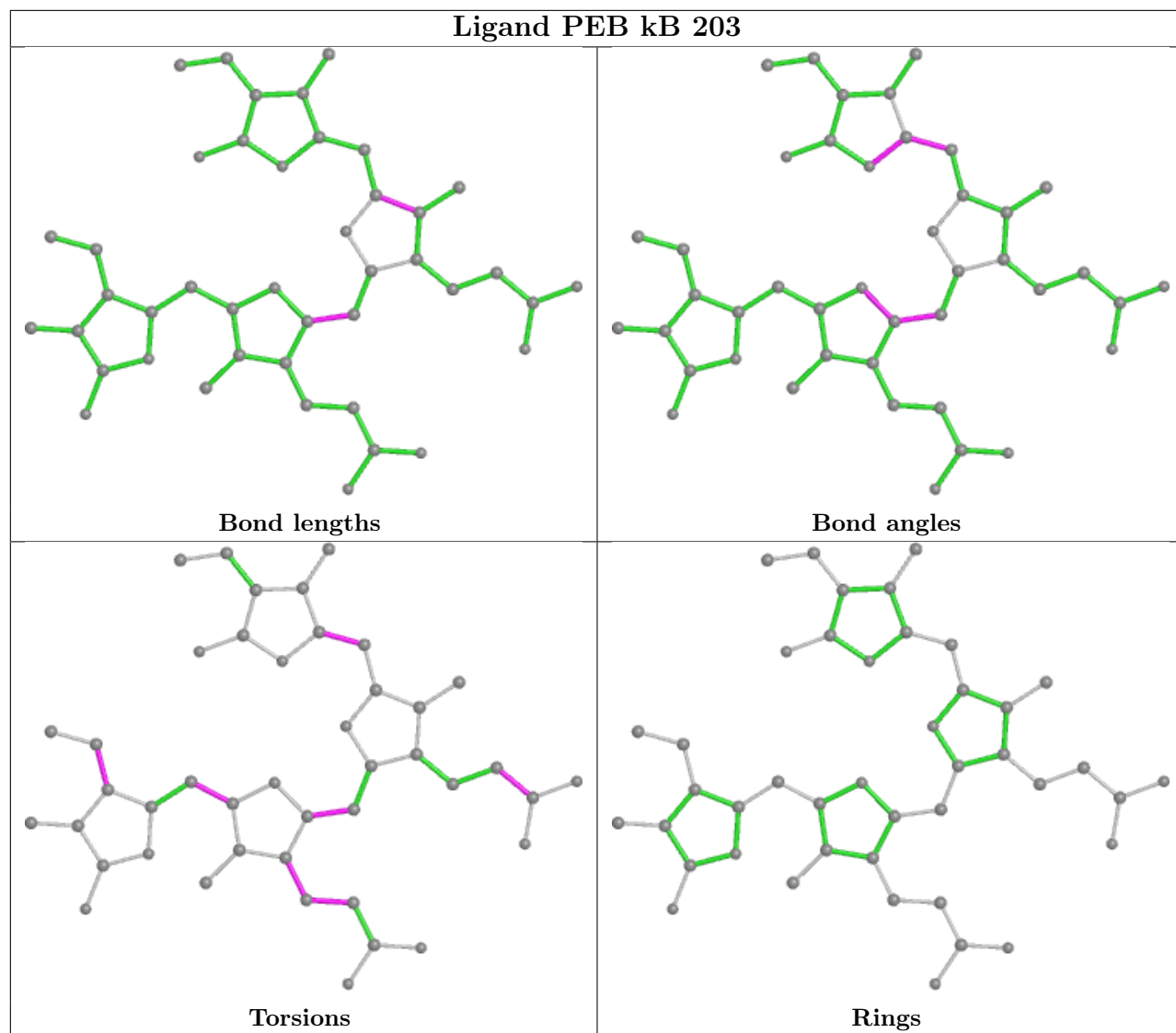


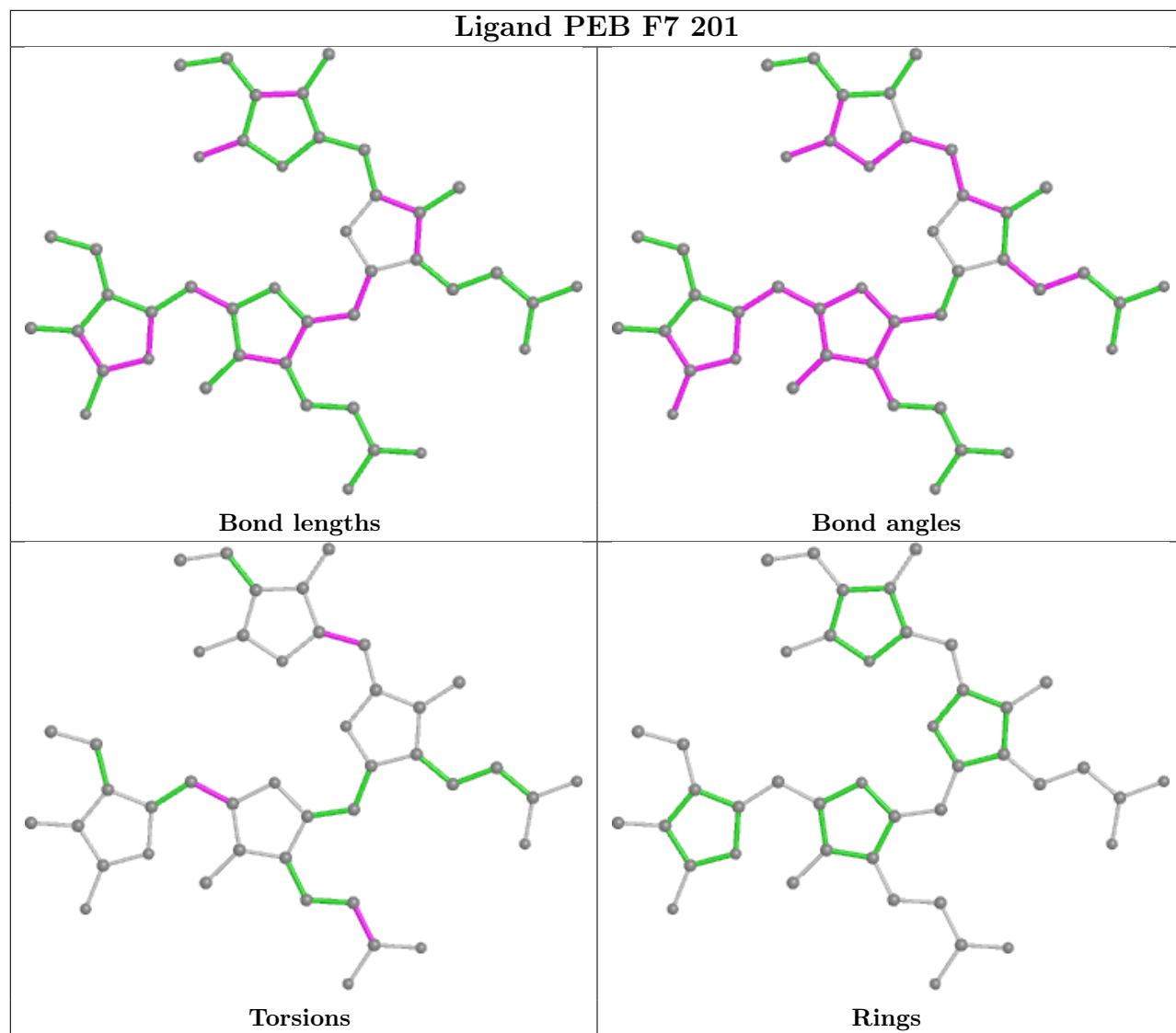


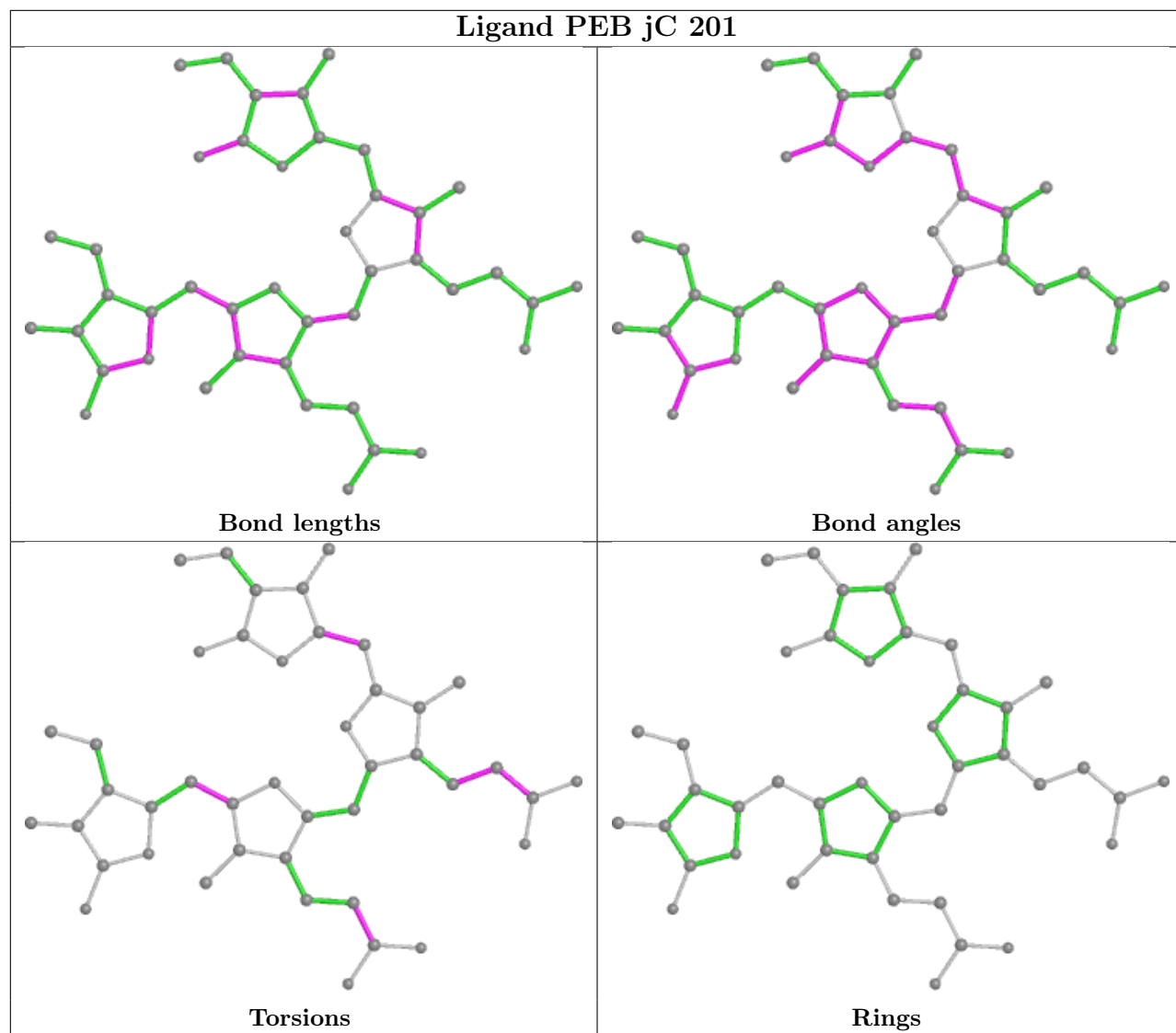


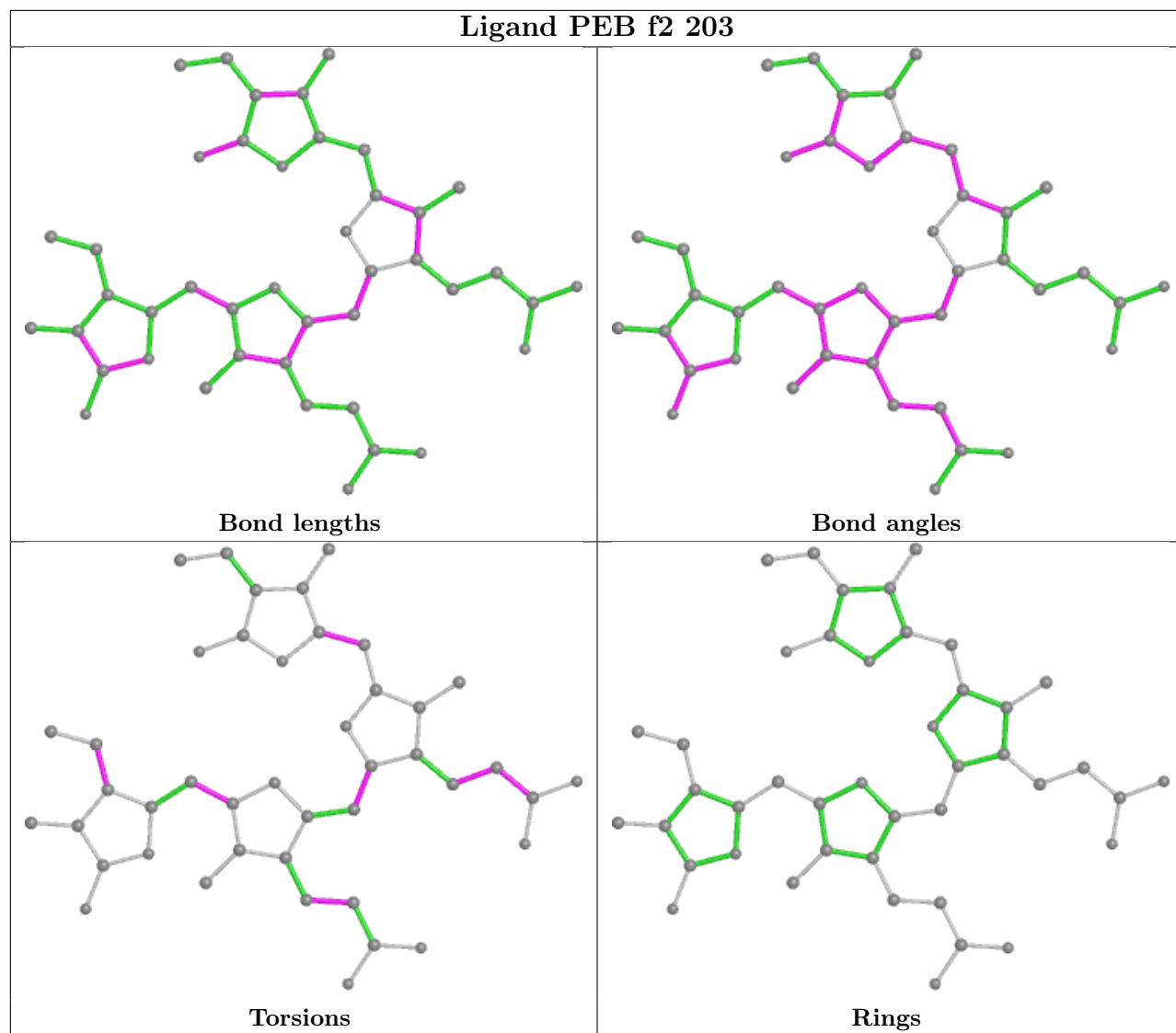


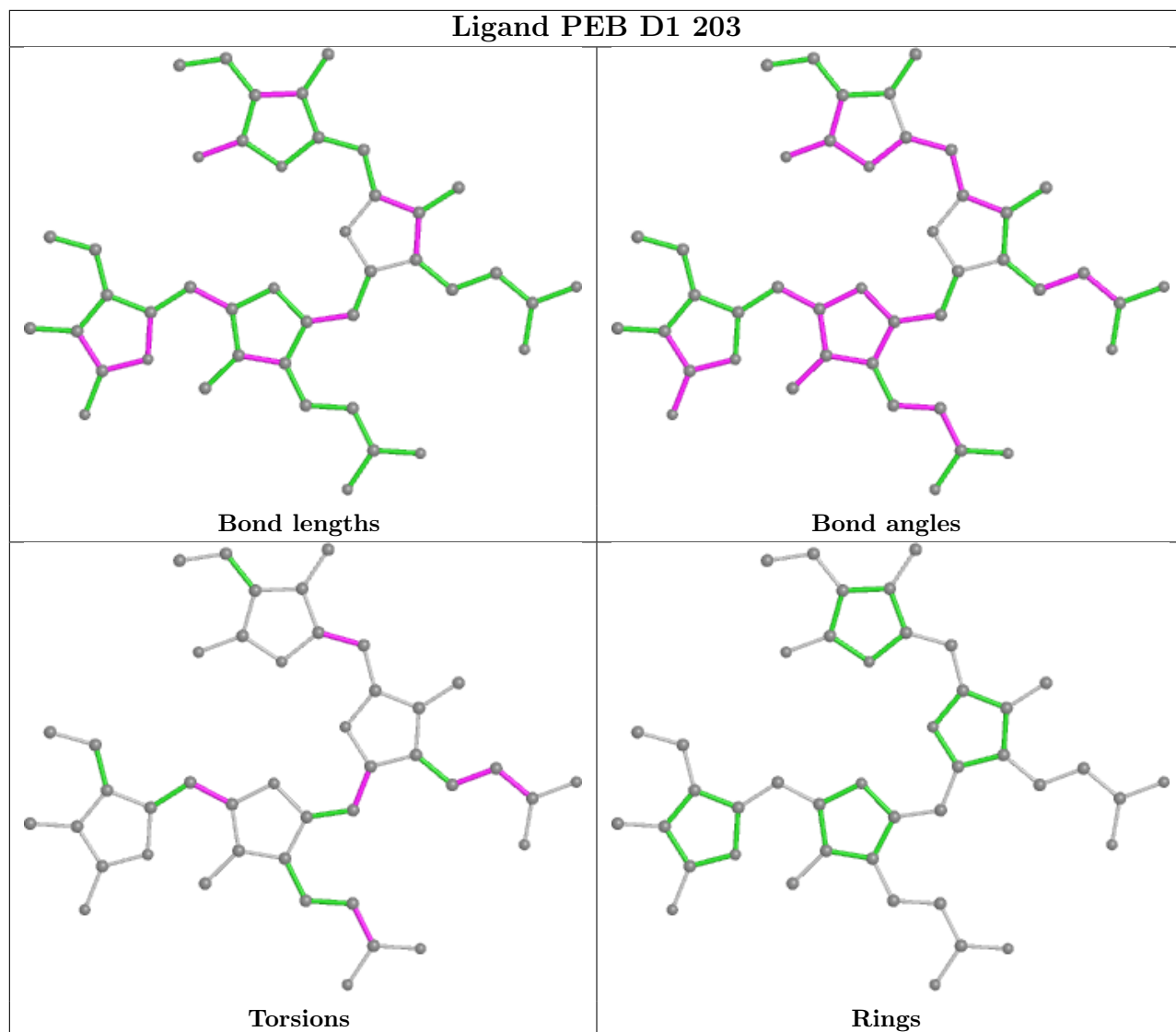


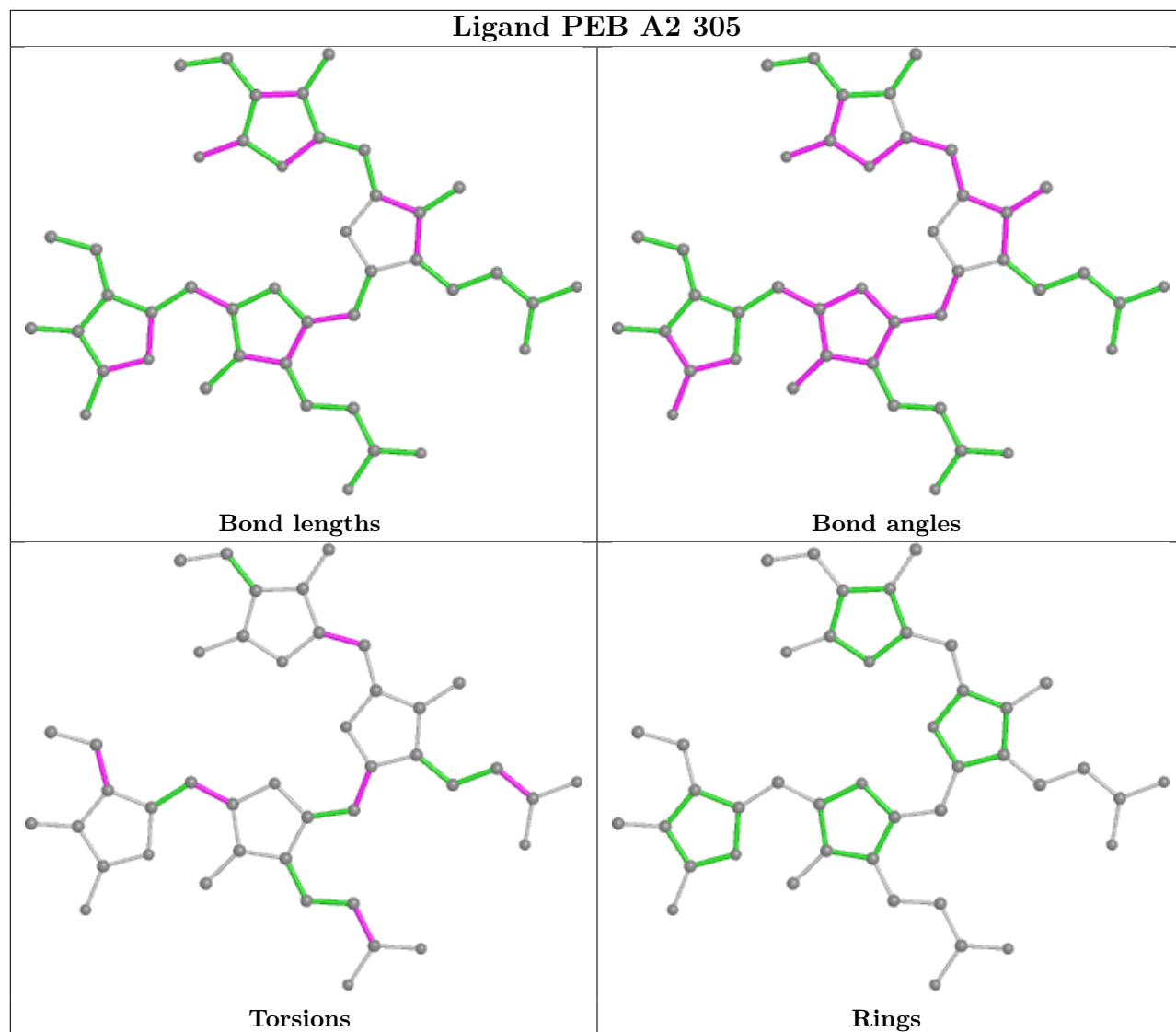


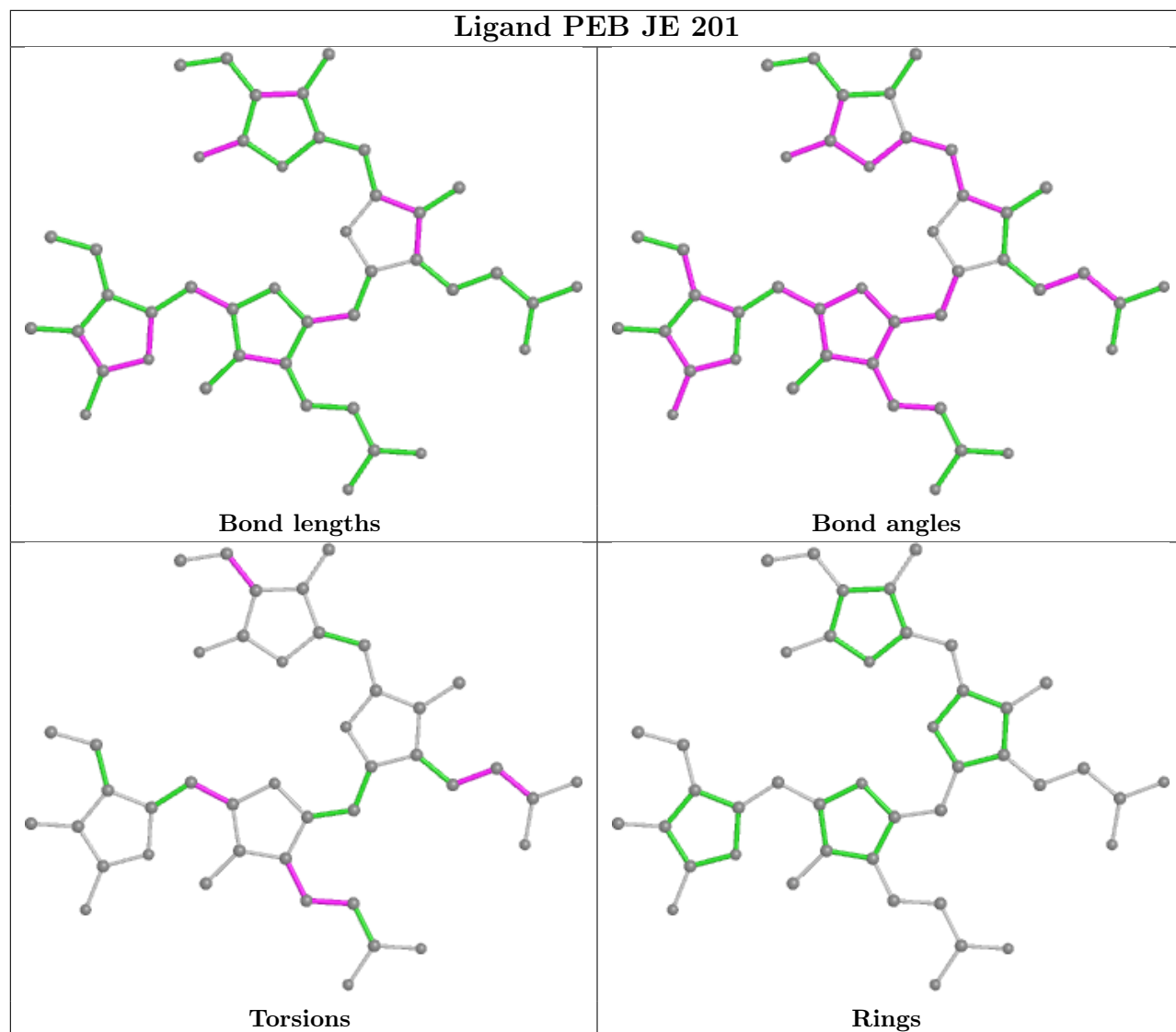


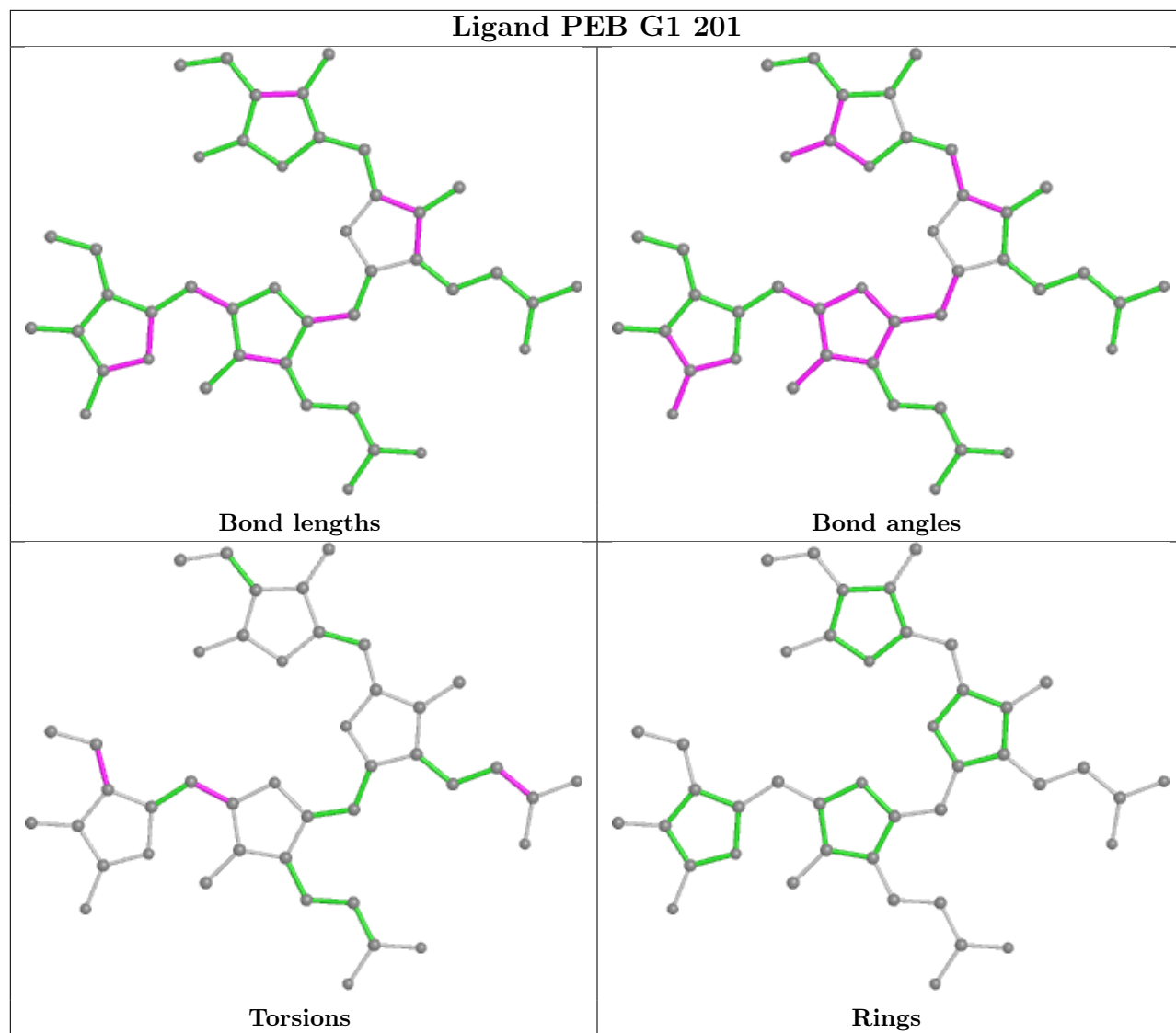


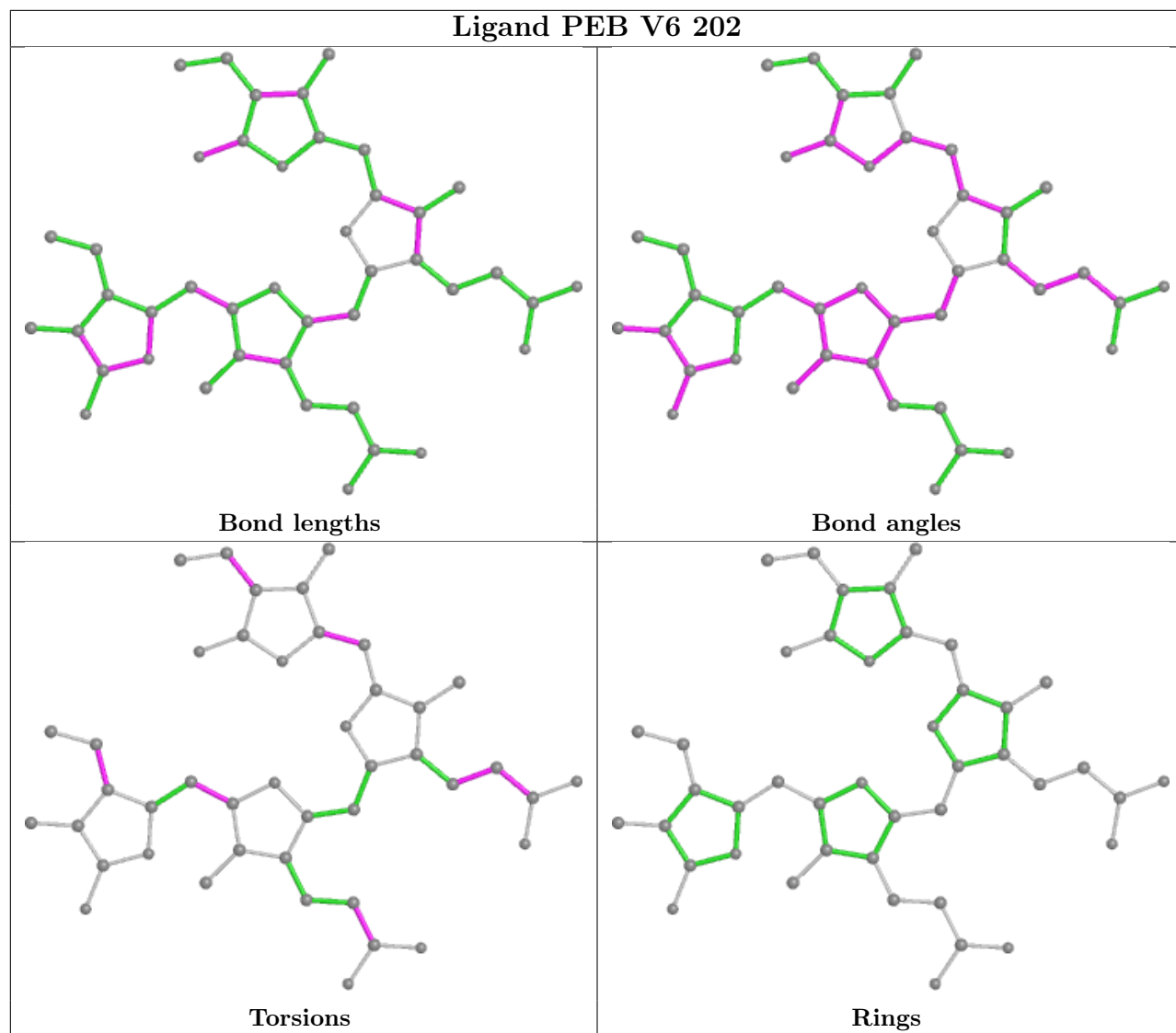


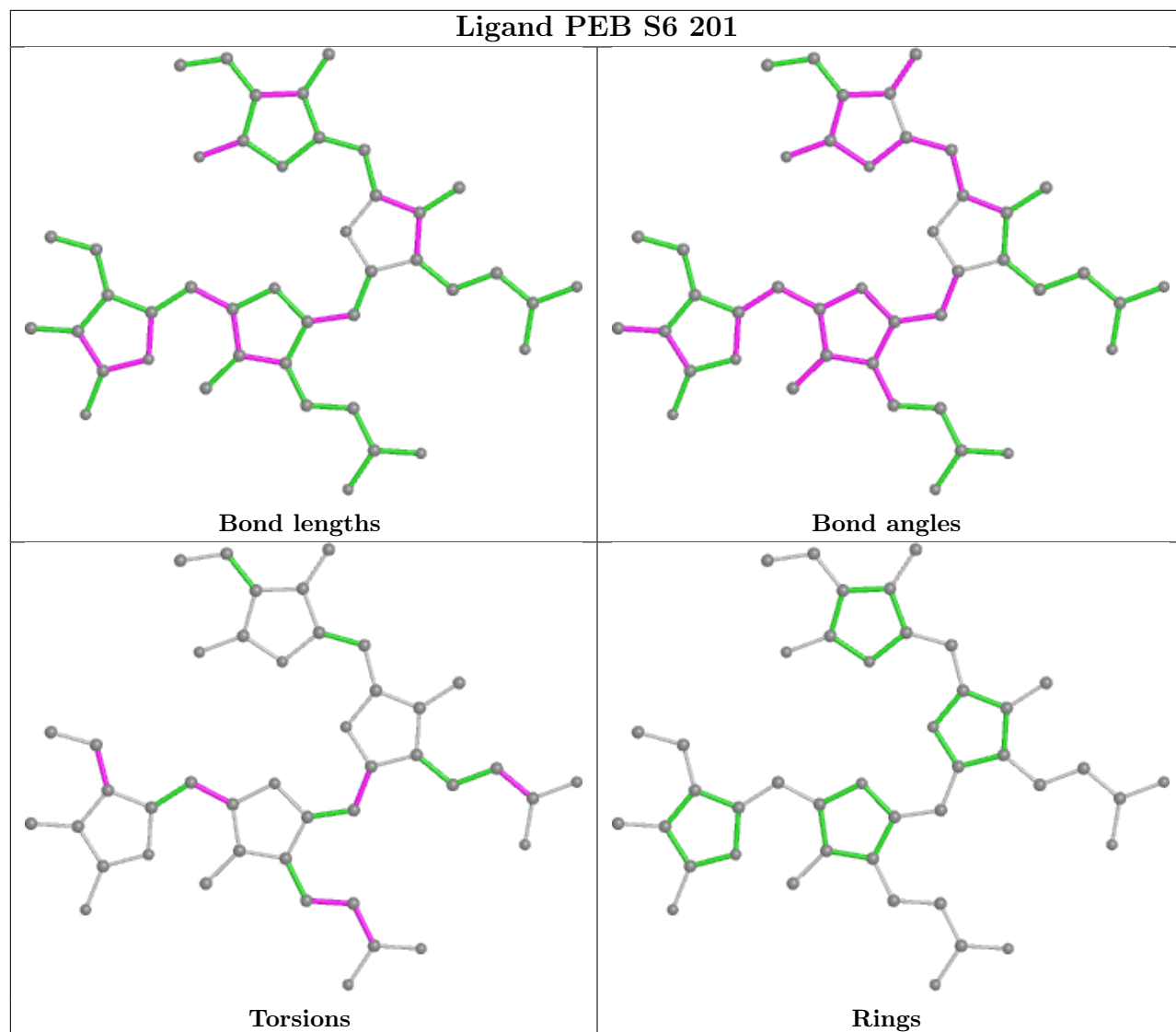


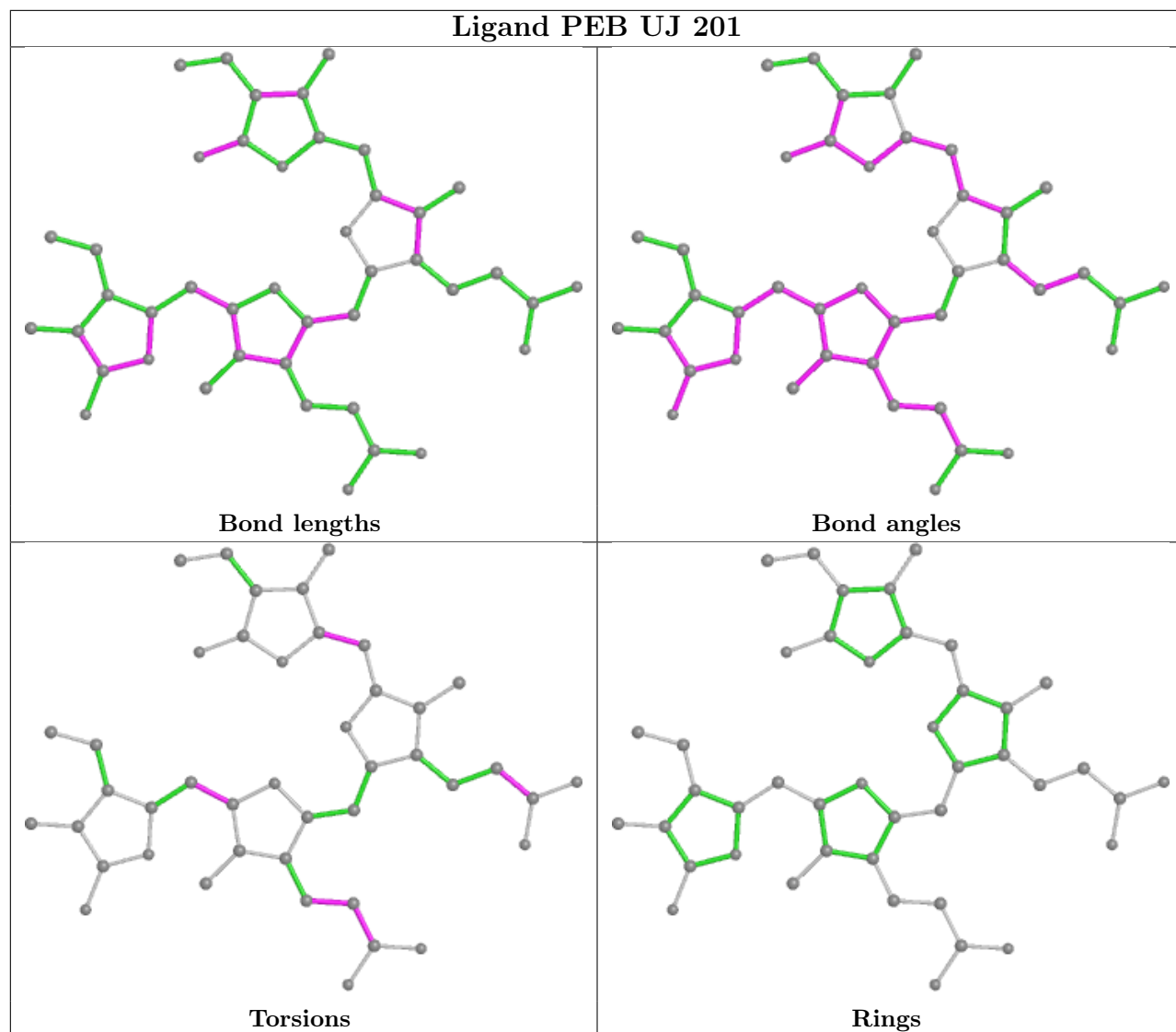


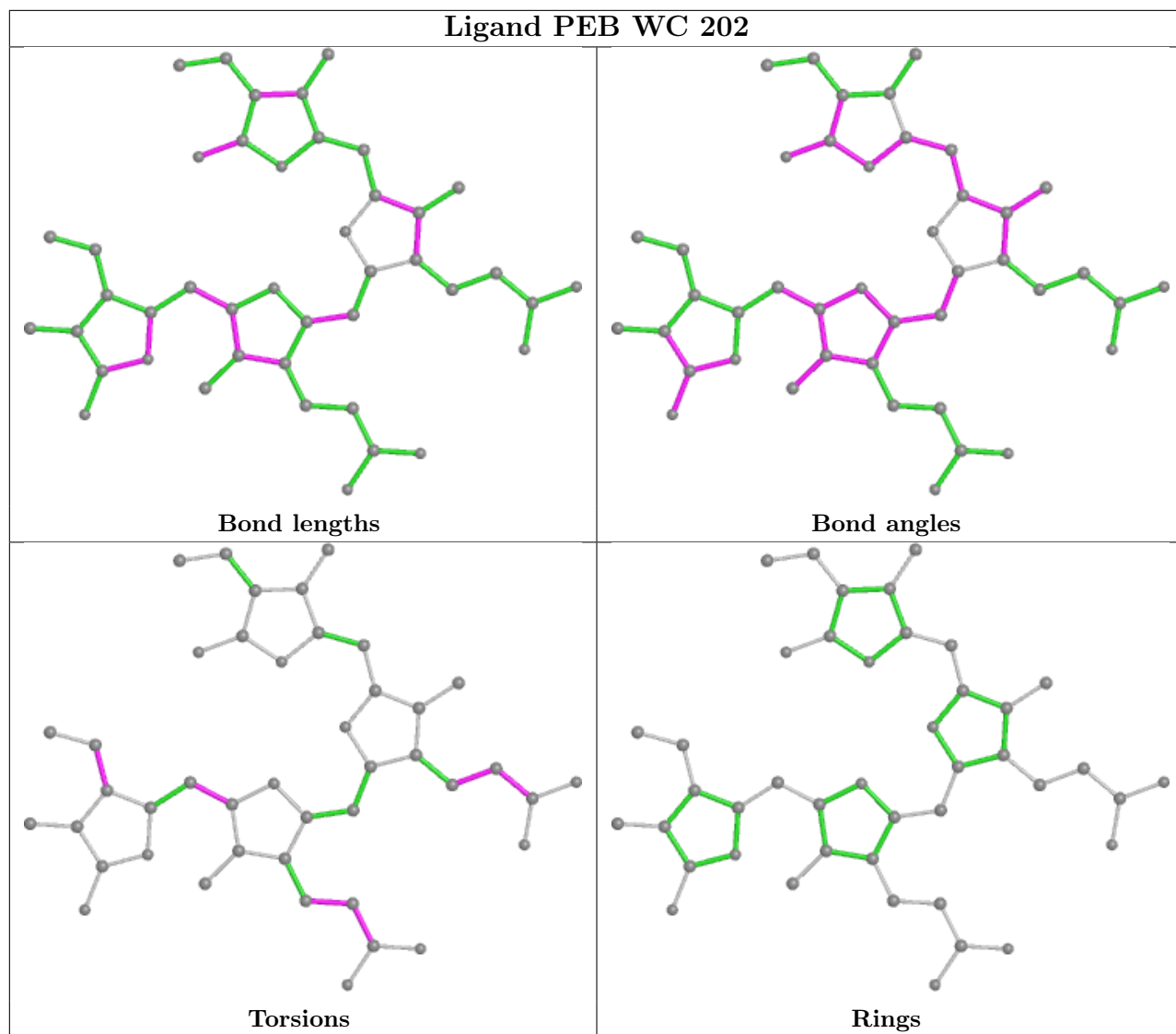


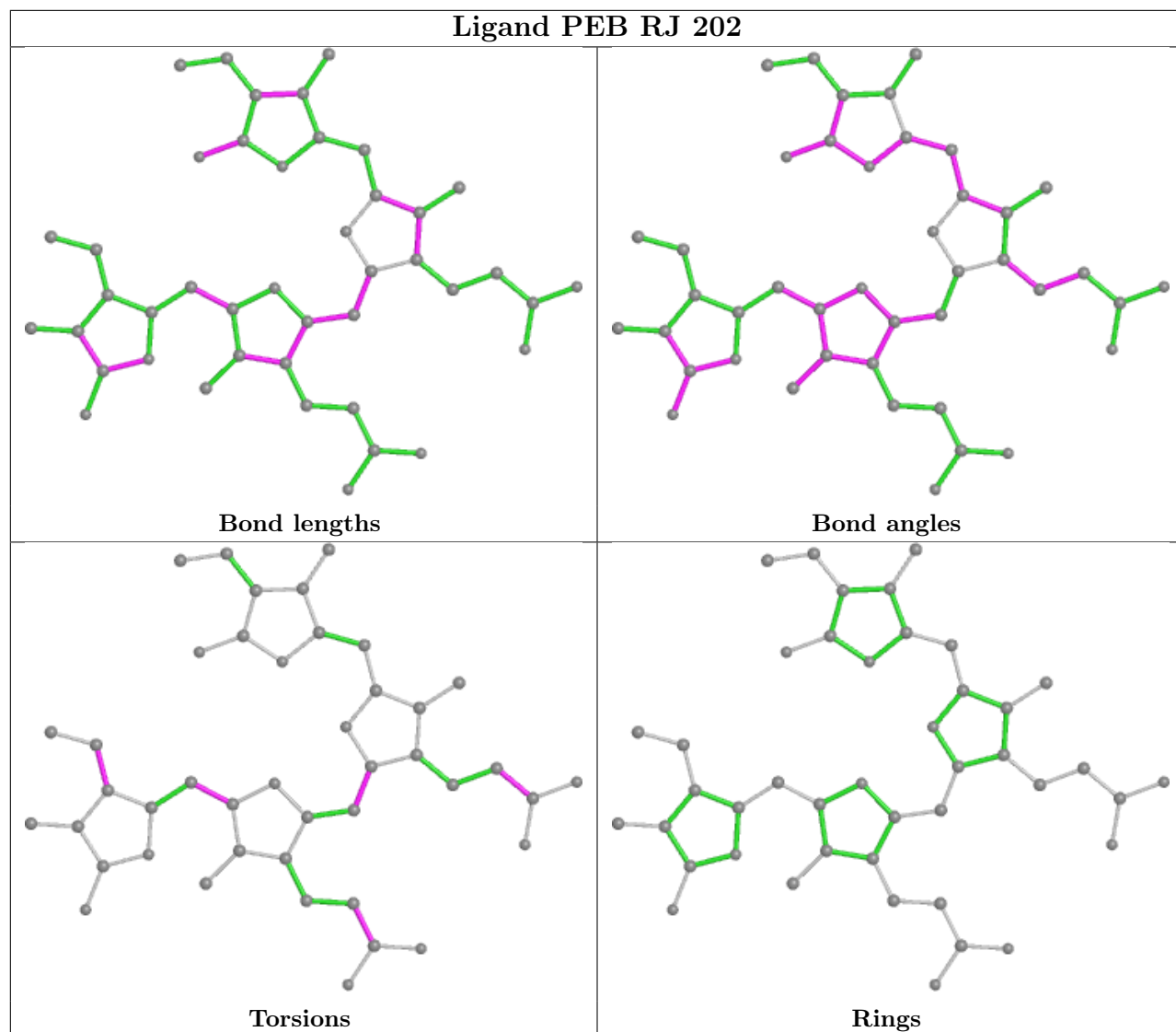


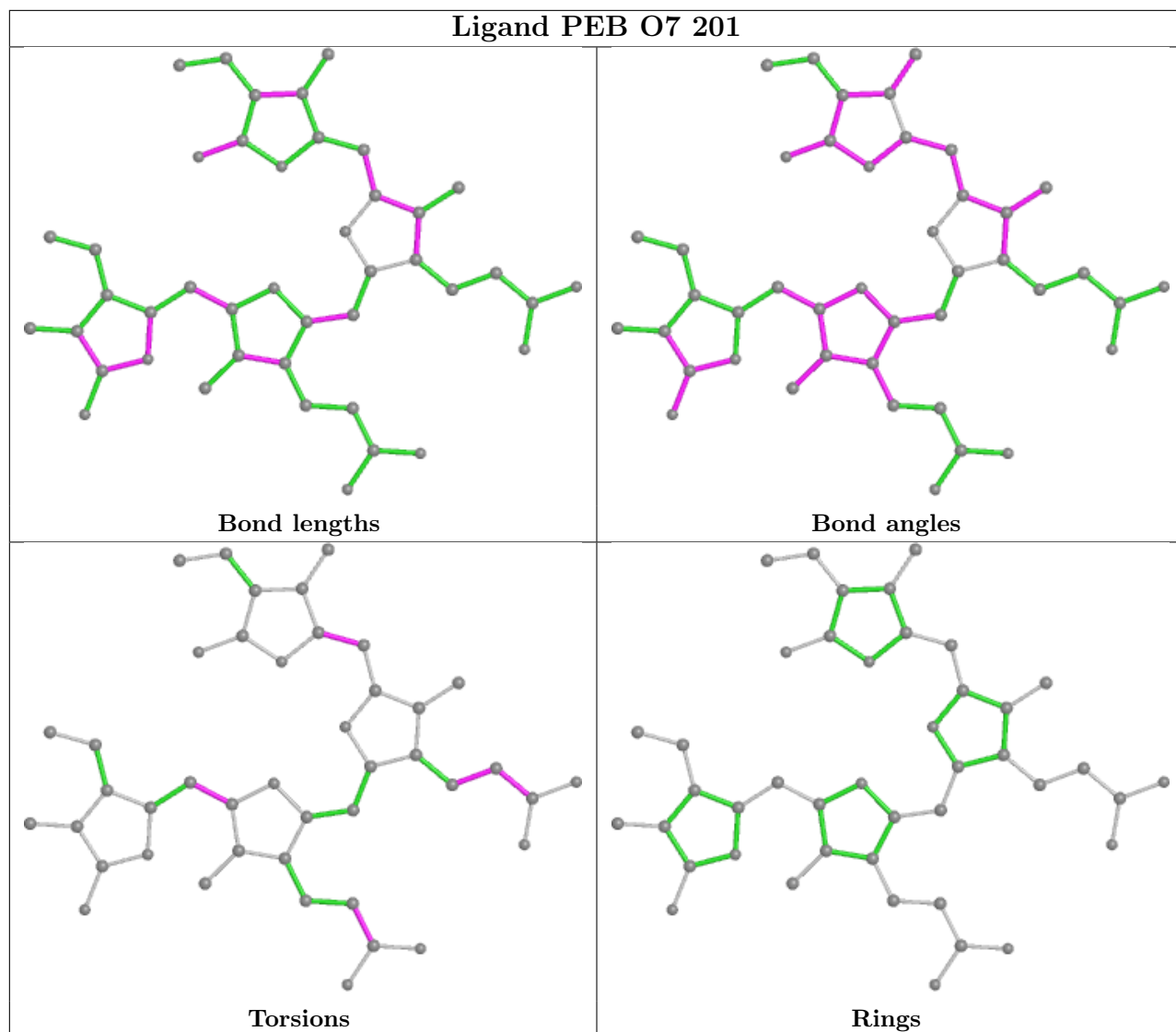


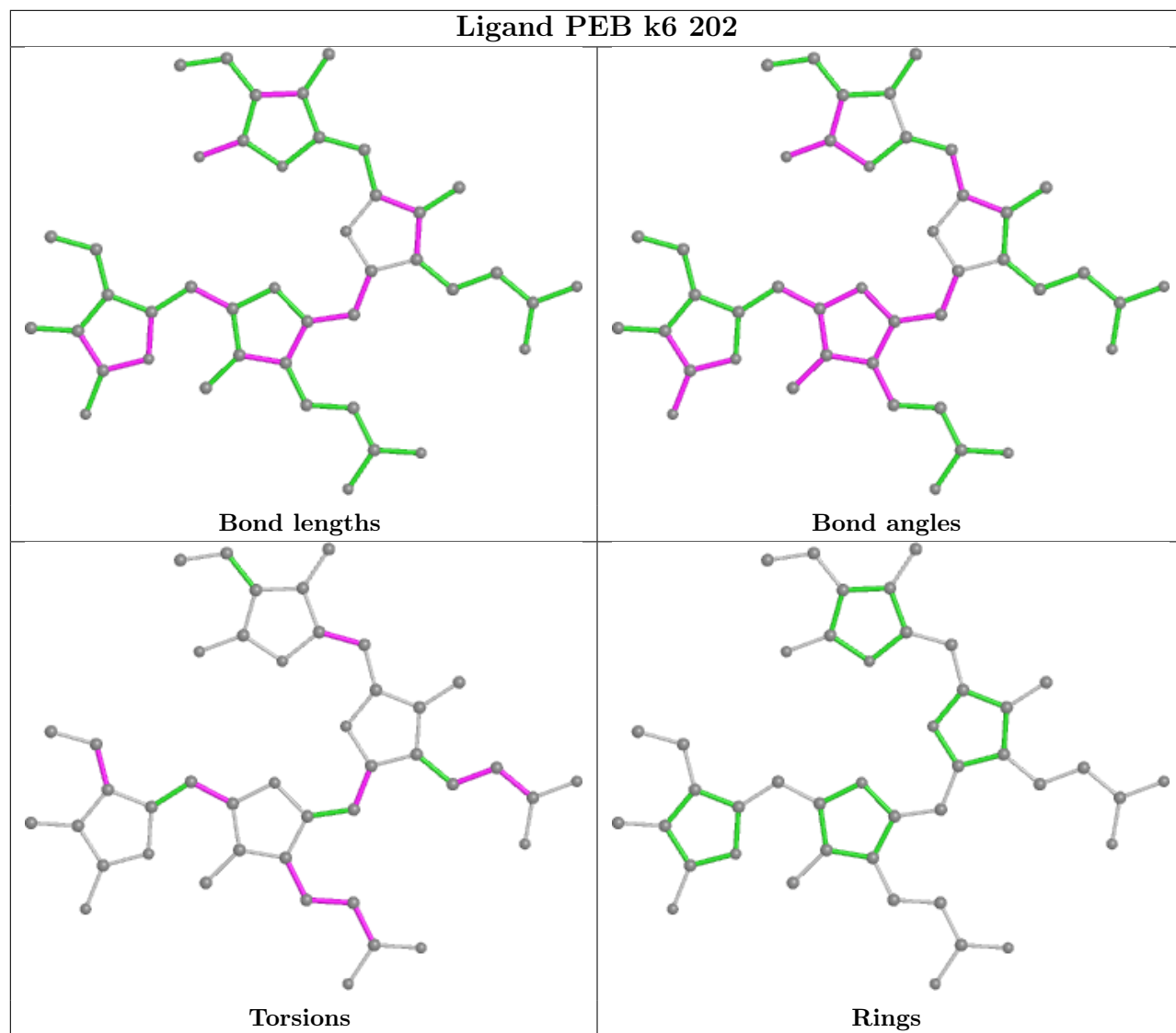


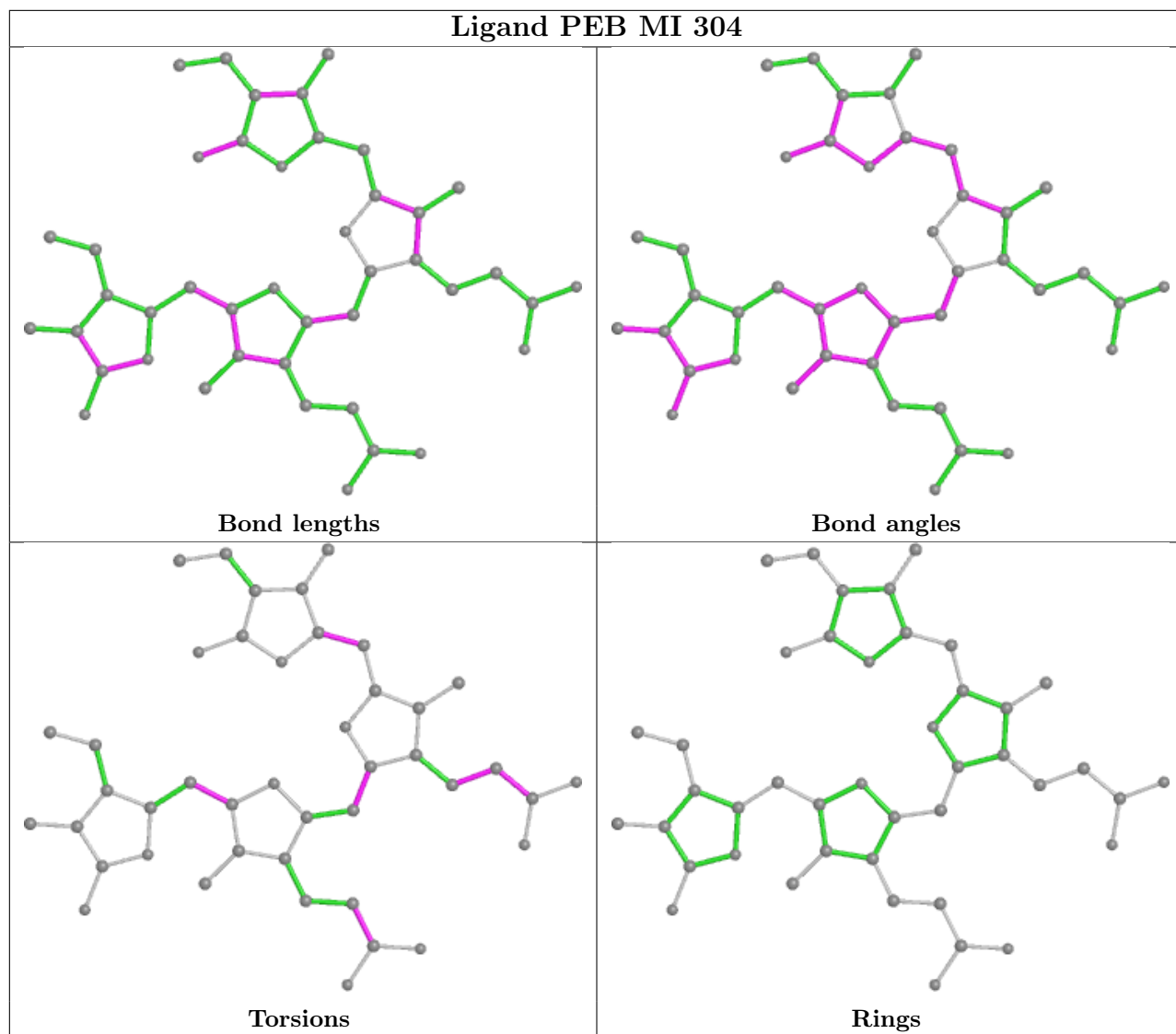


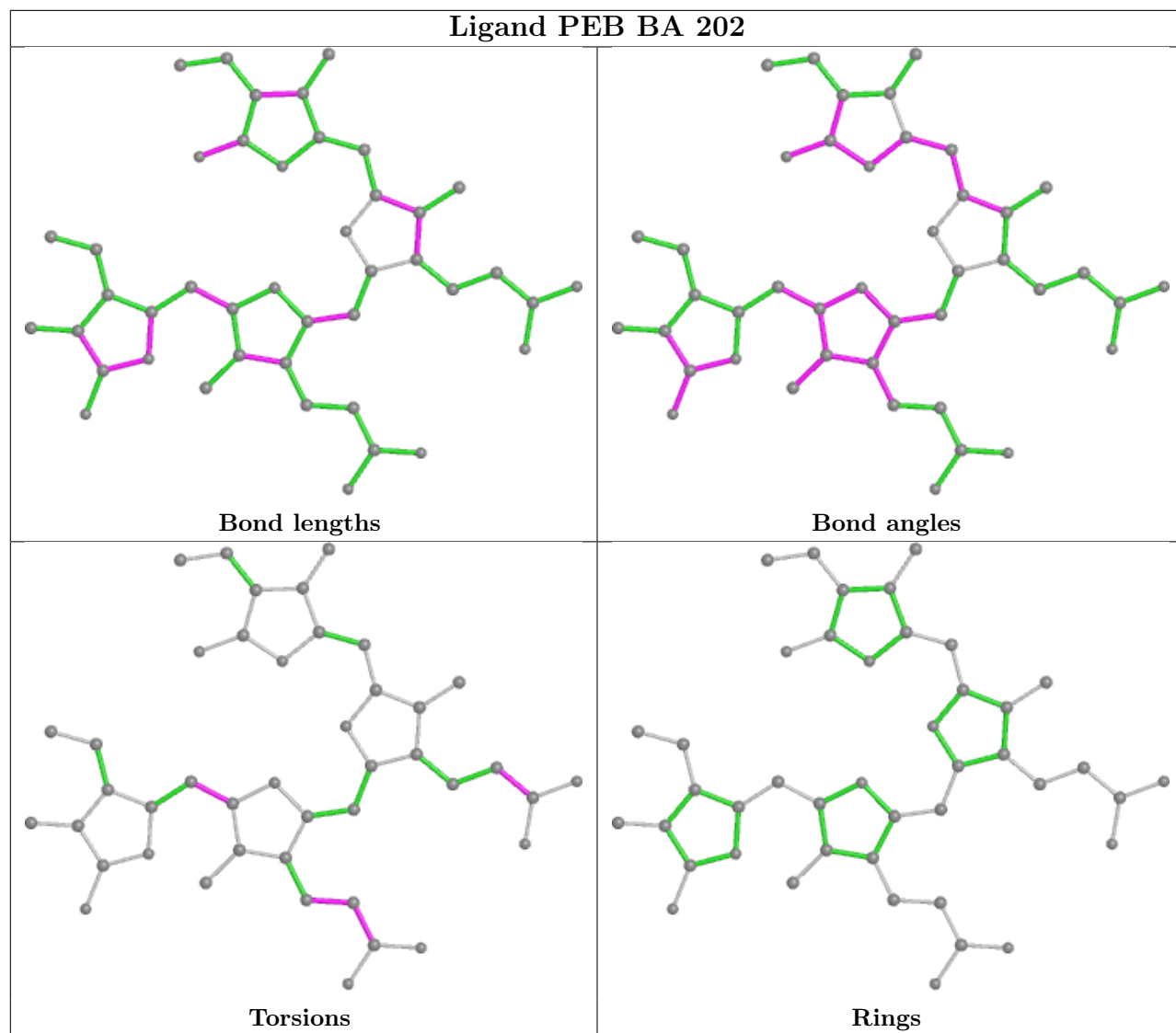


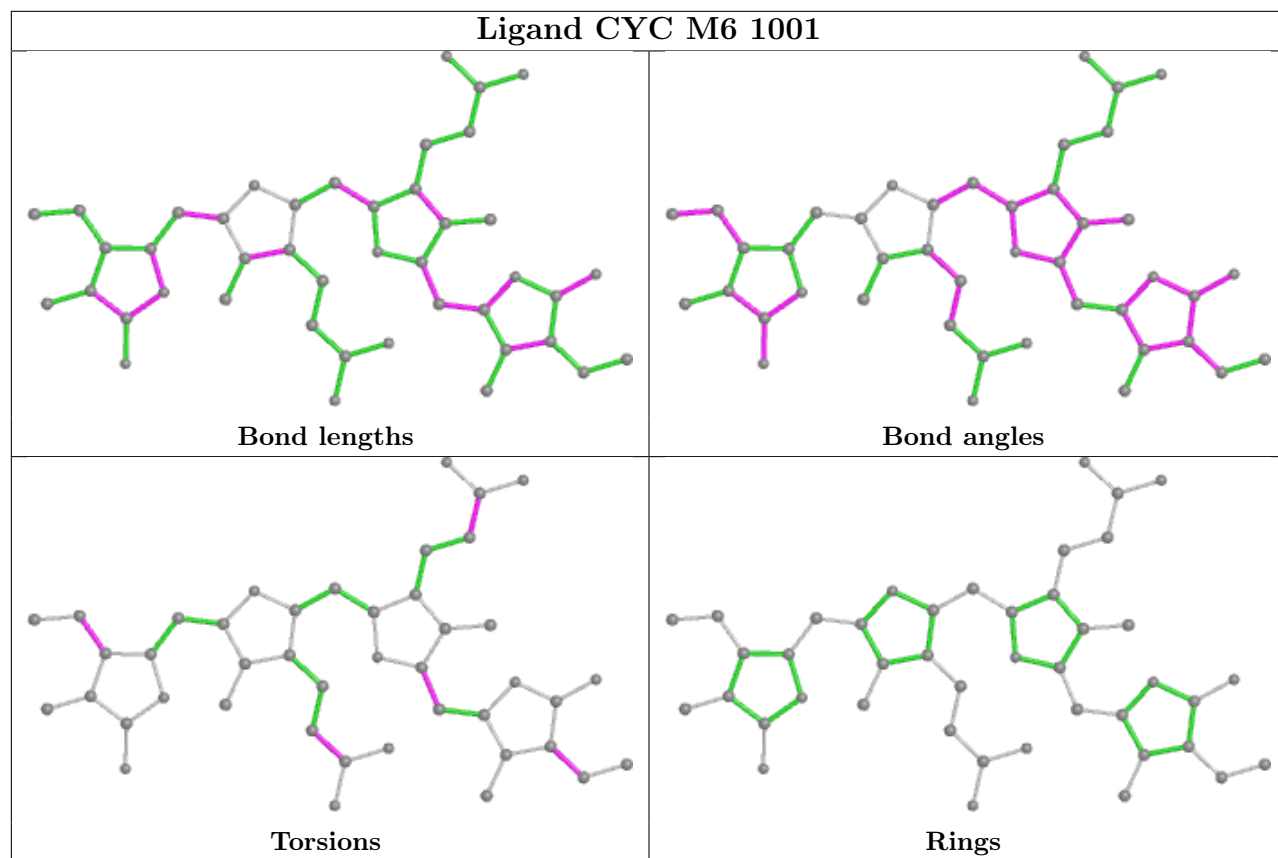


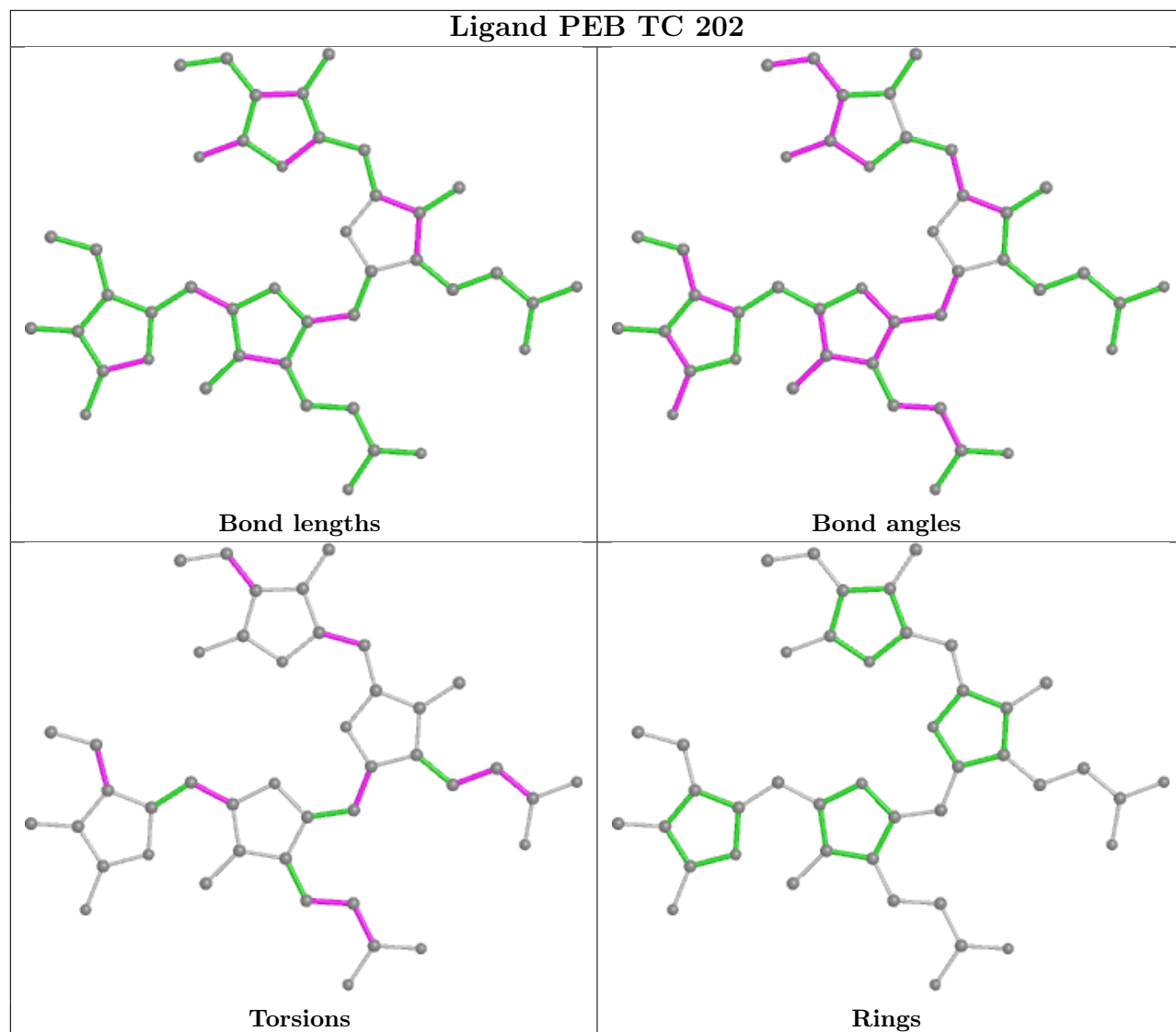


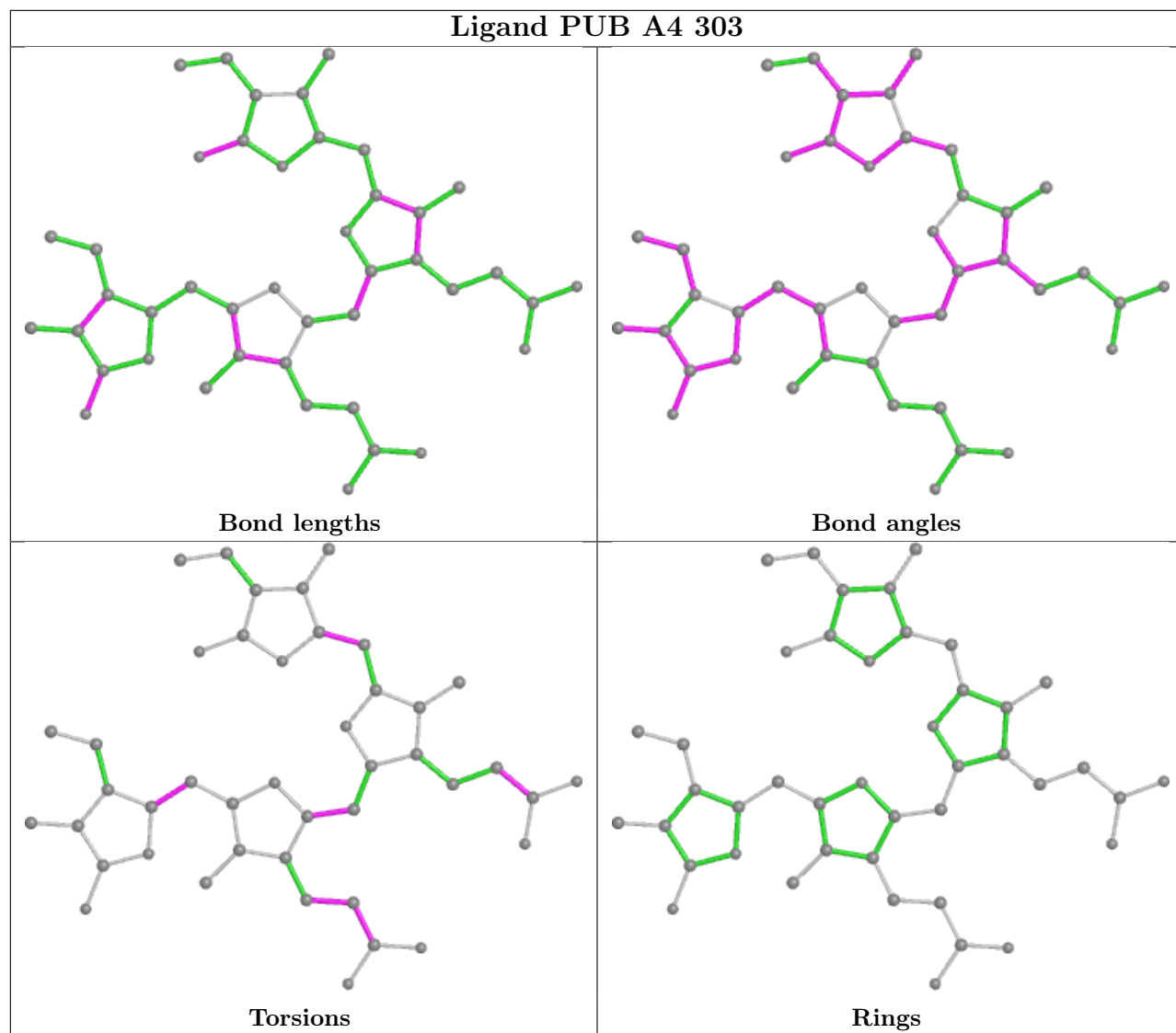


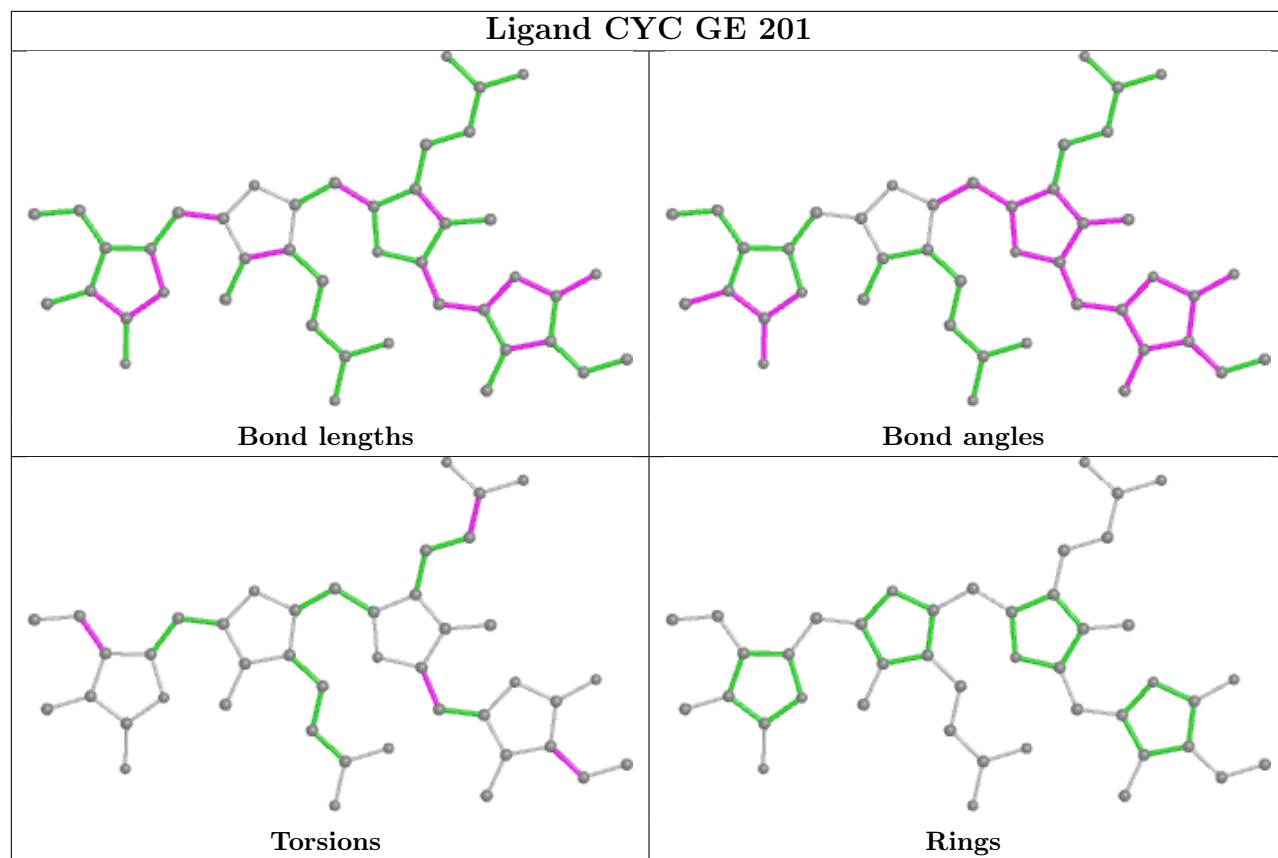


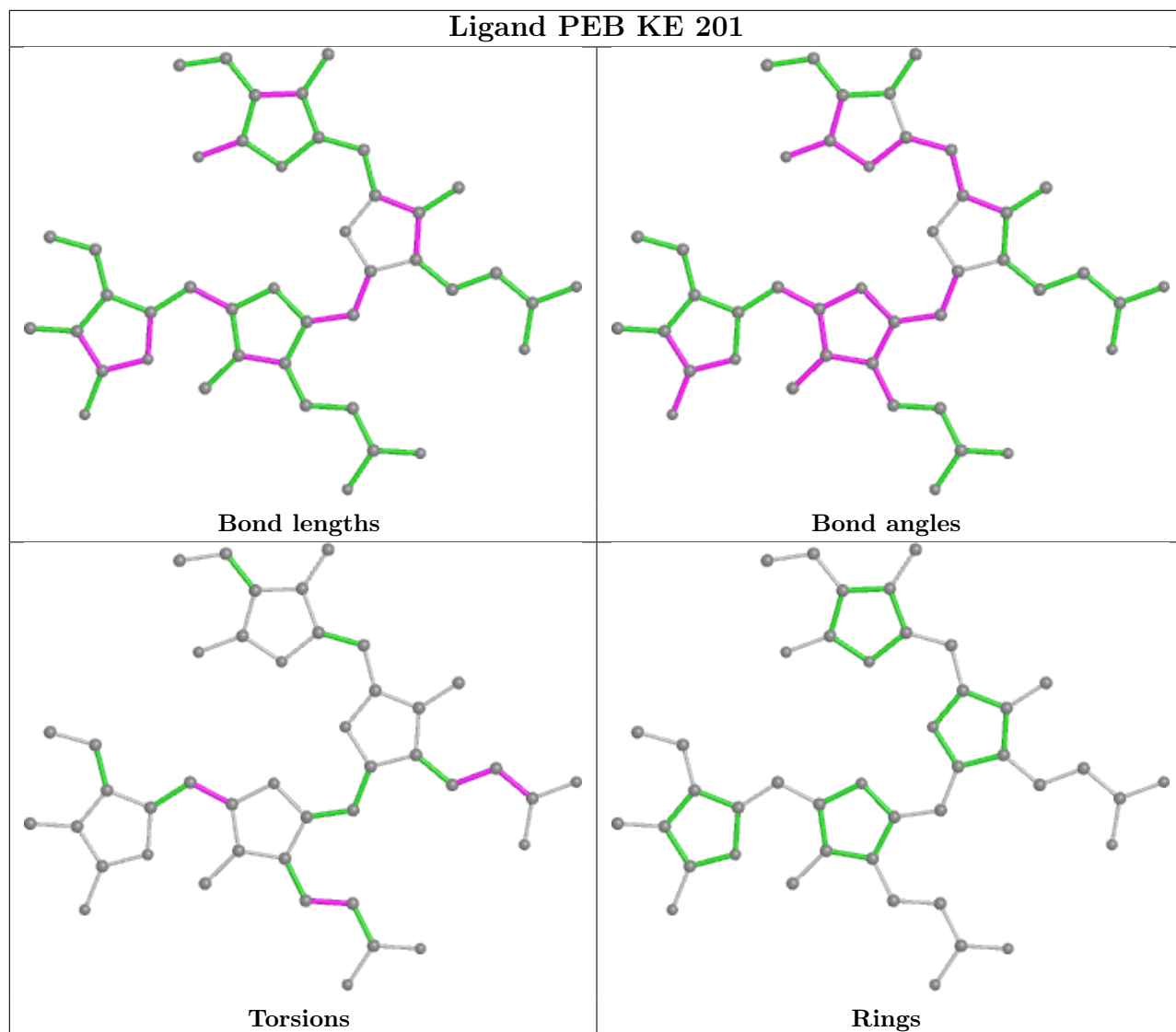


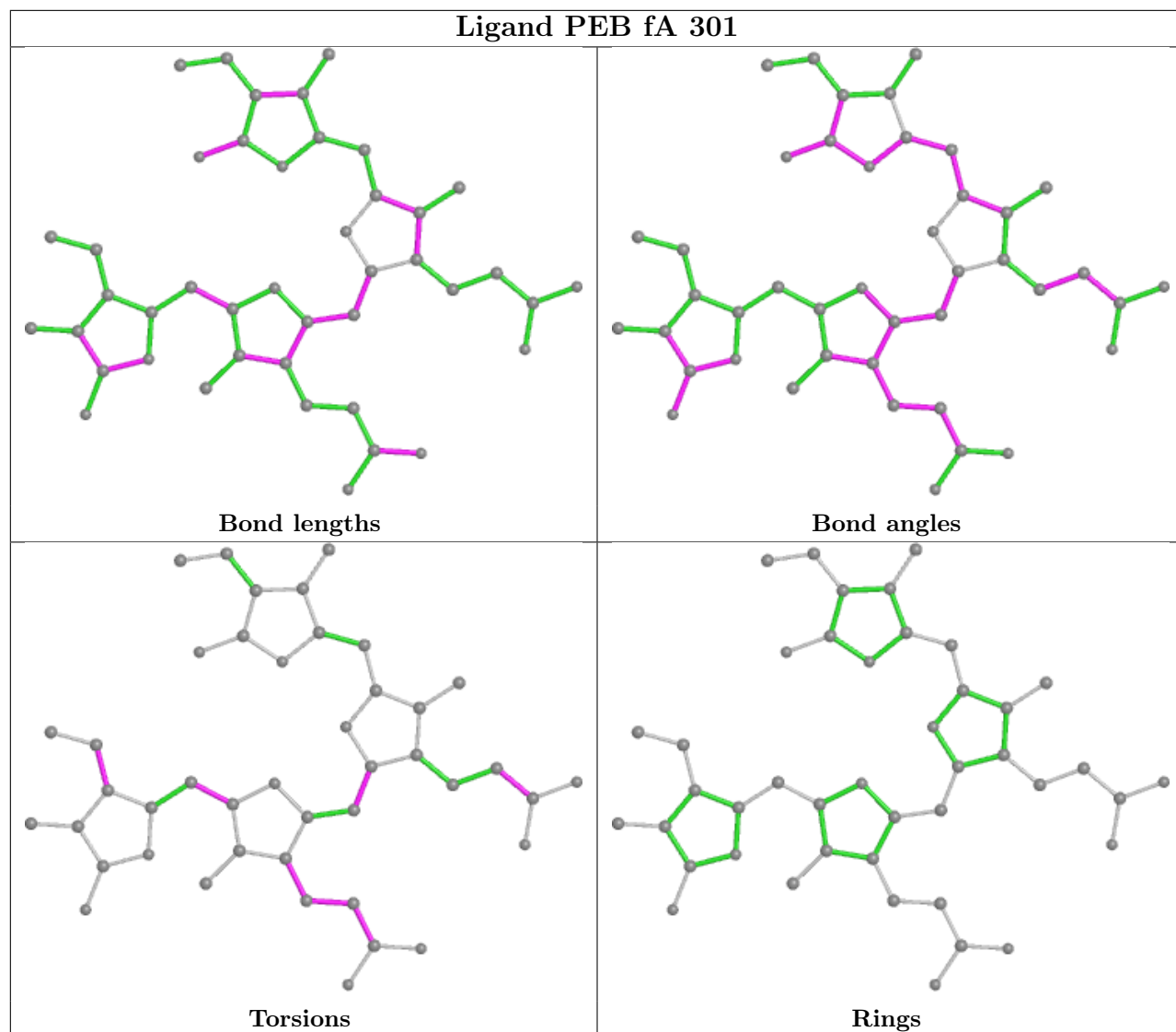


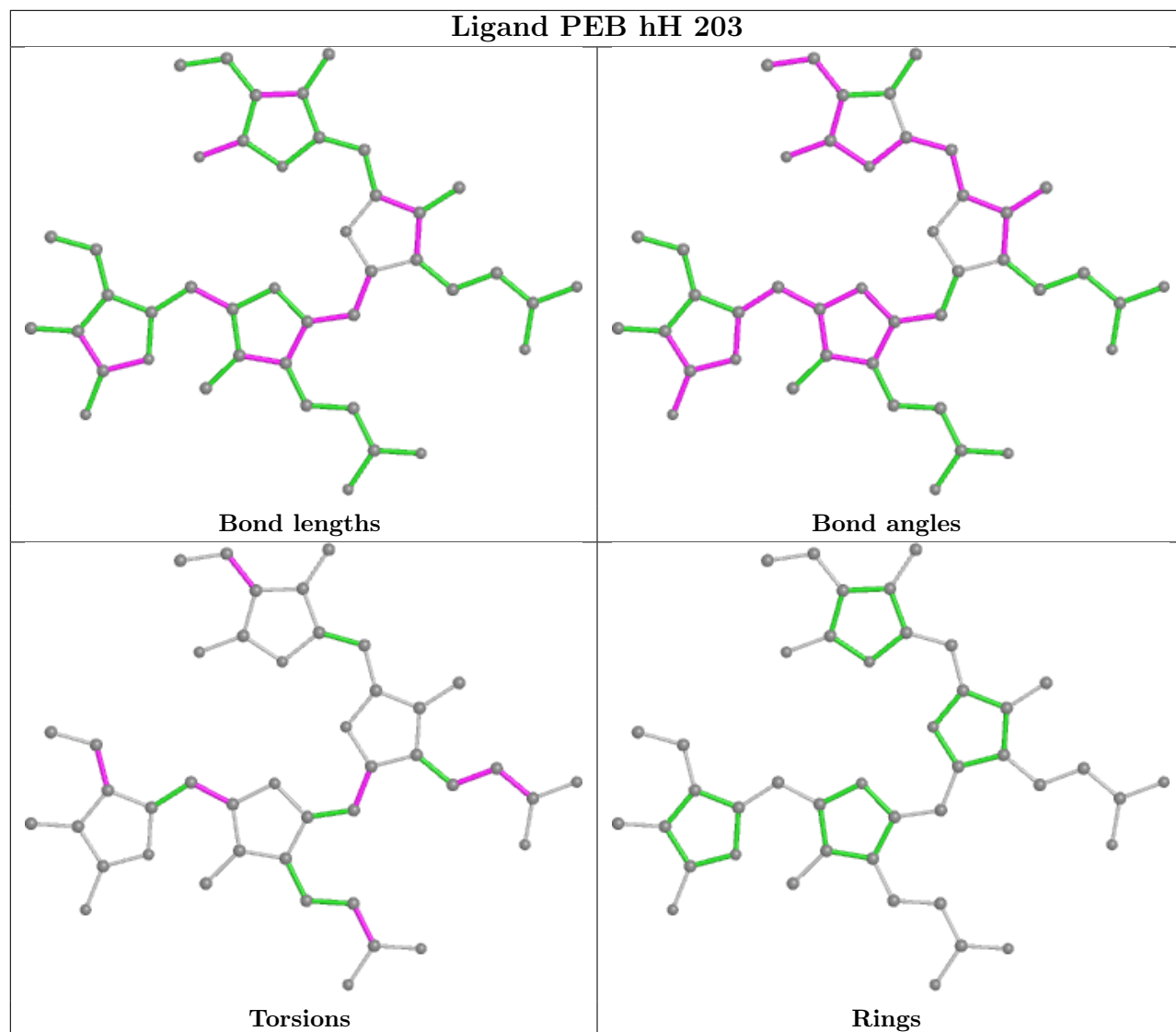


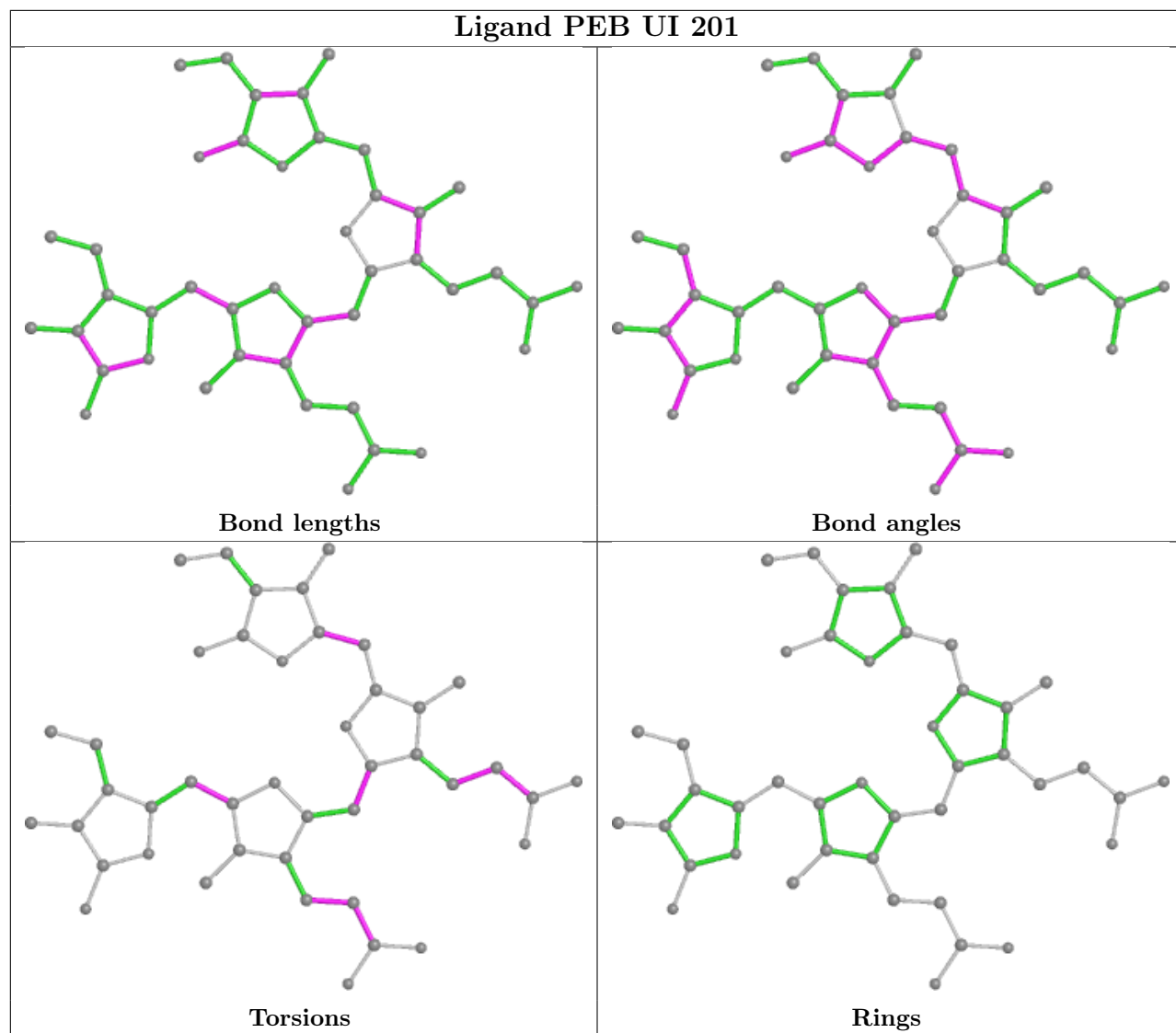


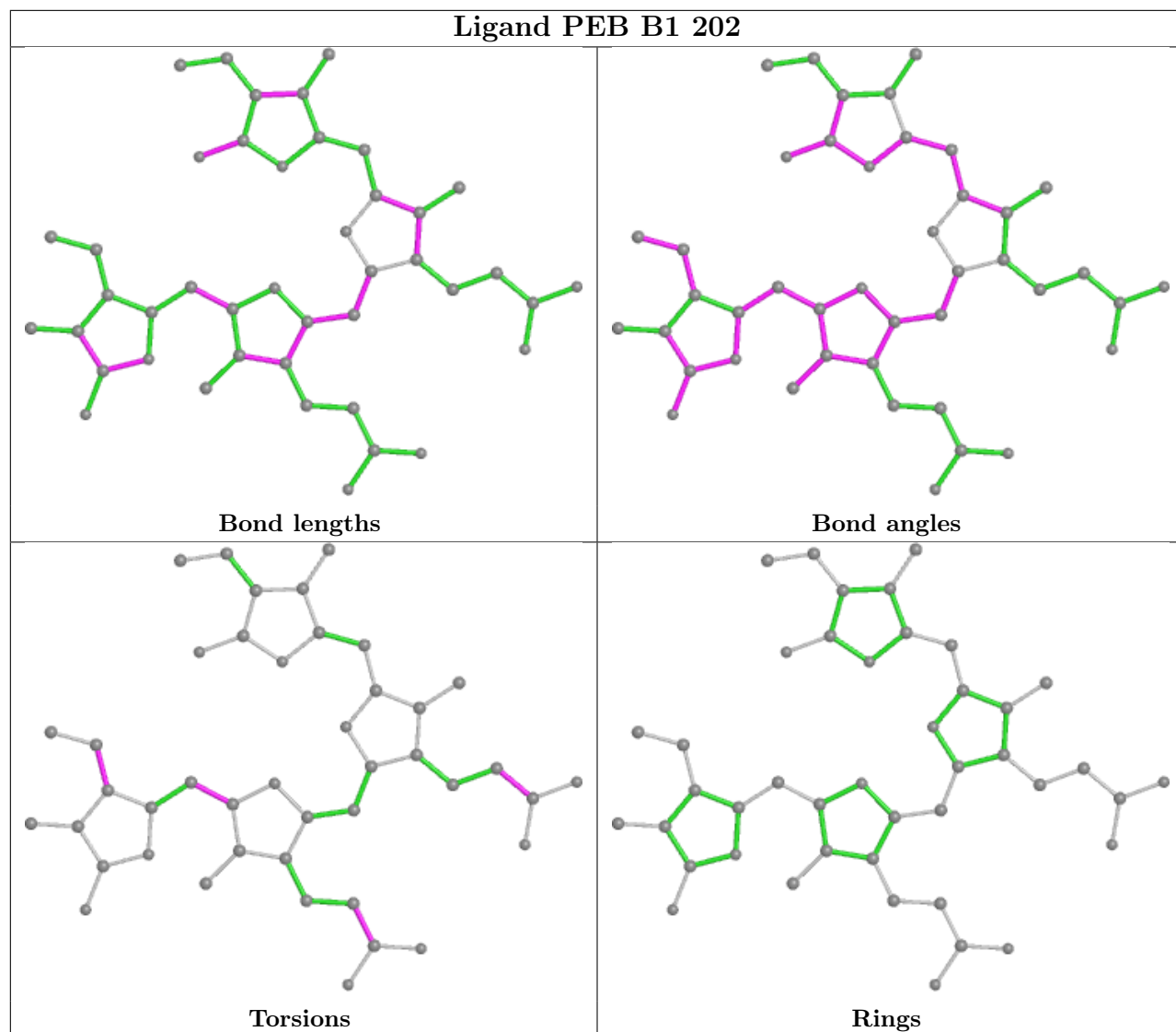


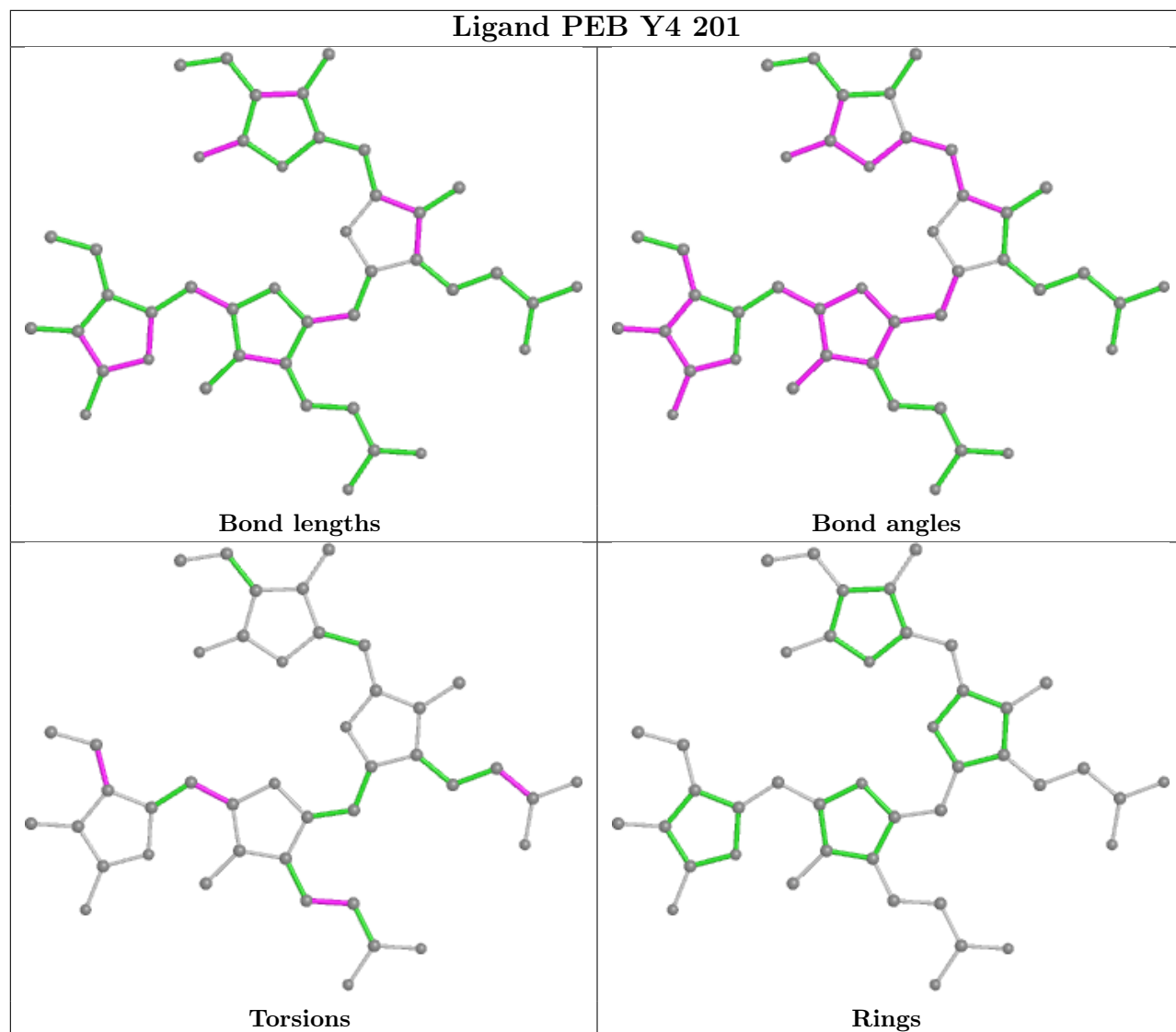


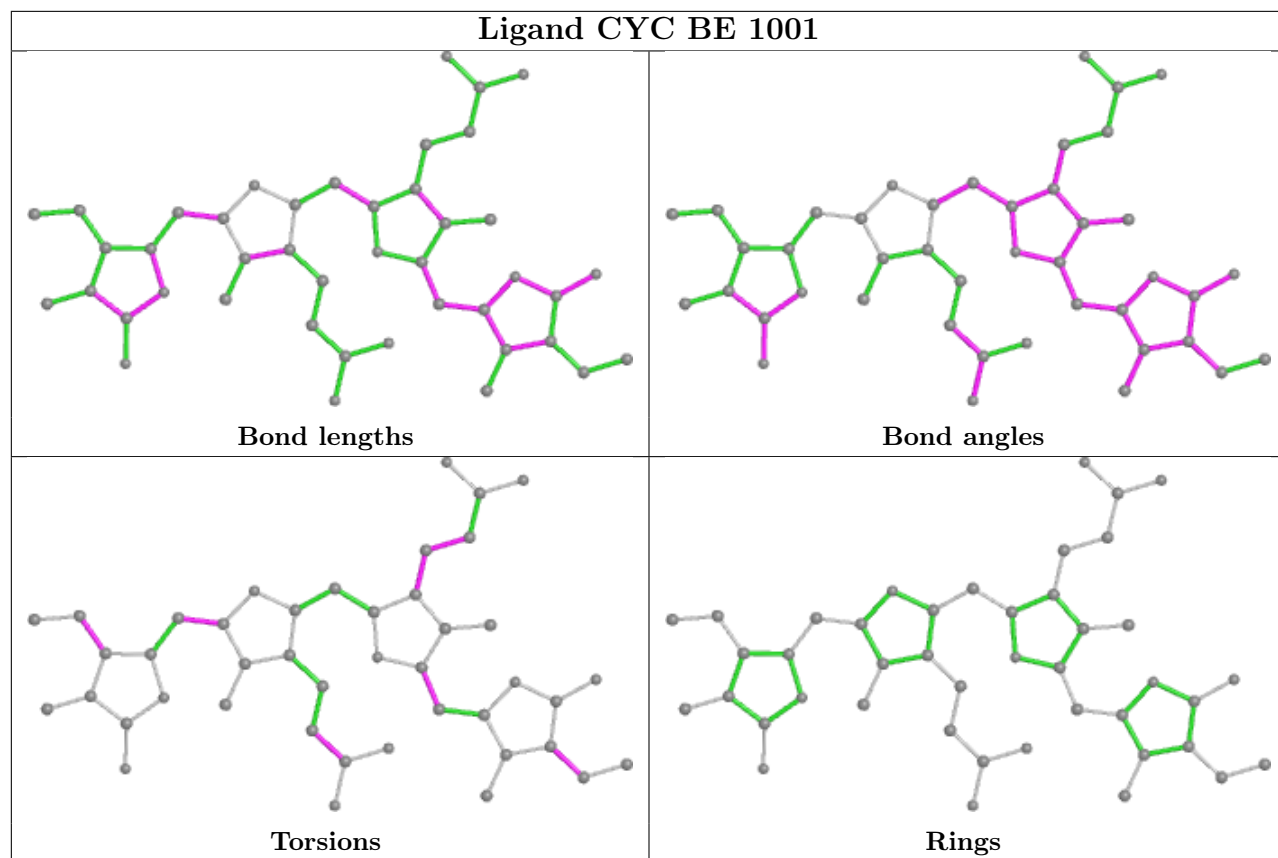


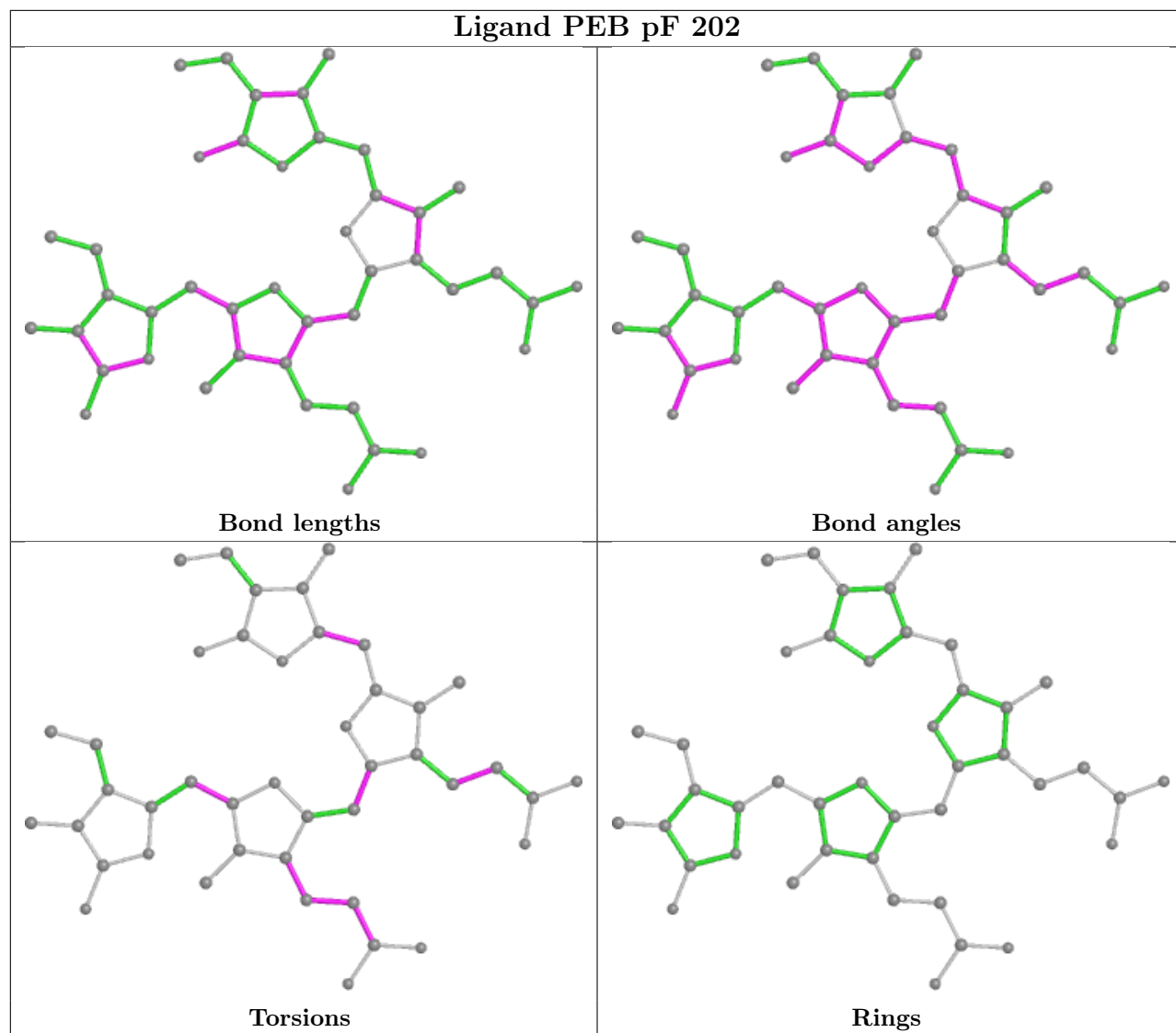


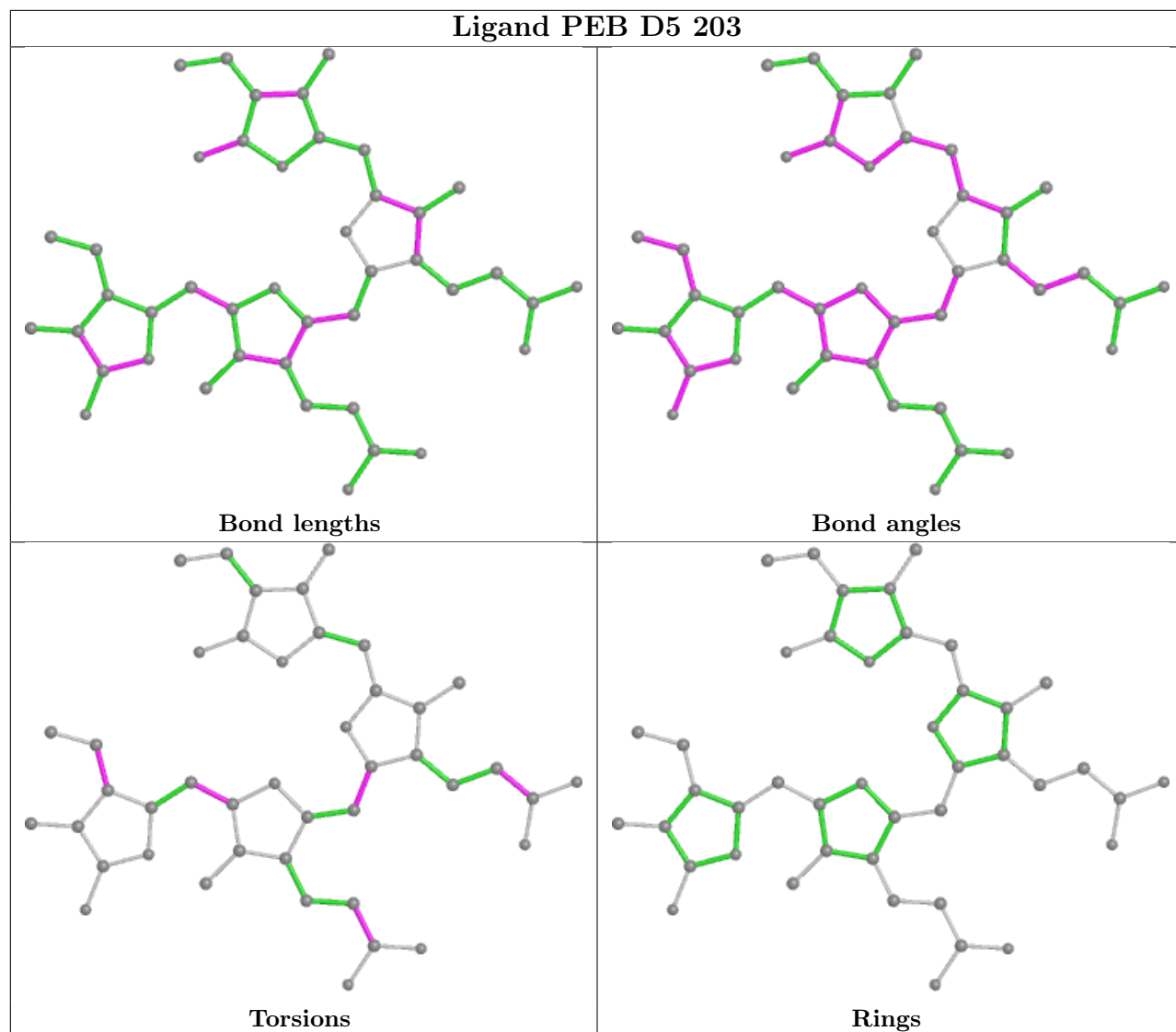


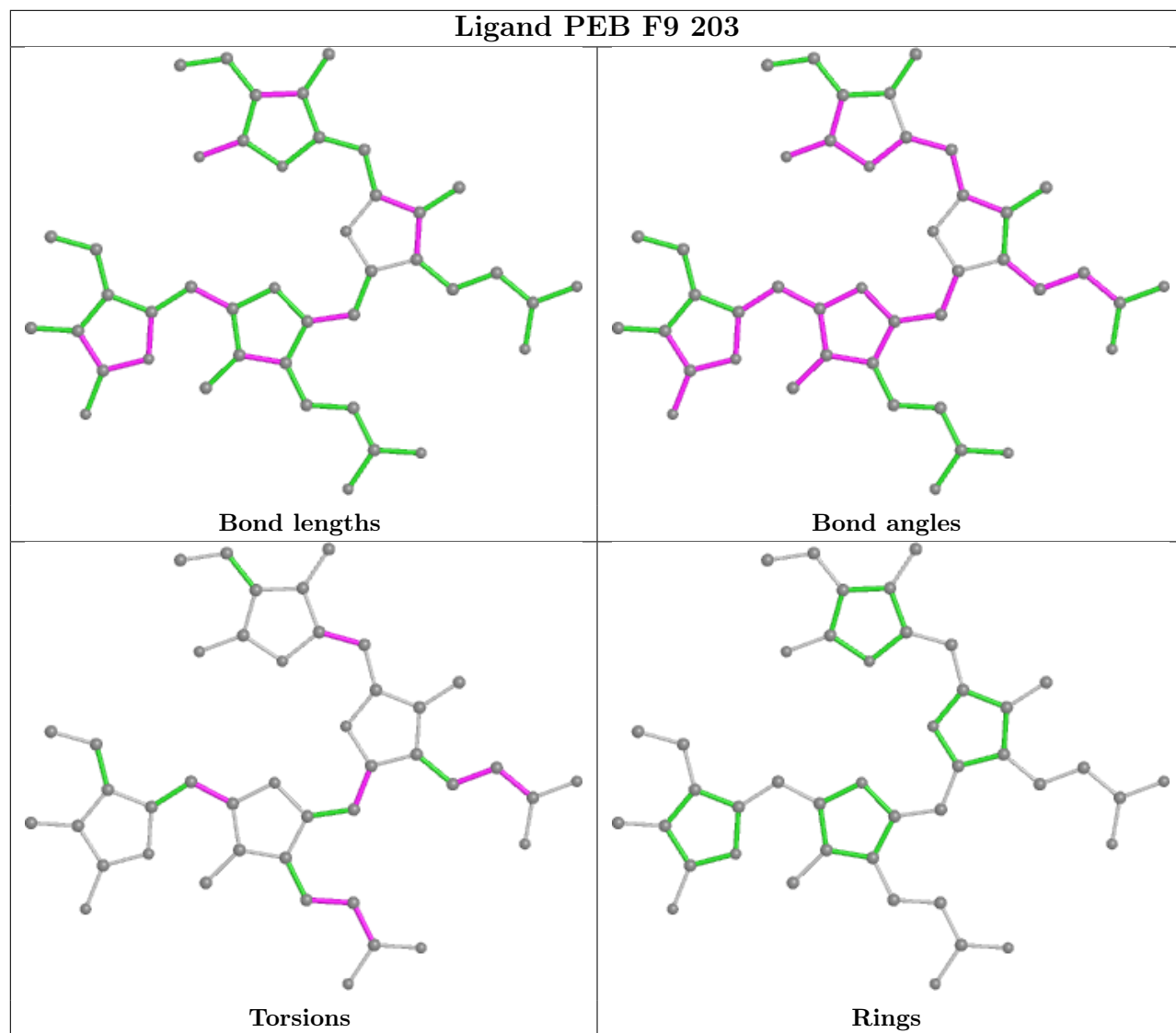


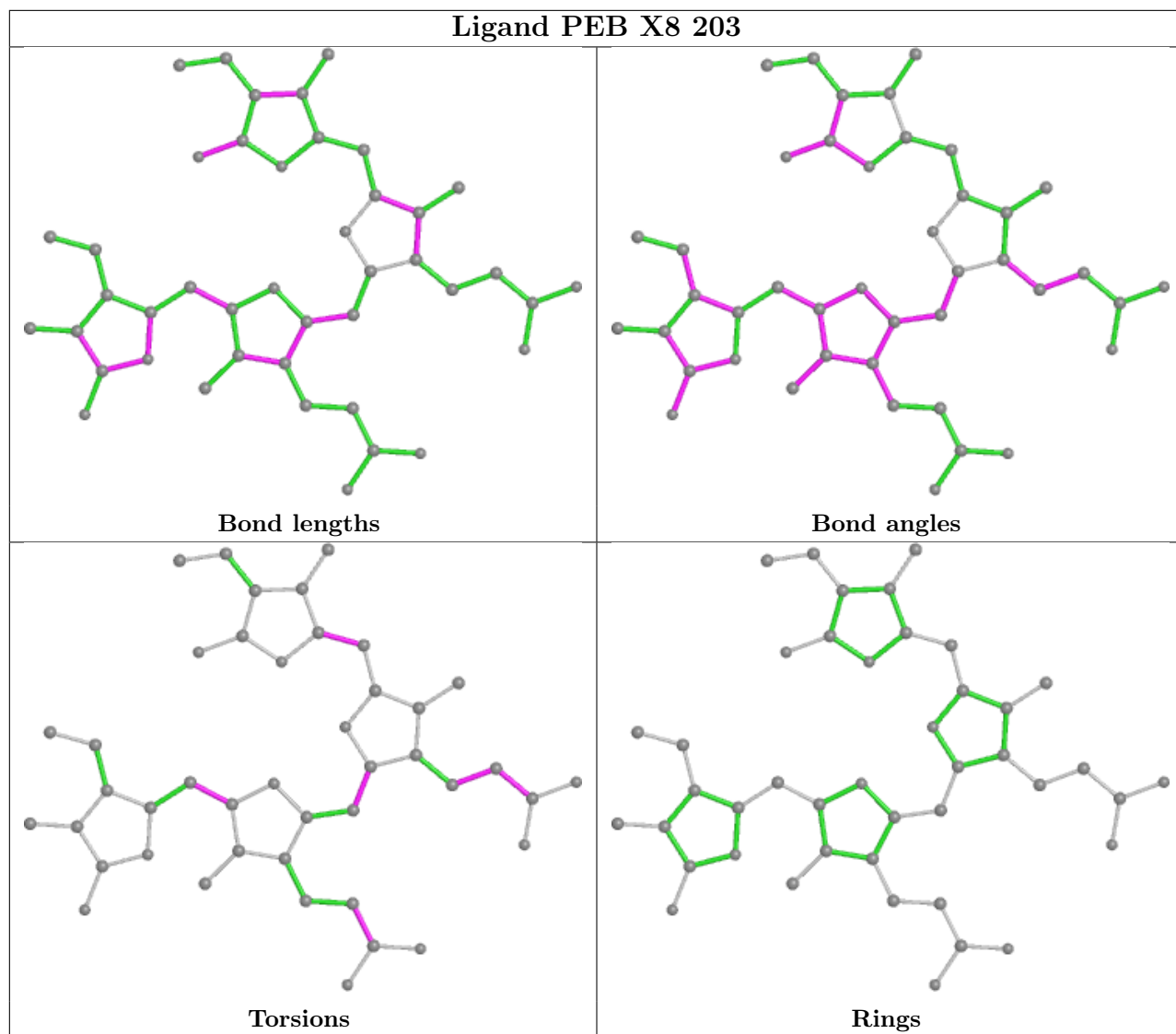


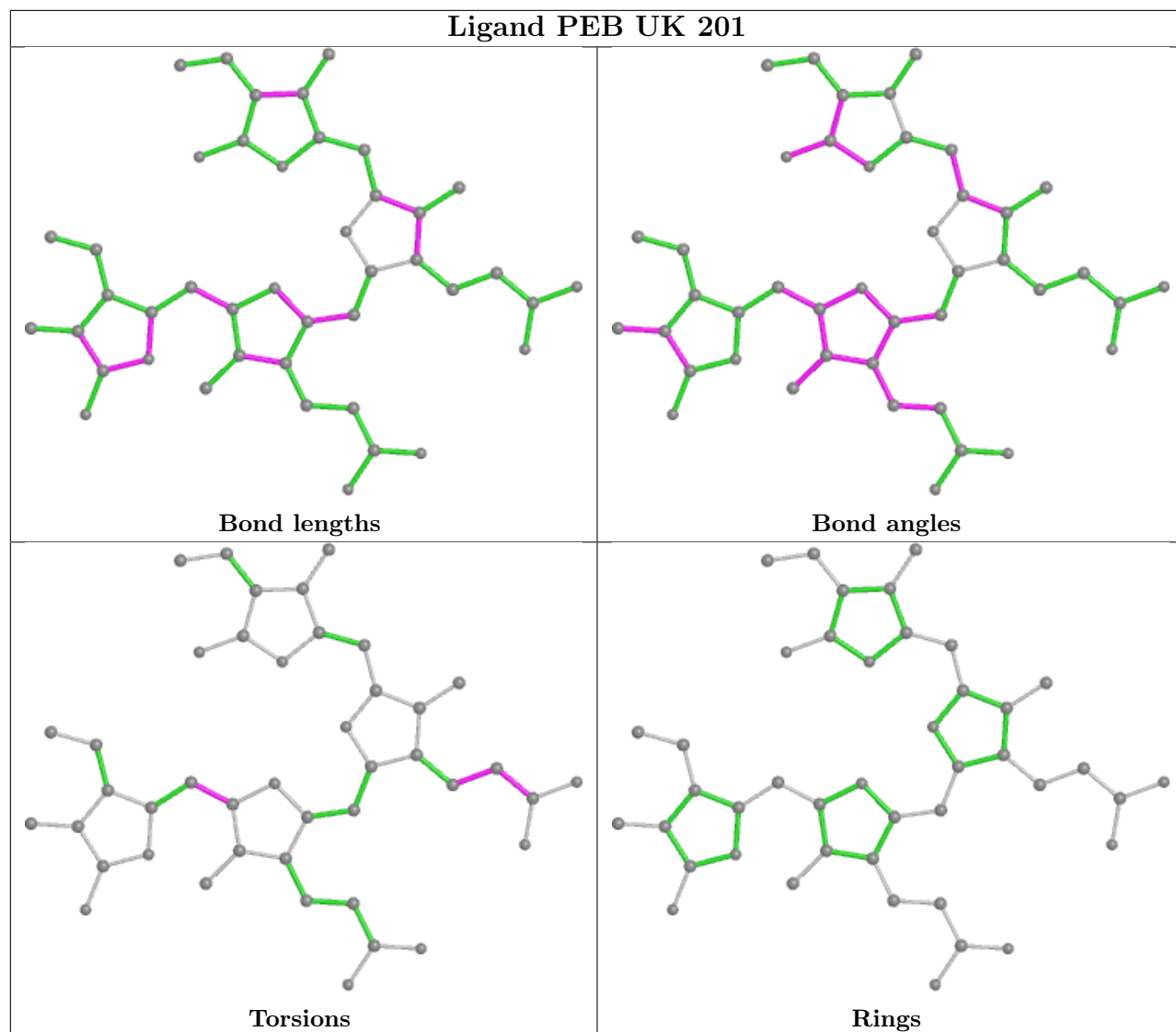


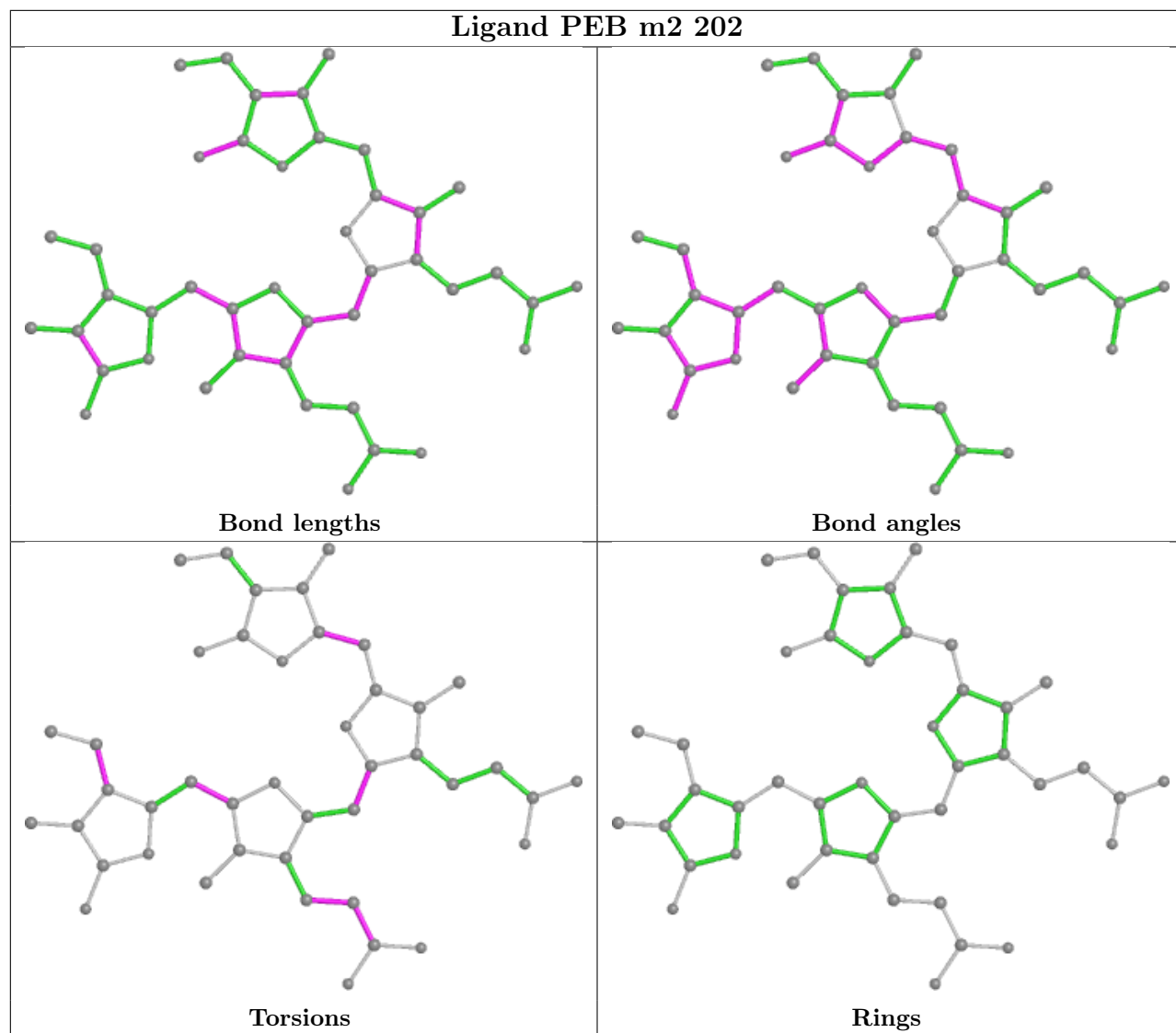


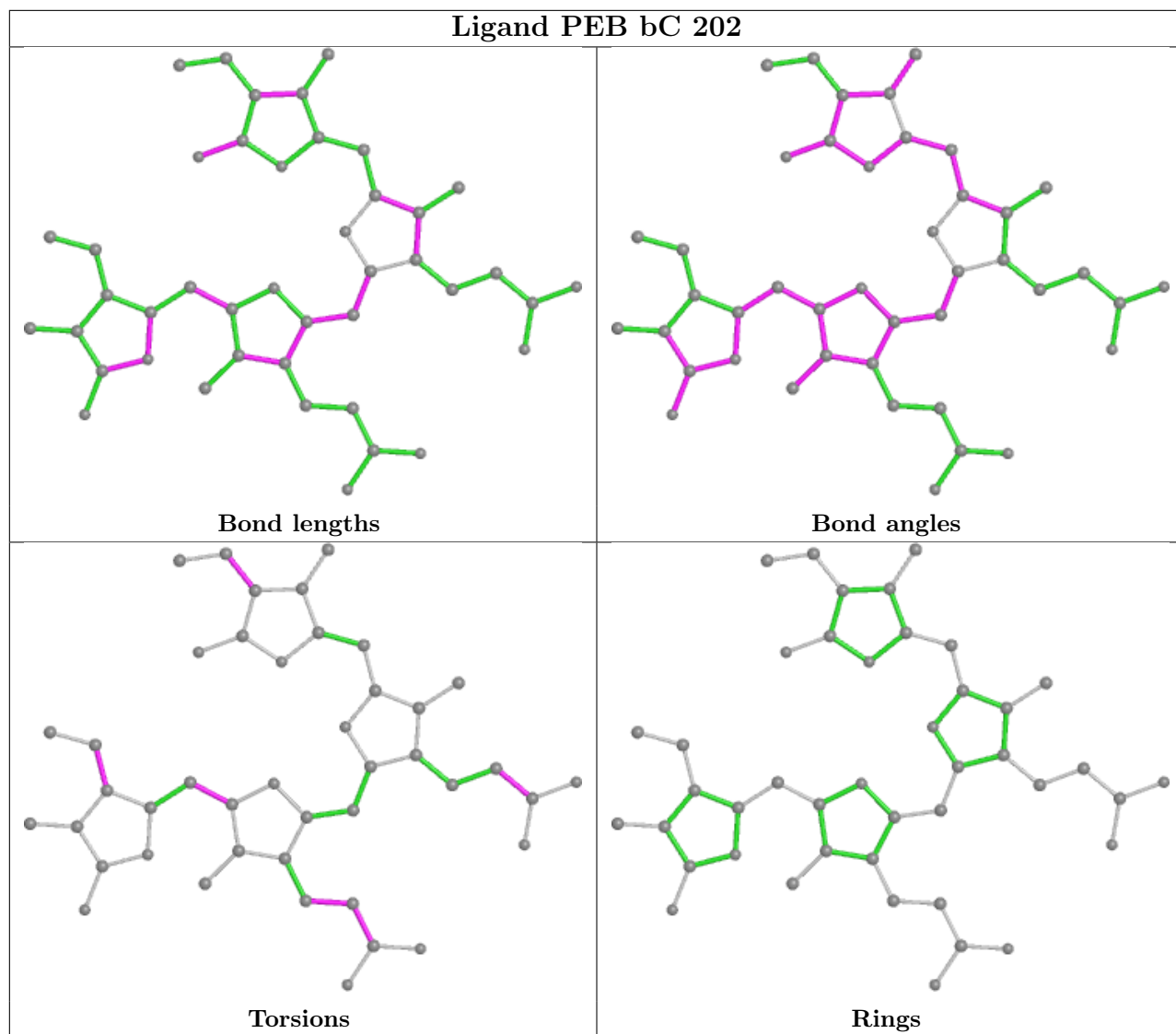


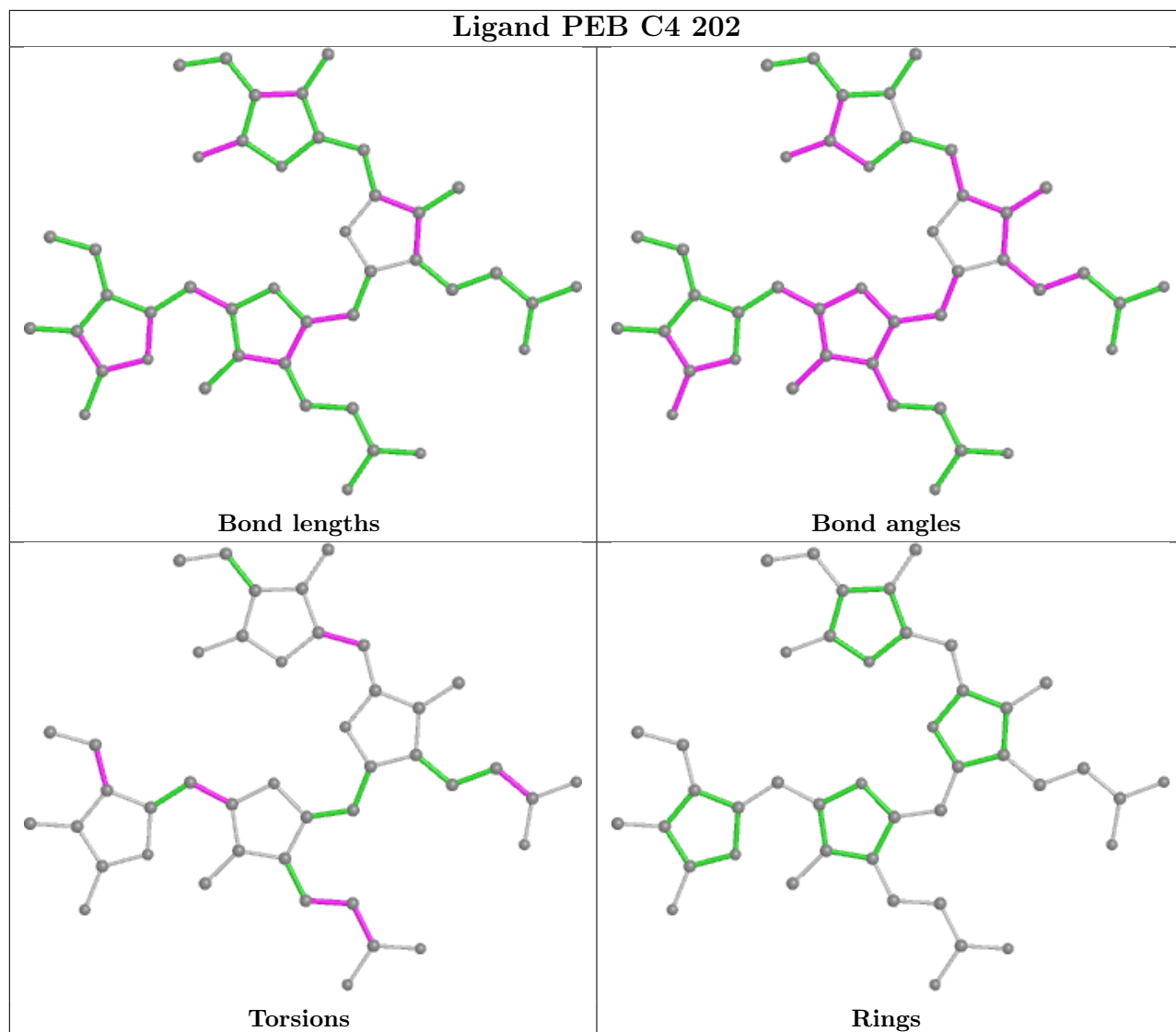


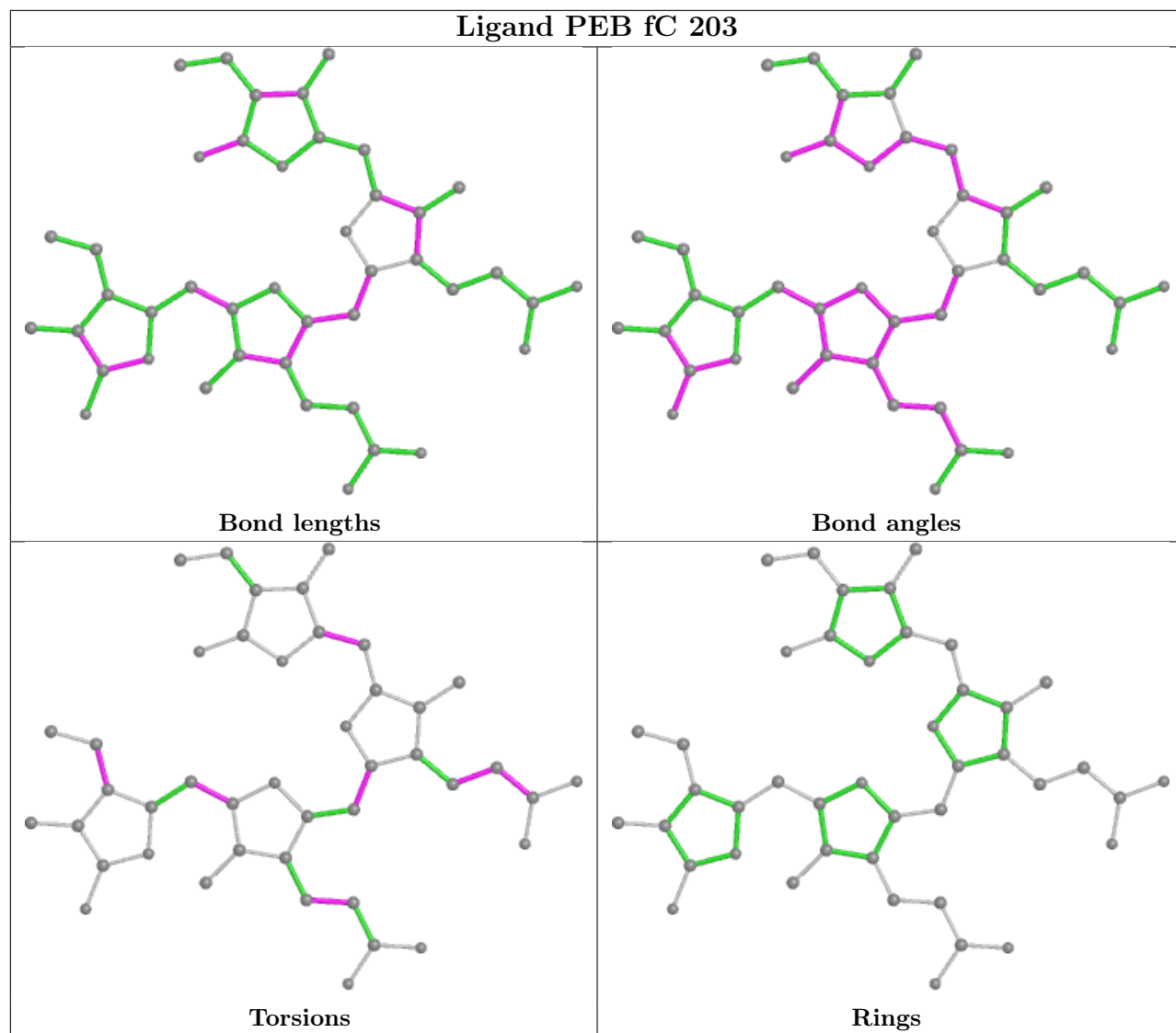


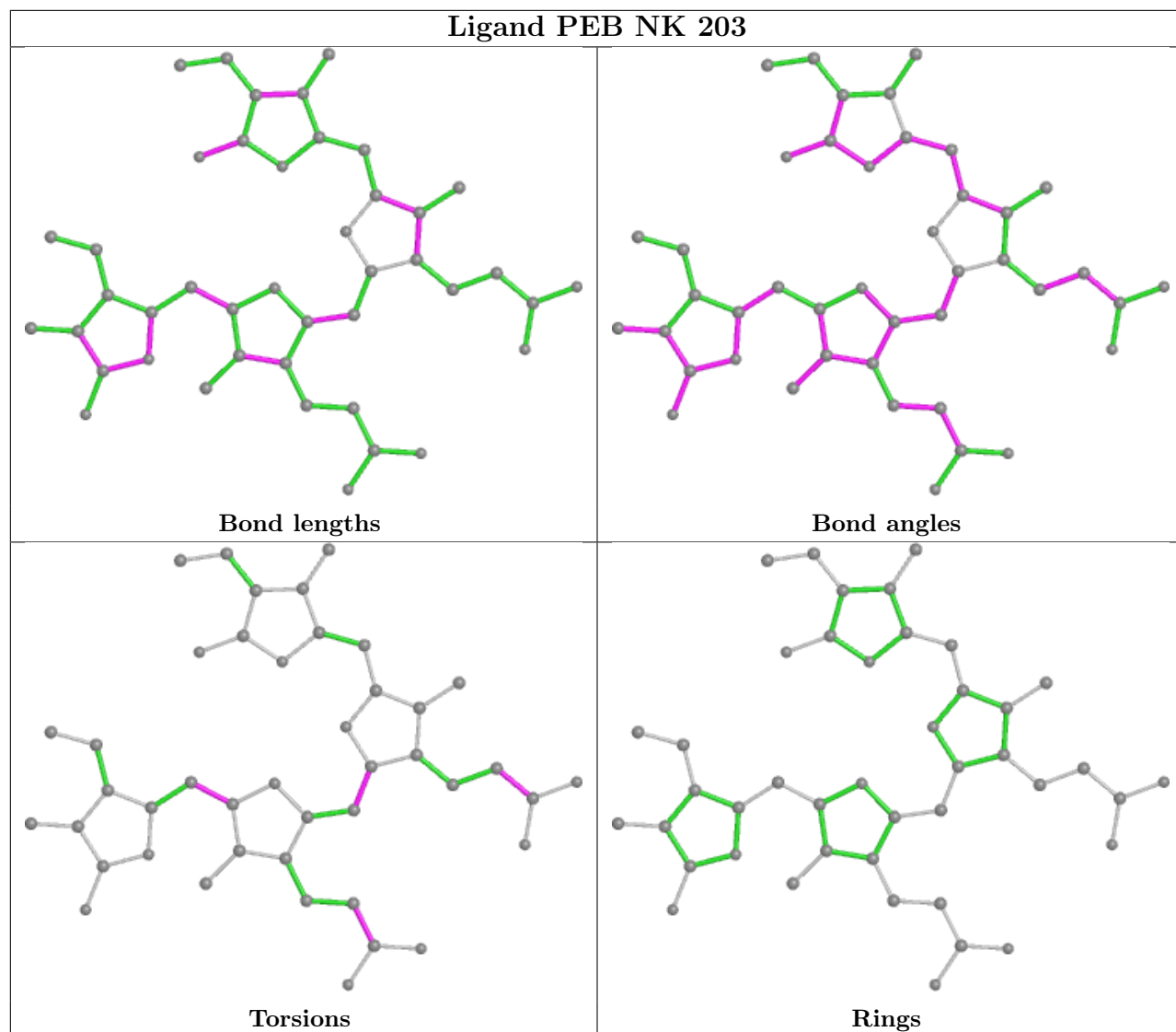


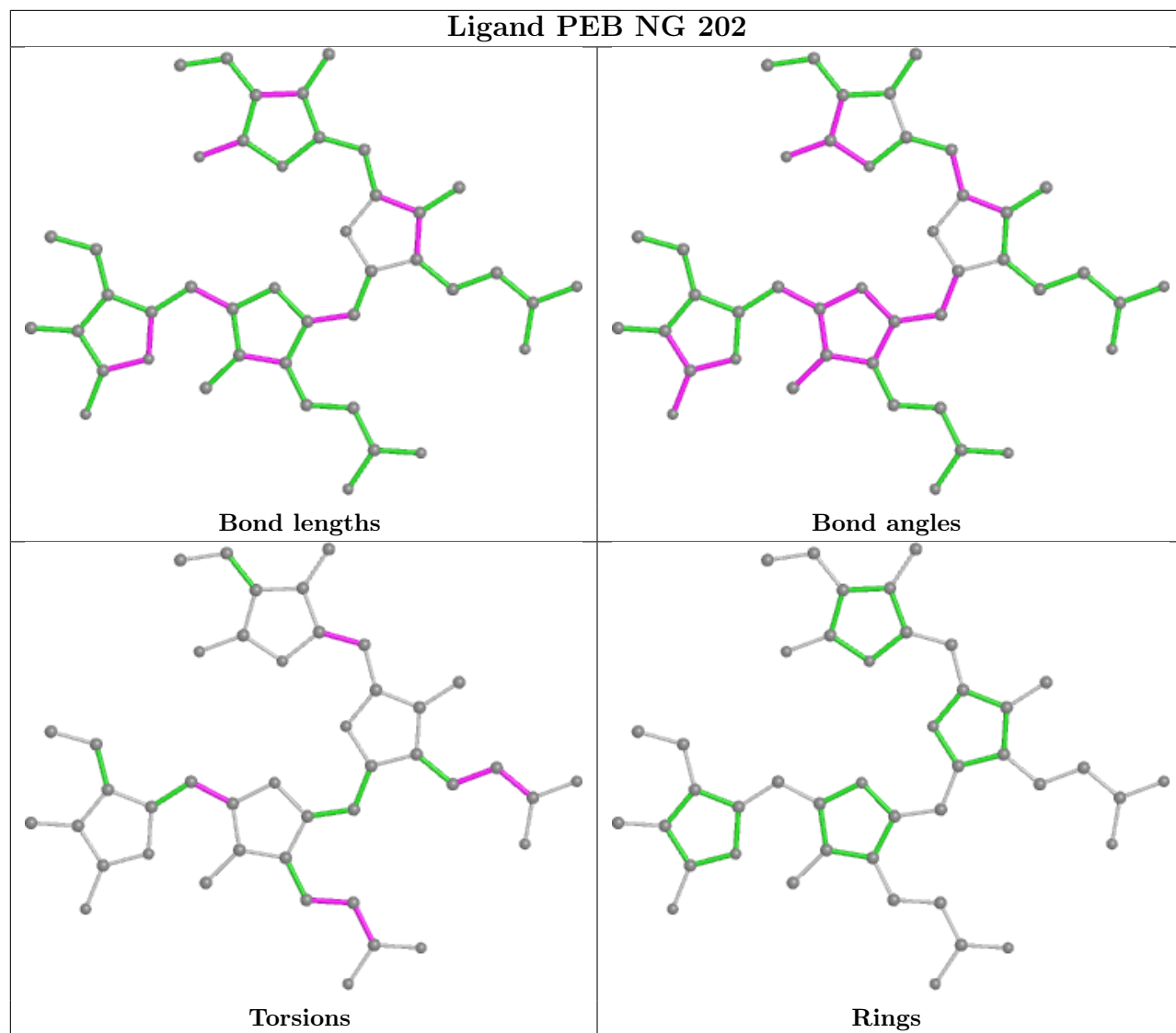


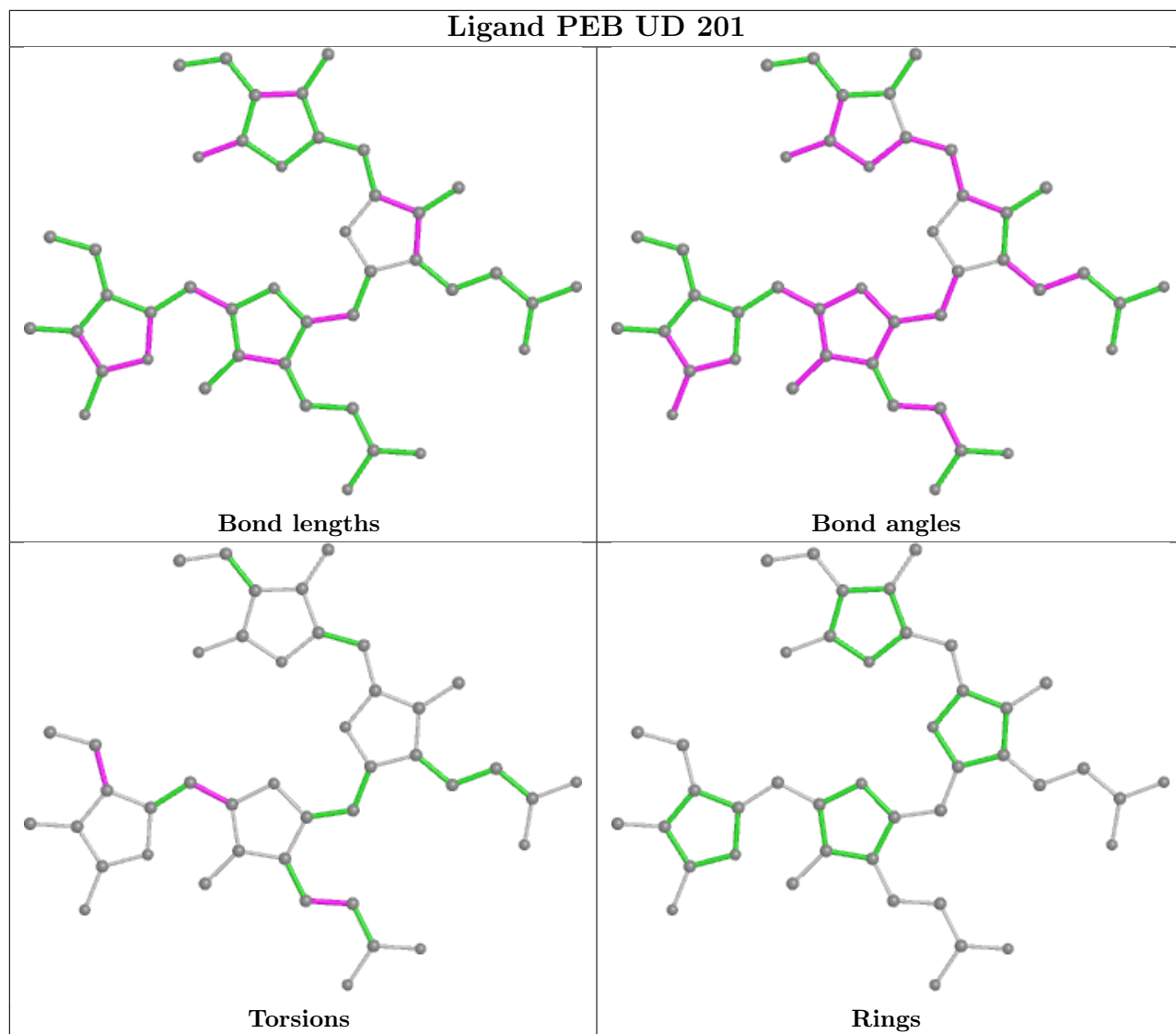


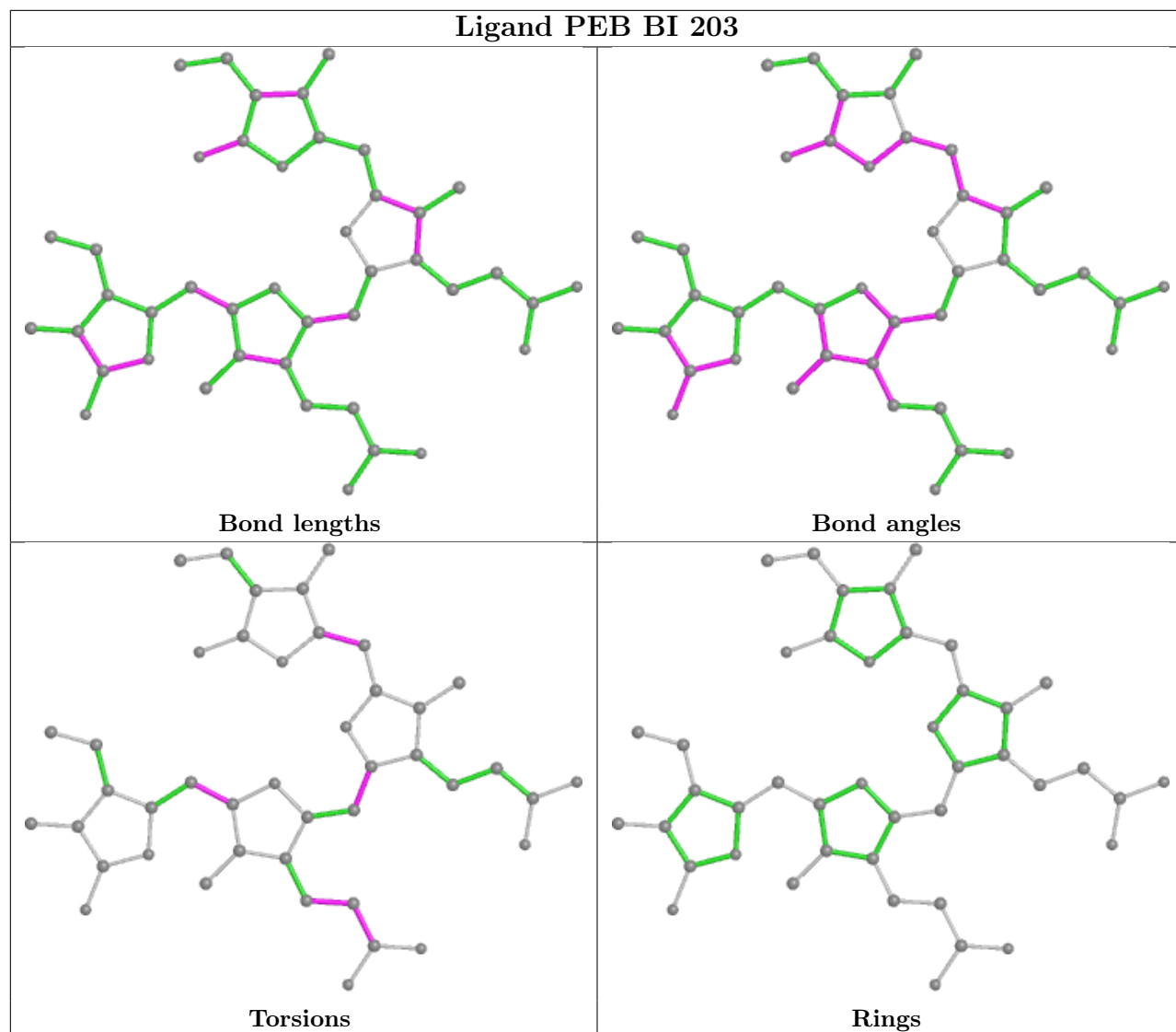


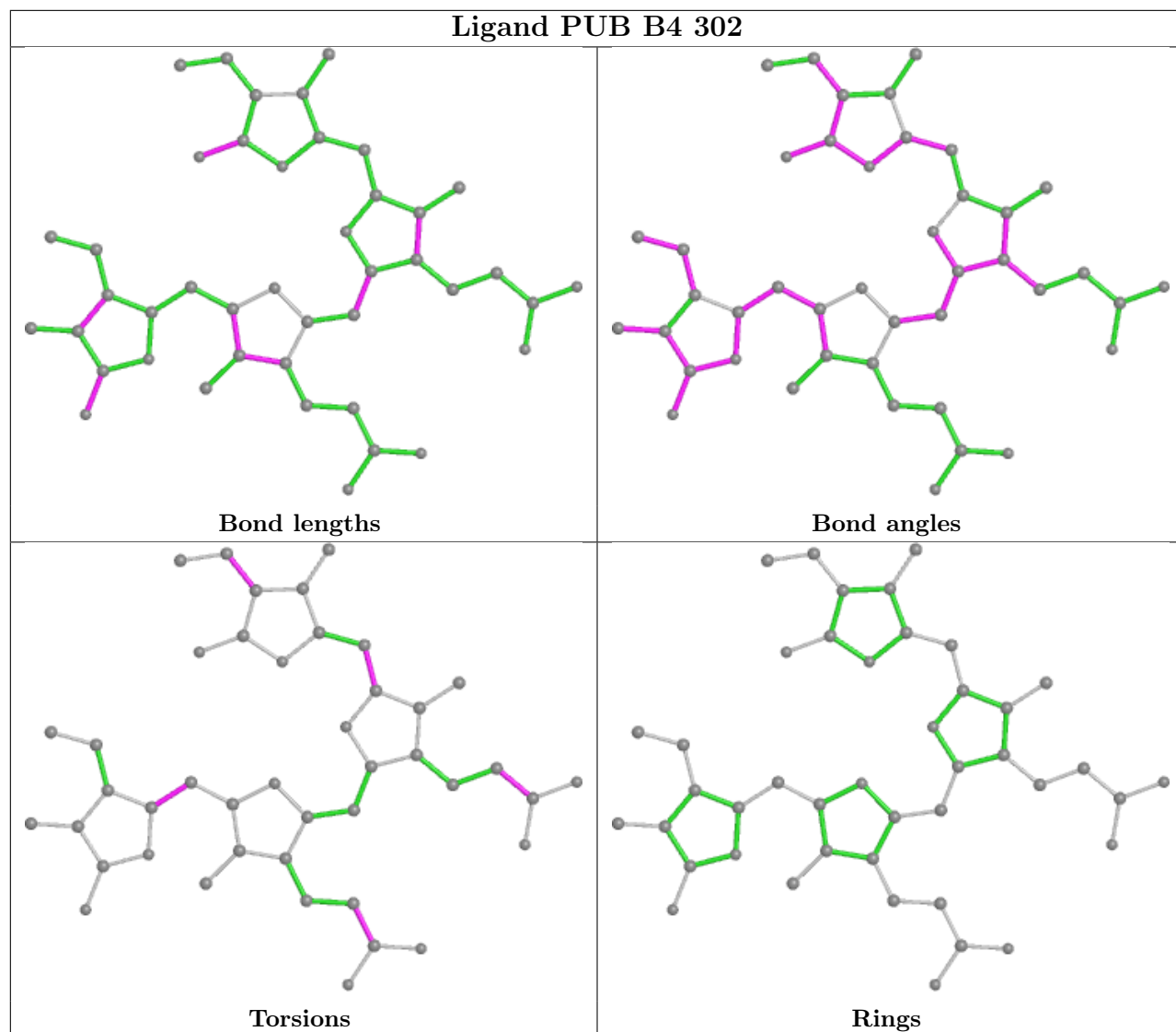


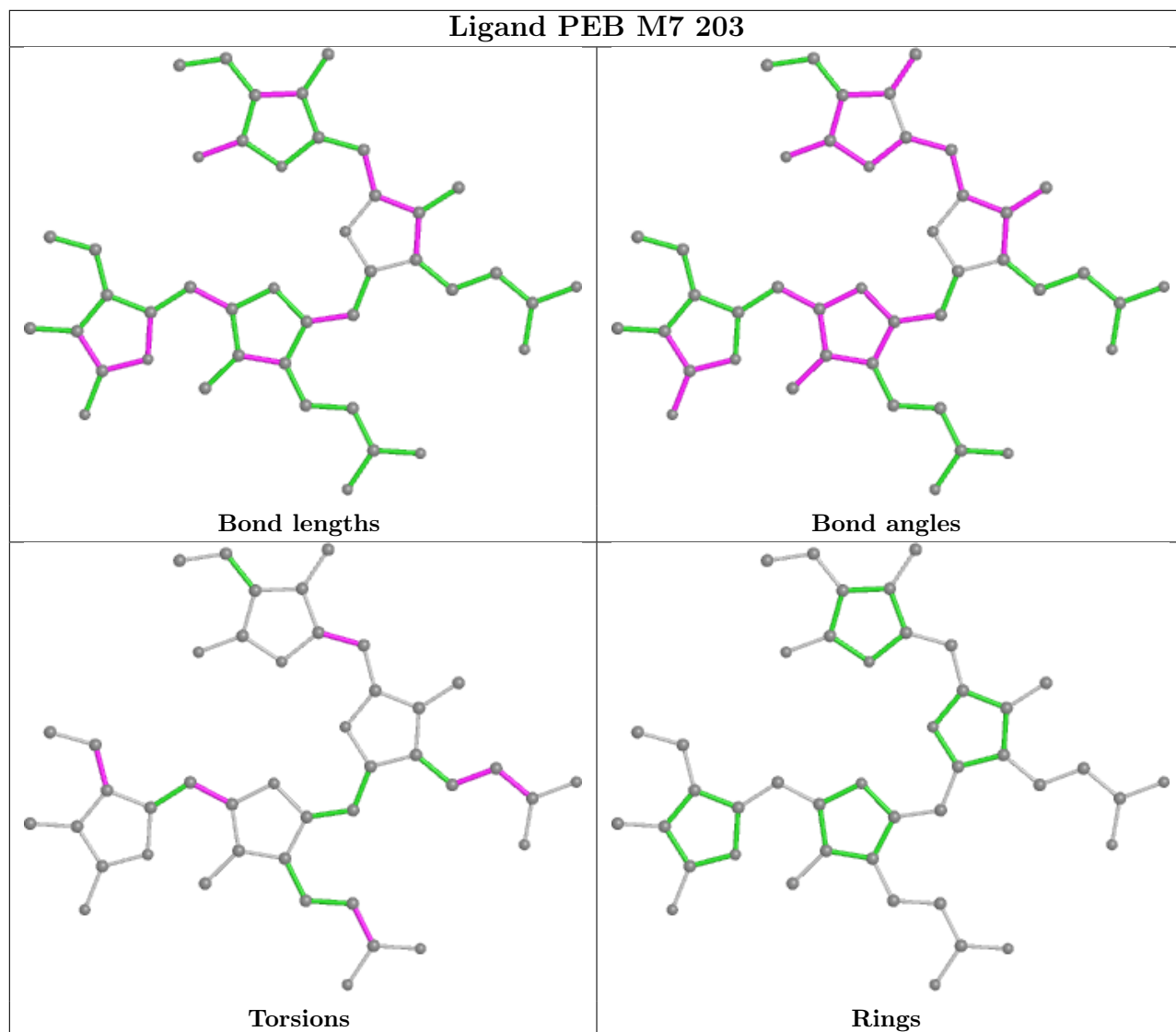


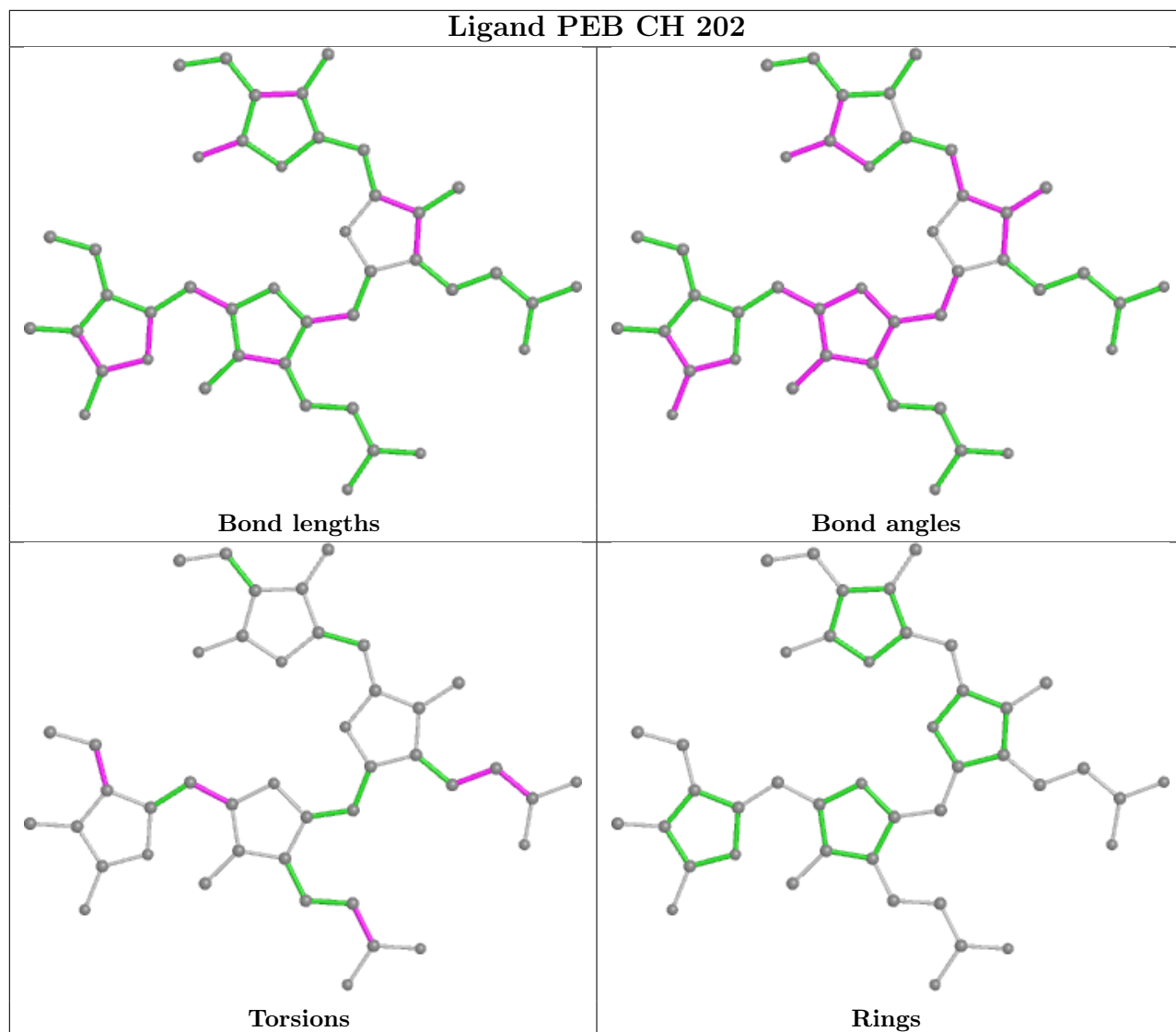


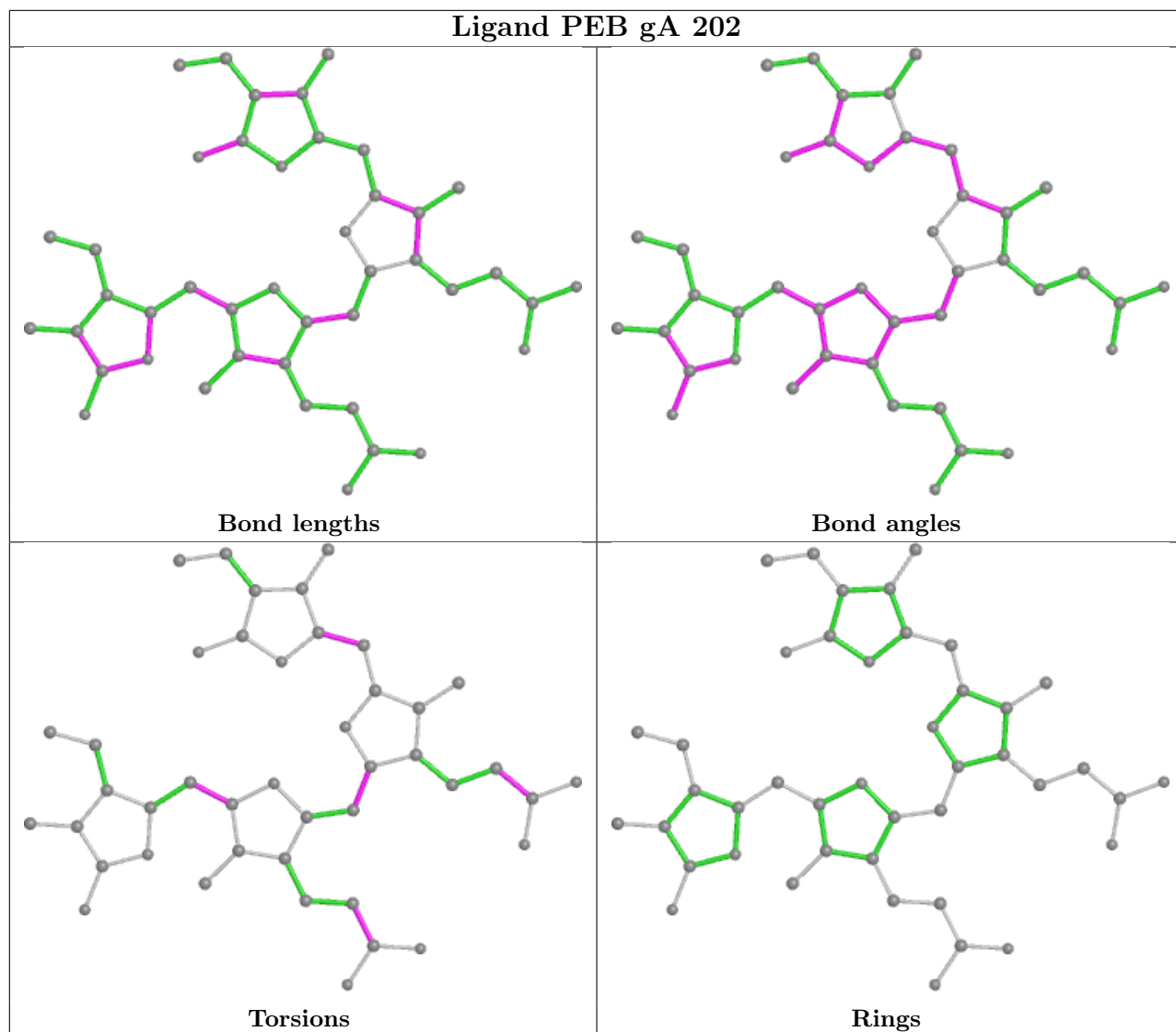


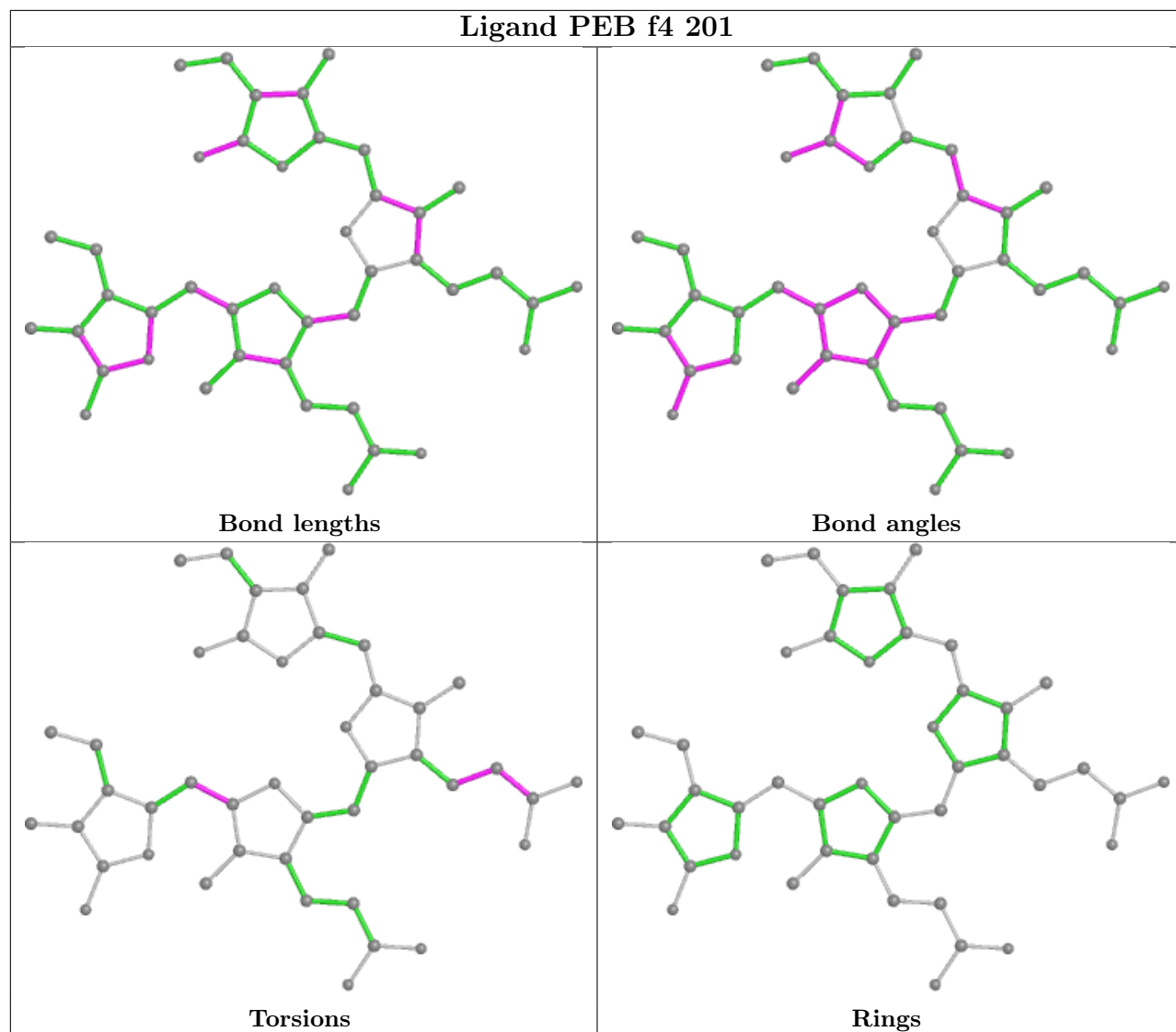


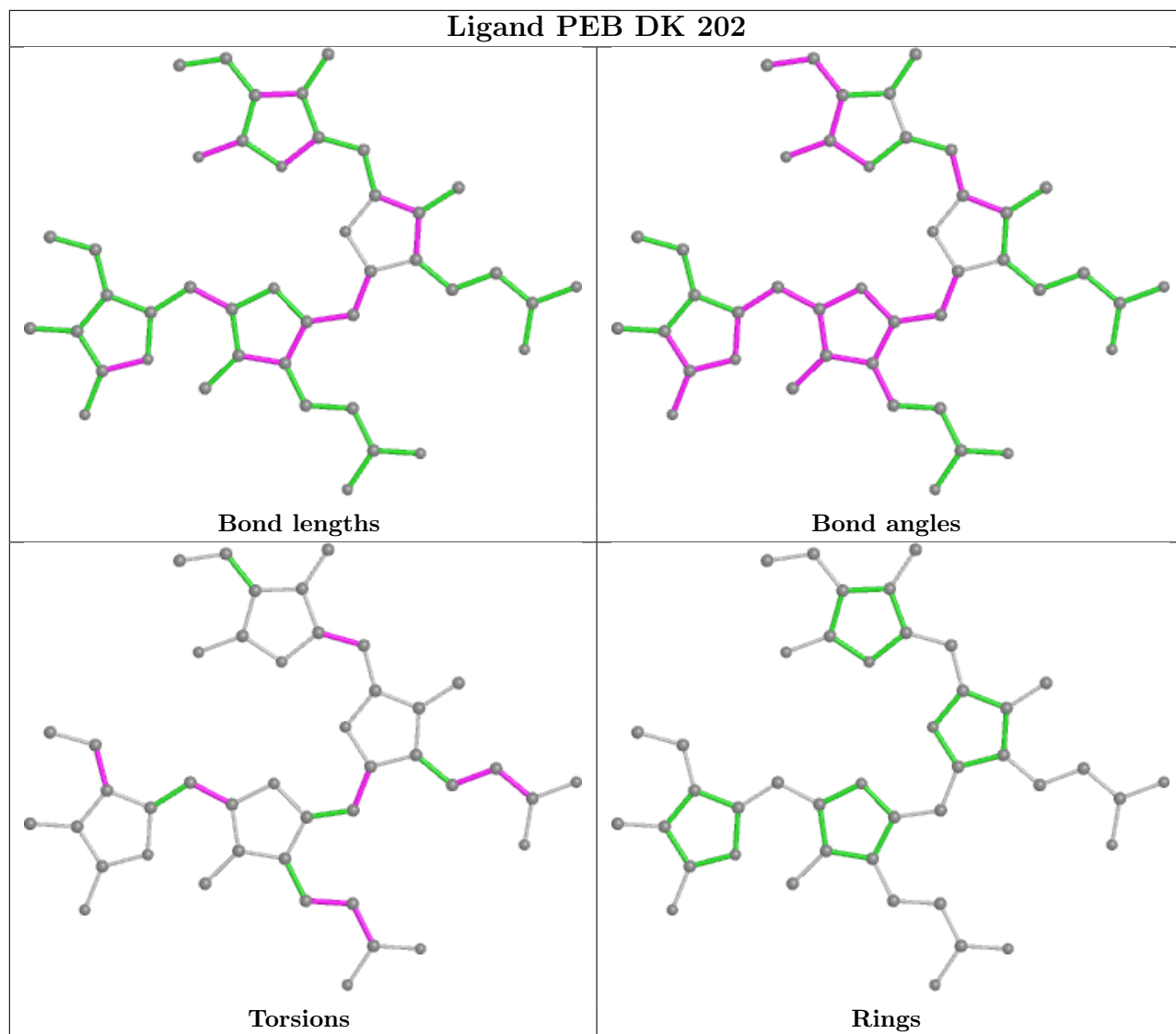


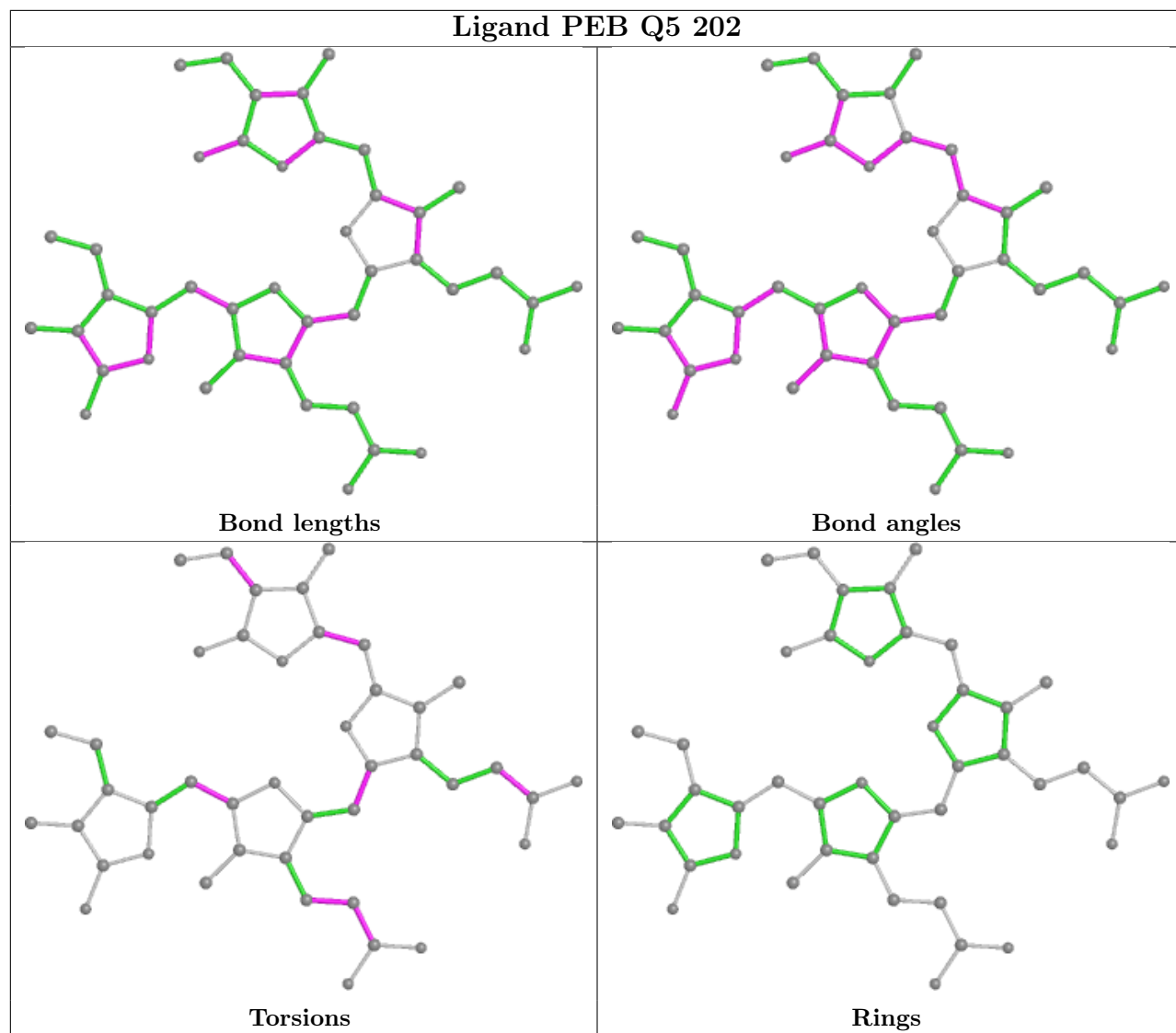


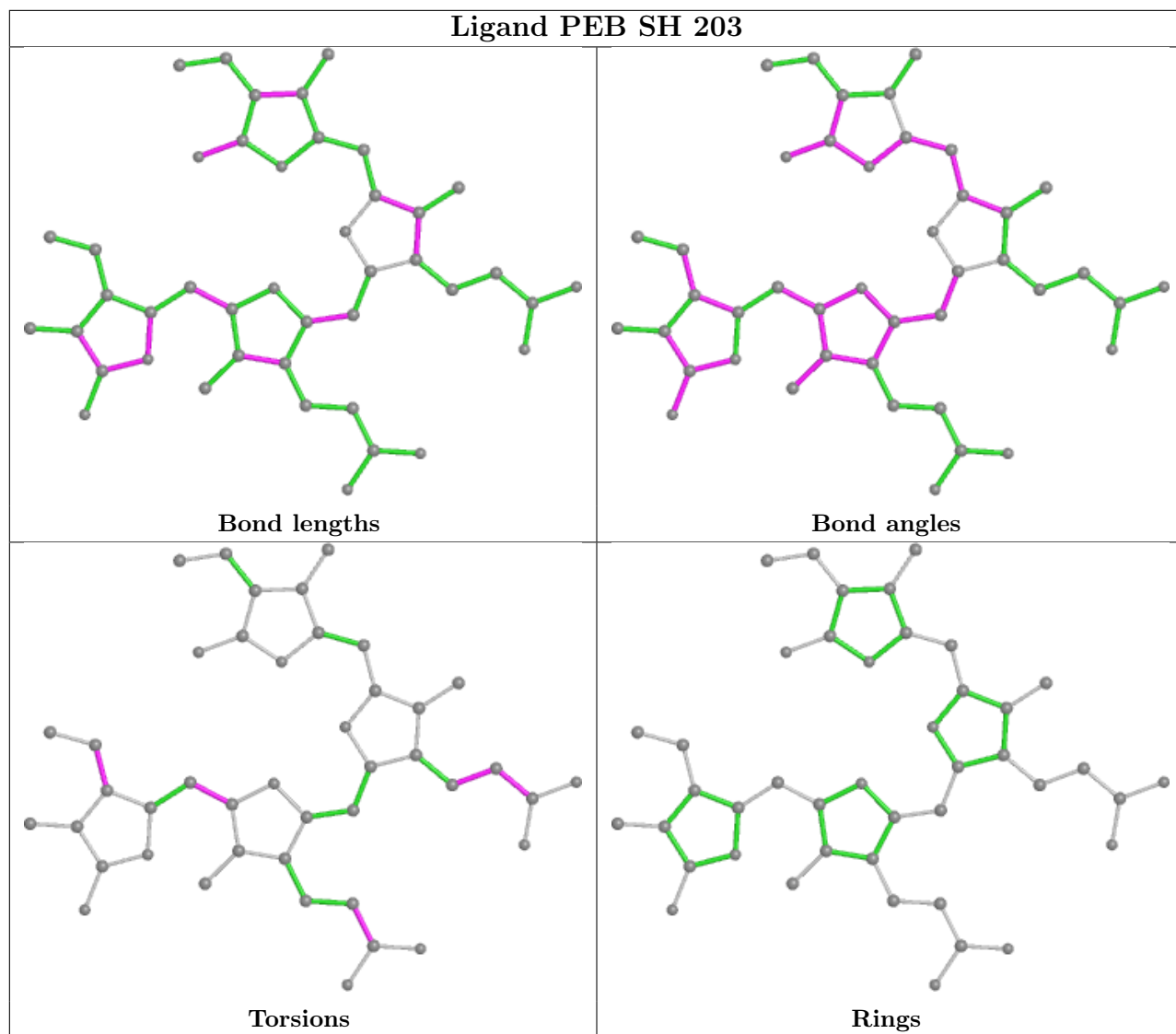


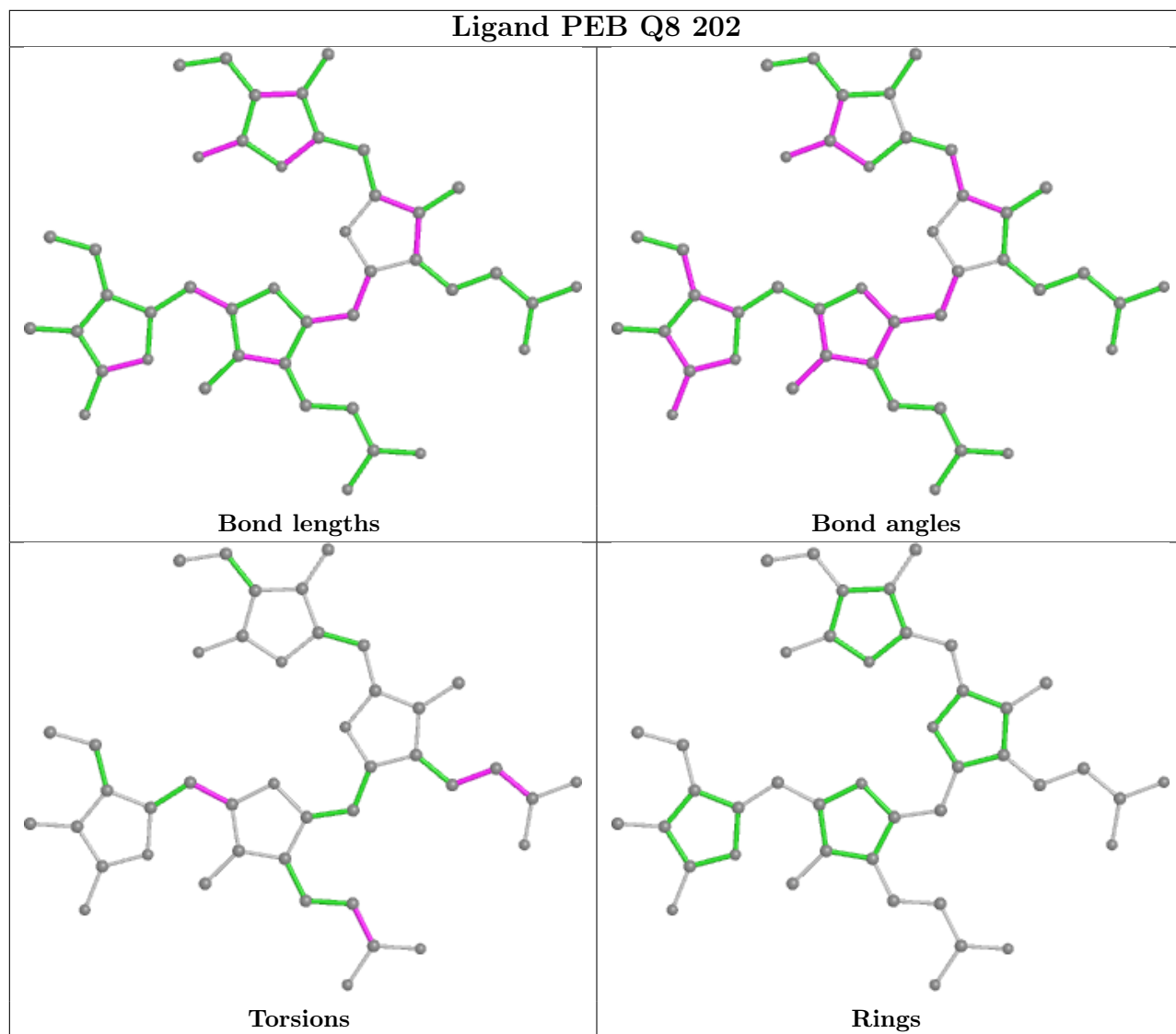


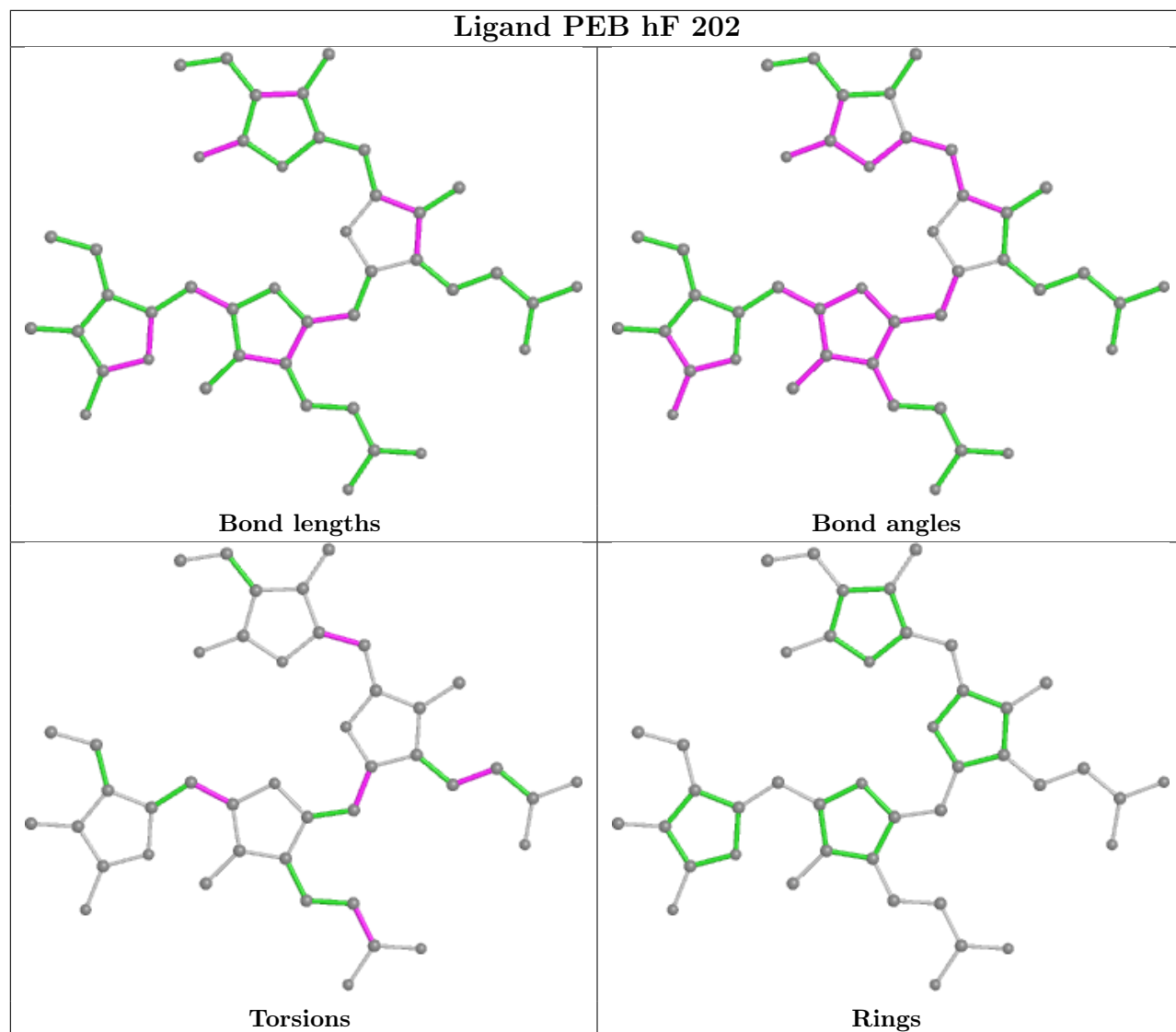


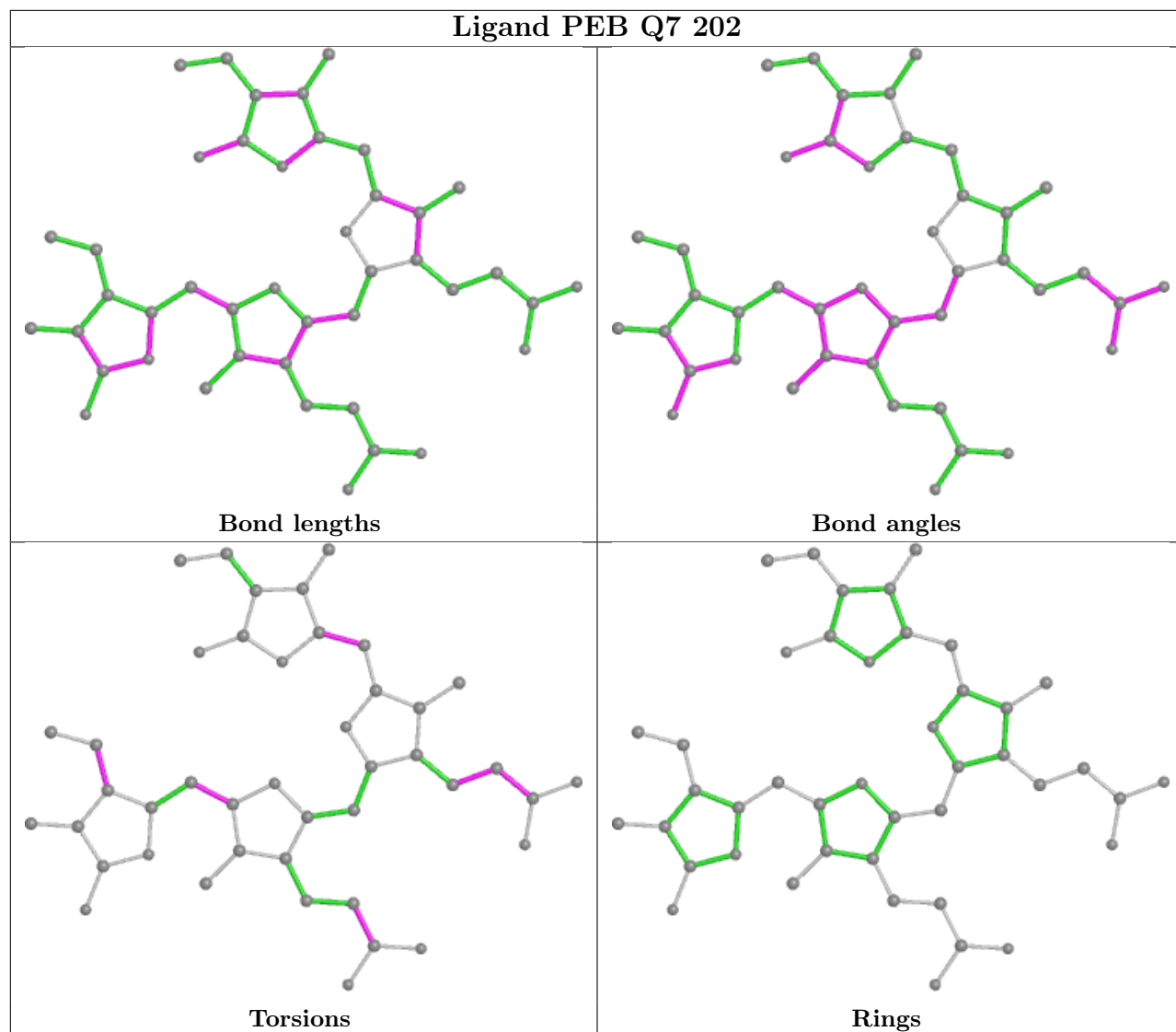


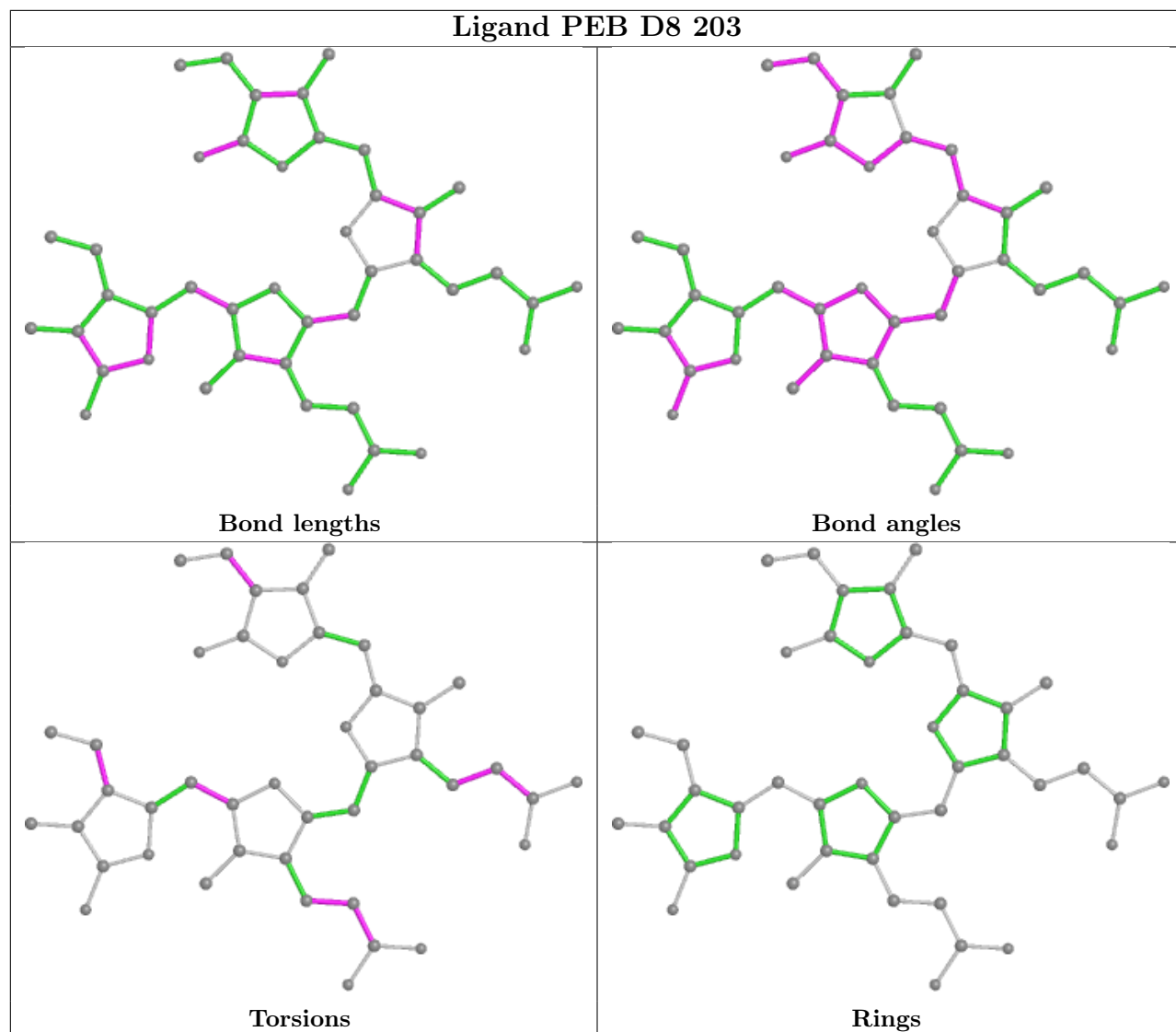


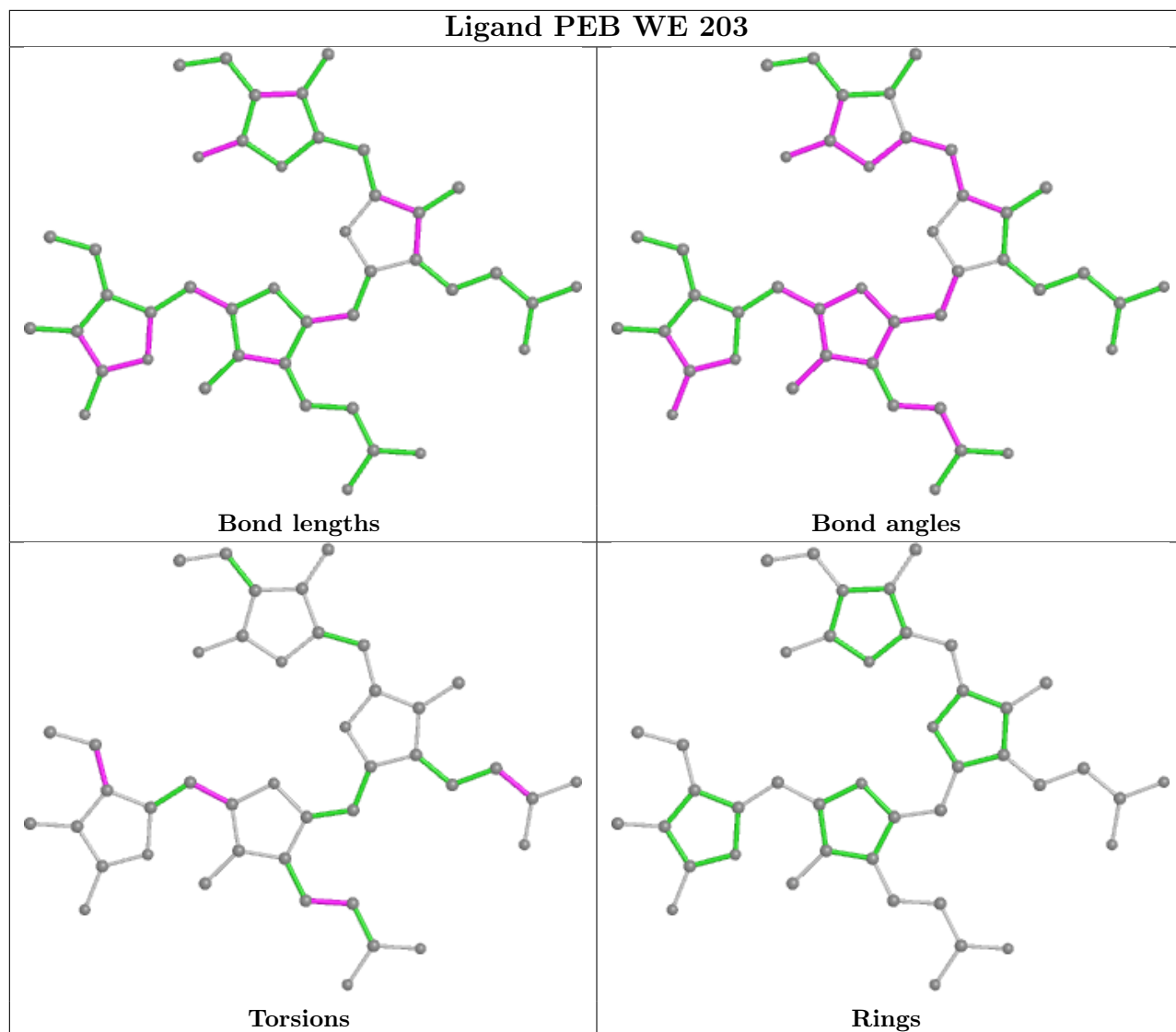


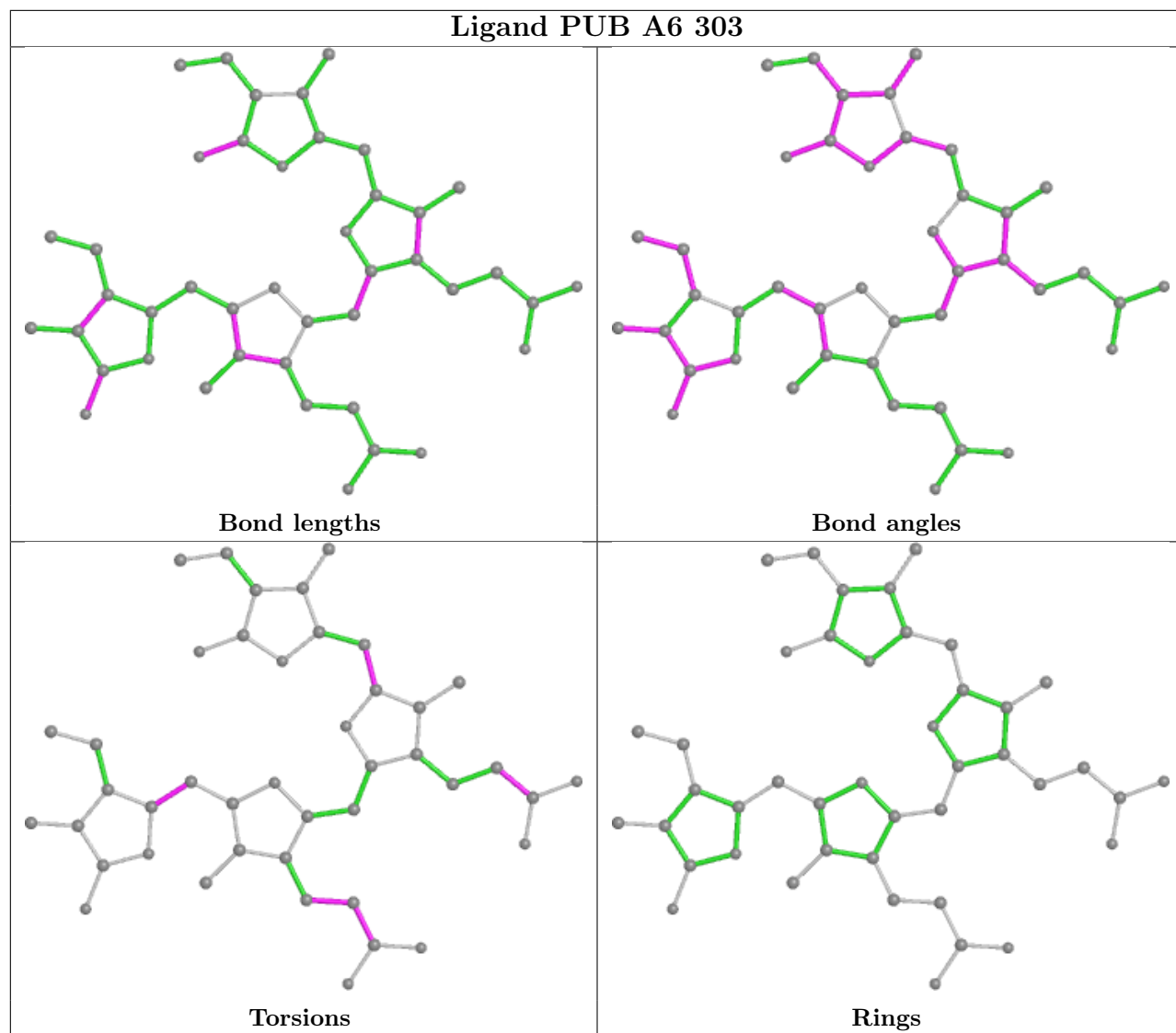


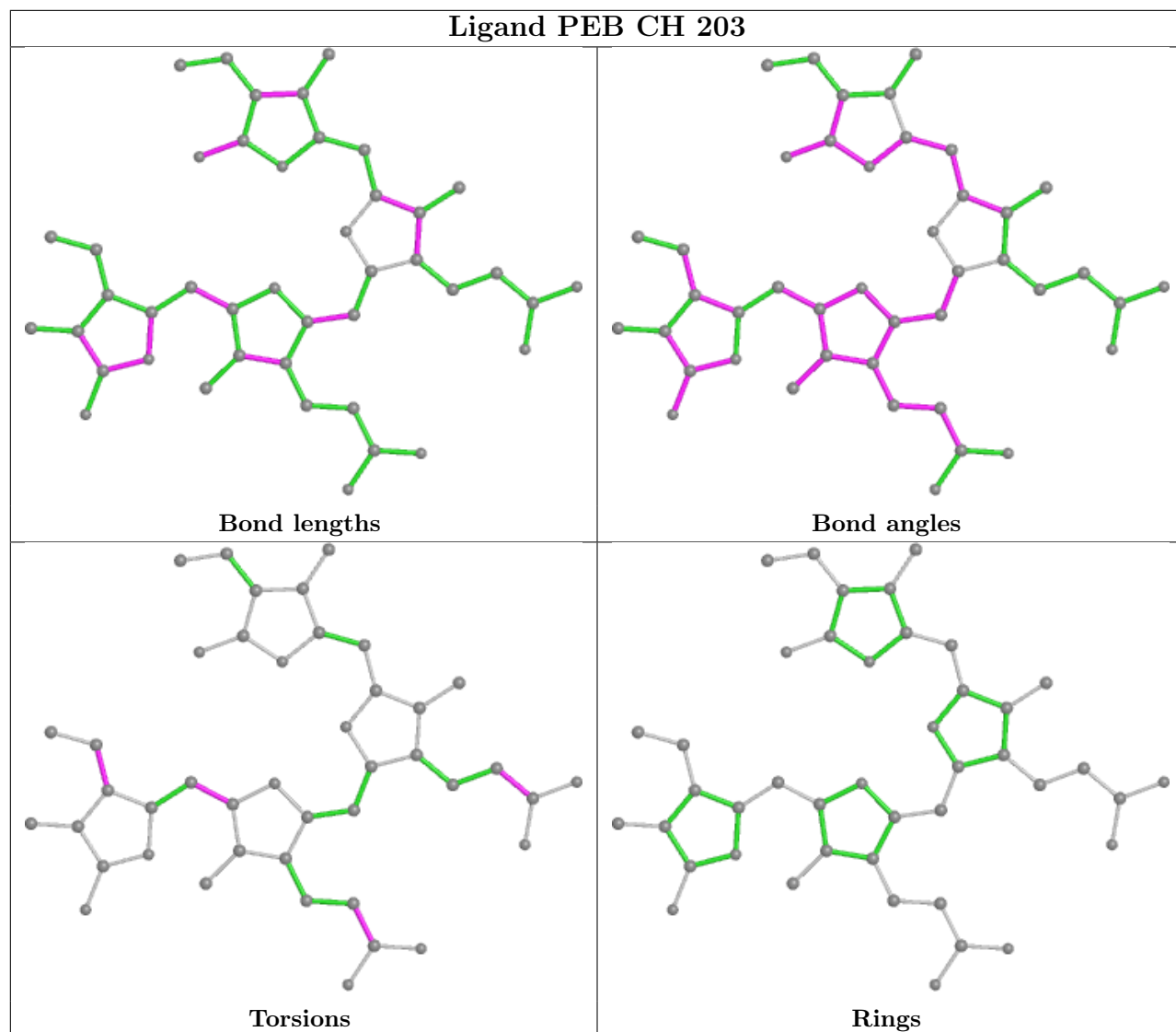


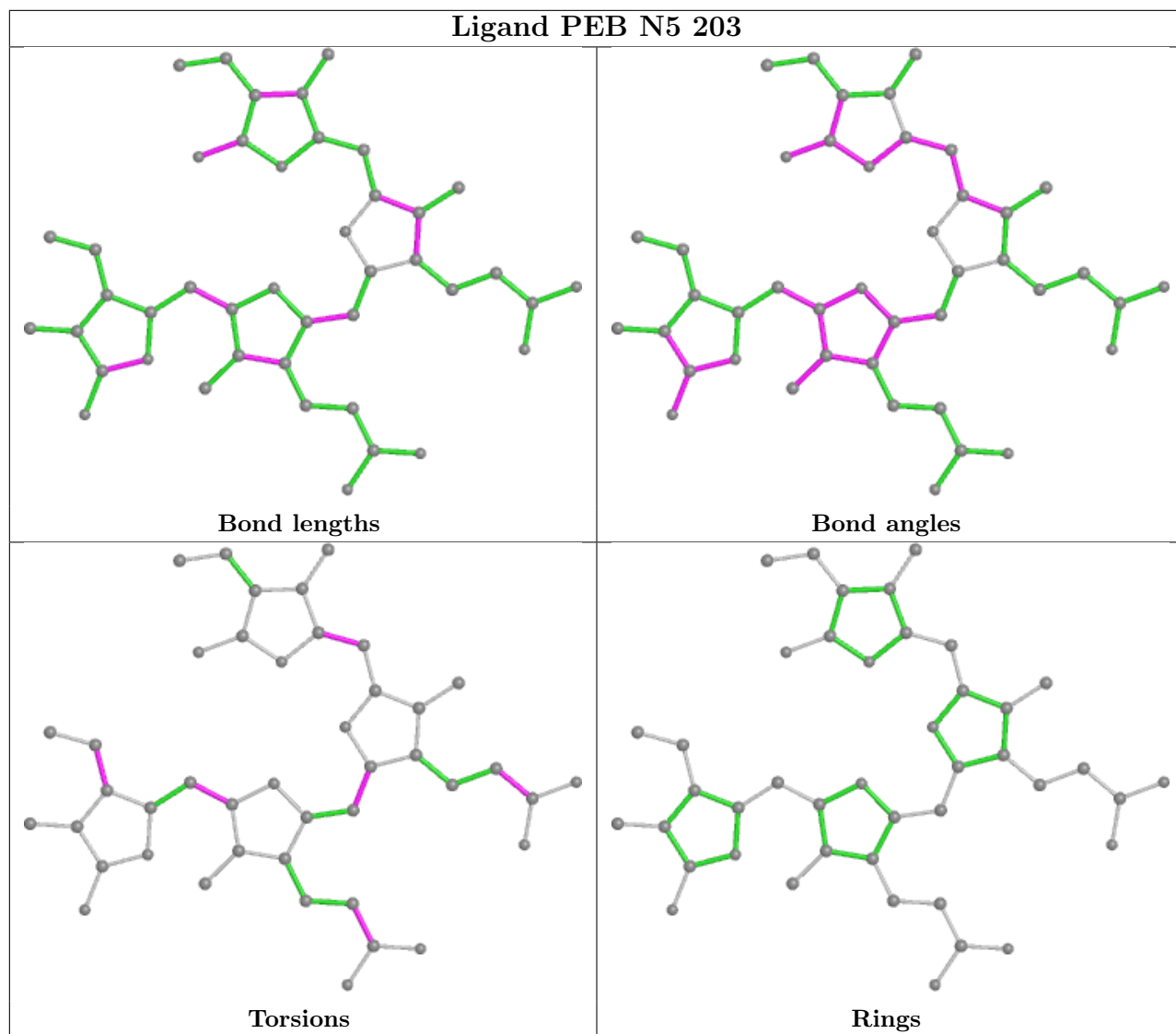


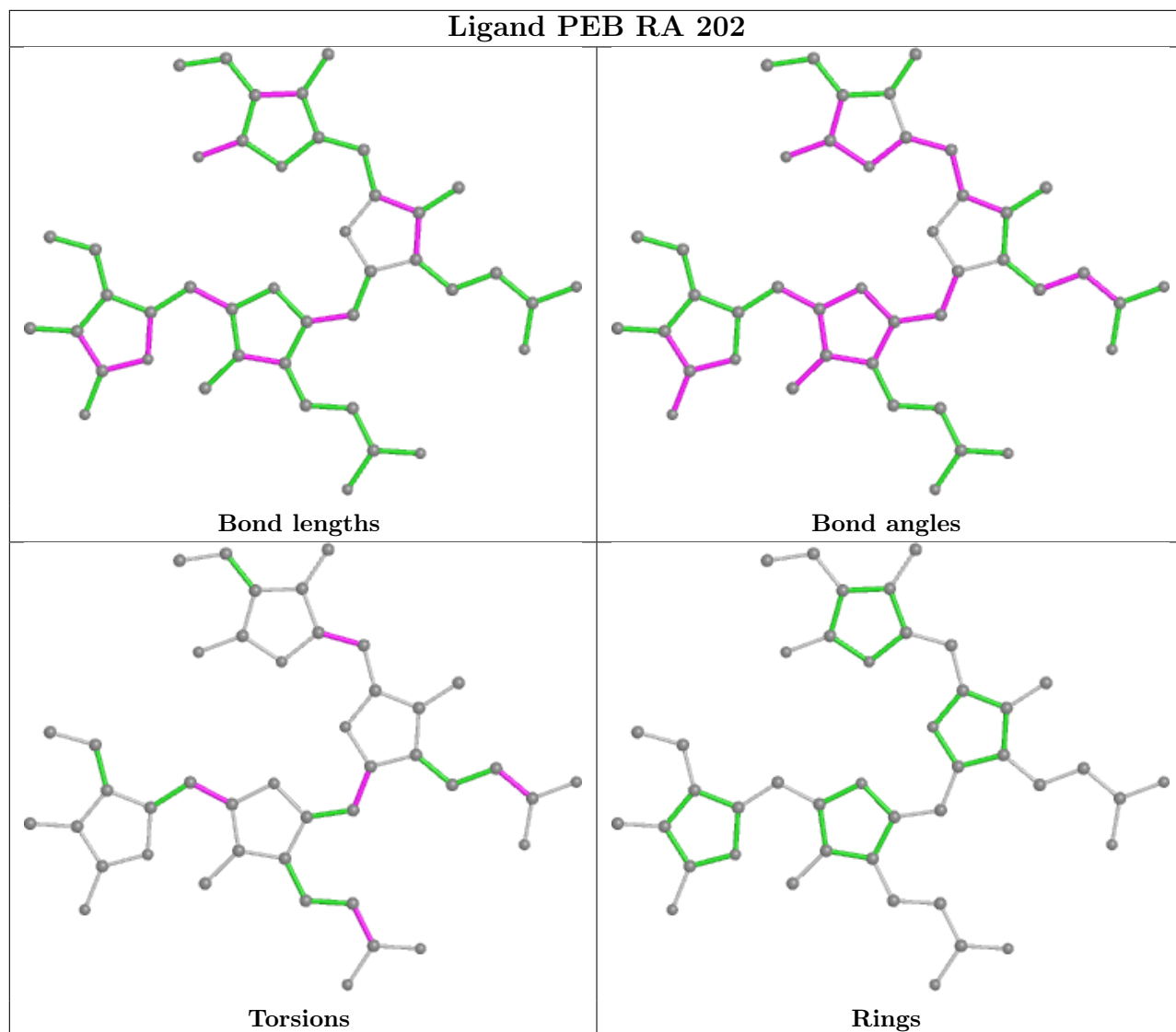


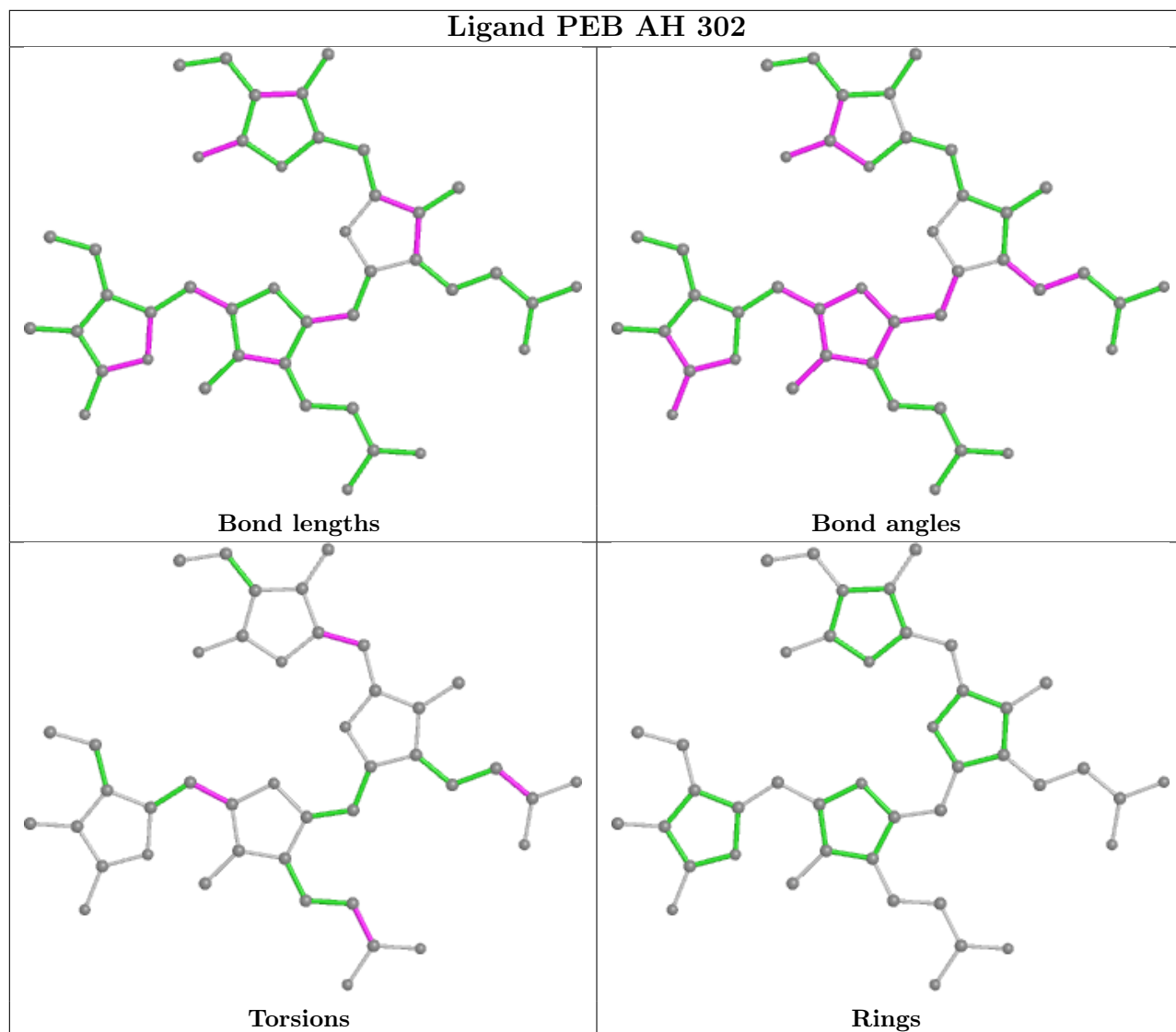


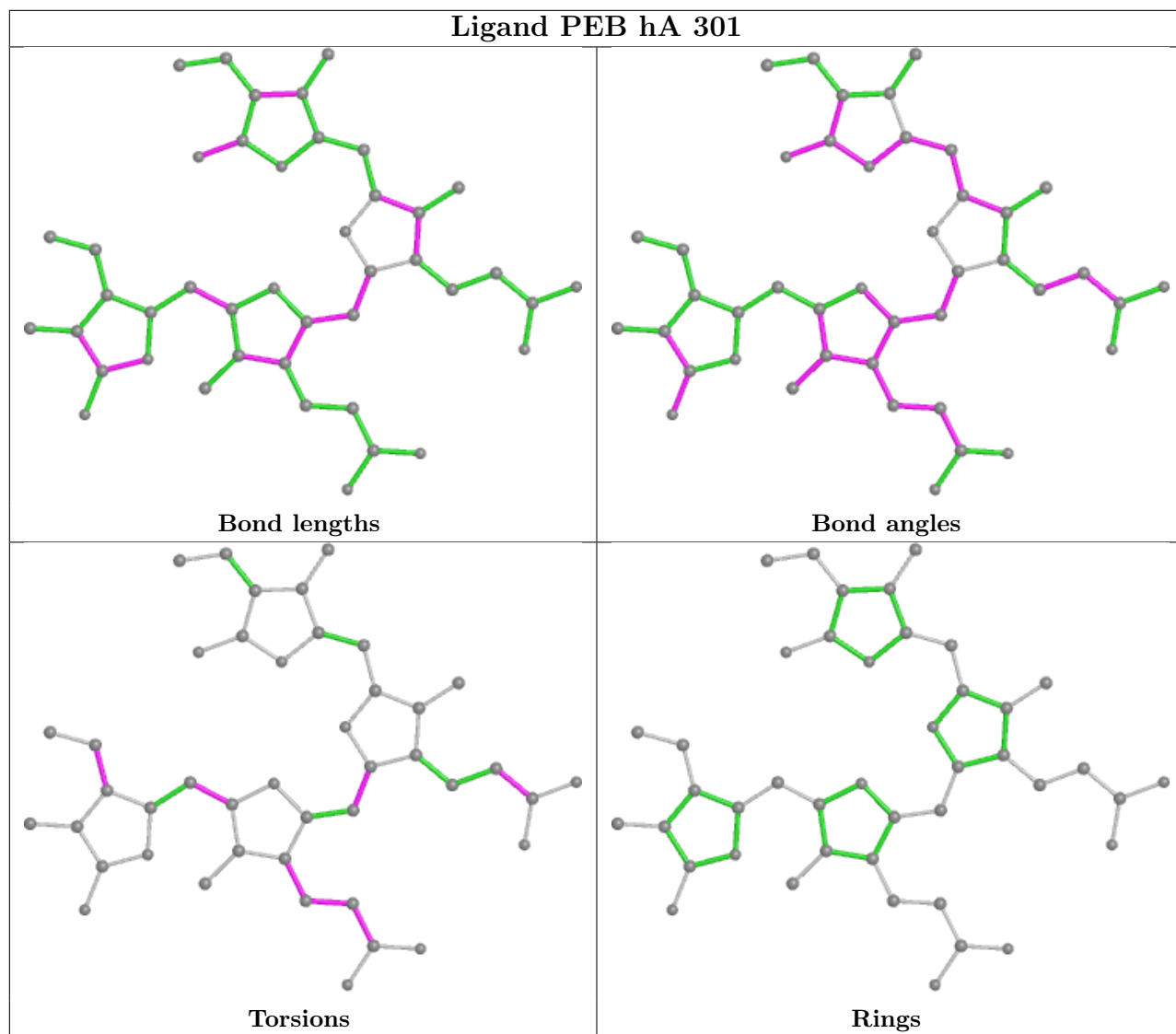


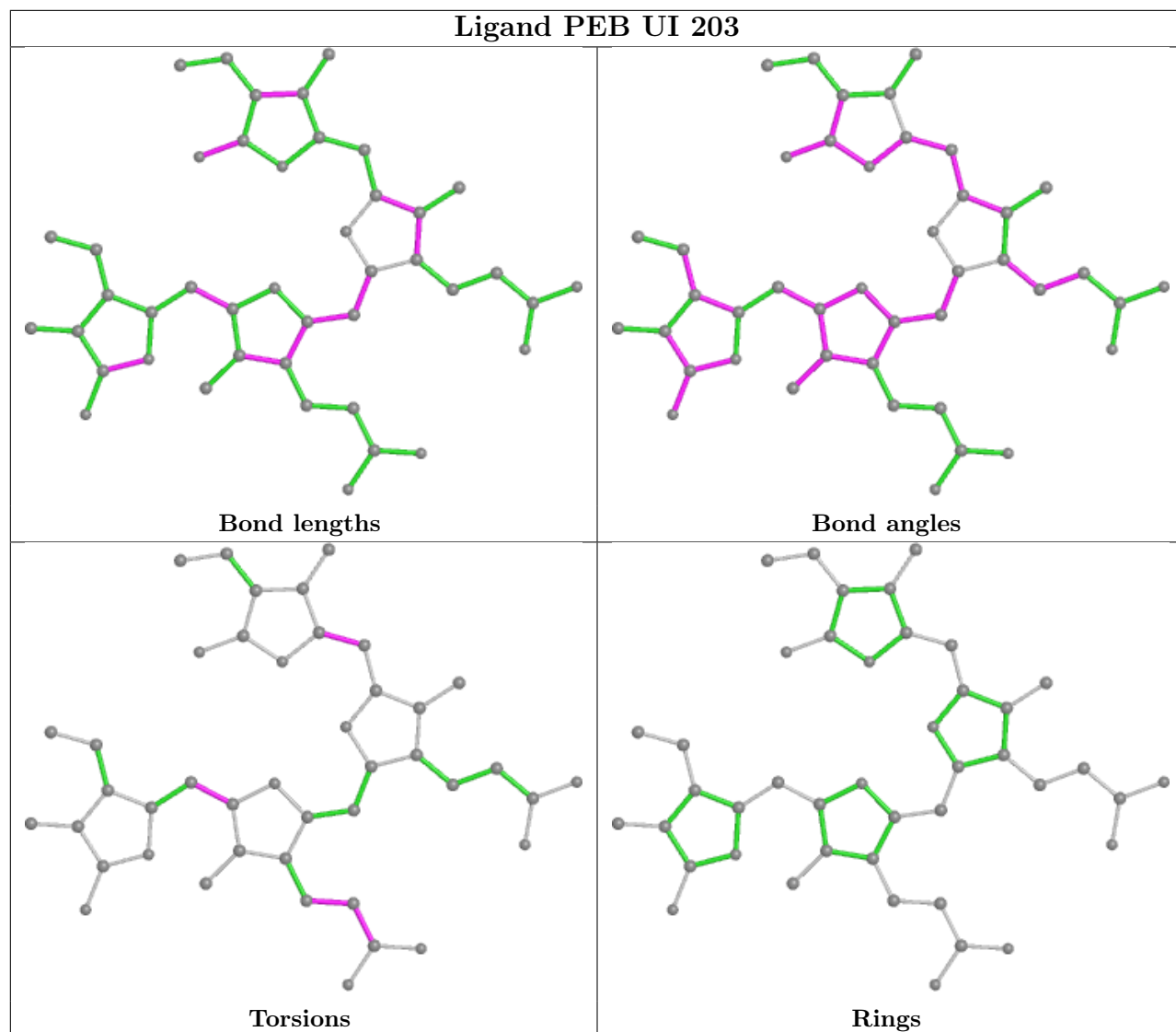


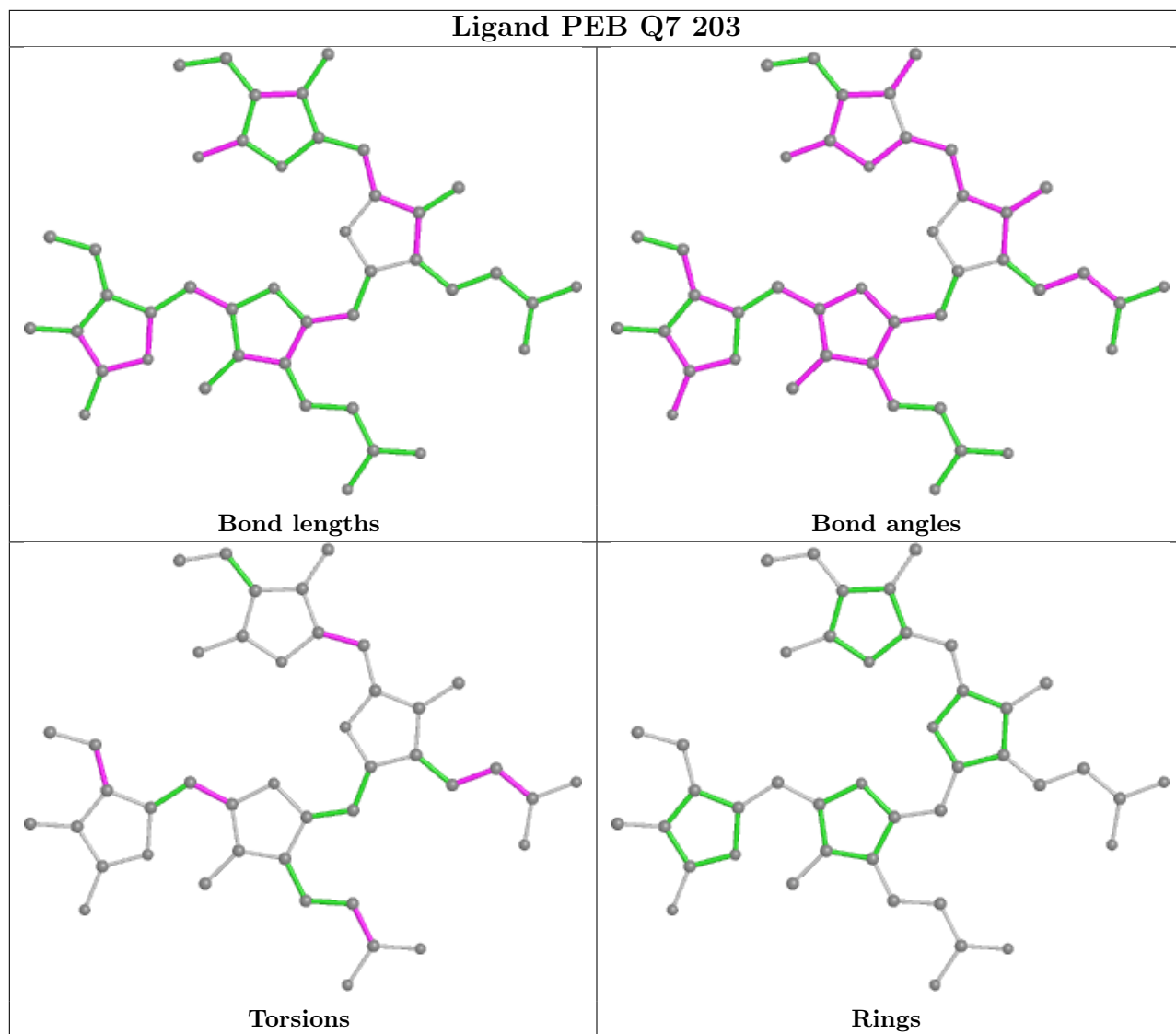


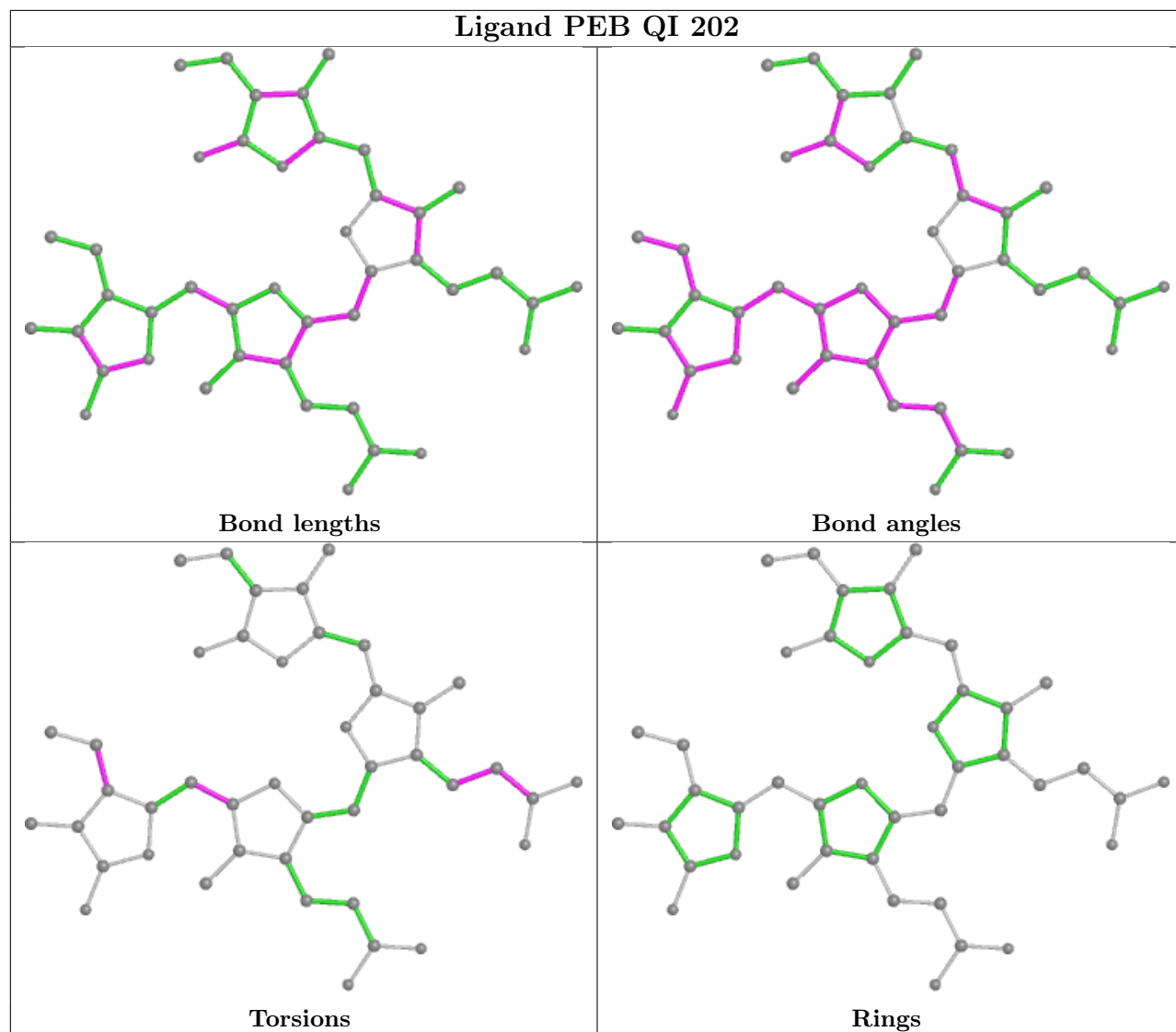


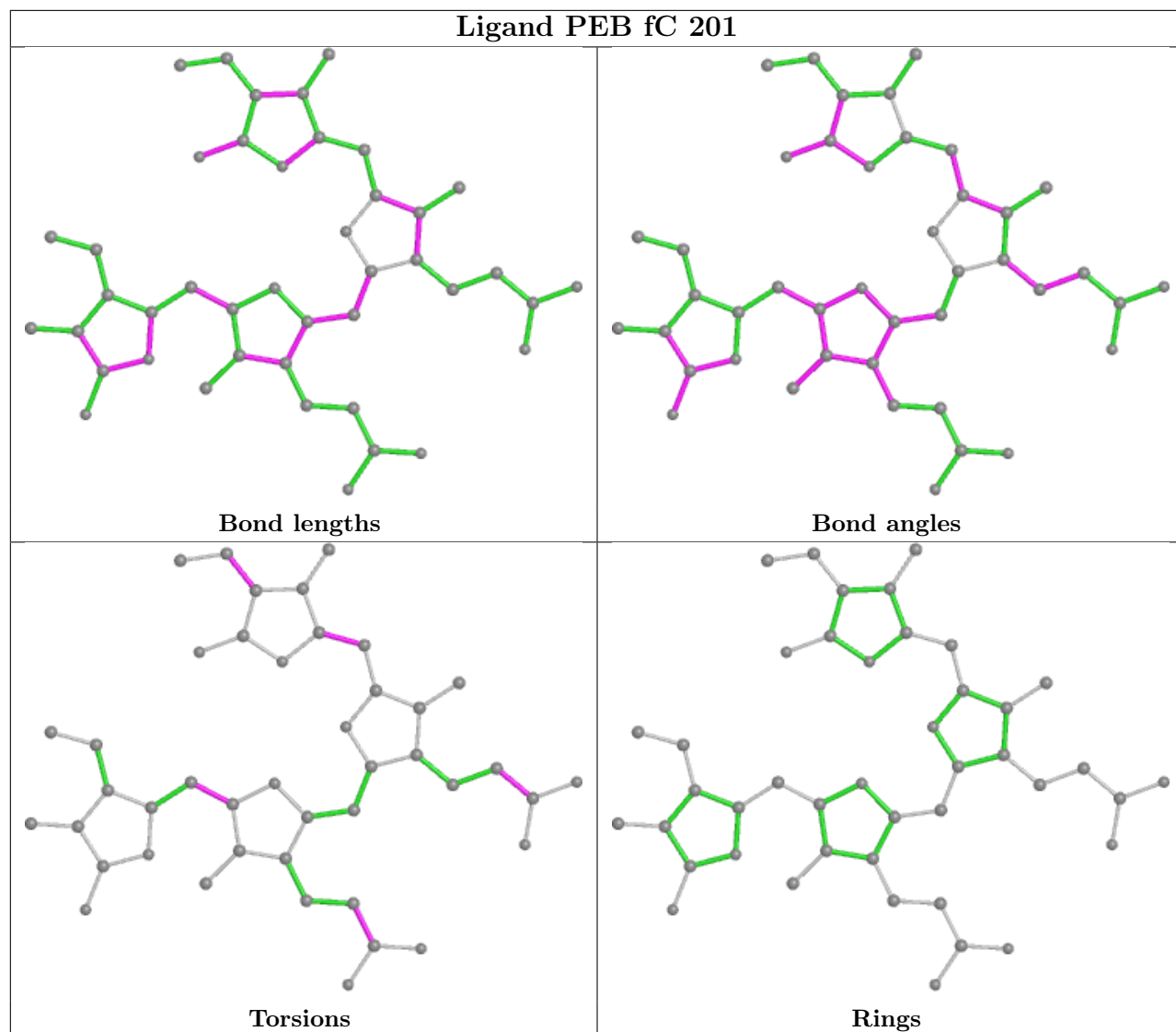


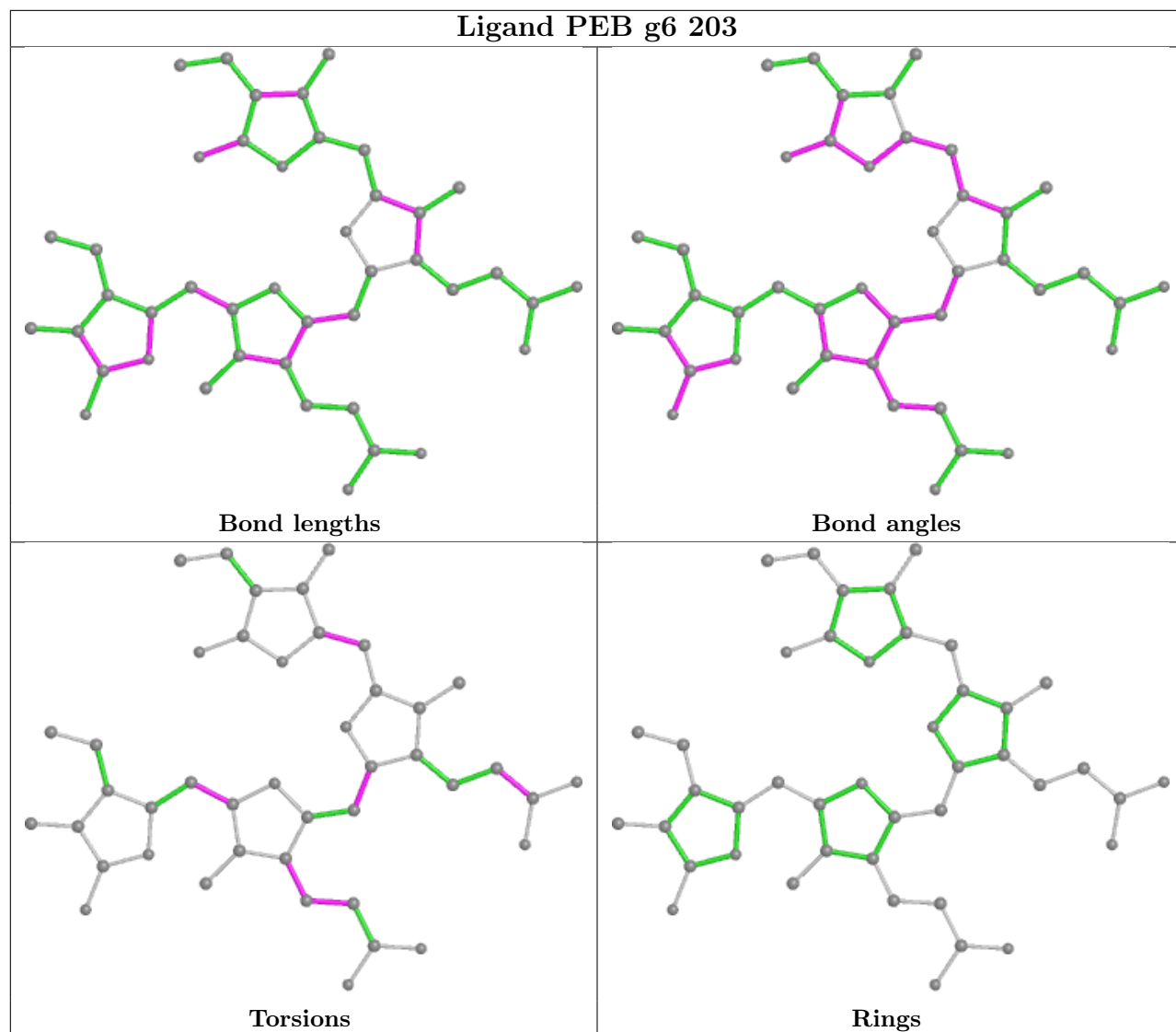


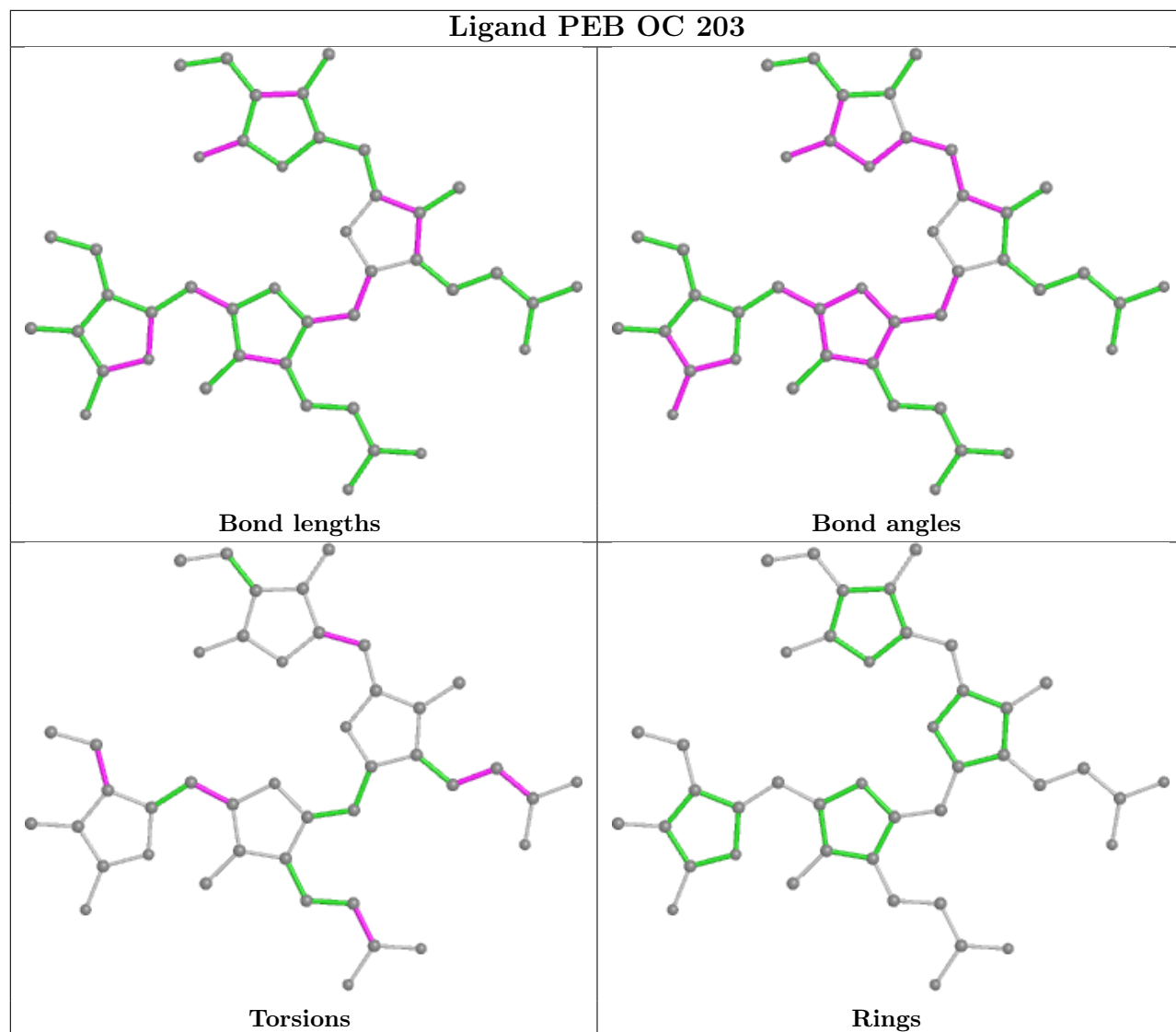


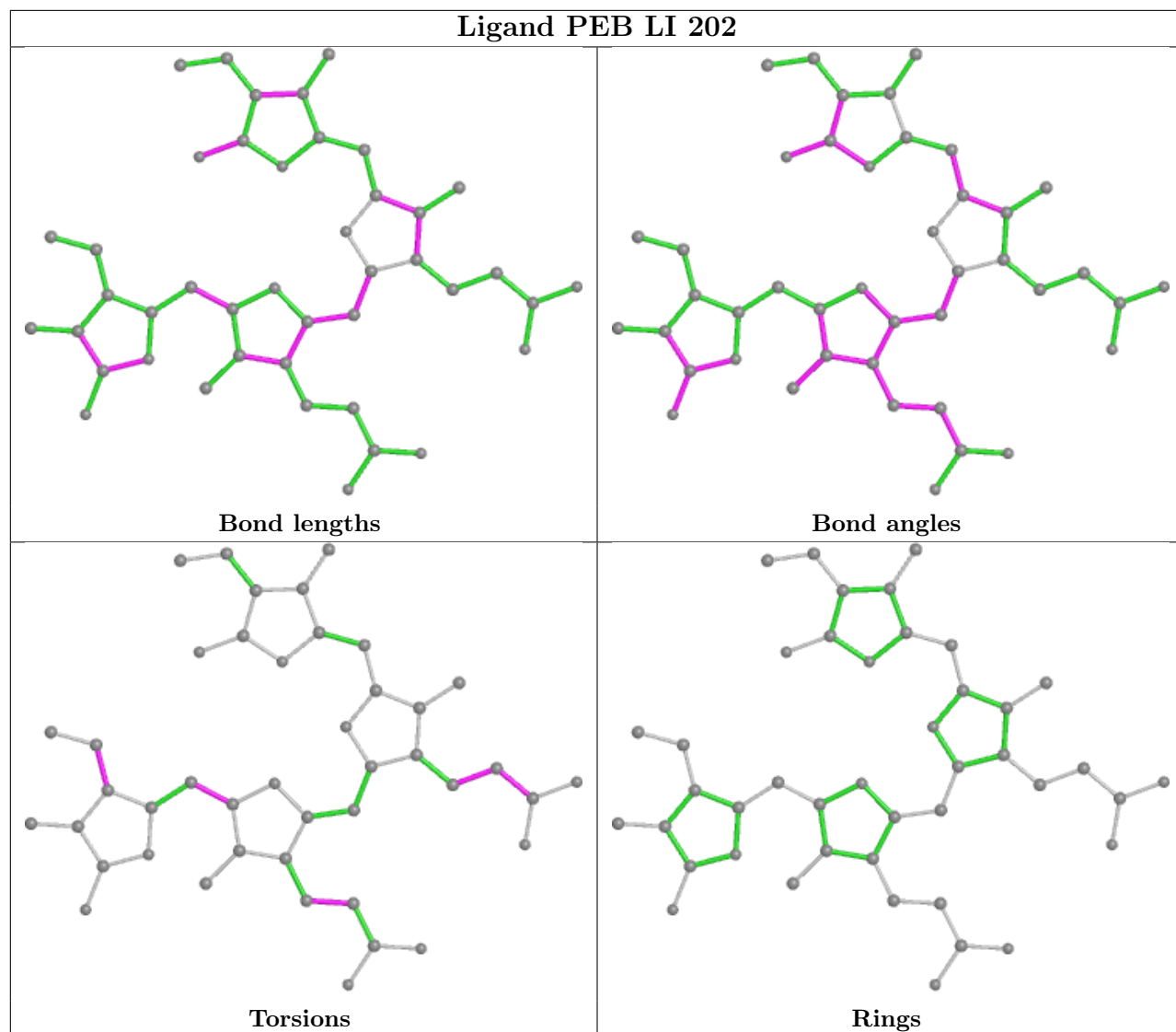


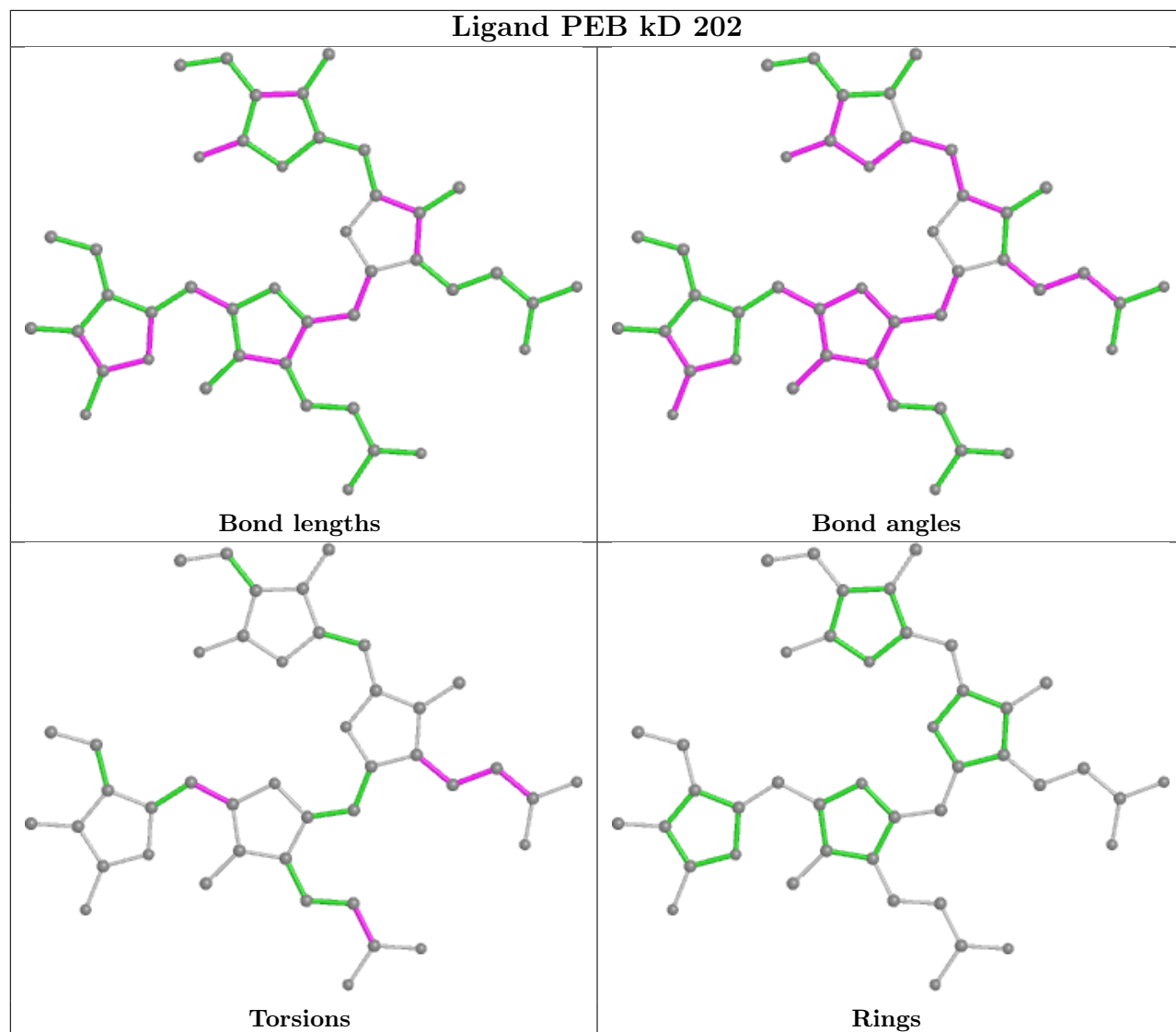


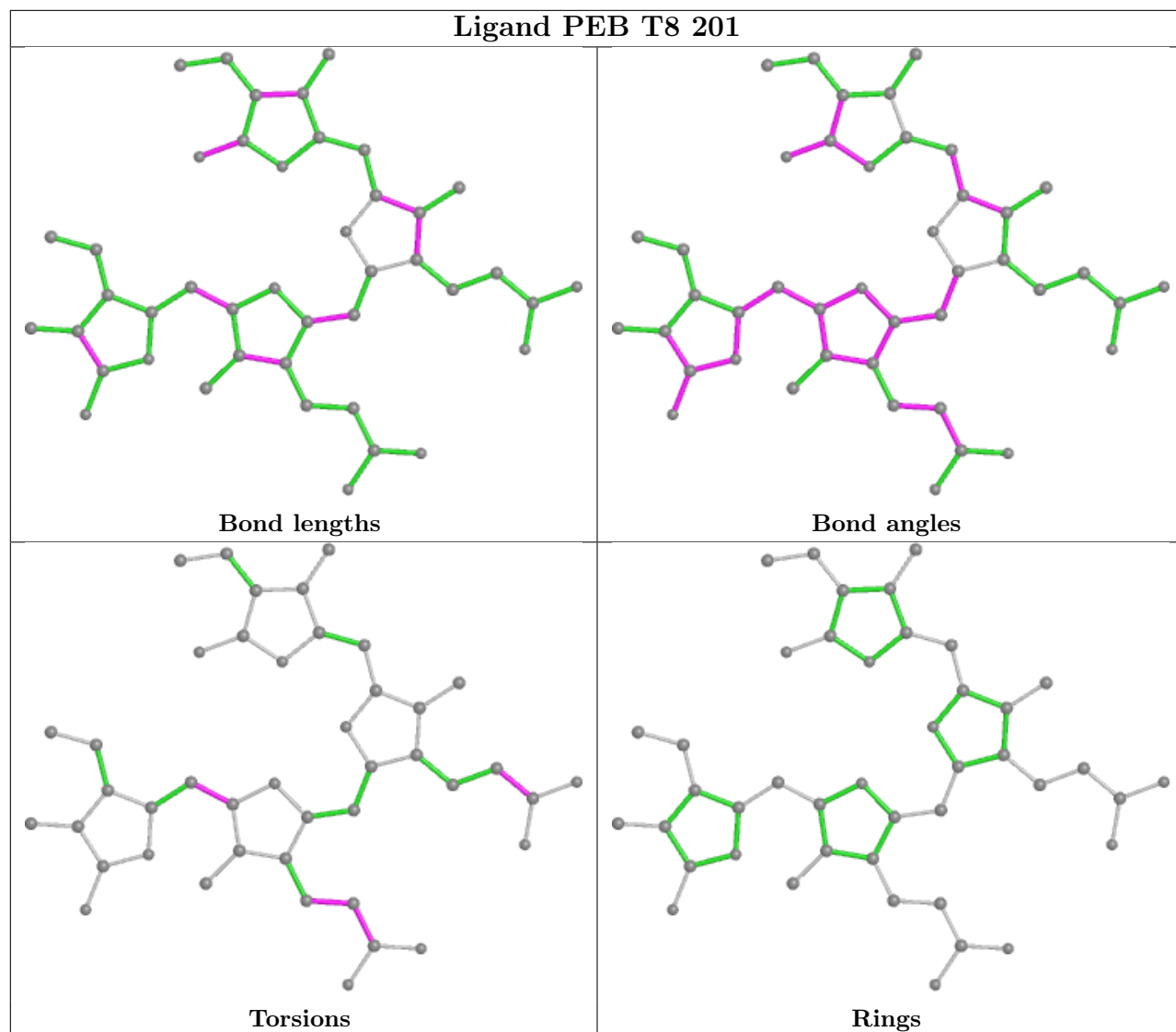


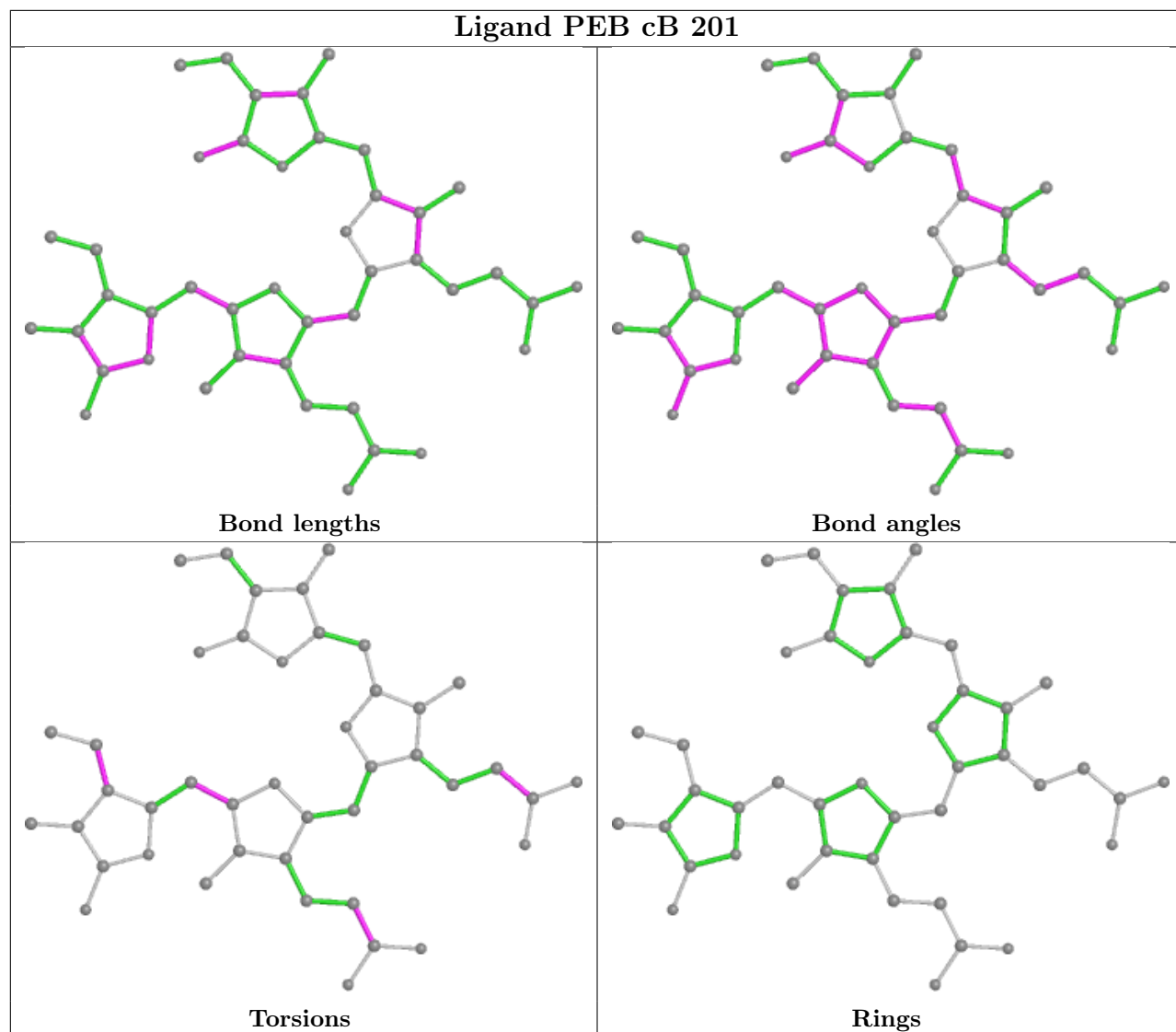


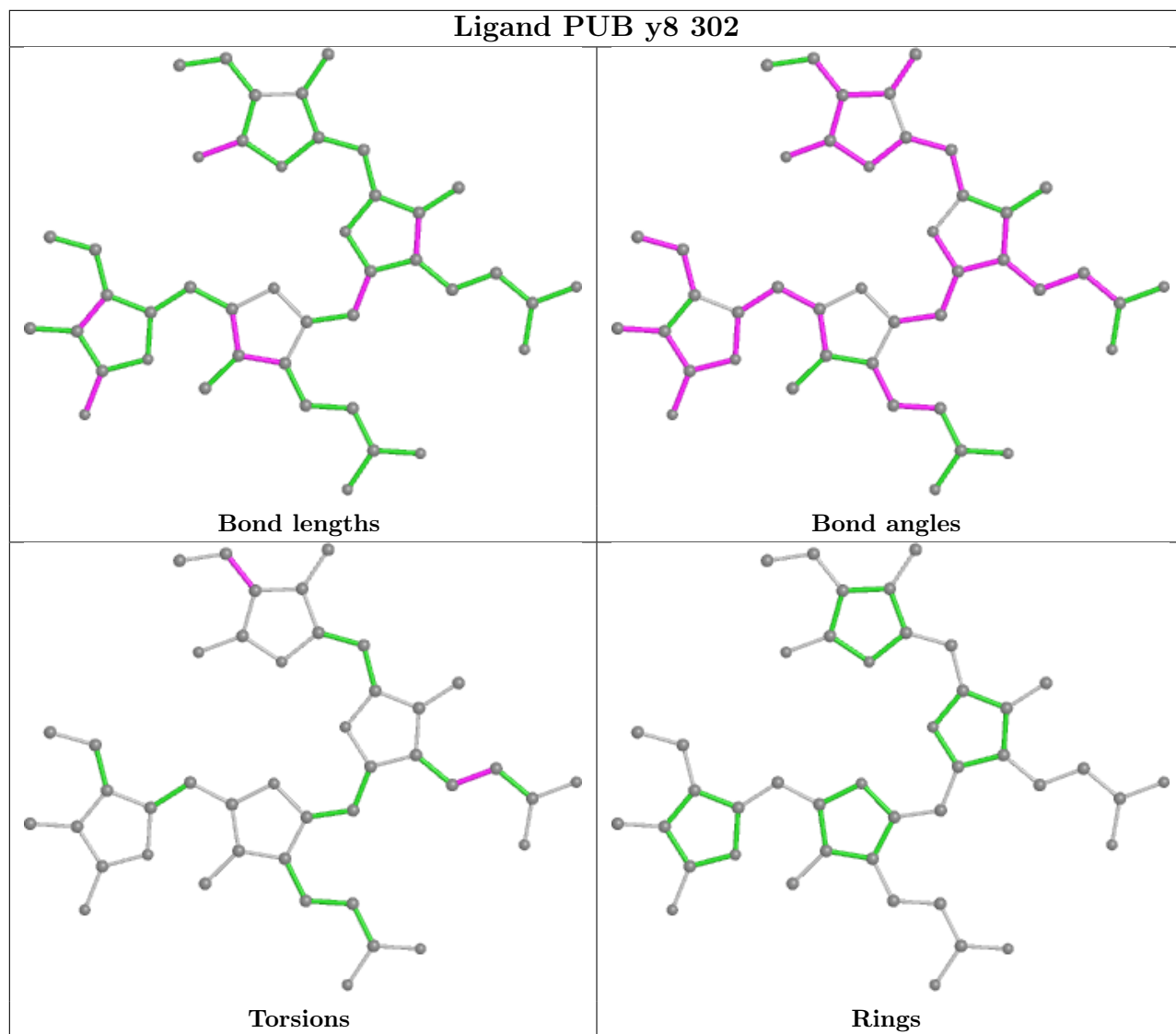


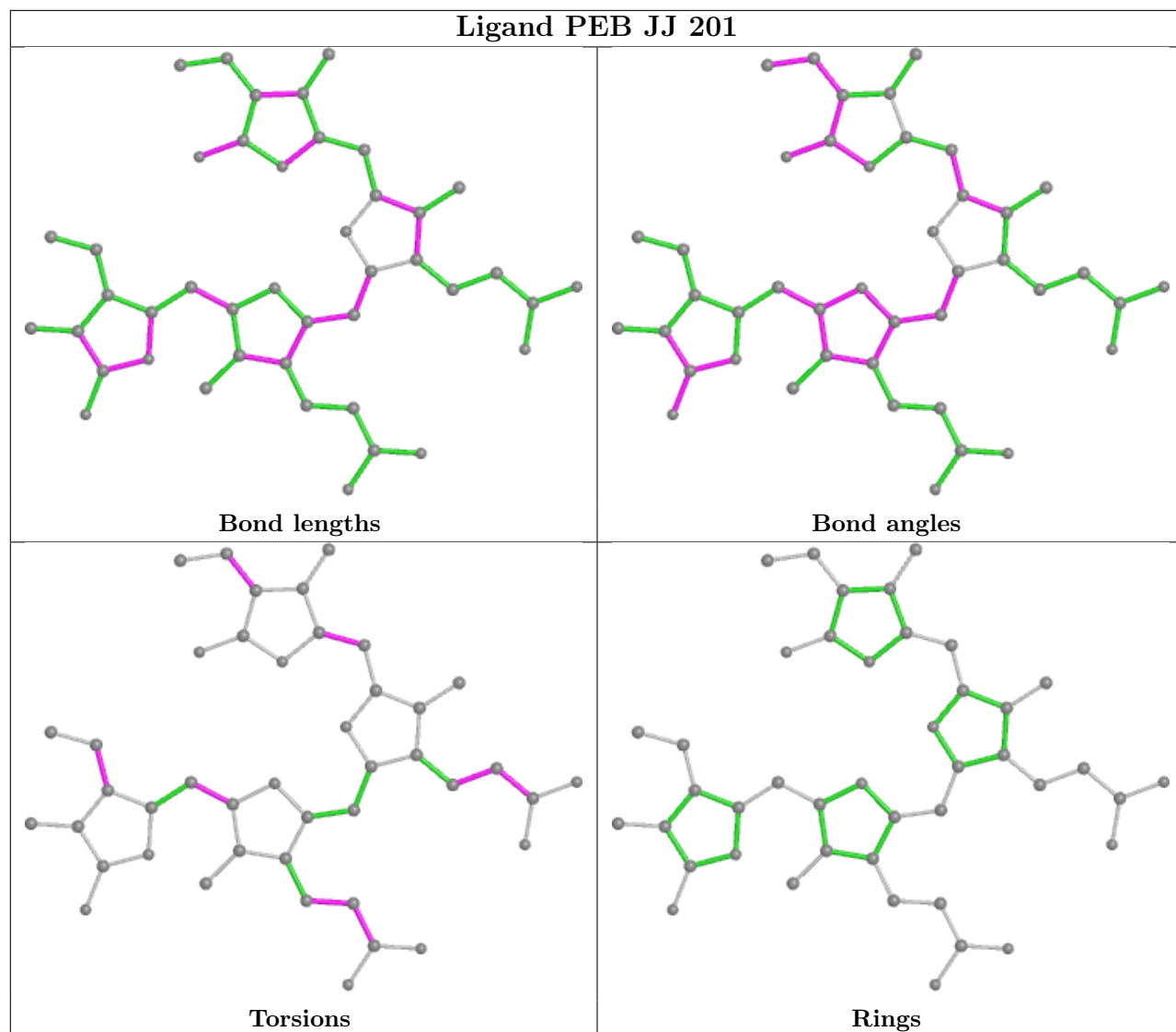


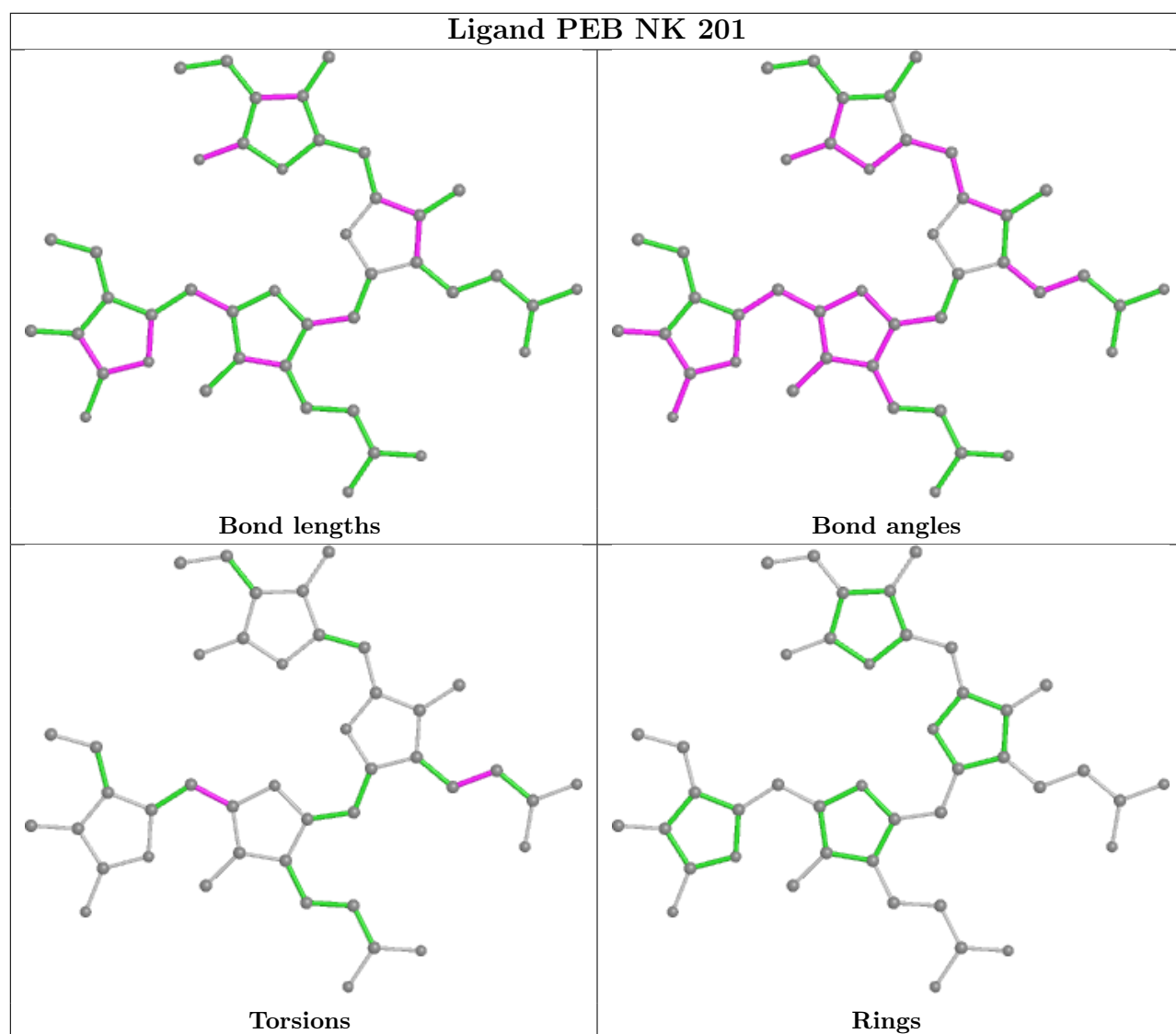


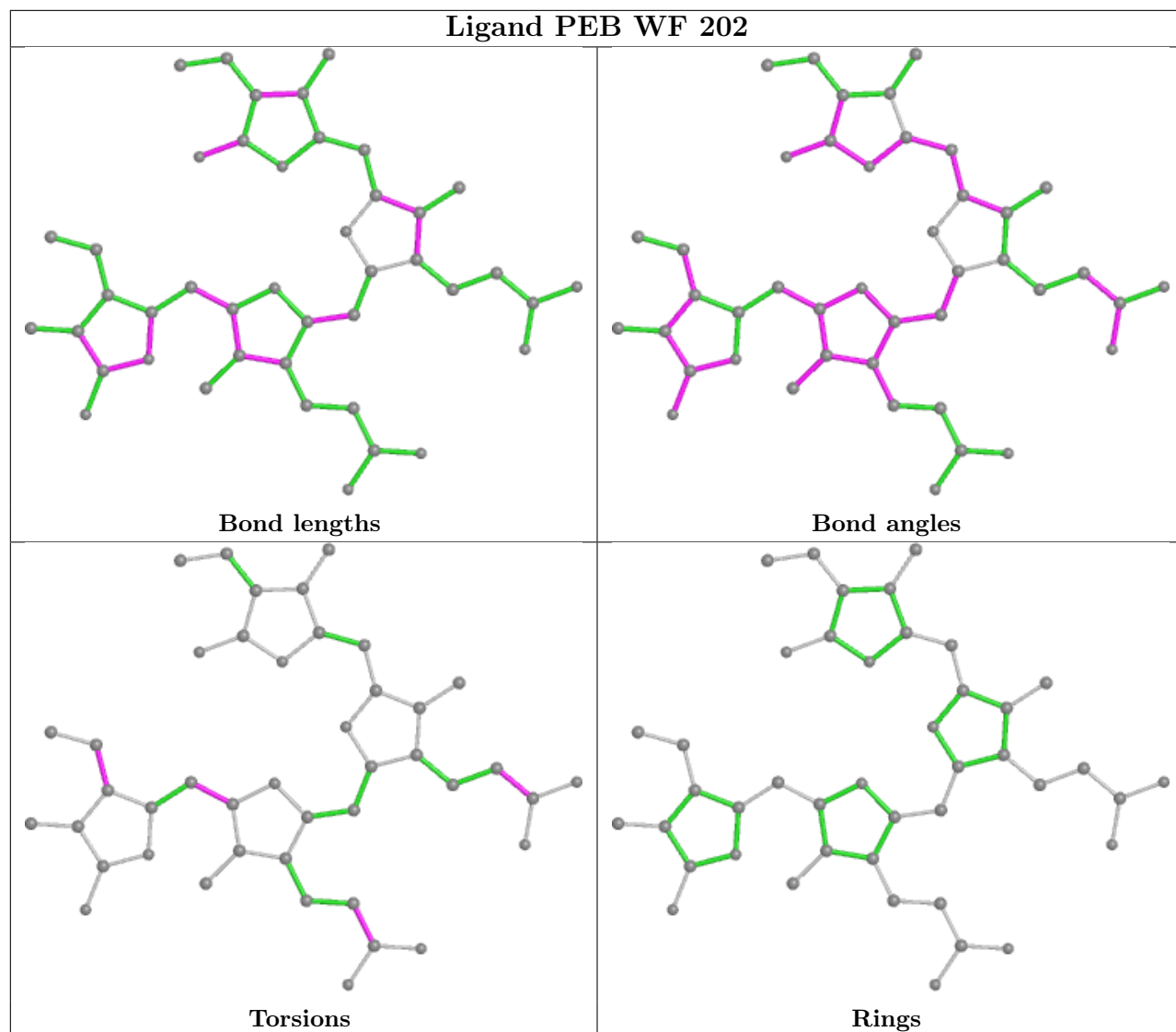


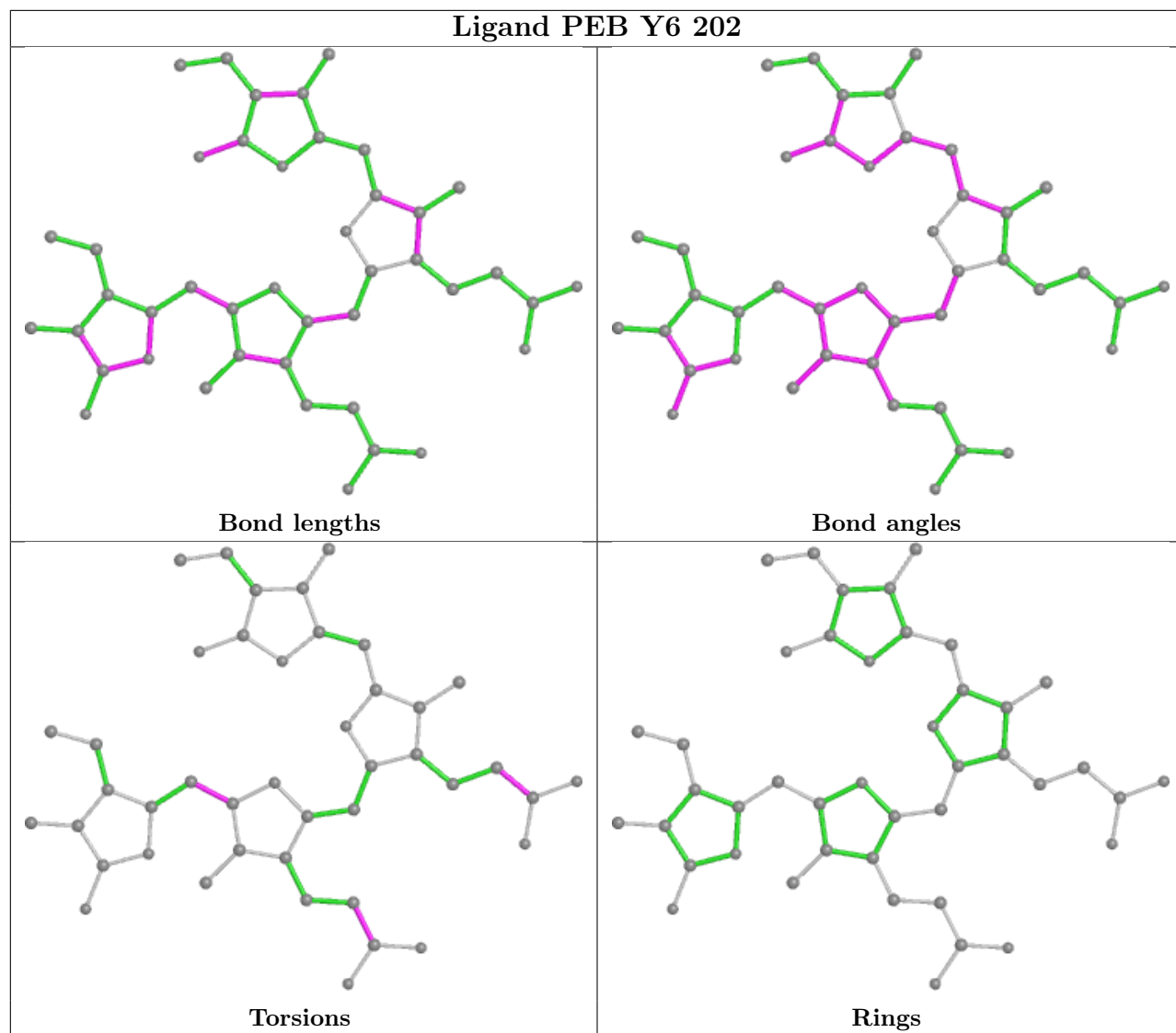


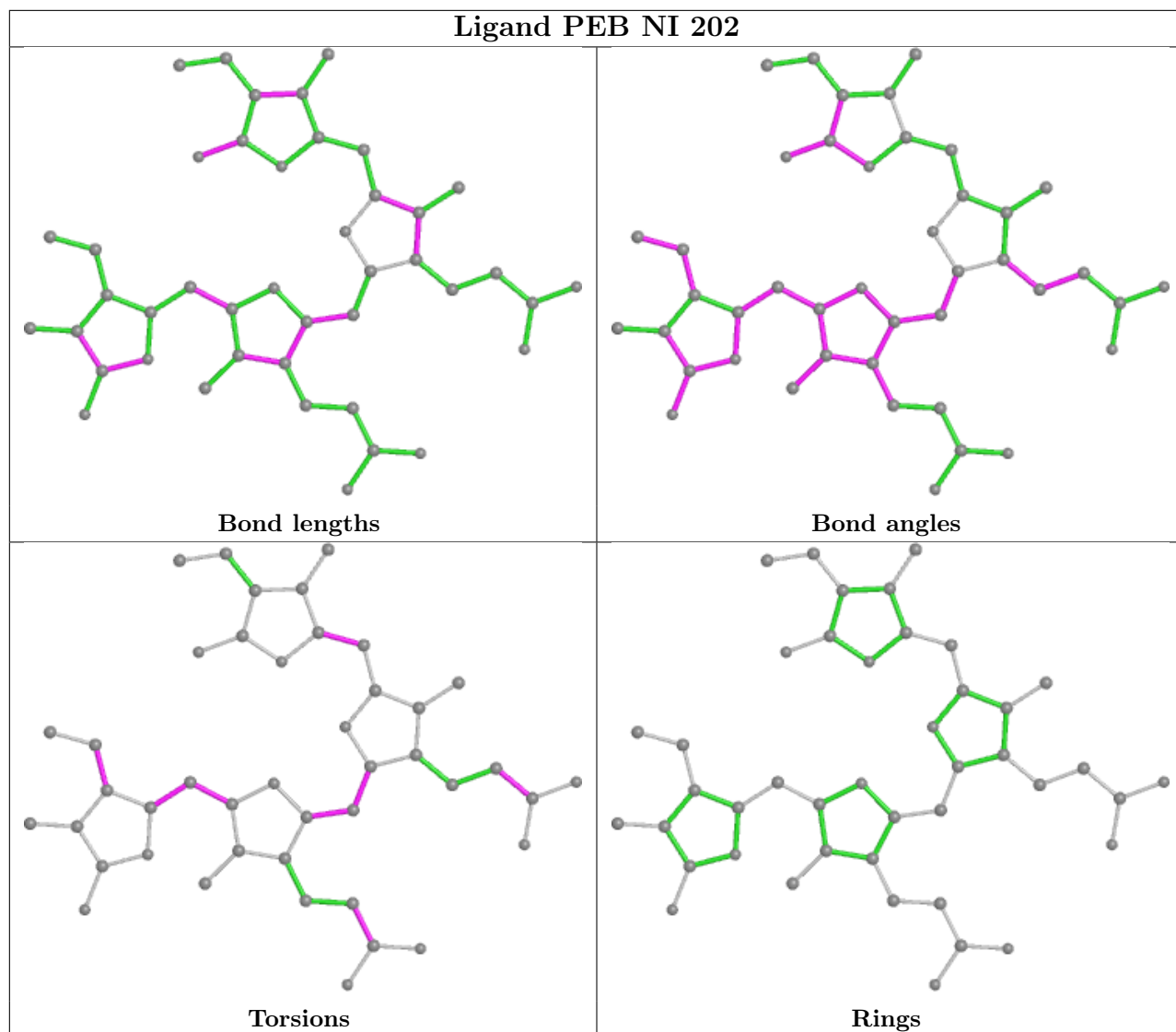


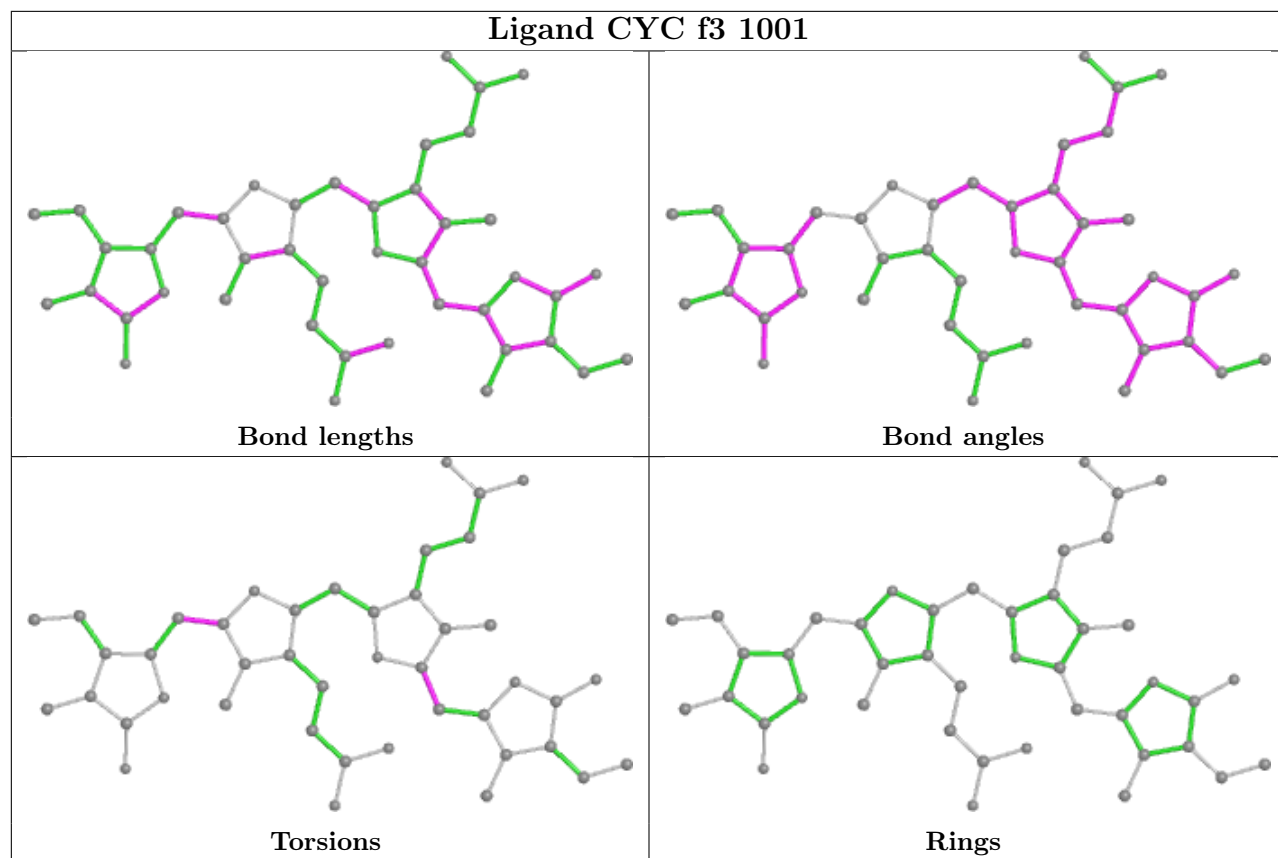


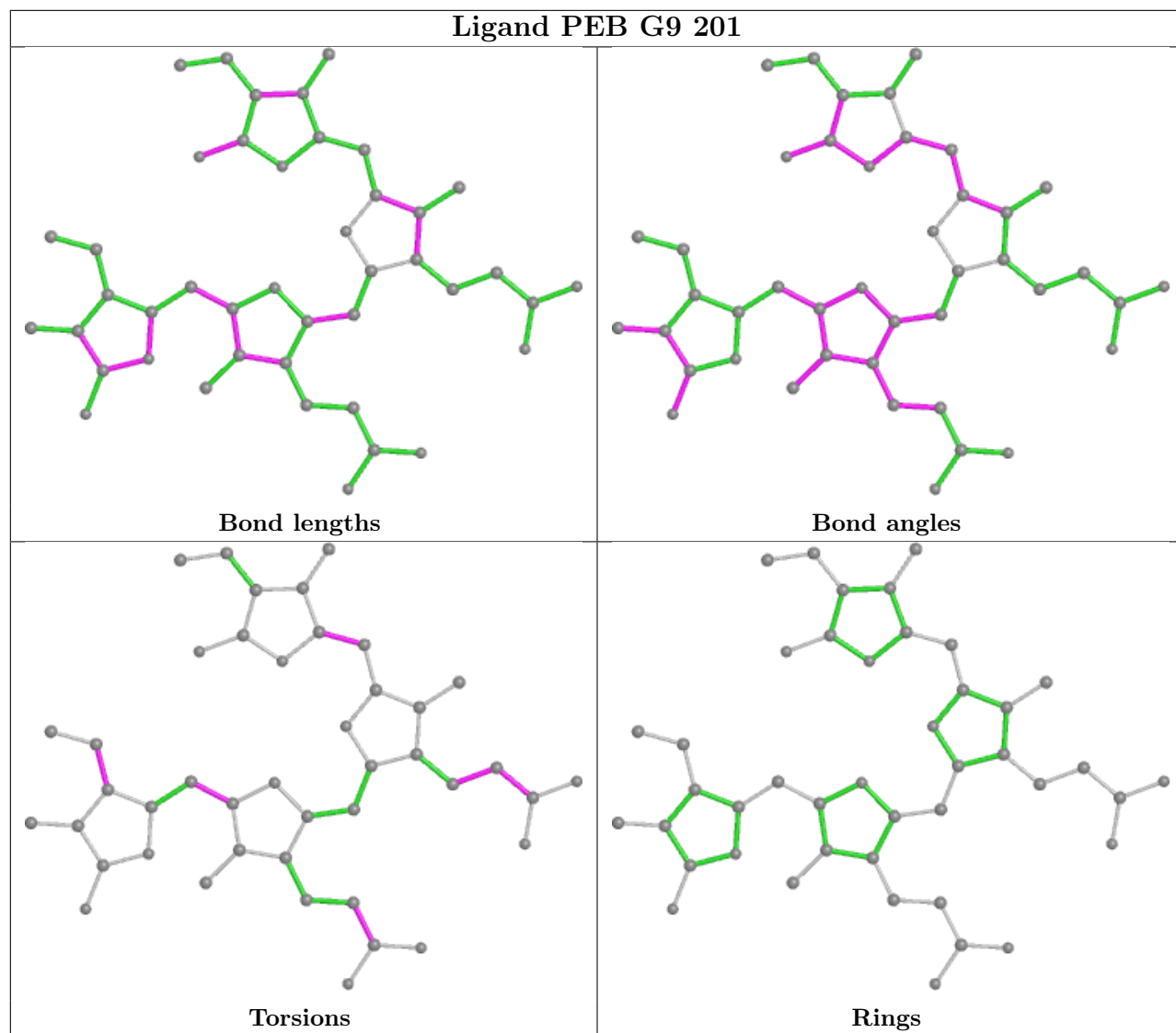


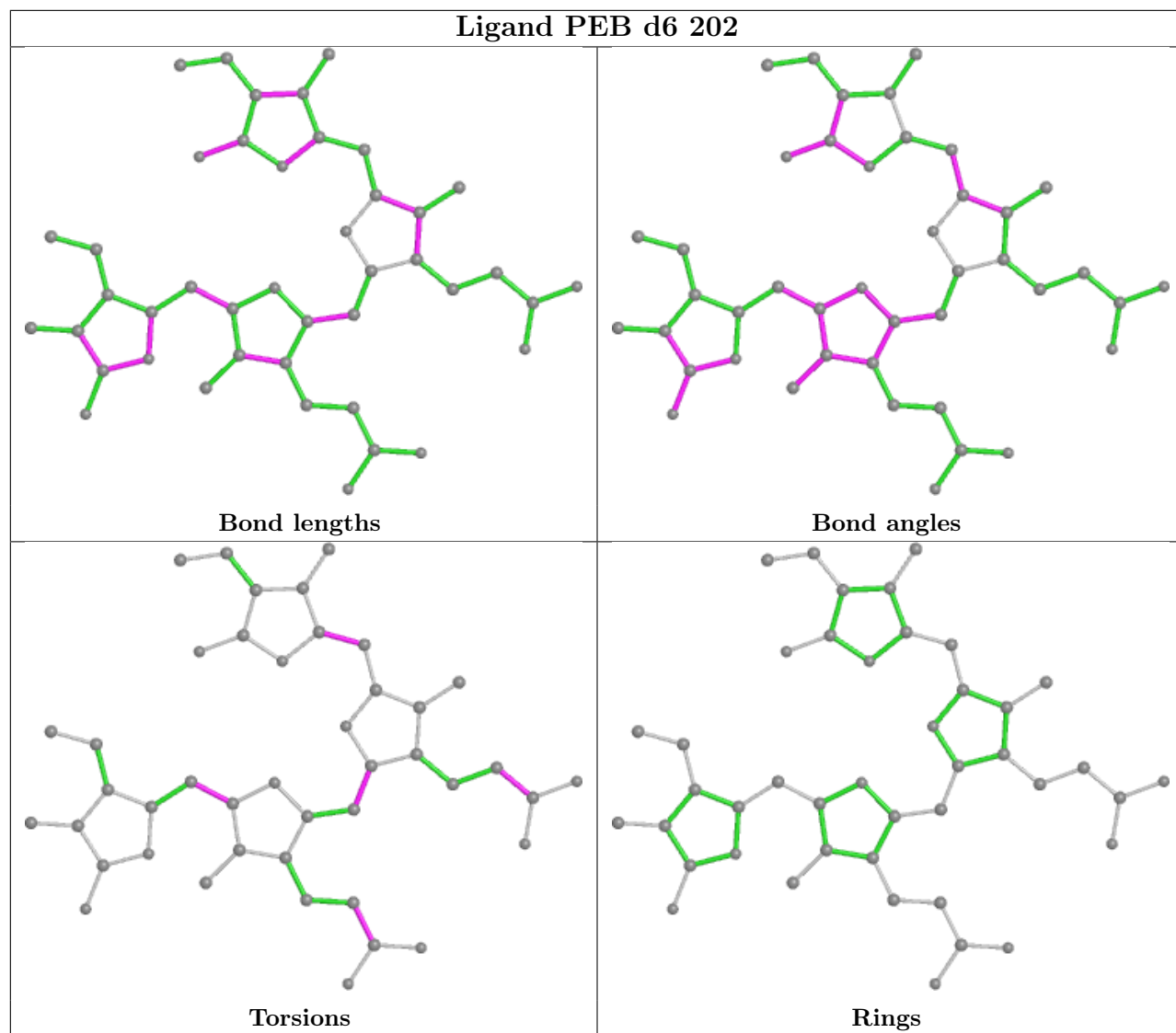


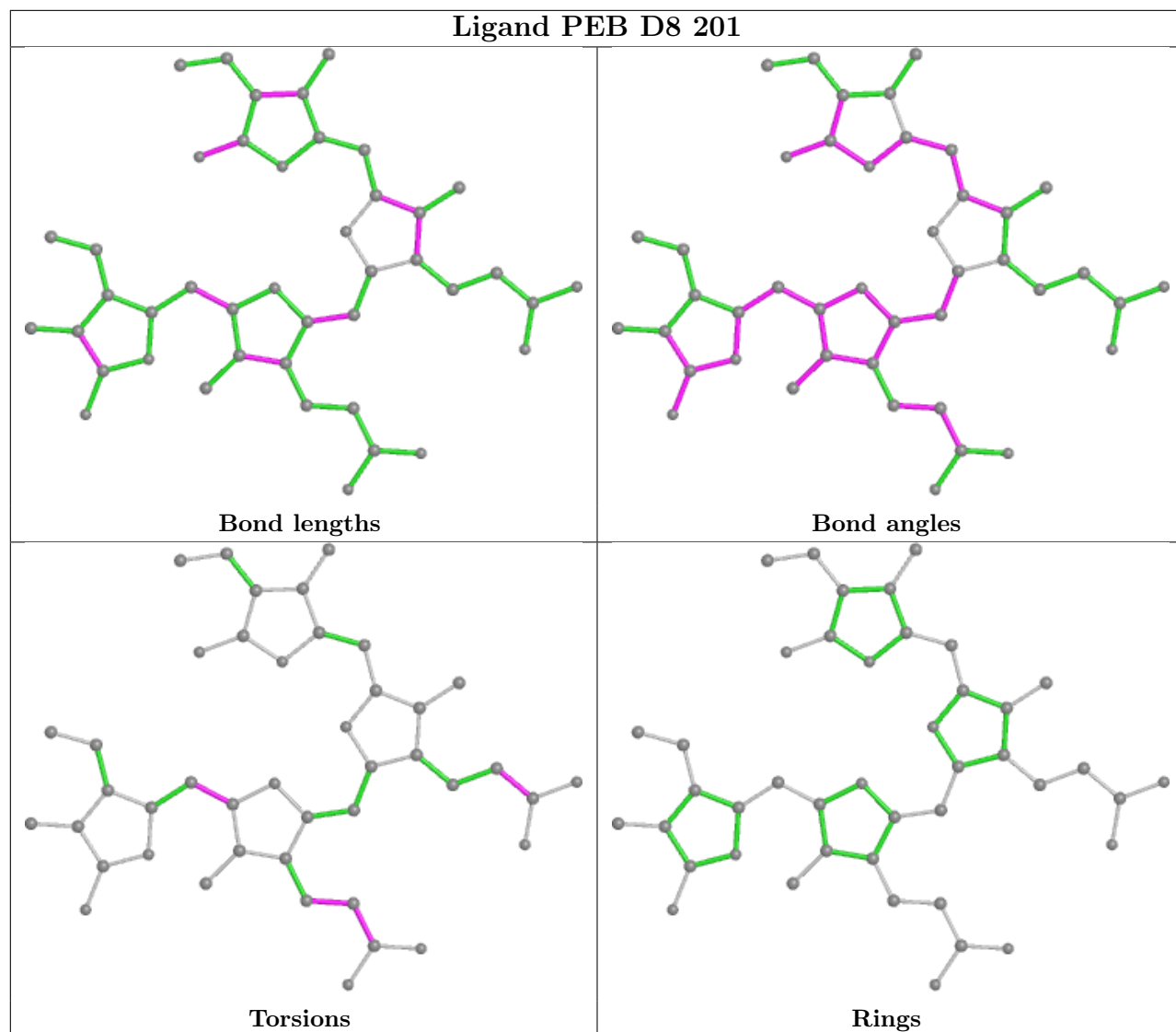


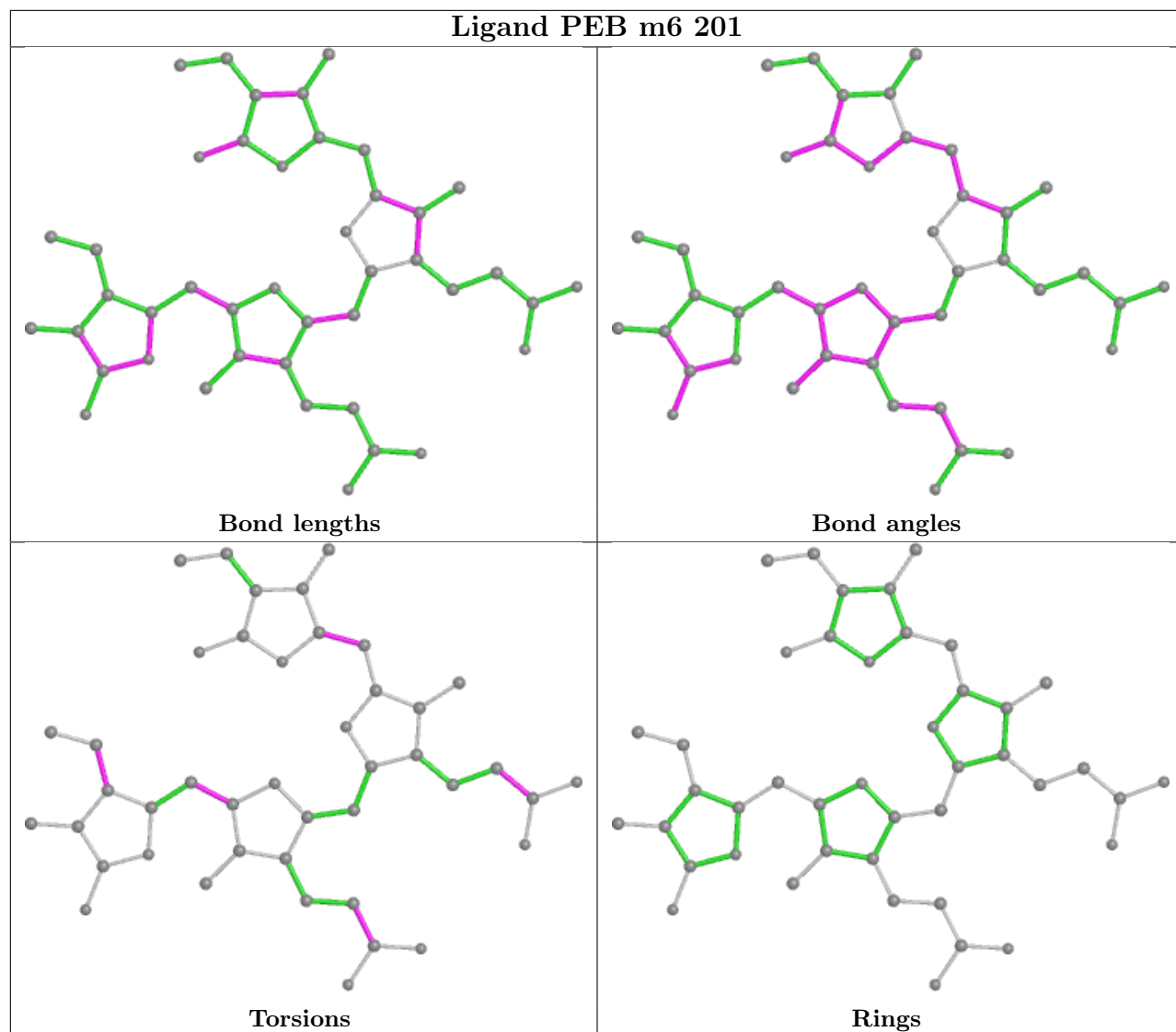


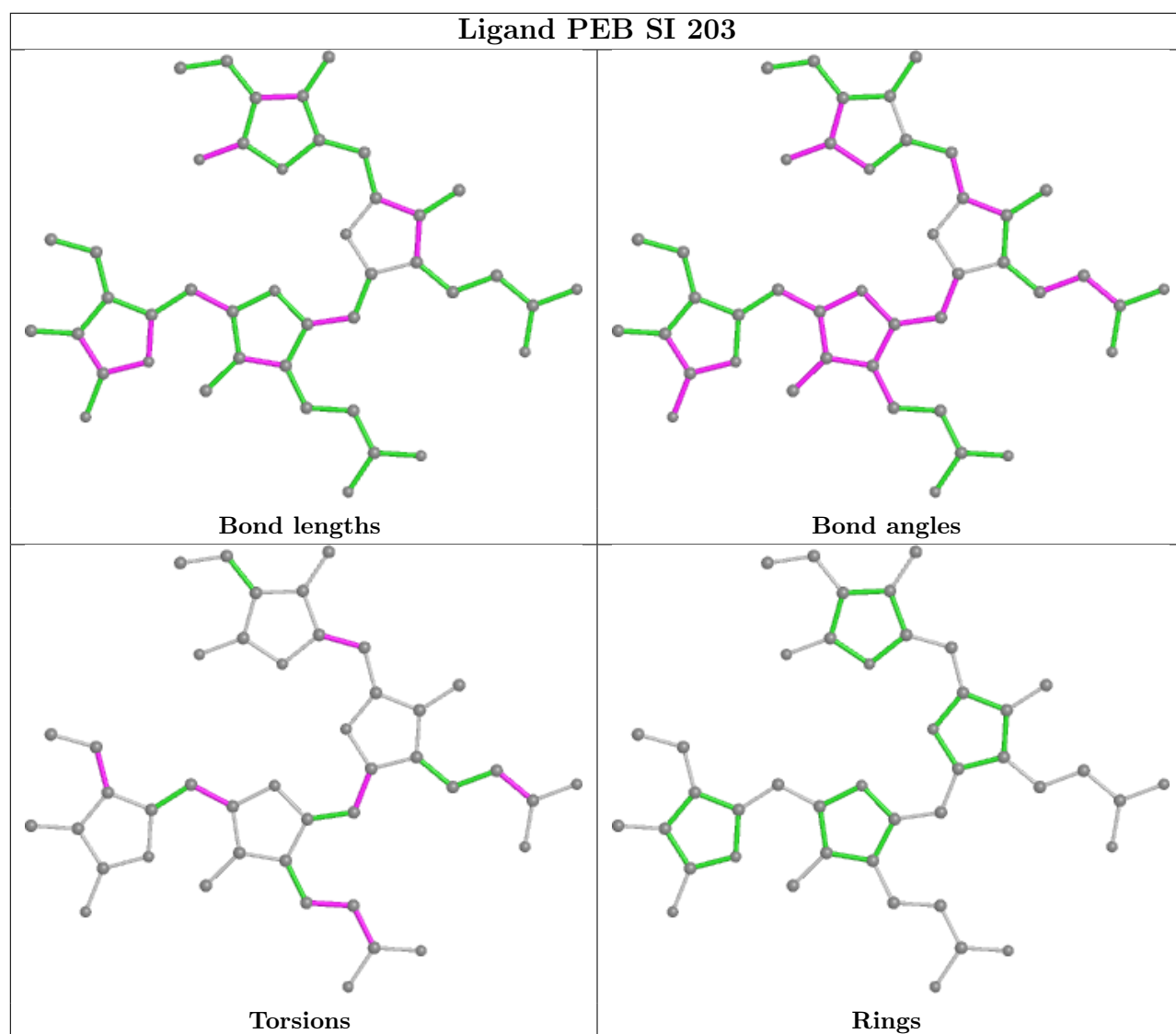


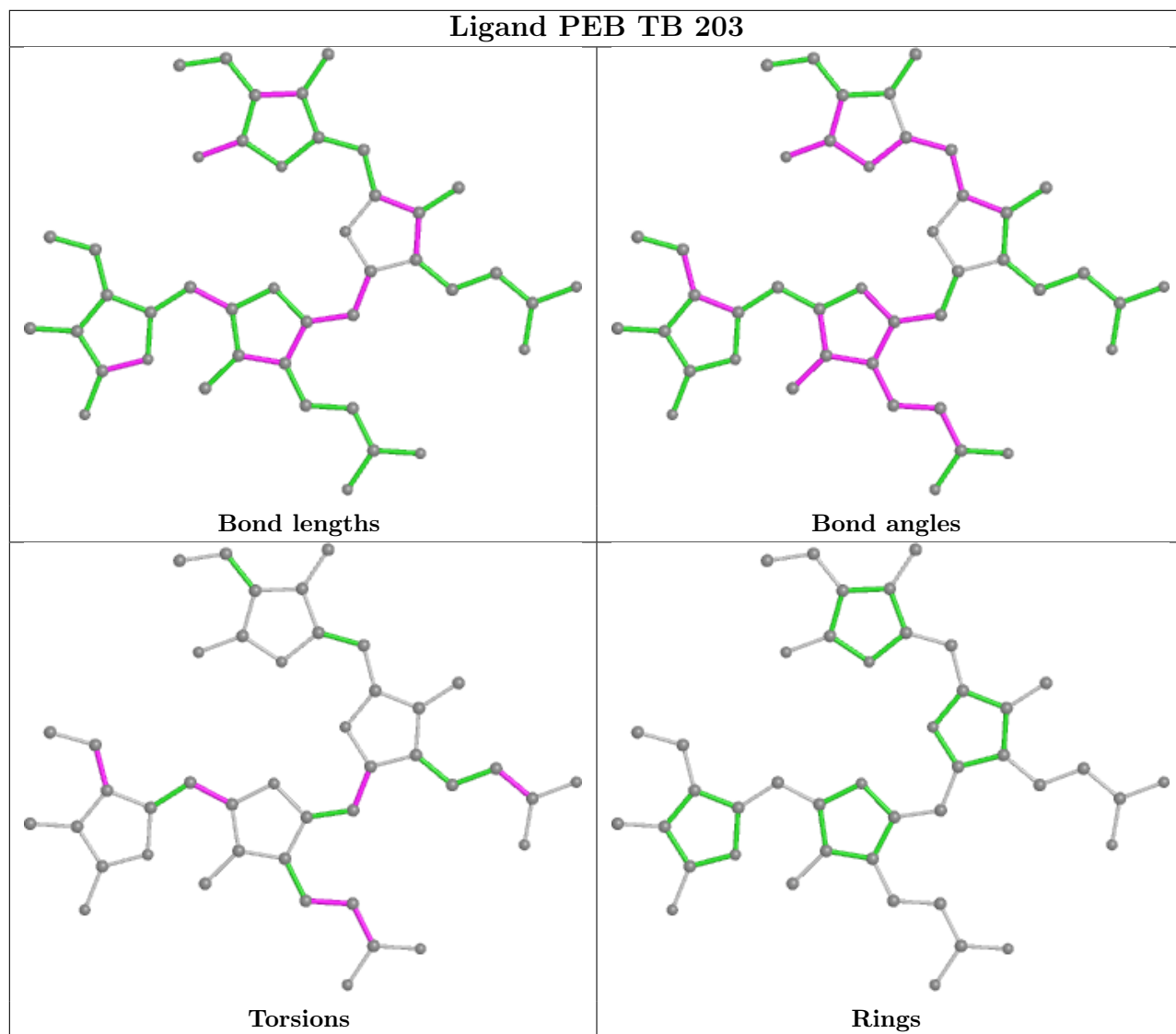


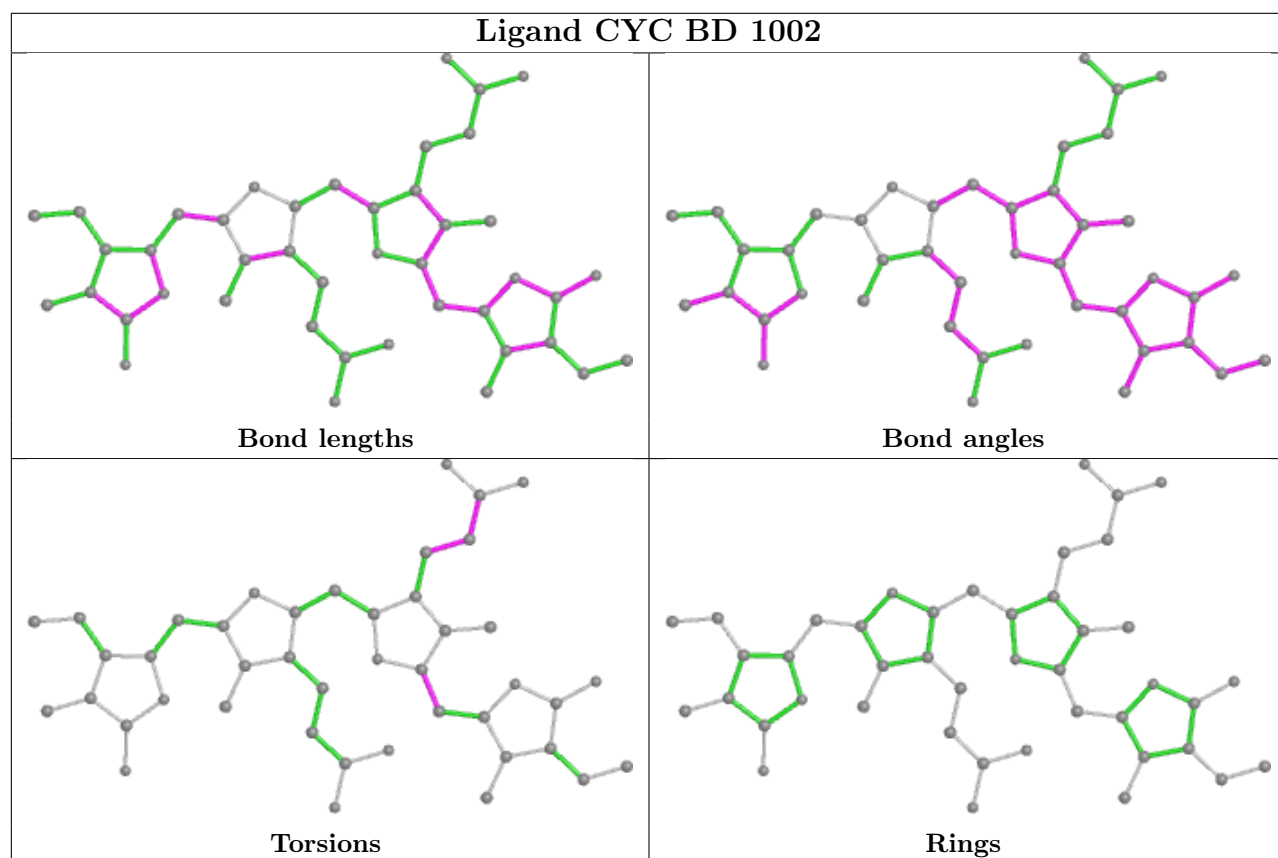
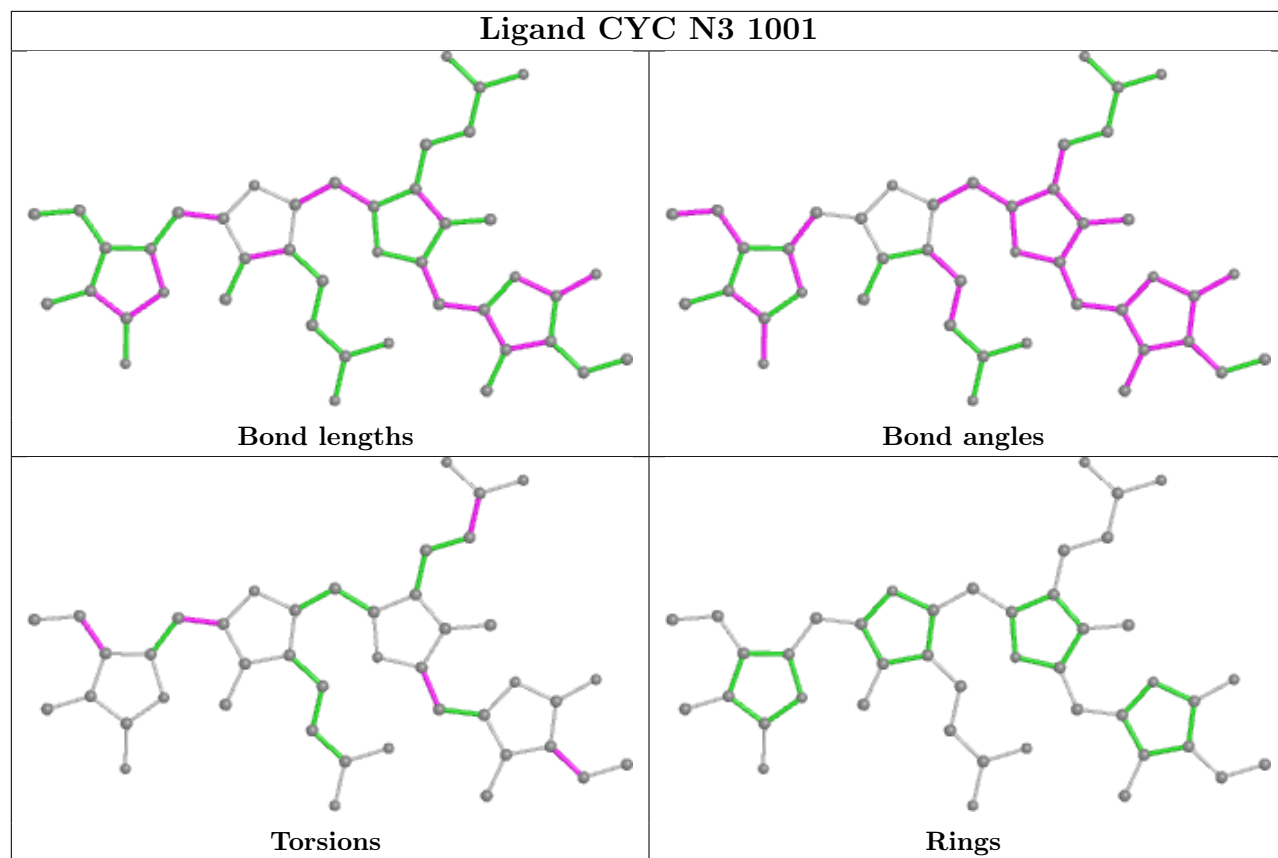


