



wwPDB EM Validation Summary Report ⓘ

Mar 26, 2024 – 02:14 PM JST

PDB ID : 7EZ
EMDB ID : EMD-31393
Title : Structure of the phycobilisome from the red alga *Porphyridium purpureum* in Middle Light
Authors : Ma, J.F.; Sui, S.-F.
Deposited on : 2021-06-02
Resolution : 3.00 Å (reported)
Based on initial model : 6KGX

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:

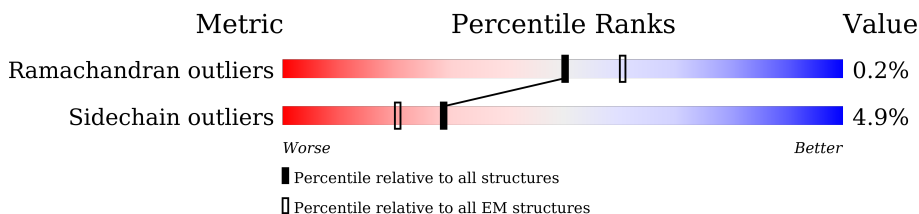
EMDB validation analysis : 0.0.1.dev70
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

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 3.00 Å.

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



Metric	Whole archive (#Entries)	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	X1	363	
1	X7	363	
1	X9	363	
1	XF	363	
1	XI	363	
1	XK	363	
2	A1	290	
2	A7	290	
2	A9	290	

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Mol	Chain	Length	Quality of chain
2	AF	290	51% 88% 11%
2	AI	290	52% 88% 11%
2	AK	290	88% 87% 11%
3	B1	232	21% 94%
3	B7	232	93% 6%
3	B9	232	93% 6%
3	BF	232	10% 99%
3	BI	232	10% 98%
3	BK	232	21% 94%
4	C1	162	74% 94% 6%
4	C7	162	93% 7%
4	C9	162	93% 7%
4	CF	162	99%
4	CI	162	99%
4	CK	162	77% 94% 6%
4	E1	162	7% 95% 5%
4	E7	162	94% 6%
4	E9	162	94% 6%
4	EF	162	99%
4	EI	162	99%
4	EK	162	7% 95% 5%
4	G1	162	53% 98%
4	G7	162	94% 6%
4	G9	162	94% 6%
4	GF	162	99%

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Mol	Chain	Length	Quality of chain
4	GI	162	99%
4	GK	162	52% 98%
4	I1	162	6% 99%
4	I7	162	93% 6%
4	I9	162	93% 6%
4	IF	162	99%
4	II	162	99%
4	IK	162	6% 99%
4	K1	162	36% 99%
4	K7	162	93% 7%
4	K9	162	93% 7%
4	KF	162	99%
4	KI	162	99%
4	KK	162	35% 98%
4	M1	162	73% 96%
4	M7	162	94% 6%
4	M9	162	94% 6%
4	MF	162	99%
4	MI	162	99%
4	MK	162	73% 96%
5	D1	172	85% 96%
5	D7	172	86% 14%
5	D9	172	86% 14%
5	DF	172	13% 99%
5	DI	172	12% 99%

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Mol	Chain	Length	Quality of chain
5	DK	172	84% 96% ..
5	F1	172	39% 94% 6% .
5	F7	172	5% 87% 13%
5	F9	172	5% 88% 12%
5	FF	172	10% 99% .
5	FI	172	9% 100%
5	FK	172	36% 93% 6% .
5	H1	172	33% 97% ..
5	H7	172	. 87% 13% .
5	H9	172	. 87% 13% .
5	HF	172	. 99% .
5	HI	172	. 99% .
5	HK	172	26% 97% ..
5	J1	172	31% 94% 6% .
5	J7	172	. 88% 12%
5	J9	172	. 88% 12%
5	JF	172	. 99% .
5	JI	172	. 99% .
5	JK	172	33% 93% 6% .
5	L1	172	10% 97% ..
5	L7	172	. 87% 13%
5	L9	172	. 87% 13%
5	LF	172	8% 98% .
5	LI	172	6% 98% .
5	LK	172	12% 97% ..

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Mol	Chain	Length	Quality of chain
5	N1	172	62% 95% 5%
5	N7	172	88% 12%
5	N9	172	88% 12%
5	NF	172	7% 98%
5	NI	172	6% 98%
5	NK	172	58% 95% 5%
6	A3	164	10% 96%
6	AA	164	100% 95% 5%
6	AC	164	100% 95%
6	AE	164	100% 95%
6	AG	164	100% 90% 9%
6	AJ	164	27% 95% 5%
6	AL	164	27% 95% 5%
6	AN	164	100% 95% 5%
6	AO	164	9% 96%
6	AQ	164	100% 90% 8%
6	B4	164	86% 89% 10%
6	BD	164	84% 89% 10%
6	C3	164	41% 95% 5%
6	CA	164	100% 95% 5%
6	CB	164	10% 99%
6	CC	164	99% 94% 5%
6	CE	164	99% 94% 5%
6	CG	164	100% 87% 11%
6	CJ	164	25% 98%

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Mol	Chain	Length	Quality of chain
6	CL	164	28% 98%
6	CM	164	11% 99%
6	CN	164	100% 95% 5%
6	CO	164	41% 95% 5%
6	CQ	164	100% 87% 11%
6	D4	164	55% 85% 14%
6	DD	164	55% 85% 14%
6	E3	164	48% 93% 7%
6	EA	164	100% 96%
6	EB	164	34% 99%
6	EC	164	100% 93% 6%
6	EE	164	100% 93% 6%
6	EG	164	100% 88% 10%
6	EJ	164	18% 99%
6	EL	164	17% 99%
6	EM	164	32% 99%
6	EN	164	100% 96%
6	EO	164	47% 93% 7%
6	EQ	164	100% 88% 10%
6	F4	164	71% 84% 16%
6	FD	164	68% 83% 16%
6	G3	164	41% 96%
6	GA	164	100% 95% 5%
6	GB	164	42% 96%
6	GC	164	96% 93% 6%

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Mol	Chain	Length	Quality of chain
6	GE	164	98% 93% 6%
6	GG	164	100% 88% 10%
6	GJ	164	6% 94% 6%
6	GL	164	5% 95% 5%
6	GM	164	41% 96% .
6	GN	164	100% 95% 5%
6	GO	164	41% 96% .
6	GQ	164	100% 88% 10%
6	H4	164	82% 85% 14%
6	HD	164	81% 85% 15%
6	I3	164	14% 93% 7%
6	IA	164	100% 95% 5%
6	IB	164	13% 99% .
6	IC	164	99% 95% ..
6	IE	164	99% 95% ..
6	IG	164	100% 89% 9%
6	IJ	164	5% 93% 7%
6	IL	164	5% 93% 7%
6	IM	164	15% 99% .
6	IN	164	100% 95% 5%
6	IO	164	16% 93% 7%
6	IQ	164	100% 89% 9%
6	J4	164	95% 87% 13%
6	J5	164	8% 97% .
6	J8	164	8% 96% .

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Mol	Chain	Length	Quality of chain
6	JD	164	95% 87% 12%
6	K3	164	94% 6%
6	KA	164	100% 95% 5%
6	KB	164	7% 99%
6	KC	164	99% 94% 6%
6	KE	164	100% 94% 6%
6	KG	164	100% 88% 10%
6	KJ	164	12% 95% 5%
6	KL	164	12% 95% 5%
6	KM	164	6% 99%
6	KN	164	100% 95% 5%
6	KO	164	94% 6%
6	KQ	164	100% 88% 10%
6	L4	164	88% 85% 13%
6	LD	164	89% 86% 13%
6	M2	164	56% 95% 5%
6	MB	164	6% 99%
6	MJ	164	46% 96%
6	ML	164	46% 96%
6	MM	164	5% 99%
6	MR	164	55% 95% 5%
6	O1	164	84% 99%
6	O2	164	13% 93% 7%
6	O7	164	6% 95% 5%
6	O9	164	9% 95% 5%

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Mol	Chain	Length	Quality of chain
6	OB	164	30% 99%
6	OF	164	10% 98%
6	OI	164	9% 98%
6	OJ	164	27% 99%
6	OK	164	85% 99%
6	OL	164	25% 99%
6	OM	164	31% 99%
6	OR	164	12% 95% 5%
6	Q1	164	77% 99%
6	Q2	164	23% 94% 6%
6	Q7	164	95% 5%
6	Q9	164	95% 5%
6	QB	164	51% 98%
6	QF	164	27% 98%
6	QI	164	26% 98%
6	QJ	164	32% 98%
6	QK	164	78% 99%
6	QL	164	33% 98%
6	QM	164	48% 98%
6	QR	164	24% 96%
6	S1	164	85% 99%
6	S2	164	18% 98%
6	S7	164	96%
6	S9	164	96%
6	SB	164	58% 99%

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Mol	Chain	Length	Quality of chain
6	SF	164	22% 98%
6	SI	164	24% 98%
6	SJ	164	16% 96%
6	SK	164	84% 99%
6	SL	164	16% 96%
6	SM	164	57% 99%
6	SR	164	19% 96%
6	U1	164	96% 99%
6	U2	164	41% 95%
6	U7	164	5% 95%
6	U9	164	7% 95%
6	UB	164	20% 99%
6	UF	164	24% 98%
6	UI	164	24% 98%
6	UJ	164	15% 96%
6	UK	164	97% 99%
6	UL	164	17% 96%
6	UM	164	18% 99%
6	UR	164	41% 95%
6	W1	164	96% 99%
6	W2	164	52% 97%
6	W7	164	96%
6	W9	164	96%
6	WB	164	8% 99%
6	WF	164	12% 98%

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Mol	Chain	Length	Quality of chain
6	WI	164	13% 98%
6	WJ	164	30% 97%
6	WK	164	96% 99%
6	WL	164	27% 97%
6	WM	164	9% 99%
6	WR	164	54% 96%
6	YB	164	11% 99%
6	YJ	164	98% 98%
6	YL	164	98% 98%
6	YM	164	10% 99%
6	Z1	164	99% 99%
6	Z7	164	5% 96%
6	Z9	164	5% 96%
6	ZF	164	8% 99%
6	ZI	164	9% 99%
6	ZK	164	99% 99%
6	aB	164	92% 99%
6	aJ	164	89% 96%
6	aL	164	87% 96%
6	aM	164	91% 99%
6	b1	164	100% 99%
6	b7	164	29% 95%
6	b9	164	29% 95%
6	bF	164	37% 98%
6	bI	164	36% 98%

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Mol	Chain	Length	Quality of chain
6	bK	164	100% 99%
6	cJ	164	93% 96%
6	cL	164	93% 95% 5%
6	d1	164	99% 99%
6	d7	164	24% 95% 5%
6	d9	164	25% 95% 5%
6	dB	164	93% 99%
6	dF	164	66% 98%
6	dI	164	68% 98%
6	dK	164	99% 99%
6	dM	164	92% 99%
6	eJ	164	90% 98%
6	eL	164	91% 98%
6	f1	164	99% 99%
6	f7	164	35% 96%
6	f9	164	37% 96%
6	fB	164	98% 99%
6	fF	164	79% 97%
6	fI	164	77% 97%
6	fK	164	99% 99%
6	fM	164	98% 99%
6	gJ	164	93% 98%
6	gL	164	93% 98%
6	h1	164	100% 98%
6	h7	164	30% 95% 5%

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Mol	Chain	Length	Quality of chain
6	h9	164	28% 95% 5%
6	hB	164	98% 99%
6	hF	164	91% 98%
6	hI	164	91% 98%
6	hK	164	100% 99%
6	hM	164	96% 99%
6	iJ	164	85% 96%
6	iL	164	86% 96%
6	j1	164	99% 99%
6	j7	164	43% 96%
6	j9	164	45% 96%
6	jB	164	98% 98%
6	jF	164	65% 98%
6	jI	164	68% 98%
6	jK	164	99% 99%
6	jM	164	97% 99%
6	kJ	164	100% 96%
6	kL	164	100% 96%
6	l1	164	100% 99%
6	l7	164	27% 95% 5%
6	l9	164	25% 96%
6	lB	164	73% 98%
6	lF	164	57% 98%
6	lI	164	57% 98%
6	lK	164	99% 99%

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Mol	Chain	Length	Quality of chain
6	lM	164	73% 97% 100%
6	mJ	164	97% 100%
6	mL	164	100% 97%
6	oJ	164	100% 98%
6	oL	164	100% 98%
6	qJ	164	100% 96%
6	qL	164	100% 96%
6	sJ	164	100% 96%
6	sL	164	100% 96%
6	uJ	164	100% 97%
6	uL	164	100% 97%
7	A5	177	100% 90% 10%
7	A8	177	100% 90% 10%
7	B3	177	18% 95% 5%
7	B5	177	79% 80% 18%
7	B8	177	80% 80% 18%
7	BA	177	100% 94% 5%
7	BC	177	100% 93% 7%
7	BE	177	100% 93% 7%
7	BG	177	100% 94% 6%
7	BJ	177	35% 97%
7	BL	177	34% 97%
7	BN	177	100% 94% 5%
7	BO	177	18% 95% 5%
7	BQ	177	100% 94% 6%

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Mol	Chain	Length	Quality of chain
7	C4	177	82% 82% 16% .
7	C5	177	100% 91% 8% .
7	C8	177	100% 91% 8% .
7	CD	177	82% 82% 16% .
7	D3	177	17% 92% 8%
7	DA	177	100% 95% . .
7	DB	177	29% 98% .
7	DC	177	98% 92% 8%
7	DE	177	98% 92% 8%
7	DG	177	100% 93% 7%
7	DJ	177	27% 98% .
7	DL	177	28% 98% .
7	DM	177	29% 98% .
7	DN	177	100% 95% . .
7	DO	177	19% 92% 8%
7	DQ	177	100% 93% 7%
7	E4	177	69% 82% 17% .
7	ED	177	69% 82% 16% .
7	F3	177	31% 93% 7%
7	F5	177	27% 80% . 18%
7	F8	177	25% 80% . 18%
7	FA	177	100% 94% 6%
7	FB	177	16% 98% .
7	FC	177	99% 90% 10%
7	FE	177	99% 90% 10%

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Mol	Chain	Length	Quality of chain
7	FG	177	100% 93% 7%
7	FJ	177	11% 93% 7%
7	FL	177	10% 93% 7%
7	FM	177	16% 98% .
7	FN	177	100% 94% 6%
7	FO	177	32% 93% 7%
7	FQ	177	100% 93% 7%
7	G4	177	90% 80% 18% .
7	G5	177	59% 80% 18%
7	G8	177	58% 80% 18%
7	GD	177	90% 81% 18% .
7	H3	177	46% 92% 8%
7	H5	177	24% 80% 18%
7	H8	177	24% 80% 18%
7	HA	177	100% 94% 6% .
7	HB	177	24% 97% .
7	HC	177	99% 90% 10%
7	HE	177	99% 90% 10%
7	HG	177	100% 93% 7%
7	HJ	177	9% 88% 12%
7	HL	177	9% 88% 12%
7	HM	177	25% 97% .
7	HN	177	100% 94% 6% .
7	HO	177	46% 92% 8%
7	HQ	177	100% 93% 7%

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Mol	Chain	Length	Quality of chain
7	I4	177	45% 88% 11%
7	I5	177	15% 89% 11%
7	I8	177	16% 89% 11%
7	ID	177	44% 88% 11%
7	J3	177	7% 93% 7%
7	JA	177	100% 95% 5%
7	JB	177	27% 97% .
7	JC	177	100% 92% 8%
7	JE	177	100% 92% 8%
7	JG	177	100% 93% 7%
7	JJ	177	12% 96% .
7	JL	177	11% 96% .
7	JM	177	27% 97% .
7	JN	177	100% 95% 5%
7	JO	177	8% 93% 7%
7	JQ	177	100% 93% 7%
7	K4	177	95% 82% 17%
7	K5	177	42% 89% 11%
7	K8	177	42% 89% 11%
7	KD	177	95% 82% 16%
7	L3	177	12% 93% 7%
7	L5	177	23% 80% 18%
7	L8	177	23% 80% 18%
7	LA	177	100% 96% ..
7	LB	177	10% 99% .

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Mol	Chain	Length	Quality of chain
7	LC	177	94% 92% 8%
7	LE	177	95% 92% 8%
7	LG	177	100% 93% 7%
7	LJ	177	10% 98% .
7	LL	177	10% 98% .
7	LM	177	10% 99% .
7	LN	177	100% 96% ..
7	LO	177	13% 93% 7%
7	LQ	177	100% 93% 7%
7	M3	177	24% 76% 7% 18%
7	M4	177	85% 83% 15% .
7	MD	177	85% 82% 16% .
7	MO	177	24% 76% 7% 18%
7	N2	177	38% 96% .
7	N3	177	48% 76% 6% 18%
7	NB	177	6% 96% .
7	NJ	177	42% 98% .
7	NL	177	44% 98% .
7	NM	177	6% 97% .
7	NO	177	47% 76% 6% 18%
7	NR	177	38% 96% .
7	P1	177	51% 98% .
7	P2	177	24% 97% ..
7	P7	177	9% 93% 7%
7	P9	177	8% 93% 7%

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Mol	Chain	Length	Quality of chain
7	PB	177	53% 99%
7	PF	177	18% 99%
7	PI	177	17% 99%
7	PJ	177	26% 95% 5%
7	PK	177	54% 98%
7	PL	177	23% 95% 5%
7	PM	177	50% 99%
7	PR	177	24% 97% ..
7	R1	177	94% 98%
7	R2	177	33% 98%
7	R7	177	. 93% 7%
7	R9	177	. 93% 7%
7	RB	177	27% 96%
7	RF	177	15% 99%
7	RI	177	15% 99%
7	RJ	177	26% 98%
7	RK	177	93% 98%
7	RL	177	25% 98%
7	RM	177	26% 96%
7	RR	177	34% 98%
7	T1	177	85% 99%
7	T2	177	10% 97% ..
7	T7	177	12% 93% 7%
7	T9	177	8% 93% 7%
7	TB	177	31% 97%

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Mol	Chain	Length	Quality of chain
7	TF	177	11% 98%
7	TI	177	12% 98%
7	TJ	177	13% 98%
7	TK	177	85% 99%
7	TL	177	14% 98%
7	TM	177	32% 97%
7	TR	177	10% 97%
7	V1	177	90% 98%
7	V2	177	64% 96%
7	V7	177	5% 94% 6%
7	V9	177	5% 94% 6%
7	VB	177	40% 97%
7	VF	177	24% 98%
7	VI	177	26% 98%
7	VJ	177	31% 99%
7	VK	177	88% 98%
7	VL	177	30% 99%
7	VM	177	41% 97%
7	VR	177	64% 96%
7	X2	177	24% 95% 5%
7	XB	177	16% 99%
7	XJ	177	16% 99%
7	XL	177	16% 99%
7	XM	177	14% 99%
7	XR	177	24% 95% 5%

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Mol	Chain	Length	Quality of chain
7	Y1	177	92%
7	Y7	177	10% 99% 7%
7	Y9	177	10% 93% 7%
7	YF	177	8% 99% .
7	YI	177	8% 99% .
7	YK	177	93% 99% .
7	ZB	177	10% 97% .
7	ZJ	177	97% 98% .
7	ZL	177	96% 98% .
7	ZM	177	10% 97% .
7	a1	177	98% 98% .
7	a7	177	10% 93% 7%
7	a9	177	11% 92% 8%
7	aF	177	22% 98% .
7	aI	177	21% 98% .
7	aK	177	98% 98% .
7	bJ	177	89% 97% .
7	bL	177	87% 97% .
7	c1	177	100% 99% .
7	c7	177	49% 93% 7%
7	c9	177	44% 93% 7%
7	cB	177	97% 98% .
7	cF	177	46% 97% .
7	cI	177	46% 97% .
7	cK	177	100% 99% .