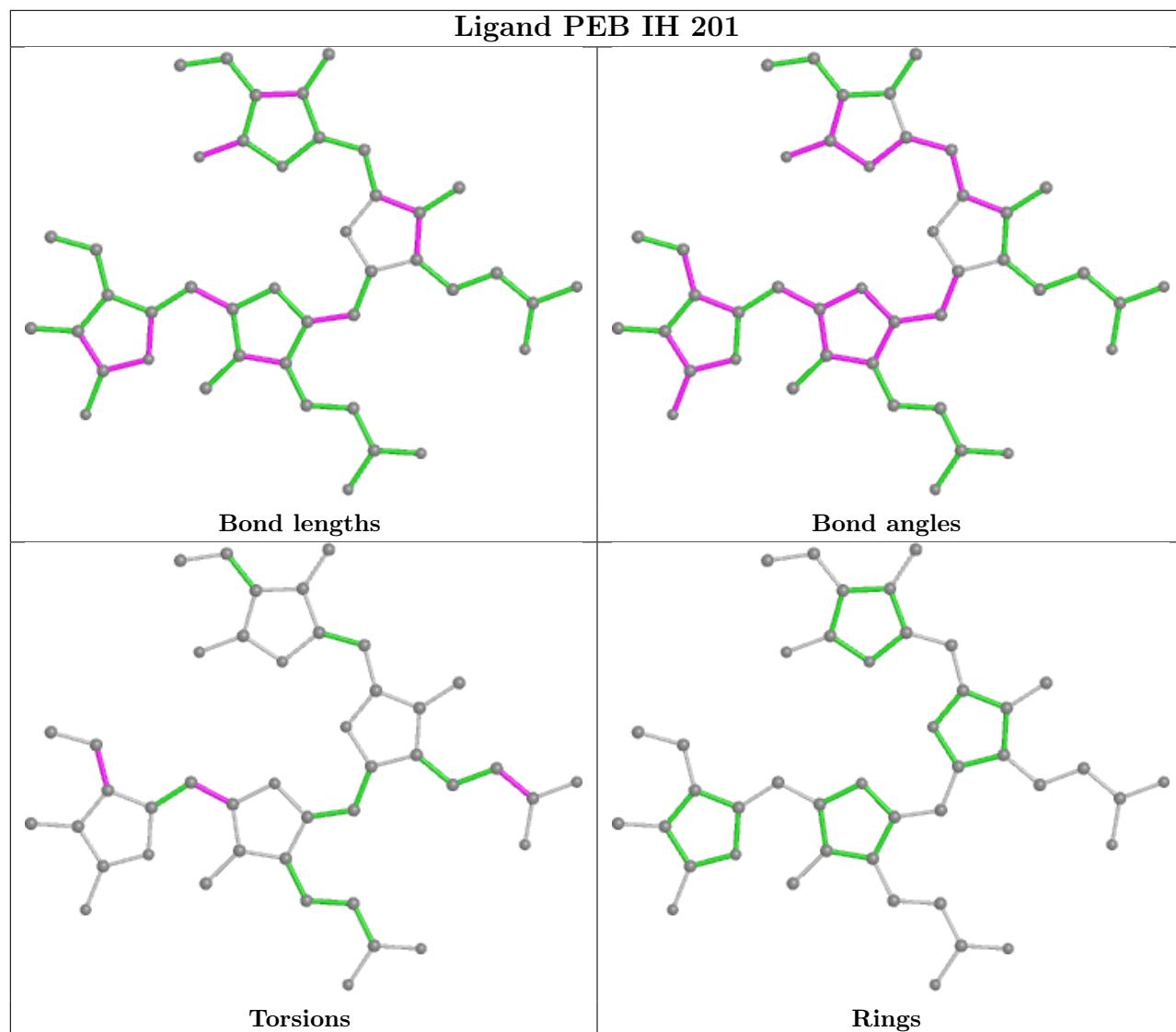


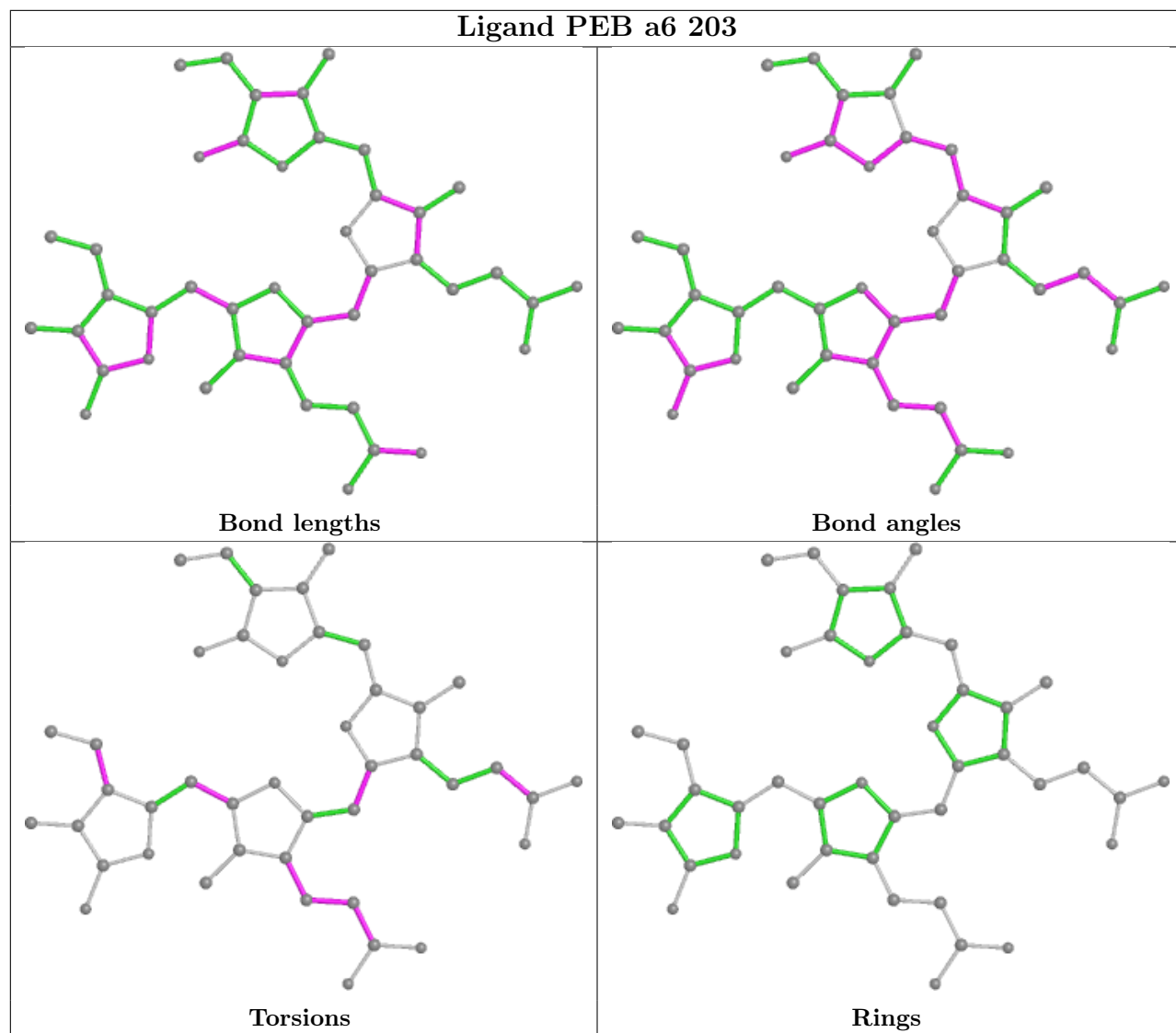


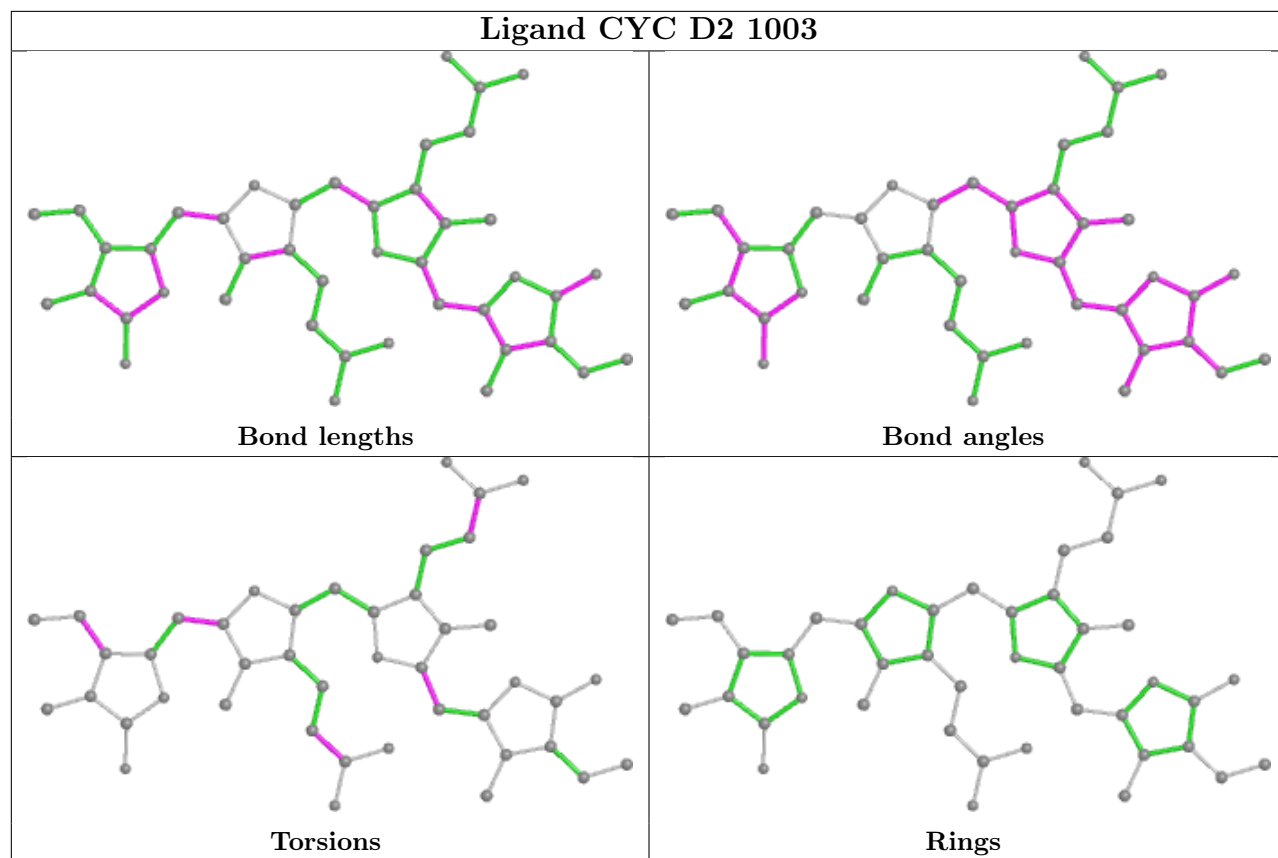


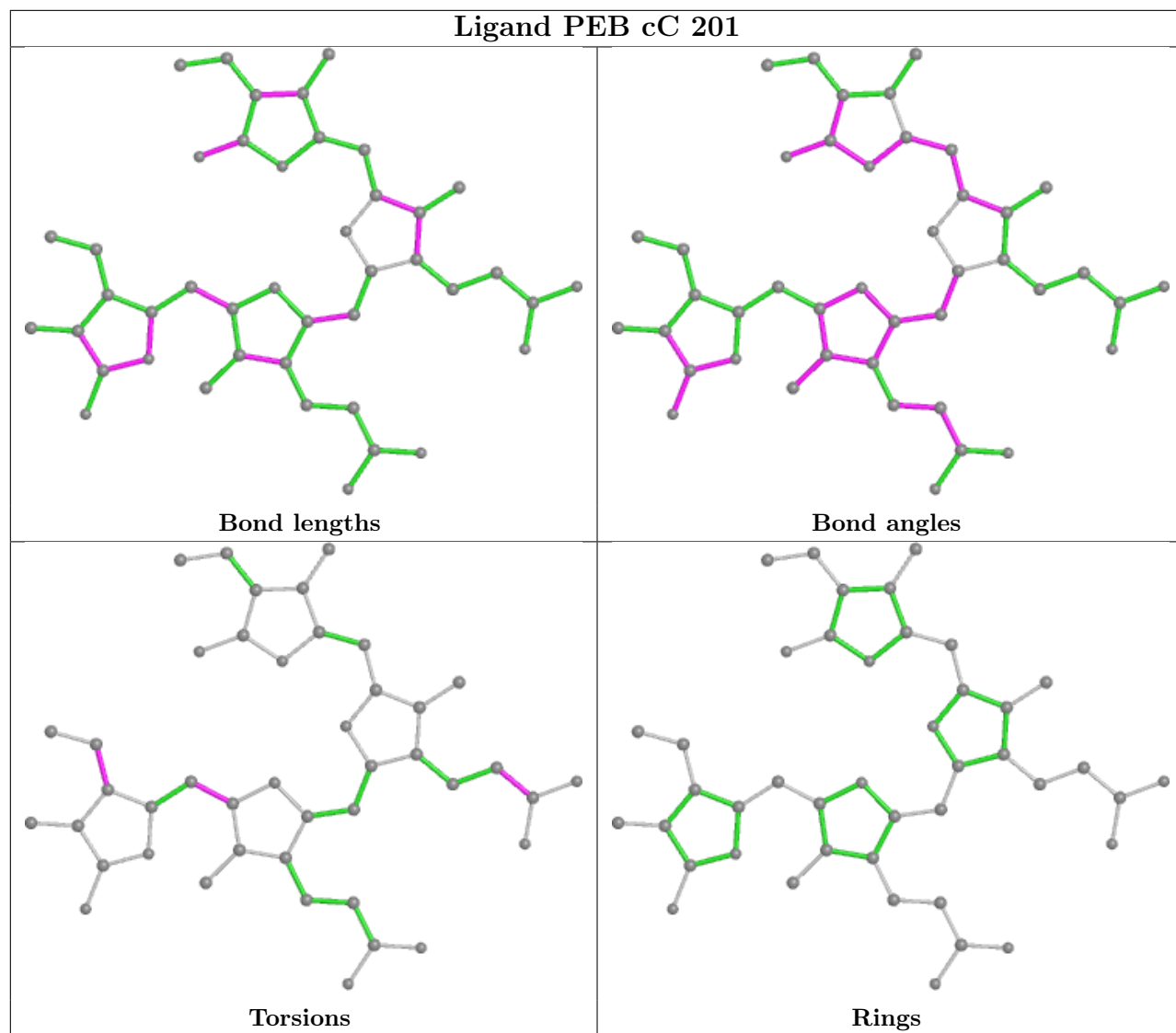


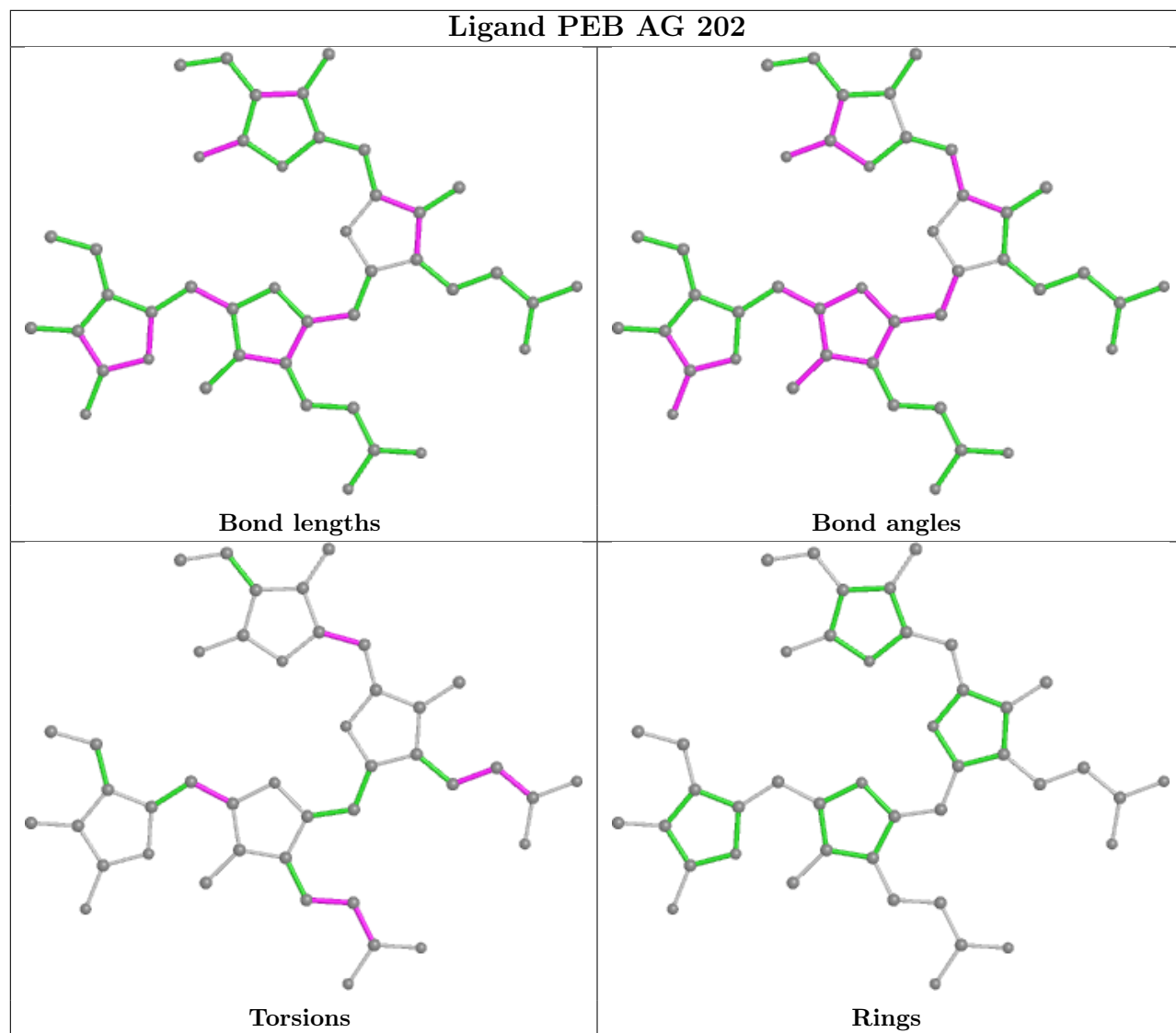


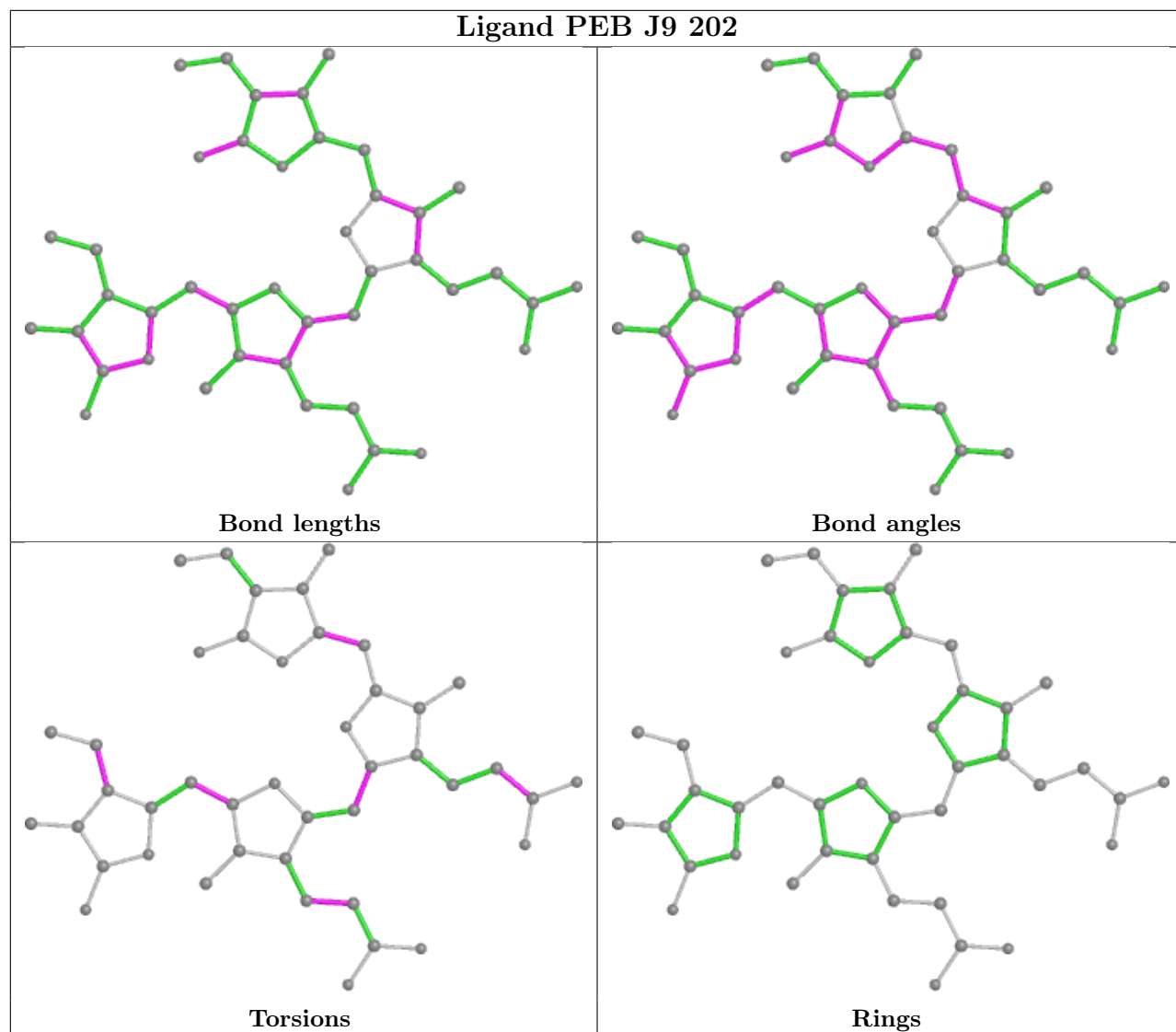


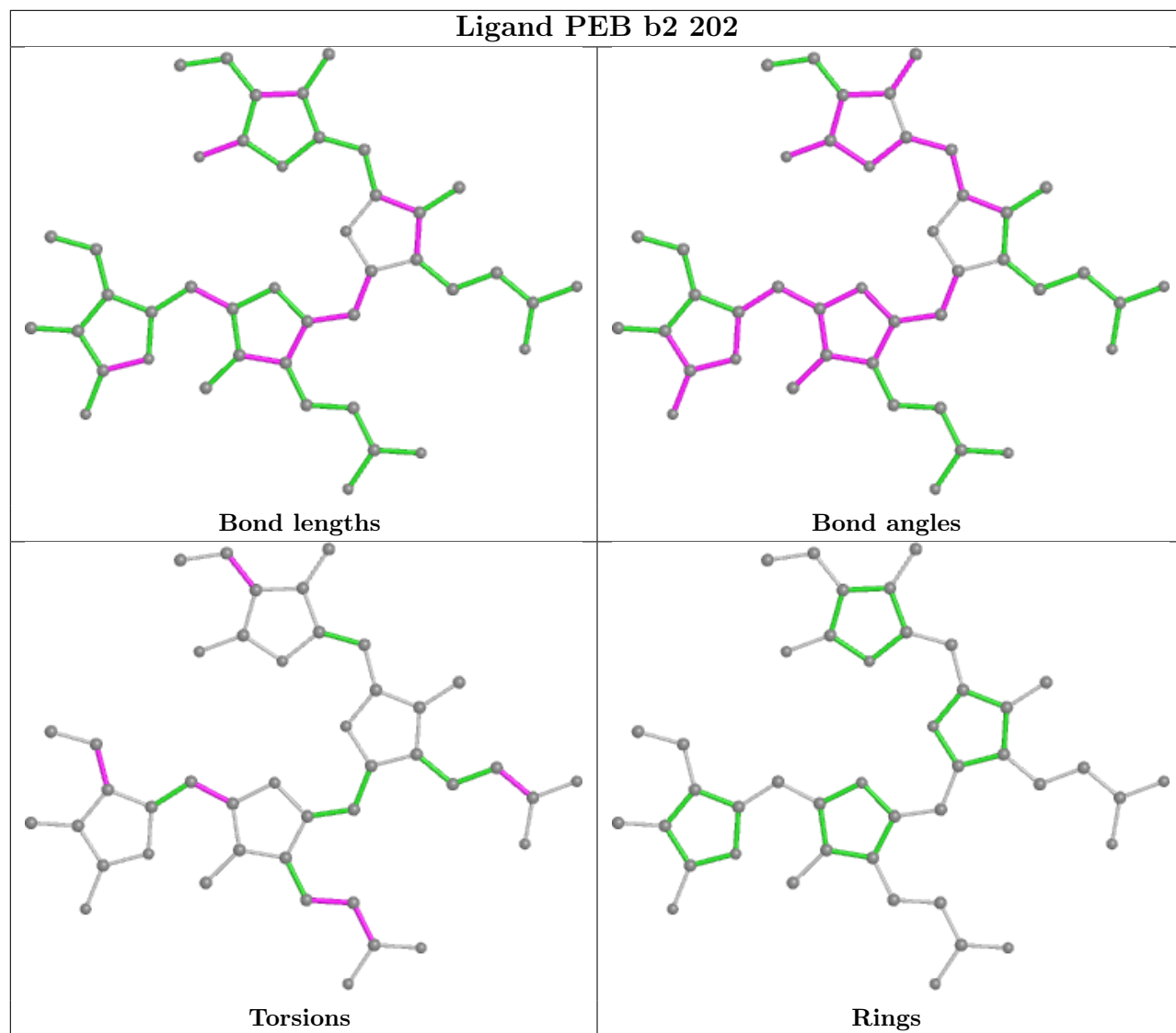


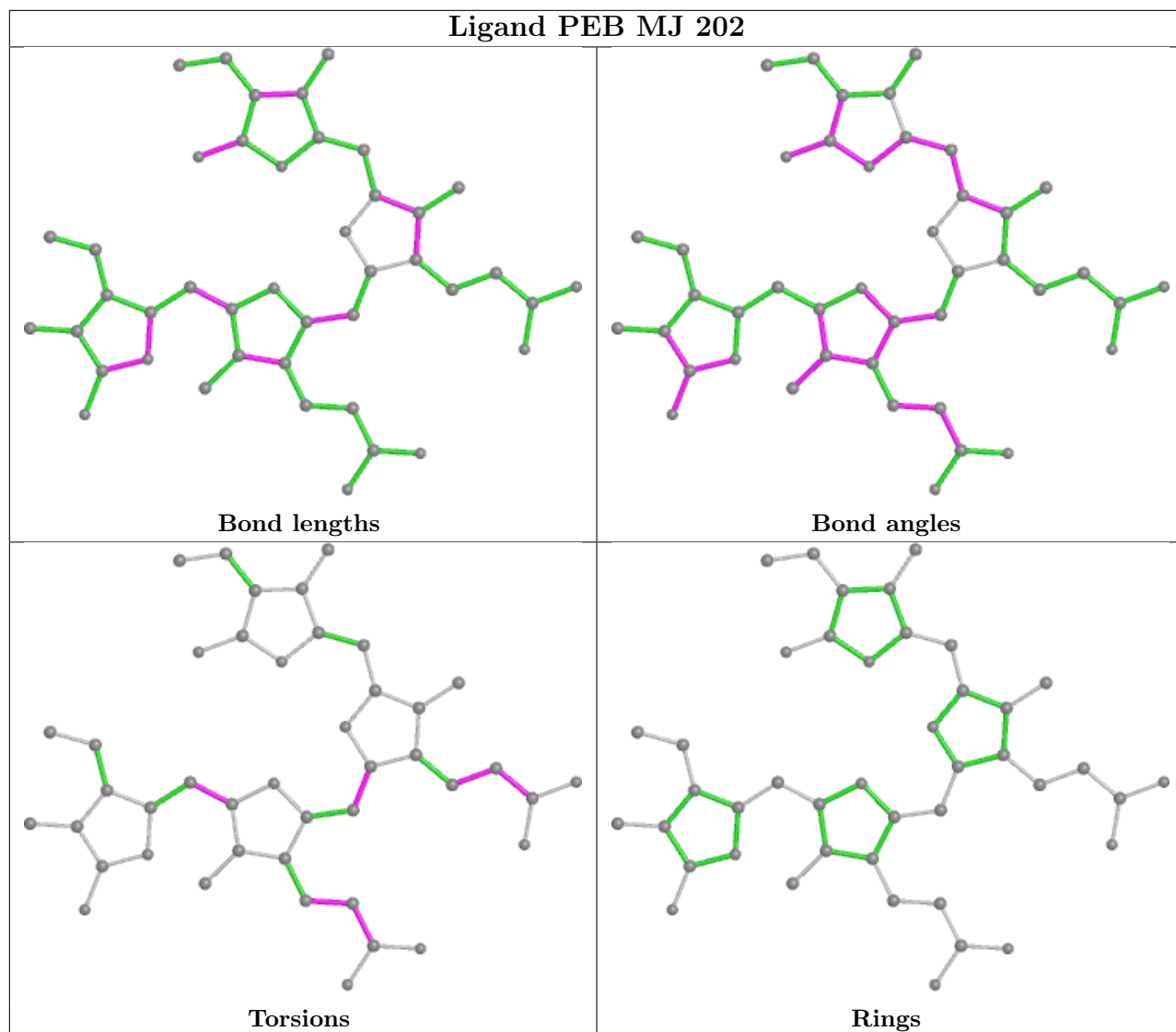


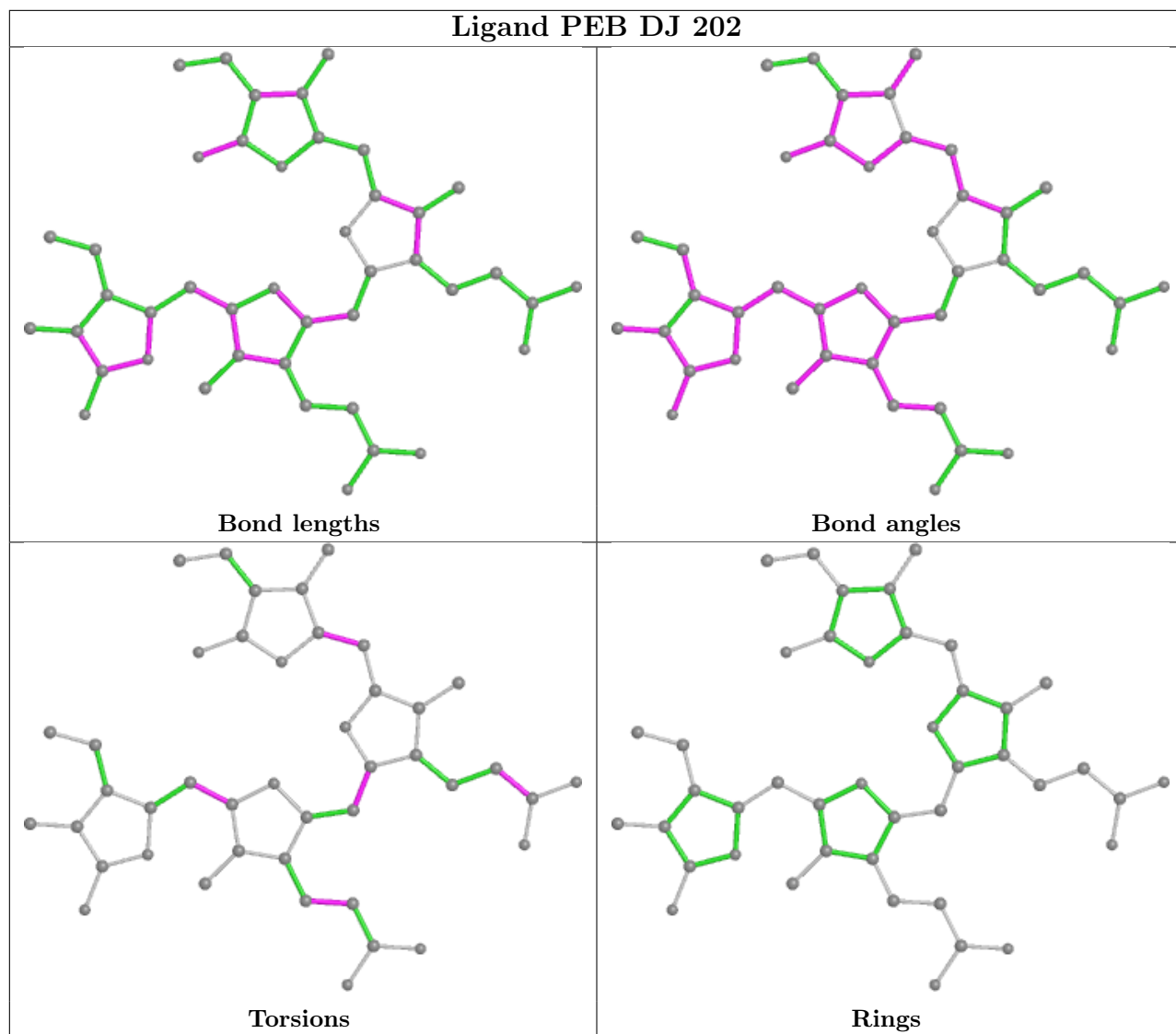


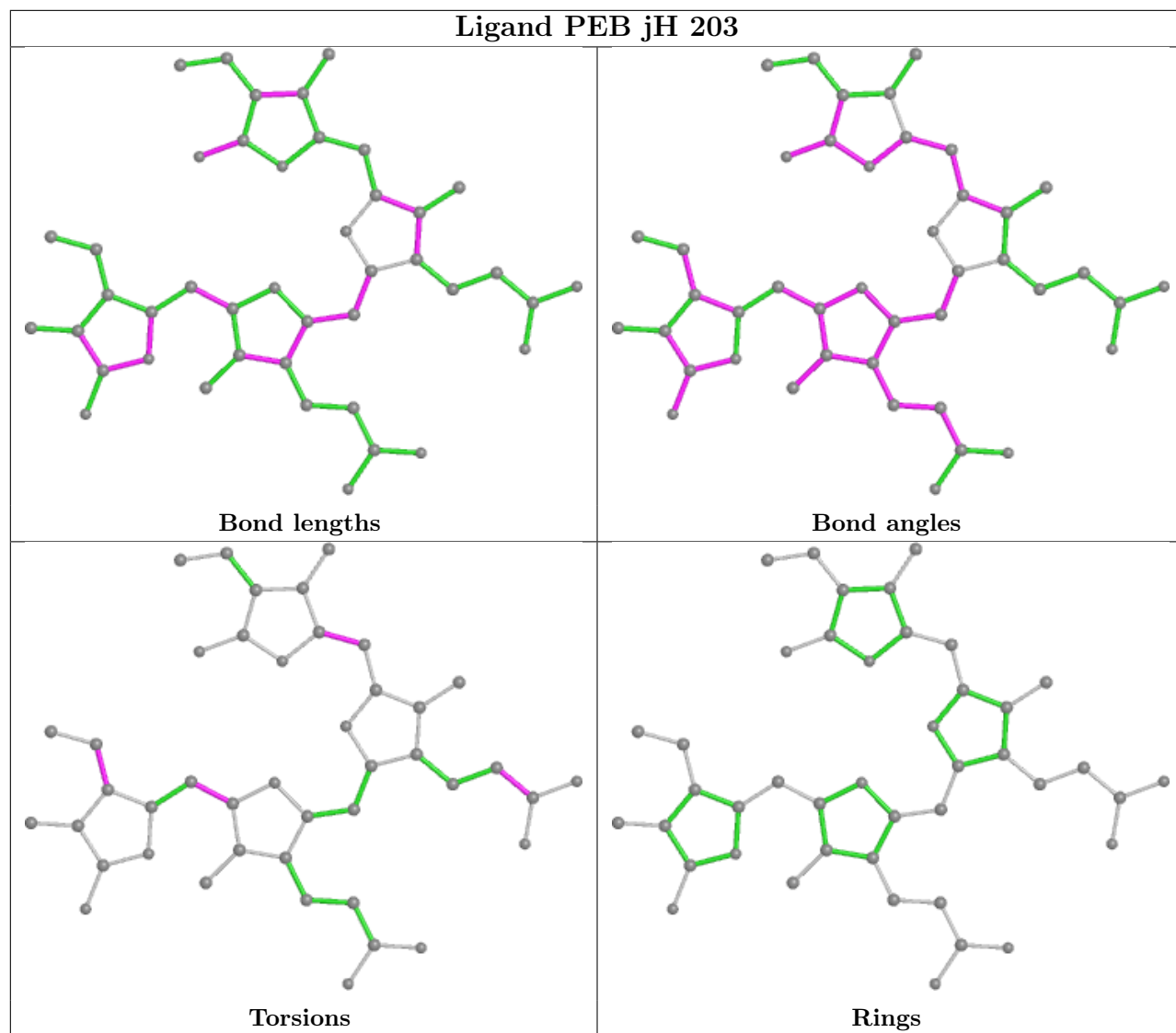


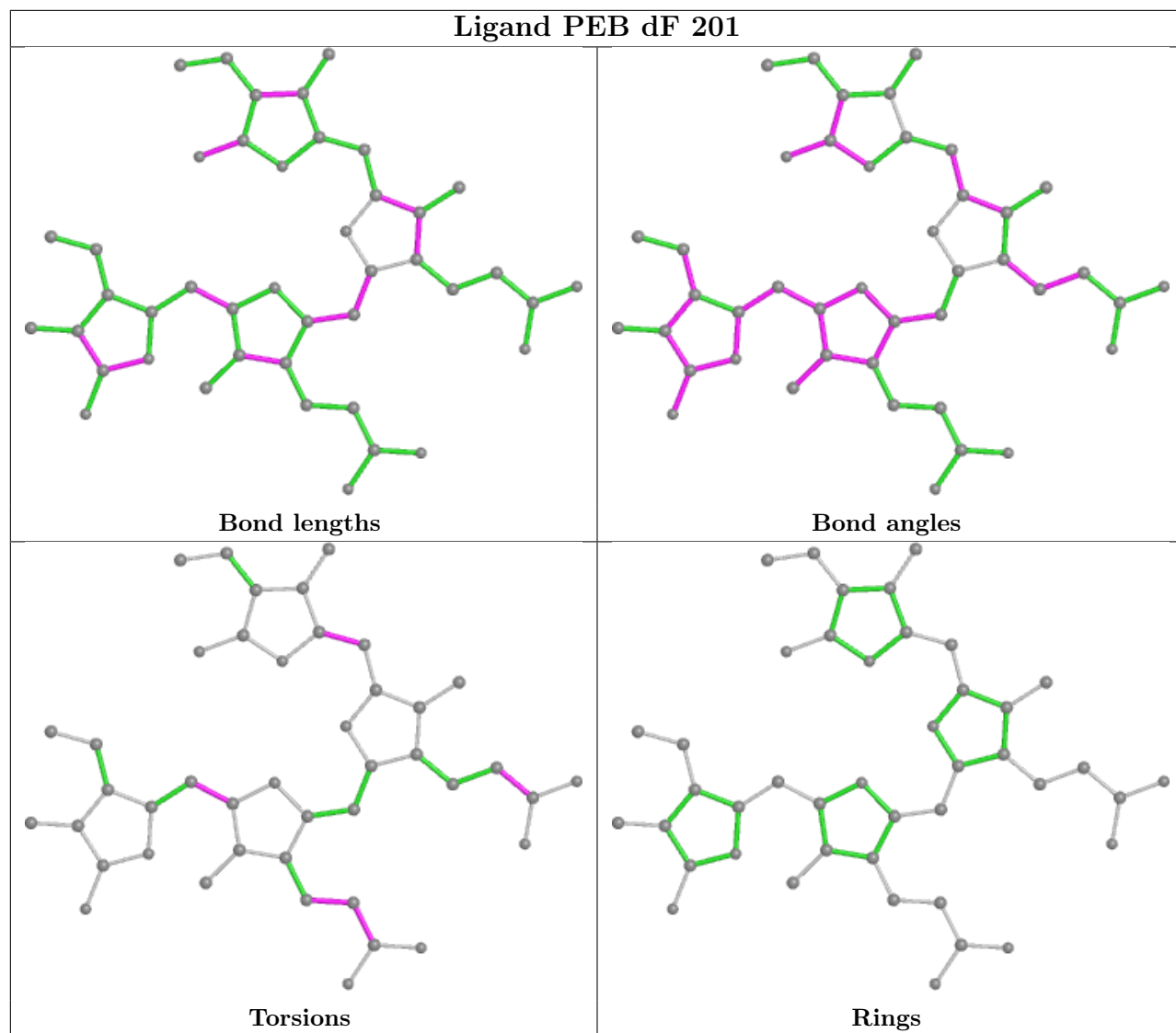


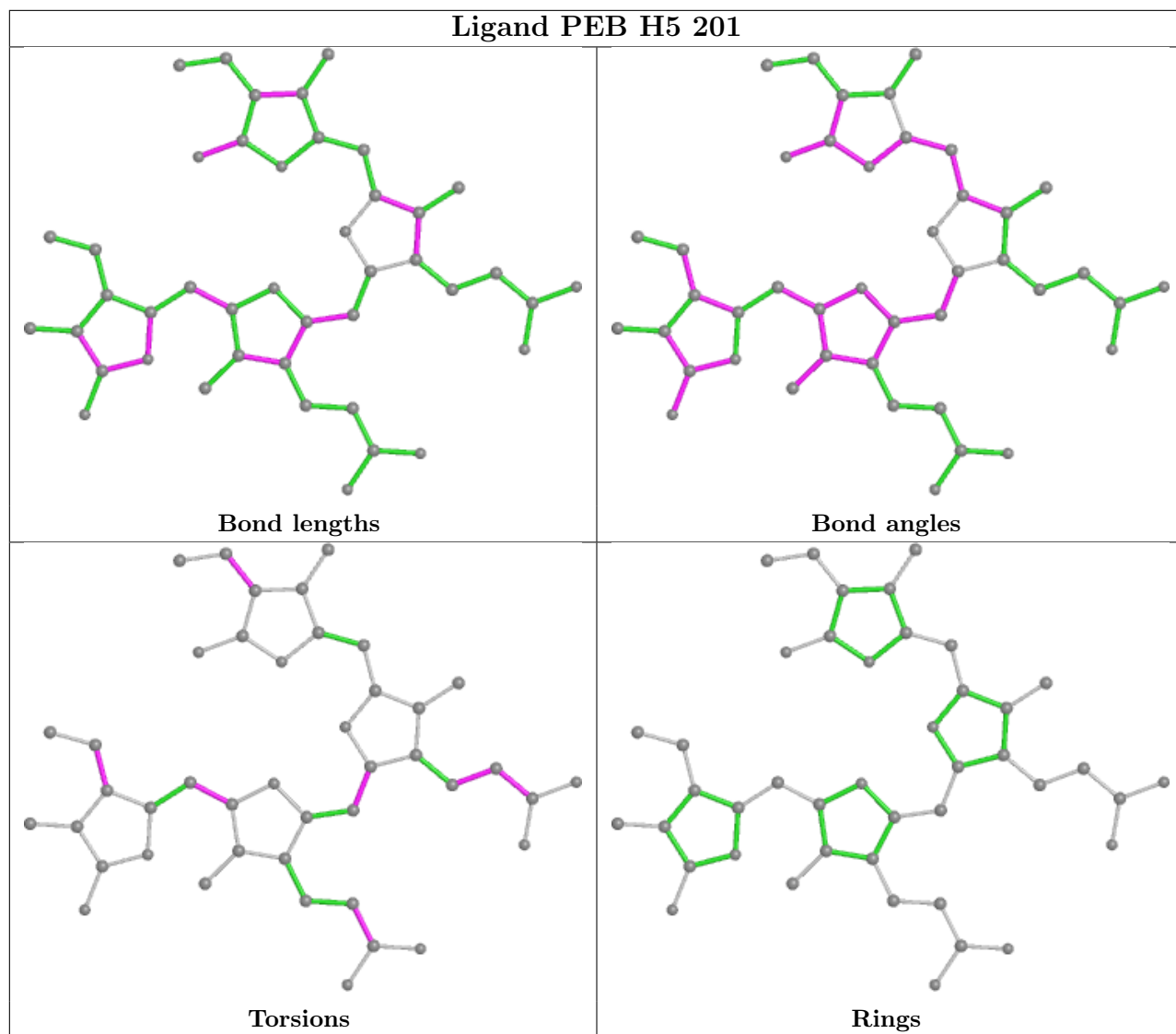


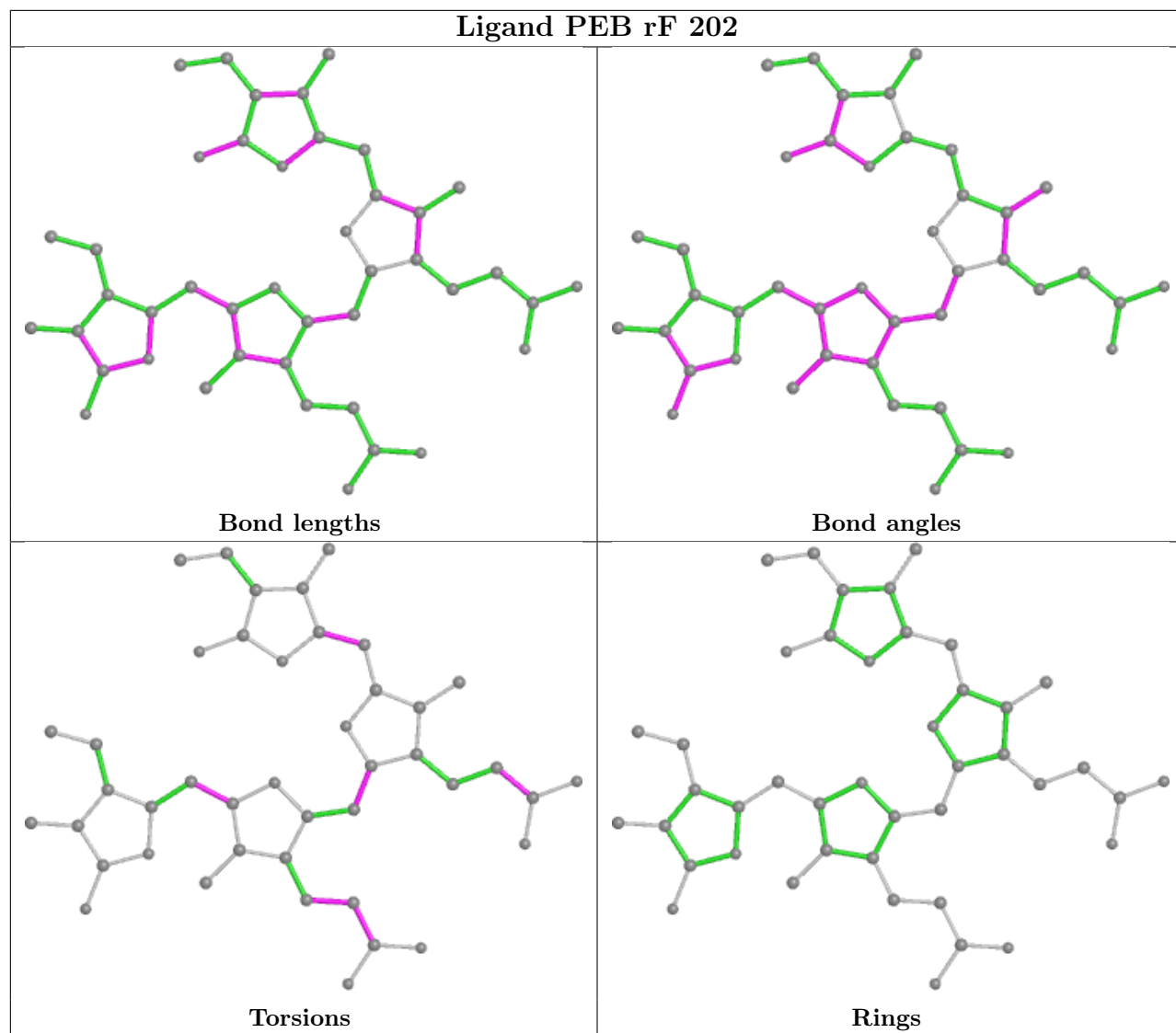


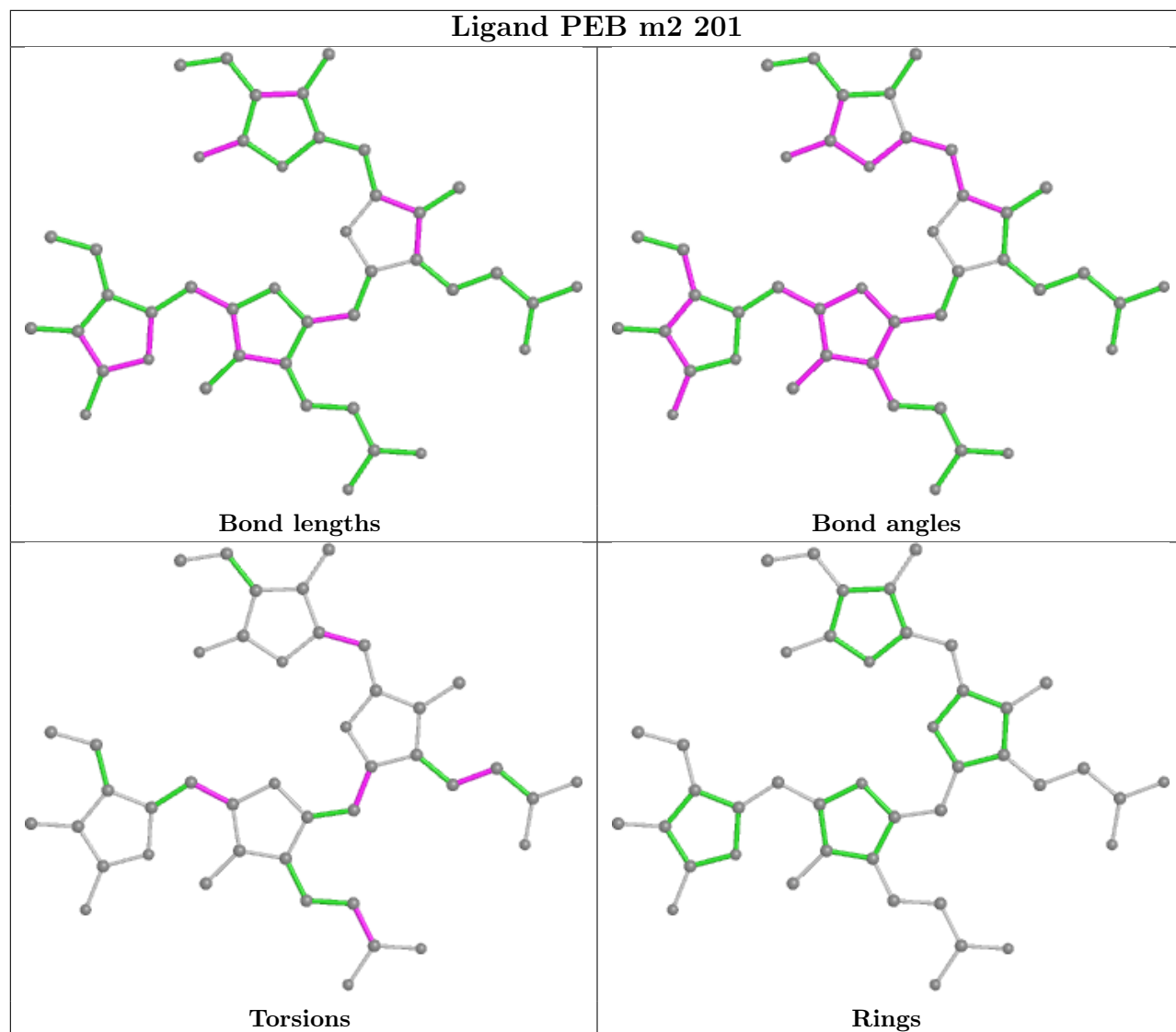


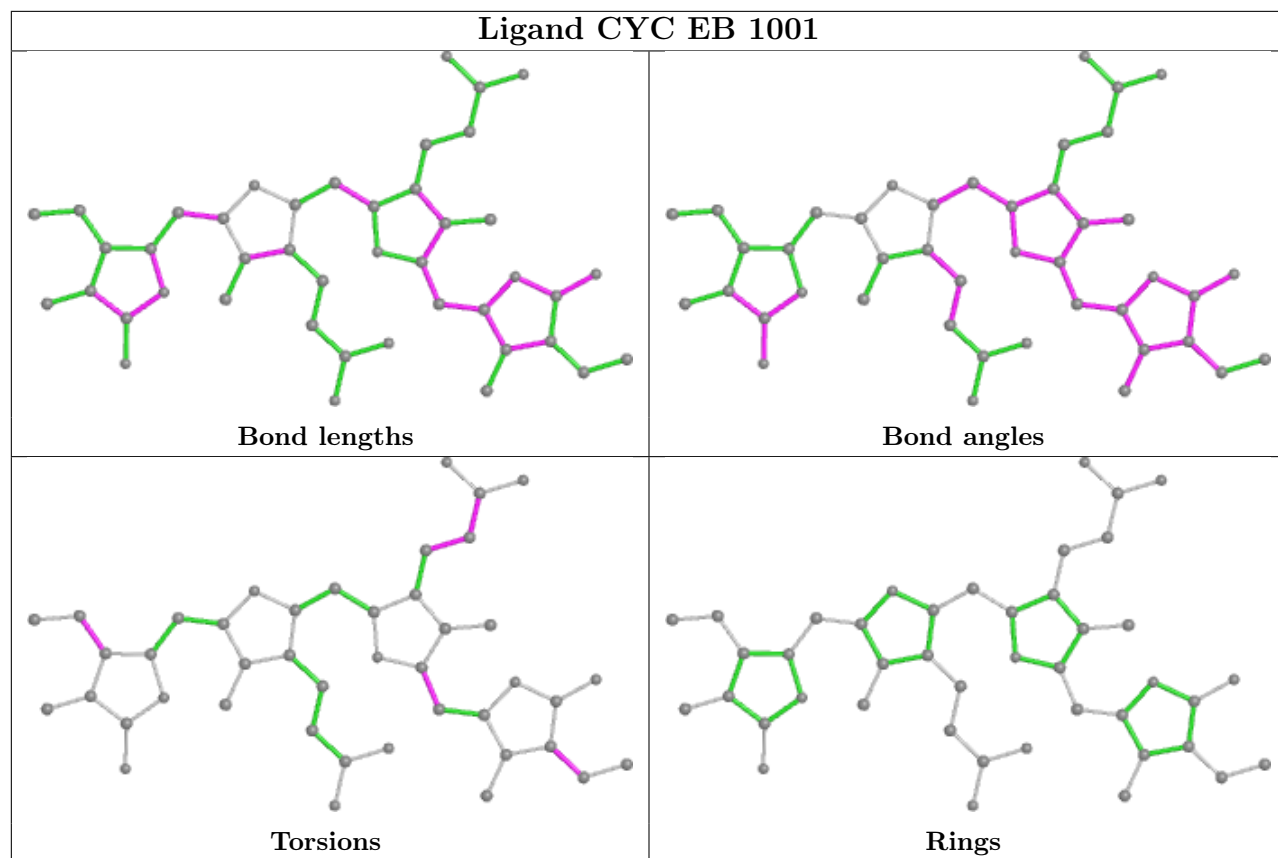


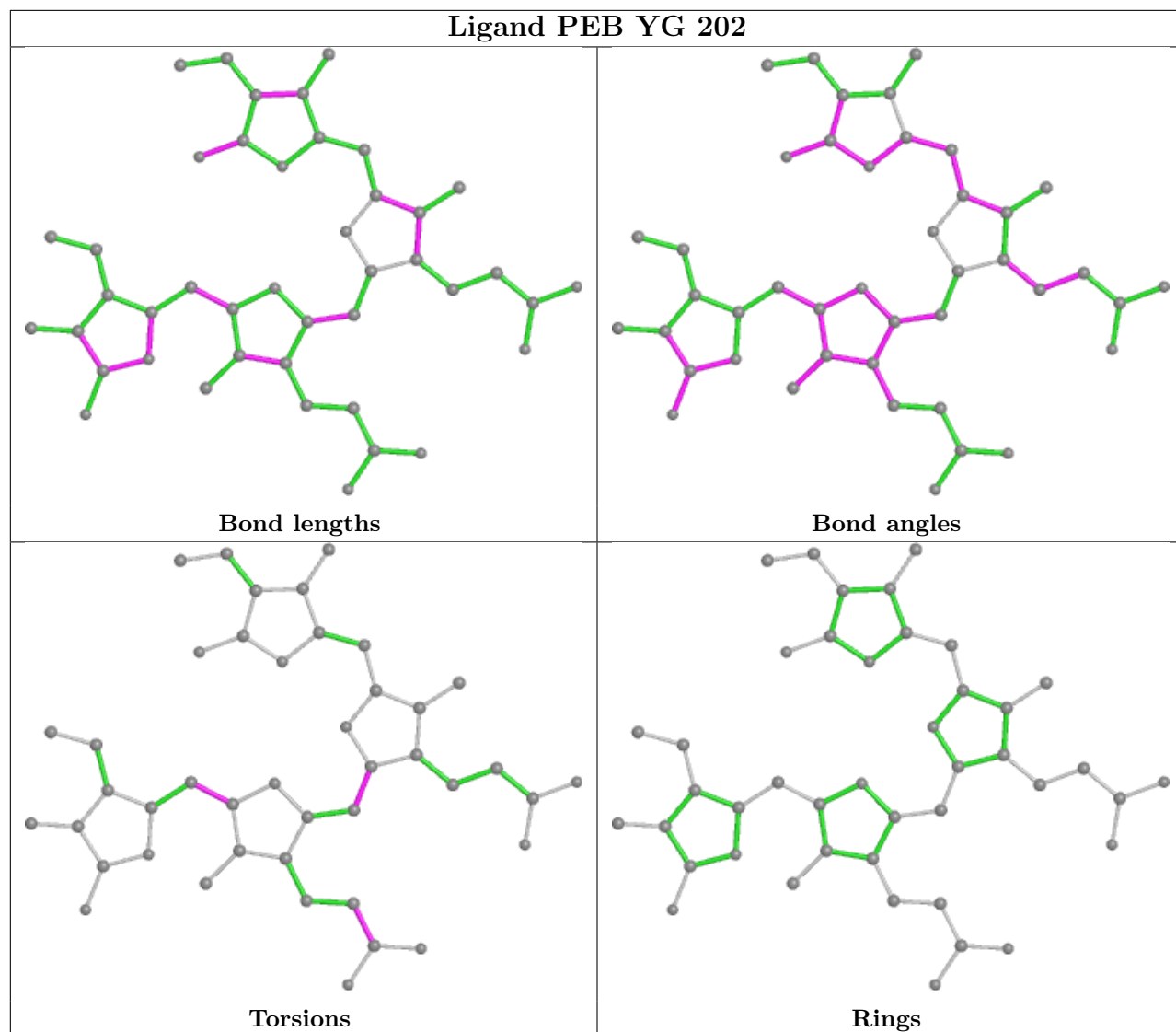


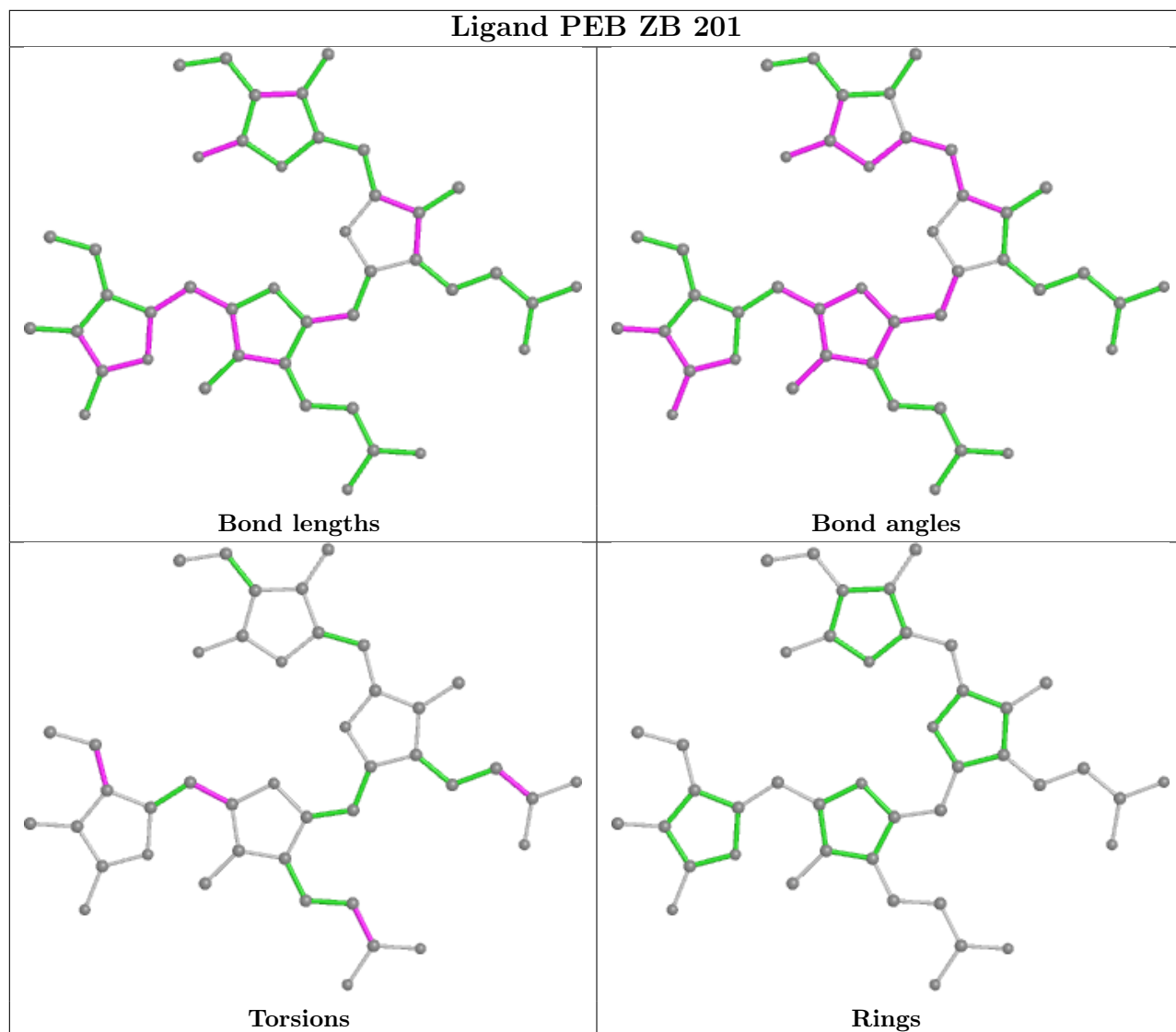


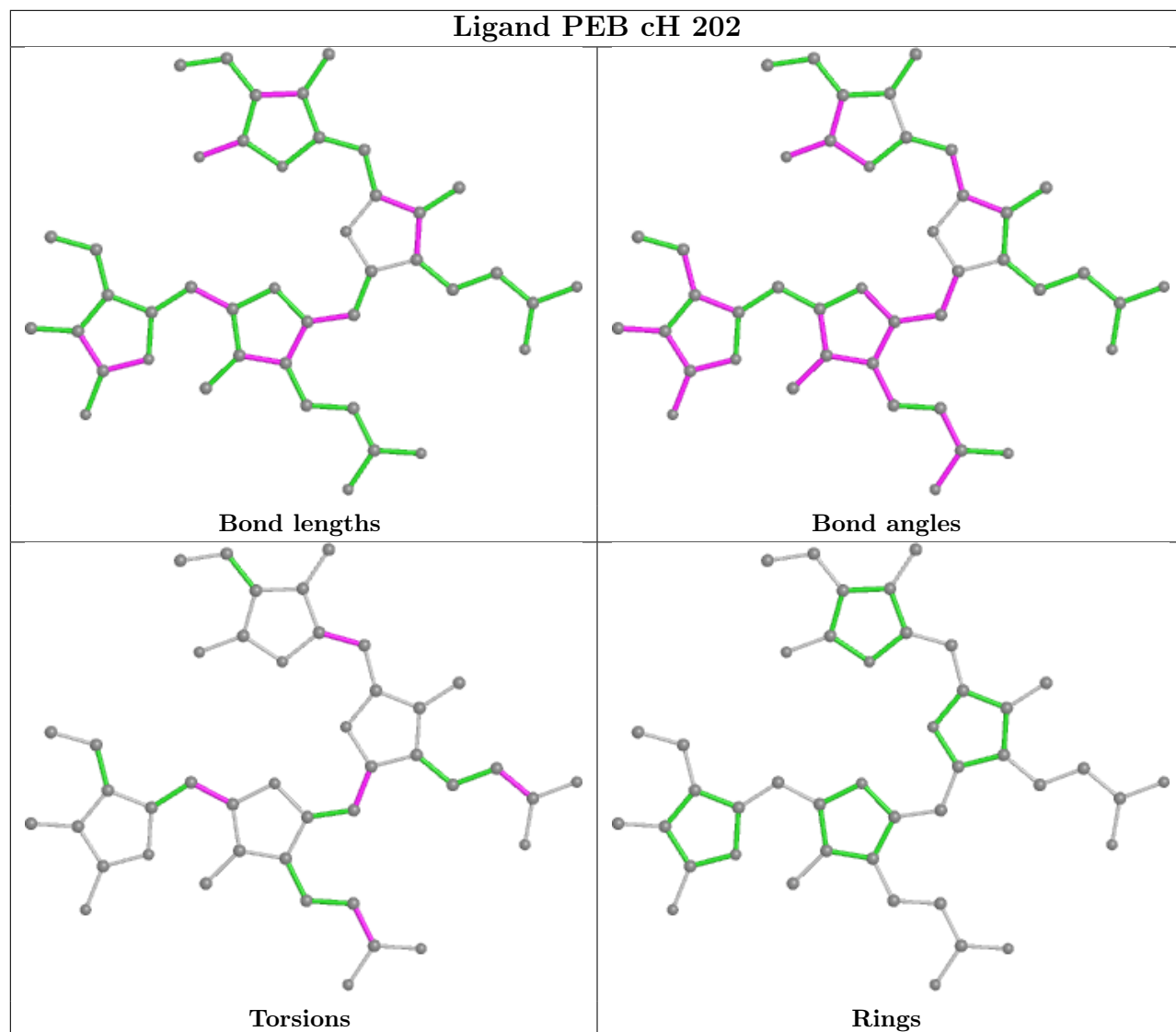


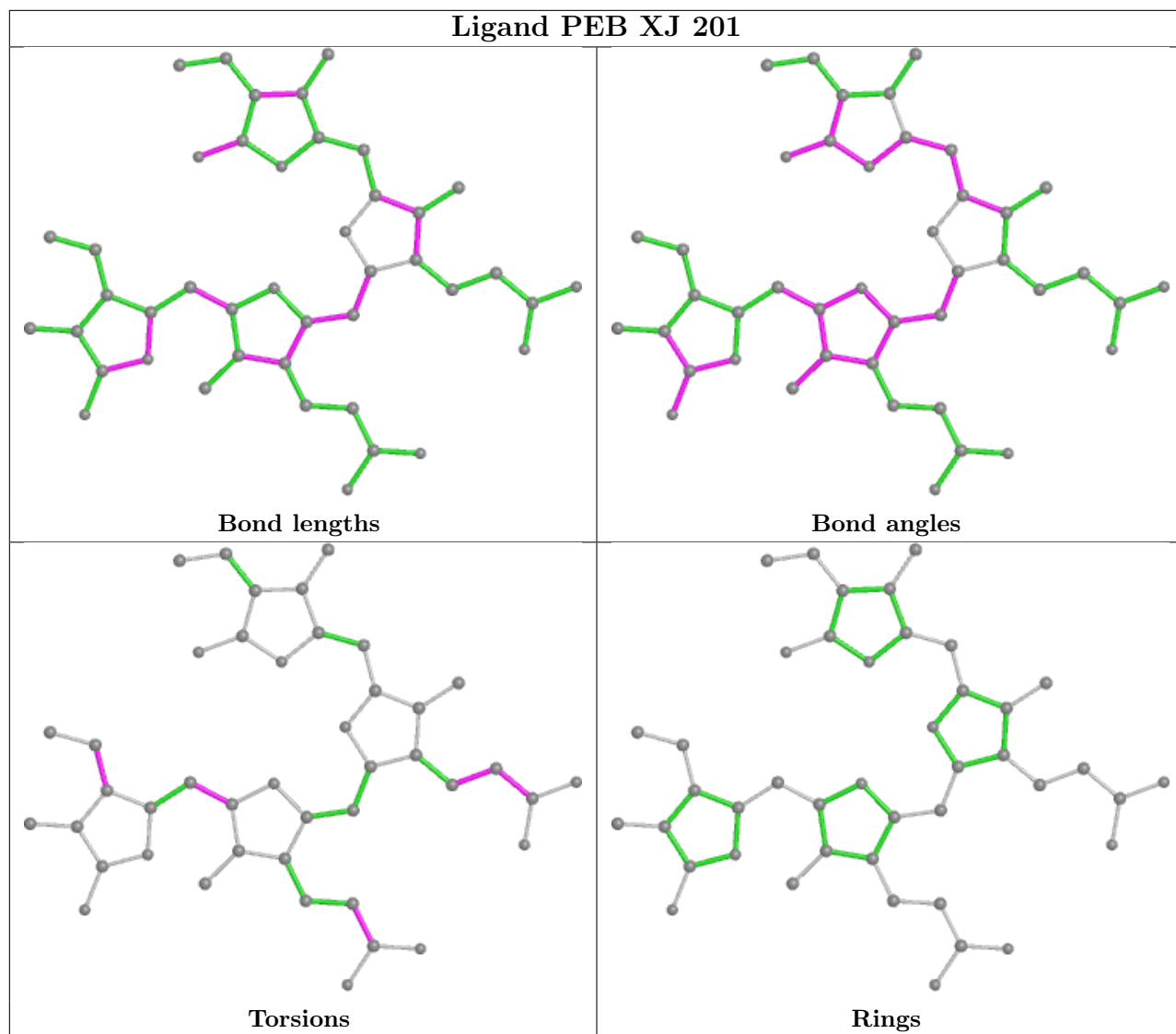


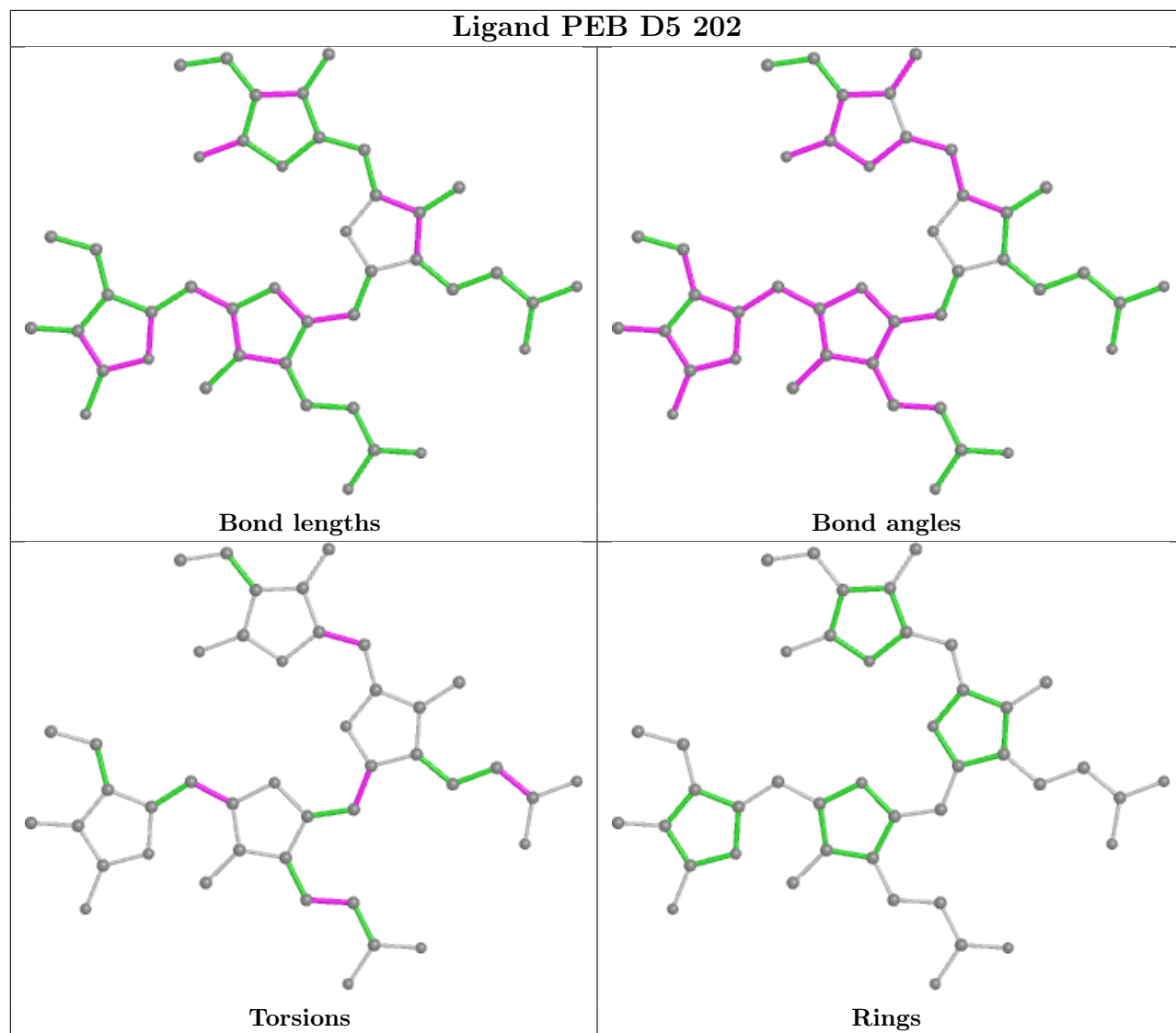


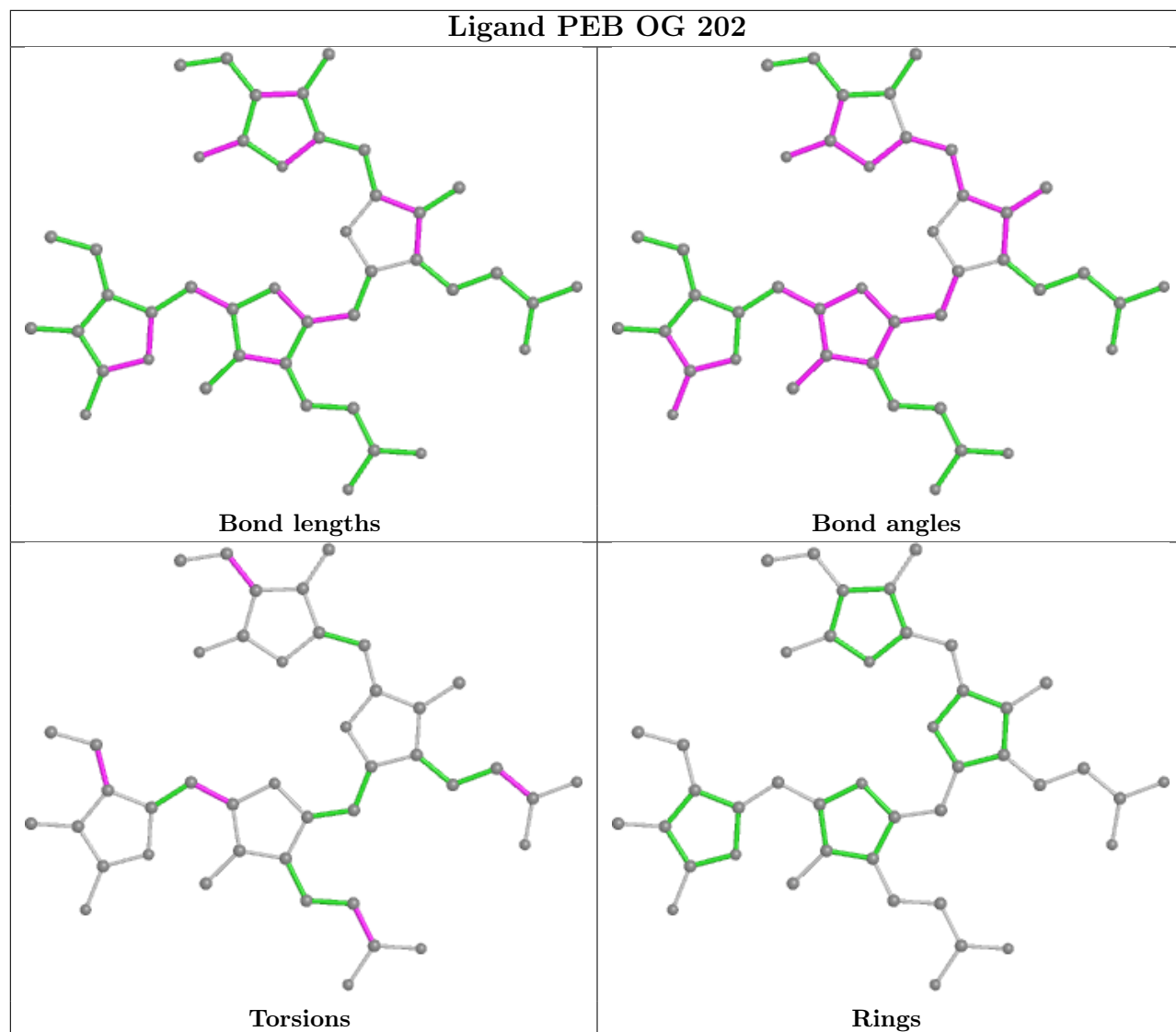


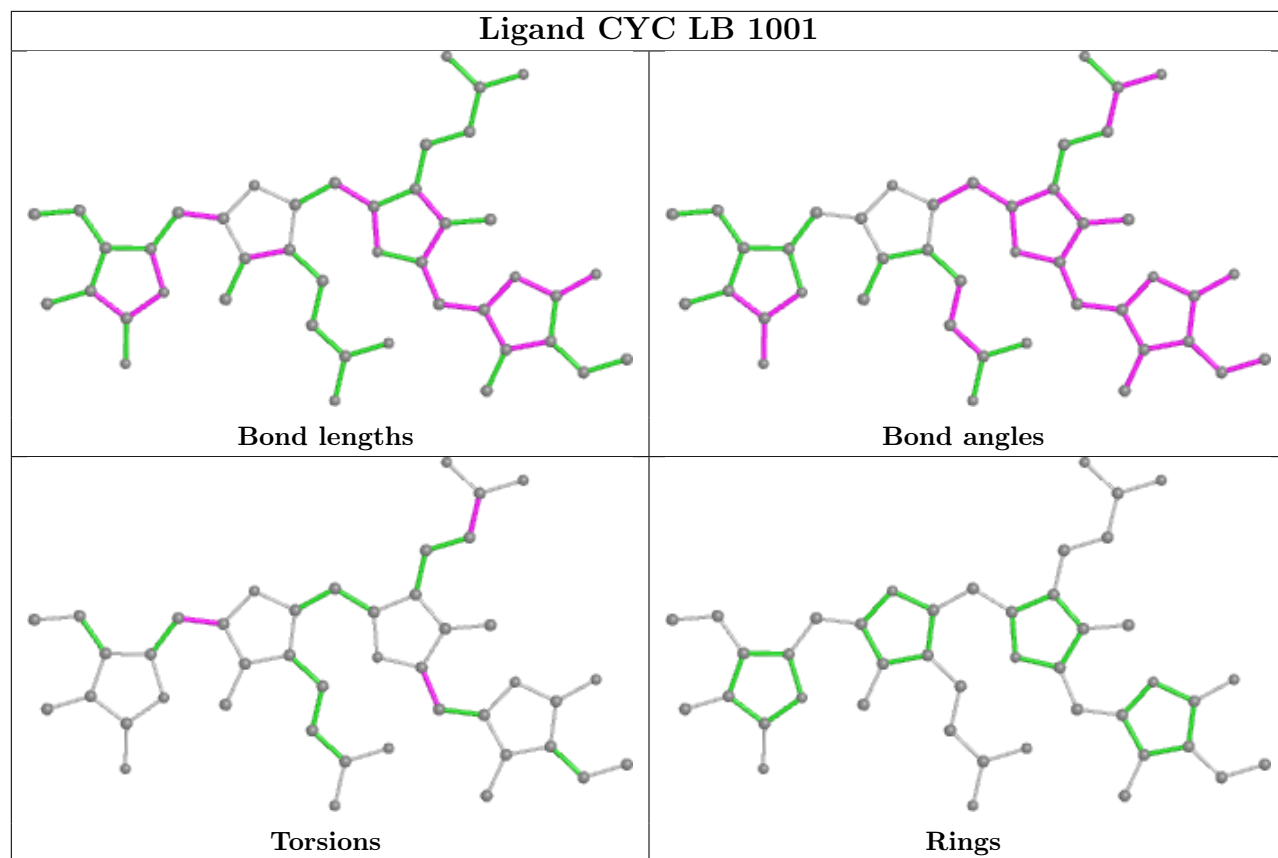


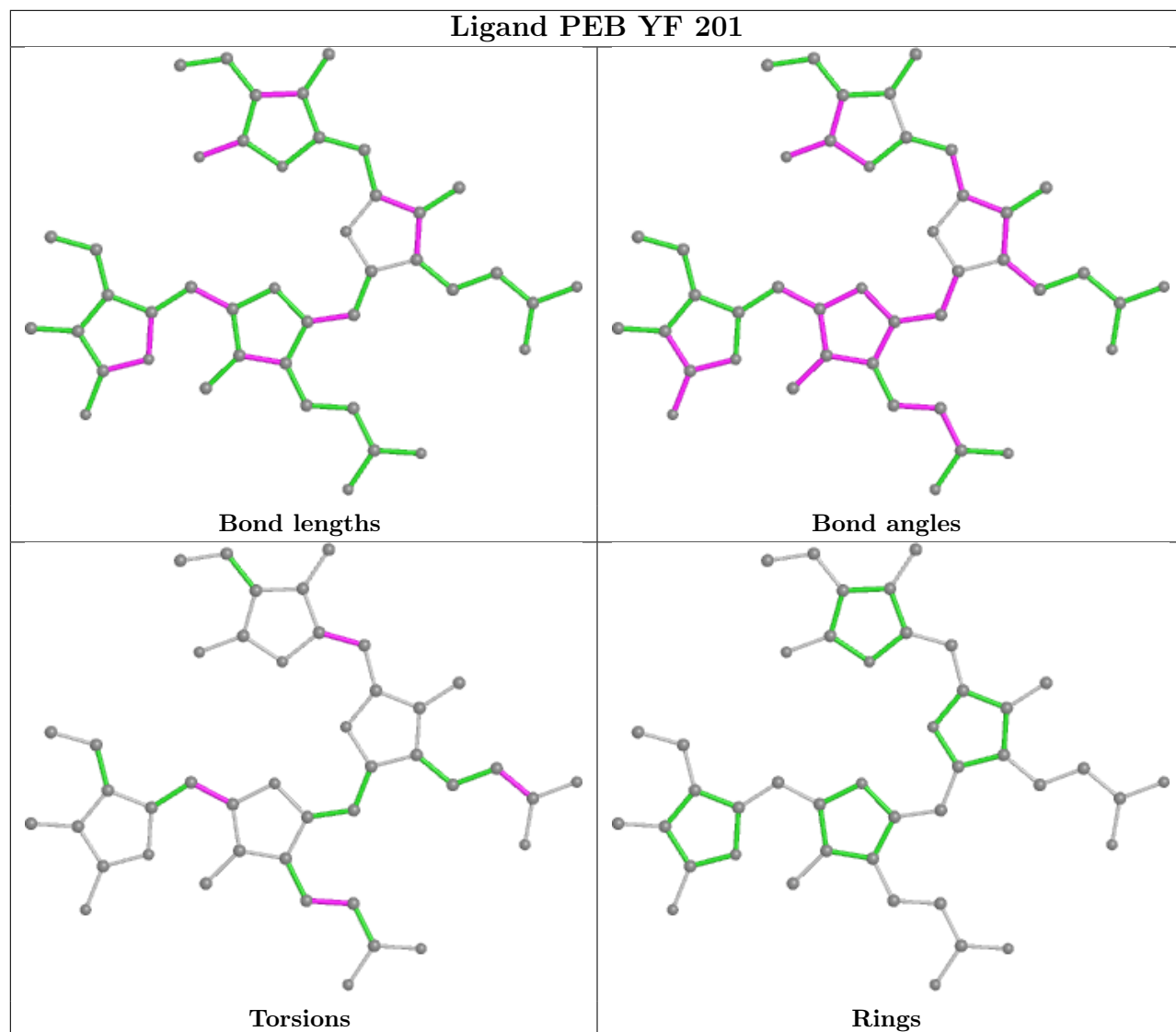


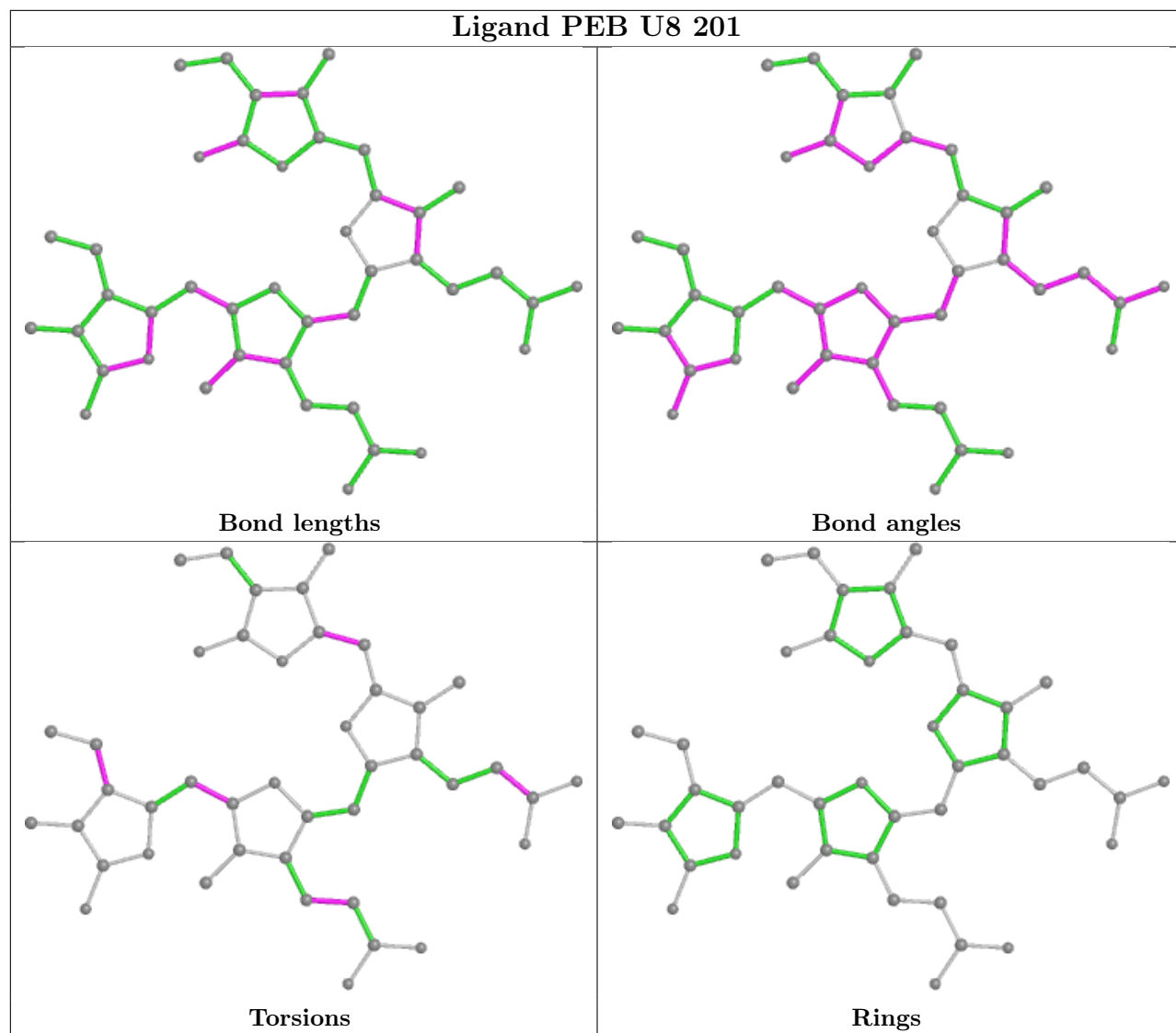


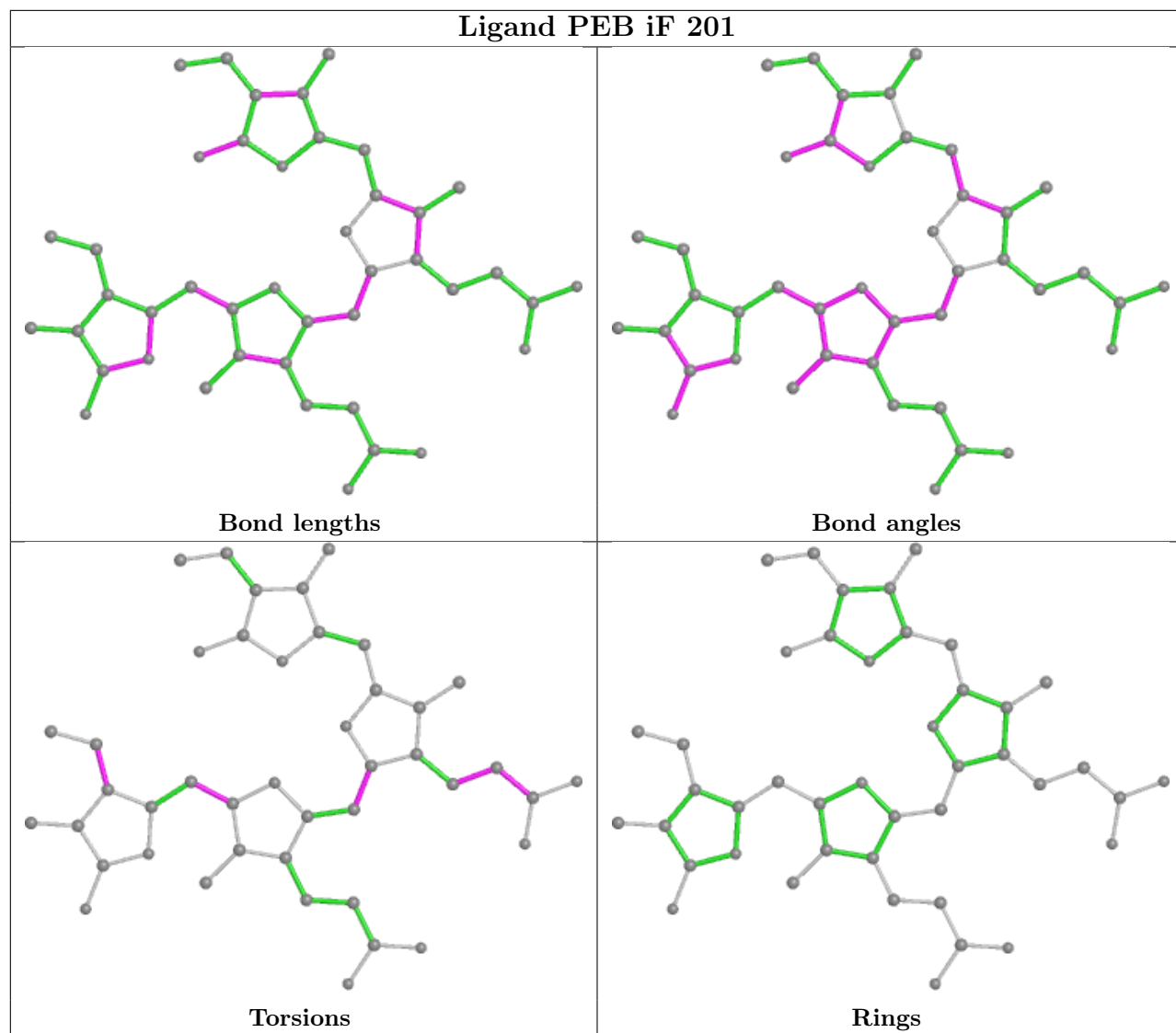


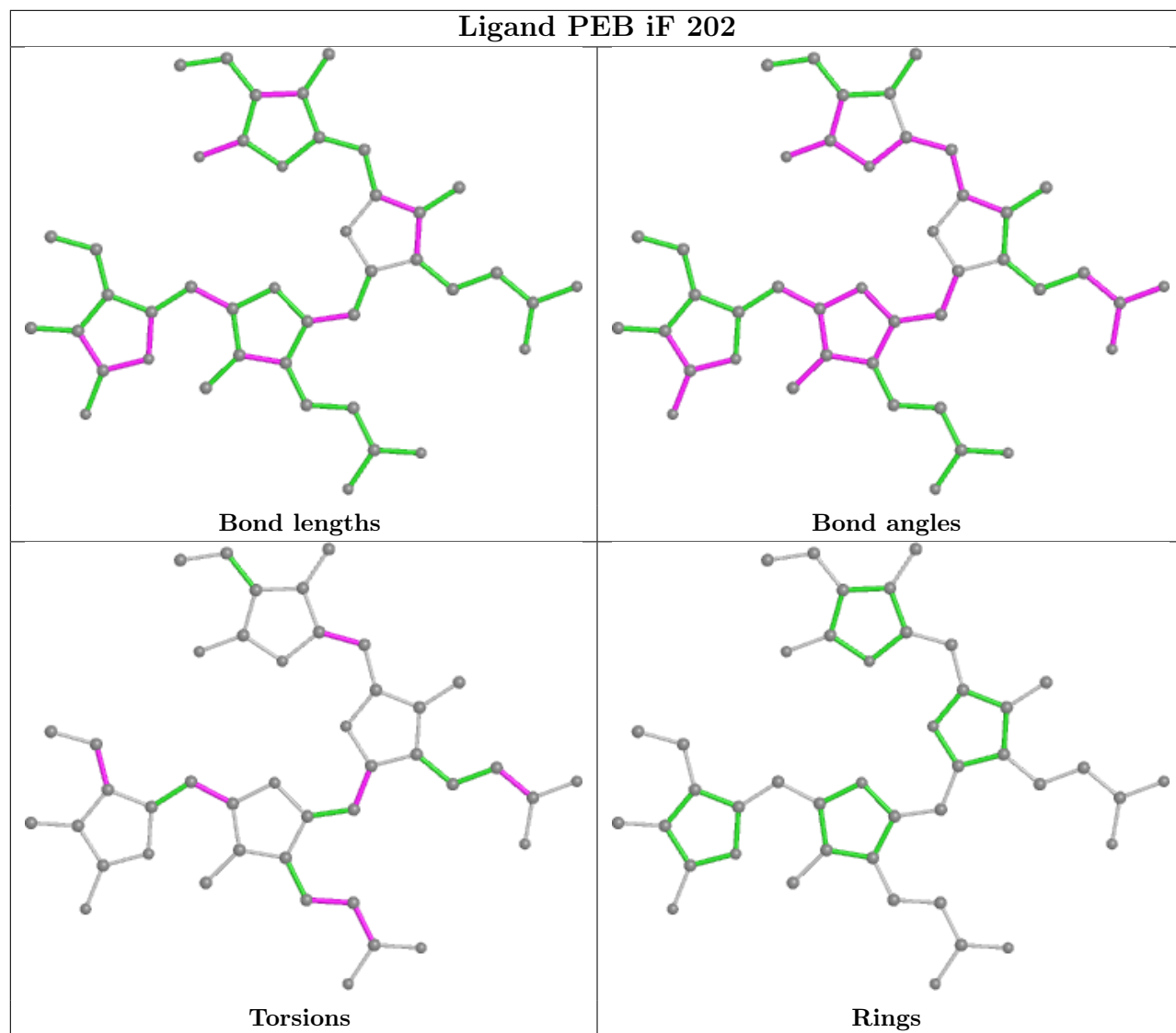


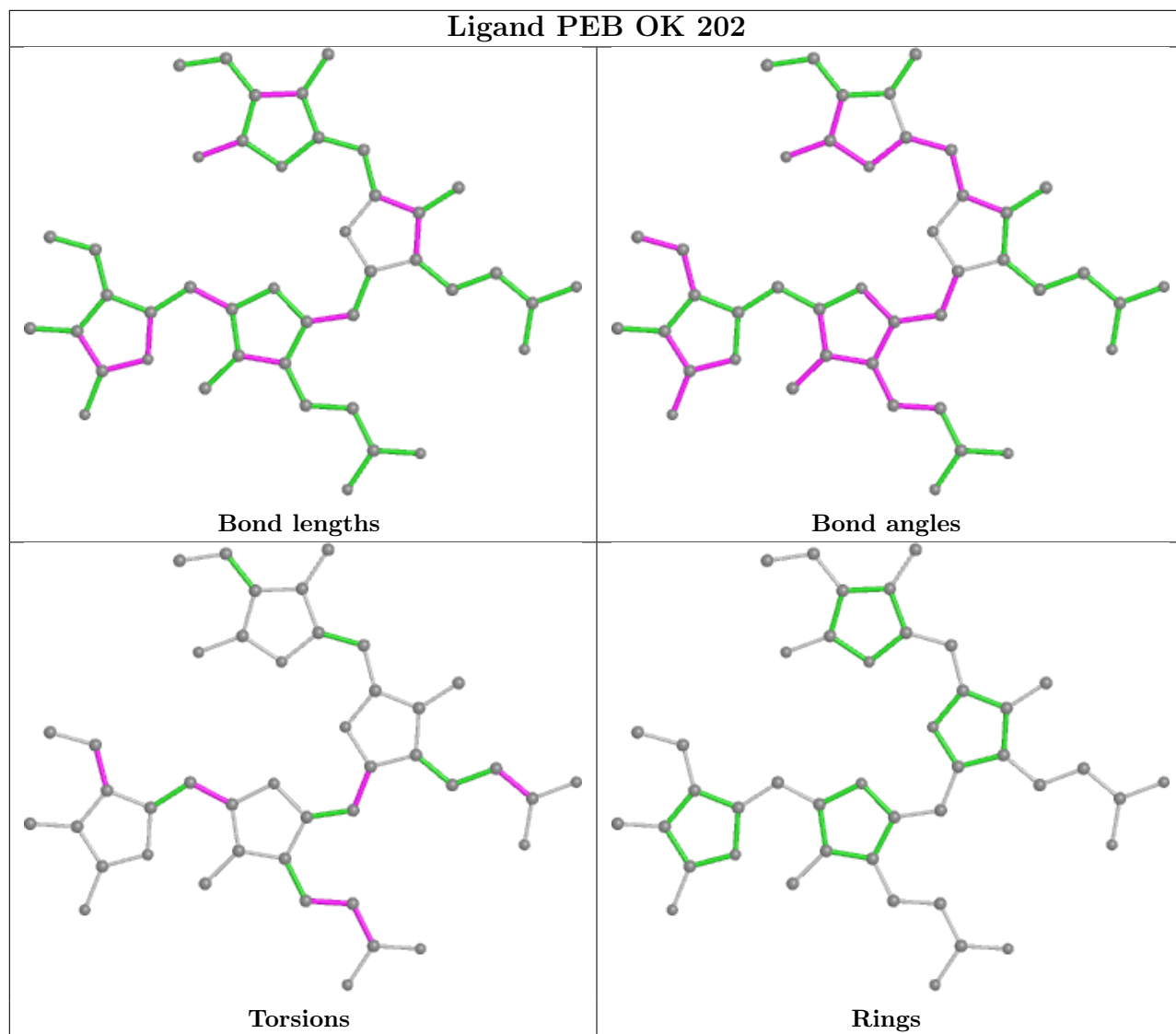


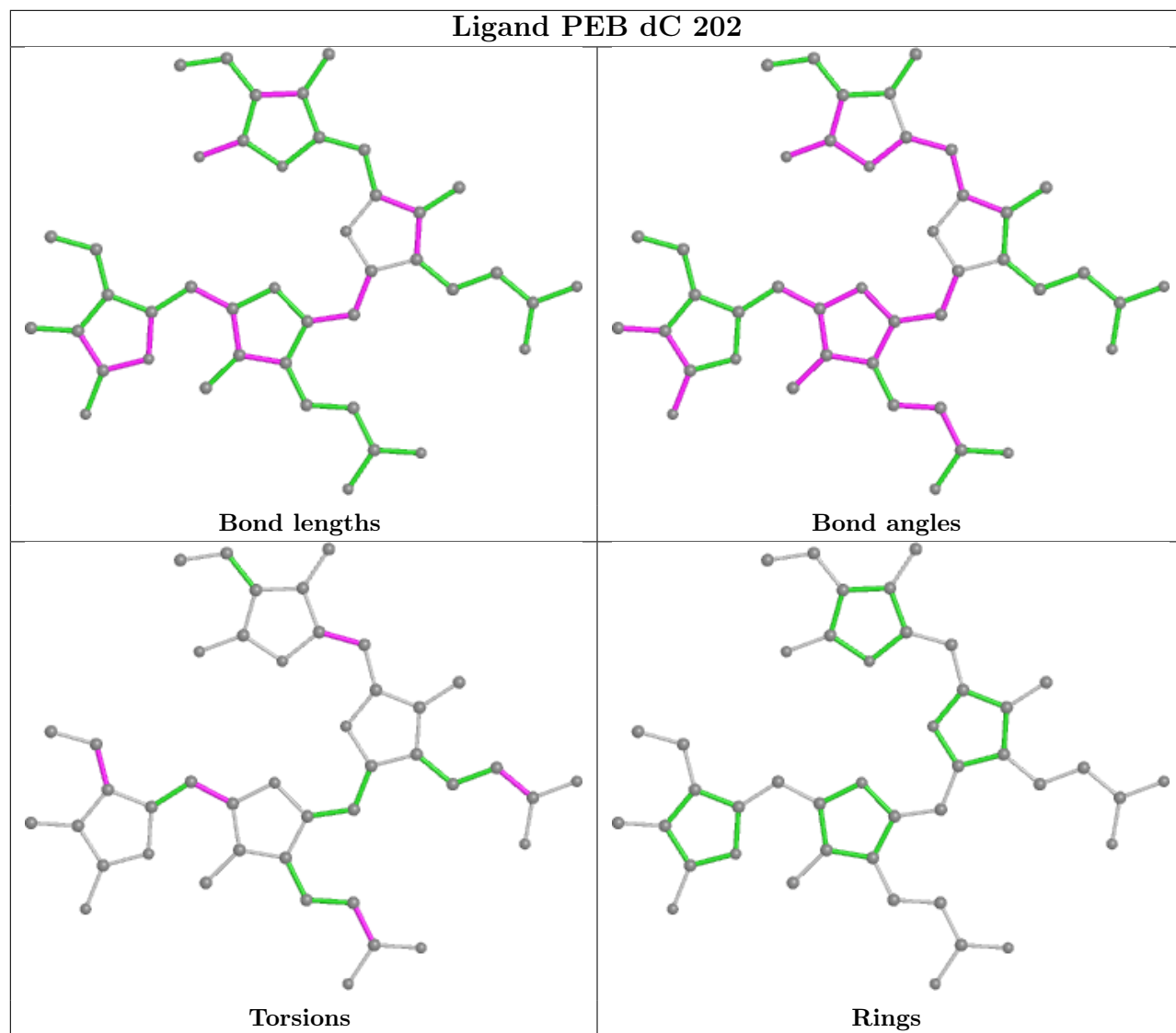


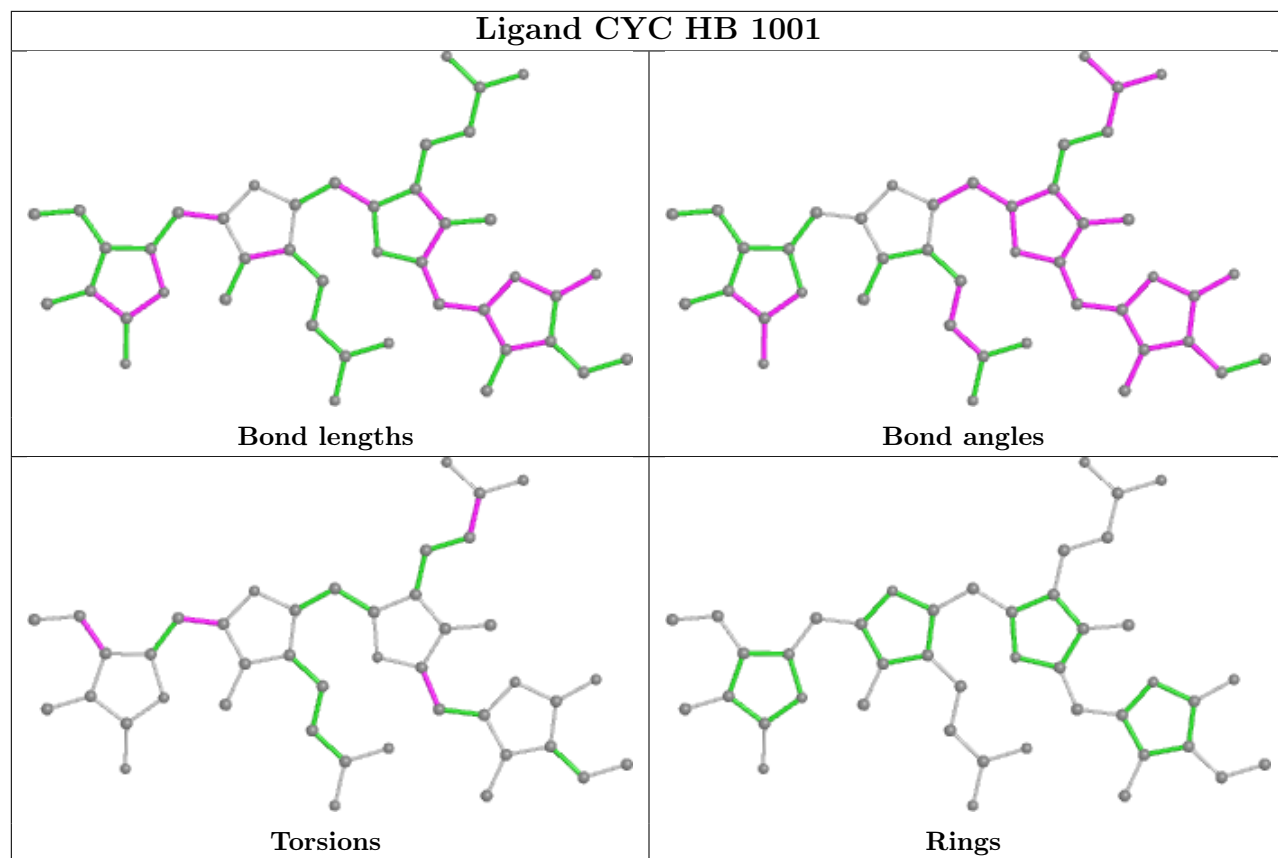


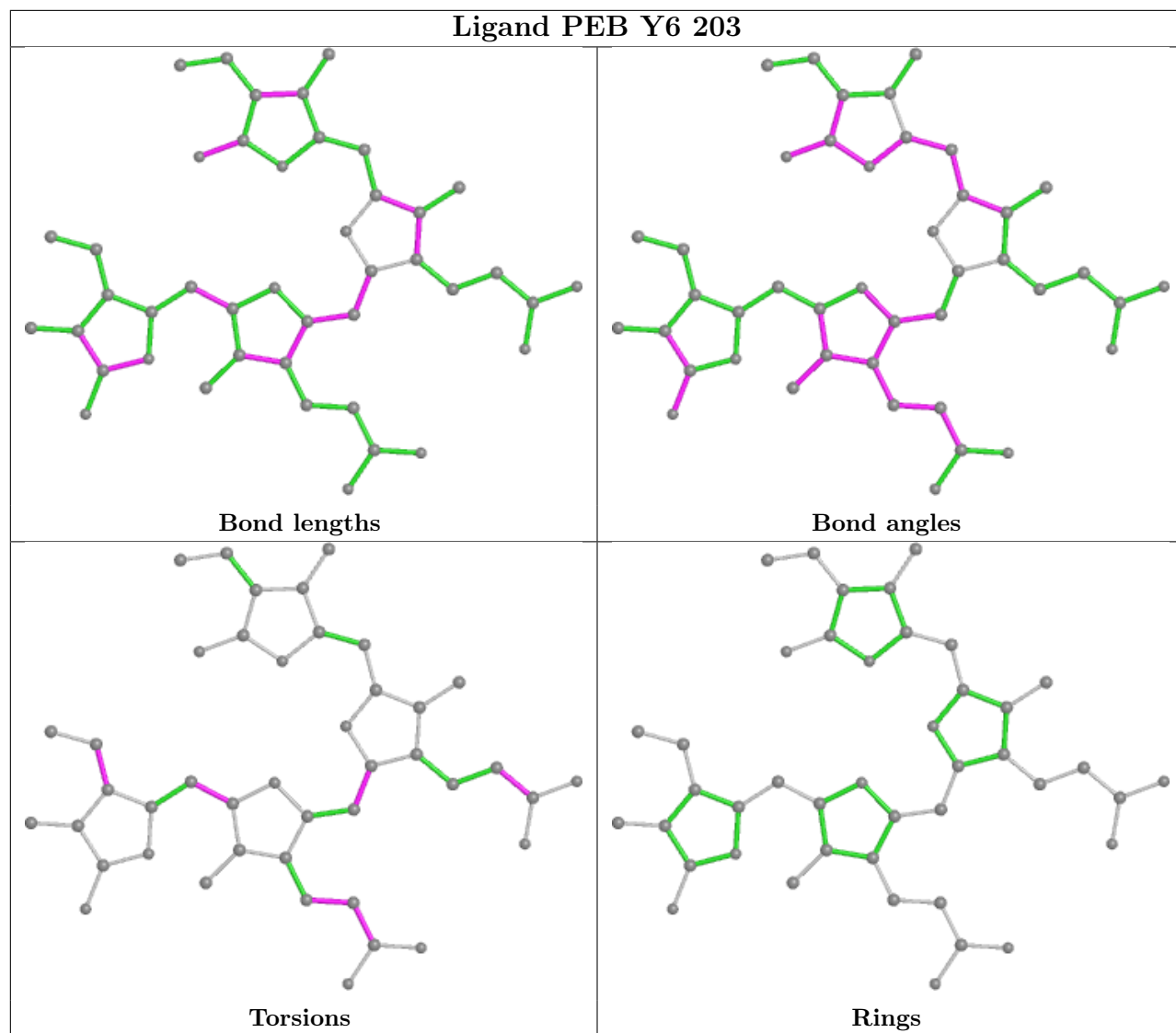


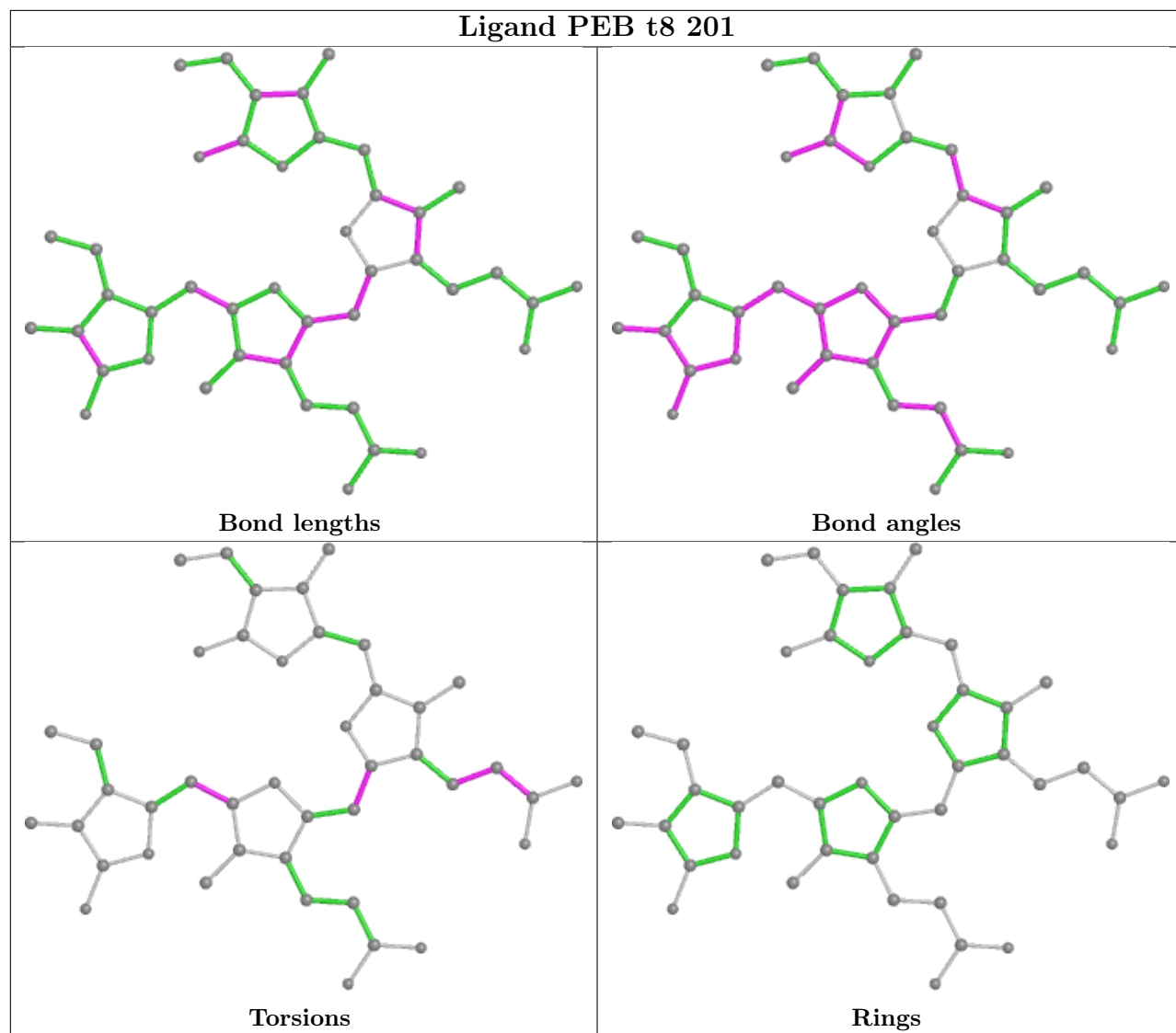


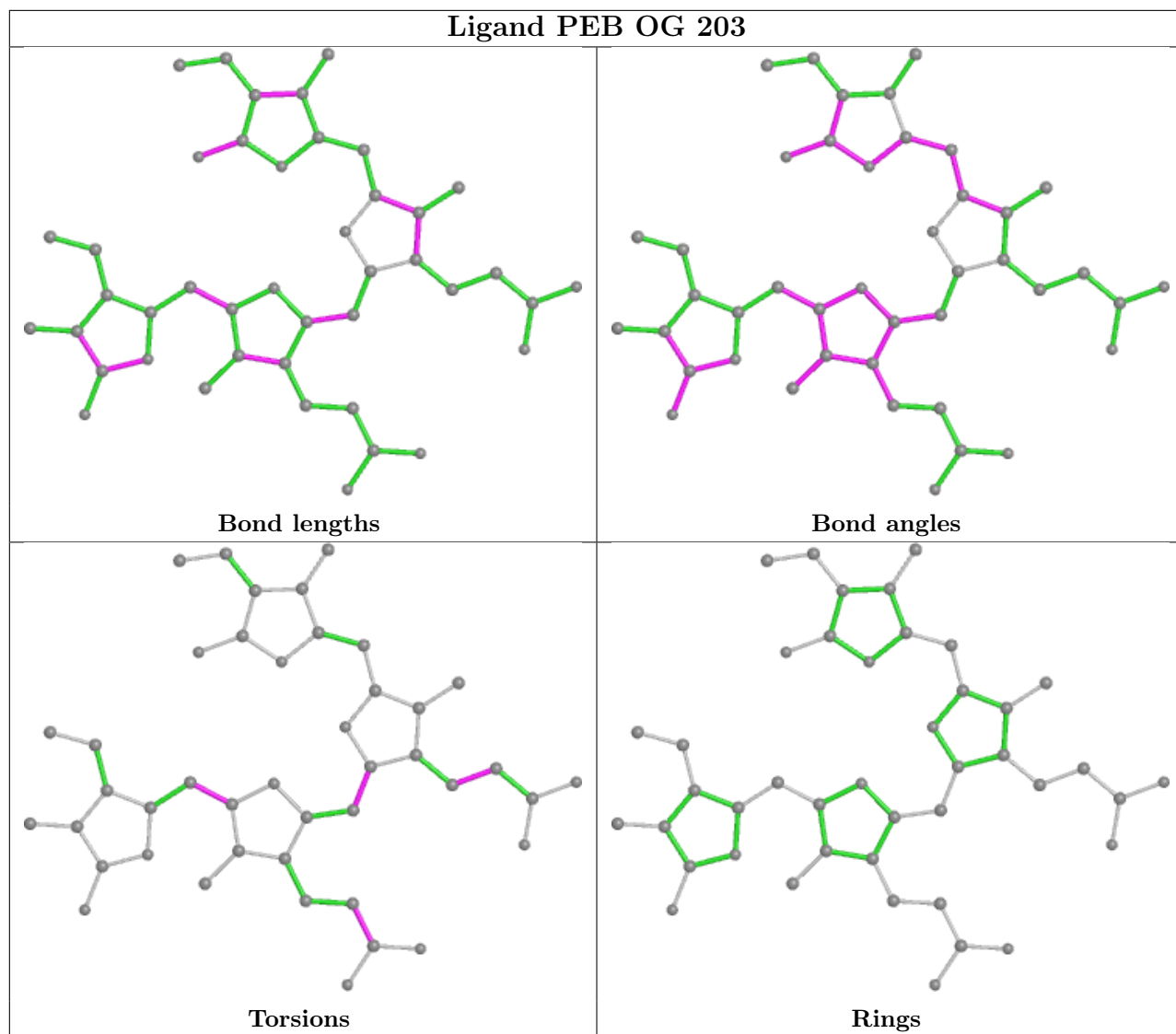


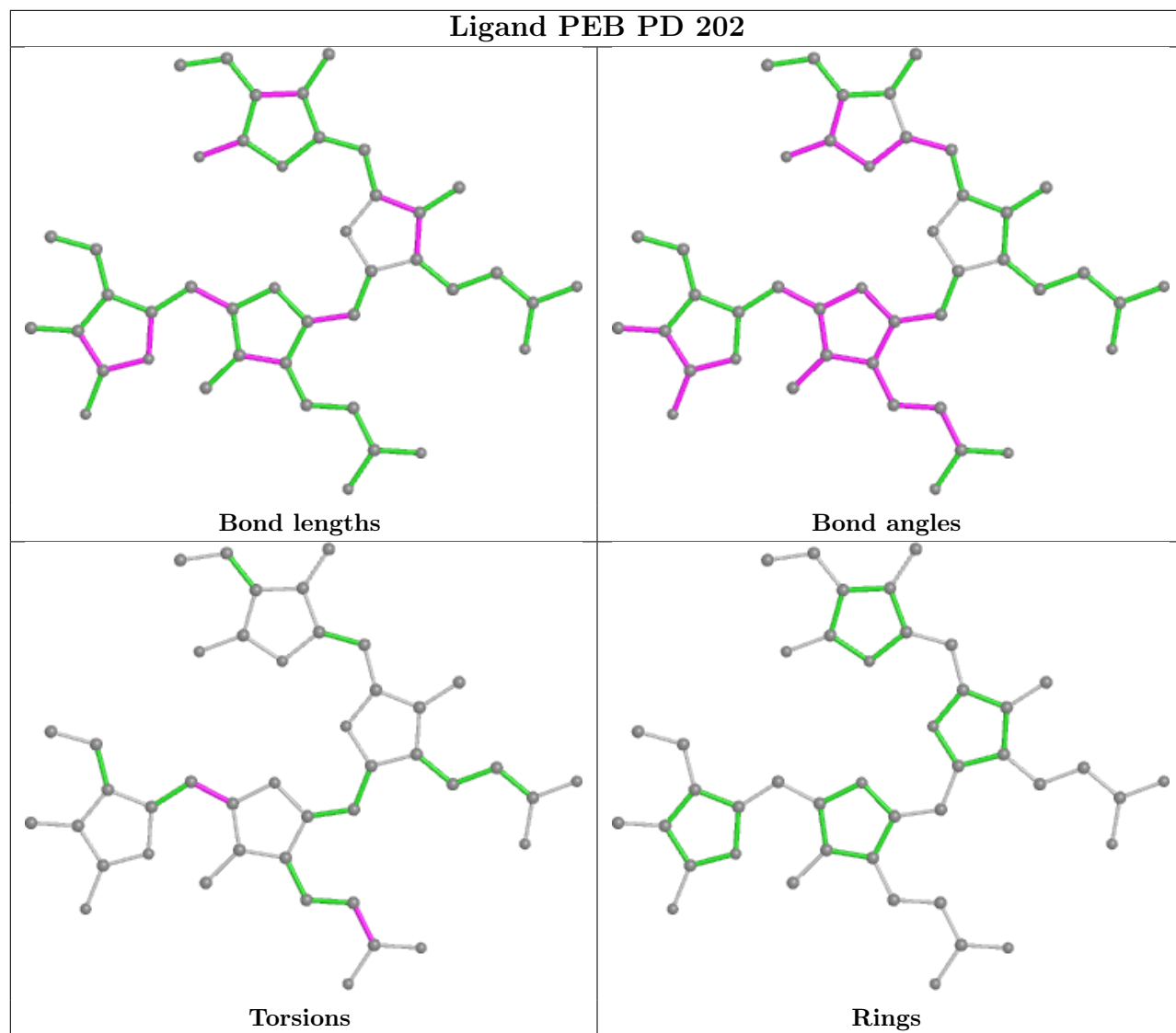


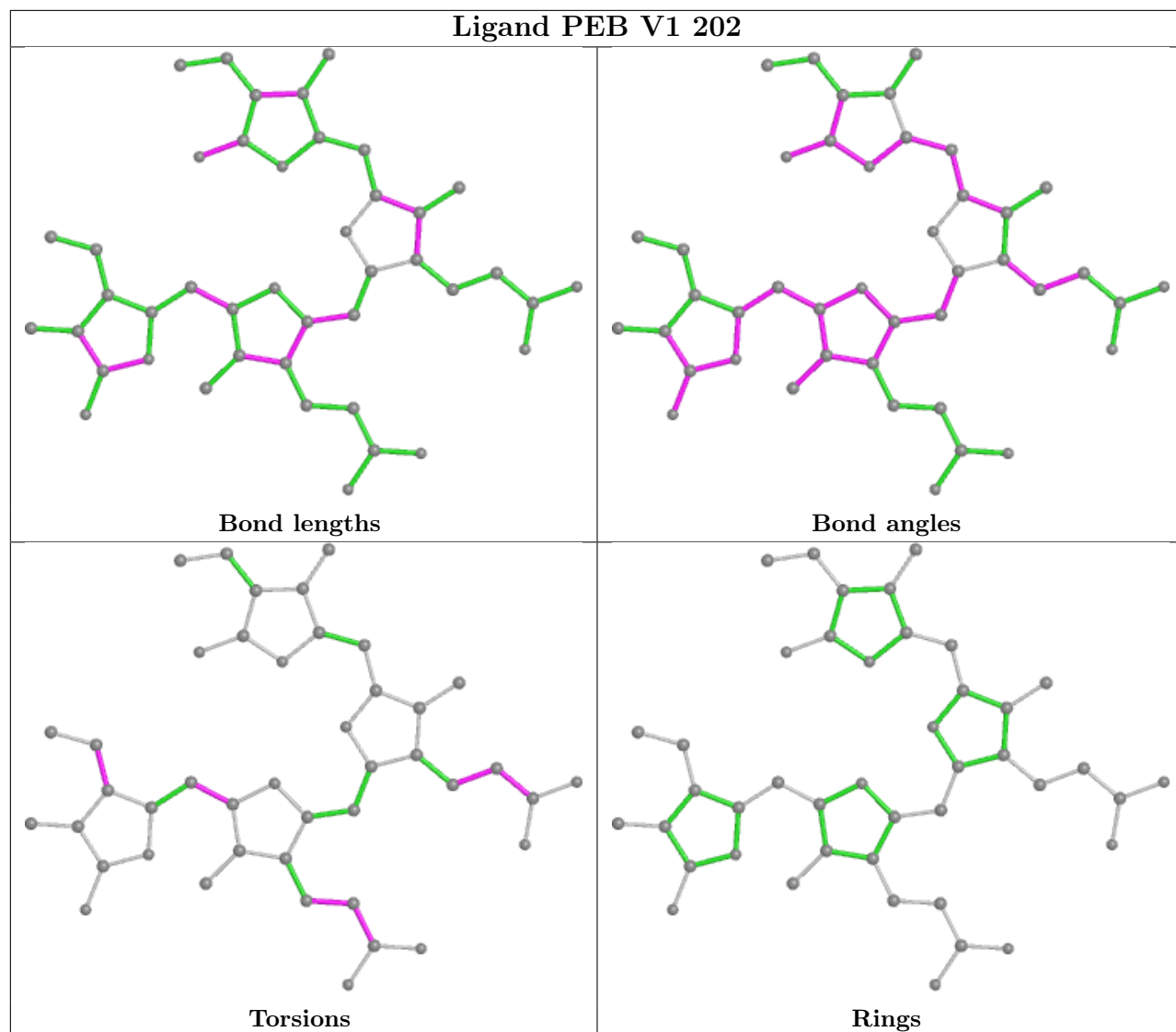


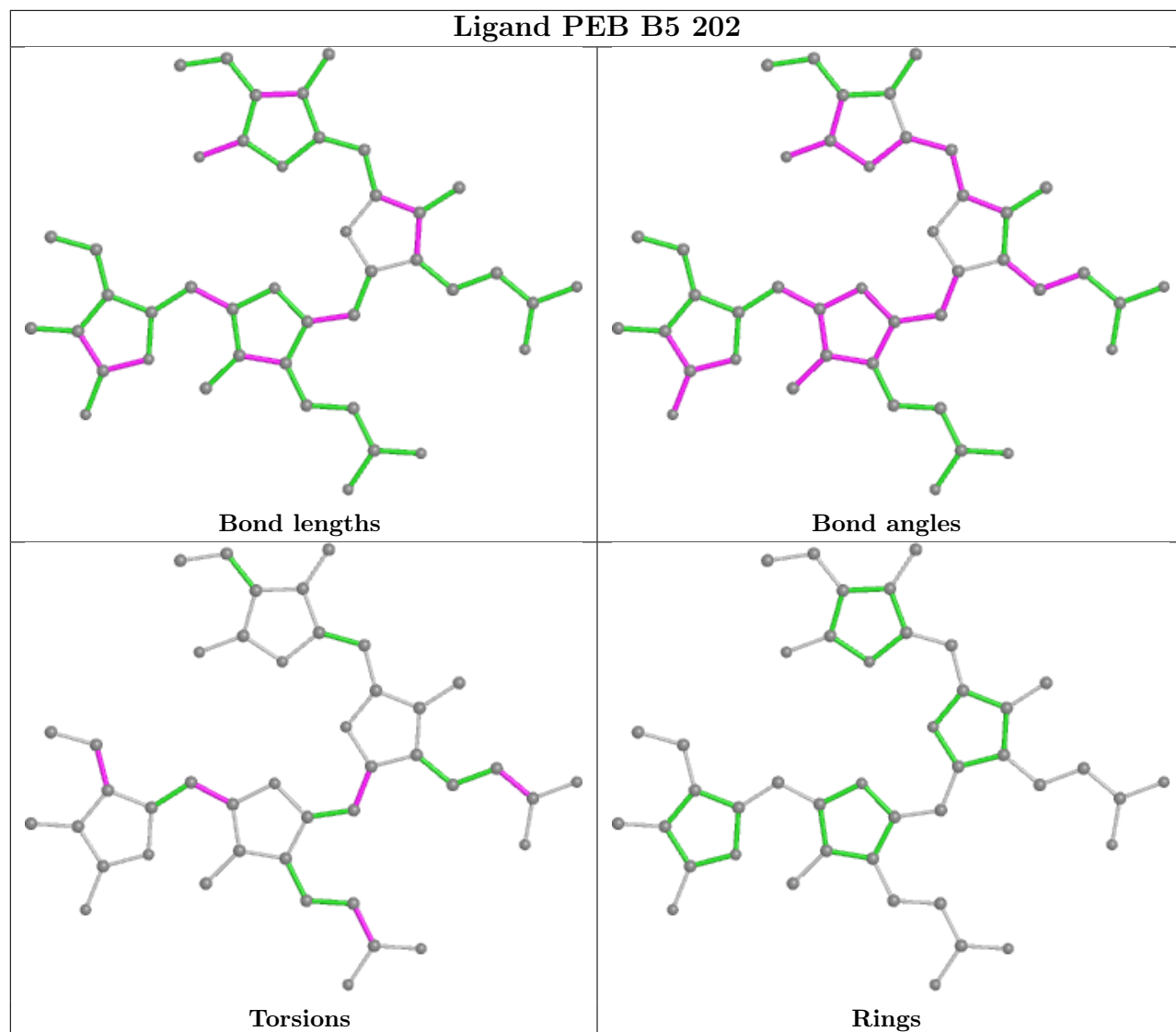


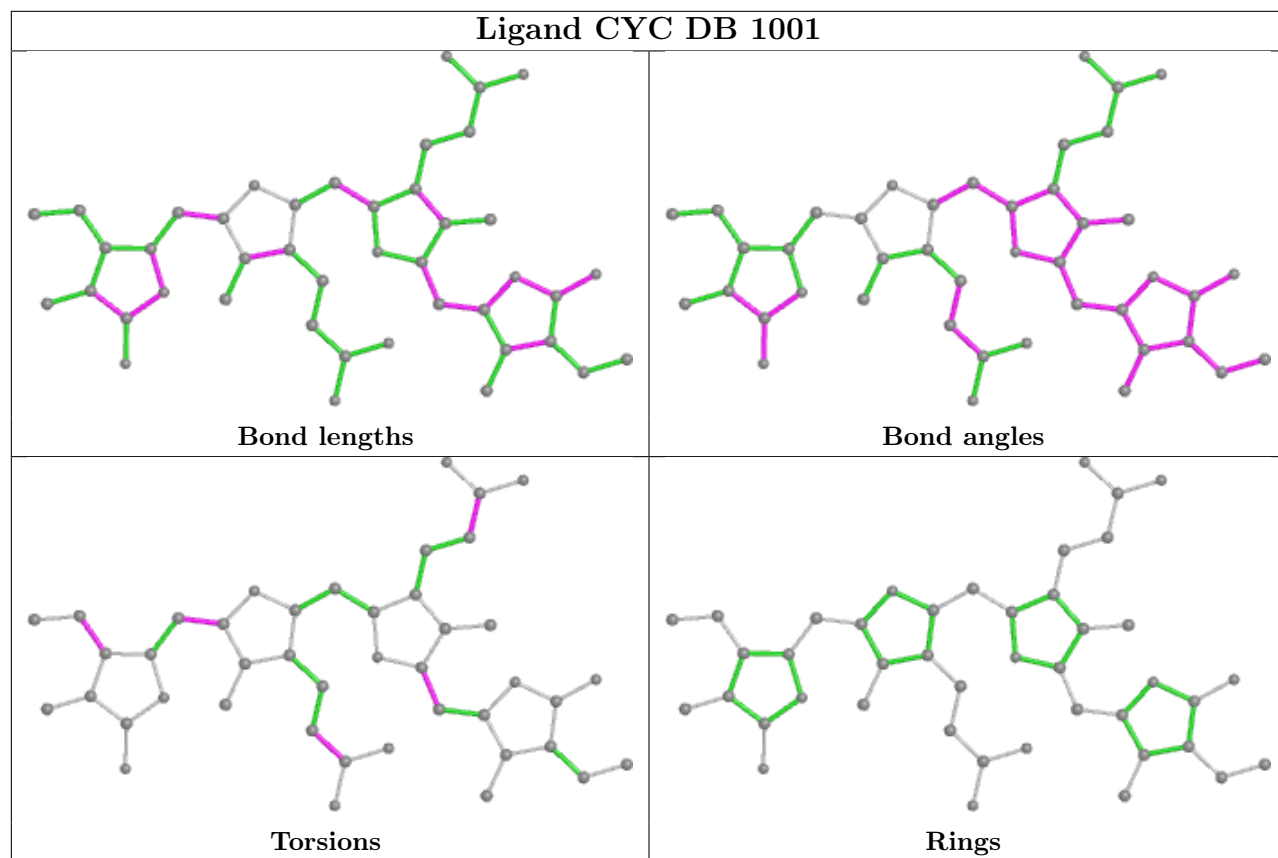


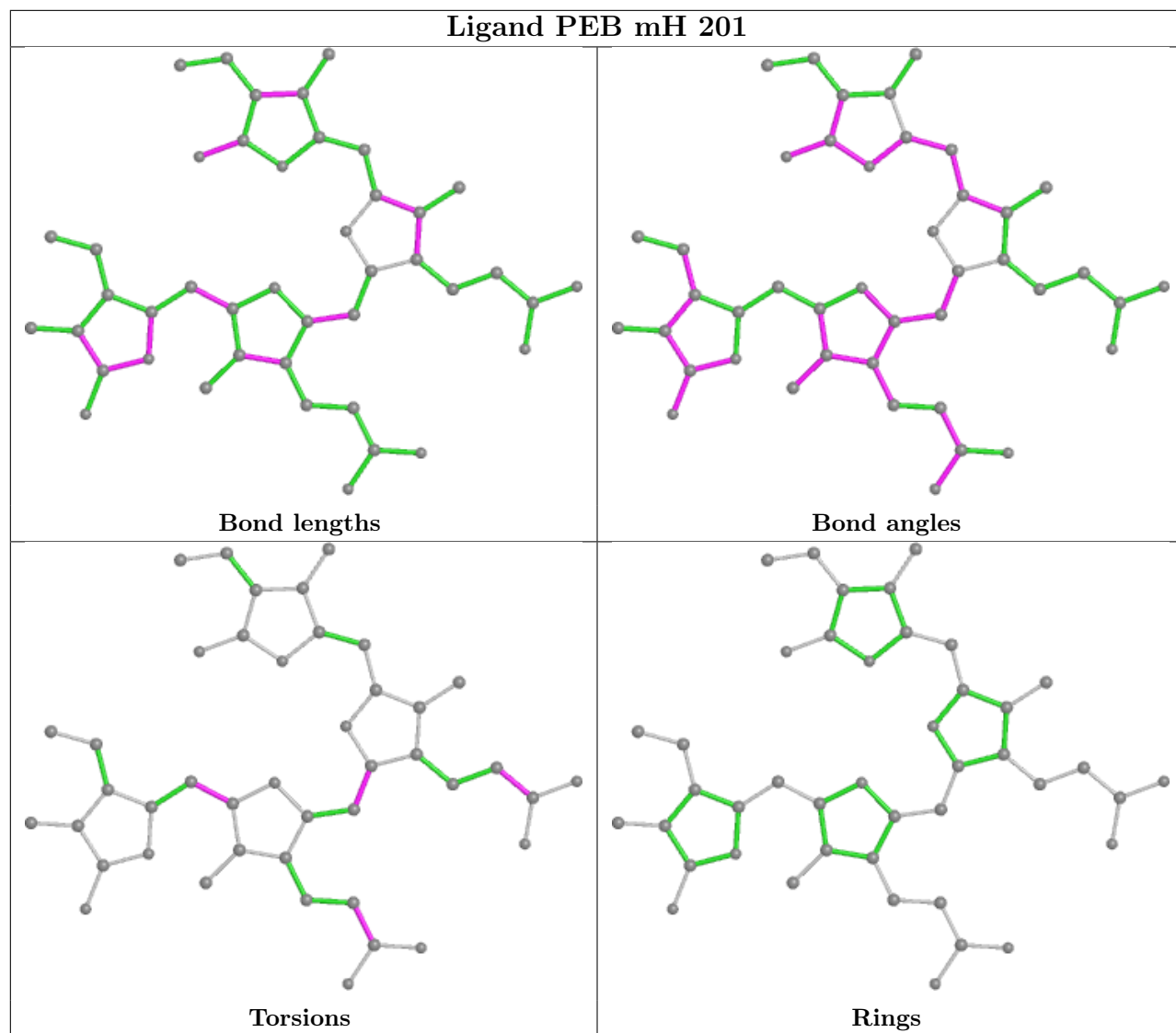


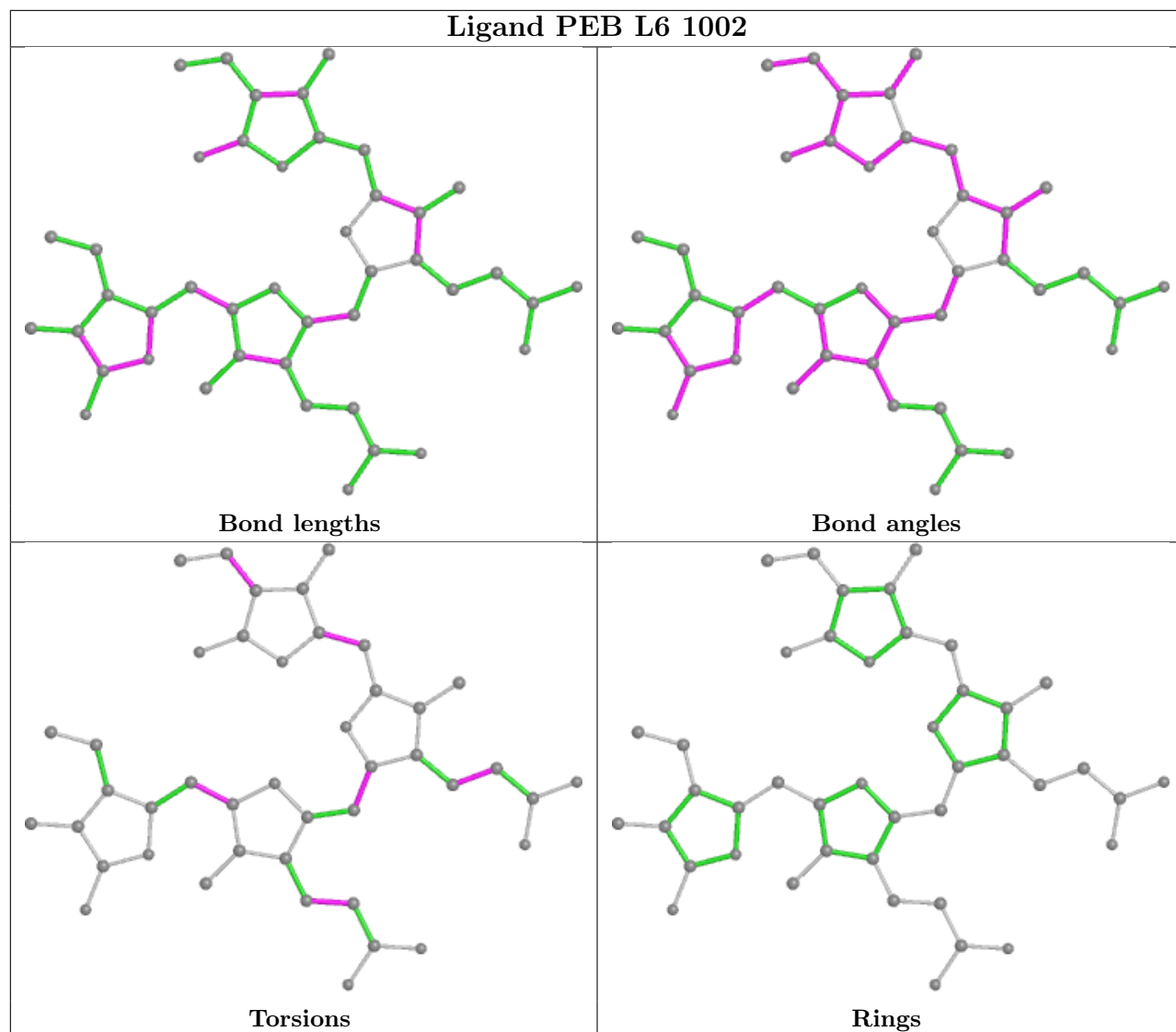


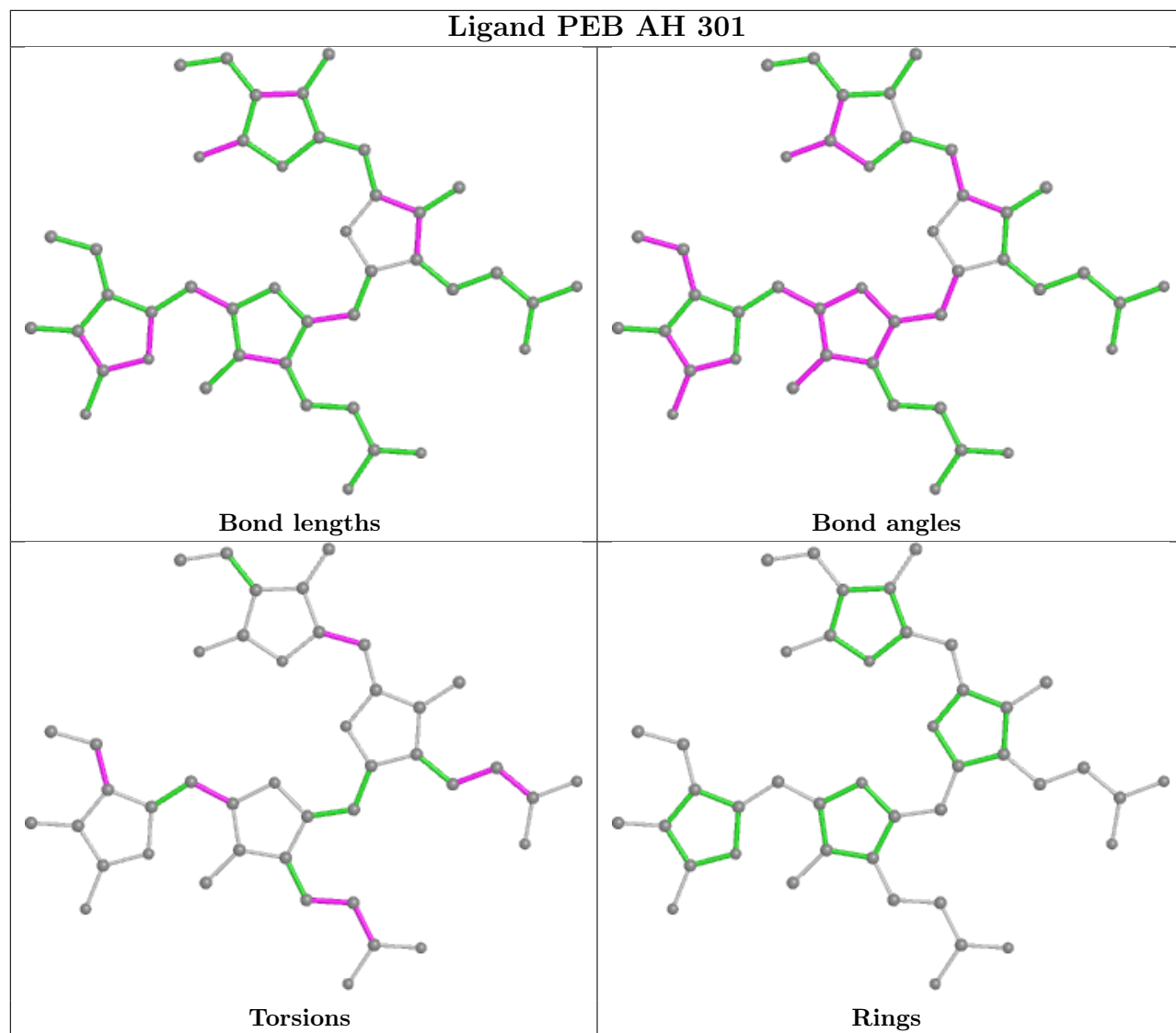


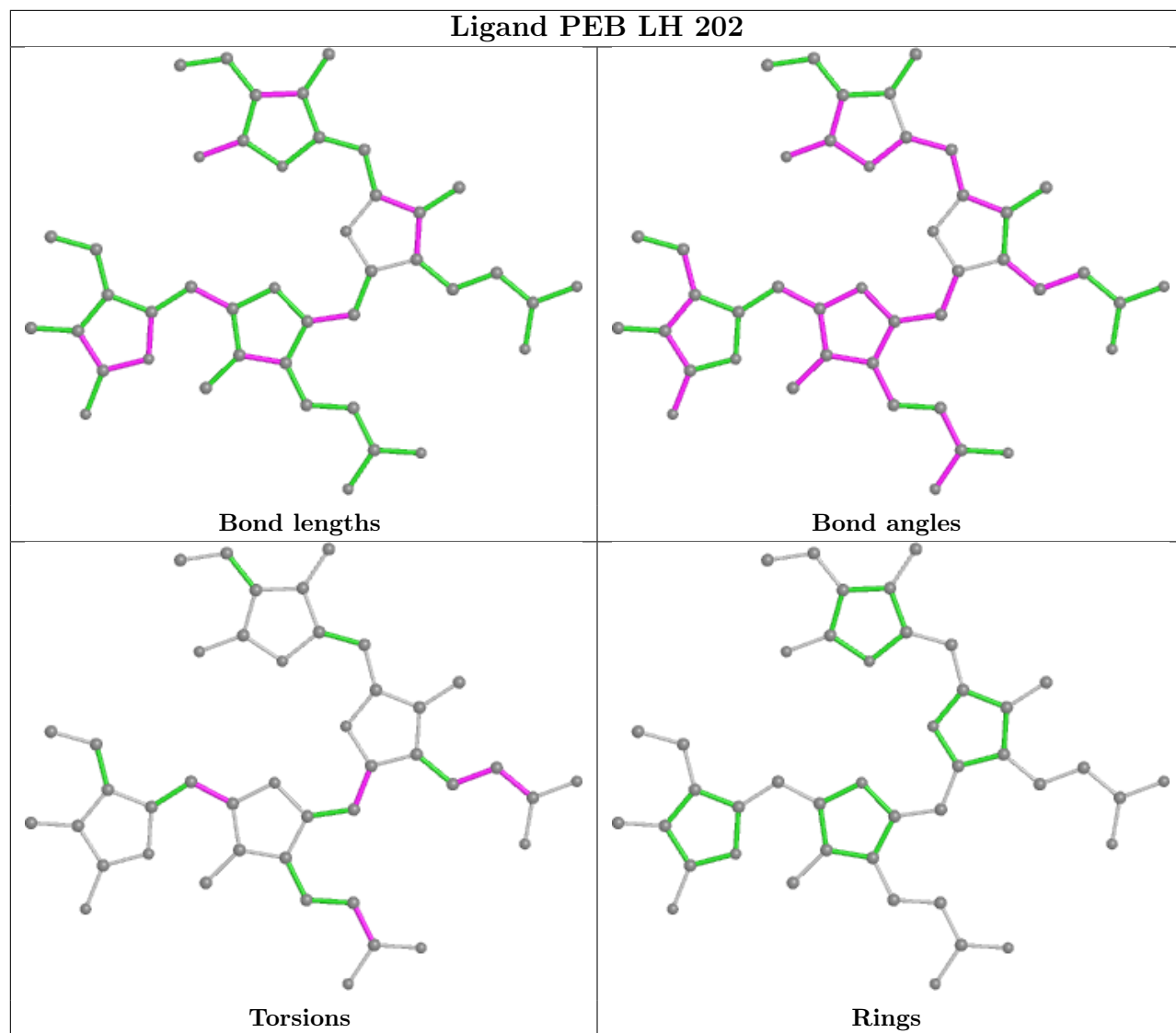


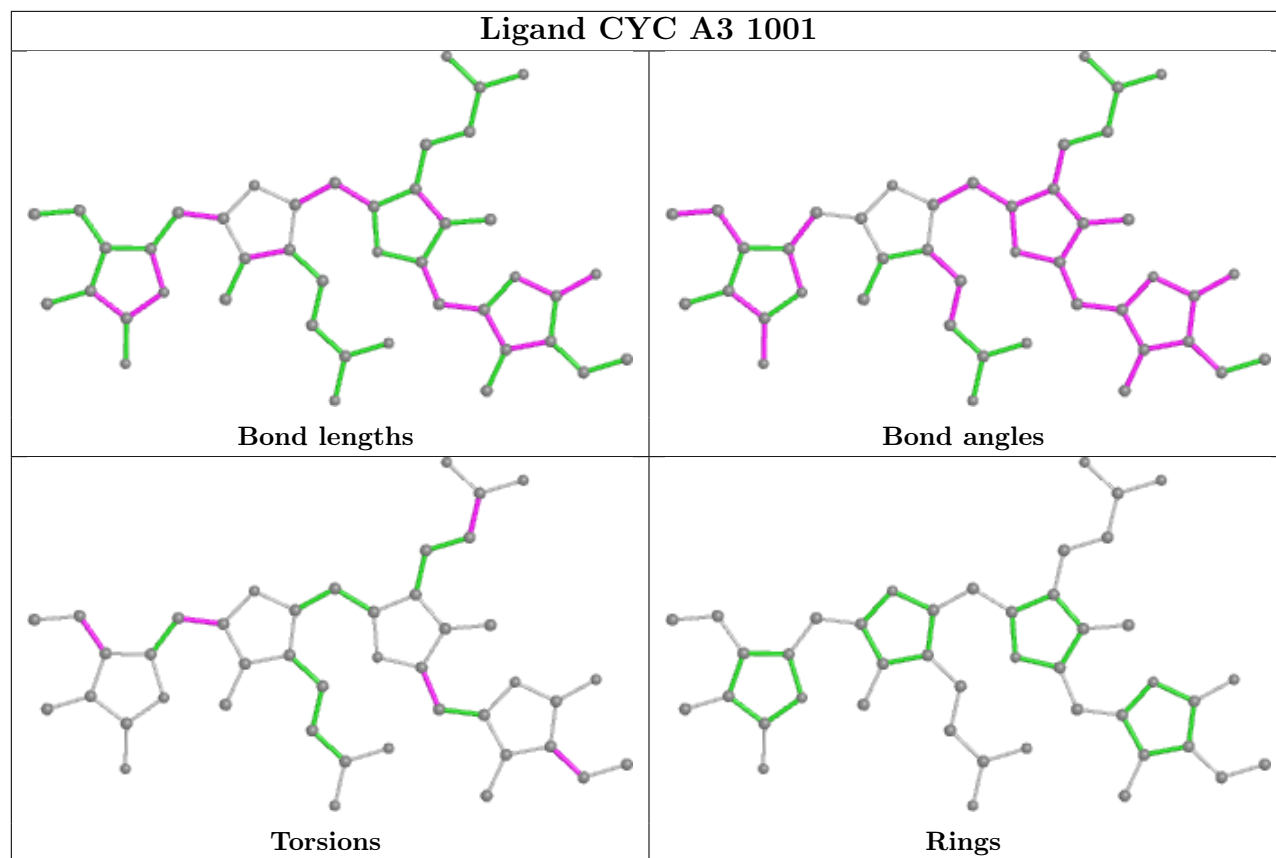


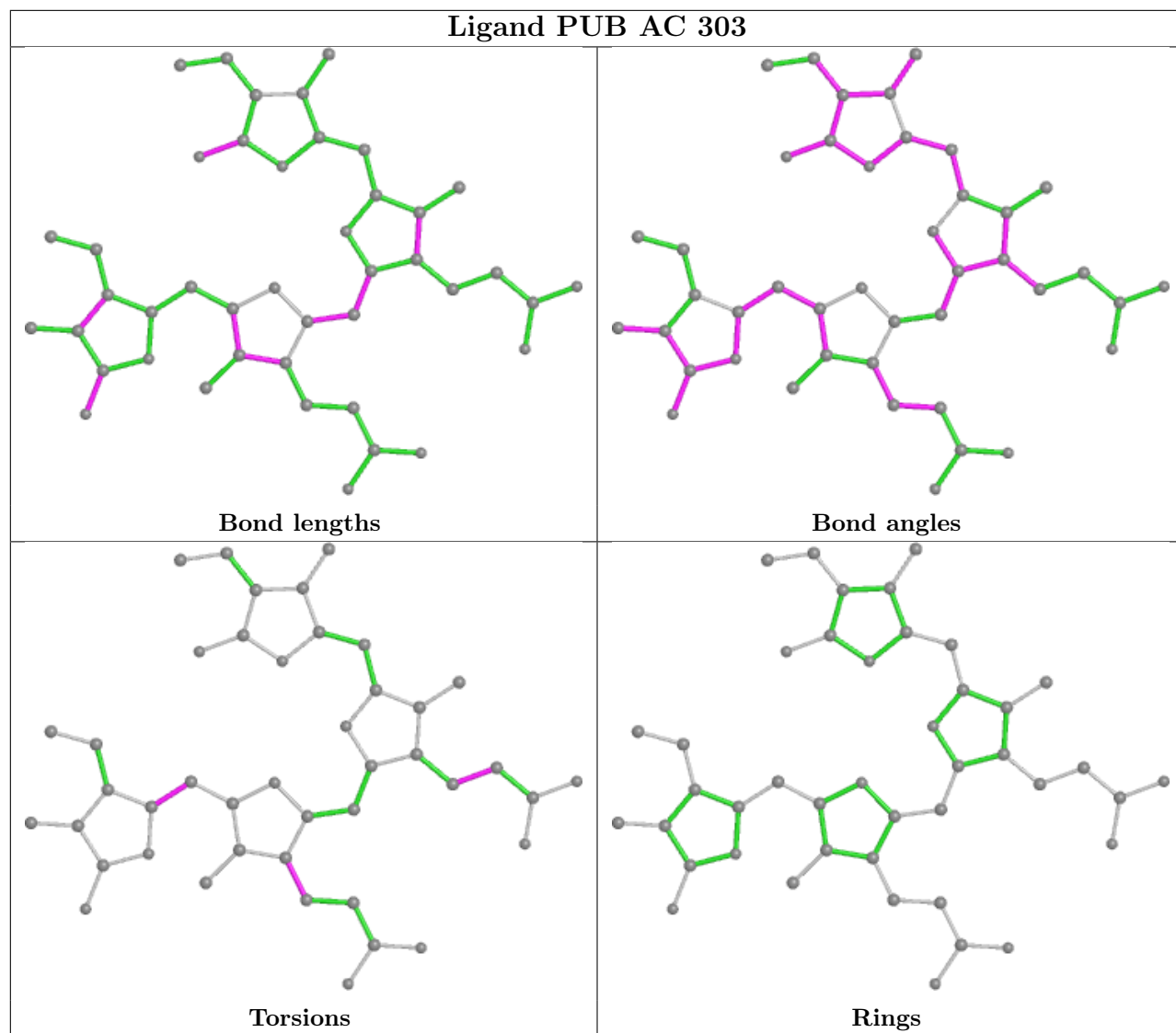


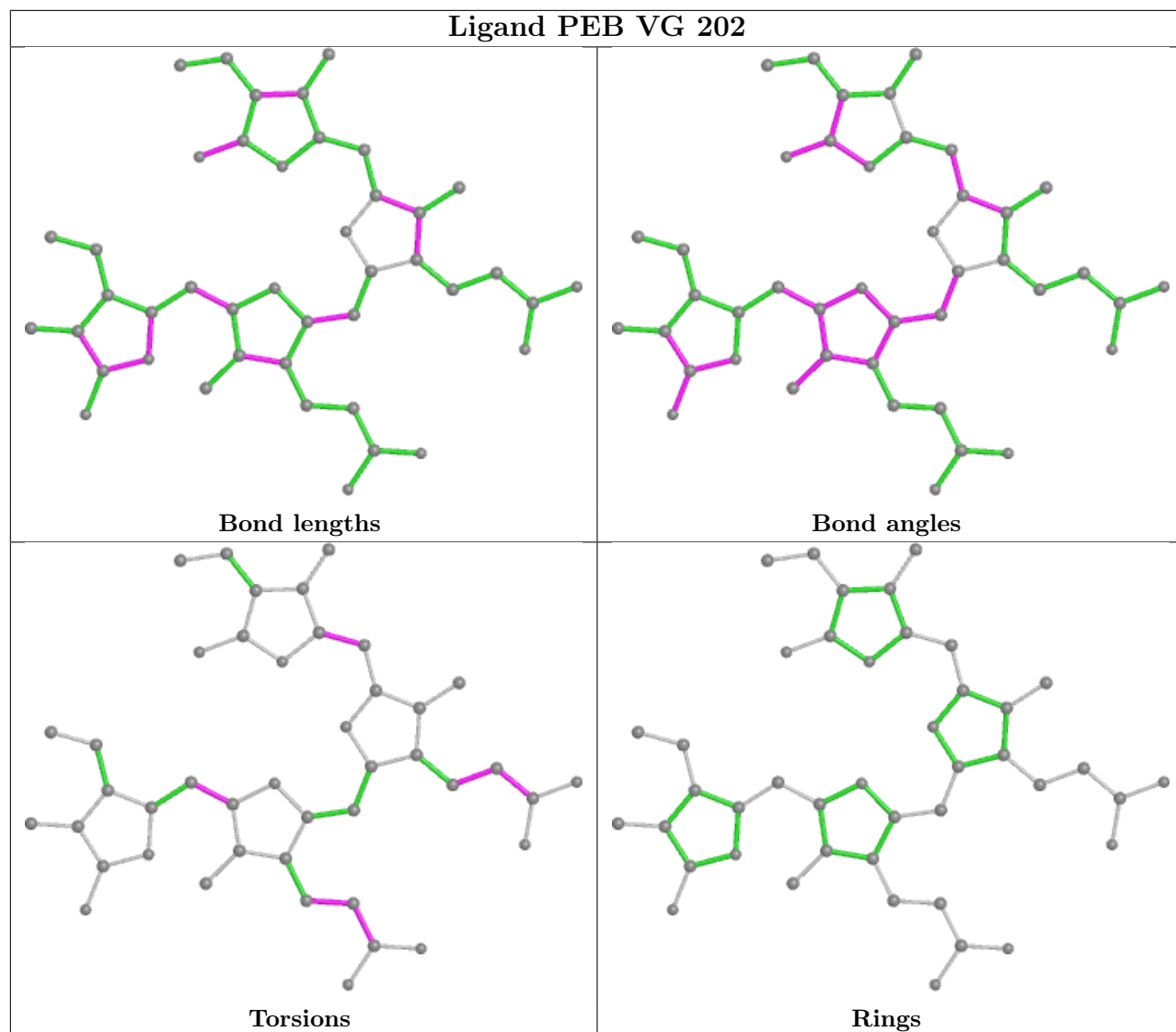


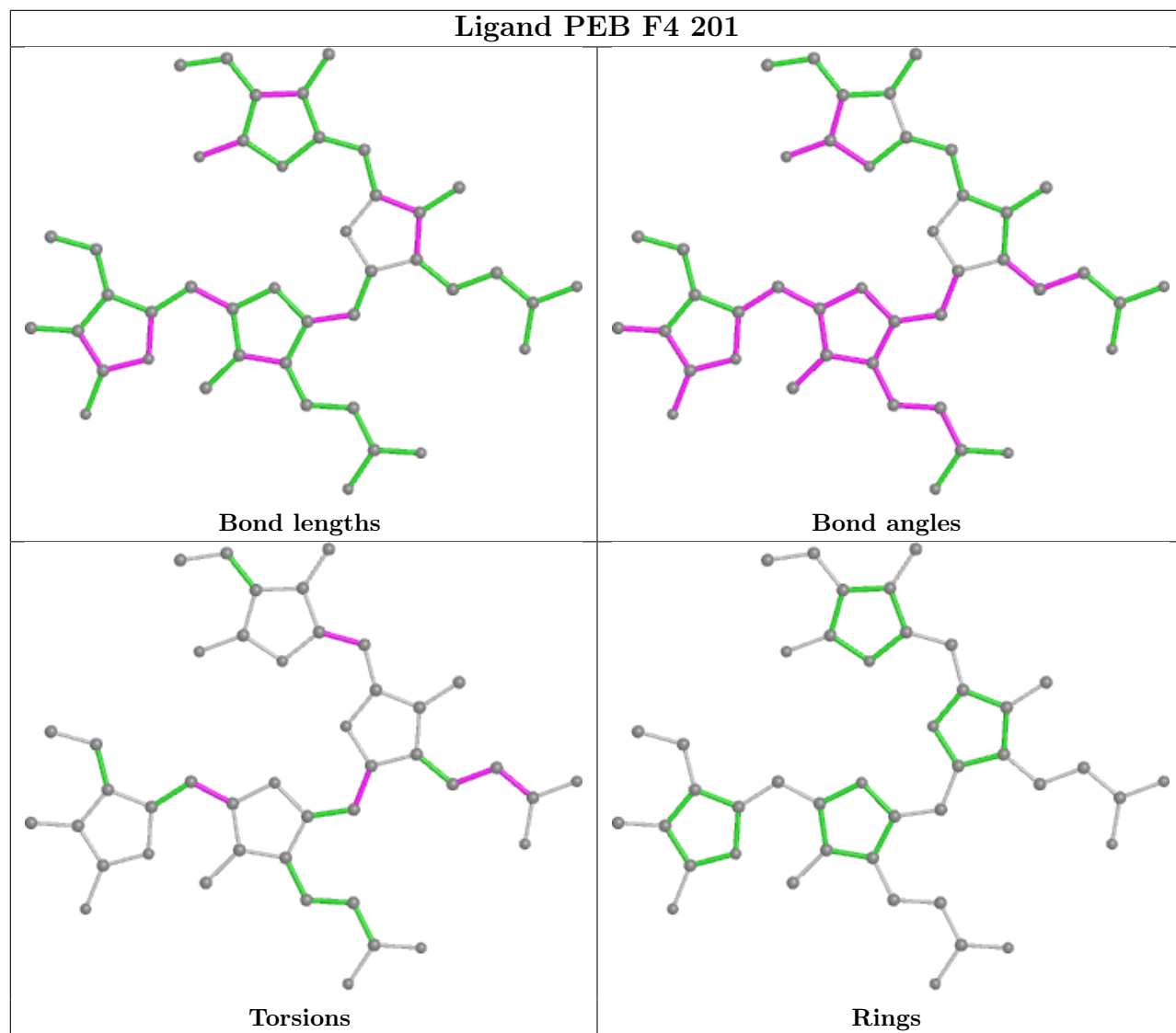


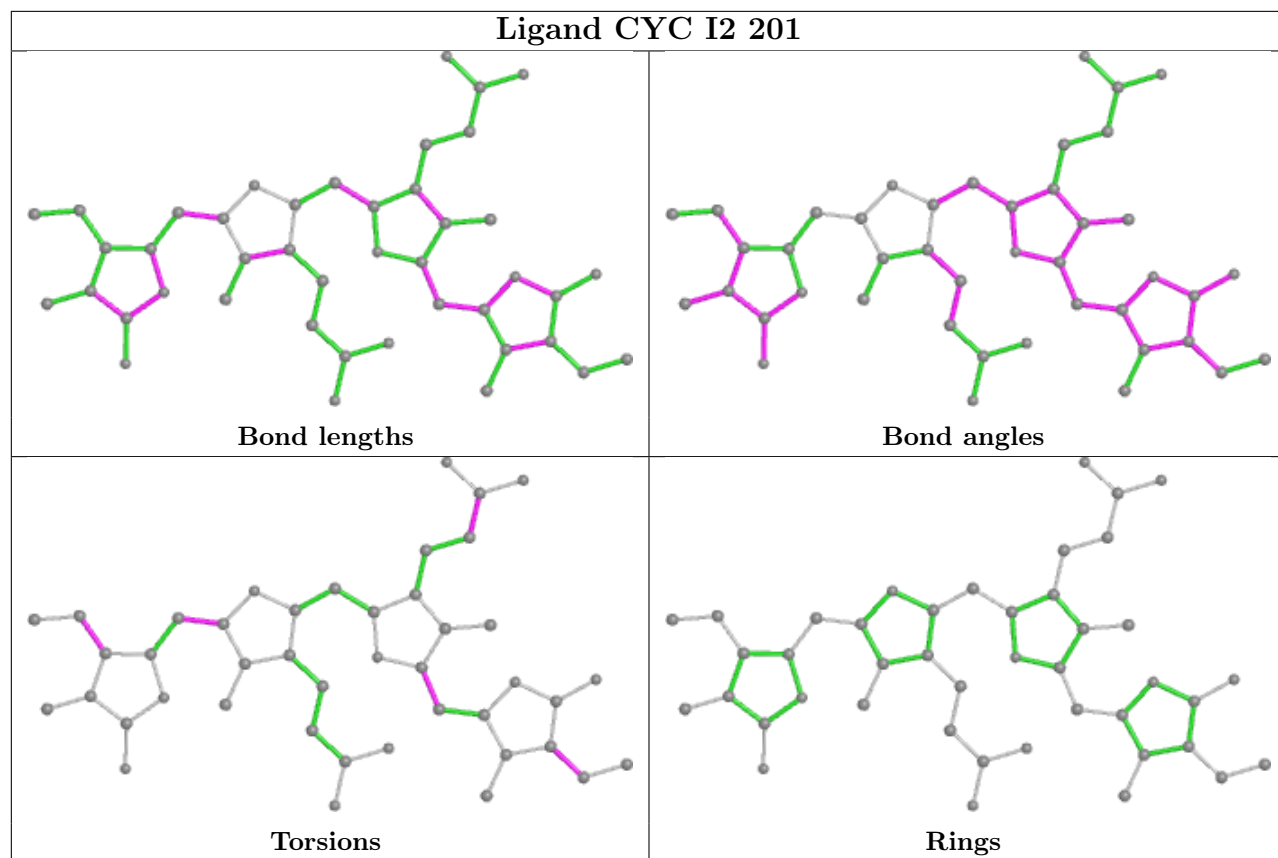


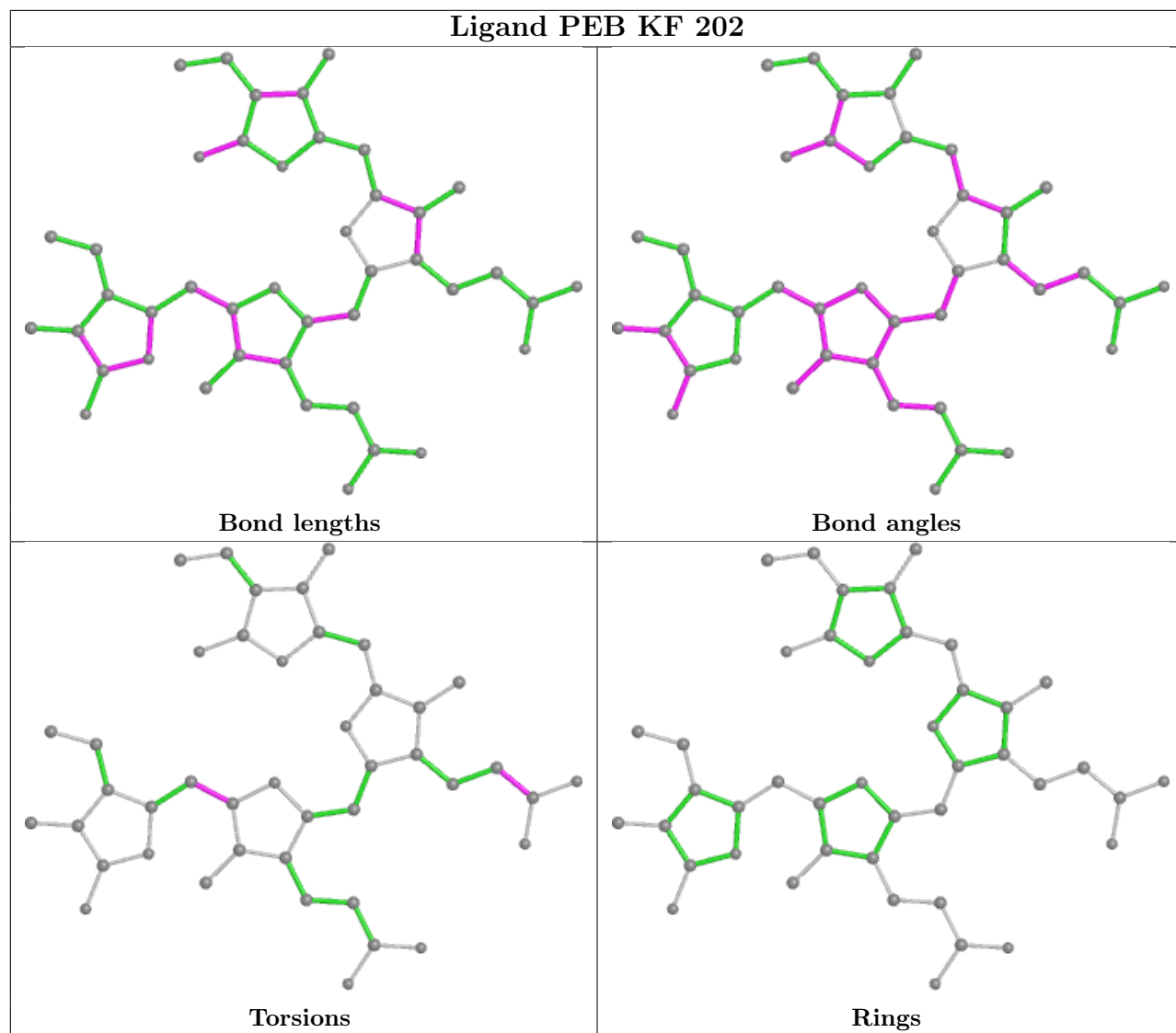


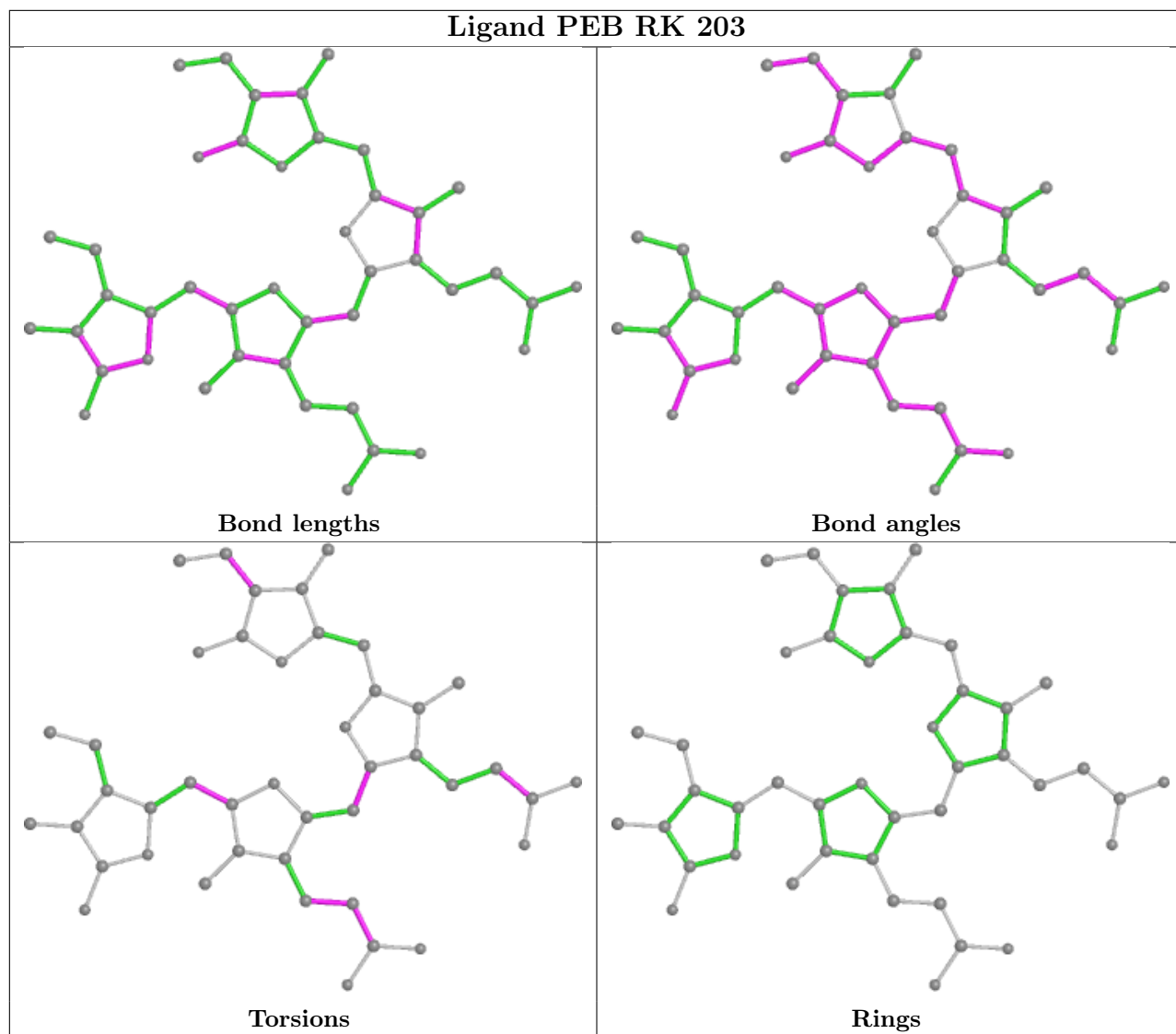


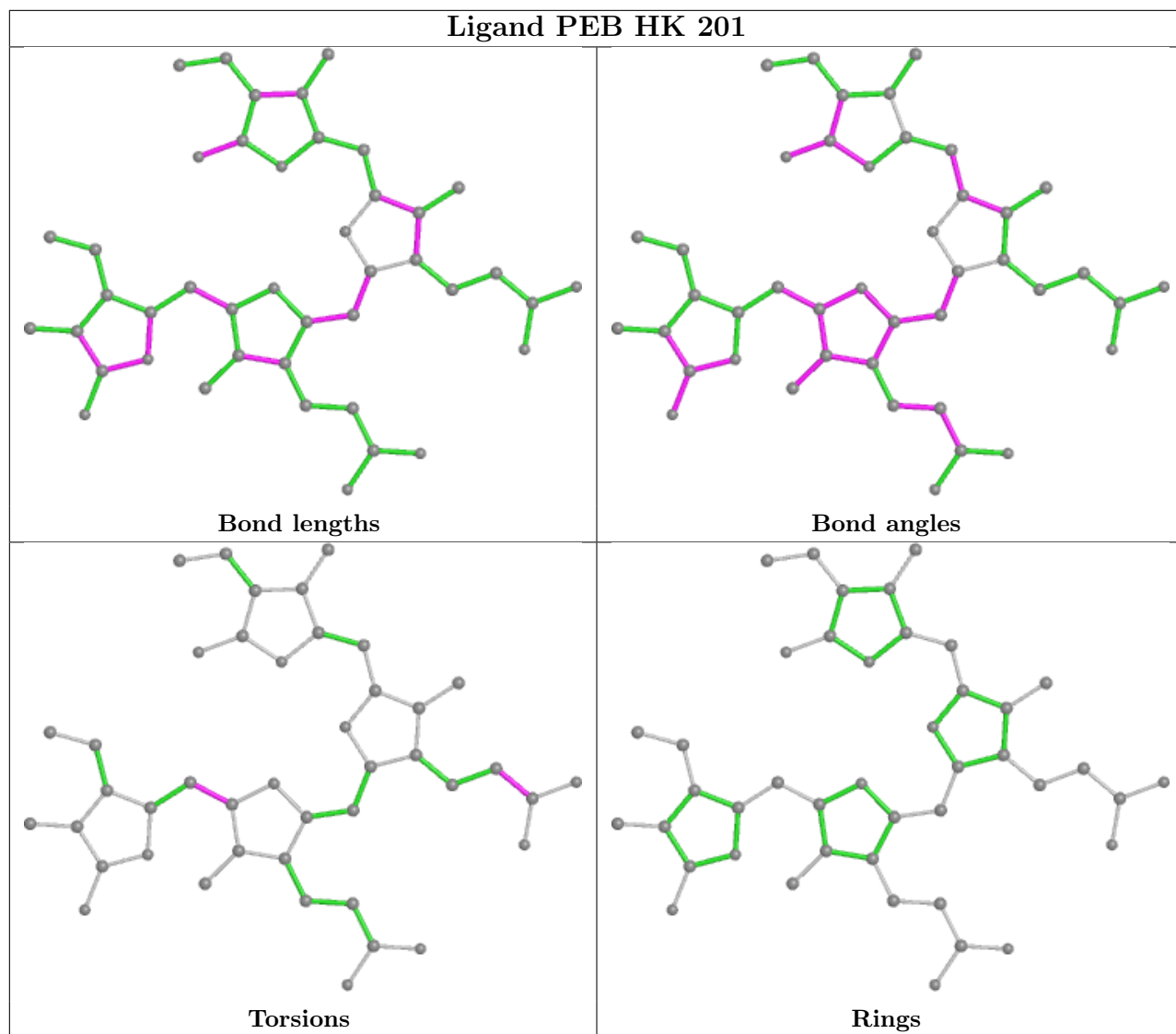


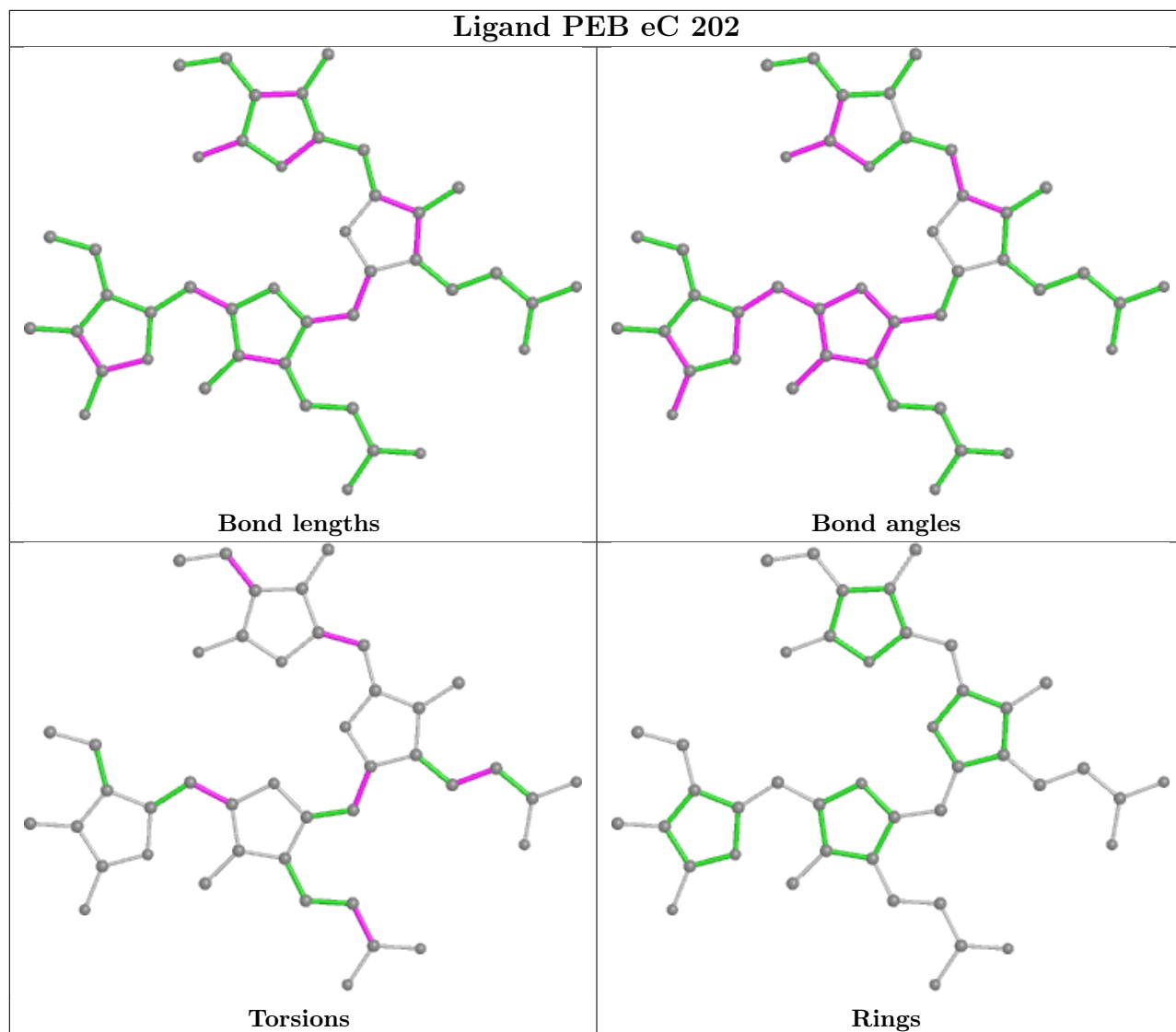


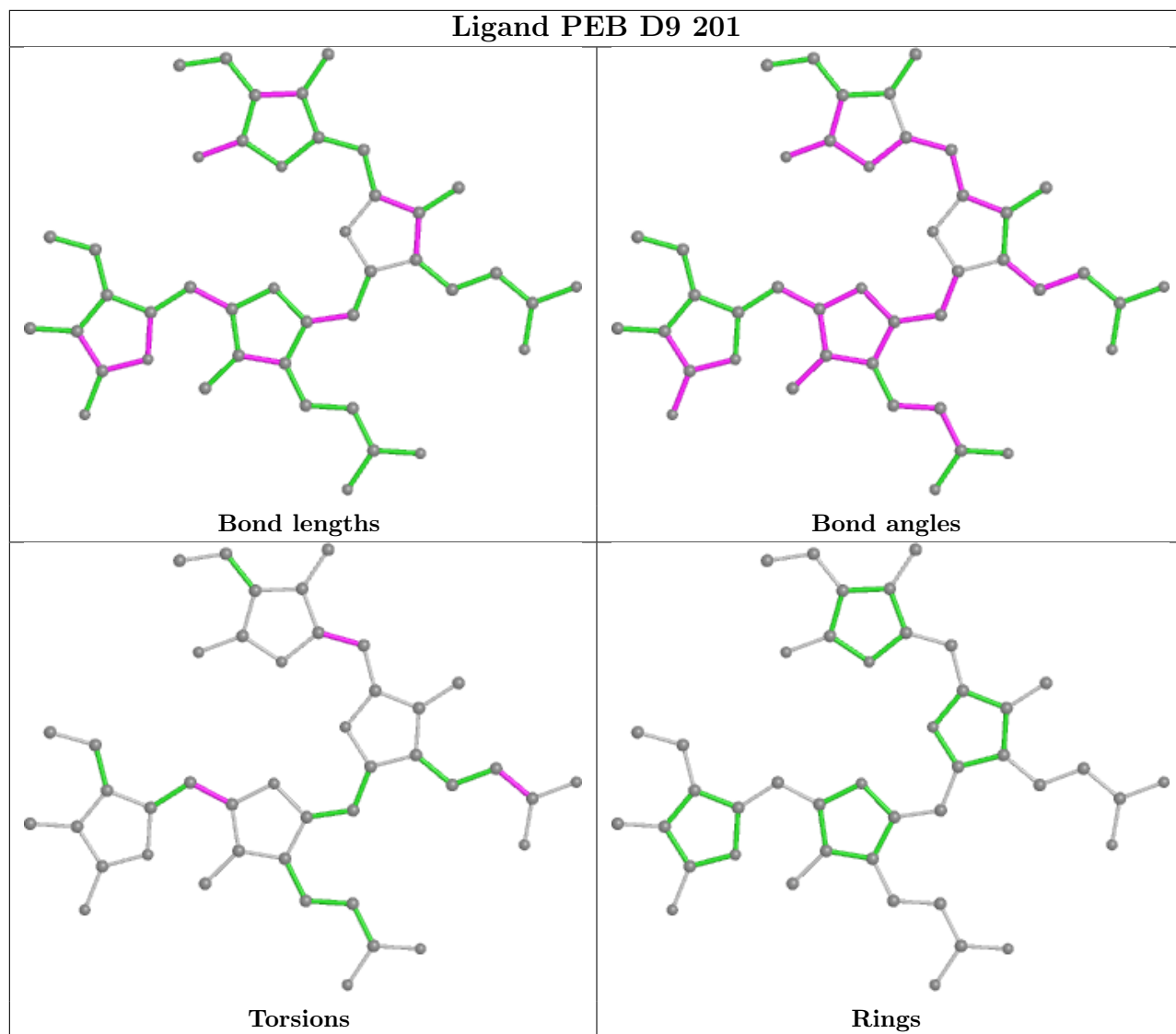


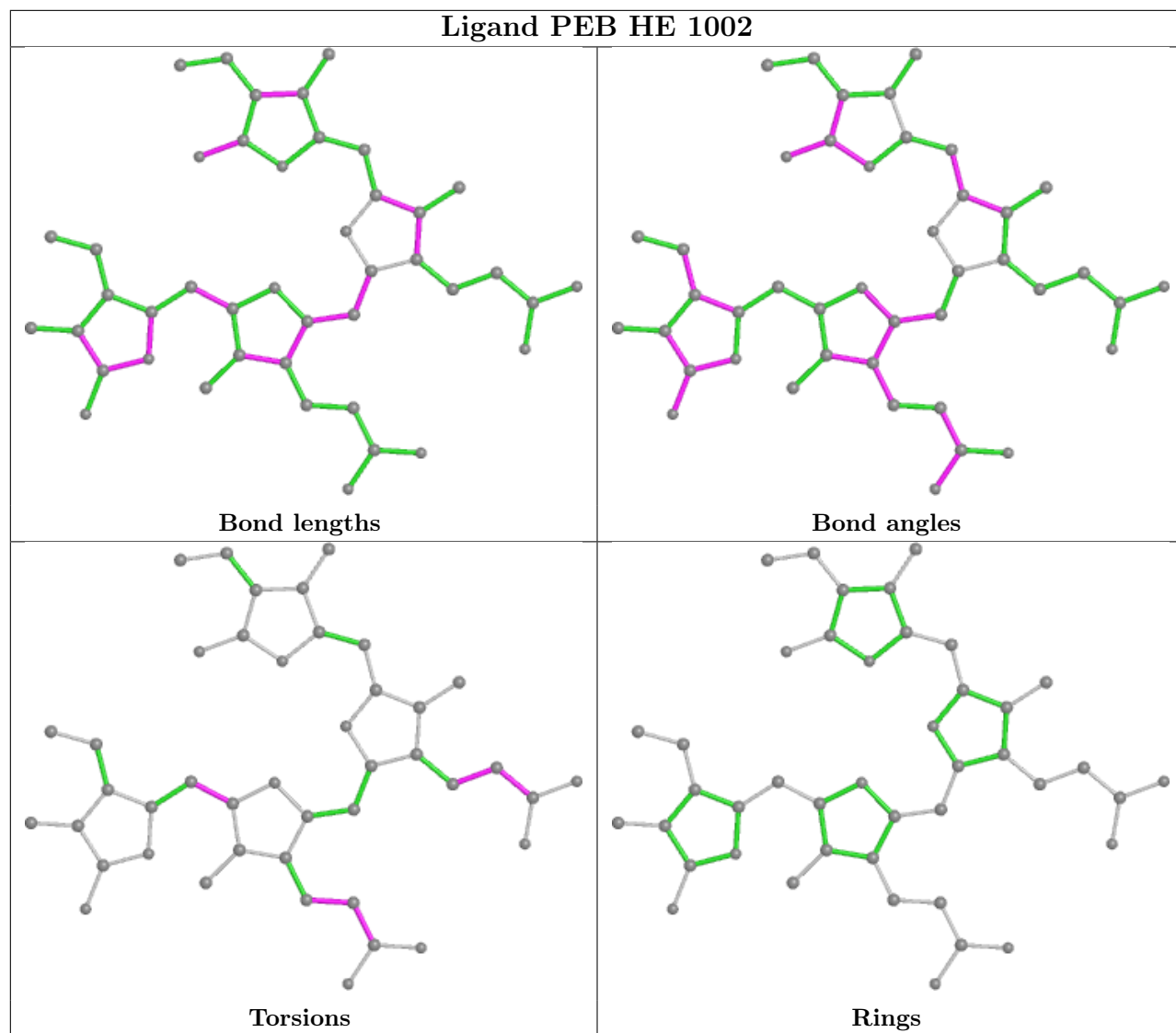


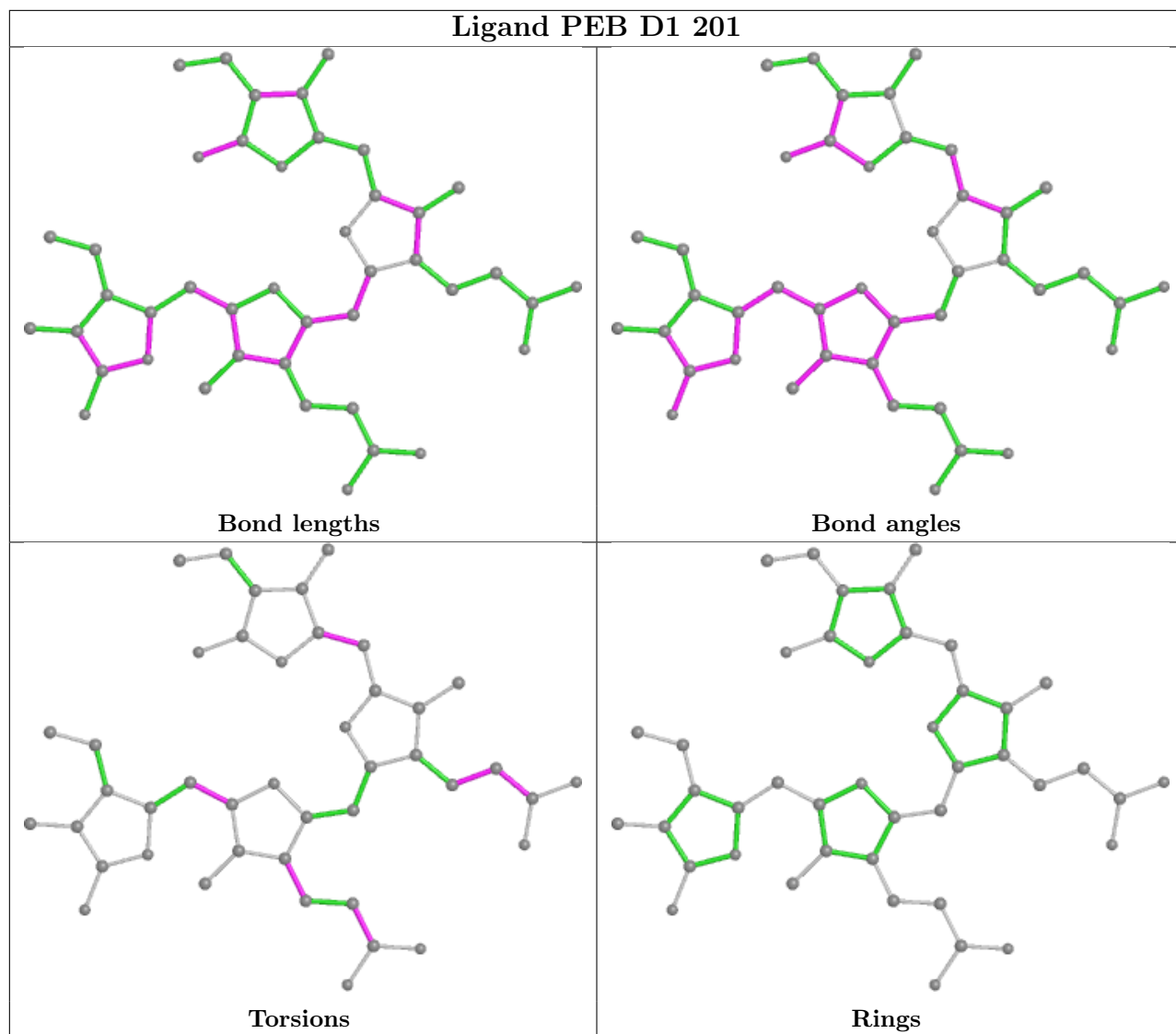


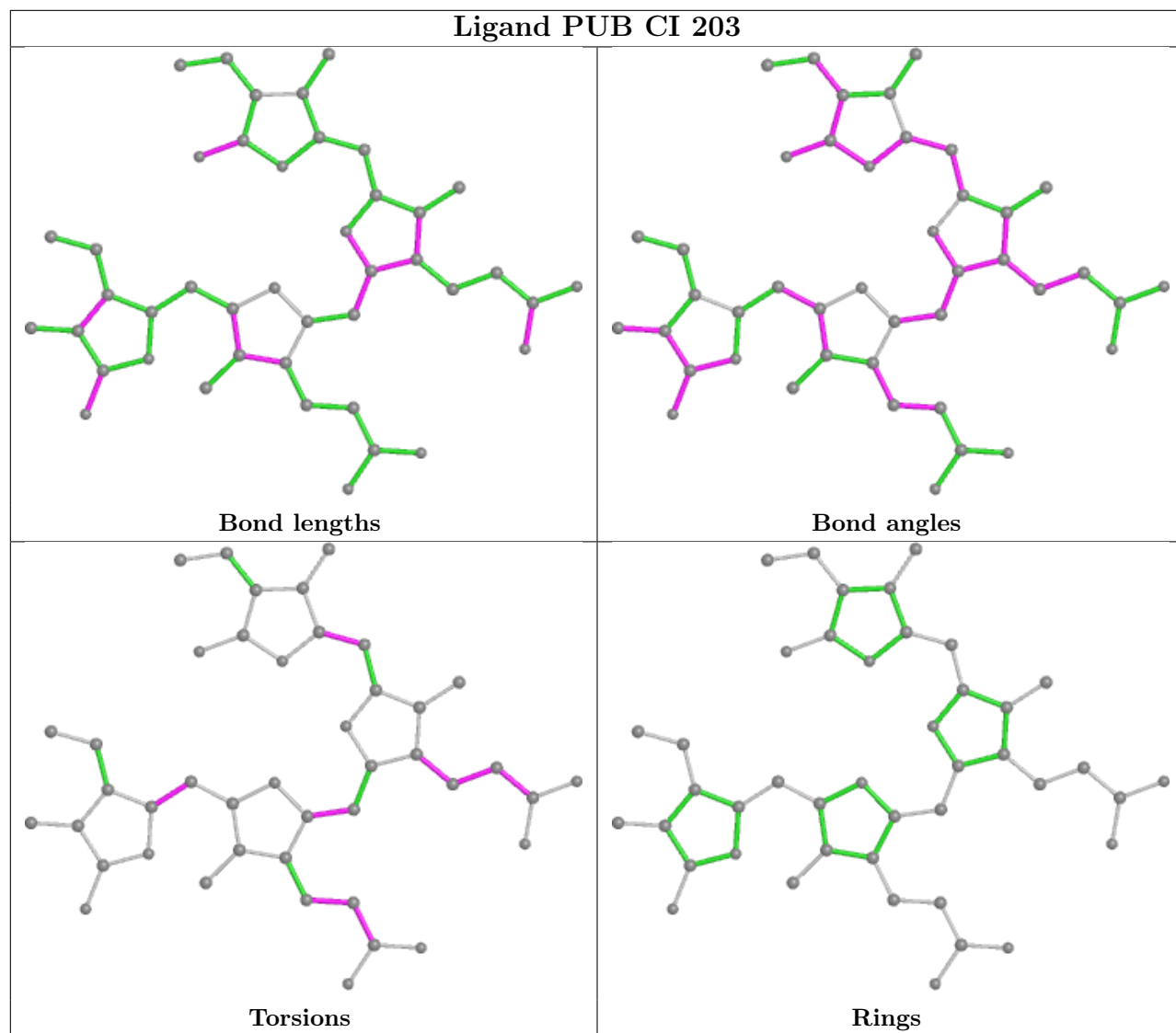


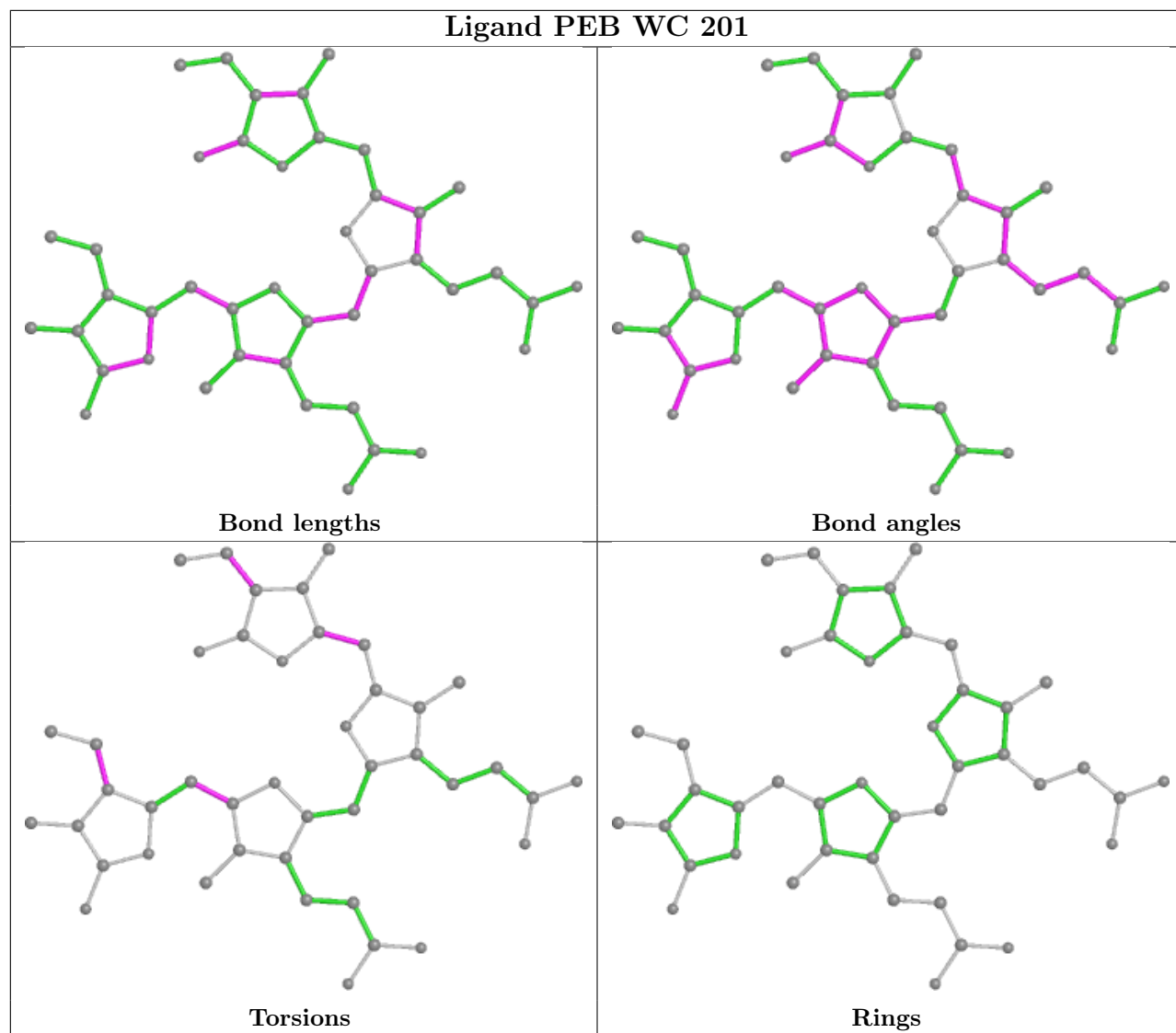


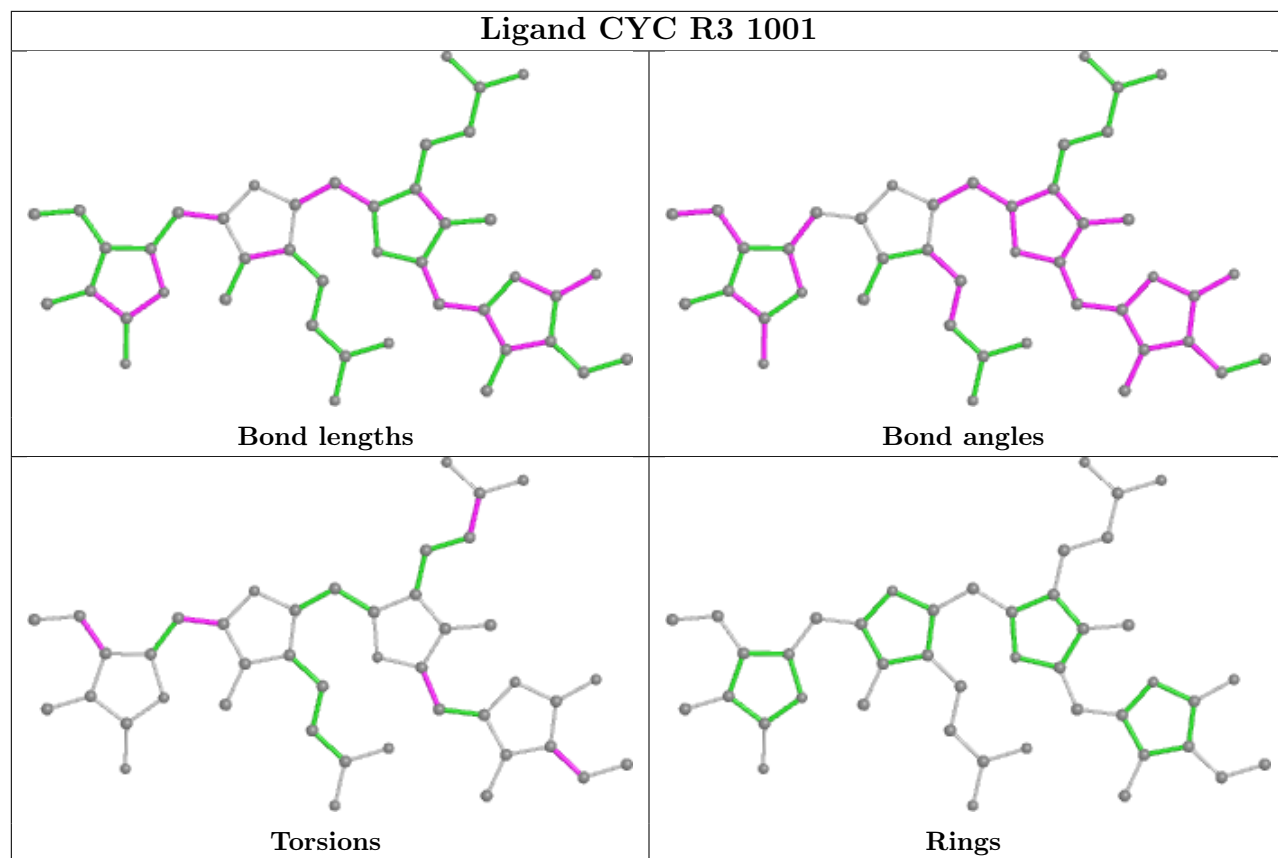


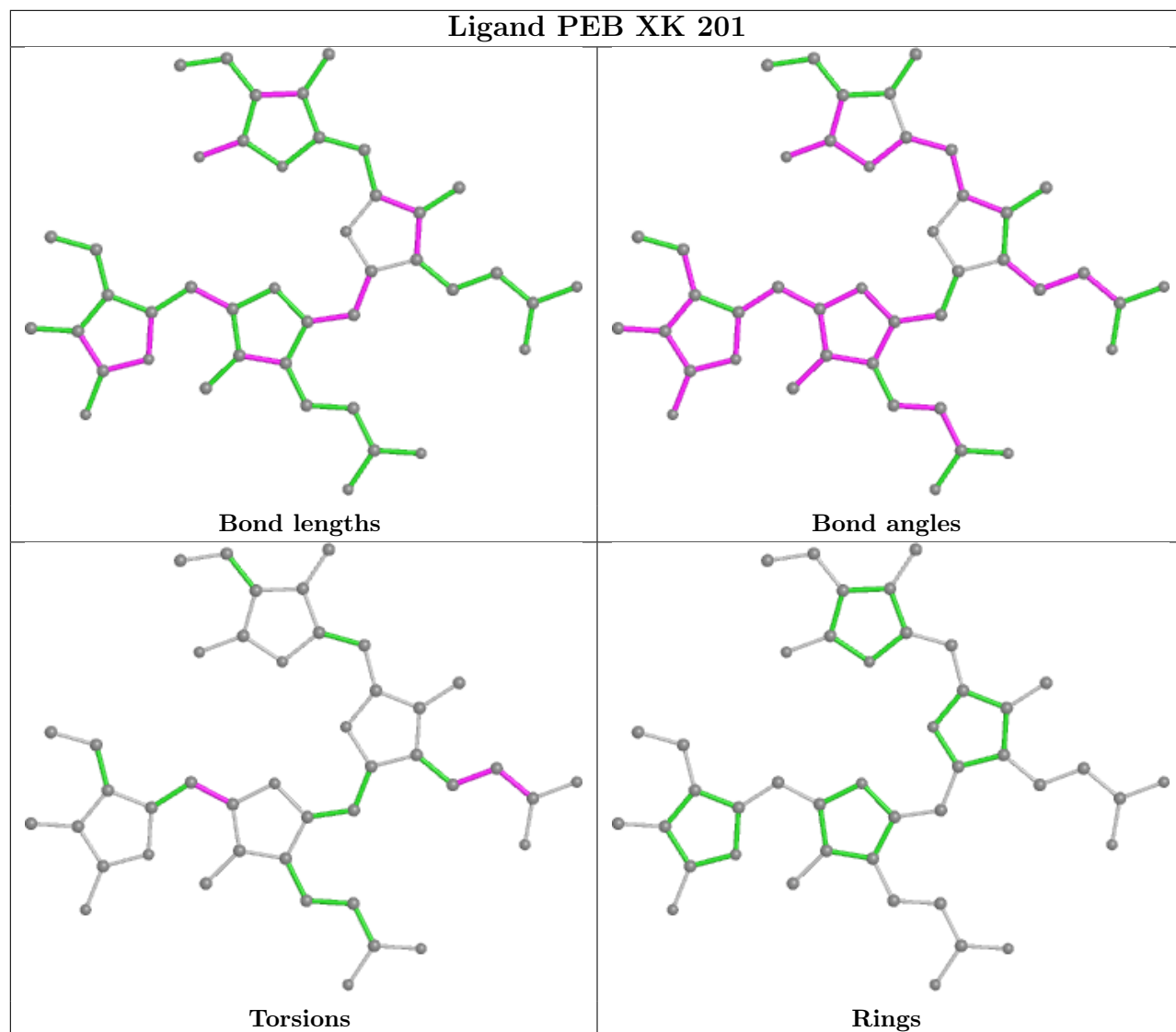


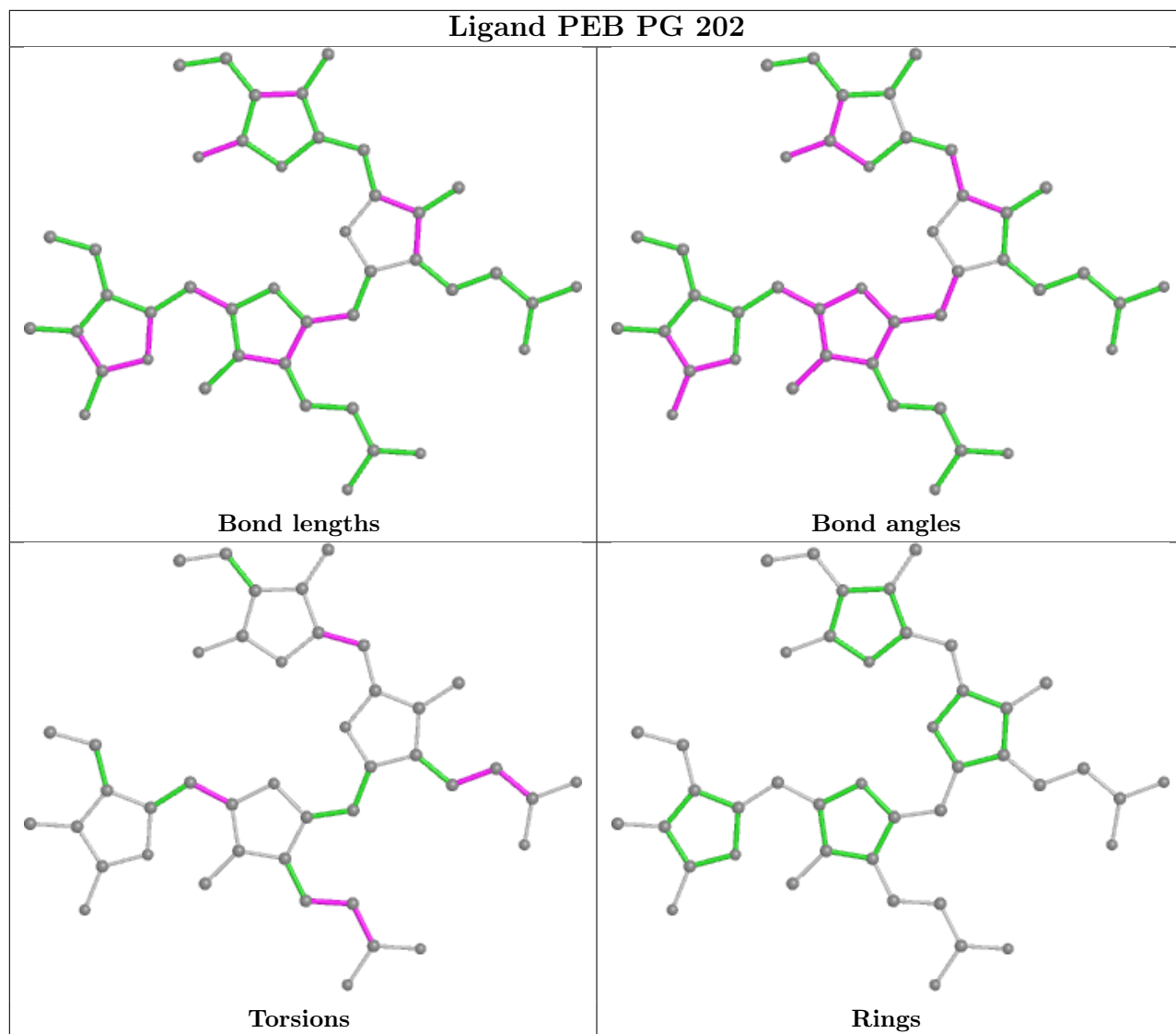


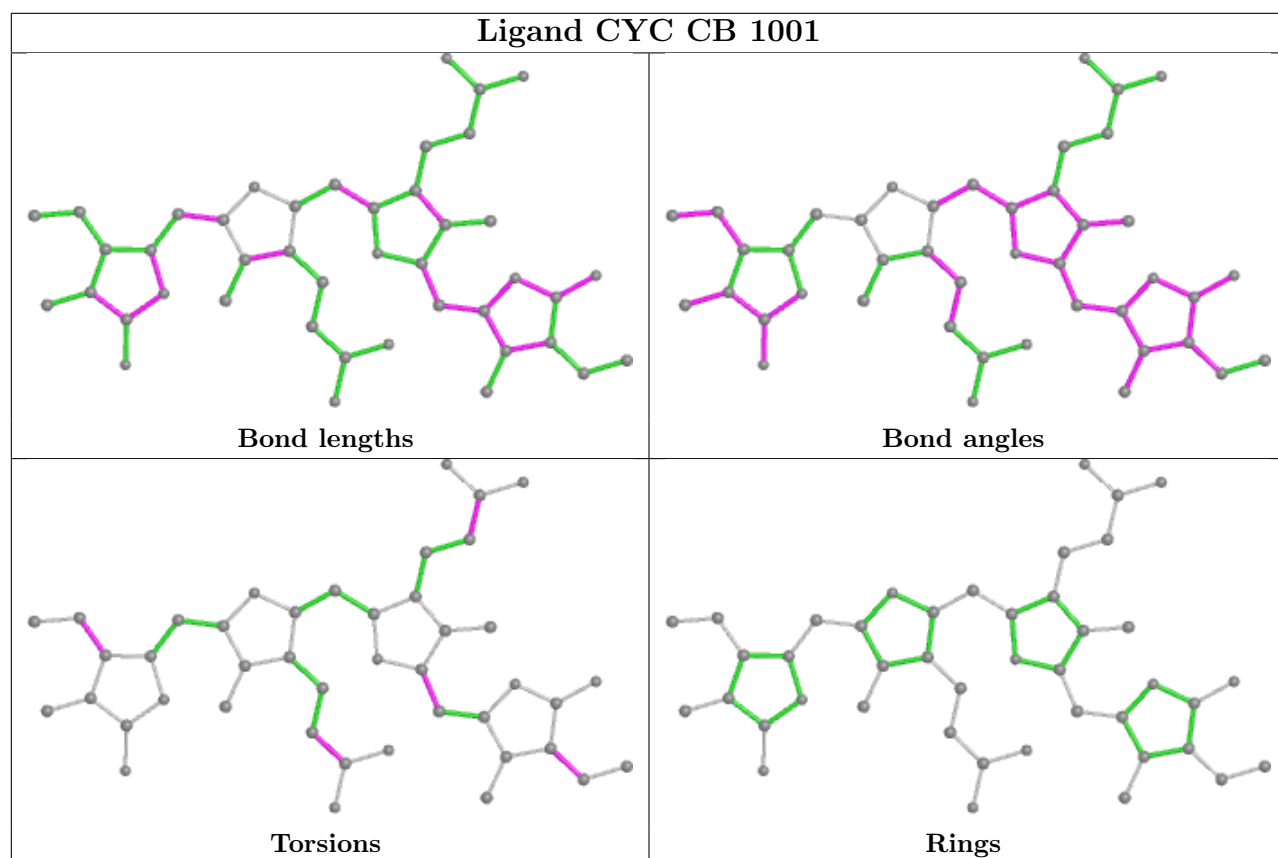
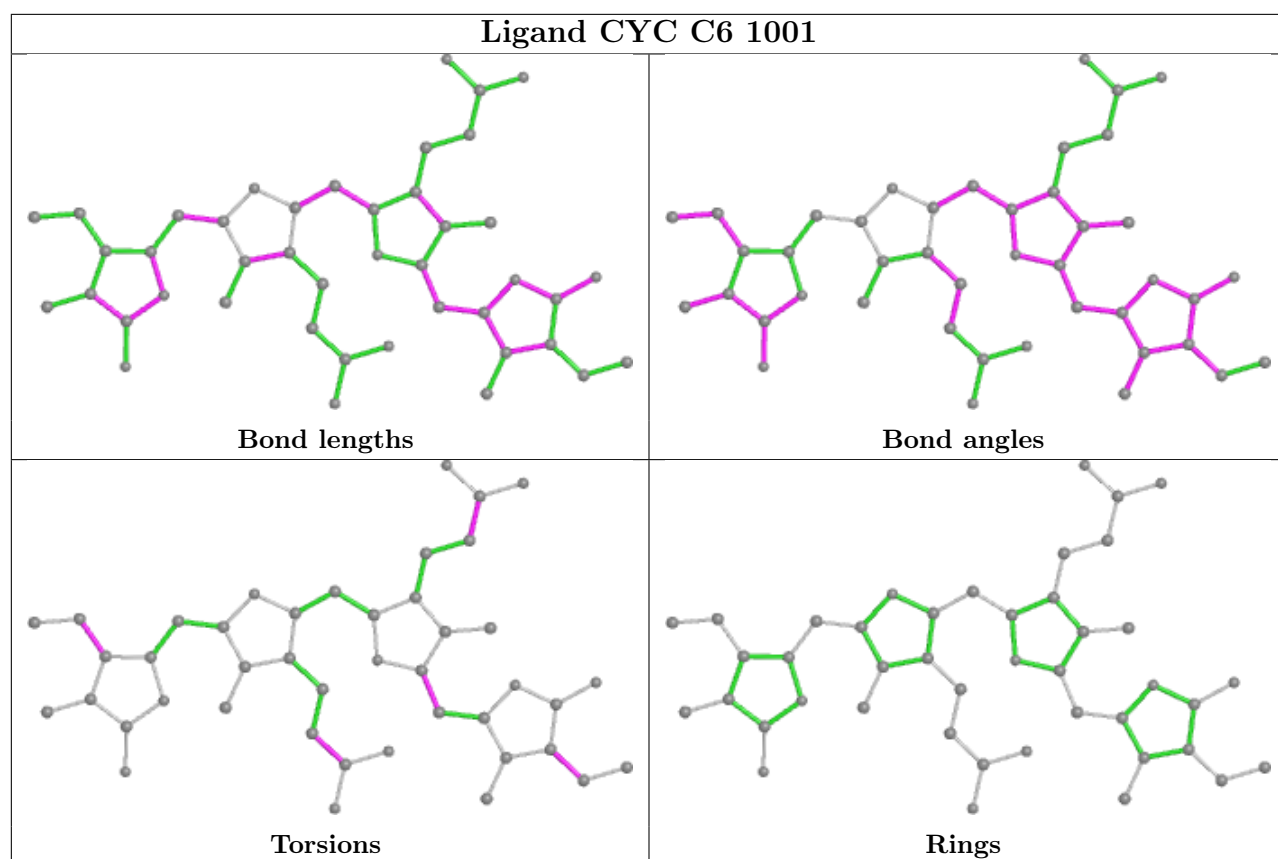


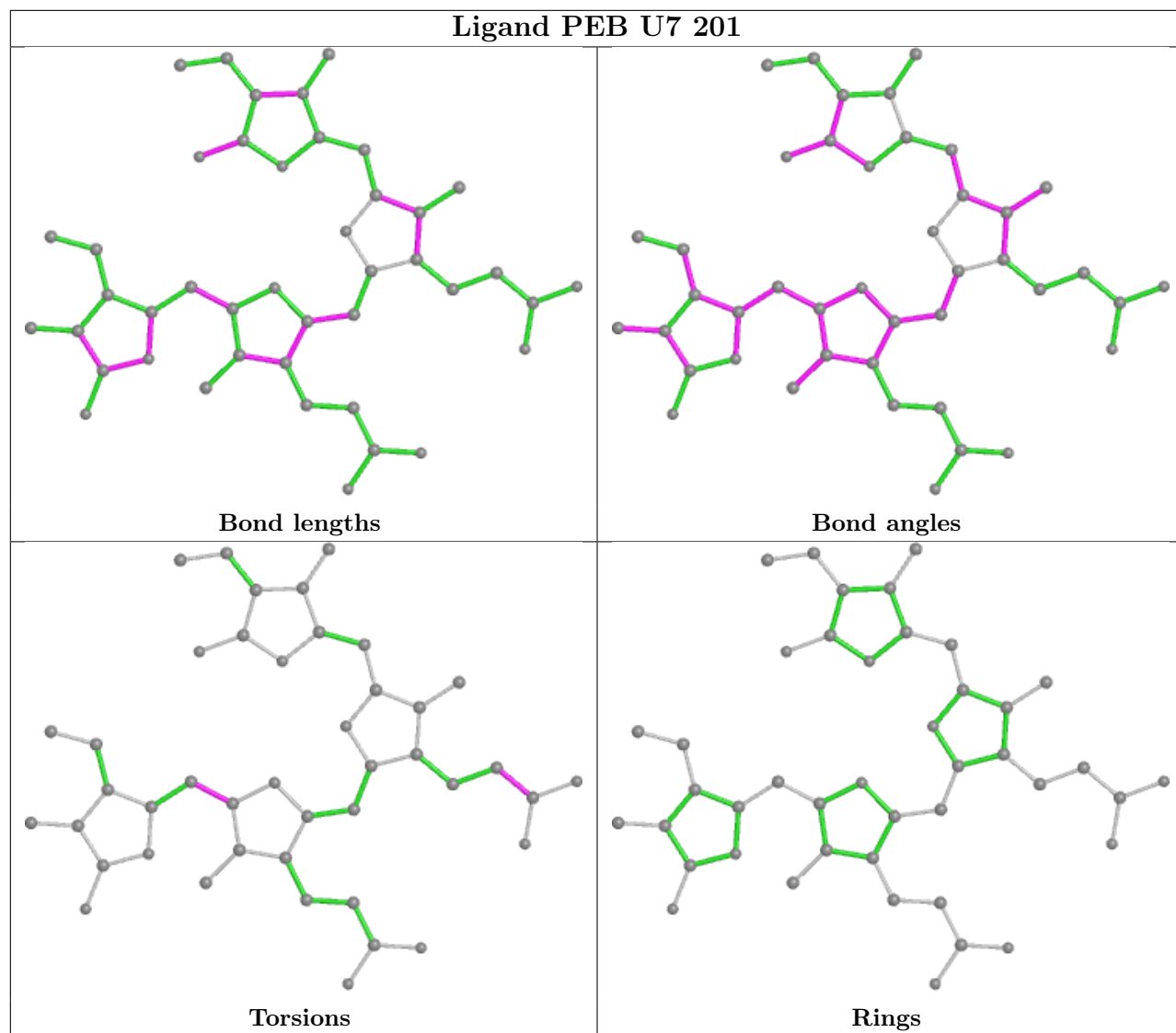


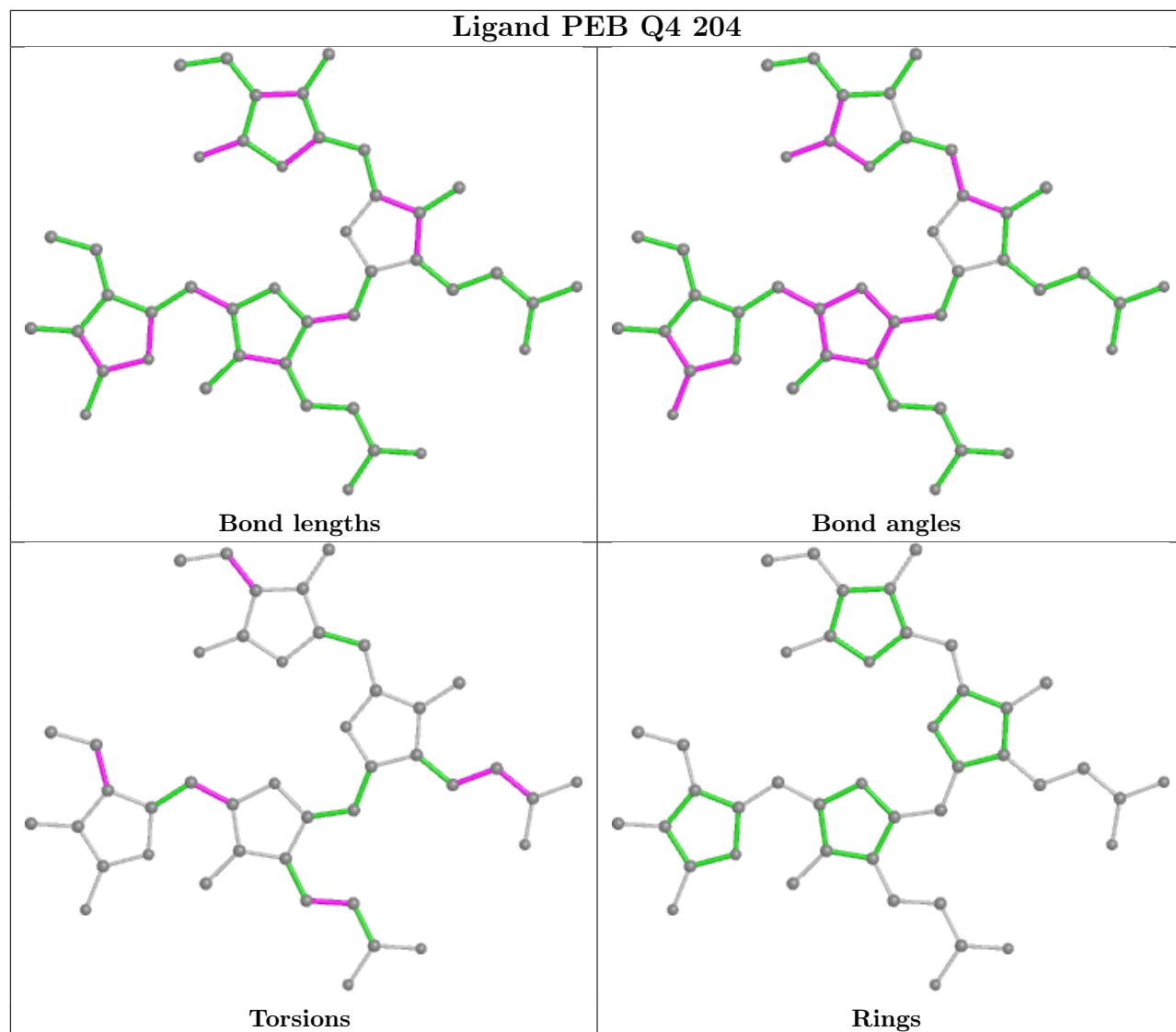


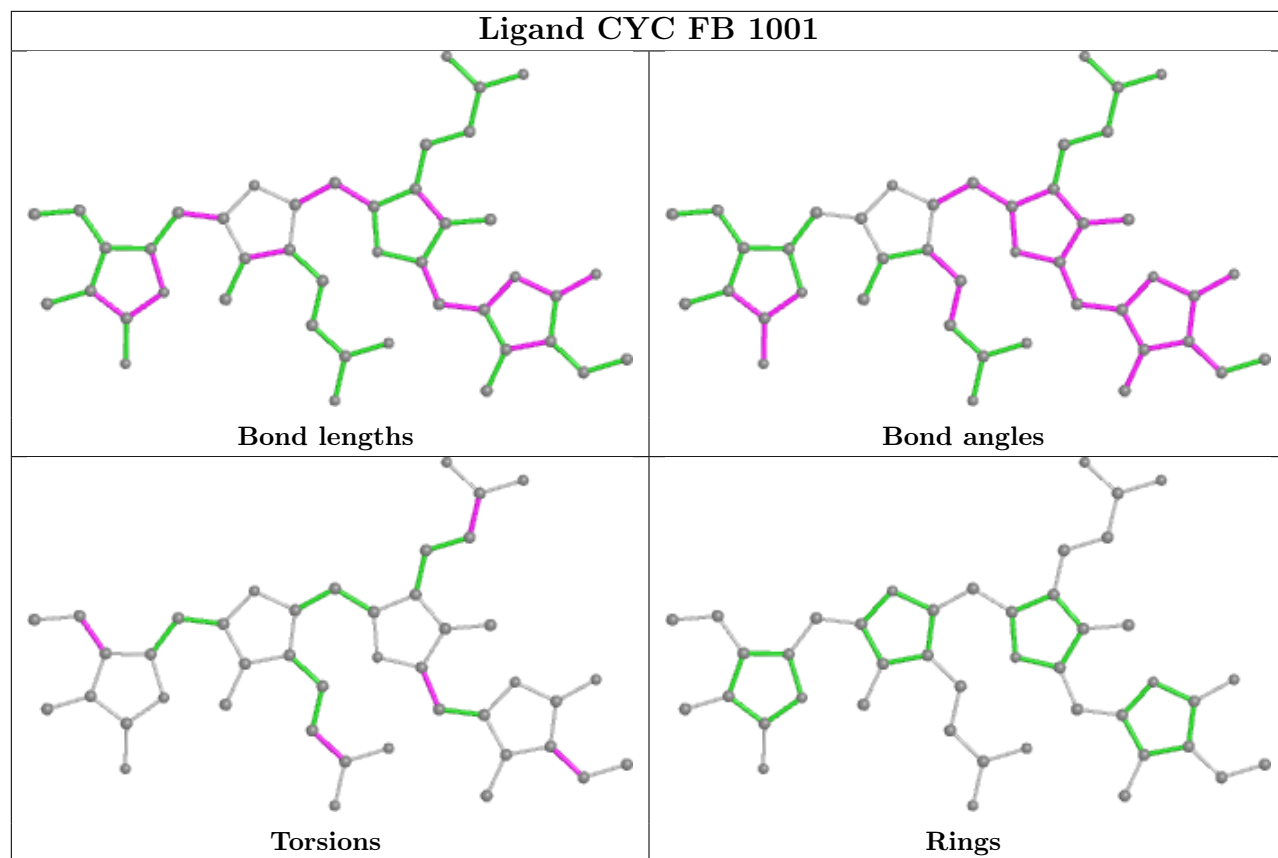


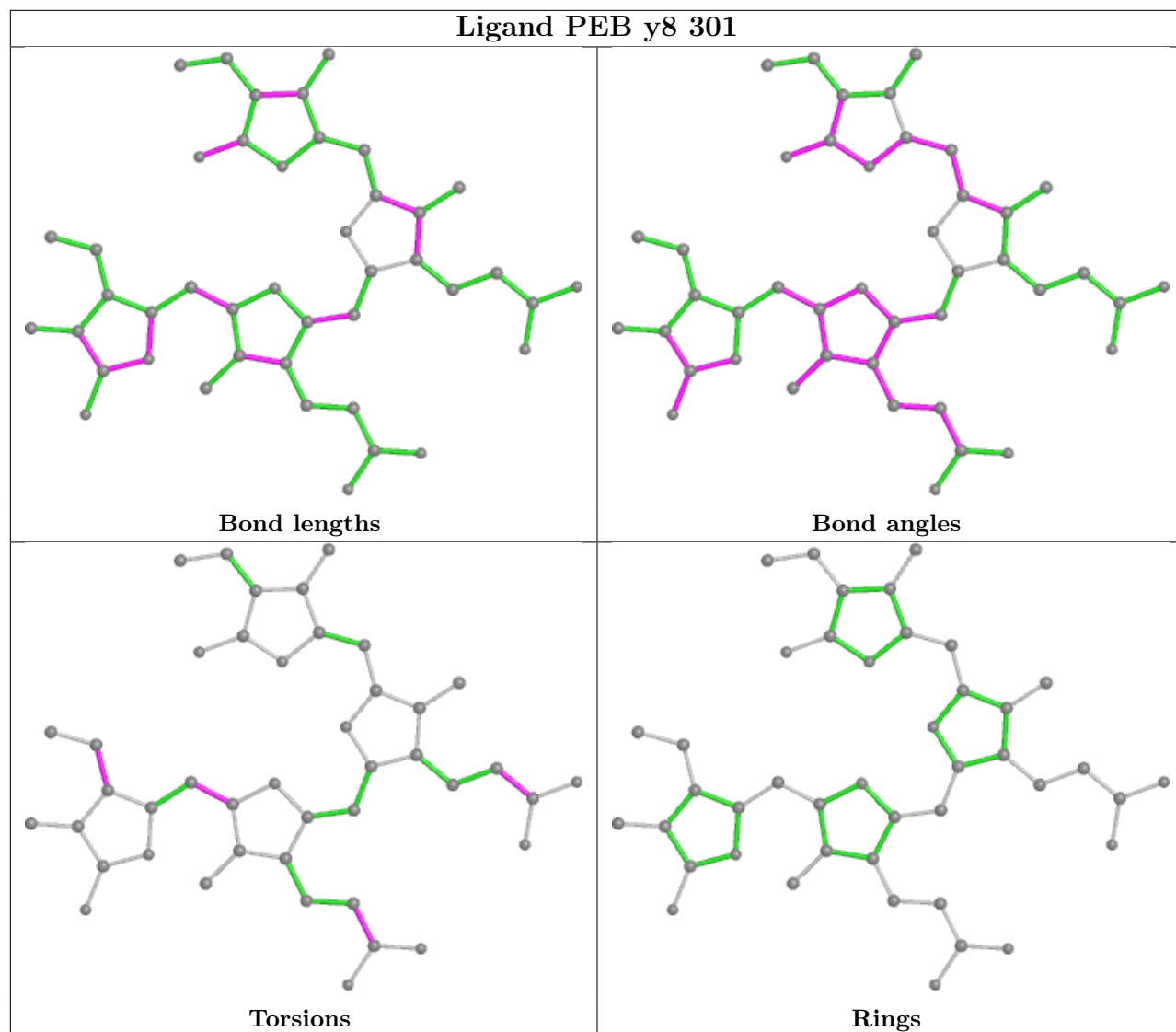


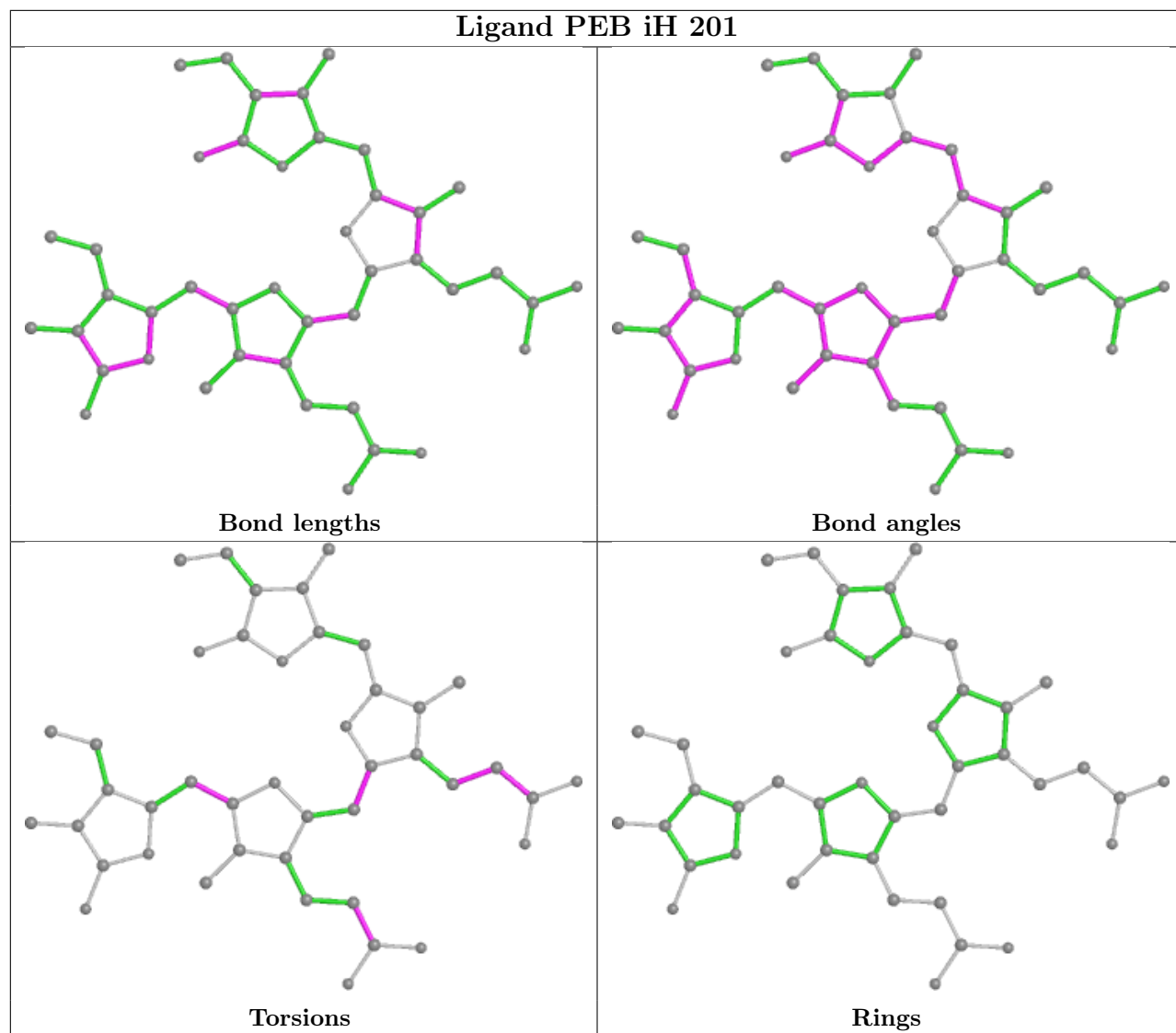


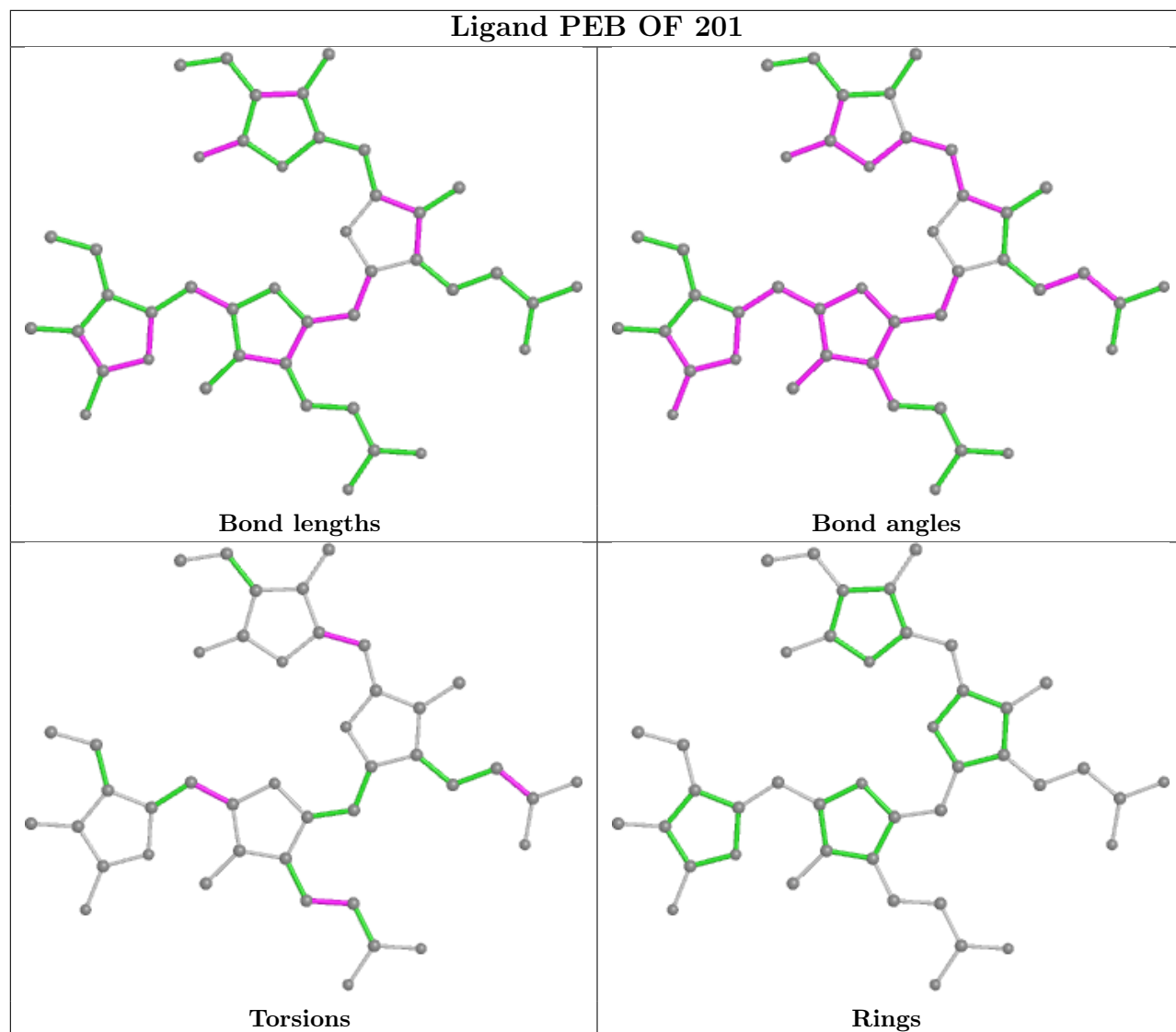


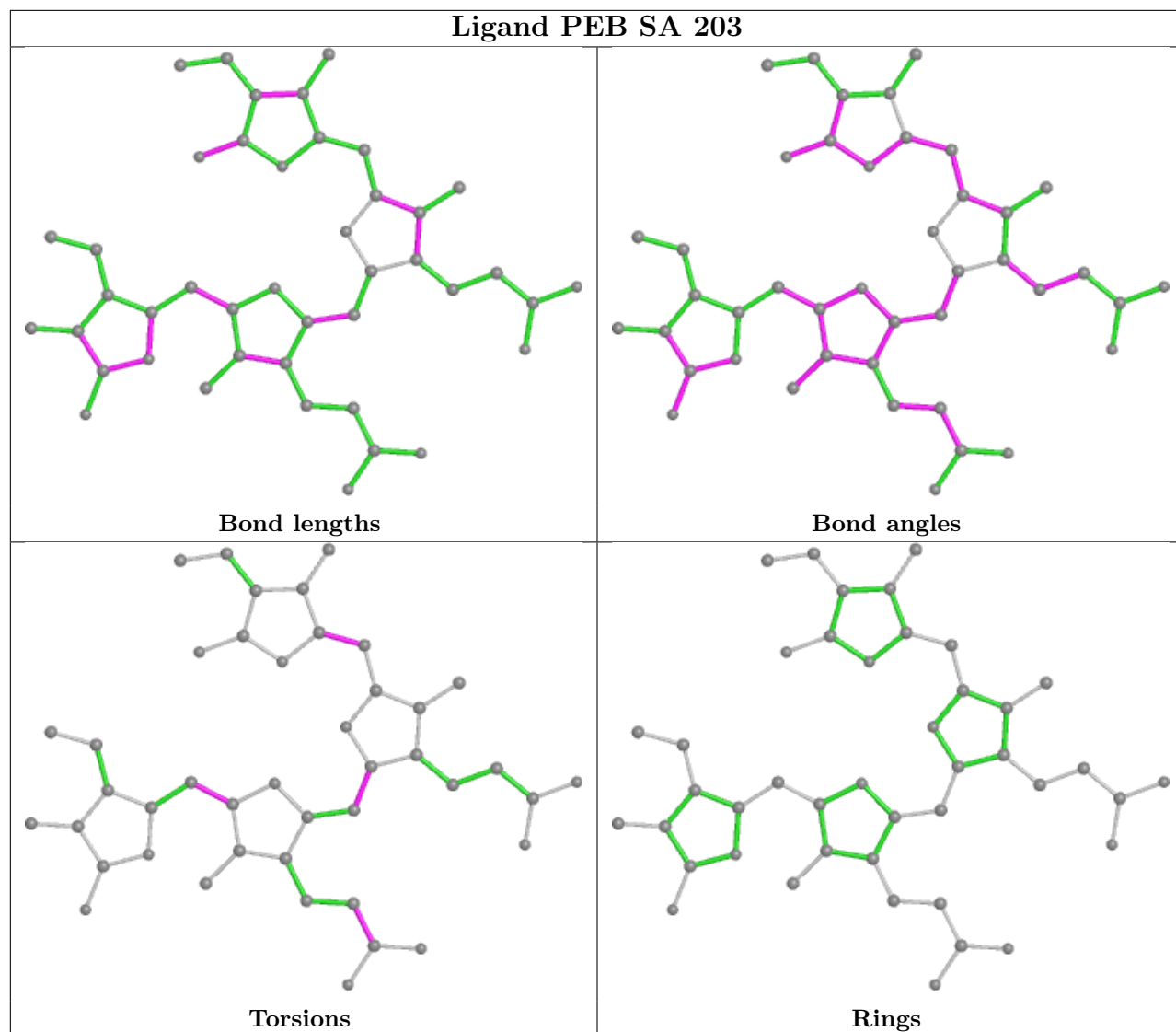


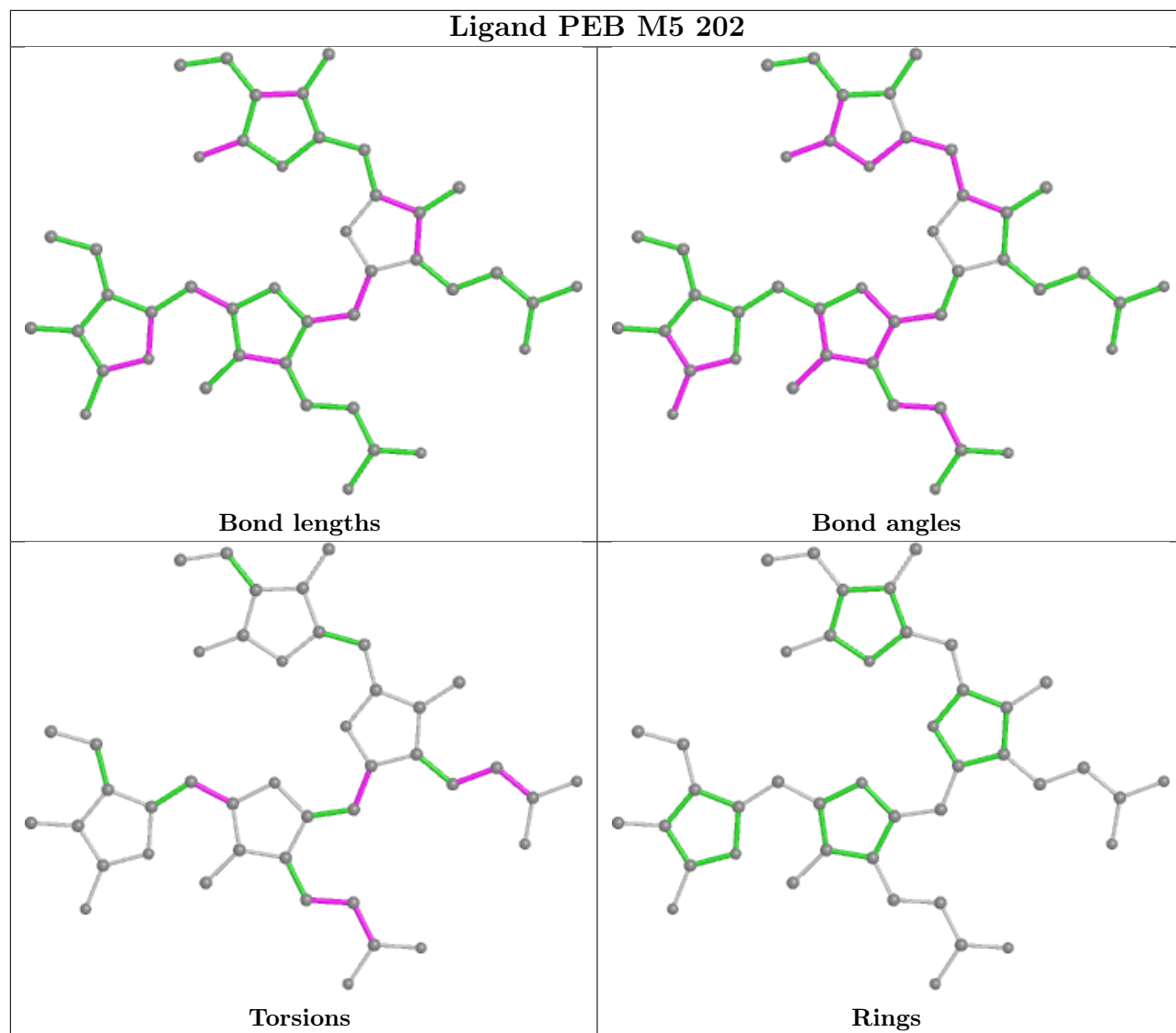


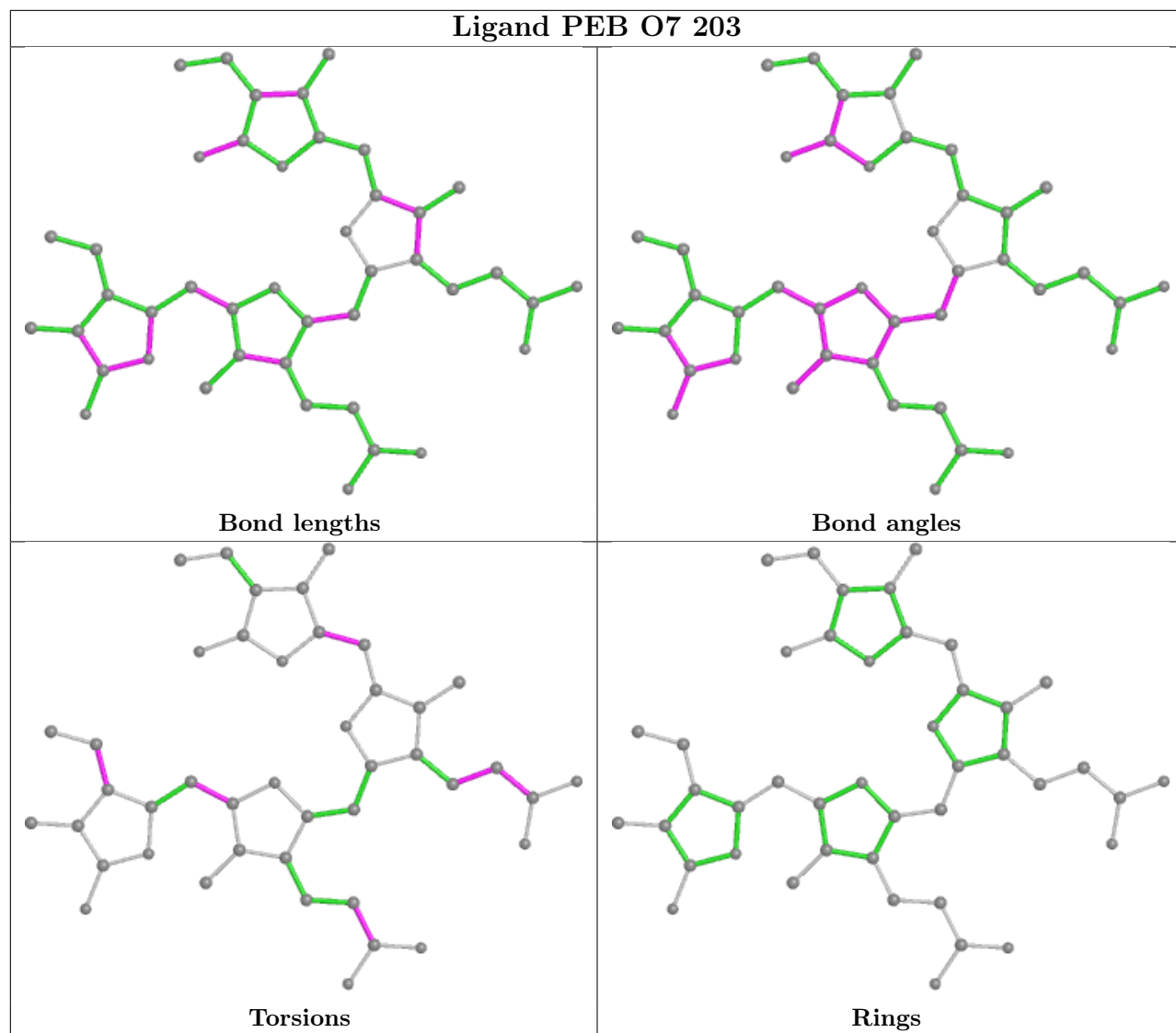


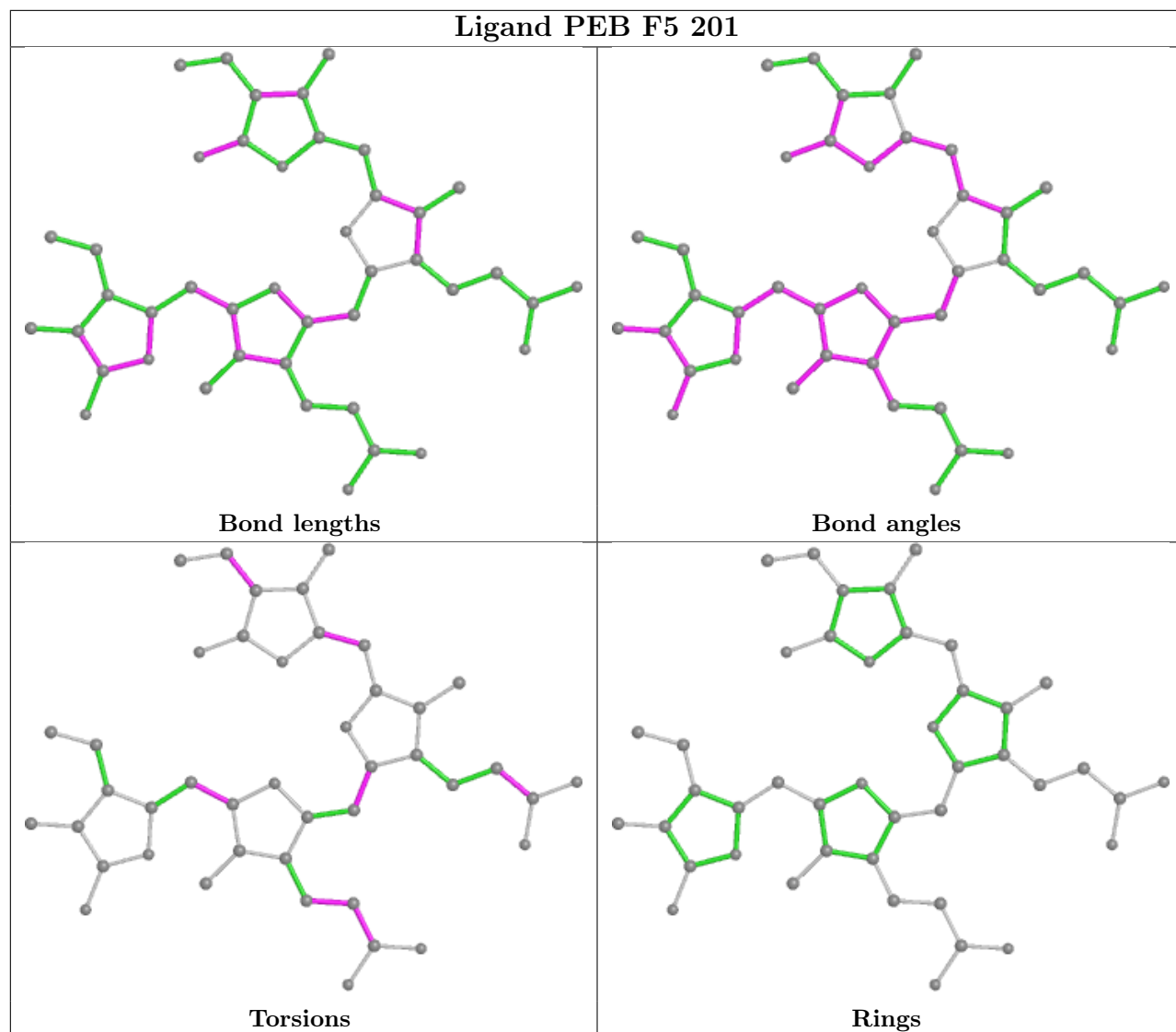


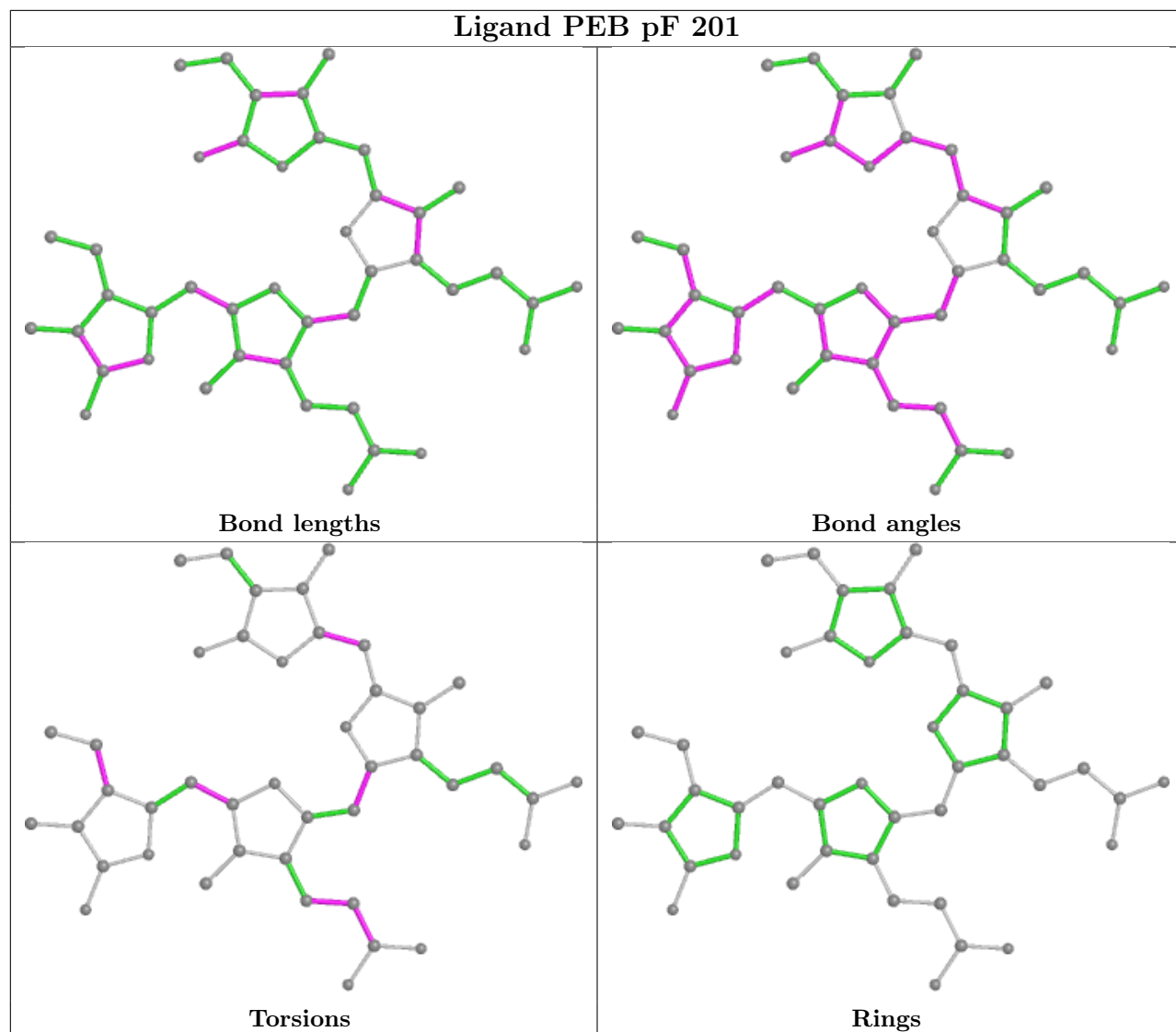


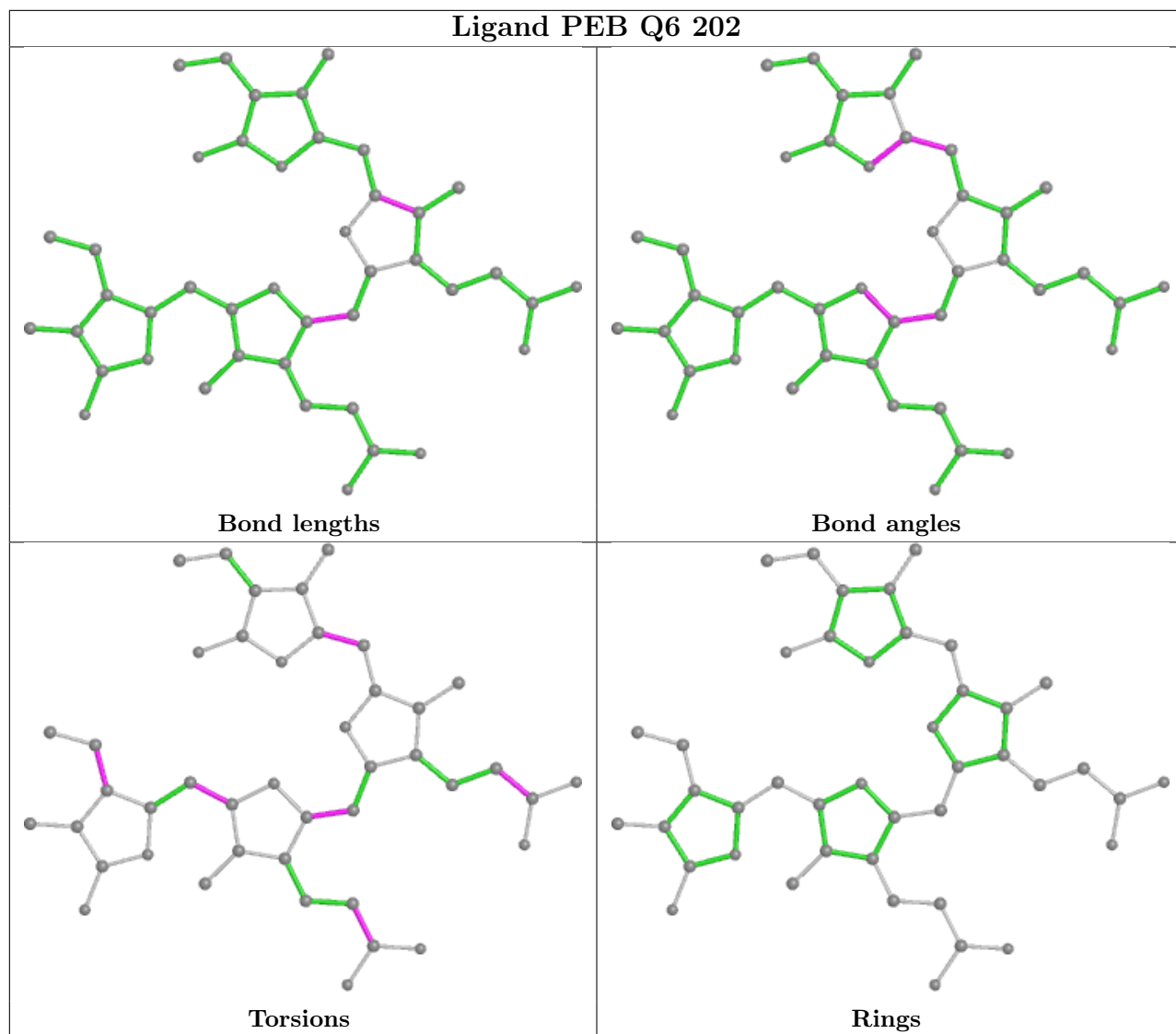


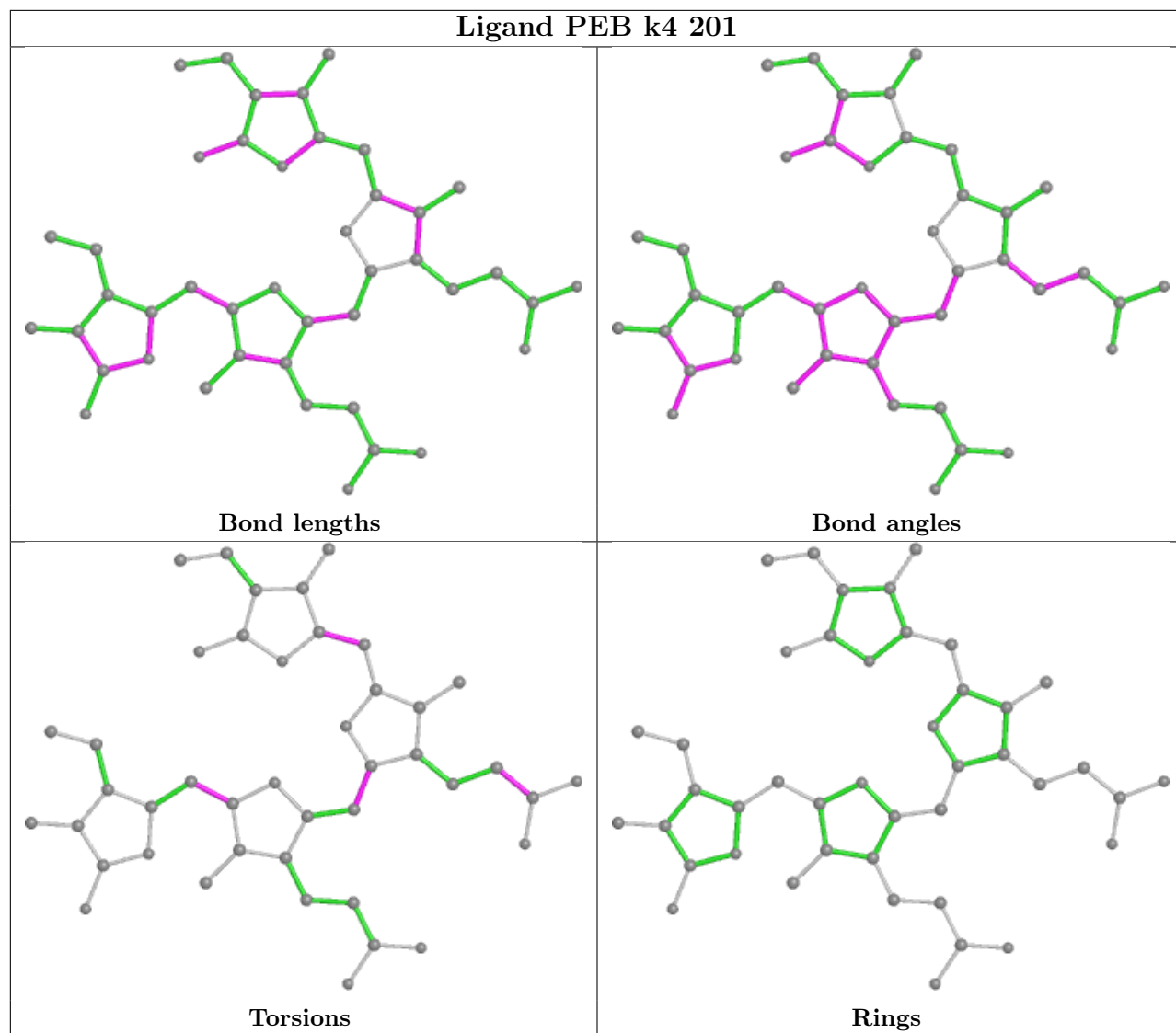


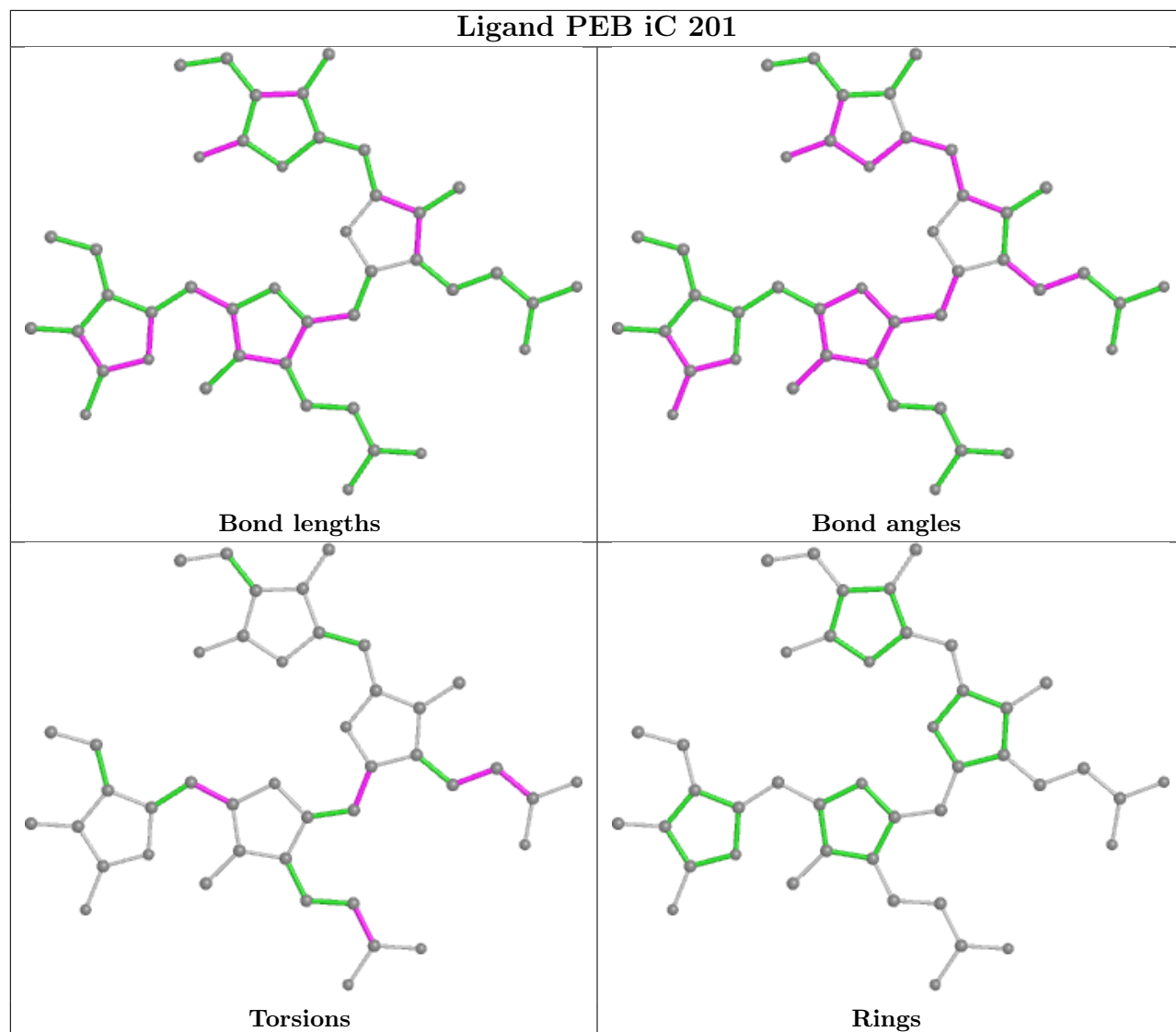


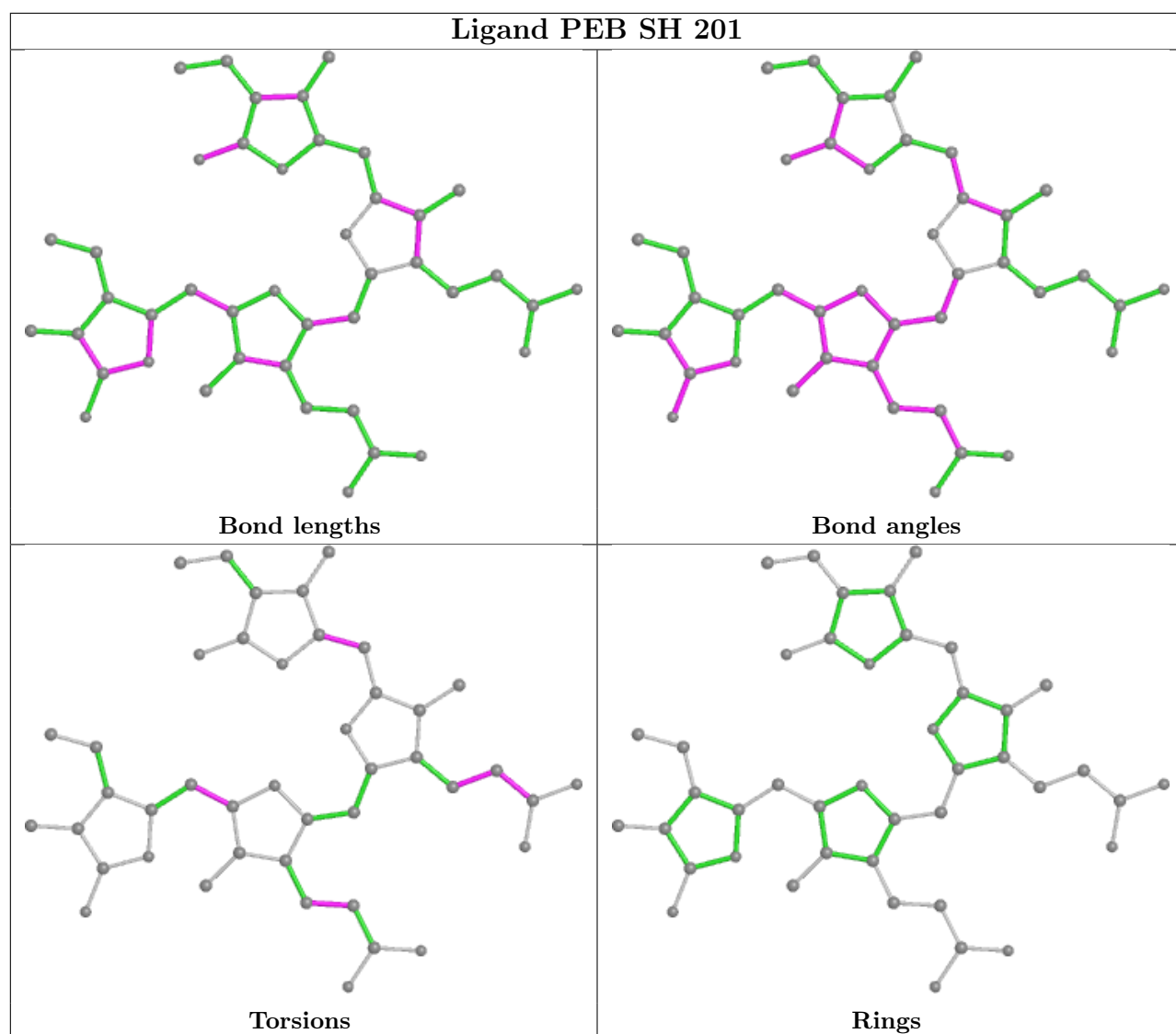


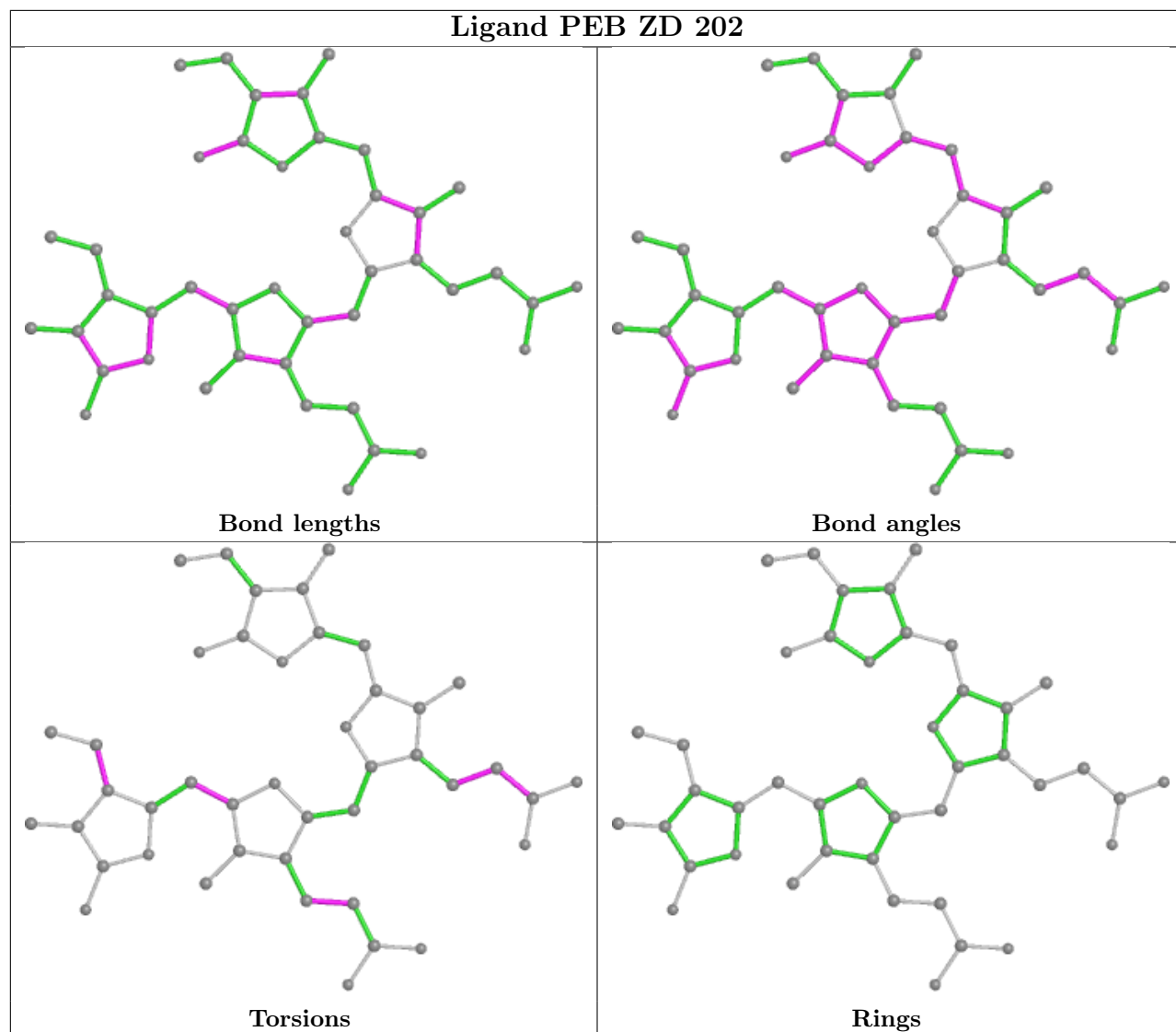


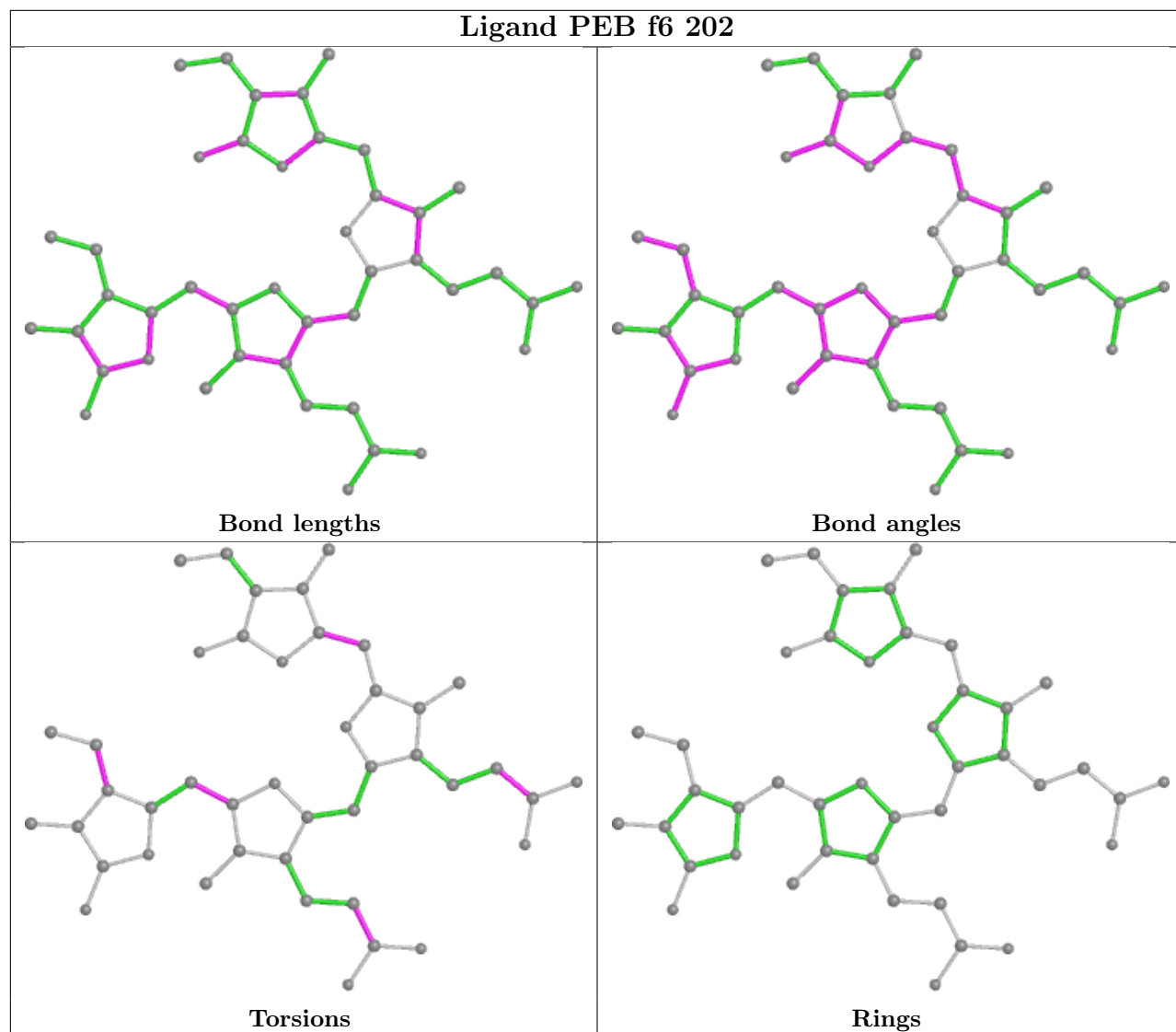


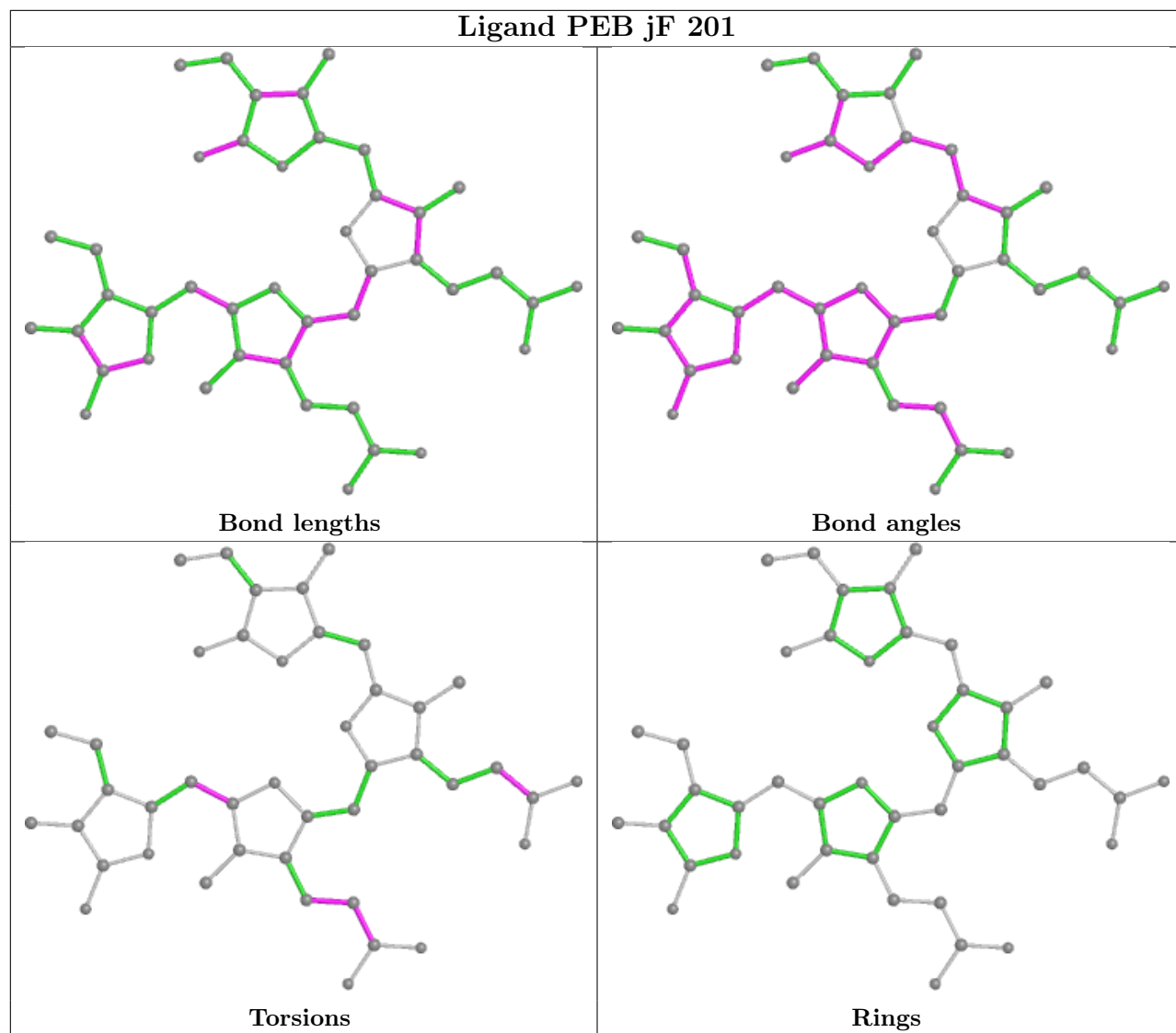


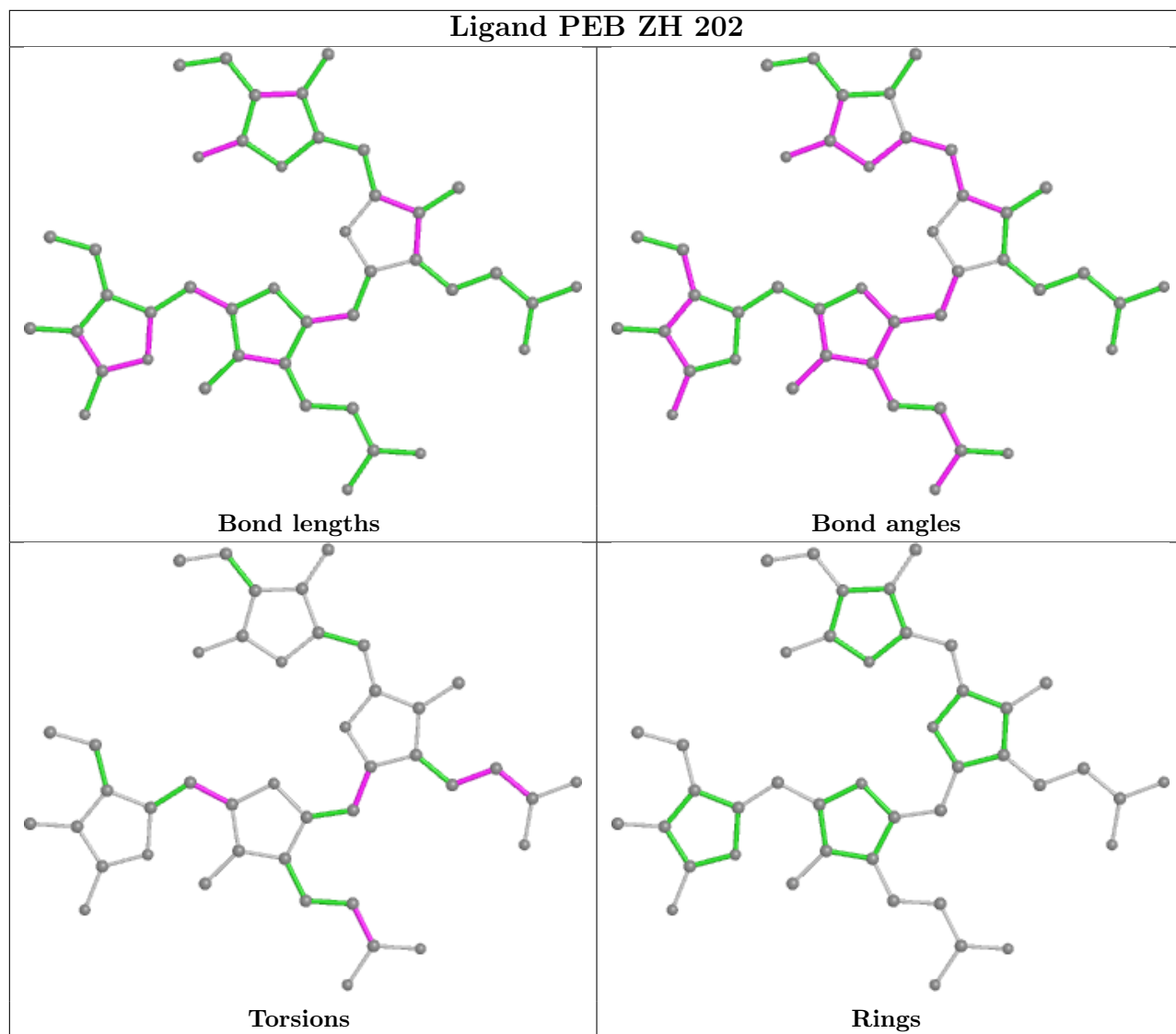


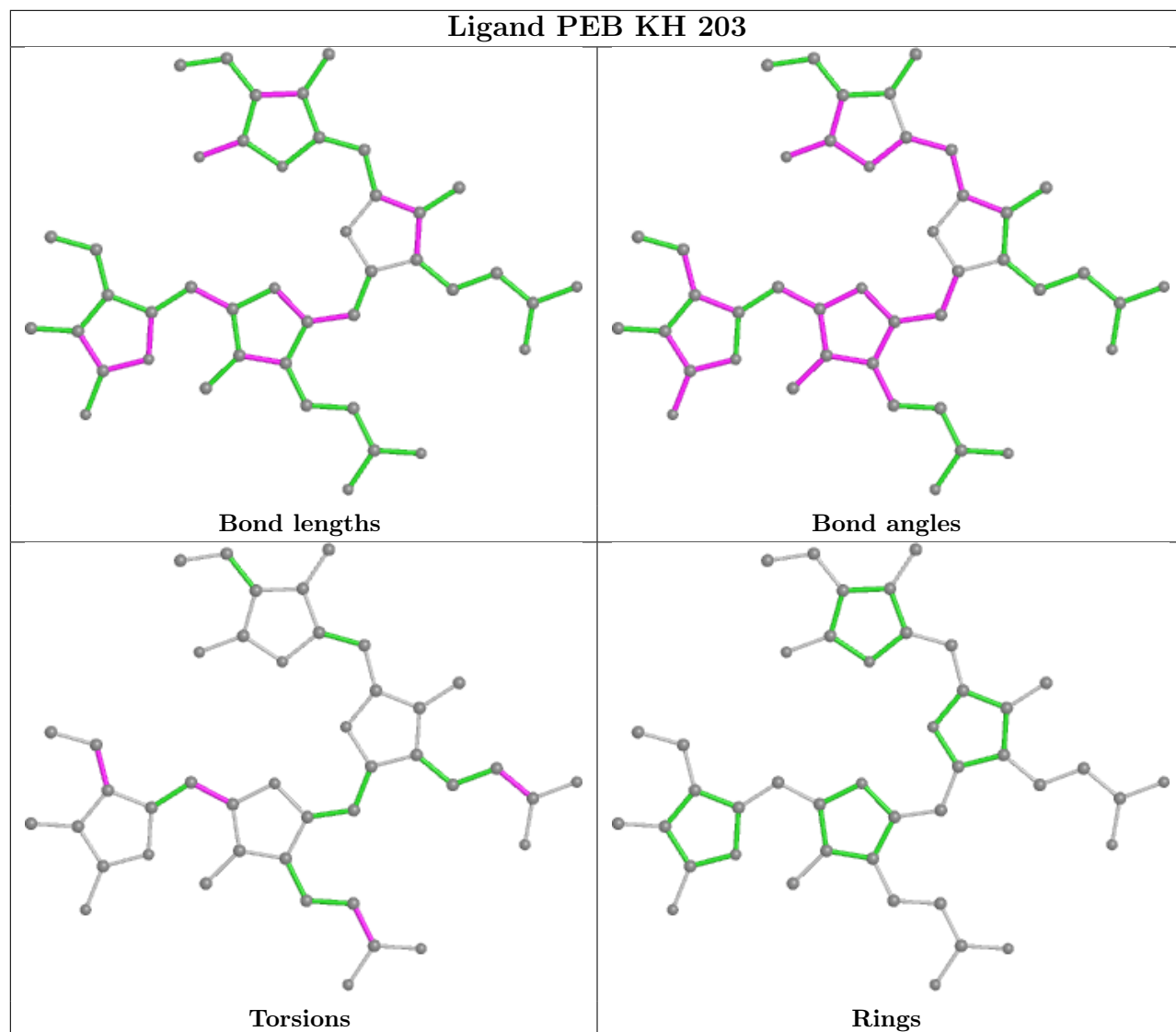


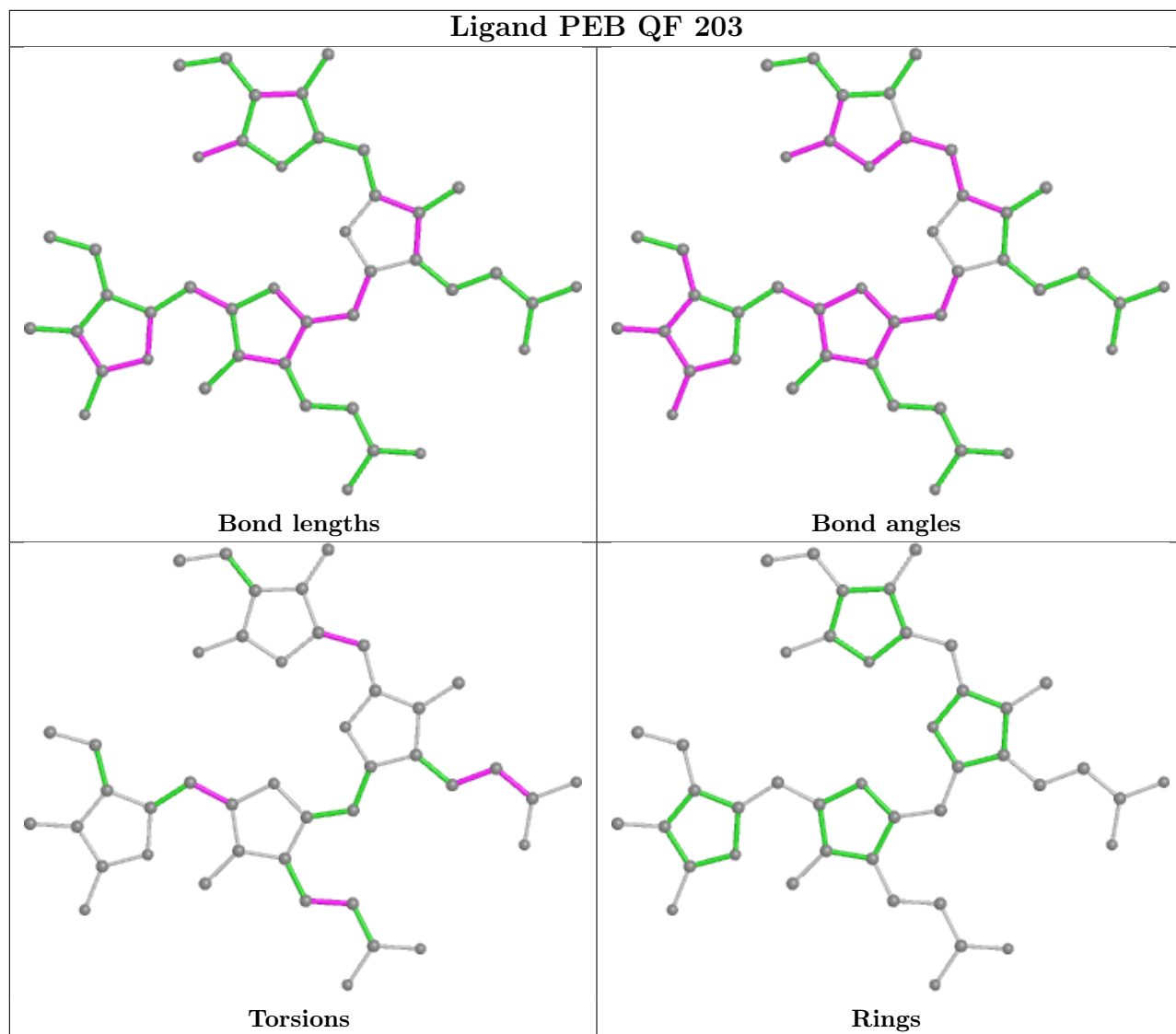


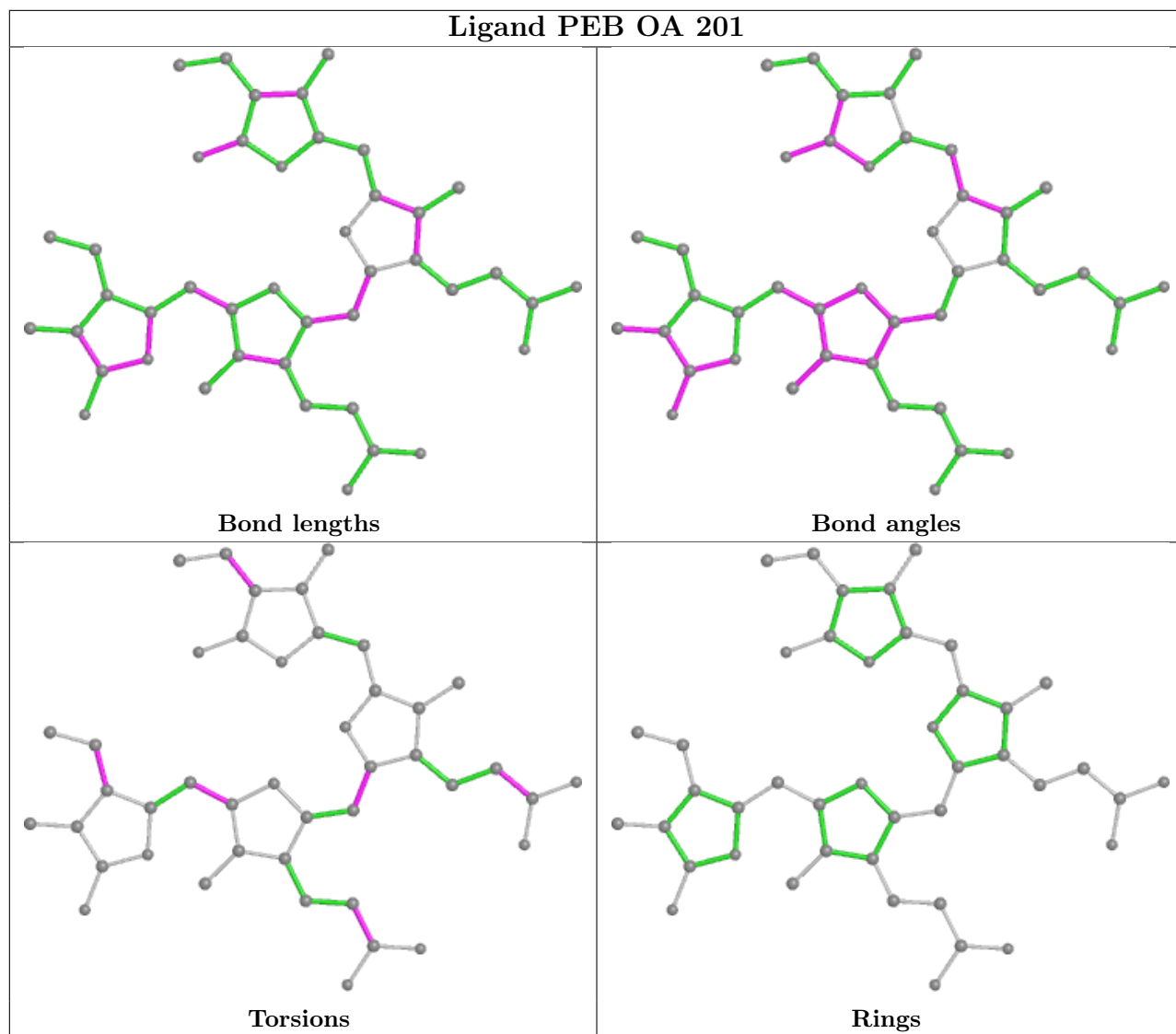


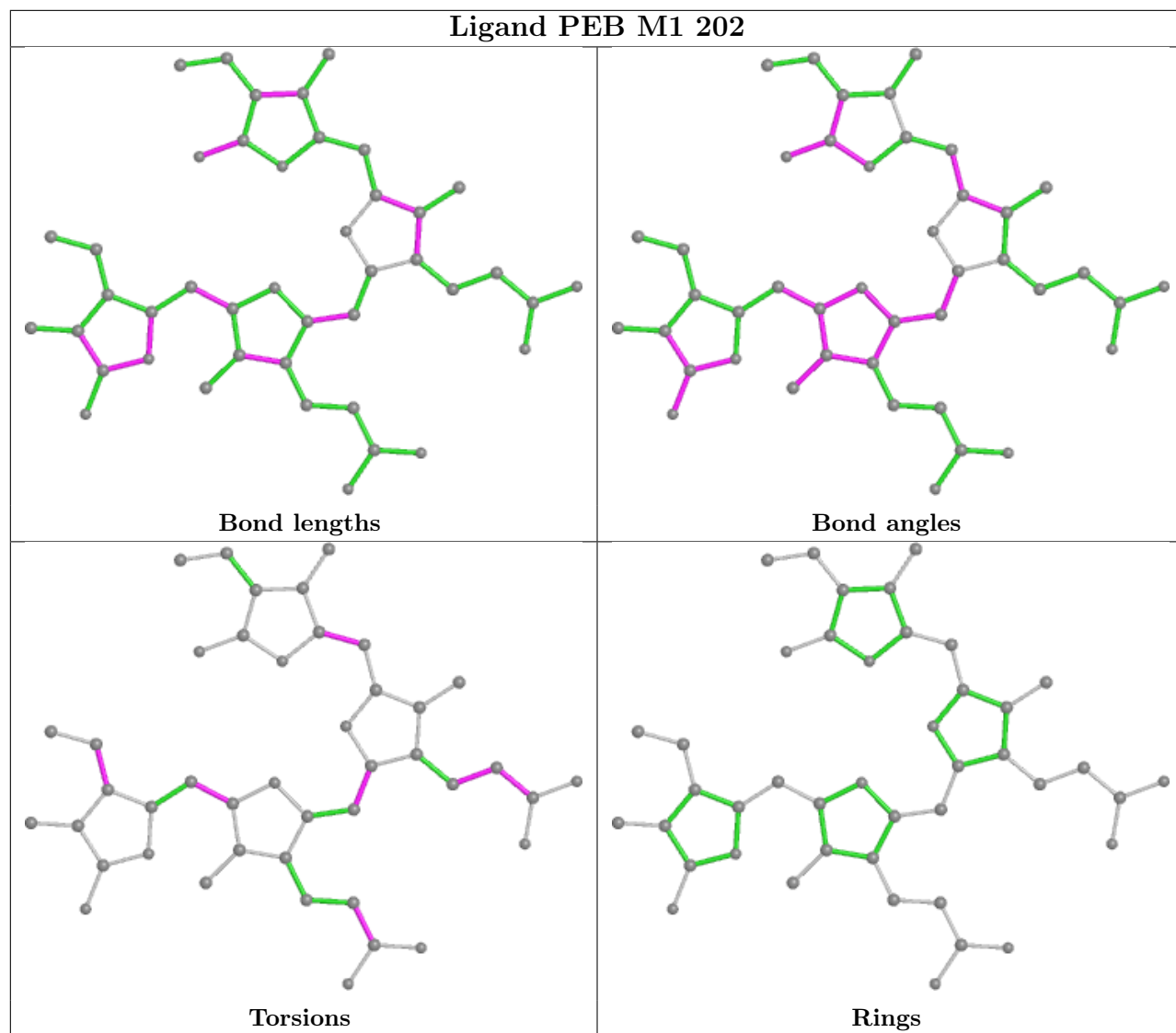


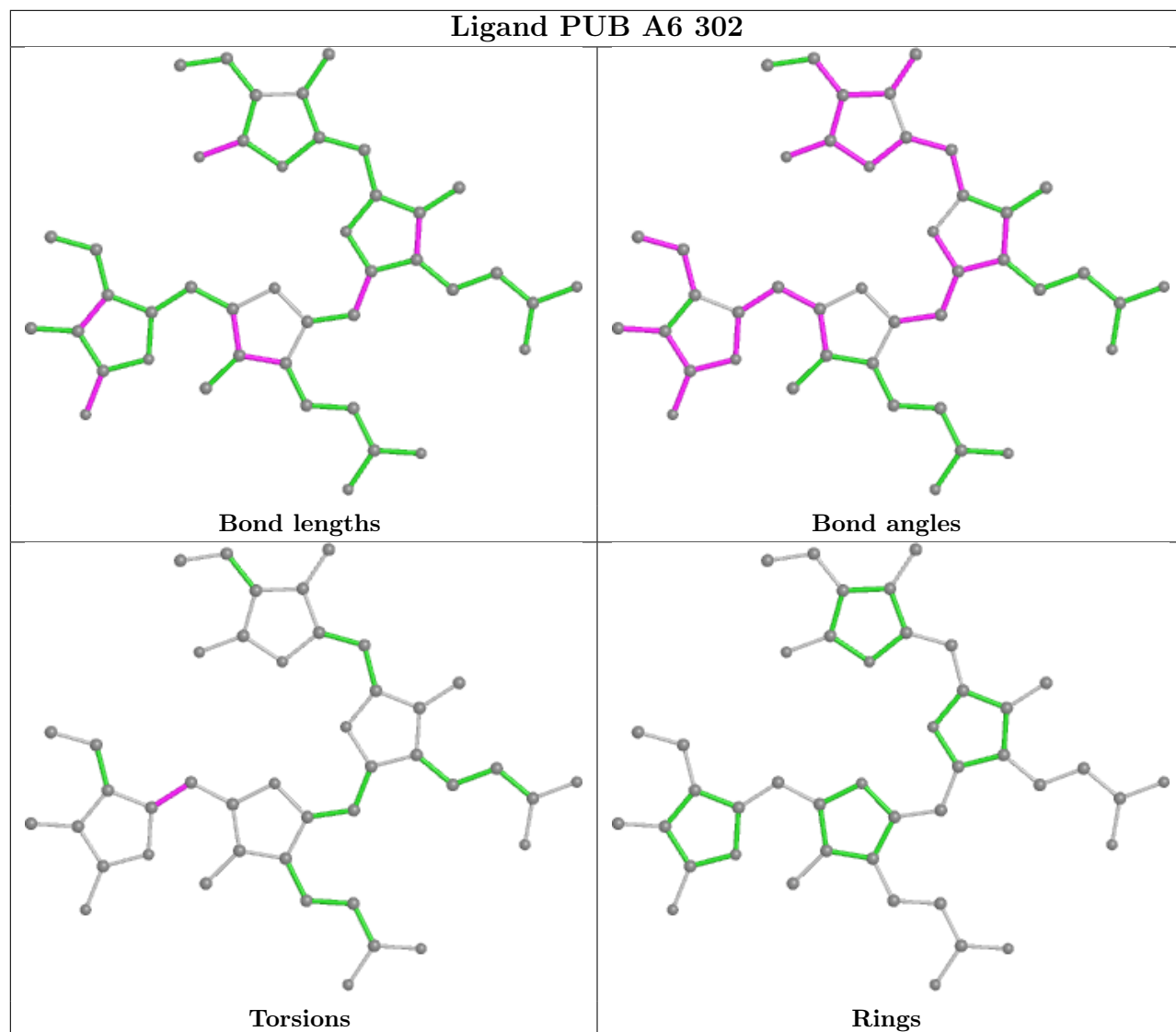


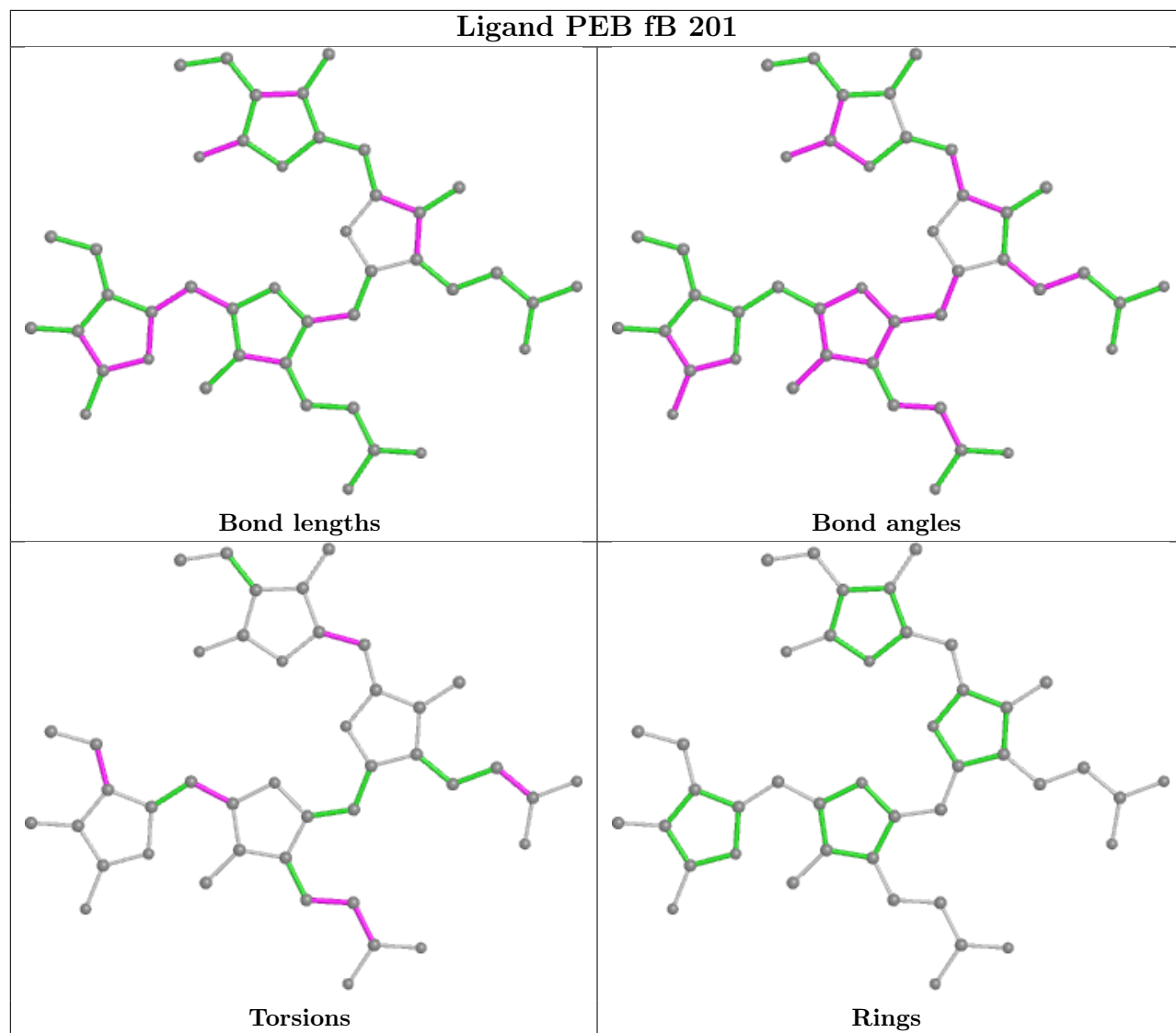


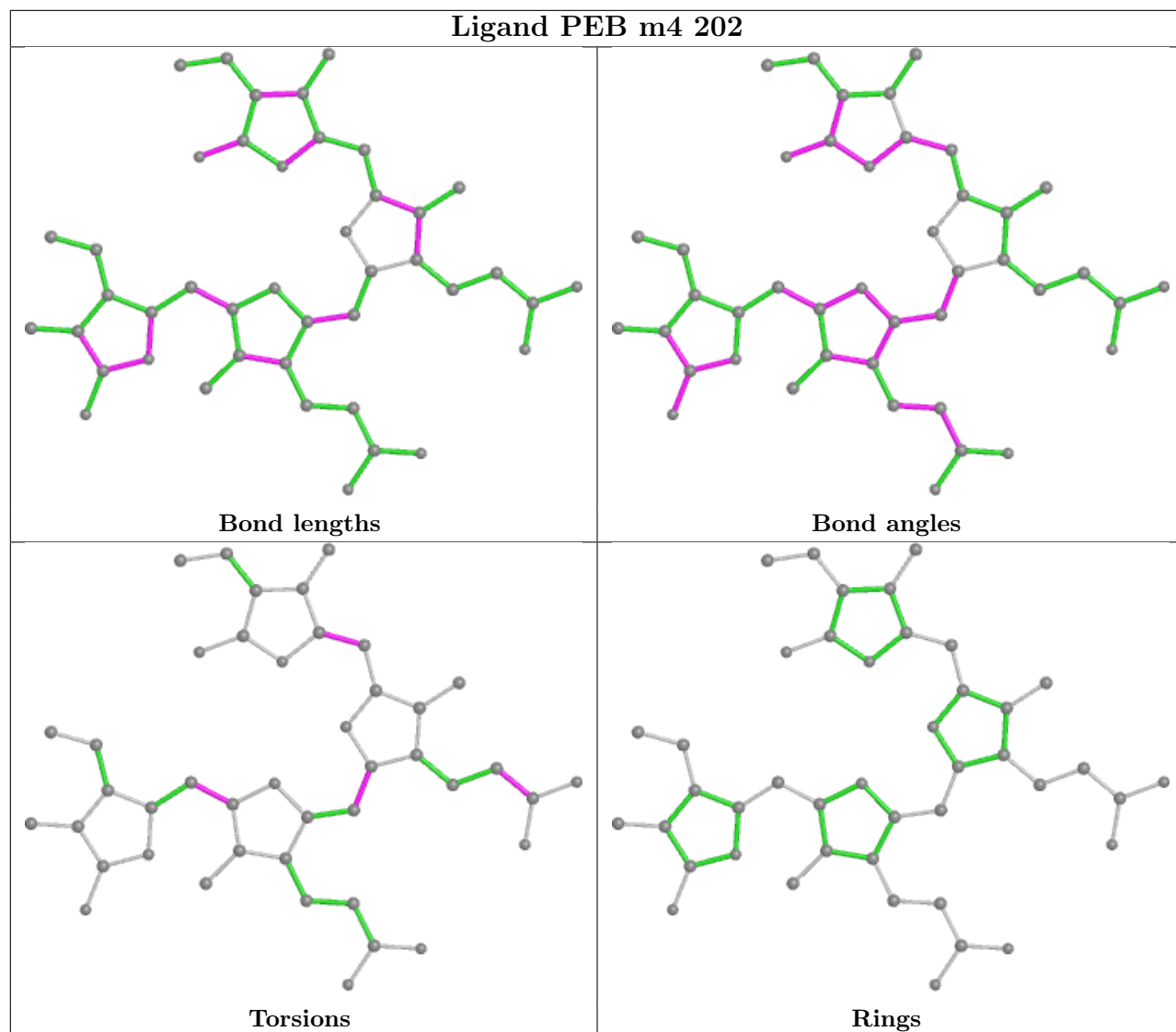


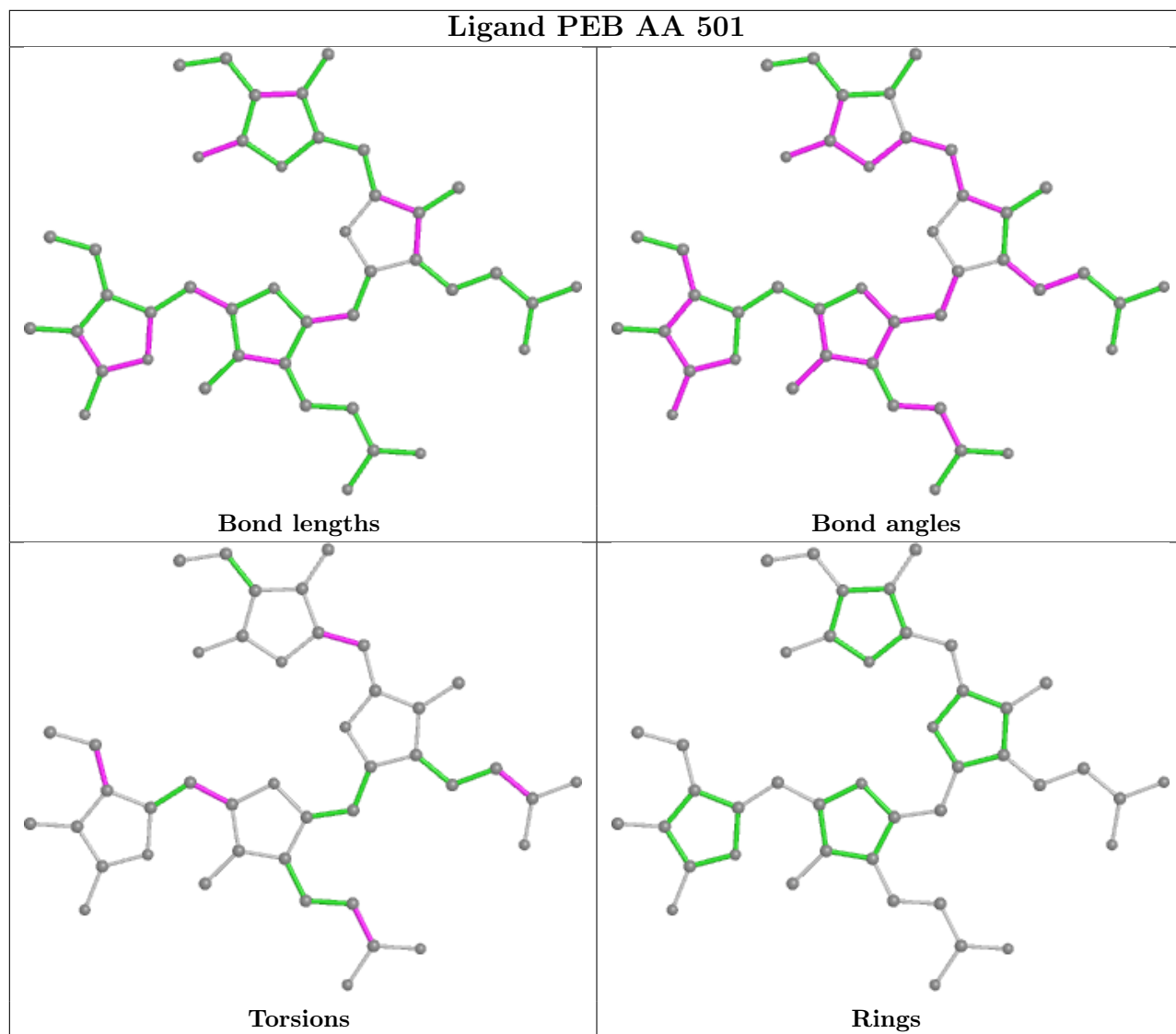


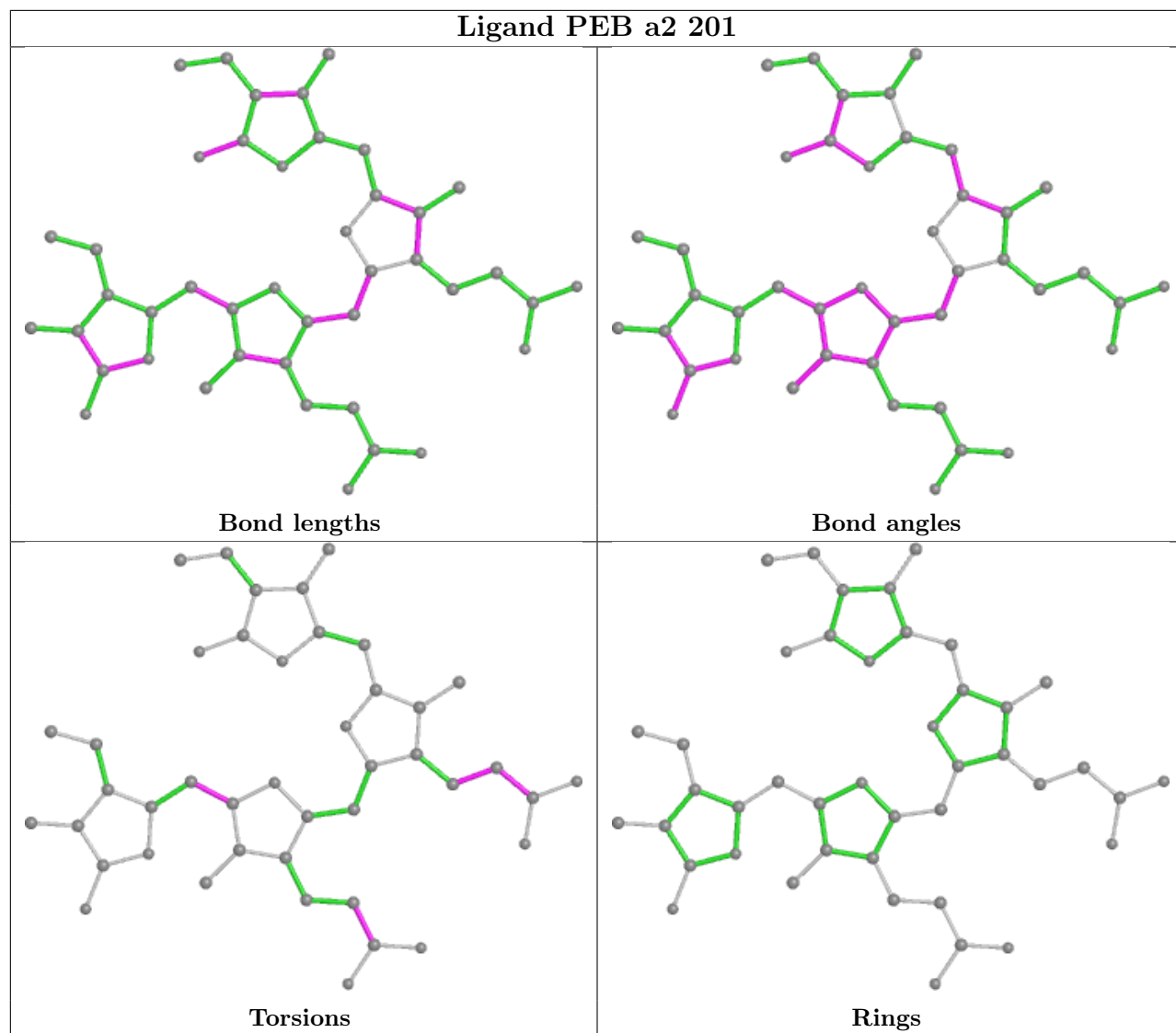


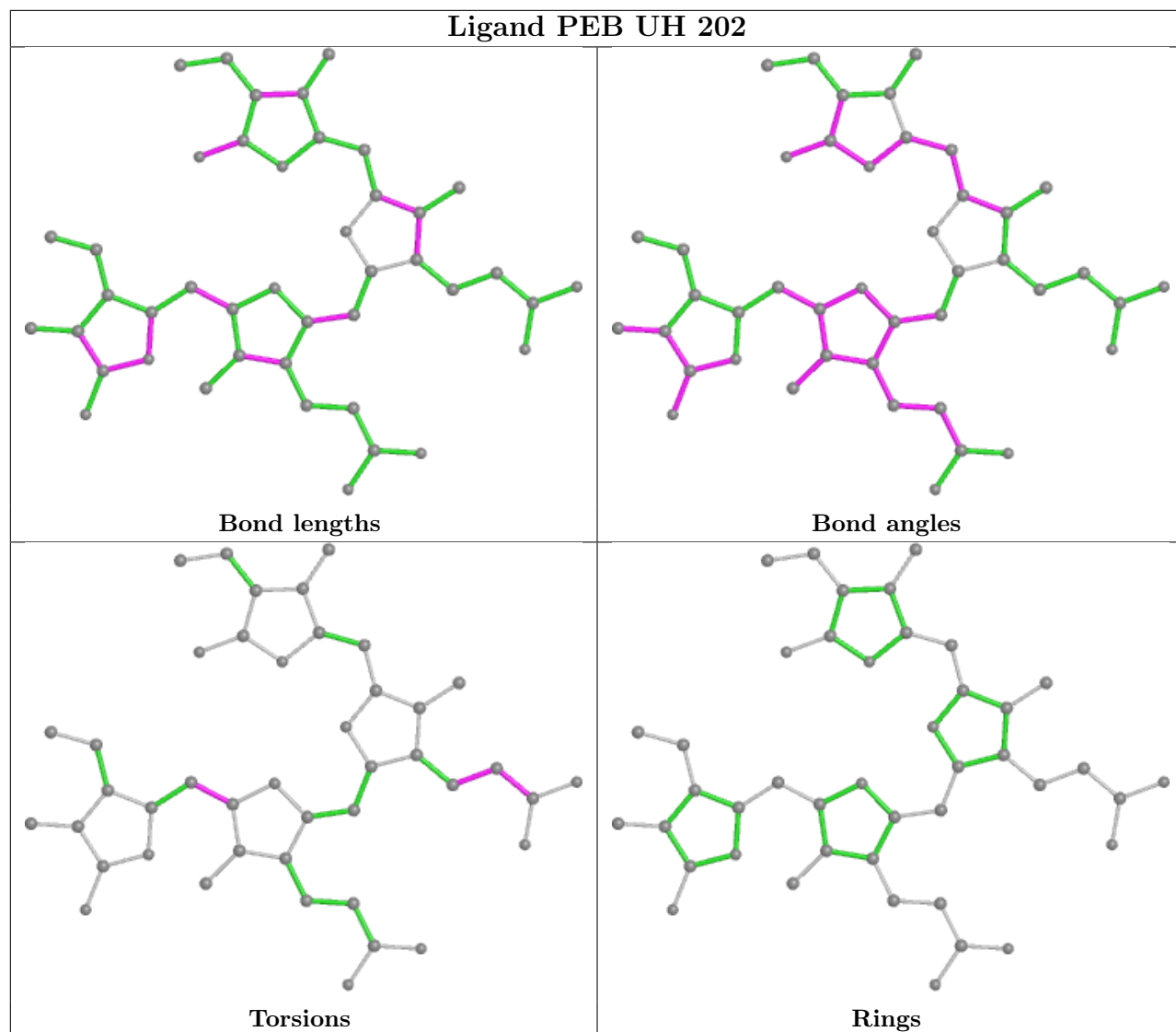


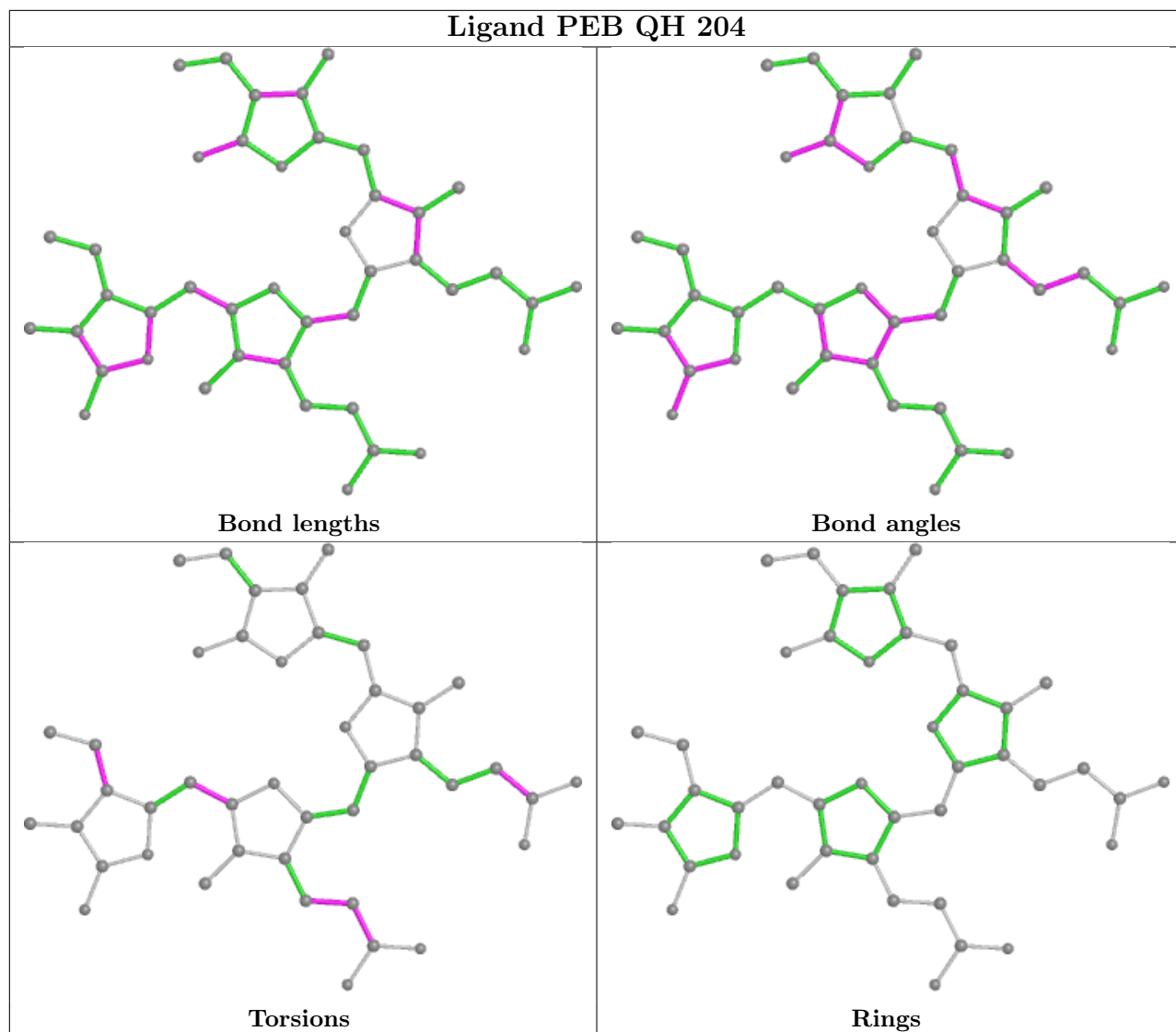


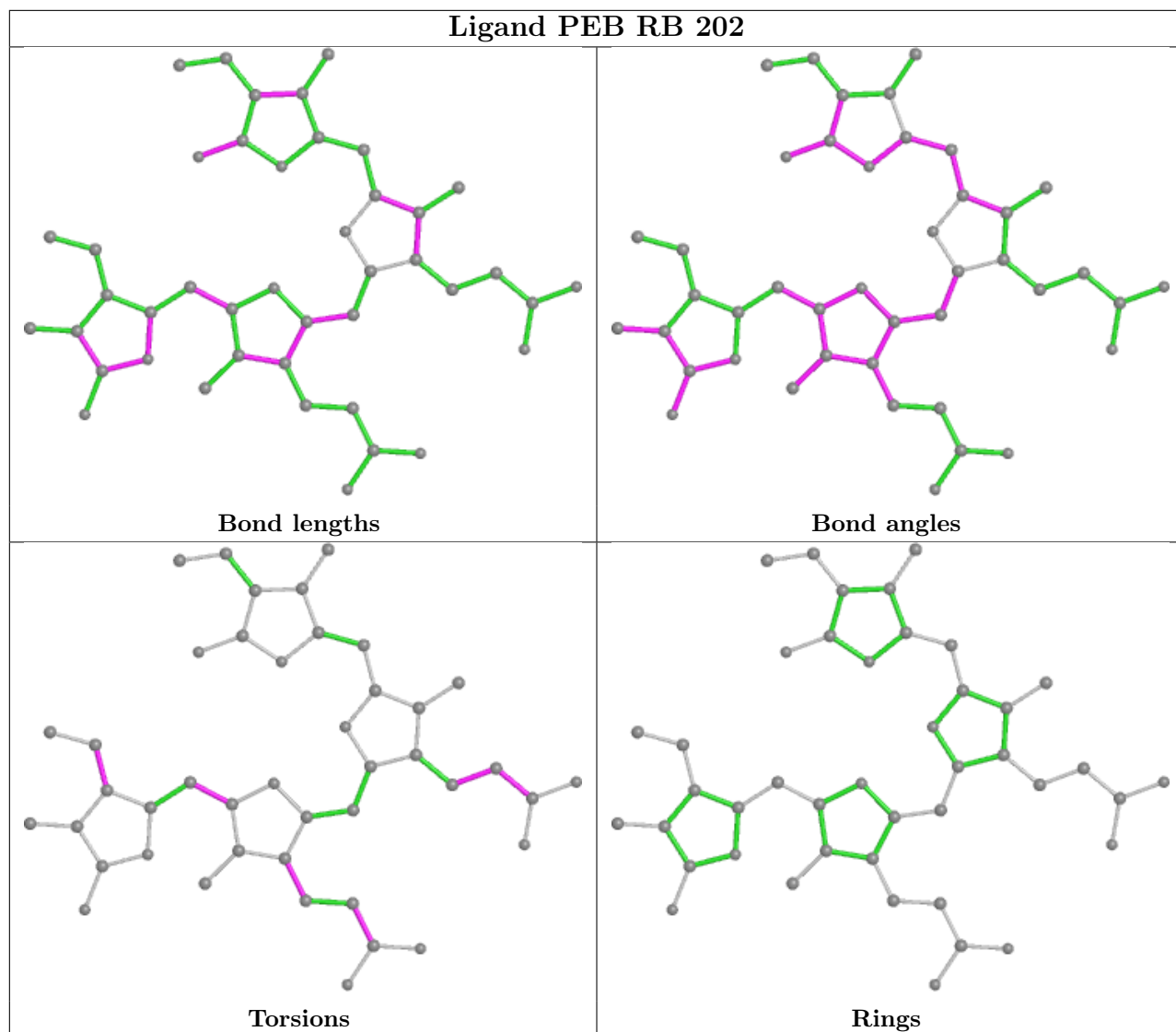


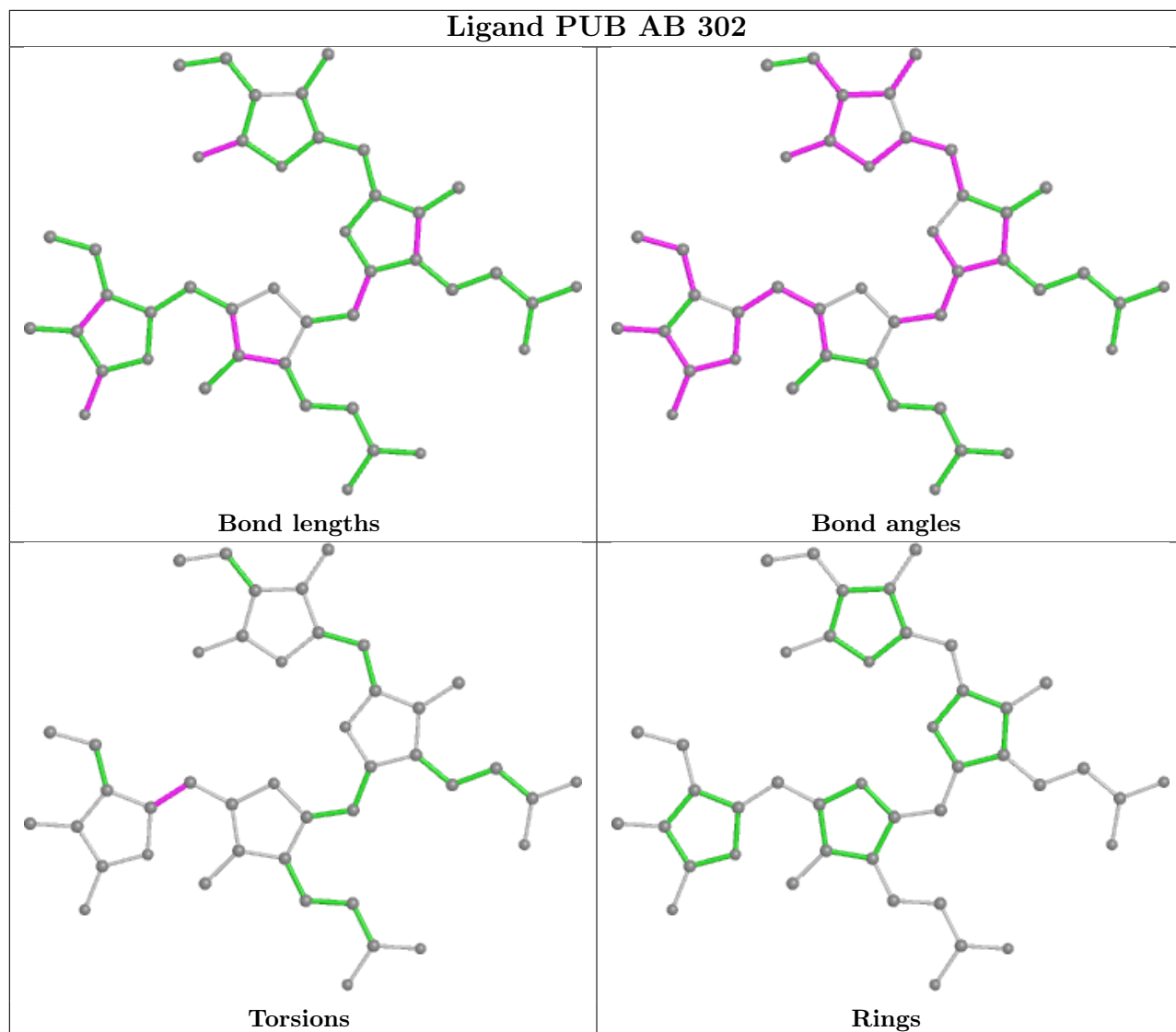


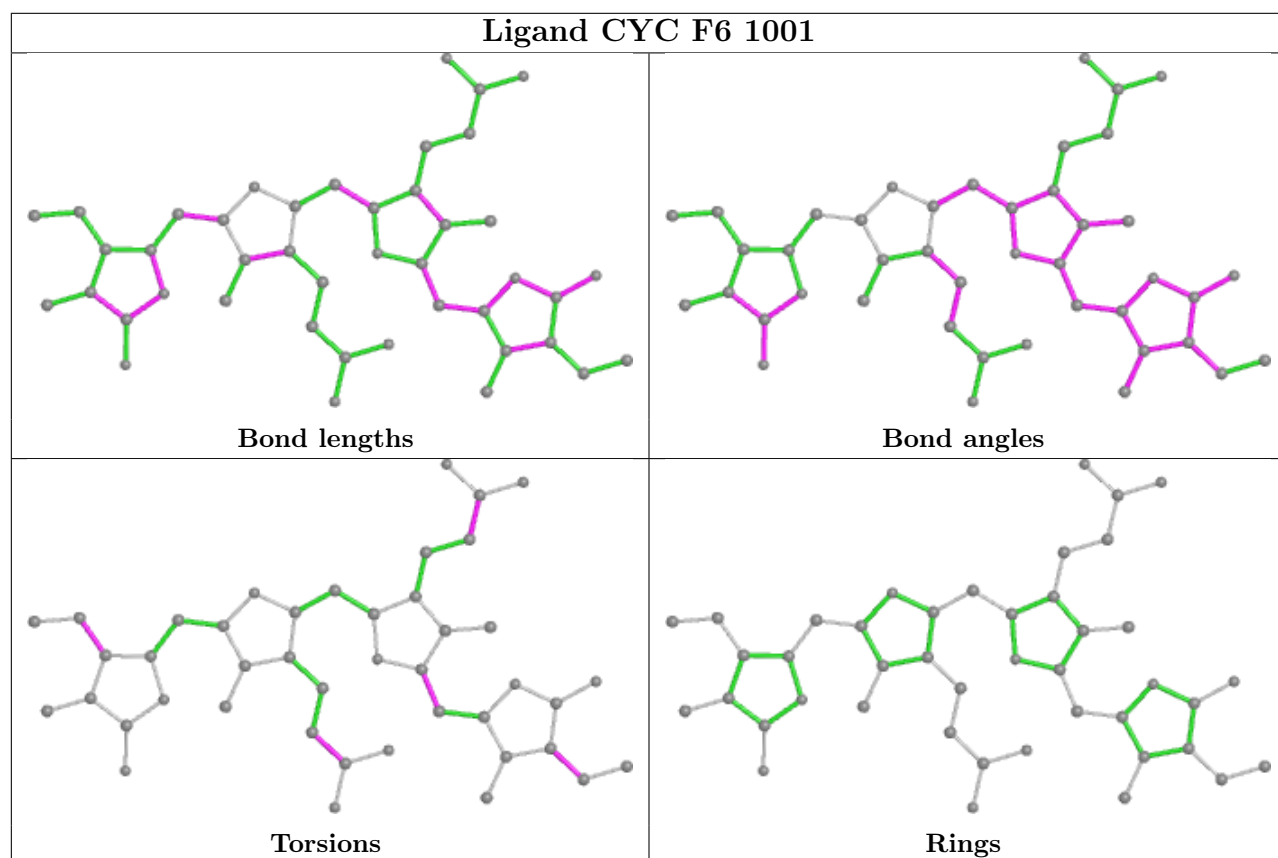
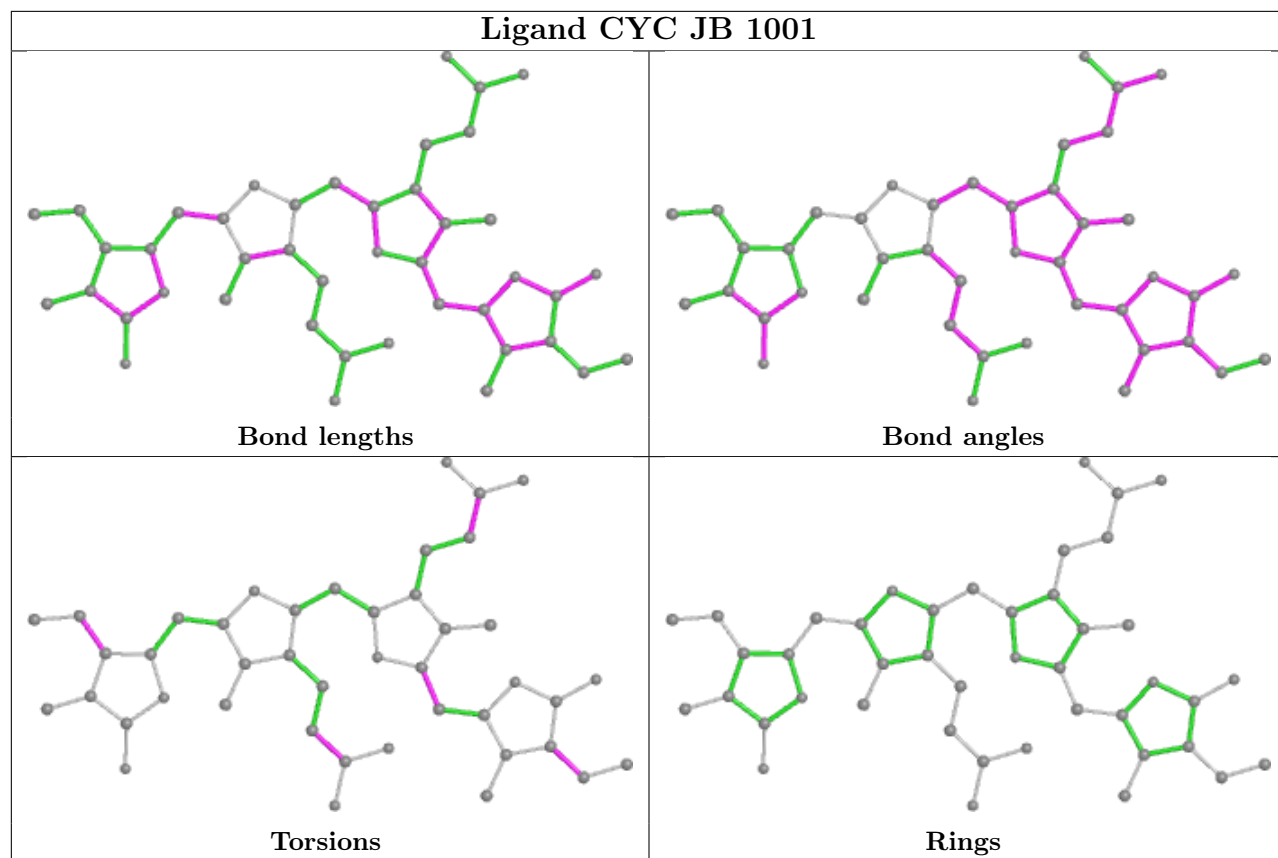


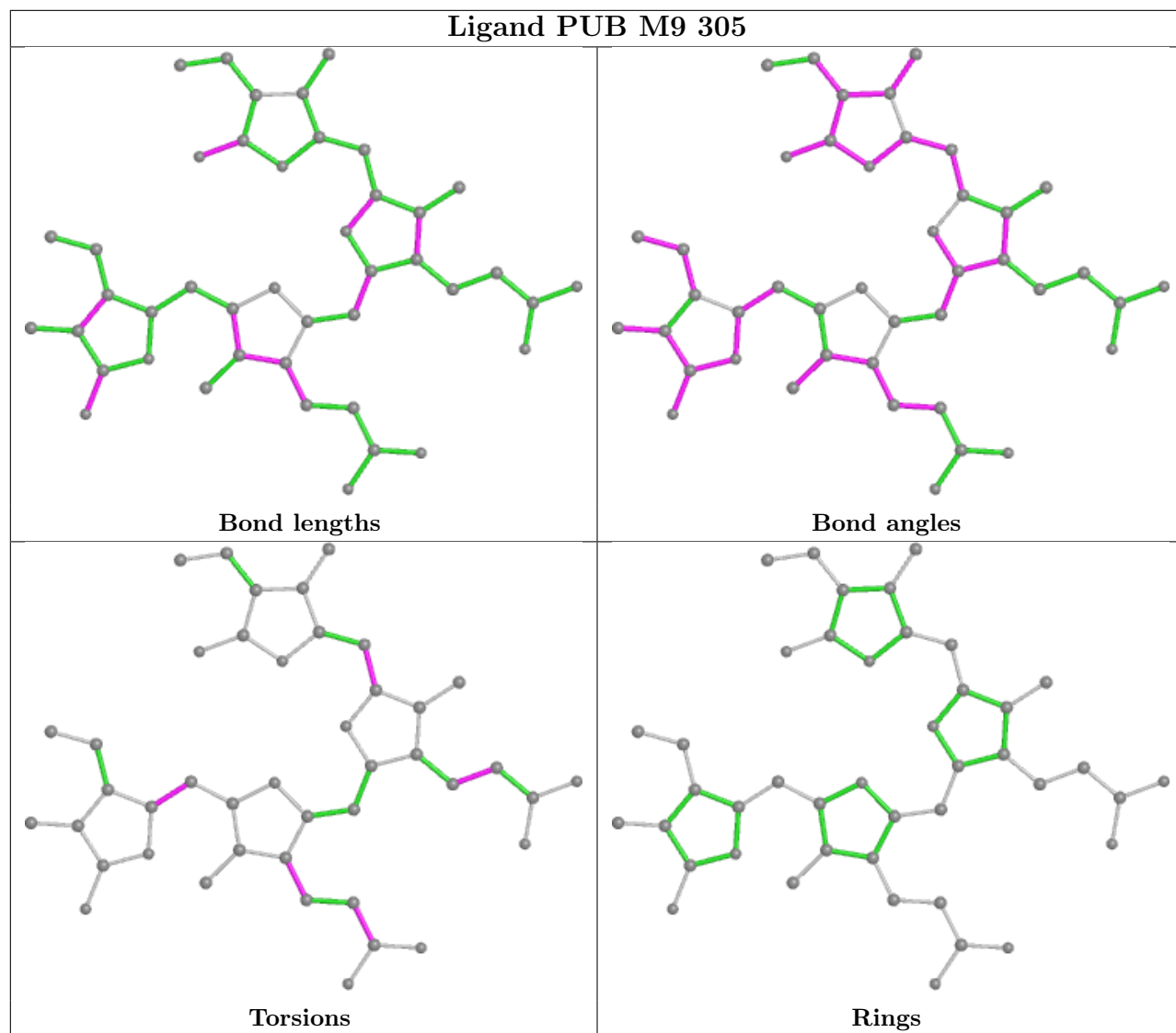


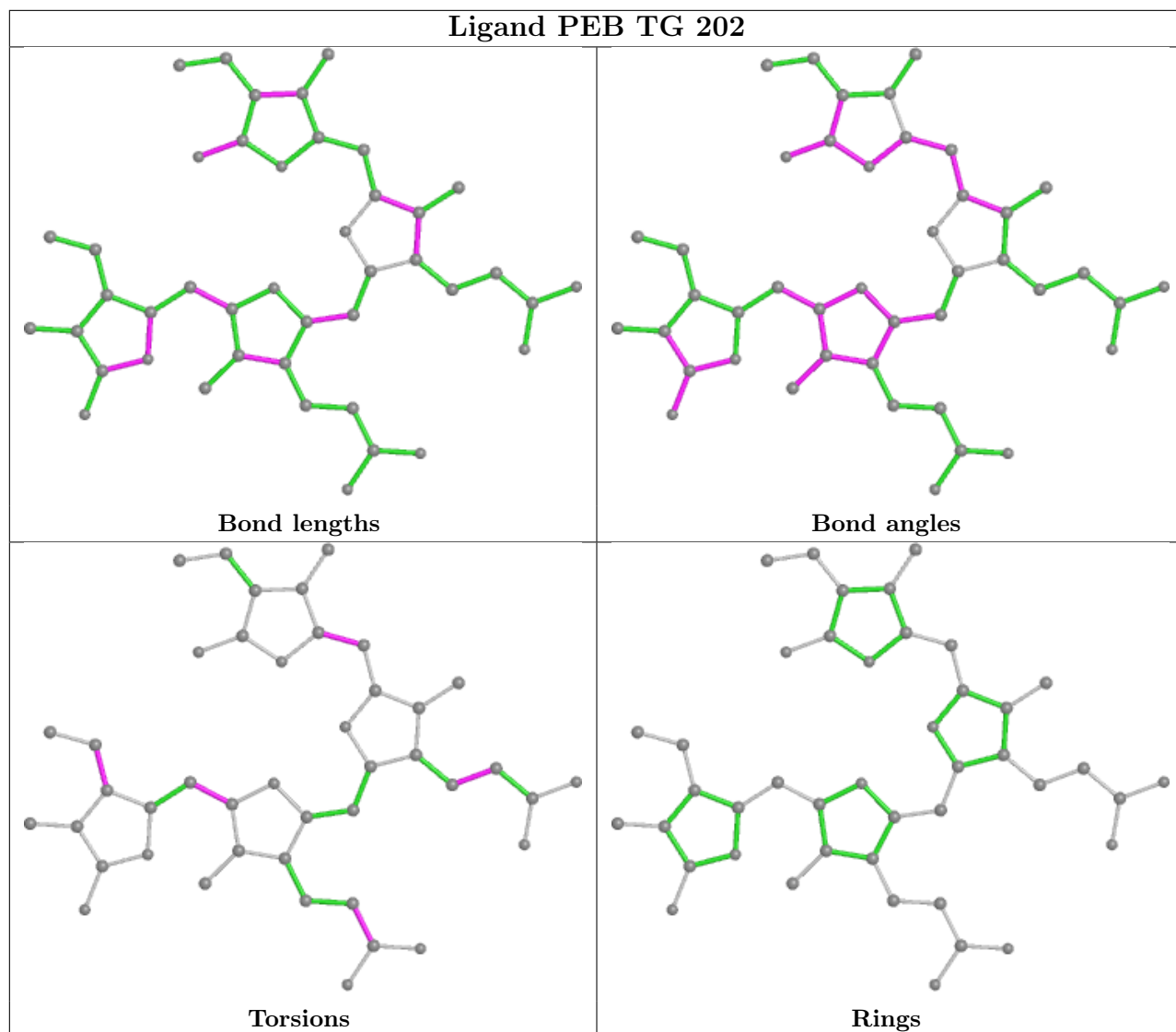


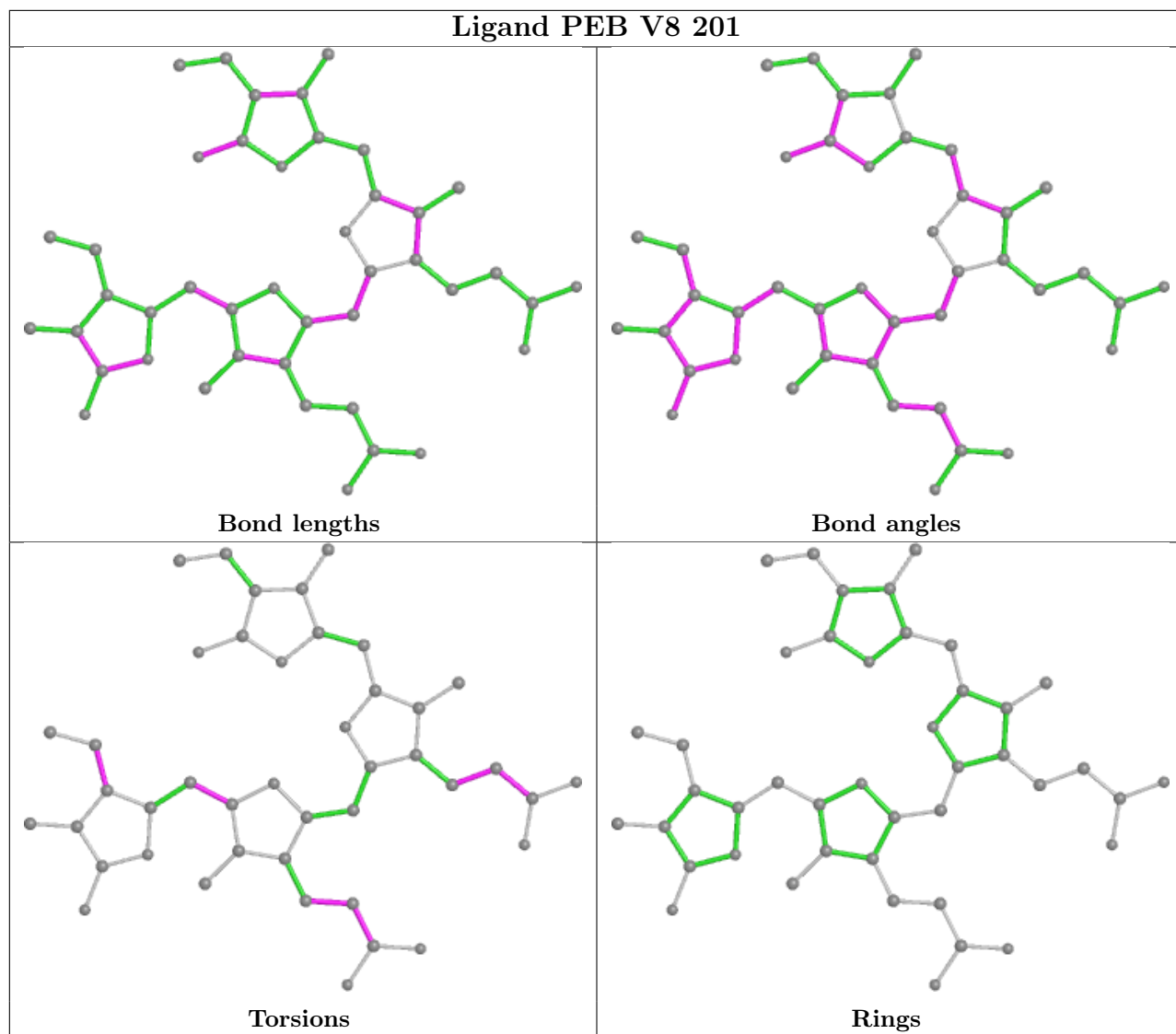


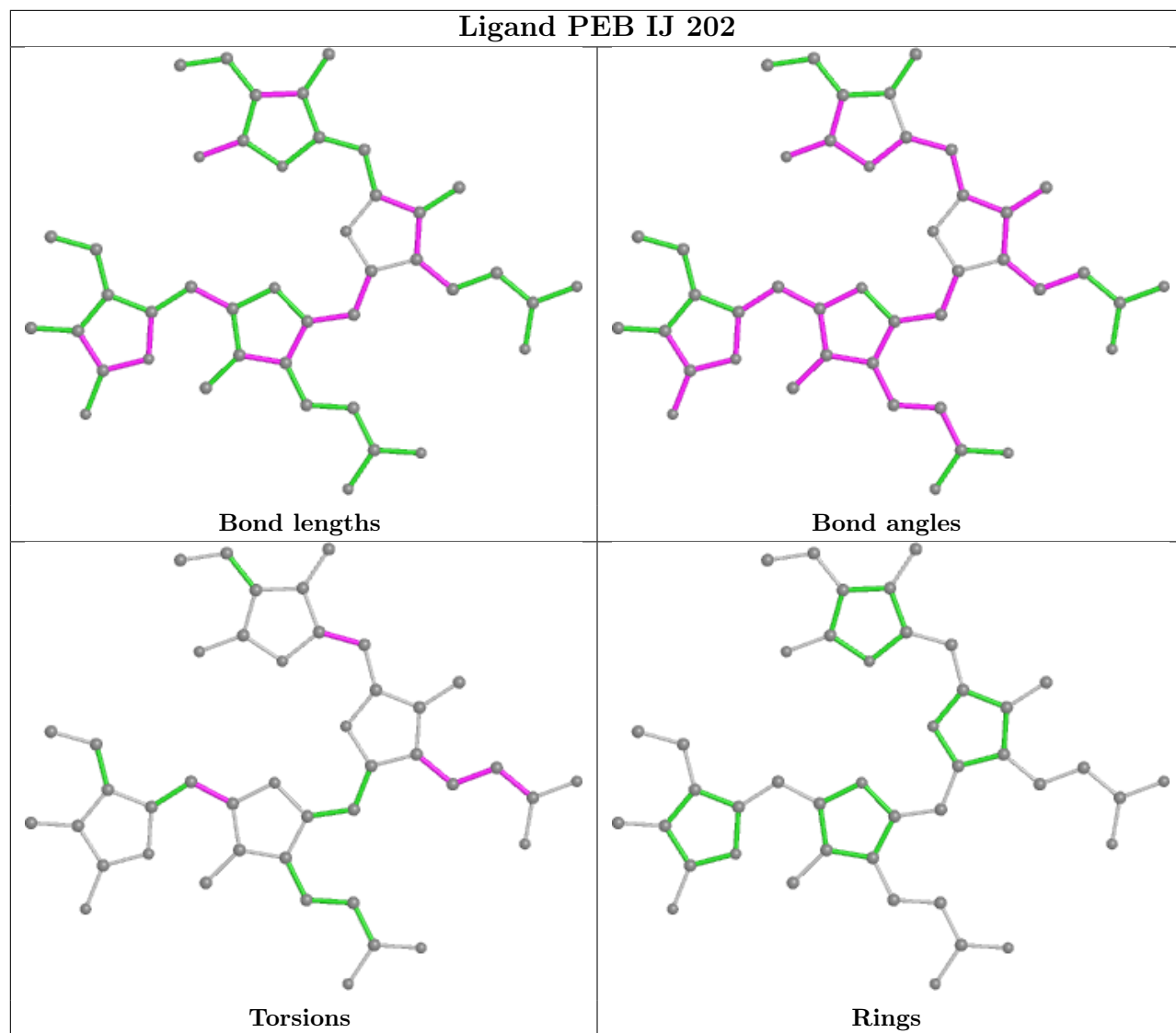


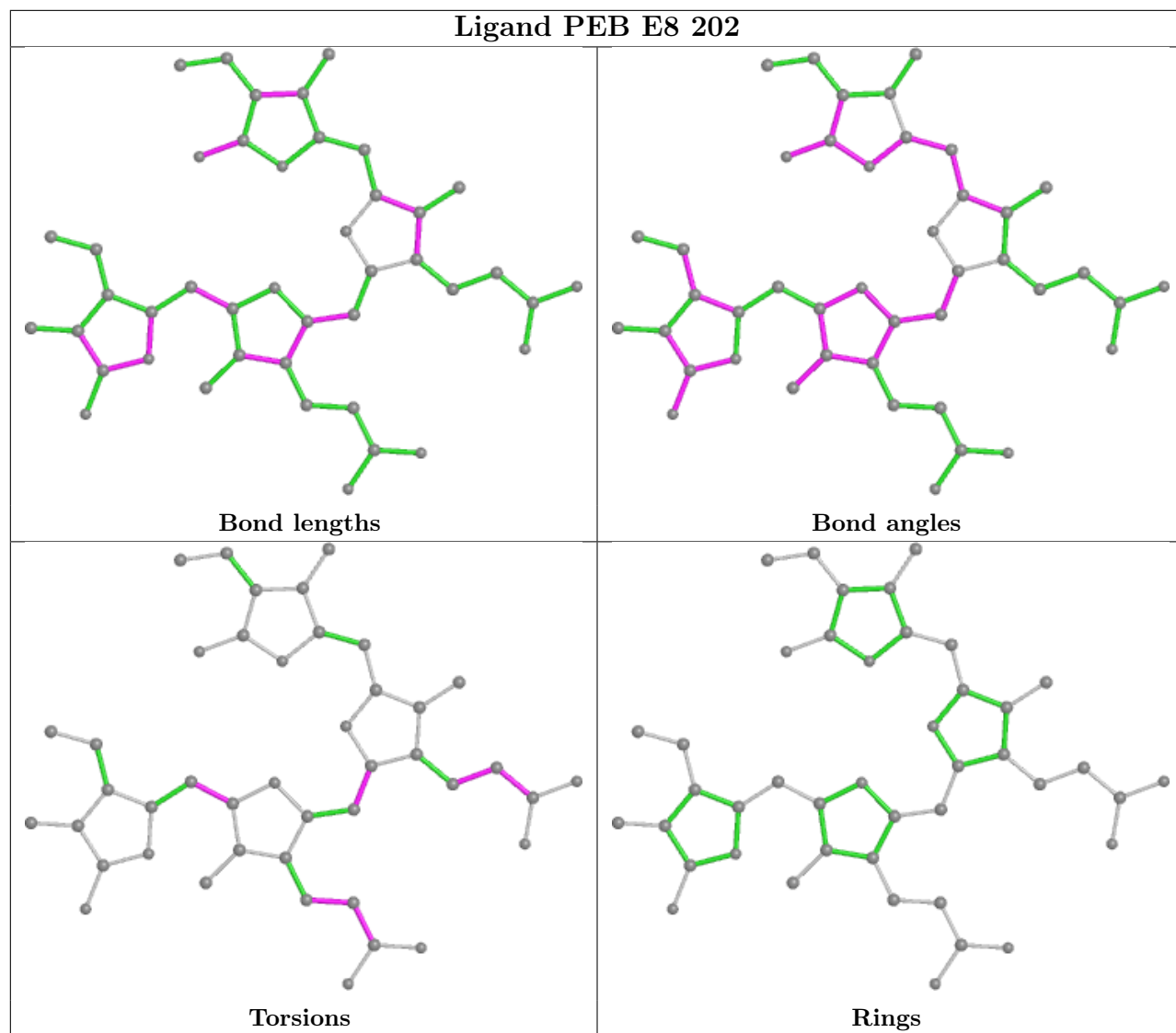


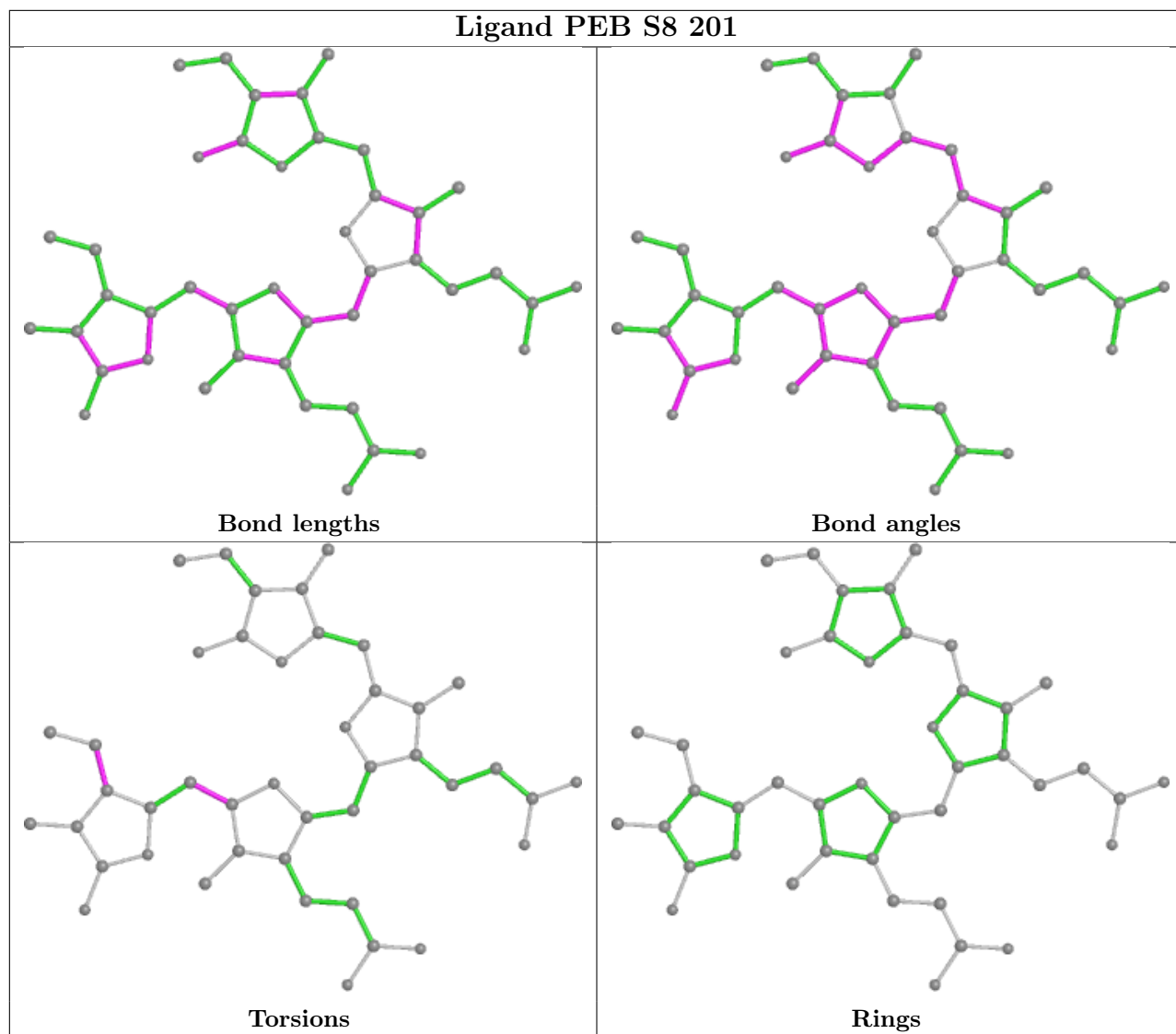


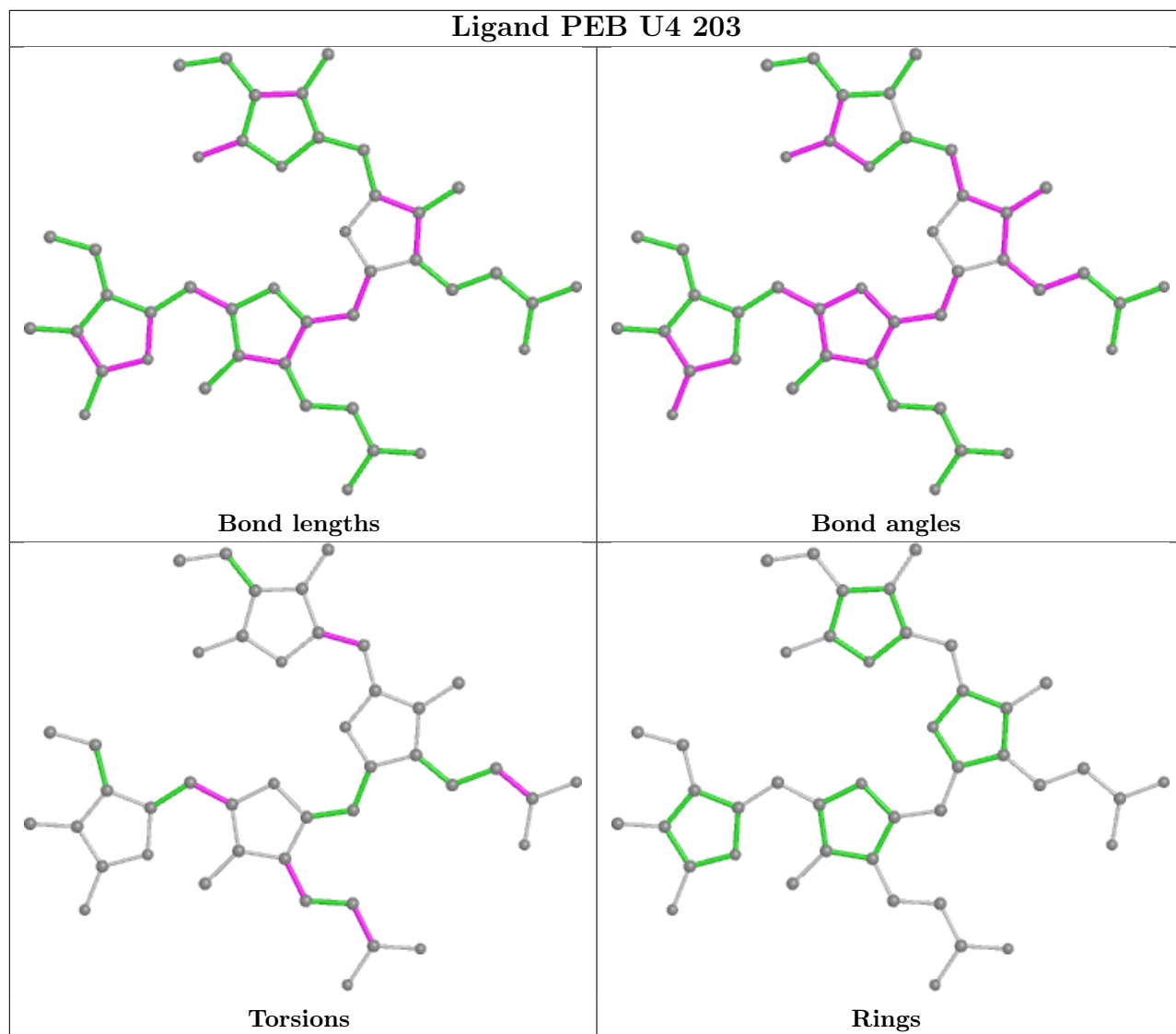


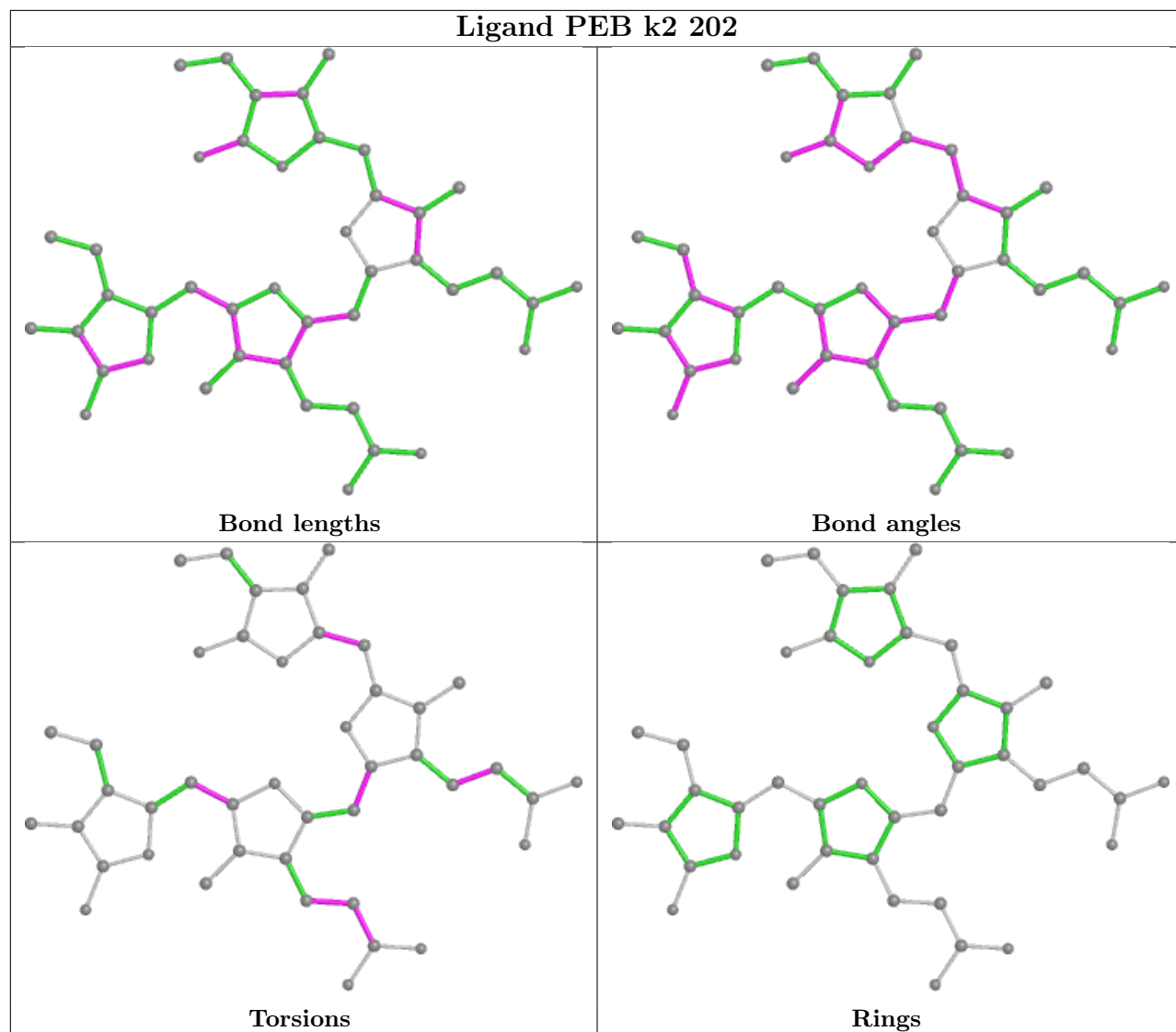


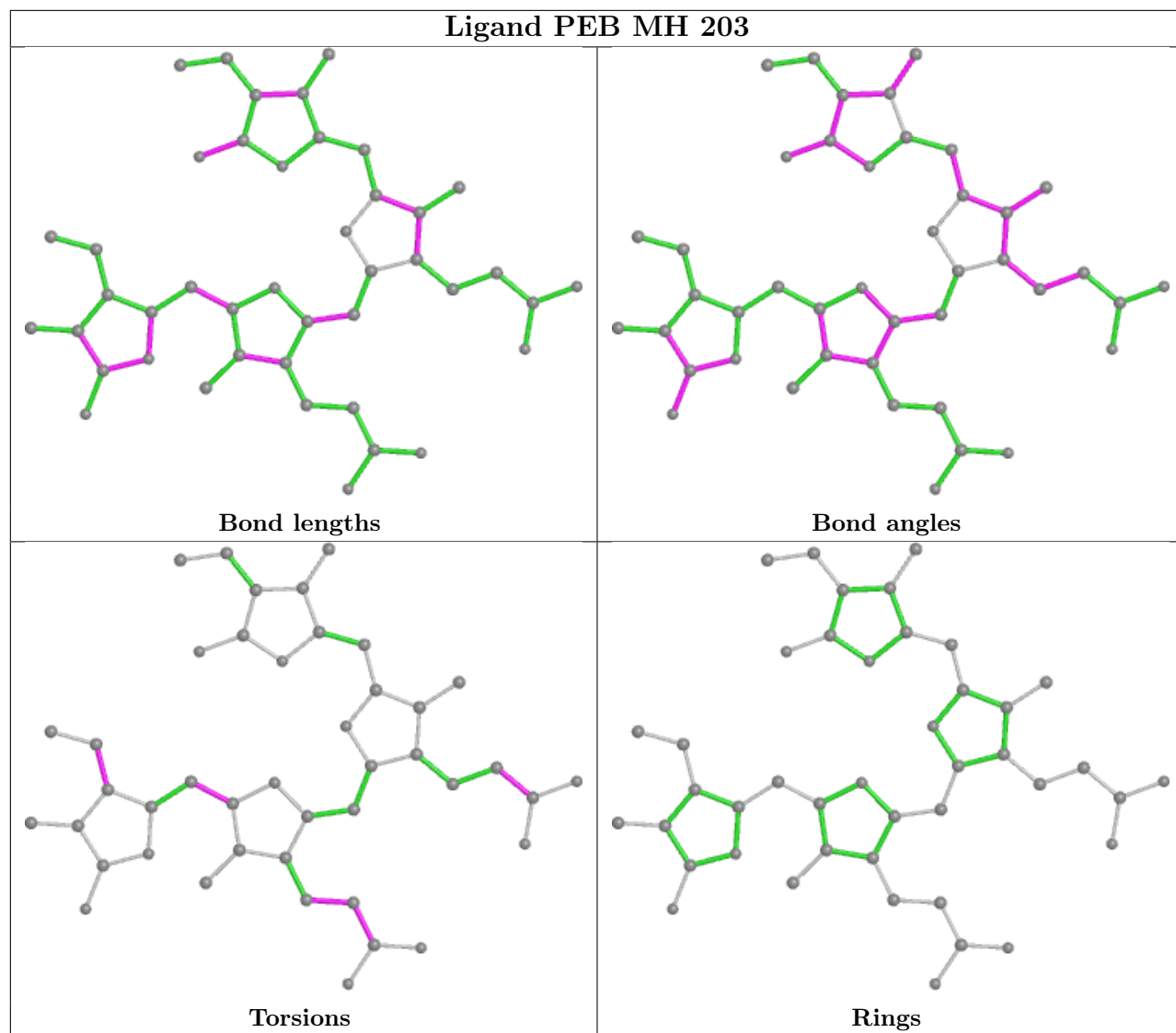


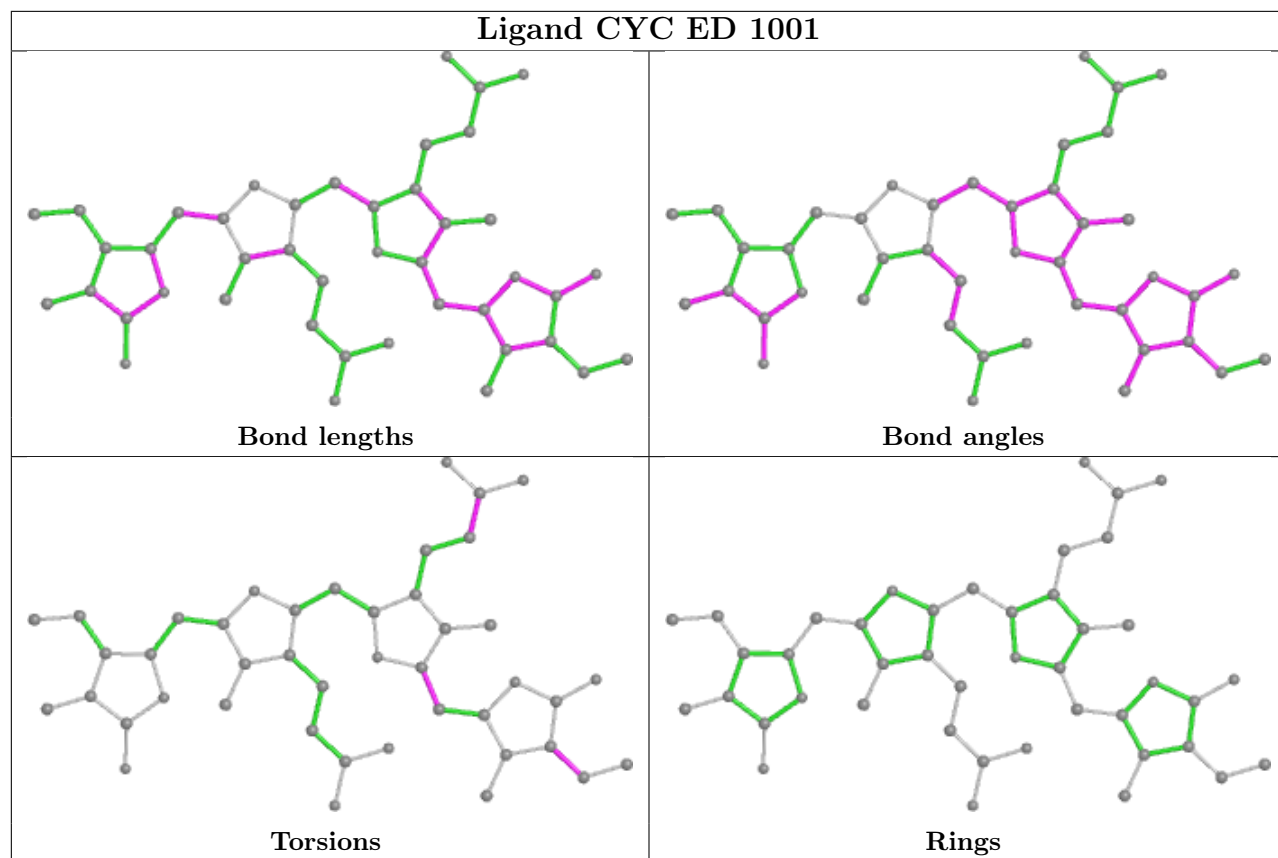


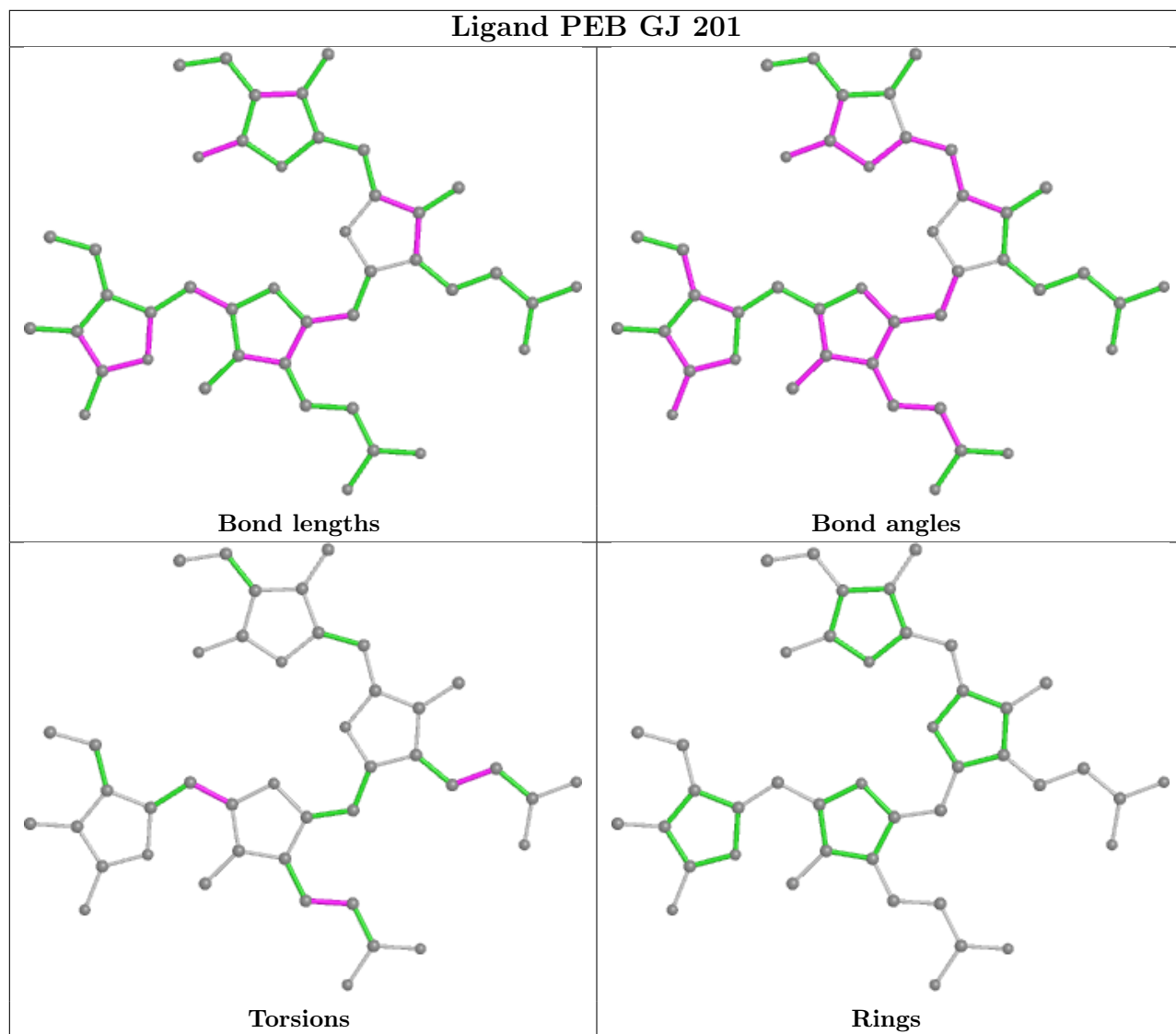


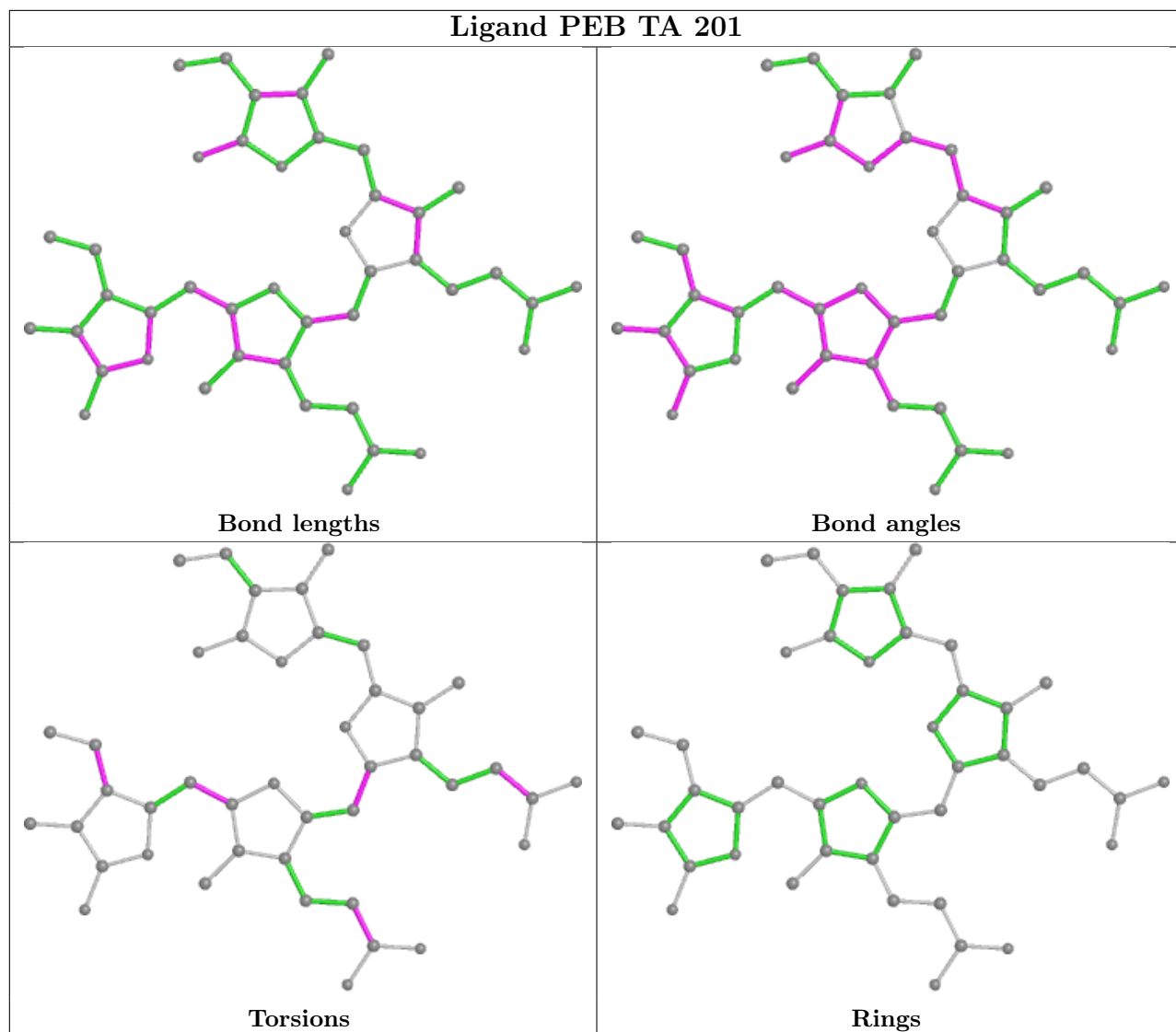


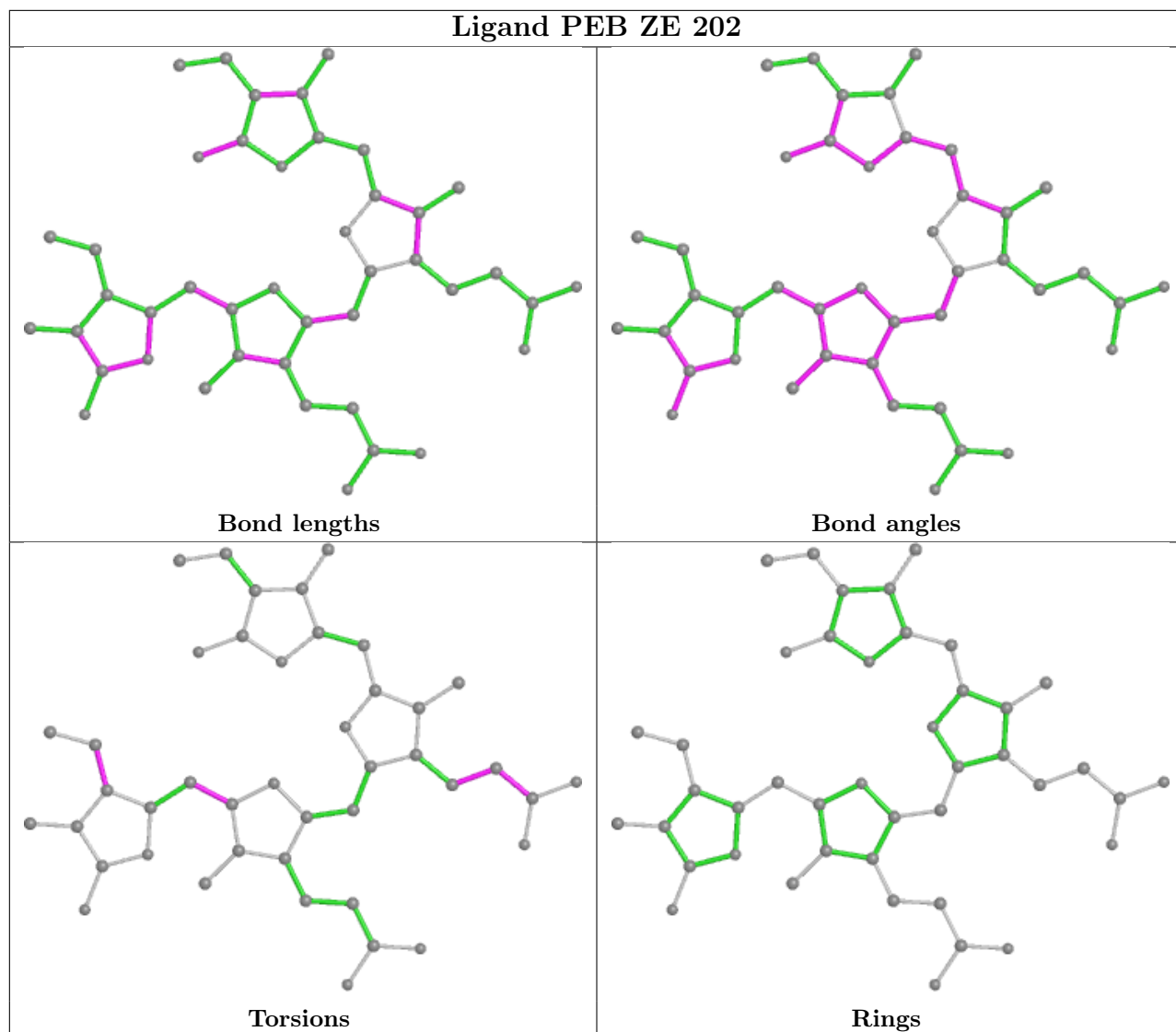


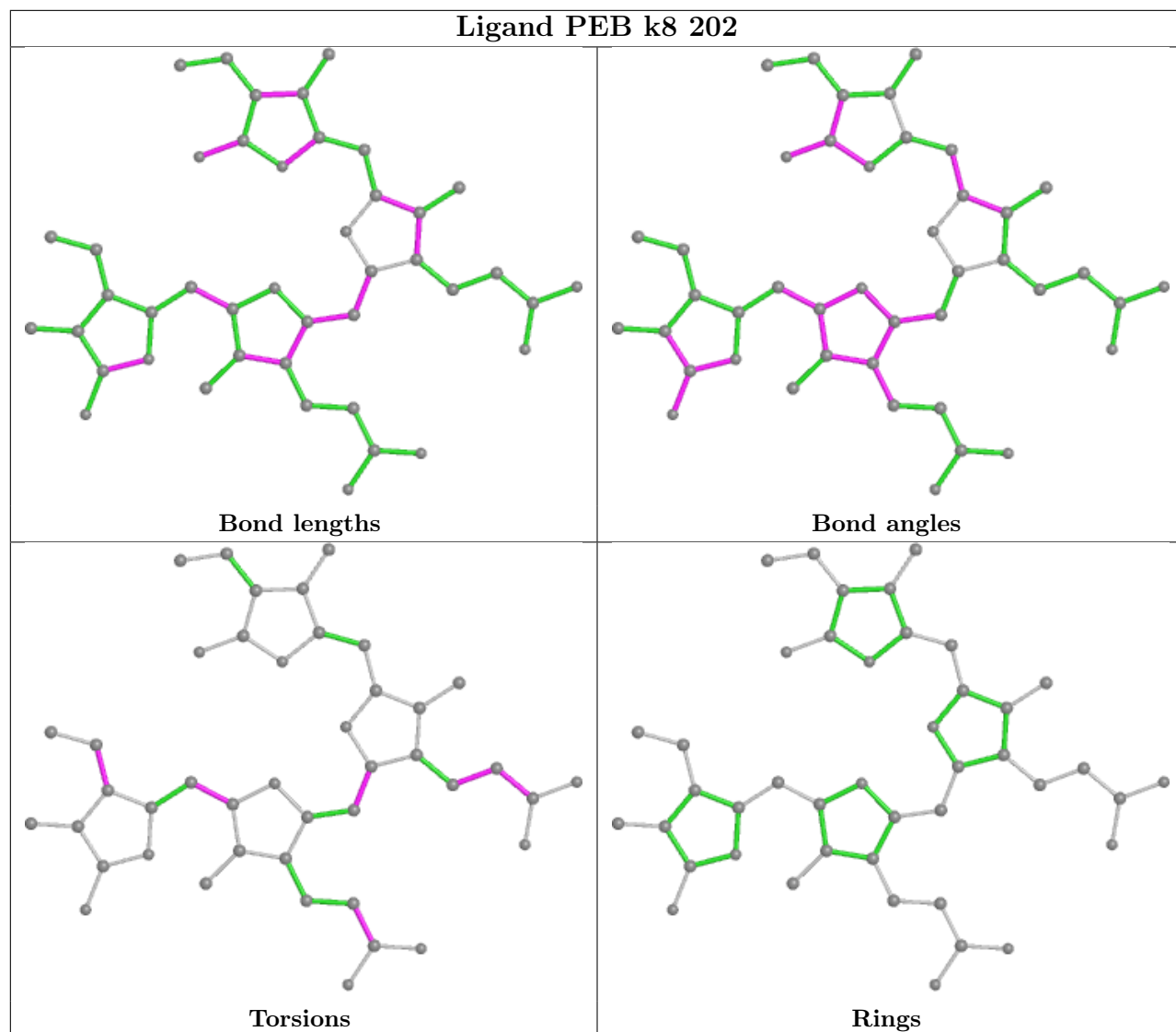


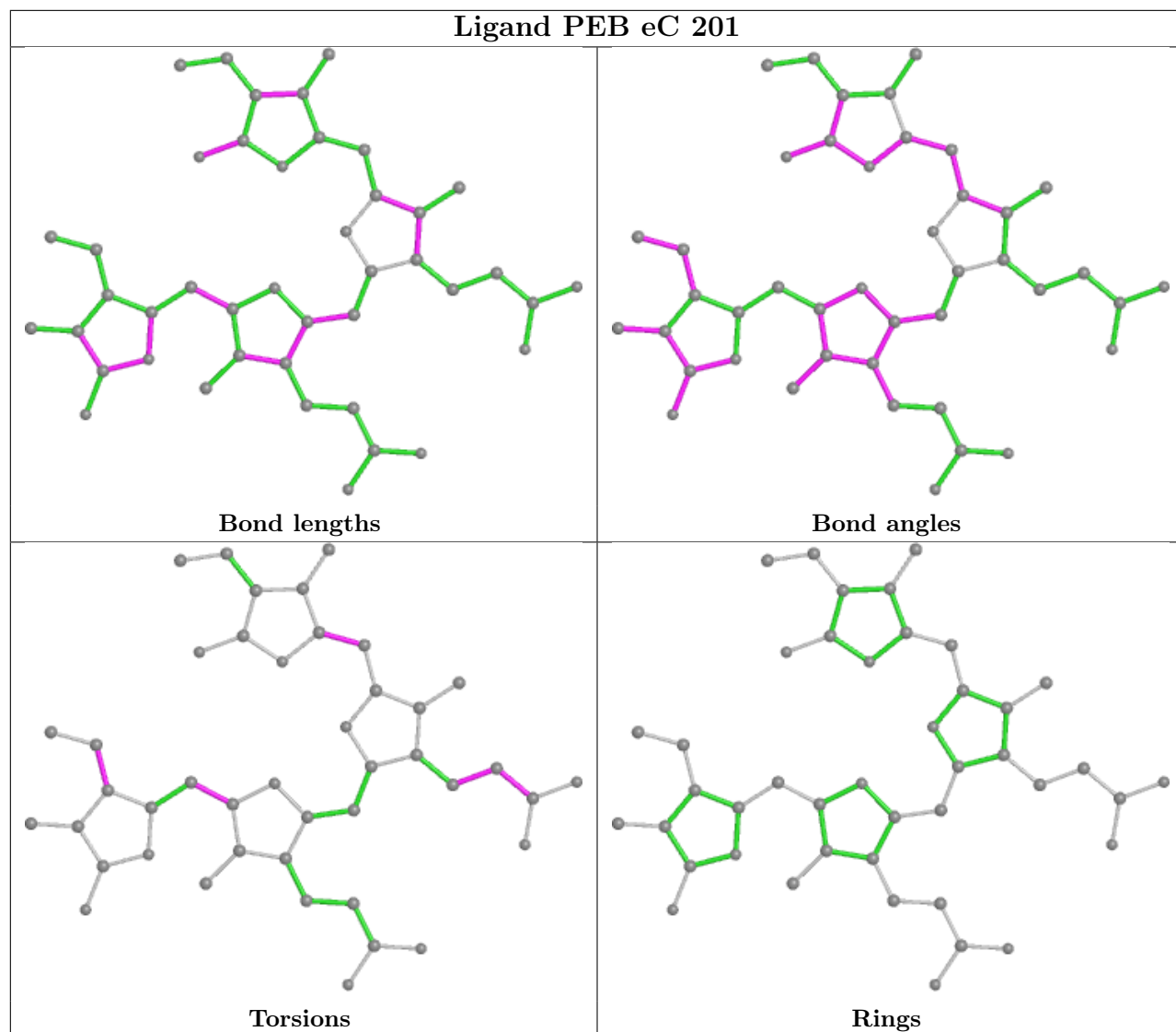


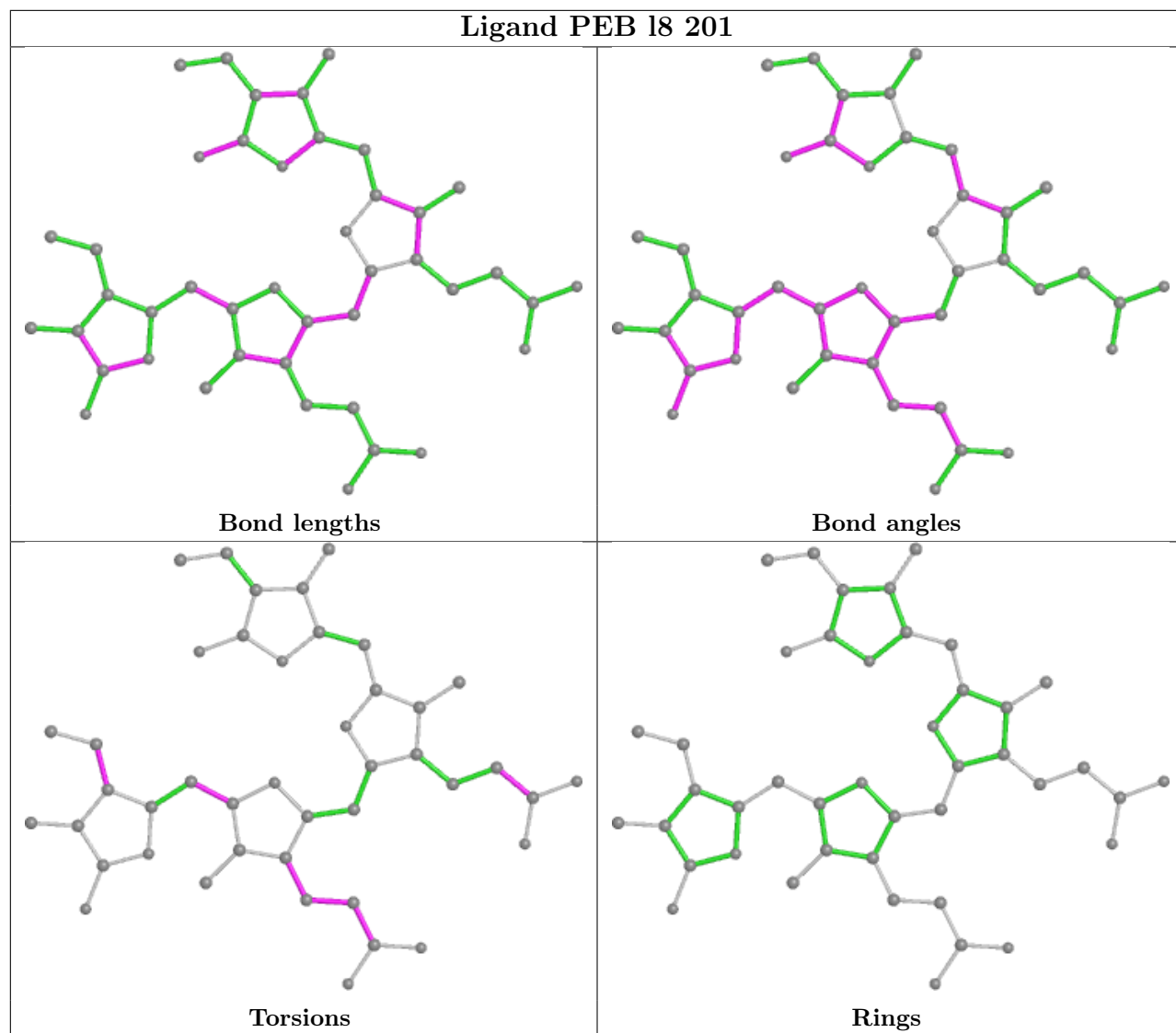


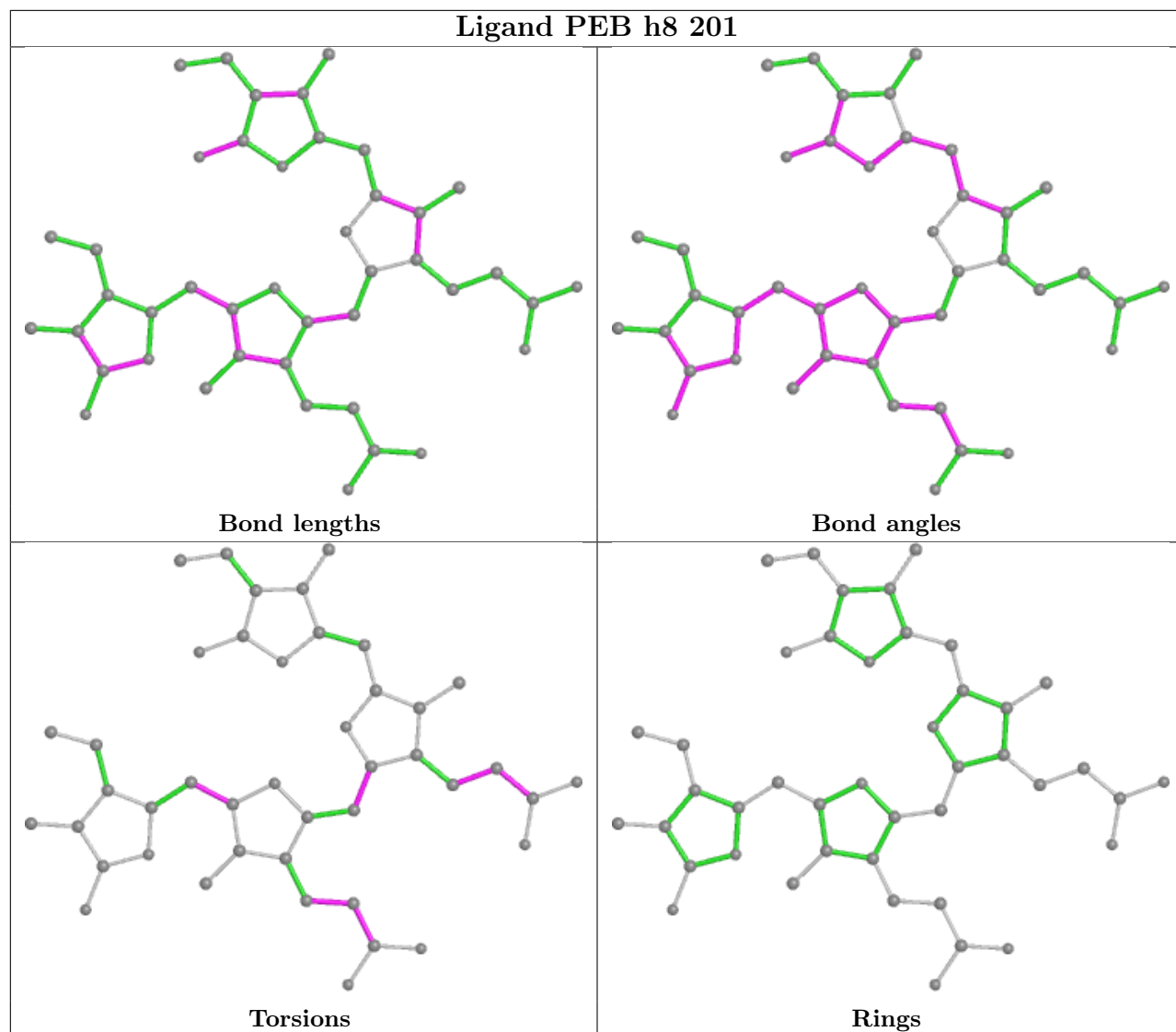


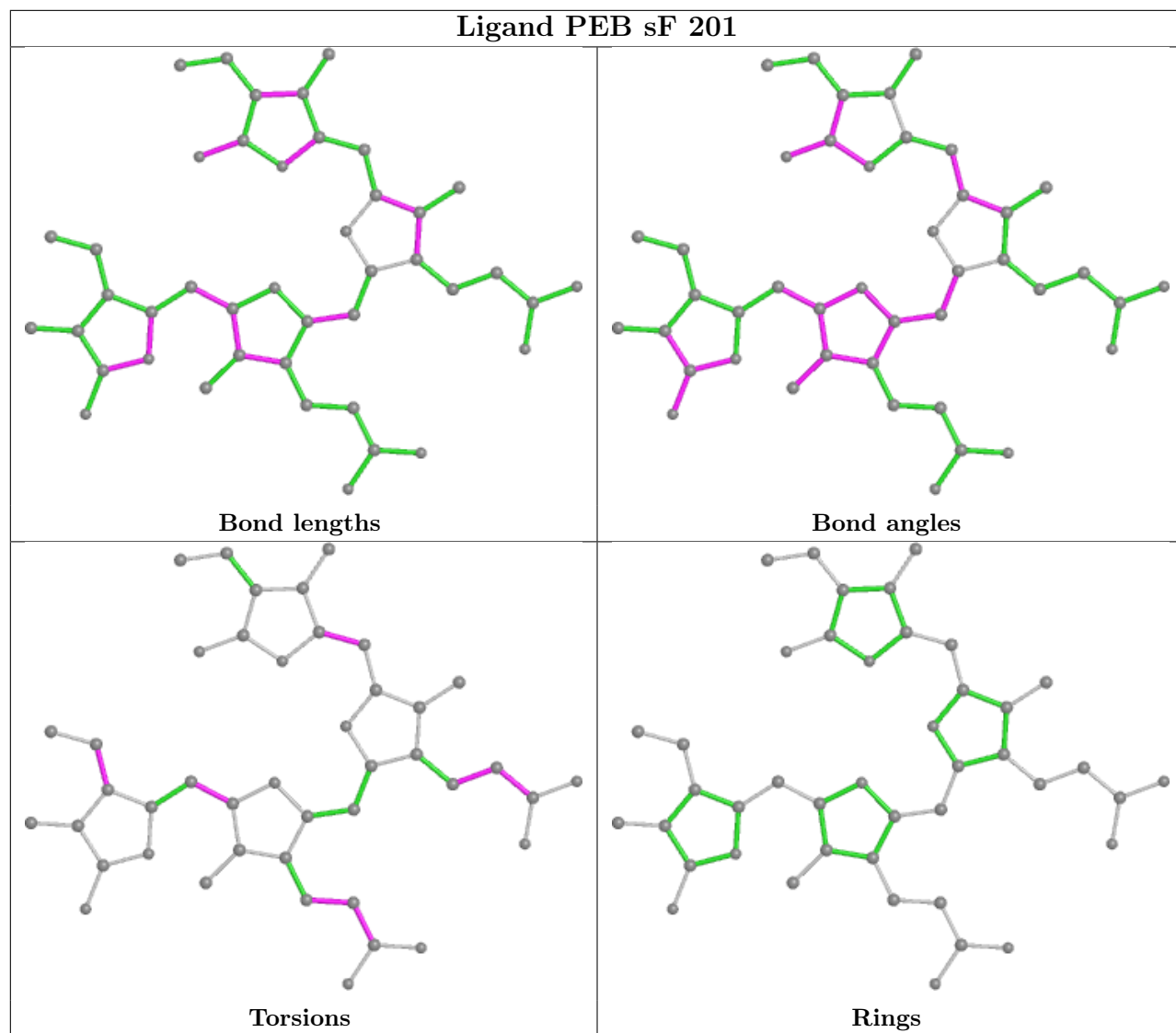


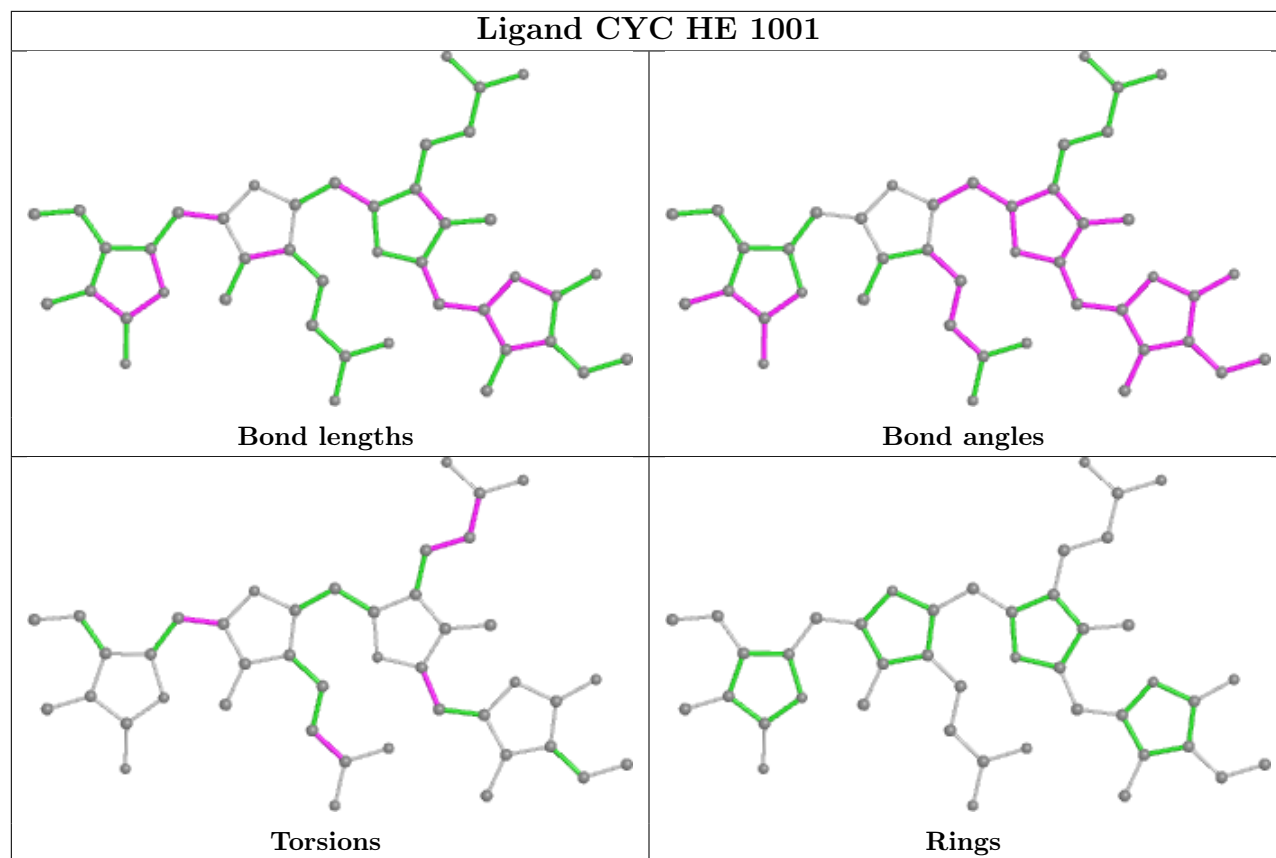


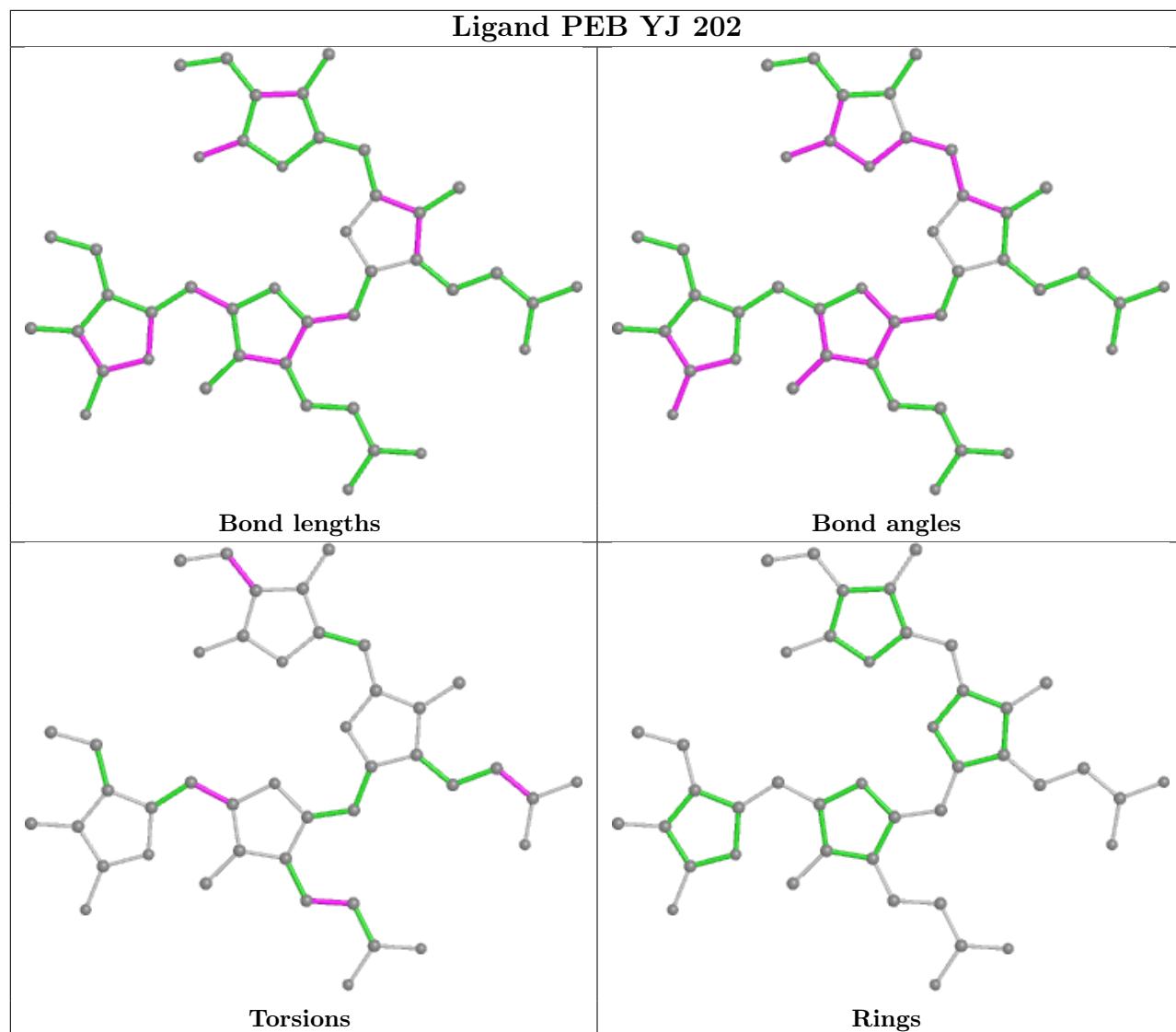


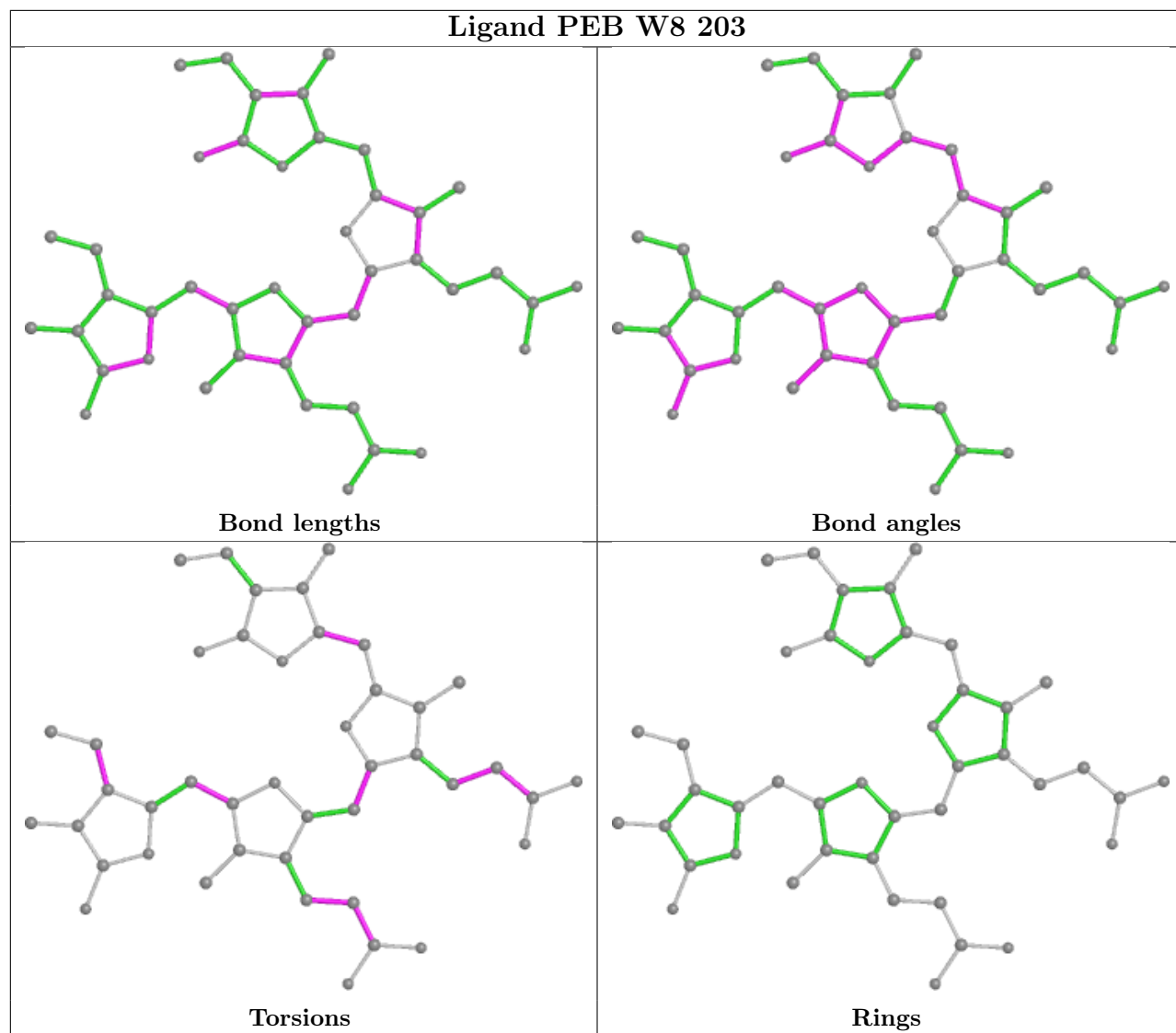


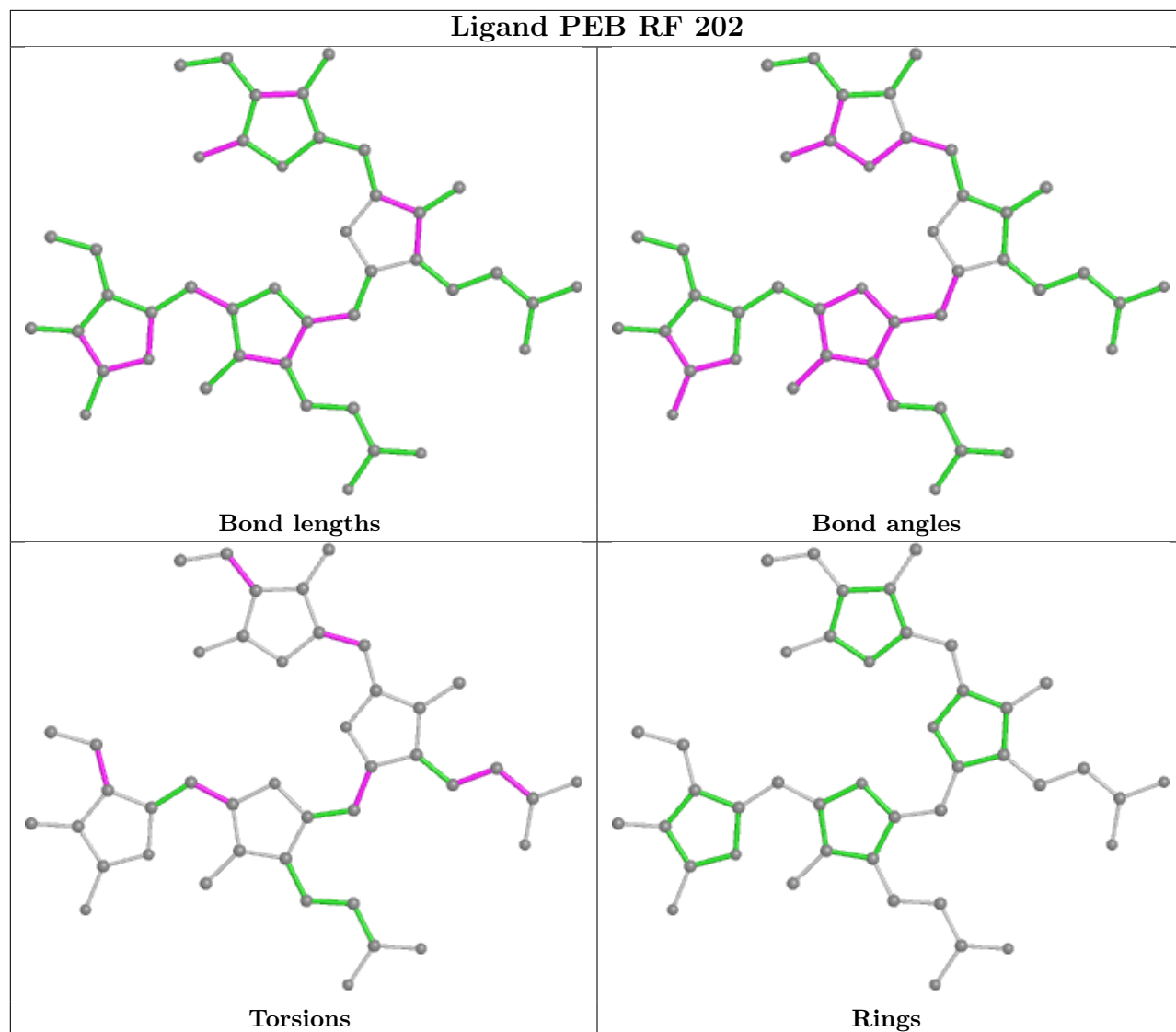


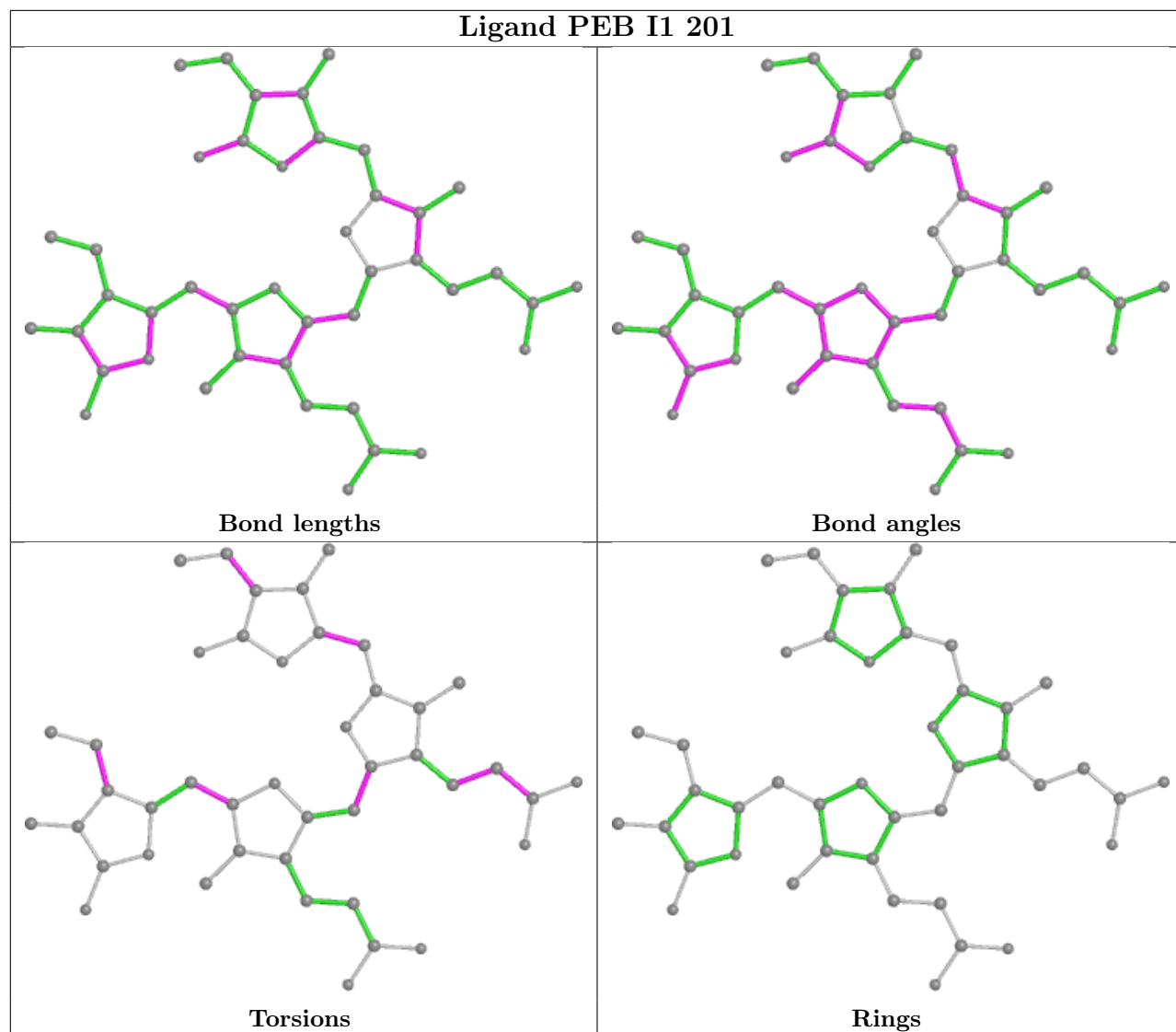


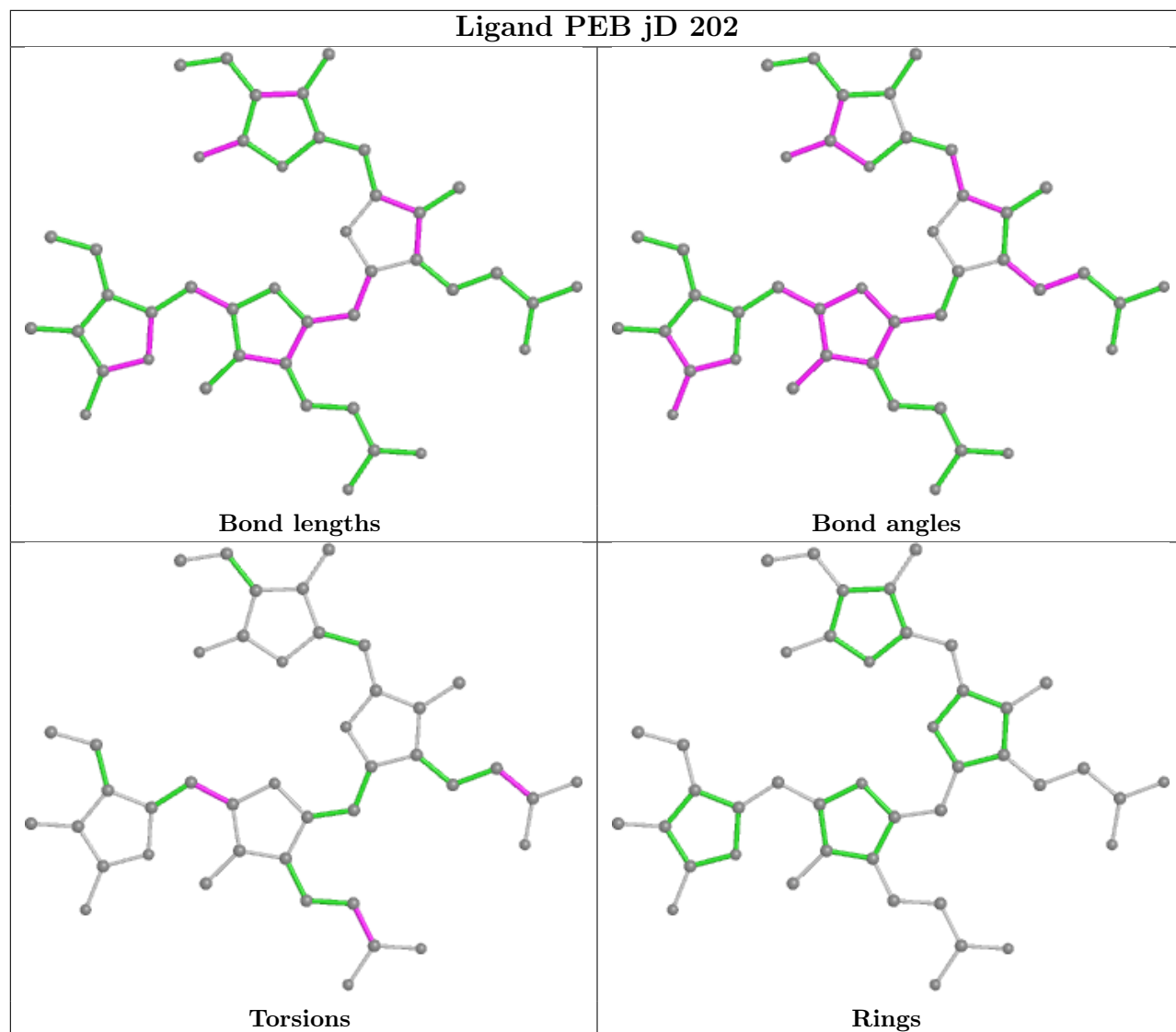


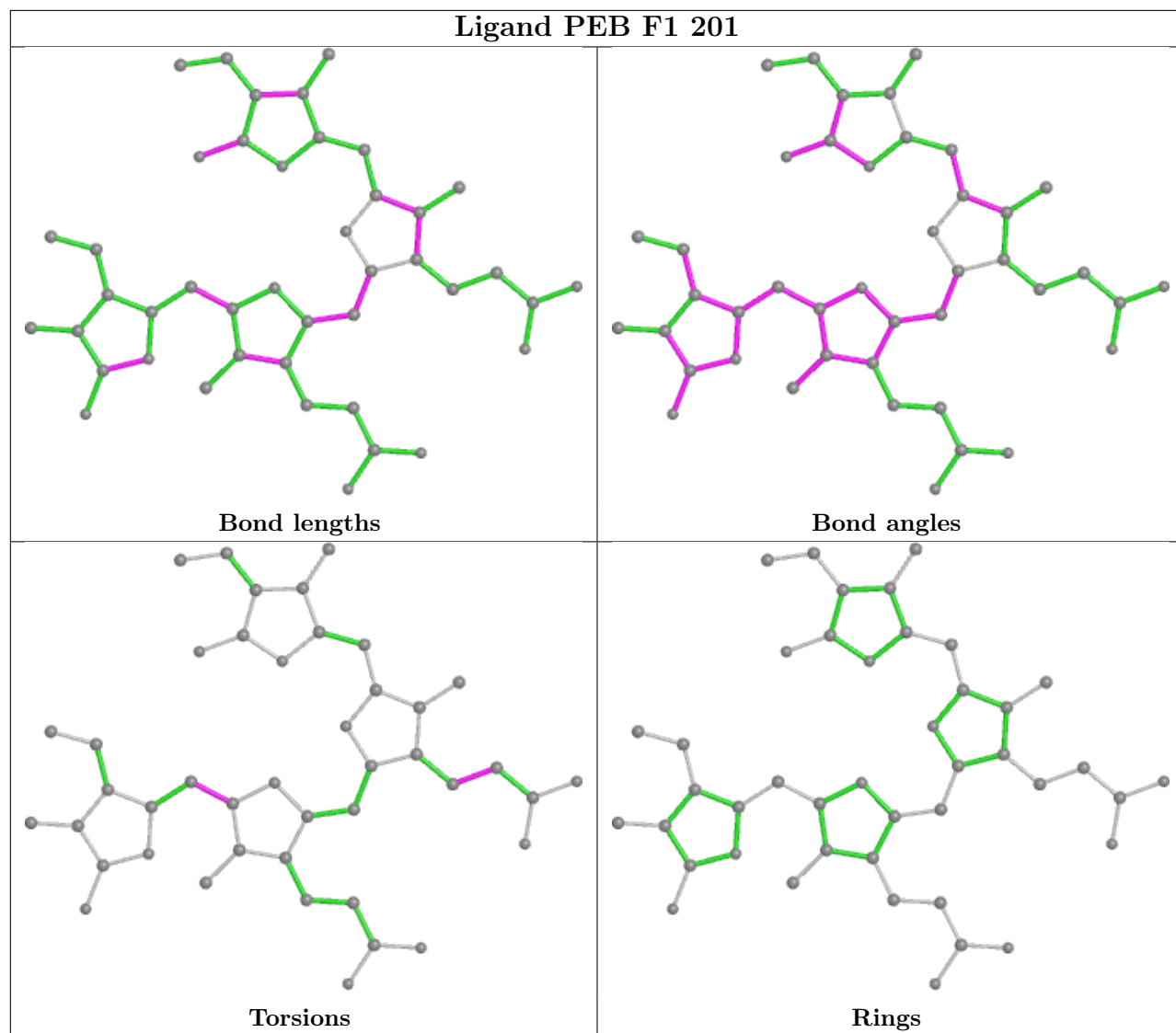


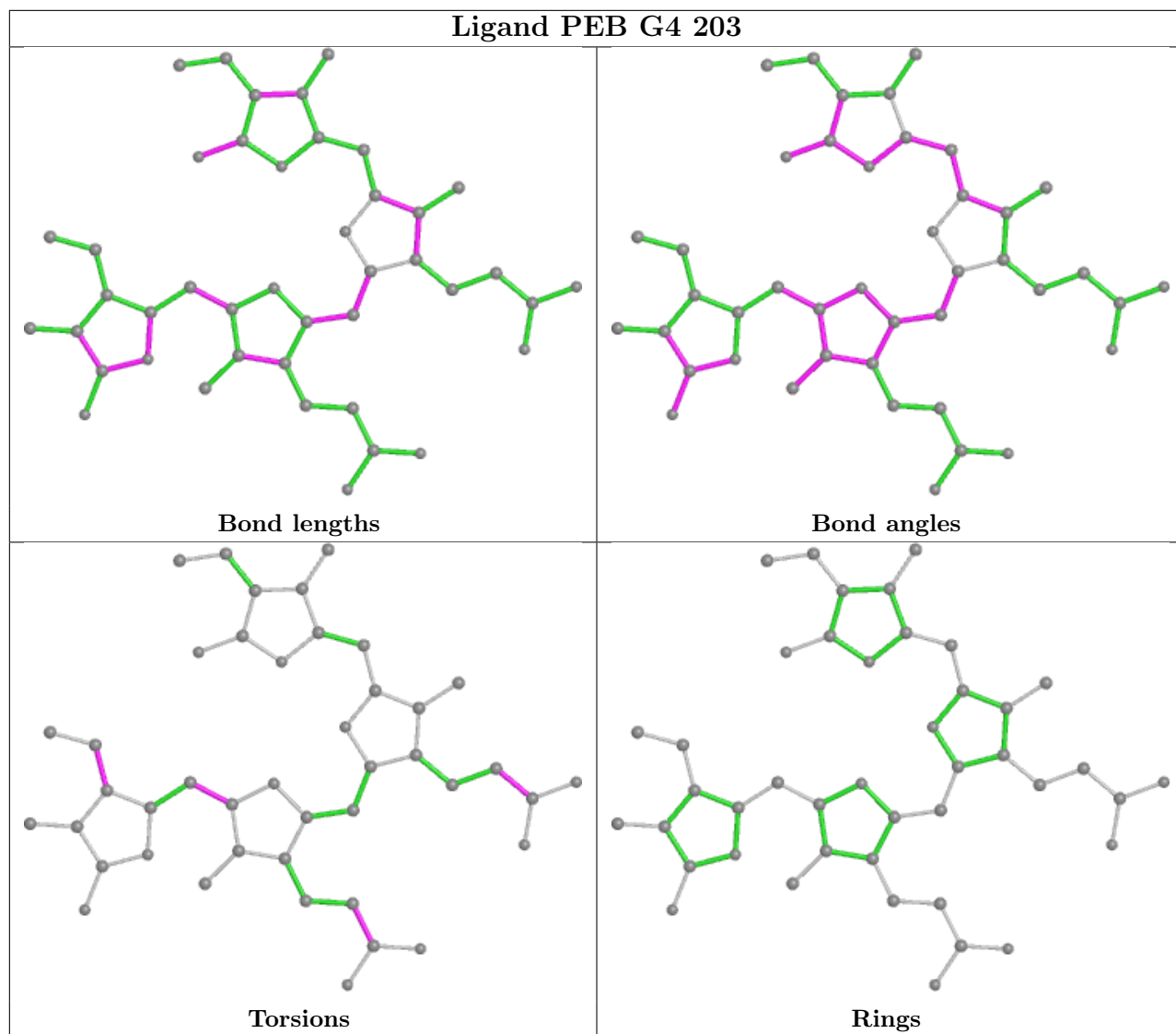


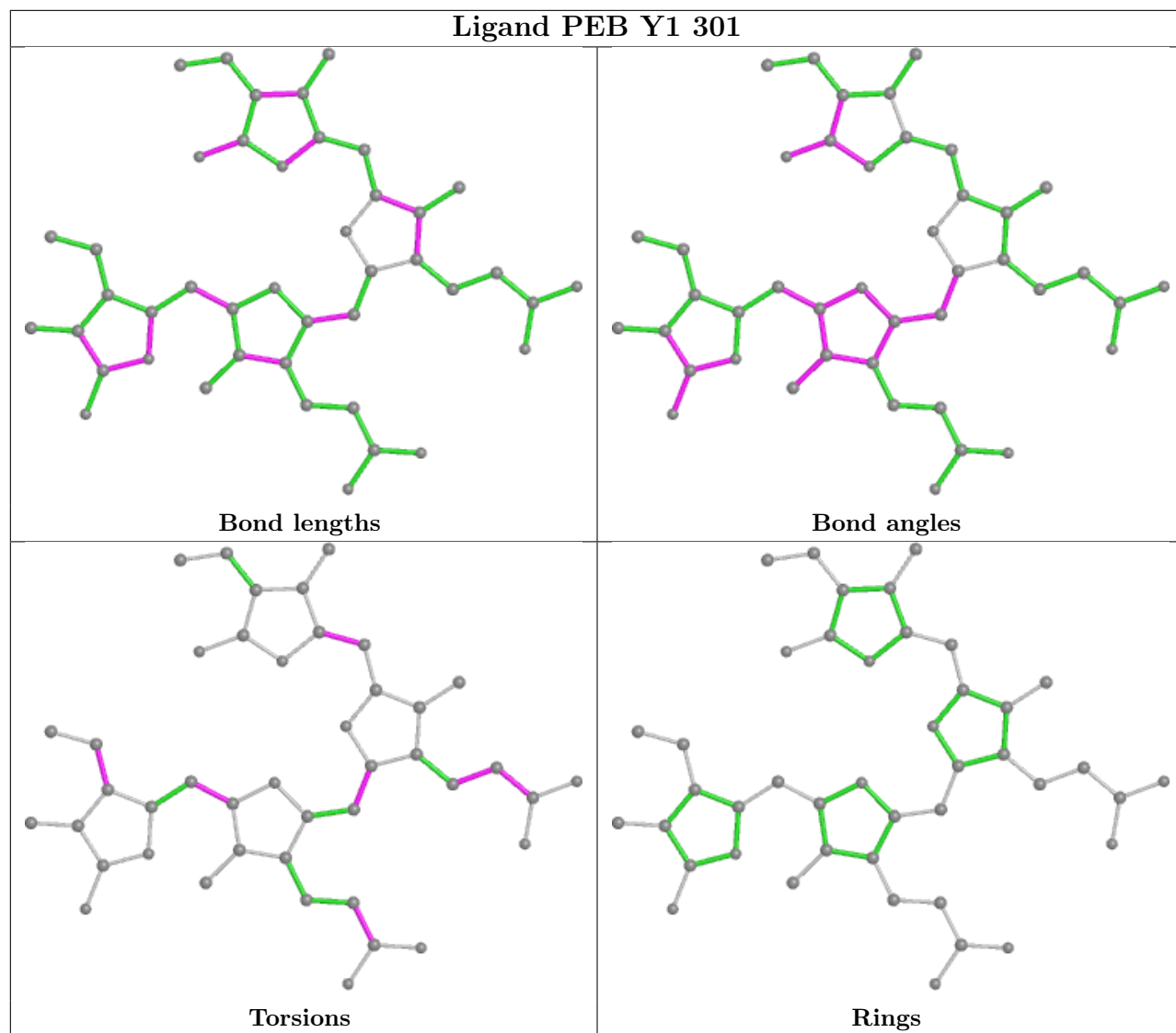


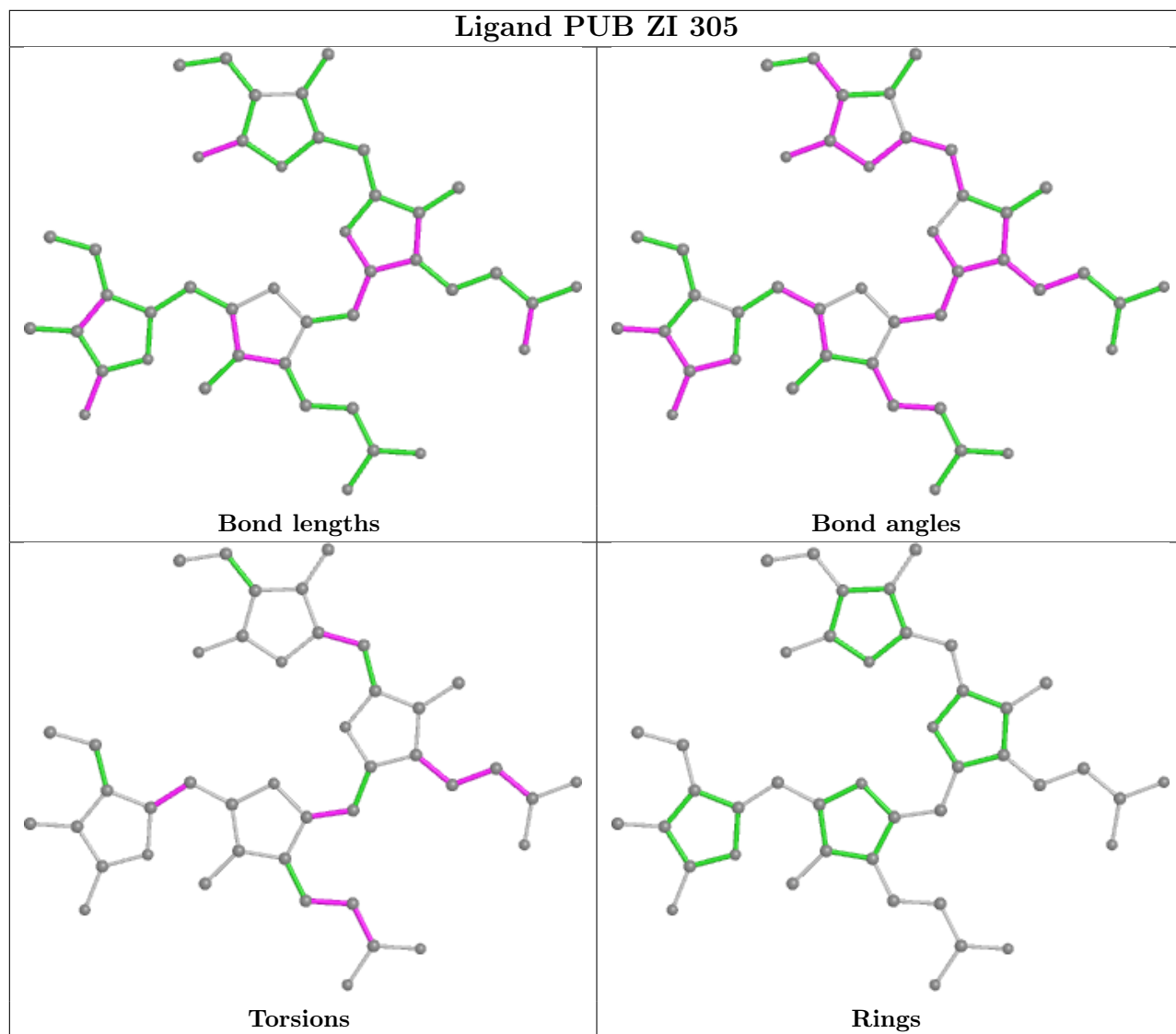


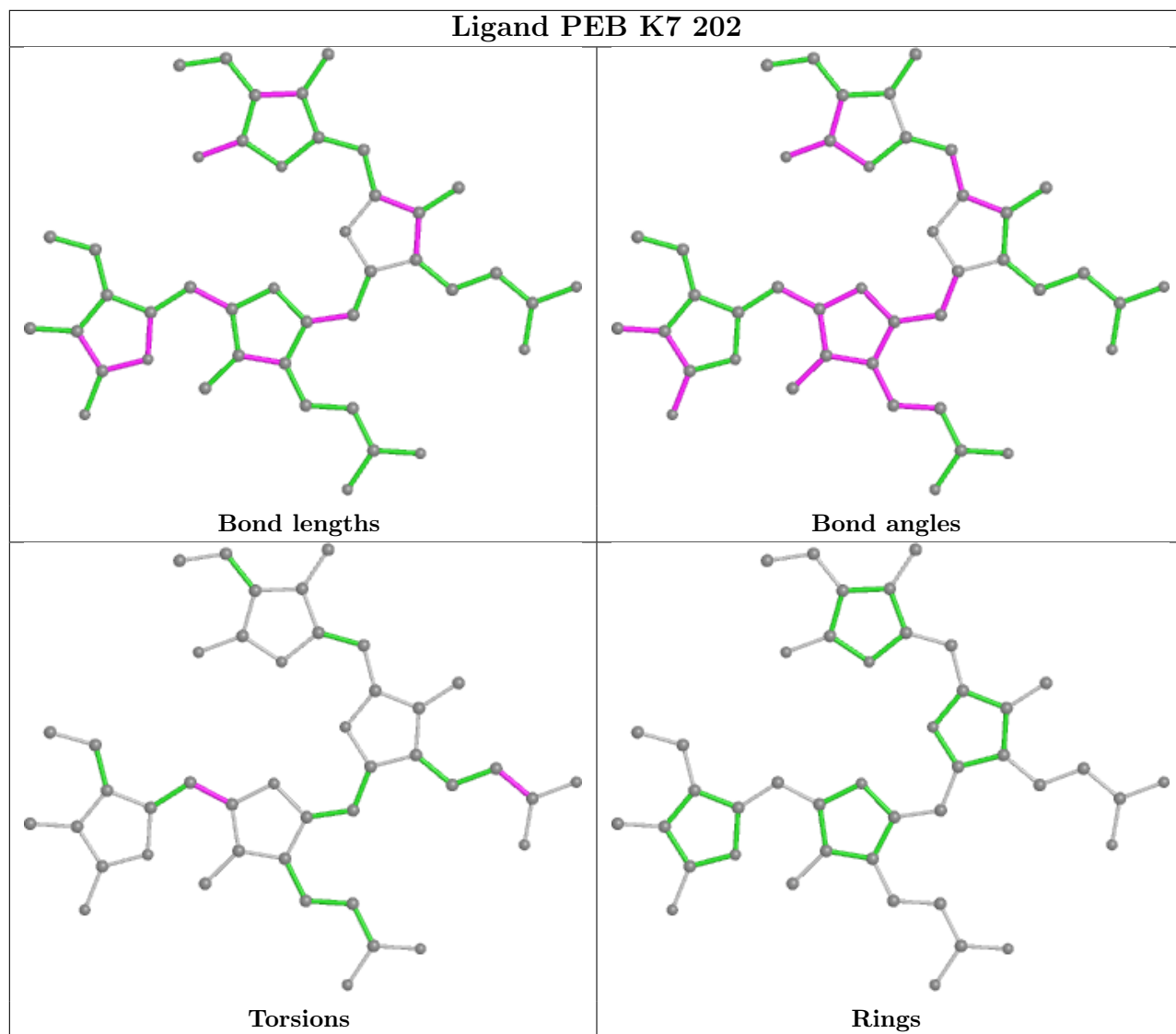


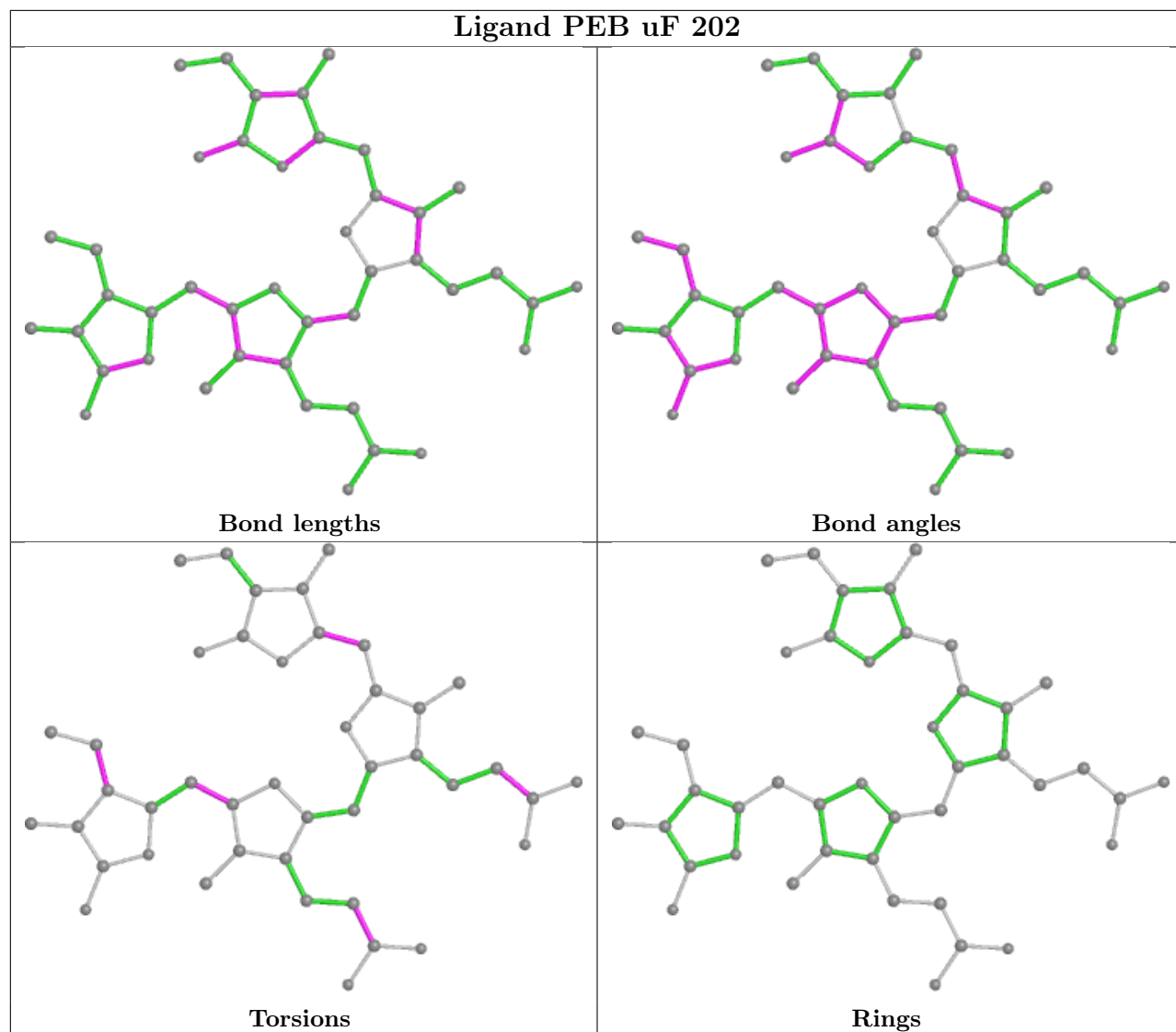


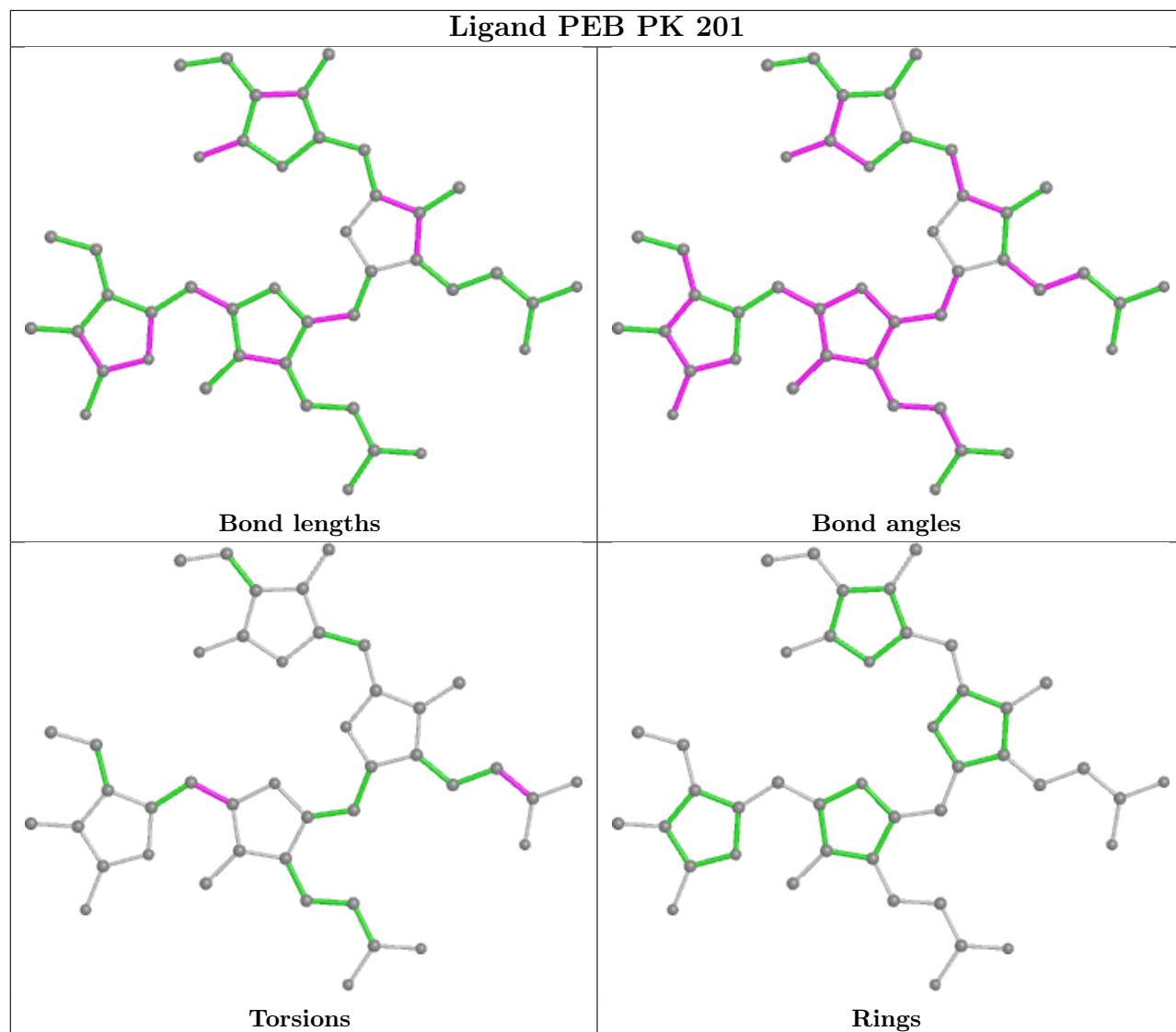


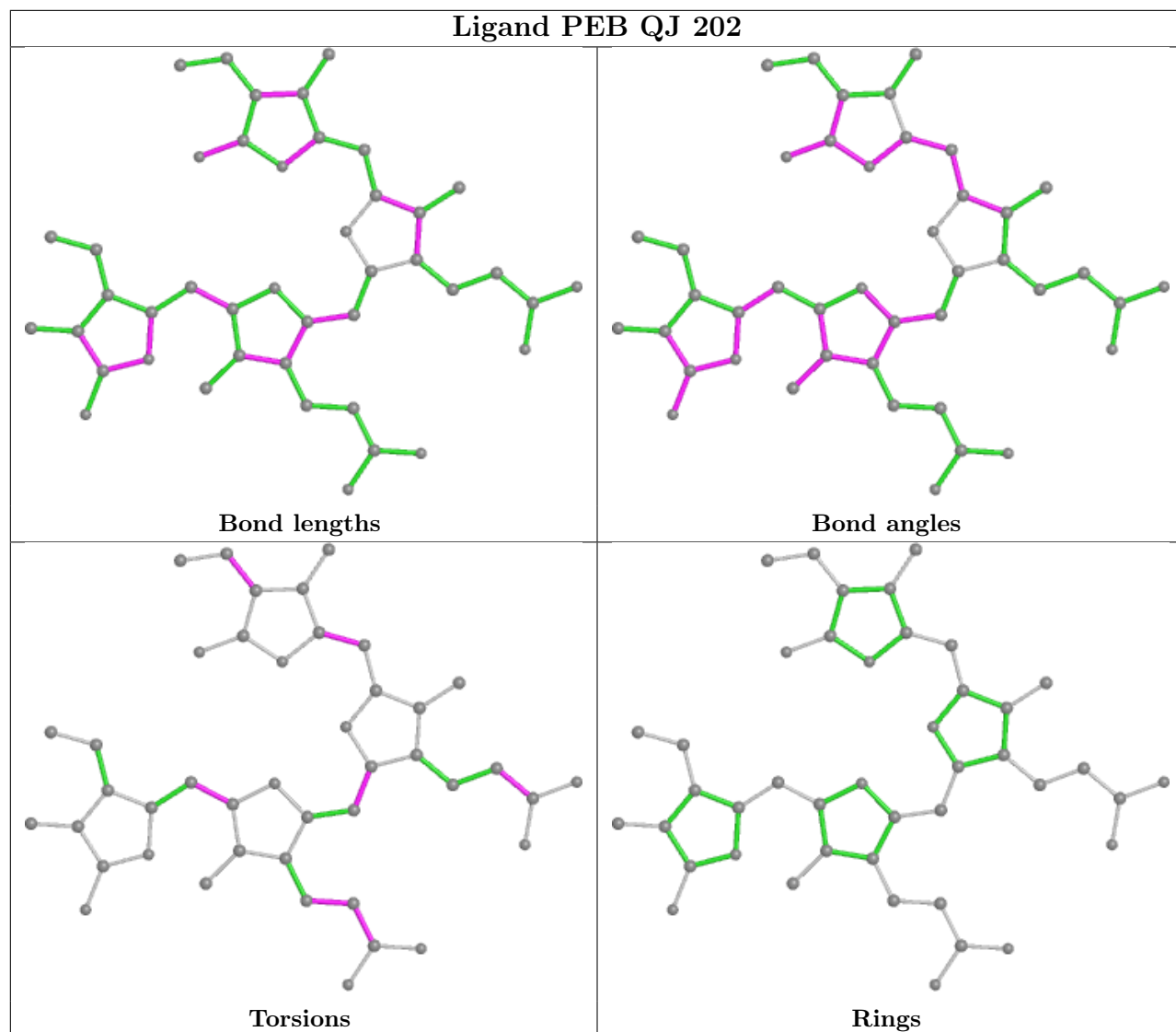


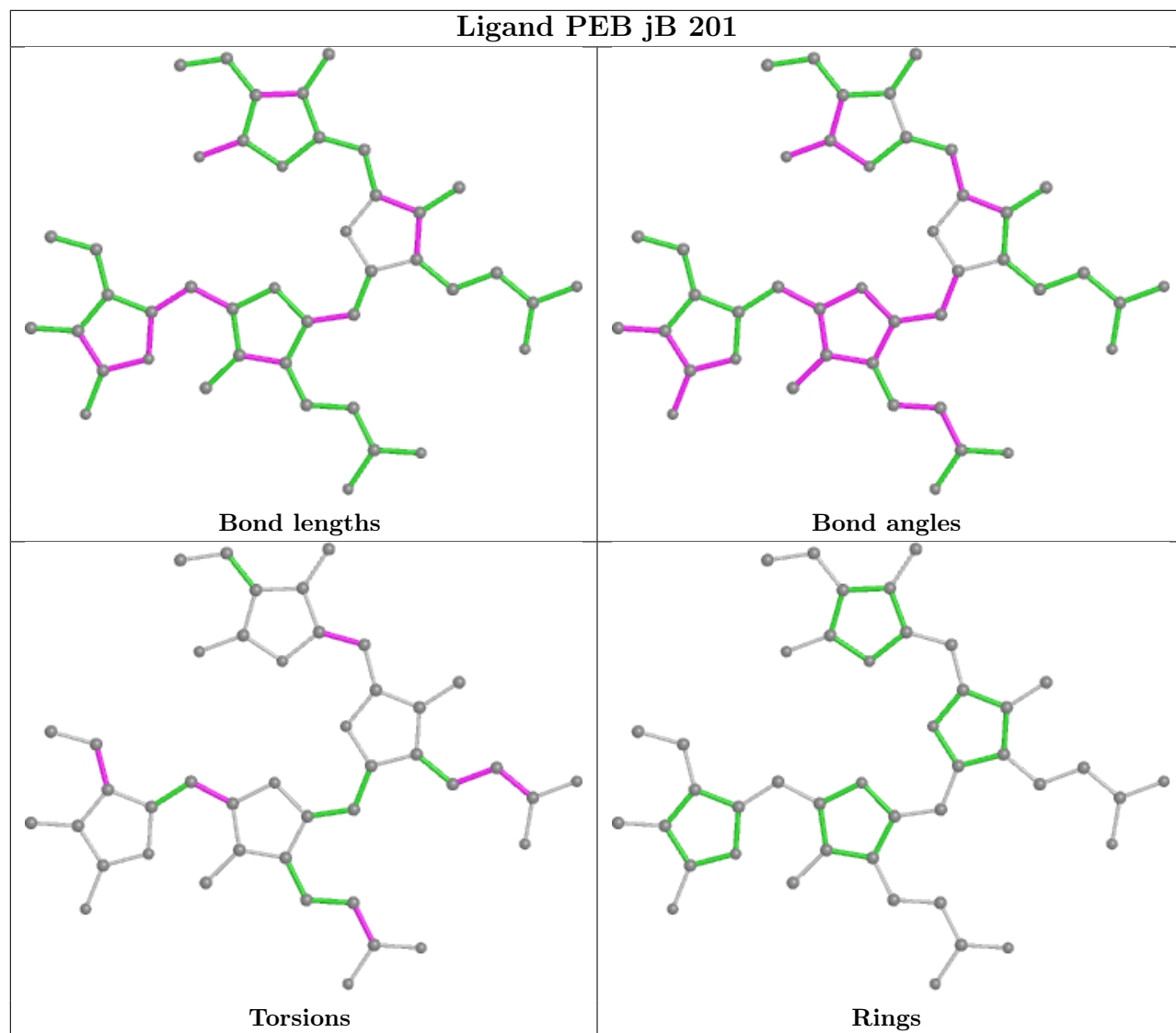


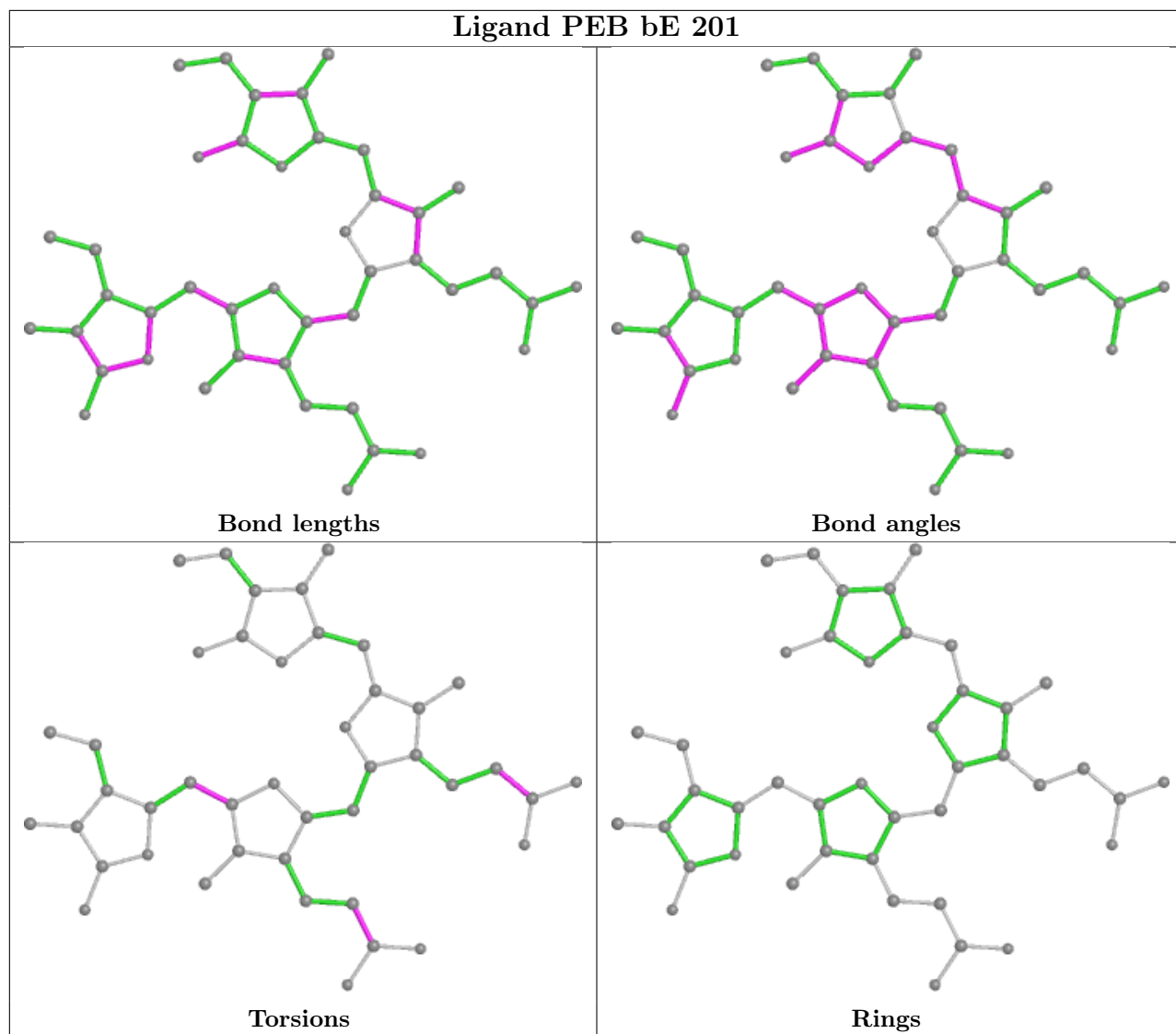


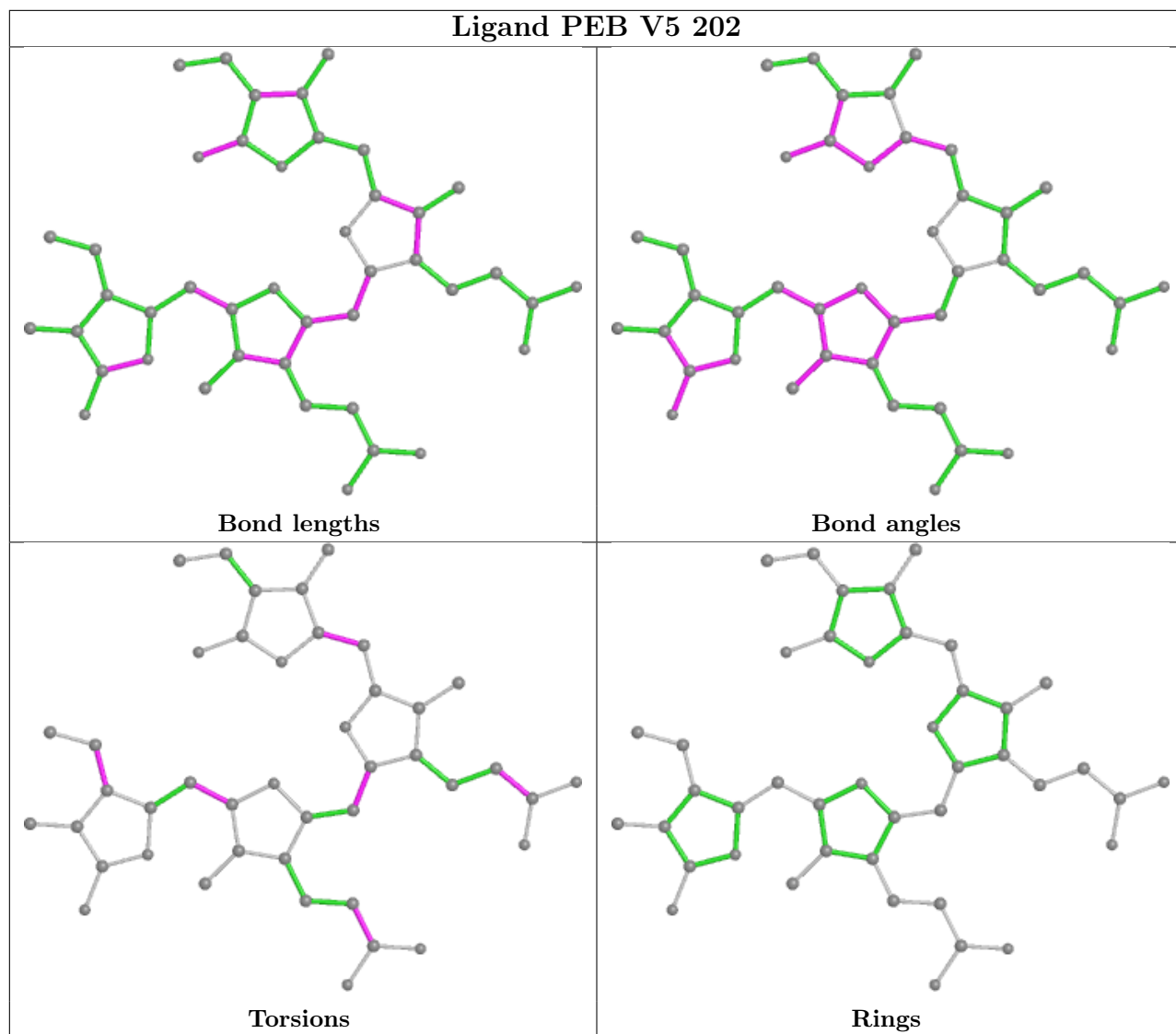


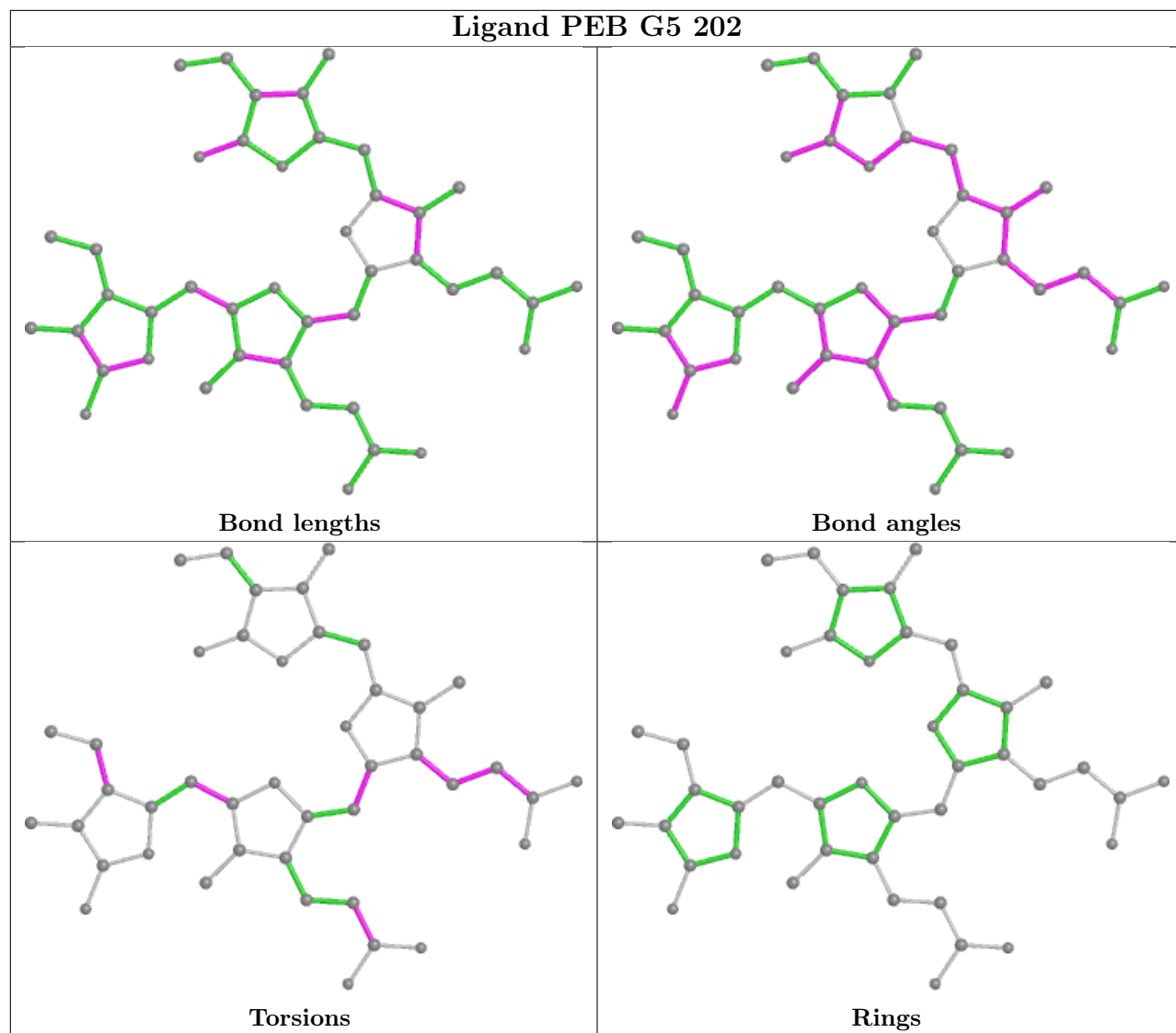


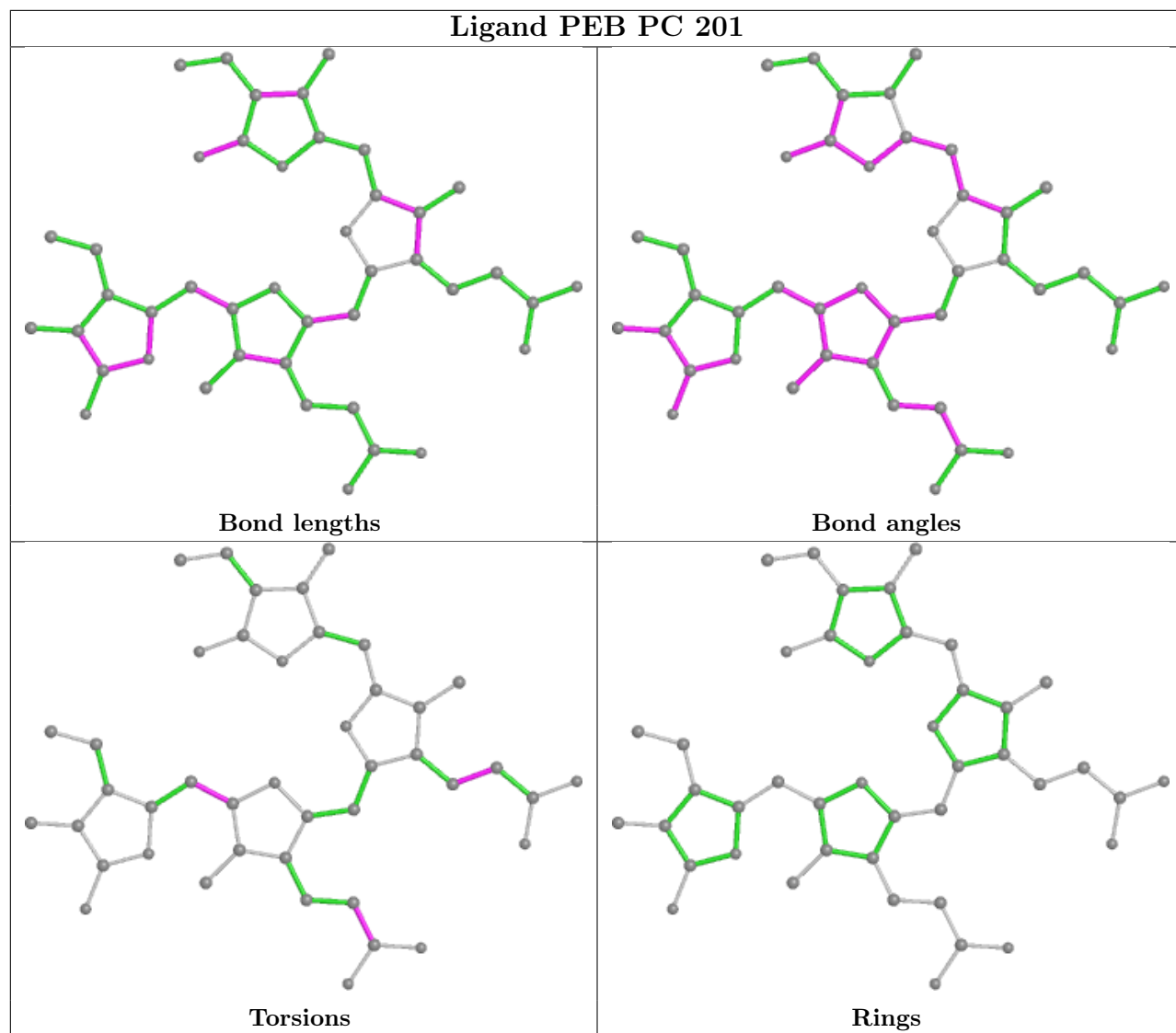


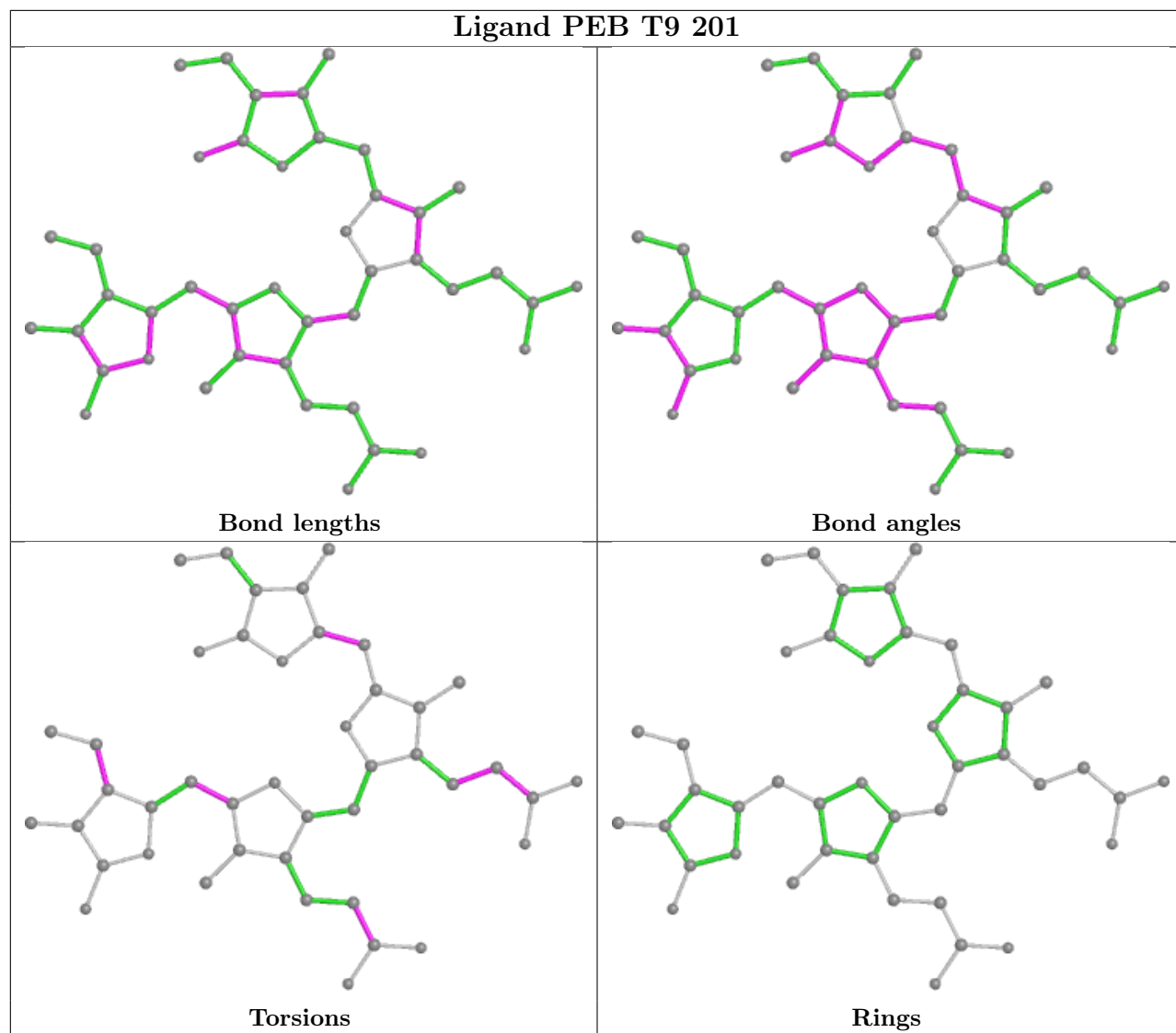


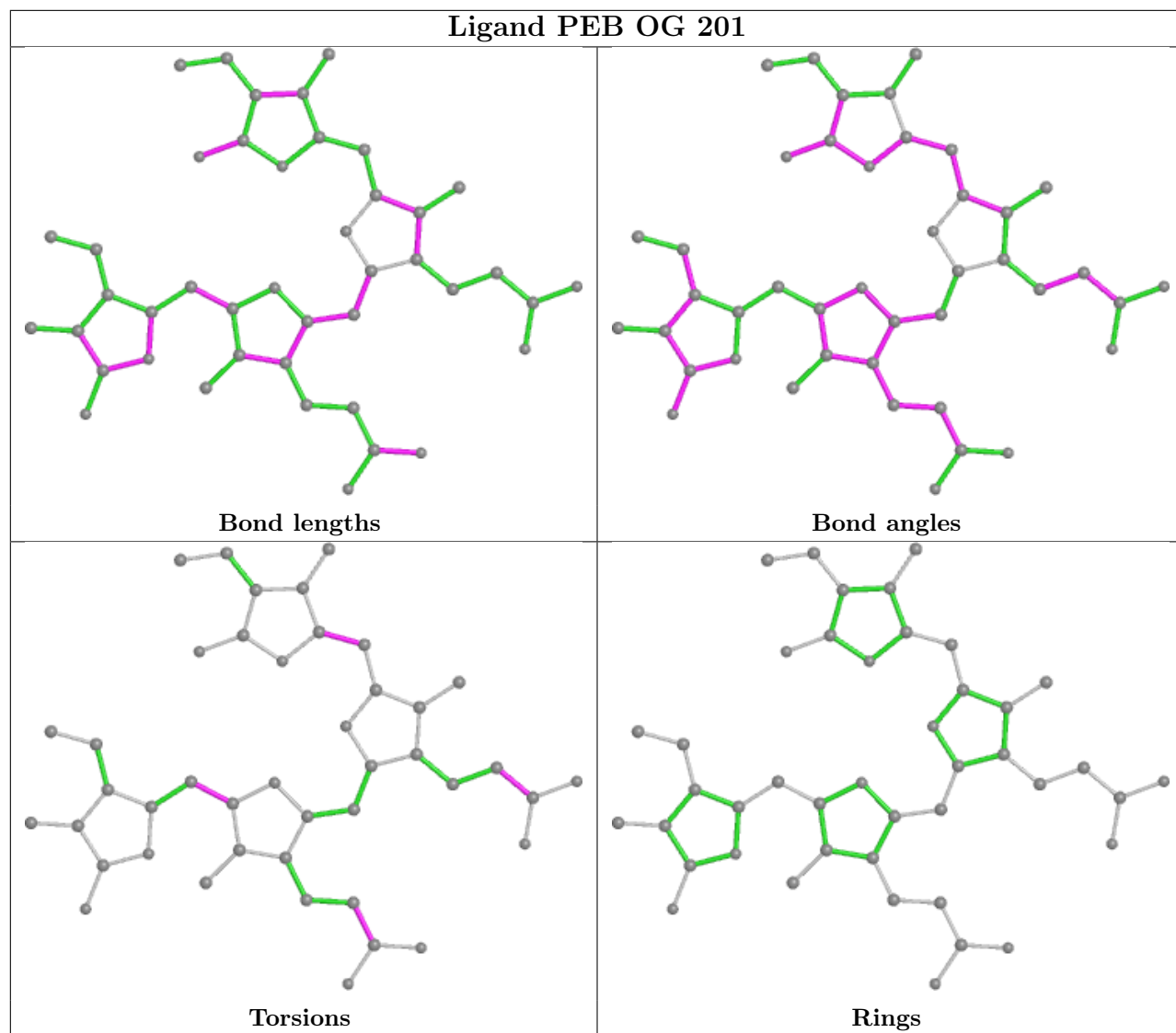


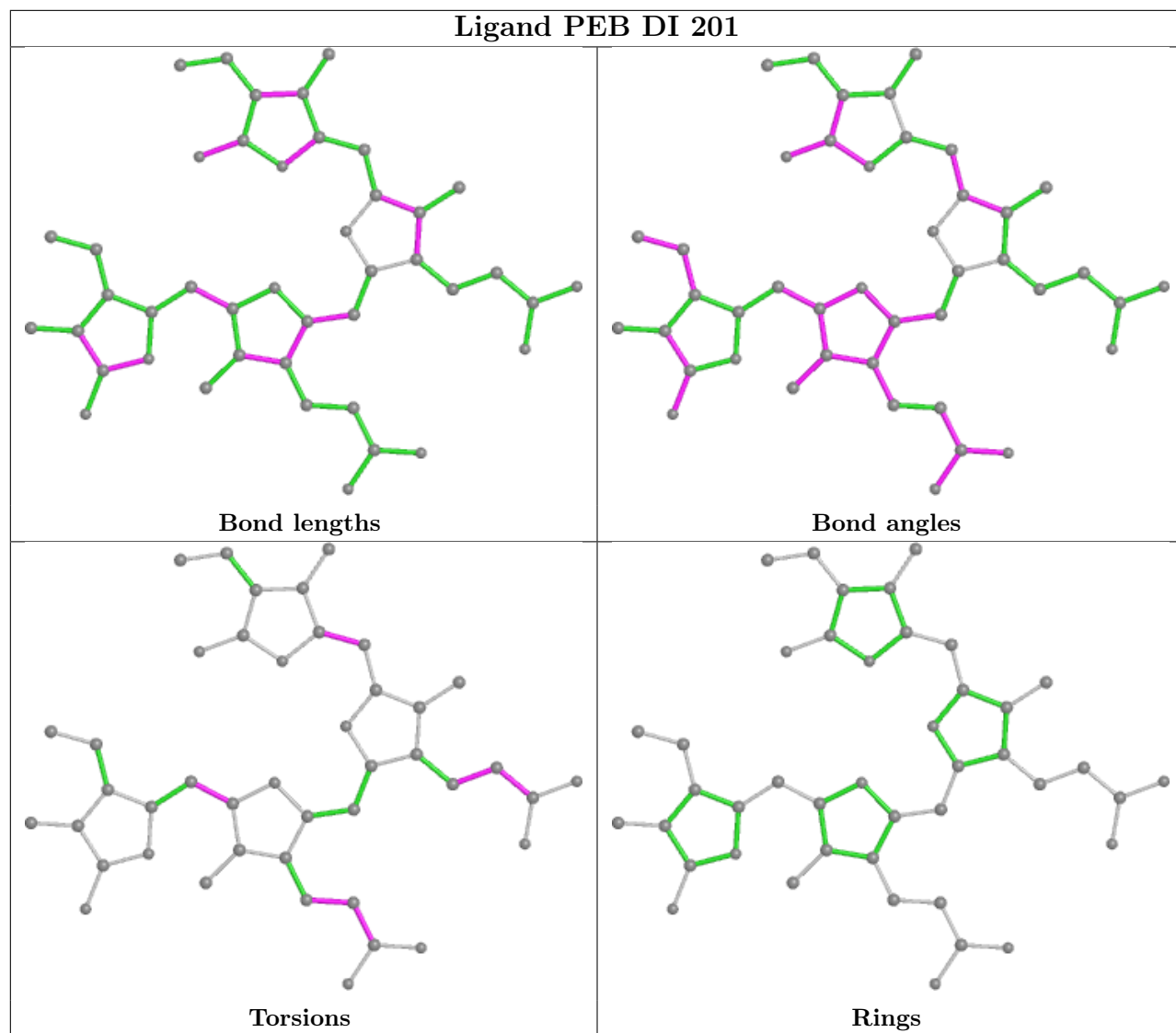


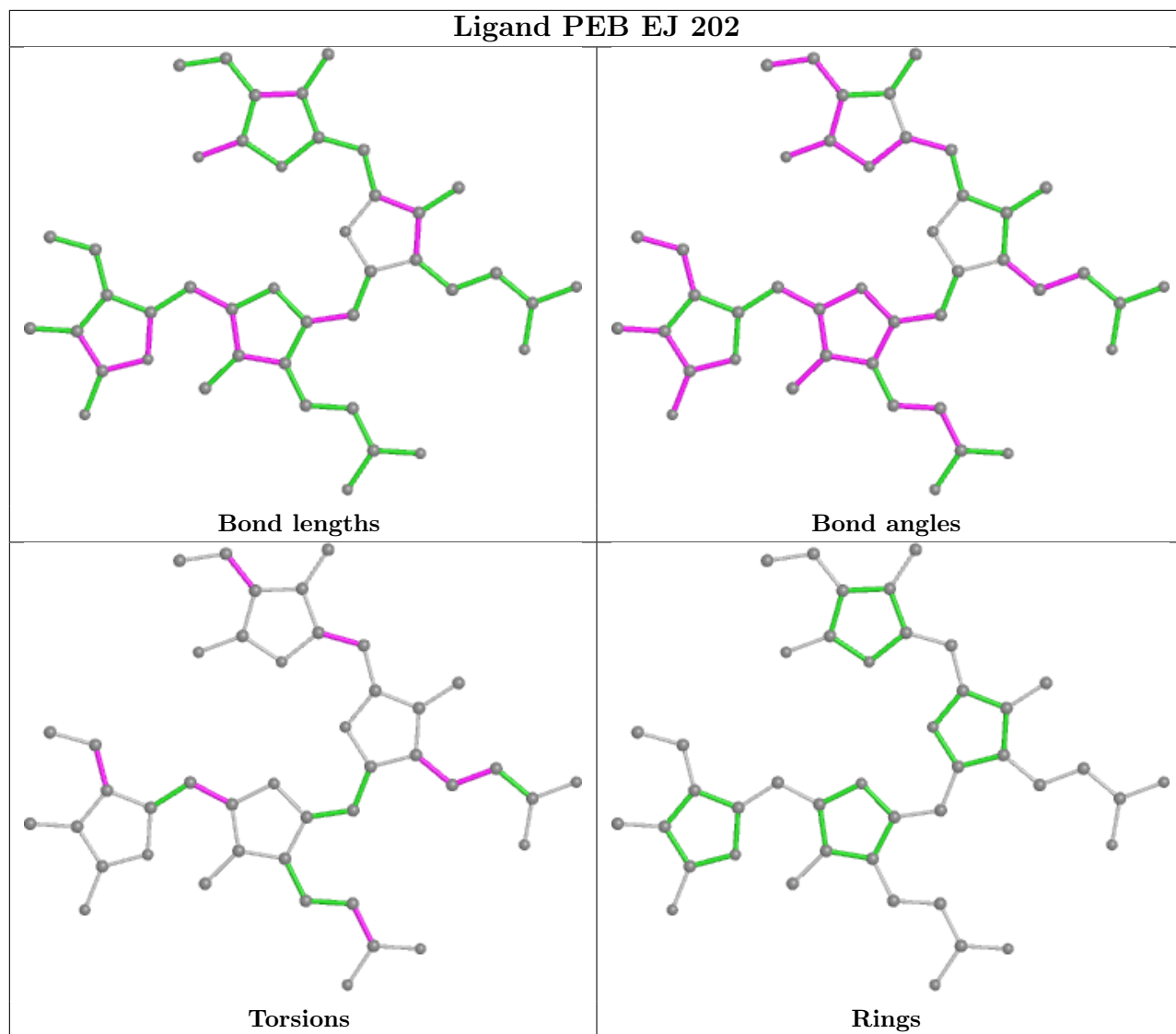


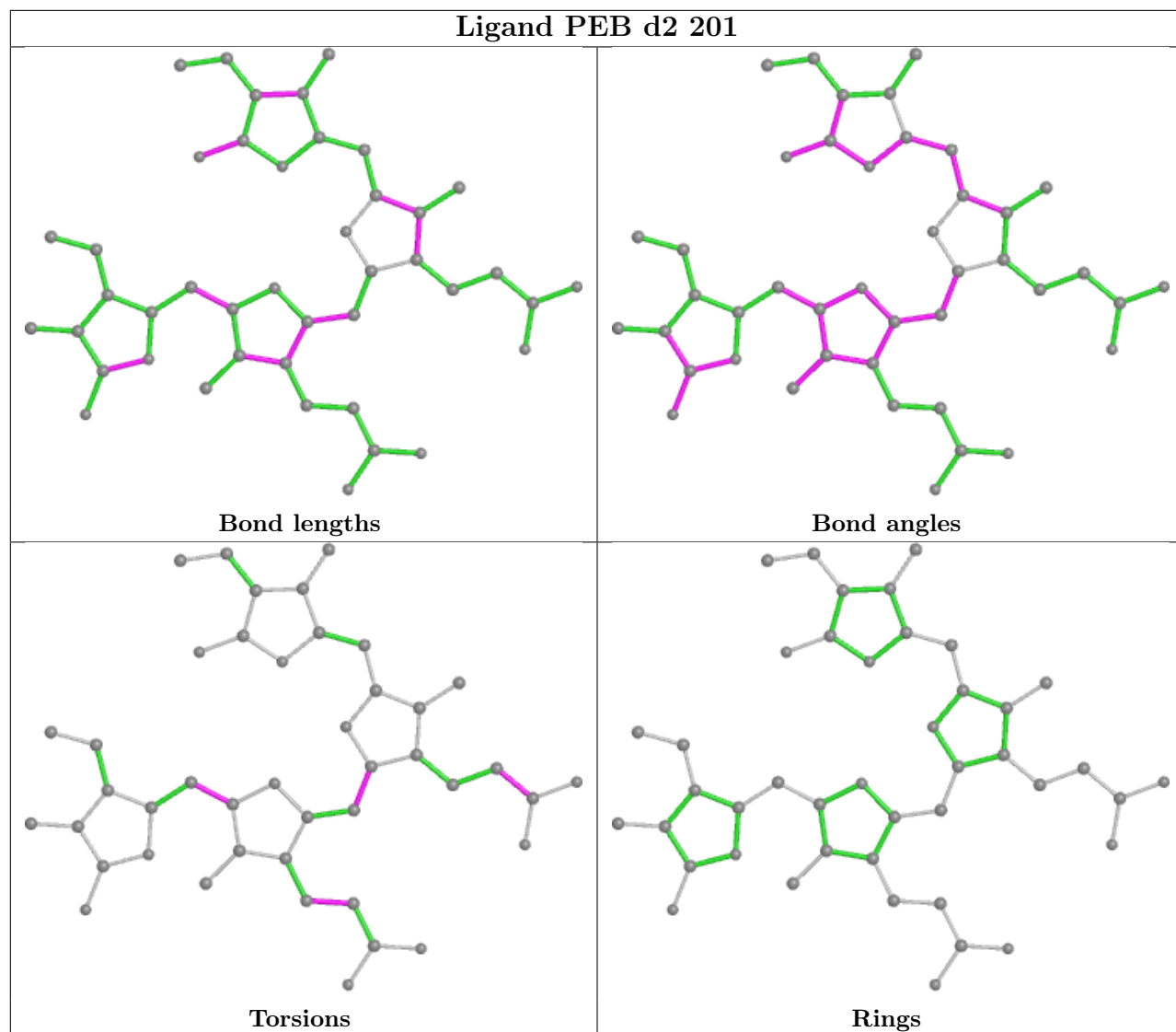


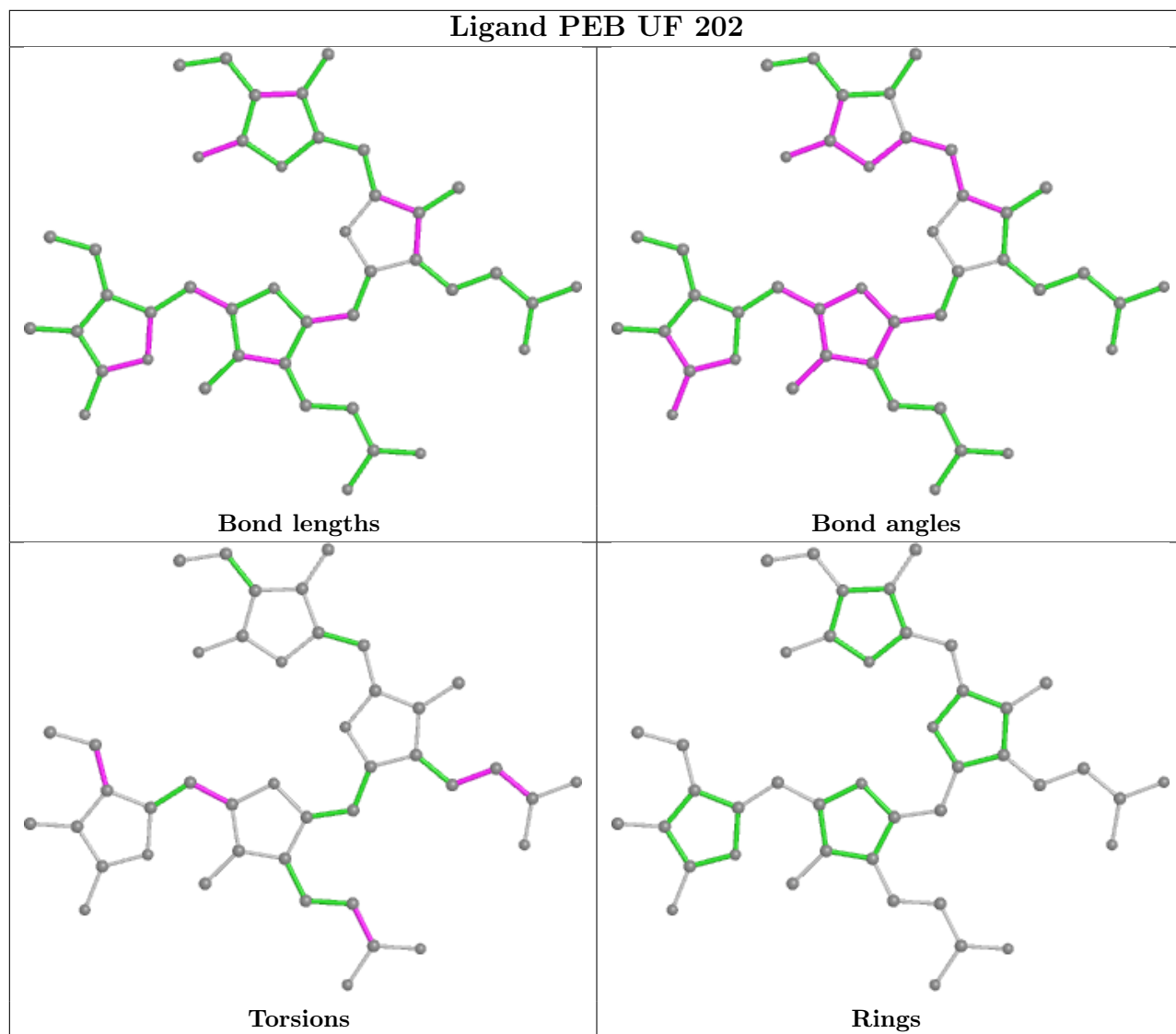


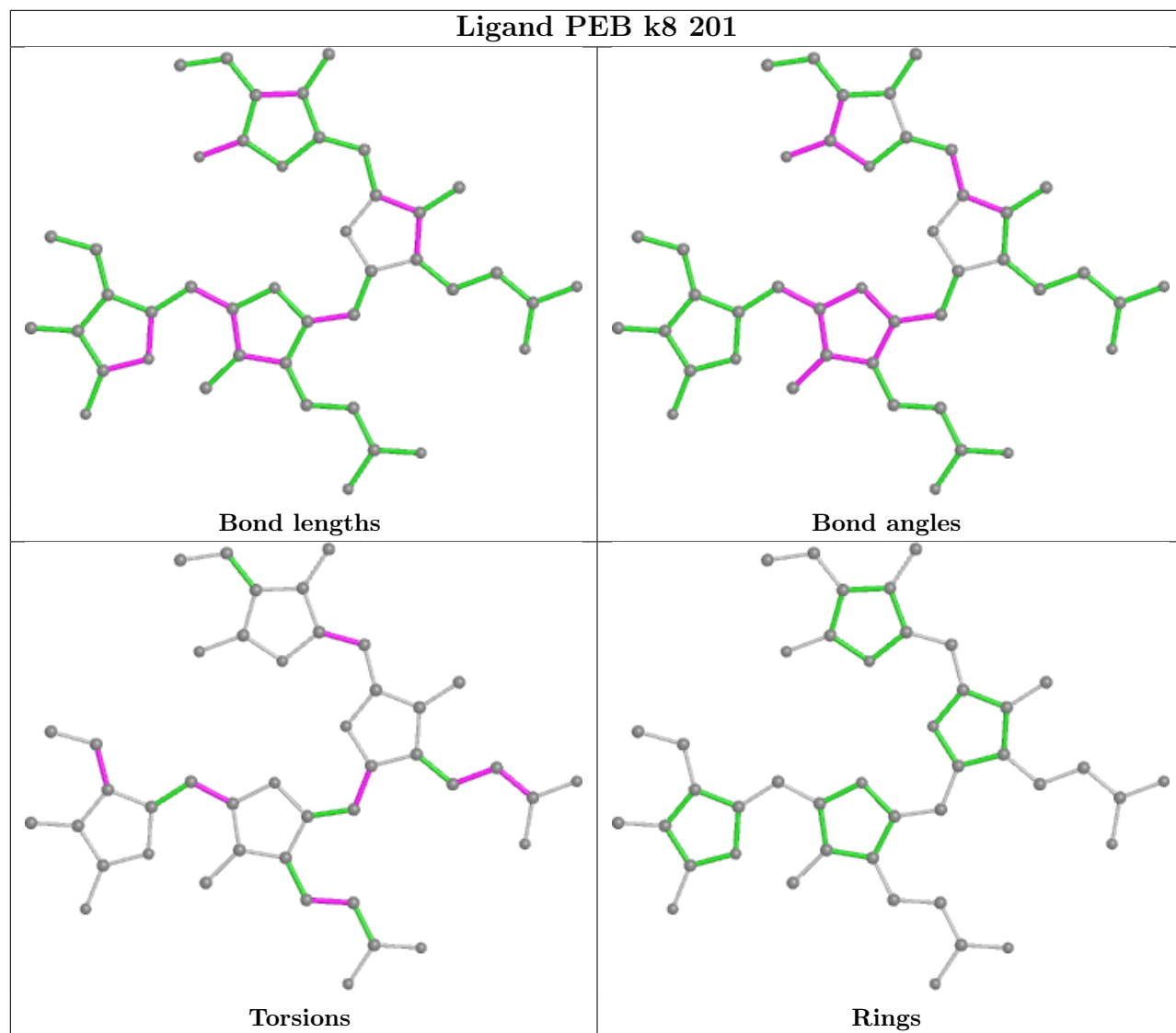


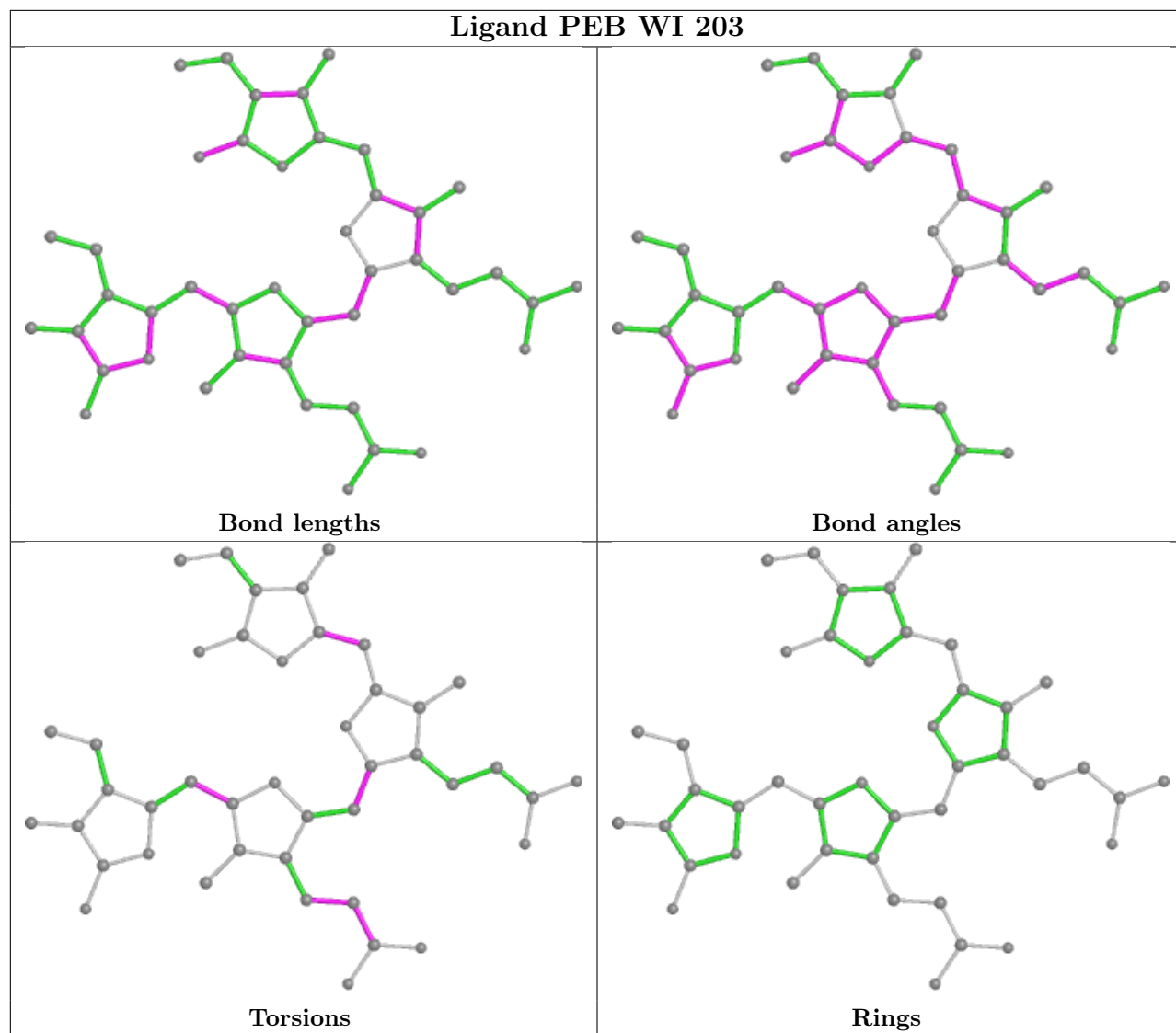


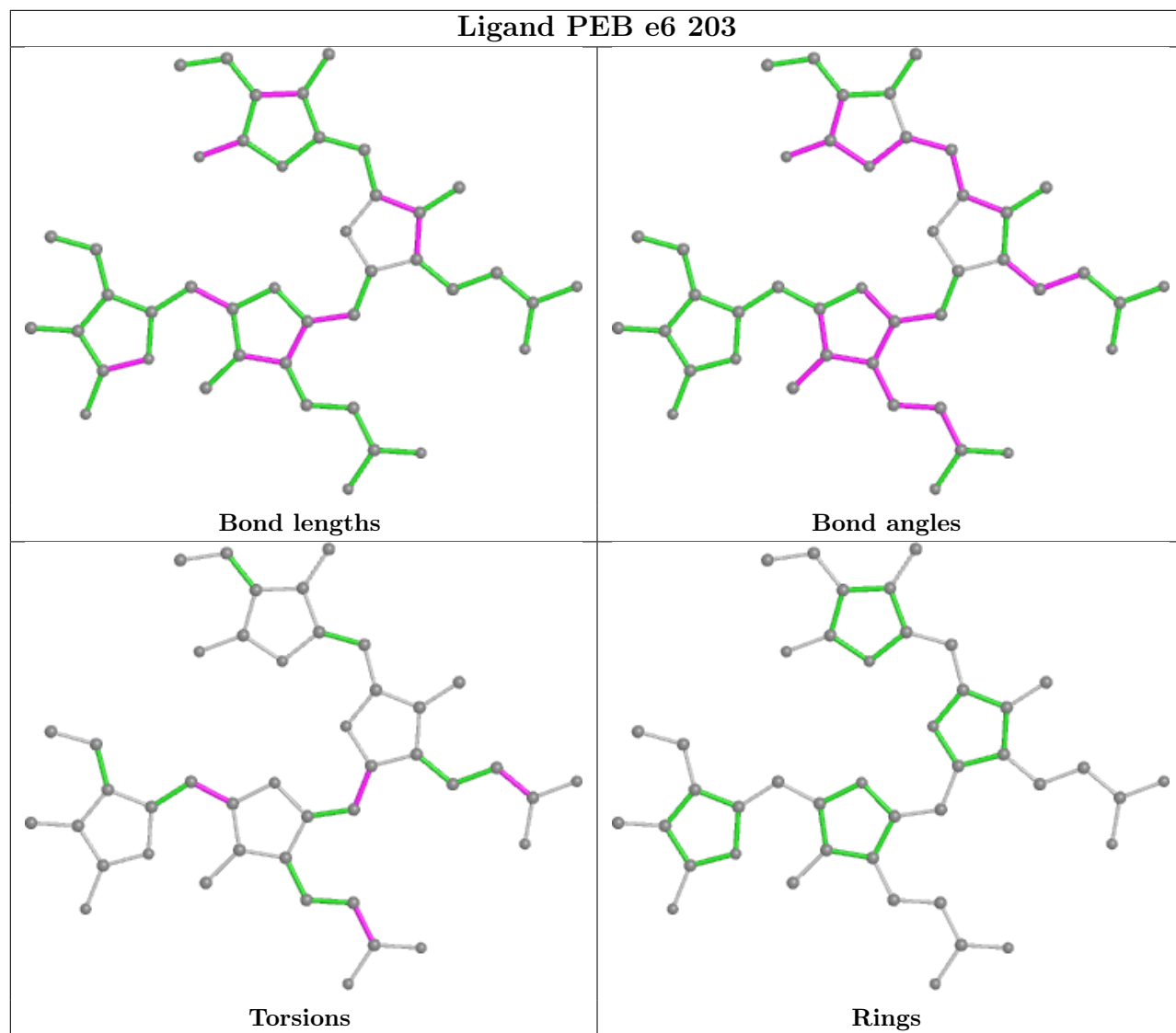


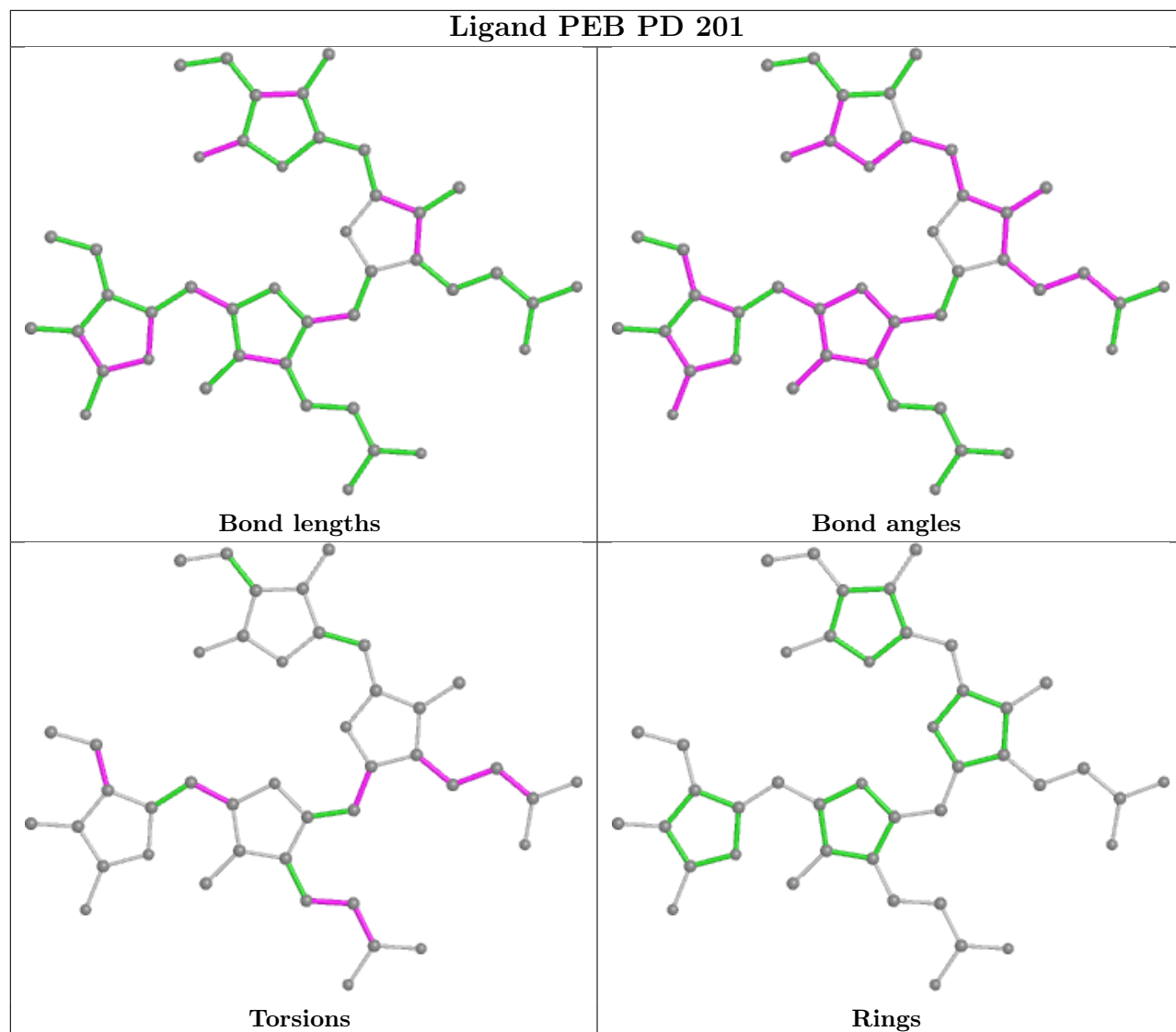


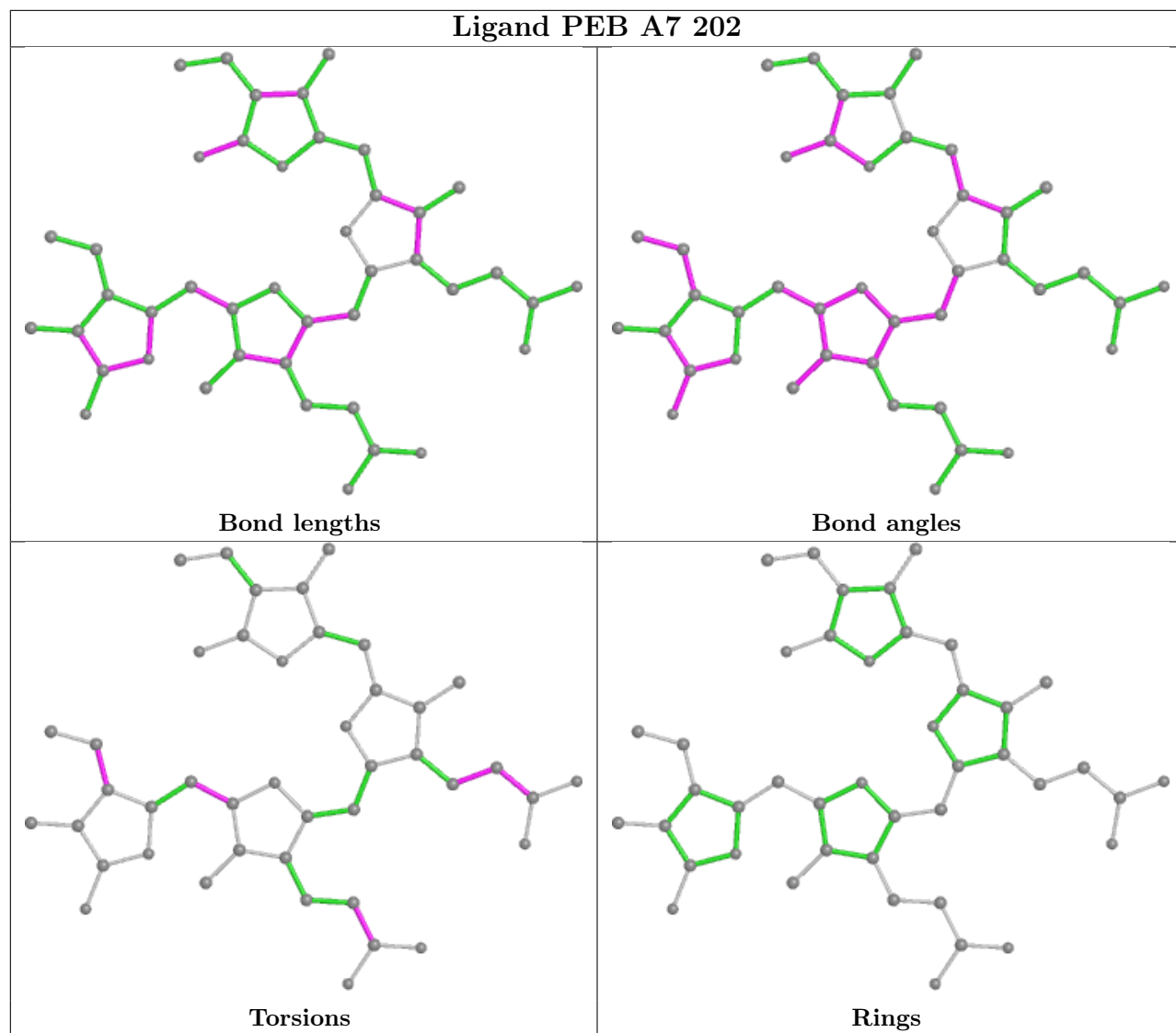


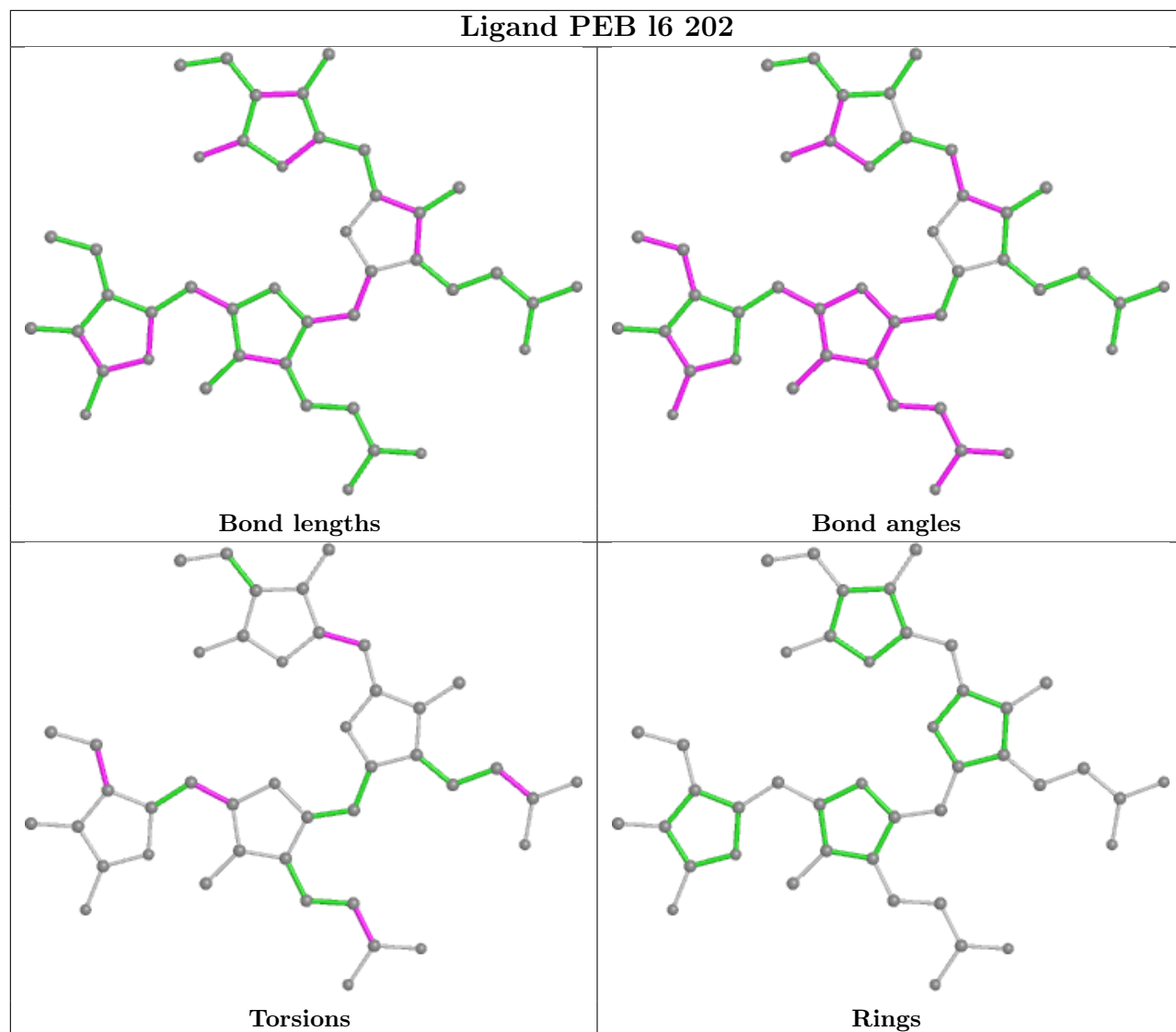


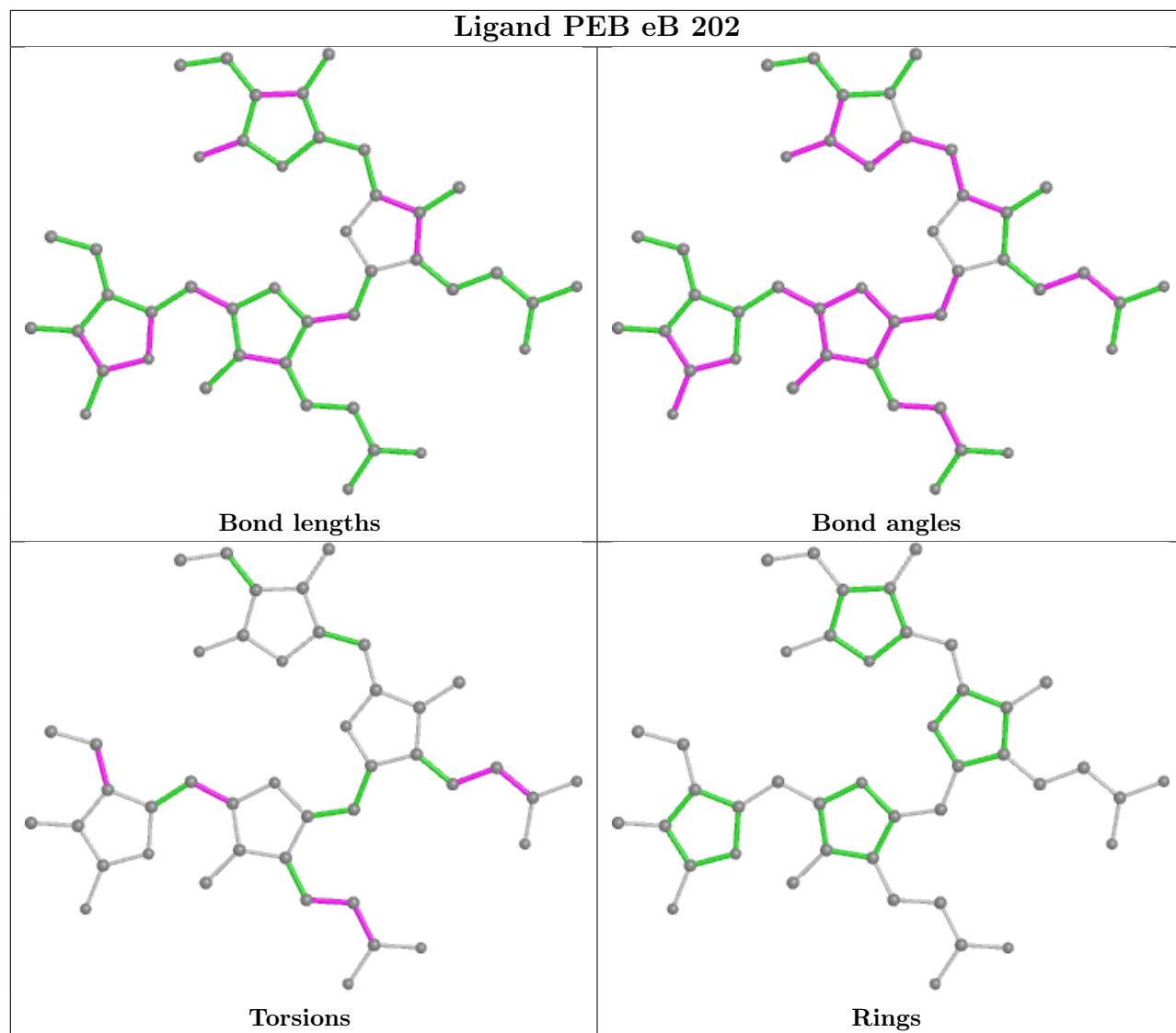


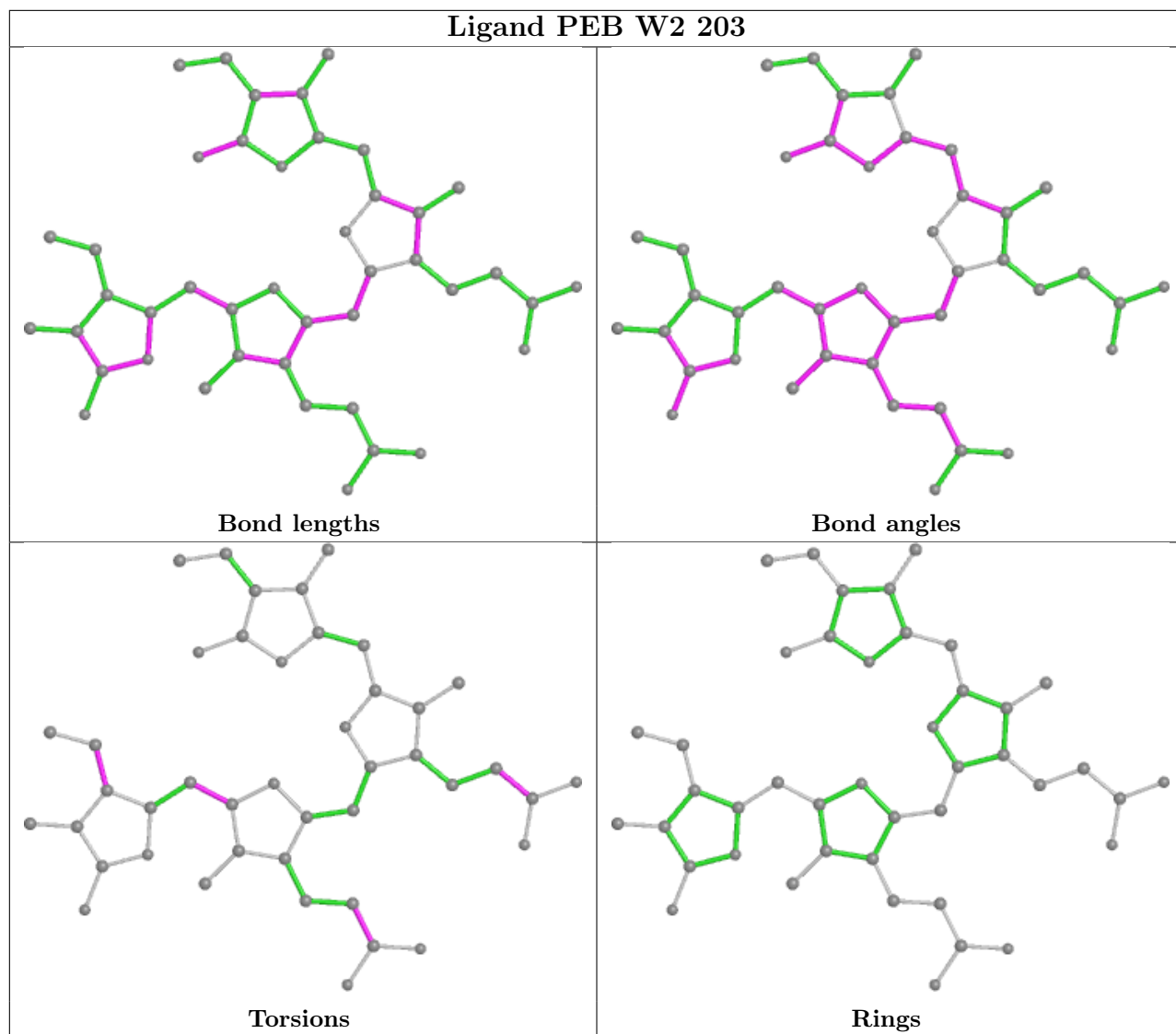


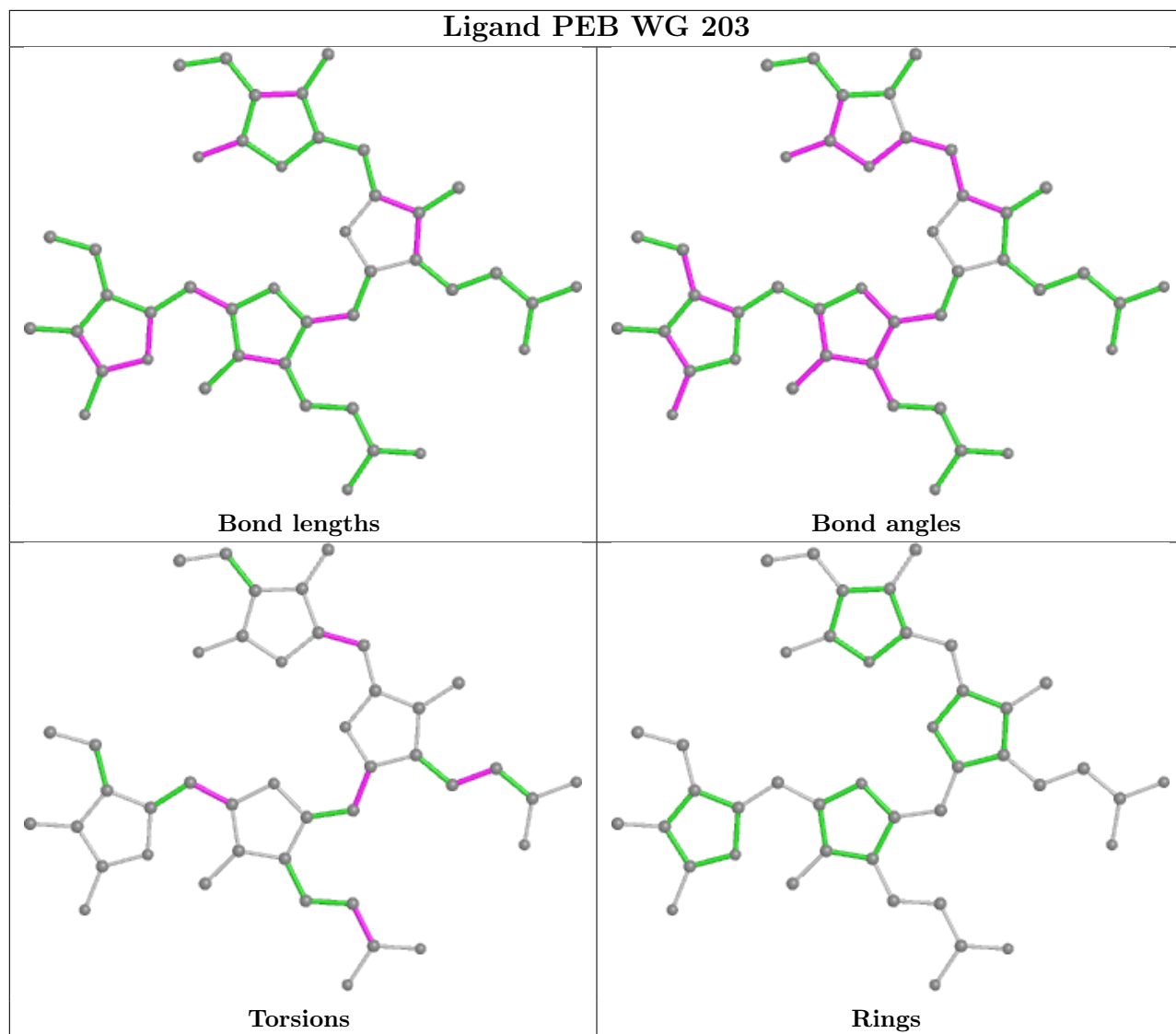


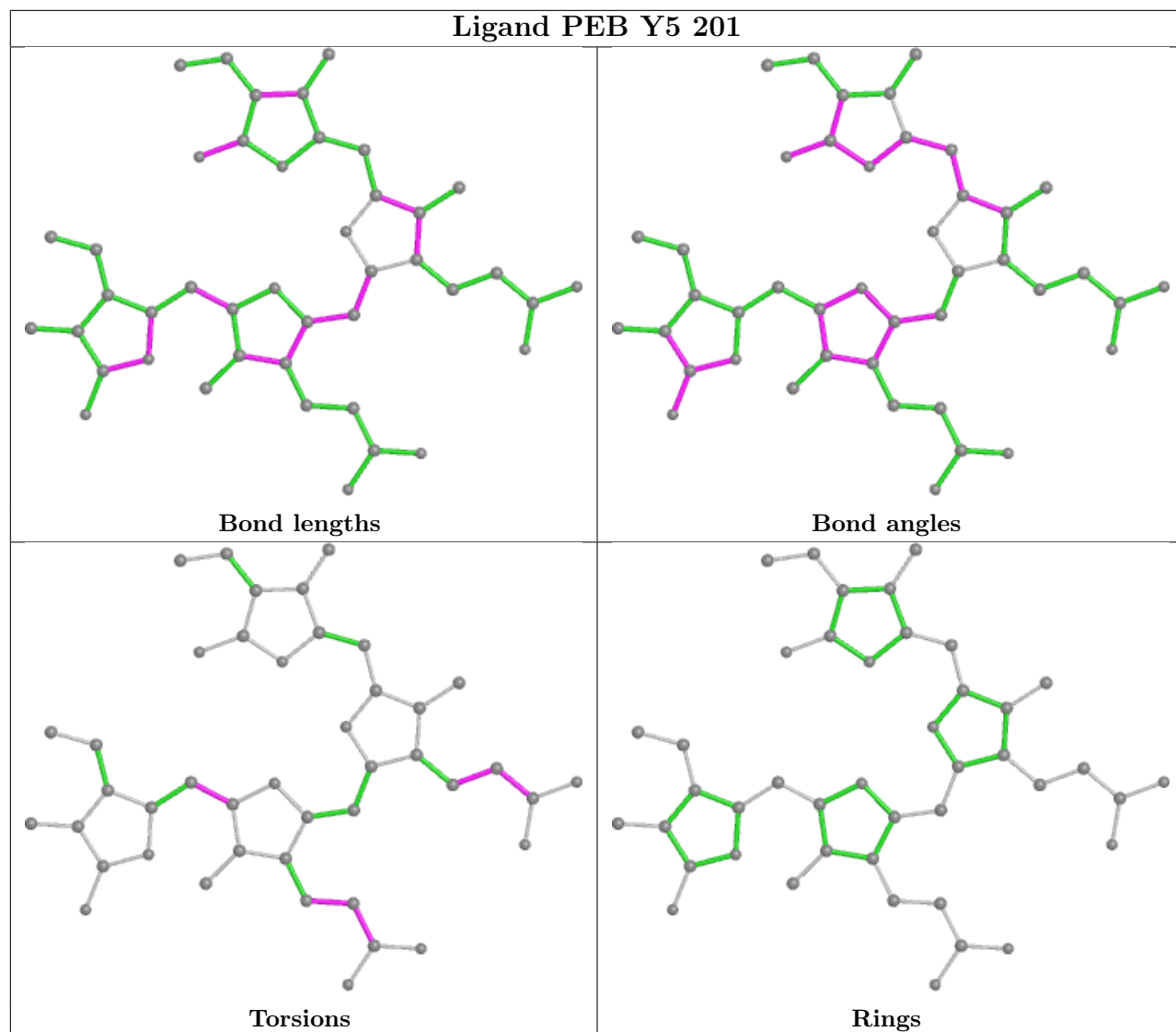


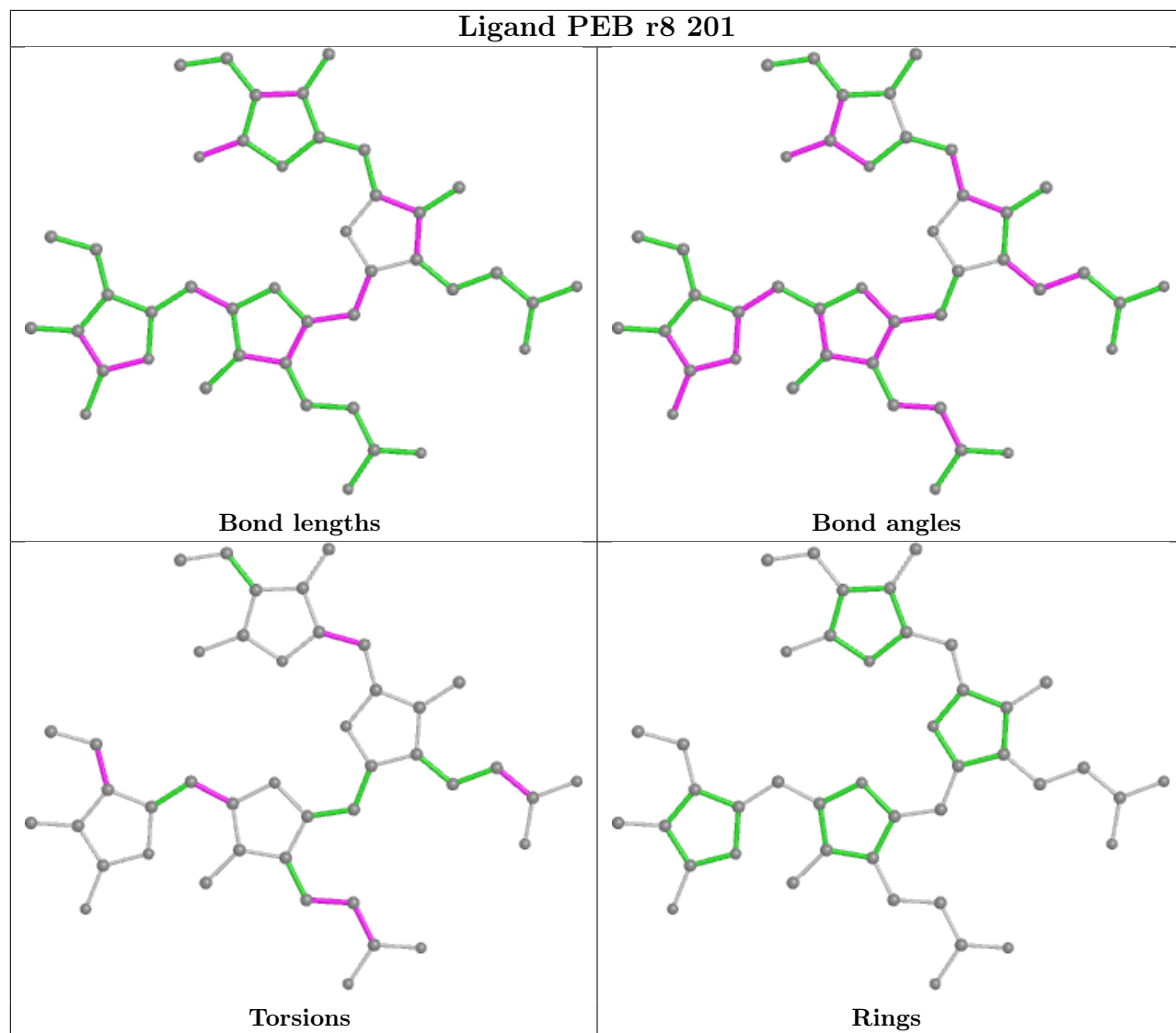


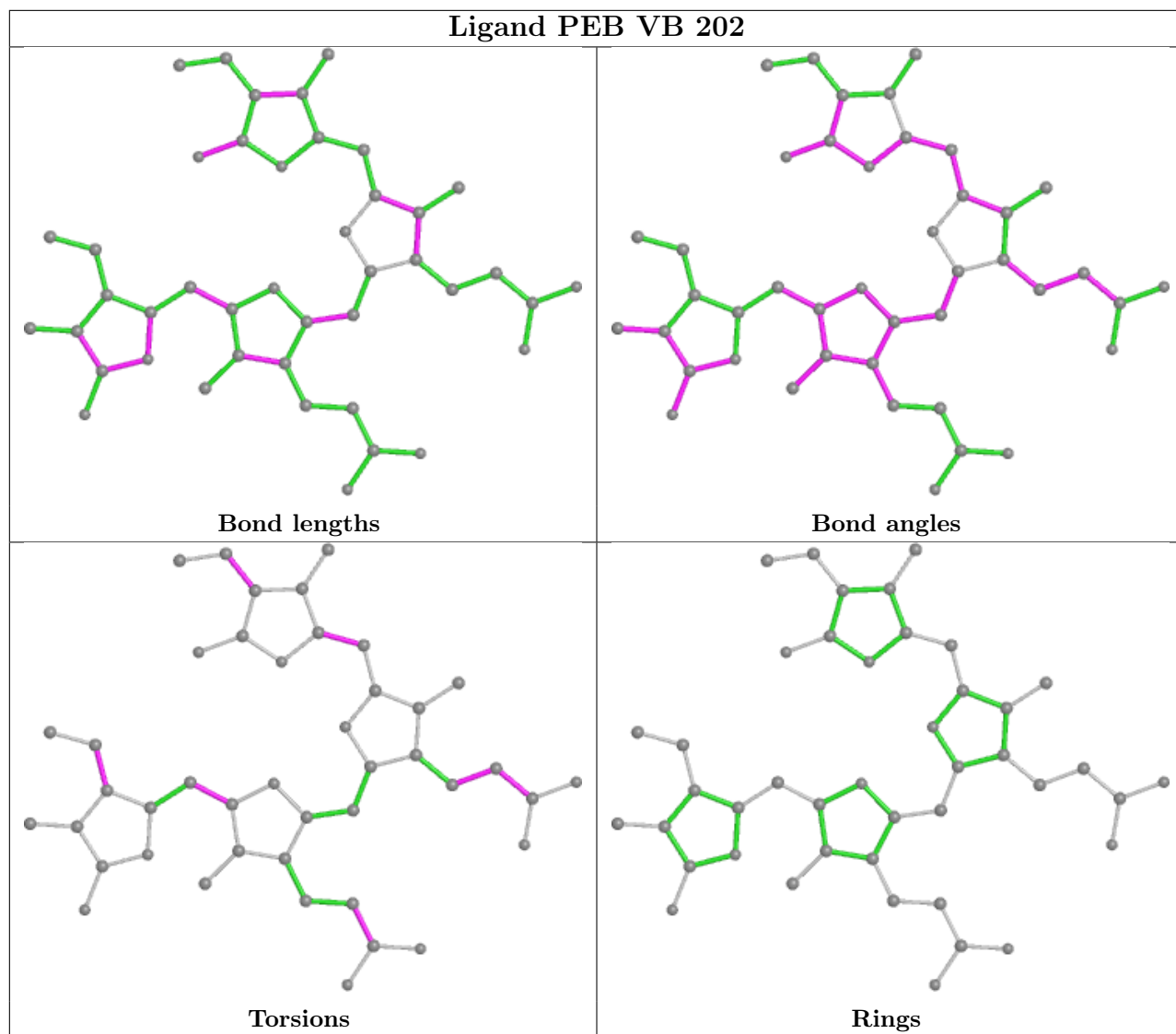


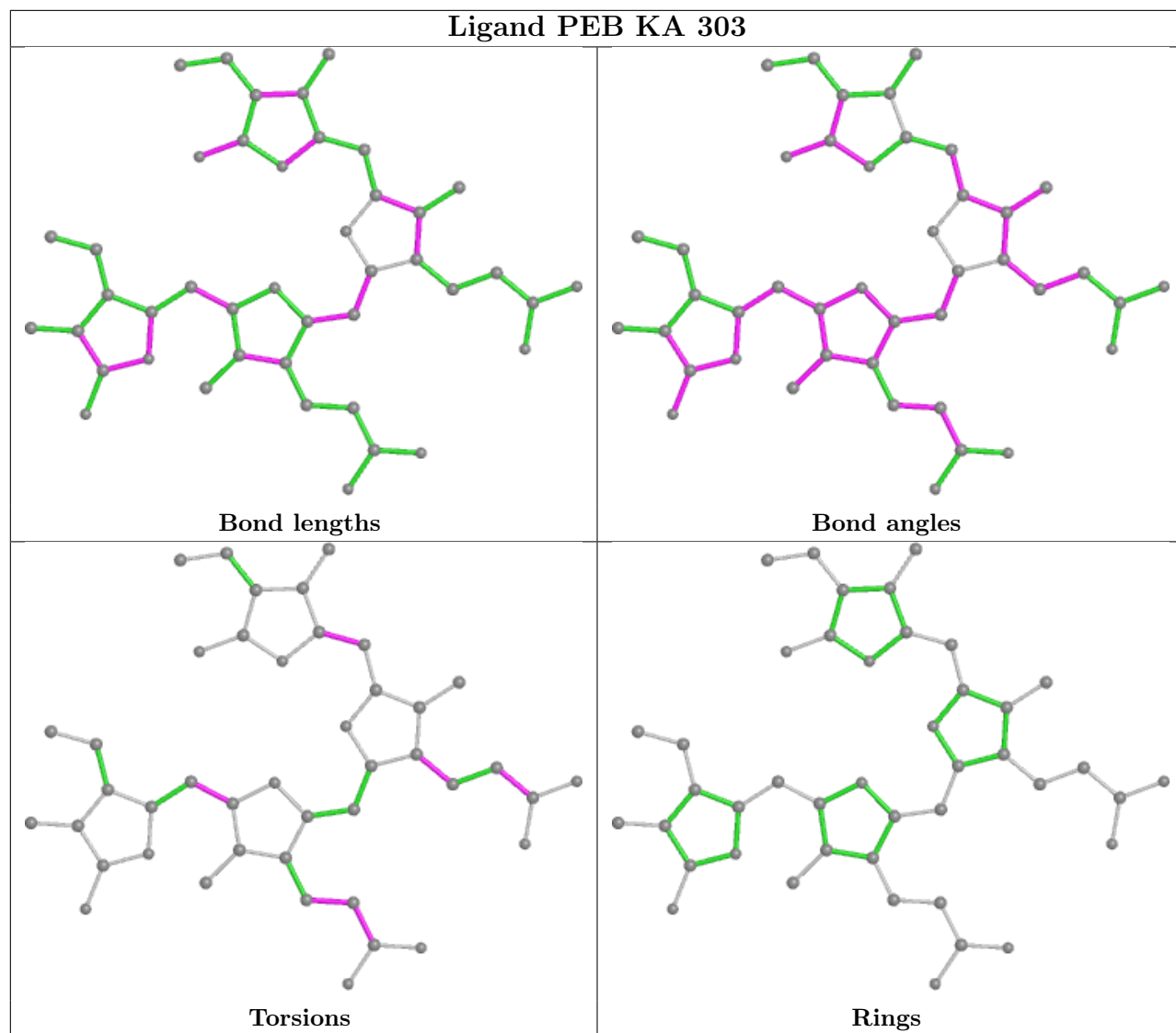


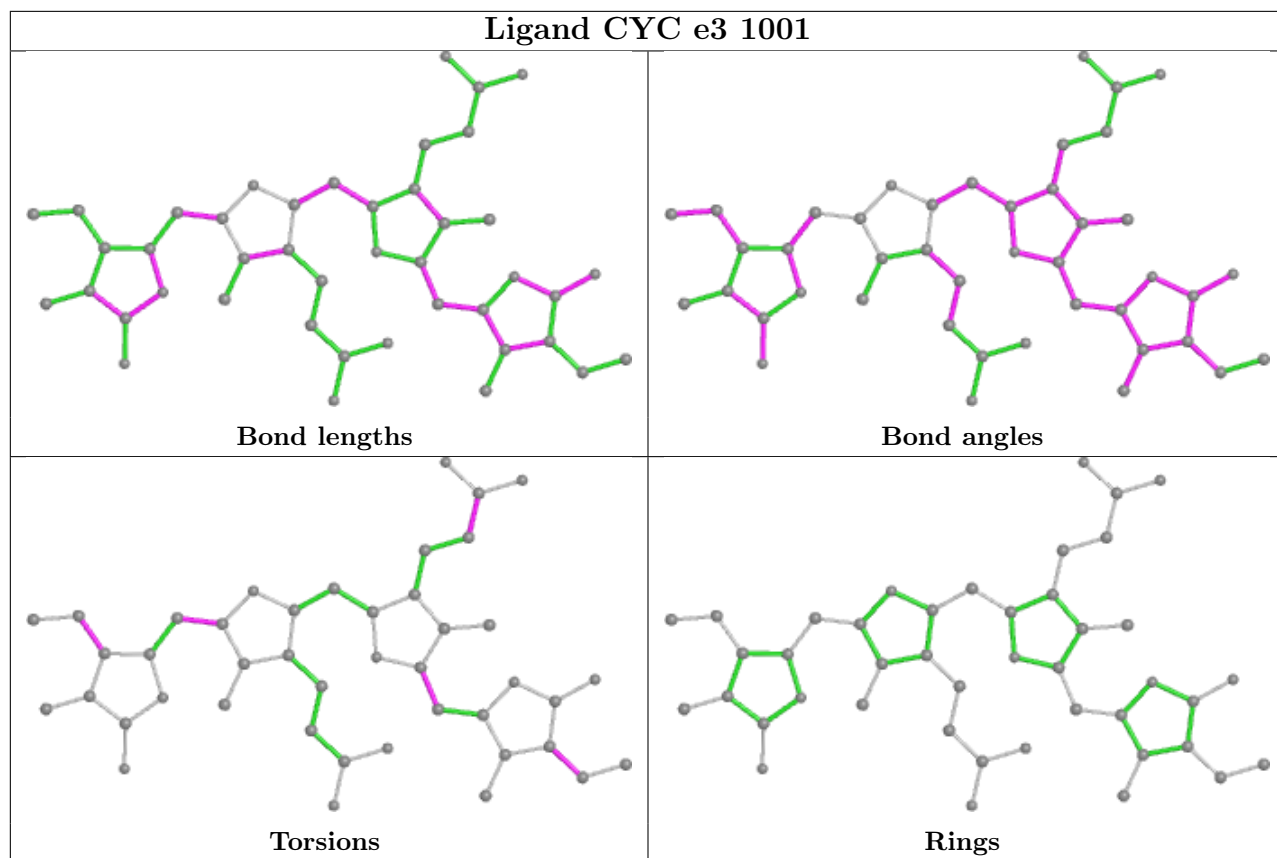


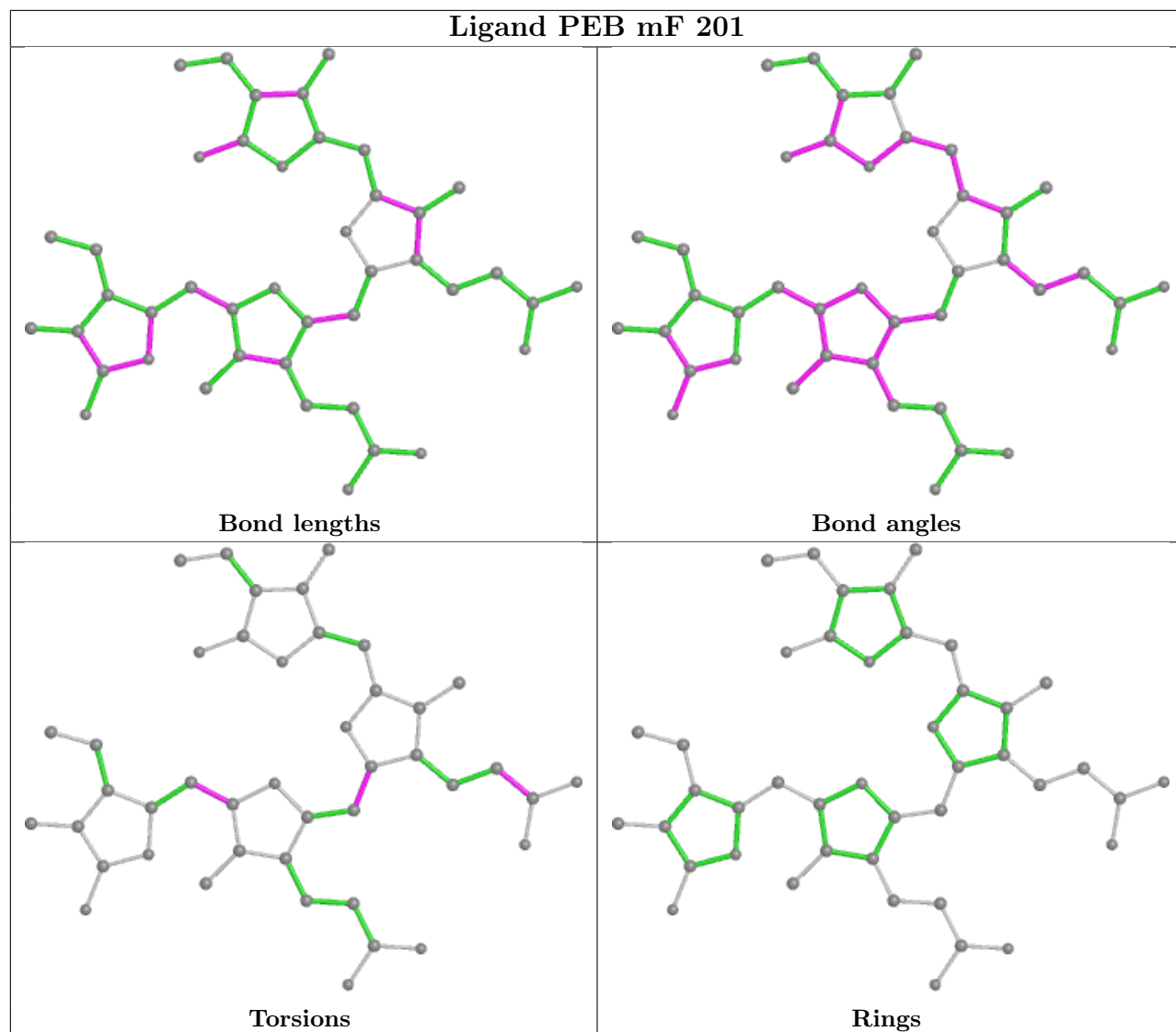


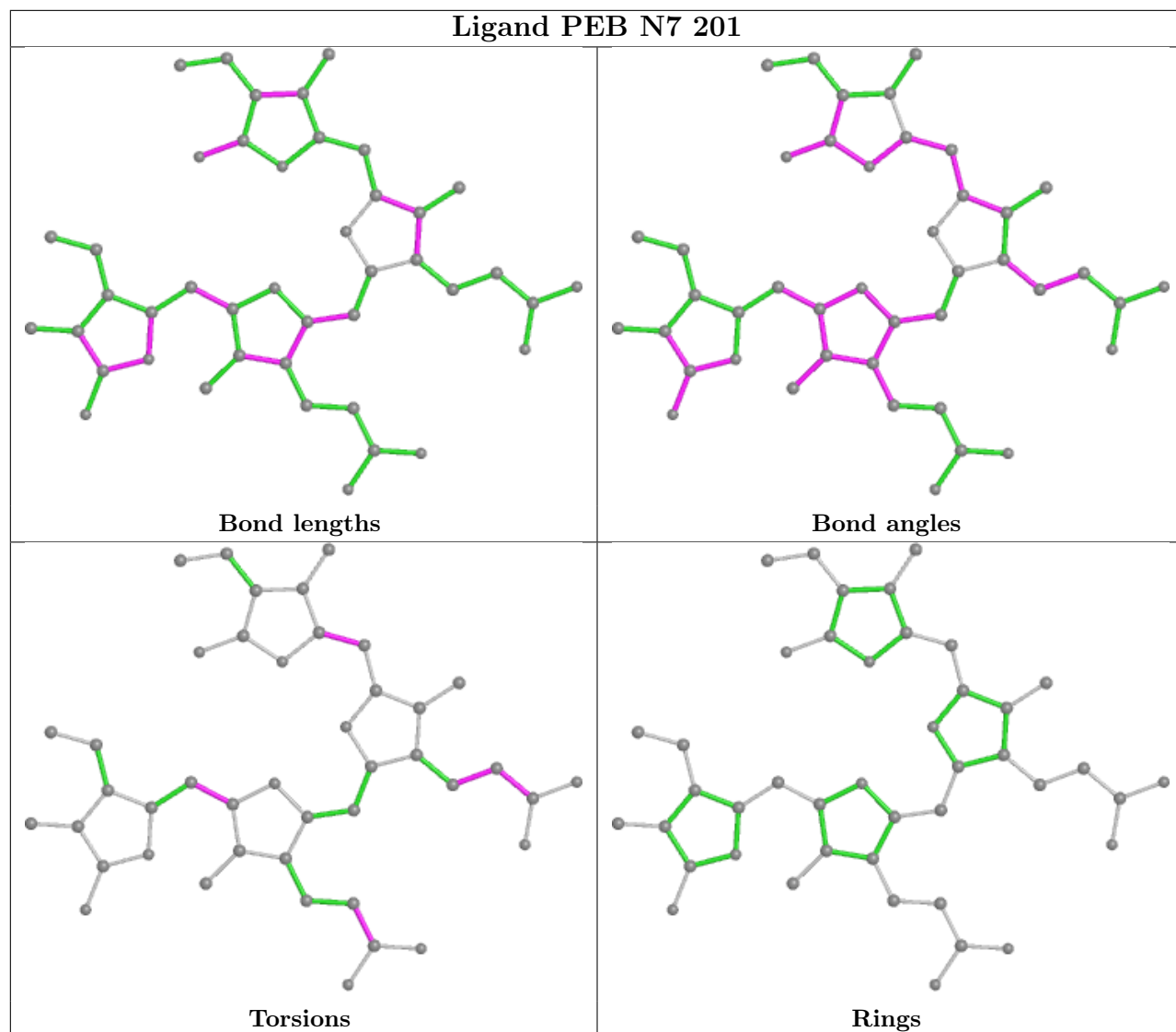


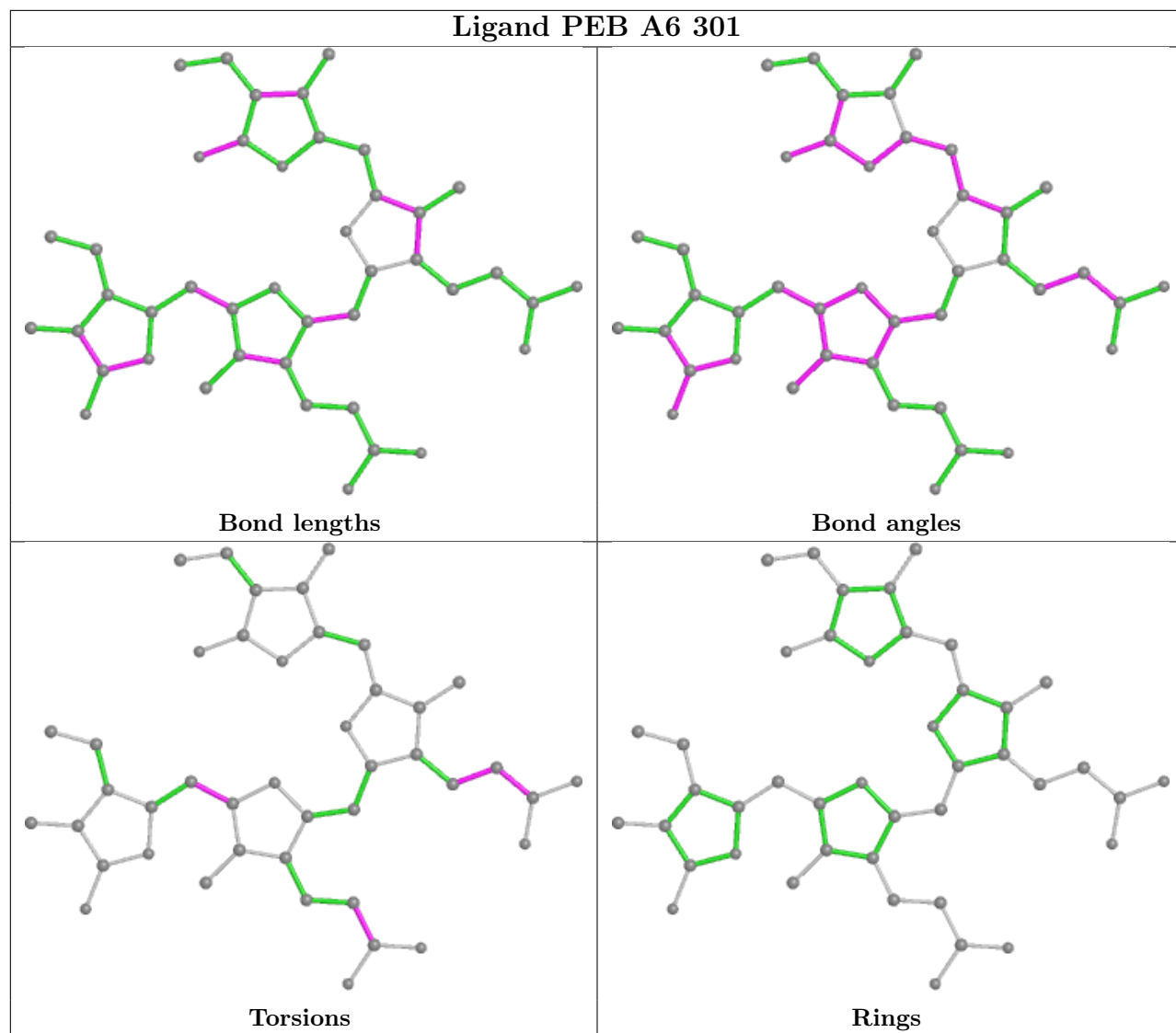


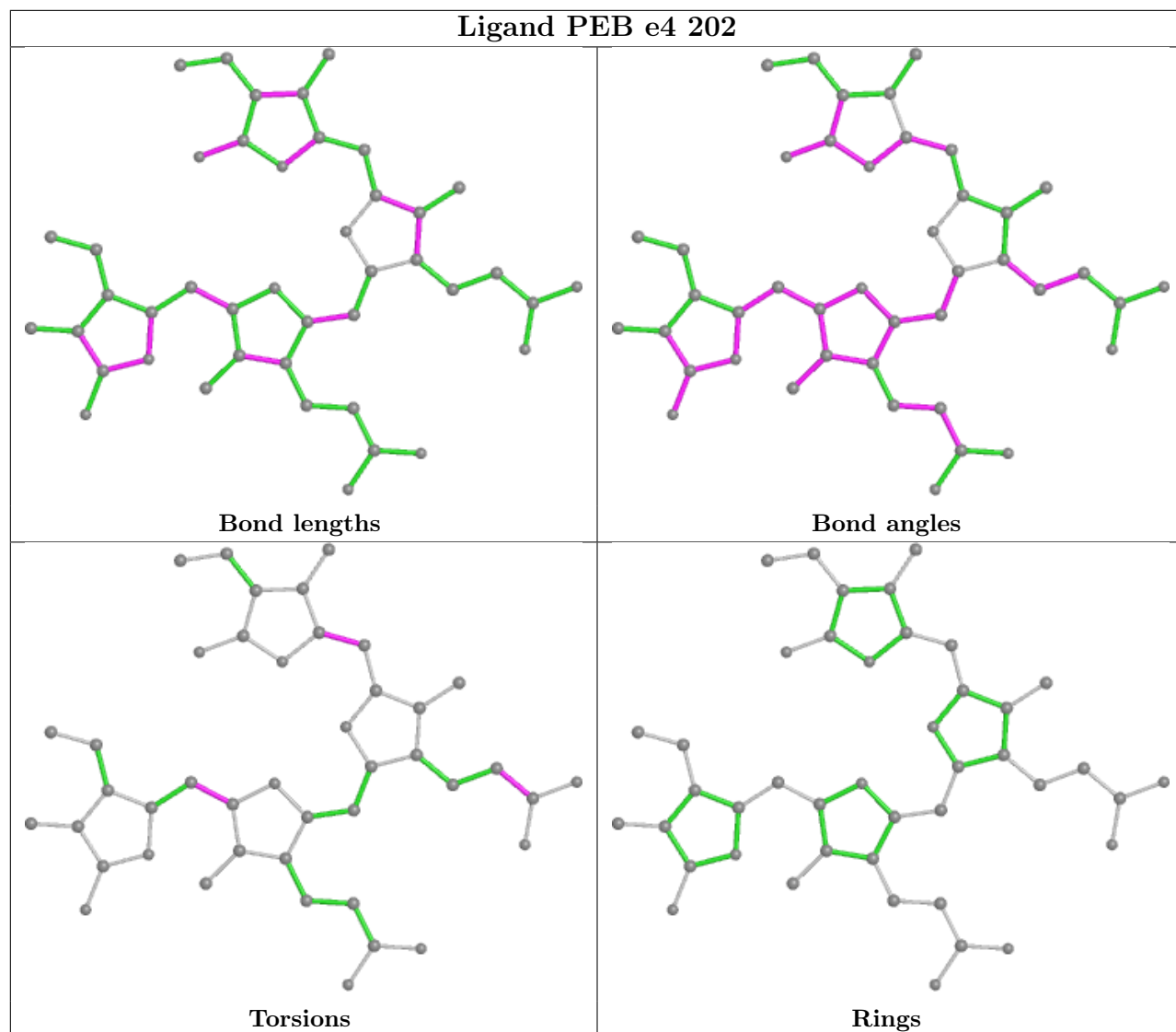


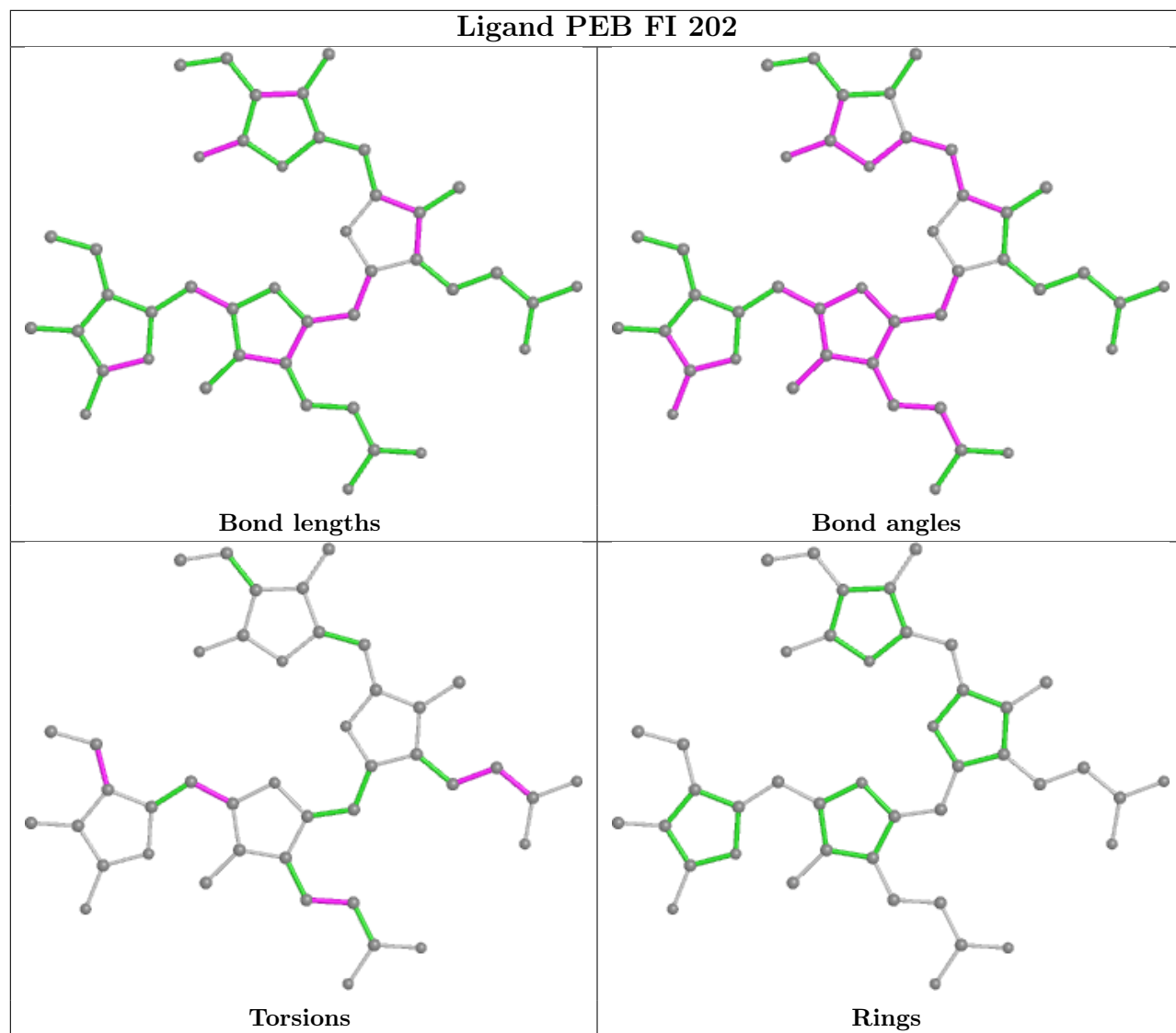


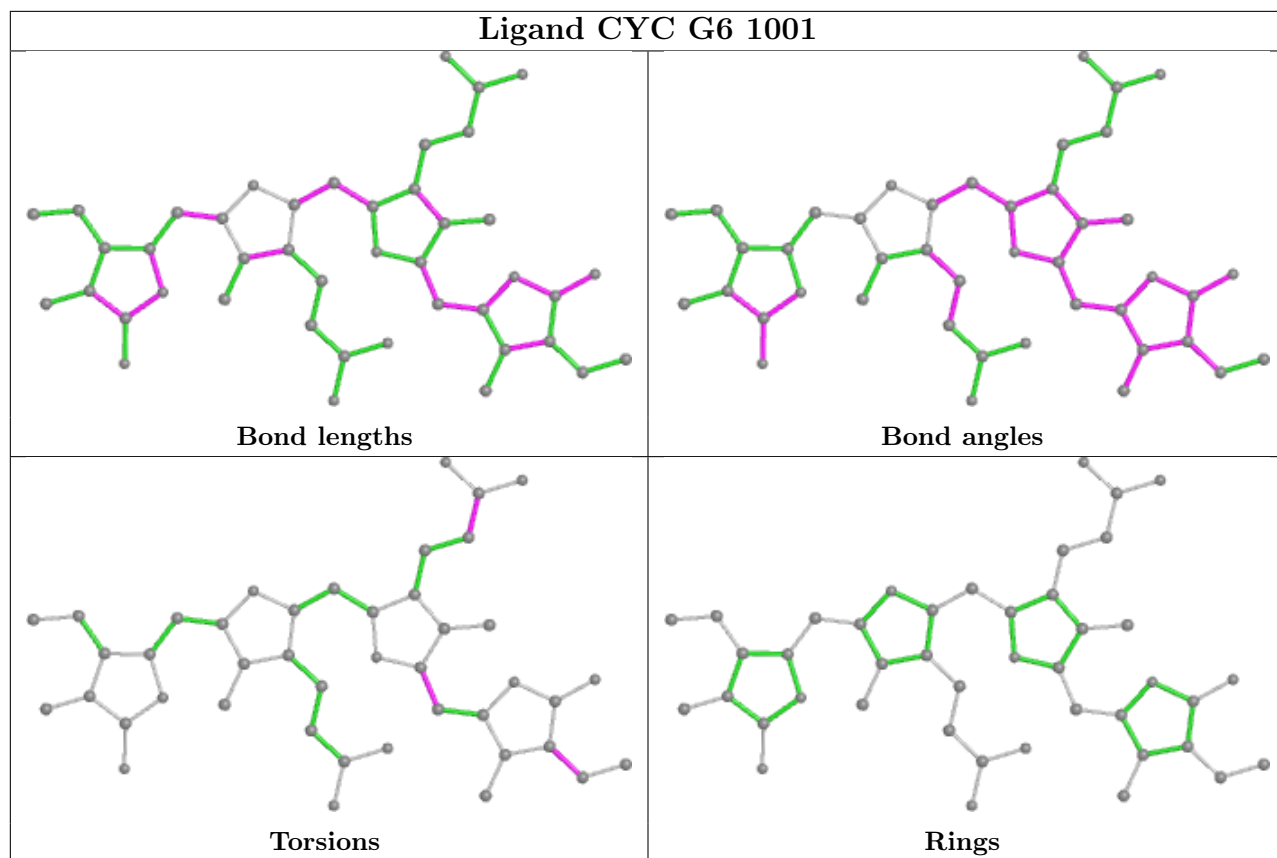


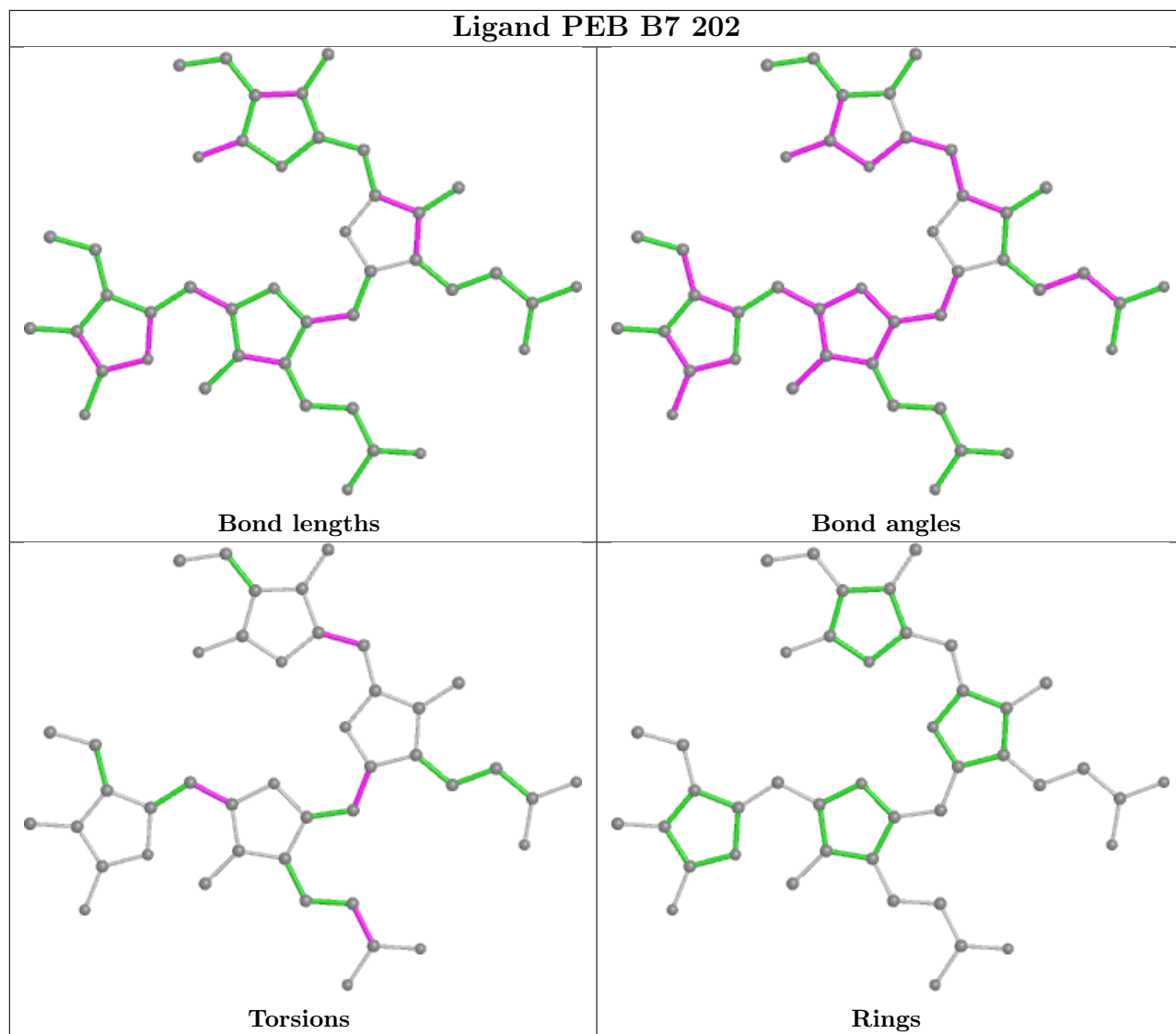


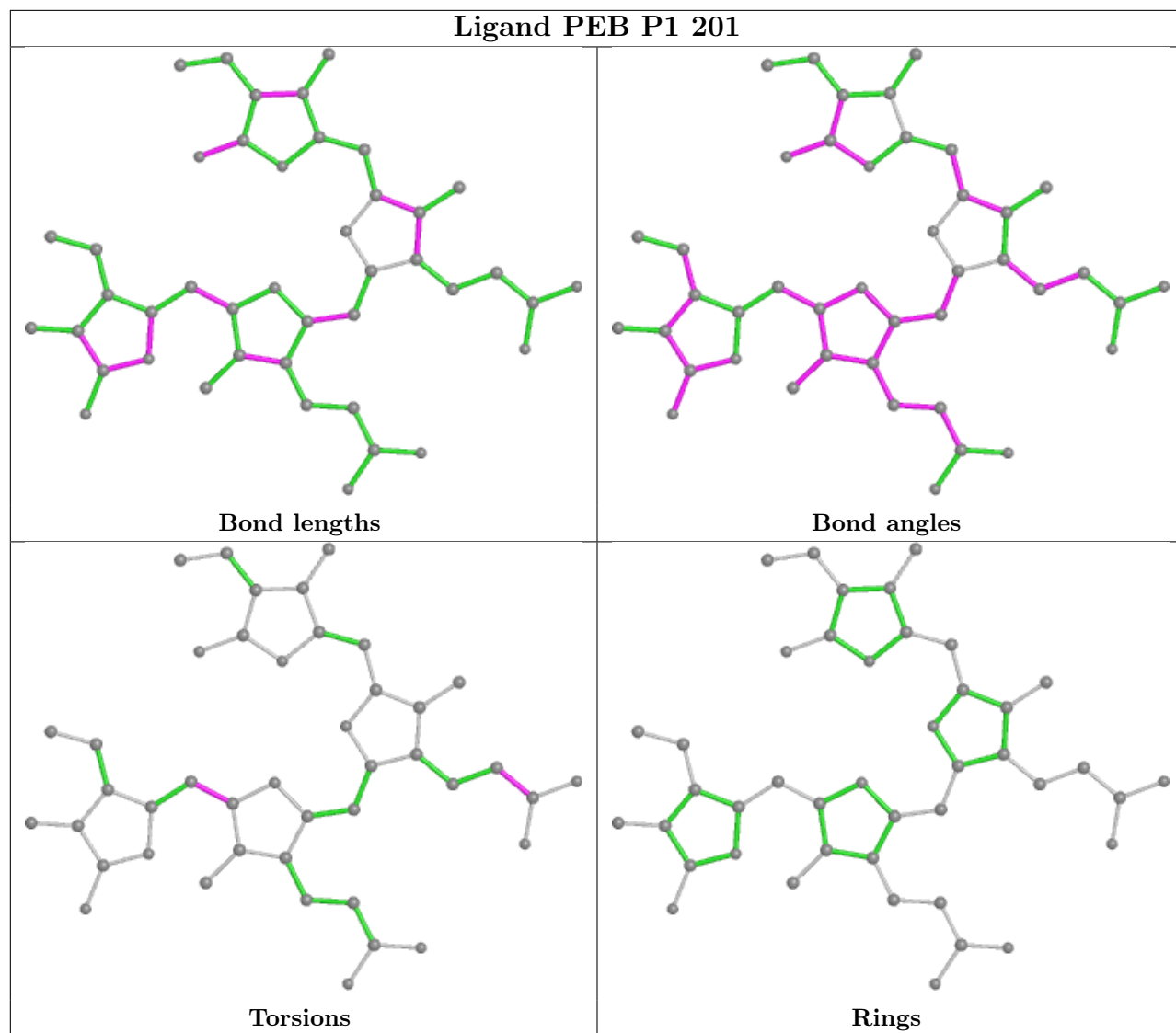


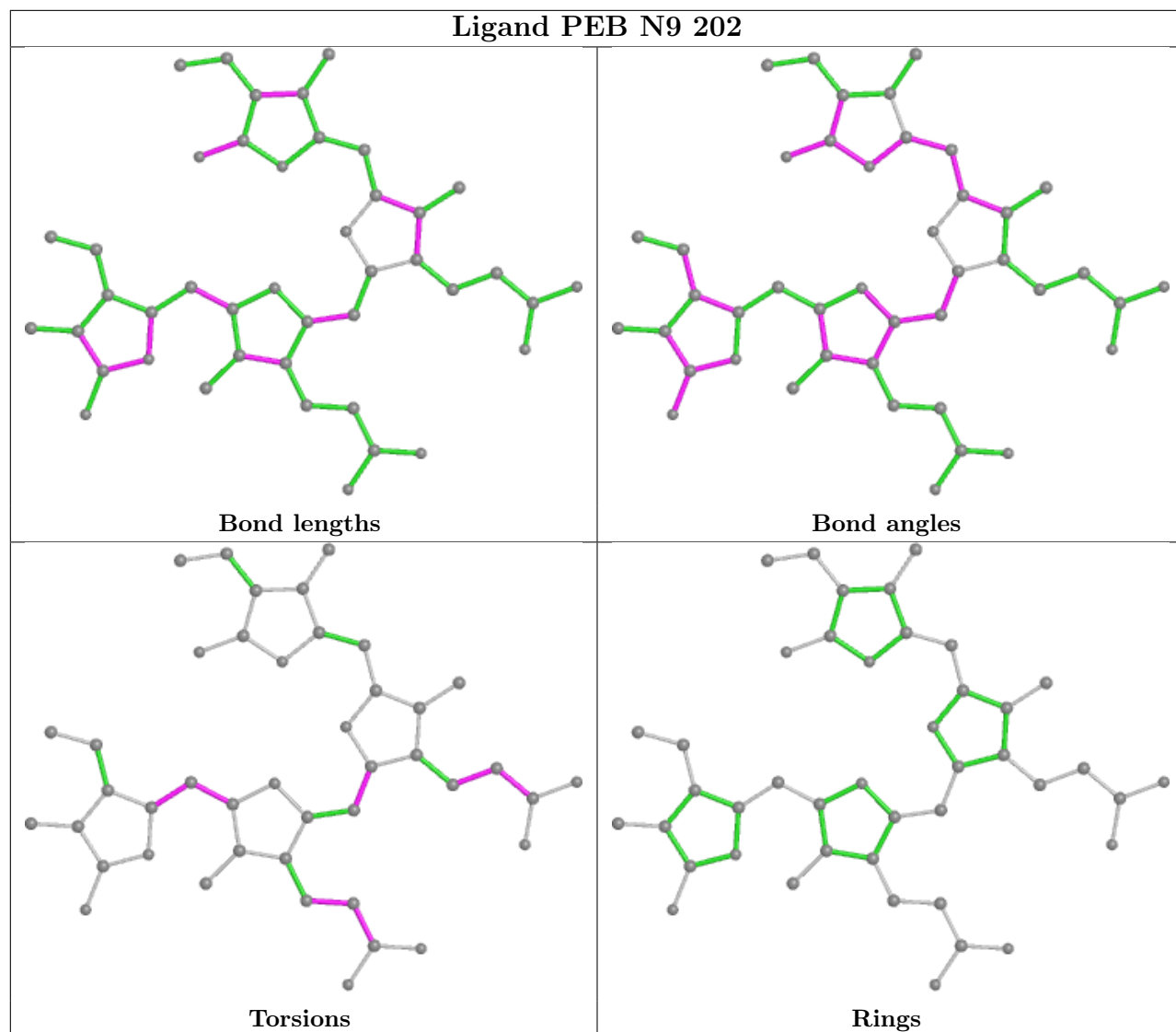


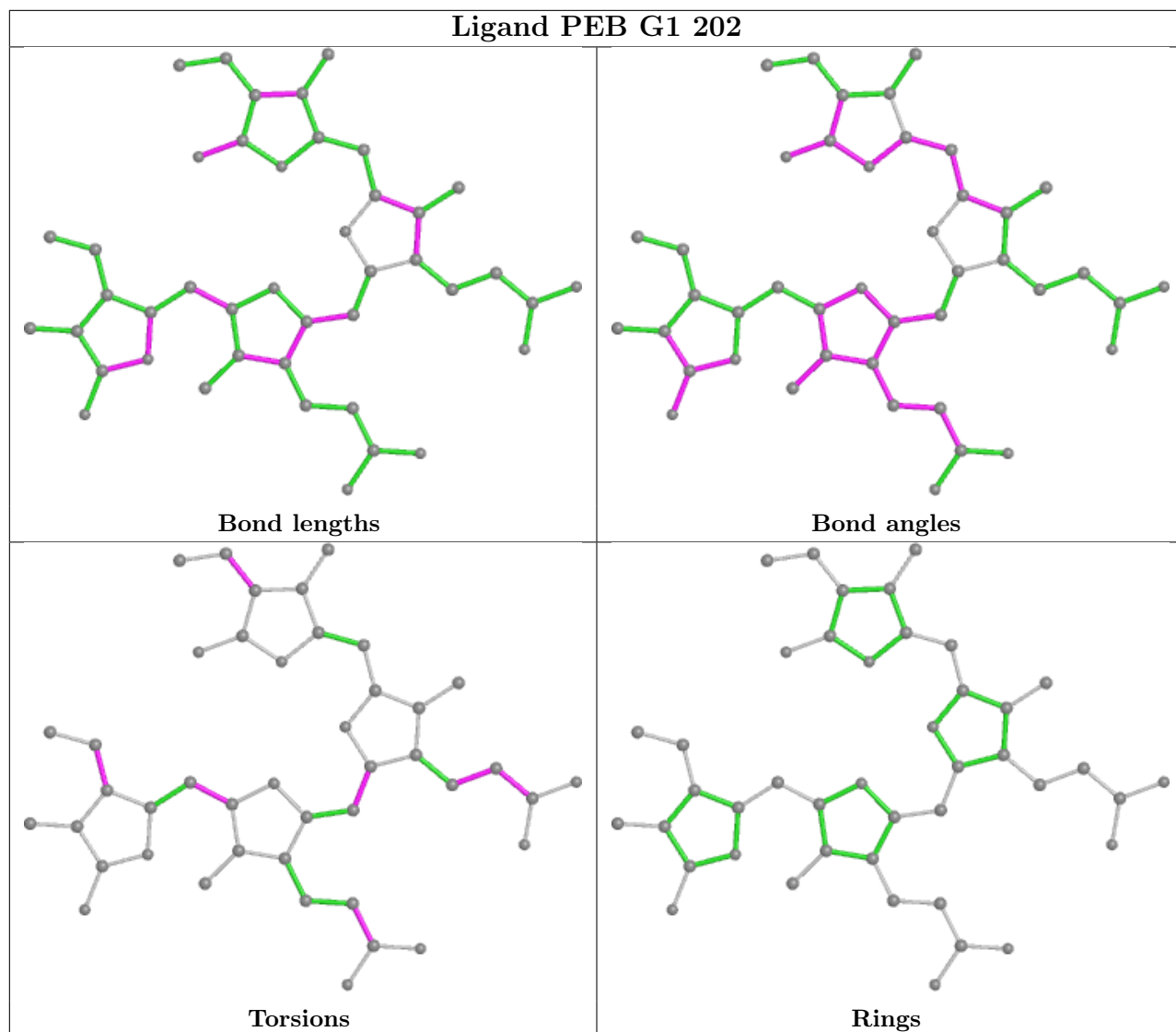


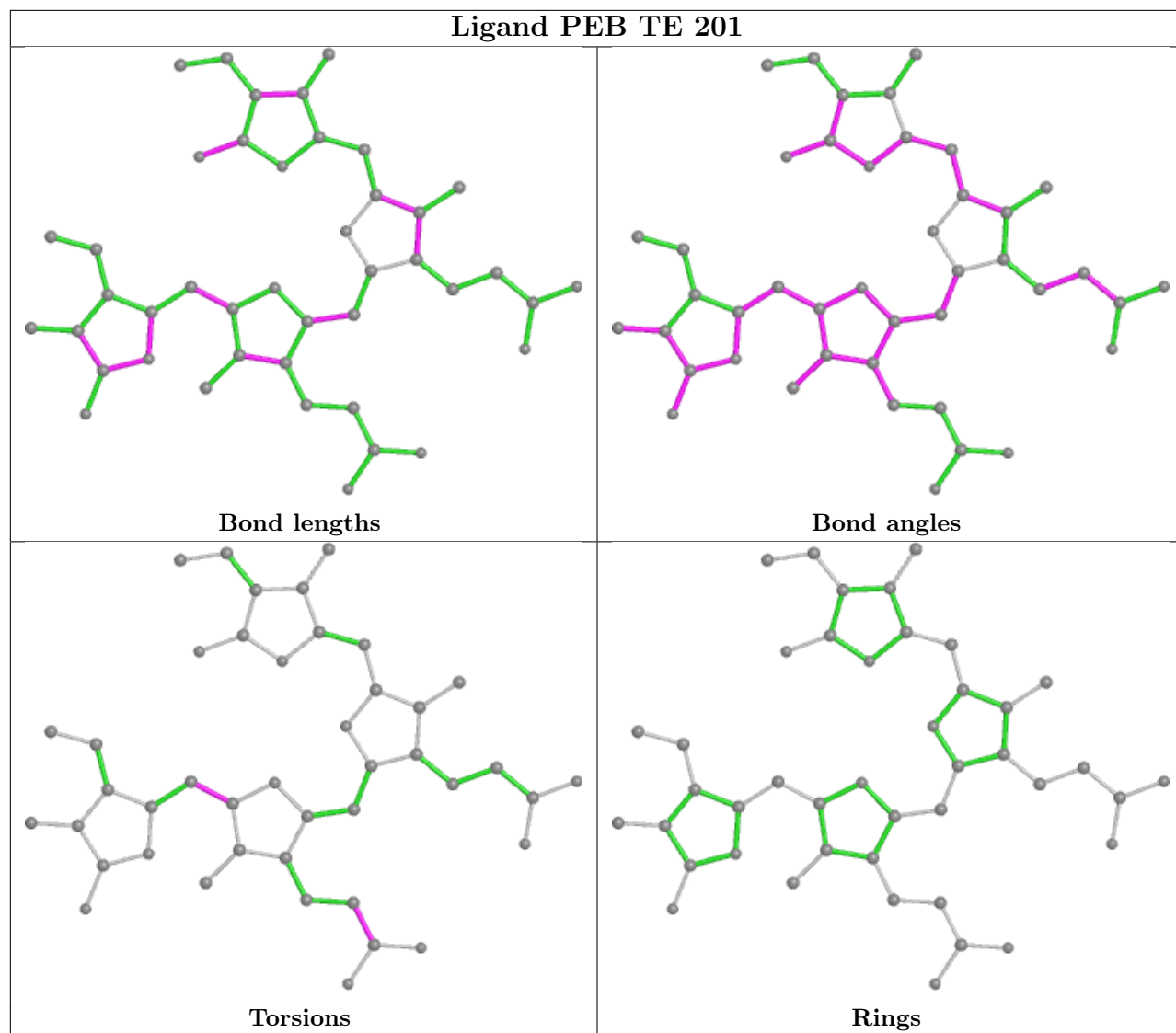


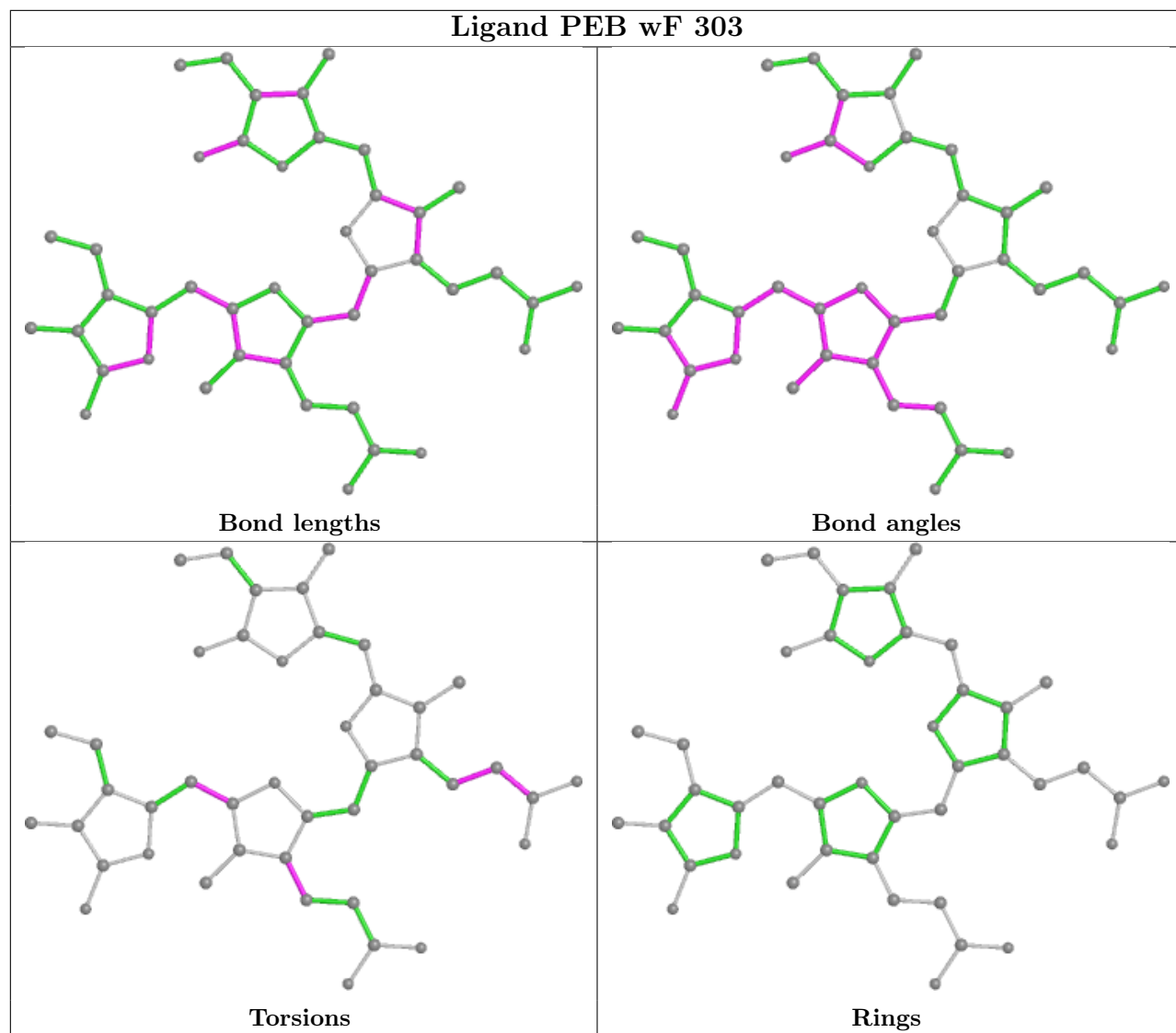


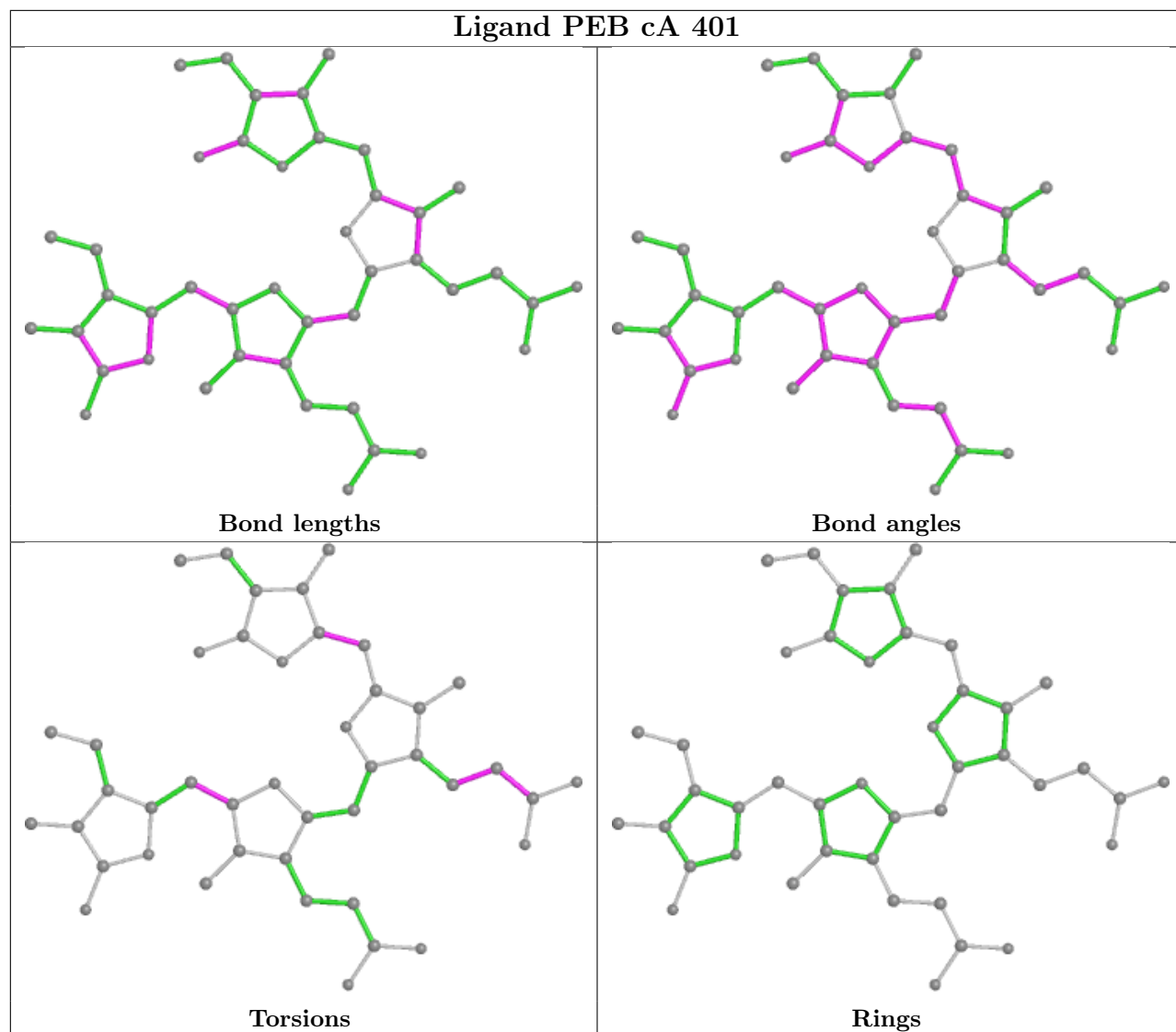


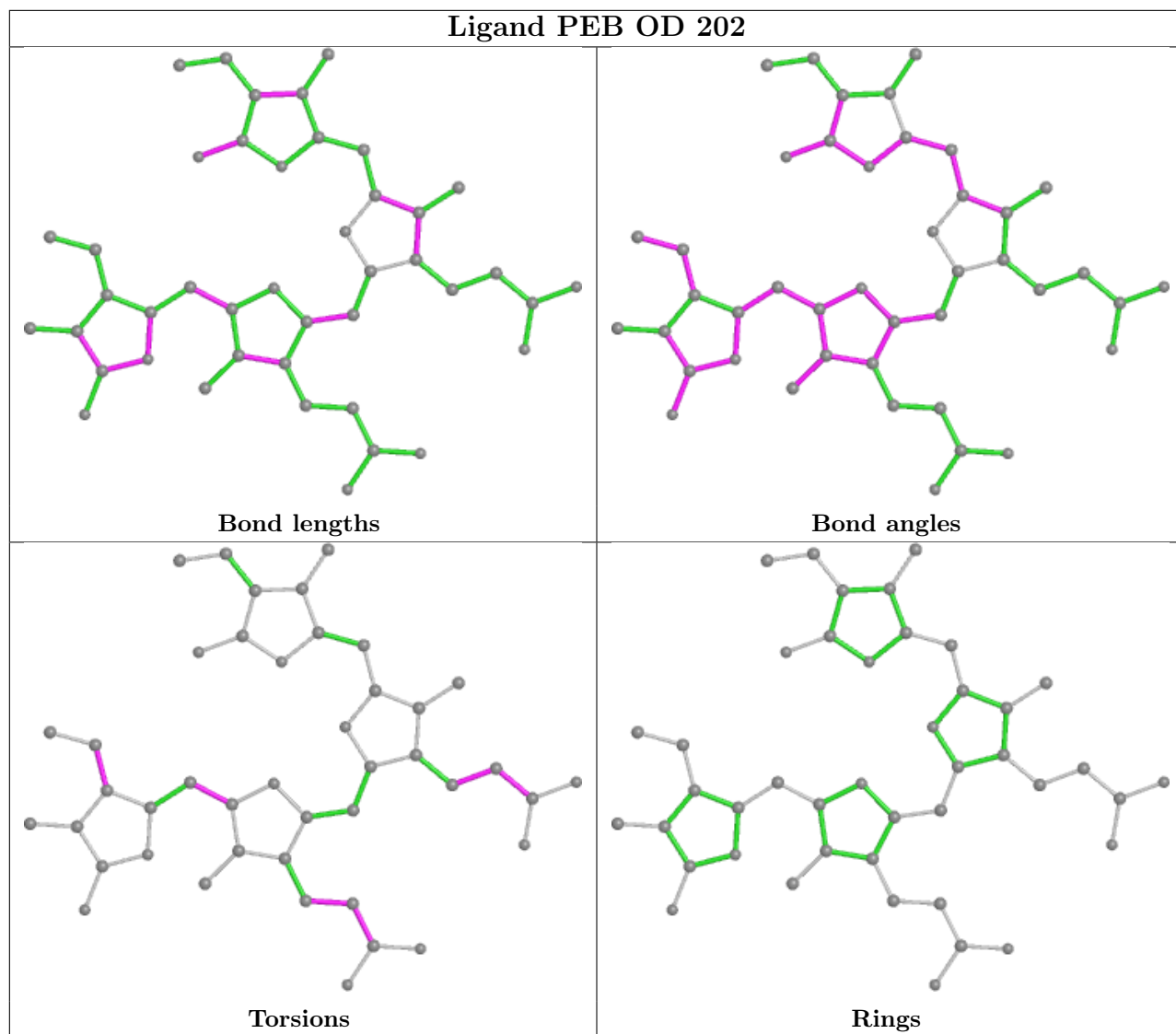


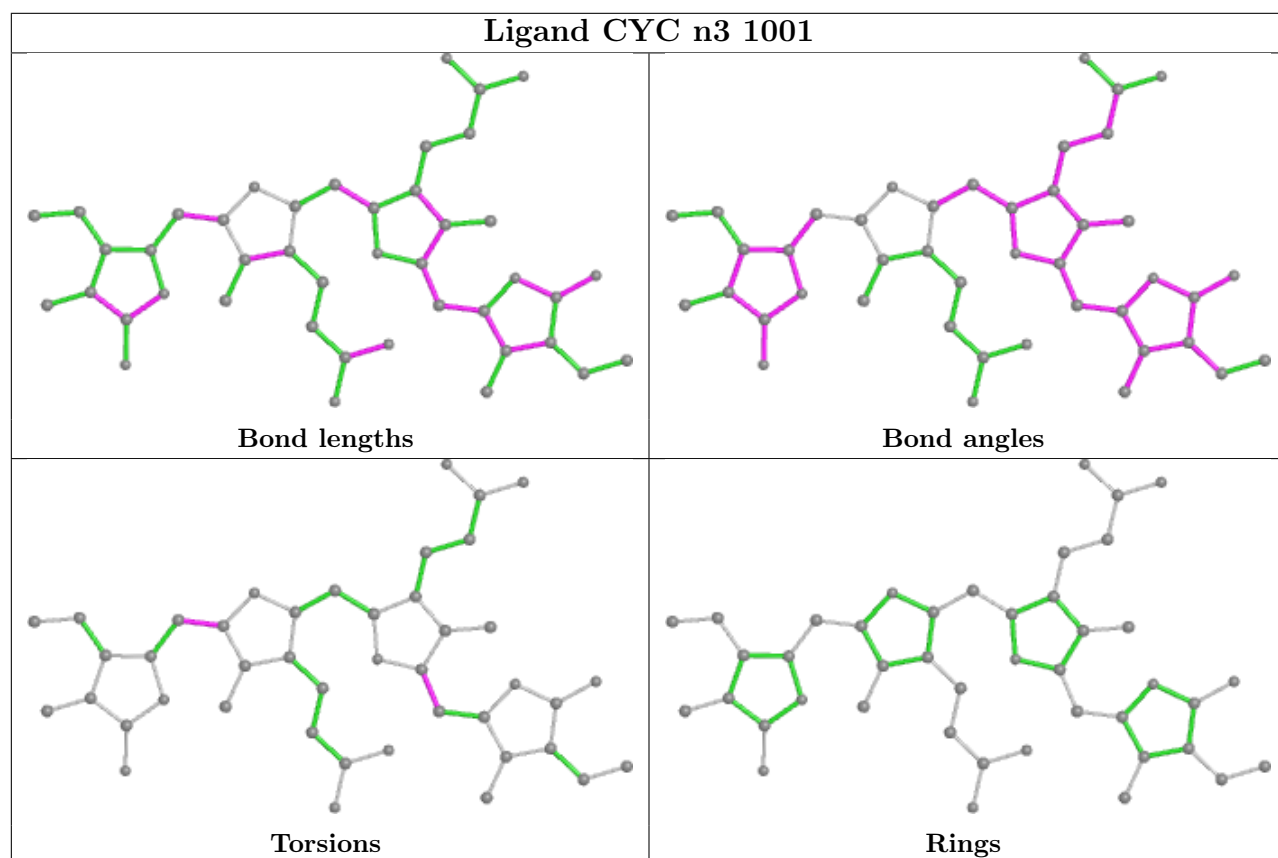
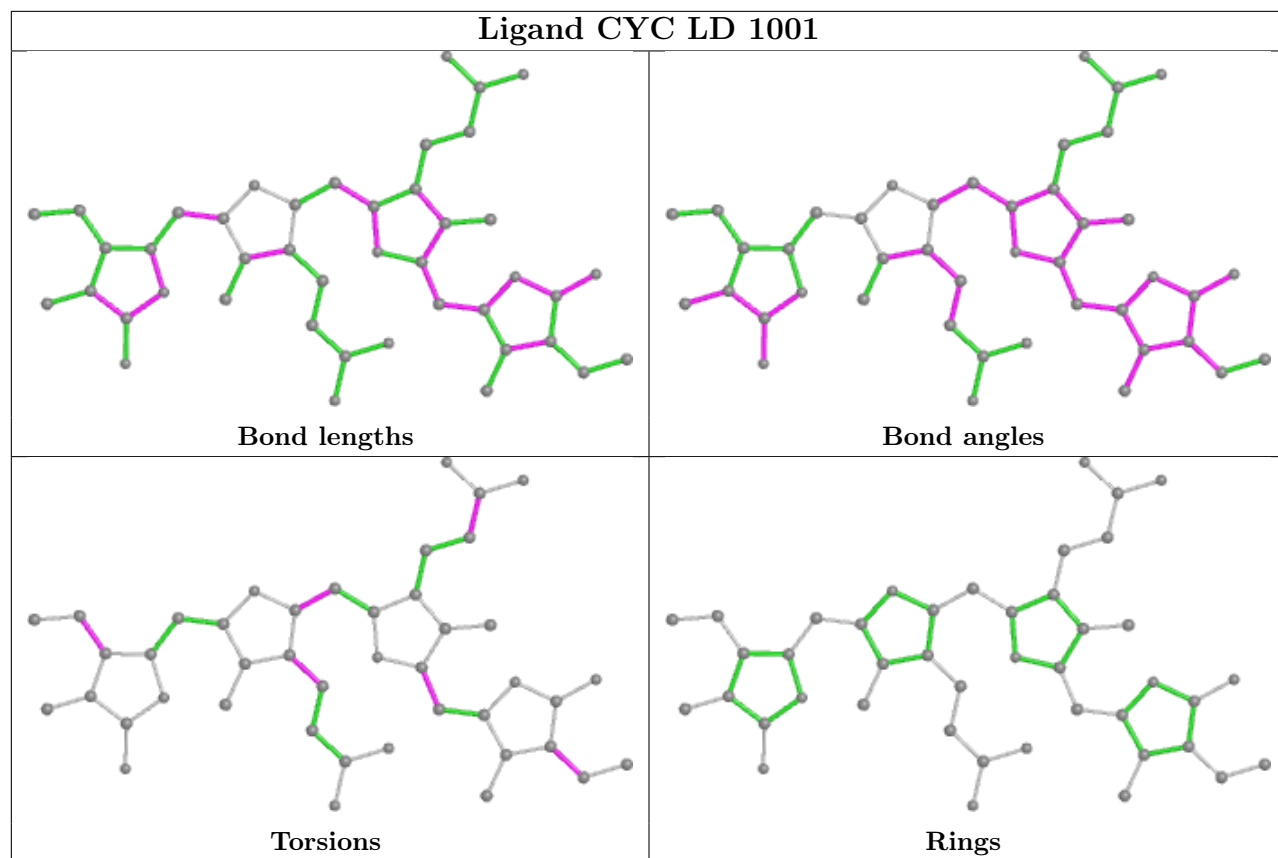