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Mol	Chain	Length	Quality of chain
7	cM	177	97% 98%
7	dJ	177	95% 98%
7	dL	177	96% 98%
7	e1	177	100% 99%
7	e7	177	16% 92% 8%
7	e9	177	16% 92% 8%
7	eB	177	64% 96%
7	eF	177	60% 98%
7	eI	177	59% 98%
7	eK	177	100% 99%
7	eM	177	66% 96%
7	fJ	177	80% 97%
7	fL	177	79% 97%
7	g1	177	99% 99%
7	g7	177	48% 93% 7%
7	g9	177	47% 93% 7%
7	gB	177	99% 96%
7	gF	177	59% 99%
7	gI	177	56% 99%
7	gK	177	99% 99%
7	gM	177	99% 96%
7	hJ	177	96% 97%
7	hL	177	96% 97%
7	i1	177	100% 99%
7	i7	177	14% 93% 7%

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Mol	Chain	Length	Quality of chain
7	i9	177	15% 93% 7%
7	iB	177	88% 98%
7	iF	177	86% 98%
7	iI	177	86% 98%
7	iK	177	100% 99%
7	iM	177	87% 98%
7	jJ	177	80% 97%
7	jL	177	81% 97%
7	k1	177	100% 99%
7	k7	177	40% 93% 7%
7	k9	177	40% 93% 7%
7	kB	177	95% 95% 5%
7	kF	177	38% 98%
7	kI	177	40% 98%
7	kK	177	100% 99%
7	kM	177	98% 95% 5%
7	lJ	177	100% 94% 6%
7	lL	177	100% 94% 6%
7	m1	177	100% 99%
7	m7	177	21% 94% 6%
7	m9	177	23% 94% 6%
7	mB	177	85% 98%
7	mF	177	80% 98%
7	mI	177	80% 98%
7	mK	177	100% 99%

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Mol	Chain	Length	Quality of chain
7	mM	177	86% 98% 100%
7	nJ	177	95% 100%
7	nL	177	95% 100%
7	pJ	177	95% 100%
7	pL	177	95% 100%
7	rJ	177	96% 100%
7	rL	177	96% 100%
7	tJ	177	95% 100%
7	tL	177	95% 100%
7	vJ	177	95% 100%
7	vL	177	95% 100%
8	e2	303	33% 79% 18%
8	eR	303	33% 79% 18%
9	O3	405	27% 91% 7%
9	OO	405	27% 91% 7%
10	d4	342	58% 85% 13%
10	dD	342	52% 85% 13%
11	D5	327	25% 75%
11	D8	327	25% 75%
12	E5	288	27% 71% 29%
12	E8	288	26% 71% 29%
13	k6	288	6% 93% 6%
13	kH	288	6% 93% 6%
14	MA	333	71% 69% 29%
14	MG	333	71% 67% 29%

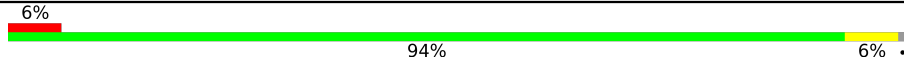
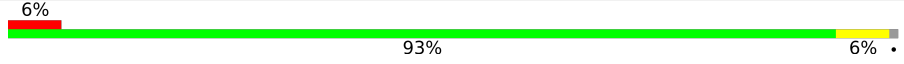
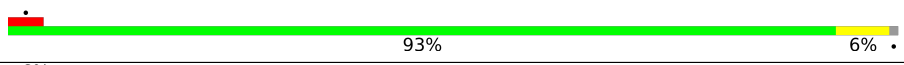
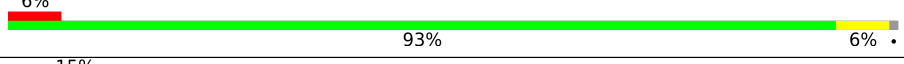
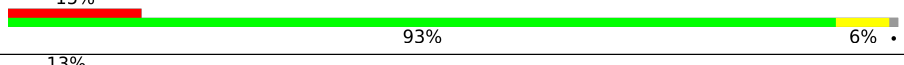
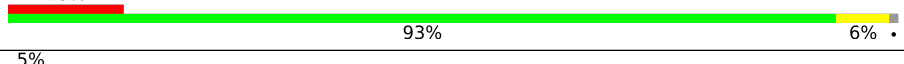
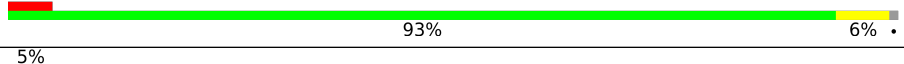
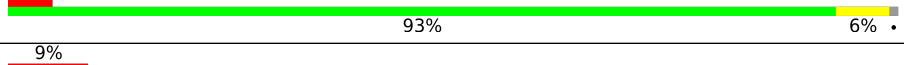
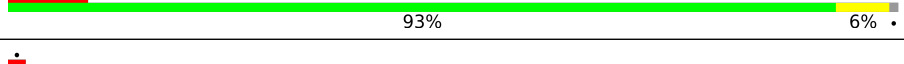
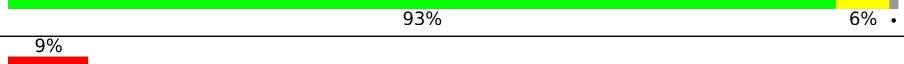
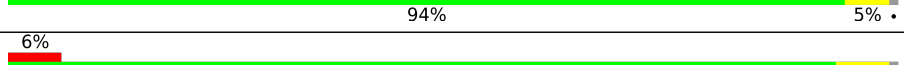
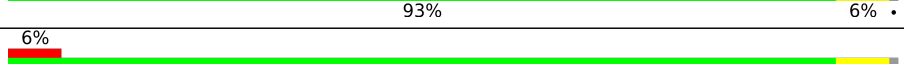
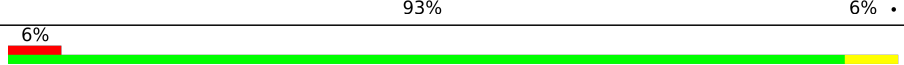
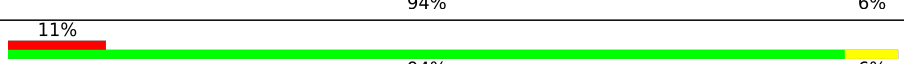
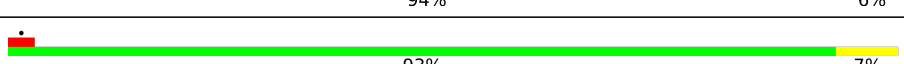
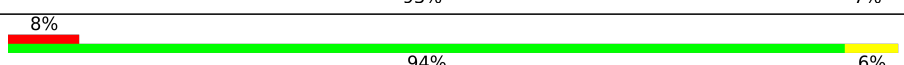
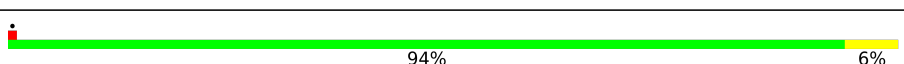
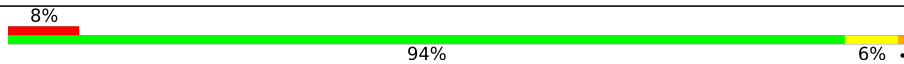
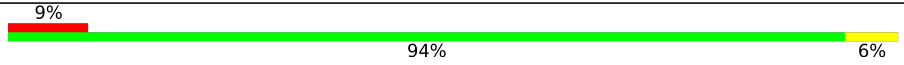
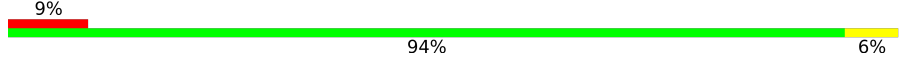
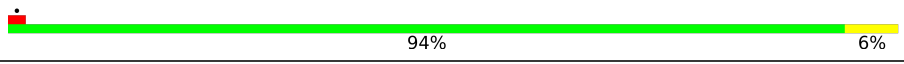
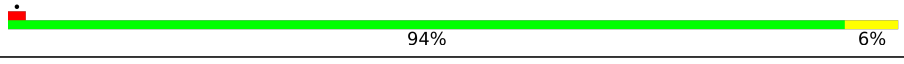
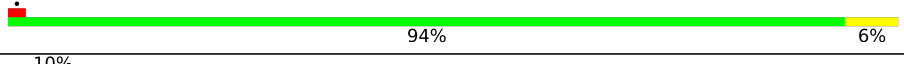
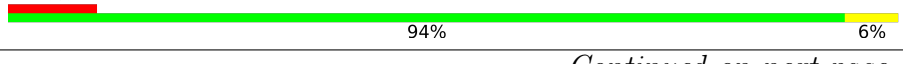

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Mol	Chain	Length	Quality of chain
14	MN	333	71% 69% 29%
14	MQ	333	71% 68% 29%
15	bB	490	9% 76% 22%
15	bM	490	9% 75% 22%
16	AB	273	76% 86% 13%
16	AM	273	77% 86% 13%
16	wJ	273	69% 79% 7% 13%
16	wL	273	68% 79% 7% 13%
16	xJ	273	87% 79% 7% 13%
16	xL	273	87% 80% 7% 13%
17	BB	290	17% 86% 14%
17	BM	290	16% 86% 14%
17	yJ	290	11% 86% 14%
17	yL	290	11% 86% 14%
18	MC	316	79% 78% 10% 11%
18	ME	316	80% 78% 9% 11%
19	zJ	498	8% 73% 26%
19	zL	498	7% 72% 26%
20	AP	161	7% 93% 6%
20	CP	161	14% 93% 6%
20	EP	161	12% 93% 6%
20	GP	161	6% 93% 6%
20	JP	161	6% 94% 6%
20	KP	161	7% 93% 6%
20	NP	161	• 93% 6%

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Mol	Chain	Length	Quality of chain
20	PP	161	 6% 94% 6%
20	RP	161	 6% 93% 6%
20	TP	161	 6% 93% 6%
20	cP	161	 6% 93% 6%
20	eP	161	 15% 93% 6%
20	gP	161	 13% 93% 6%
20	iP	161	 5% 93% 6%
20	lP	161	 5% 93% 6%
20	mP	161	 9% 93% 6%
20	pP	161	 6% 93% 6%
20	rP	161	 9% 94% 5%
20	tP	161	 6% 93% 6%
20	vP	161	 6% 93% 6%
21	BP	161	 6% 94% 6%
21	DP	161	 11% 94% 6%
21	FP	161	 6% 93% 7%
21	HP	161	 8% 94% 6%
21	IP	161	 6% 94% 6%
21	LP	161	 8% 94% 6%
21	MP	161	 9% 94% 6%
21	OP	161	 9% 94% 6%
21	QP	161	 6% 94% 6%
21	SP	161	 6% 94% 6%
21	UP	161	 6% 94% 6%
21	dP	161	 10% 94% 6%

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Mol	Chain	Length	Quality of chain
21	fP	161	94% 6%
21	hP	161	94% 6%
21	jP	161	94% 6%
21	kP	161	94% 6%
21	nP	161	94% 6%
21	oP	161	93% 7%
21	qP	161	94% 6%
21	sP	161	94% 6%
21	uP	161	94% 6%
21	wP	161	94% 6%
22	VP	161	98% ...
22	xP	161	98% ...
23	WP	173	100%
23	yP	173	100%
24	XP	132	69% 30%
24	zP	132	69% 30%
25	1P	879	95% ..
25	YP	879	95% ..
26	2P	159	82% 17%
26	ZP	159	81% 17%
27	3P	288	85% 12%
27	aP	288	85% 12%
28	4P	253	80% 18%
28	bP	253	80% 18%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
21	MEN	LP	71	-	X	-	-
21	MEN	jP	71	-	X	-	-
21	MEN	kP	71	-	X	-	-