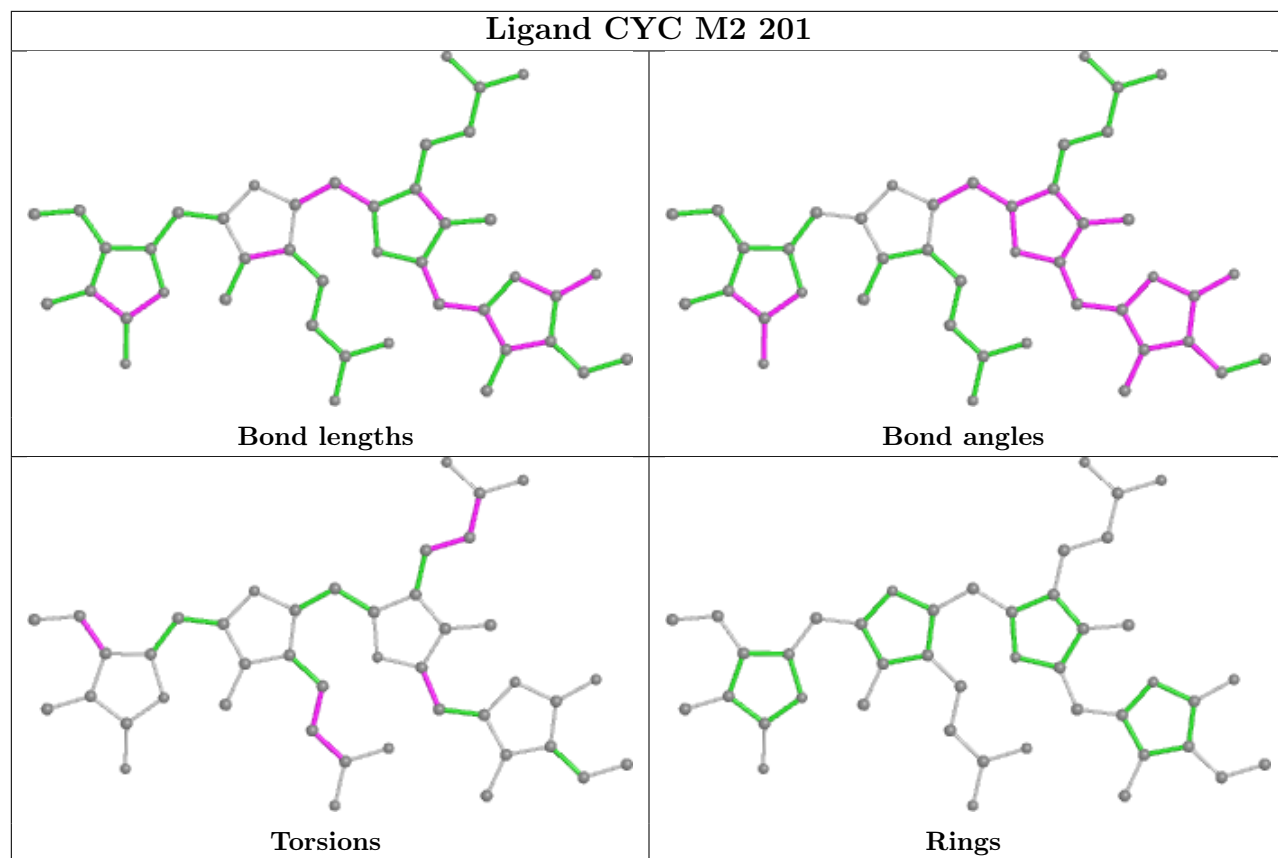


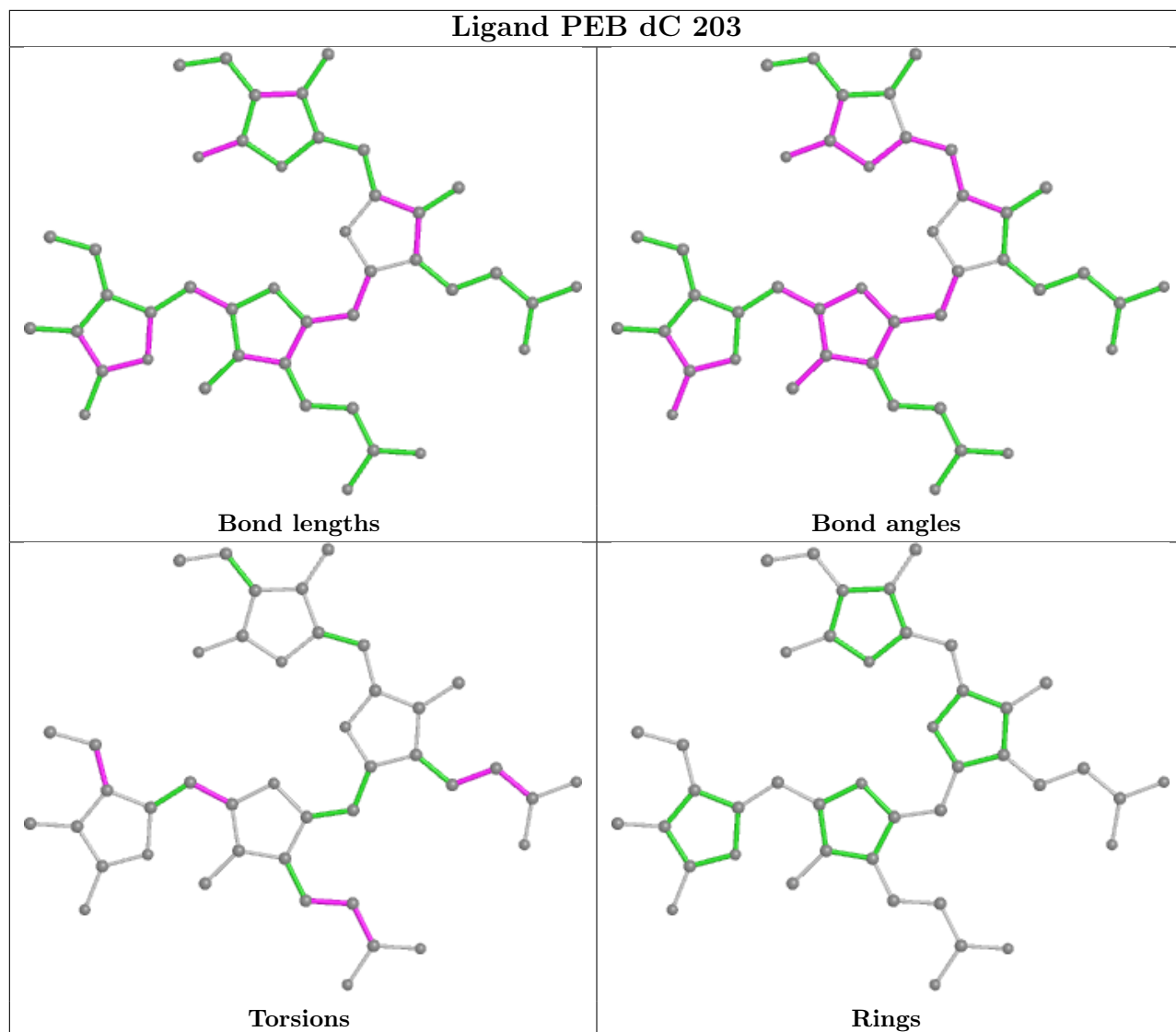


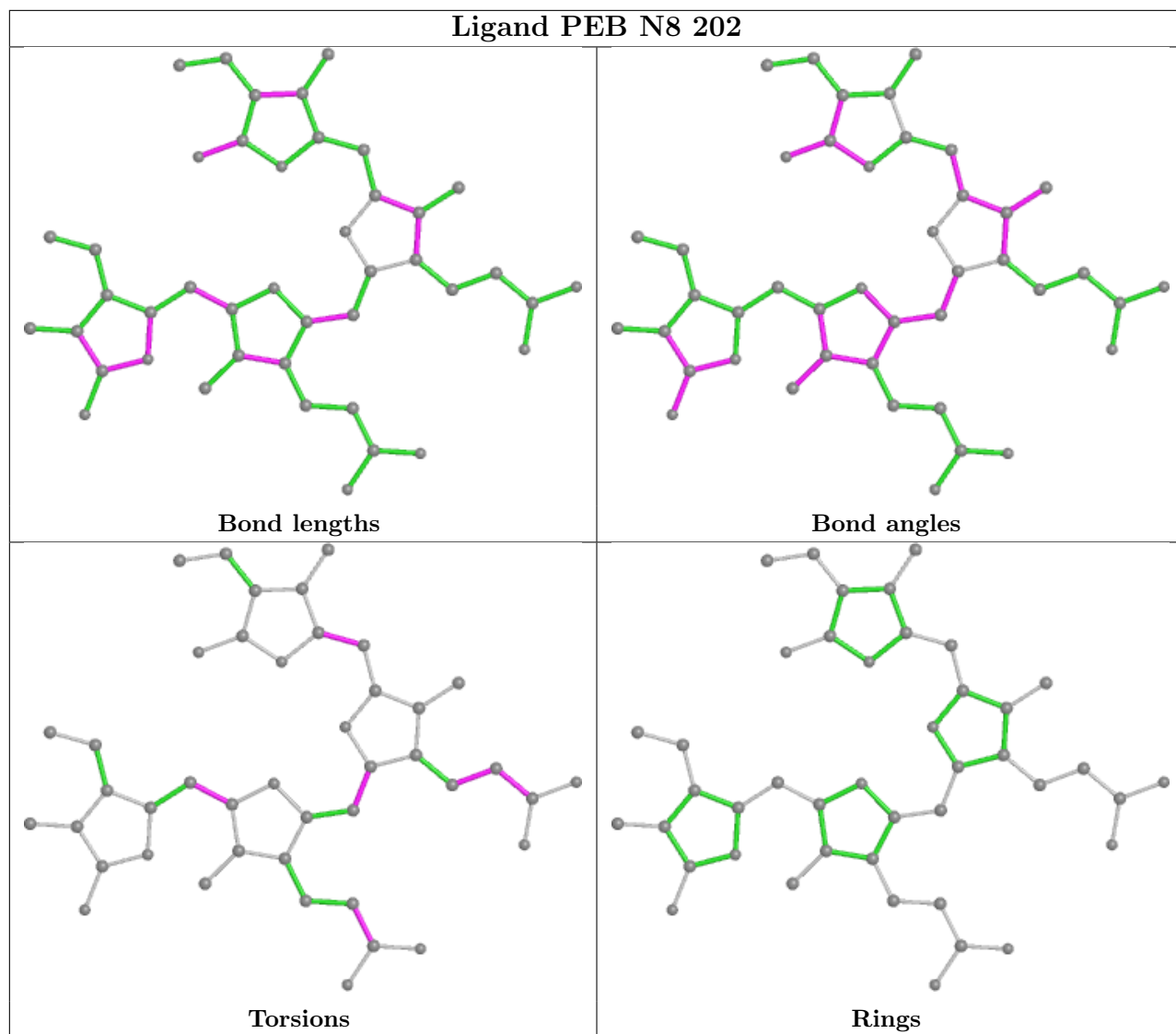


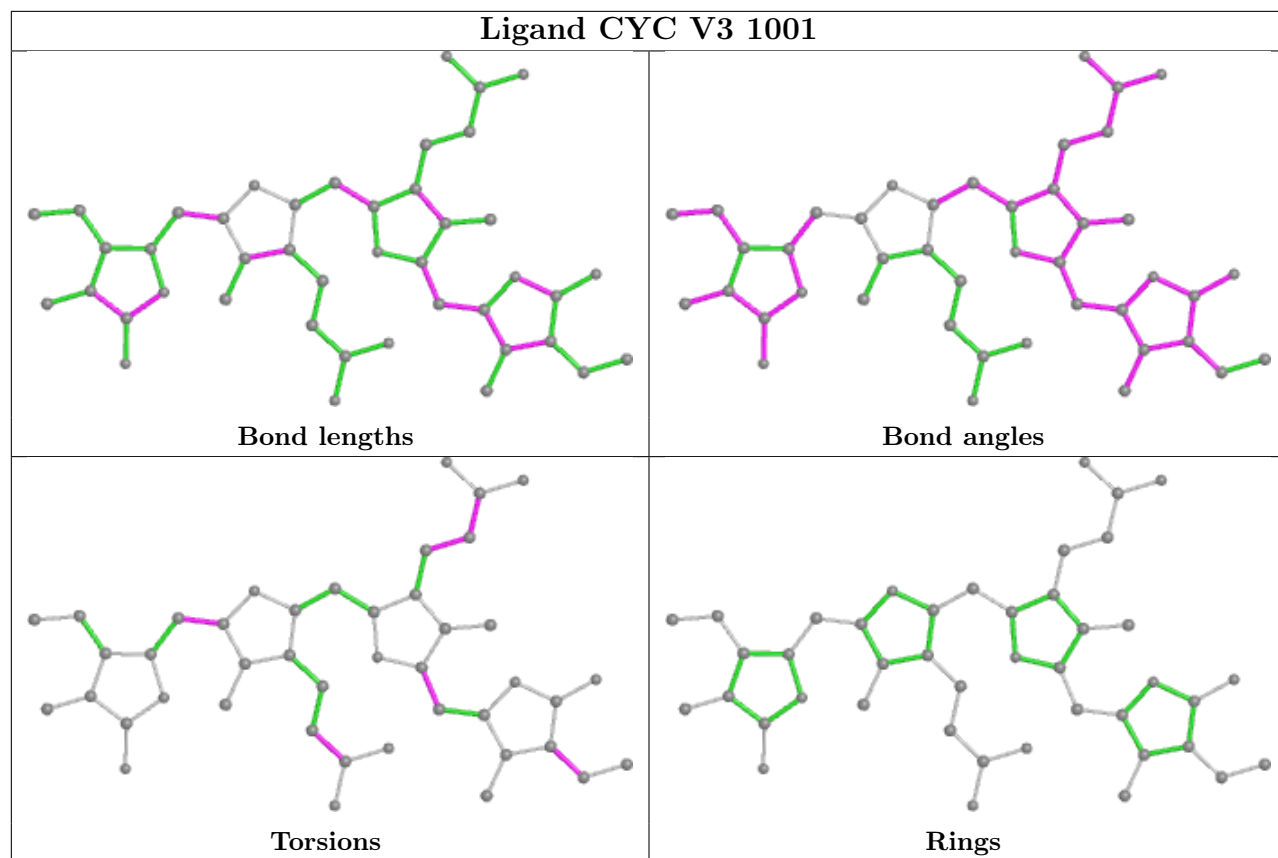


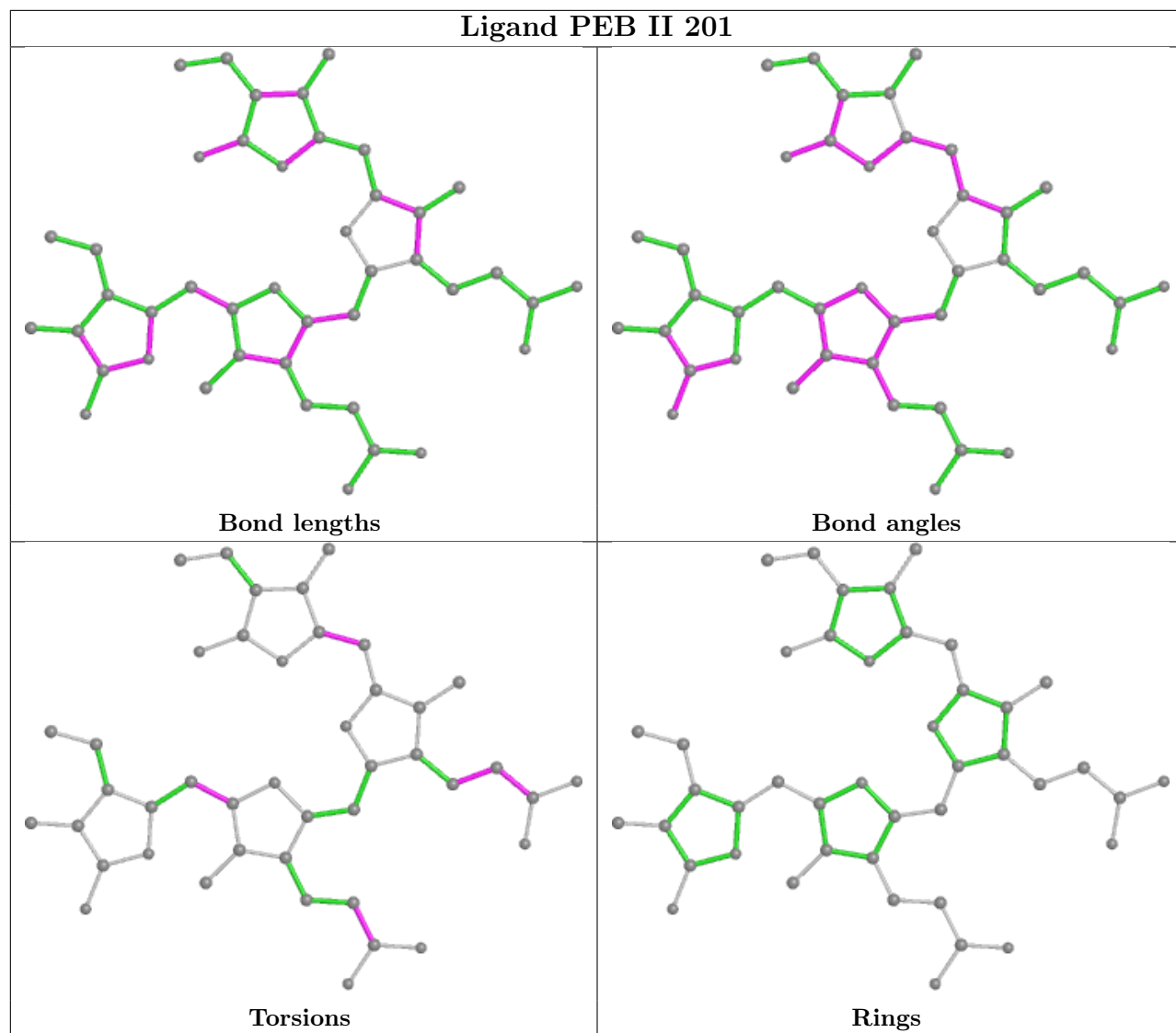


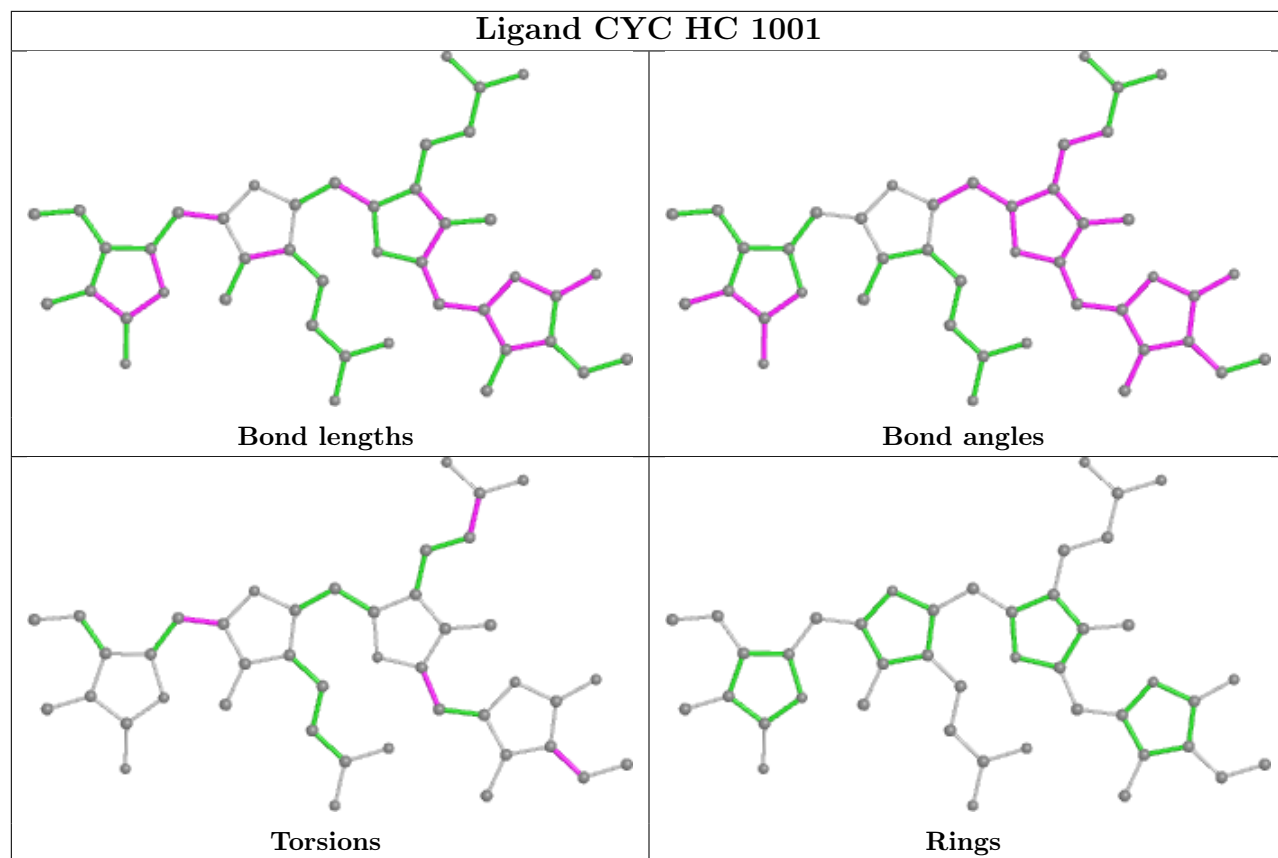


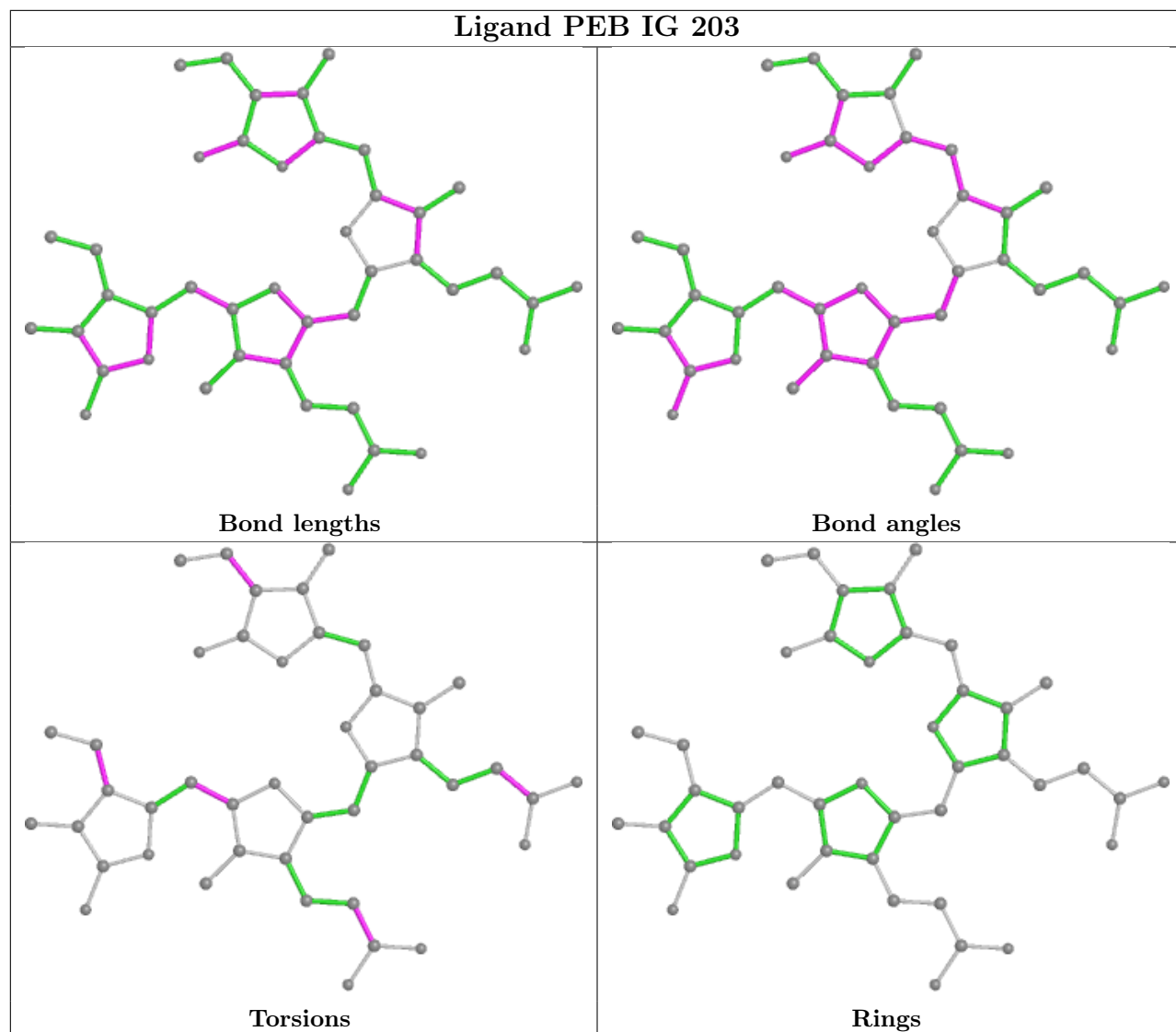


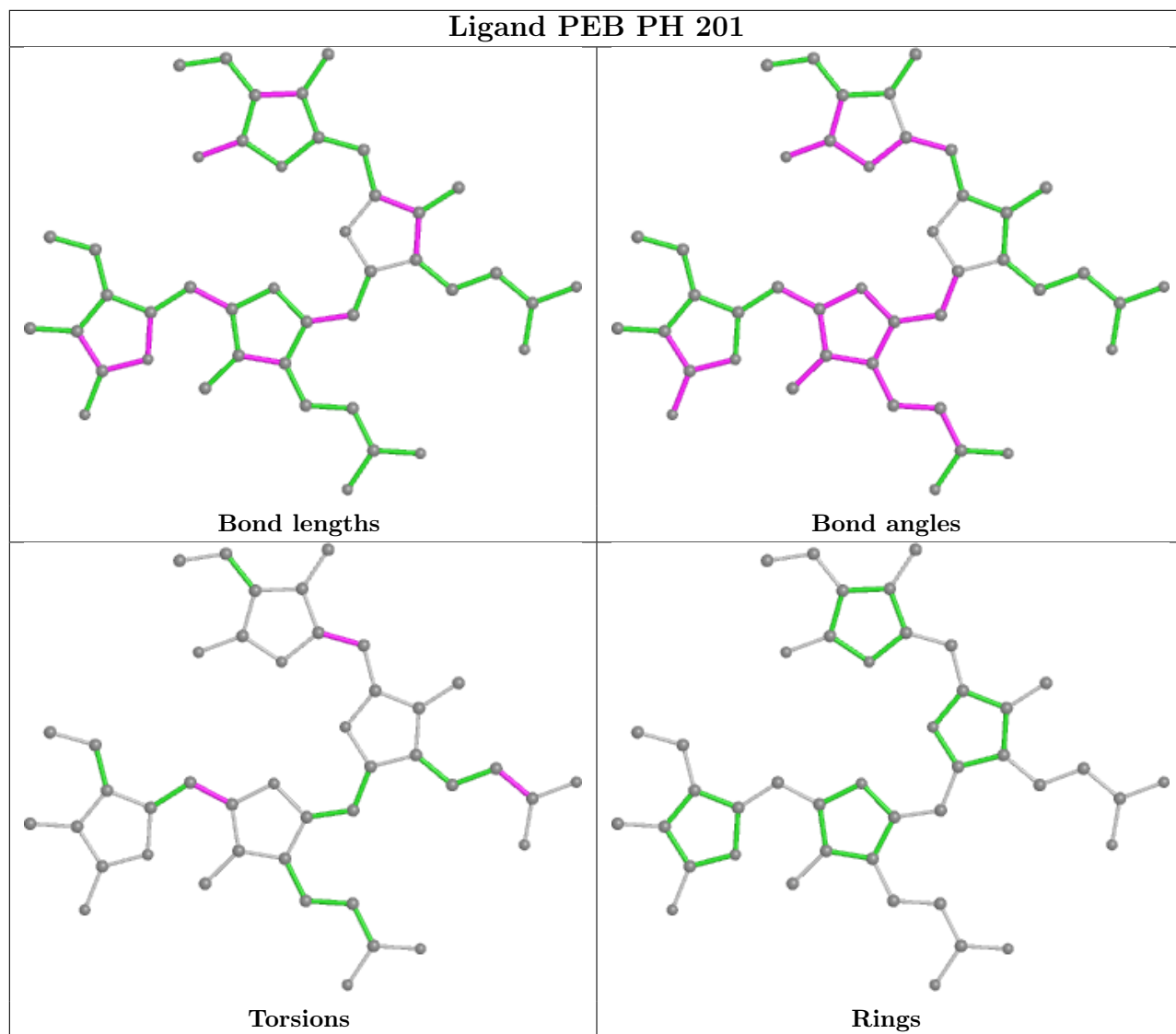


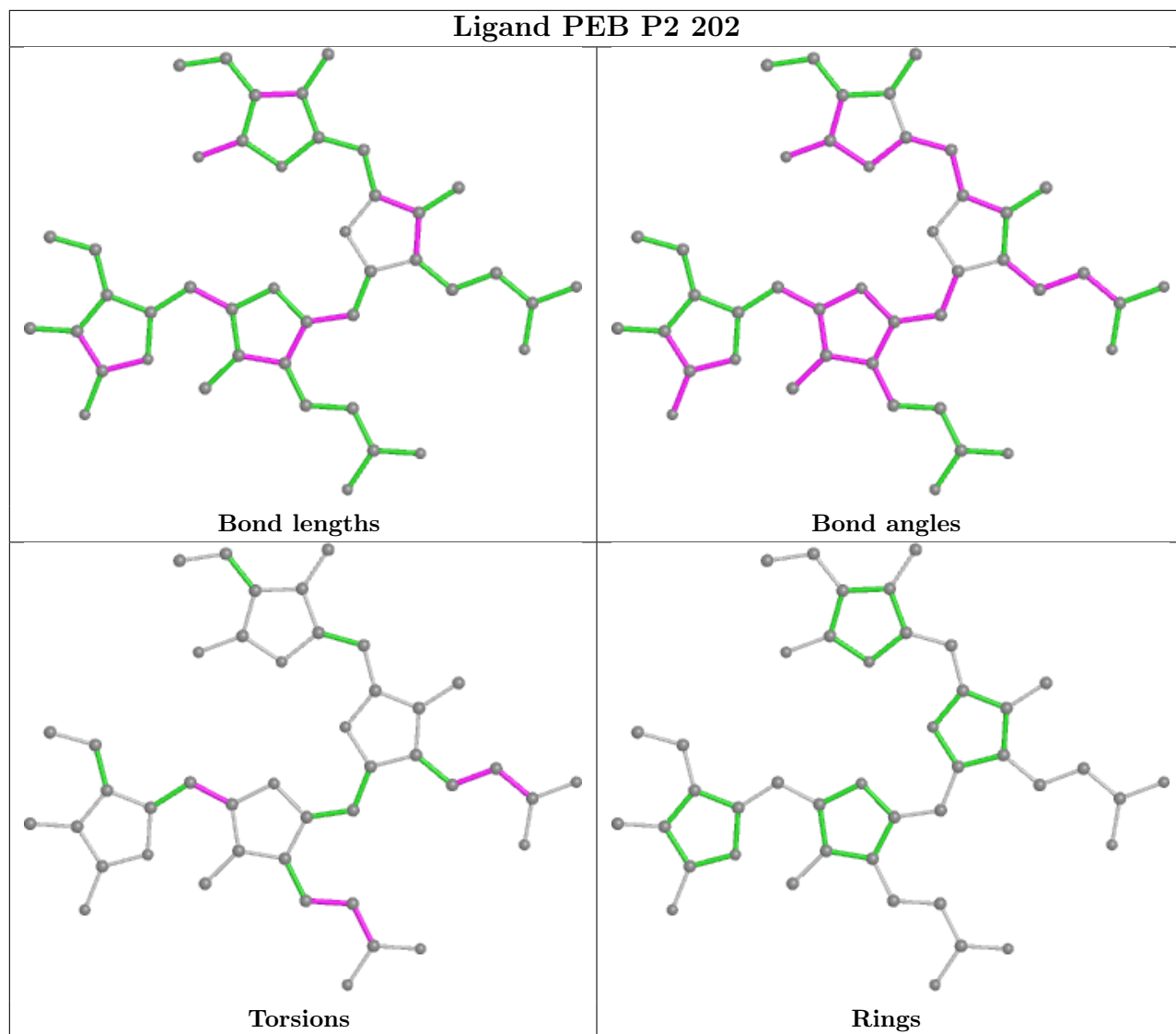


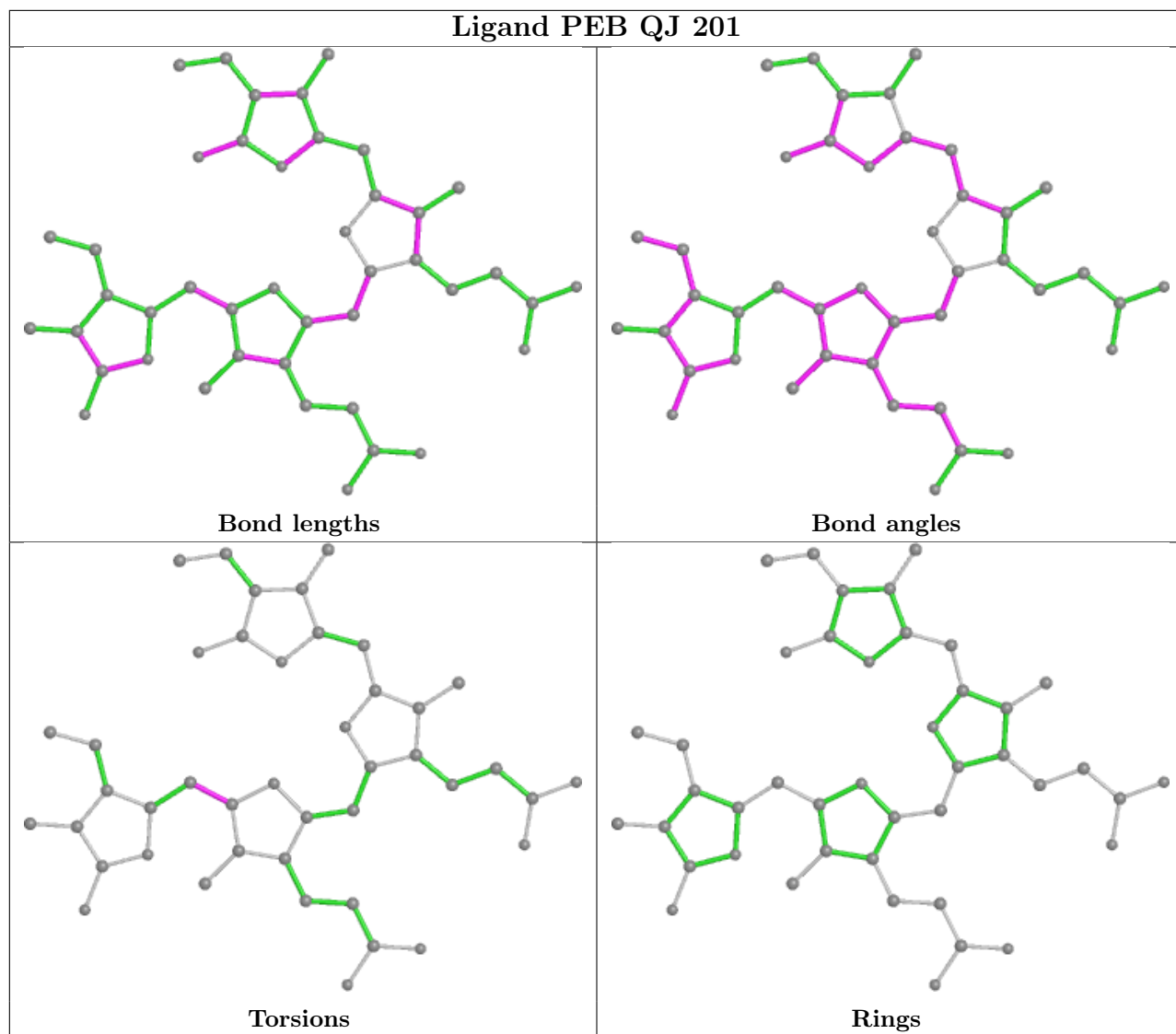


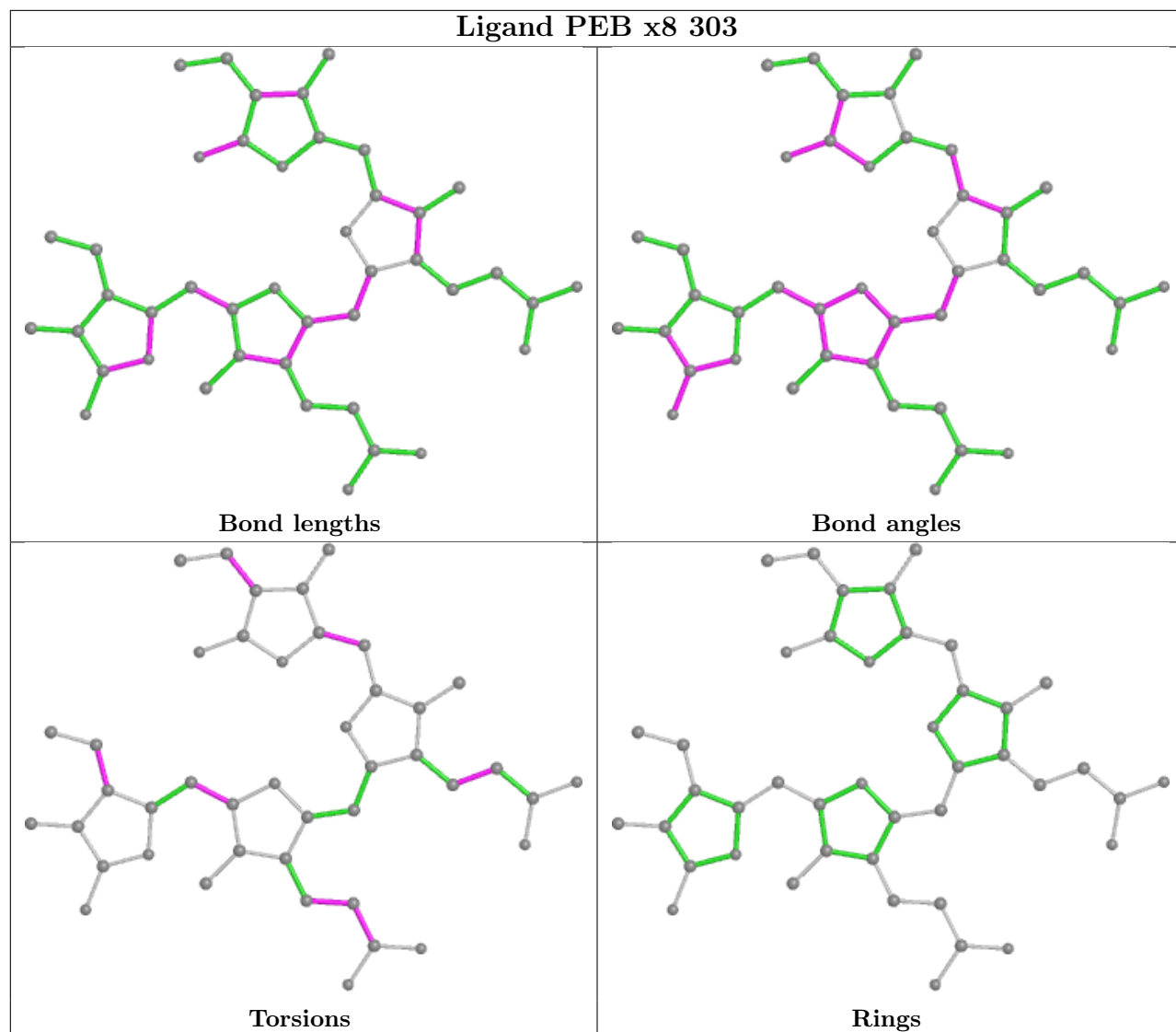


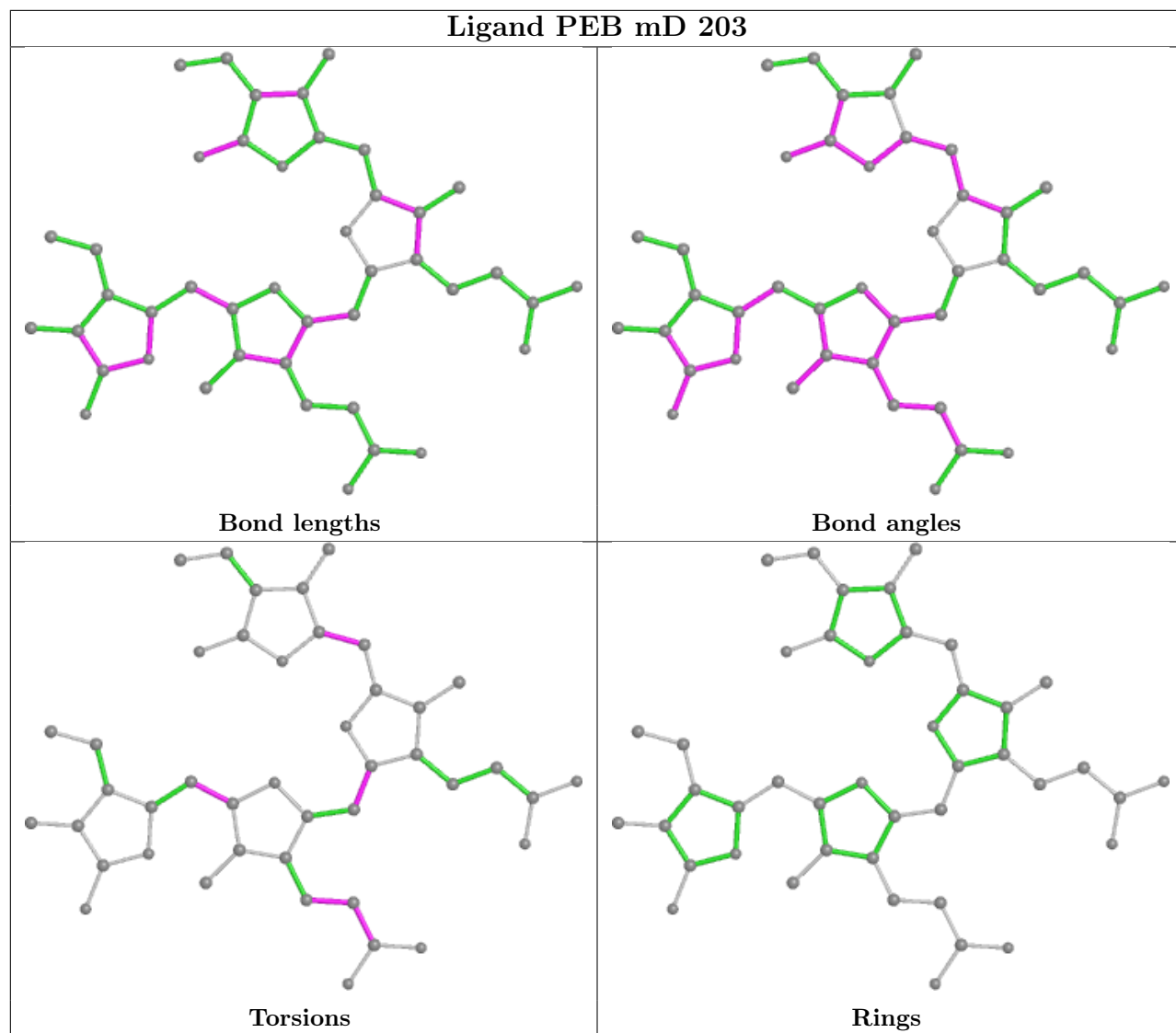


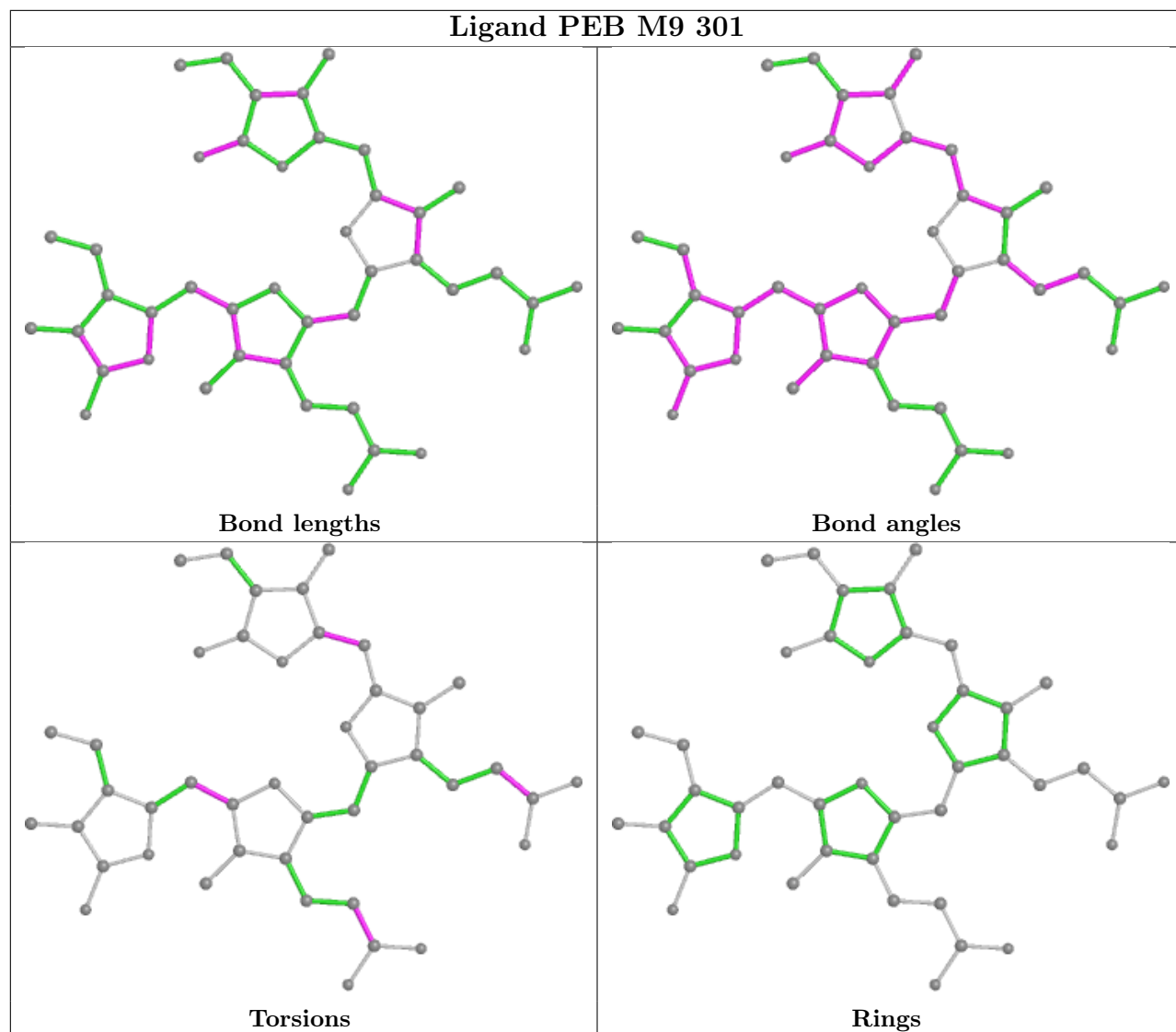


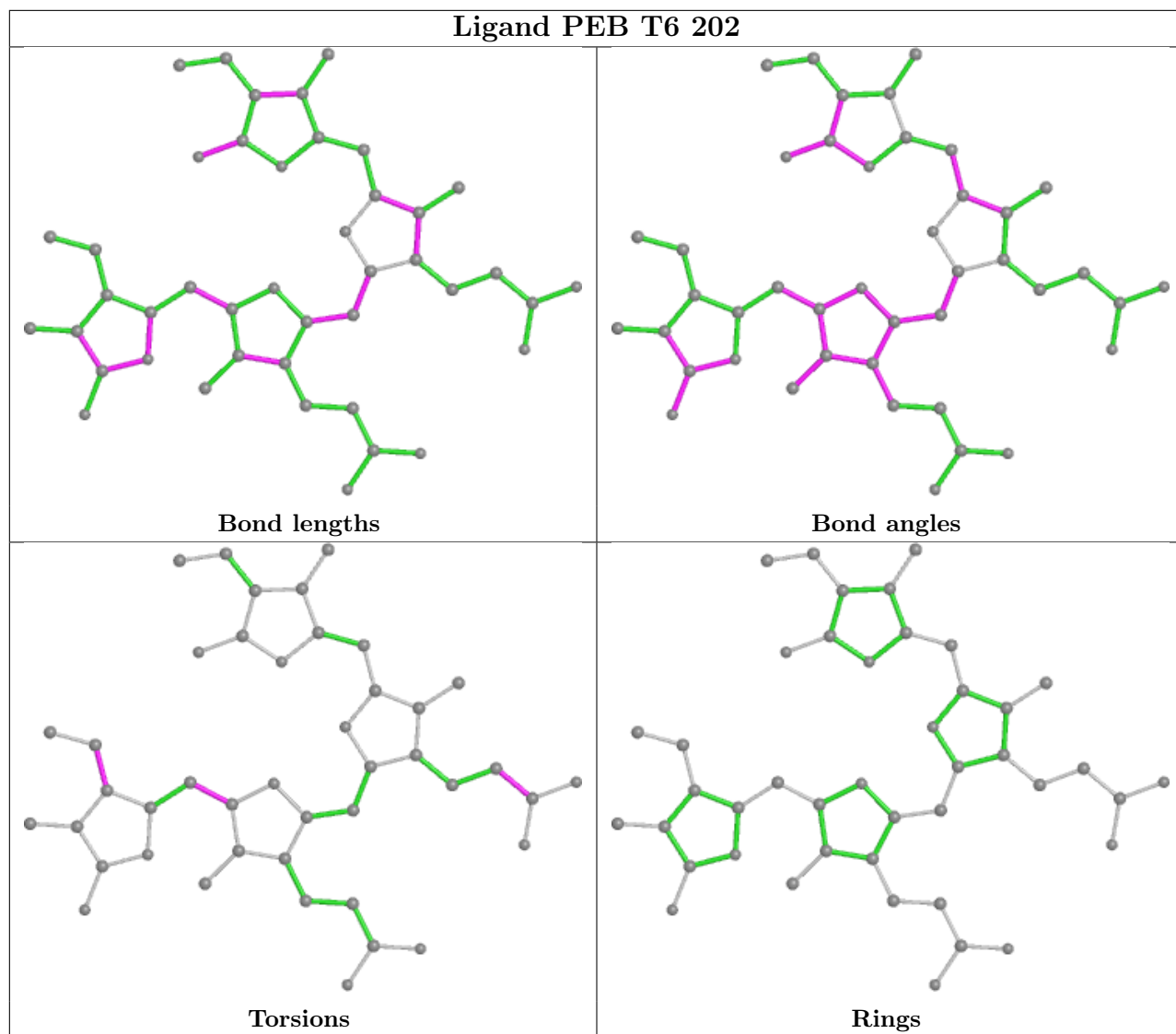


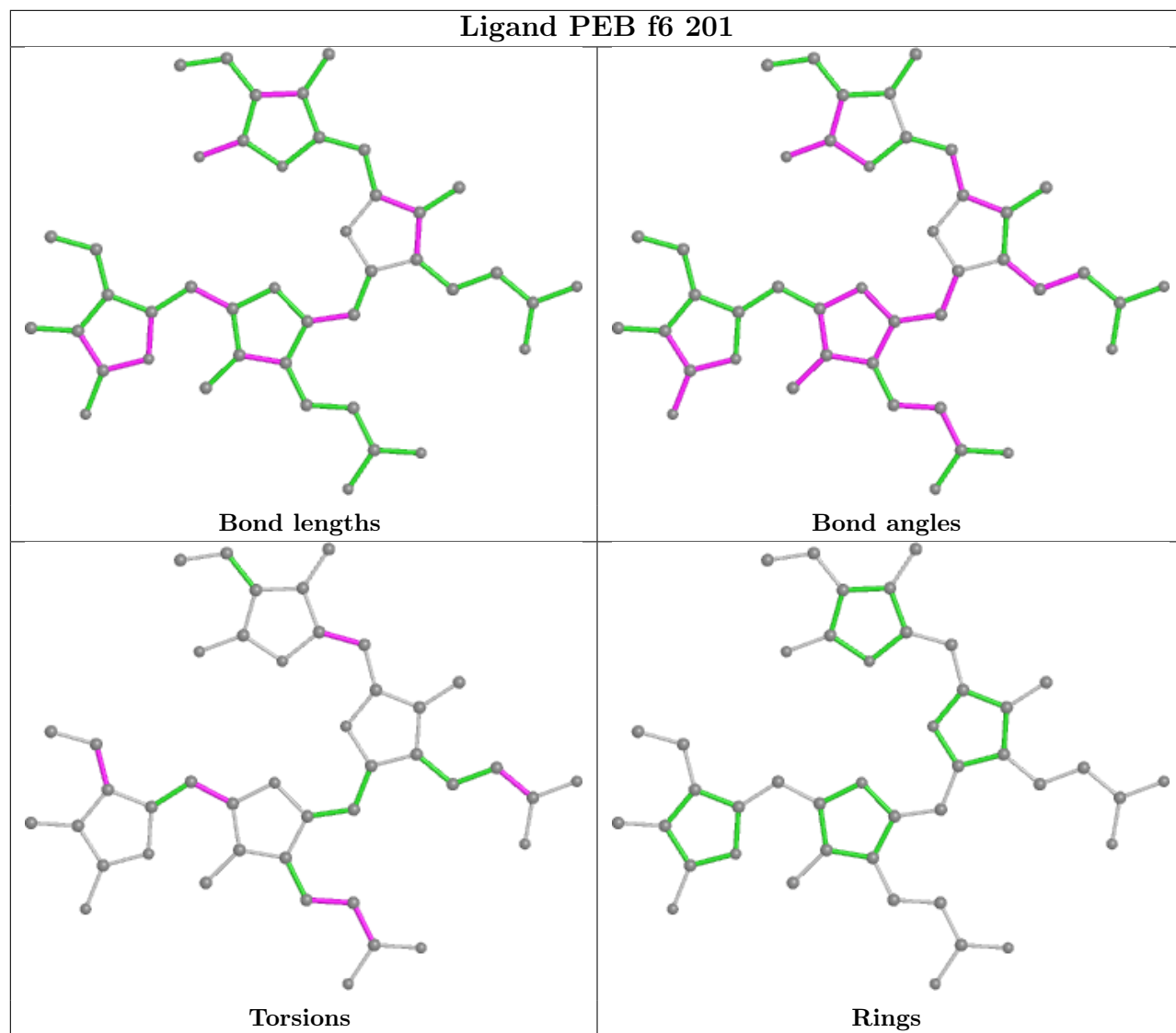


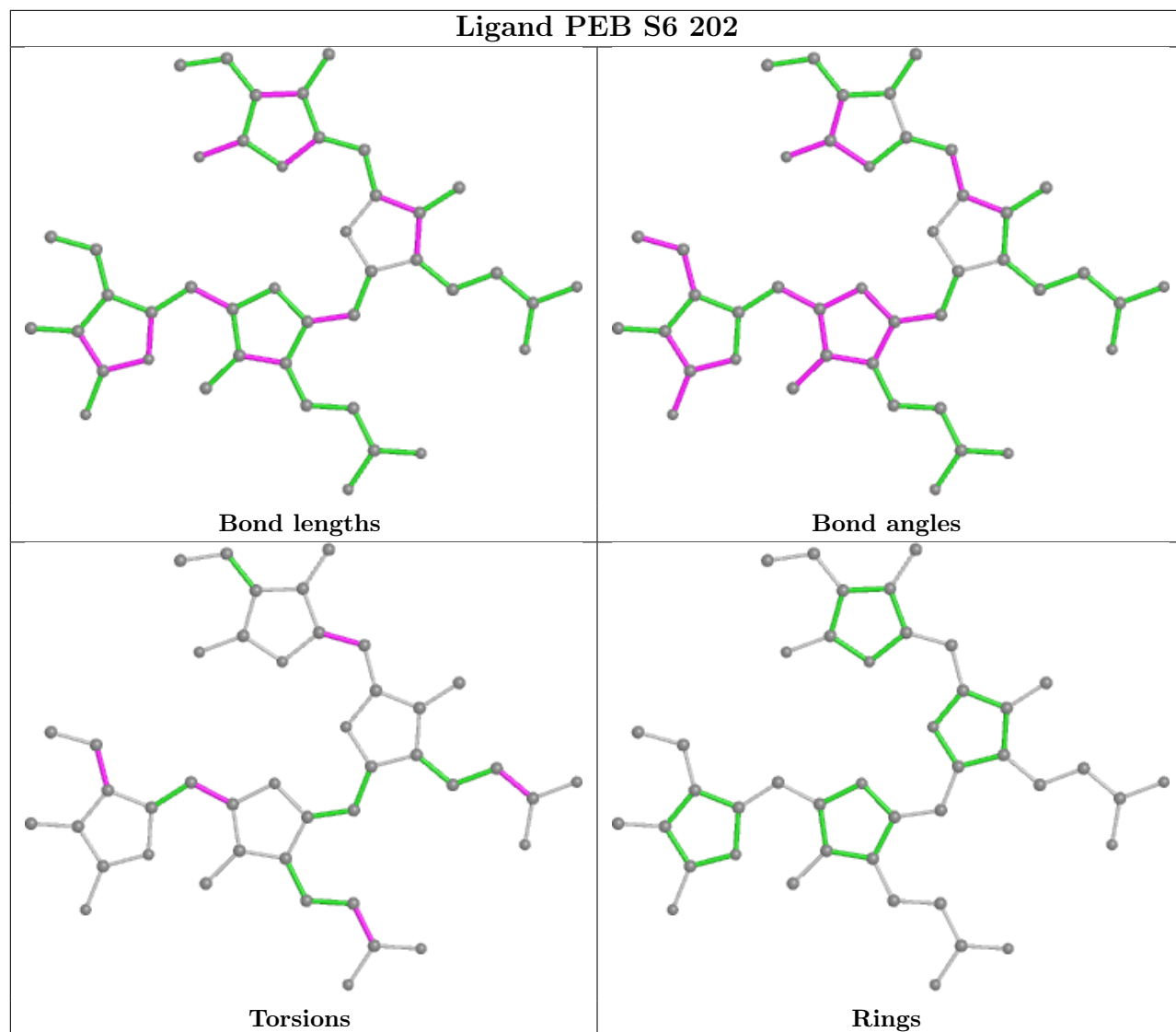


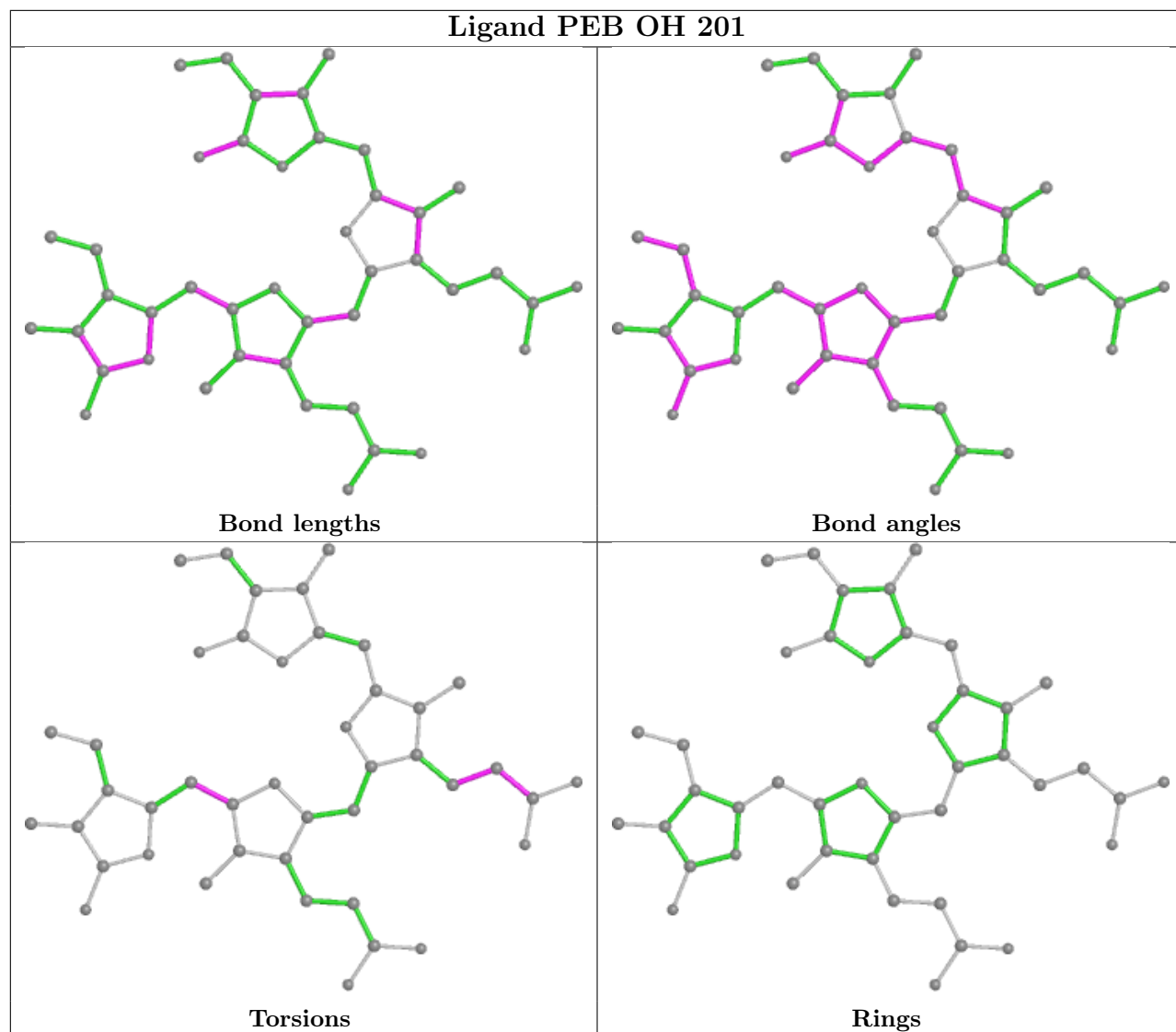


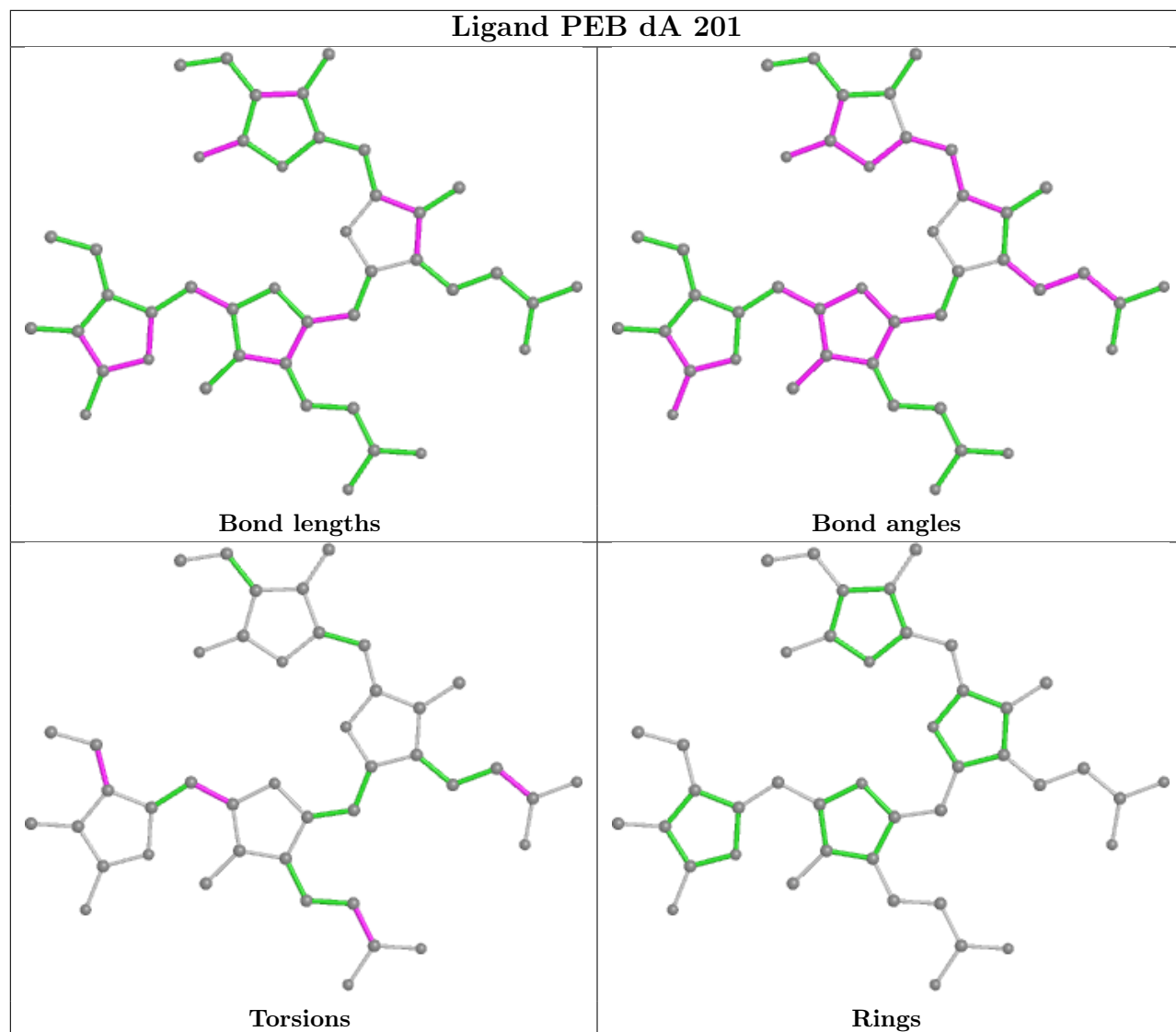


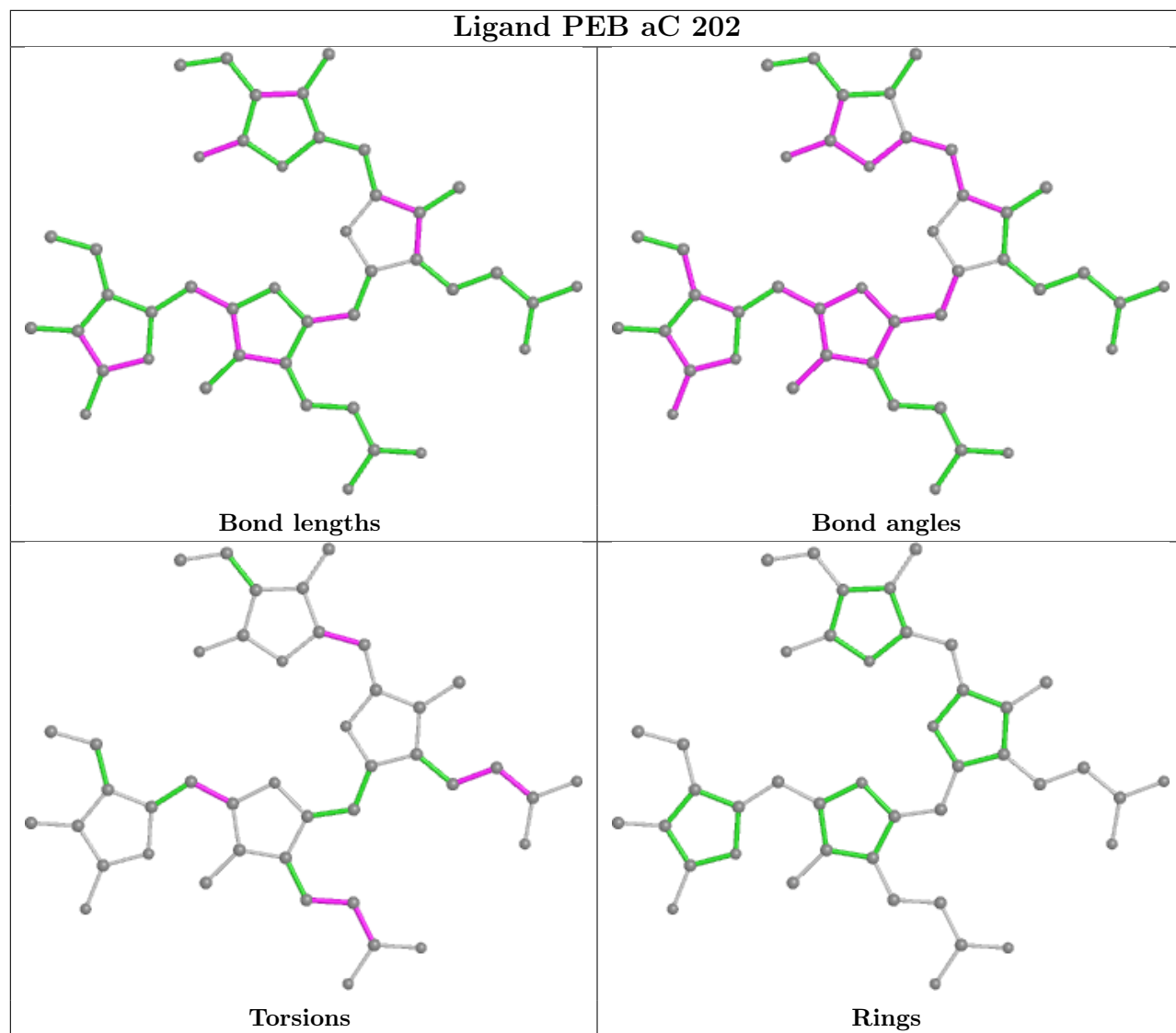


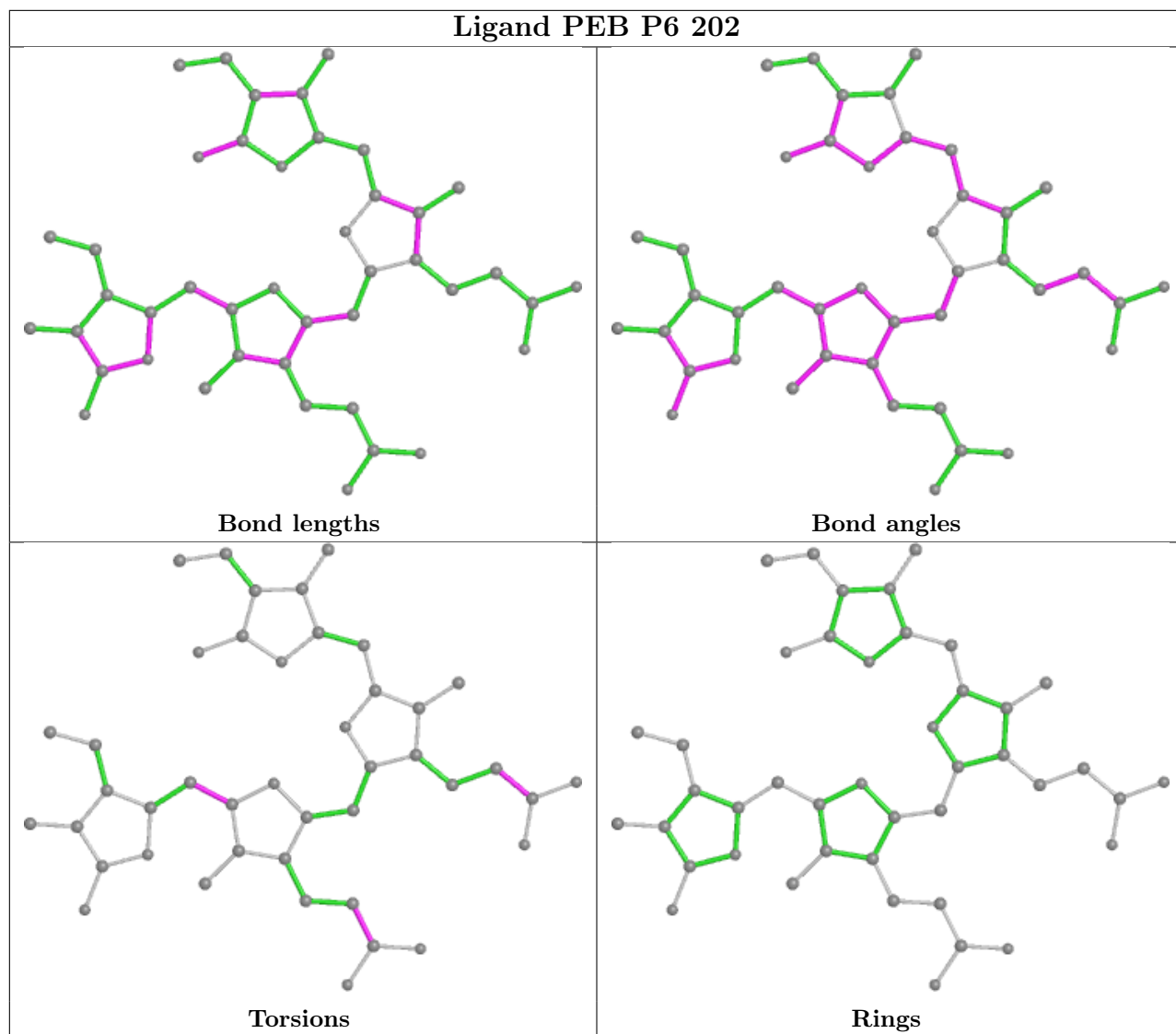


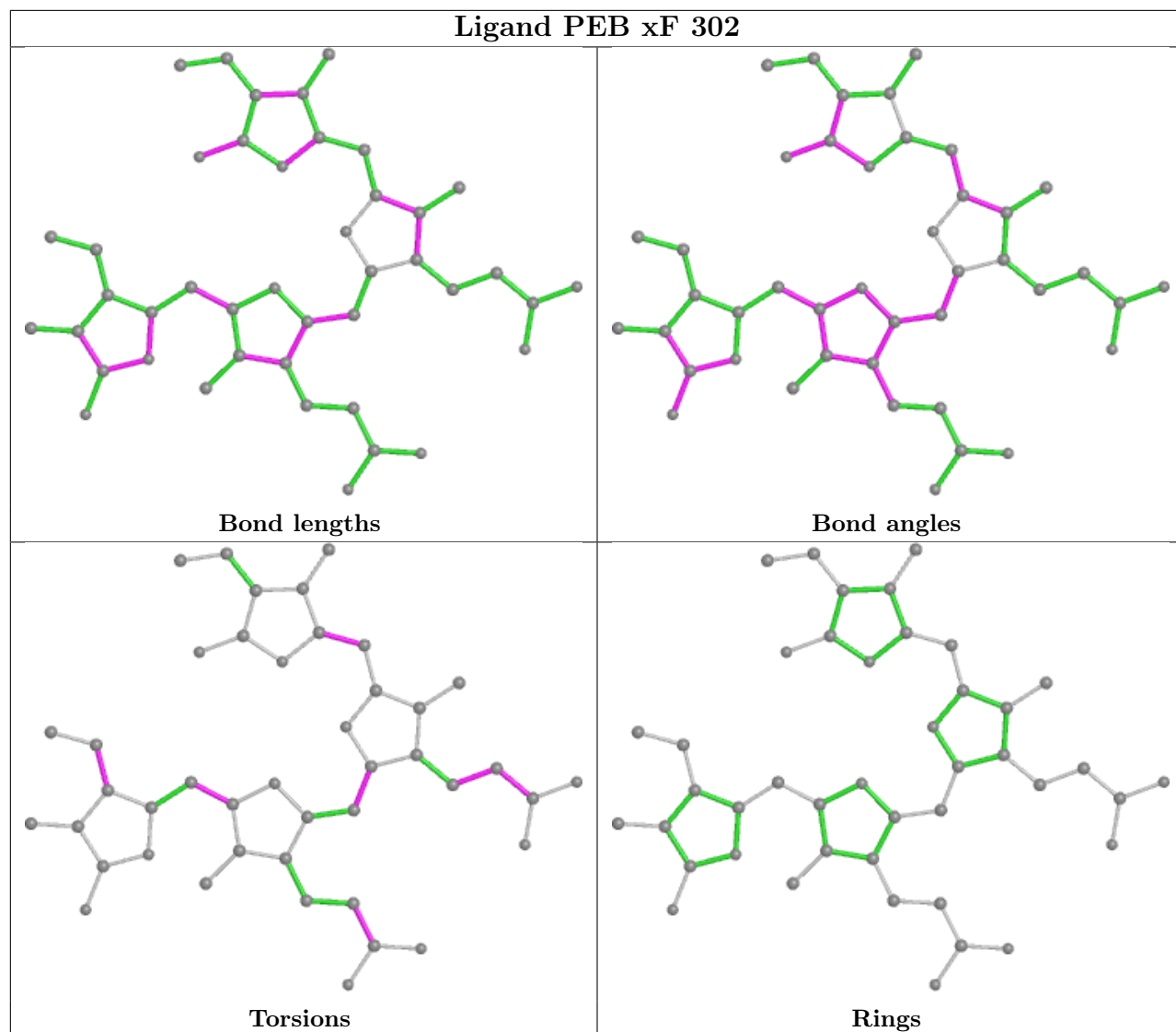


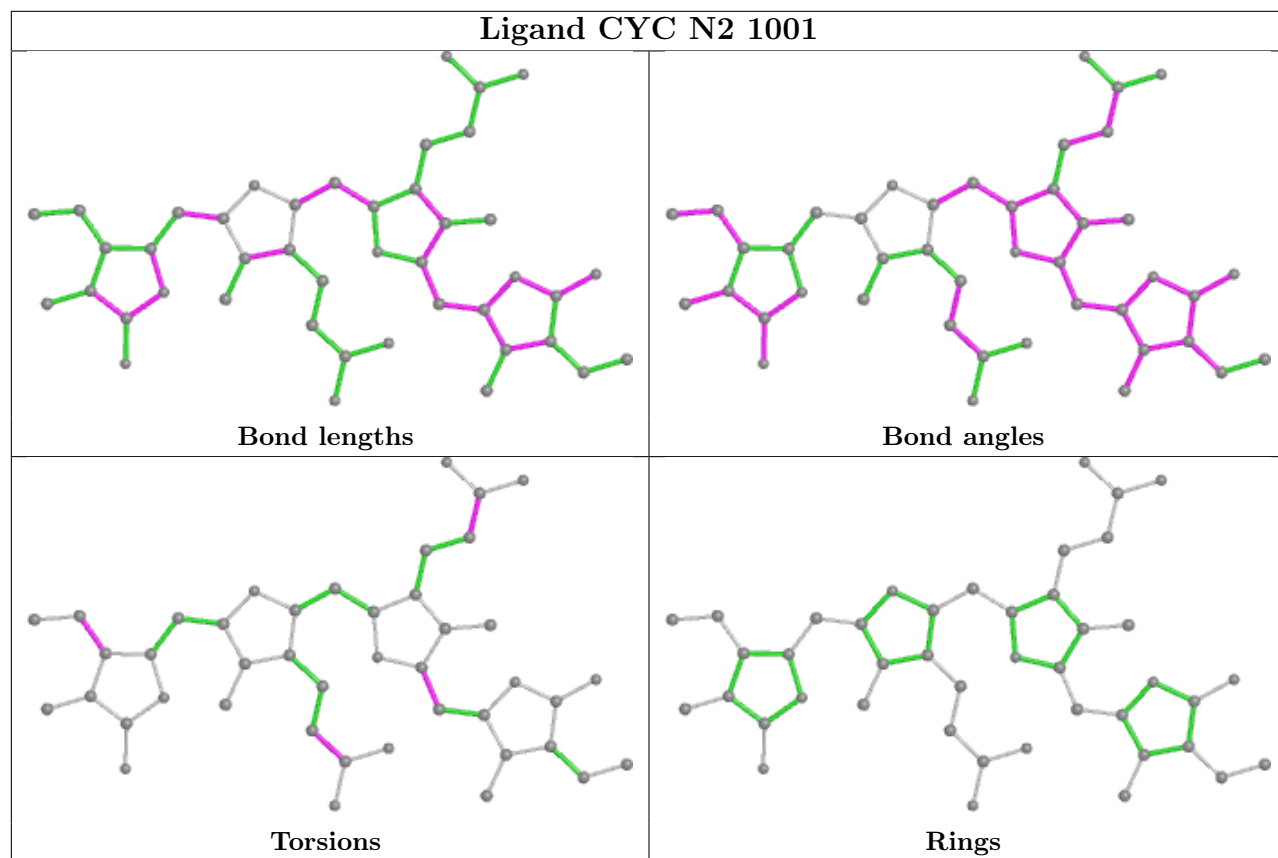


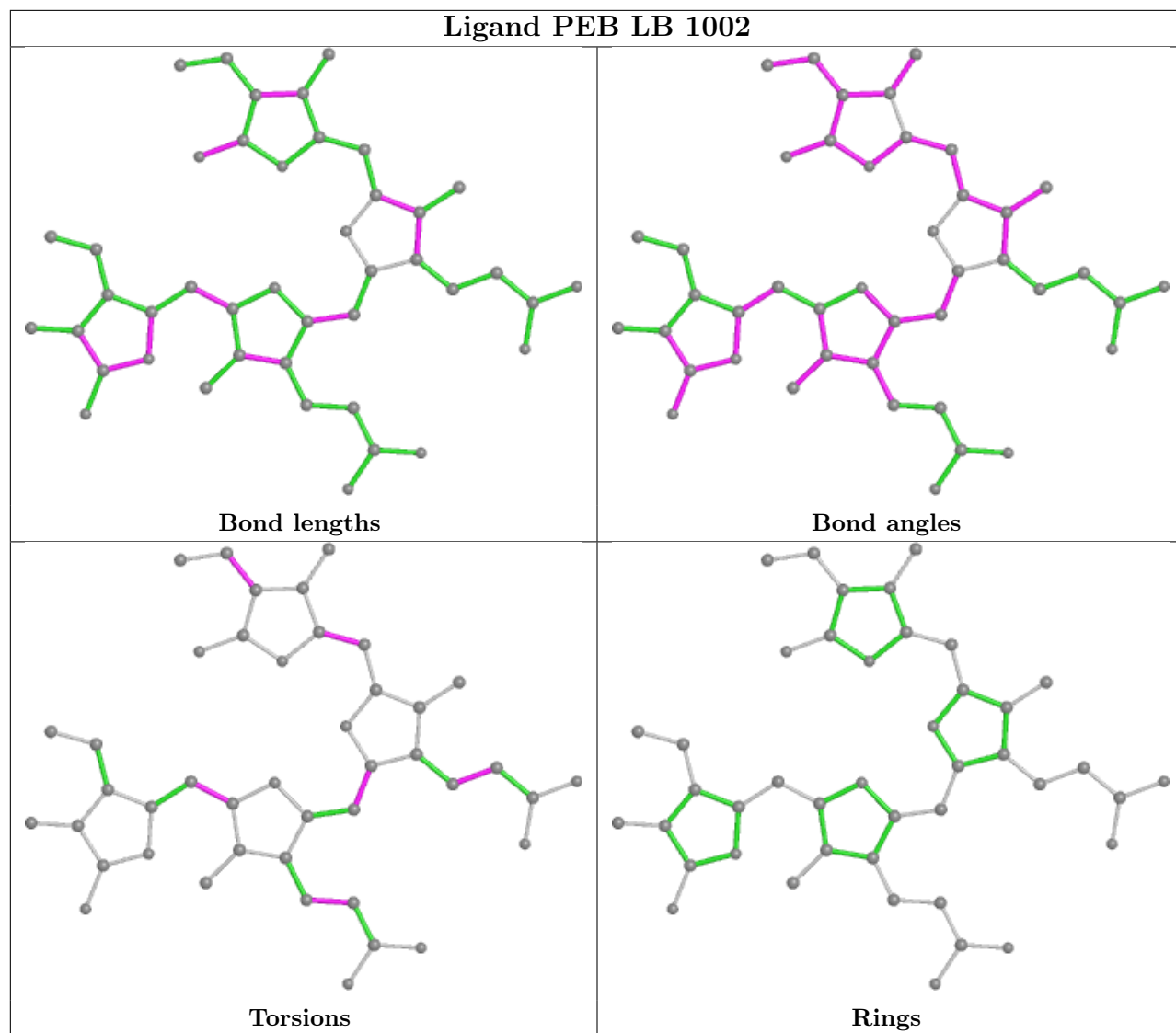


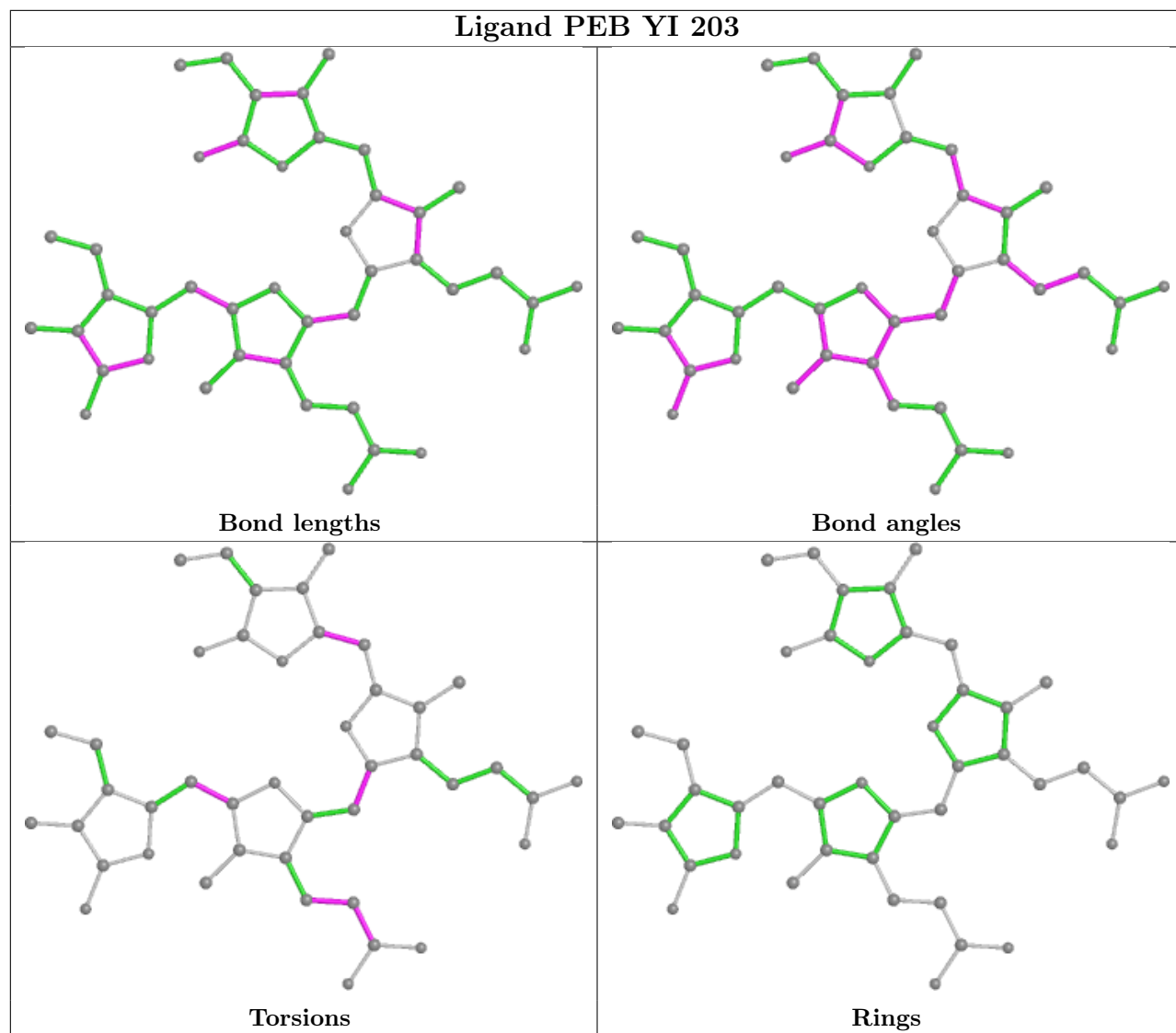


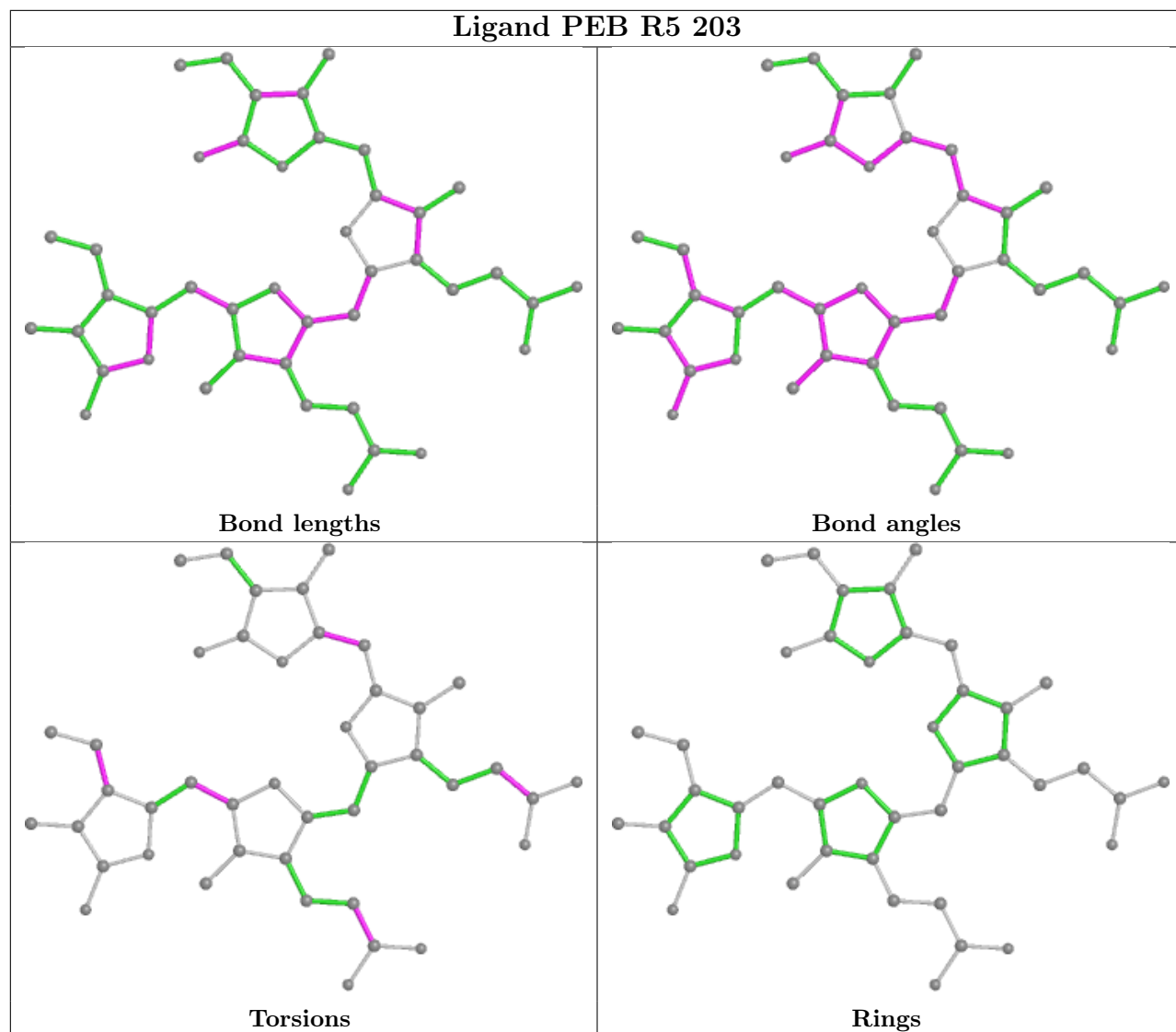


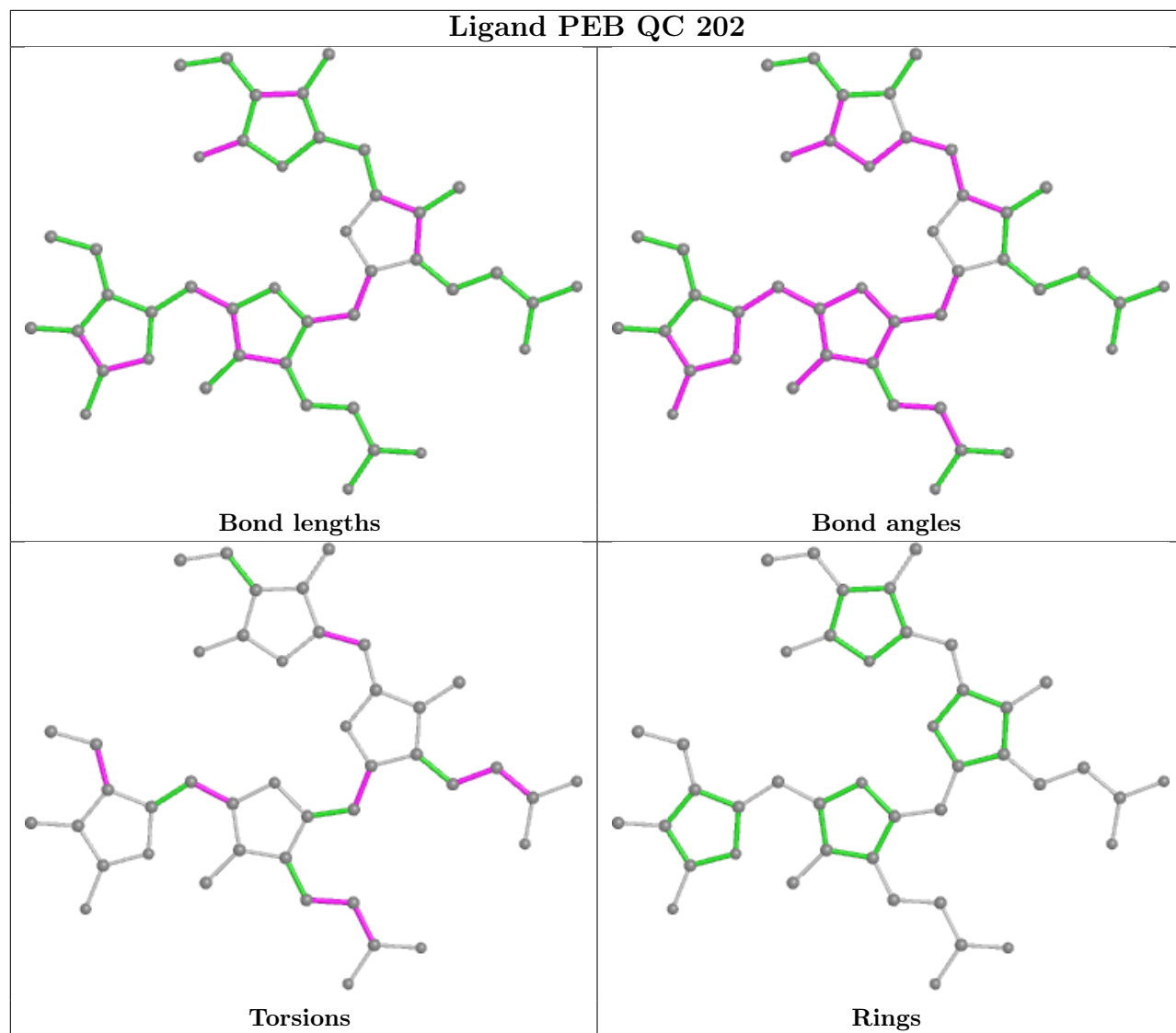


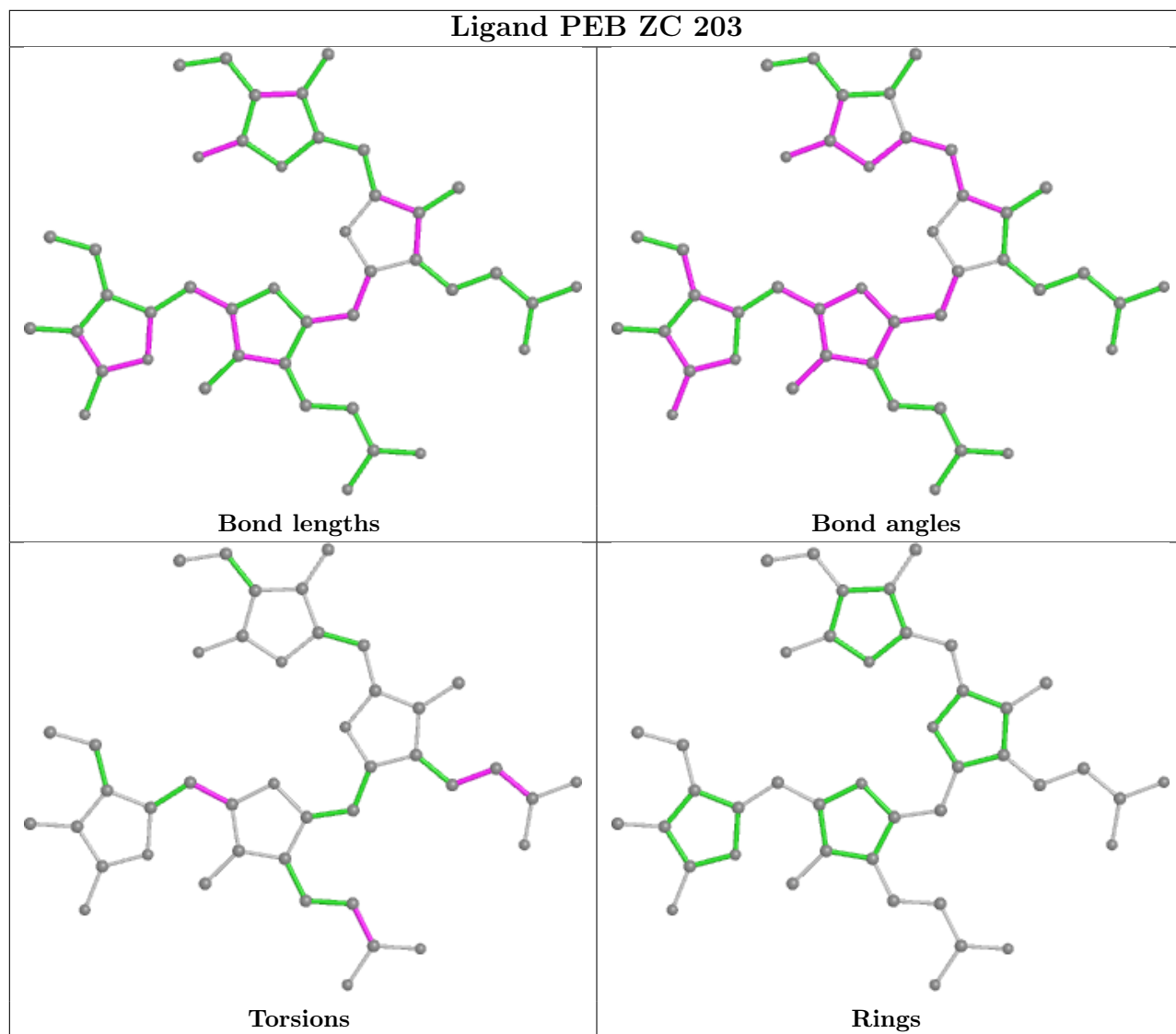


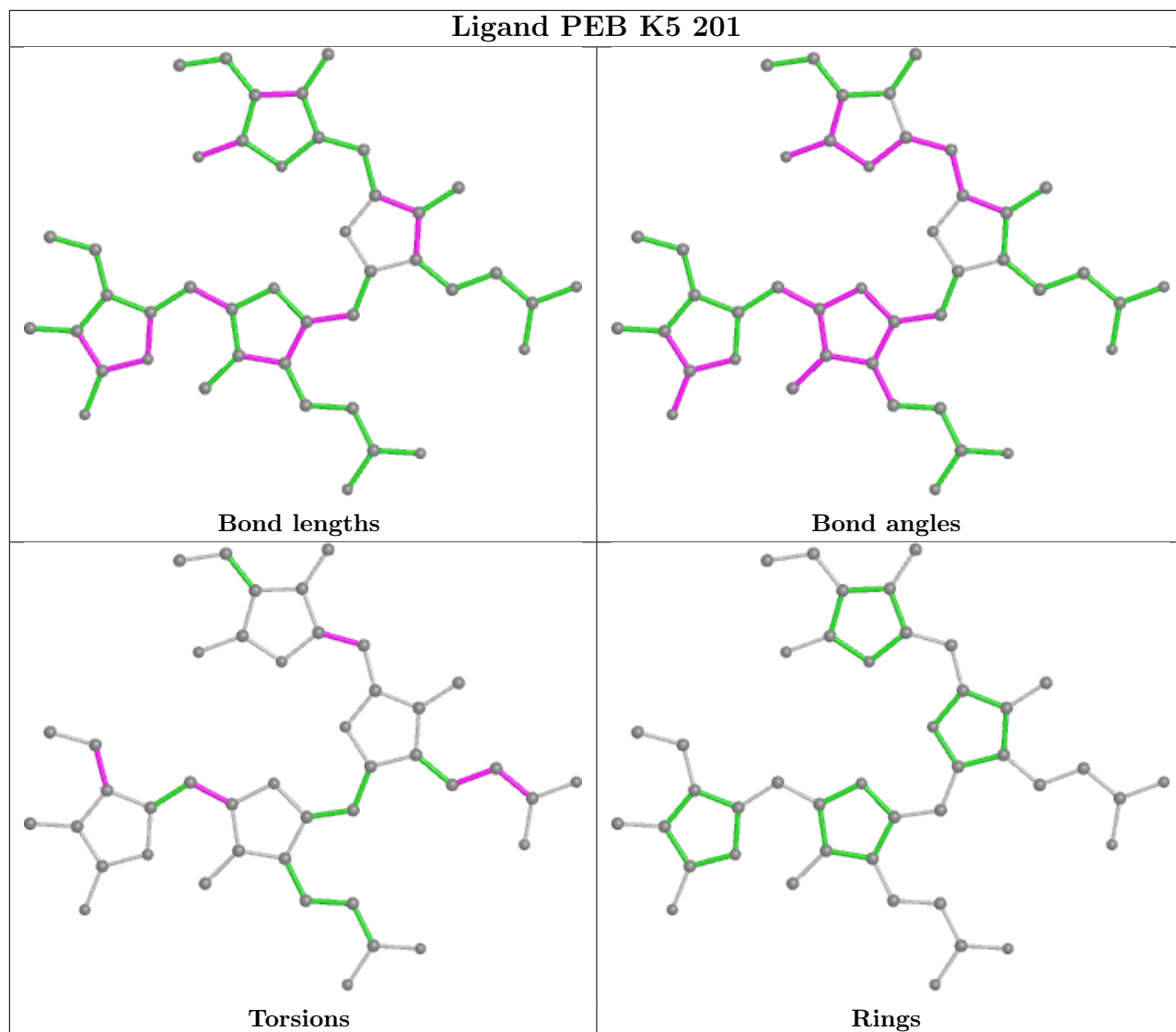


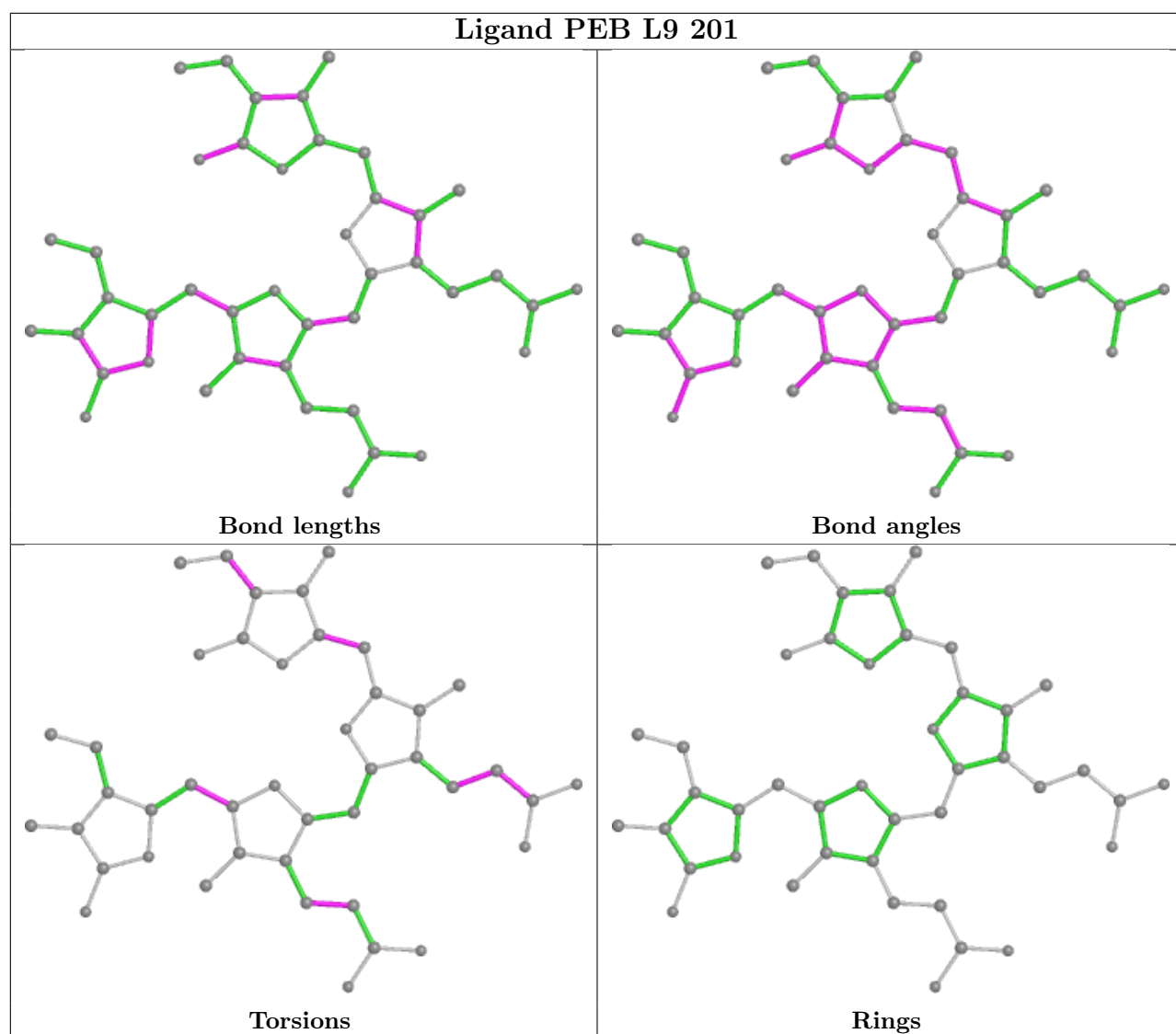


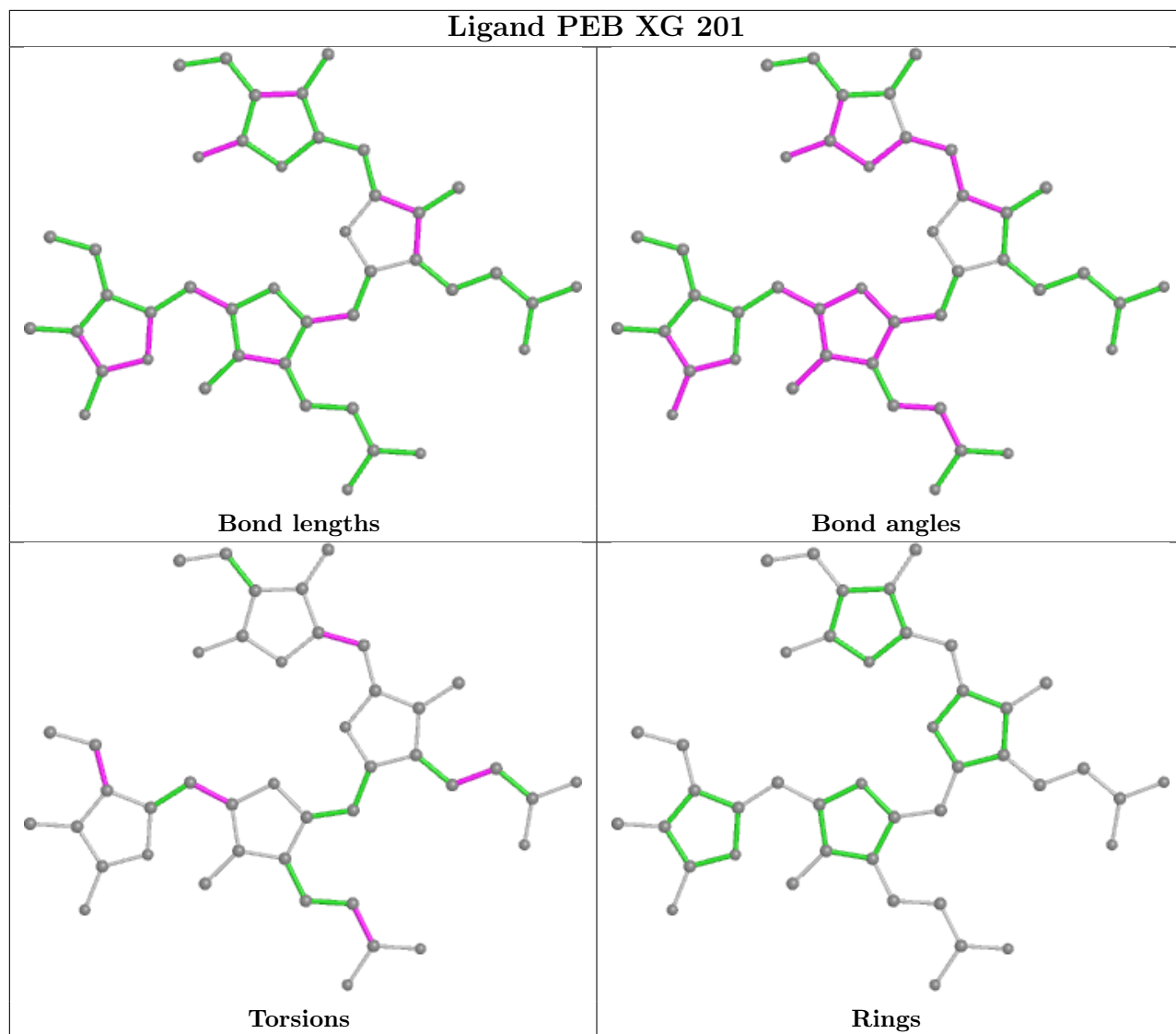


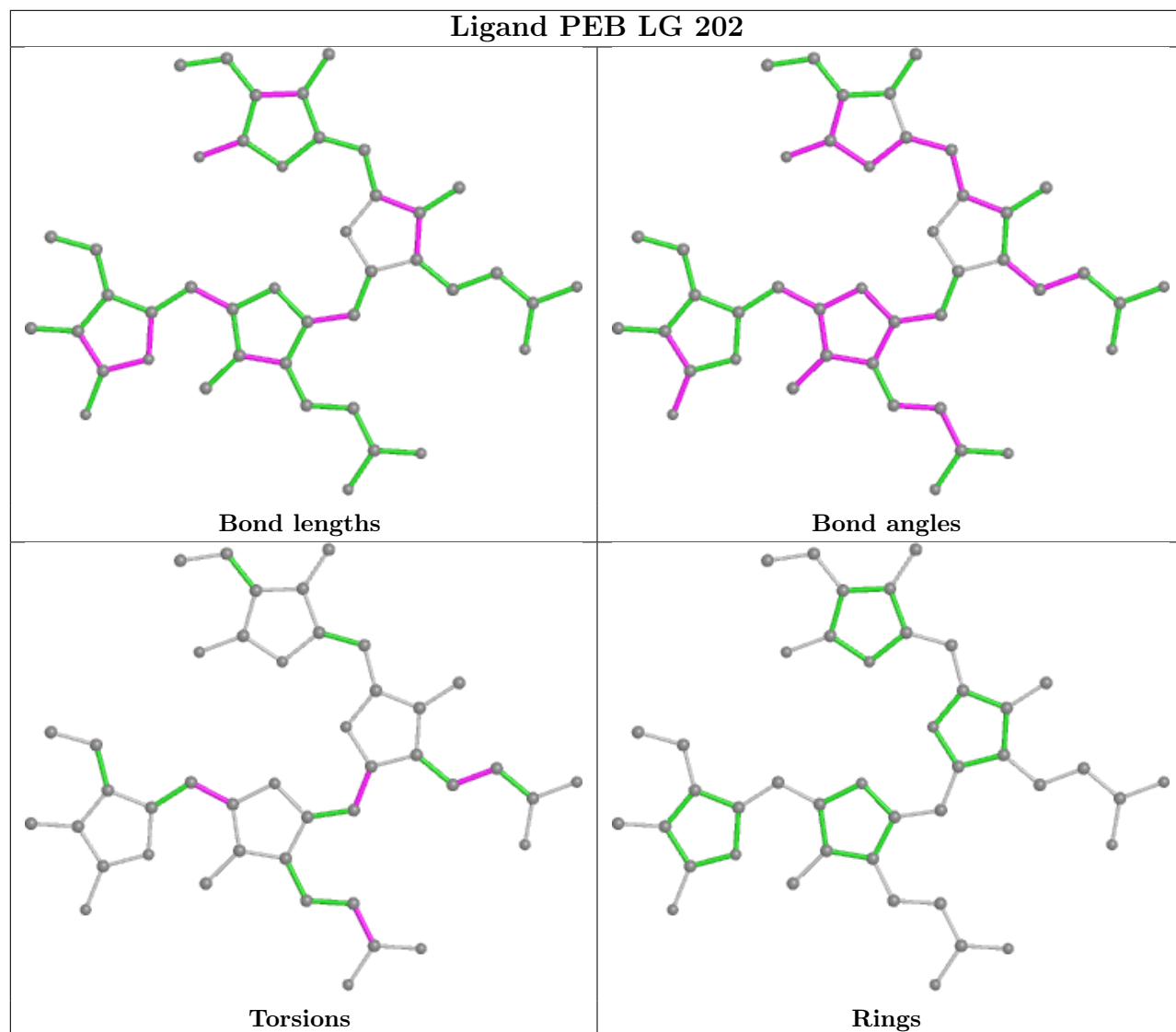


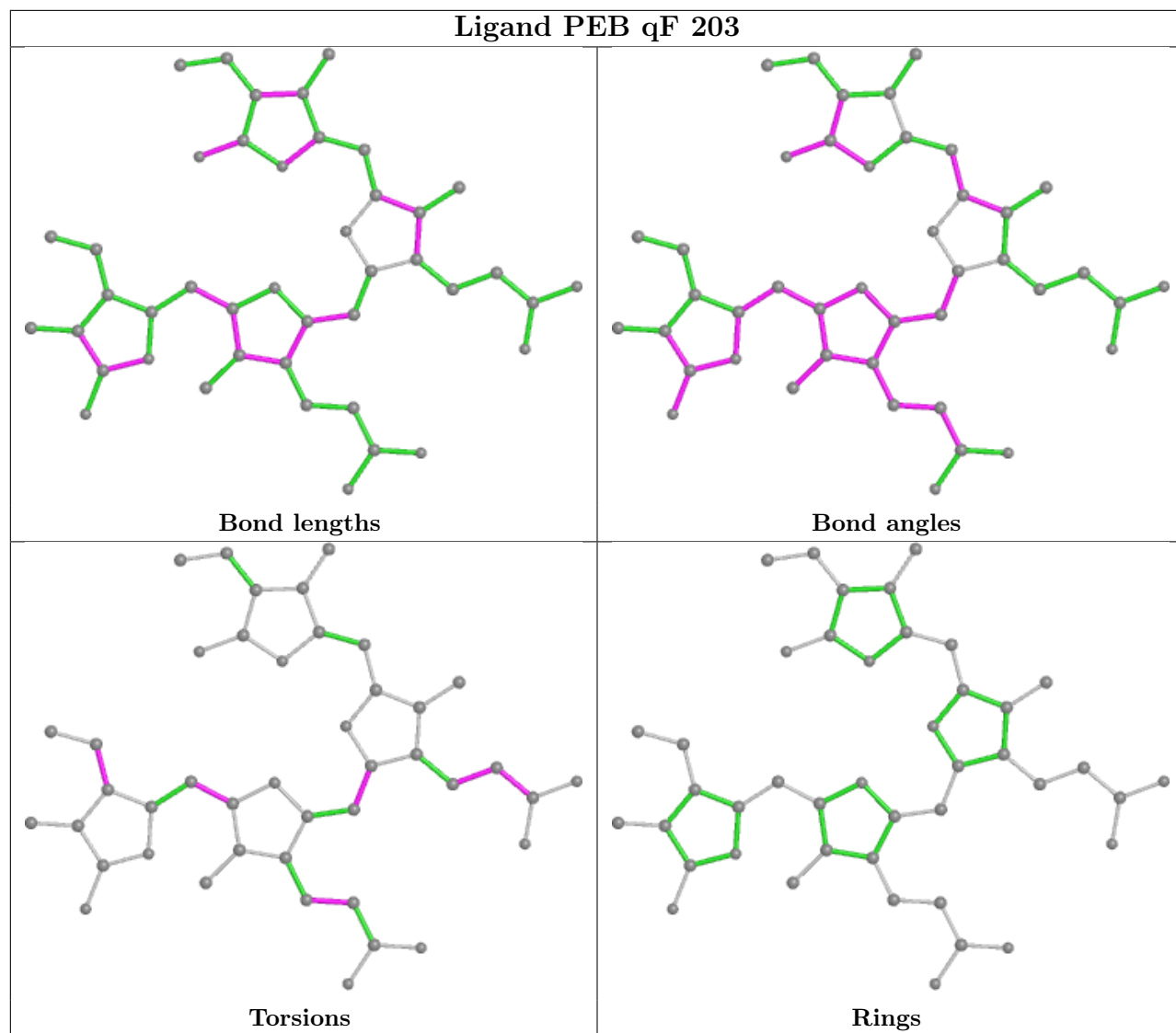


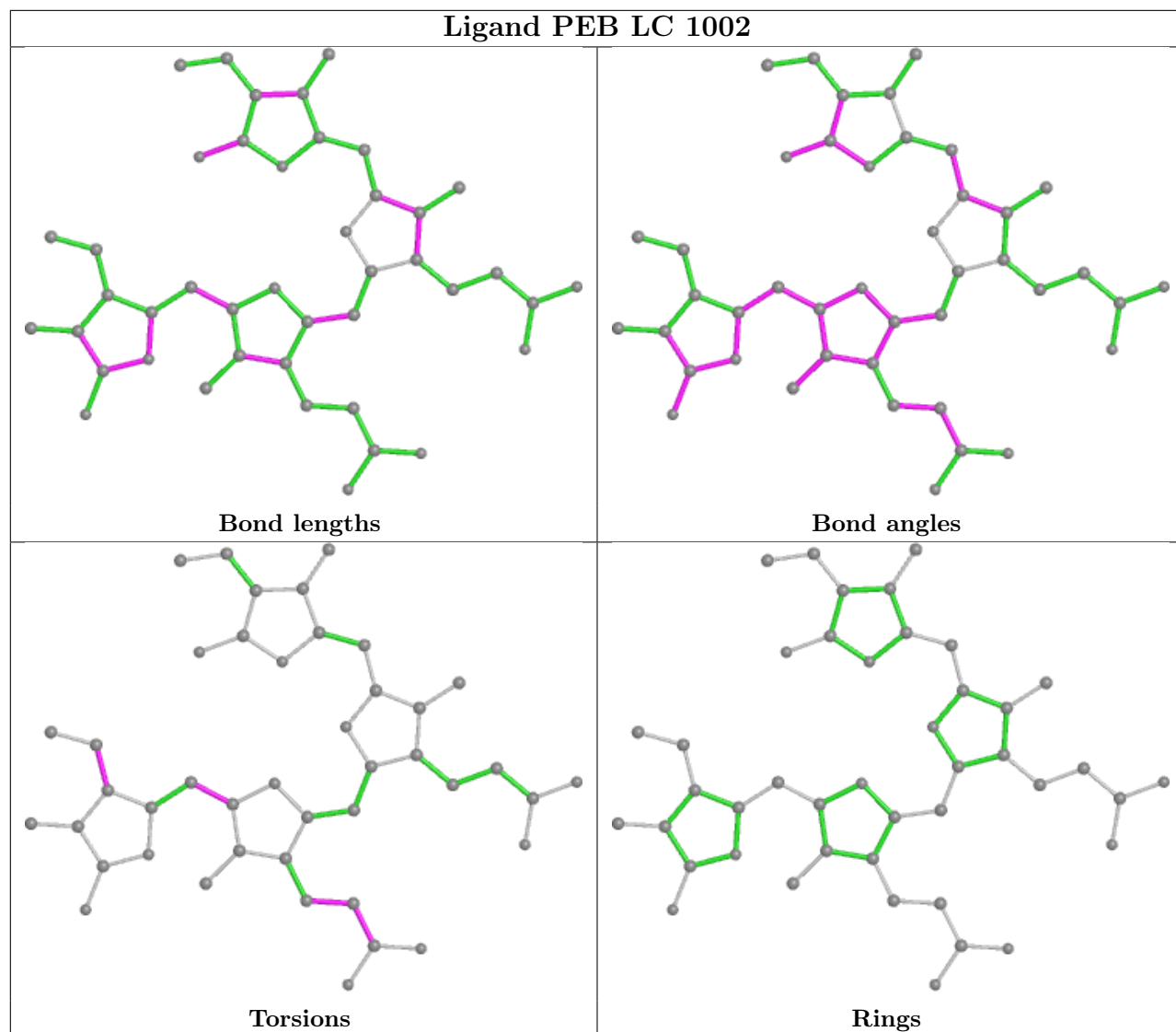


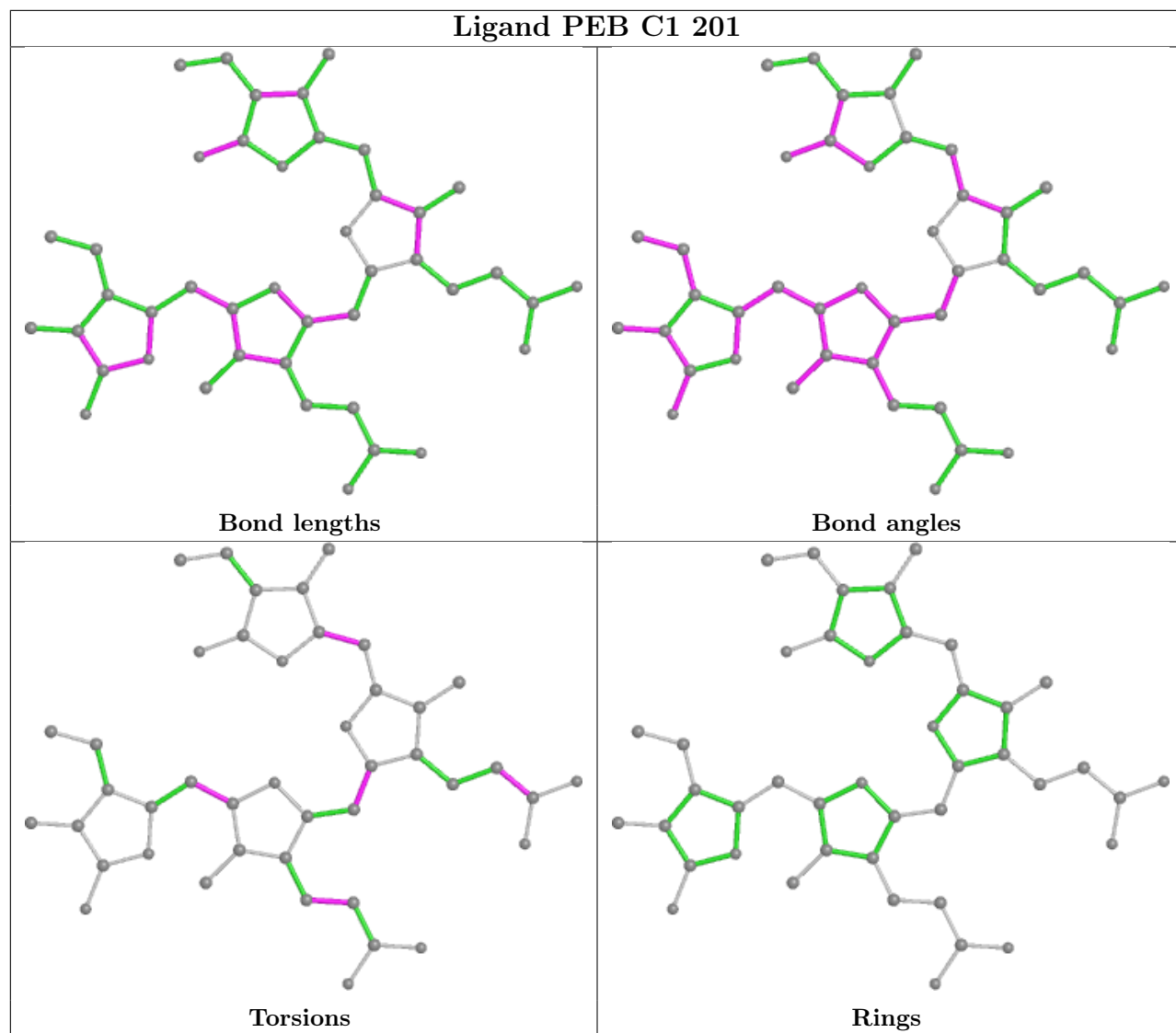


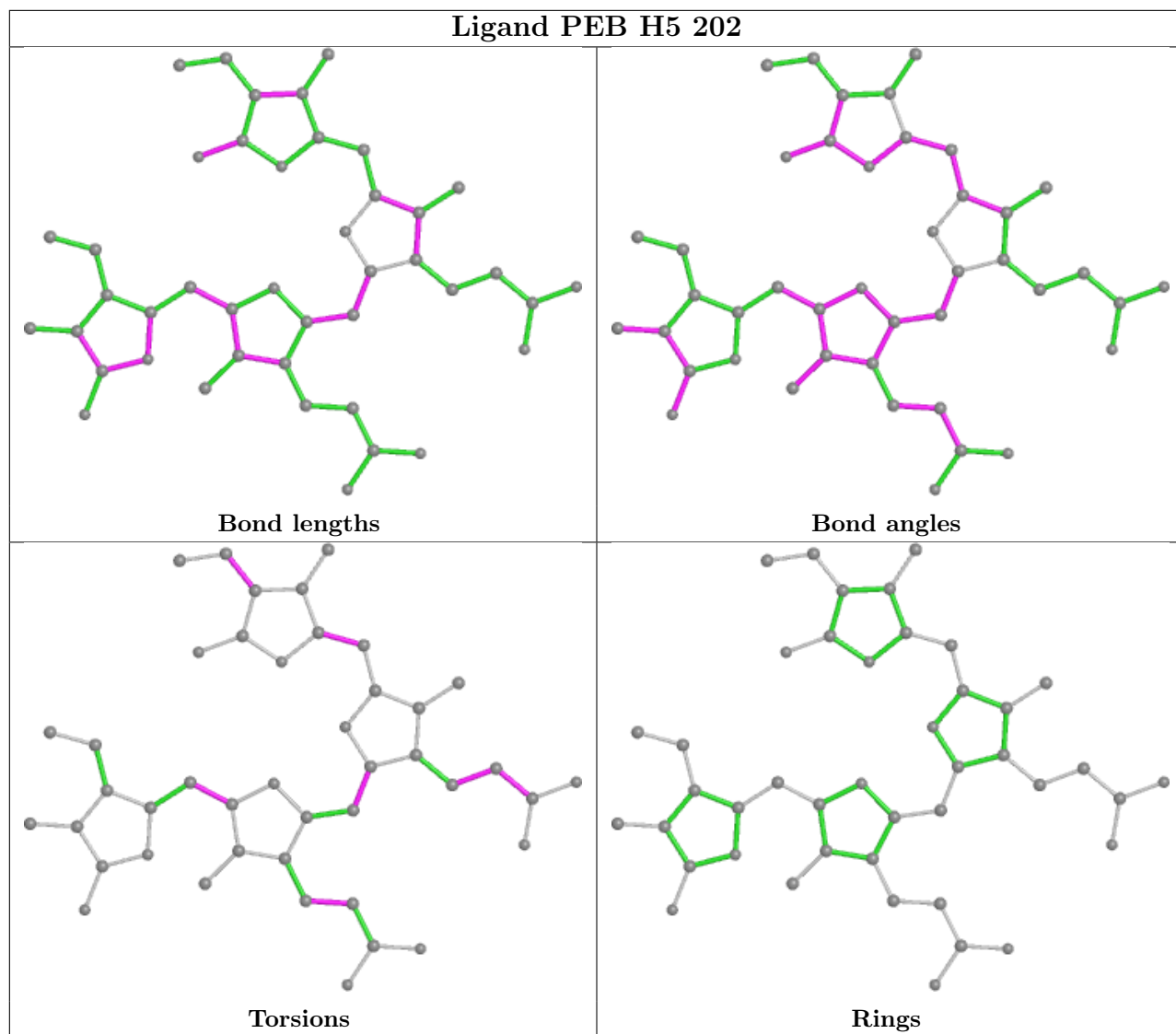


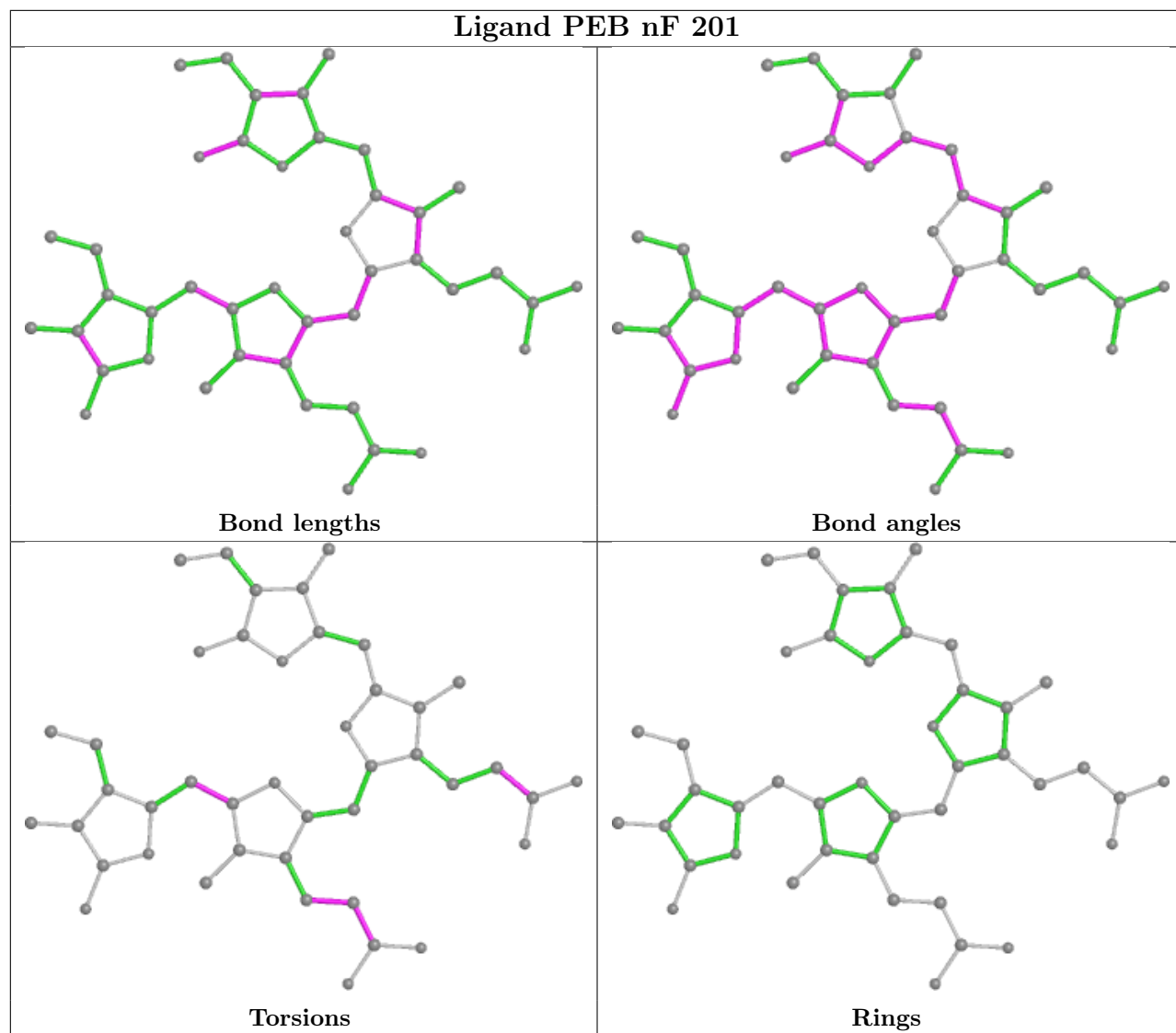


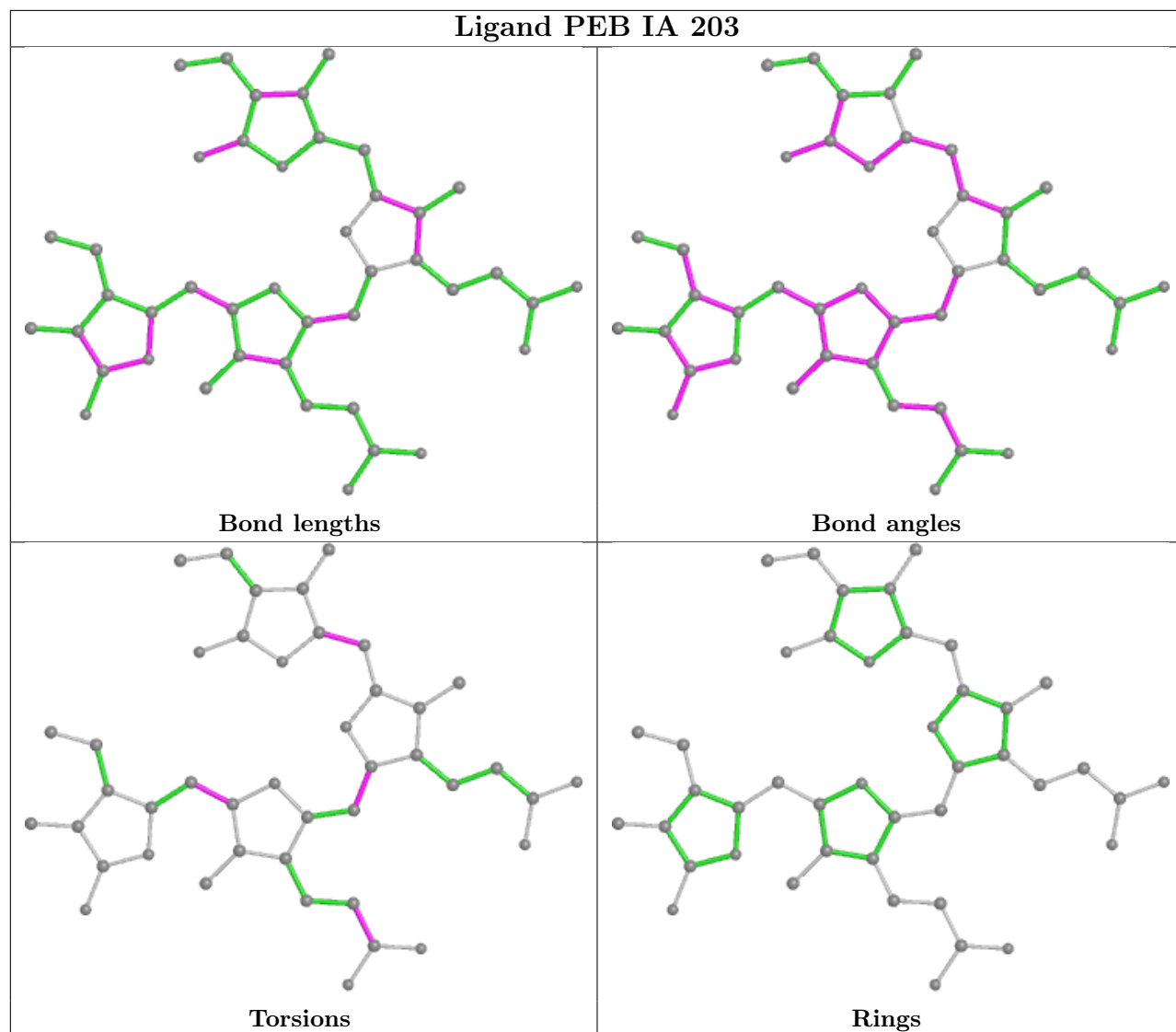


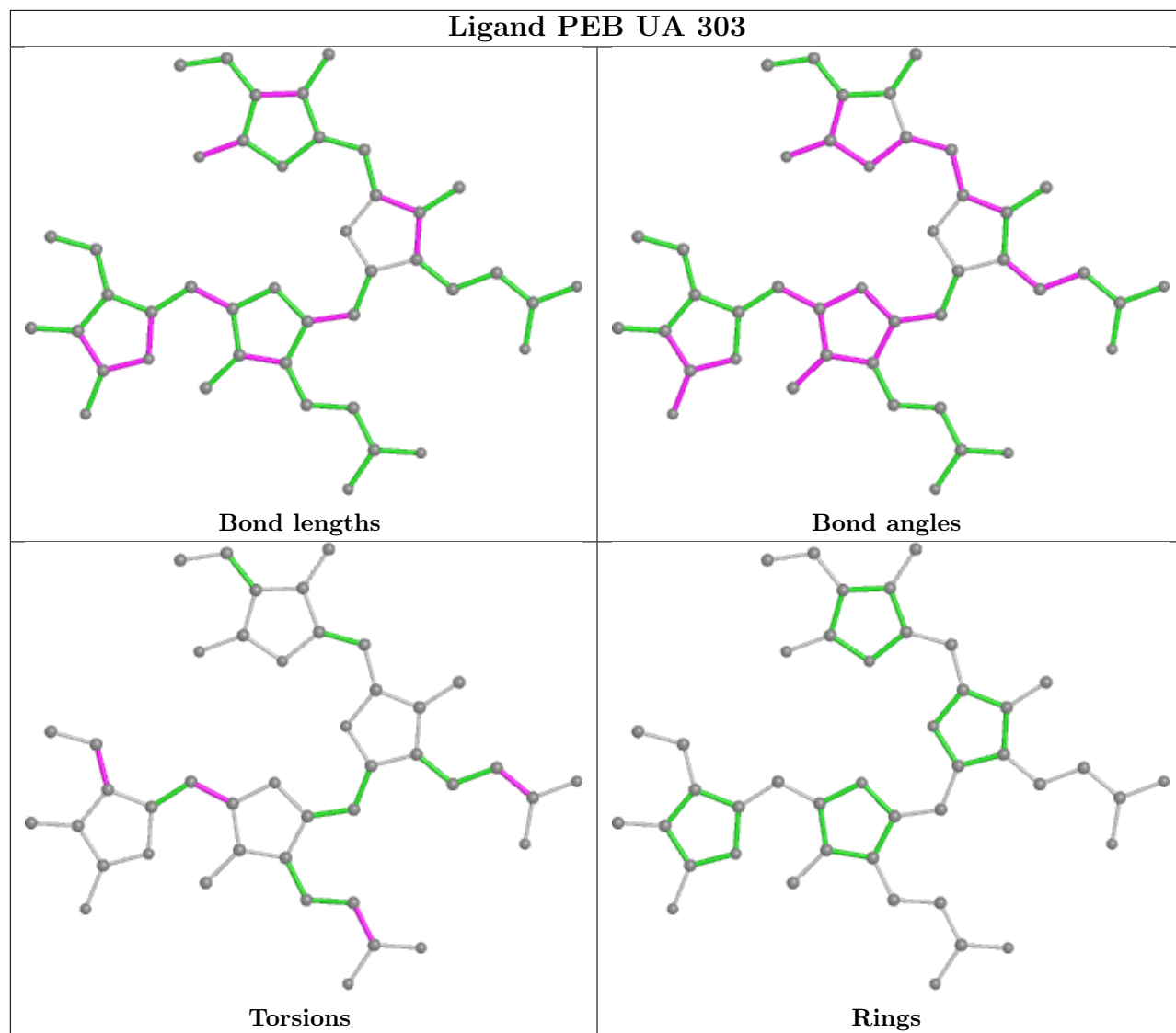


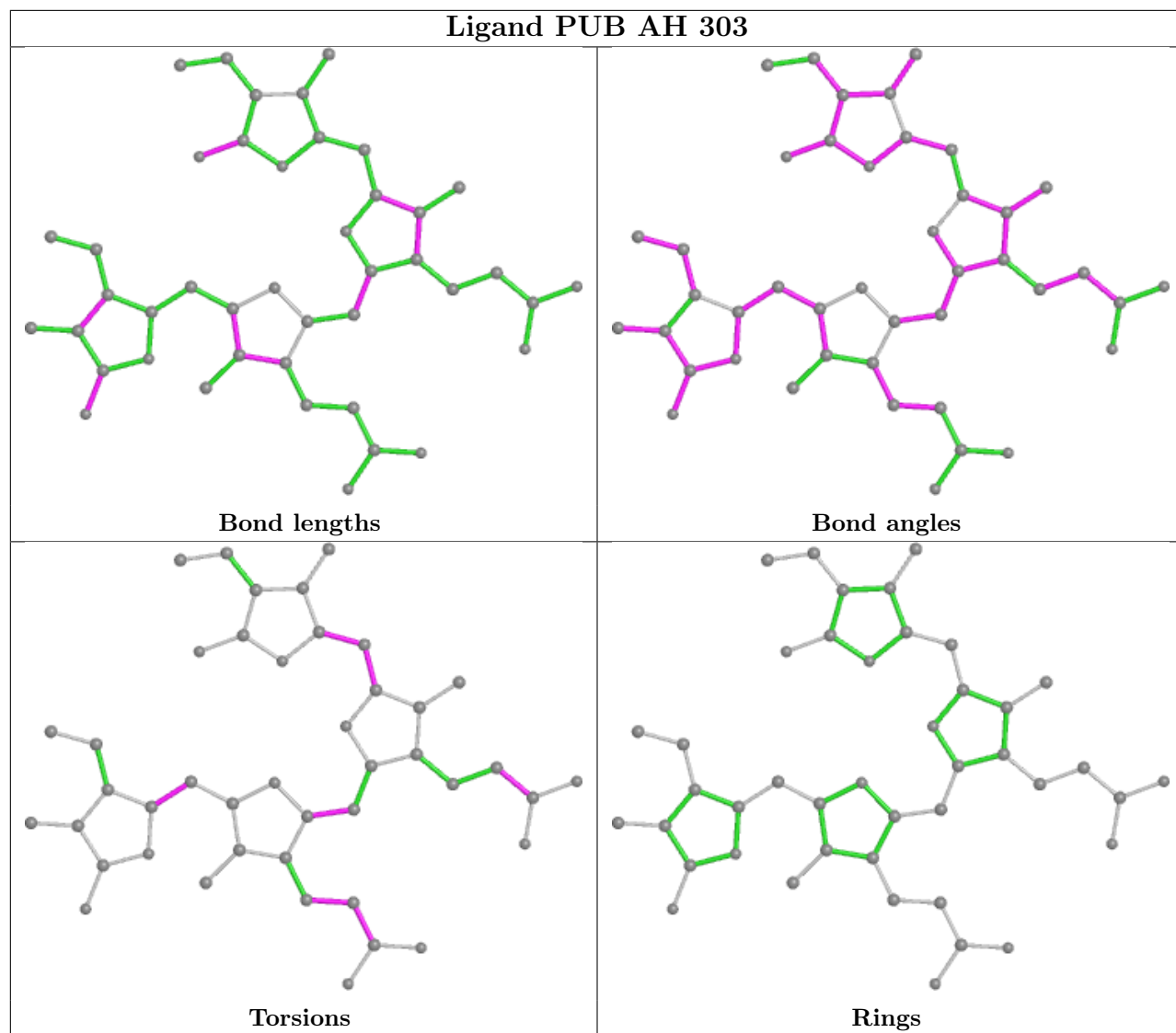


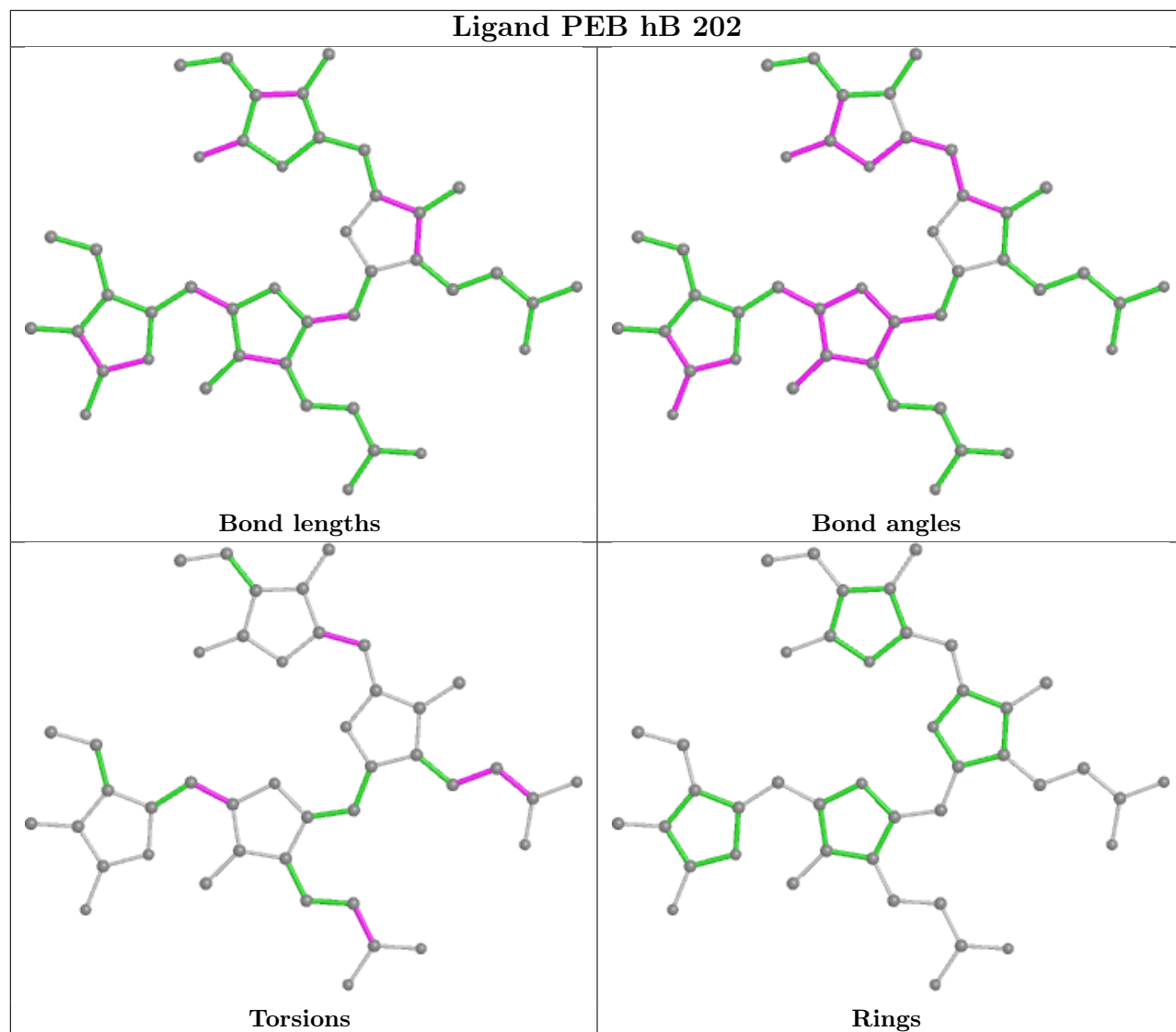


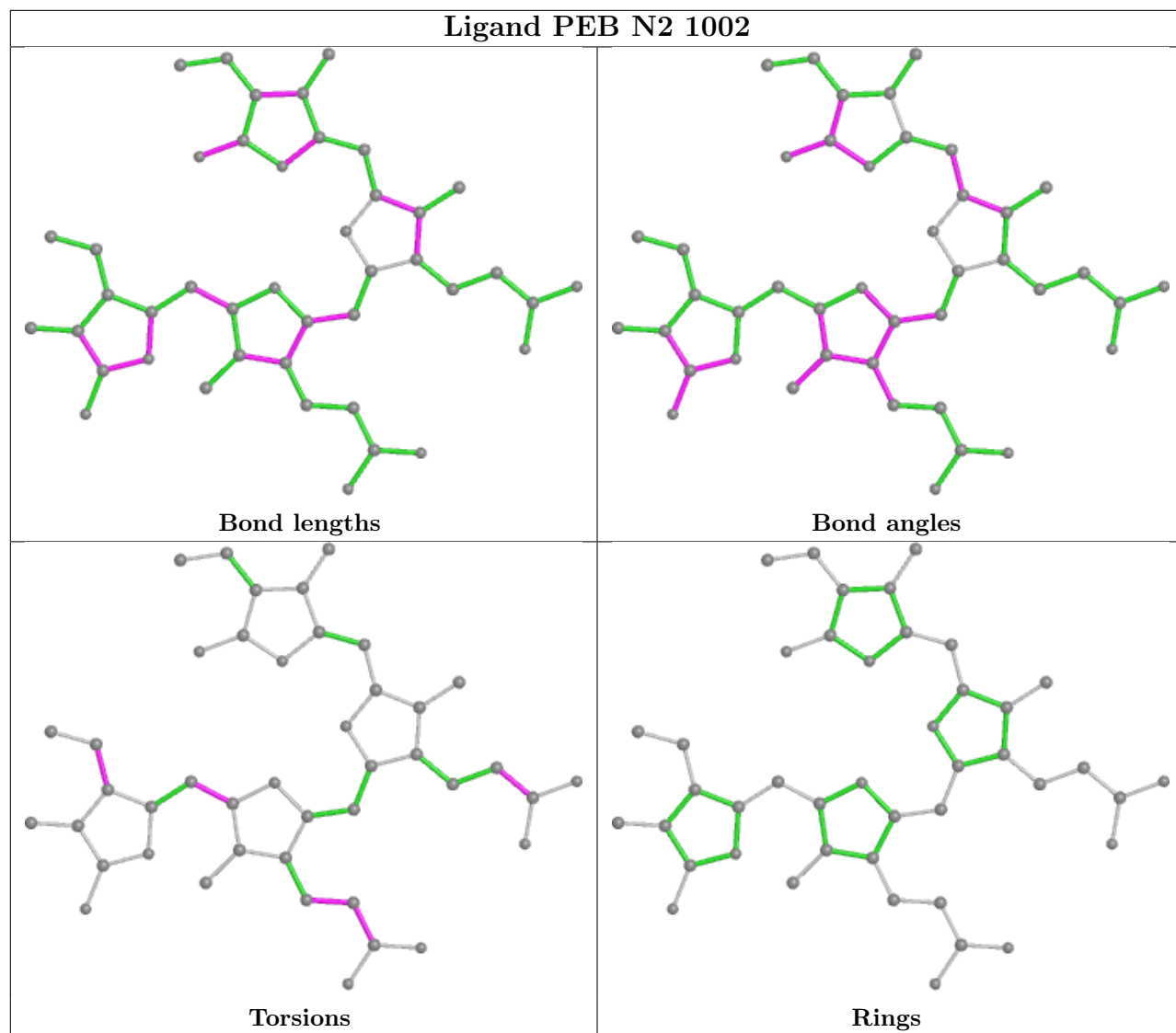


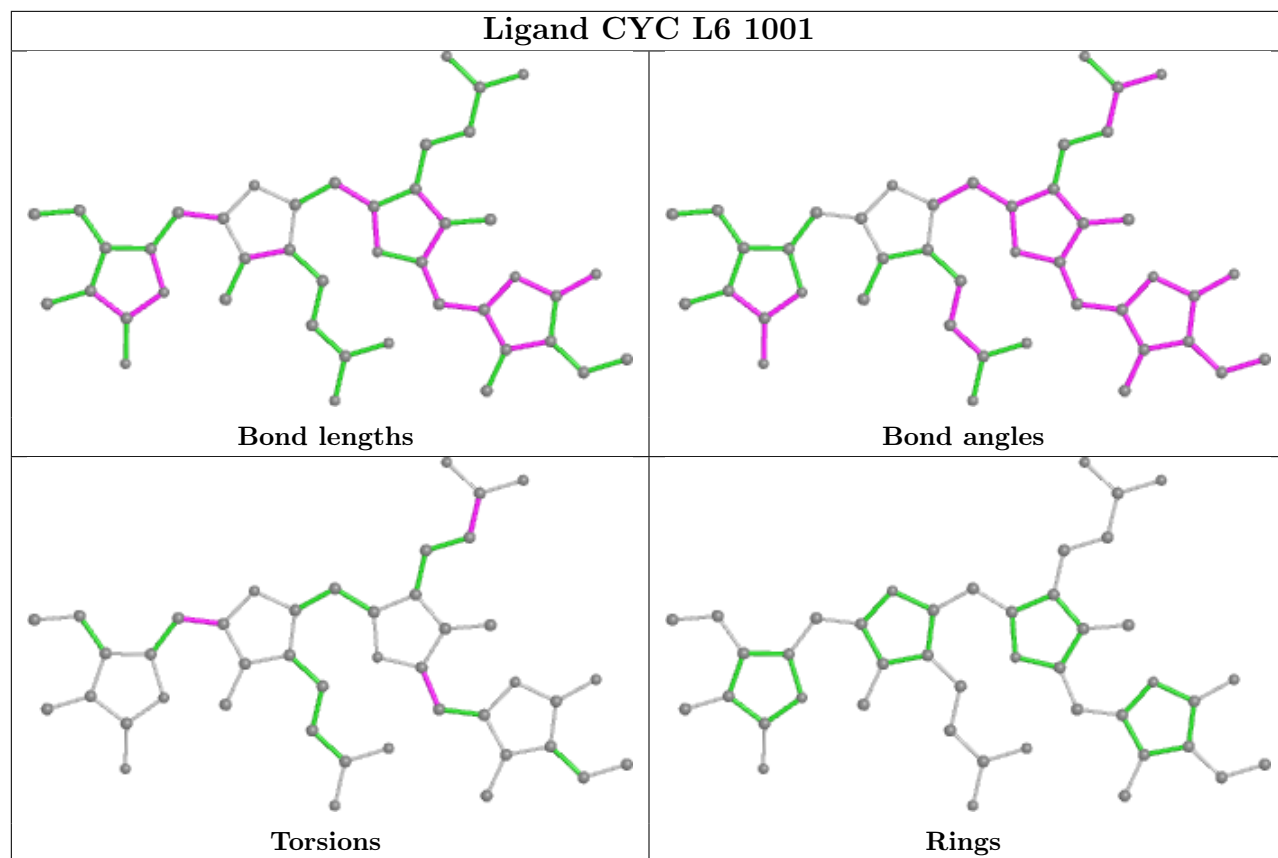


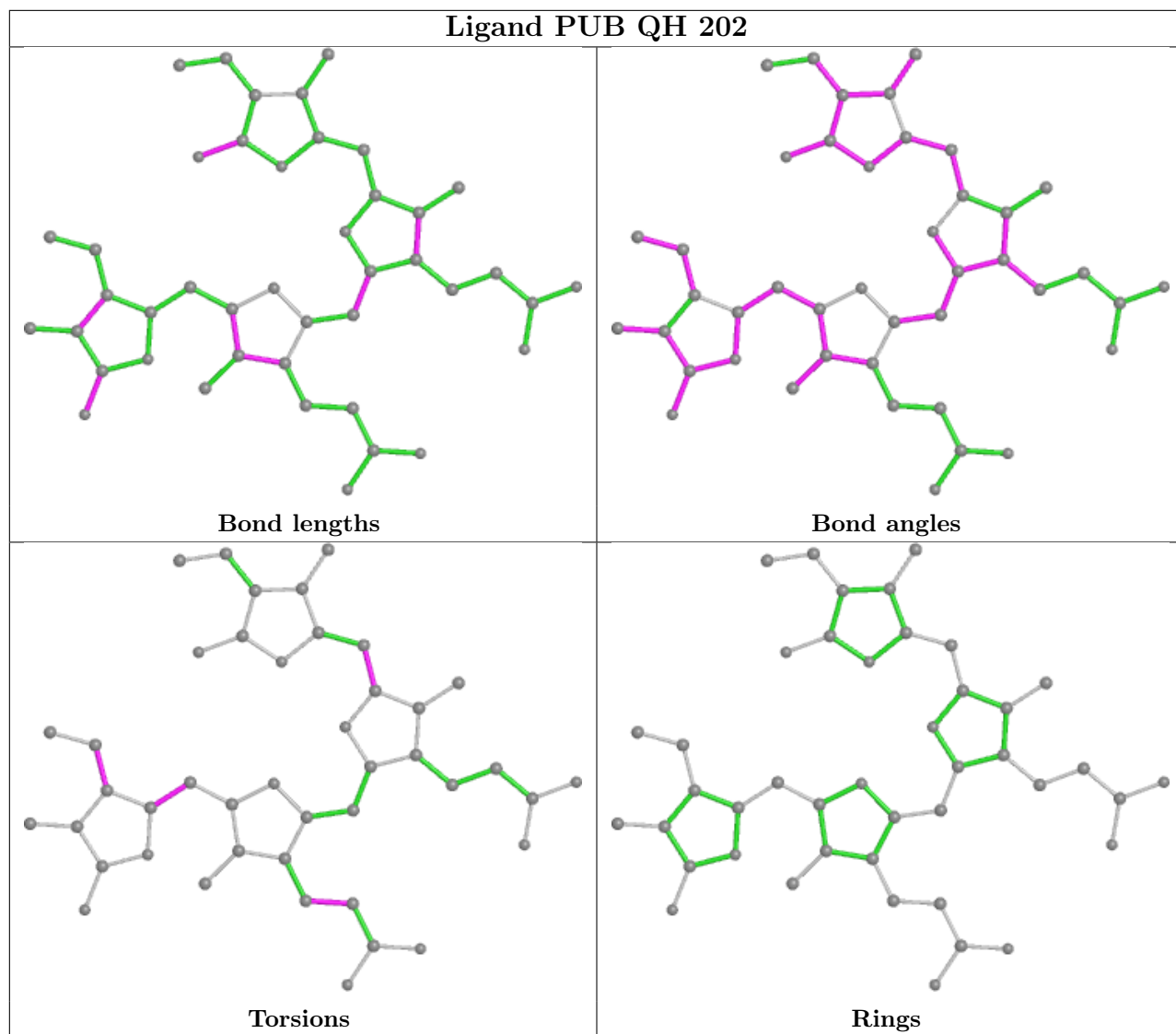


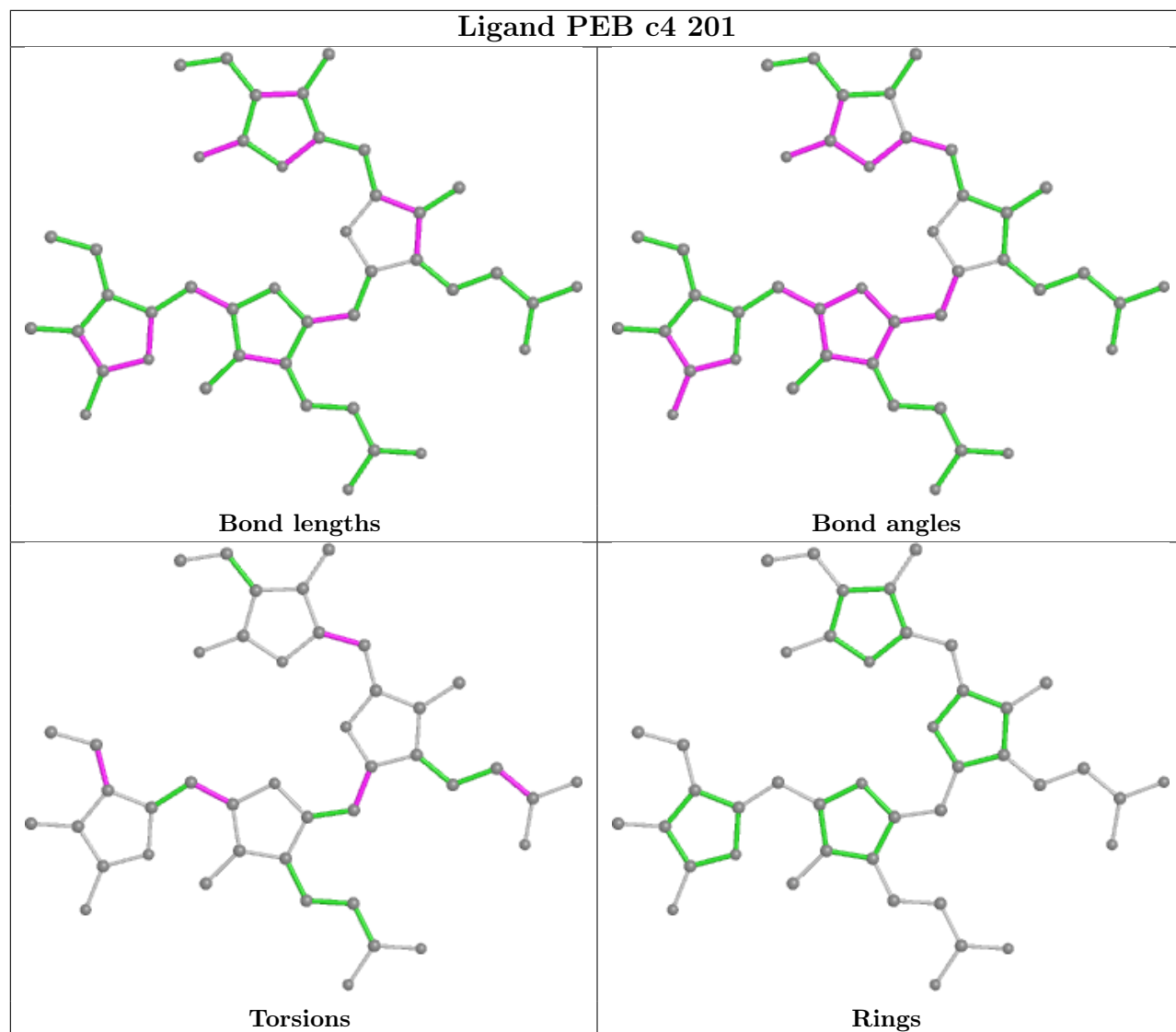


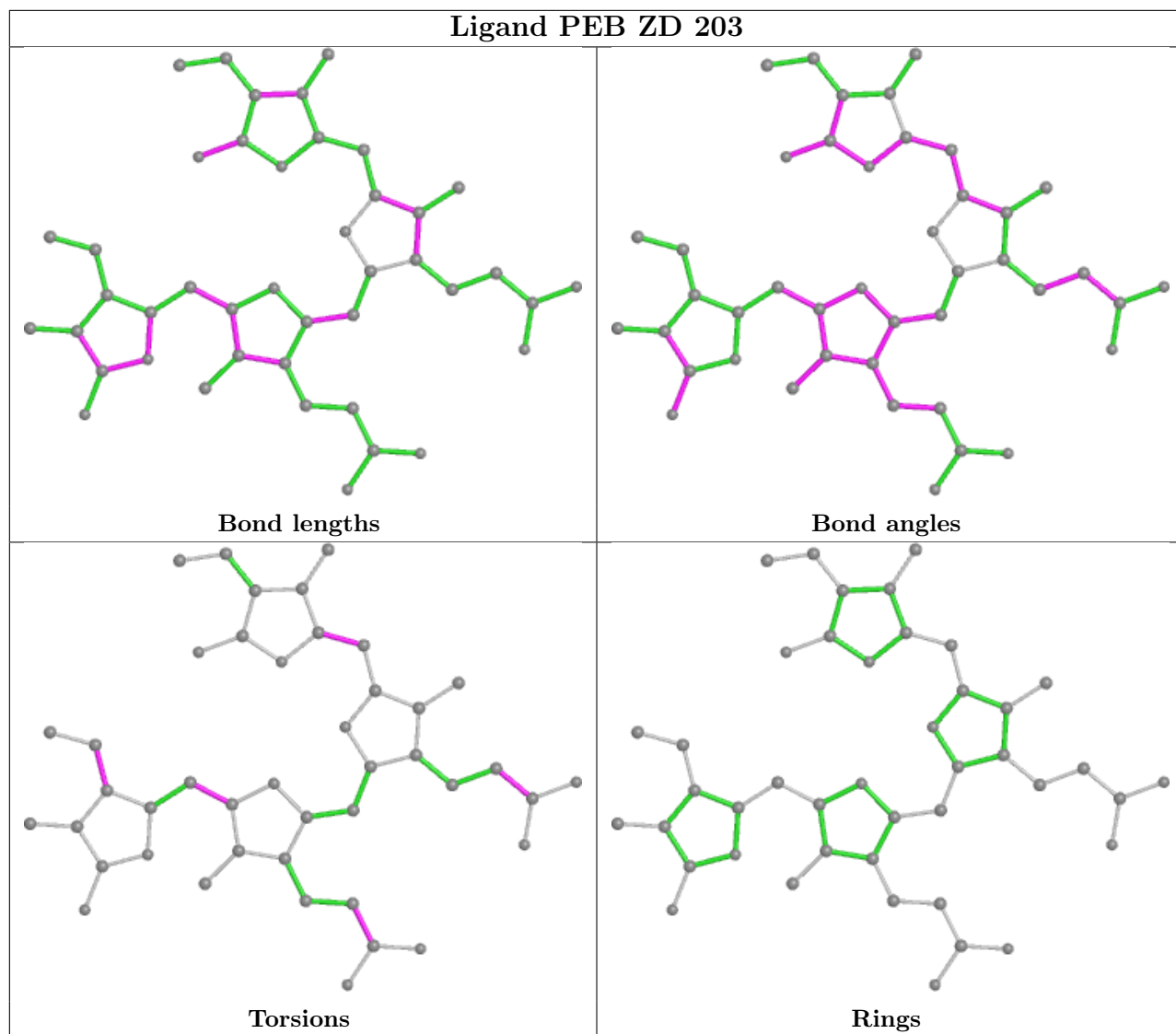


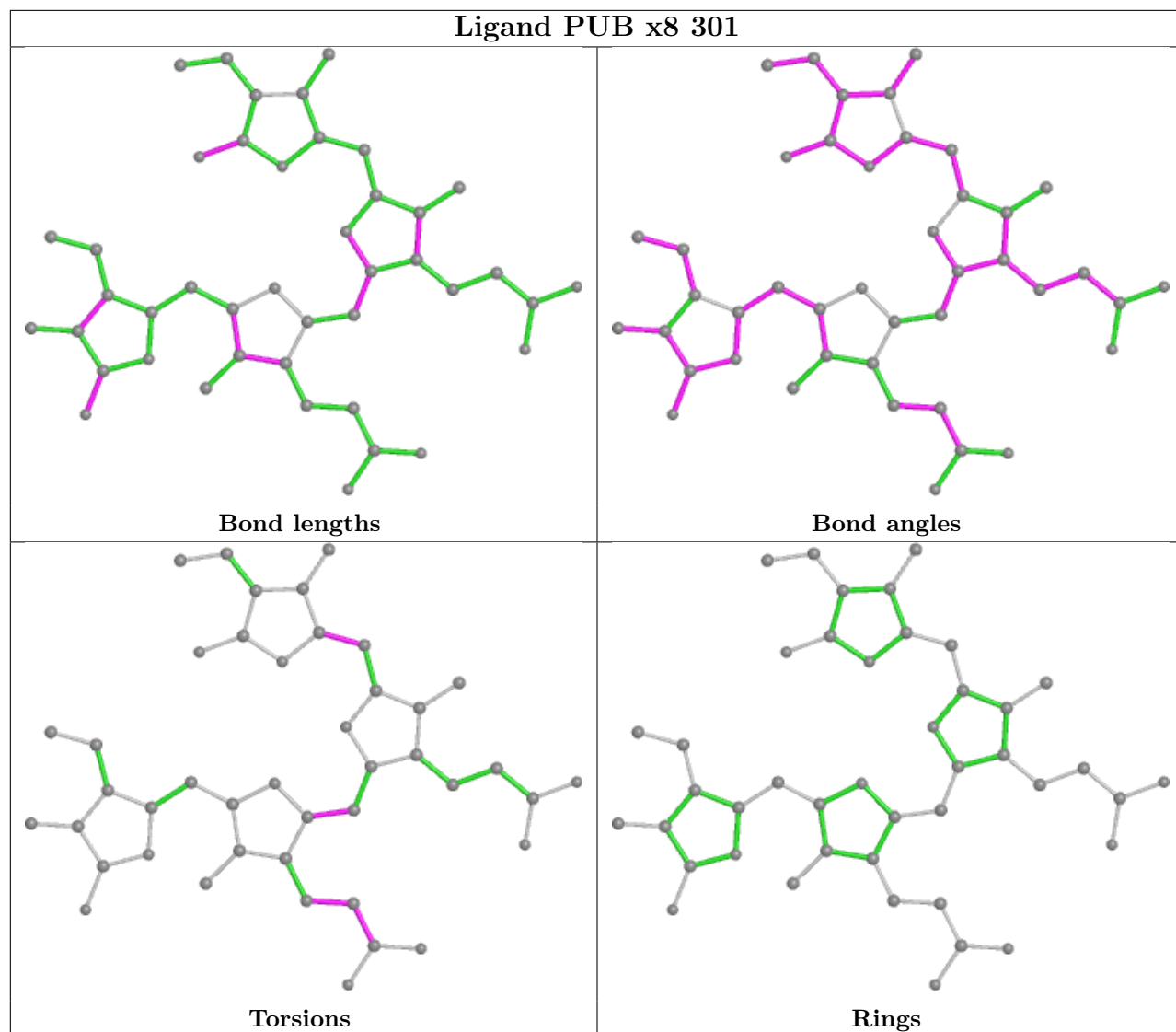


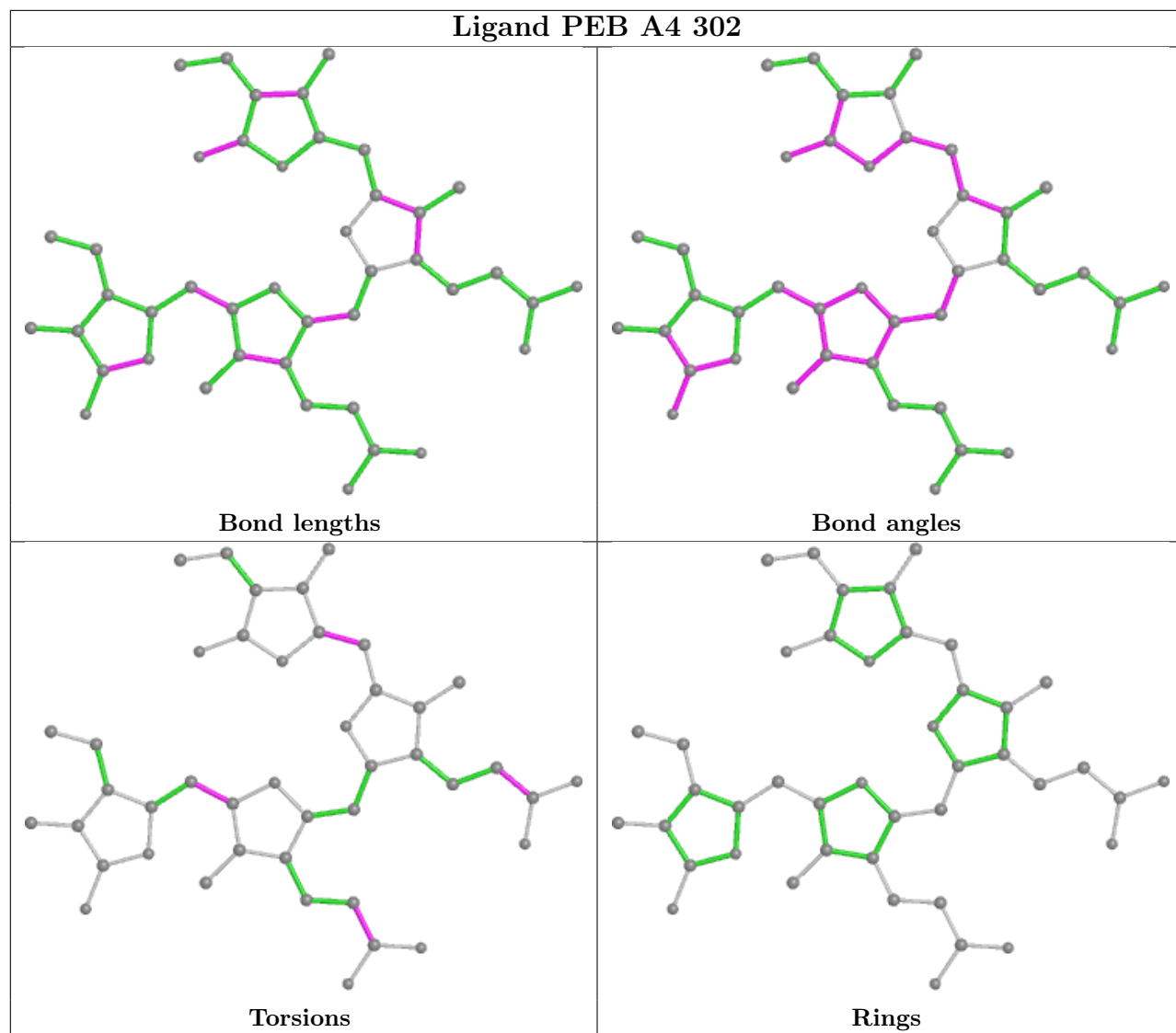


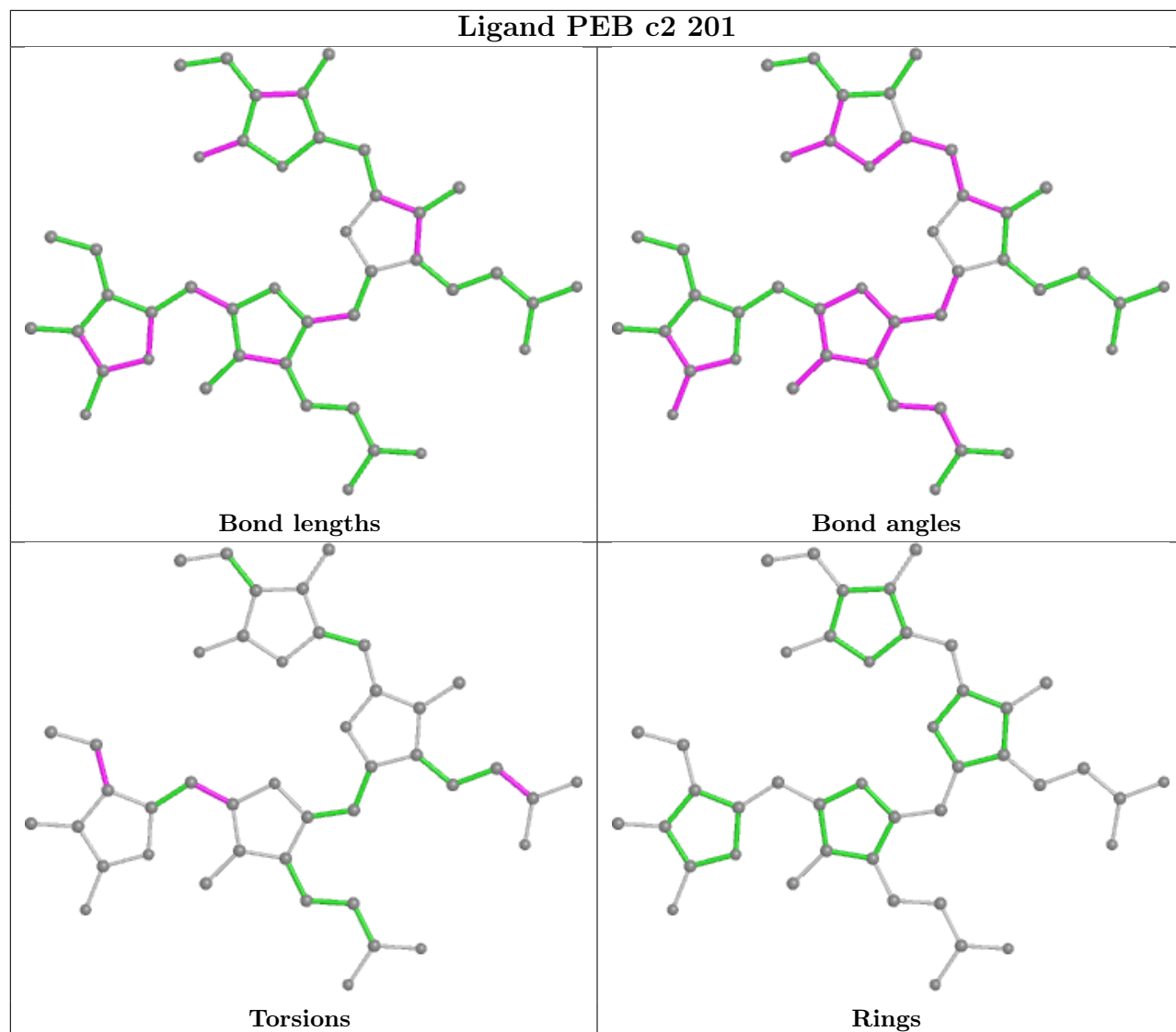


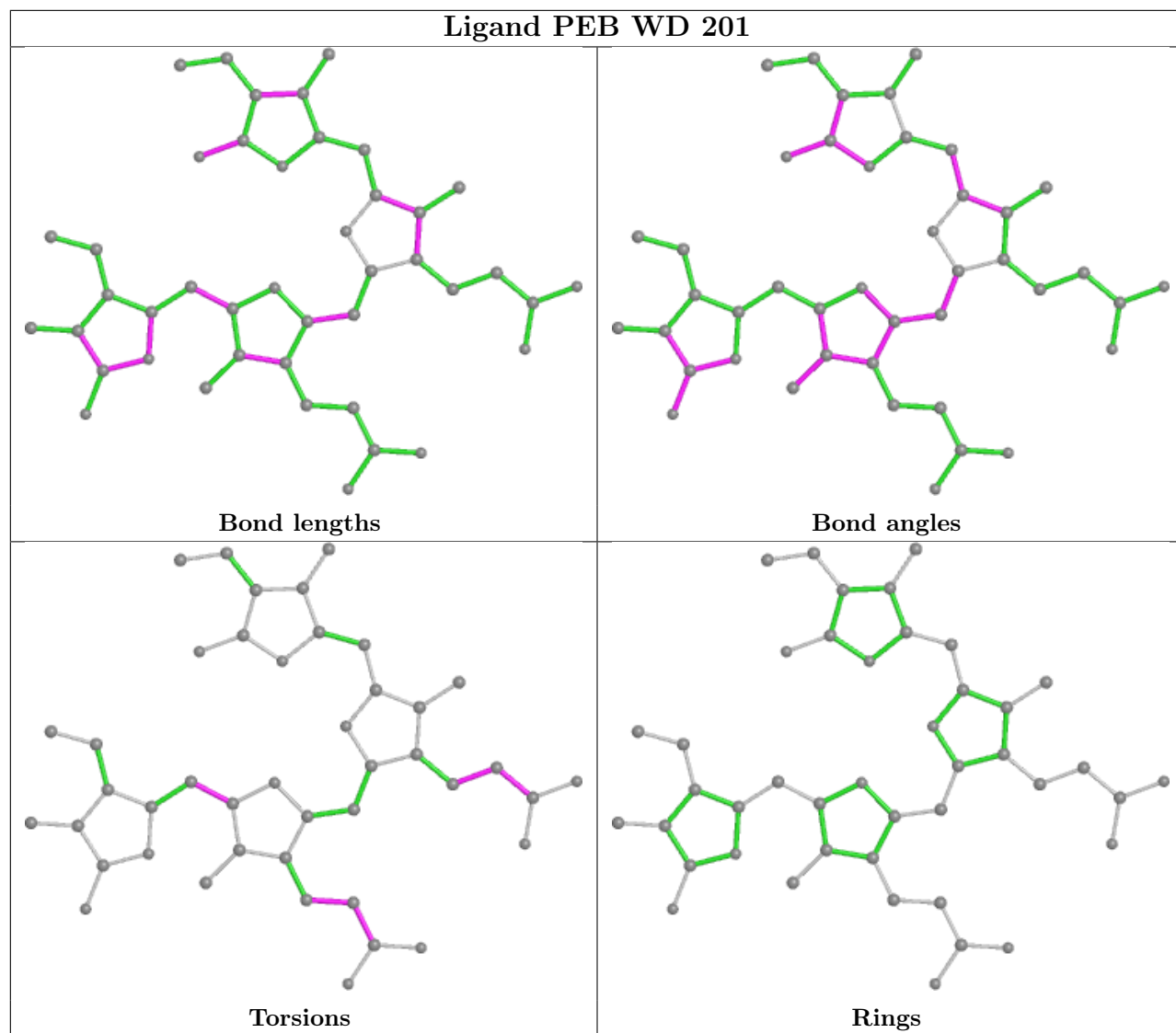


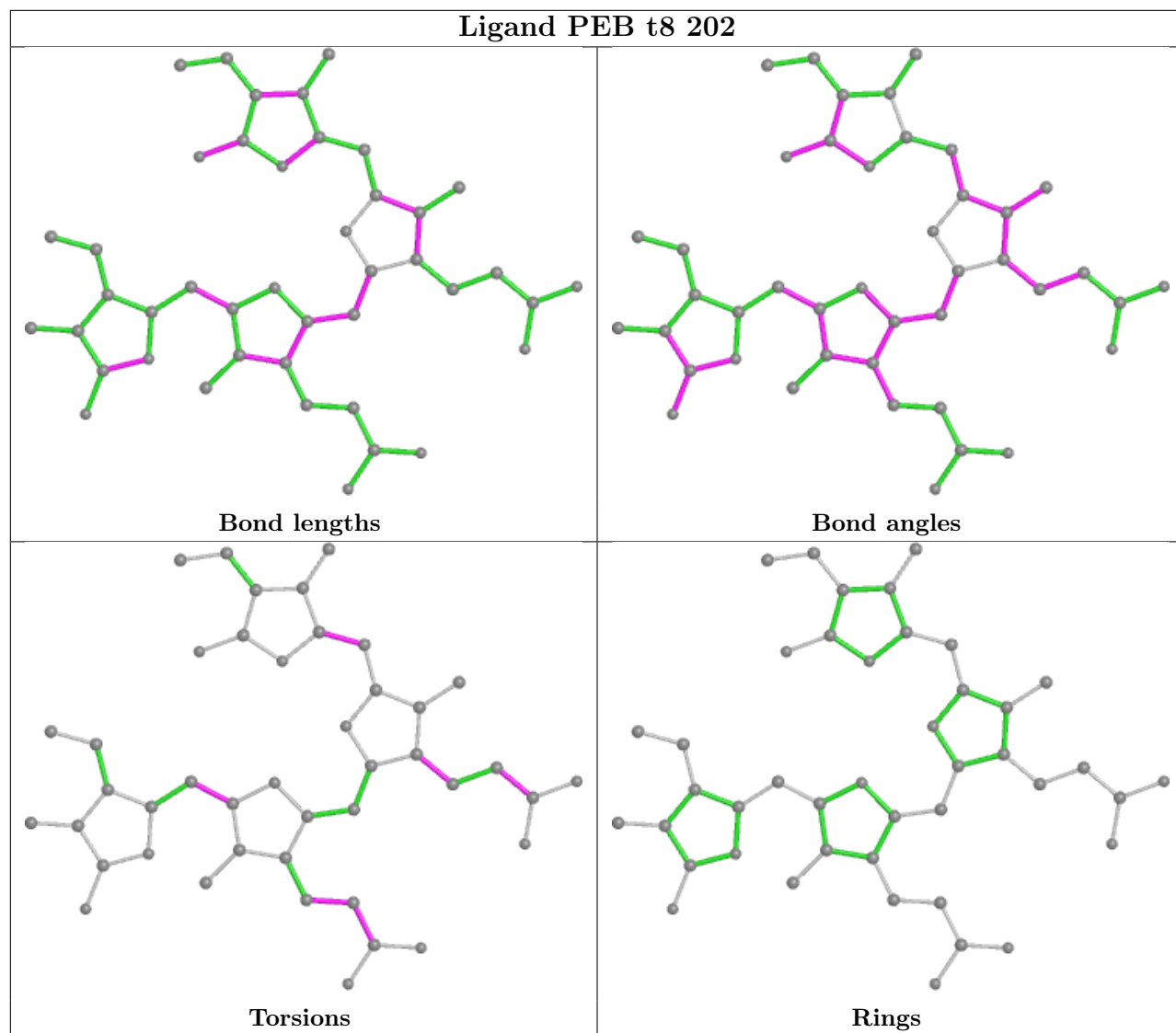


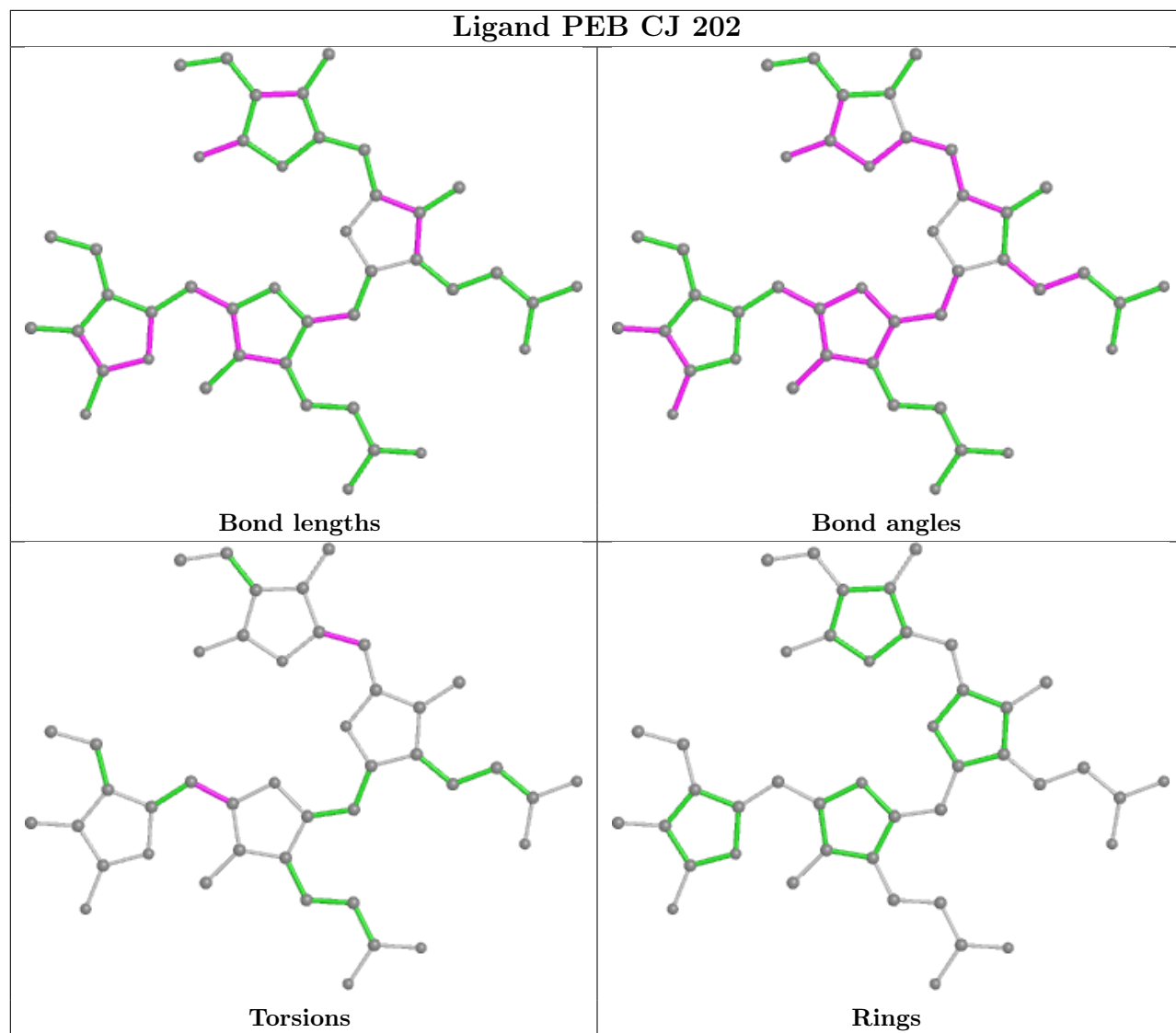


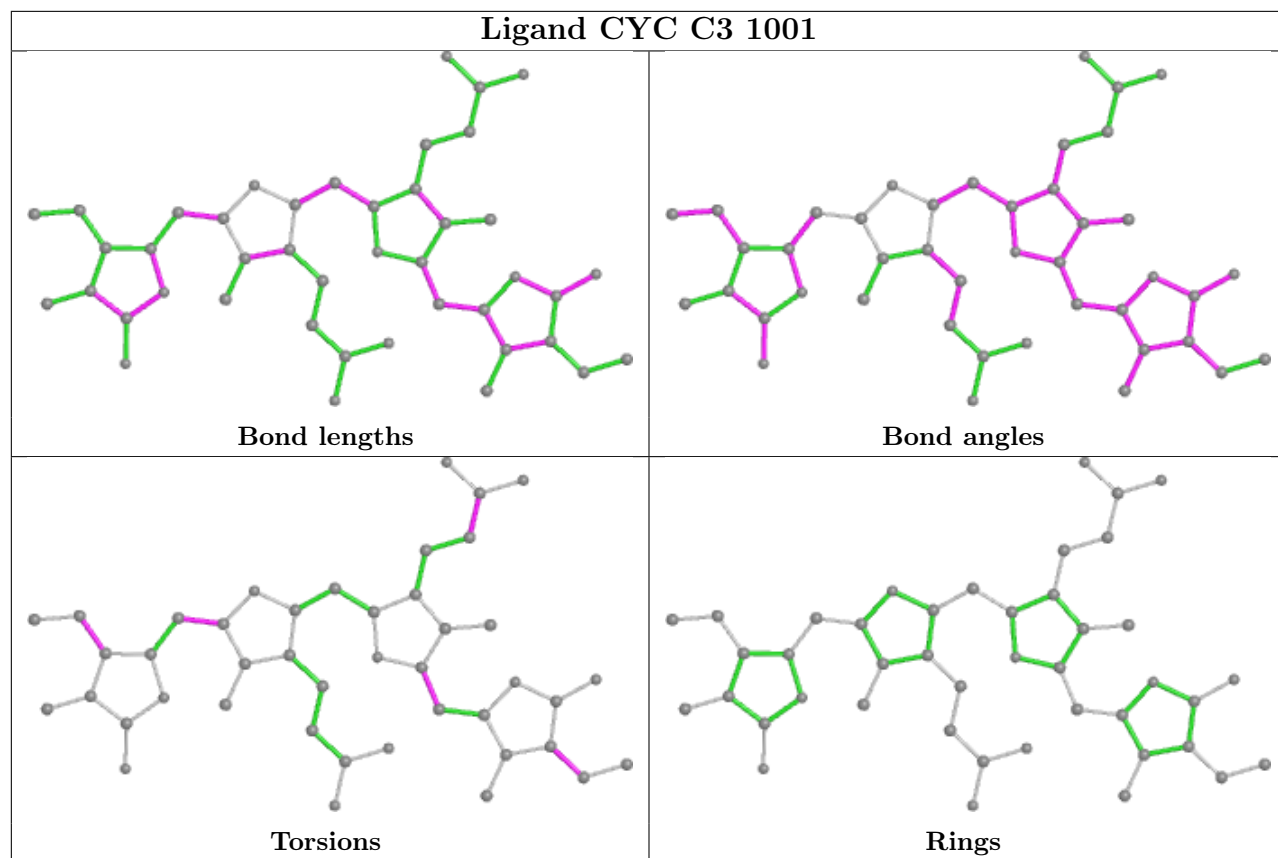


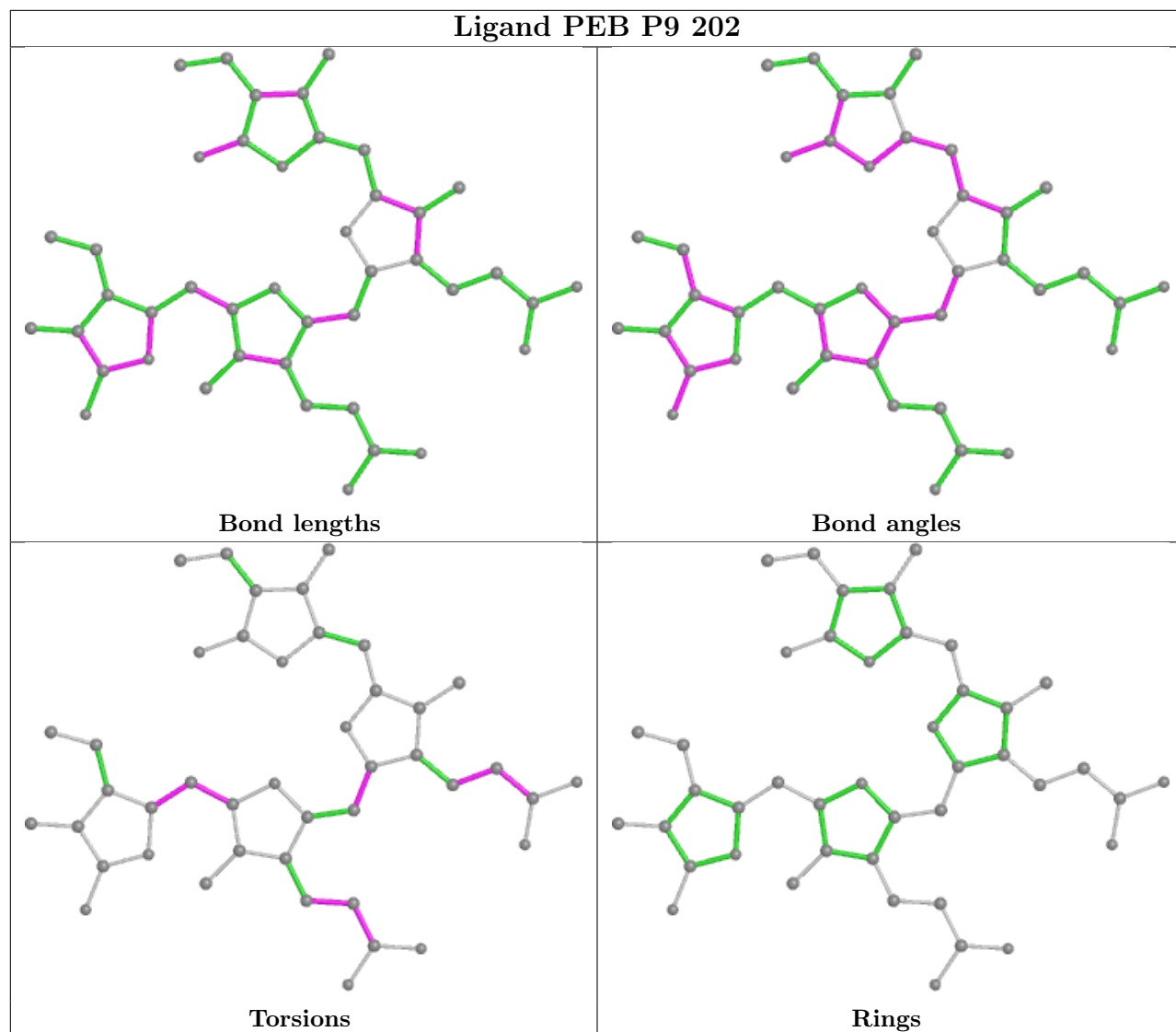


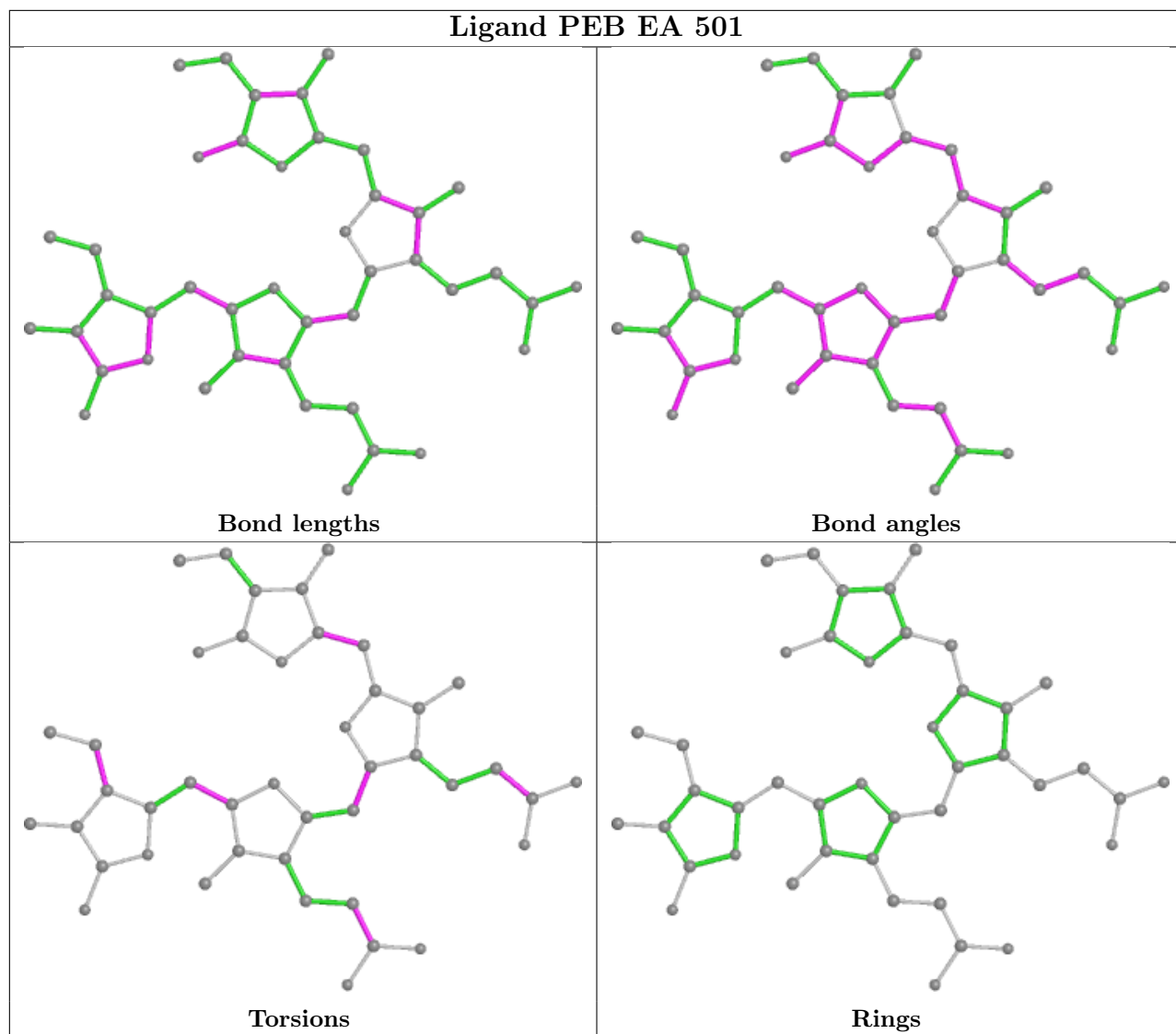


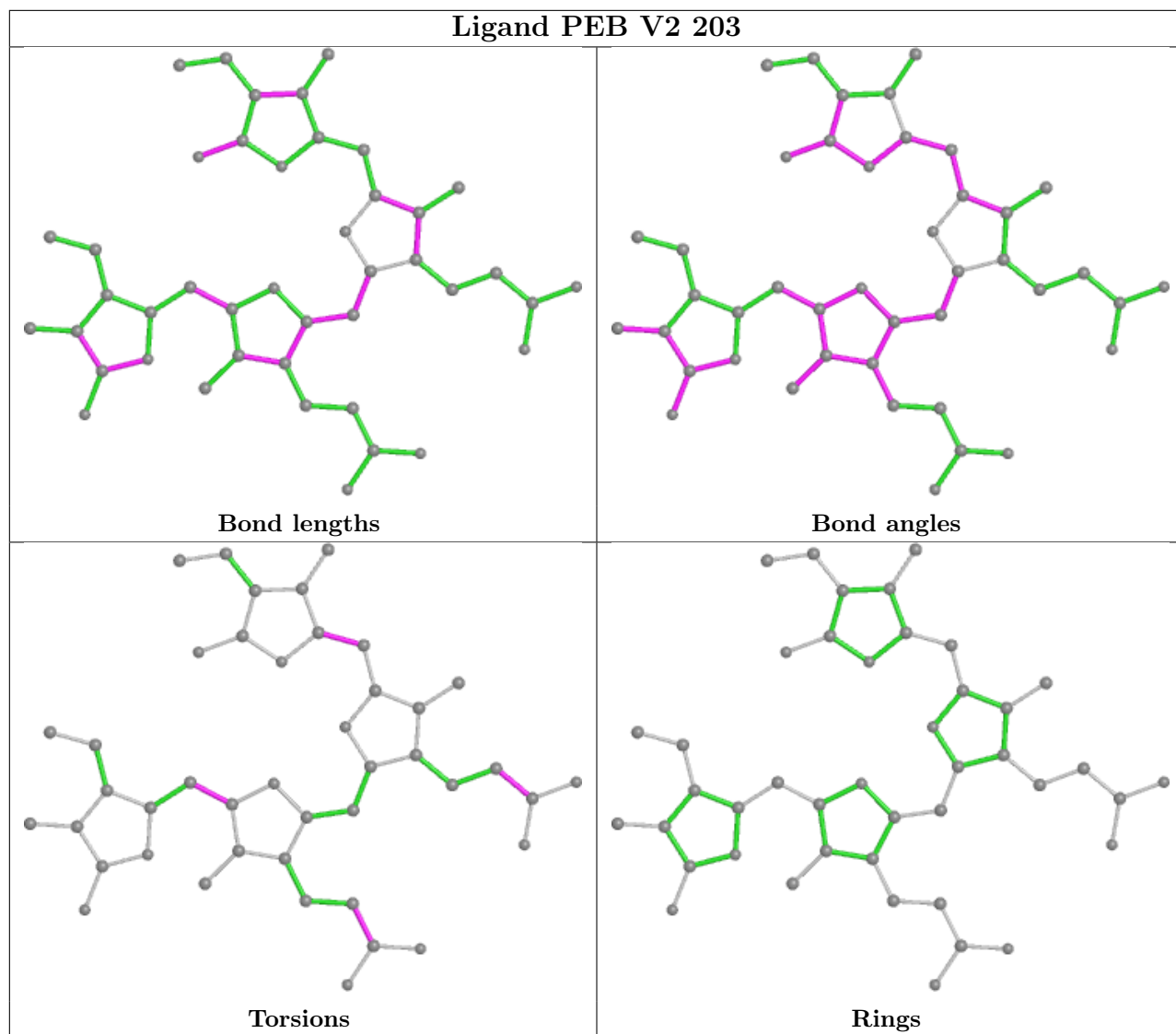


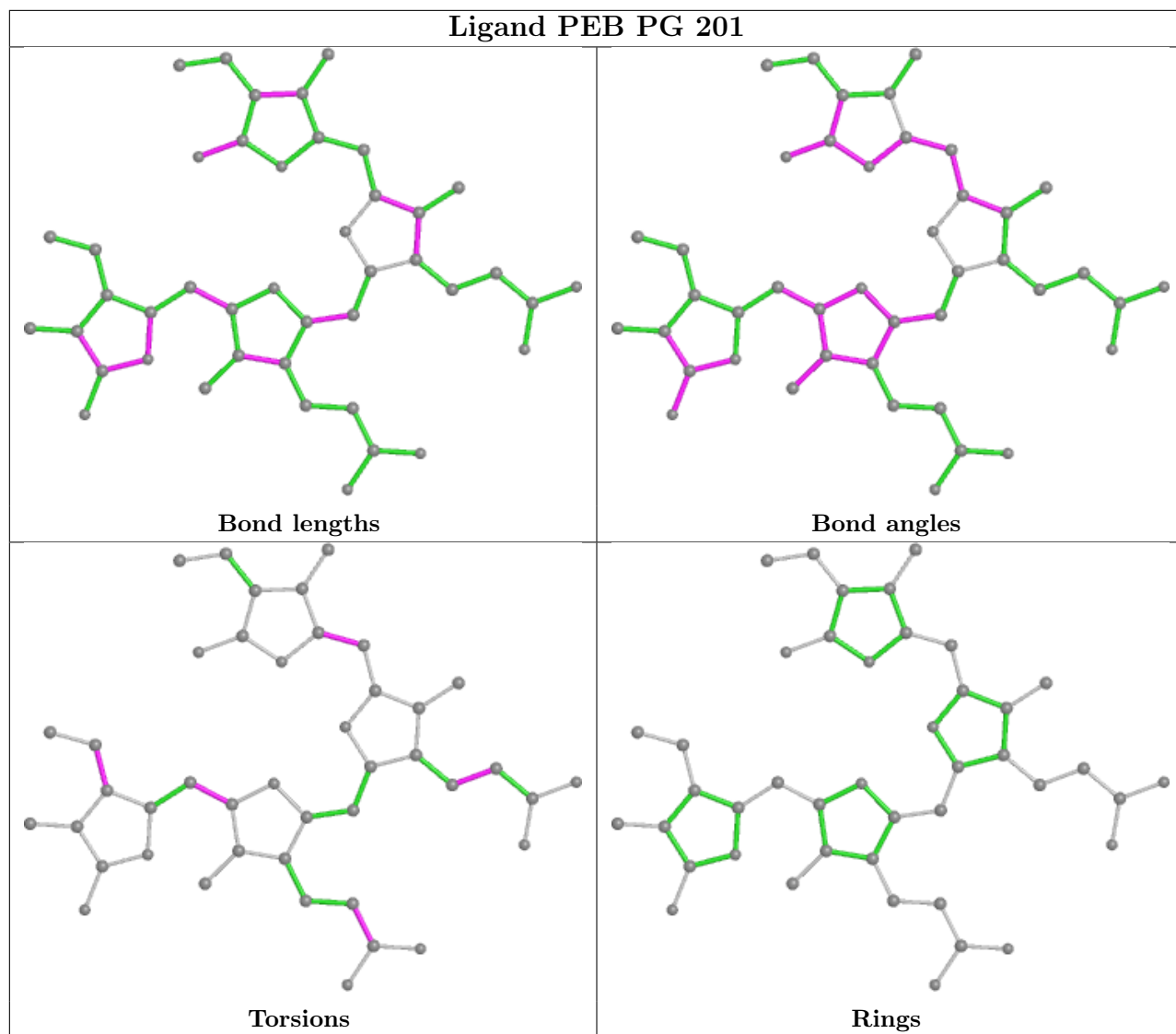


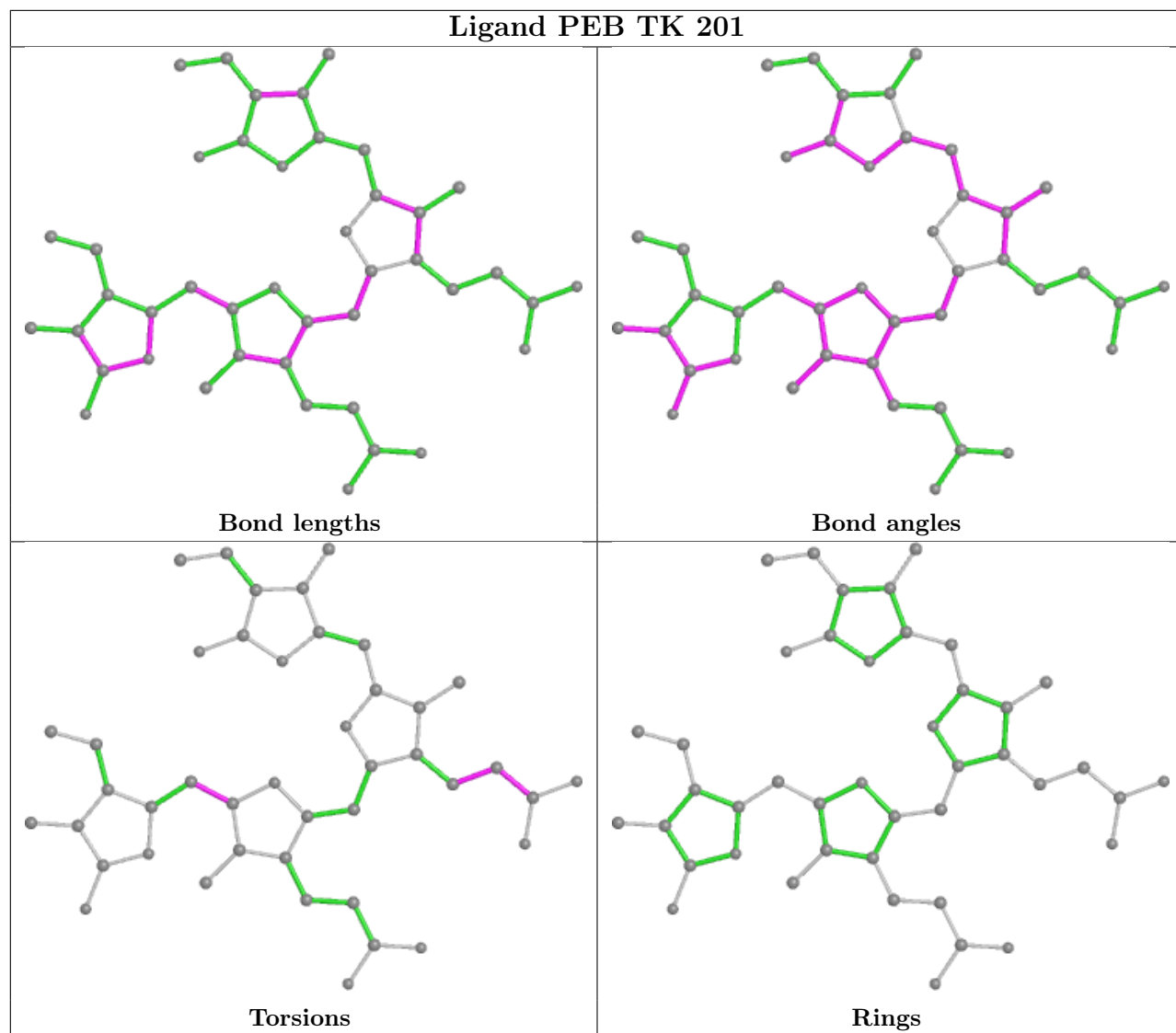


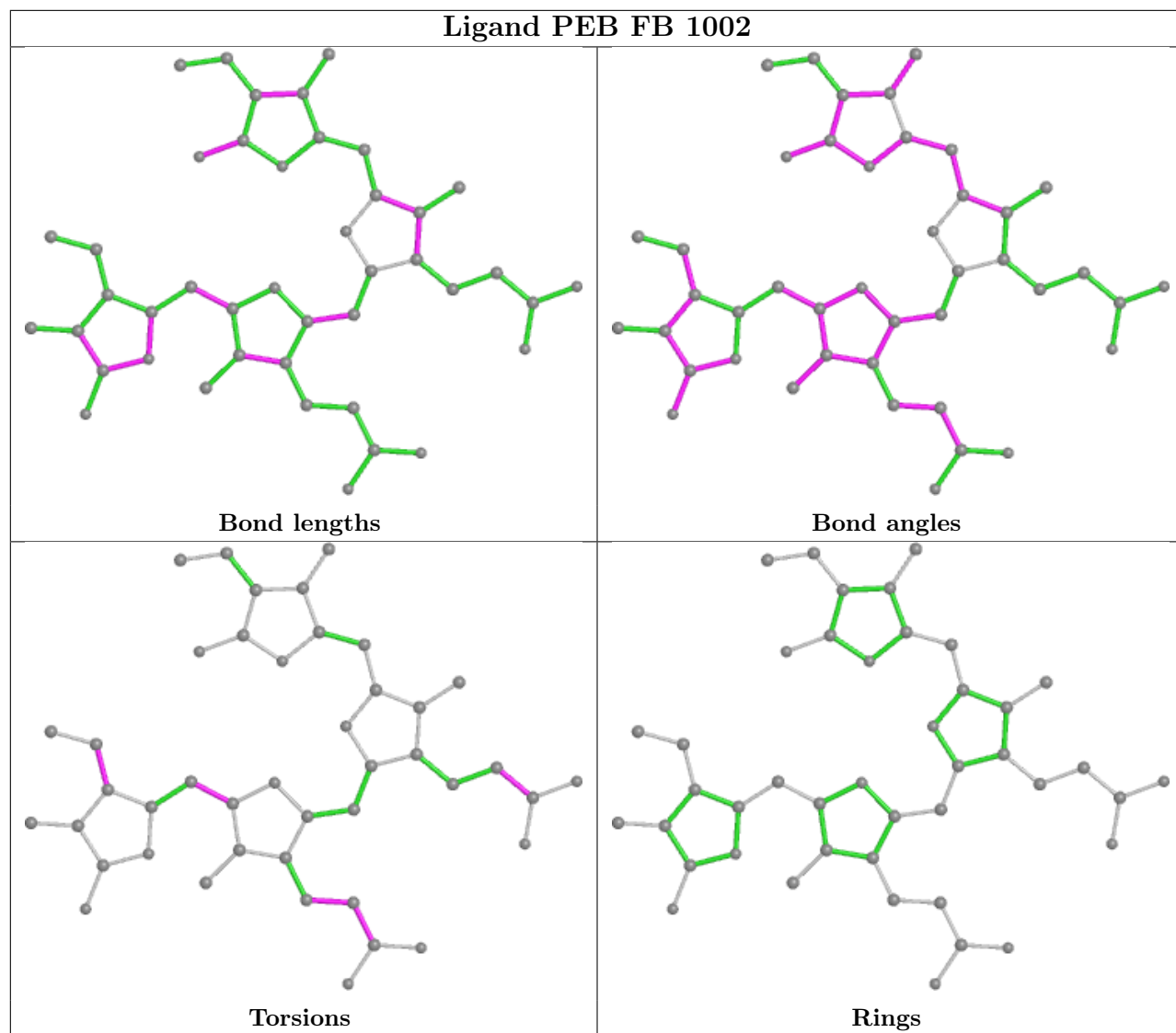


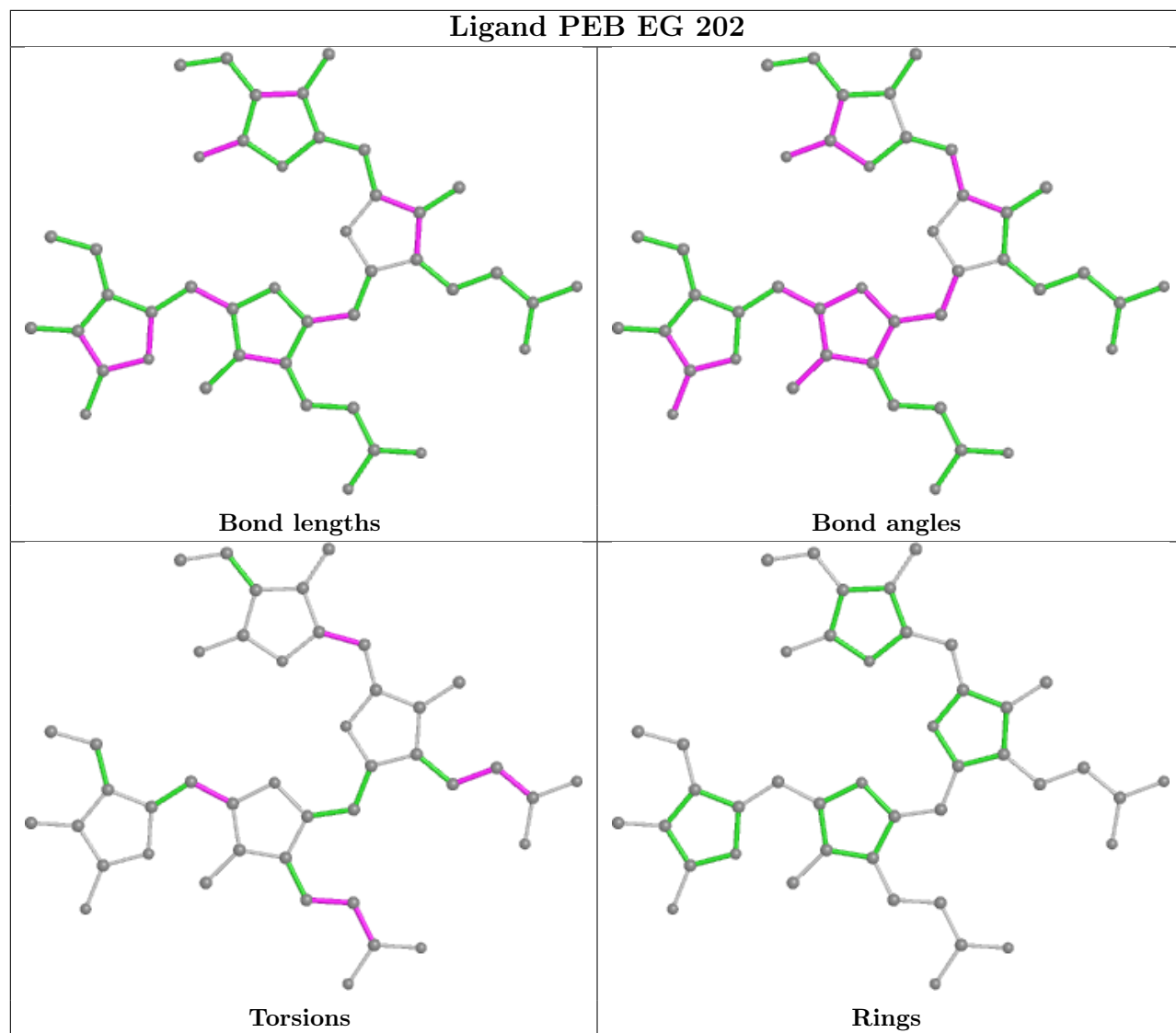


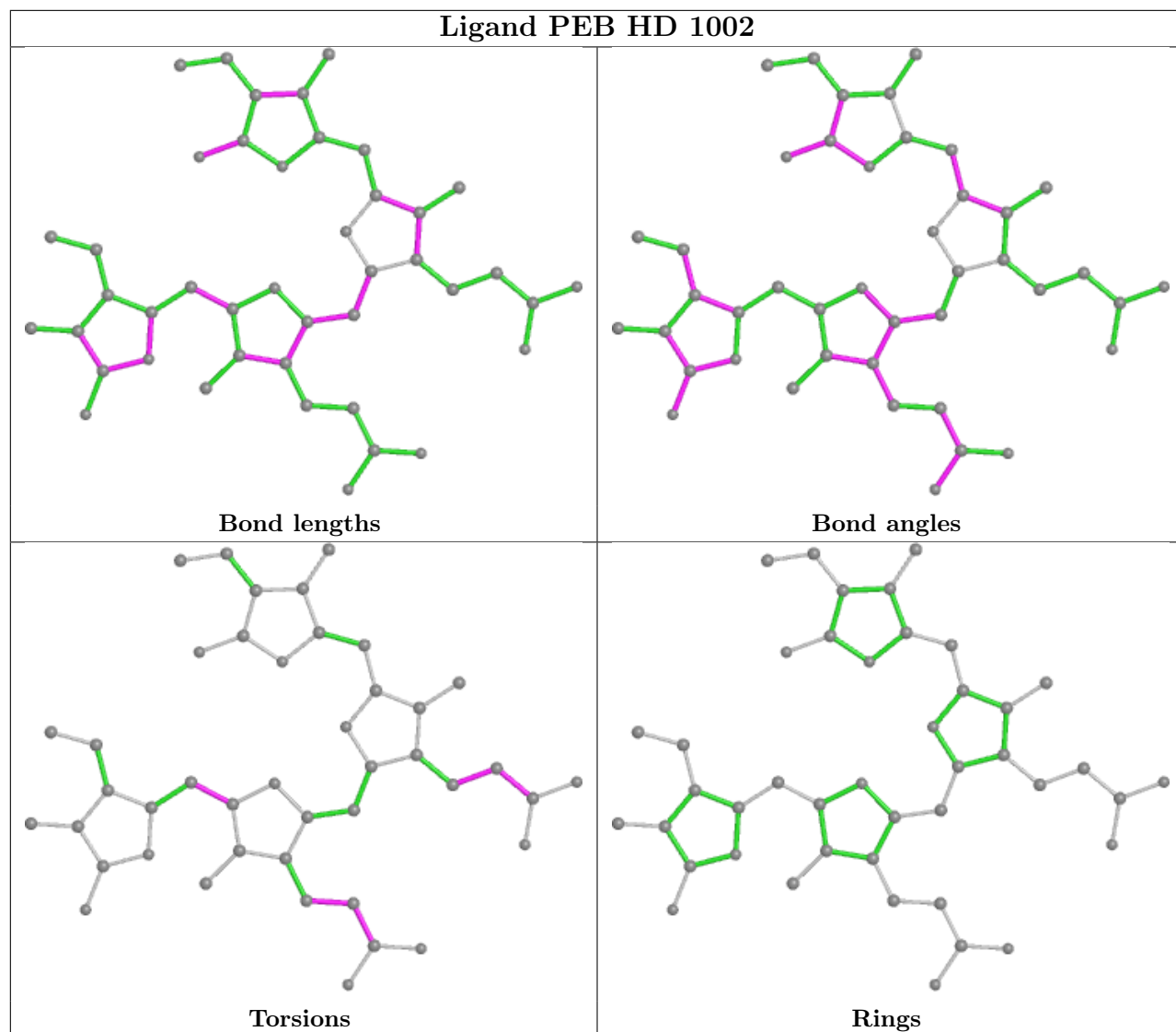


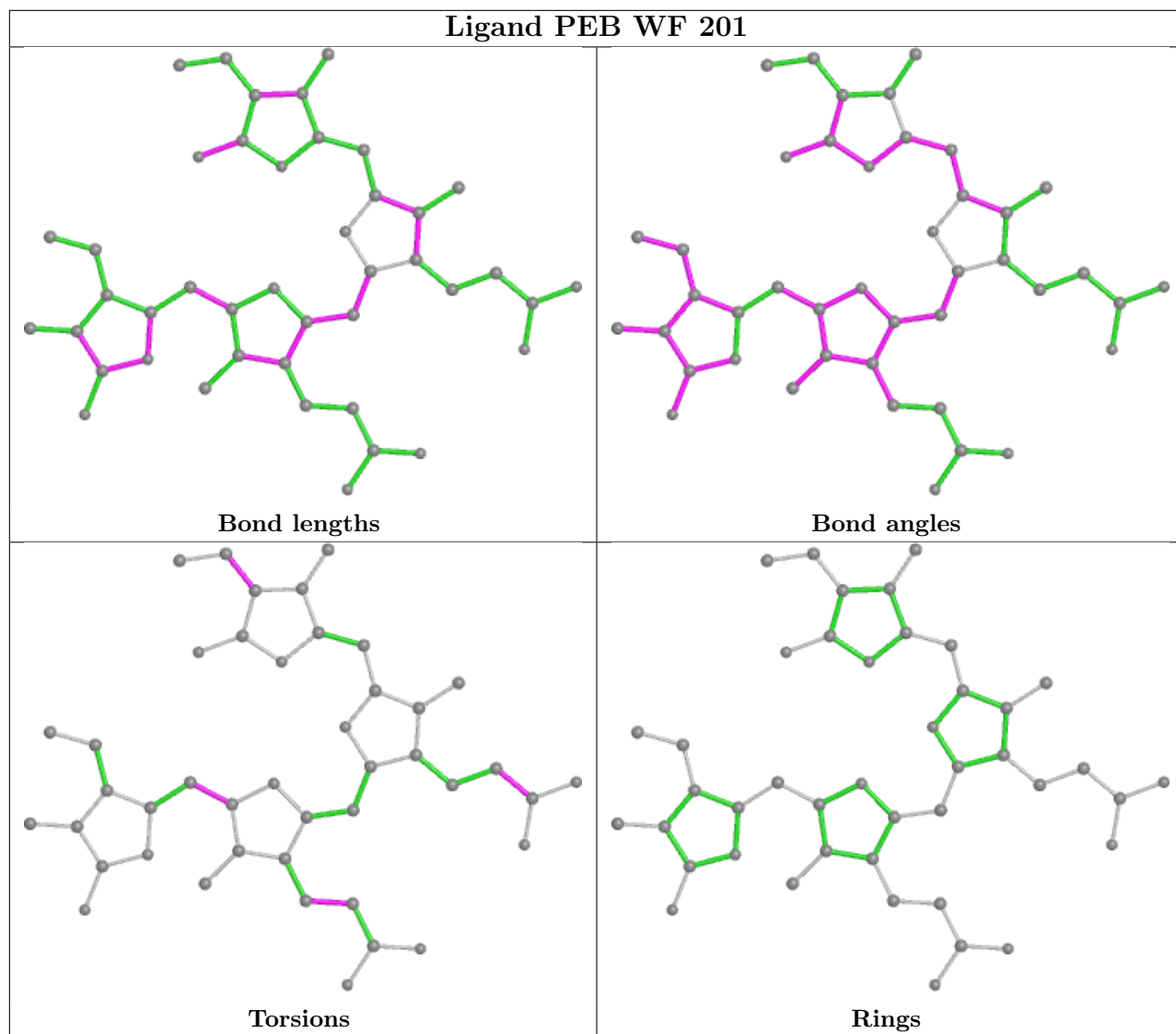


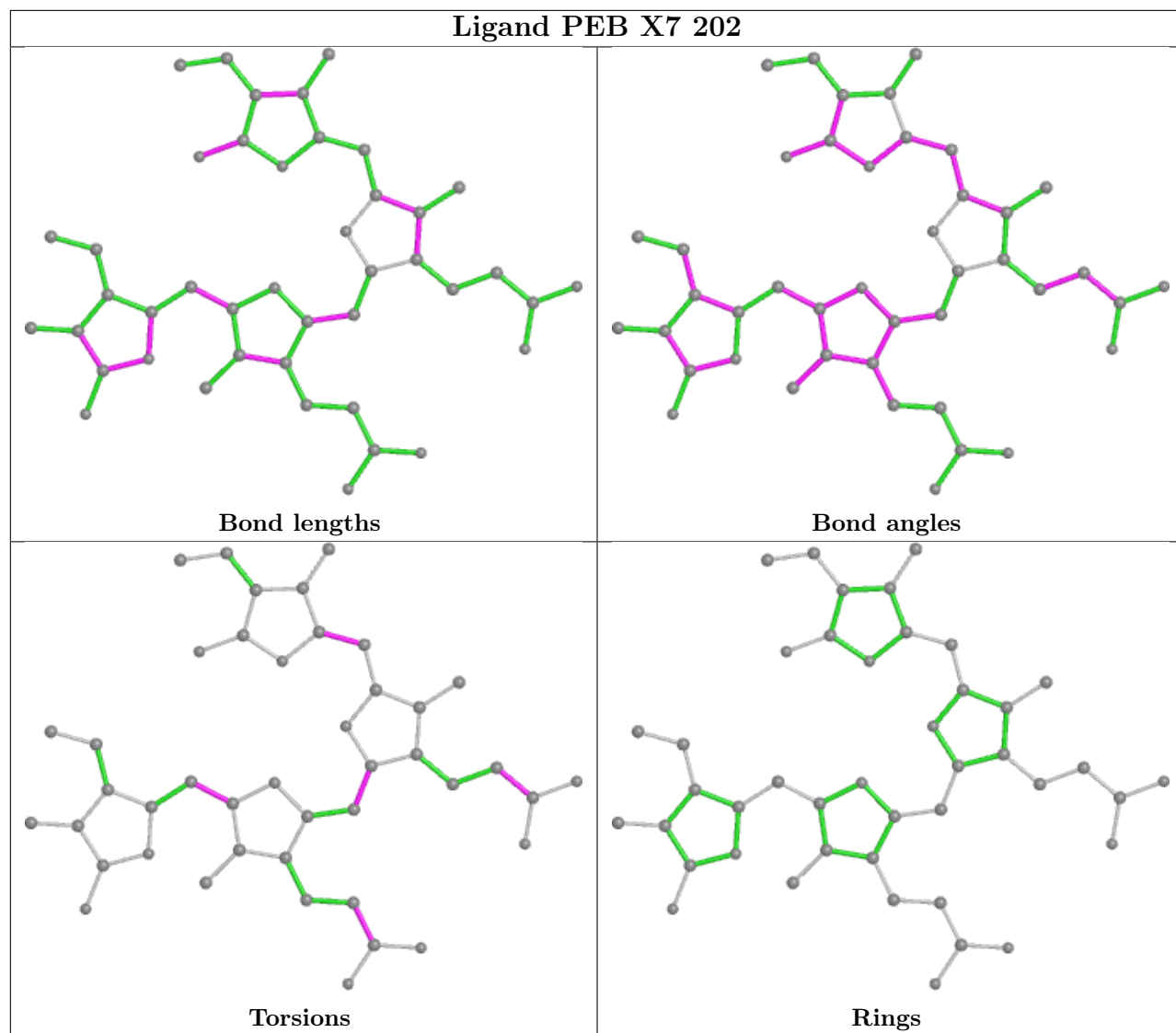


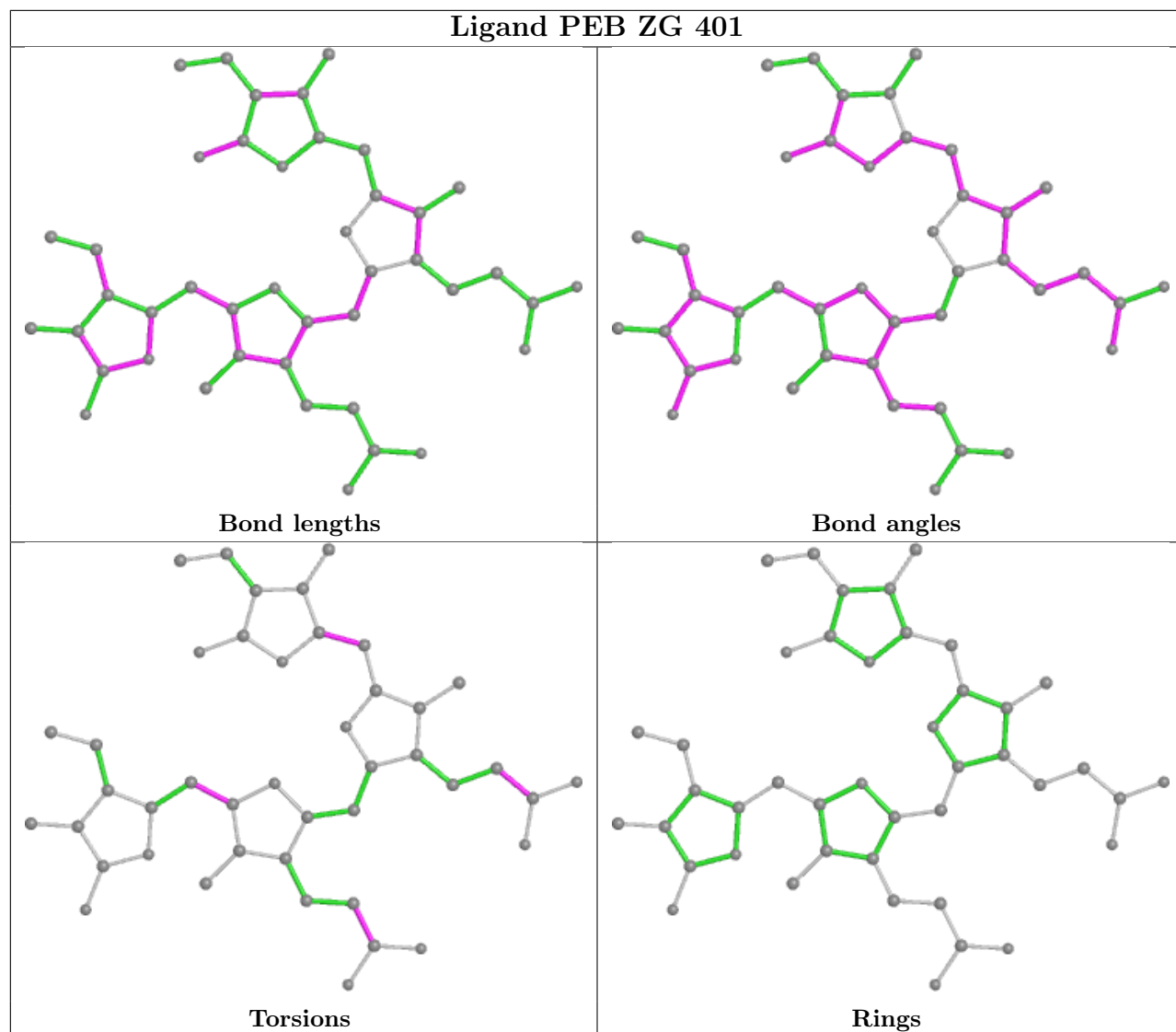


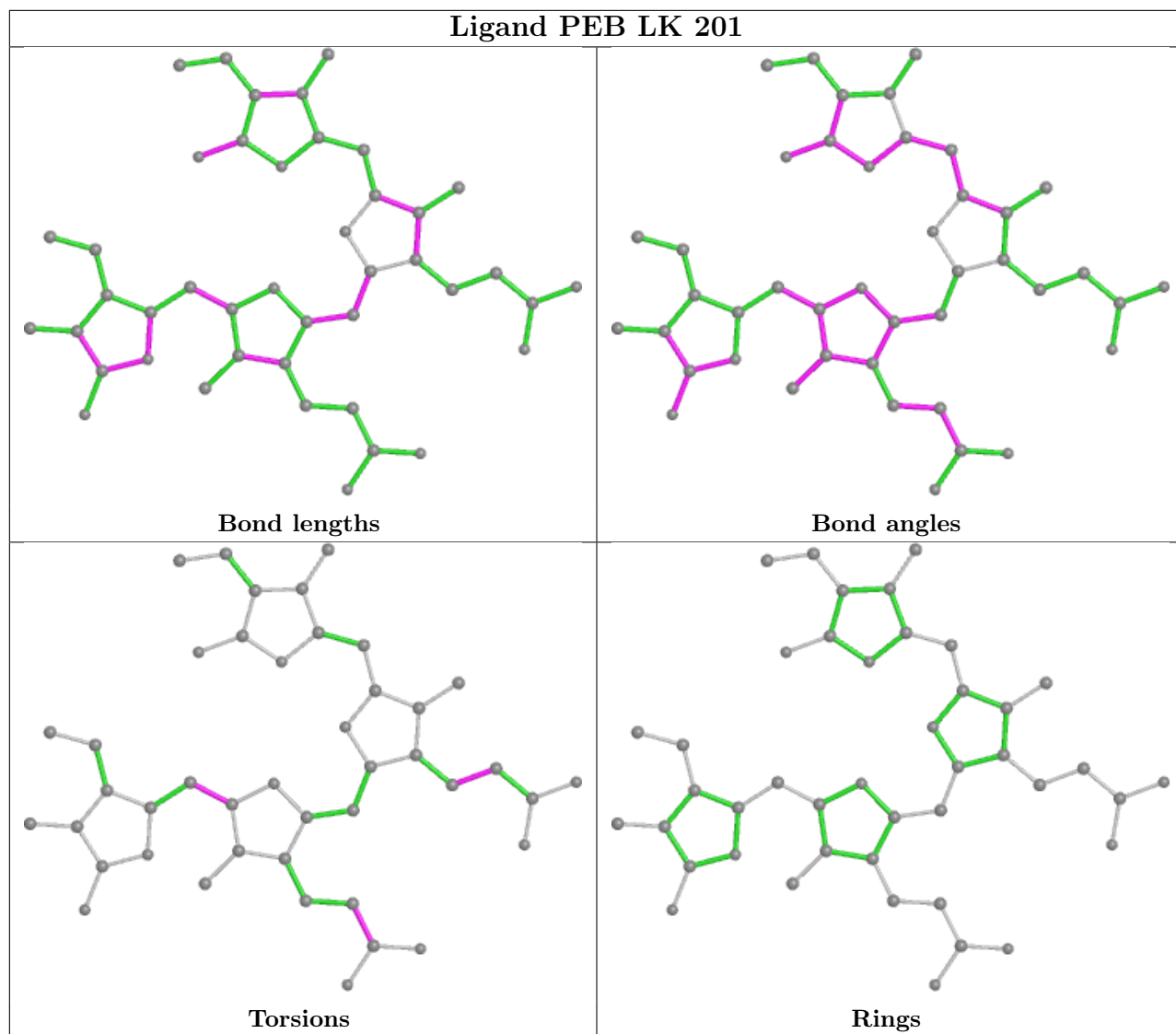


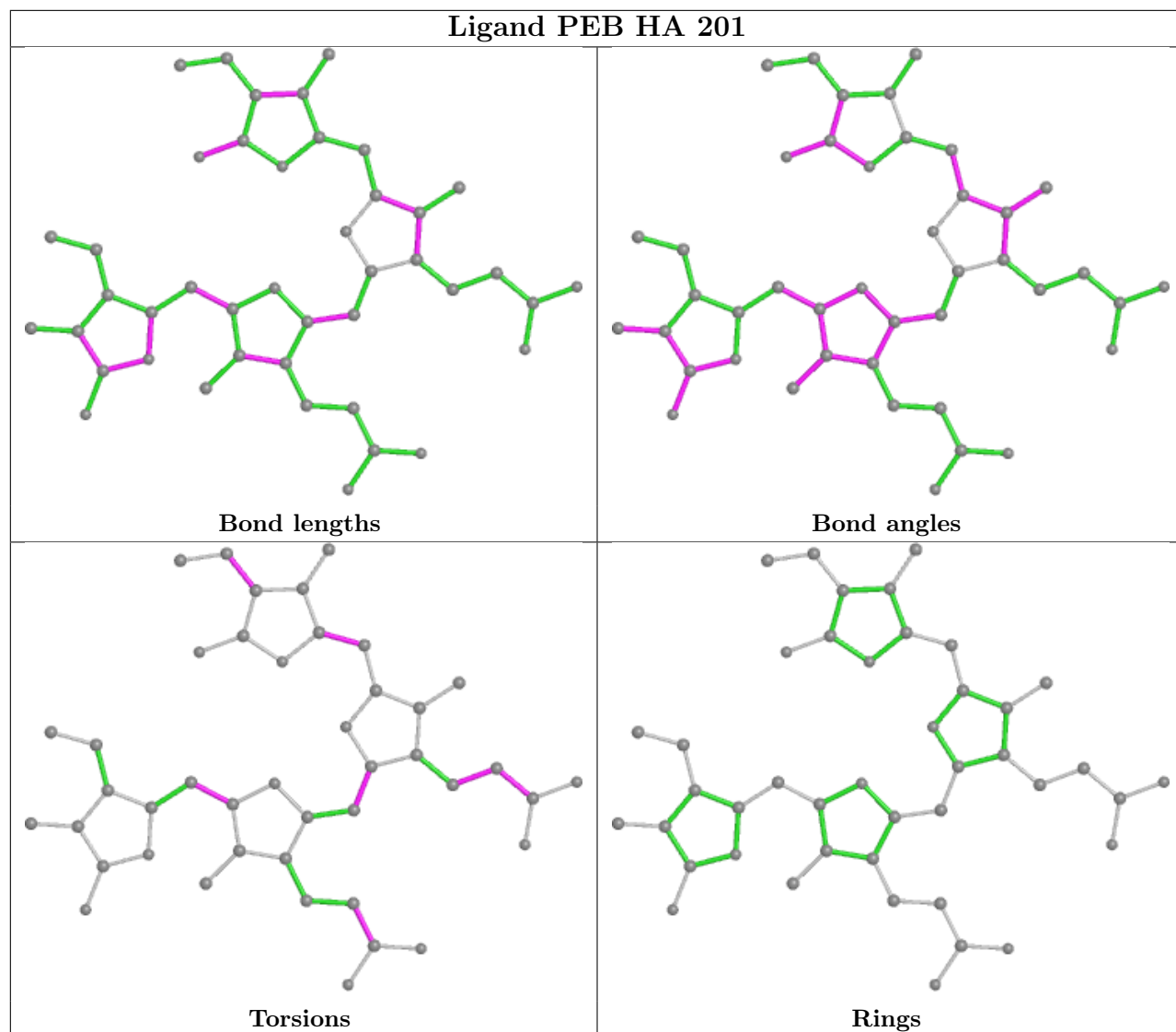


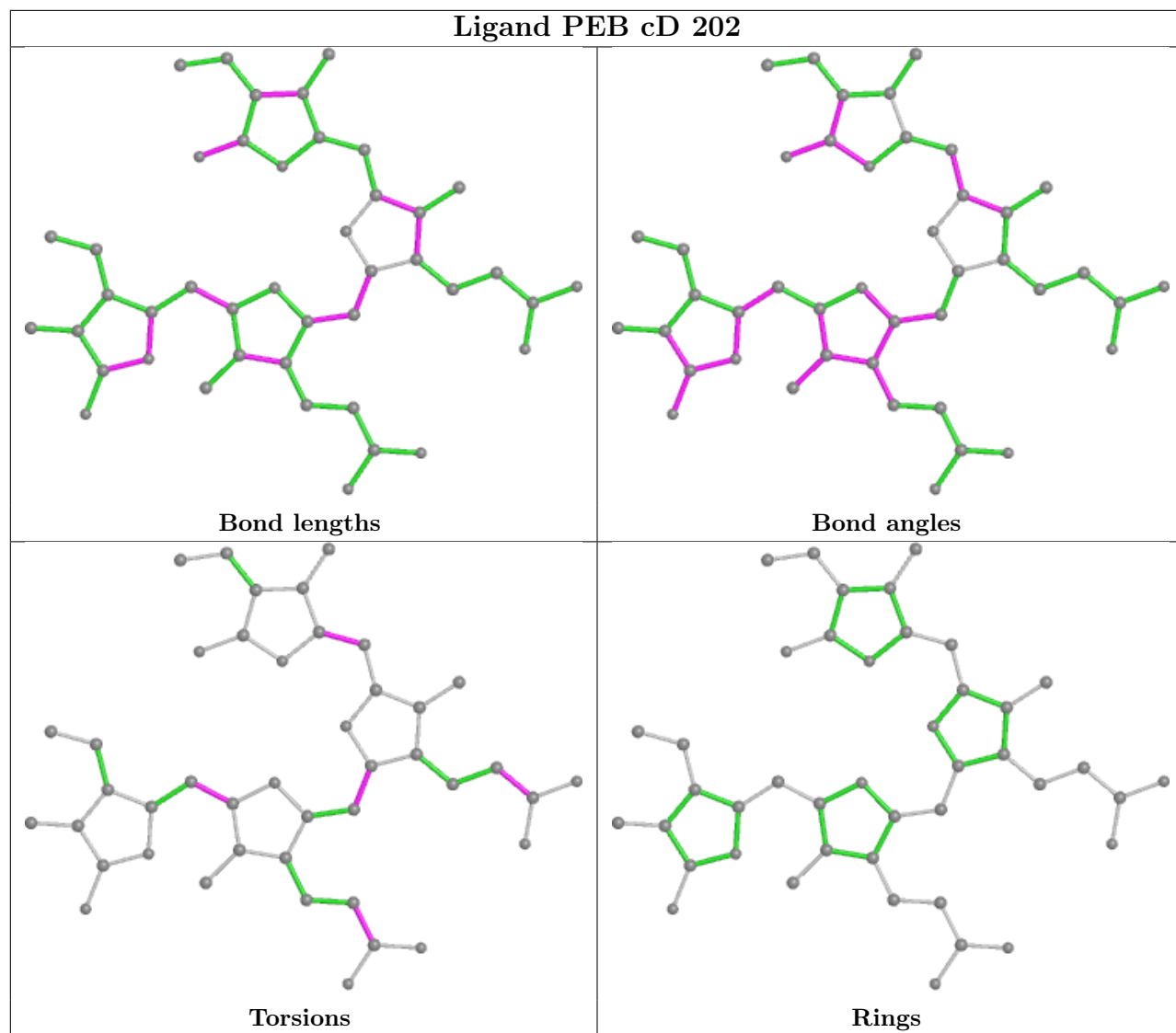


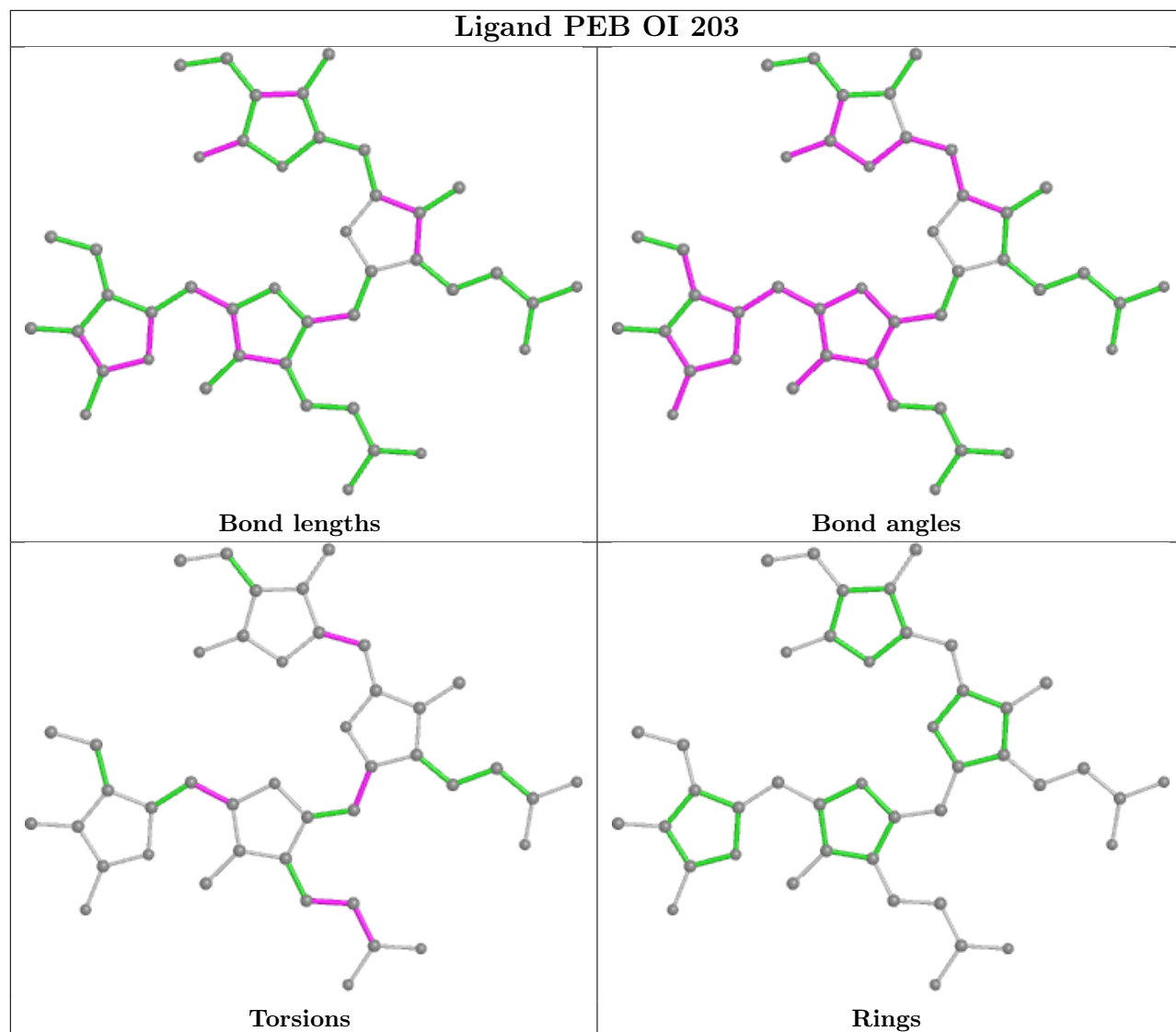


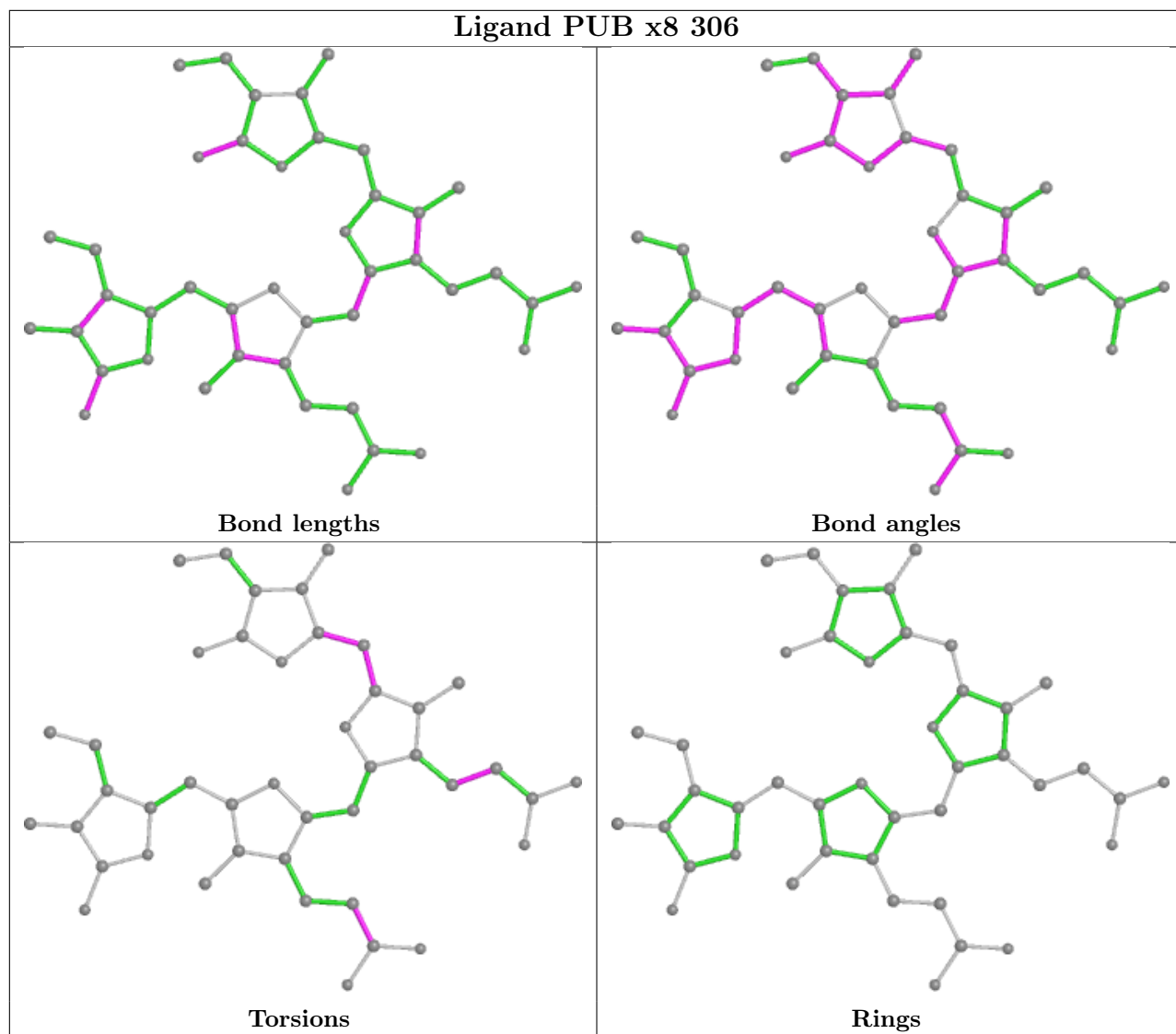


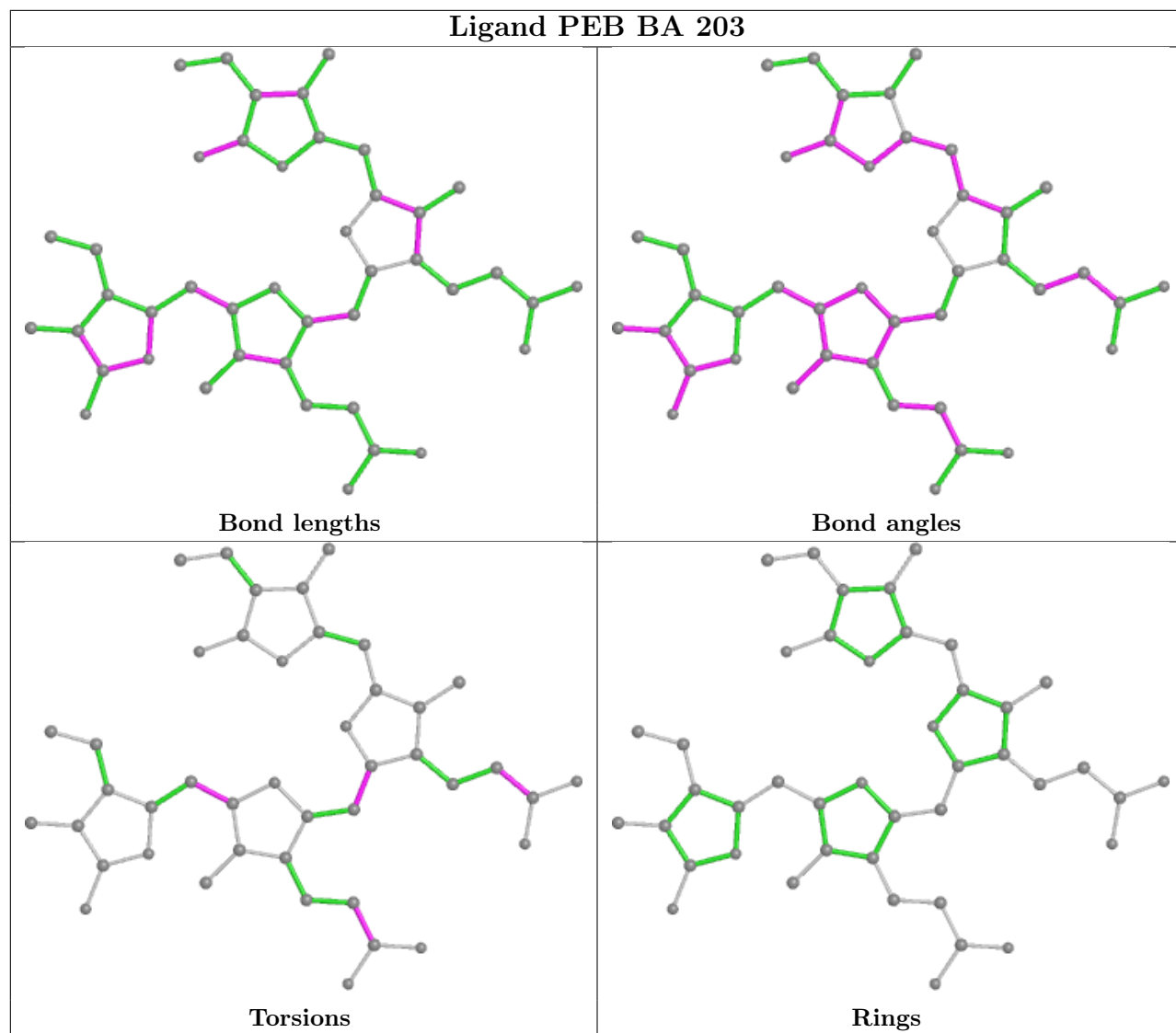


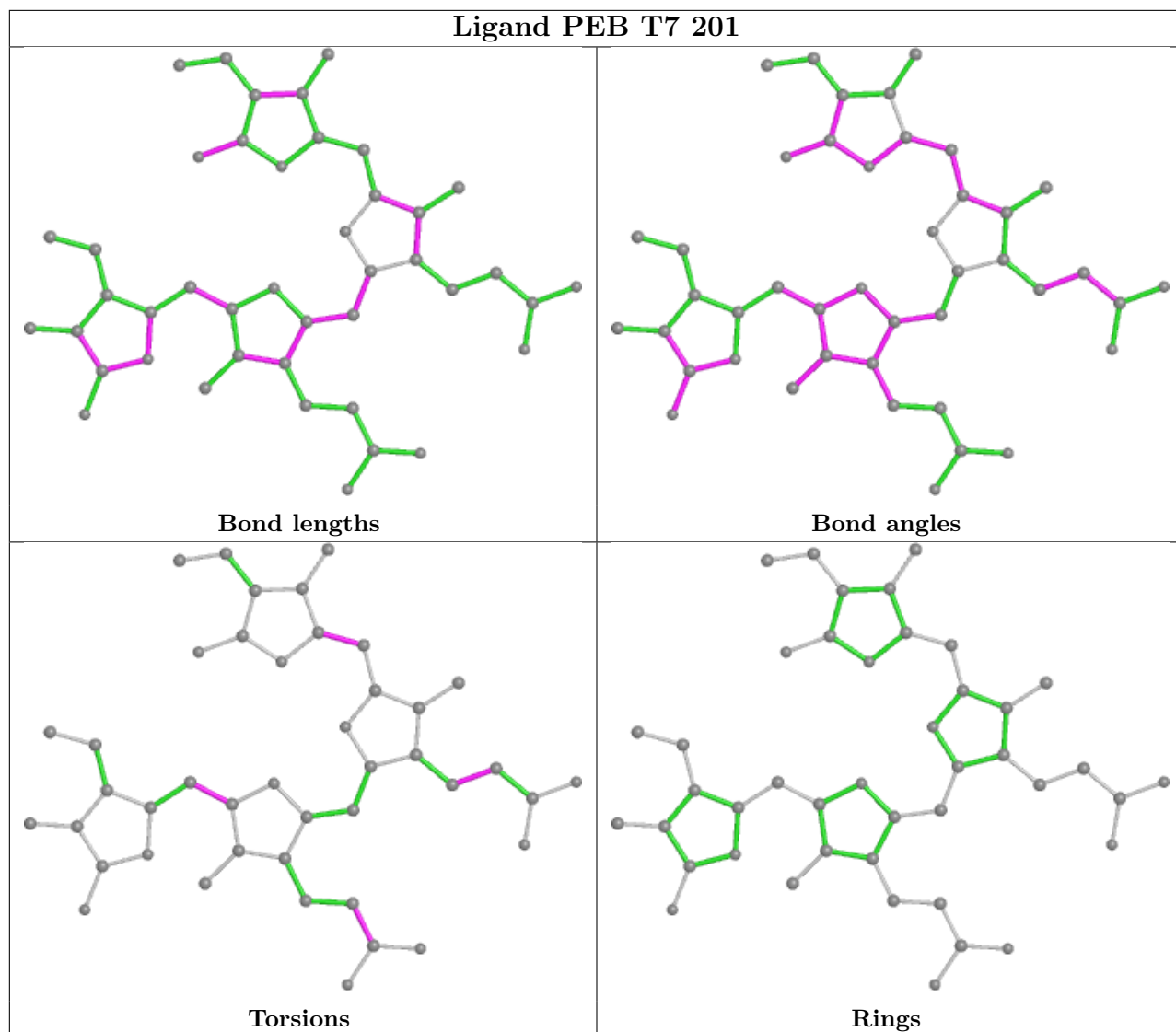


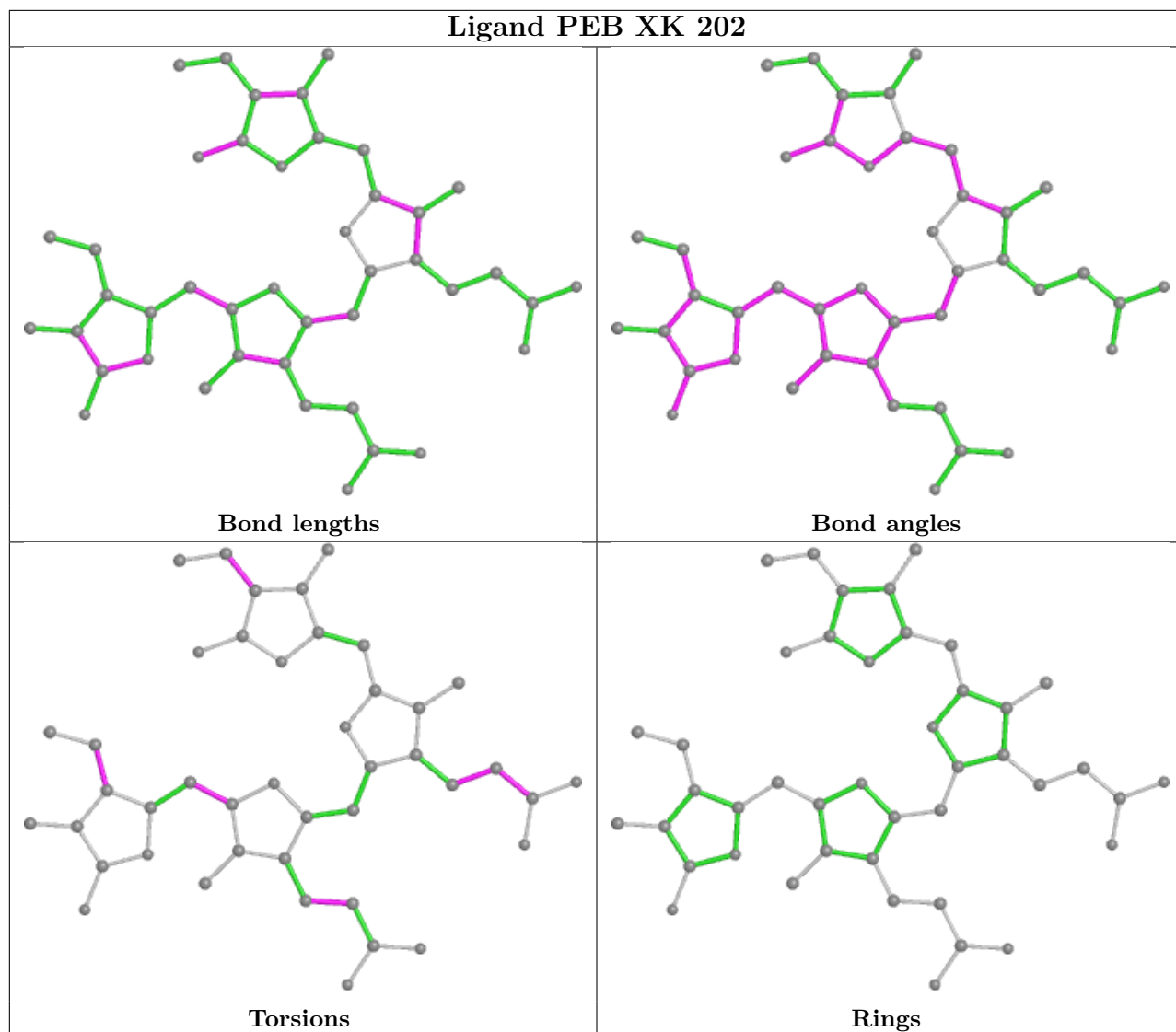


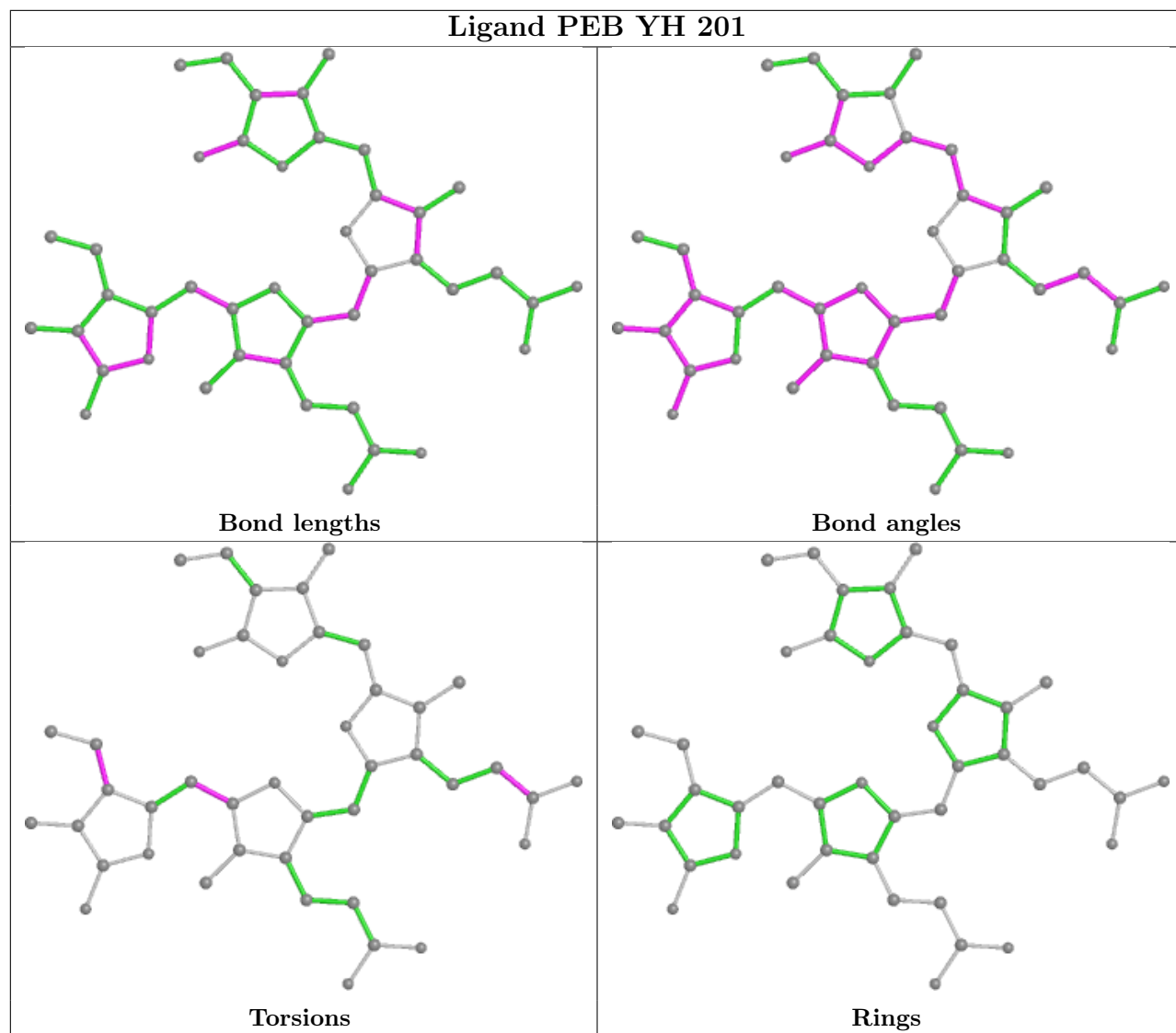


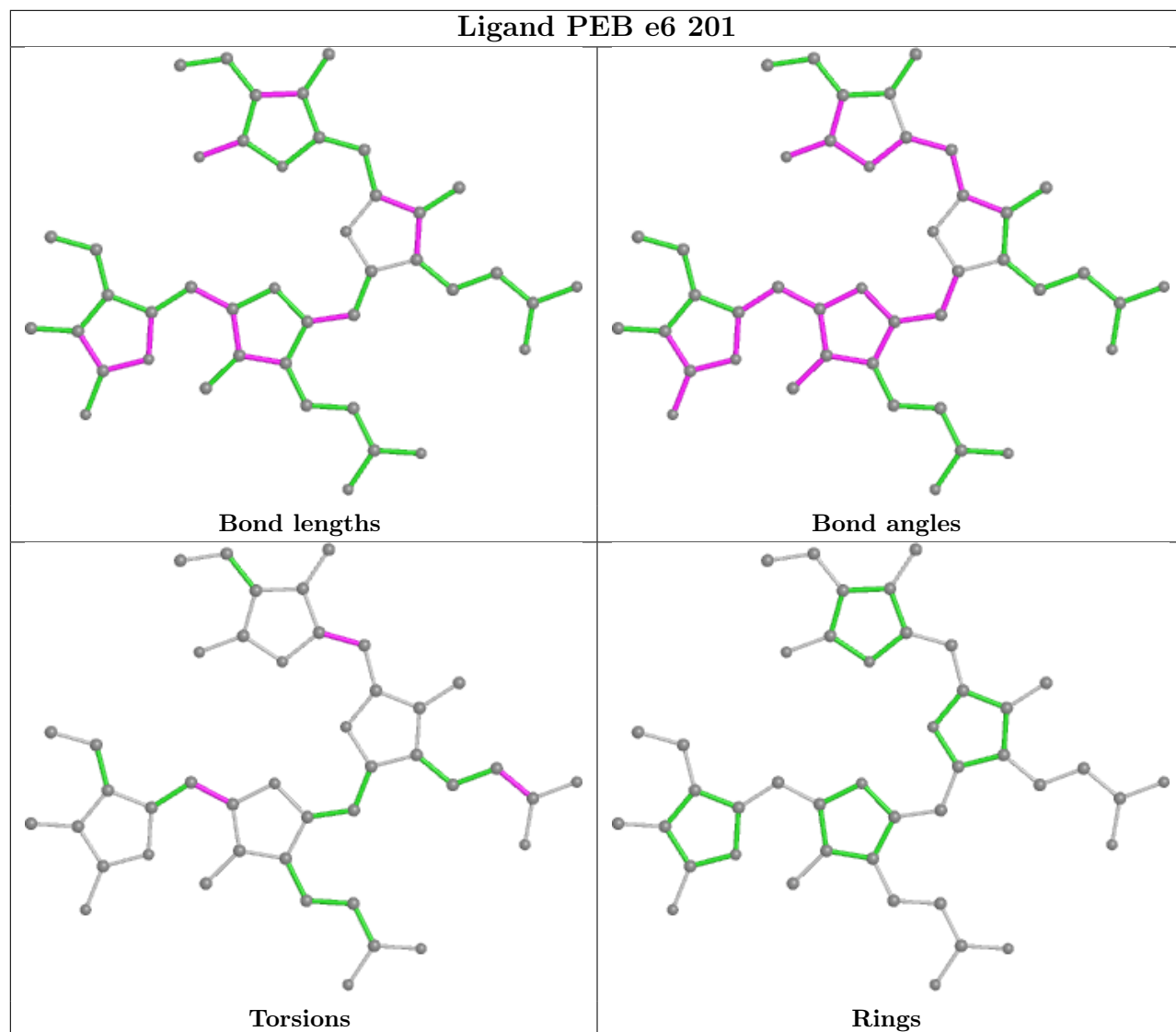


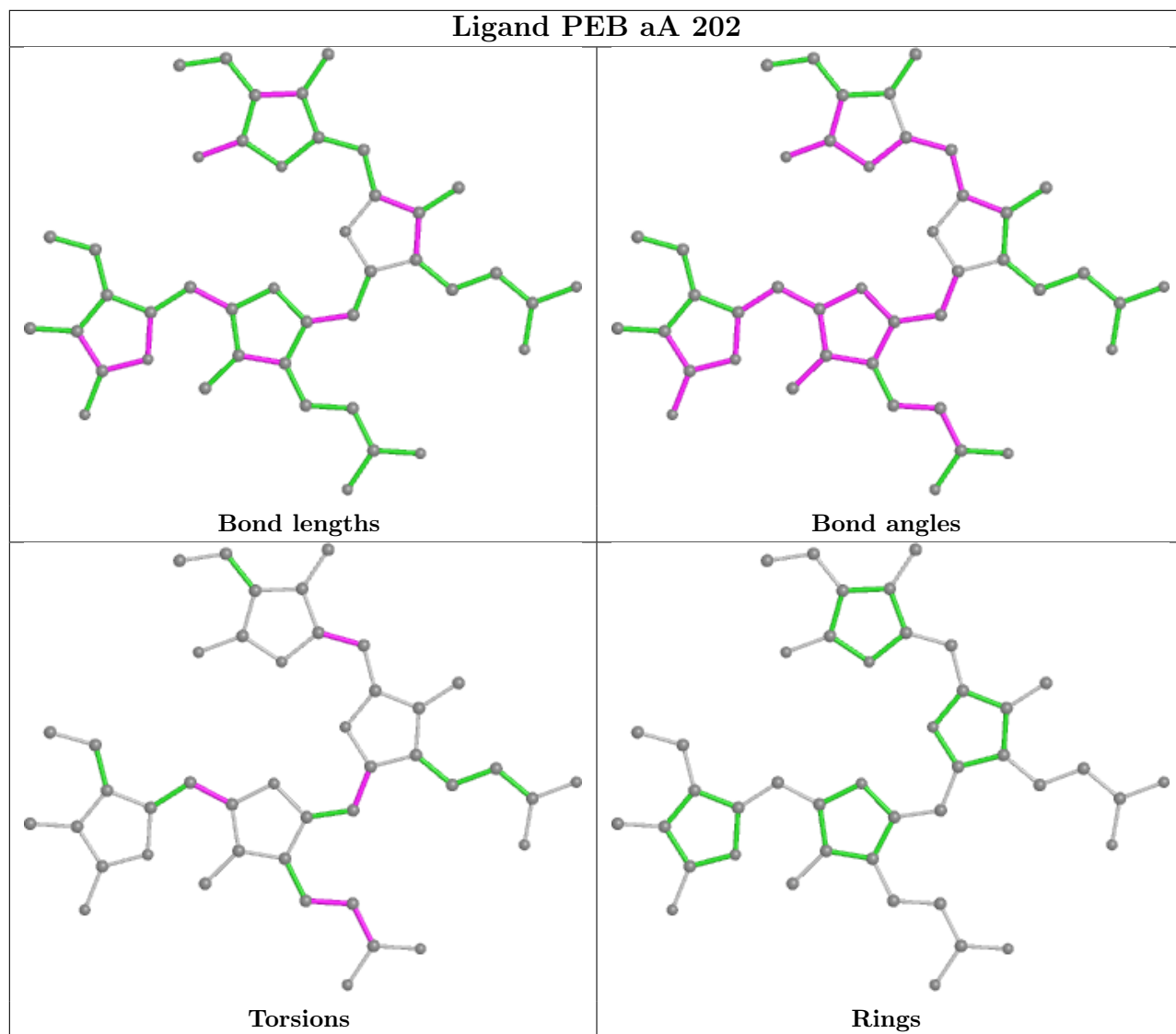


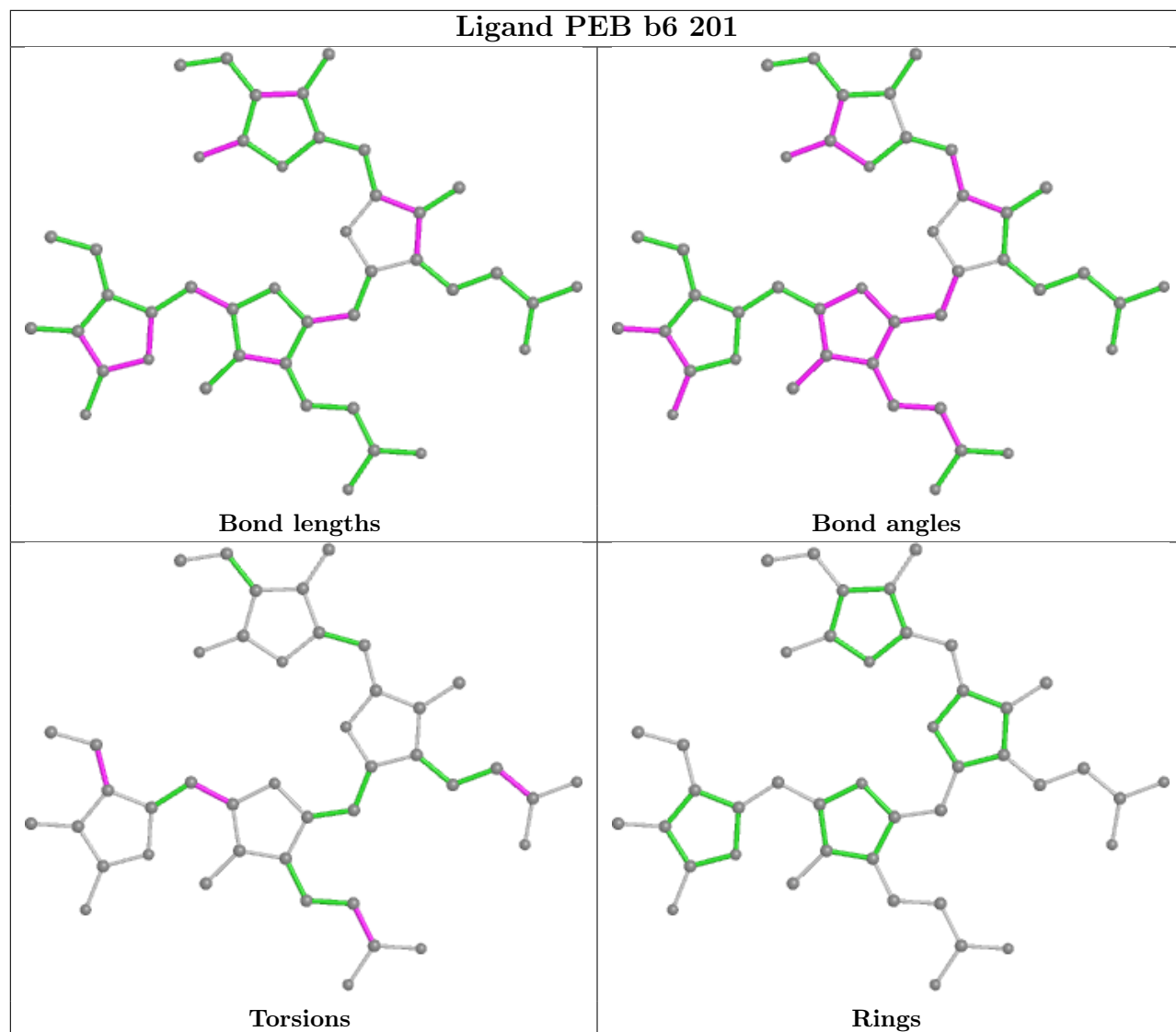


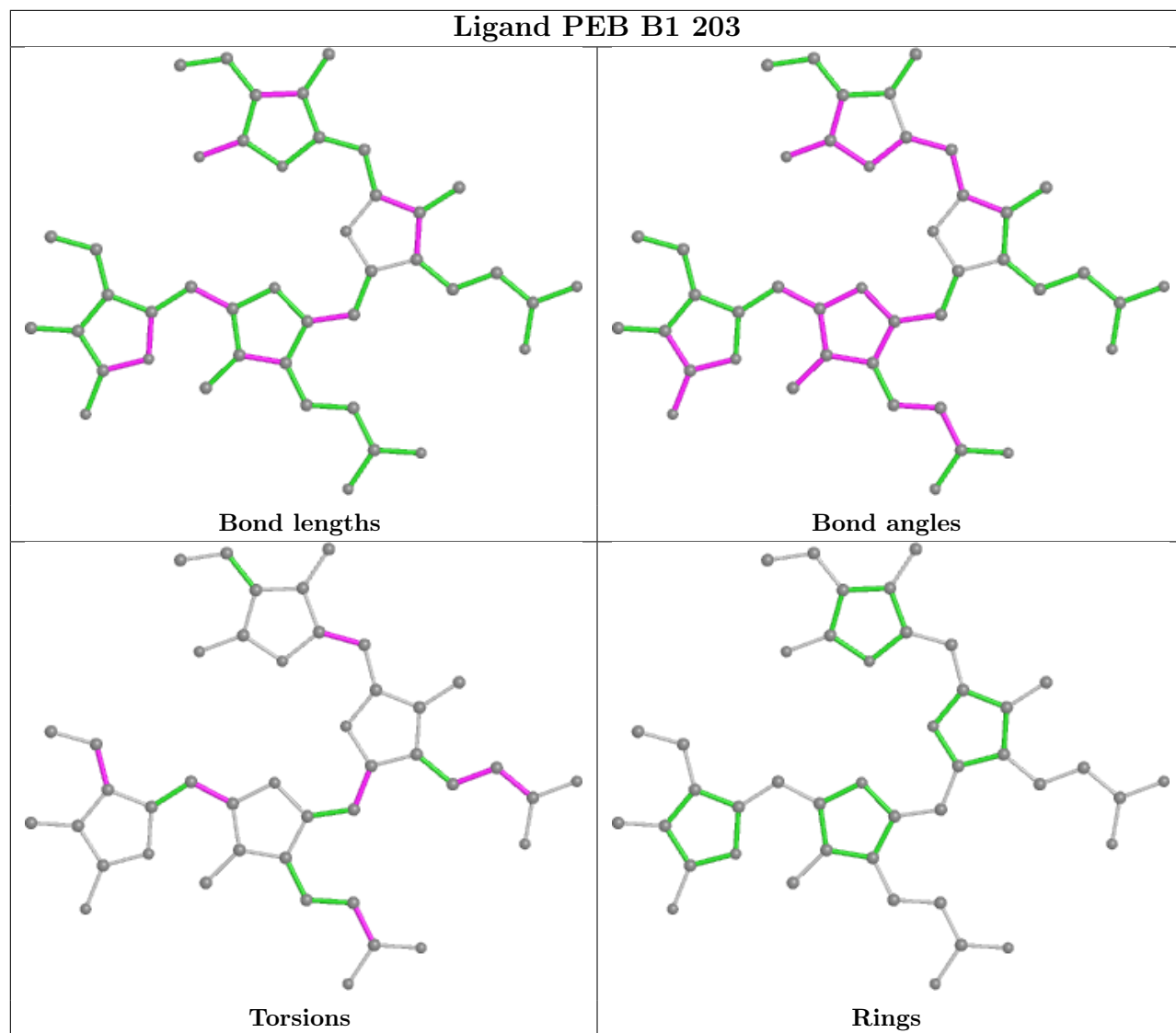


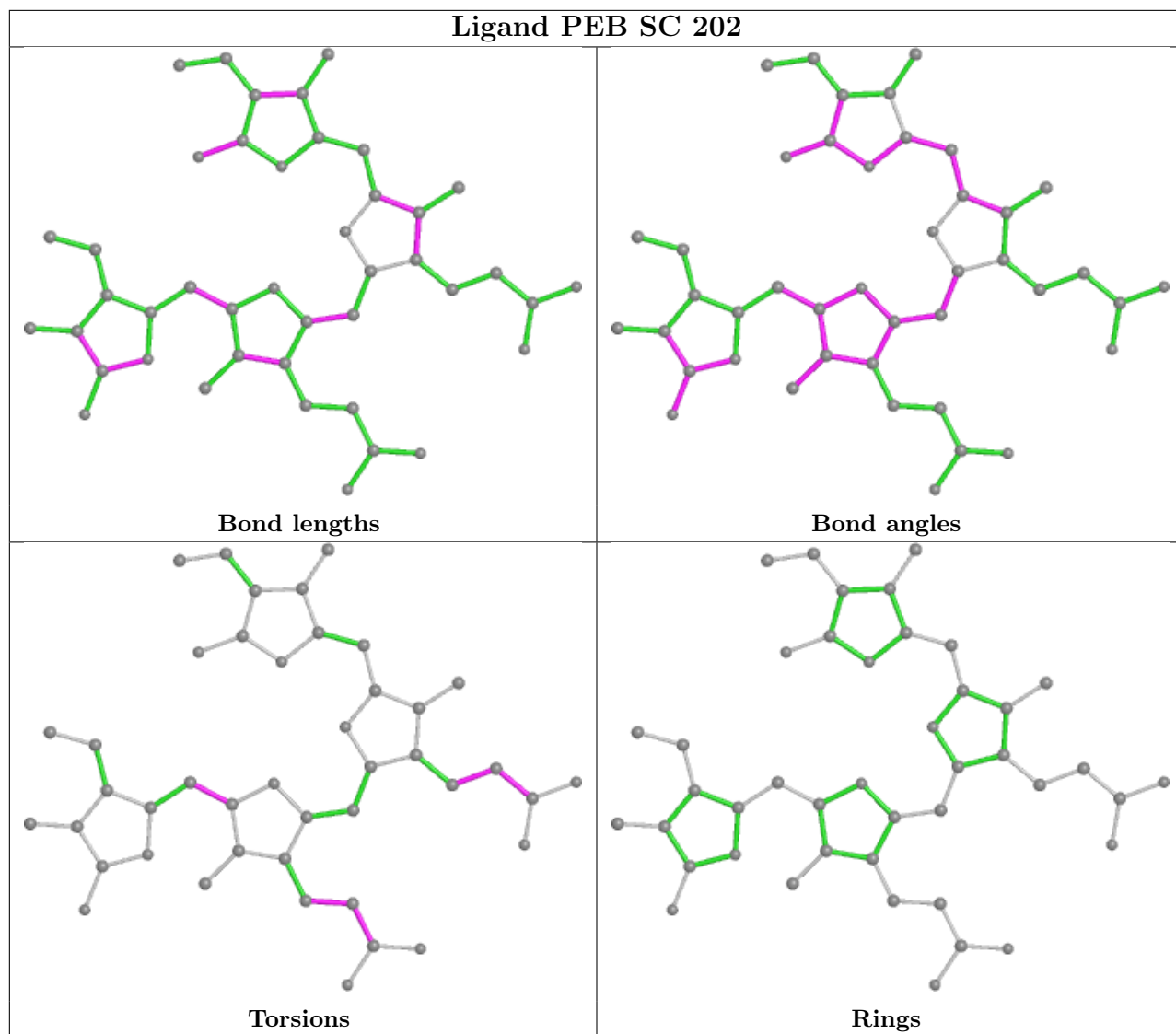


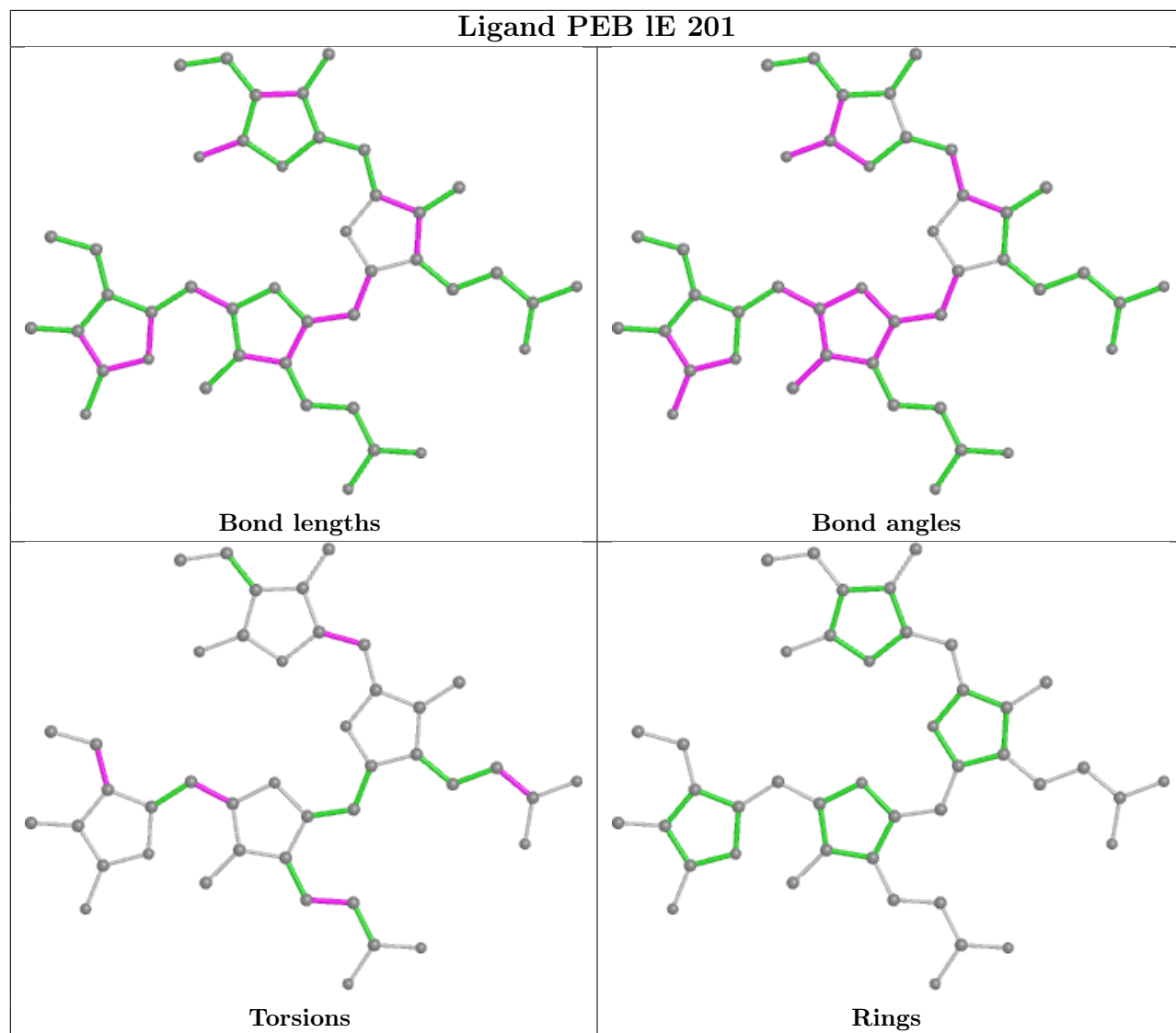


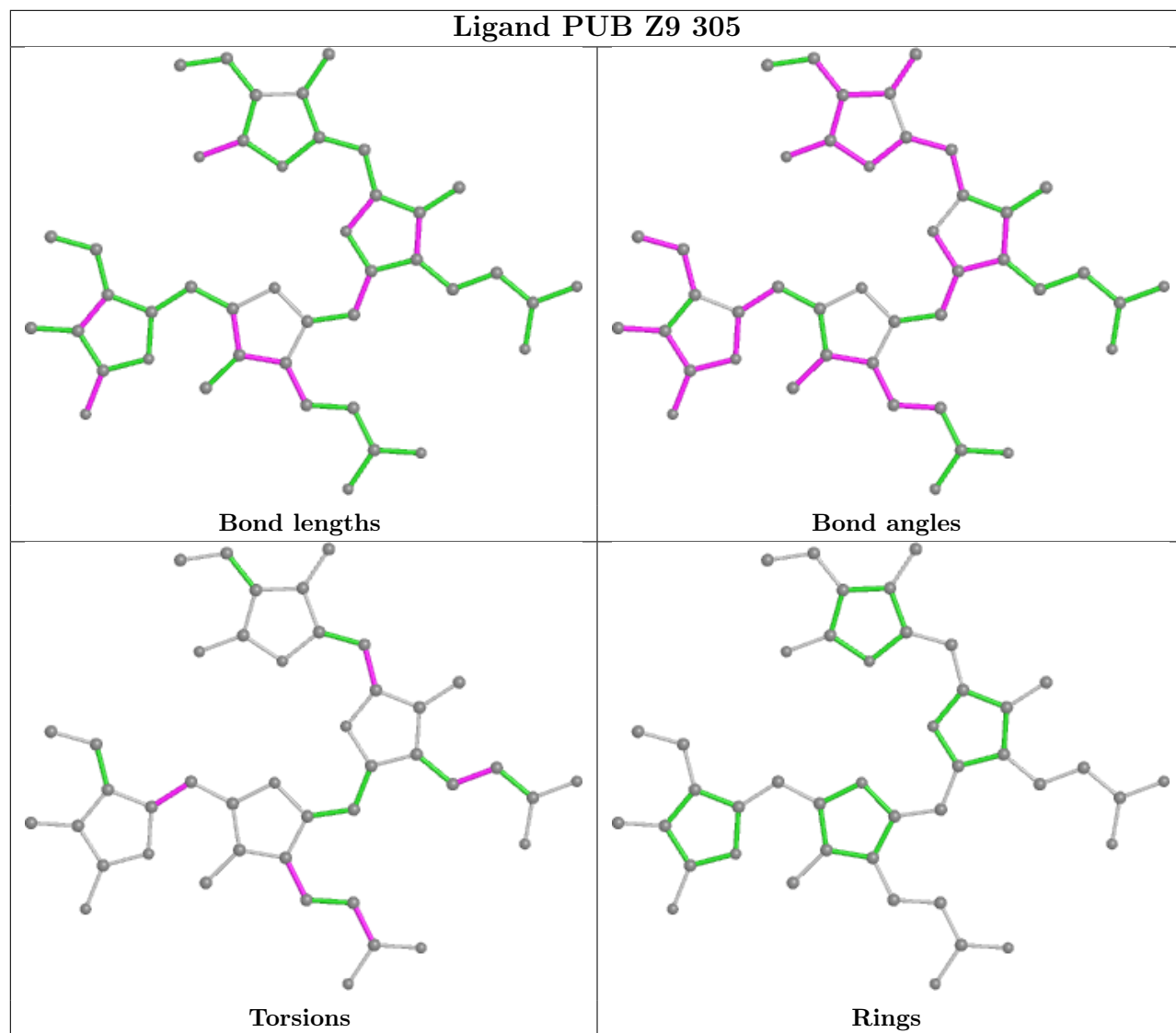


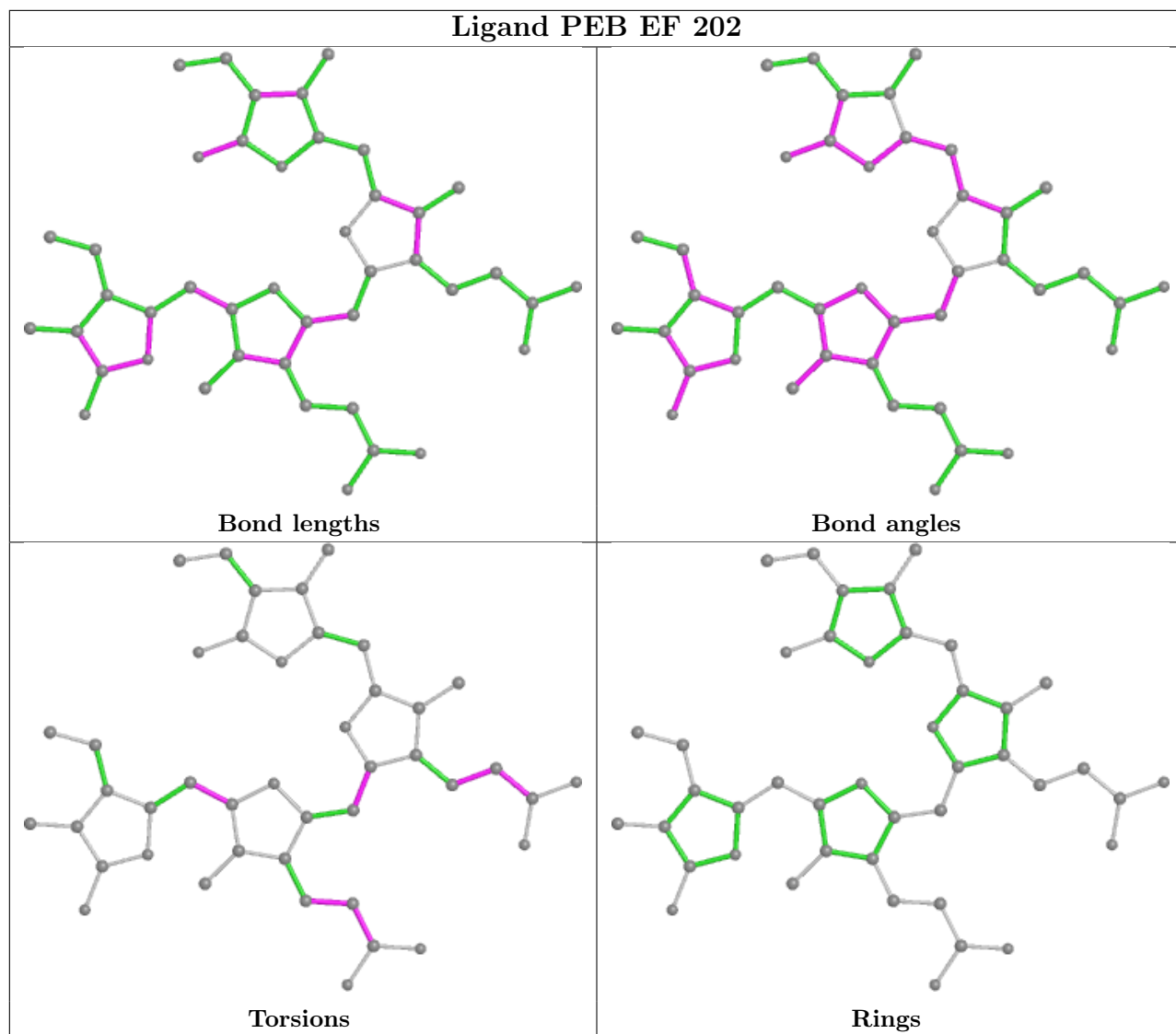


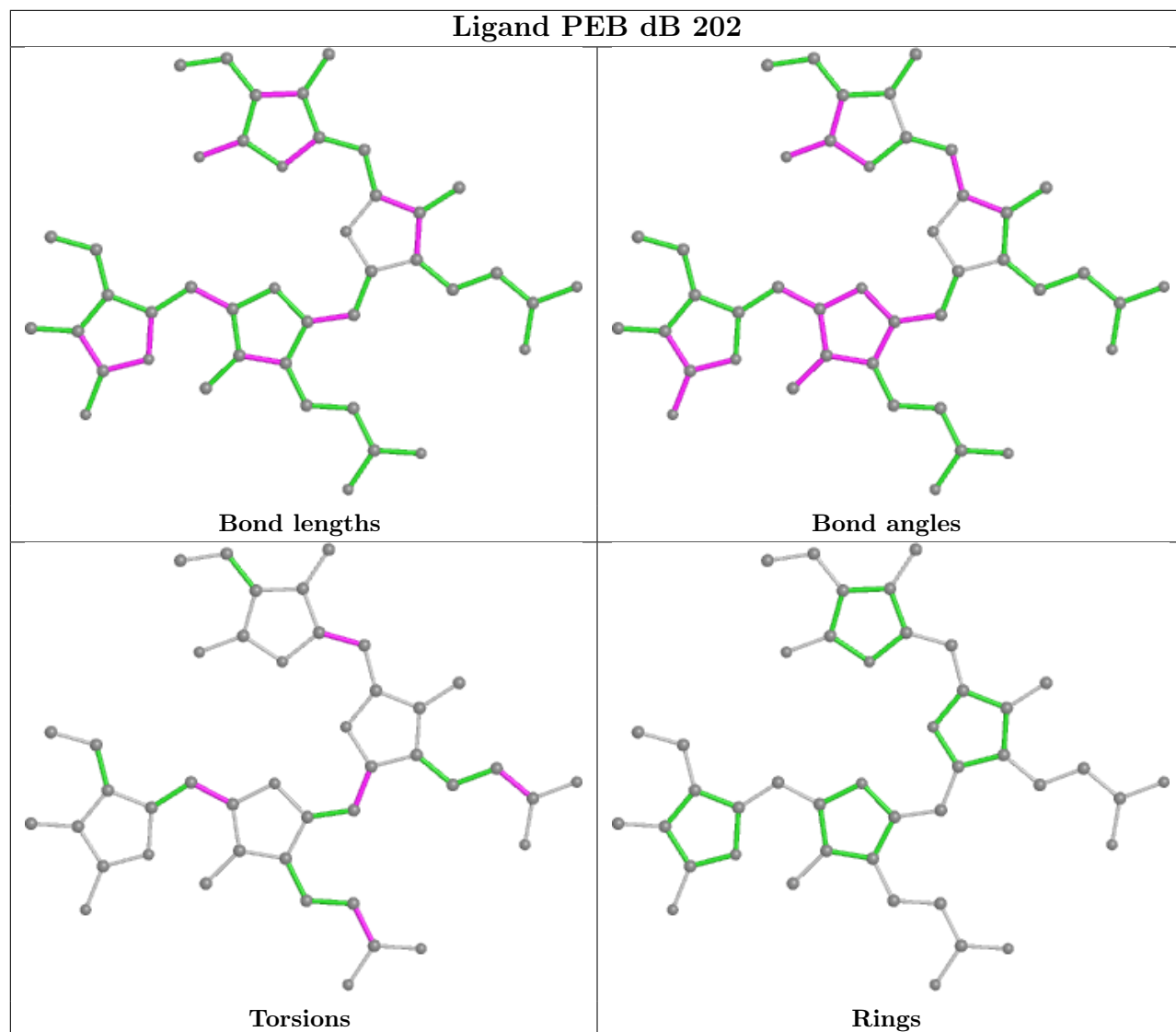


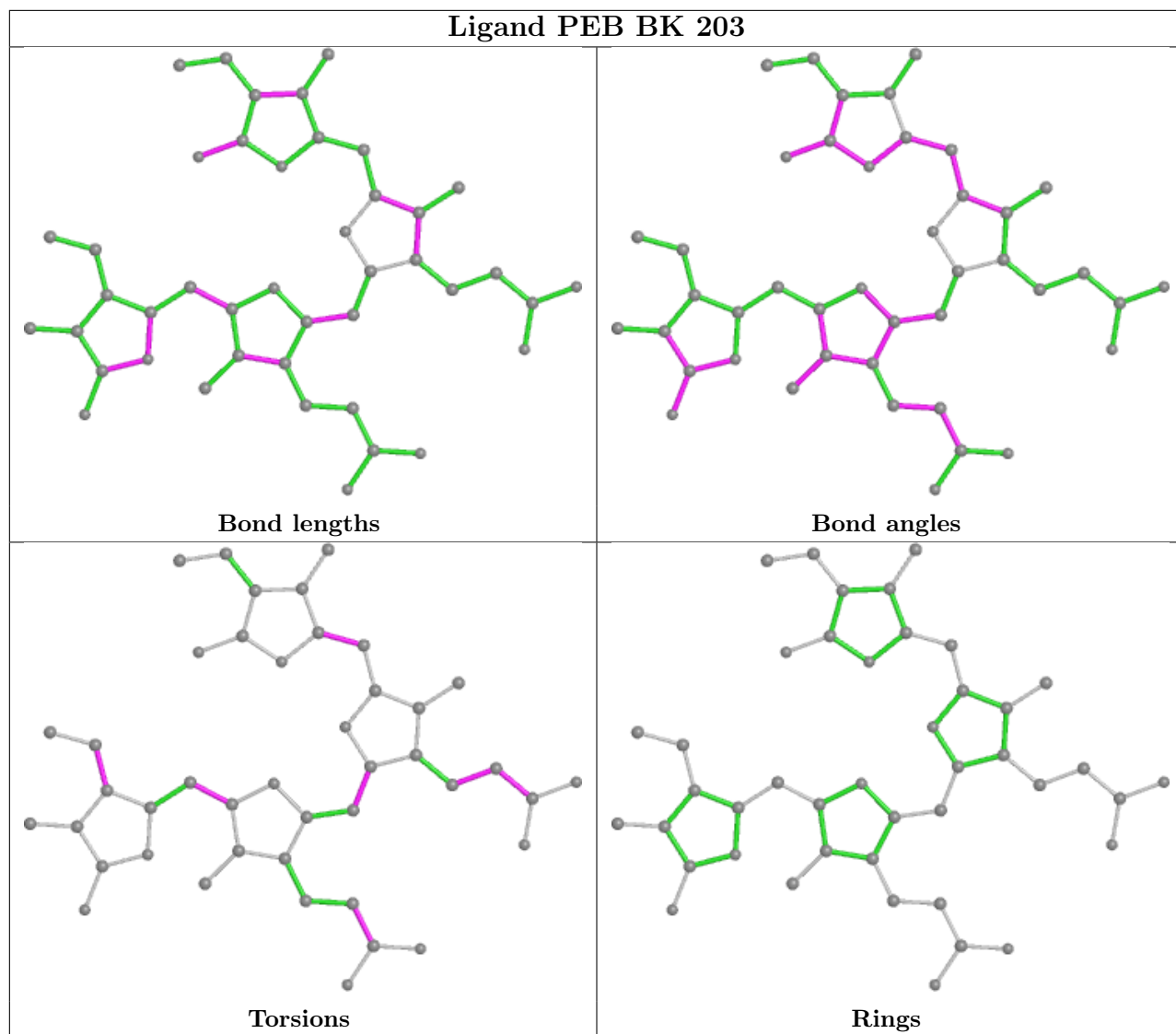


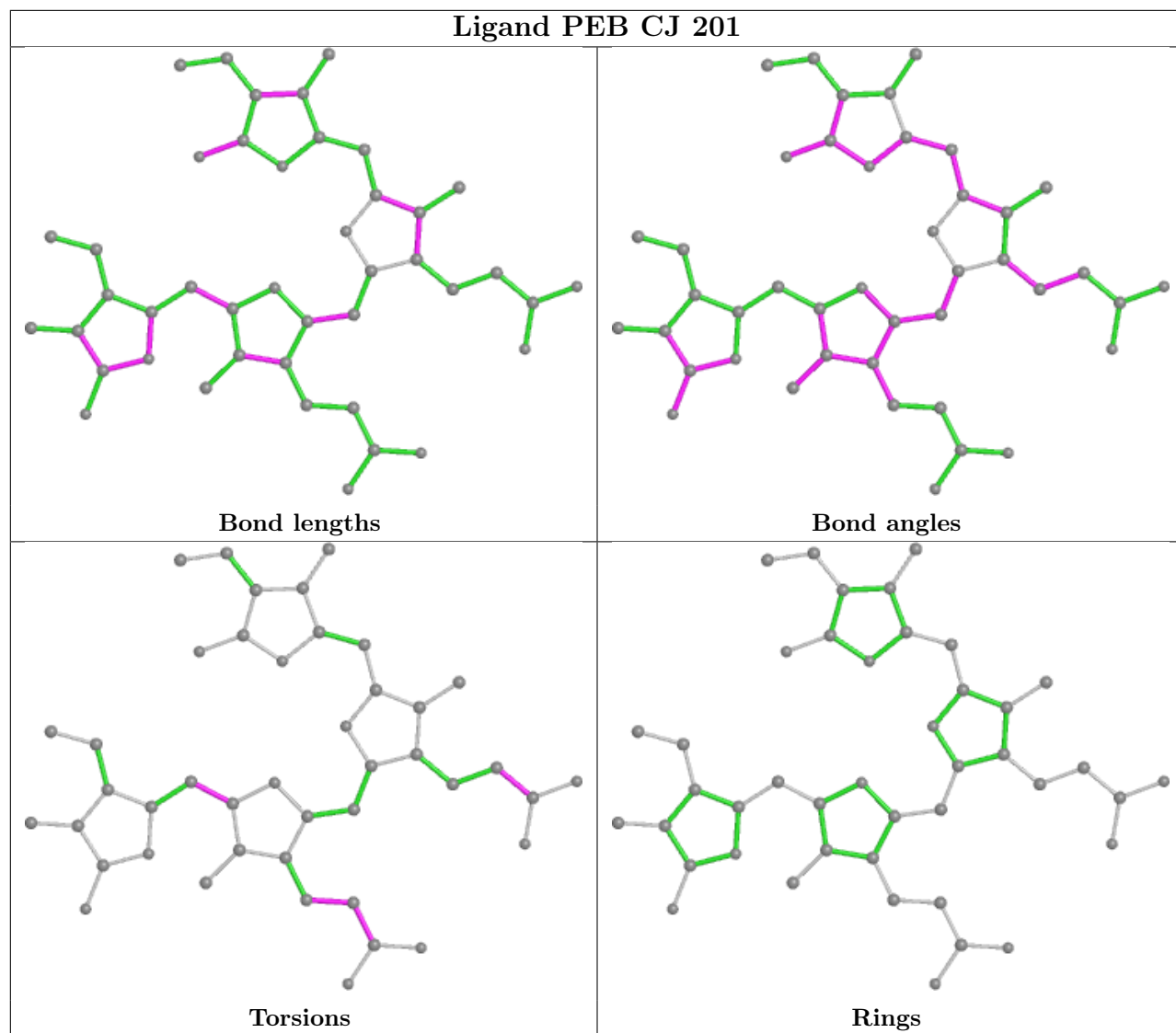


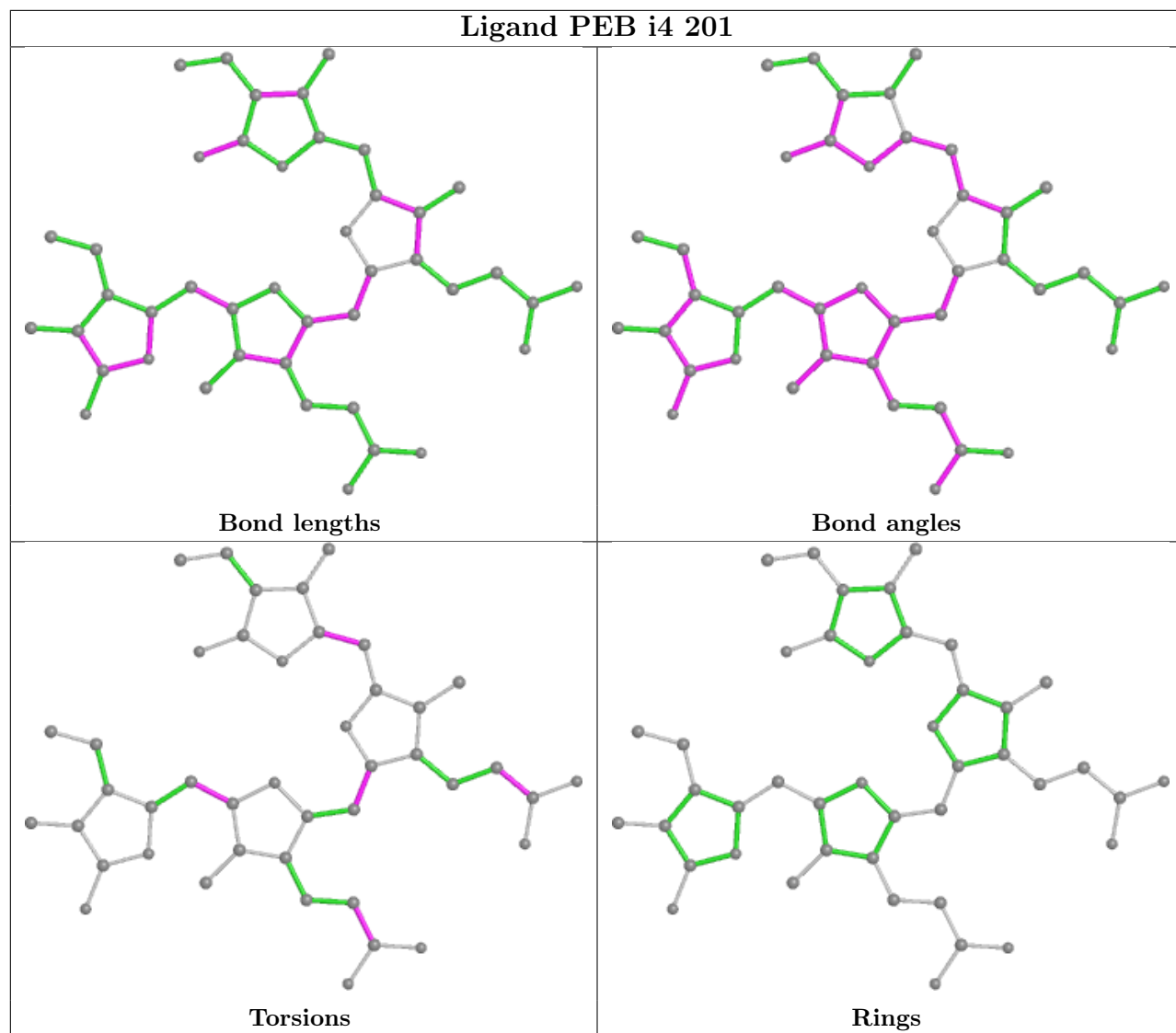


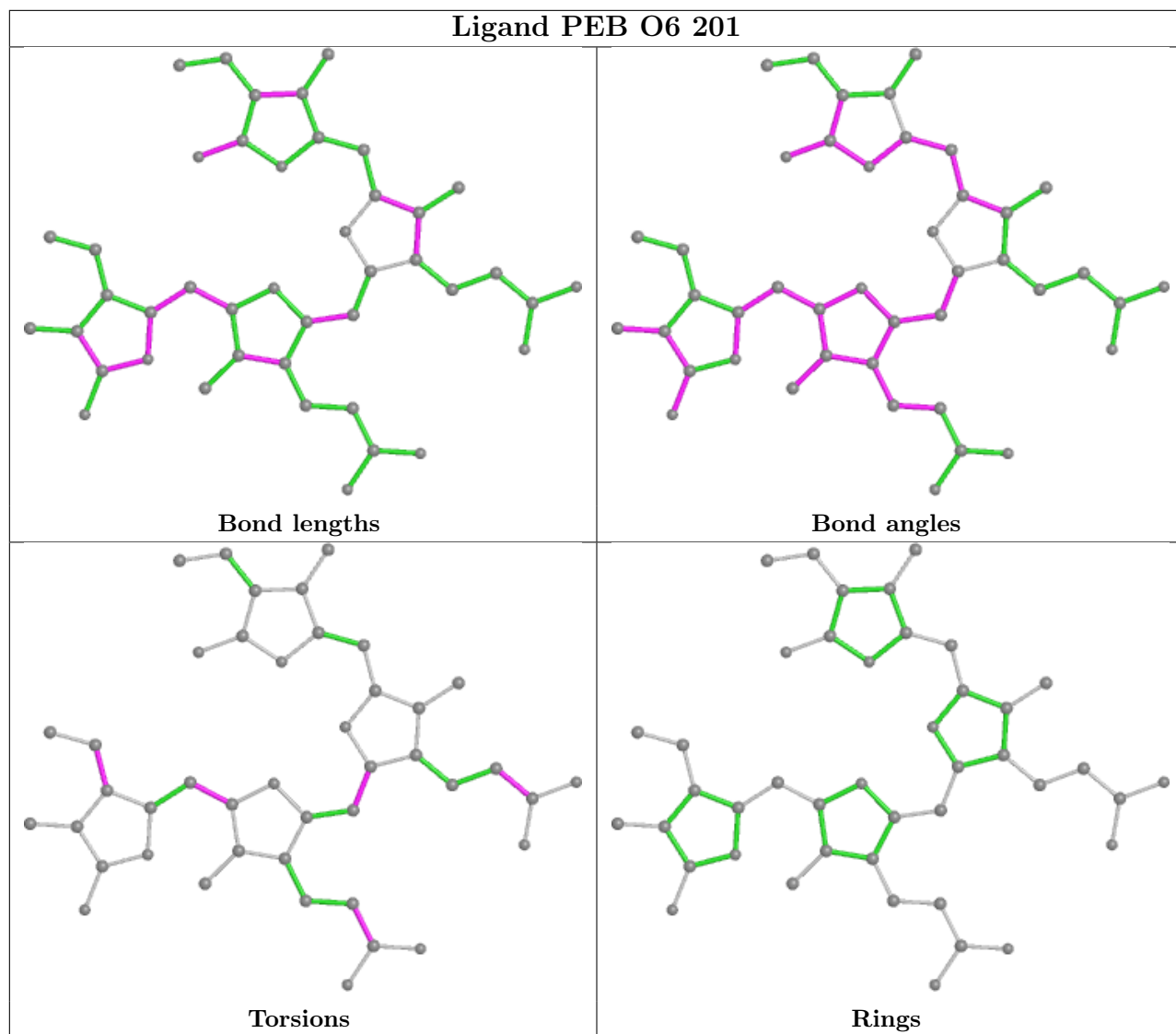


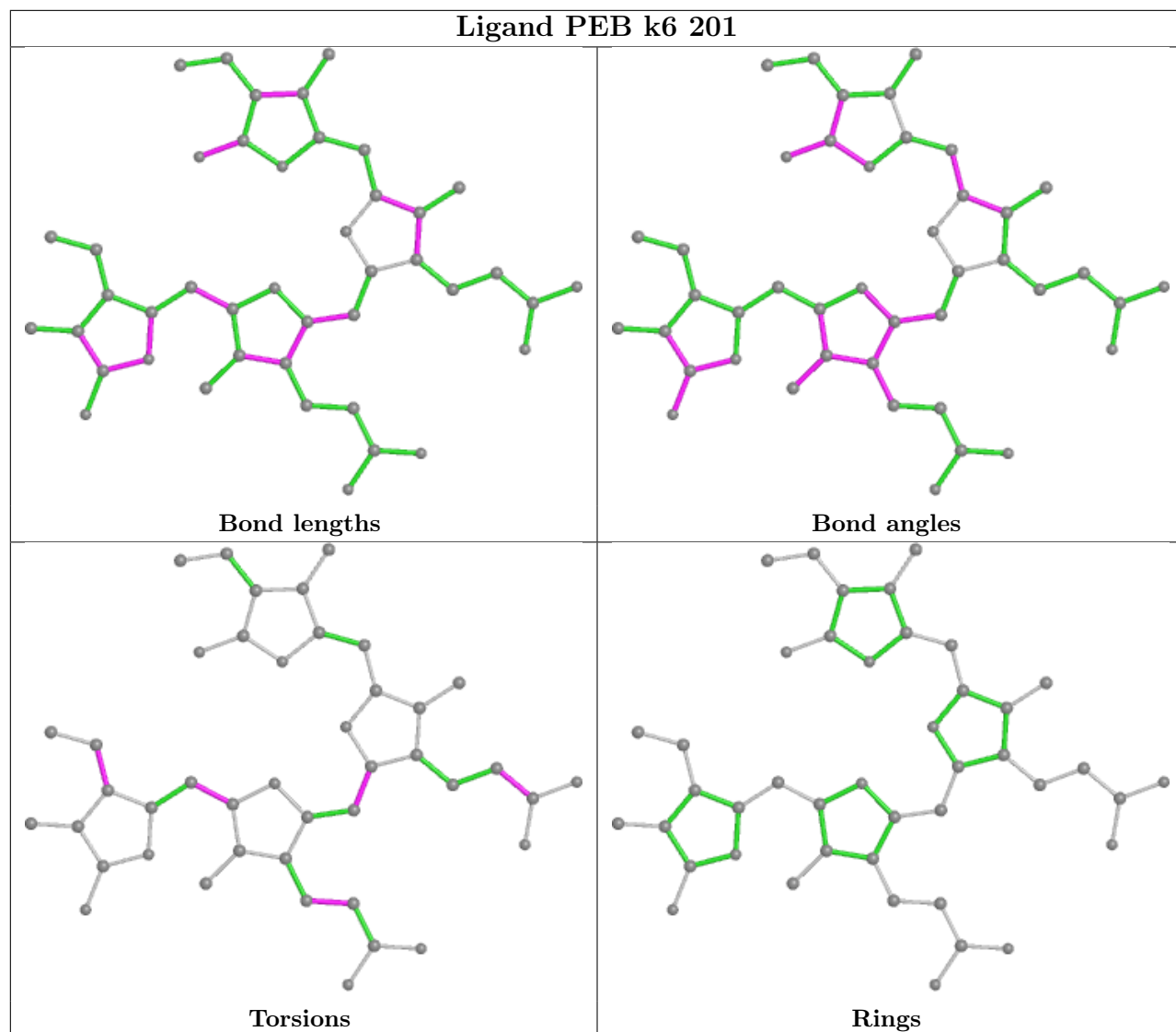


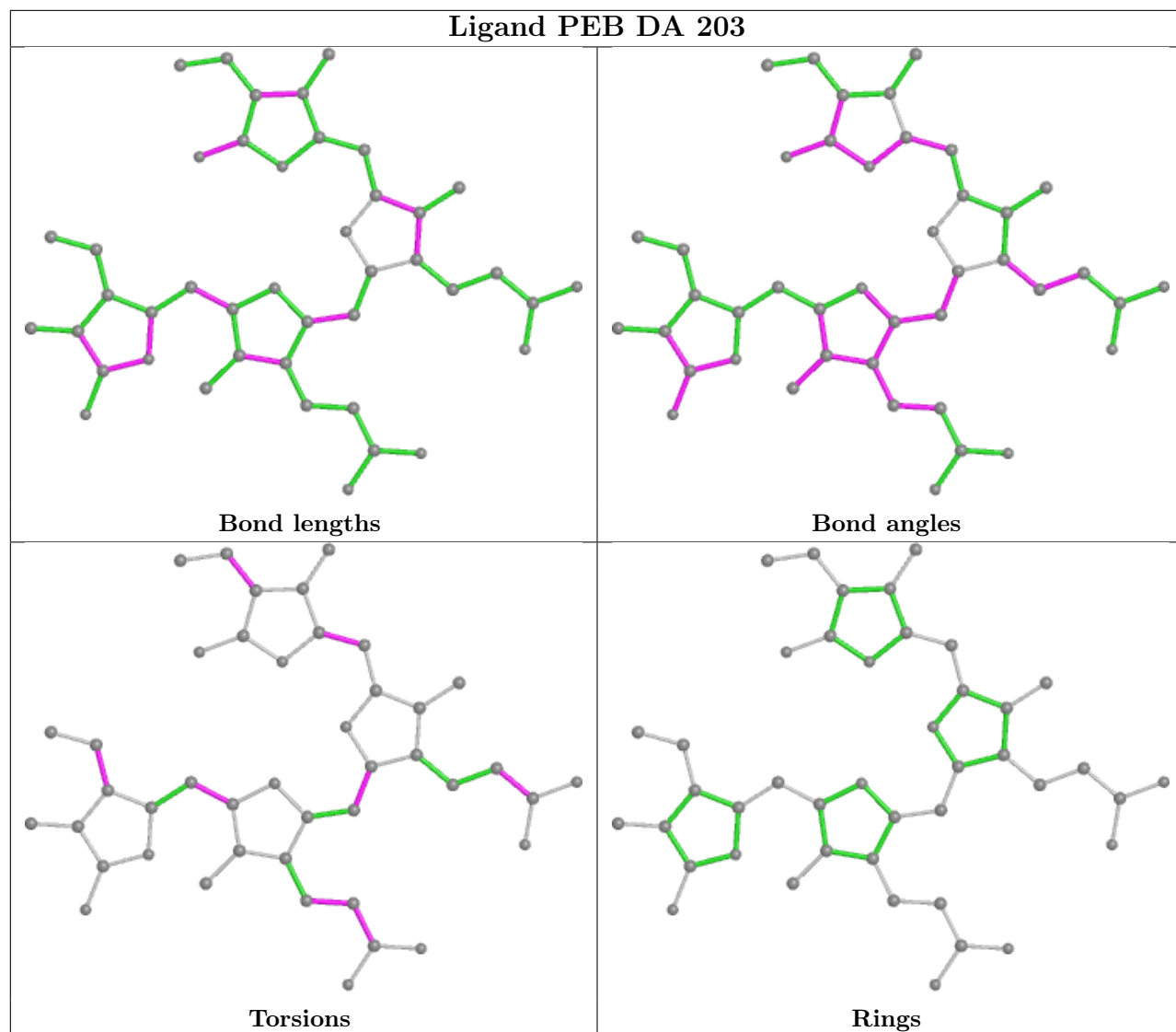


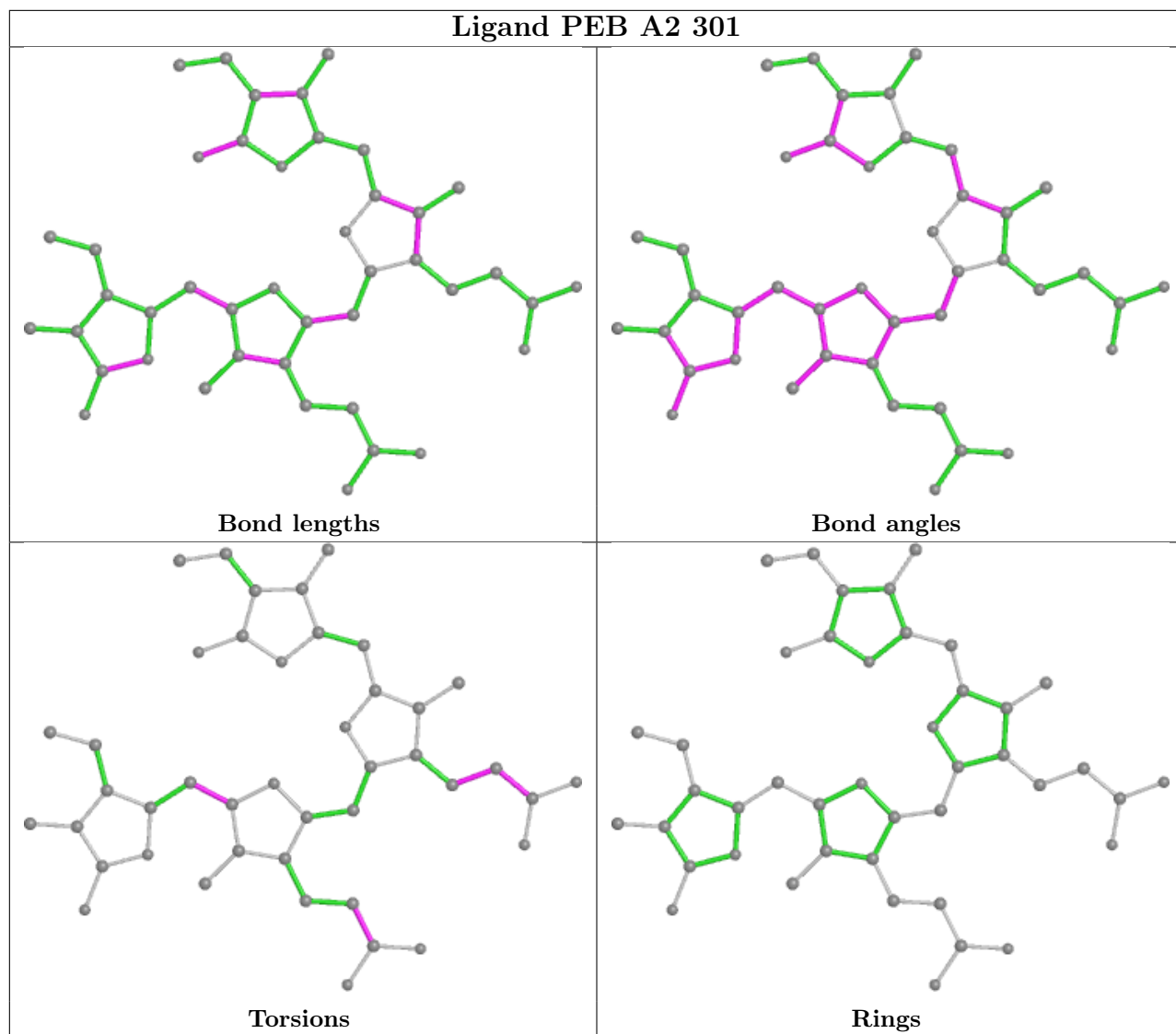


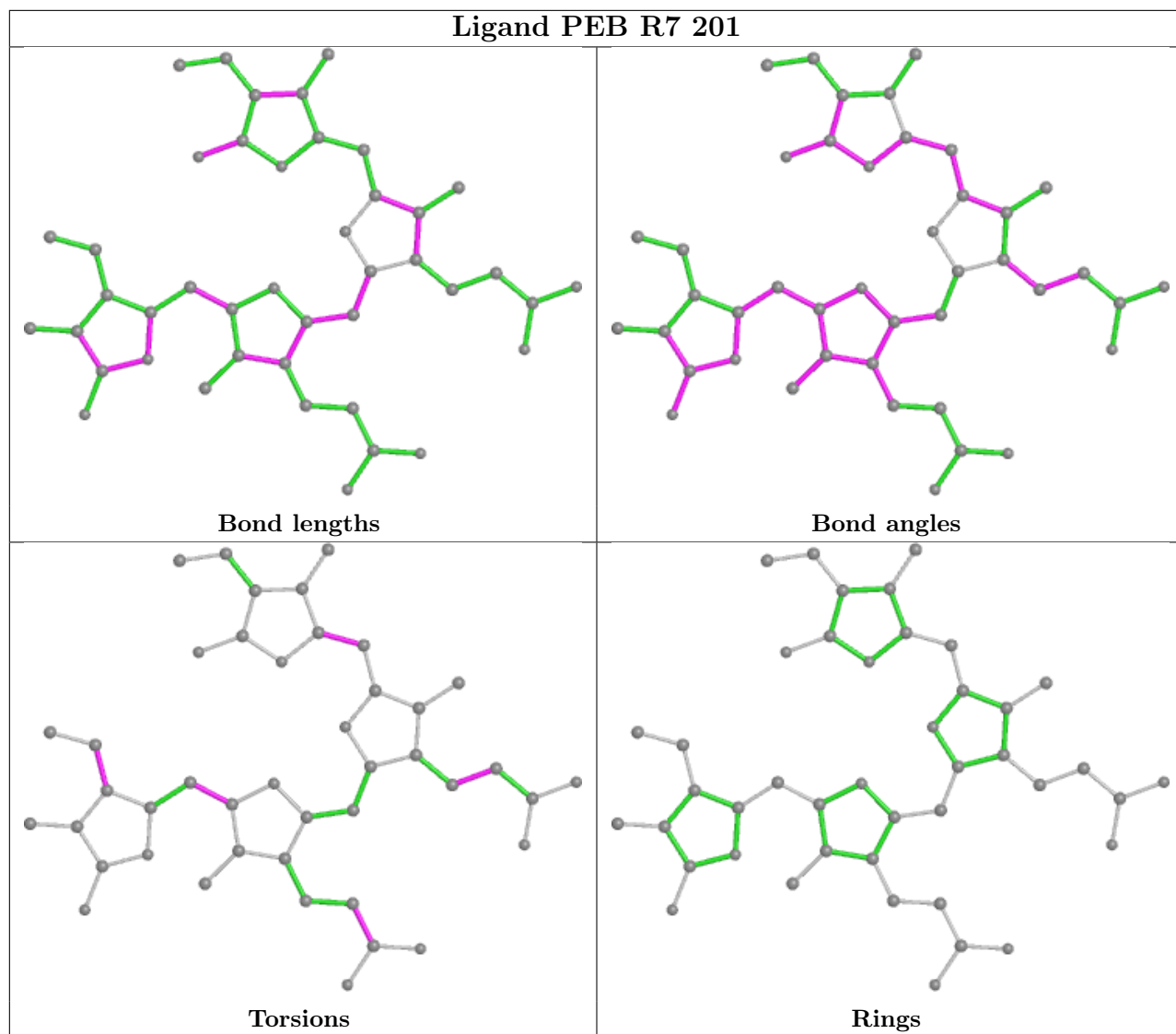


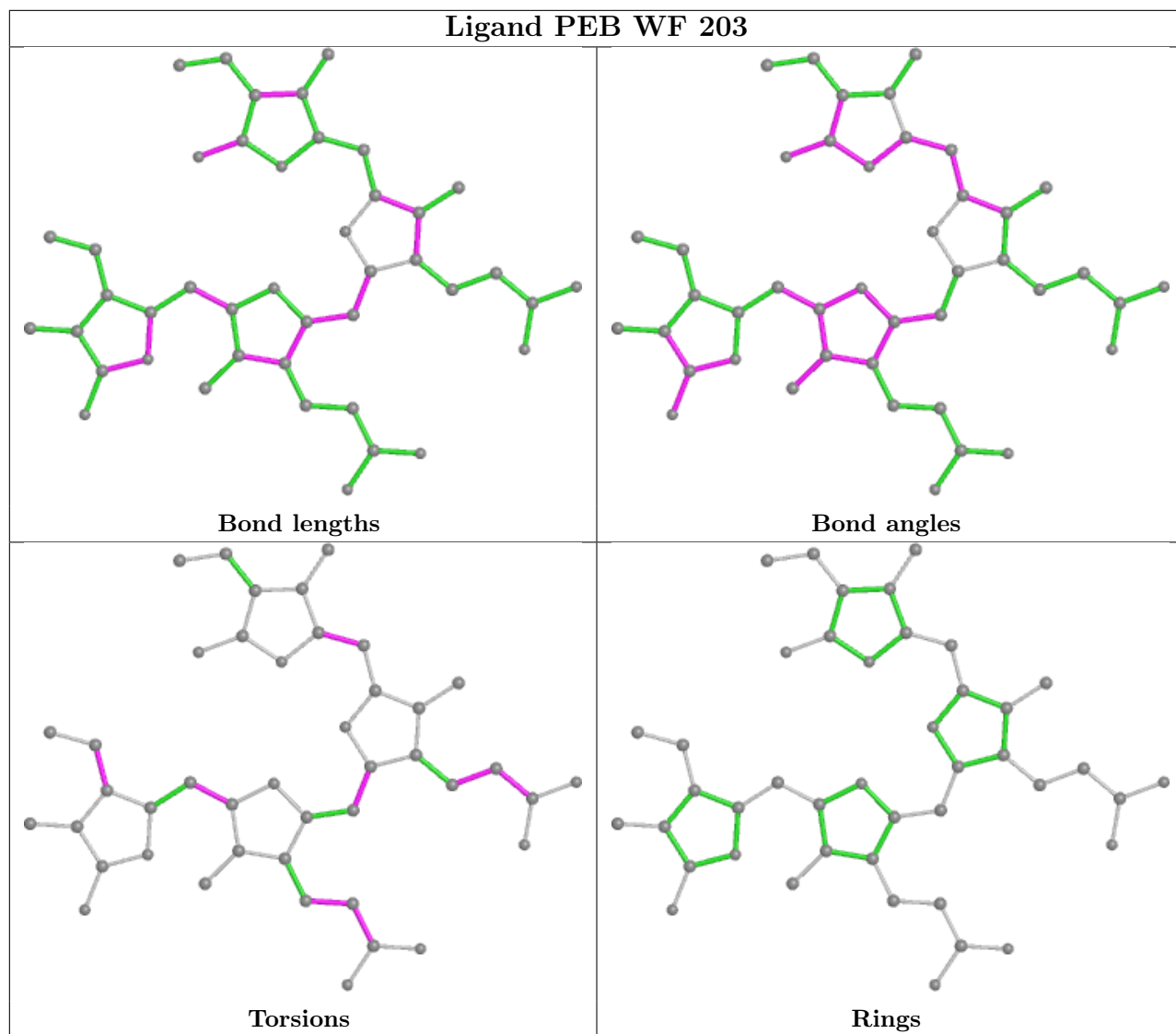


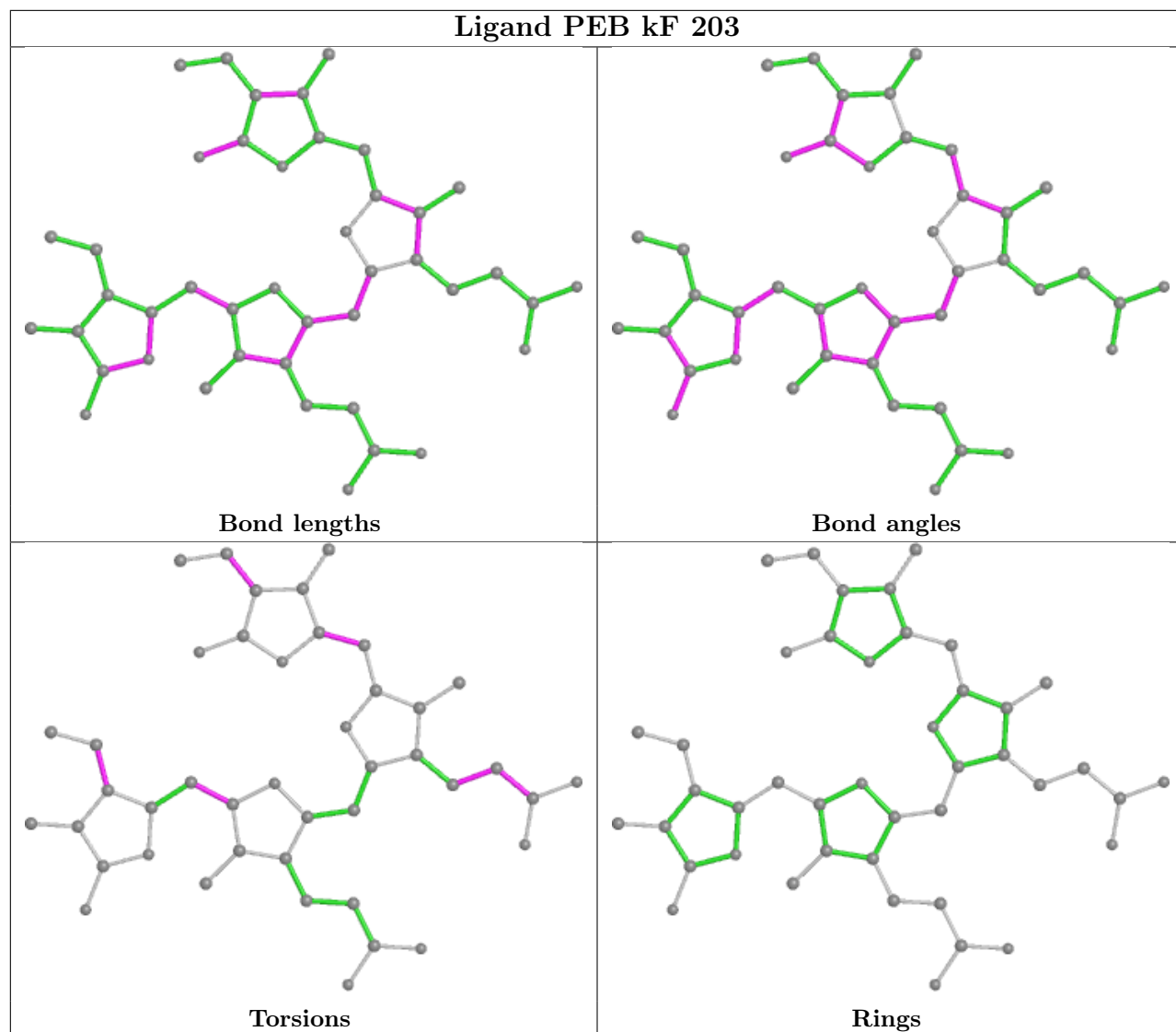


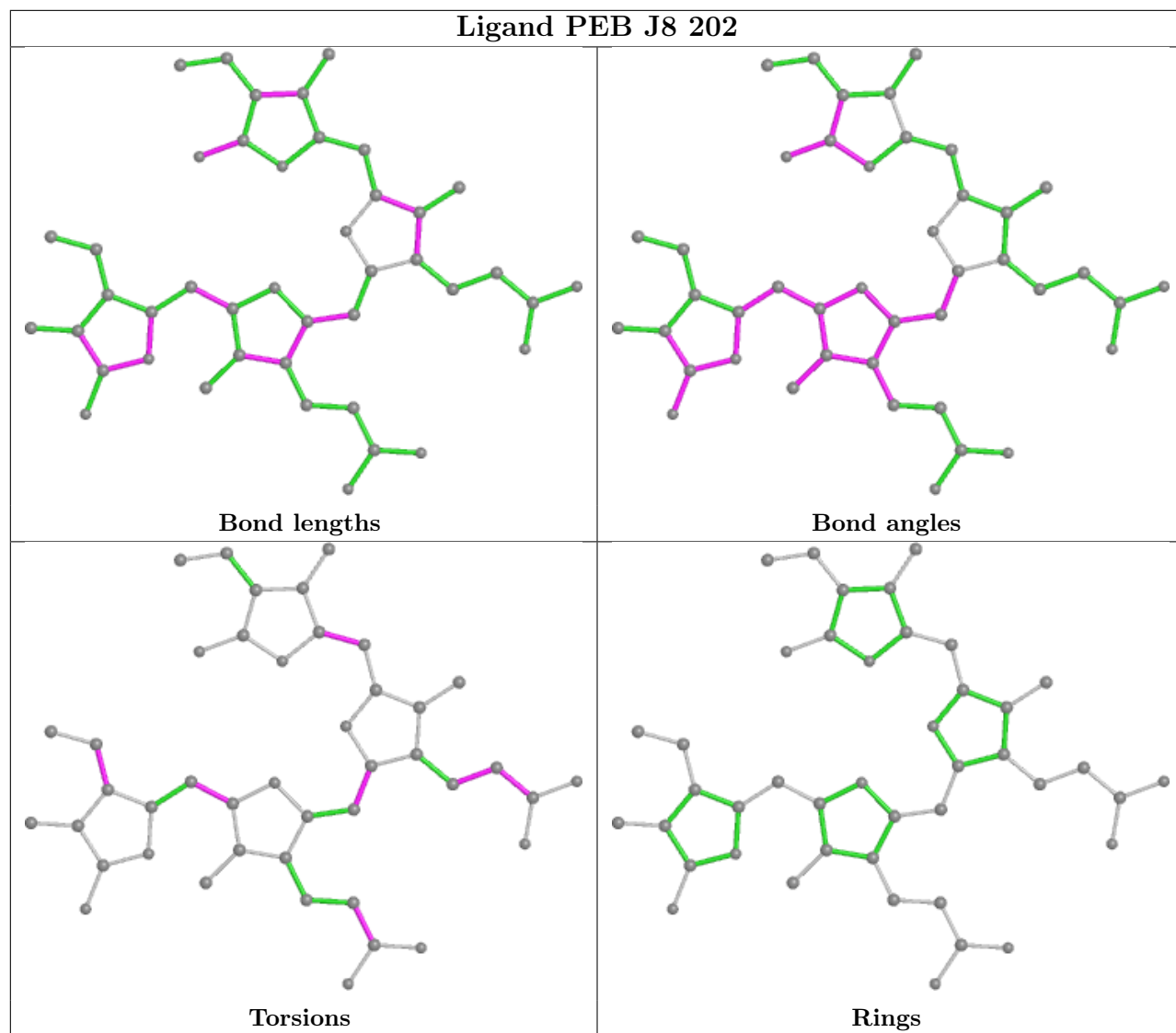


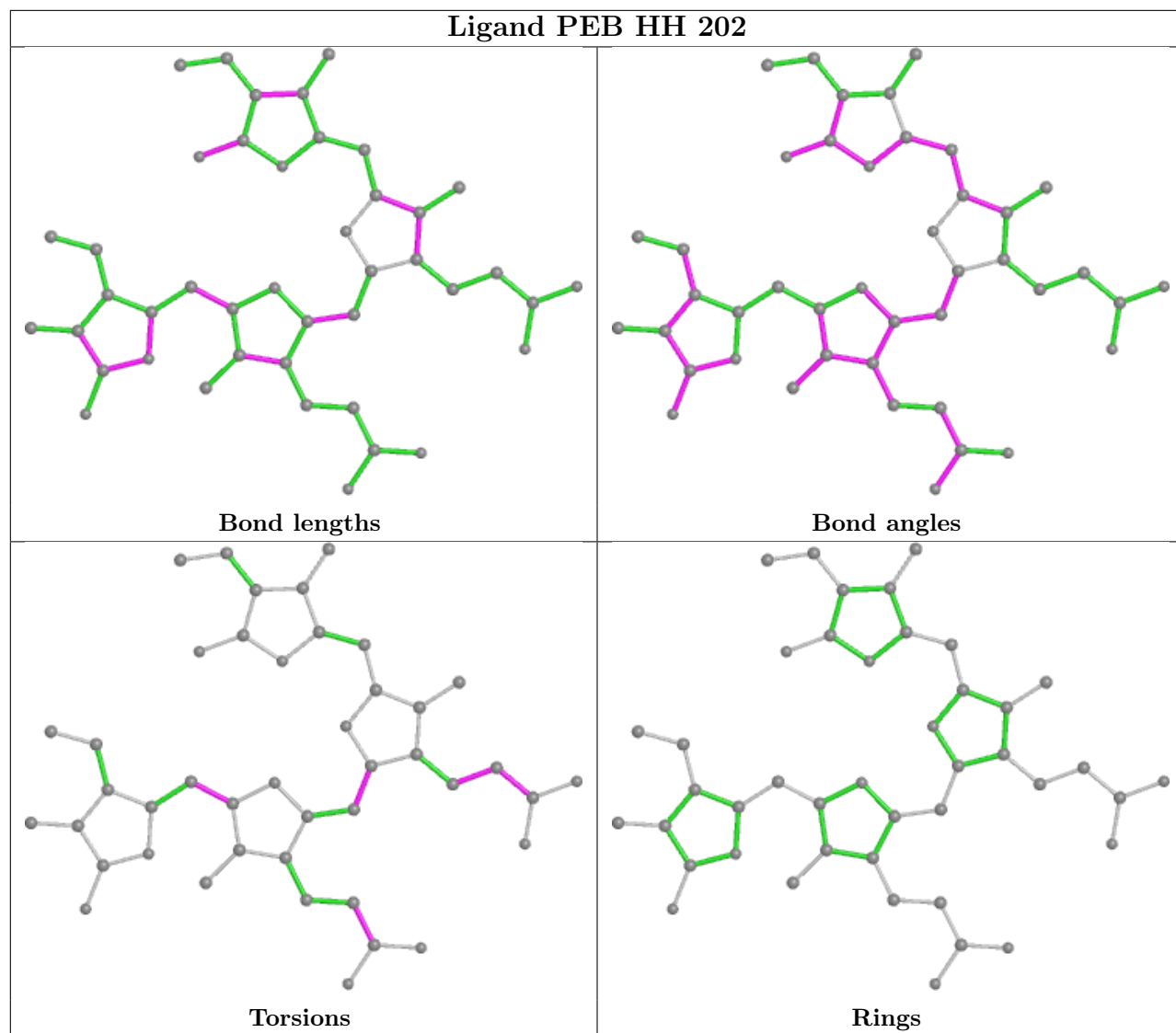


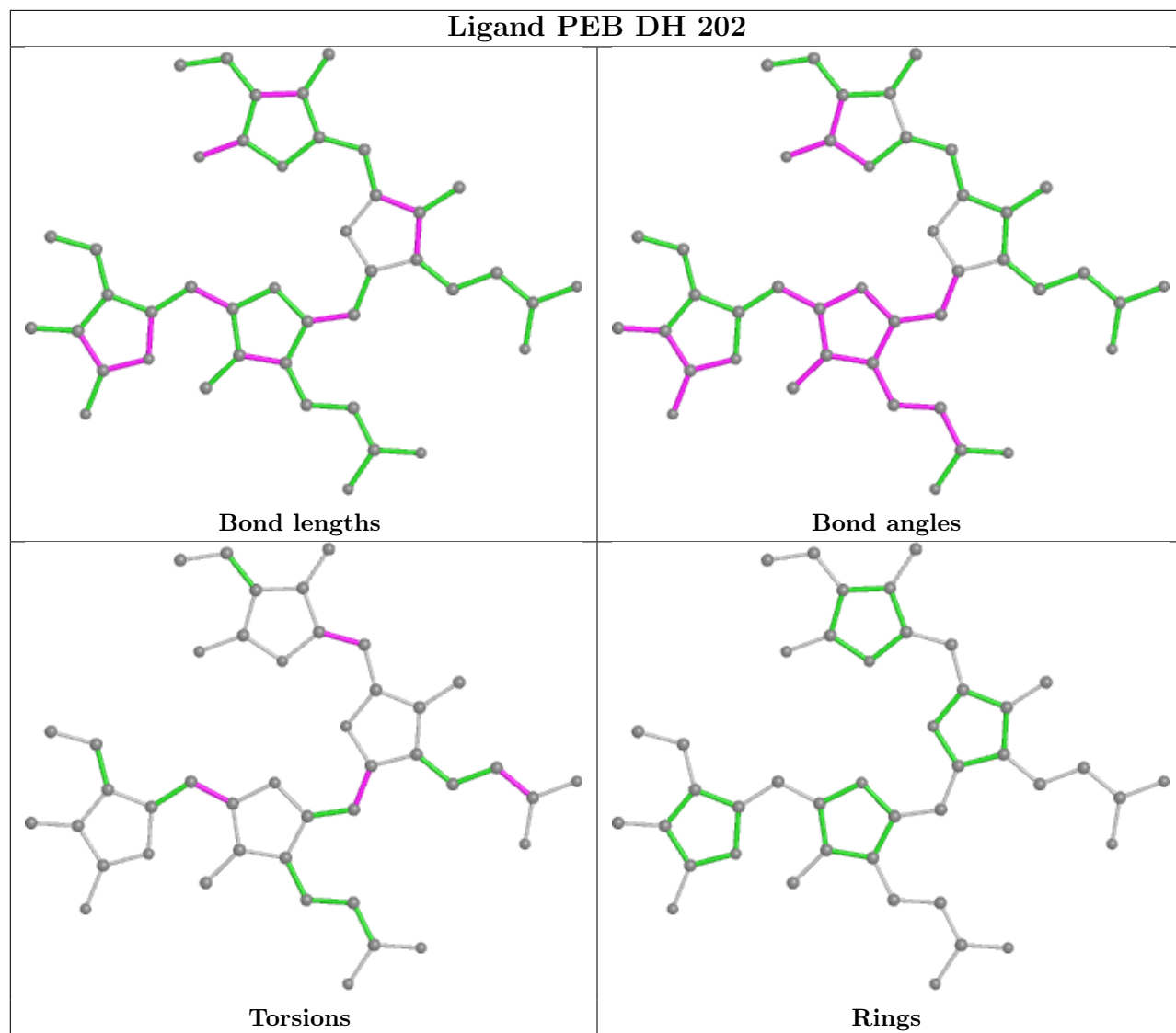


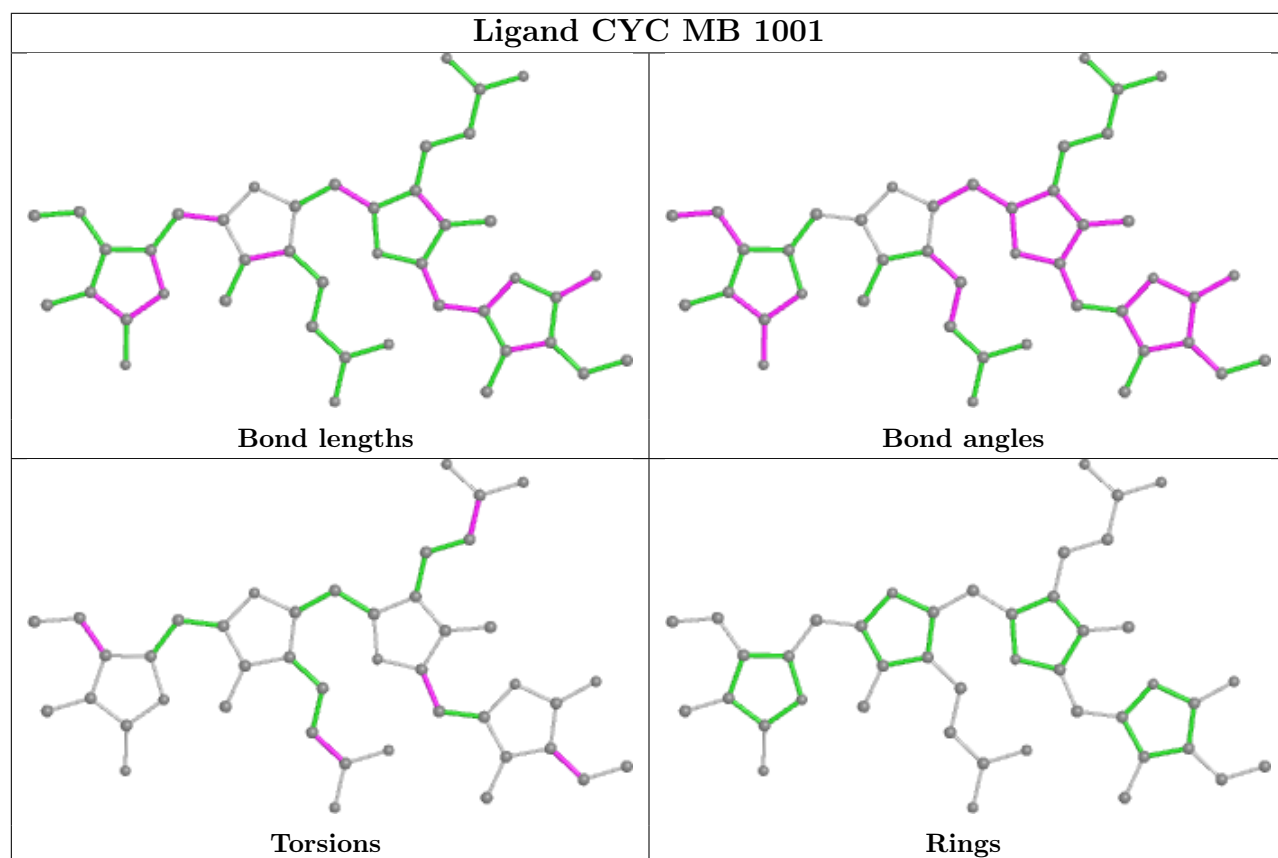
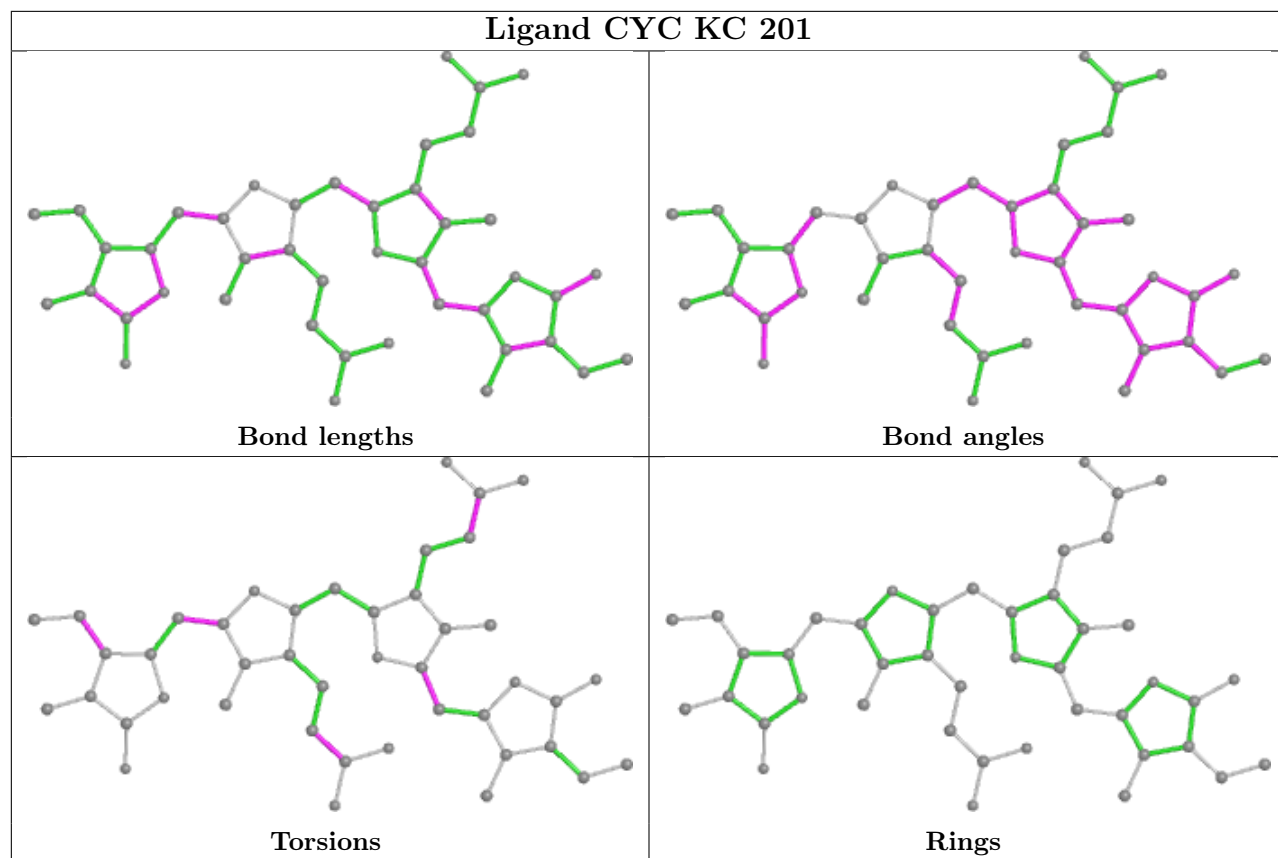


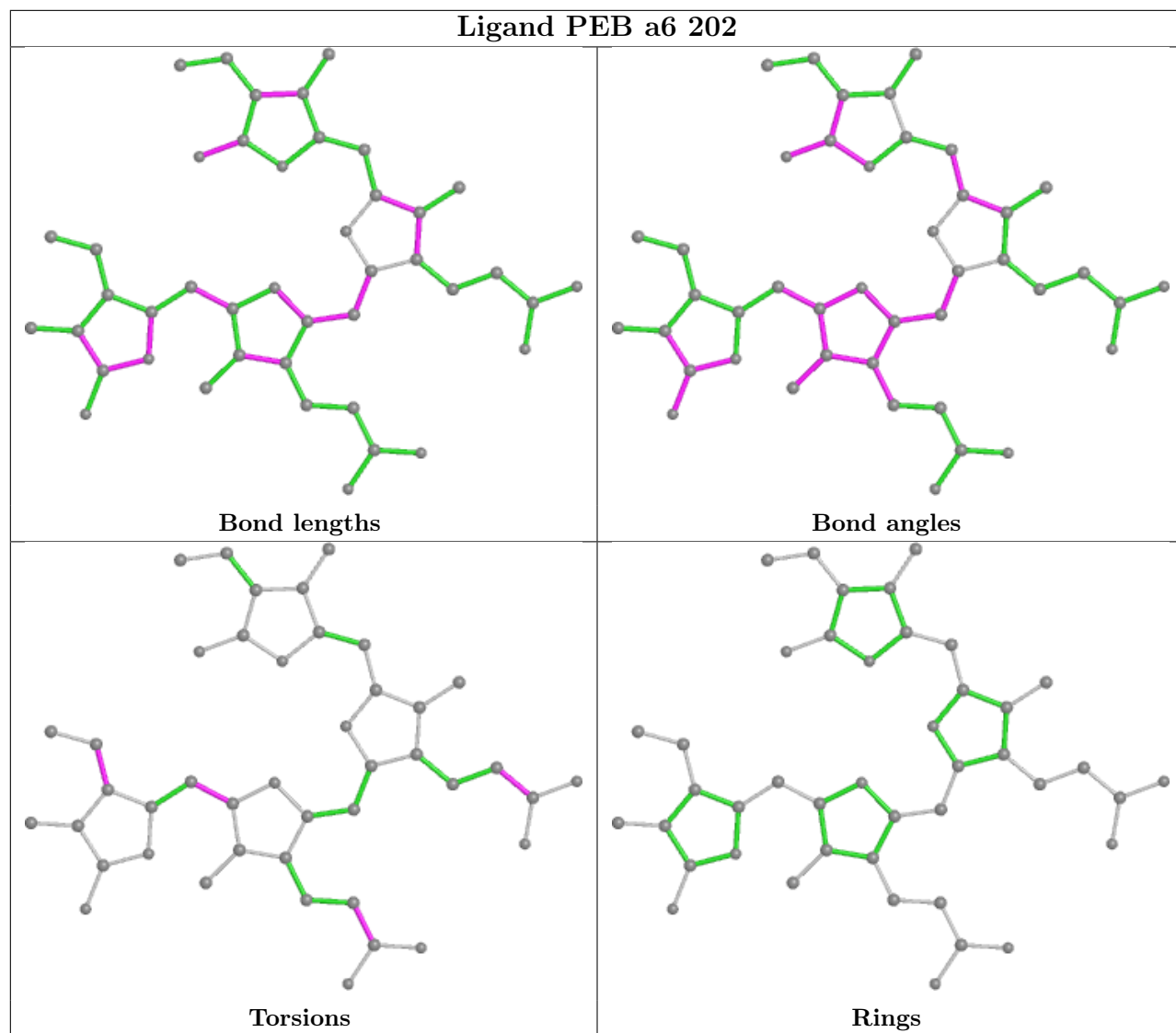


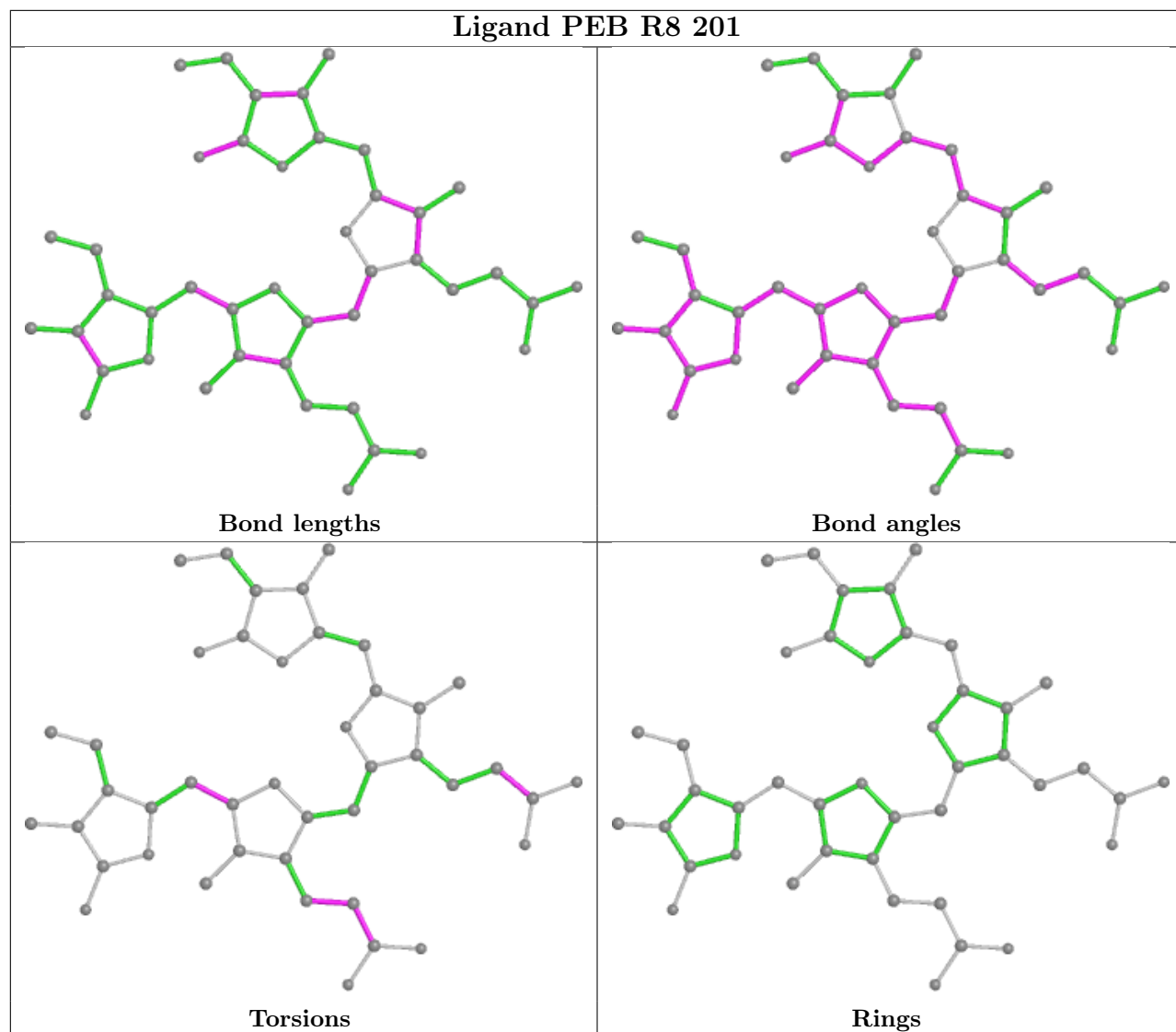


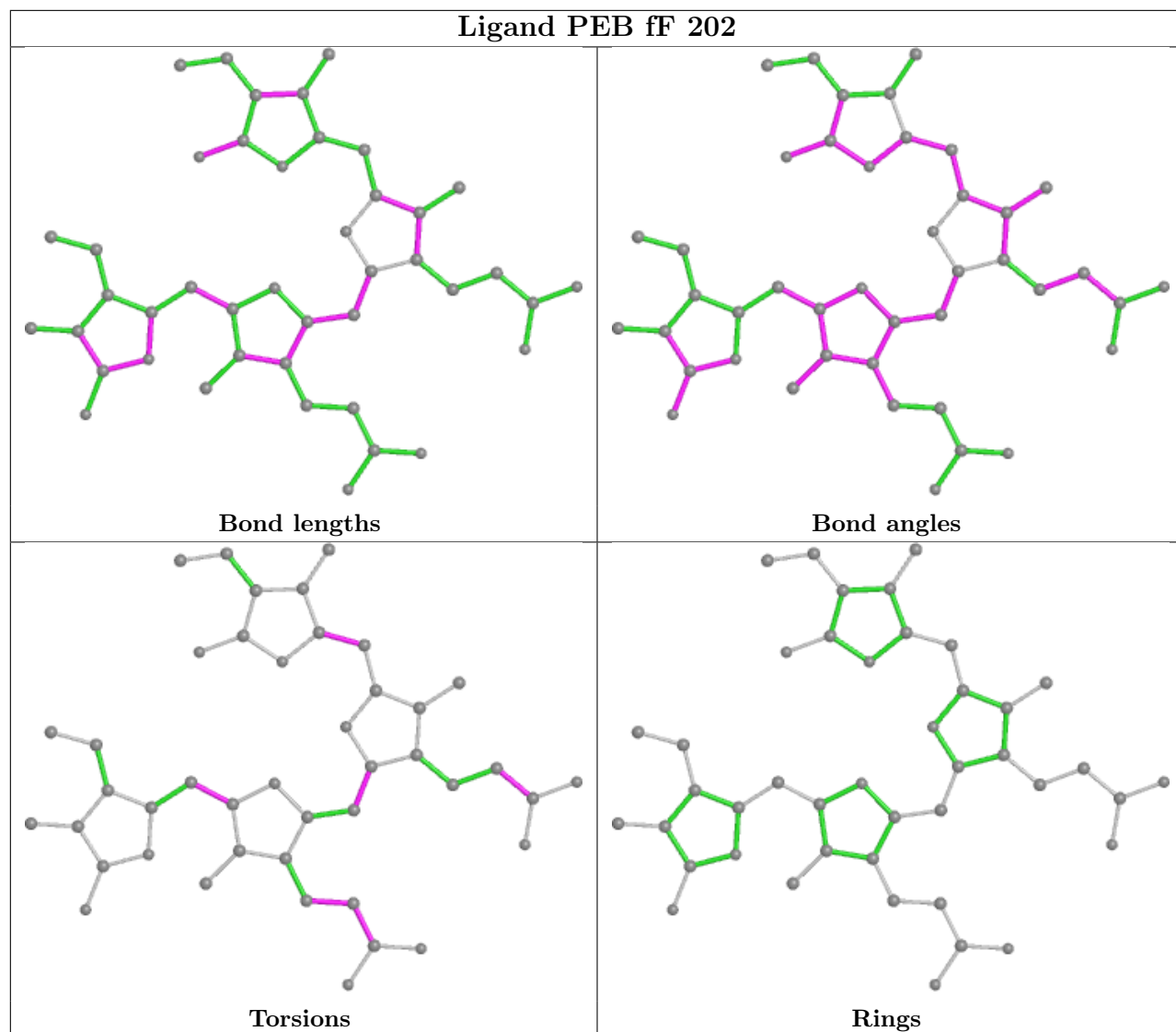


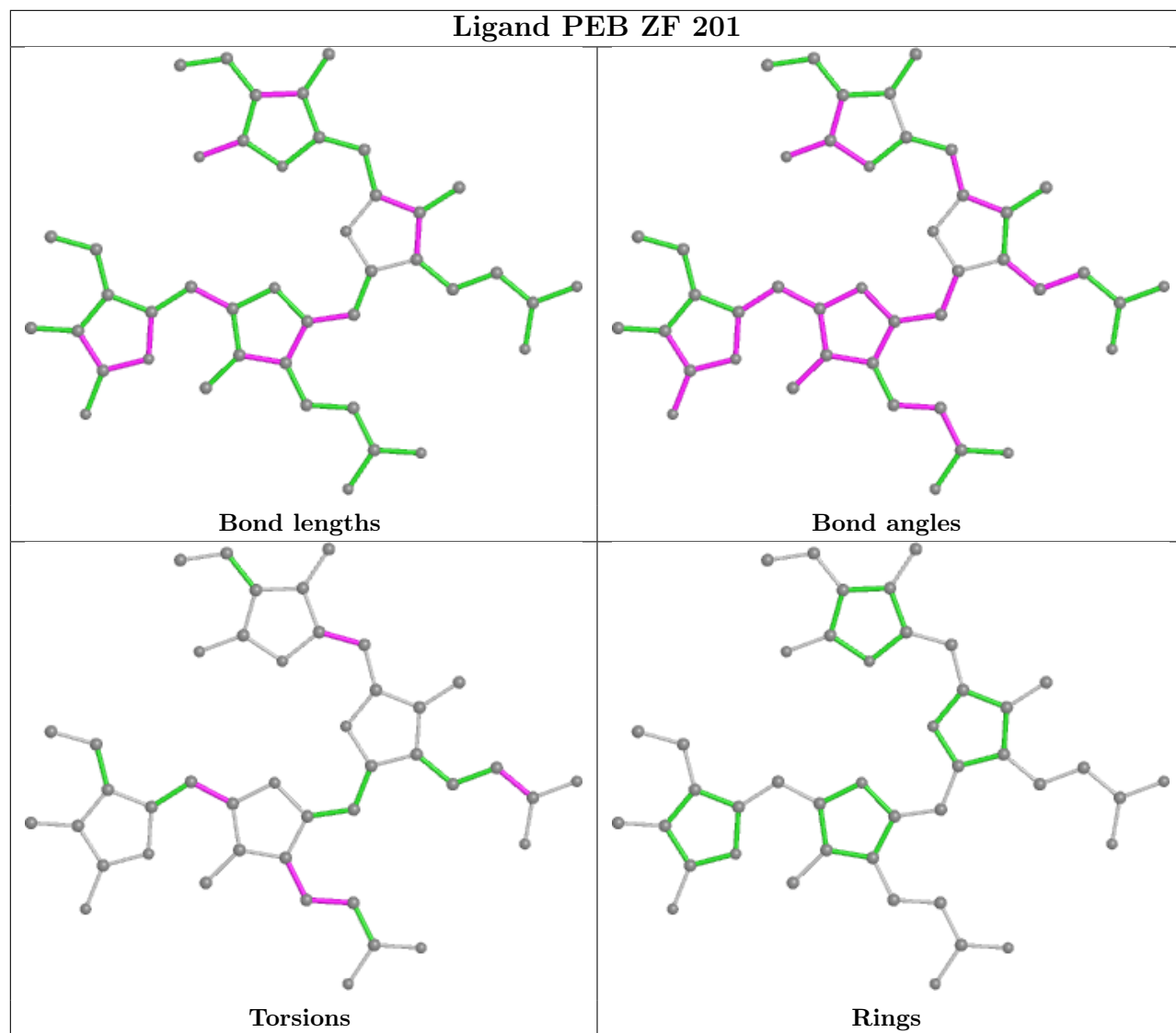


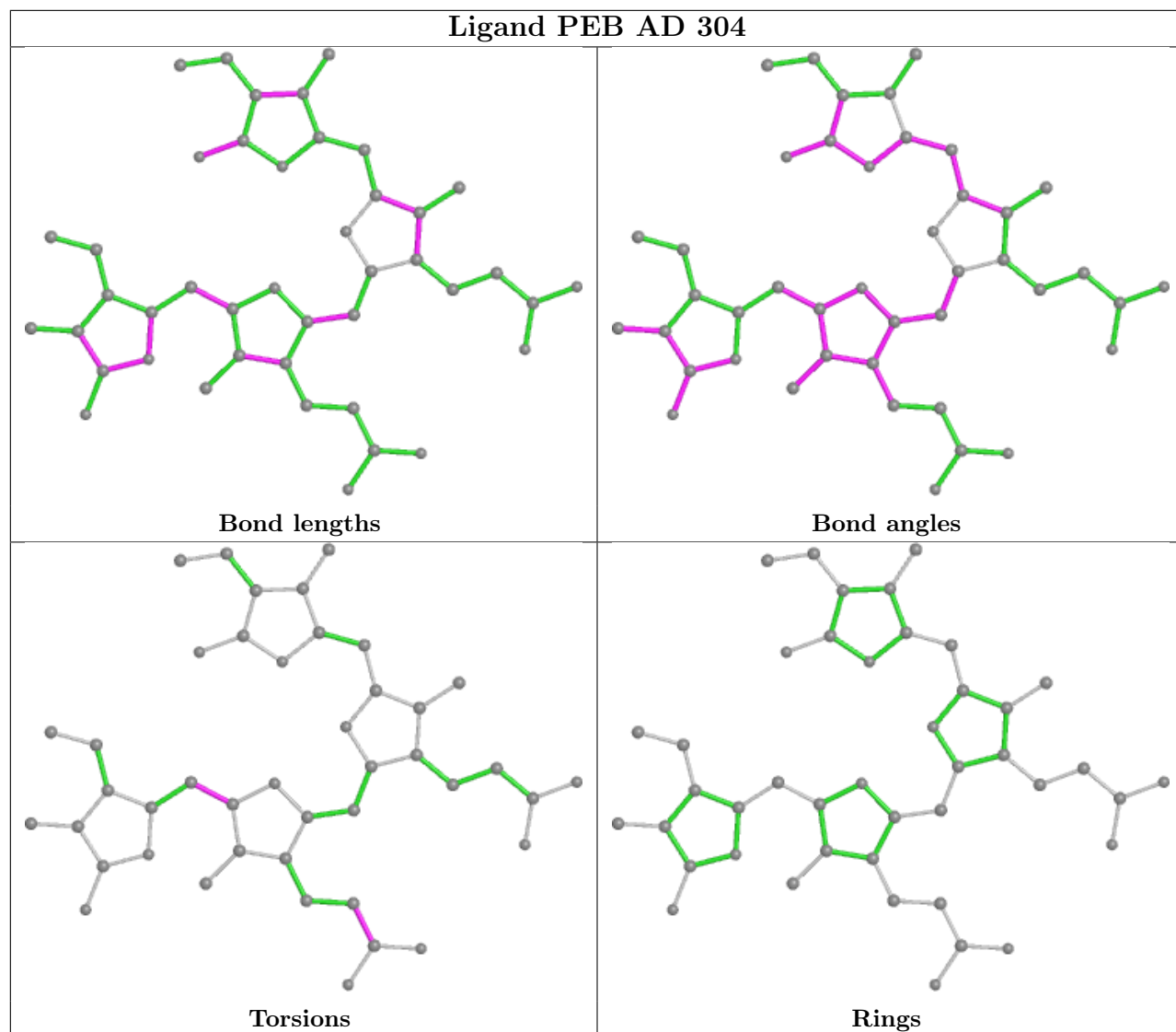


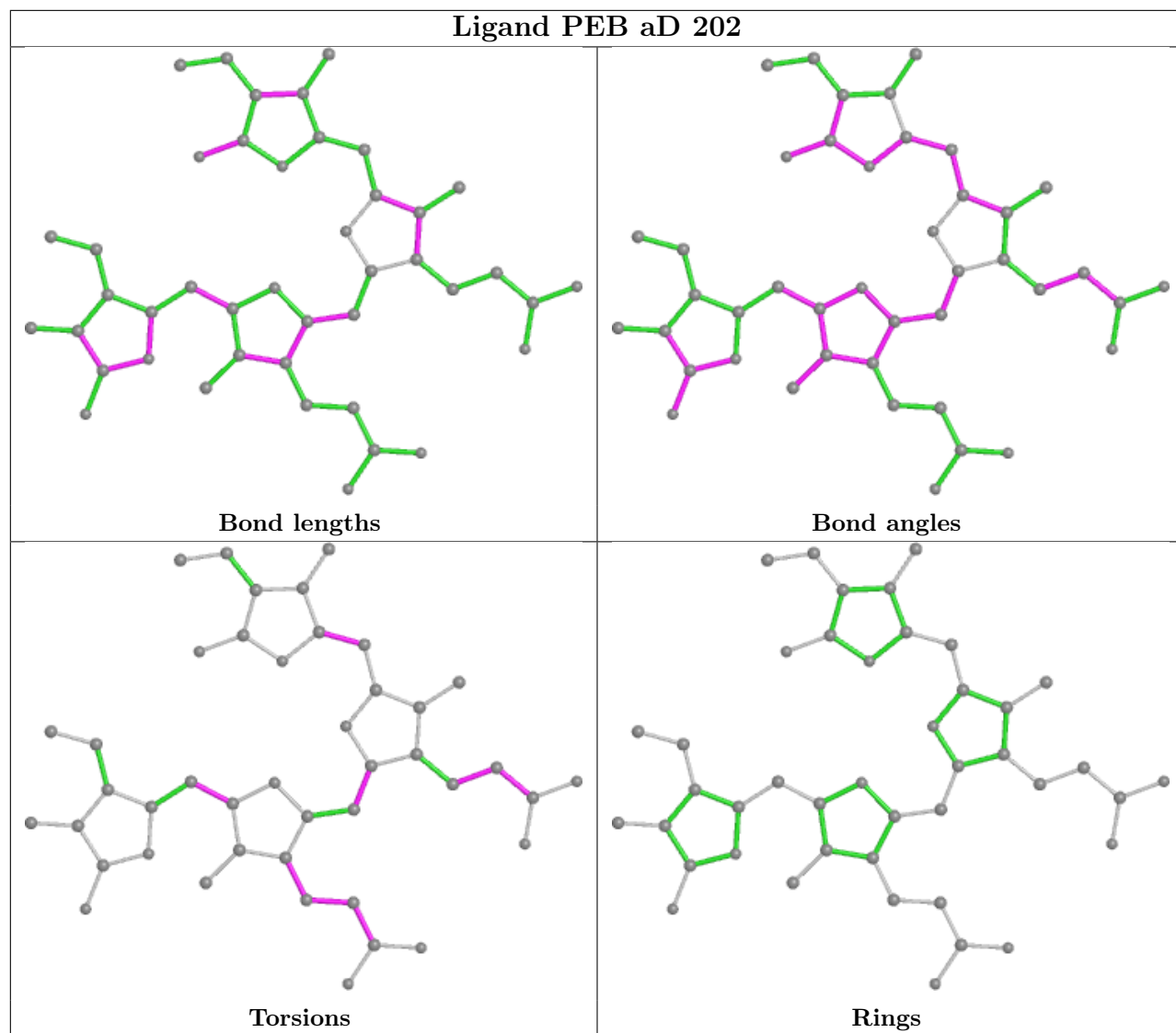


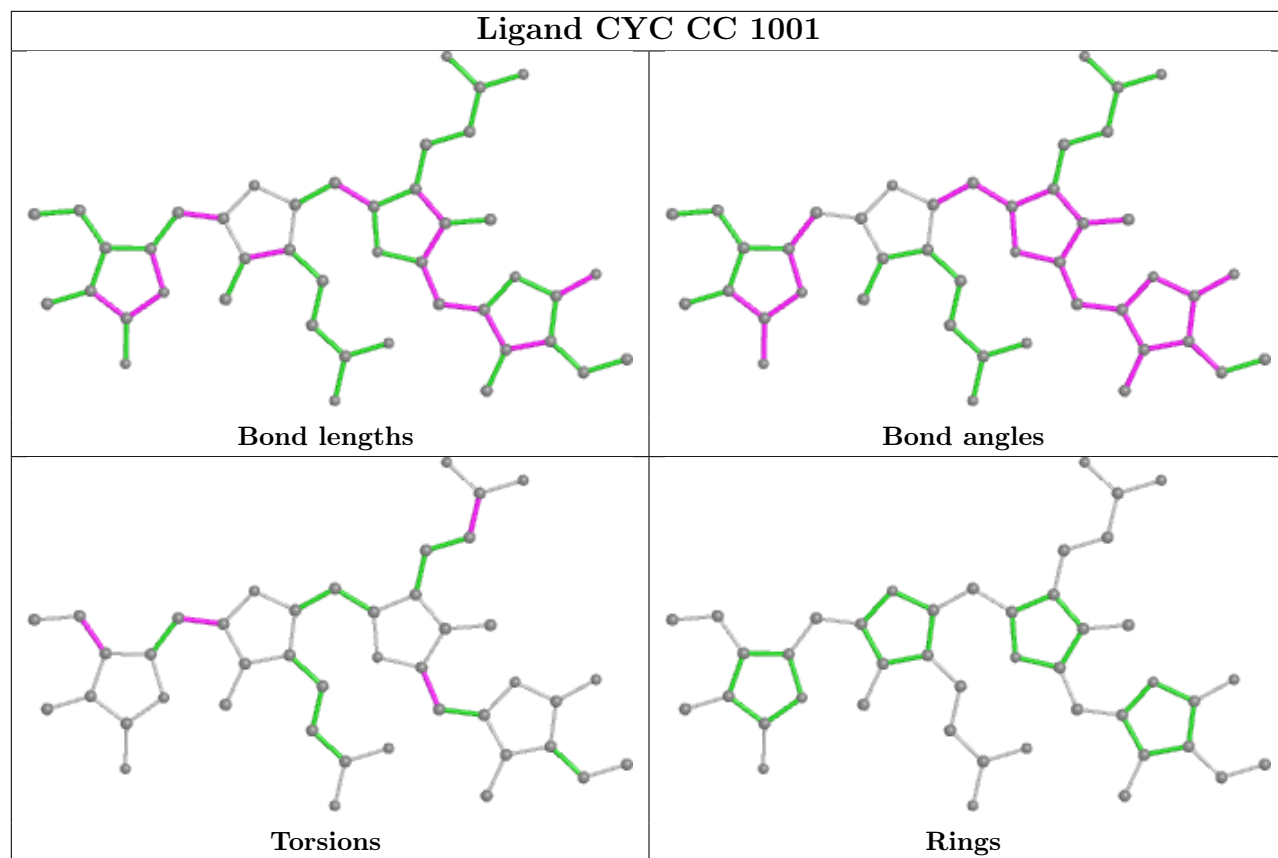


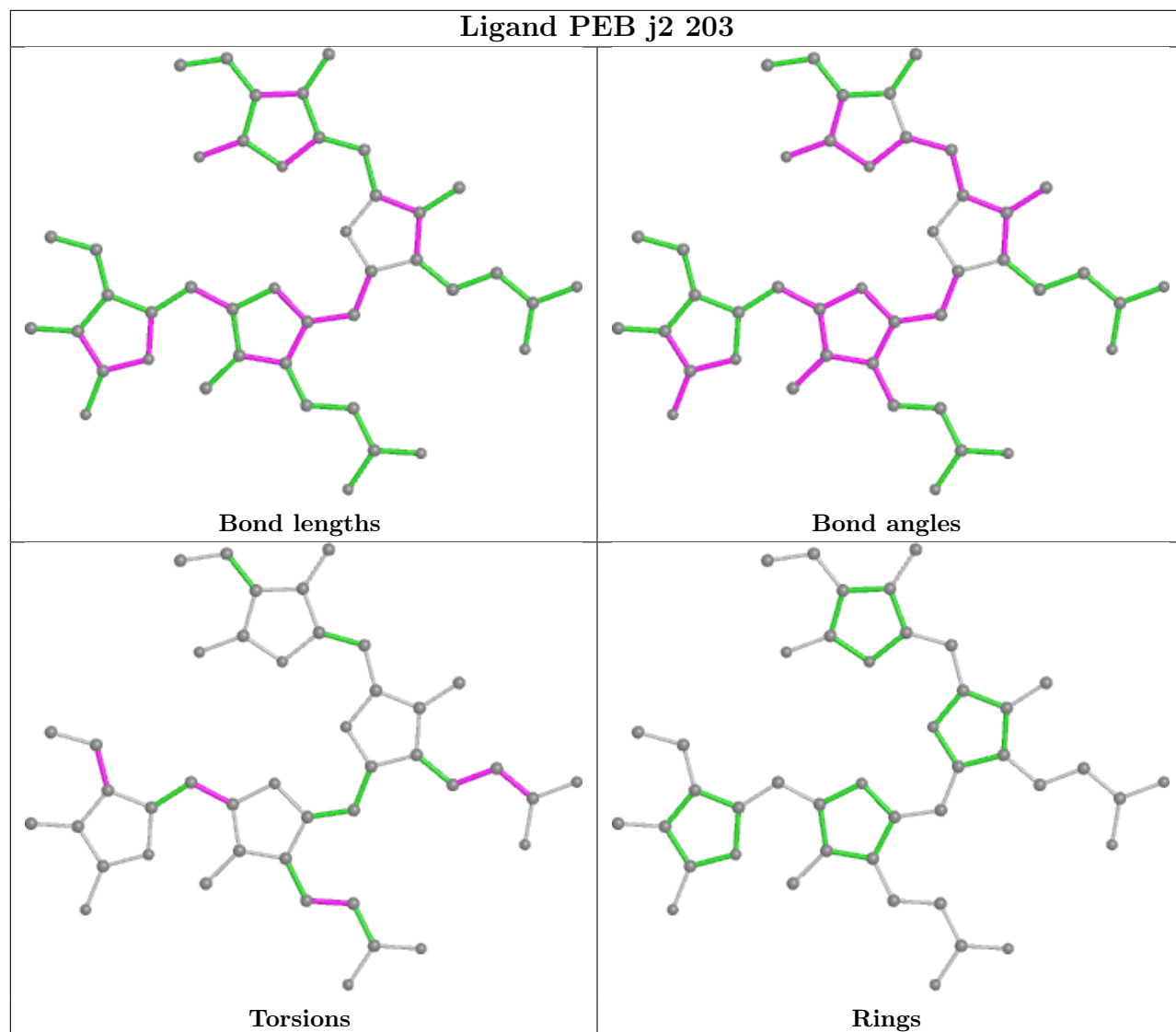


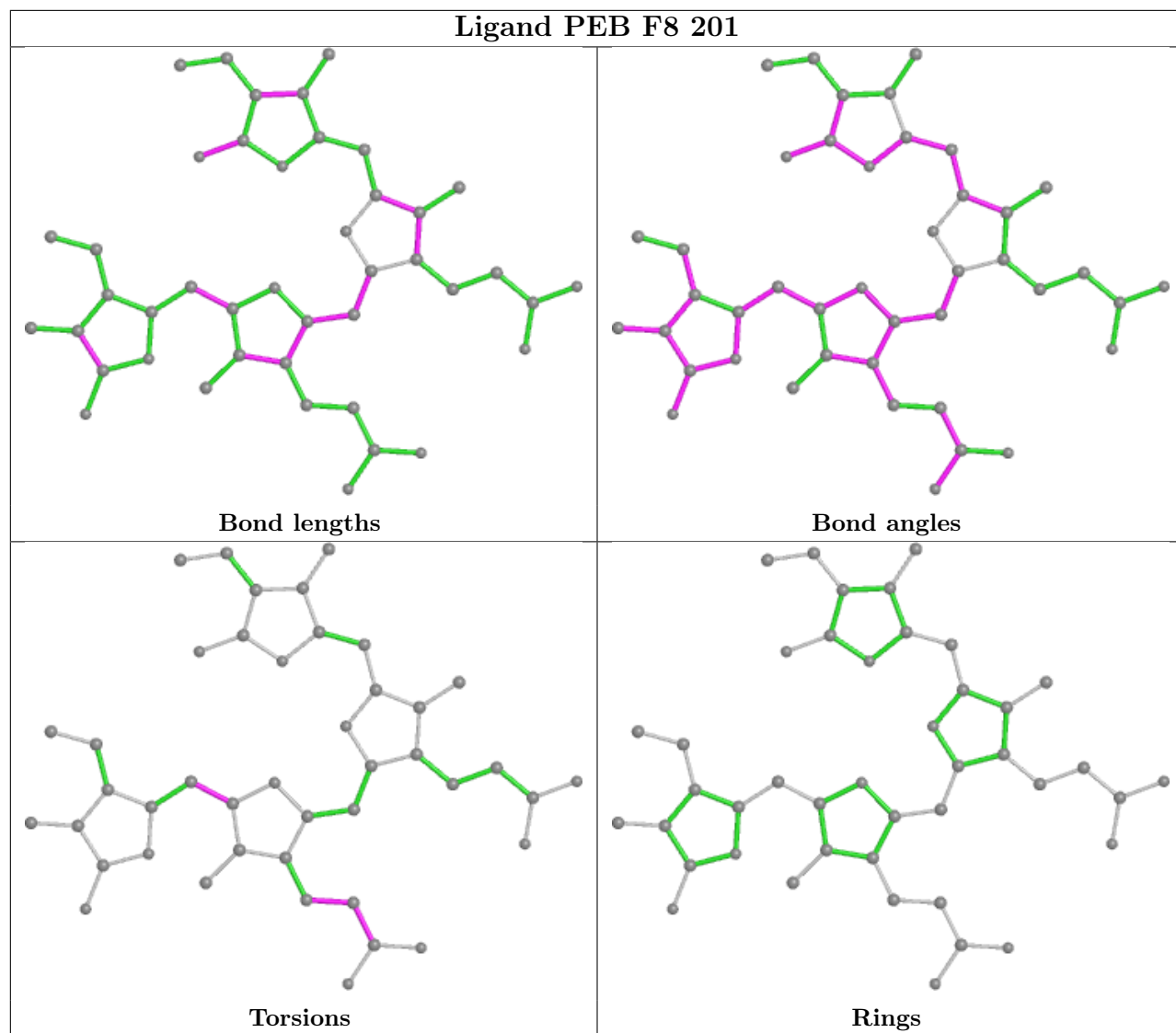


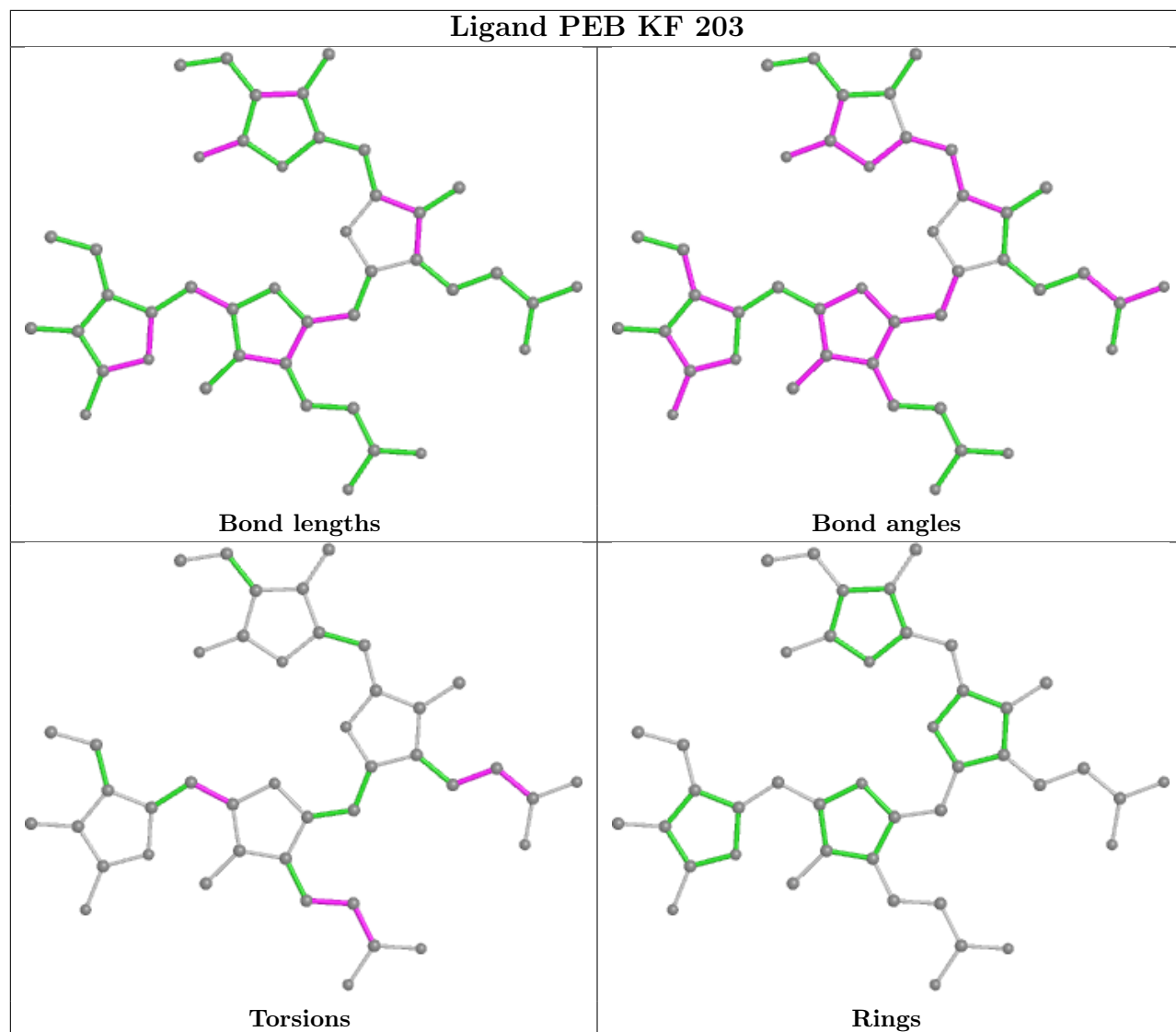


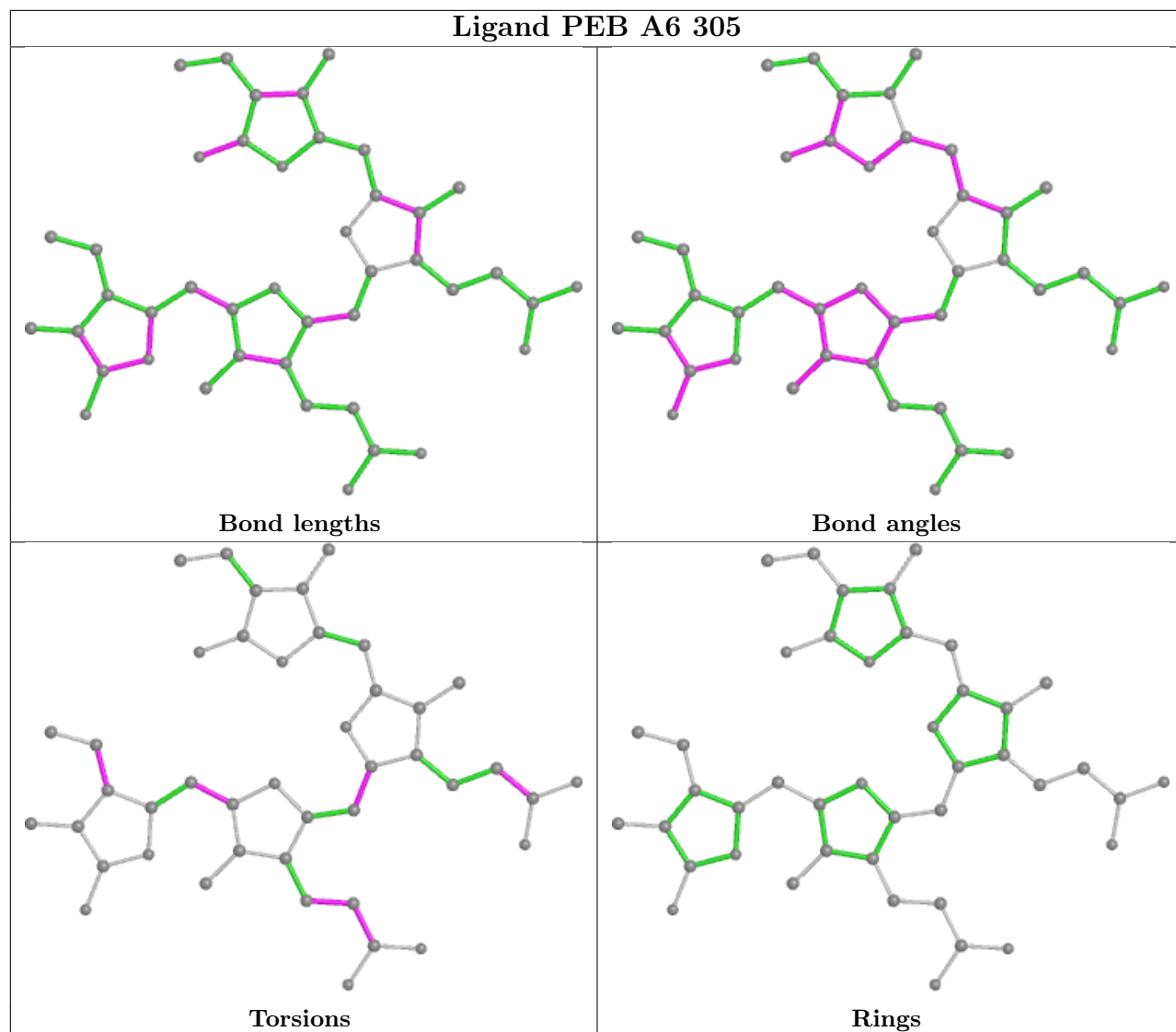


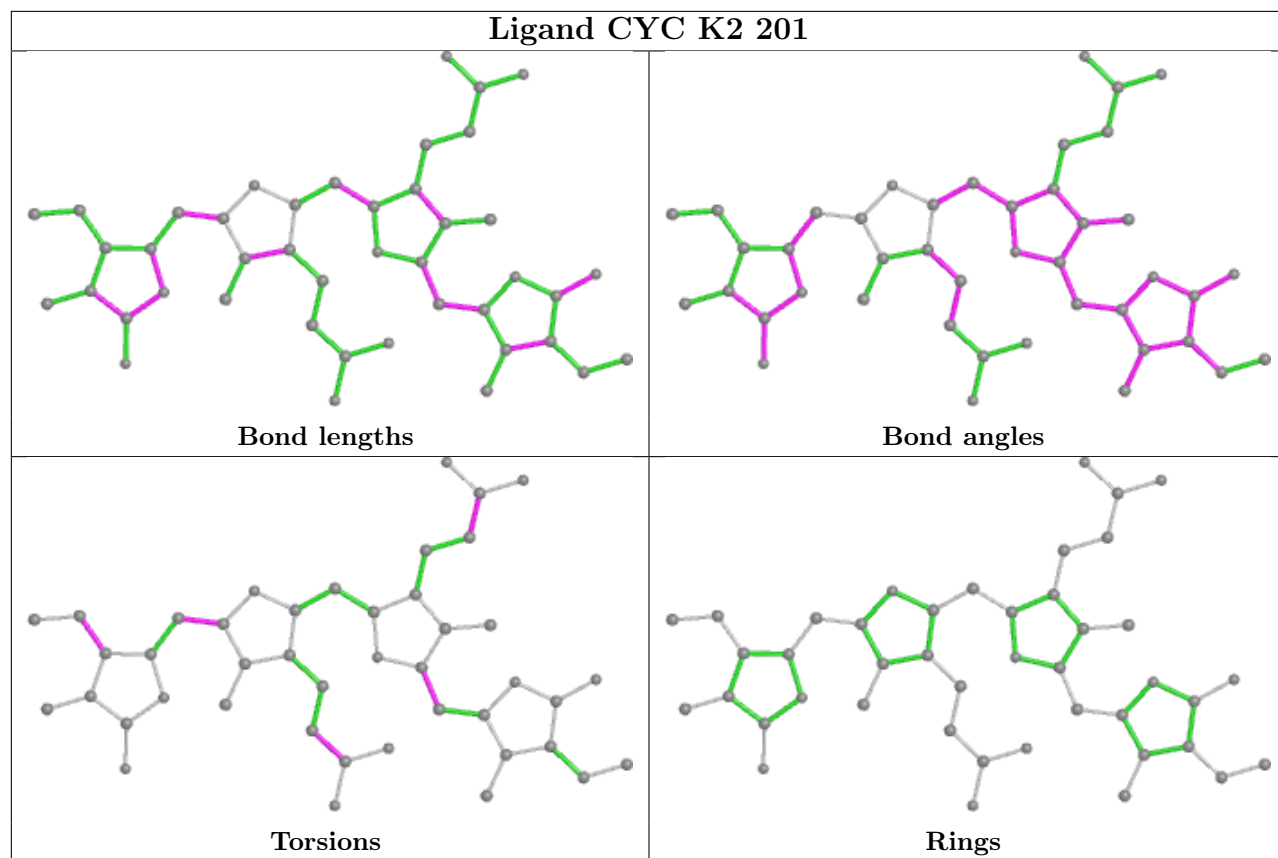


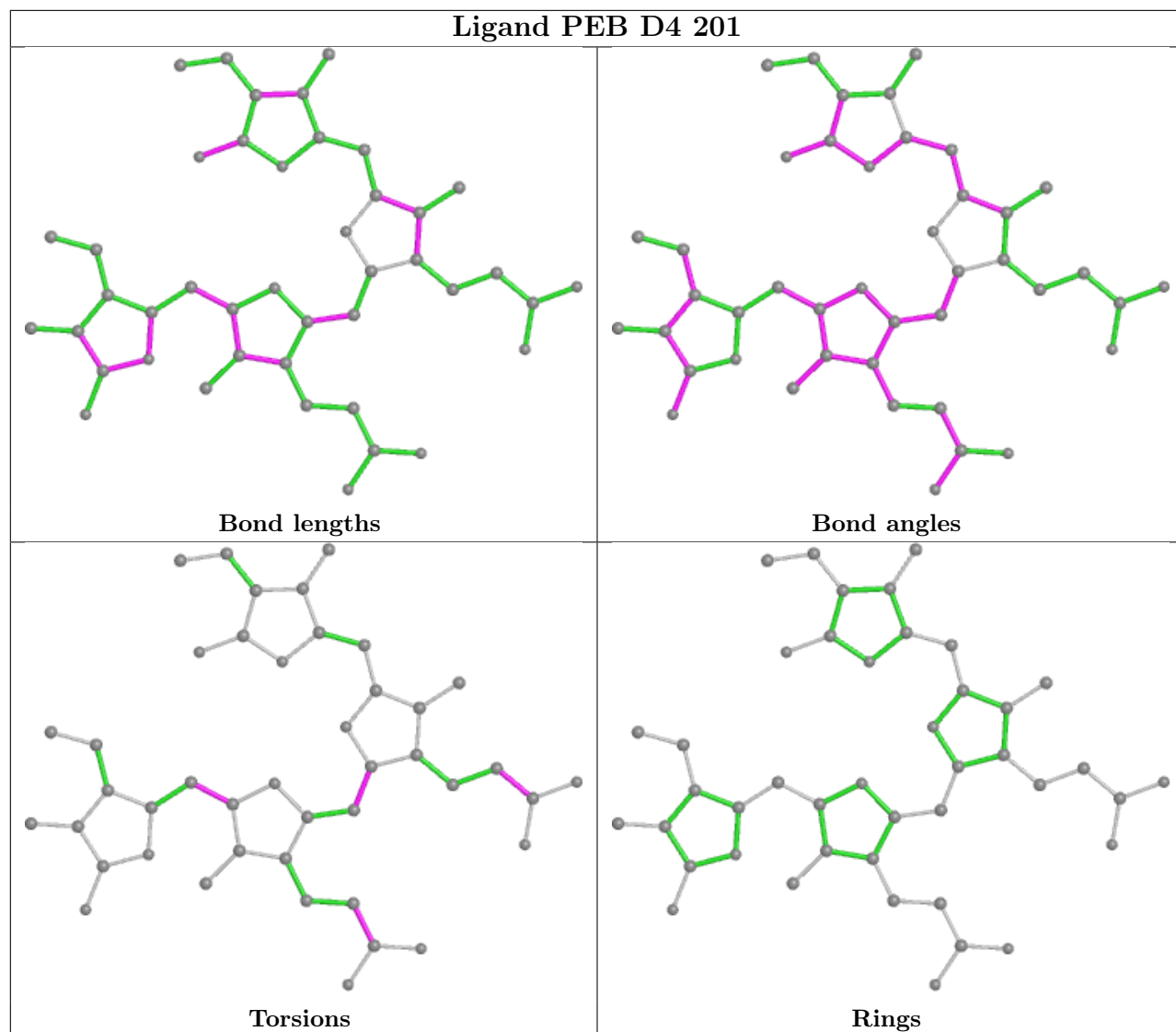


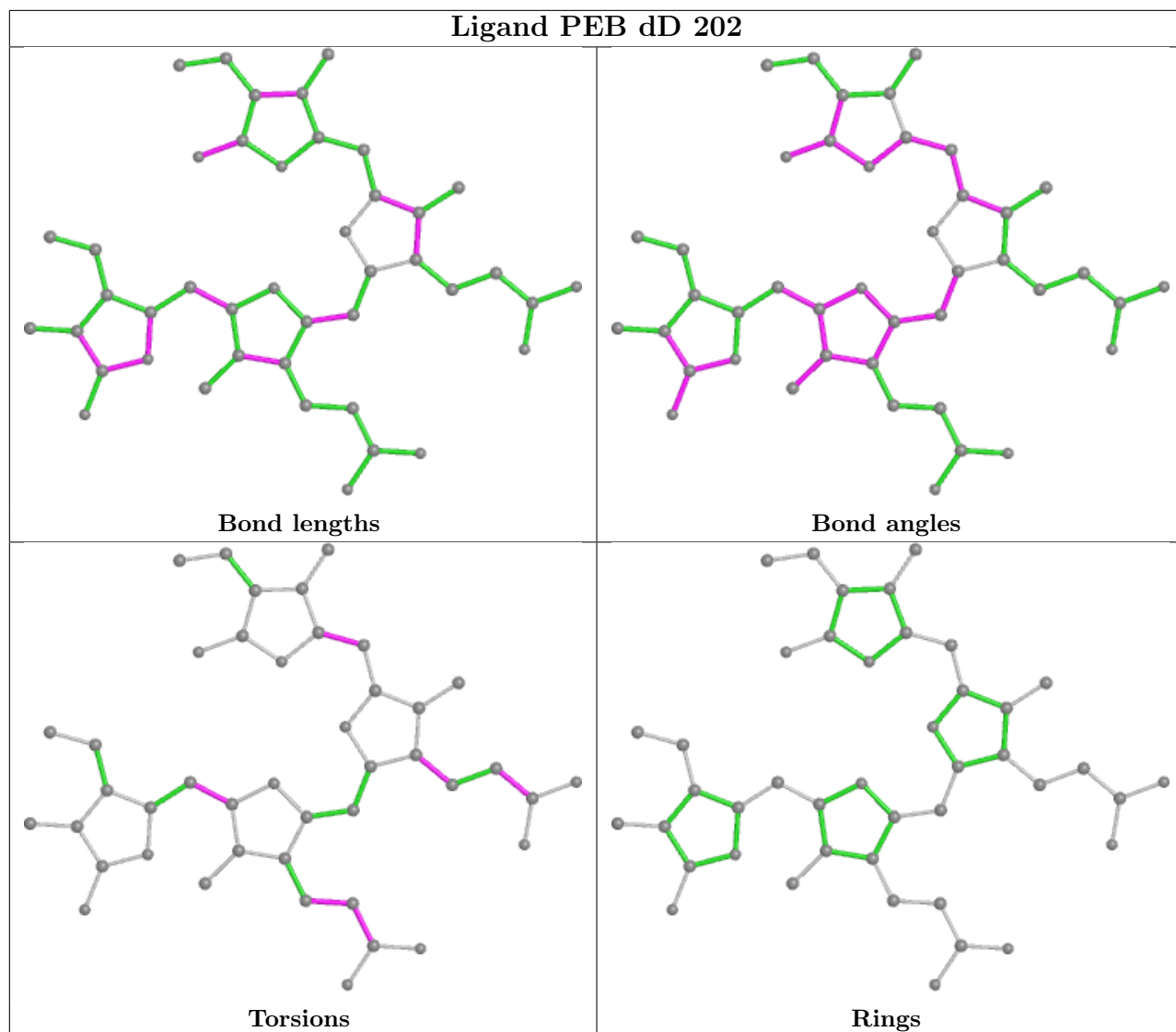


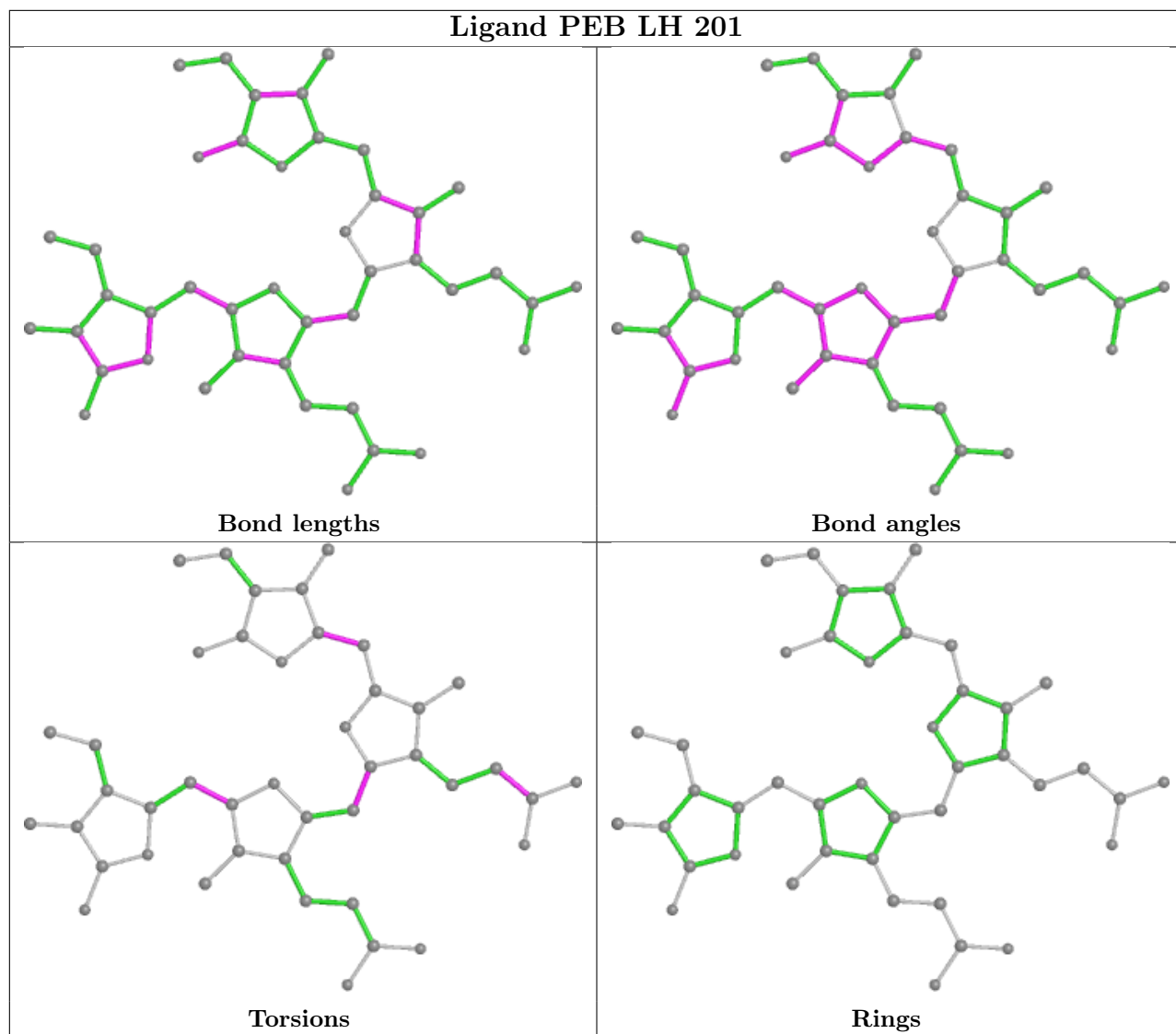


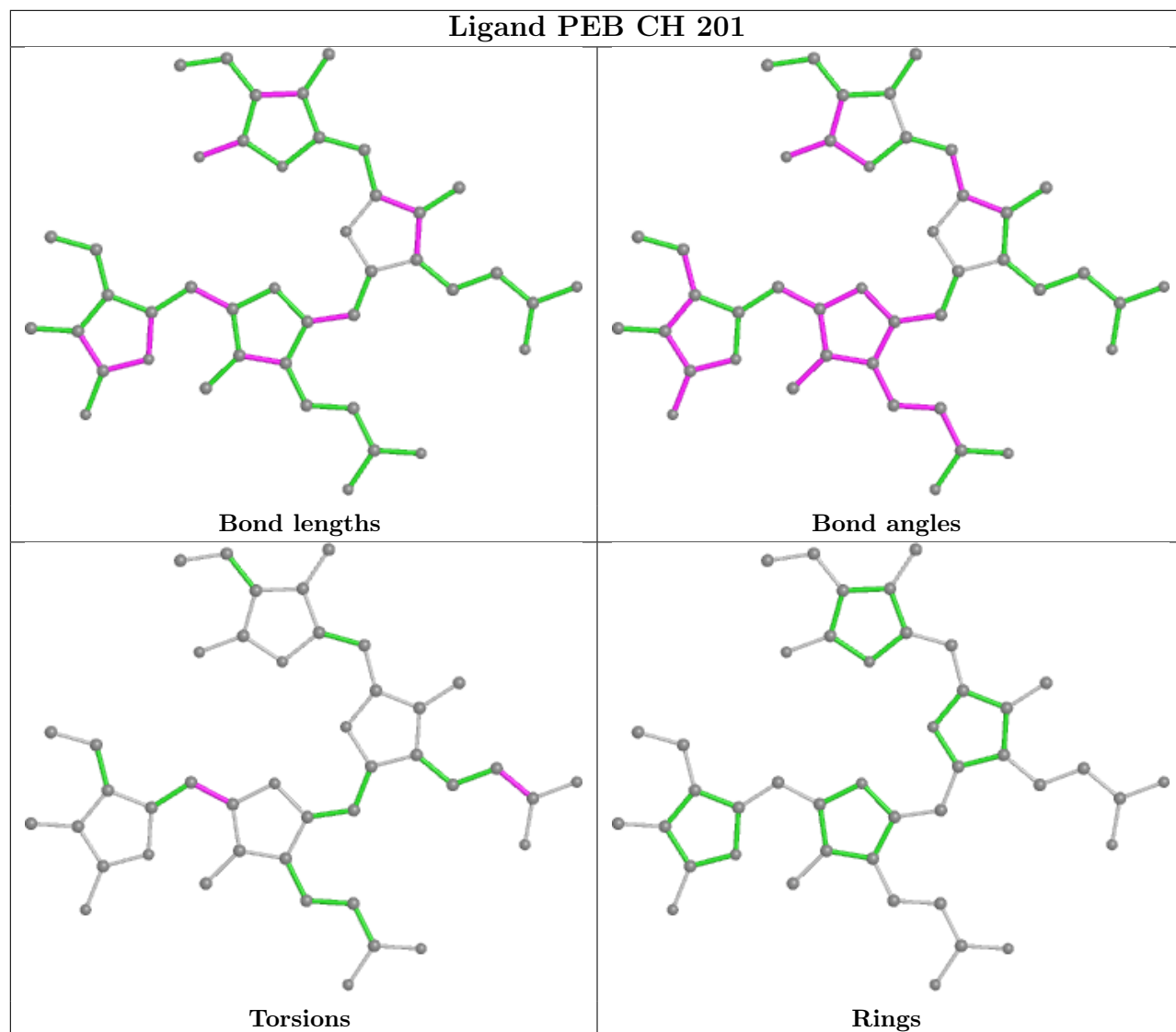


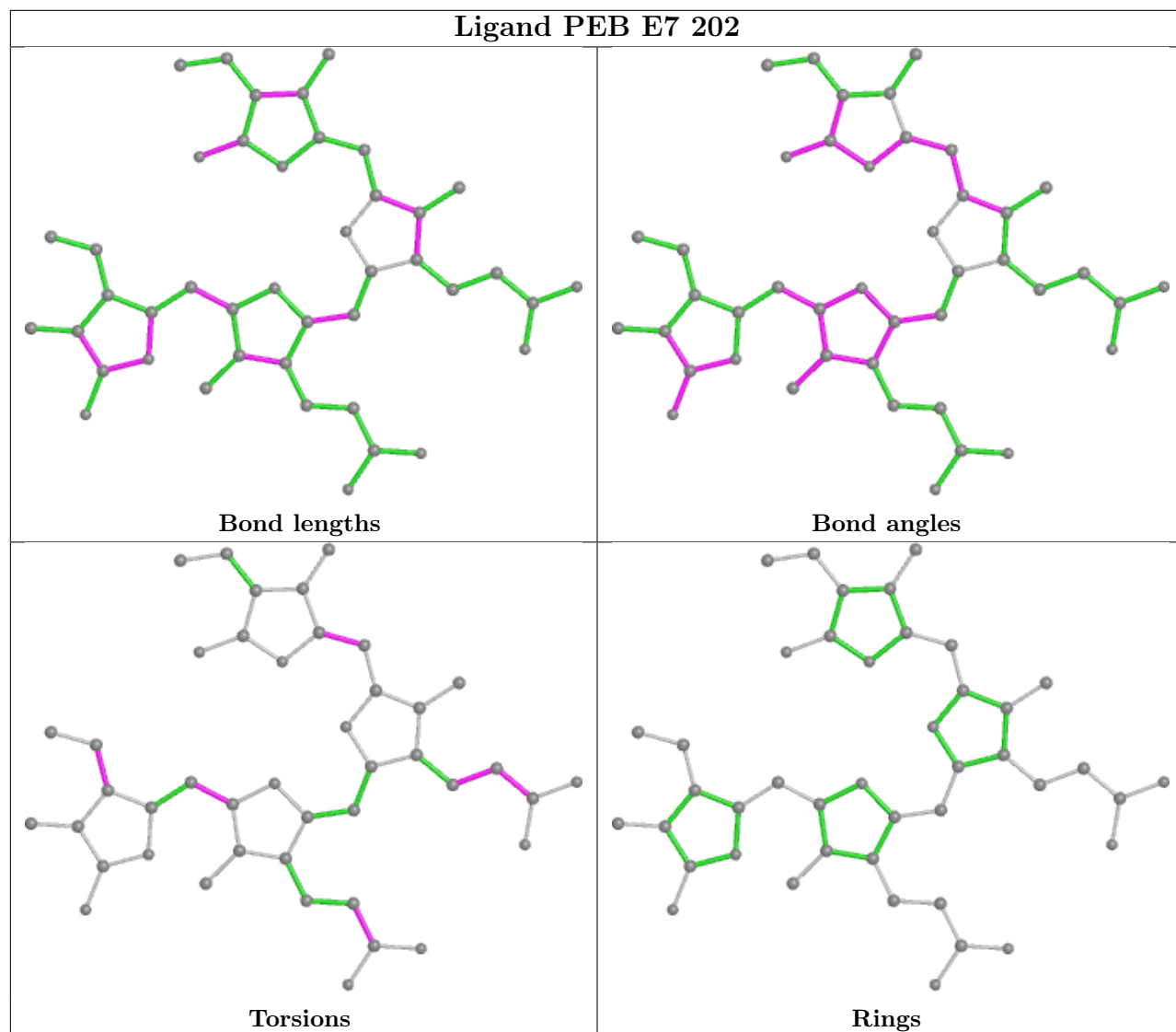


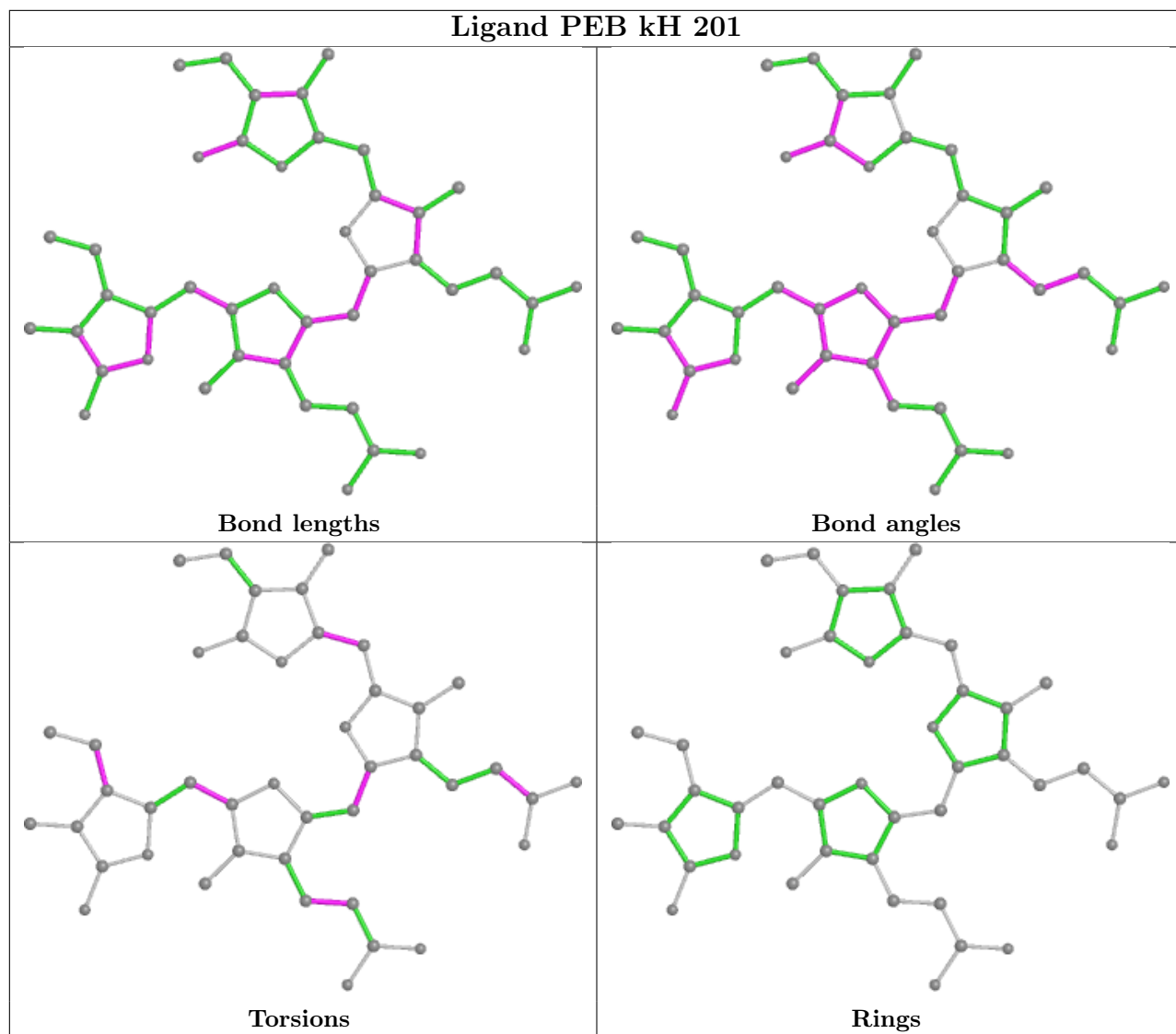


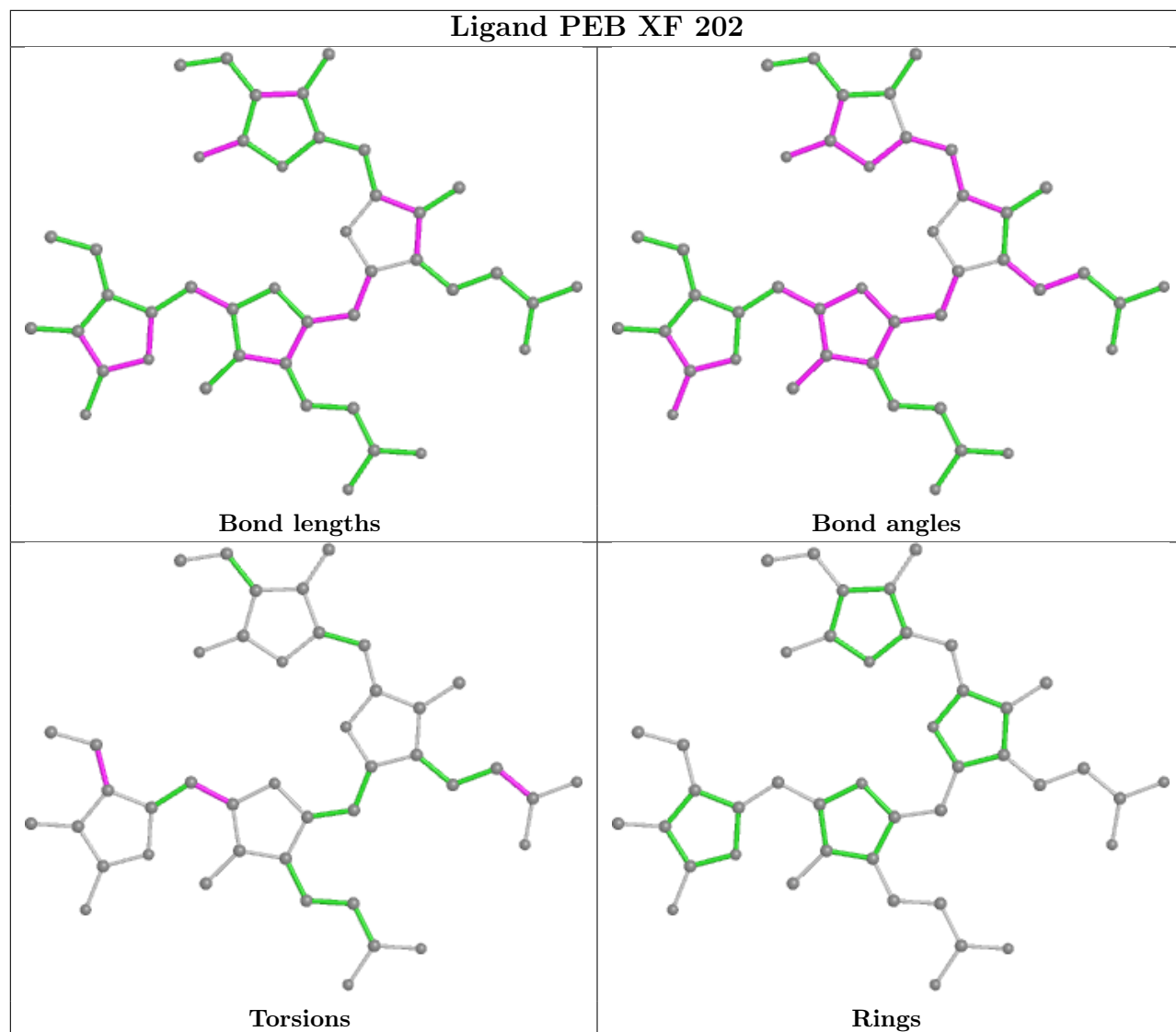


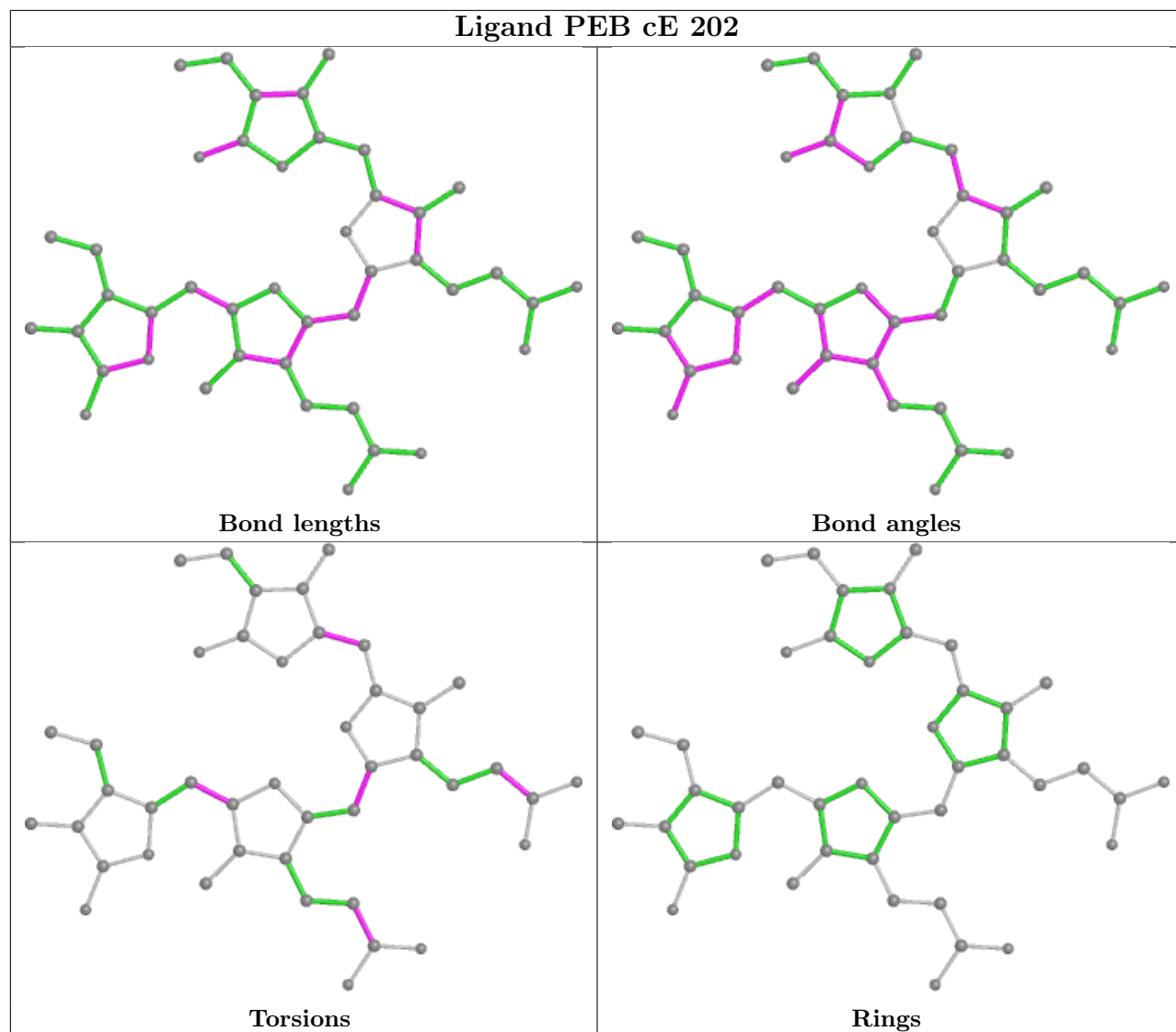


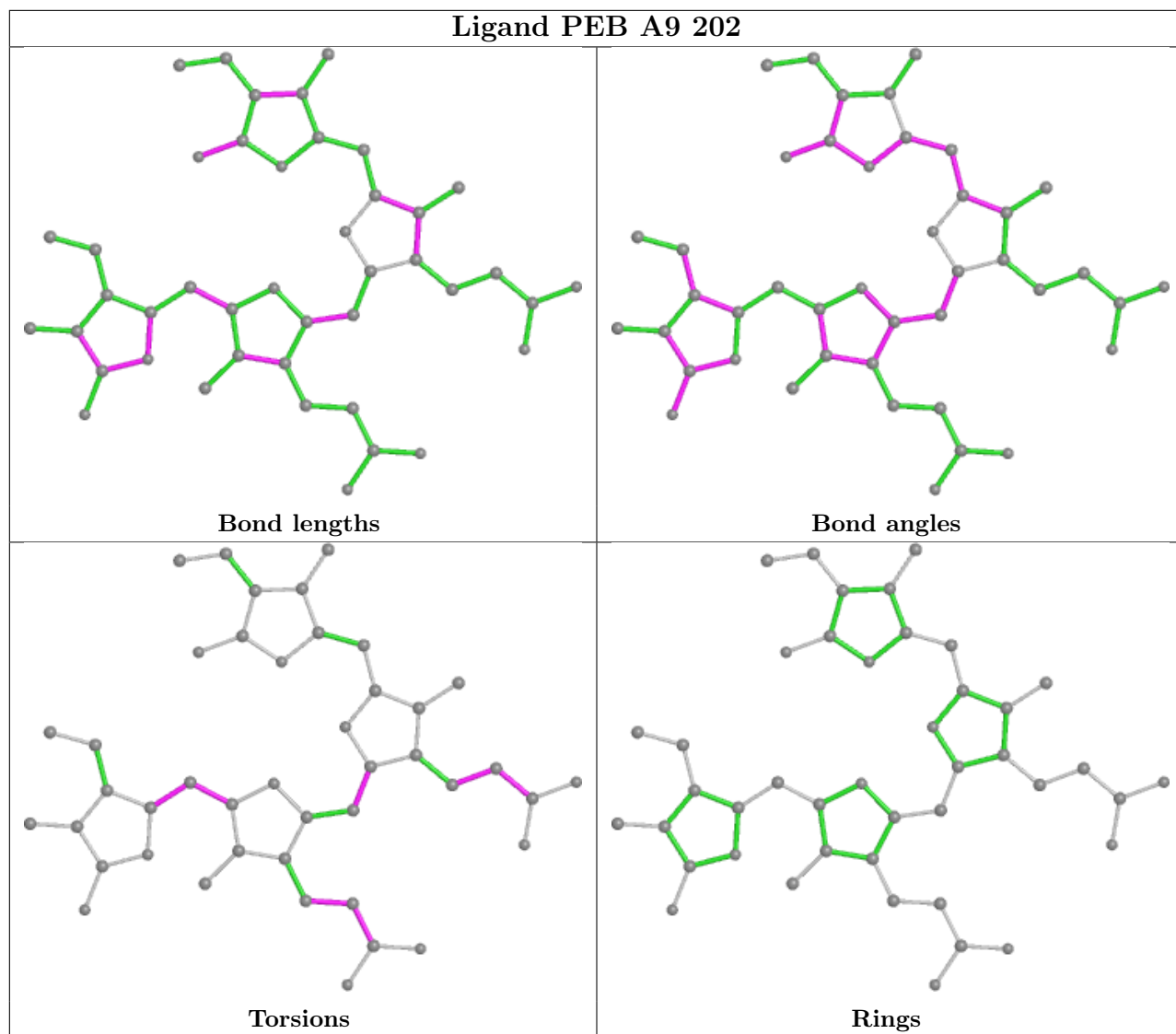


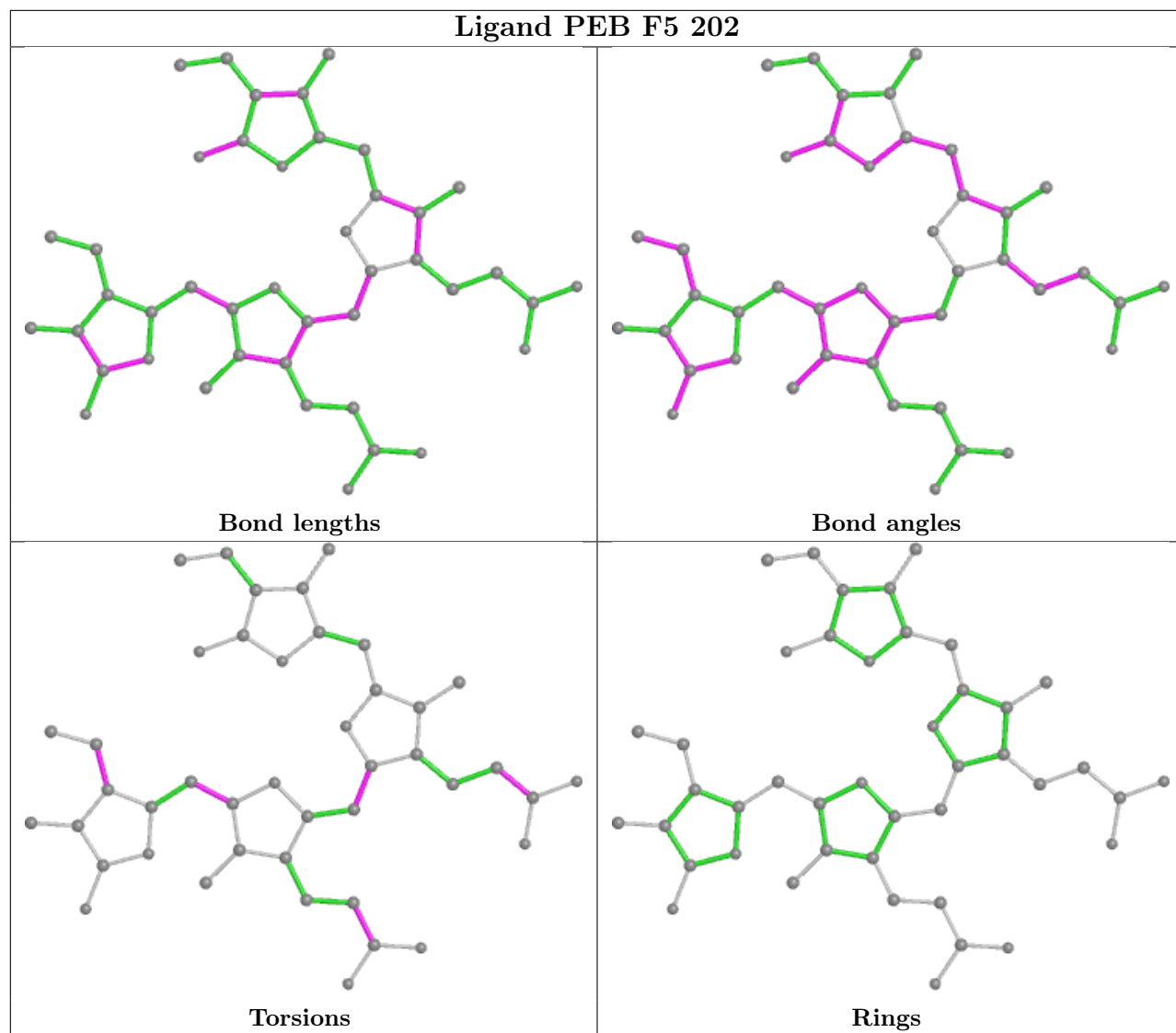


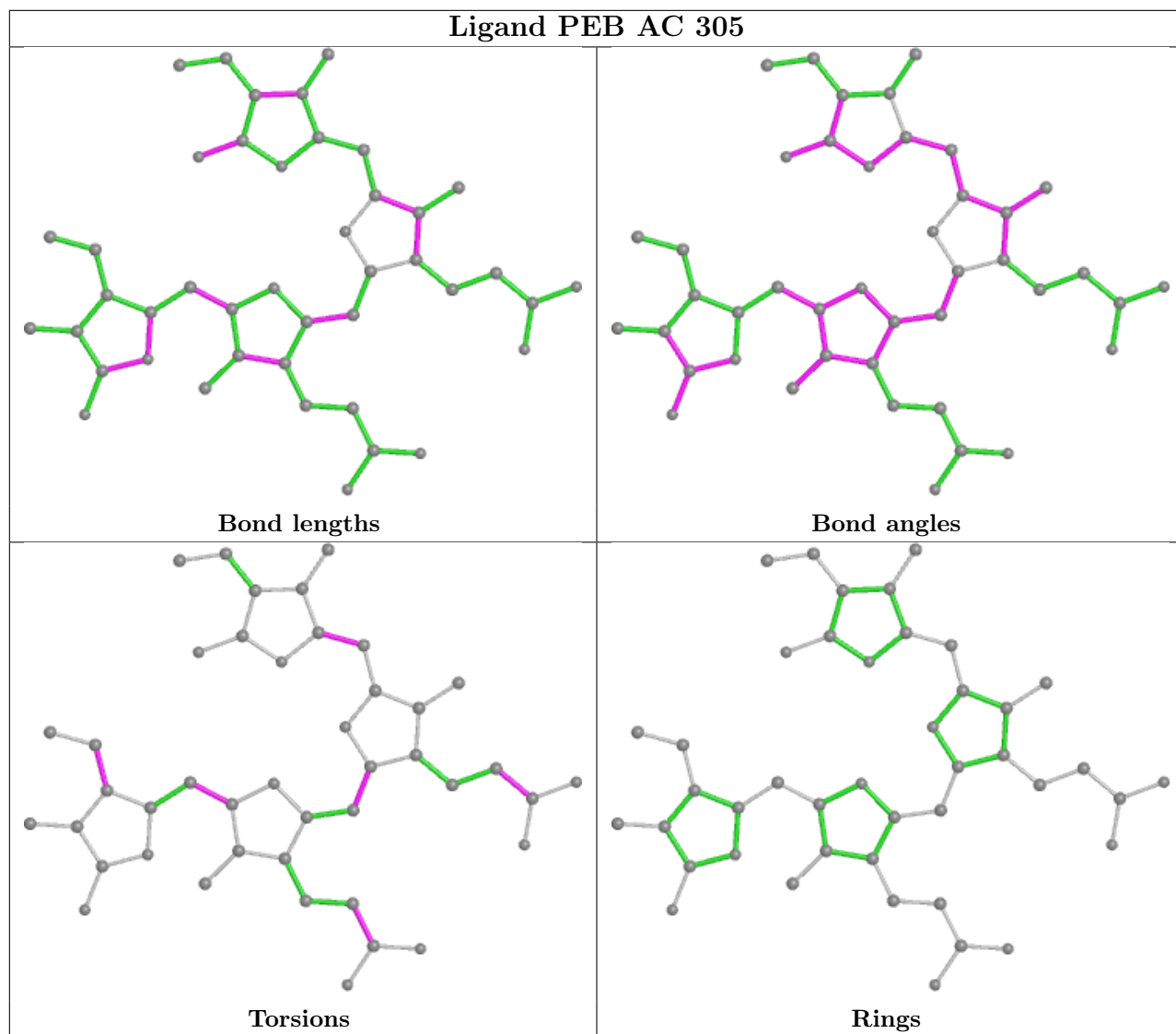


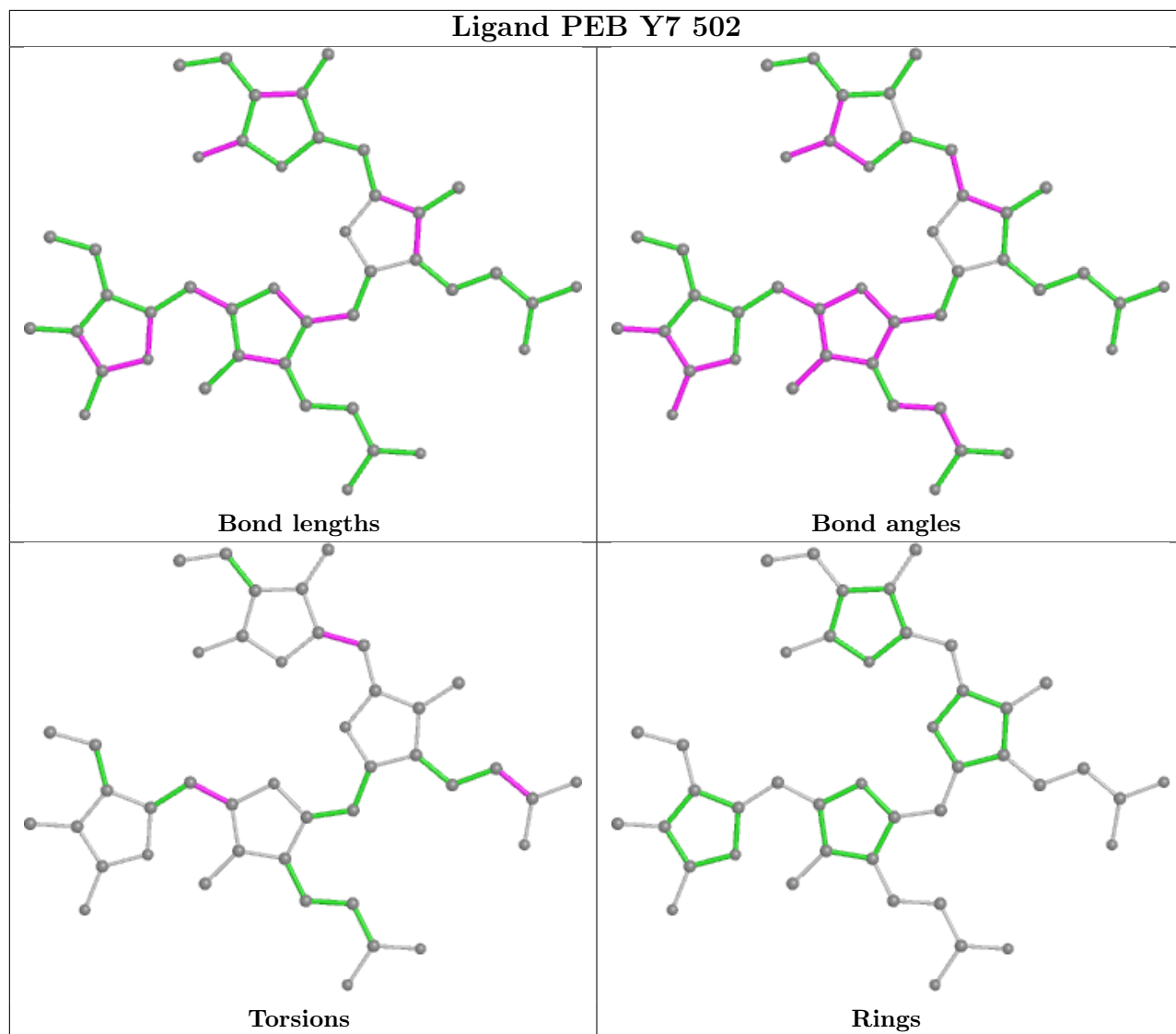


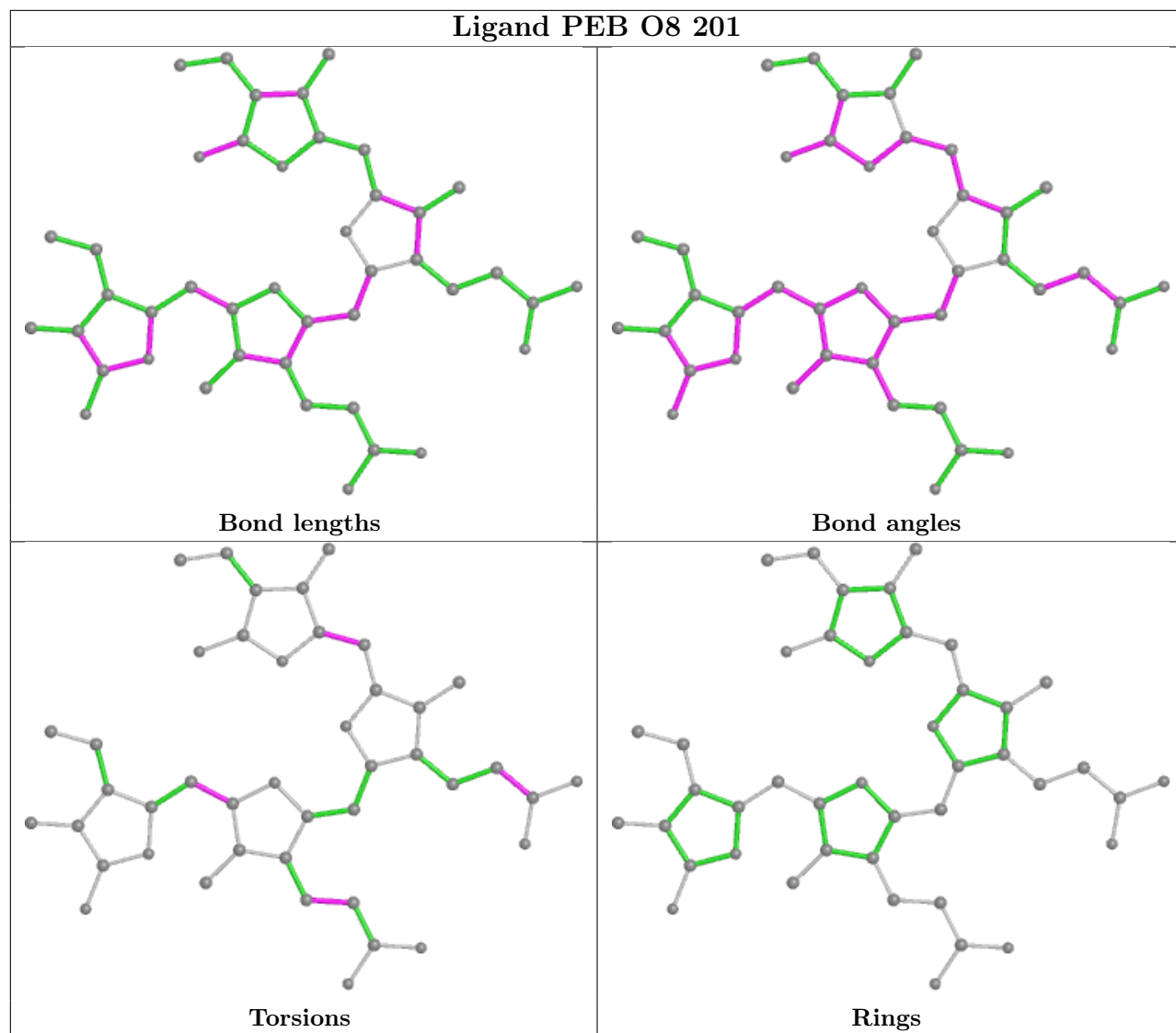


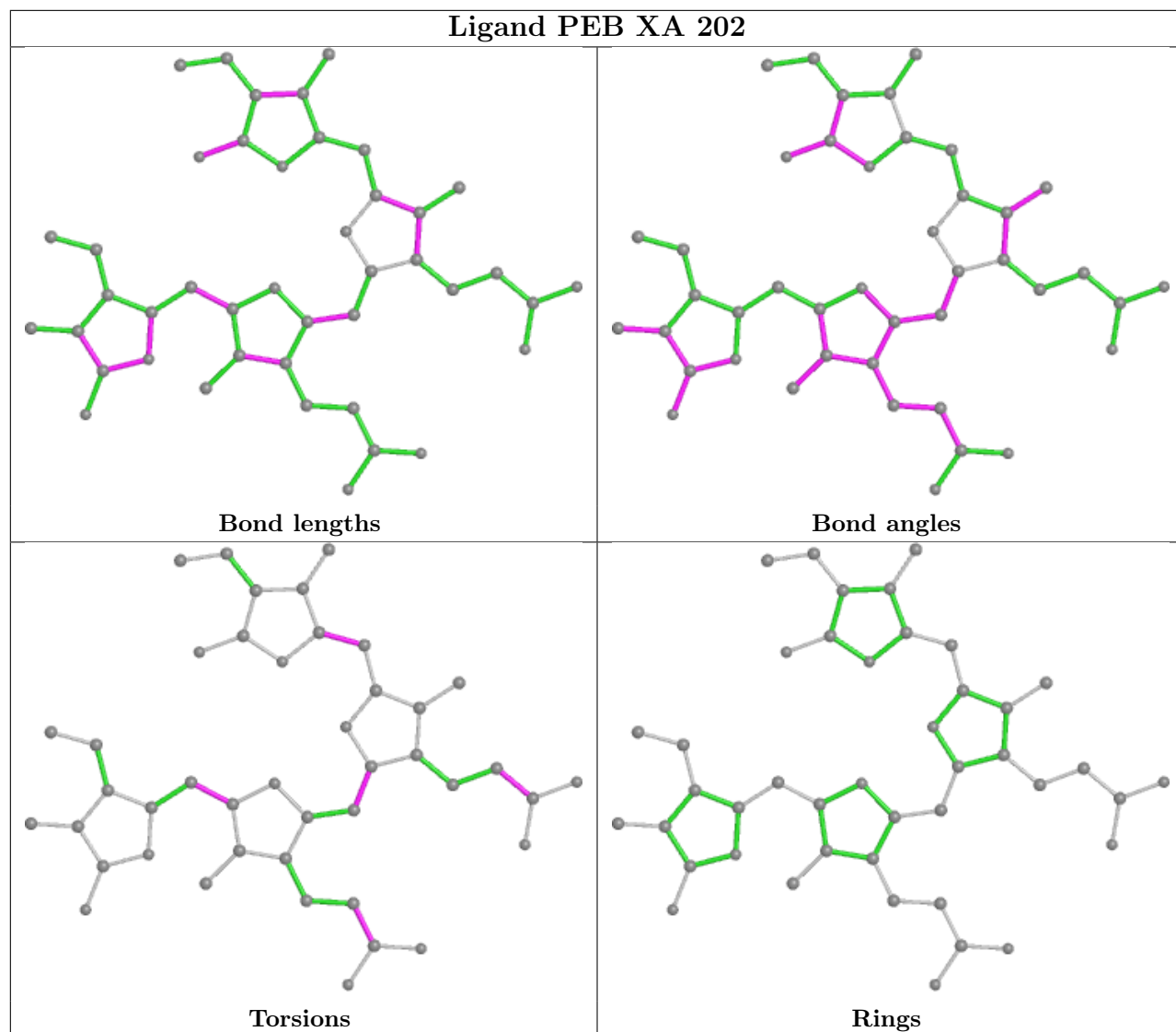


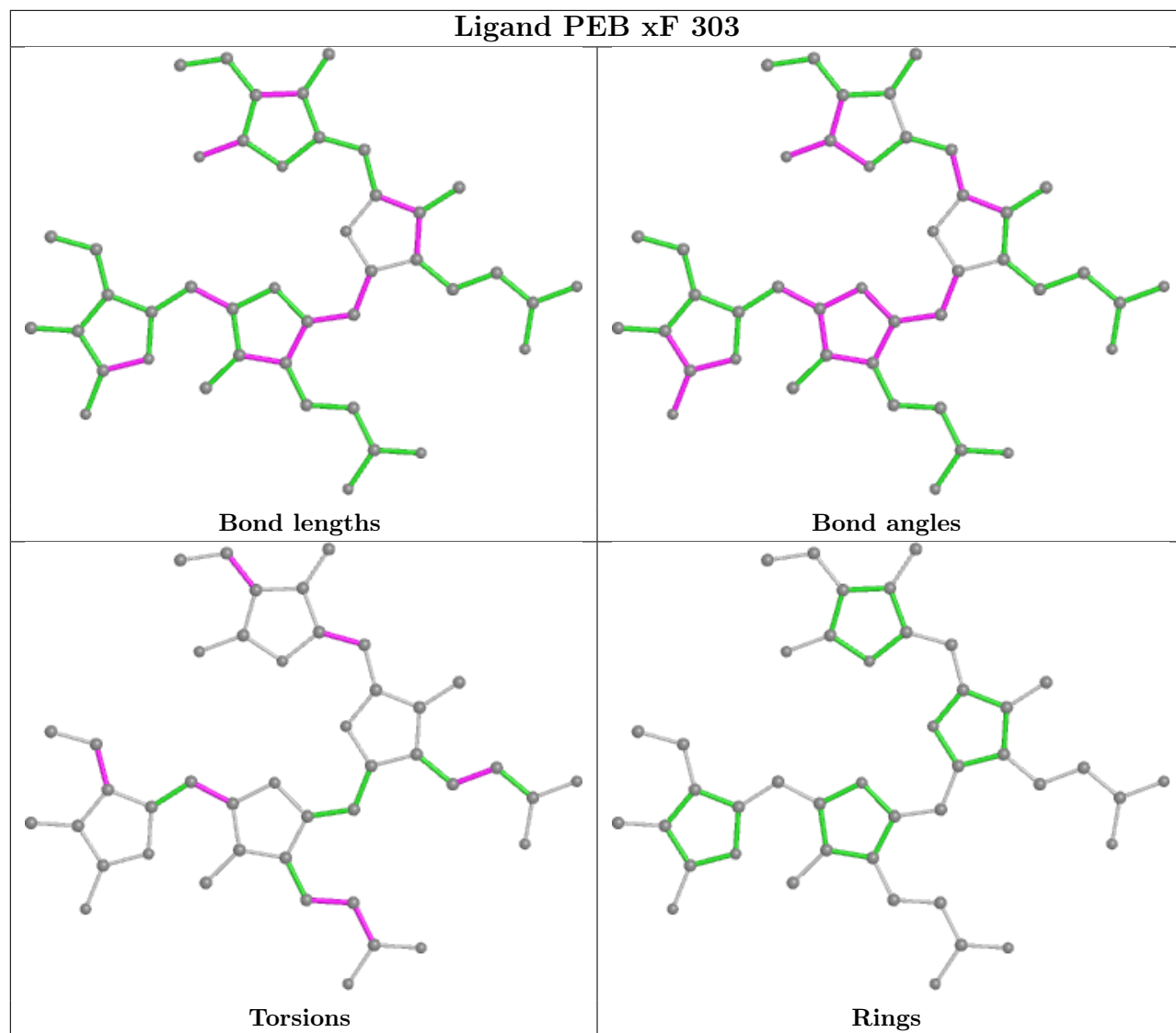


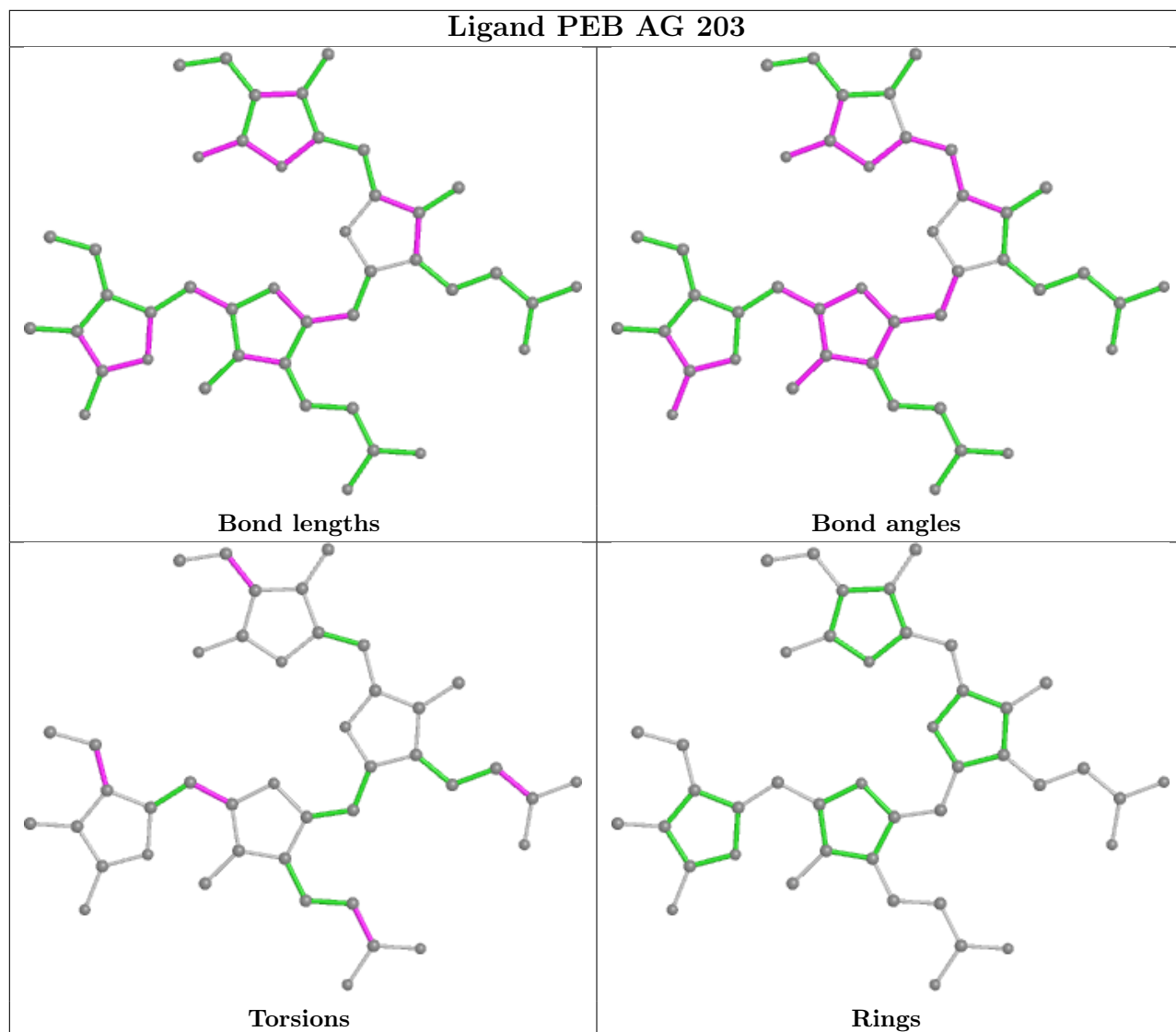


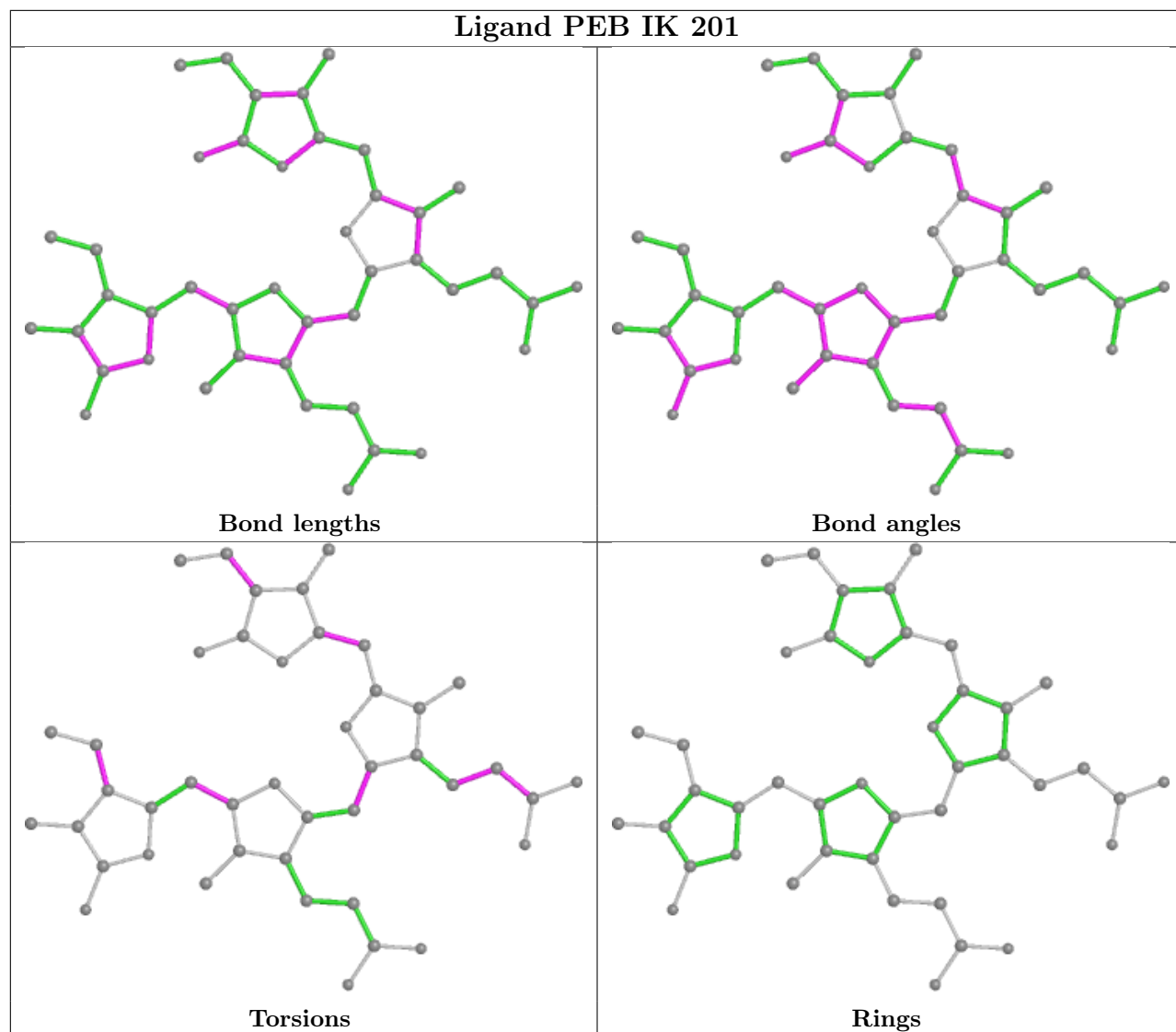


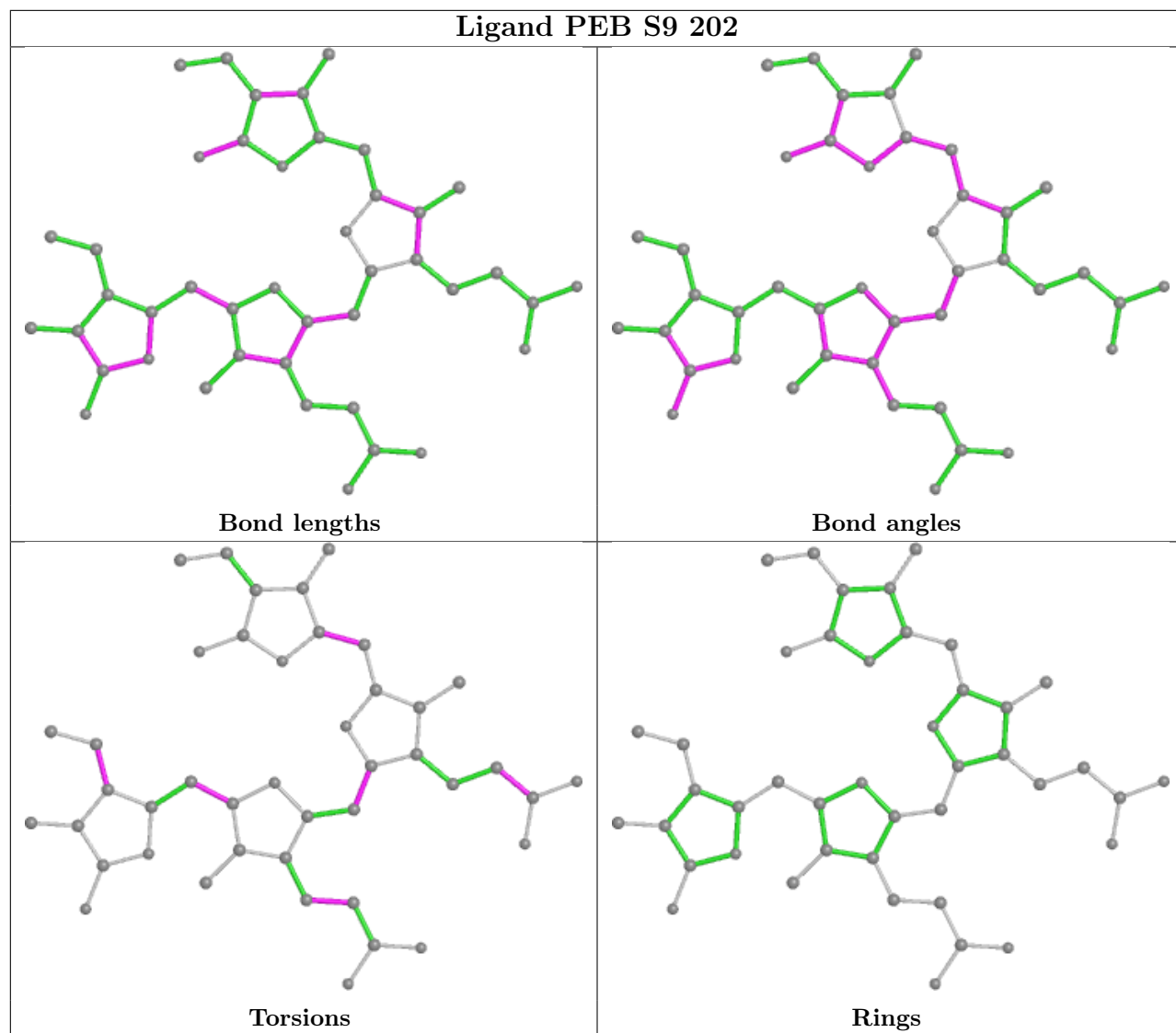


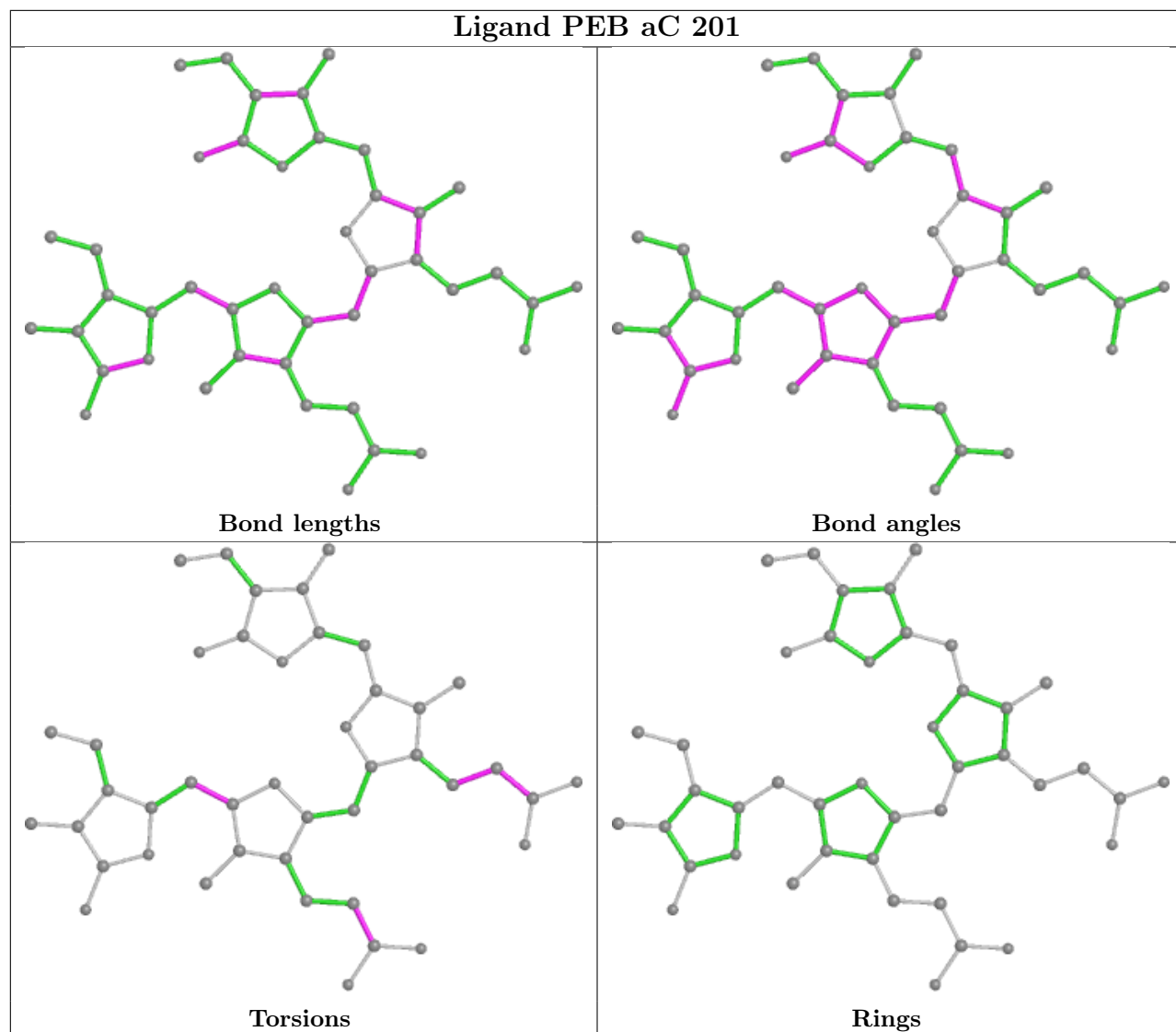


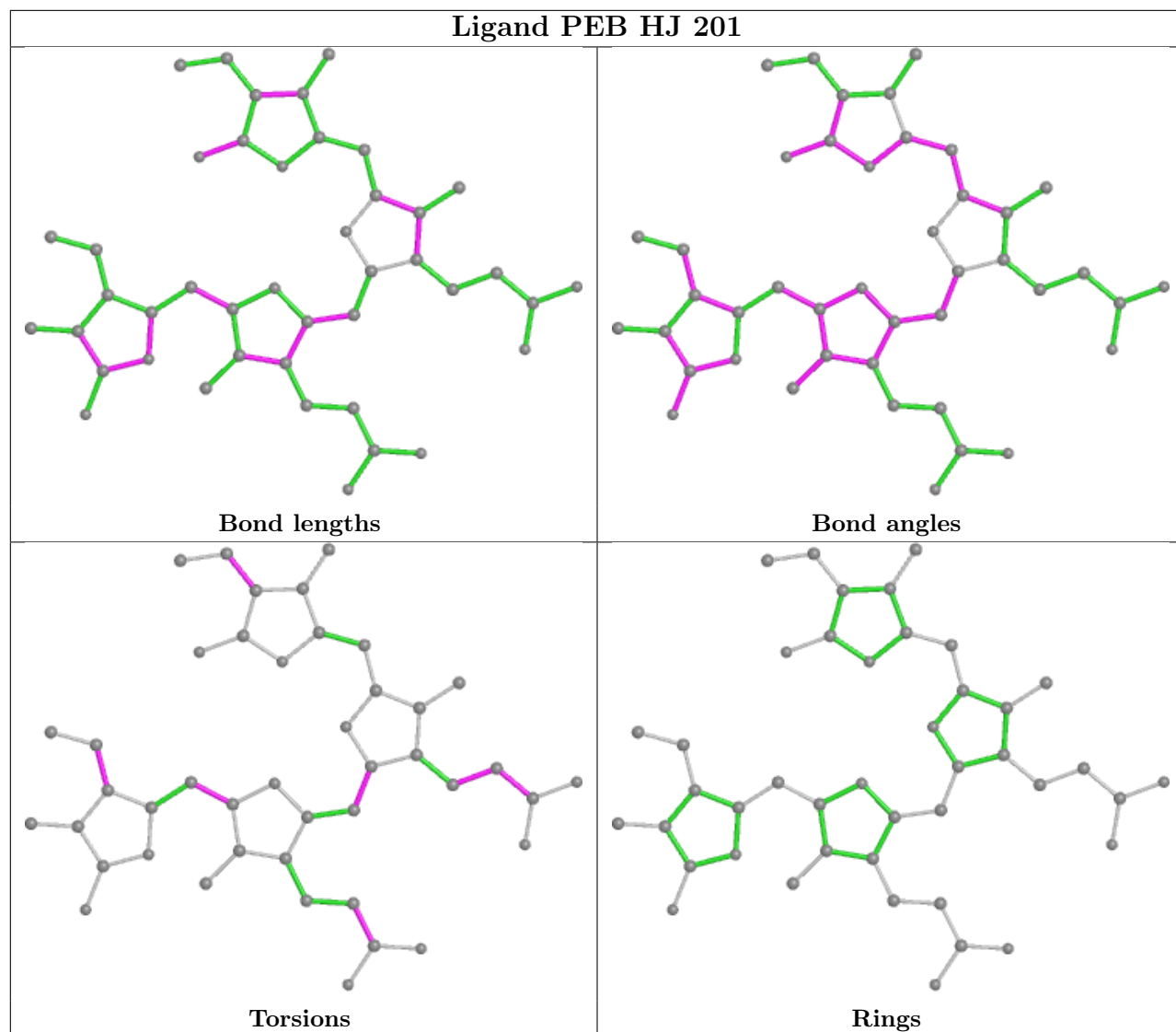


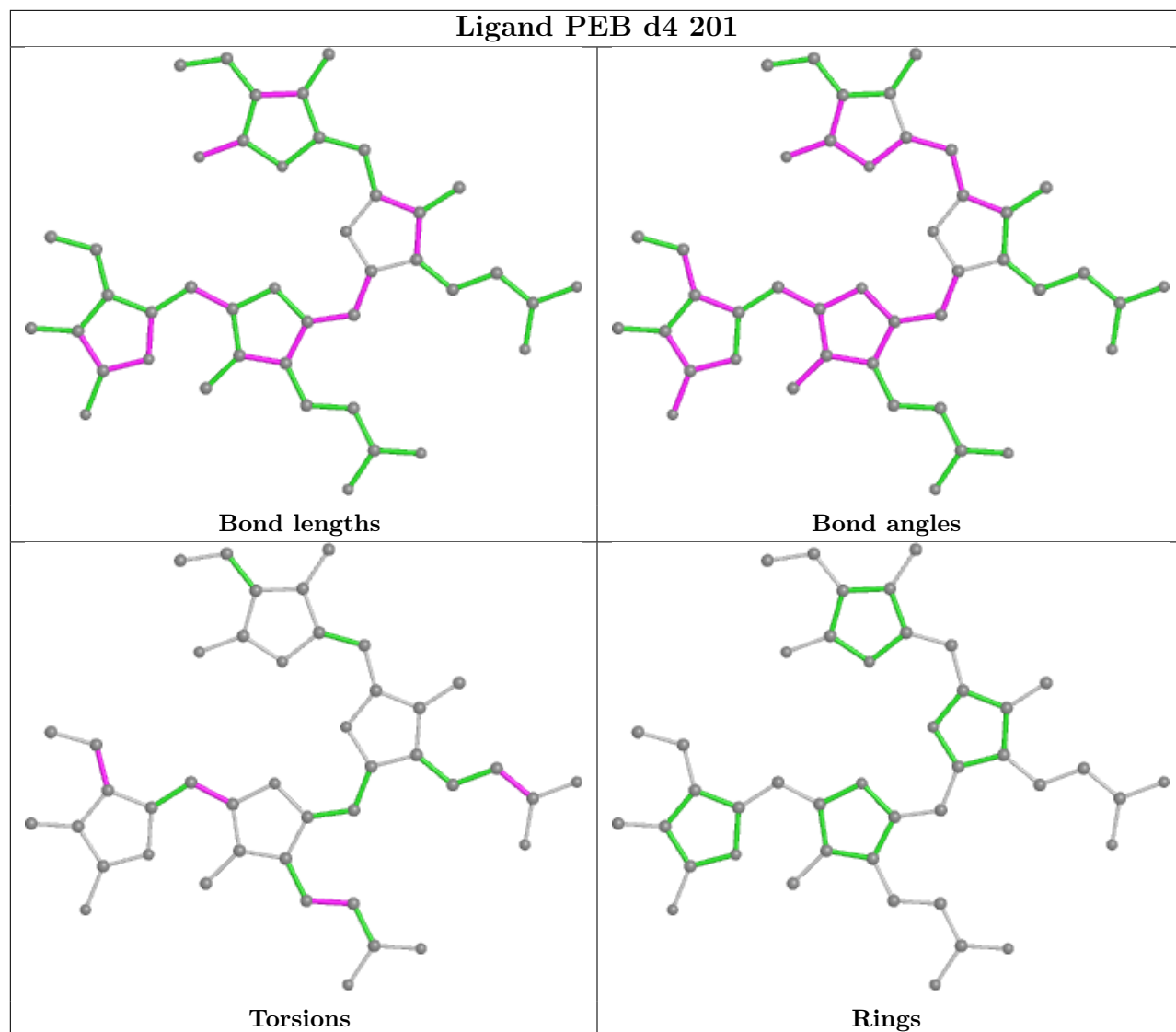


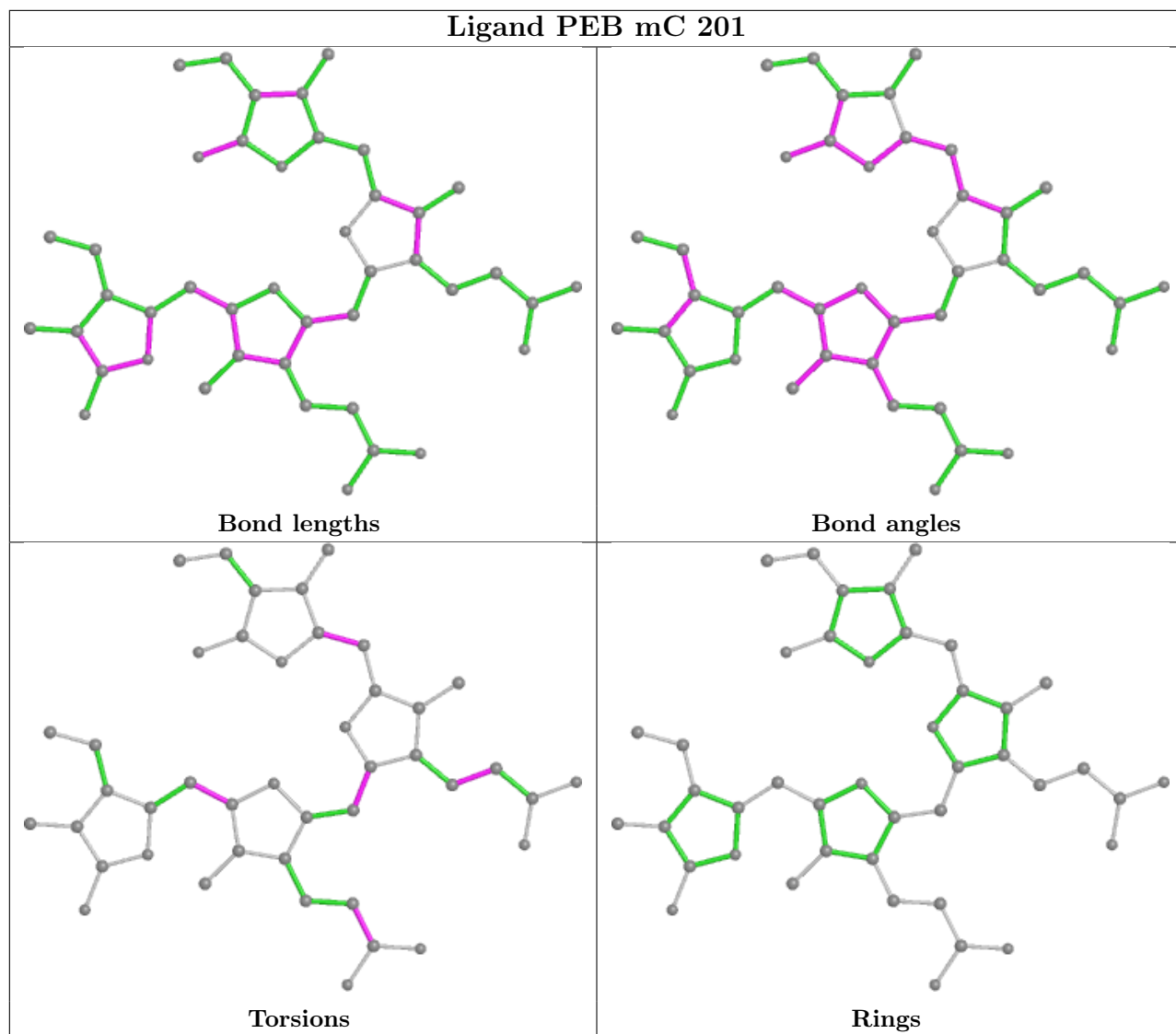


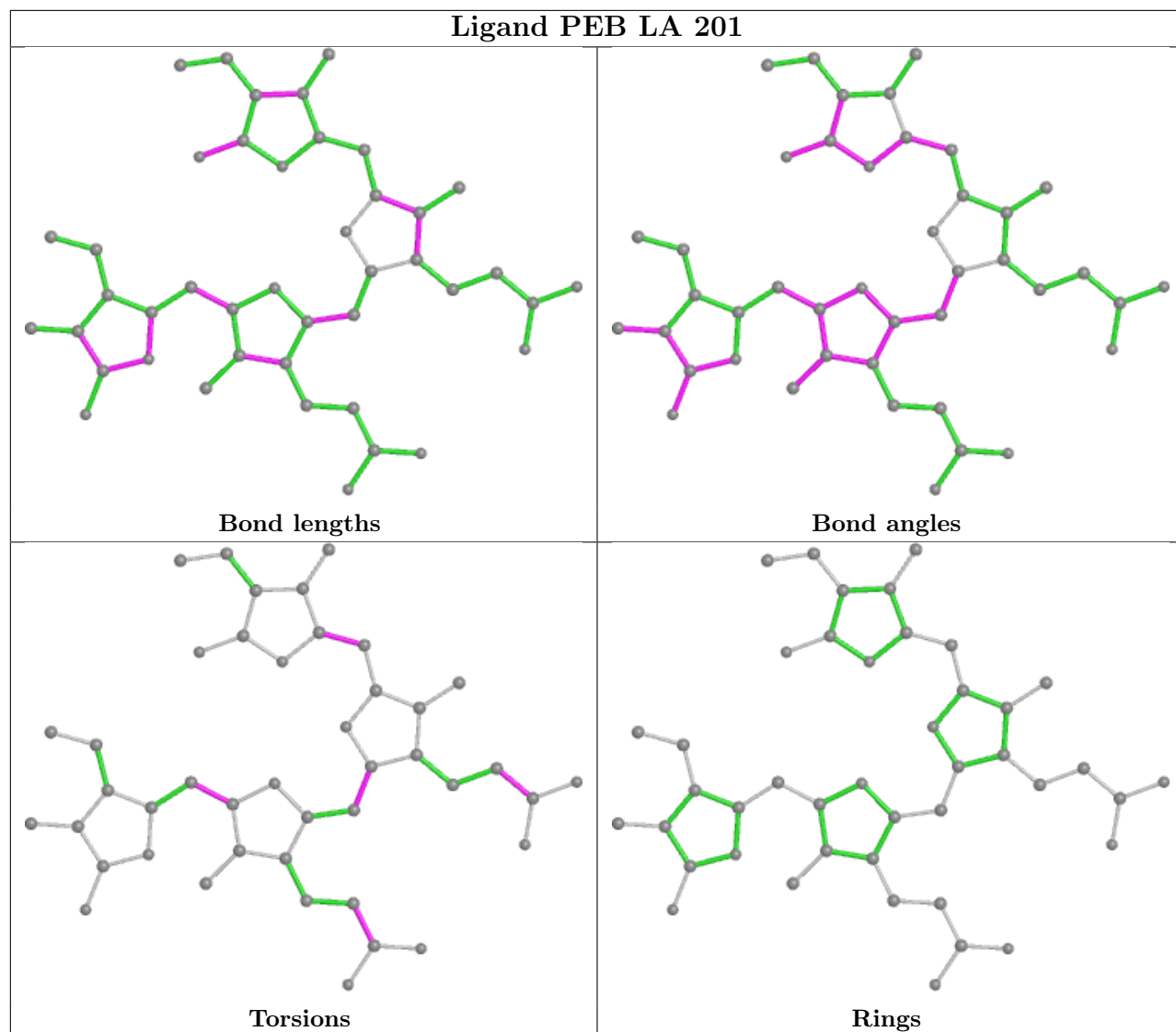


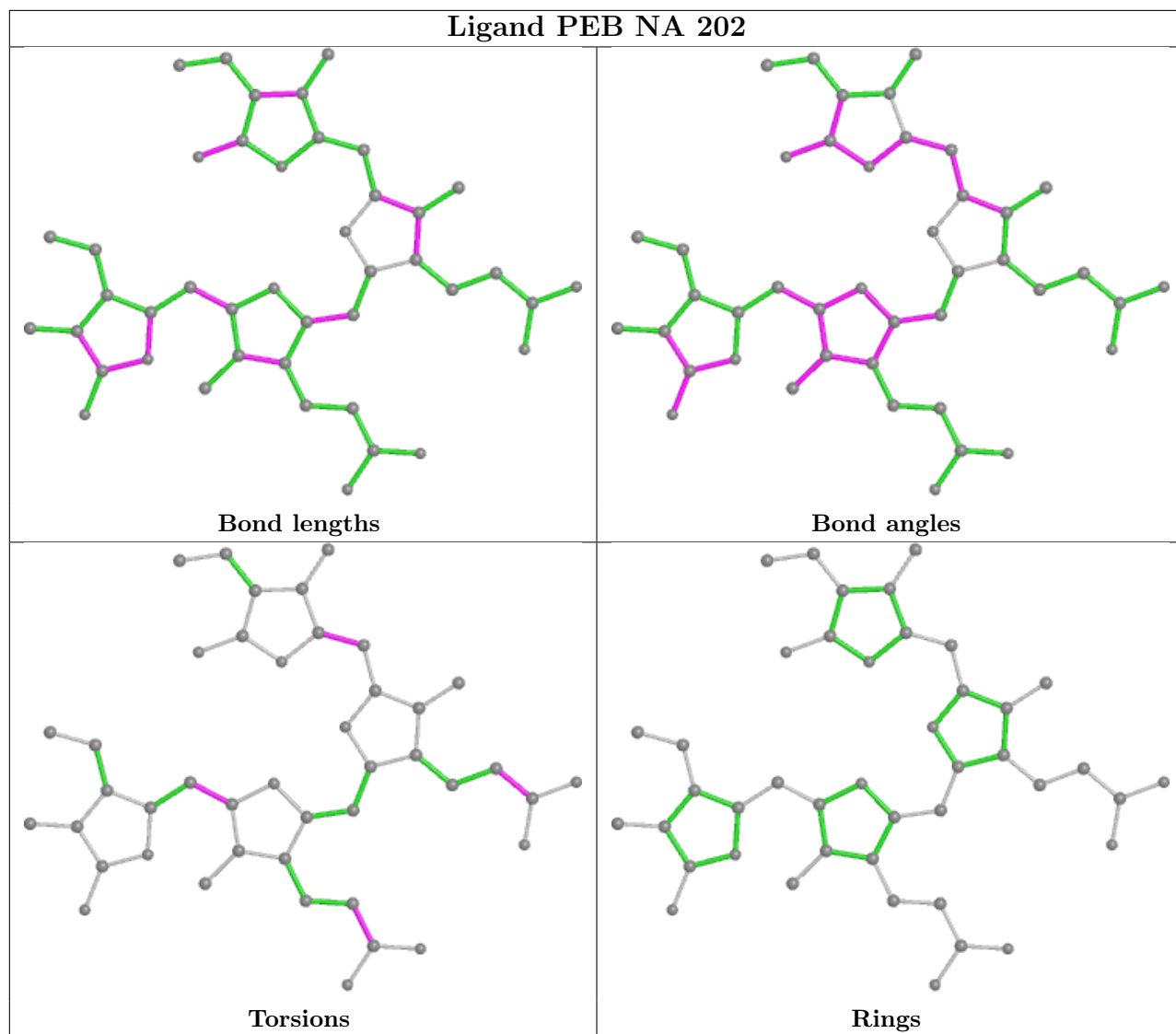


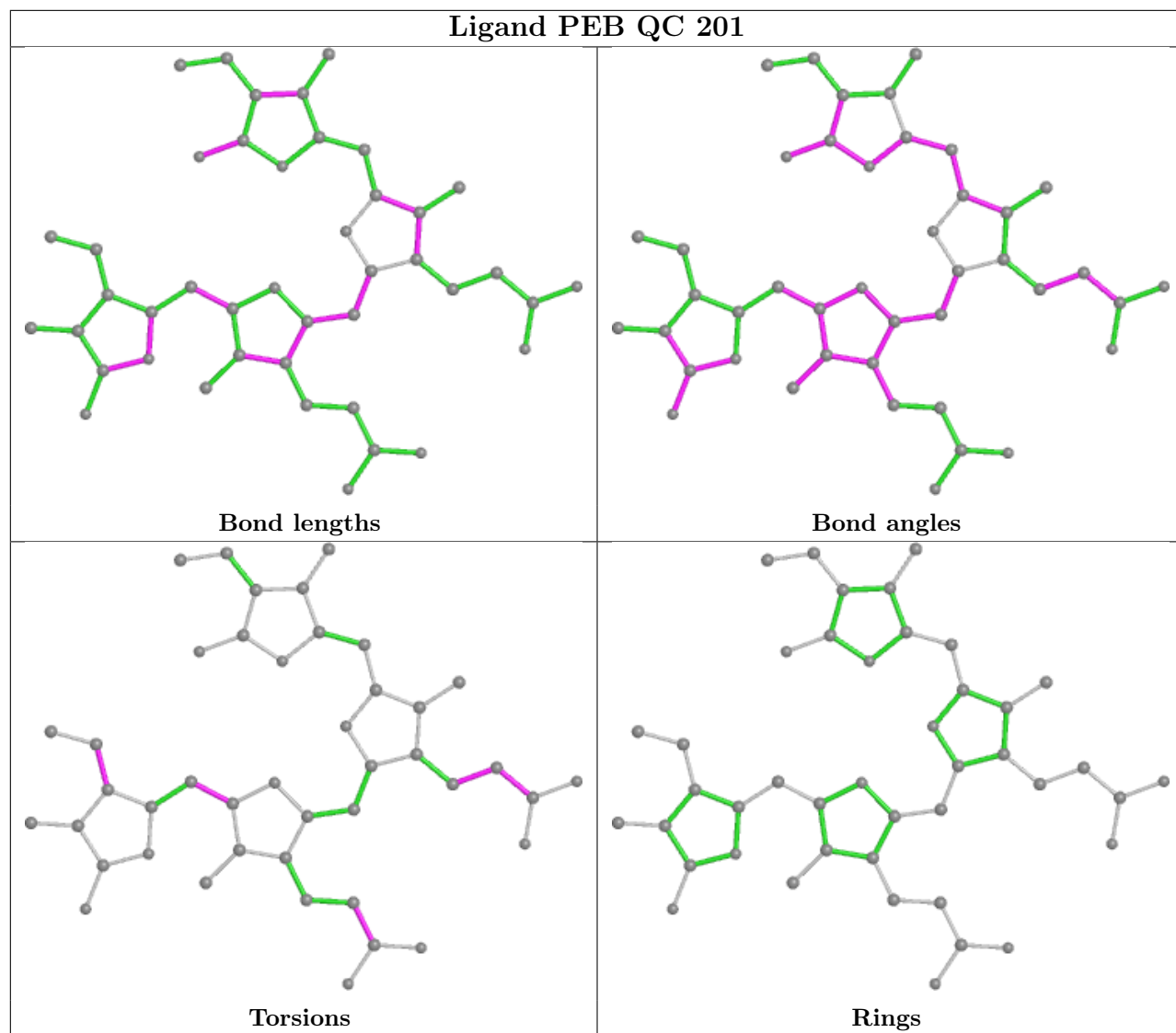


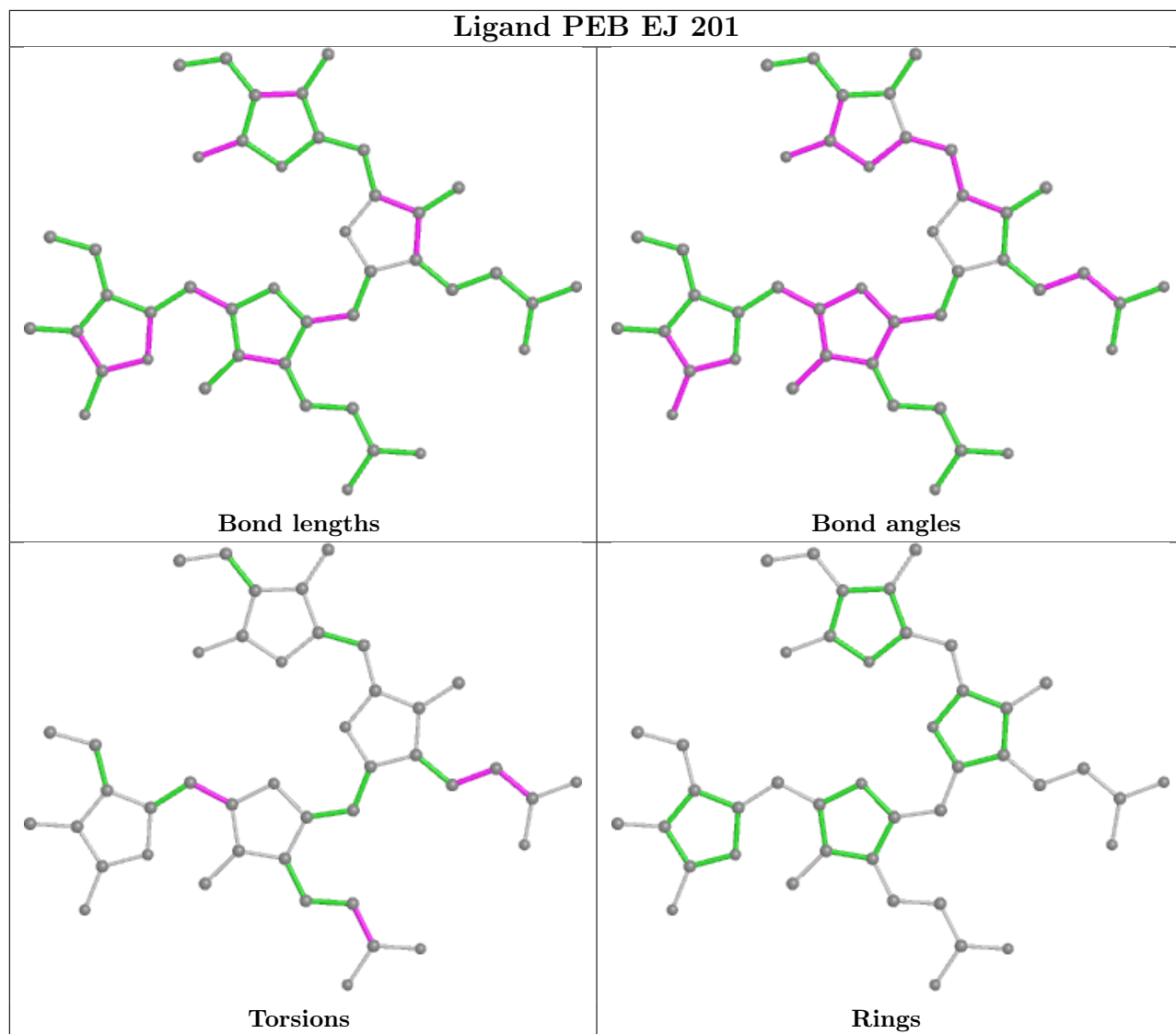


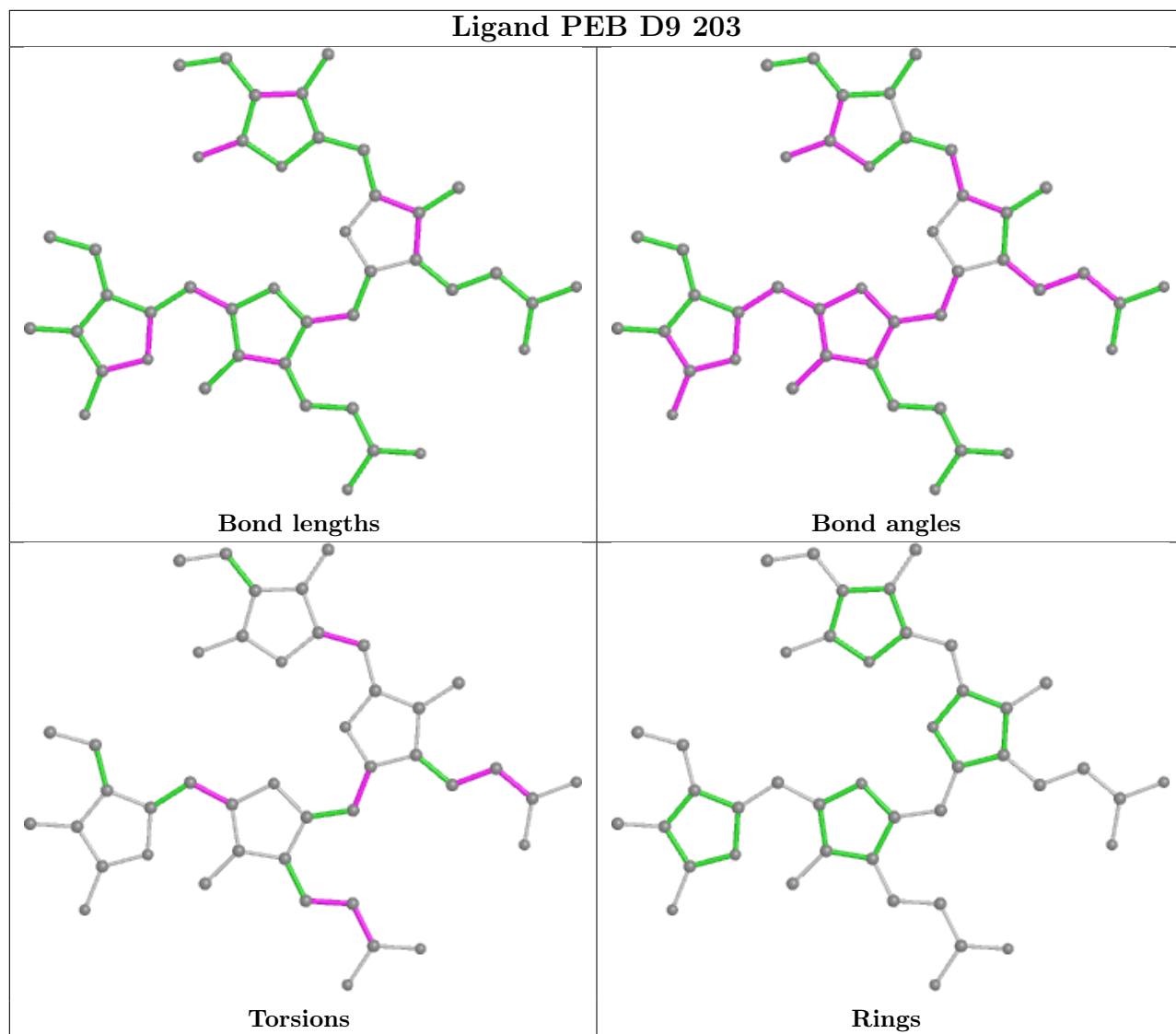


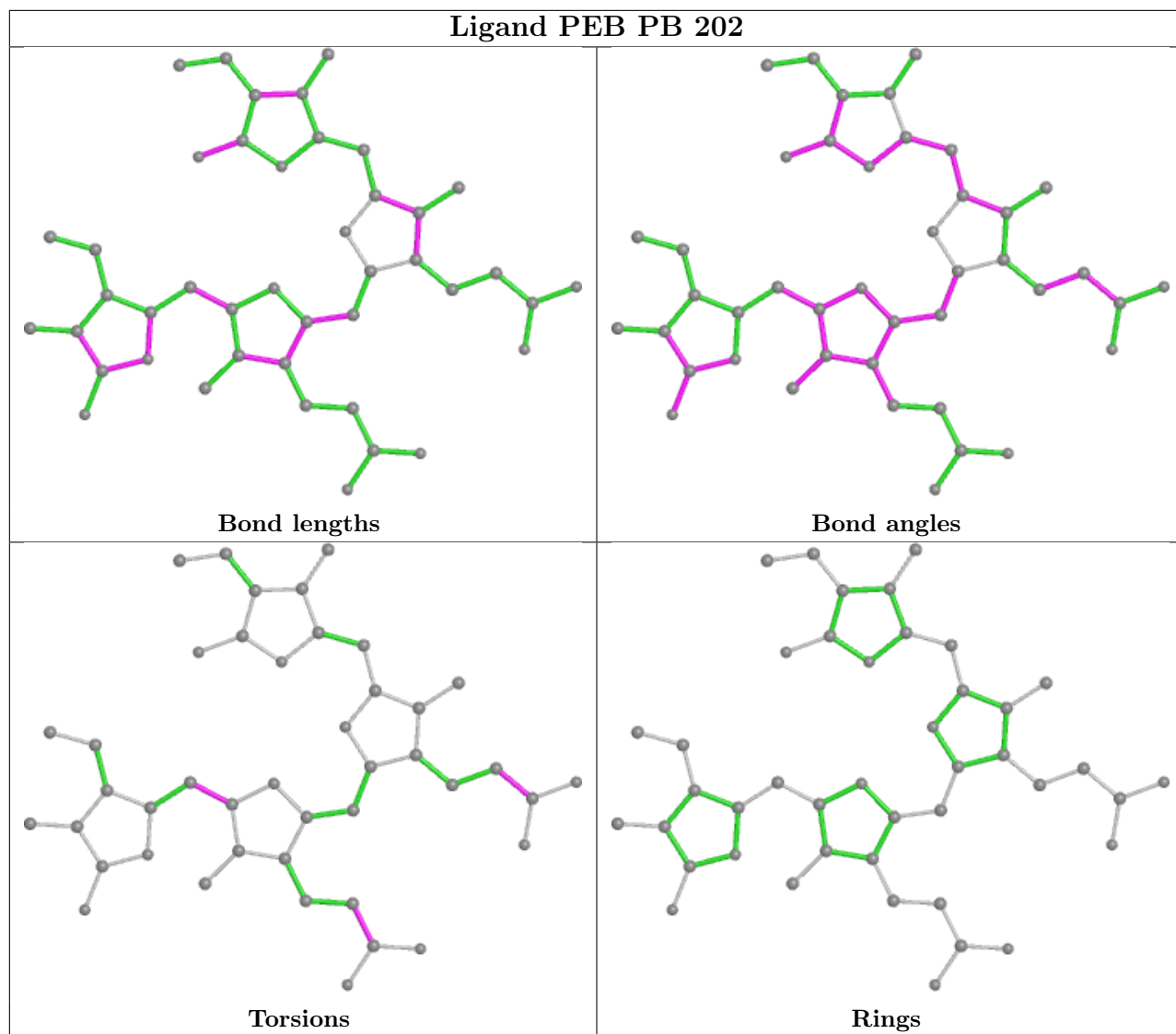


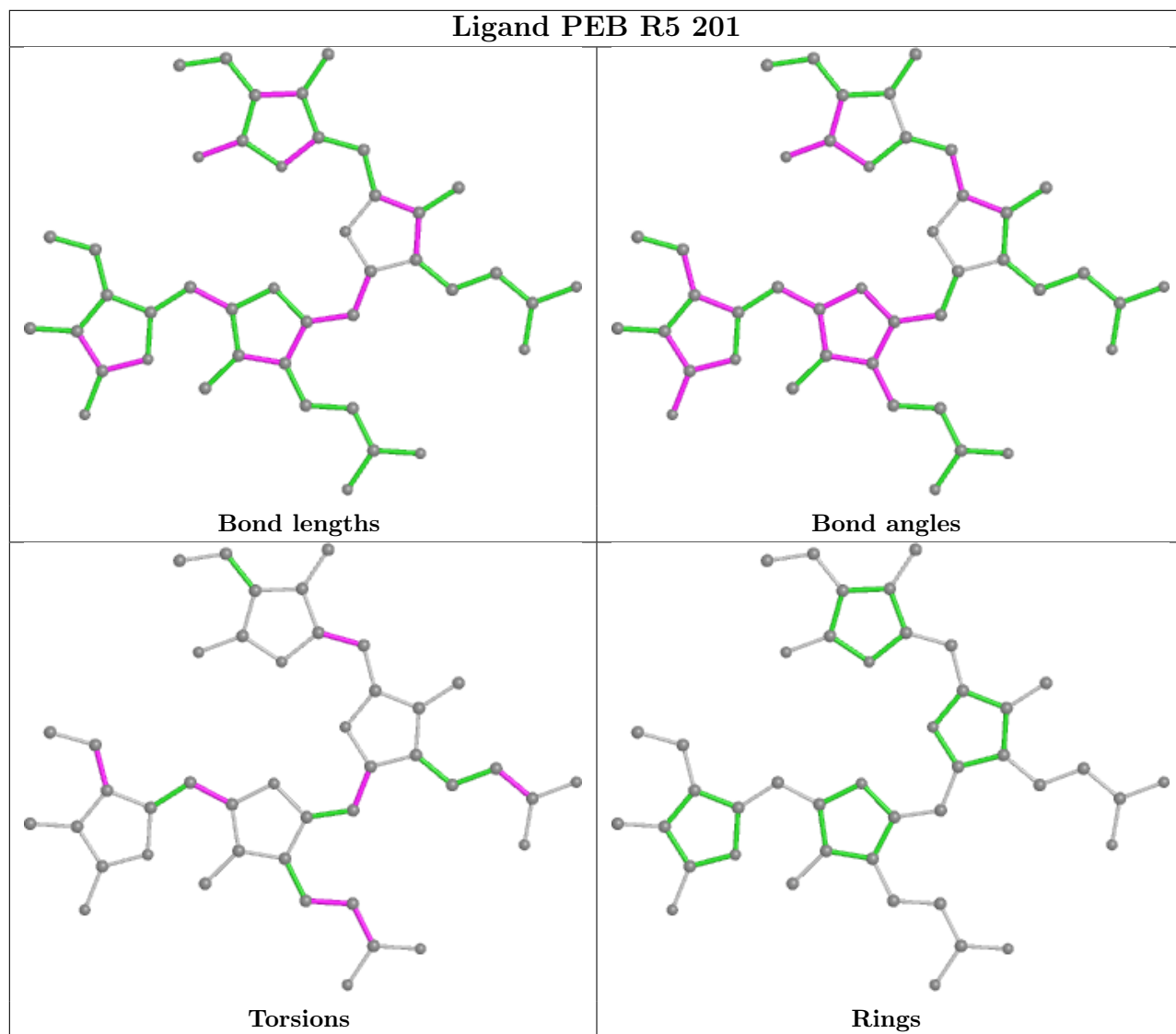


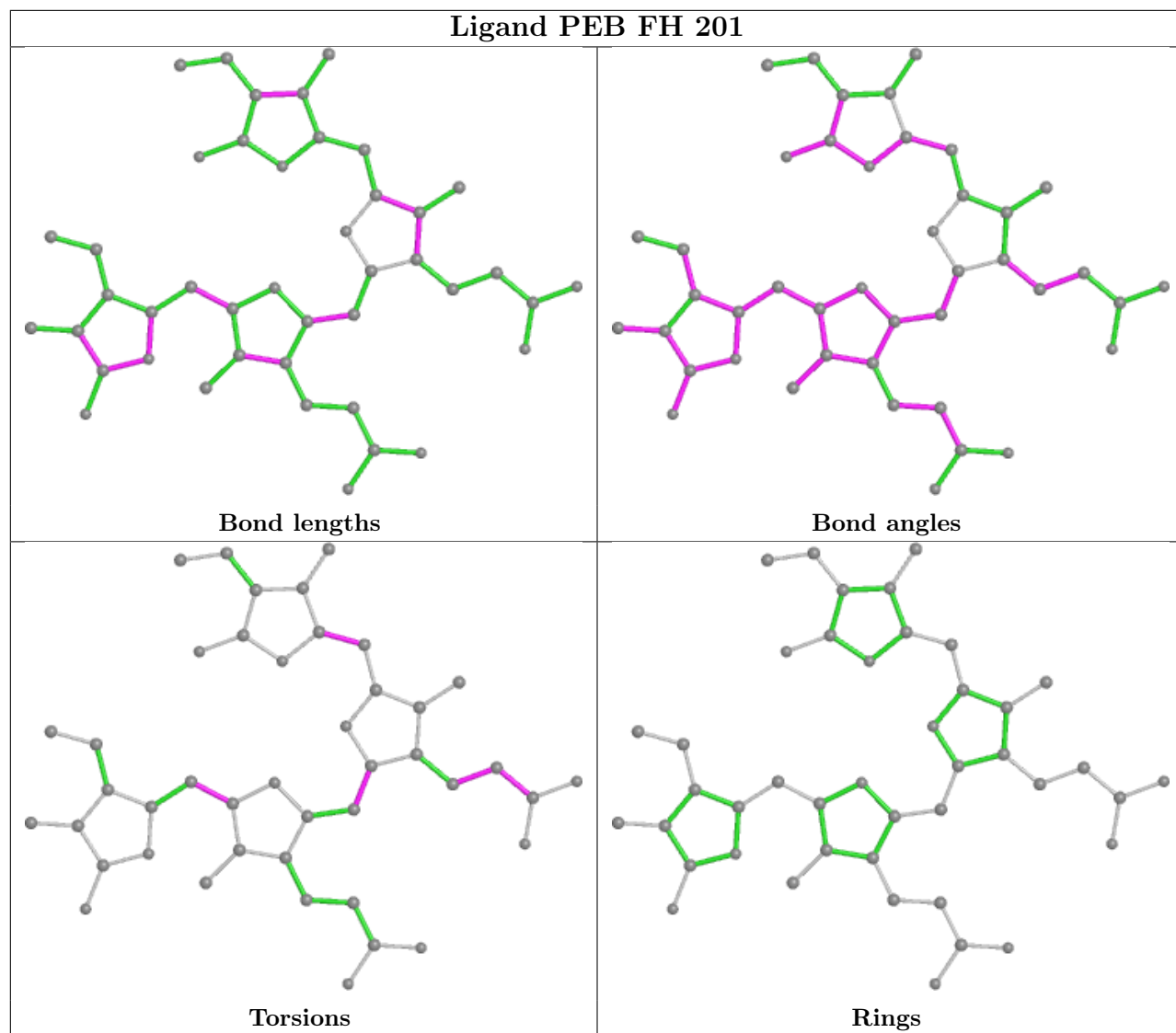


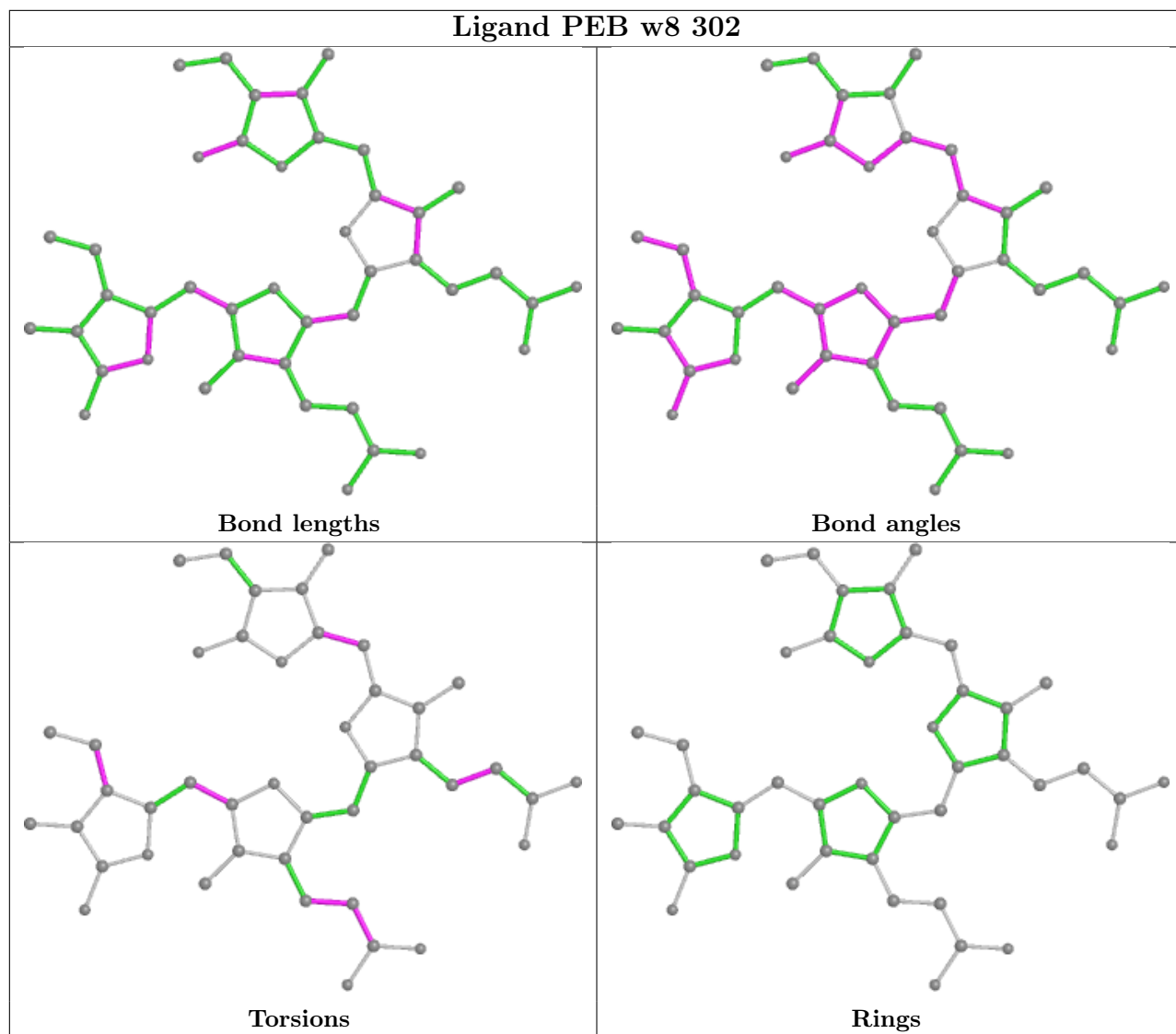


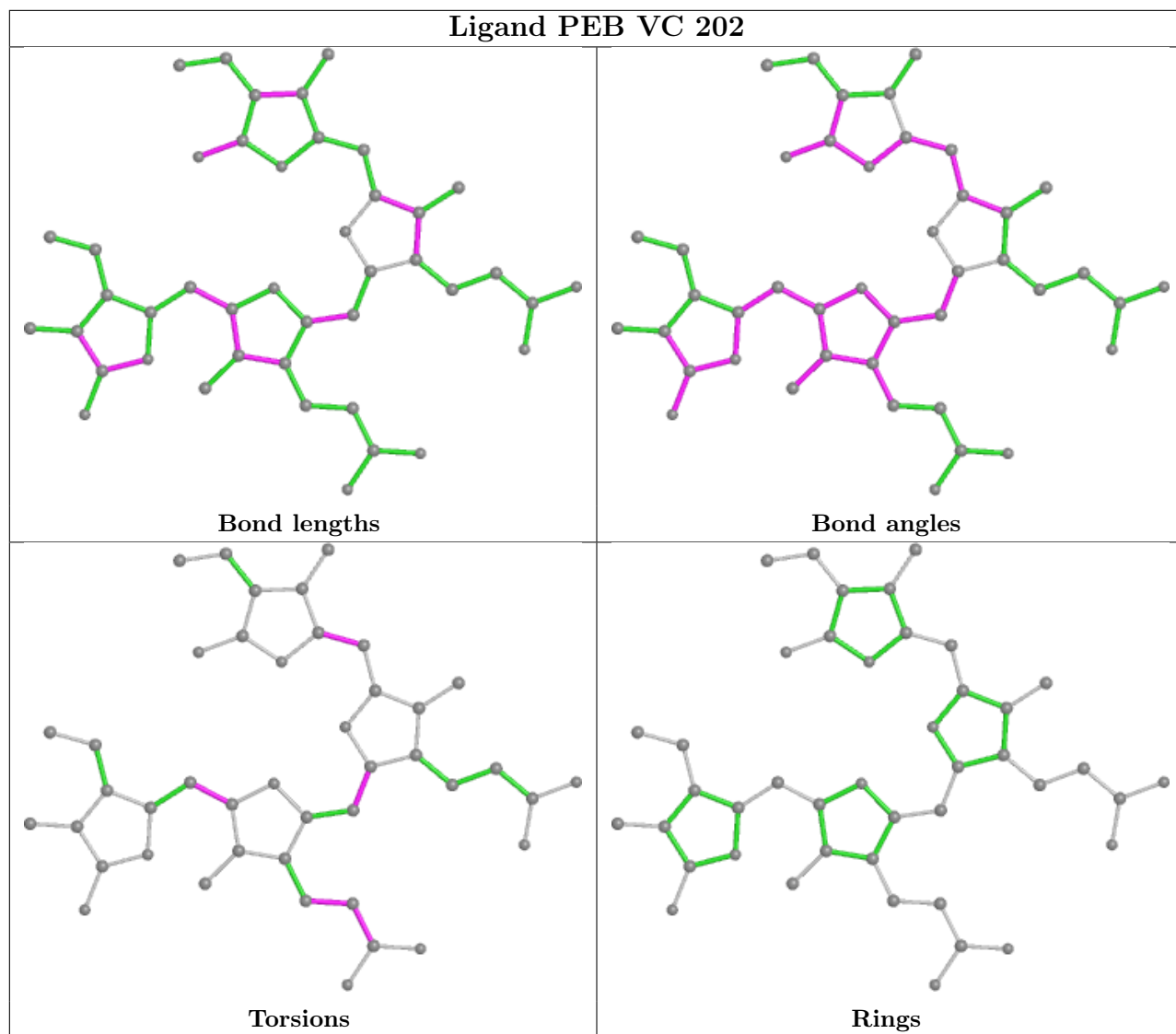


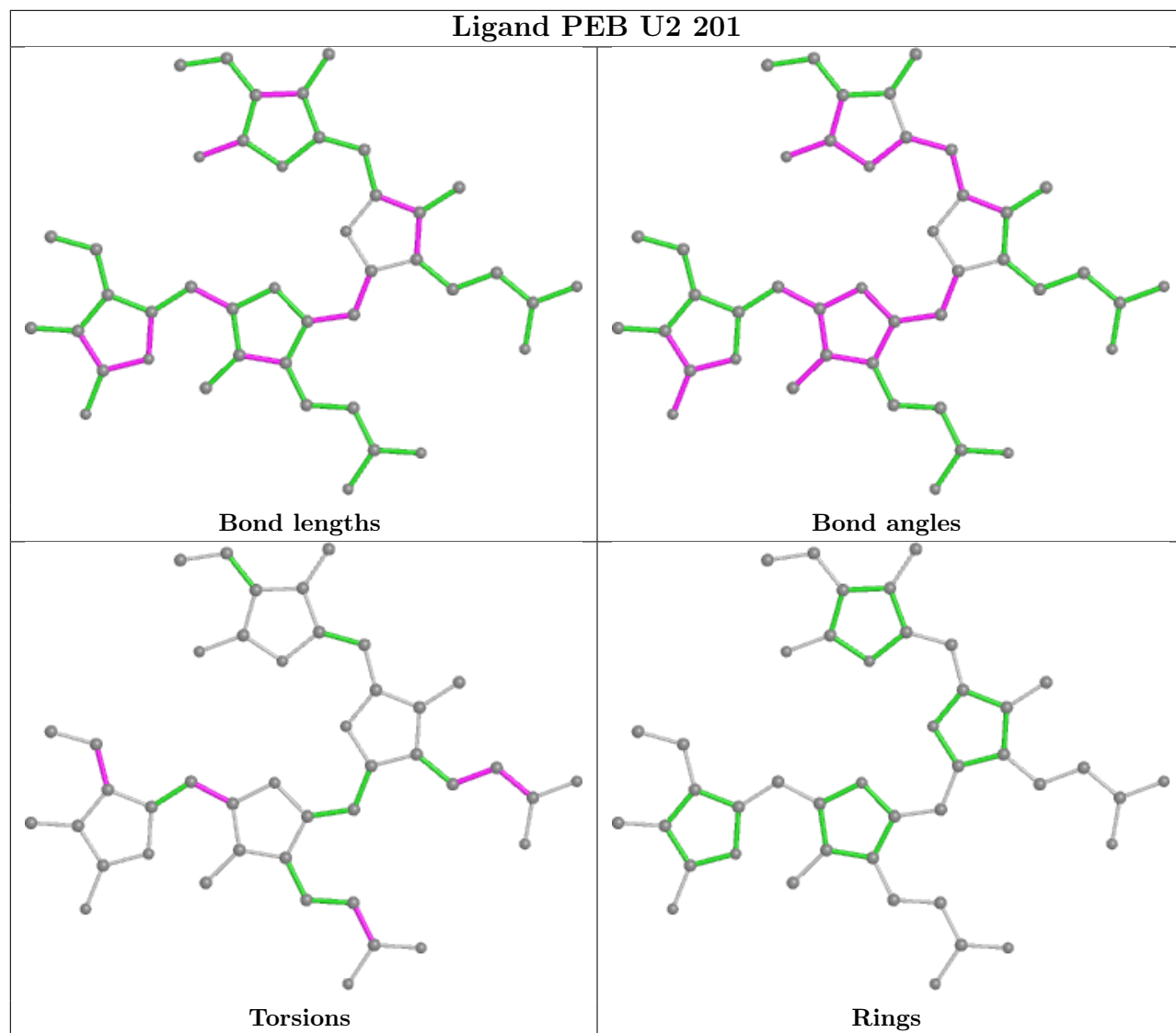


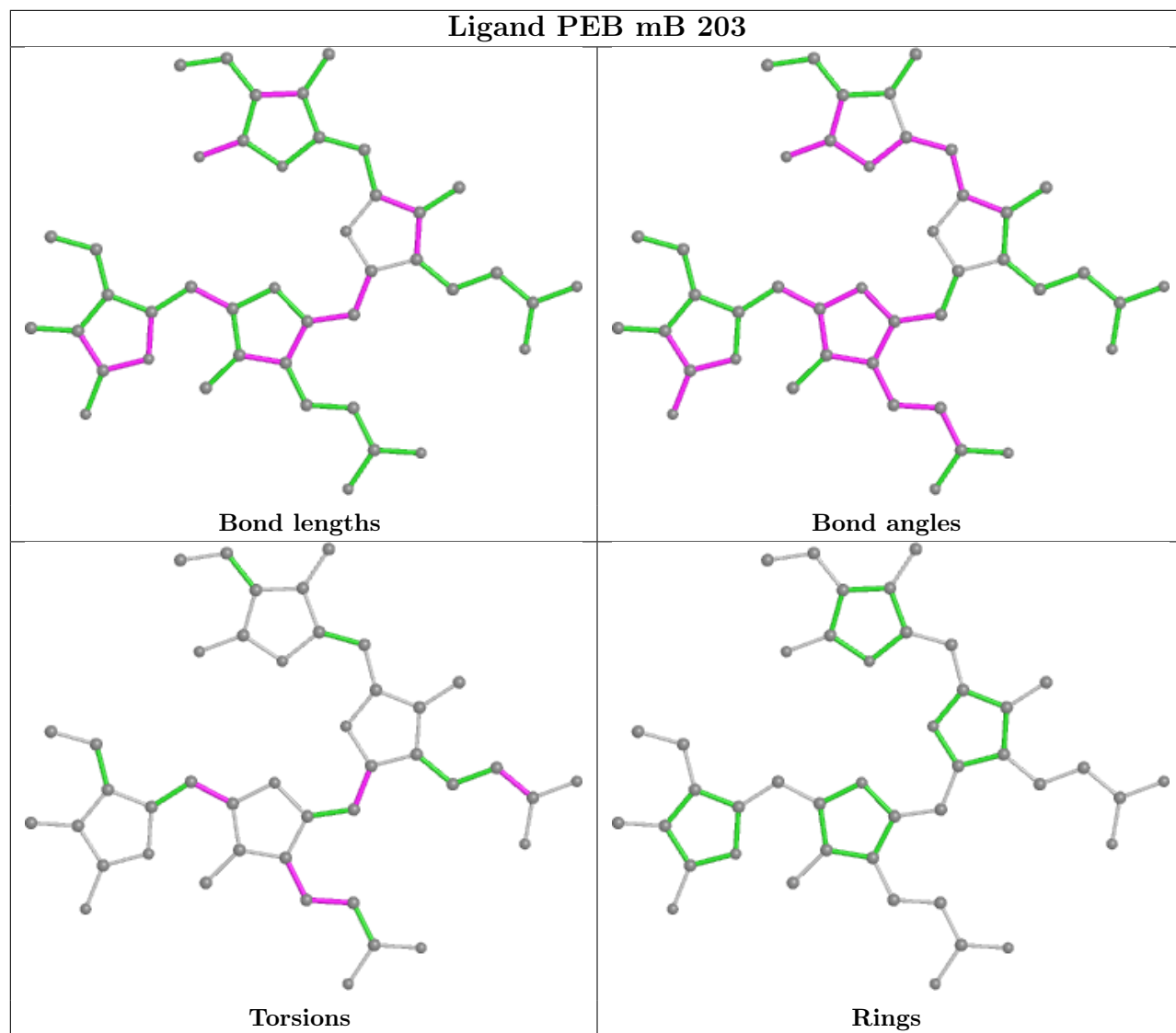


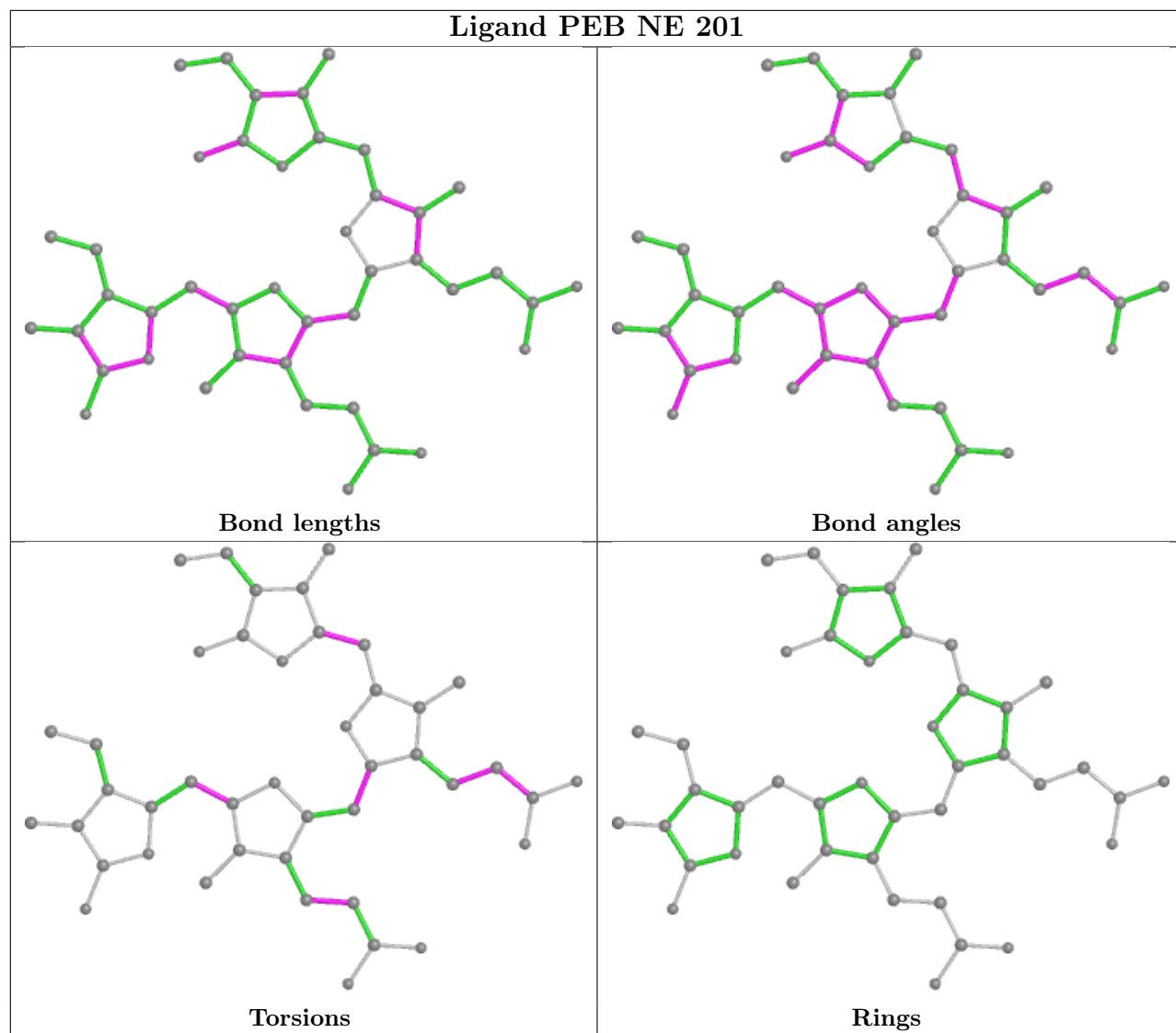


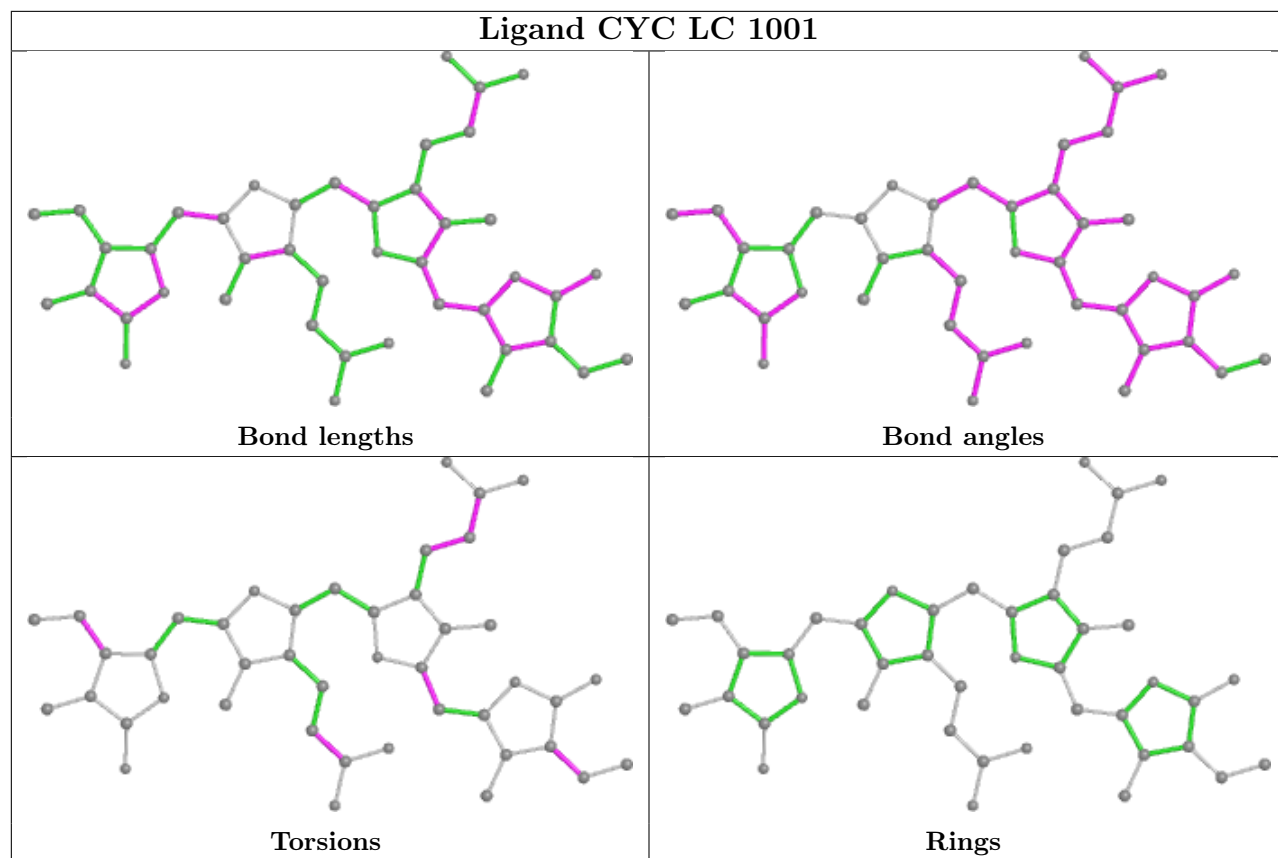


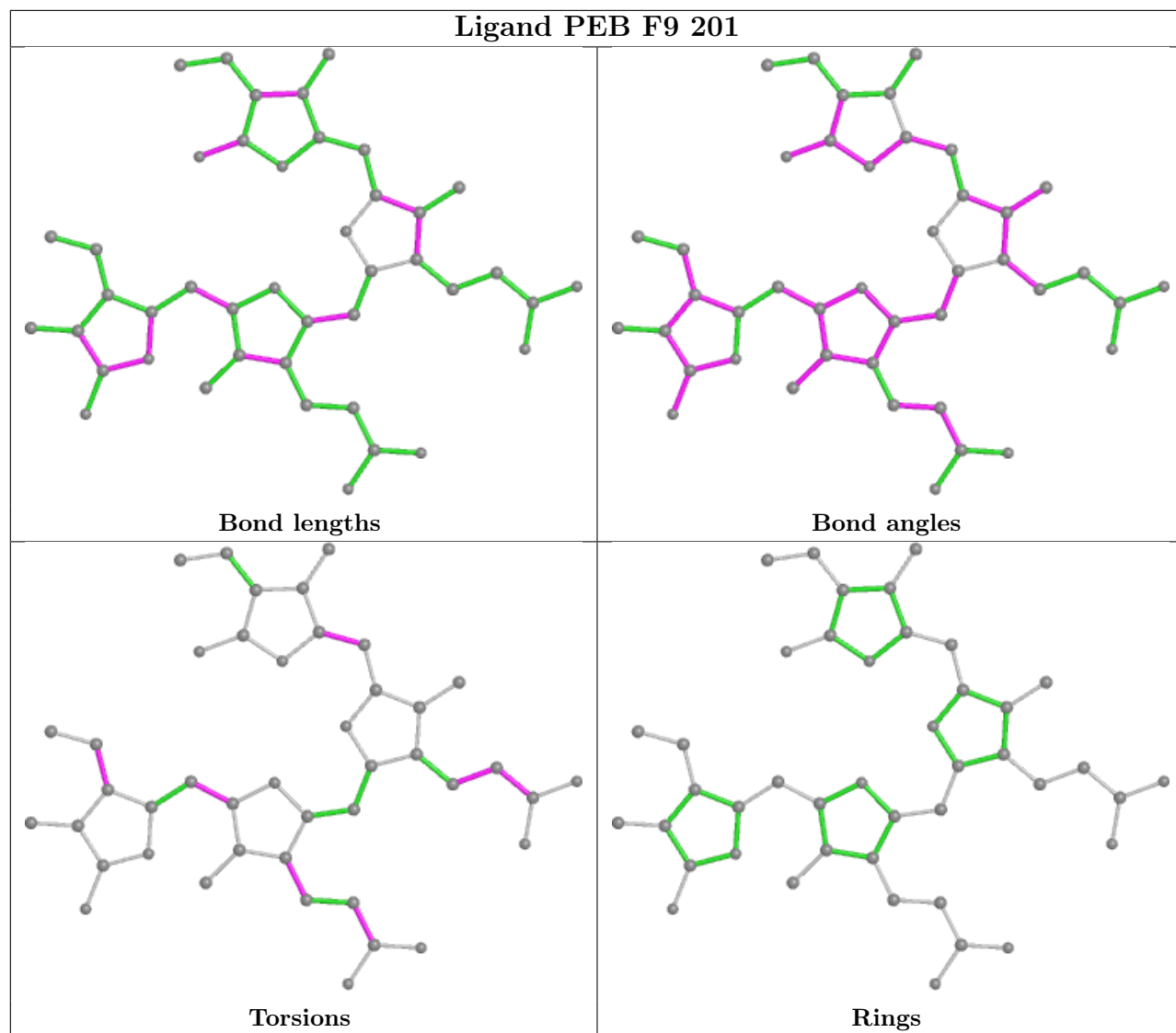


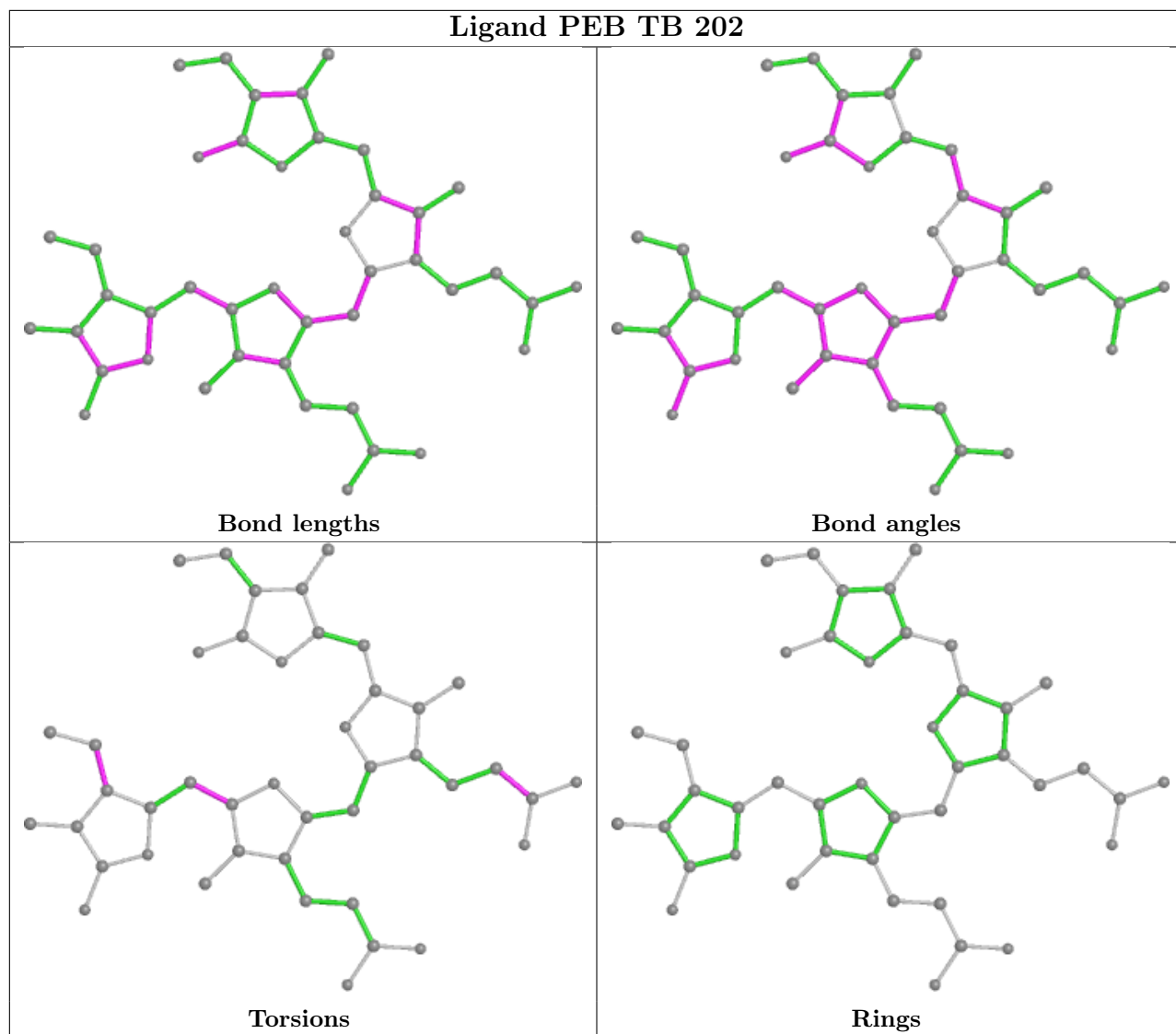


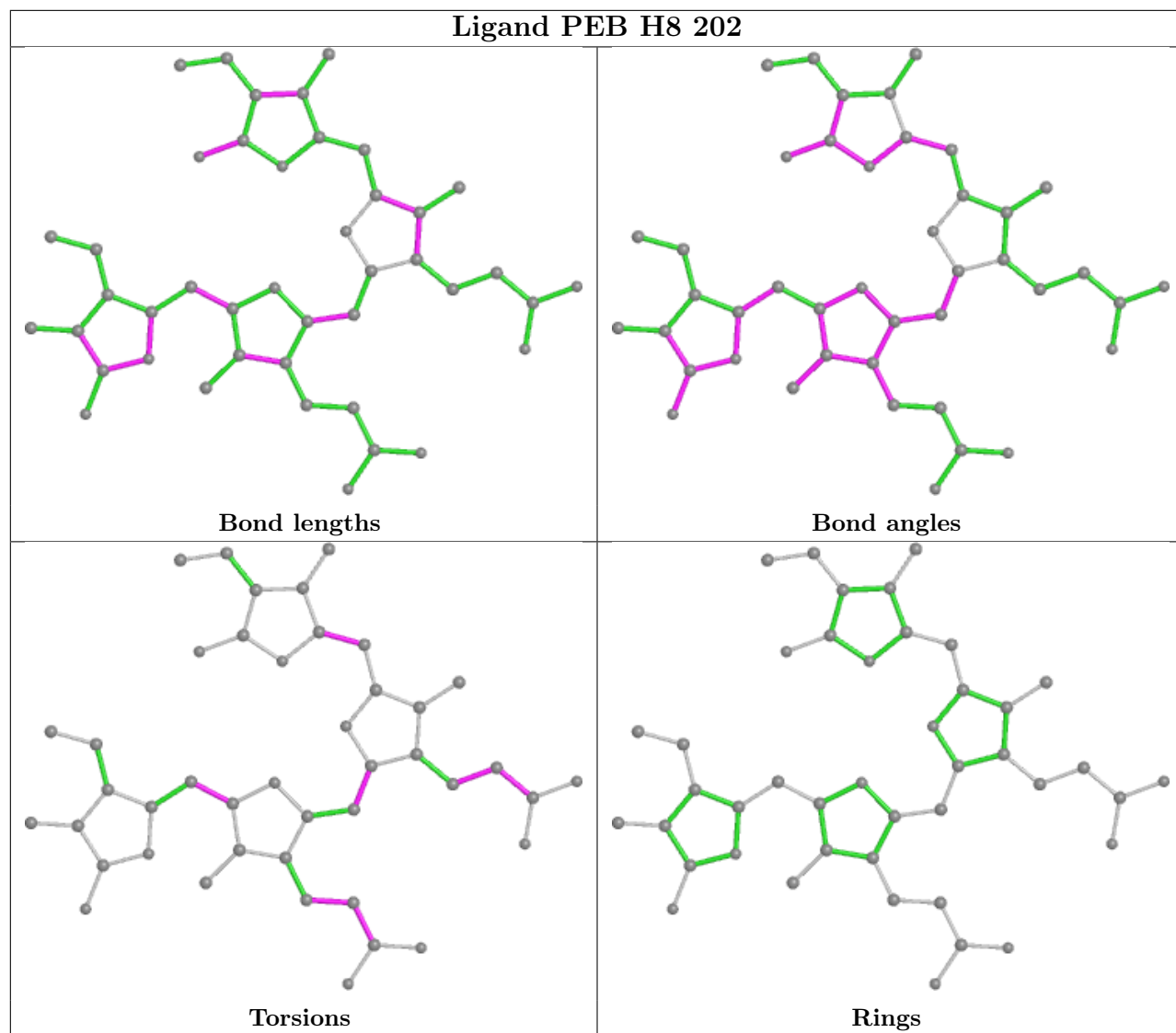


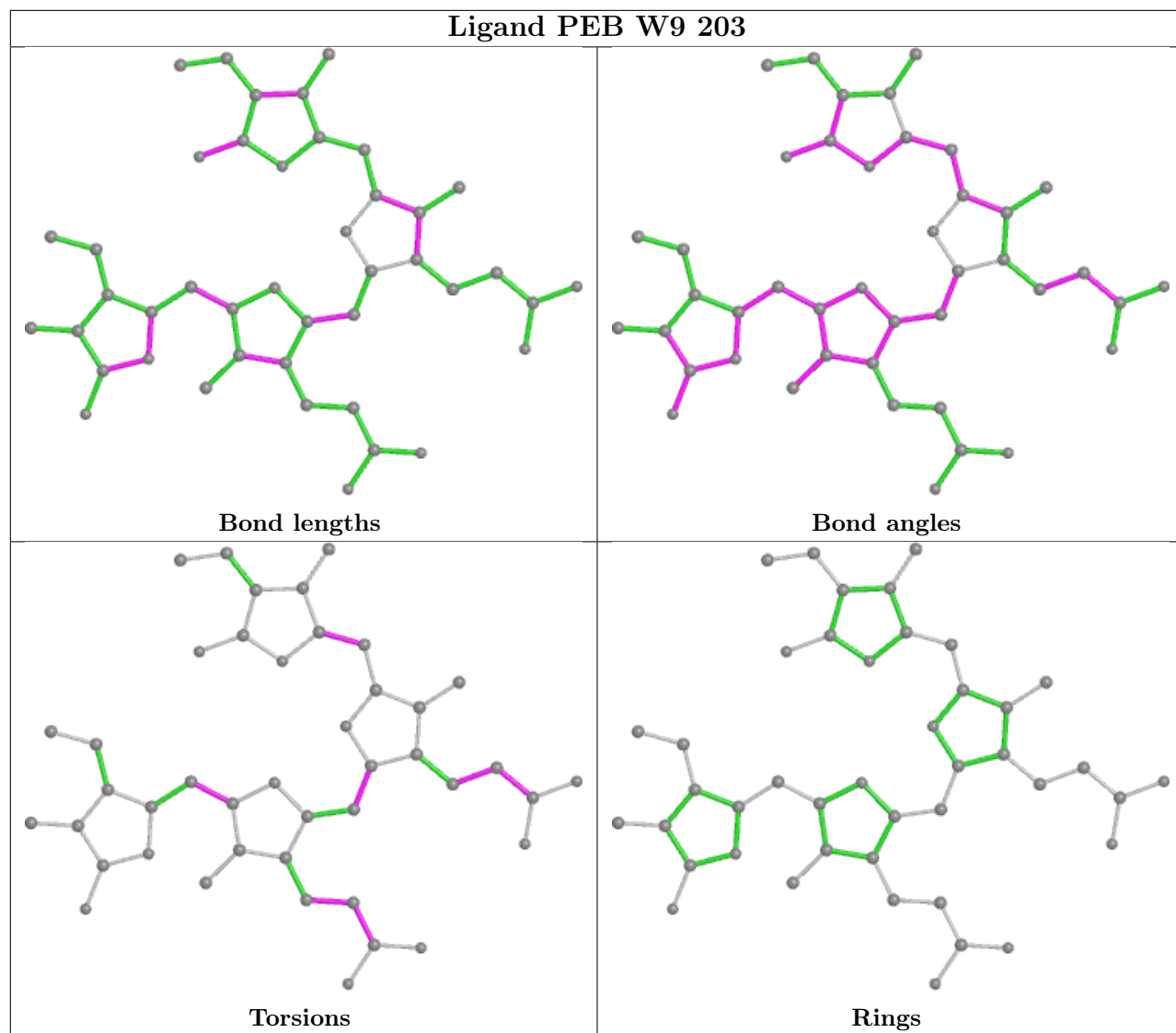


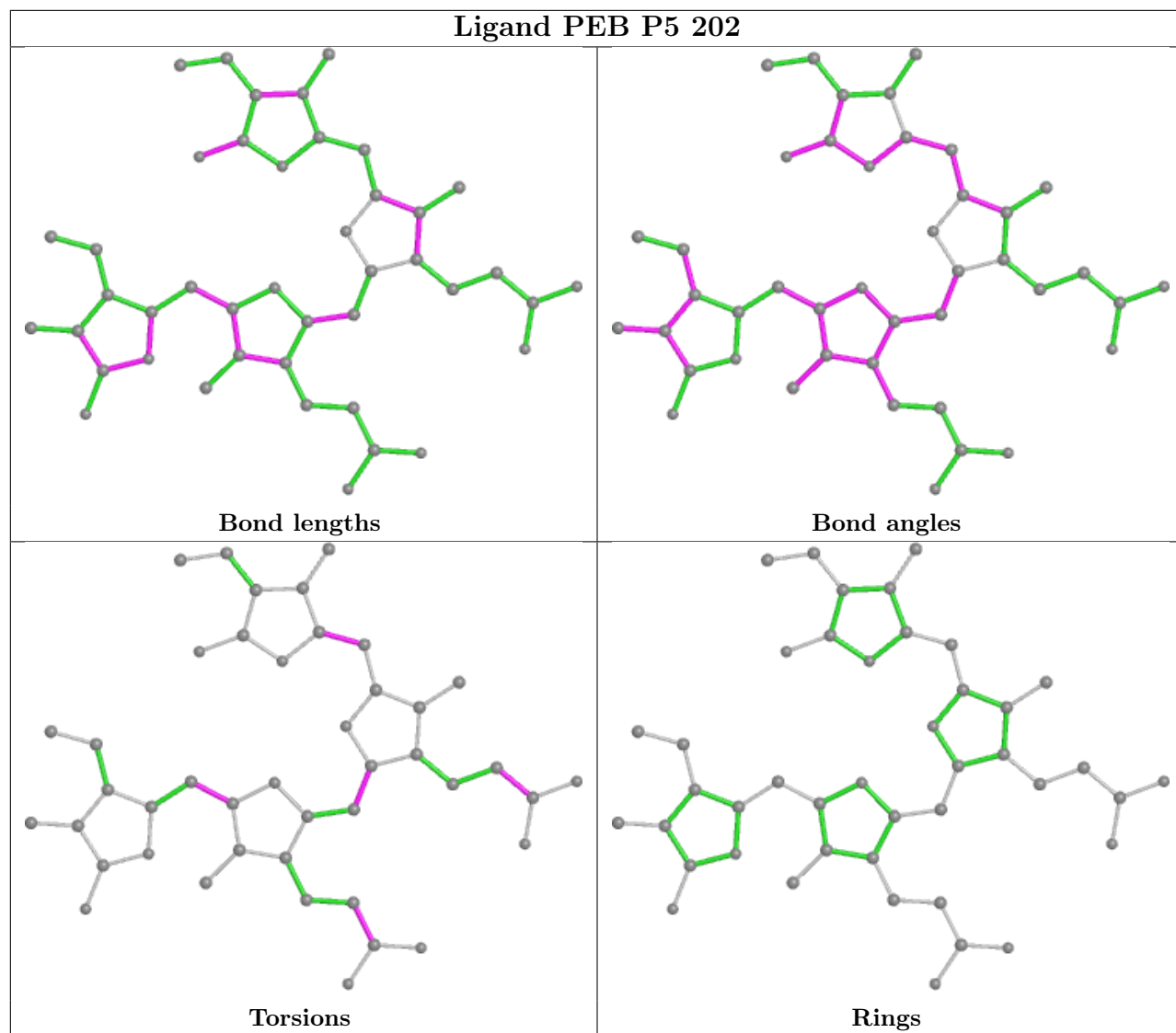


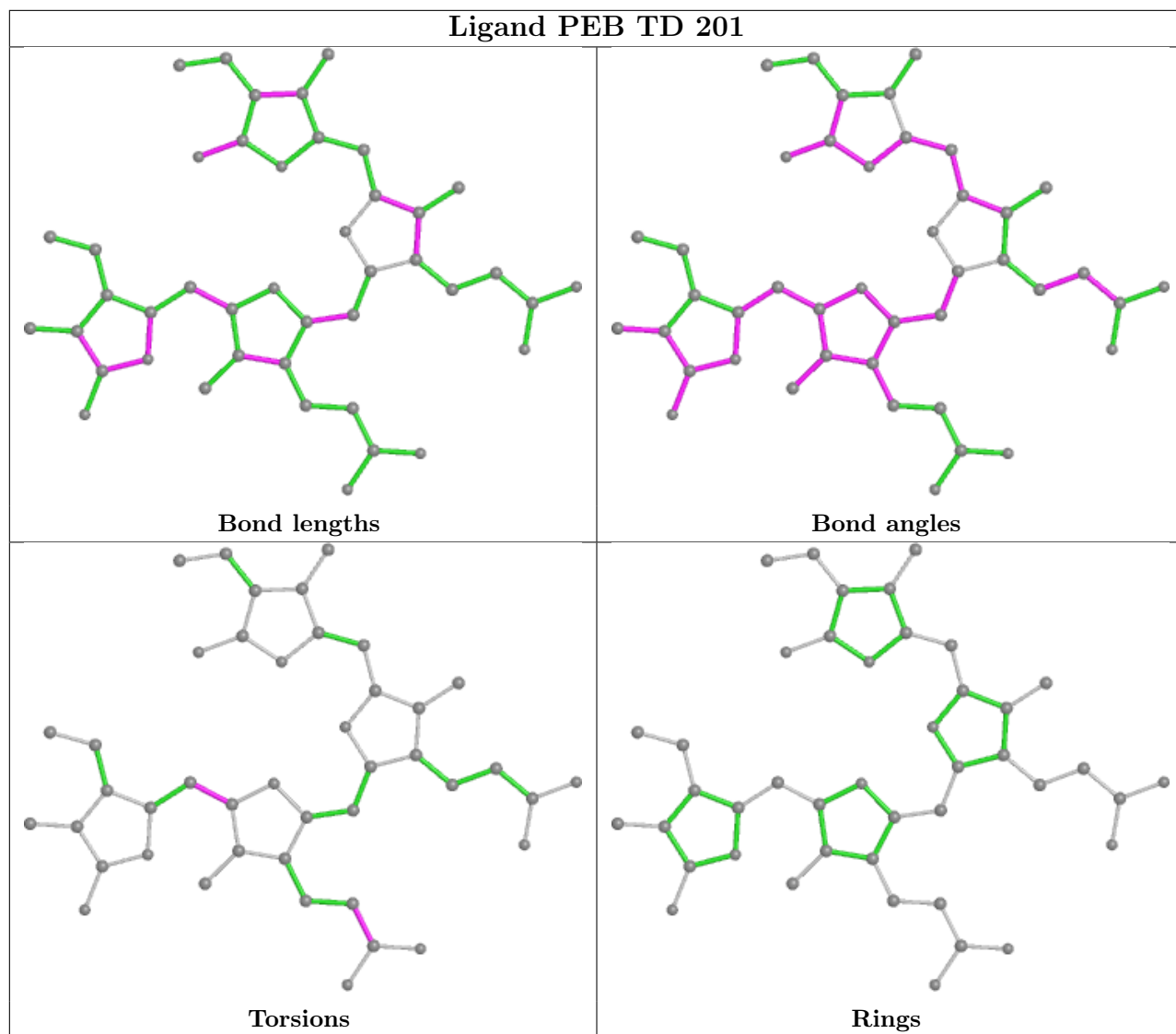


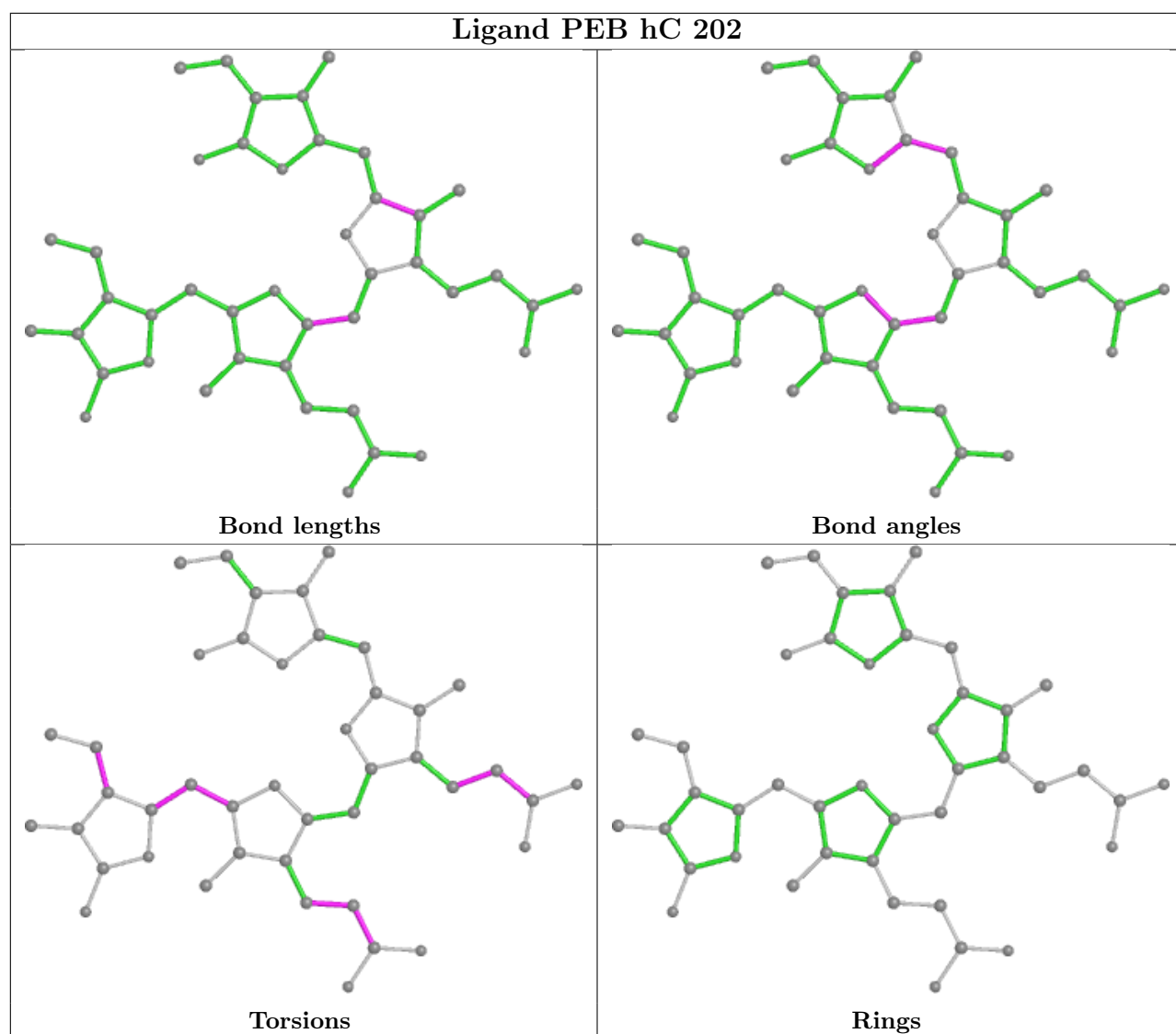


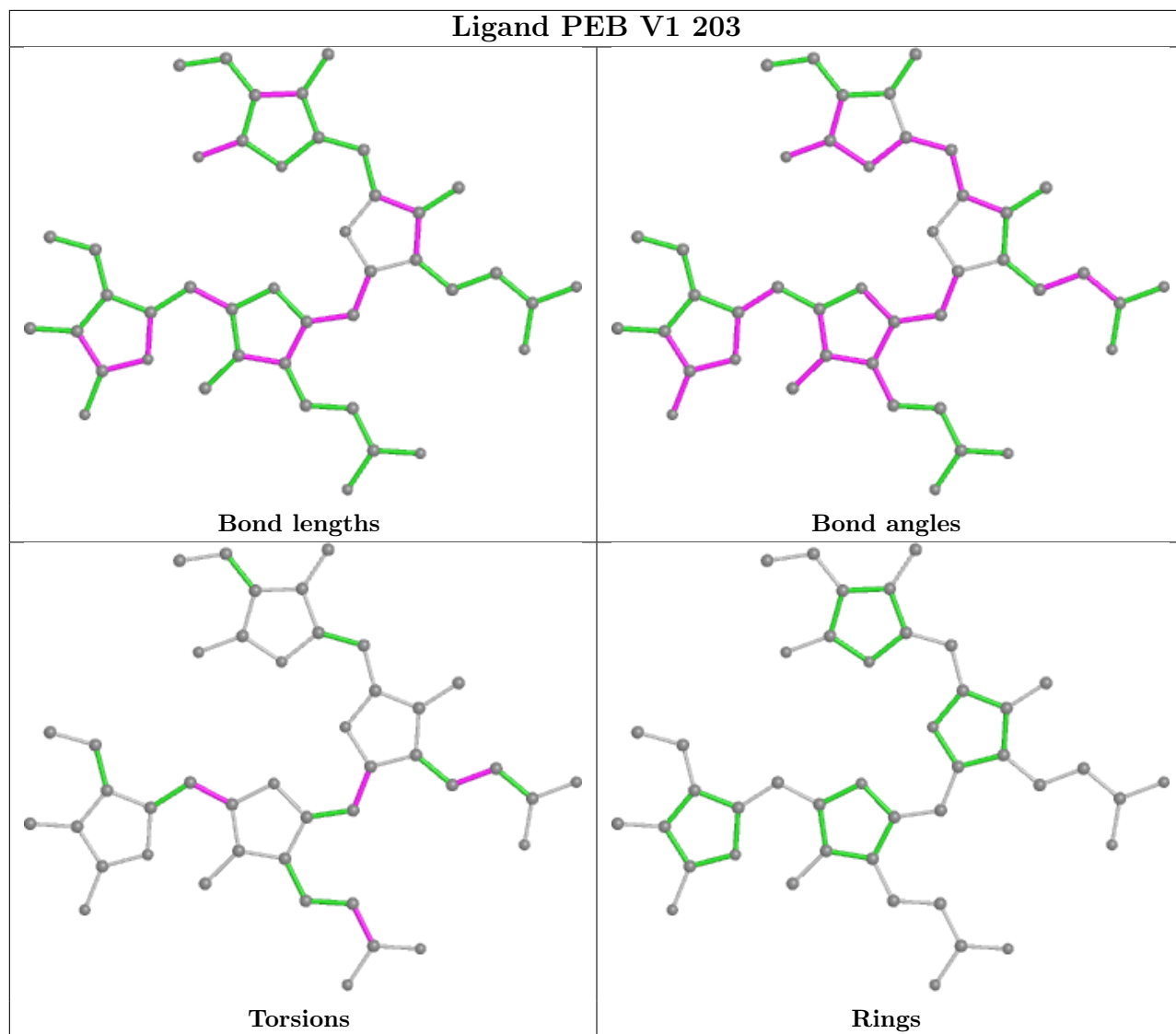


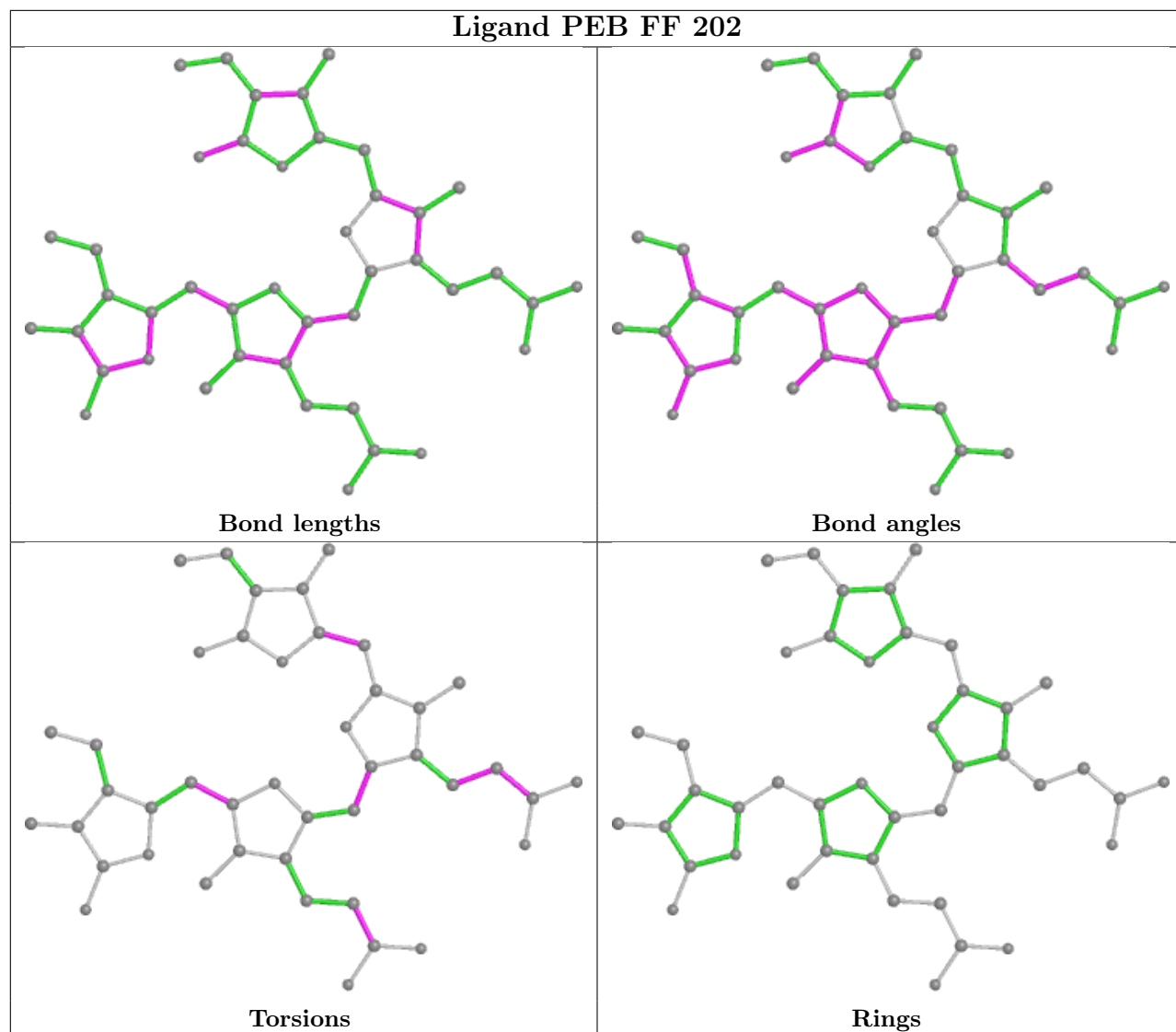


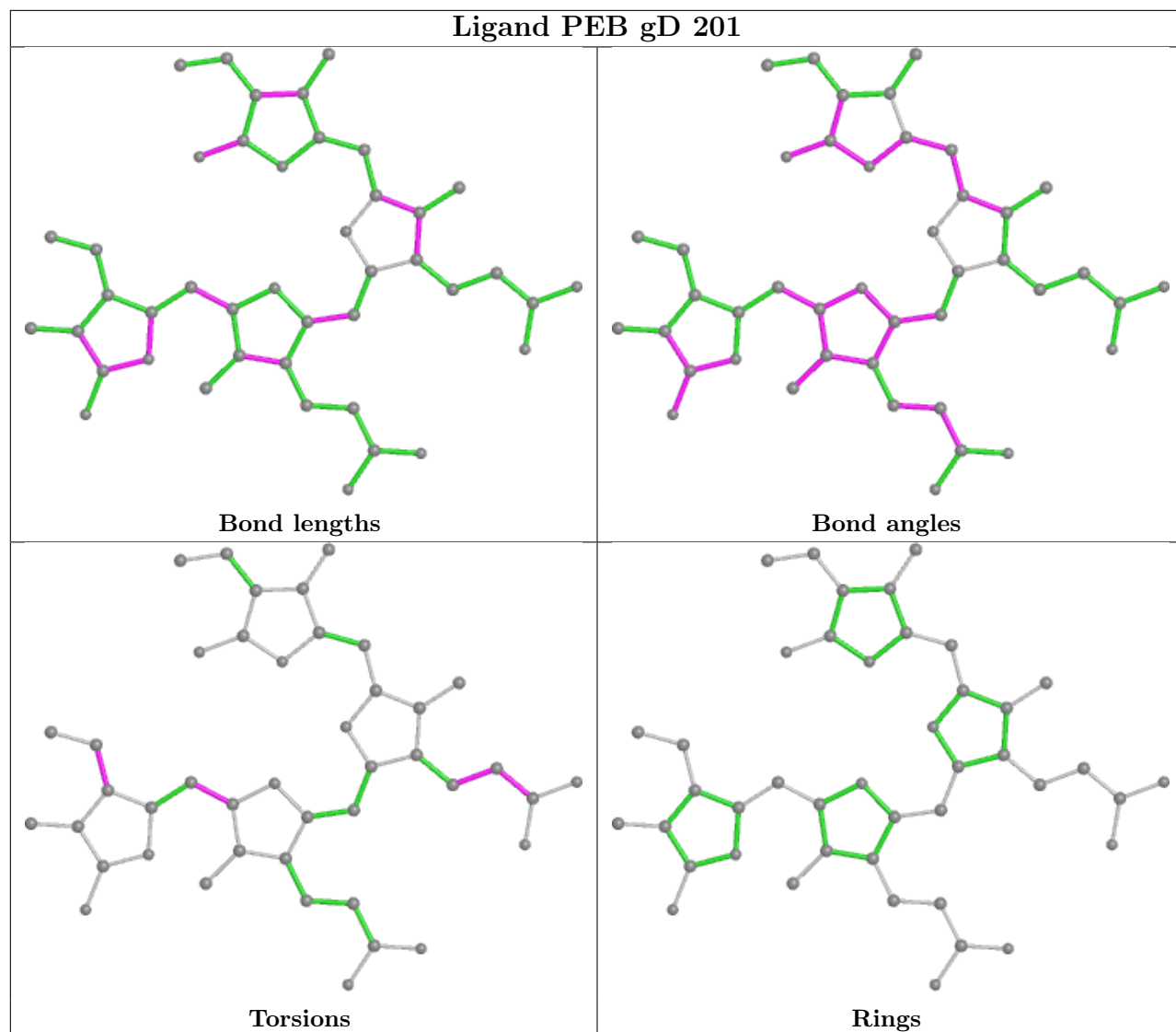


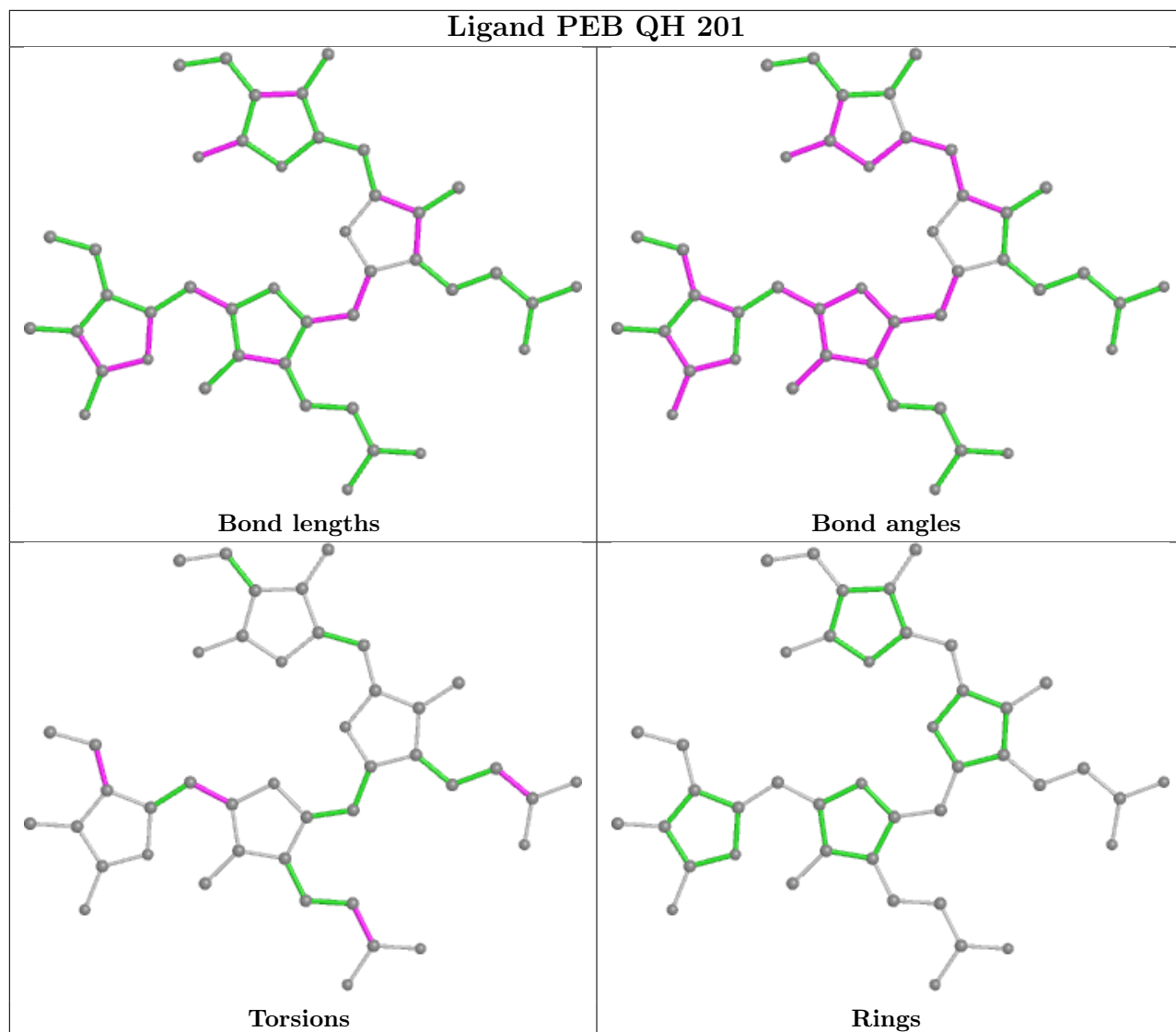


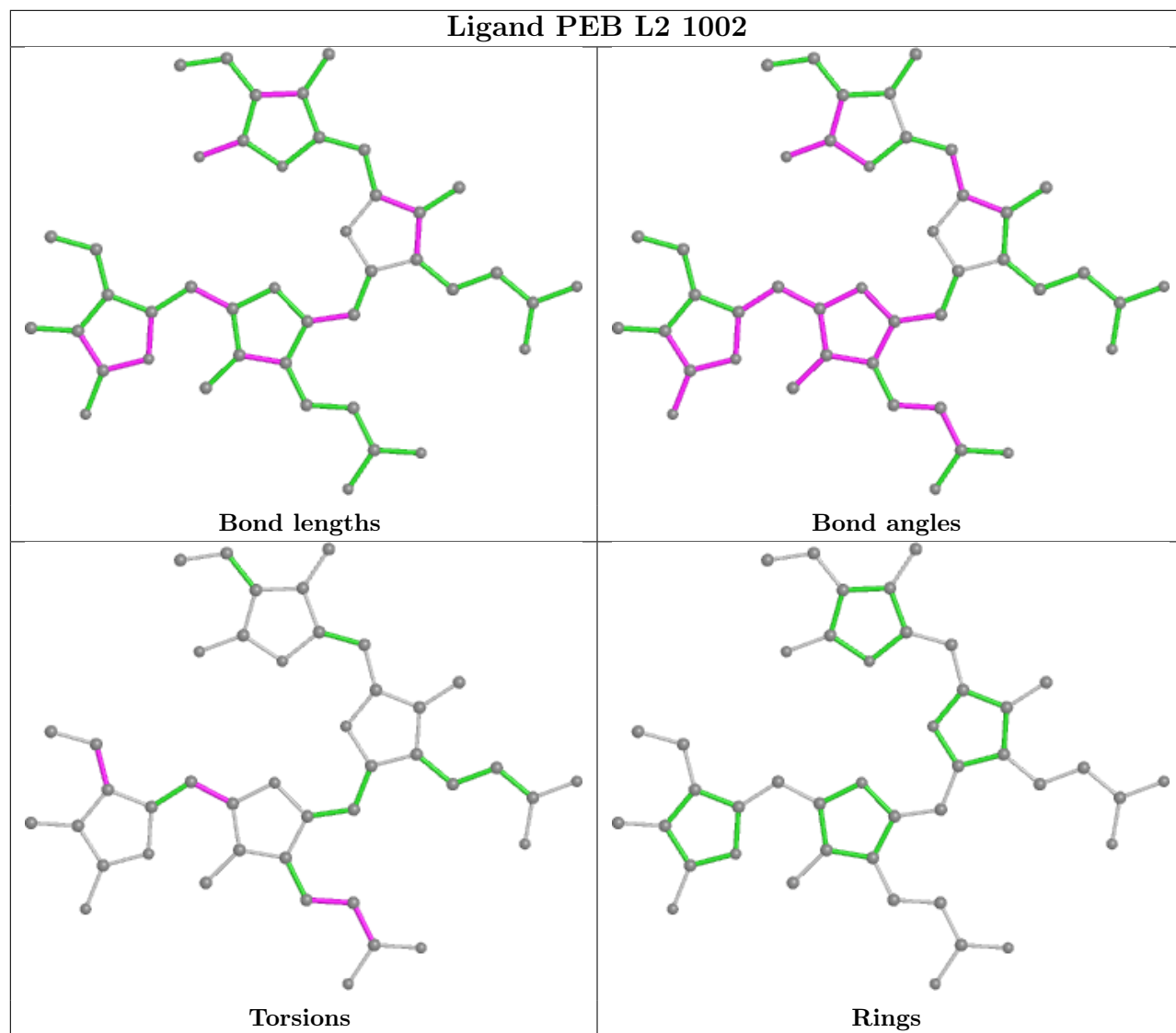


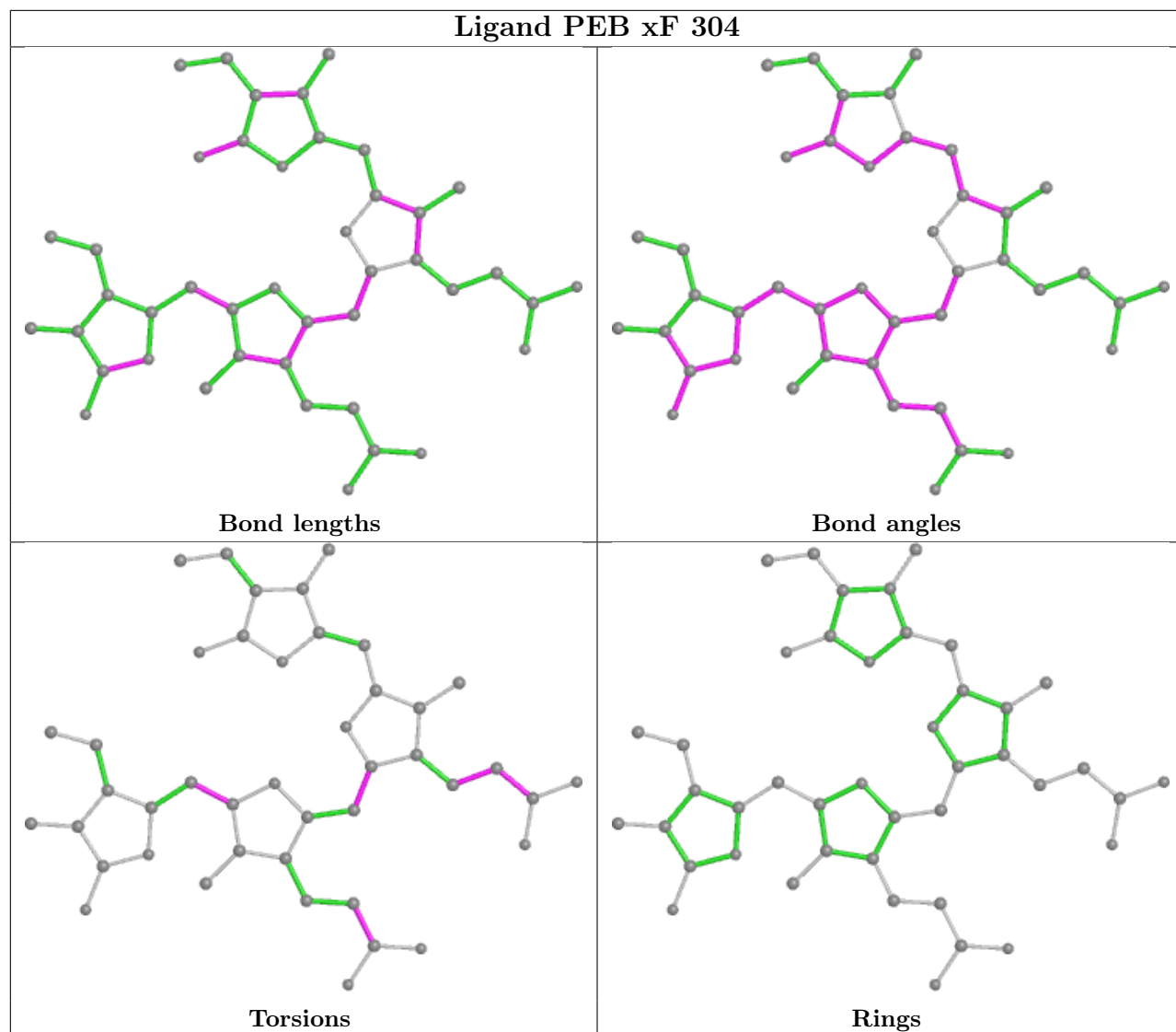


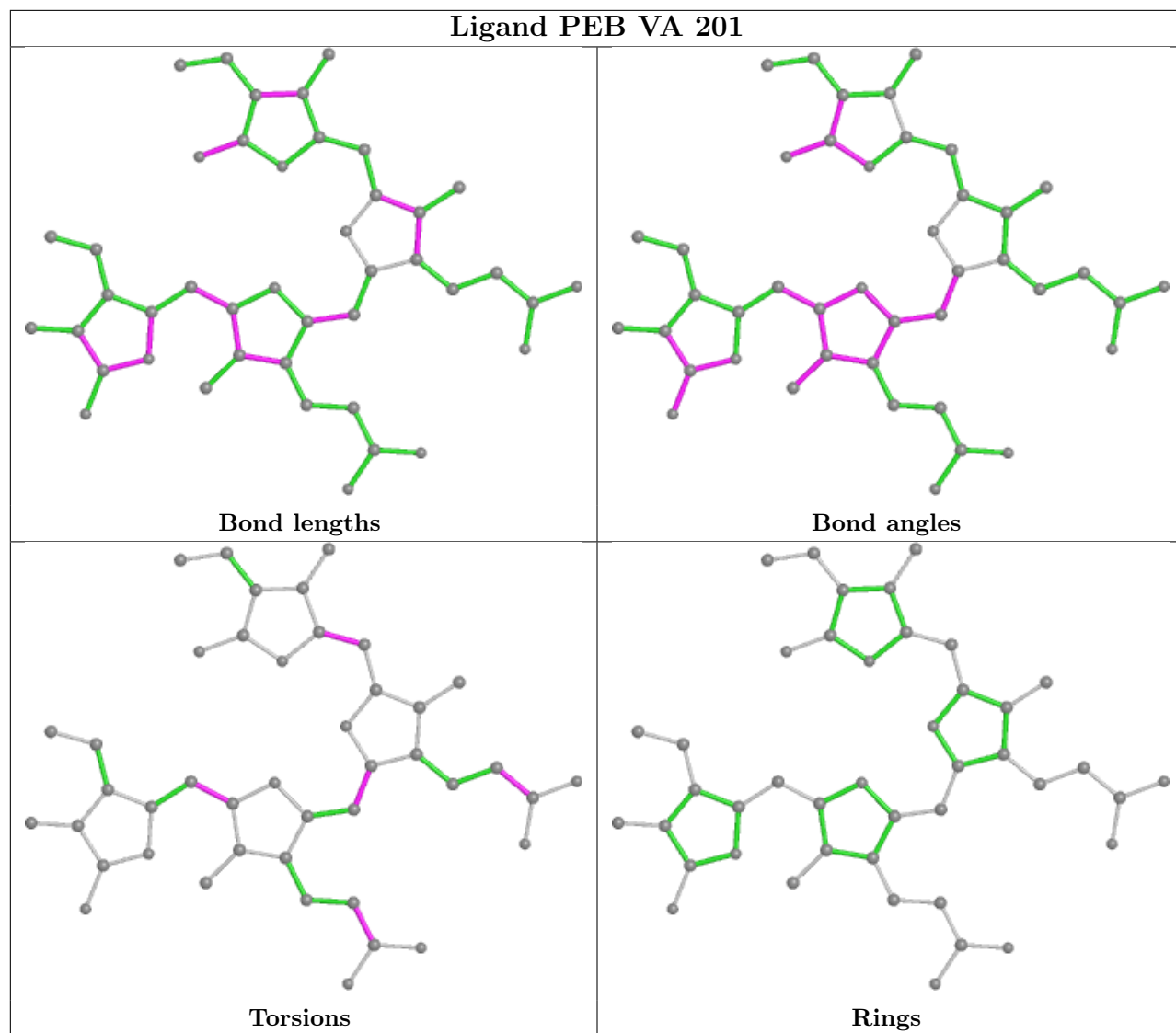


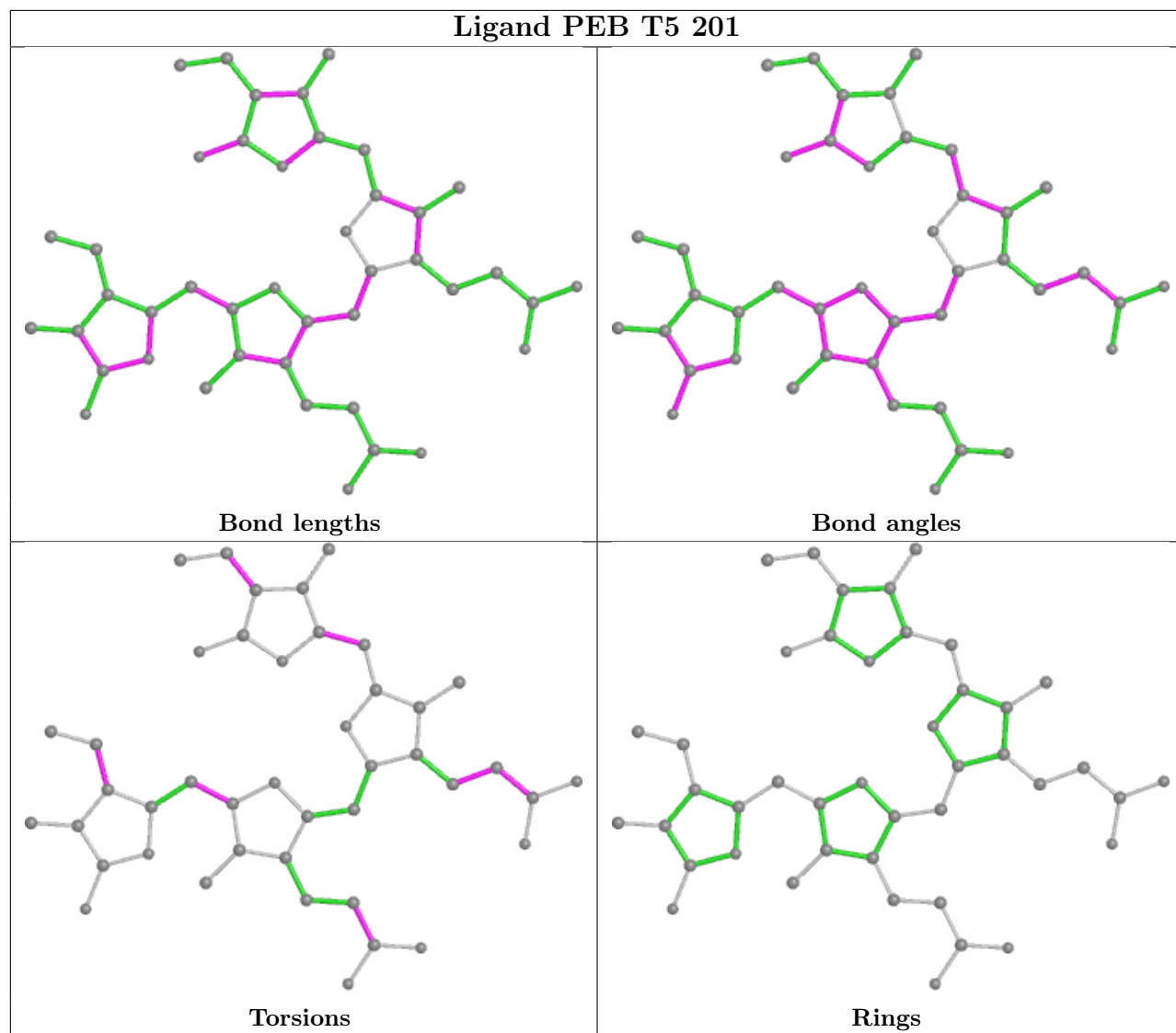


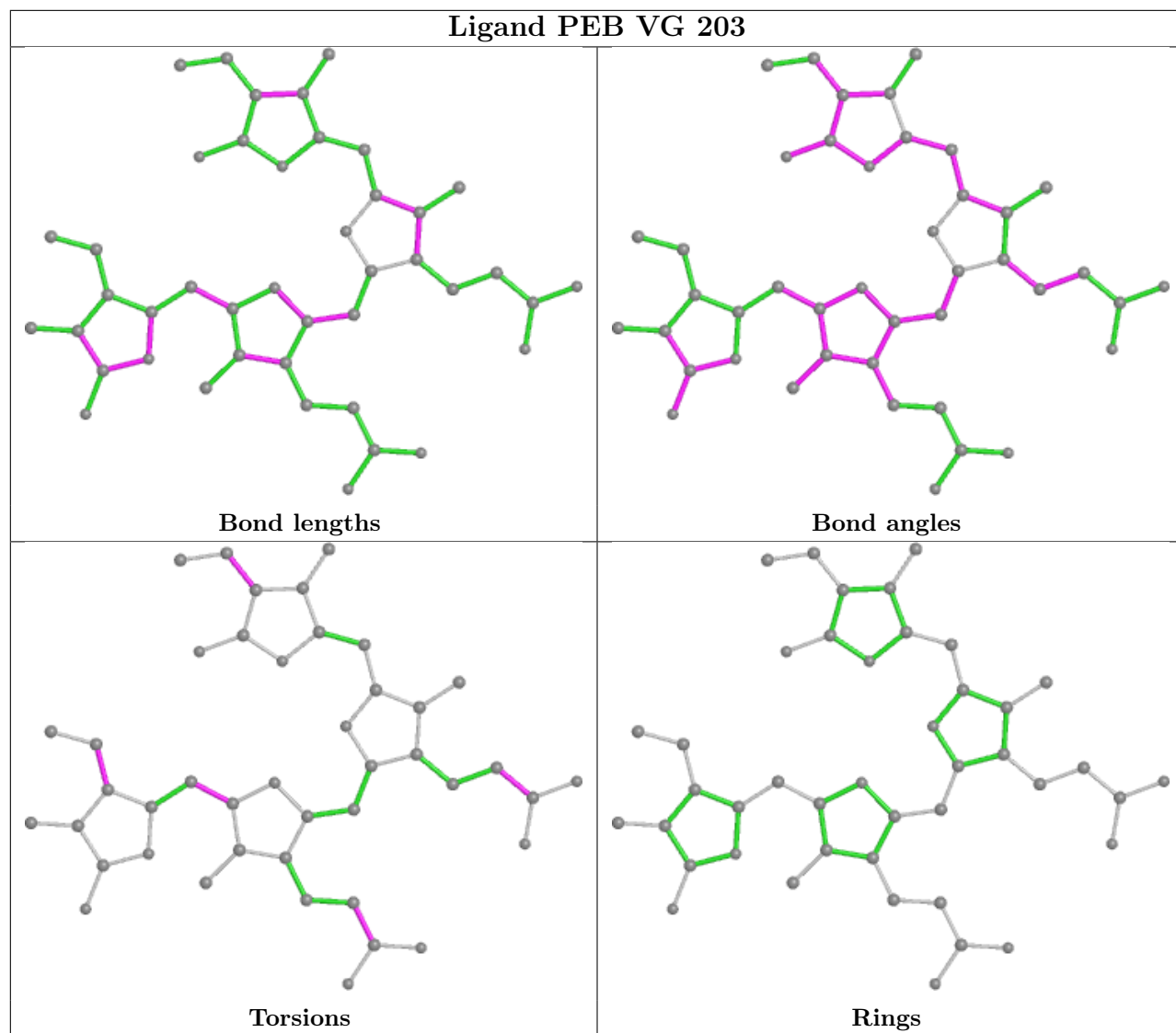


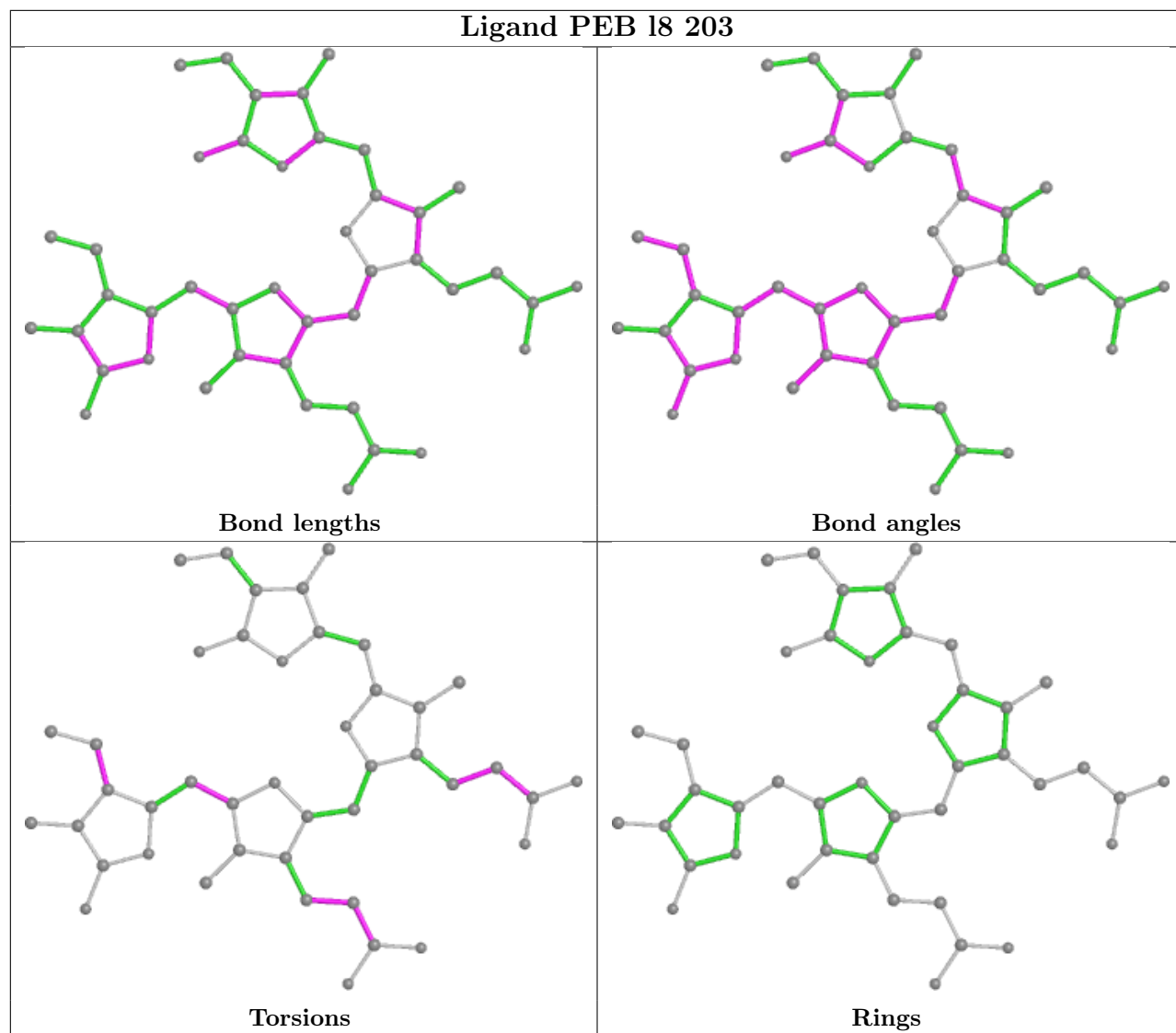


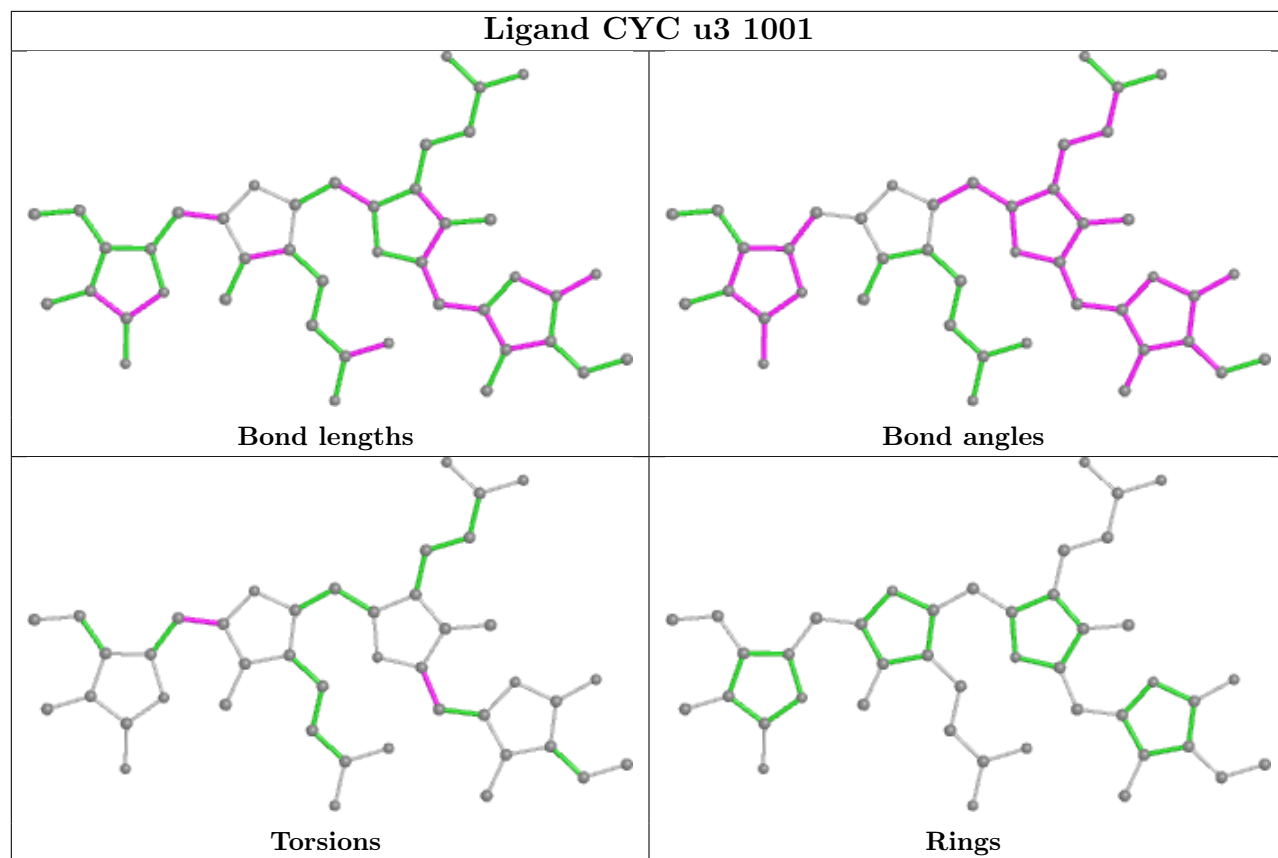


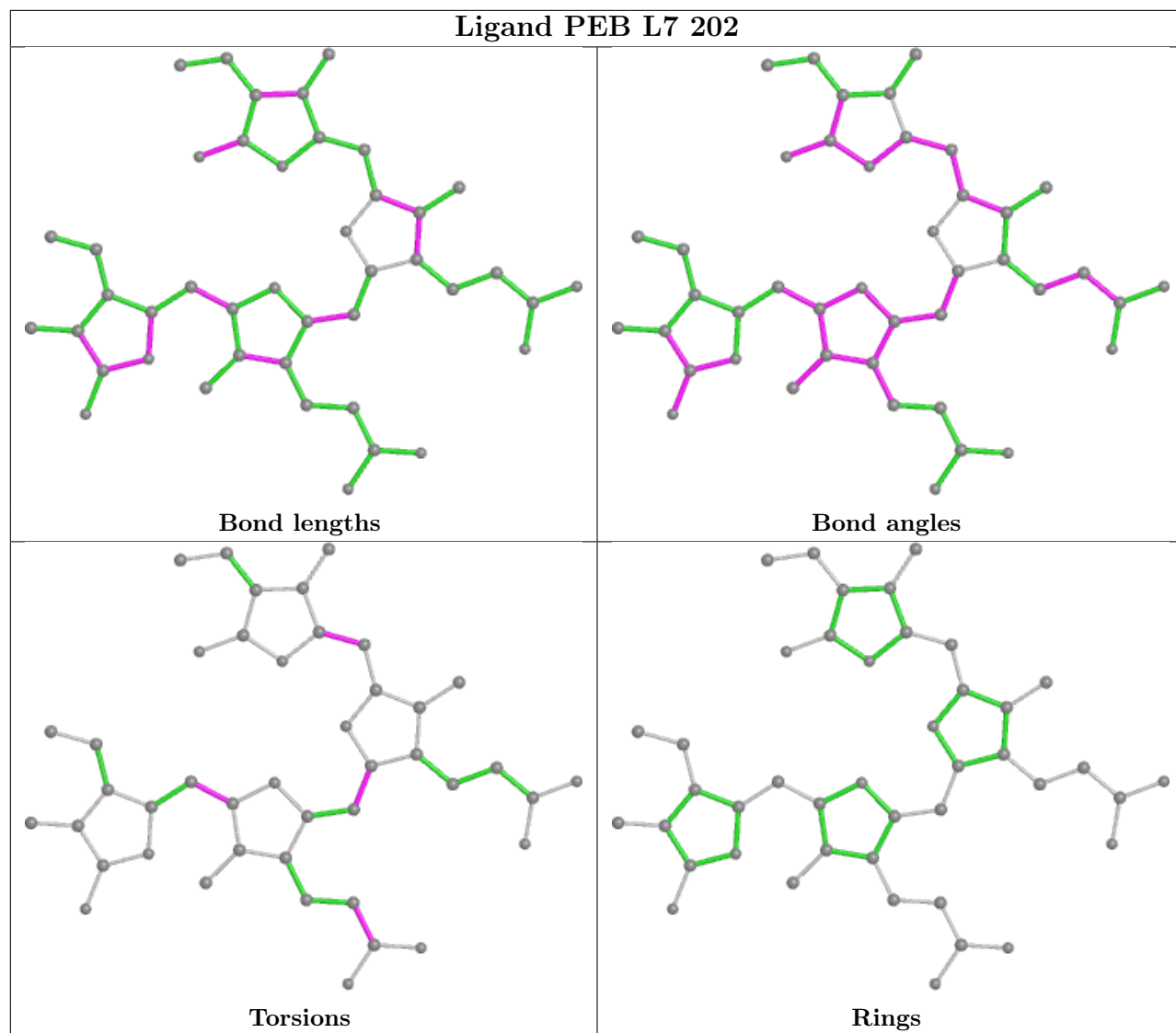


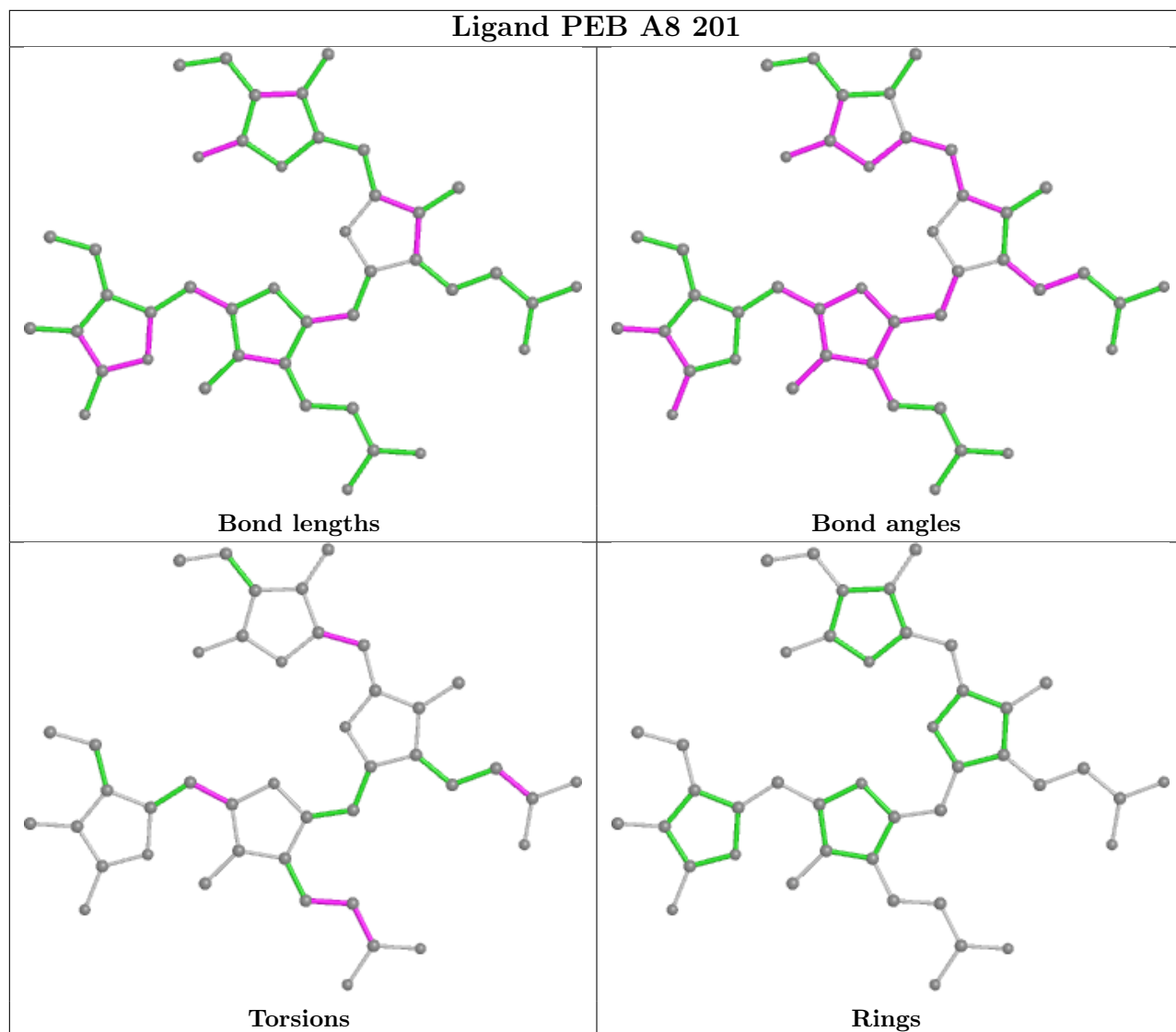


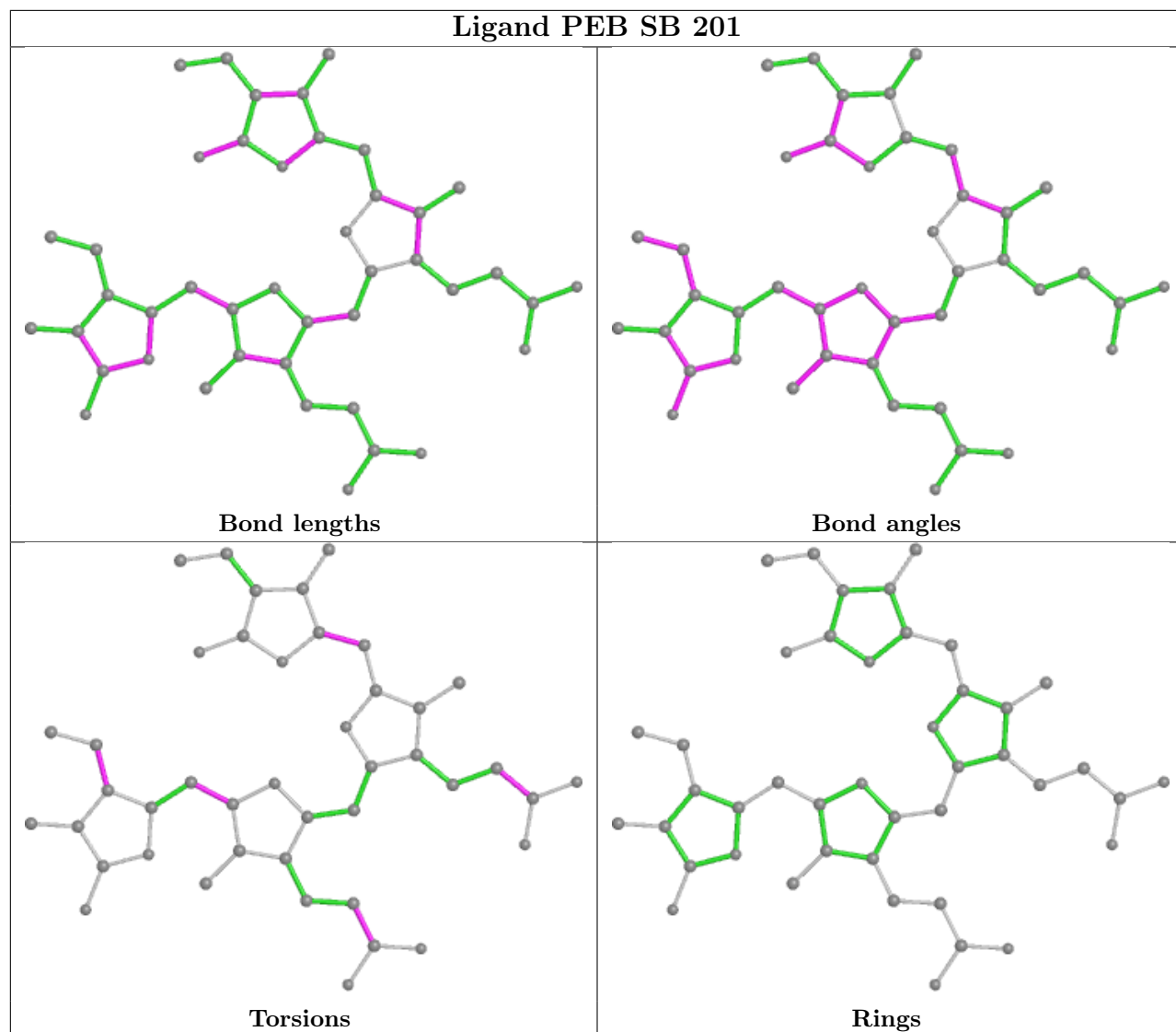


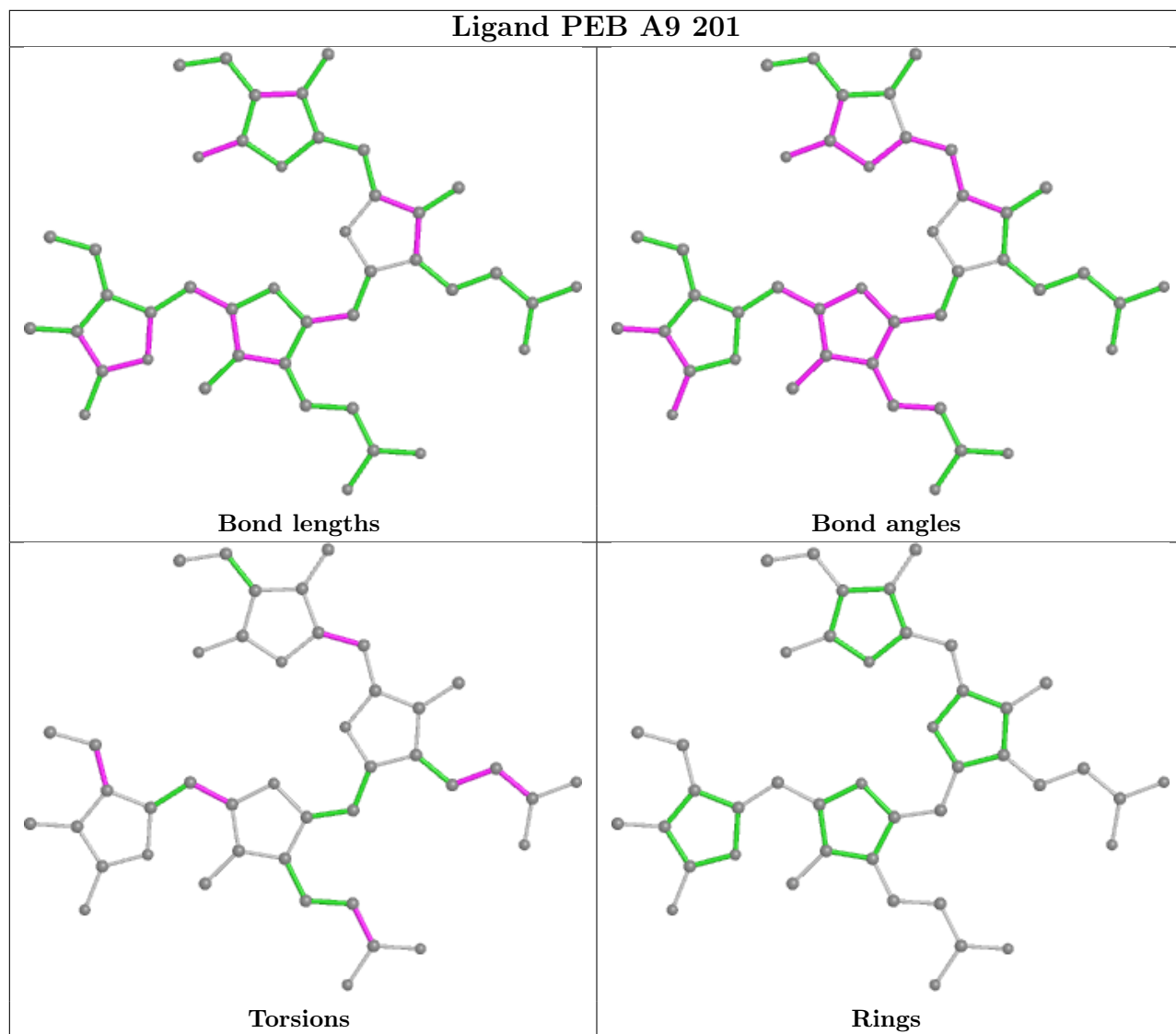


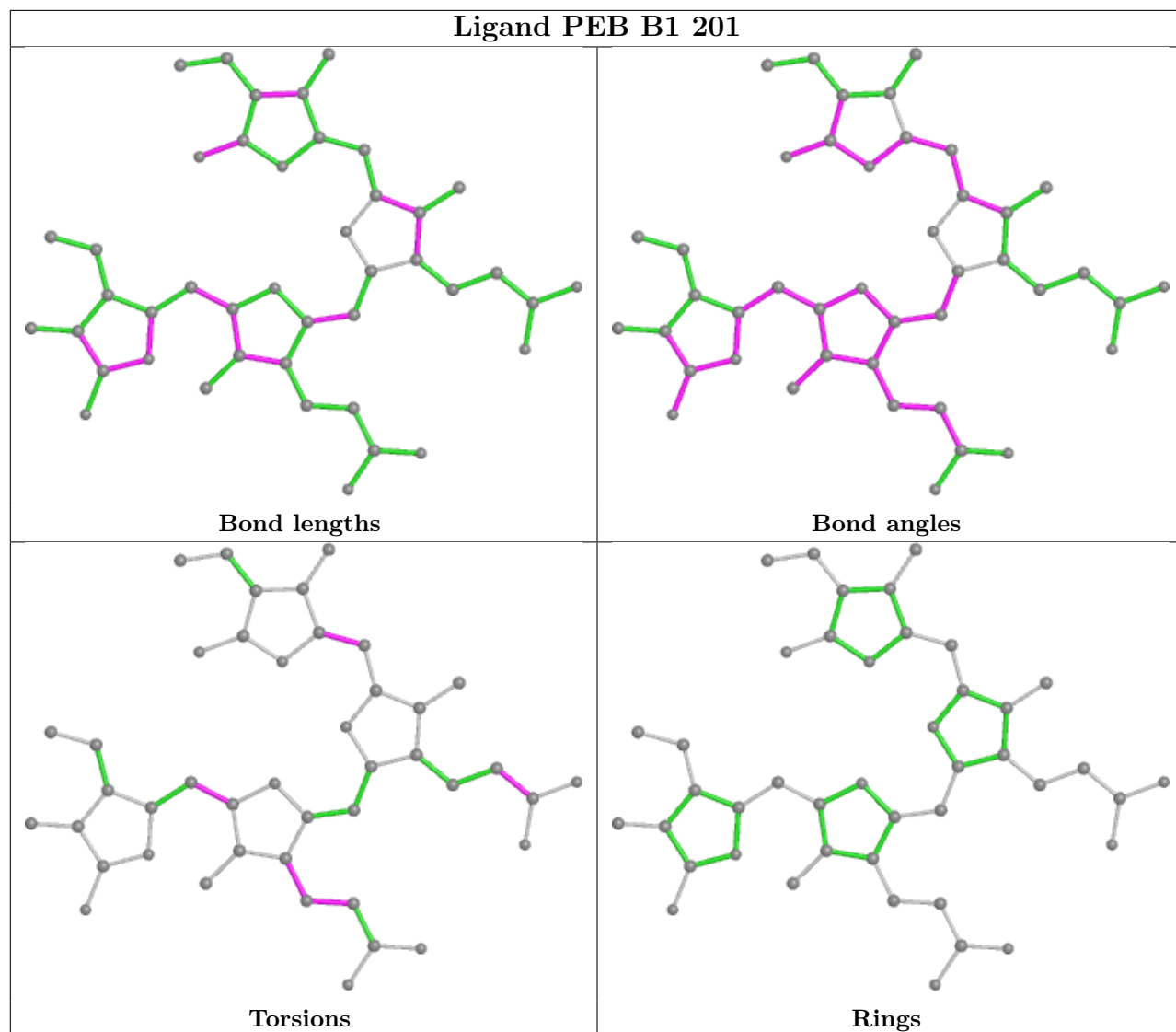


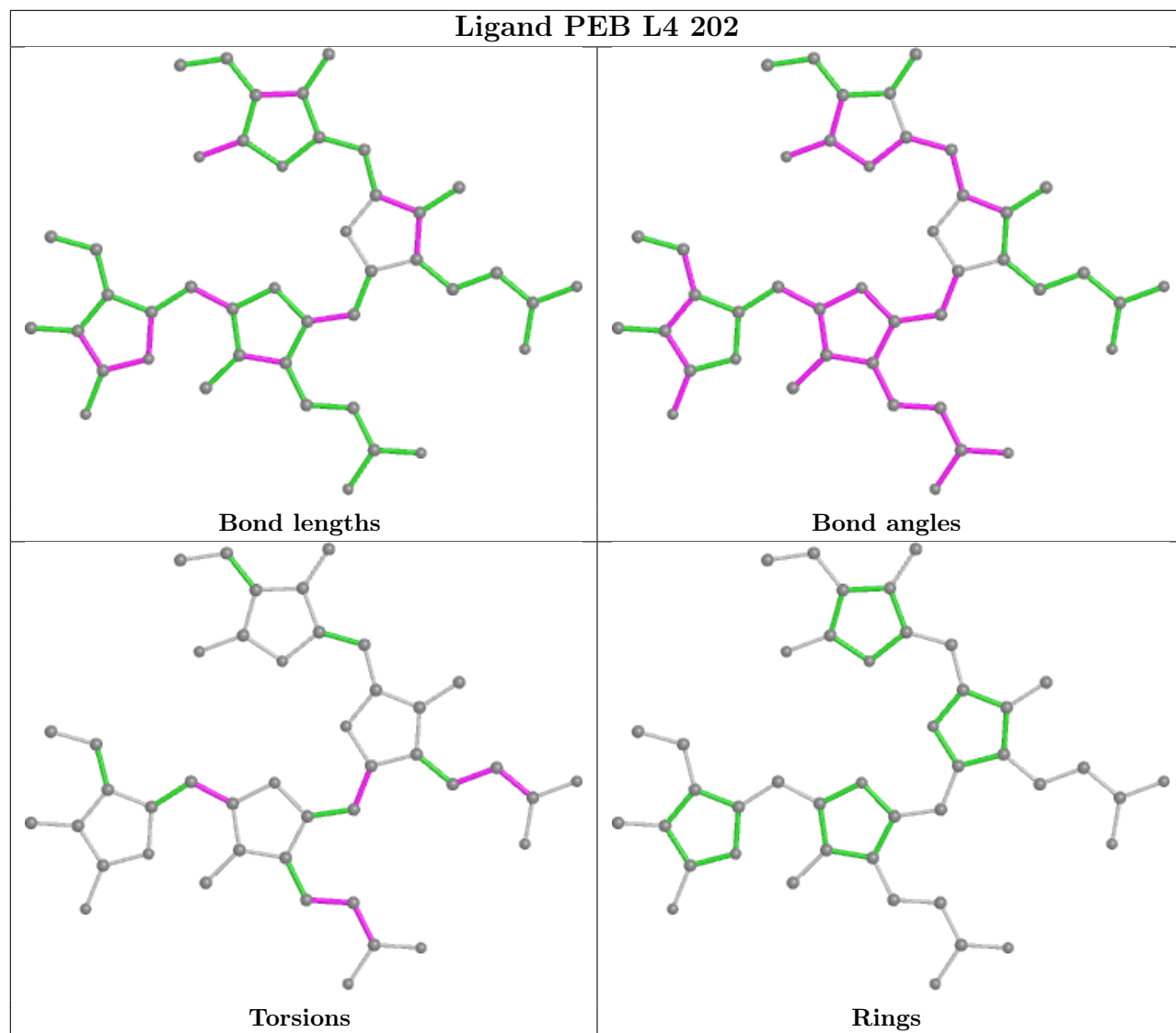


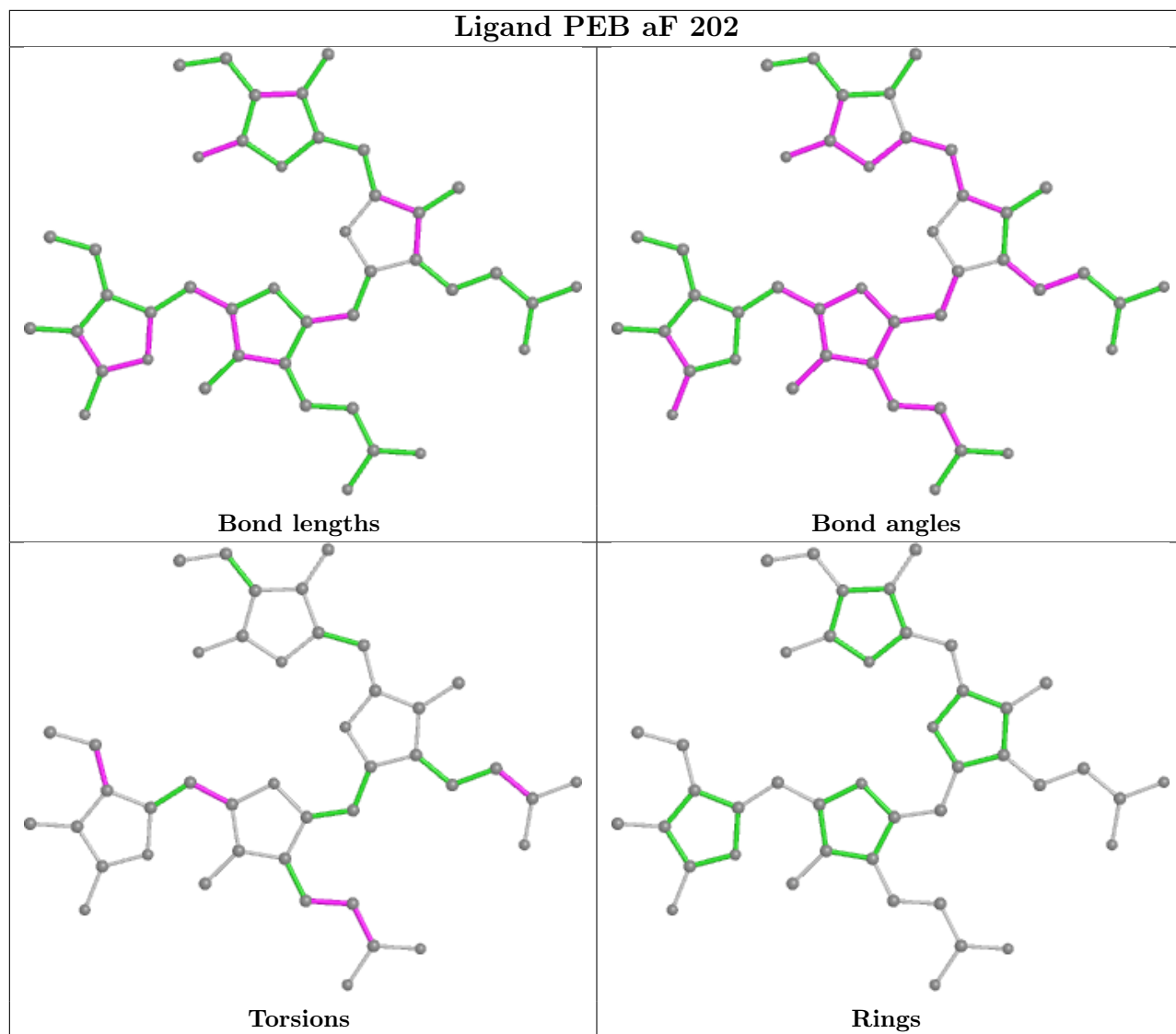


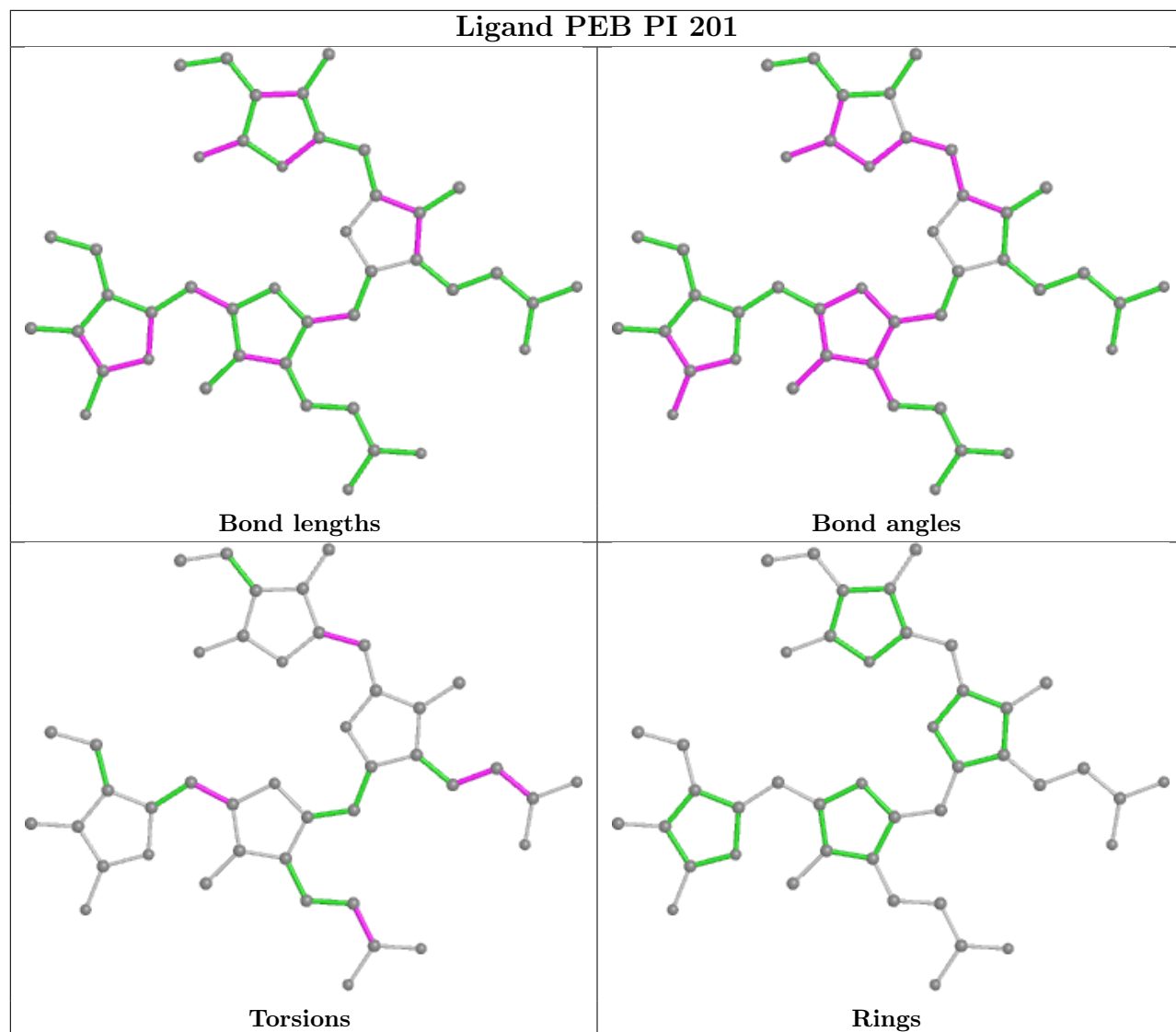


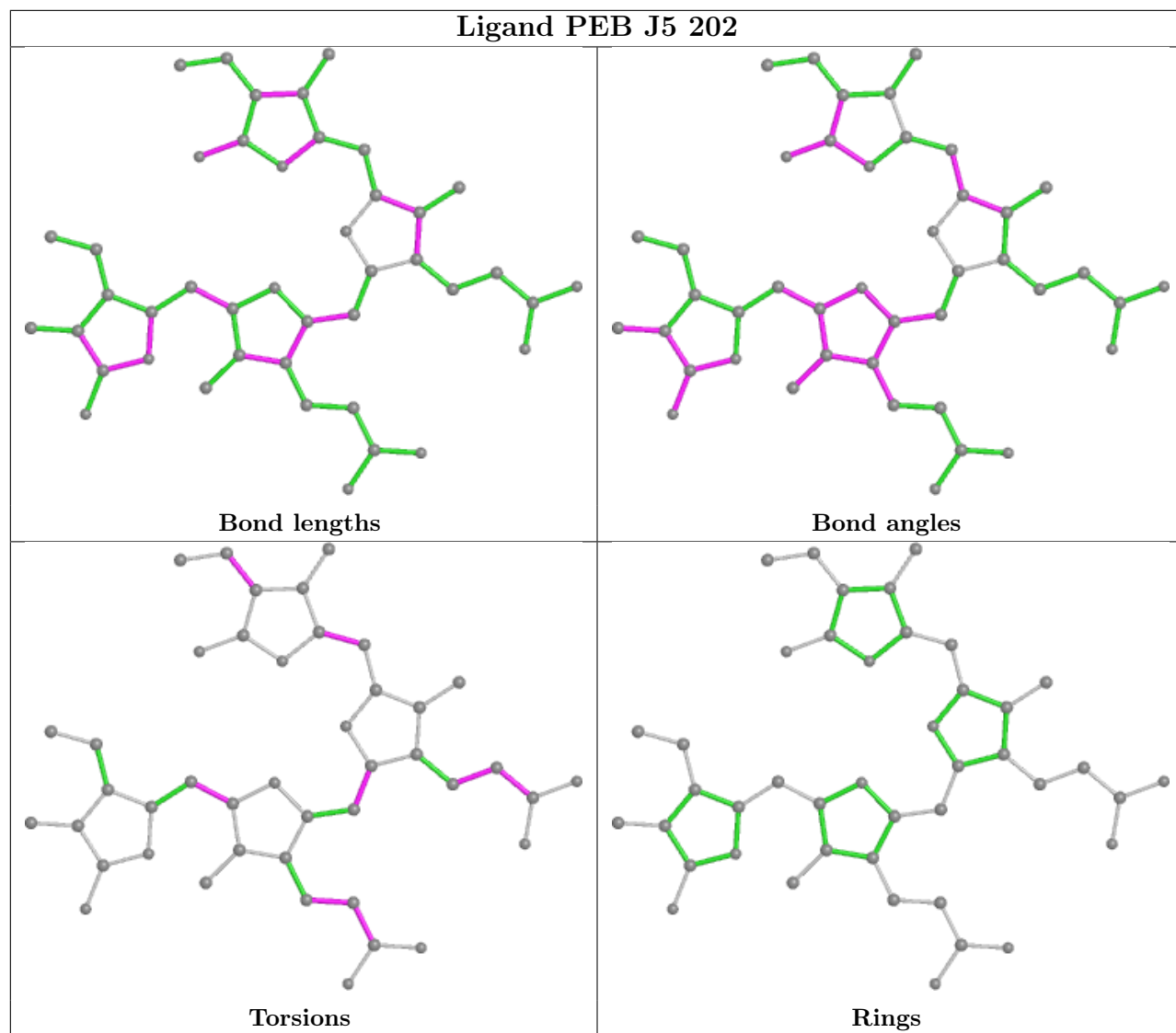


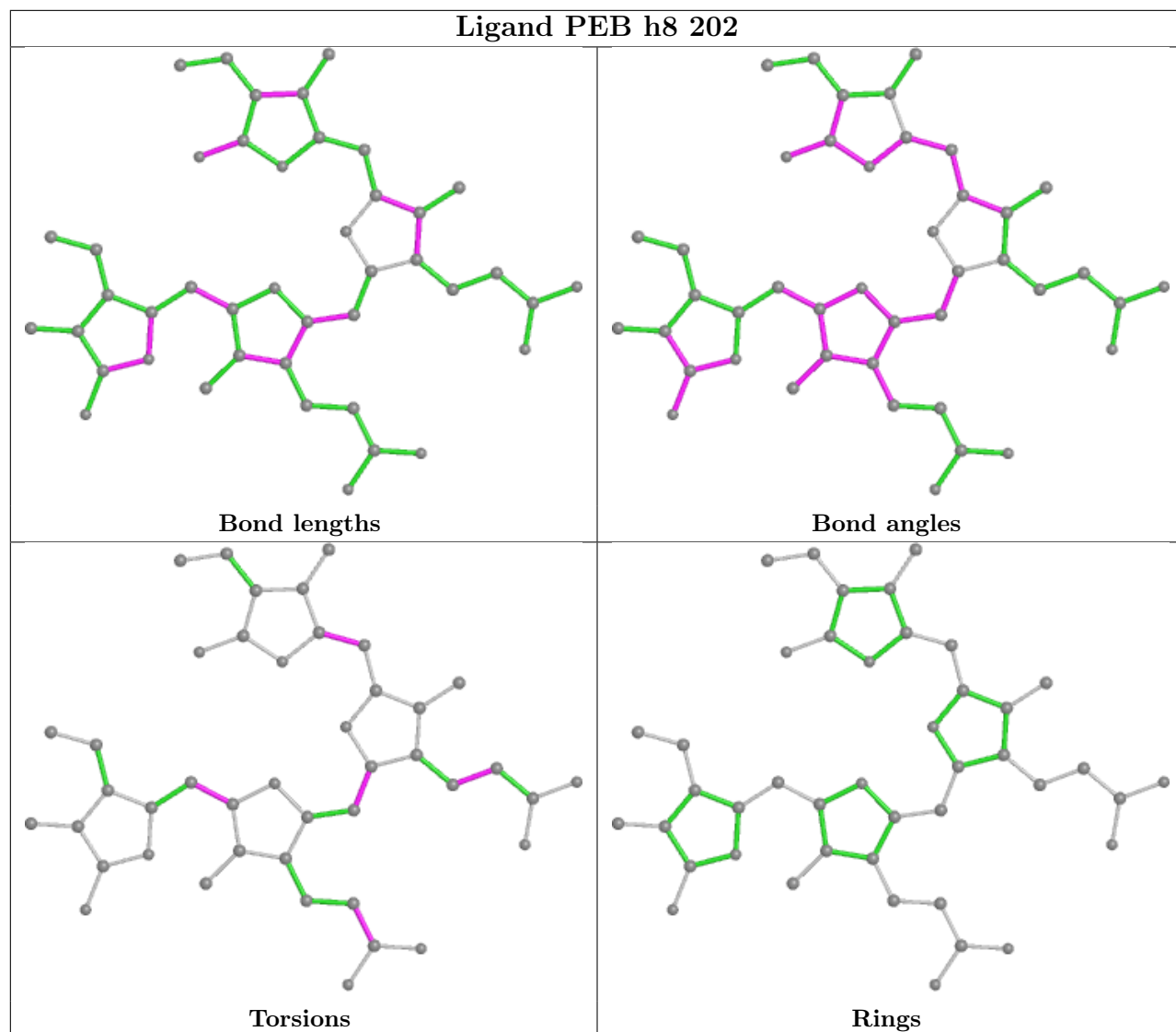


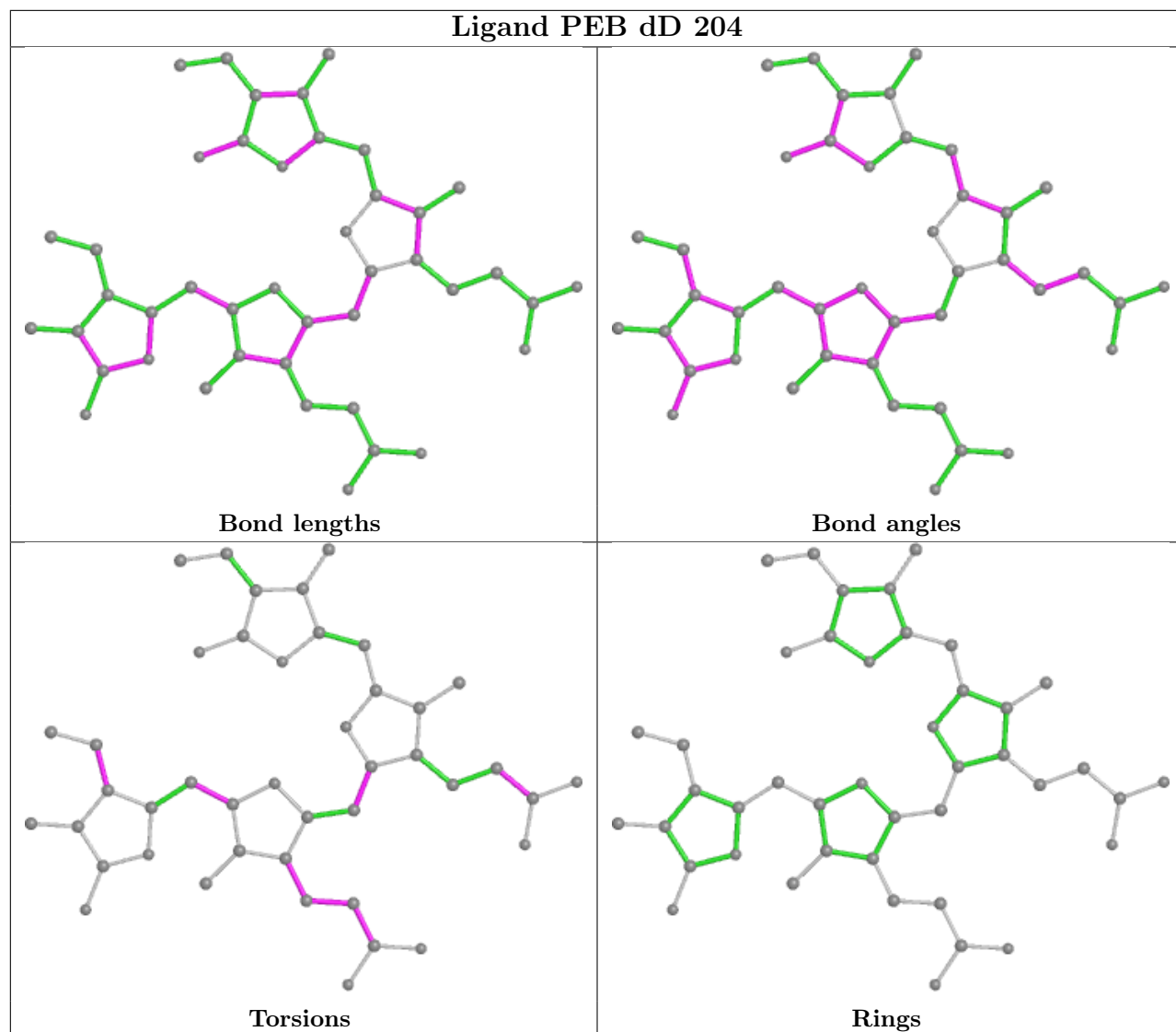


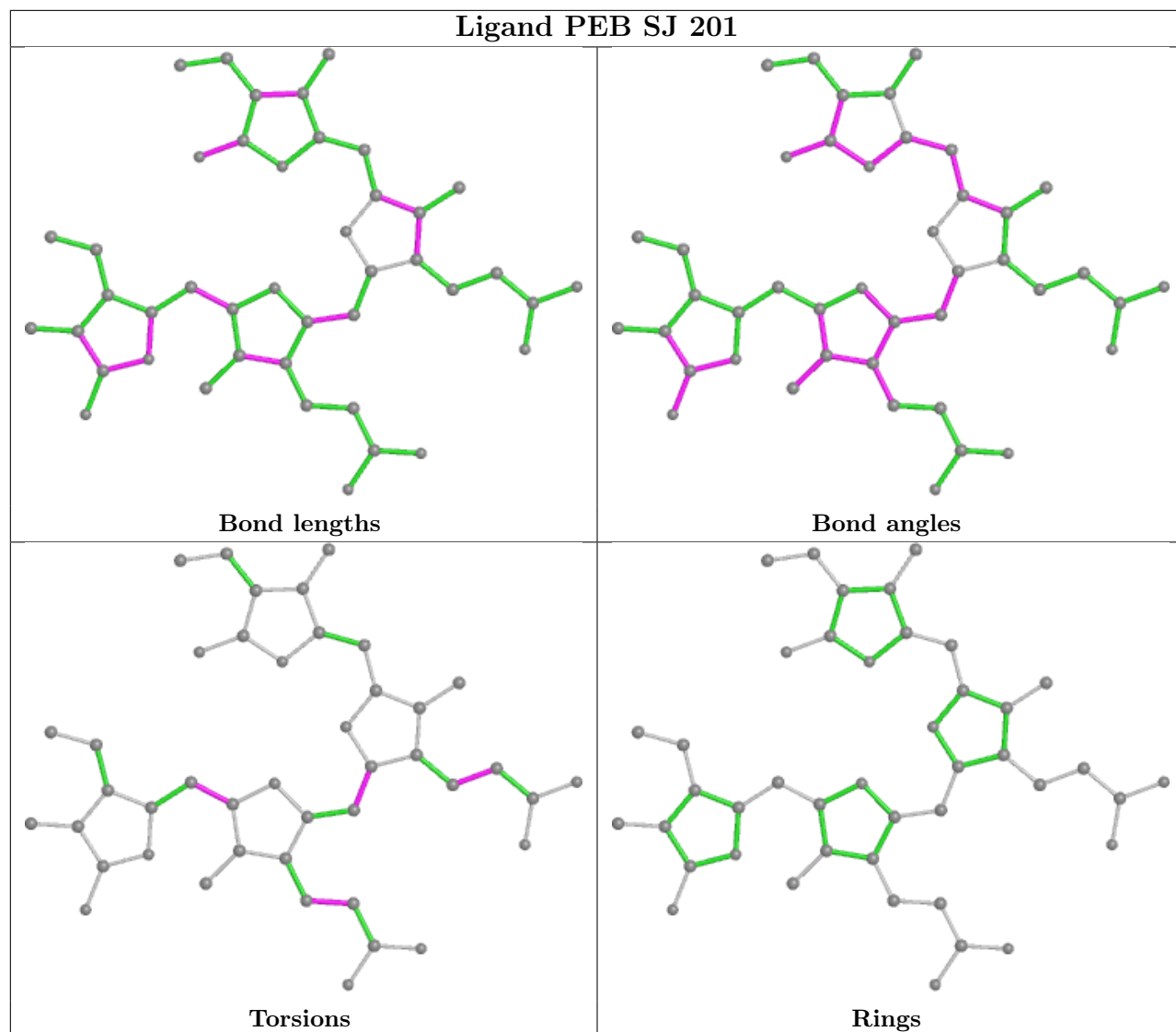


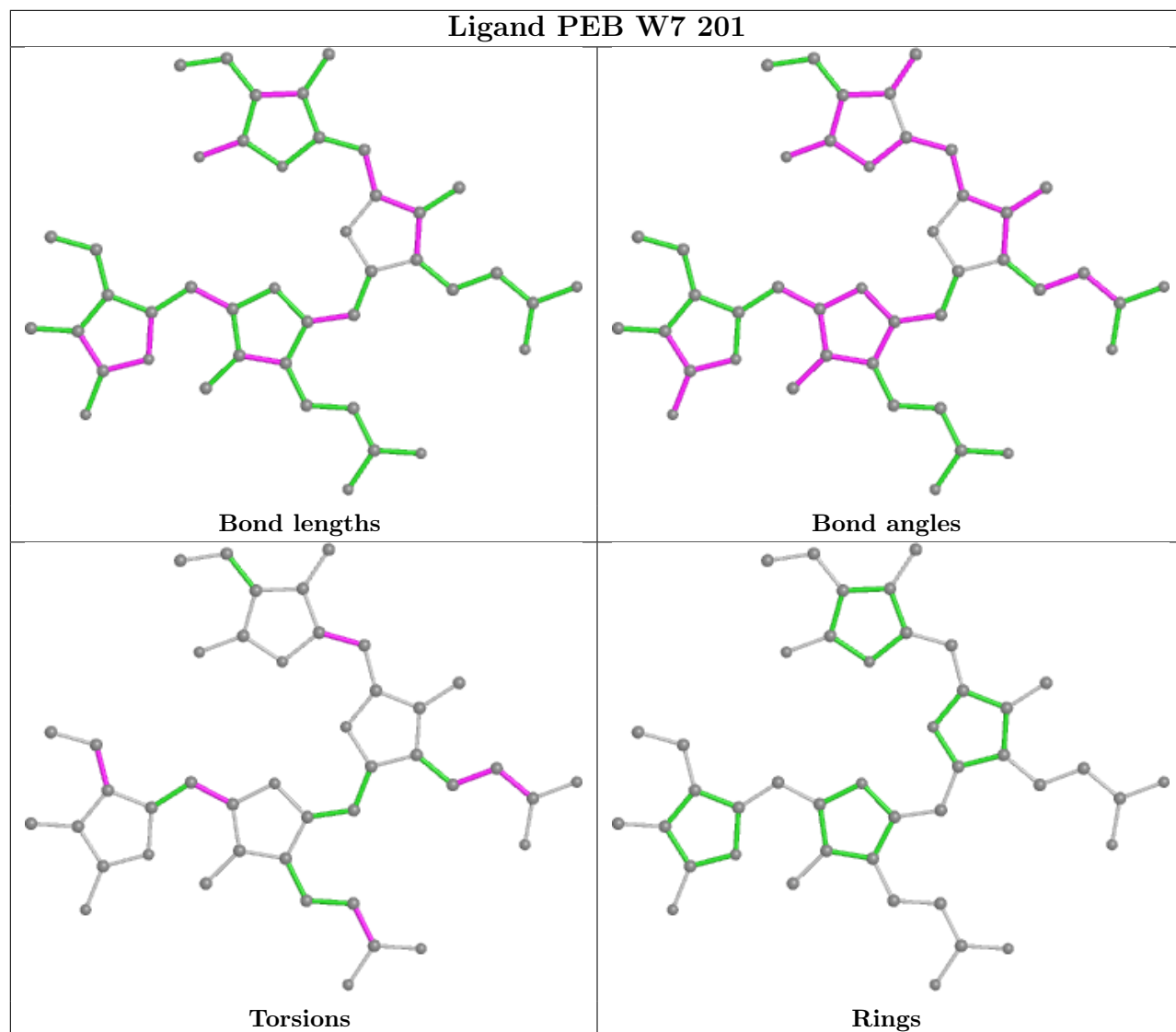


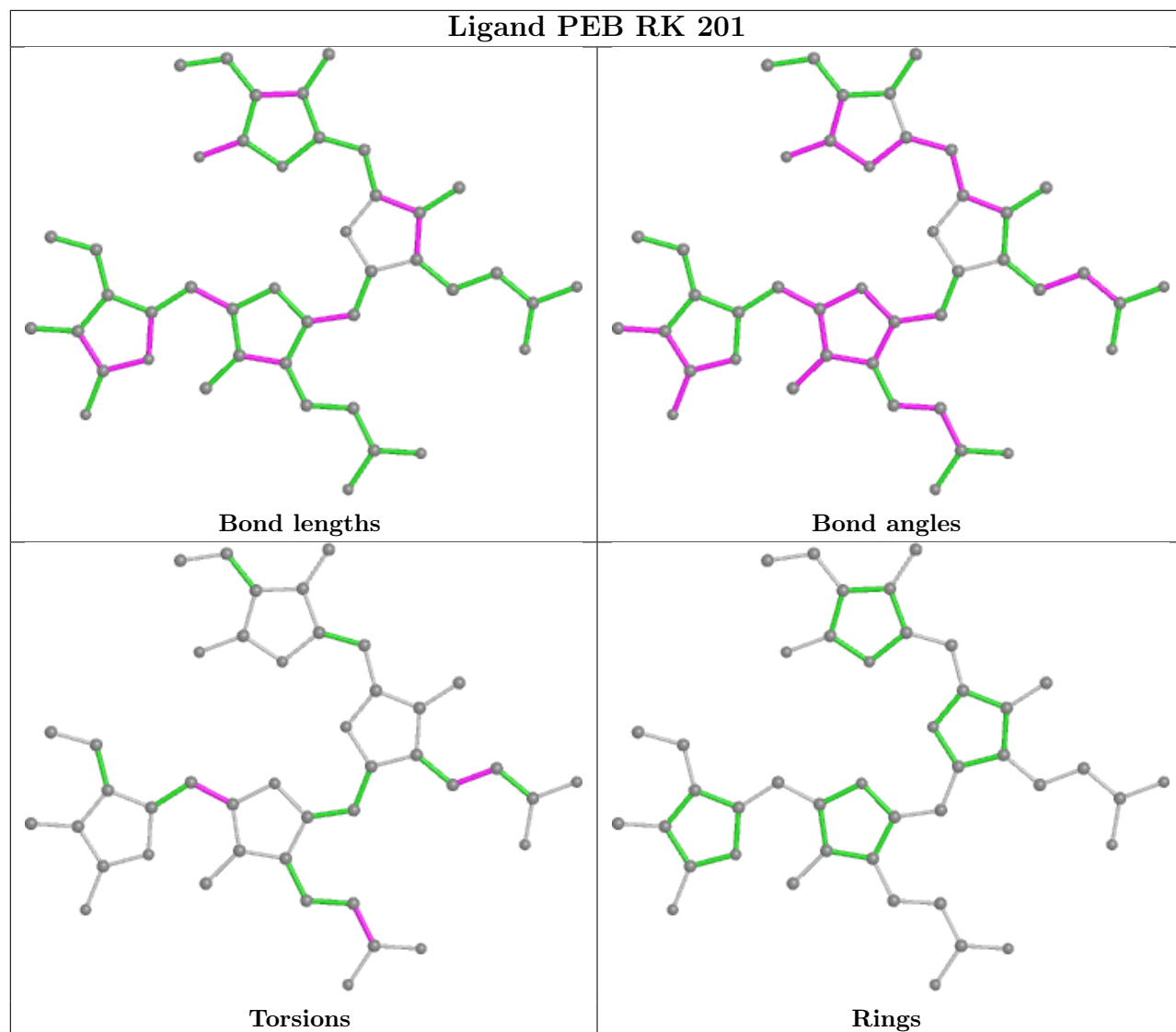


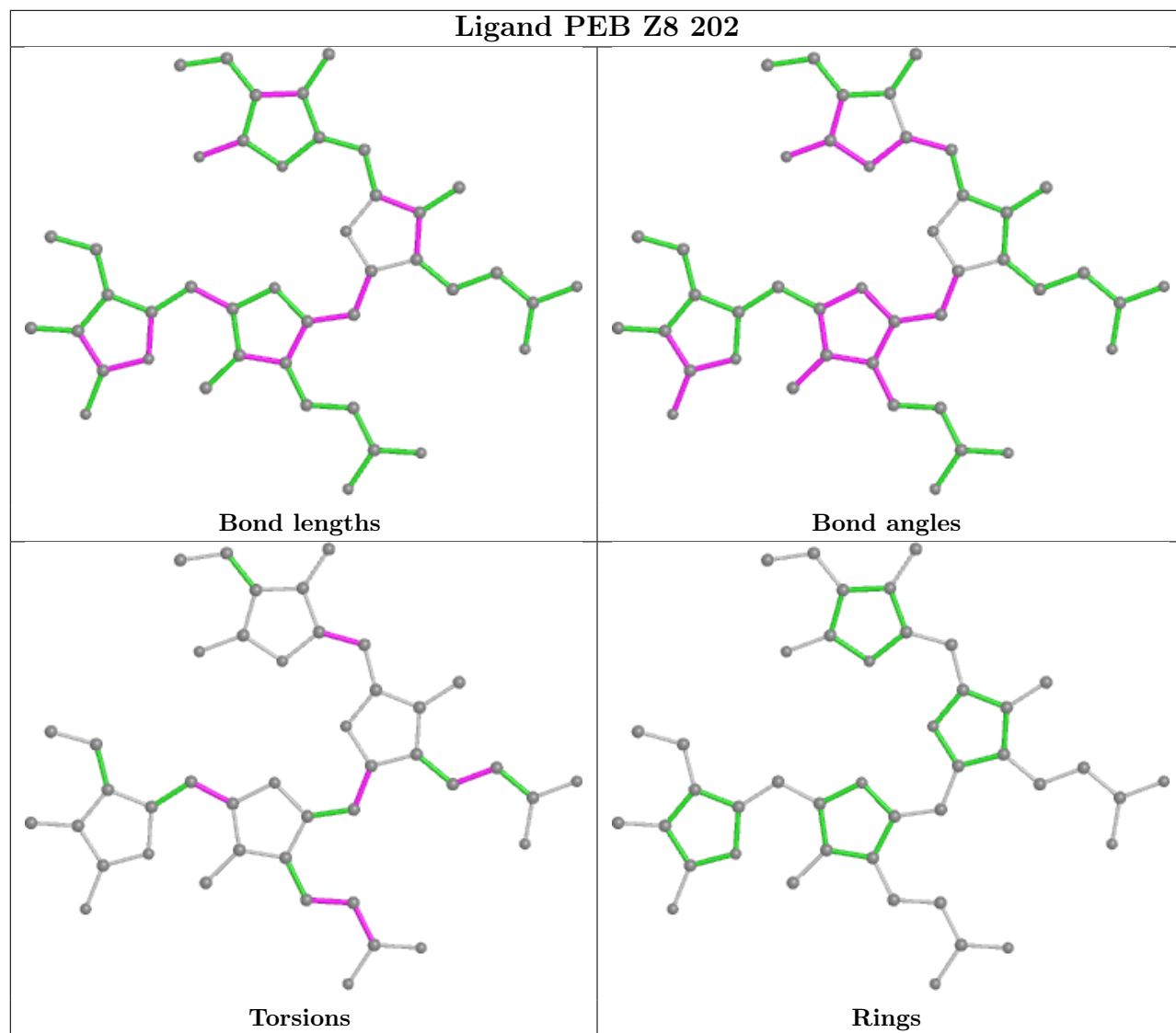


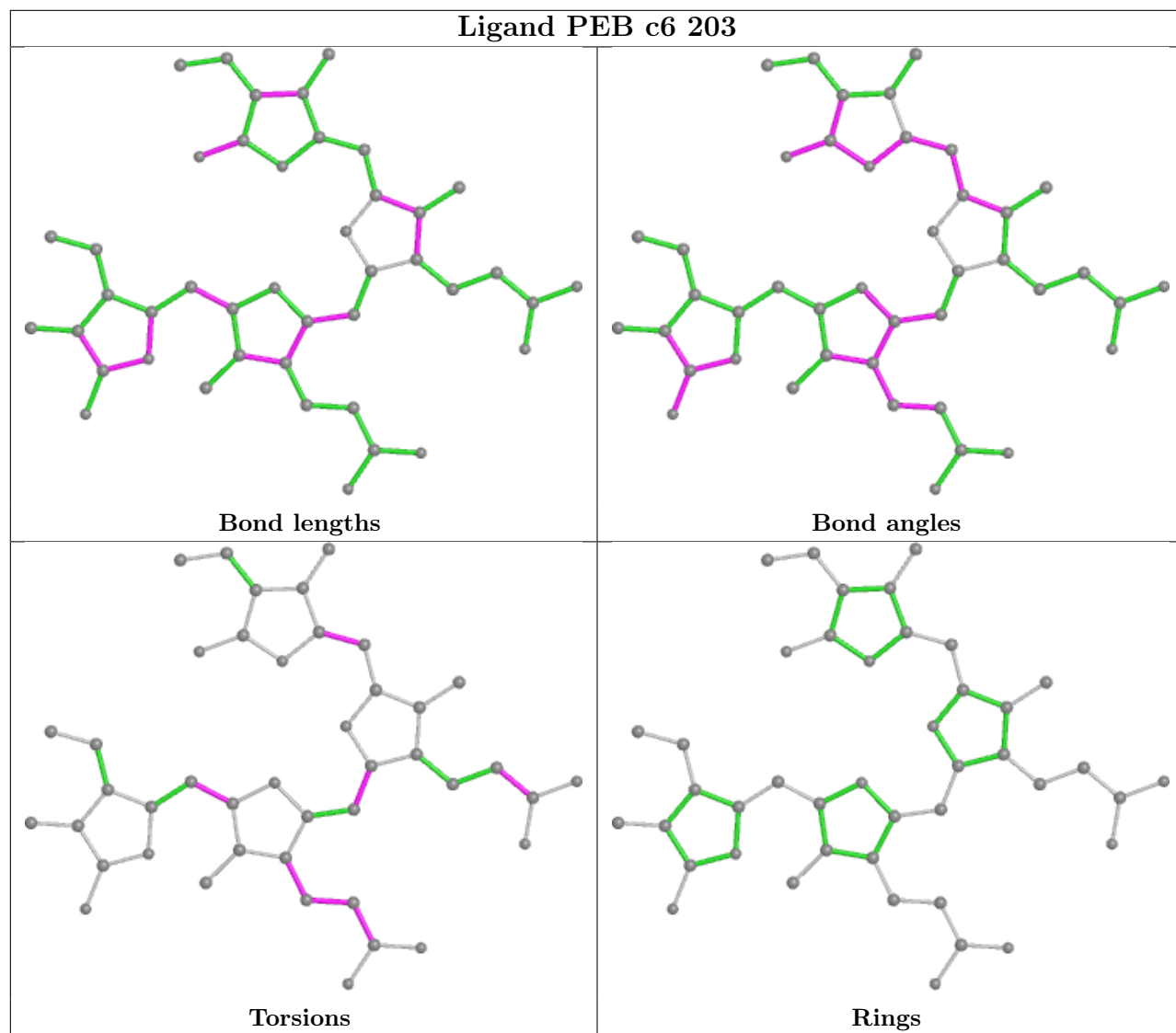


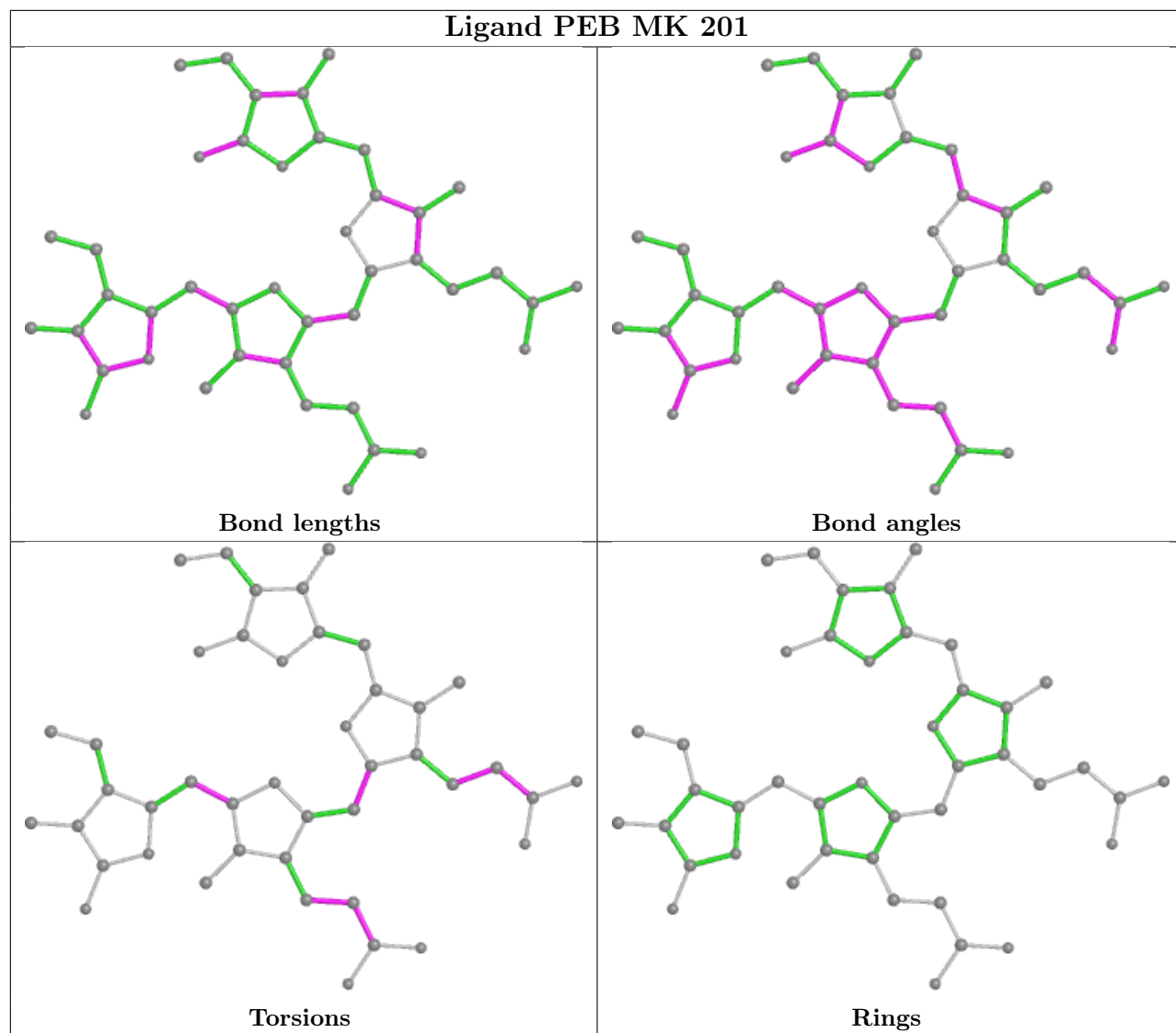


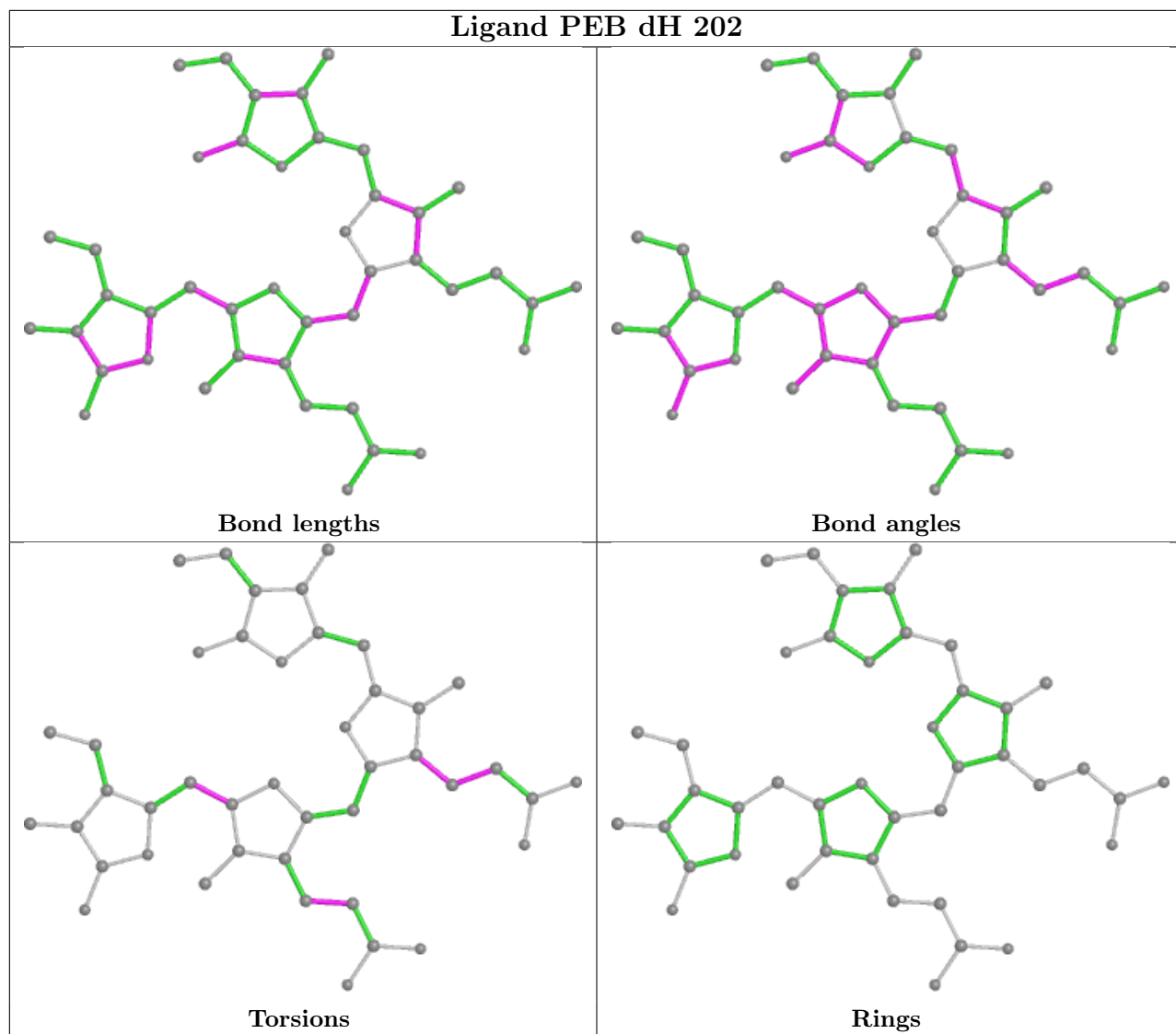


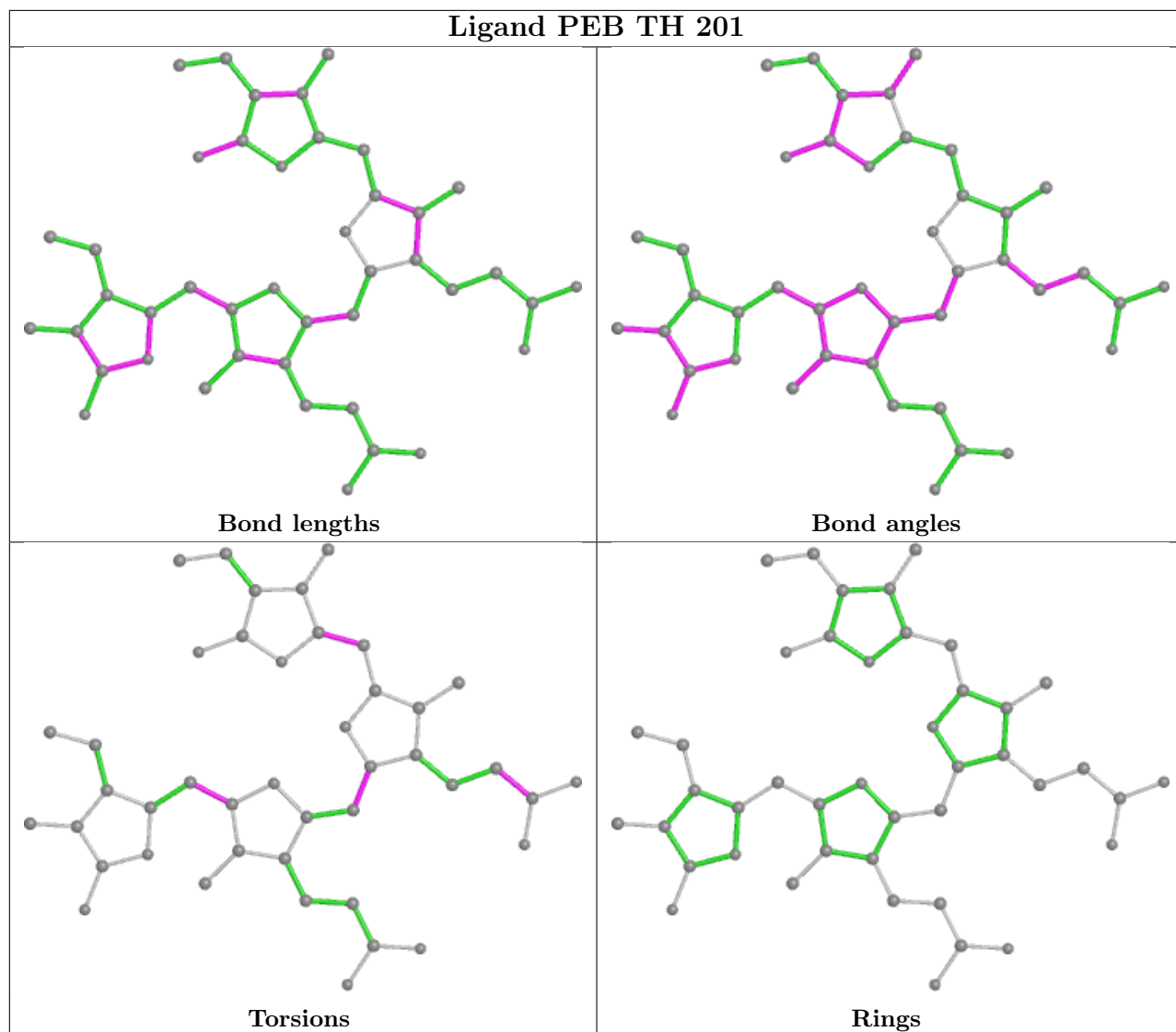


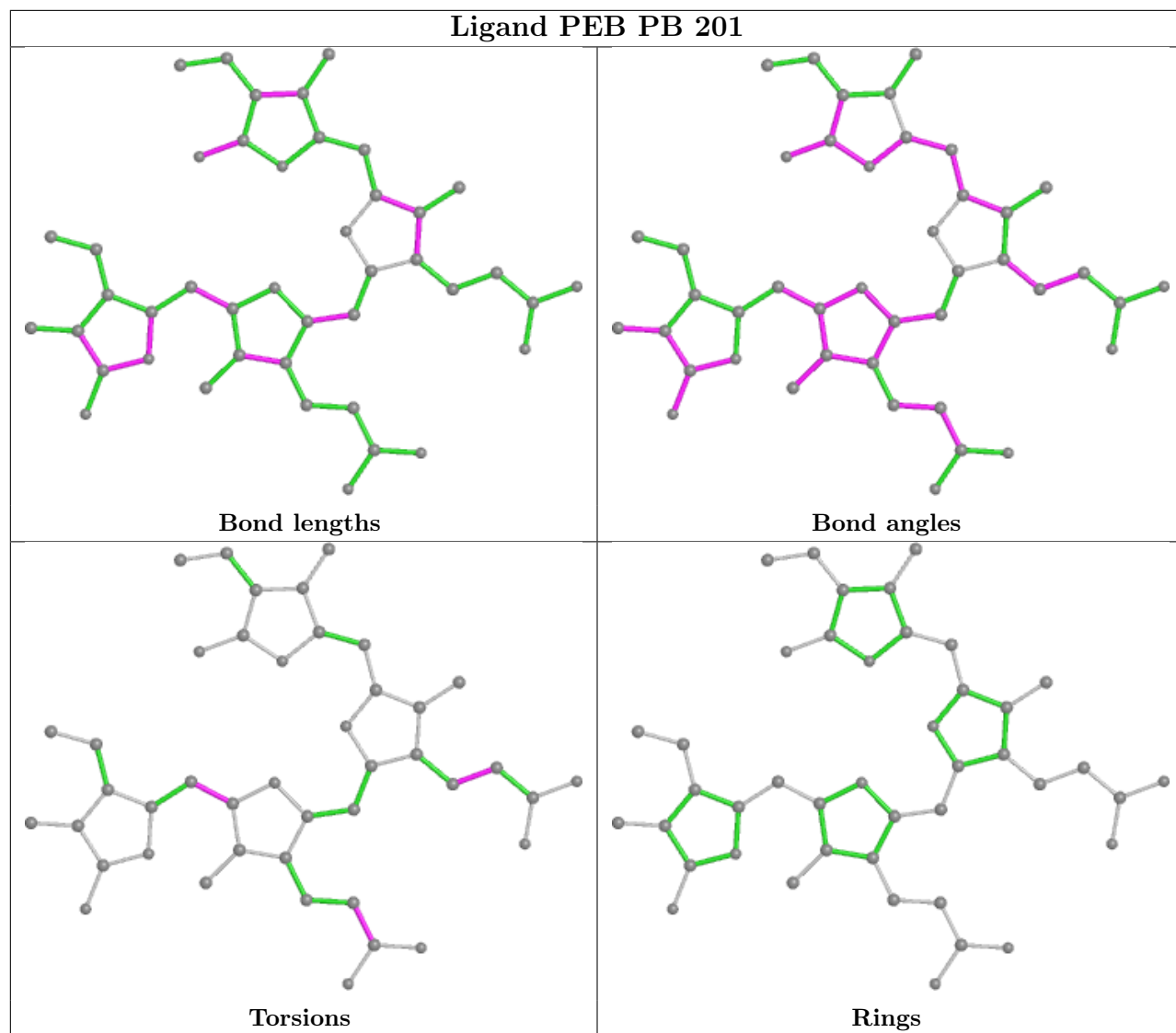


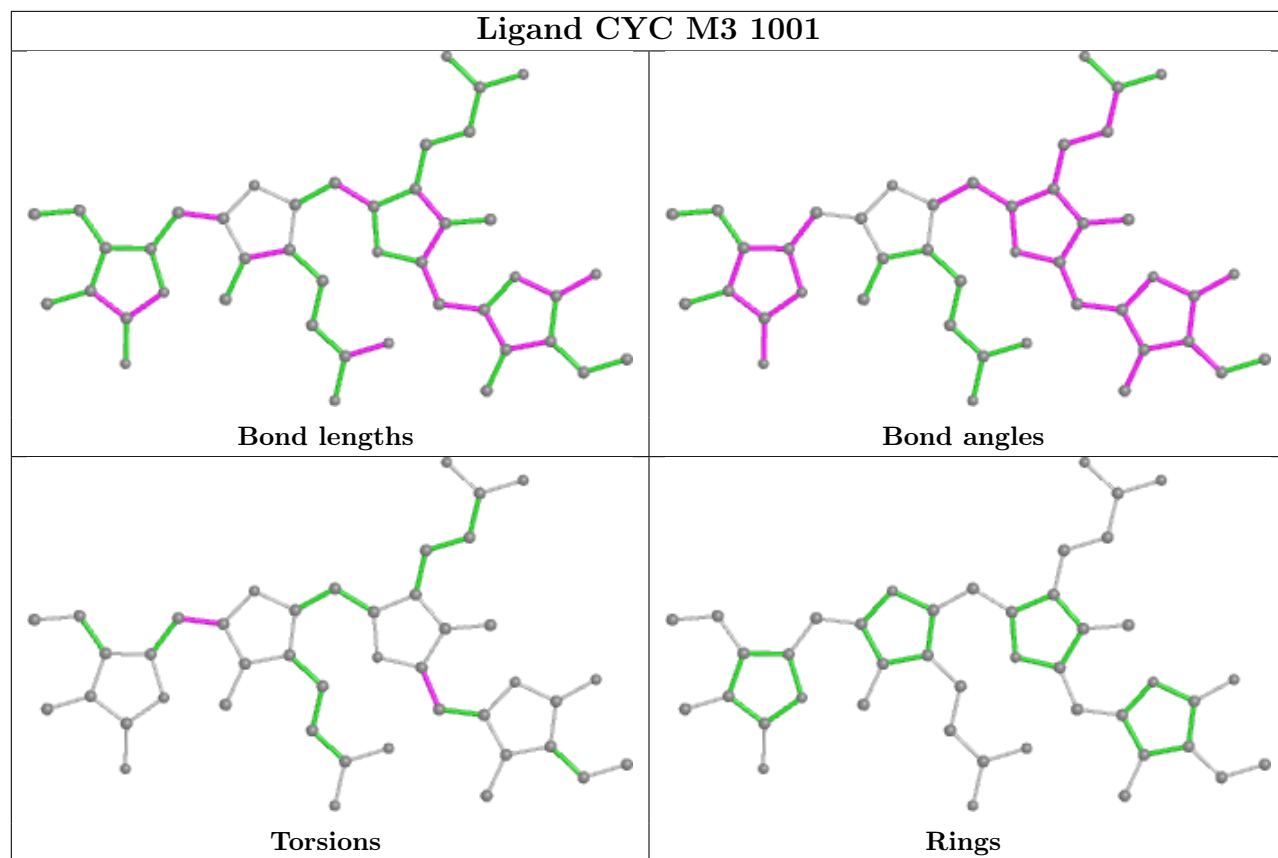


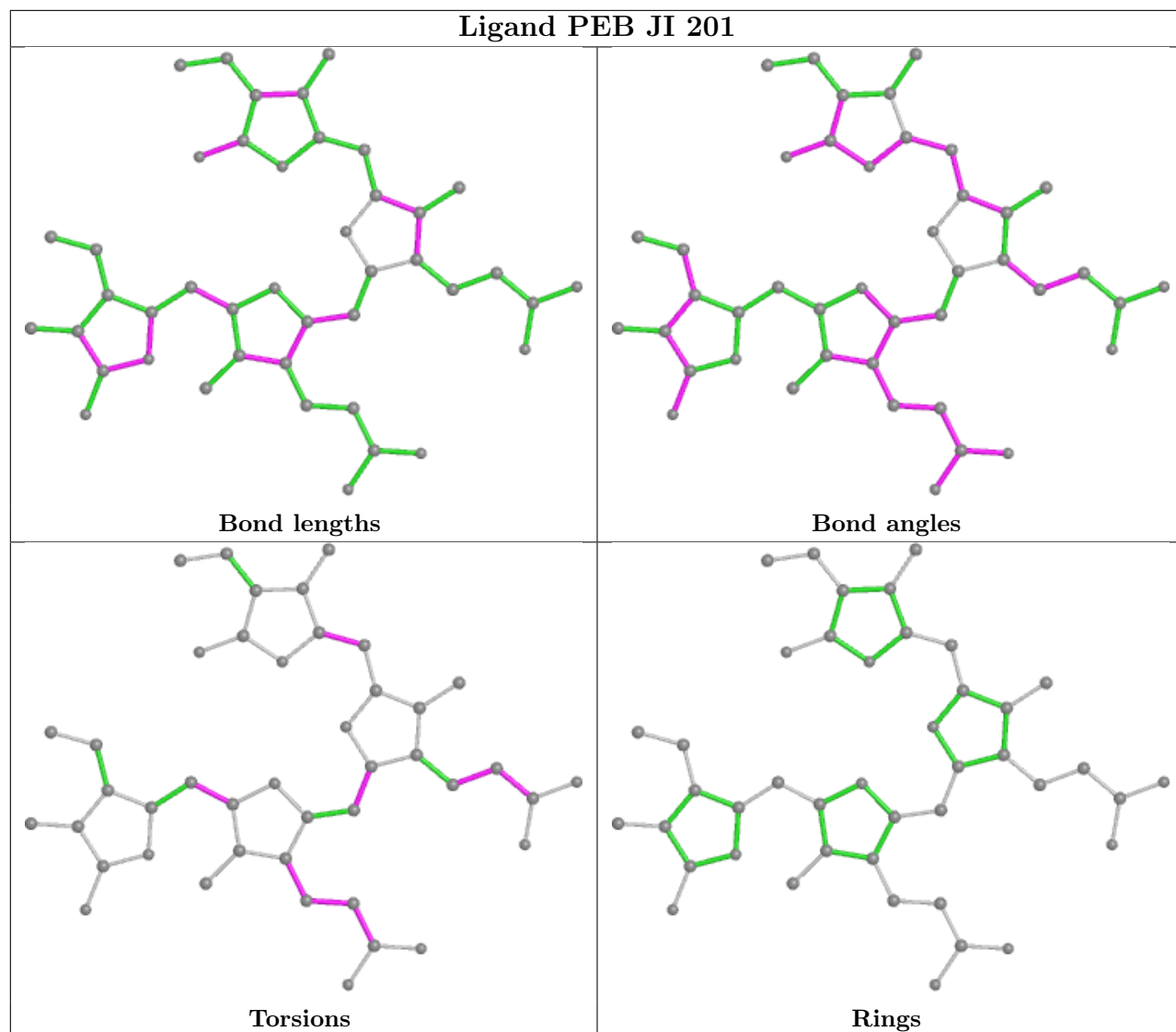


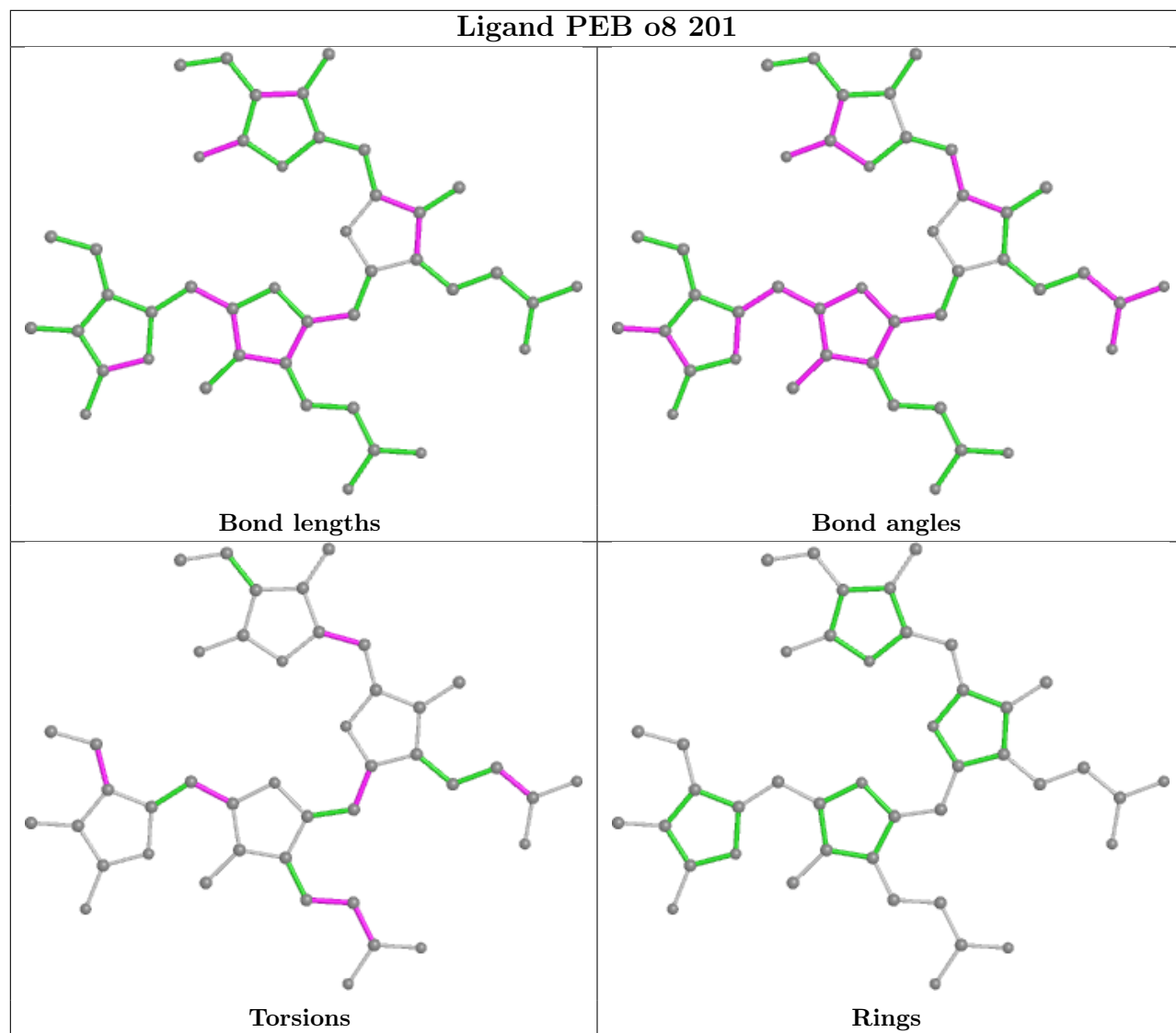


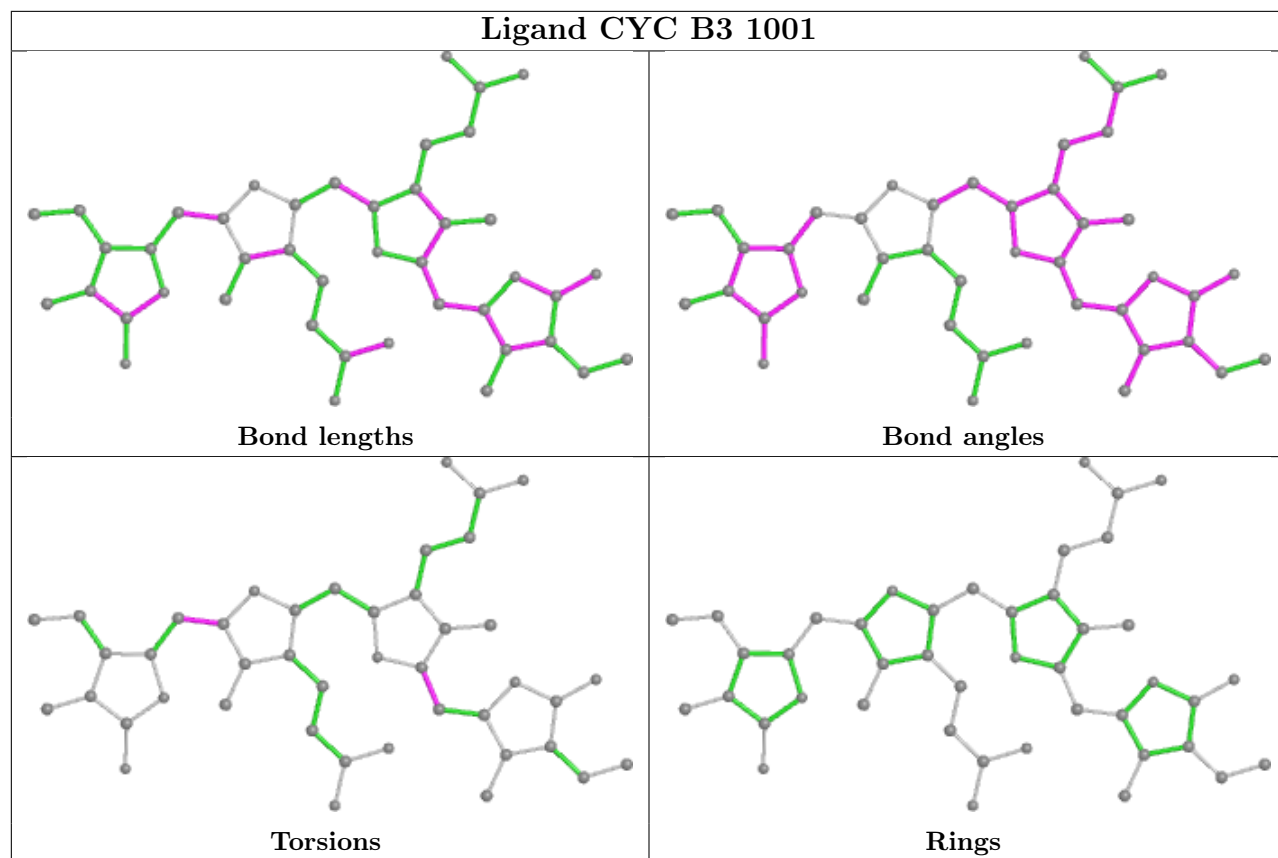


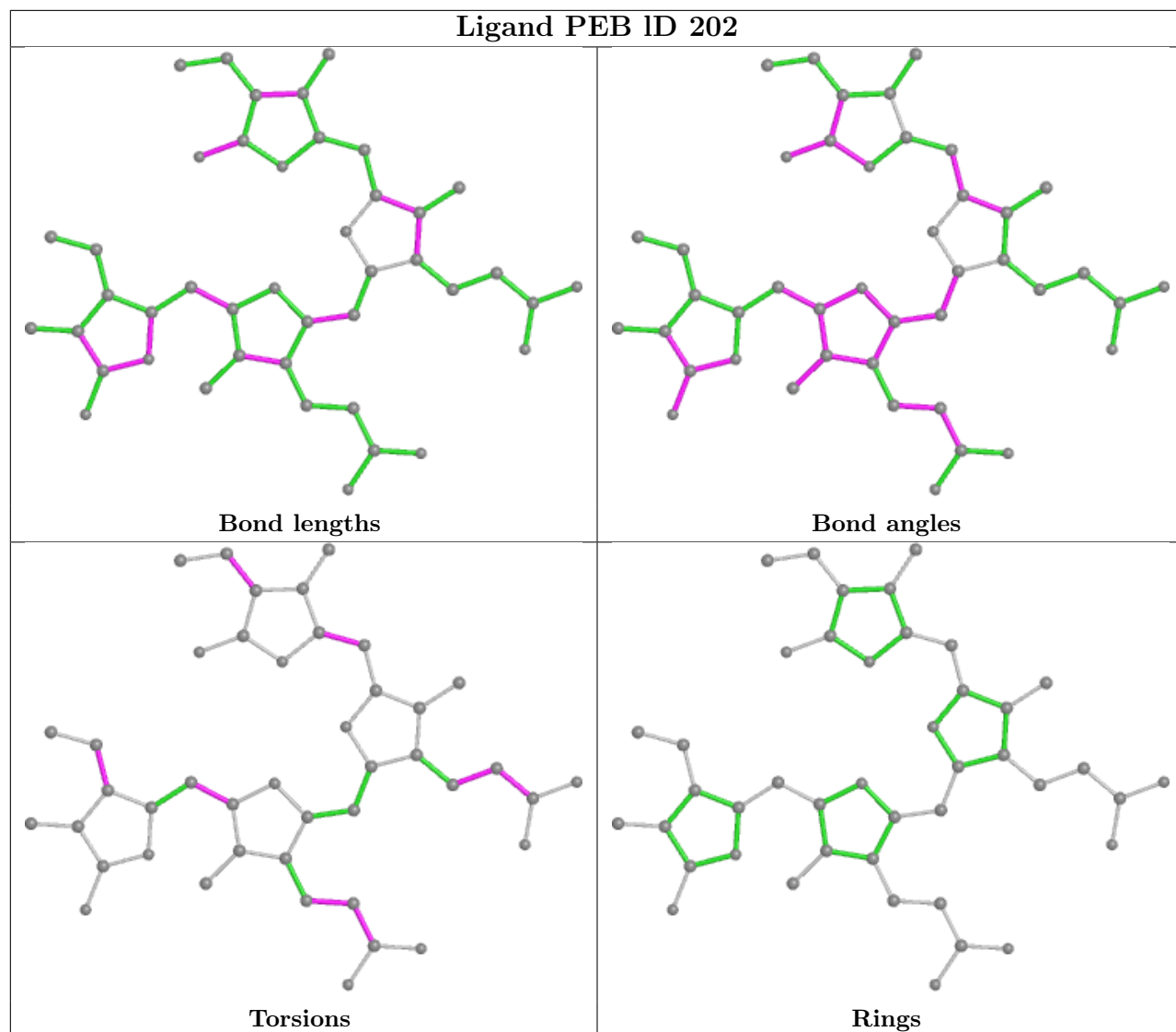


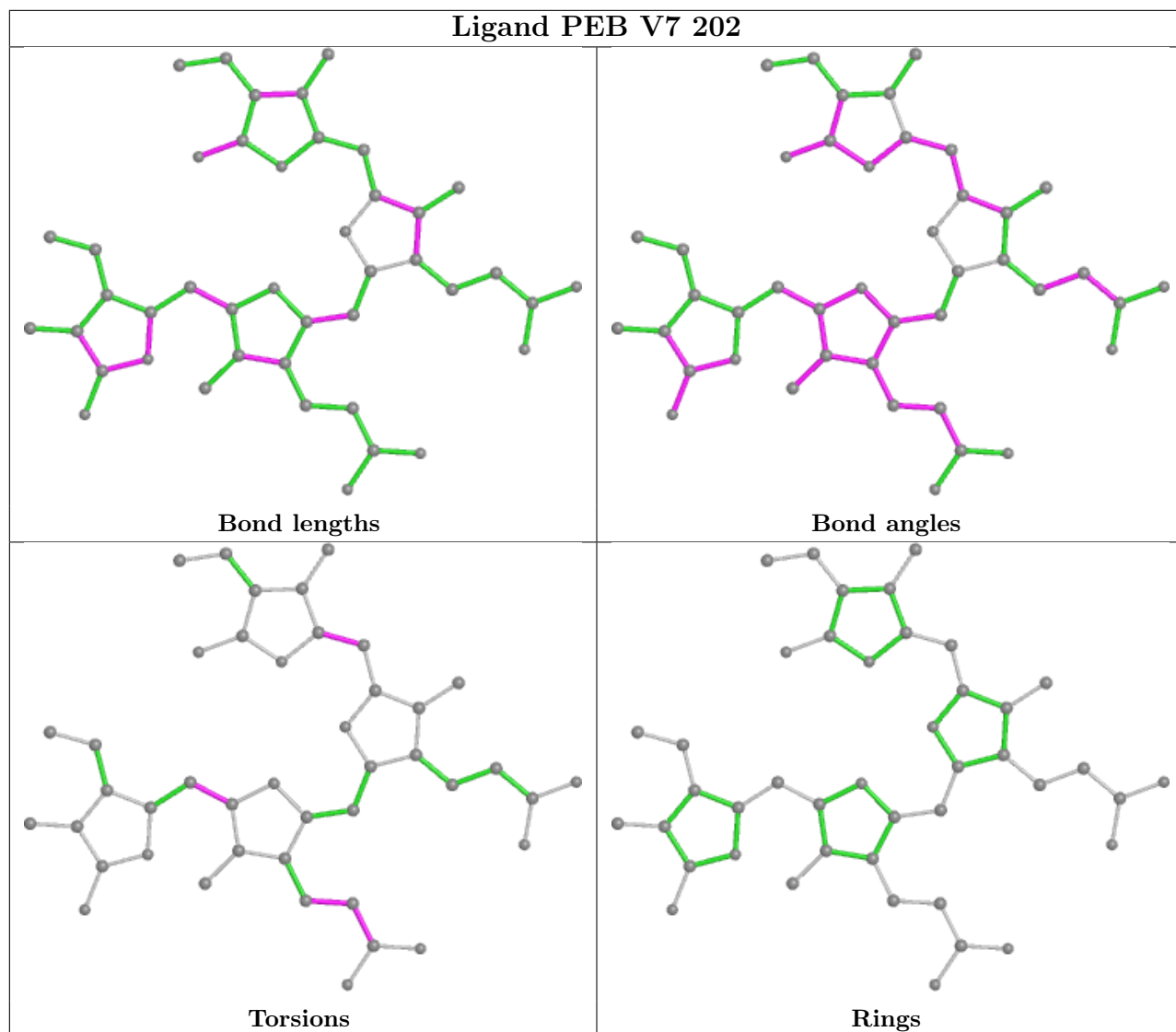


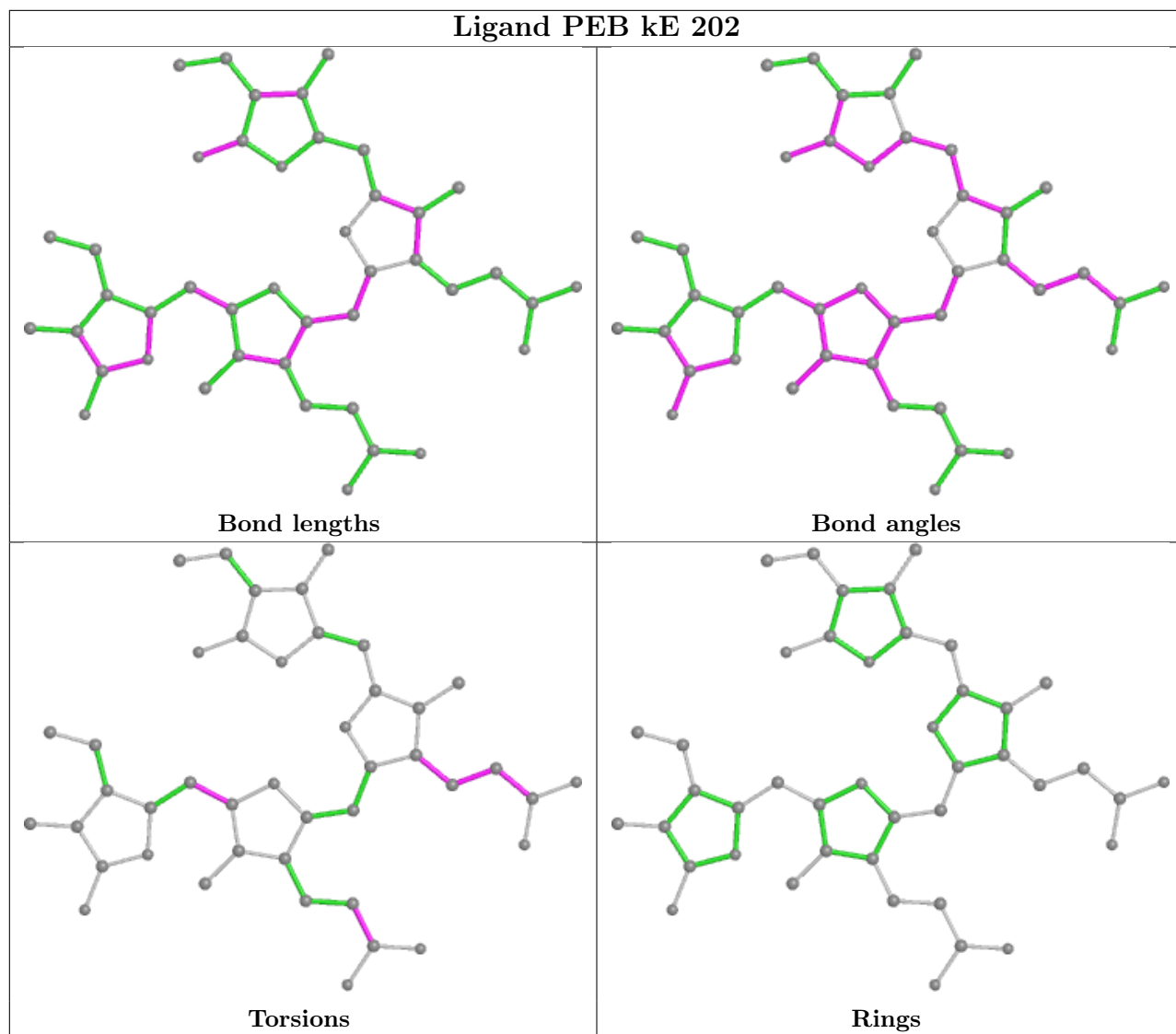


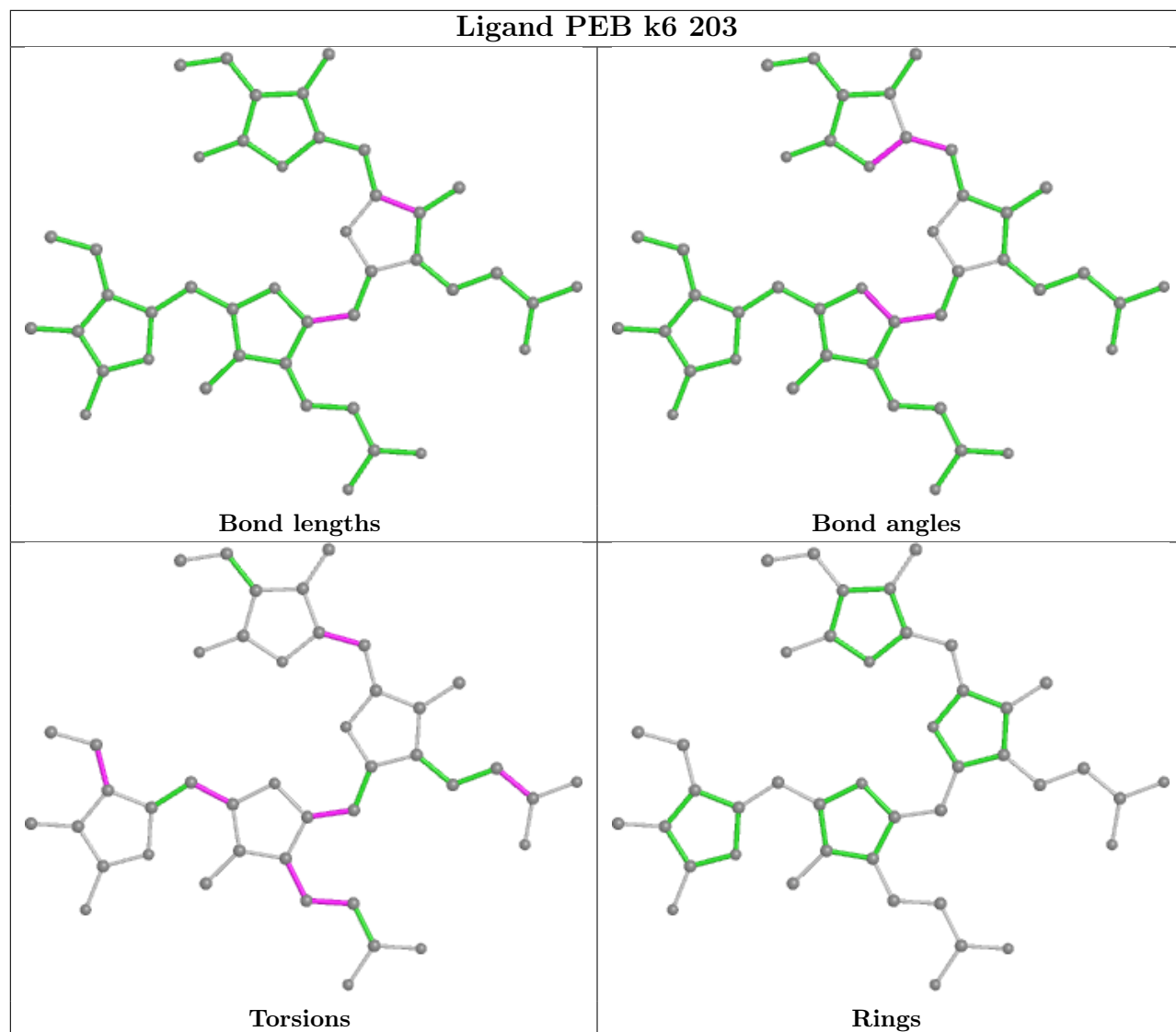


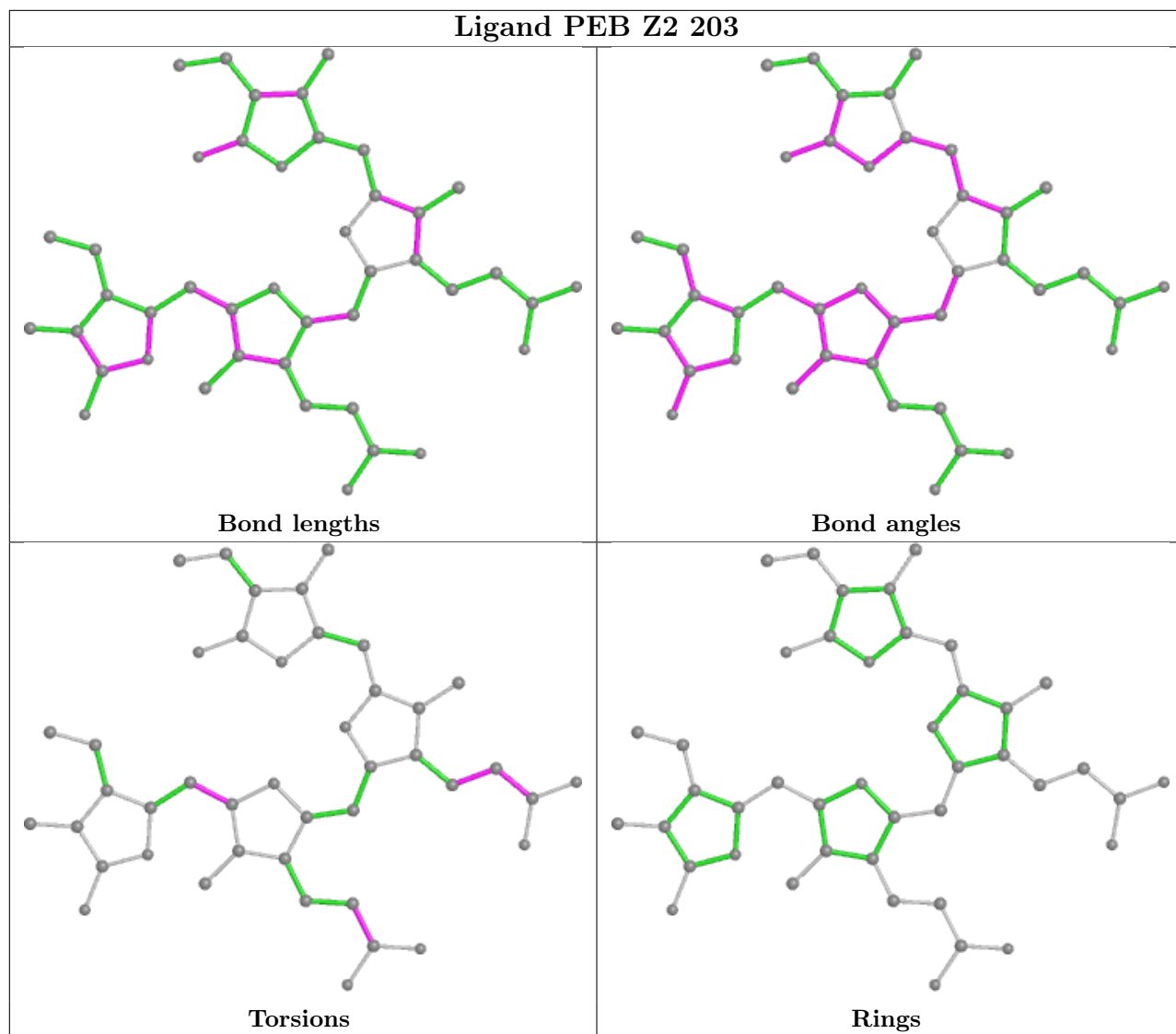


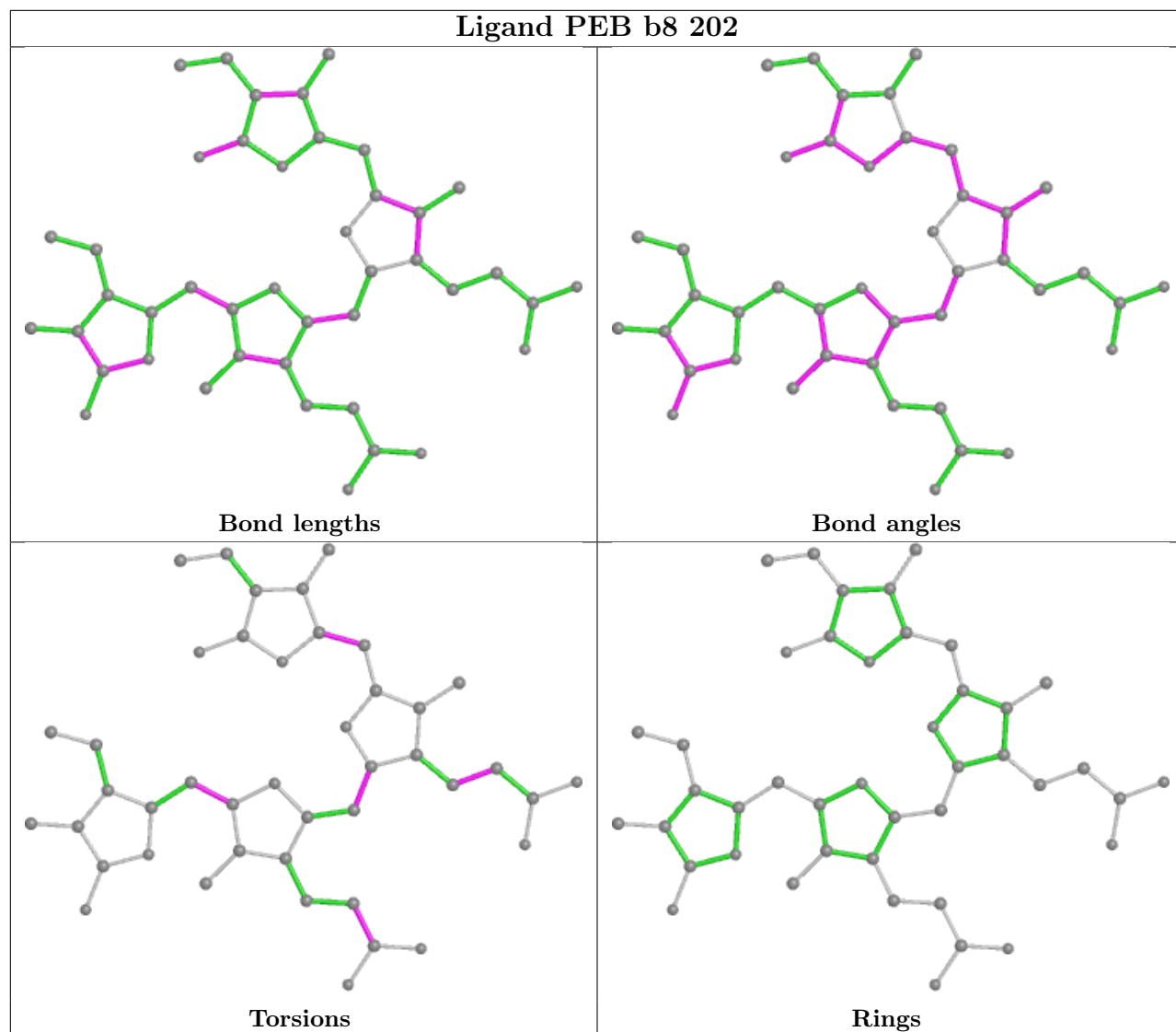


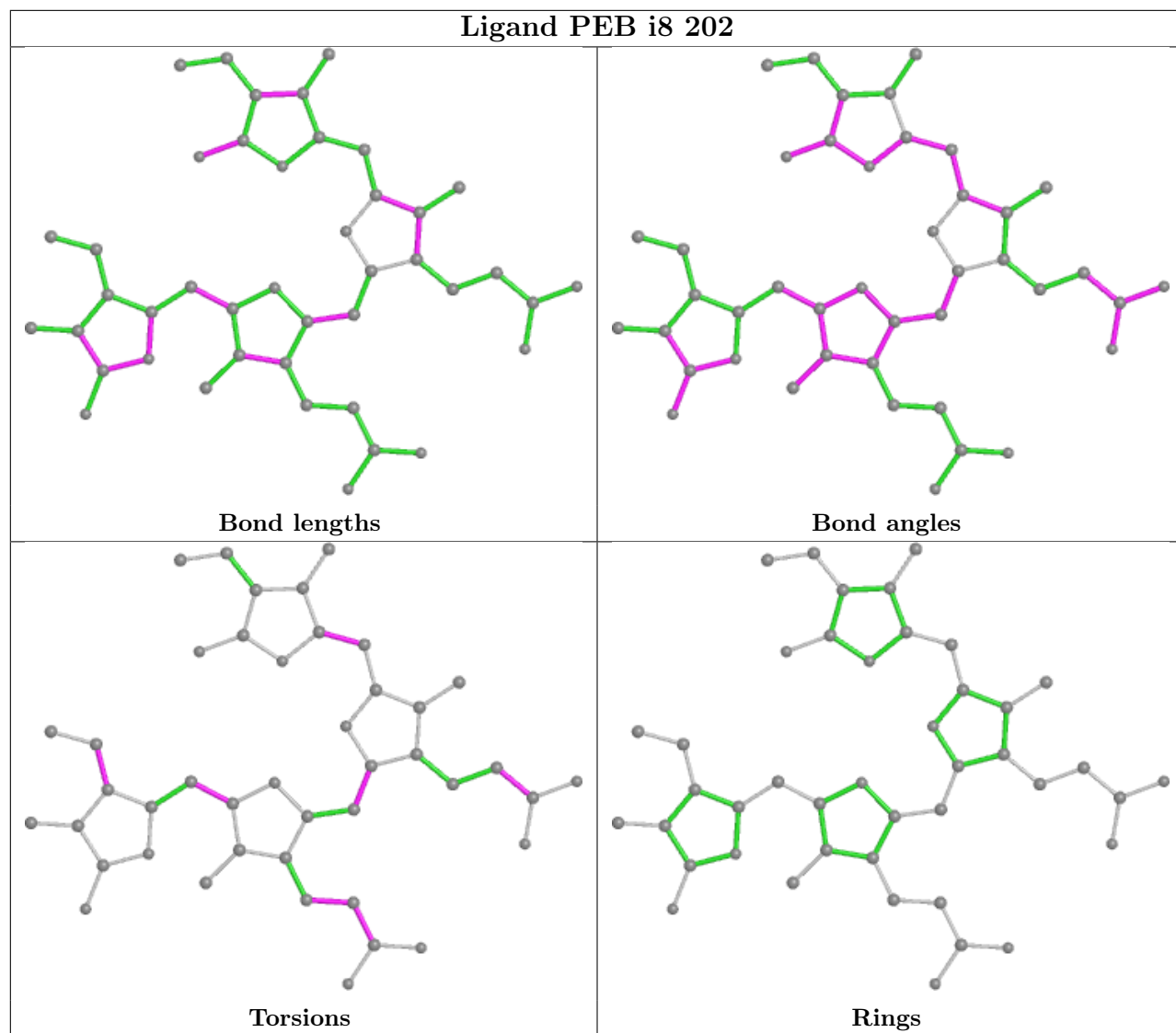


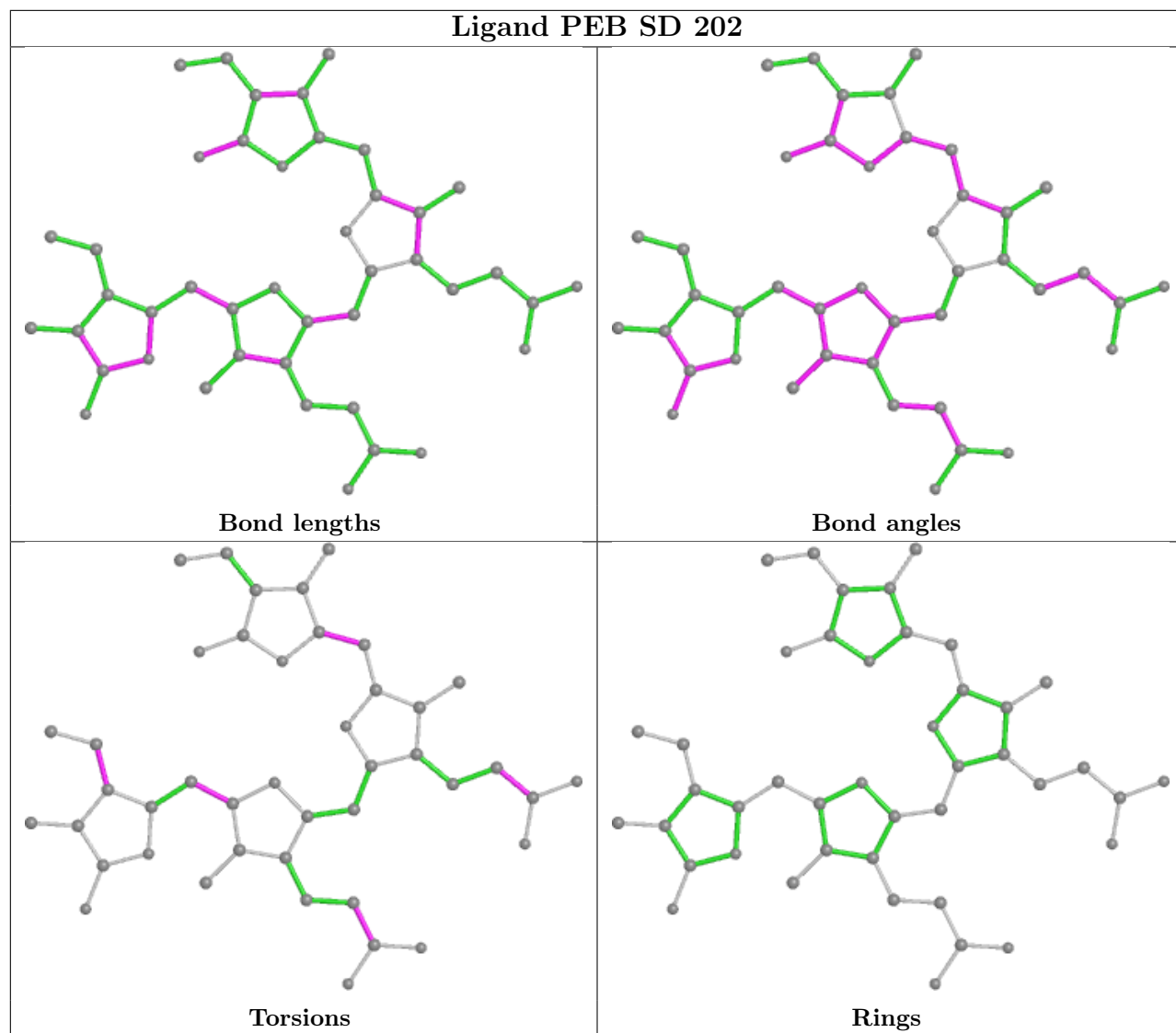


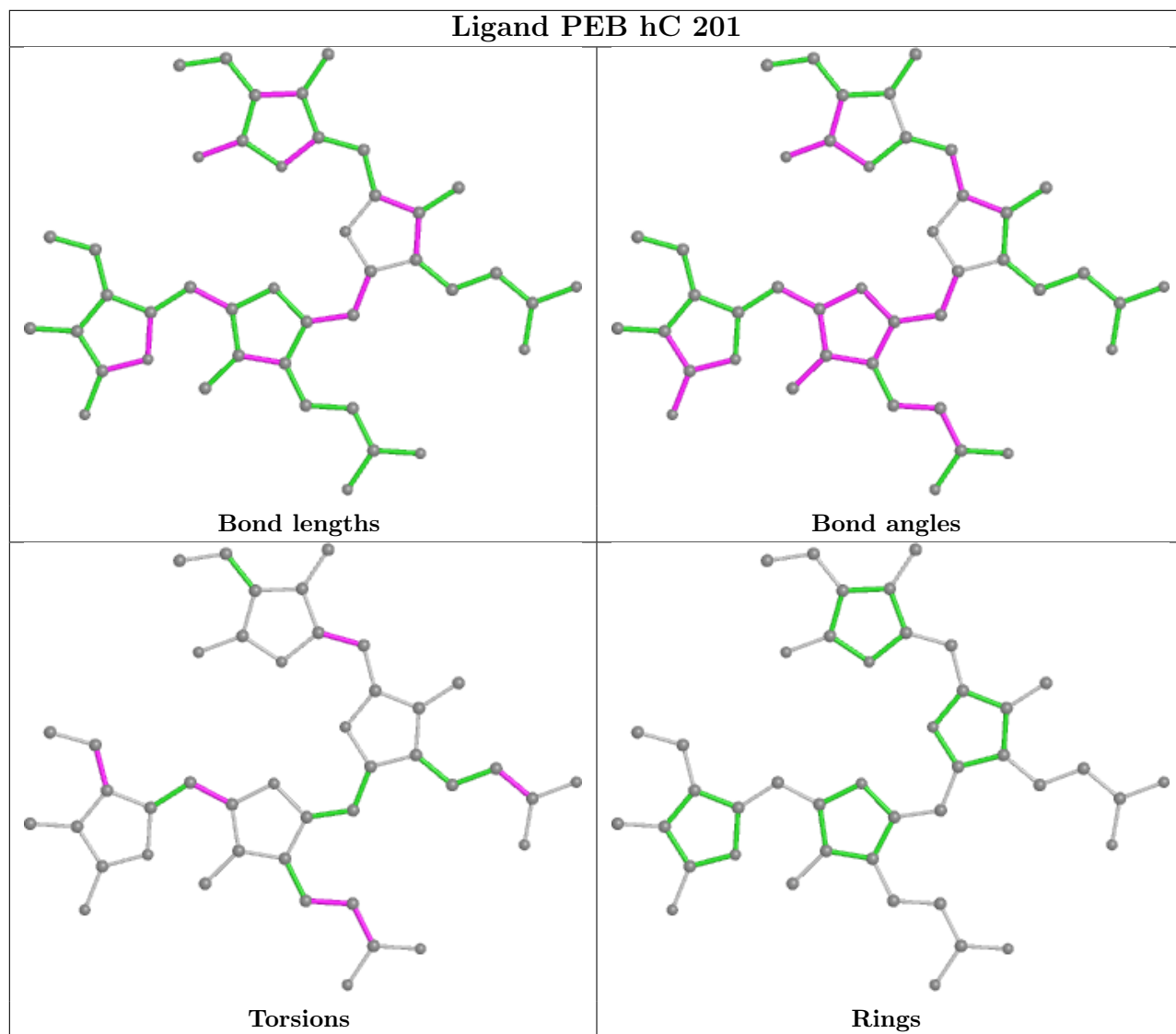


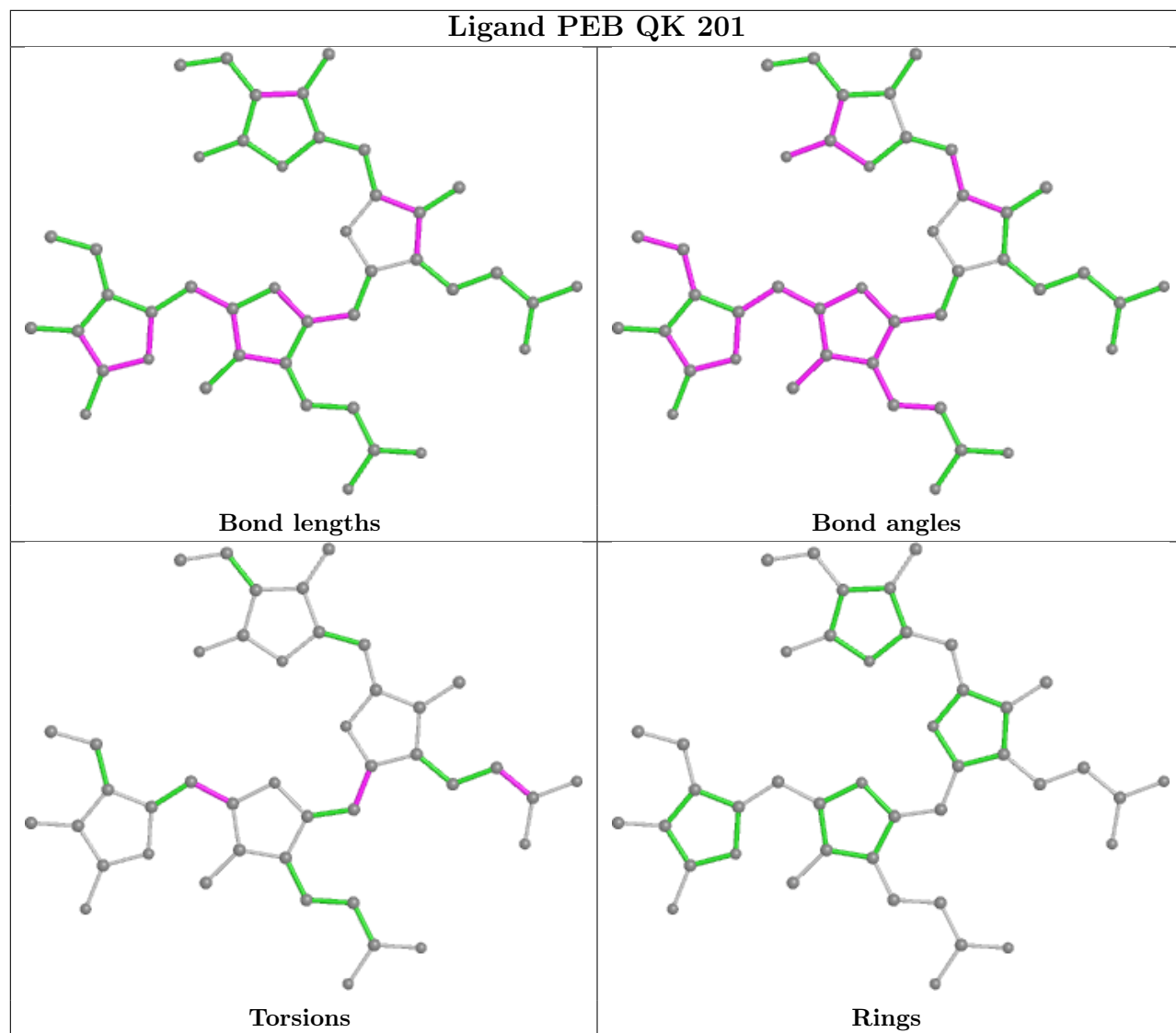


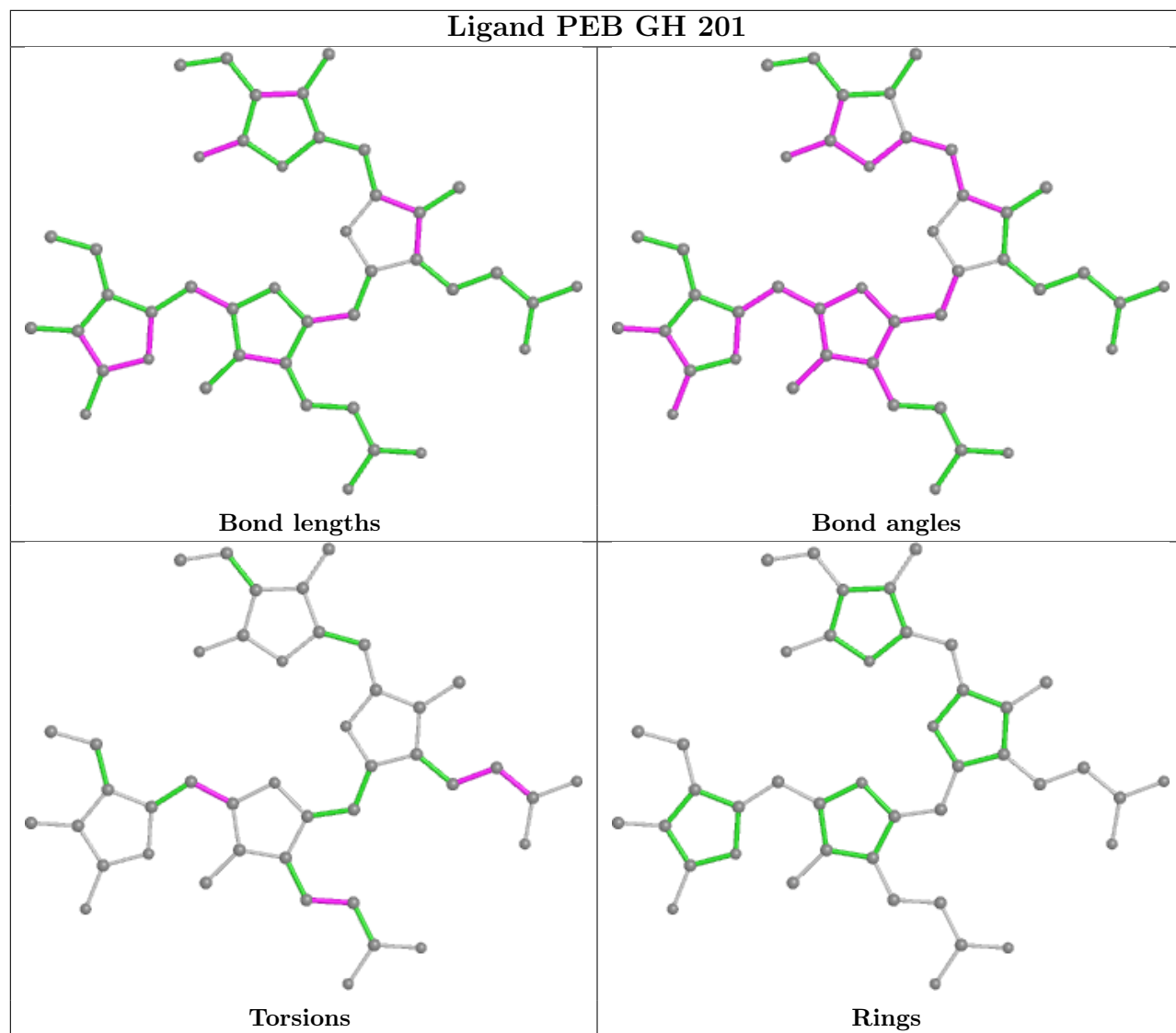


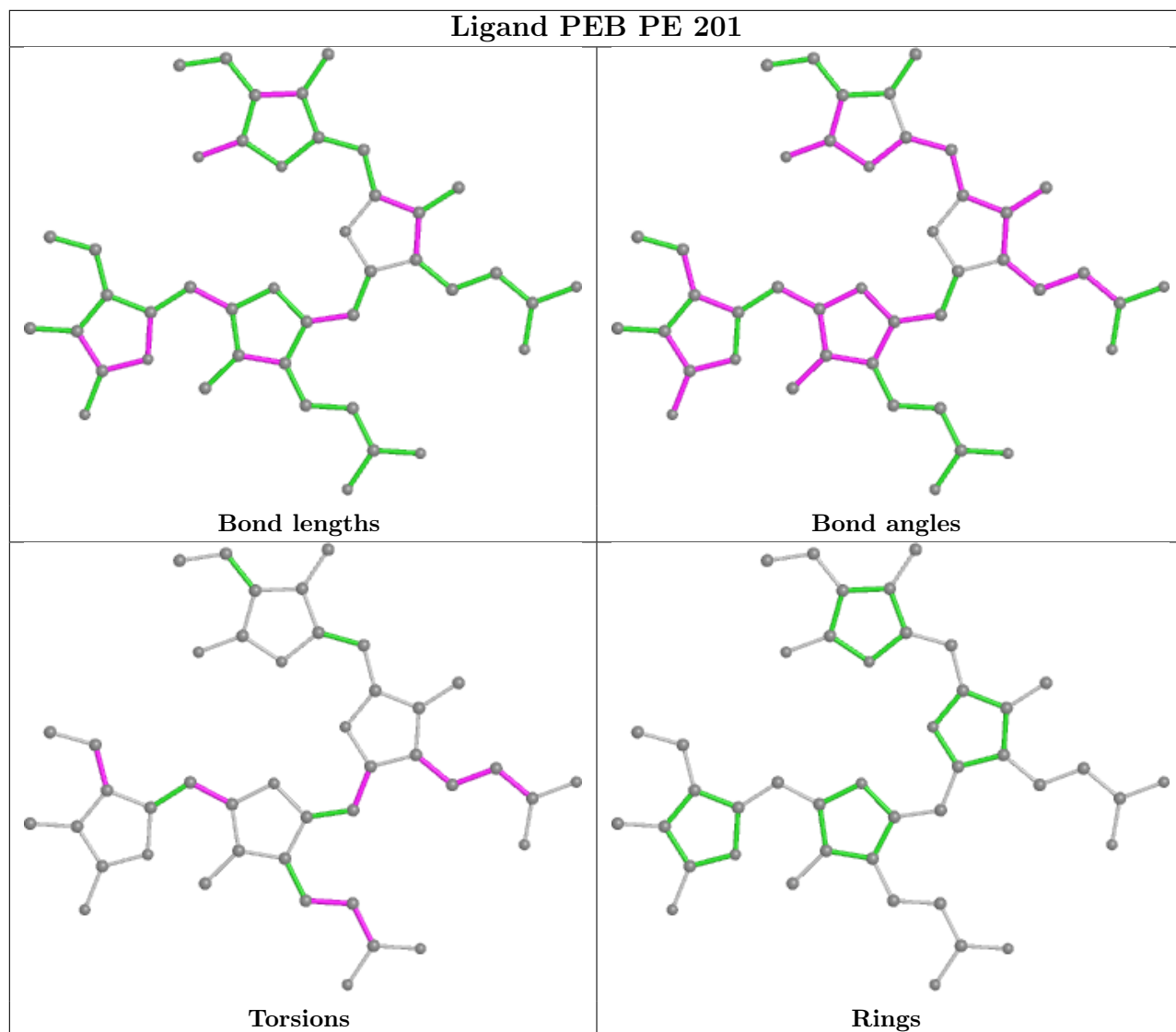


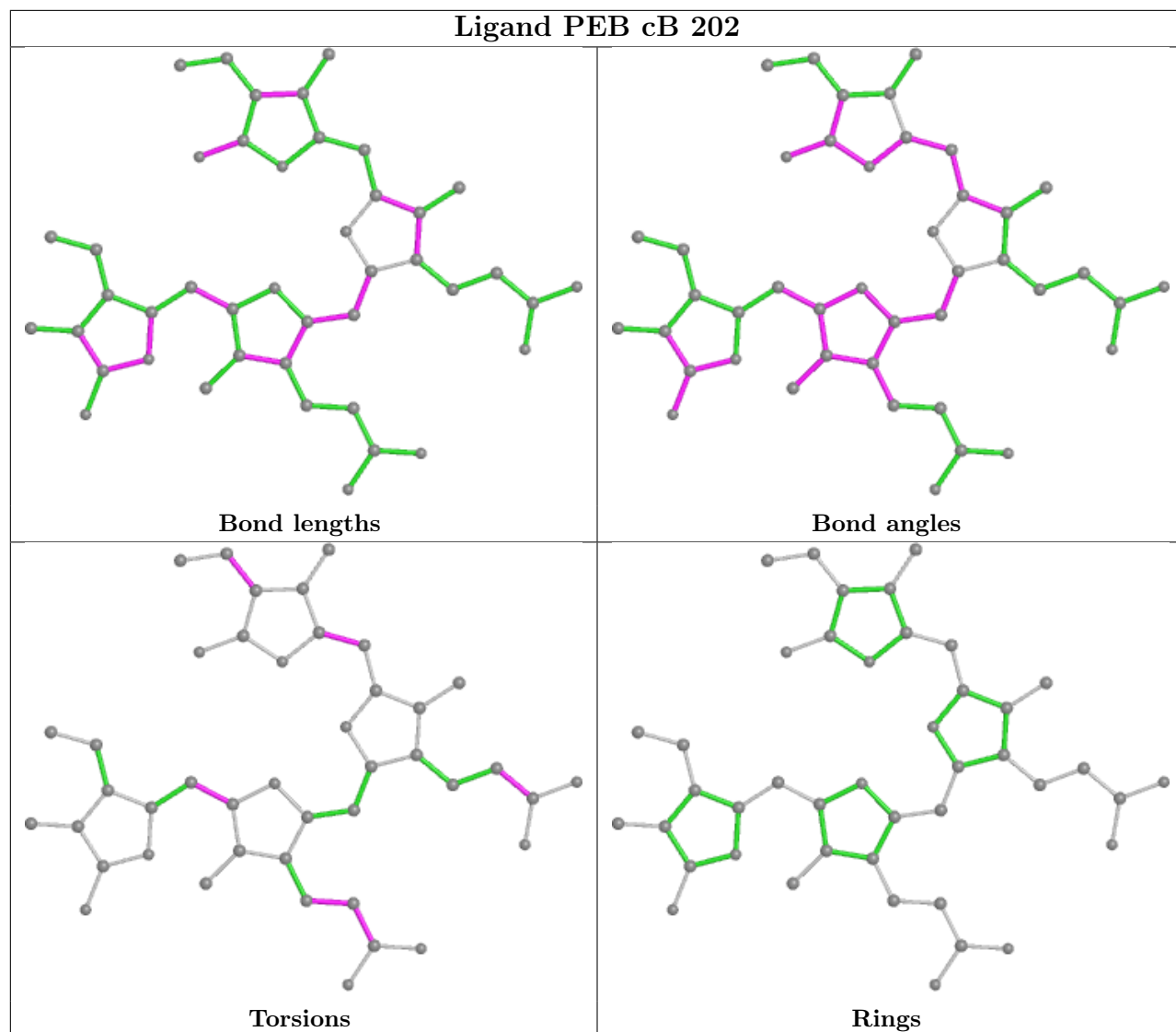


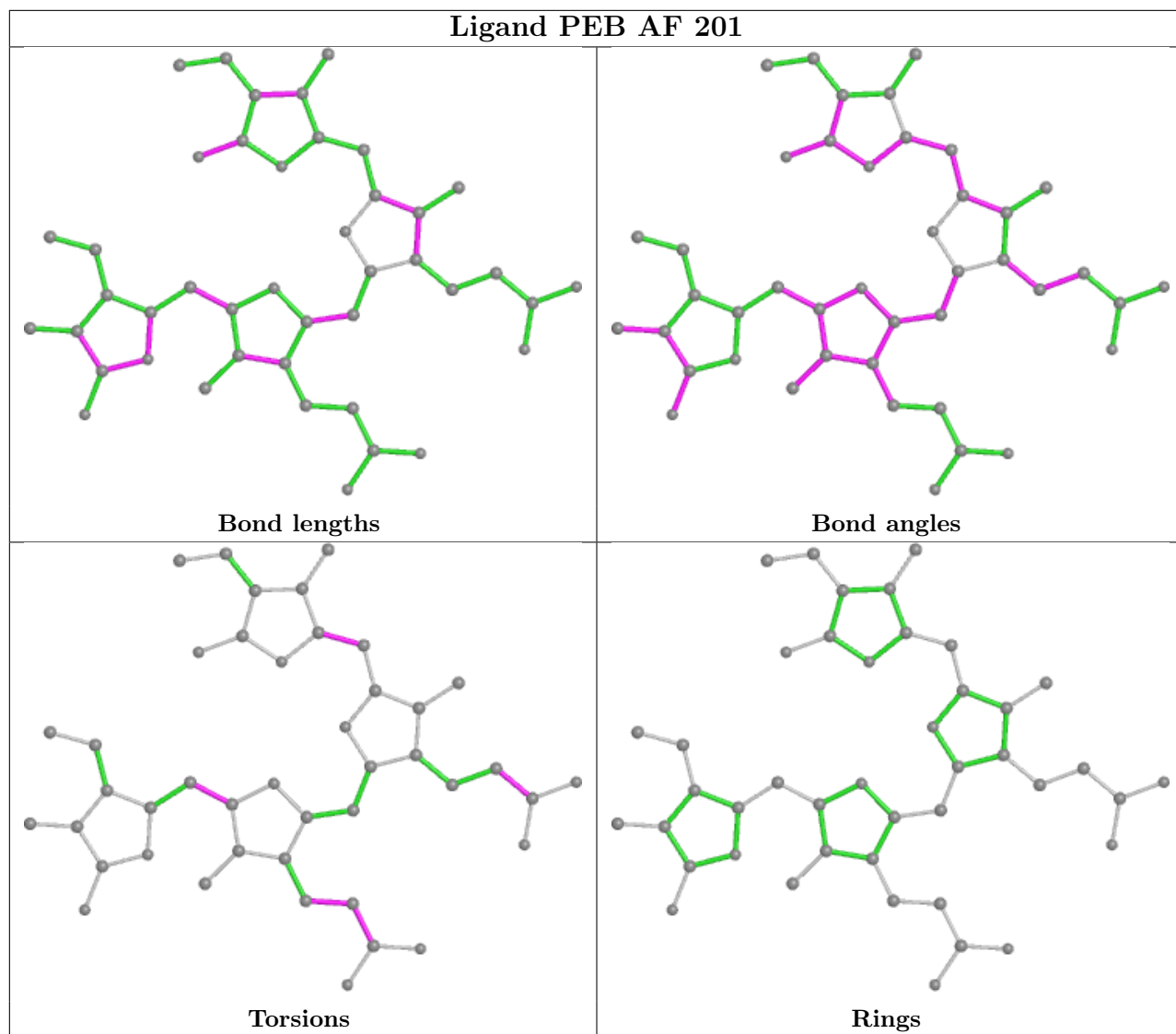


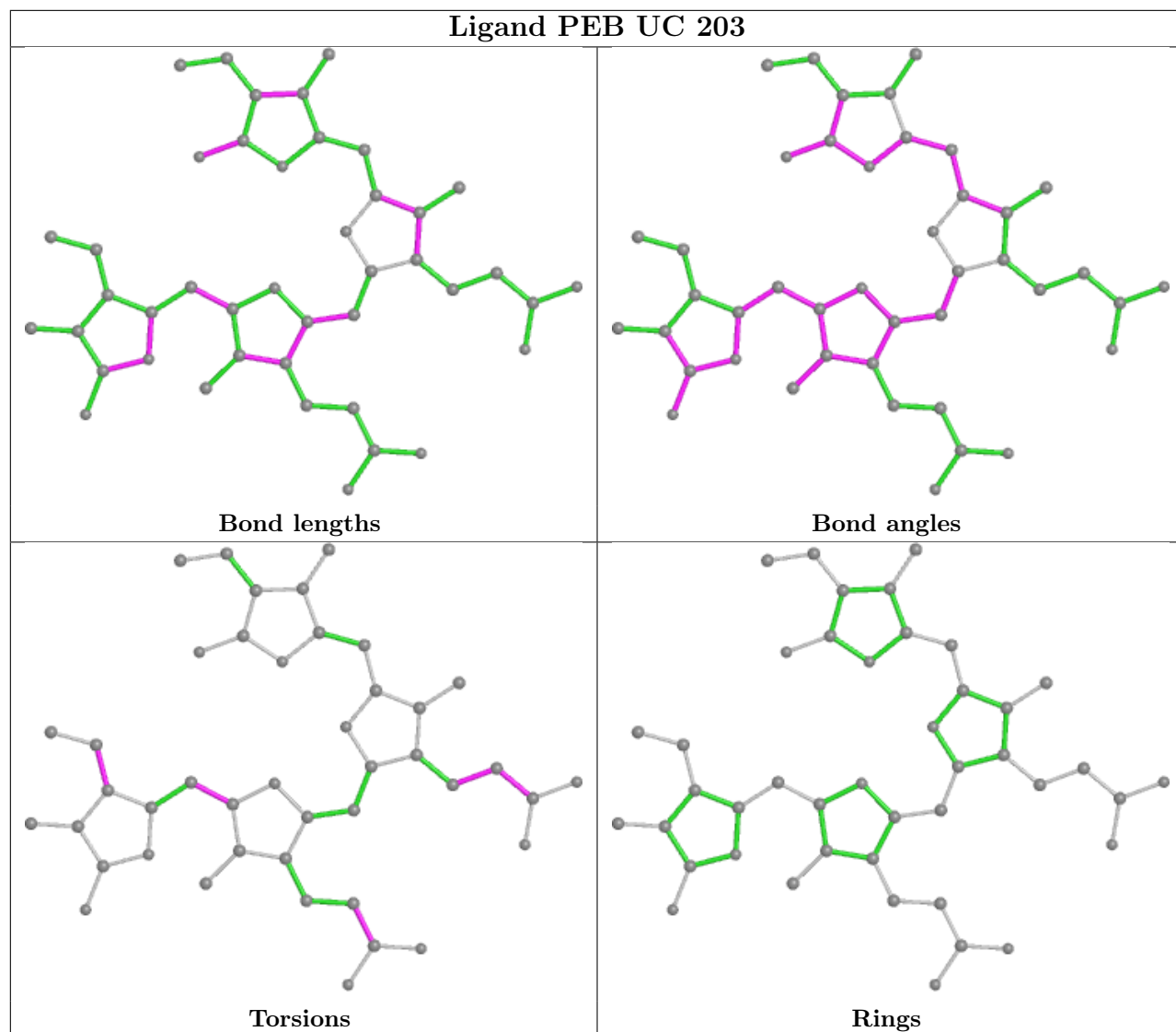


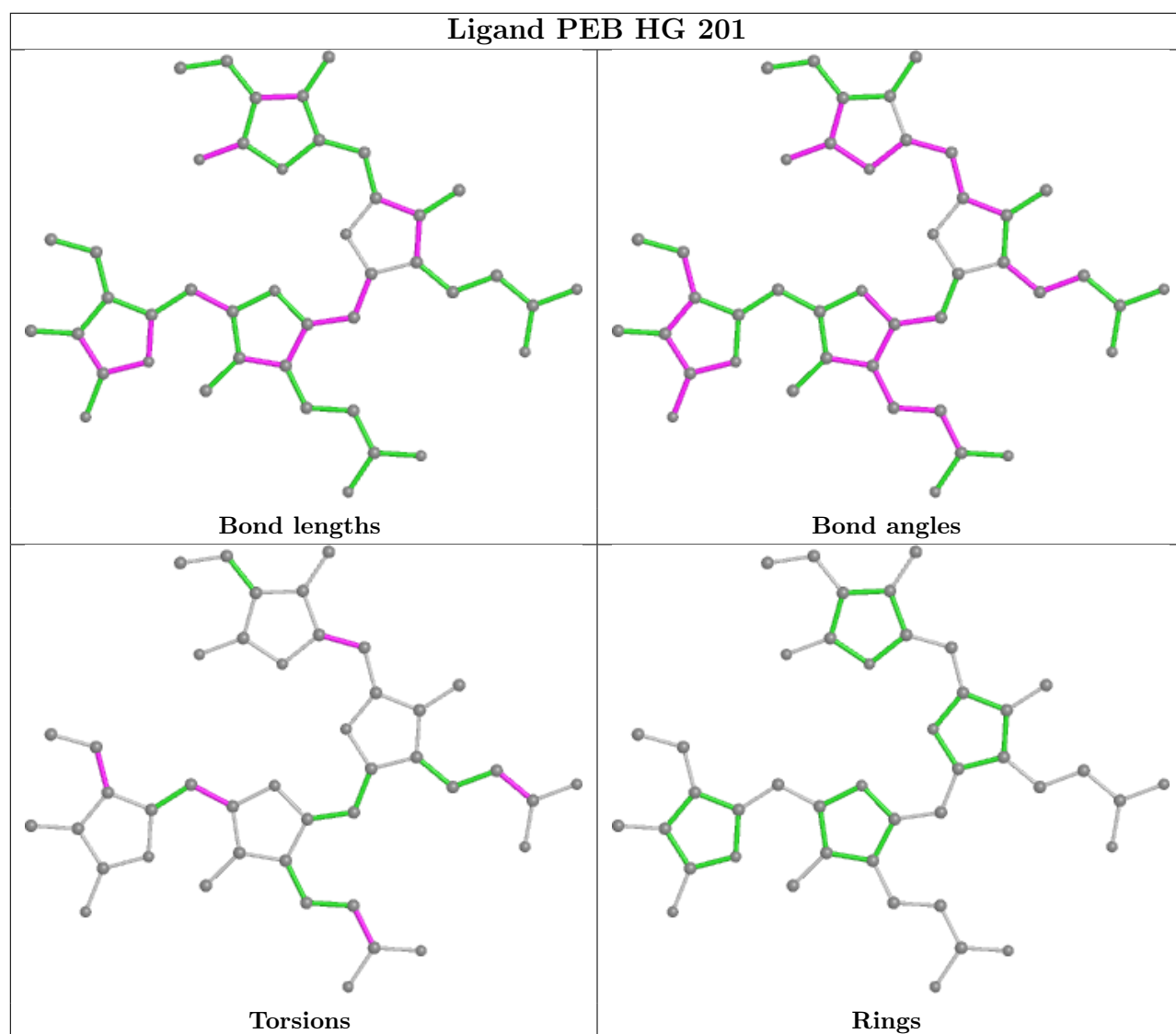


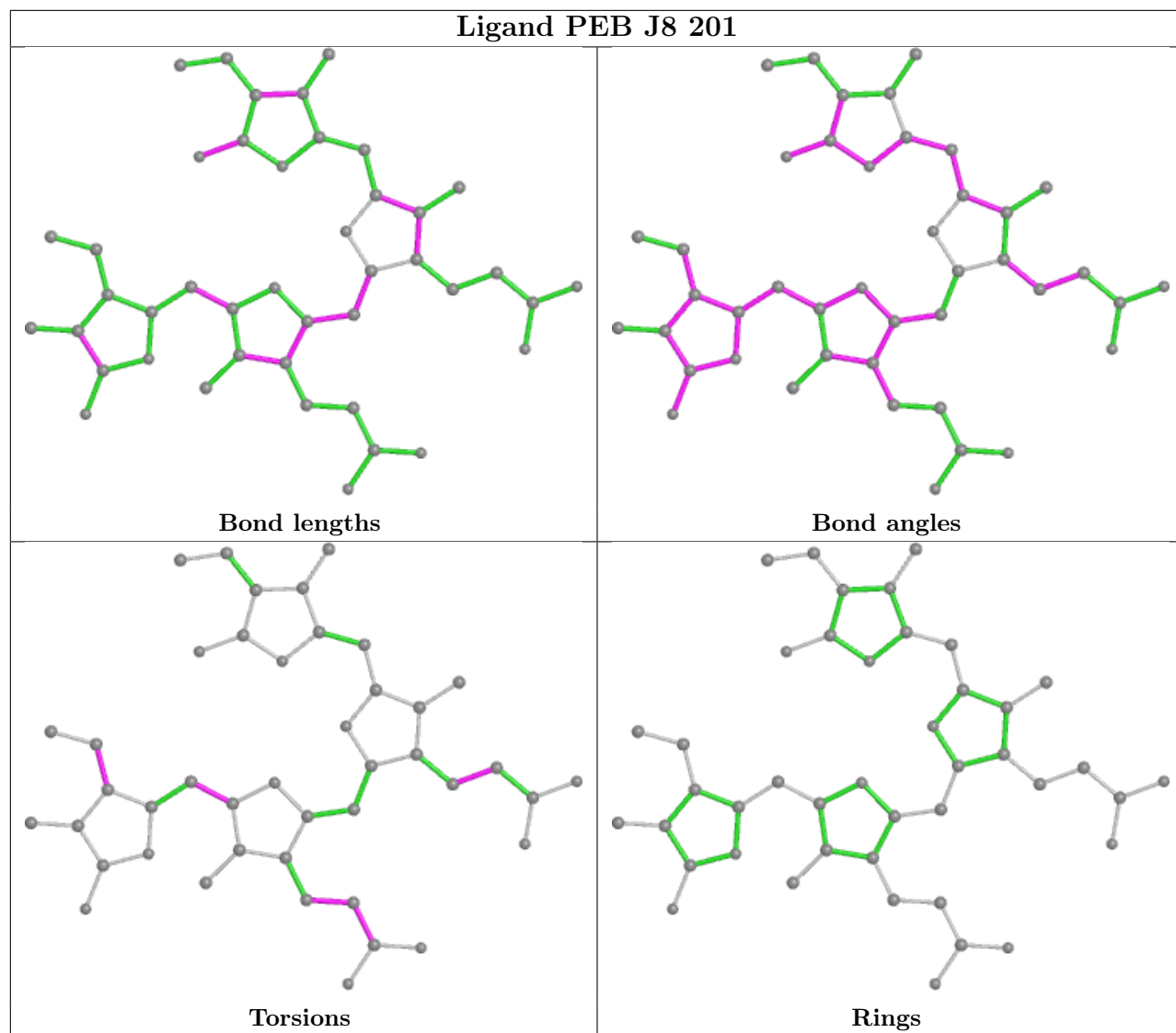


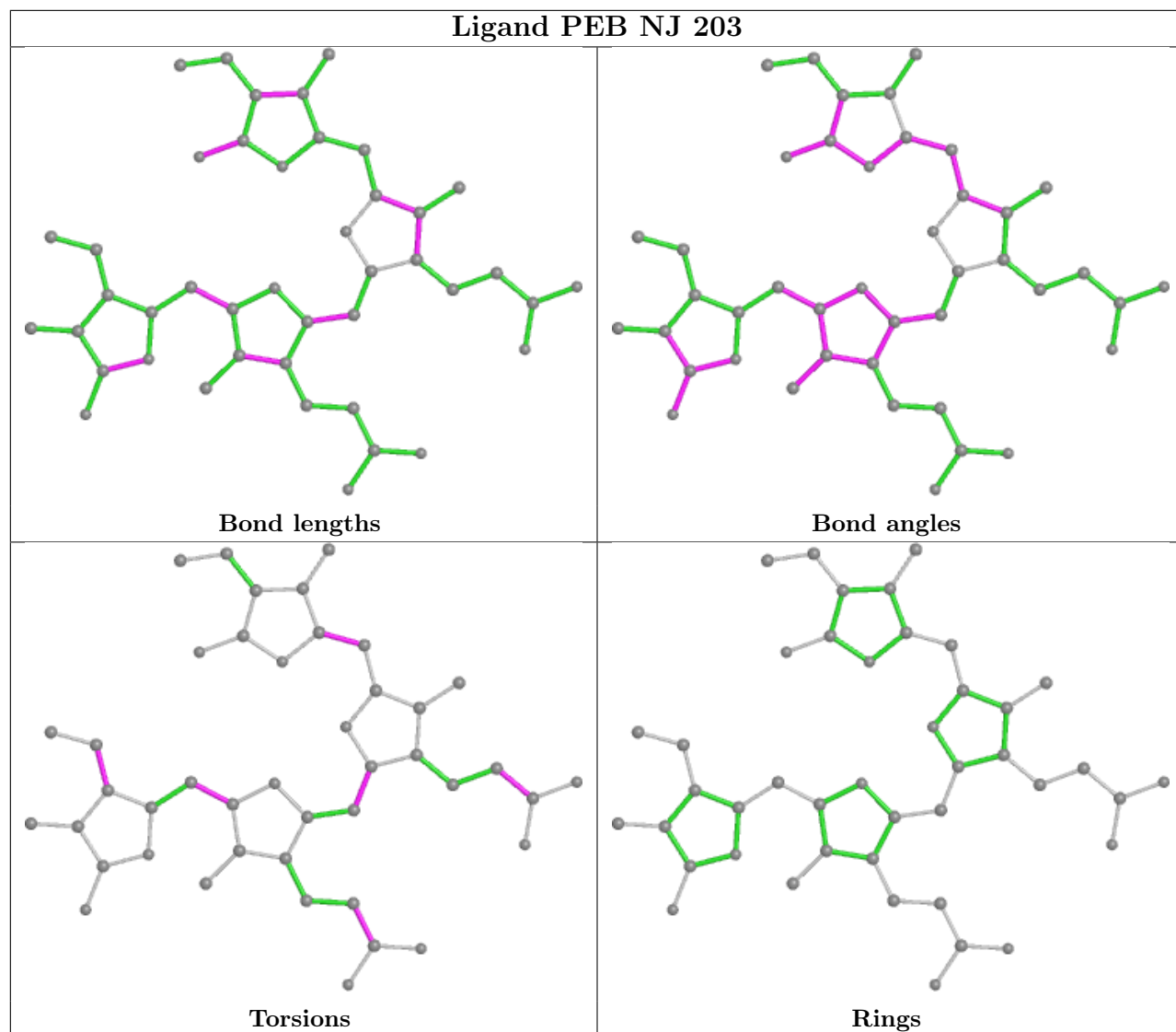


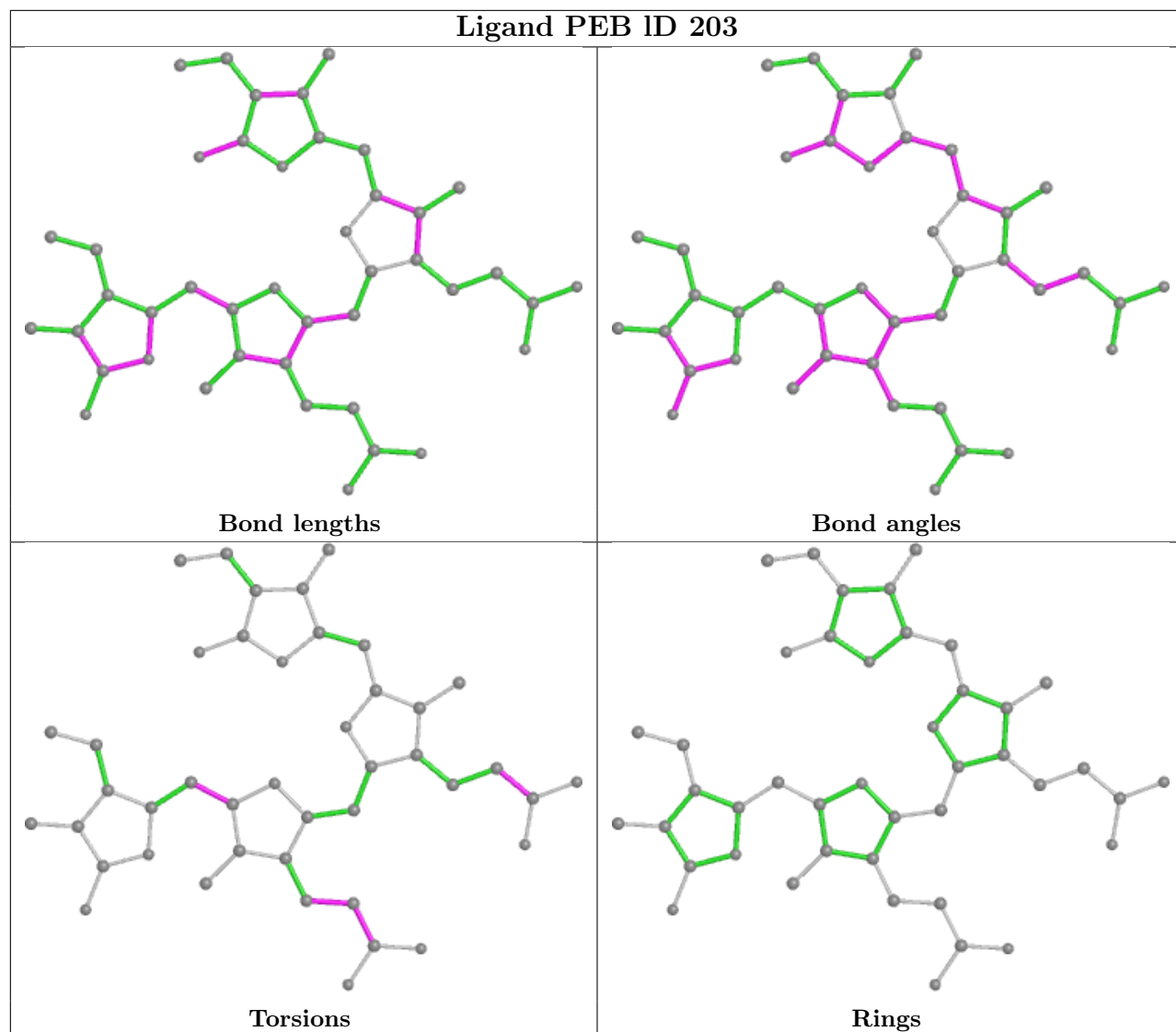


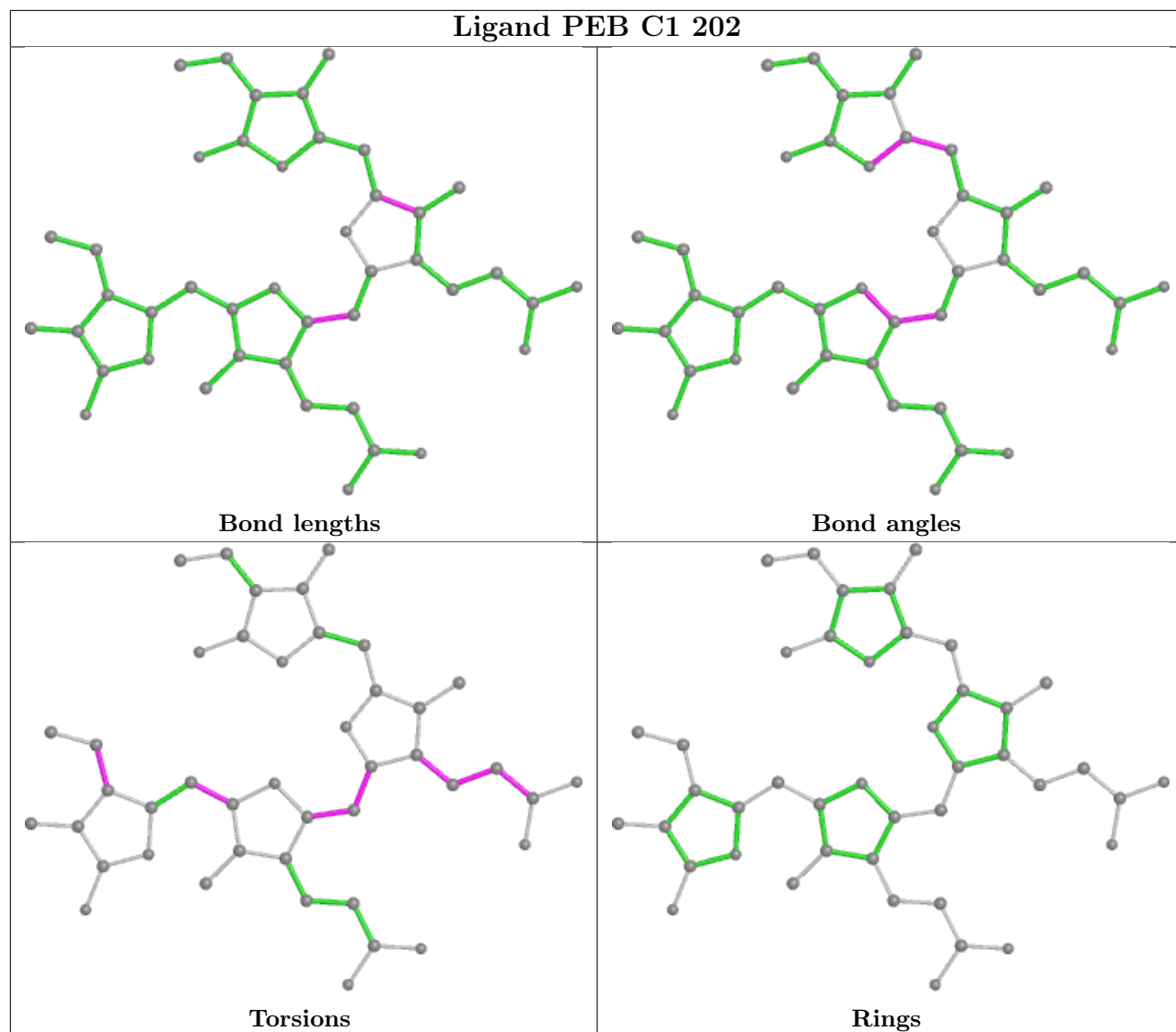


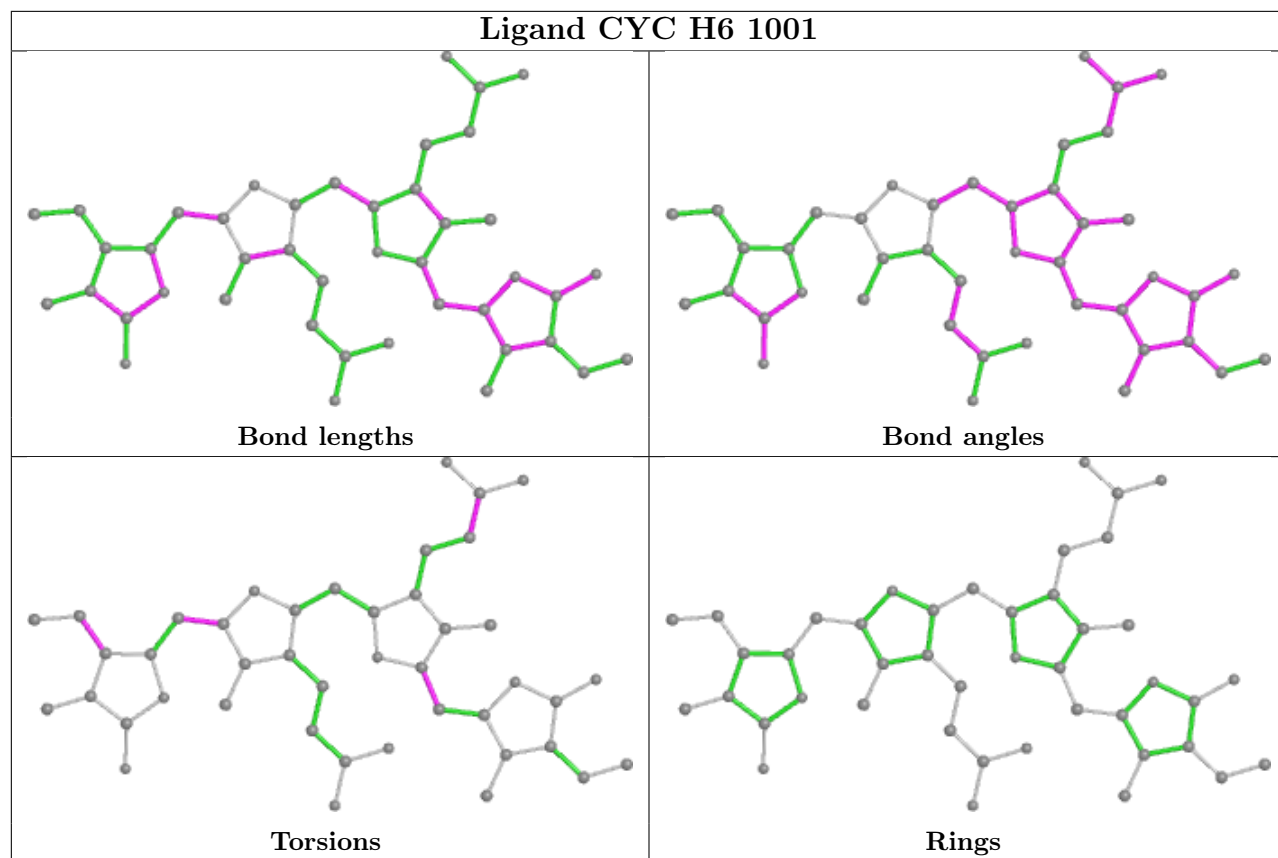


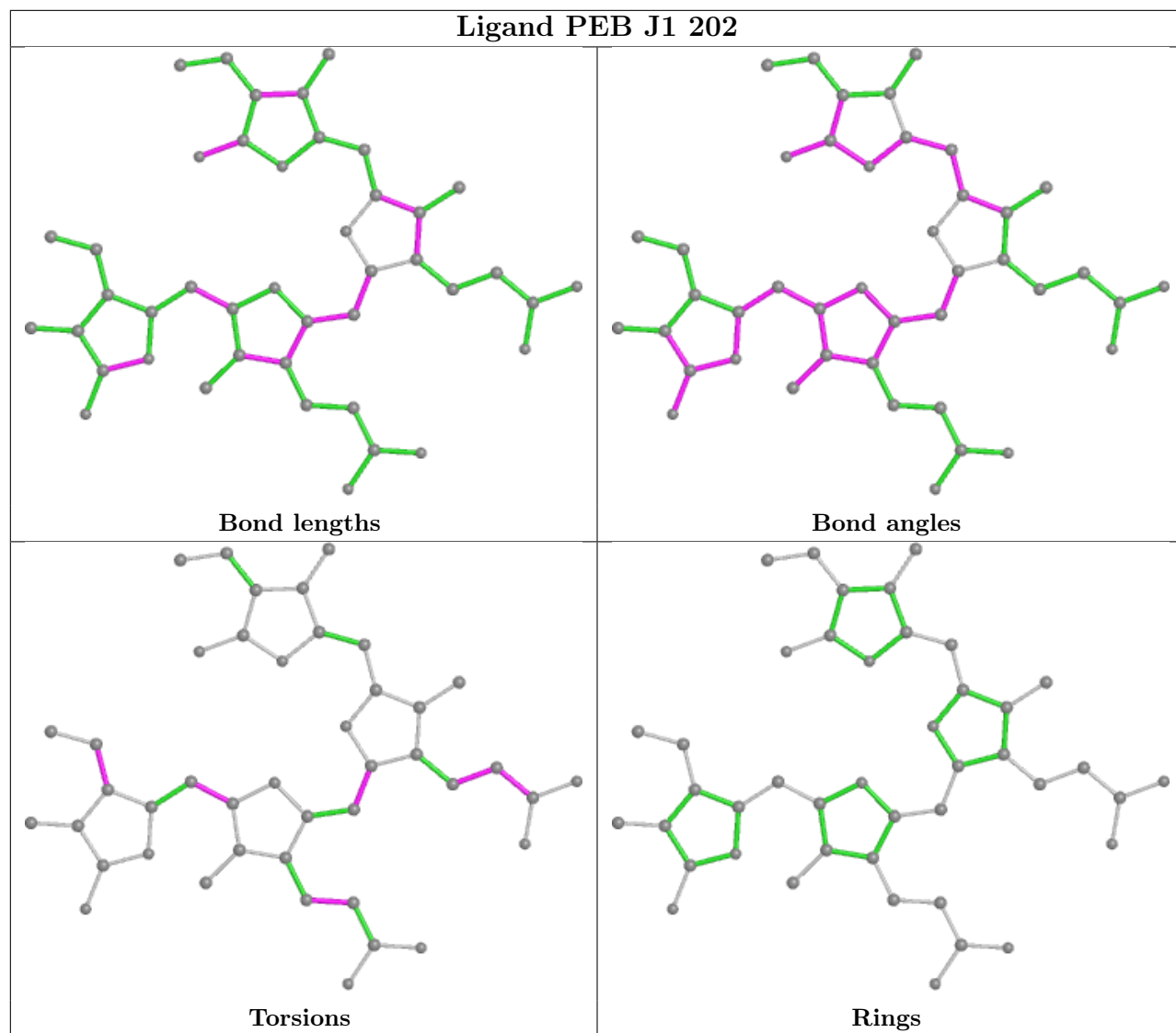


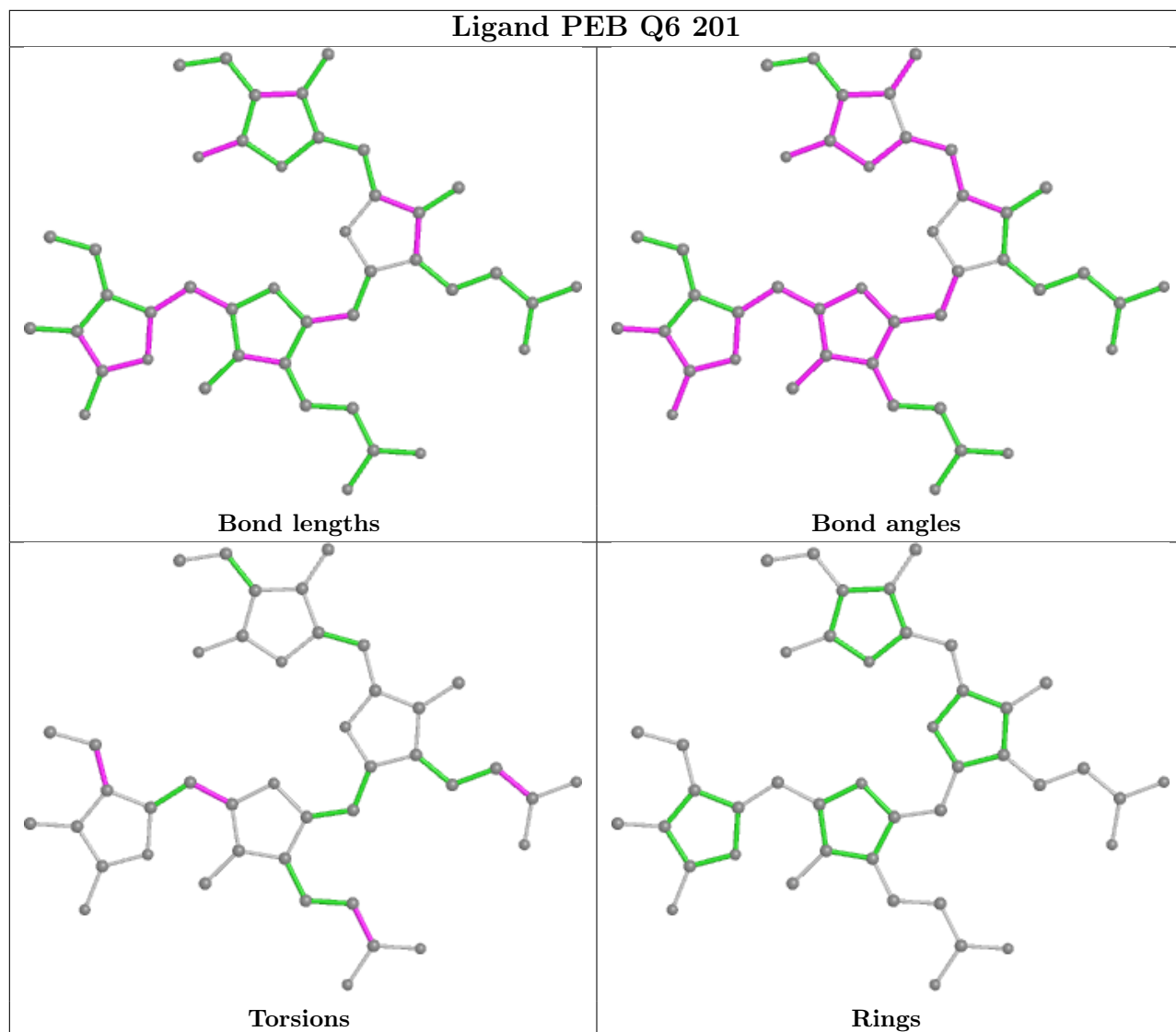


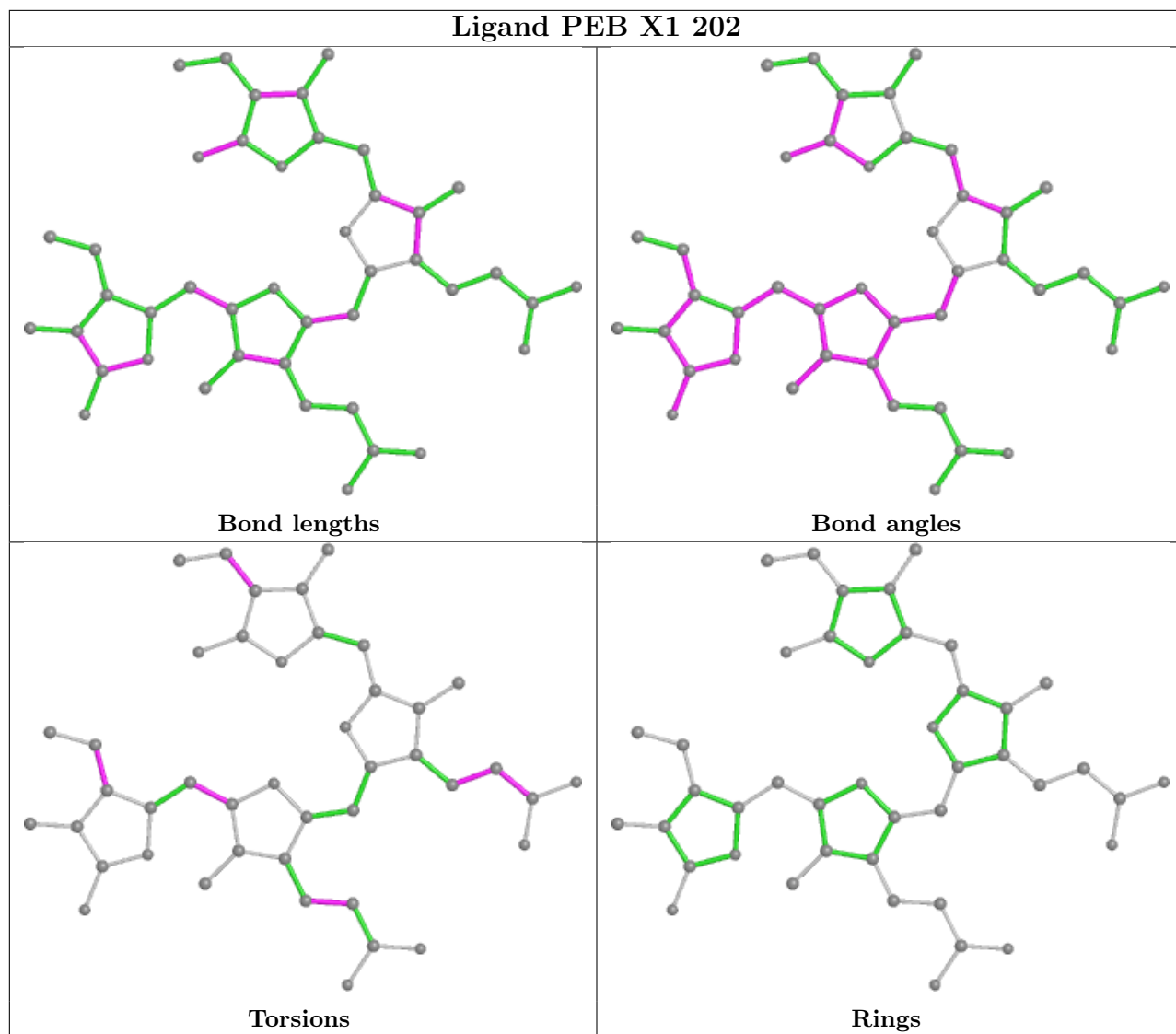


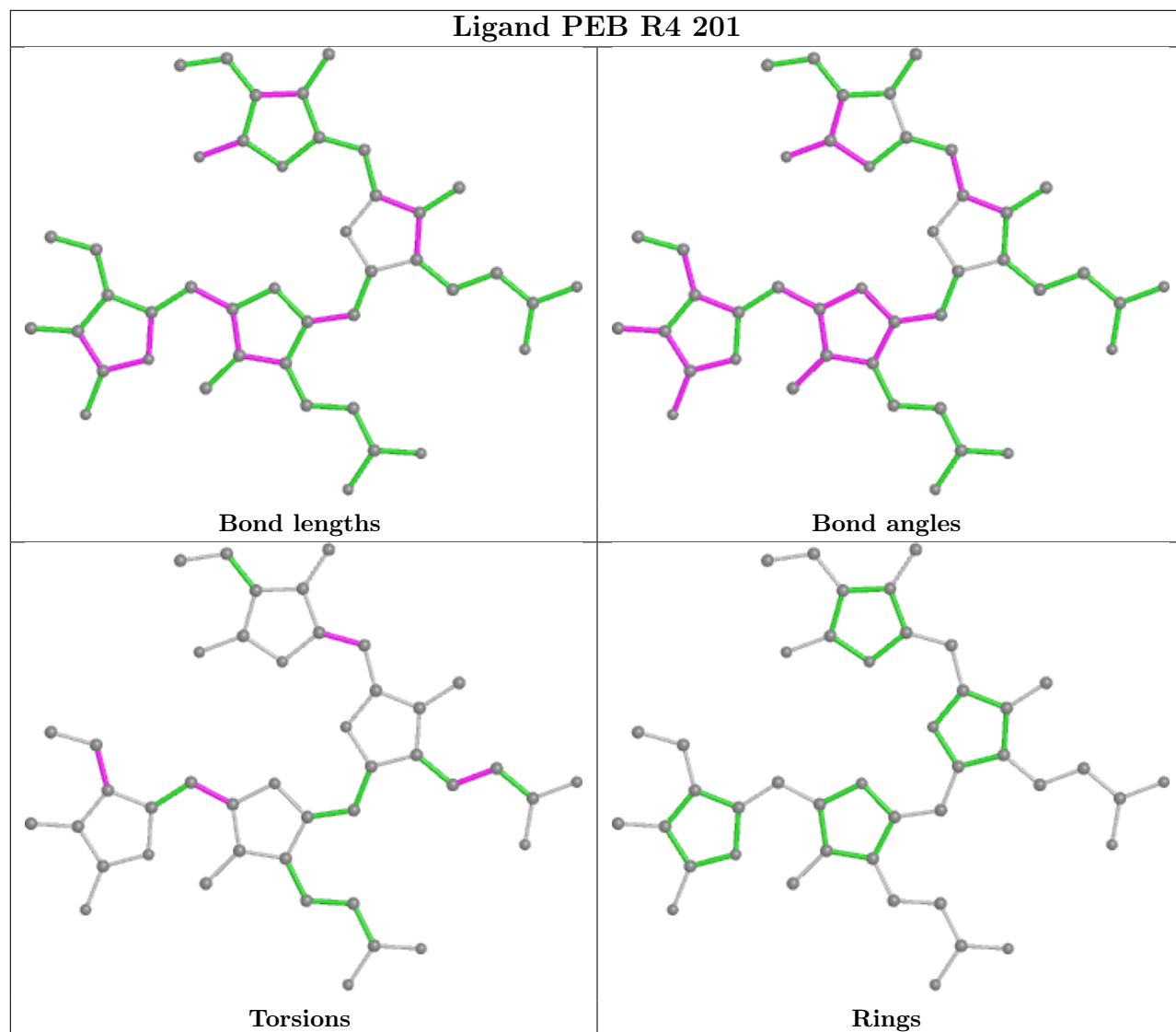


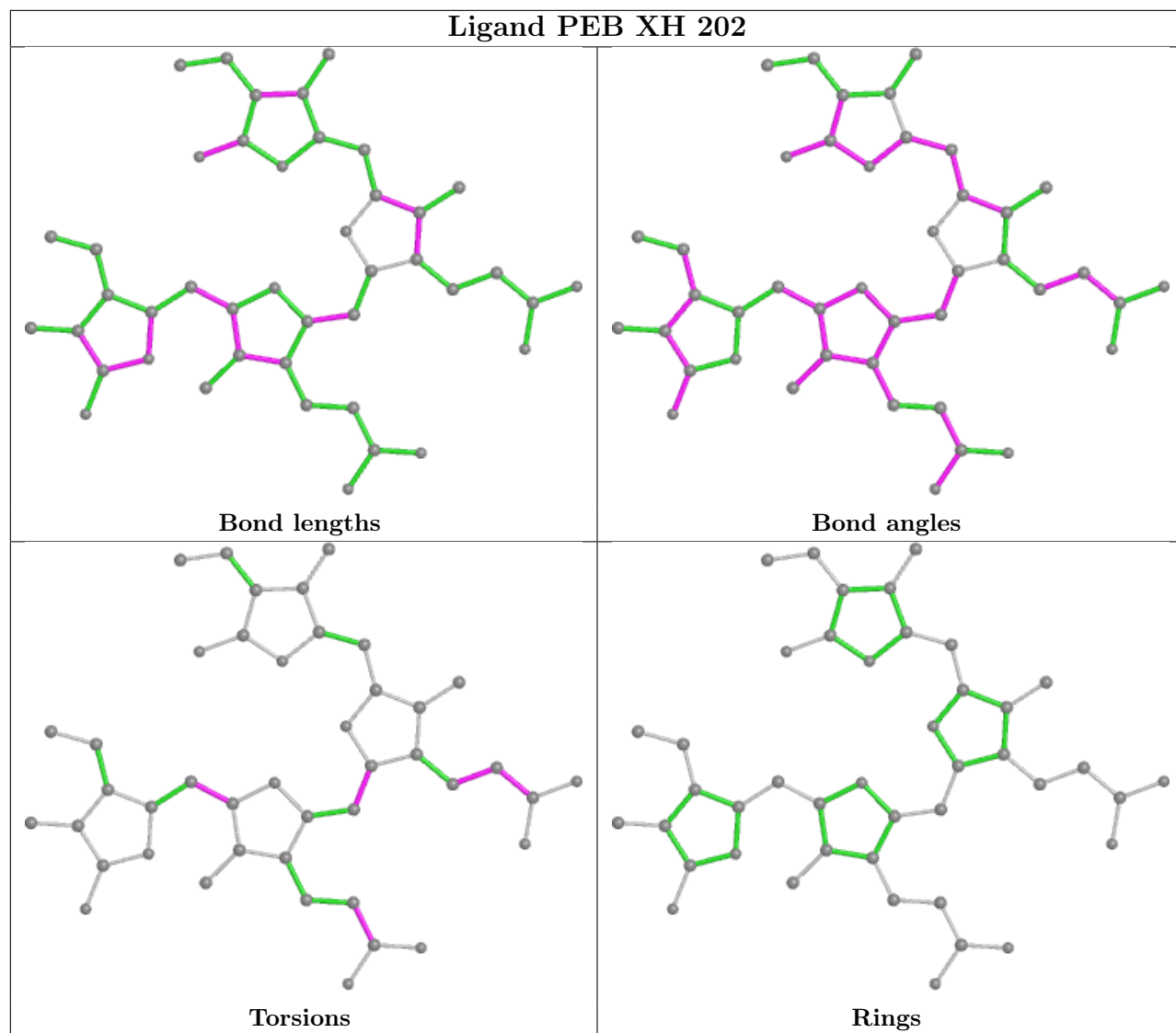


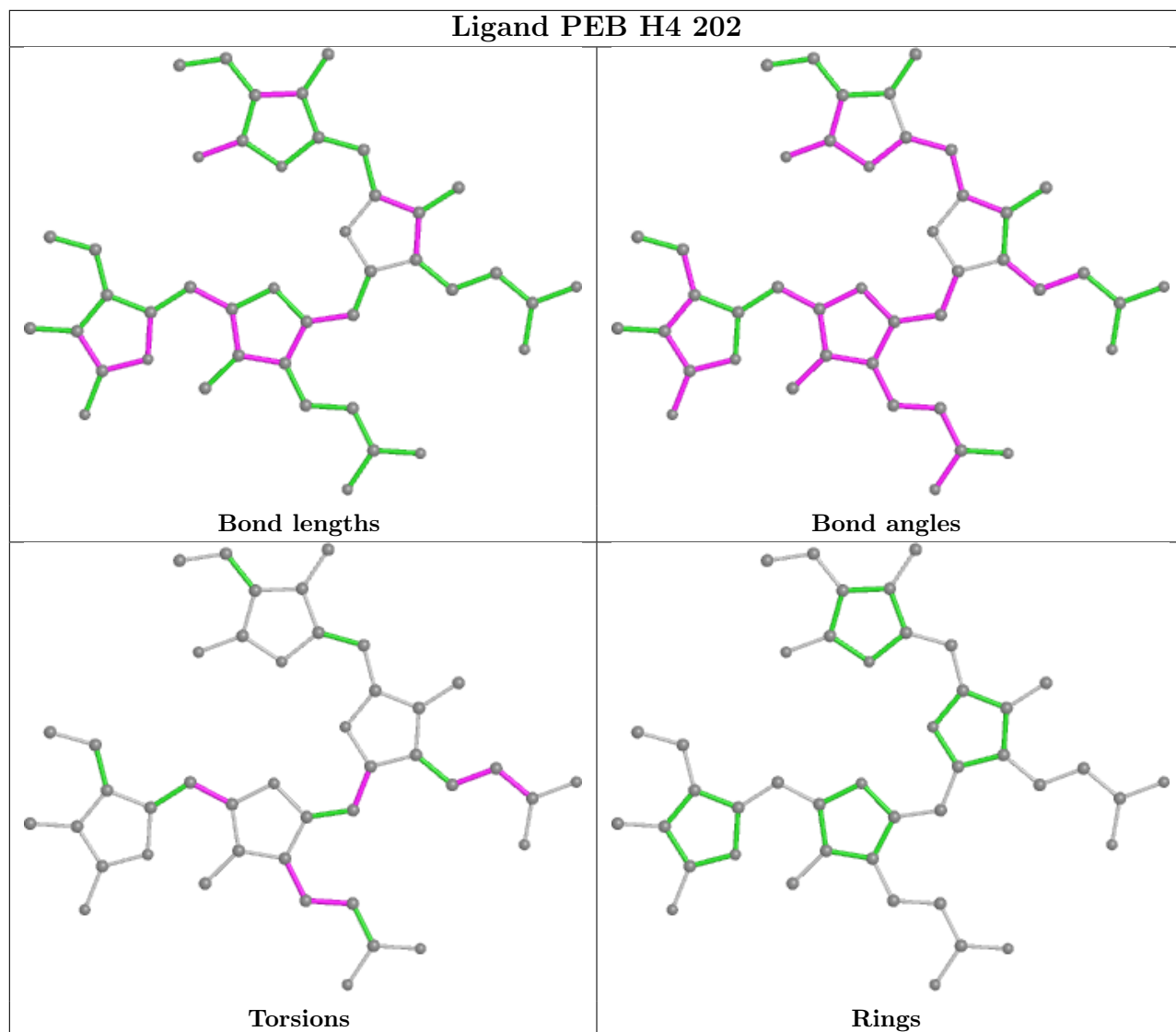


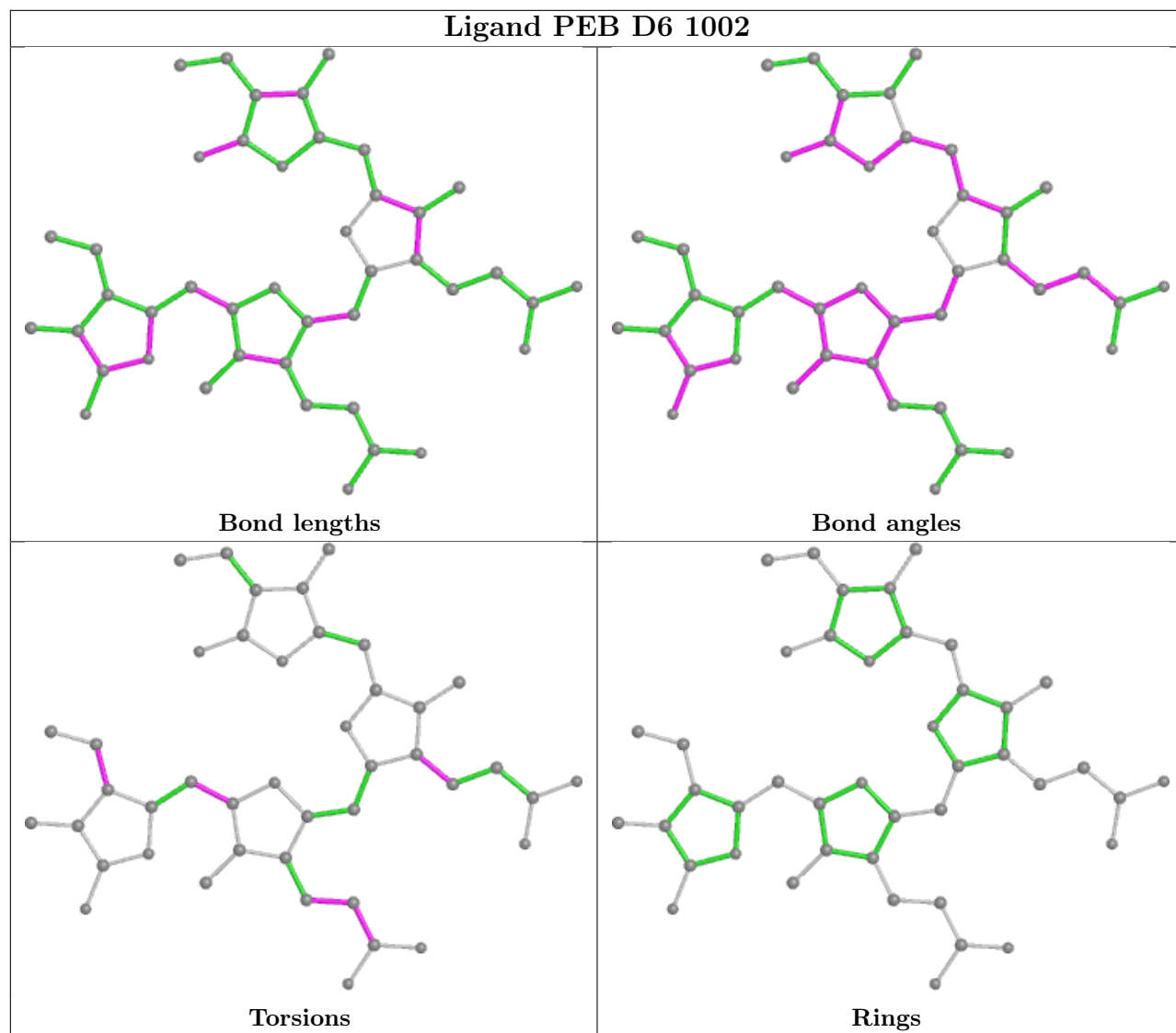


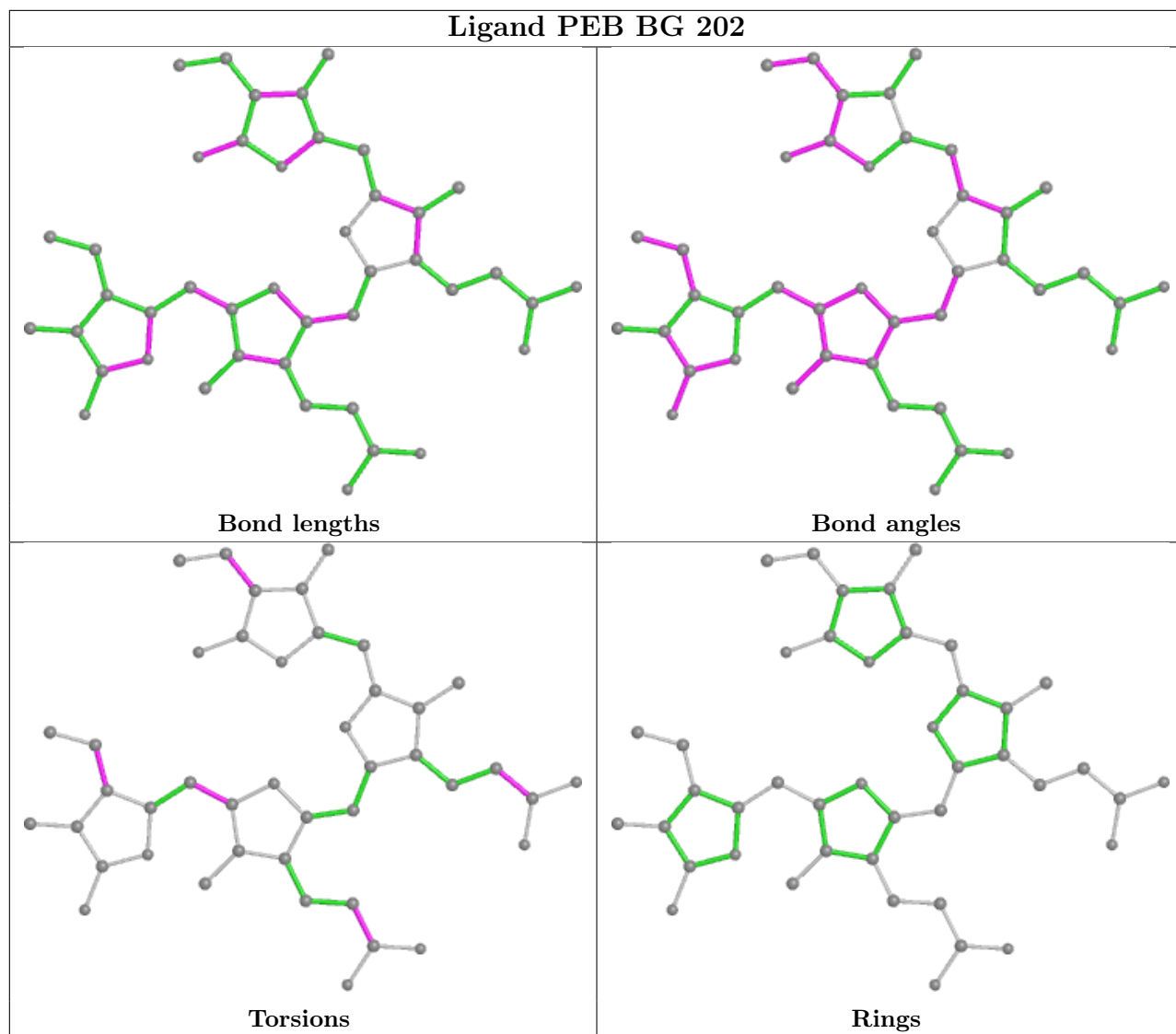


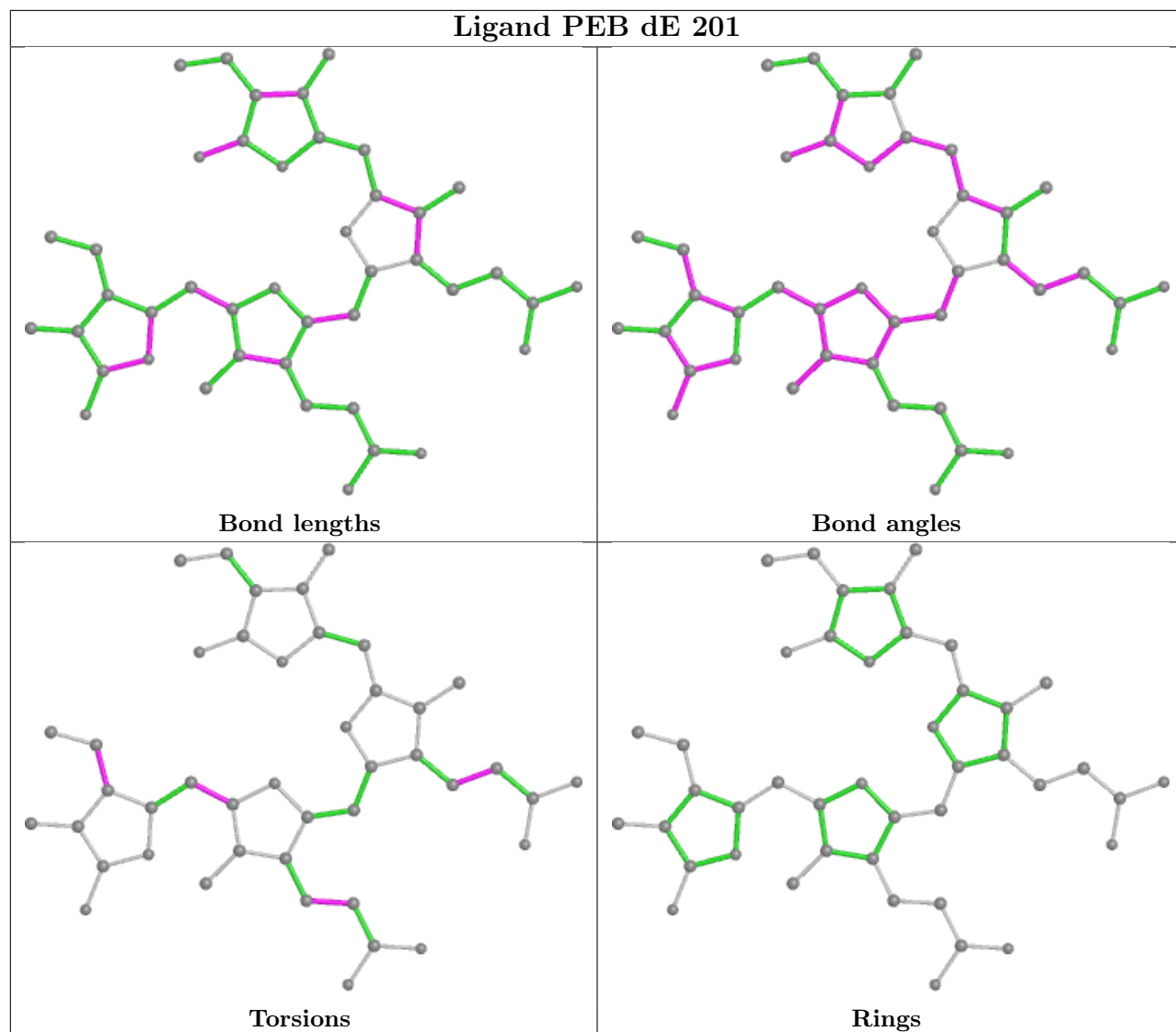


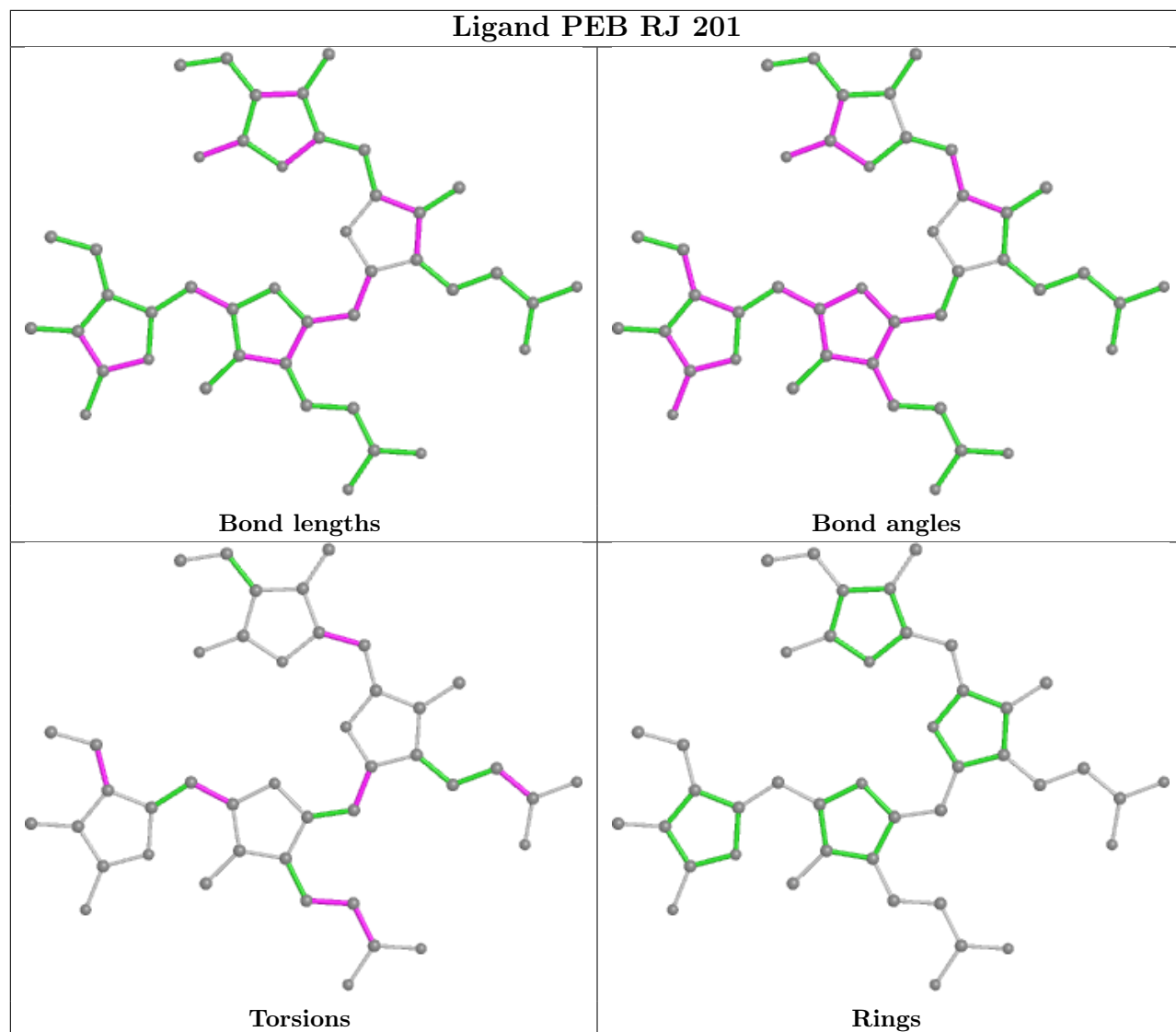


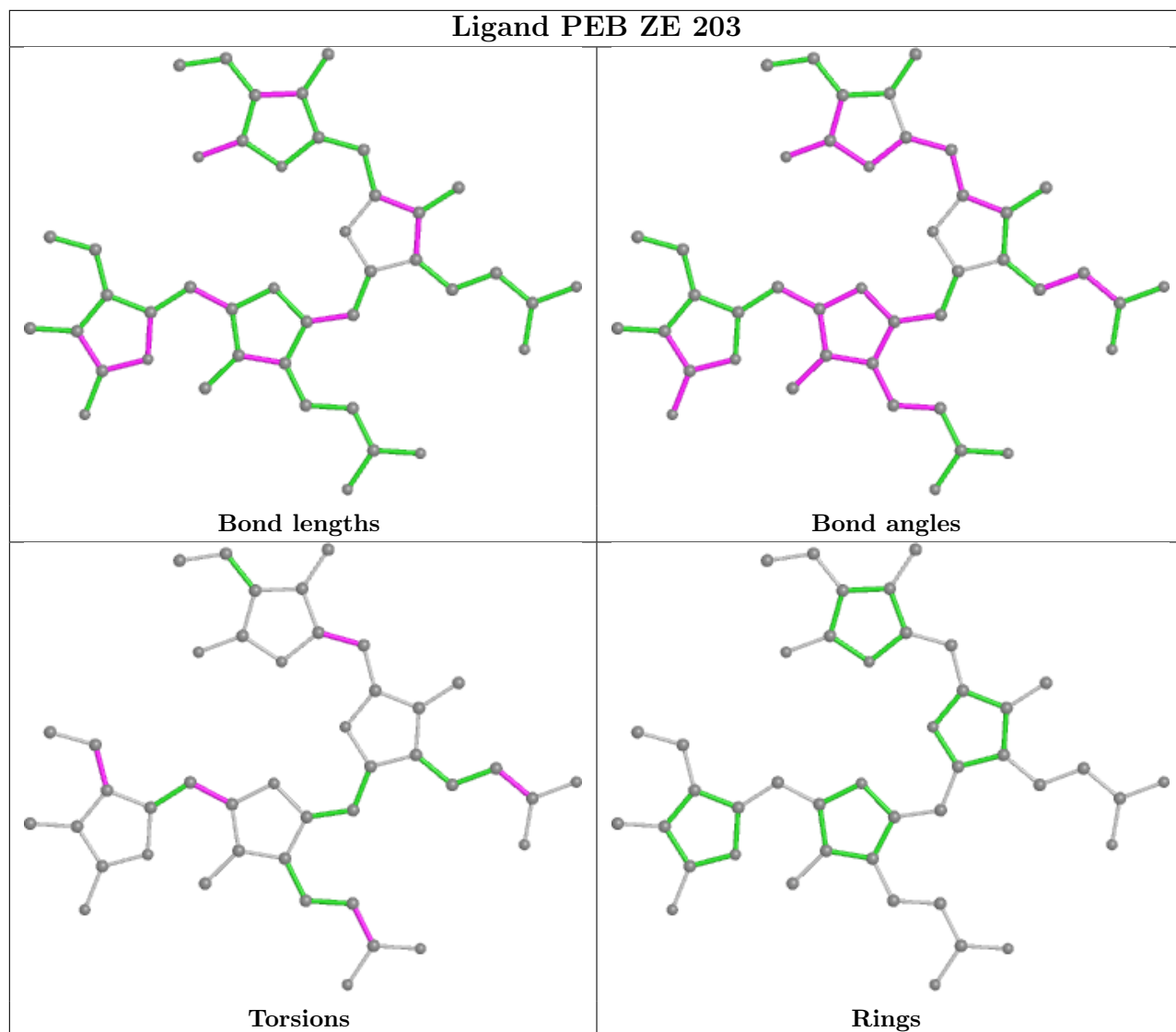


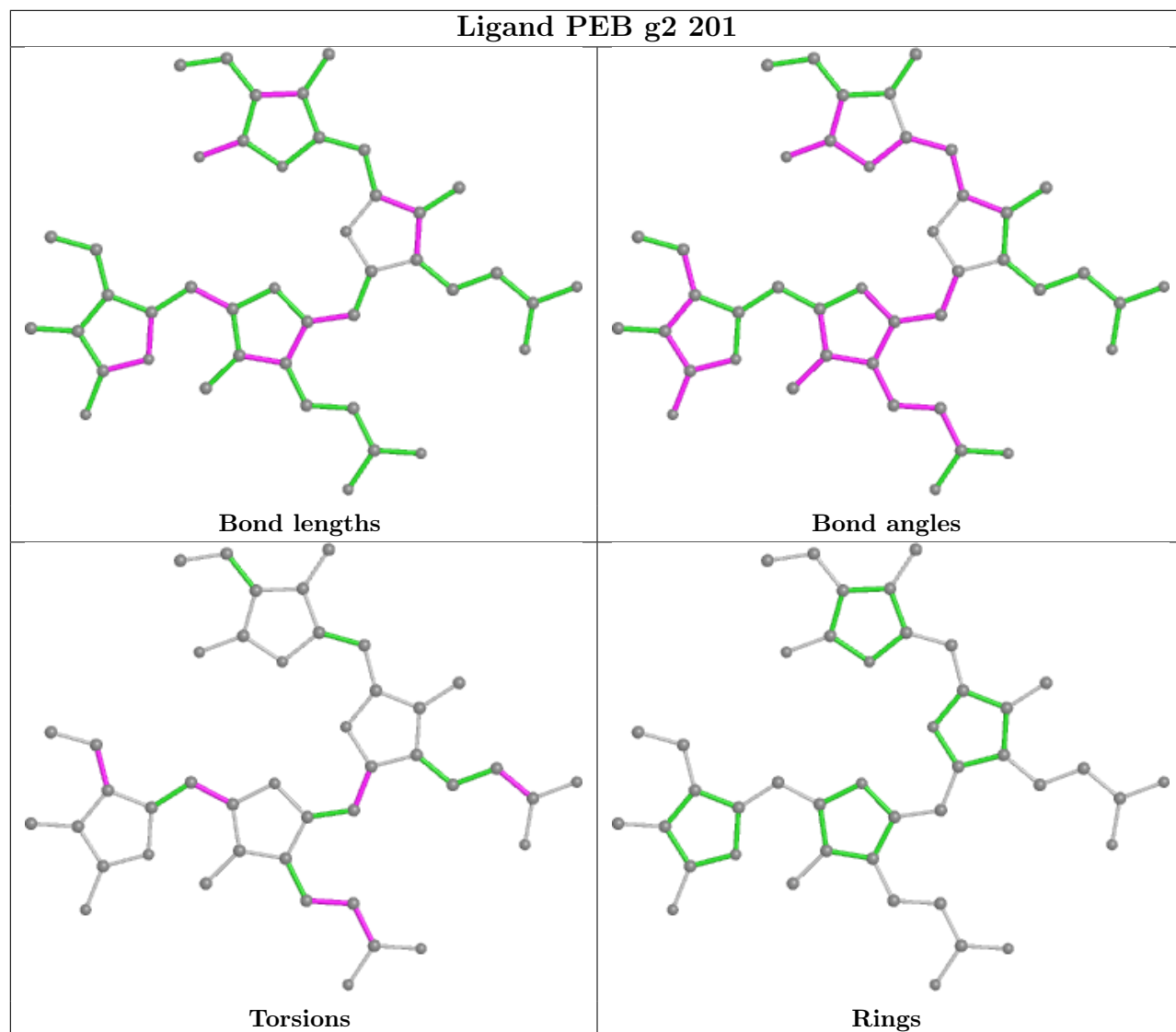


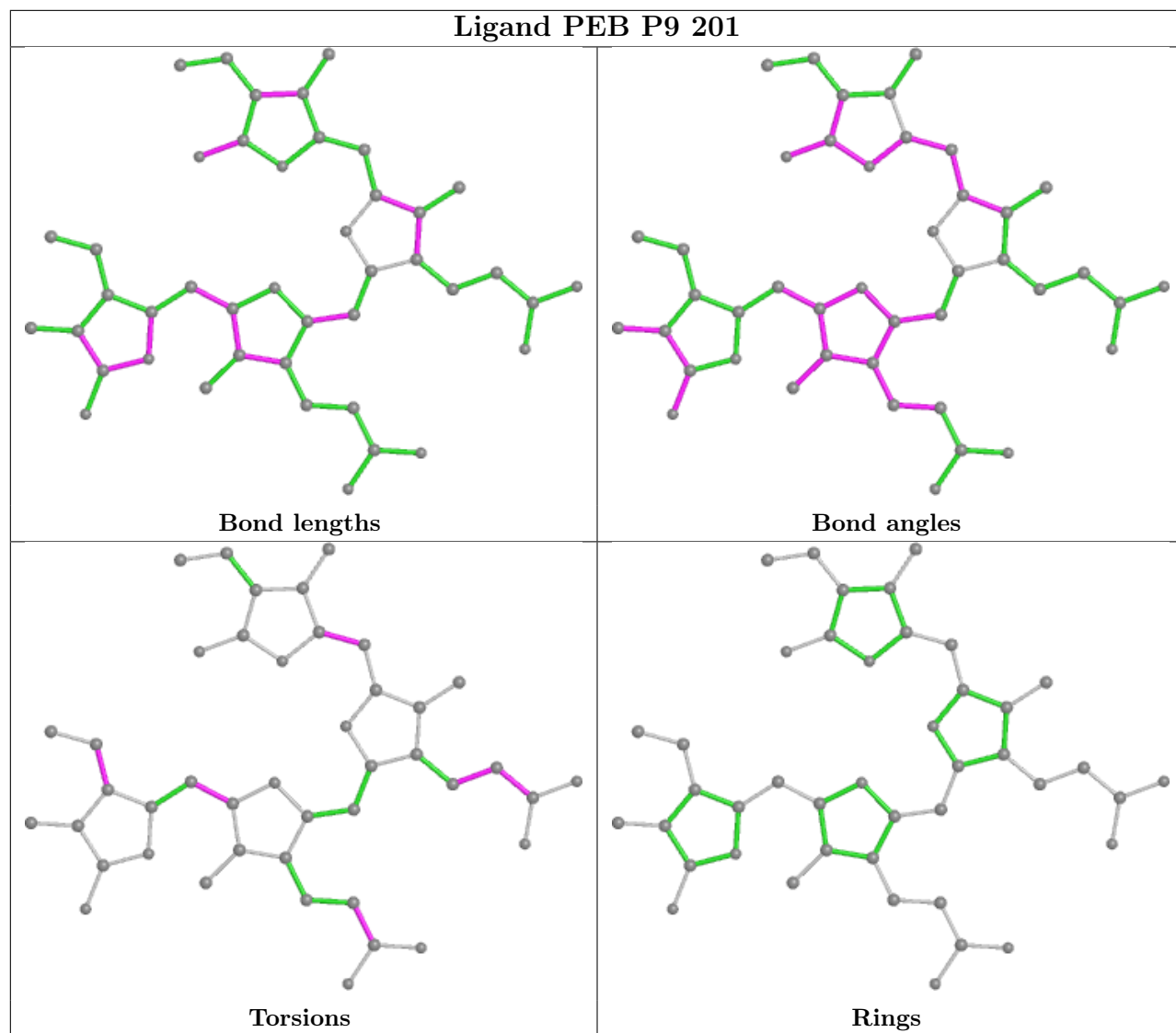


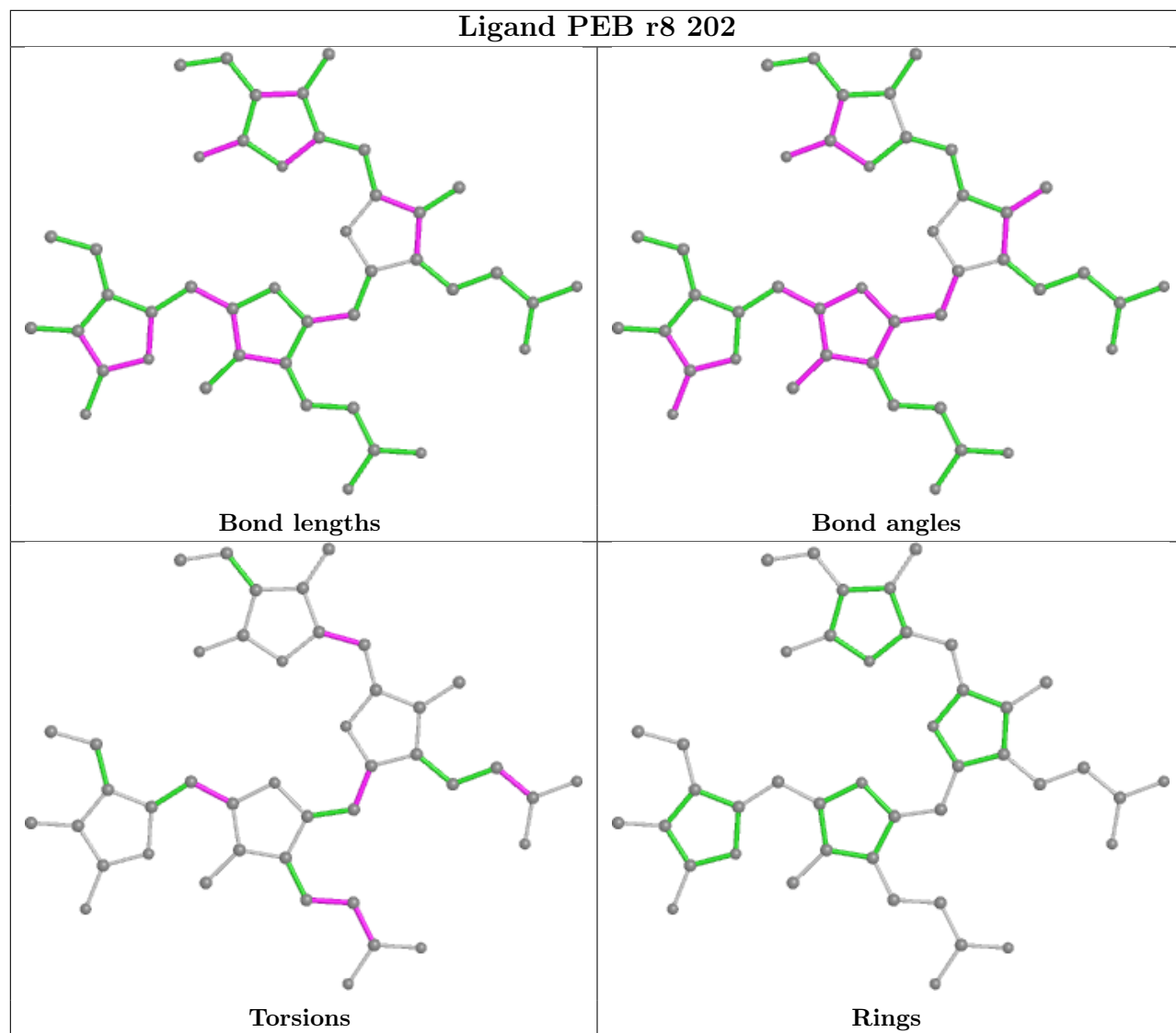


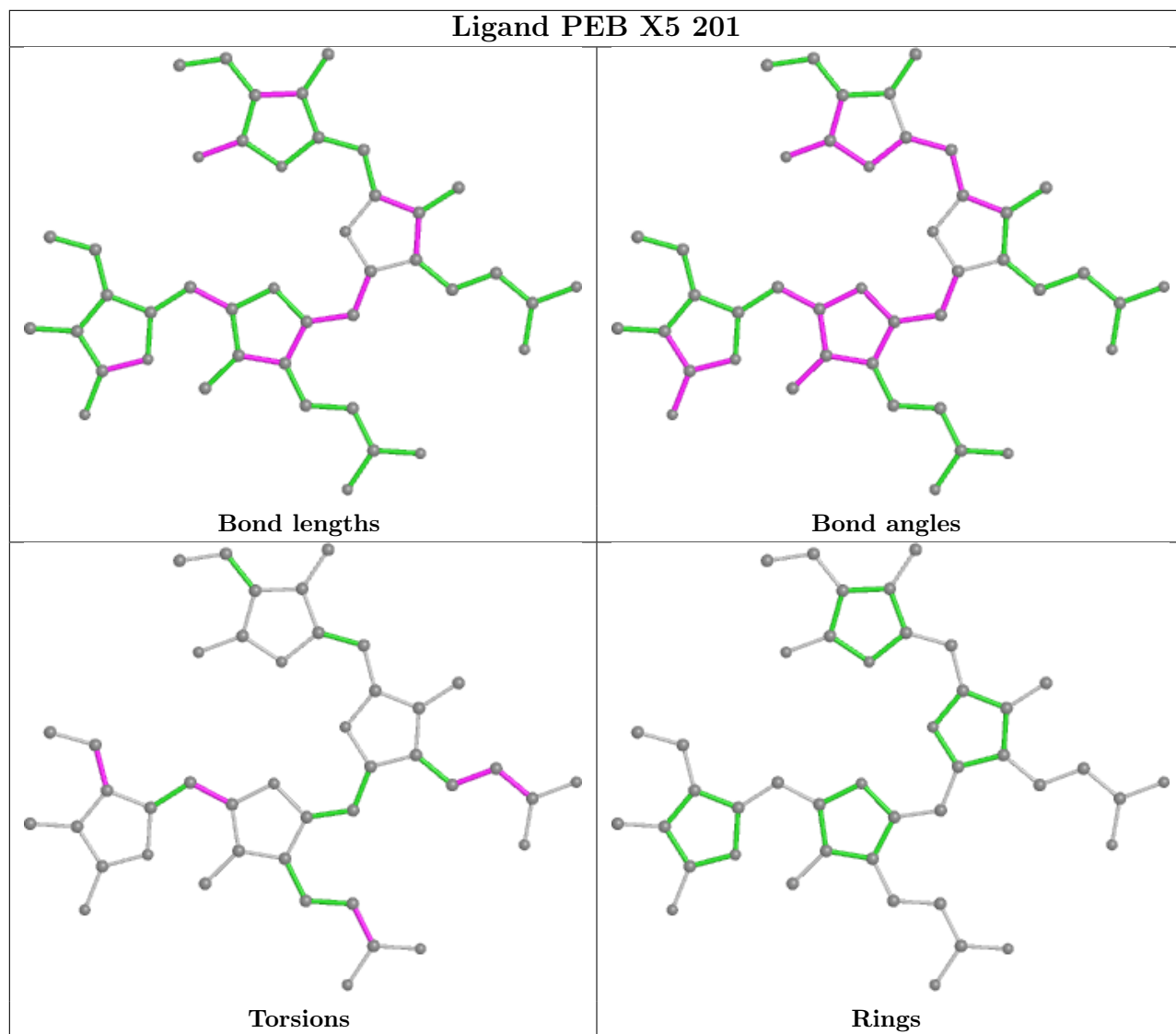


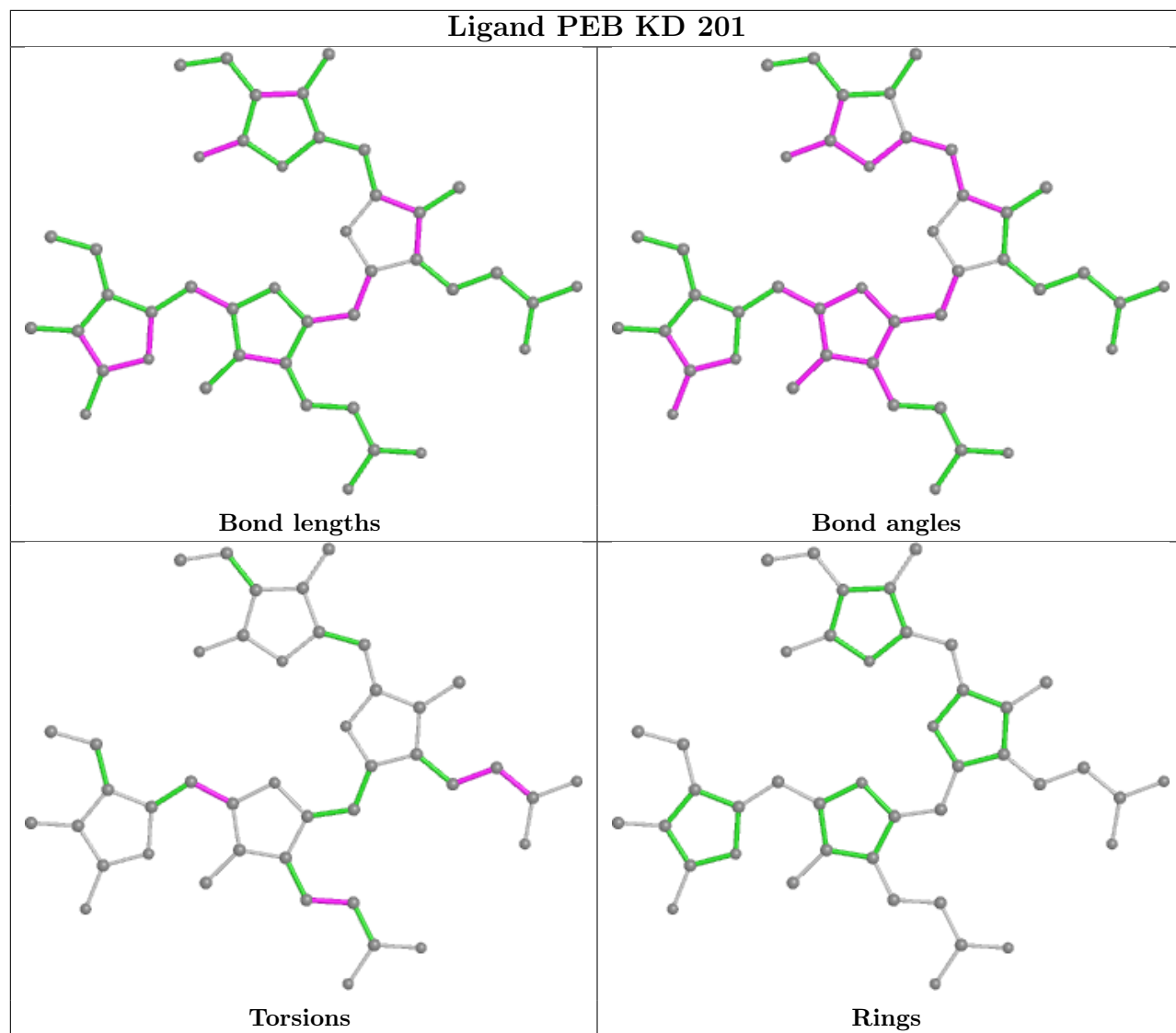


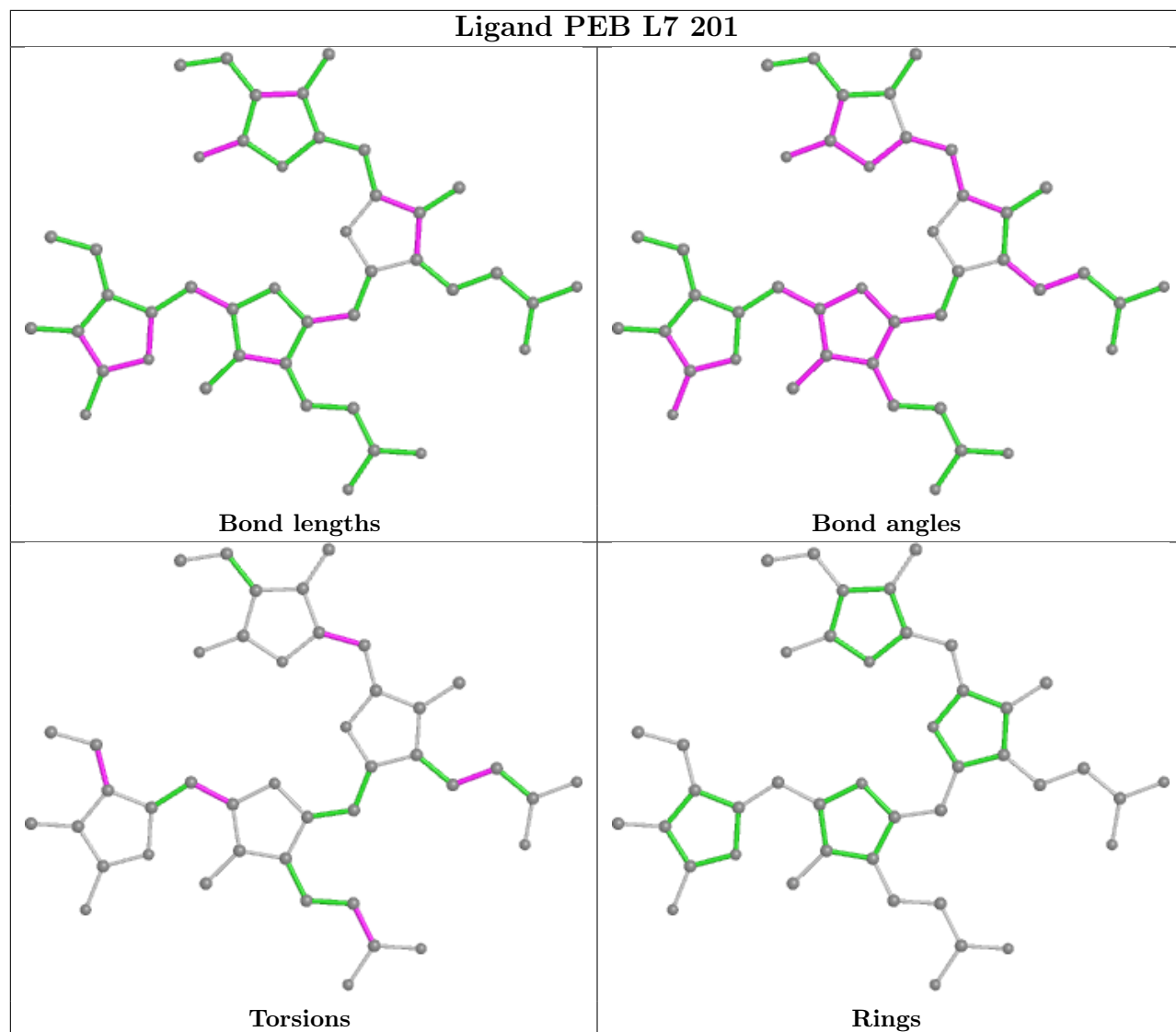


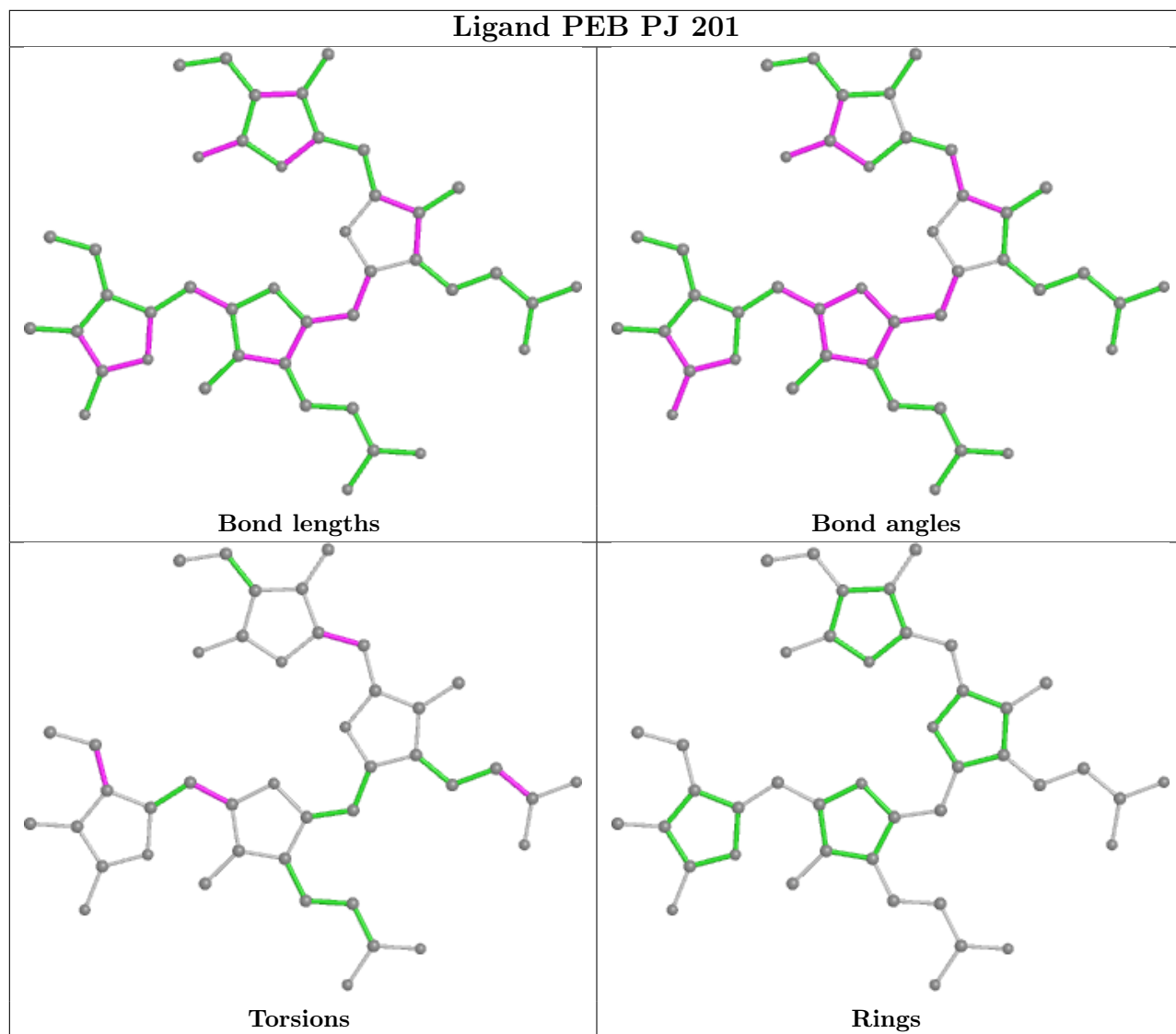


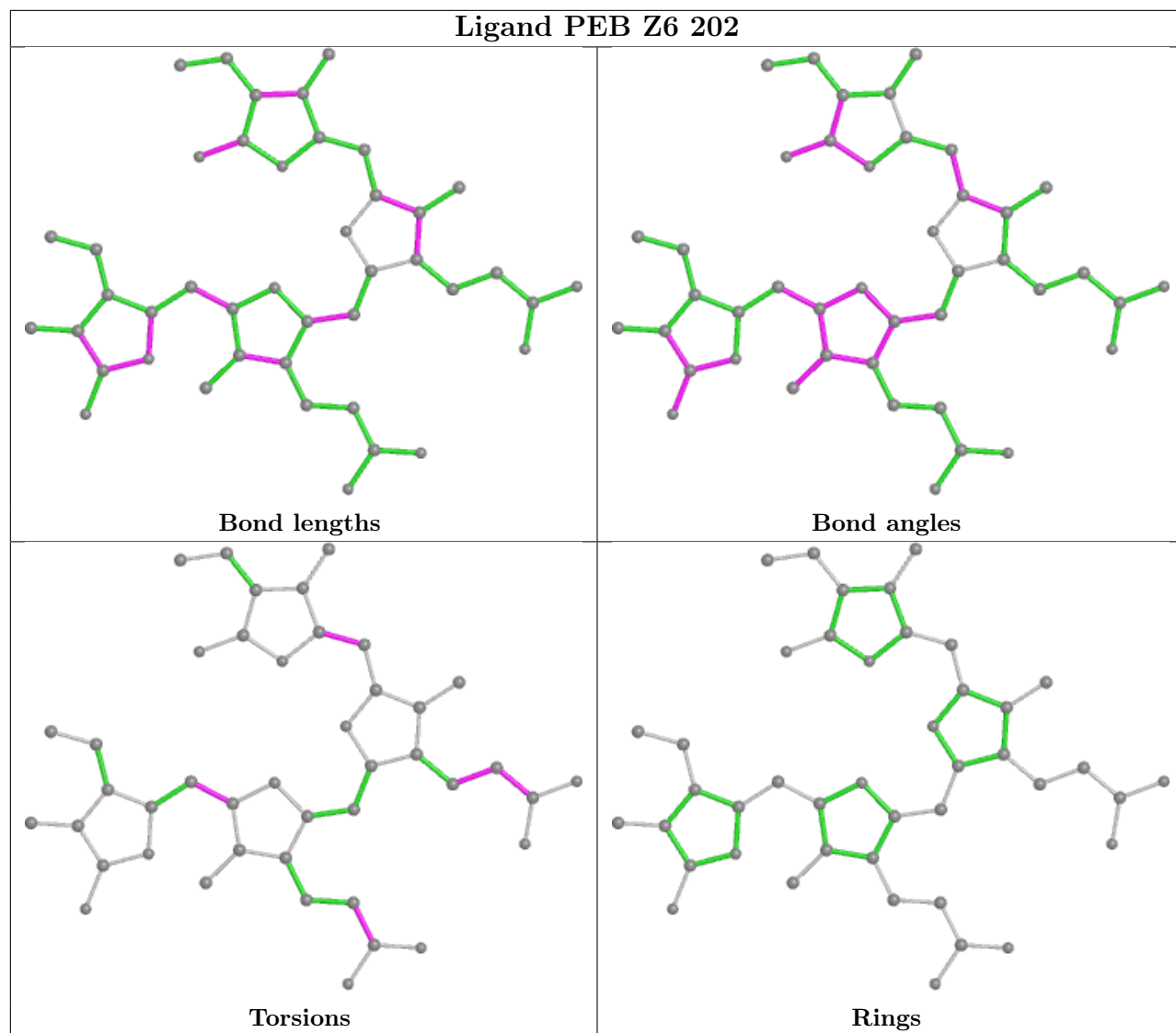


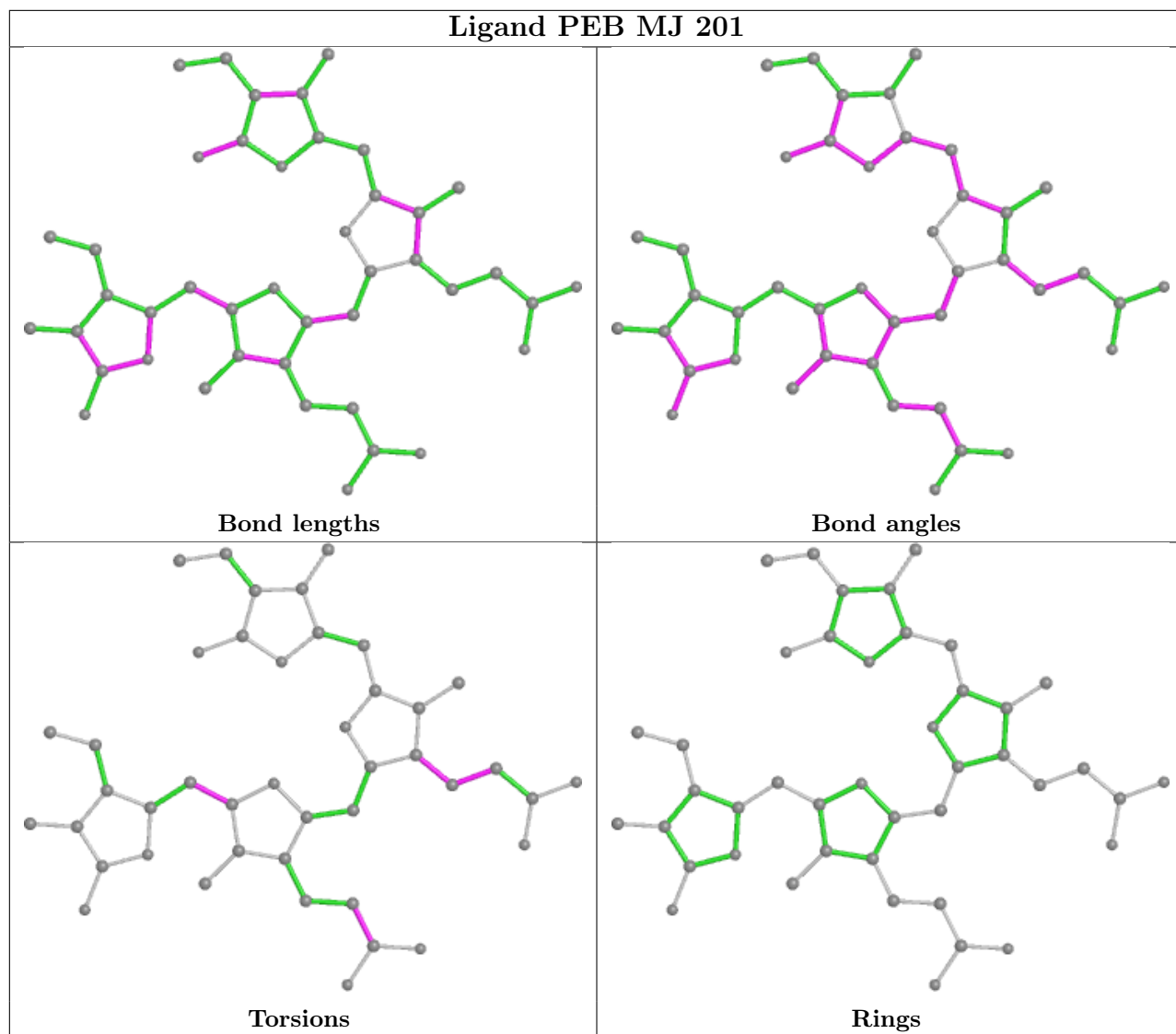


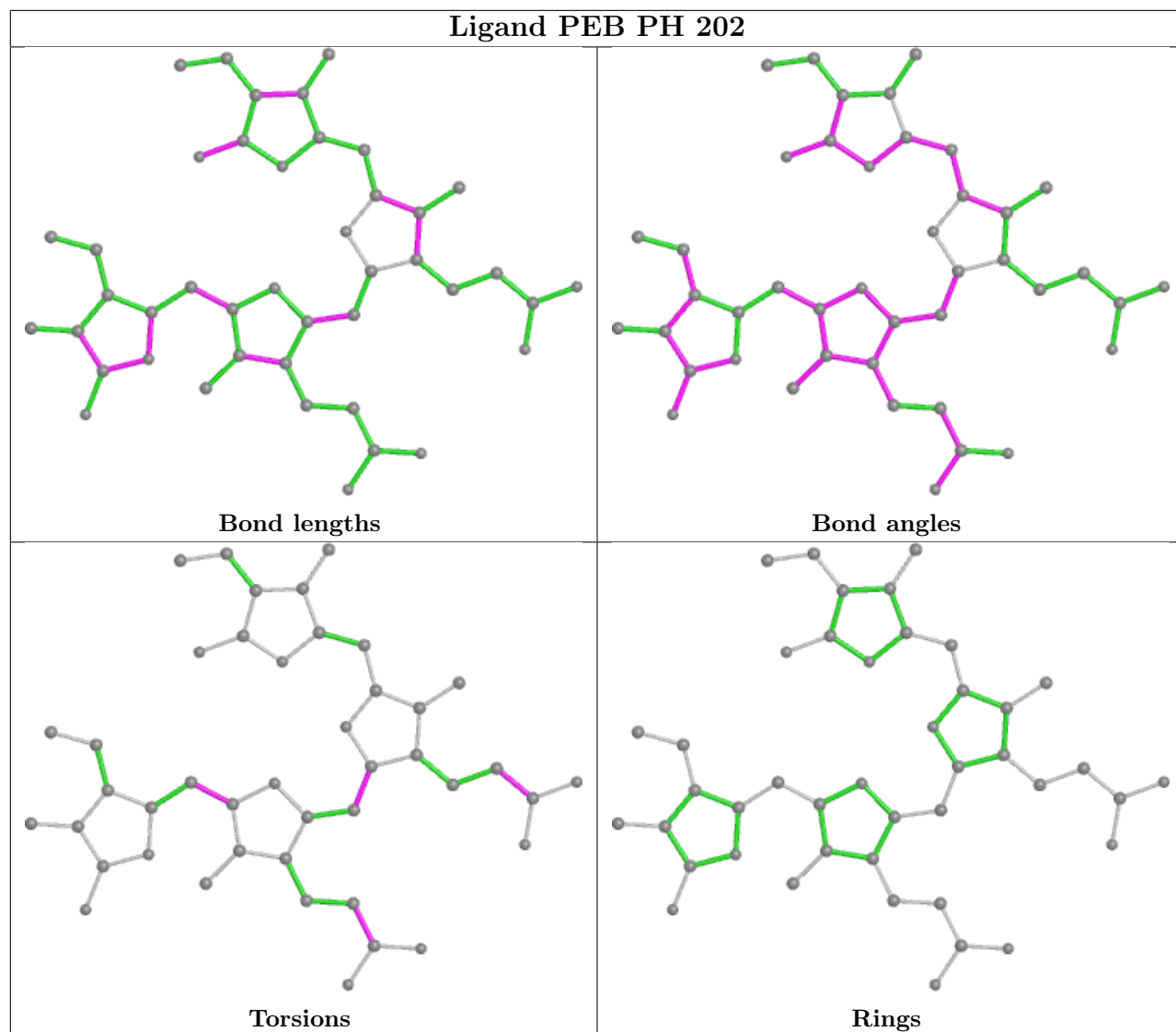


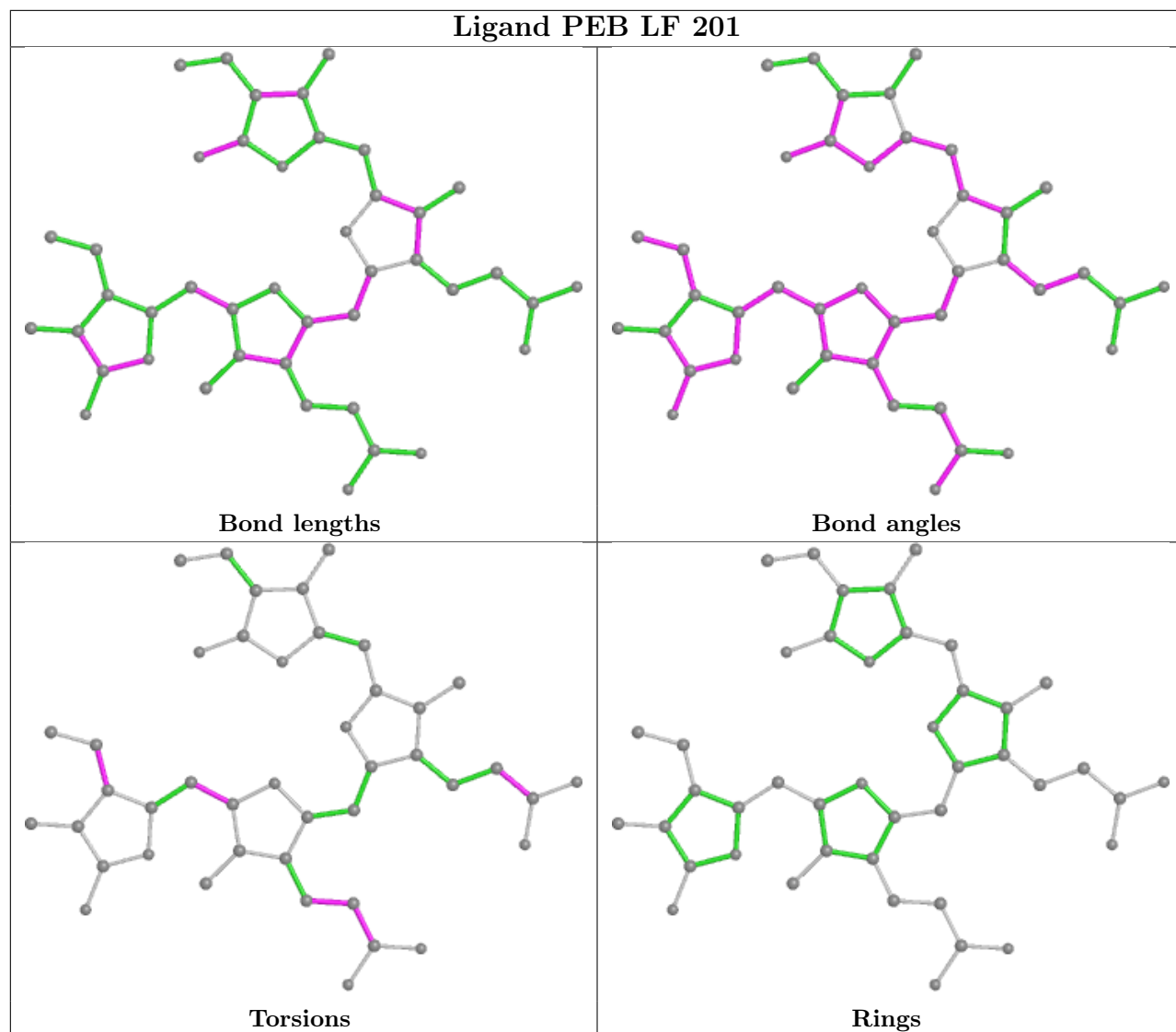


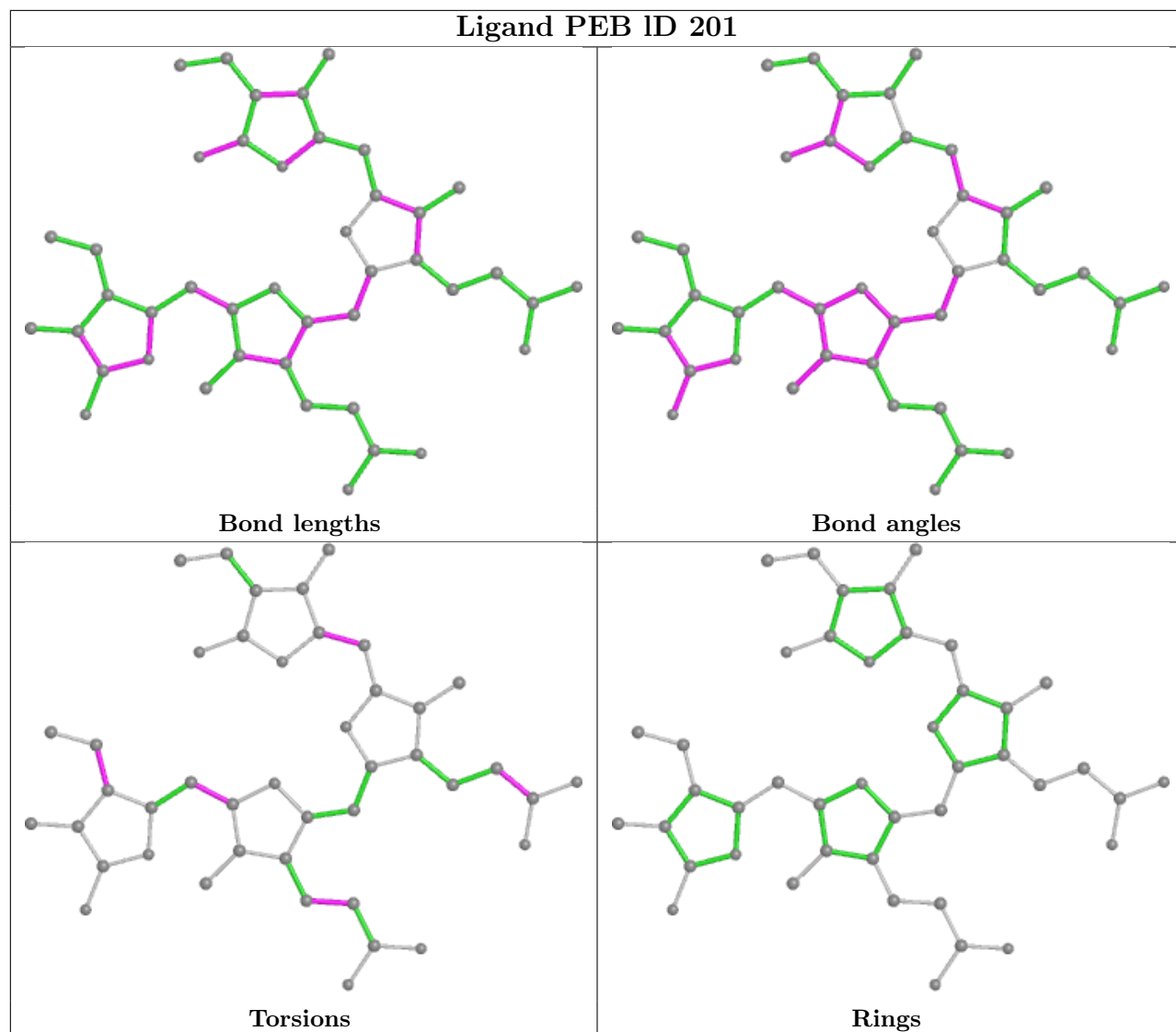


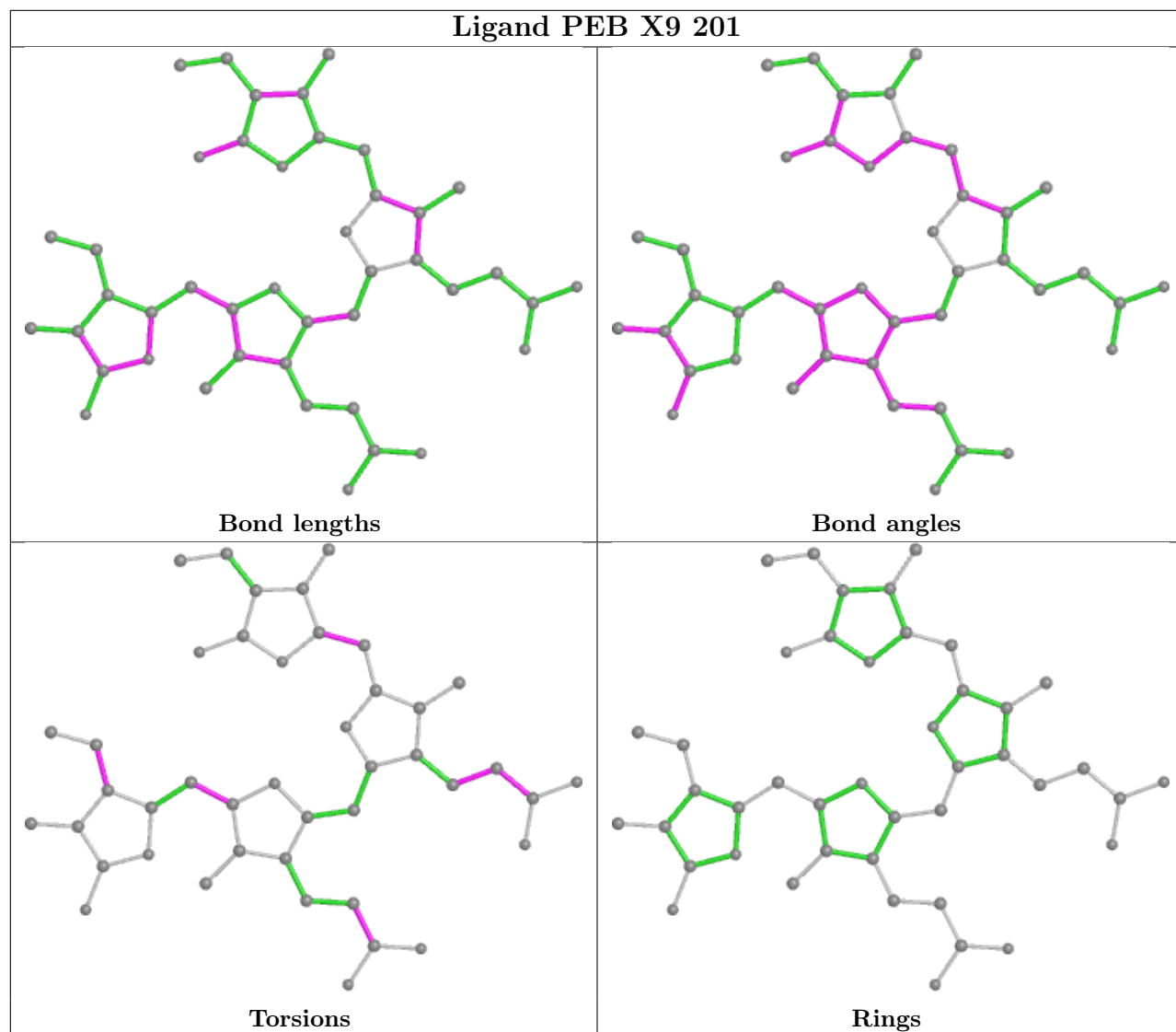


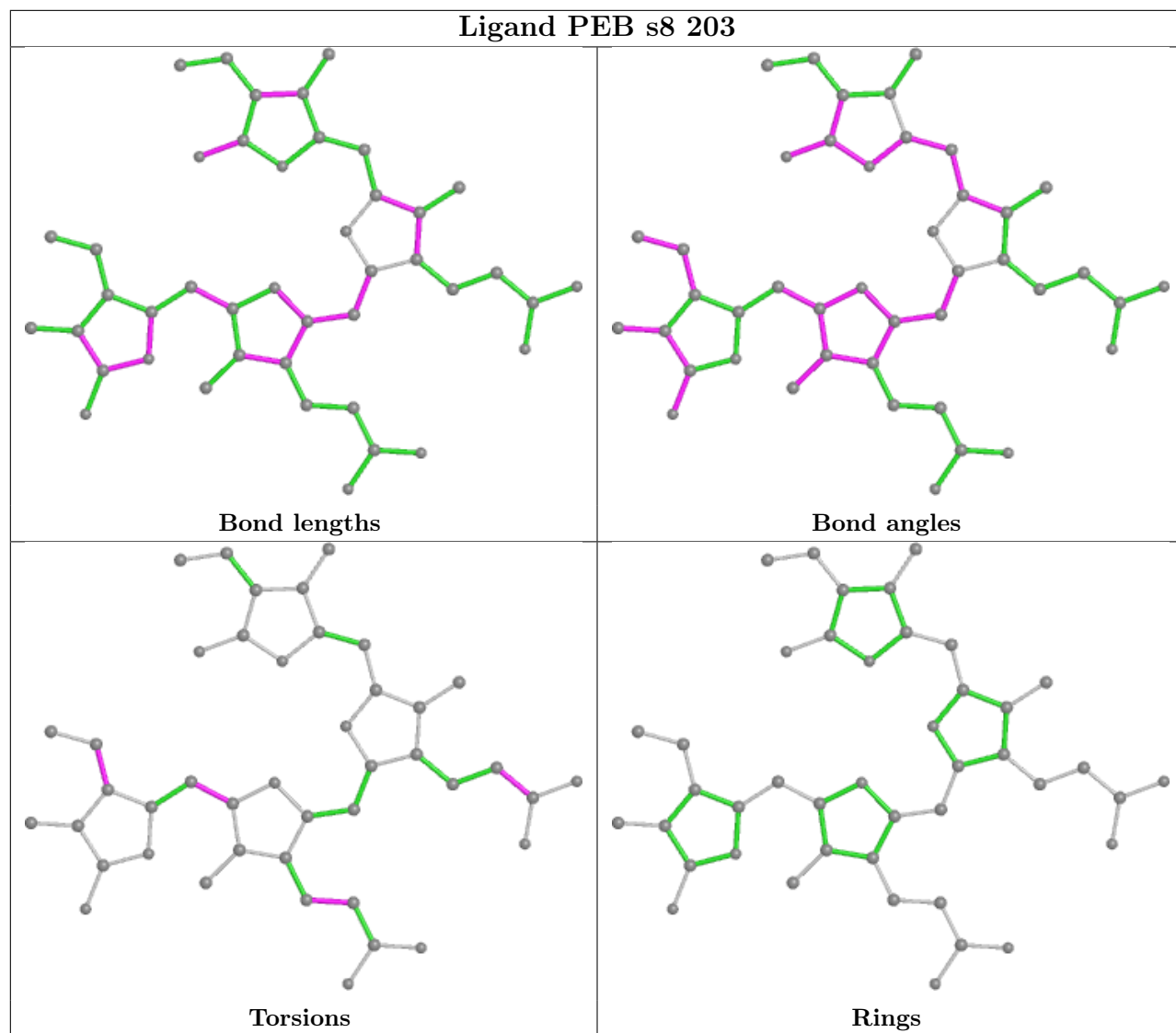


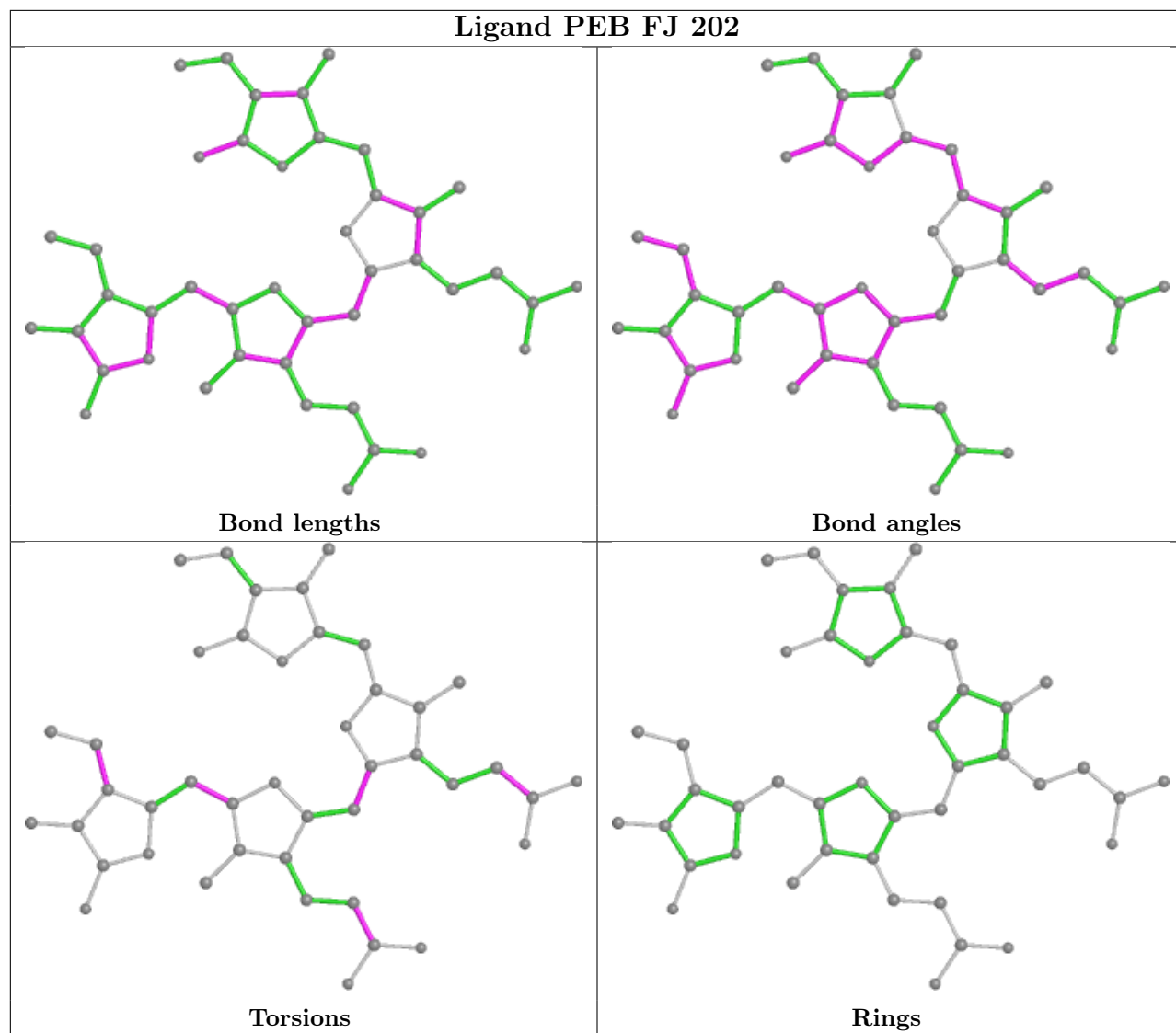


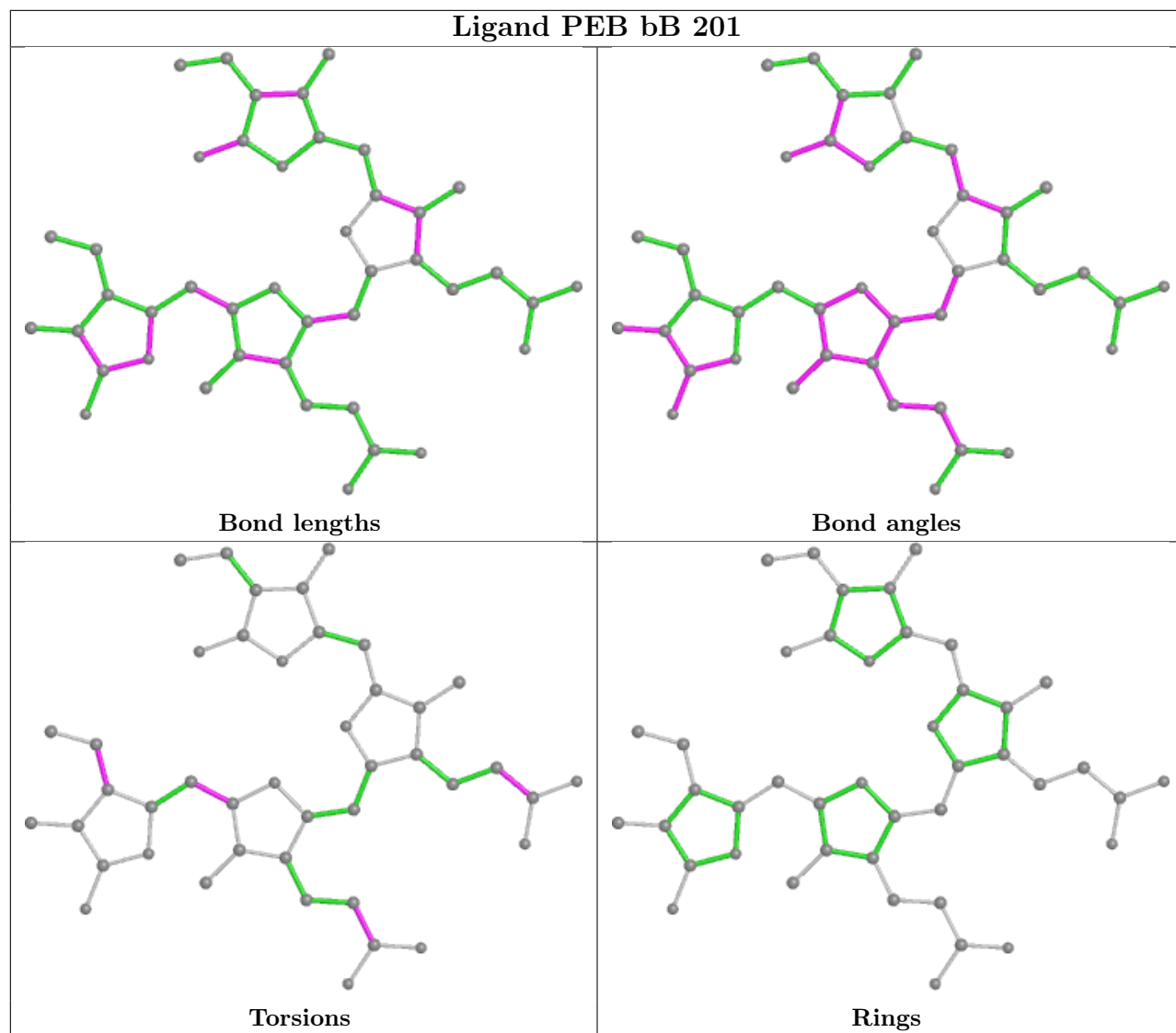


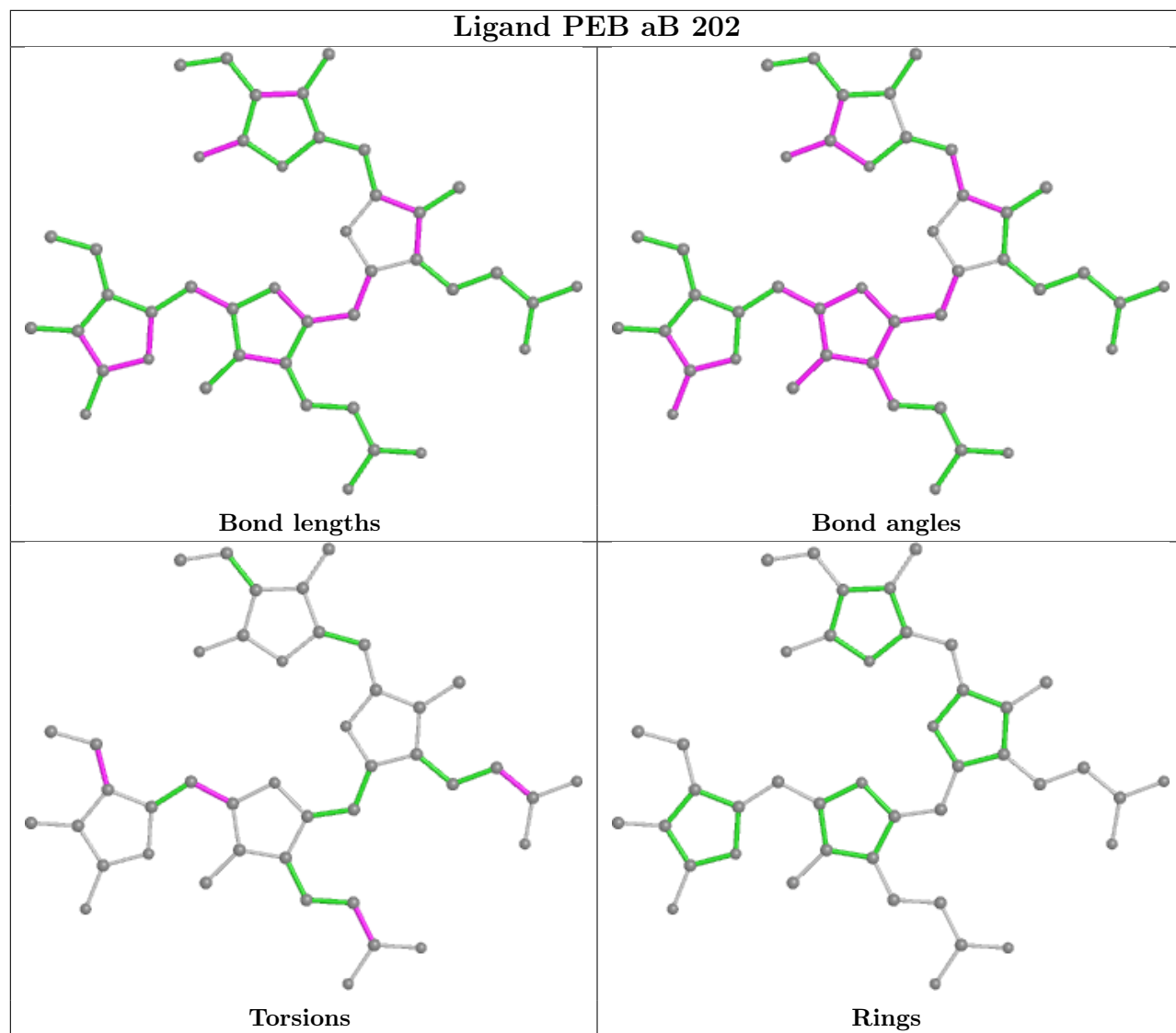


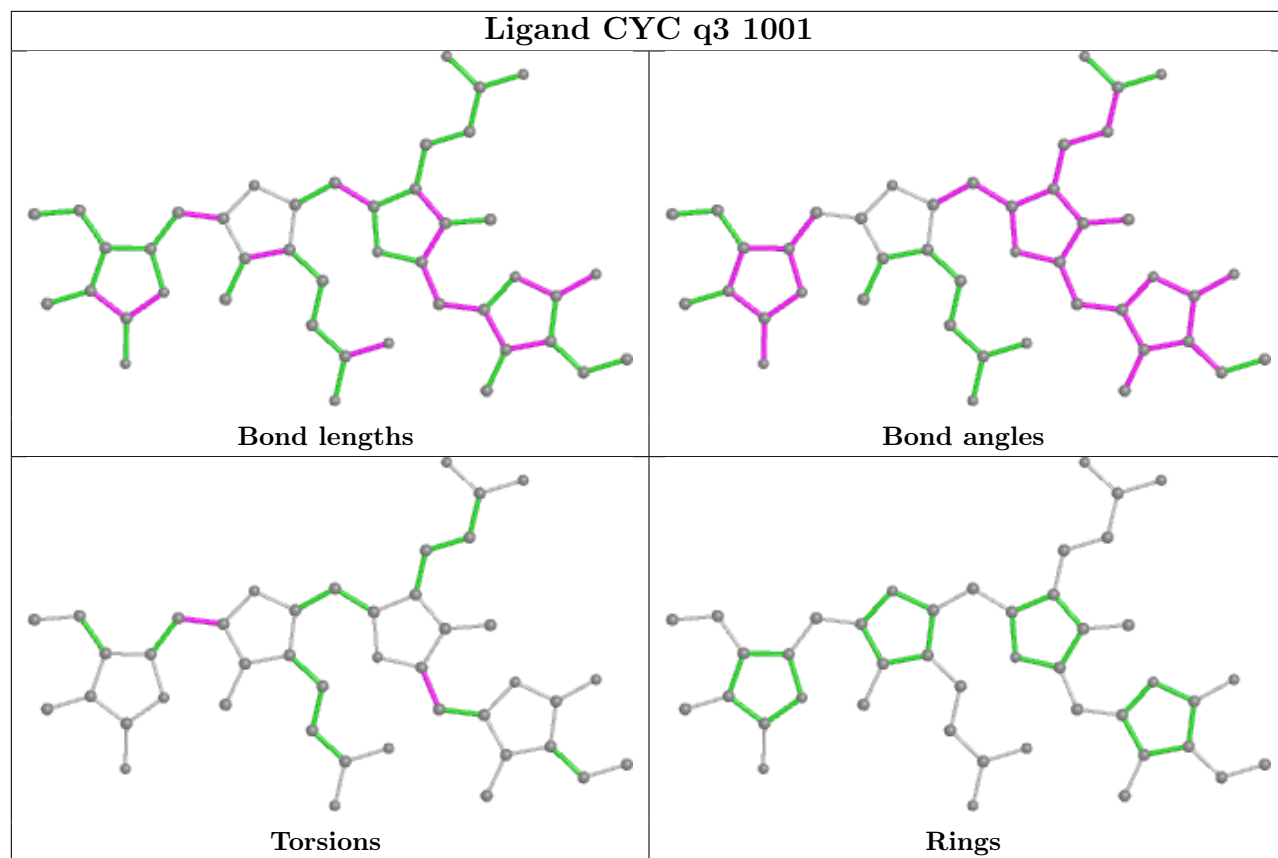


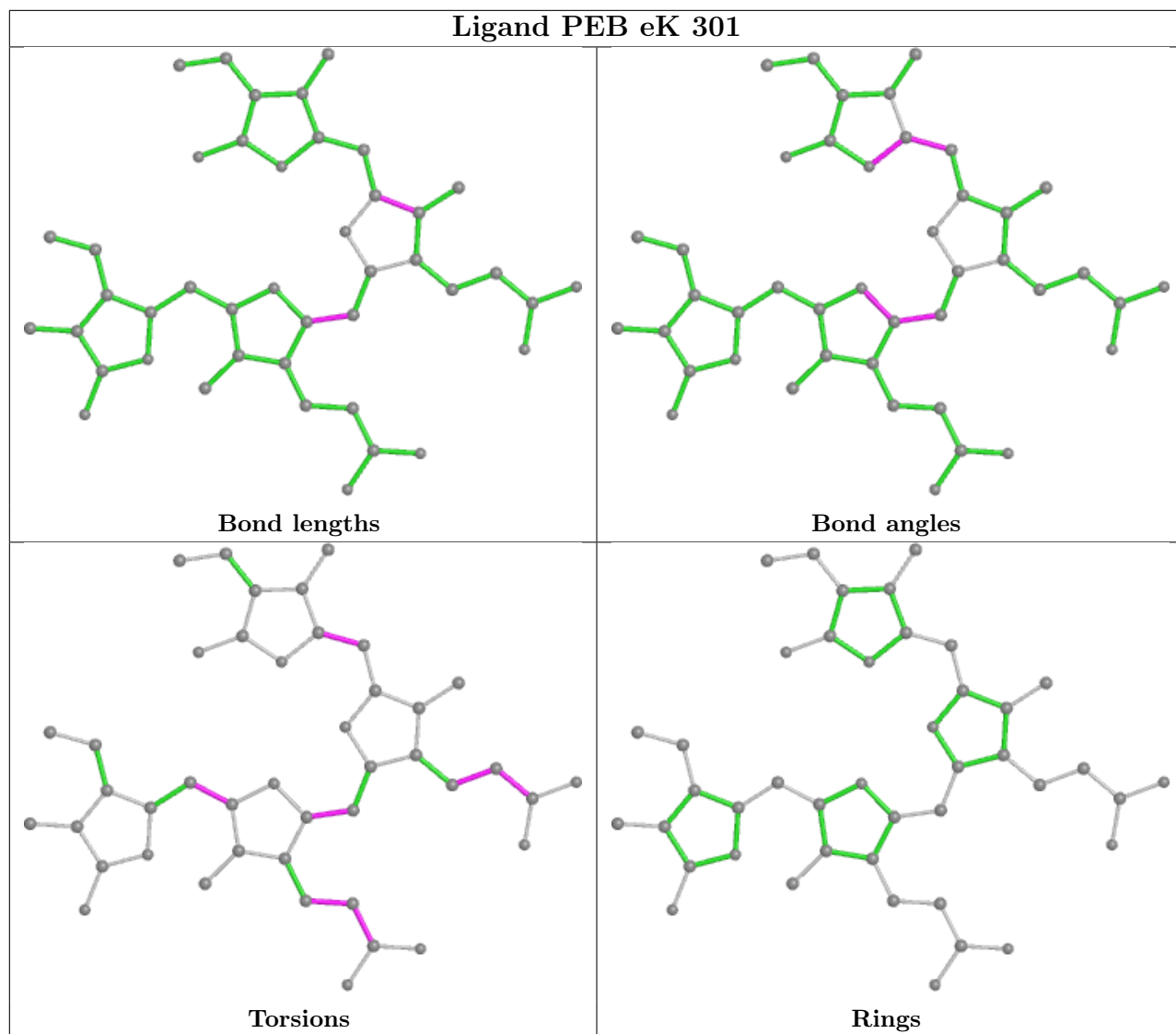


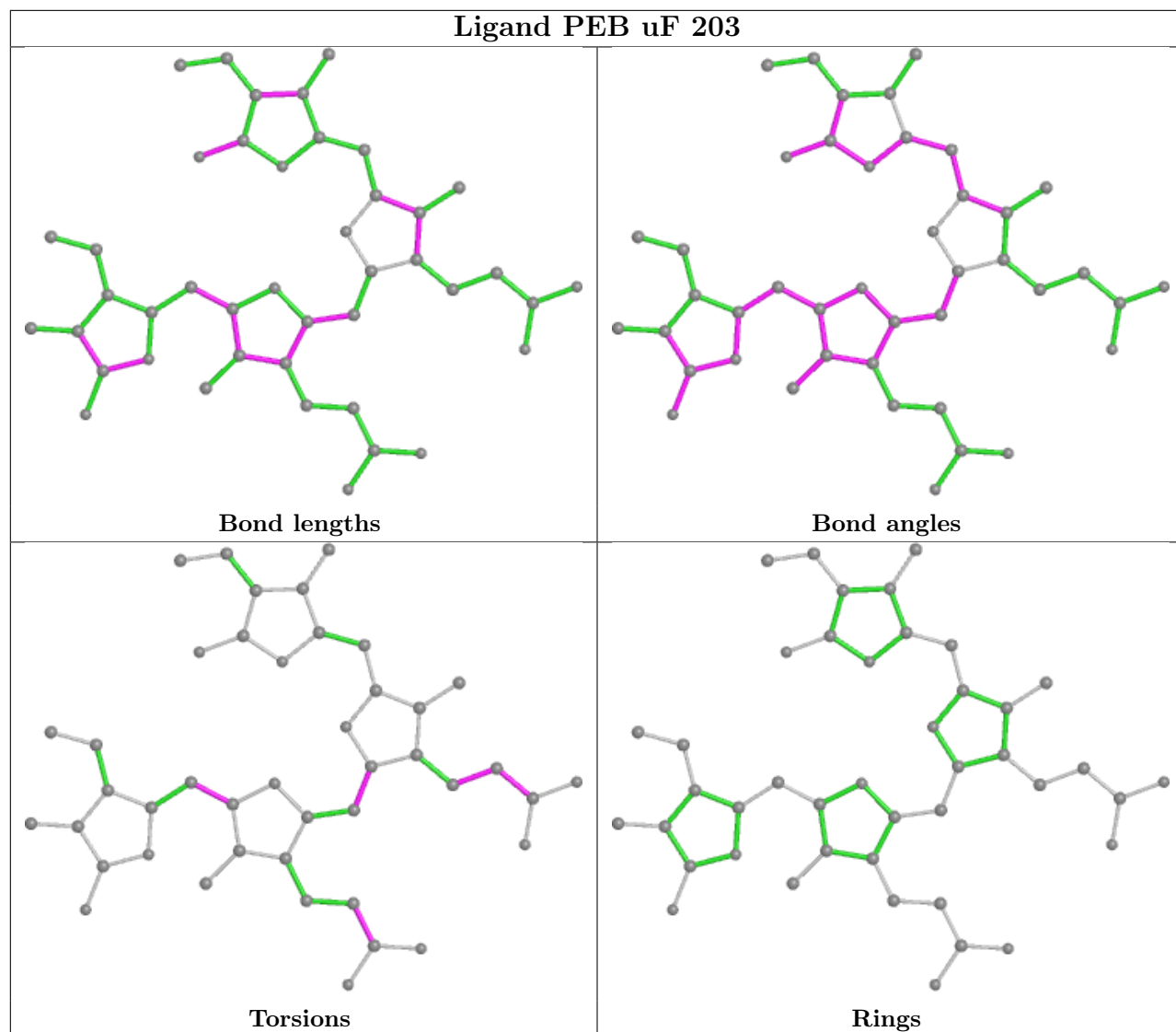


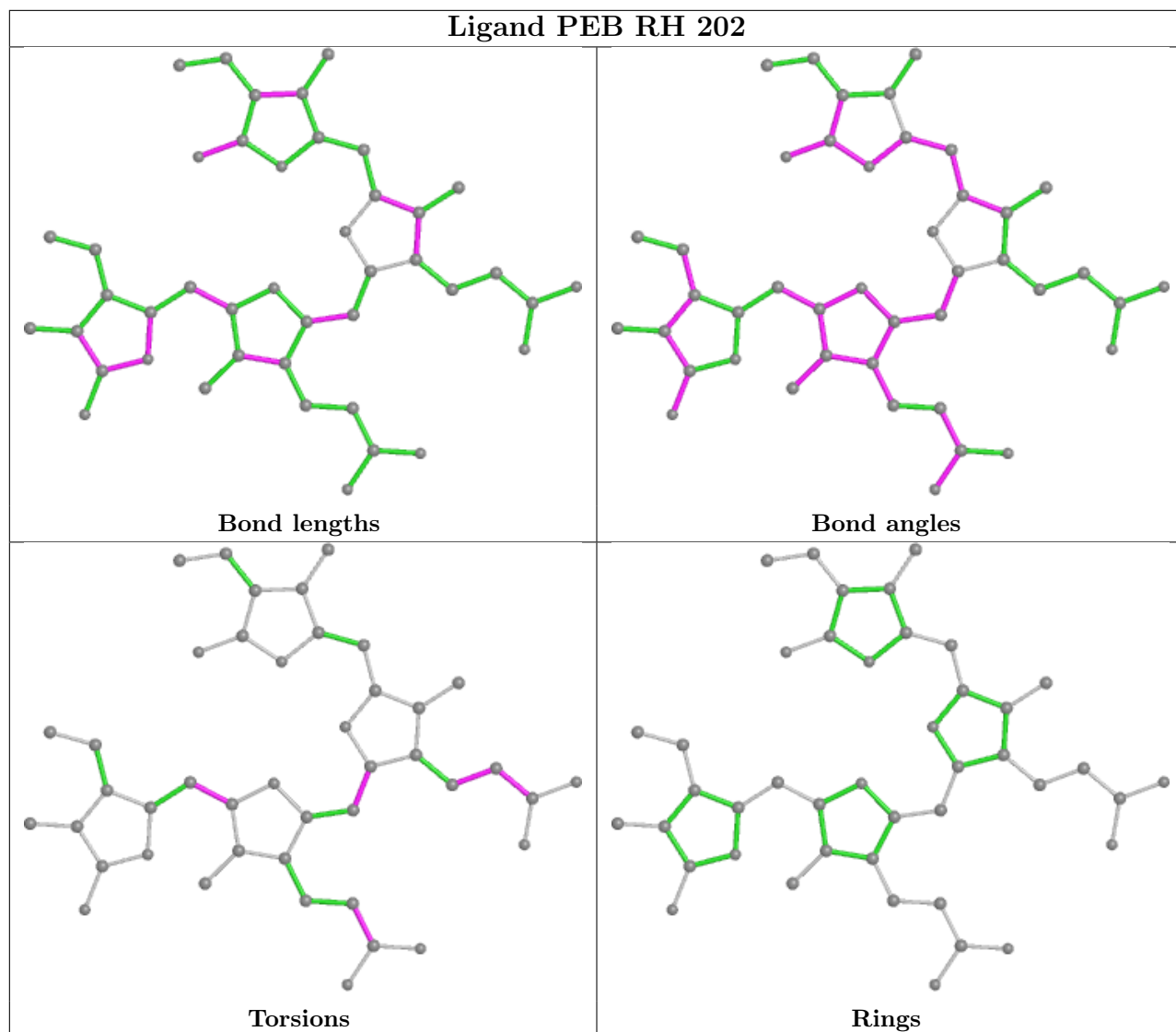


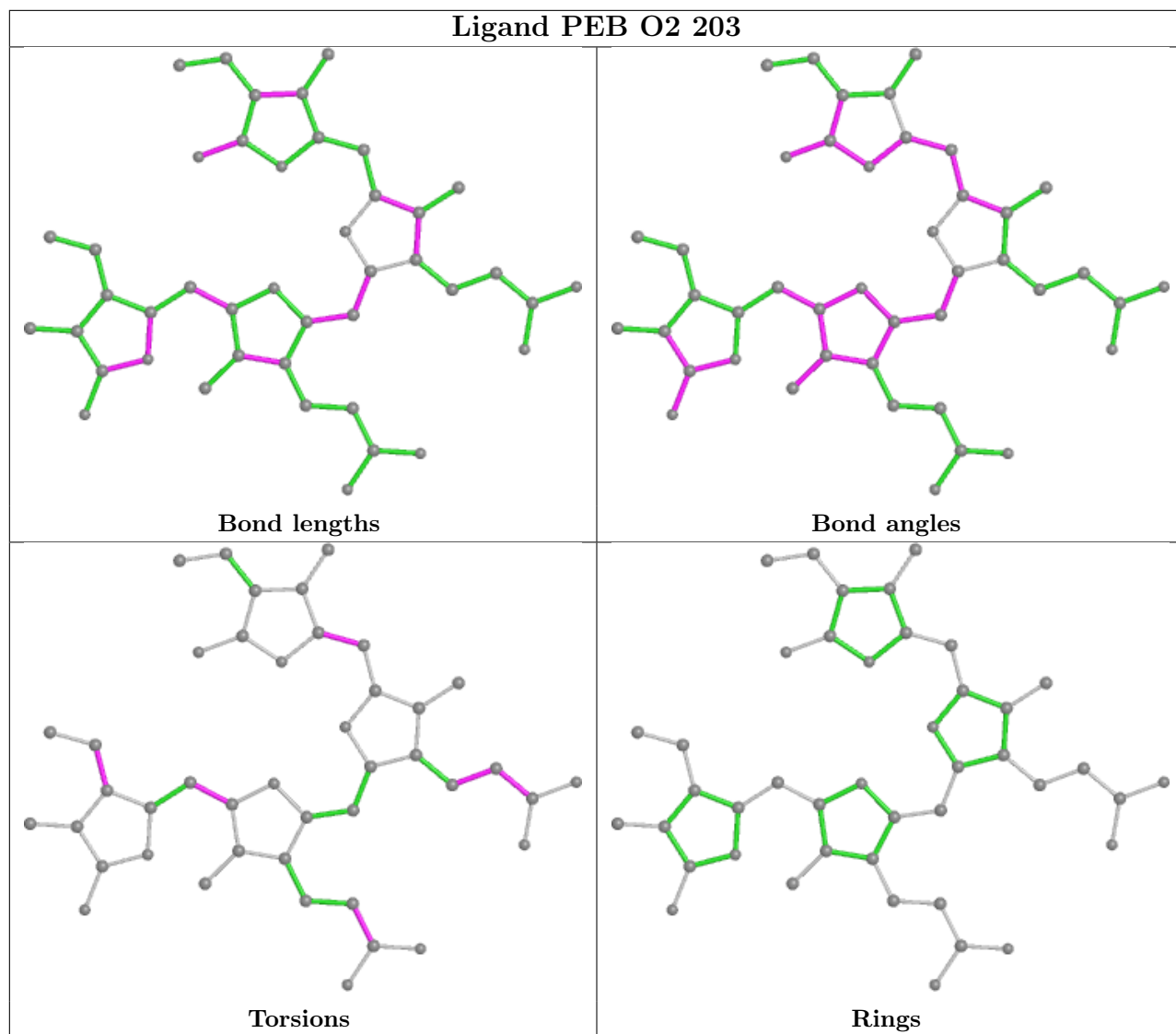


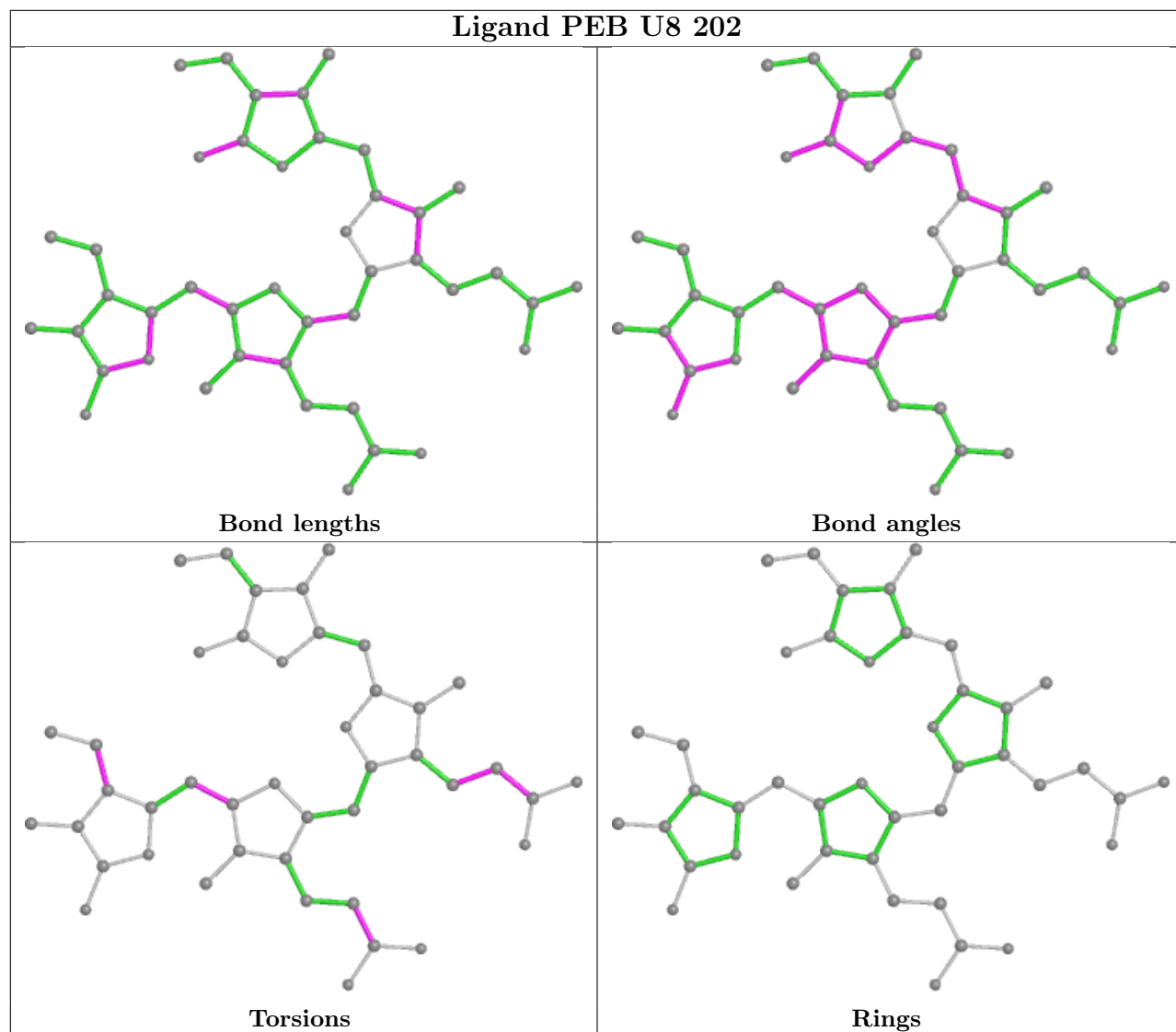


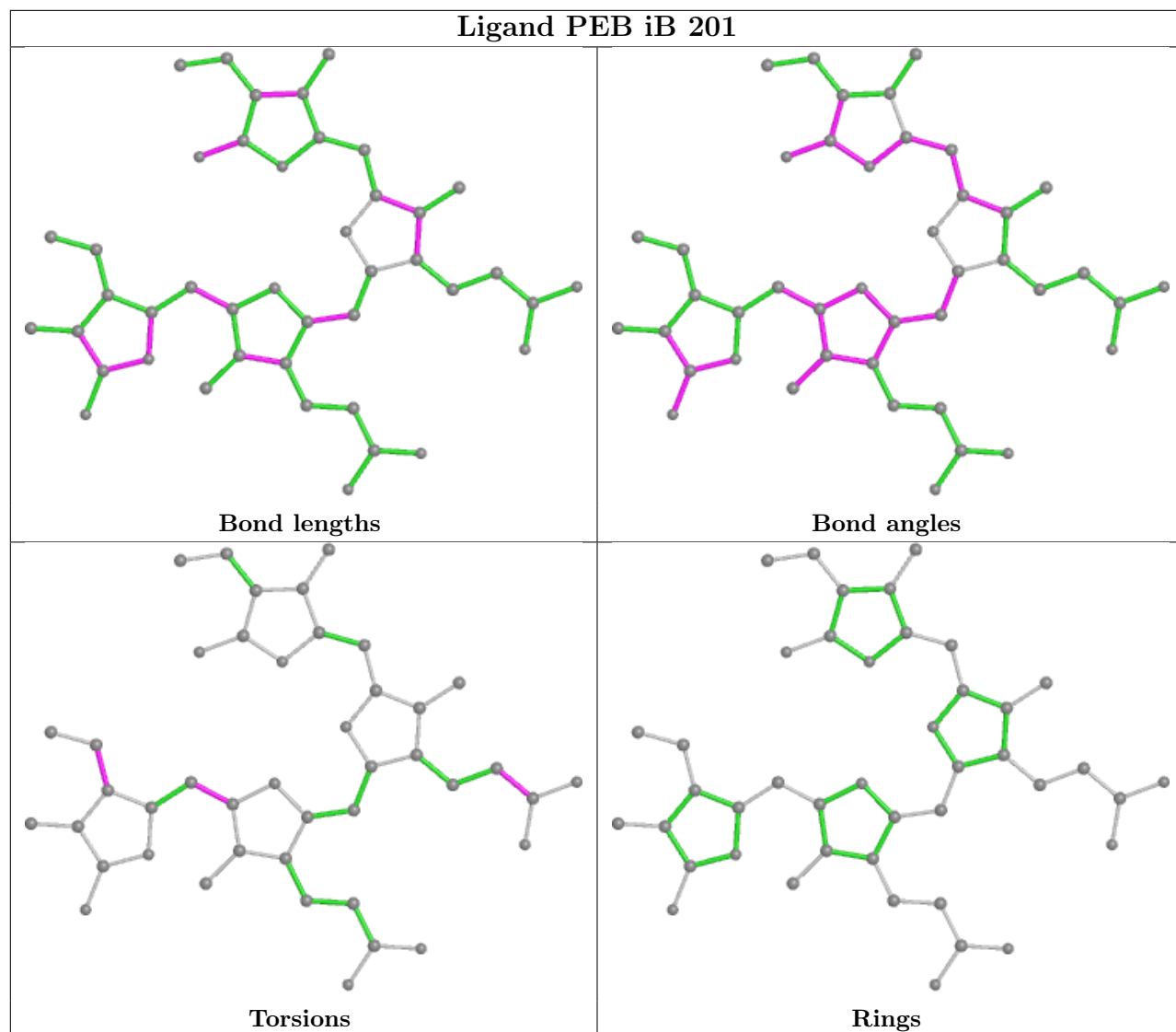


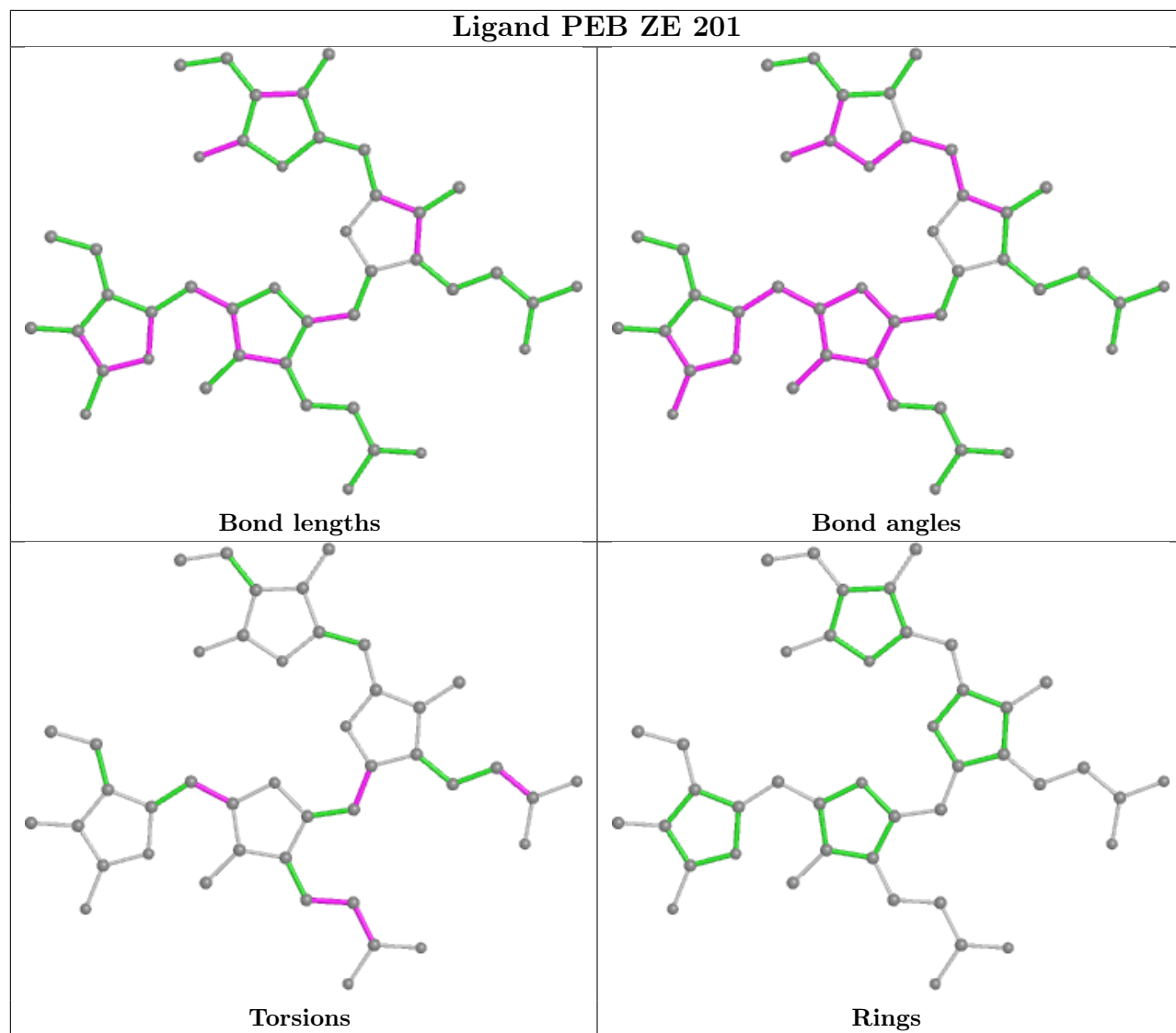


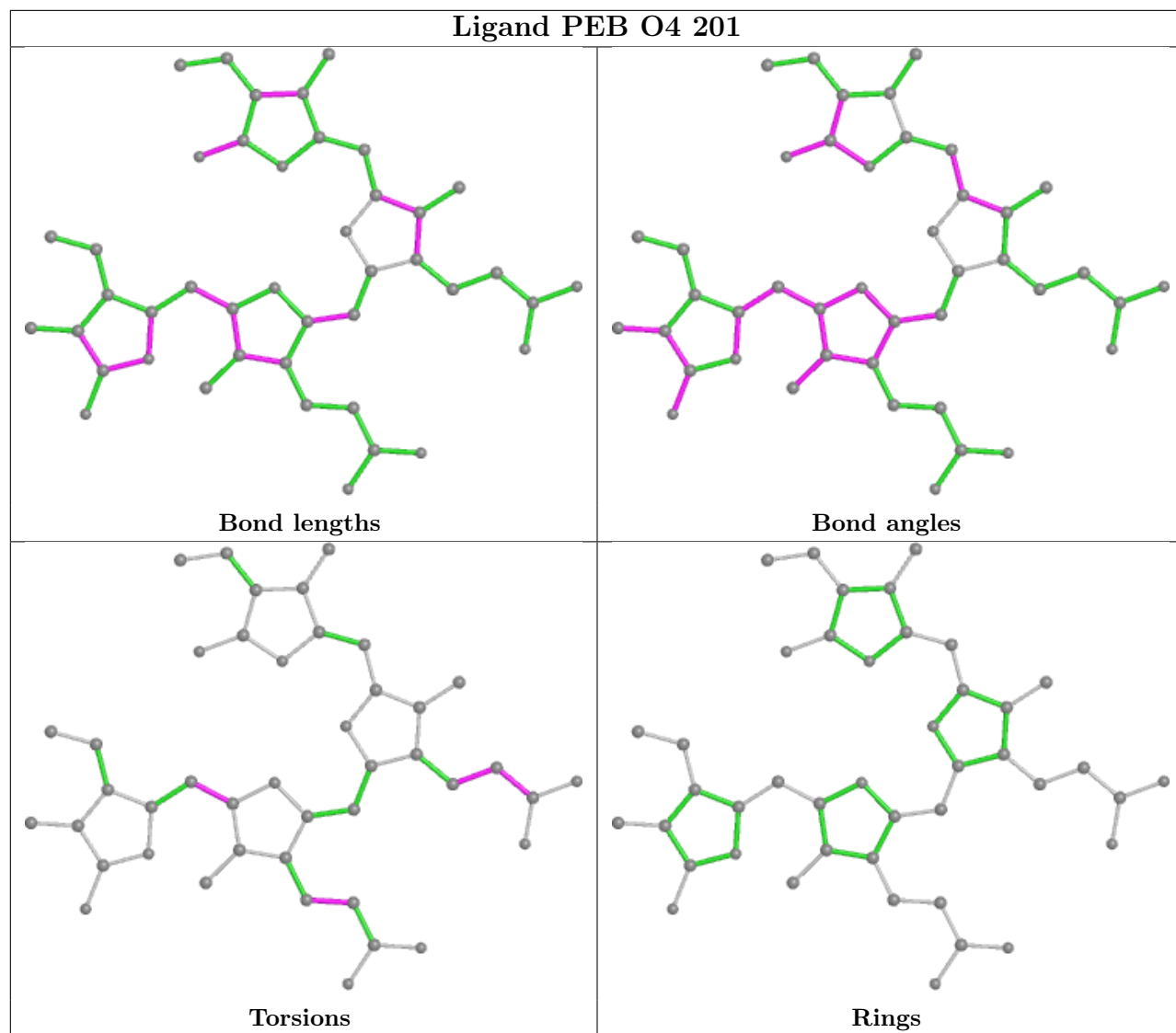


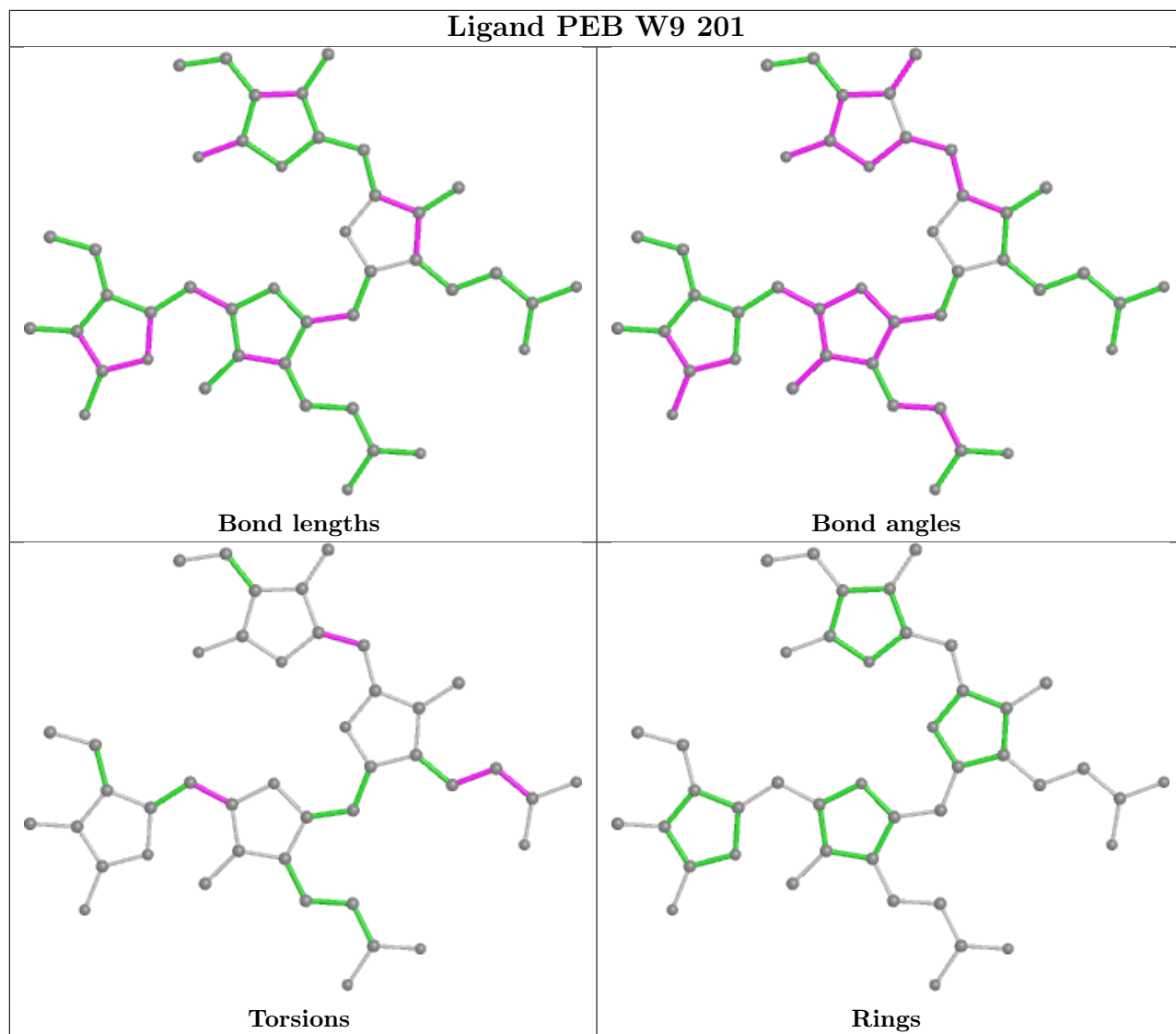


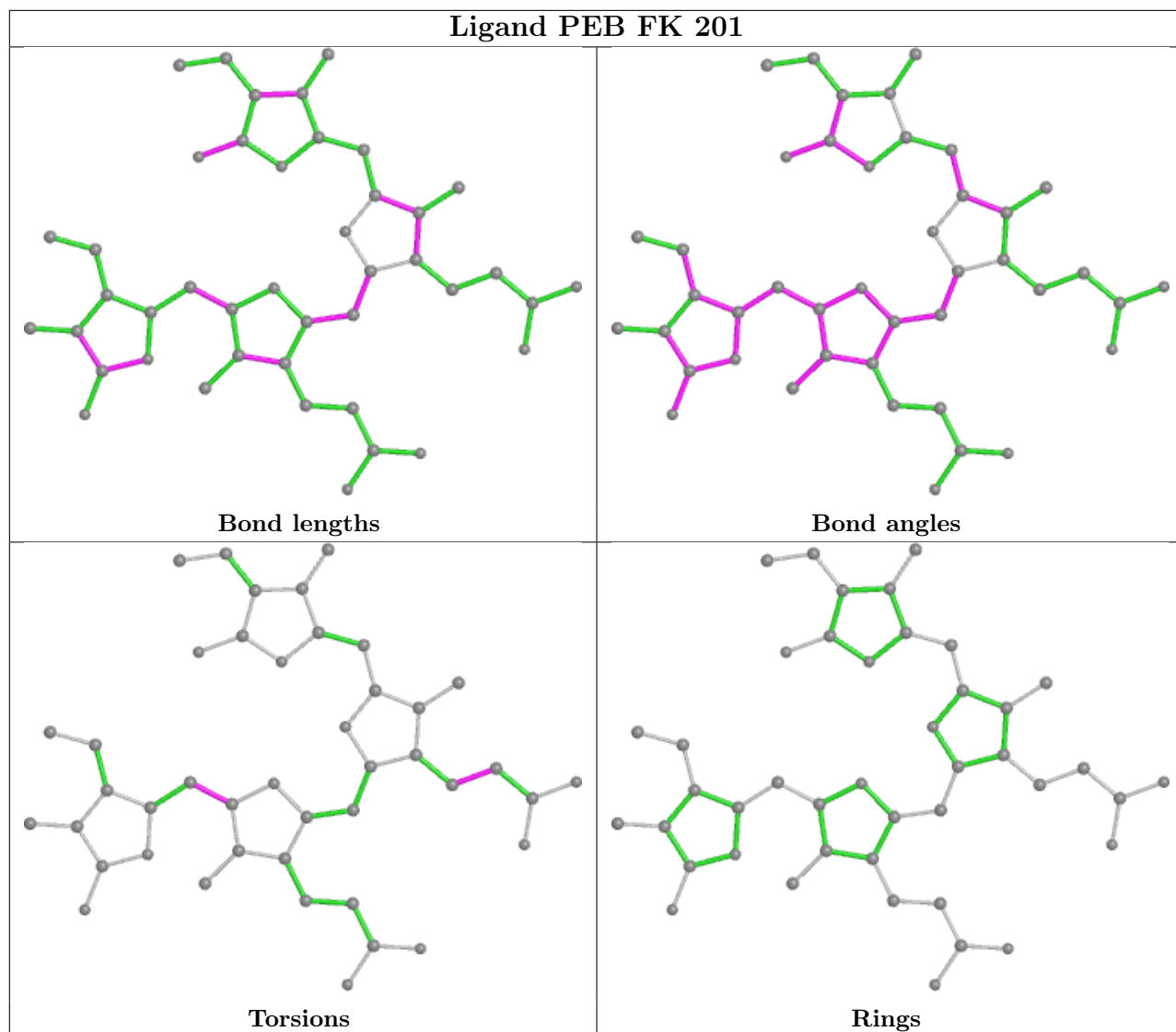


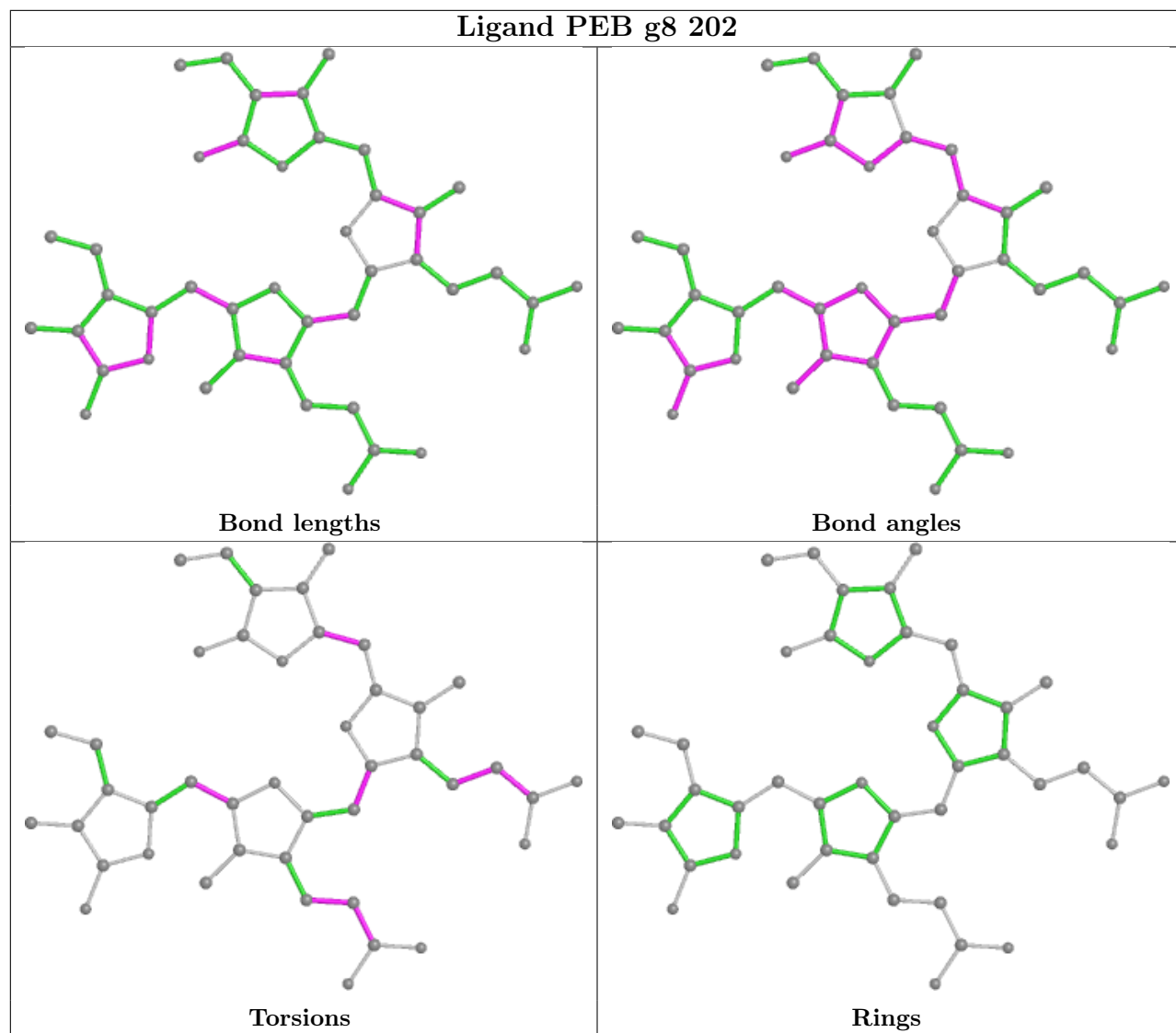


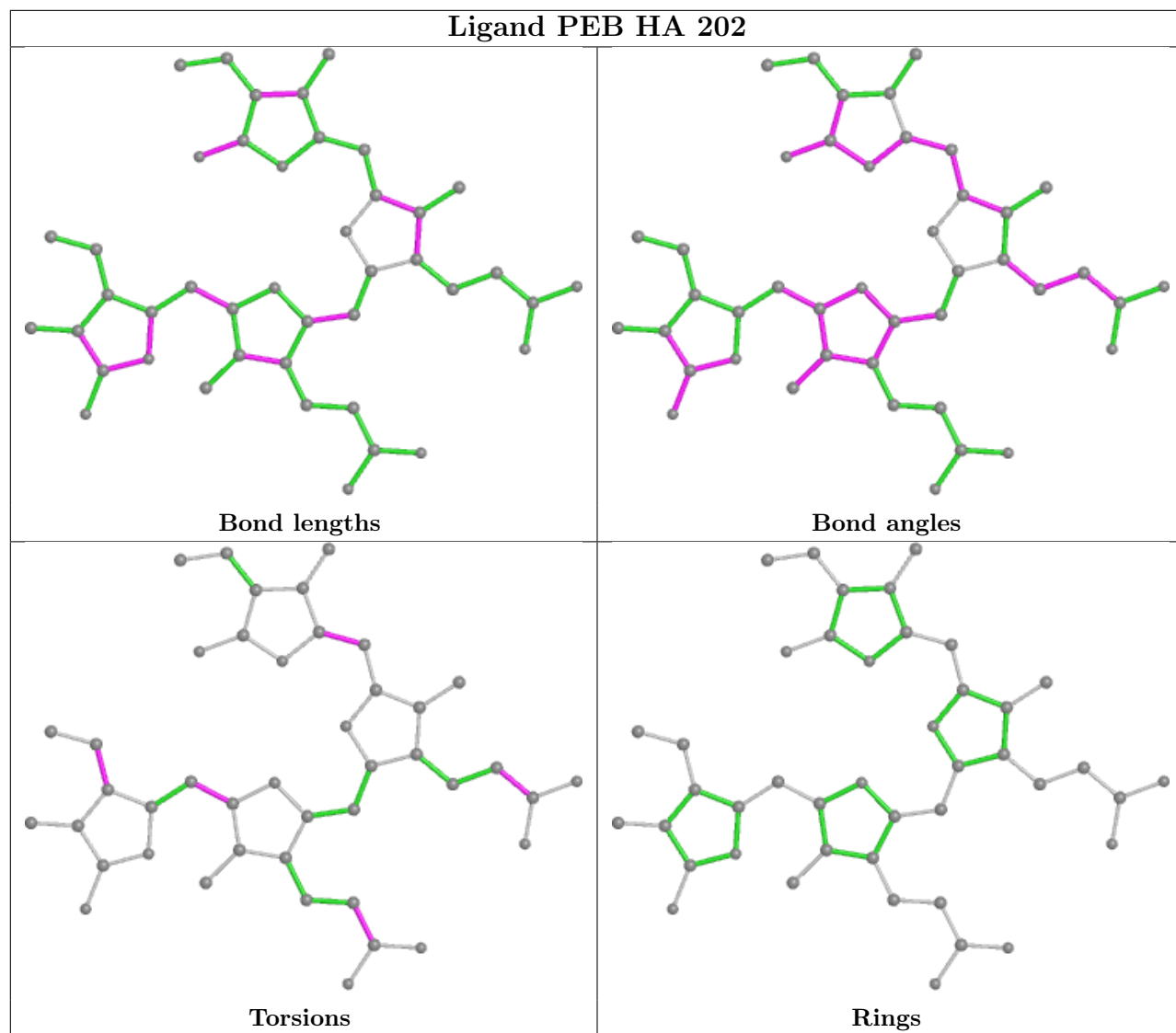


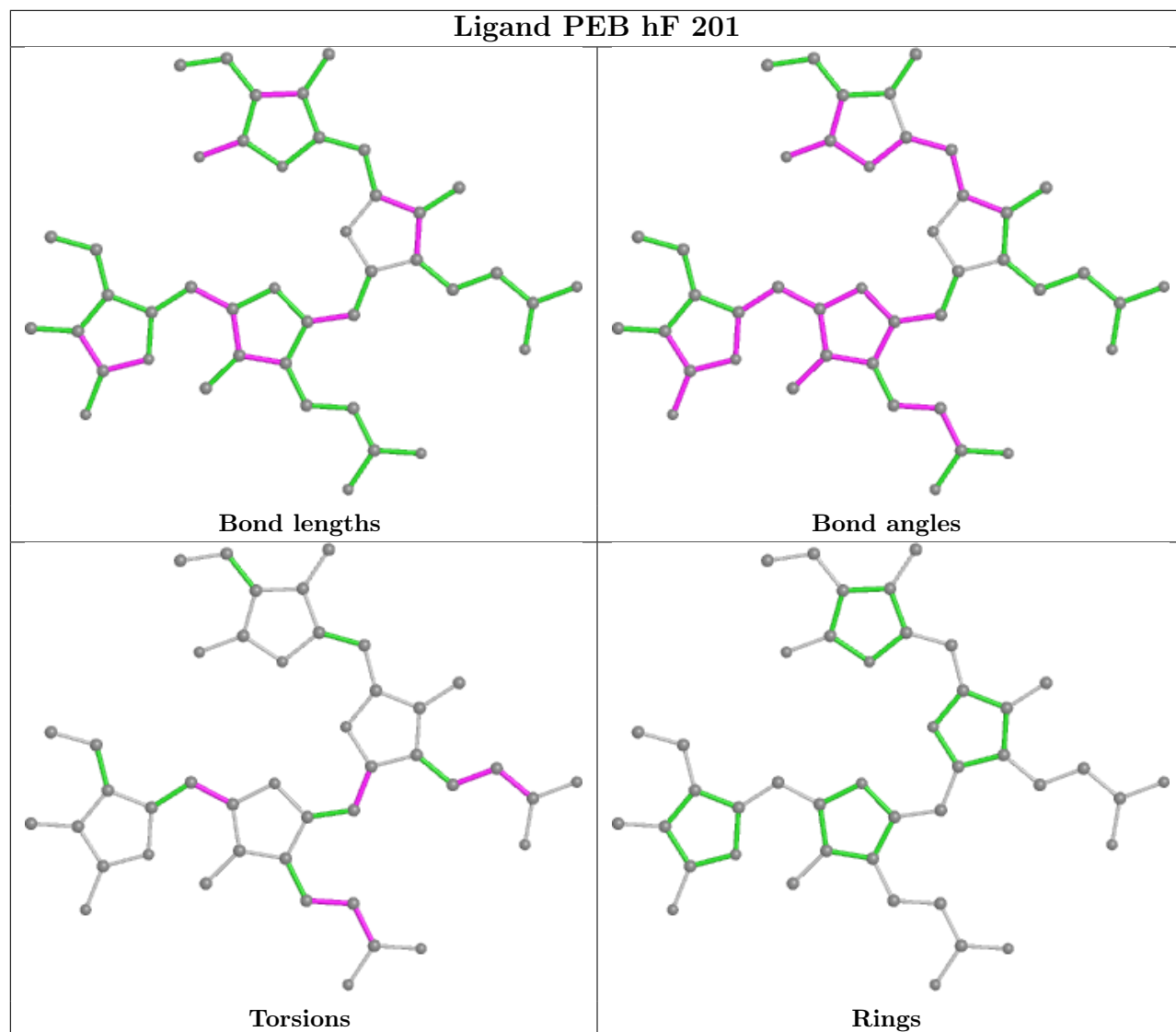


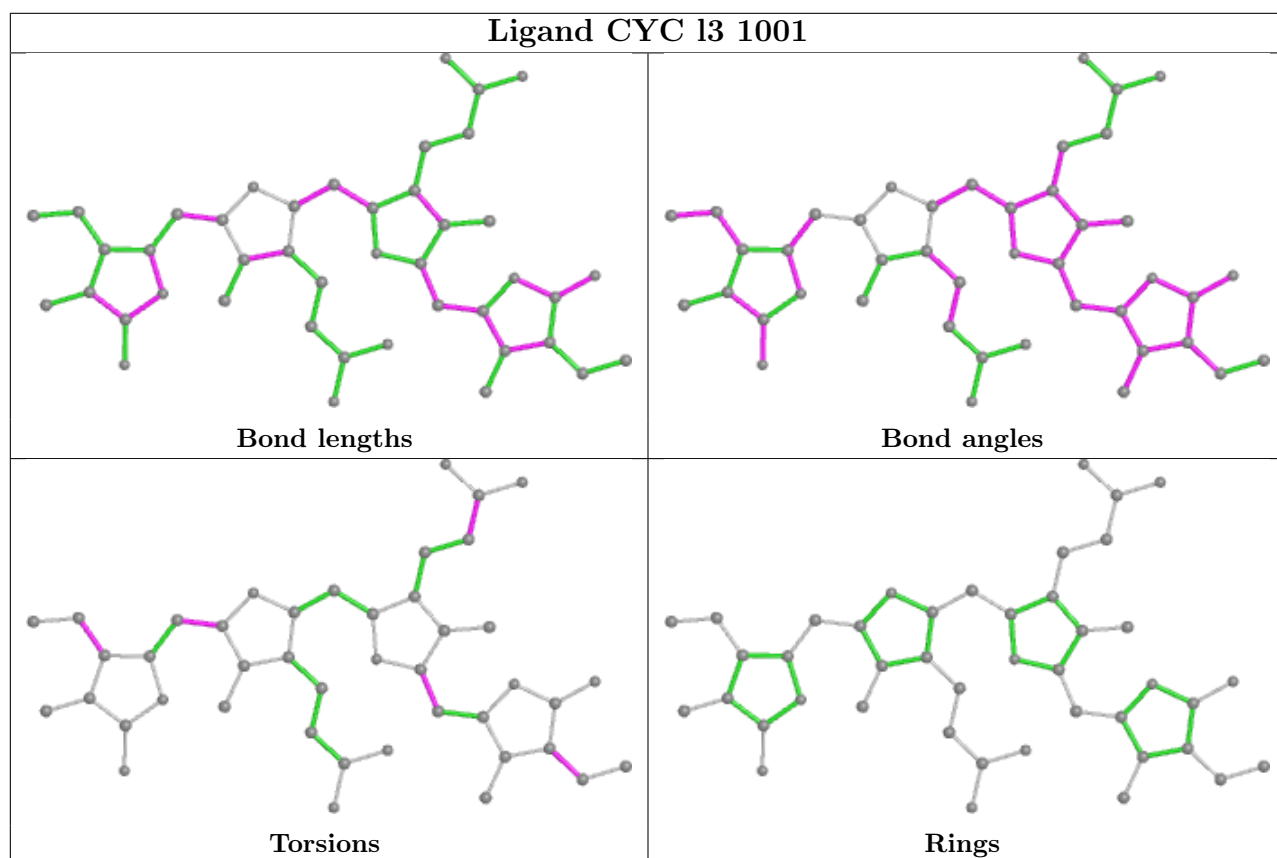
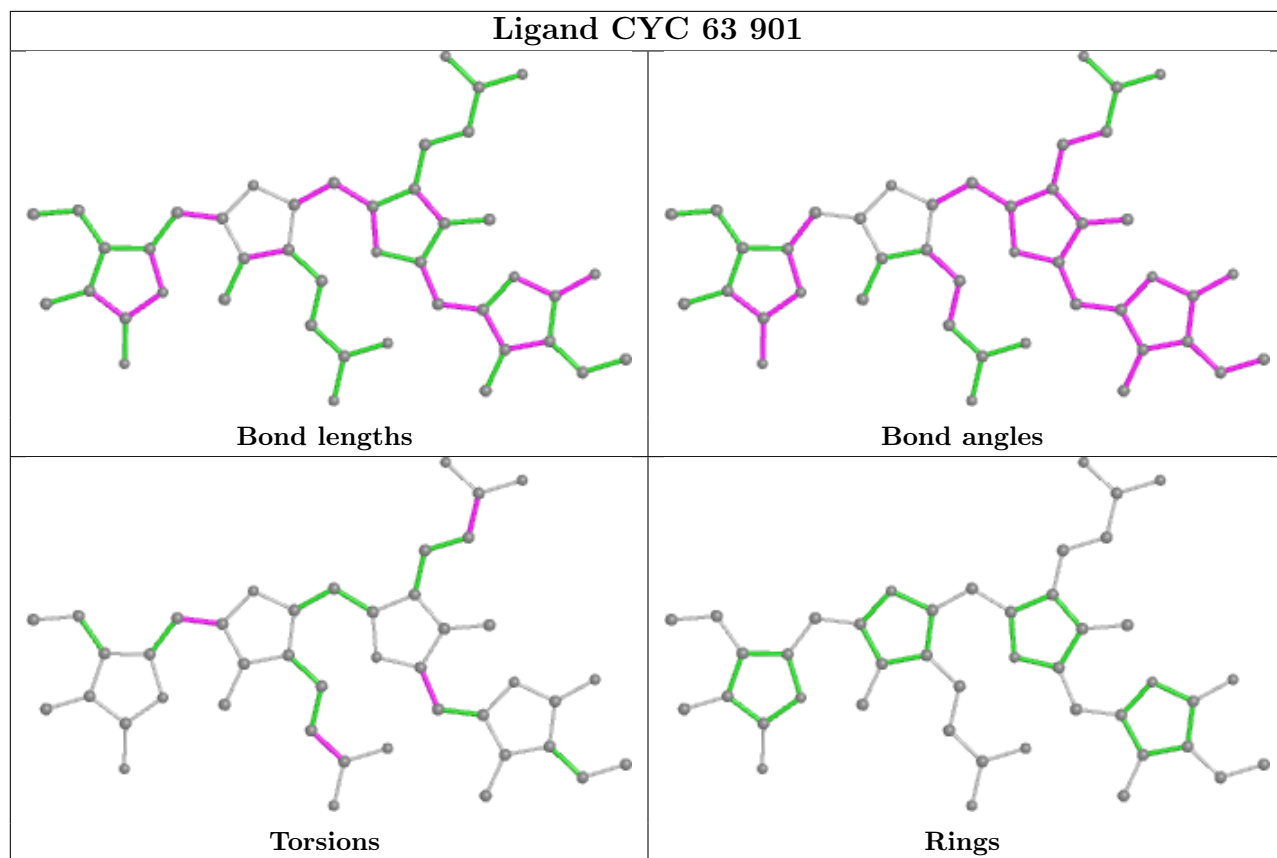