2 Entry composition [i](#)

There are 32 unique types of molecules in this entry. The entry contains 944670 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X1	324	2527	1603	431	486	7	0	0
1	X7	324	2527	1603	431	486	7	0	0
1	X9	324	2527	1603	431	486	7	0	0
1	XF	324	2527	1603	431	486	7	0	0
1	XI	324	2523	1600	430	486	7	0	0
1	XK	324	2527	1603	431	486	7	0	0

- Molecule 2 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	A1	257	1987	1226	368	378	15	0	0
2	A7	257	1987	1226	368	378	15	0	0
2	A9	257	1987	1226	368	378	15	0	0
2	AF	257	1987	1226	368	378	15	0	0
2	AI	257	1987	1226	368	378	15	0	0
2	AK	257	1987	1226	368	378	15	0	0

- Molecule 3 is a protein called Phycobilisome rod-core linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B1	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		
3	B7	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		
3	B9	230	Total	C	N	O	S	0	0
			1889	1206	331	348	4		
3	BF	231	Total	C	N	O	S	0	0
			1897	1212	332	349	4		
3	BI	231	Total	C	N	O	S	0	0
			1897	1212	332	349	4		
3	BK	227	Total	C	N	O	S	0	0
			1874	1197	328	345	4		

- Molecule 4 is a protein called C-phycoyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	G1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	I1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	K1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	M1	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	C7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	G7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	I7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	K7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	M7	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	C9	162	Total	C	N	O	S	0	0
			1228	773	209	240	6		
4	E9	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		
4	G9	162	1228	773	209	240	6	0	0
4	I9	162	1228	773	209	240	6	0	0
4	K9	162	1228	773	209	240	6	0	0
4	M9	162	1228	773	209	240	6	0	0
4	CF	162	1228	773	209	240	6	0	0
4	EF	162	1228	773	209	240	6	0	0
4	GF	162	1228	773	209	240	6	0	0
4	IF	162	1228	773	209	240	6	0	0
4	KF	162	1228	773	209	240	6	0	0
4	MF	162	1228	773	209	240	6	0	0
4	CI	162	1228	773	209	240	6	0	0
4	EI	162	1228	773	209	240	6	0	0
4	GI	162	1228	773	209	240	6	0	0
4	II	162	1228	773	209	240	6	0	0
4	KI	162	1228	773	209	240	6	0	0
4	MI	162	1228	773	209	240	6	0	0
4	CK	162	1228	773	209	240	6	0	0
4	EK	162	1228	773	209	240	6	0	0
4	GK	162	1228	773	209	240	6	0	0
4	IK	162	1228	773	209	240	6	0	0
4	KK	162	1228	773	209	240	6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	MK	162	1228	773	209	240	6	0	0

- Molecule 5 is a protein called C-phycoyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	D1	172	1272	786	224	253	9	0	0
5	F1	172	1272	786	224	253	9	0	0
5	H1	172	1272	786	224	253	9	0	0
5	J1	172	1272	786	224	253	9	0	0
5	L1	172	1272	786	224	253	9	0	0
5	N1	172	1272	786	224	253	9	0	0
5	D7	172	1272	786	224	253	9	0	0
5	F7	172	1272	786	224	253	9	0	0
5	H7	172	1272	786	224	253	9	0	0
5	J7	172	1272	786	224	253	9	0	0
5	L7	172	1272	786	224	253	9	0	0
5	N7	172	1272	786	224	253	9	0	0
5	D9	172	1272	786	224	253	9	0	0
5	F9	172	1272	786	224	253	9	0	0
5	H9	172	1272	786	224	253	9	0	0
5	J9	172	1272	786	224	253	9	0	0
5	L9	172	1272	786	224	253	9	0	0
5	N9	172	1272	786	224	253	9	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	DF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NF	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	DI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NI	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	DK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	FK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	HK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	JK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	LK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		
5	NK	172	Total	C	N	O	S	0	0
			1272	786	224	253	9		

- Molecule 6 is a protein called Phycoerythrin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	O1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l1	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	M2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	Q2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	U2	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	W2	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	A3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	C3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	E3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	G3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	I3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	K3	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	B4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	D4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	F4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	H4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	J4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	L4	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	J5	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Q7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l7	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	J8	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	O9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Q9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	S9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	U9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	W9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	Z9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	b9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	d9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	f9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	h9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	j9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	l9	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KA	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	GB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lB	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KC	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	BD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	DD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	FD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	HD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	JD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	LD	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KE	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	fF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lF	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KG	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jI	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	II	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	cJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	eJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	gJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	iJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	kJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	mJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	oJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	qJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	sJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	uJ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ZK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	bK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lK	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	ML	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	cL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	eL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	gL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	iL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	kL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	mL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	oL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	qL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	sL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	uL	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	GM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	QM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	UM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	WM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	YM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	aM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	dM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	fM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	hM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	jM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	lM	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	KN	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KO	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	AQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	CQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	EQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	GQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	IQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	KQ	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	MR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	OR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	QR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		
6	SR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	UR	164	Total	C	N	O	S	0	0
			1249	779	219	244	7		
6	WR	164	Total	C	N	O	S	0	0
			1250	779	219	245	7		

- Molecule 7 is a protein called B-phycoerythrin beta chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	P1	177	1294	800	225	257	12	0	0
7	R1	177	1294	800	225	257	12	0	0
7	T1	177	1294	800	225	257	12	0	0
7	V1	177	1300	804	225	259	12	2	0
7	Y1	177	1294	800	225	257	12	0	0
7	a1	177	1294	800	225	257	12	0	0
7	c1	177	1294	800	225	257	12	0	0
7	e1	177	1294	800	225	257	12	0	0
7	g1	177	1294	800	225	257	12	0	0
7	i1	177	1297	802	225	258	12	1	0
7	k1	177	1294	800	225	257	12	0	0
7	m1	177	1294	800	225	257	12	0	0
7	N2	177	1294	800	225	257	12	0	0
7	P2	177	1297	802	225	258	12	1	0
7	R2	177	1294	800	225	257	12	0	0
7	T2	177	1294	800	225	257	12	0	0
7	V2	177	1294	800	225	257	12	0	0
7	X2	177	1294	800	225	257	12	0	0
7	B3	177	1294	800	225	257	12	0	0
7	D3	177	1294	800	225	257	12	0	0
7	F3	177	1294	800	225	257	12	0	0
7	H3	177	1294	800	225	257	12	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	J3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L3	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	M3	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	N3	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	C4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	E4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	G4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	I4	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	K4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	M4	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	B5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	F5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	G5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	H5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	I5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	K5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L5	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	A5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	C5	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	P7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	R7	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		
7	T7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	Y7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	a7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	c7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	e7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	g7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	i7	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	k7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	m7	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	B8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	F8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	G8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	H8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	I8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	K8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	L8	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	A8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	C8	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	P9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	R9	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		
7	T9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	V9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	Y9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	a9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	c9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	e9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	g9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	i9	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	k9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	m9	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HA	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LA	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	FB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	HB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	JB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	LB	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		
7	NB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	PB	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	TB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	VB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	XB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	ZB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	cB	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	eB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	gB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	iB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	kB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	mB	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	BC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LC	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	CD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	ED	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		
7	GD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	ID	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	KD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	MD	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LE	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VF	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iF	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kF	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		
7	mF	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HG	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LG	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VI	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iI	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	mI	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DJ	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		
7	FJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	RJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	ZJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	bJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	dJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	fJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	hJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	jJ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	lJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	nJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	pJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	rJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	tJ	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		
7	vJ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VK	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	YK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	aK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	cK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	eK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	gK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	iK	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	kK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	mK	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PL	177	Total 1297	C 802	N 225	O 258	S 12	1	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	RL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XL	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	ZL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	bL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	dL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	fL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	hL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	jL	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	lL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	nL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	pL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	rL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	tL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	vL	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	FM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	HM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	JM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	LM	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		
7	NM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	PM	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	RM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	TM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	VM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	XM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	ZM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	cM	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	eM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	gM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	iM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	kM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	mM	177	Total 1300	C 804	N 225	O 259	S 12	2	0
7	BN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HN	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LN	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	BO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DO	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		
7	FO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	JO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LO	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	MO	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	NO	146	Total 1065	C 654	N 187	O 213	S 11	0	0
7	BQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	DQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	FQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	HQ	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	JQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	LQ	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	NR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	PR	177	Total 1297	C 802	N 225	O 258	S 12	1	0
7	RR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	TR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	VR	177	Total 1294	C 800	N 225	O 257	S 12	0	0
7	XR	177	Total 1294	C 800	N 225	O 257	S 12	0	0

- Molecule 8 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	e2	248	Total 1932	C 1217	N 336	O 369	S 10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	eR	248	1932	1217	336	369	10	0	0

- Molecule 9 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	O3	375	2873	1809	488	563	13	0	0
9	OO	375	2873	1809	488	563	13	0	0

- Molecule 10 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	d4	297	2293	1425	407	450	11	0	0
10	dD	297	2293	1425	407	450	11	0	0

- Molecule 11 is a protein called CaRSPs2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	D5	81	654	417	113	122	2	0	0
11	D8	81	654	417	113	122	2	0	0

- Molecule 12 is a protein called CaRSPs1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	E5	205	1580	1004	278	289	9	0	0
12	E8	205	1580	1004	278	289	9	0	0

- Molecule 13 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	k6	285	2182	1399	369	404	10	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	kH	285	2182	1399	369	404	10	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	MA	238	1851	1140	348	348	15	0	0
14	MG	238	1851	1140	348	348	15	0	0
14	MN	238	1851	1140	348	348	15	0	0
14	MQ	238	1851	1140	348	348	15	0	0

- Molecule 15 is a protein called Phycobilisome 32.1 kDa linker polypeptide, phycocyanin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	bB	380	2961	1867	514	565	15	0	0
15	bM	380	2961	1867	514	565	15	0	0

- Molecule 16 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	AB	238	1814	1122	335	342	15	0	0
16	wJ	238	1814	1122	335	342	15	0	0
16	xJ	238	1814	1122	335	342	15	0	0
16	wL	238	1814	1122	335	342	15	0	0
16	xL	238	1814	1122	335	342	15	0	0
16	AM	238	1814	1122	335	342	15	0	0

- Molecule 17 is a protein called R-phycoerythrin gamma chain, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	BB	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	yJ	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	yL	250	Total 1902	C 1184	N 346	O 358	S 14	0	0
17	BM	250	Total 1902	C 1184	N 346	O 358	S 14	0	0

- Molecule 18 is a protein called Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	MC	280	Total 2196	C 1391	N 382	O 413	S 10	0	0
18	ME	280	Total 2196	C 1391	N 382	O 413	S 10	0	0