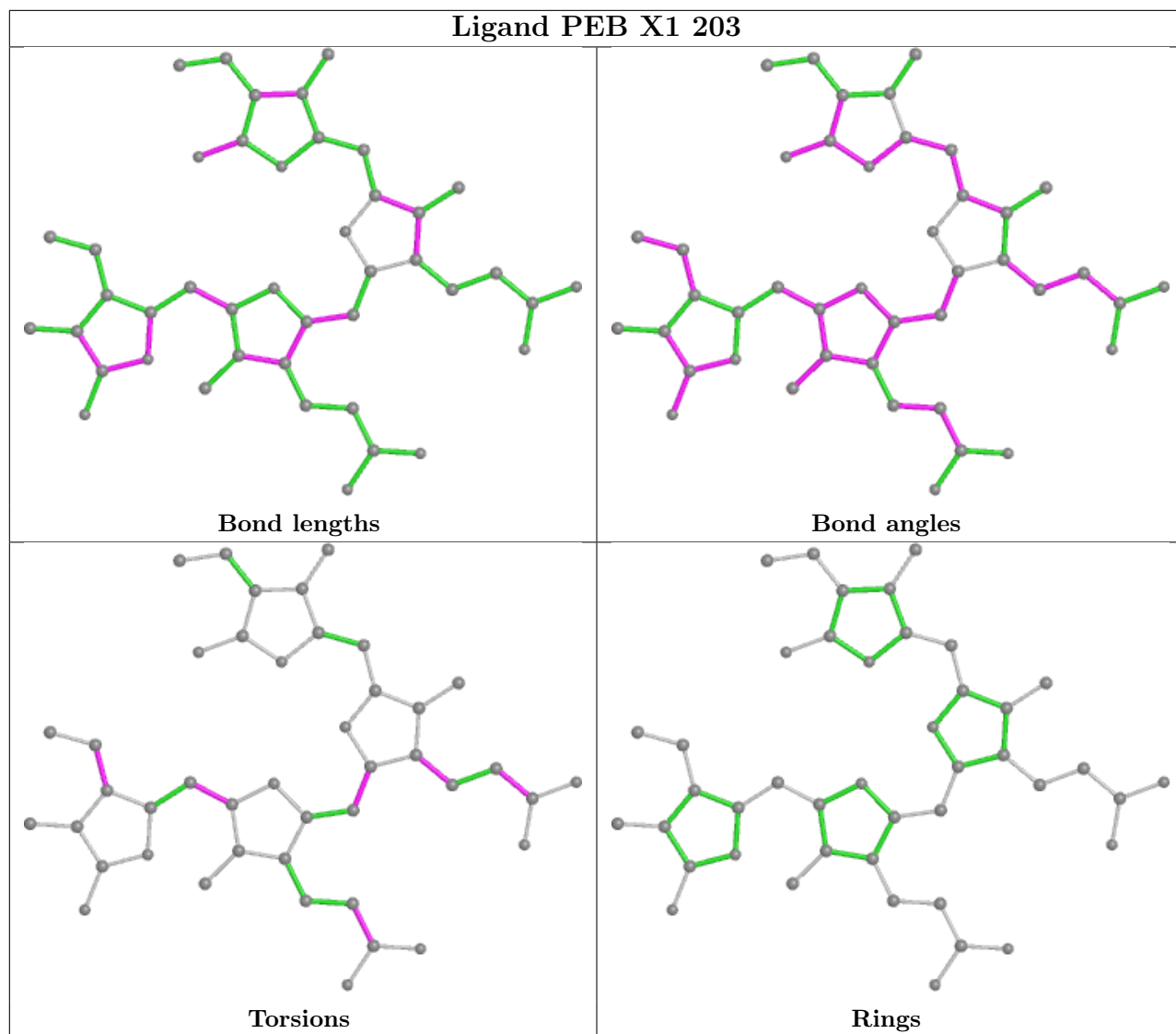


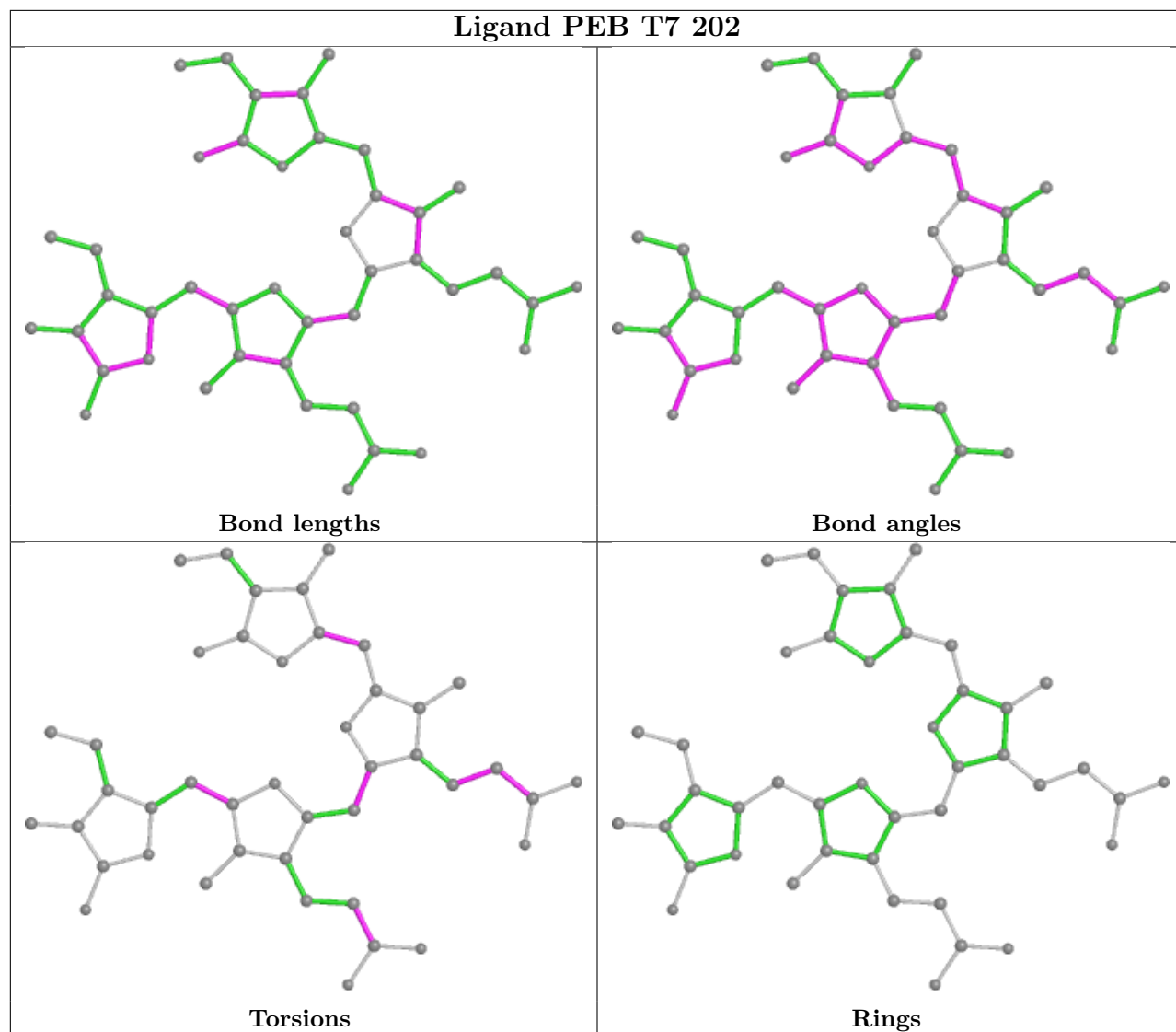


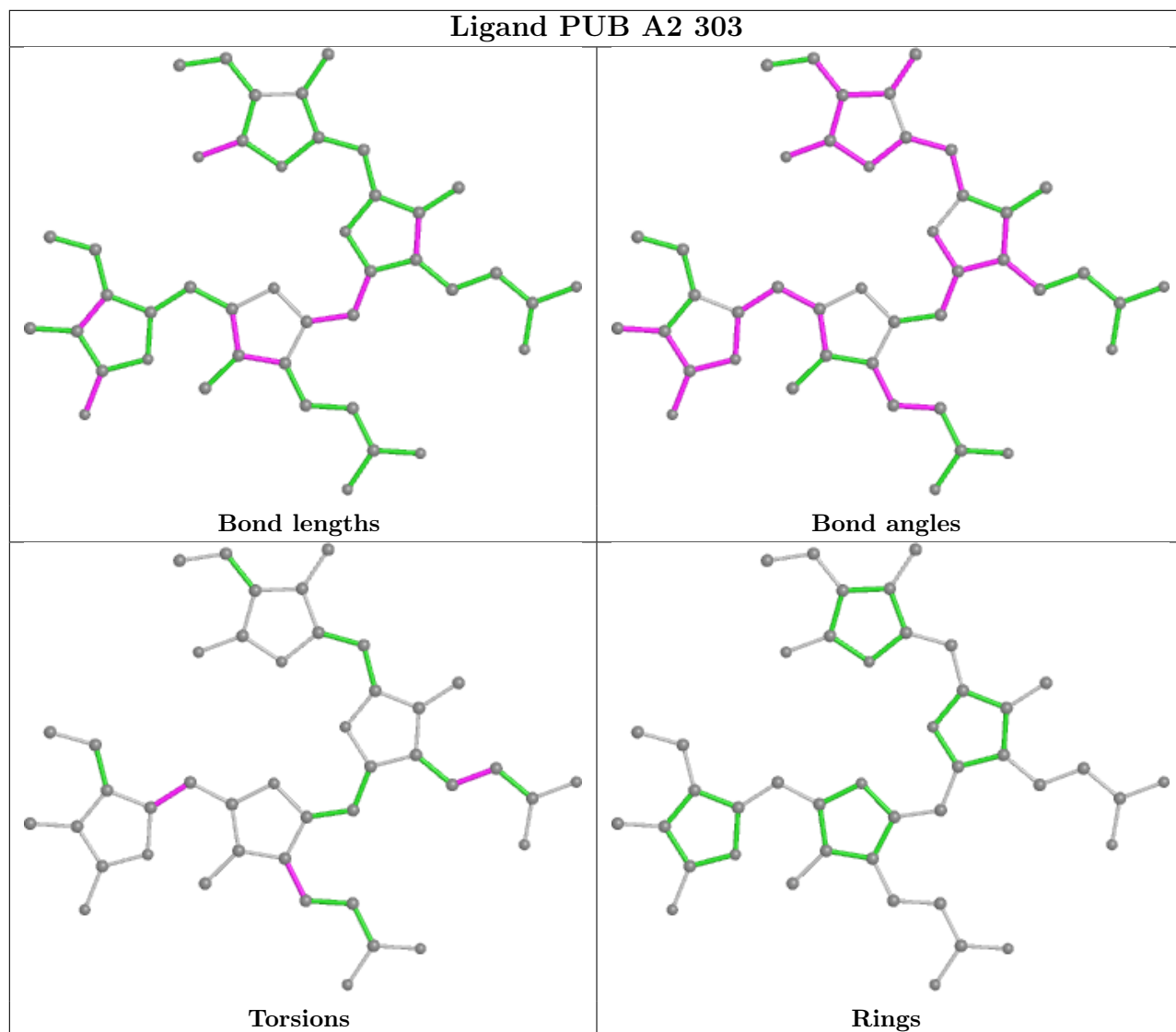


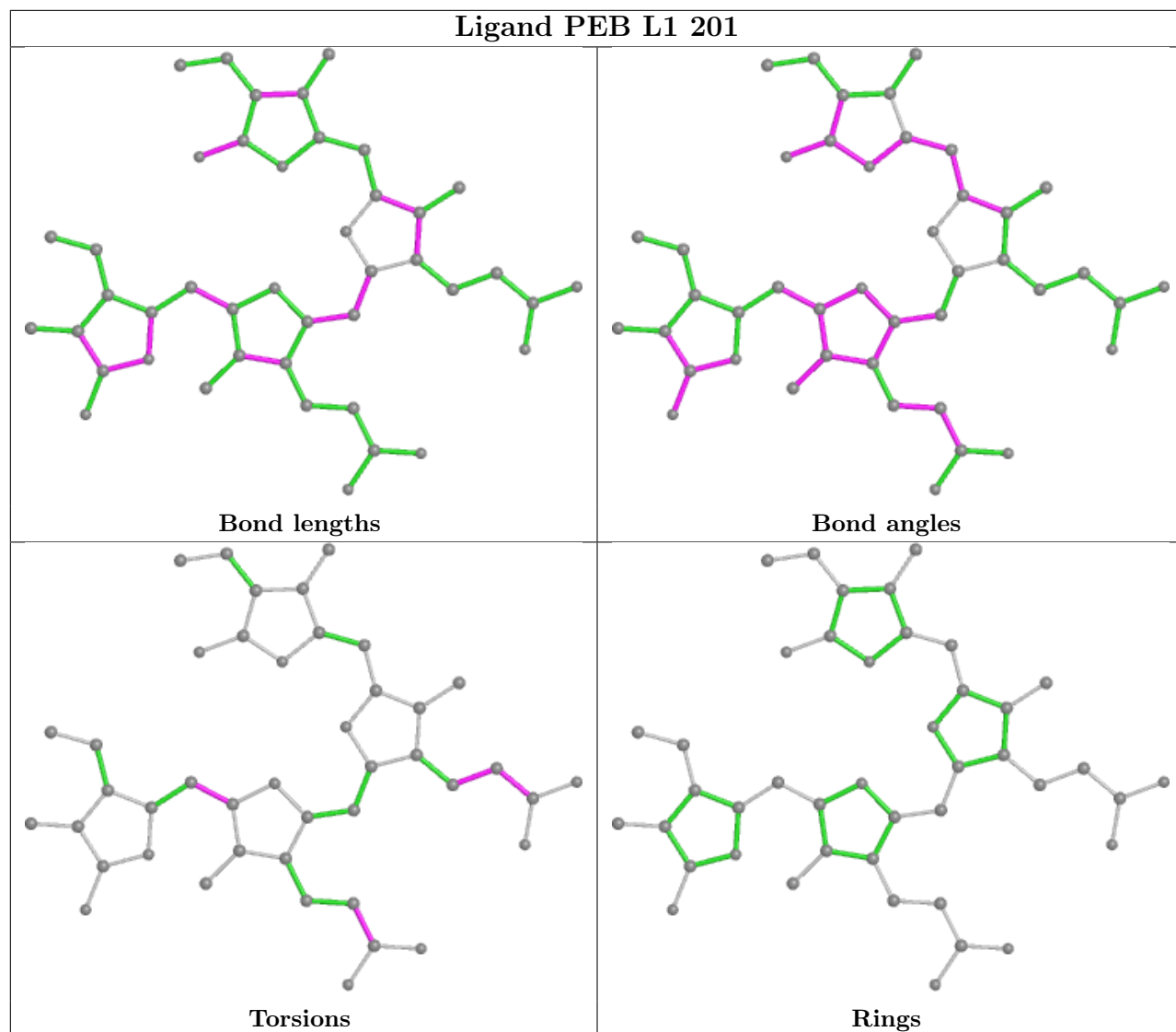


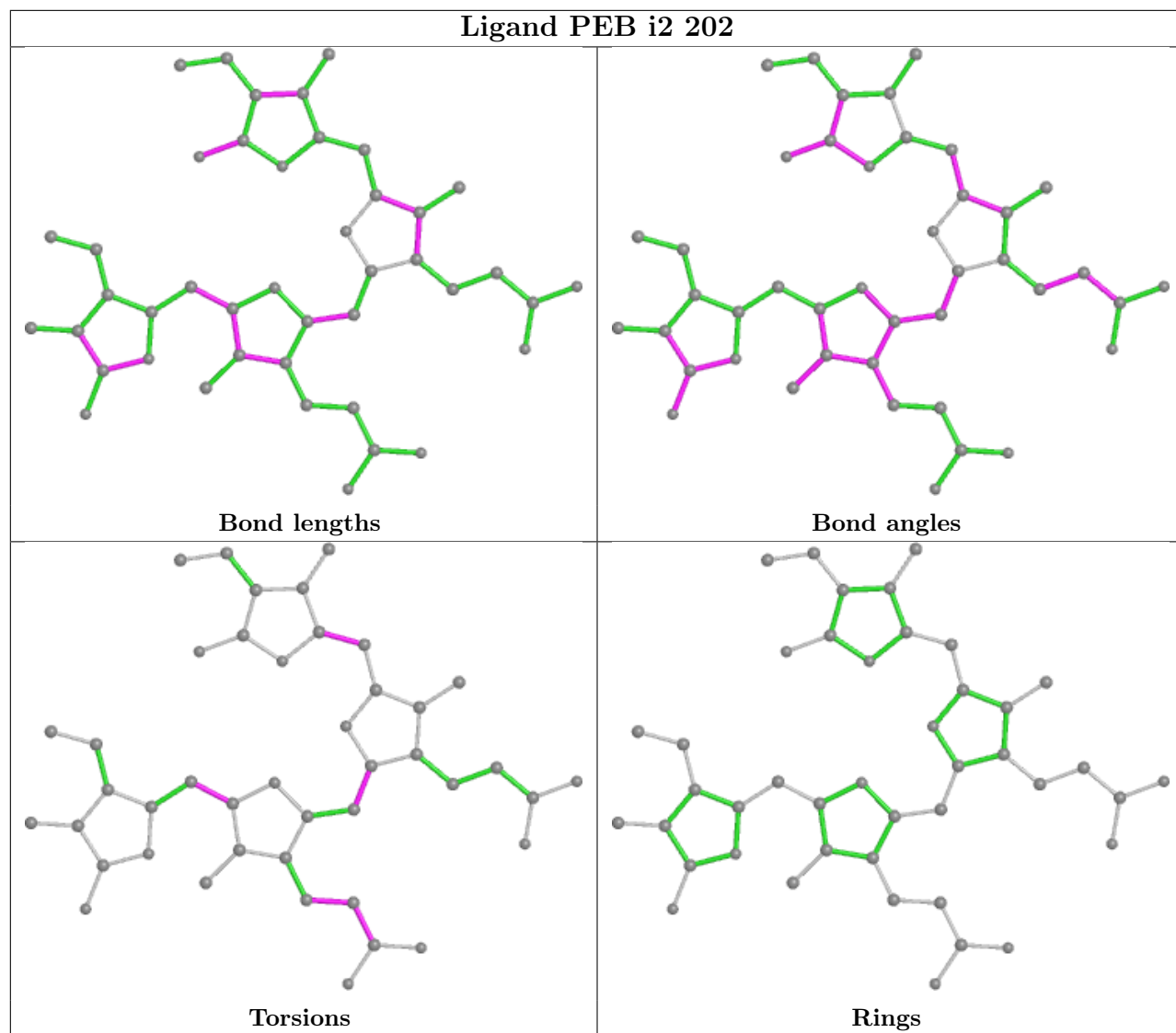


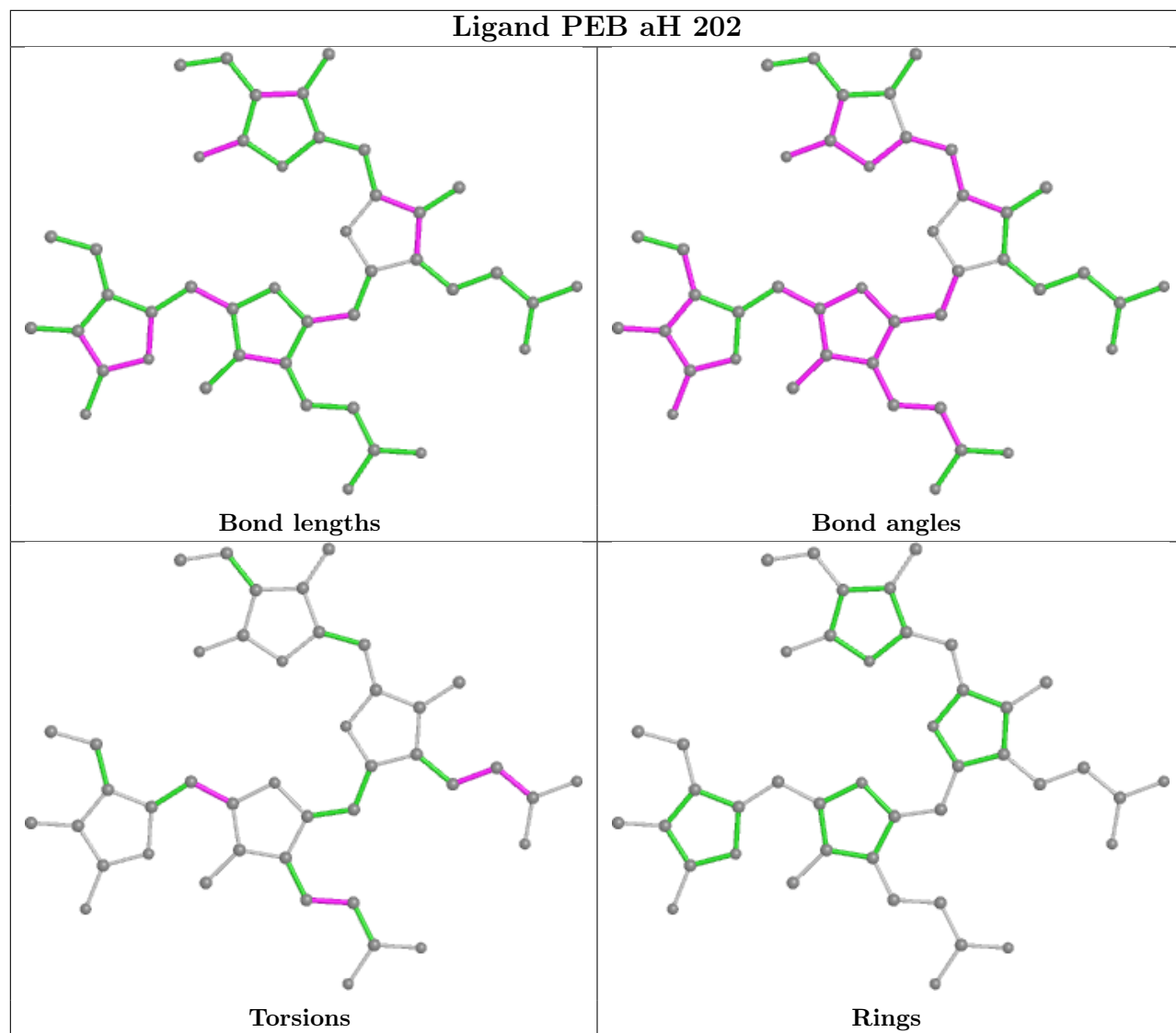


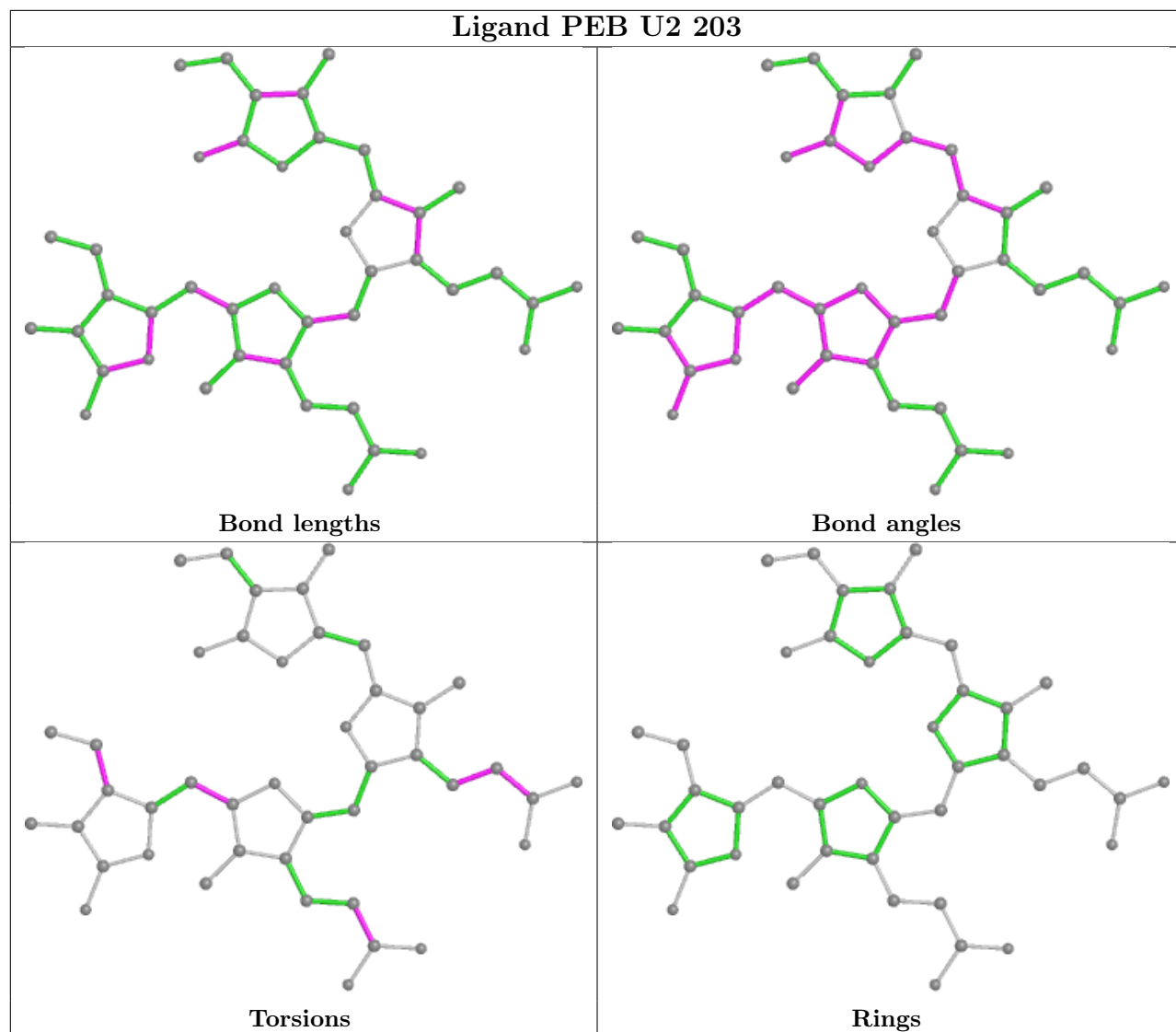


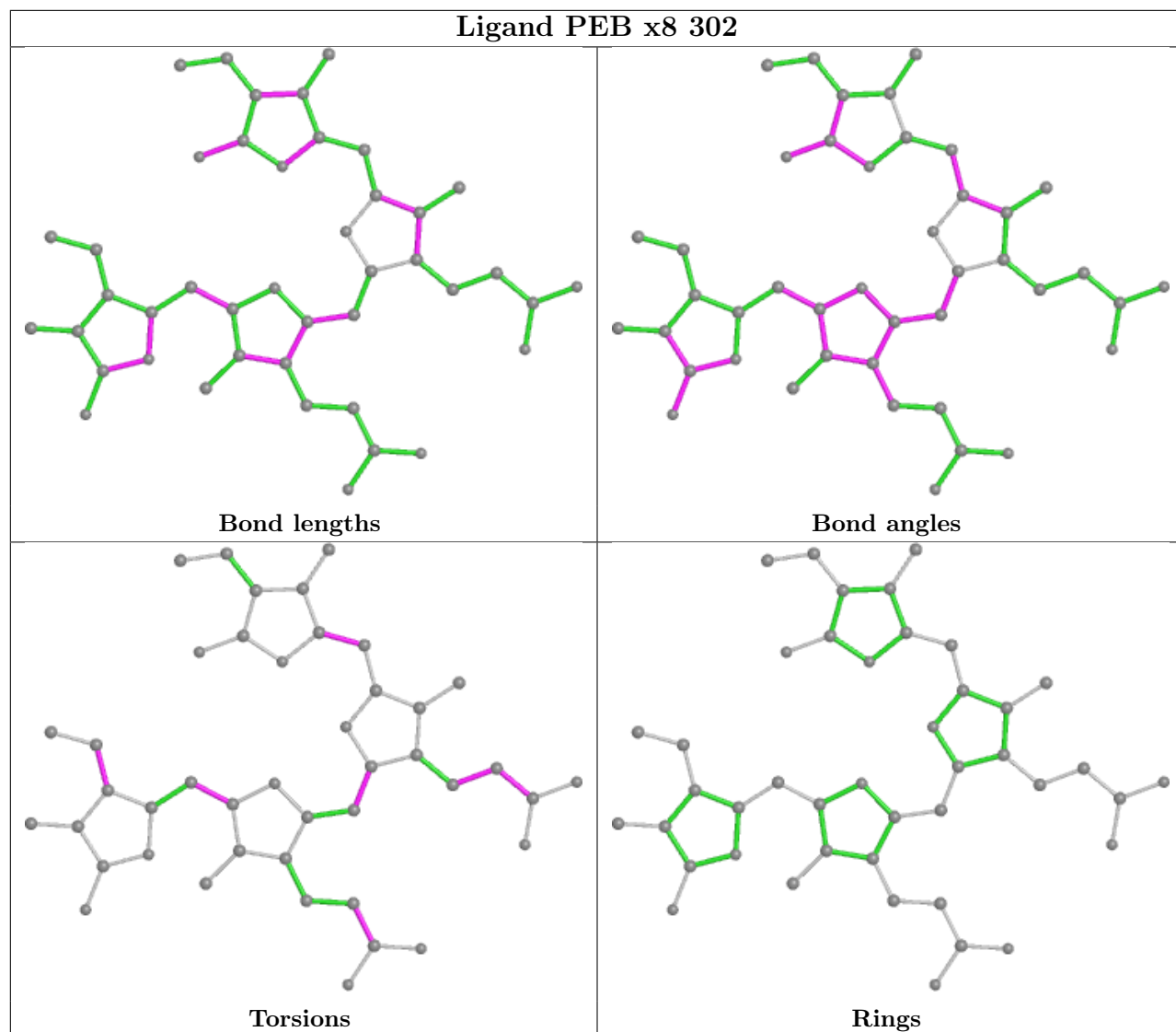


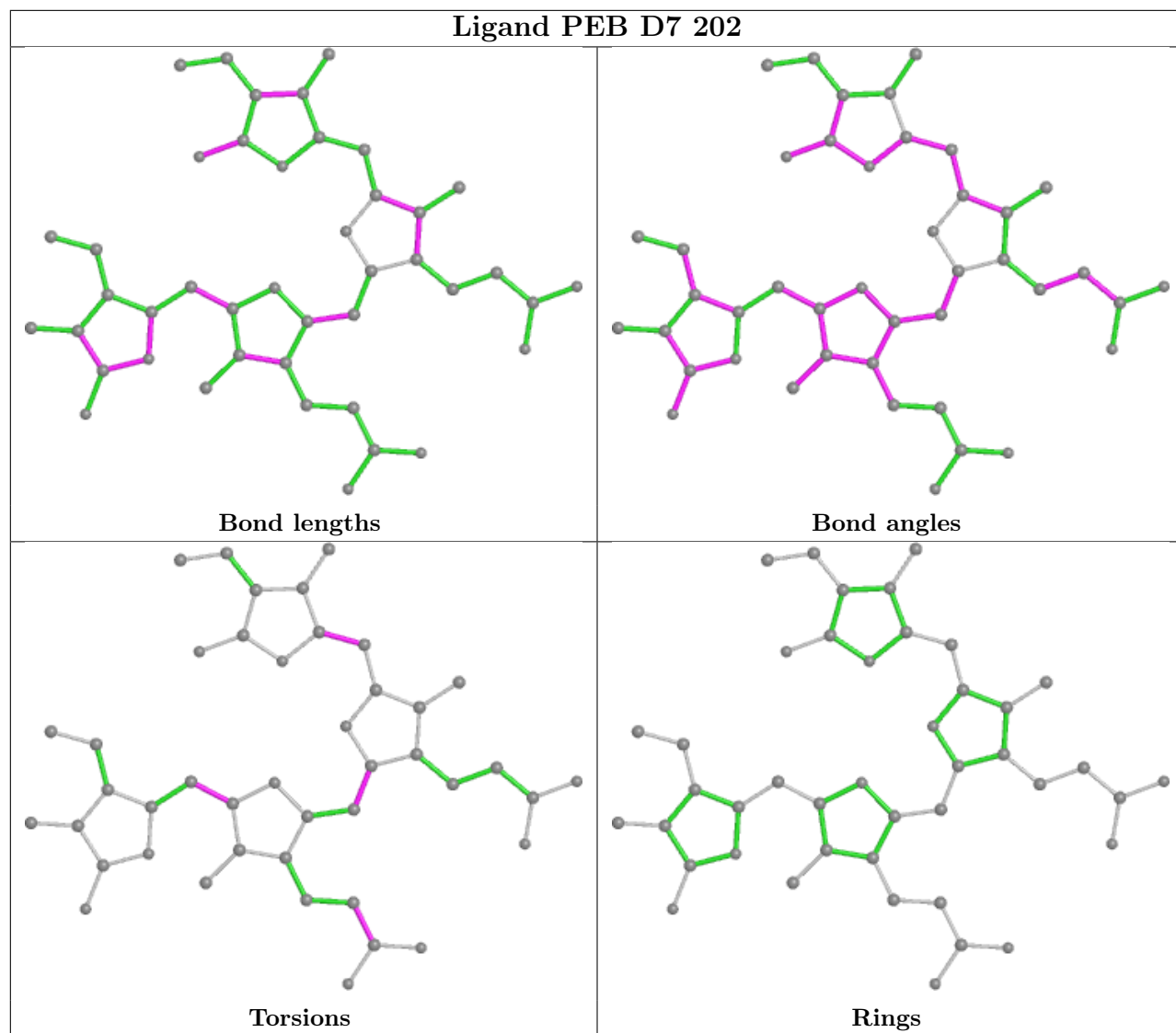


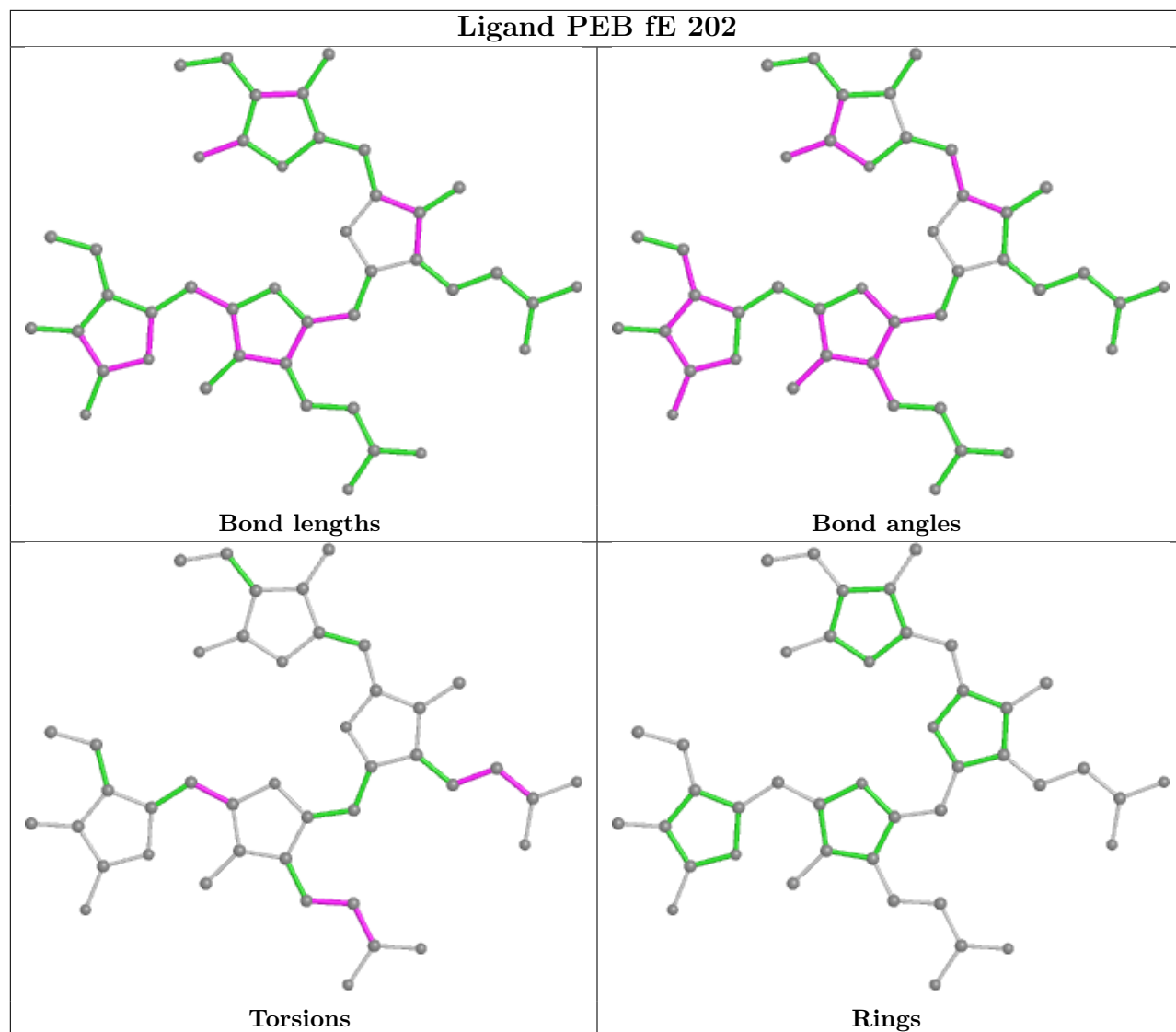


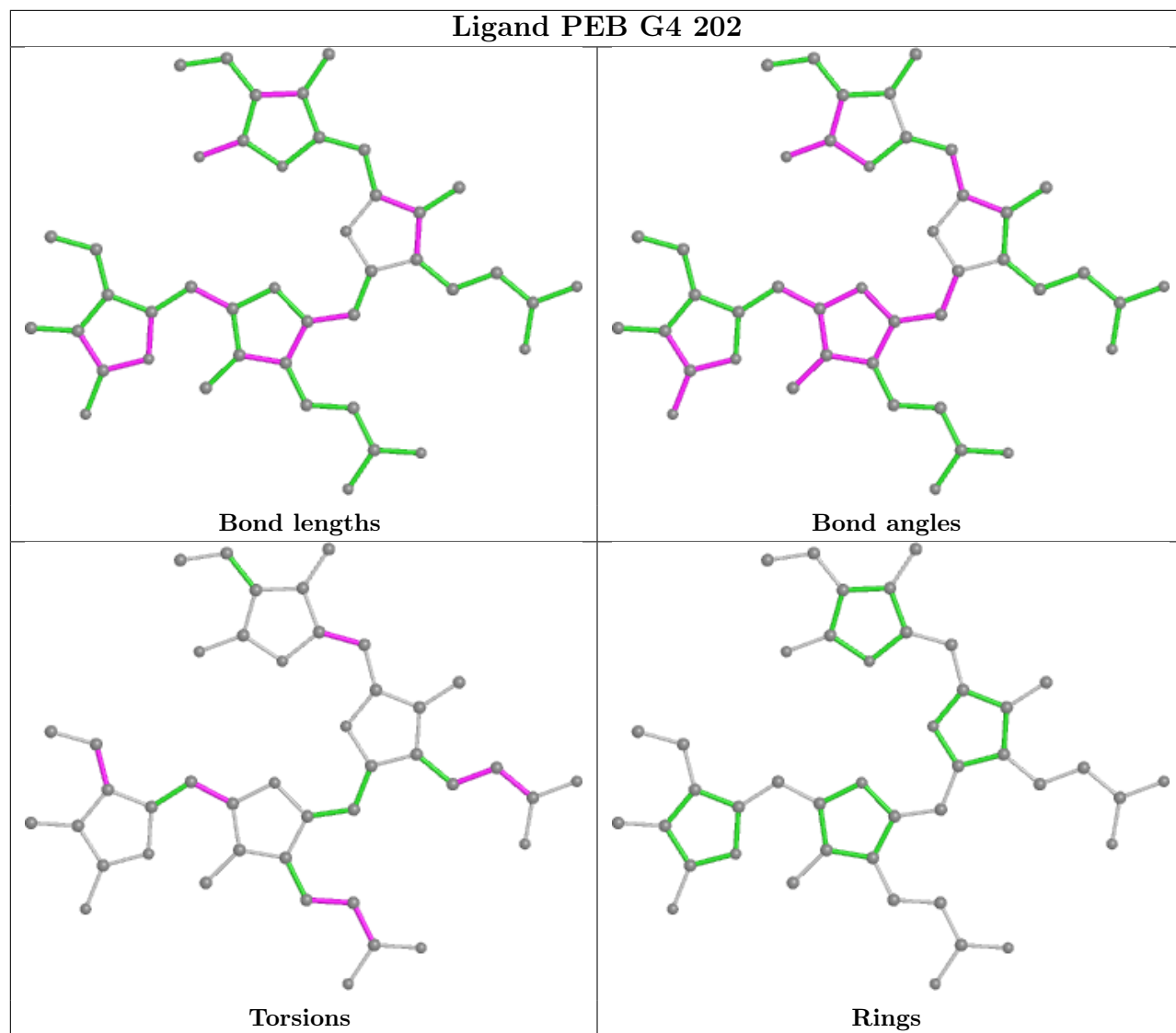


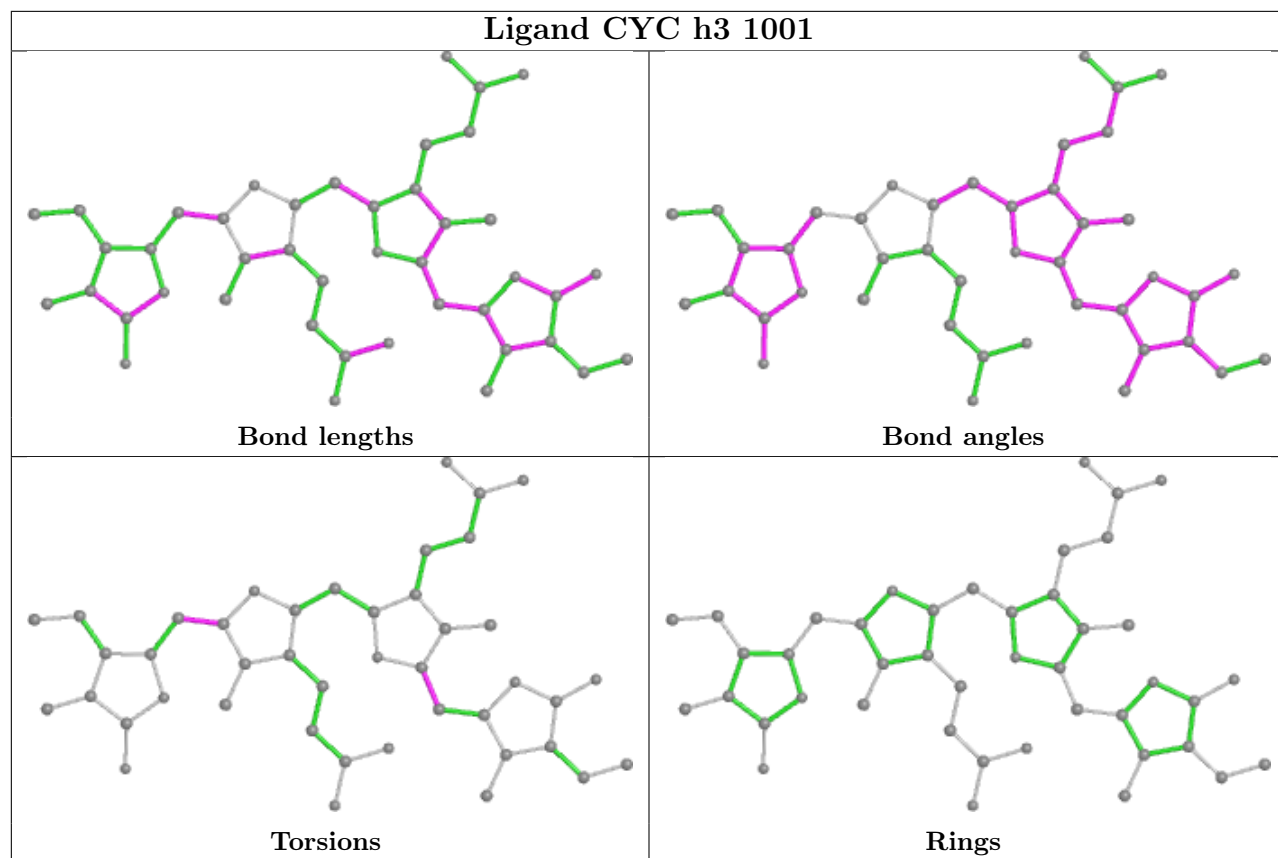


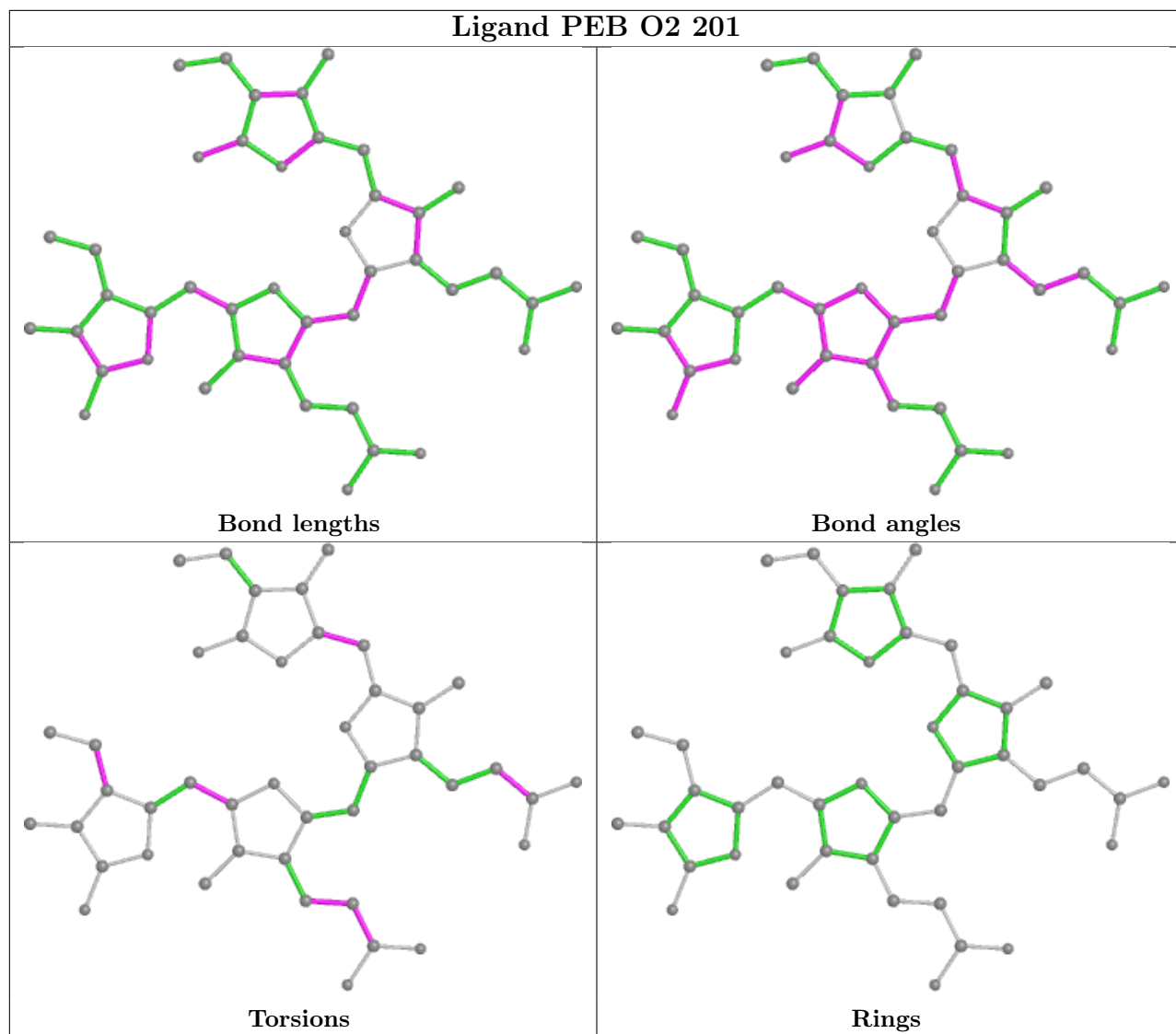


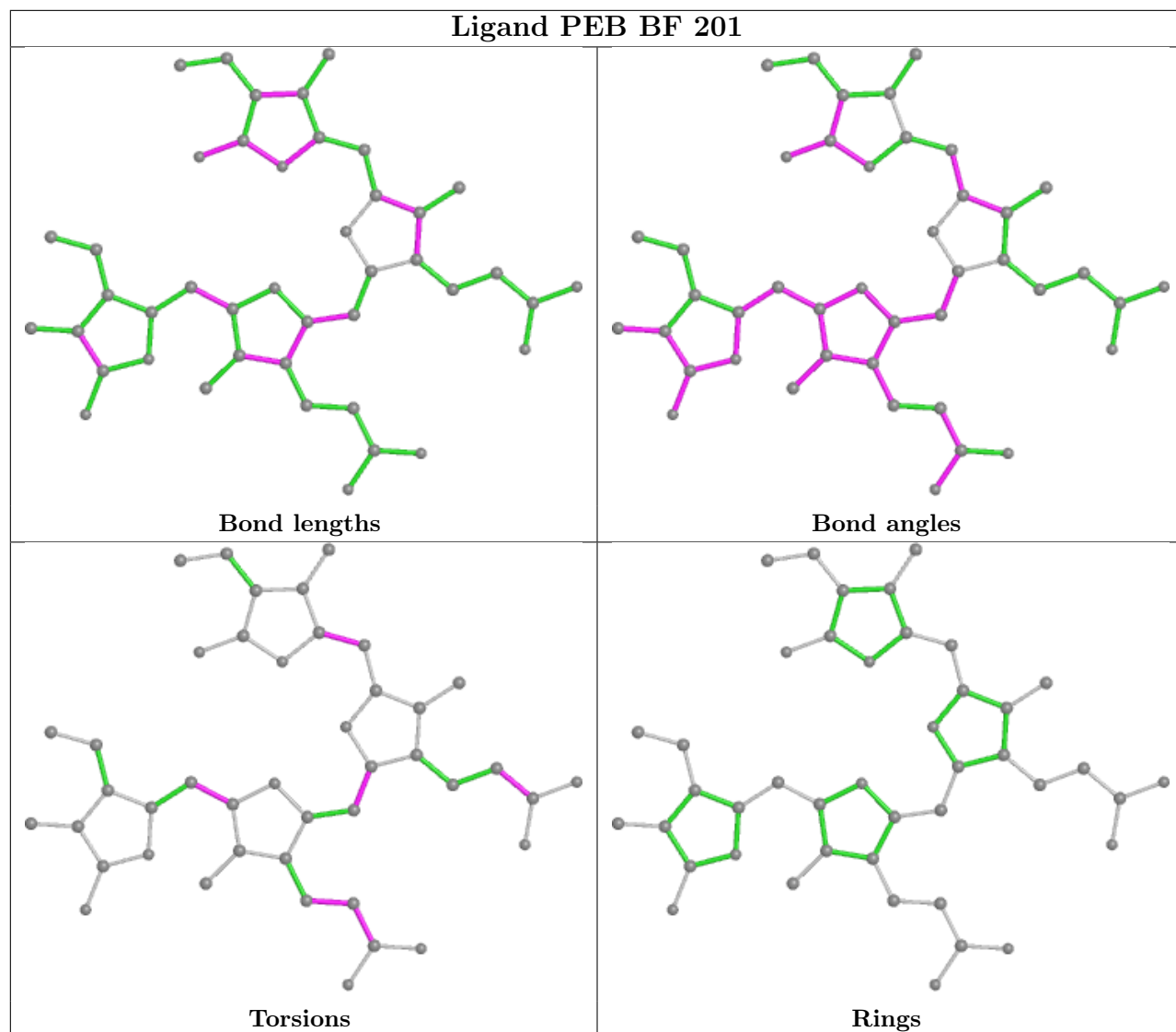


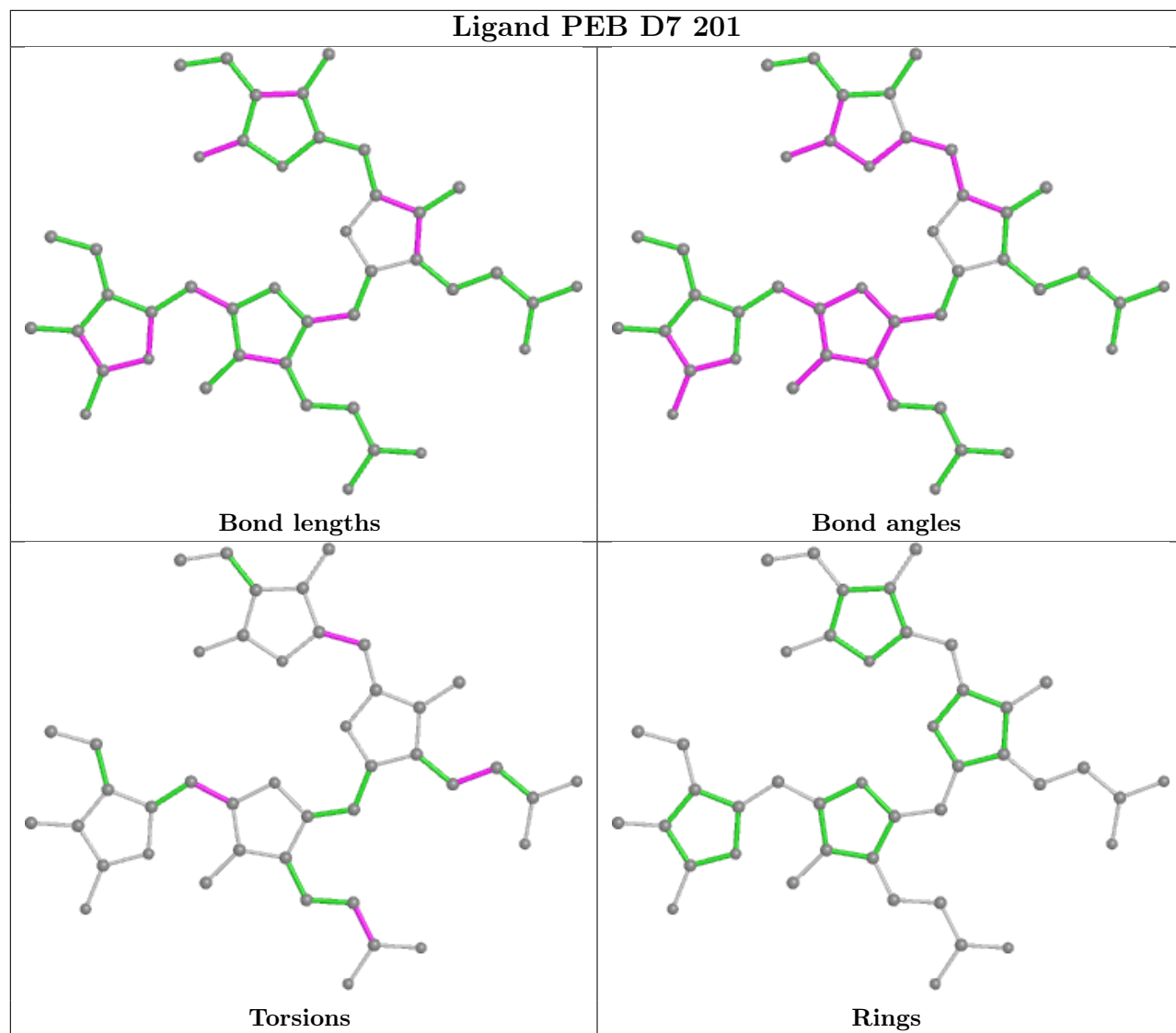


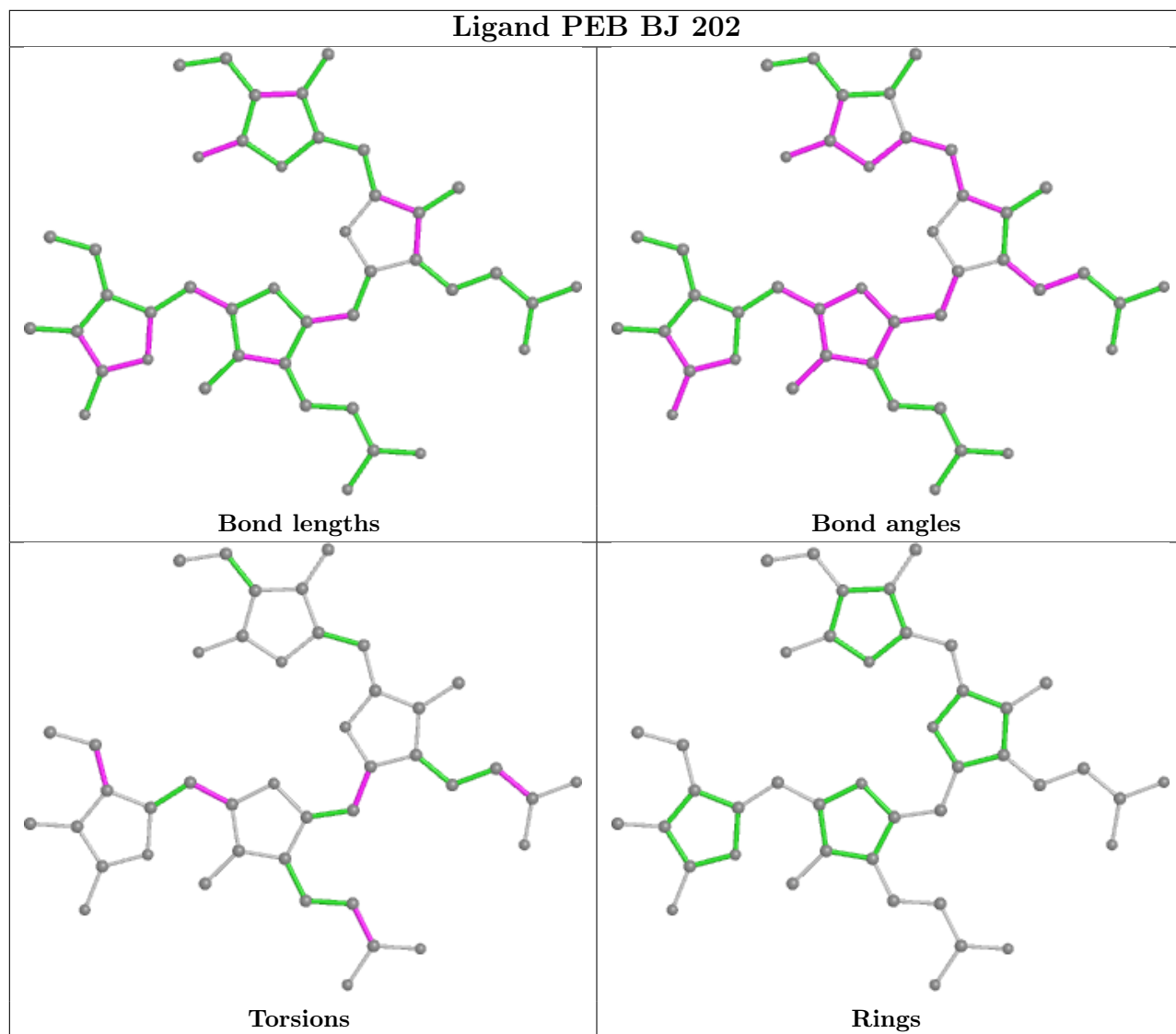


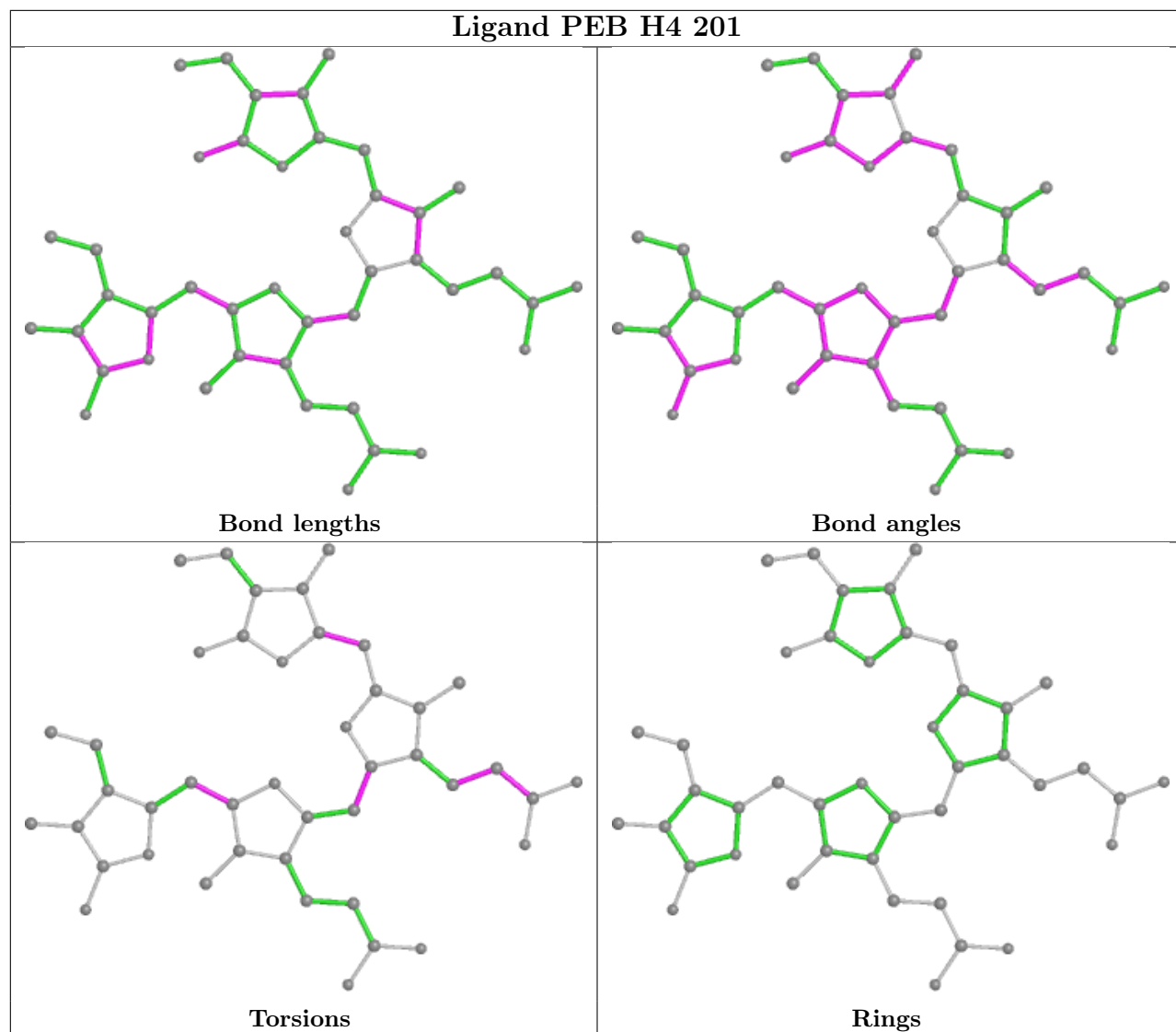


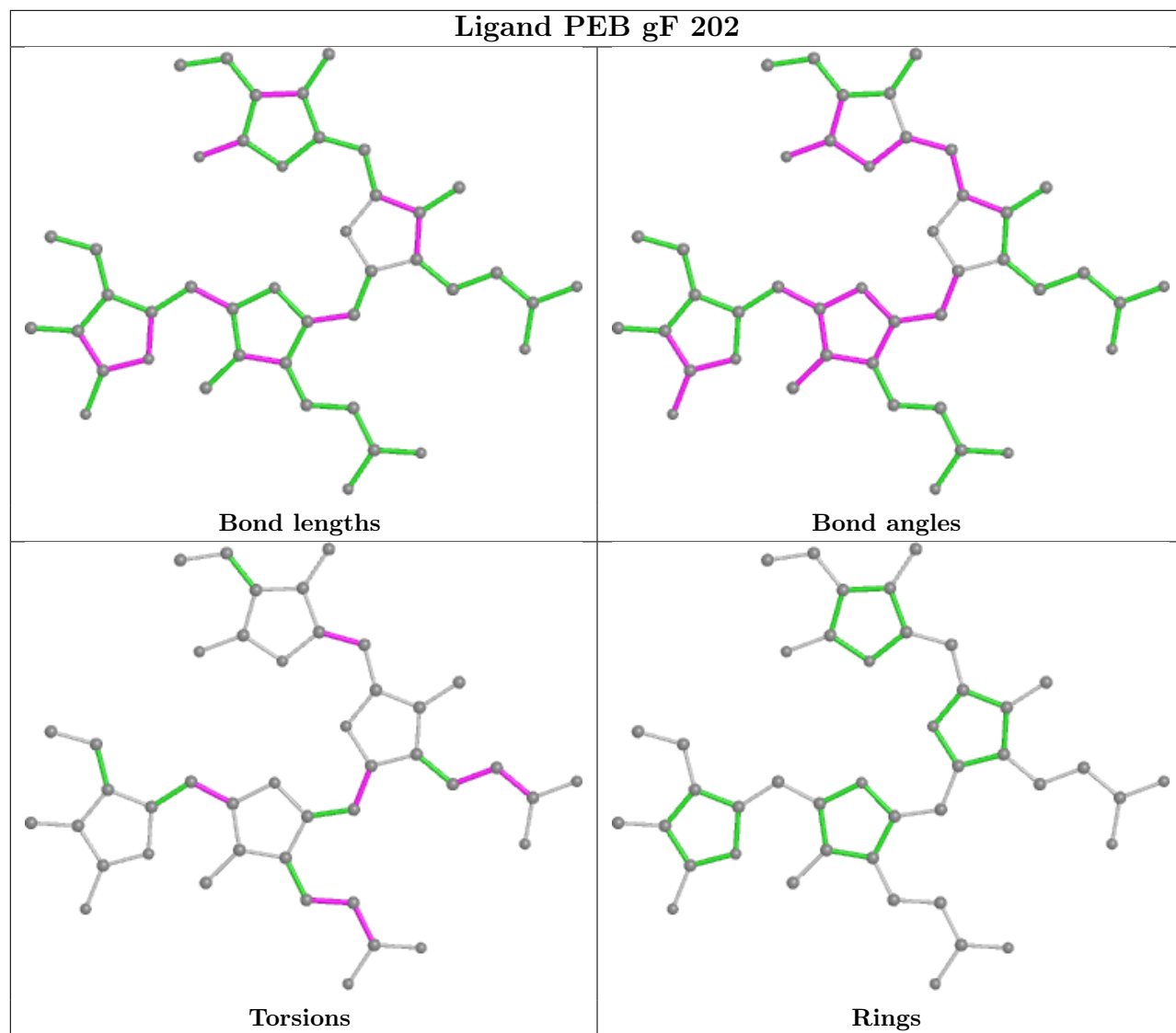


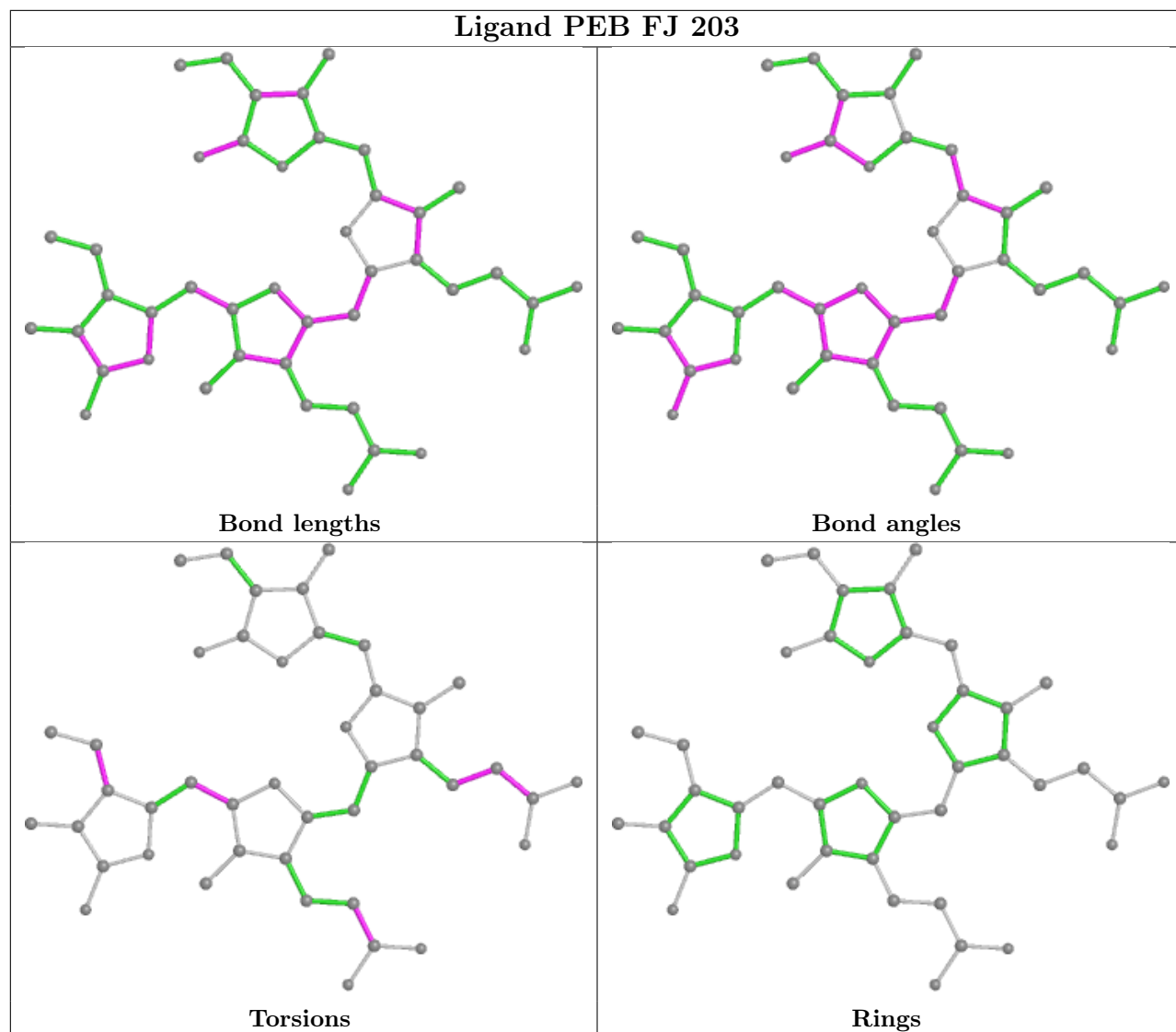


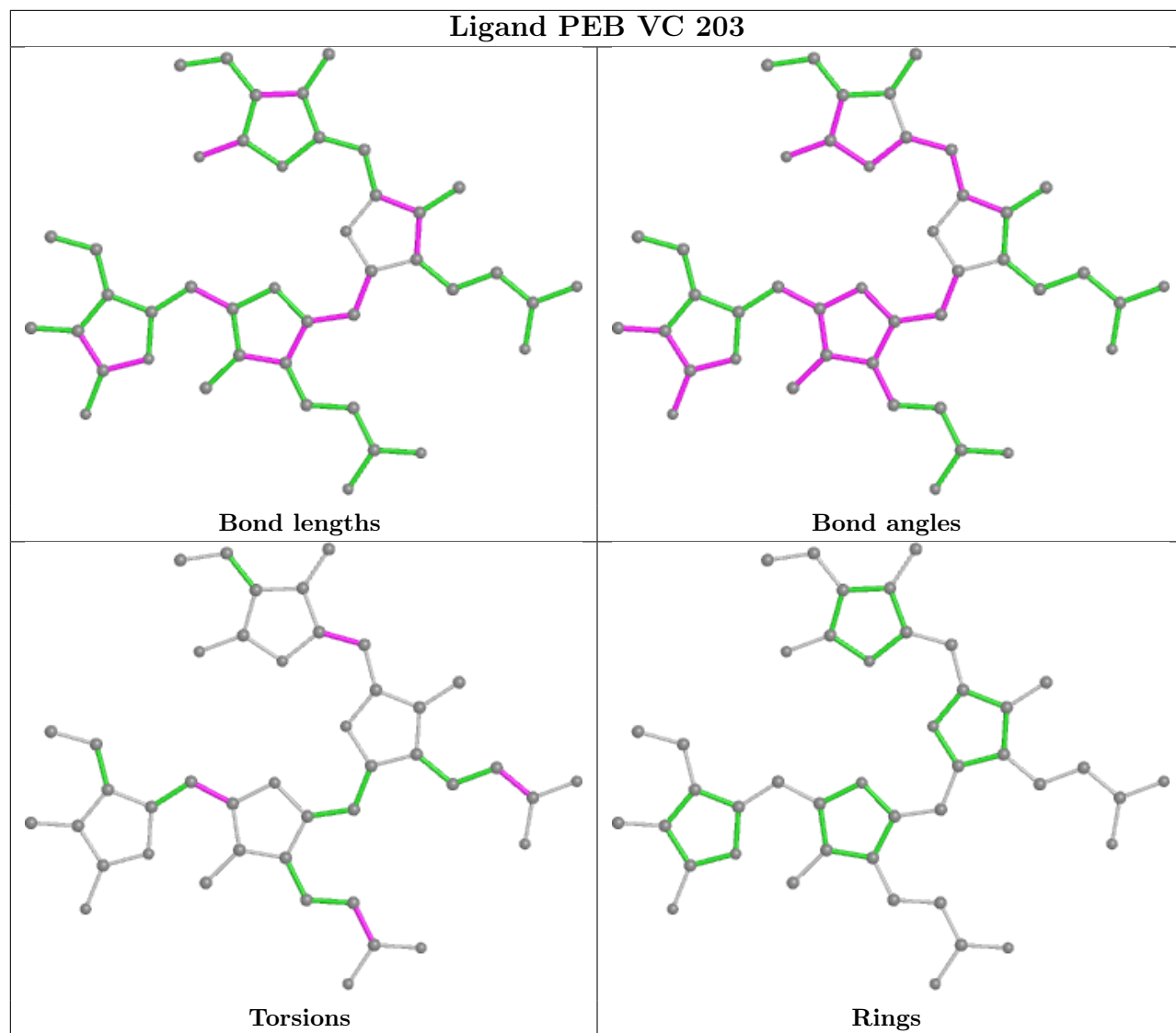


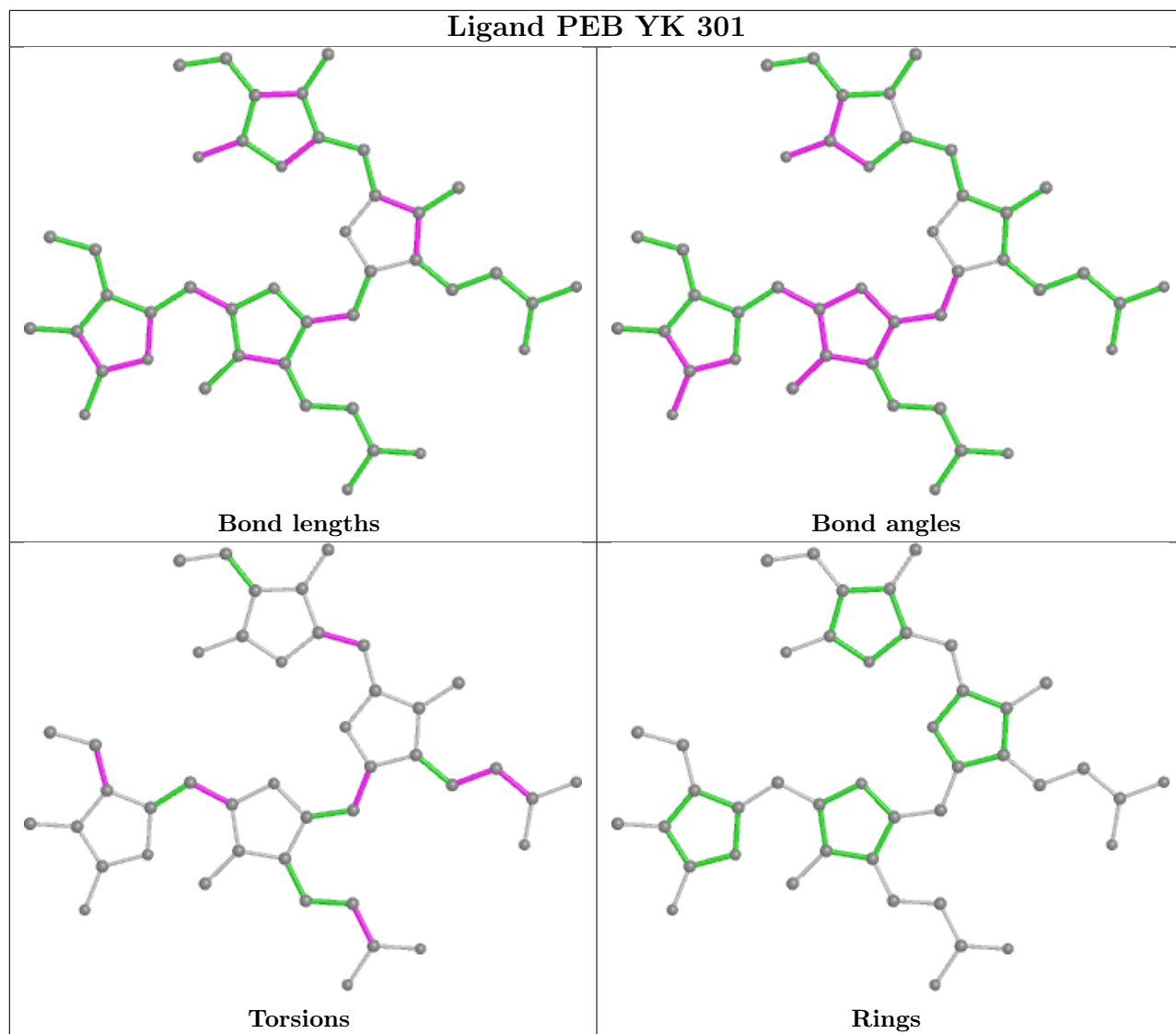


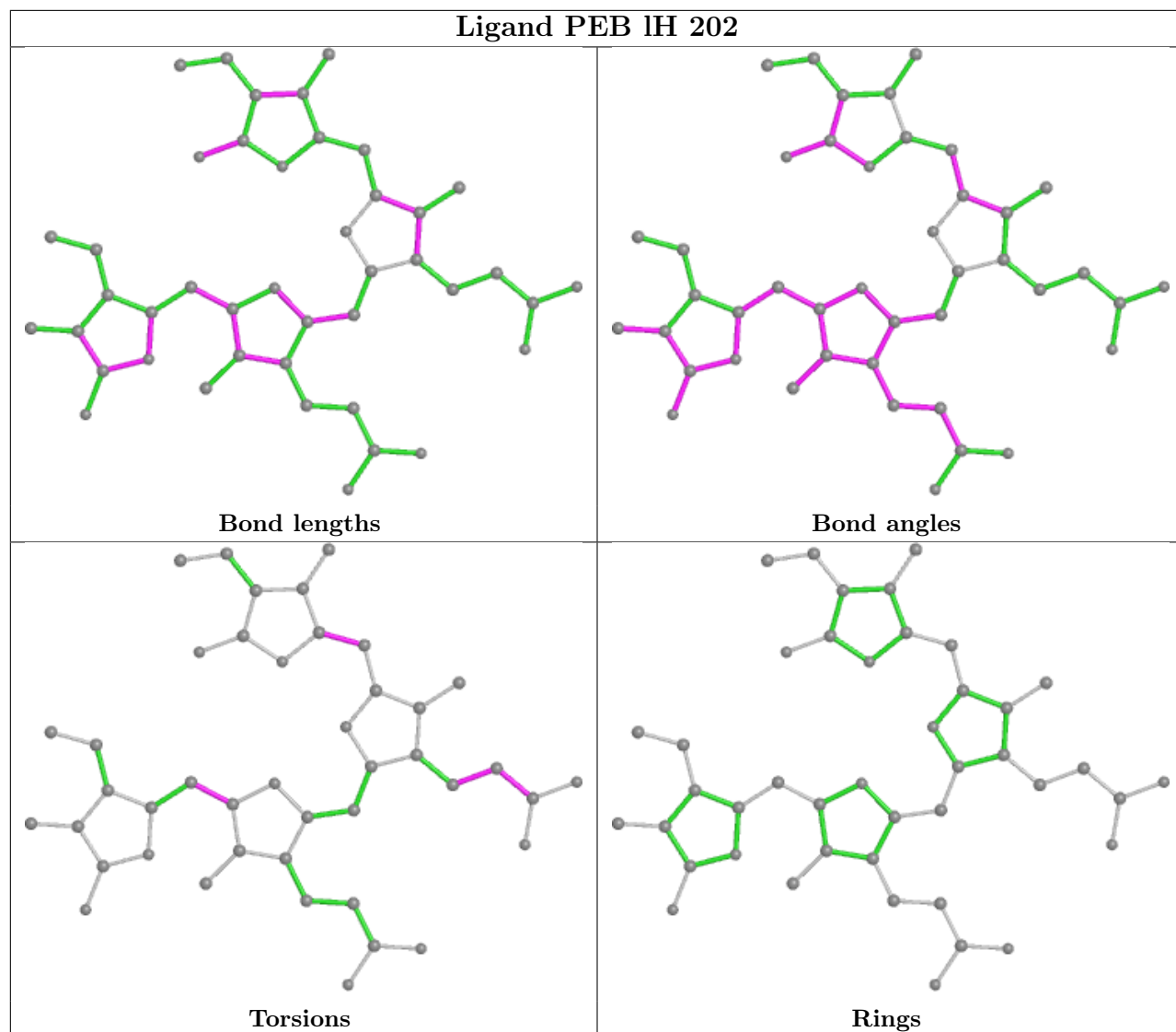


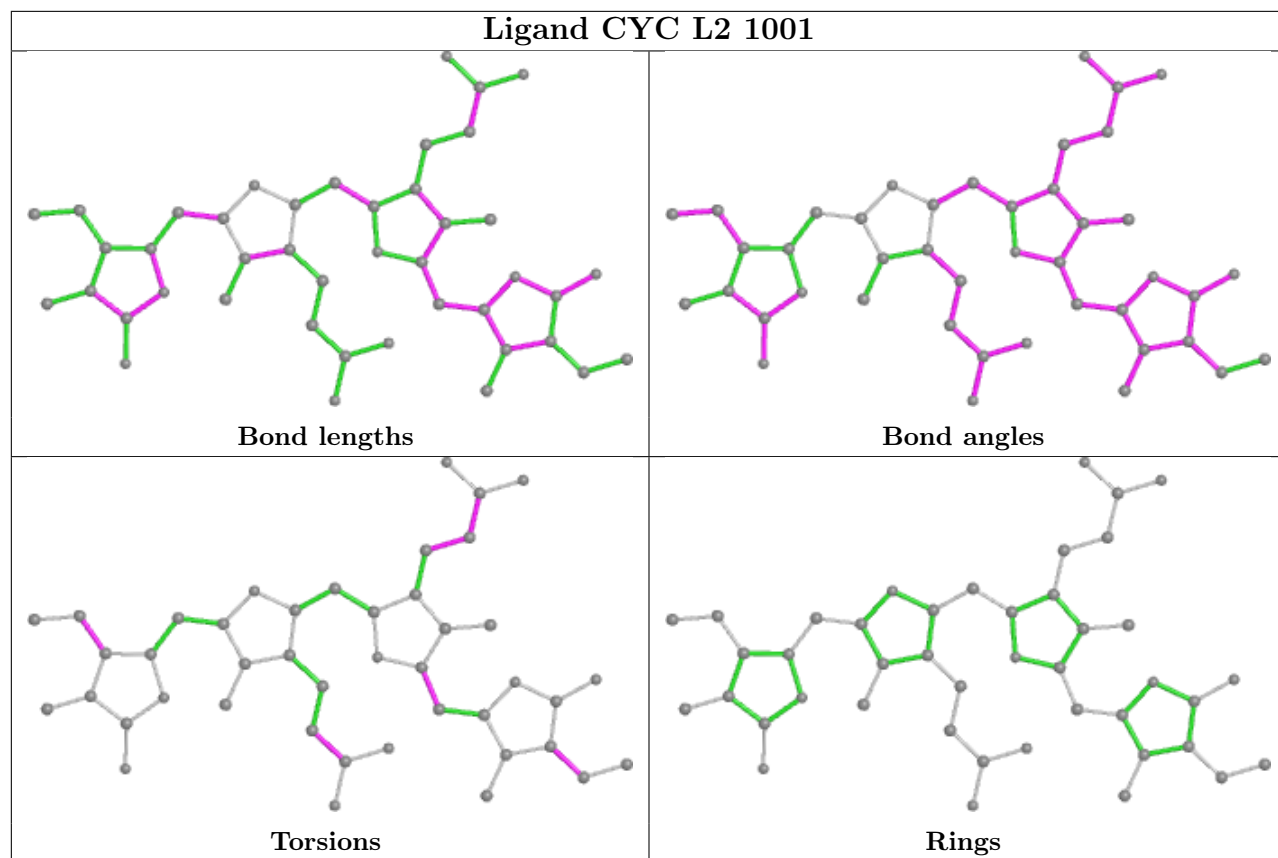


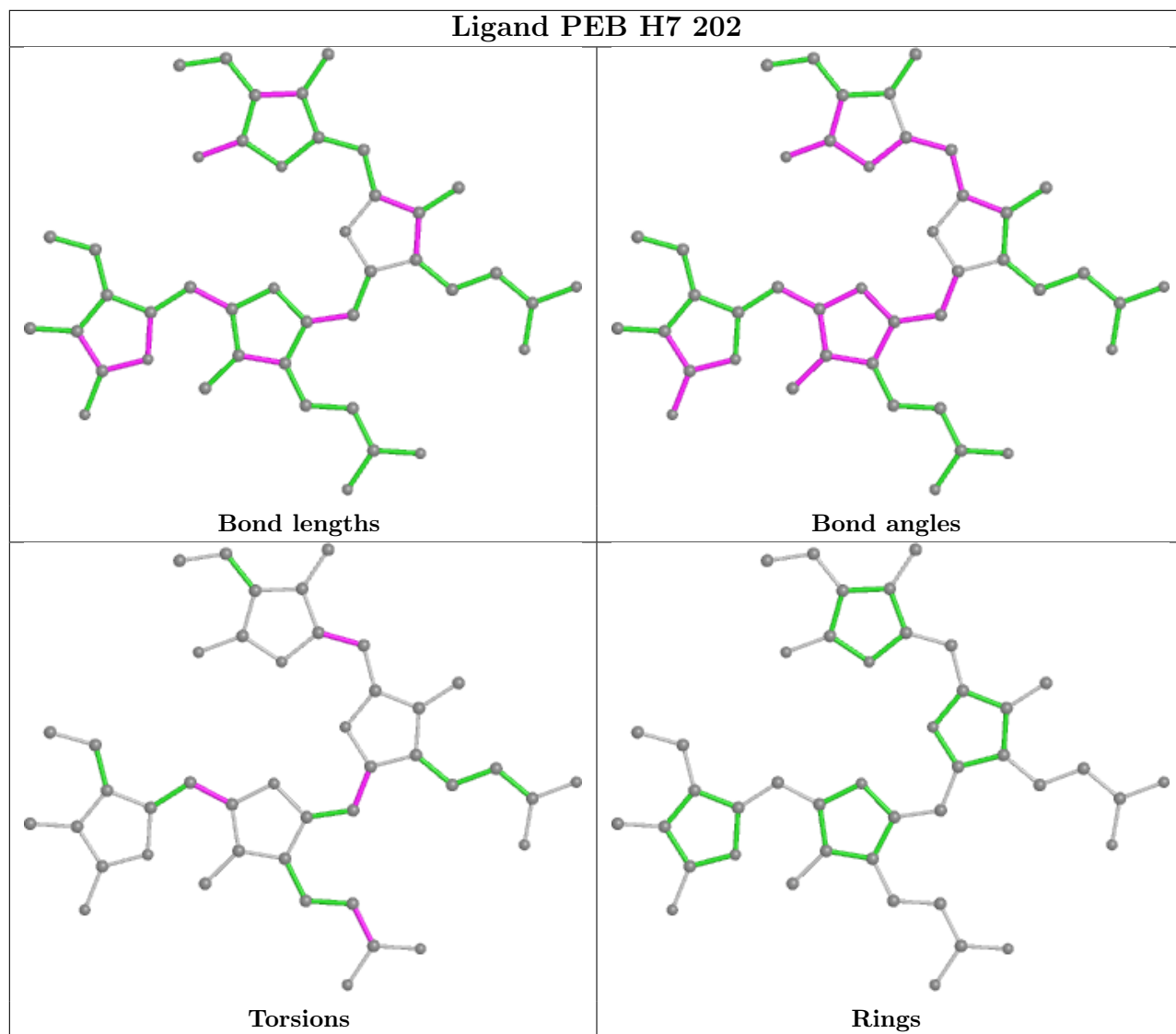


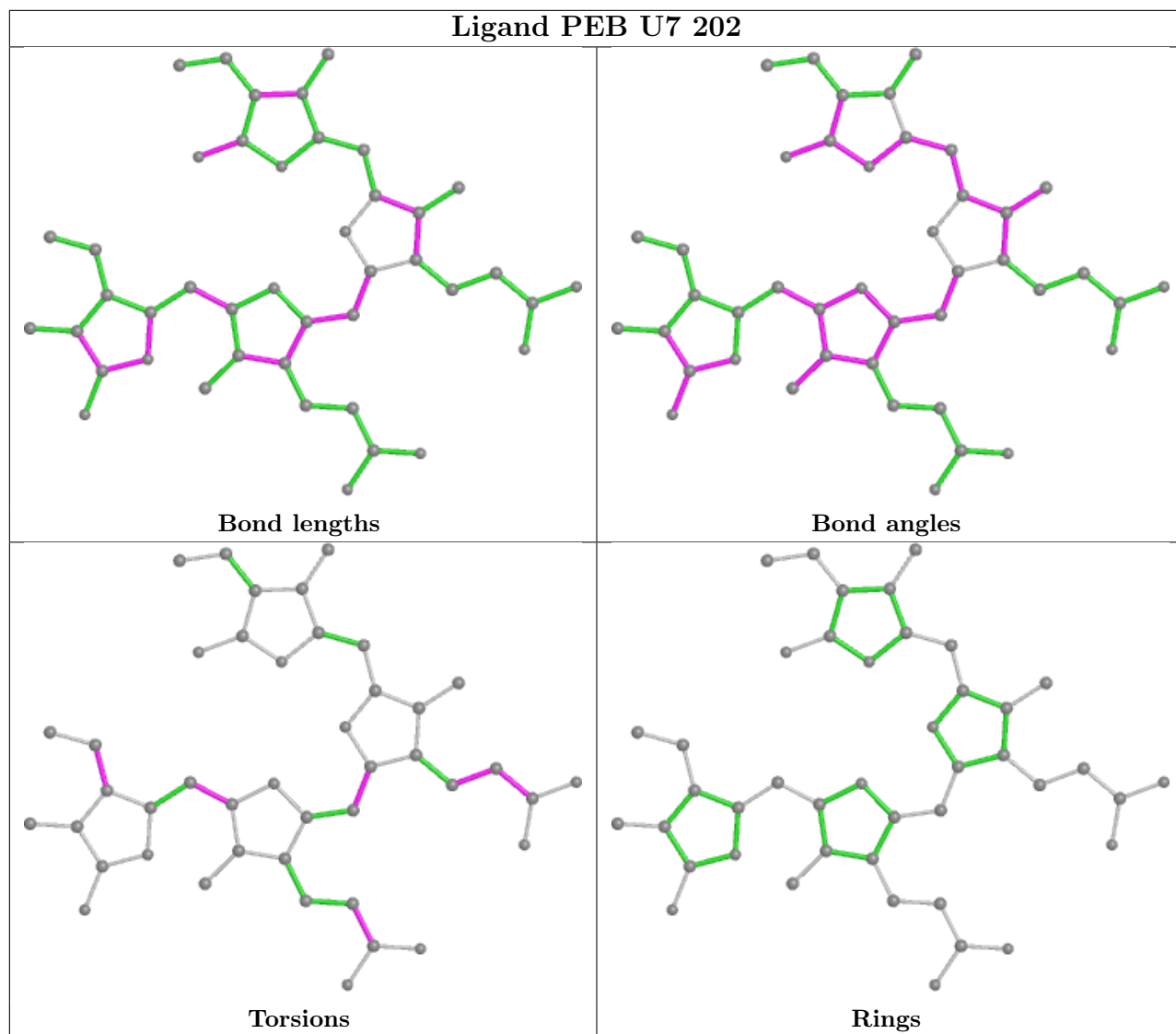


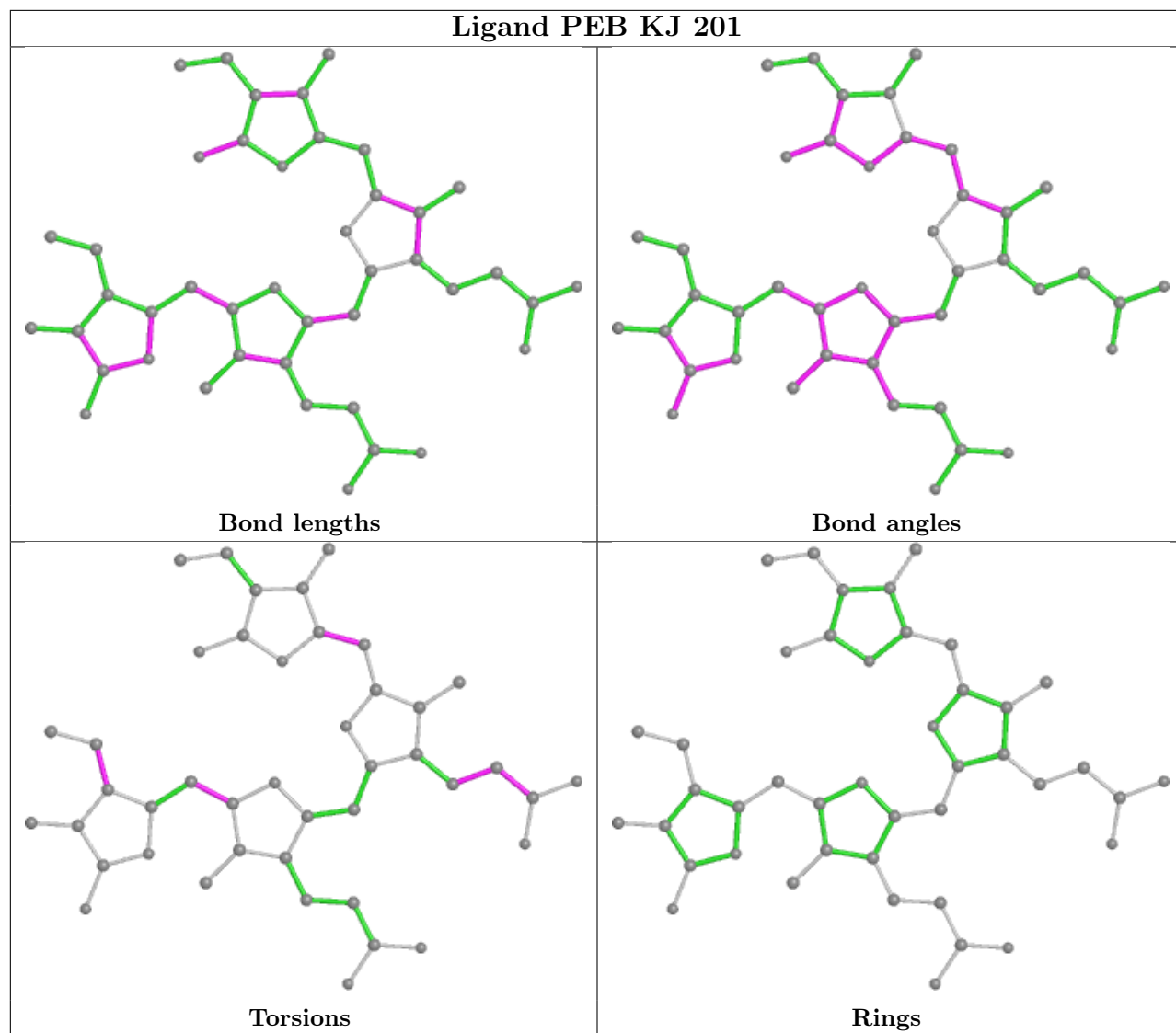


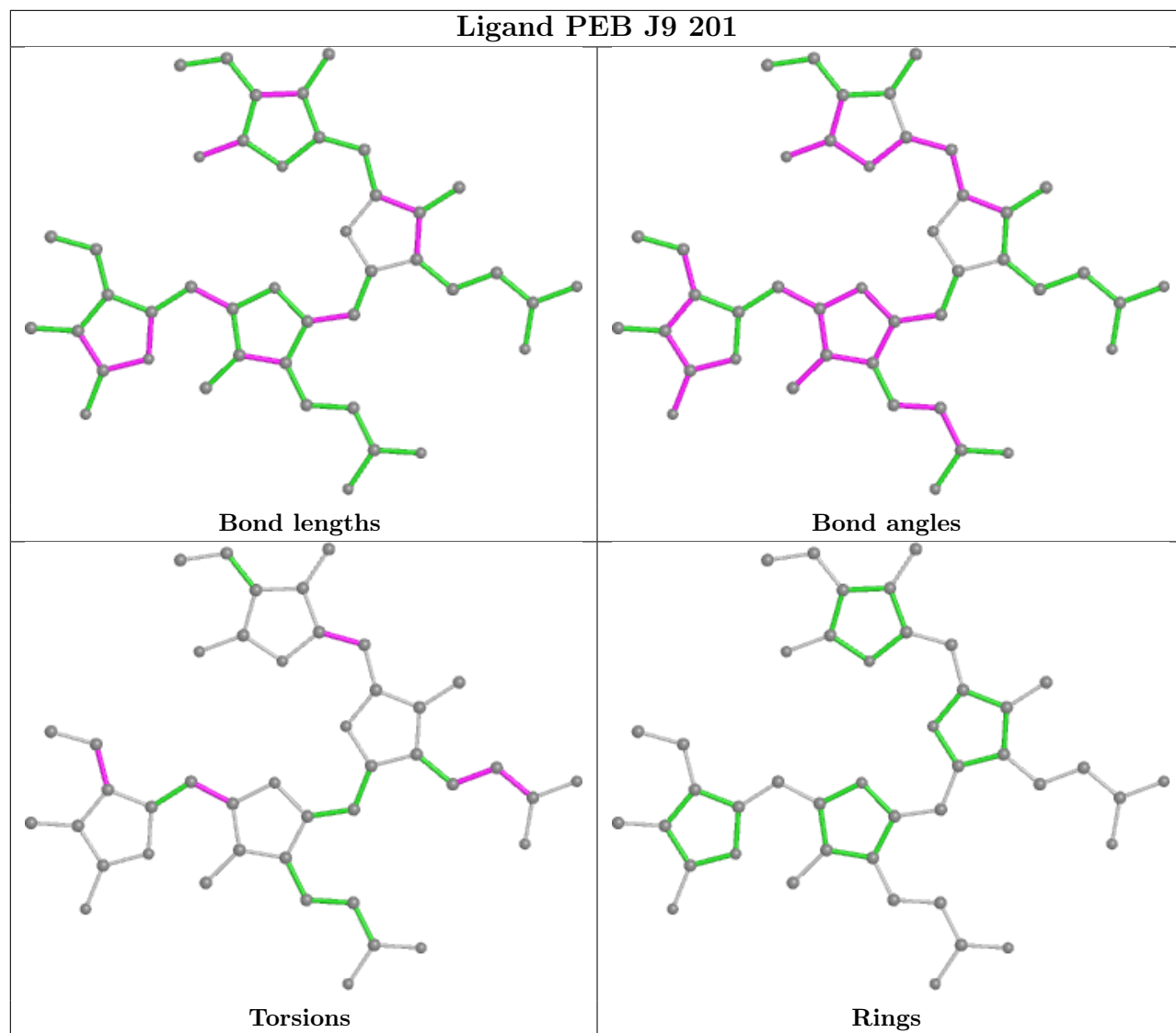


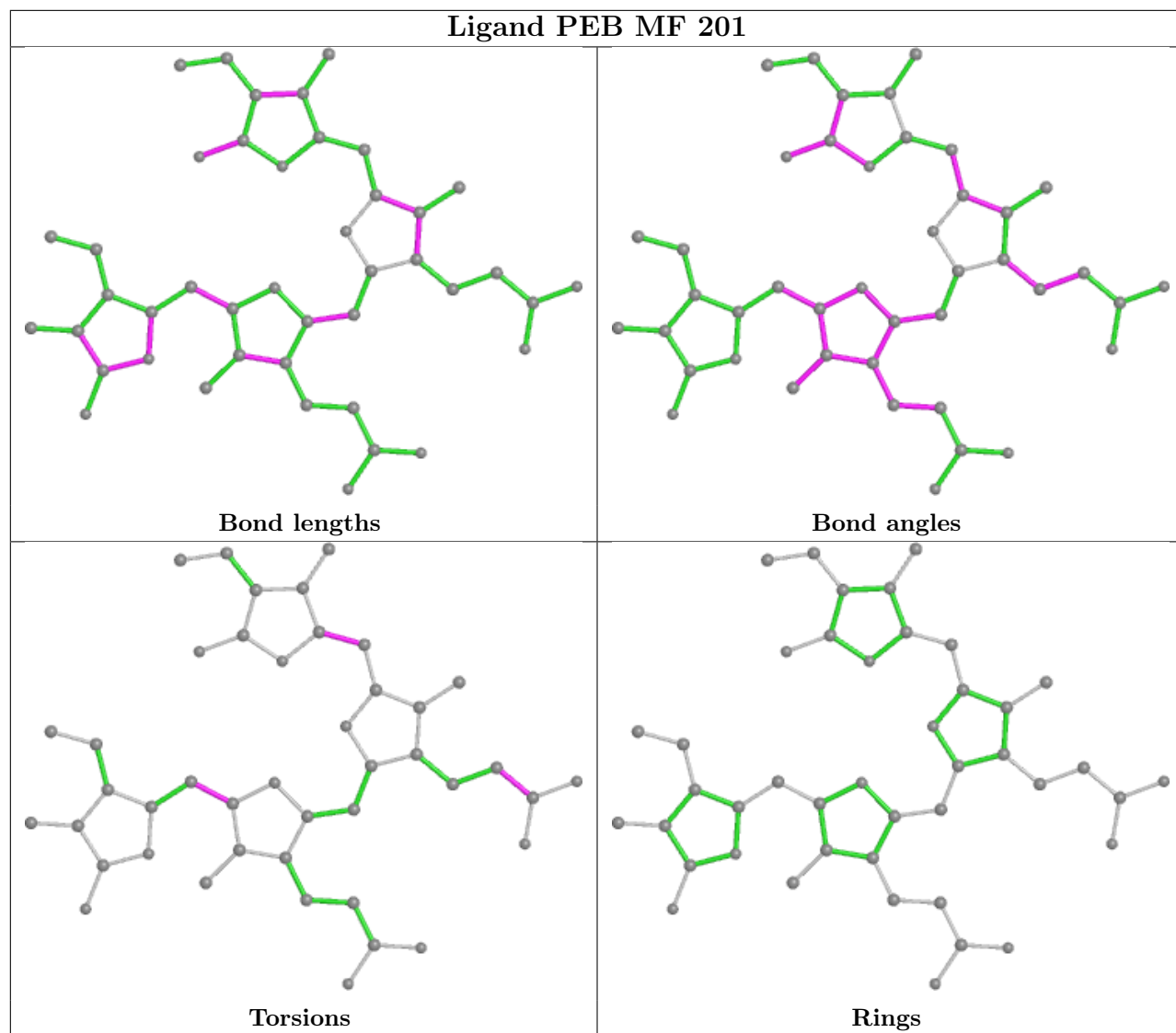


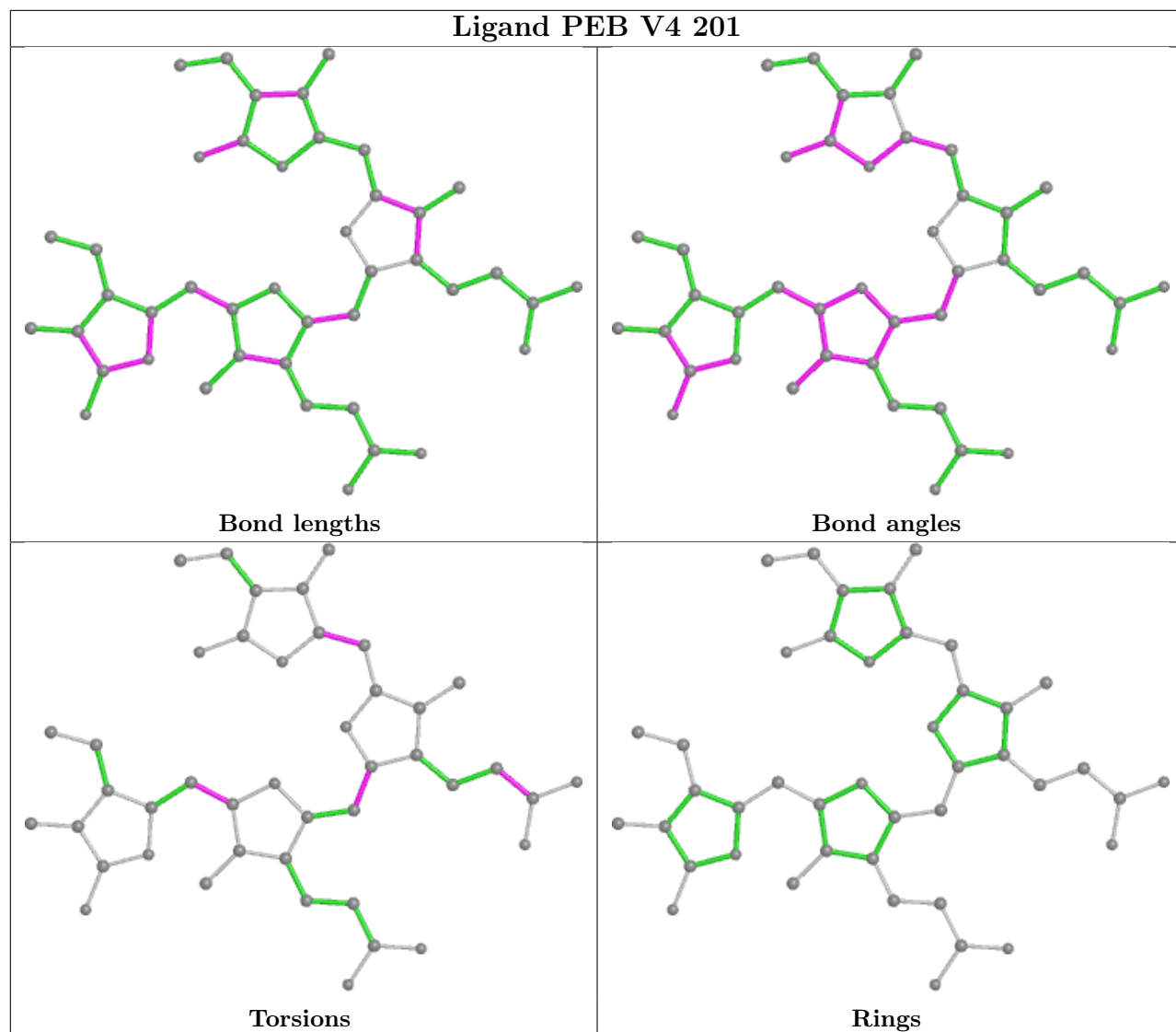


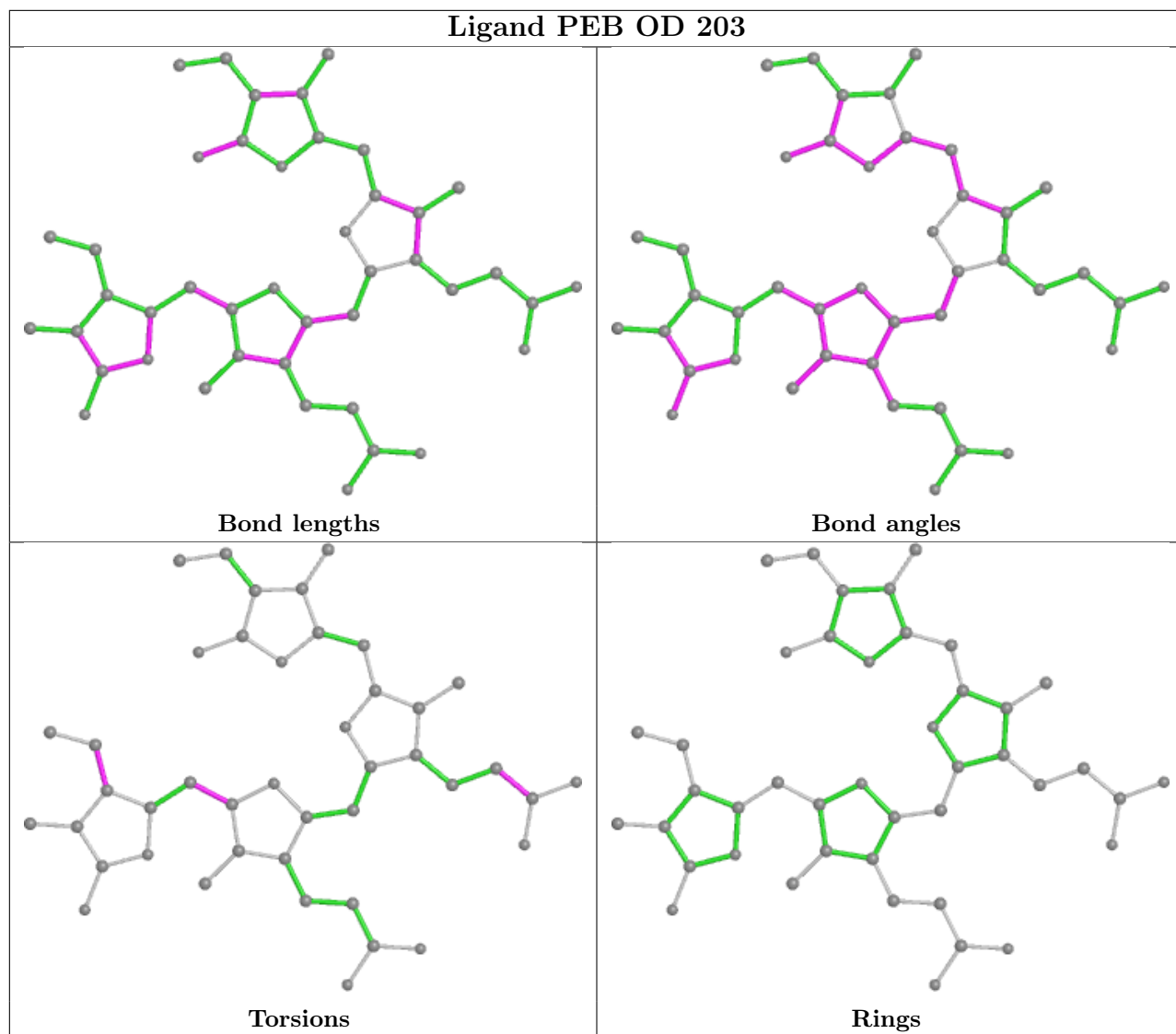


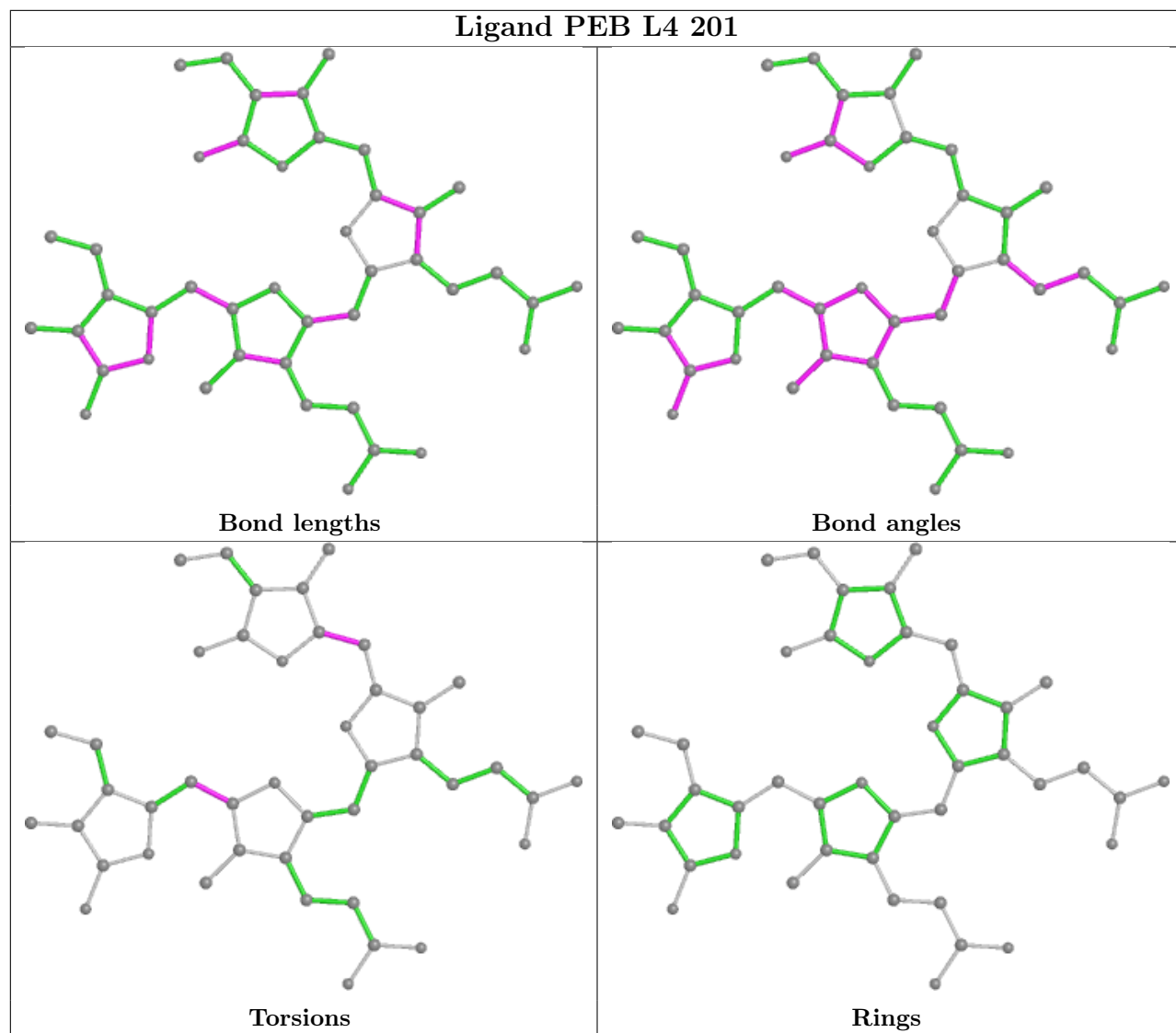


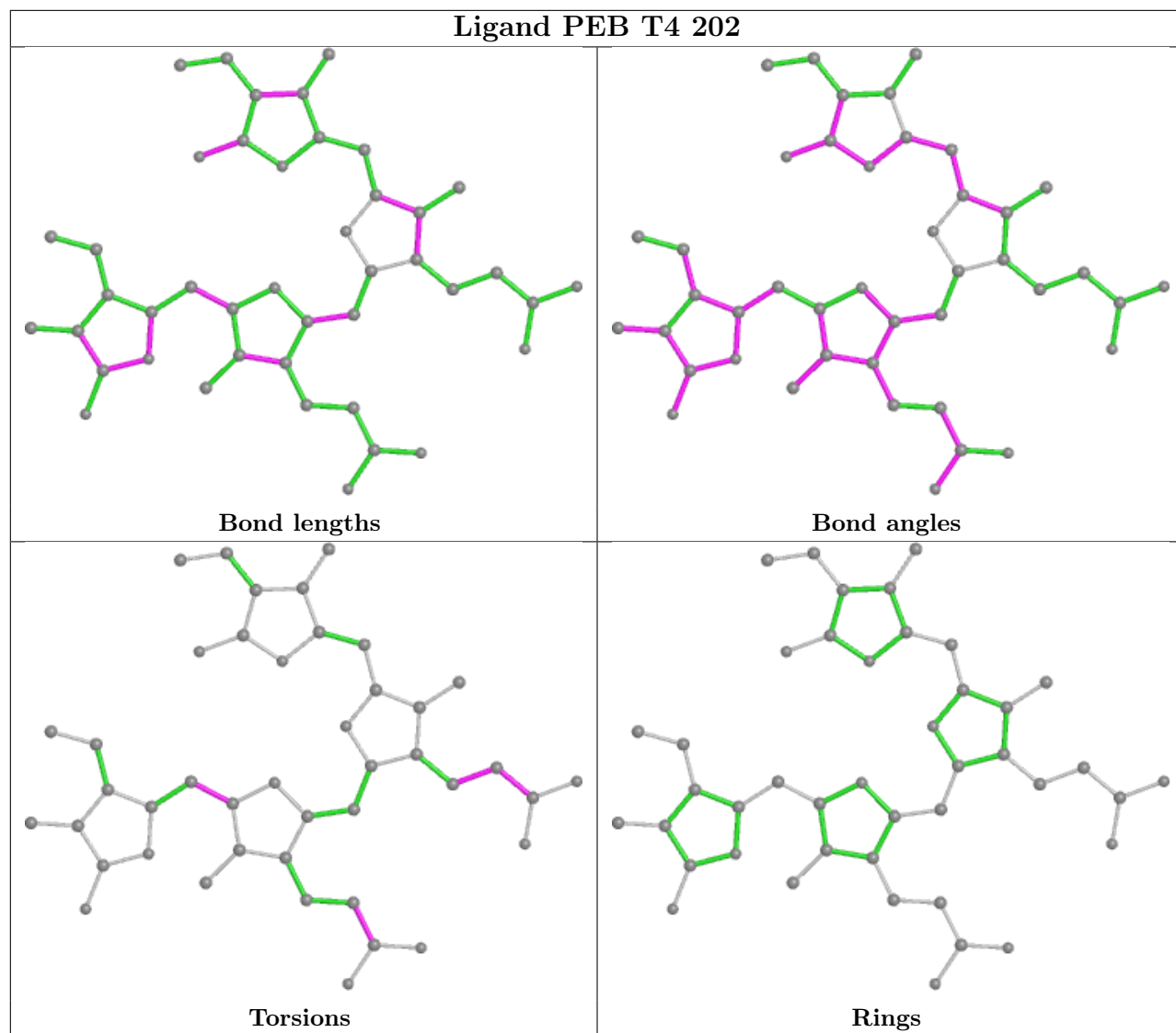


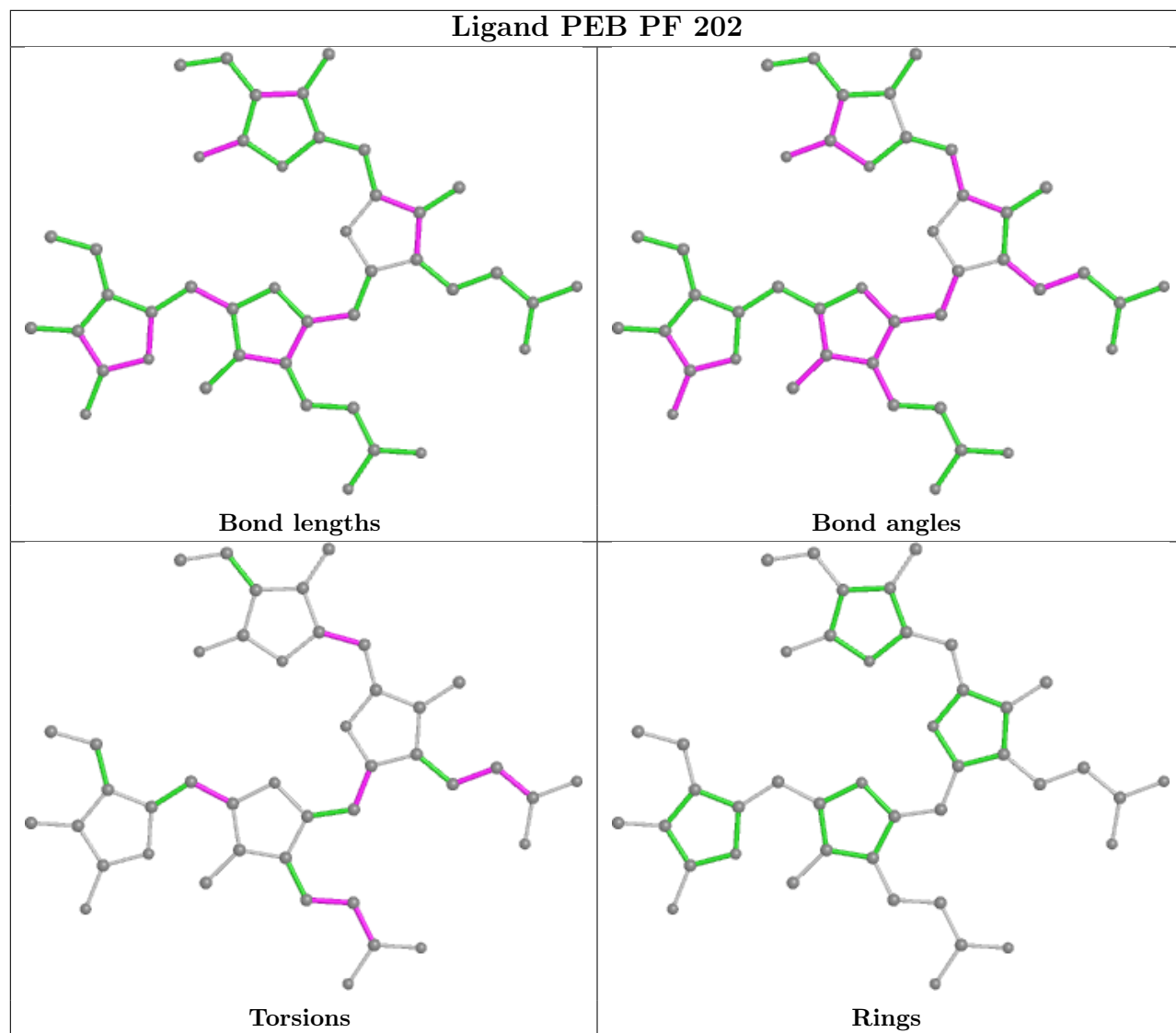


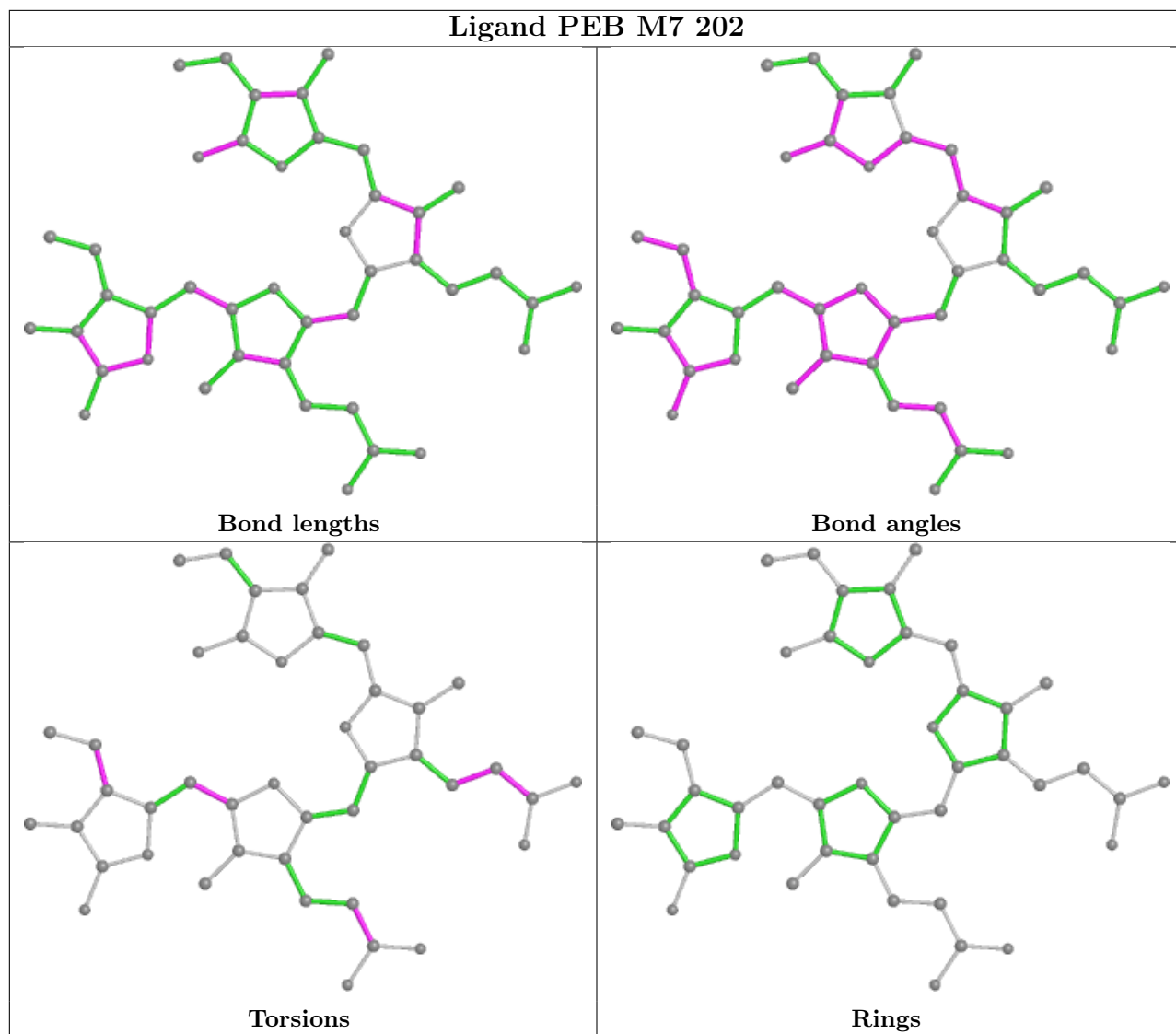


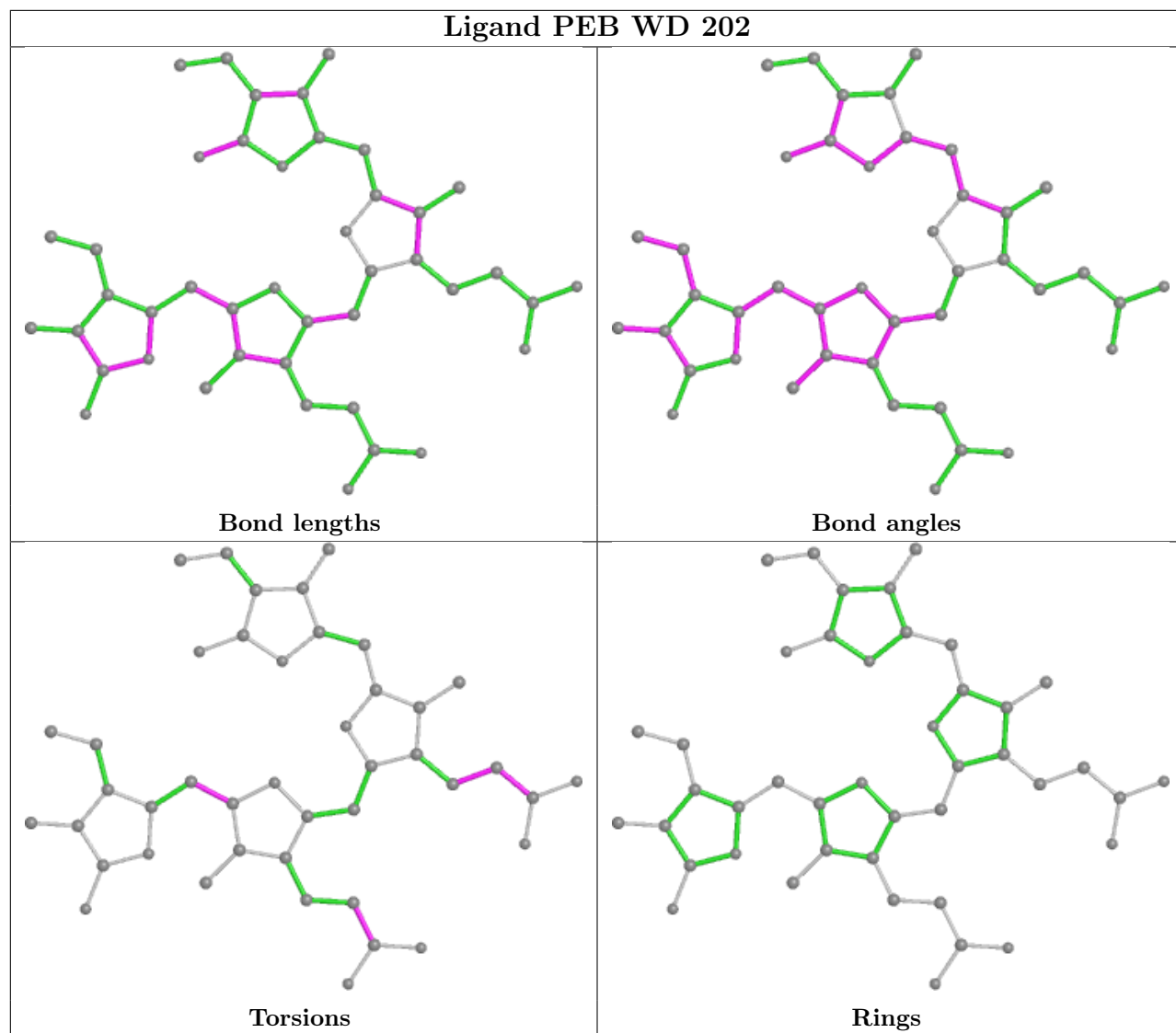


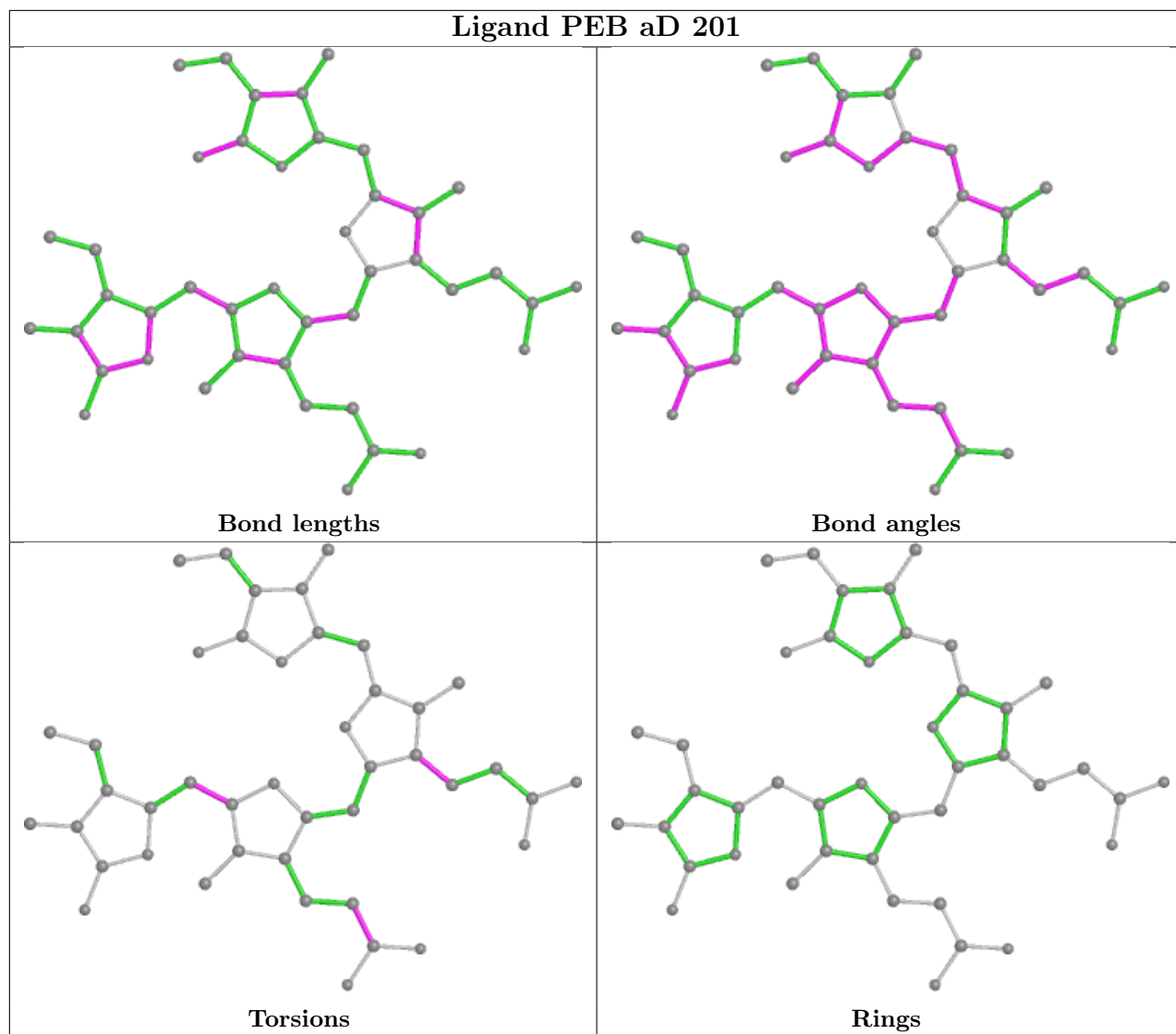


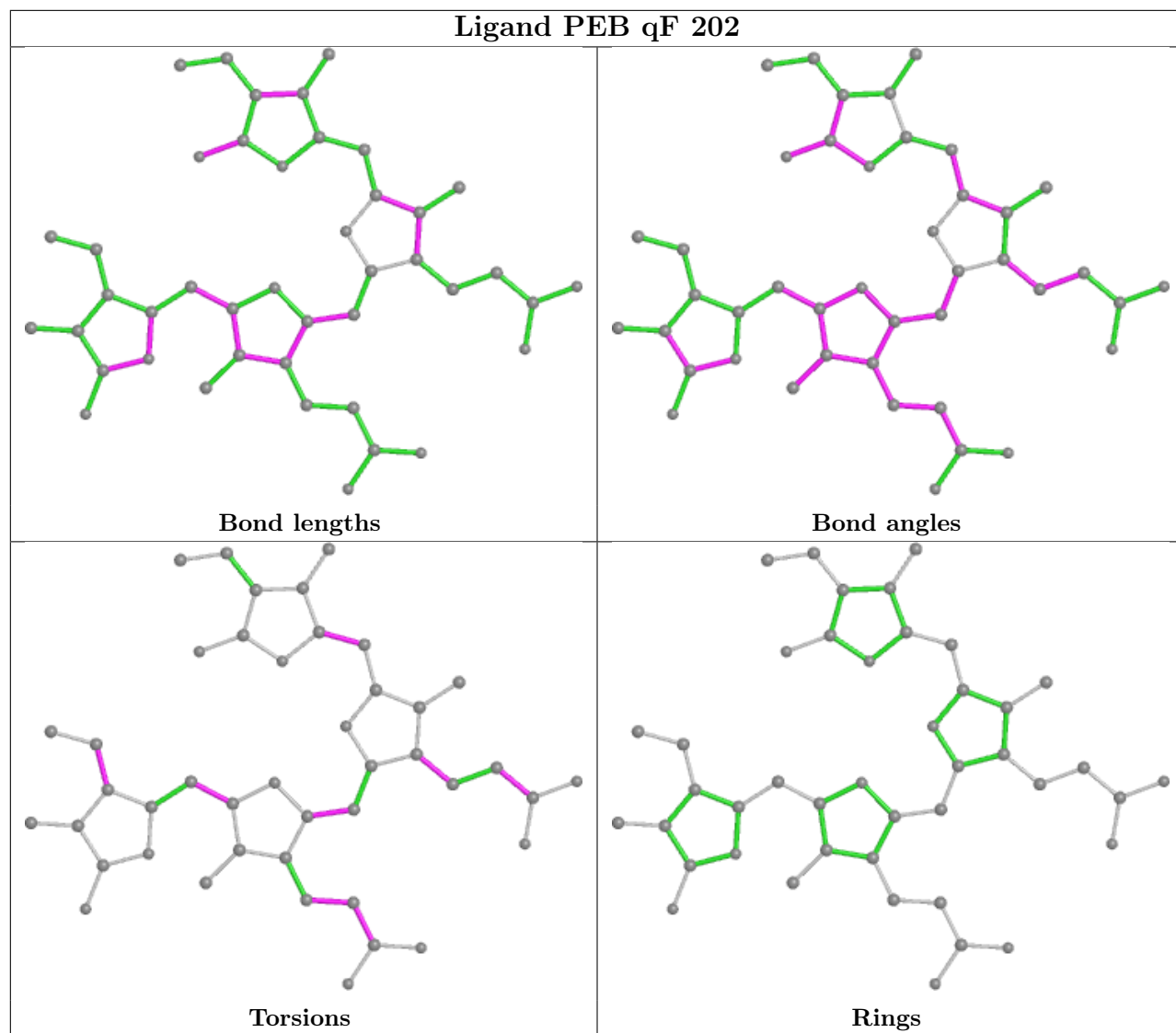


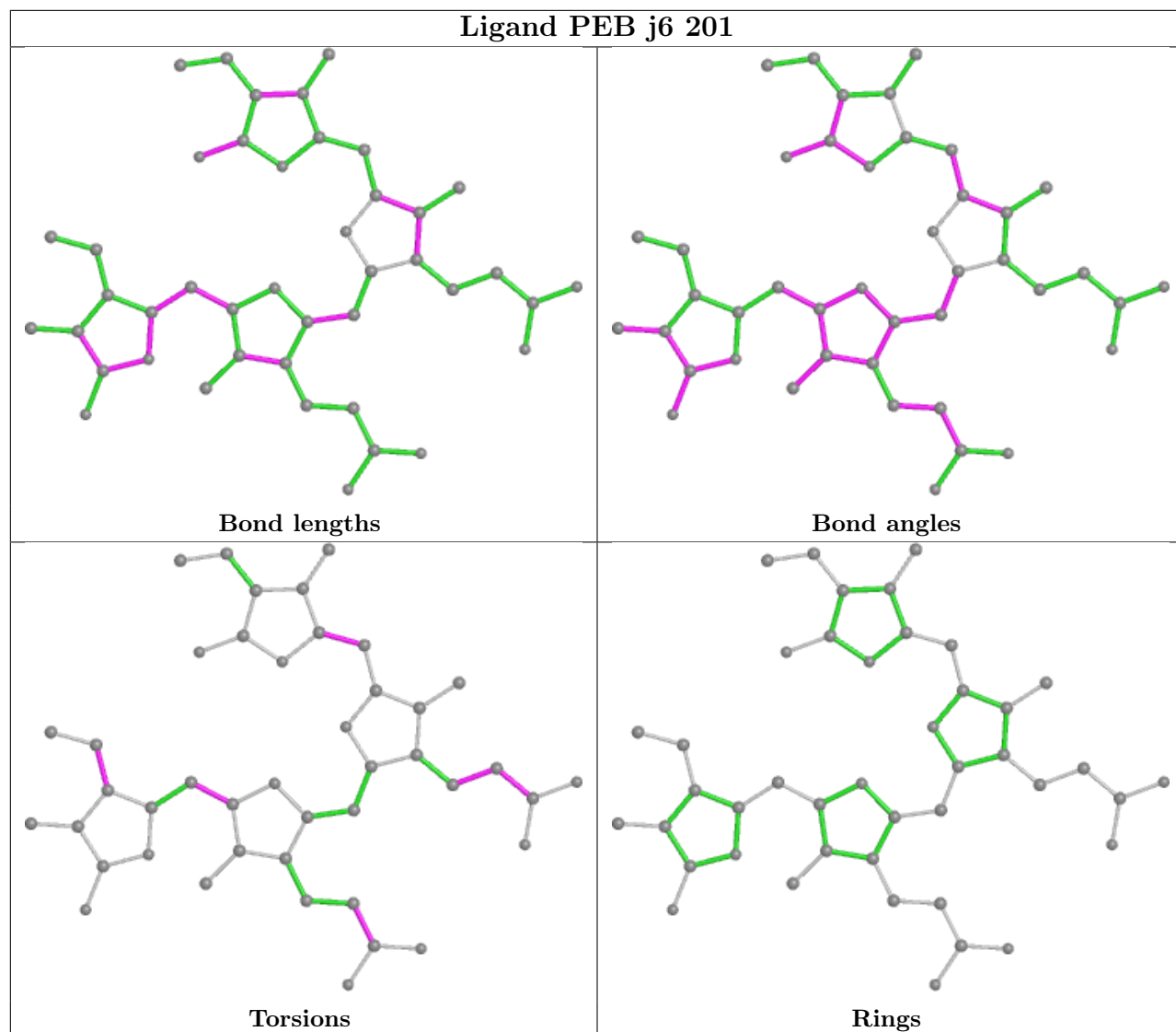


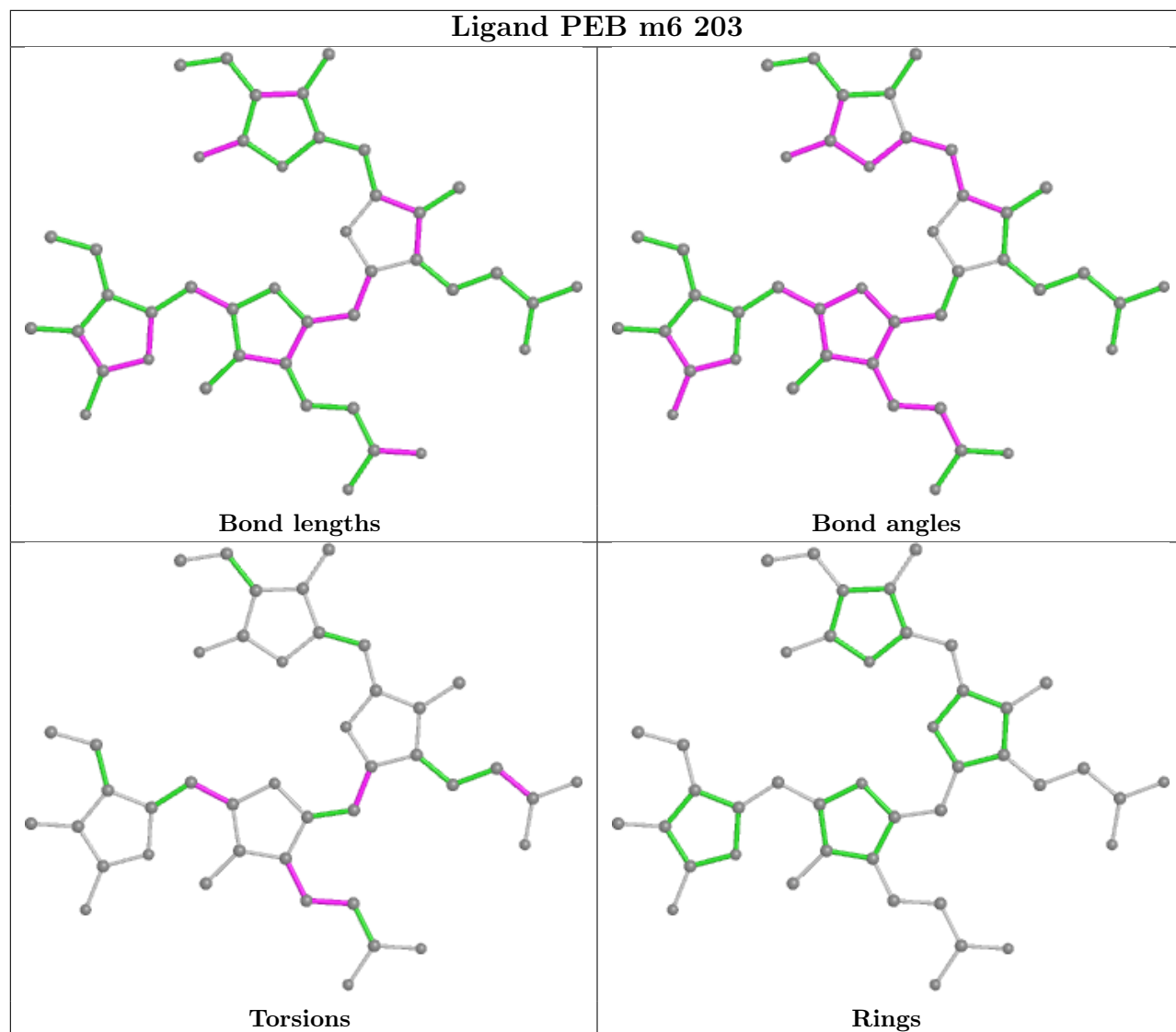


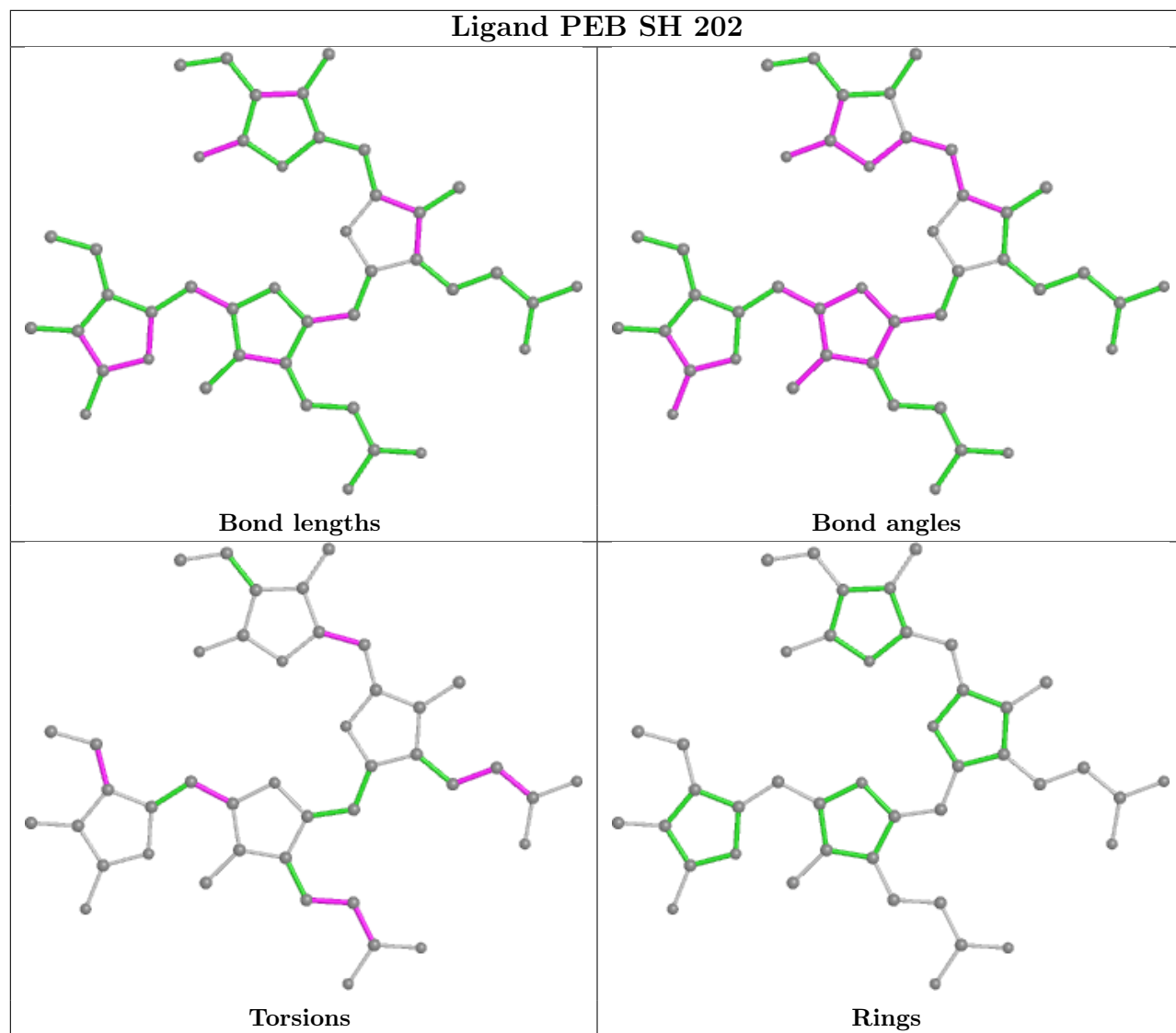


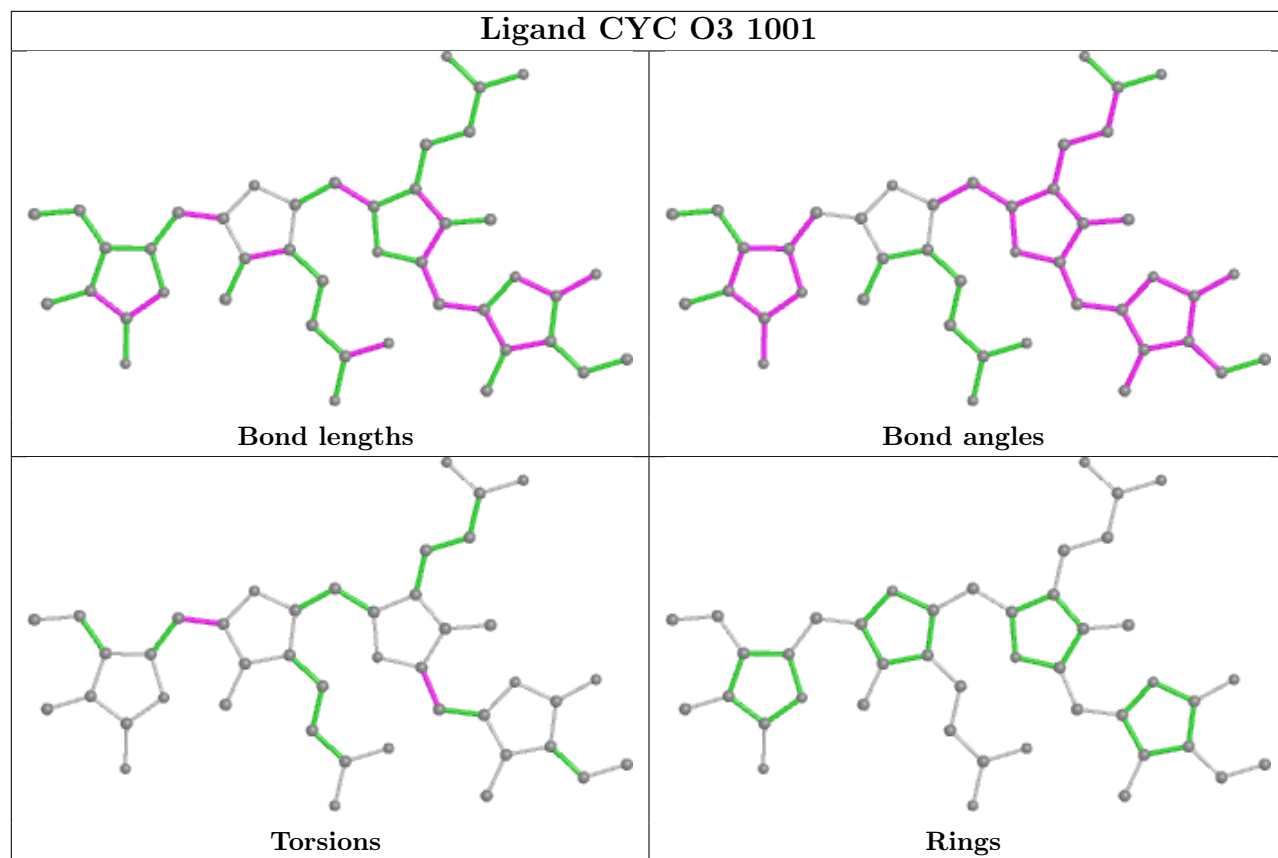


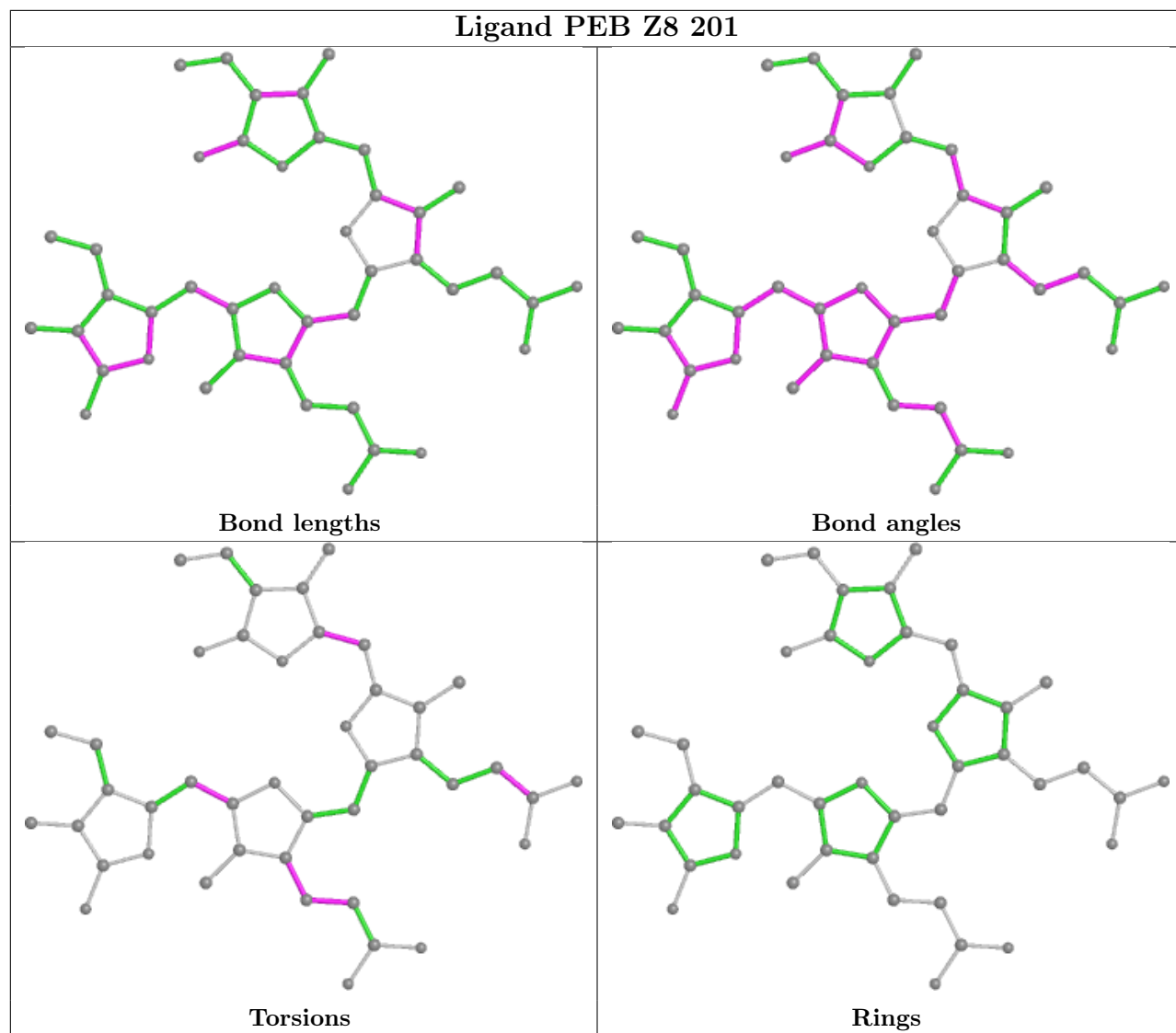


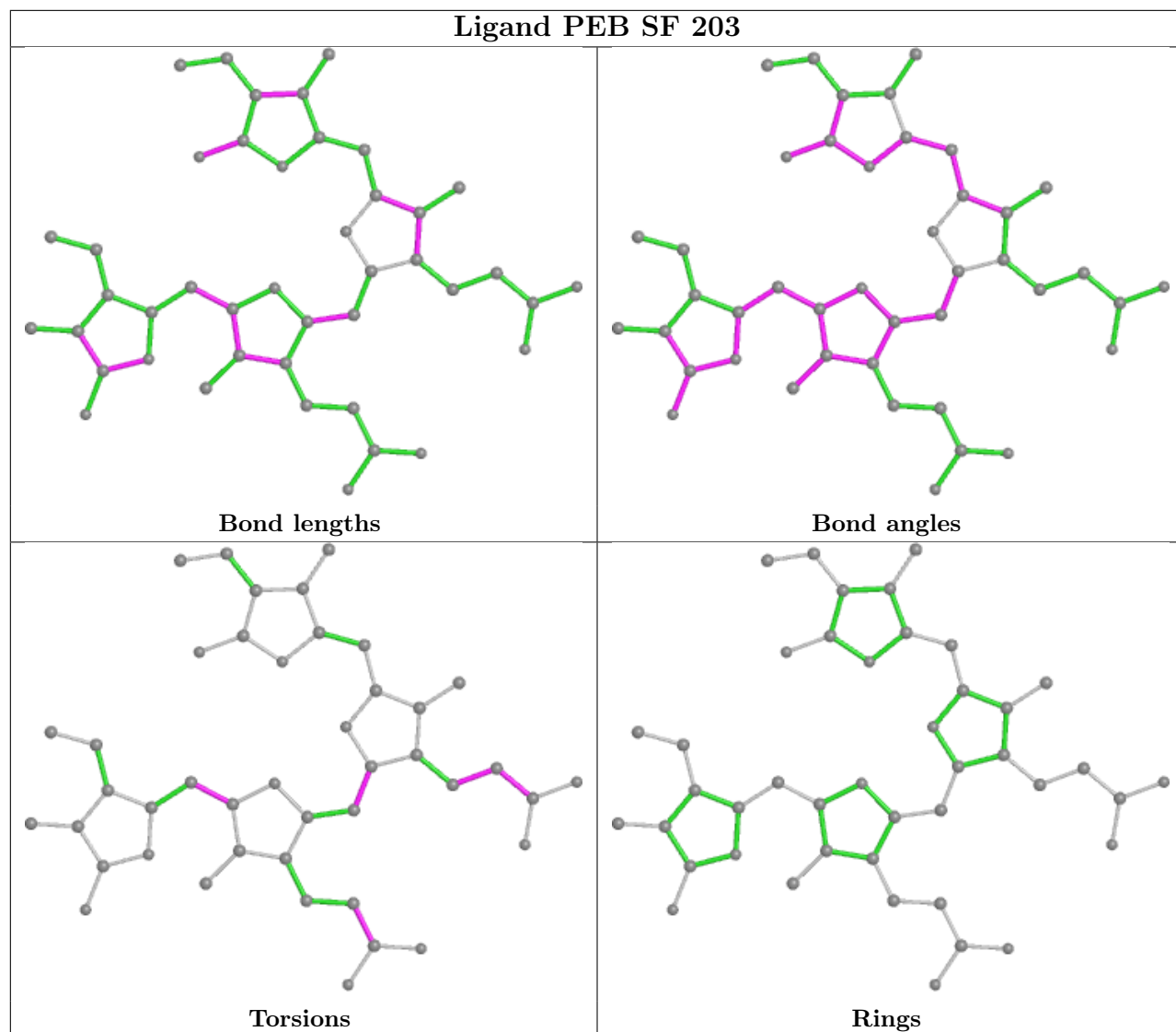


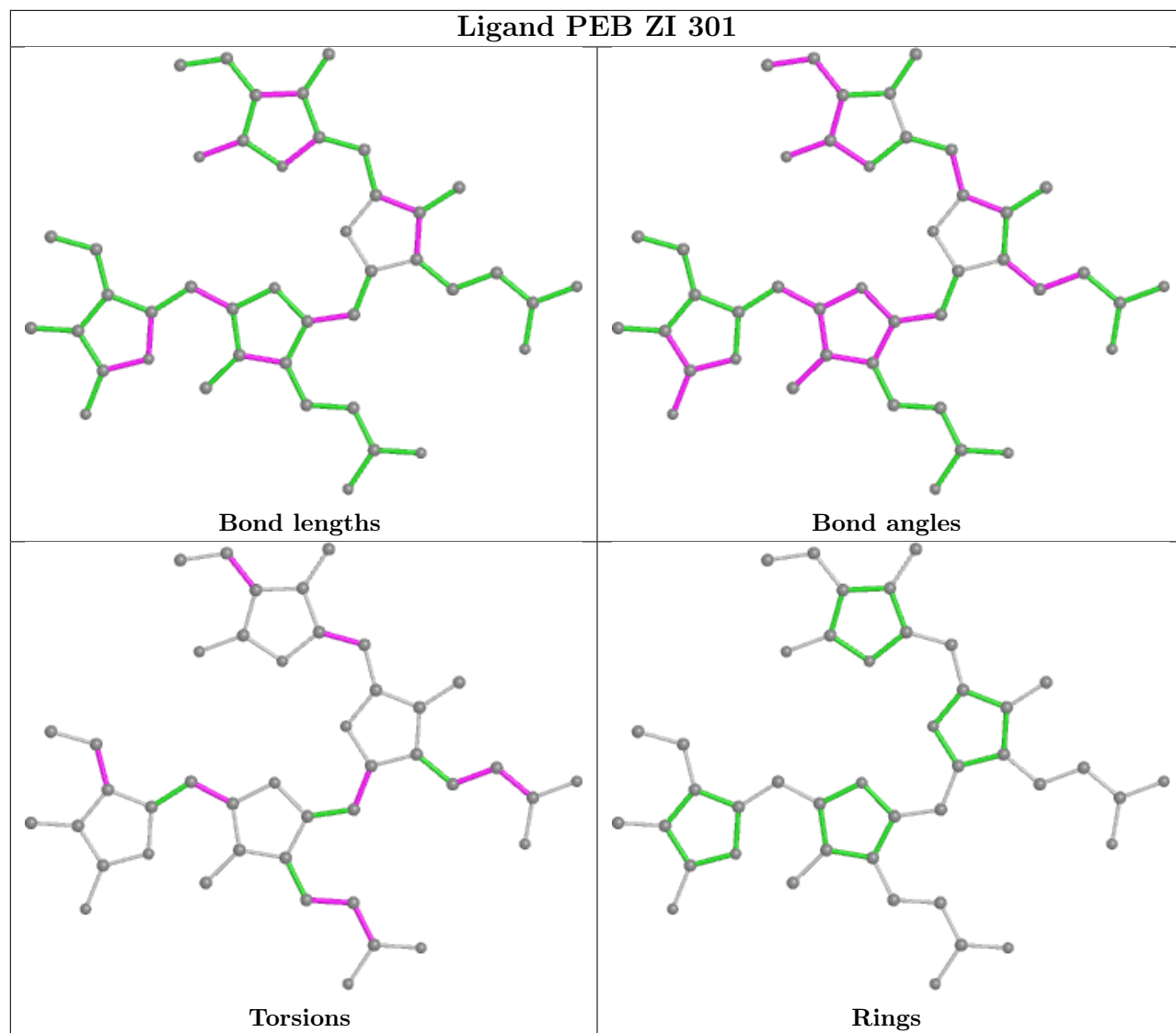


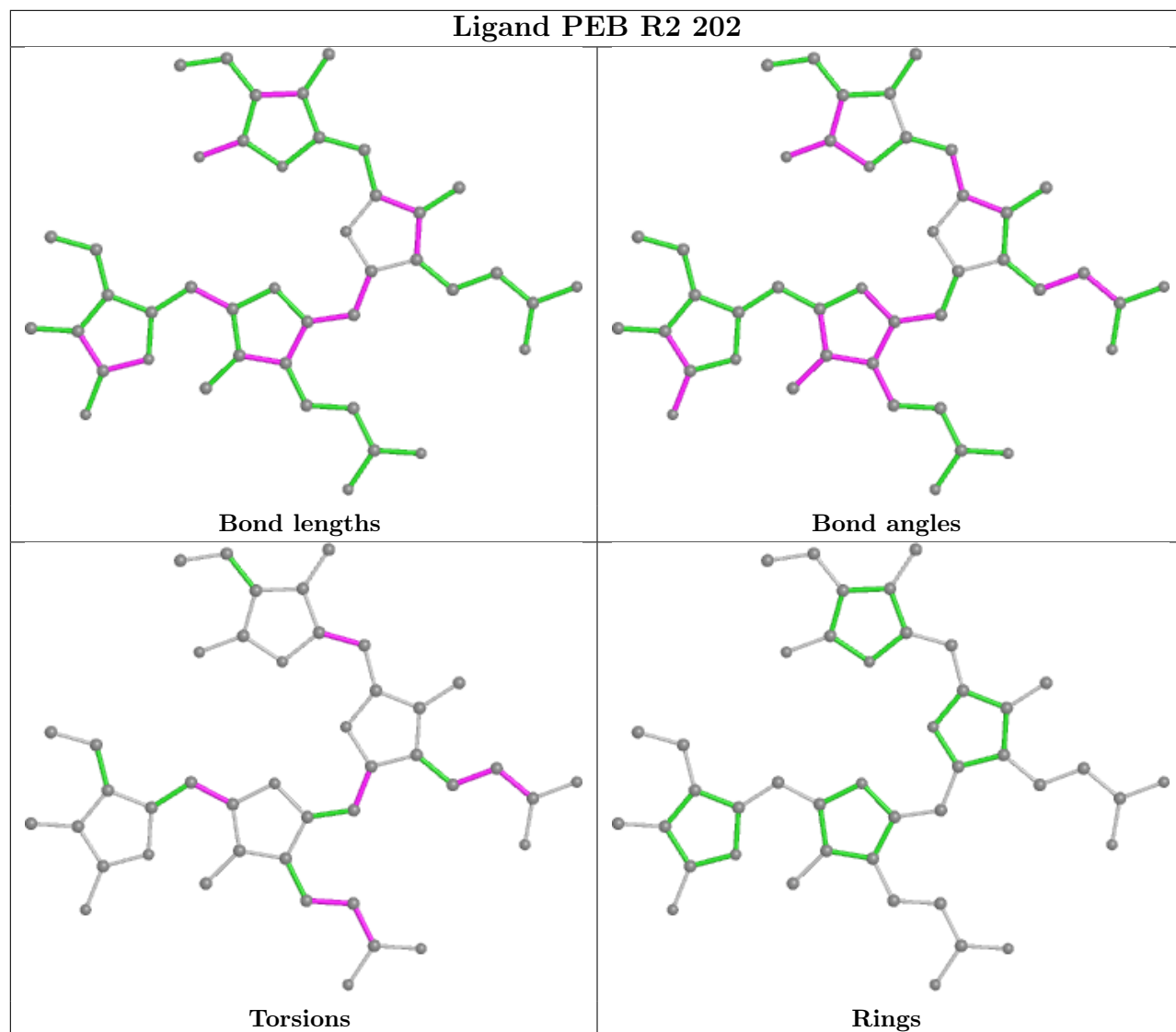


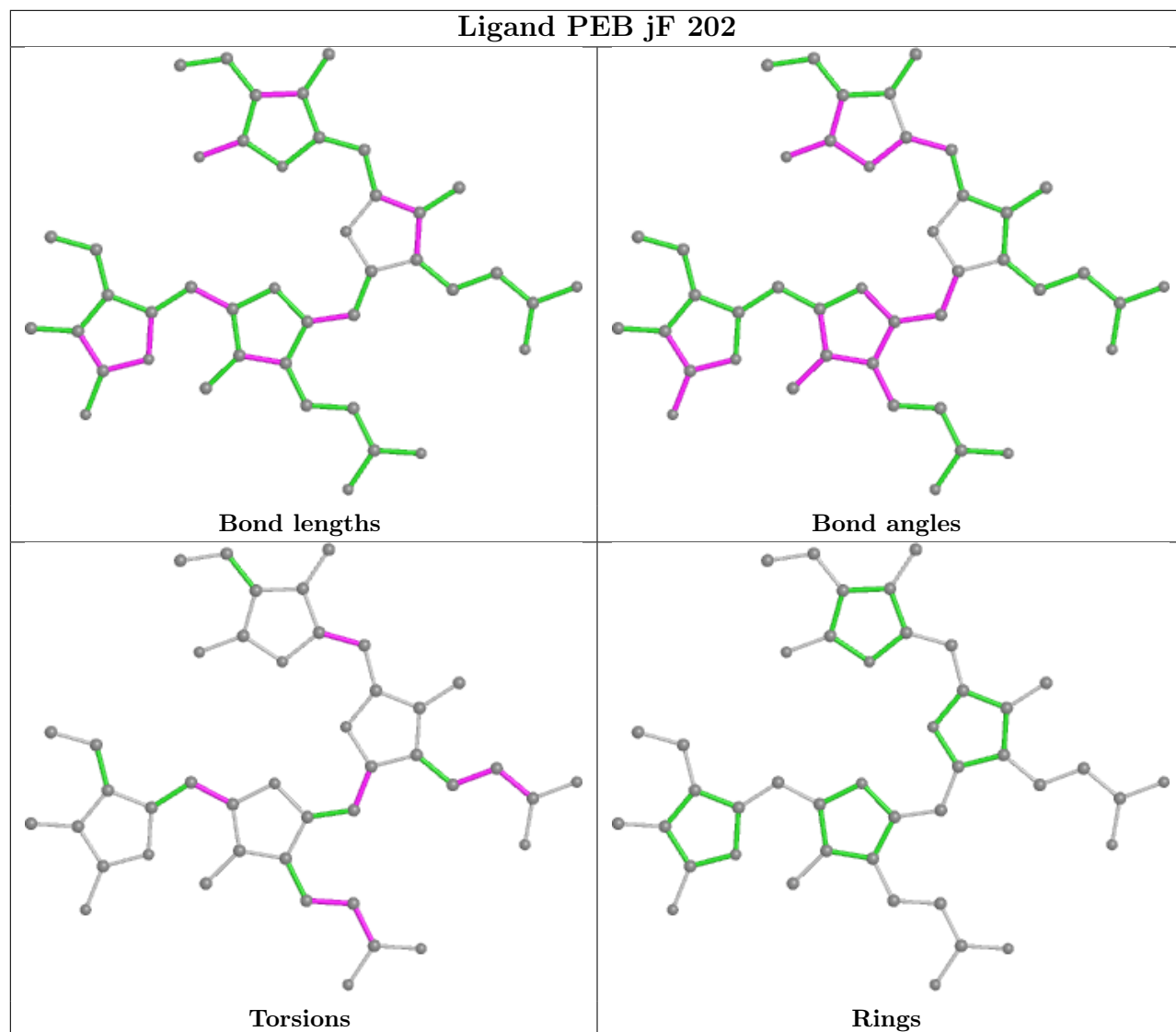


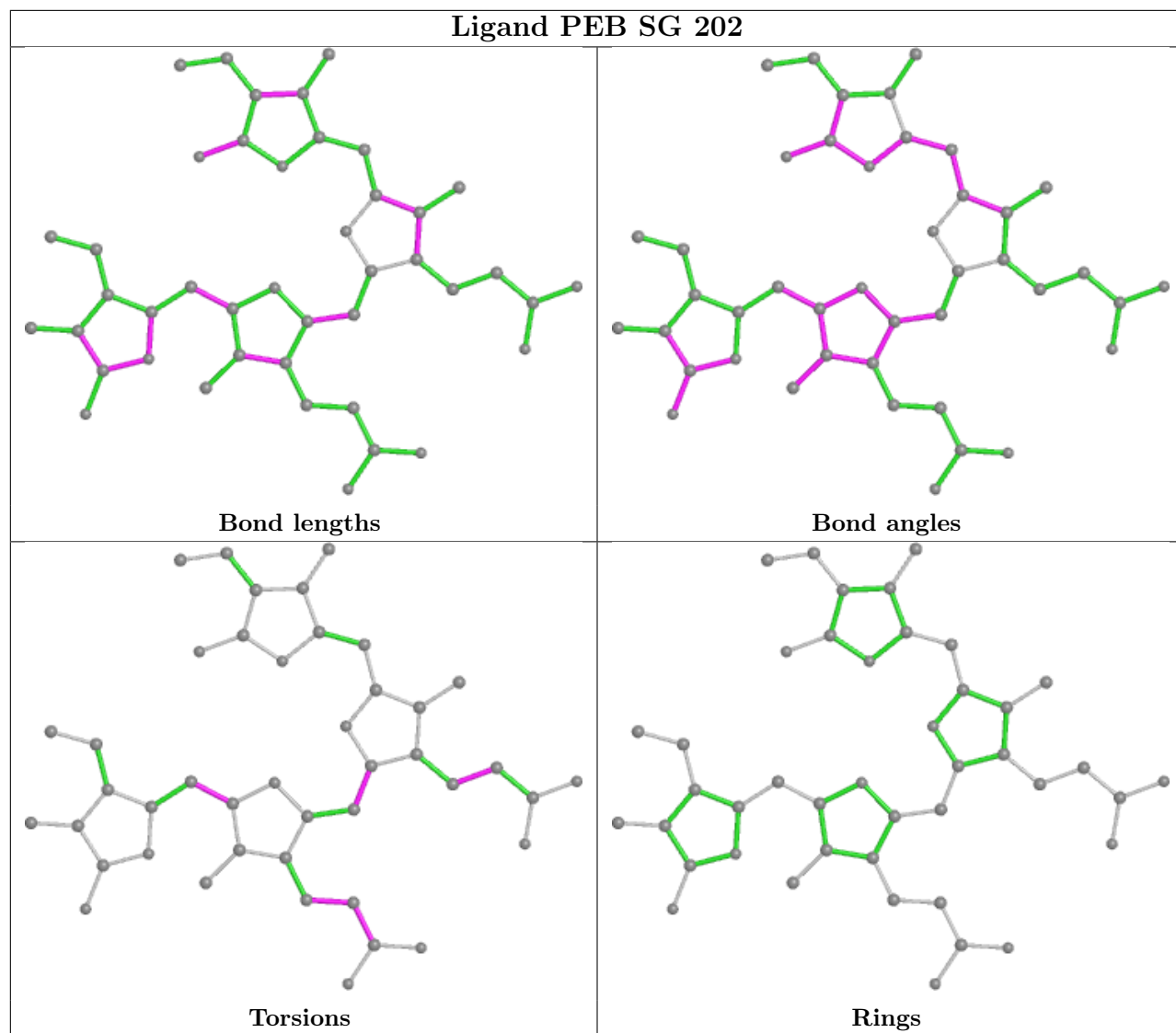


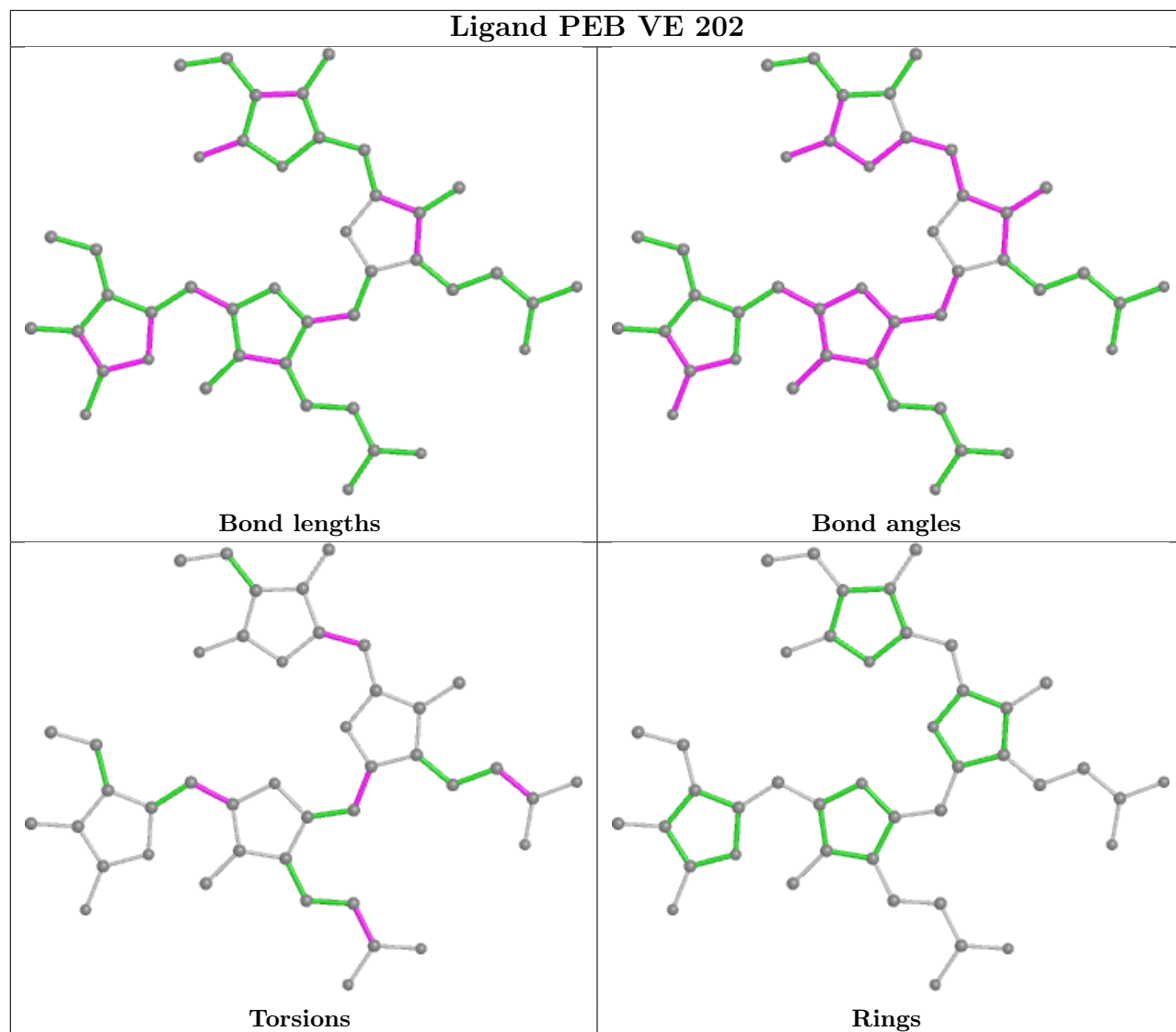


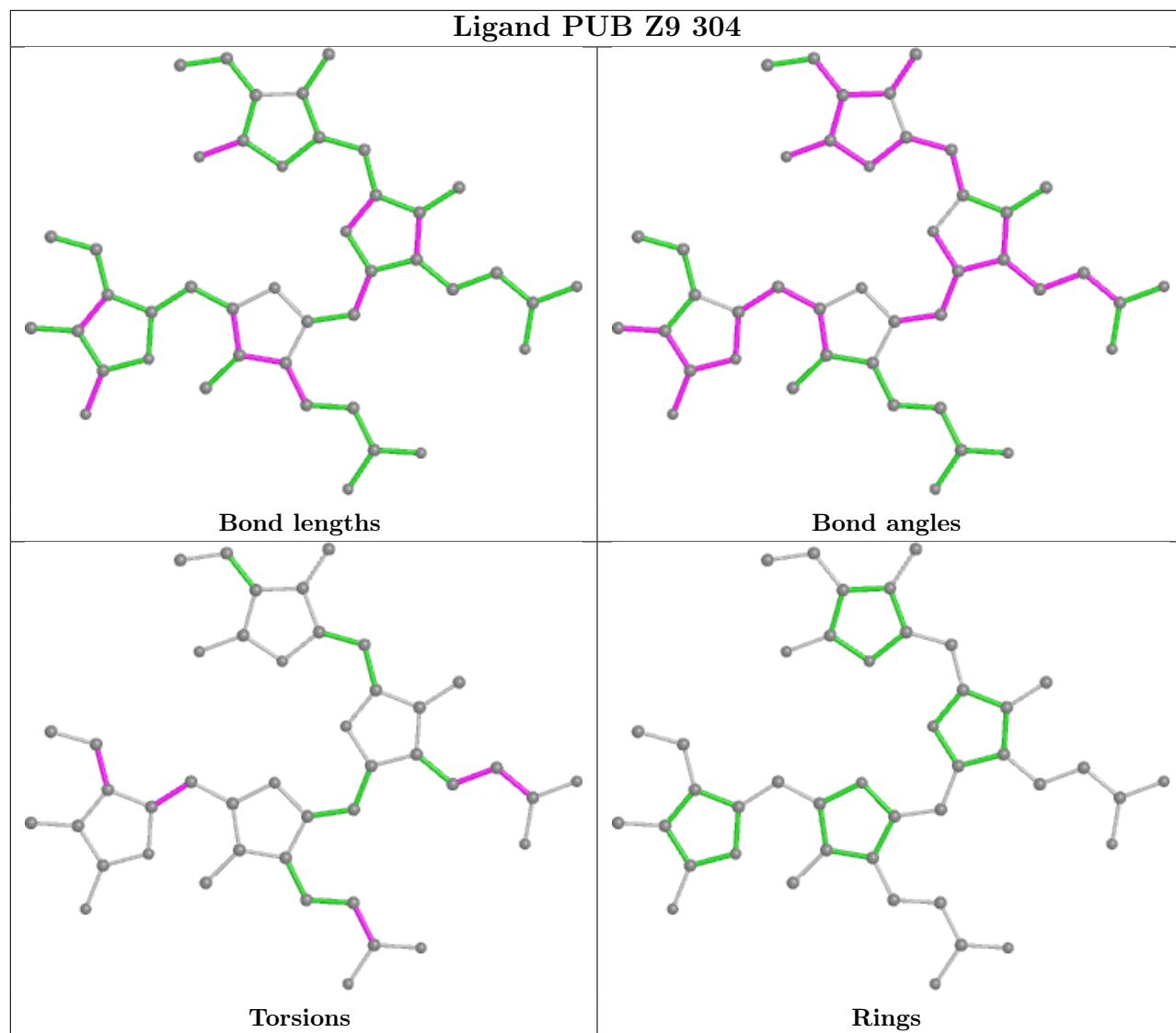


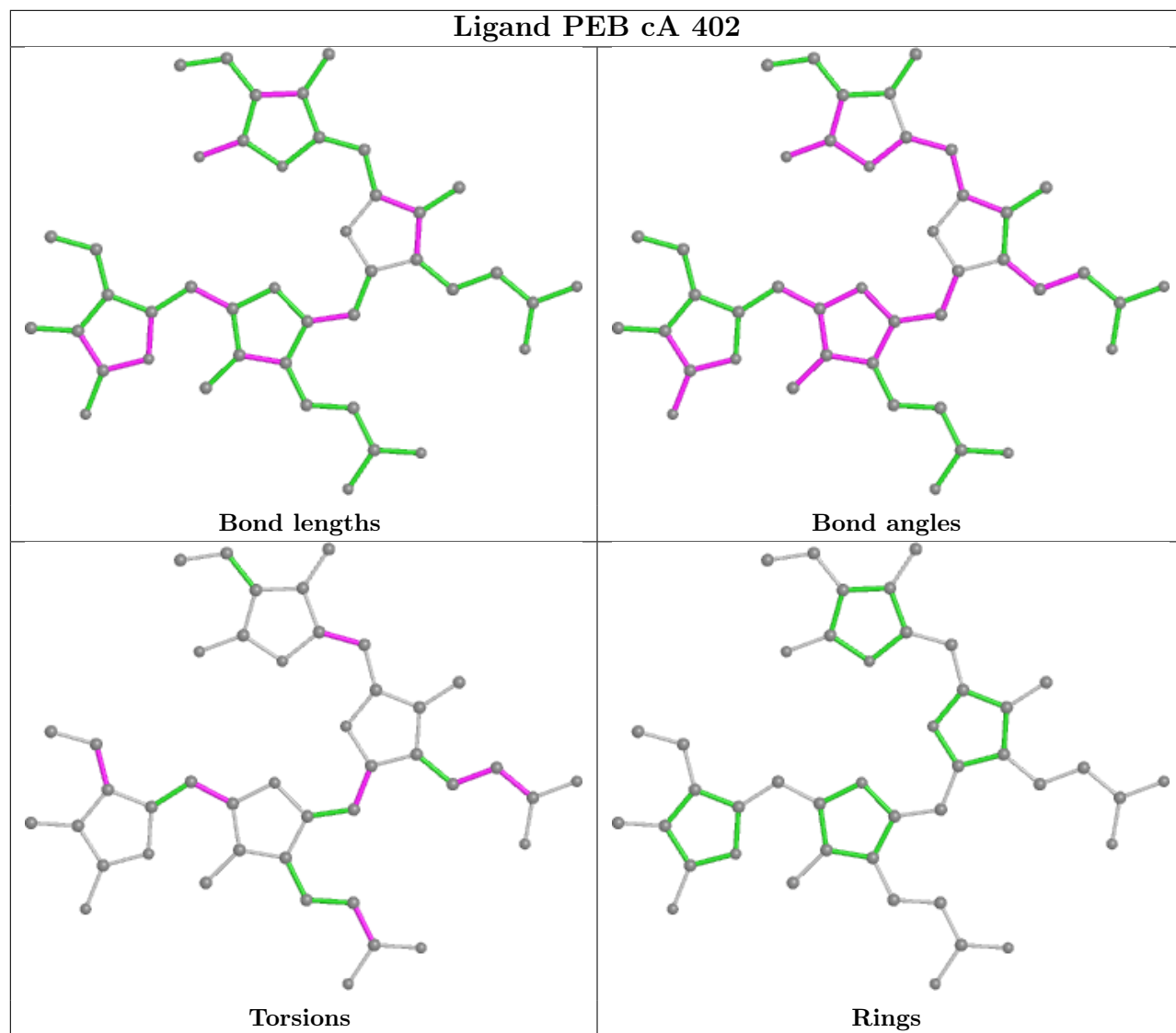


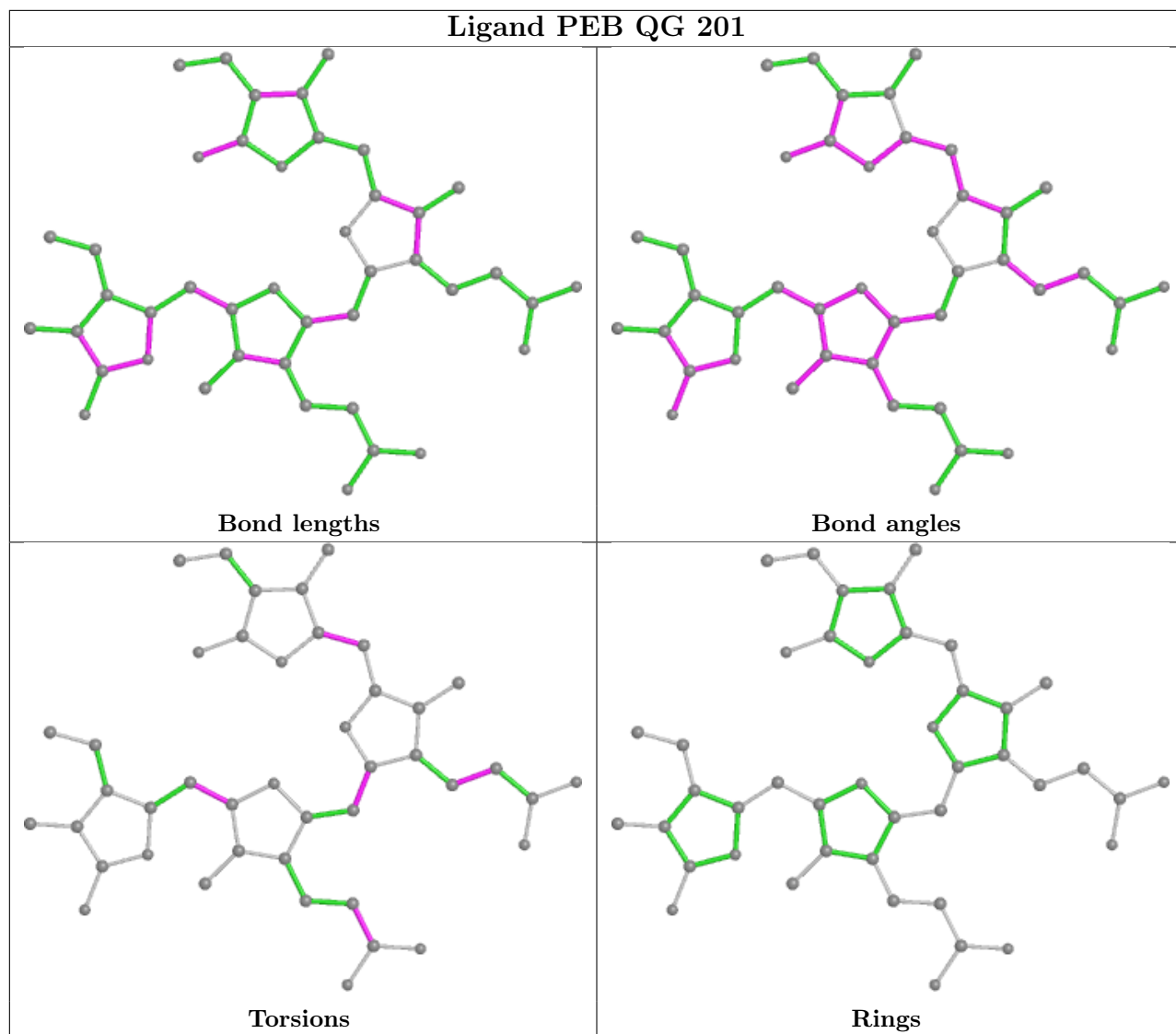


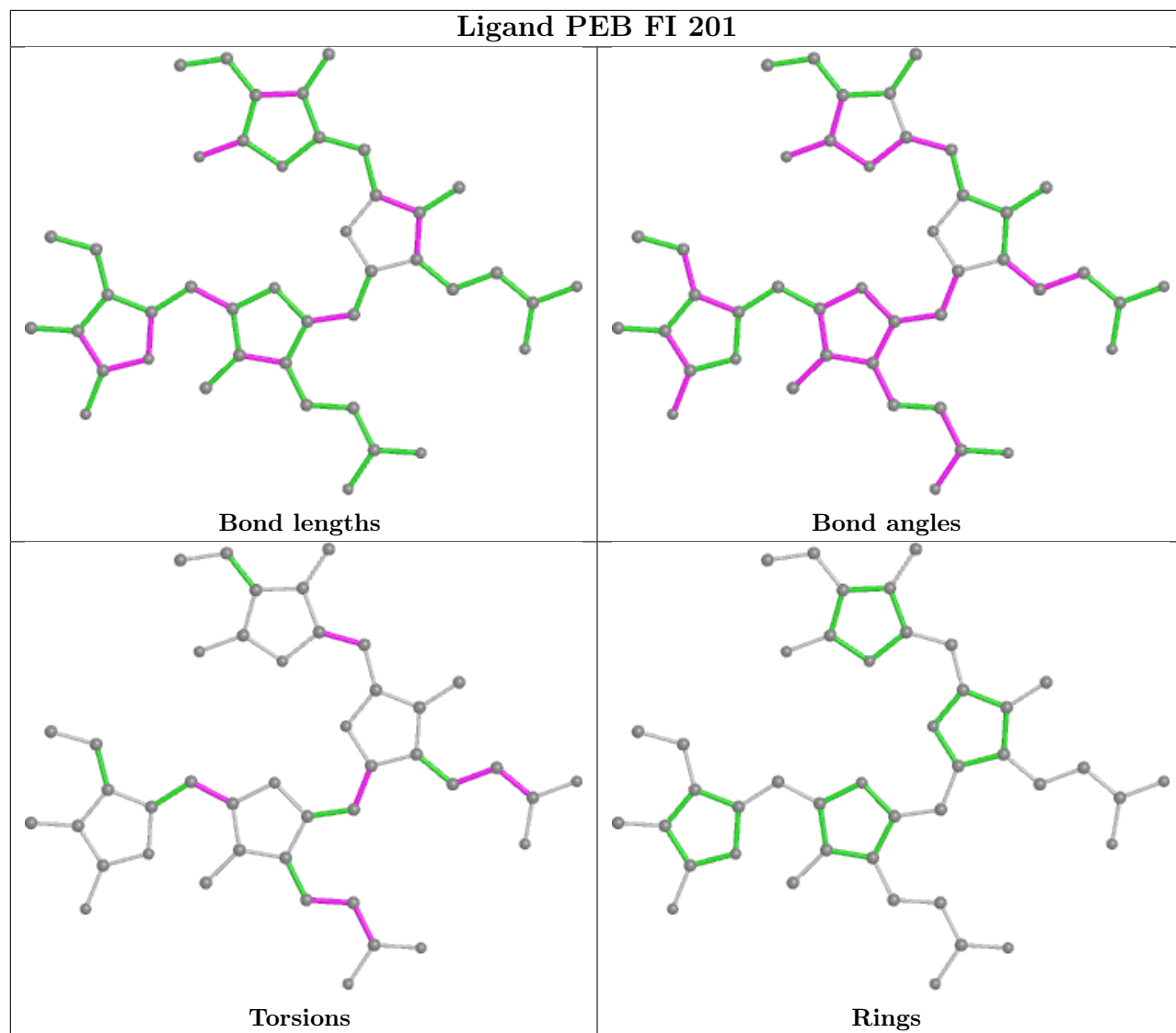


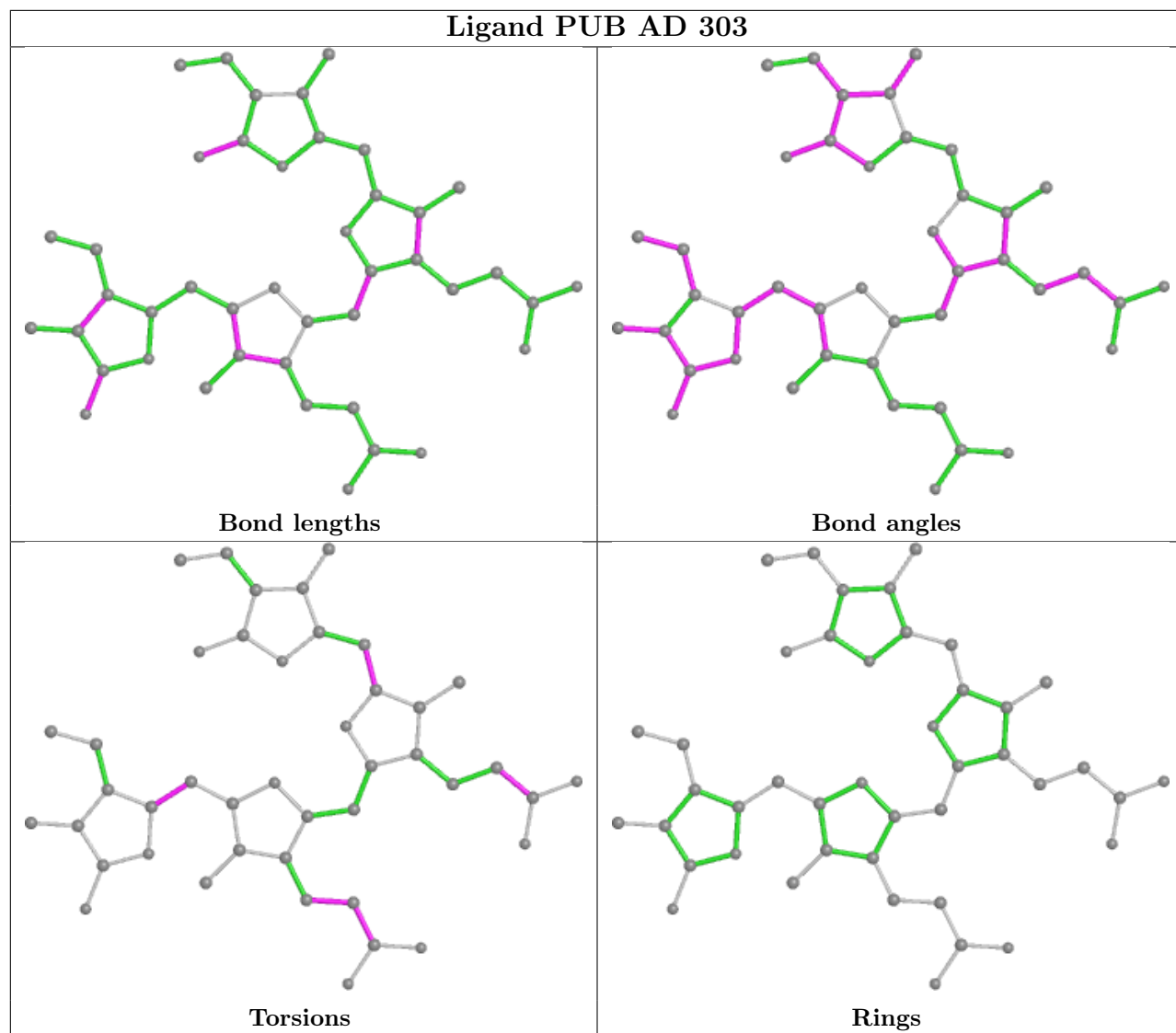


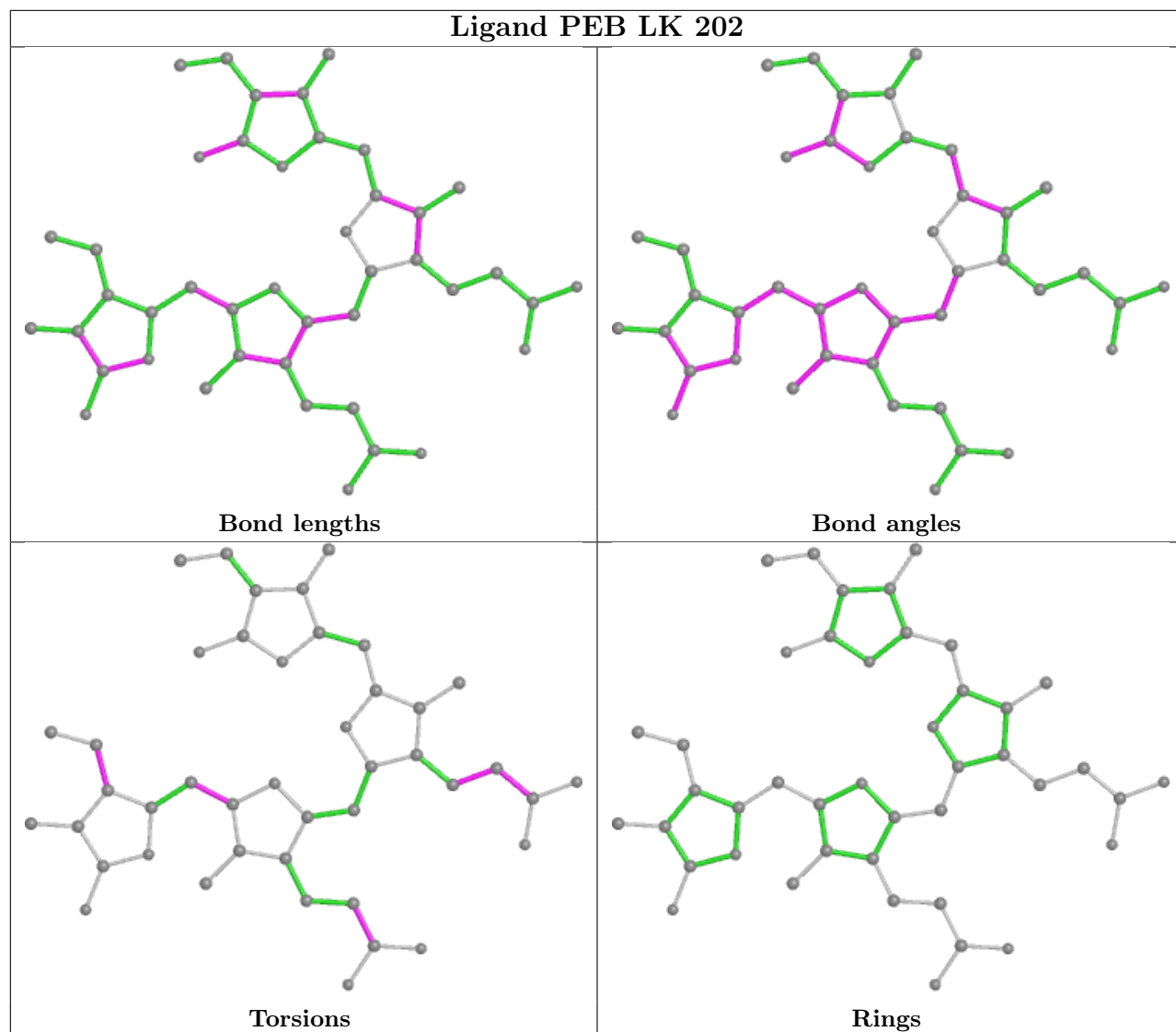


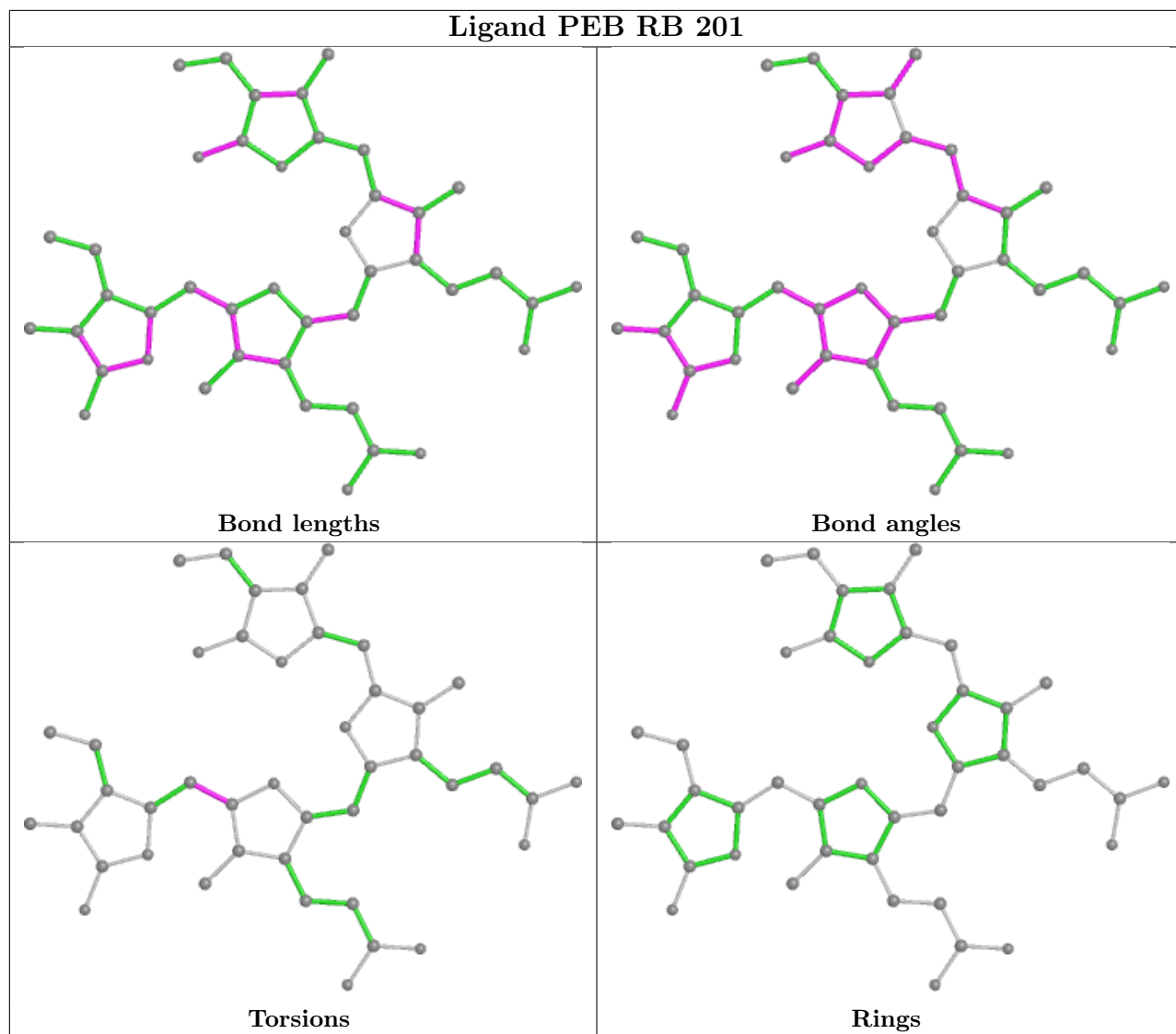


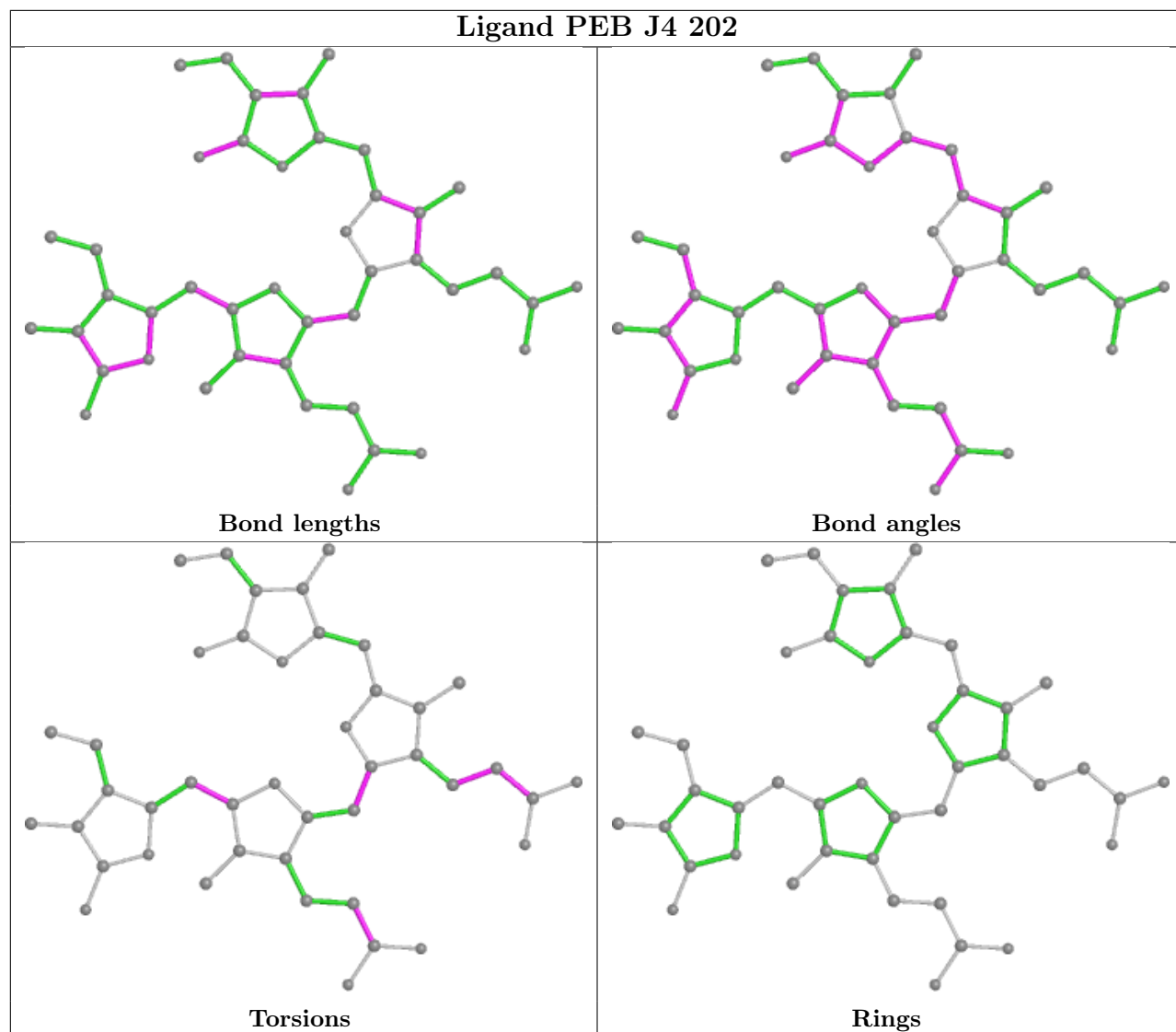


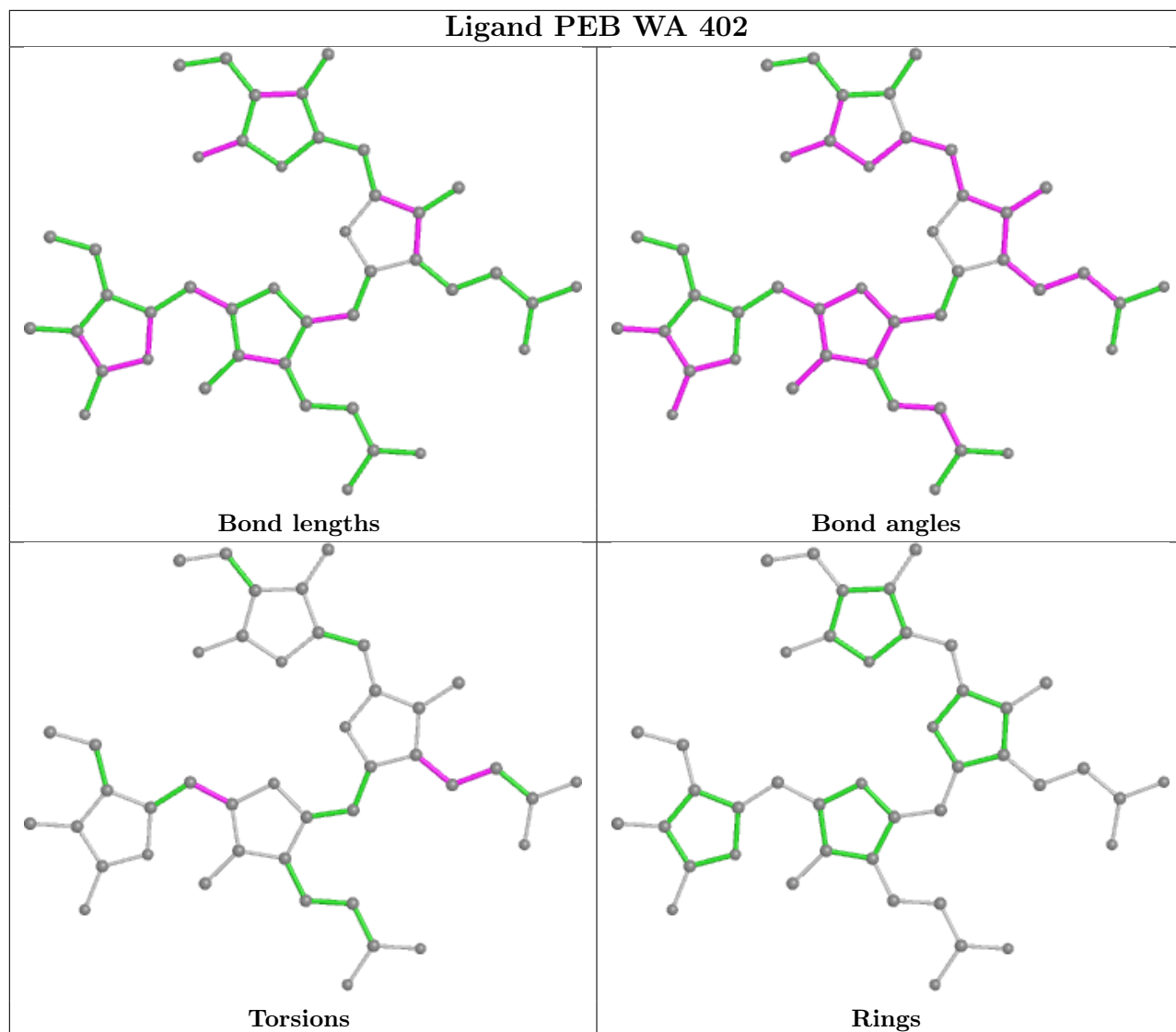


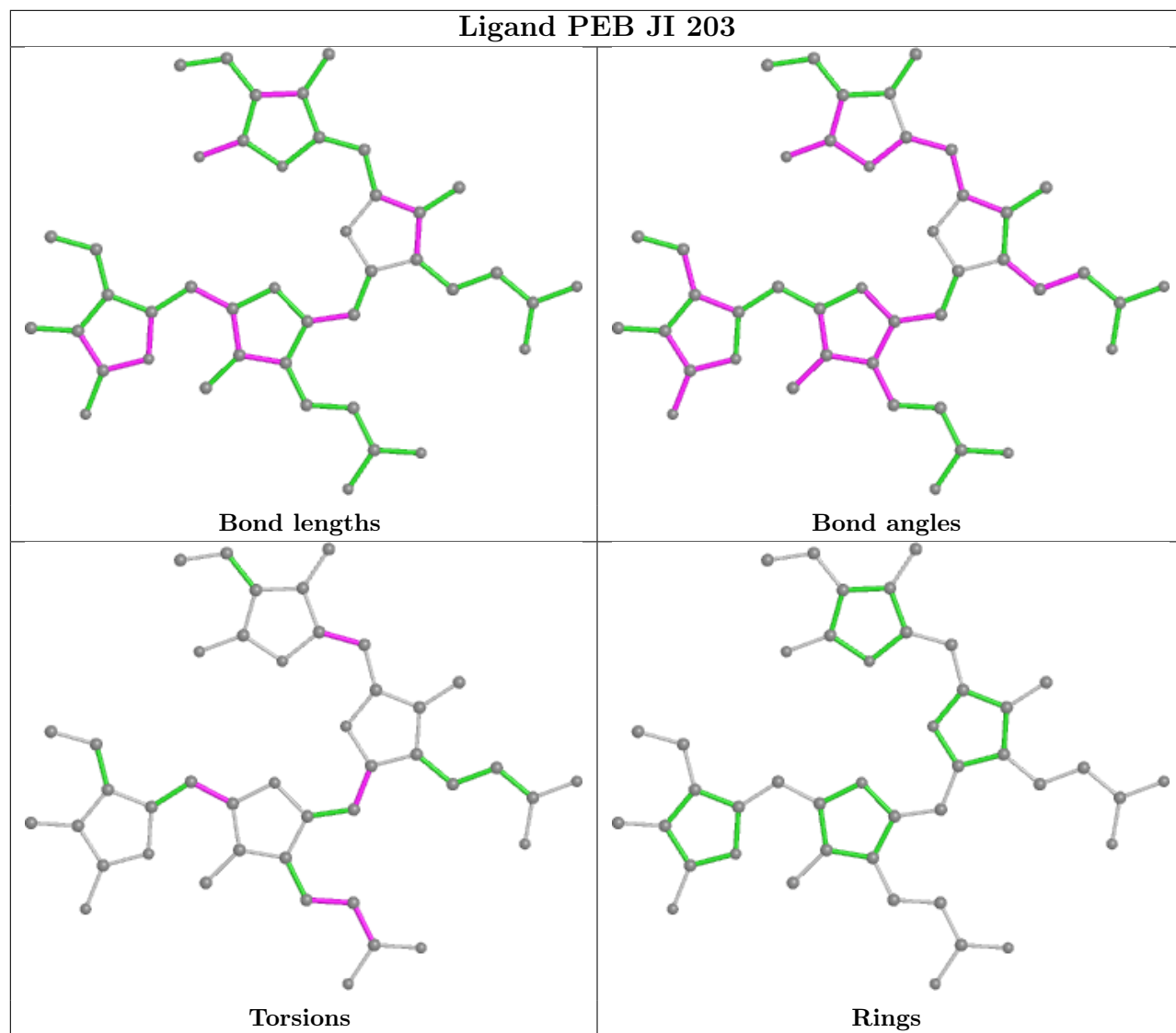


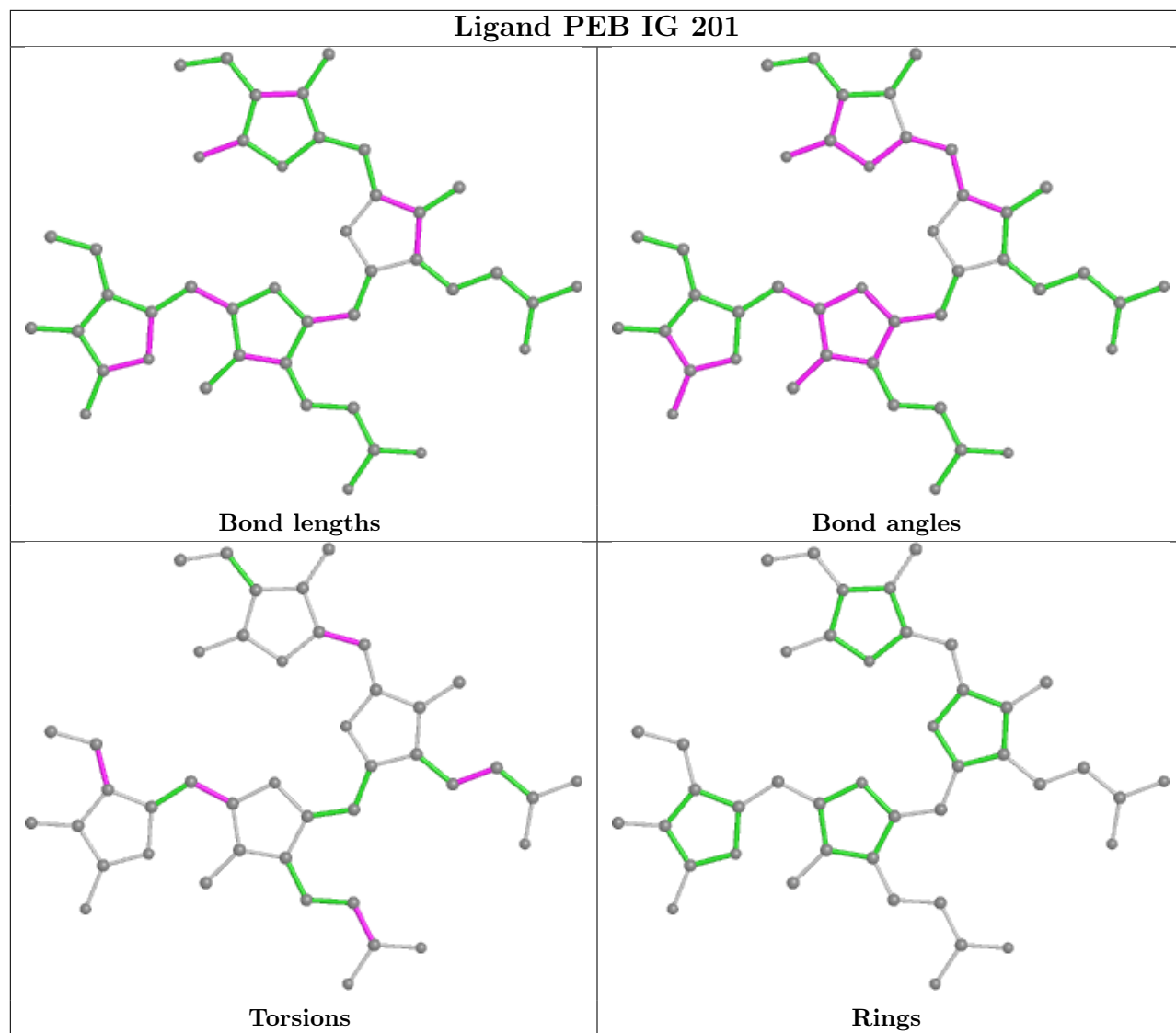


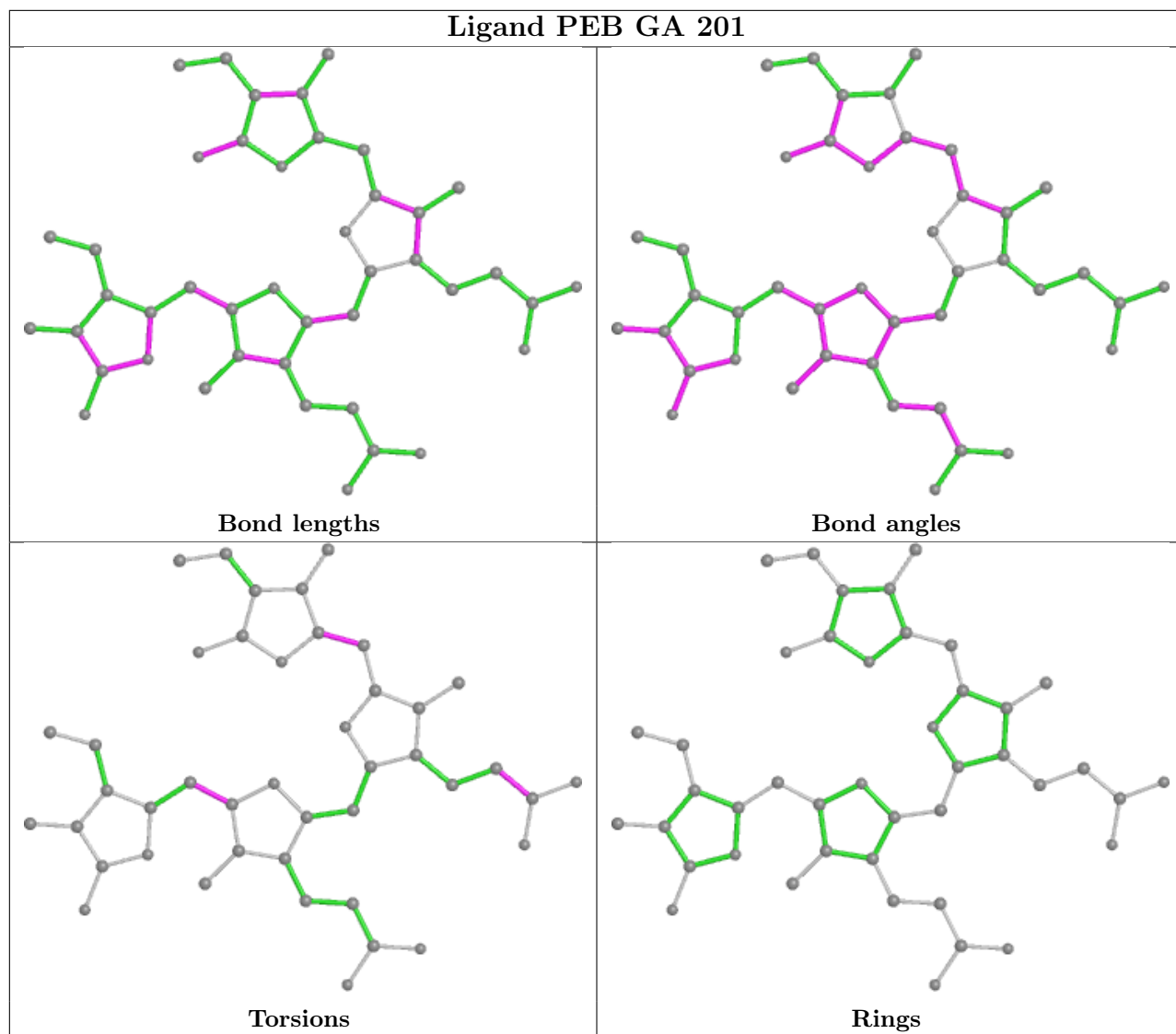


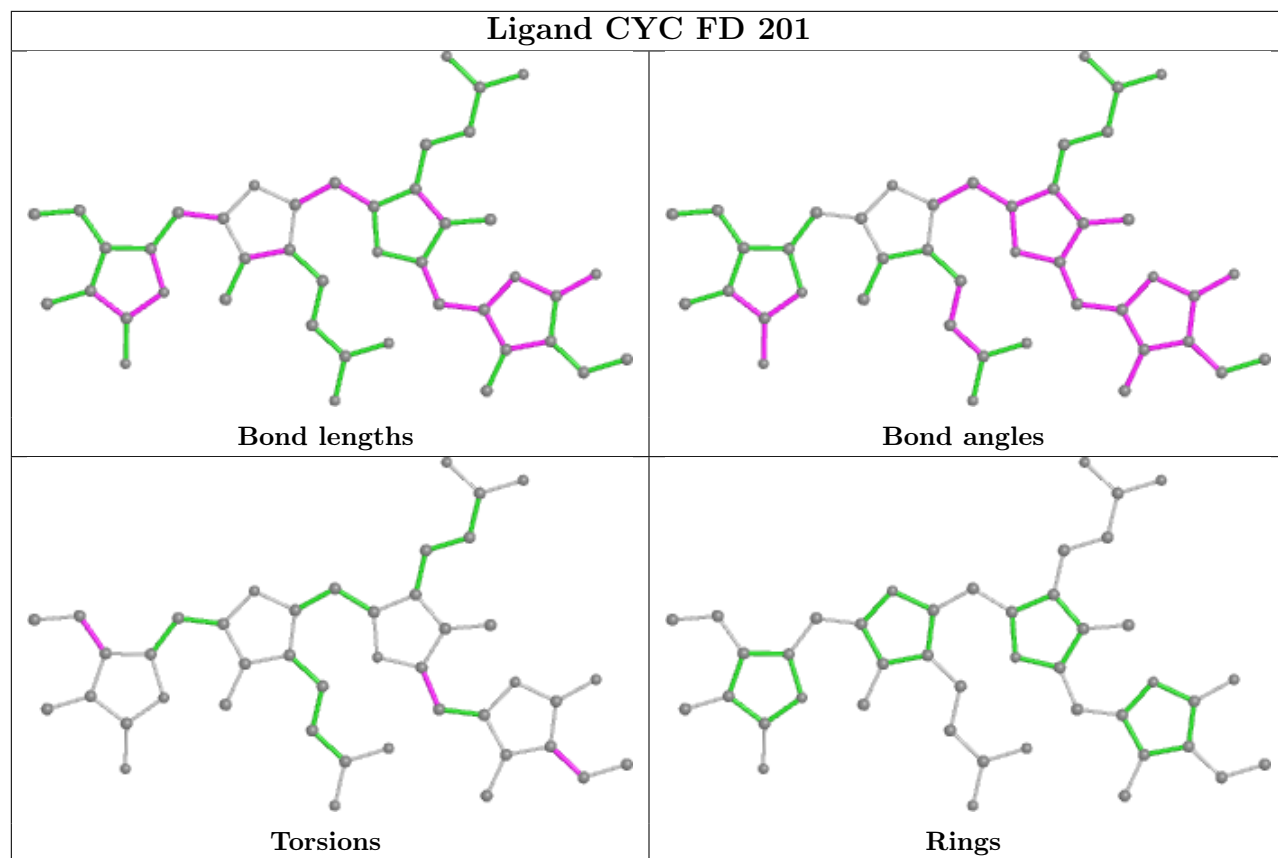


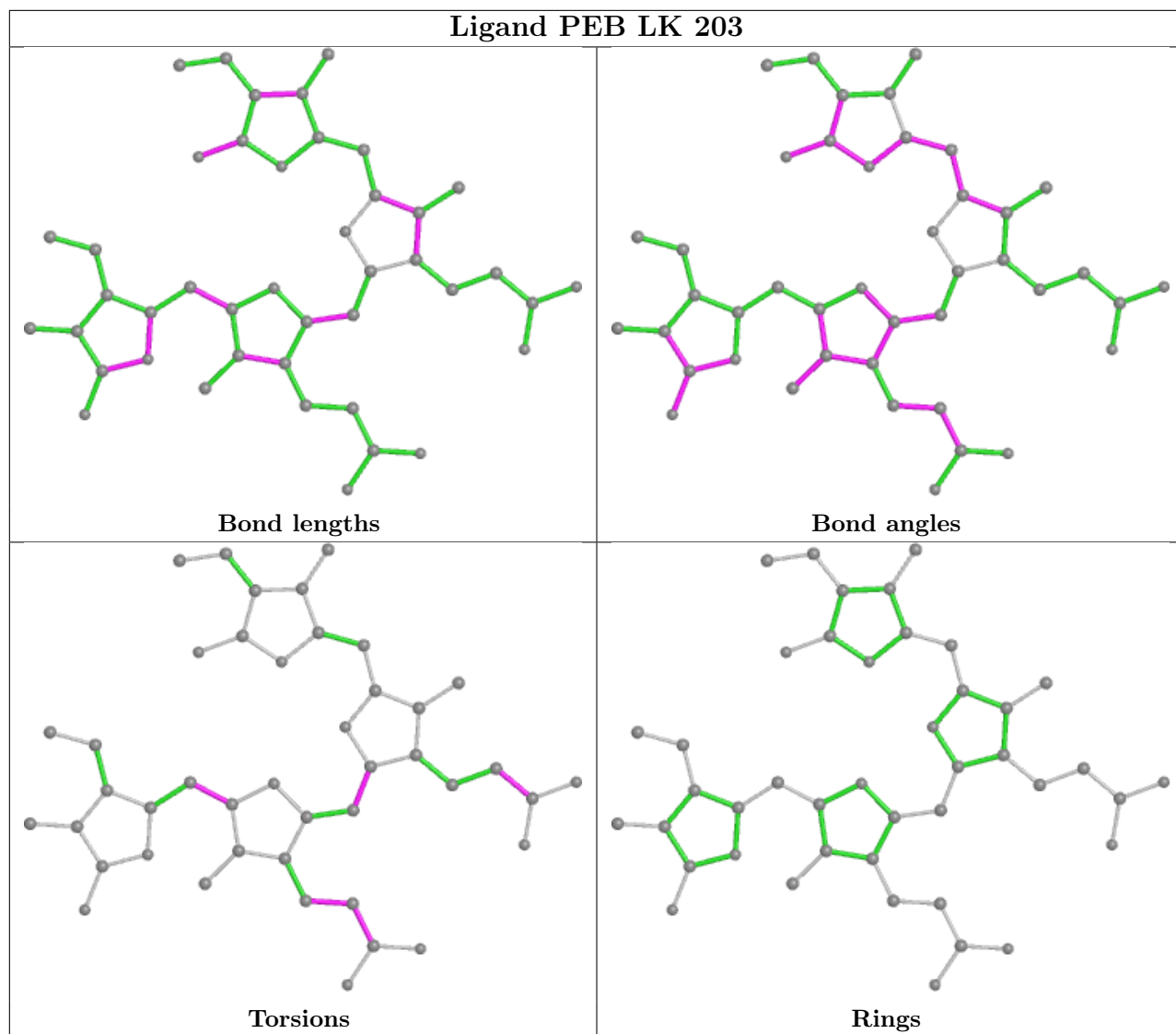


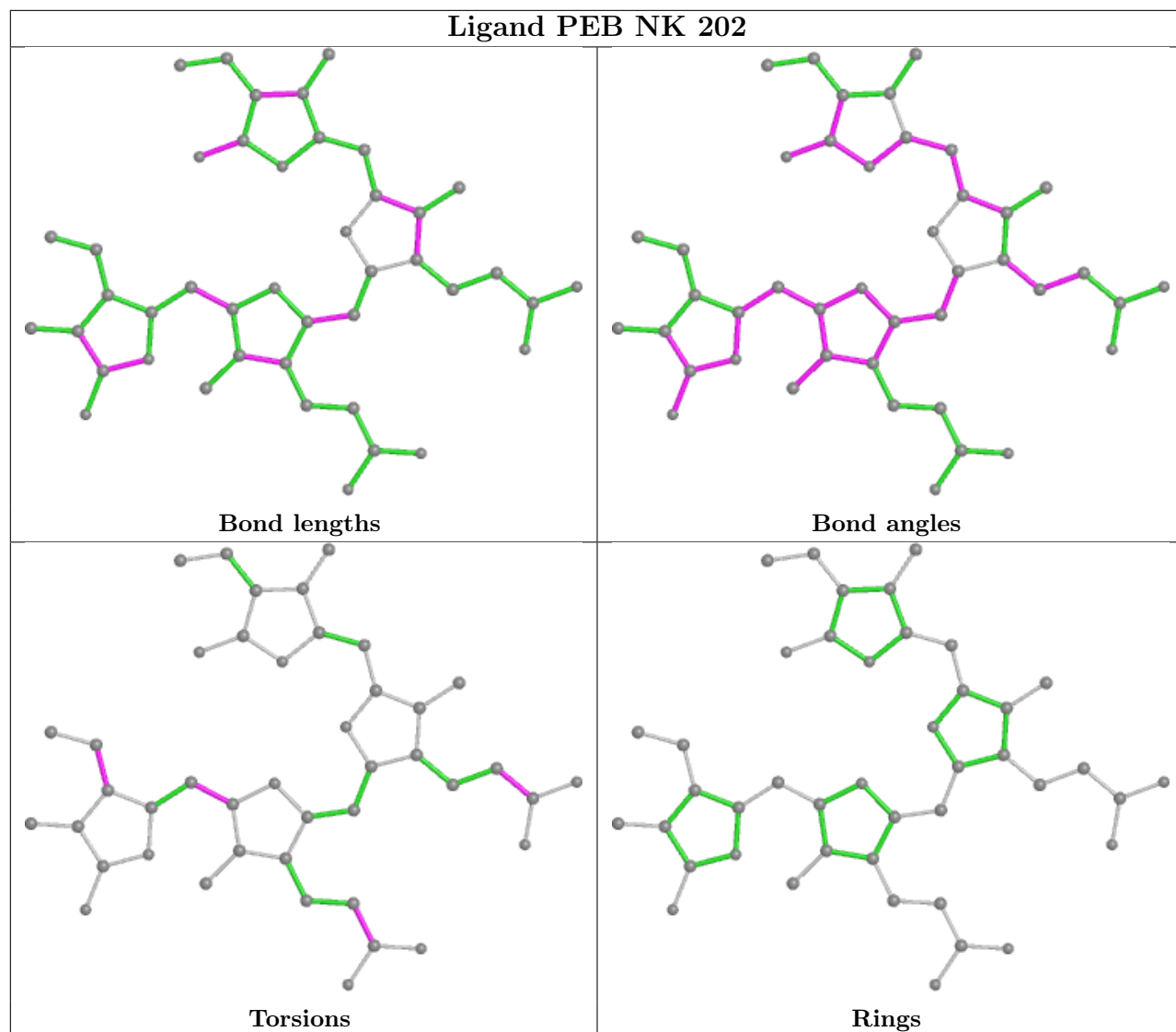


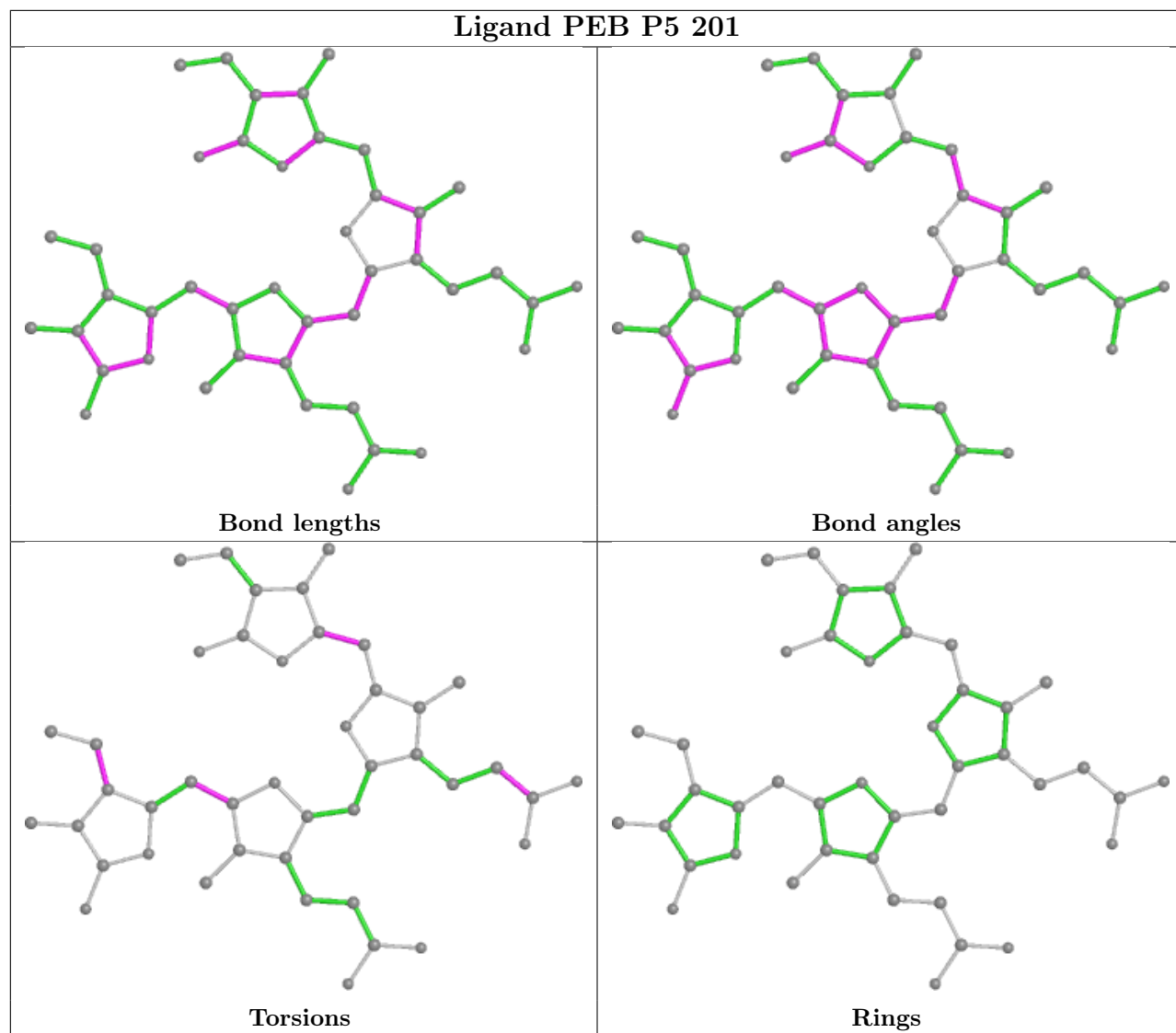


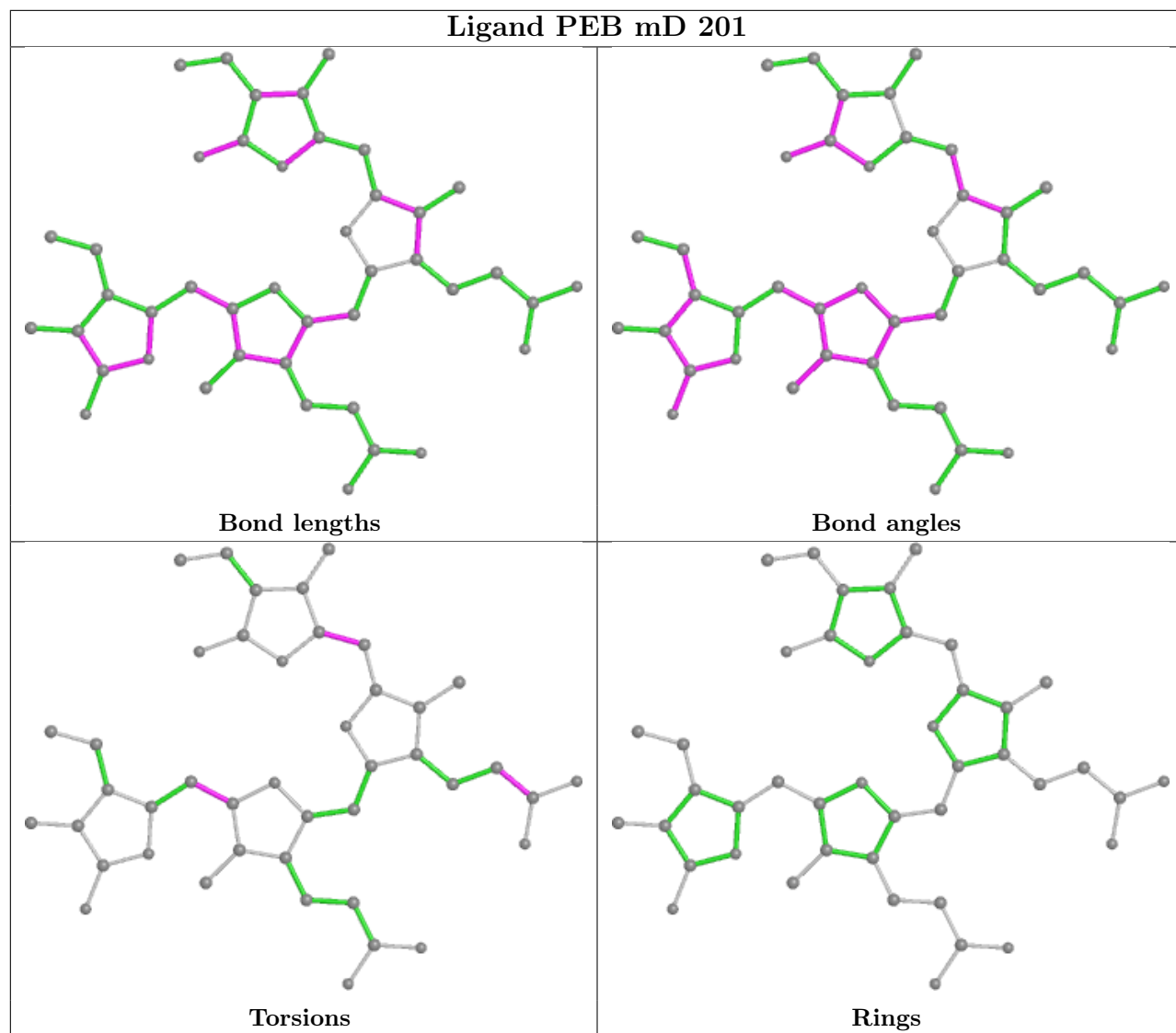


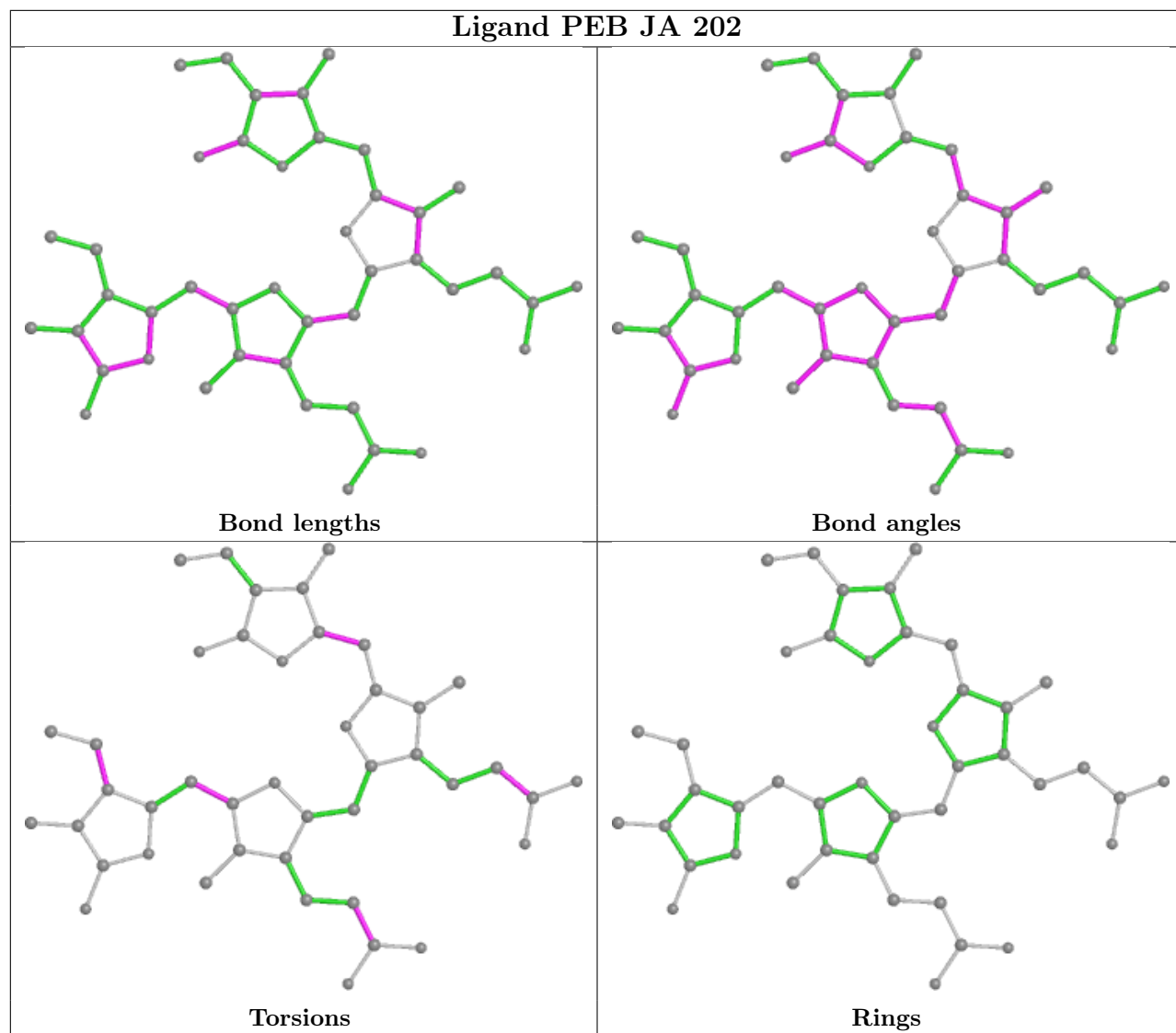


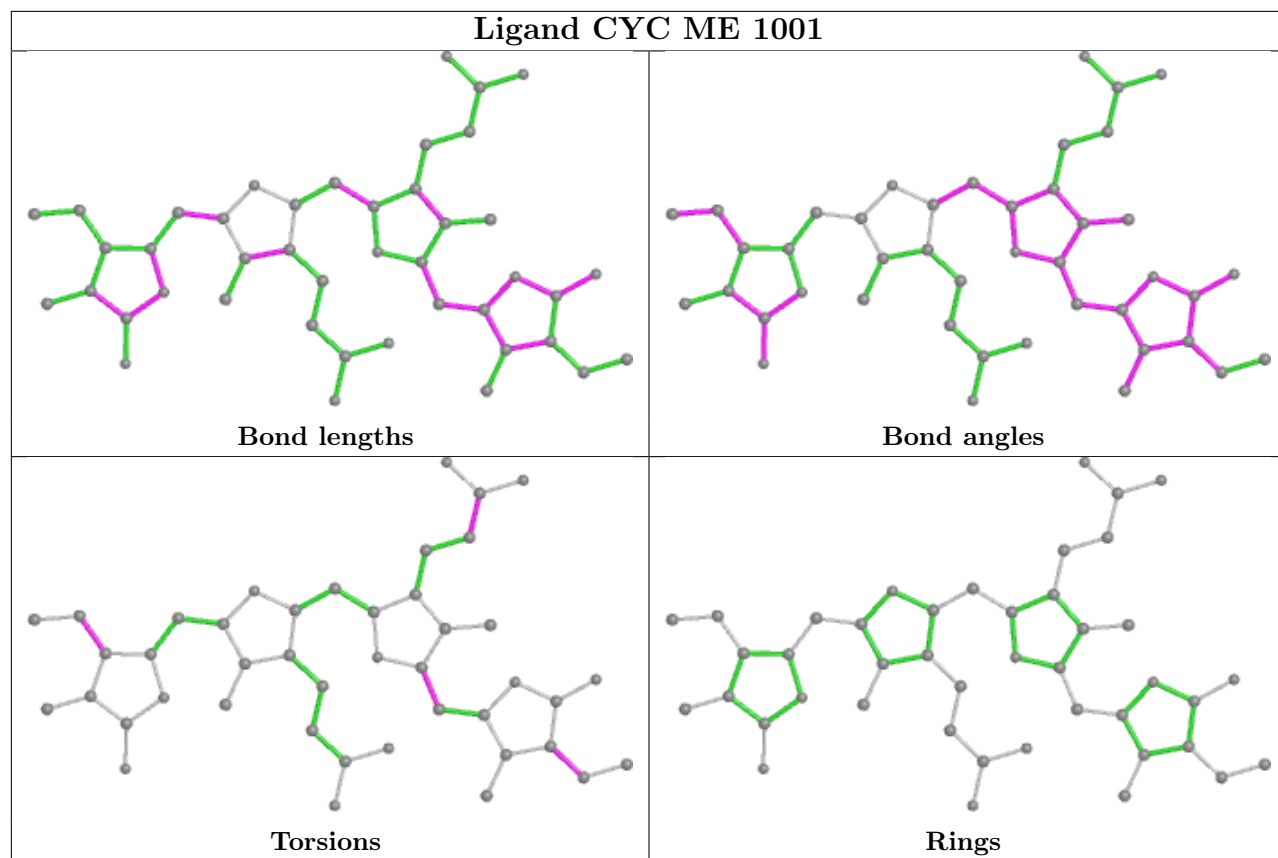


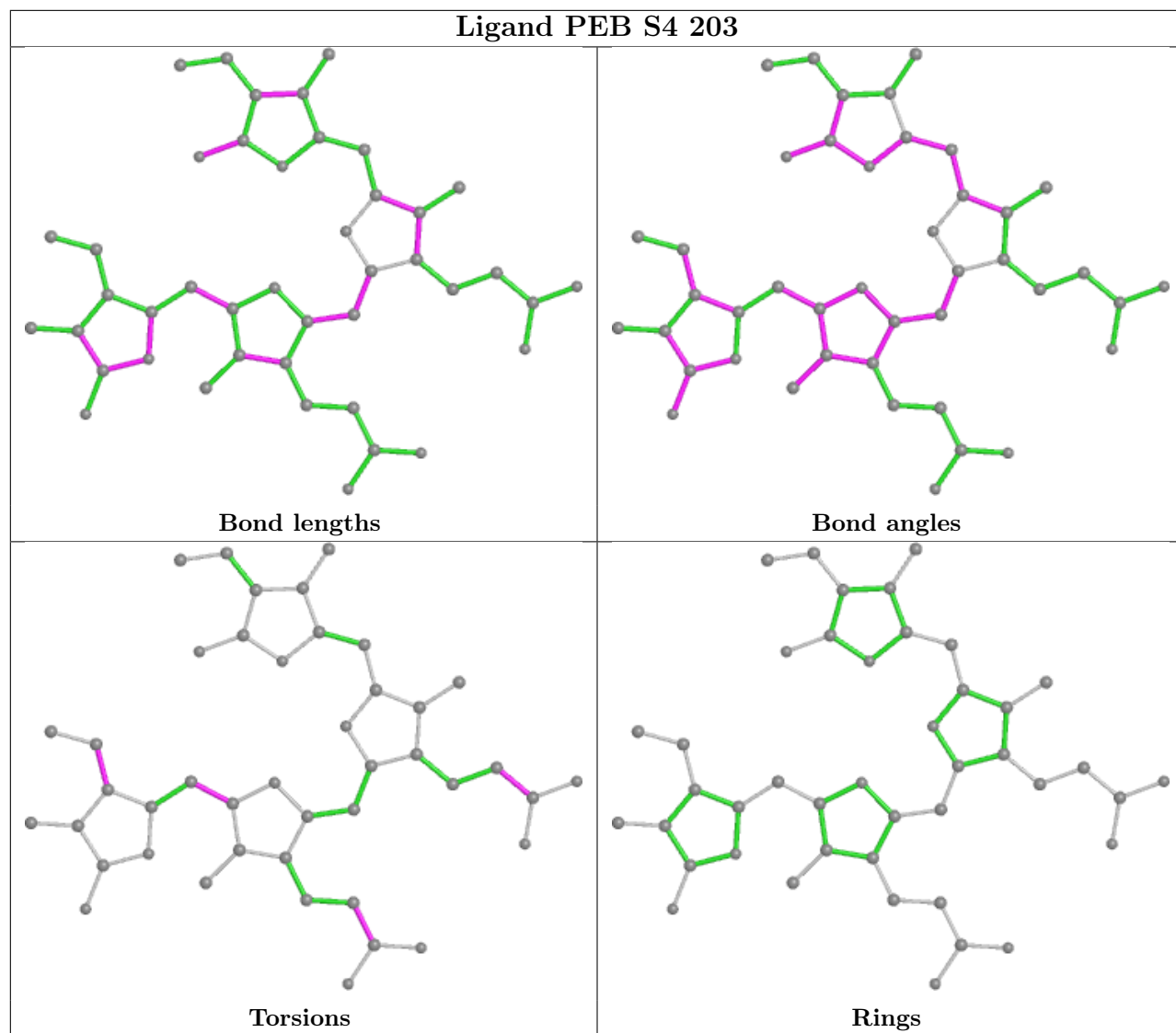


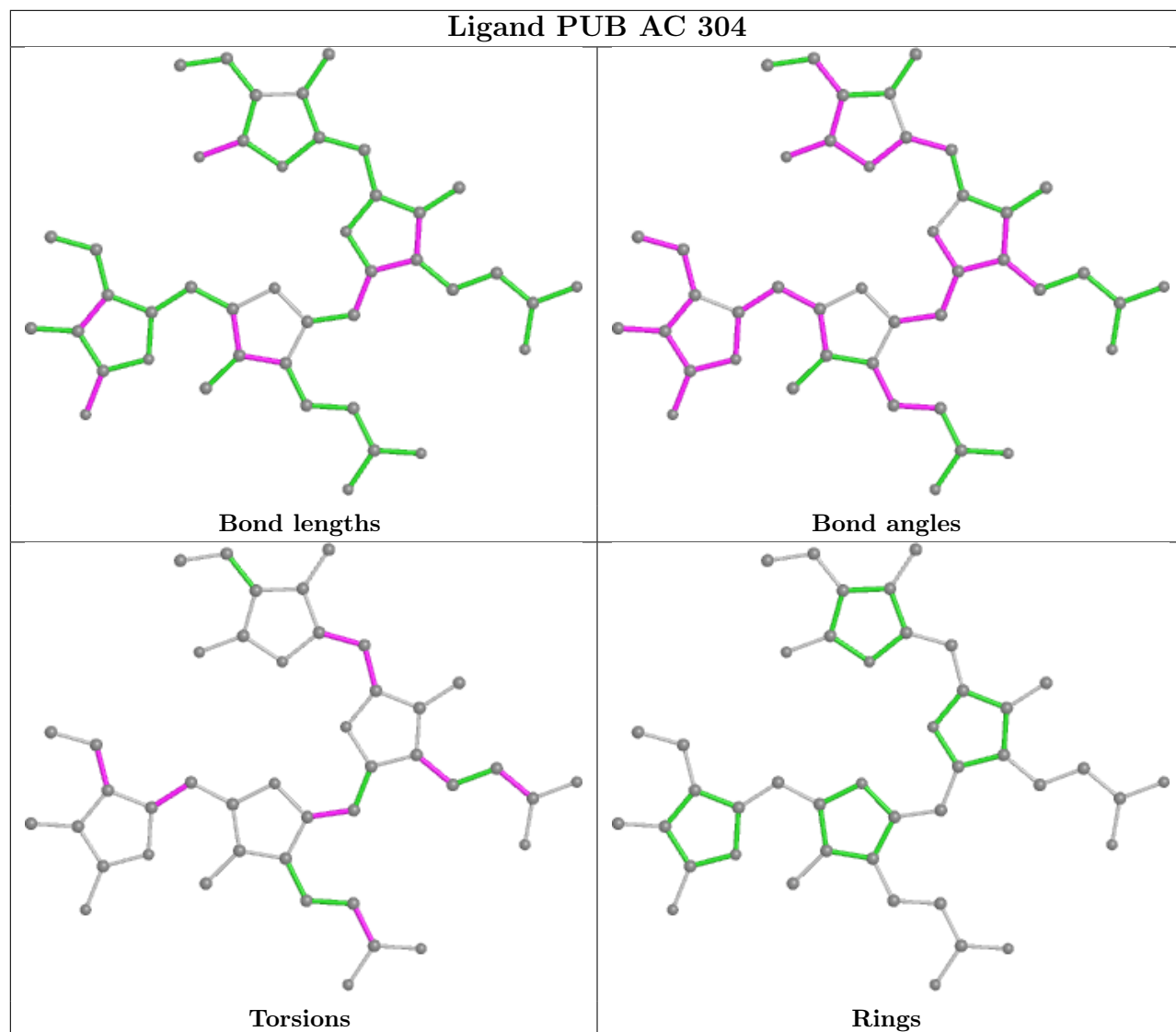


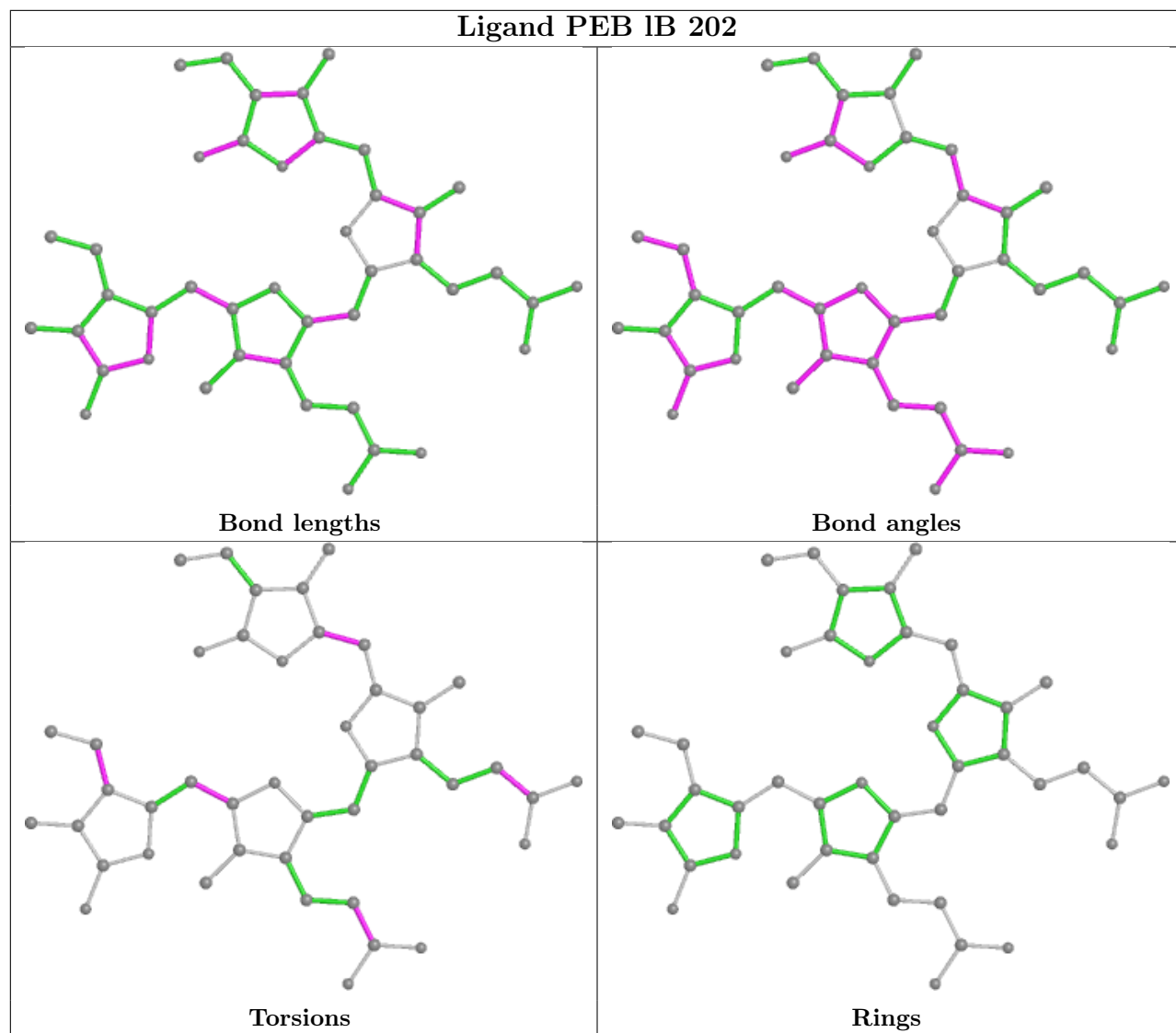


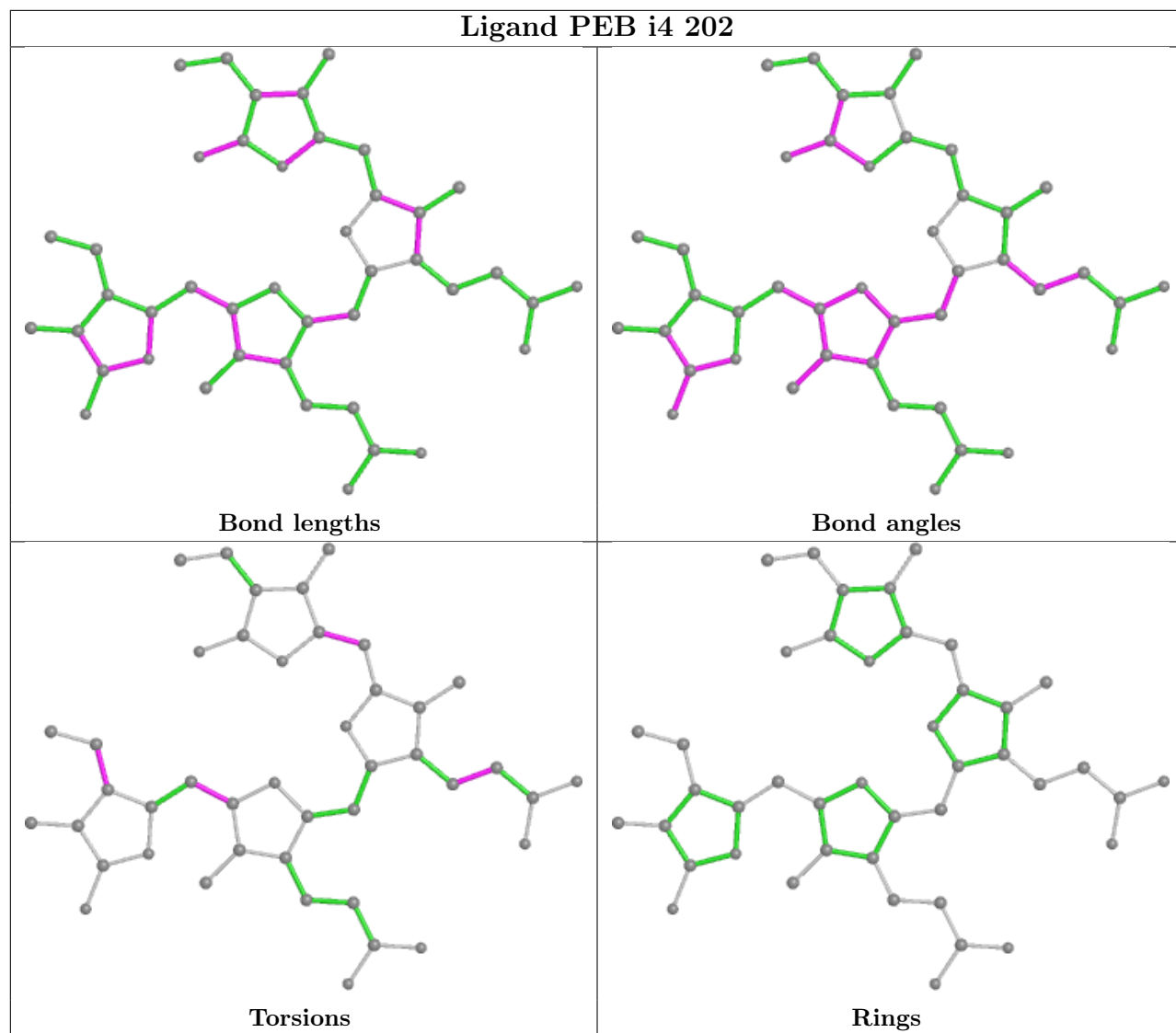


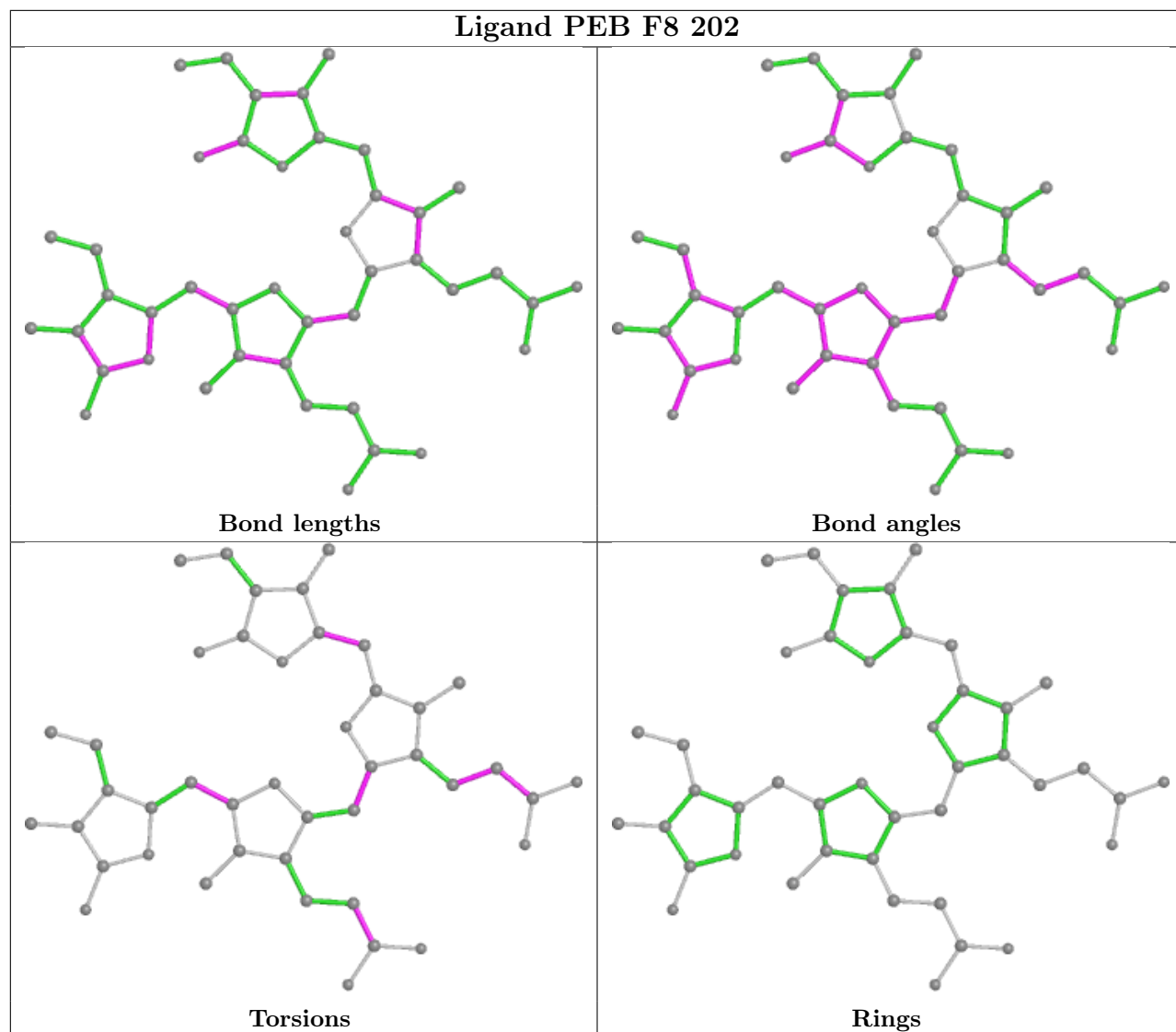


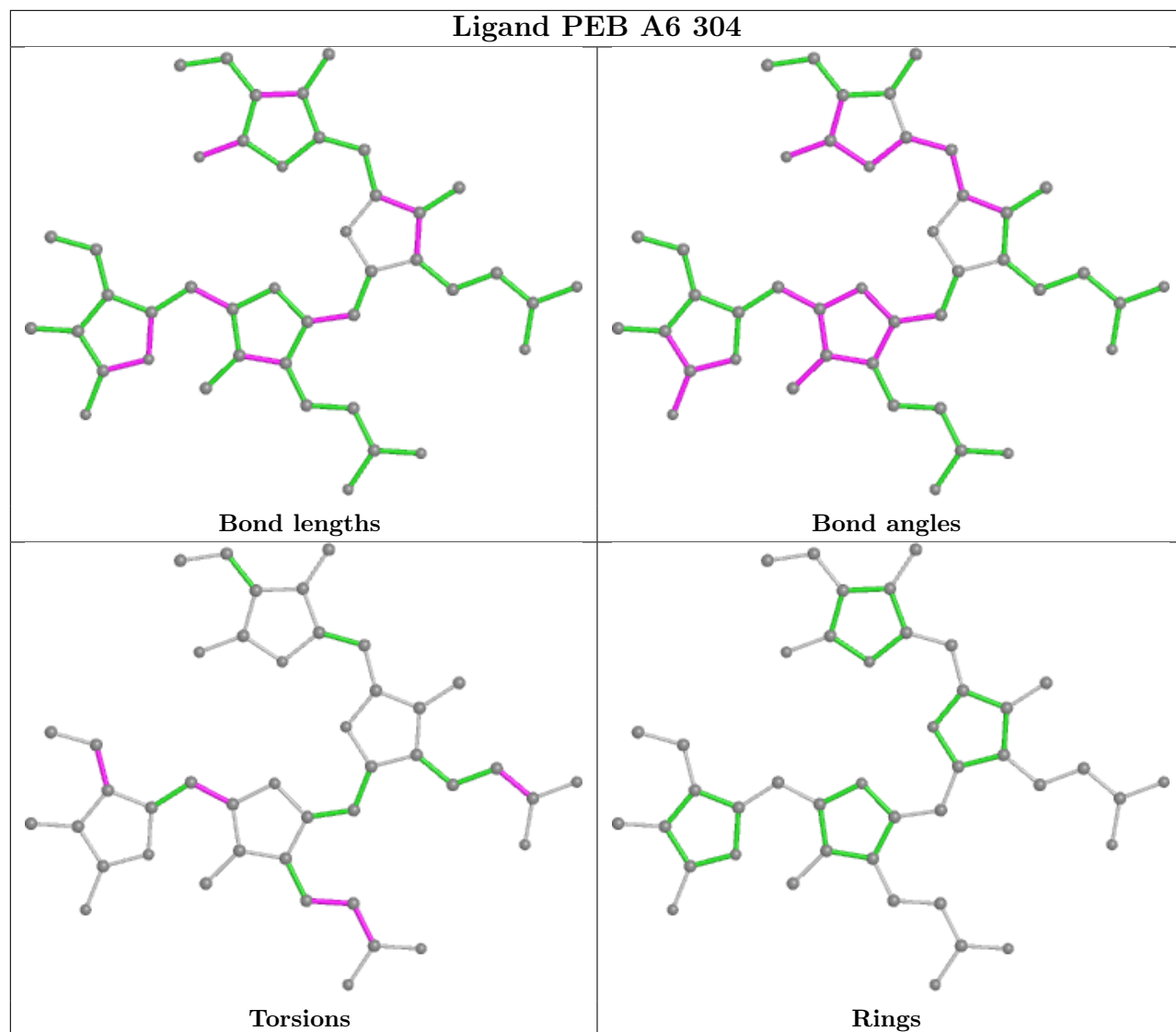


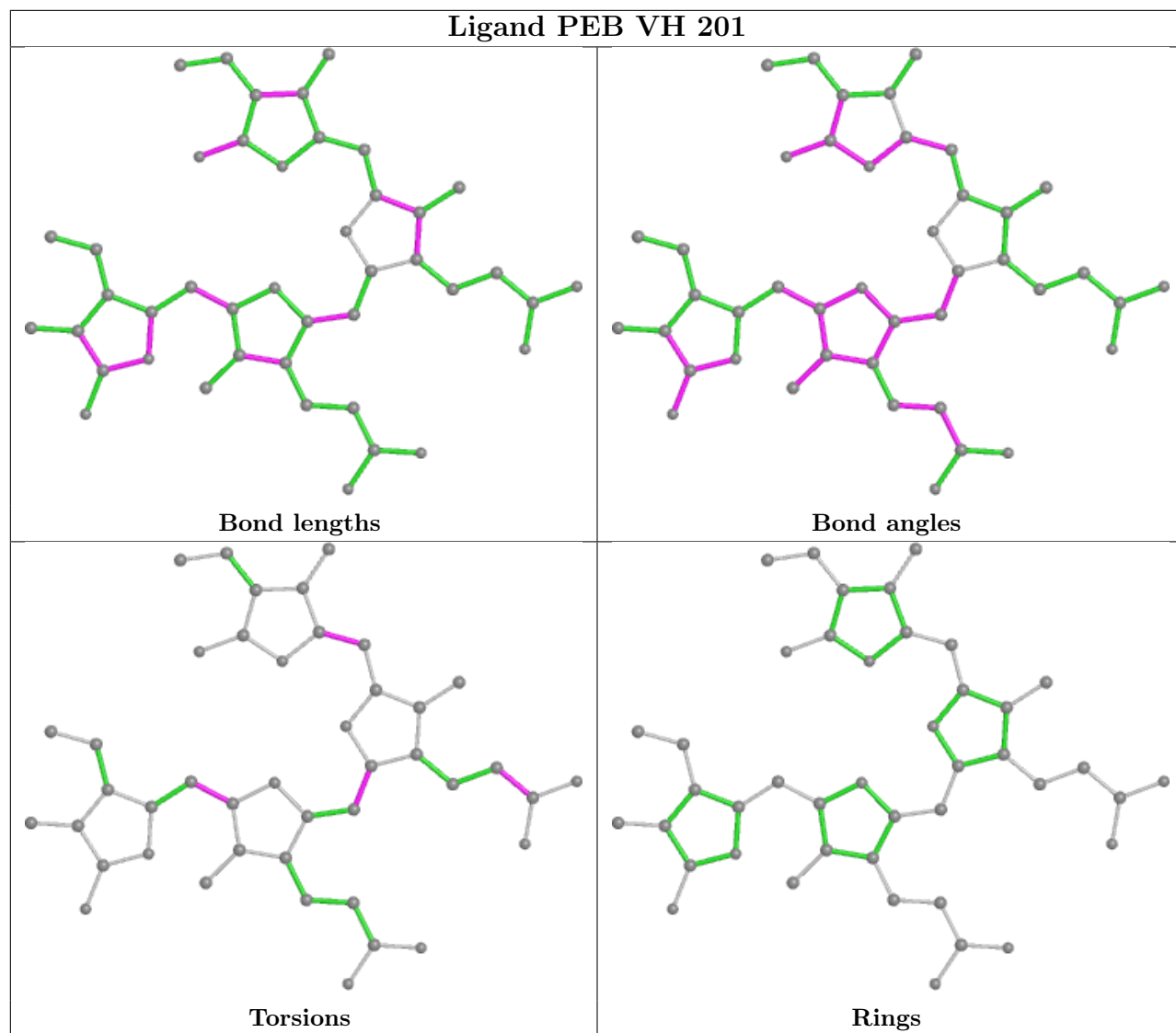


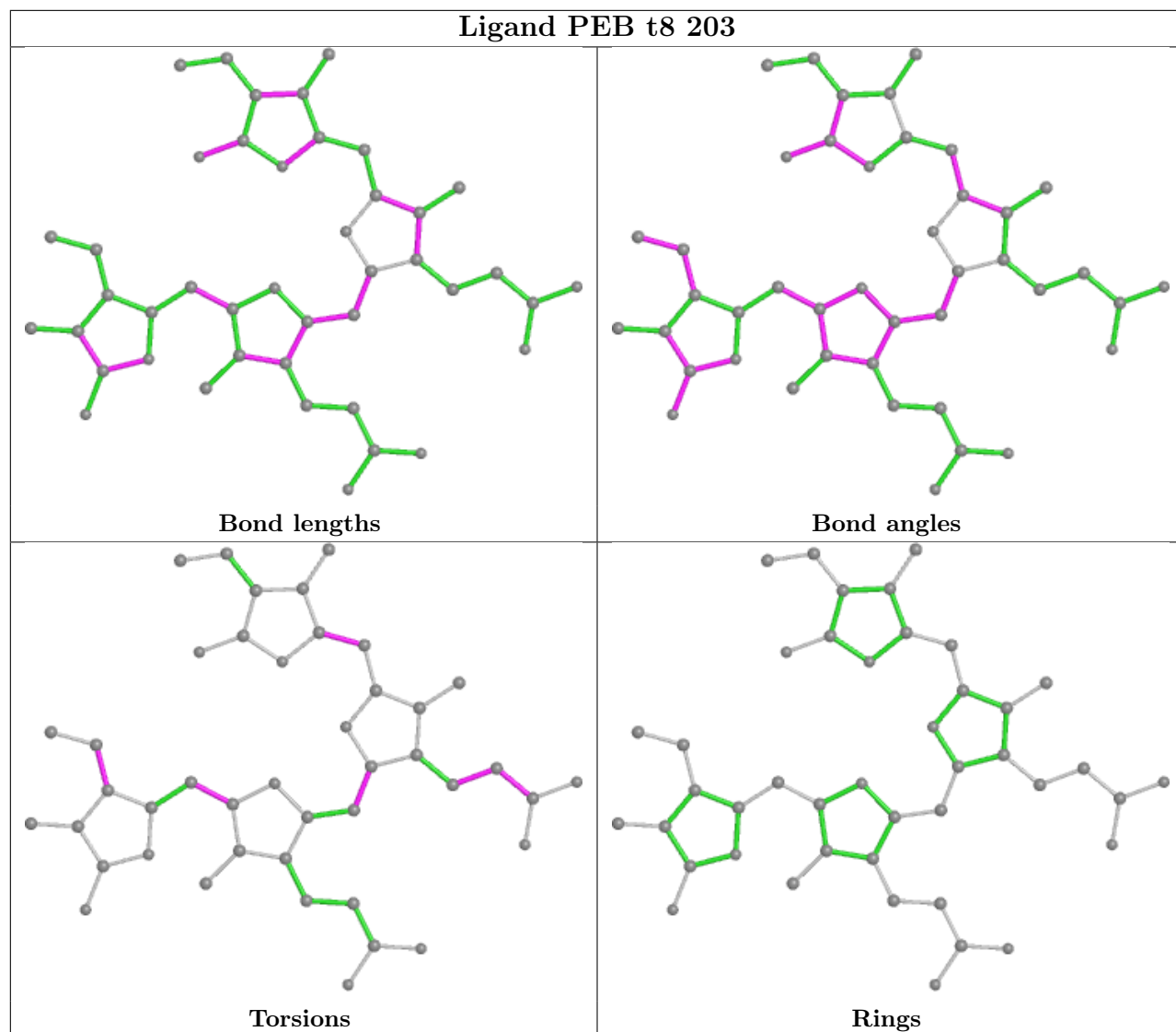


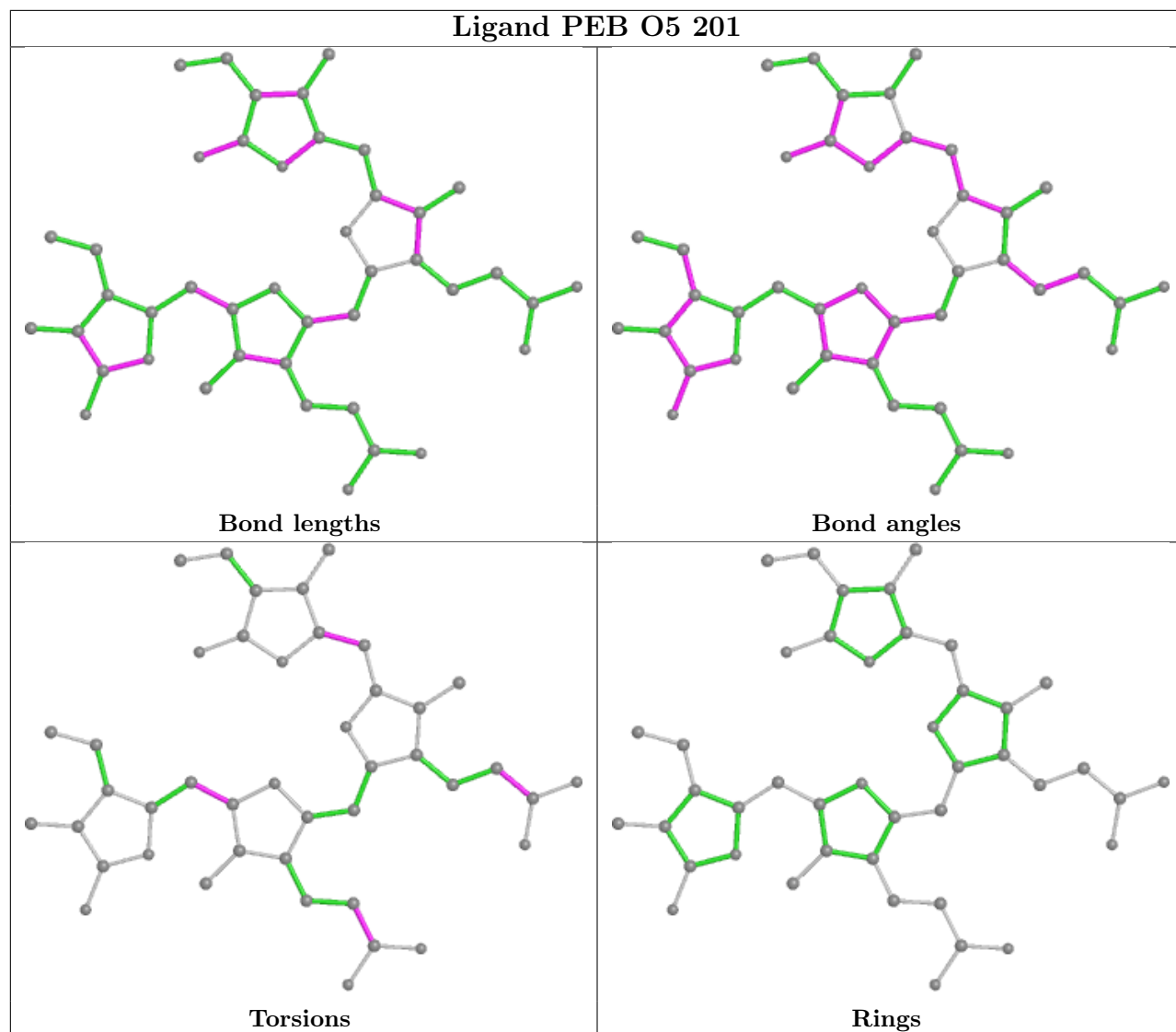


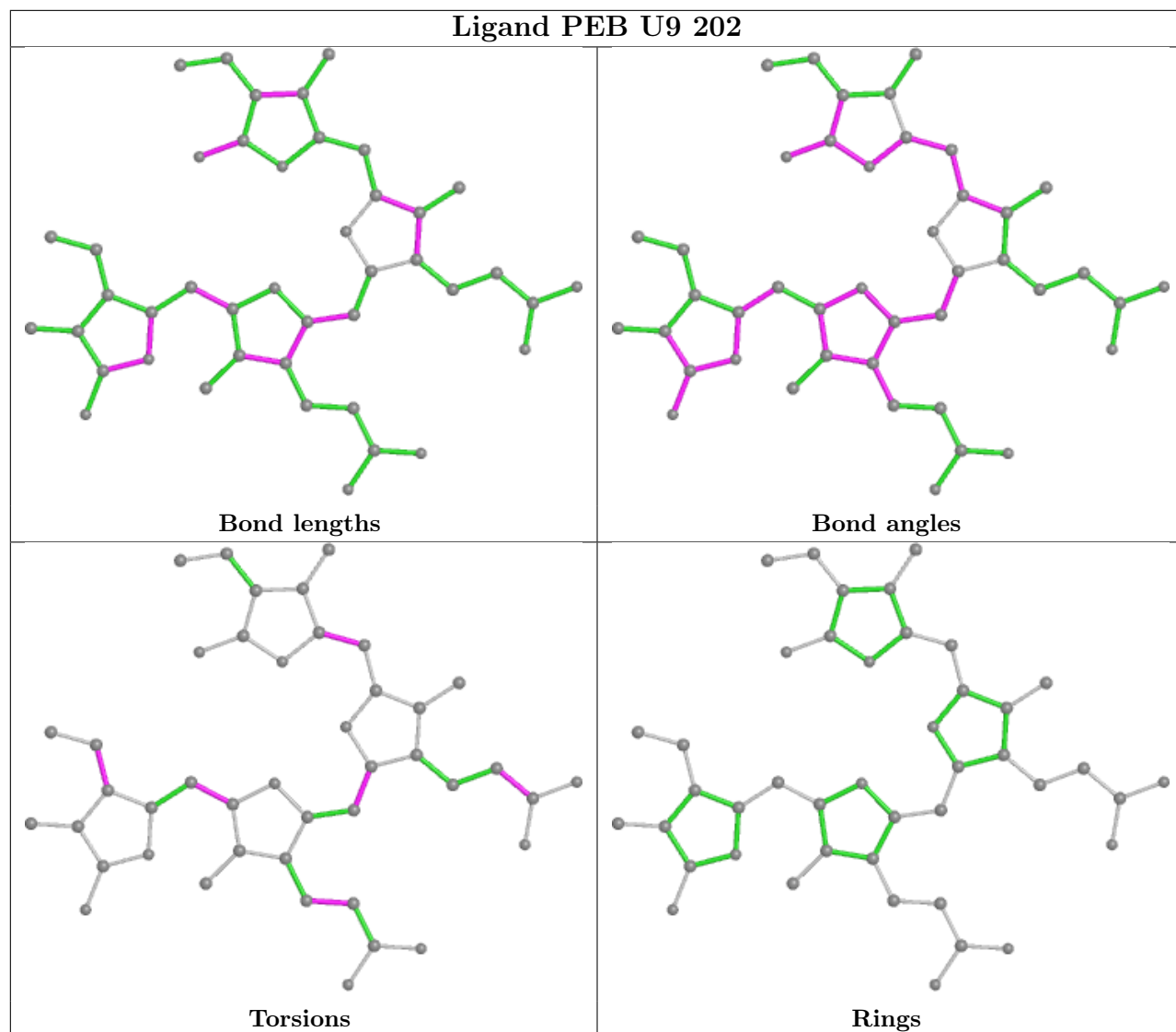


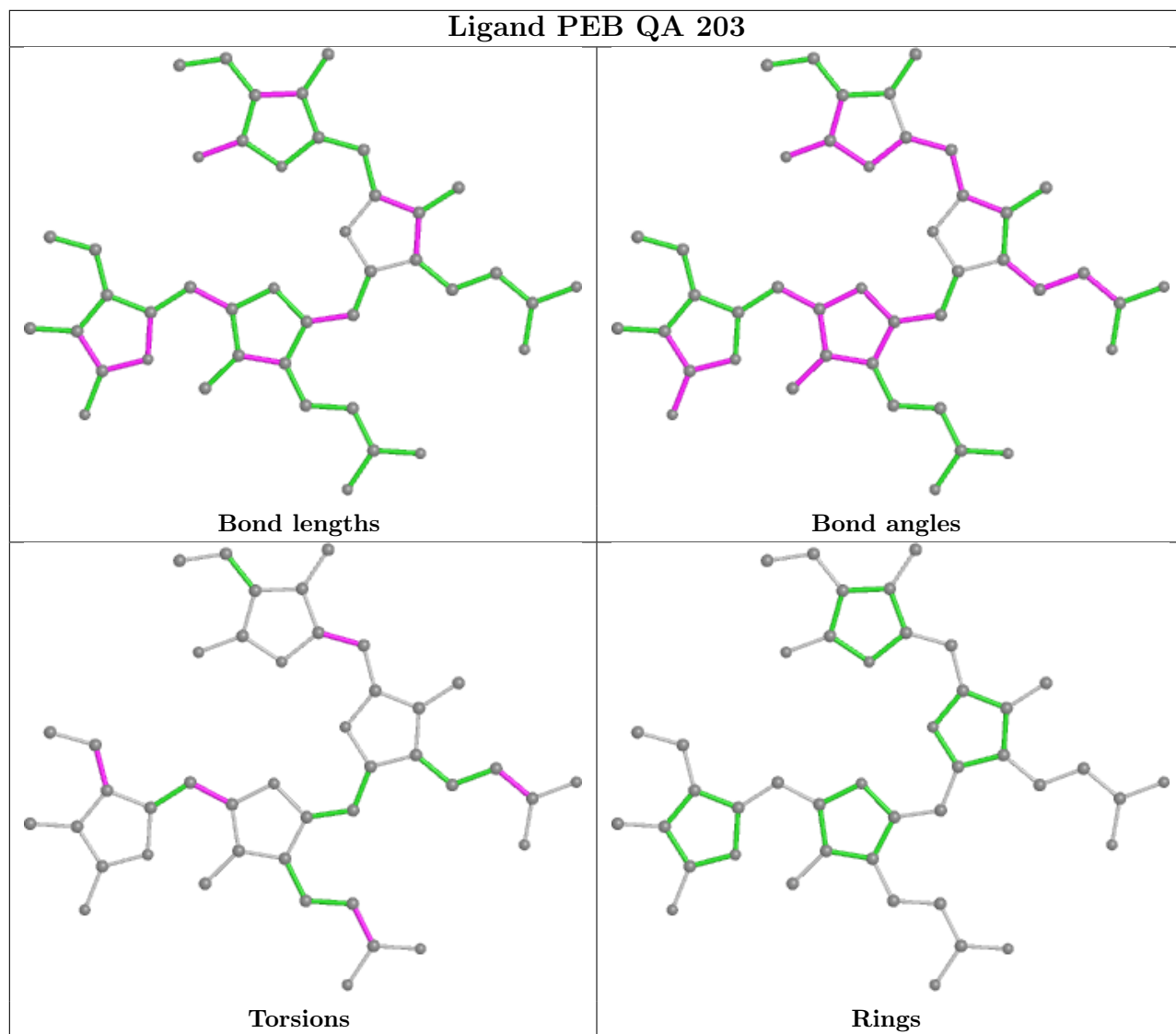


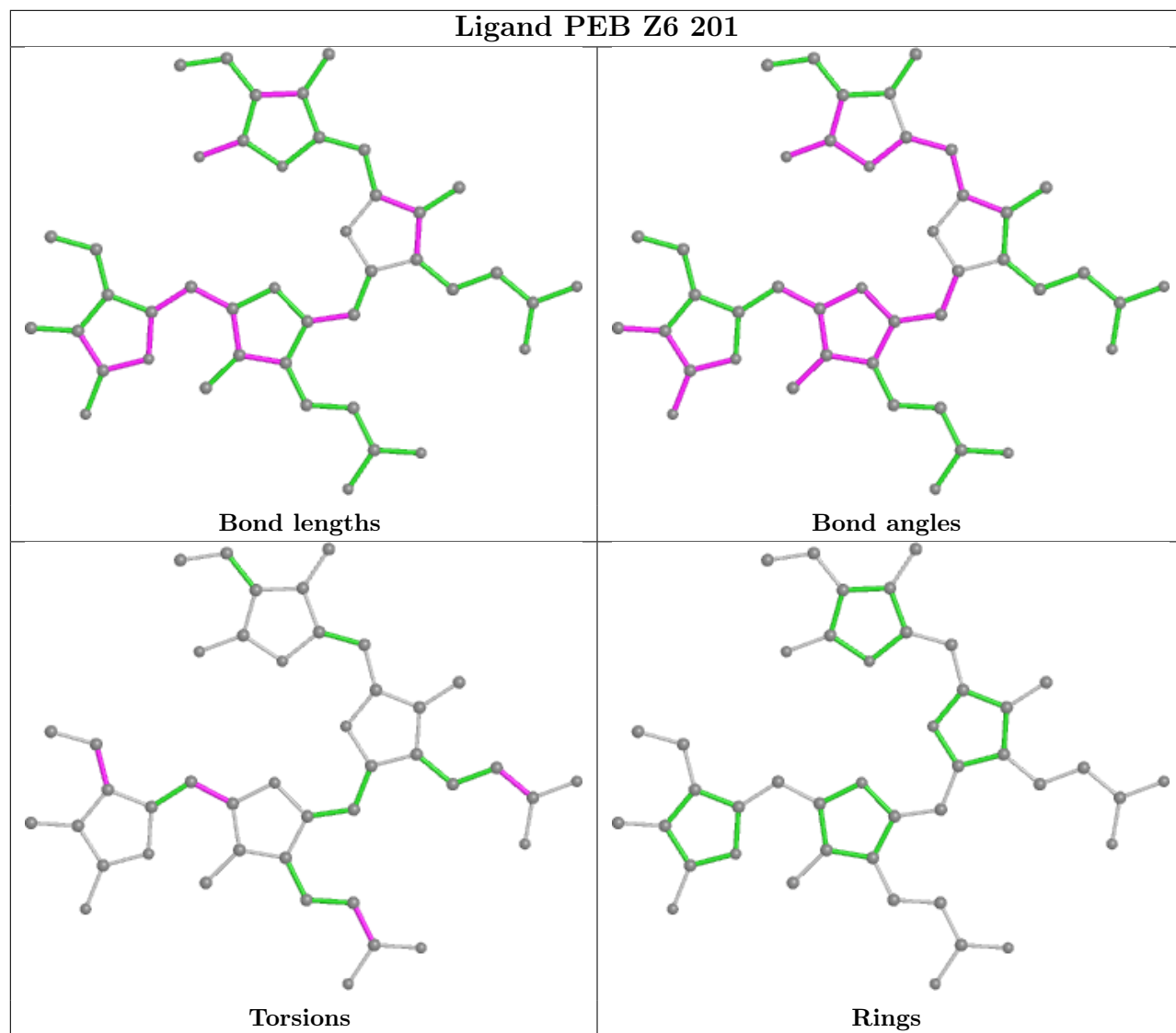


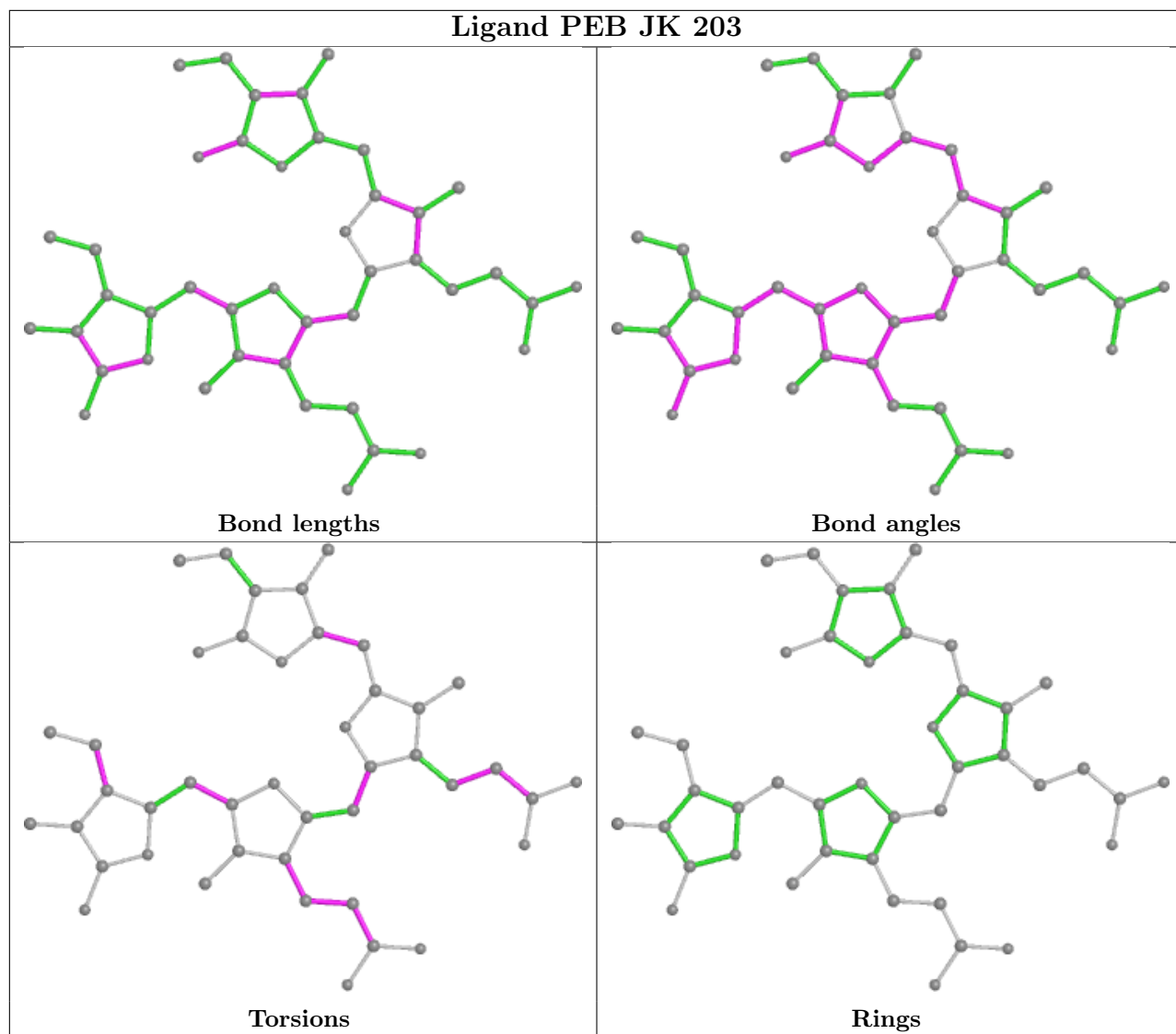


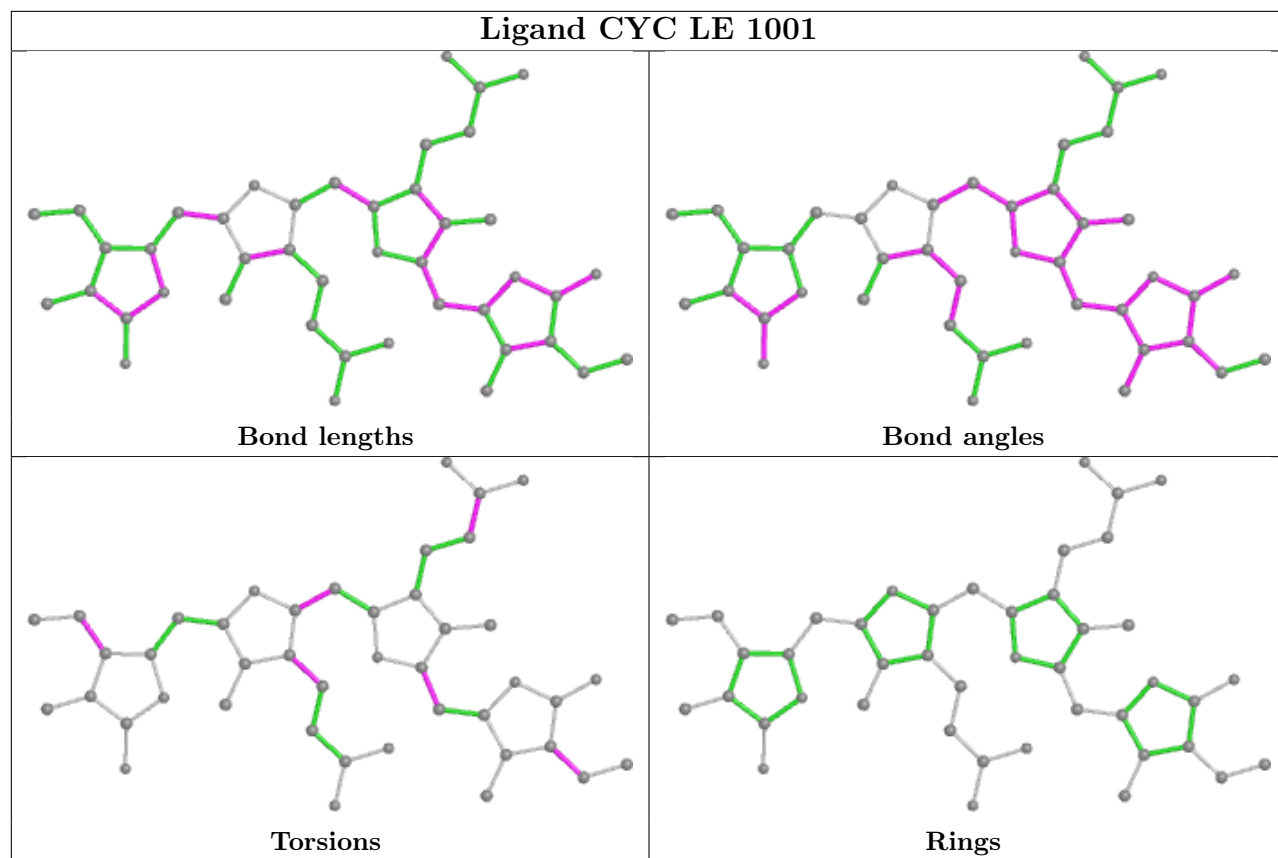


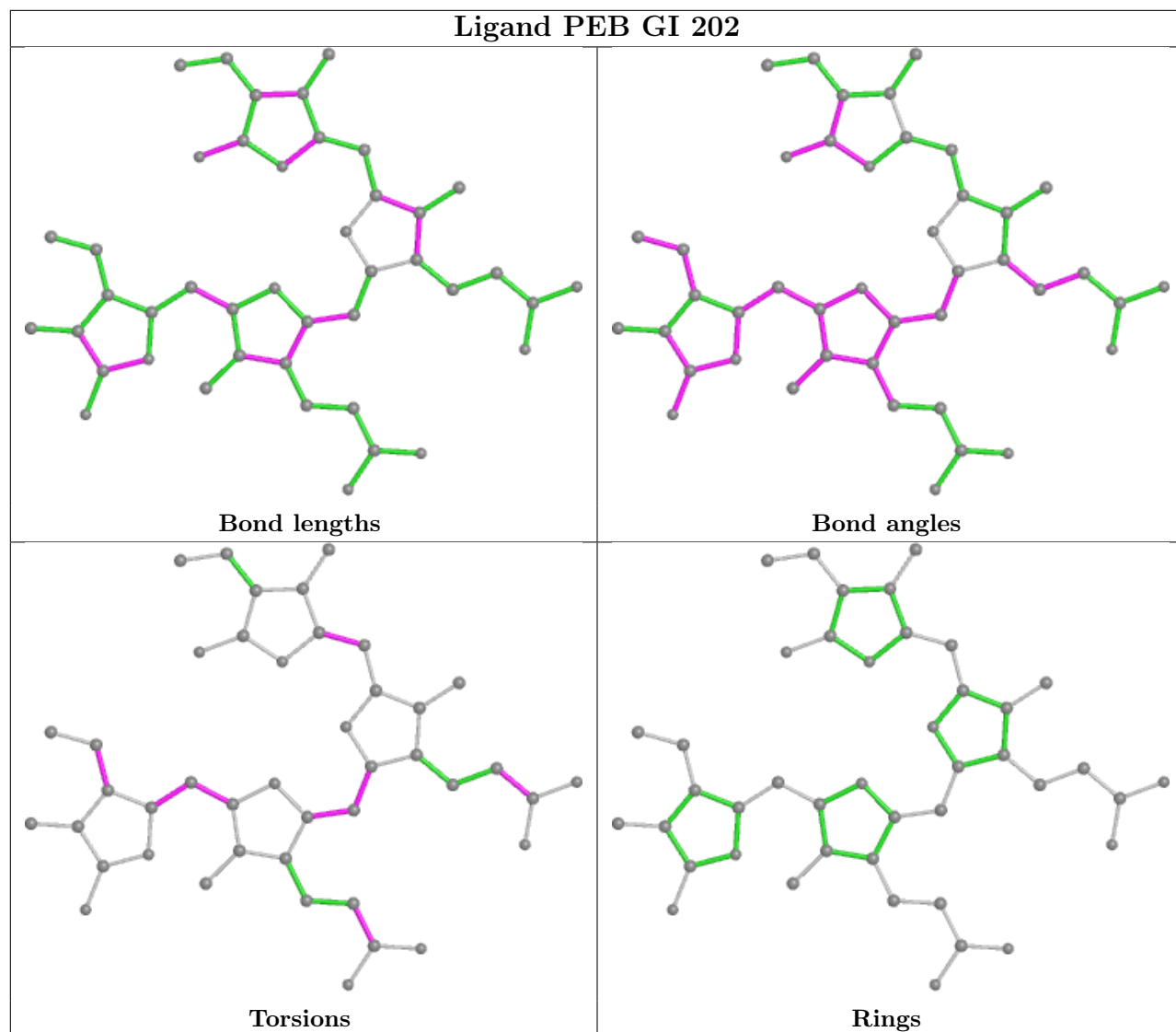


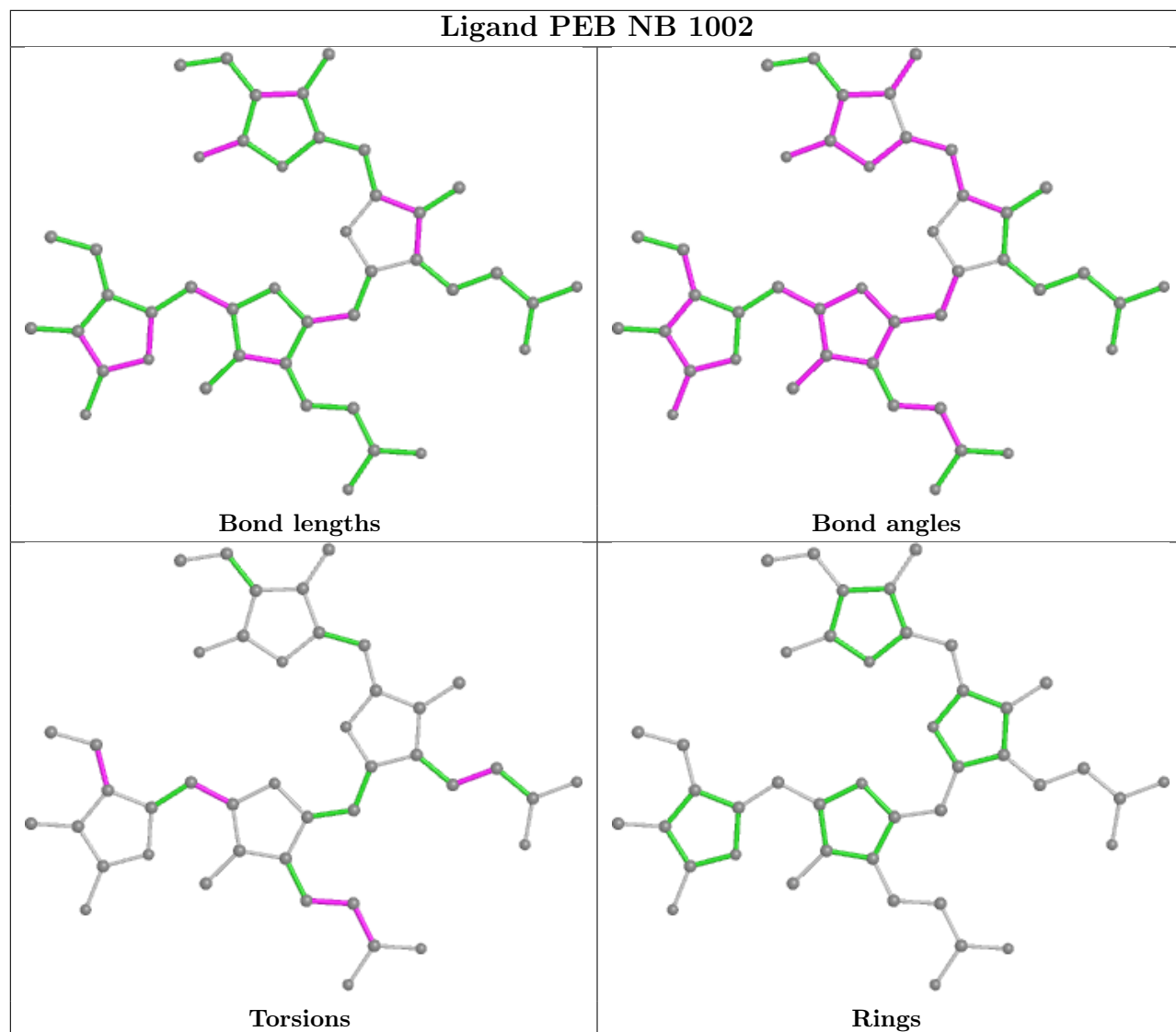


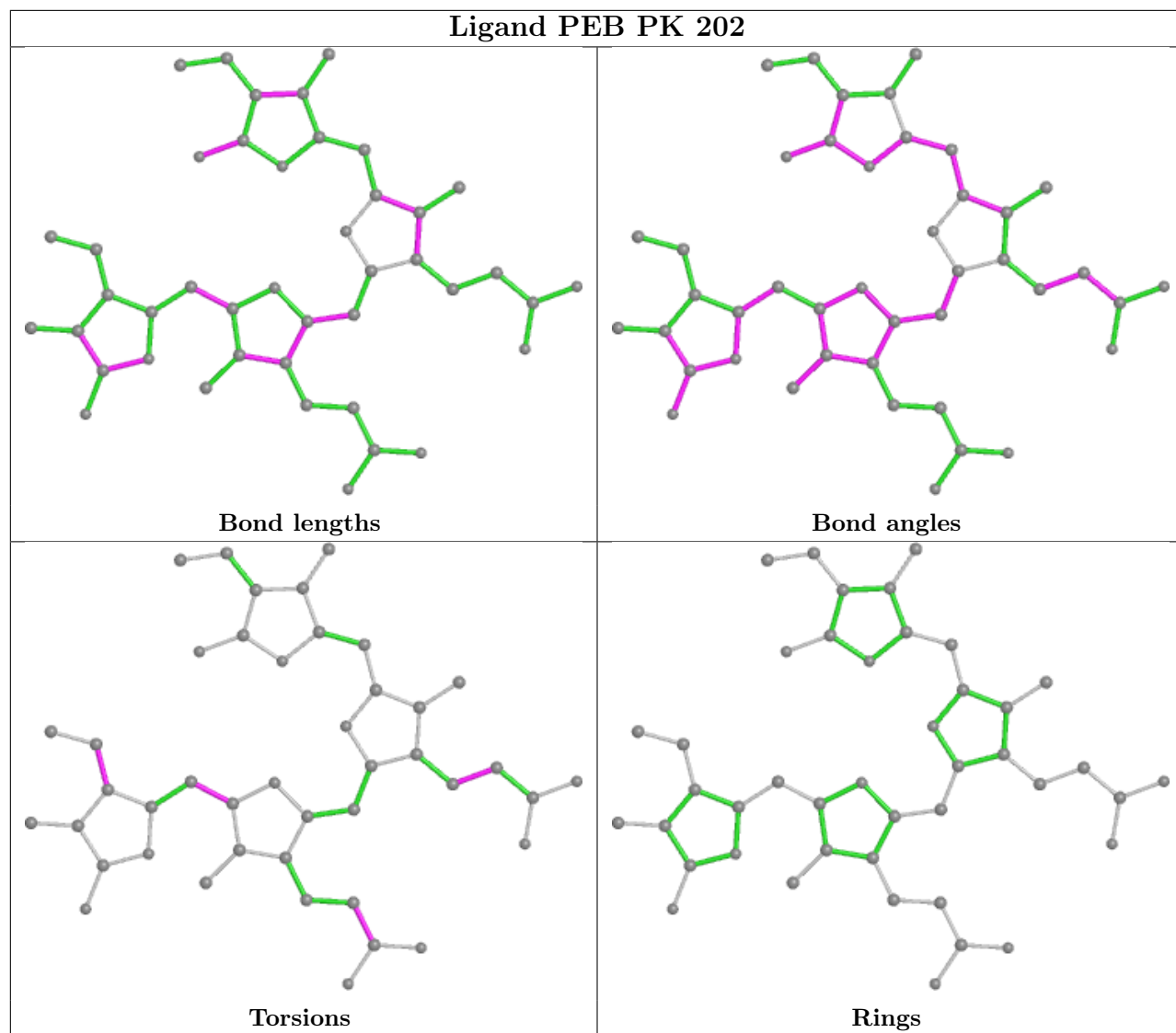


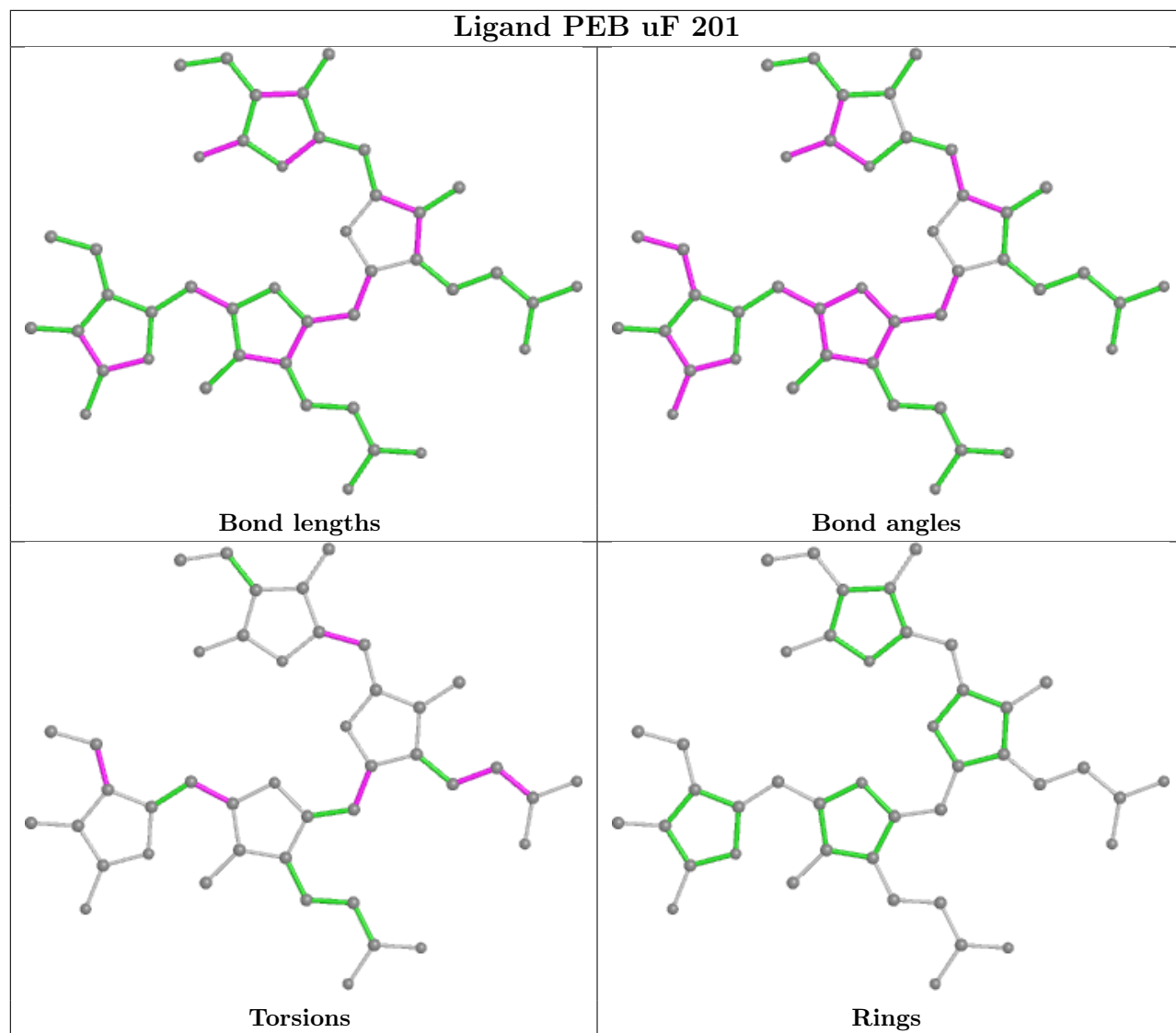


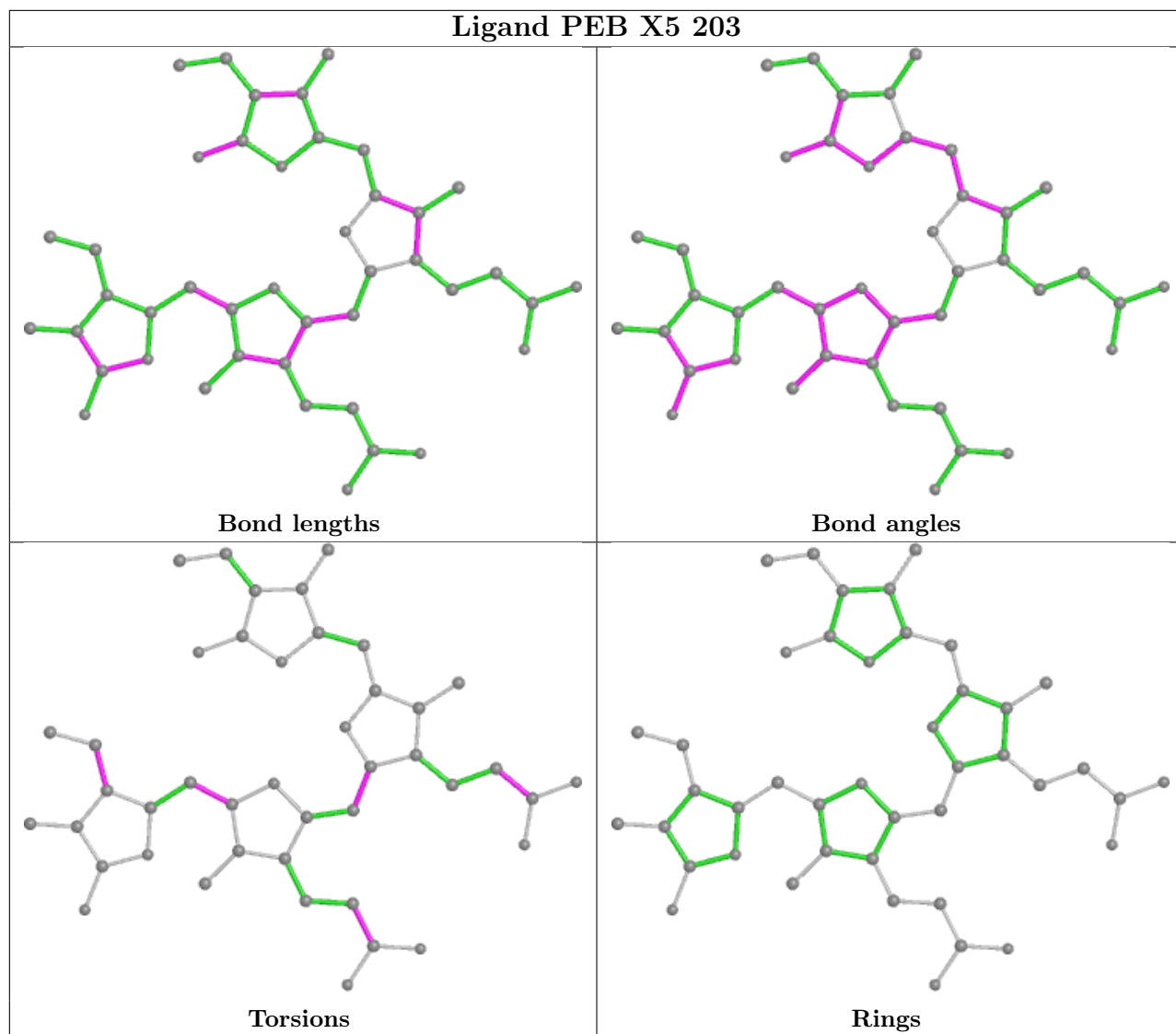


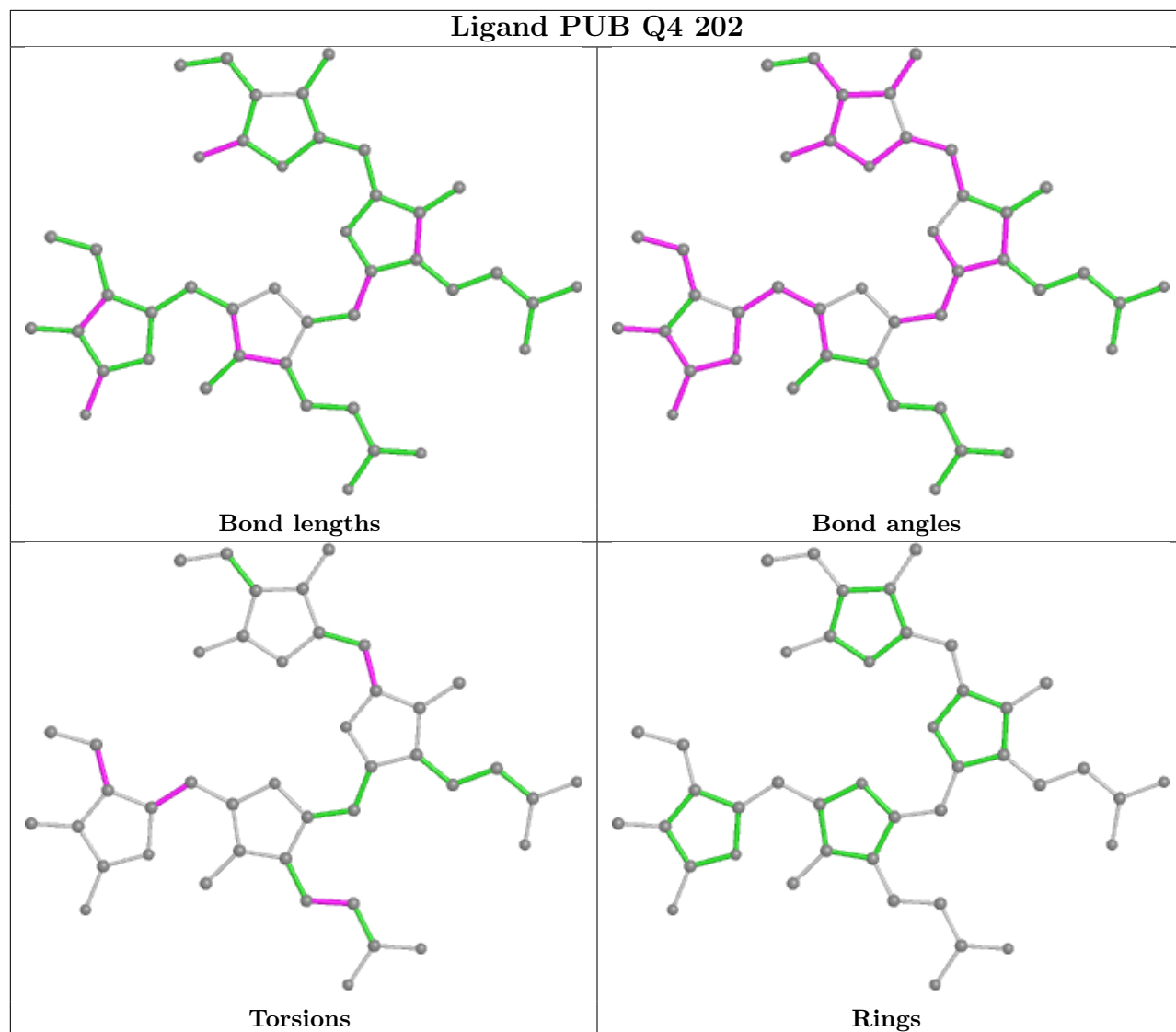


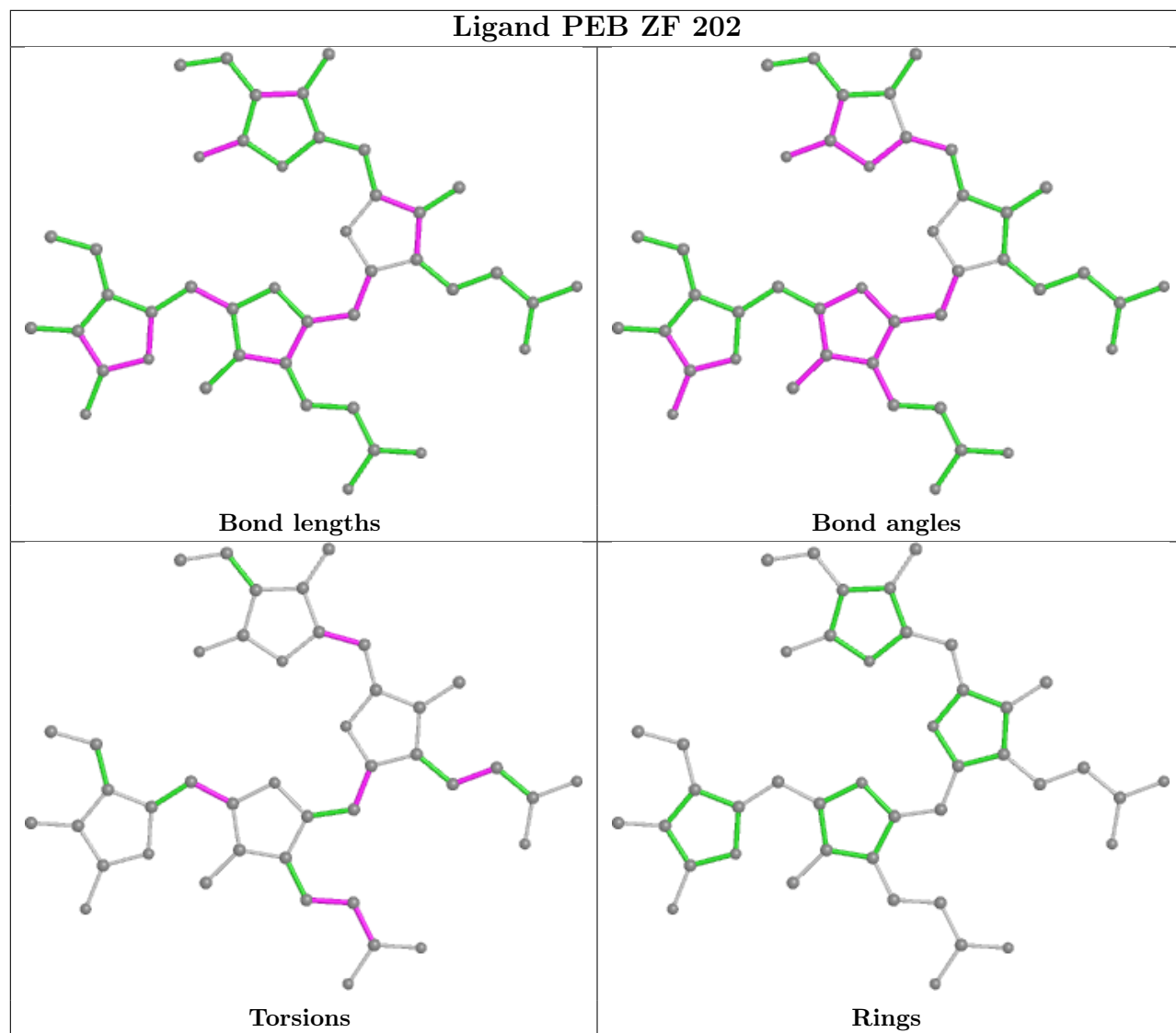


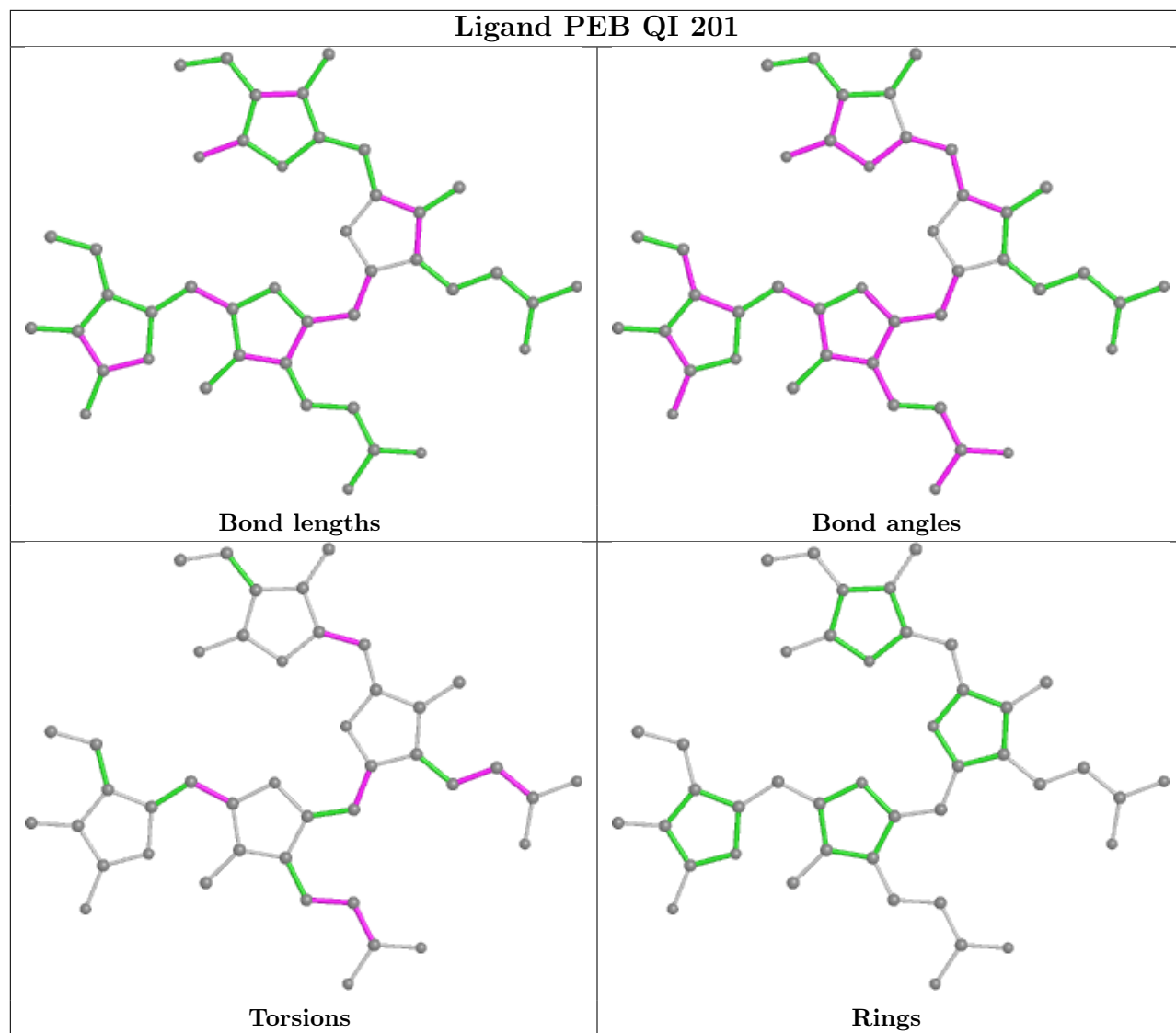


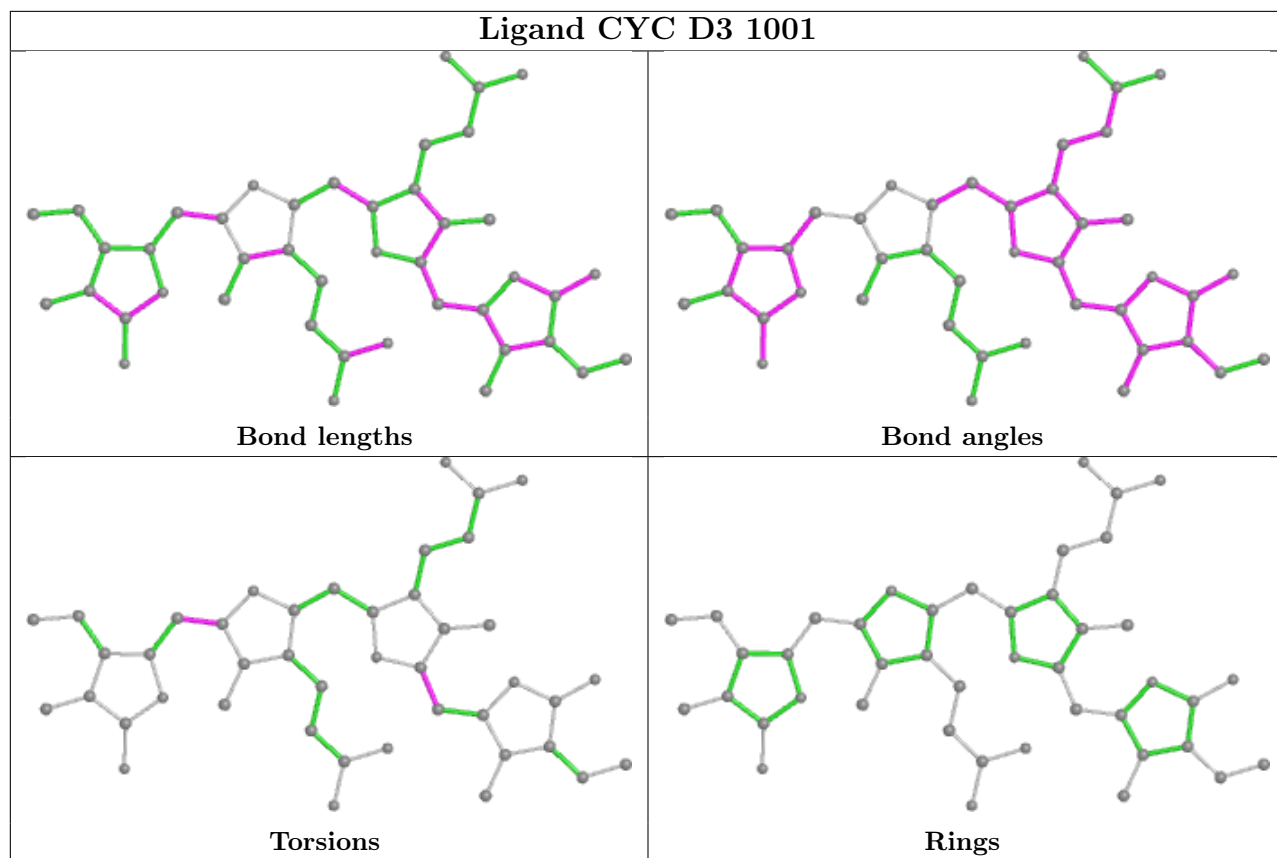


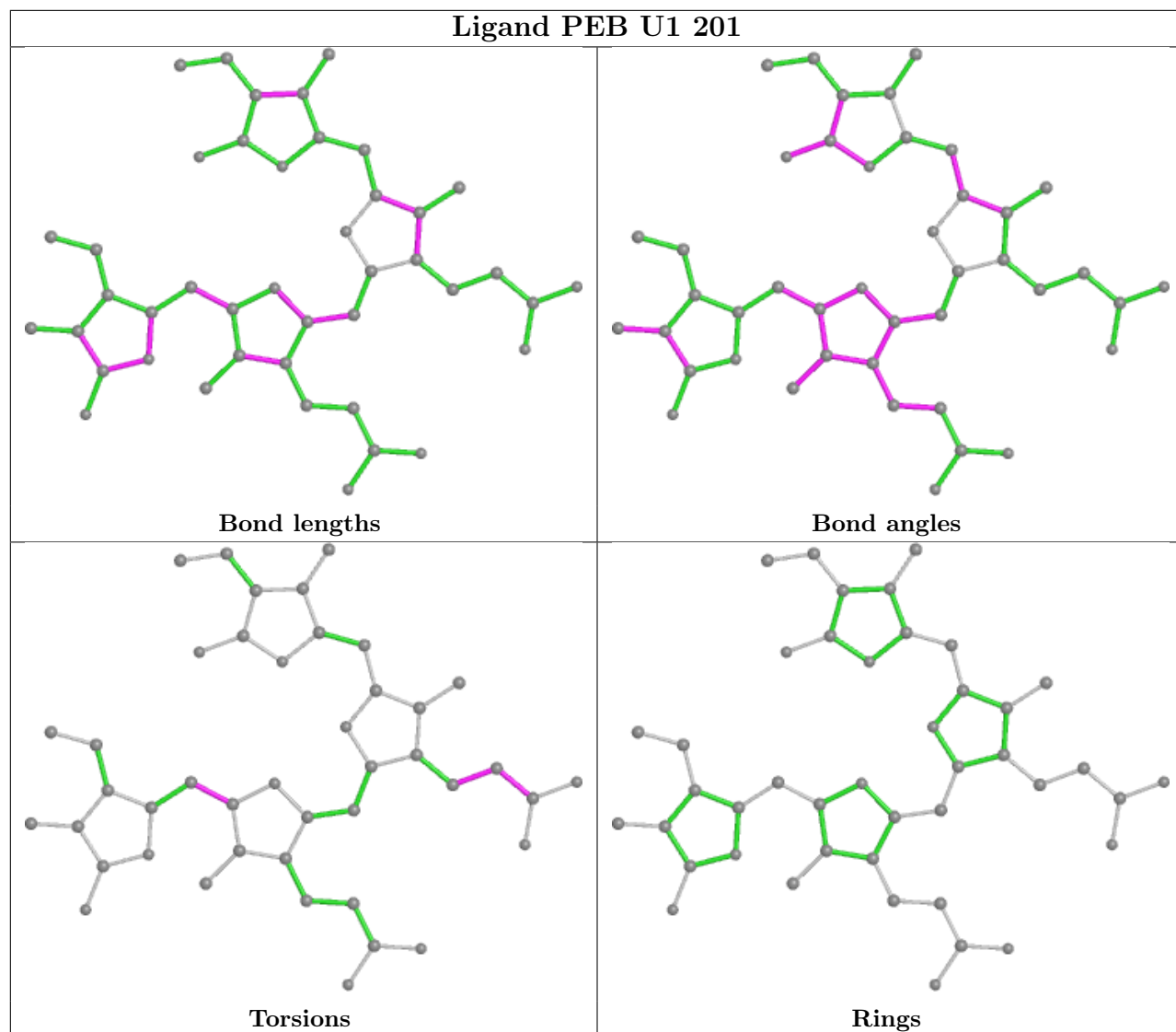


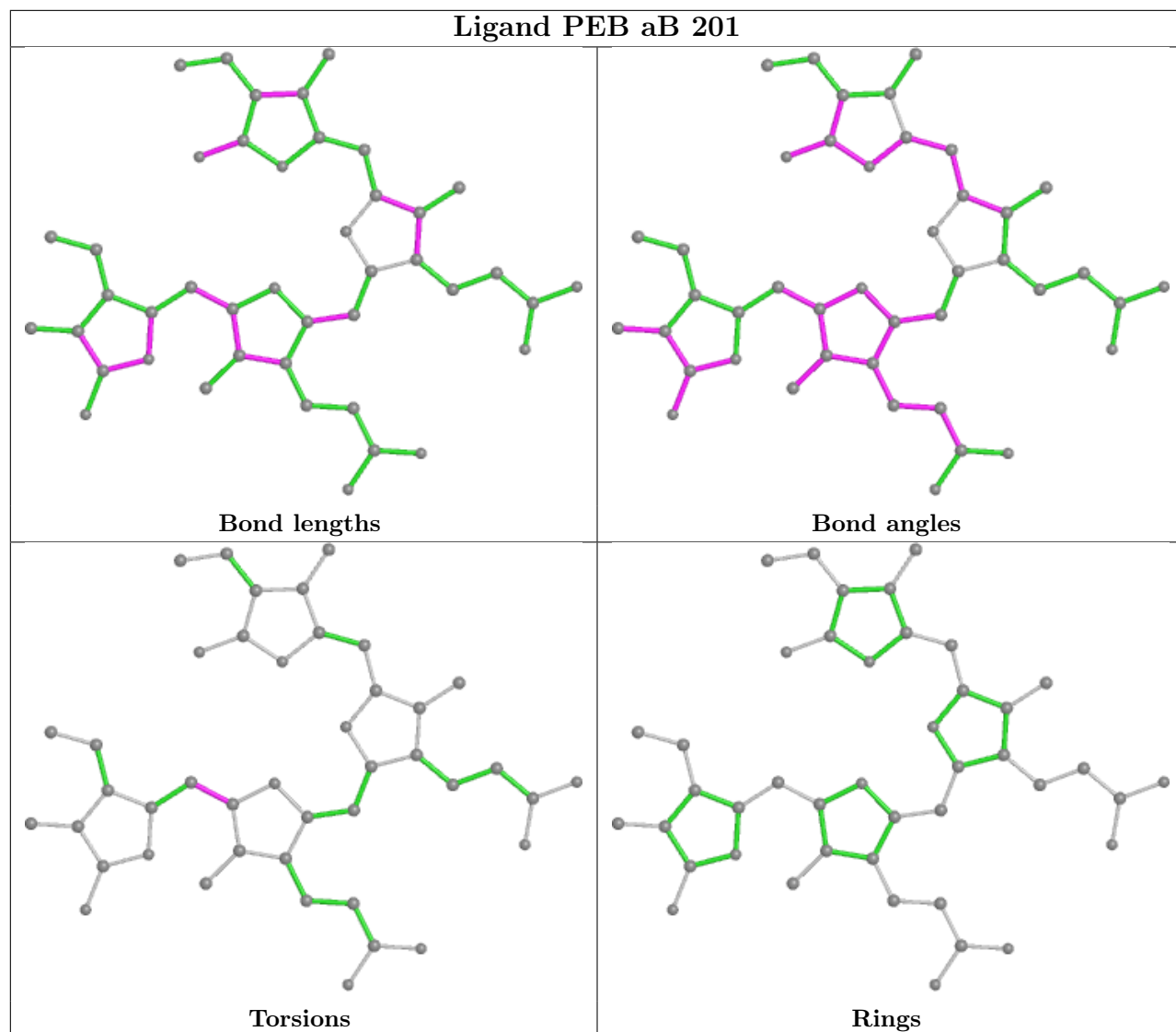


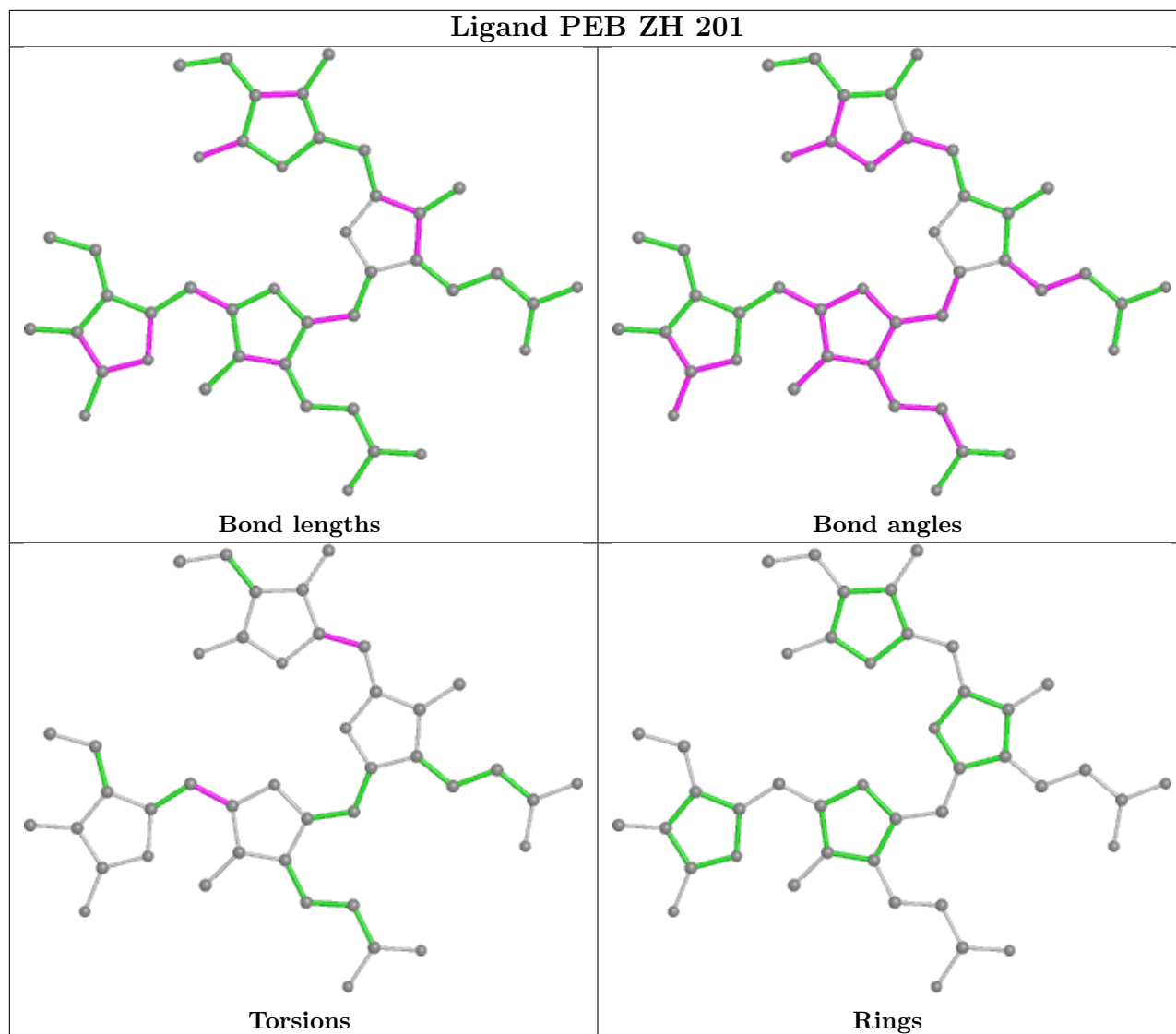


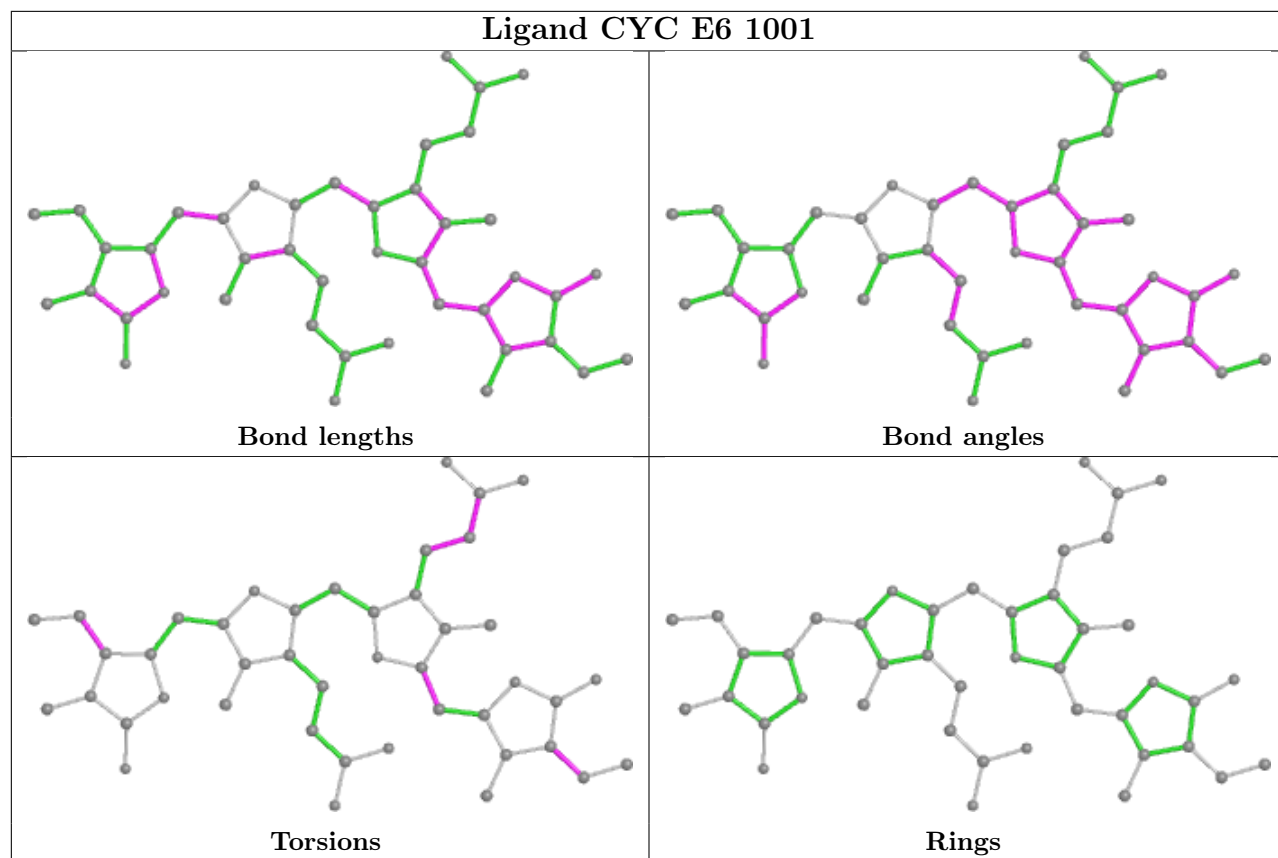


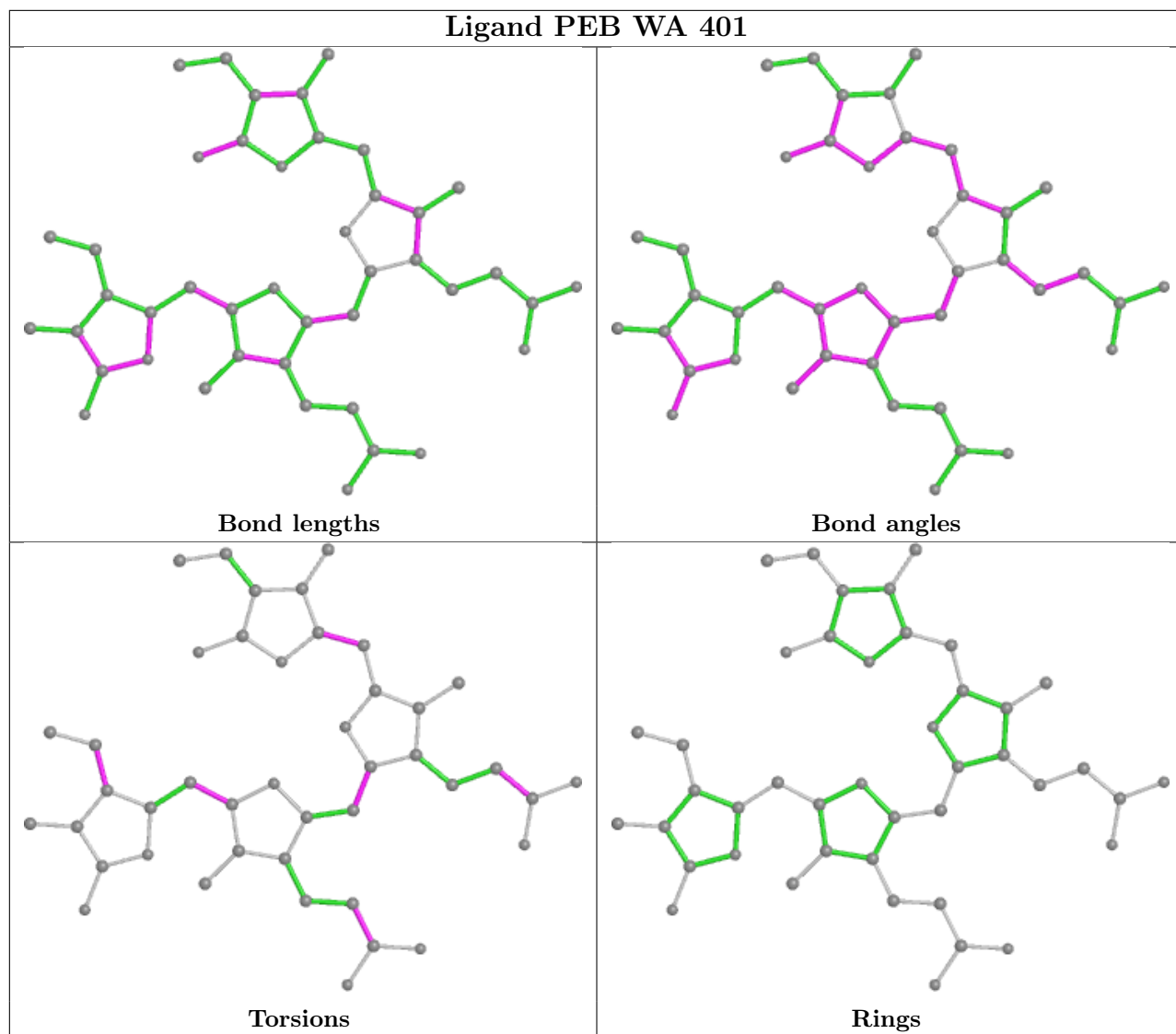


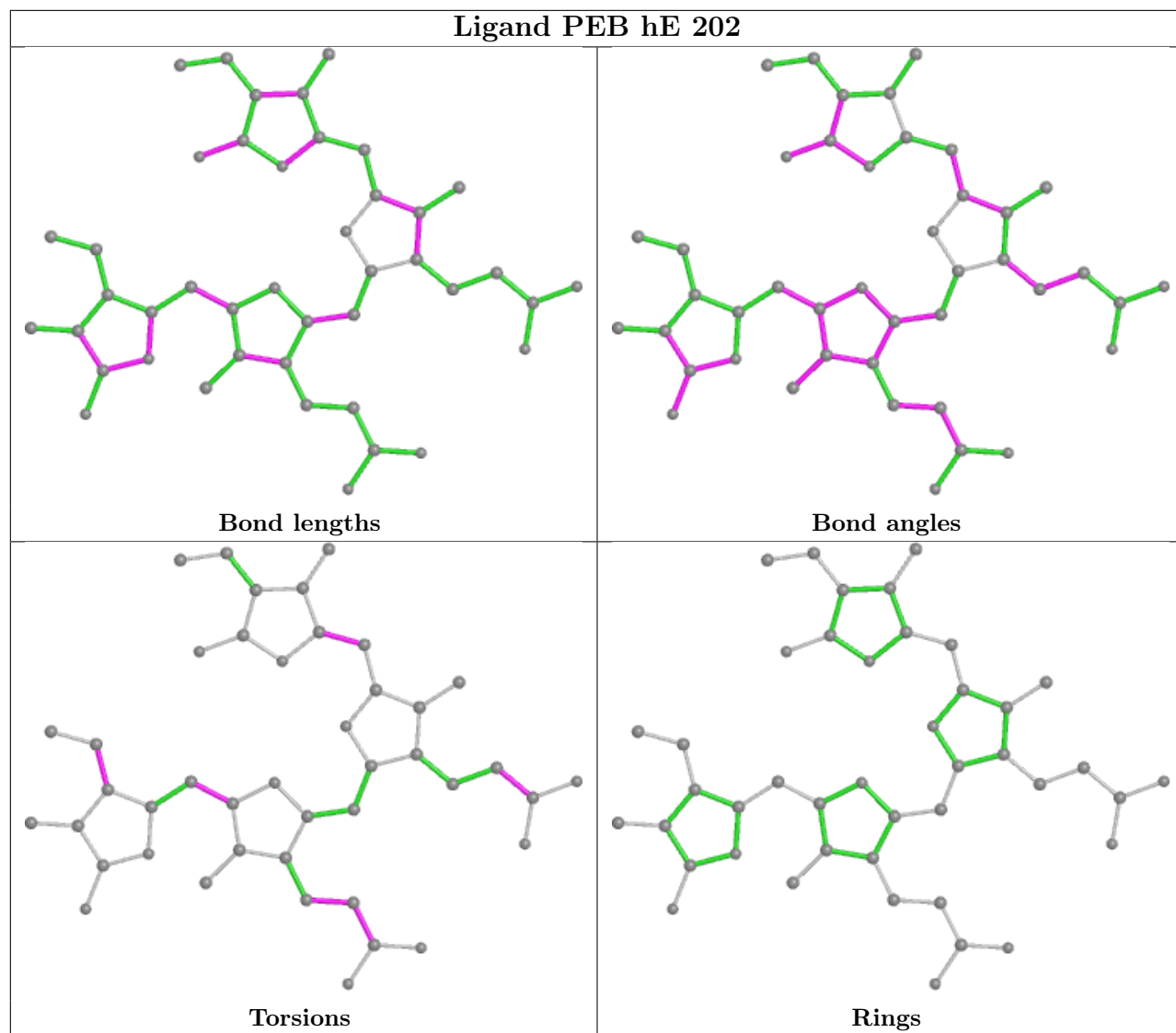


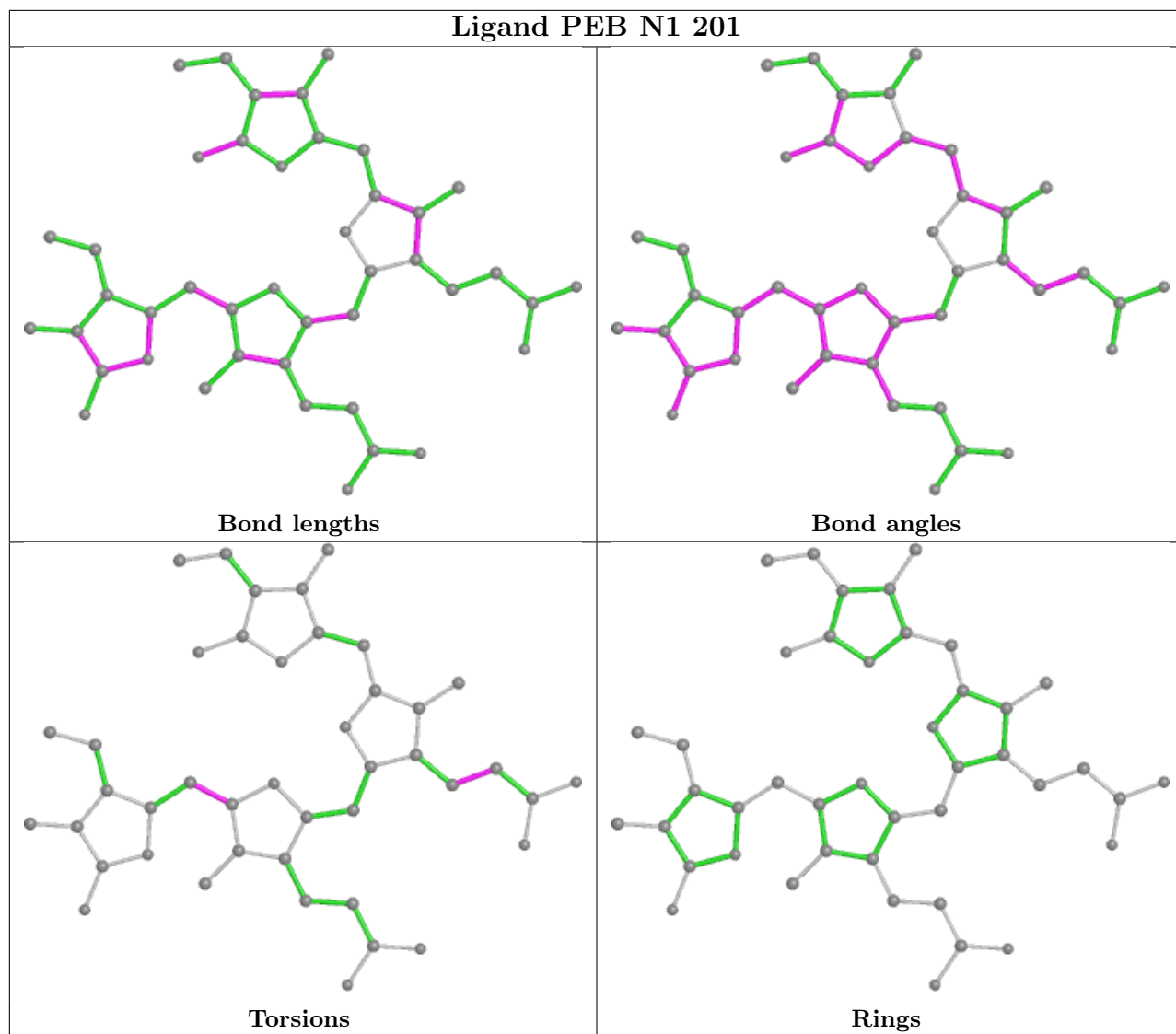


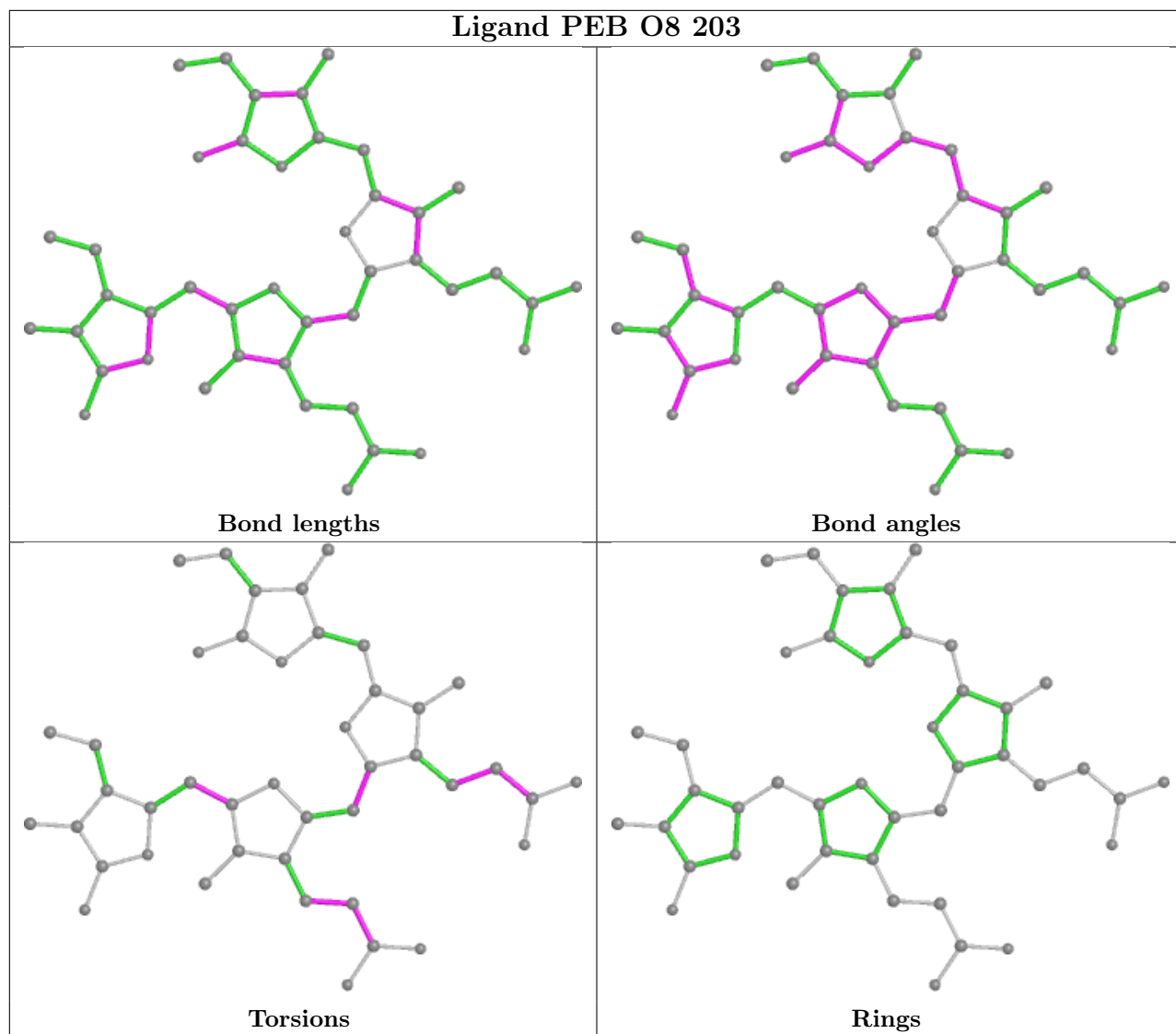


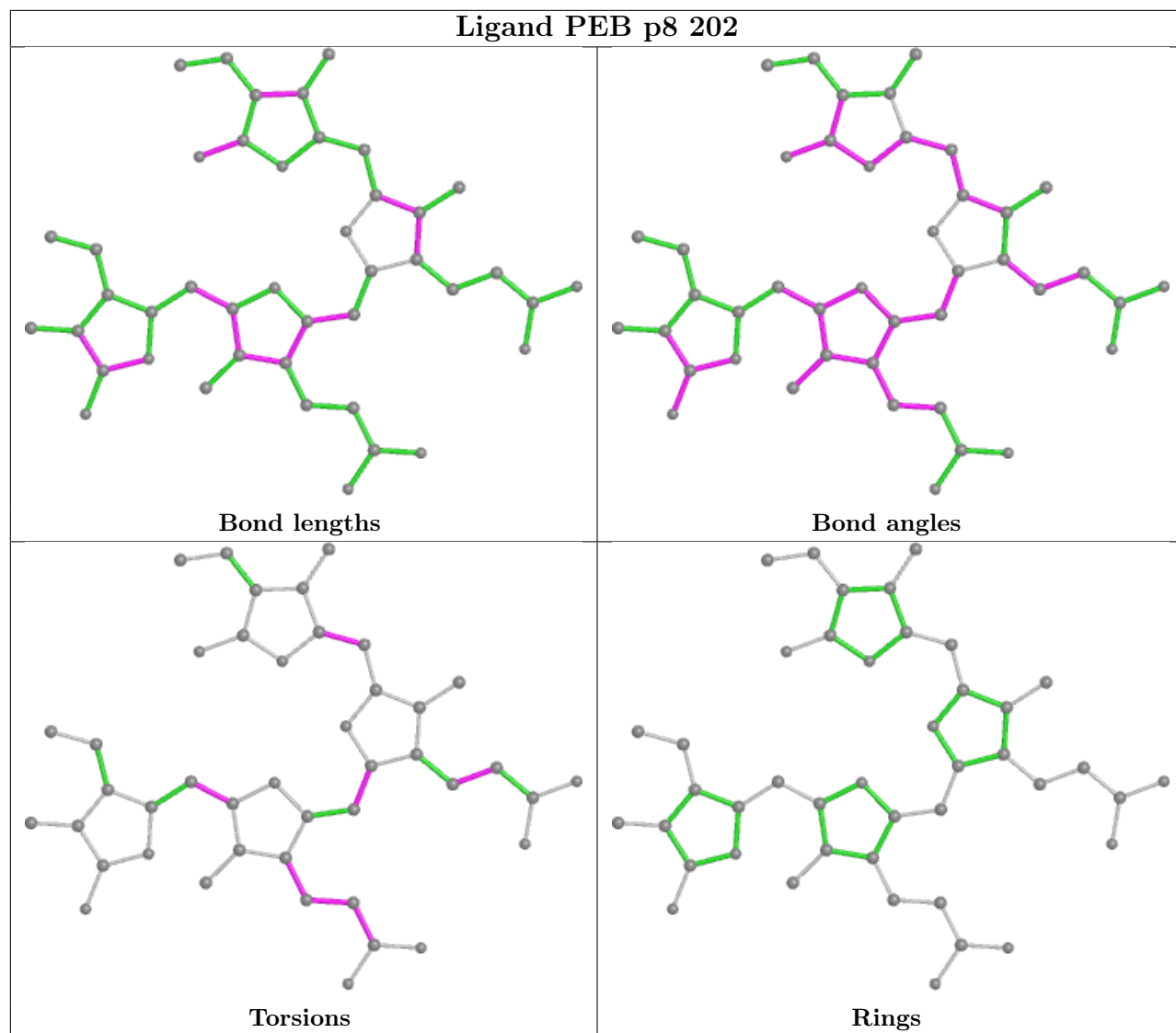


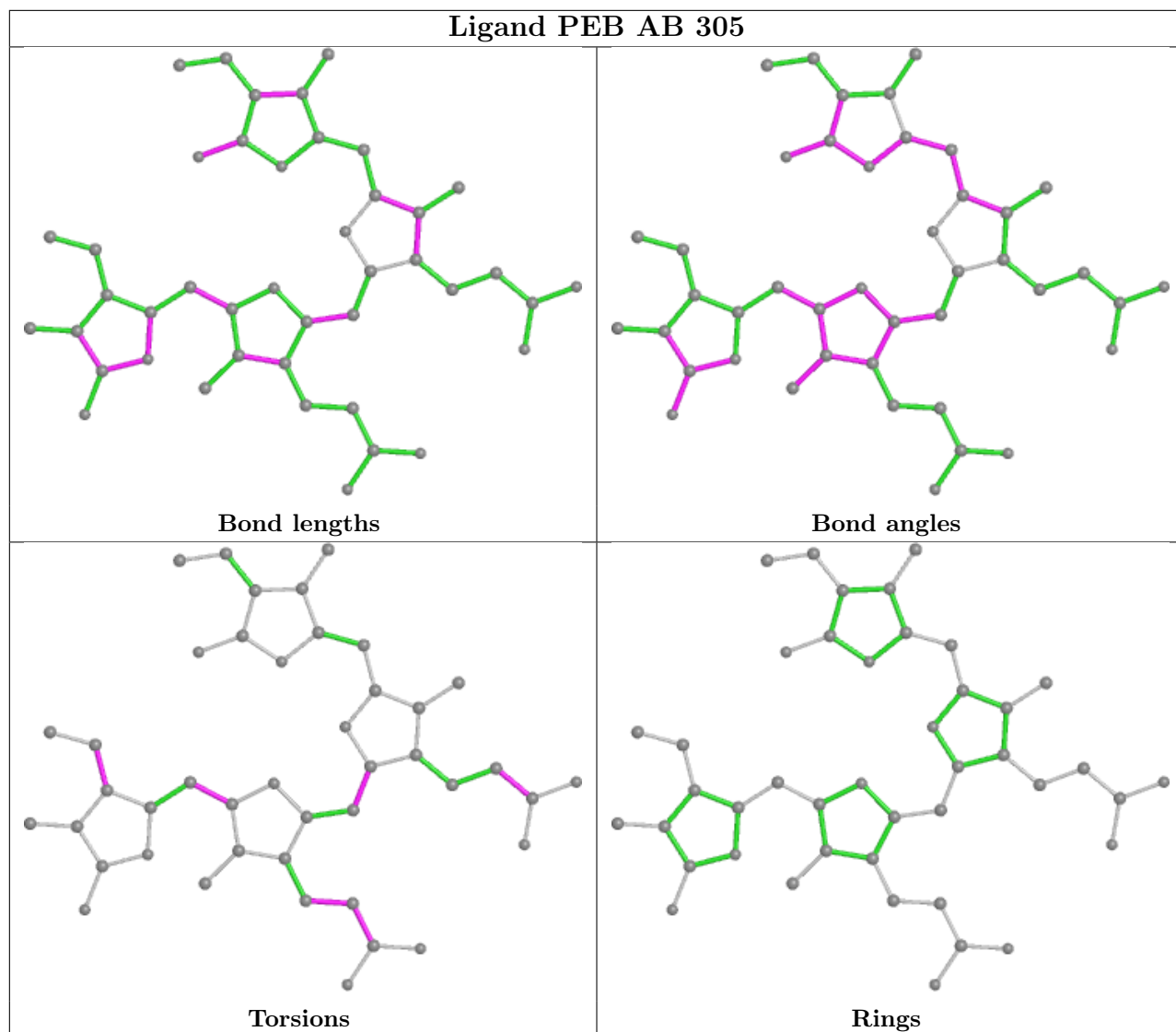


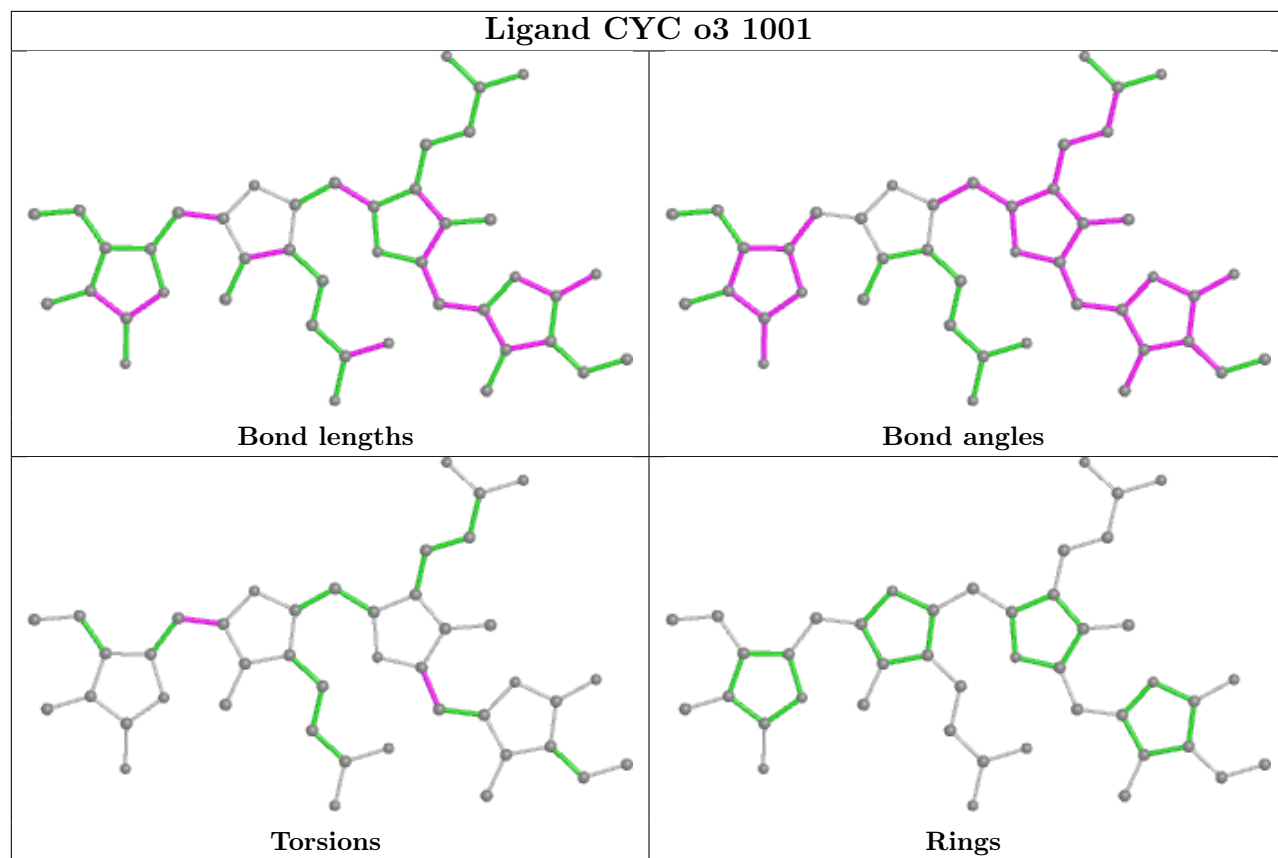


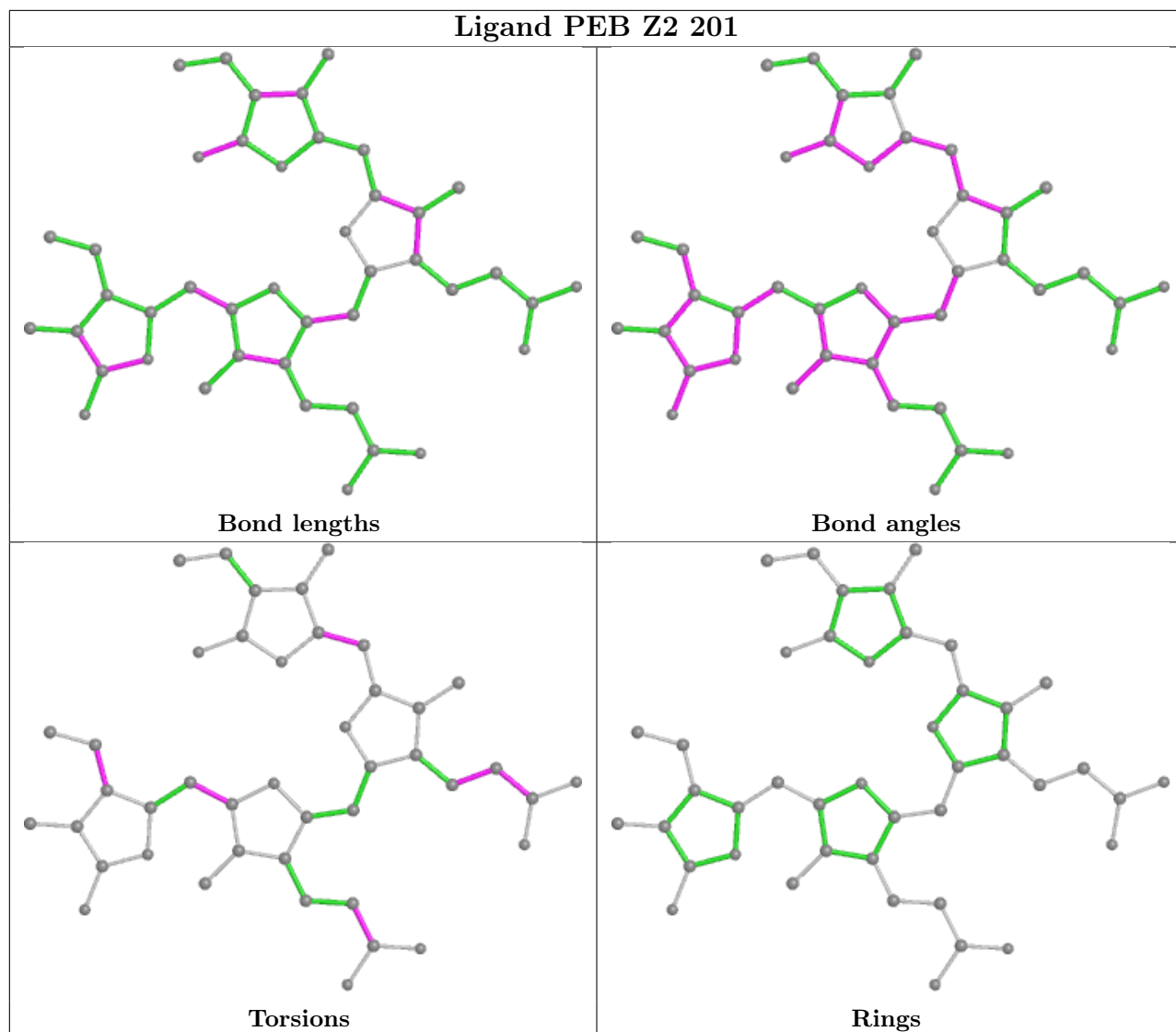


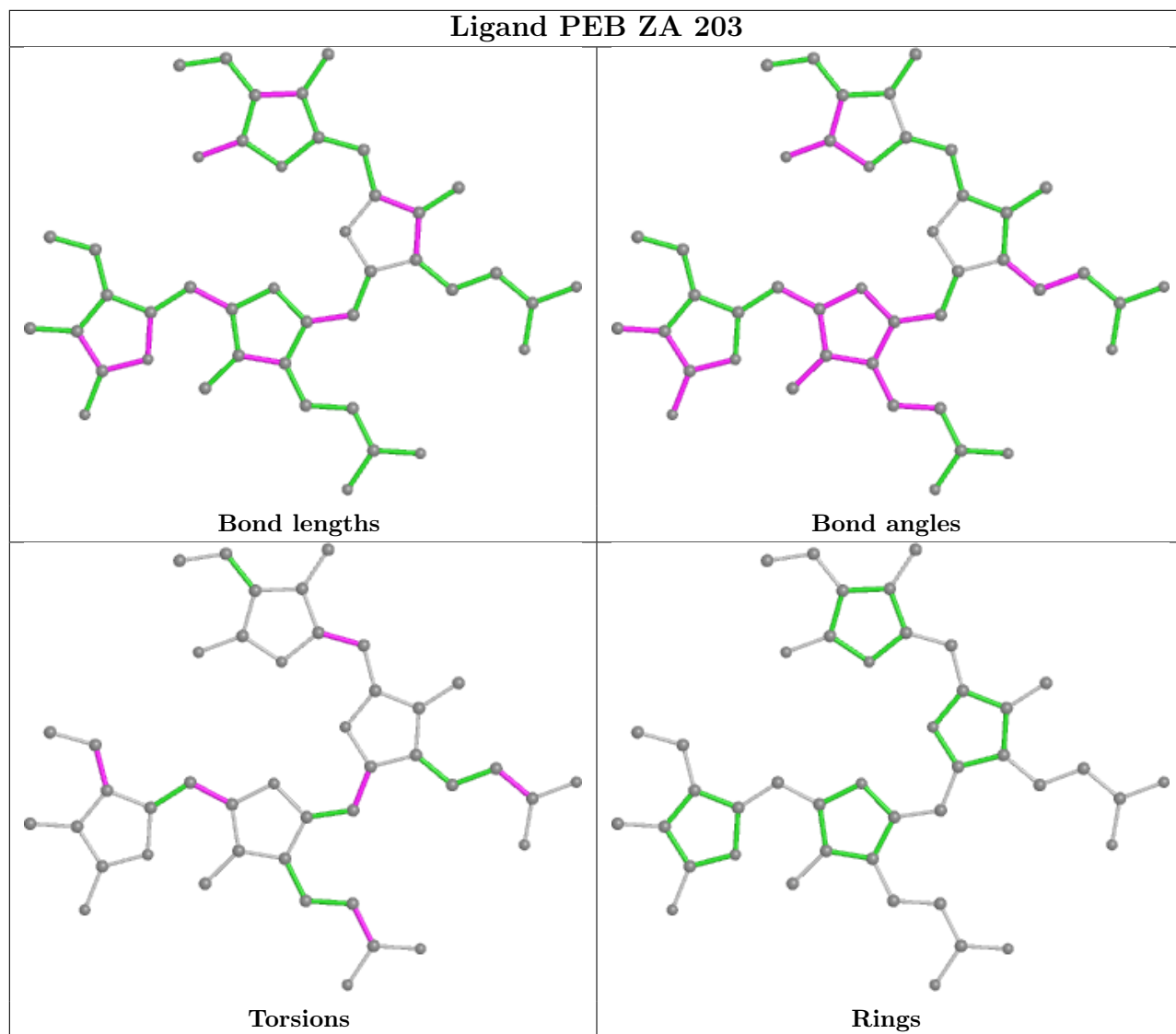


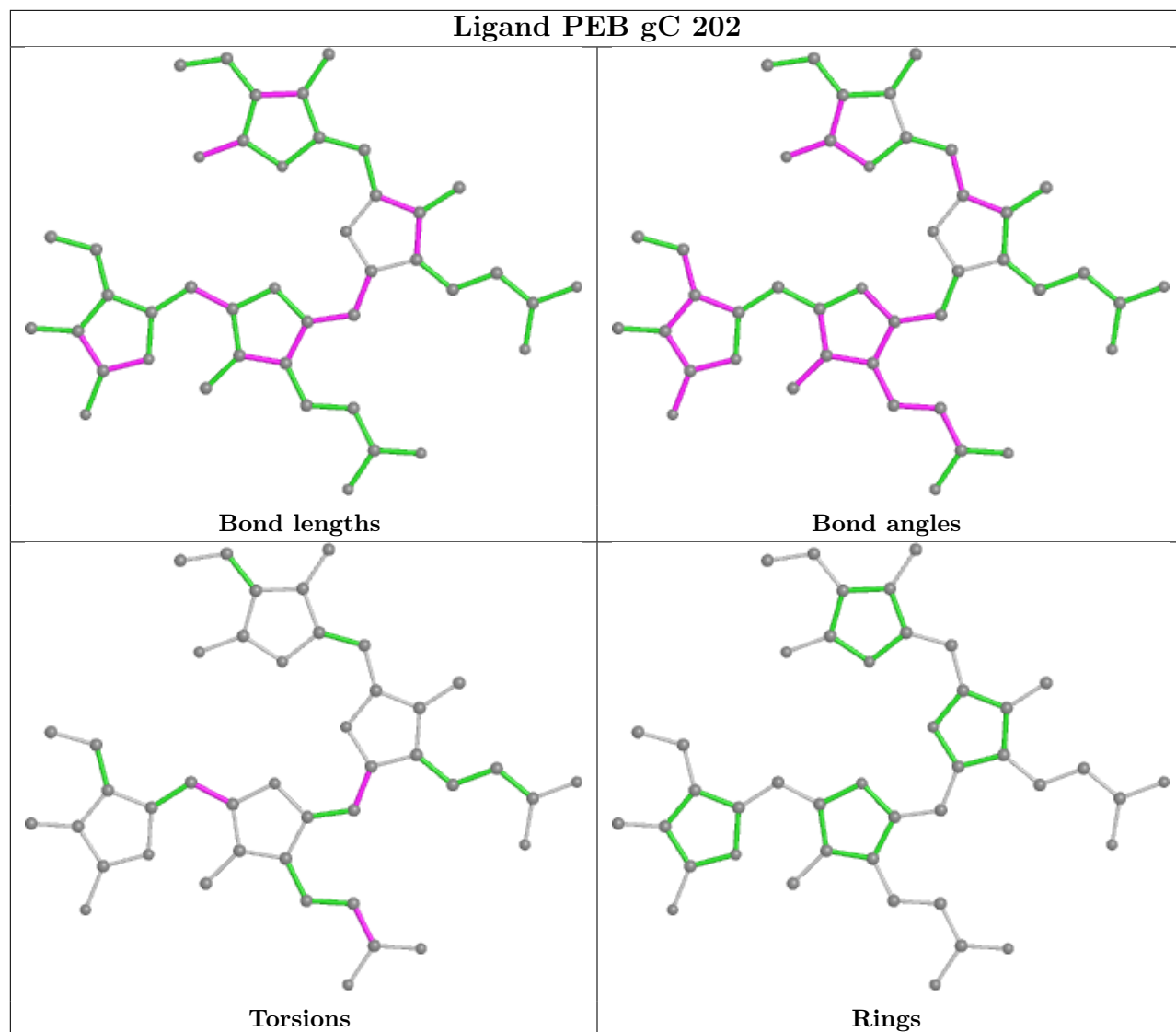


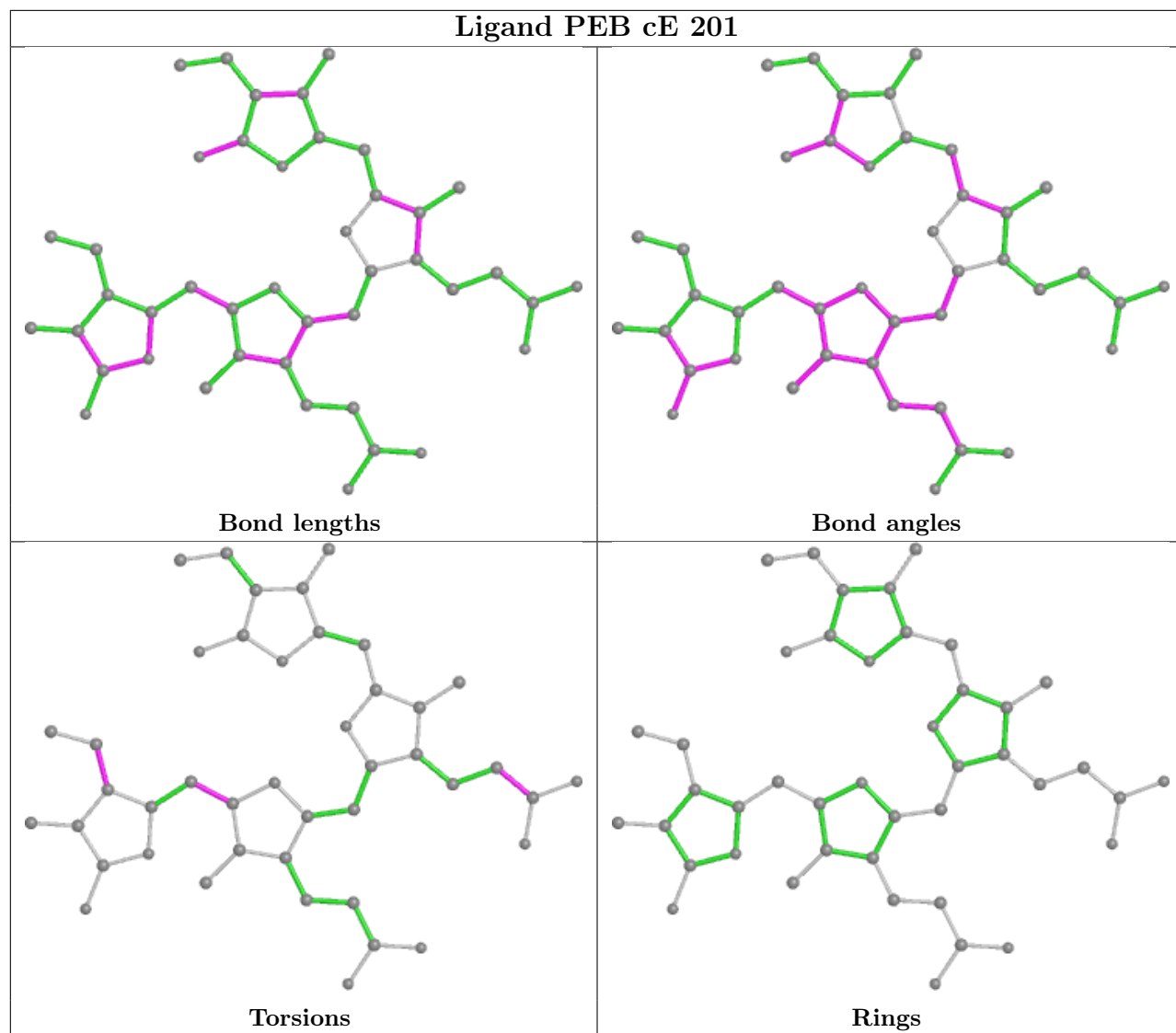


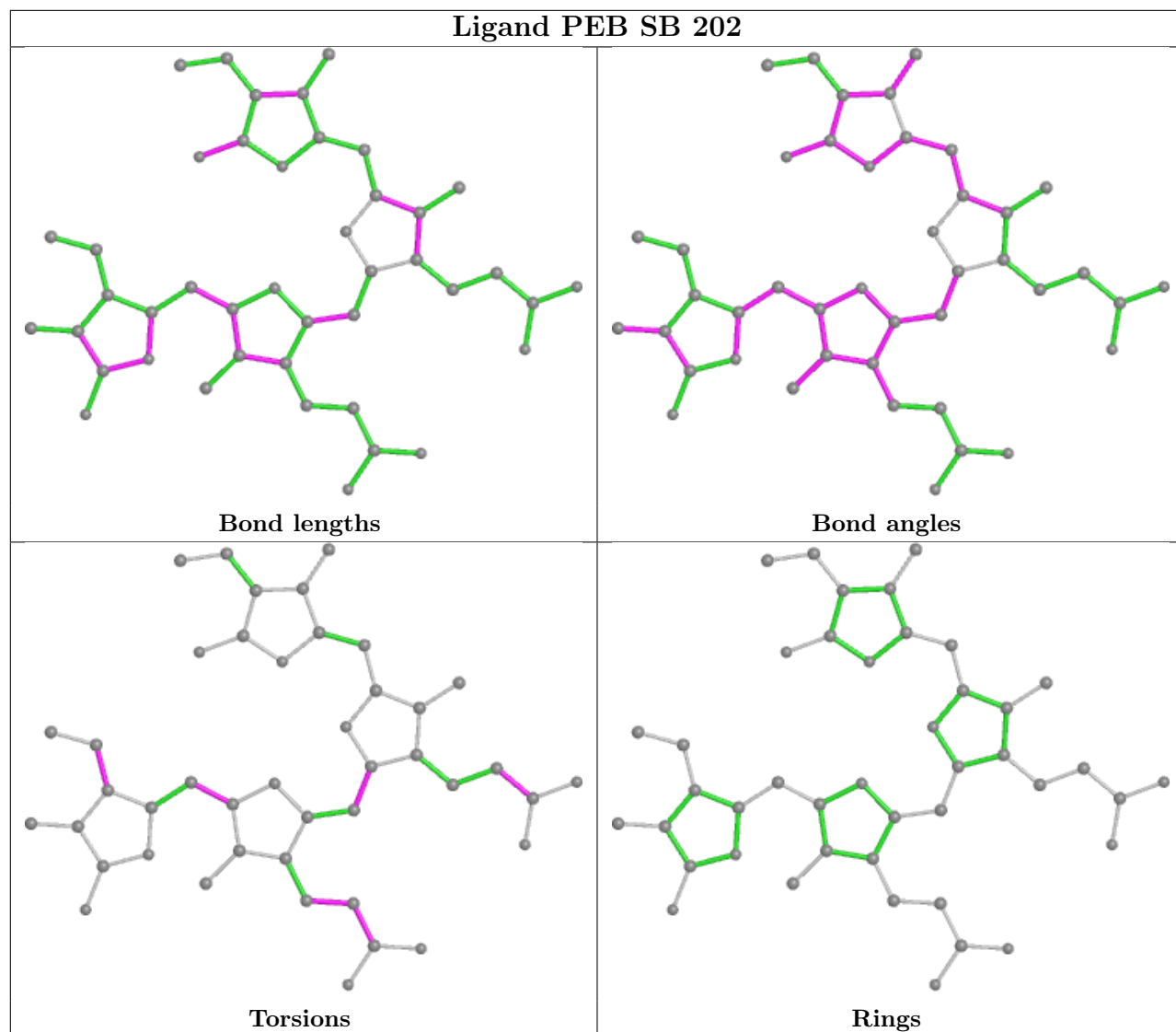


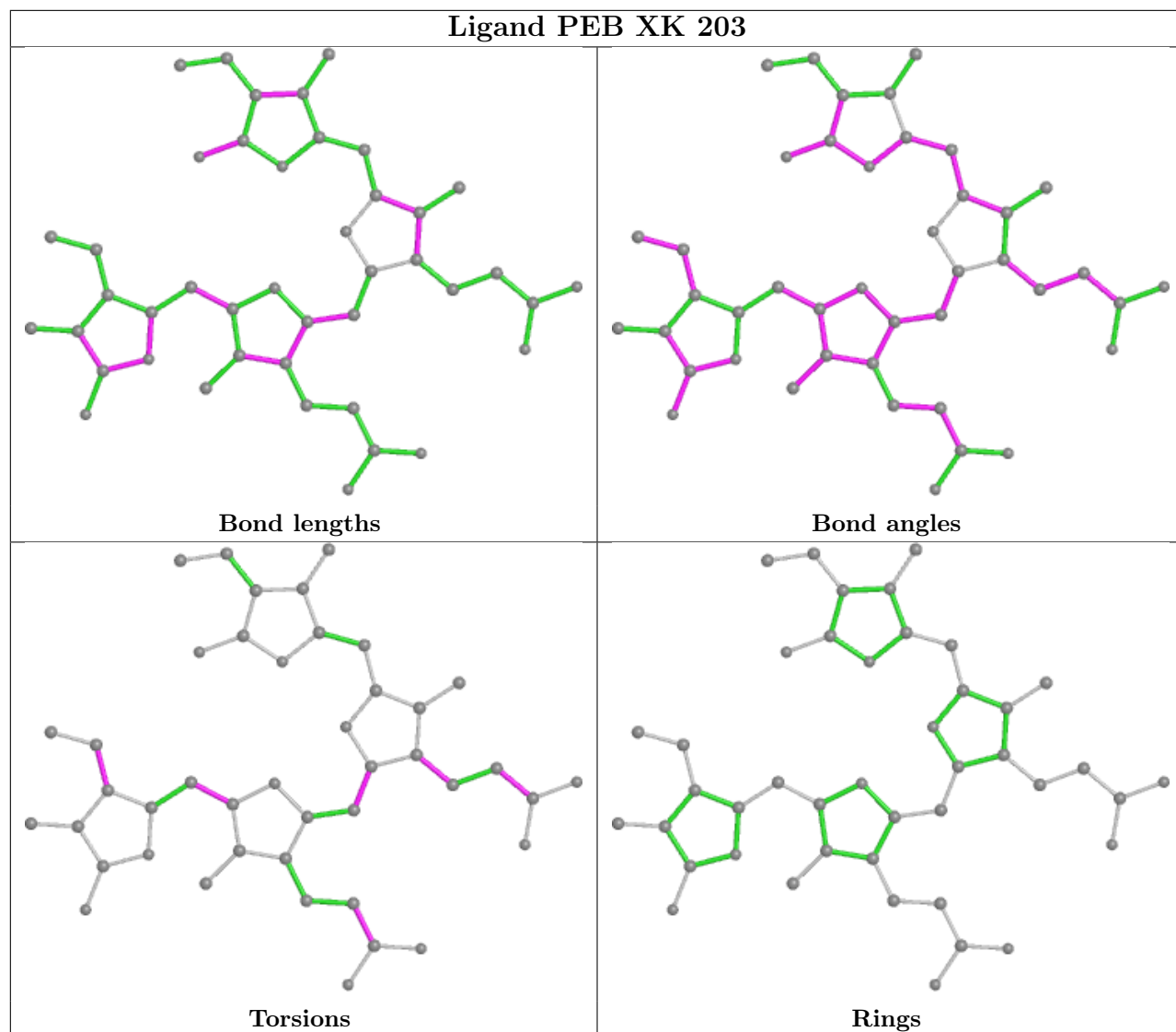


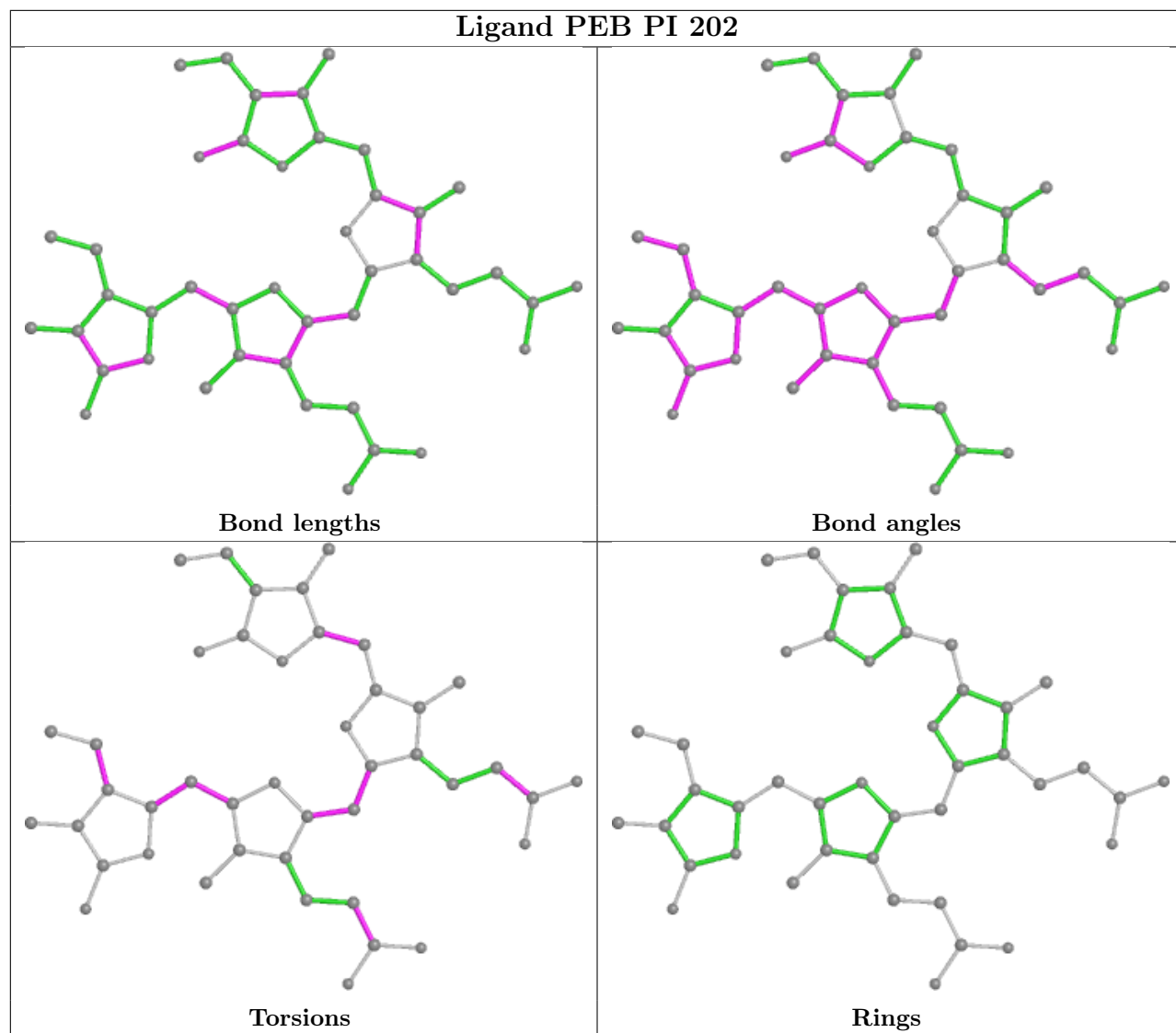


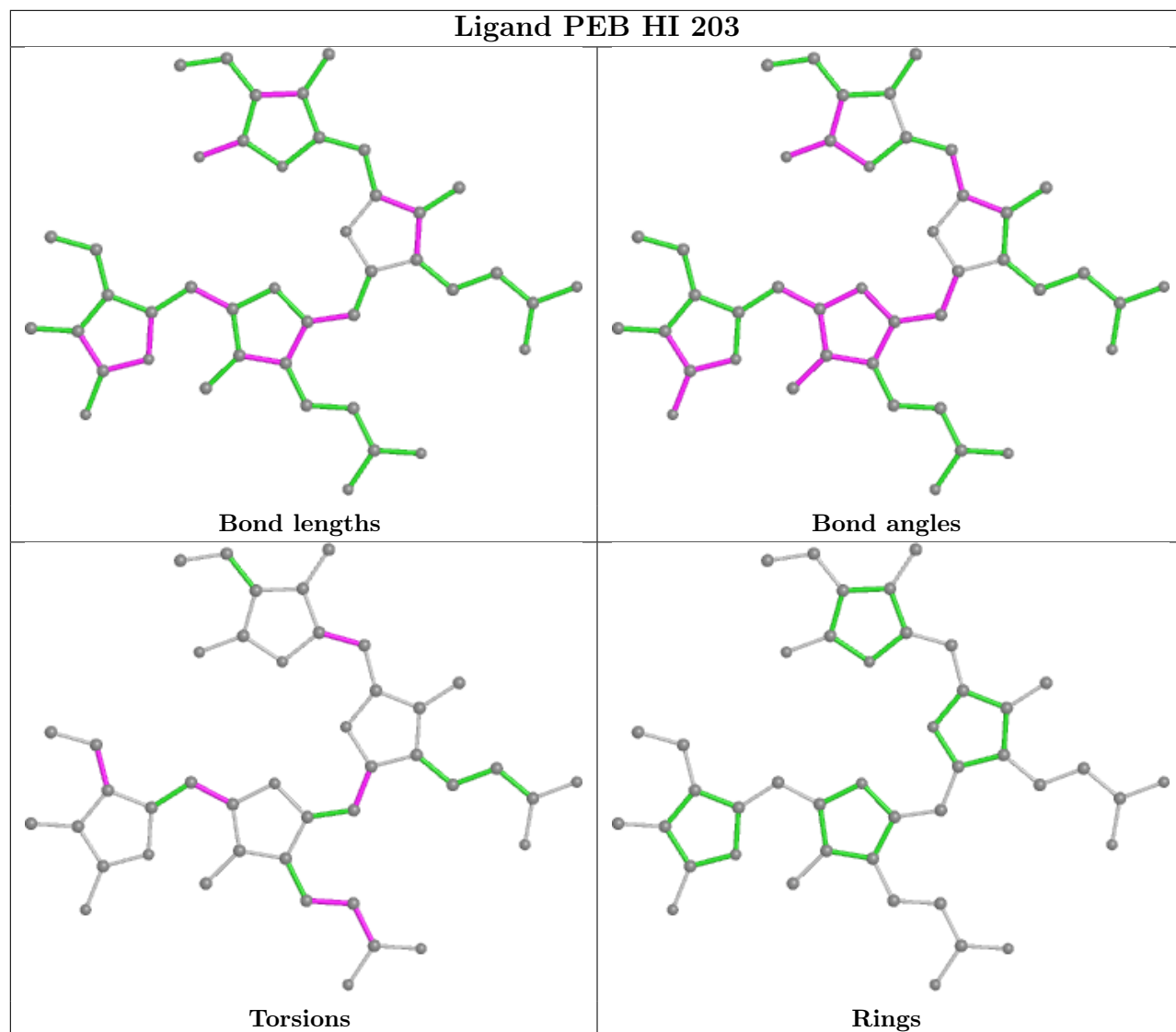


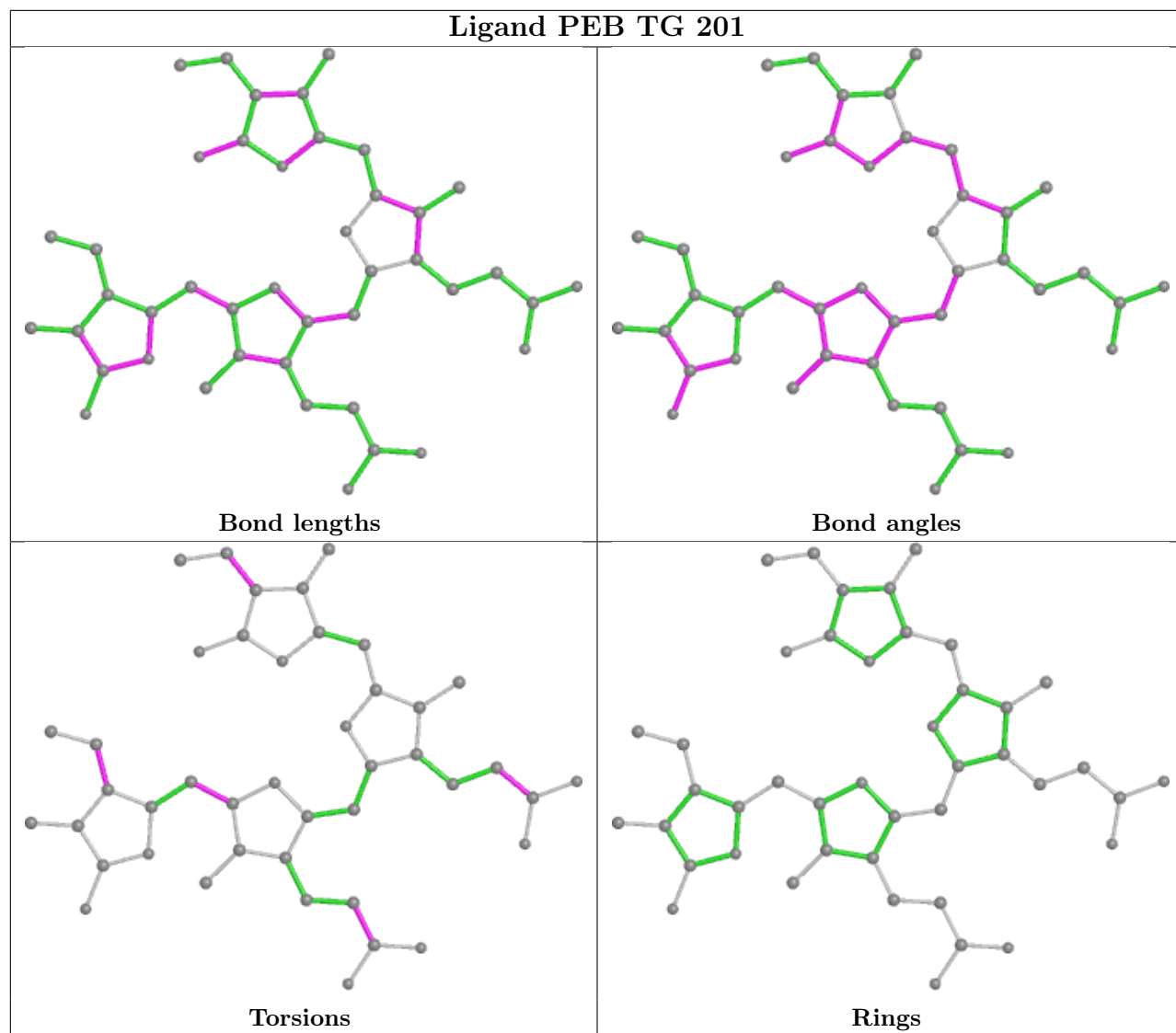


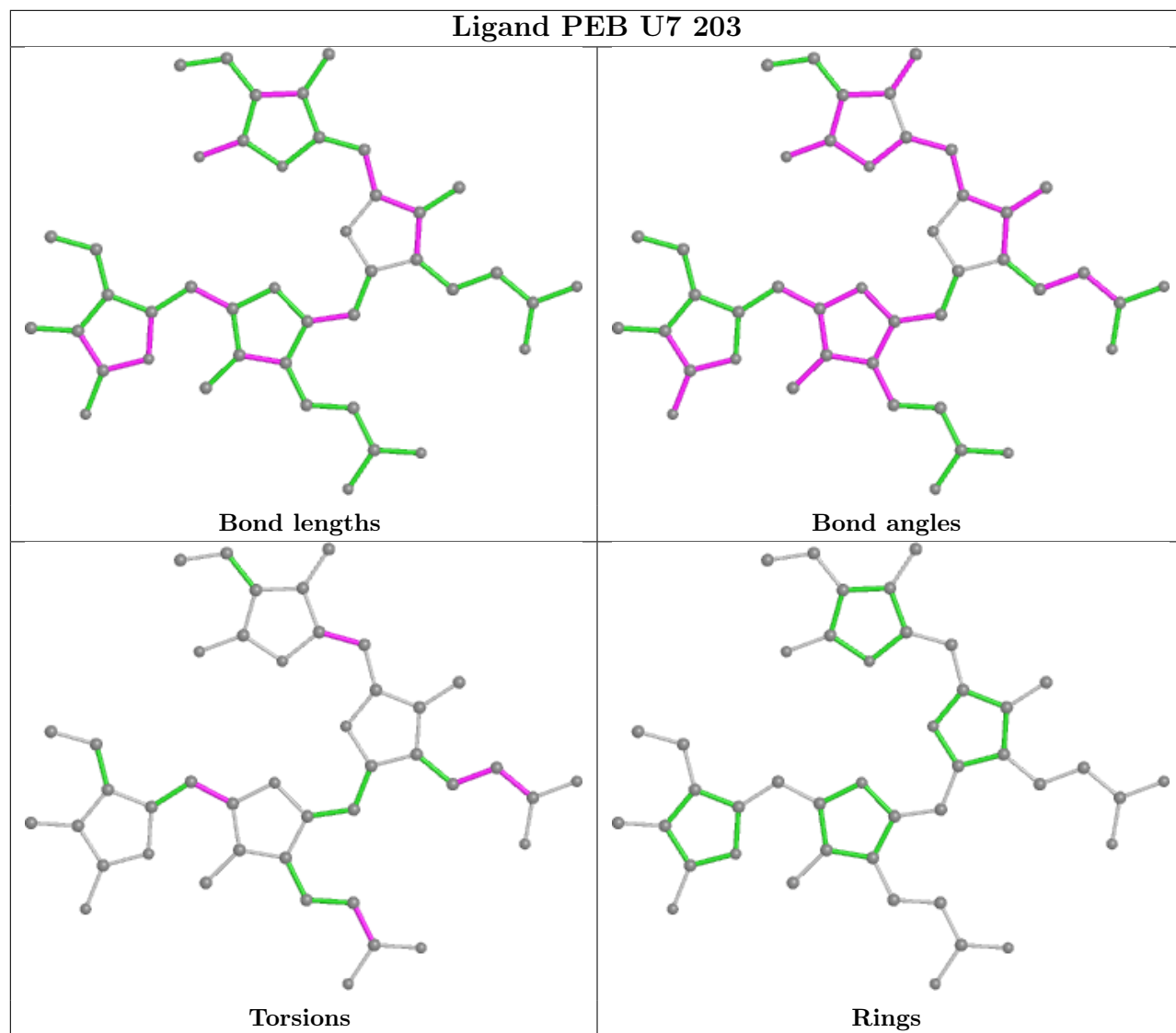


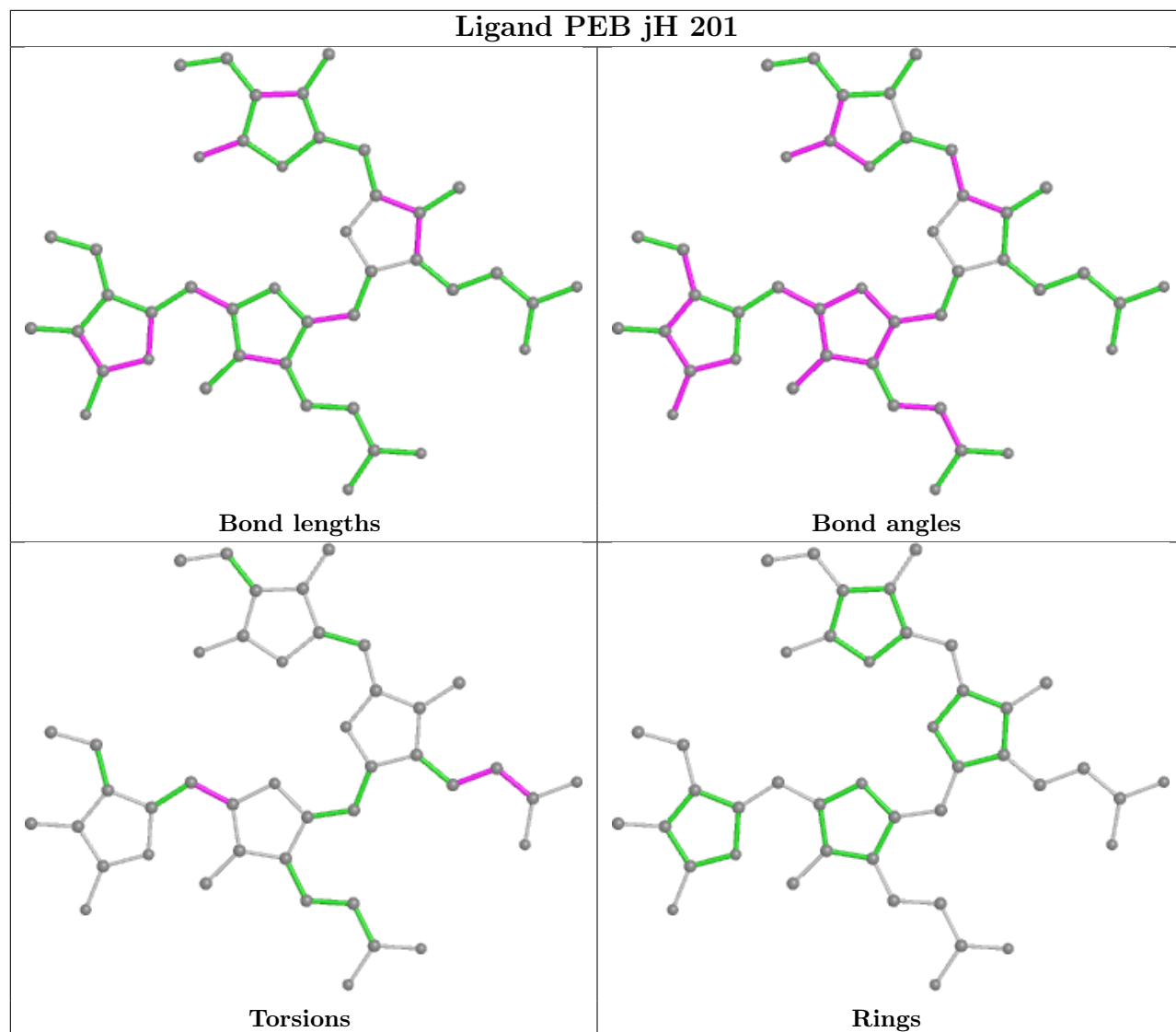


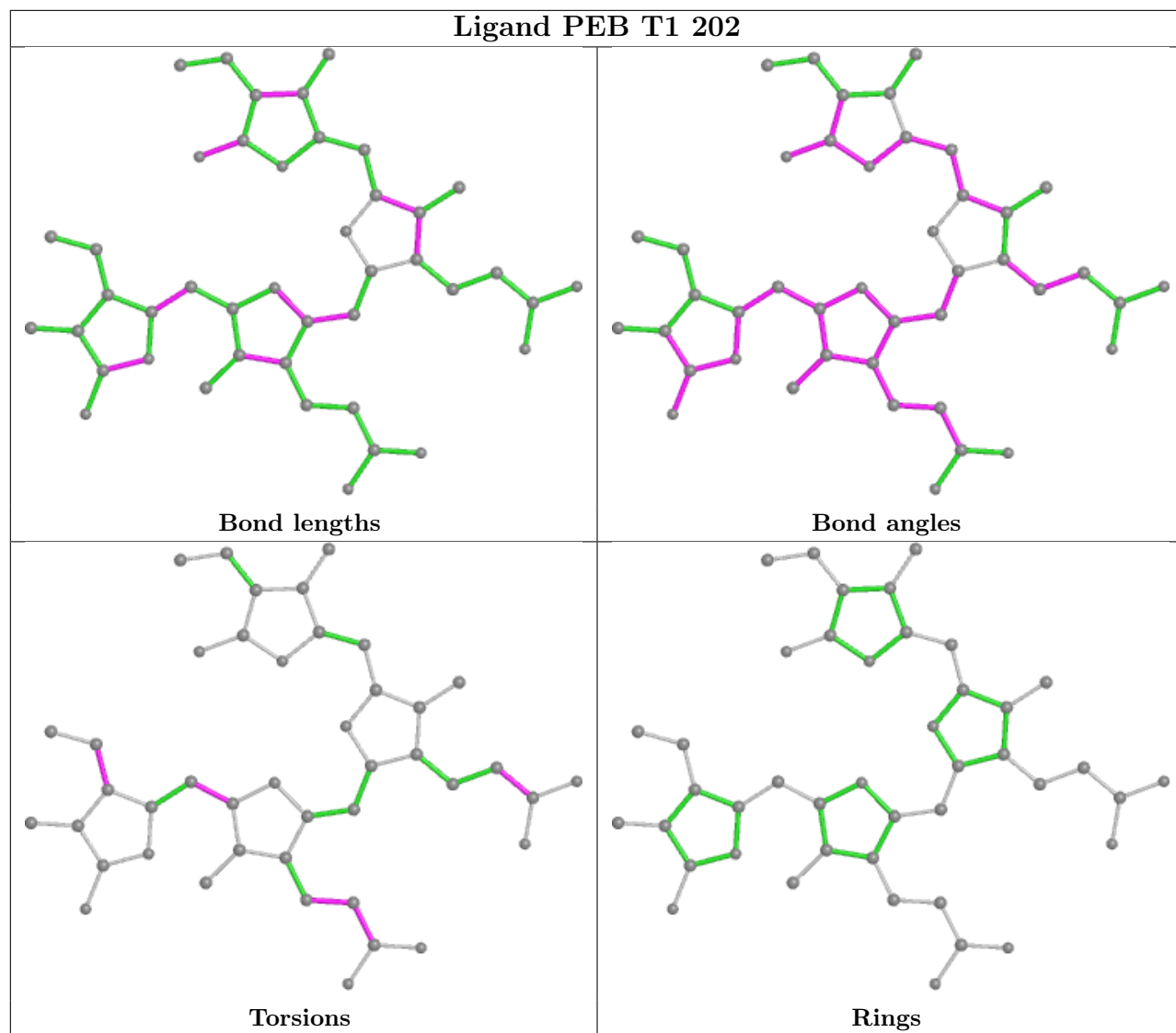


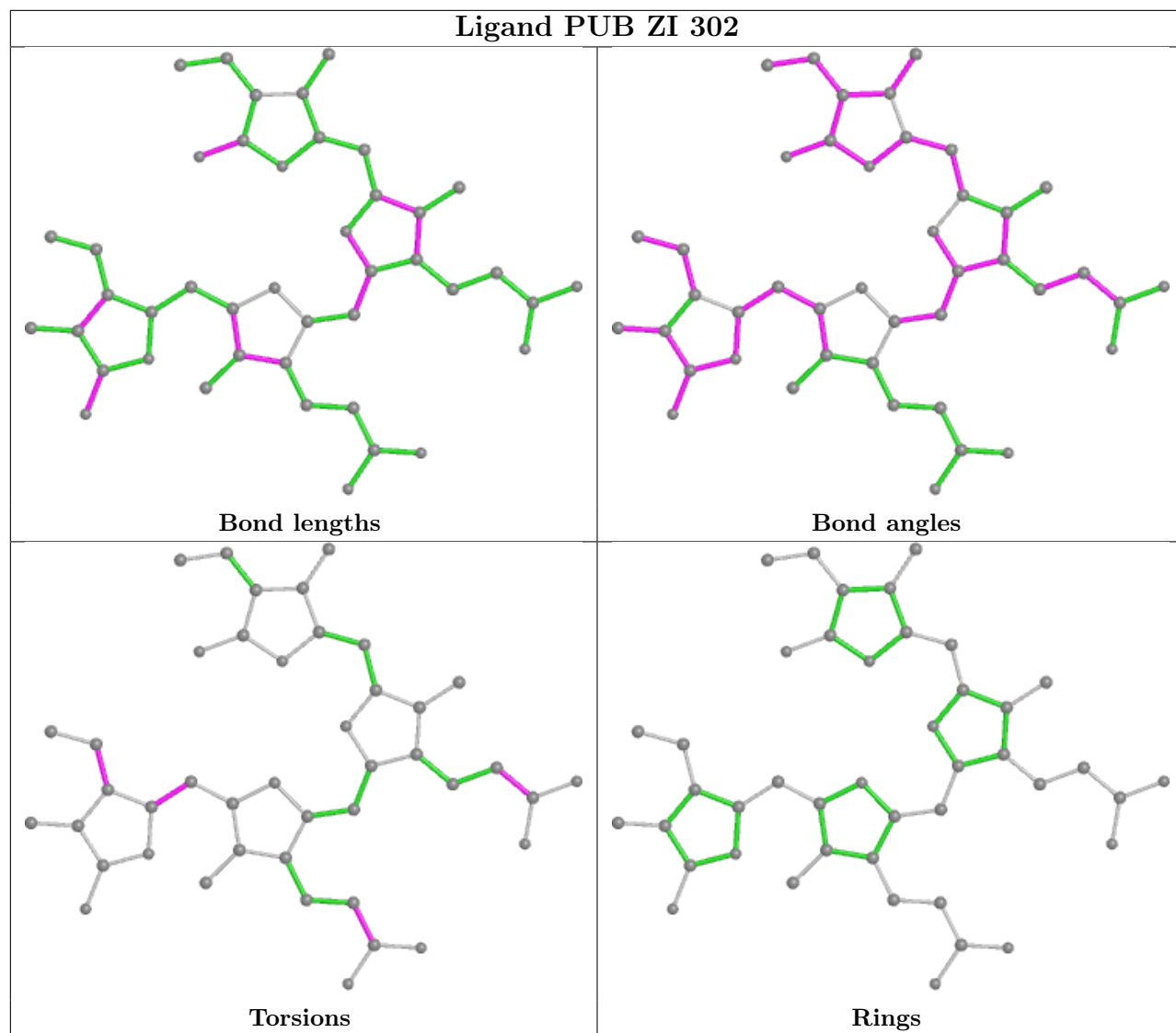


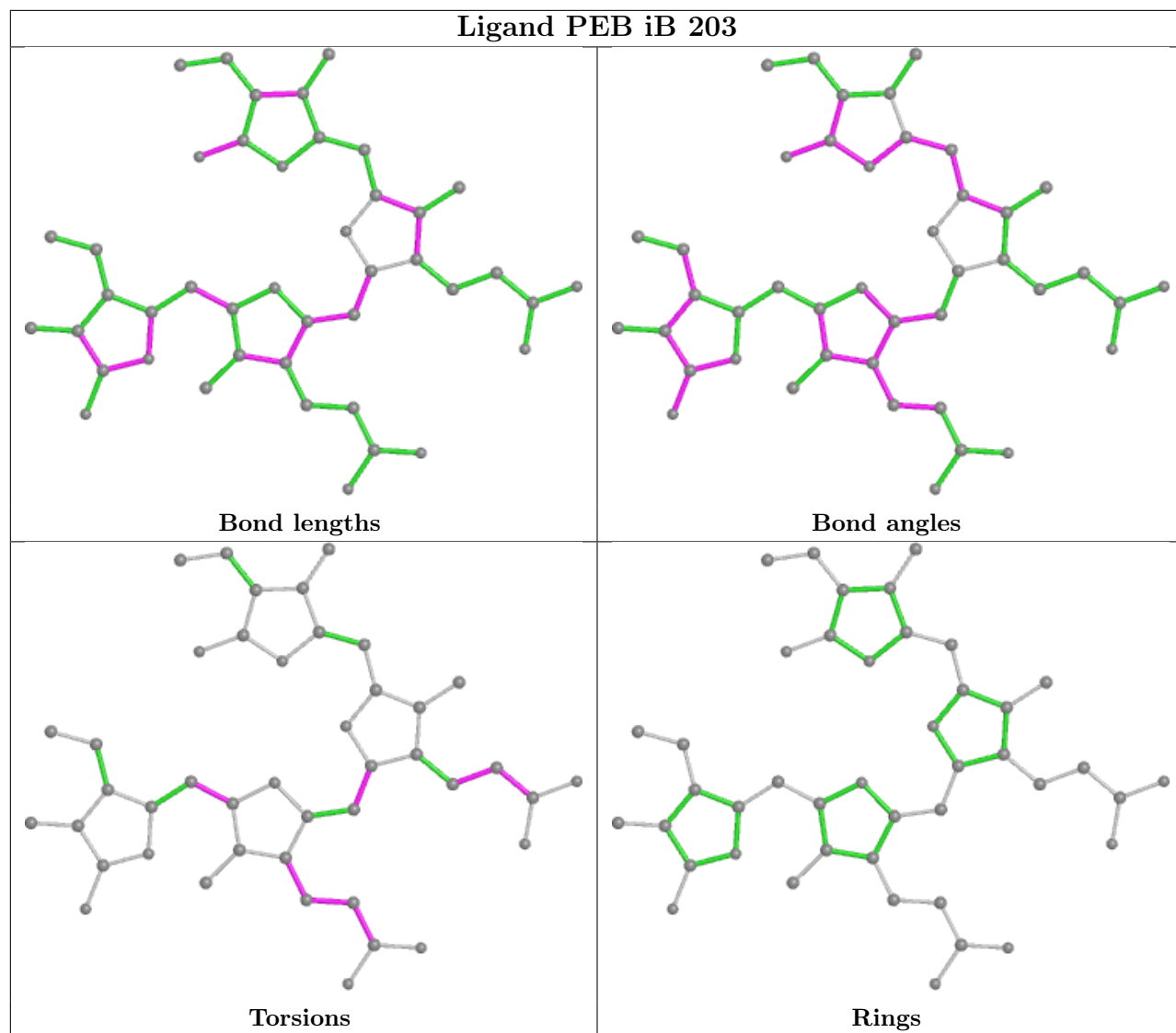


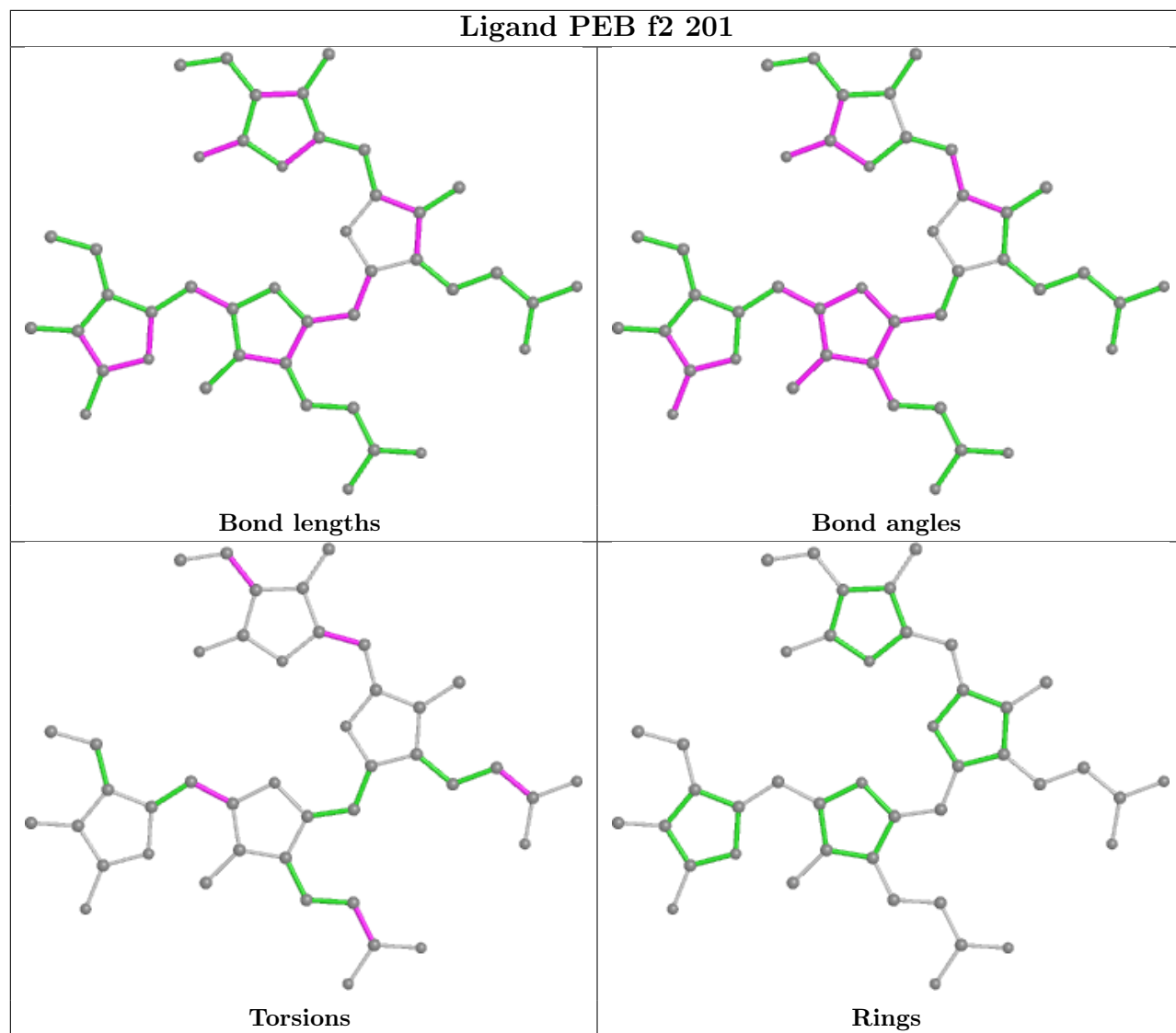


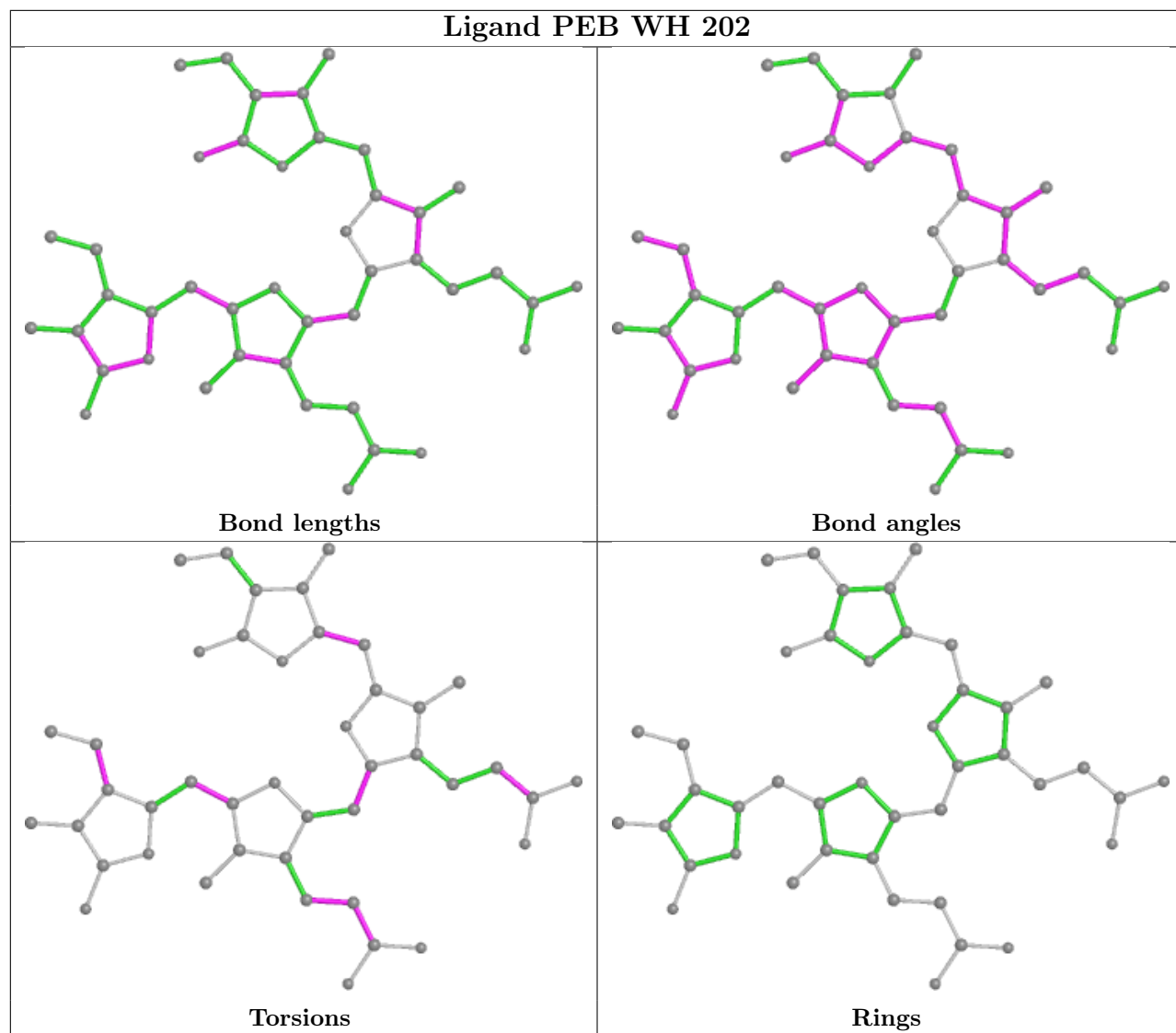


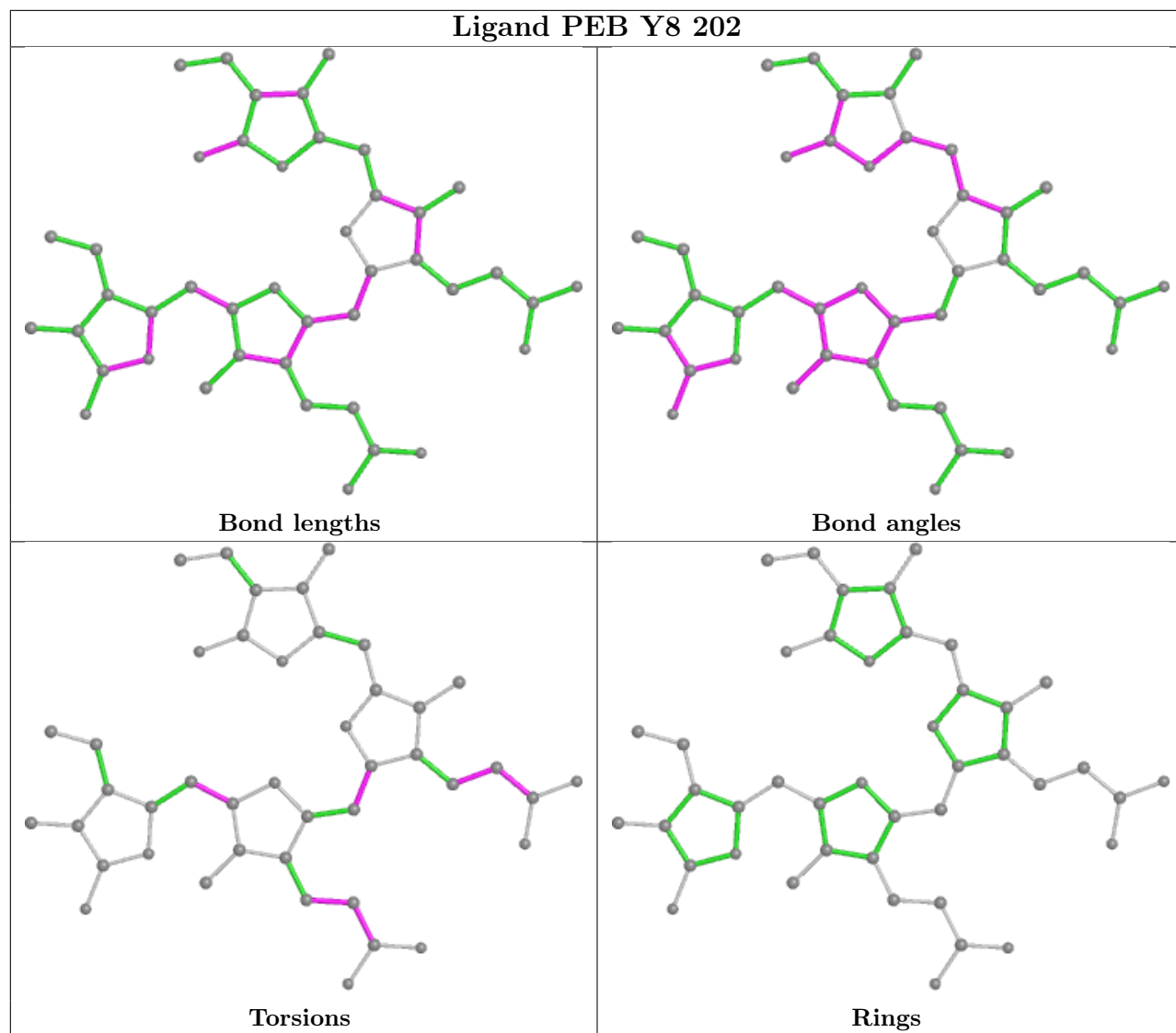


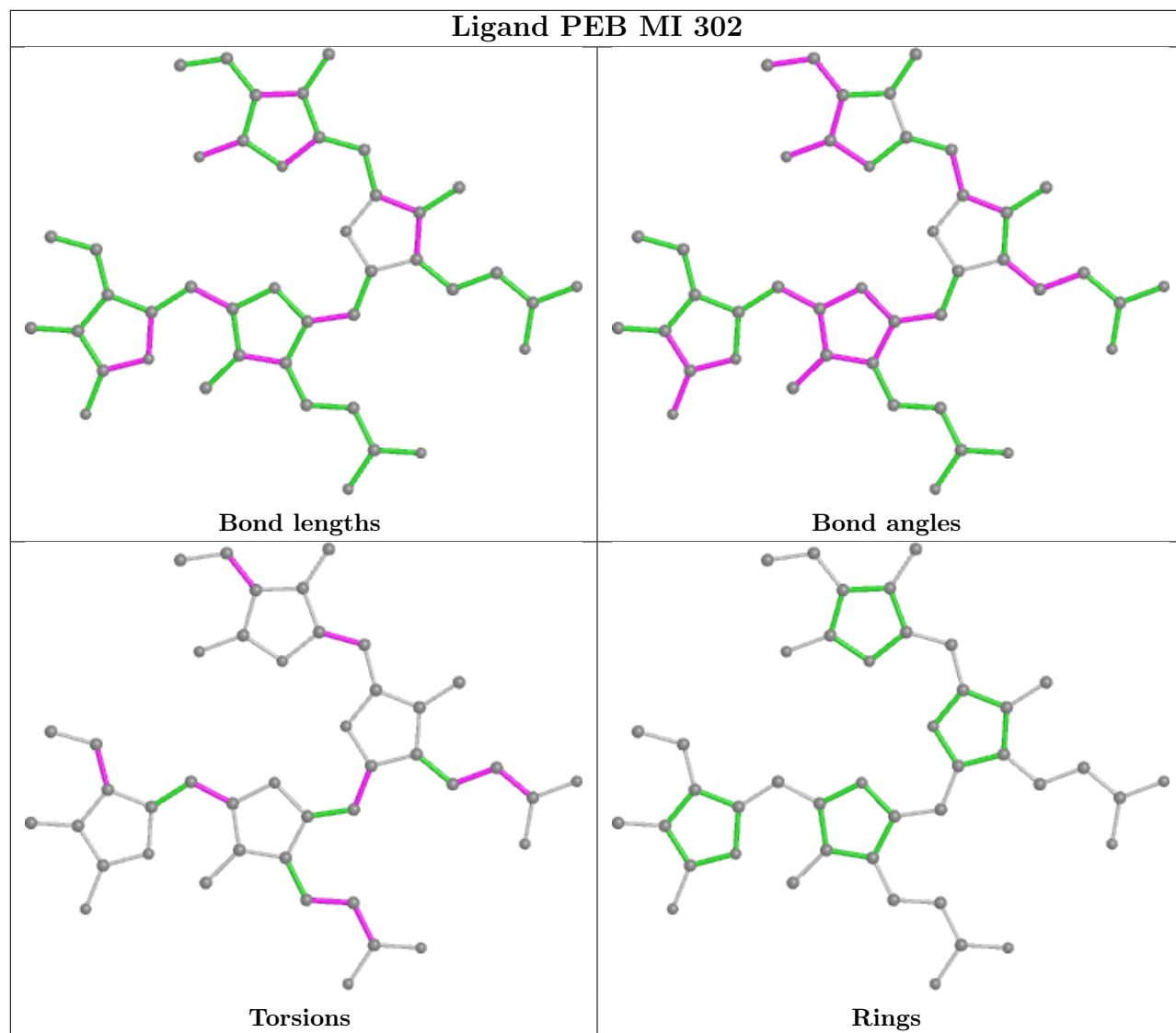


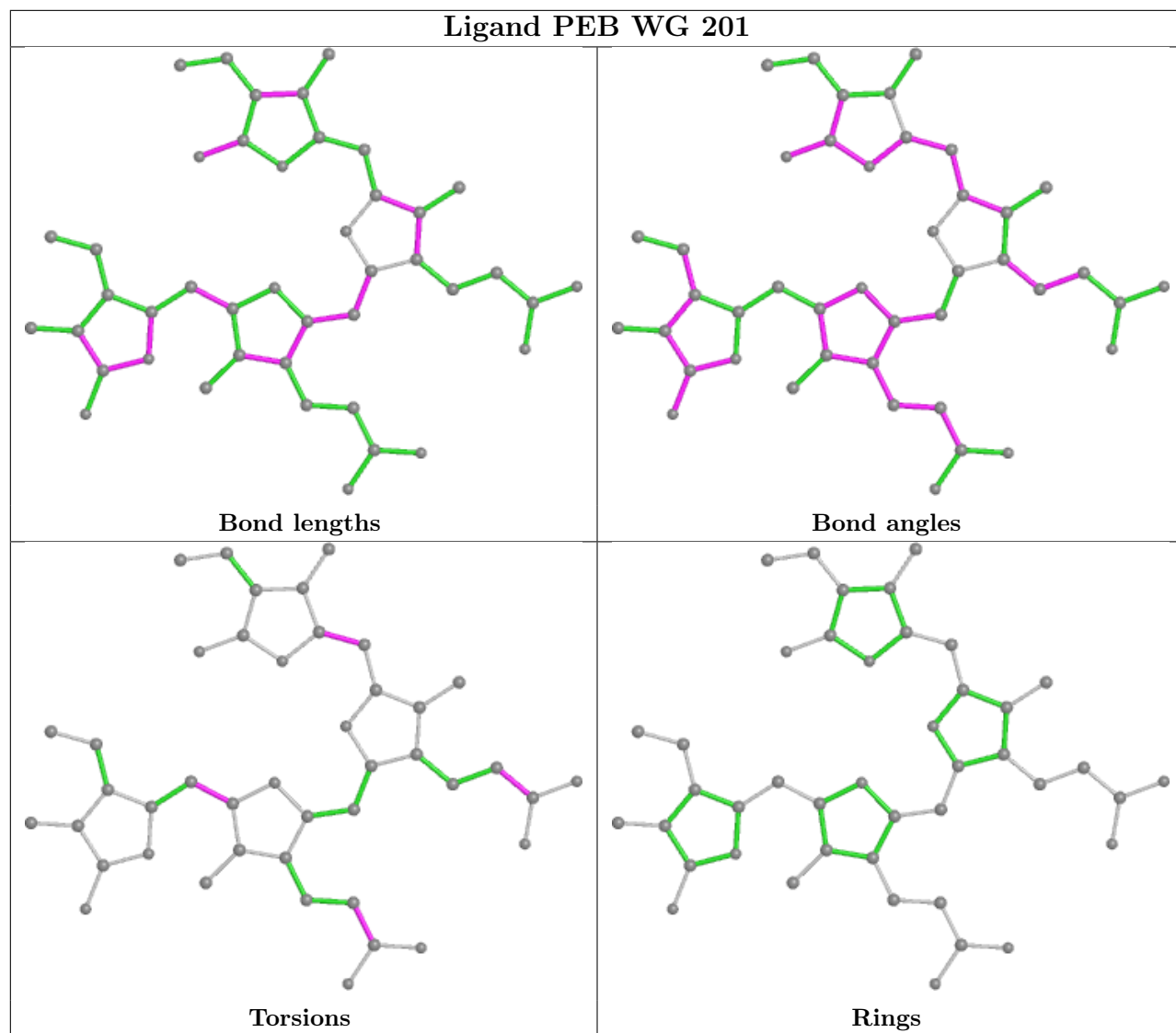


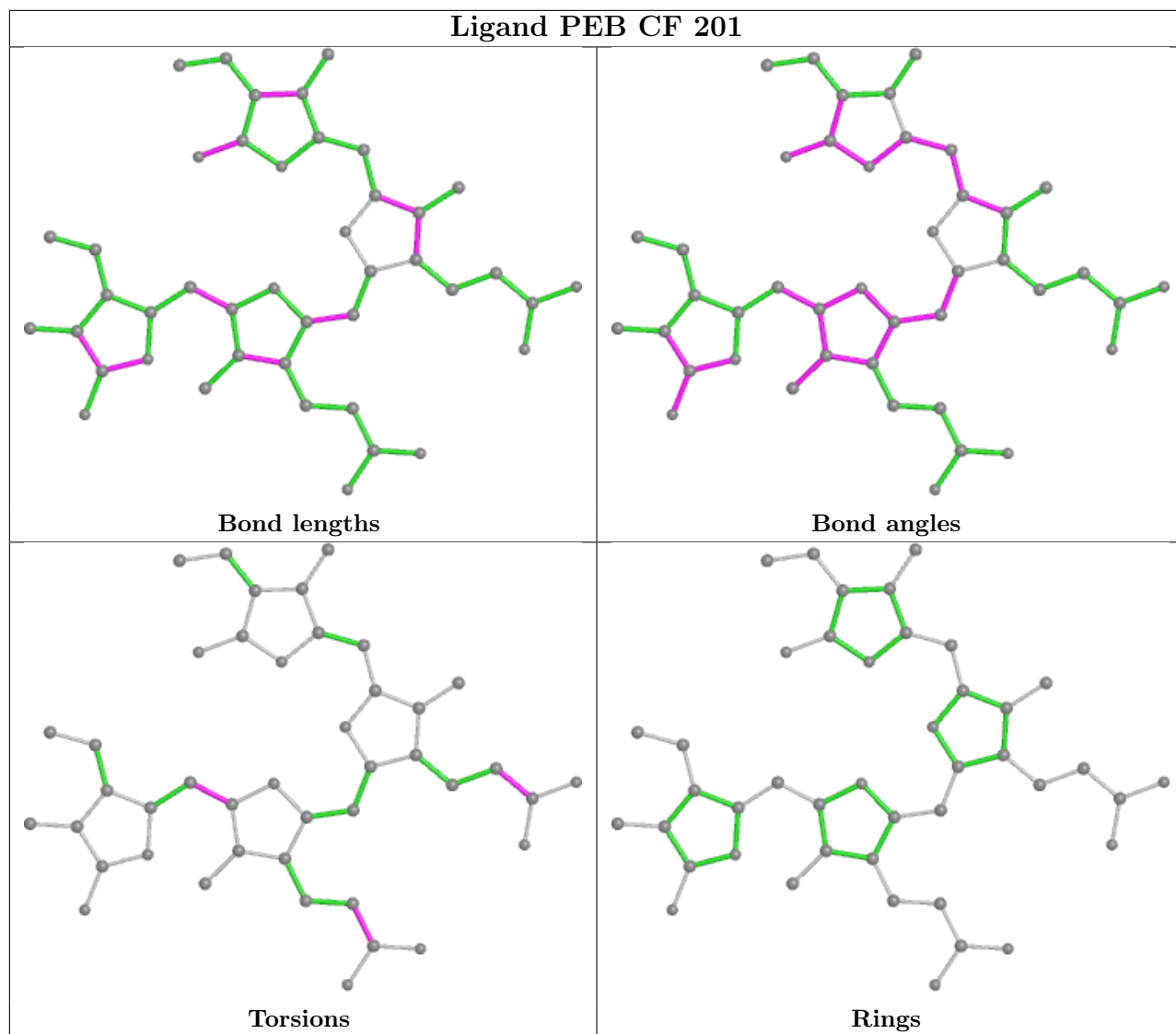


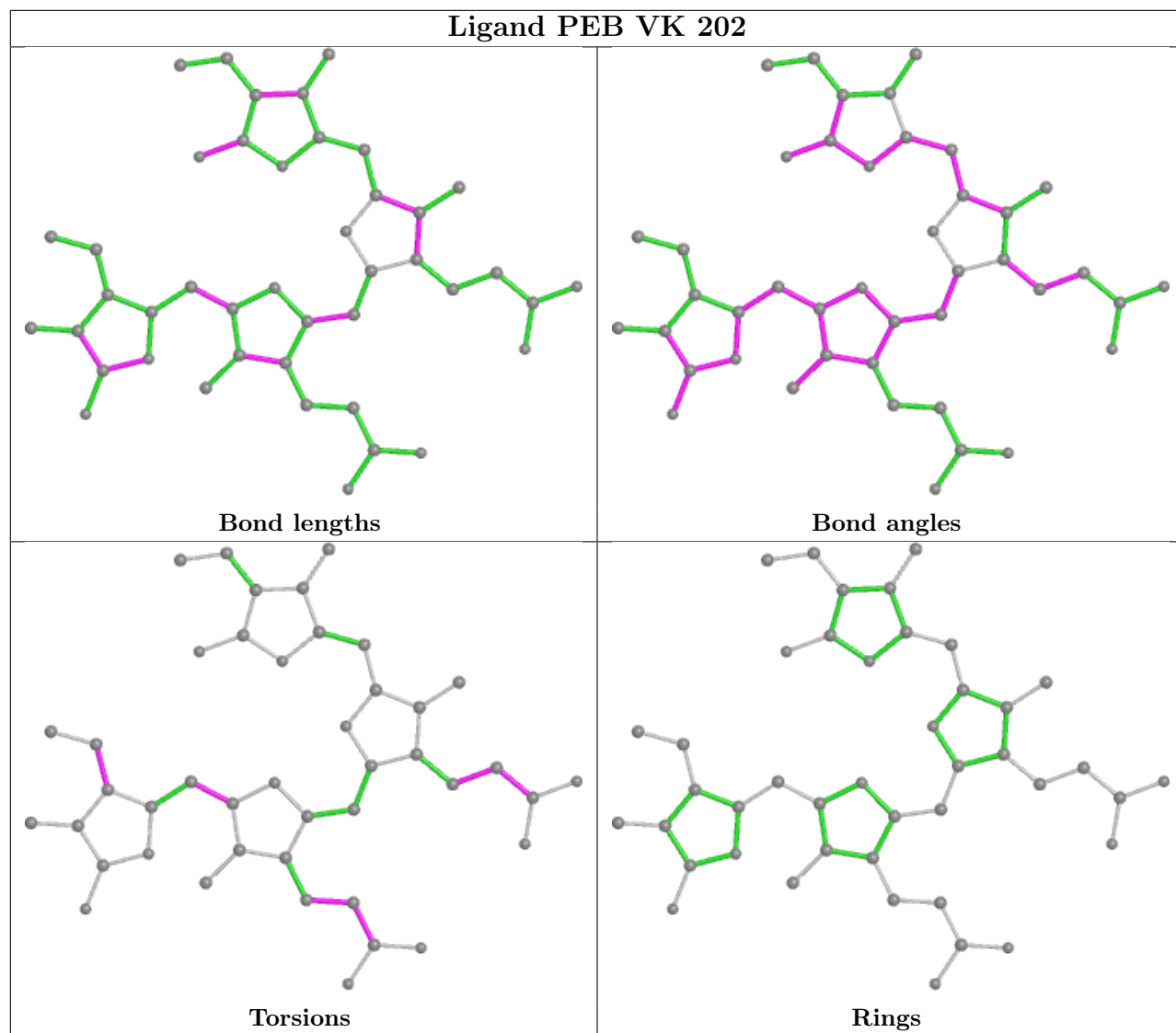


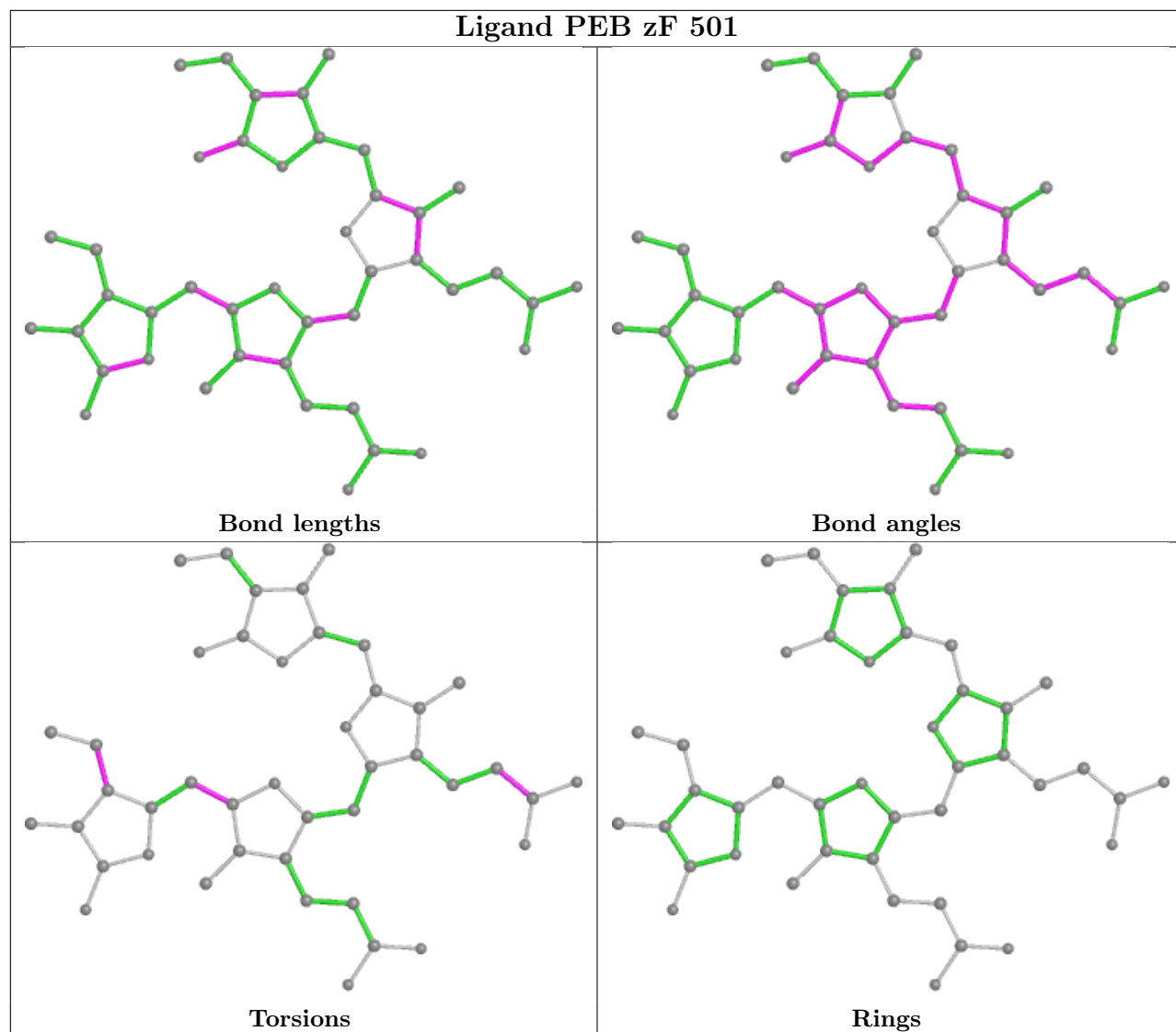


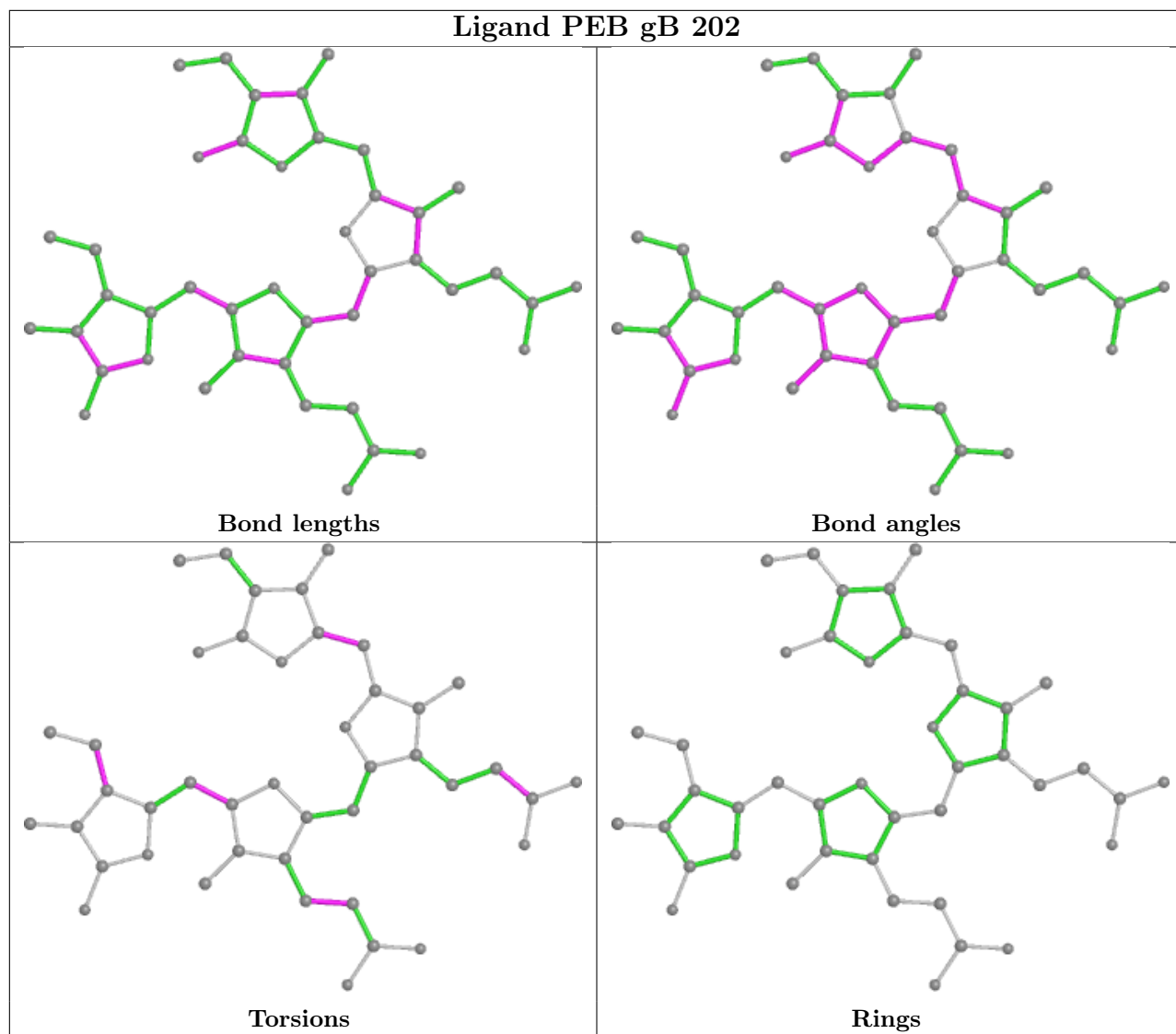


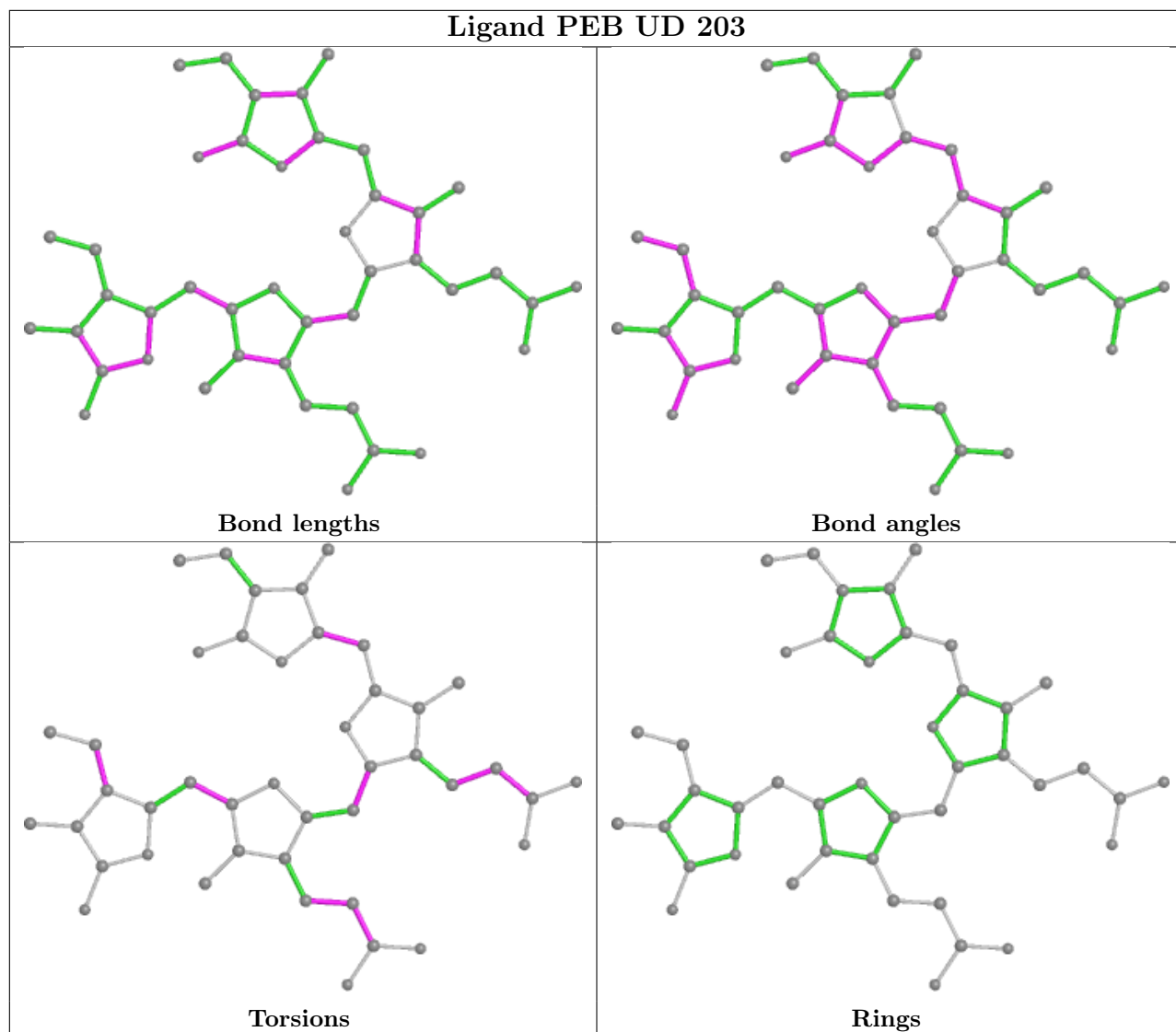


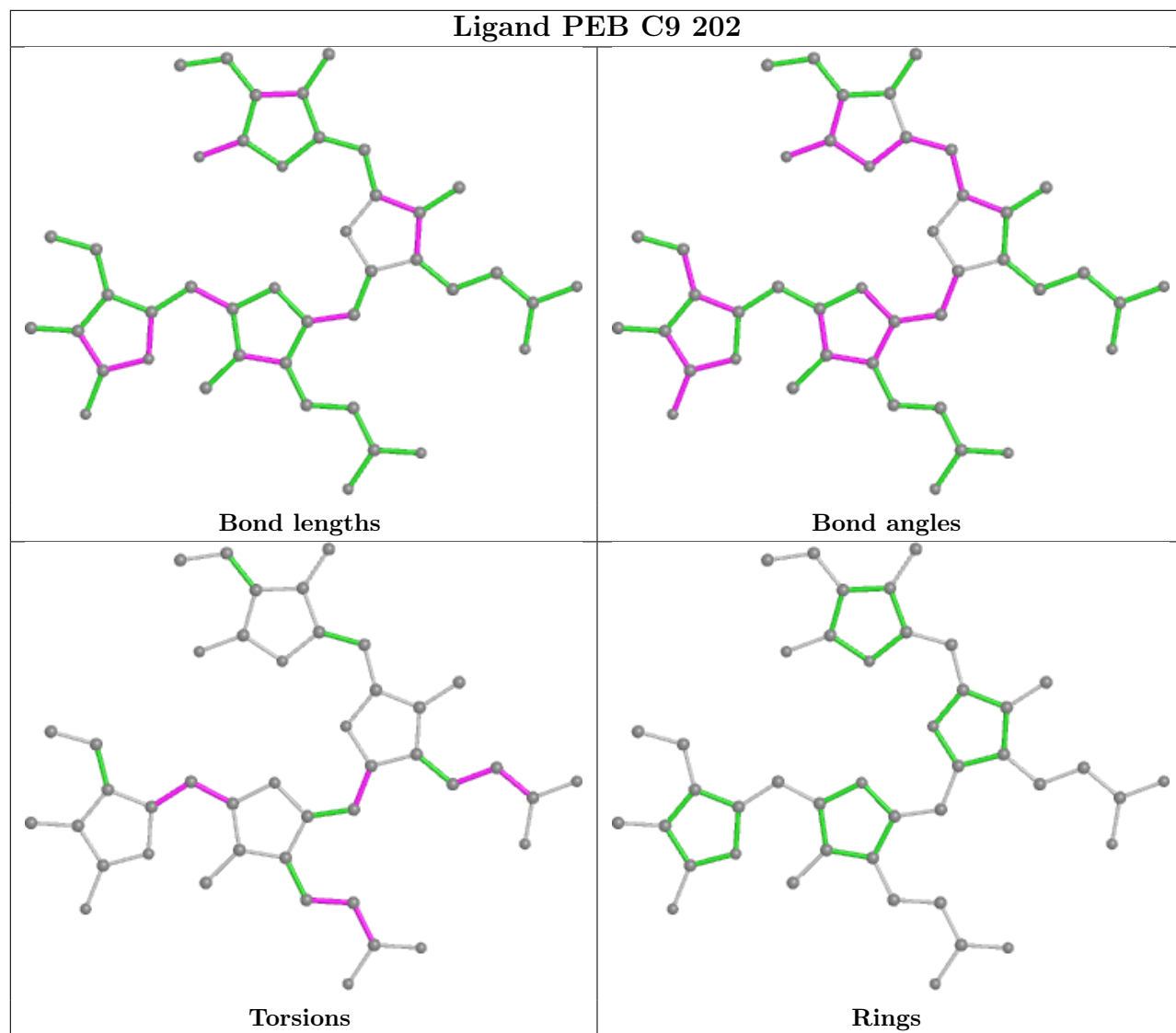