- Molecule 19 is a protein called Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	zJ	370	Total 2901	C 1833	N 514	O 540	S 14	0	0
19	zL	370	Total 2901	C 1833	N 514	O 540	S 14	0	0

- Molecule 20 is a protein called Allophycocyanin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	AP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	CP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	EP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	GP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	JP	160	Total 1225	C 768	N 211	O 239	S 7	0	0
20	KP	160	Total 1225	C 768	N 211	O 239	S 7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	NP	160	1225	768	211	239	7	0	0
20	PP	160	1225	768	211	239	7	0	0
20	RP	160	1225	768	211	239	7	0	0
20	TP	160	1225	768	211	239	7	0	0
20	cP	160	1225	768	211	239	7	0	0
20	eP	160	1225	768	211	239	7	0	0
20	gP	160	1225	768	211	239	7	0	0
20	iP	160	1225	768	211	239	7	0	0
20	lP	160	1225	768	211	239	7	0	0
20	mP	160	1225	768	211	239	7	0	0
20	pP	160	1225	768	211	239	7	0	0
20	rP	160	1225	768	211	239	7	0	0
20	tP	160	1225	768	211	239	7	0	0
20	vP	160	1225	768	211	239	7	0	0

- Molecule 21 is a protein called Allophycocyanin beta subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	DP	161	1220	767	206	240	7	0	0
21	FP	161	1220	767	206	240	7	0	0
21	BP	161	1220	767	206	240	7	0	0
21	HP	161	1220	767	206	240	7	0	0
21	IP	161	1220	767	206	240	7	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
21	LP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	MP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	OP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	QP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	SP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	UP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	dP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	fP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	hP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	jP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	kP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	nP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	oP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	qP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	sP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	uP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		
21	wP	161	Total	C	N	O	S	0	0
			1220	767	206	240	7		

- Molecule 22 is a protein called Allophycocyanin gamma subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	VP	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		
22	xP	160	Total	C	N	O	S	0	0
			1260	808	207	240	5		

- Molecule 23 is a protein called Allophycocyanin beta 18 subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	WP	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		
23	yP	173	Total	C	N	O	S	0	0
			1376	881	230	261	4		

- Molecule 24 is a protein called Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	XP	92	Total	C	N	O	S	0	0
			720	453	127	135	5		
24	zP	92	Total	C	N	O	S	0	0
			720	453	127	135	5		

- Molecule 25 is a protein called Phycobilisome linker polypeptide.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	YP	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		
25	1P	844	Total	C	N	O	S	0	0
			6756	4328	1169	1245	14		

- Molecule 26 is a protein called Lrc4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	ZP	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		
26	2P	132	Total	C	N	O	S	0	0
			1004	631	179	191	3		

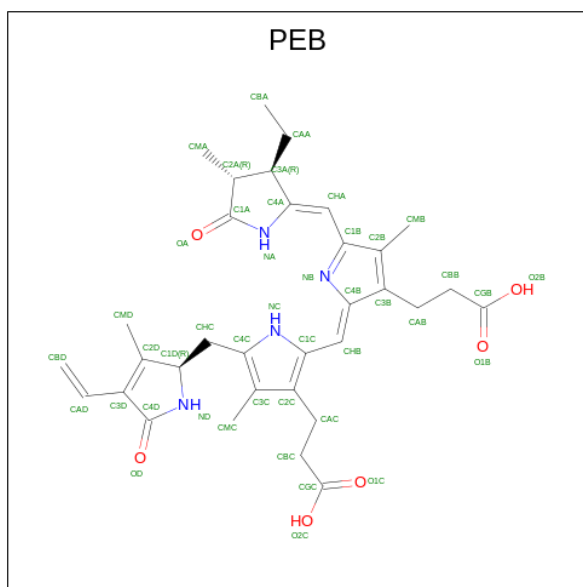
- Molecule 27 is a protein called LRC5.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	aP	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		
27	3P	253	Total	C	N	O	S	0	0
			1897	1190	325	375	7		

- Molecule 28 is a protein called FAS1 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	bP	207	1537	985	260	287	5	0	0
28	4P	207	1537	985	260	287	5	0	0

- Molecule 29 is PHYCOERYTHROBILIN (three-letter code: PEB) (formula: C₃₃H₄₀N₄O₆).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	A1	1	43	33	4	6	0
29	A1	1	43	33	4	6	0
29	A1	1	43	33	4	6	0
29	D1	1	43	33	4	6	0
29	F1	1	43	33	4	6	0
29	H1	1	43	33	4	6	0
29	J1	1	43	33	4	6	0
29	L1	1	43	33	4	6	0
29	N1	1	43	33	4	6	0
29	O1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	O1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	P1	1	43	33	4	6	0
29	Q1	1	43	33	4	6	0
29	Q1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	R1	1	43	33	4	6	0
29	S1	1	43	33	4	6	0
29	S1	1	43	33	4	6	0
29	T1	1	43	33	4	6	0
29	T1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	U1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	V1	1	43	33	4	6	0
29	W1	1	43	33	4	6	0
29	W1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	Y1	1	43	33	4	6	0
29	Y1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	Z1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	a1	1	43	33	4	6	0
29	b1	1	43	33	4	6	0
29	b1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	c1	1	43	33	4	6	0
29	d1	1	43	33	4	6	0
29	d1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	e1	1	43	33	4	6	0
29	f1	1	43	33	4	6	0
29	f1	1	43	33	4	6	0
29	g1	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	g1	1	43	33	4	6	0
29	g1	1	43	33	4	6	0
29	h1	1	43	33	4	6	0
29	h1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	i1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	j1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	k1	1	43	33	4	6	0
29	l1	1	43	33	4	6	0
29	l1	1	43	33	4	6	0
29	m1	1	43	33	4	6	0
29	m1	1	43	33	4	6	0
29	e2	1	43	33	4	6	0
29	e2	1	43	33	4	6	0
29	M2	1	43	33	4	6	0
29	M2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	N2	1	43	33	4	6	0
29	N2	1	43	33	4	6	0
29	N2	1	43	33	4	6	0
29	O2	1	43	33	4	6	0
29	O2	1	43	33	4	6	0
29	P2	1	43	33	4	6	0
29	P2	1	43	33	4	6	0
29	Q2	1	43	33	4	6	0
29	Q2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	R2	1	43	33	4	6	0
29	S2	1	43	33	4	6	0
29	S2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	T2	1	43	33	4	6	0
29	U2	1	43	33	4	6	0
29	U2	1	43	33	4	6	0
29	V2	1	43	33	4	6	0
29	V2	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	V2	1	43	33	4	6	0
29	W2	1	43	33	4	6	0
29	W2	1	43	33	4	6	0
29	X2	1	43	33	4	6	0
29	X2	1	43	33	4	6	0
29	A3	1	43	33	4	6	0
29	A3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	B3	1	43	33	4	6	0
29	C3	1	43	33	4	6	0
29	C3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	D3	1	43	33	4	6	0
29	E3	1	43	33	4	6	0
29	E3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	F3	1	43	33	4	6	0
29	G3	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	G3	1	43	33	4	6	0
29	H3	1	43	33	4	6	0
29	H3	1	43	33	4	6	0
29	H3	1	43	33	4	6	0
29	I3	1	43	33	4	6	0
29	I3	1	43	33	4	6	0
29	I3	1	43	33	4	6	0
29	J3	1	43	33	4	6	0
29	J3	1	43	33	4	6	0
29	J3	1	43	33	4	6	0
29	K3	1	43	33	4	6	0
29	K3	1	43	33	4	6	0
29	L3	1	43	33	4	6	0
29	L3	1	43	33	4	6	0
29	M3	1	43	33	4	6	0
29	M3	1	43	33	4	6	0
29	M3	1	43	33	4	6	0
29	N3	1	43	33	4	6	0
29	N3	1	43	33	4	6	0
29	N3	1	43	33	4	6	0
29	B4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	B4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	C4	1	43	33	4	6	0
29	D4	1	43	33	4	6	0
29	D4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	E4	1	43	33	4	6	0
29	F4	1	43	33	4	6	0
29	F4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	G4	1	43	33	4	6	0
29	H4	1	43	33	4	6	0
29	H4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	I4	1	43	33	4	6	0
29	J4	1	43	33	4	6	0
29	J4	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	K4	1	43	33	4	6	0
29	K4	1	43	33	4	6	0
29	K4	1	43	33	4	6	0
29	L4	1	43	33	4	6	0
29	L4	1	43	33	4	6	0
29	M4	1	43	33	4	6	0
29	M4	1	43	33	4	6	0
29	M4	1	43	33	4	6	0
29	B5	1	43	33	4	6	0
29	B5	1	43	33	4	6	0
29	B5	1	43	33	4	6	0
29	F5	1	43	33	4	6	0
29	F5	1	43	33	4	6	0
29	F5	1	43	33	4	6	0
29	G5	1	43	33	4	6	0
29	G5	1	43	33	4	6	0
29	G5	1	43	33	4	6	0
29	H5	1	43	33	4	6	0
29	H5	1	43	33	4	6	0
29	H5	1	43	33	4	6	0
29	I5	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	I5	1	43	33	4	6	0
29	I5	1	43	33	4	6	0
29	J5	1	43	33	4	6	0
29	J5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	K5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	L5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	A5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	C5	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	A7	1	43	33	4	6	0
29	D7	1	43	33	4	6	0
29	F7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	H7	1	43	33	4	6	0
29	J7	1	43	33	4	6	0
29	L7	1	43	33	4	6	0
29	N7	1	43	33	4	6	0
29	O7	1	43	33	4	6	0
29	O7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	P7	1	43	33	4	6	0
29	Q7	1	43	33	4	6	0
29	Q7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	R7	1	43	33	4	6	0
29	S7	1	43	33	4	6	0
29	S7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	T7	1	43	33	4	6	0
29	U7	1	43	33	4	6	0
29	U7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	V7	1	43	33	4	6	0
29	V7	1	43	33	4	6	0
29	V7	1	43	33	4	6	0
29	W7	1	43	33	4	6	0
29	W7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Y7	1	43	33	4	6	0
29	Z7	1	43	33	4	6	0
29	Z7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	a7	1	43	33	4	6	0
29	b7	1	43	33	4	6	0
29	b7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	c7	1	43	33	4	6	0
29	d7	1	43	33	4	6	0
29	d7	1	43	33	4	6	0
29	e7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	e7	1	43	33	4	6	0
29	e7	1	43	33	4	6	0
29	f7	1	43	33	4	6	0
29	f7	1	43	33	4	6	0
29	g7	1	43	33	4	6	0
29	g7	1	43	33	4	6	0
29	g7	1	43	33	4	6	0
29	h7	1	43	33	4	6	0
29	h7	1	43	33	4	6	0
29	i7	1	43	33	4	6	0
29	i7	1	43	33	4	6	0
29	i7	1	43	33	4	6	0
29	j7	1	43	33	4	6	0
29	j7	1	43	33	4	6	0
29	k7	1	43	33	4	6	0
29	k7	1	43	33	4	6	0
29	k7	1	43	33	4	6	0
29	l7	1	43	33	4	6	0
29	l7	1	43	33	4	6	0
29	m7	1	43	33	4	6	0
29	m7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	m7	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	B8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	F8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	G8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	H8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	I8	1	43	33	4	6	0
29	J8	1	43	33	4	6	0
29	J8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0
29	K8	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	L8	1	43	33	4	6	0
29	L8	1	43	33	4	6	0
29	L8	1	43	33	4	6	0
29	A8	1	43	33	4	6	0
29	A8	1	43	33	4	6	0
29	A8	1	43	33	4	6	0
29	C8	1	43	33	4	6	0
29	C8	1	43	33	4	6	0
29	C8	1	43	33	4	6	0
29	A9	1	43	33	4	6	0
29	A9	1	43	33	4	6	0
29	A9	1	43	33	4	6	0
29	D9	1	43	33	4	6	0
29	F9	1	43	33	4	6	0
29	H9	1	43	33	4	6	0
29	J9	1	43	33	4	6	0
29	L9	1	43	33	4	6	0
29	N9	1	43	33	4	6	0
29	O9	1	43	33	4	6	0
29	O9	1	43	33	4	6	0
29	P9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	P9	1	43	33	4	6	0
29	P9	1	43	33	4	6	0
29	Q9	1	43	33	4	6	0
29	Q9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	R9	1	43	33	4	6	0
29	S9	1	43	33	4	6	0
29	S9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	T9	1	43	33	4	6	0
29	U9	1	43	33	4	6	0
29	U9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	V9	1	43	33	4	6	0
29	W9	1	43	33	4	6	0
29	W9	1	43	33	4	6	0
29	Y9	1	43	33	4	6	0
29	Y9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	Y9	1	43	33	4	6	0
29	Z9	1	43	33	4	6	0
29	Z9	1	43	33	4	6	0
29	a9	1	43	33	4	6	0
29	a9	1	43	33	4	6	0
29	a9	1	43	33	4	6	0
29	b9	1	43	33	4	6	0
29	b9	1	43	33	4	6	0
29	c9	1	43	33	4	6	0
29	c9	1	43	33	4	6	0
29	c9	1	43	33	4	6	0
29	d9	1	43	33	4	6	0
29	d9	1	43	33	4	6	0
29	e9	1	43	33	4	6	0
29	e9	1	43	33	4	6	0
29	e9	1	43	33	4	6	0
29	f9	1	43	33	4	6	0
29	f9	1	43	33	4	6	0
29	g9	1	43	33	4	6	0
29	g9	1	43	33	4	6	0
29	g9	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	h9	1	43	33	4	6	0
29	h9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	i9	1	43	33	4	6	0
29	j9	1	43	33	4	6	0
29	j9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	k9	1	43	33	4	6	0
29	l9	1	43	33	4	6	0
29	l9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	m9	1	43	33	4	6	0
29	AA	1	43	33	4	6	0
29	AA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	BA	1	43	33	4	6	0
29	CA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	CA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	DA	1	43	33	4	6	0
29	EA	1	43	33	4	6	0
29	EA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	FA	1	43	33	4	6	0
29	GA	1	43	33	4	6	0
29	GA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	HA	1	43	33	4	6	0
29	IA	1	43	33	4	6	0
29	IA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	JA	1	43	33	4	6	0
29	KA	1	43	33	4	6	0
29	KA	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	LA	1	43	33	4	6	0
29	LA	1	43	33	4	6	0
29	LA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	MA	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	AB	1	43	33	4	6	0
29	BB	1	43	33	4	6	0
29	CB	1	43	33	4	6	0
29	CB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	DB	1	43	33	4	6	0
29	EB	1	43	33	4	6	0
29	EB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	FB	1	43	33	4	6	0
29	GB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	GB	1	43	33	4	6	0
29	HB	1	43	33	4	6	0
29	HB	1	43	33	4	6	0
29	HB	1	43	33	4	6	0
29	IB	1	43	33	4	6	0
29	IB	1	43	33	4	6	0
29	JB	1	43	33	4	6	0
29	JB	1	43	33	4	6	0
29	JB	1	43	33	4	6	0
29	KB	1	43	33	4	6	0
29	KB	1	43	33	4	6	0
29	KB	1	43	33	4	6	0
29	LB	1	43	33	4	6	0
29	LB	1	43	33	4	6	0
29	LB	1	43	33	4	6	0
29	MB	1	43	33	4	6	0
29	MB	1	43	33	4	6	0
29	NB	1	43	33	4	6	0
29	NB	1	43	33	4	6	0
29	OB	1	43	33	4	6	0
29	OB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	PB	1	43	33	4	6	0
29	PB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	QB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	RB	1	43	33	4	6	0
29	SB	1	43	33	4	6	0
29	SB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	TB	1	43	33	4	6	0
29	UB	1	43	33	4	6	0
29	UB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	VB	1	43	33	4	6	0
29	WB	1	43	33	4	6	0
29	WB	1	43	33	4	6	0
29	XB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	XB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	YB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	ZB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	aB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	cB	1	43	33	4	6	0
29	dB	1	43	33	4	6	0
29	dB	1	43	33	4	6	0
29	eB	1	43	33	4	6	0
29	eB	1	43	33	4	6	0
29	fB	1	43	33	4	6	0
29	fB	1	43	33	4	6	0
29	gB	1	43	33	4	6	0
29	gB	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	gB	1	43	33	4	6	0
29	hB	1	43	33	4	6	0
29	hB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	iB	1	43	33	4	6	0
29	jB	1	43	33	4	6	0
29	jB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	kB	1	43	33	4	6	0
29	lB	1	43	33	4	6	0
29	lB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	mB	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	AC	1	43	33	4	6	0
29	BC	1	43	33	4	6	0
29	BC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	BC	1	43	33	4	6	0
29	CC	1	43	33	4	6	0
29	CC	1	43	33	4	6	0
29	DC	1	43	33	4	6	0
29	DC	1	43	33	4	6	0
29	EC	1	43	33	4	6	0
29	EC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	FC	1	43	33	4	6	0
29	GC	1	43	33	4	6	0
29	GC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	HC	1	43	33	4	6	0
29	IC	1	43	33	4	6	0
29	IC	1	43	33	4	6	0
29	JC	1	43	33	4	6	0
29	JC	1	43	33	4	6	0
29	KC	1	43	33	4	6	0
29	KC	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	KC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	LC	1	43	33	4	6	0
29	dD	1	43	33	4	6	0
29	BD	1	43	33	4	6	0
29	BD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	CD	1	43	33	4	6	0
29	DD	1	43	33	4	6	0
29	DD	1	43	33	4	6	0
29	ED	1	43	33	4	6	0
29	ED	1	43	33	4	6	0
29	FD	1	43	33	4	6	0
29	FD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	GD	1	43	33	4	6	0
29	HD	1	43	33	4	6	0
29	HD	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	ID	1	43	33	4	6	0
29	ID	1	43	33	4	6	0
29	ID	1	43	33	4	6	0
29	JD	1	43	33	4	6	0
29	JD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	KD	1	43	33	4	6	0
29	LD	1	43	33	4	6	0
29	LD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	MD	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	AE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	BE	1	43	33	4	6	0
29	CE	1	43	33	4	6	0
29	CE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	DE	1	43	33	4	6	0
29	DE	1	43	33	4	6	0
29	EE	1	43	33	4	6	0
29	EE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	FE	1	43	33	4	6	0
29	GE	1	43	33	4	6	0
29	GE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	HE	1	43	33	4	6	0
29	IE	1	43	33	4	6	0
29	IE	1	43	33	4	6	0
29	JE	1	43	33	4	6	0
29	JE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	KE	1	43	33	4	6	0
29	LE	1	43	33	4	6	0
29	LE	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	LE	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	AF	1	43	33	4	6	0
29	DF	1	43	33	4	6	0
29	FF	1	43	33	4	6	0
29	HF	1	43	33	4	6	0
29	JF	1	43	33	4	6	0
29	LF	1	43	33	4	6	0
29	NF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	OF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	PF	1	43	33	4	6	0
29	QF	1	43	33	4	6	0
29	QF	1	43	33	4	6	0
29	RF	1	43	33	4	6	0
29	RF	1	43	33	4	6	0
29	SF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	SF	1	43	33	4	6	0
29	TF	1	43	33	4	6	0
29	TF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	UF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	VF	1	43	33	4	6	0
29	WF	1	43	33	4	6	0
29	WF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	YF	1	43	33	4	6	0
29	ZF	1	43	33	4	6	0
29	ZF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	aF	1	43	33	4	6	0
29	bF	1	43	33	4	6	0
29	bF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	cF	1	43	33	4	6	0
29	cF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	dF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	eF	1	43	33	4	6	0
29	fF	1	43	33	4	6	0
29	fF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	gF	1	43	33	4	6	0
29	hF	1	43	33	4	6	0
29	hF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	iF	1	43	33	4	6	0
29	jF	1	43	33	4	6	0
29	jF	1	43	33	4	6	0
29	kF	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	kF	1	43	33	4	6	0
29	kF	1	43	33	4	6	0
29	lF	1	43	33	4	6	0
29	lF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	mF	1	43	33	4	6	0
29	AG	1	43	33	4	6	0
29	AG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	BG	1	43	33	4	6	0
29	CG	1	43	33	4	6	0
29	CG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	DG	1	43	33	4	6	0
29	EG	1	43	33	4	6	0
29	EG	1	43	33	4	6	0
29	FG	1	43	33	4	6	0
29	FG	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	FG	1	43	33	4	6	0
29	GG	1	43	33	4	6	0
29	GG	1	43	33	4	6	0
29	HG	1	43	33	4	6	0
29	HG	1	43	33	4	6	0
29	HG	1	43	33	4	6	0
29	IG	1	43	33	4	6	0
29	IG	1	43	33	4	6	0
29	JG	1	43	33	4	6	0
29	JG	1	43	33	4	6	0
29	JG	1	43	33	4	6	0
29	KG	1	43	33	4	6	0
29	KG	1	43	33	4	6	0
29	LG	1	43	33	4	6	0
29	LG	1	43	33	4	6	0
29	LG	1	43	33	4	6	0
29	MG	1	43	33	4	6	0
29	MG	1	43	33	4	6	0
29	MG	1	43	33	4	6	0
29	AI	1	43	33	4	6	0
29	AI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	AI	1	43	33	4	6	0
29	DI	1	43	33	4	6	0
29	FI	1	43	33	4	6	0
29	HI	1	43	33	4	6	0
29	JI	1	43	33	4	6	0
29	LI	1	43	33	4	6	0
29	NI	1	43	33	4	6	0
29	OI	1	43	33	4	6	0
29	OI	1	43	33	4	6	0
29	OI	1	43	33	4	6	0
29	PI	1	43	33	4	6	0
29	PI	1	43	33	4	6	0
29	PI	1	43	33	4	6	0
29	QI	1	43	33	4	6	0
29	QI	1	43	33	4	6	0
29	RI	1	43	33	4	6	0
29	RI	1	43	33	4	6	0
29	SI	1	43	33	4	6	0
29	SI	1	43	33	4	6	0
29	TI	1	43	33	4	6	0
29	TI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	UI	1	43	33	4	6	0
29	UI	1	43	33	4	6	0
29	UI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	VI	1	43	33	4	6	0
29	WI	1	43	33	4	6	0
29	WI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	YI	1	43	33	4	6	0
29	ZI	1	43	33	4	6	0
29	ZI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	aI	1	43	33	4	6	0
29	bI	1	43	33	4	6	0
29	bI	1	43	33	4	6	0
29	cI	1	43	33	4	6	0
29	cI	1	43	33	4	6	0
29	dI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	dI	1	43	33	4	6	0
29	dI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	eI	1	43	33	4	6	0
29	fI	1	43	33	4	6	0
29	fI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	gI	1	43	33	4	6	0
29	hI	1	43	33	4	6	0
29	hI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	iI	1	43	33	4	6	0
29	jI	1	43	33	4	6	0
29	jI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	kI	1	43	33	4	6	0
29	lI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	lI	1	43	33	4	6	0
29	mI	1	43	33	4	6	0
29	mI	1	43	33	4	6	0
29	mI	1	43	33	4	6	0
29	AJ	1	43	33	4	6	0
29	AJ	1	43	33	4	6	0
29	AJ	1	43	33	4	6	0
29	BJ	1	43	33	4	6	0
29	BJ	1	43	33	4	6	0
29	BJ	1	43	33	4	6	0
29	CJ	1	43	33	4	6	0
29	CJ	1	43	33	4	6	0
29	DJ	1	43	33	4	6	0
29	DJ	1	43	33	4	6	0
29	EJ	1	43	33	4	6	0
29	EJ	1	43	33	4	6	0
29	FJ	1	43	33	4	6	0
29	FJ	1	43	33	4	6	0
29	FJ	1	43	33	4	6	0
29	GJ	1	43	33	4	6	0
29	GJ	1	43	33	4	6	0