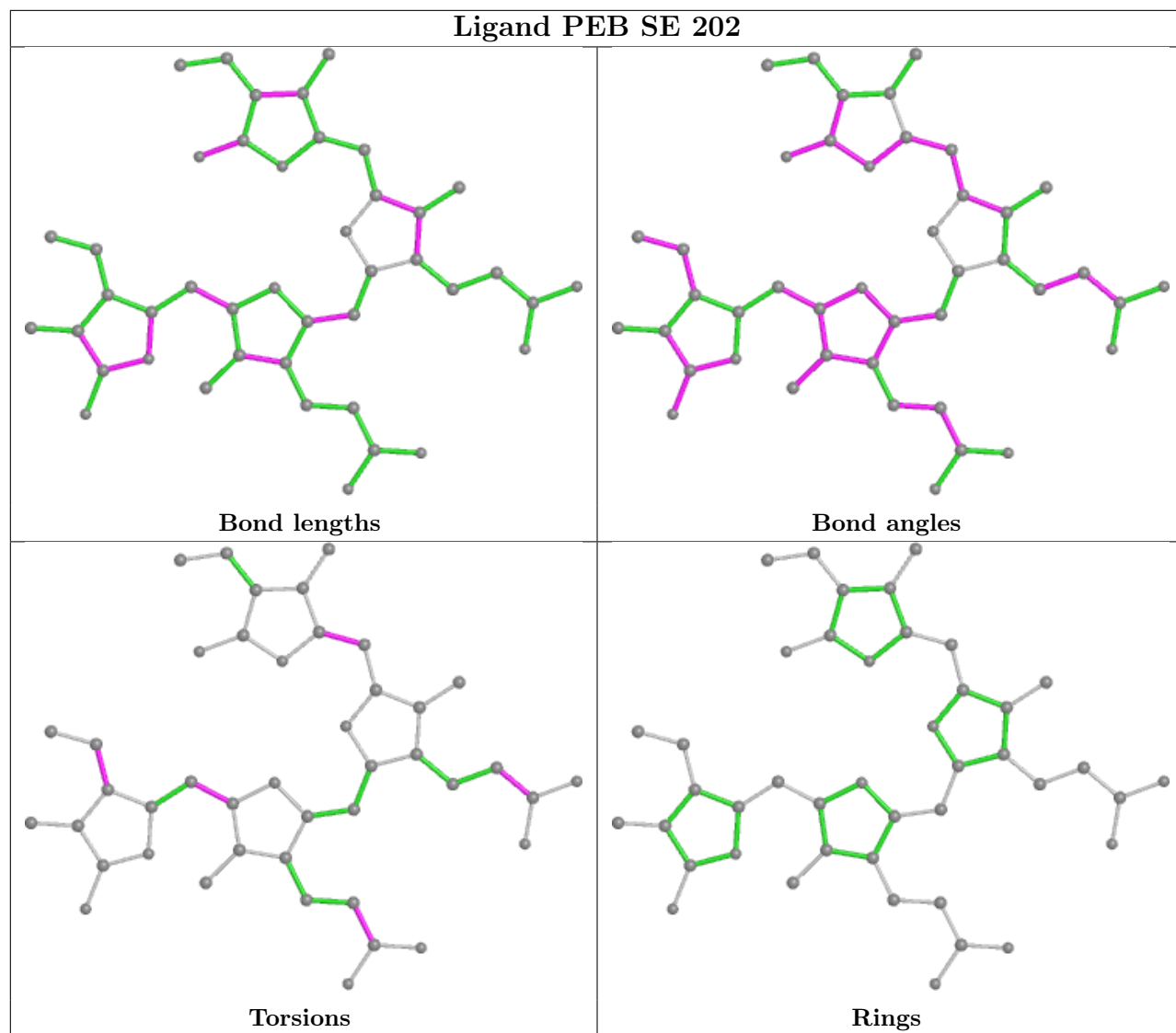


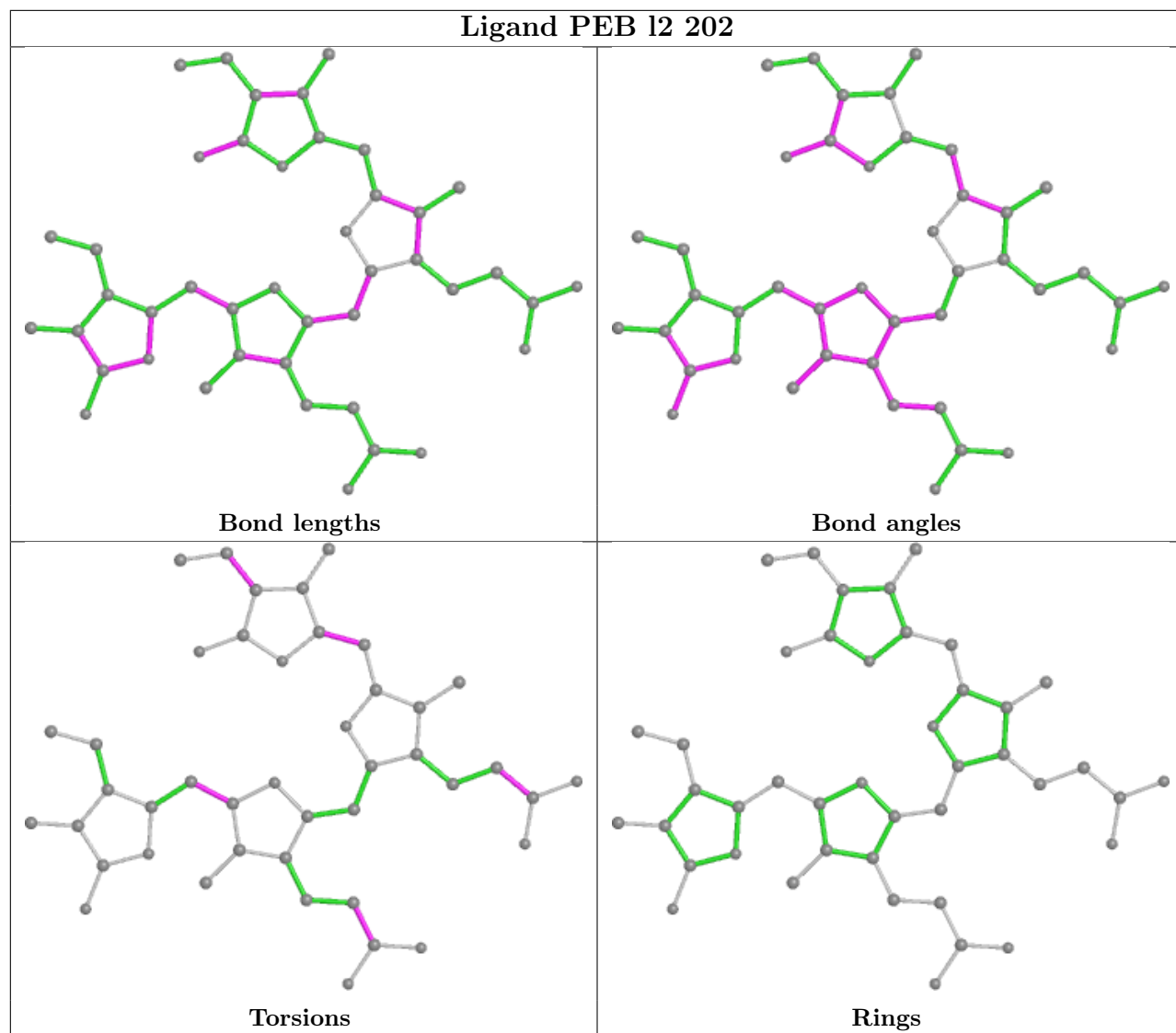


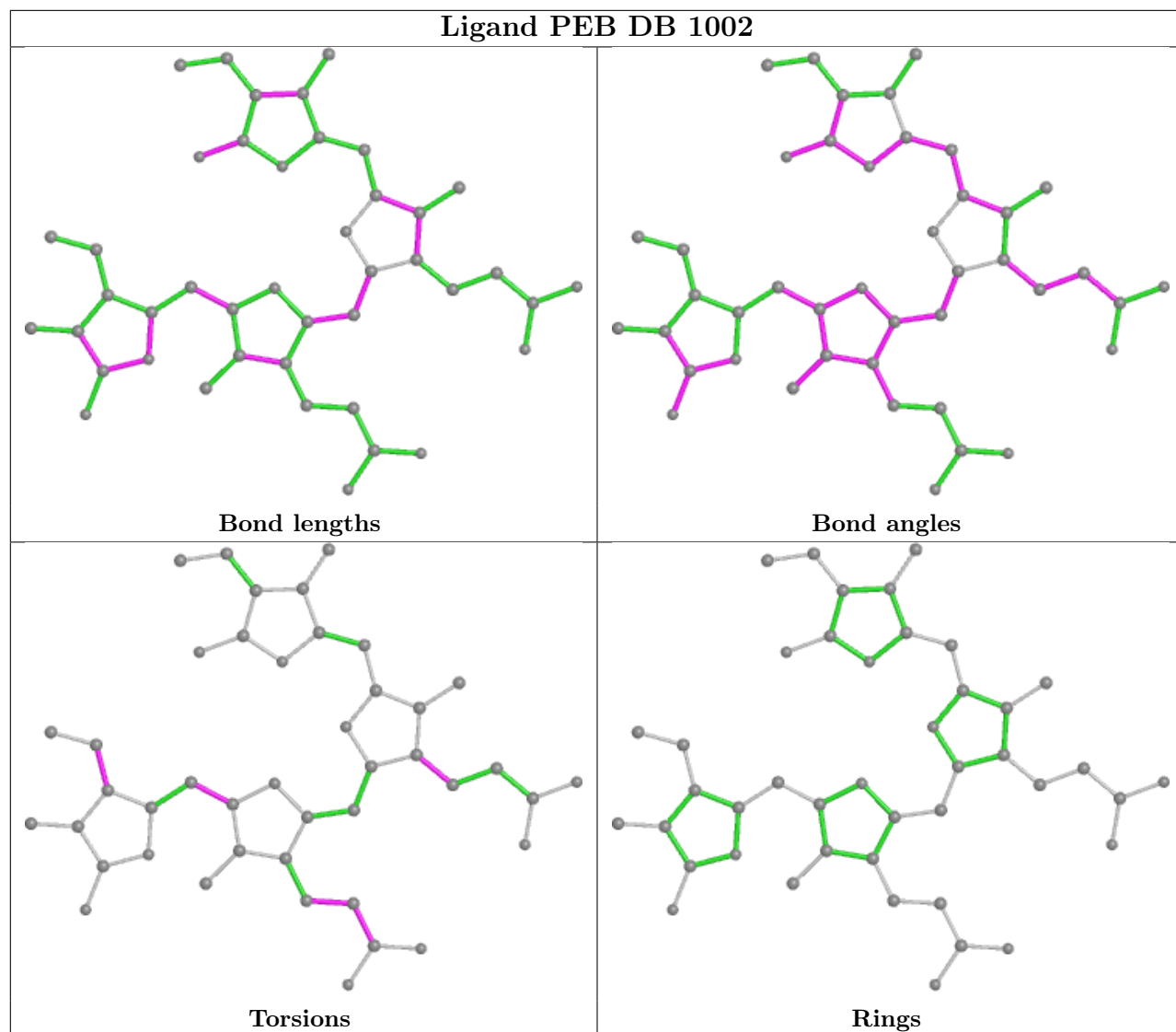


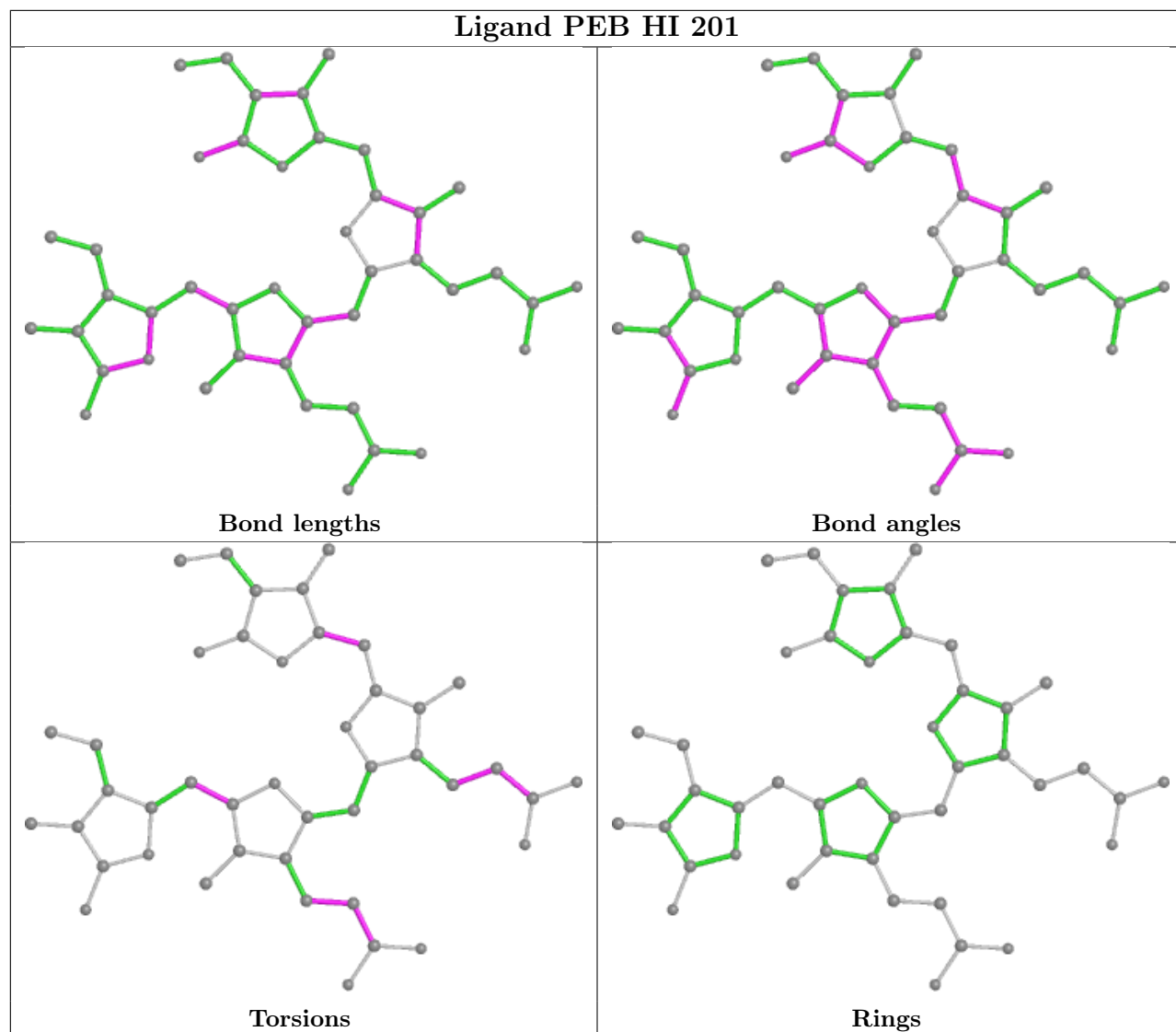


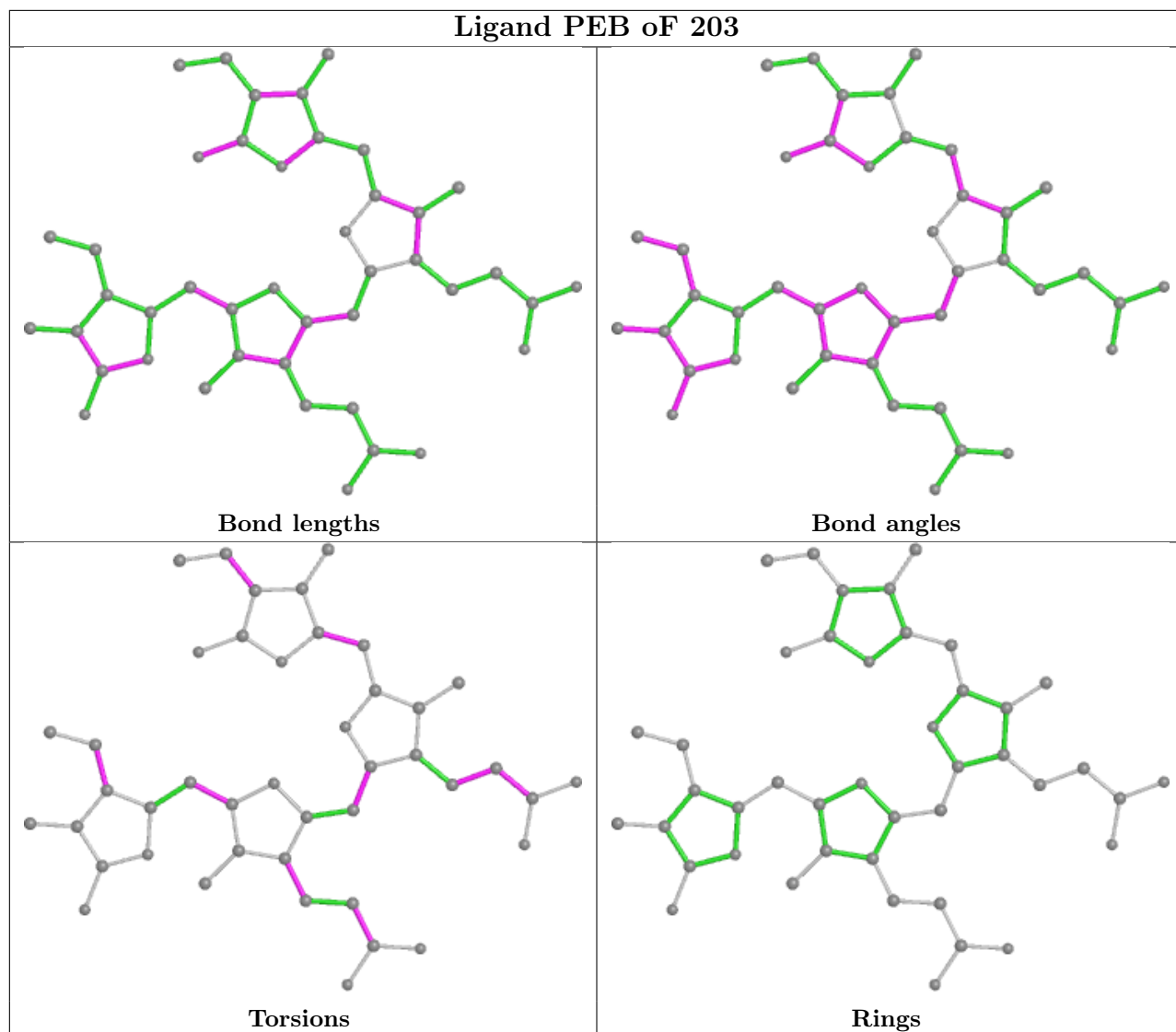


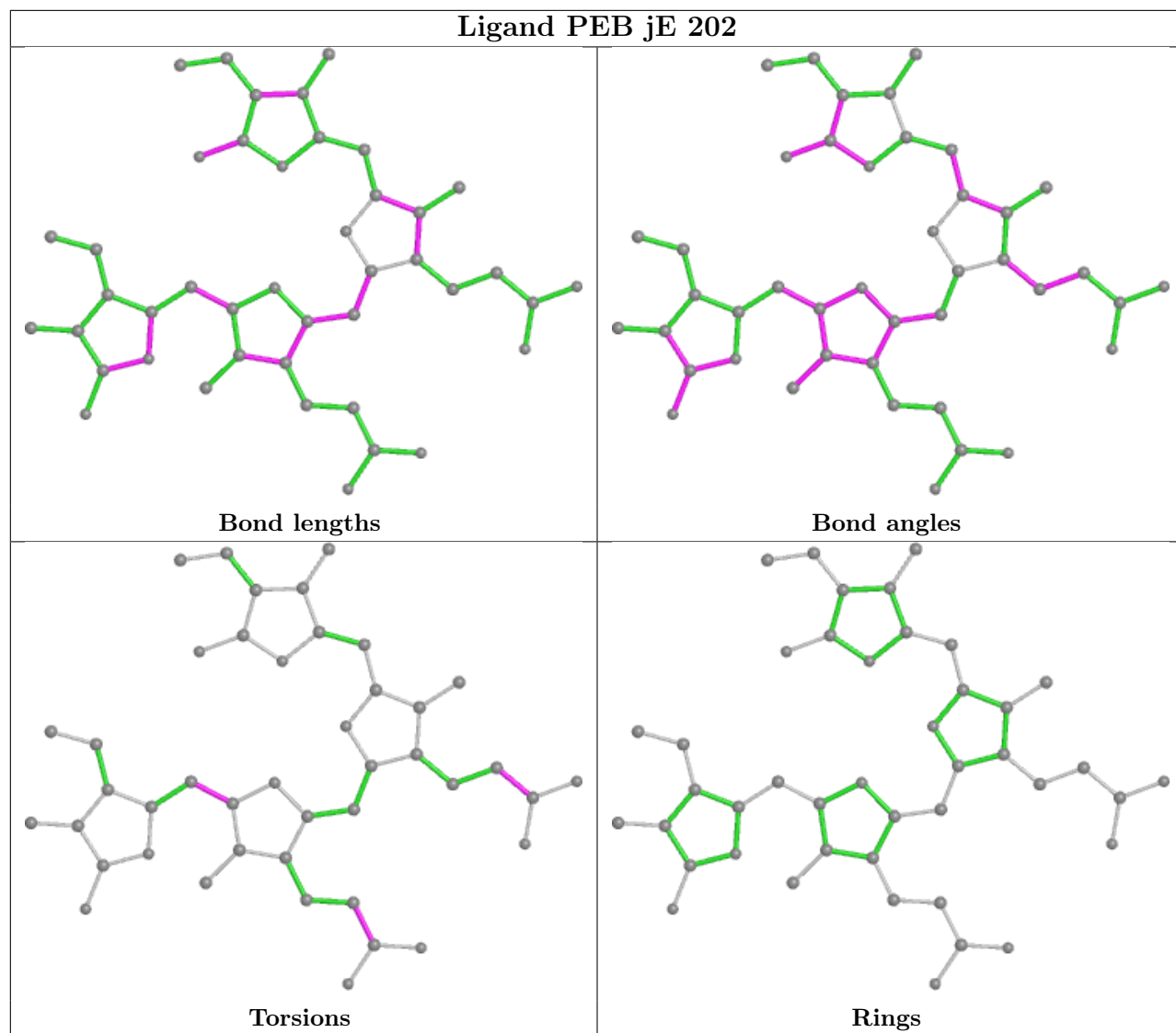


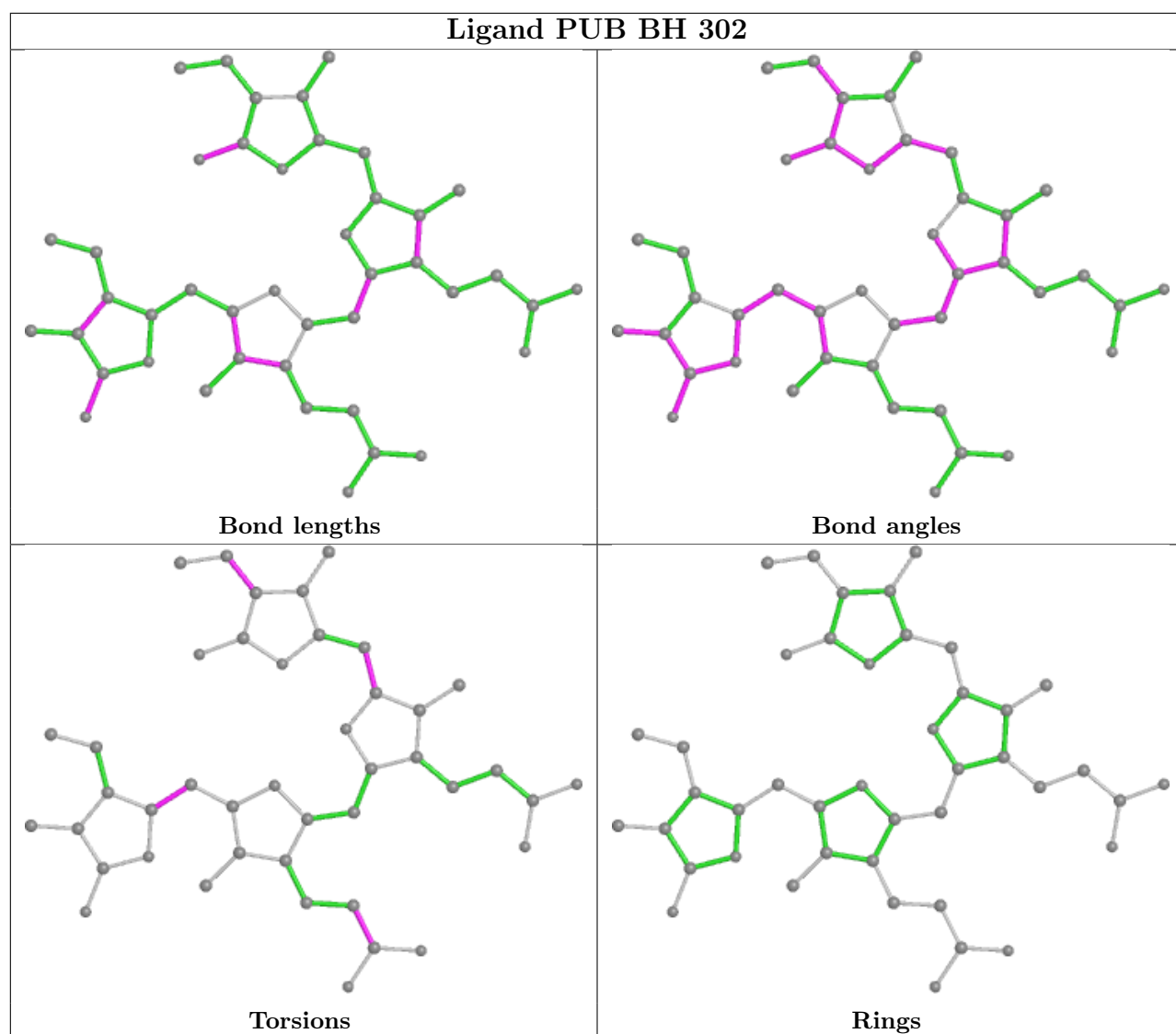


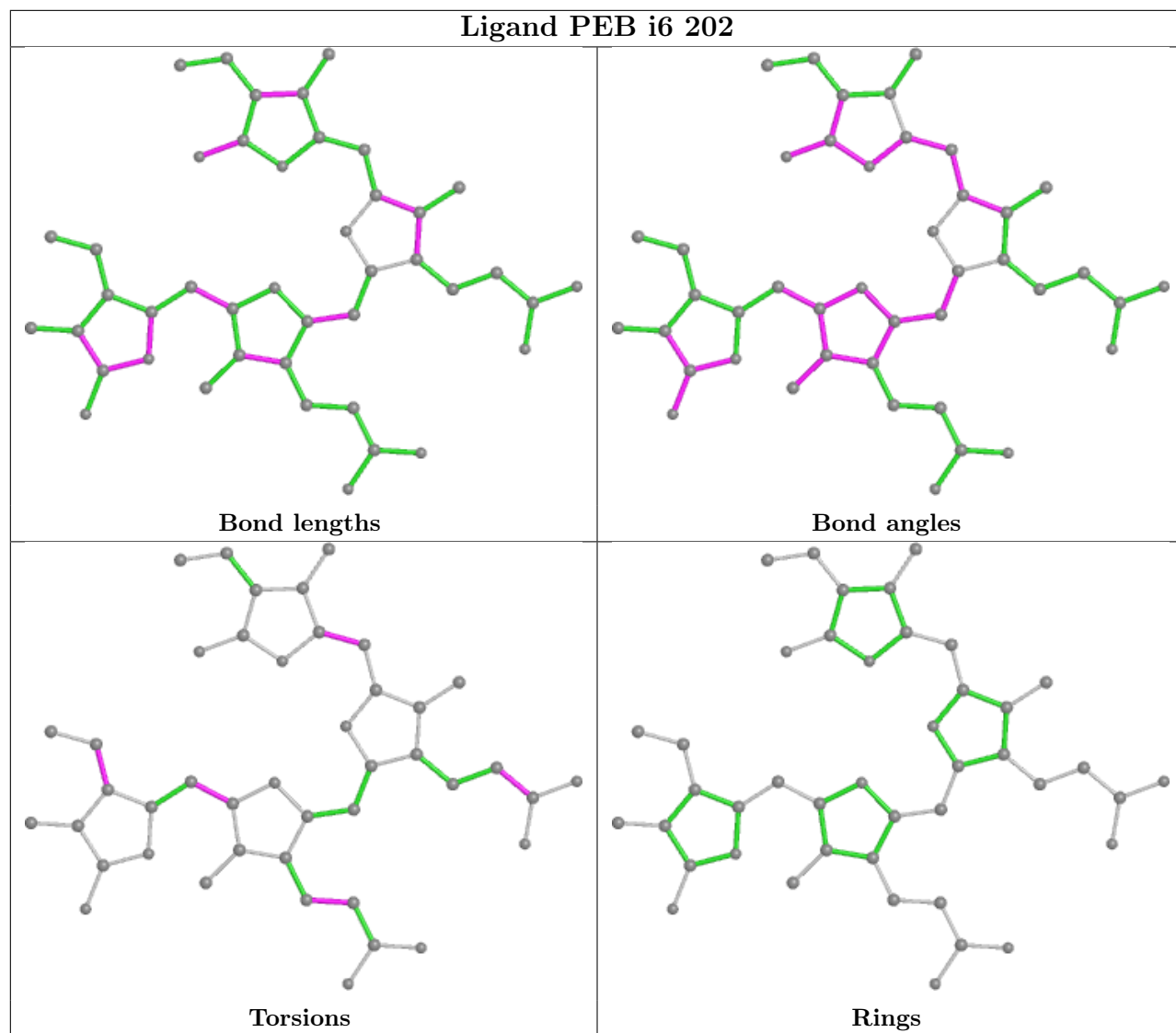


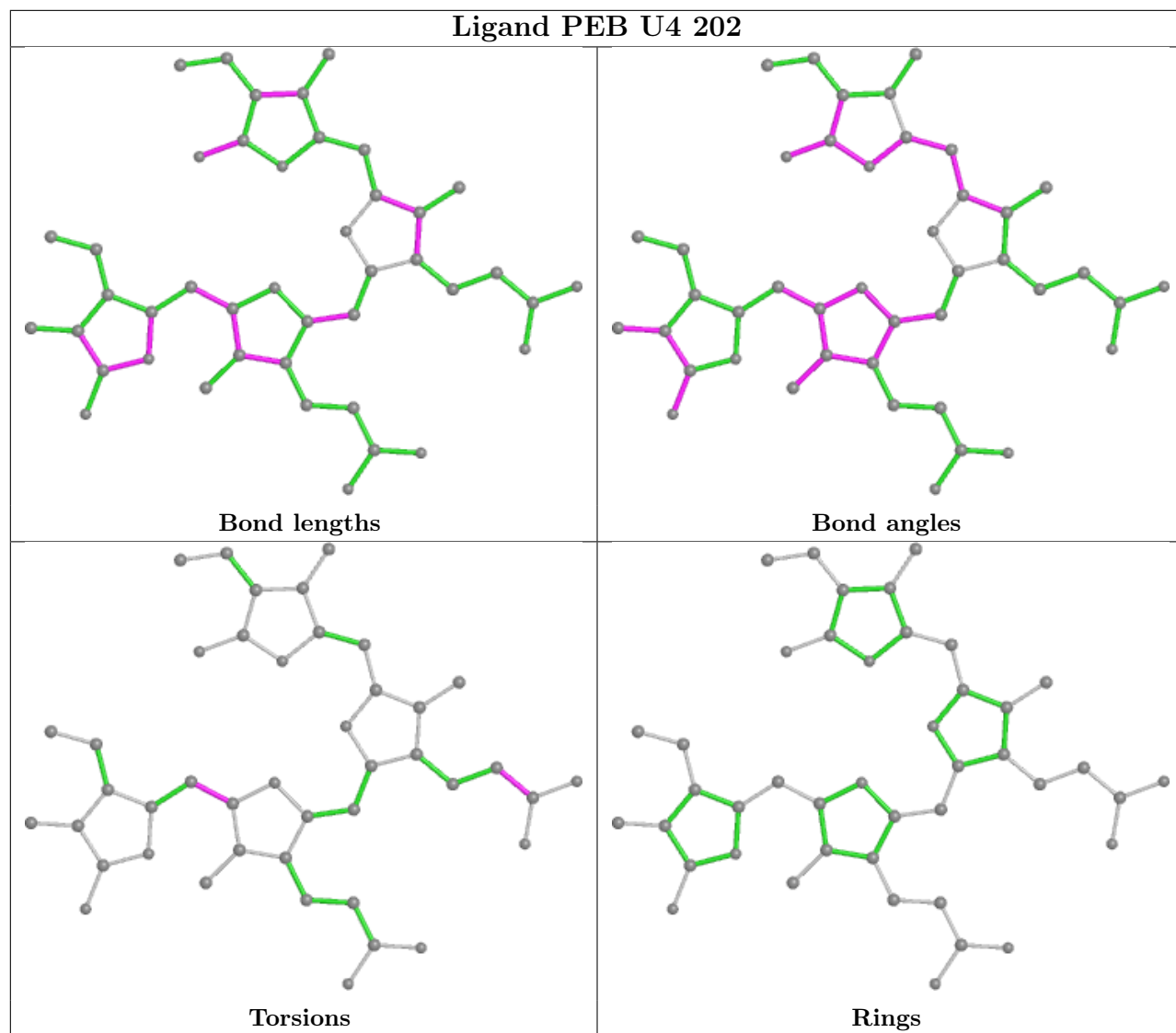


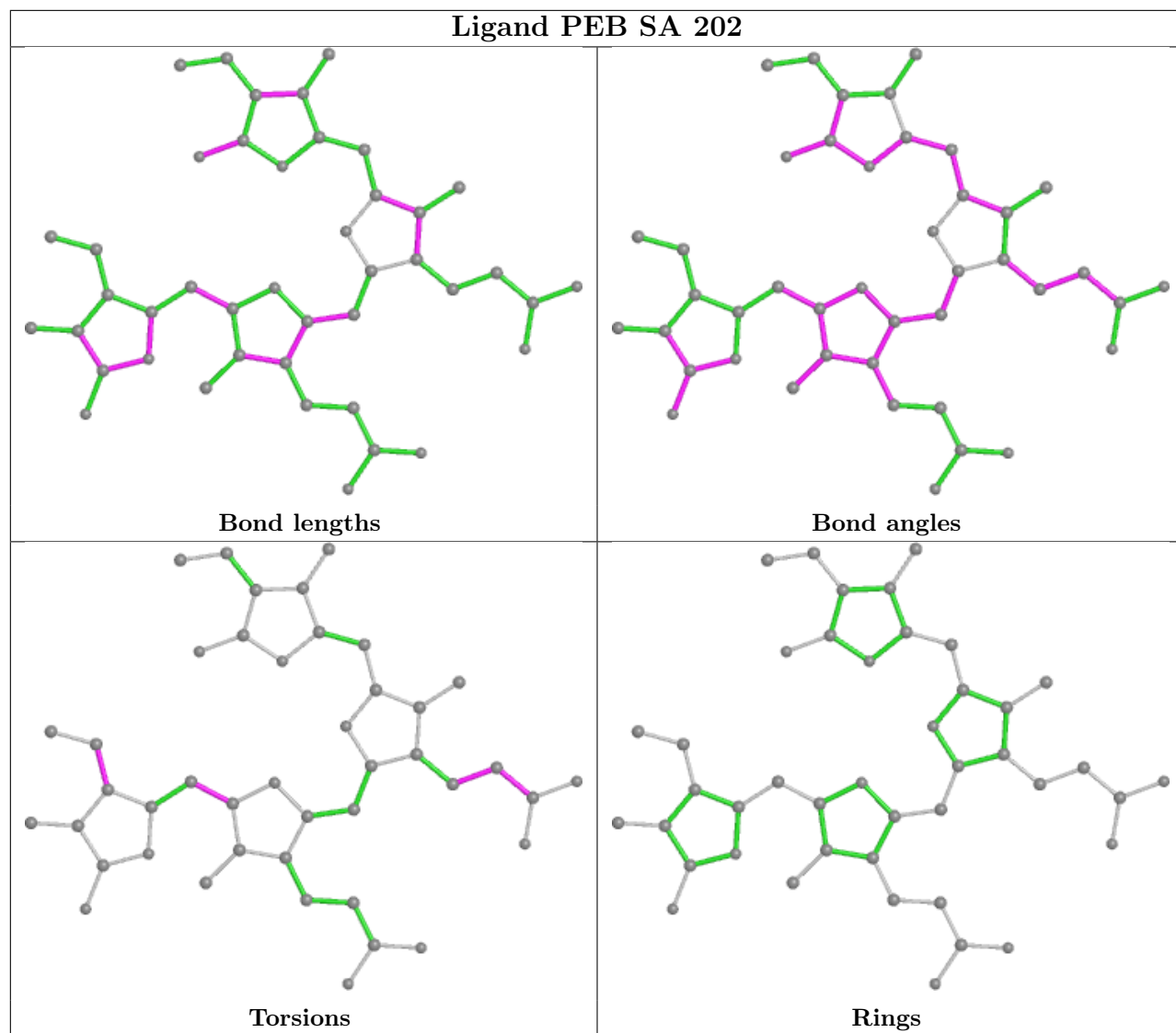


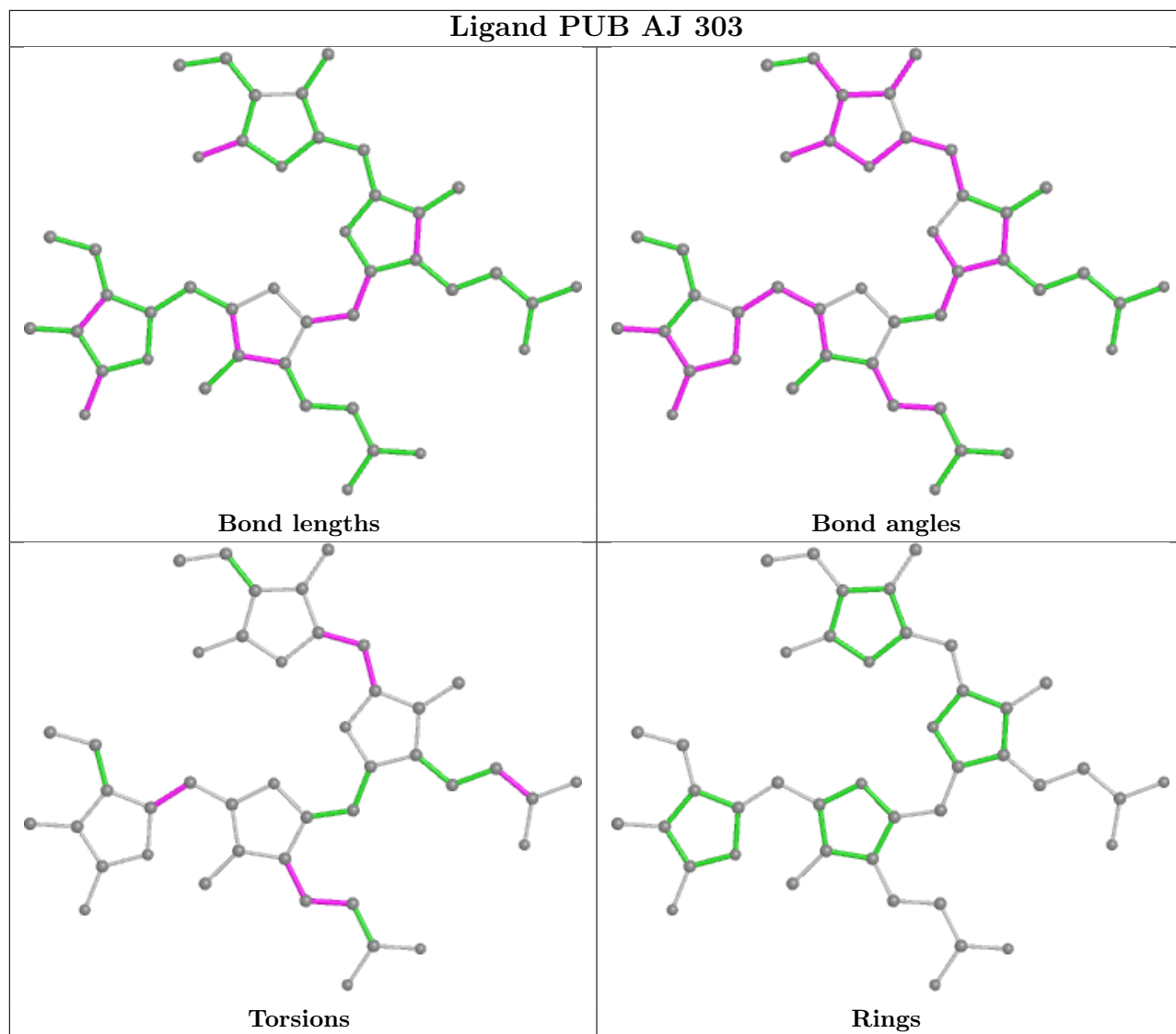


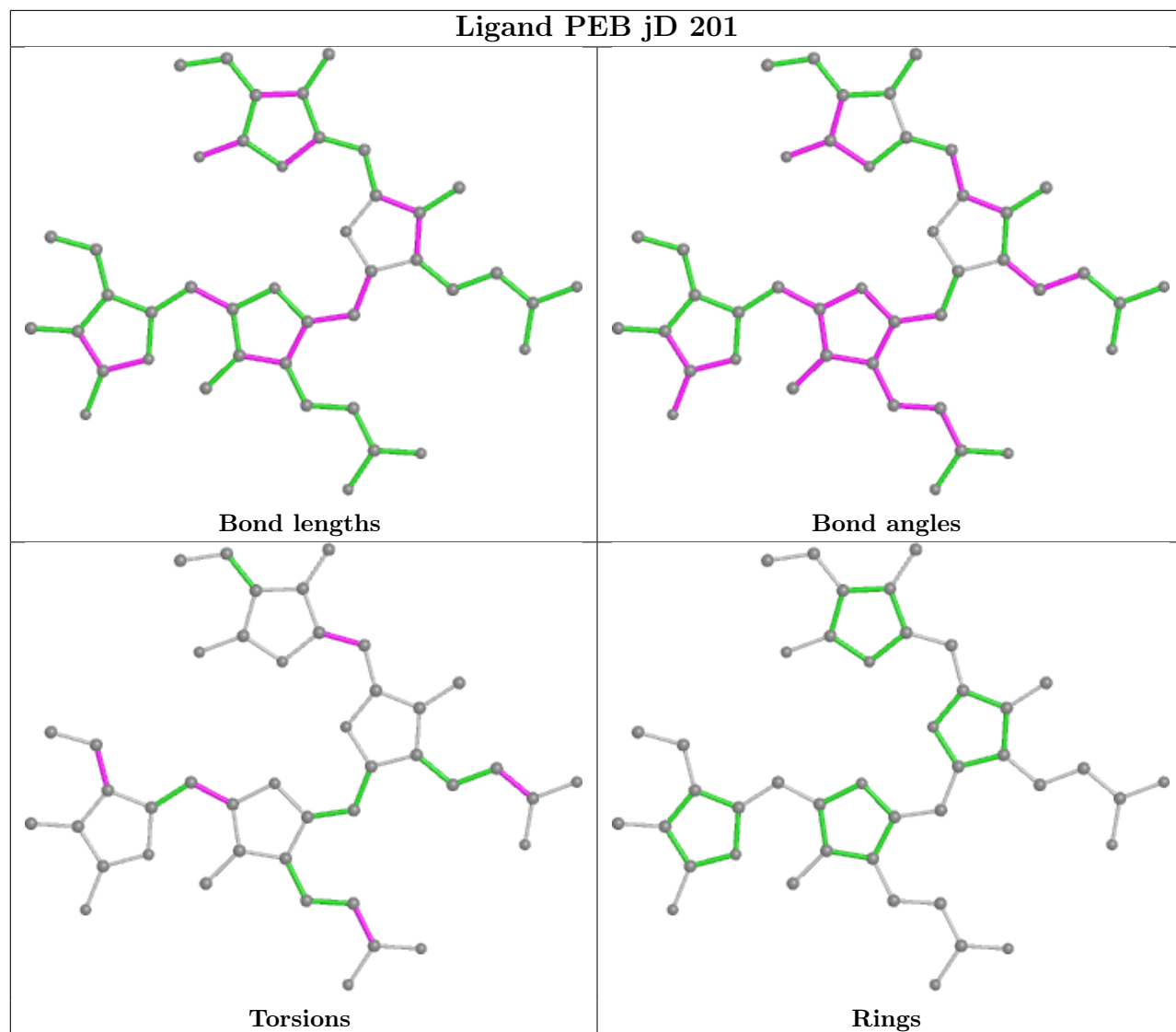


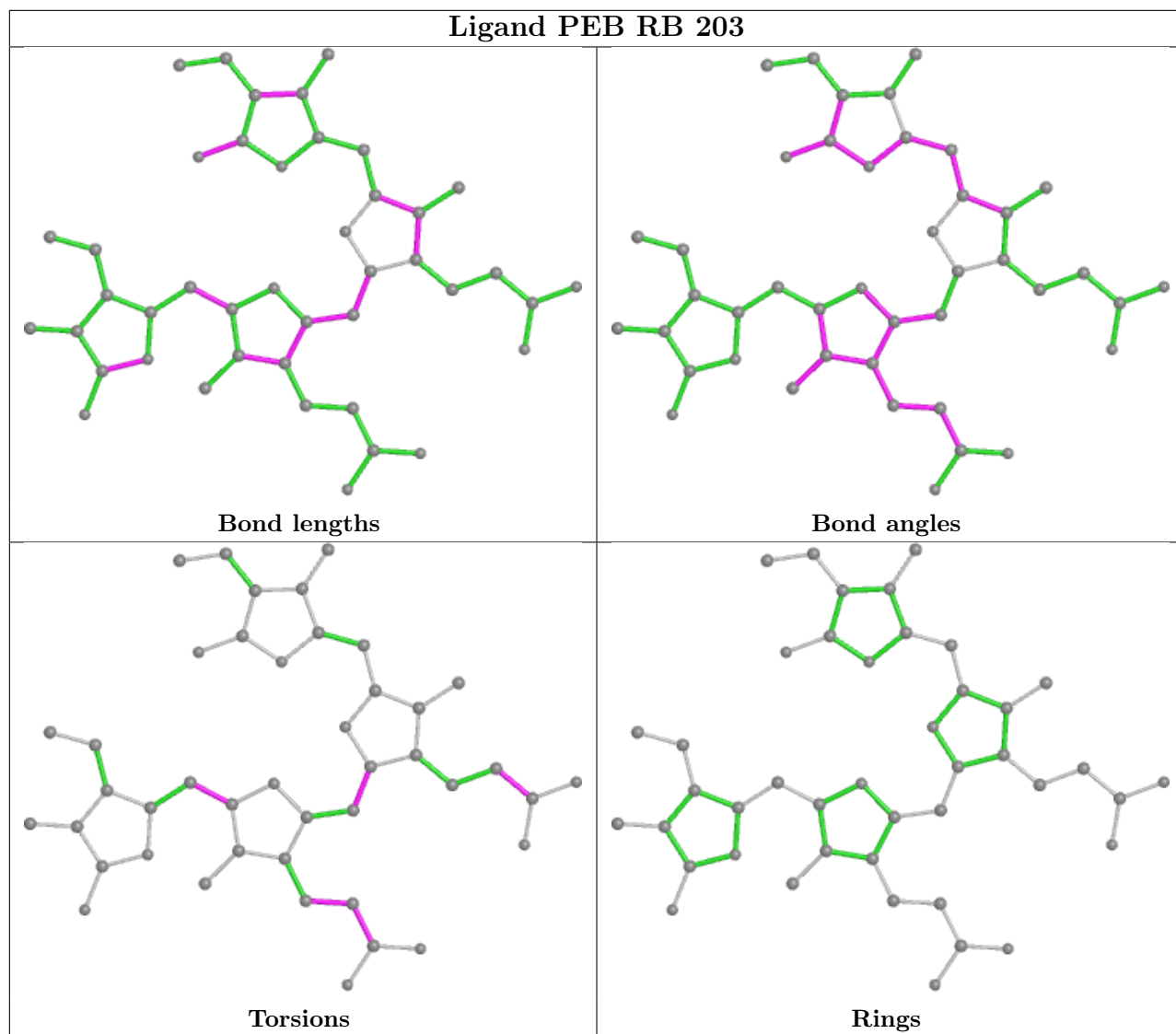


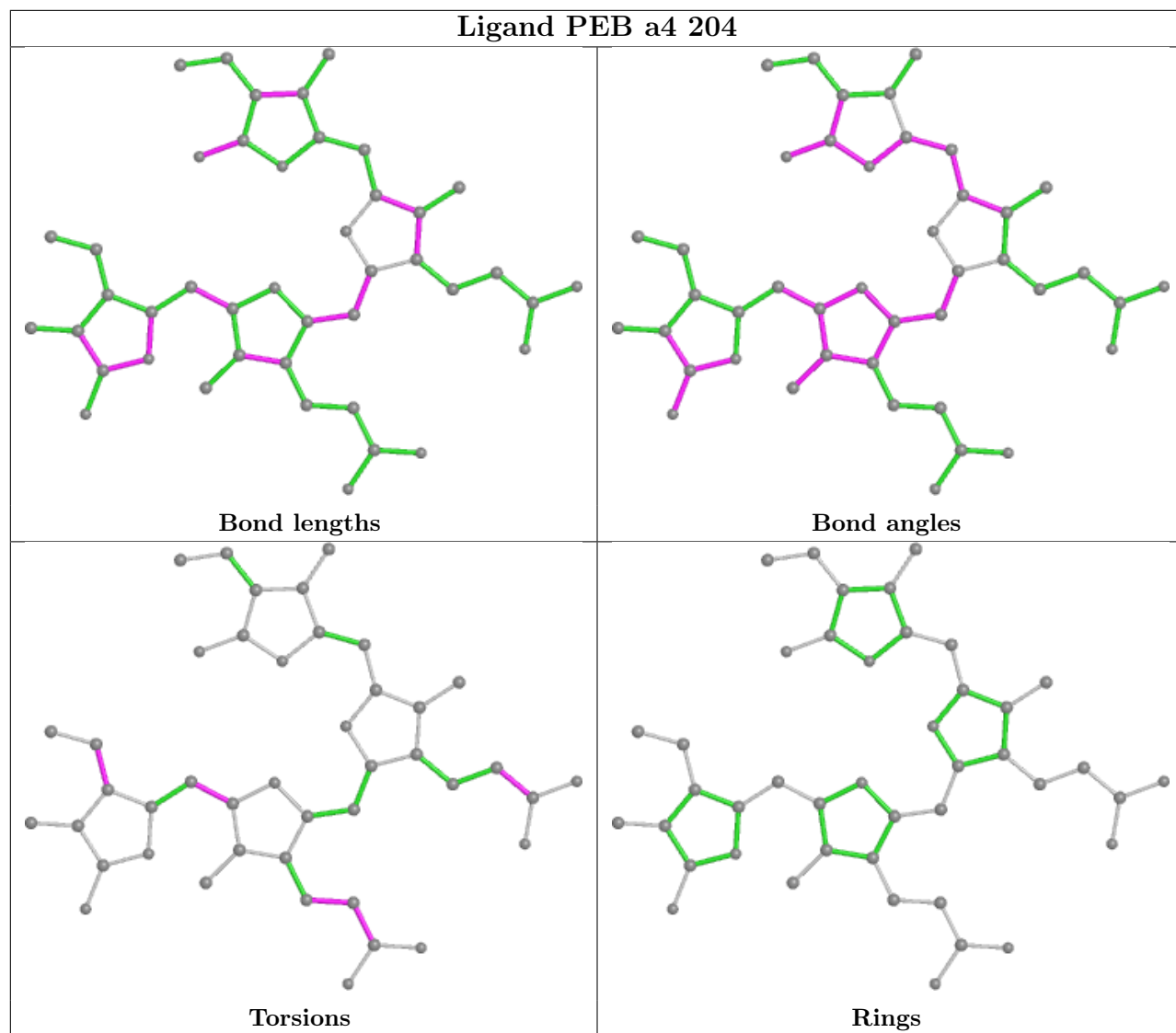


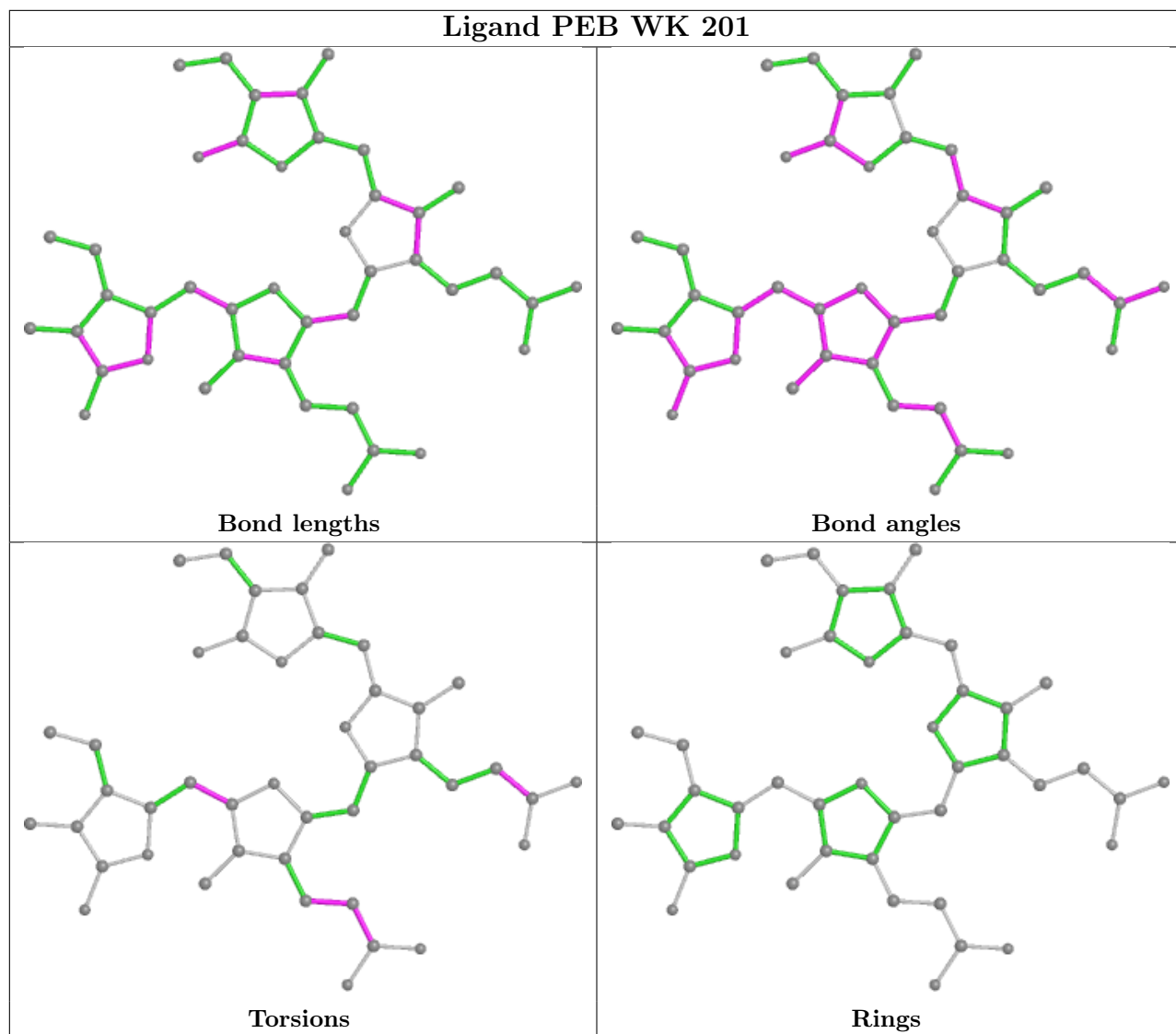


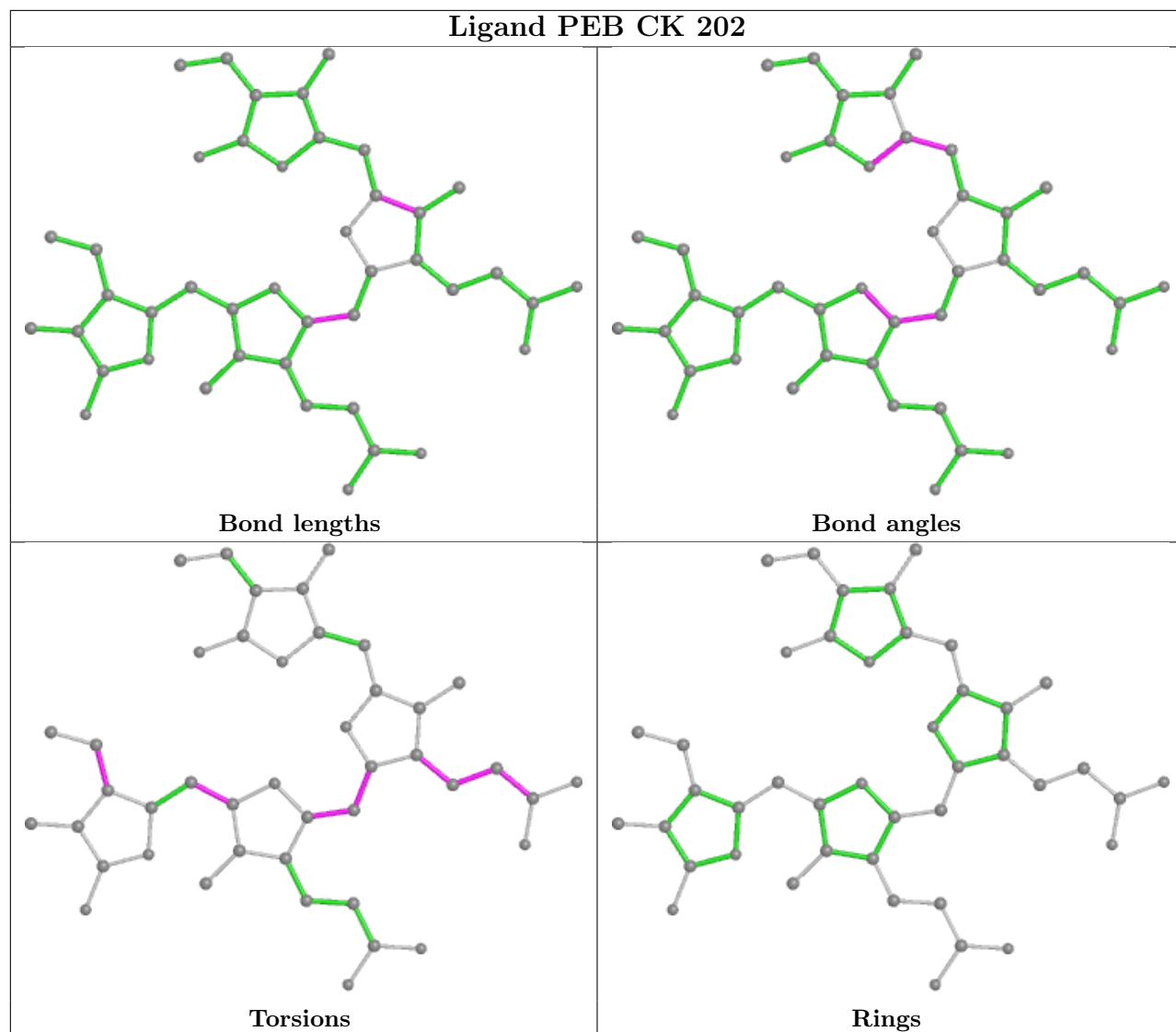


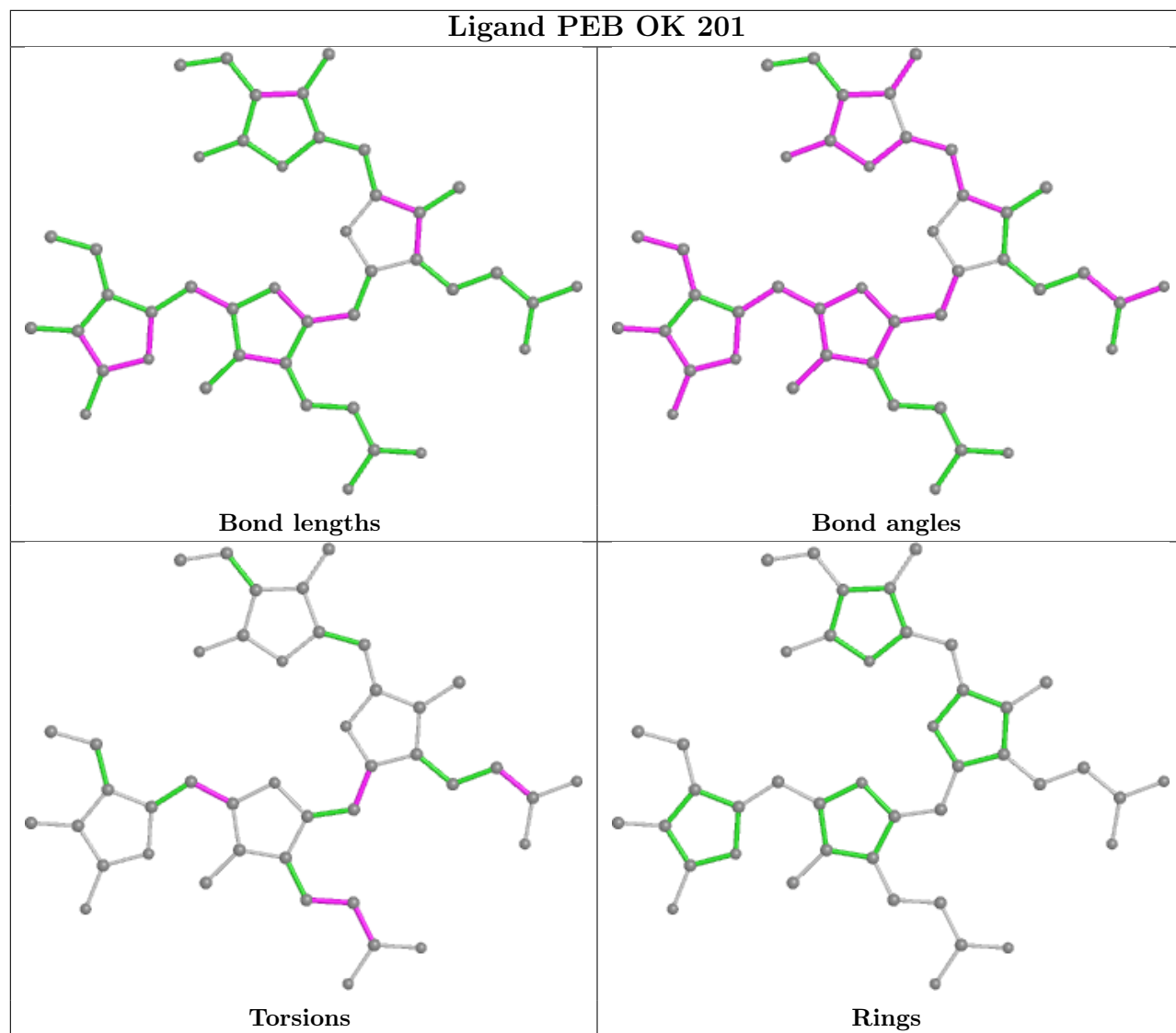


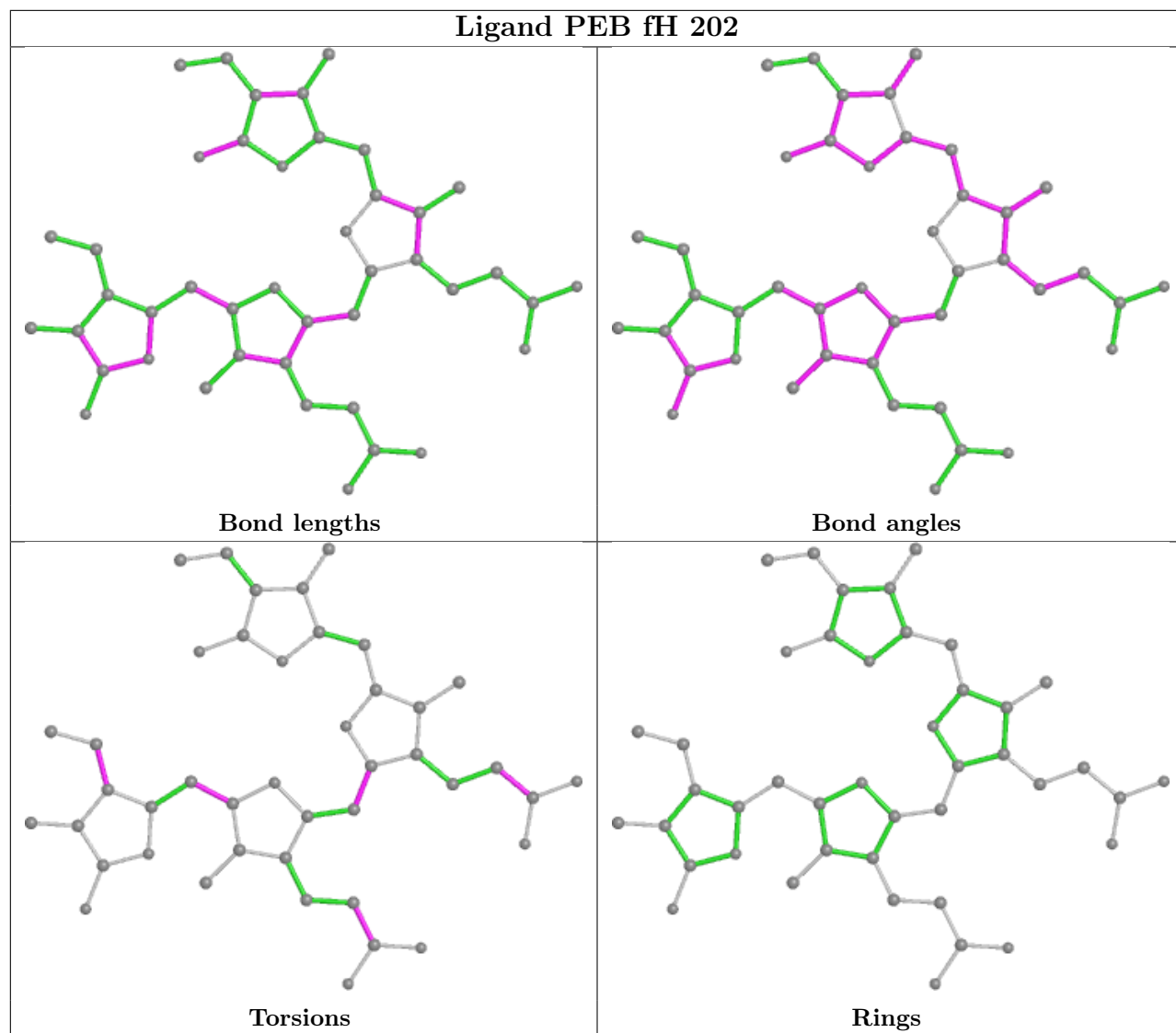


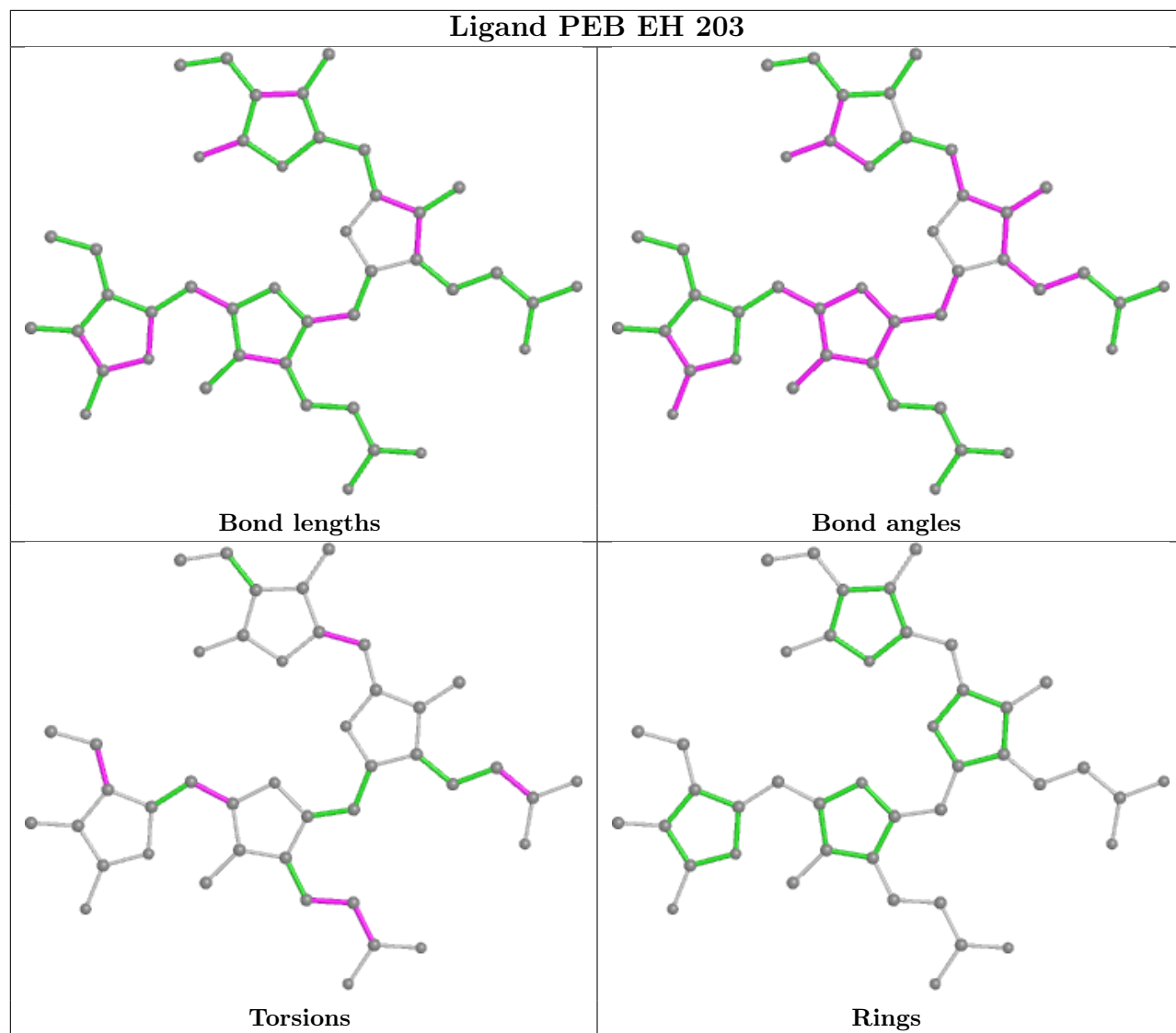


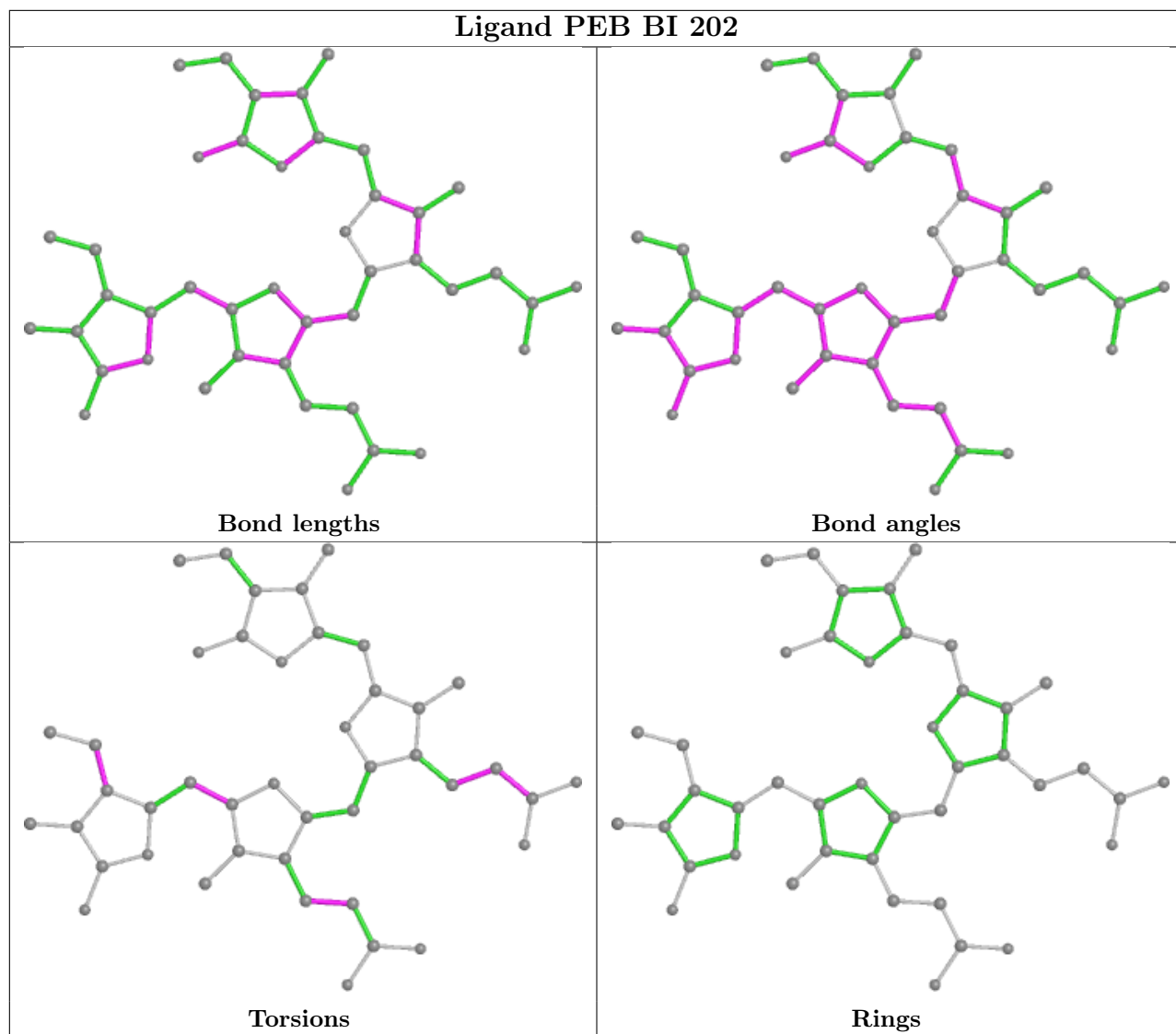


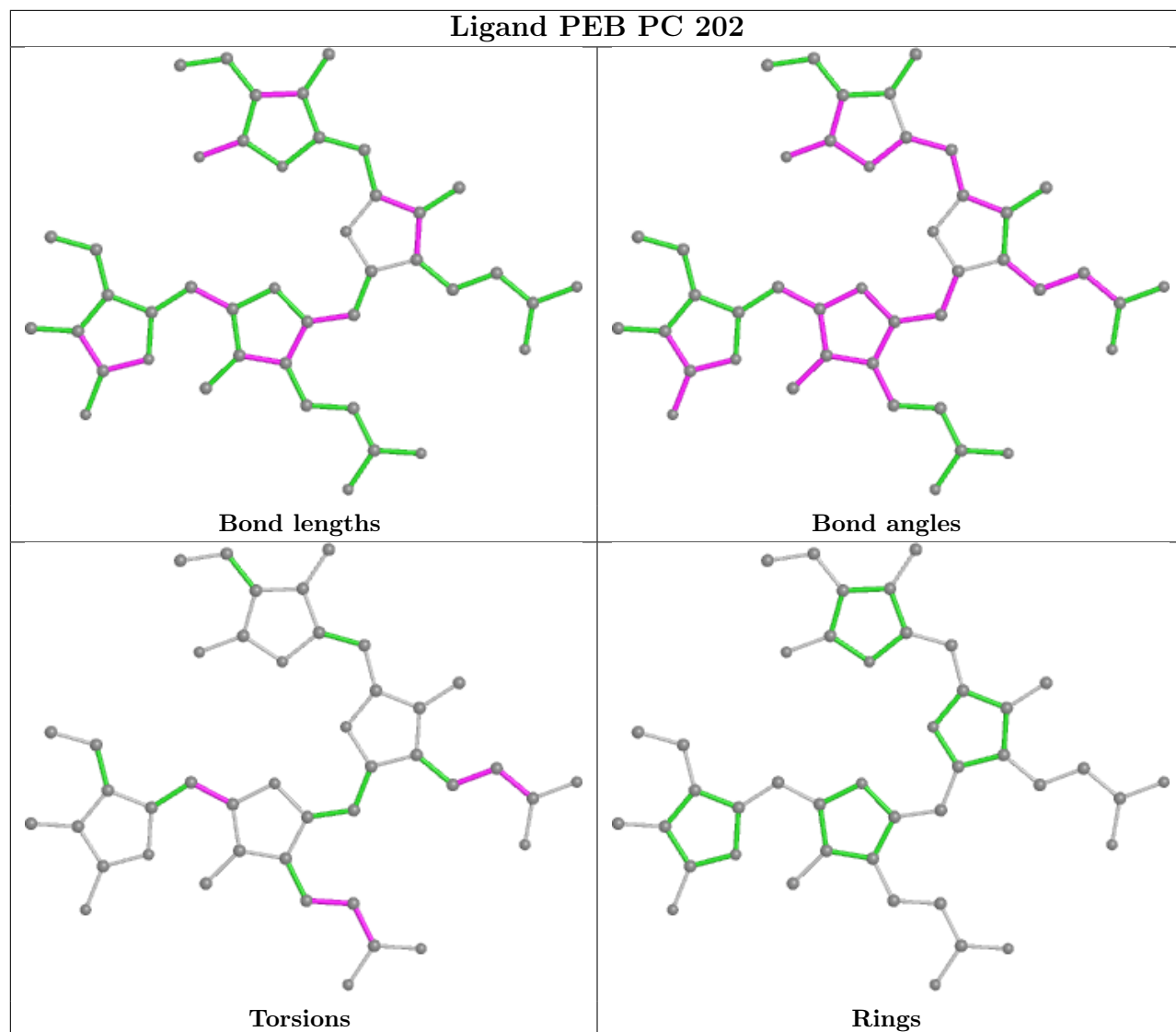


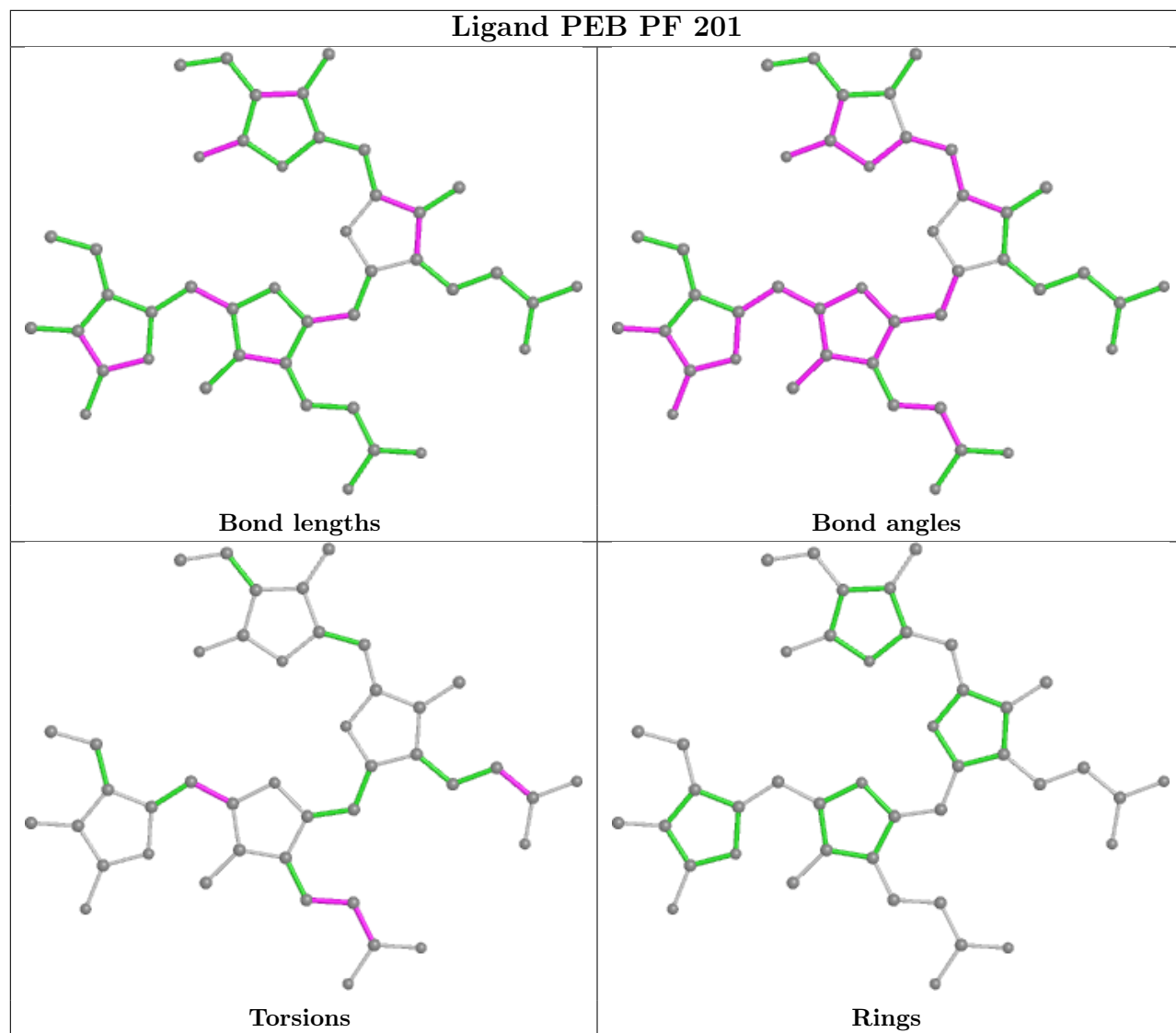


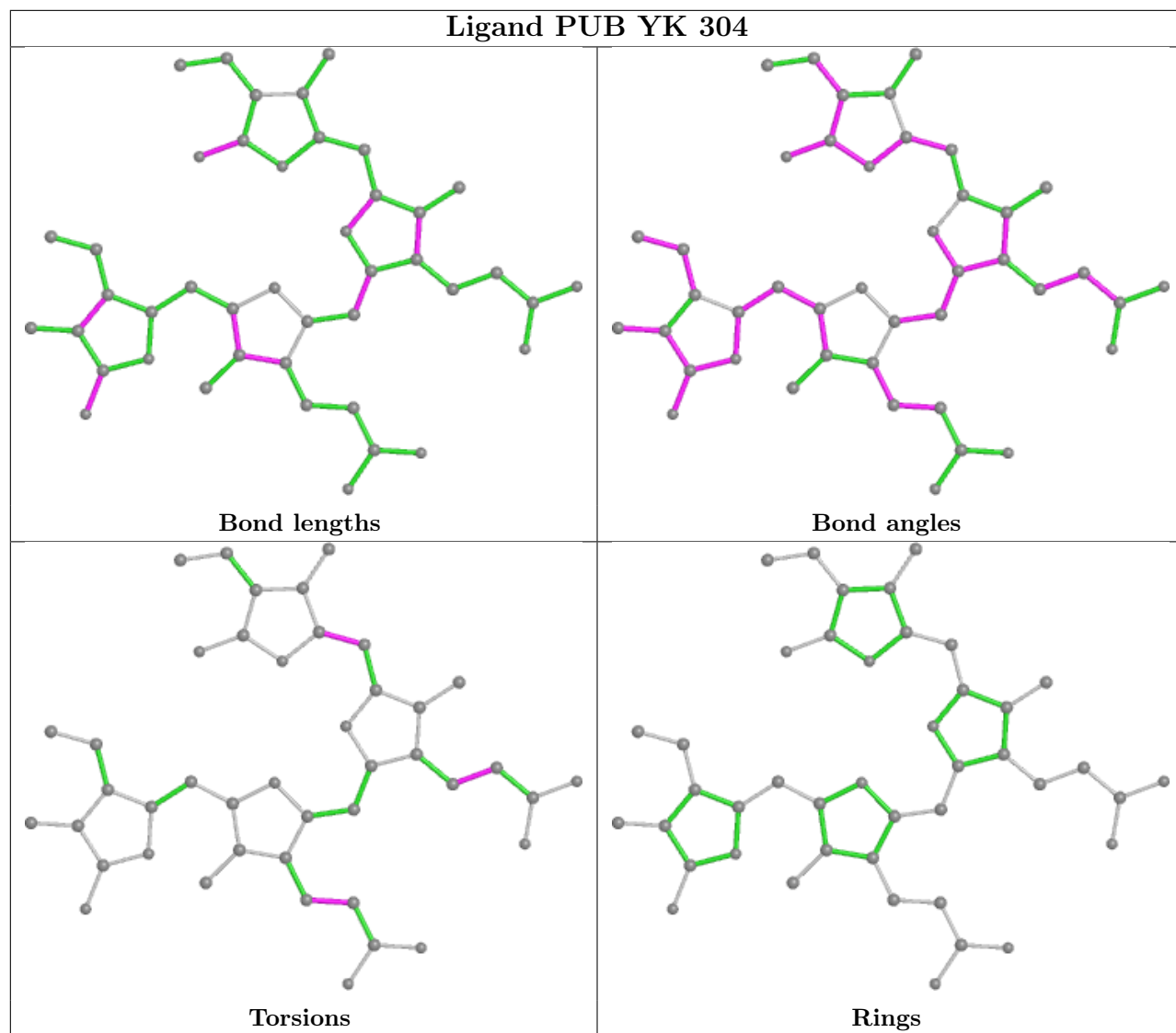


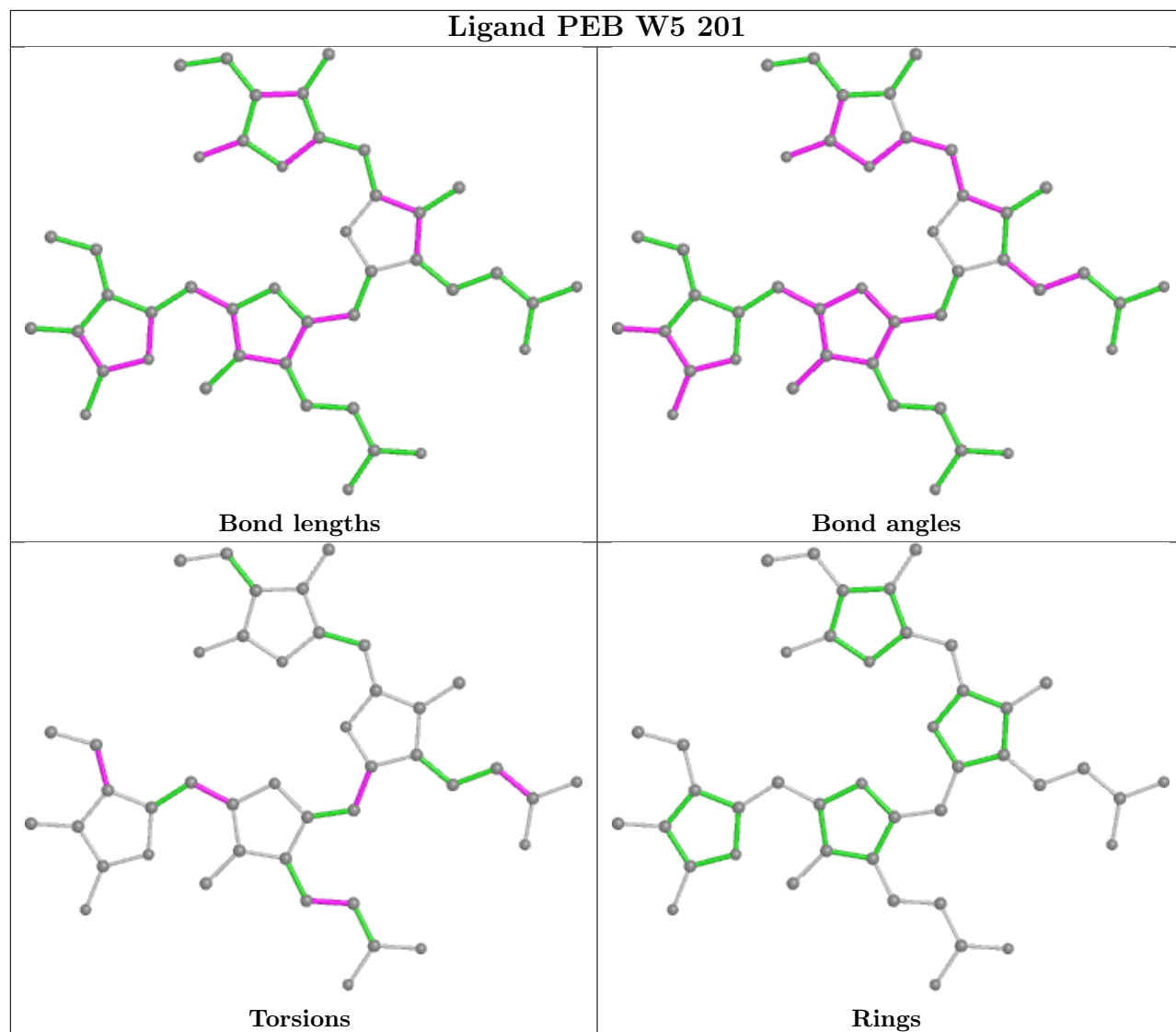


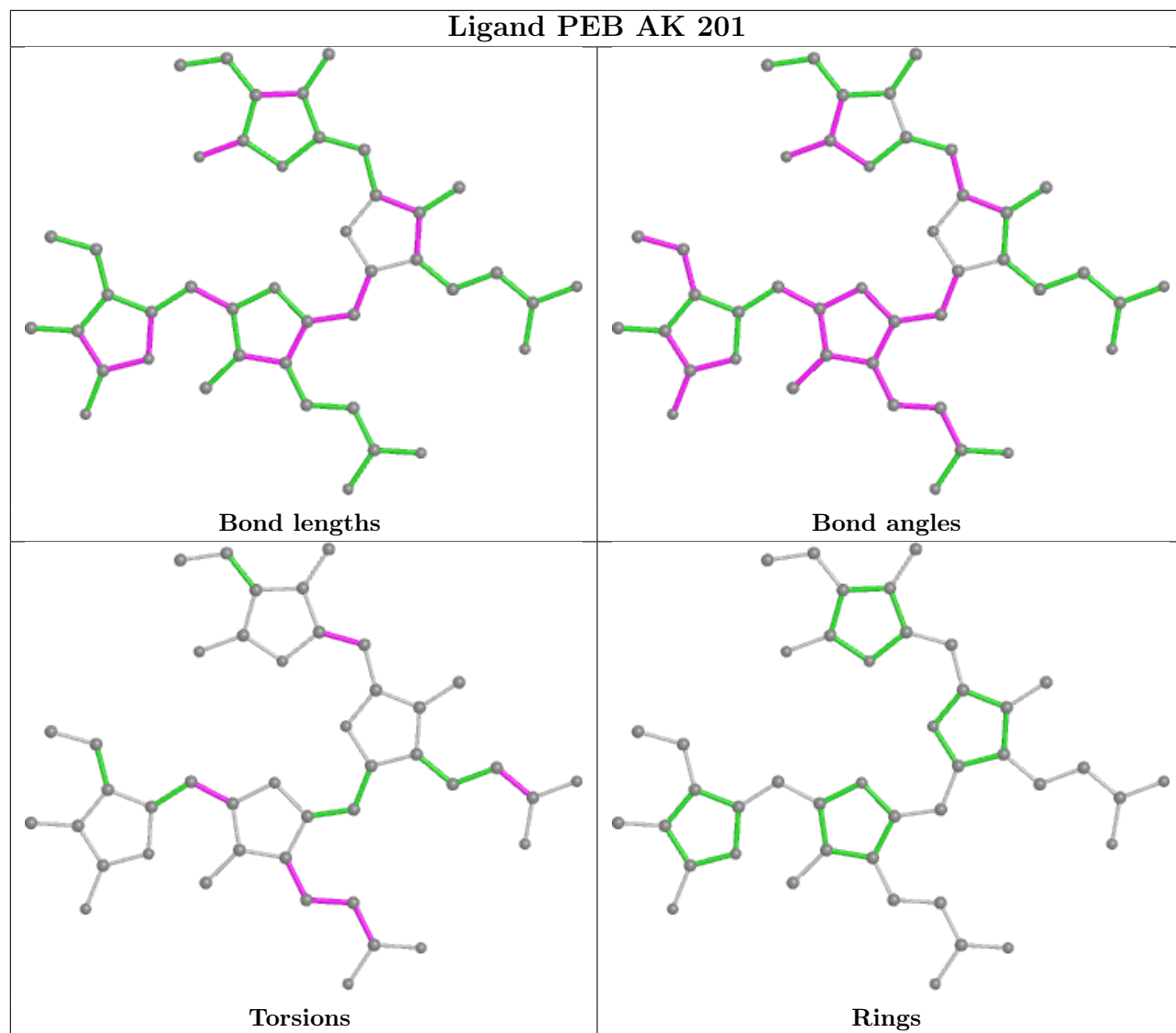


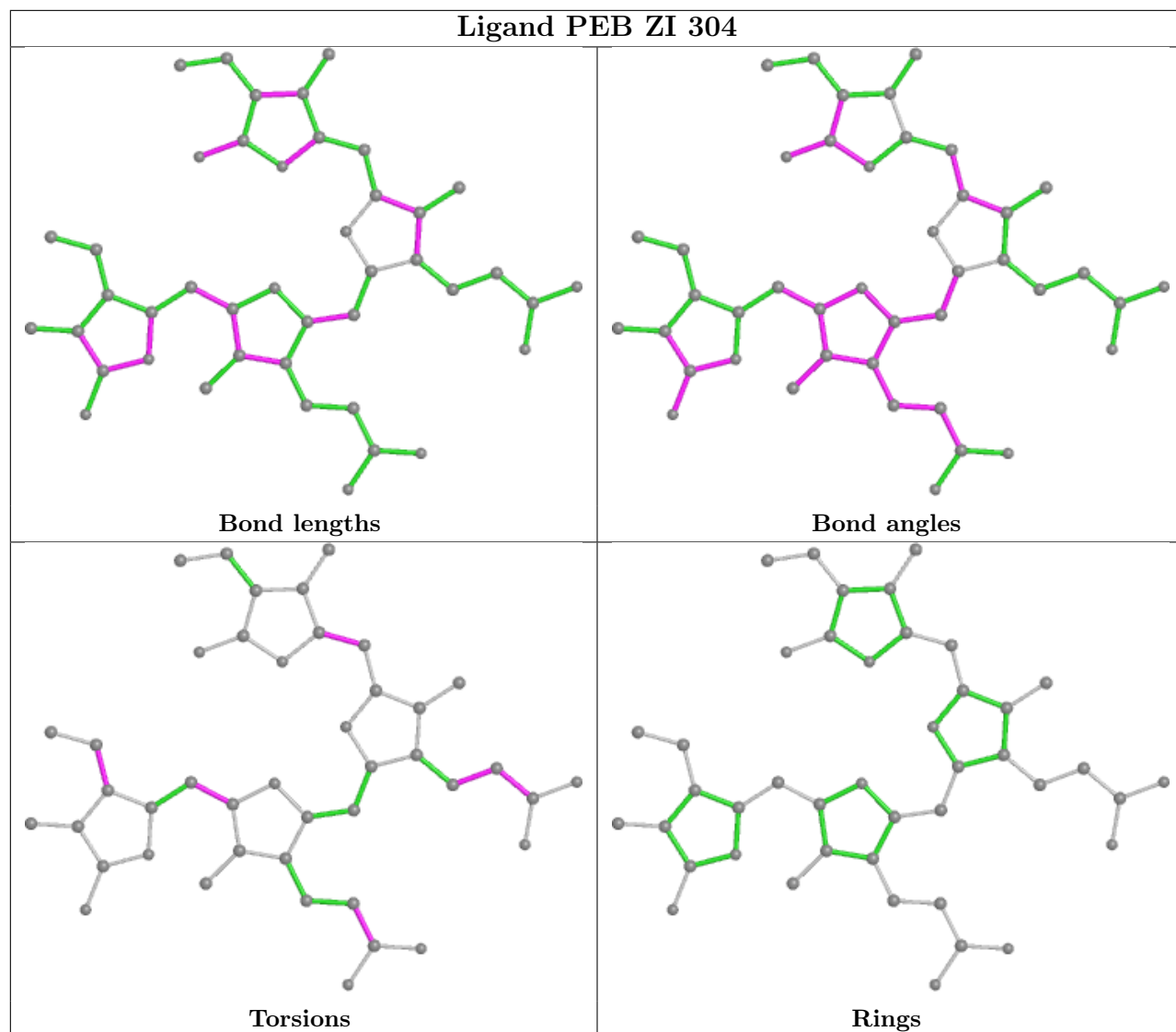


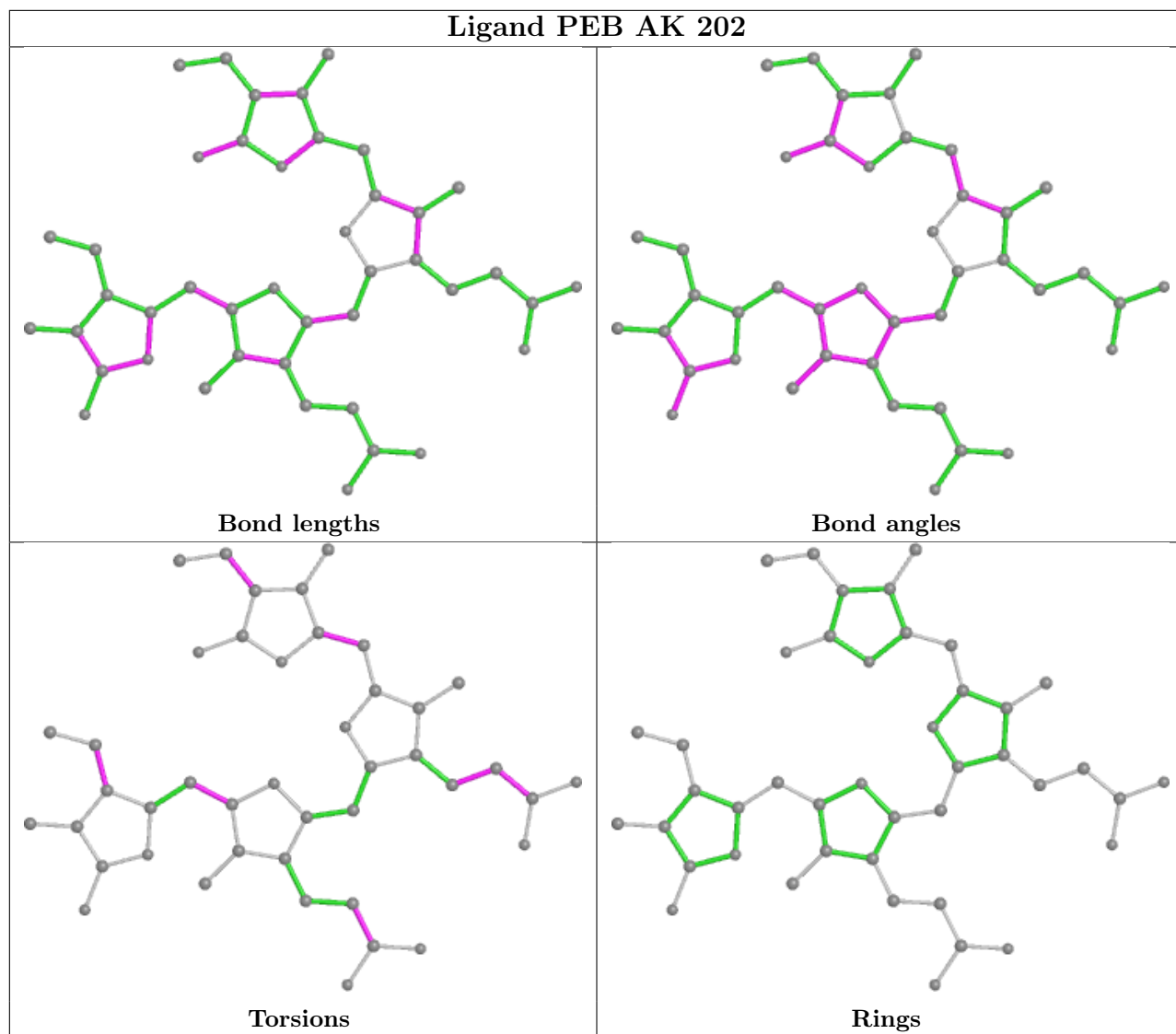


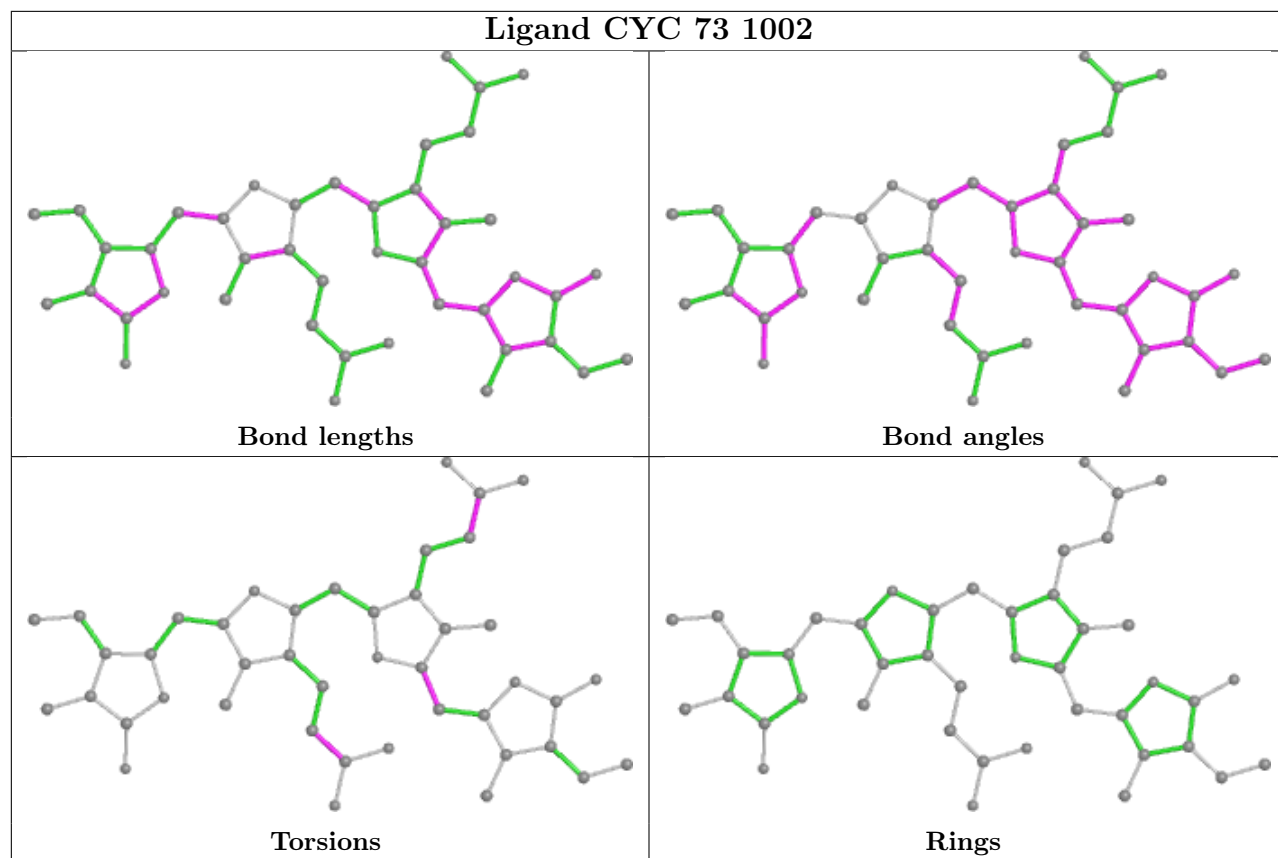


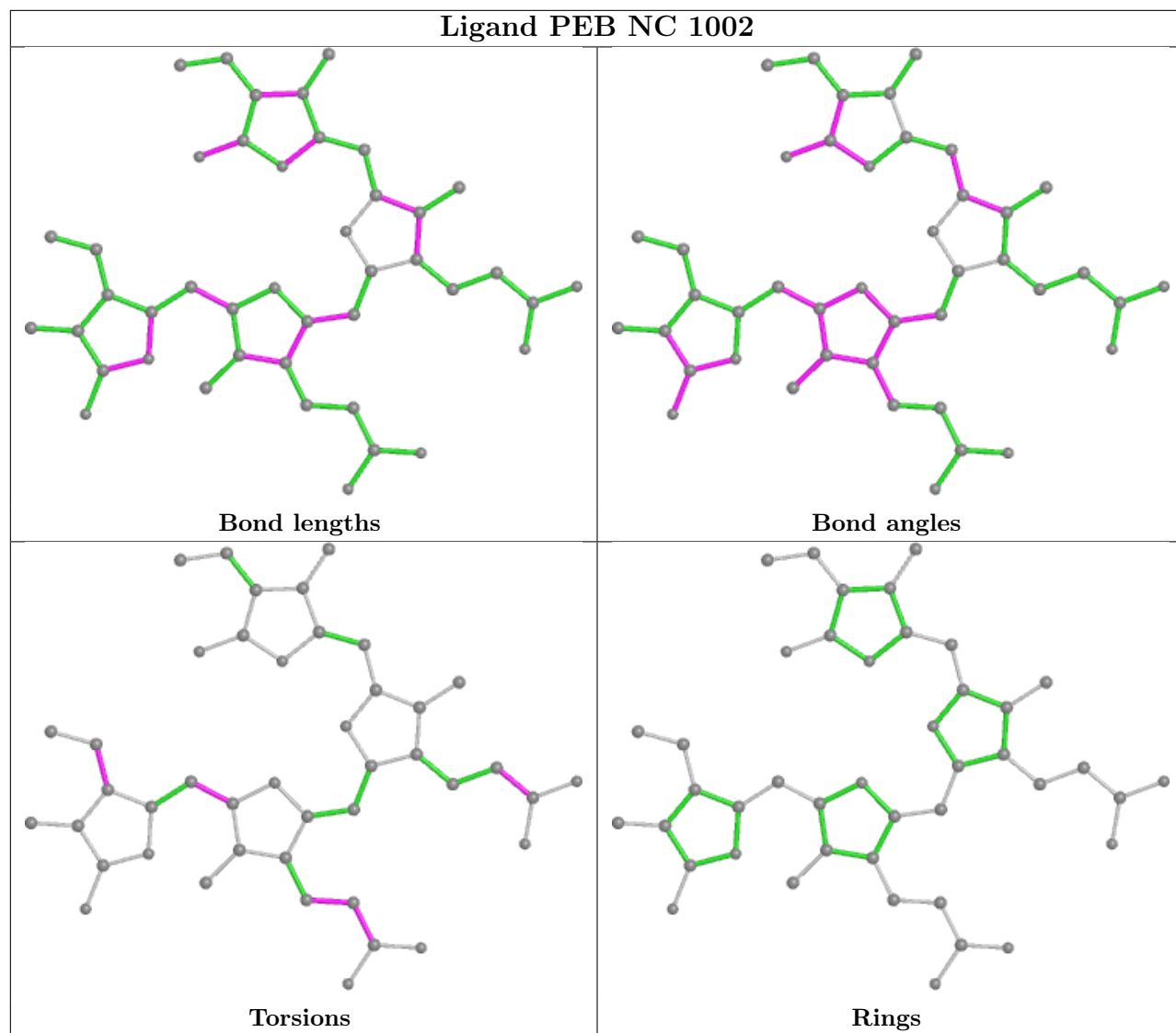


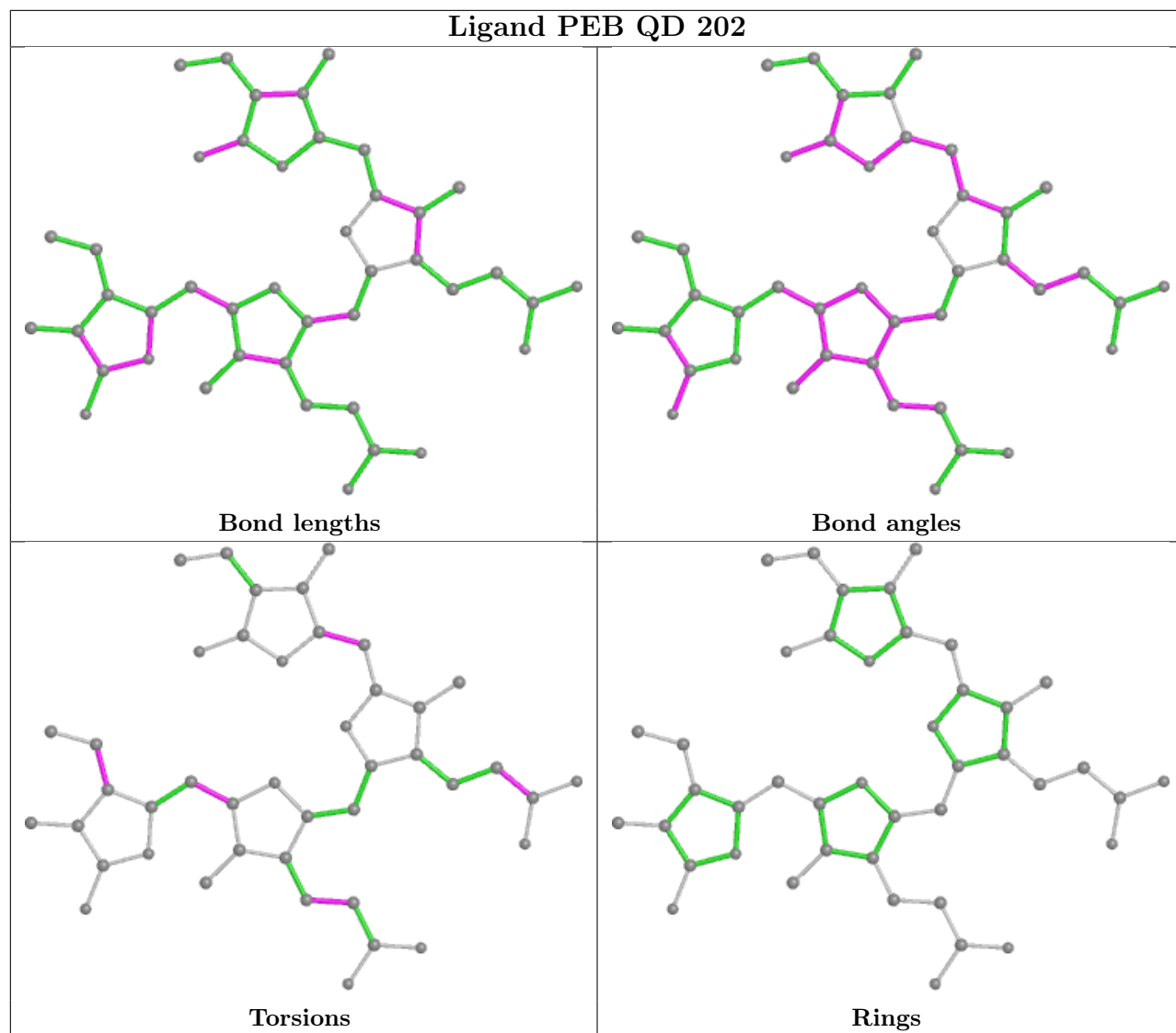


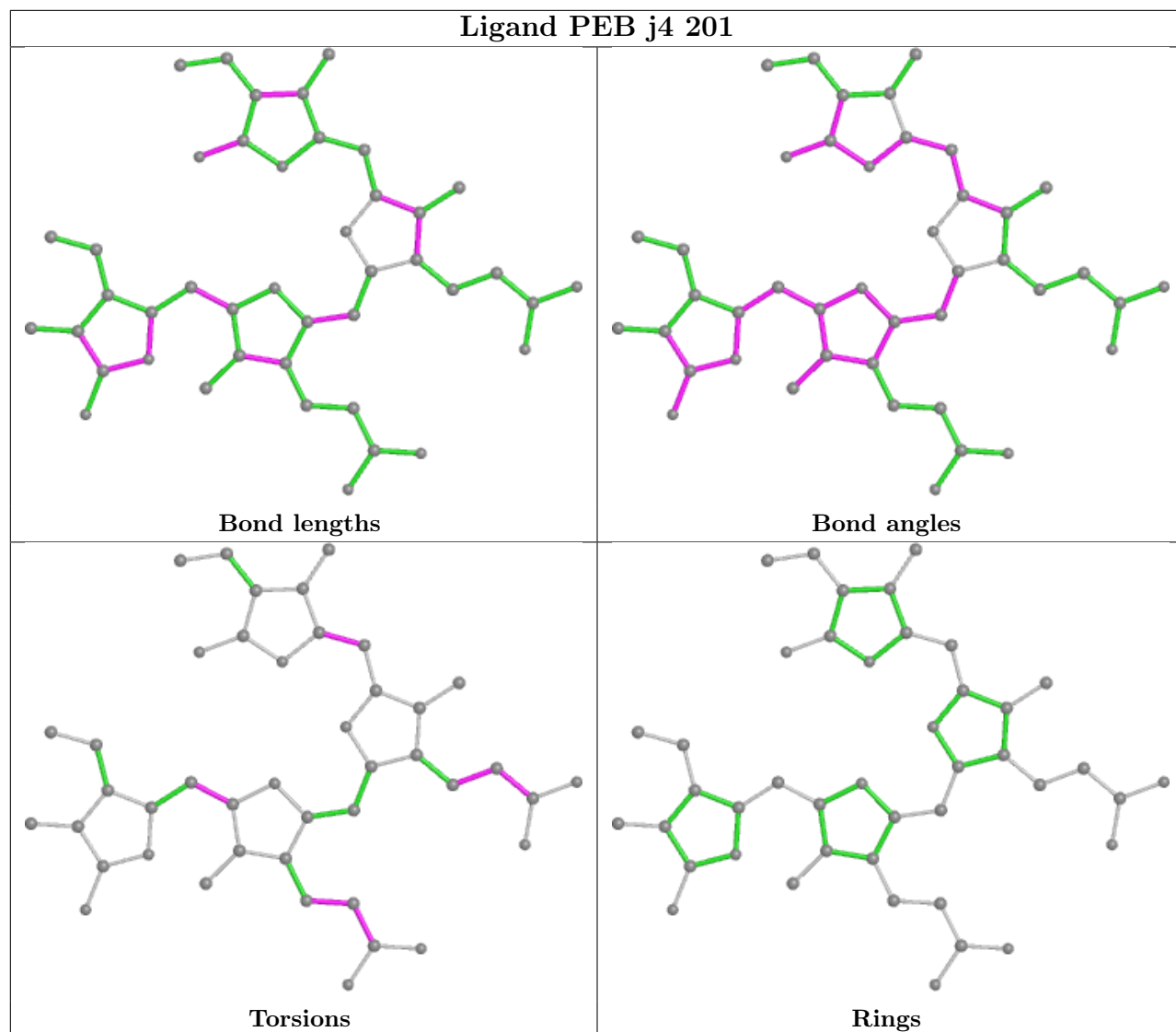


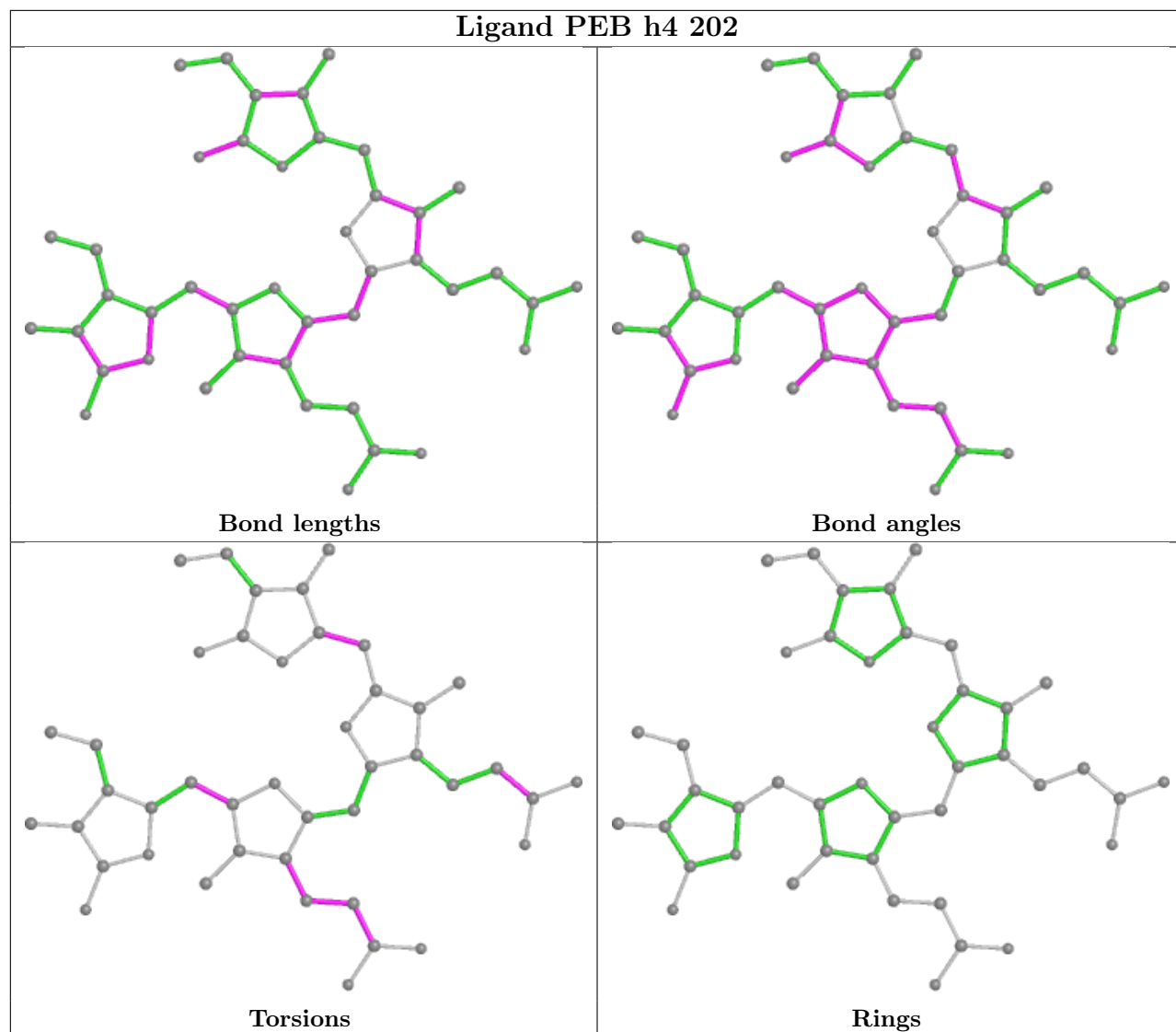


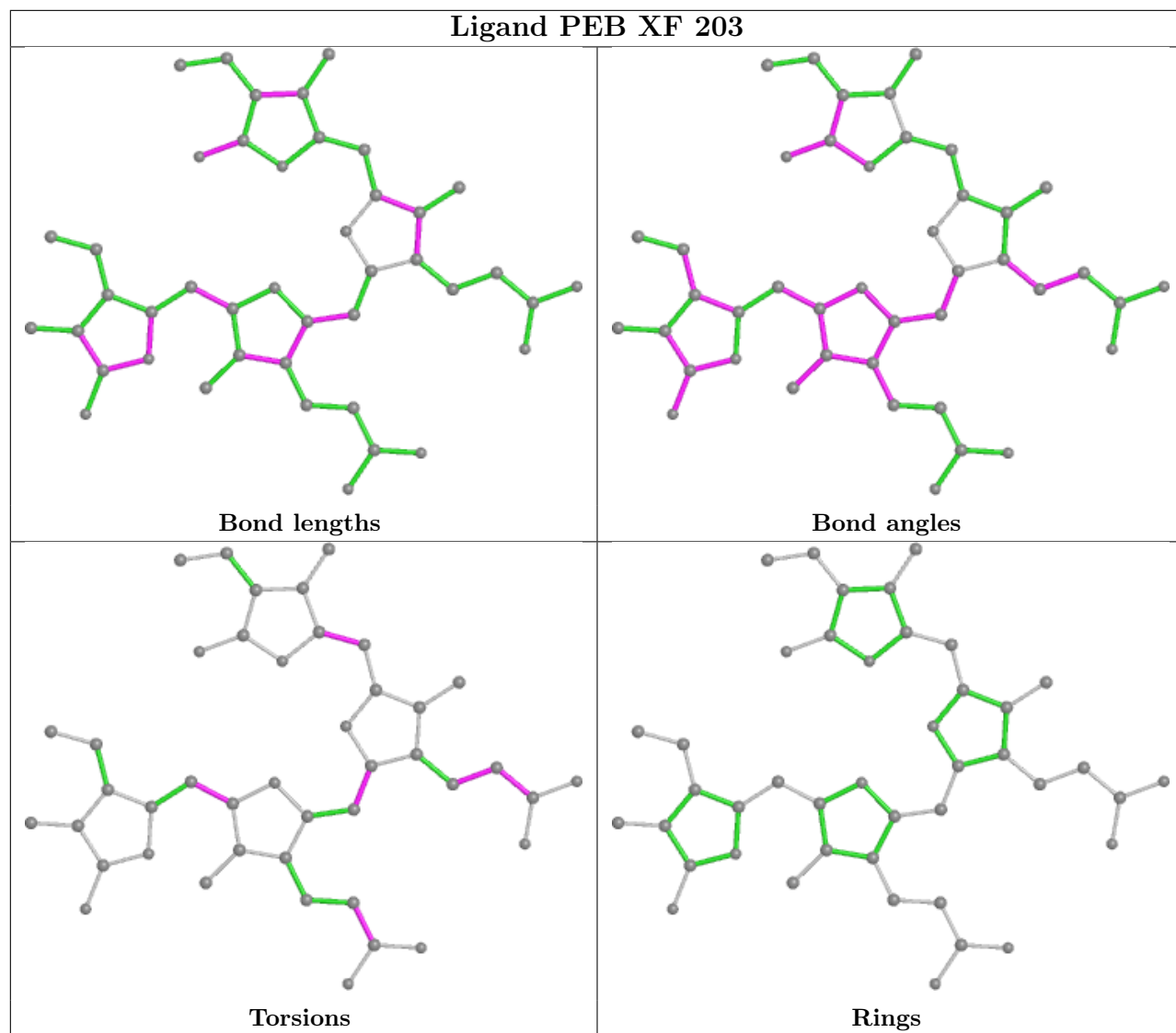


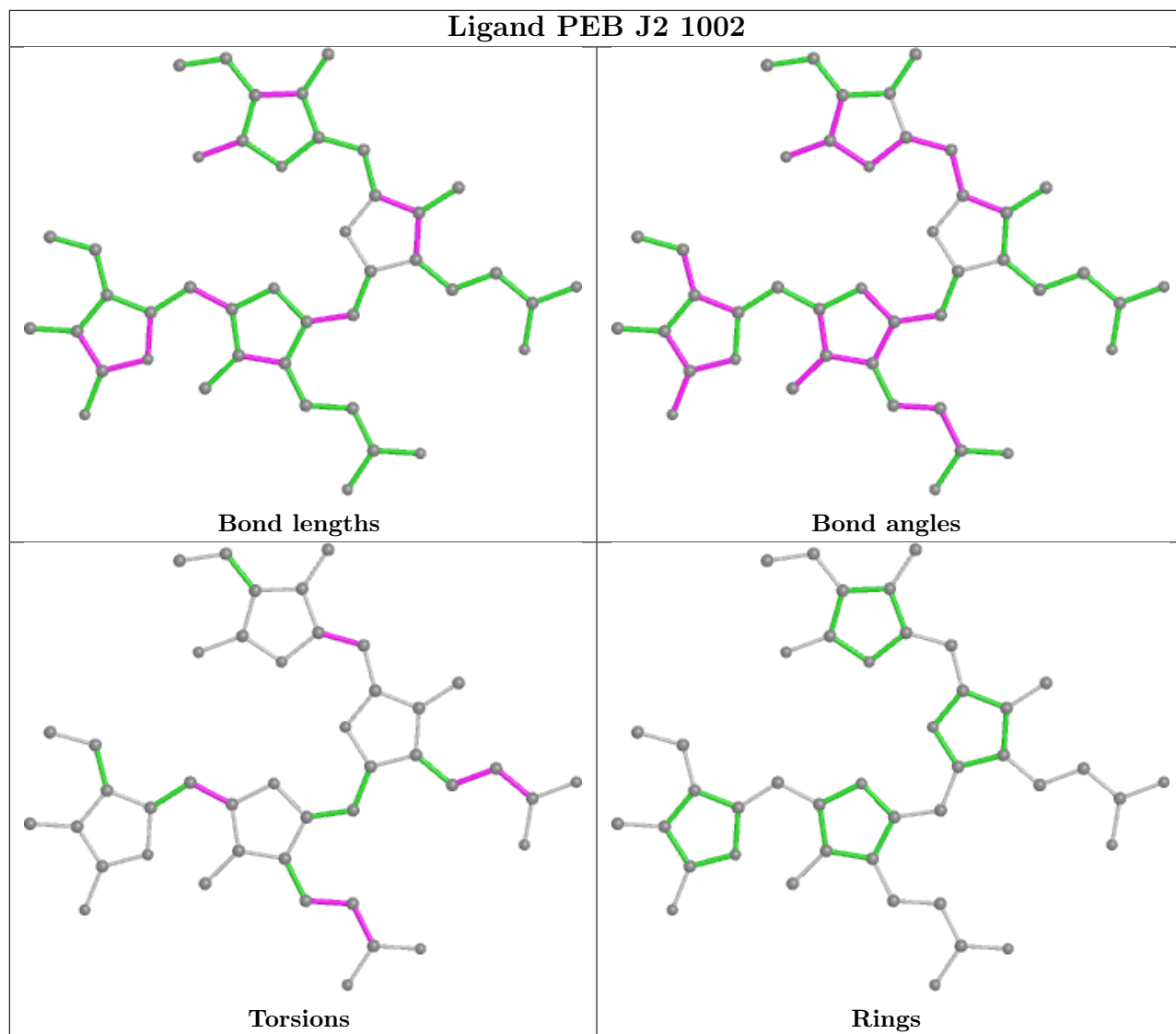


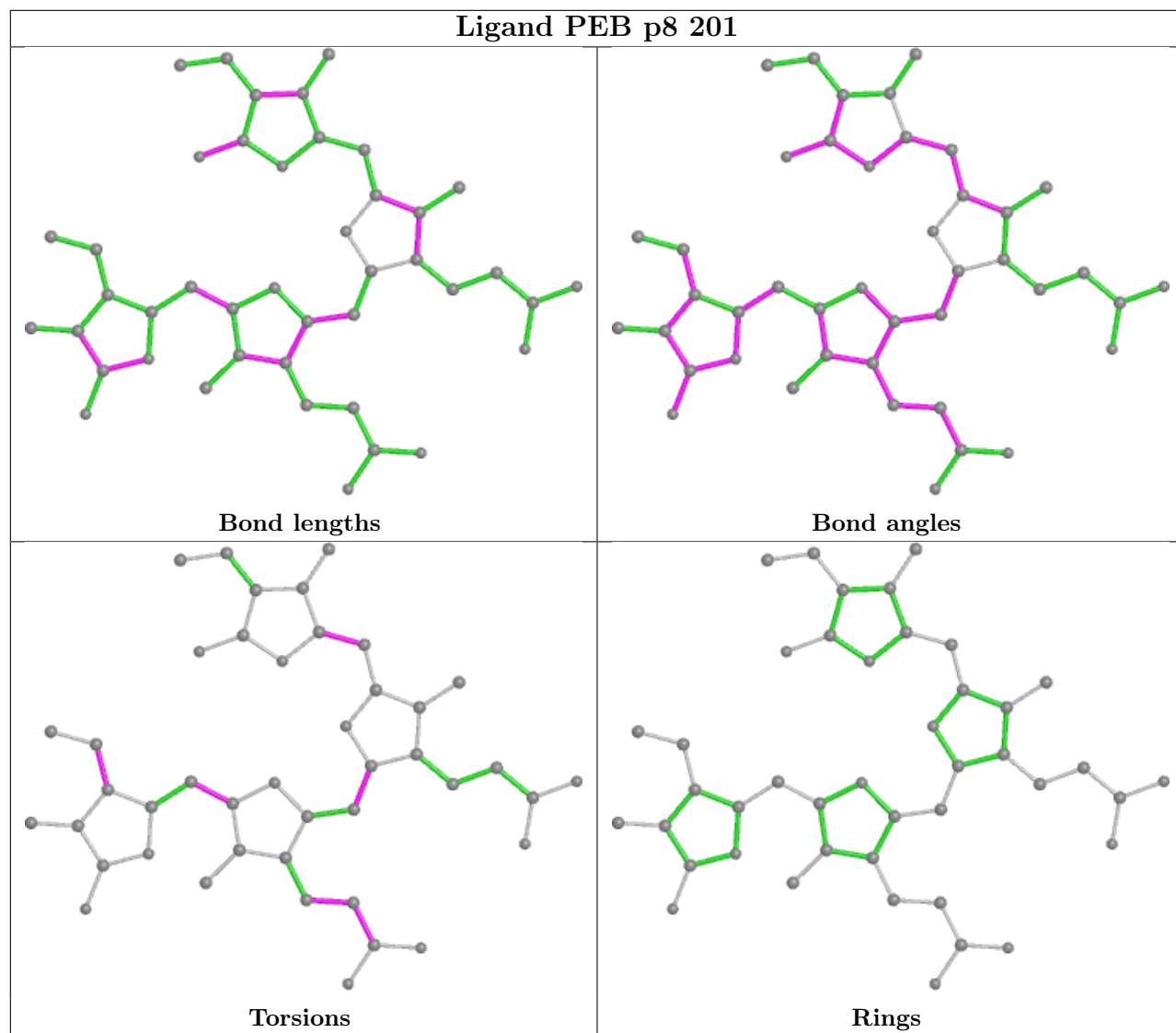


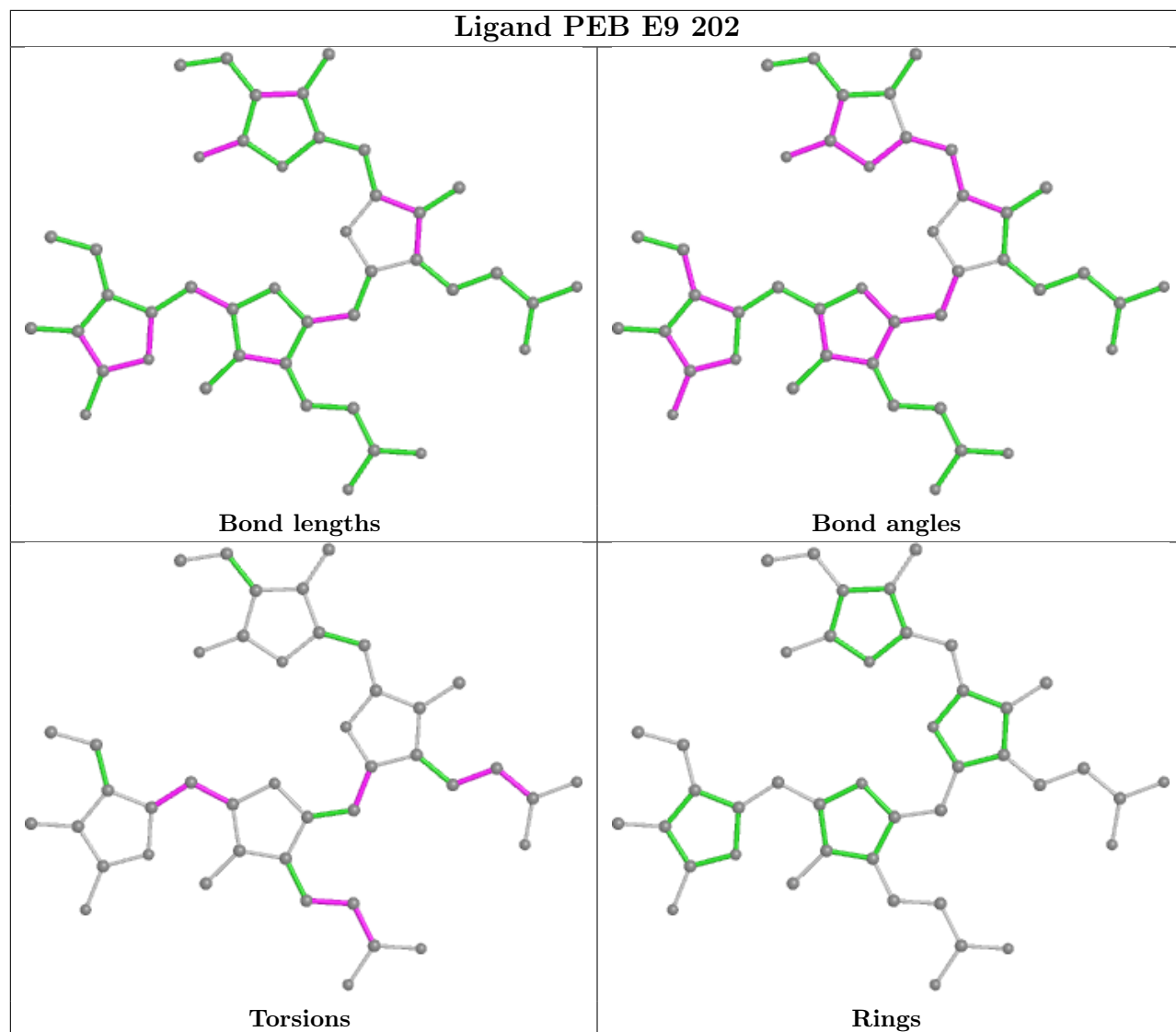


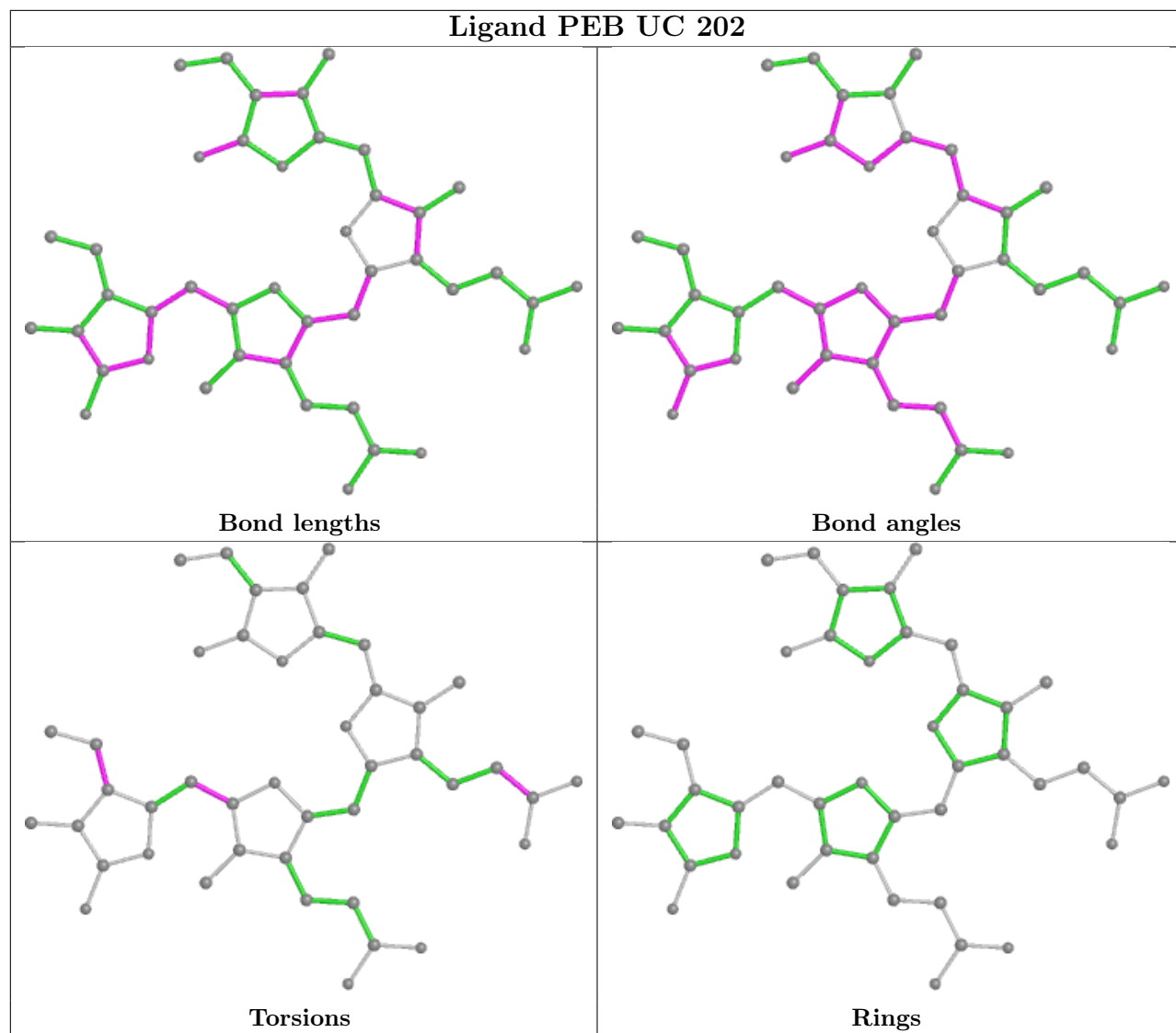


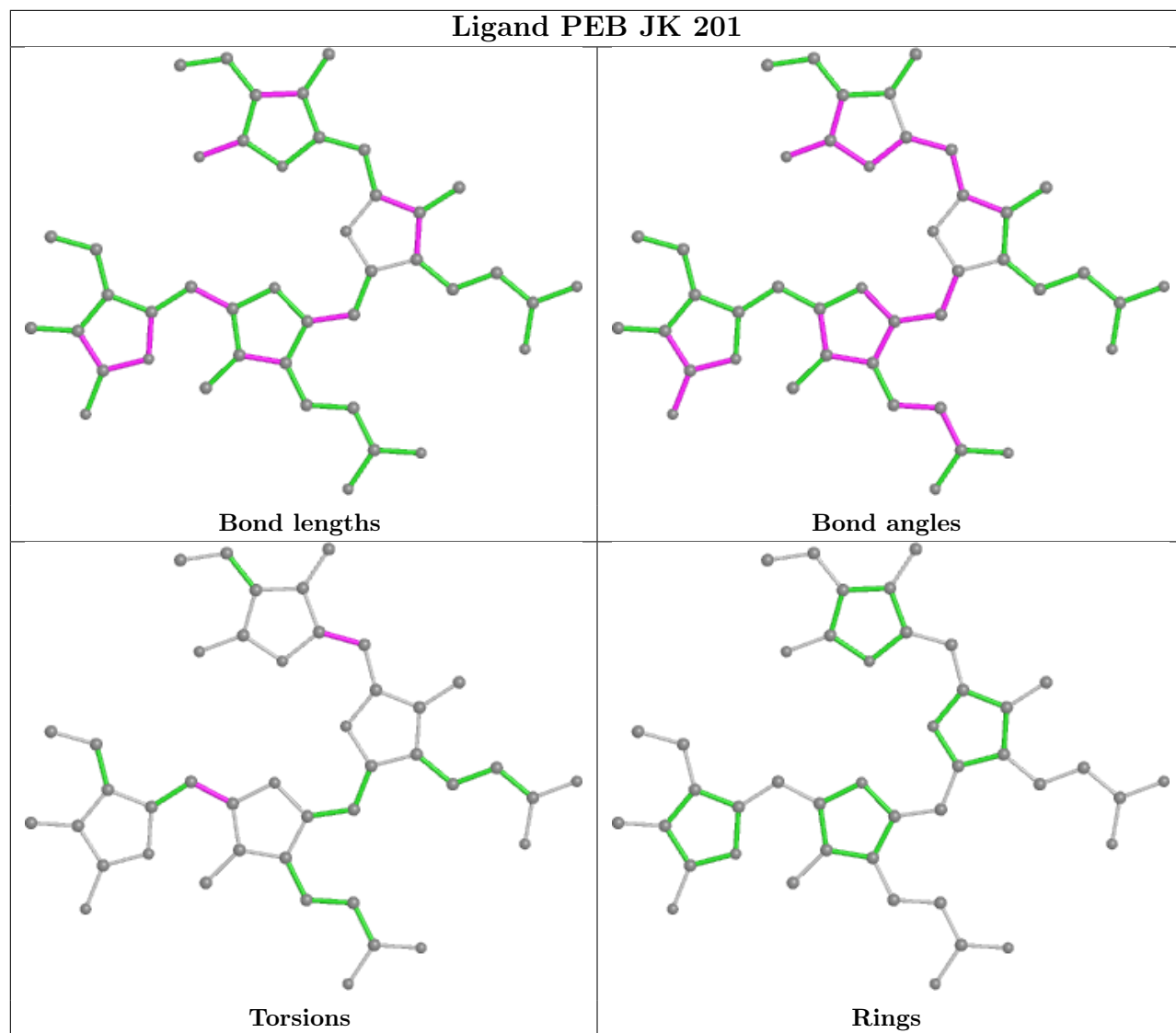


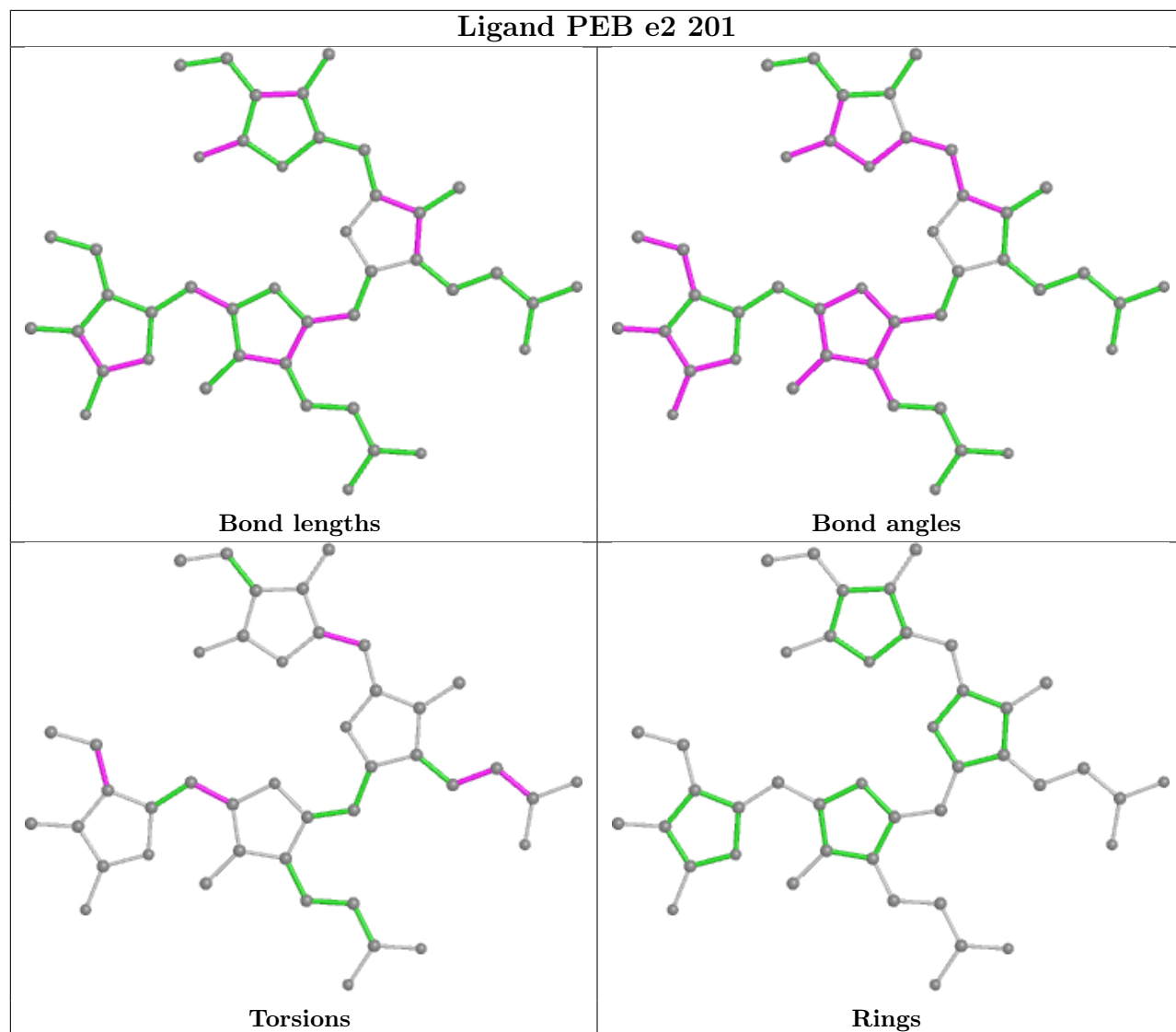


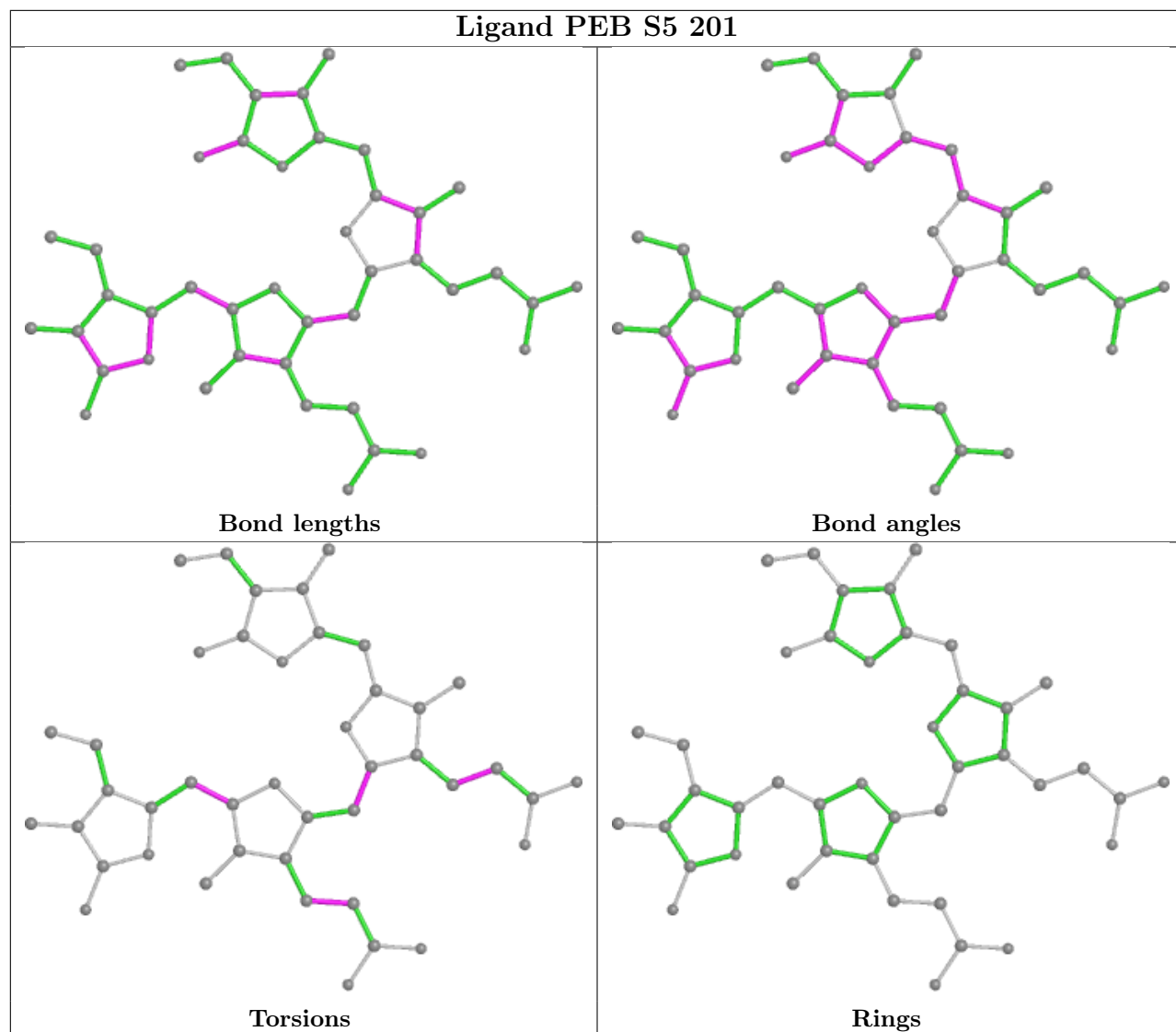


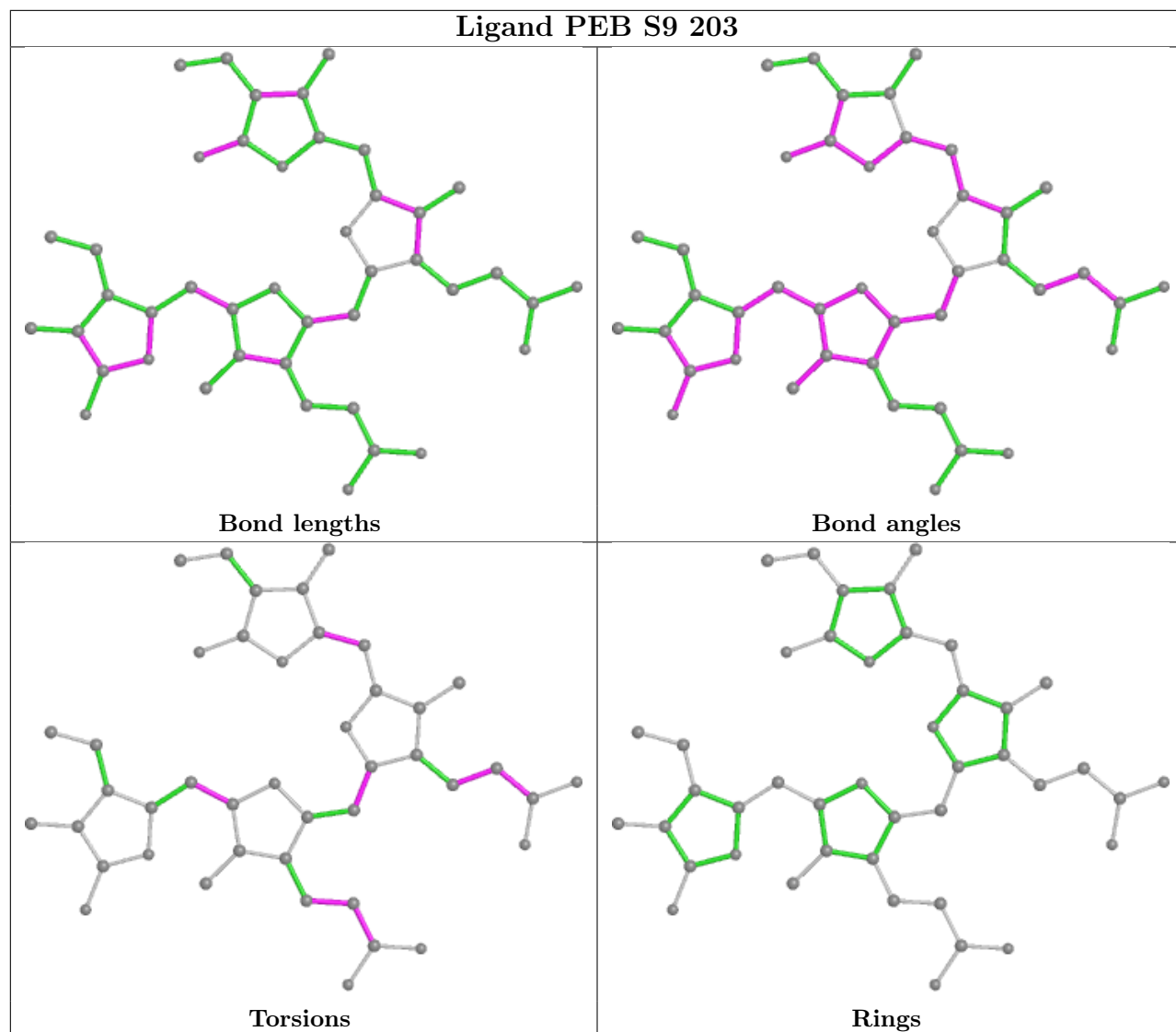


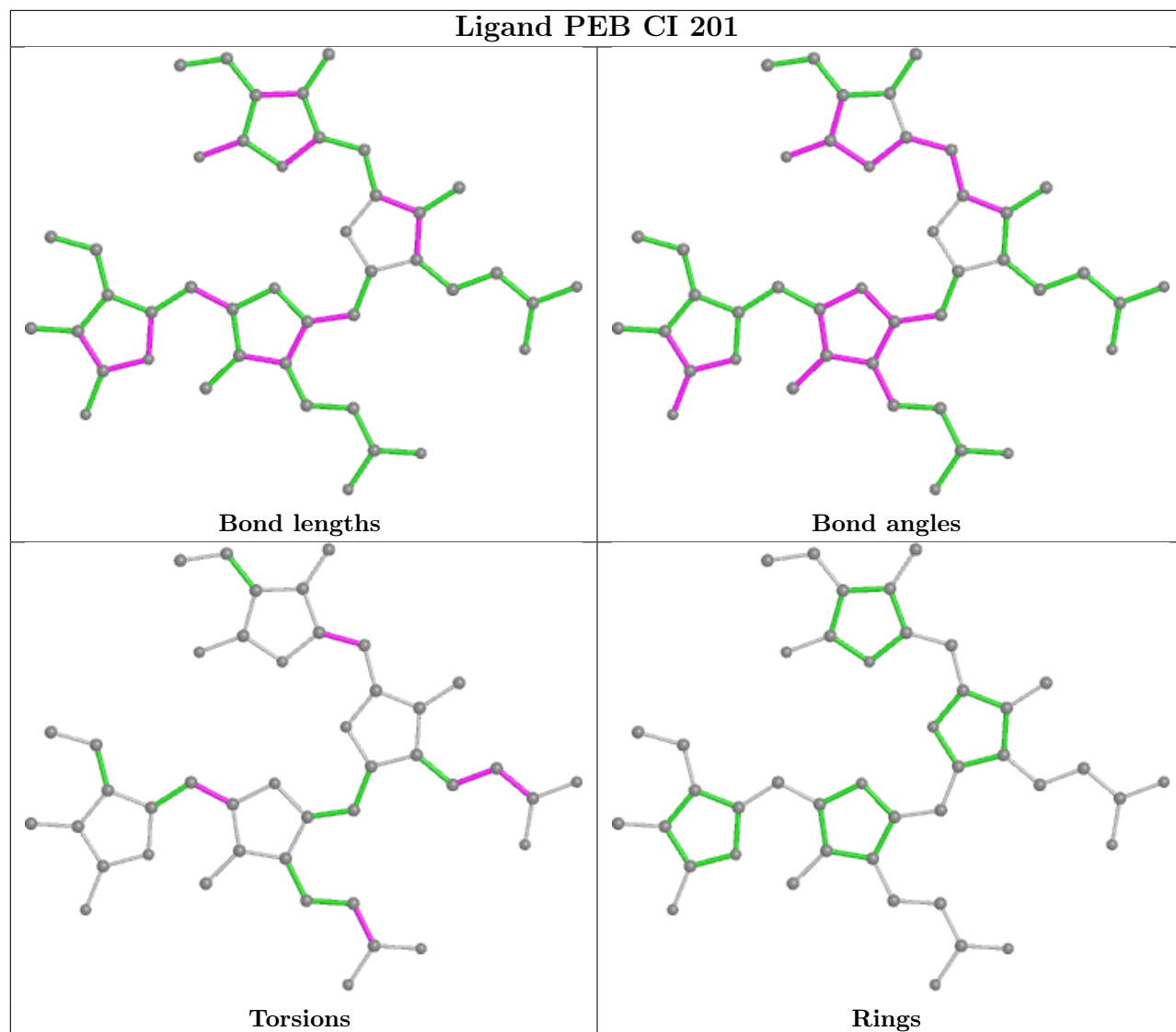


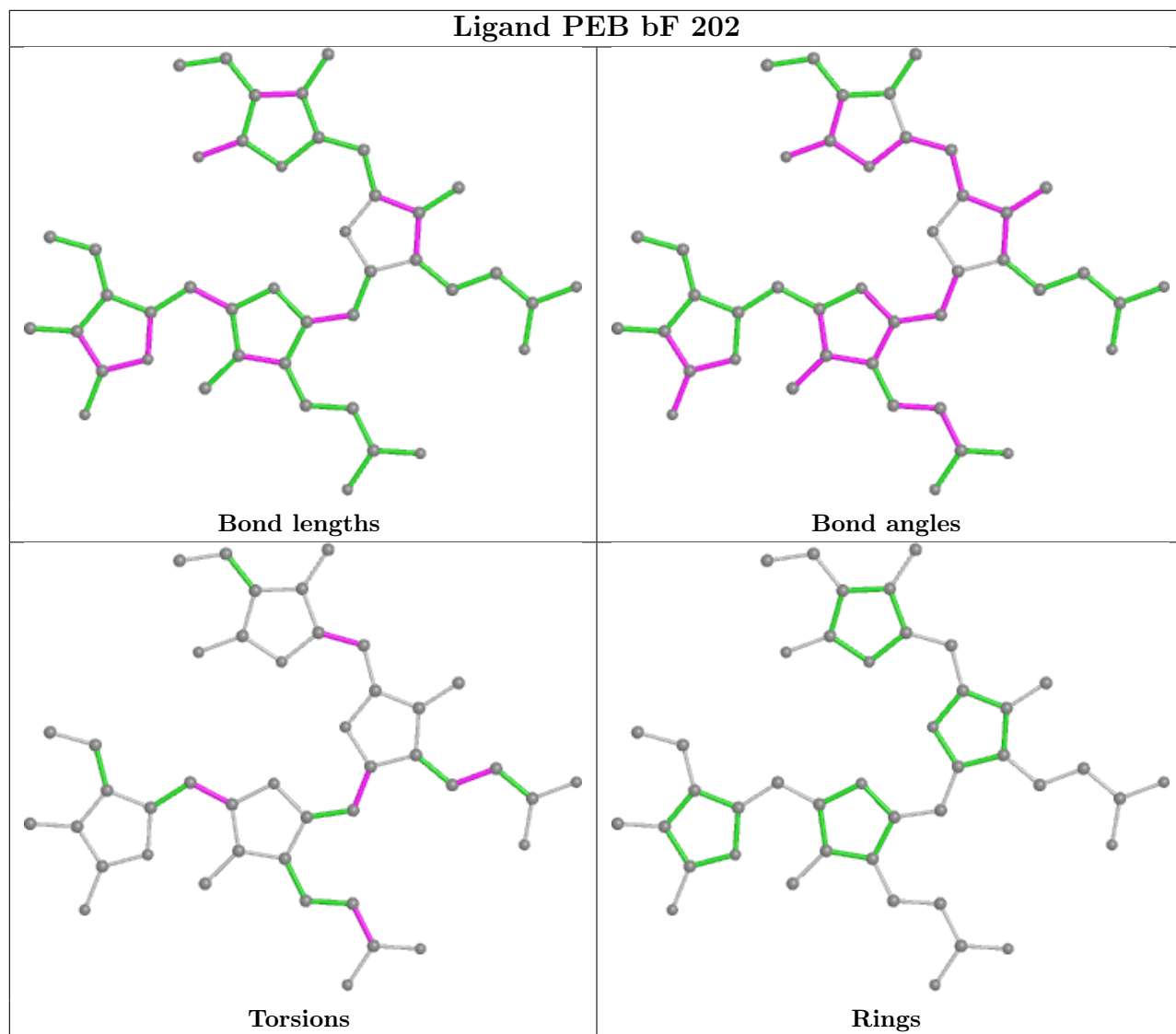


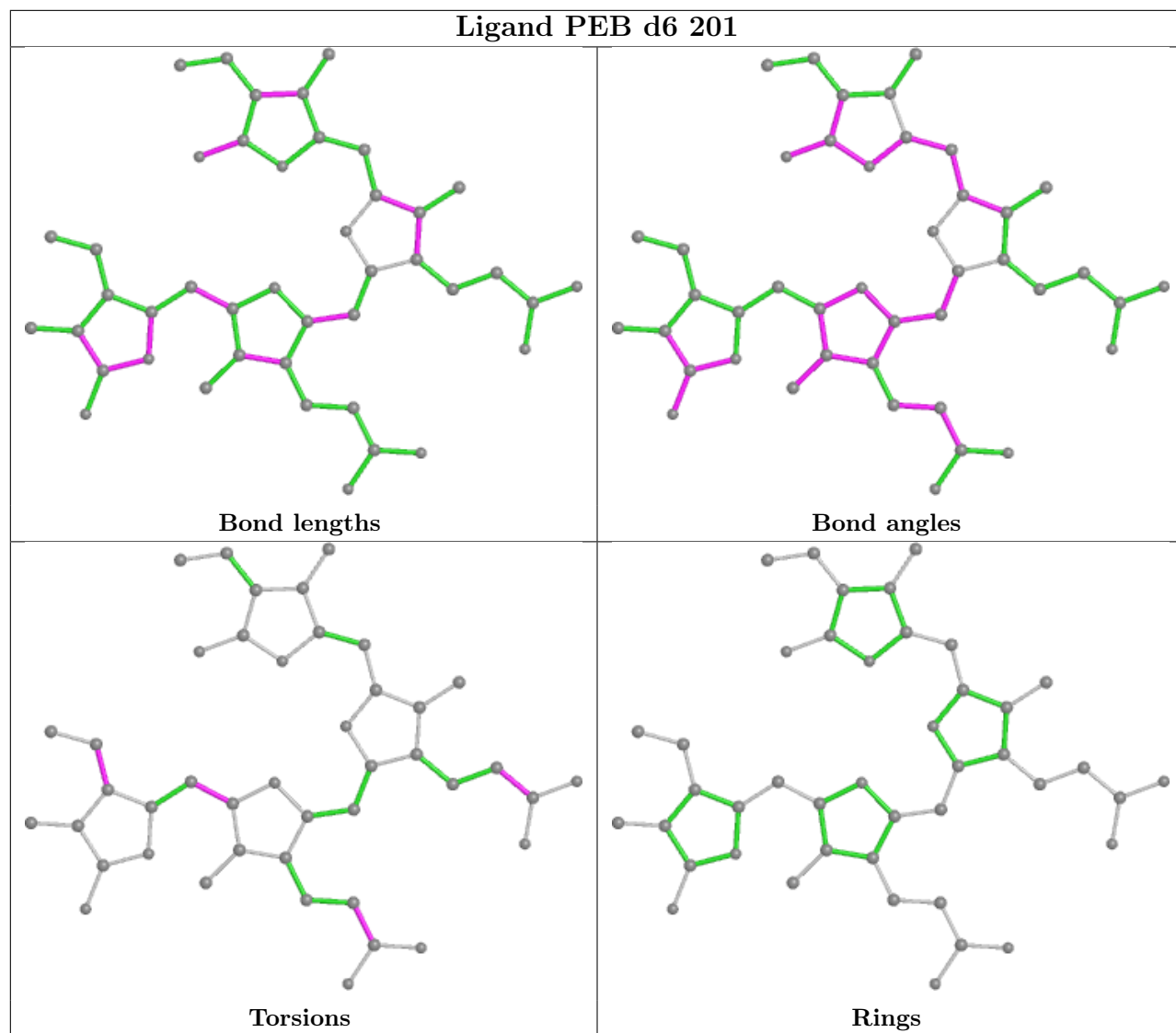


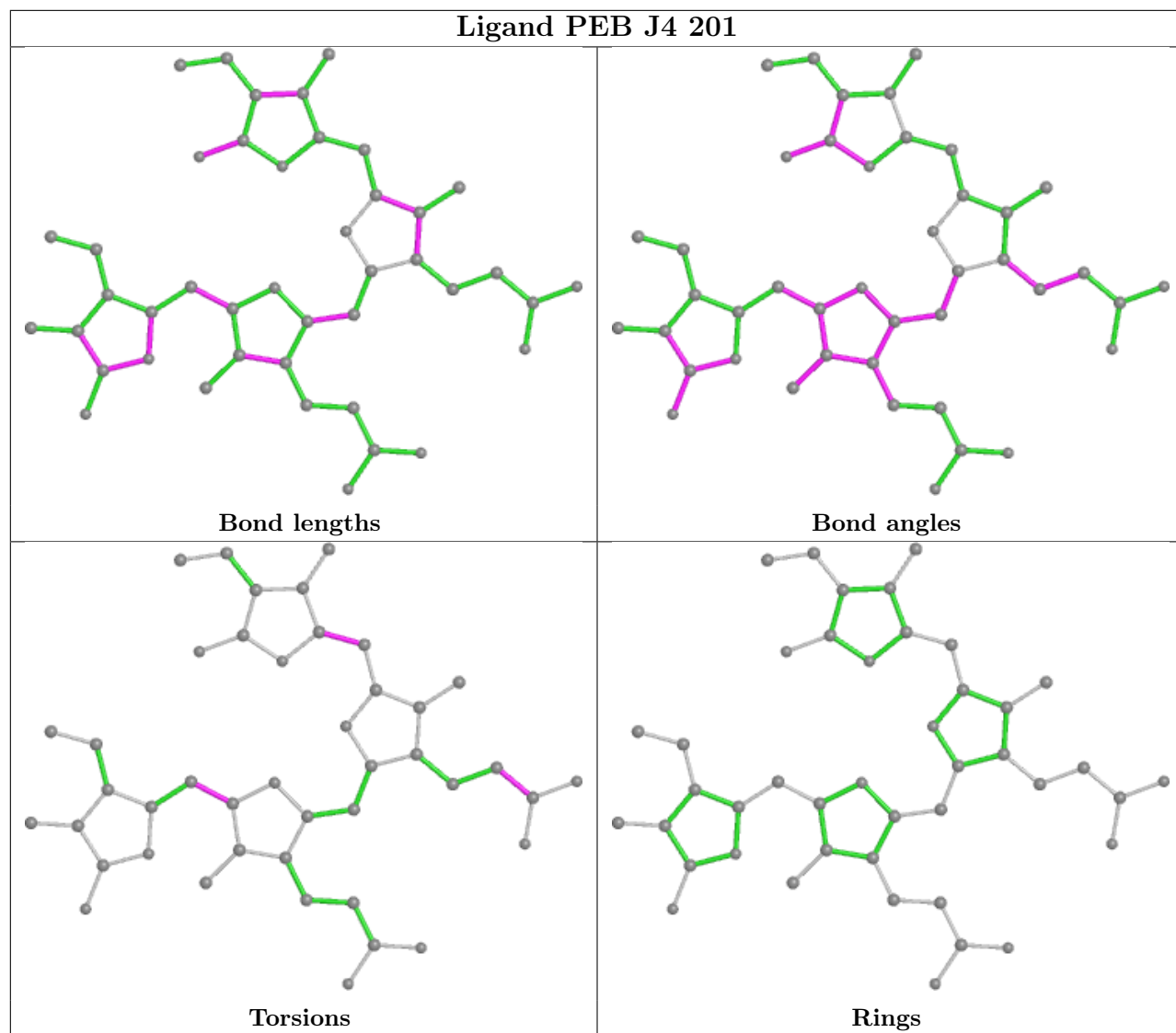


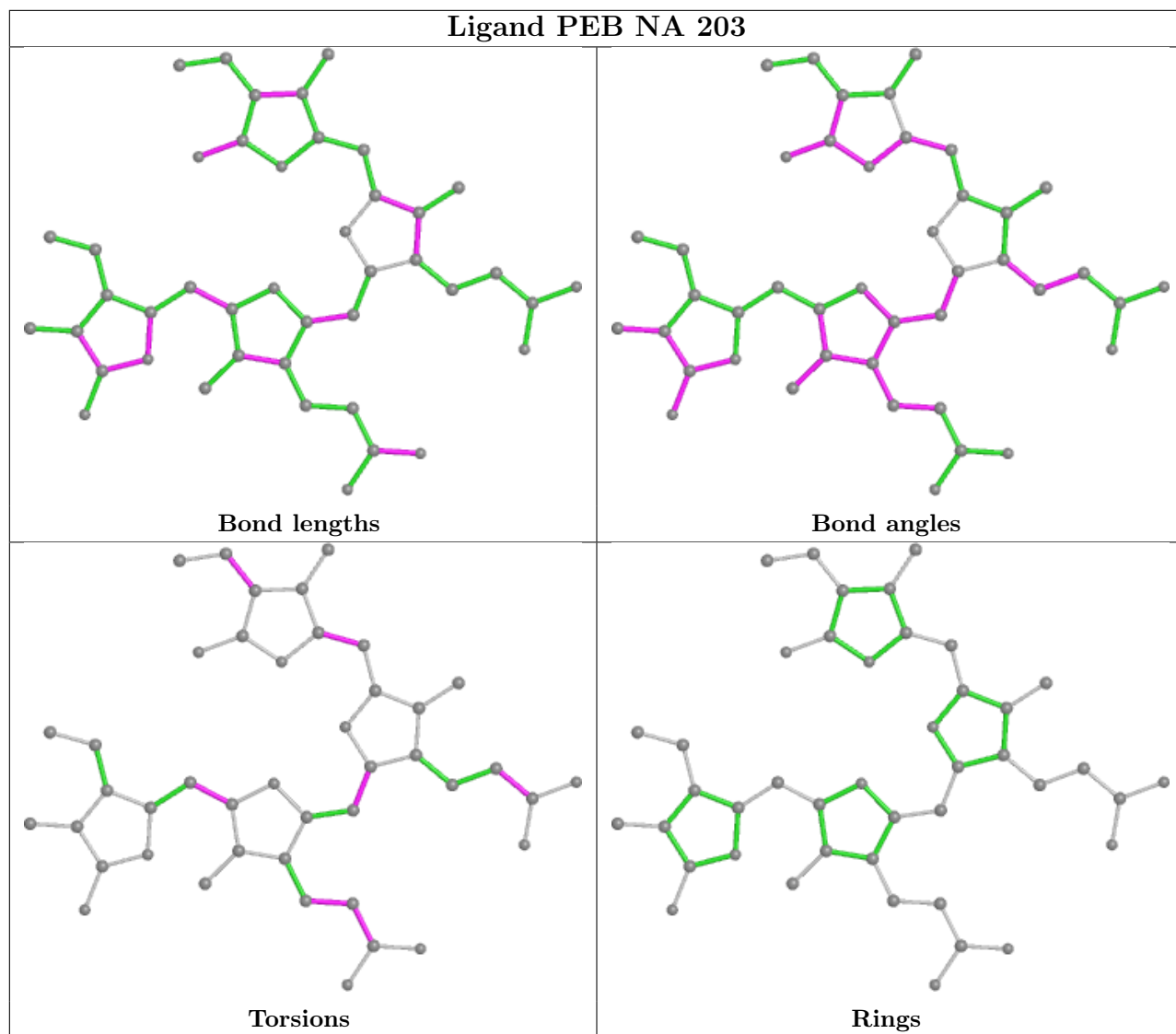


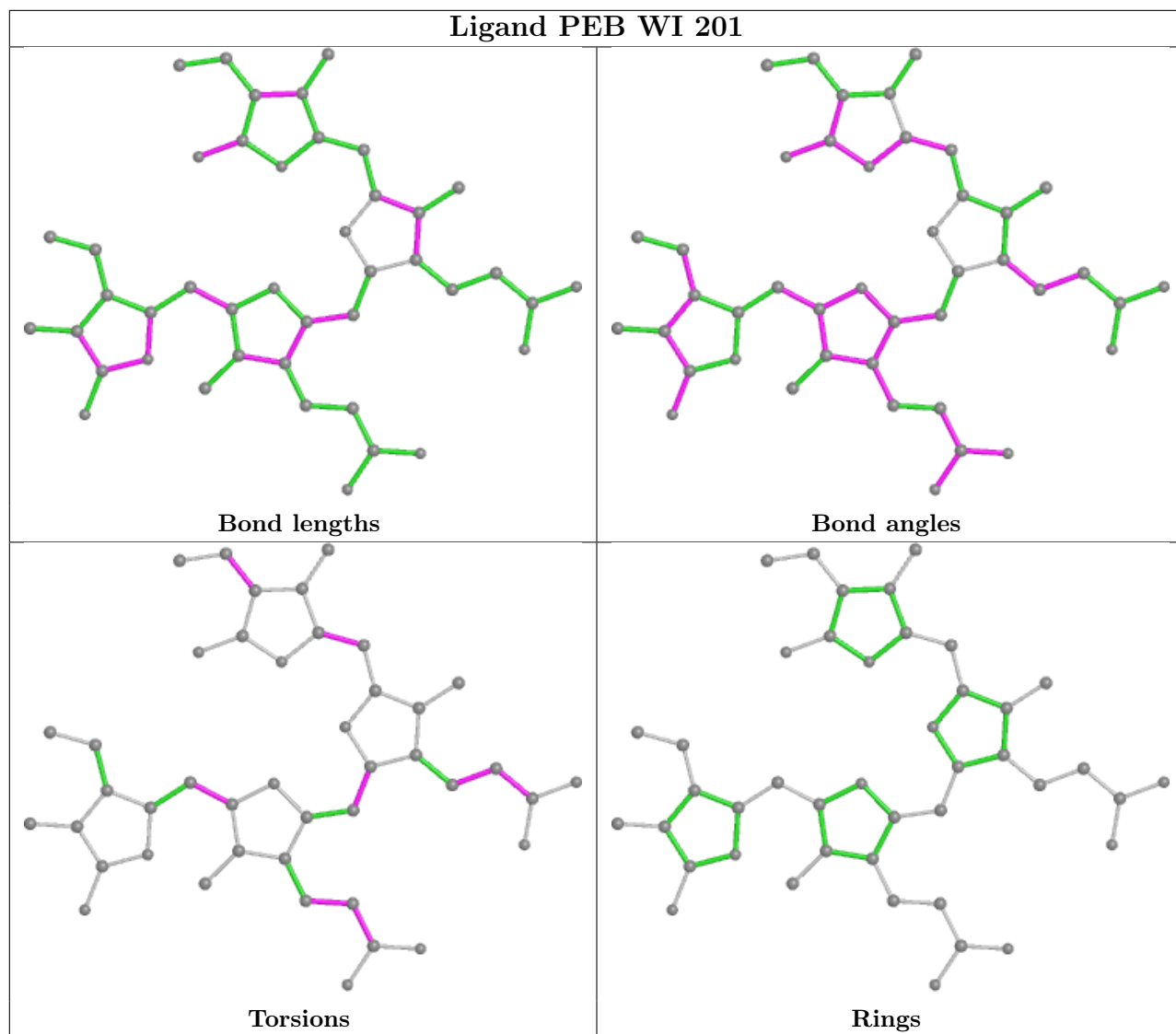


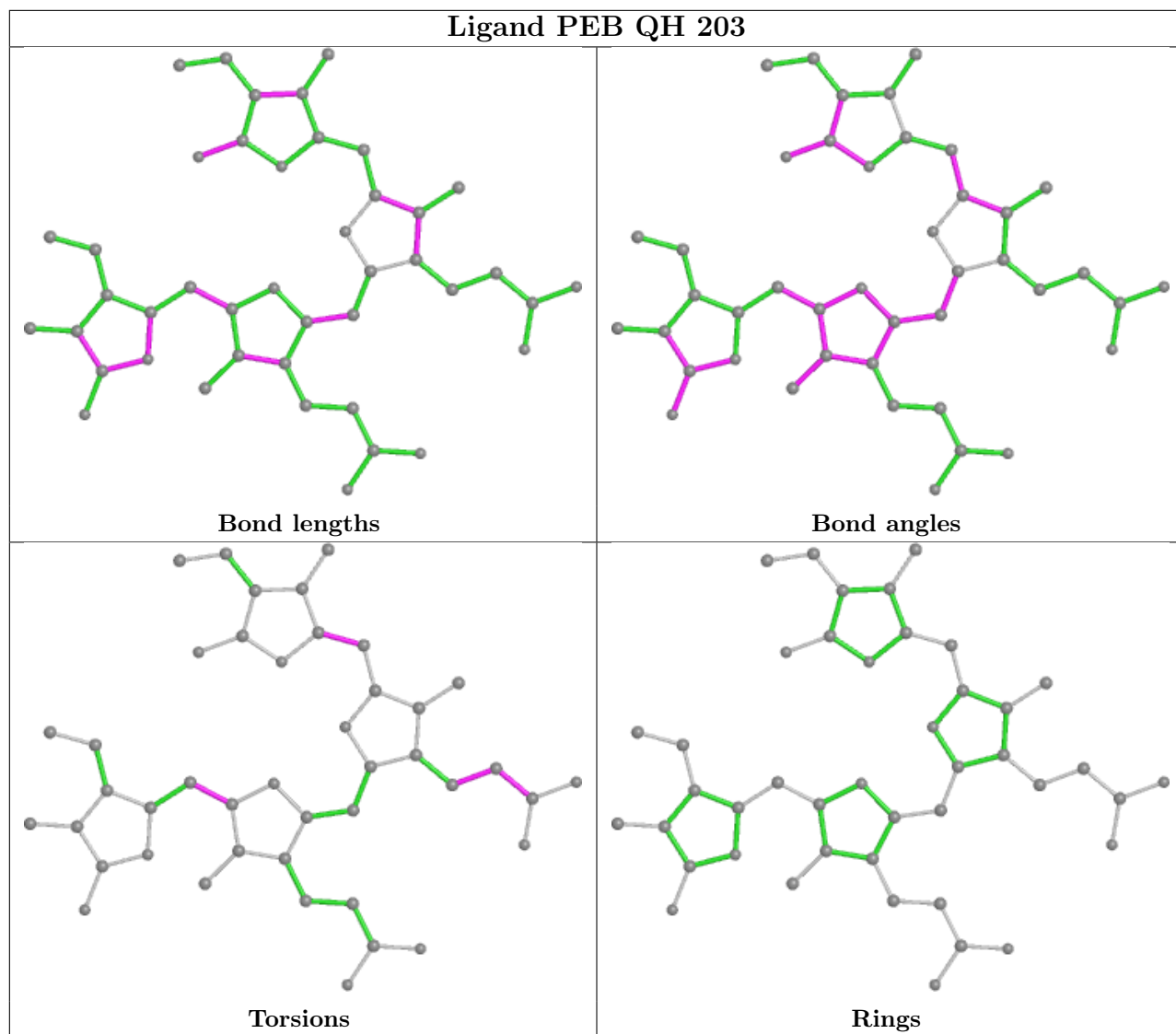


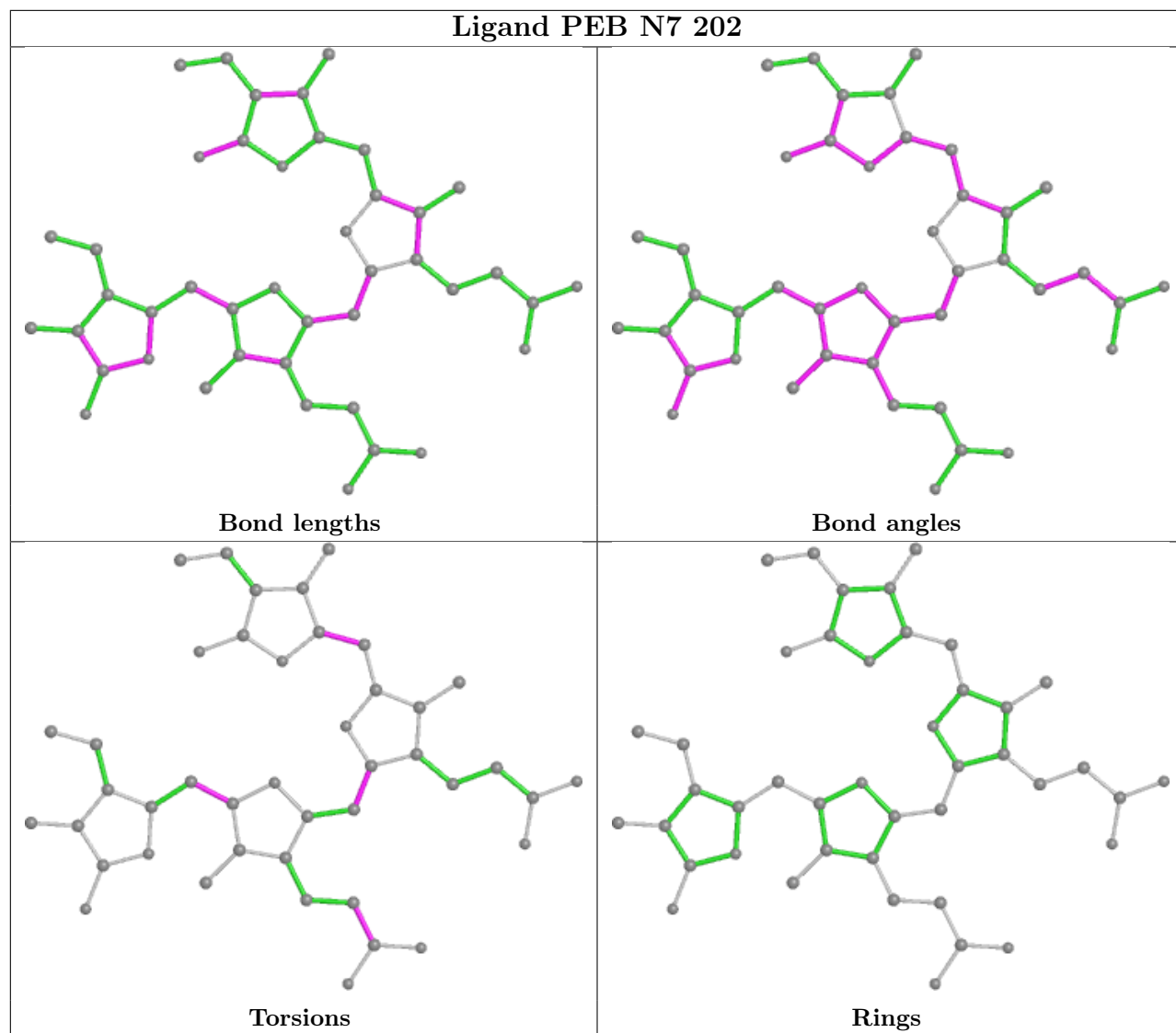


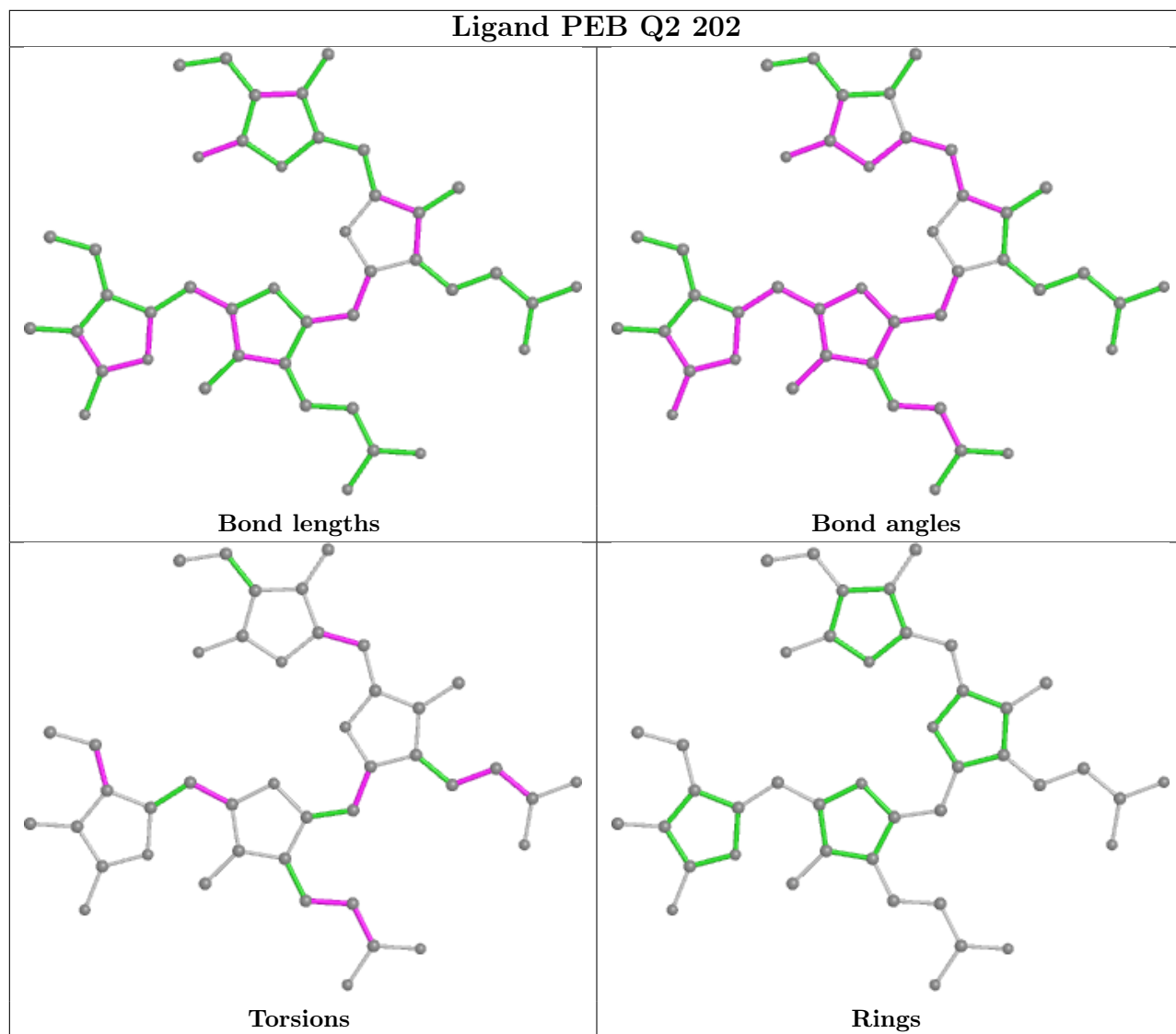


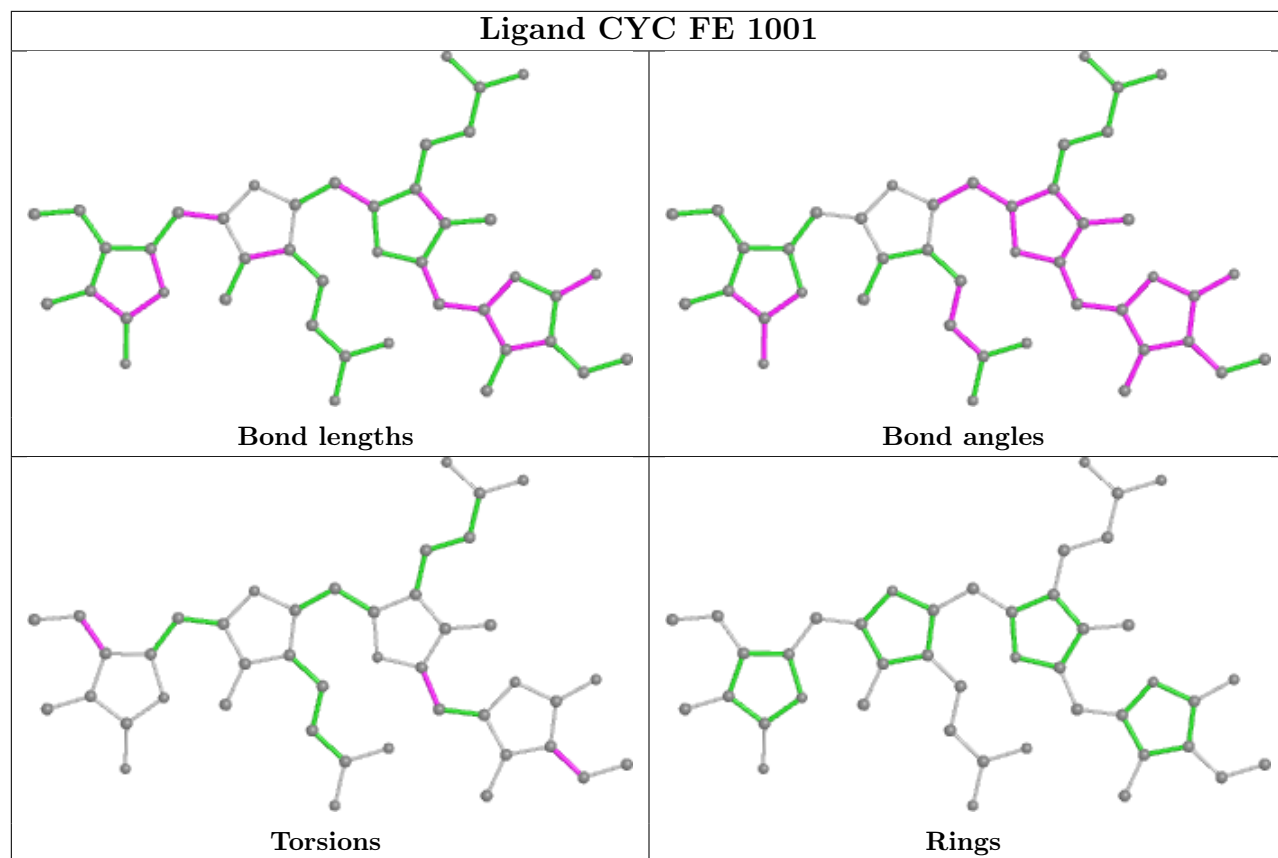


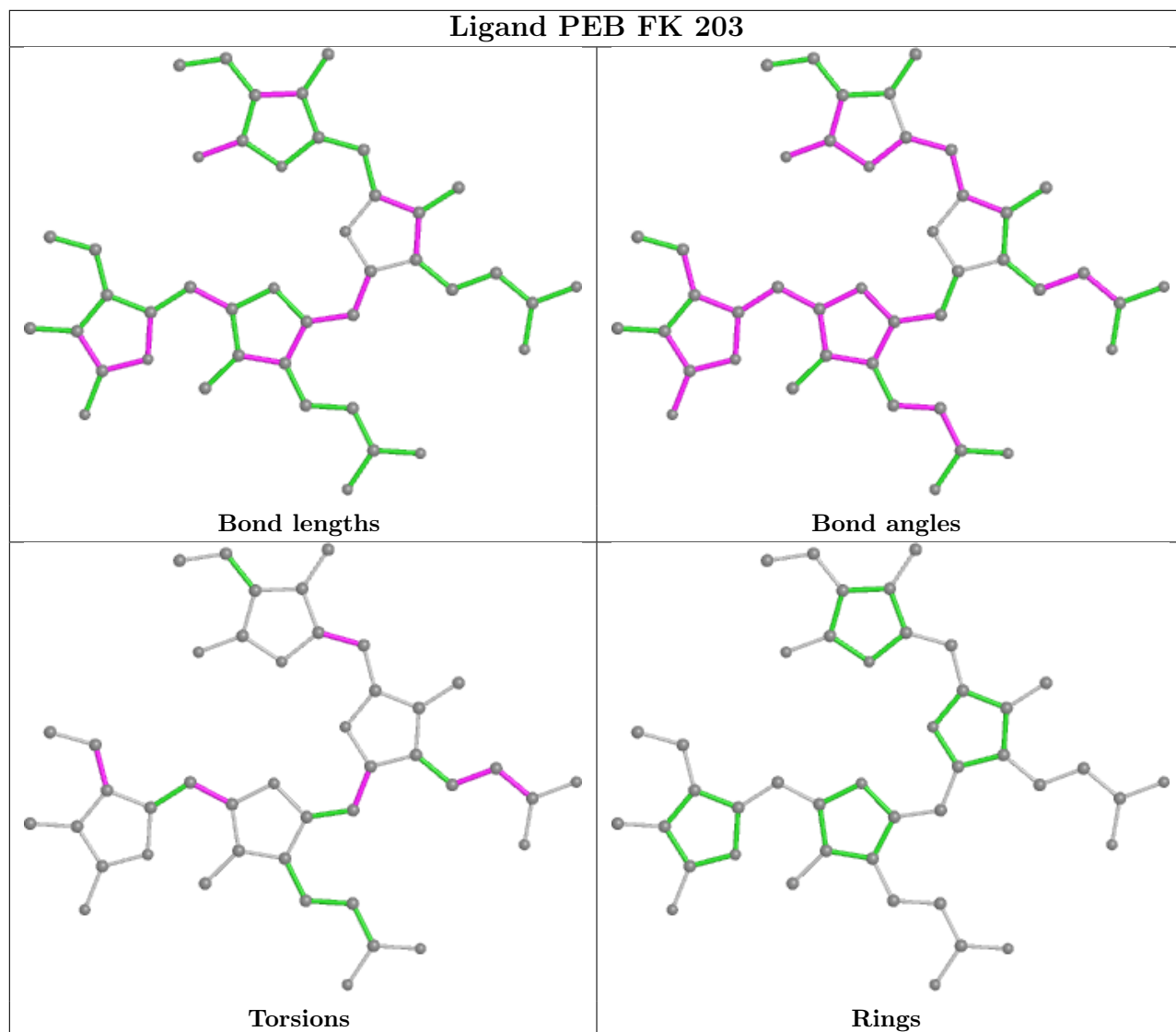


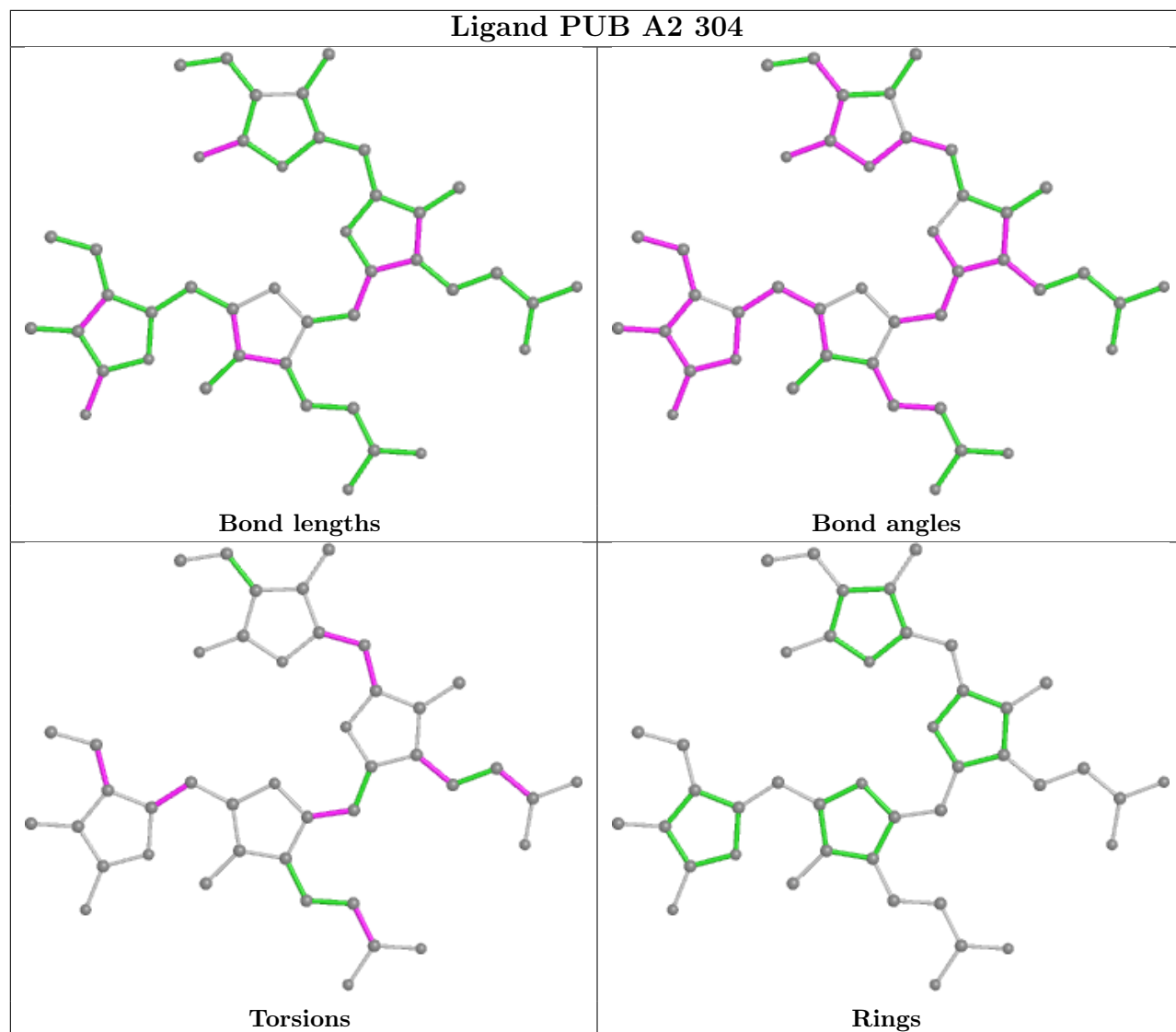


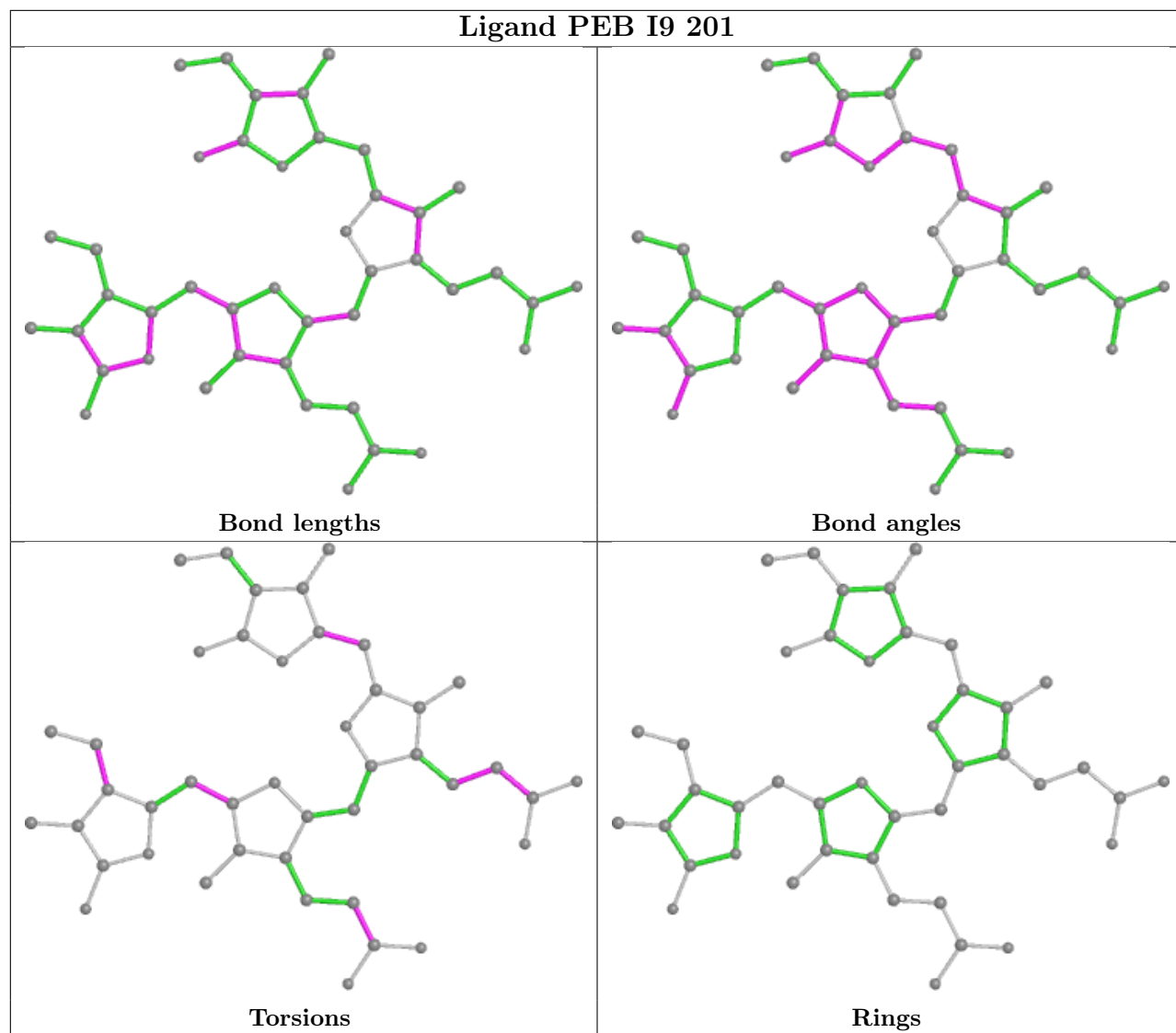


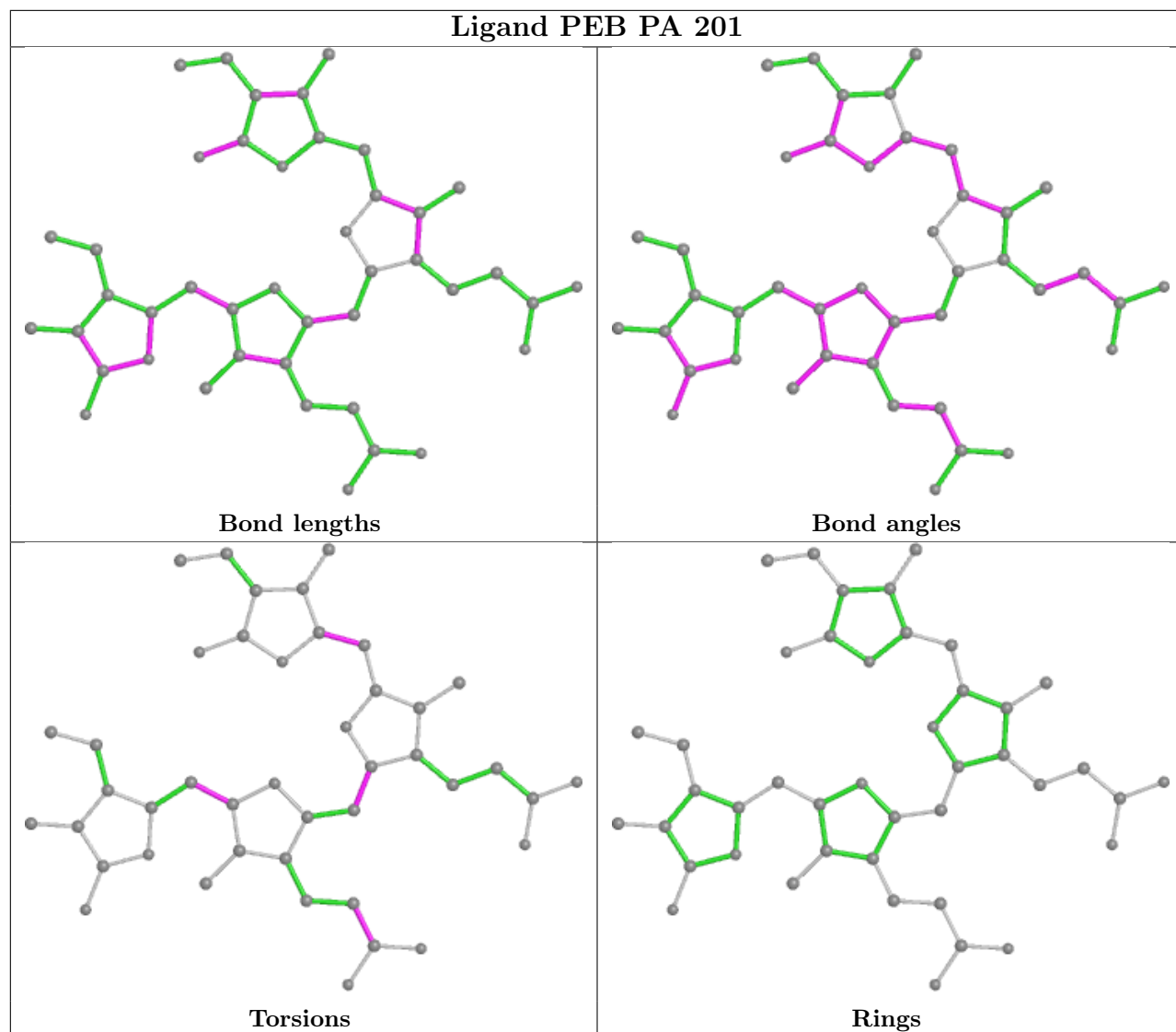


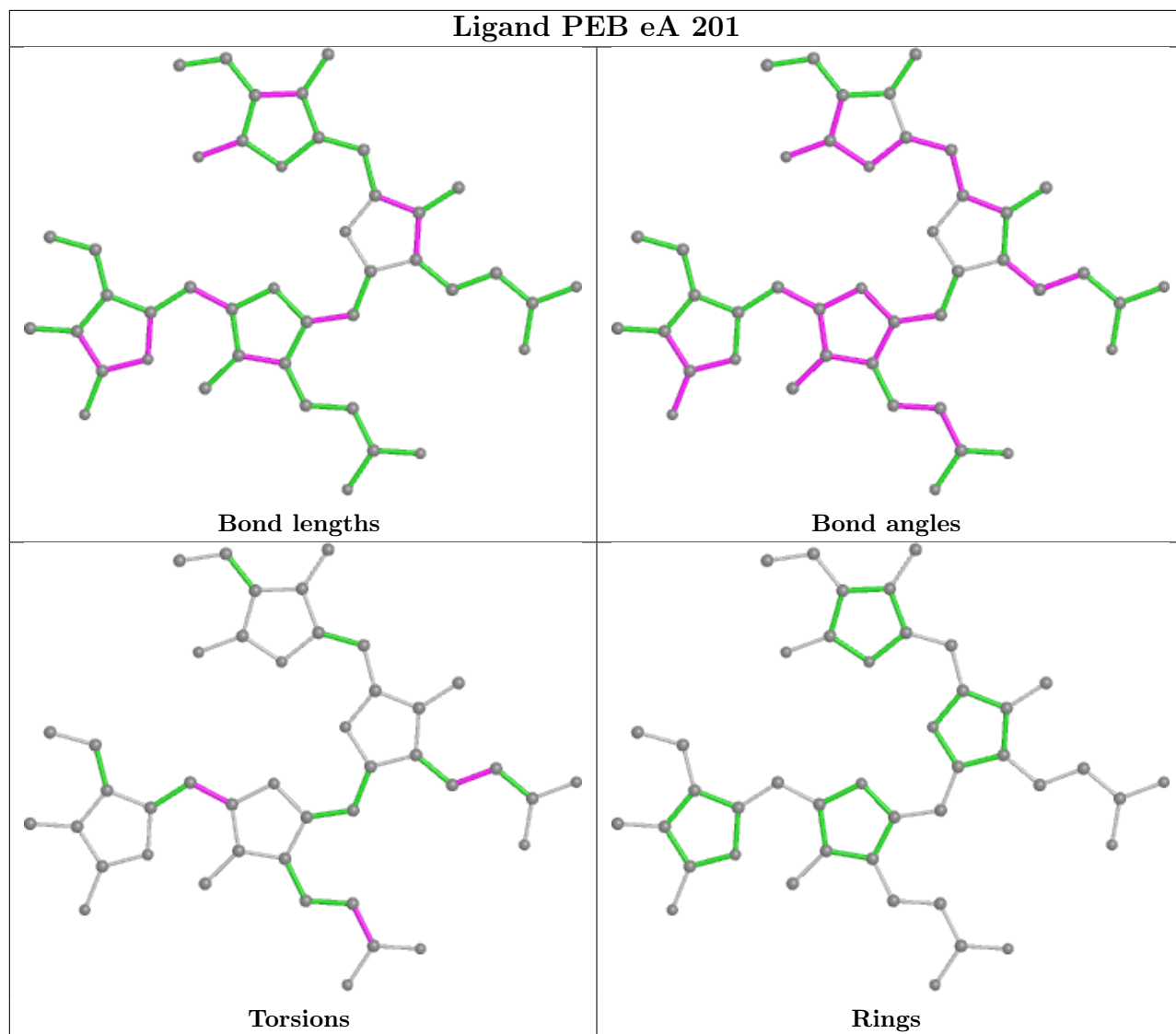


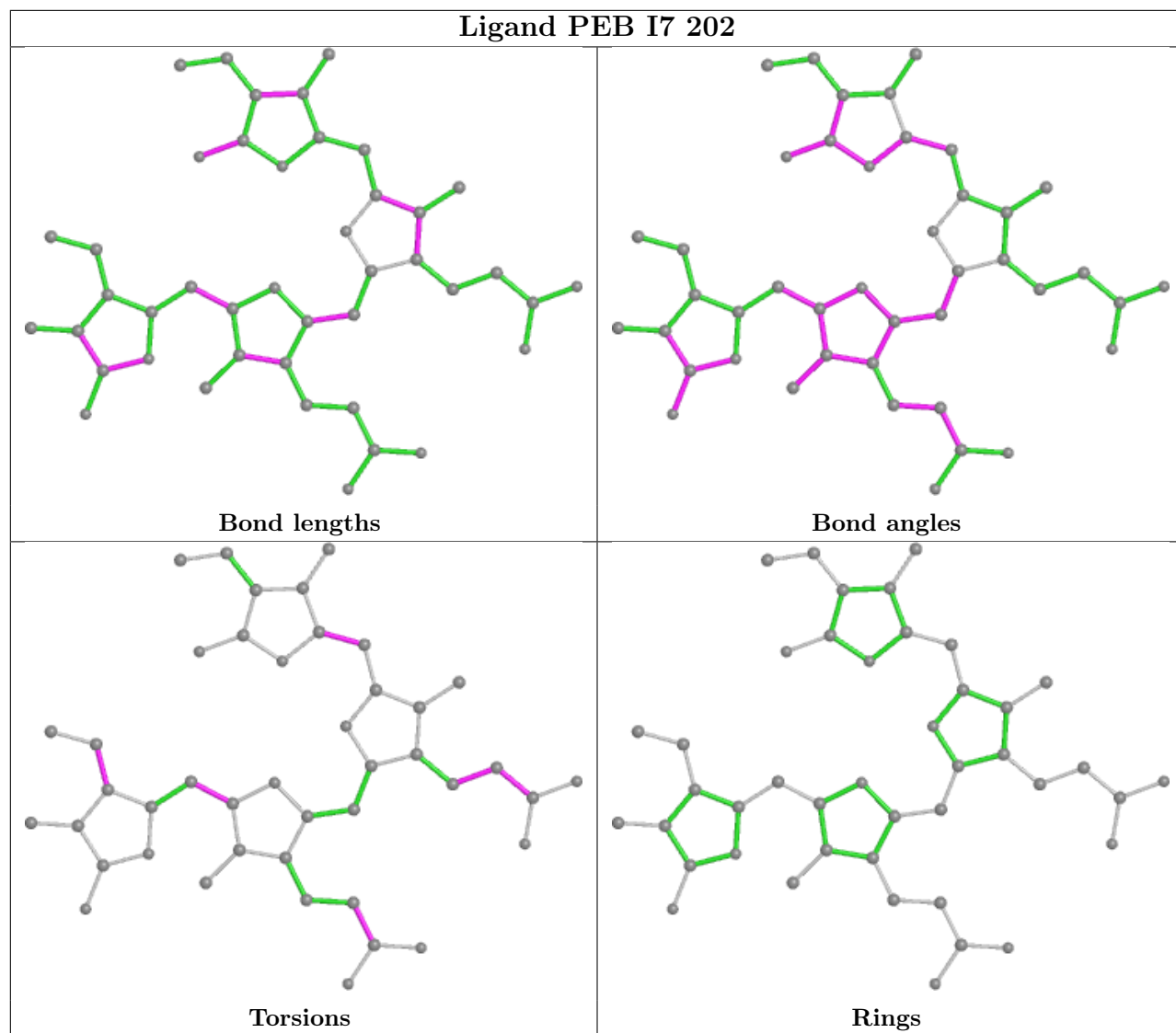


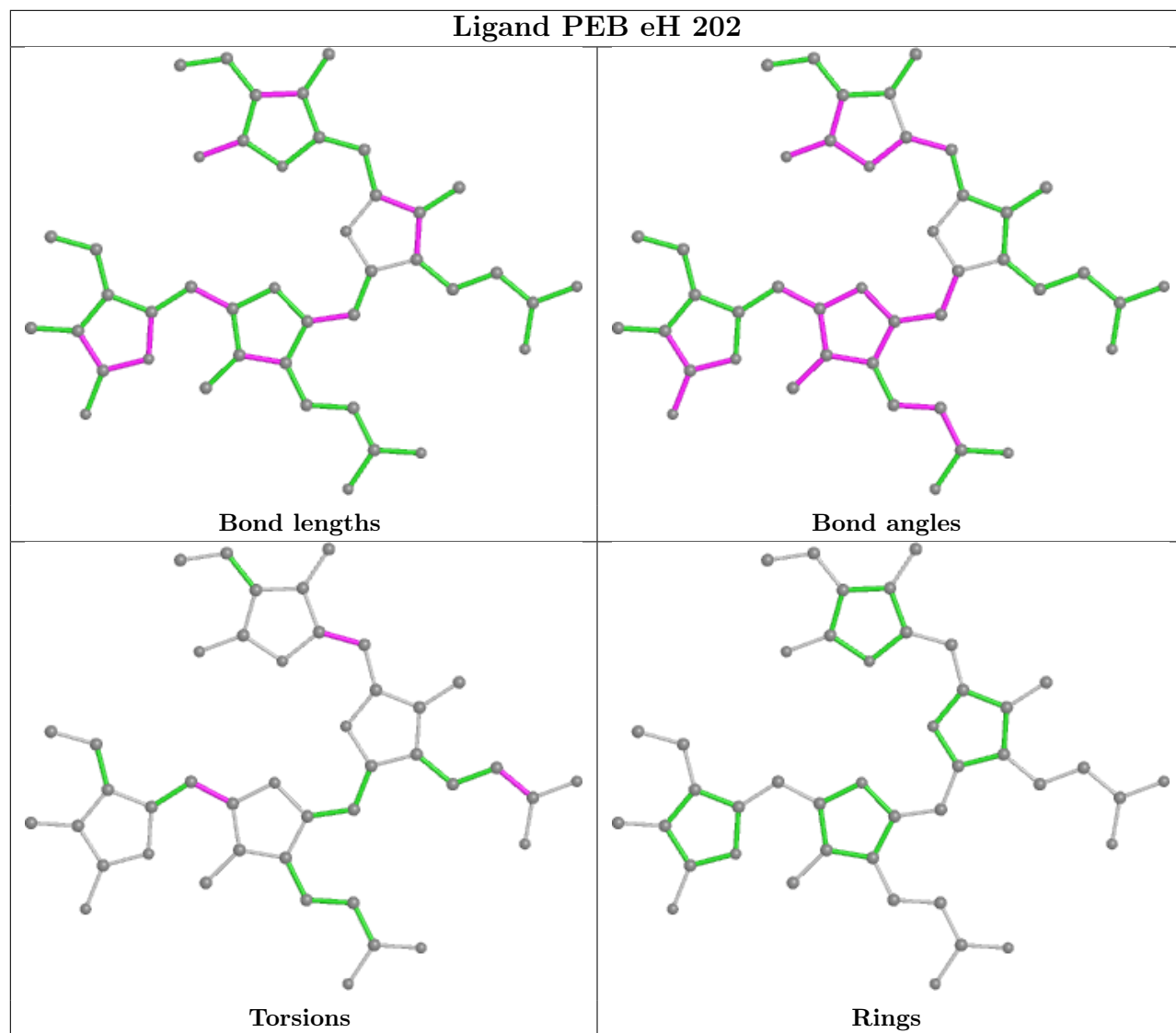


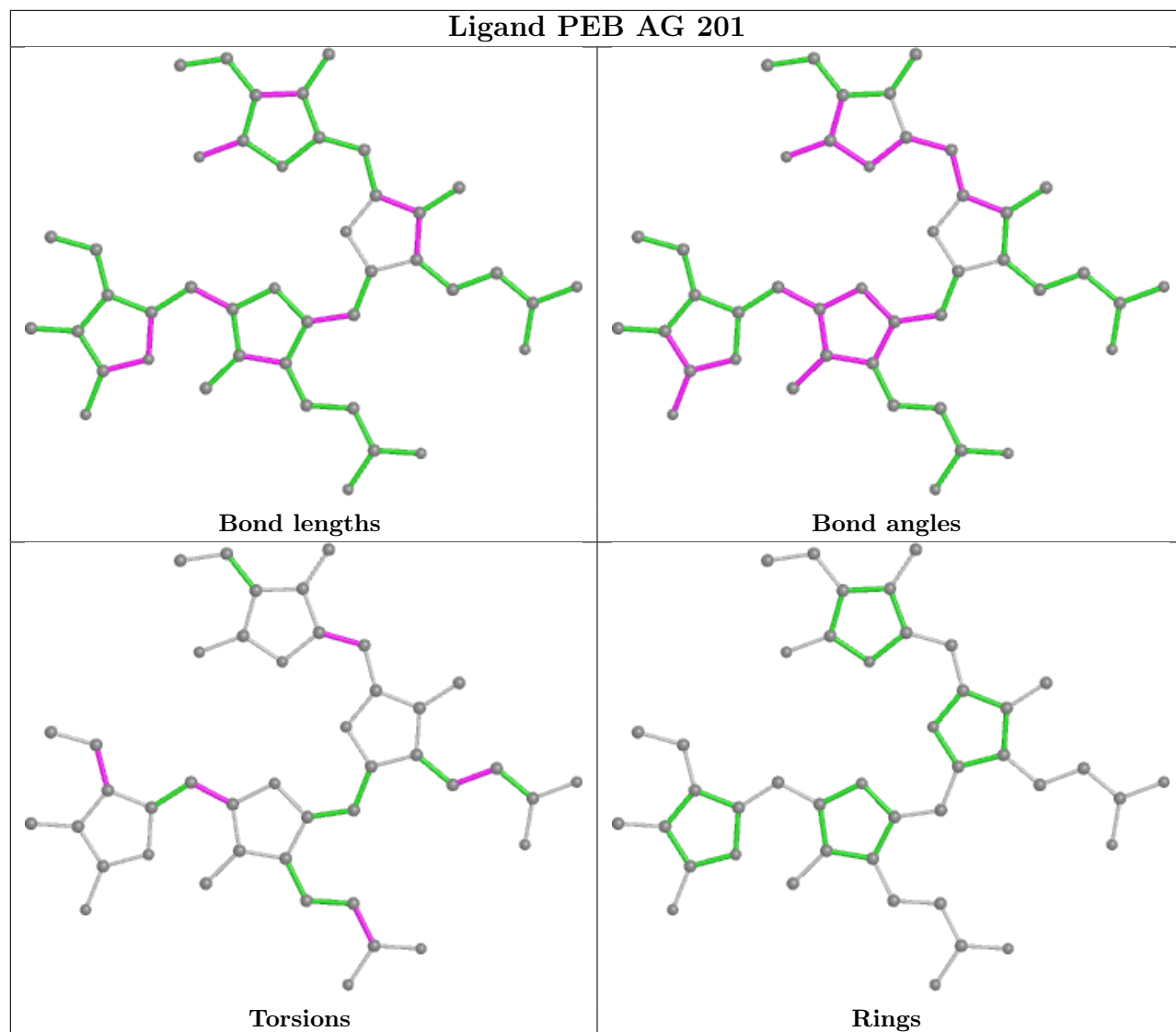


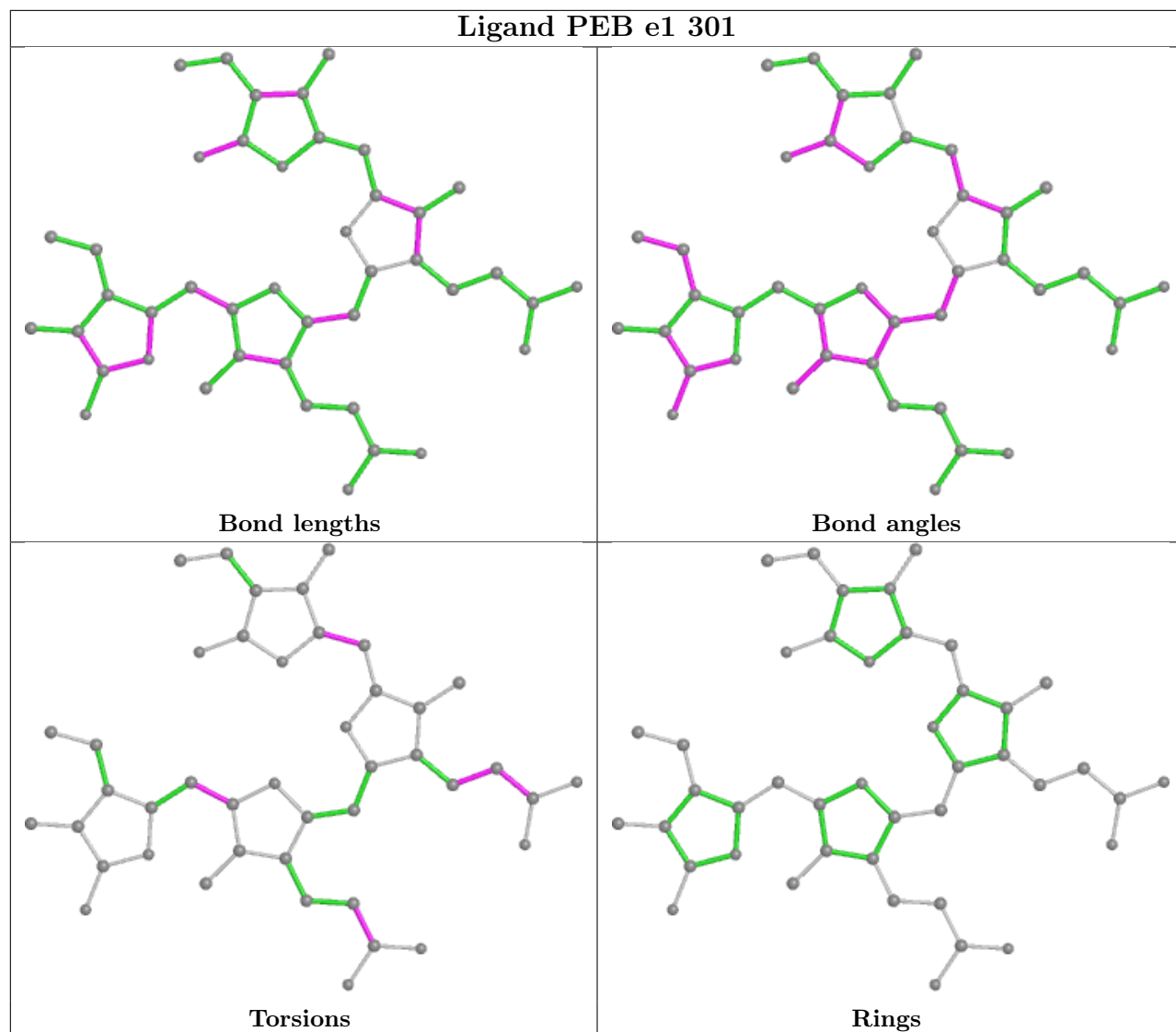


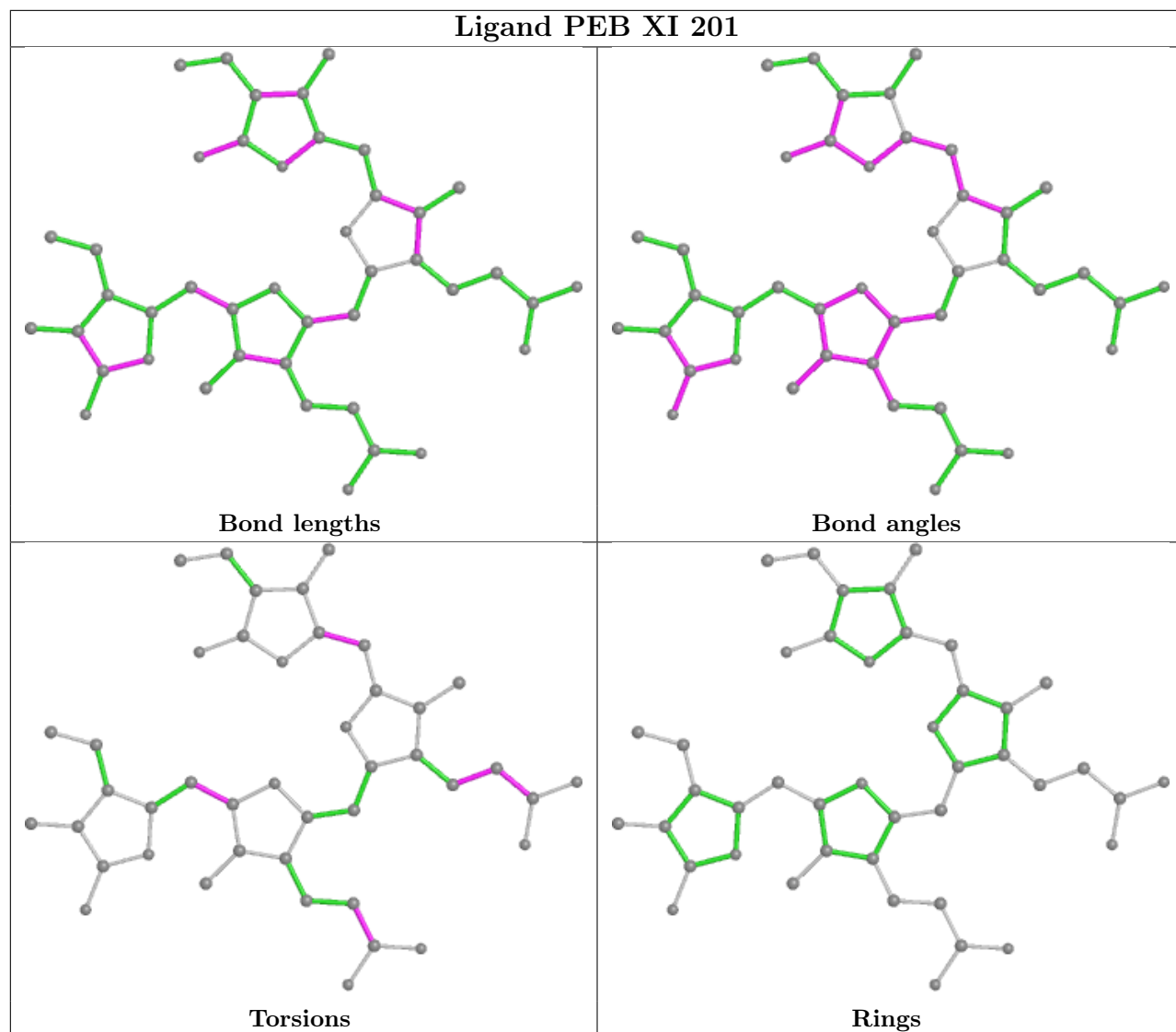


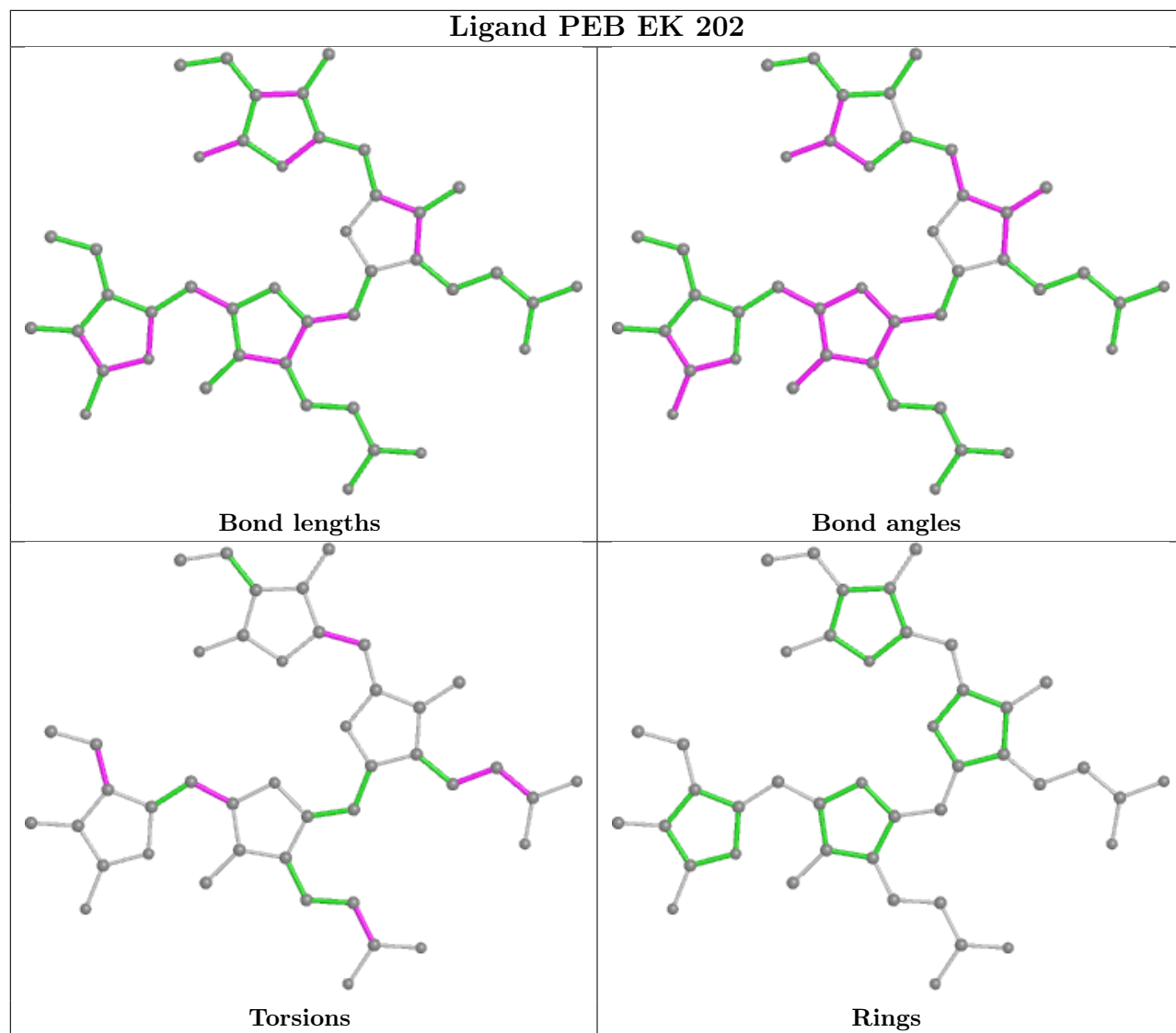


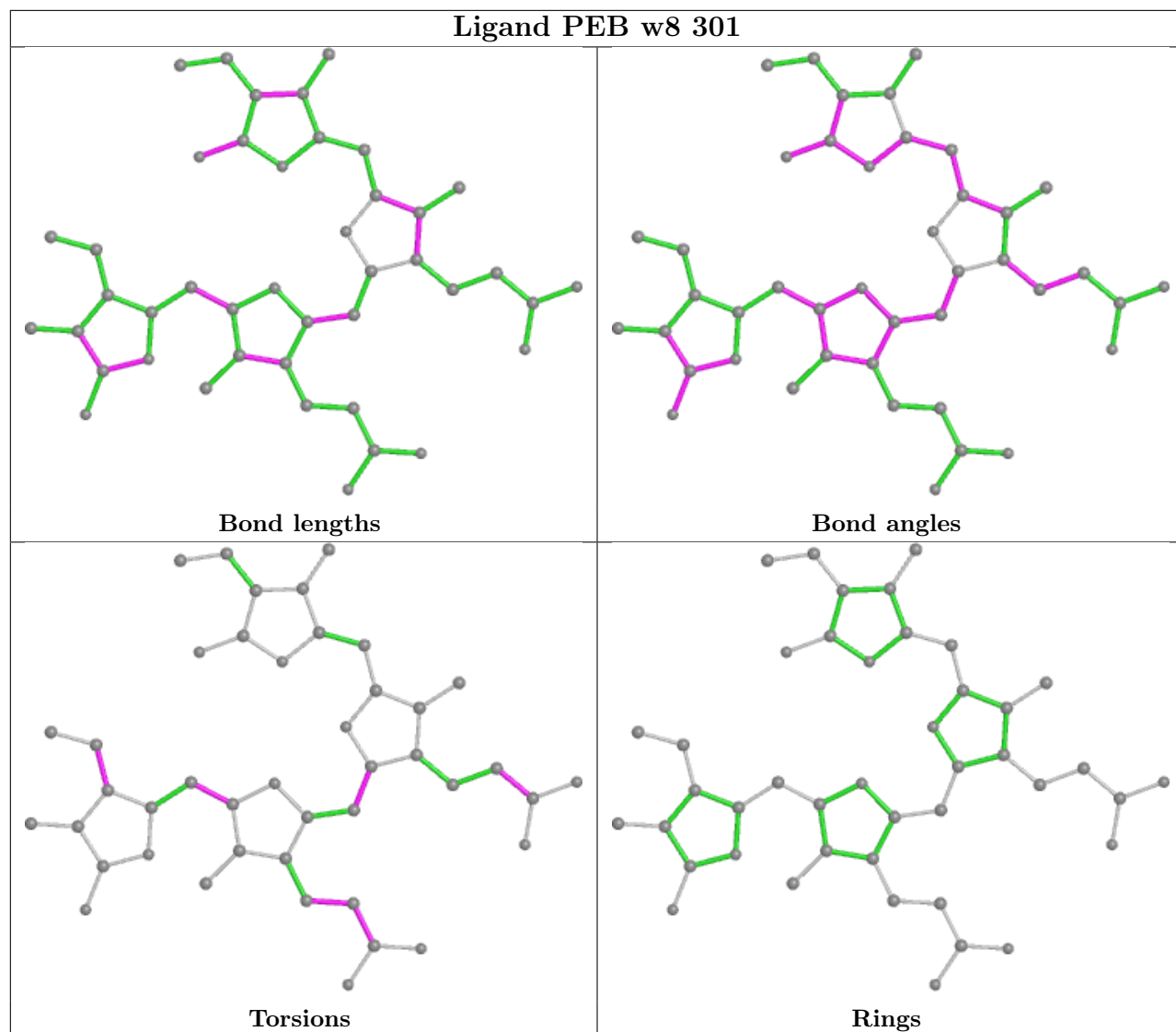


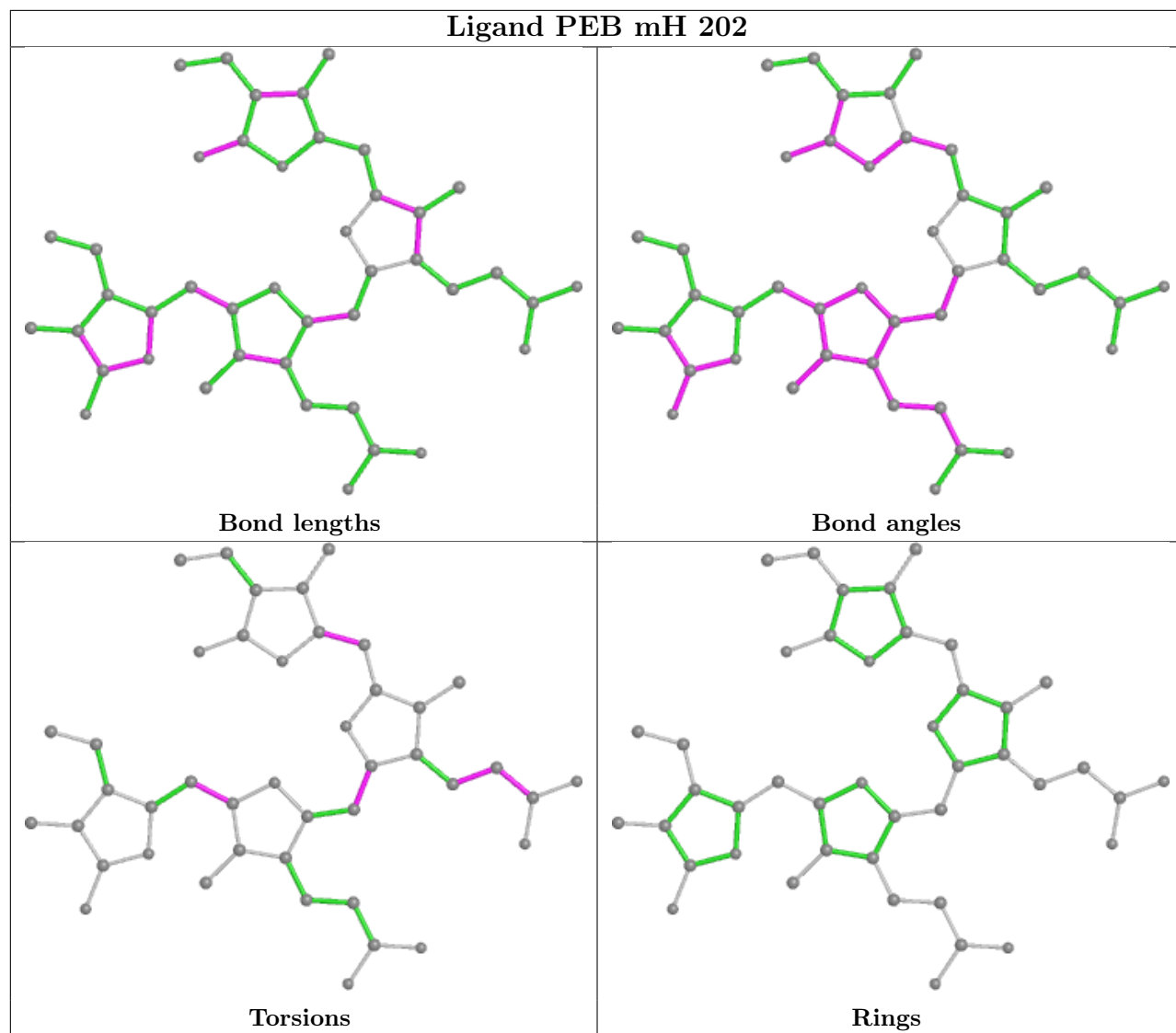


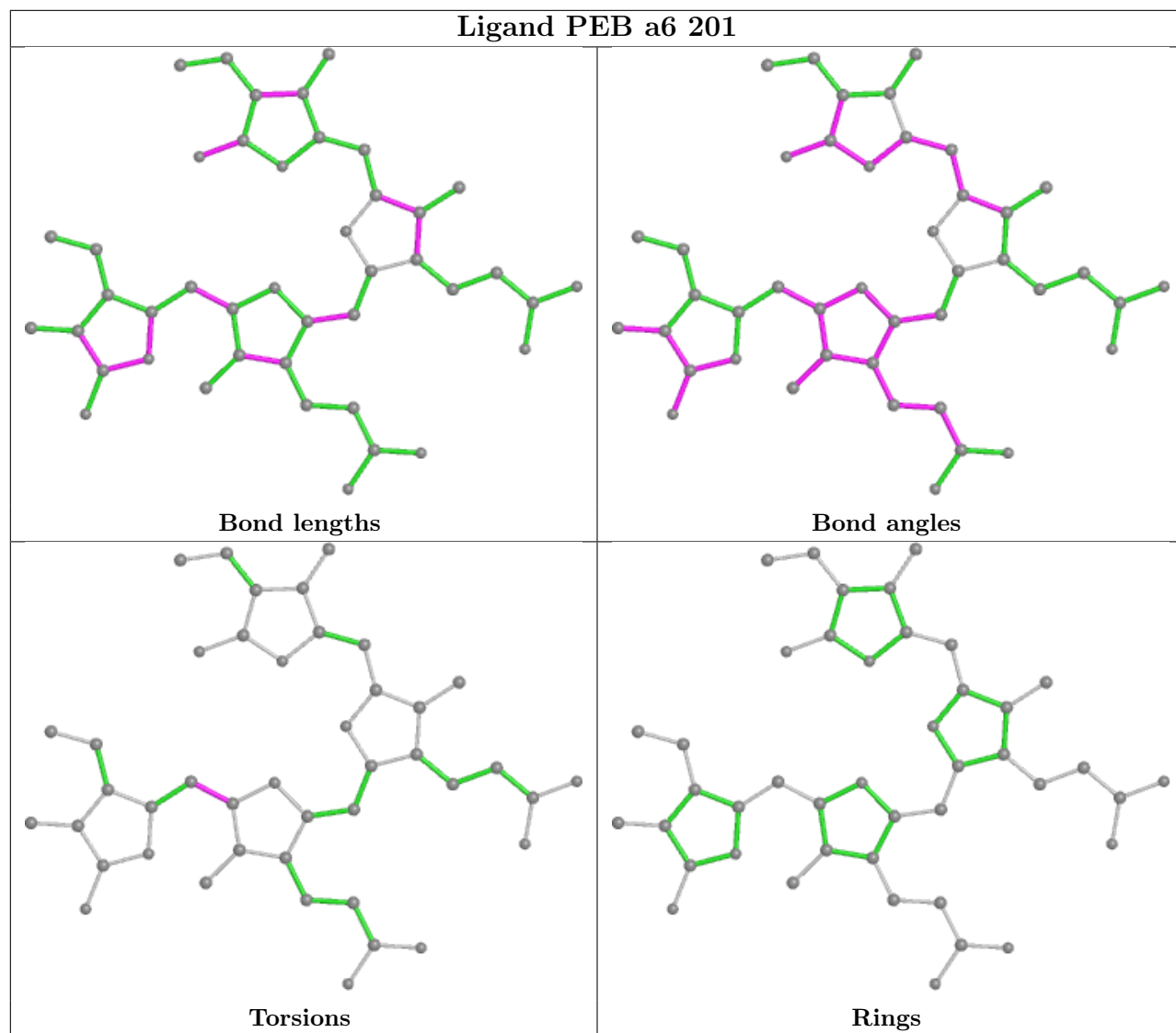


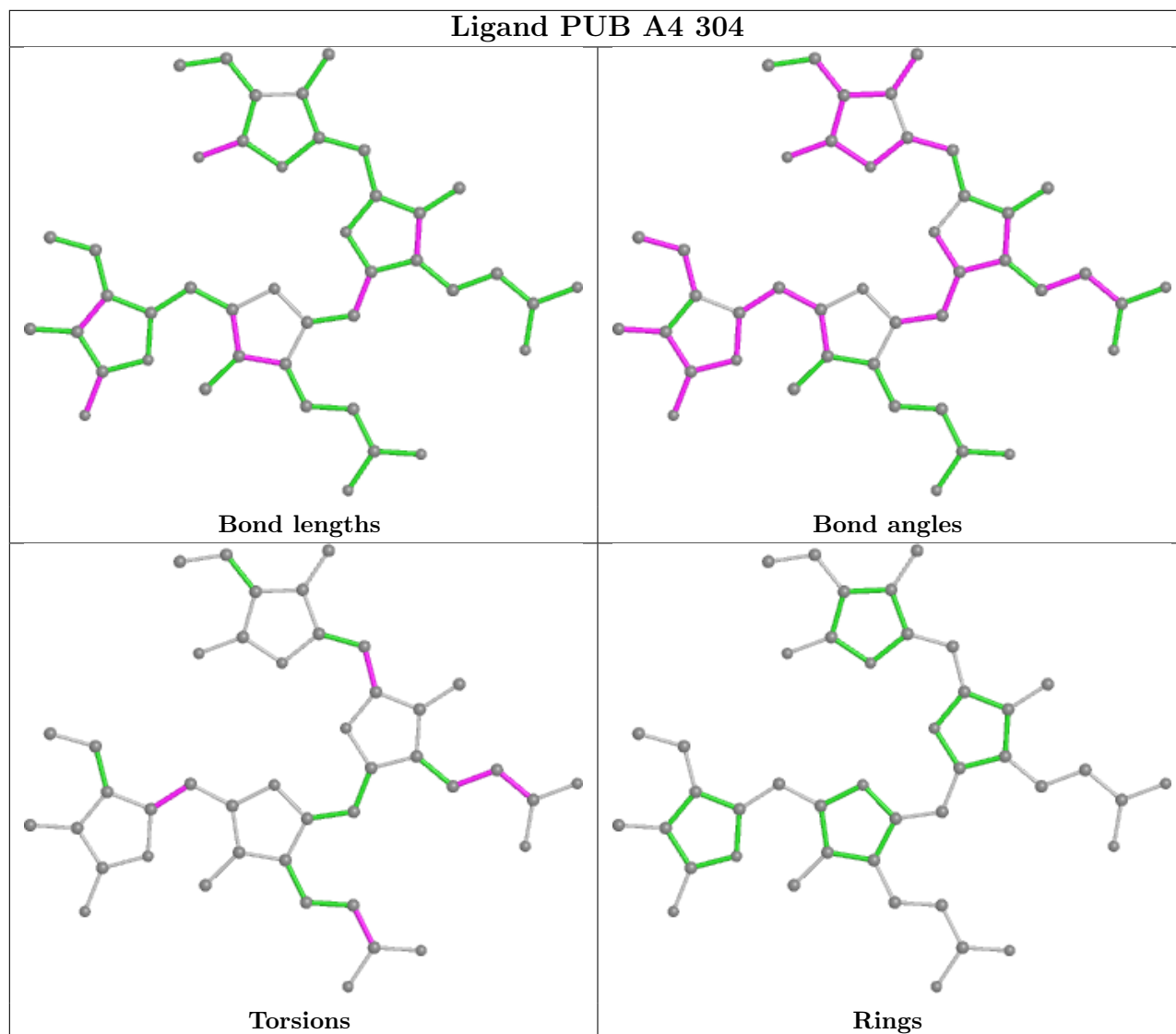


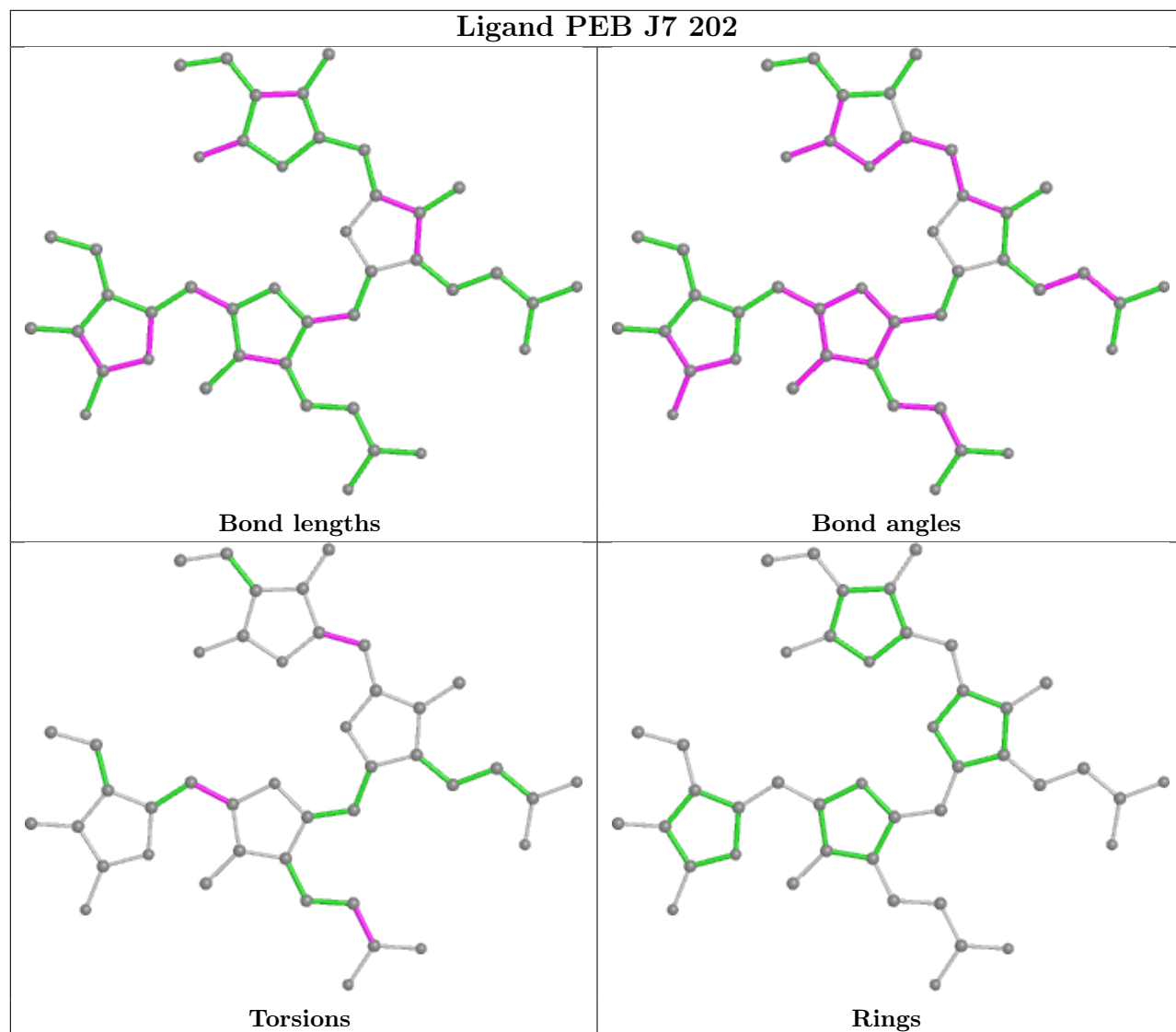


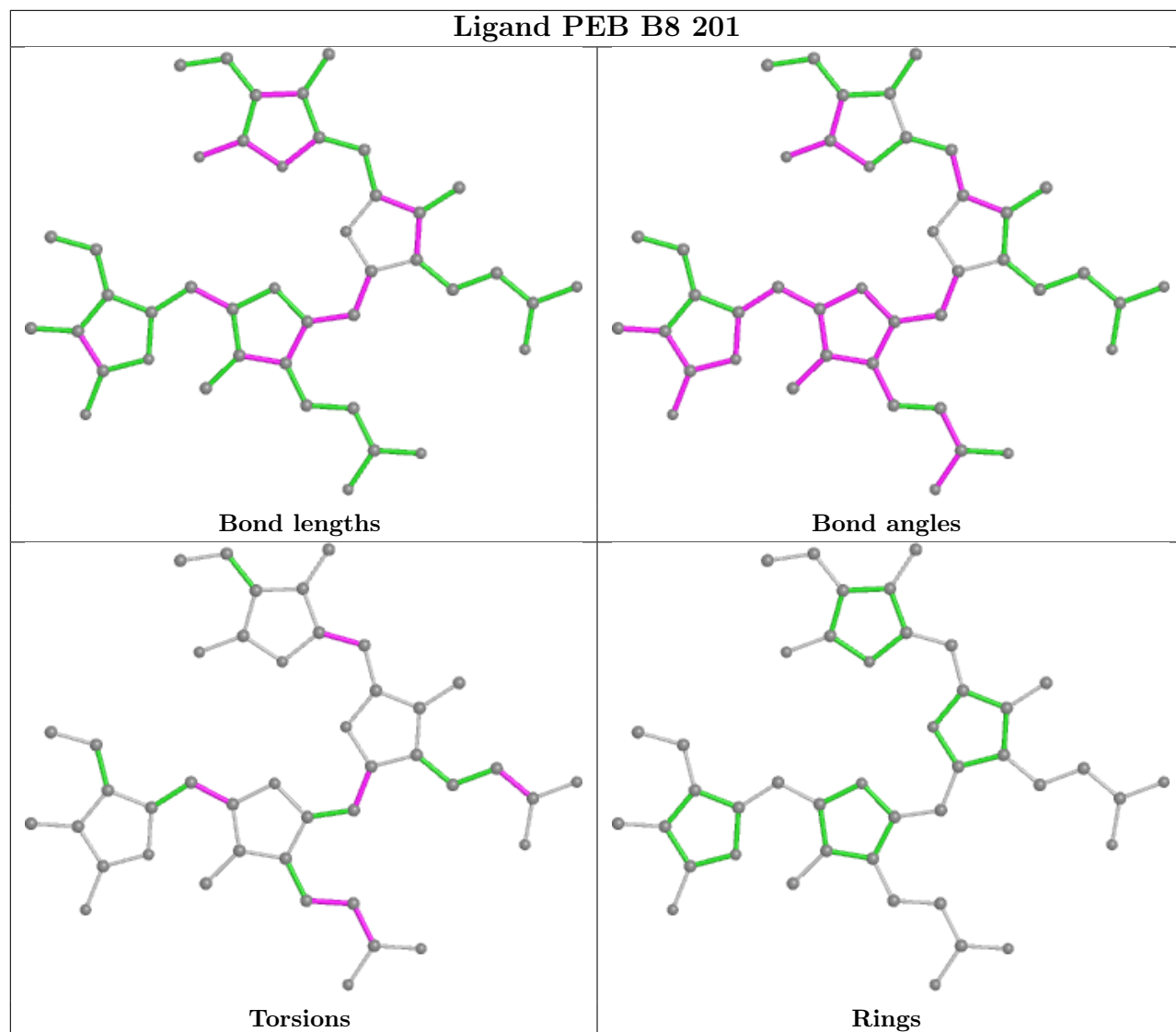


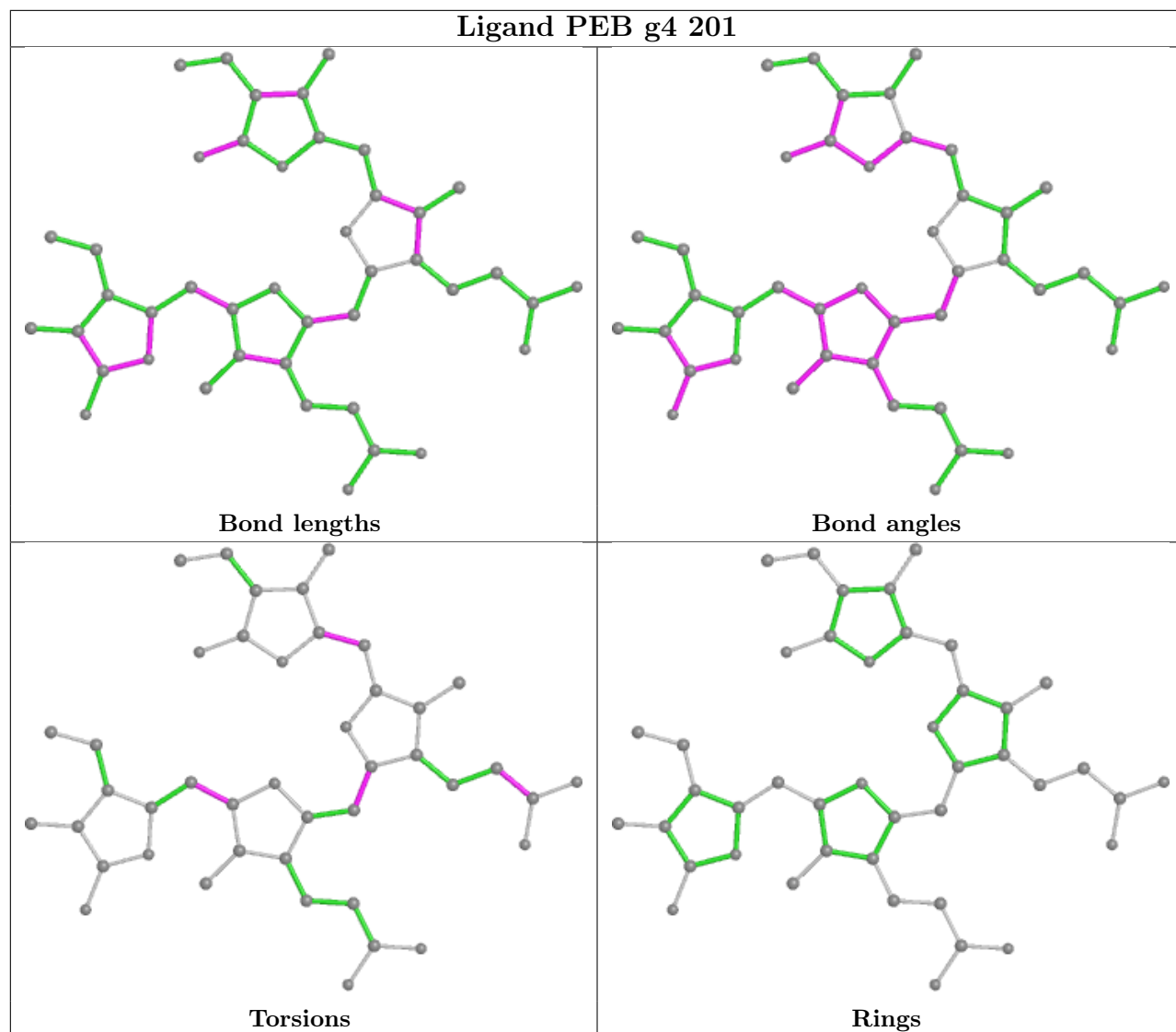


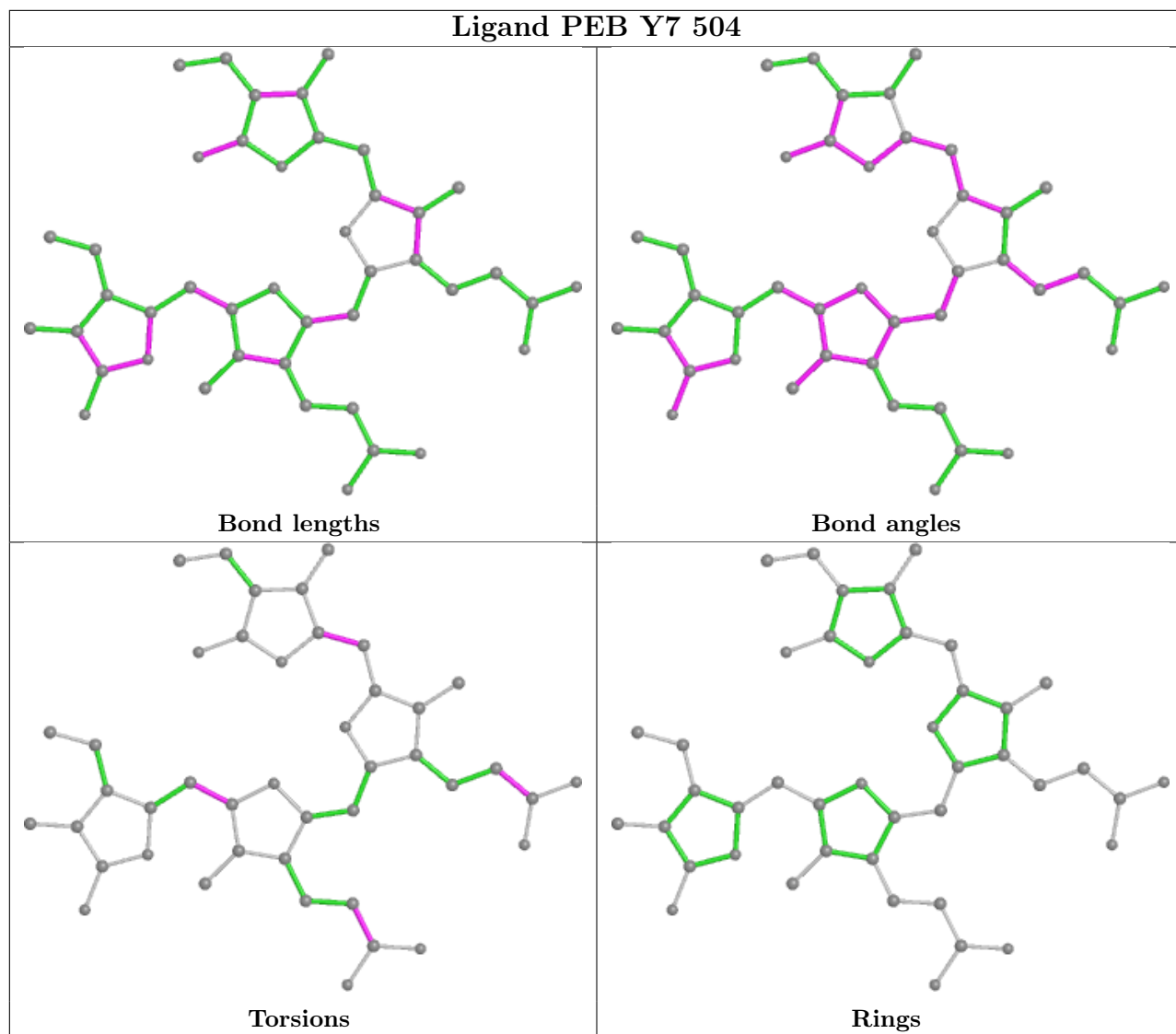


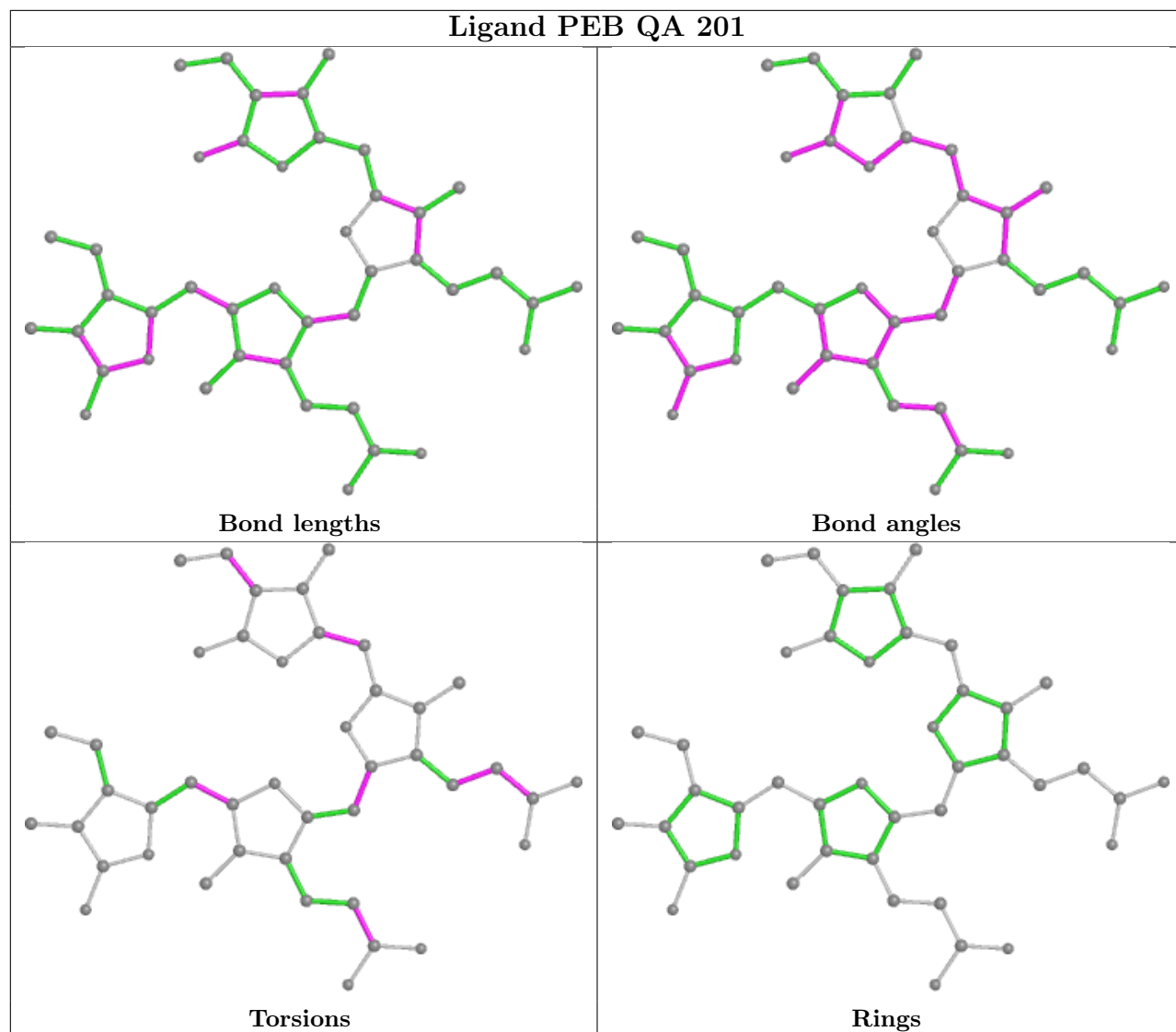


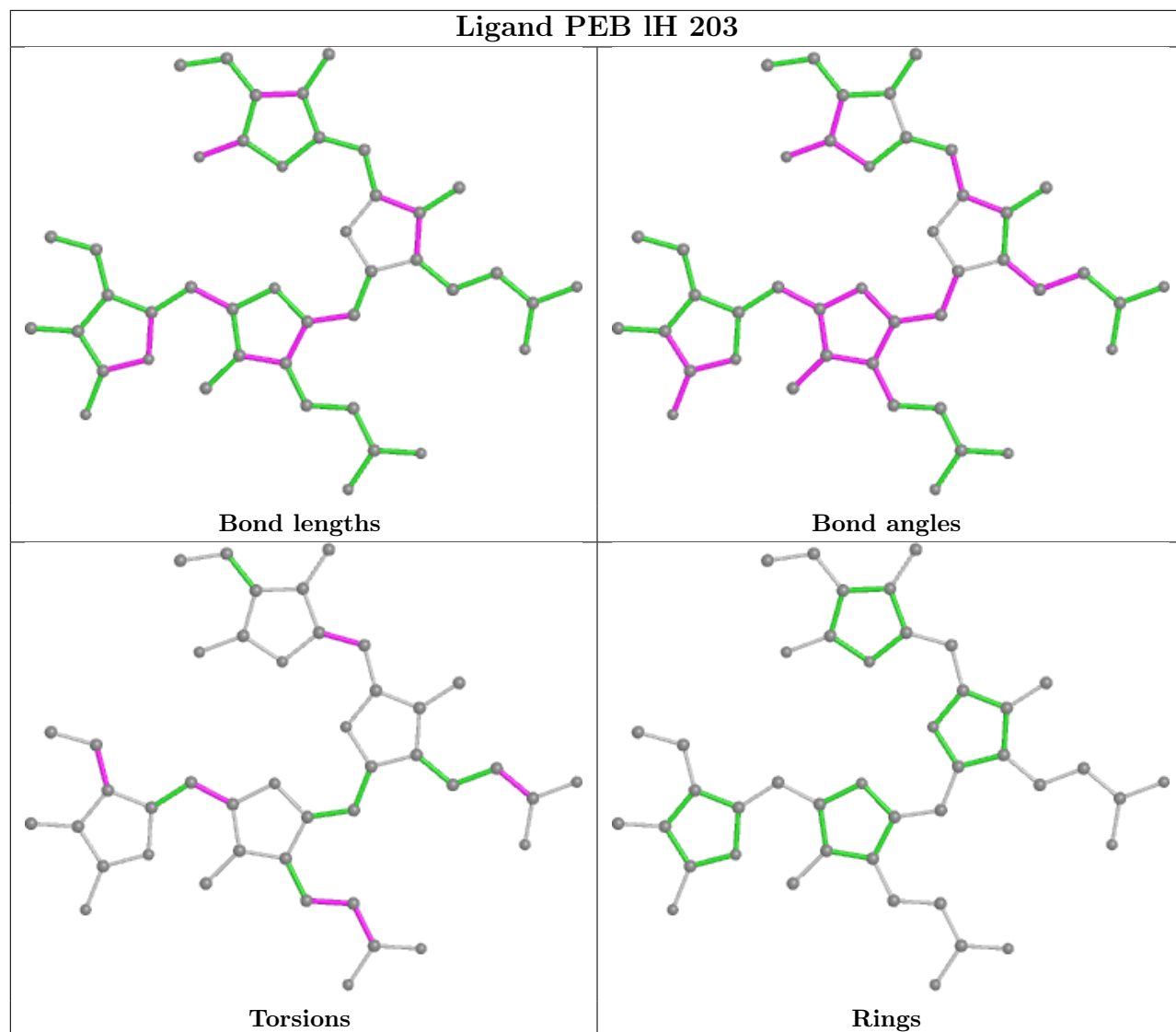


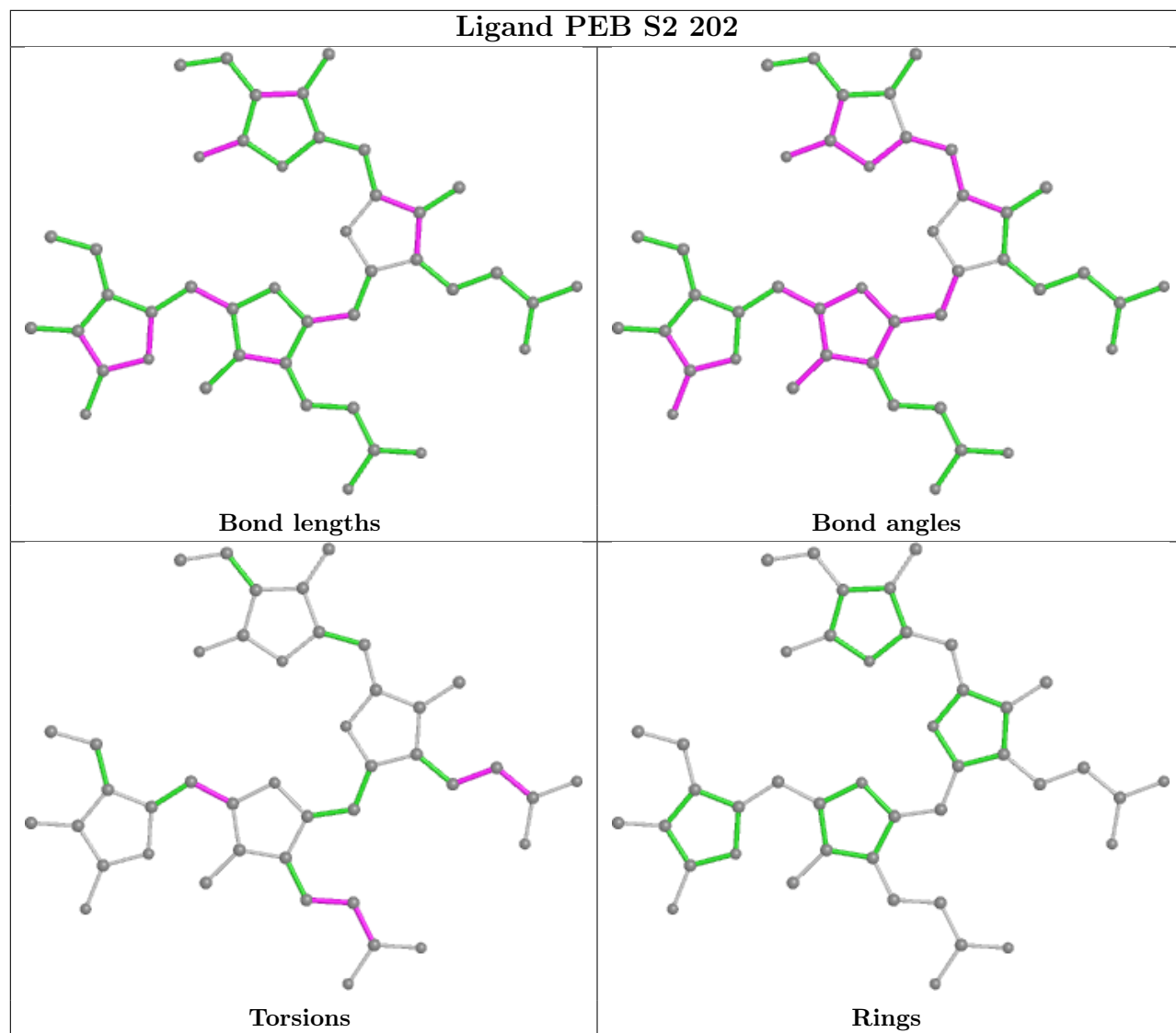


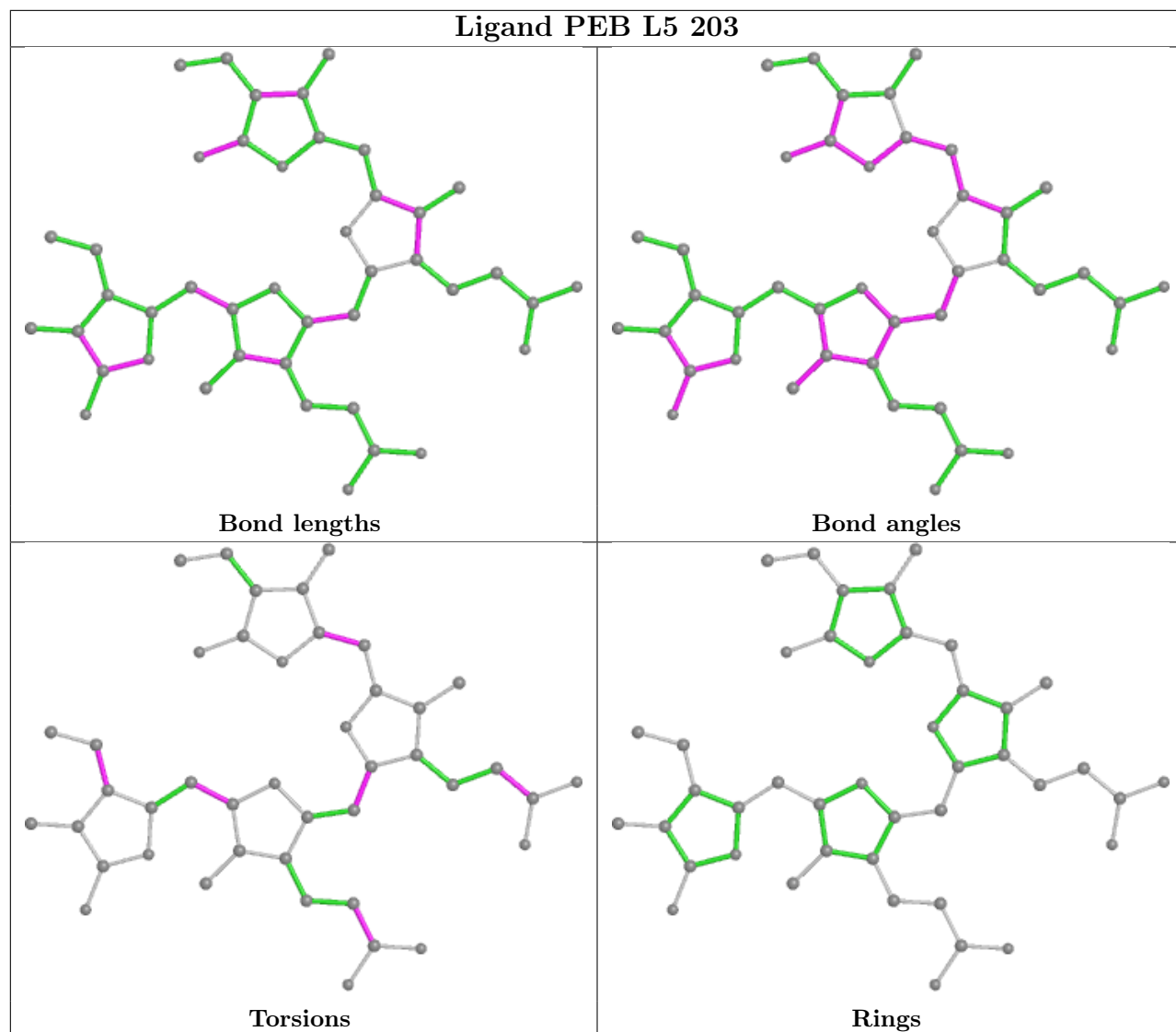


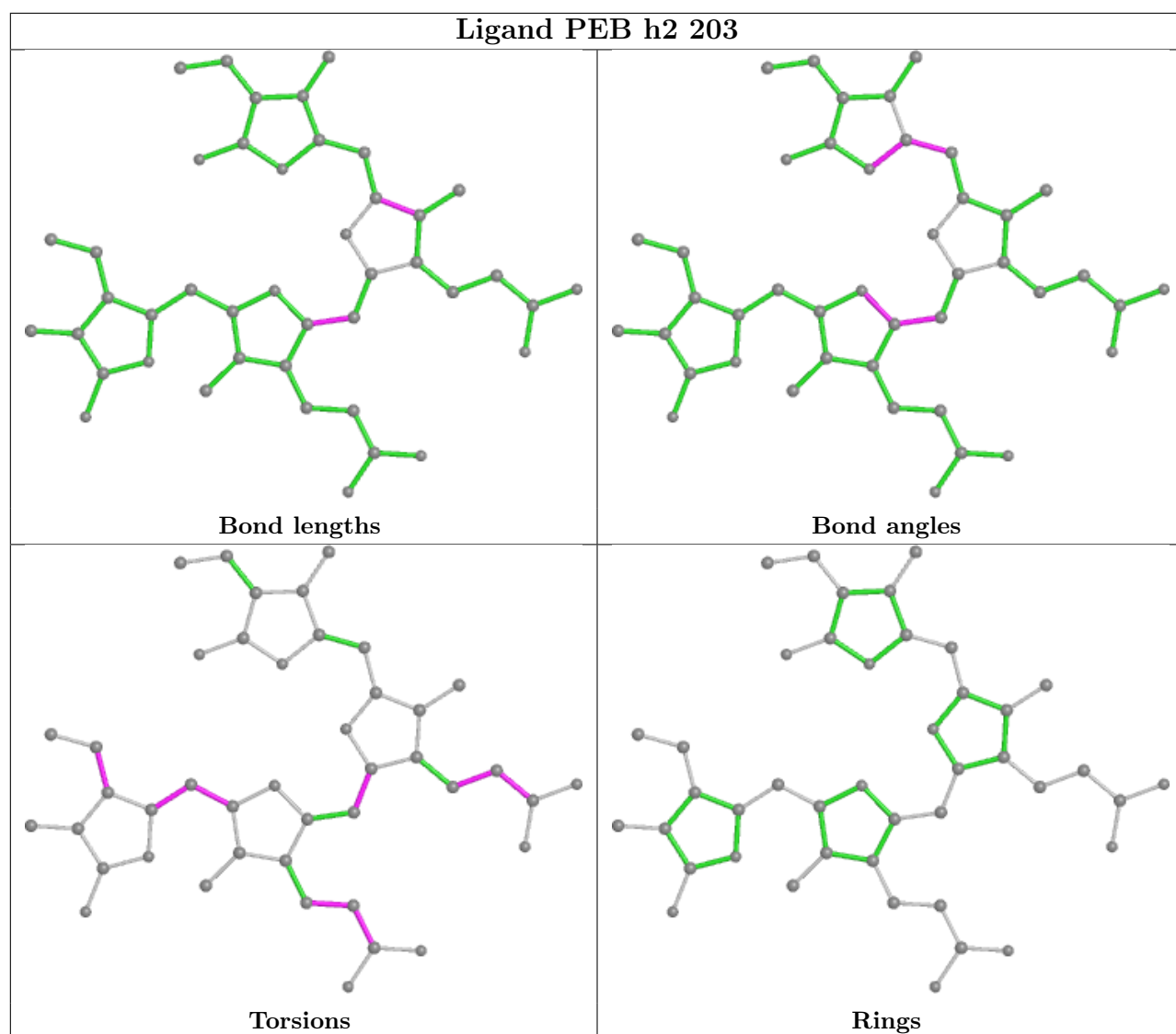


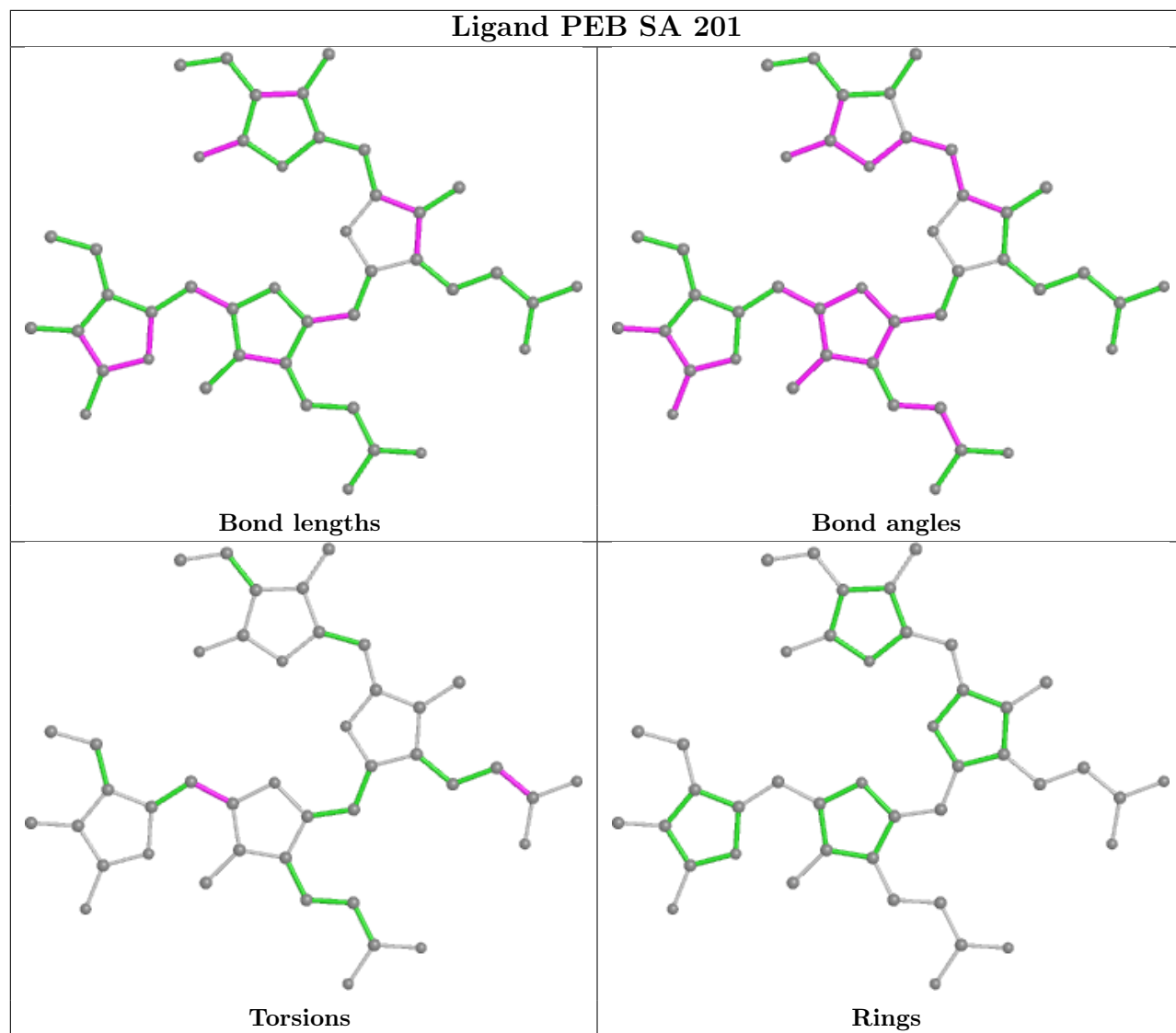


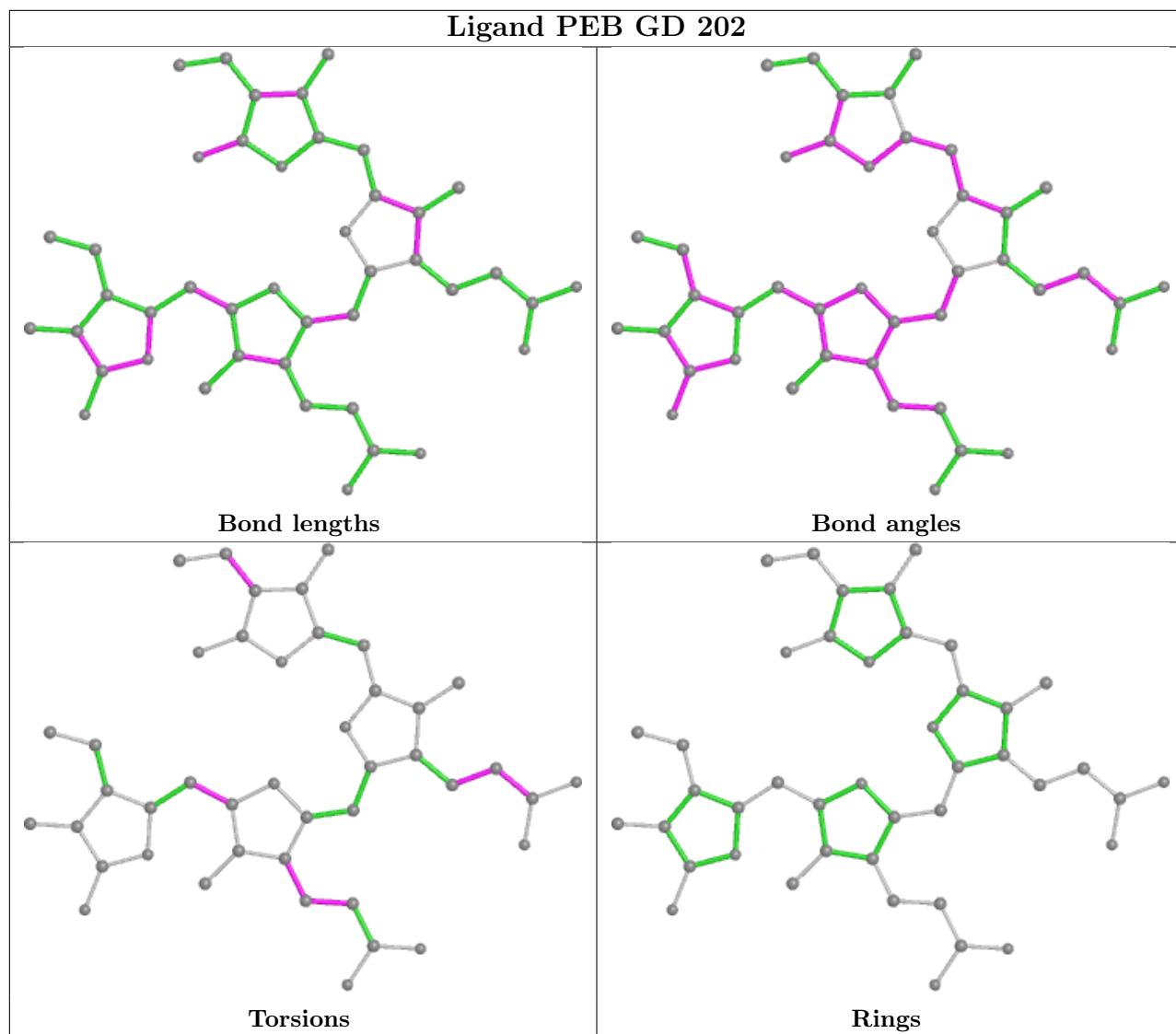


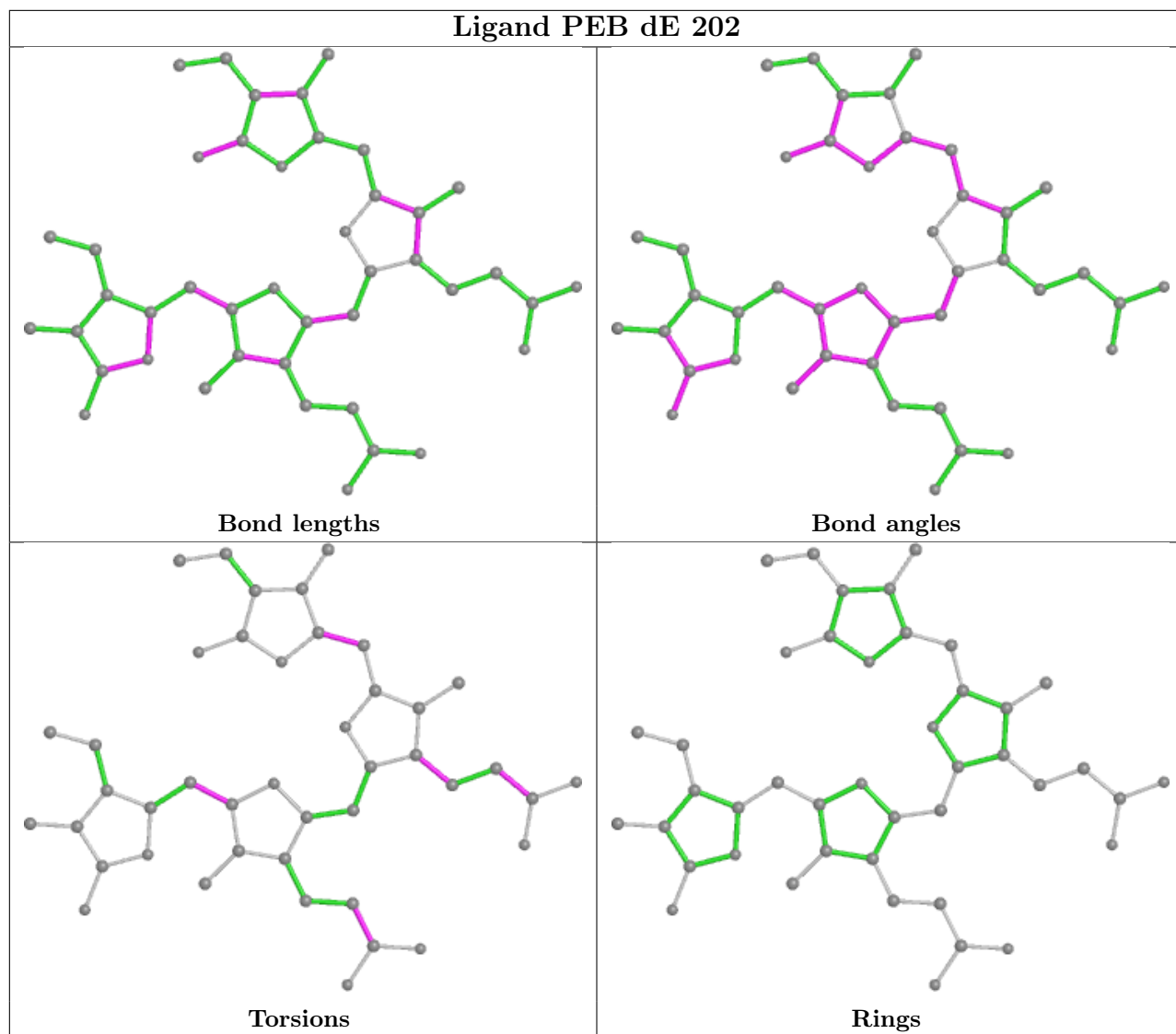


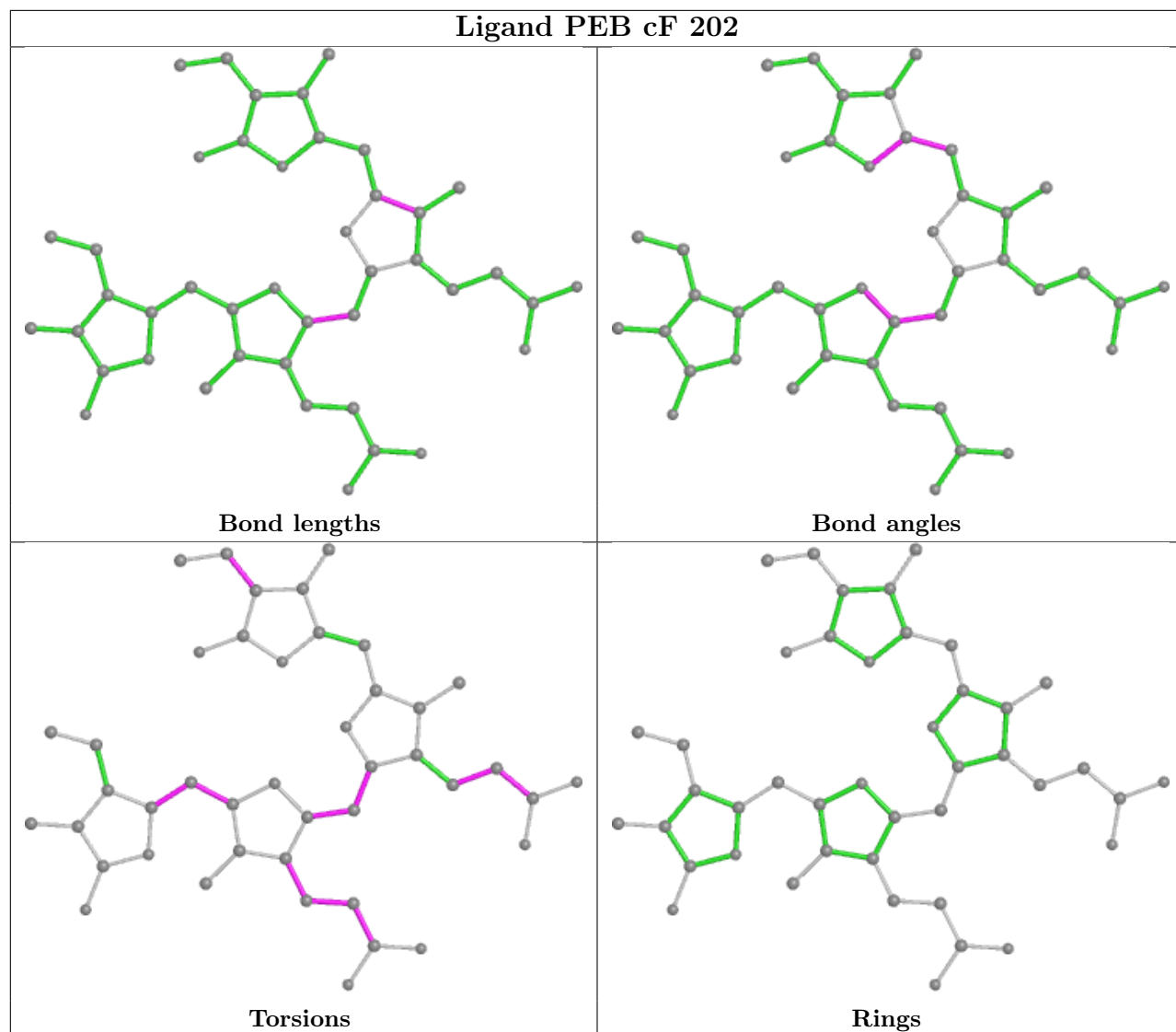


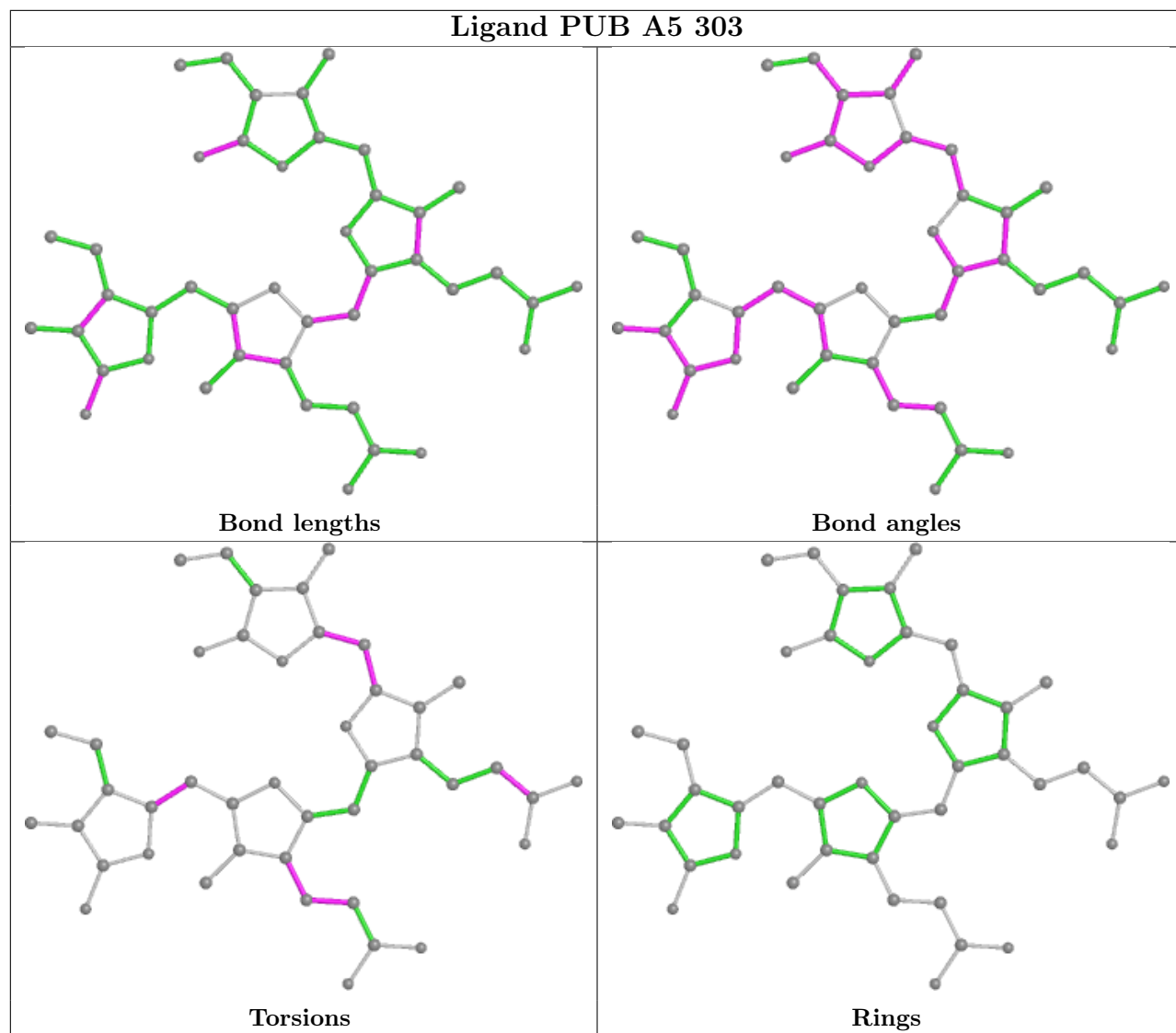


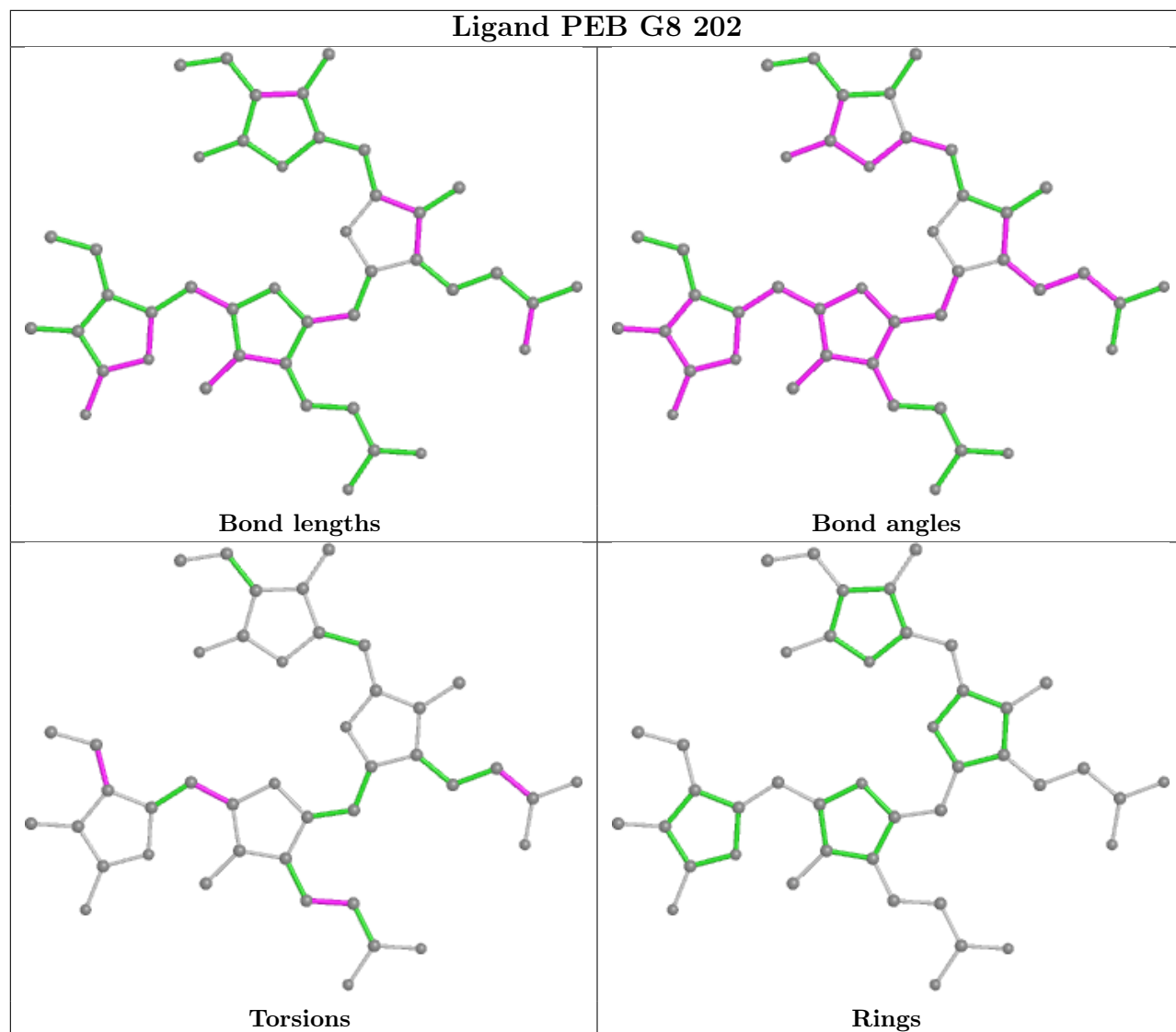


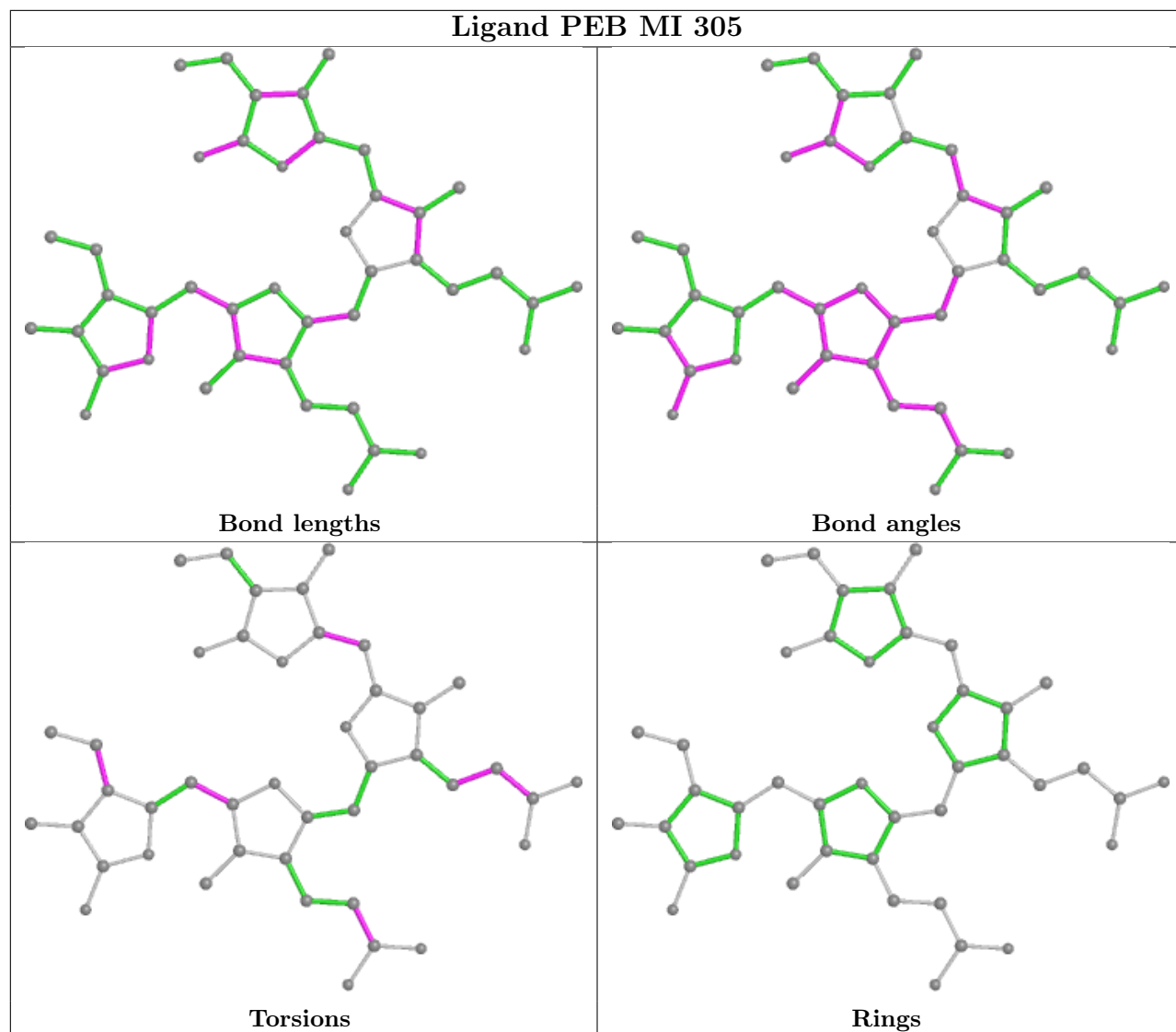


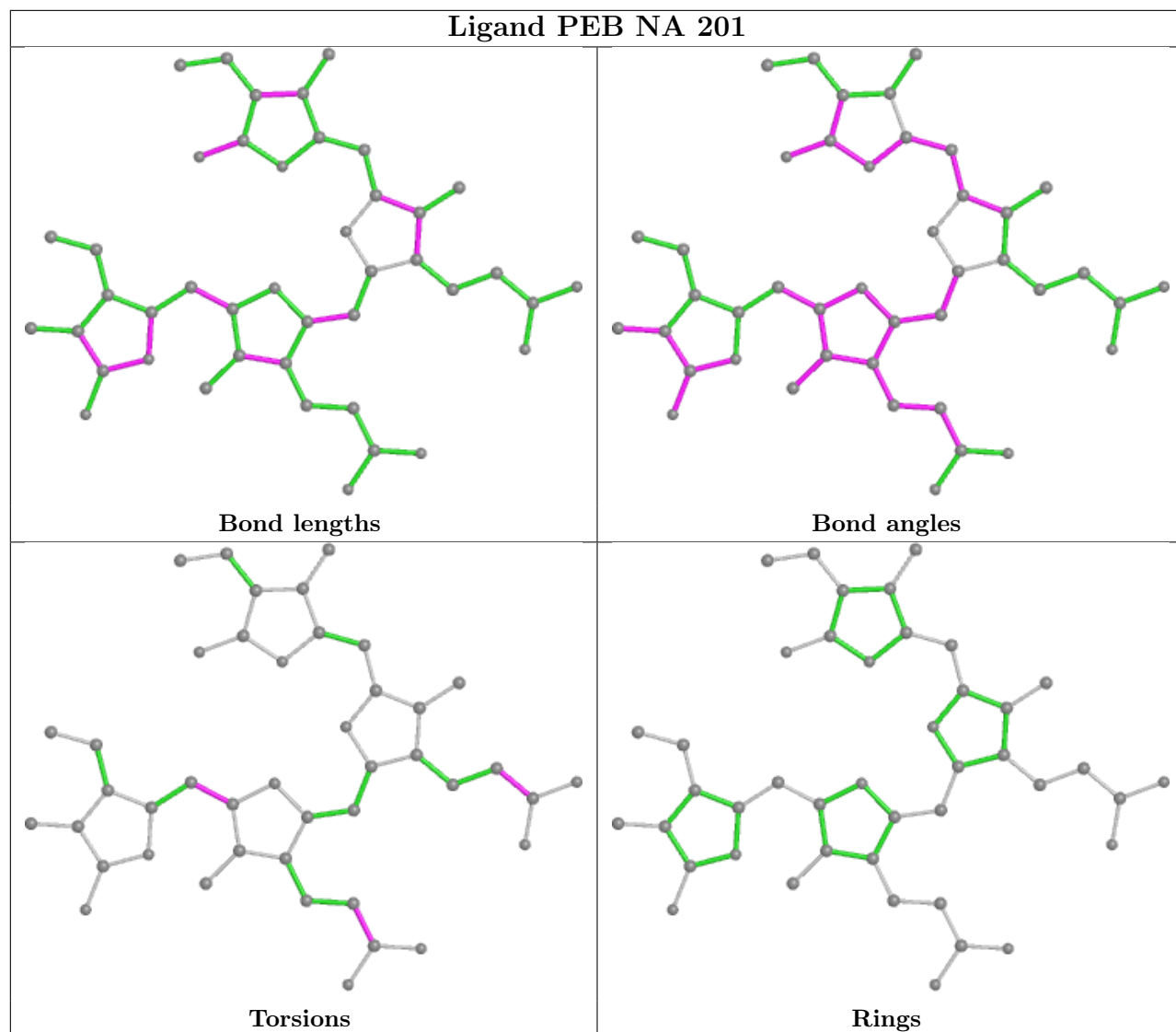


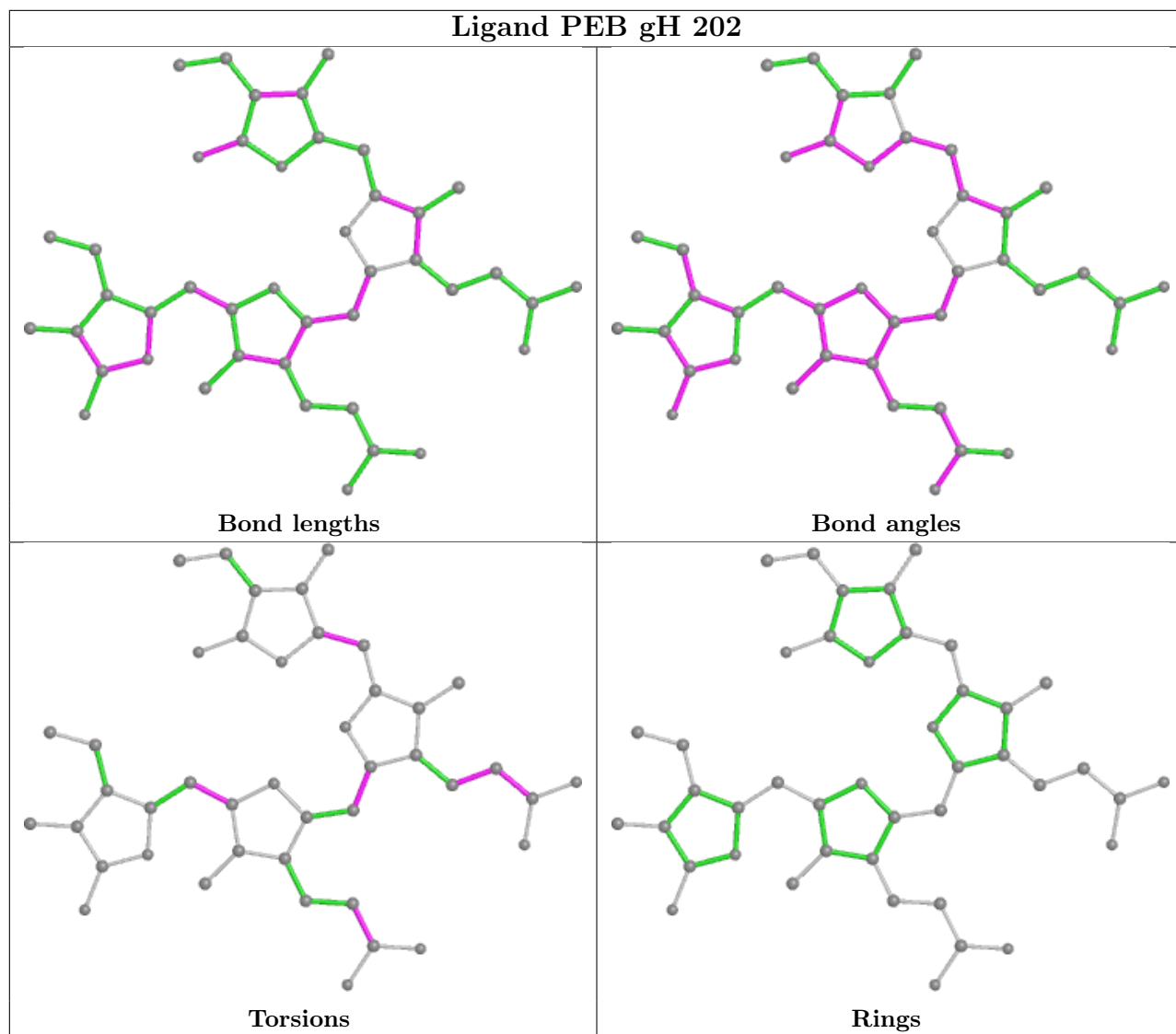


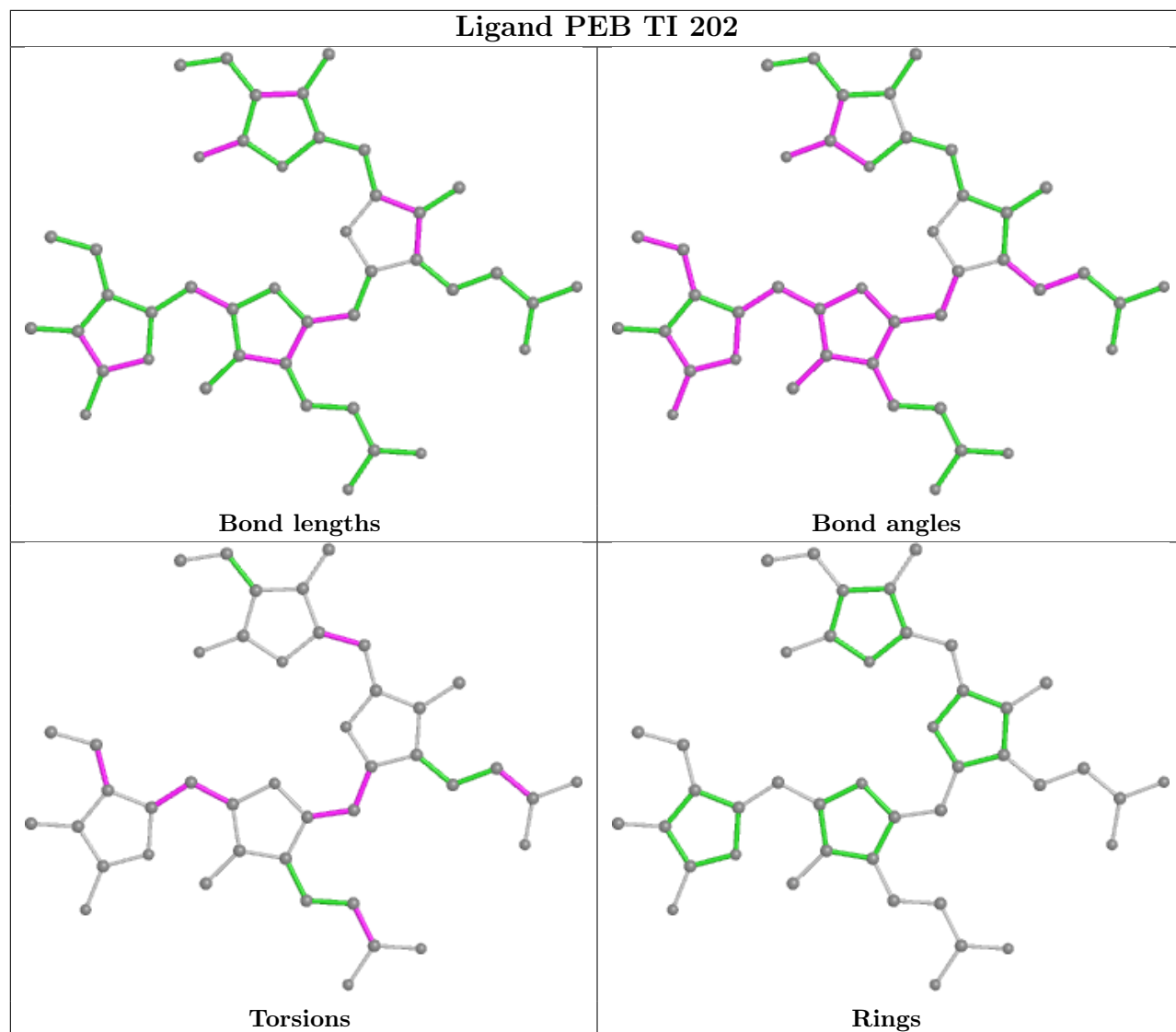


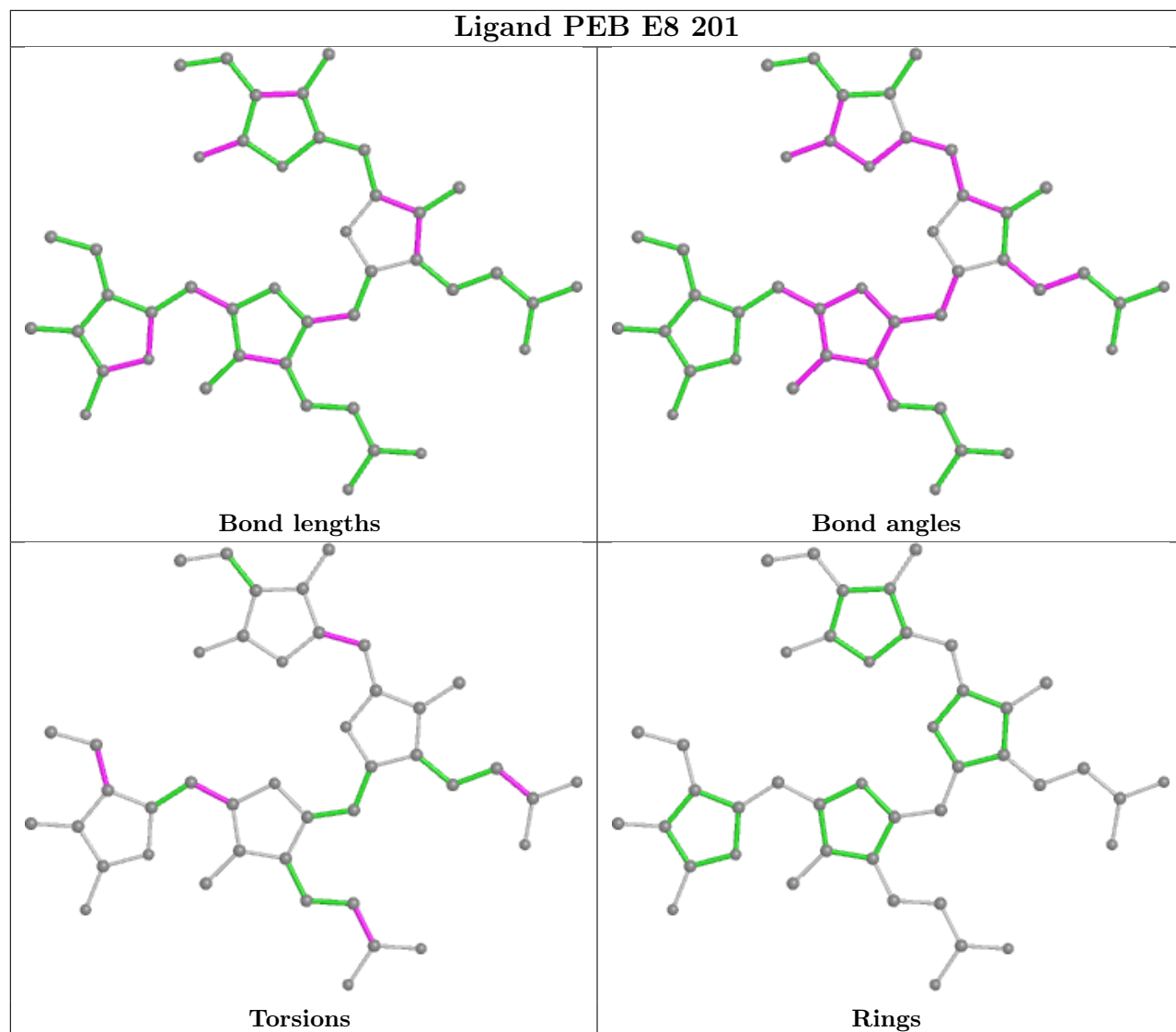


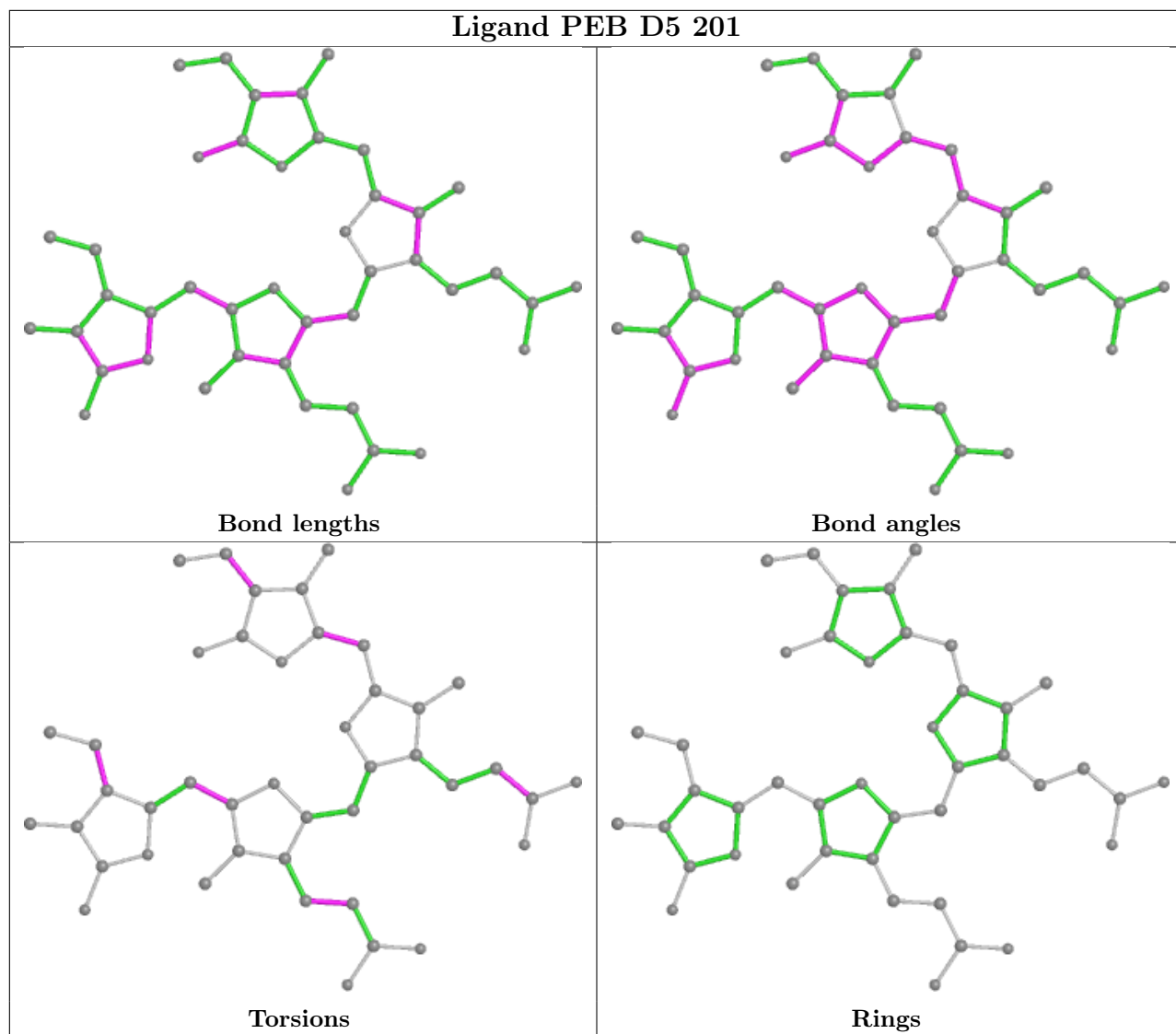


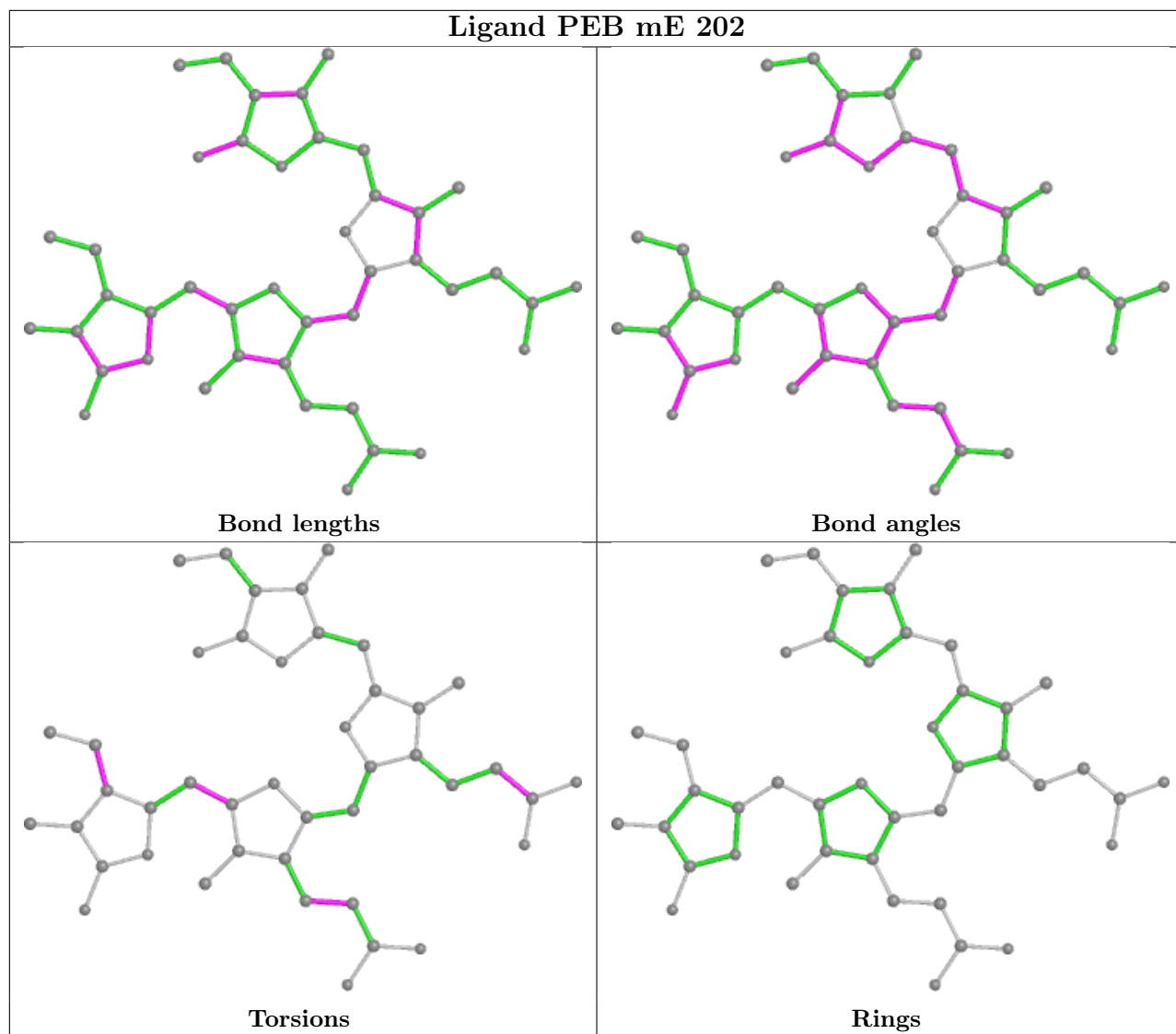


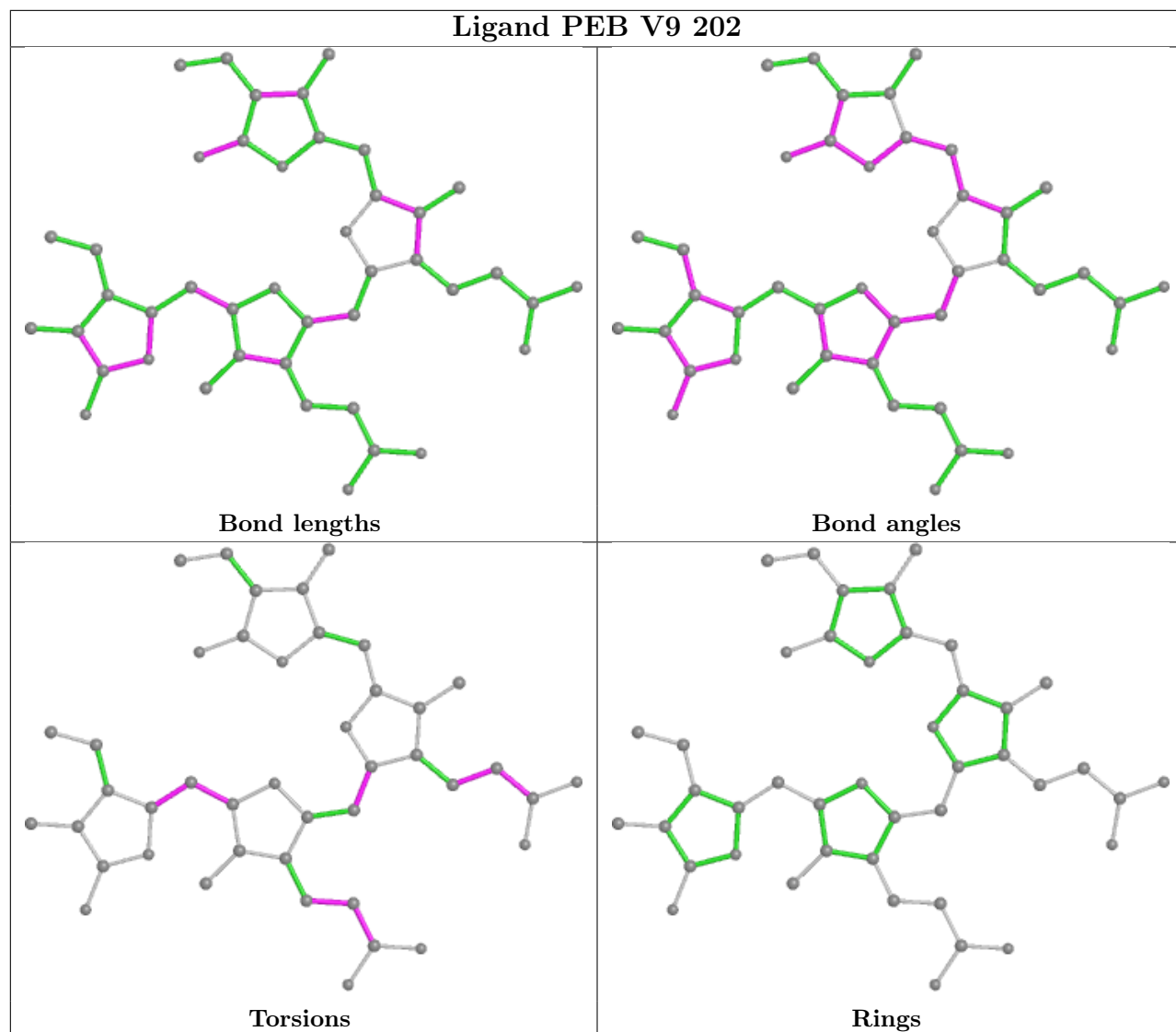


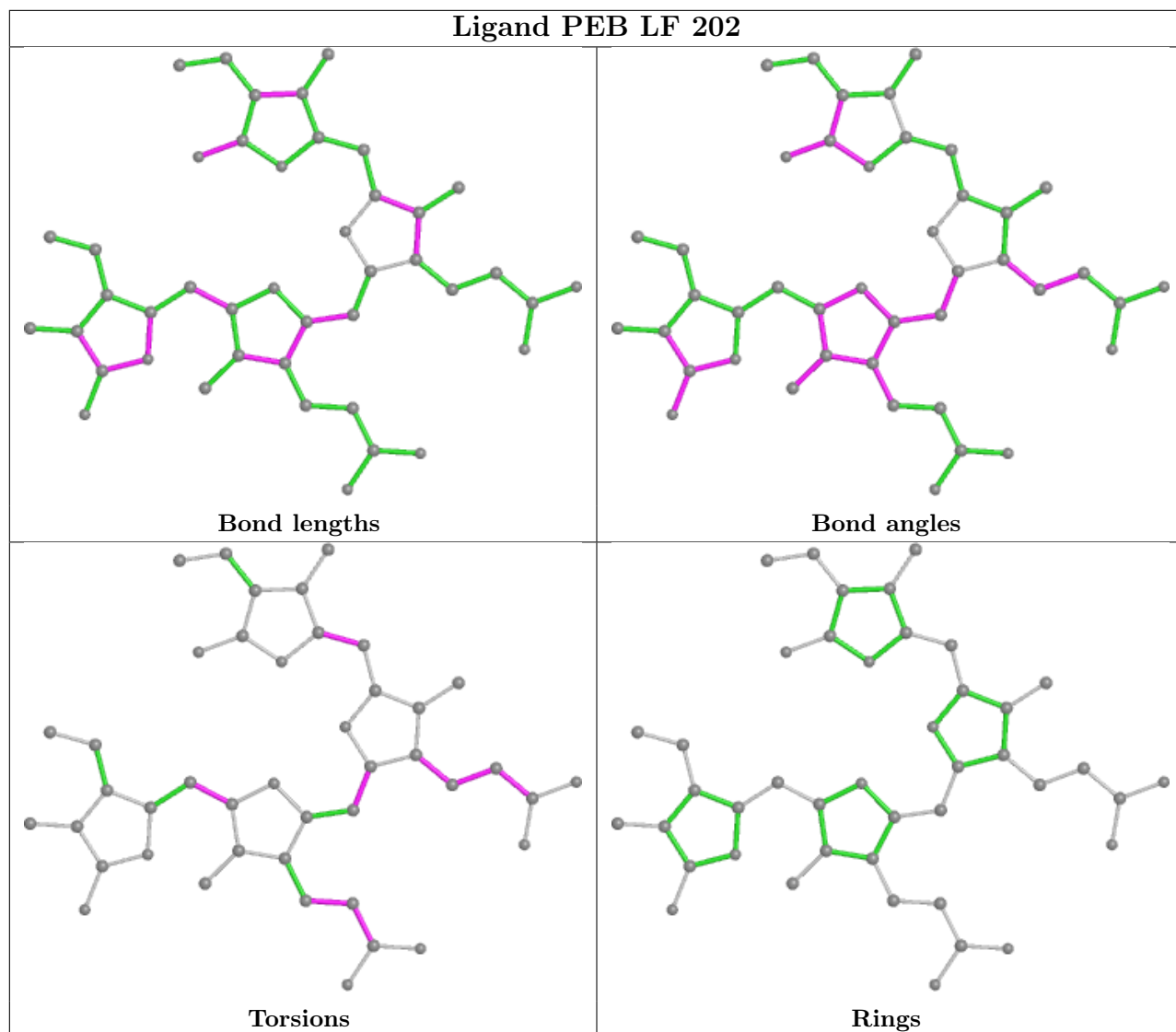


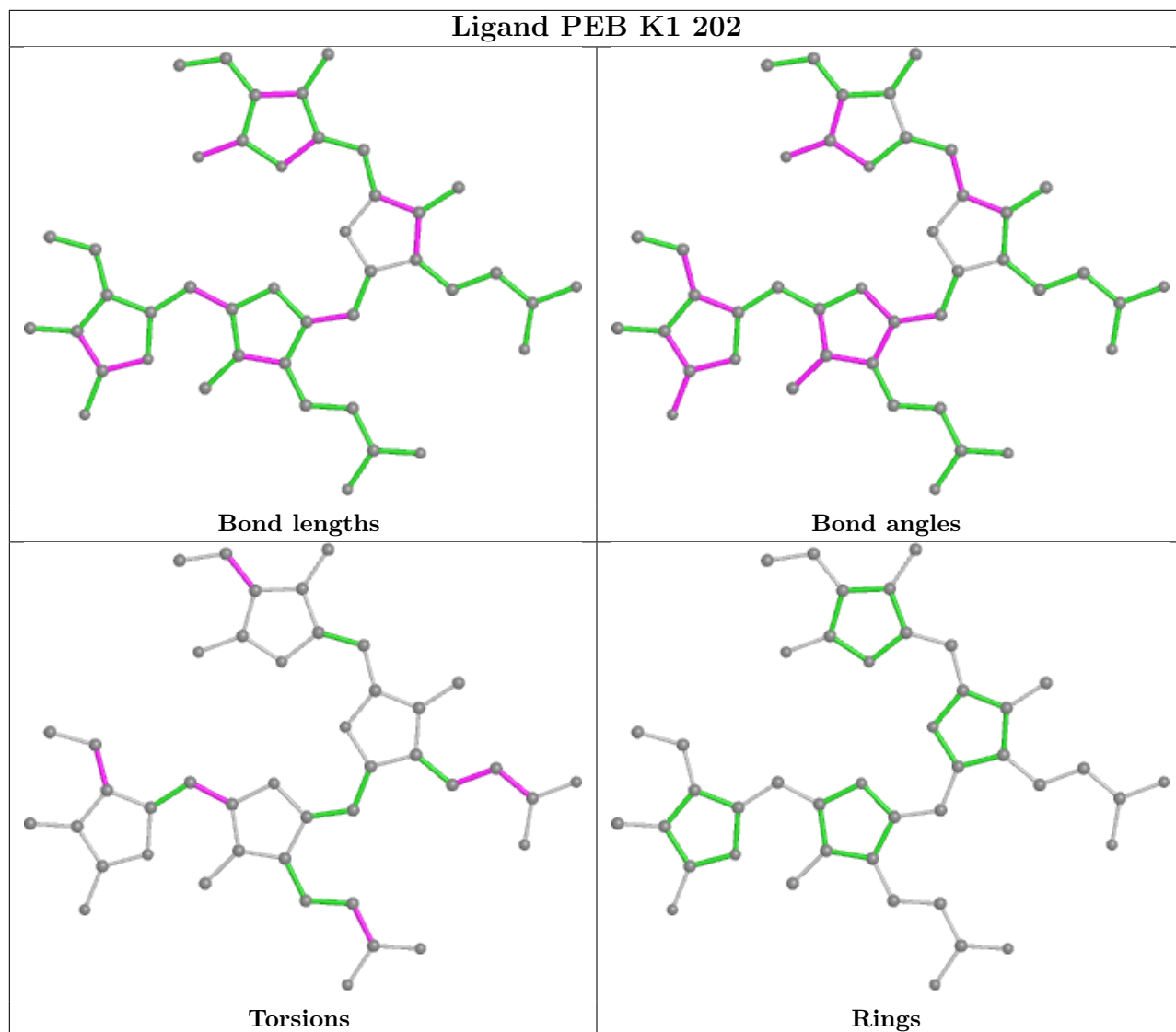


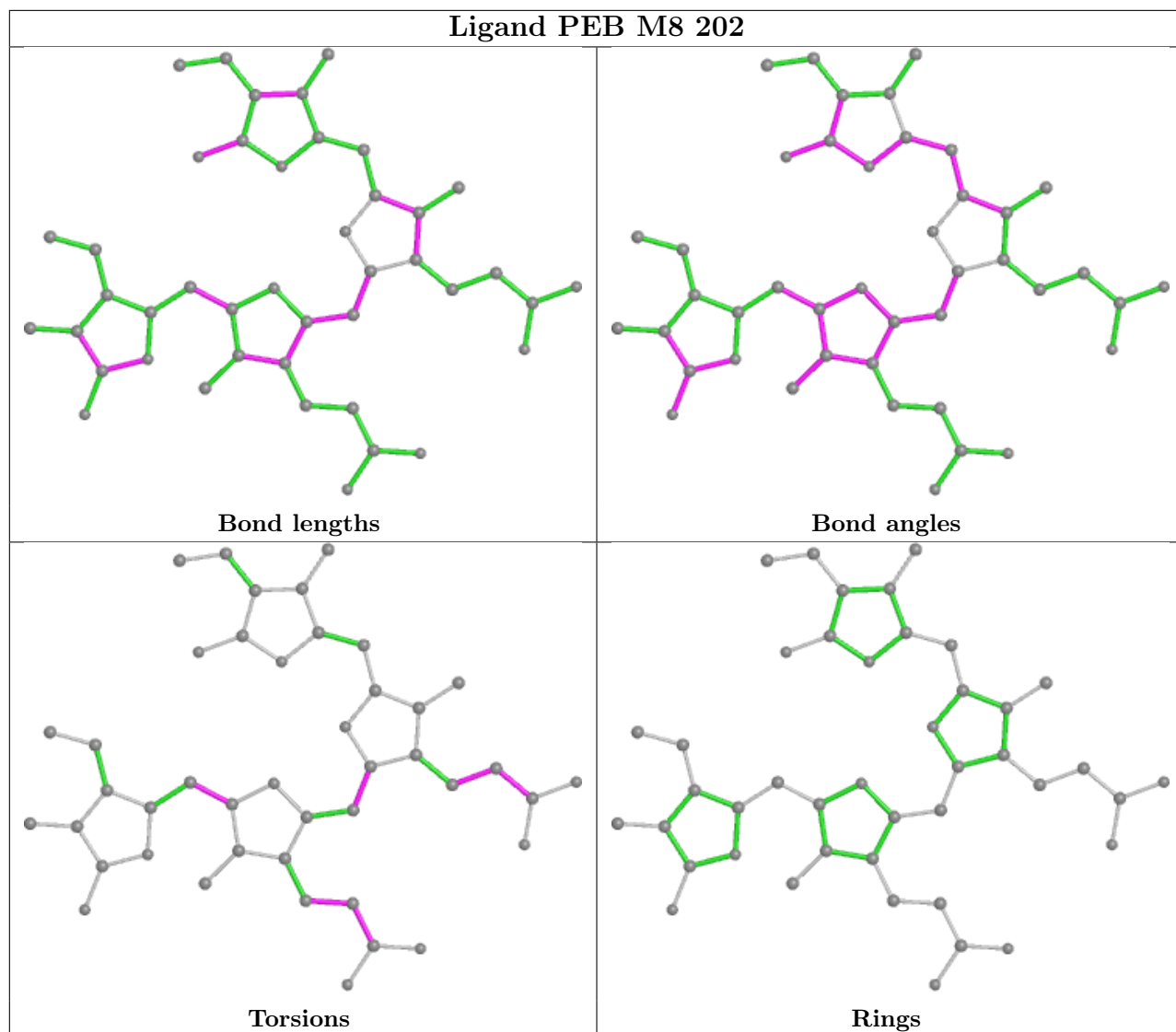


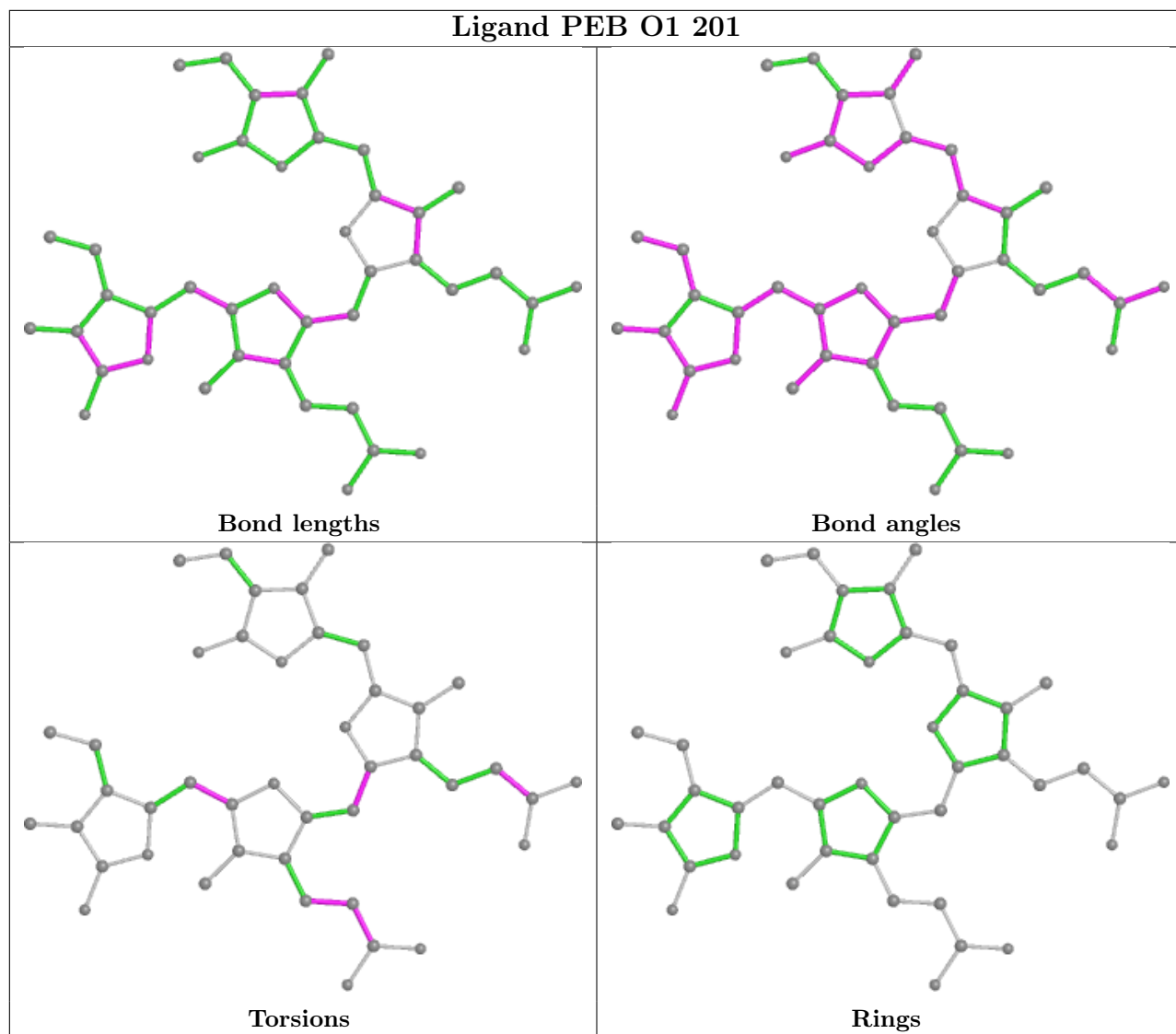


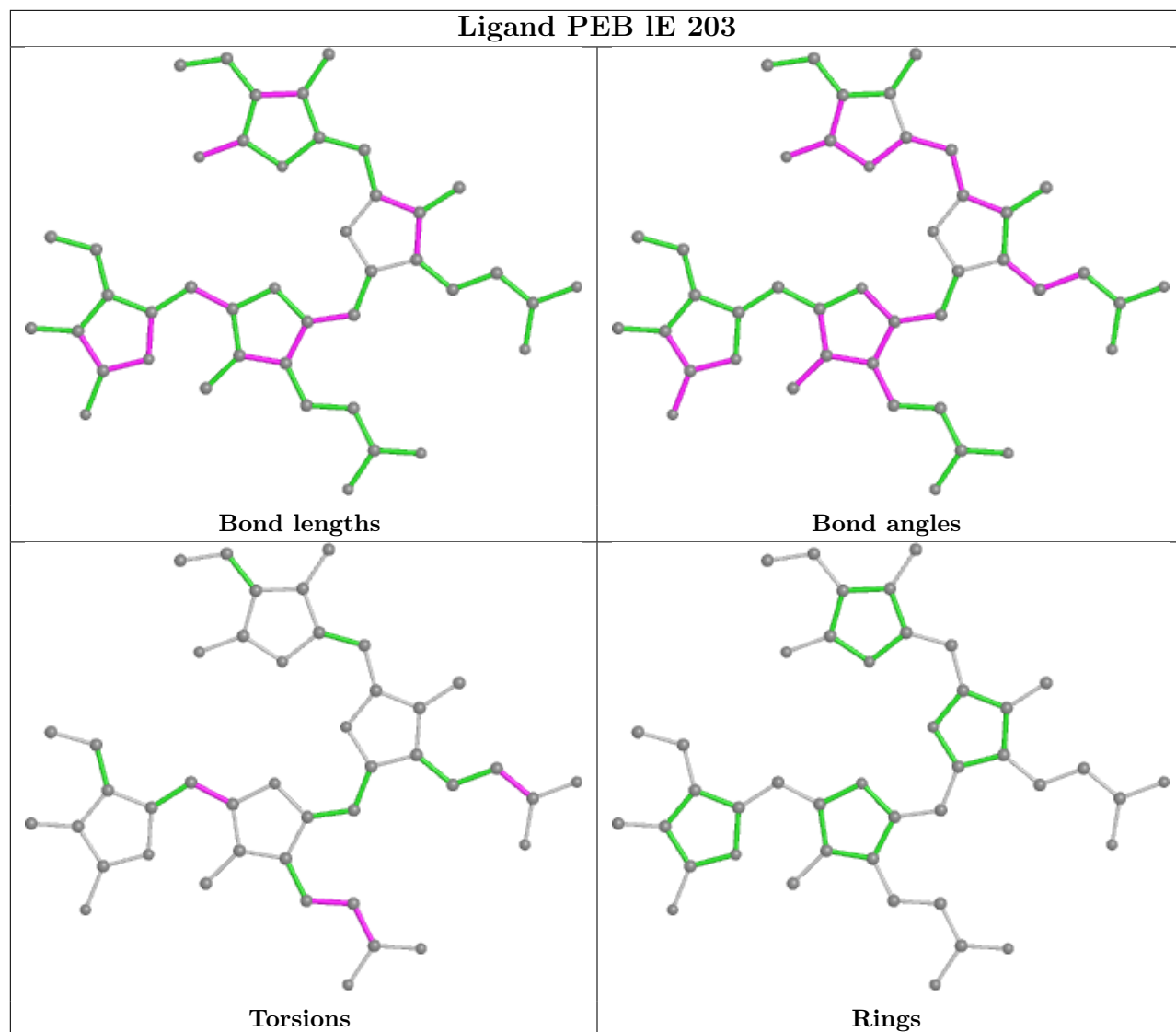


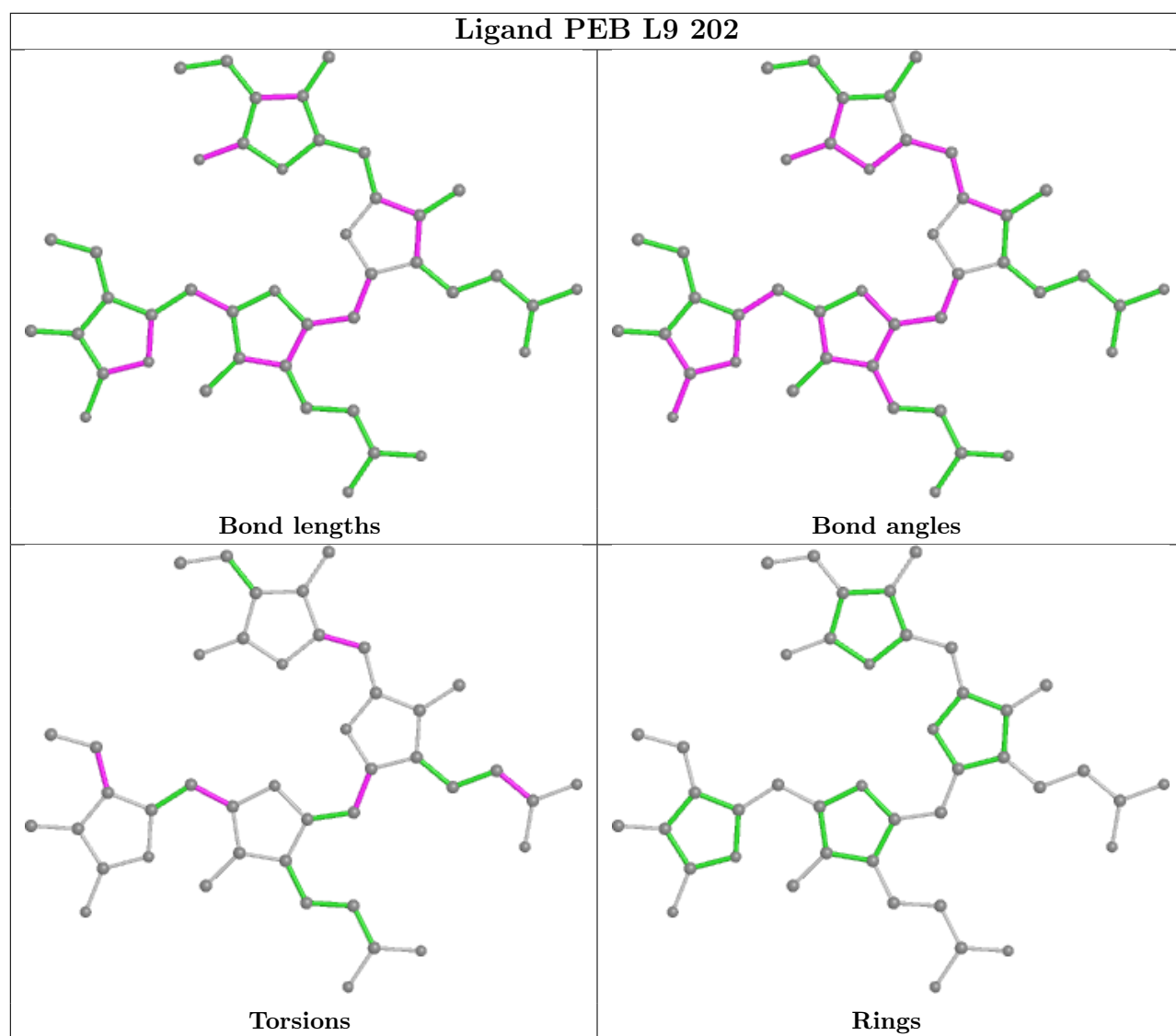


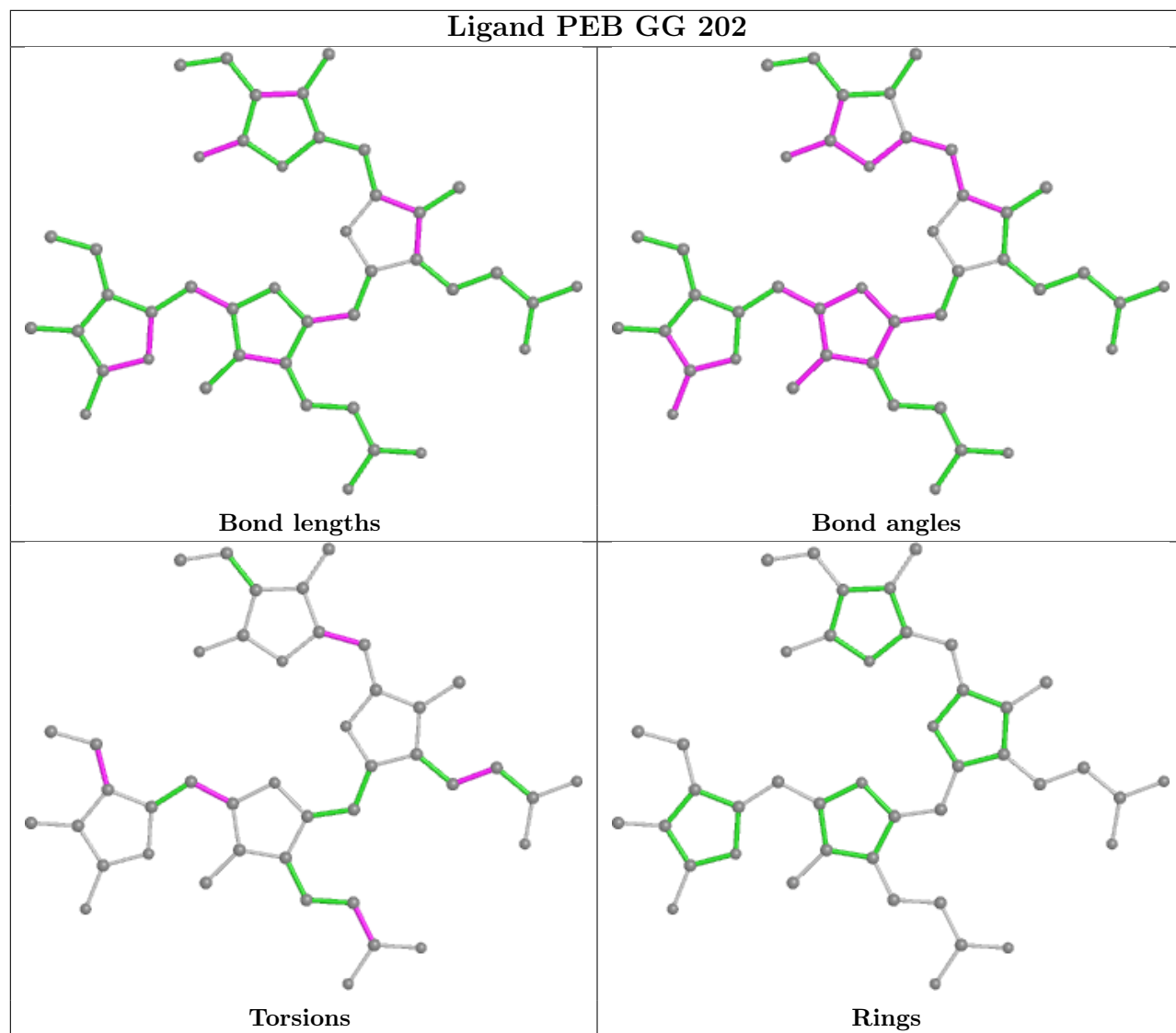


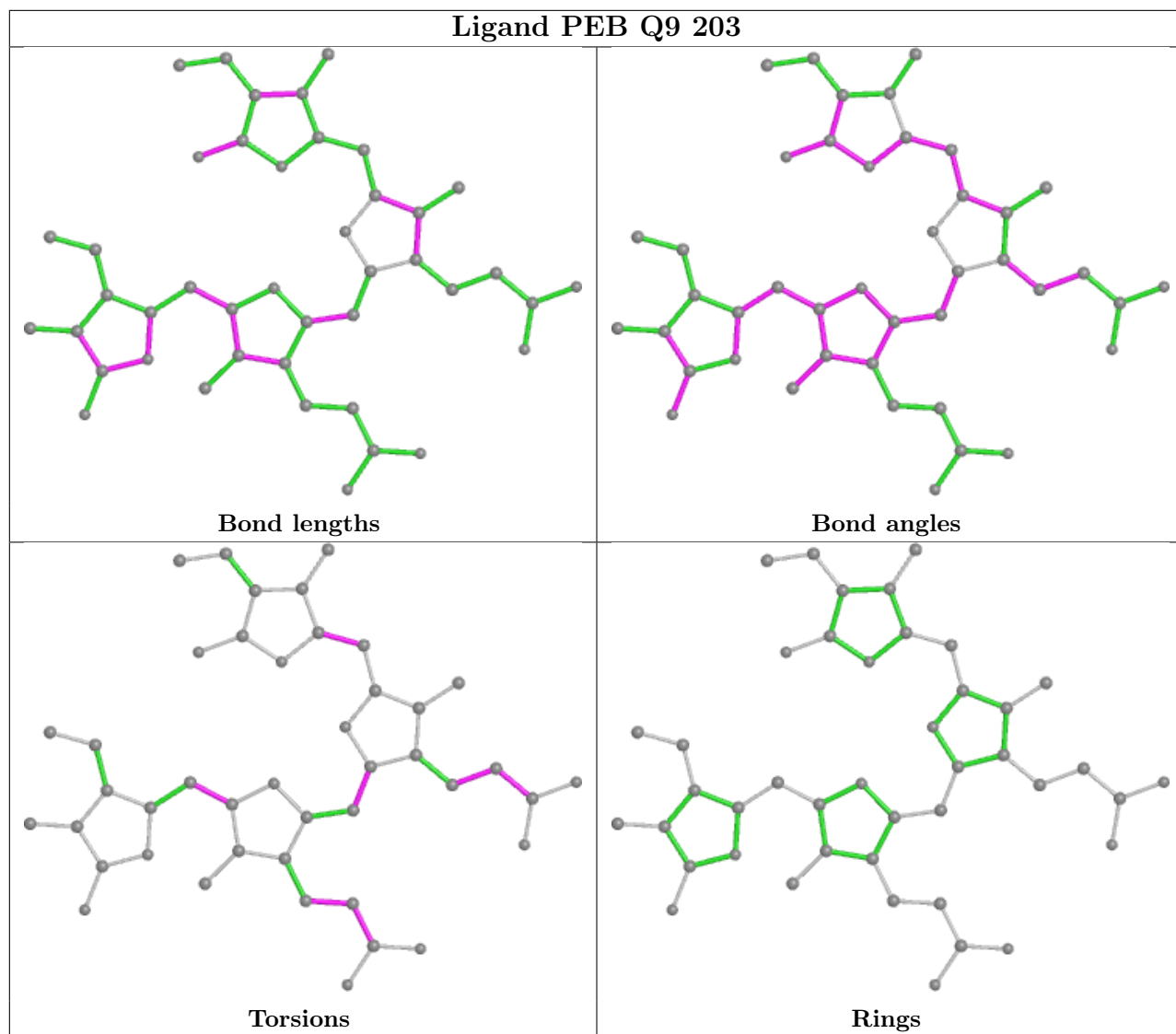


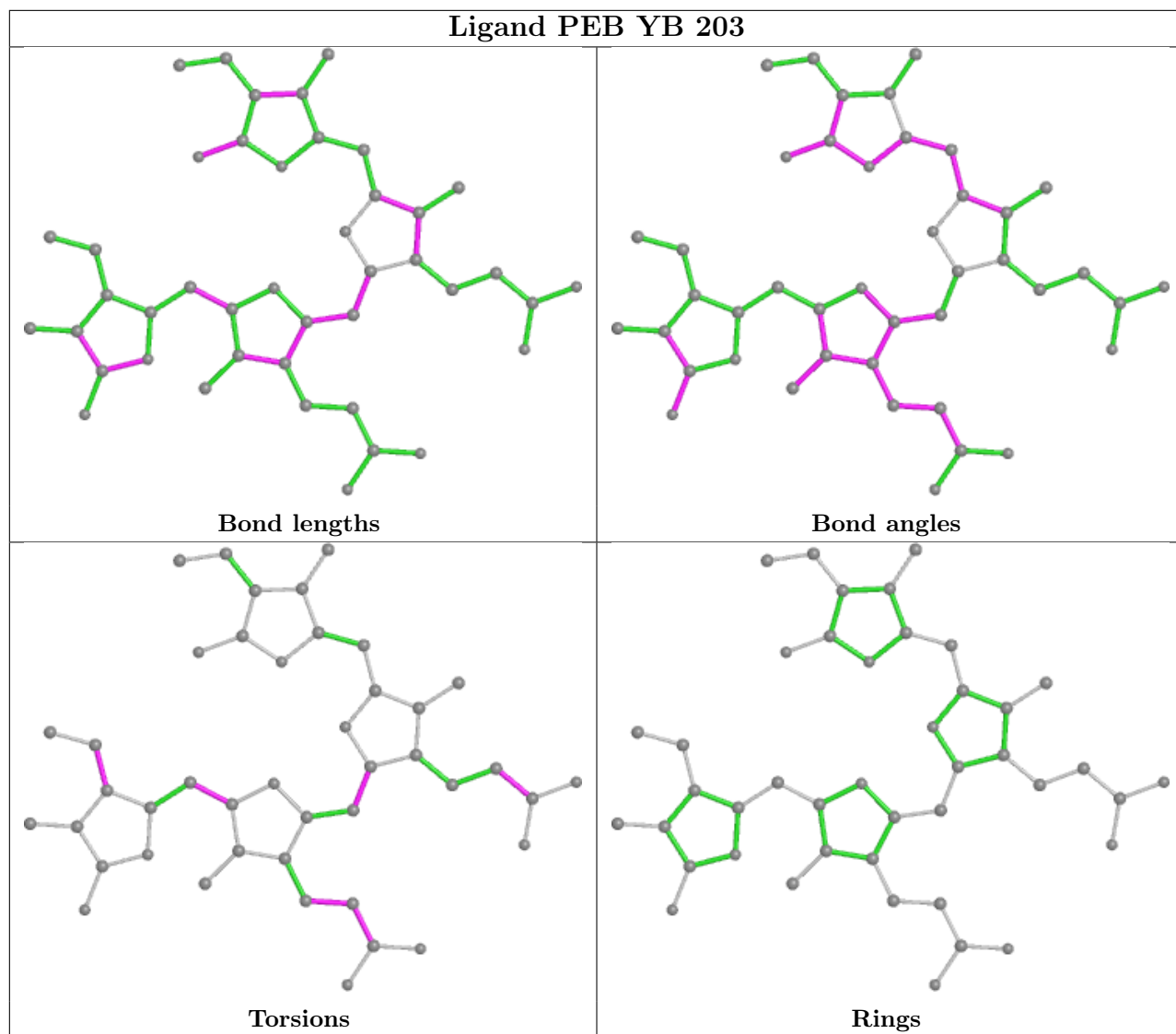


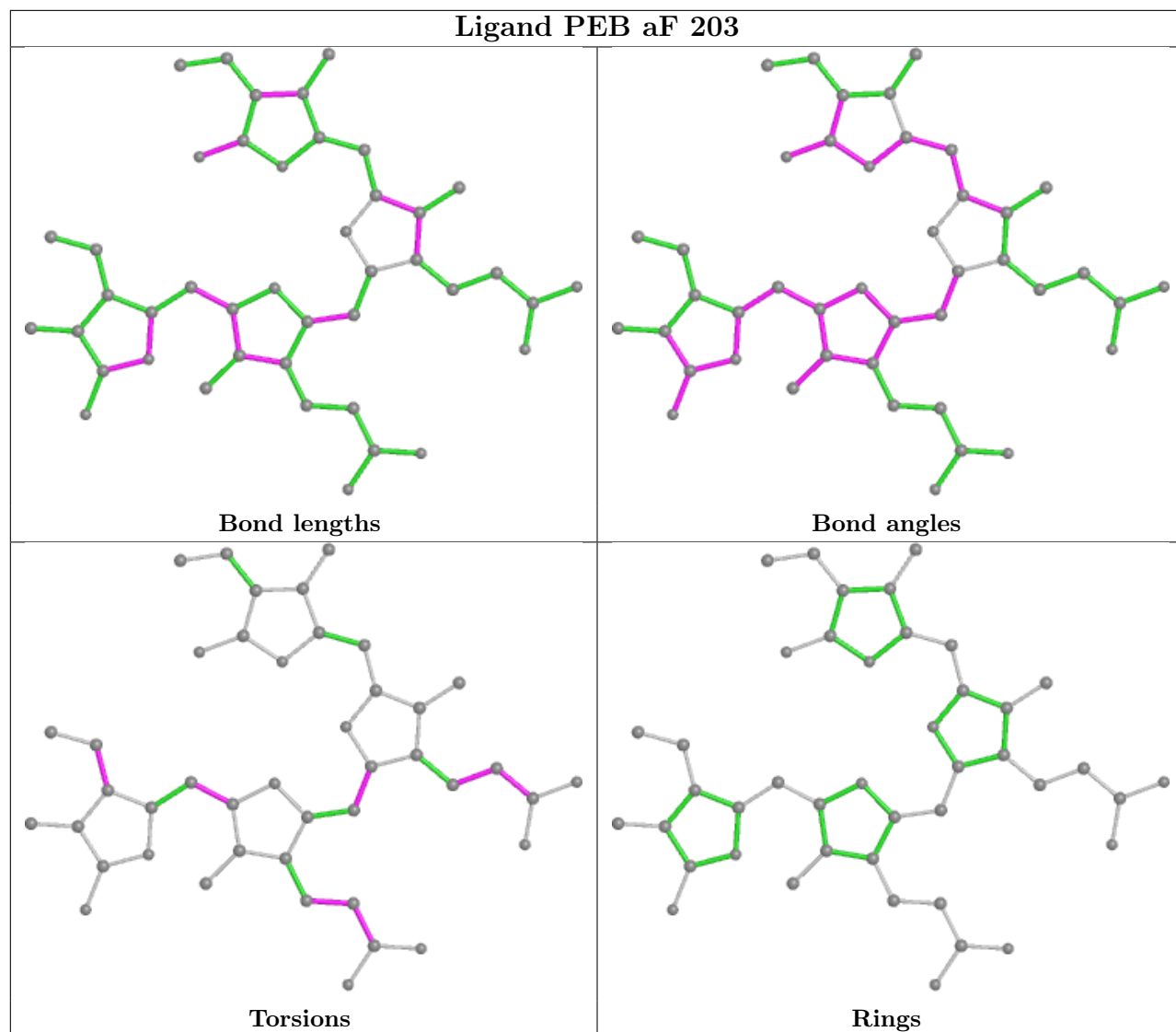


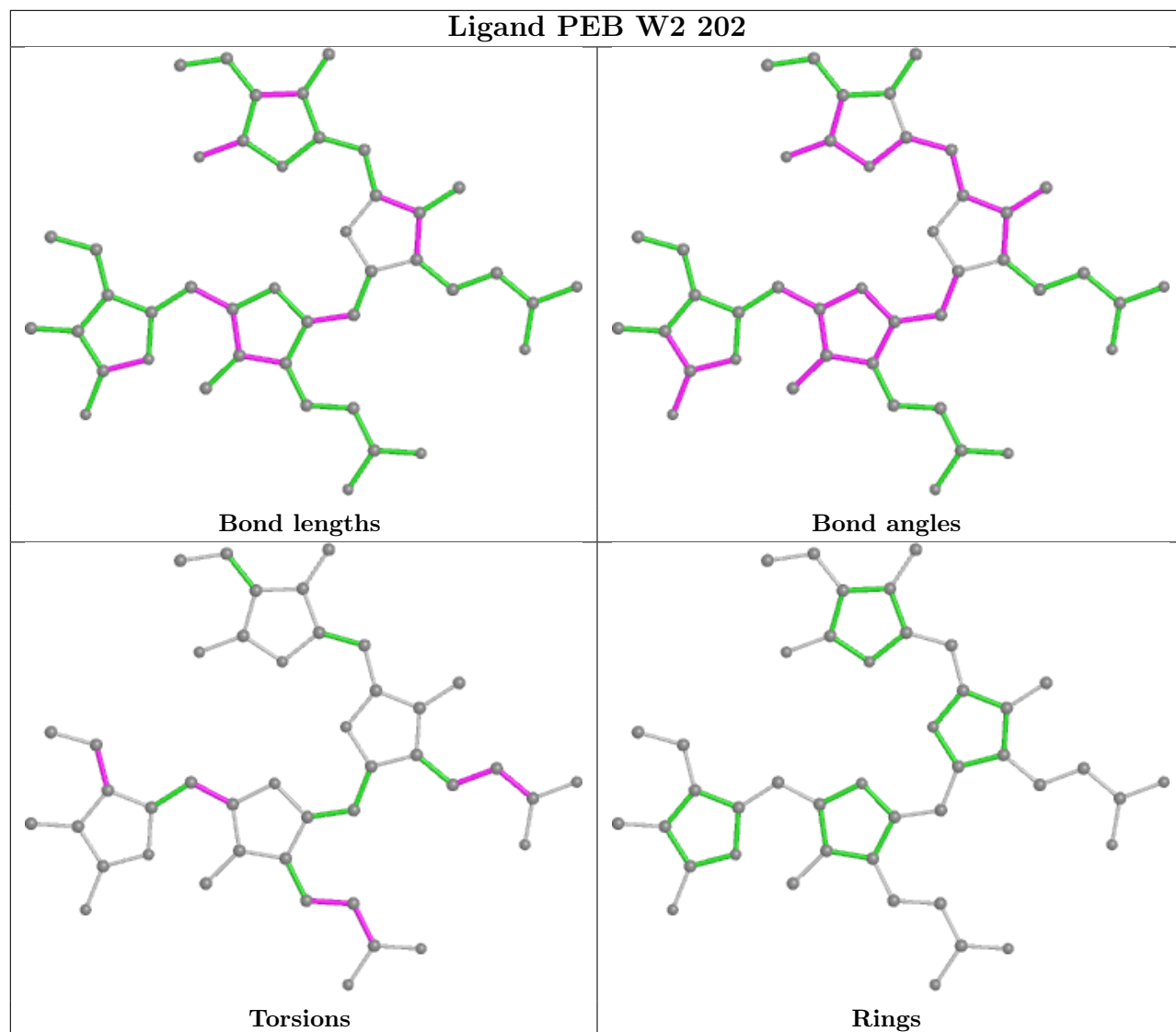


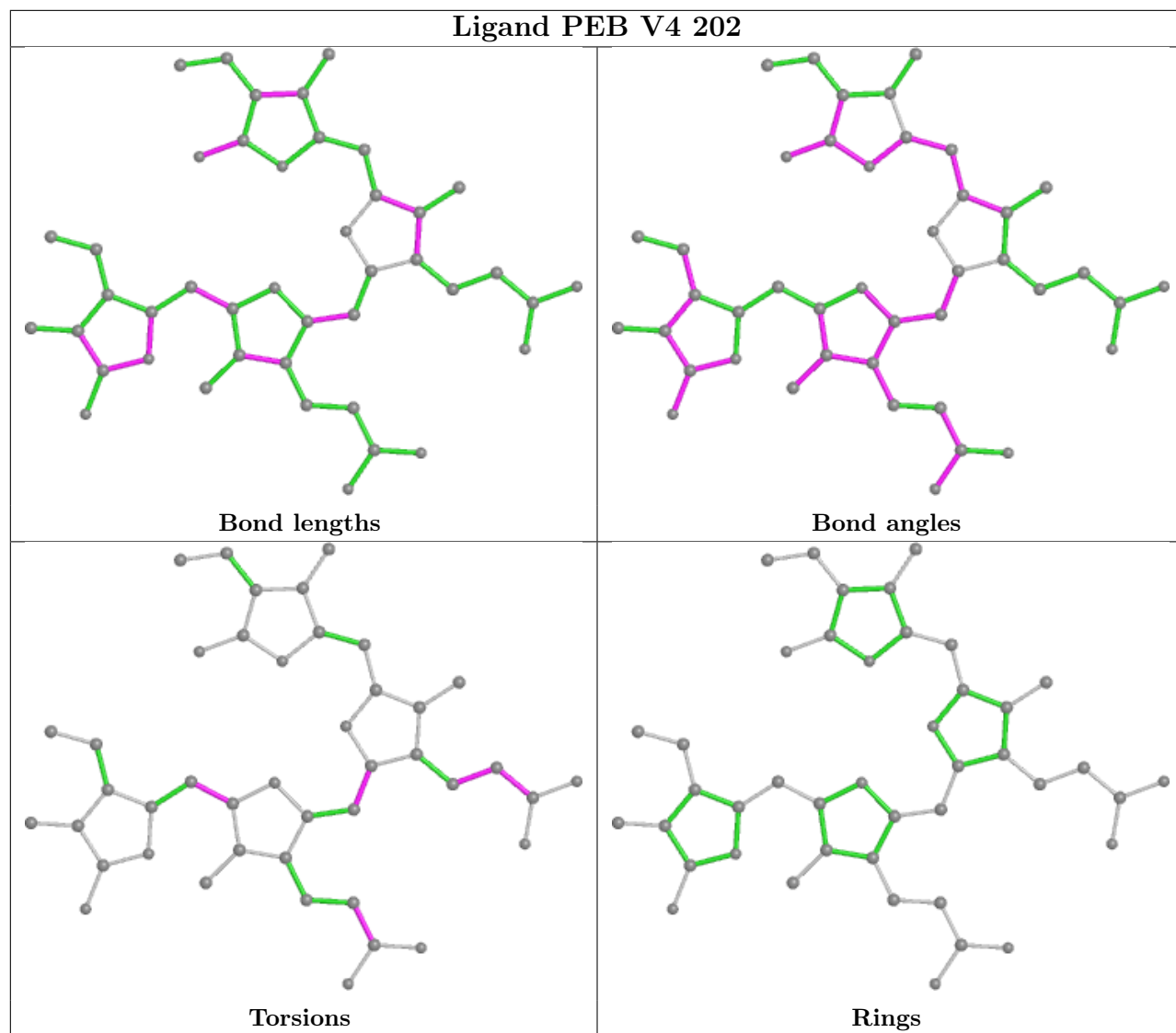


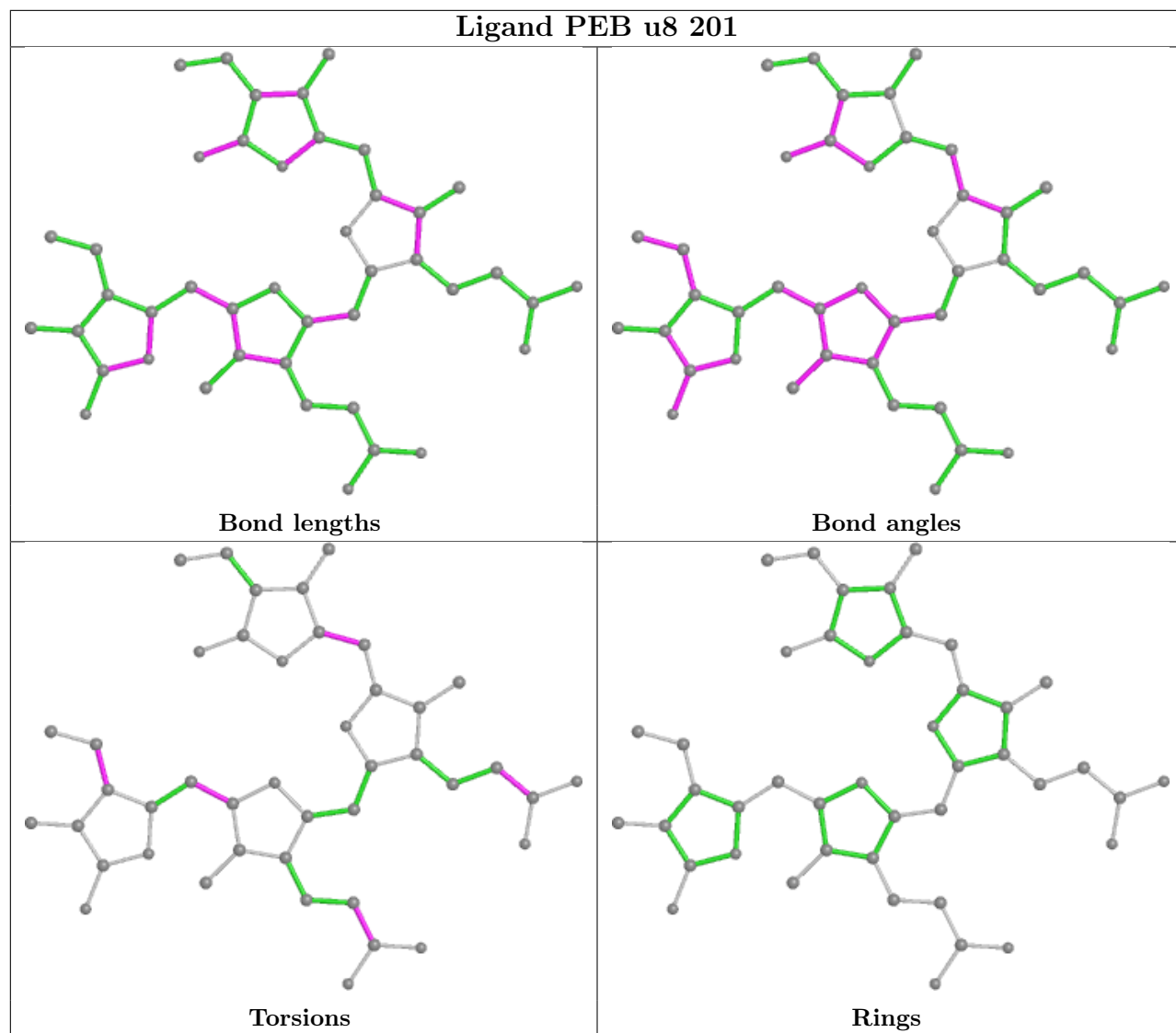


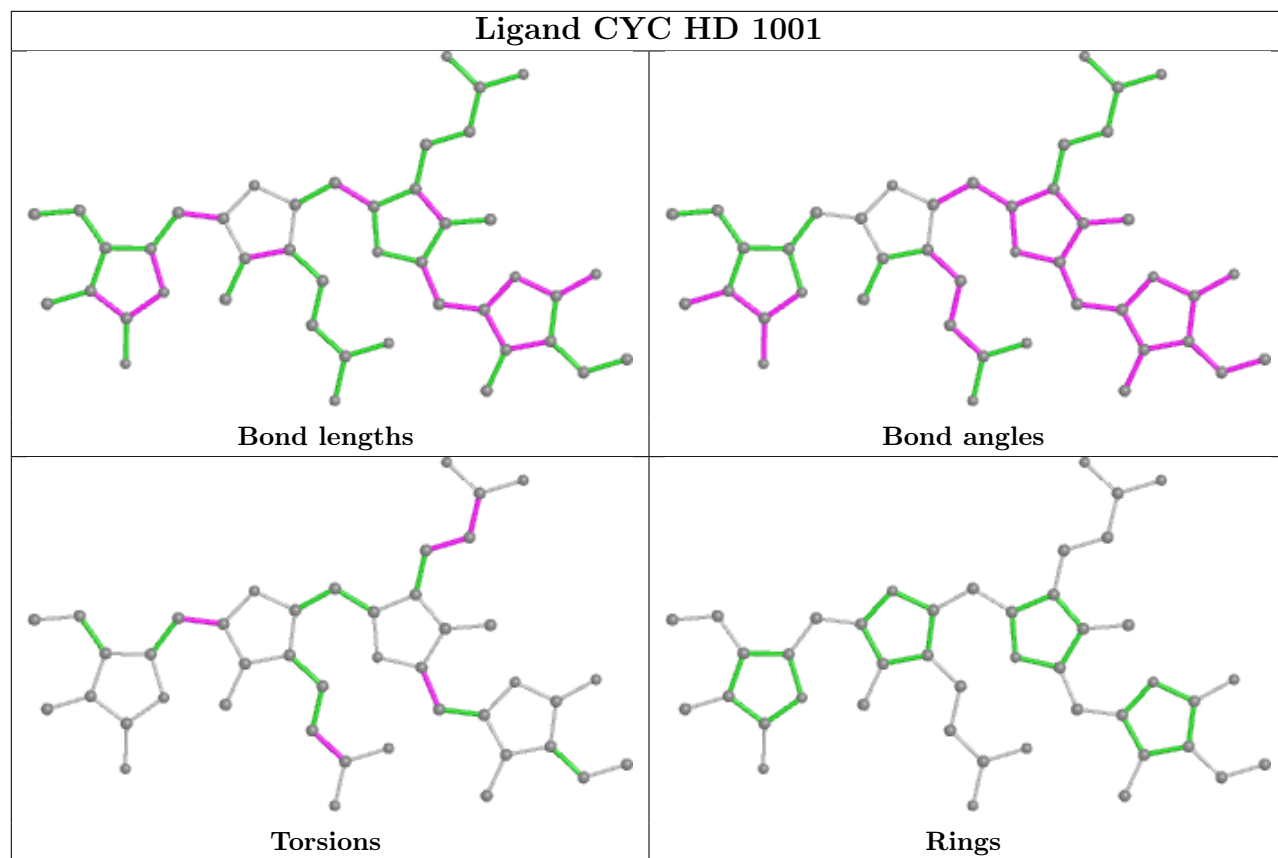


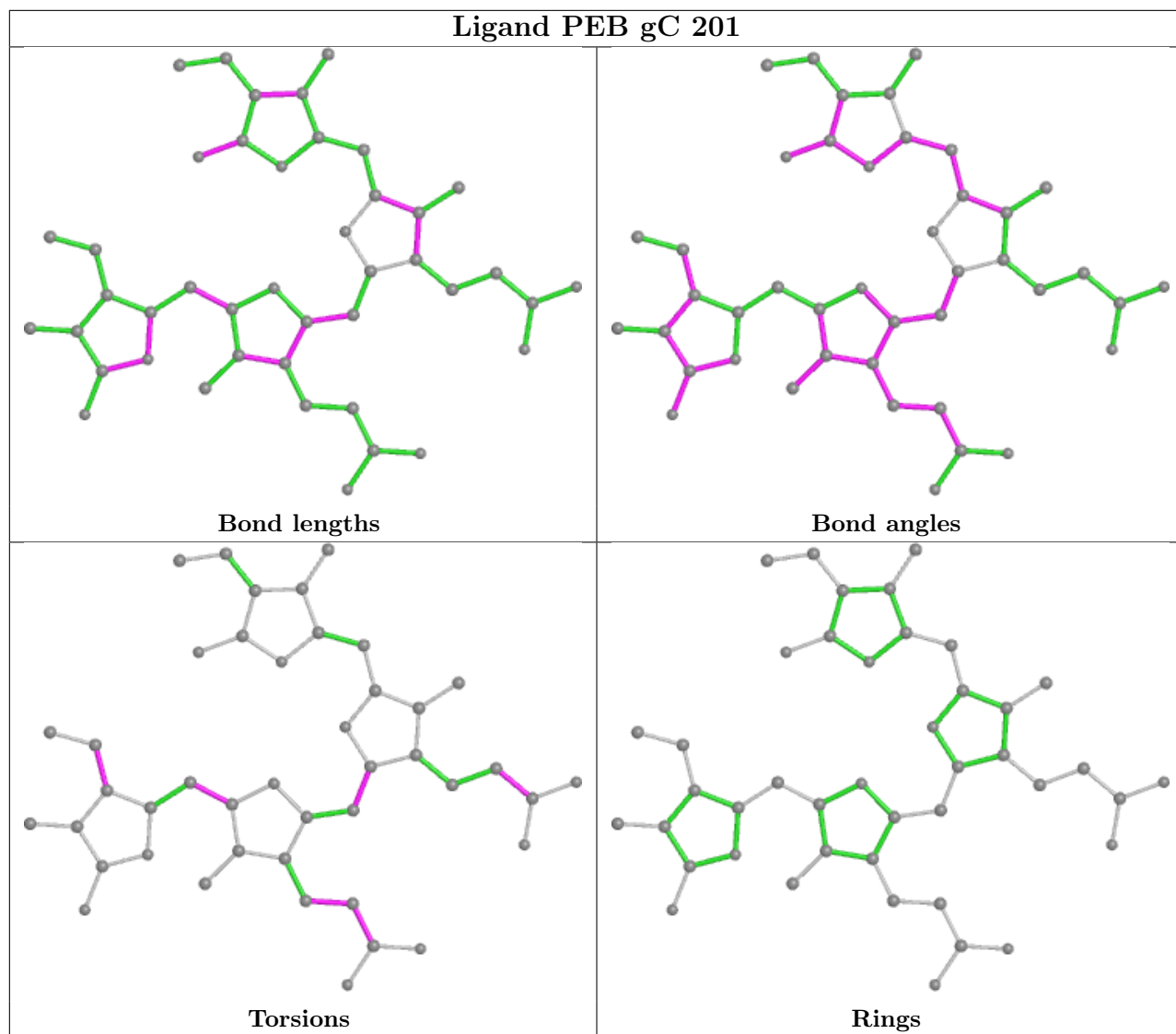


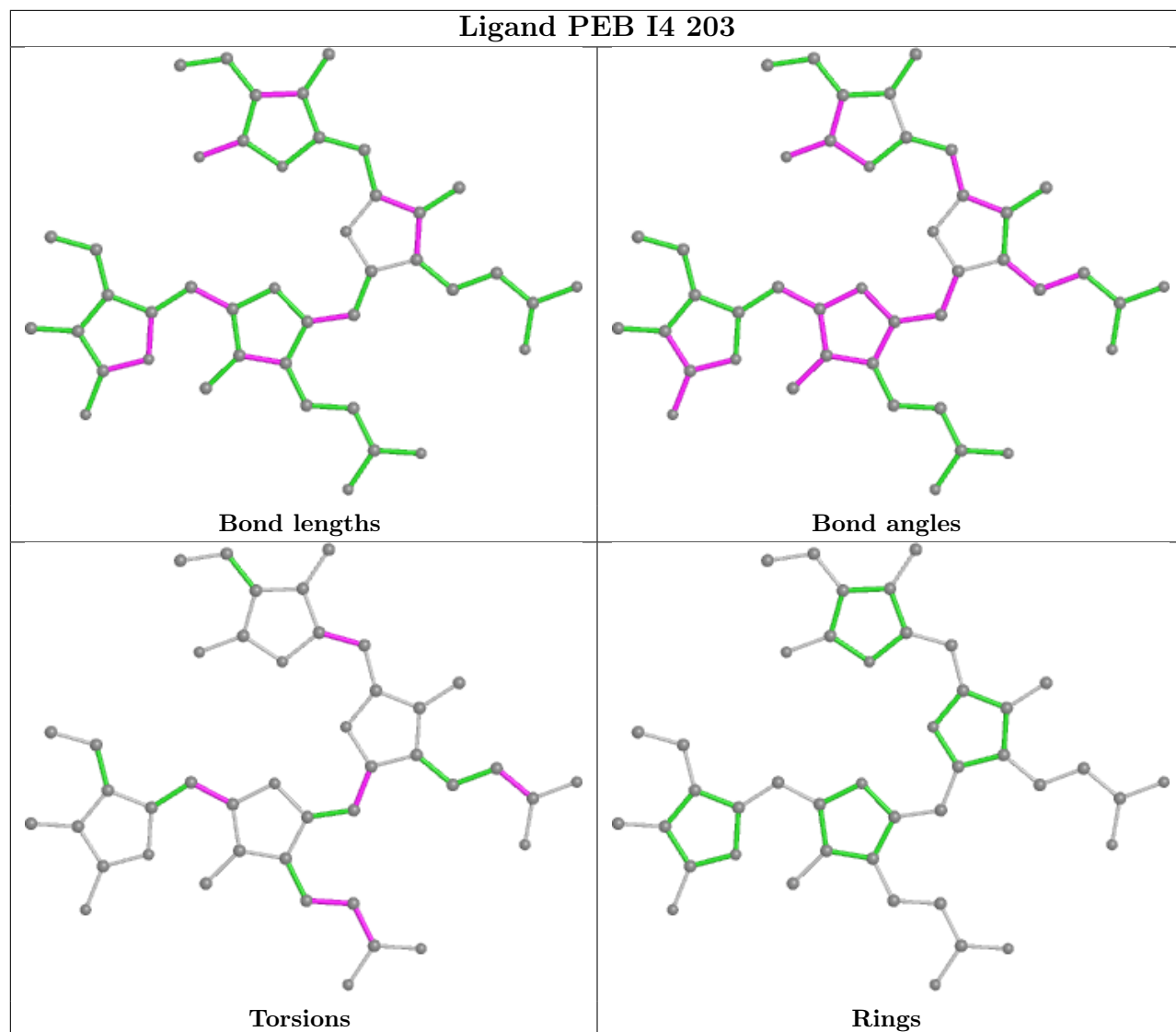


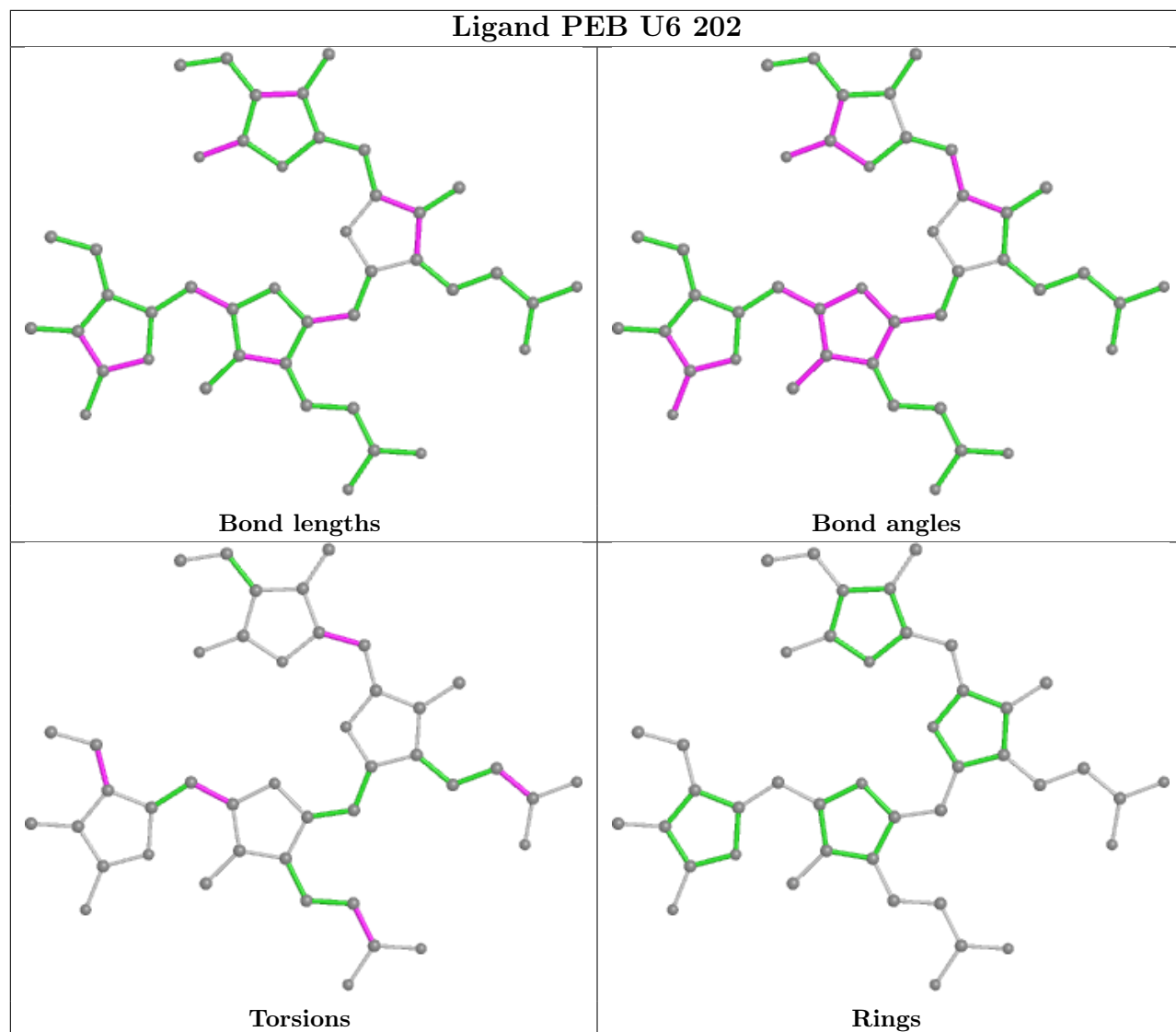


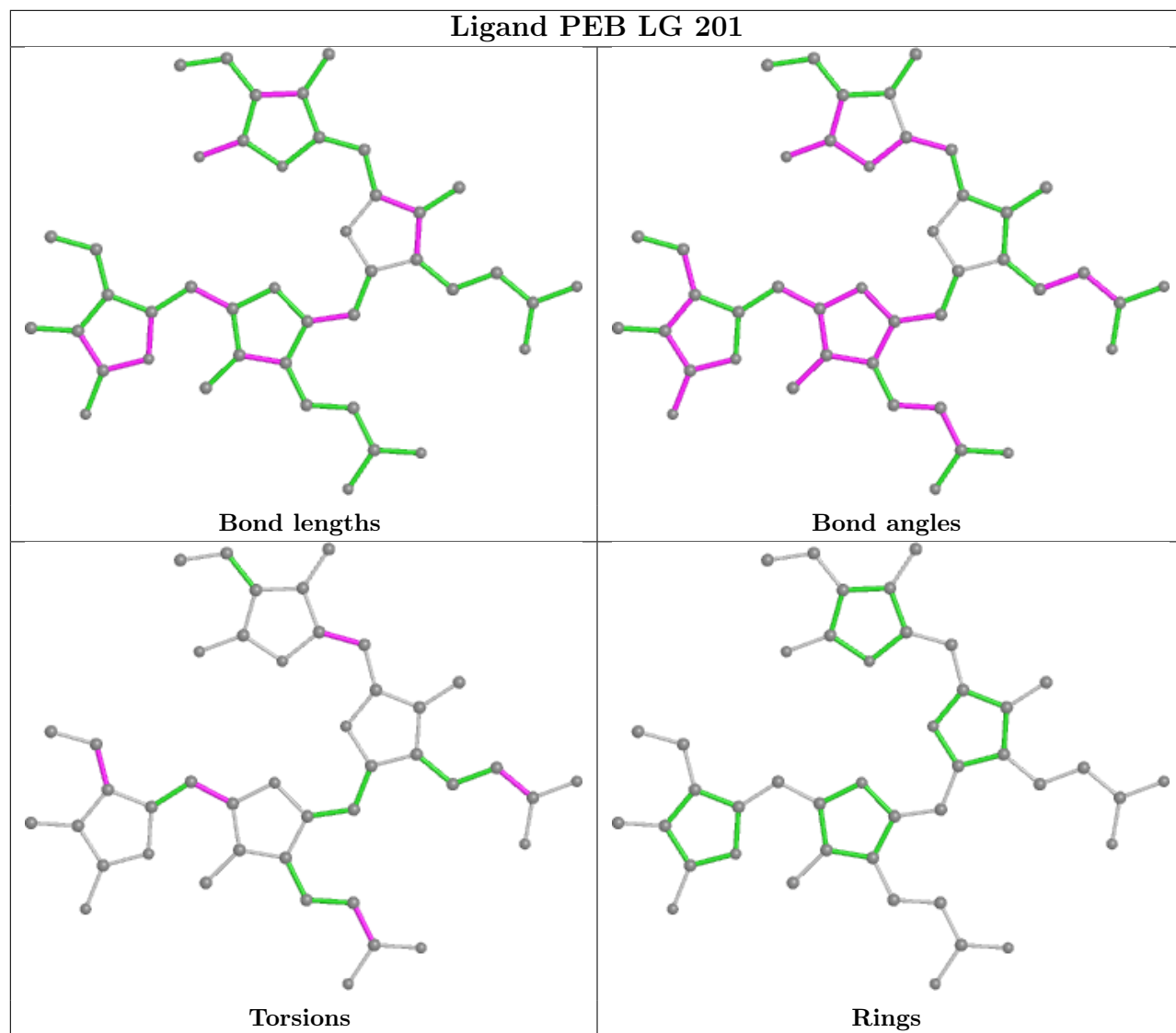


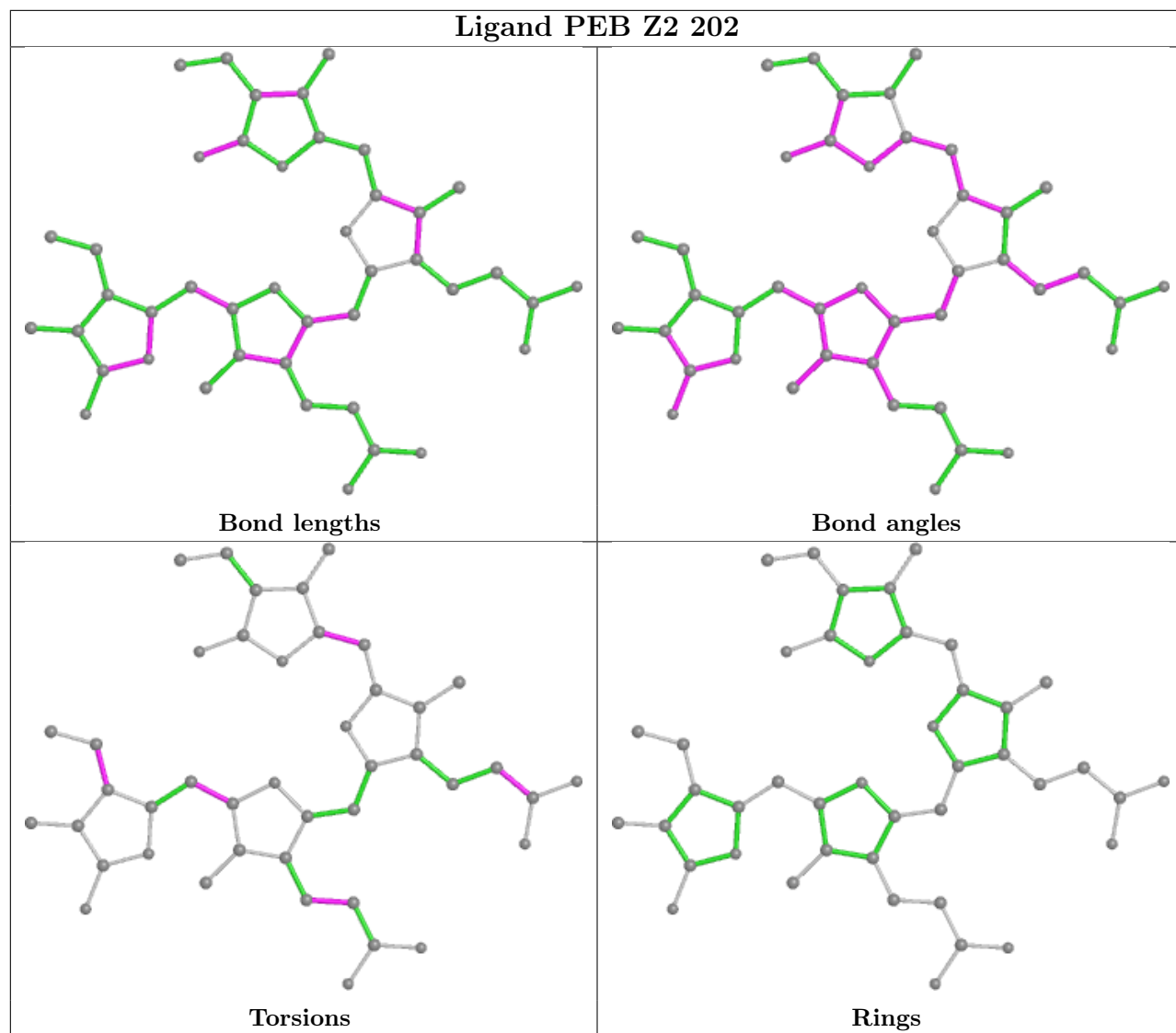


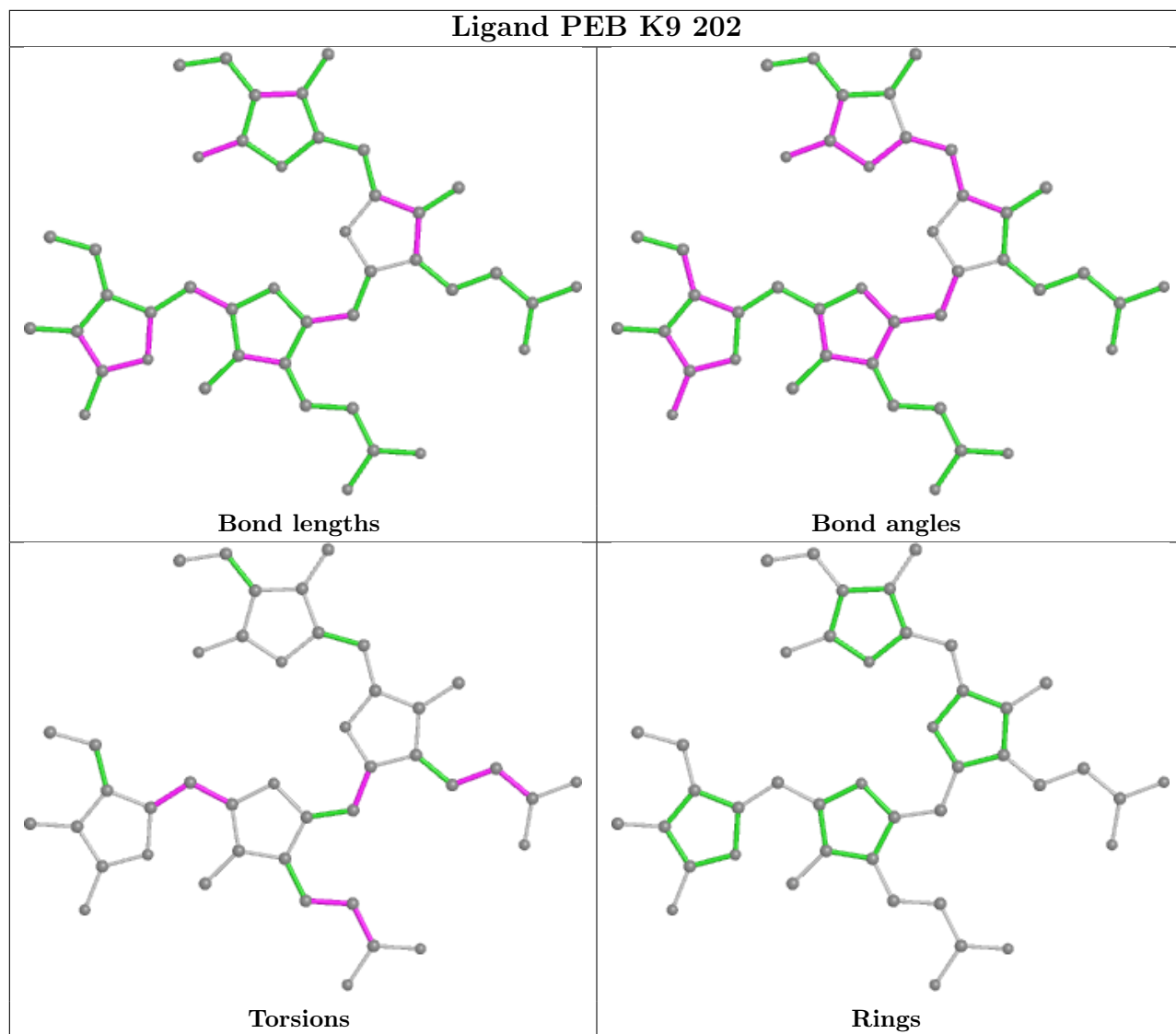


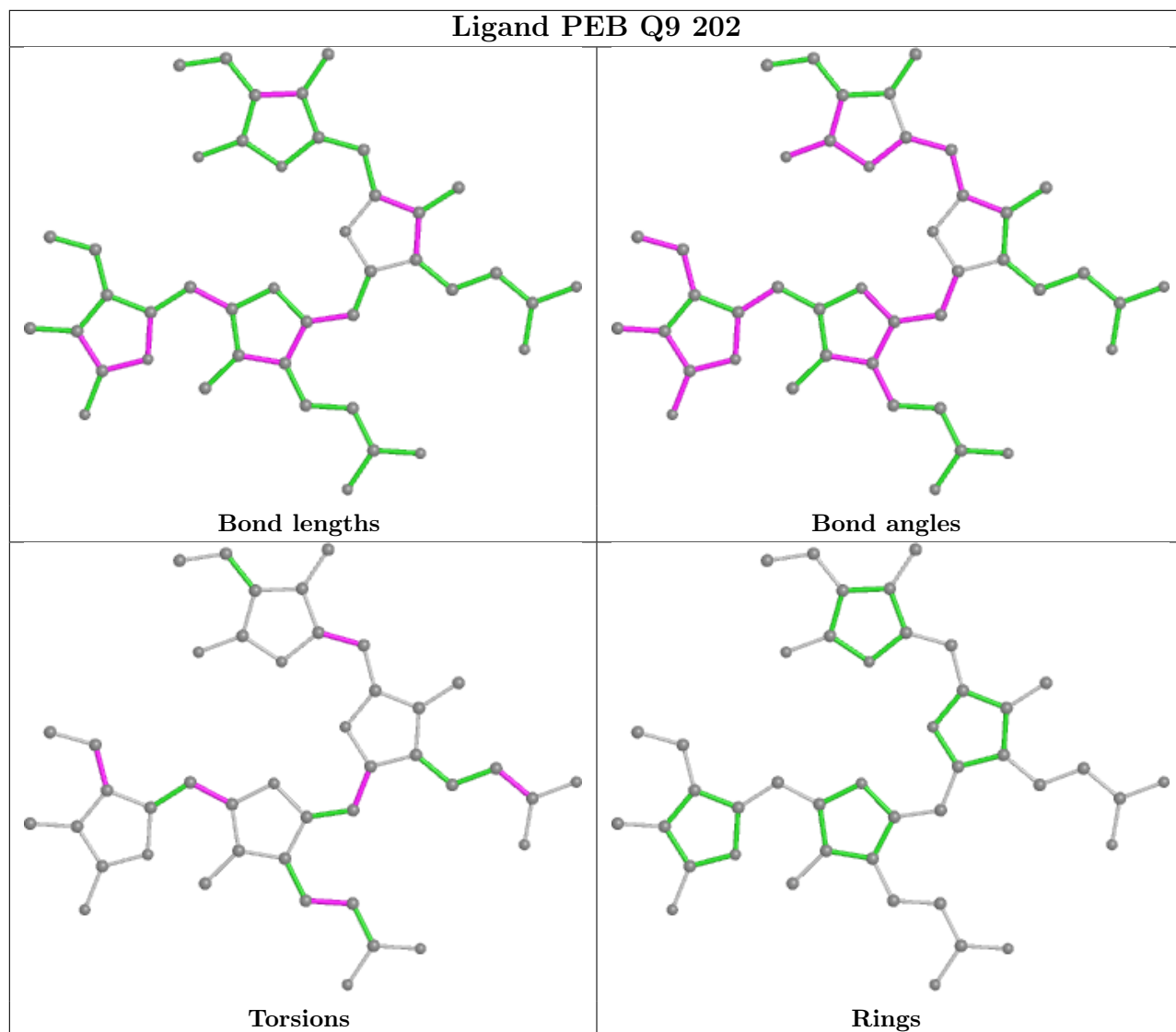


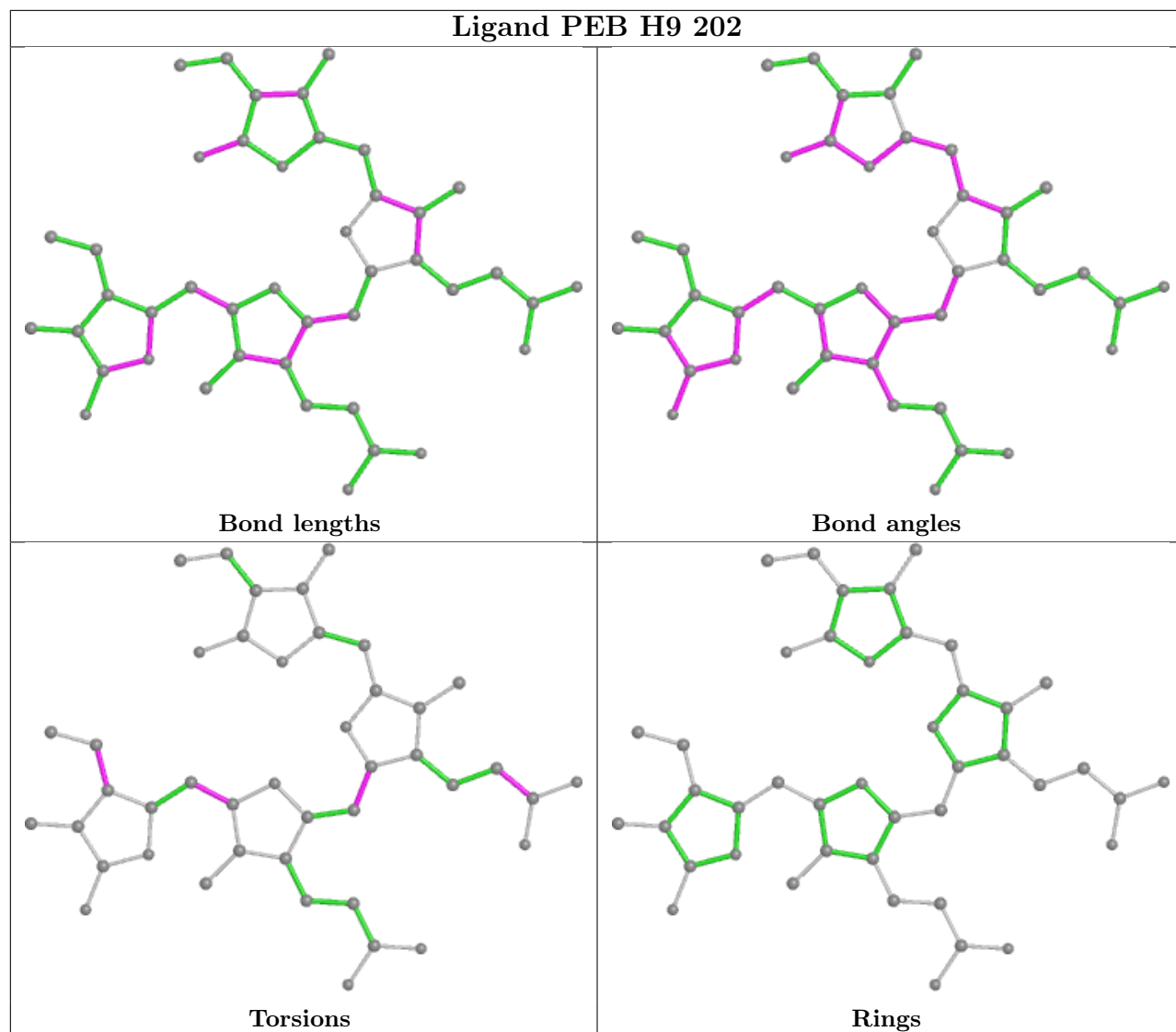


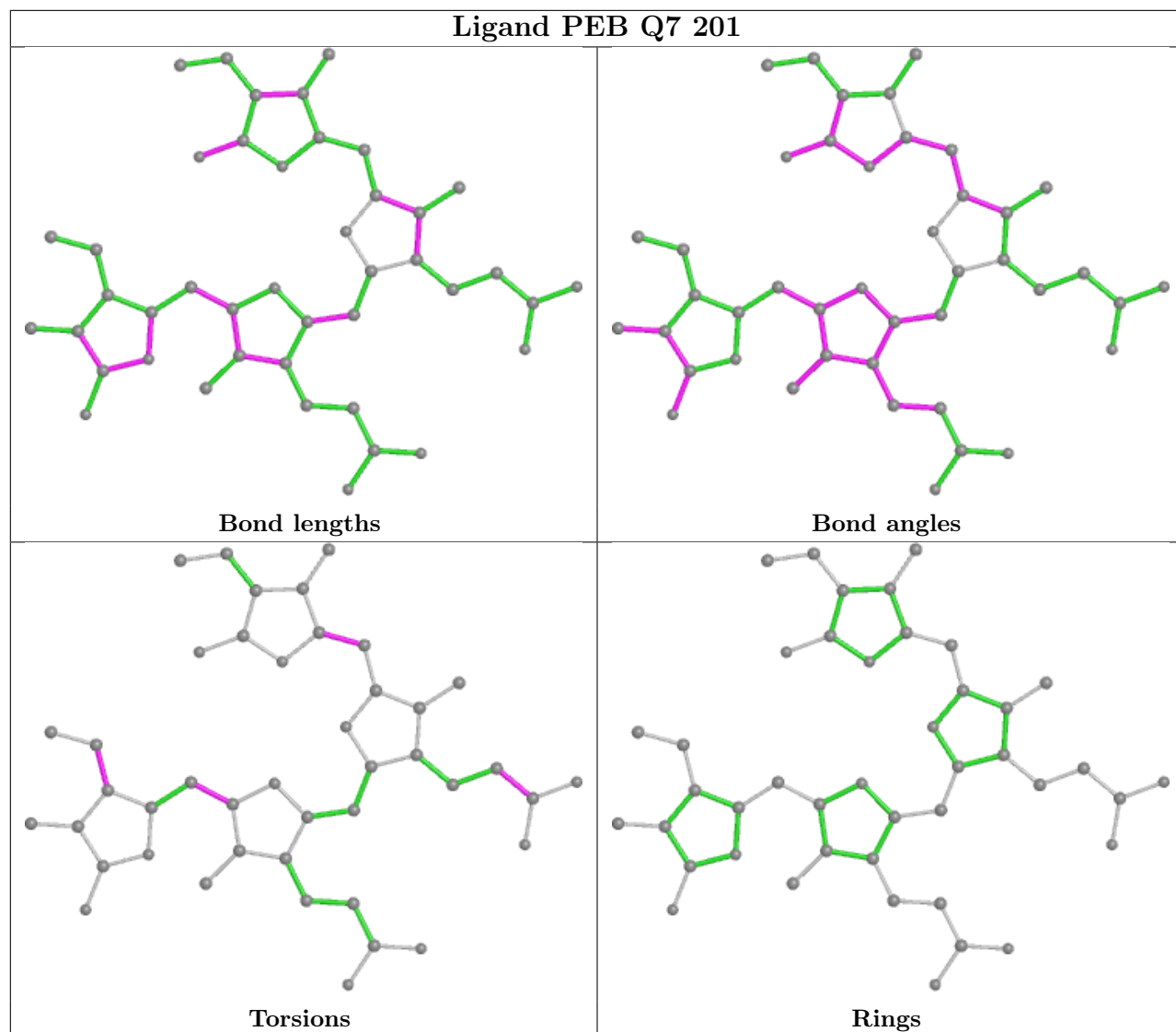


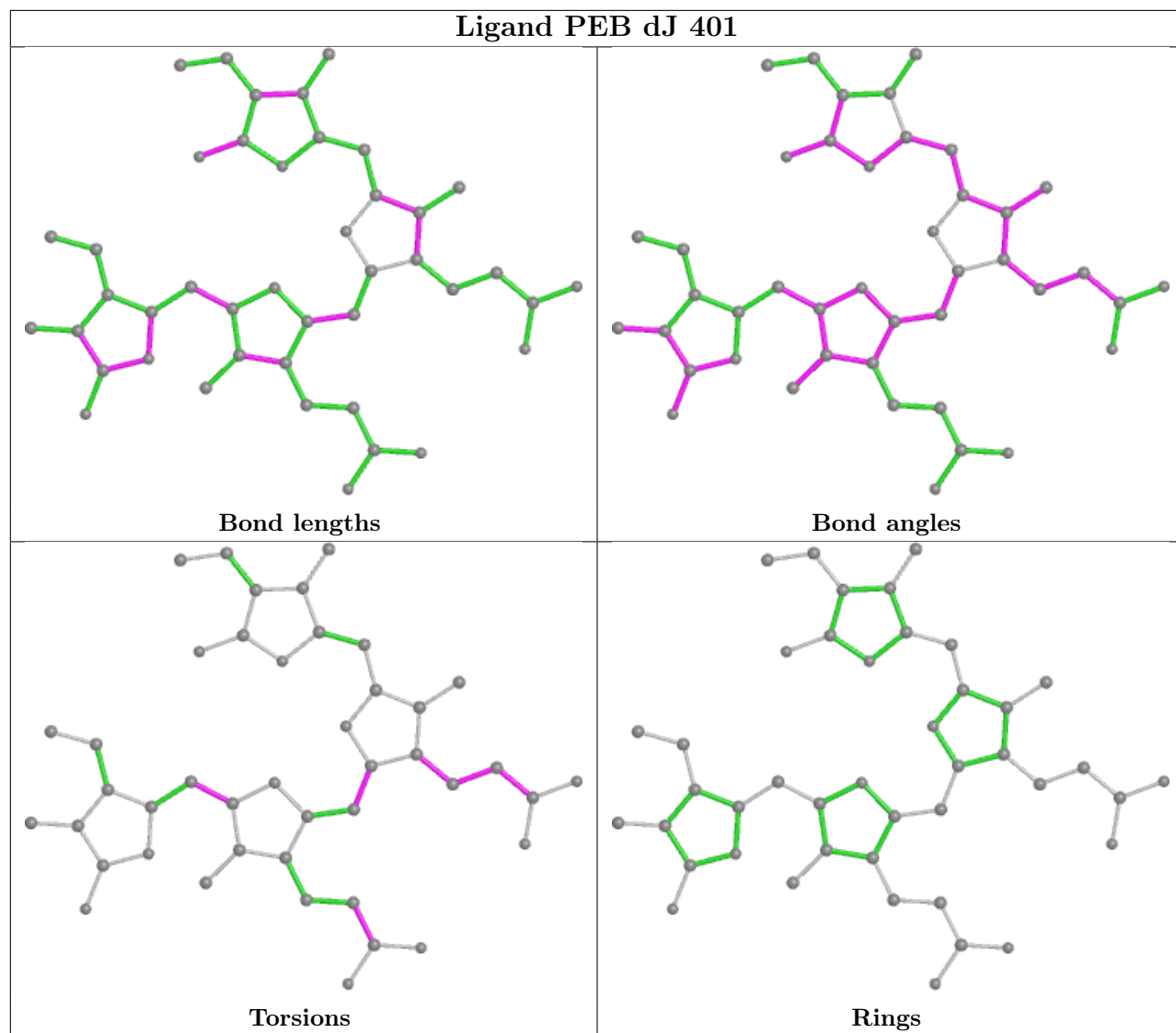


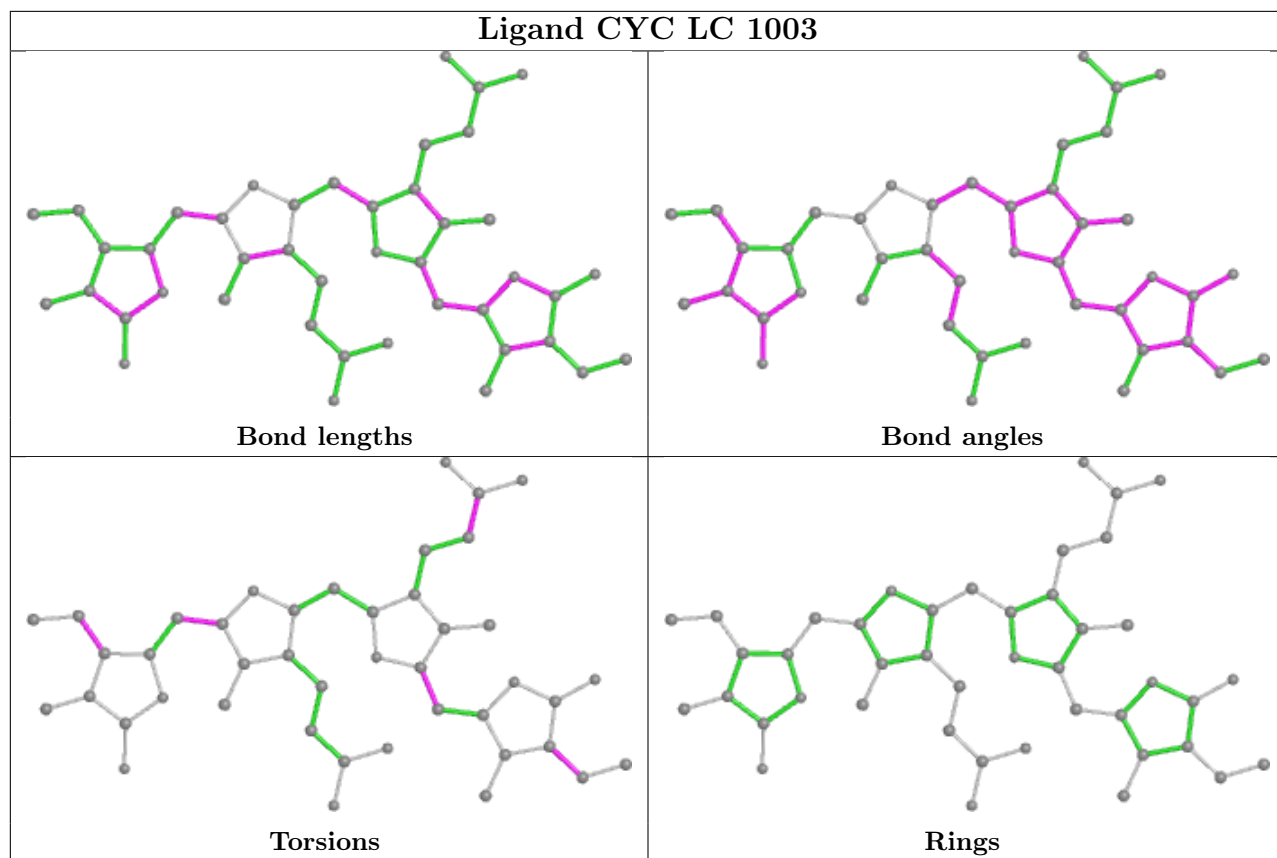


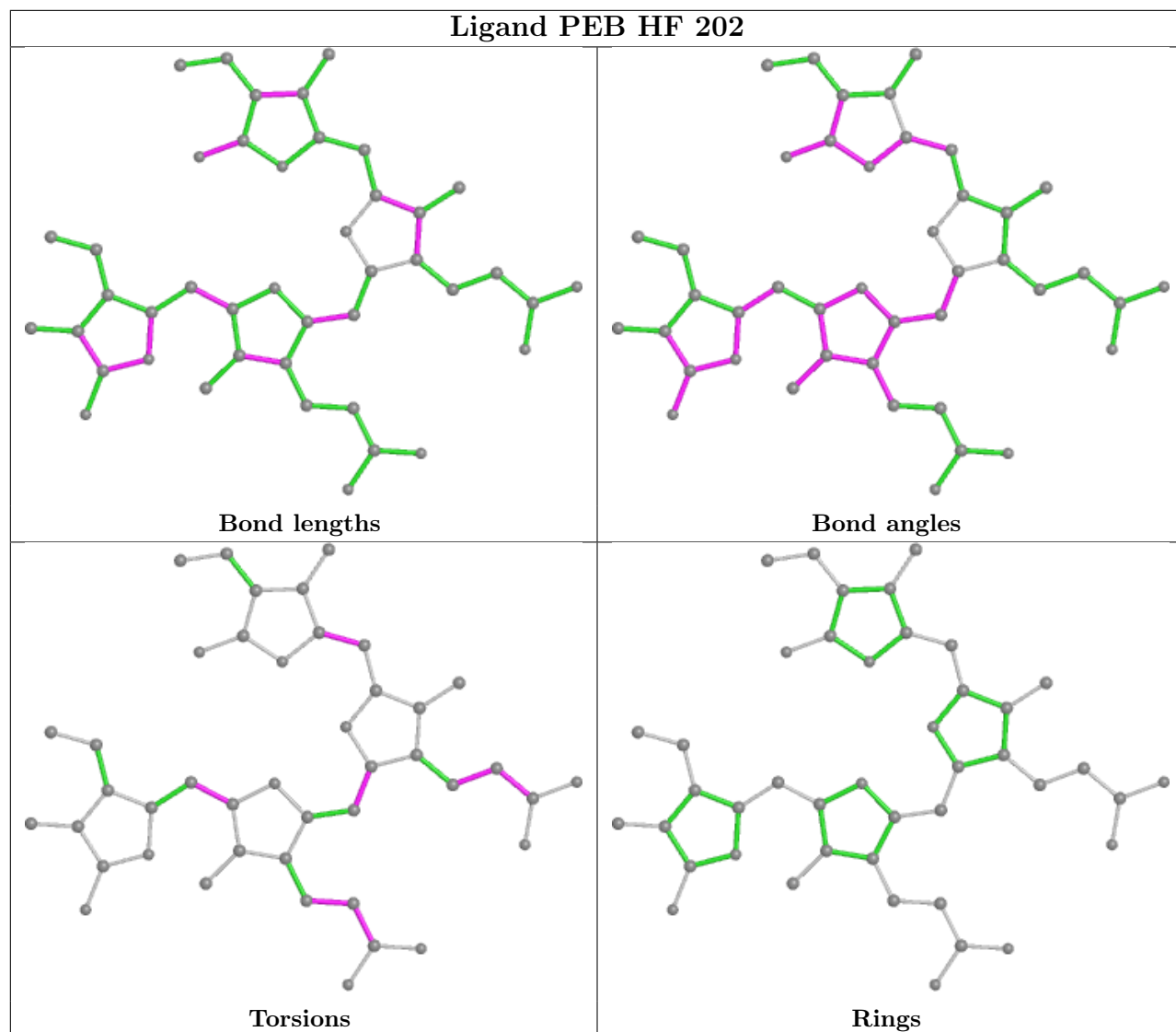


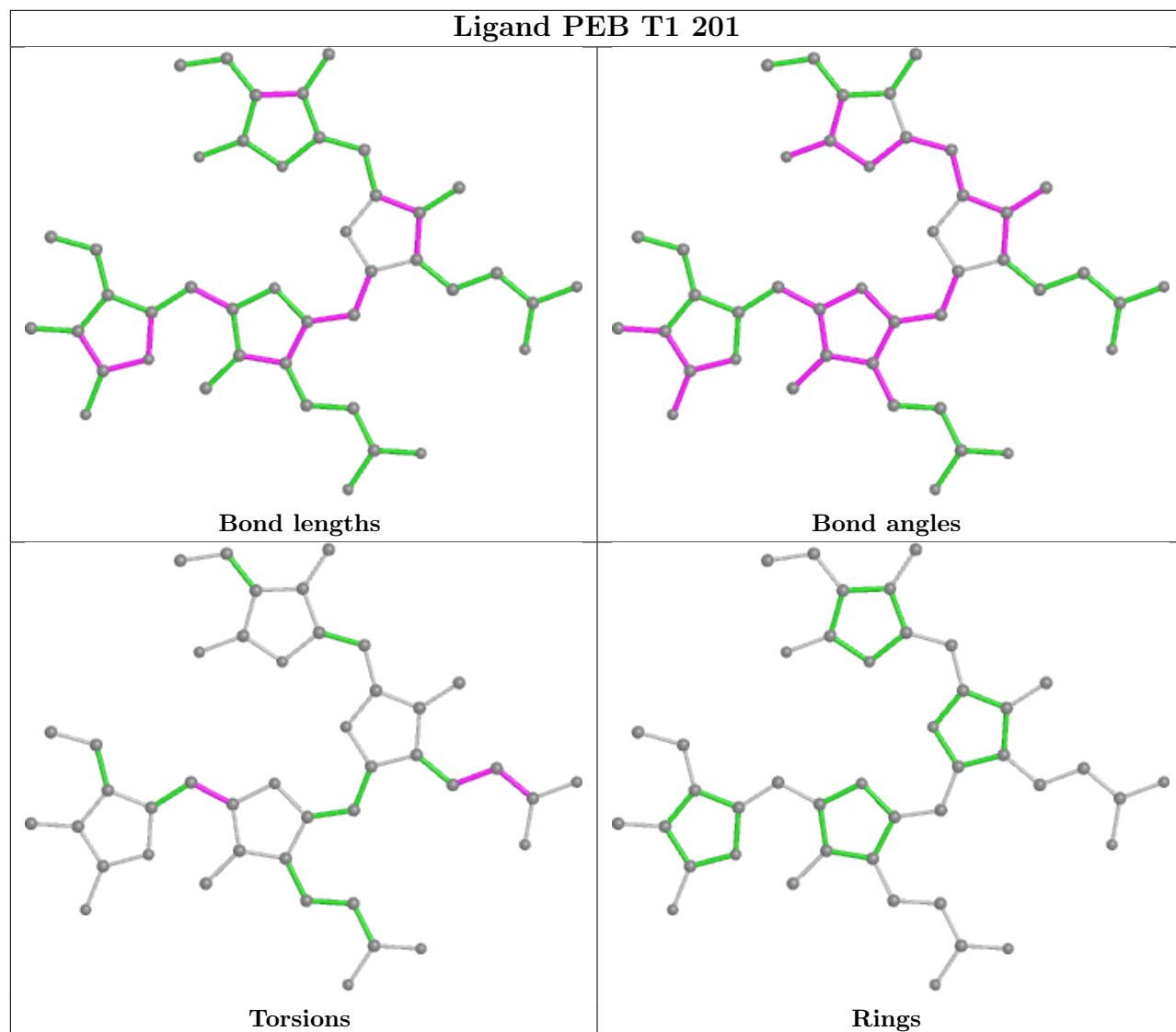


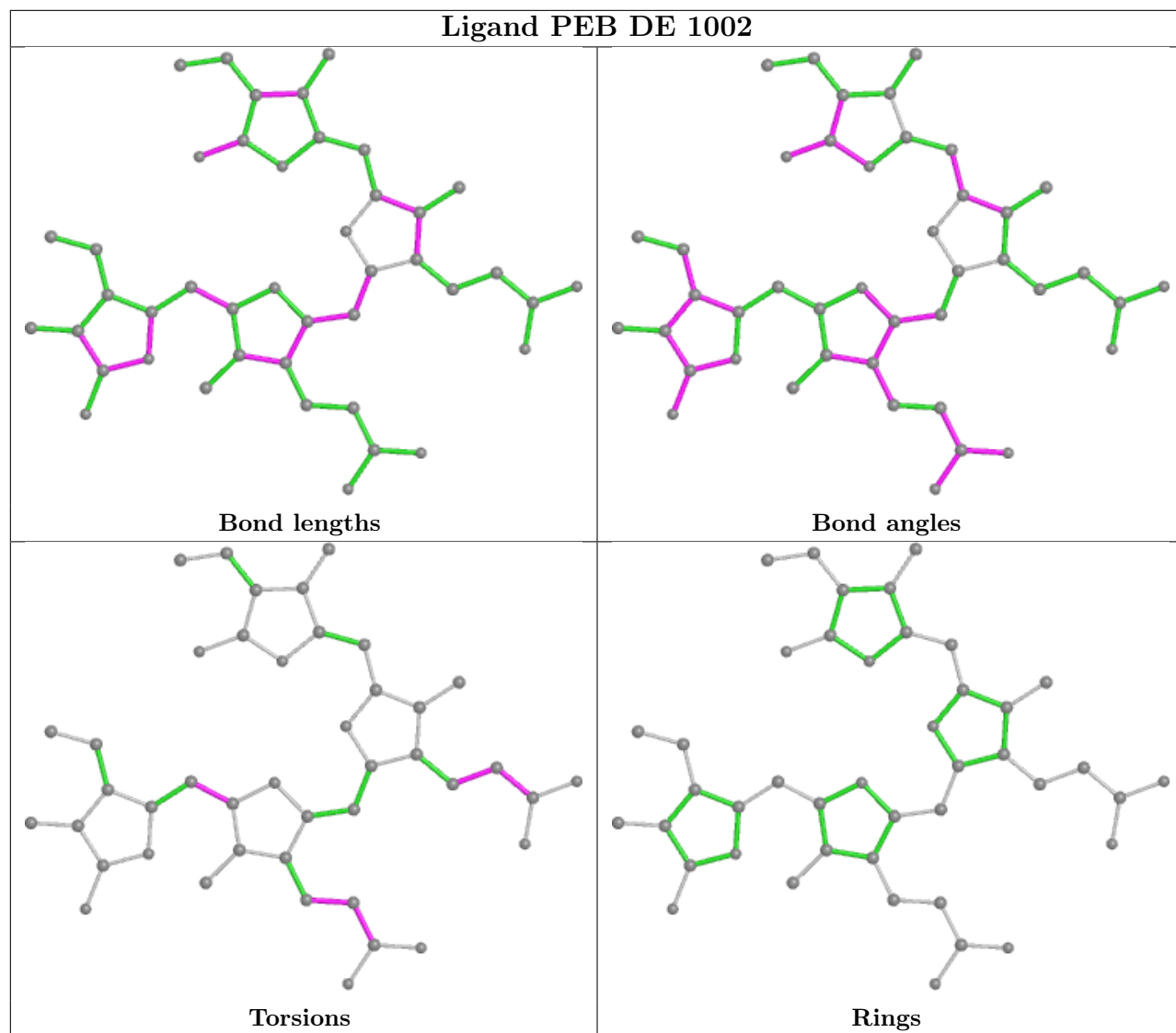


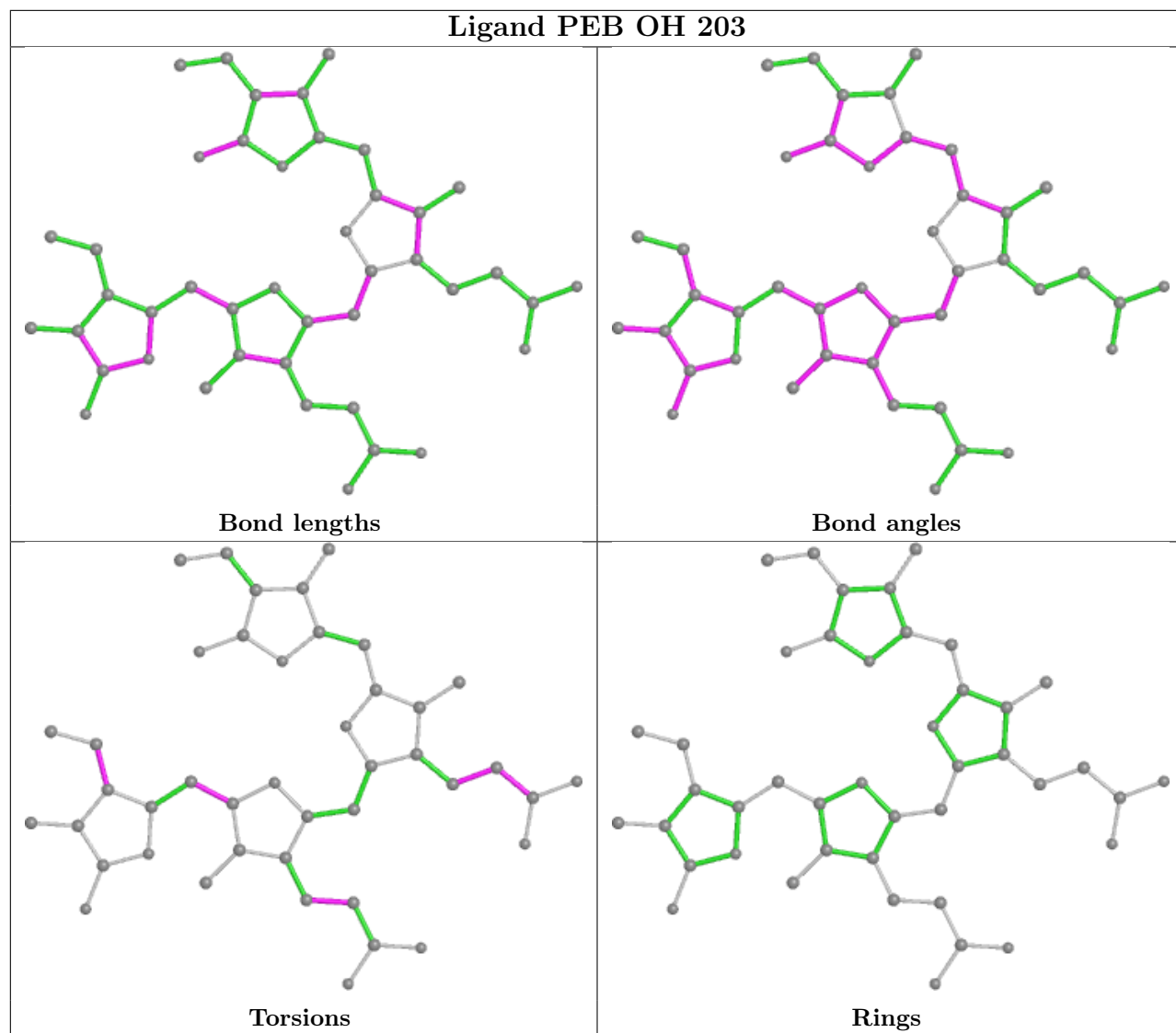


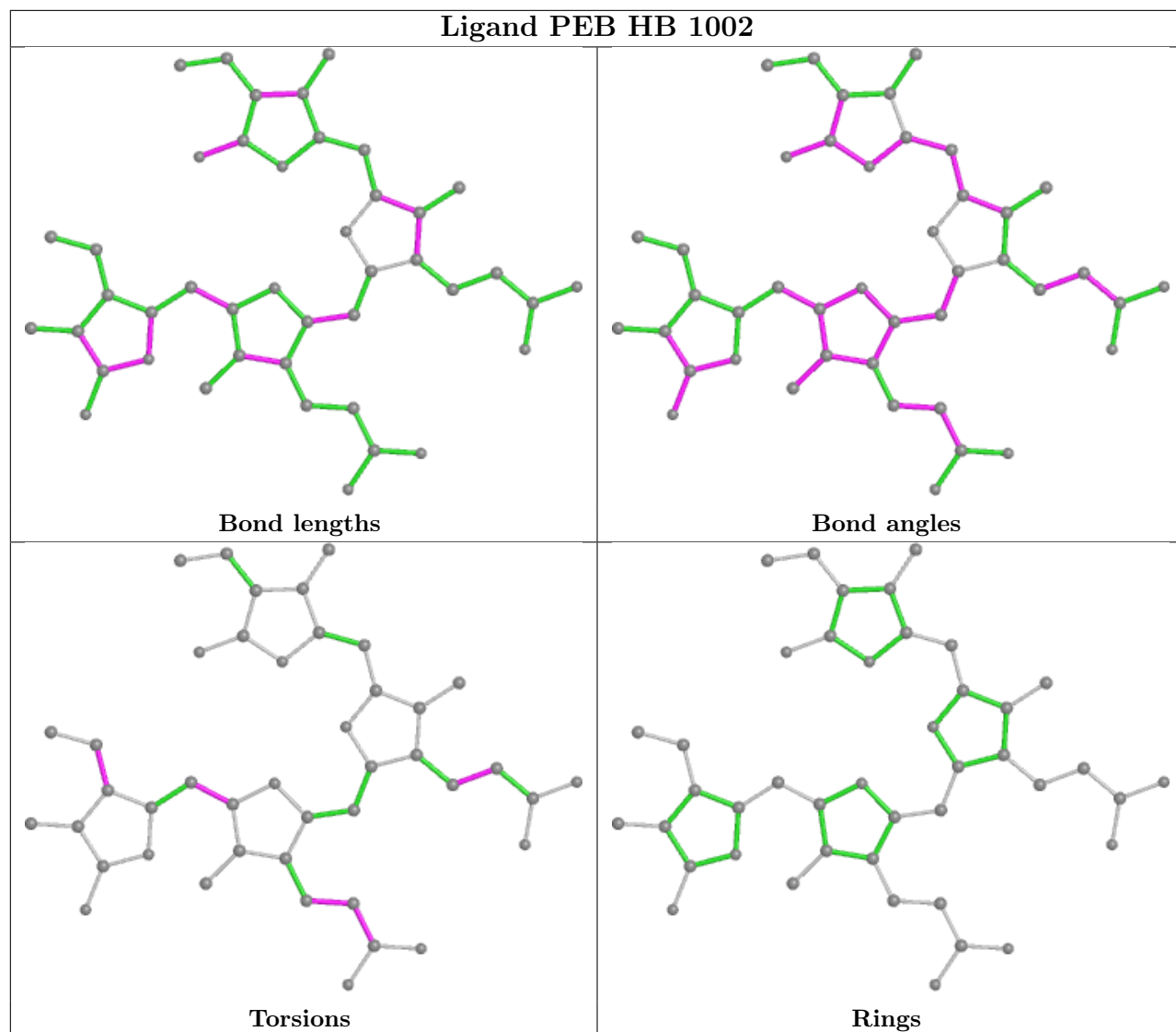


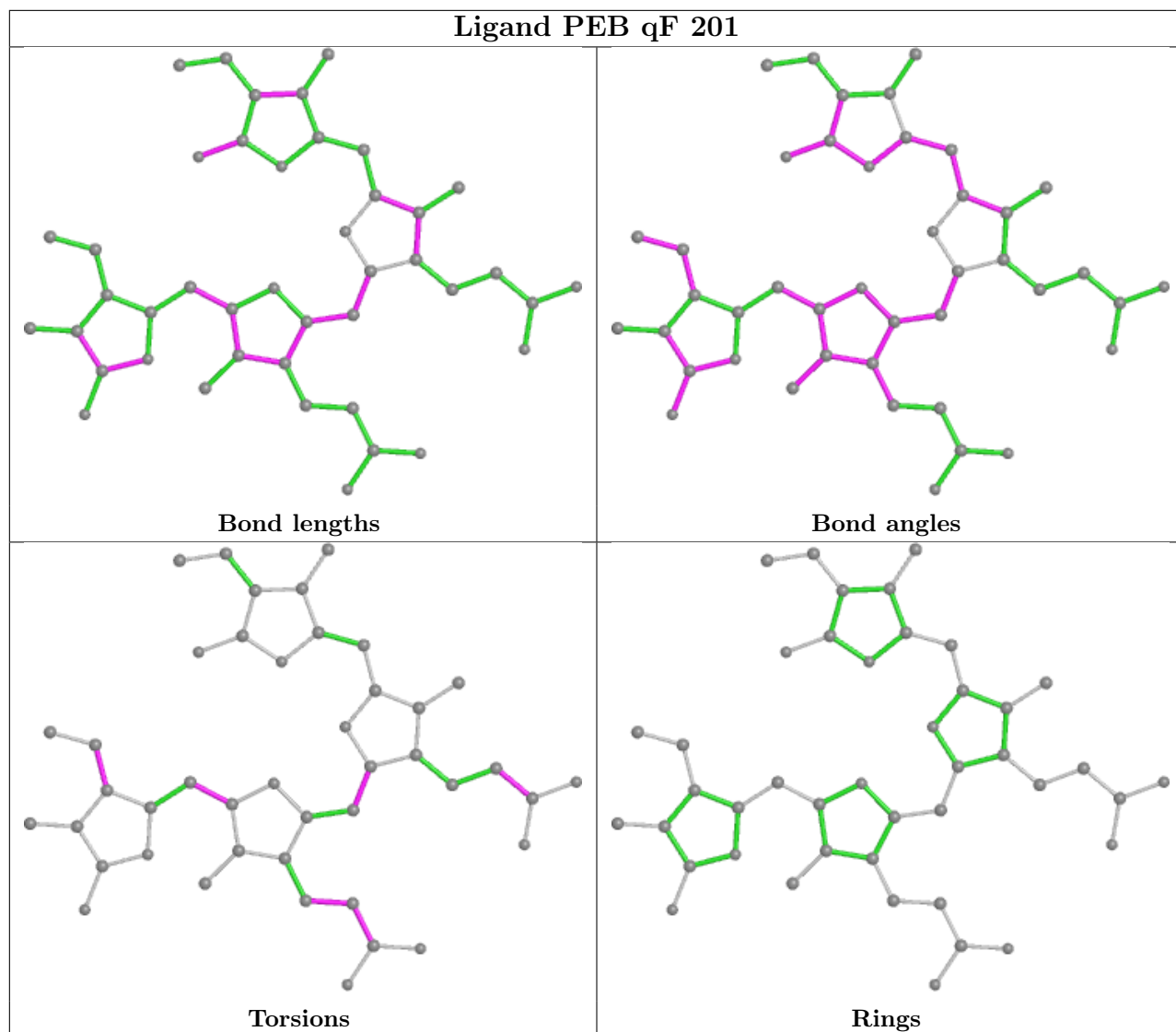


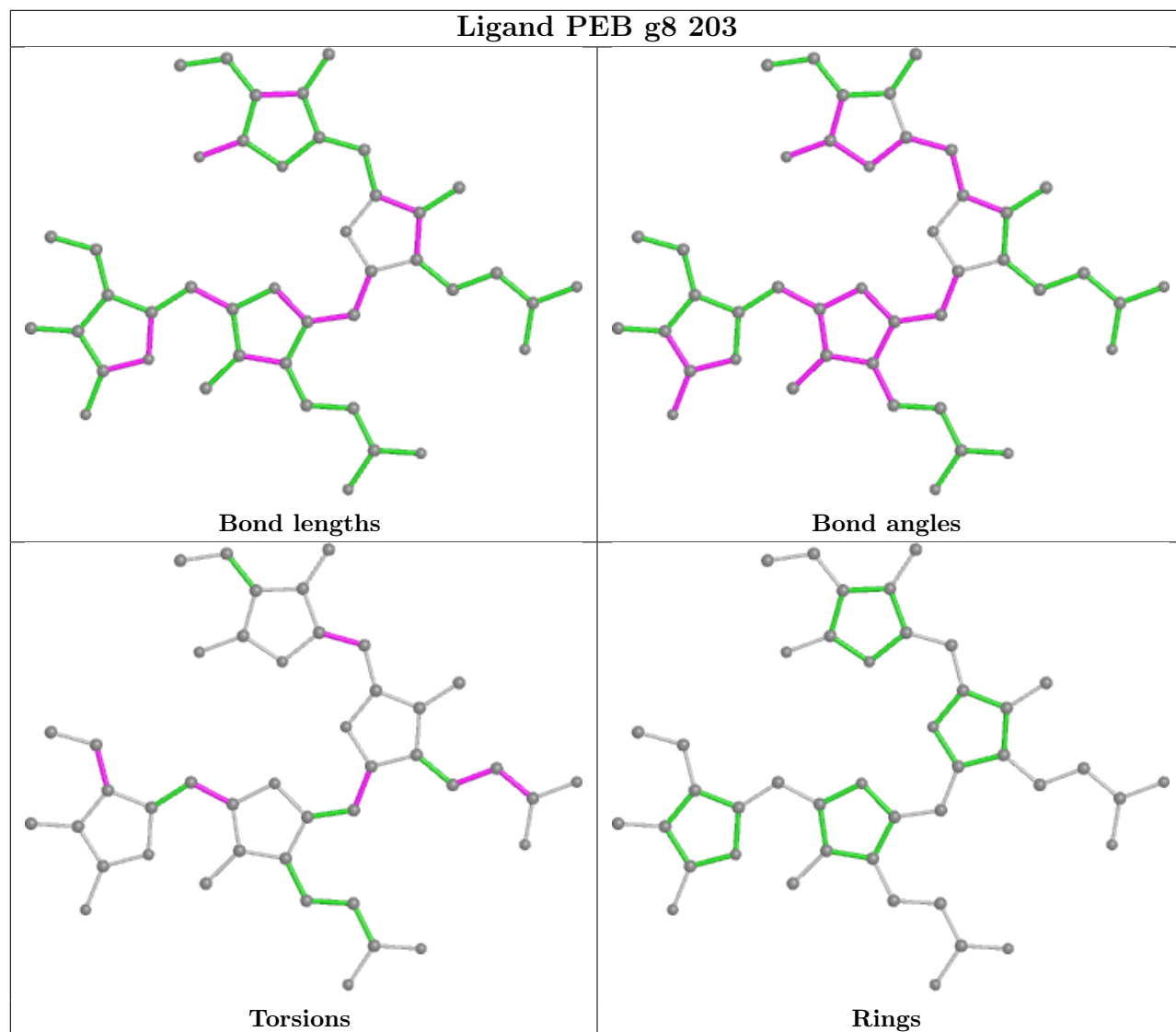


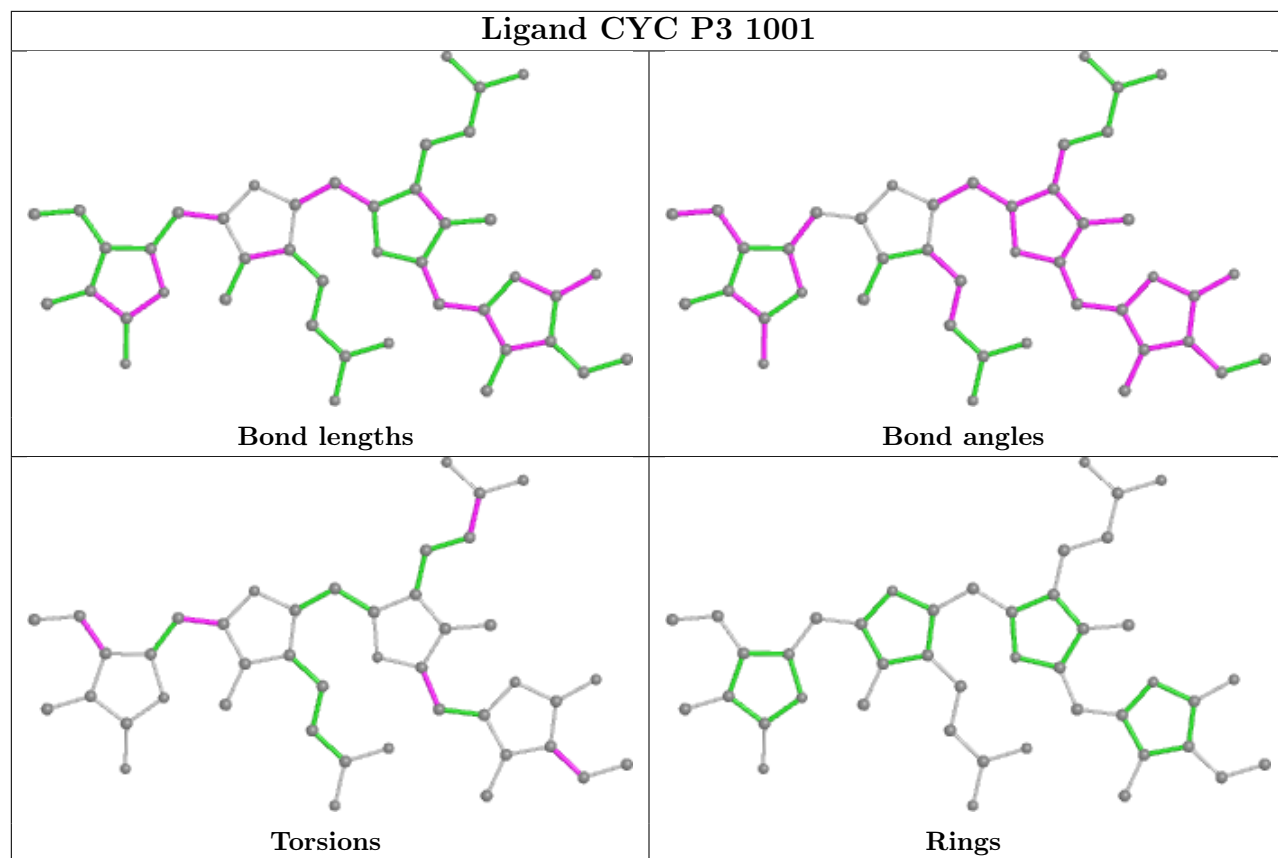


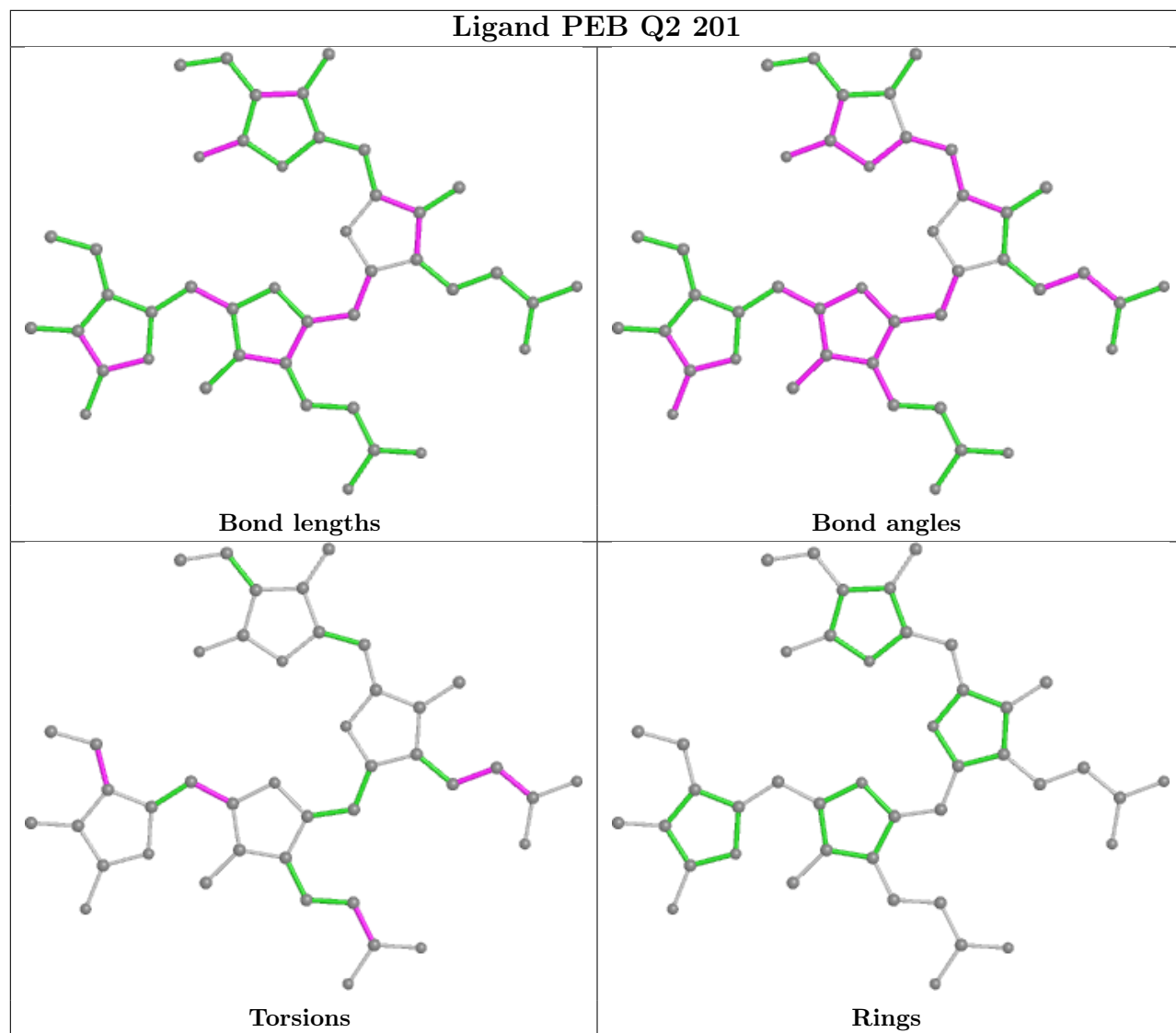


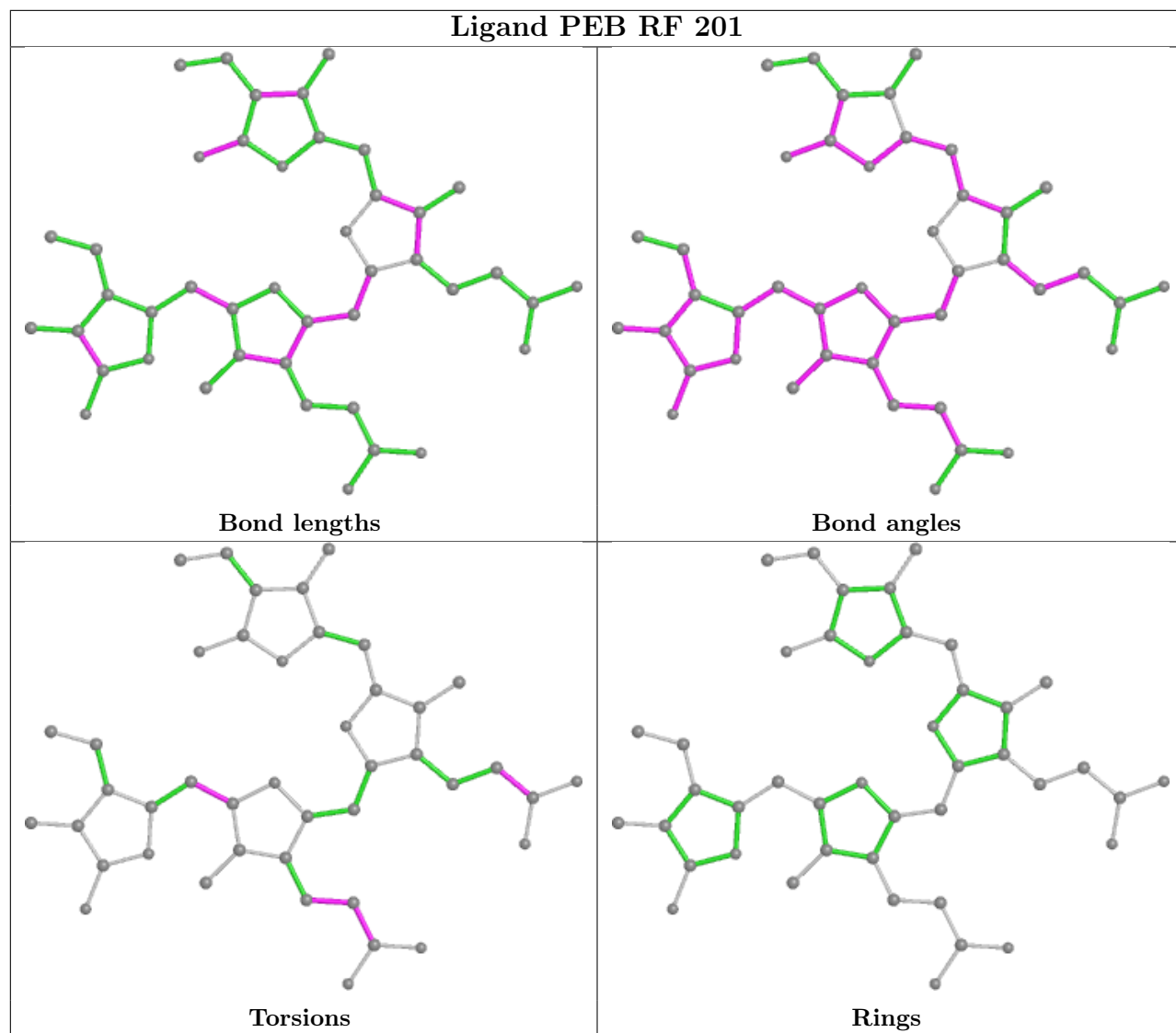


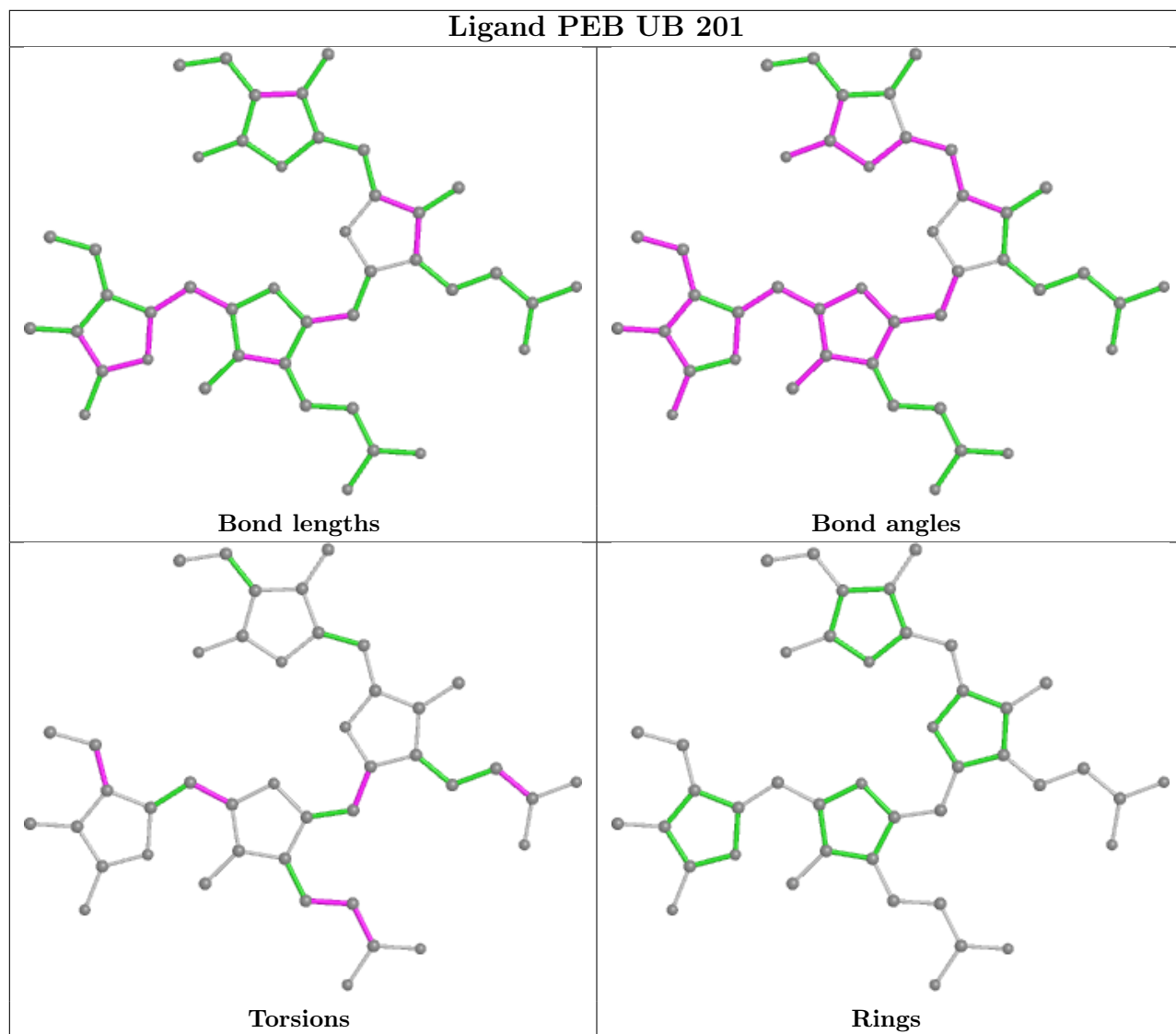


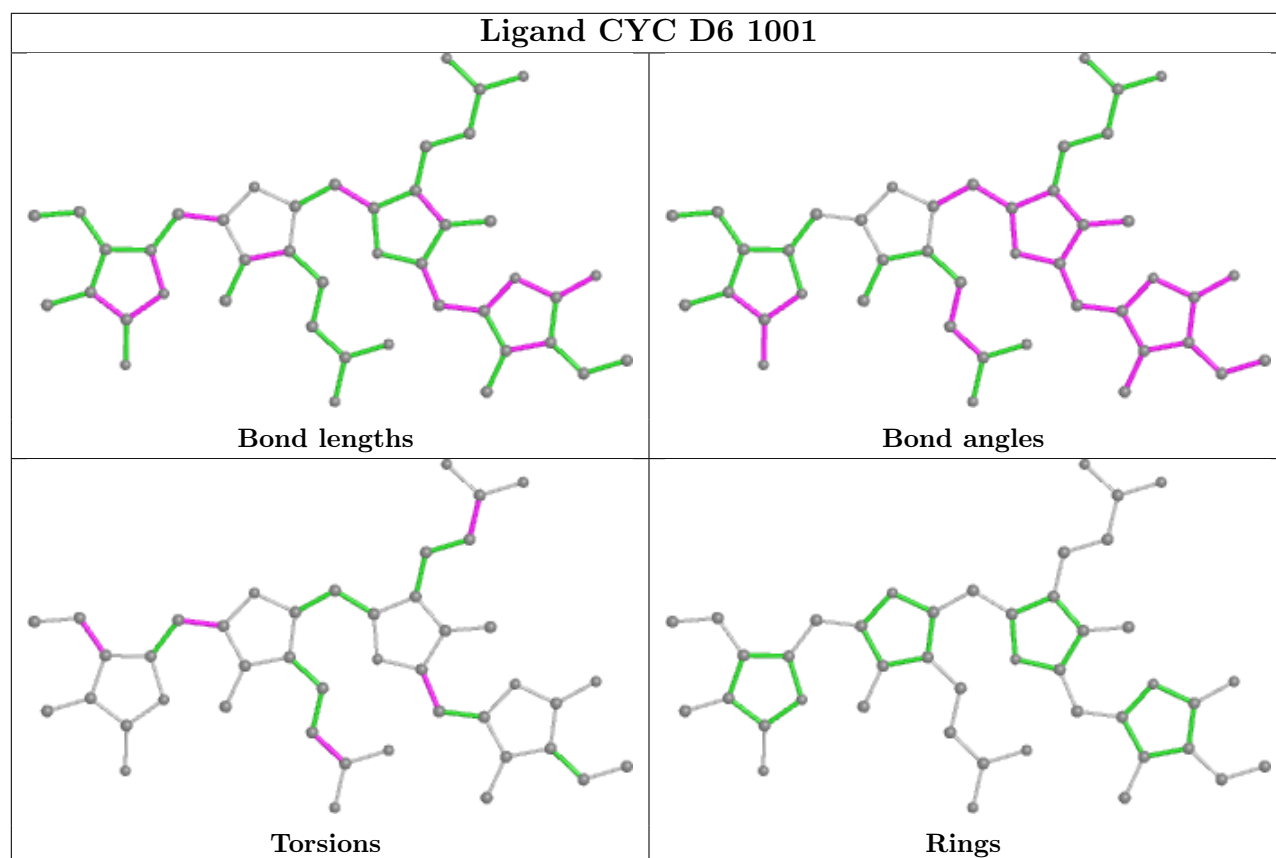
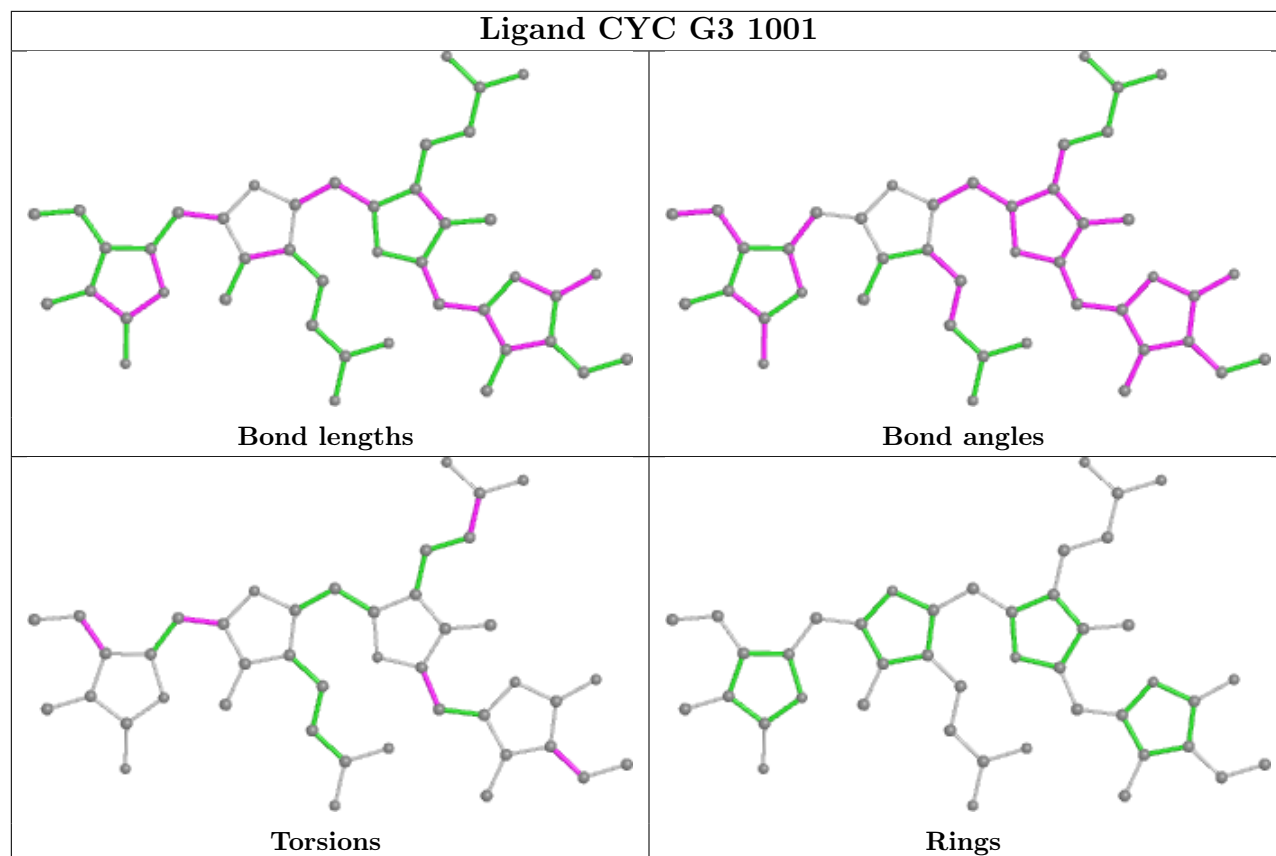