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

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	PJ	1	43	33	4	6	0
29	QJ	1	43	33	4	6	0
29	QJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	RJ	1	43	33	4	6	0
29	SJ	1	43	33	4	6	0
29	SJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	TJ	1	43	33	4	6	0
29	UJ	1	43	33	4	6	0
29	UJ	1	43	33	4	6	0
29	VJ	1	43	33	4	6	0
29	VJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	WJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0
29	XJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	YJ	1	43	33	4	6	0
29	YJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	ZJ	1	43	33	4	6	0
29	aJ	1	43	33	4	6	0
29	aJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	bJ	1	43	33	4	6	0
29	cJ	1	43	33	4	6	0
29	cJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	dJ	1	43	33	4	6	0
29	eJ	1	43	33	4	6	0
29	eJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	fJ	1	43	33	4	6	0
29	gJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	gJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	hJ	1	43	33	4	6	0
29	iJ	1	43	33	4	6	0
29	iJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	jJ	1	43	33	4	6	0
29	kJ	1	43	33	4	6	0
29	kJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	lJ	1	43	33	4	6	0
29	mJ	1	43	33	4	6	0
29	mJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	nJ	1	43	33	4	6	0
29	oJ	1	43	33	4	6	0
29	oJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	pJ	1	43	33	4	6	0
29	pJ	1	43	33	4	6	0
29	pJ	1	43	33	4	6	0
29	qJ	1	43	33	4	6	0
29	qJ	1	43	33	4	6	0
29	rJ	1	43	33	4	6	0
29	rJ	1	43	33	4	6	0
29	rJ	1	43	33	4	6	0
29	sJ	1	43	33	4	6	0
29	sJ	1	43	33	4	6	0
29	sJ	1	43	33	4	6	0
29	tJ	1	43	33	4	6	0
29	tJ	1	43	33	4	6	0
29	uJ	1	43	33	4	6	0
29	uJ	1	43	33	4	6	0
29	uJ	1	43	33	4	6	0
29	vJ	1	43	33	4	6	0
29	vJ	1	43	33	4	6	0
29	wJ	1	43	33	4	6	0
29	wJ	1	43	33	4	6	0
29	wJ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	xJ	1	43	33	4	6	0
29	xJ	1	43	33	4	6	0
29	xJ	1	43	33	4	6	0
29	yJ	1	43	33	4	6	0
29	zJ	1	43	33	4	6	0
29	AK	1	43	33	4	6	0
29	AK	1	43	33	4	6	0
29	AK	1	43	33	4	6	0
29	DK	1	43	33	4	6	0
29	FK	1	43	33	4	6	0
29	HK	1	43	33	4	6	0
29	JK	1	43	33	4	6	0
29	LK	1	43	33	4	6	0
29	NK	1	43	33	4	6	0
29	OK	1	43	33	4	6	0
29	OK	1	43	33	4	6	0
29	PK	1	43	33	4	6	0
29	PK	1	43	33	4	6	0
29	PK	1	43	33	4	6	0
29	QK	1	43	33	4	6	0
29	QK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	RK	1	Total 43	C 33	N 4	O 6	0
29	RK	1	Total 43	C 33	N 4	O 6	0
29	RK	1	Total 43	C 33	N 4	O 6	0
29	SK	1	Total 43	C 33	N 4	O 6	0
29	SK	1	Total 43	C 33	N 4	O 6	0
29	TK	1	Total 43	C 33	N 4	O 6	0
29	TK	1	Total 43	C 33	N 4	O 6	0
29	UK	1	Total 43	C 33	N 4	O 6	0
29	UK	1	Total 43	C 33	N 4	O 6	0
29	UK	1	Total 43	C 33	N 4	O 6	0
29	VK	1	Total 43	C 33	N 4	O 6	0
29	VK	1	Total 43	C 33	N 4	O 6	0
29	VK	1	Total 43	C 33	N 4	O 6	0
29	WK	1	Total 43	C 33	N 4	O 6	0
29	WK	1	Total 43	C 33	N 4	O 6	0
29	YK	1	Total 43	C 33	N 4	O 6	0
29	YK	1	Total 43	C 33	N 4	O 6	0
29	ZK	1	Total 43	C 33	N 4	O 6	0
29	ZK	1	Total 43	C 33	N 4	O 6	0
29	ZK	1	Total 43	C 33	N 4	O 6	0
29	aK	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	aK	1	43	33	4	6	0
29	aK	1	43	33	4	6	0
29	bK	1	43	33	4	6	0
29	bK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	cK	1	43	33	4	6	0
29	dK	1	43	33	4	6	0
29	dK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	eK	1	43	33	4	6	0
29	fK	1	43	33	4	6	0
29	fK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	gK	1	43	33	4	6	0
29	hK	1	43	33	4	6	0
29	hK	1	43	33	4	6	0
29	iK	1	43	33	4	6	0
29	iK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	iK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	jK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	kK	1	Total 43	C 33	N 4	O 6	0
29	lK	1	Total 43	C 33	N 4	O 6	0
29	lK	1	Total 43	C 33	N 4	O 6	0
29	mK	1	Total 43	C 33	N 4	O 6	0
29	mK	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	AL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	BL	1	Total 43	C 33	N 4	O 6	0
29	CL	1	Total 43	C 33	N 4	O 6	0
29	CL	1	Total 43	C 33	N 4	O 6	0
29	DL	1	Total 43	C 33	N 4	O 6	0
29	DL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	EL	1	43	33	4	6	0
29	EL	1	43	33	4	6	0
29	FL	1	43	33	4	6	0
29	FL	1	43	33	4	6	0
29	FL	1	43	33	4	6	0
29	GL	1	43	33	4	6	0
29	GL	1	43	33	4	6	0
29	HL	1	43	33	4	6	0
29	HL	1	43	33	4	6	0
29	IL	1	43	33	4	6	0
29	IL	1	43	33	4	6	0
29	IL	1	43	33	4	6	0
29	JL	1	43	33	4	6	0
29	JL	1	43	33	4	6	0
29	JL	1	43	33	4	6	0
29	KL	1	43	33	4	6	0
29	KL	1	43	33	4	6	0
29	LL	1	43	33	4	6	0
29	LL	1	43	33	4	6	0
29	ML	1	43	33	4	6	0
29	ML	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	NL	1	43	33	4	6	0
29	NL	1	43	33	4	6	0
29	NL	1	43	33	4	6	0
29	OL	1	43	33	4	6	0
29	OL	1	43	33	4	6	0
29	PL	1	43	33	4	6	0
29	PL	1	43	33	4	6	0
29	PL	1	43	33	4	6	0
29	QL	1	43	33	4	6	0
29	QL	1	43	33	4	6	0
29	RL	1	43	33	4	6	0
29	RL	1	43	33	4	6	0
29	RL	1	43	33	4	6	0
29	SL	1	43	33	4	6	0
29	SL	1	43	33	4	6	0
29	TL	1	43	33	4	6	0
29	TL	1	43	33	4	6	0
29	TL	1	43	33	4	6	0
29	UL	1	43	33	4	6	0
29	UL	1	43	33	4	6	0
29	VL	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	WL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	XL	1	43	33	4	6	0
29	YL	1	43	33	4	6	0
29	YL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	ZL	1	43	33	4	6	0
29	aL	1	43	33	4	6	0
29	aL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	bL	1	43	33	4	6	0
29	cL	1	43	33	4	6	0
29	cL	1	43	33	4	6	0
29	dL	1	43	33	4	6	0
29	dL	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	dL	1	43	33	4	6	0
29	eL	1	43	33	4	6	0
29	eL	1	43	33	4	6	0
29	fL	1	43	33	4	6	0
29	fL	1	43	33	4	6	0
29	fL	1	43	33	4	6	0
29	gL	1	43	33	4	6	0
29	gL	1	43	33	4	6	0
29	hL	1	43	33	4	6	0
29	hL	1	43	33	4	6	0
29	hL	1	43	33	4	6	0
29	iL	1	43	33	4	6	0
29	iL	1	43	33	4	6	0
29	jL	1	43	33	4	6	0
29	jL	1	43	33	4	6	0
29	jL	1	43	33	4	6	0
29	kL	1	43	33	4	6	0
29	kL	1	43	33	4	6	0
29	lL	1	43	33	4	6	0
29	lL	1	43	33	4	6	0
29	lL	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	mL	1	Total 43	C 33	N 4	O 6	0
29	mL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	nL	1	Total 43	C 33	N 4	O 6	0
29	oL	1	Total 43	C 33	N 4	O 6	0
29	oL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	pL	1	Total 43	C 33	N 4	O 6	0
29	qL	1	Total 43	C 33	N 4	O 6	0
29	qL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	rL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	sL	1	Total 43	C 33	N 4	O 6	0
29	tL	1	Total 43	C 33	N 4	O 6	0
29	tL	1	Total 43	C 33	N 4	O 6	0
29	uL	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	uL	1	43	33	4	6	0
29	uL	1	43	33	4	6	0
29	vL	1	43	33	4	6	0
29	vL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	wL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	xL	1	43	33	4	6	0
29	yL	1	43	33	4	6	0
29	zL	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	AM	1	43	33	4	6	0
29	BM	1	43	33	4	6	0
29	CM	1	43	33	4	6	0
29	CM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0
29	DM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	EM	1	43	33	4	6	0
29	EM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	FM	1	43	33	4	6	0
29	GM	1	43	33	4	6	0
29	GM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	HM	1	43	33	4	6	0
29	IM	1	43	33	4	6	0
29	IM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	JM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	KM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0
29	LM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MM	1	43	33	4	6	0
29	MM	1	43	33	4	6	0
29	NM	1	43	33	4	6	0
29	NM	1	43	33	4	6	0
29	OM	1	43	33	4	6	0
29	OM	1	43	33	4	6	0
29	PM	1	43	33	4	6	0
29	PM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	QM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	RM	1	43	33	4	6	0
29	SM	1	43	33	4	6	0
29	SM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	TM	1	43	33	4	6	0
29	UM	1	43	33	4	6	0
29	VM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VM	1	43	33	4	6	0
29	VM	1	43	33	4	6	0
29	WM	1	43	33	4	6	0
29	WM	1	43	33	4	6	0
29	XM	1	43	33	4	6	0
29	XM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	YM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	ZM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	aM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	cM	1	43	33	4	6	0
29	dM	1	43	33	4	6	0
29	dM	1	43	33	4	6	0
29	eM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	eM	1	43	33	4	6	0
29	fM	1	43	33	4	6	0
29	fM	1	43	33	4	6	0
29	gM	1	43	33	4	6	0
29	gM	1	43	33	4	6	0
29	gM	1	43	33	4	6	0
29	hM	1	43	33	4	6	0
29	hM	1	43	33	4	6	0
29	iM	1	43	33	4	6	0
29	iM	1	43	33	4	6	0
29	iM	1	43	33	4	6	0
29	jM	1	43	33	4	6	0
29	jM	1	43	33	4	6	0
29	kM	1	43	33	4	6	0
29	kM	1	43	33	4	6	0
29	kM	1	43	33	4	6	0
29	lM	1	43	33	4	6	0
29	lM	1	43	33	4	6	0
29	mM	1	43	33	4	6	0
29	mM	1	43	33	4	6	0
29	mM	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	AN	1	43	33	4	6	0
29	AN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	BN	1	43	33	4	6	0
29	CN	1	43	33	4	6	0
29	CN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	DN	1	43	33	4	6	0
29	EN	1	43	33	4	6	0
29	EN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	FN	1	43	33	4	6	0
29	GN	1	43	33	4	6	0
29	GN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	HN	1	43	33	4	6	0
29	IN	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	IN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	JN	1	43	33	4	6	0
29	KN	1	43	33	4	6	0
29	KN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	LN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	MN	1	43	33	4	6	0
29	AO	1	43	33	4	6	0
29	AO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	BO	1	43	33	4	6	0
29	CO	1	43	33	4	6	0
29	CO	1	43	33	4	6	0
29	DO	1	43	33	4	6	0
29	DO	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	DO	1	43	33	4	6	0
29	EO	1	43	33	4	6	0
29	EO	1	43	33	4	6	0
29	FO	1	43	33	4	6	0
29	FO	1	43	33	4	6	0
29	FO	1	43	33	4	6	0
29	GO	1	43	33	4	6	0
29	GO	1	43	33	4	6	0
29	HO	1	43	33	4	6	0
29	HO	1	43	33	4	6	0
29	HO	1	43	33	4	6	0
29	IO	1	43	33	4	6	0
29	IO	1	43	33	4	6	0
29	IO	1	43	33	4	6	0
29	JO	1	43	33	4	6	0
29	JO	1	43	33	4	6	0
29	JO	1	43	33	4	6	0
29	KO	1	43	33	4	6	0
29	KO	1	43	33	4	6	0
29	LO	1	43	33	4	6	0
29	LO	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MO	1	43	33	4	6	0
29	MO	1	43	33	4	6	0
29	MO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	NO	1	43	33	4	6	0
29	AQ	1	43	33	4	6	0
29	AQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	BQ	1	43	33	4	6	0
29	CQ	1	43	33	4	6	0
29	CQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	DQ	1	43	33	4	6	0
29	EQ	1	43	33	4	6	0
29	EQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0
29	FQ	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	GQ	1	43	33	4	6	0
29	GQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	HQ	1	43	33	4	6	0
29	IQ	1	43	33	4	6	0
29	IQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	JQ	1	43	33	4	6	0
29	KQ	1	43	33	4	6	0
29	KQ	1	43	33	4	6	0
29	LQ	1	43	33	4	6	0
29	LQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	MQ	1	43	33	4	6	0
29	eR	1	43	33	4	6	0
29	MR	1	43	33	4	6	0