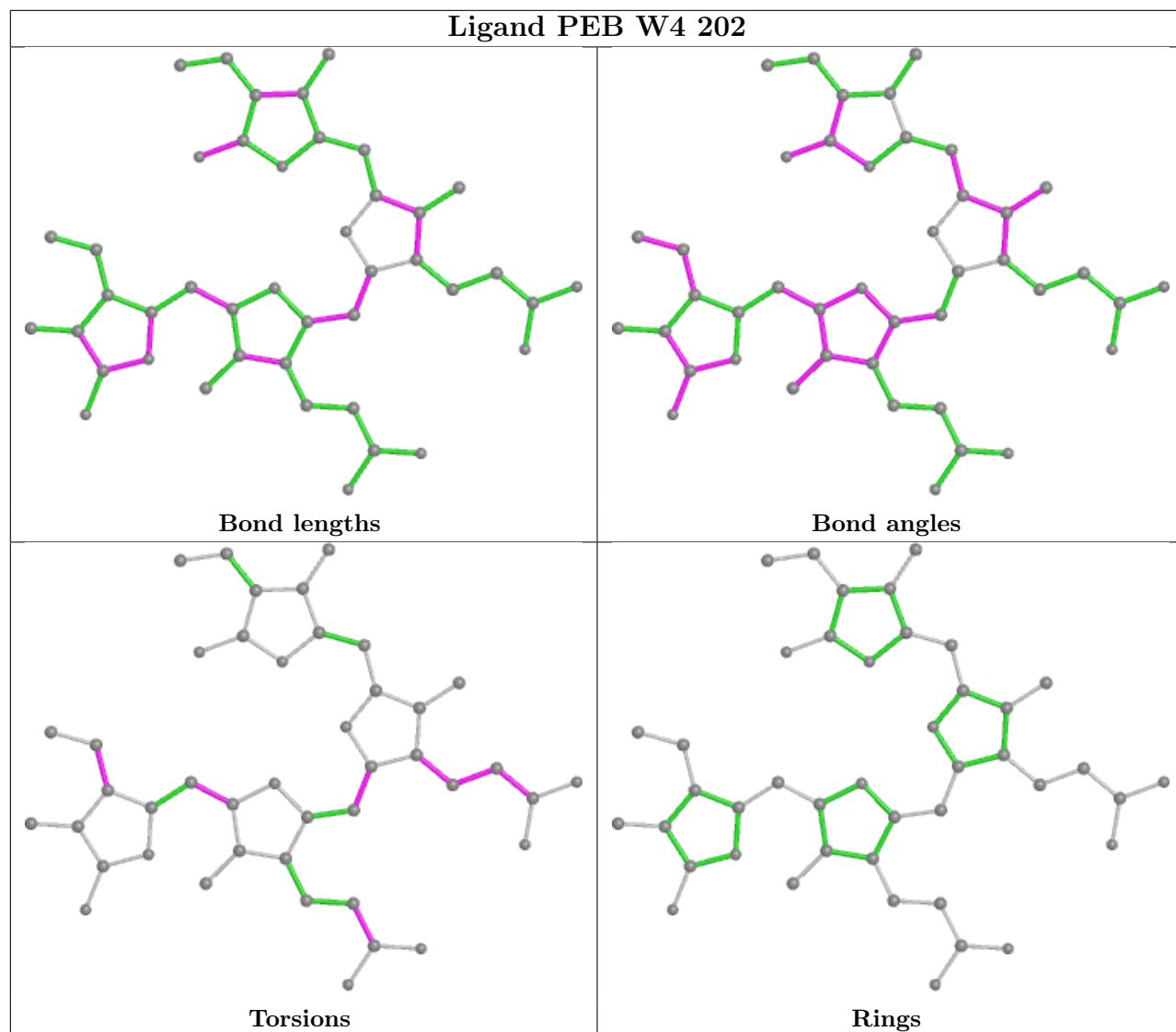


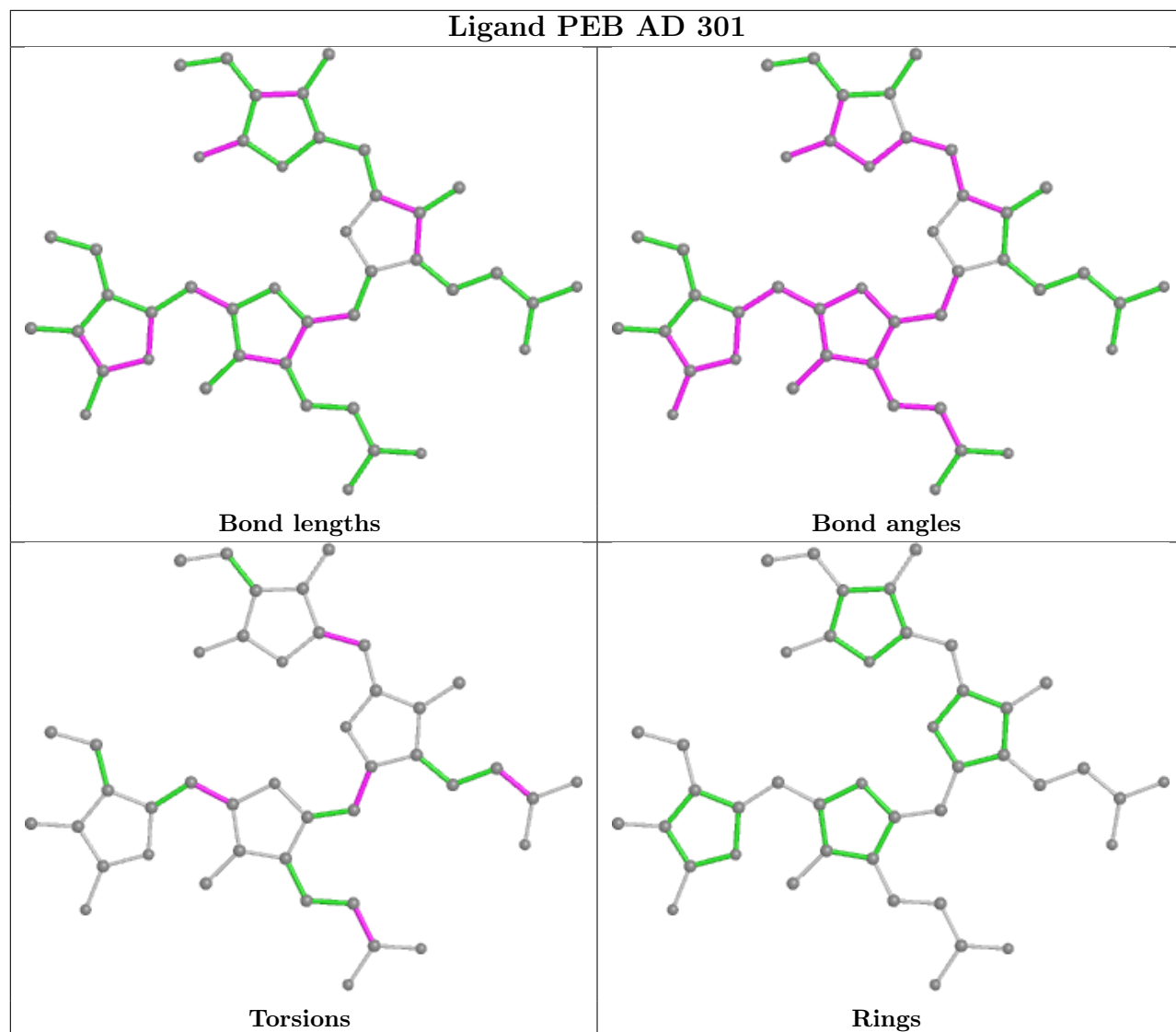


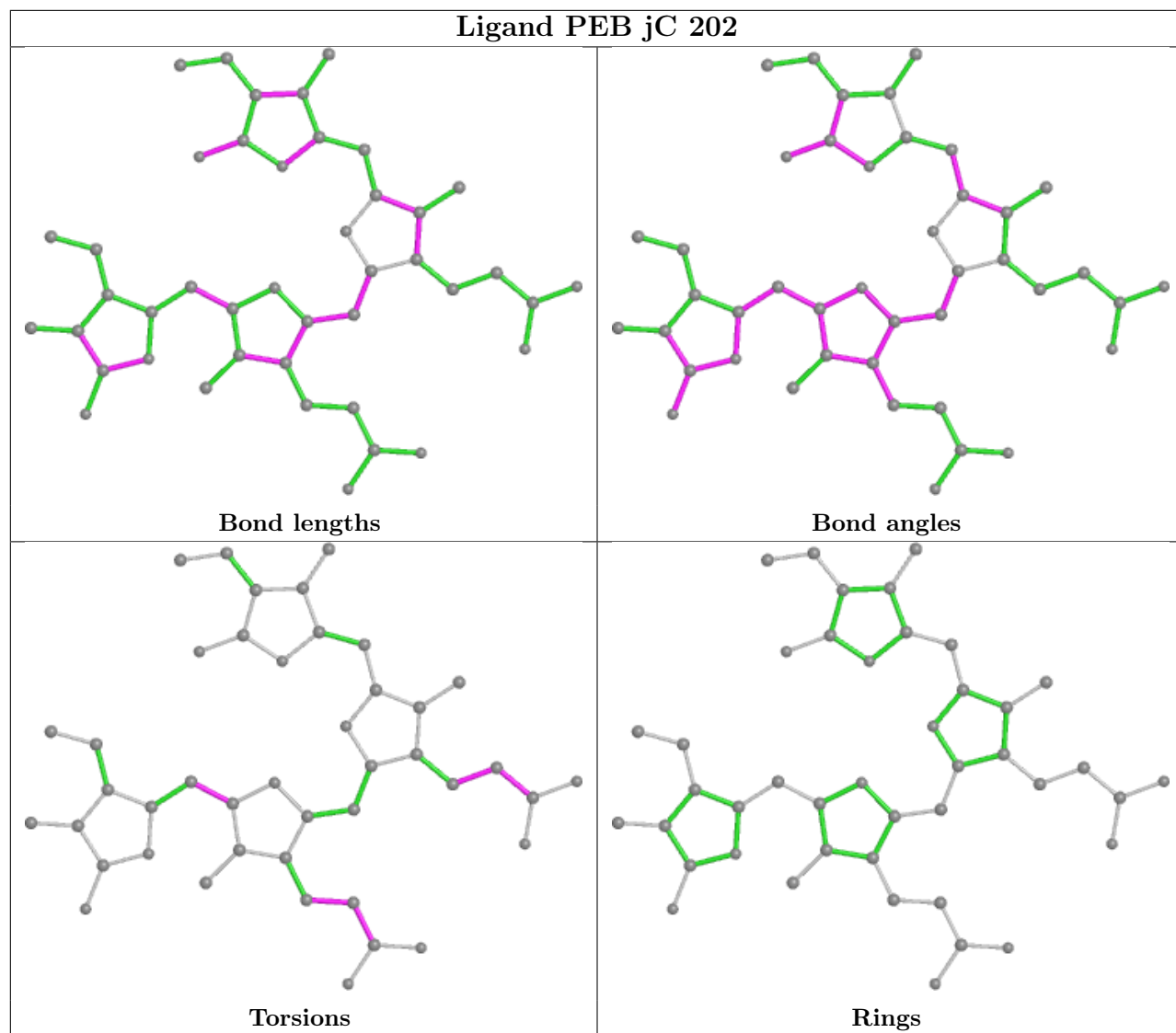


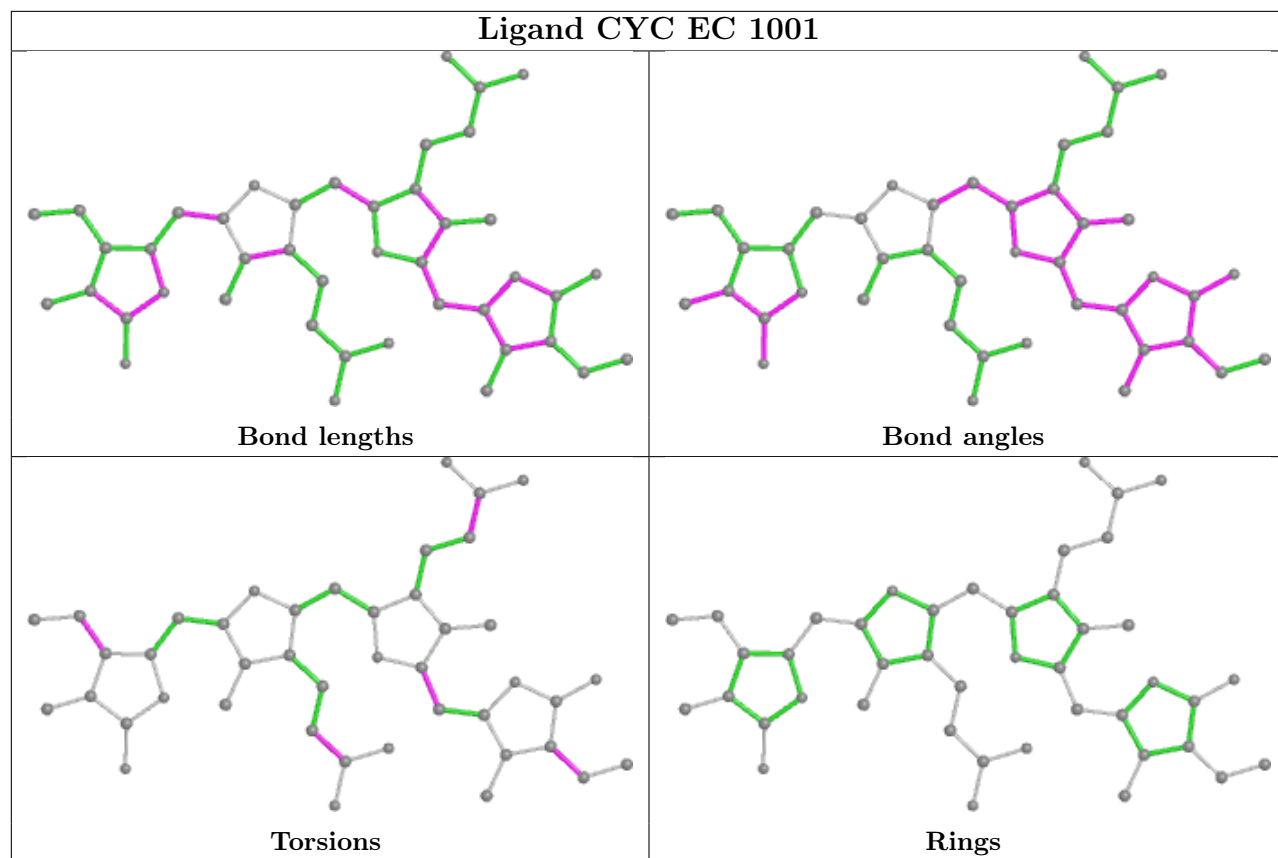


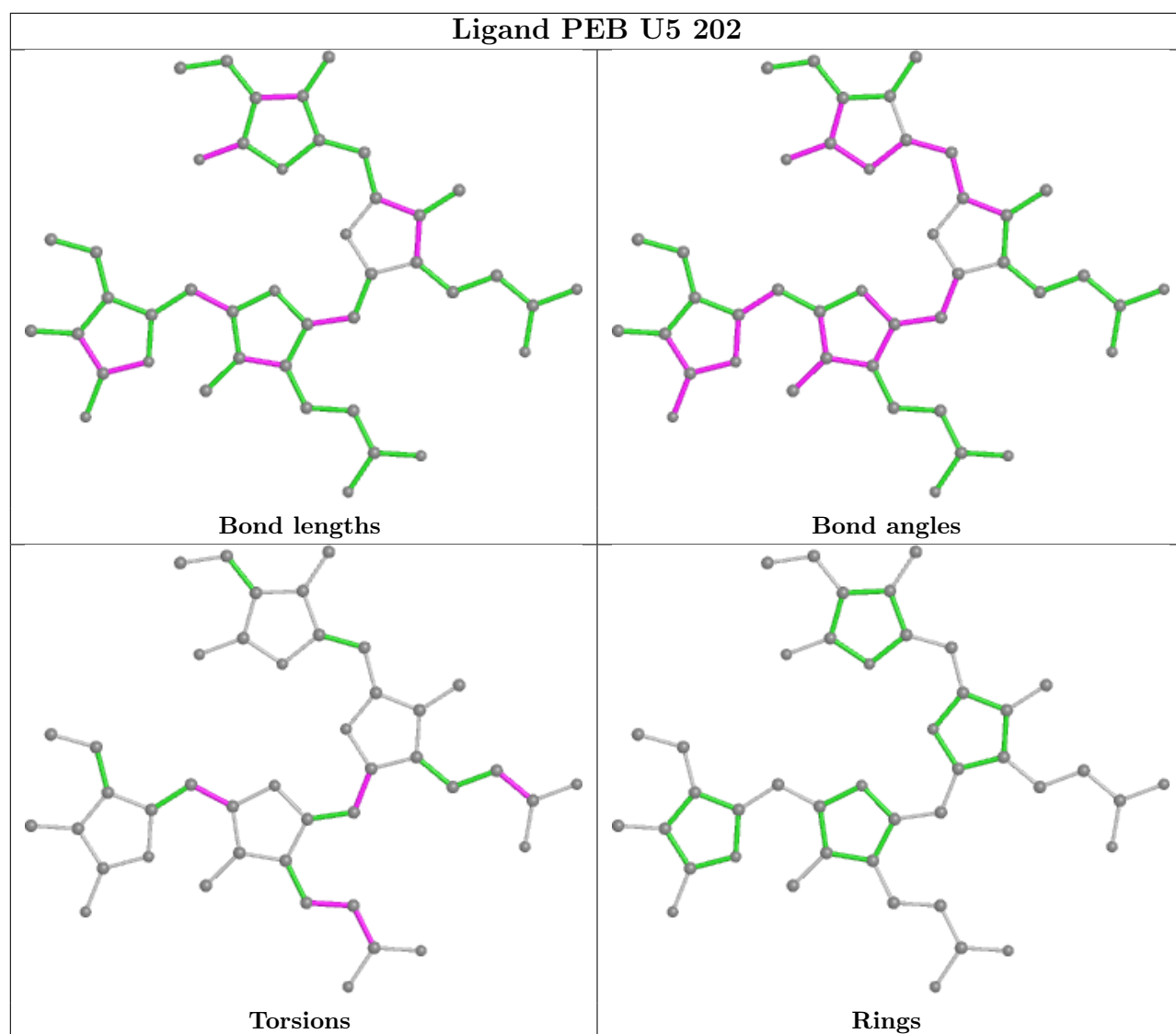


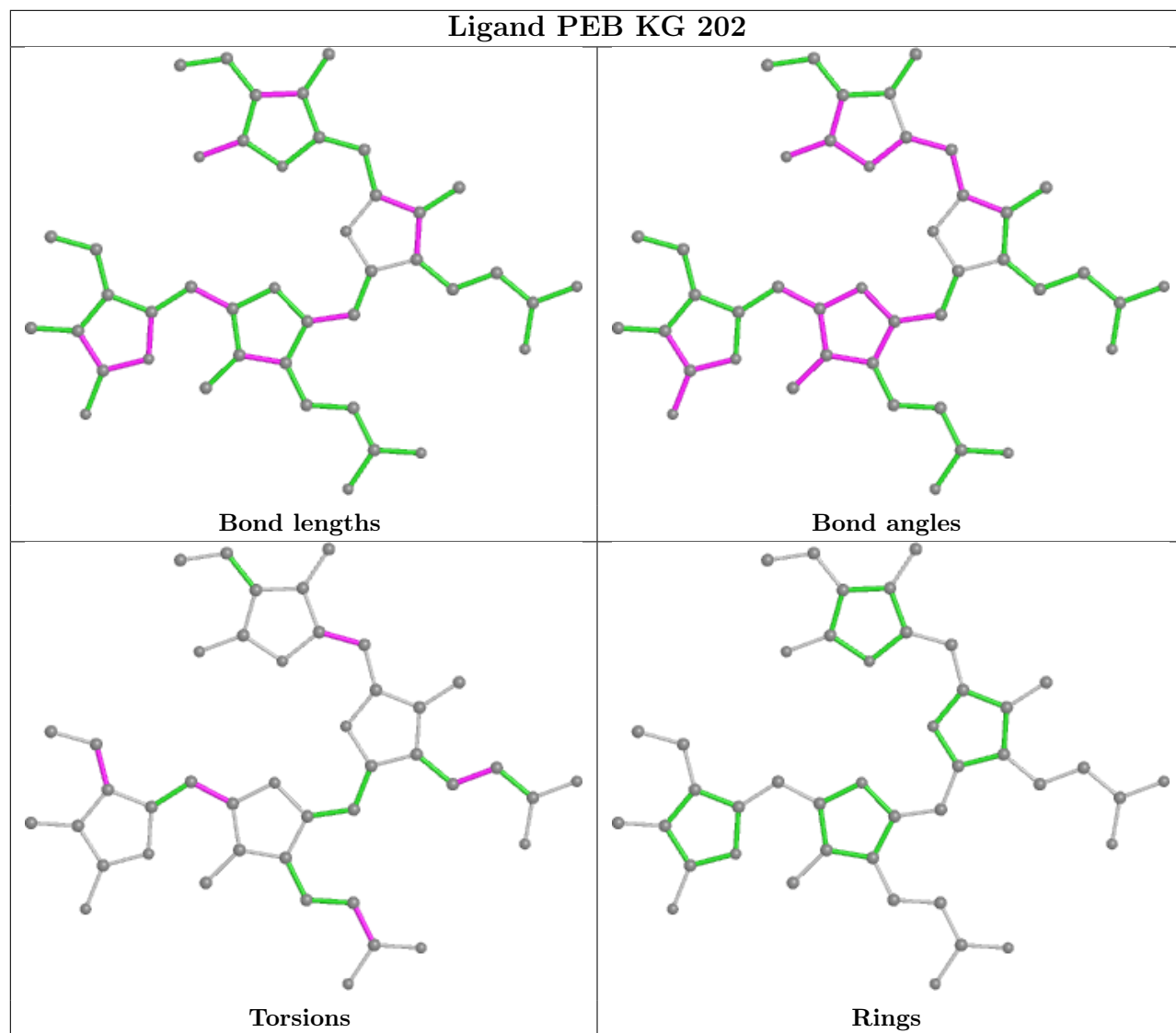


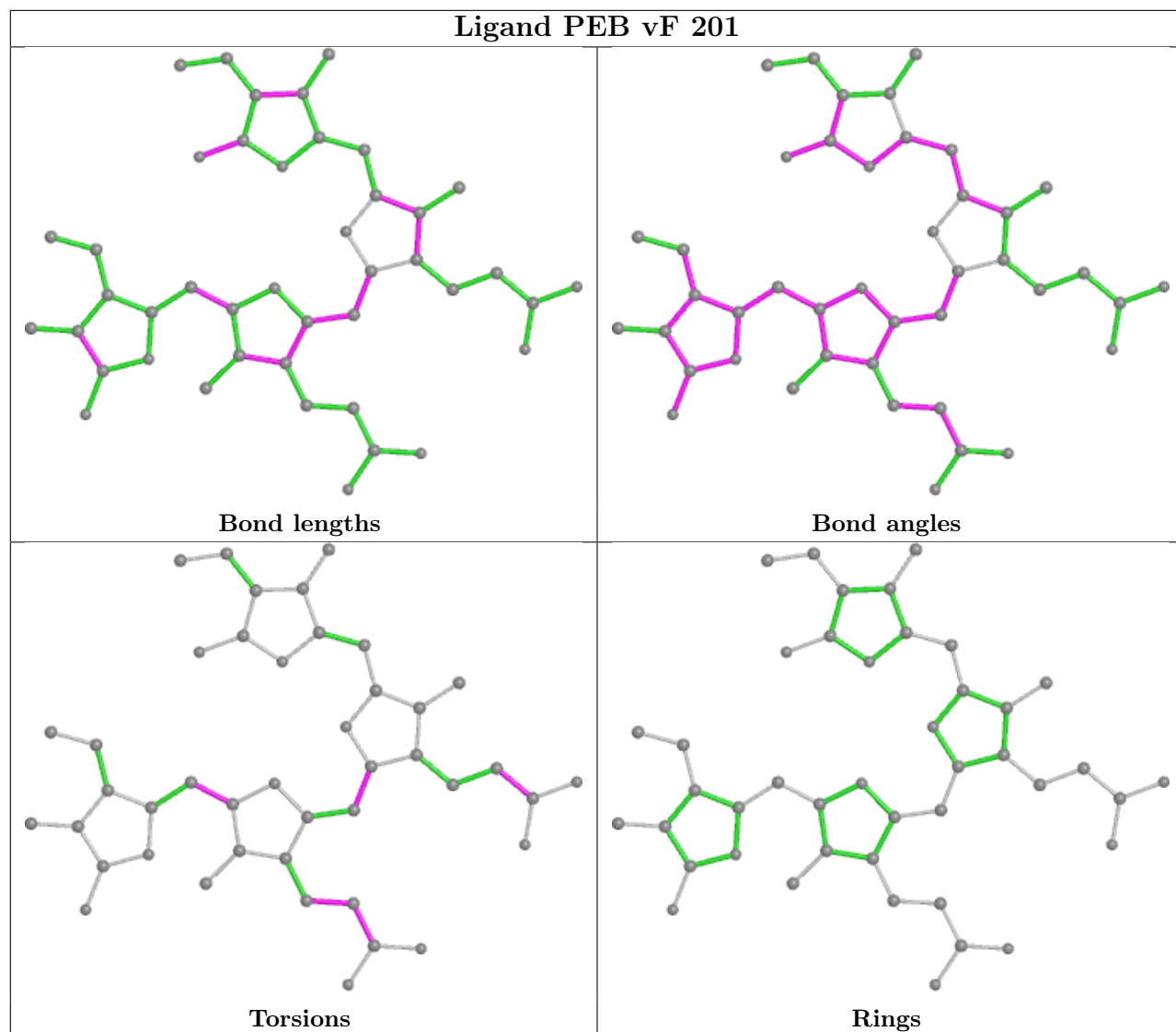


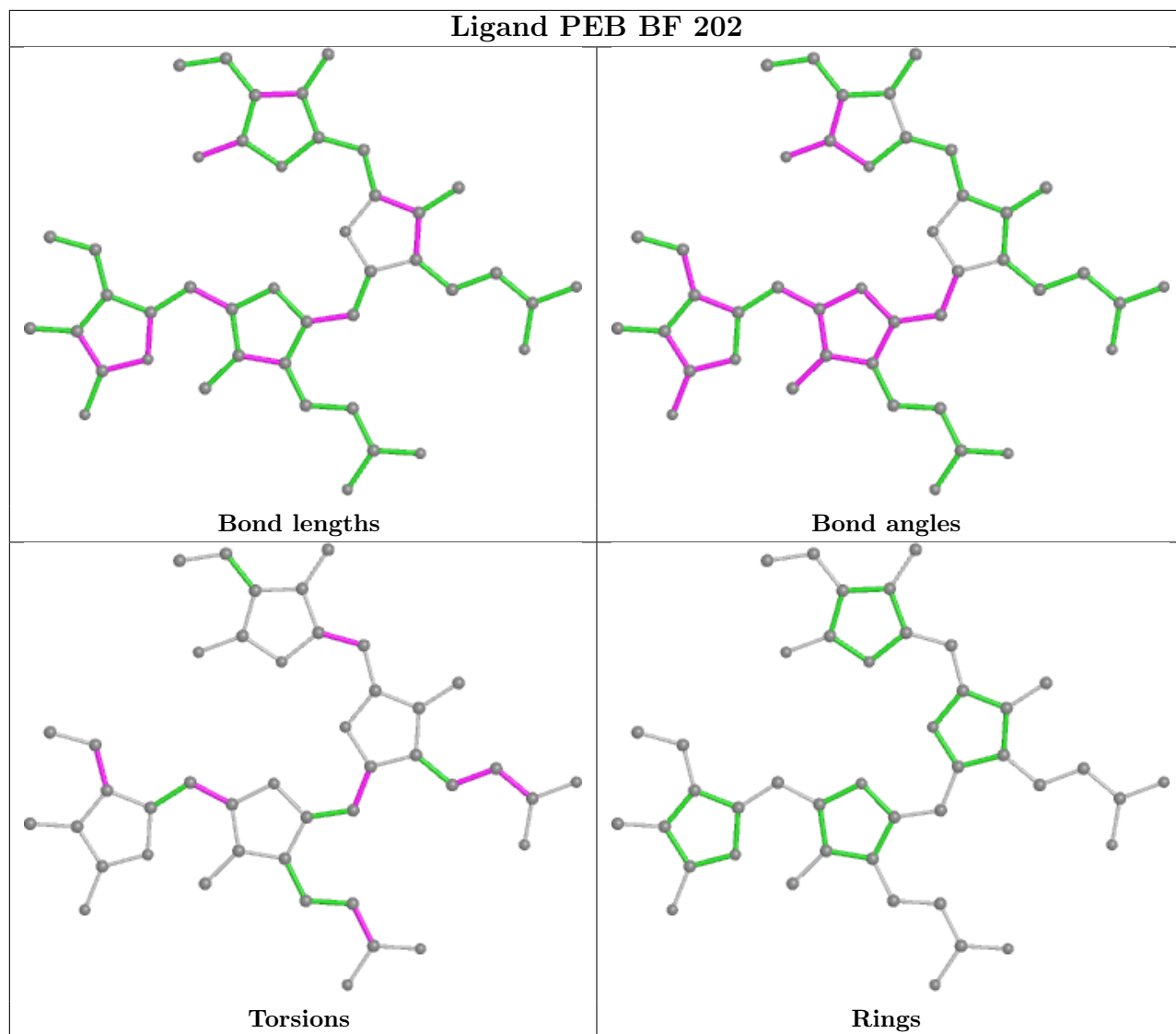


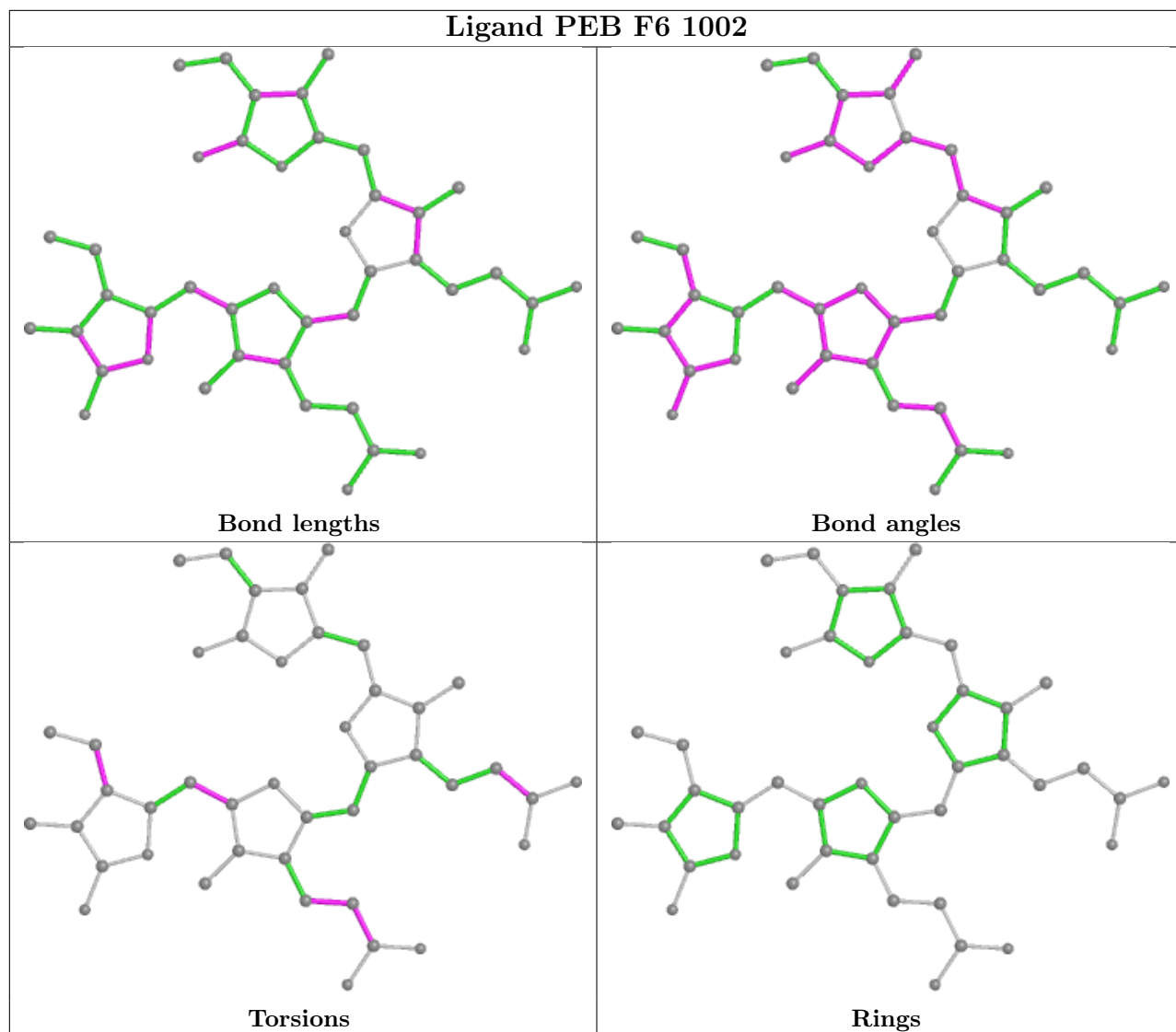


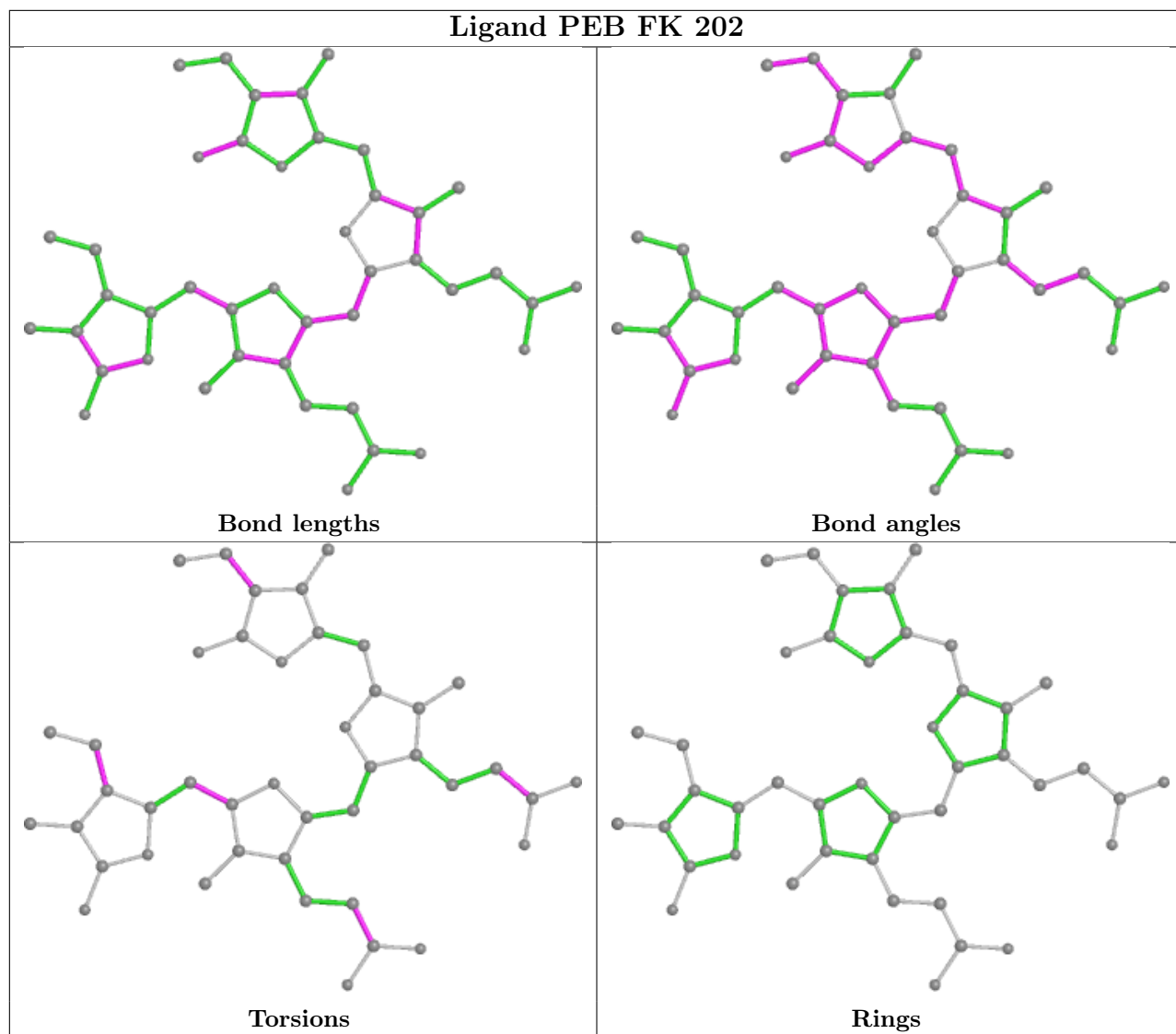


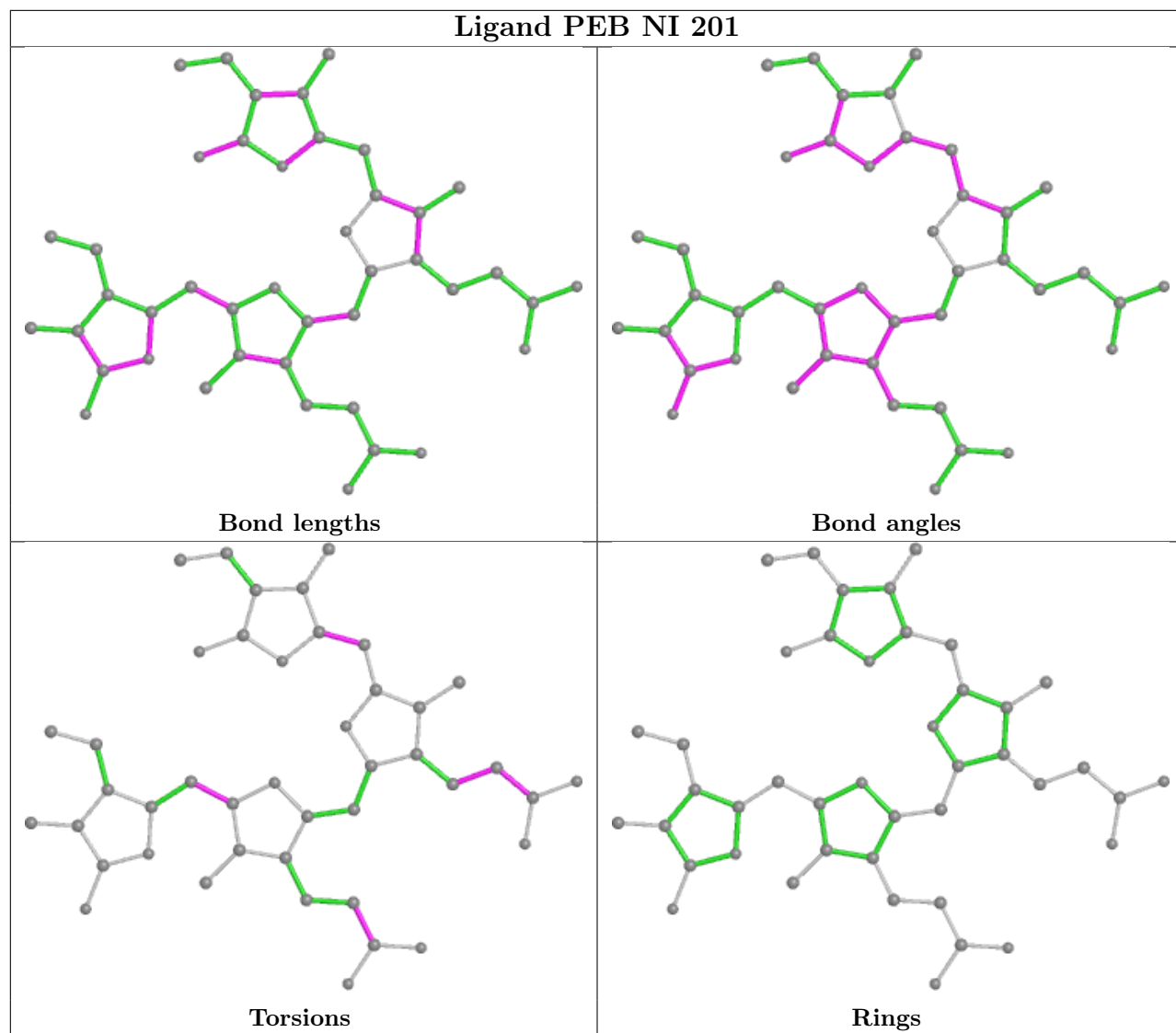


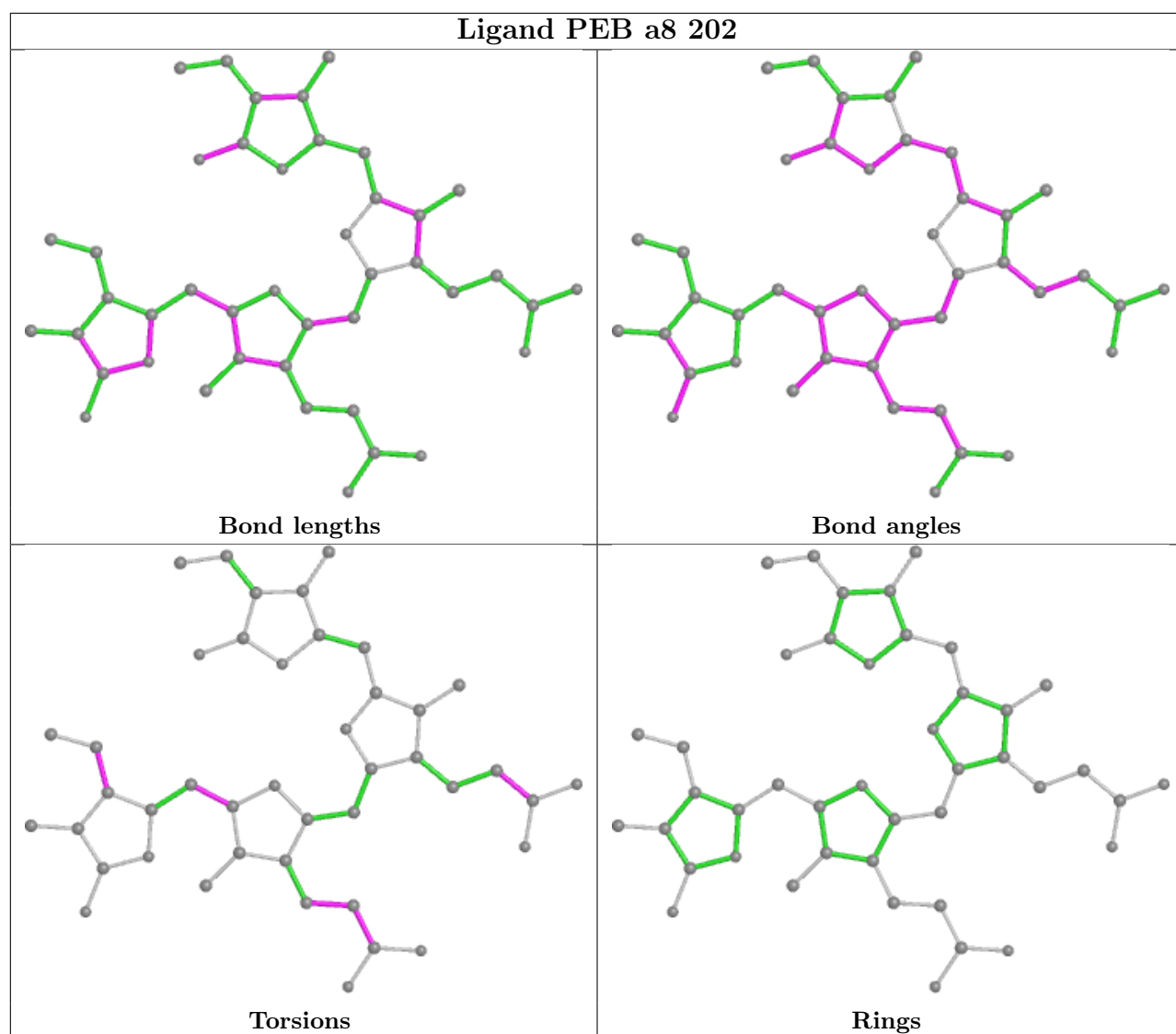


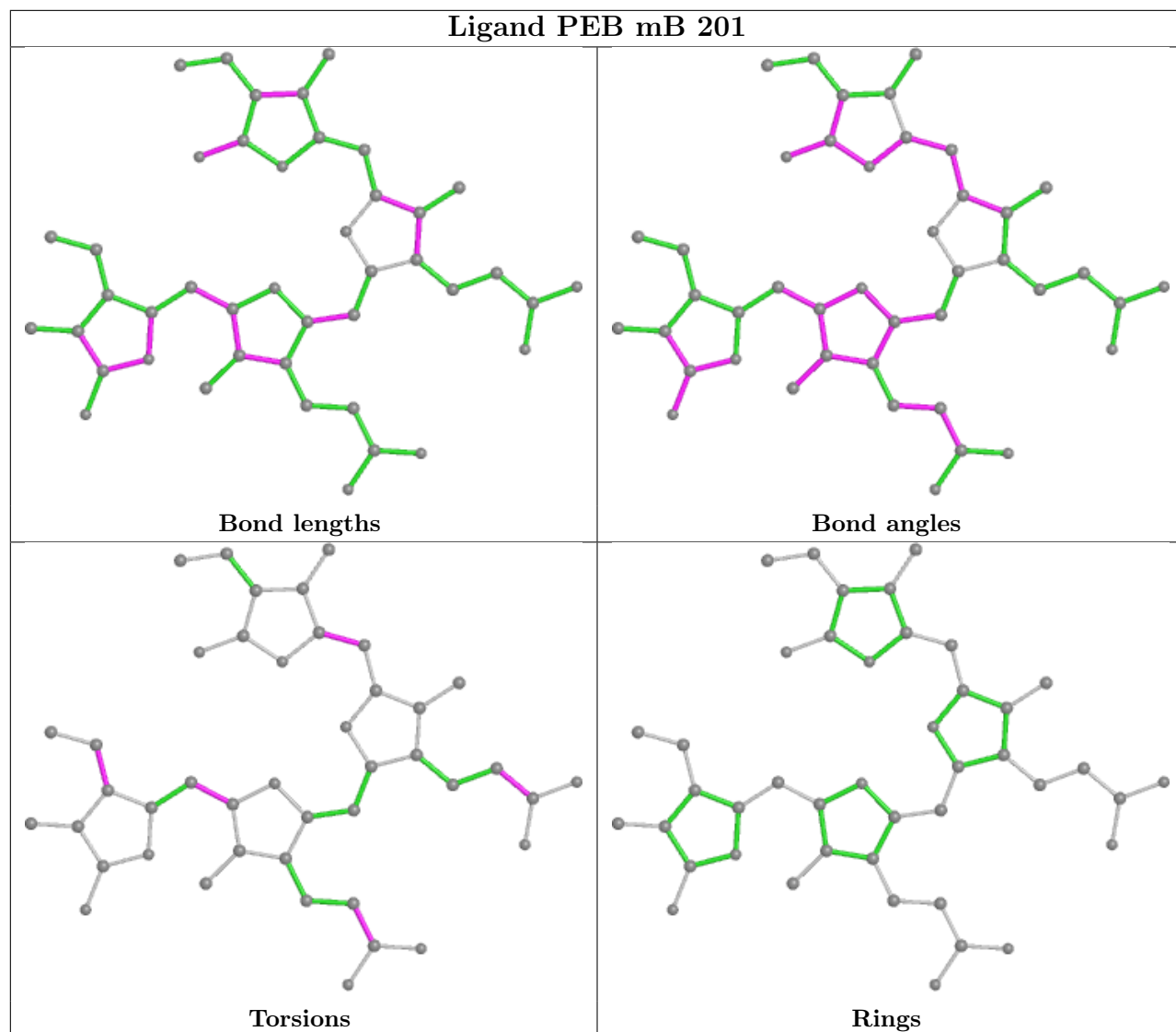


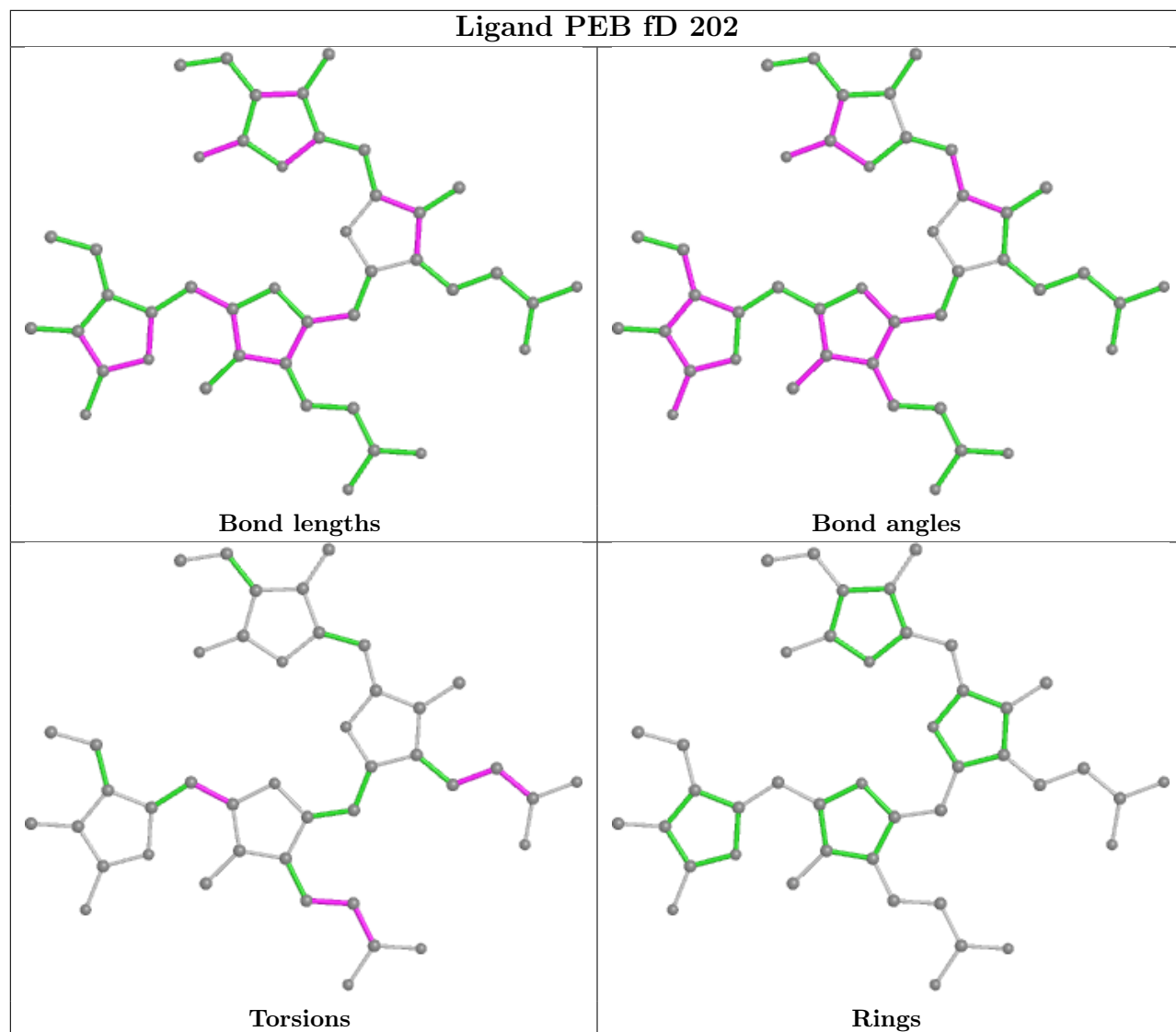


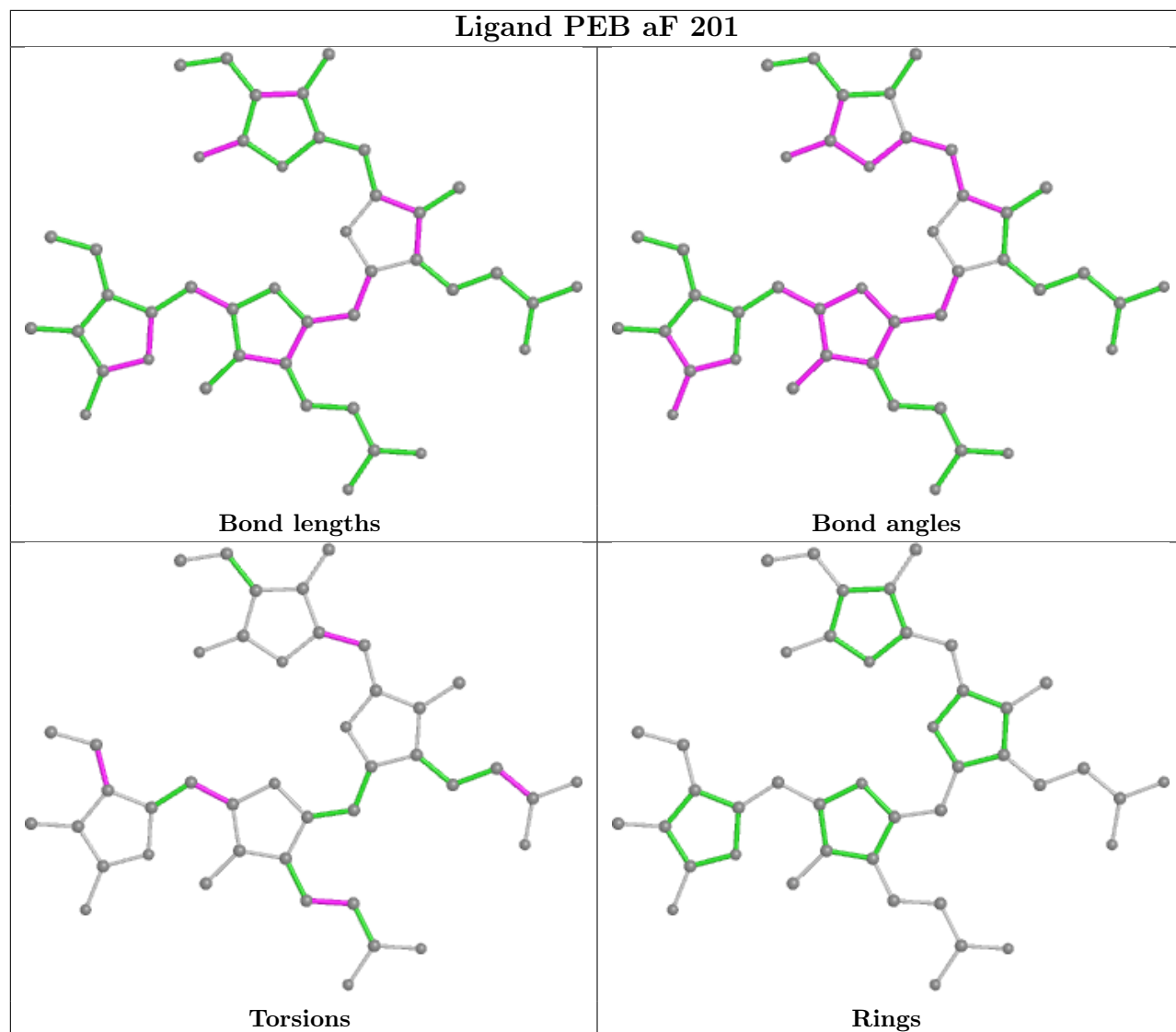


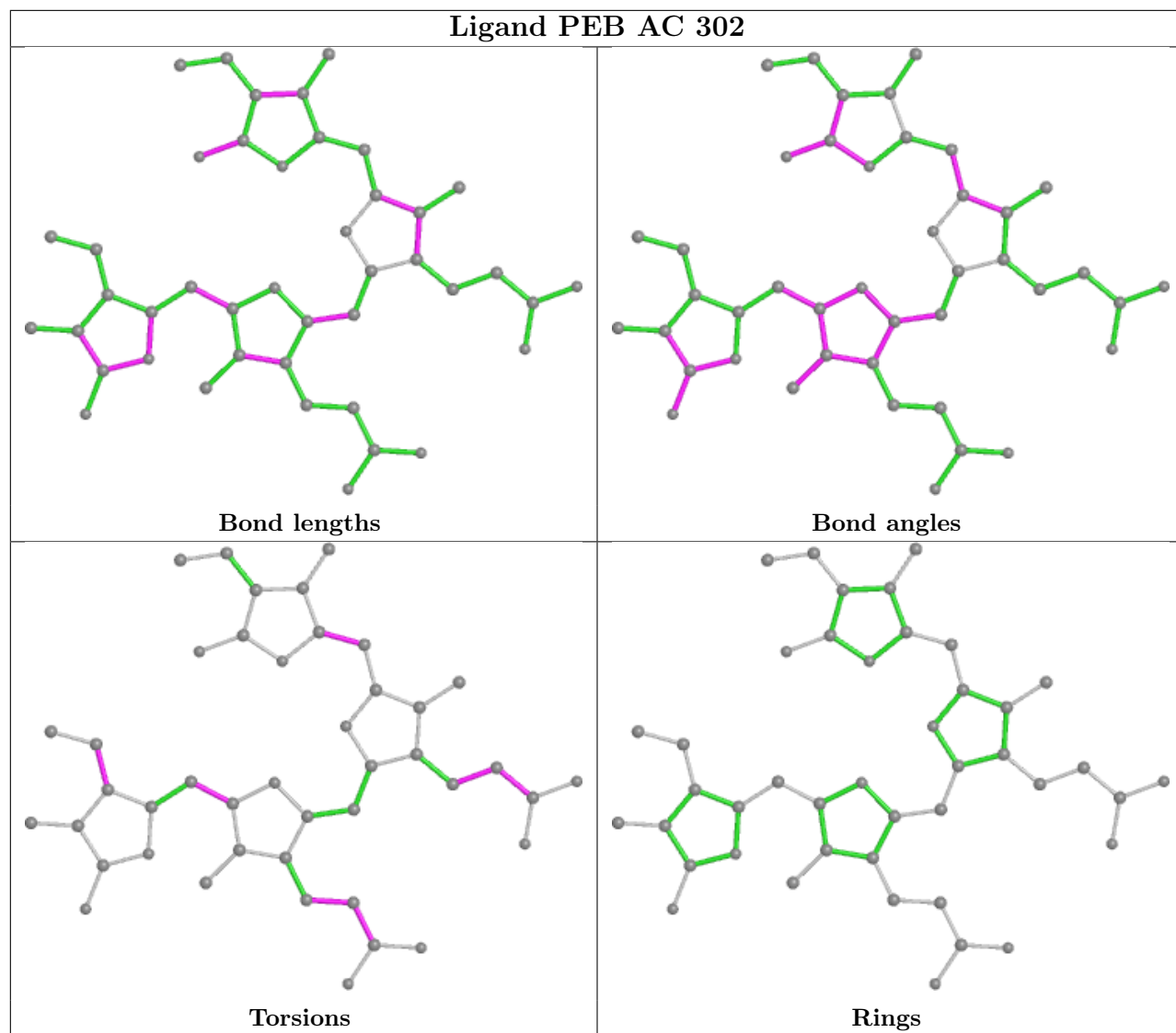


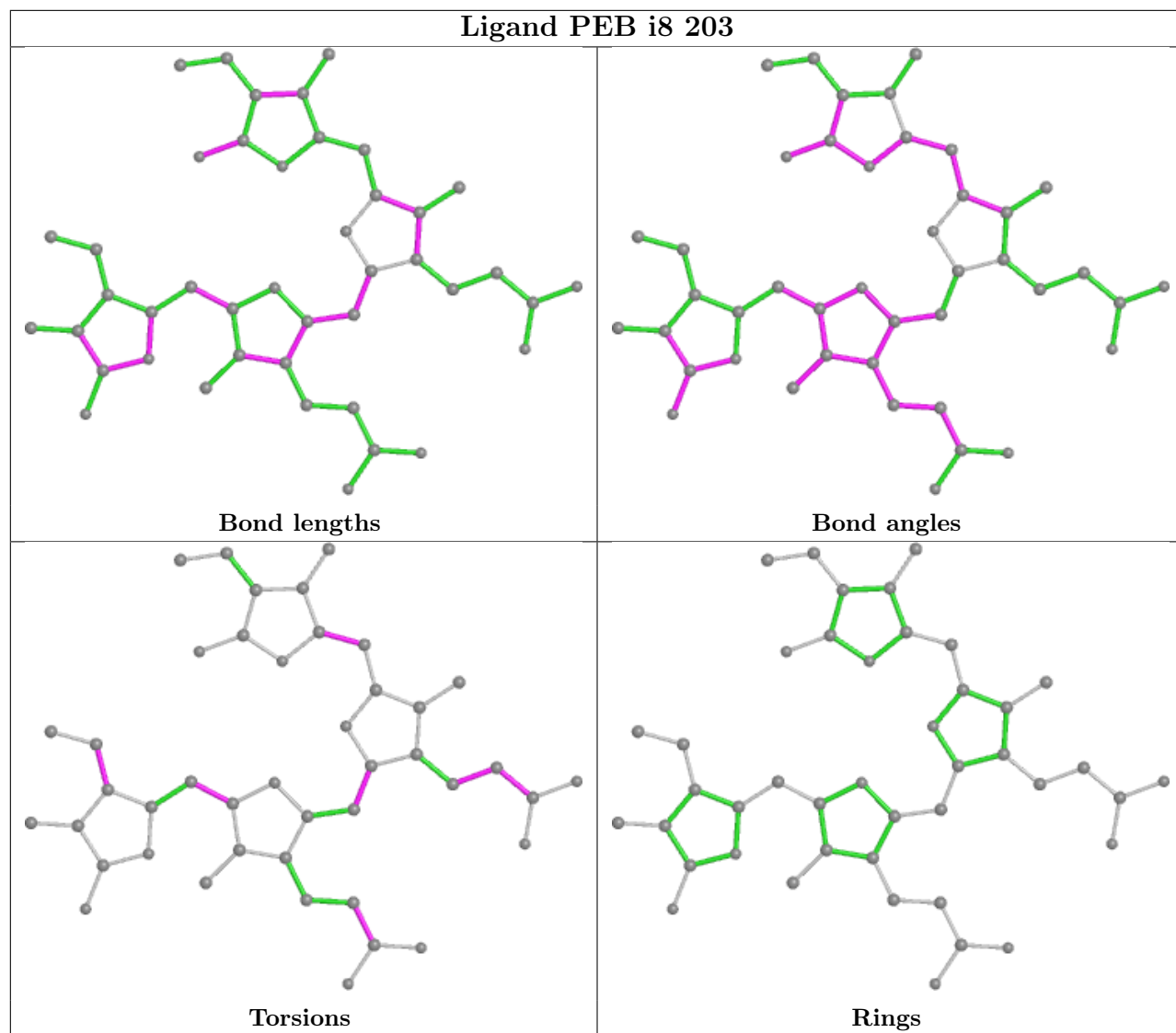


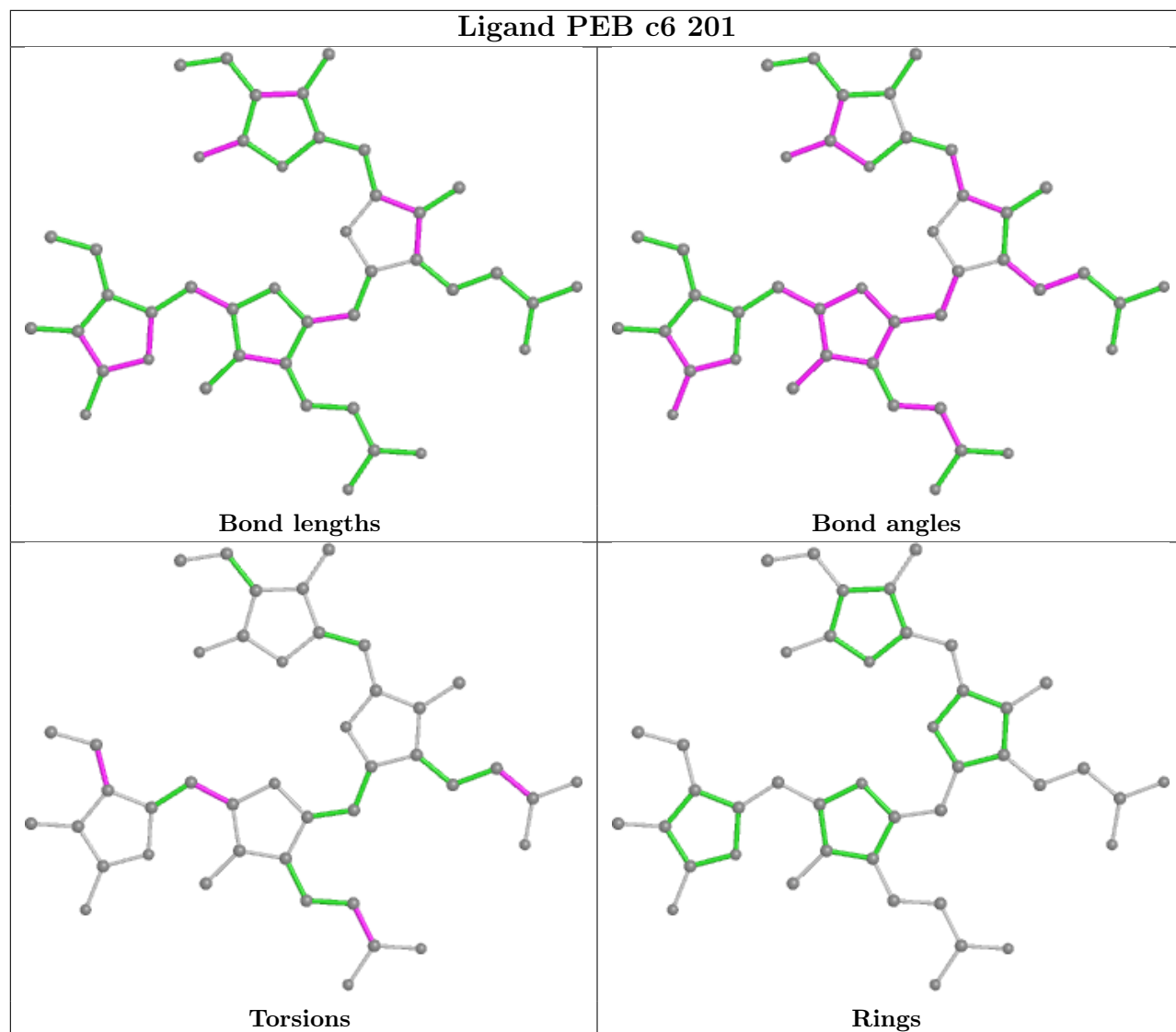


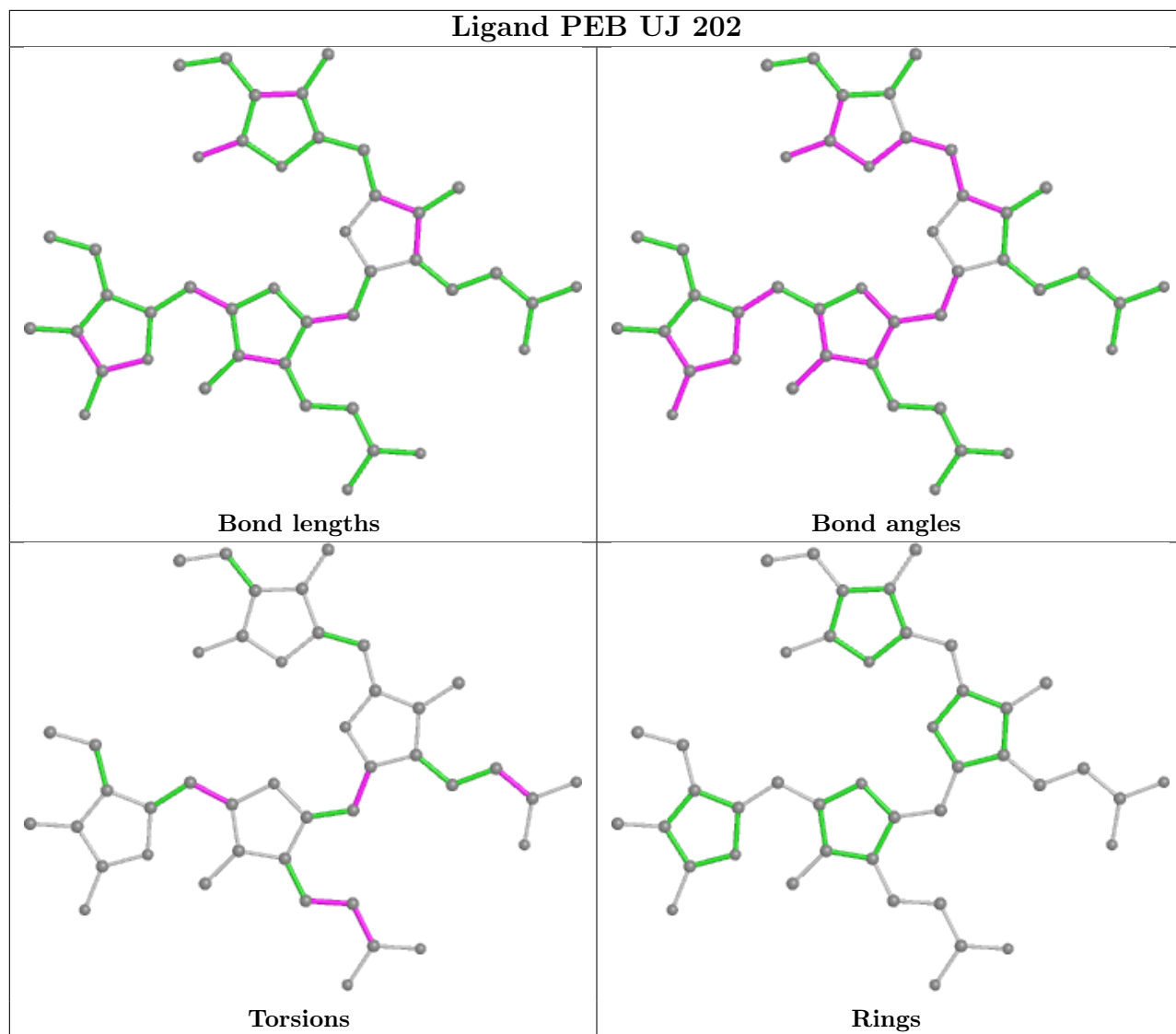


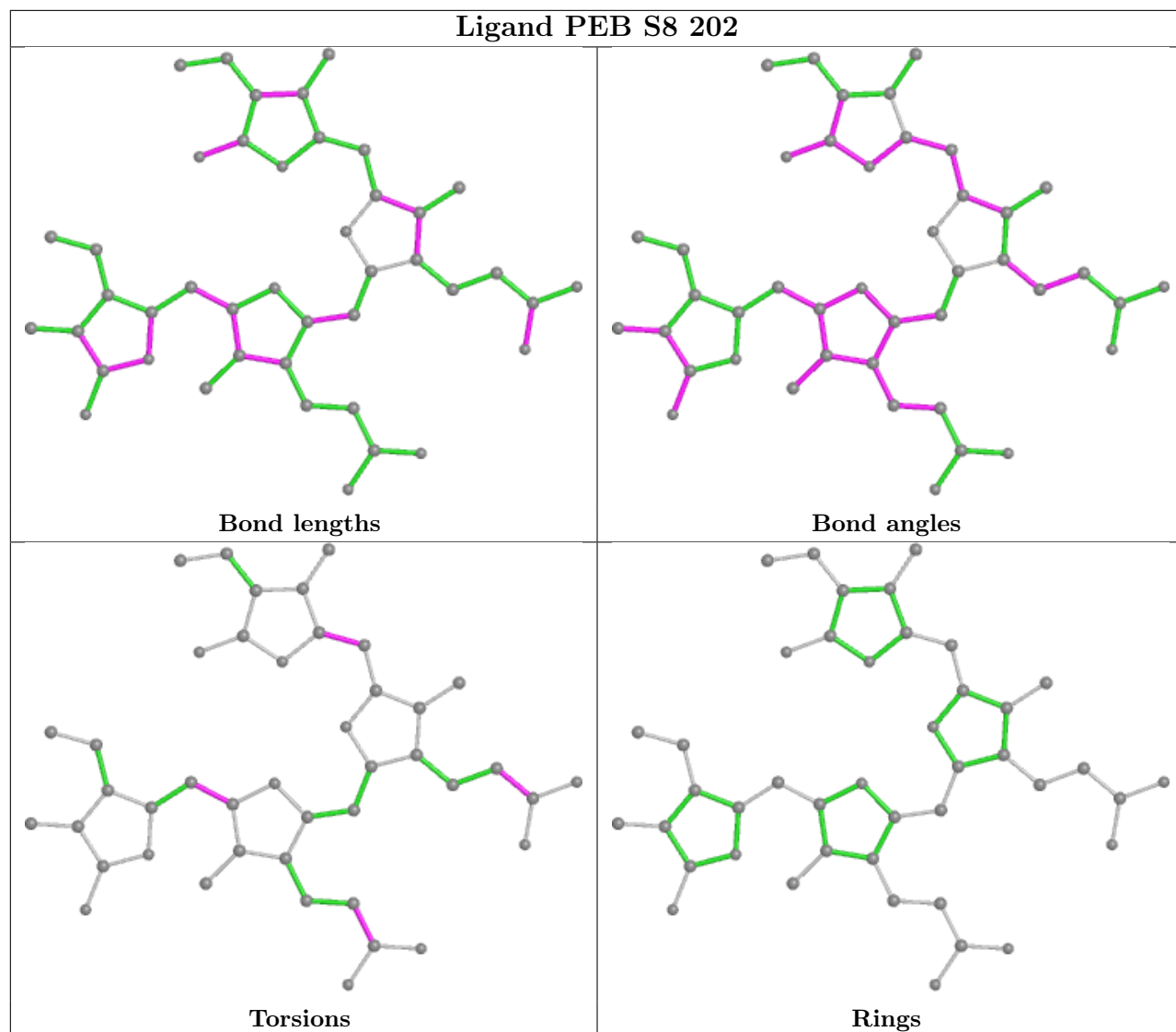


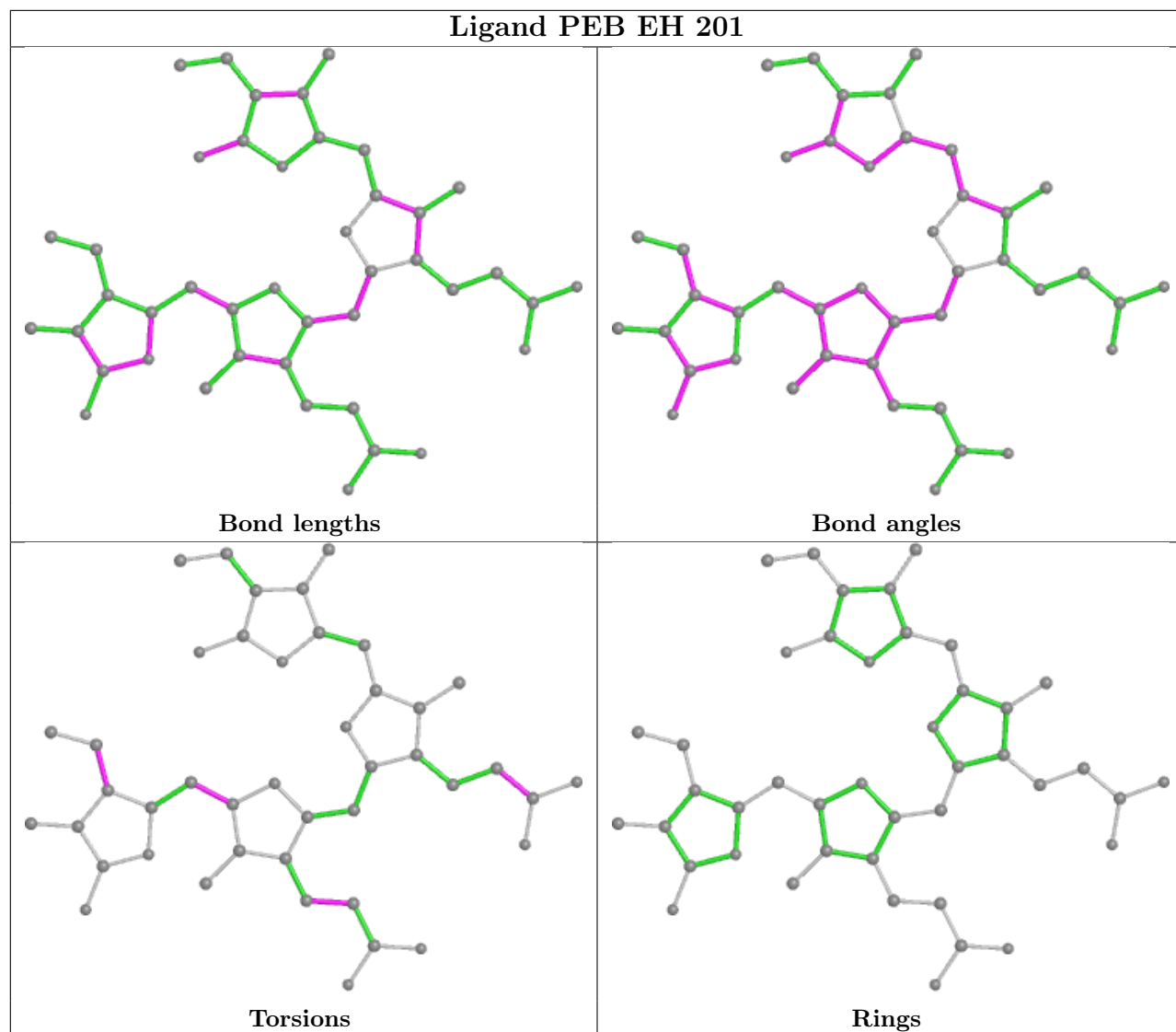


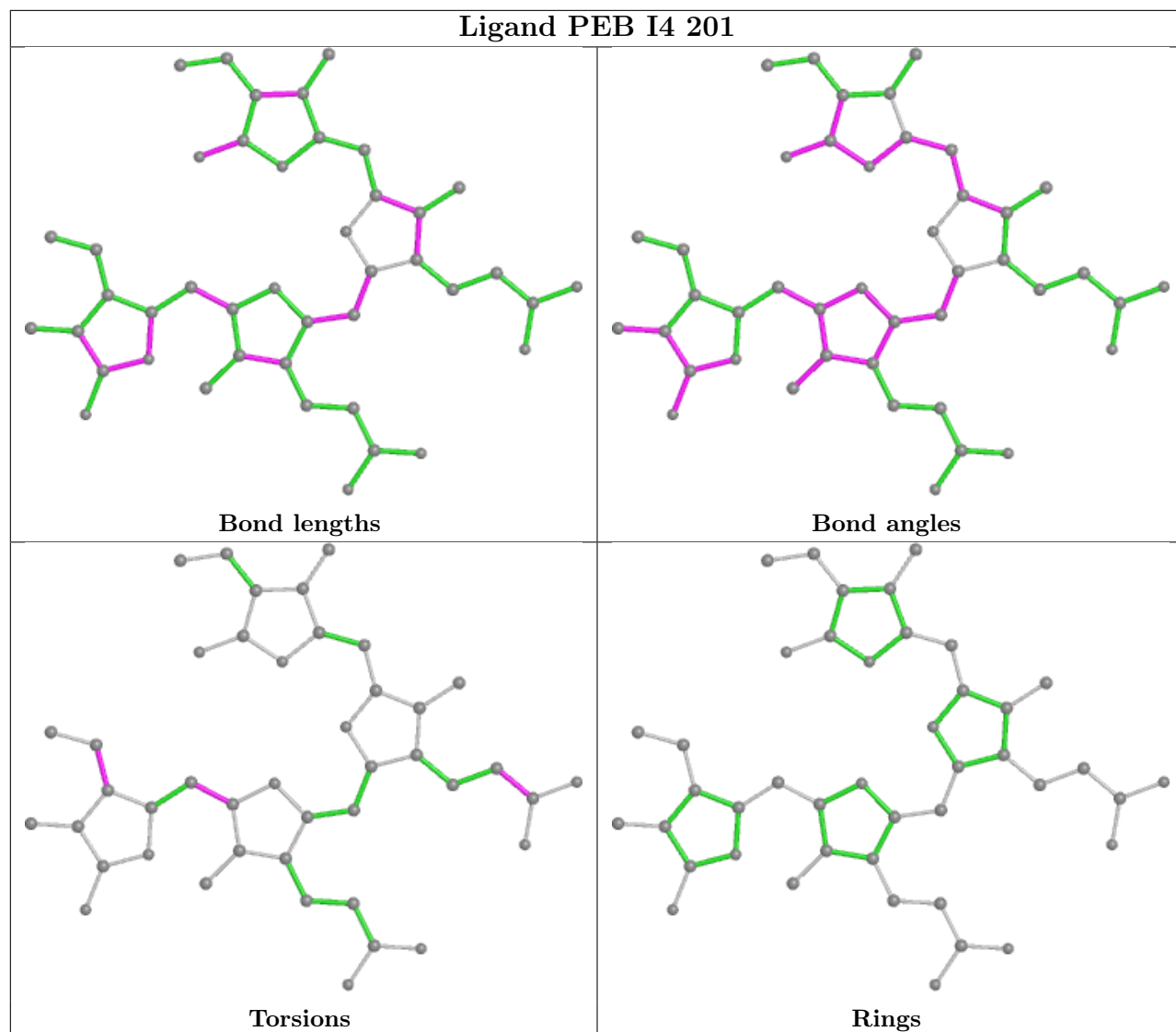


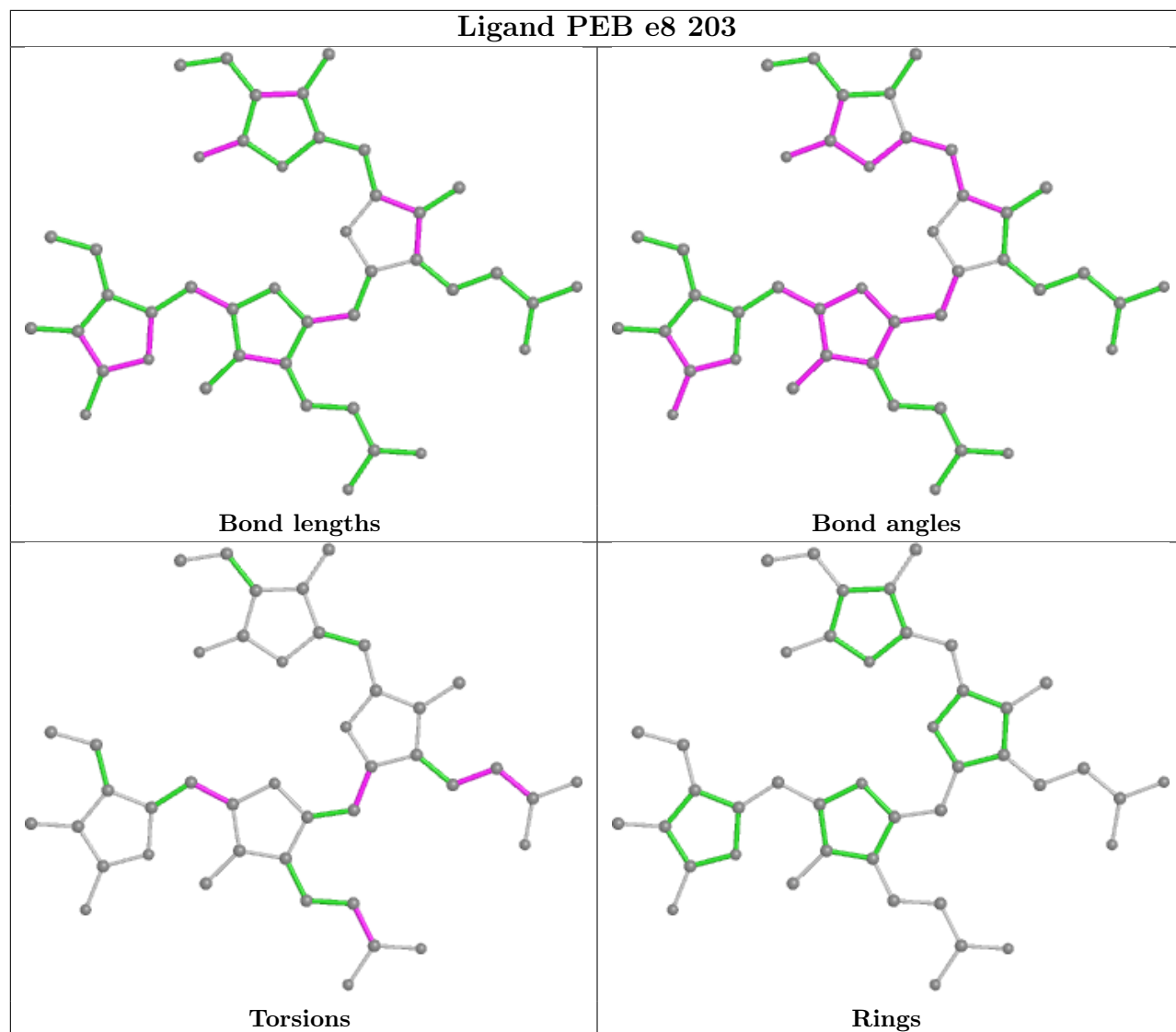


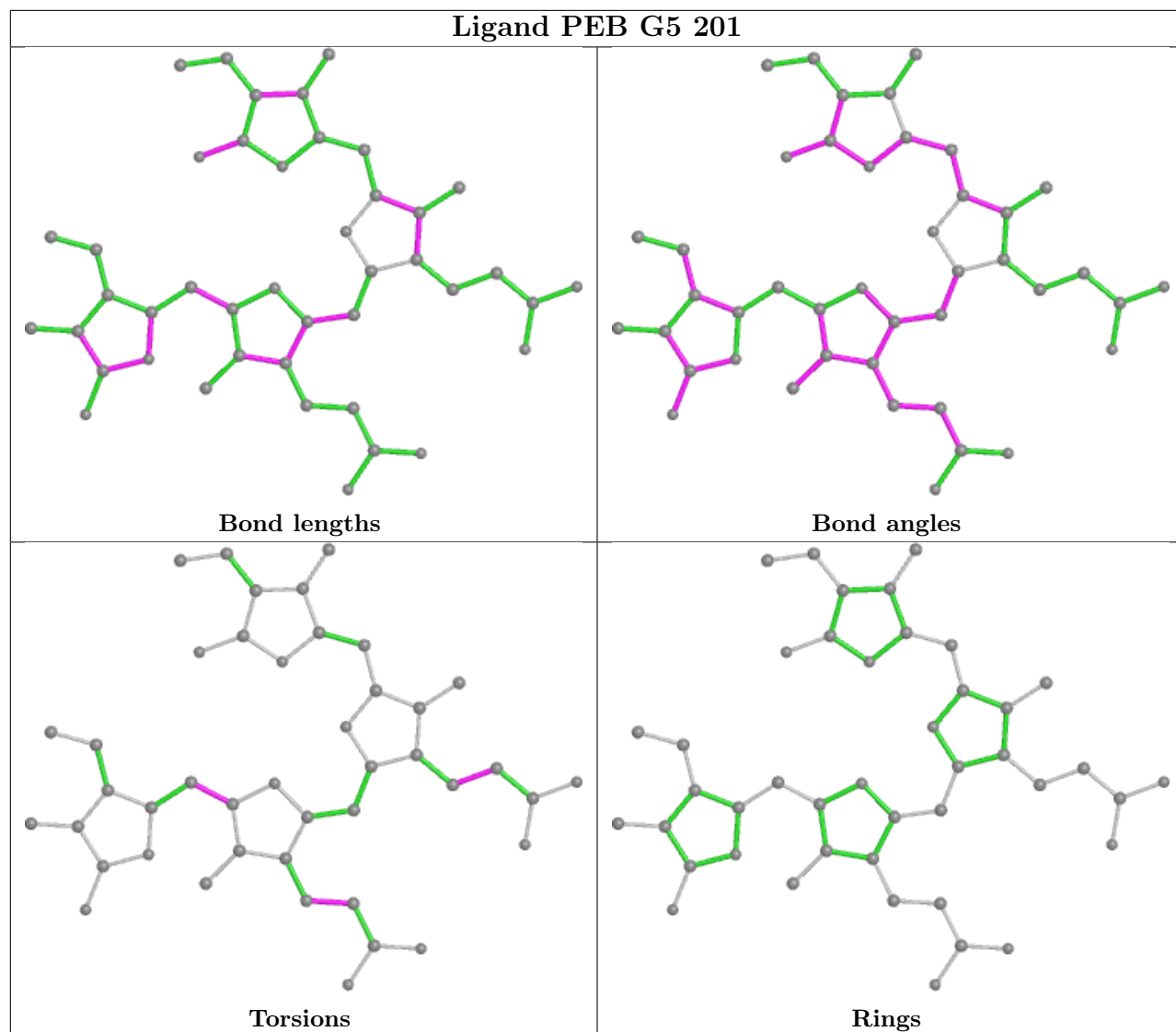


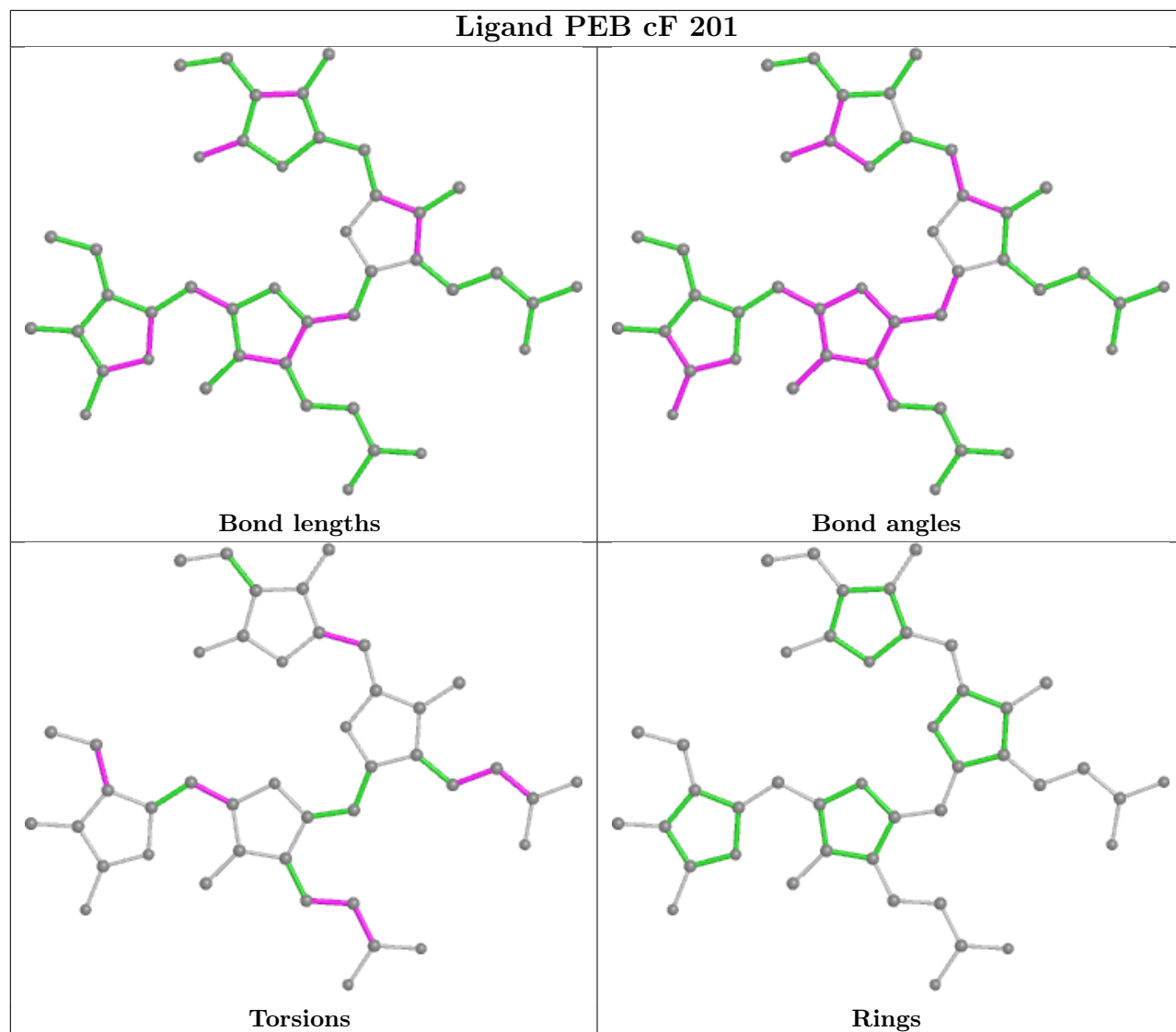


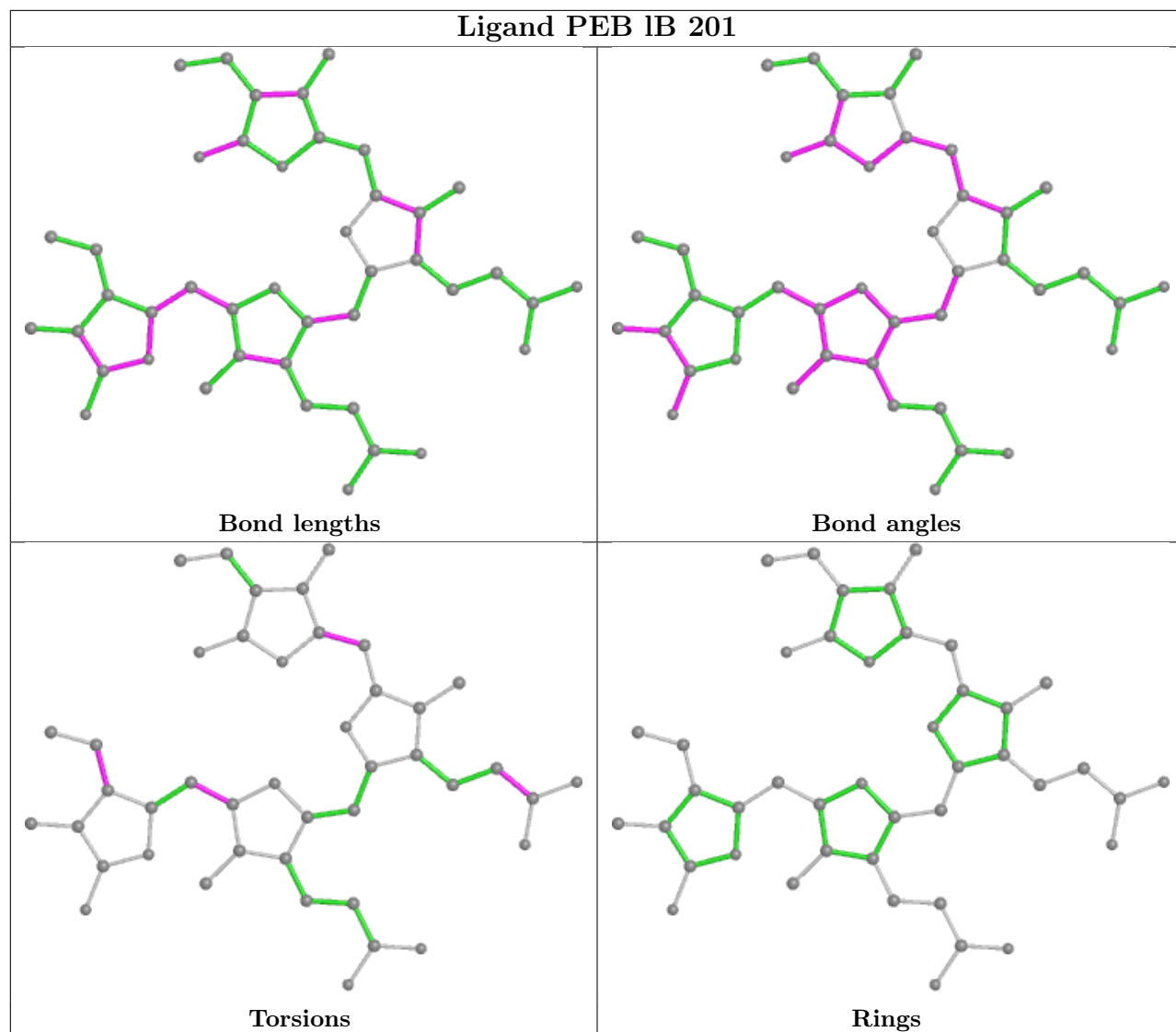


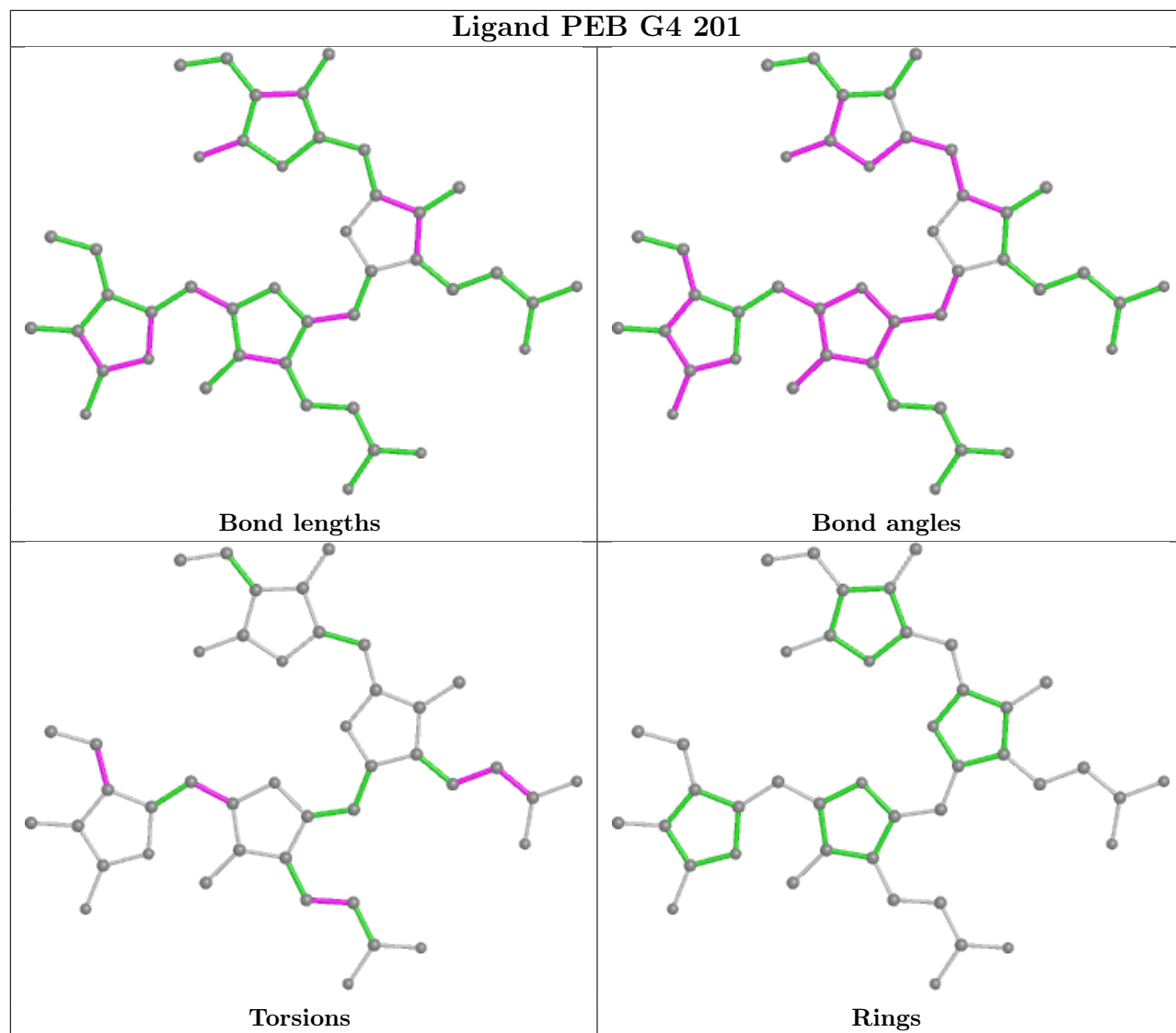


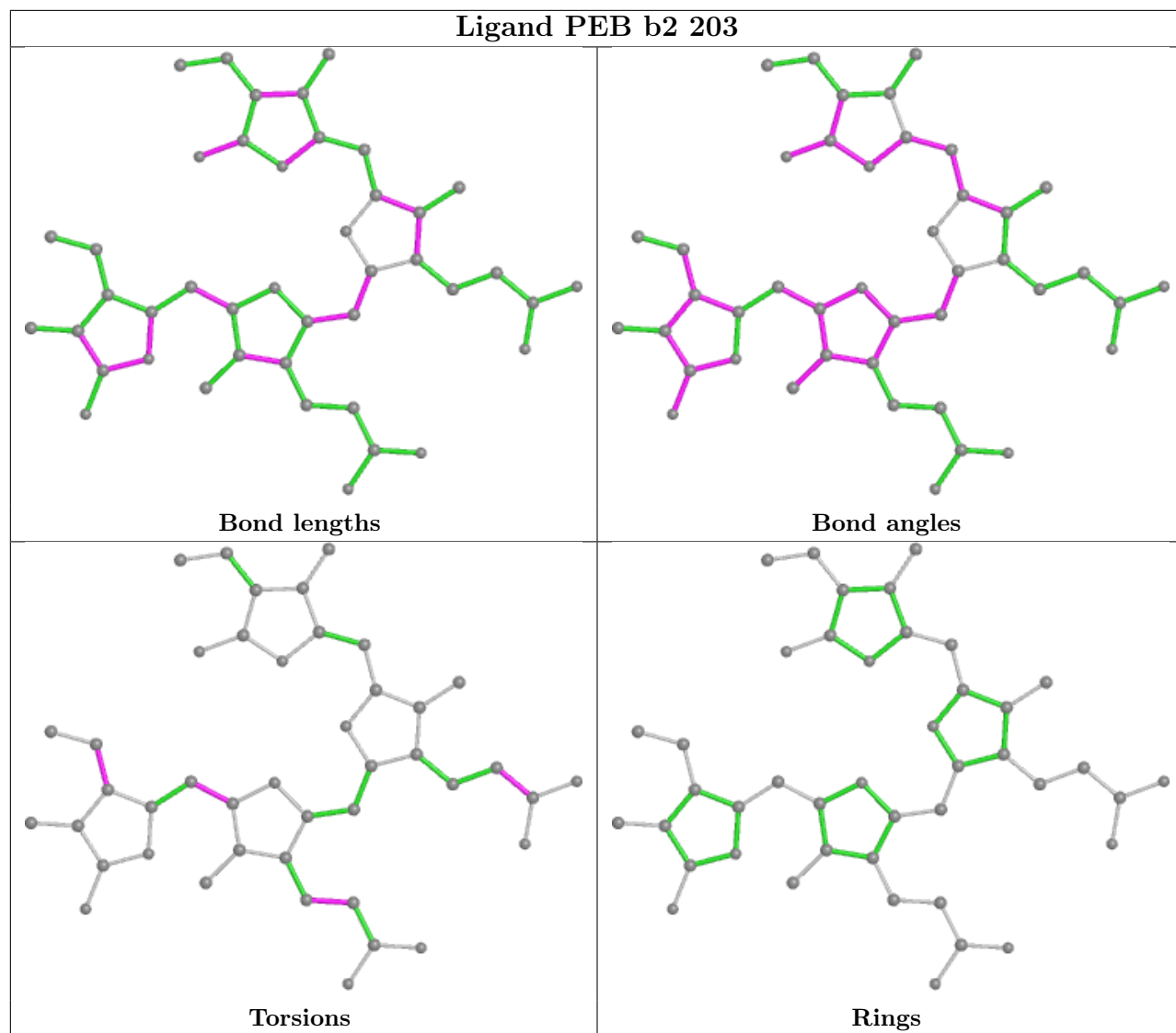


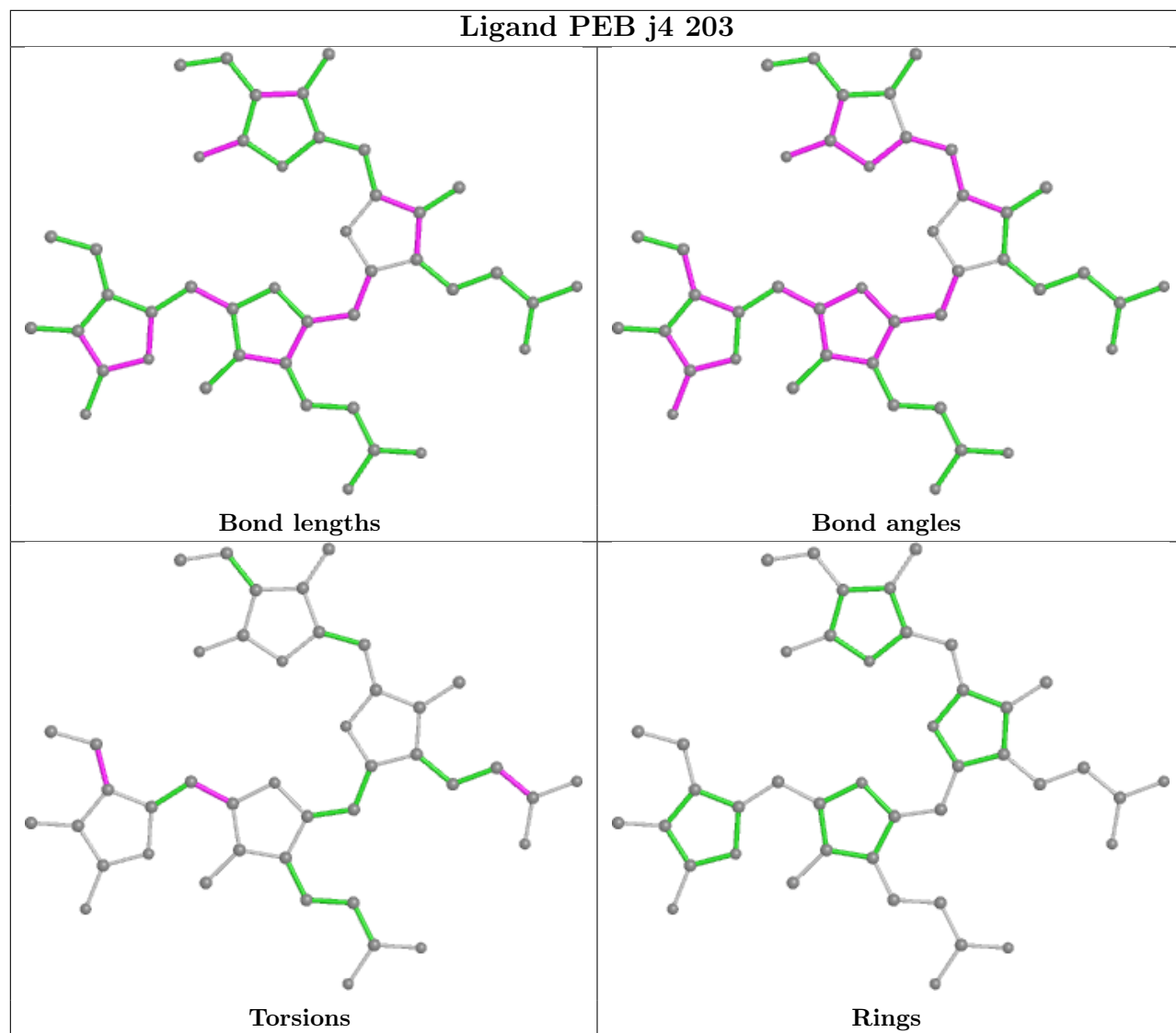


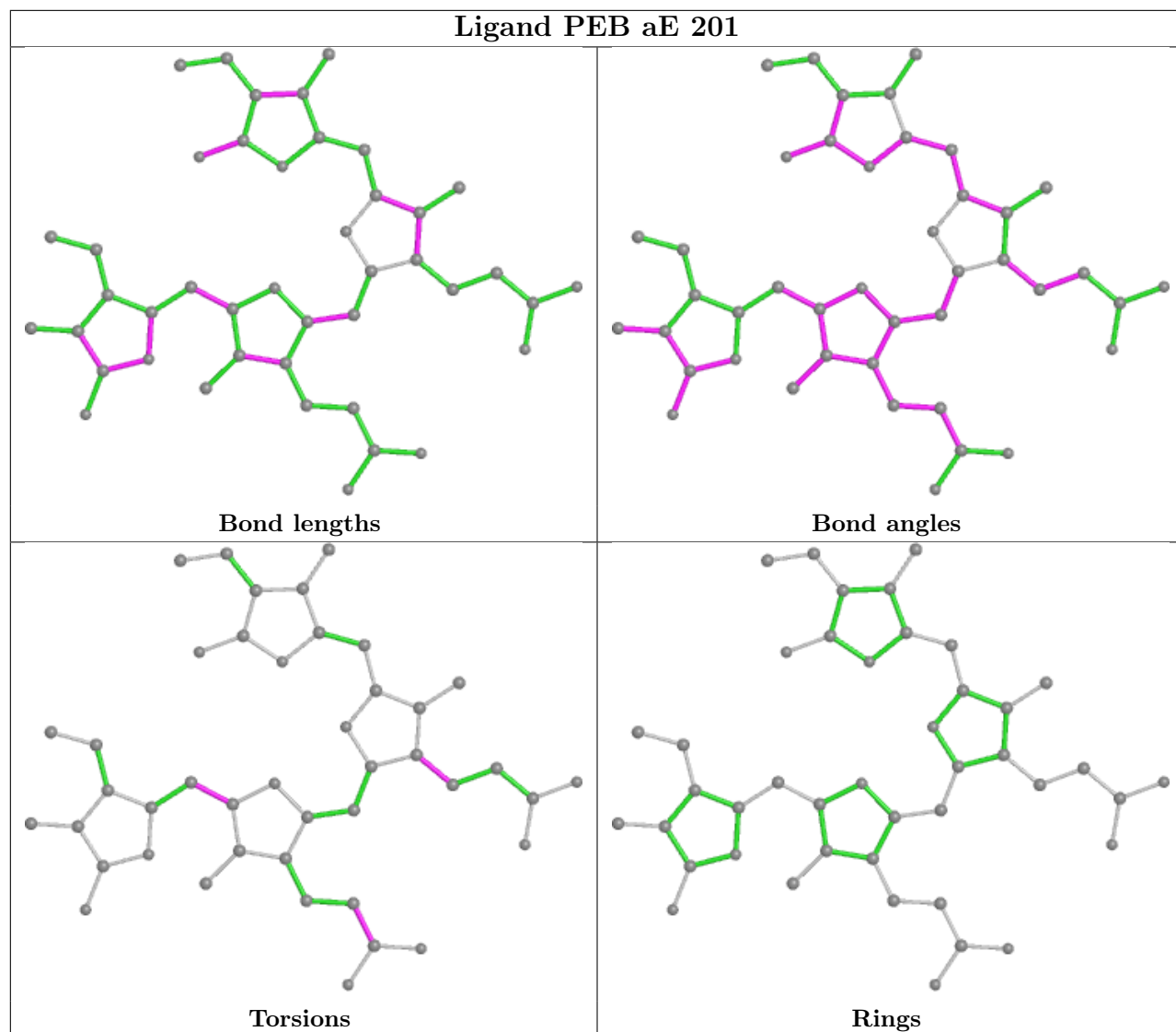


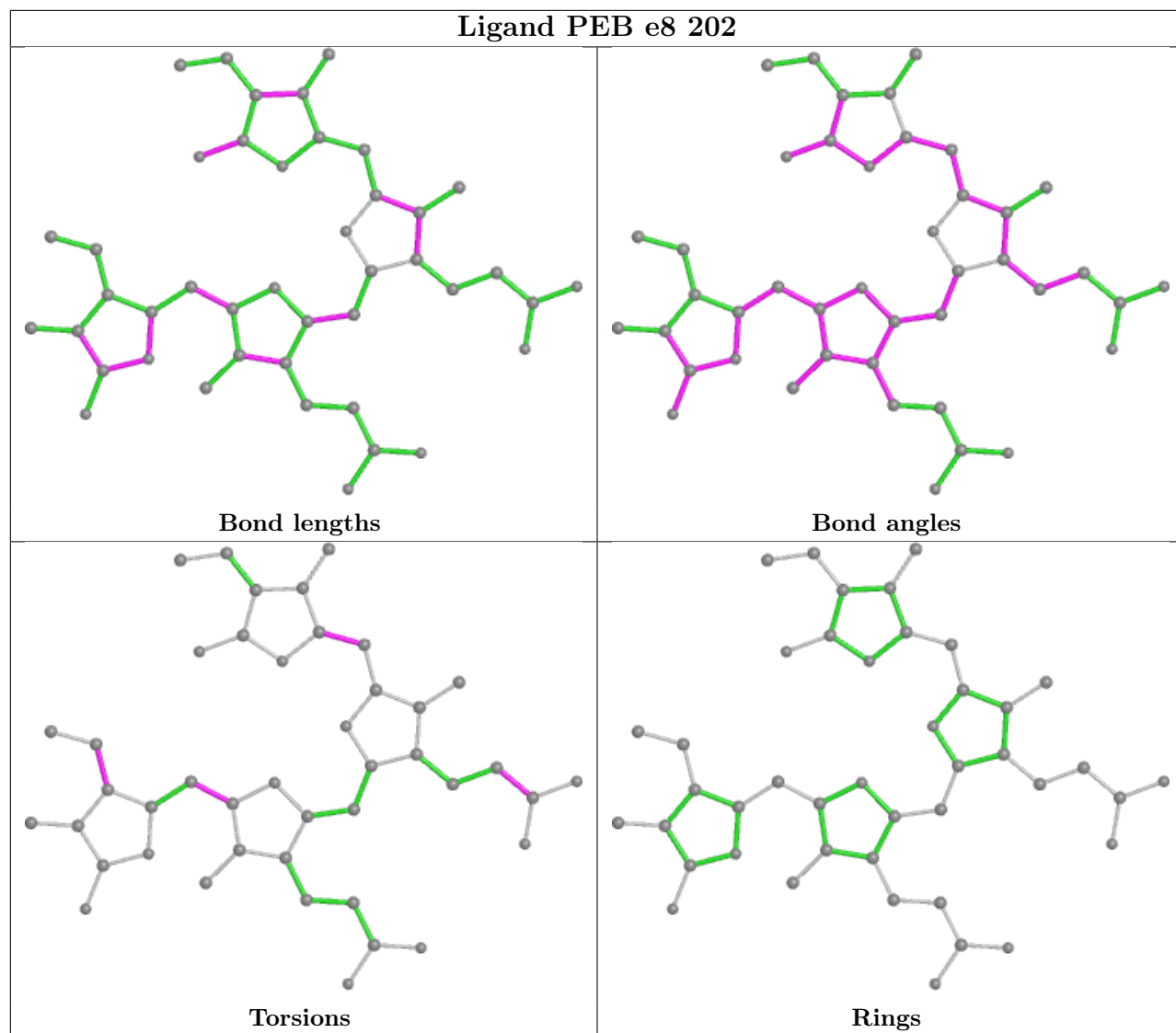


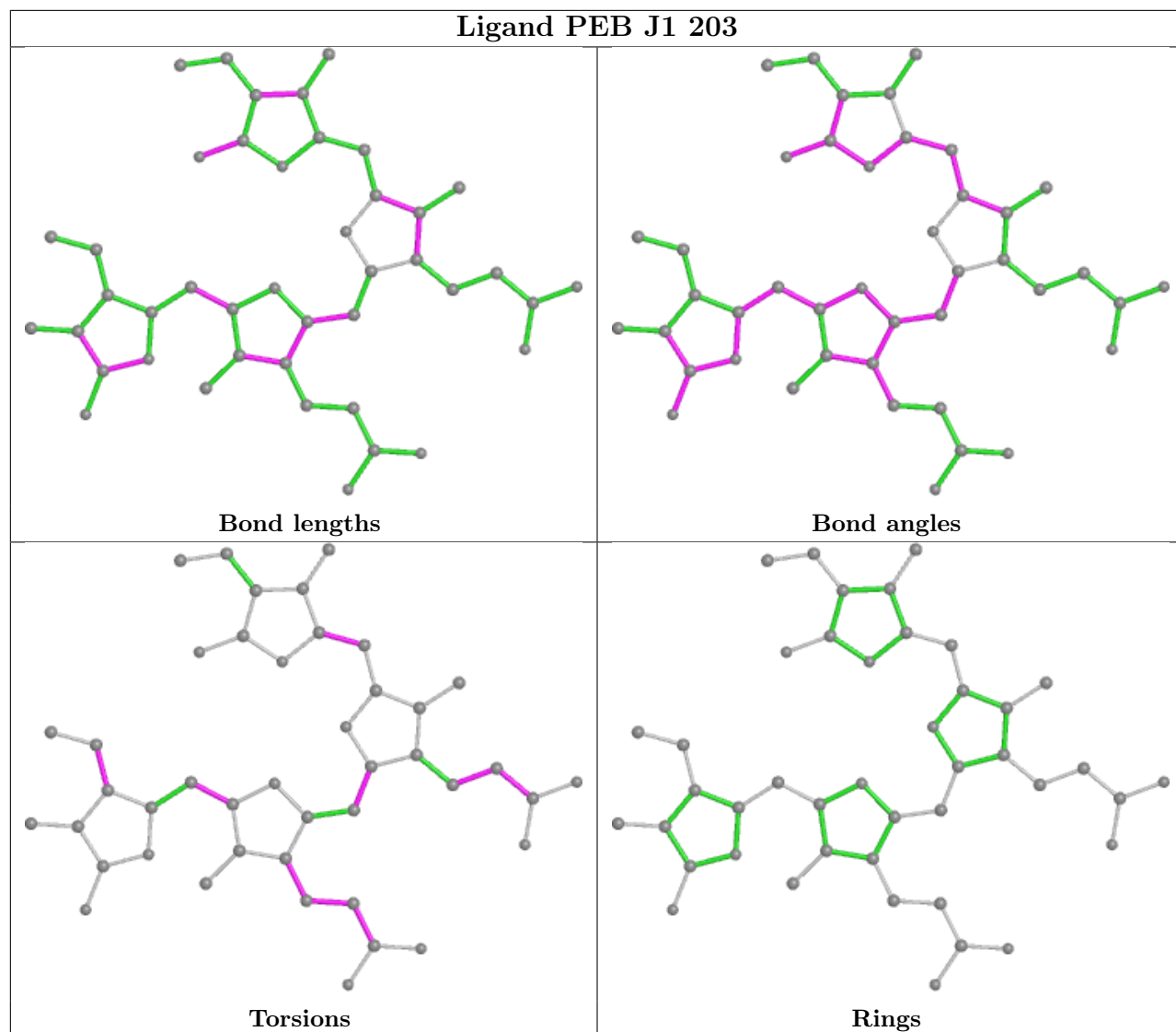


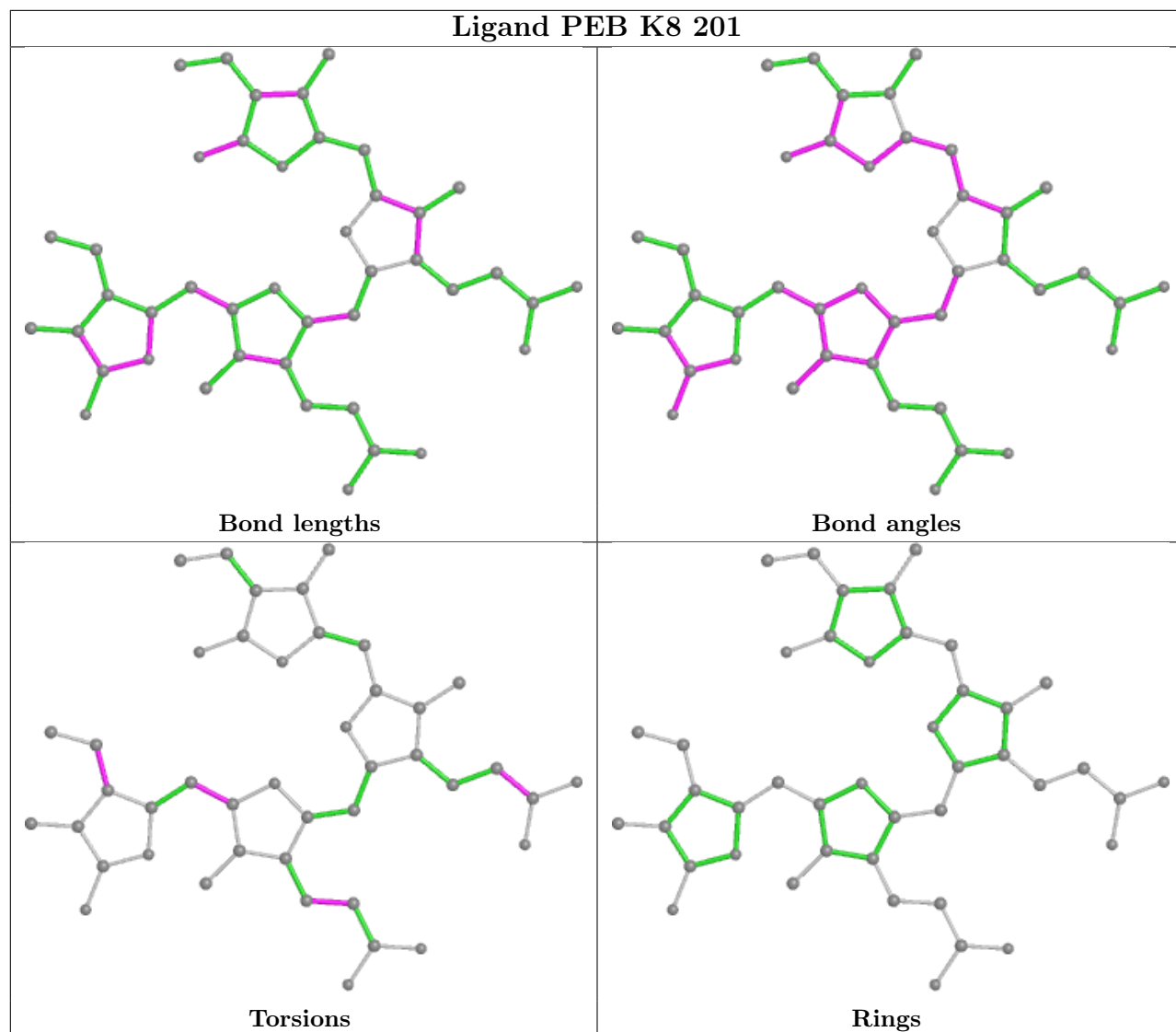


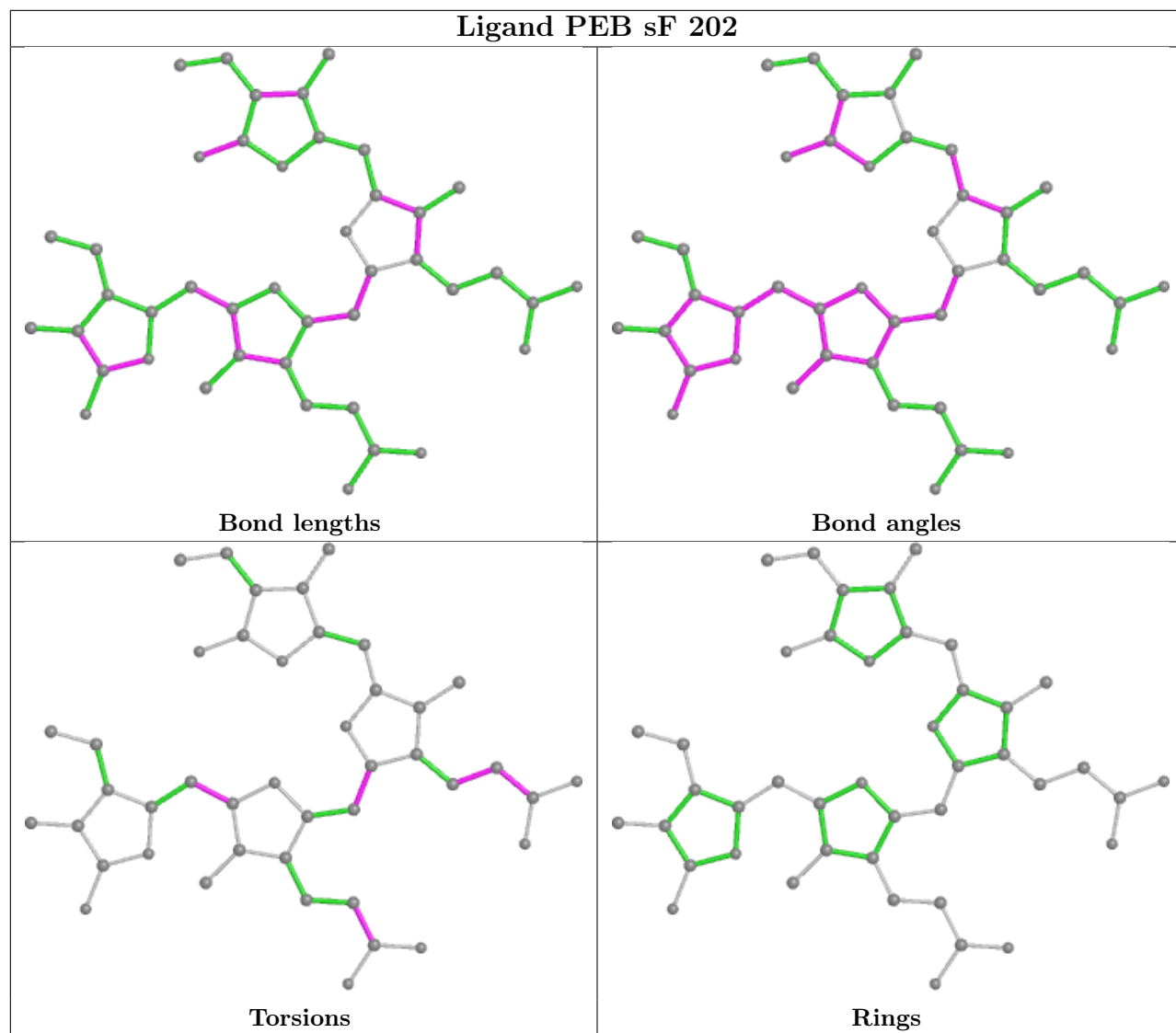


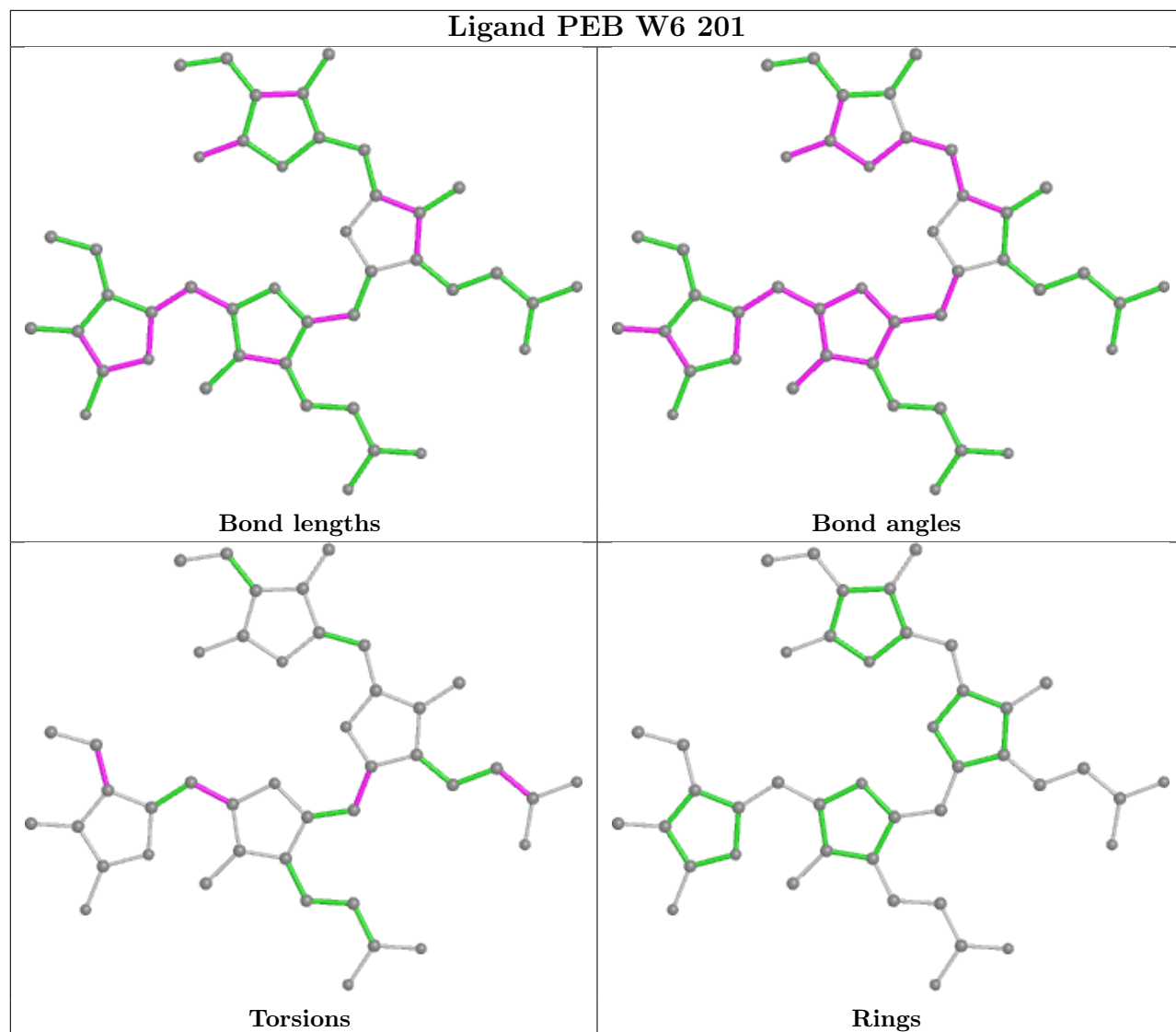


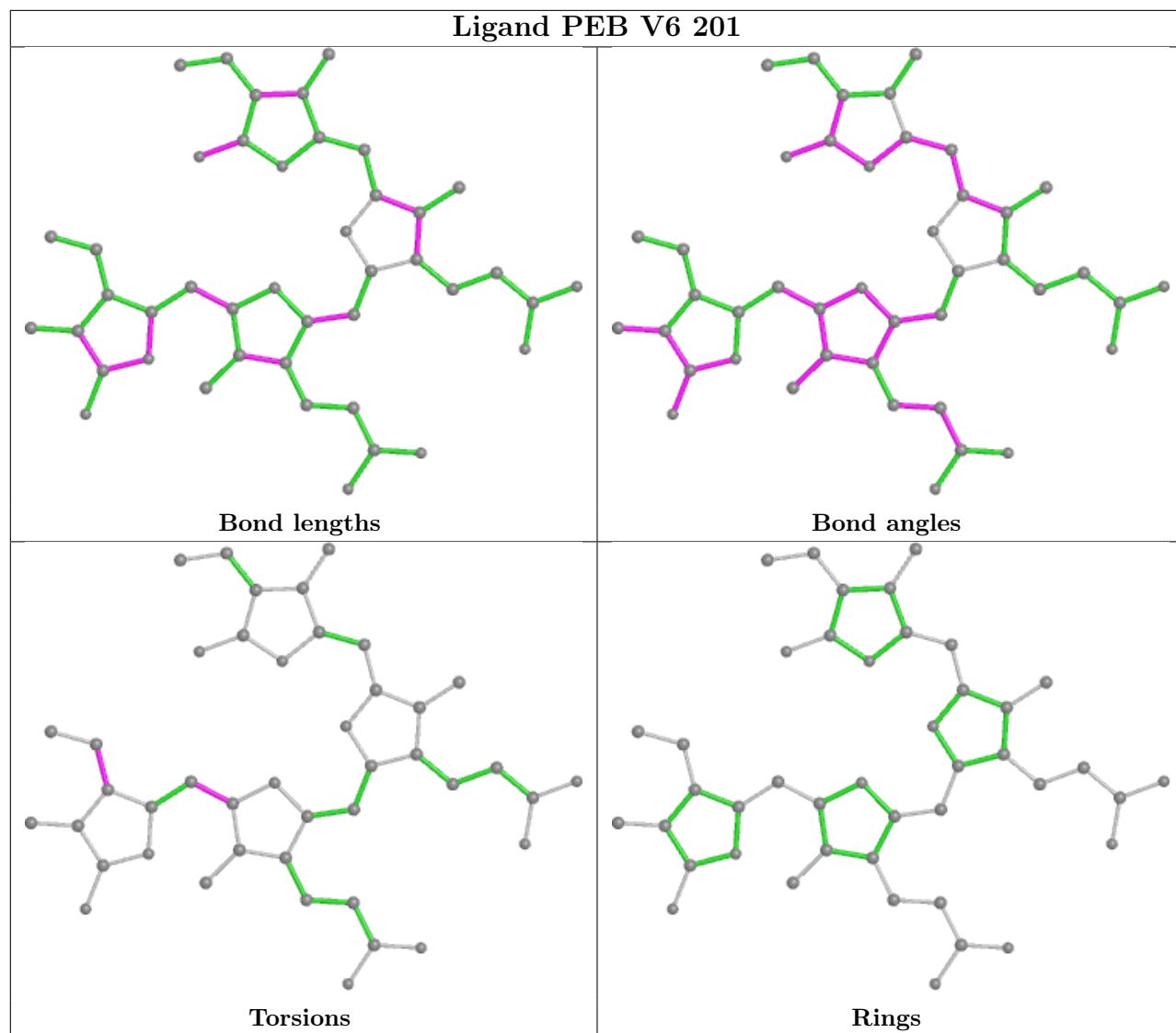


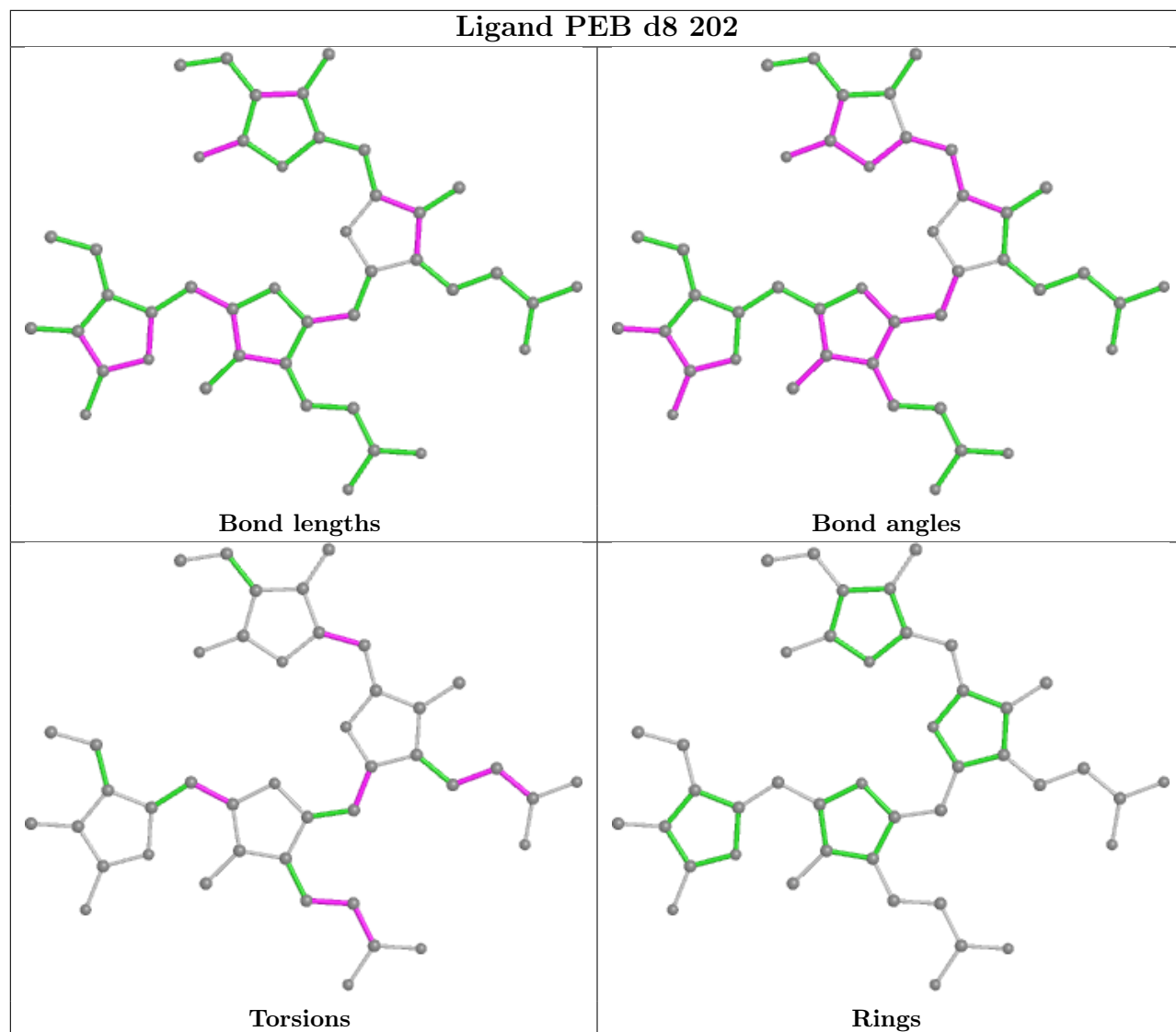


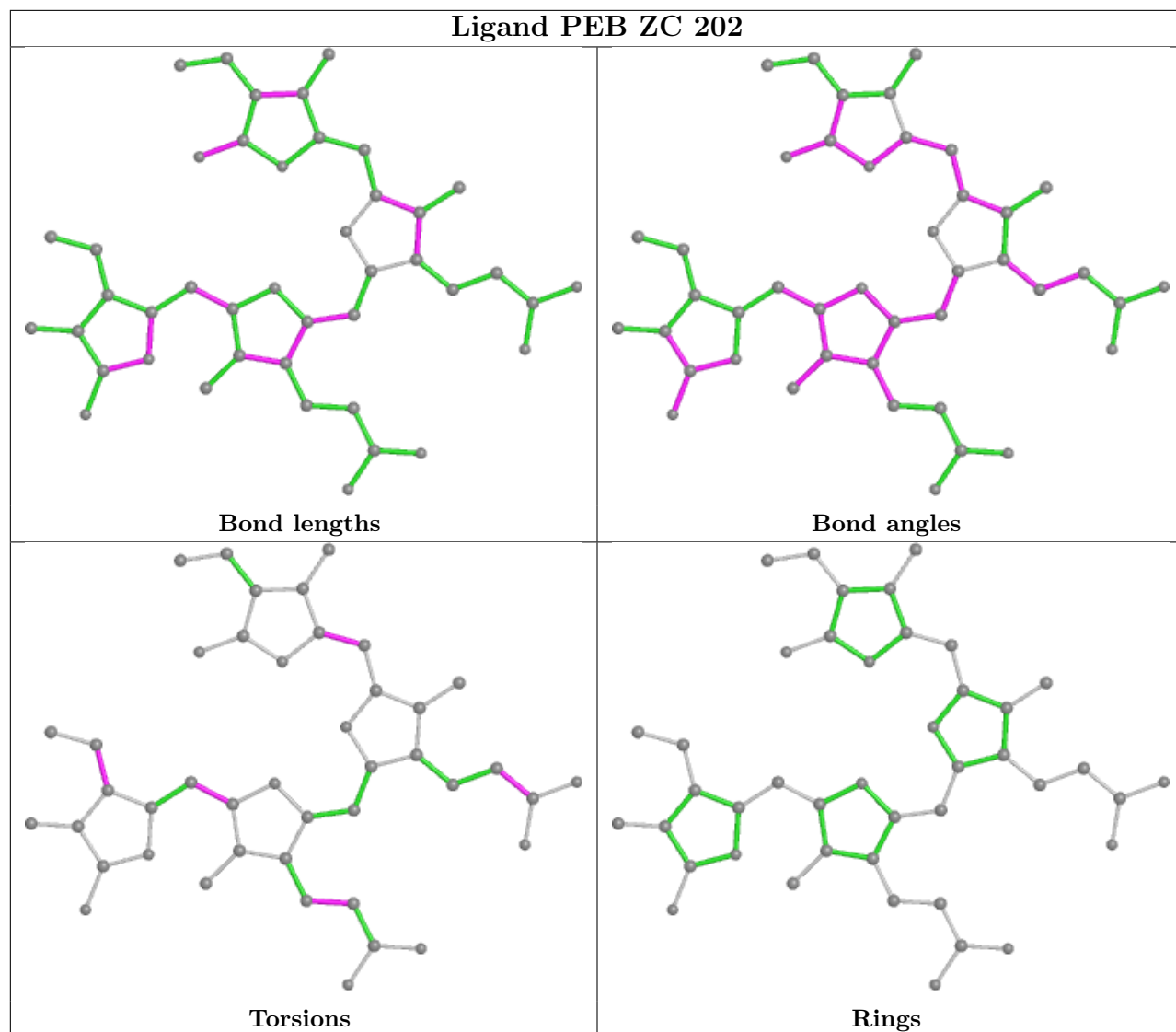


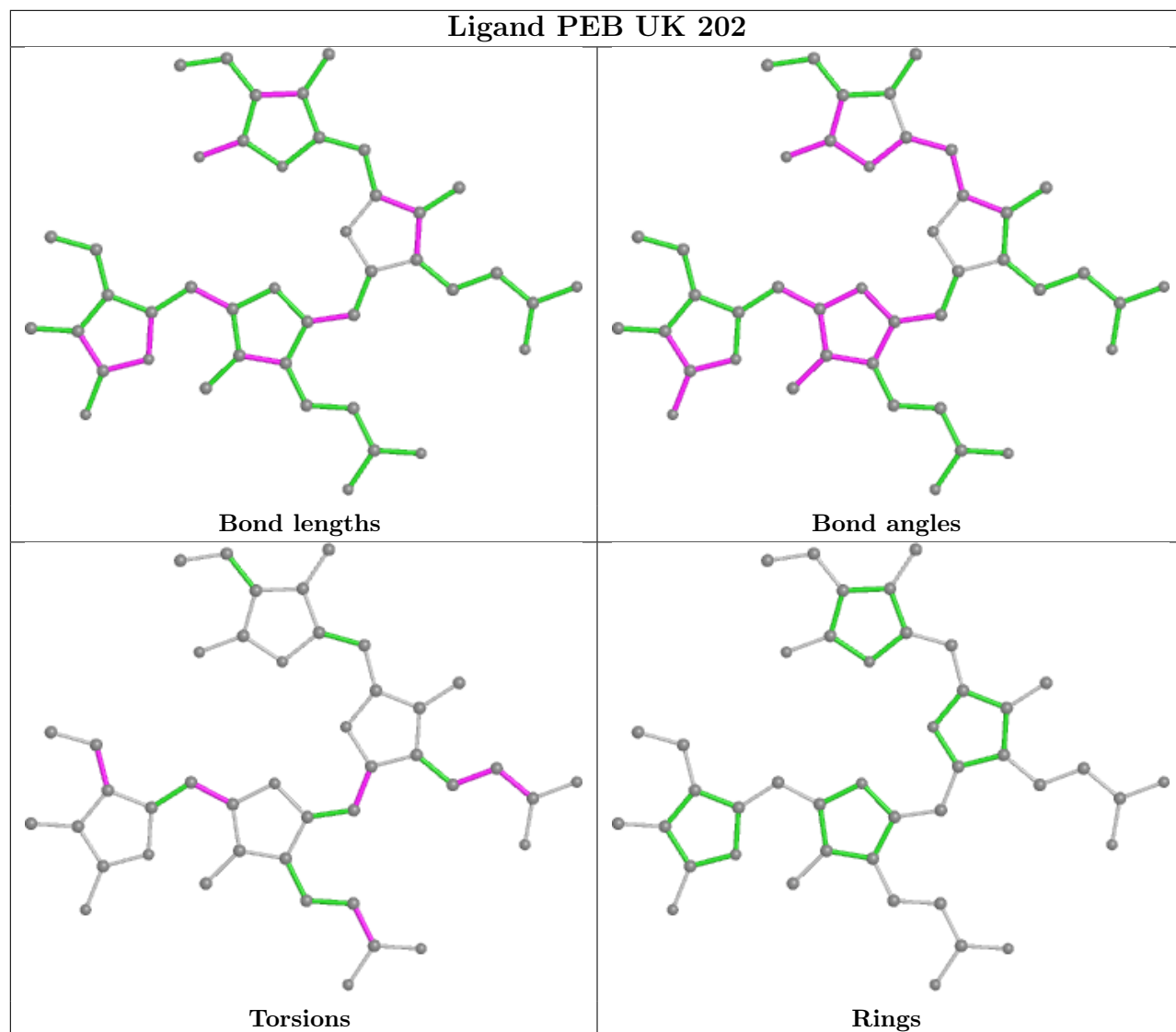


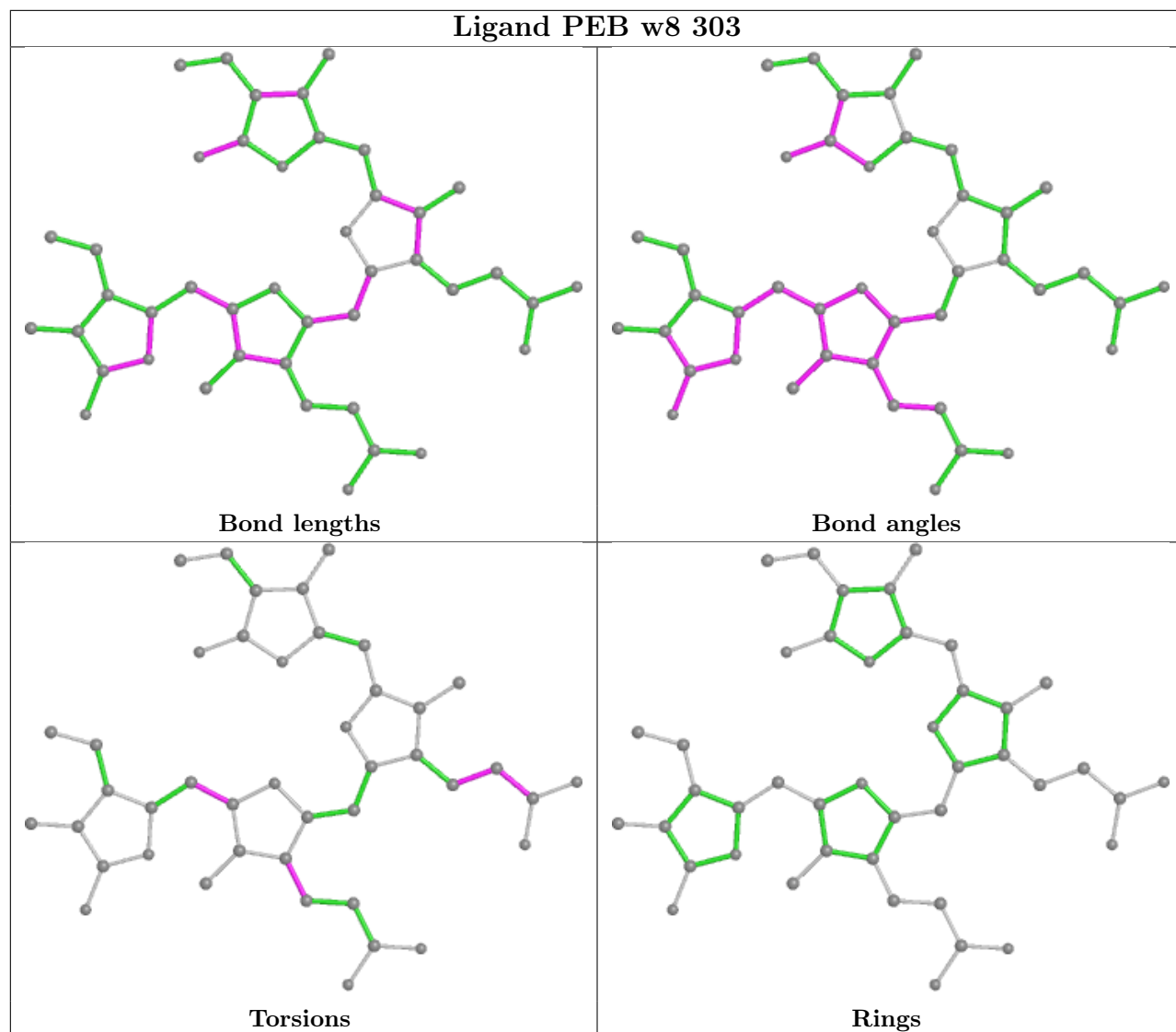


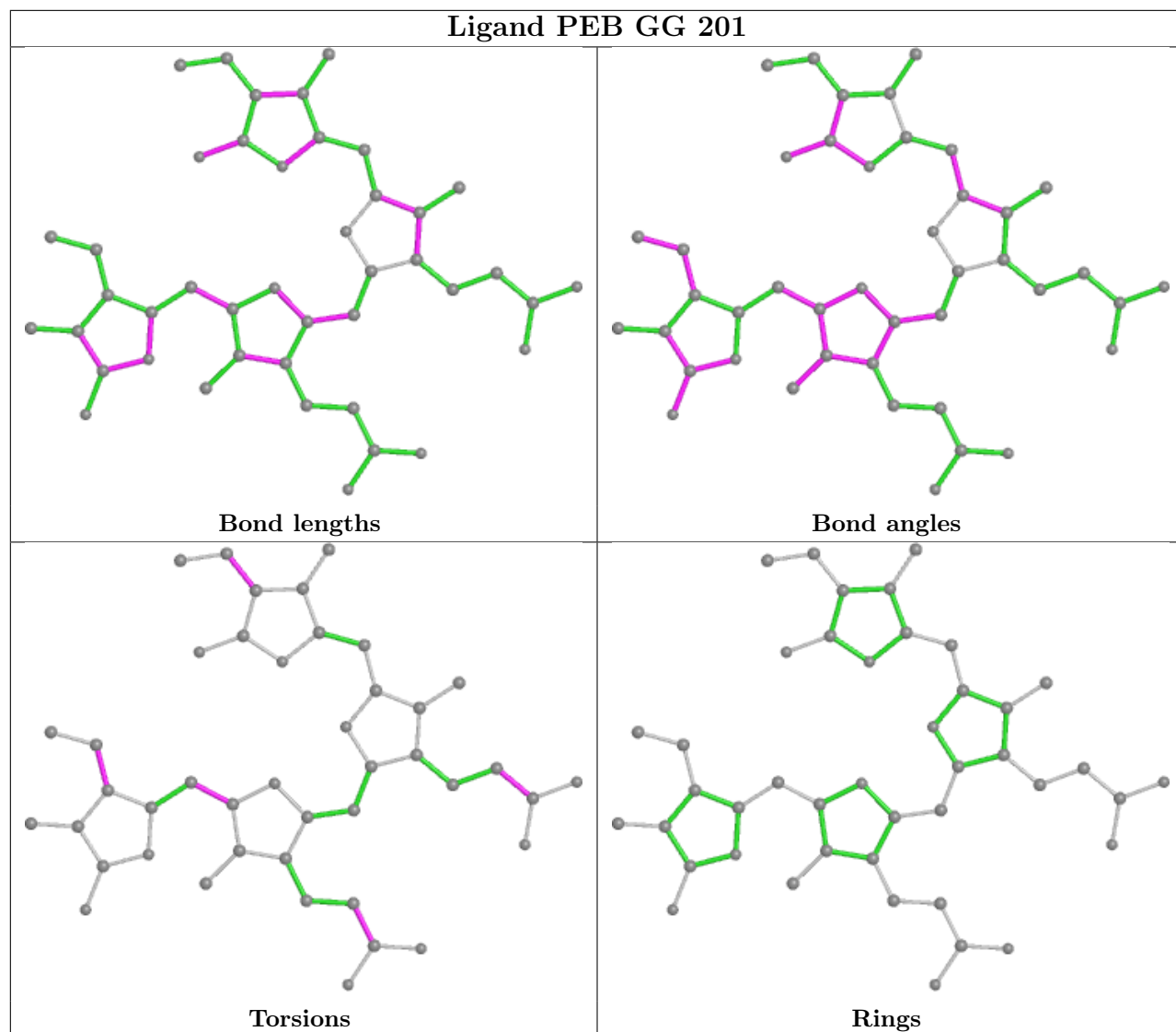


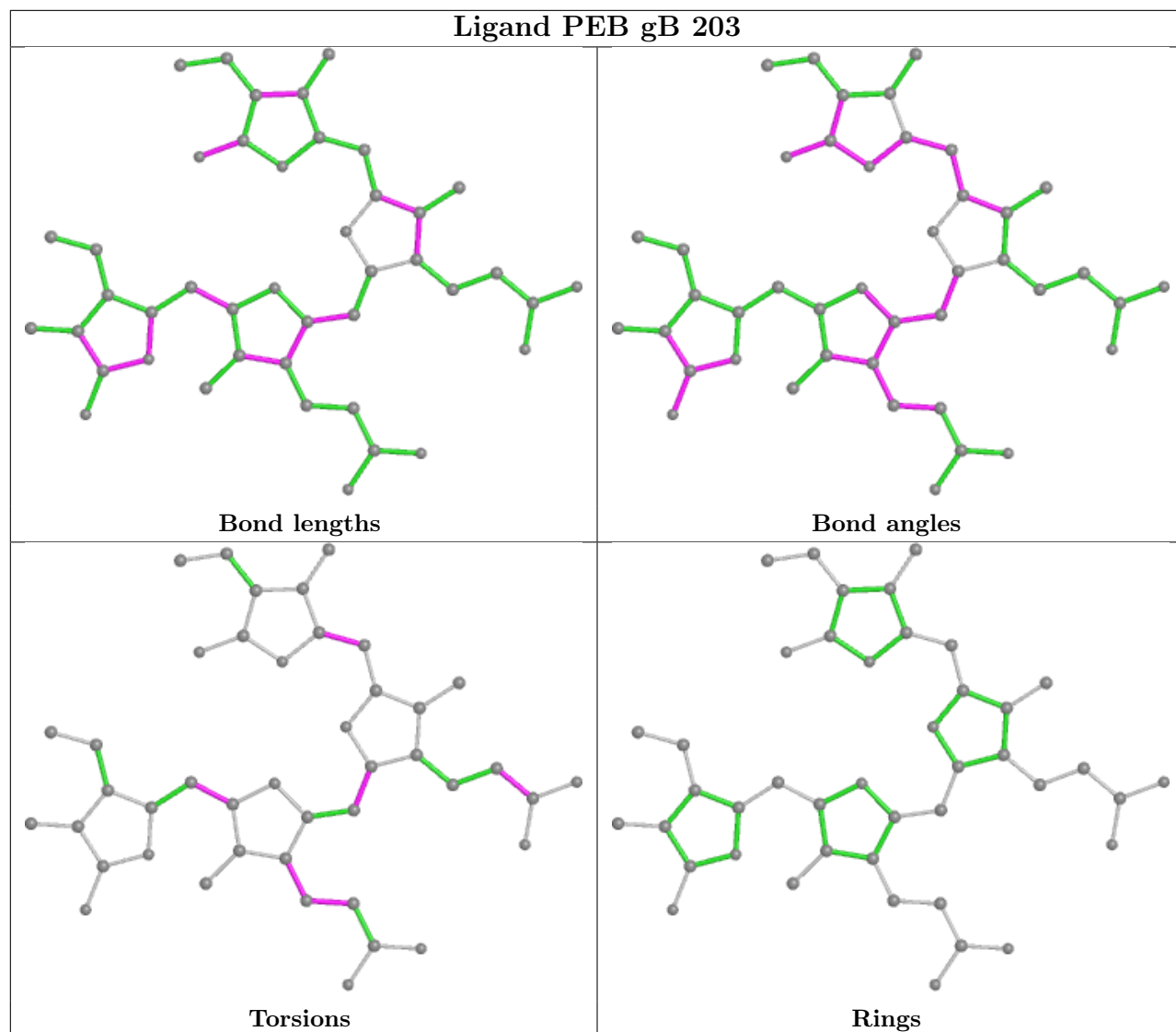


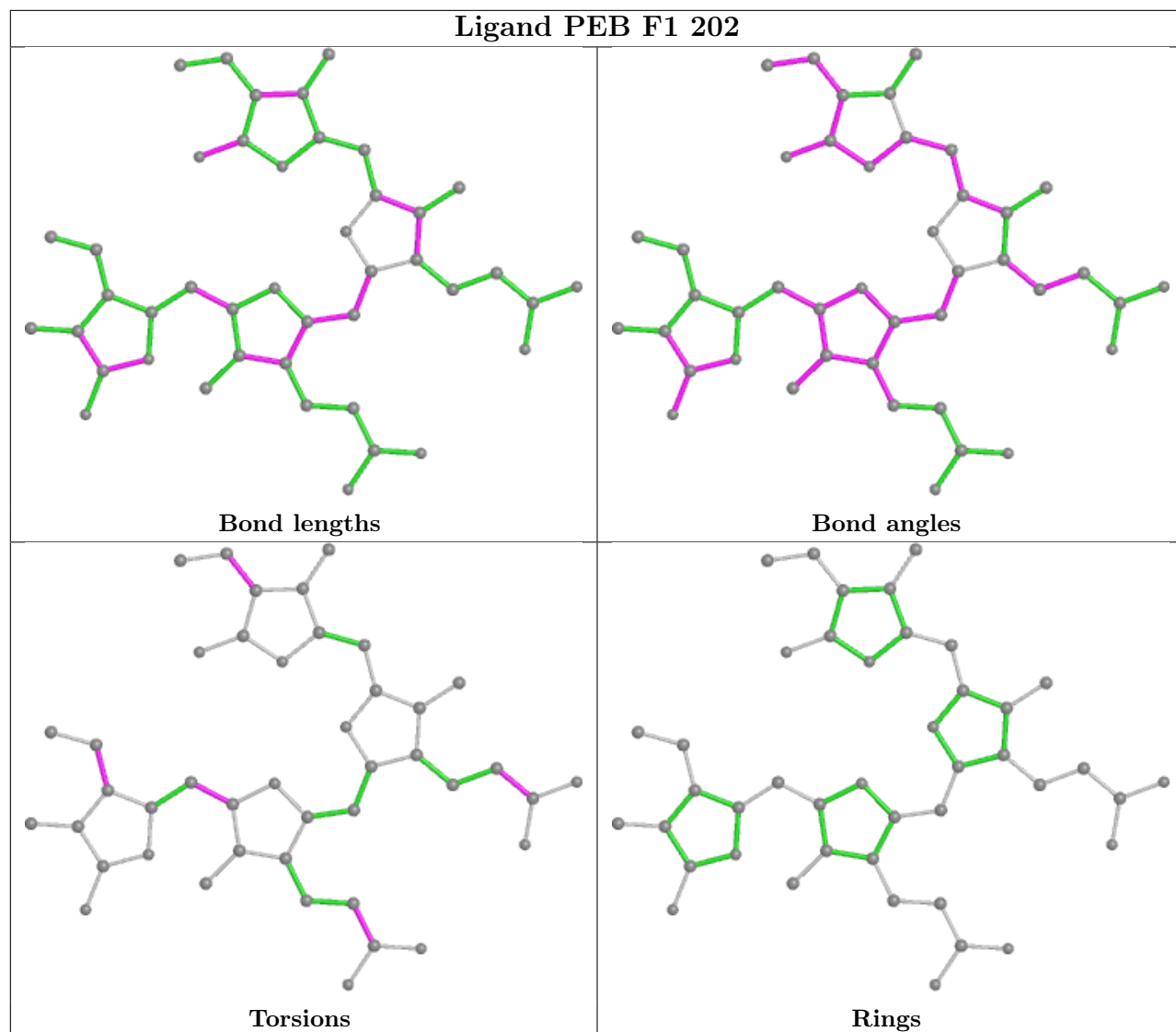


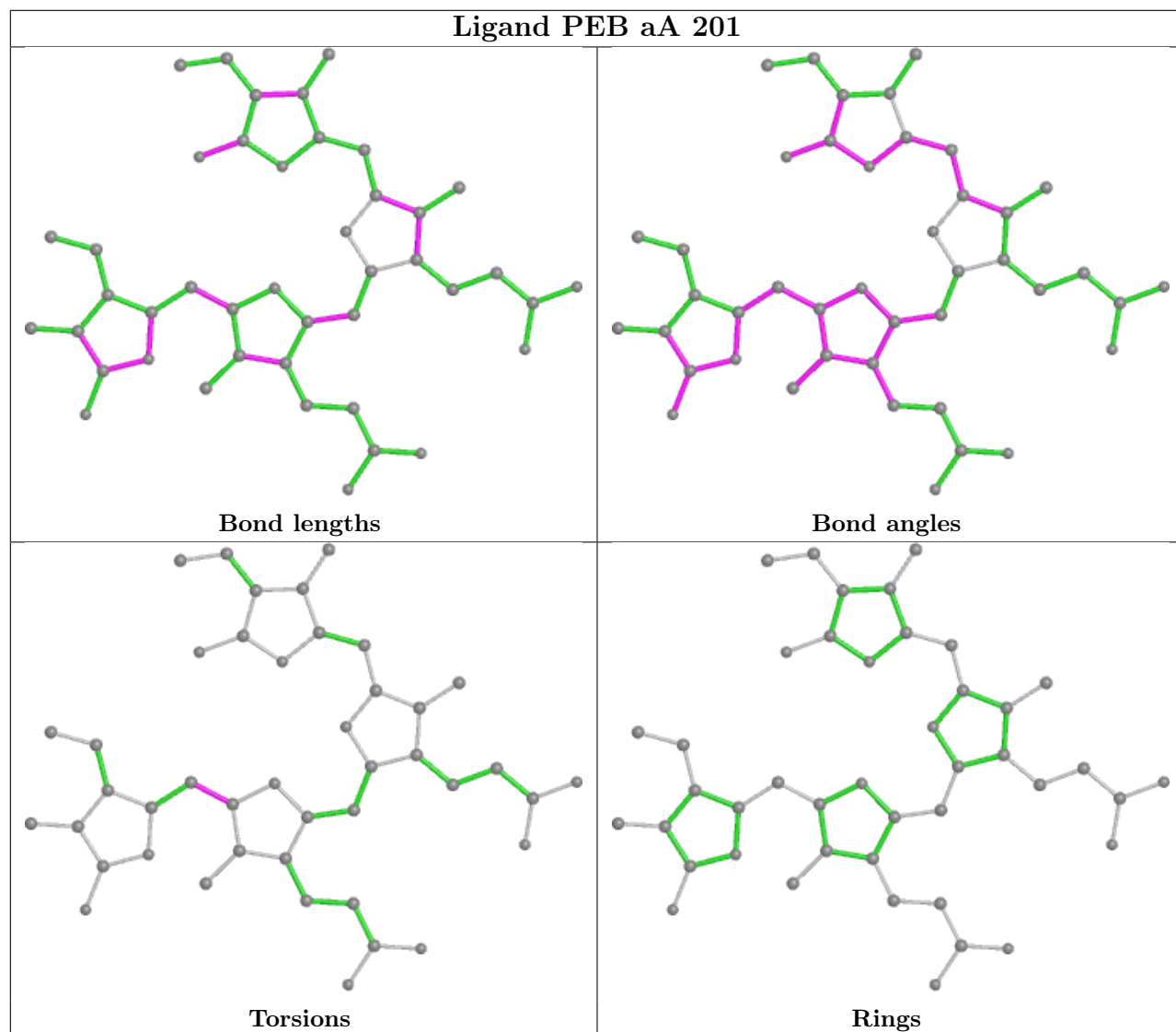


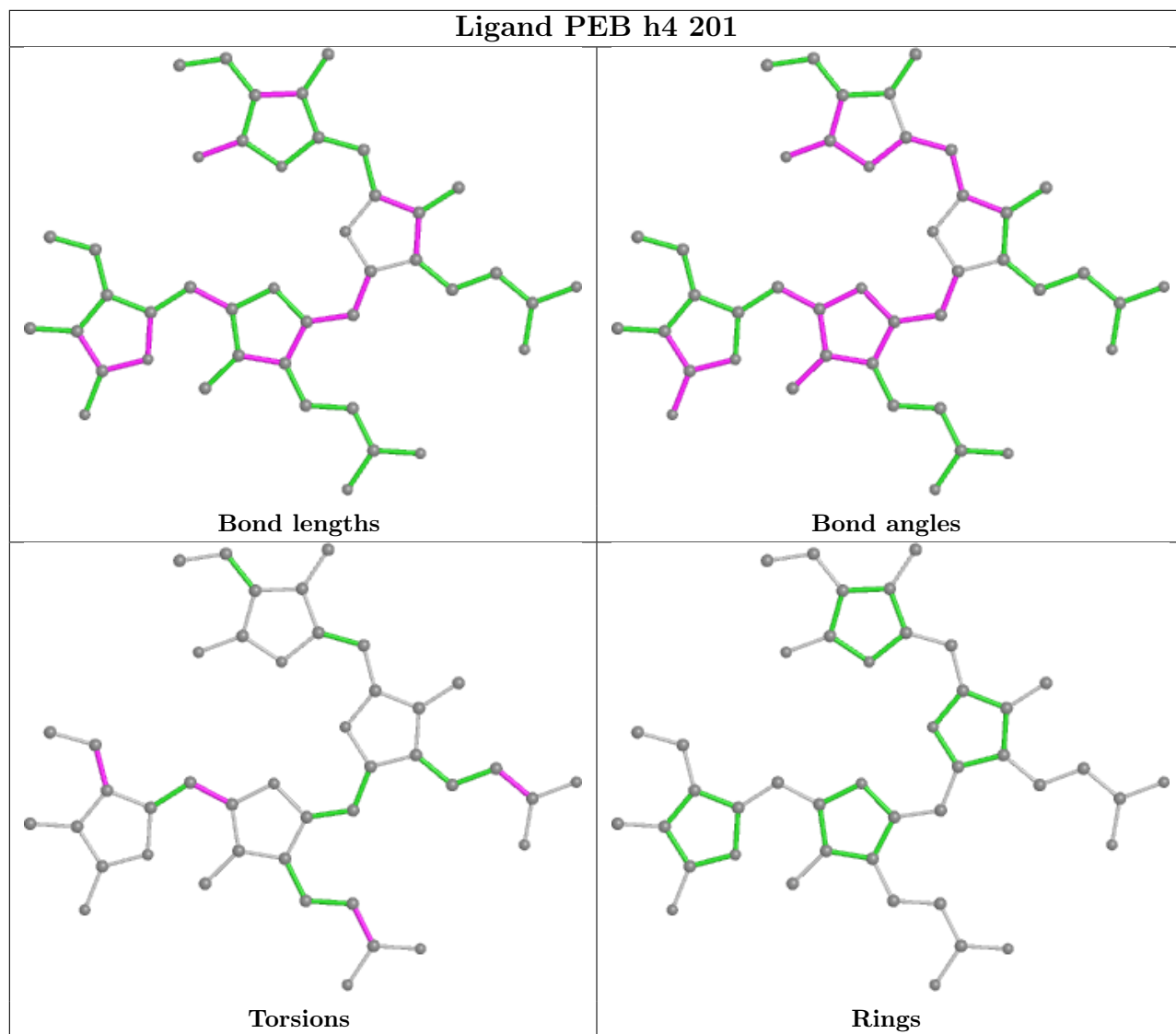


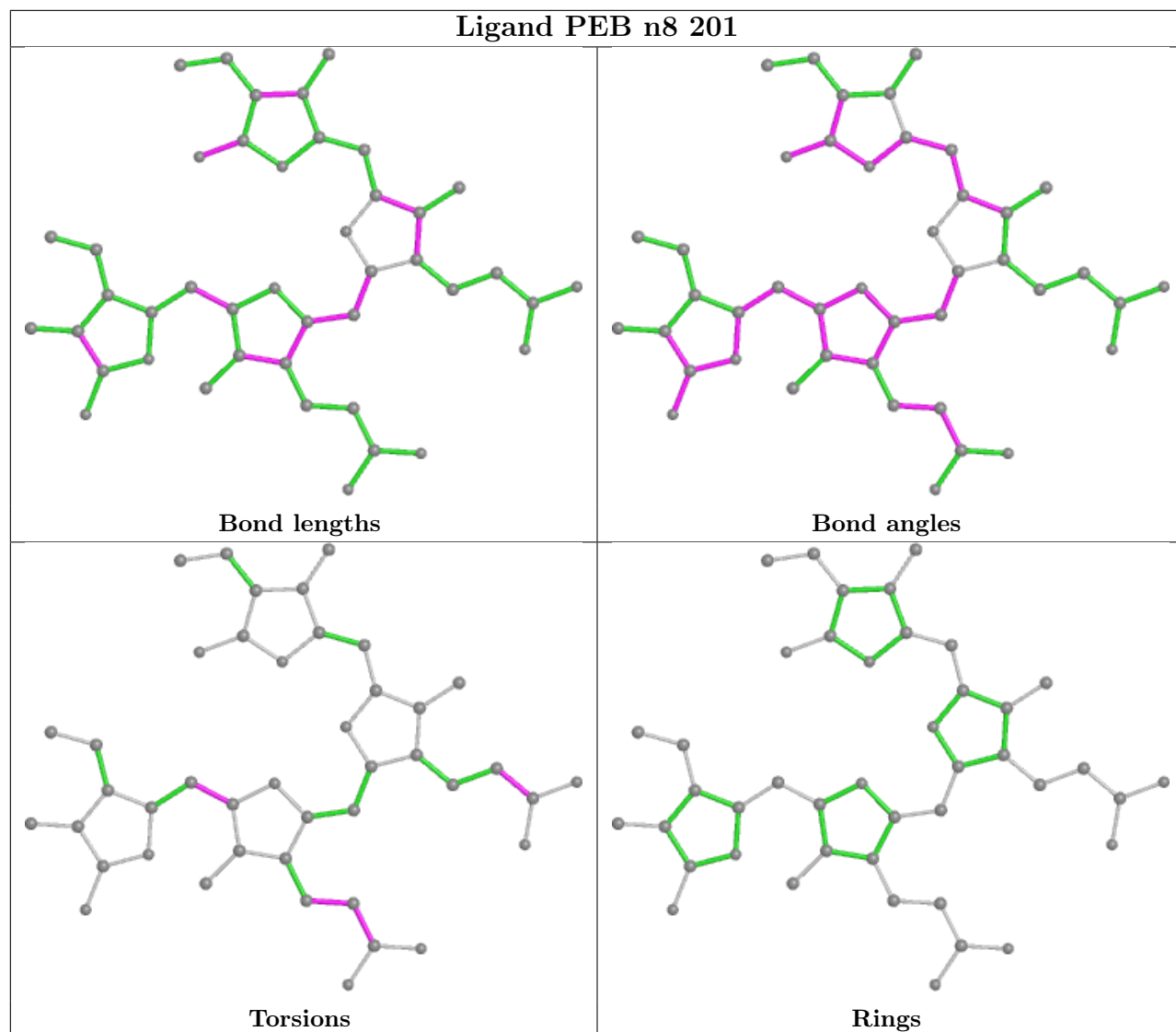


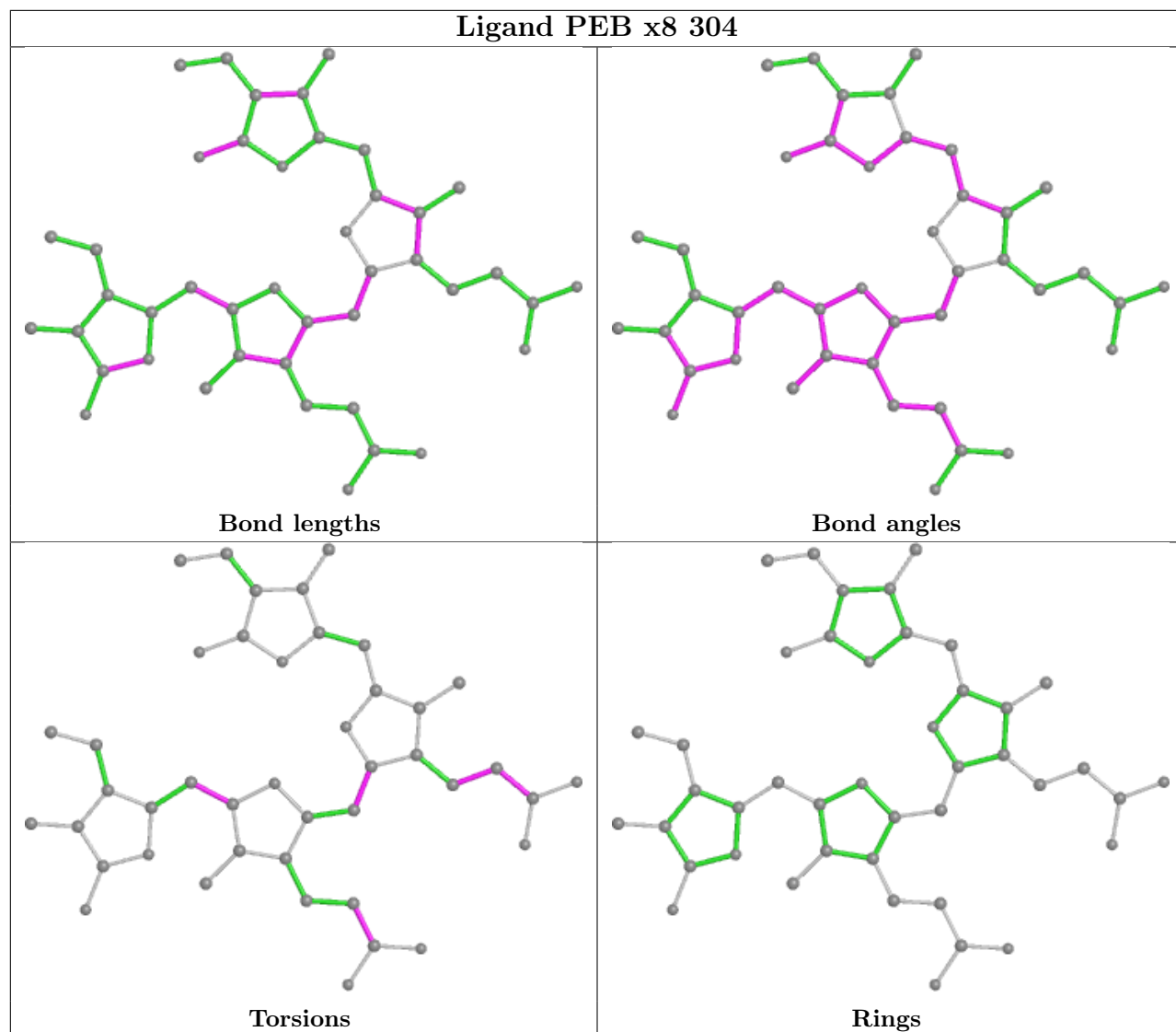


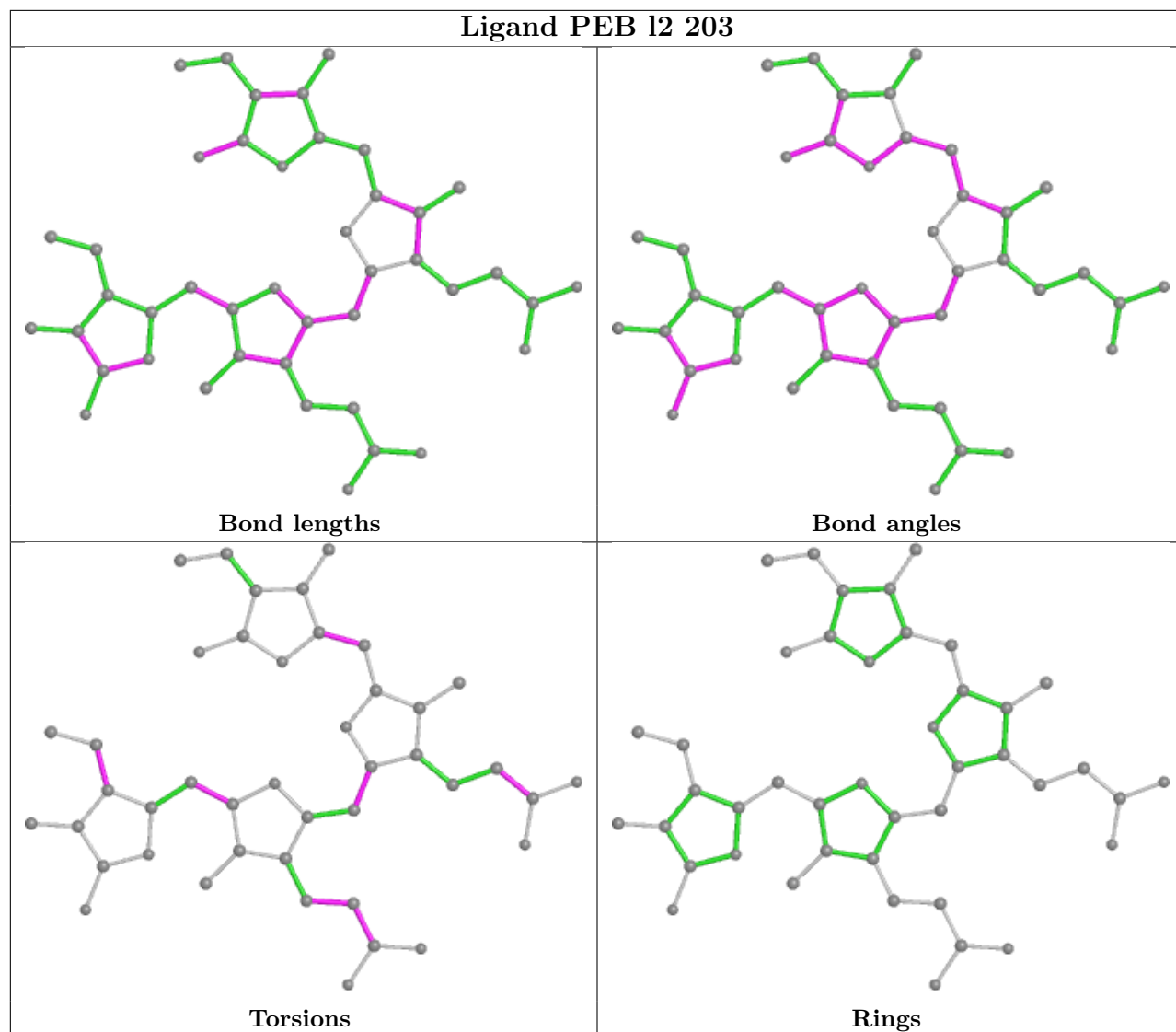


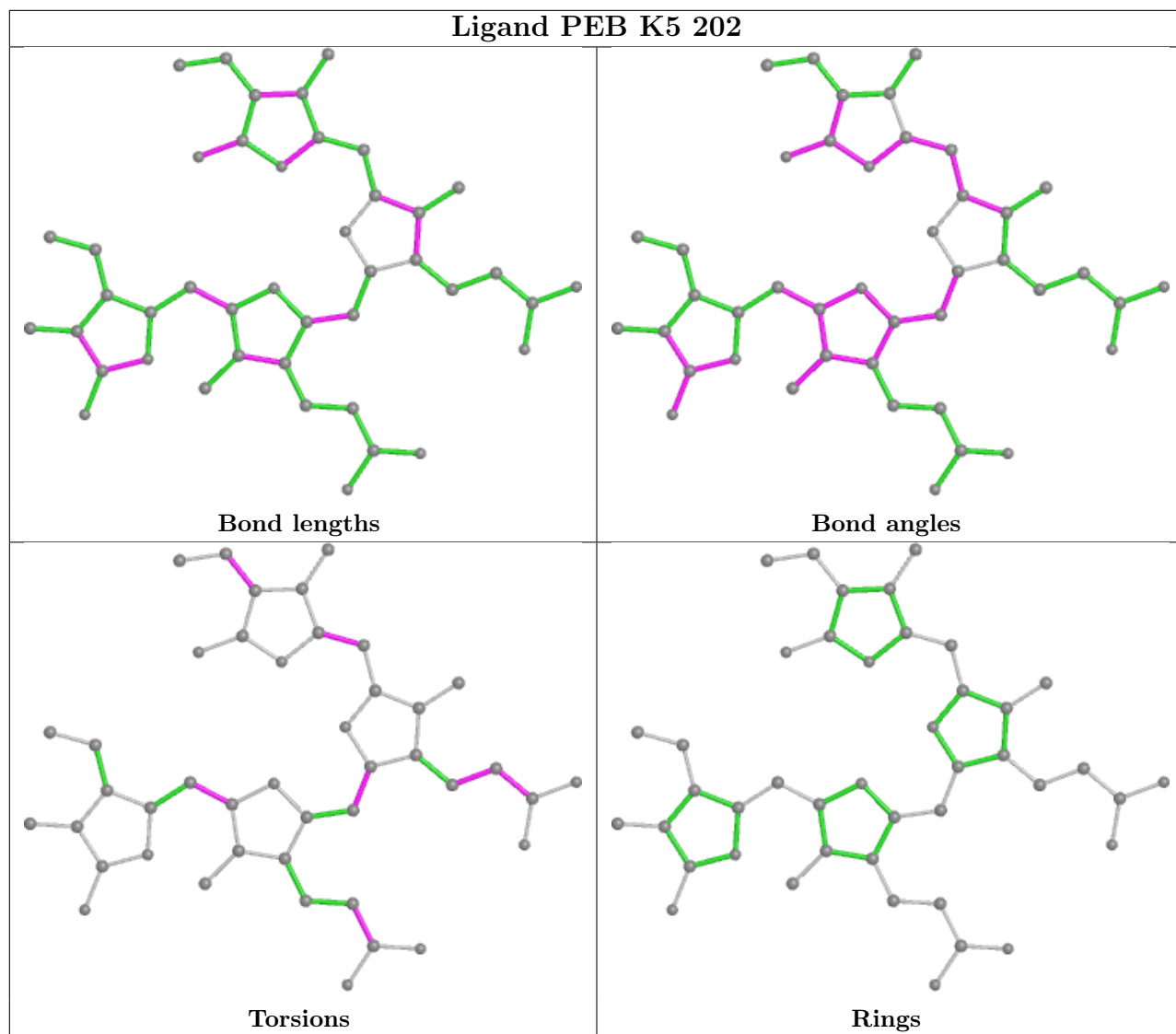


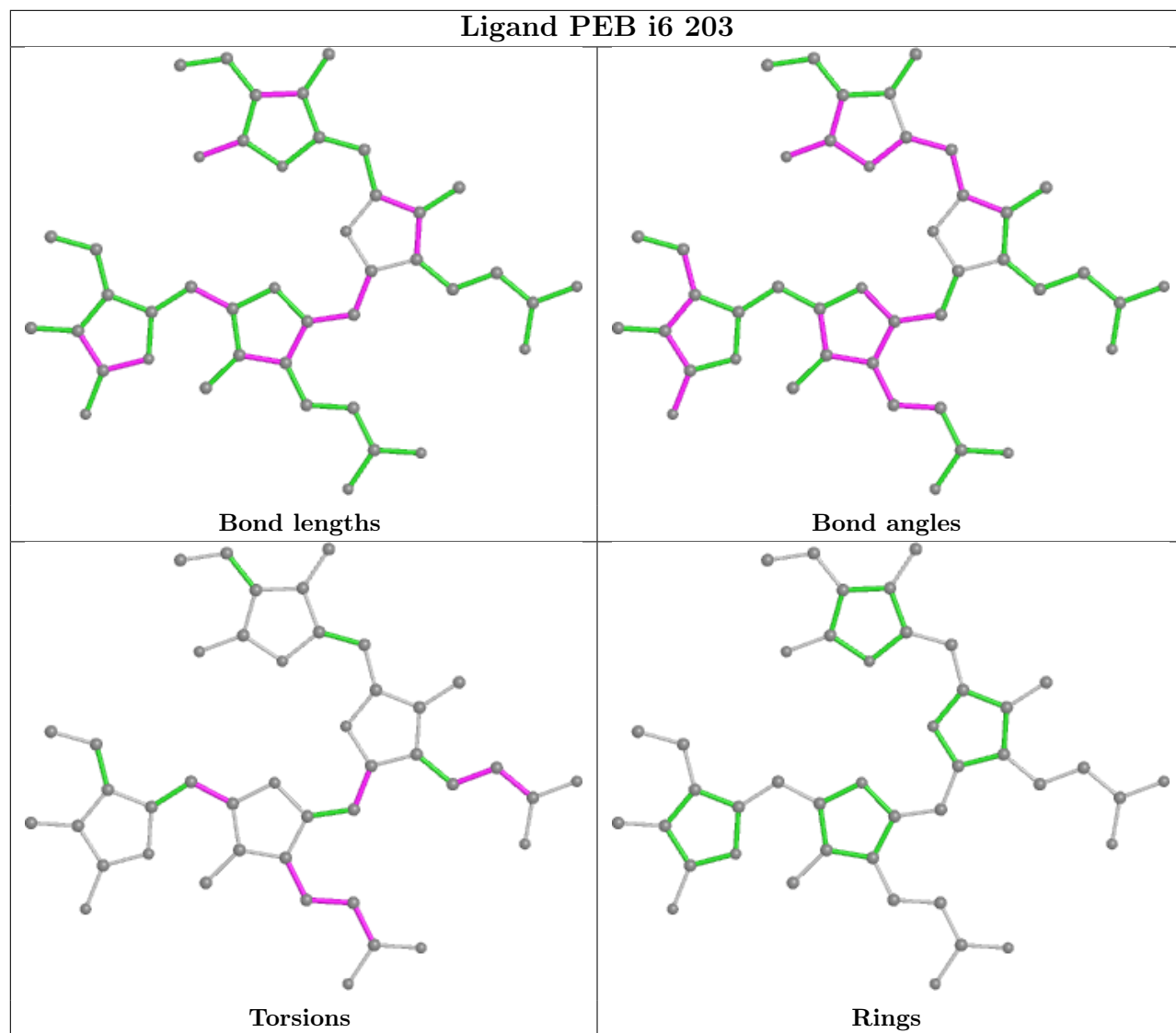


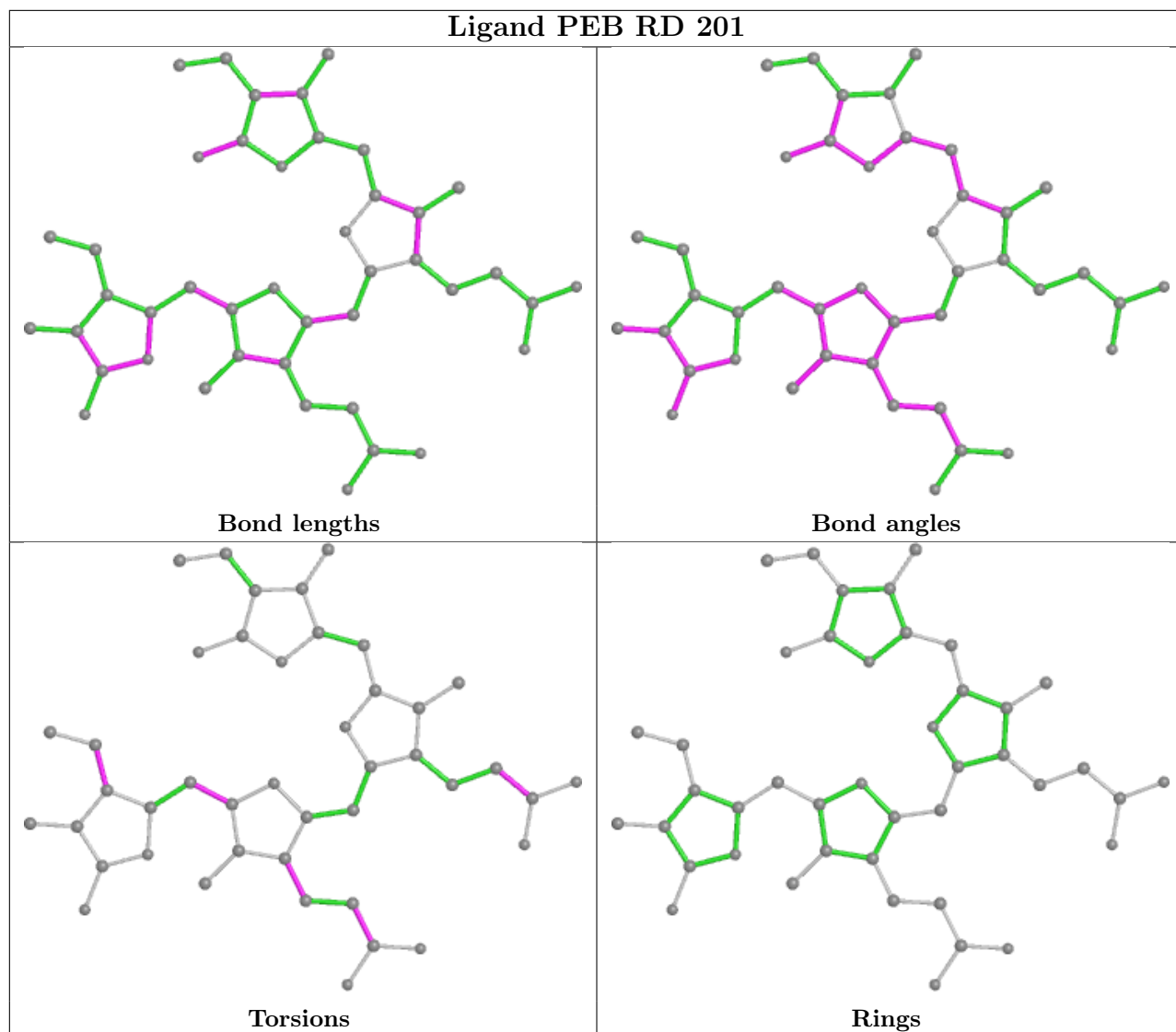


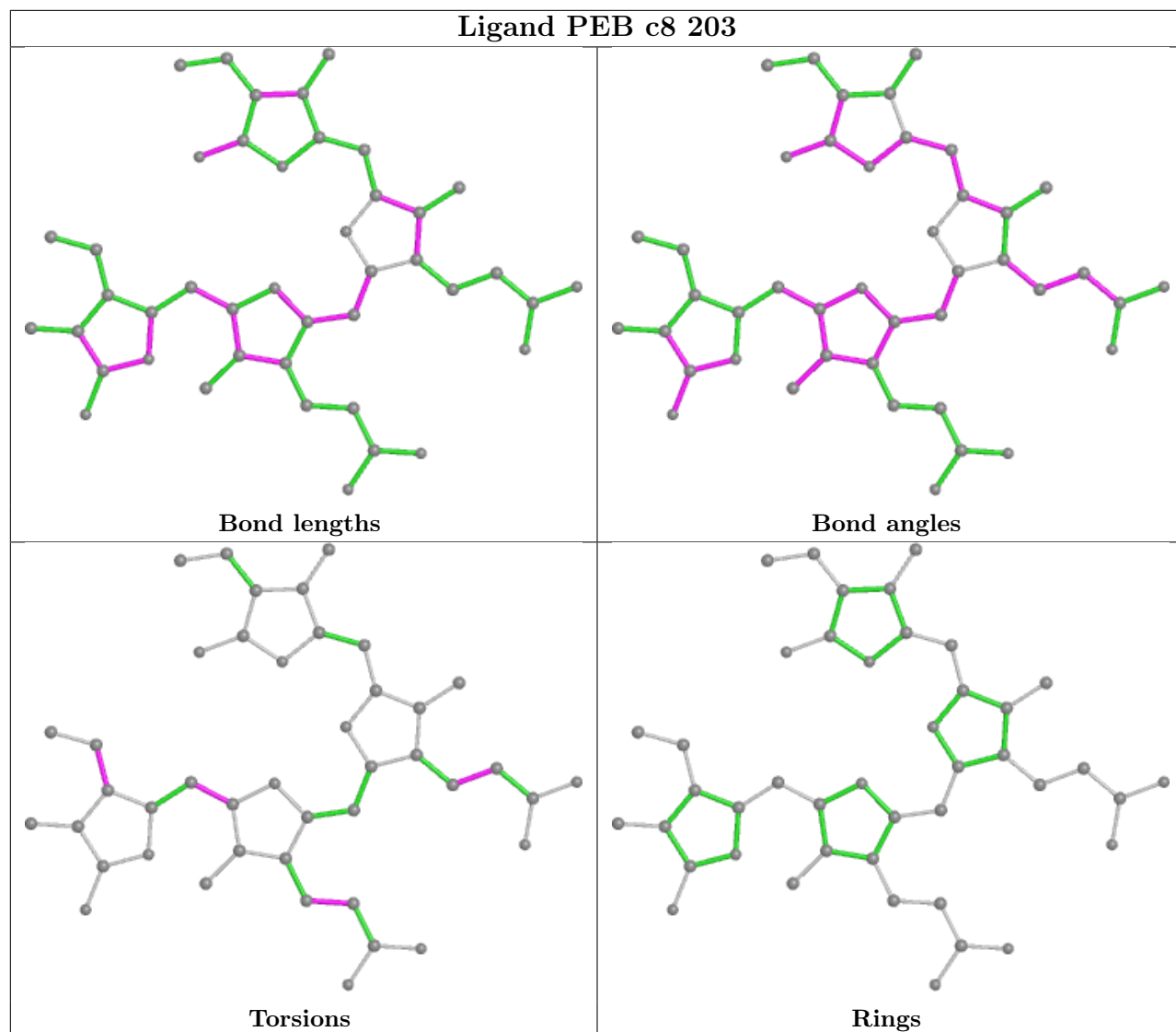


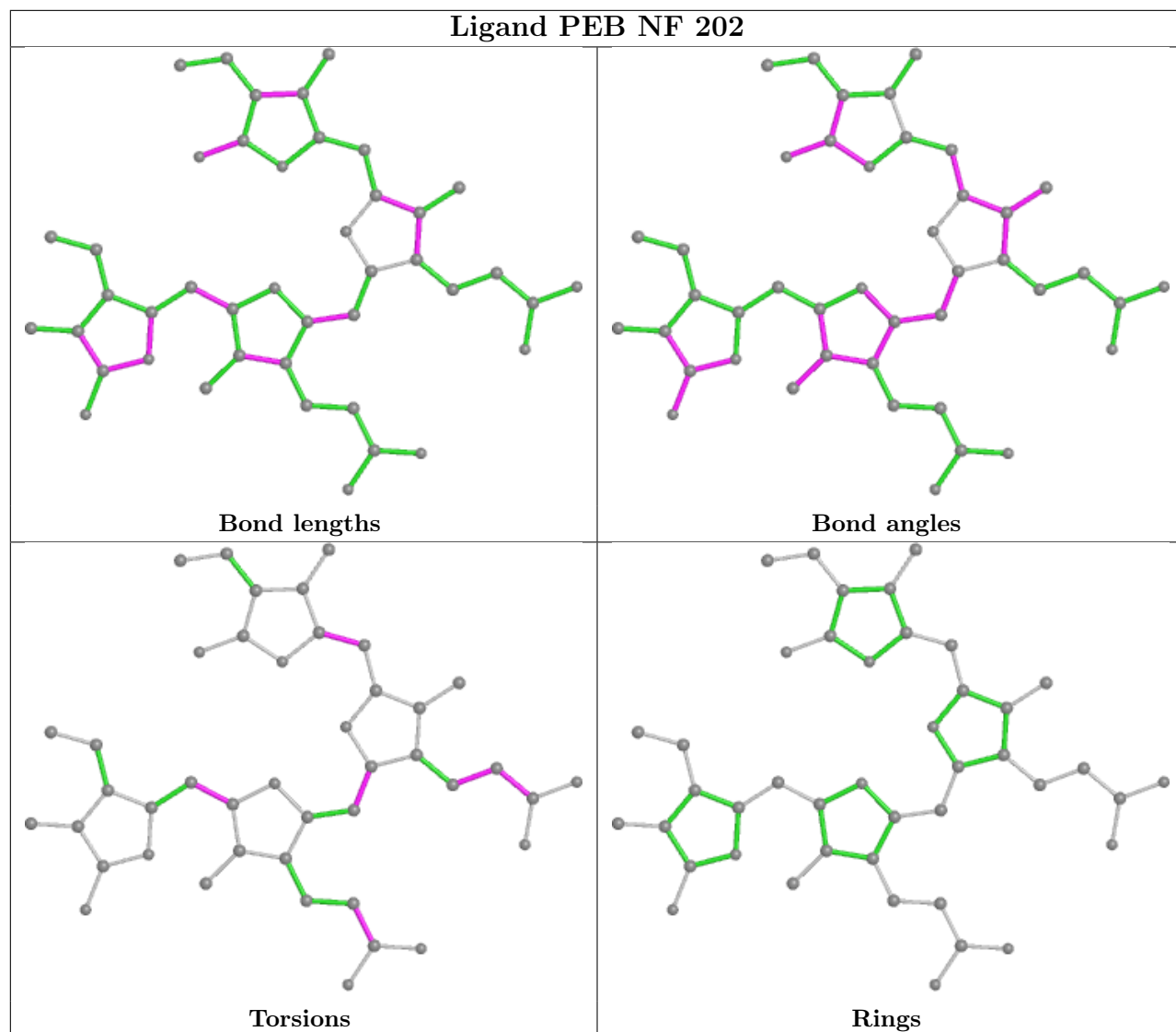


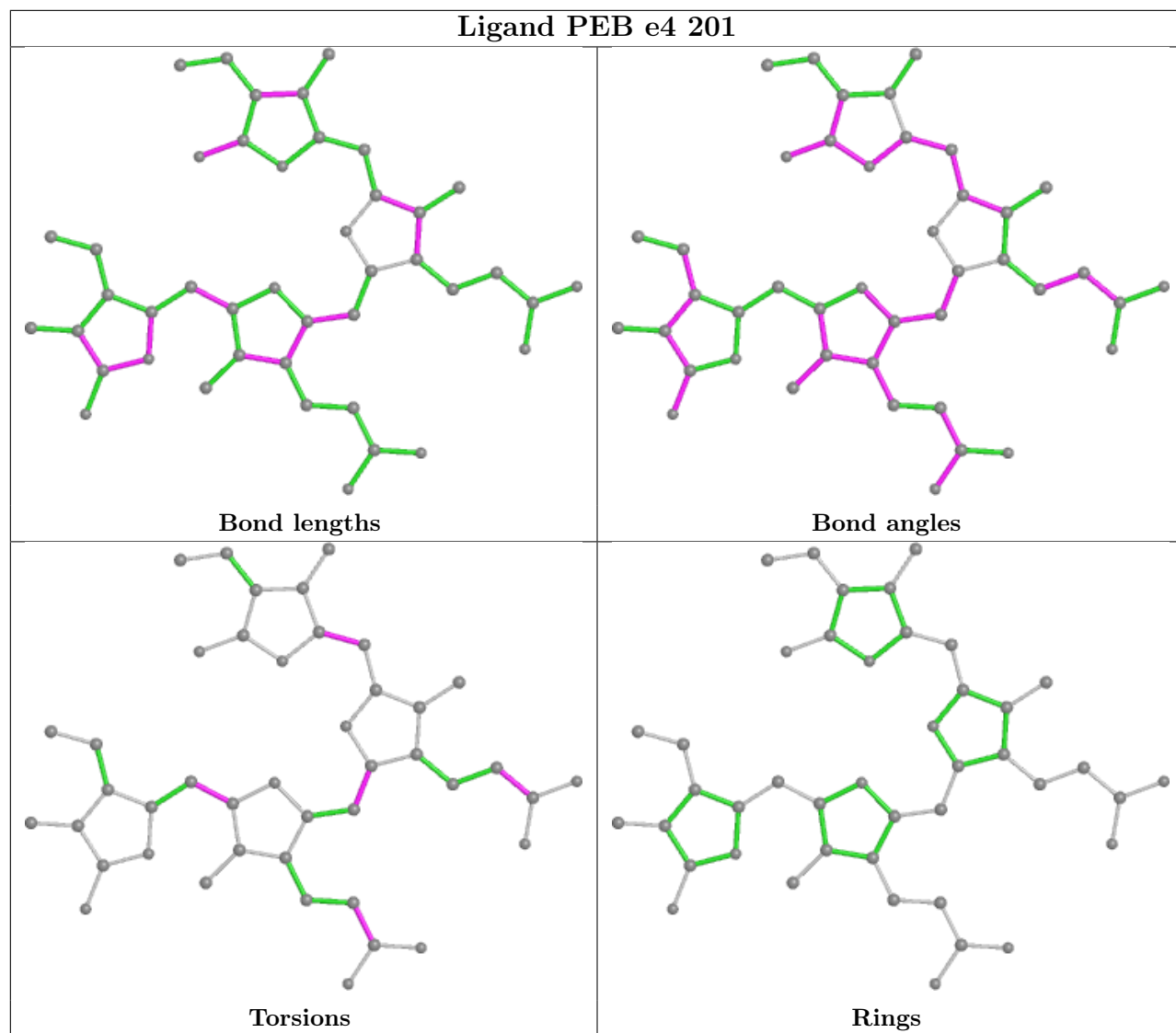


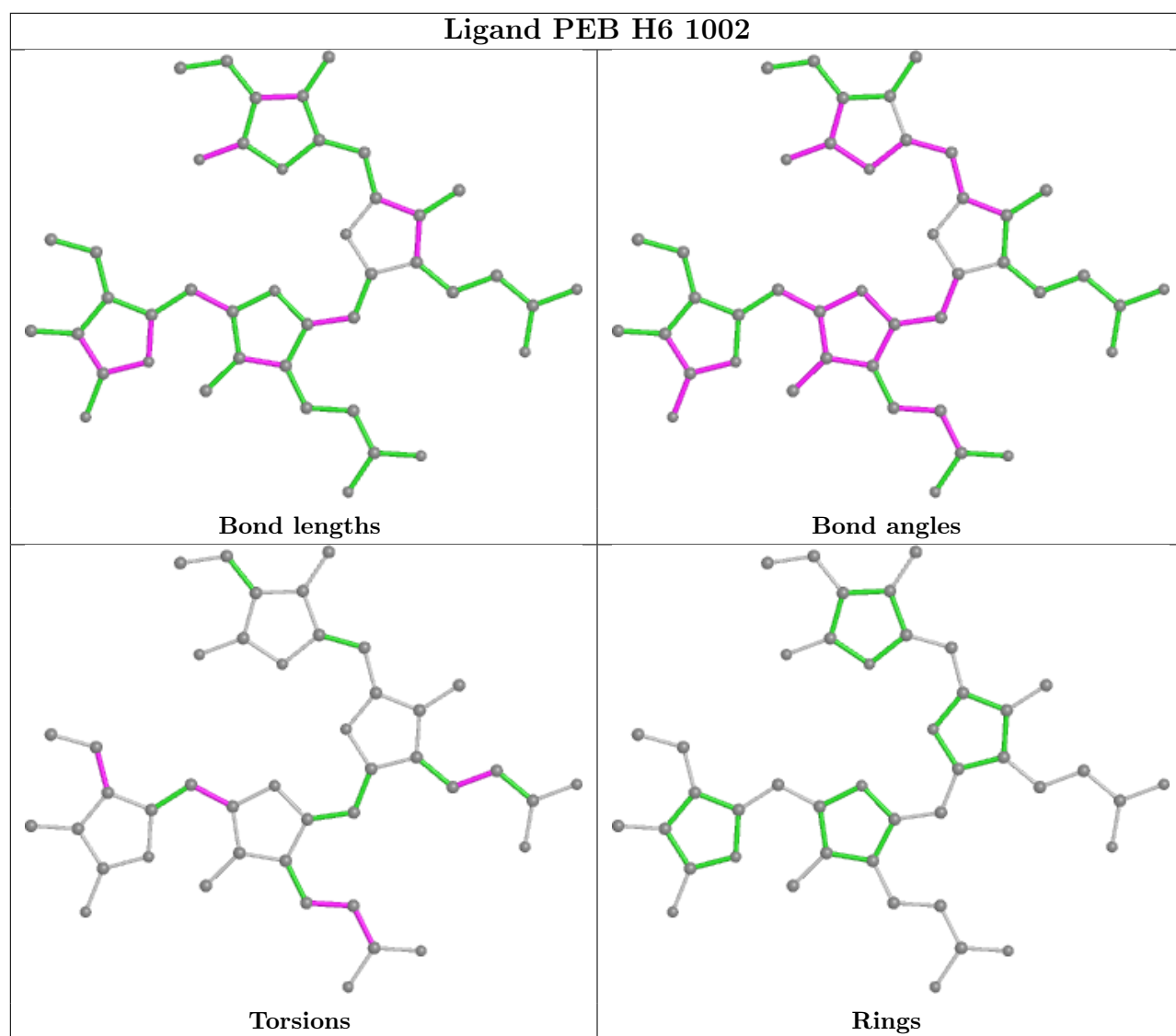


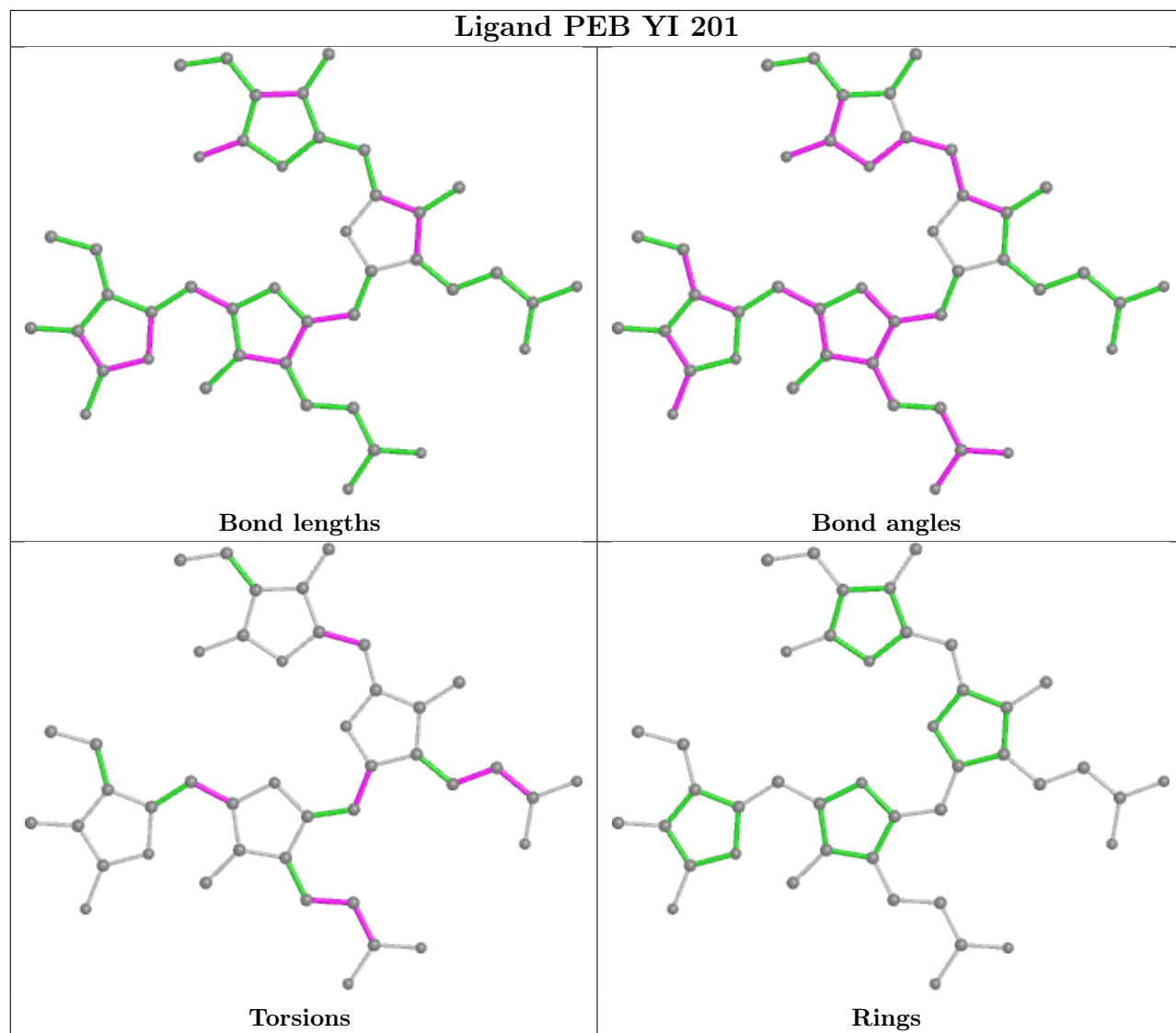


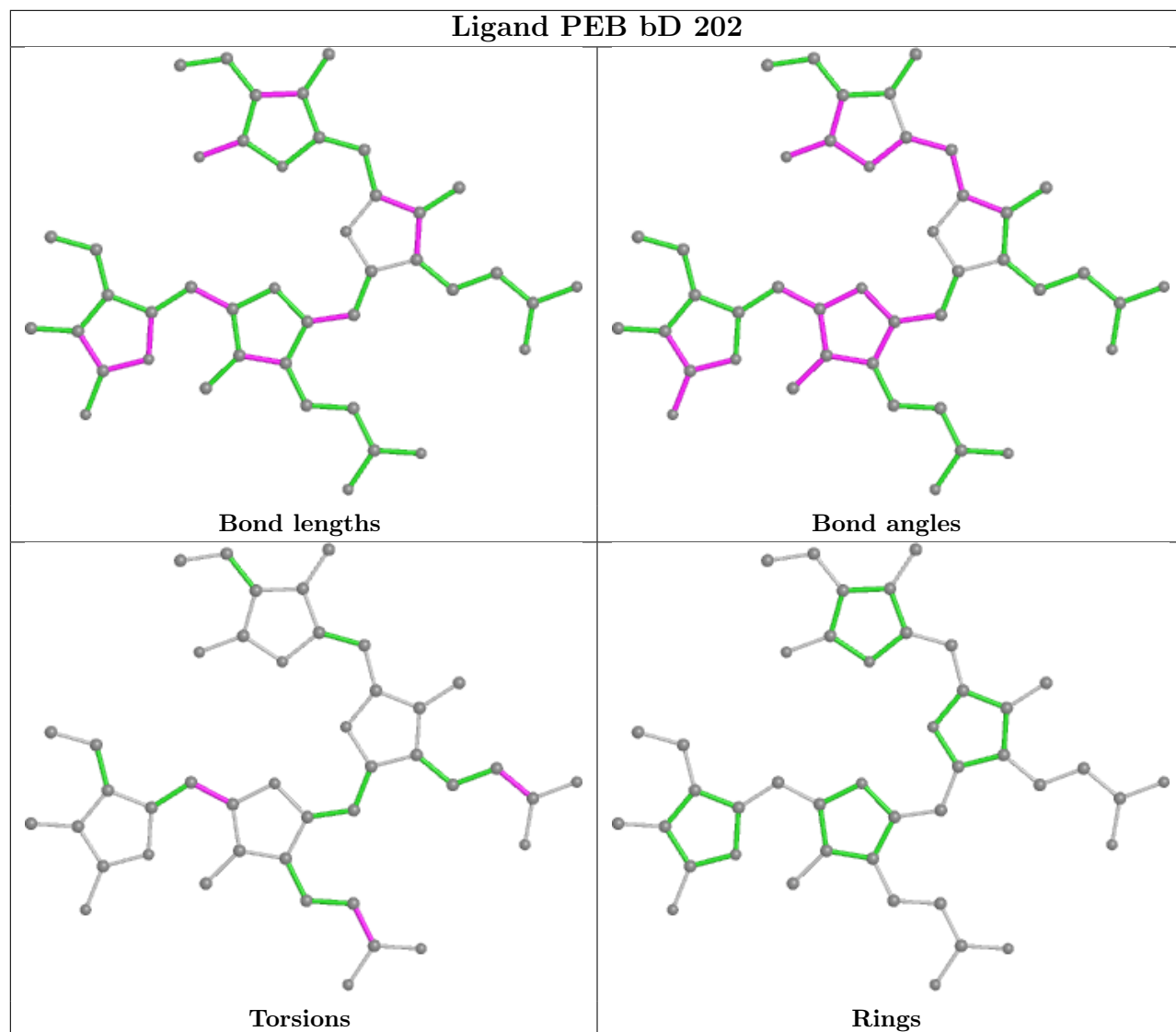


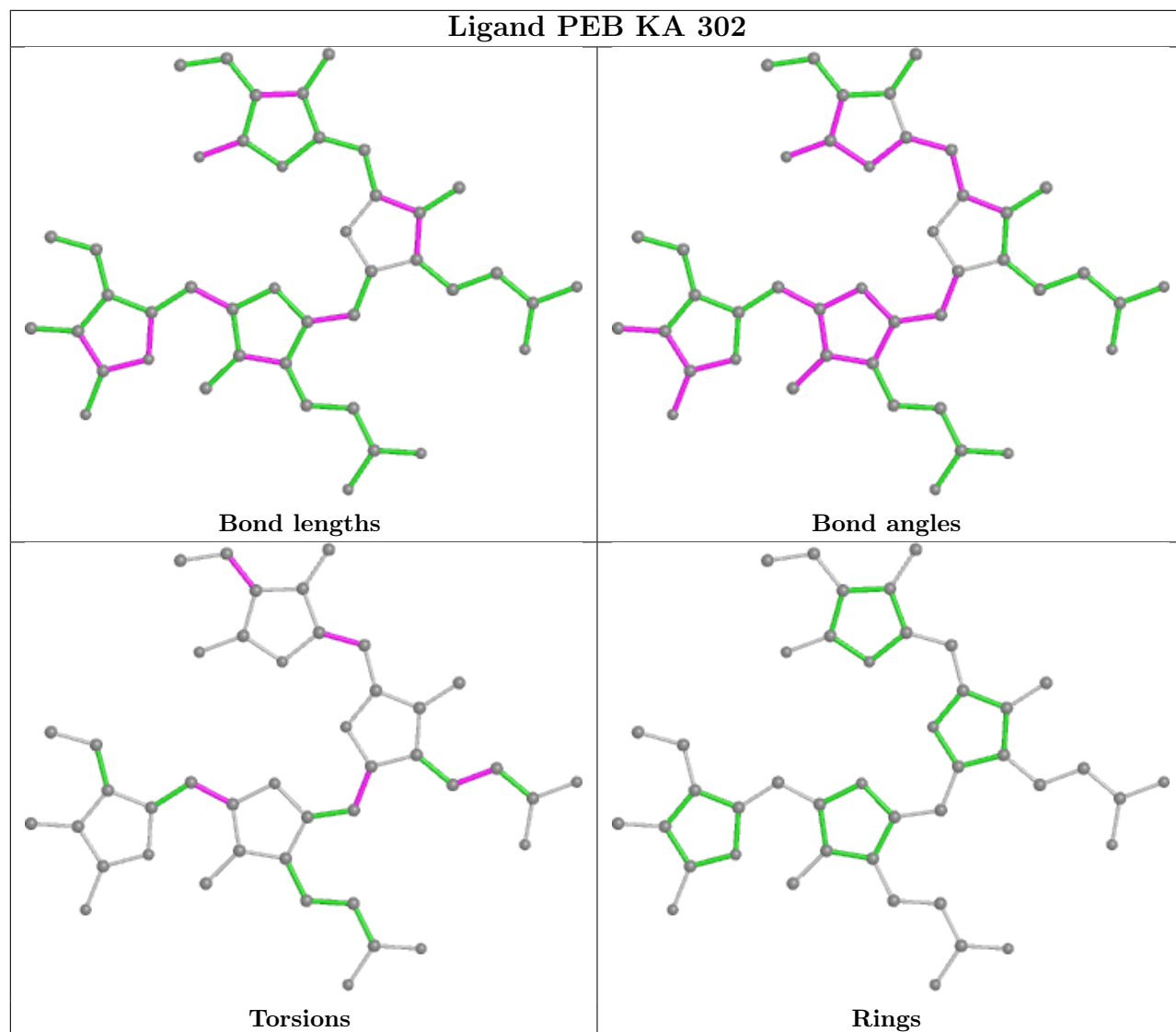


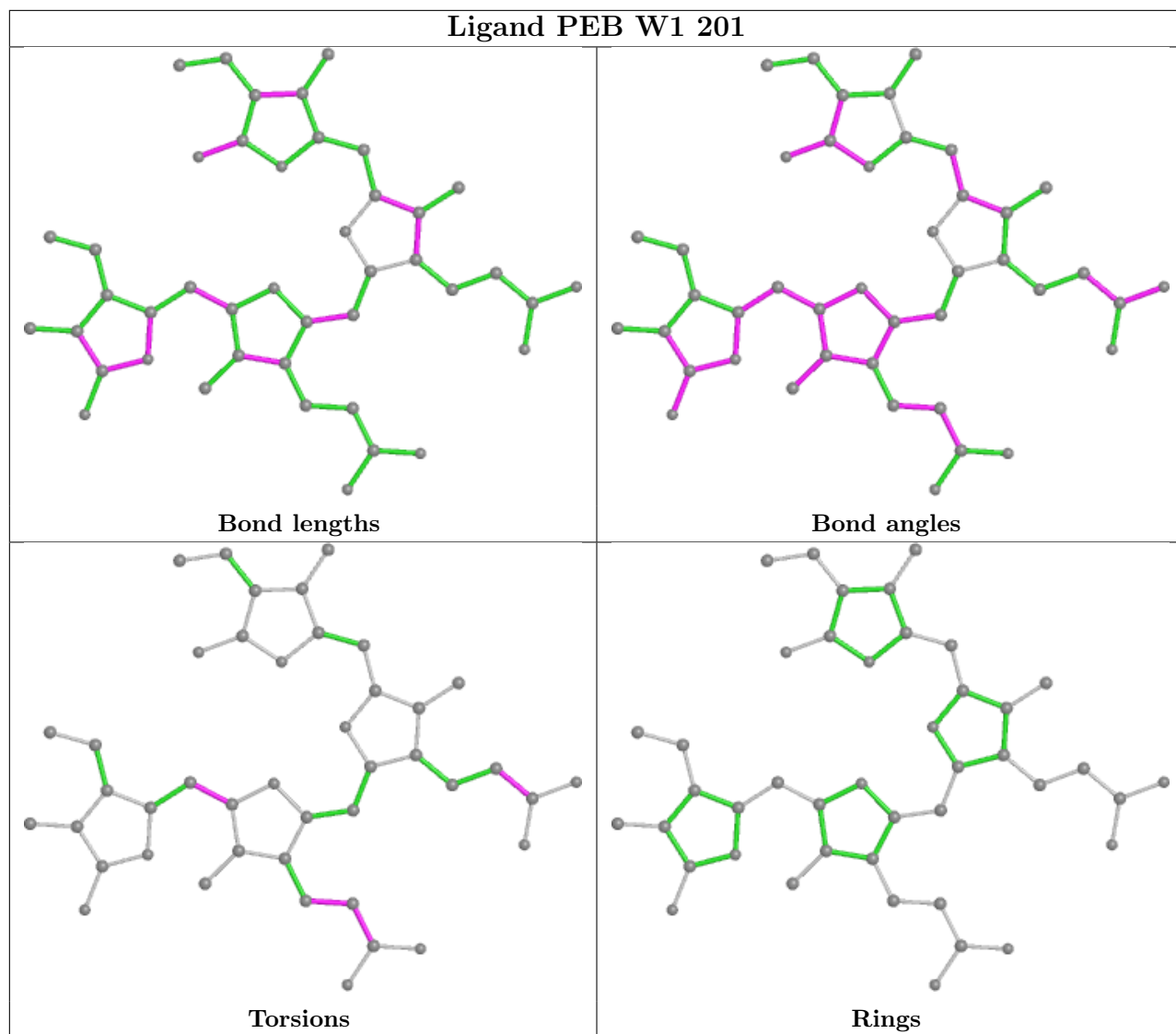


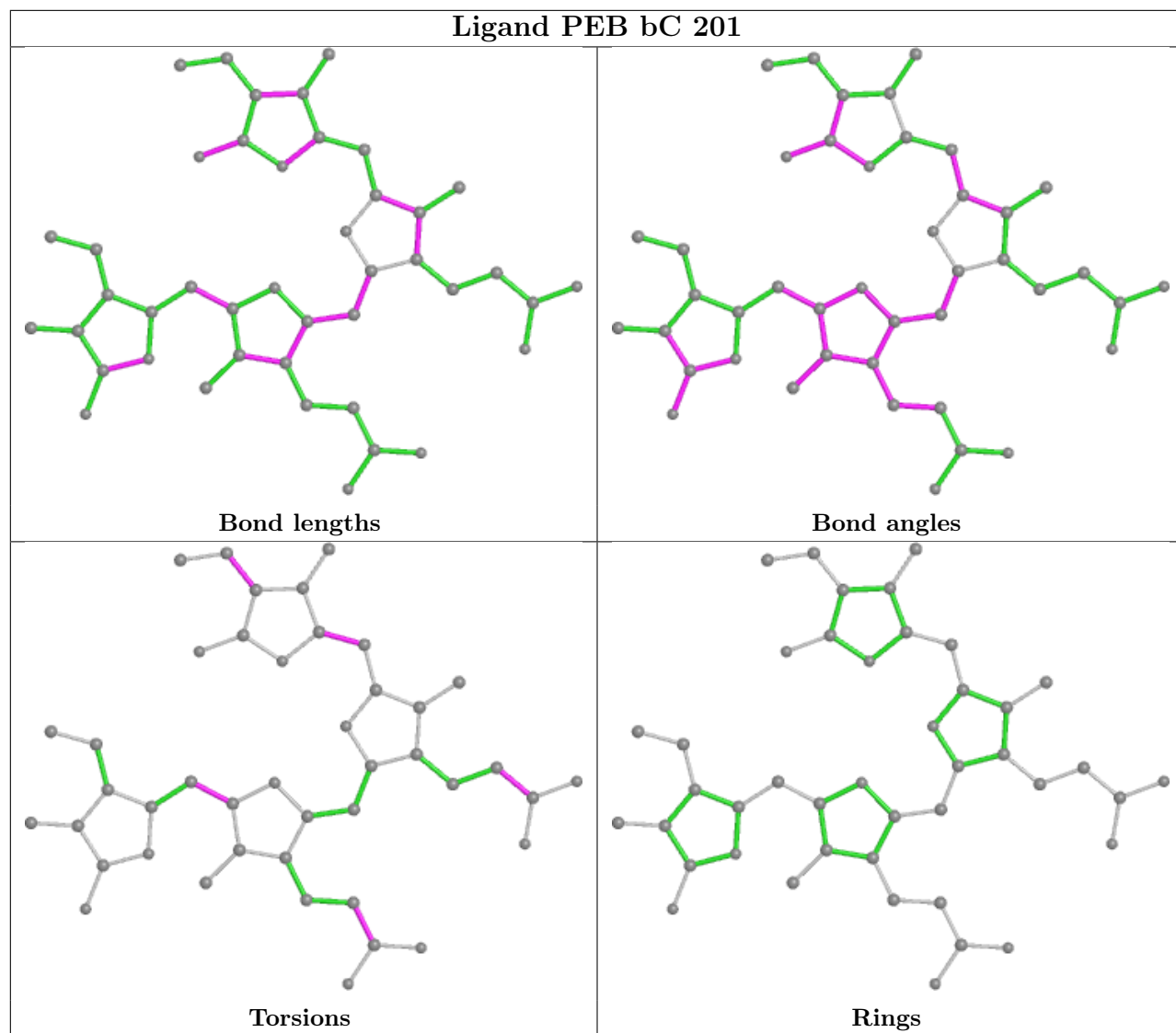


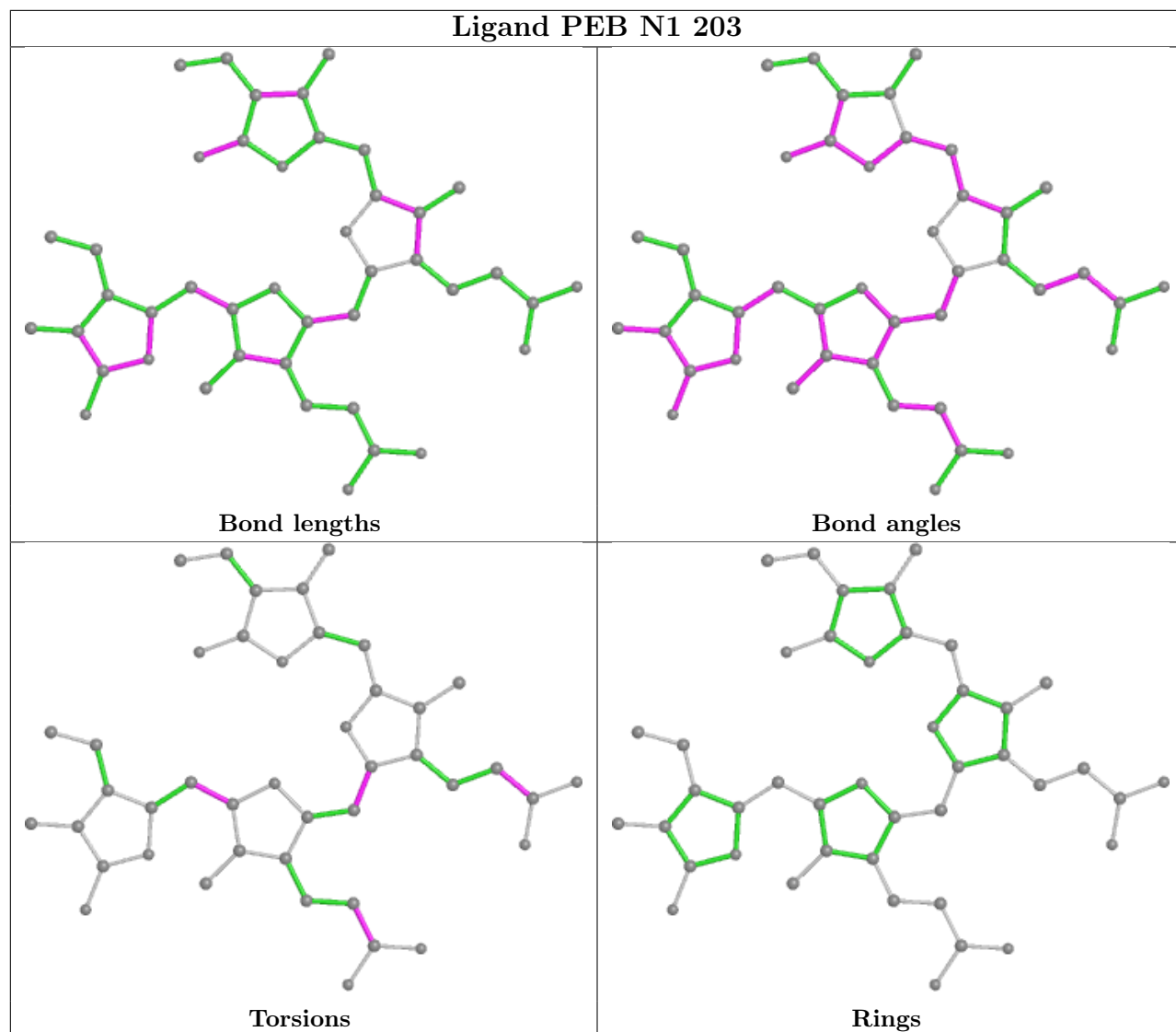


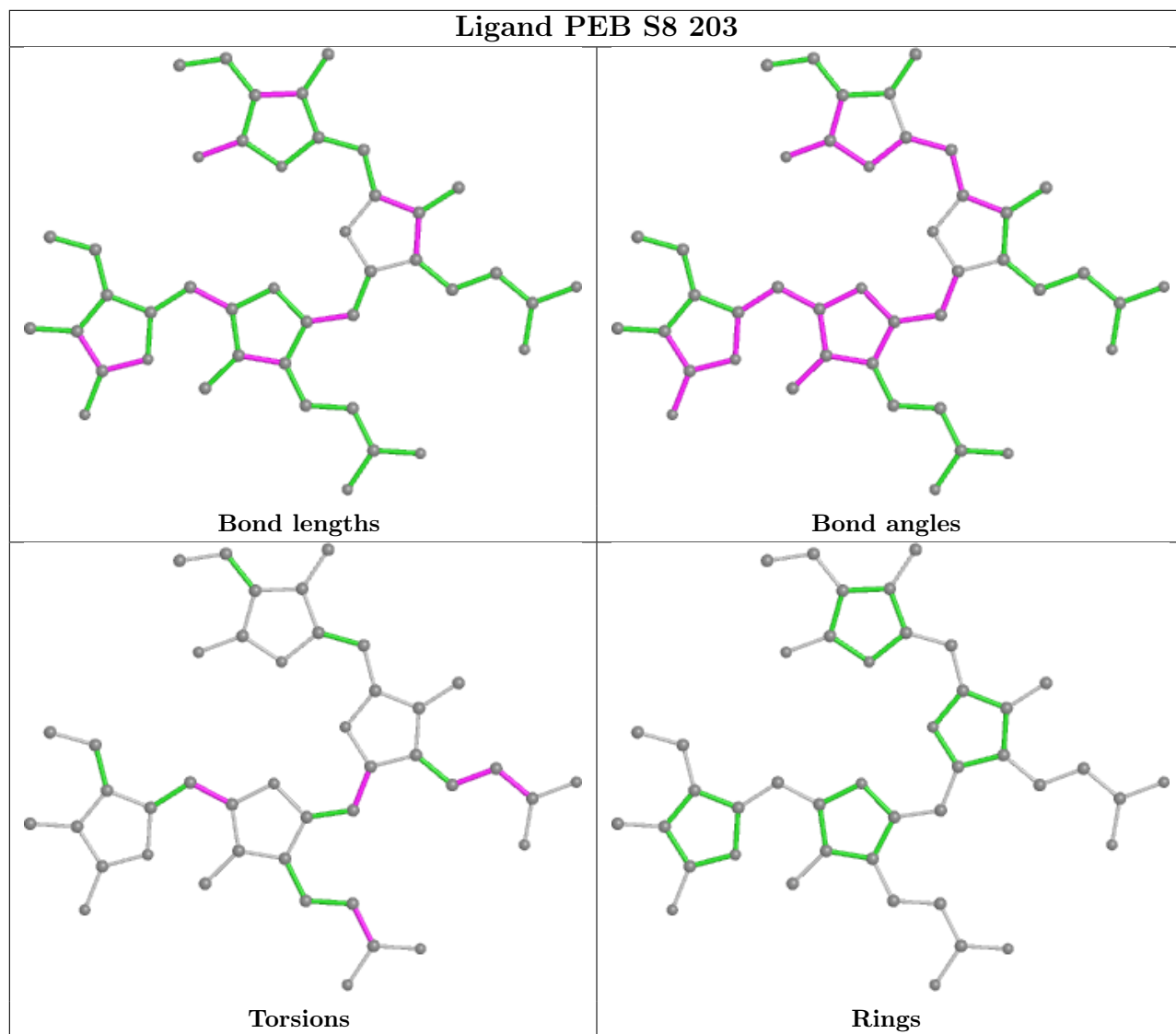


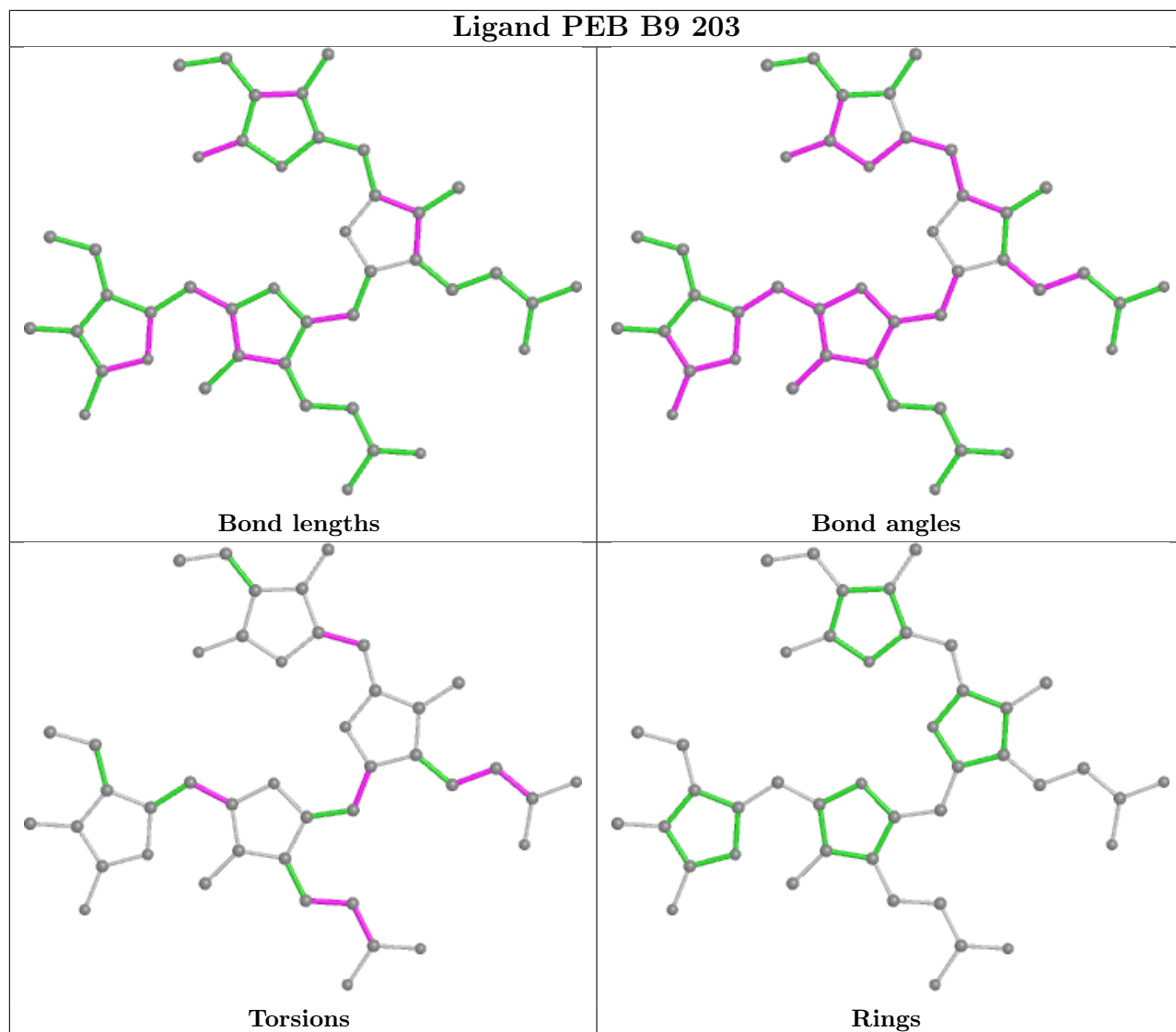


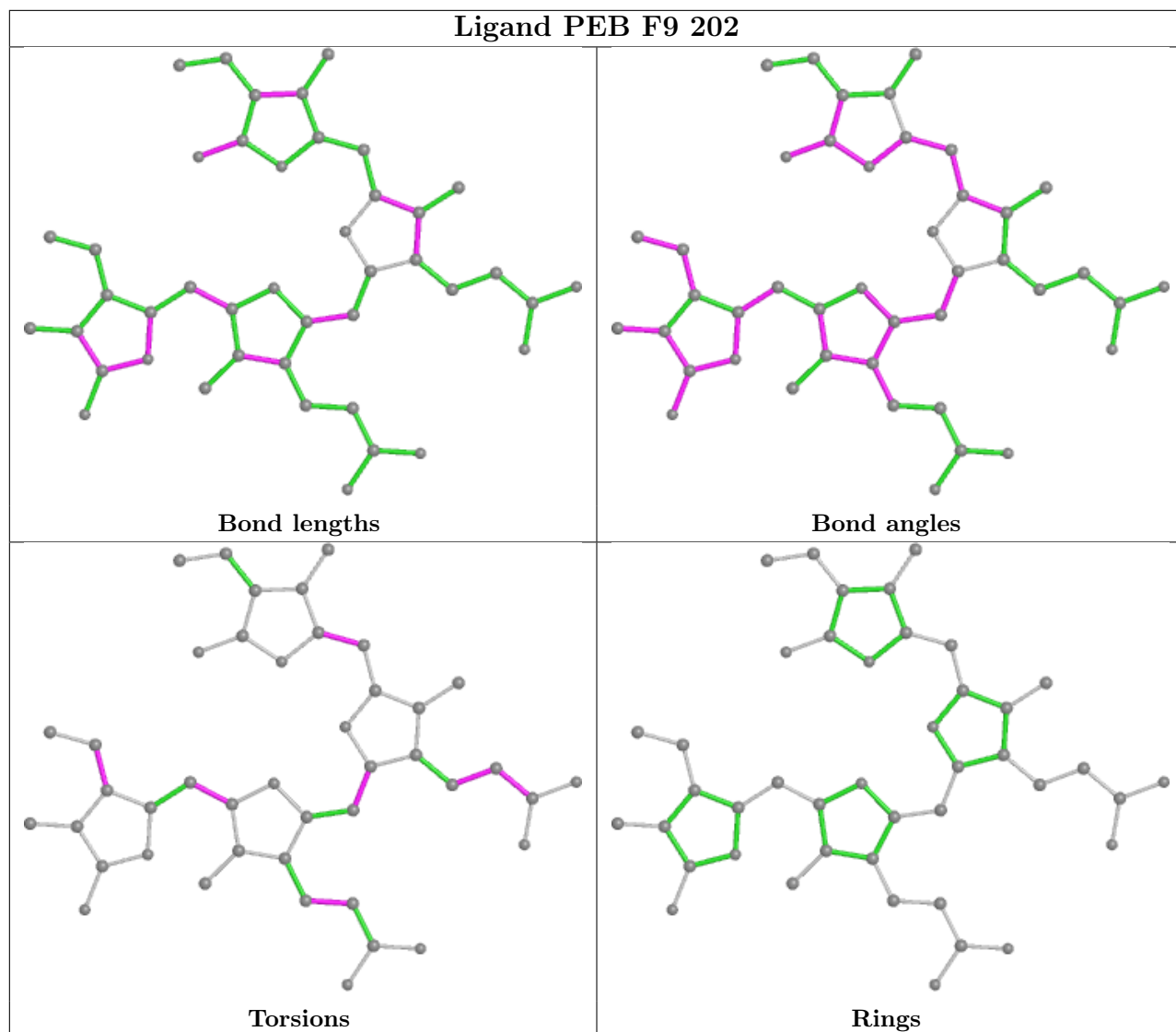


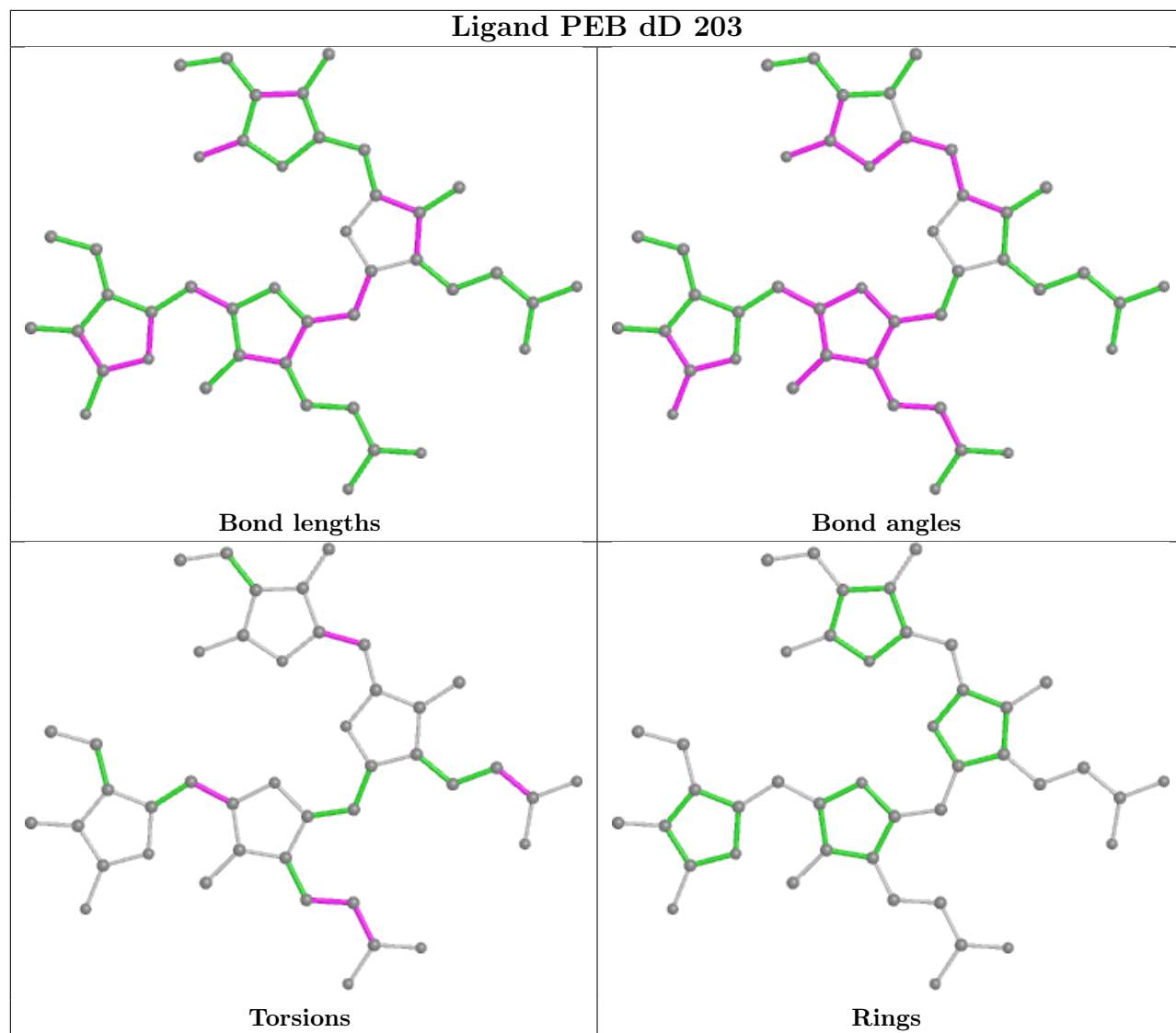


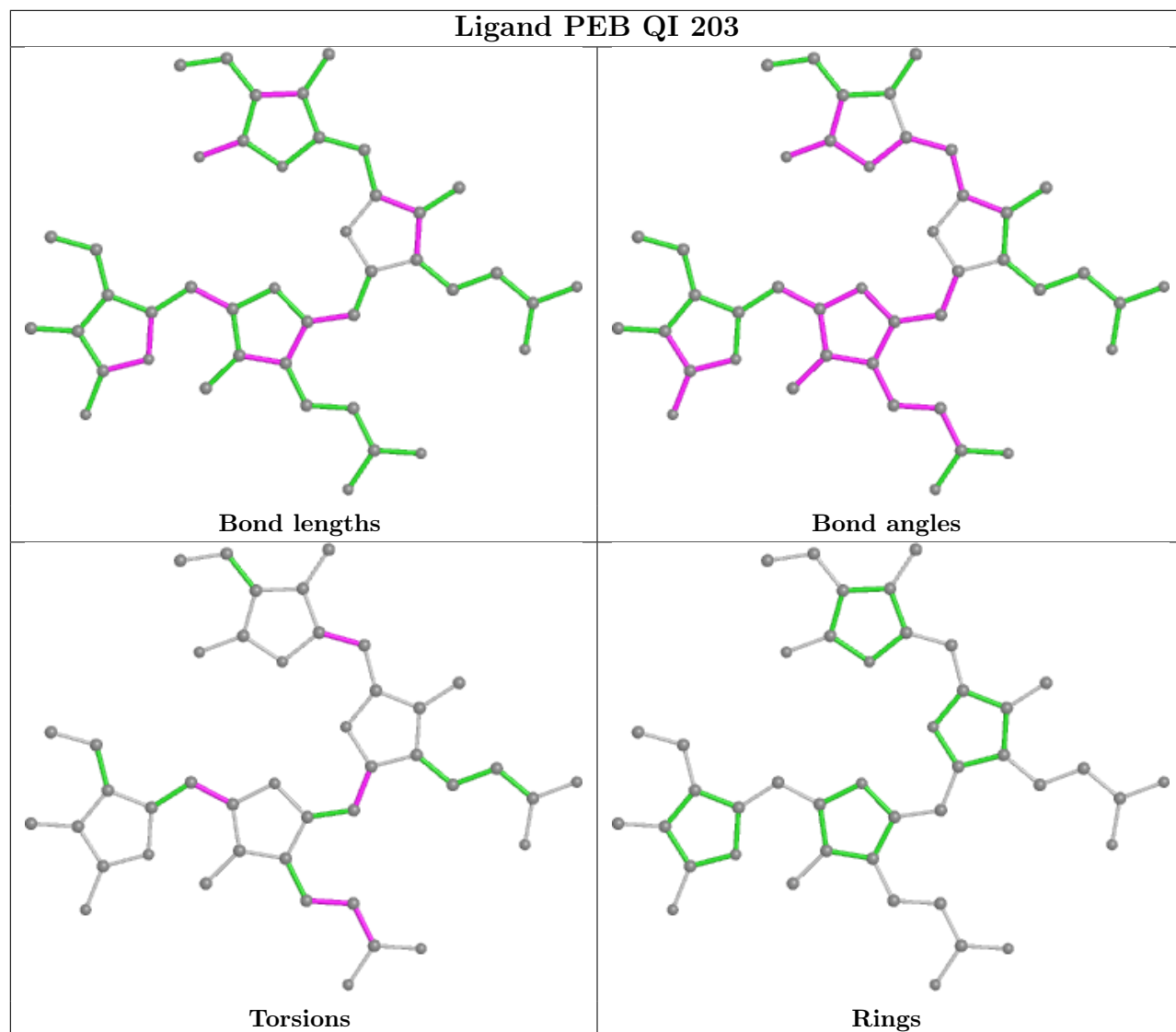


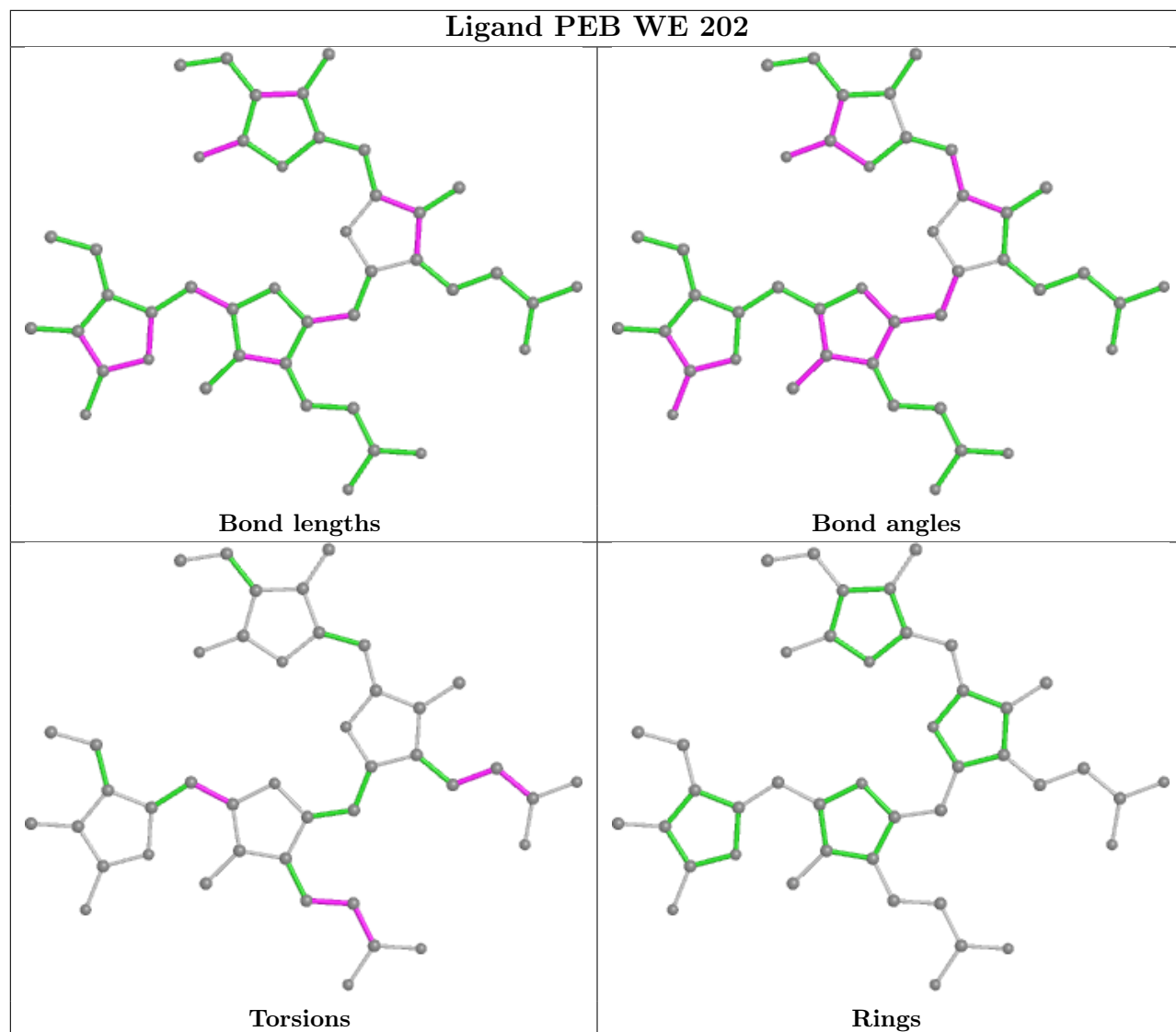


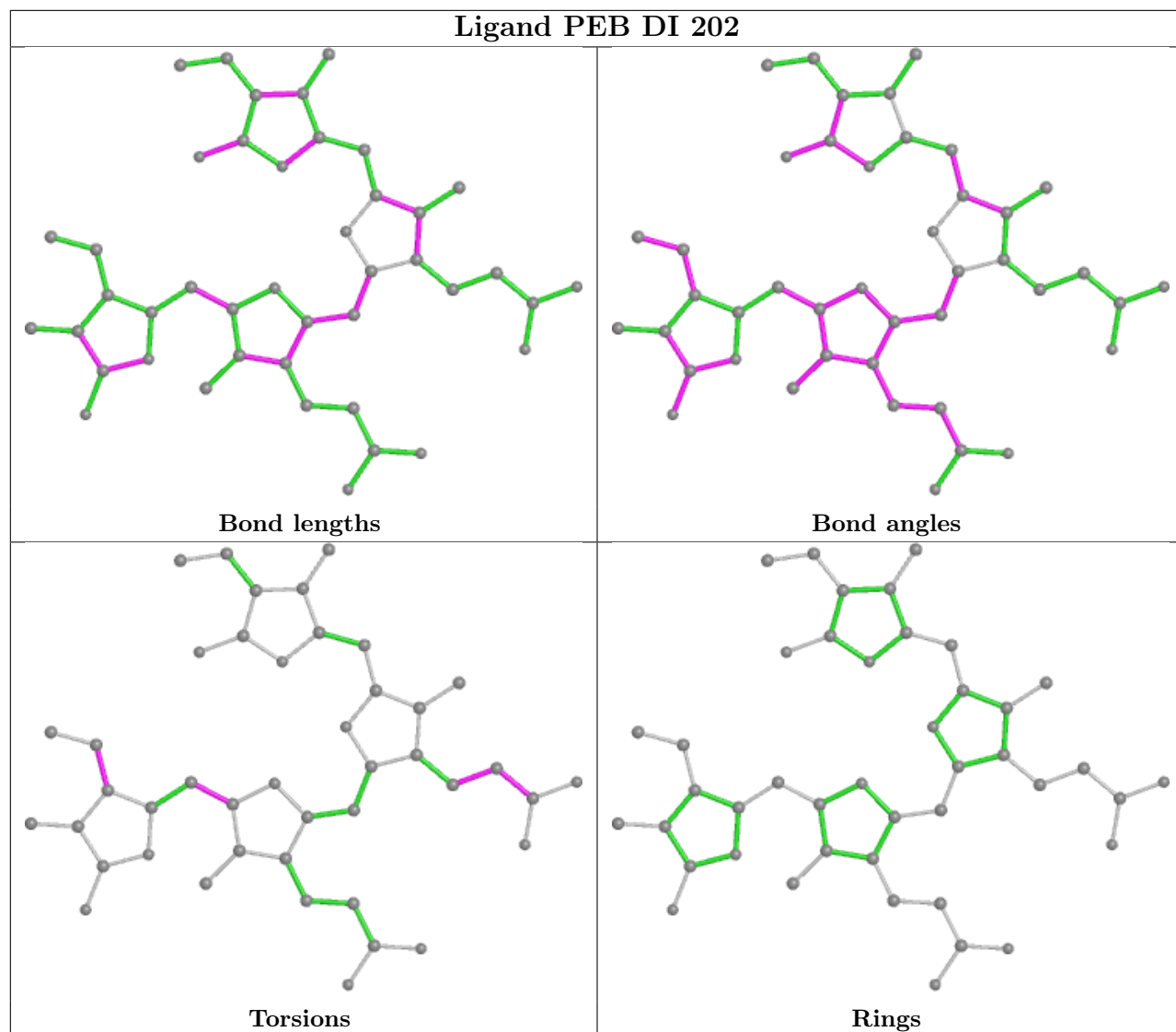


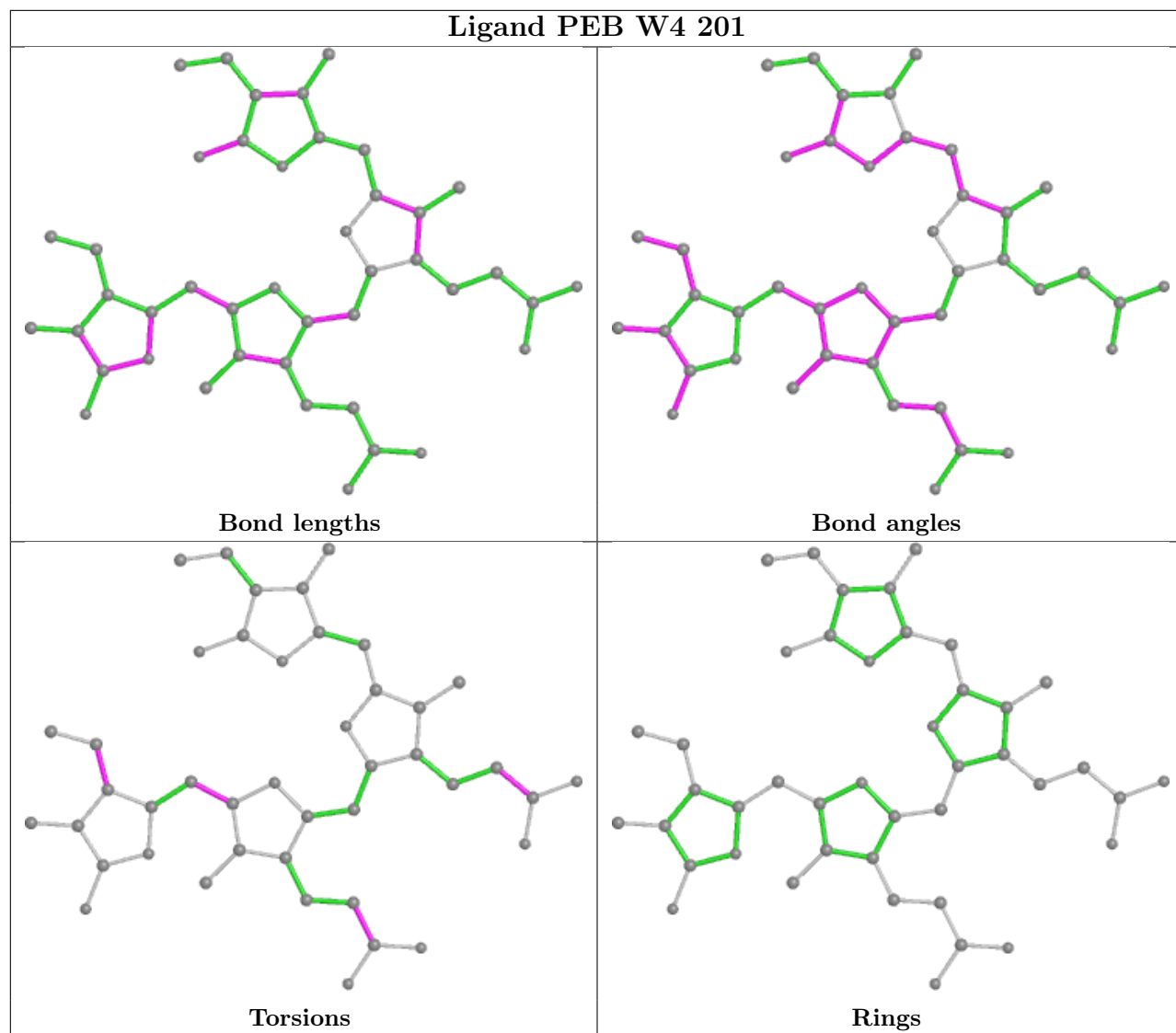


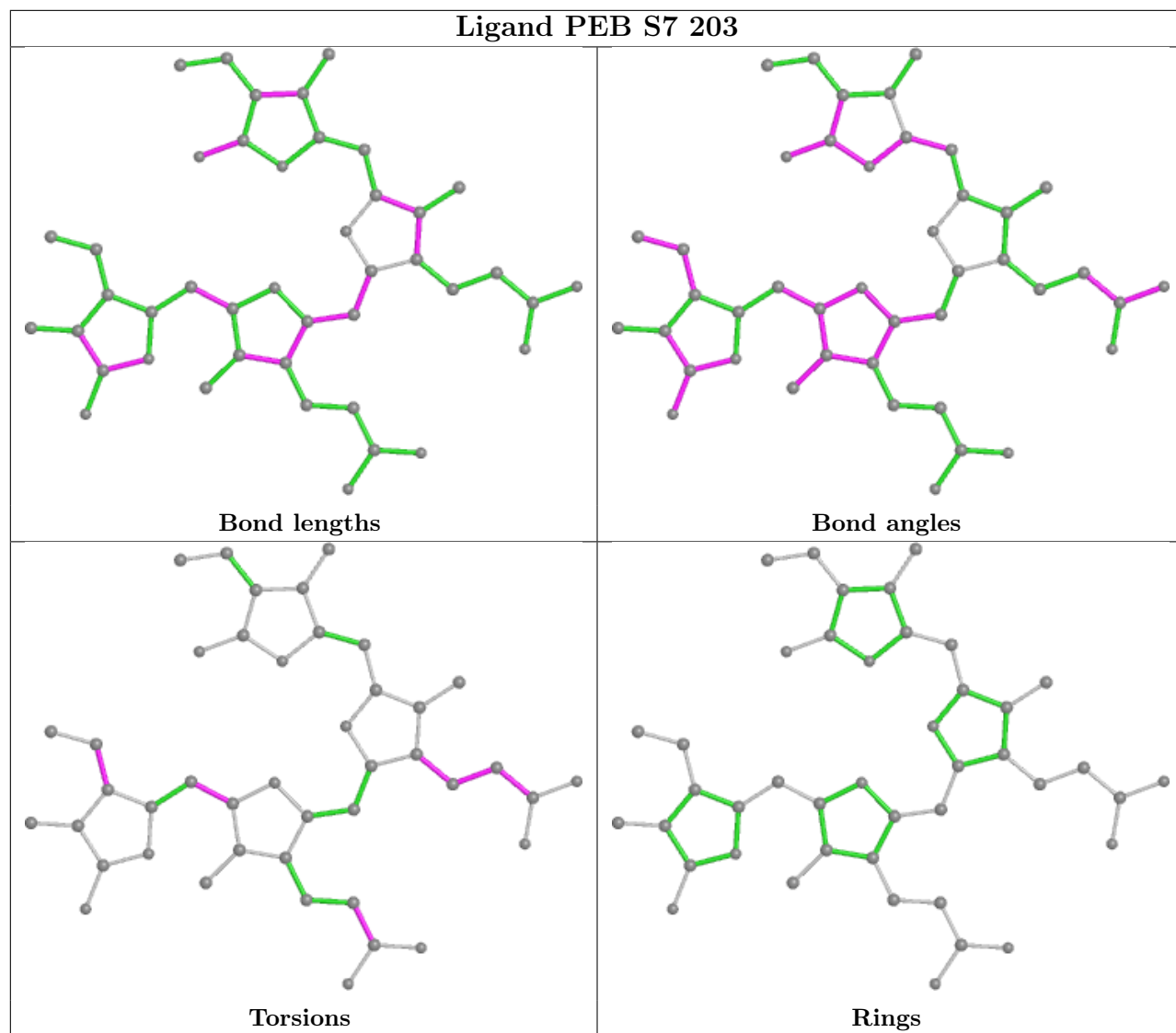


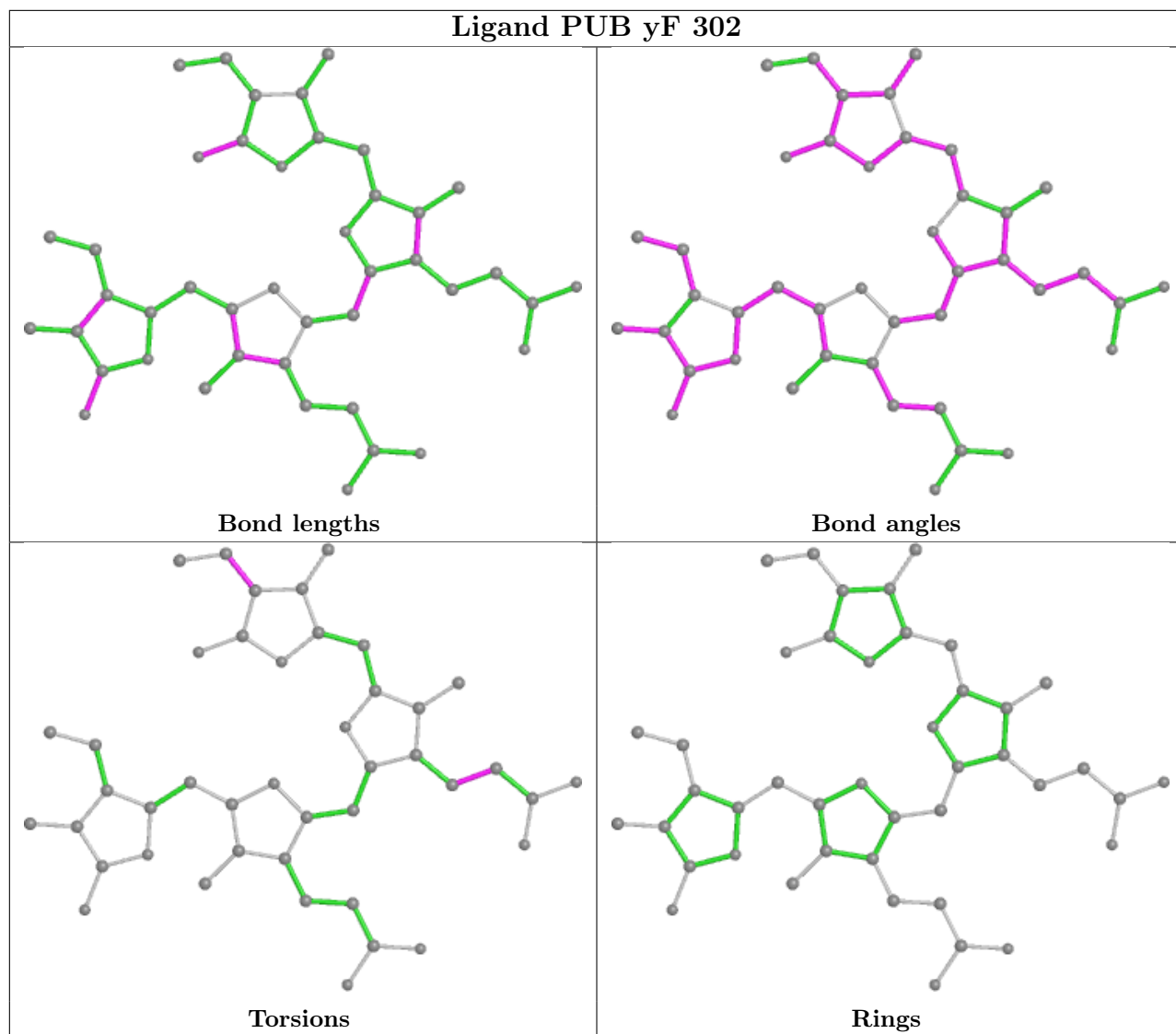


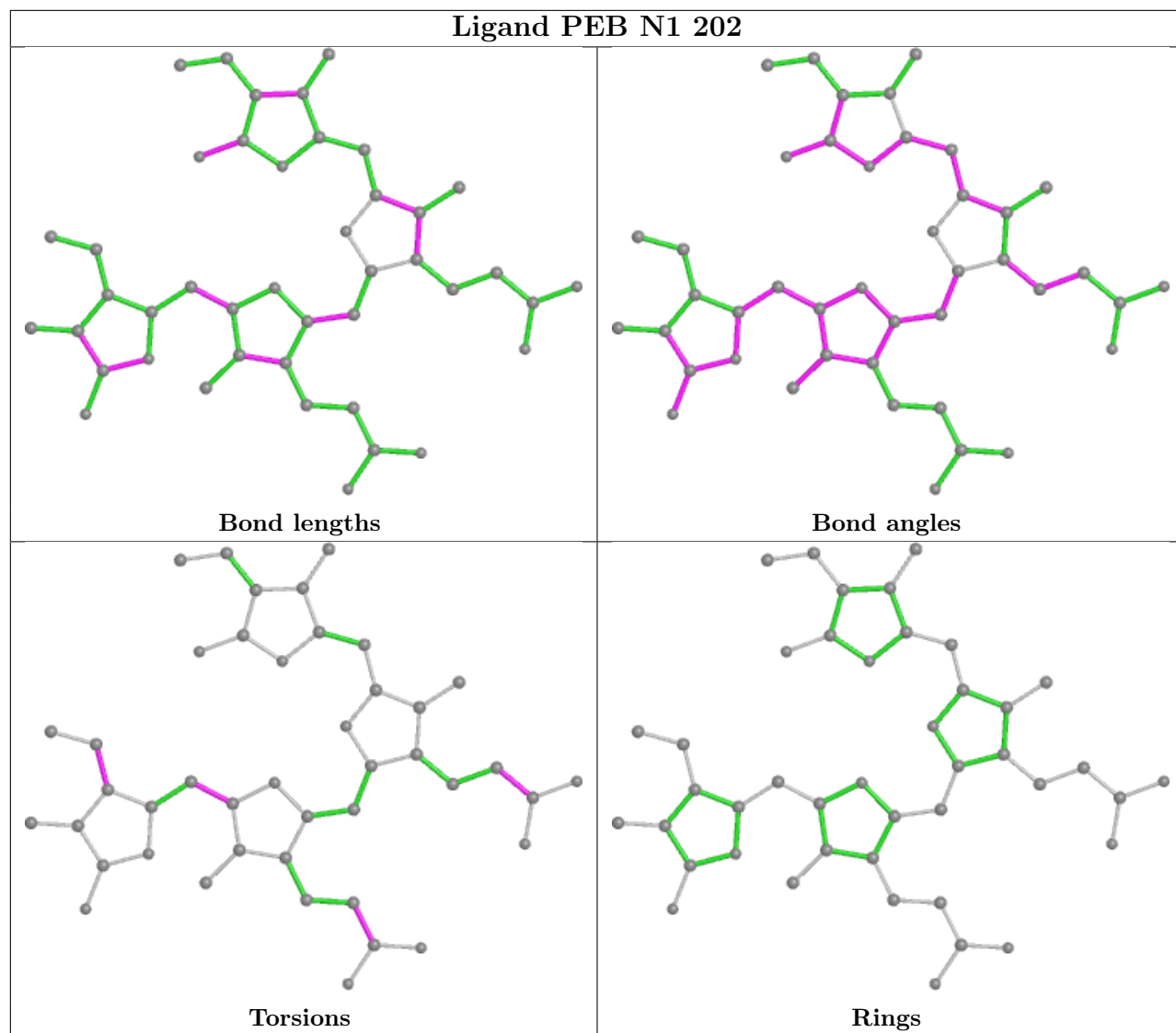


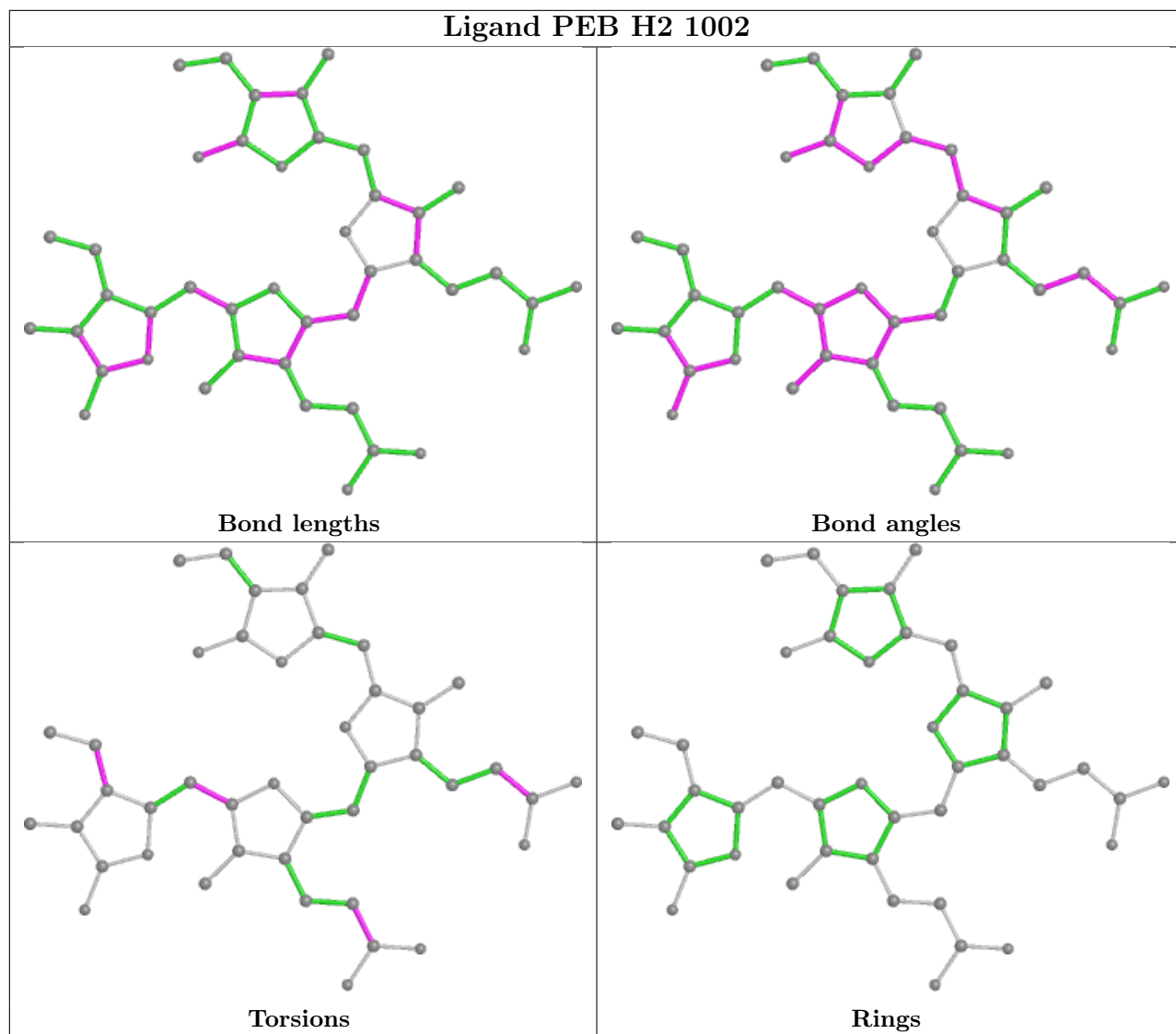


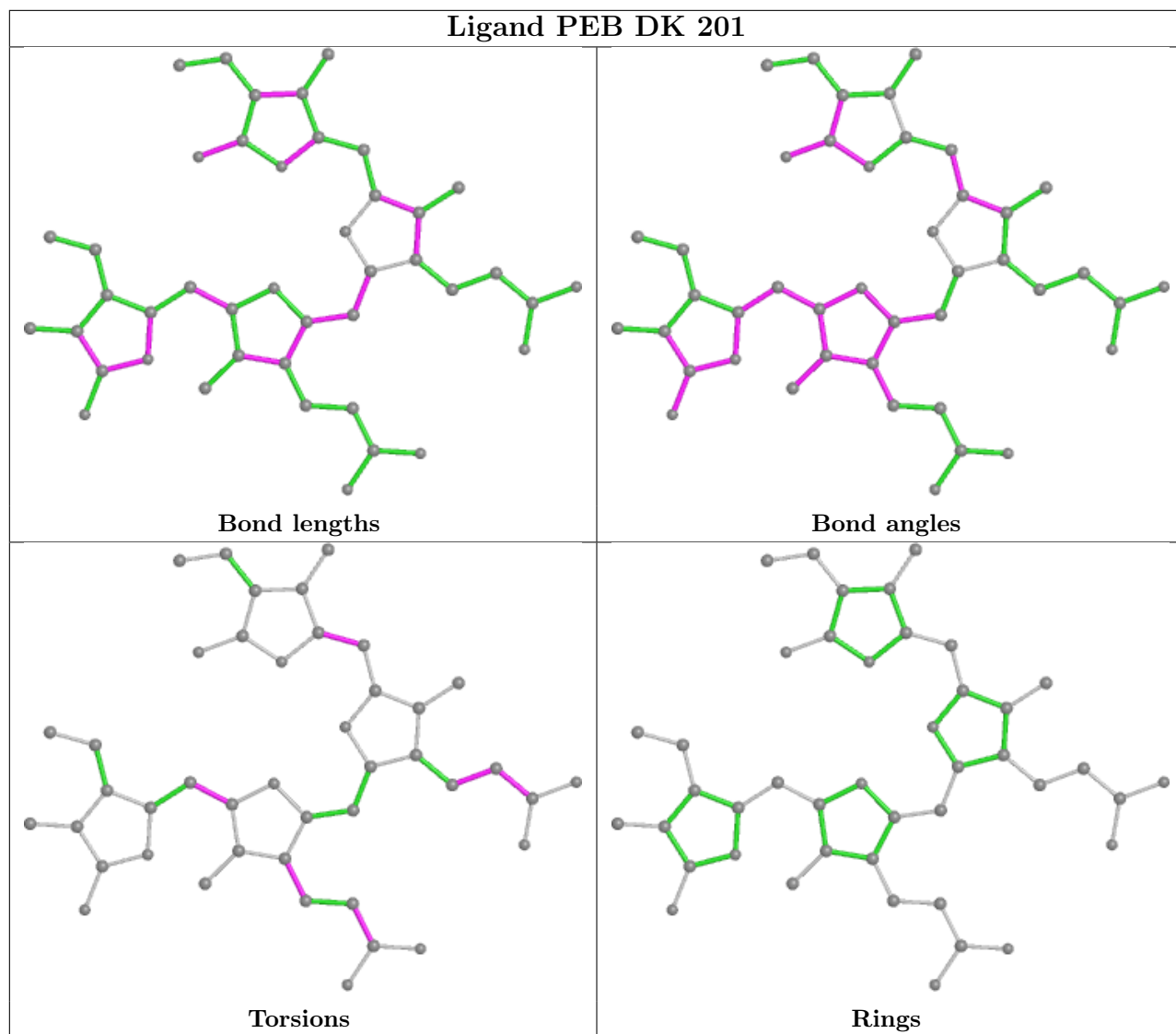


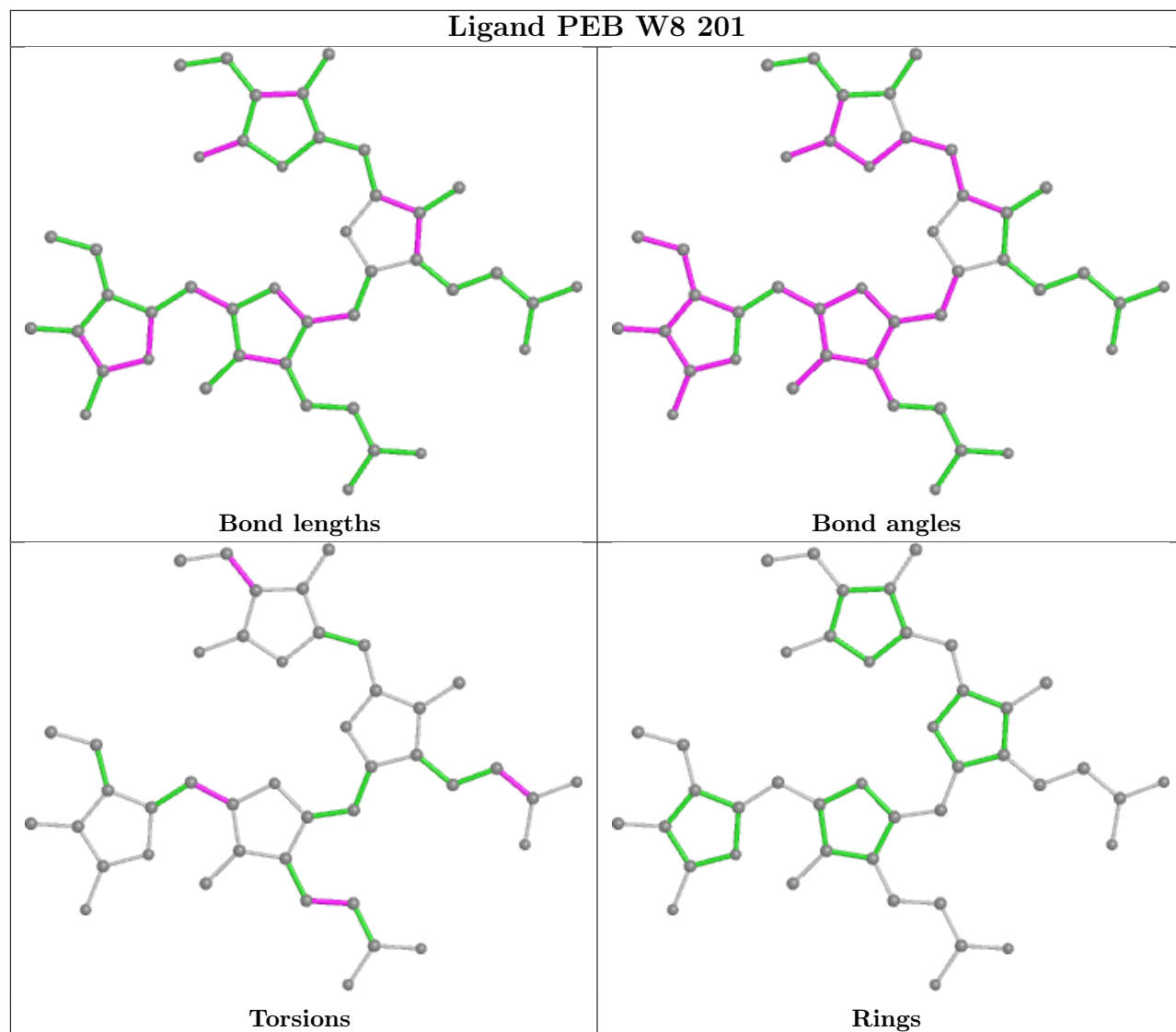


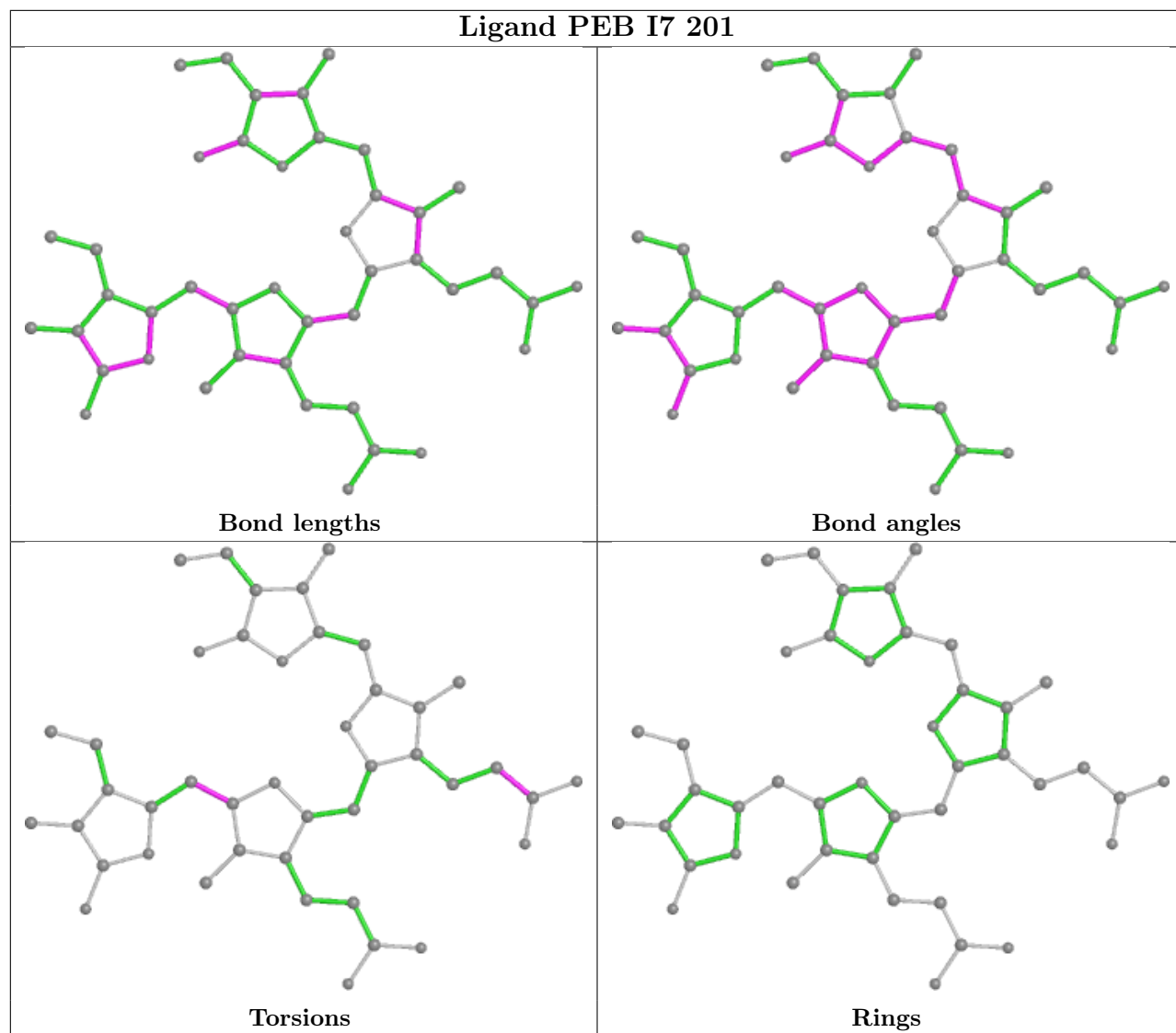


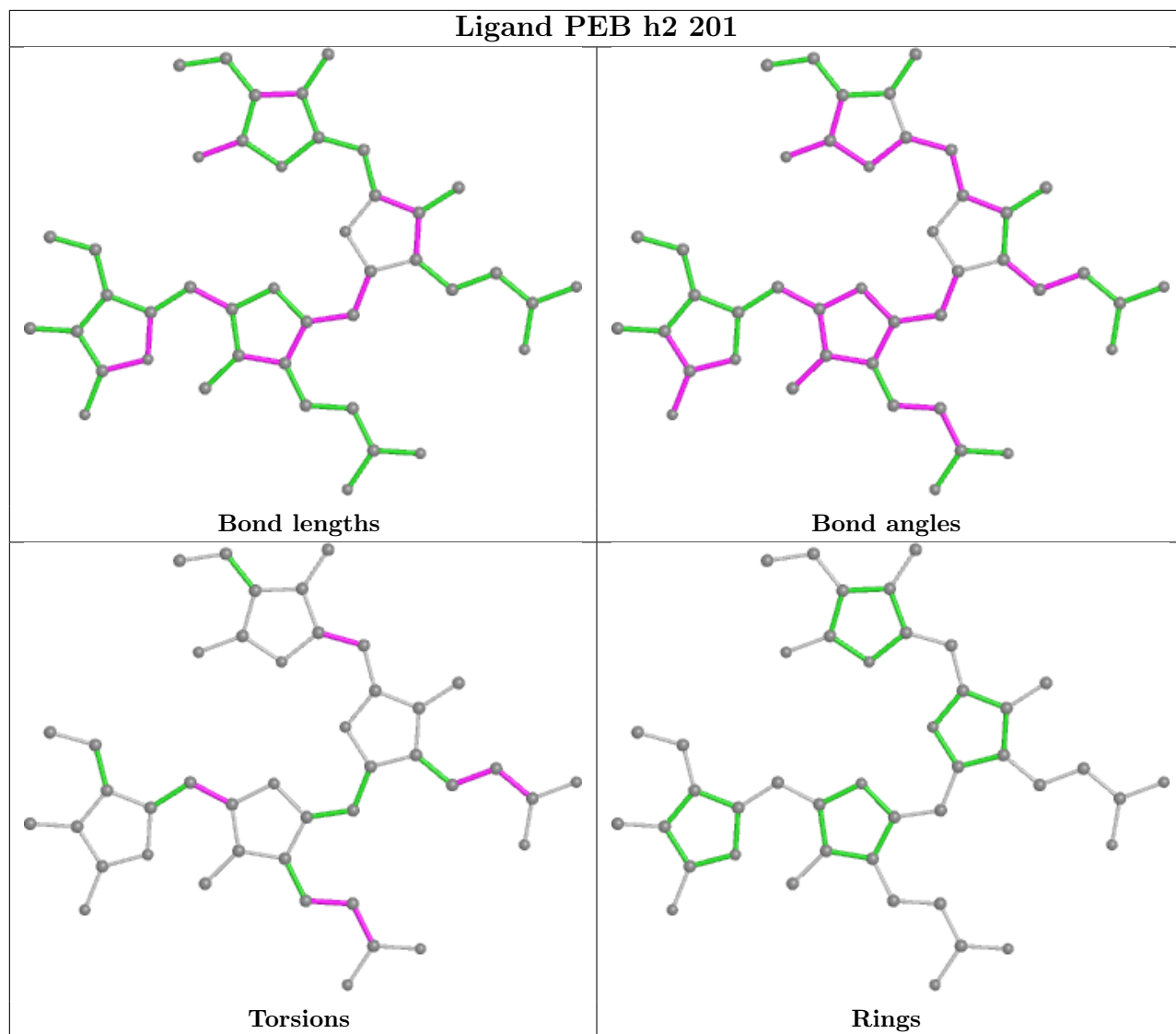


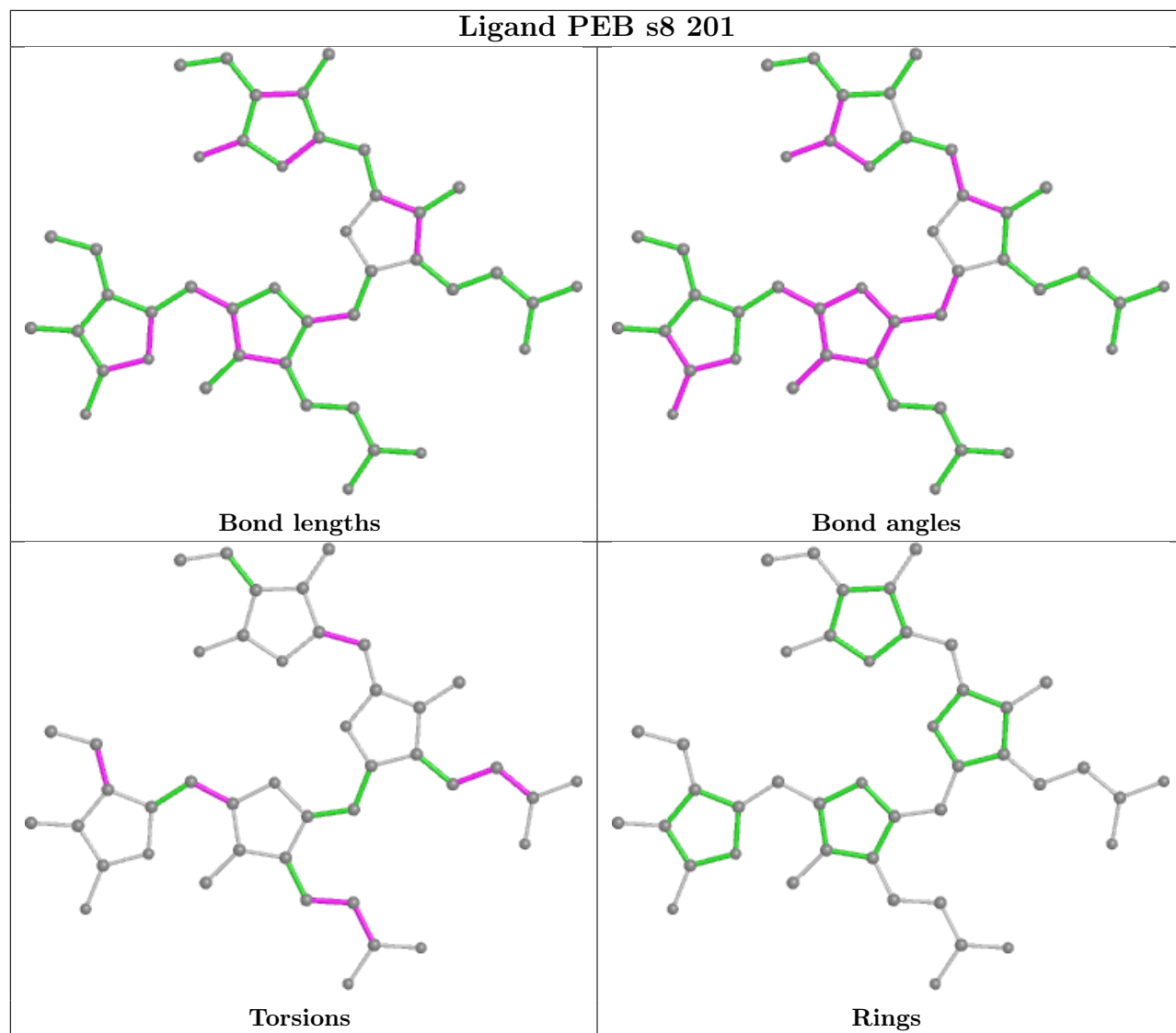


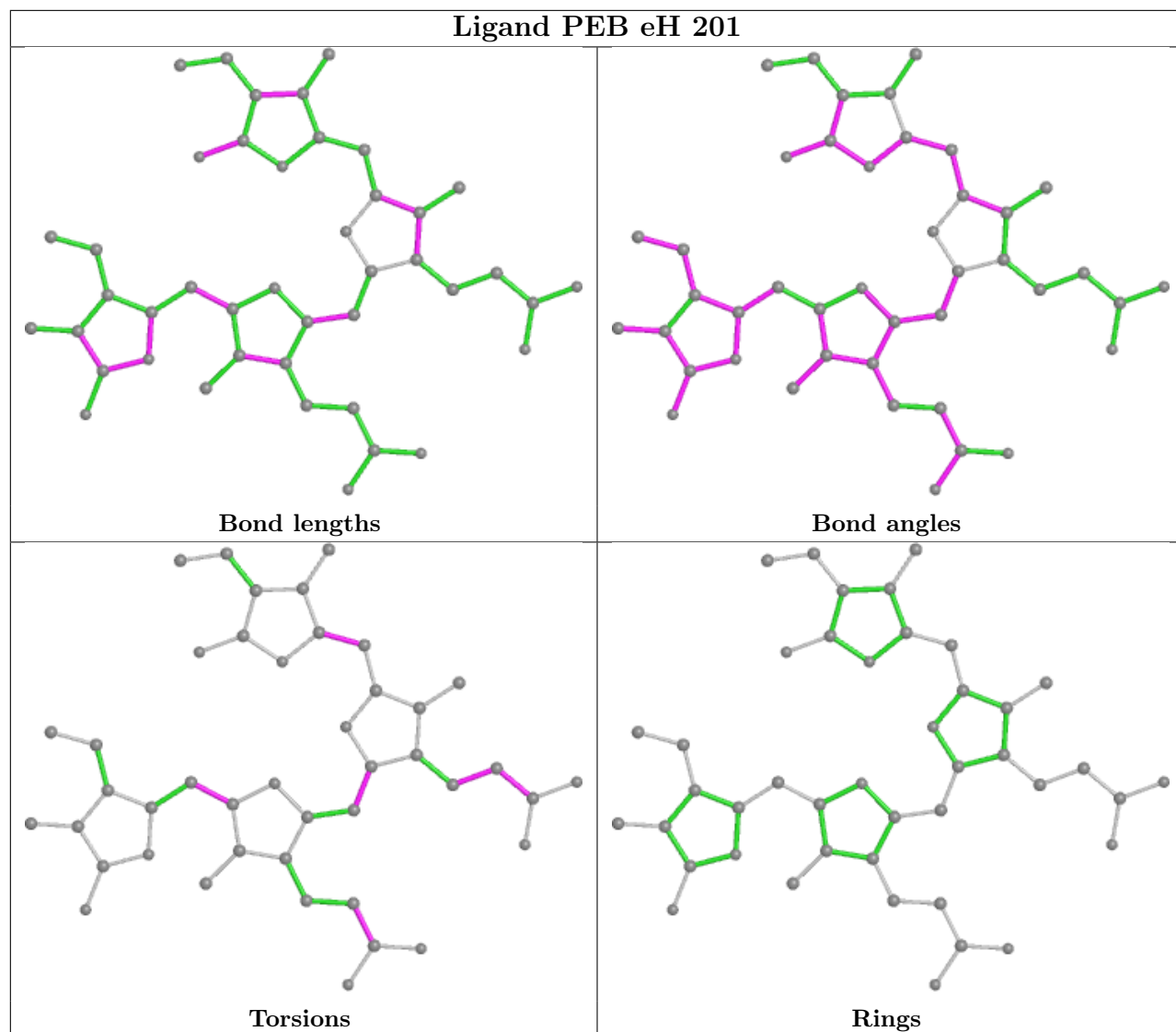


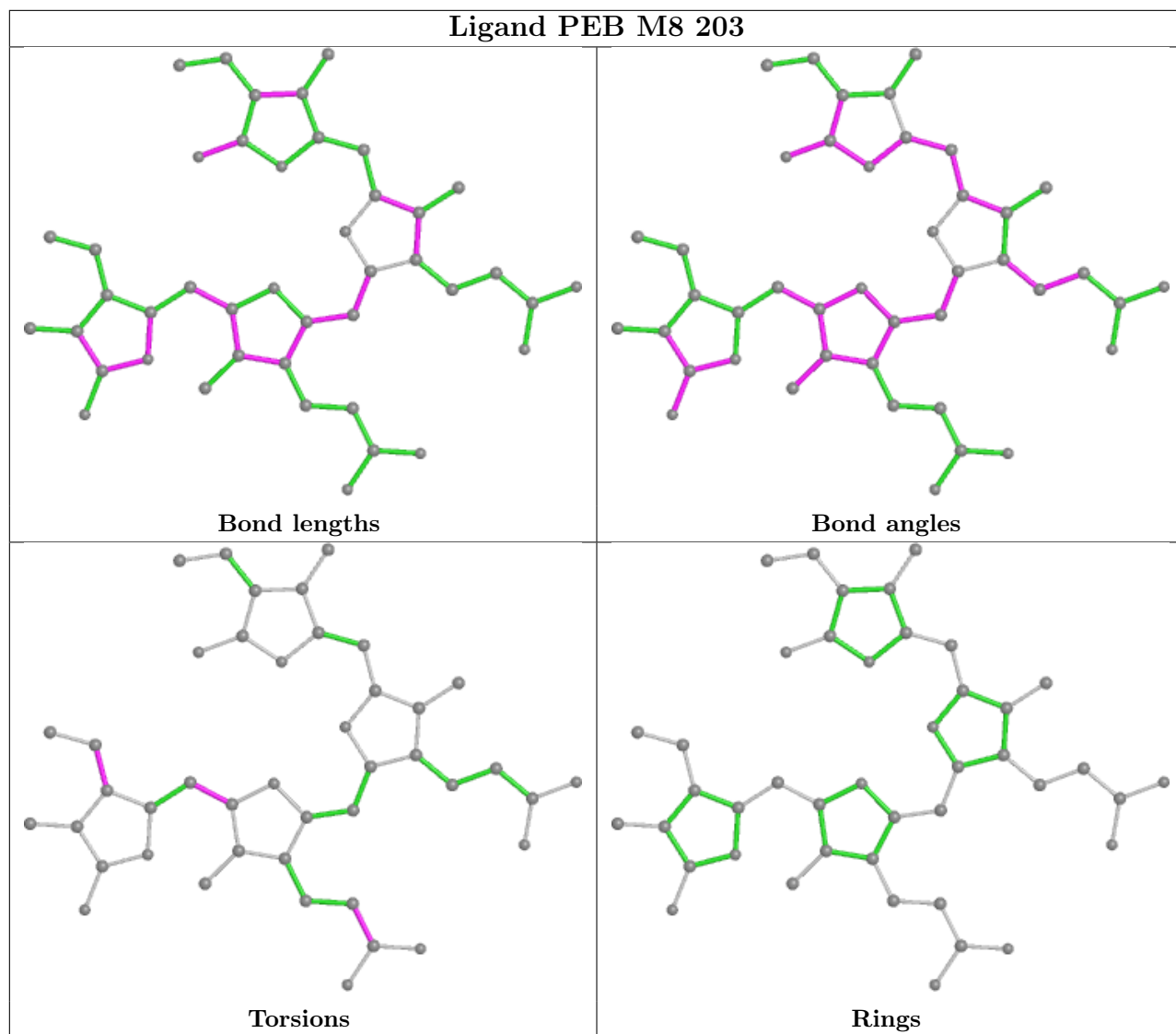


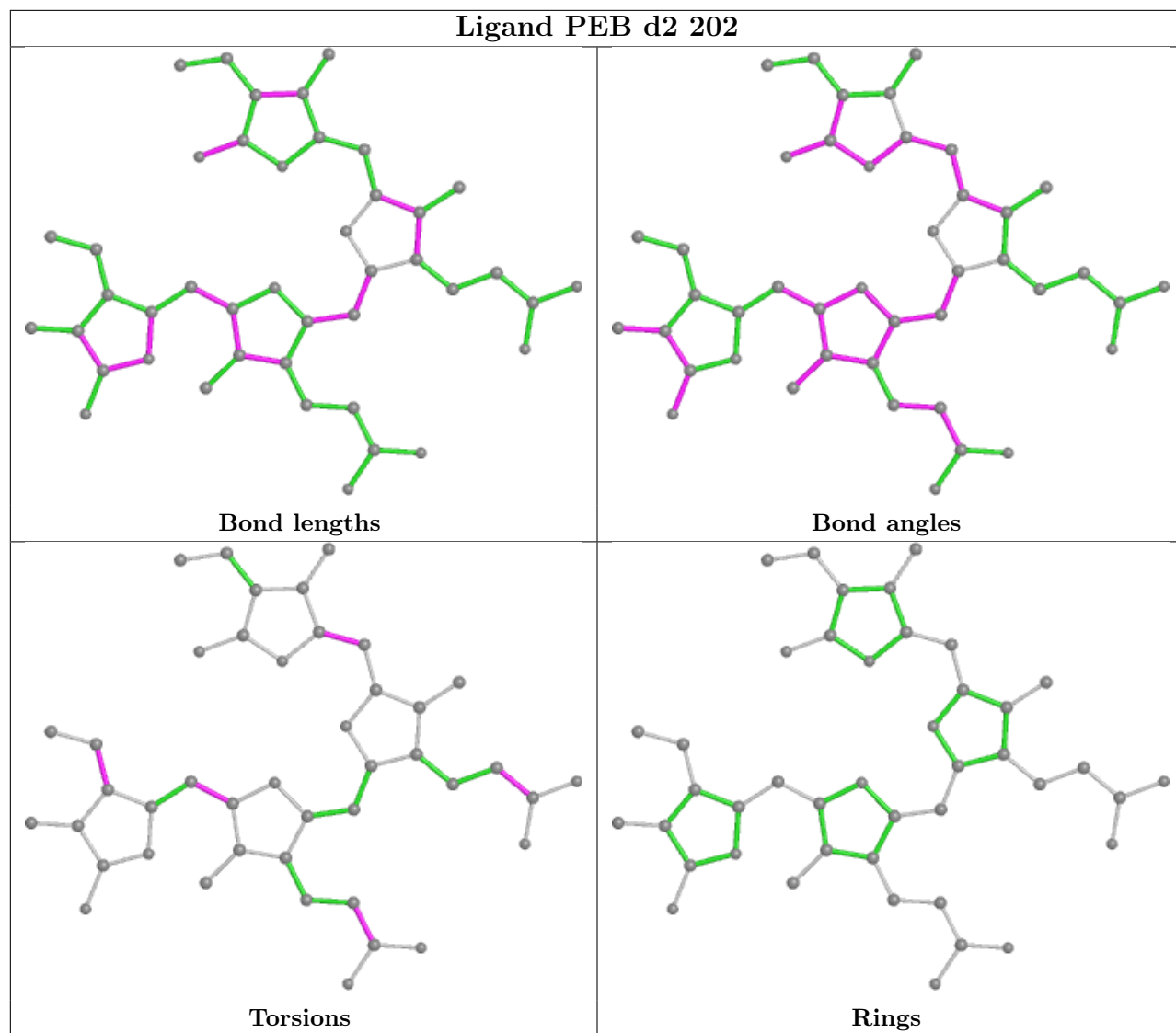


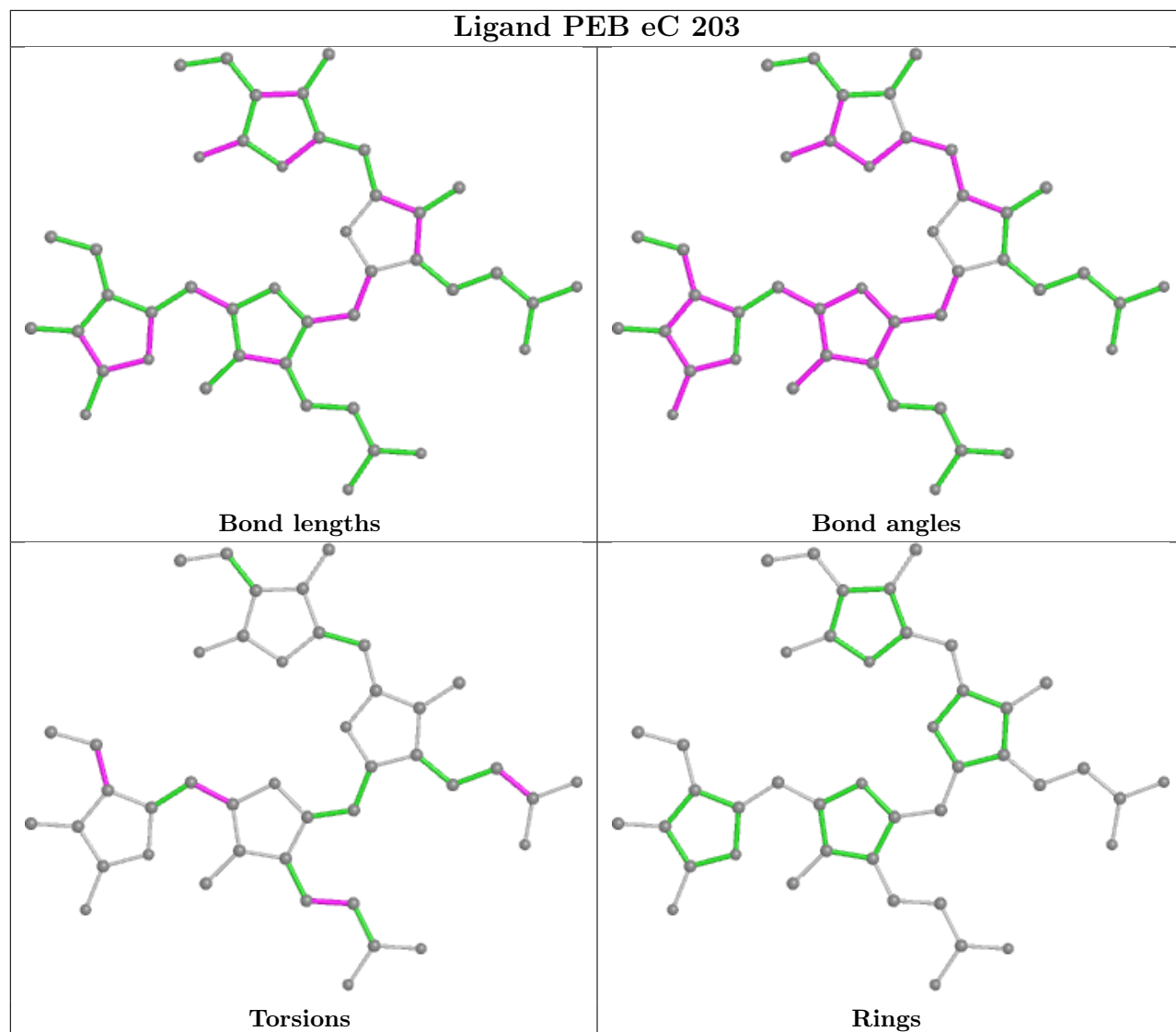


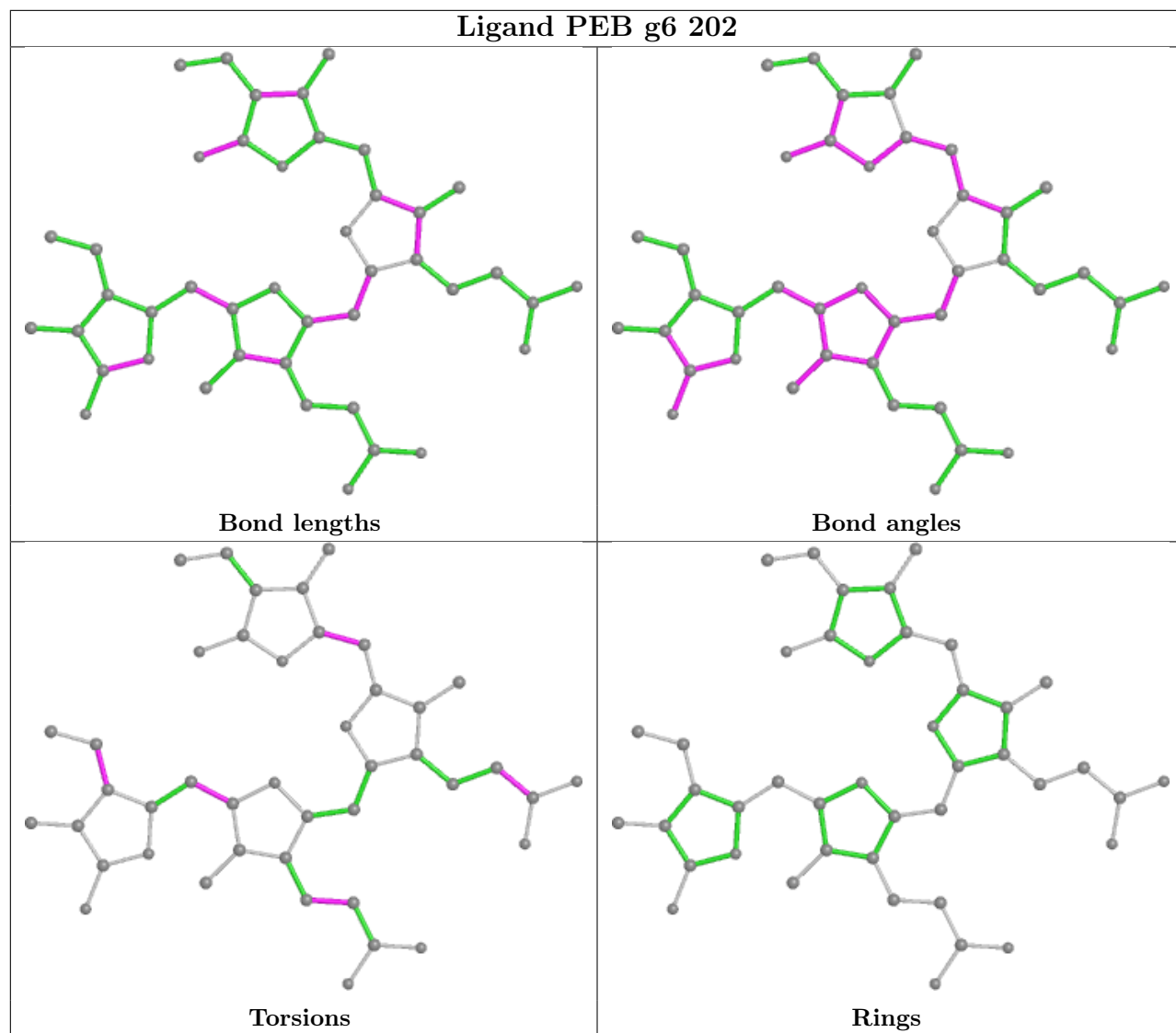


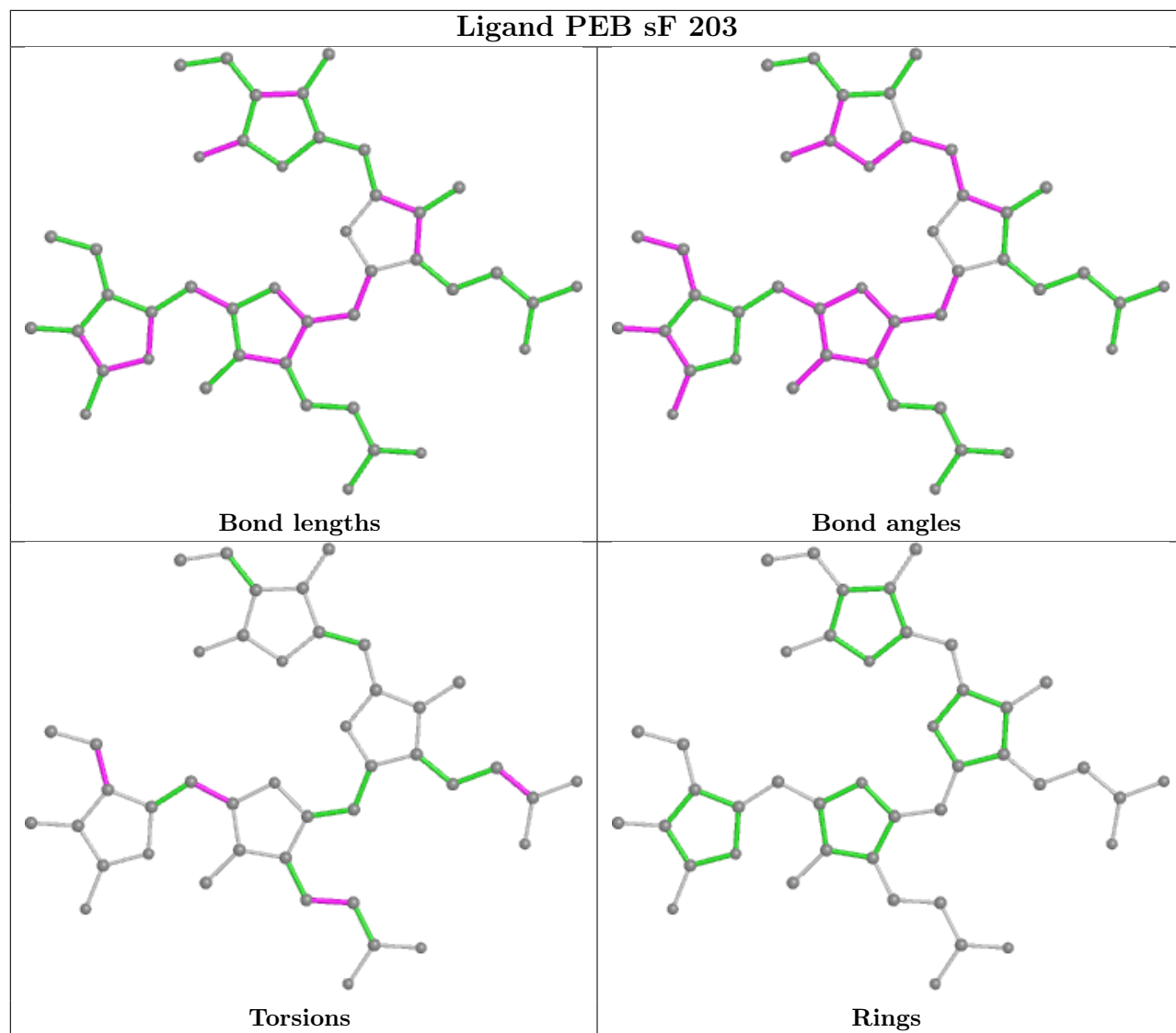


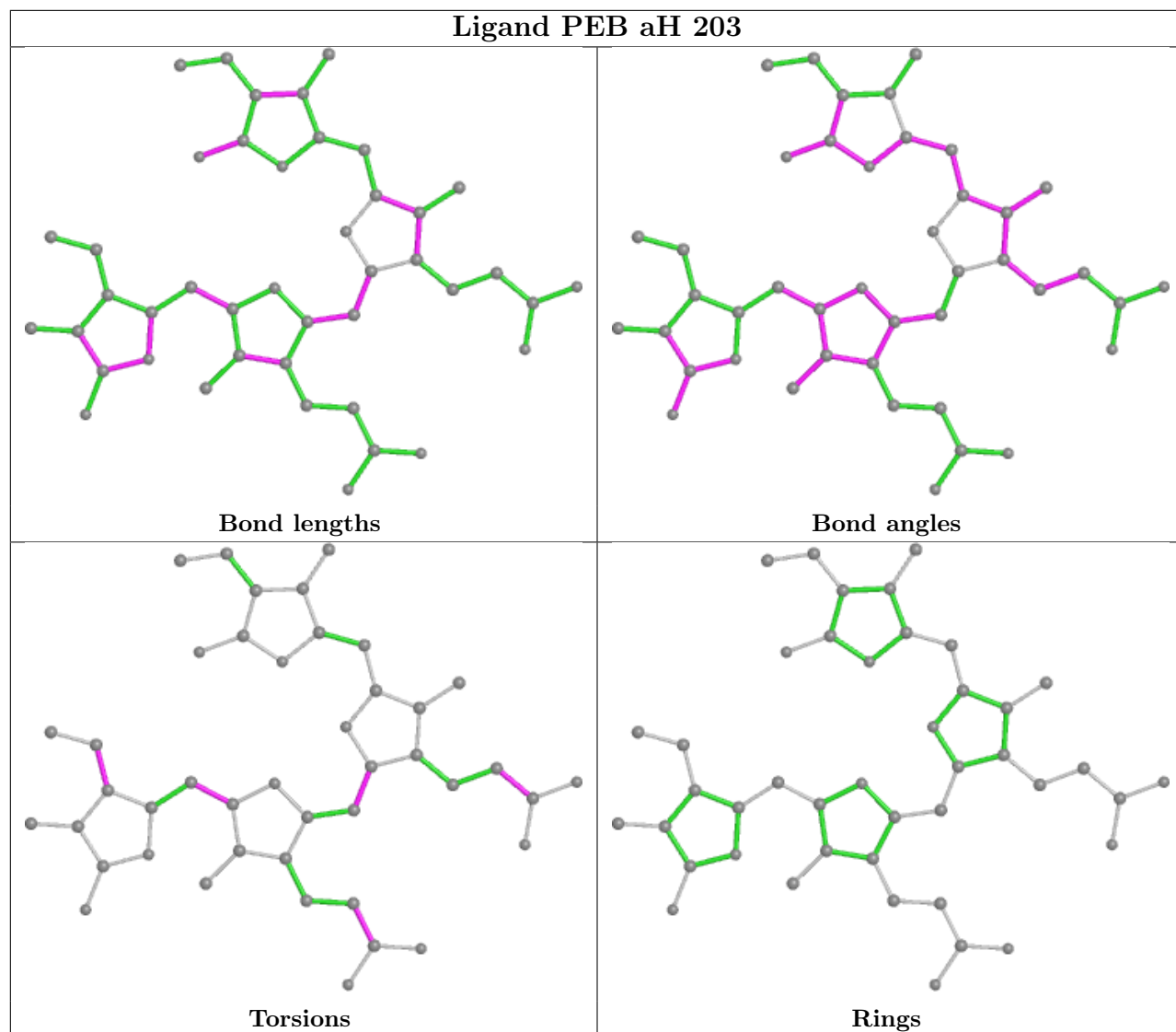


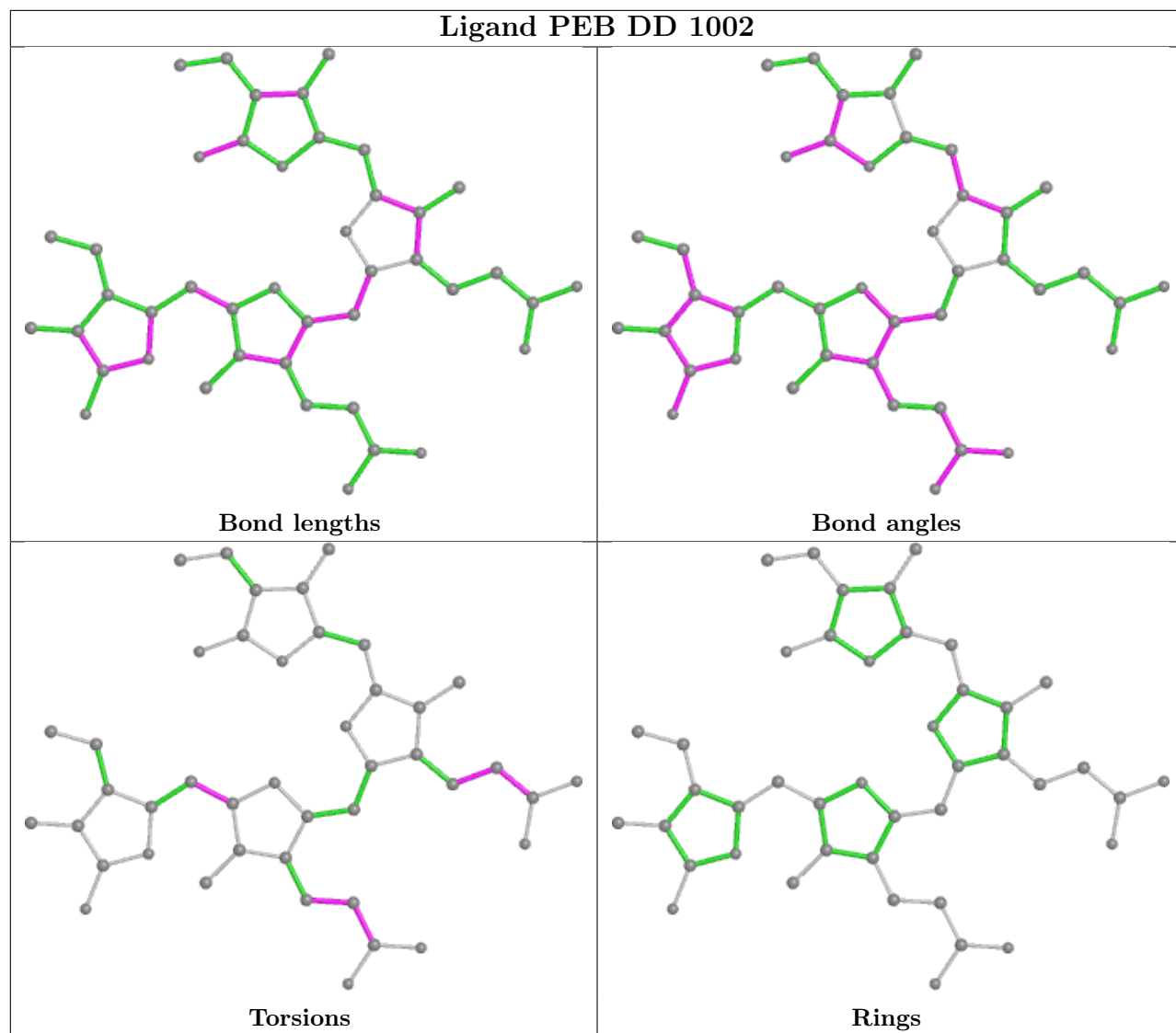


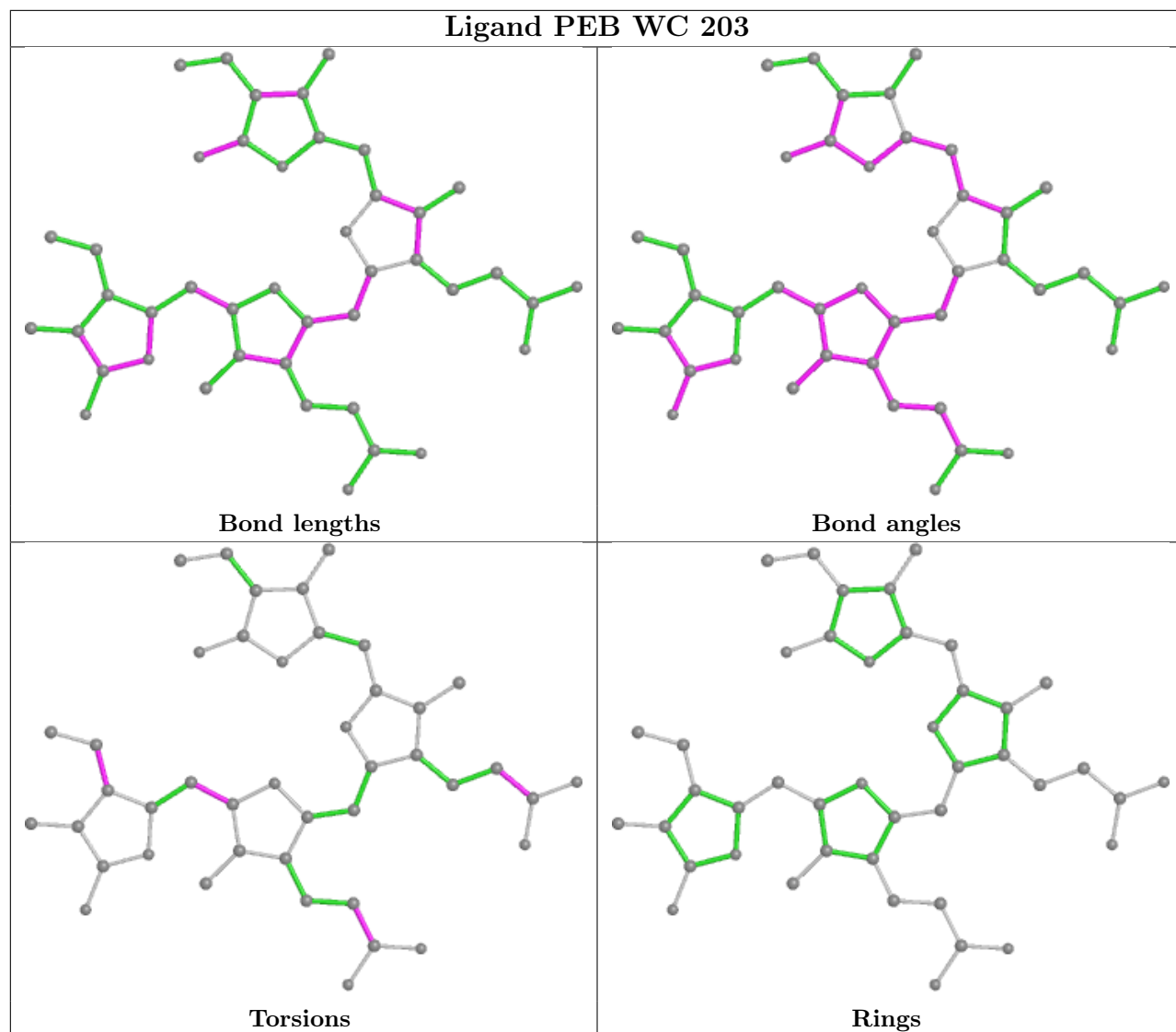


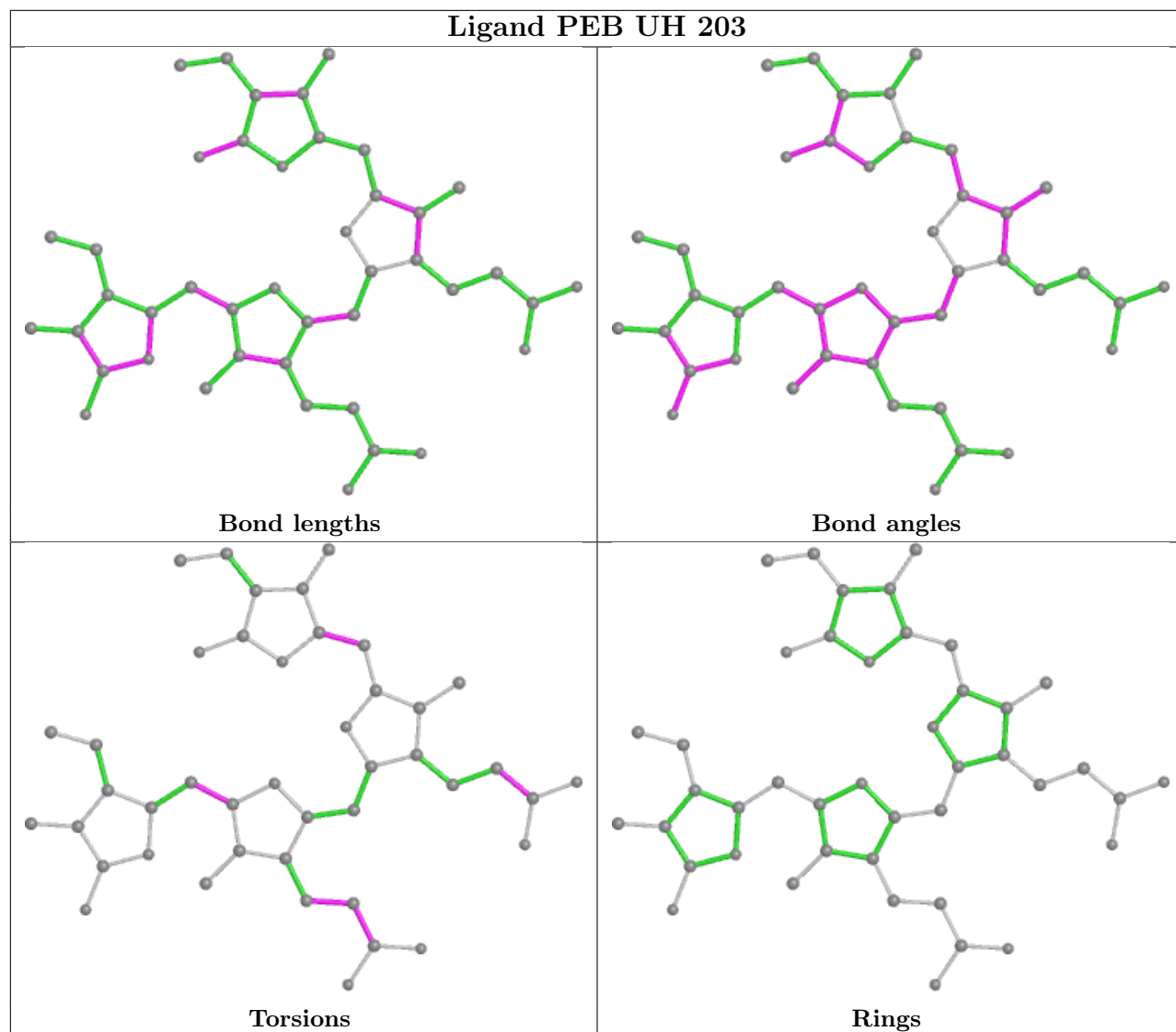


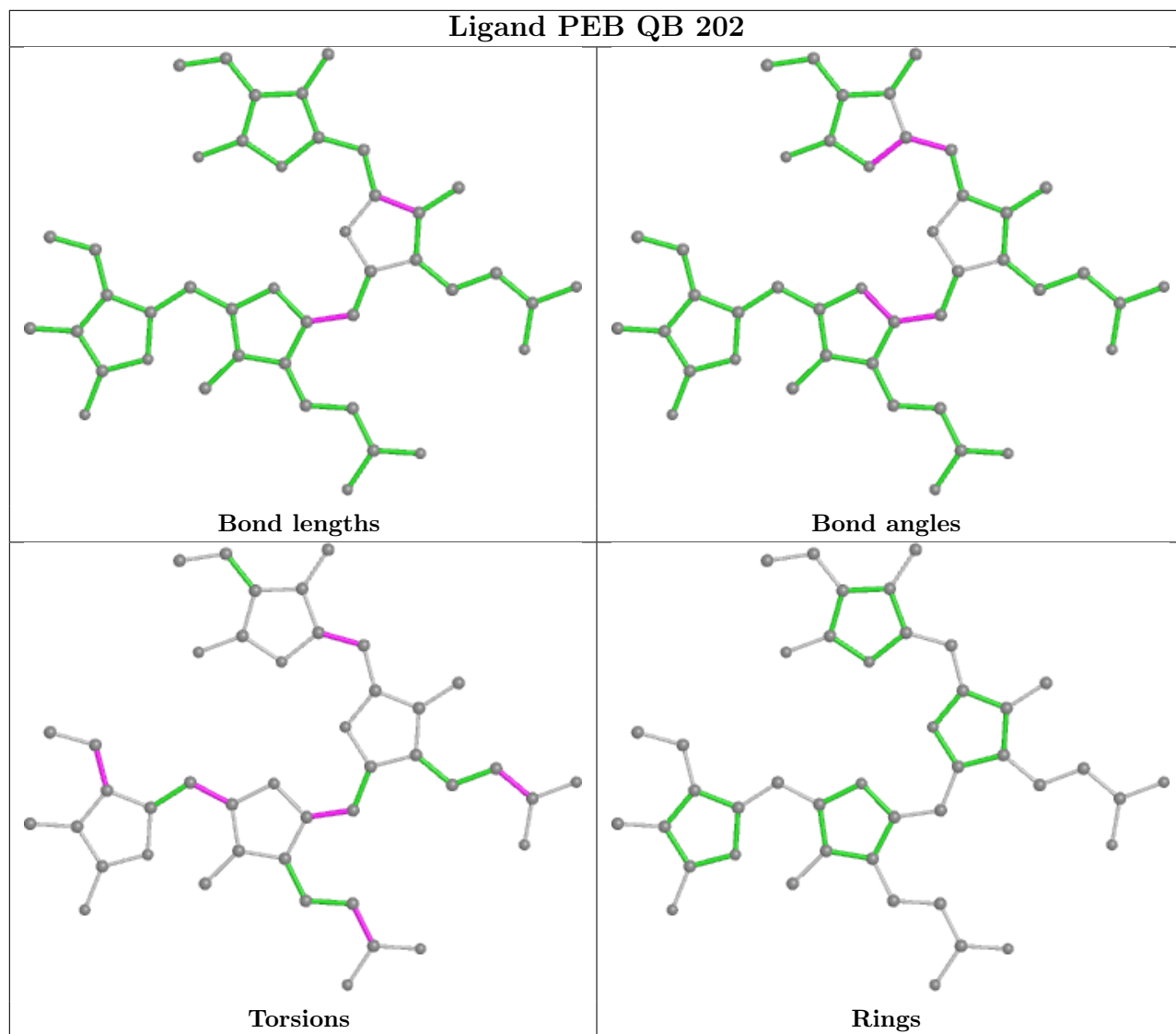


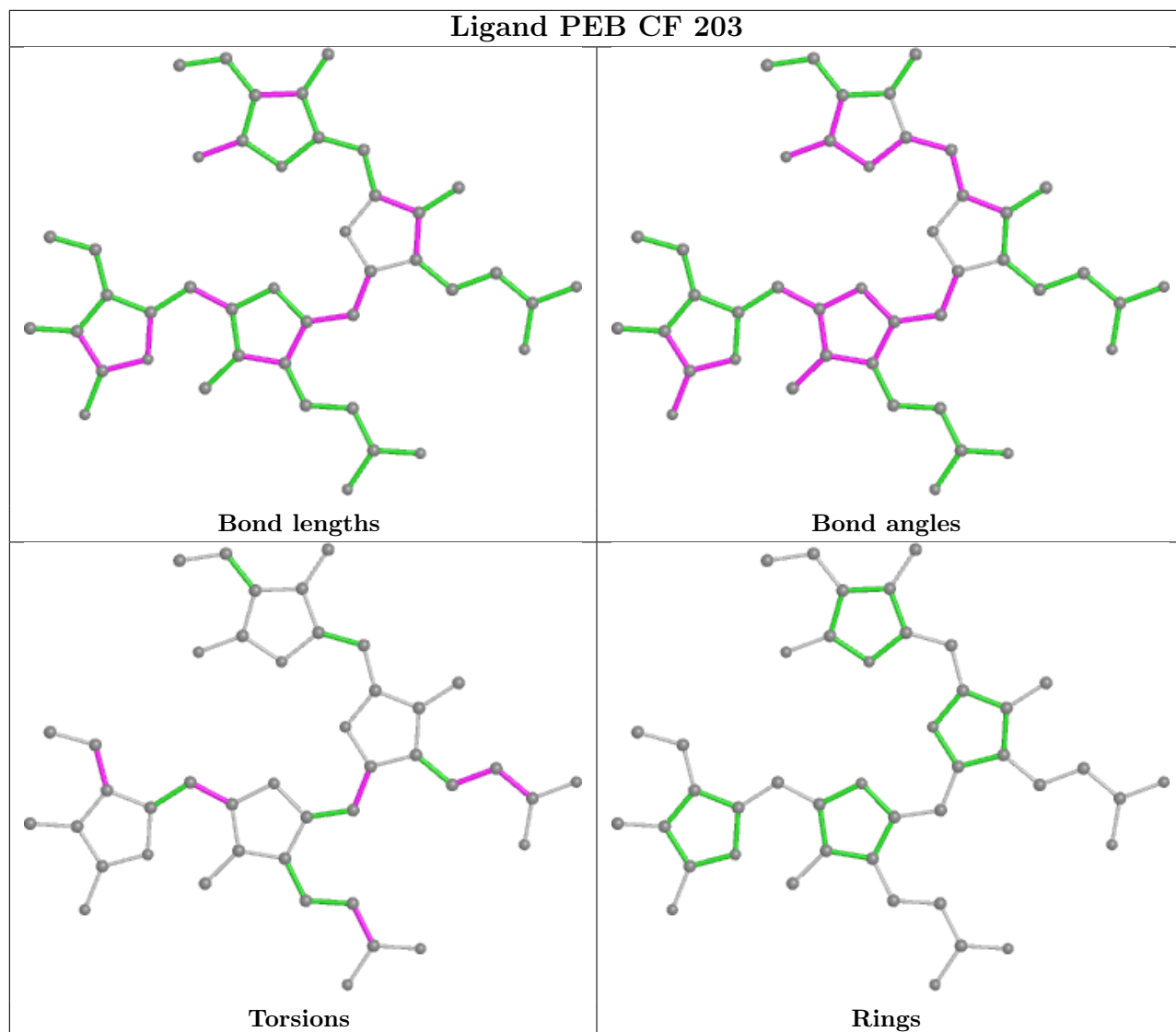


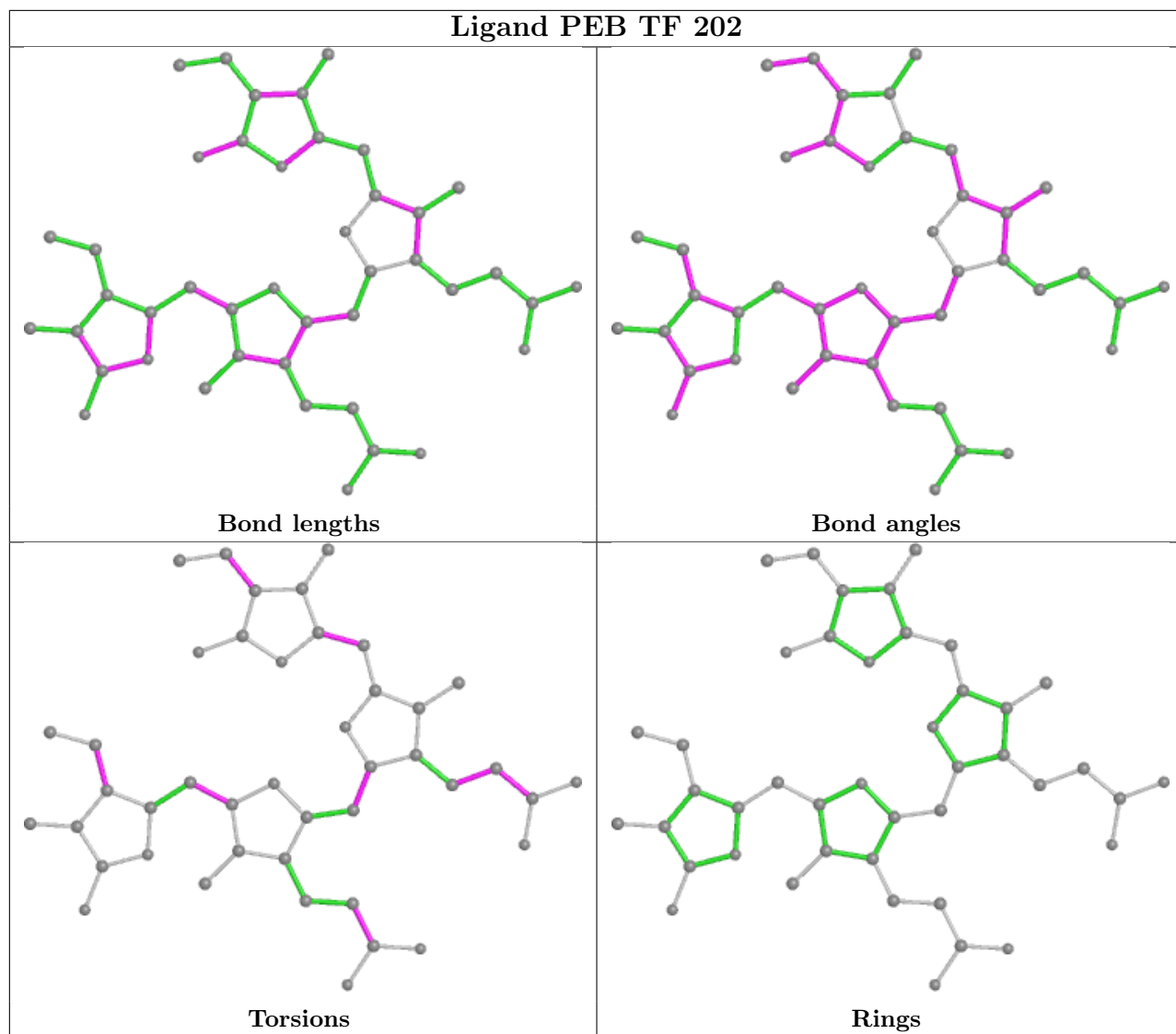


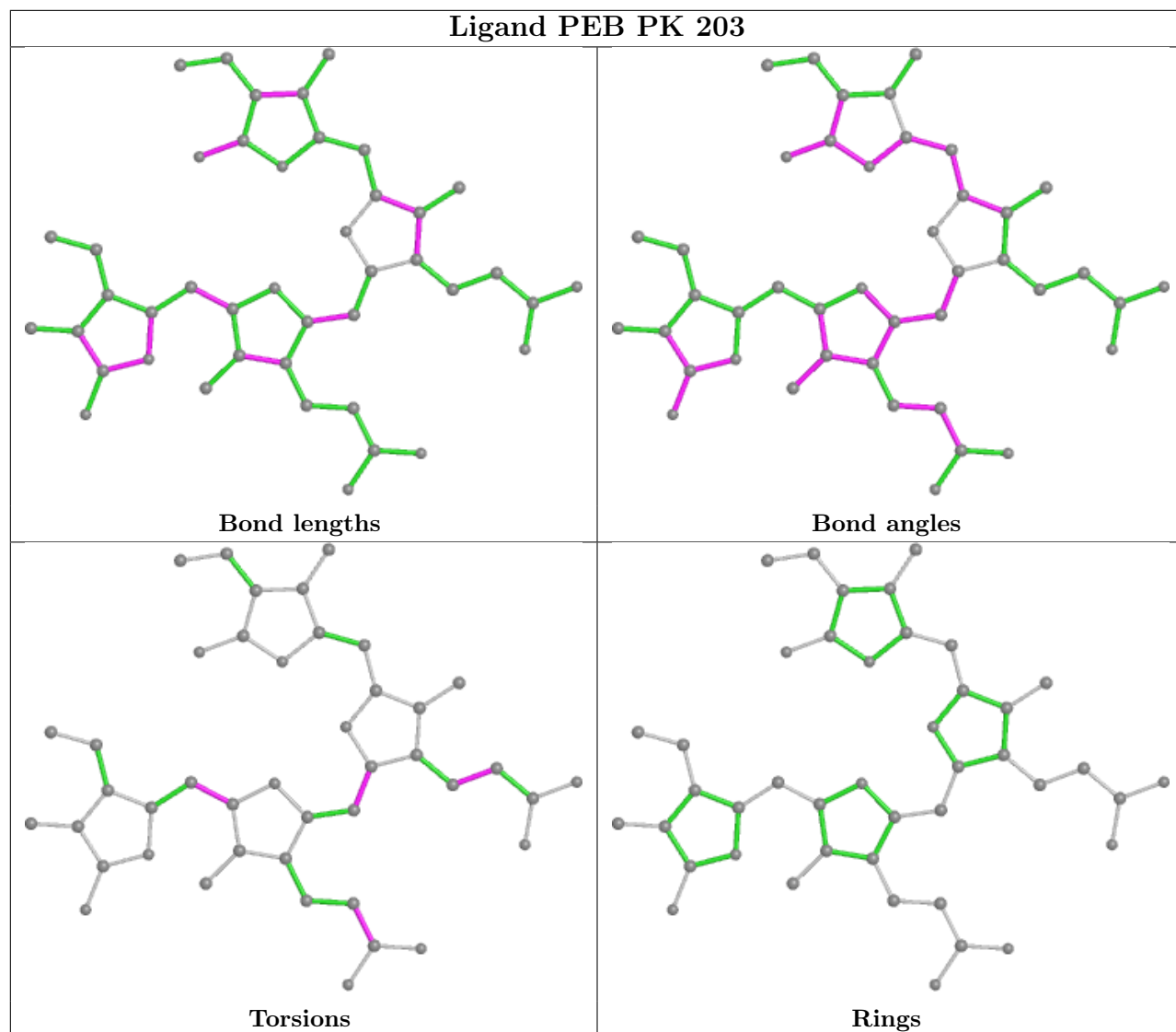


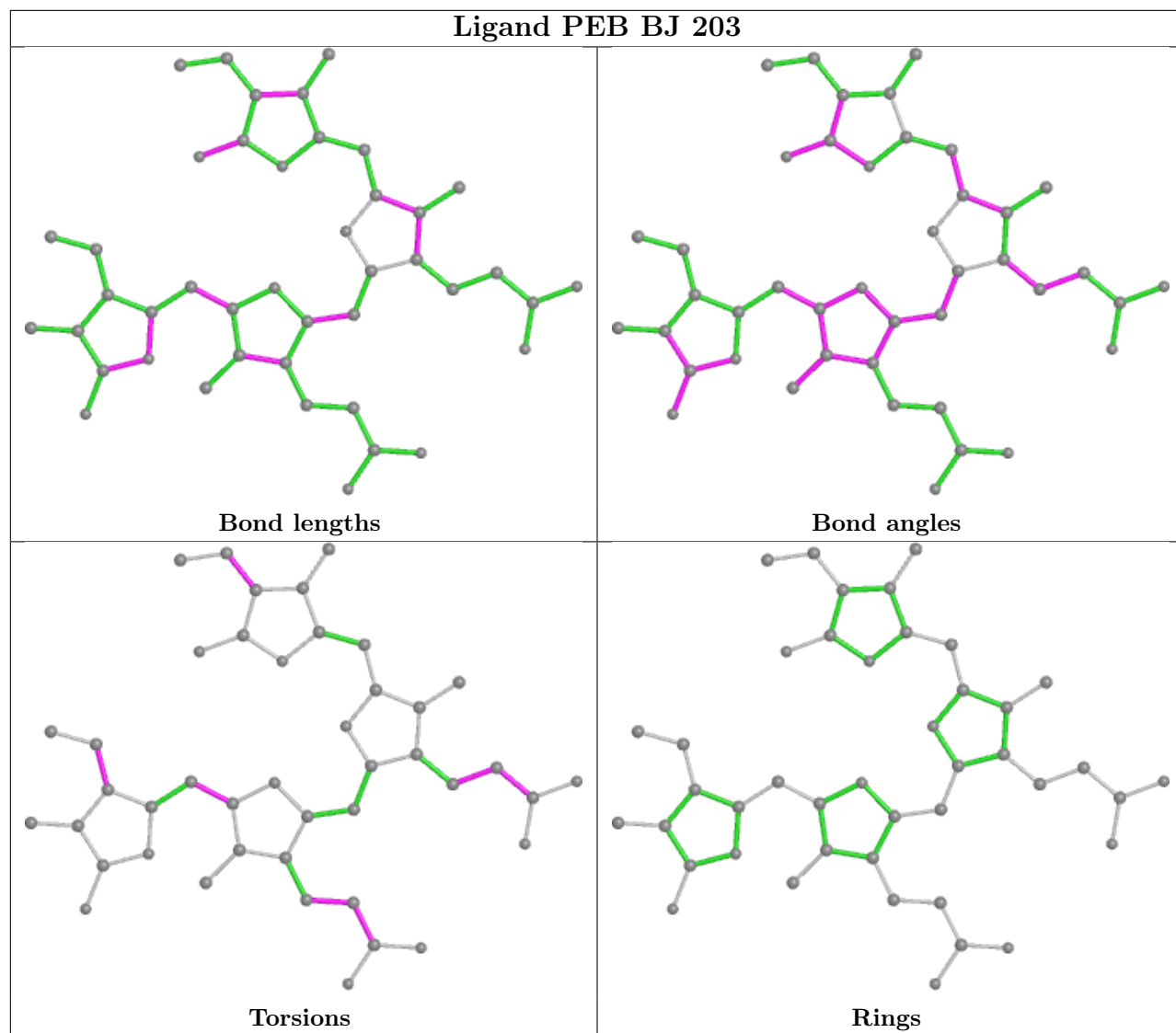


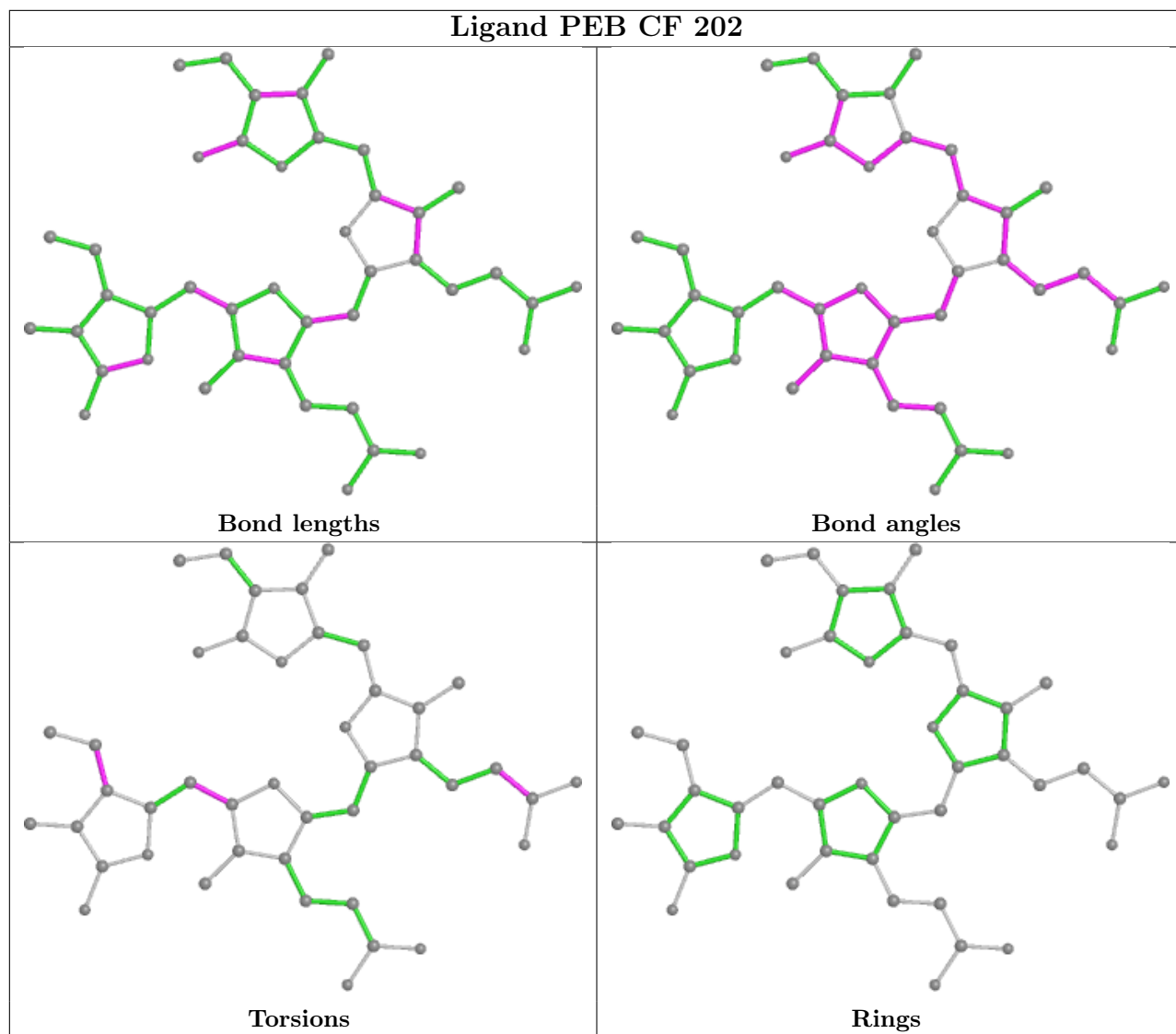


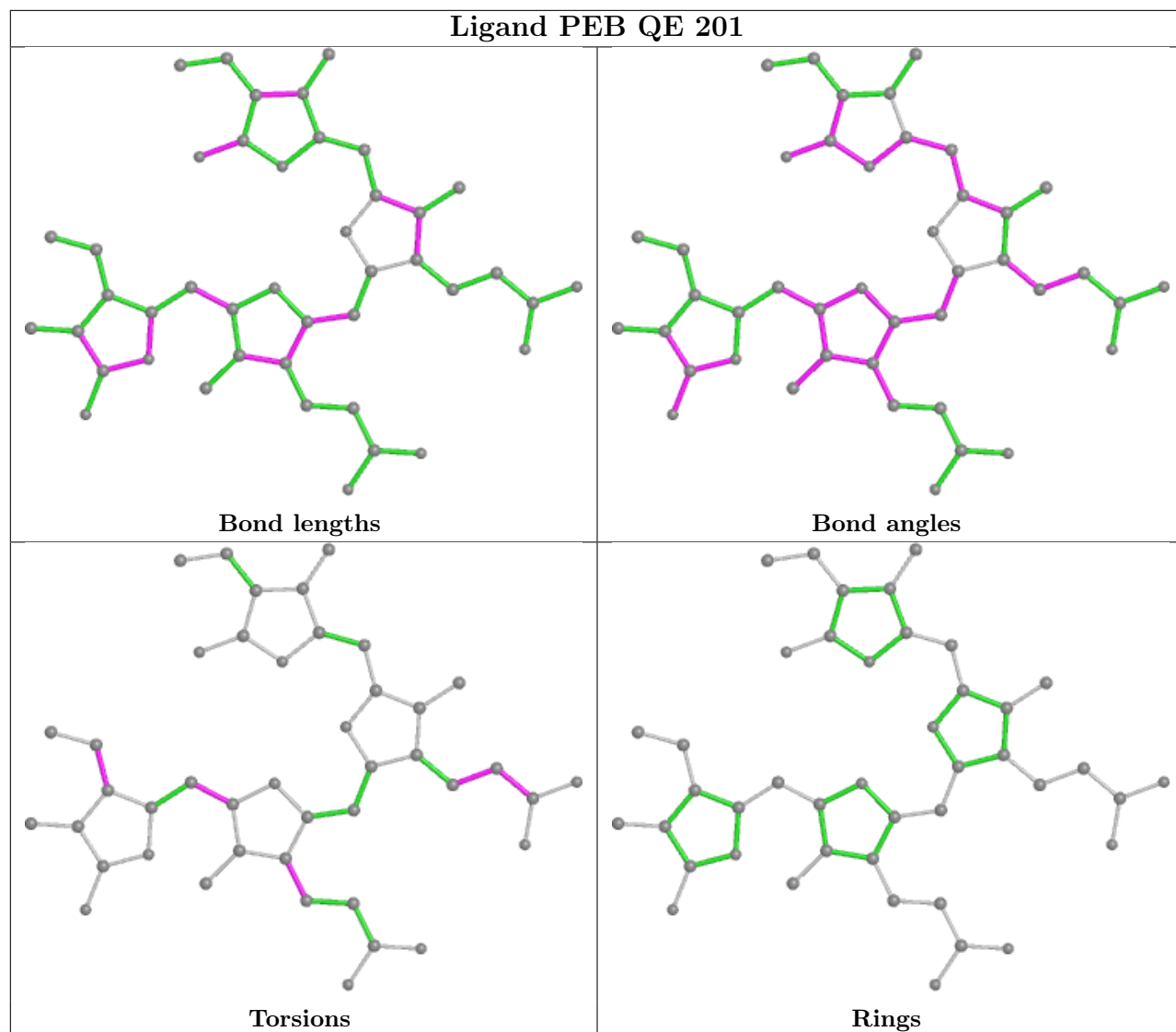


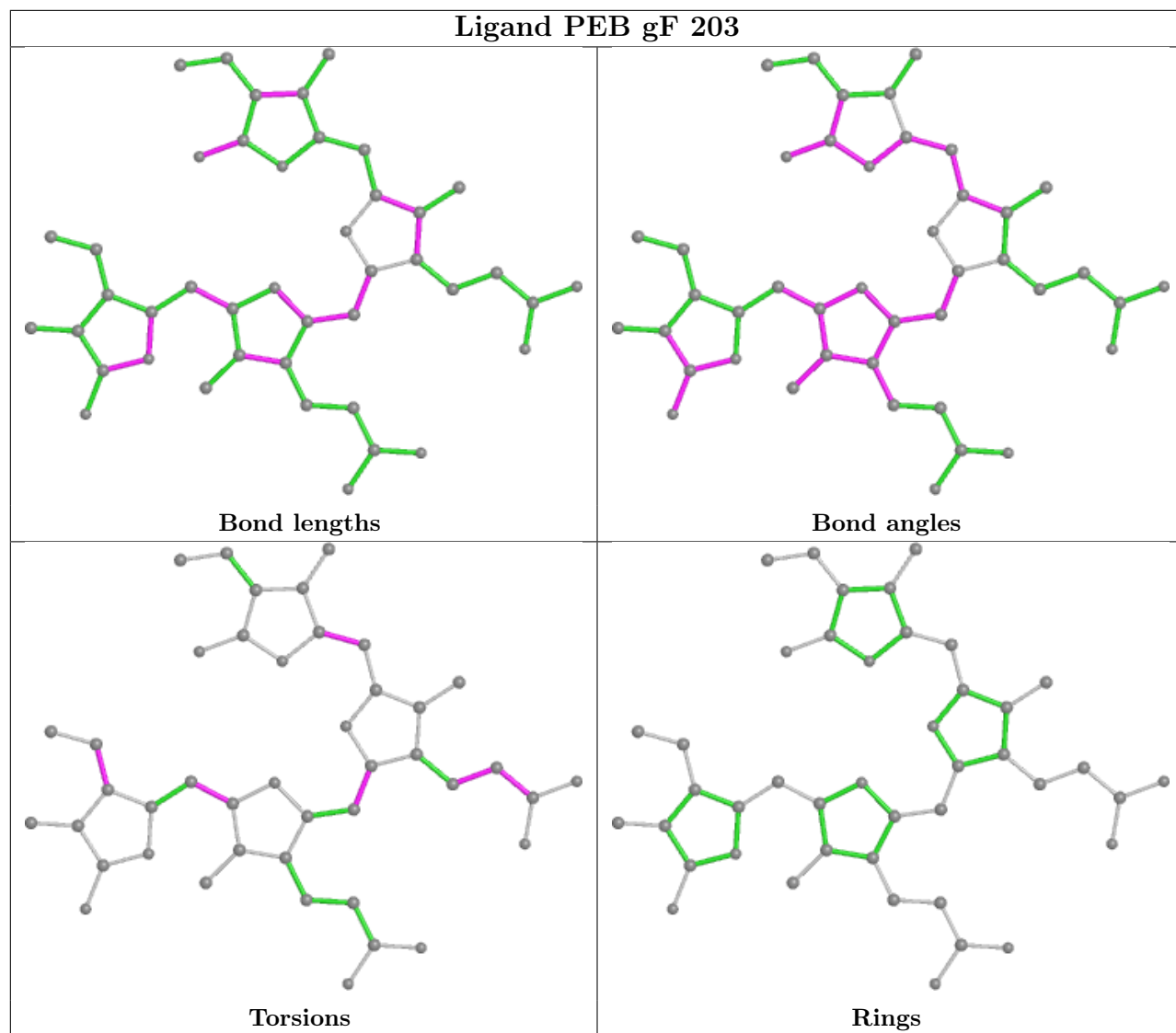


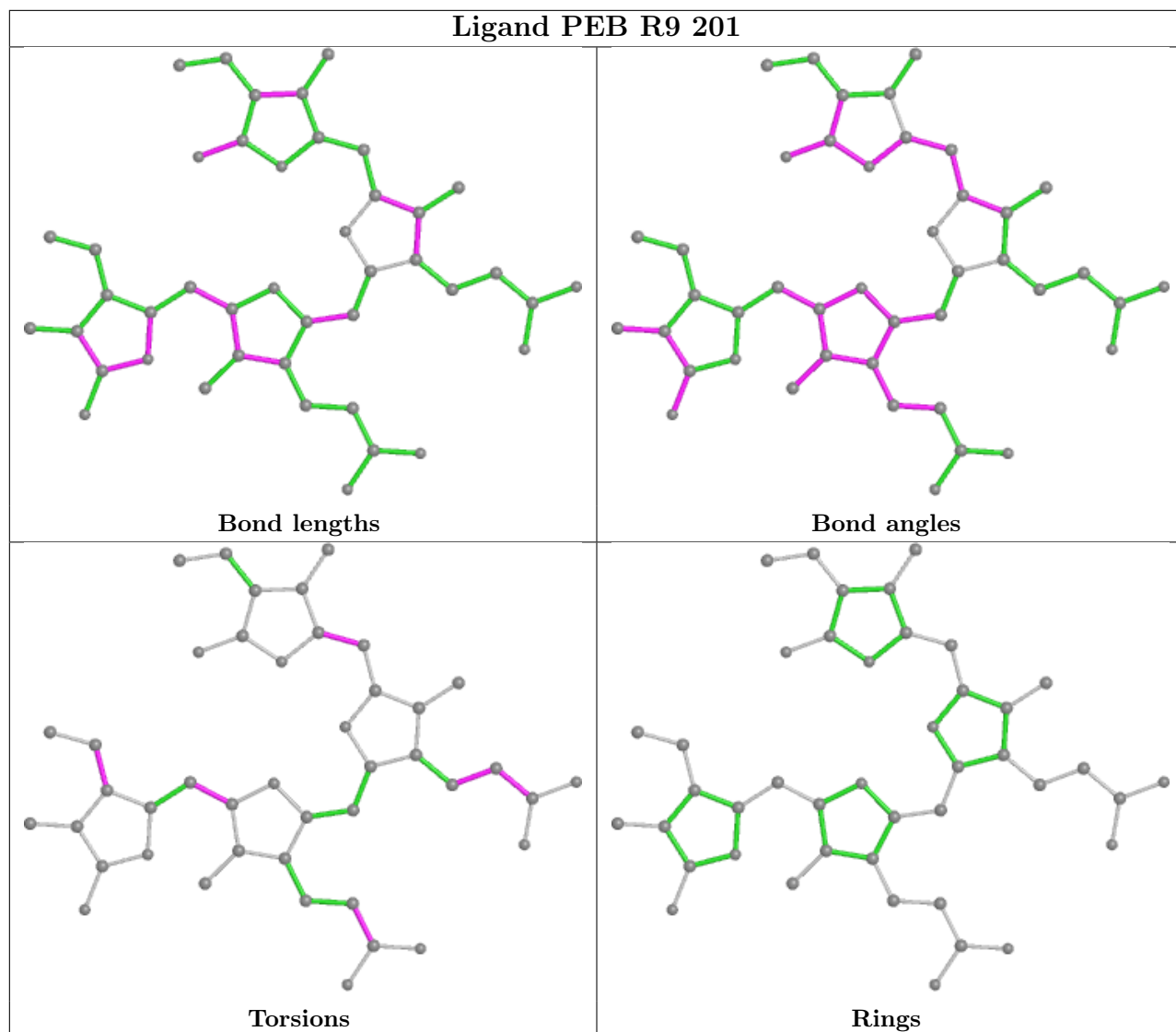


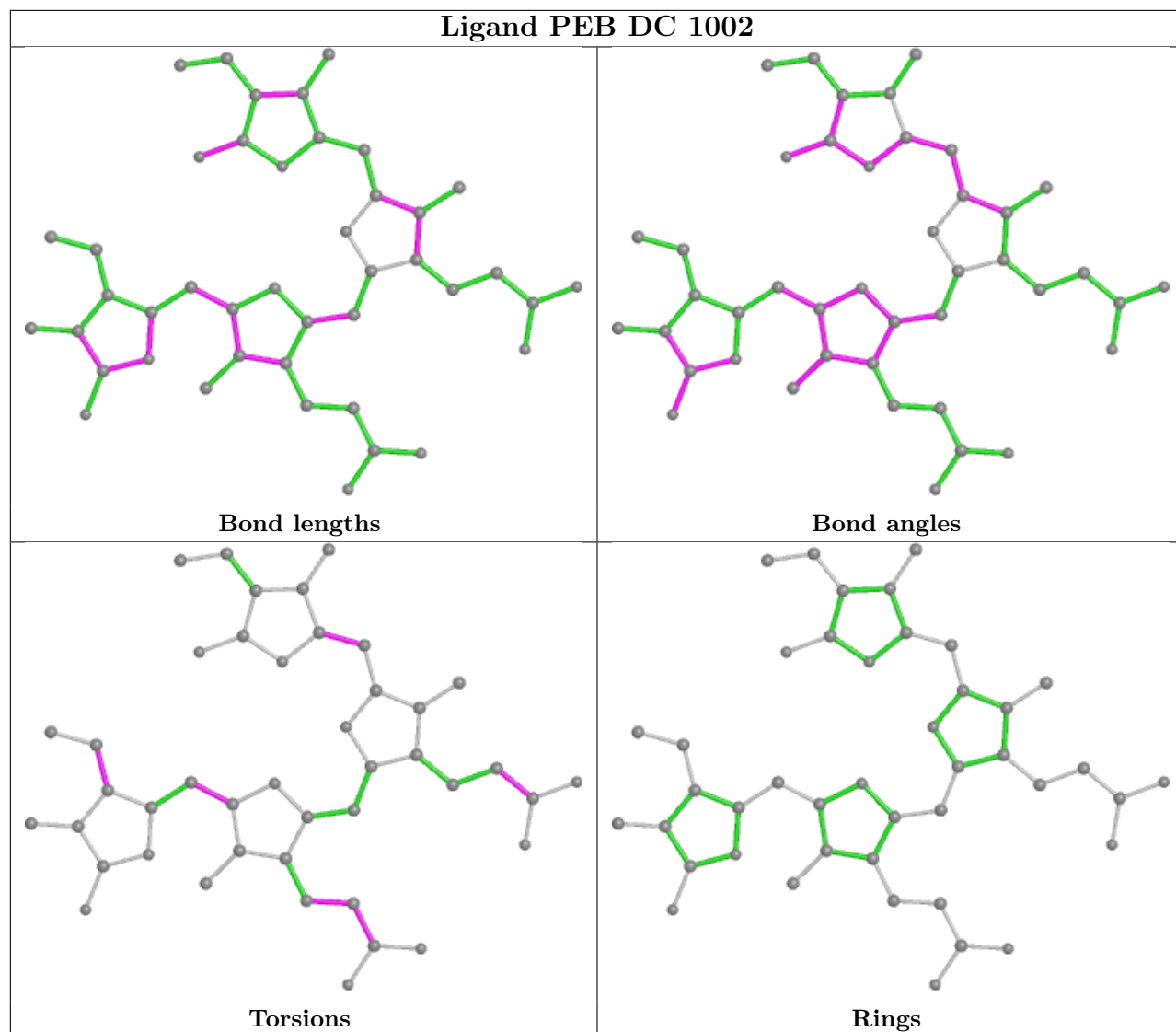


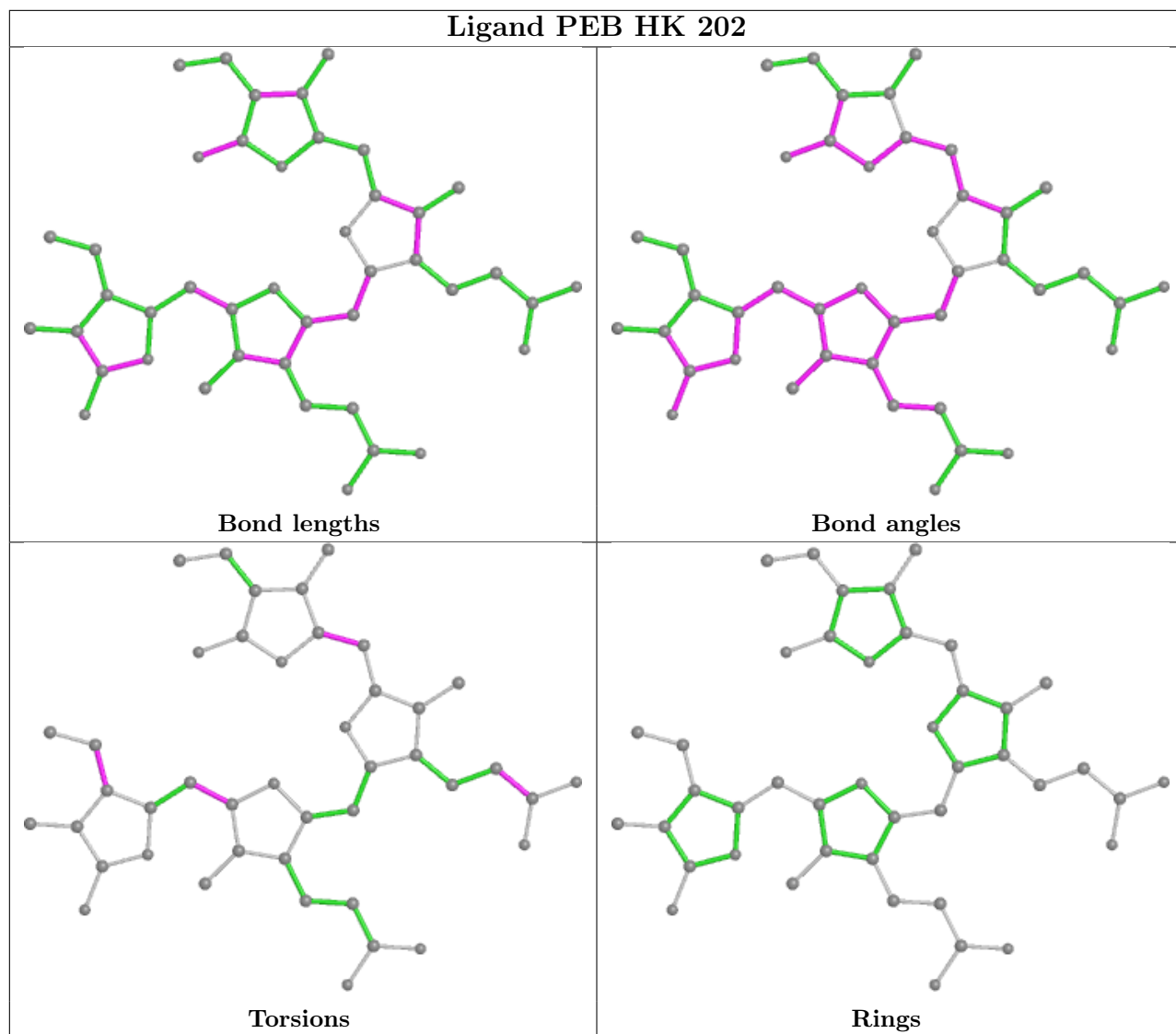


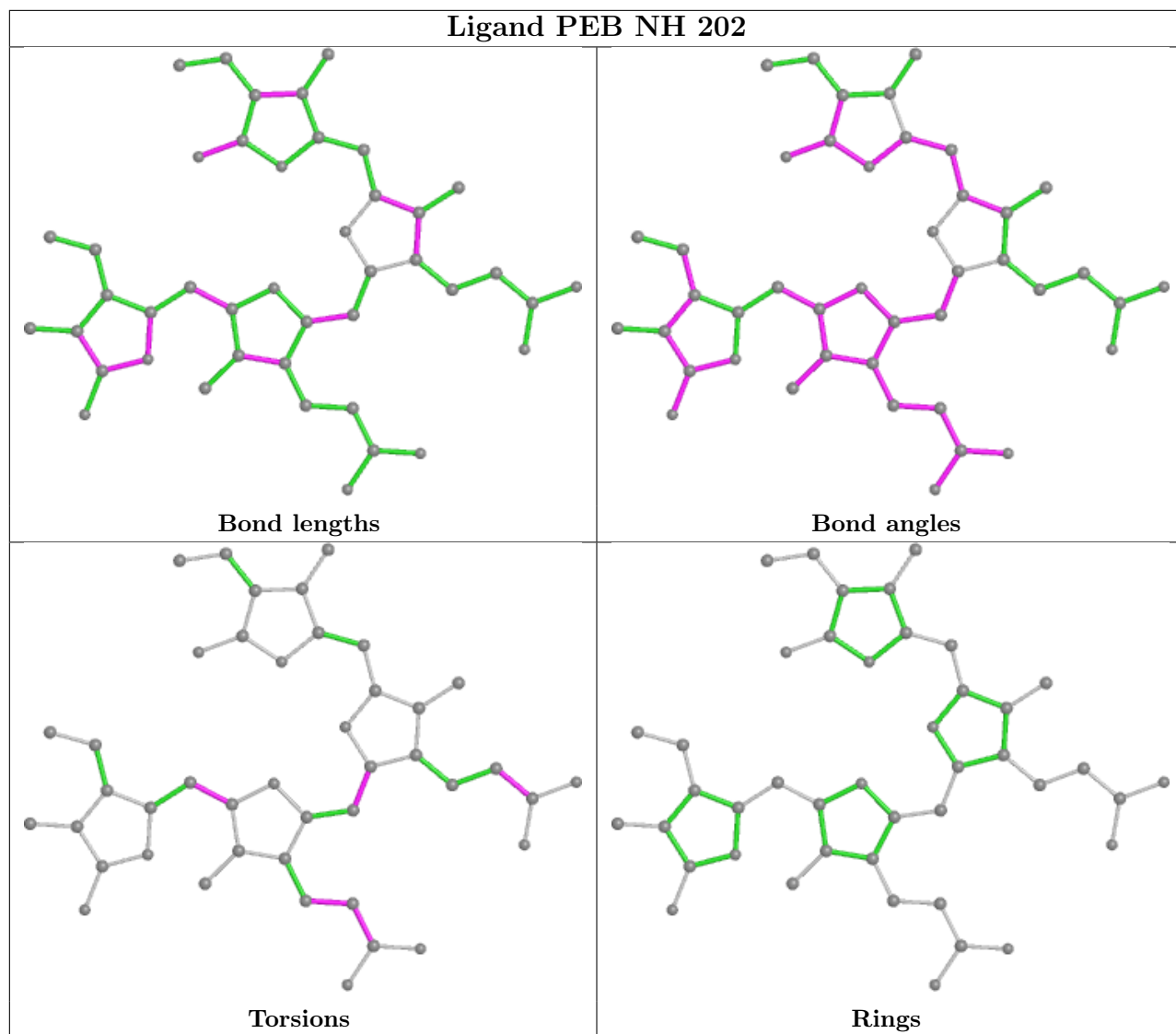


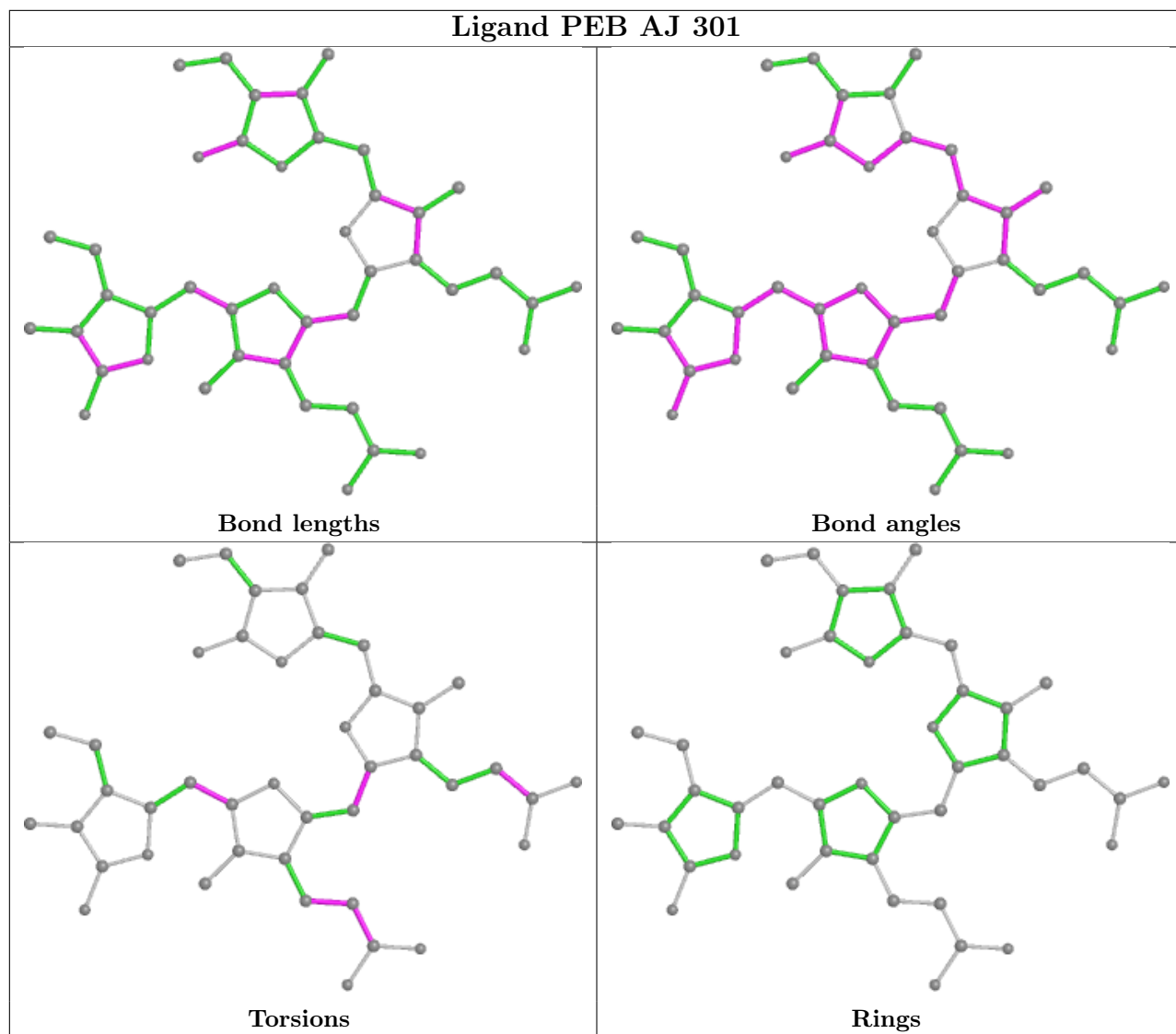


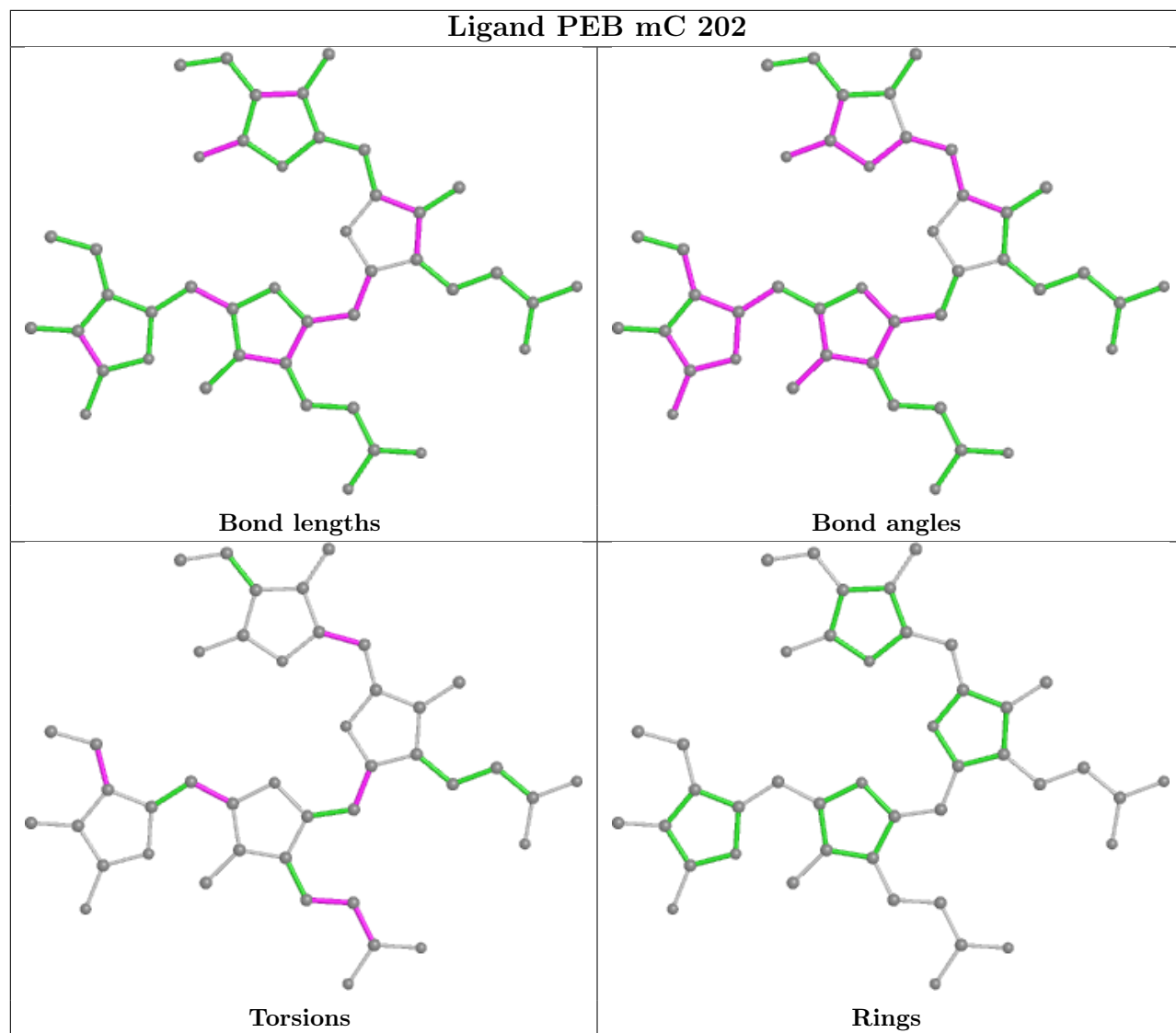


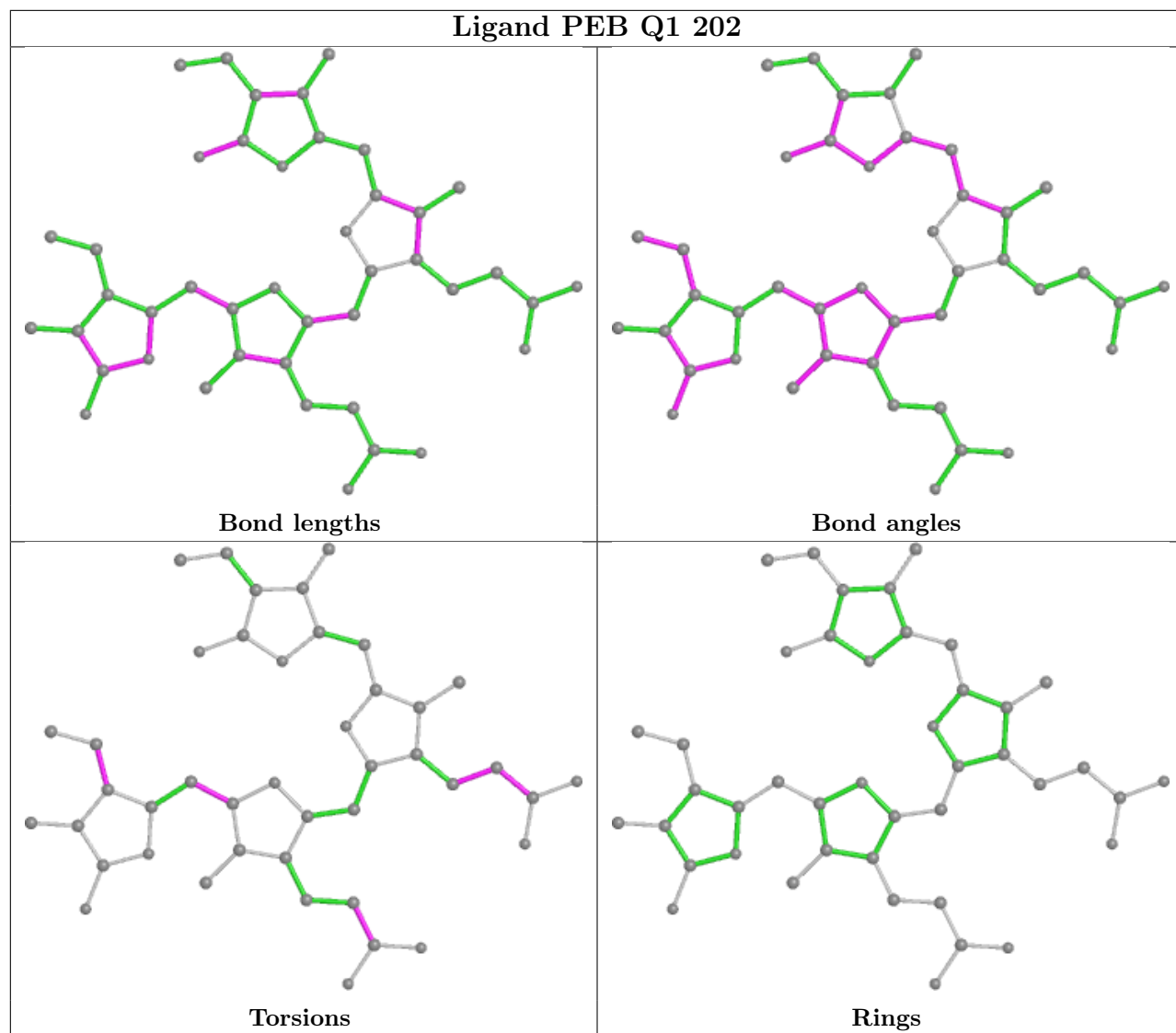


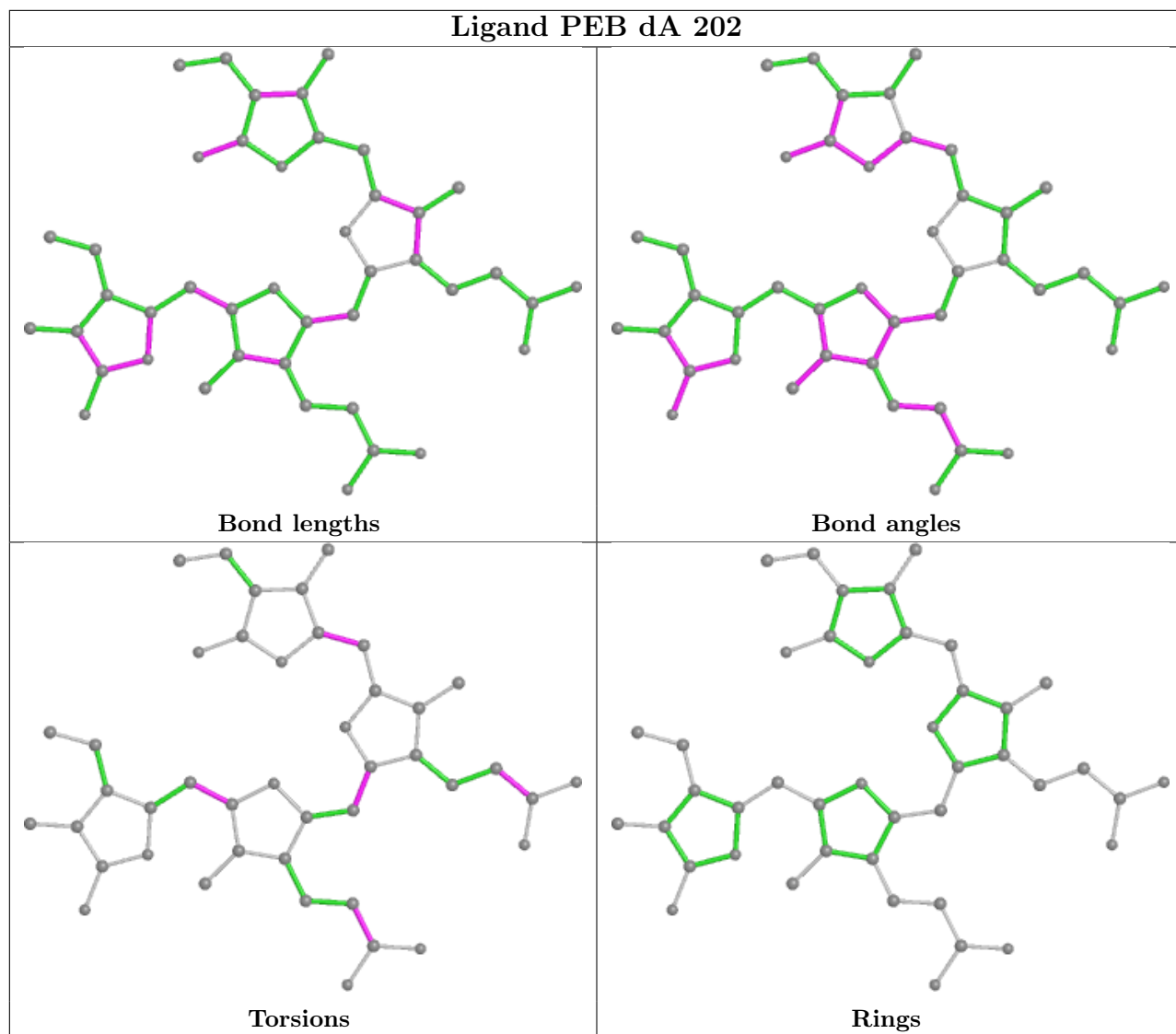


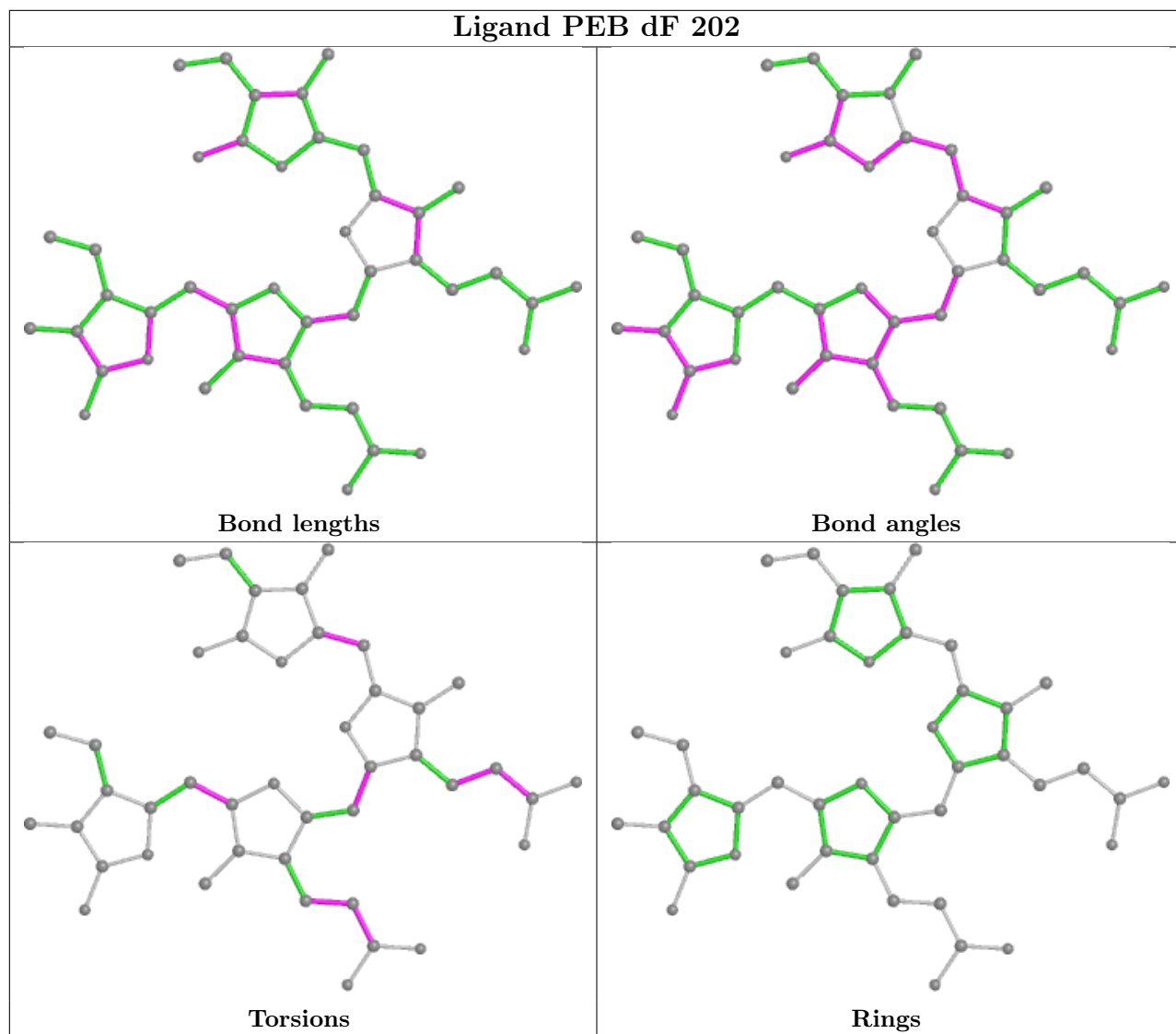


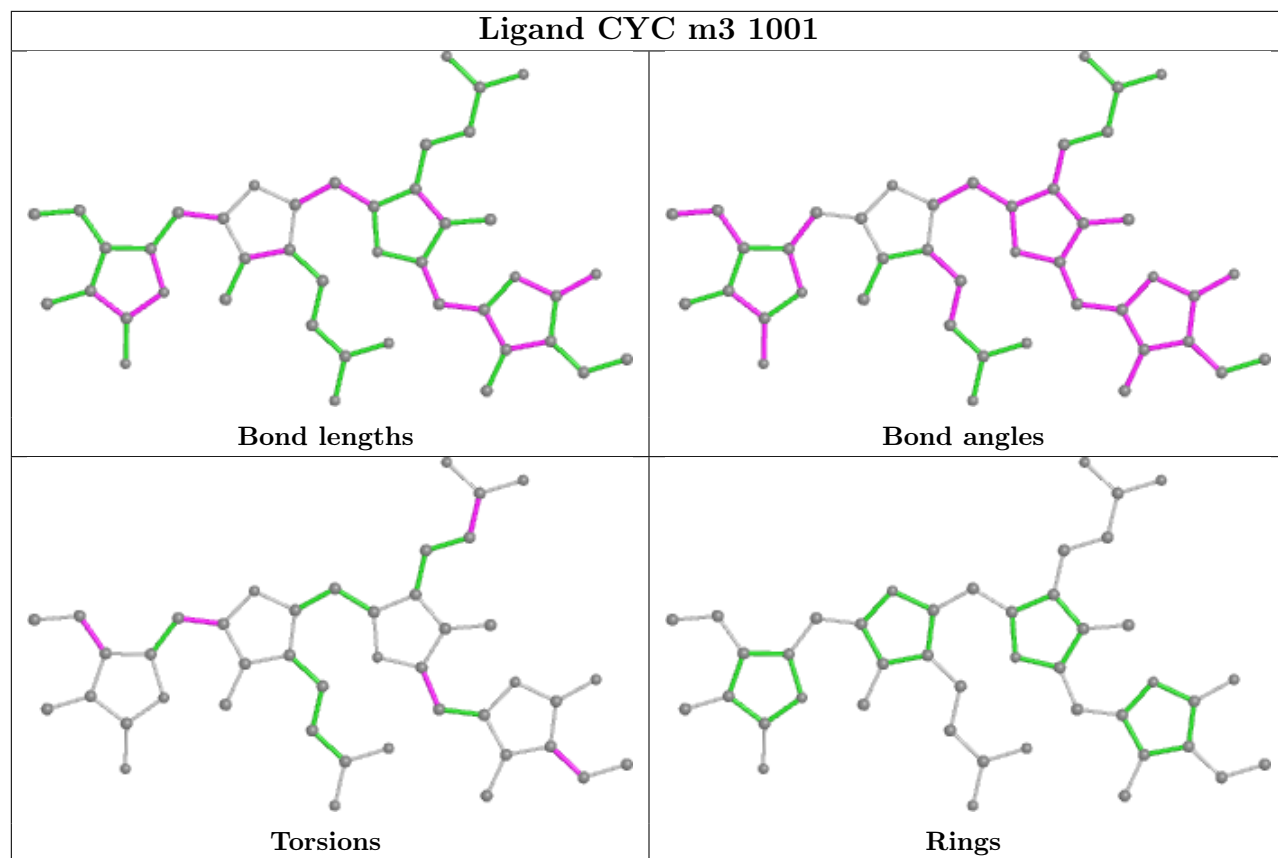


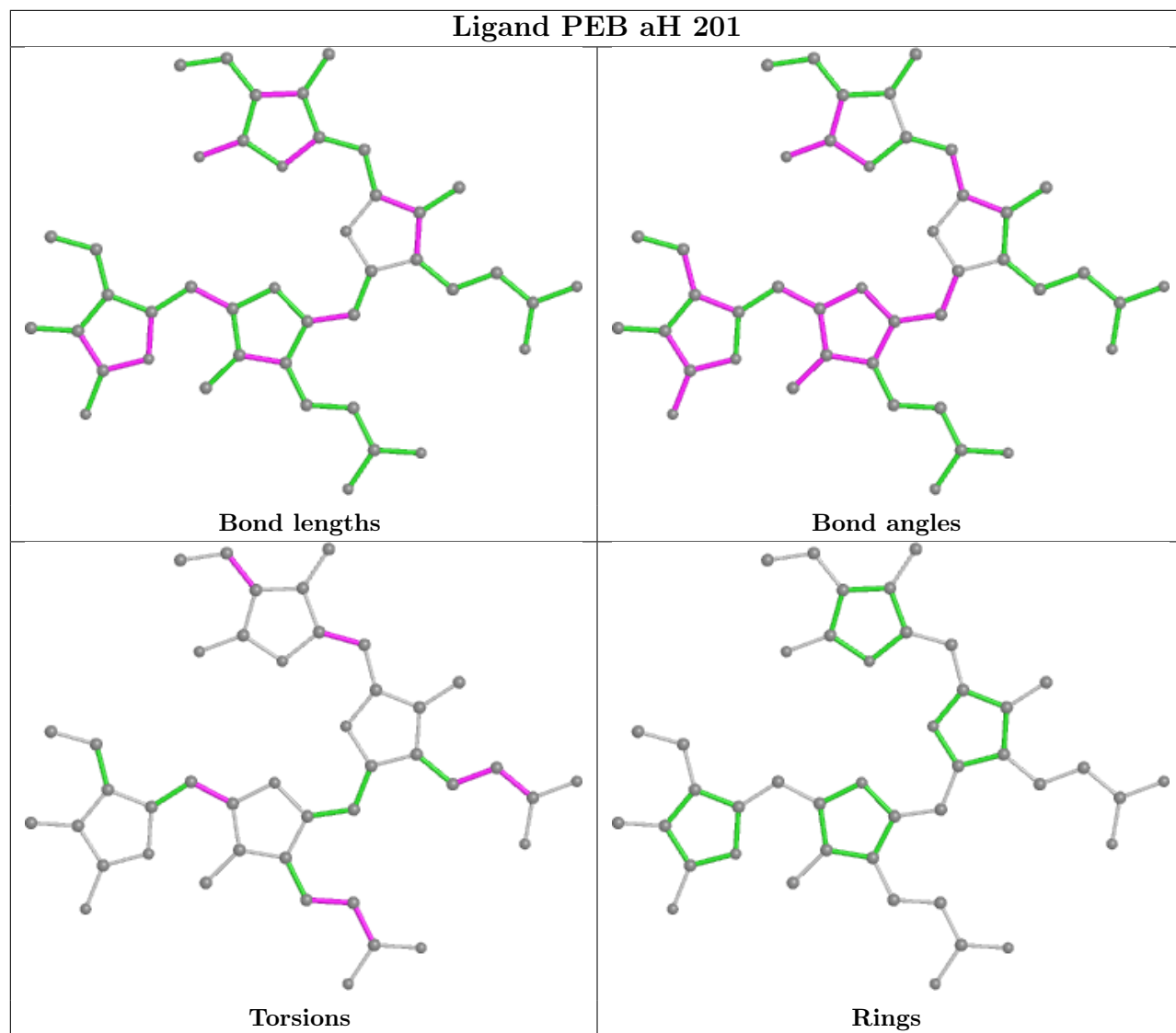


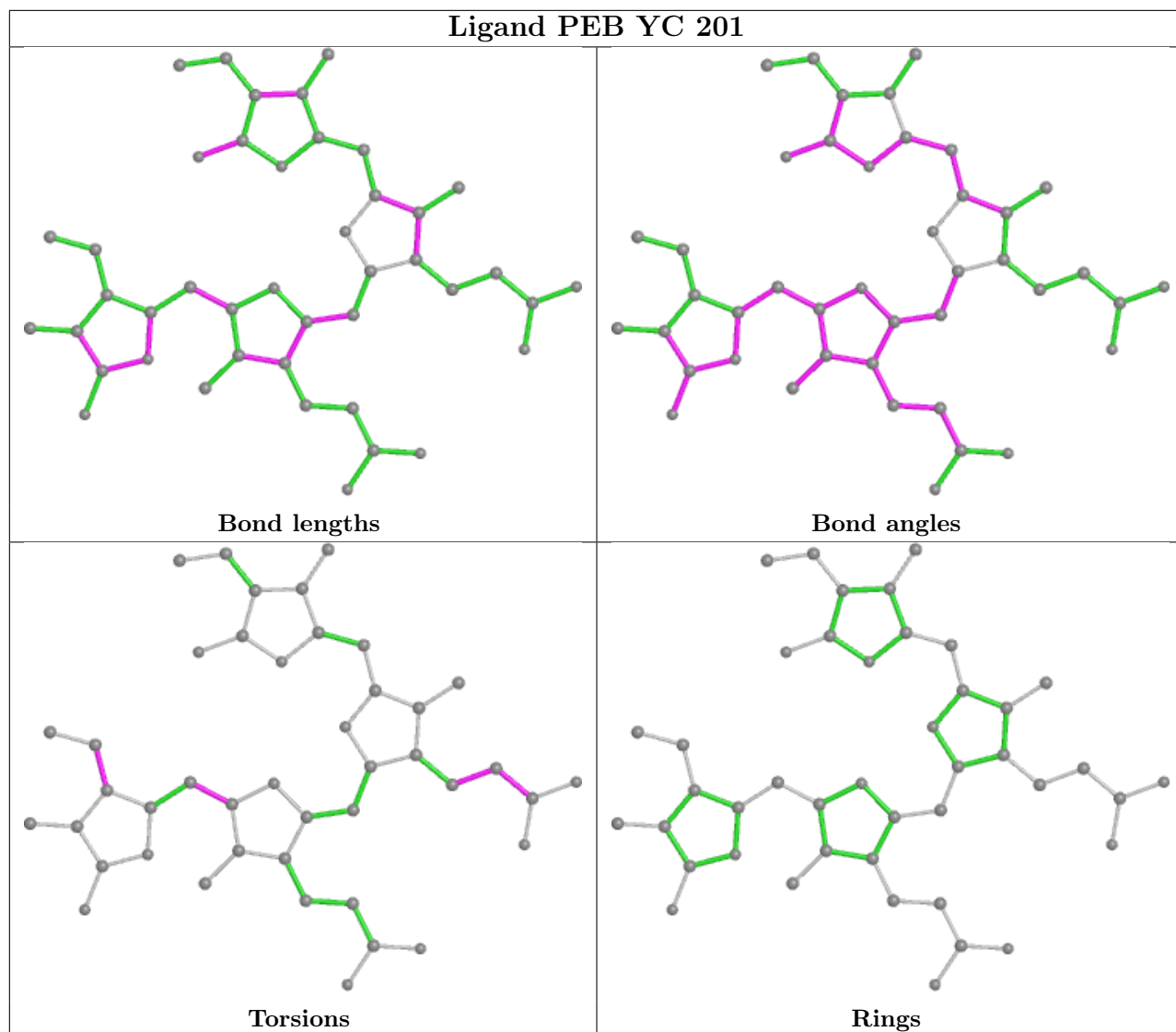


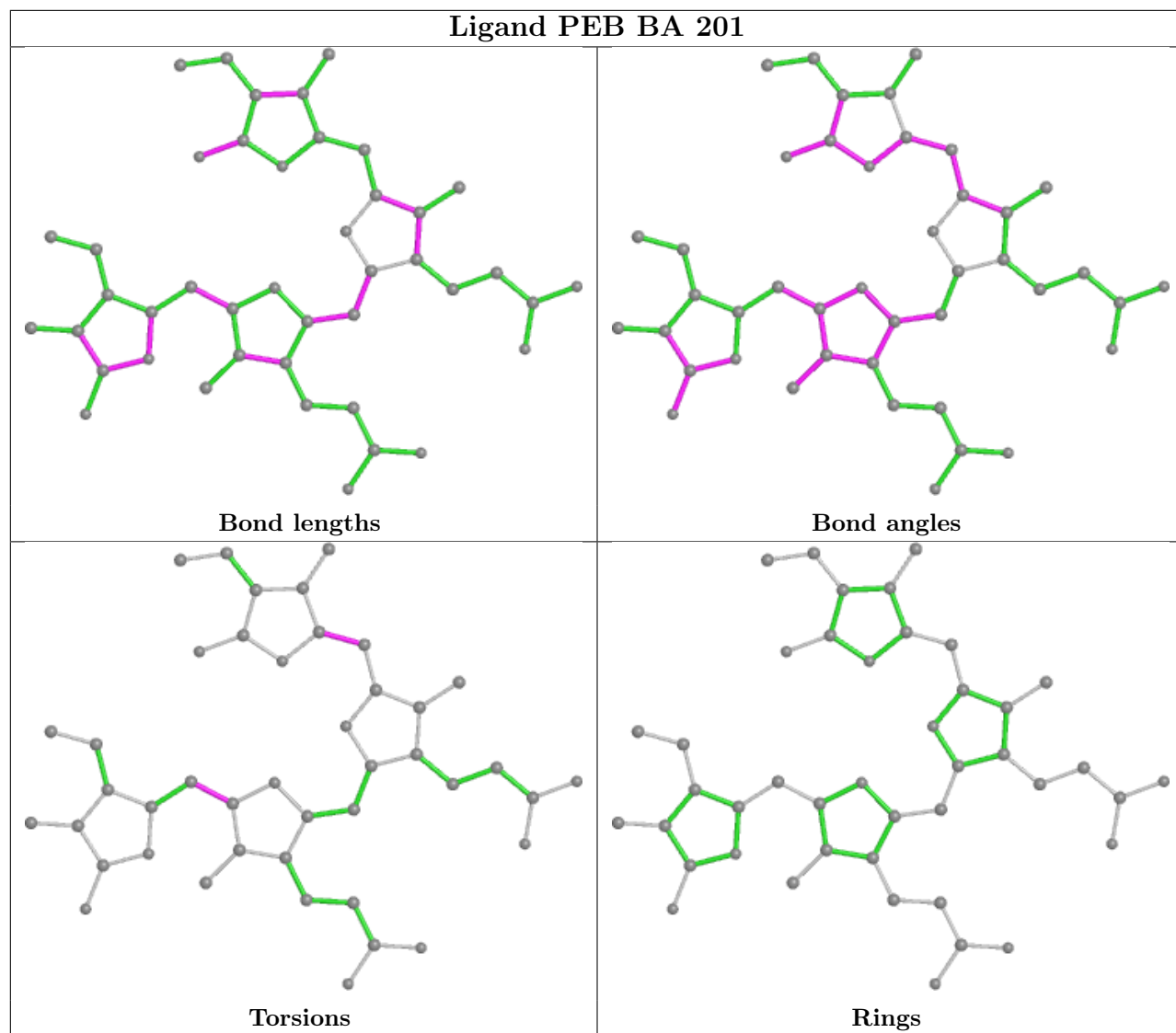


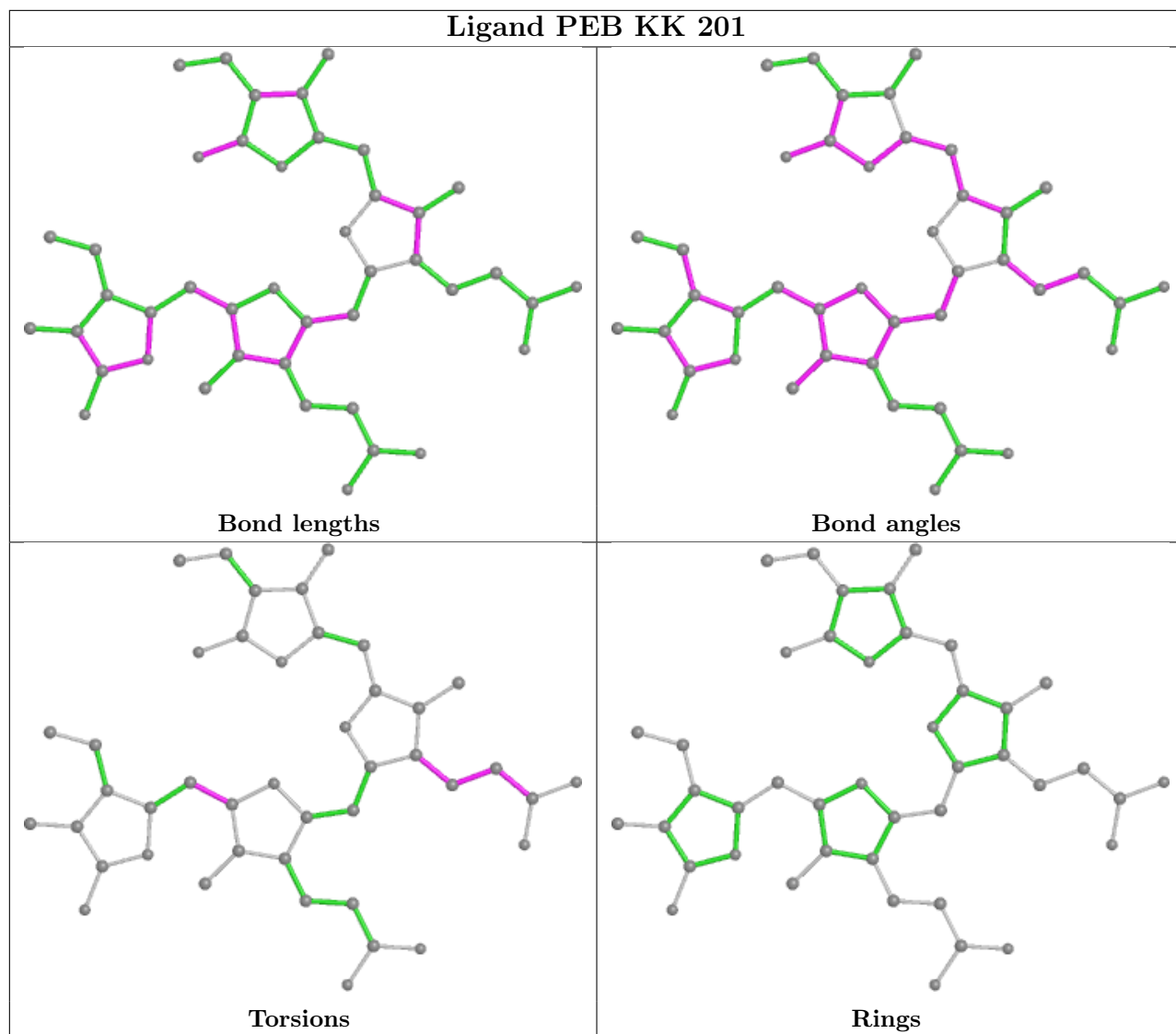


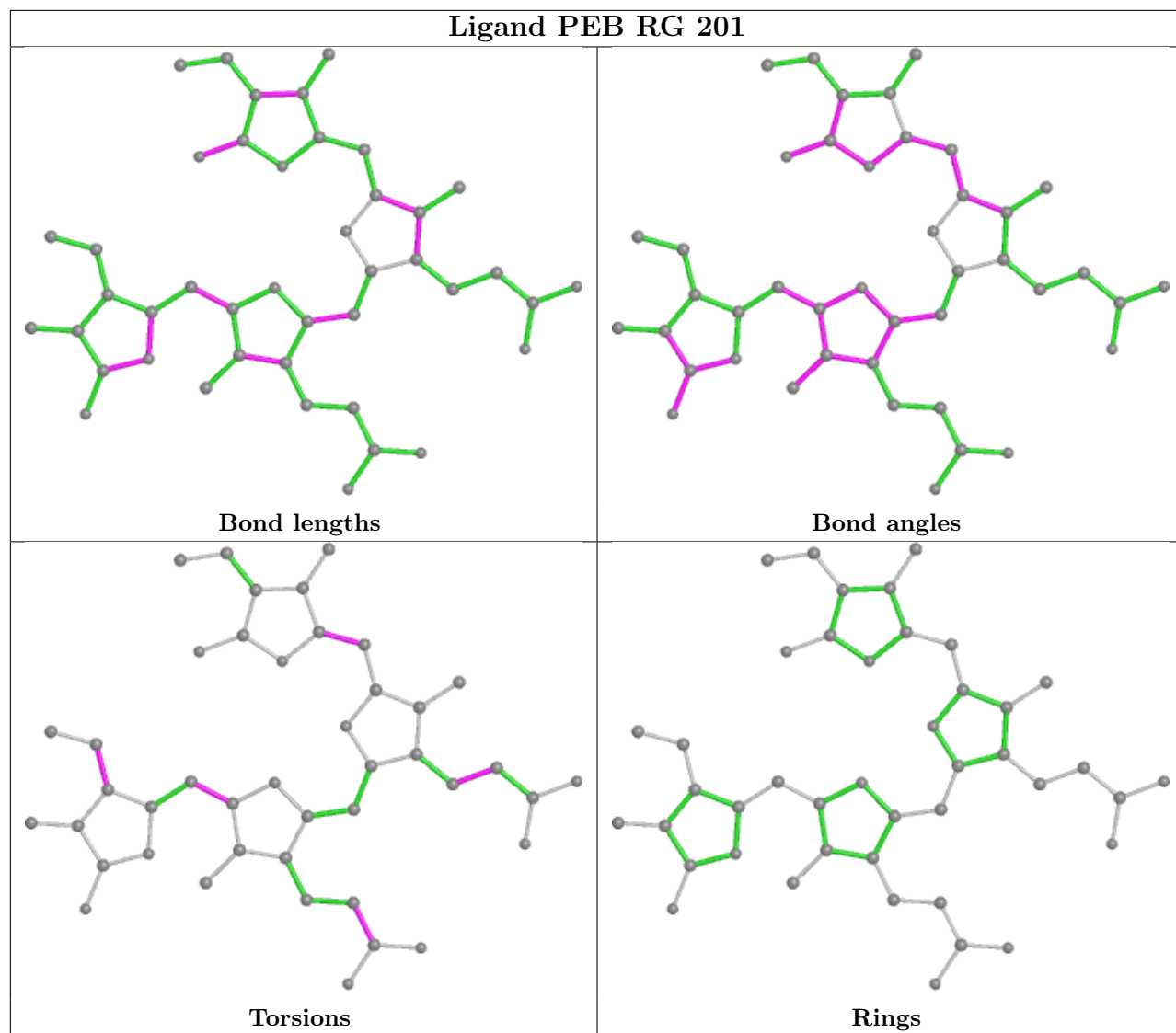


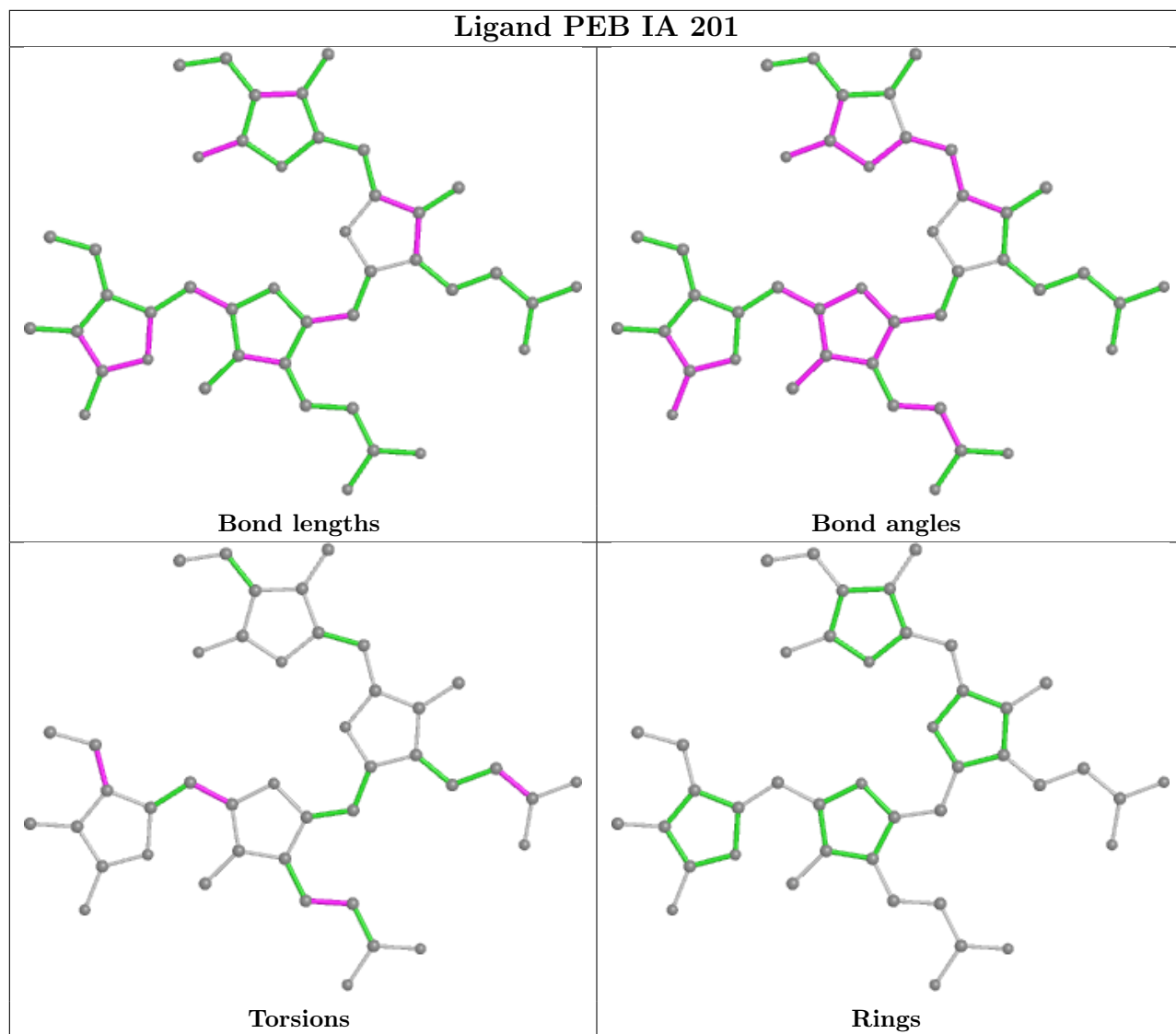


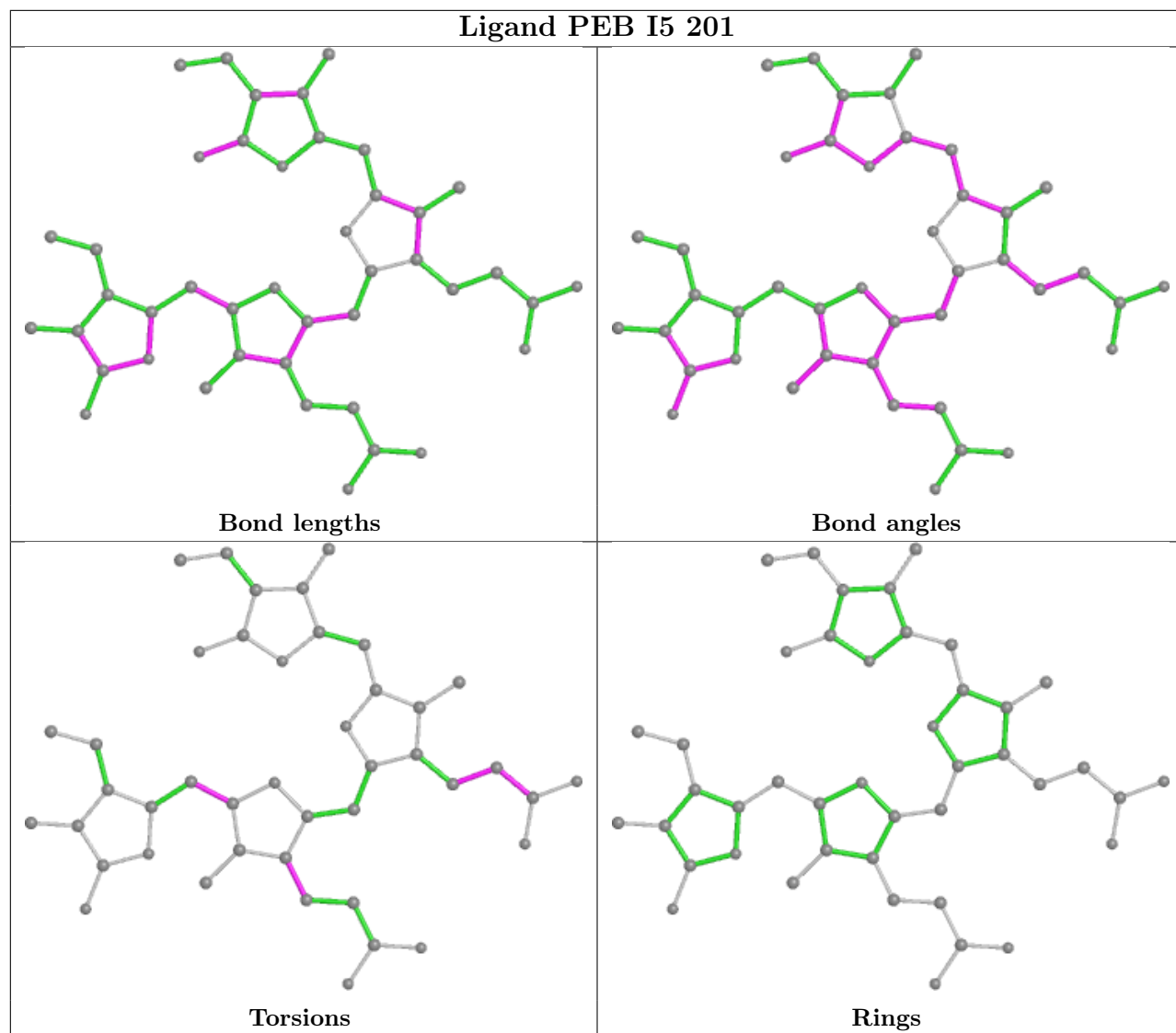


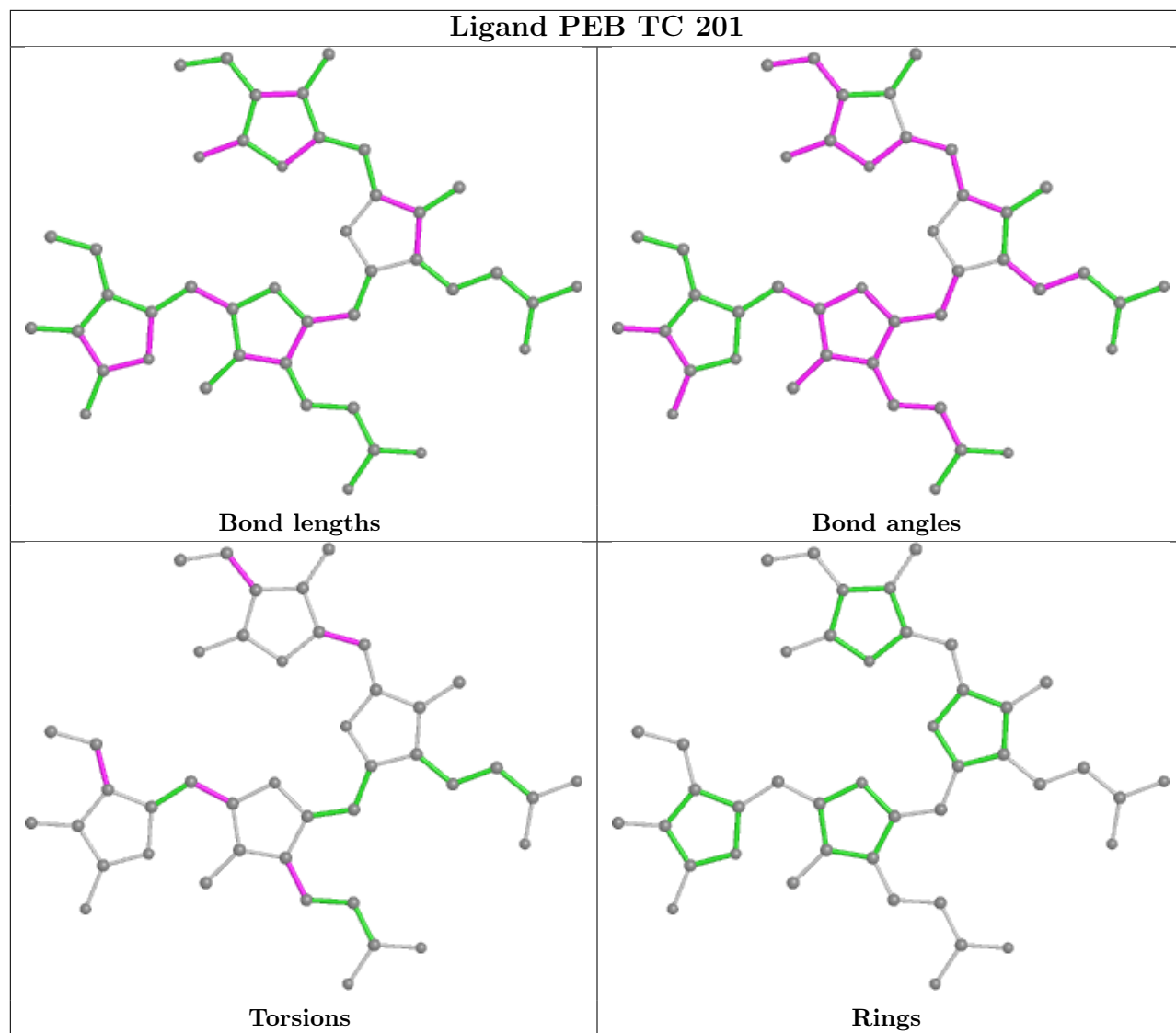


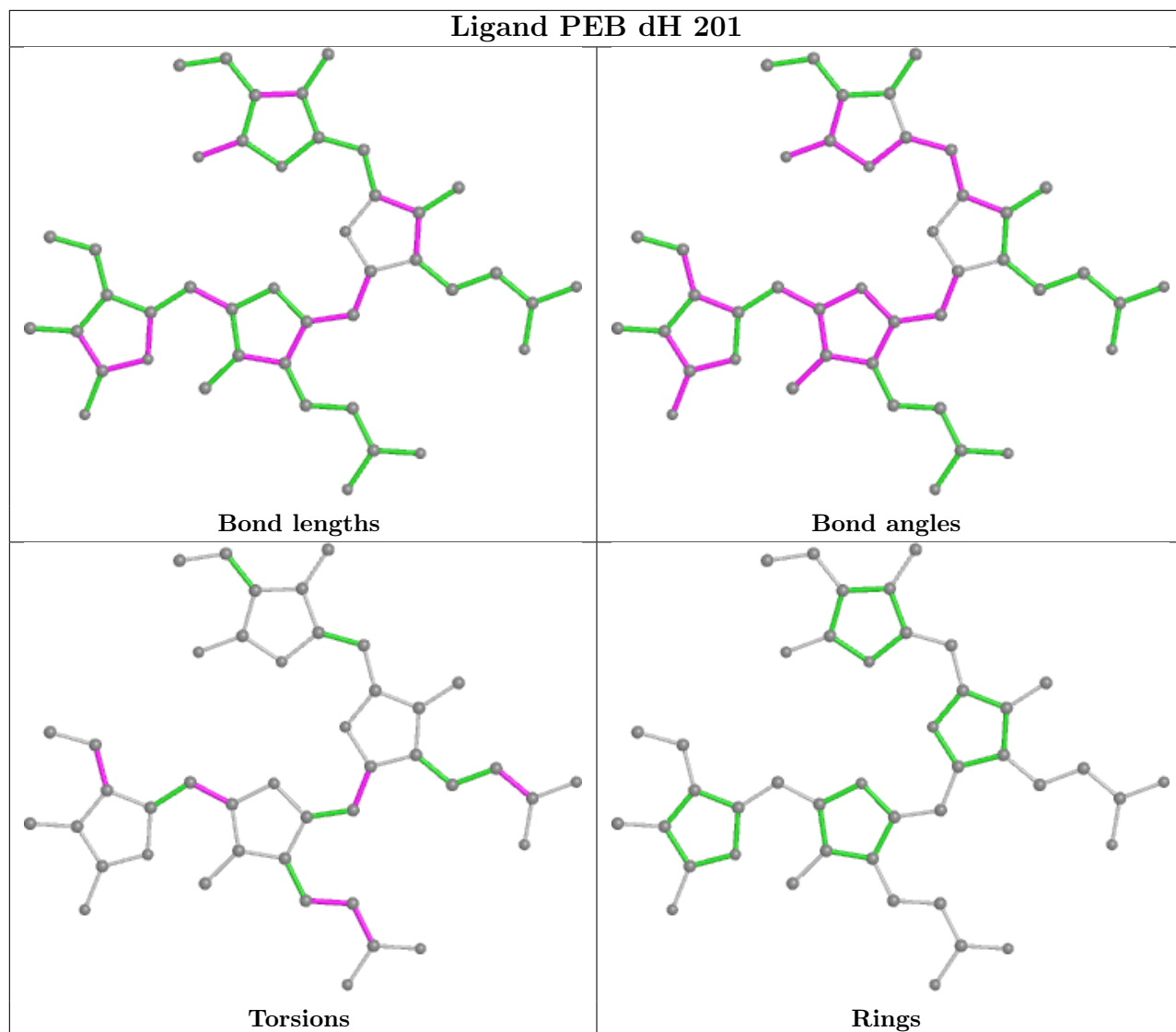


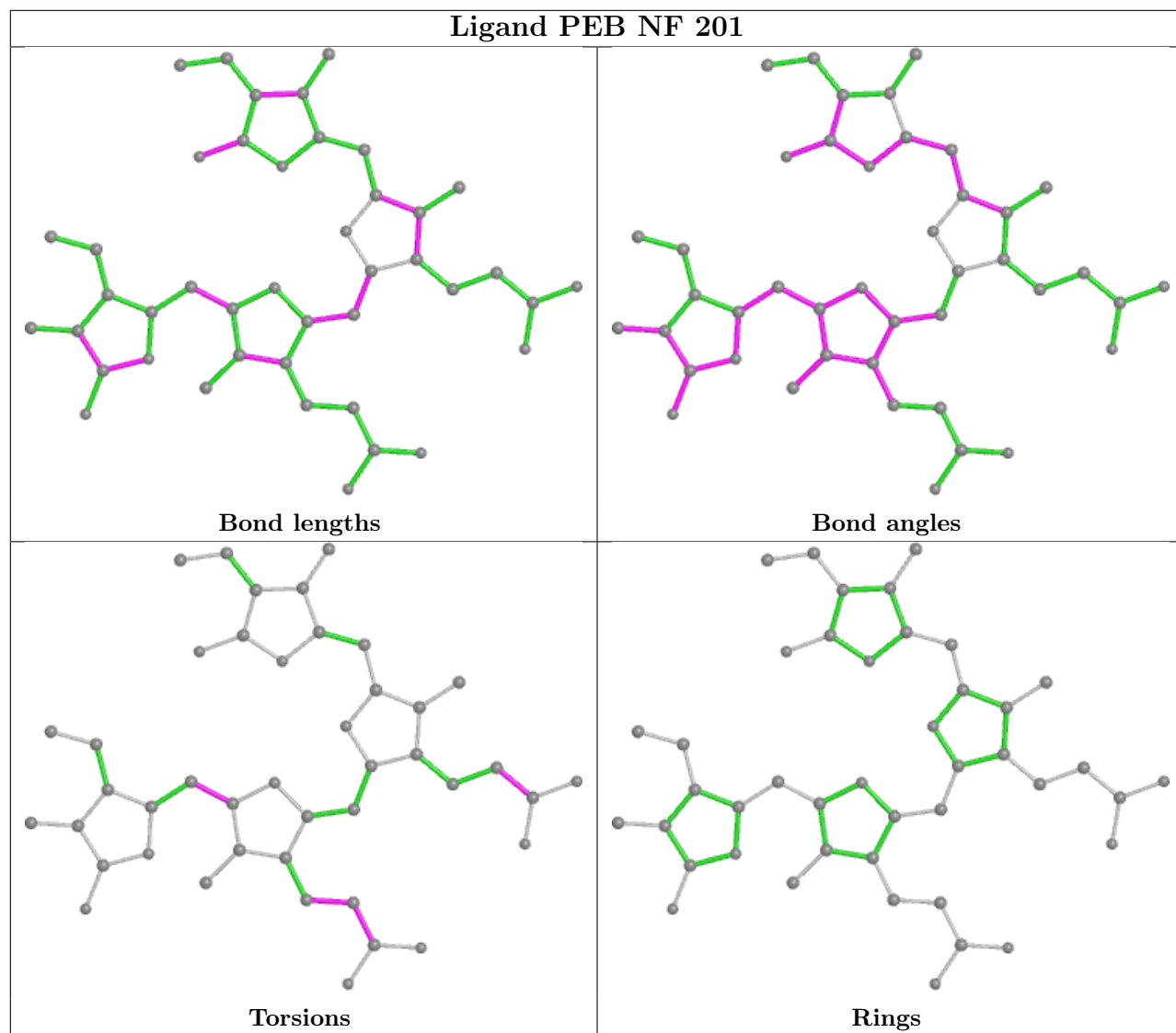


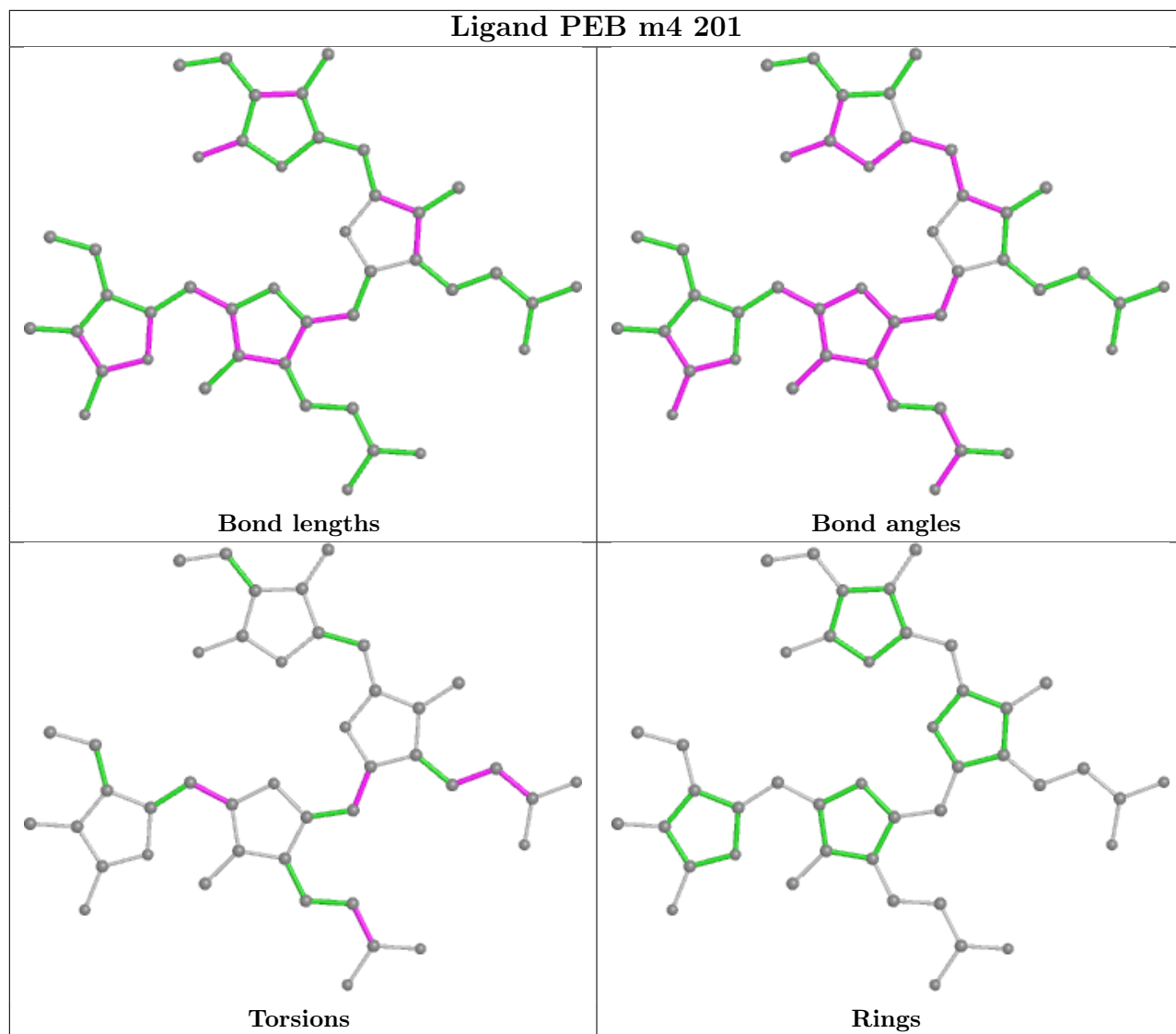


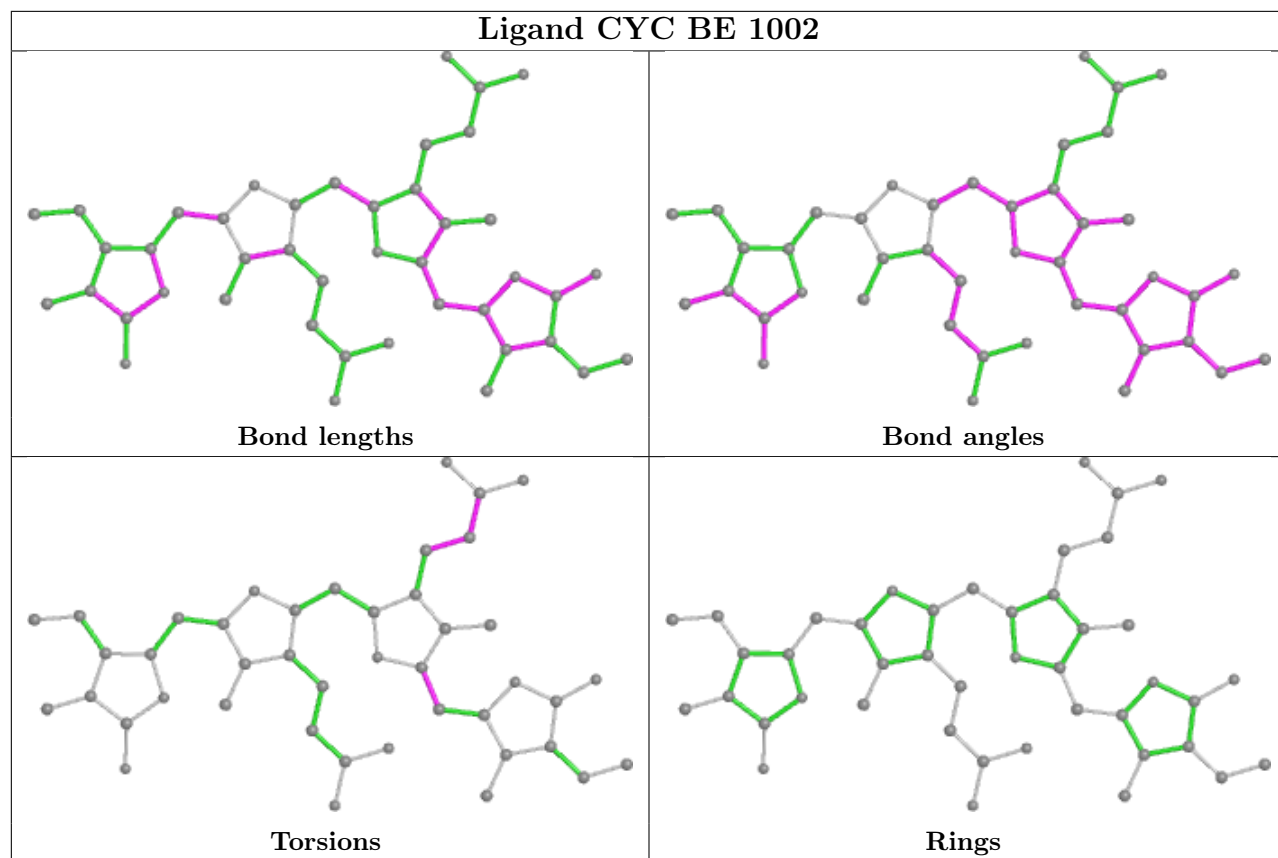


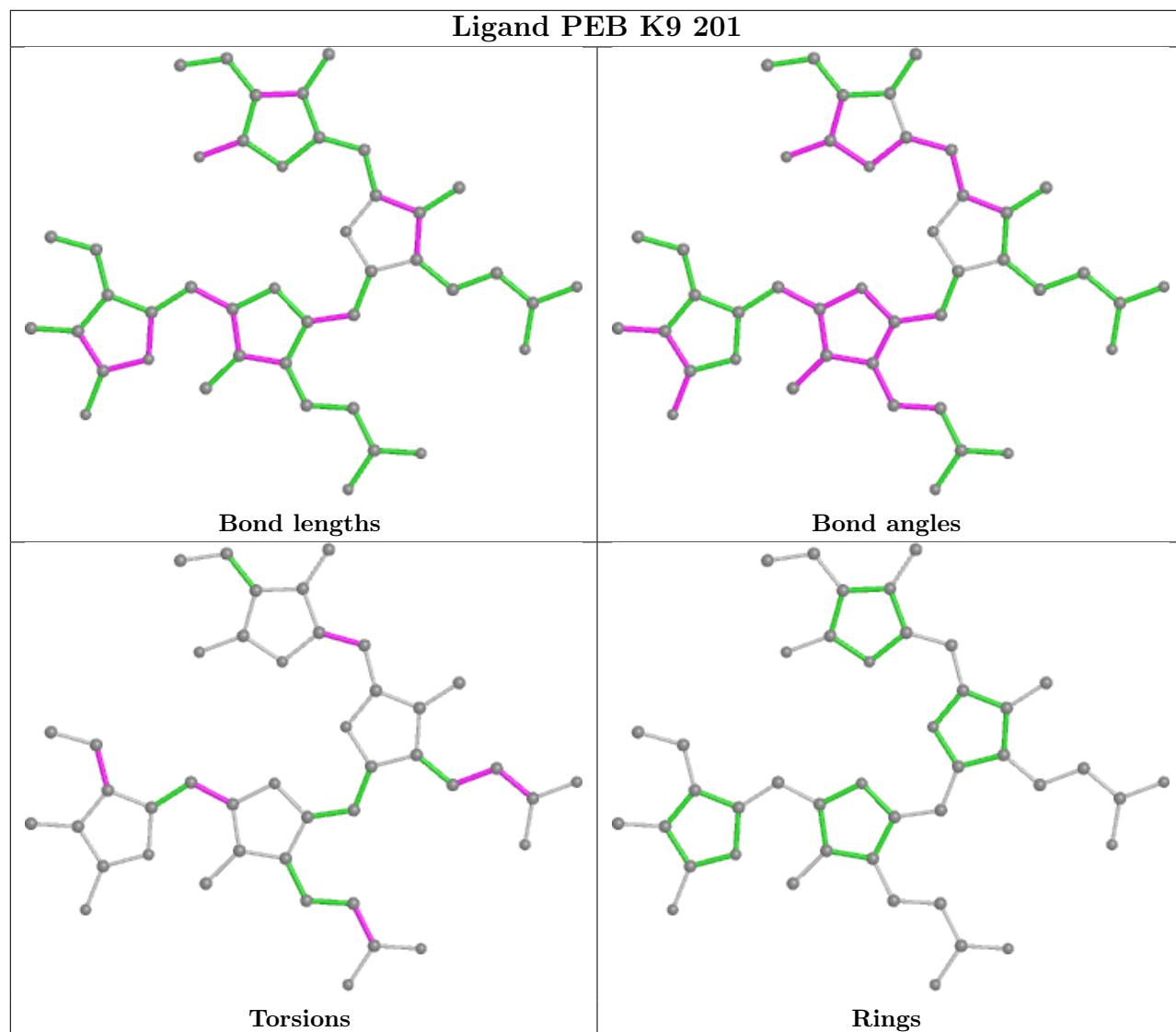


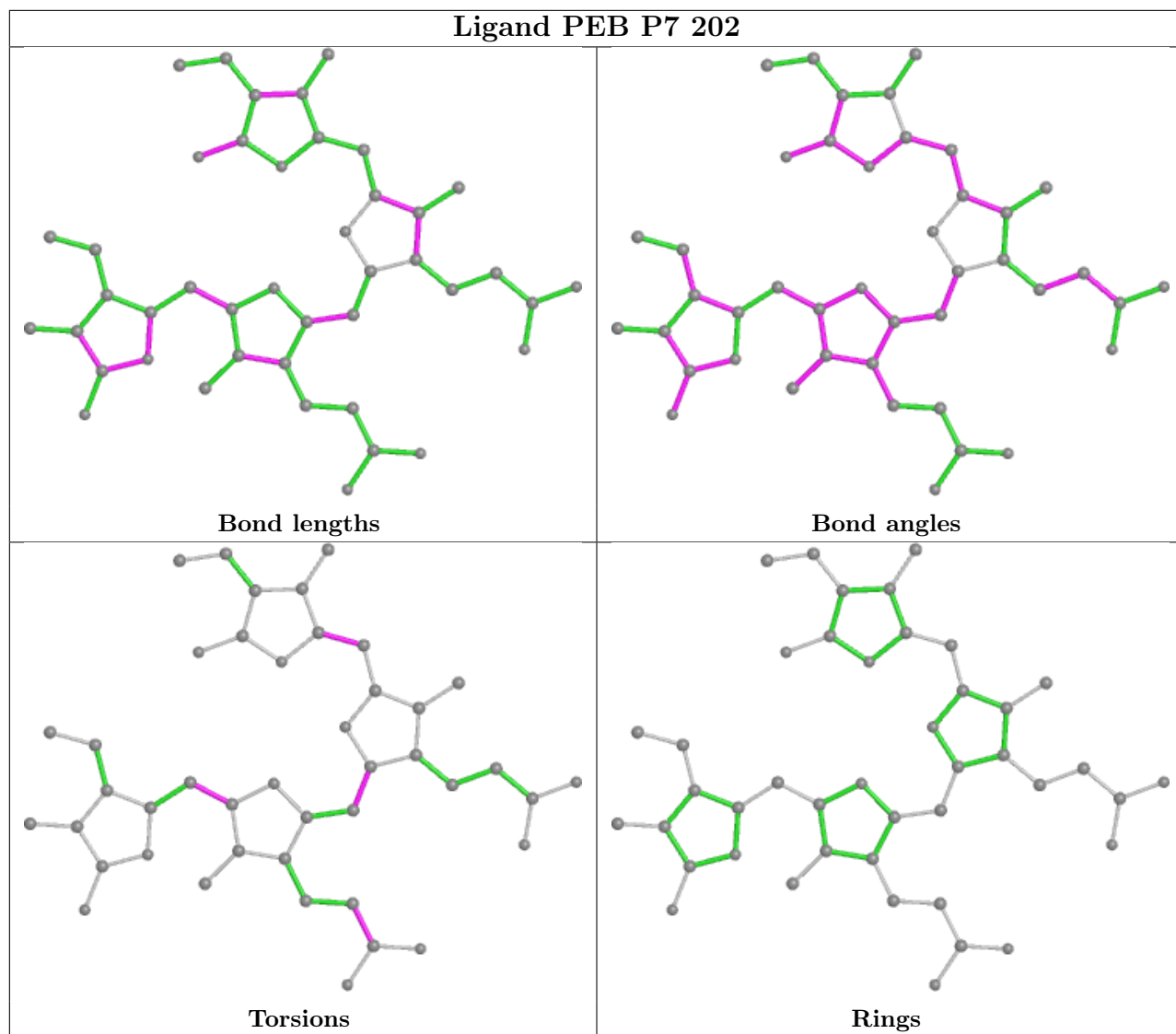


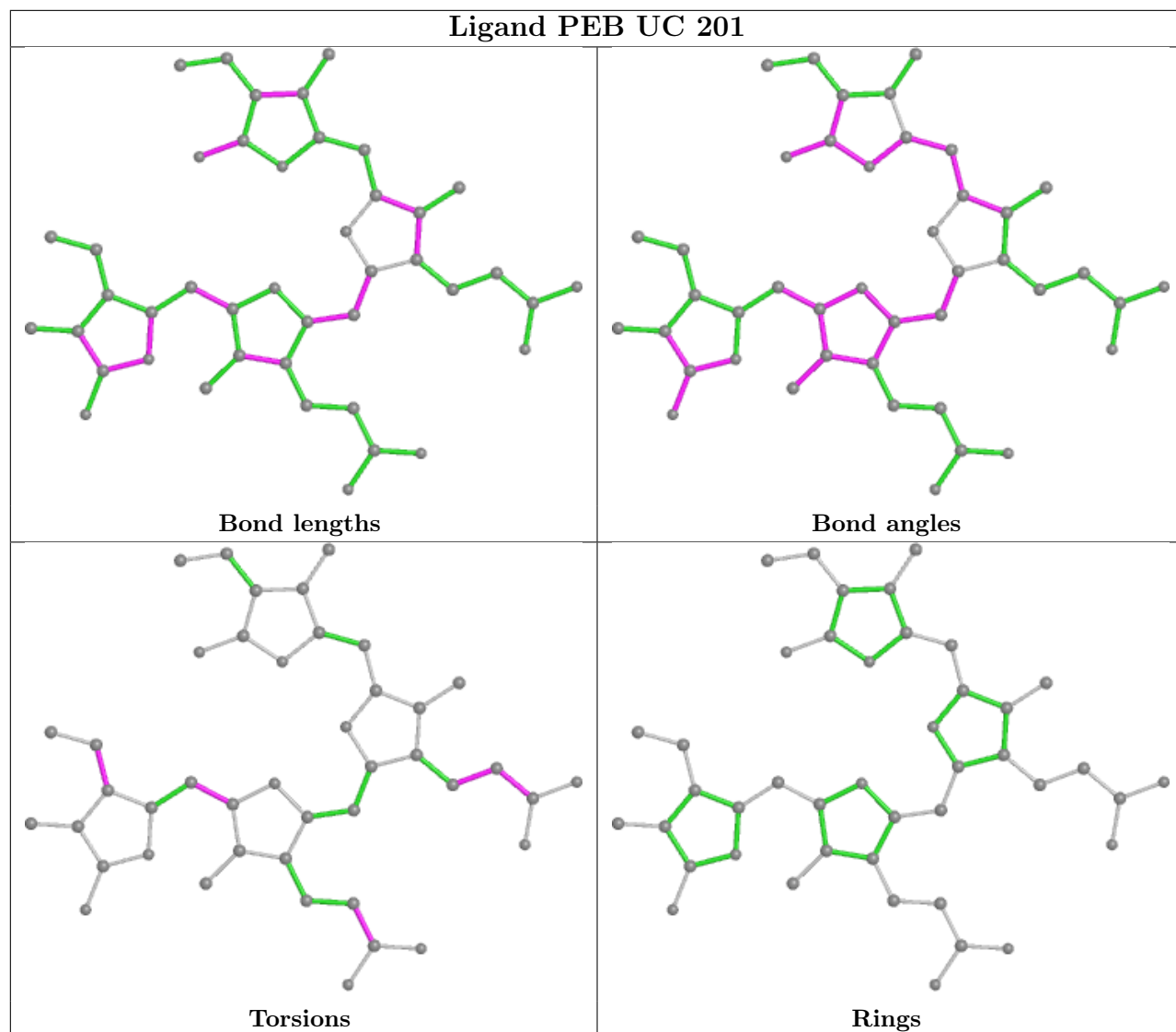


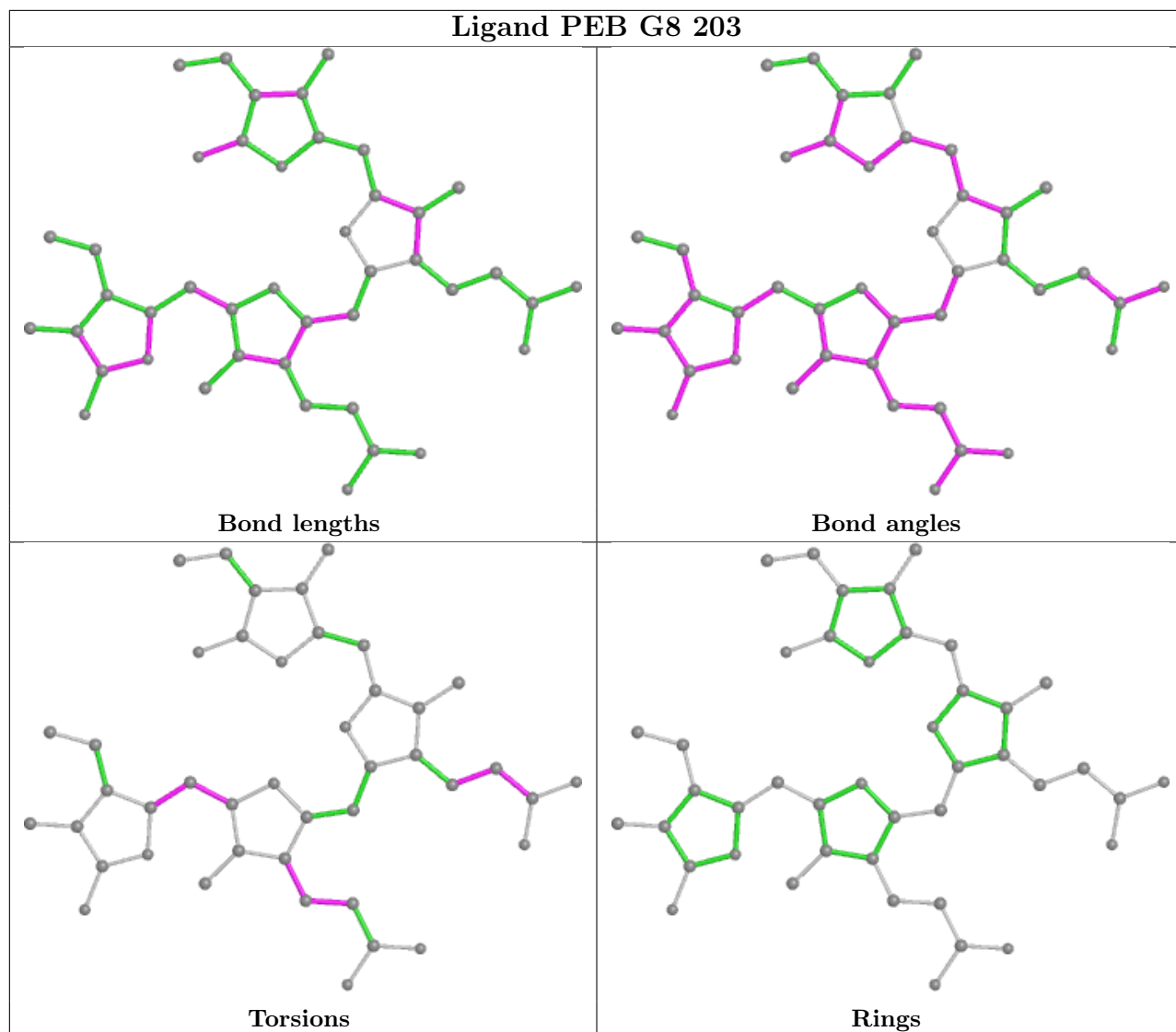


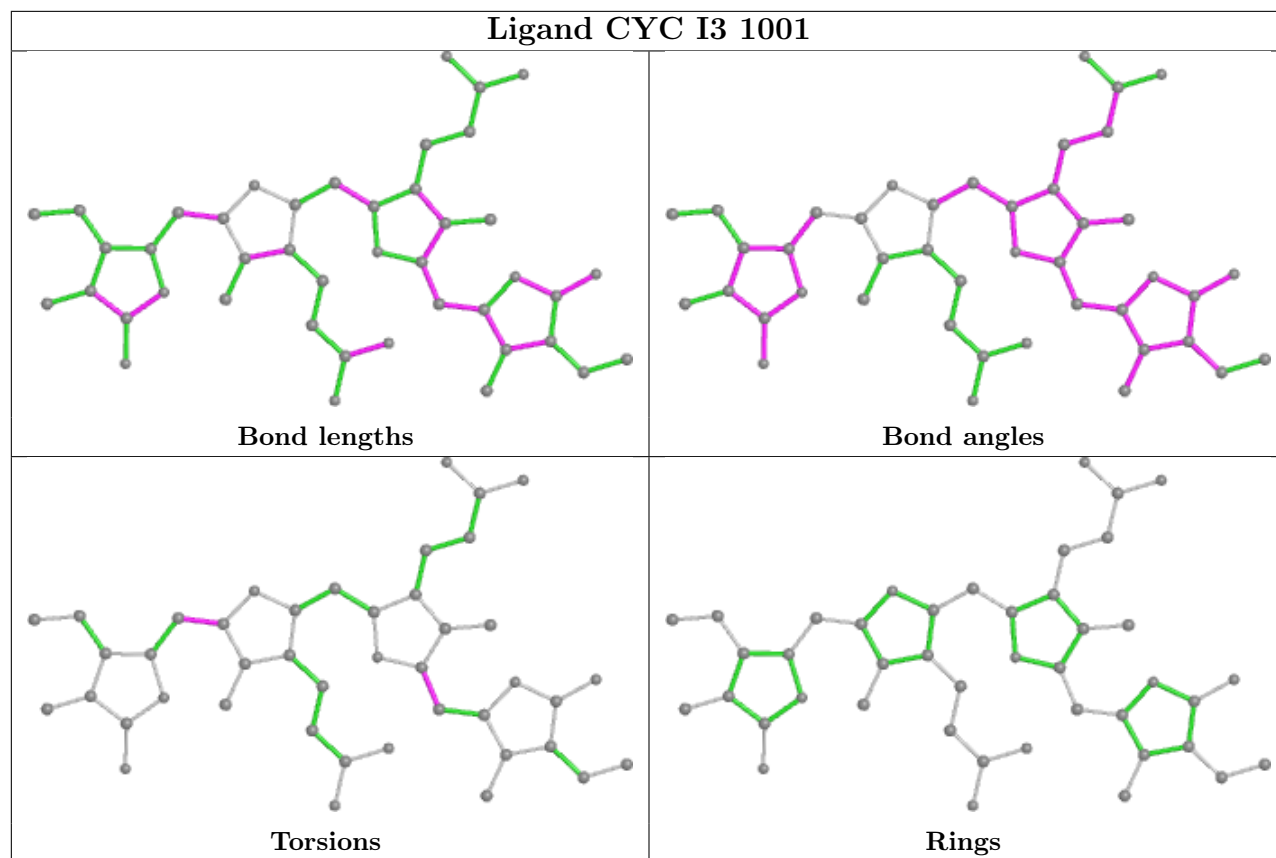


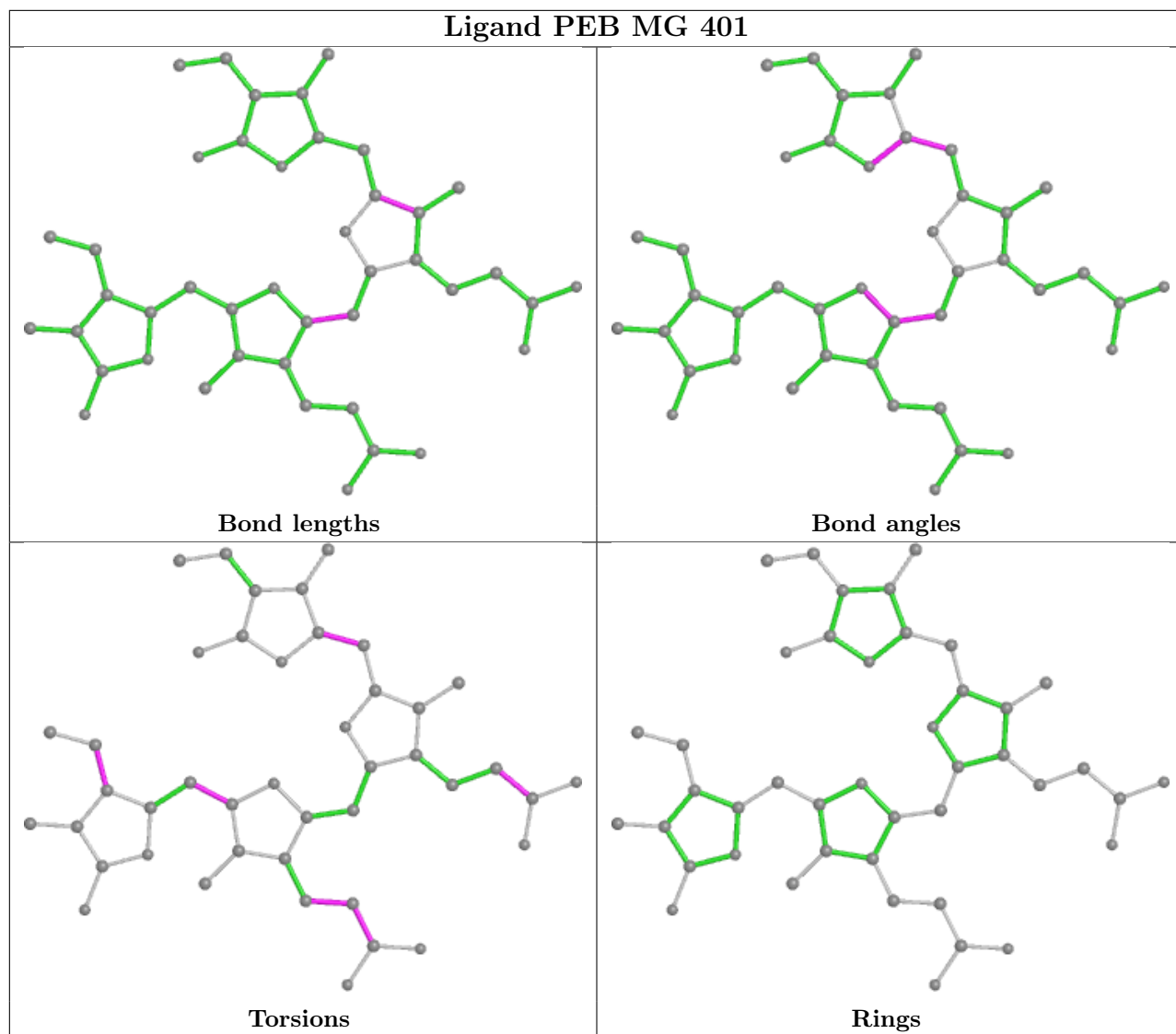


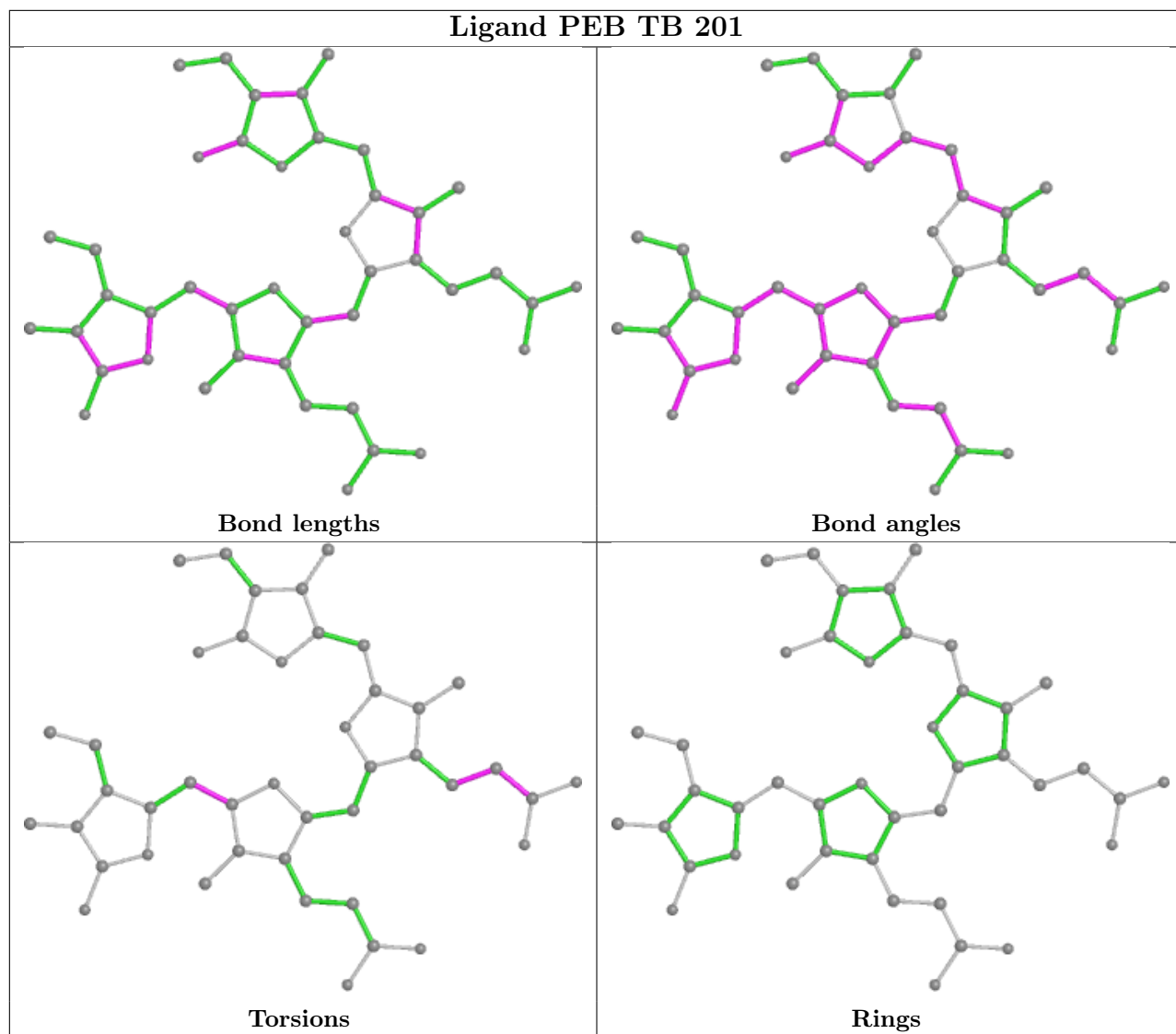


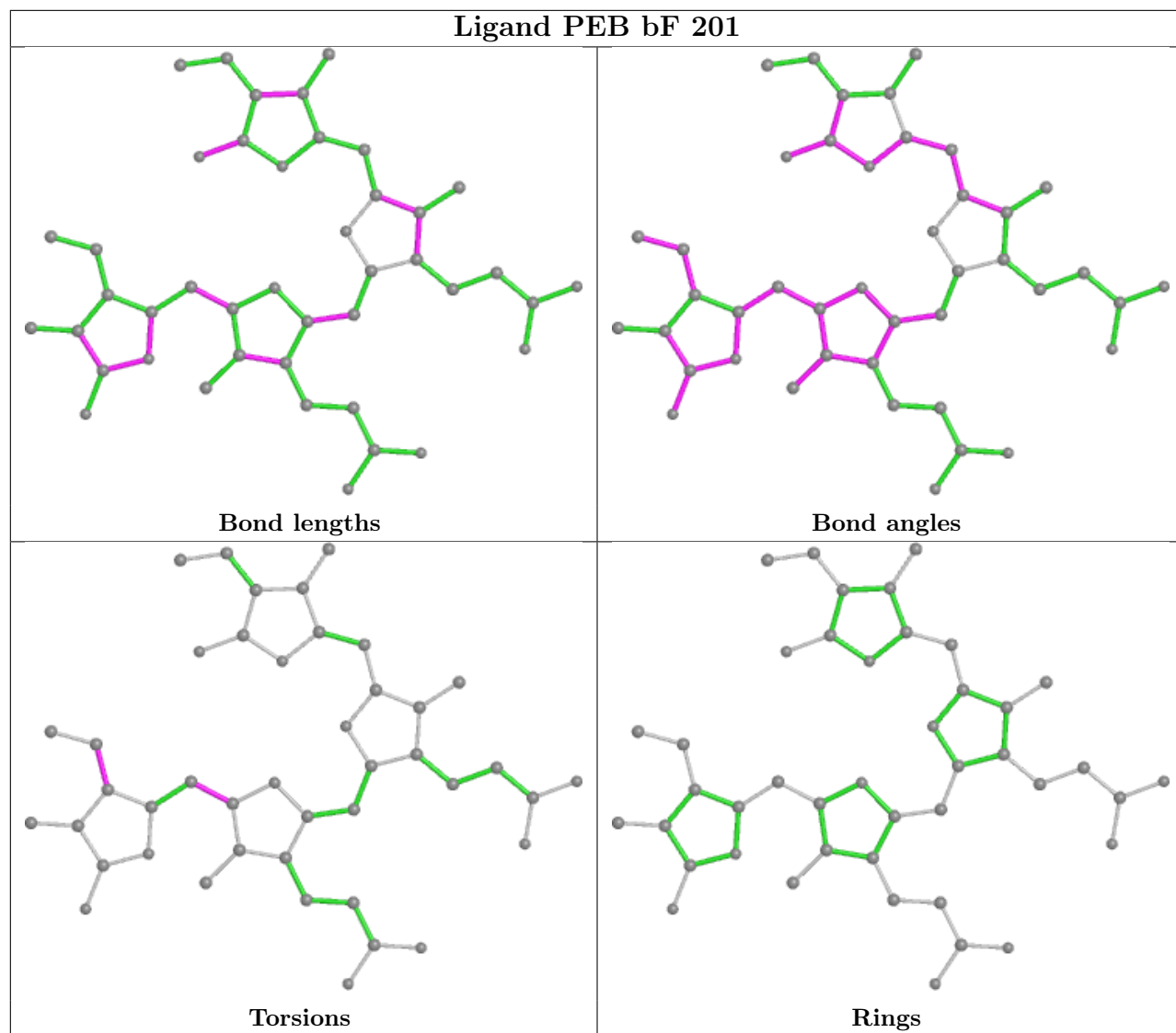


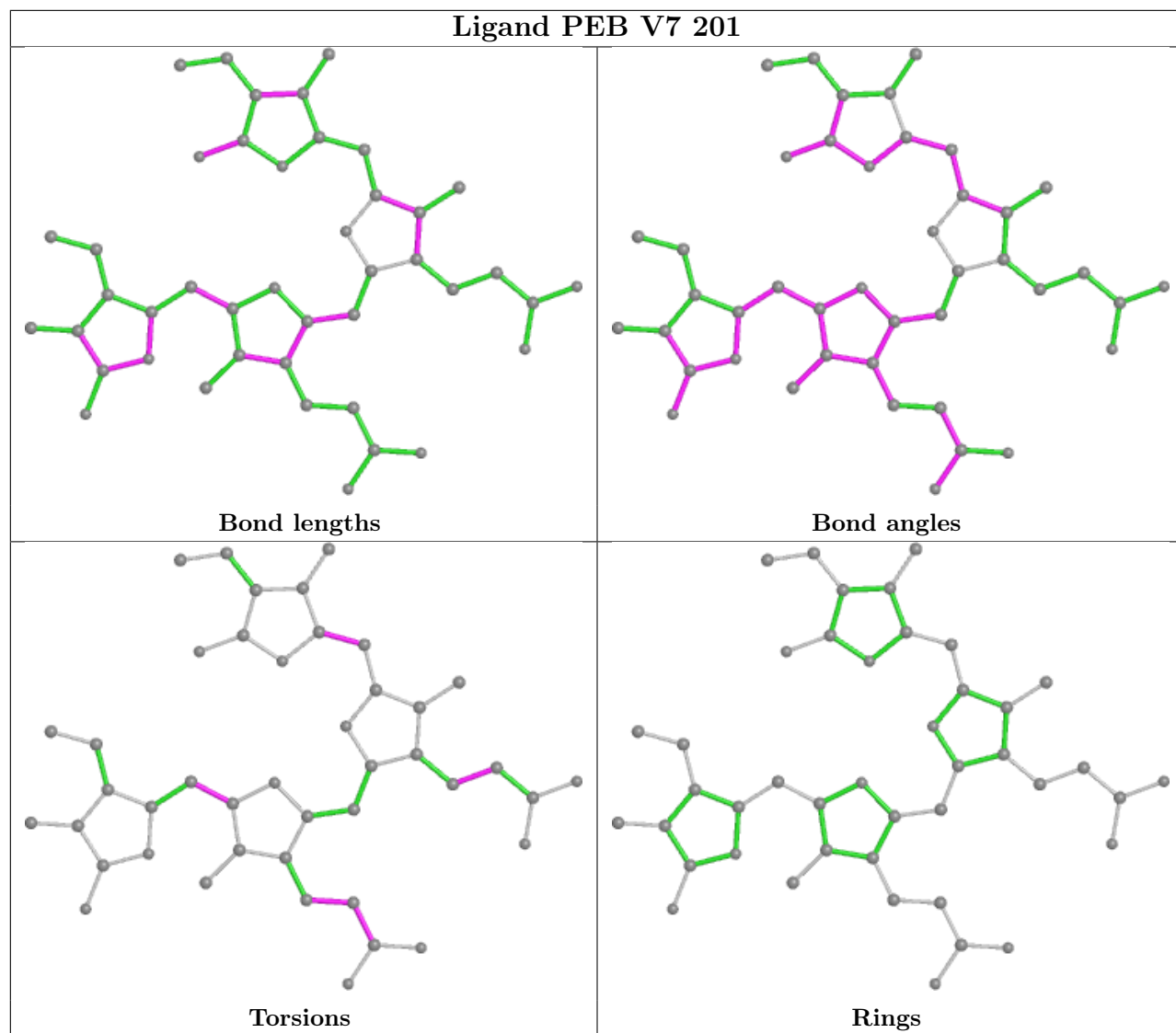


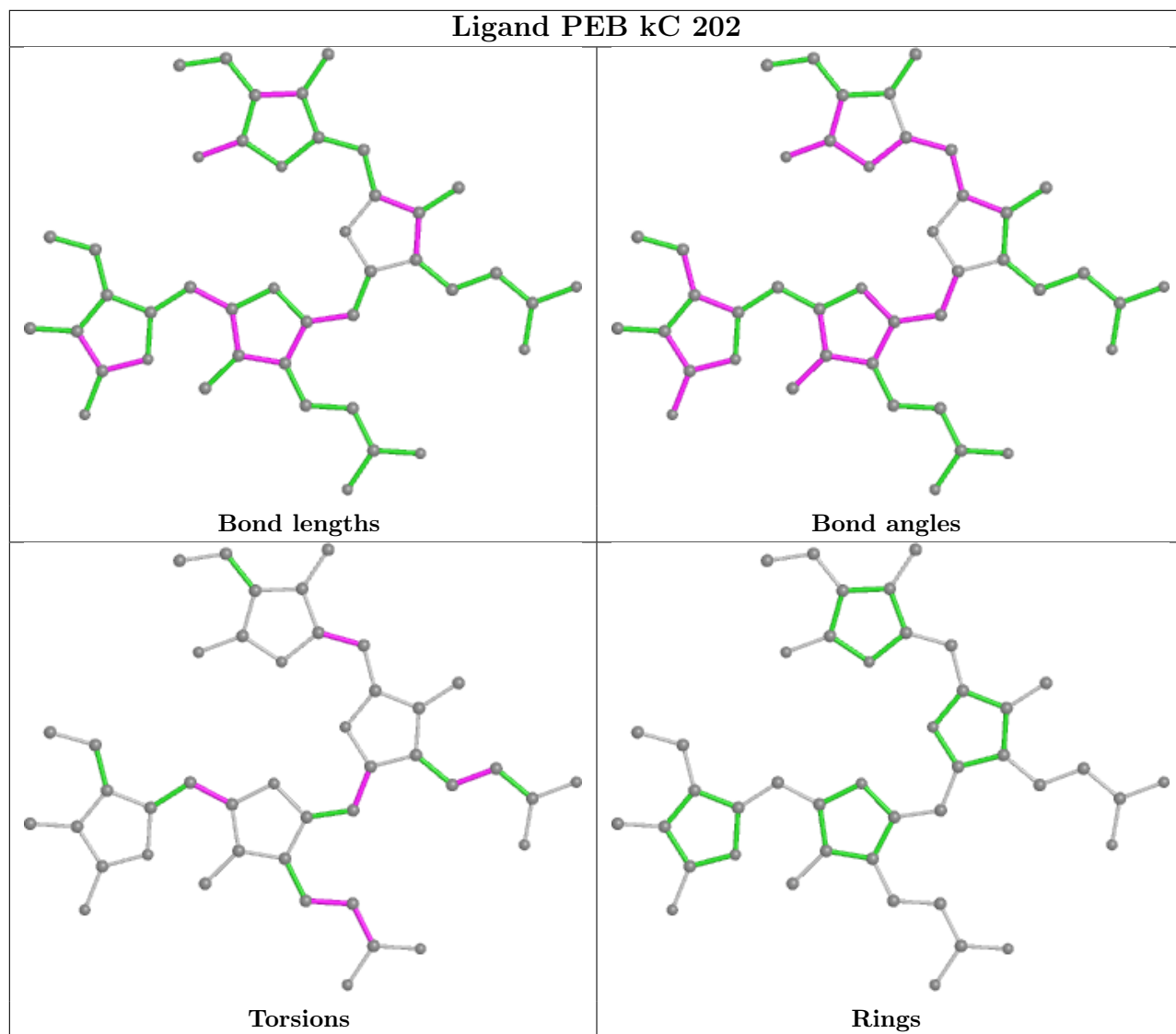


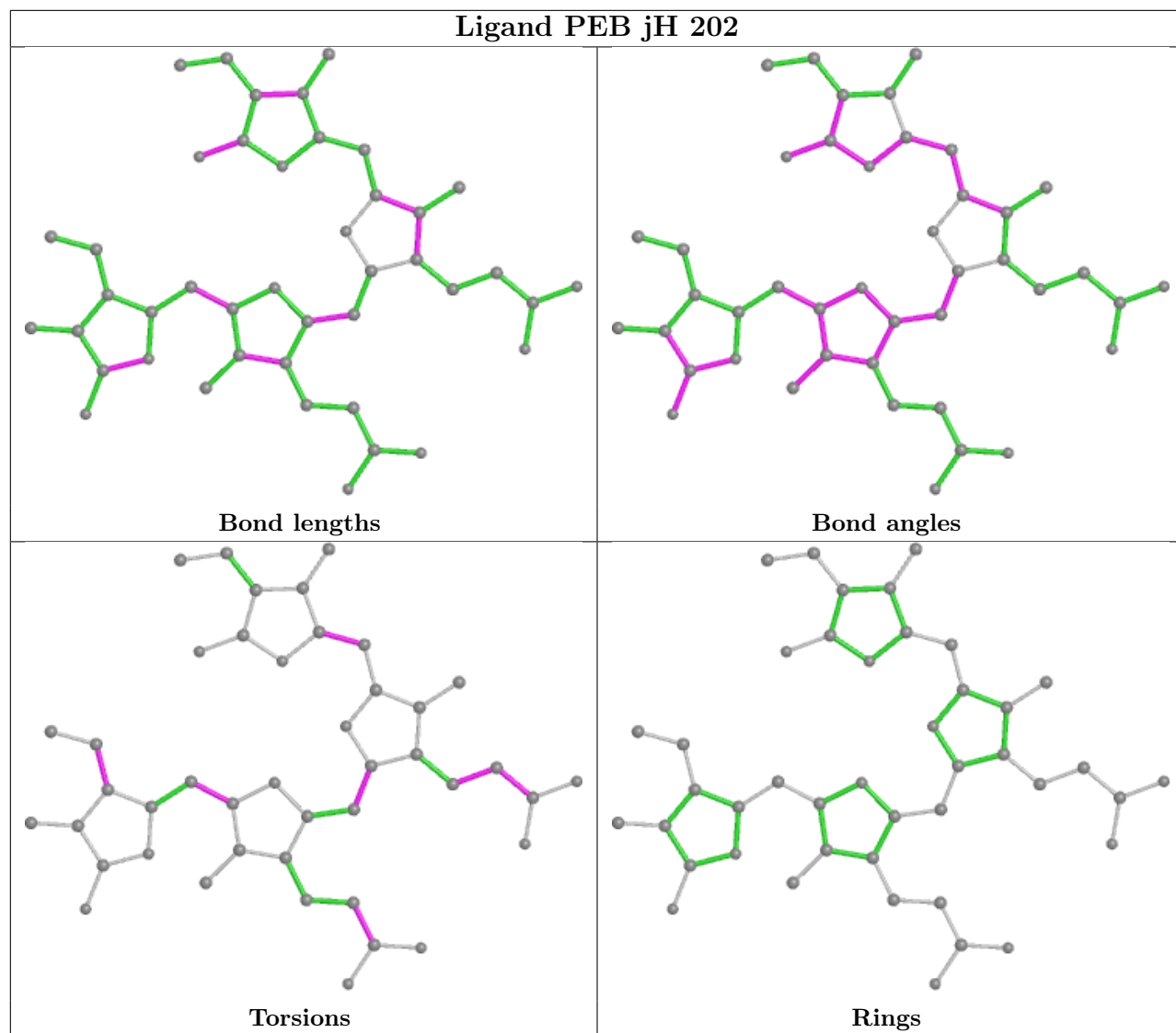


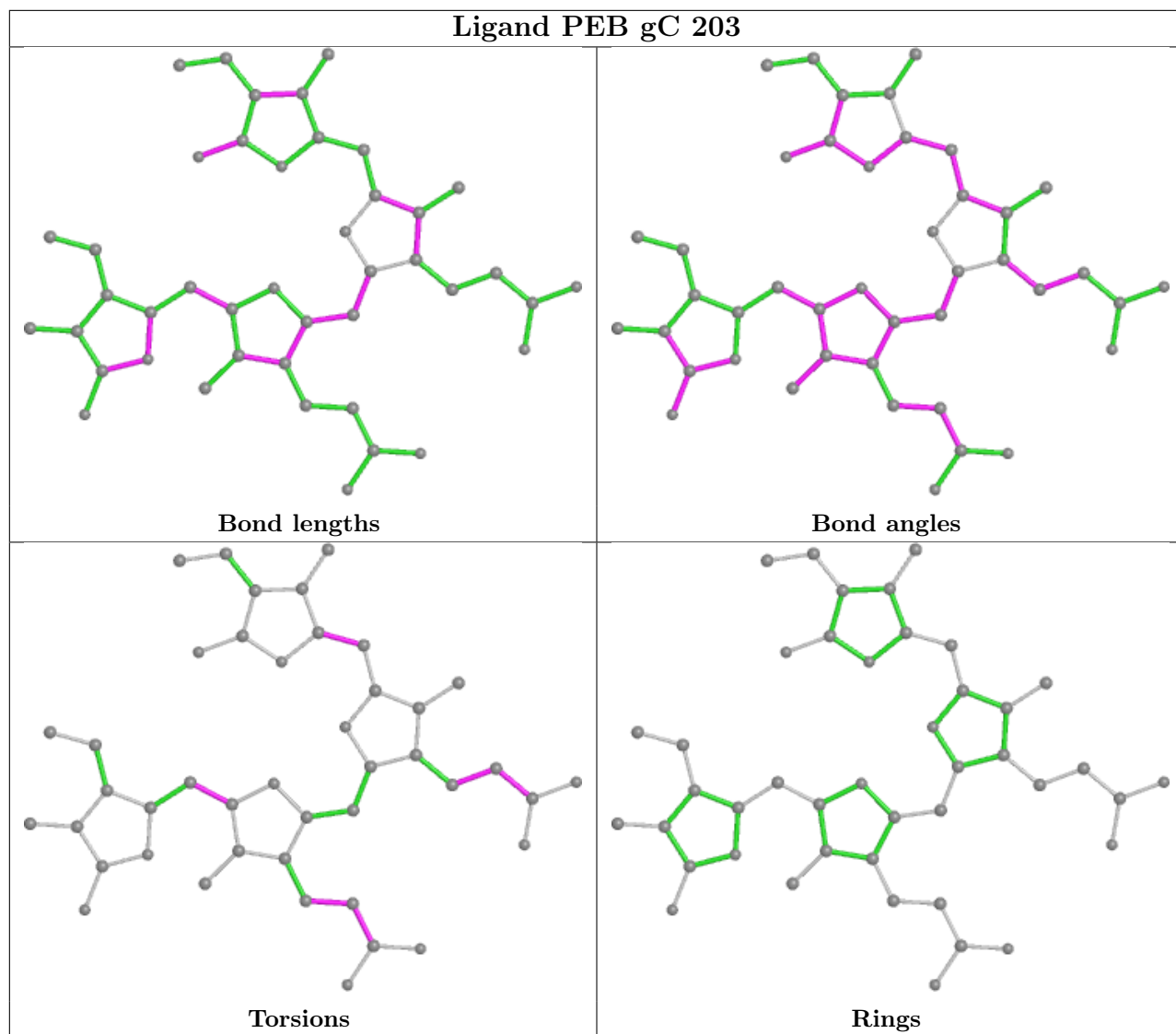


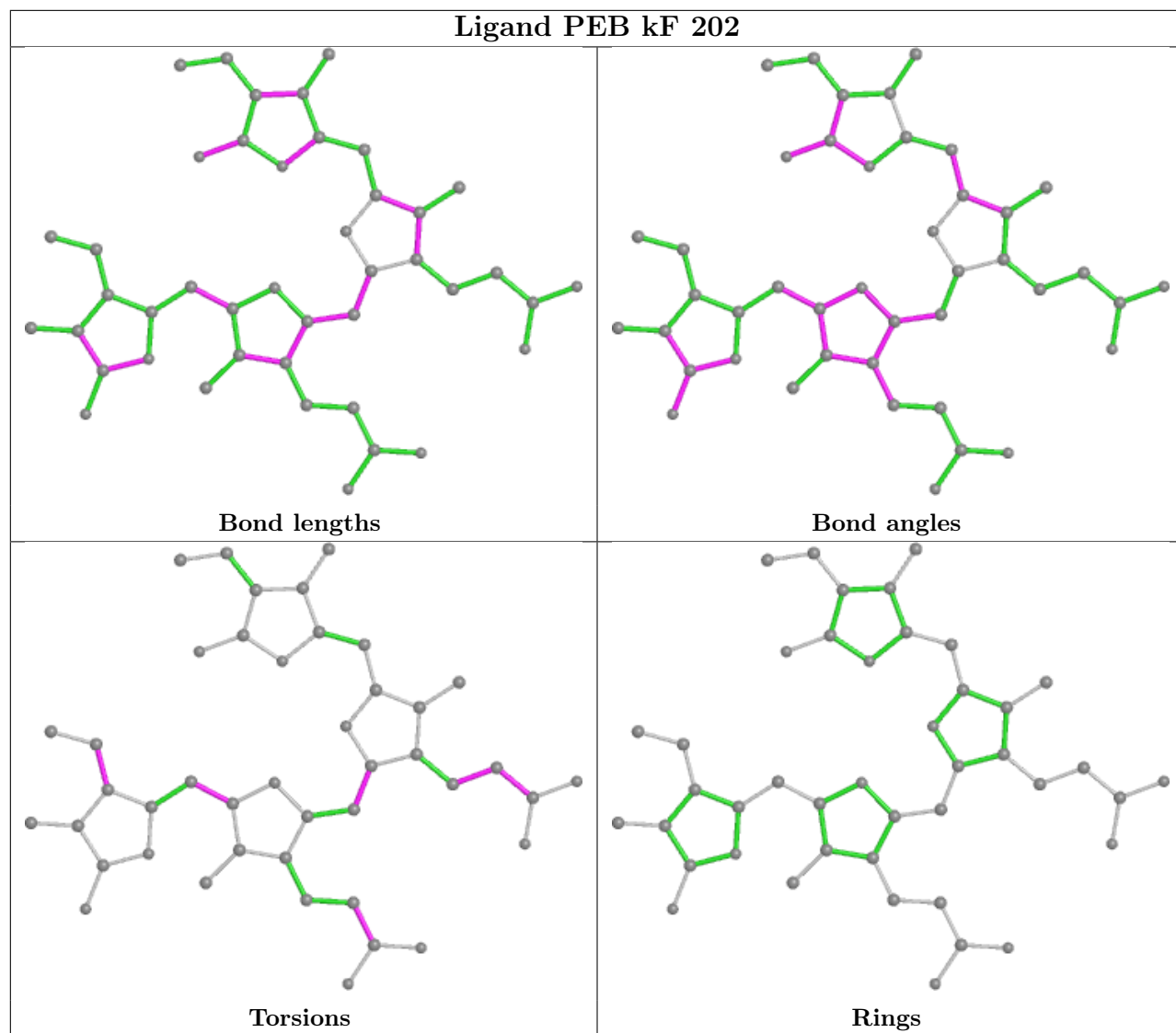


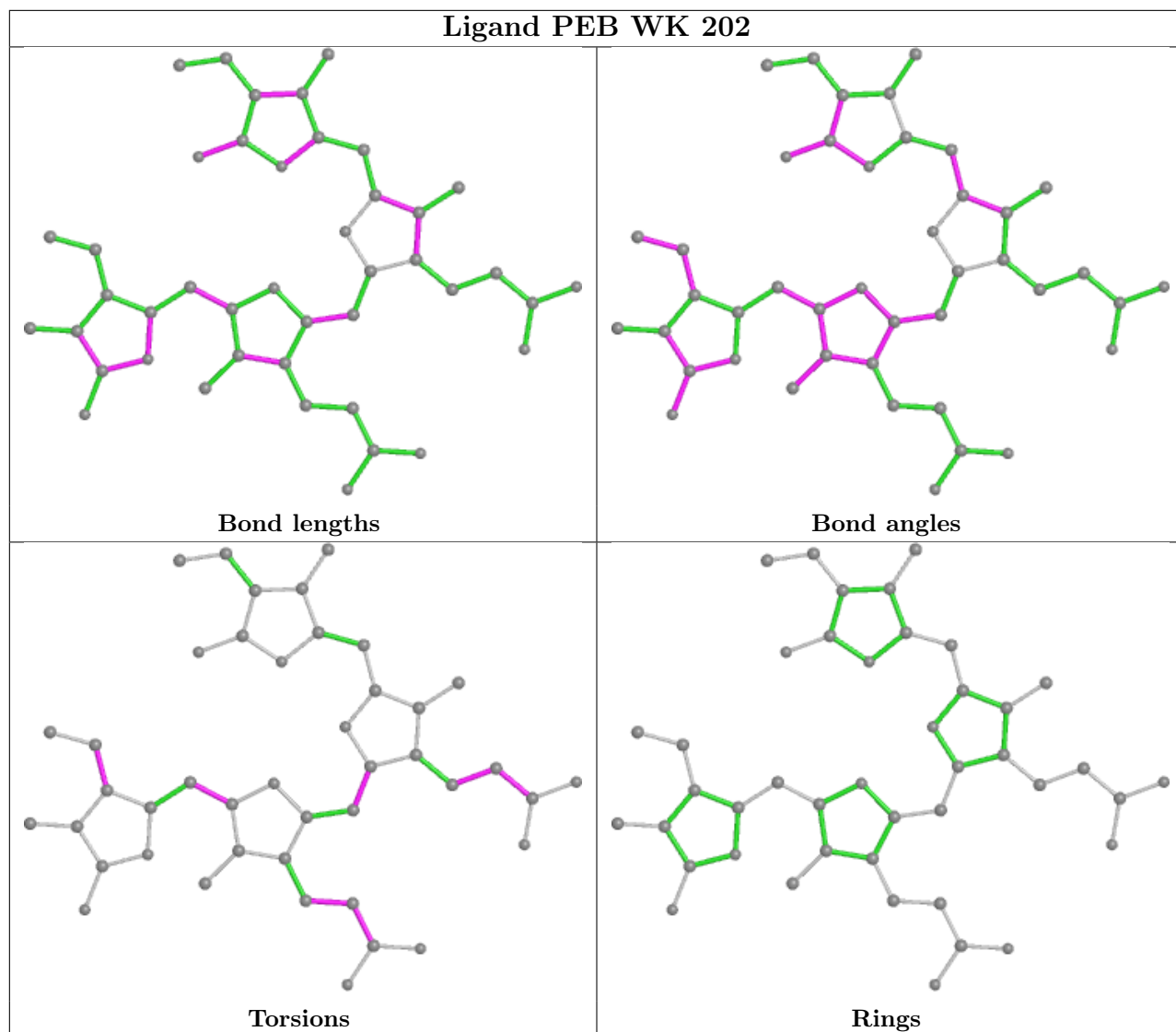


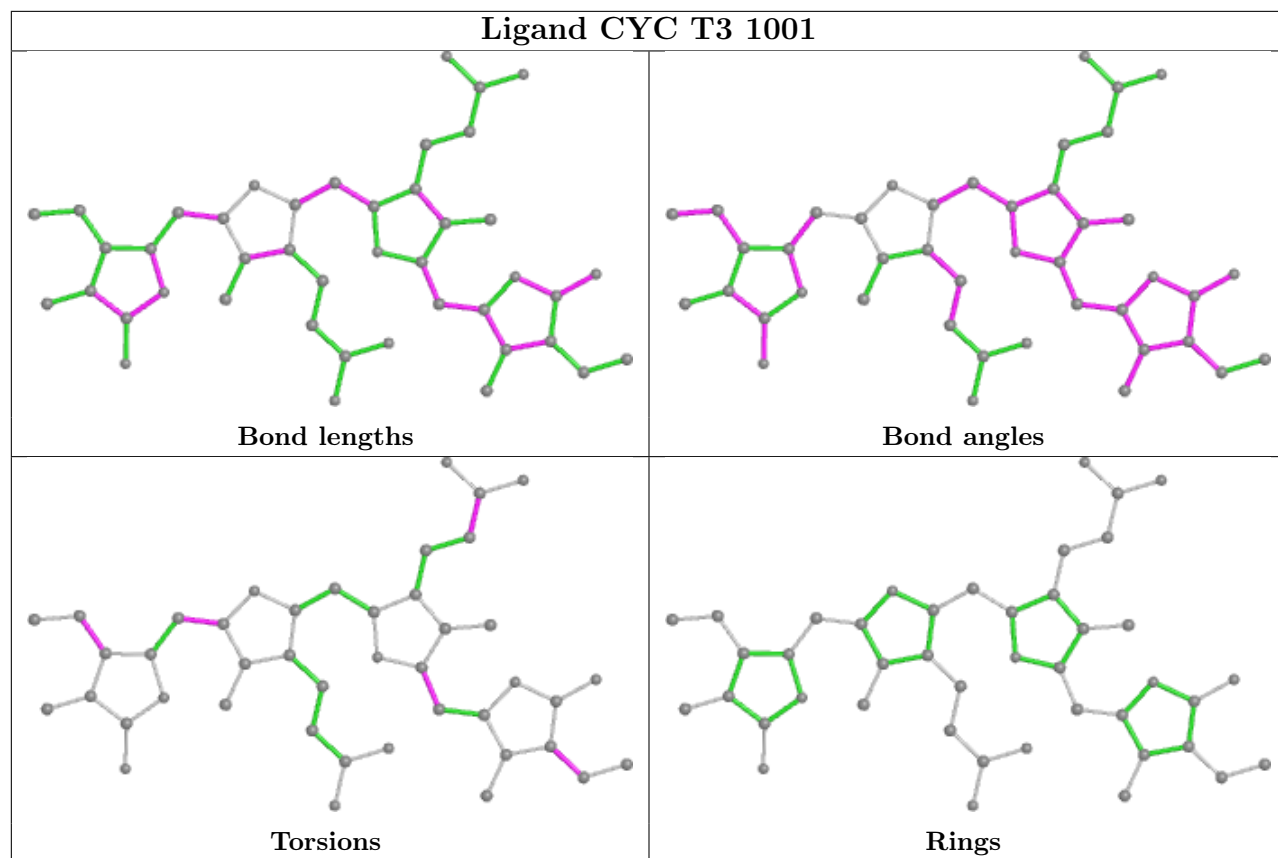


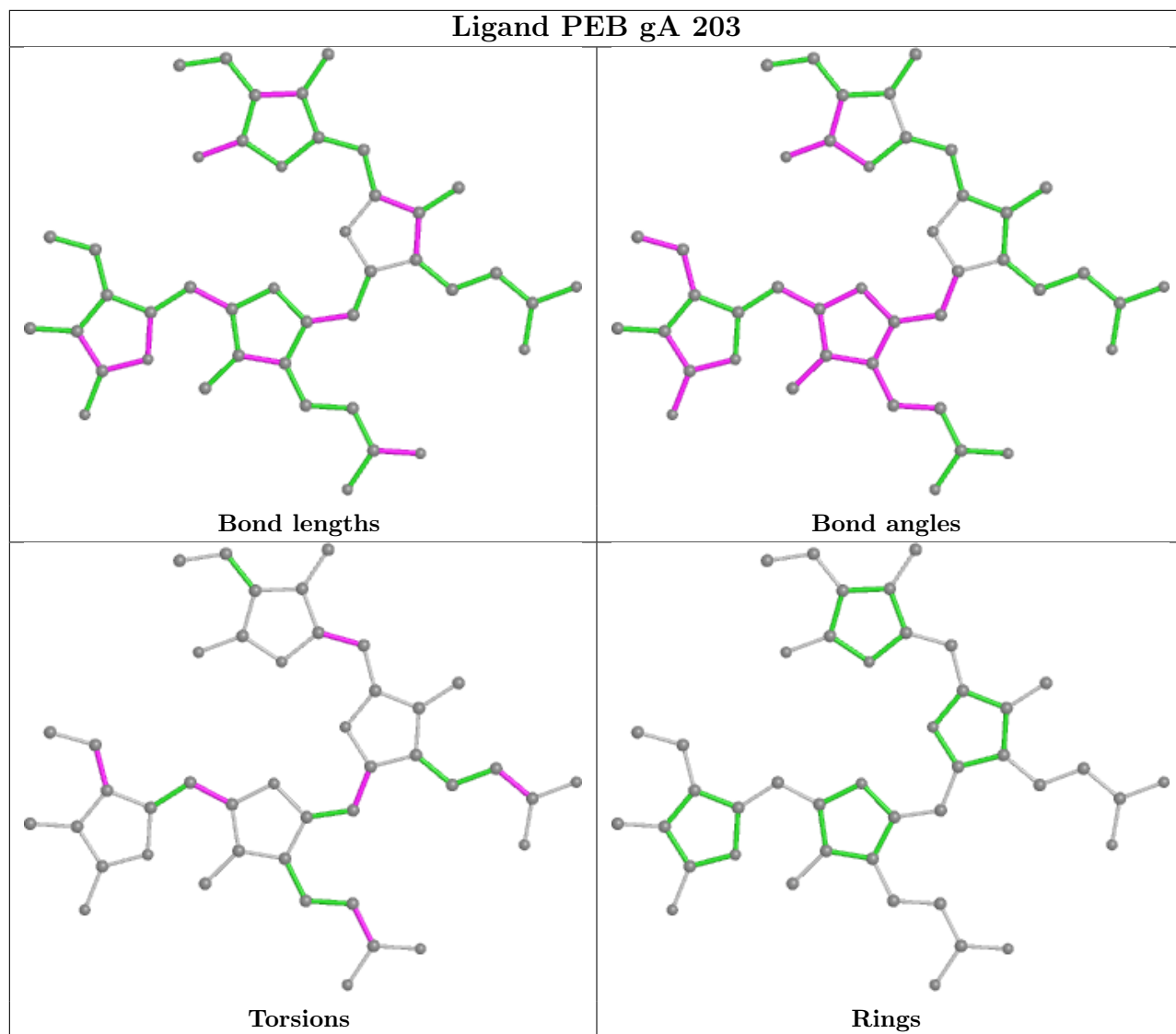


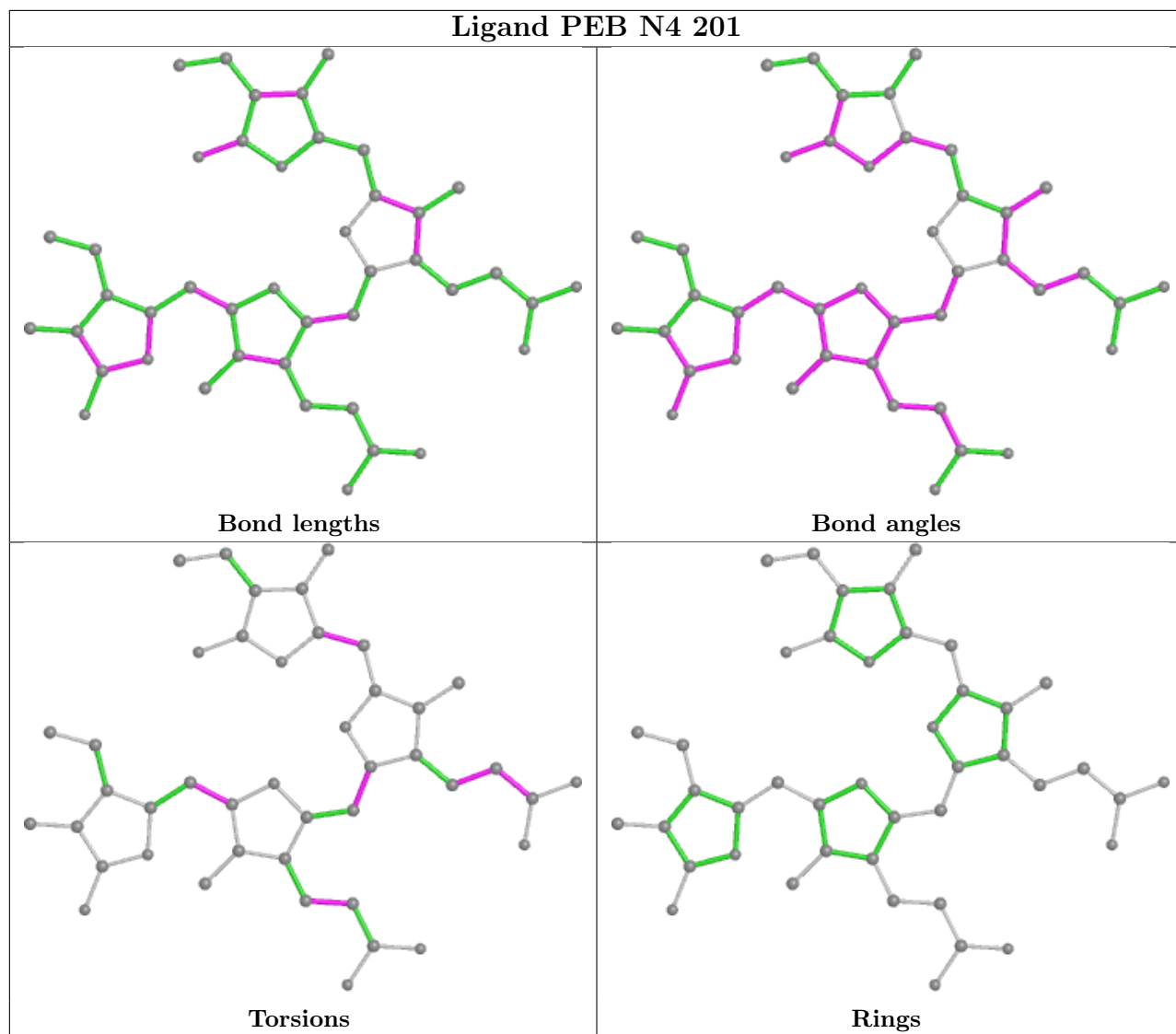


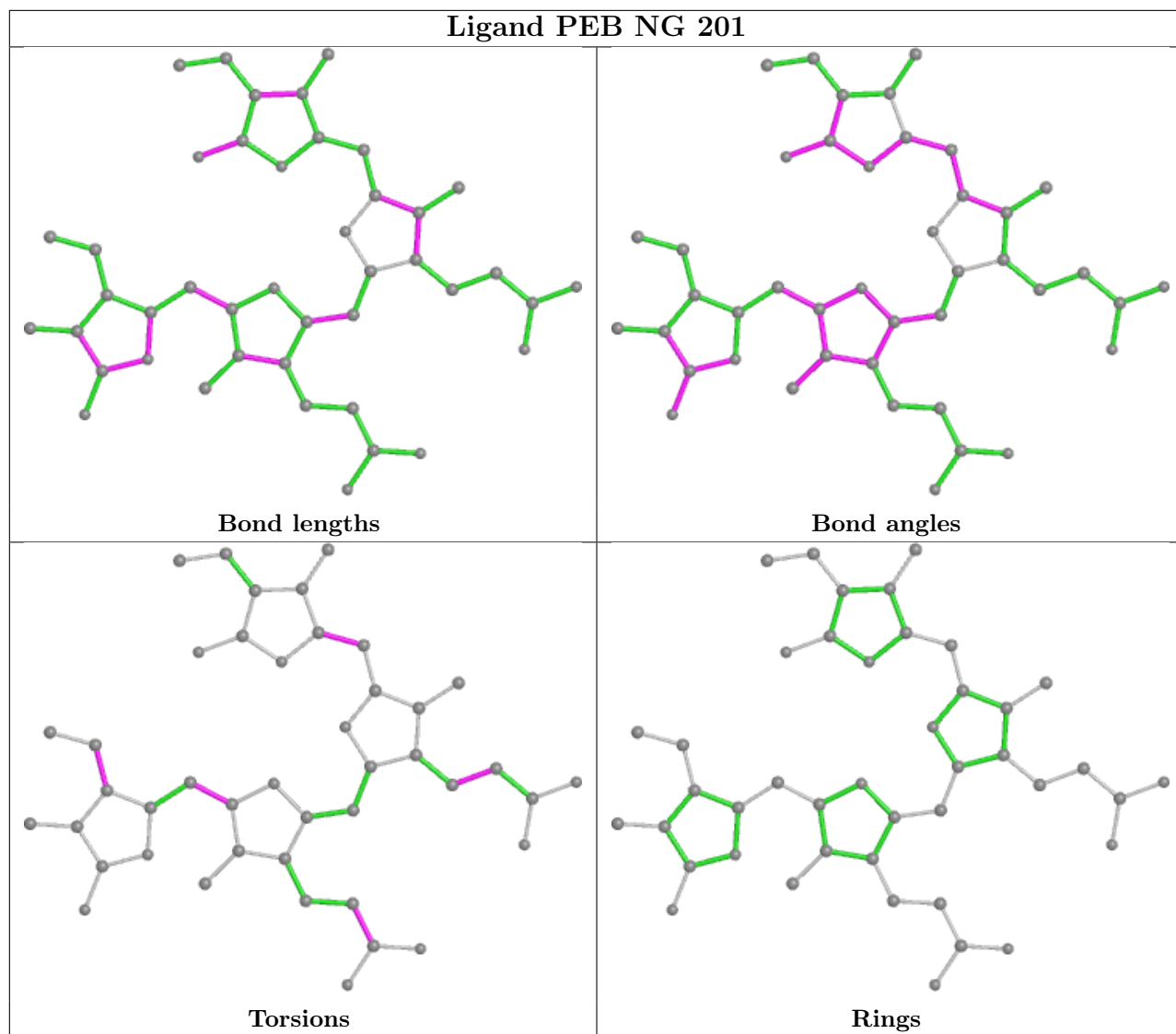


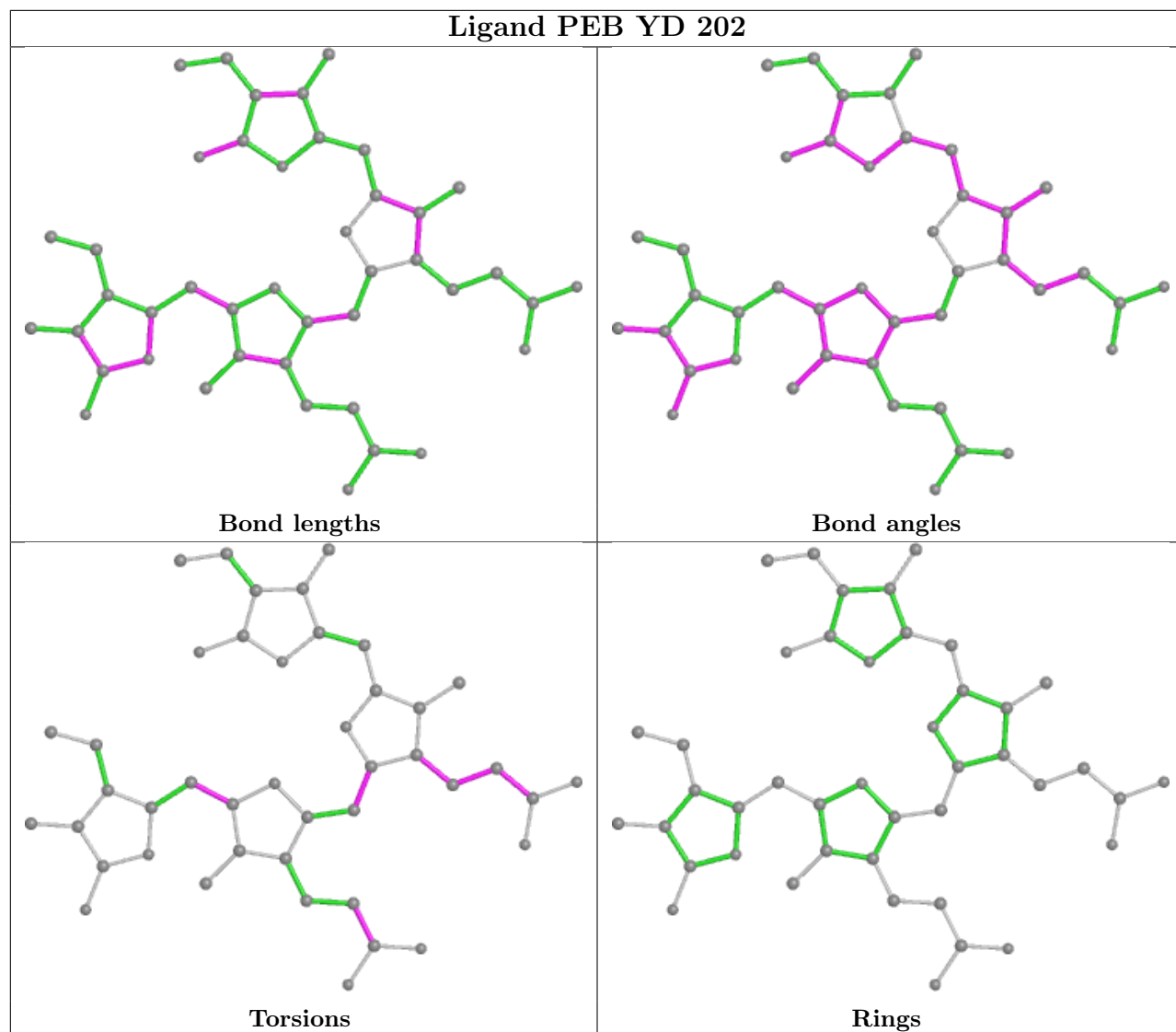


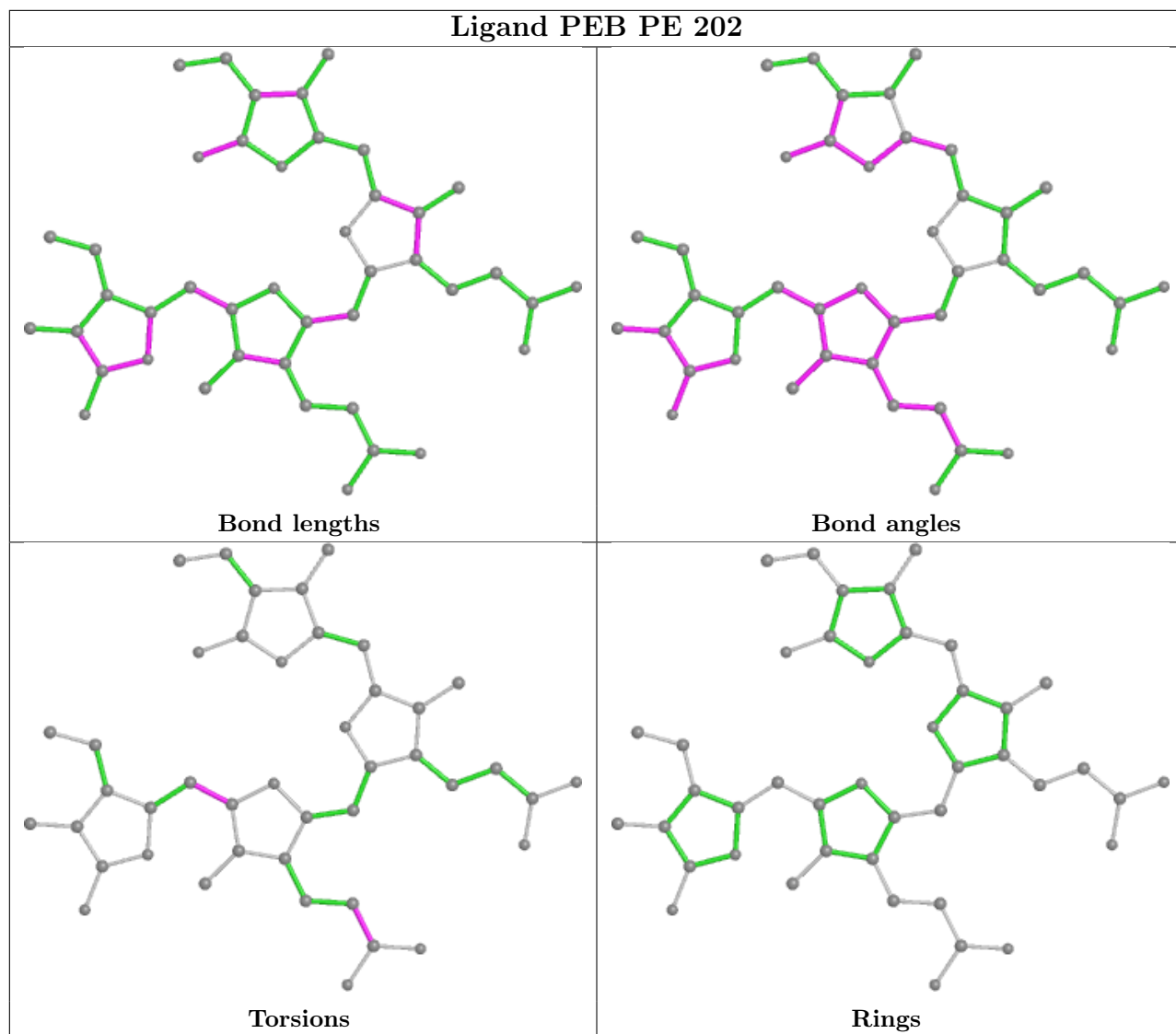


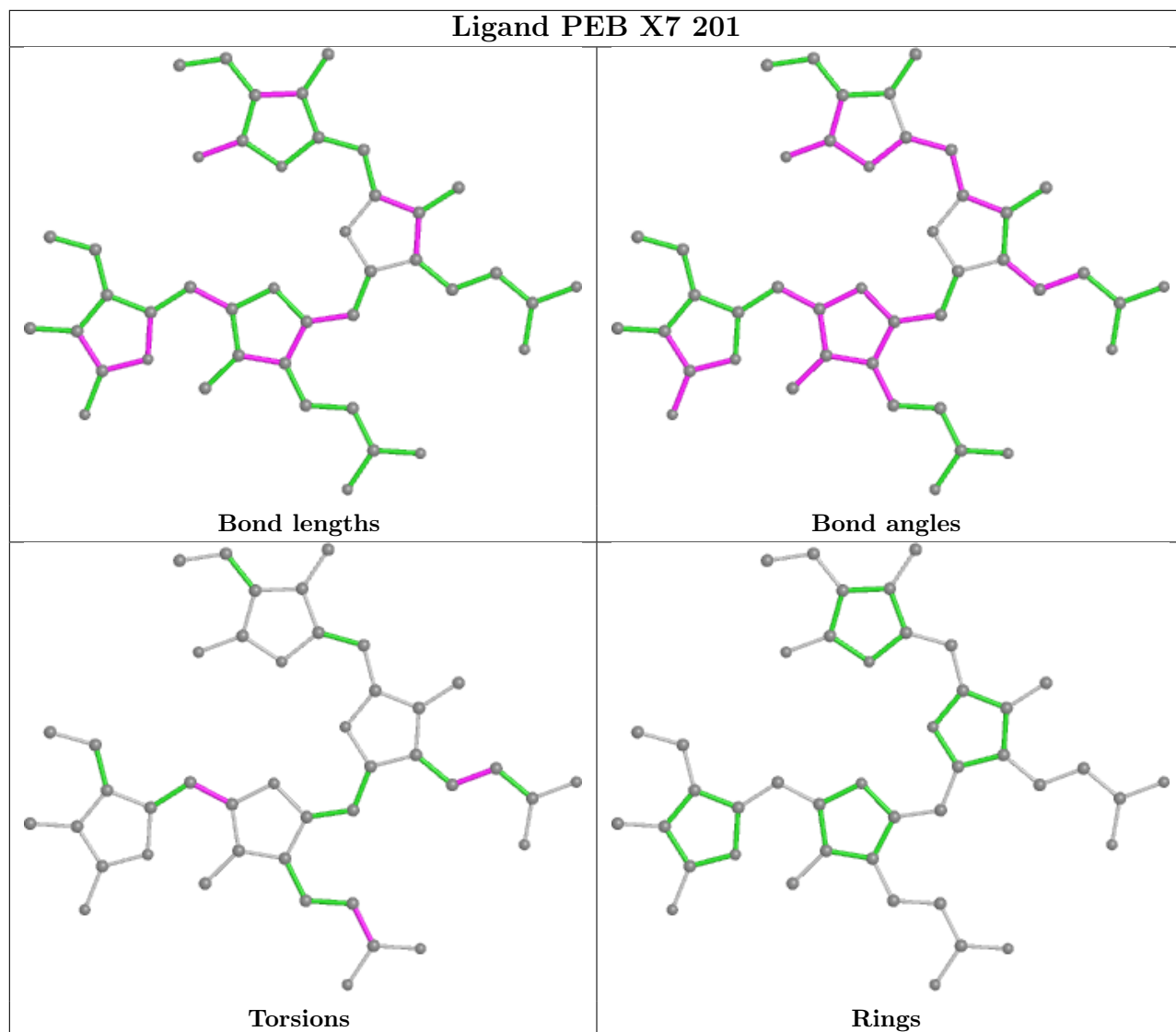


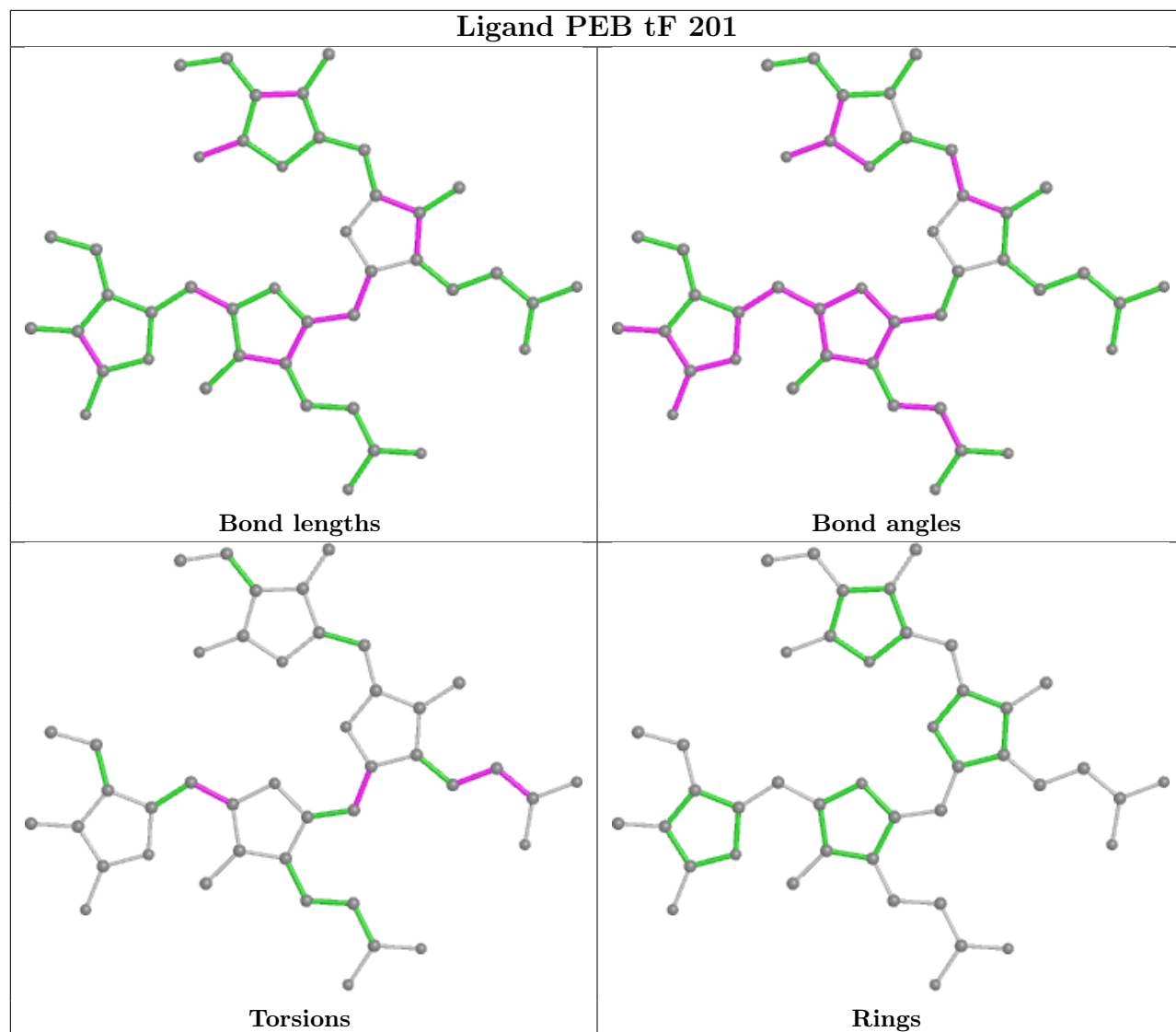


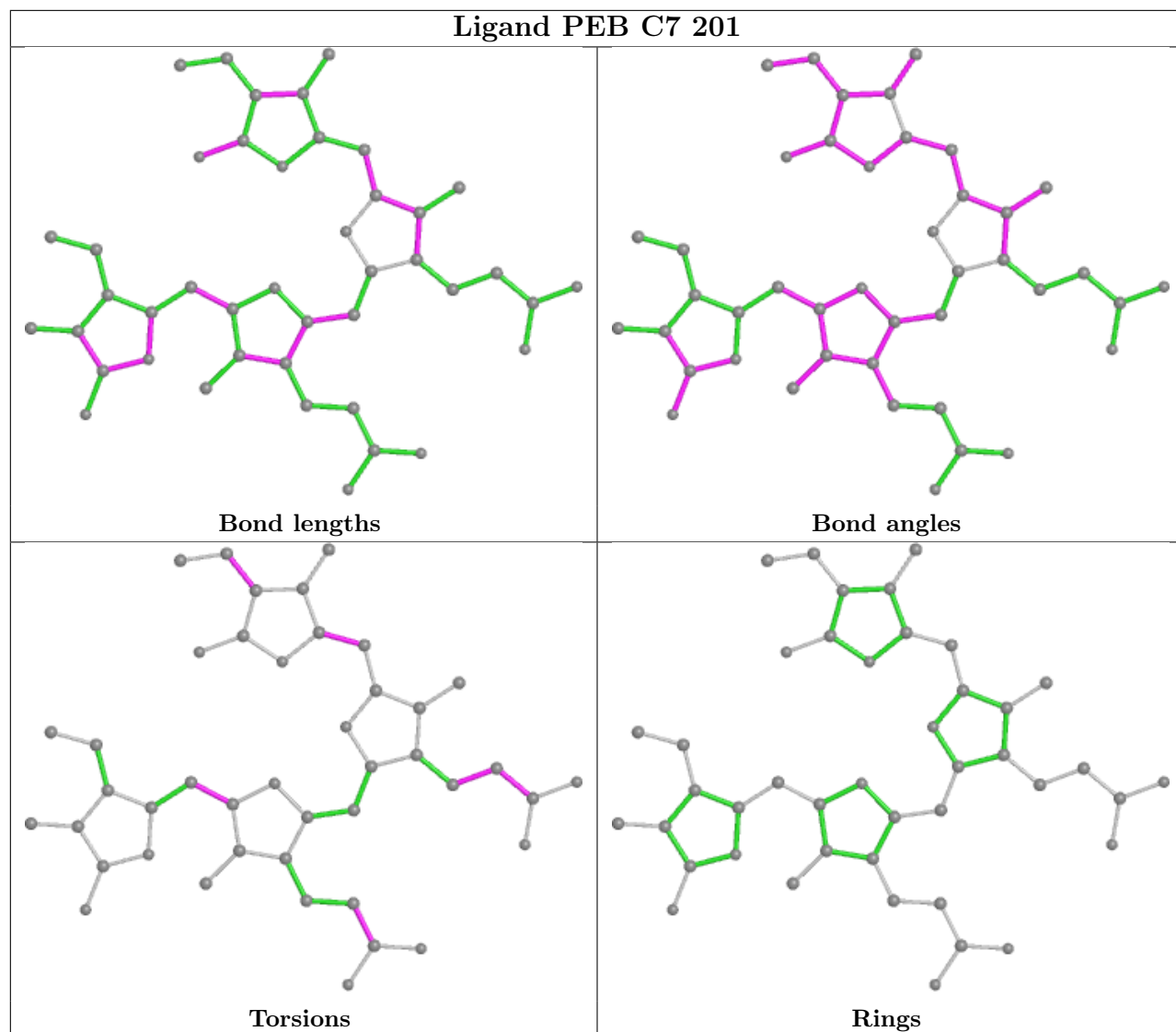


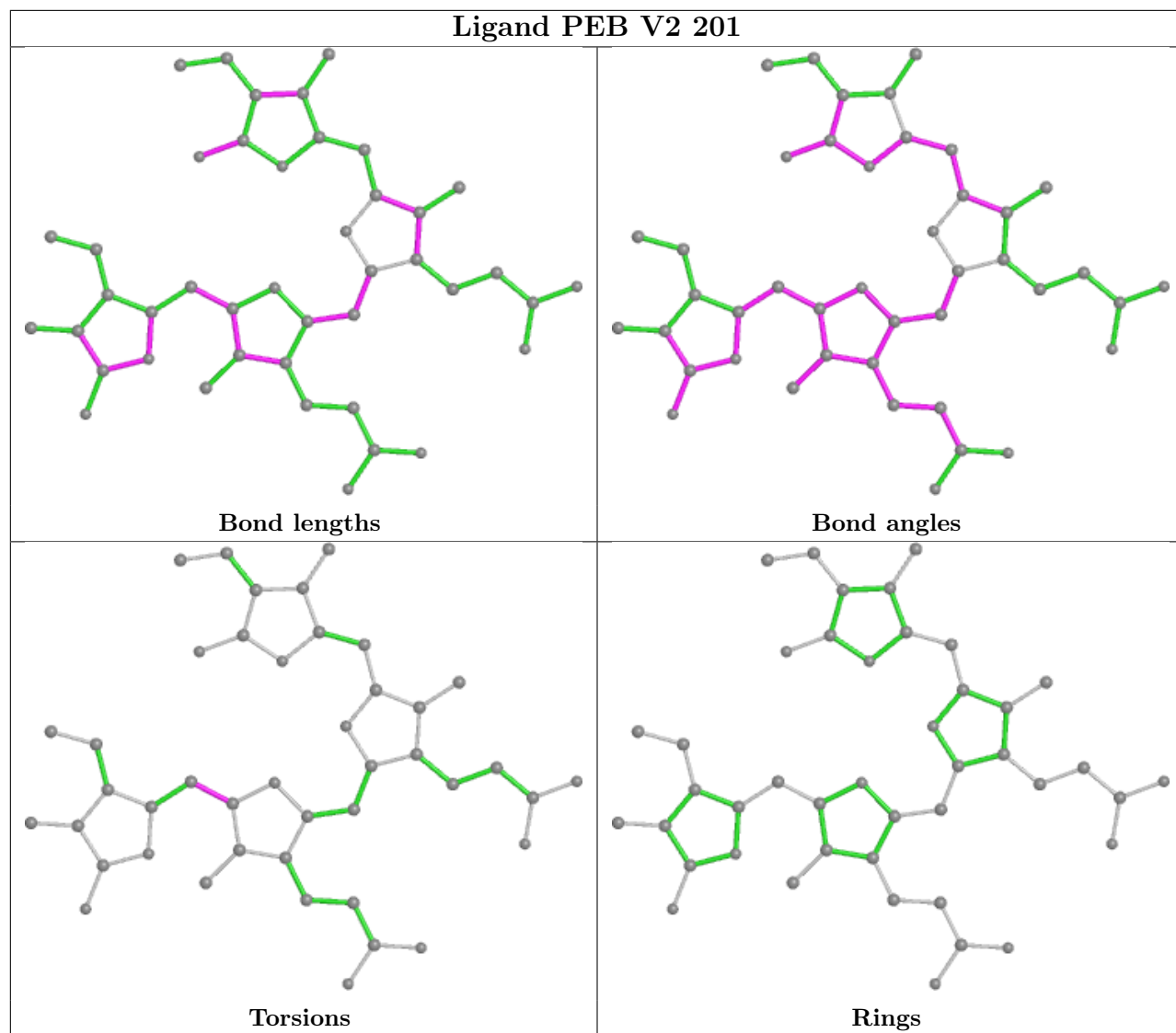


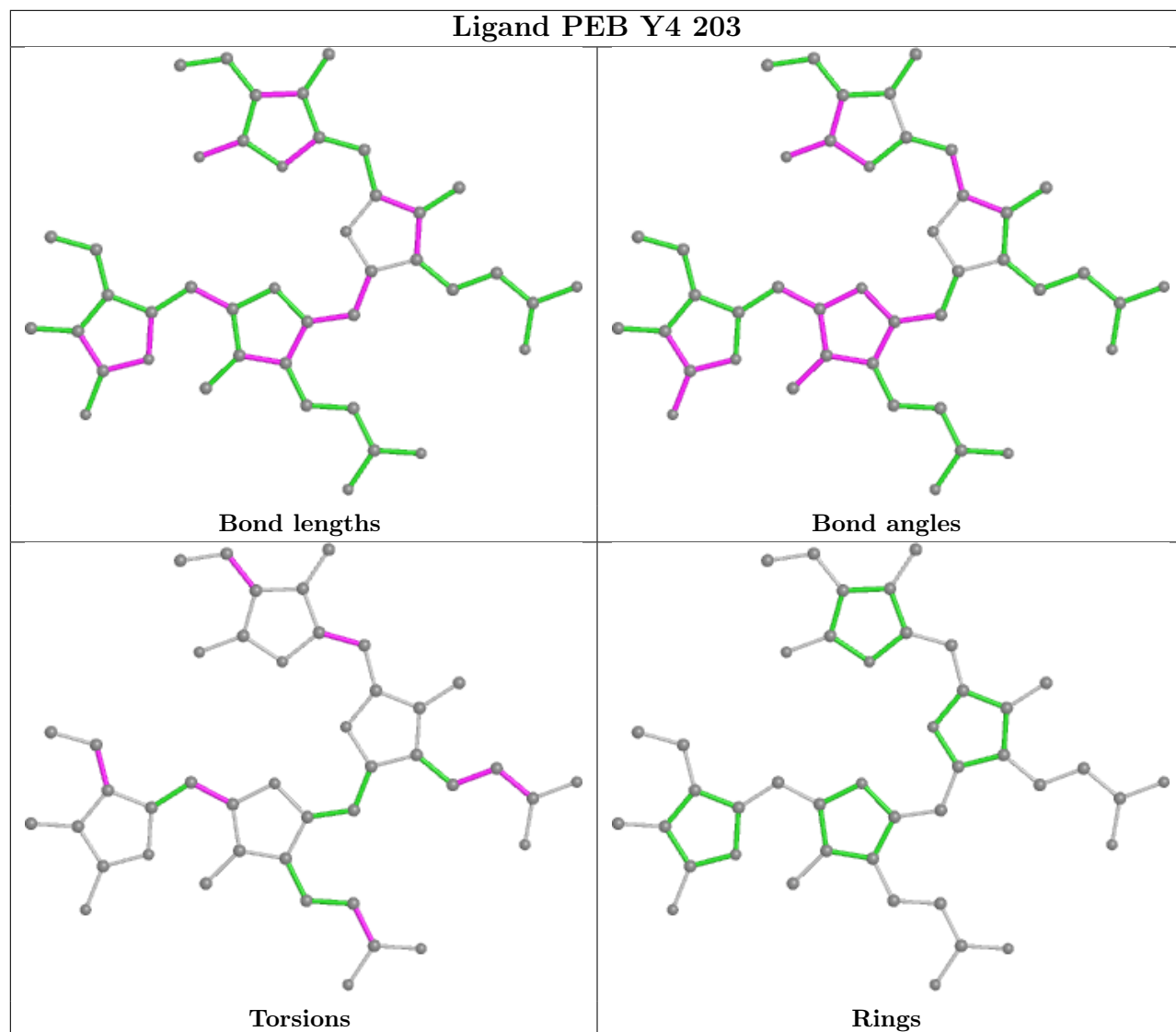


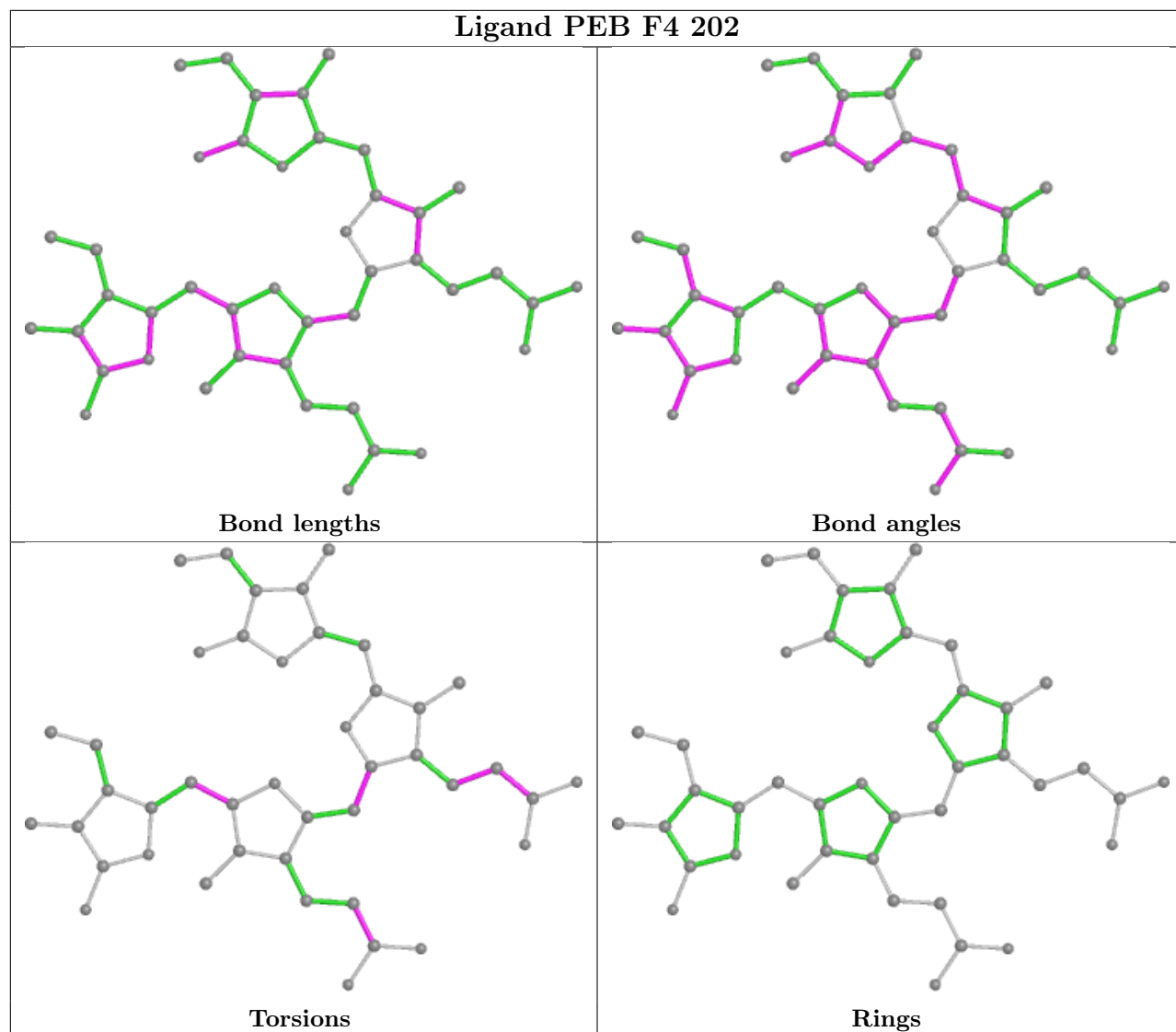


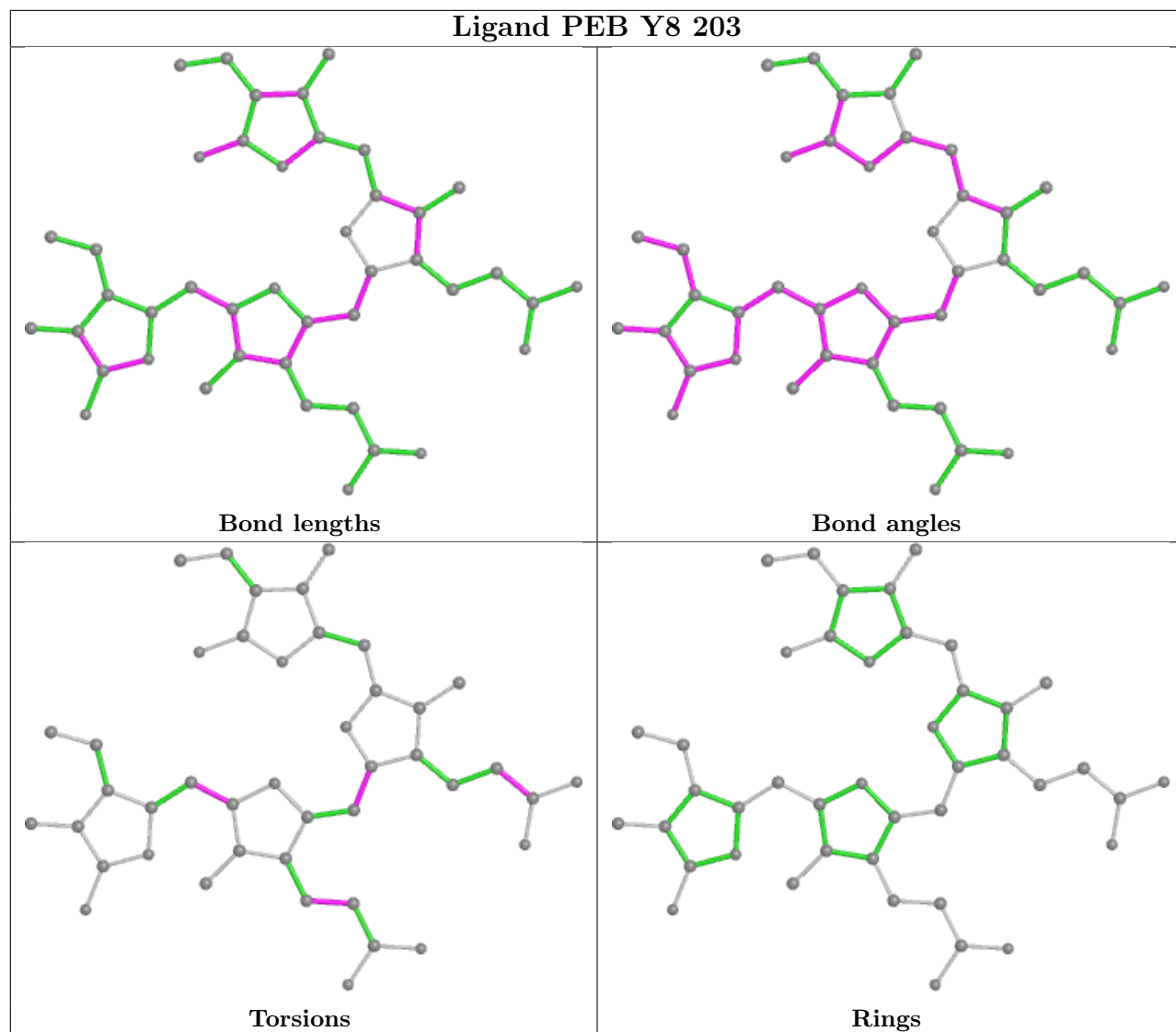


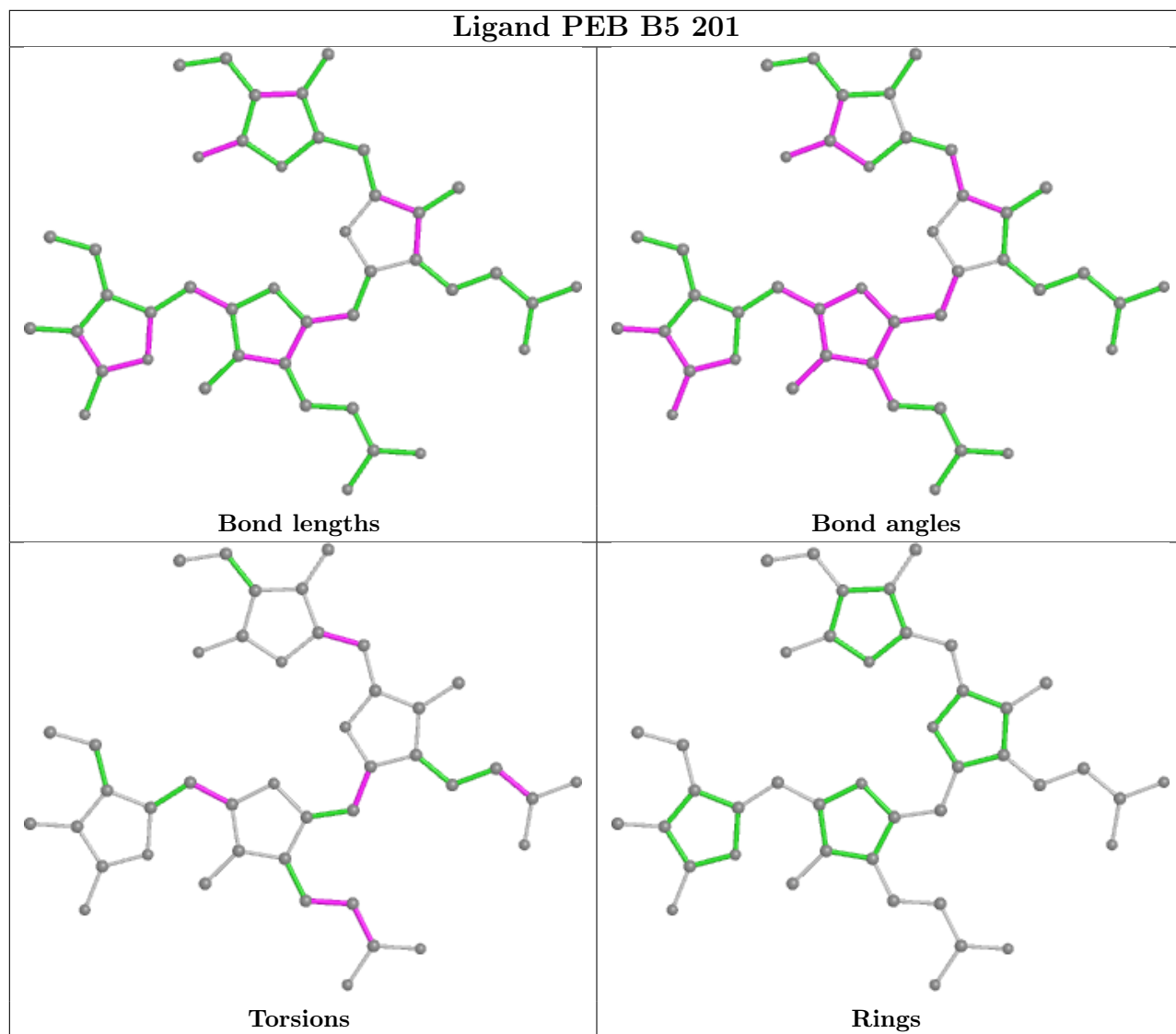


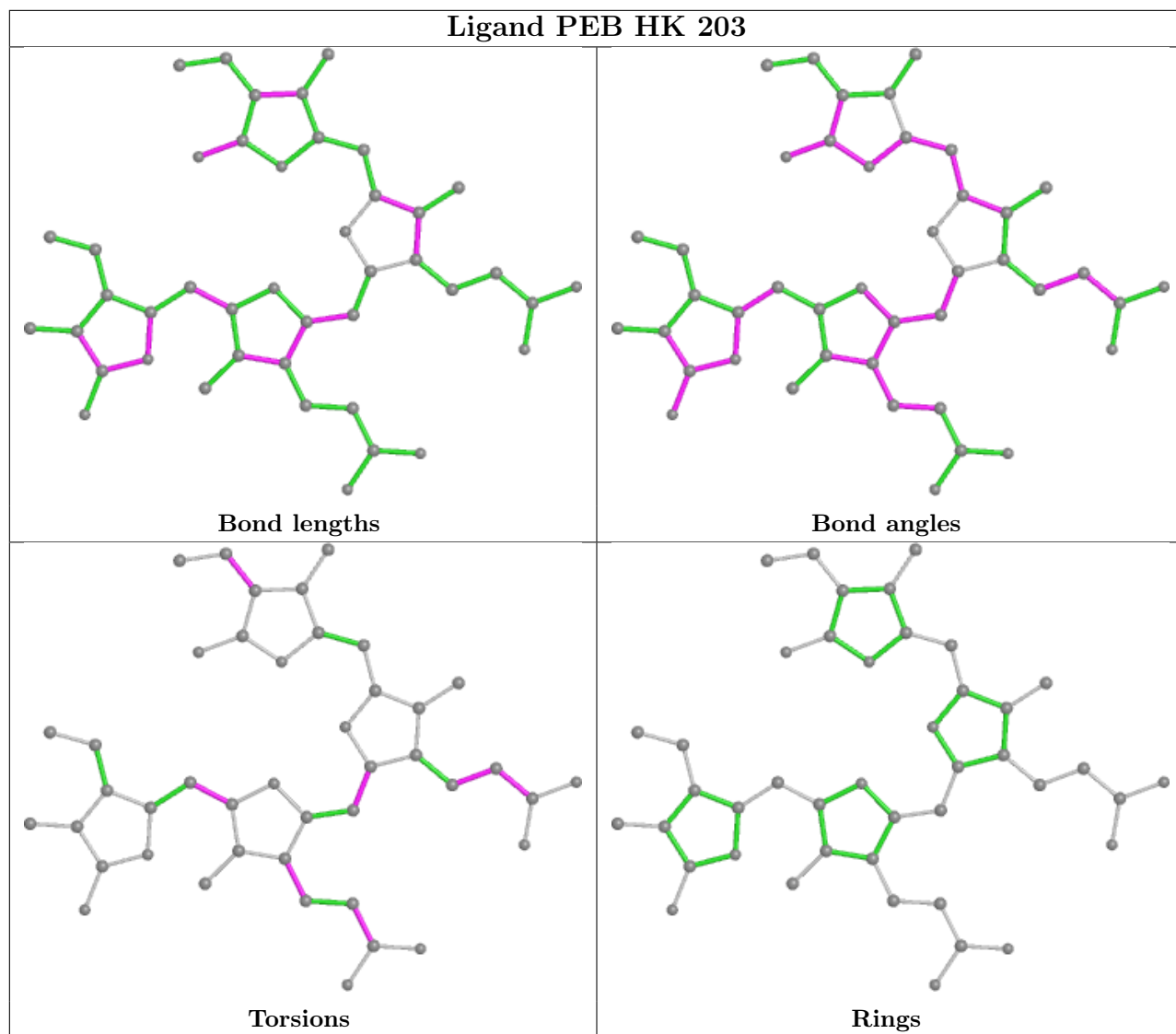


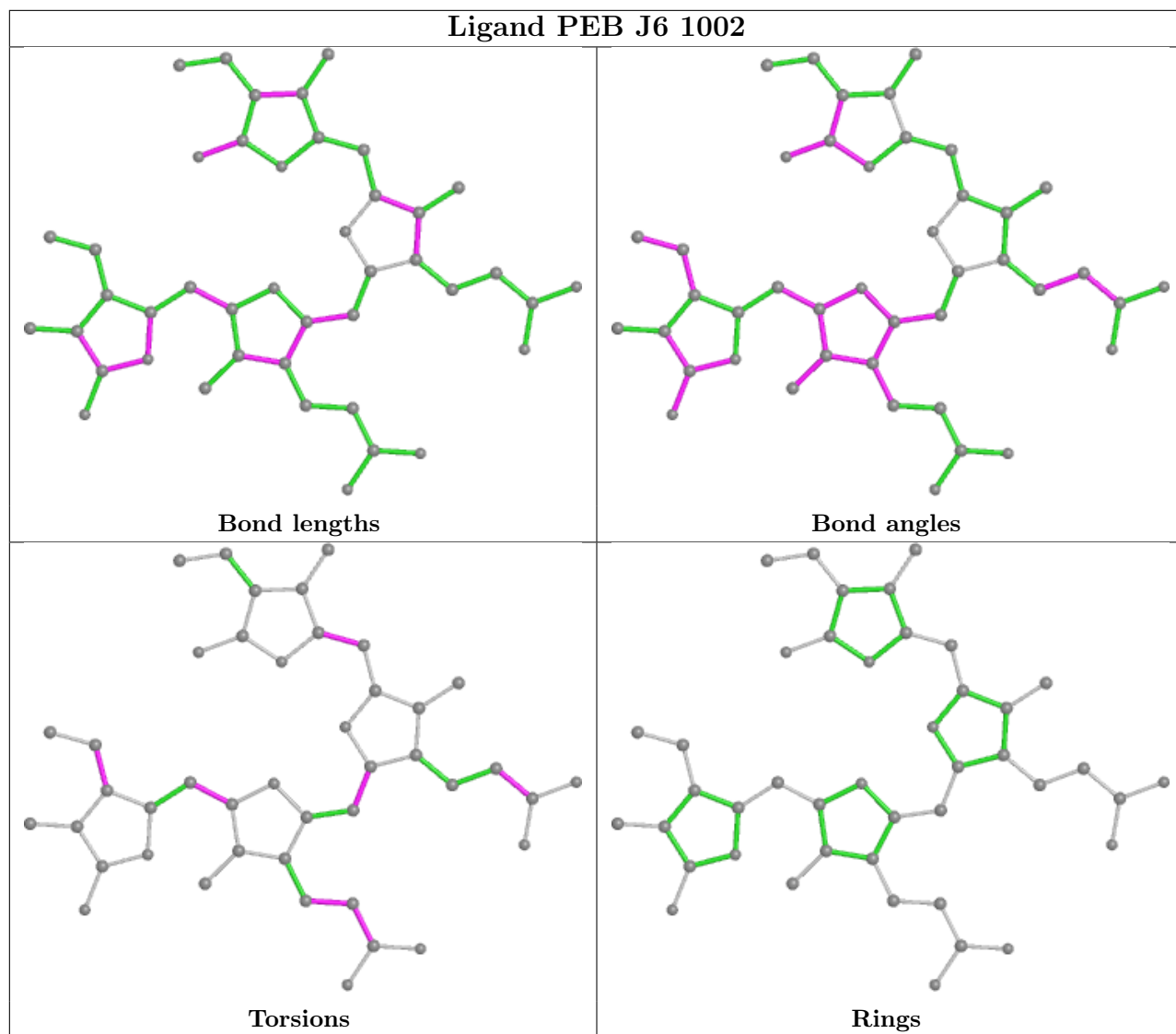


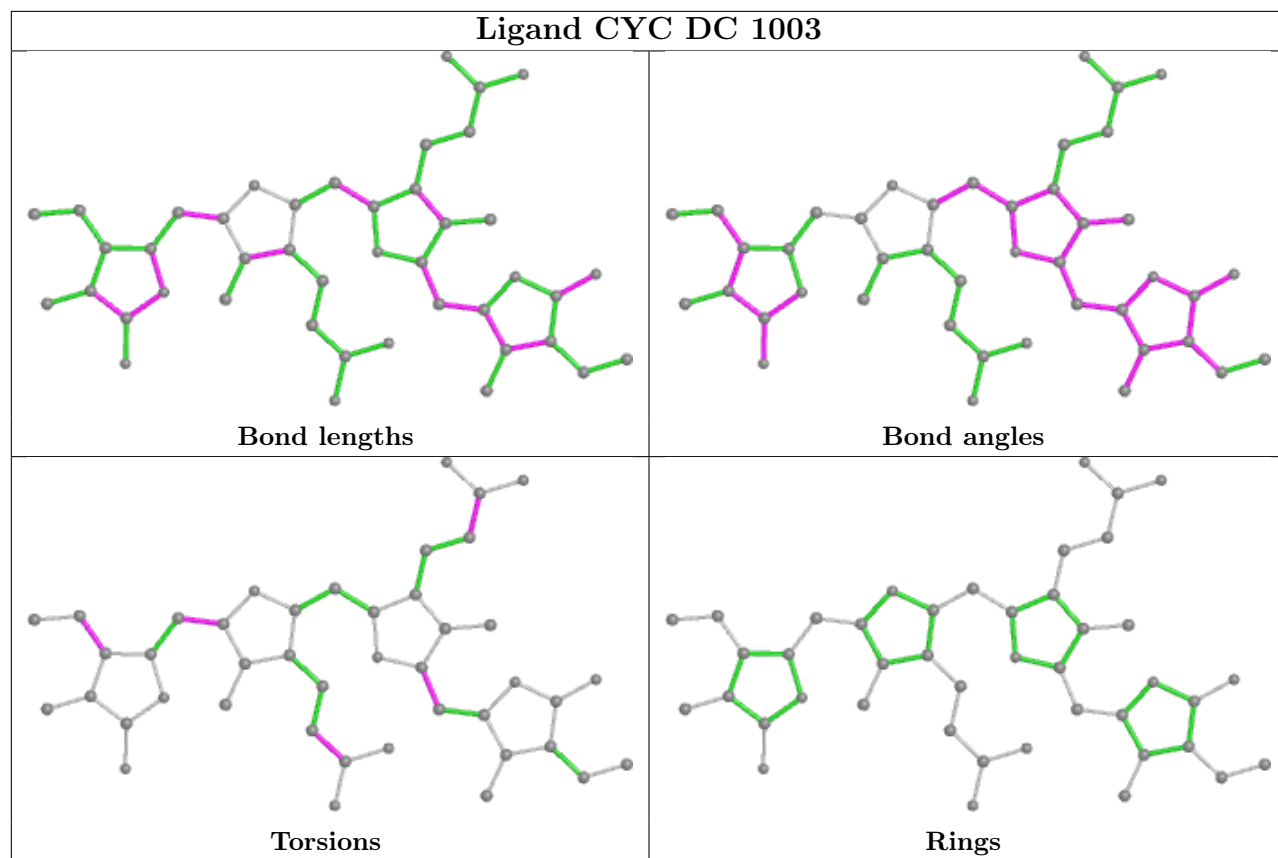


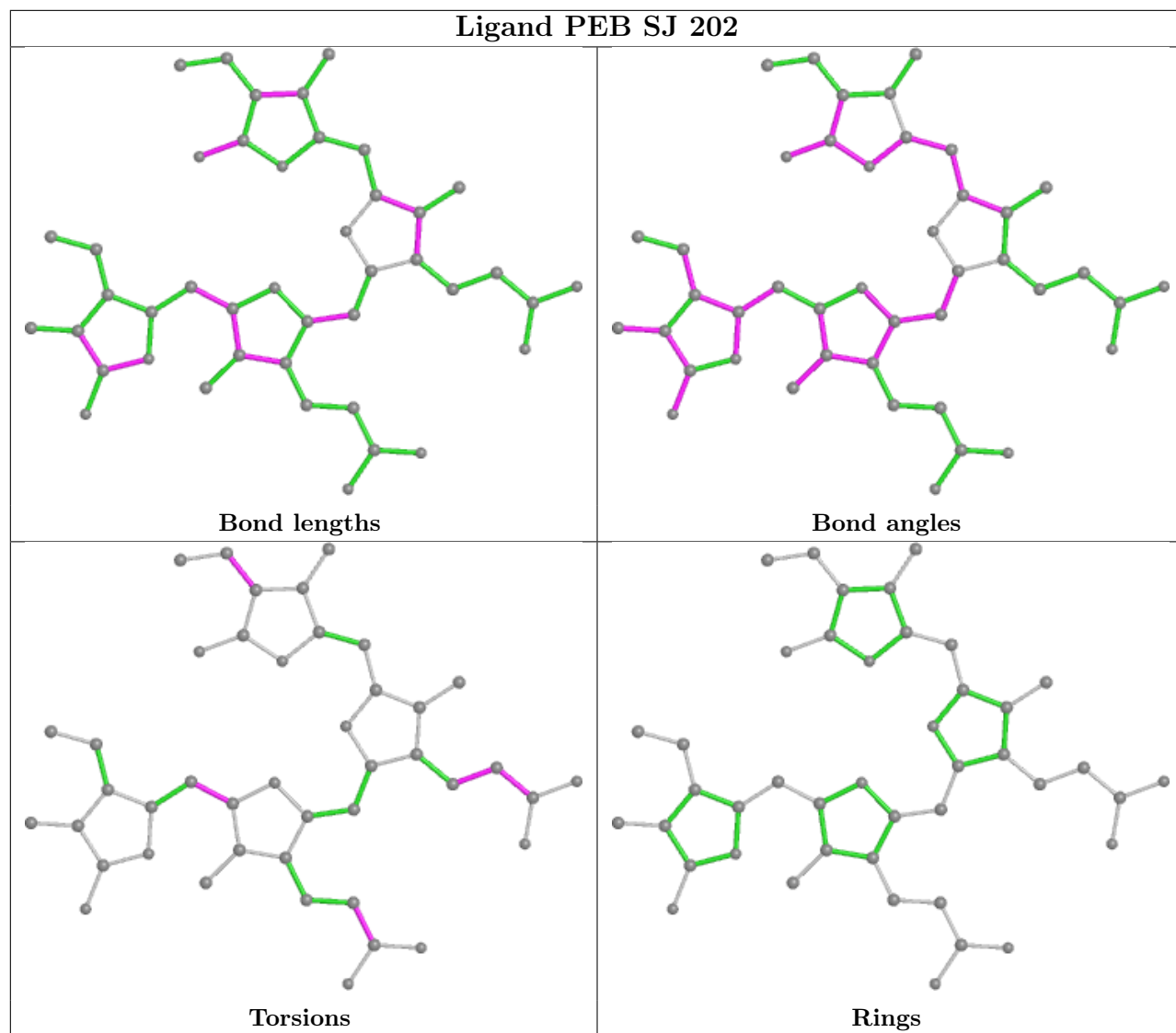


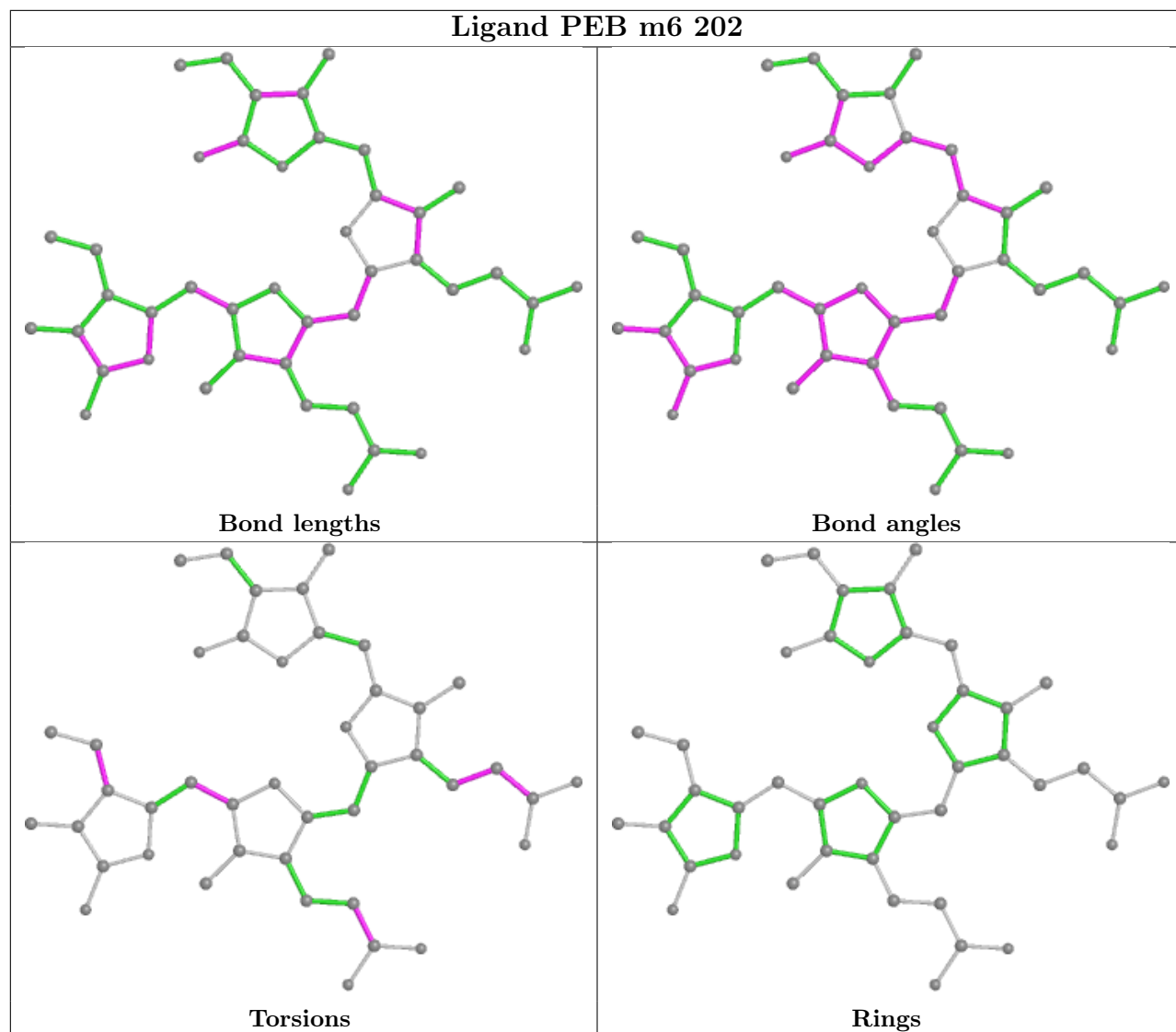


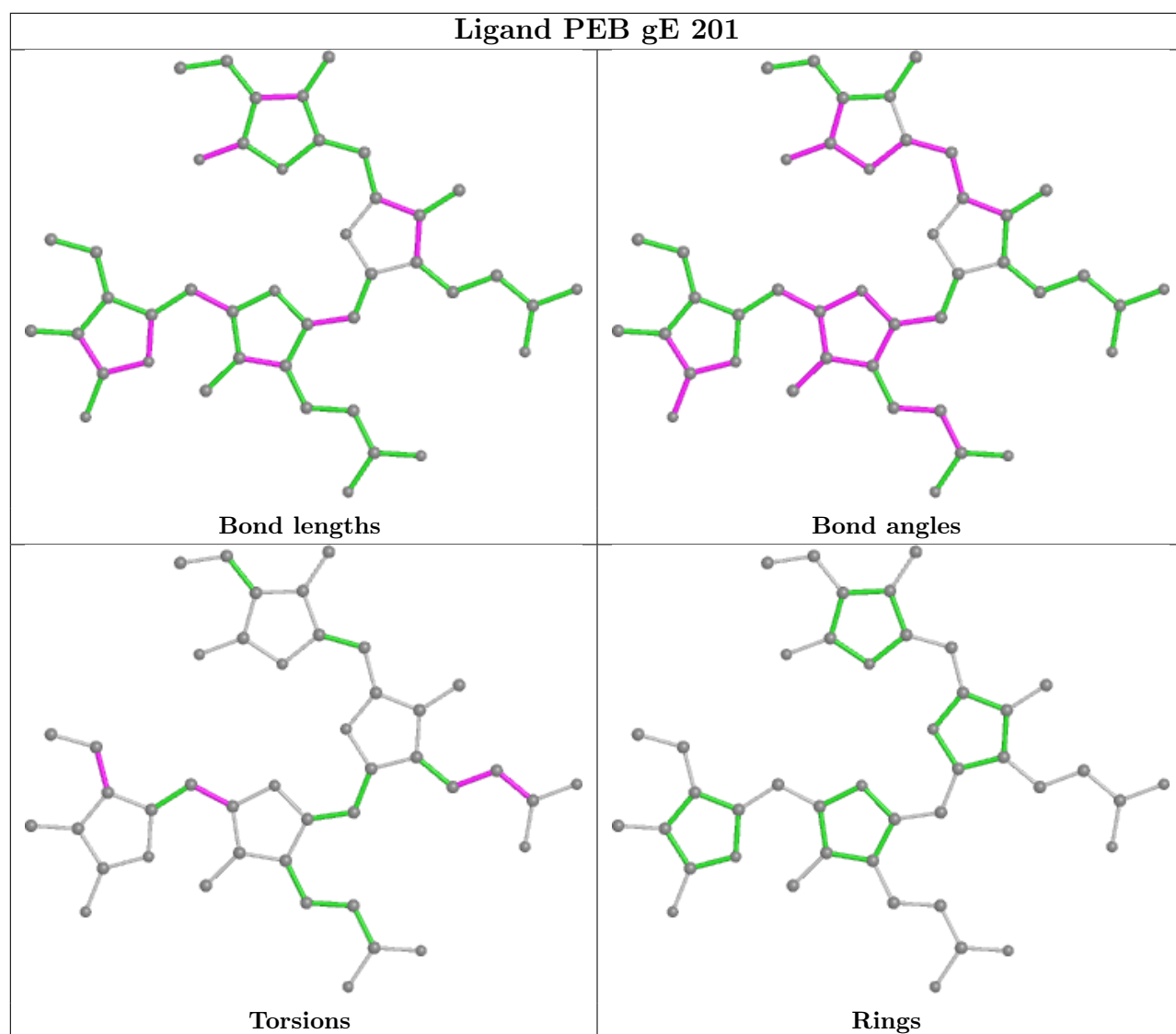


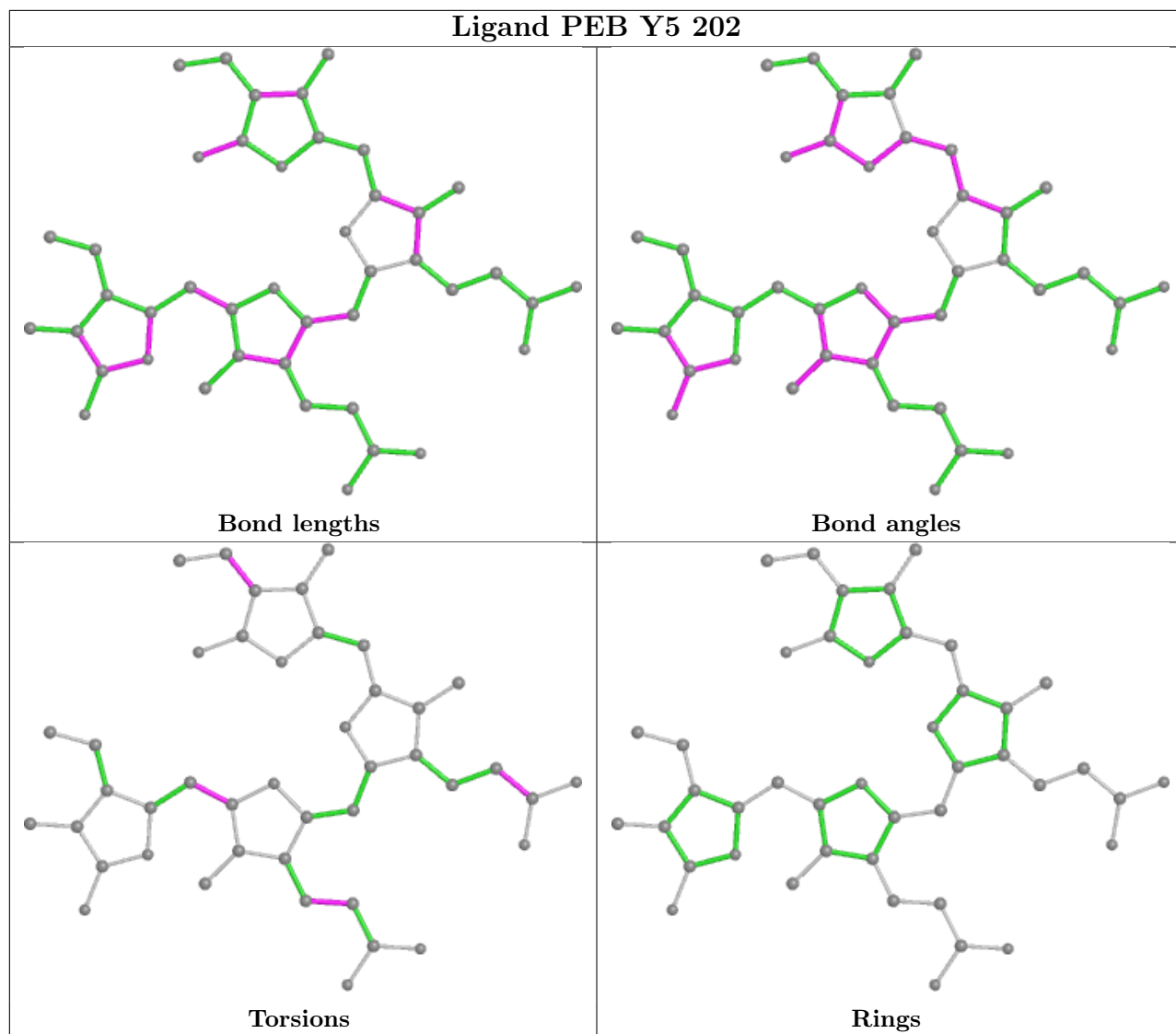


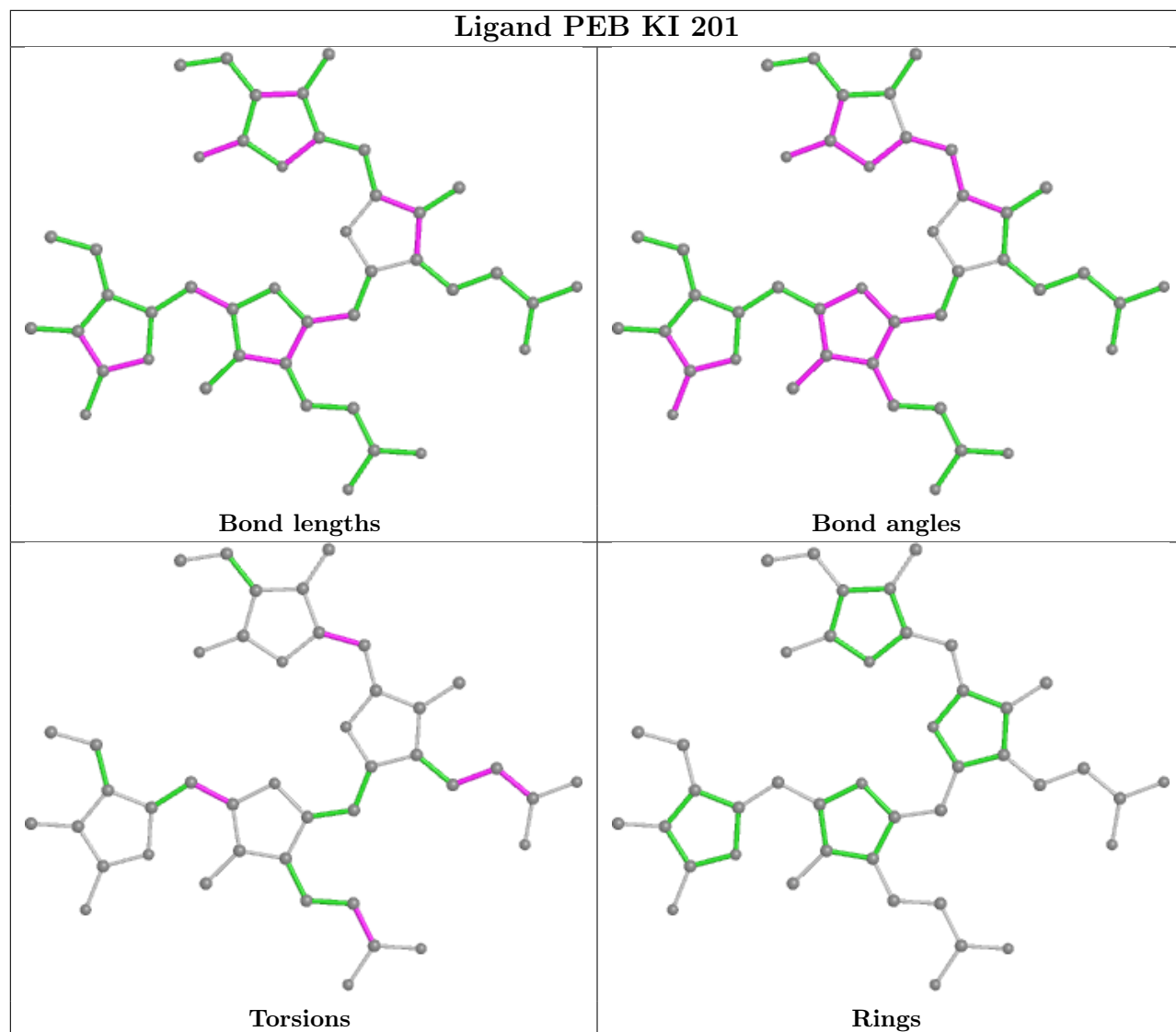


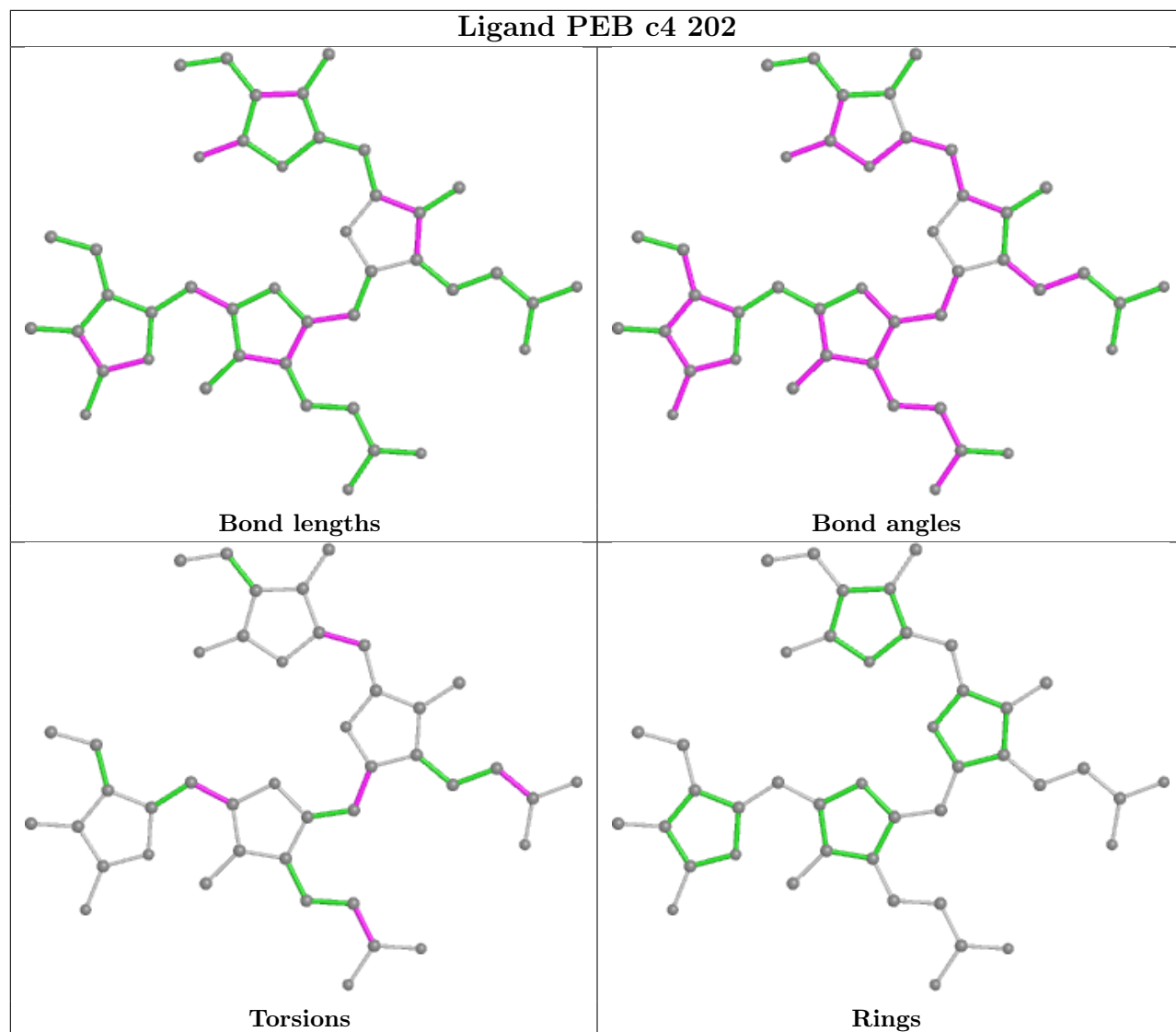


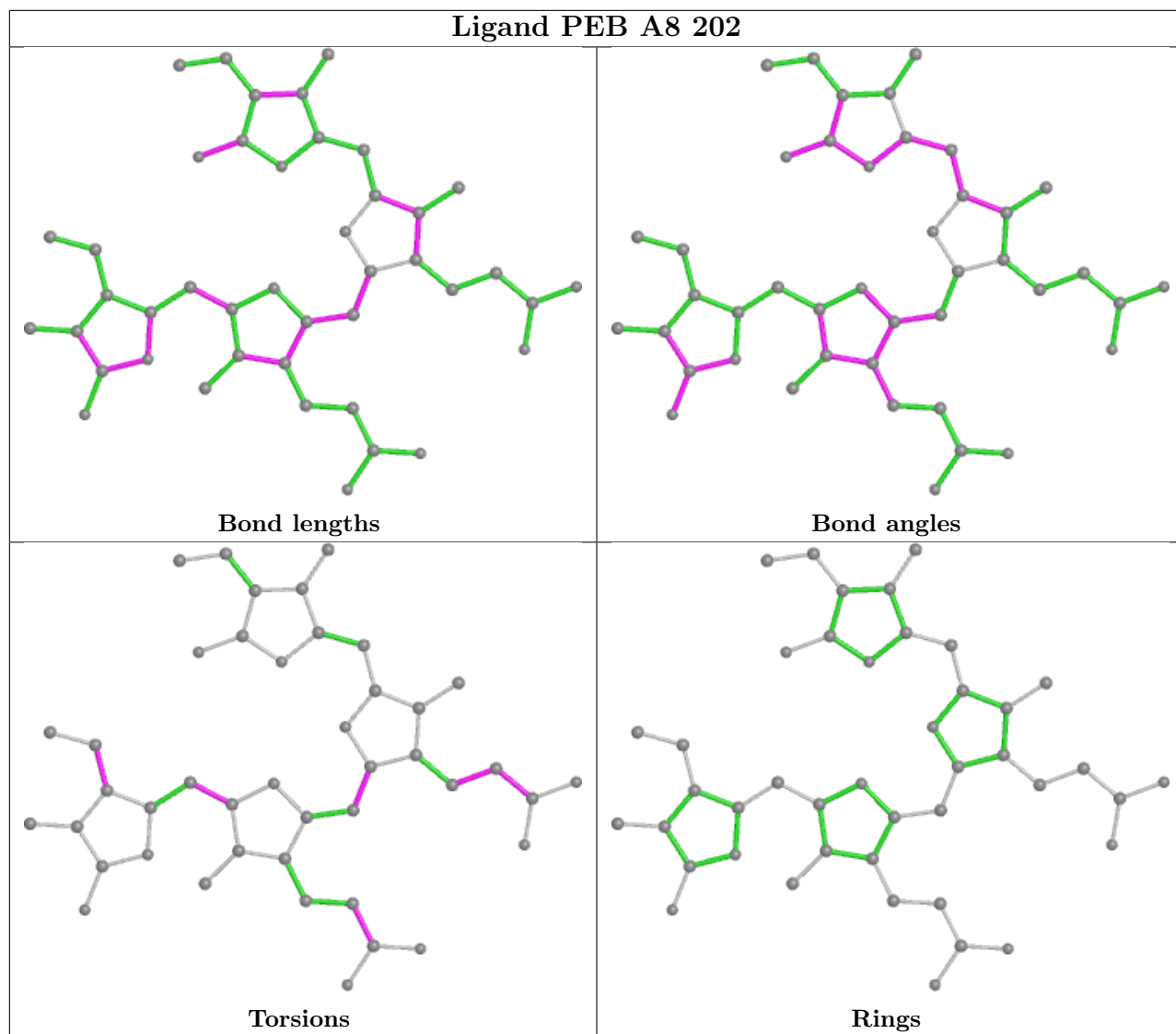


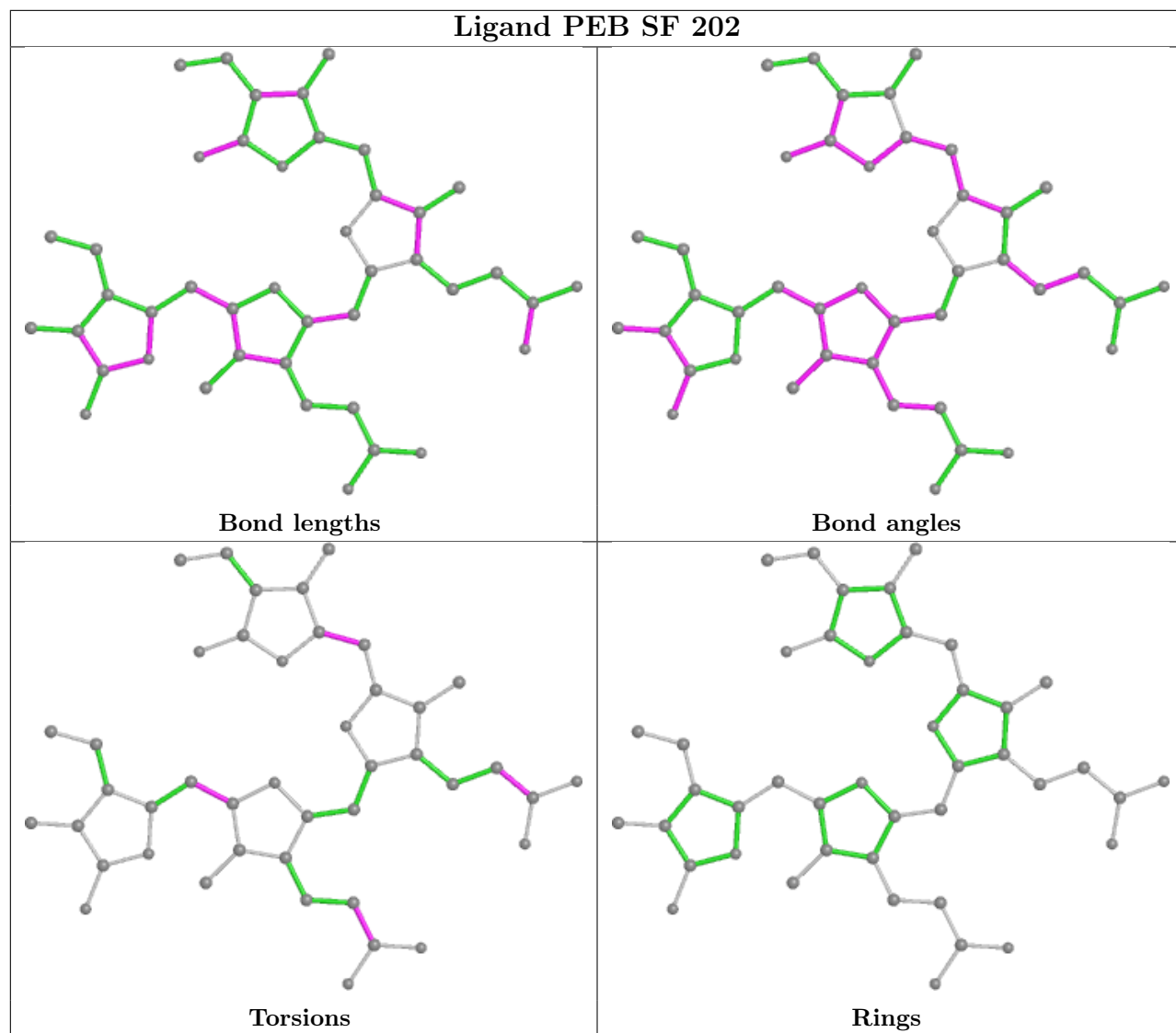


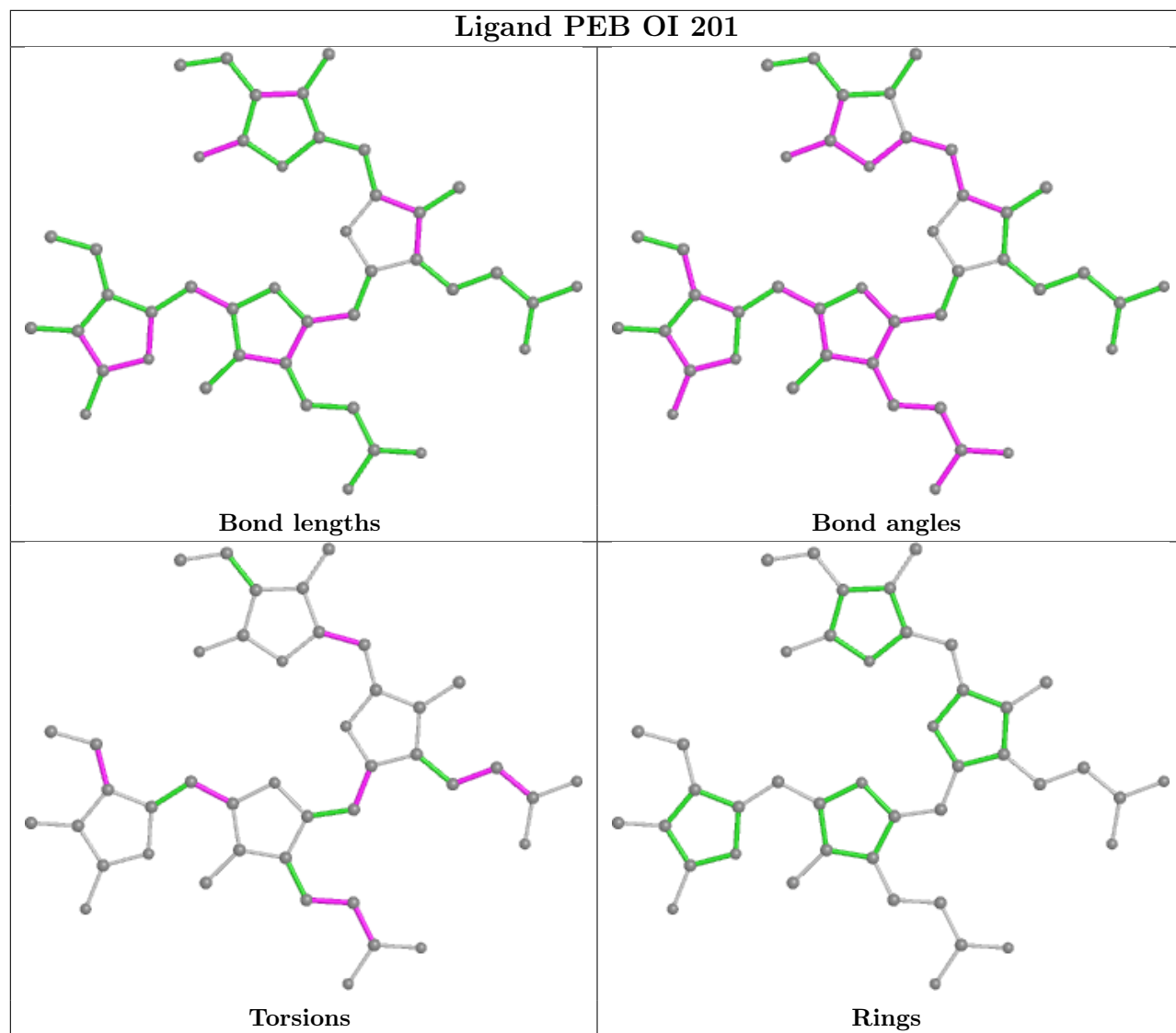


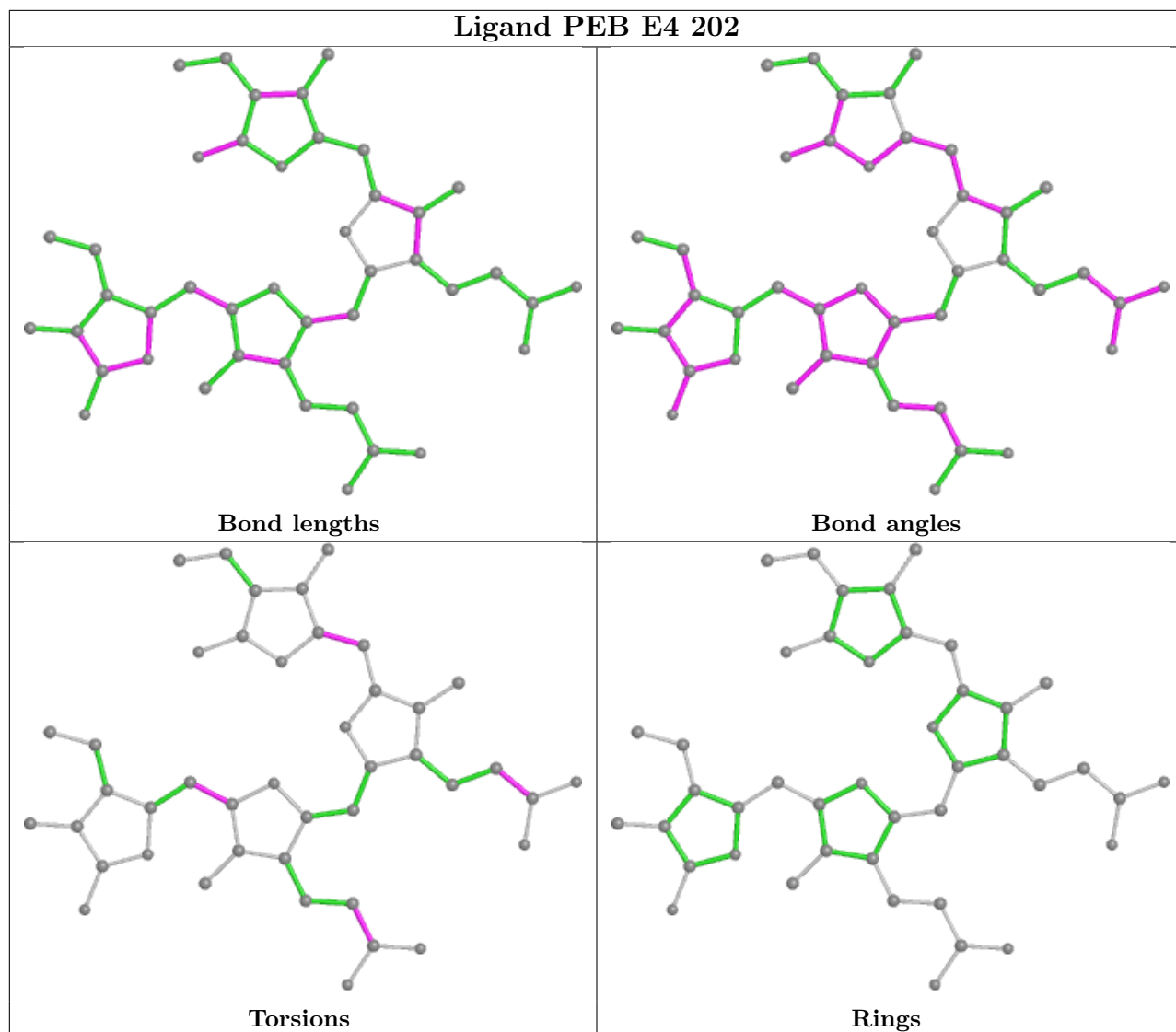


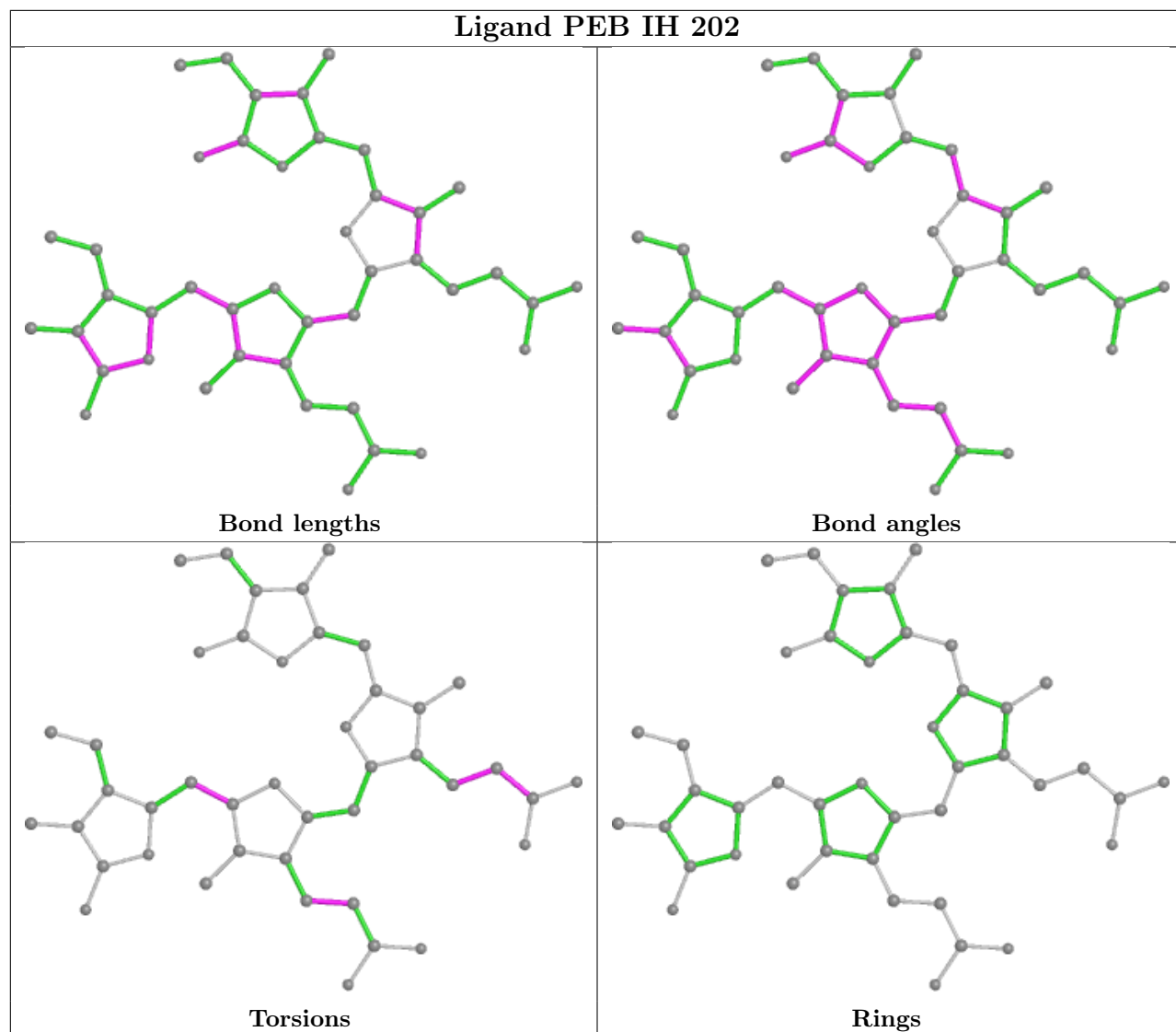


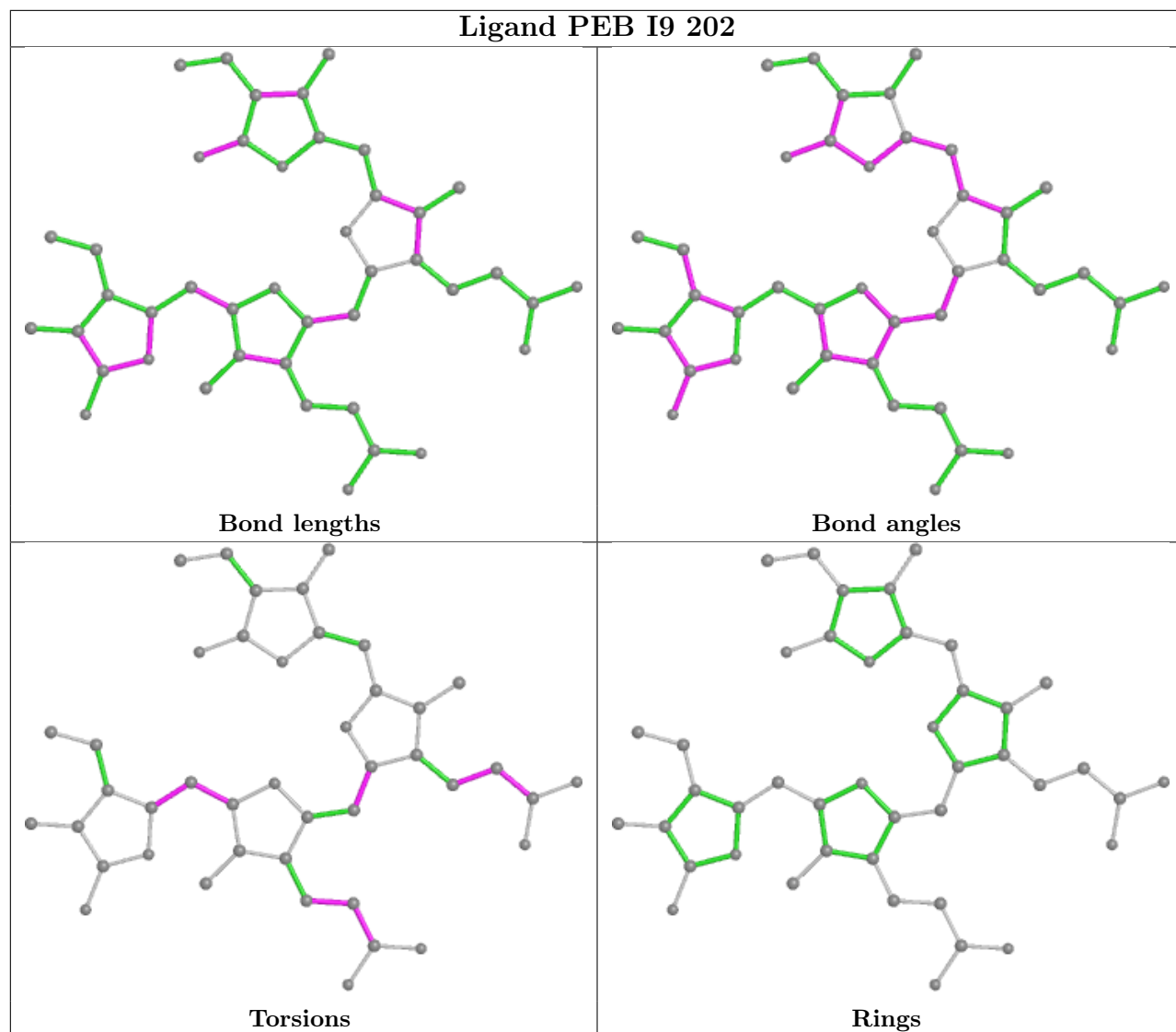


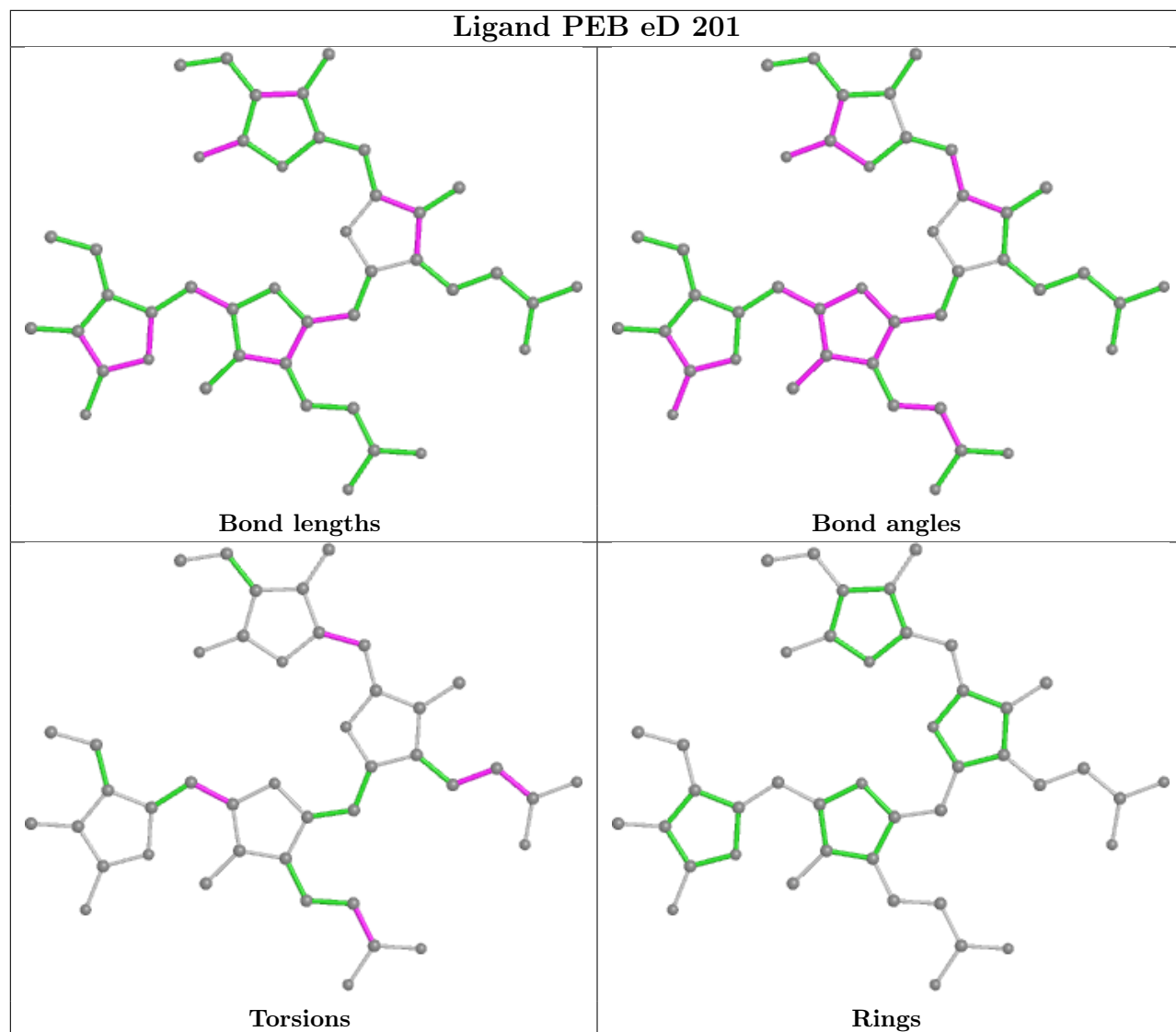


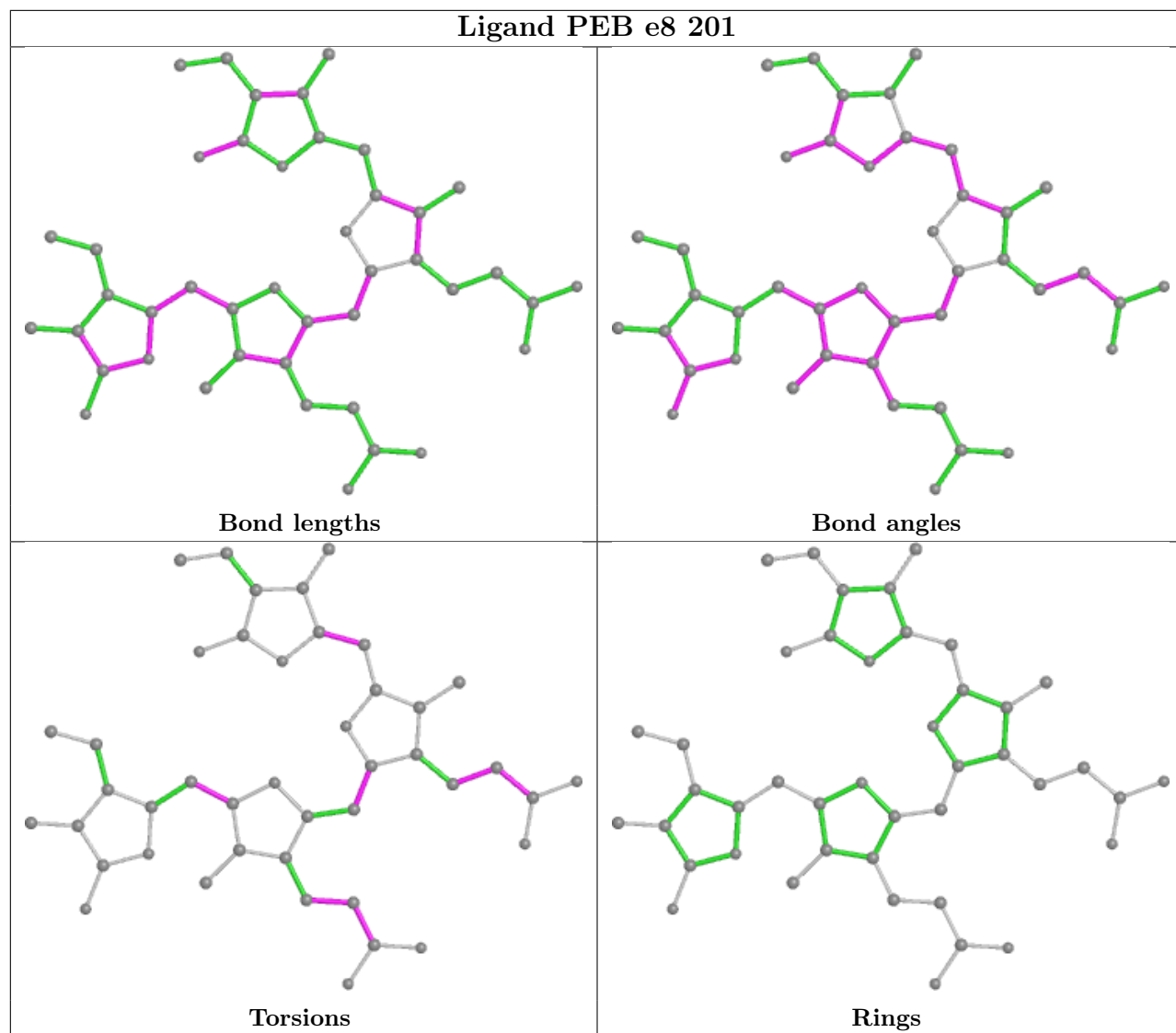


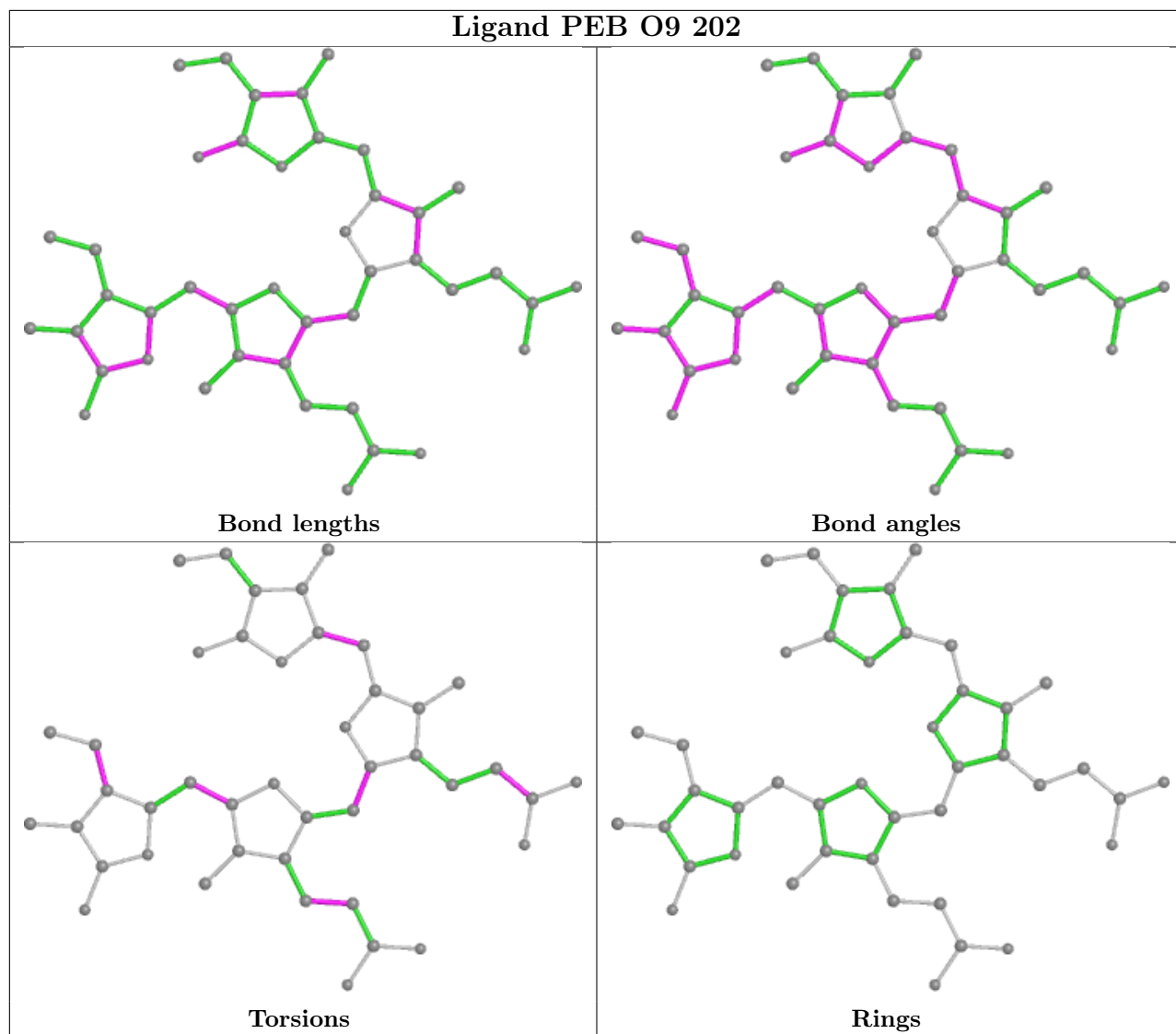


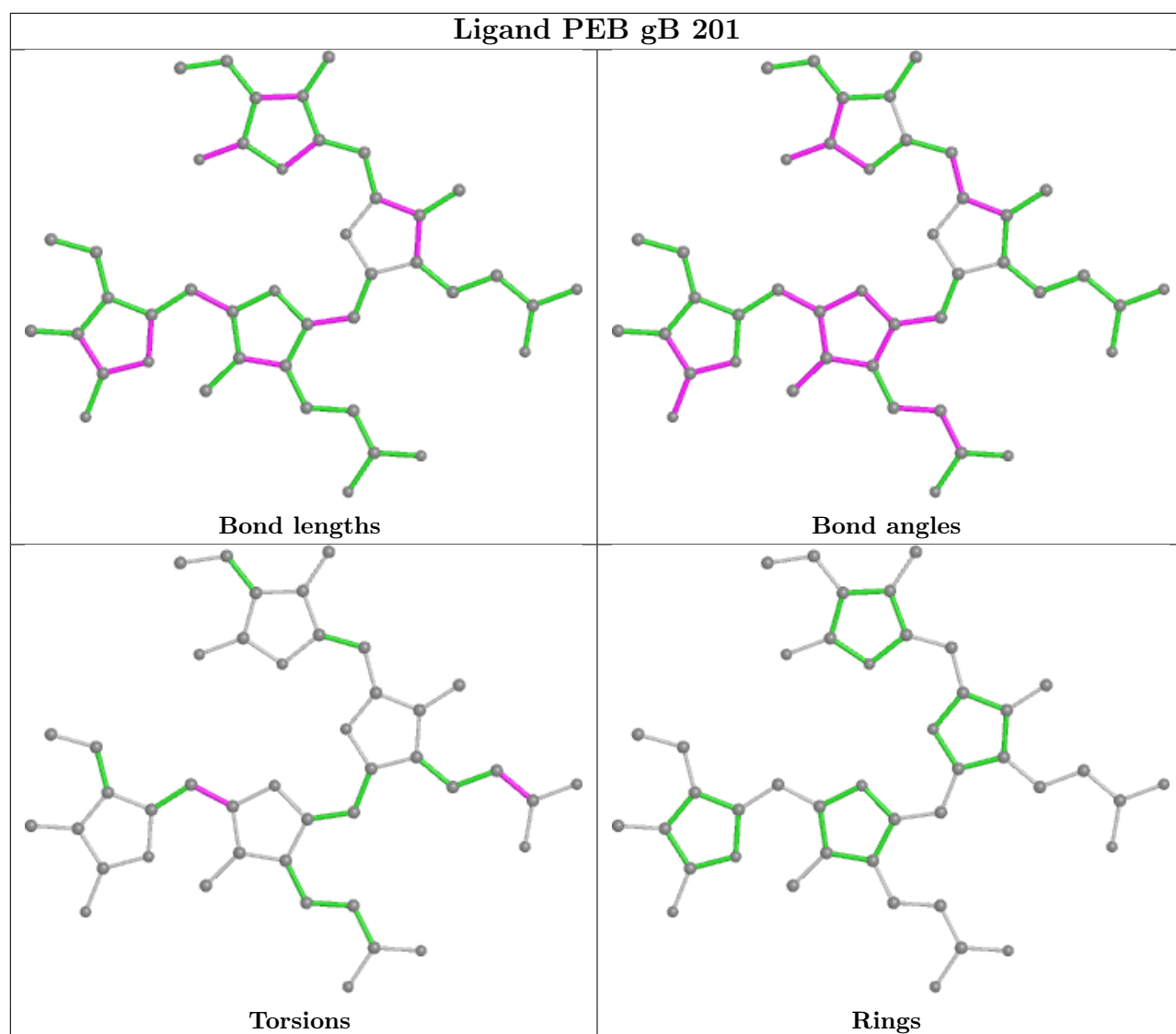












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

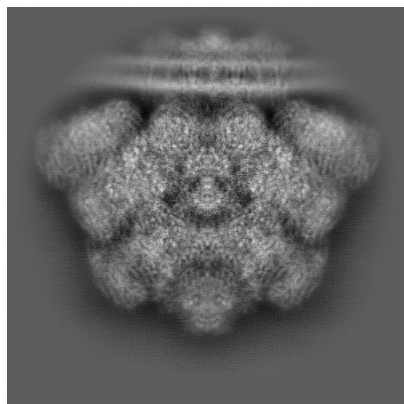
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-33605. These allow visual inspection of the internal detail of the map and identification of artifacts.

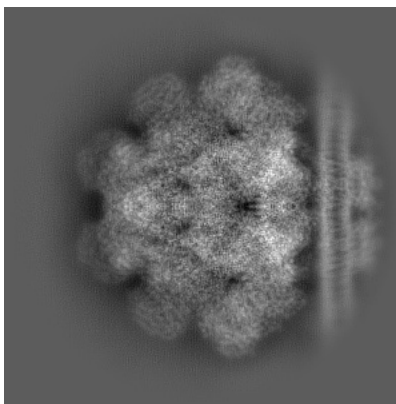
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

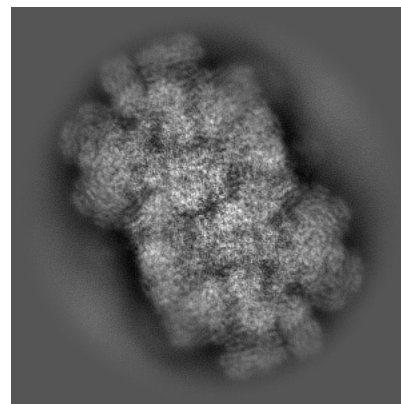
6.1.1 Primary map



X

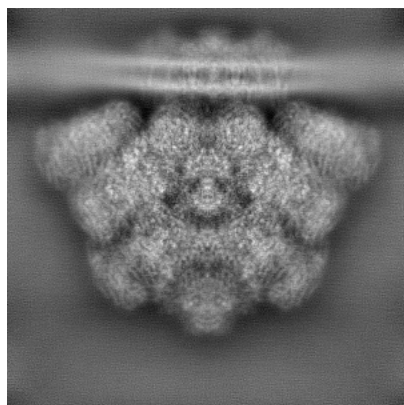


Y

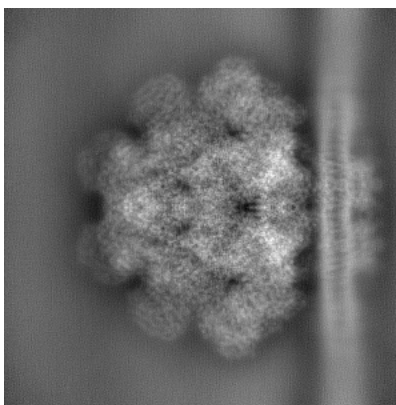


Z

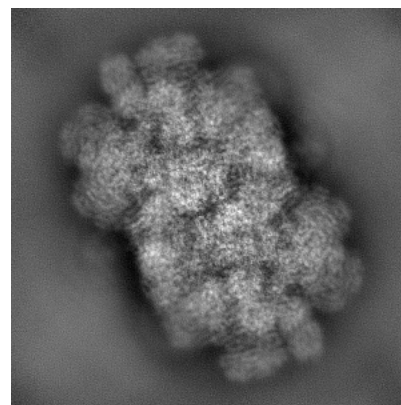
6.1.2 Raw map



X



Y

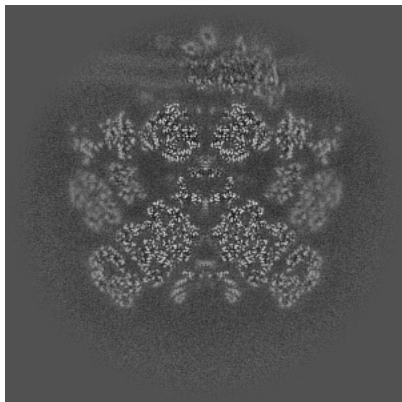


Z

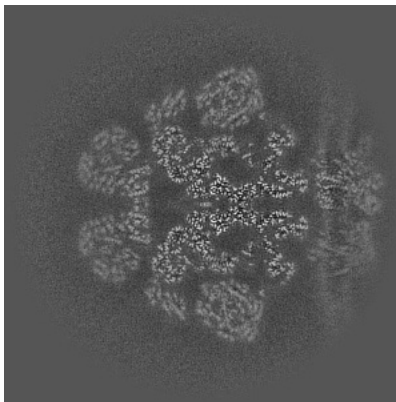
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

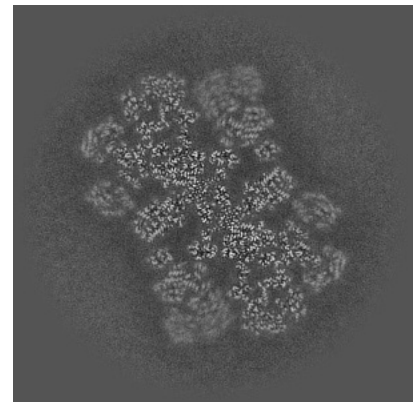
6.2.1 Primary map



X Index: 192

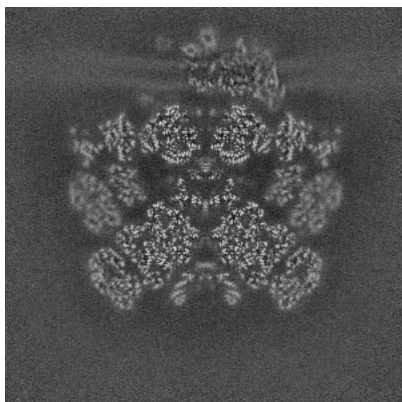


Y Index: 192

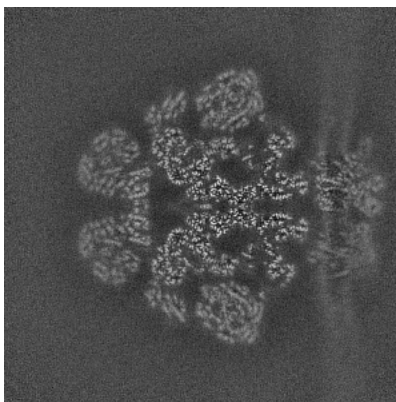


Z Index: 192

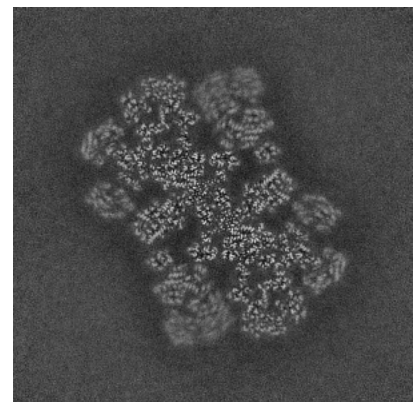
6.2.2 Raw map



X Index: 192



Y Index: 192

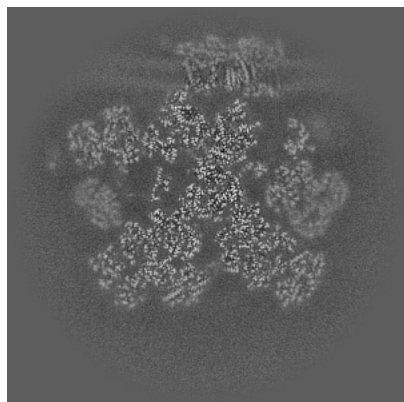


Z Index: 192

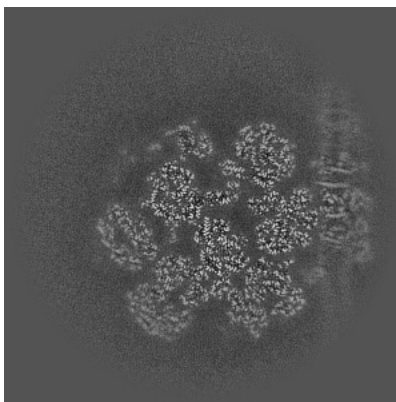
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

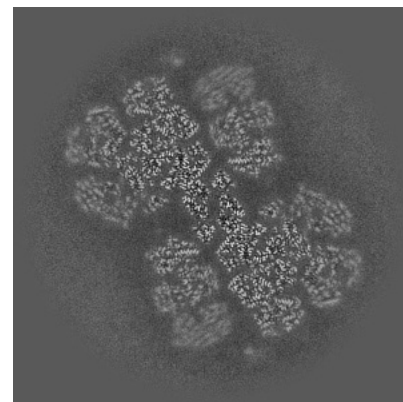
6.3.1 Primary map



X Index: 199

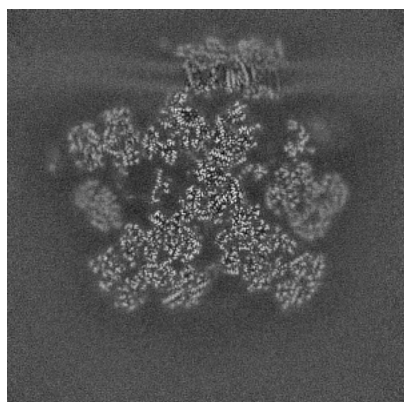


Y Index: 222

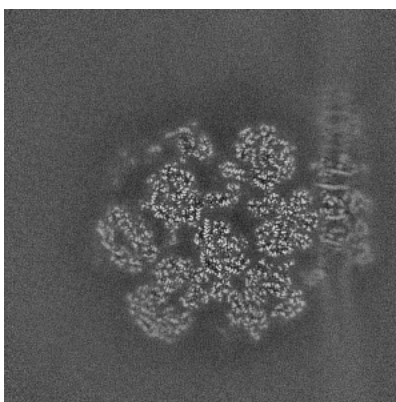


Z Index: 208

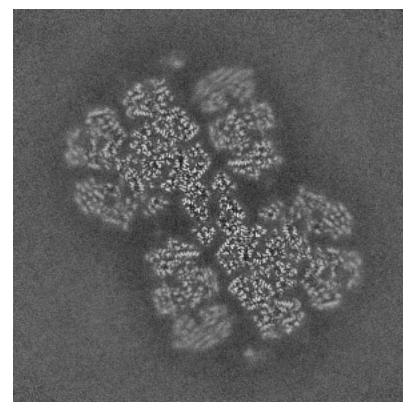
6.3.2 Raw map



X Index: 199



Y Index: 222

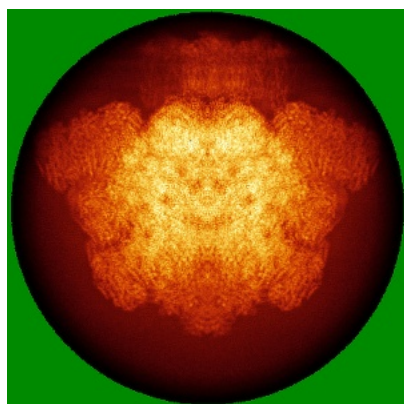


Z Index: 208

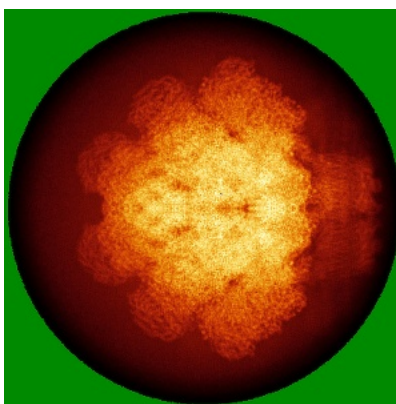
The images above show the largest variance slices of the map in three orthogonal directions.

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

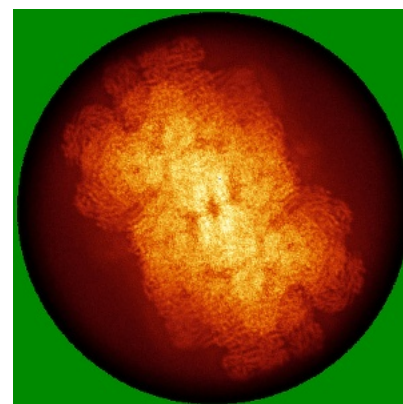
6.4.1 Primary map



X

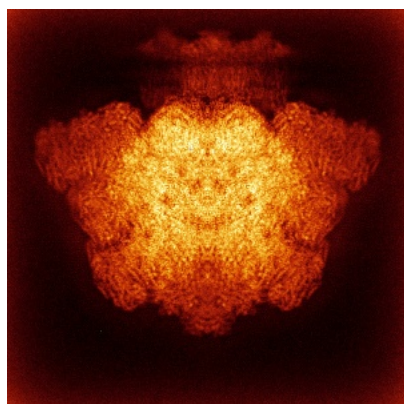


Y

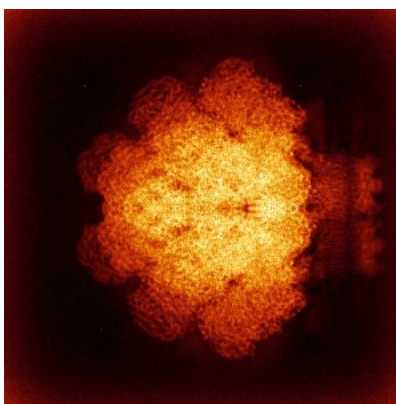


Z

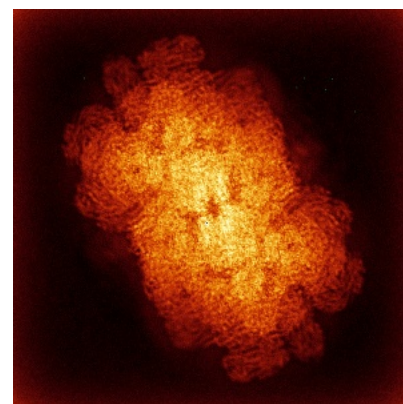
6.4.2 Raw map



X



Y

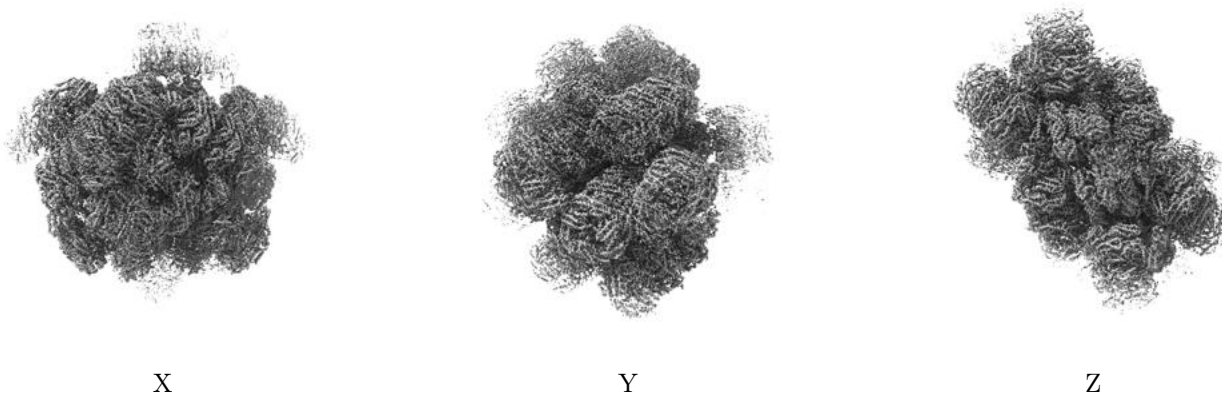


Z

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

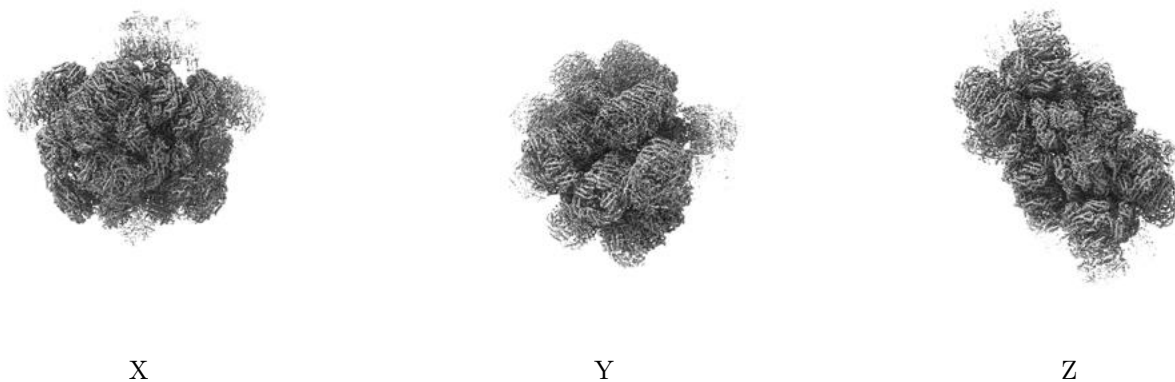
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.36. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

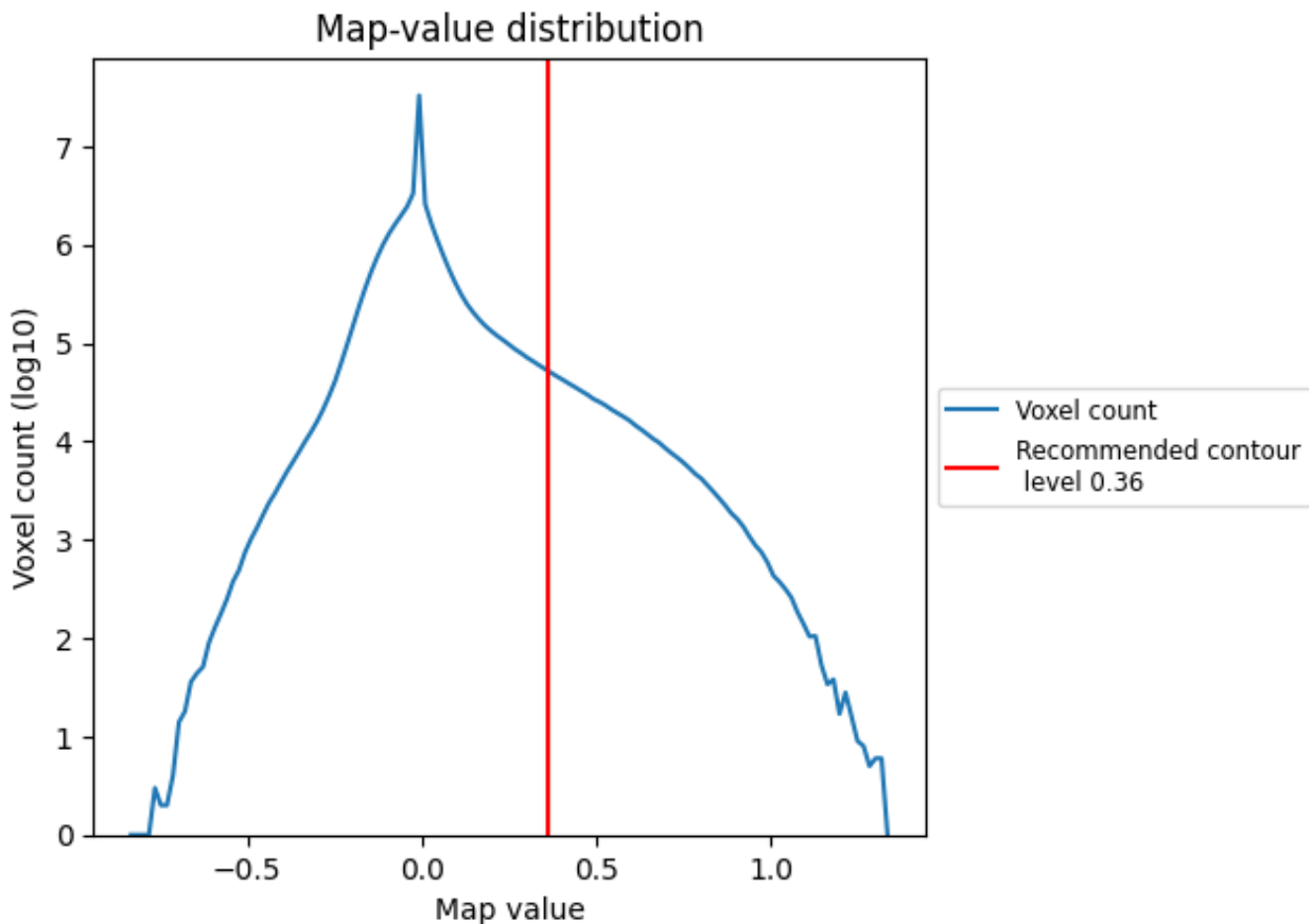
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

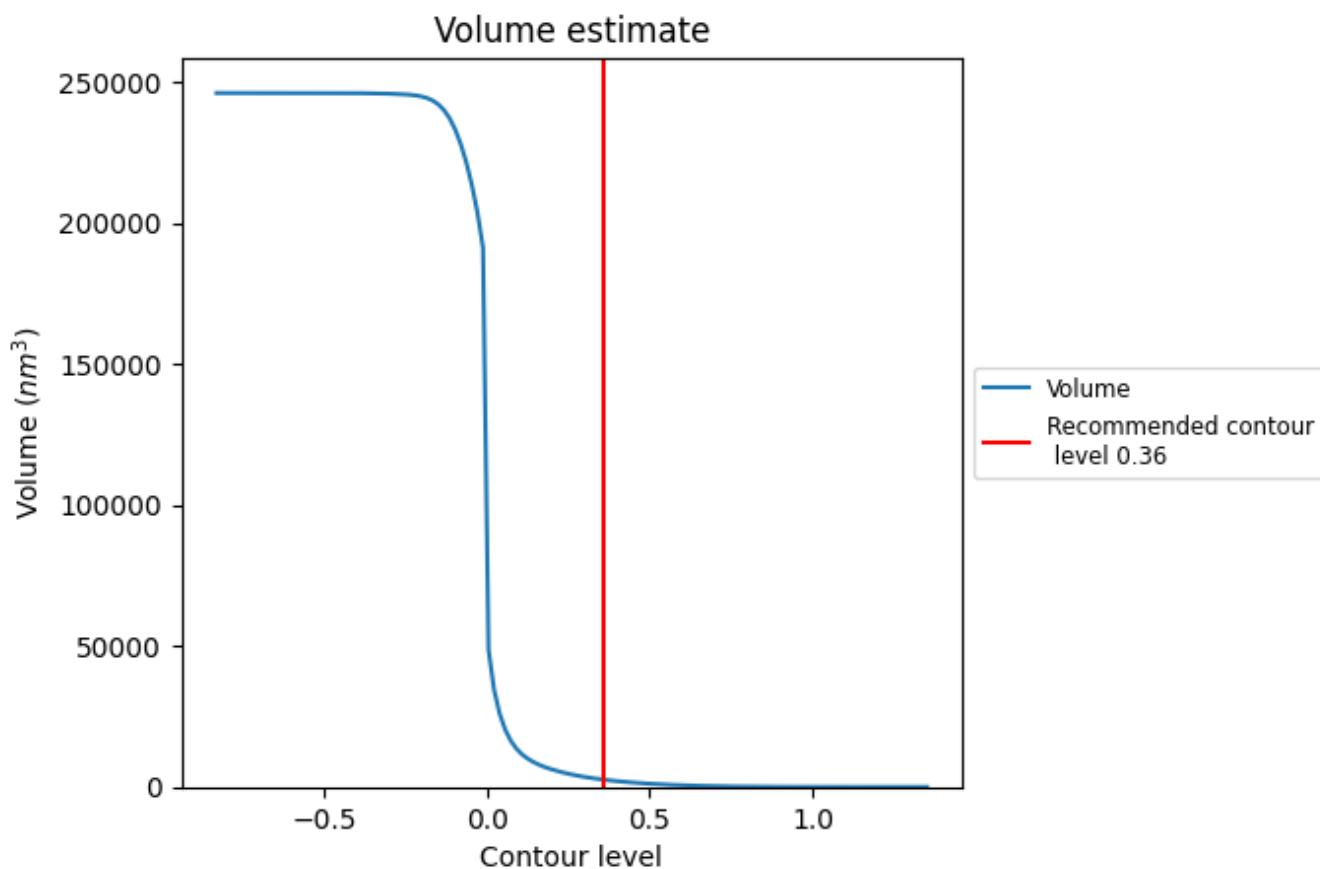
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

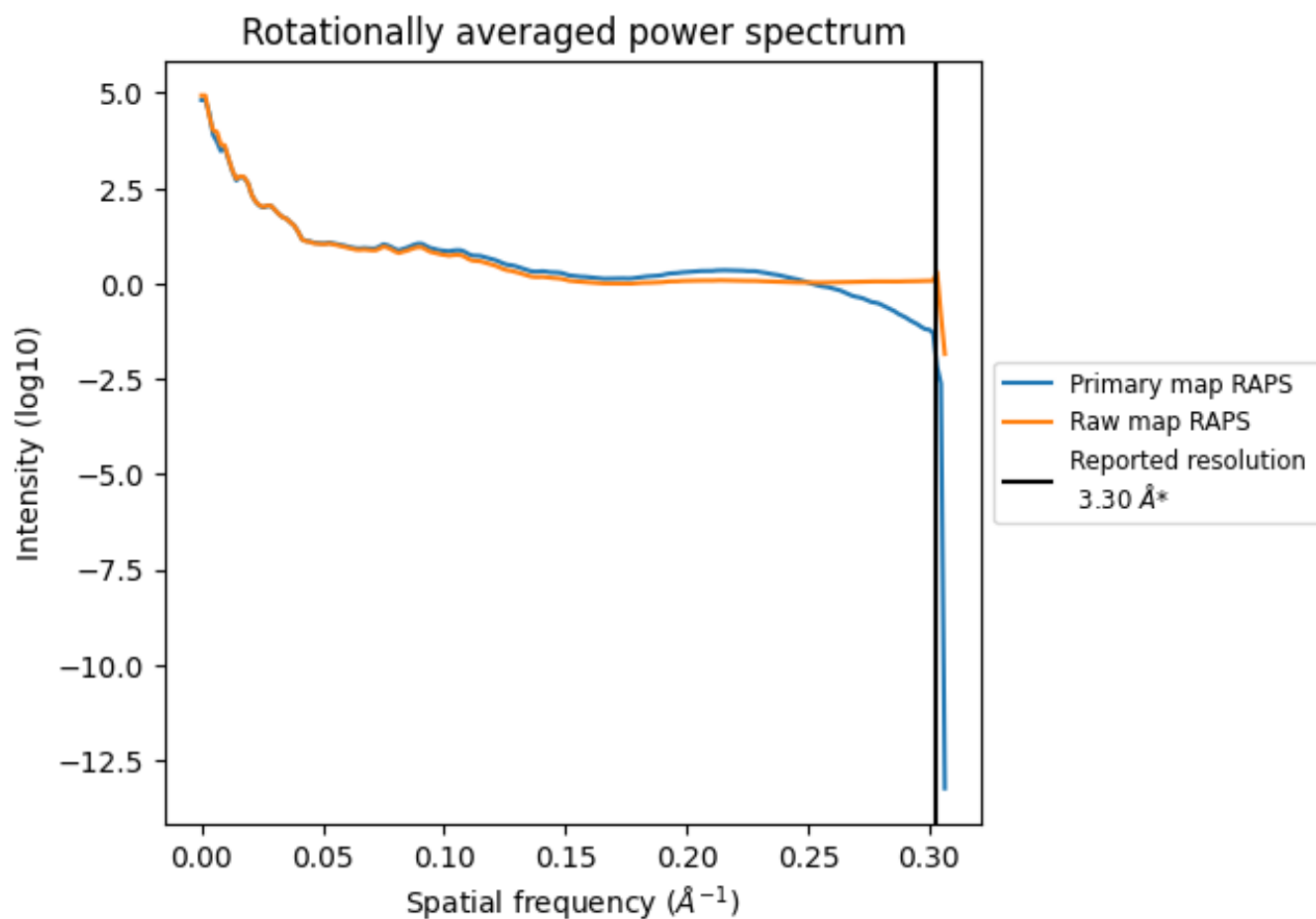
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 2558 nm^3 ; this corresponds to an approximate mass of 2311 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](#)

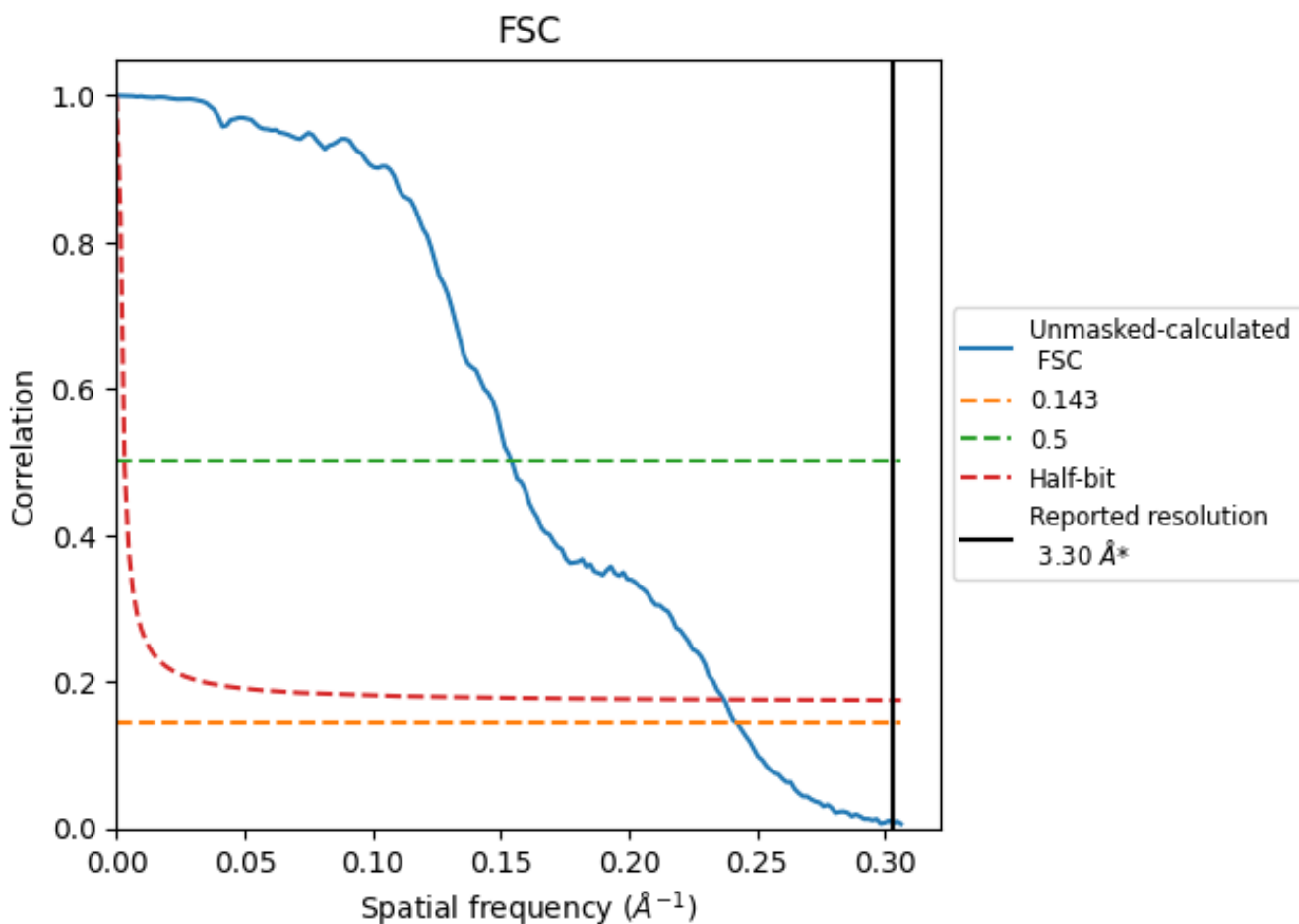


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

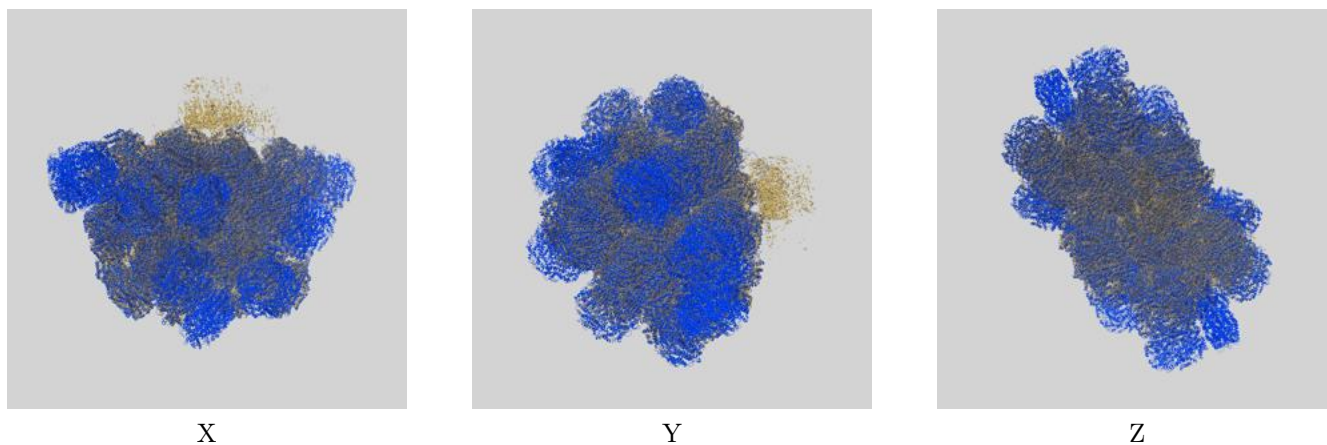
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.13	6.48	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.13 differs from the reported value 3.3 by more than 10 %

9 Map-model fit [i](#)

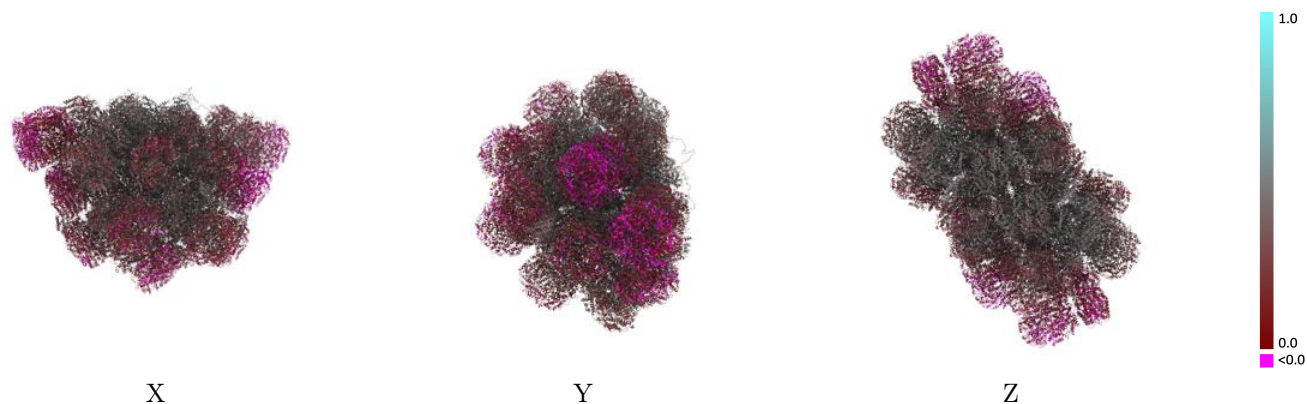
This section contains information regarding the fit between EMDB map EMD-33605 and PDB model 7Y4L. Per-residue inclusion information can be found in section 3 on page 148.

9.1 Map-model overlay [i](#)



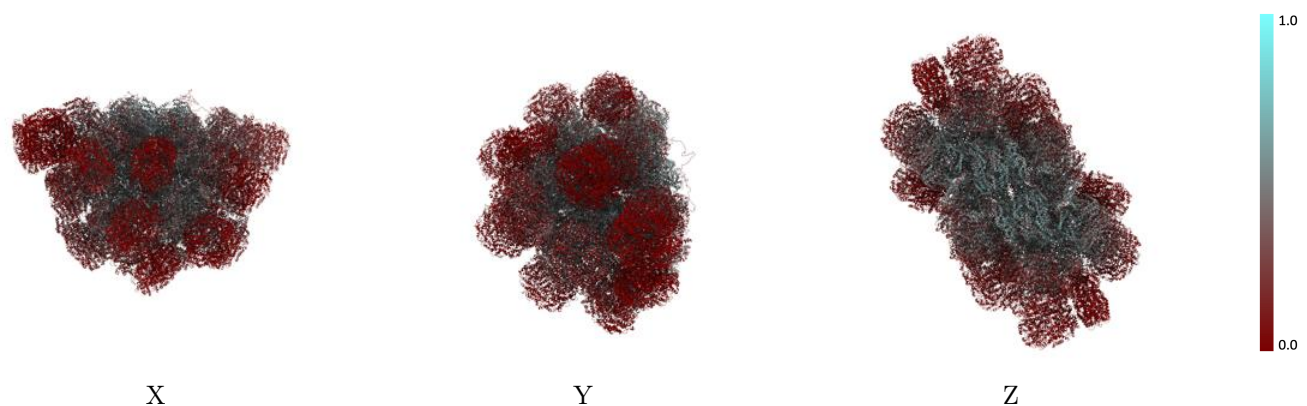
The images above show the 3D surface view of the map at the recommended contour level 0.36 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



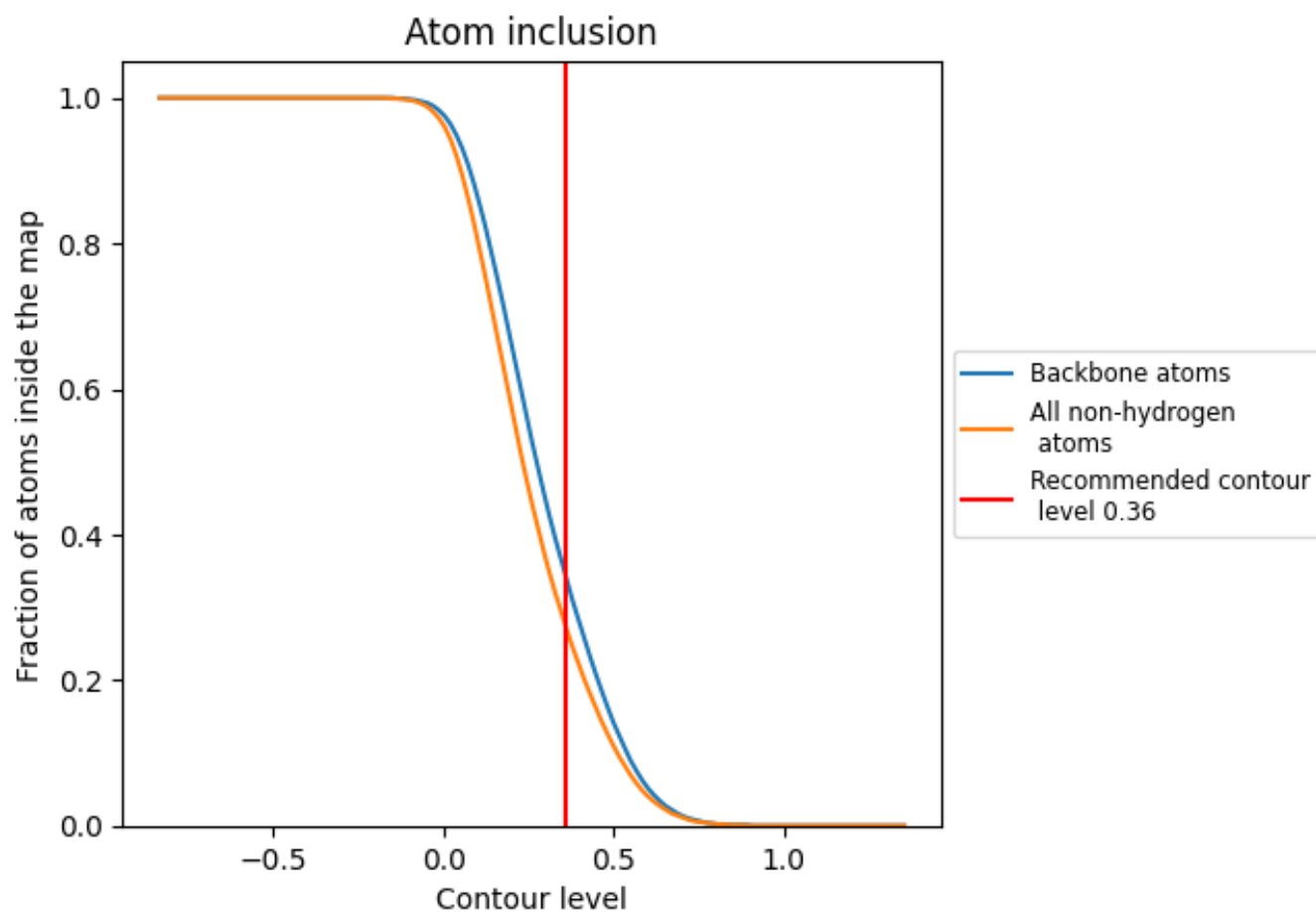
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.36).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 34% of all backbone atoms, 27% 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 (0.36) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.2730	 0.3190
23	 0.4580	 0.4200
33	 0.4920	 0.4620
43	 0.5080	 0.4620
53	 0.2940	 0.3020
63	 0.5340	 0.4730
73	 0.5280	 0.4670
A1	 0.0230	 0.1710
A2	 0.0170	 0.1260
A3	 0.4830	 0.4290
A4	 0.1620	 0.3810
A5	 0.0080	 0.1970
A6	 0.2760	 0.2730
A7	 0.5000	 0.4520
A8	 0.3350	 0.3210
A9	 0.0150	 0.2390
AA	 0.4330	 0.4300
AB	 0.2900	 0.2760
AC	 0.0140	 0.1300
AD	 0.2390	 0.2760
AE	 0.2430	 0.2860
AF	 0.3480	 0.3410
AG	 0.0130	 0.1900
AH	 0.1670	 0.3890
AI	 0.0000	 0.0670
AJ	 0.0090	 0.1900
AK	 0.0200	 0.1620
B1	 0.0340	 0.1590
B2	 0.3760	 0.3580
B3	 0.5560	 0.4400
B4	 0.3850	 0.4520
B5	 0.1990	 0.3100
B6	 0.5330	 0.4150
B7	 0.4670	 0.4480
B8	 0.3630	 0.3650























































































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Chain	Atom inclusion	Q-score
B9	0.0380	0.3050
BA	0.3690	0.4570
BB	0.5370	0.4270
BC	0.3710	0.3570
BD	0.4870	0.4010
BE	0.5020	0.4220
BF	0.3810	0.3810
BG	0.0070	0.2120
BH	0.3900	0.4590
BI	0.0000	0.1260
BJ	0.2010	0.3100
BK	0.0420	0.1620
C1	0.0720	0.2500
C2	0.2230	0.2830
C3	0.5200	0.4040
C4	0.4620	0.4560
C5	0.2710	0.3700
C6	0.5500	0.4090
C7	0.3760	0.4080
C8	0.3520	0.3130
C9	0.0140	0.2000
CA	0.3210	0.3990
CB	0.5500	0.4160
CC	0.2180	0.2850
CD	0.4800	0.3840
CE	0.4870	0.3960
CF	0.3440	0.3220
CG	0.0370	0.2420
CH	0.4760	0.4610
CI	0.0000	0.0680
CJ	0.2710	0.3640
CK	0.0760	0.2500
D1	0.0710	0.2850
D2	0.2400	0.2940
D3	0.5410	0.4050
D4	0.3920	0.4340
D5	0.3230	0.3890
D6	0.5350	0.4490
D7	0.4720	0.4520
D8	0.3450	0.3230
D9	0.0190	0.2720
DA	0.4490	0.4680

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Chain	Atom inclusion	Q-score
DB	 0.5370	 0.4540
DC	 0.2210	 0.2940
DD	 0.4930	 0.4200
DE	 0.5050	 0.4280
DF	 0.3480	 0.3290
DG	 0.0550	 0.3000
DH	 0.4010	 0.4400
DI	 0.0000	 0.1170
DJ	 0.3170	 0.3900
DK	 0.0710	 0.2860
E1	 0.0360	 0.2260
E2	 0.4710	 0.4130
E3	 0.5120	 0.4130
E4	 0.4140	 0.4260
E5	 0.2770	 0.3790
E6	 0.5200	 0.3920
E7	 0.3540	 0.3880
E8	 0.4120	 0.3570
E9	 0.0380	 0.2580
EA	 0.4090	 0.4230
EB	 0.5200	 0.3880
EC	 0.4860	 0.4080
ED	 0.4960	 0.4060
EE	 0.4970	 0.4010
EF	 0.3970	 0.3620
EG	 0.0040	 0.2170
EH	 0.4000	 0.4220
EI	 0.0000	 0.1420
EJ	 0.2900	 0.3770
EK	 0.0290	 0.2090
F1	 0.0260	 0.1750
F2	 0.3720	 0.3970
F3	 0.5320	 0.4560
F4	 0.5070	 0.4630
F5	 0.2960	 0.3470
F6	 0.5320	 0.4190
F7	 0.4290	 0.4180
F8	 0.4870	 0.4290
F9	 0.1170	 0.3560
FA	 0.3620	 0.4310
FB	 0.5270	 0.4130
FC	 0.3780	 0.3970

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Chain	Atom inclusion	Q-score
FD	0.4810	0.4080
FE	0.4820	0.4100
FF	0.4740	0.4230
FG	0.0280	0.2640
FH	0.5010	0.4620
FI	0.0090	0.2770
FJ	0.2910	0.3630
FK	0.0270	0.1610
G1	0.0420	0.2280
G2	0.2910	0.2940
G3	0.5540	0.4330
G4	0.3640	0.4180
G5	0.1710	0.3100
G6	0.5470	0.4230
G7	0.3520	0.3790
G8	0.4680	0.3740
G9	0.0590	0.3090
GA	0.3810	0.4520
GB	0.5400	0.4280
GC	0.2850	0.2860
GD	0.5580	0.4340
GE	0.5510	0.4300
GF	0.4620	0.3600
GG	0.0830	0.3050
GH	0.3610	0.4090
GI	0.0030	0.1960
GJ	0.1780	0.3150
GK	0.0450	0.2290
H1	0.1290	0.3280
H2	0.3590	0.3440
H3	0.5290	0.4400
H4	0.3890	0.4520
H5	0.2230	0.2940
H6	0.5240	0.4270
H7	0.3510	0.4030
H8	0.4500	0.3630
H9	0.0460	0.2850
HA	0.3920	0.4530
HB	0.5240	0.4230
HC	0.3510	0.3290
HD	0.5170	0.4350
HE	0.5210	0.4330

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Chain	Atom inclusion	Q-score
HF	0.4440	0.3640
HG	0.0720	0.3130
HH	0.3830	0.4480
HI	0.0010	0.1820
HJ	0.2340	0.2940
HK	0.1310	0.3340
I1	0.0340	0.1720
I2	0.3960	0.3210
I3	0.5630	0.4590
I4	0.4230	0.4480
I5	0.3760	0.3910
I6	0.4850	0.3640
I7	0.4430	0.4300
I8	0.4650	0.4120
I9	0.0510	0.3070
IA	0.4960	0.4690
IB	0.4940	0.3680
IC	0.3840	0.3210
ID	0.5200	0.4030
IE	0.5220	0.4060
IF	0.4670	0.4050
IG	0.0460	0.2790
IH	0.4140	0.4410
II	0.0060	0.1600
IJ	0.3770	0.3940
IK	0.0370	0.1700
J1	0.0250	0.1600
J2	0.3380	0.3010
J3	0.5190	0.4390
J4	0.4410	0.4450
J5	0.1400	0.2560
J6	0.4970	0.3750
J7	0.5210	0.4680
J8	0.4300	0.4120
J9	0.0390	0.3360
JA	0.4950	0.4660
JB	0.4870	0.3740
JC	0.3460	0.3210
JD	0.5170	0.3800
JE	0.5170	0.3870
JF	0.4270	0.4090
JG	0.0110	0.2170

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Chain	Atom inclusion	Q-score
JH	0.4280	0.4390
JI	0.0000	0.1690
JJ	0.1430	0.2390
JK	0.0220	0.1630
K1	0.0400	0.1870
K2	0.3430	0.3590
K3	0.5080	0.4270
K4	0.4570	0.4700
K5	0.1360	0.2850
K6	0.4840	0.3430
K7	0.5290	0.4600
K8	0.4060	0.3570
K9	0.0210	0.2760
KA	0.3040	0.4210
KB	0.4780	0.3410
KC	0.3430	0.3570
KD	0.4530	0.3580
KE	0.4390	0.3350
KF	0.3970	0.3530
KG	0.0150	0.2230
KH	0.4750	0.4780
KI	0.0000	0.0900
KJ	0.1480	0.2880
KK	0.0400	0.1960
L1	0.0730	0.2700
L2	0.4340	0.3710
L3	0.5780	0.4490
L4	0.4940	0.4820
L5	0.1660	0.2770
L6	0.4780	0.3410
L7	0.4670	0.4440
L8	0.4630	0.3800
L9	0.0480	0.3190
LA	0.2260	0.3790
LB	0.4690	0.3360
LC	0.4400	0.3630
LD	0.4900	0.3760
LE	0.4860	0.3760
LF	0.4610	0.3700
LG	0.1260	0.3510
LH	0.4980	0.4850
LI	0.0000	0.1580

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Chain	Atom inclusion	Q-score
LJ	0.1710	0.2790
LK	0.0680	0.2670
M1	0.2830	0.3300
M2	0.2480	0.2630
M3	0.5060	0.4200
M4	0.5250	0.4820
M5	0.2090	0.2910
M6	0.5100	0.4020
M7	0.5120	0.4550
M8	0.2270	0.2690
M9	0.0890	0.3430
MA	0.3360	0.4050
MB	0.5330	0.4140
MC	0.2360	0.2590
MD	0.5160	0.3960
ME	0.5200	0.3960
MF	0.2490	0.2730
MG	0.1300	0.3430
MH	0.5310	0.4860
MI	0.0430	0.2350
MJ	0.2230	0.3080
MK	0.2860	0.3300
N1	0.3730	0.3770
N2	0.2590	0.2790
N3	0.5330	0.4510
N4	0.5440	0.4900
N5	0.0010	0.1170
N6	0.5110	0.3900
N7	0.4730	0.4480
N8	0.2470	0.3000
N9	0.0130	0.2110
NA	0.4310	0.4560
NB	0.5130	0.3950
NC	0.2460	0.2860
ND	0.4890	0.3990
NE	0.4700	0.3720
NF	0.2620	0.3180
NG	0.0110	0.2020
NH	0.5480	0.4940
NI	0.0000	0.0690
NJ	0.0020	0.0980
NK	0.3740	0.3760





















































































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Chain	Atom inclusion	Q-score
O1	0.4420	0.3940
O2	0.1540	0.2440
O3	0.5470	0.4400
O4	0.3440	0.4200
O5	0.0020	0.1040
O6	0.4320	0.3810
O7	0.3880	0.4060
O8	0.3070	0.3150
O9	0.0400	0.3000
OA	0.3650	0.4390
OB	0.4380	0.3870
OC	0.1390	0.2530
OD	0.4410	0.3990
OE	0.4490	0.4000
OF	0.3180	0.3250
OG	0.0190	0.2210
OH	0.3660	0.4230
OI	0.0000	0.1680
OJ	0.0020	0.1230
OK	0.4310	0.3810
P1	0.3800	0.3700
P2	0.2890	0.3610
P3	0.5470	0.4290
P4	0.2770	0.4160
P5	0.0070	0.1840
P6	0.4370	0.3900
P7	0.4740	0.4540
P8	0.3250	0.3410
P9	0.0180	0.2110
PA	0.4430	0.4460
PB	0.4540	0.3980
PC	0.2960	0.3720
PD	0.4690	0.4330
PE	0.4750	0.4320
PF	0.3430	0.3620
PG	0.0330	0.2480
PH	0.3090	0.4210
PI	0.0000	0.0730
PJ	0.0060	0.1880
PK	0.3830	0.3730
Q1	0.4490	0.4200
Q2	0.1750	0.2560





















































































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Chain	Atom inclusion	Q-score
Q3	 0.5790	 0.4620
Q4	 0.3130	 0.4050
Q5	 0.0040	 0.2180
Q6	 0.4900	 0.4110
Q7	 0.3580	 0.3930
Q8	 0.3390	 0.3600
Q9	 0.0090	 0.2610
QA	 0.3920	 0.4390
QB	 0.4880	 0.4120
QC	 0.1760	 0.2630
QD	 0.3760	 0.3570
QE	 0.3850	 0.3540
QF	 0.3390	 0.3500
QG	 0.0660	 0.2920
QH	 0.3070	 0.3980
QI	 0.0000	 0.1280
QJ	 0.0050	 0.1970
QK	 0.4390	 0.4180
R1	 0.4120	 0.4090
R2	 0.1000	 0.2220
R3	 0.5360	 0.4360
R4	 0.3960	 0.4410
R5	 0.0030	 0.1330
R6	 0.5040	 0.4450
R7	 0.4280	 0.4280
R8	 0.3580	 0.3980
R9	 0.0470	 0.2490
RA	 0.2230	 0.3350
RB	 0.5200	 0.4460
RC	 0.0890	 0.2080
RD	 0.3780	 0.3760
RE	 0.3930	 0.3790
RF	 0.3550	 0.3850
RG	 0.0220	 0.2090
RH	 0.3940	 0.4400
RI	 0.0000	 0.1620
RJ	 0.0020	 0.1130
RK	 0.4030	 0.4080
S1	 0.4300	 0.4090
S2	 0.1950	 0.2700
S3	 0.5810	 0.4490
S4	 0.2520	 0.4060

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Chain	Atom inclusion	Q-score
S5	 0.0030	 0.0870
S6	 0.4800	 0.4000
S7	 0.3600	 0.3900
S8	 0.4030	 0.4050
S9	 0.1040	 0.3480
SA	 0.5040	 0.4760
SB	 0.4720	 0.3990
SC	 0.2080	 0.2720
SD	 0.3730	 0.3570
SE	 0.3790	 0.3540
SF	 0.4090	 0.3880
SG	 0.0370	 0.2640
SH	 0.2420	 0.3970
SI	 0.0070	 0.2910
SJ	 0.0040	 0.1090
SK	 0.4290	 0.4110
T1	 0.4840	 0.4290
T2	 0.2210	 0.3060
T3	 0.5560	 0.4280
T4	 0.3650	 0.4420
T5	 0.0040	 0.1130
T6	 0.4670	 0.4040
T7	 0.3630	 0.4070
T8	 0.4240	 0.4200
T9	 0.0720	 0.3000
TA	 0.4870	 0.4650
TB	 0.4540	 0.4010
TC	 0.2190	 0.3090
TD	 0.4550	 0.4140
TE	 0.4670	 0.4150
TF	 0.4230	 0.4150
TG	 0.0780	 0.3140
TH	 0.3730	 0.4460
TI	 0.0010	 0.1930
TJ	 0.0040	 0.1110
TK	 0.4910	 0.4330
U1	 0.3270	 0.3520
U2	 0.1090	 0.2100
U3	 0.5910	 0.4680
U4	 0.3750	 0.4470
U5	 0.0200	 0.2490
U6	 0.4980	 0.4100





















































































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Chain	Atom inclusion	Q-score
U7	█ 0.4530	█ 0.4320
U8	█ 0.3980	█ 0.3830
U9	█ 0.0390	█ 0.2800
UA	█ 0.2940	█ 0.3960
UB	█ 0.4900	█ 0.4040
UC	█ 0.1070	█ 0.2060
UD	█ 0.3760	█ 0.3470
UE	█ 0.3830	█ 0.3480
UF	█ 0.4070	█ 0.3860
UG	█ 0.0770	█ 0.3100
UH	█ 0.3900	█ 0.4420
UI	█ 0.0010	█ 0.2030
UJ	█ 0.0140	█ 0.2350
UK	█ 0.3370	█ 0.3570
V1	█ 0.2940	█ 0.3420
V2	█ 0.1140	█ 0.2080
V3	█ 0.5190	█ 0.4390
V4	█ 0.2960	█ 0.4240
V5	█ 0.0010	█ 0.1090
V6	█ 0.5100	█ 0.4490
V7	█ 0.5240	█ 0.4700
V8	█ 0.3210	█ 0.3420
V9	█ 0.0520	█ 0.3030
VA	█ 0.2230	█ 0.3580
VB	█ 0.5190	█ 0.4470
VC	█ 0.1230	█ 0.2340
VD	█ 0.3410	█ 0.3380
VE	█ 0.3450	█ 0.3340
VF	█ 0.3260	█ 0.3450
VG	█ 0.0460	█ 0.2830
VH	█ 0.3090	█ 0.4230
VI	█ 0.0060	█ 0.1420
VJ	█ 0.0020	█ 0.0970
VK	█ 0.2890	█ 0.3450
W1	█ 0.3070	█ 0.3180
W2	█ 0.1140	█ 0.2290
W3	█ 0.5590	█ 0.4510
W4	█ 0.5000	█ 0.4810
W5	█ 0.0000	█ 0.1130
W6	█ 0.4700	█ 0.3920
W7	█ 0.5340	█ 0.4670
W8	█ 0.3270	█ 0.3270

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Chain	Atom inclusion	Q-score
W9	 0.0390	 0.3280
WA	 0.2110	 0.3810
WB	 0.4830	 0.3920
WC	 0.1150	 0.2200
WD	 0.4290	 0.3700
WE	 0.4230	 0.3670
WF	 0.3460	 0.3450
WG	 0.0110	 0.2070
WH	 0.4970	 0.4790
WI	 0.0000	 0.1600
WJ	 0.0010	 0.1000
WK	 0.3090	 0.3300
X1	 0.3810	 0.3690
X2	 0.2280	 0.3540
X3	 0.5520	 0.4890
X4	 0.4240	 0.4570
X5	 0.0060	 0.1380
X6	 0.5310	 0.4690
X7	 0.4650	 0.4460
X8	 0.4320	 0.4240
X9	 0.0270	 0.2770
XA	 0.2860	 0.3740
XB	 0.5340	 0.4670
XC	 0.2340	 0.3580
XD	 0.4770	 0.4550
XE	 0.4890	 0.4540
XF	 0.4470	 0.4270
XG	 0.0200	 0.2190
XH	 0.4190	 0.4560
XI	 0.0010	 0.1000
XJ	 0.0040	 0.1380
XK	 0.3830	 0.3730
Y1	 0.1000	 0.2730
Y2	 0.1730	 0.2900
Y3	 0.3000	 0.3740
Y4	 0.4610	 0.4670
Y5	 0.0040	 0.1990
Y6	 0.4700	 0.4020
Y7	 0.4570	 0.4350
Y8	 0.0240	 0.0880
Y9	 0.0460	 0.3060
YA	 0.3620	 0.4350

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Chain	Atom inclusion	Q-score
YB	█ 0.4730	█ 0.4030
YC	█ 0.1600	█ 0.2910
YD	█ 0.4900	█ 0.4360
YE	█ 0.4930	█ 0.4320
YF	█ 0.0410	█ 0.0960
YG	█ 0.1390	█ 0.3500
YH	█ 0.4680	█ 0.4690
YI	█ 0.0010	█ 0.1760
YJ	█ 0.0080	█ 0.2050
YK	█ 0.1000	█ 0.2720
Z2	█ 0.0670	█ 0.1710
Z3	█ 0.4550	█ 0.4420
Z4	█ 0.4610	█ 0.4760
Z6	█ 0.4930	█ 0.4260
Z8	█ 0.0430	█ 0.0910
Z9	█ 0.0940	█ 0.3250
ZA	█ 0.0130	█ 0.3860
ZB	█ 0.4860	█ 0.4280
ZC	█ 0.0580	█ 0.1830
ZD	█ 0.4460	█ 0.3780
ZE	█ 0.4400	█ 0.3680
ZF	█ 0.0530	█ 0.1170
ZG	█ 0.1450	█ 0.3230
ZH	█ 0.4670	█ 0.4750
ZI	█ 0.0360	█ 0.2190
a2	█ 0.0660	█ 0.1980
a3	█ 0.5050	█ 0.4670
a4	█ 0.1870	█ 0.3830
a6	█ 0.5210	█ 0.4560
a8	█ 0.0820	█ 0.1670
aA	█ 0.4430	█ 0.4550
aB	█ 0.5360	█ 0.4570
aC	█ 0.0530	█ 0.1990
aD	█ 0.3840	█ 0.3650
aE	█ 0.3970	█ 0.3640
aF	█ 0.1060	█ 0.1710
aH	█ 0.1860	█ 0.3810
b2	█ 0.0150	█ 0.0830
b3	█ 0.4840	█ 0.4210
b4	█ 0.4710	█ 0.4740
b6	█ 0.2010	█ 0.1880
b7	█ 0.4500	█ 0.4390

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Chain	Atom inclusion	Q-score
b8	0.1340	0.2420
bA	0.2020	0.3110
bB	0.2070	0.1860
bC	0.0110	0.0960
bD	0.2460	0.2580
bE	0.2440	0.2530
bF	0.1550	0.2500
bH	0.4760	0.4730
c2	0.0250	0.1330
c3	0.4840	0.4260
c4	0.0870	0.3240
c6	0.1760	0.1460
c8	0.0800	0.1950
cA	0.2080	0.3720
cB	0.1670	0.1660
cC	0.0300	0.1250
cD	0.2400	0.2850
cE	0.2460	0.2890
cF	0.1050	0.1930
cH	0.0930	0.3020
d2	0.0120	0.0550
d3	0.5510	0.4110
d4	0.1290	0.3690
d5	0.3140	0.3690
d6	0.2500	0.2440
d8	0.0720	0.1930
dA	0.2630	0.3550
dB	0.2560	0.2540
dC	0.0090	0.0680
dD	0.1620	0.1940
dE	0.1590	0.1960
dF	0.0870	0.2170
dH	0.1450	0.3710
dJ	0.3240	0.3800
e1	0.4210	0.4080
e2	0.0010	0.0360
e3	0.5150	0.4000
e4	0.3170	0.4470
e6	0.3090	0.2970
e8	0.1070	0.2430
eA	0.3360	0.4270
eB	0.3440	0.3120

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Chain	Atom inclusion	Q-score
eC	0.0010	0.0460
eD	0.1840	0.1820
eE	0.1760	0.1730
eF	0.1190	0.2480
eH	0.3040	0.4390
eK	0.4130	0.4050
f2	0.0310	0.0620
f3	0.5260	0.4570
f4	0.0590	0.3000
f6	0.1850	0.1800
f8	0.1680	0.2790
fA	0.5050	0.4870
fB	0.1900	0.1820
fC	0.0290	0.0730
fD	0.1650	0.2180
fE	0.1720	0.2260
fF	0.1900	0.2830
fH	0.0610	0.2940
g2	0.0210	0.1380
g3	0.5070	0.4130
g4	0.0270	0.3020
g6	0.1610	0.1670
g8	0.1170	0.2460
gA	0.0170	0.3540
gB	0.1690	0.1560
gC	0.0200	0.1360
gD	0.2230	0.2890
gE	0.2340	0.2870
gF	0.1340	0.2400
gH	0.0380	0.2980
h2	0.0040	0.0660
h3	0.5320	0.4270
h4	0.0710	0.3280
h6	0.2460	0.2360
h8	0.0410	0.1460
hA	0.5020	0.4780
hB	0.2430	0.2300
hC	0.0020	0.0760
hD	0.1410	0.1820
hE	0.1490	0.1890
hF	0.0520	0.1620
hH	0.0720	0.3150

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Chain	Atom inclusion	Q-score
i2	0.0070	0.0520
i3	0.5520	0.4350
i4	0.1360	0.3760
i6	0.3130	0.2930
i8	0.1110	0.2090
iB	0.3150	0.2940
iC	0.0050	0.0570
iD	0.1190	0.1660
iE	0.1260	0.1680
iF	0.1260	0.2200
iH	0.1570	0.3760
j2	0.0000	0.0960
j3	0.5480	0.4320
j4	0.0720	0.3110
j6	0.2120	0.1930
j8	0.2220	0.3400
jB	0.2030	0.2070
jC	0.0000	0.0900
jD	0.1660	0.2070
jE	0.1900	0.2050
jF	0.2390	0.3450
jH	0.0770	0.3240
k2	0.0120	0.1000
k3	0.5620	0.4610
k4	0.1250	0.3510
k6	0.1920	0.1900
k8	0.0000	0.0070
kB	0.2160	0.1840
kC	0.0060	0.1050
kD	0.2720	0.2810
kE	0.2790	0.2910
kF	0.0000	0.0180
kH	0.1510	0.3350
l2	0.0000	0.0670
l3	0.5210	0.4440
l4	0.2840	0.4050
l6	0.2690	0.2870
l8	0.0000	0.0360
lB	0.2730	0.2630
lC	0.0000	0.0660
lD	0.2110	0.2410
lE	0.1920	0.2010





















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Chain	Atom inclusion	Q-score
lF	0.0010	0.0570
lH	0.2730	0.4000
m2	0.0000	0.0770
m3	0.5180	0.4310
m4	0.1680	0.3930
m6	0.3190	0.3040
m8	0.0050	0.0600
mB	0.3080	0.2990
mC	0.0000	0.0540
mD	0.1220	0.1340
mE	0.1350	0.1340
mF	0.0070	0.0510
mH	0.1880	0.3960
n3	0.5770	0.4430
n8	0.0010	0.0320
nF	0.0000	0.0520
o3	0.5080	0.4310
o8	0.0000	0.0700
oF	0.0000	0.0730
p3	0.5360	0.4520
p8	0.0050	0.0770
pF	0.0040	0.0830
q3	0.5500	0.4130
q8	0.0020	0.0930
qF	0.0020	0.0950
r3	0.5550	0.4370
r8	0.0020	0.1390
rF	0.0050	0.1430
s3	0.5720	0.4510
s8	0.0000	0.0330
sF	0.0020	0.0510
t3	0.5350	0.4320
t8	0.0000	0.0220
tF	0.0000	0.0350
u3	0.5820	0.4480
u8	0.0000	0.0130
uF	0.0000	0.0200
v3	0.5720	0.4330
v8	0.0040	0.0930
vF	0.0070	0.0940
w3	0.5910	0.4680
w8	0.1670	0.2850

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Chain	Atom inclusion	Q-score
wF	 0.1590	 0.2810
x3	 0.5350	 0.4550
x8	 0.0020	 0.0850
xF	 0.0010	 0.0760
y3	 0.5530	 0.4760
y8	 0.4000	 0.4280
yF	 0.4200	 0.4290
z3	 0.5360	 0.4830
z8	 0.3560	 0.3440
zF	 0.2710	 0.2250