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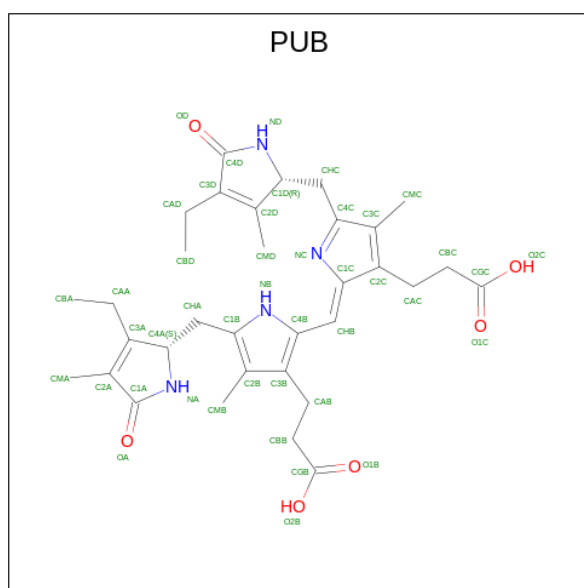
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	MR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	NR	1	43	33	4	6	0
29	OR	1	43	33	4	6	0
29	OR	1	43	33	4	6	0
29	PR	1	43	33	4	6	0
29	PR	1	43	33	4	6	0
29	QR	1	43	33	4	6	0
29	QR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	RR	1	43	33	4	6	0
29	SR	1	43	33	4	6	0
29	SR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	TR	1	43	33	4	6	0
29	UR	1	43	33	4	6	0
29	UR	1	43	33	4	6	0
29	VR	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
29	VR	1	Total 43	C 33	N 4	O 6	0
29	VR	1	Total 43	C 33	N 4	O 6	0
29	WR	1	Total 43	C 33	N 4	O 6	0
29	WR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0
29	XR	1	Total 43	C 33	N 4	O 6	0

- Molecule 30 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	
30	A1	1	Total 43	C 33	N 4	O 6	0
30	A1	1	Total 43	C 33	N 4	O 6	0
30	A7	1	Total 43	C 33	N 4	O 6	0
30	A7	1	Total 43	C 33	N 4	O 6	0

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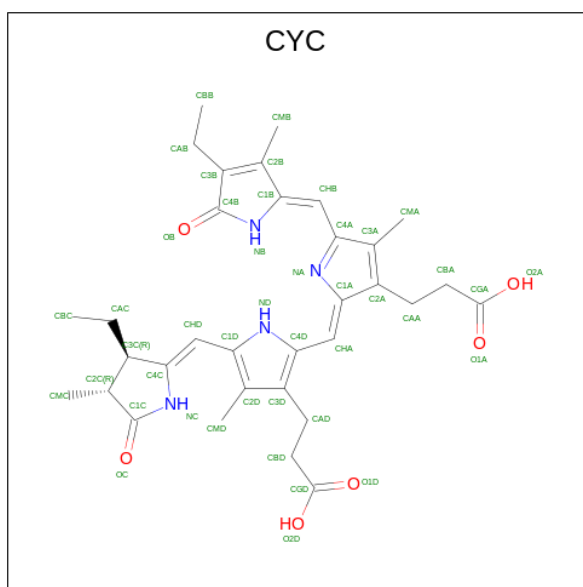
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	A9	1	43	33	4	6	0
30	A9	1	43	33	4	6	0
30	MA	1	43	33	4	6	0
30	MA	1	43	33	4	6	0
30	AB	1	43	33	4	6	0
30	AB	1	43	33	4	6	0
30	BB	1	43	33	4	6	0
30	QB	1	43	33	4	6	0
30	AF	1	43	33	4	6	0
30	AF	1	43	33	4	6	0
30	MG	1	43	33	4	6	0
30	MG	1	43	33	4	6	0
30	AI	1	43	33	4	6	0
30	AI	1	43	33	4	6	0
30	wJ	1	43	33	4	6	0
30	wJ	1	43	33	4	6	0
30	xJ	1	43	33	4	6	0
30	xJ	1	43	33	4	6	0
30	yJ	1	43	33	4	6	0
30	yJ	1	43	33	4	6	0
30	AK	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
30	AK	1	43	33	4	6	0
30	wL	1	43	33	4	6	0
30	wL	1	43	33	4	6	0
30	xL	1	43	33	4	6	0
30	xL	1	43	33	4	6	0
30	yL	1	43	33	4	6	0
30	yL	1	43	33	4	6	0
30	AM	1	43	33	4	6	0
30	AM	1	43	33	4	6	0
30	BM	1	43	33	4	6	0
30	QM	1	43	33	4	6	0
30	MN	1	43	33	4	6	0
30	MN	1	43	33	4	6	0
30	MQ	1	43	33	4	6	0
30	MQ	1	43	33	4	6	0

- Molecule 31 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$).



Mol	Chain	Residues	Atoms			AltConf	
			Total	C	N		O
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	E1	1	43	33	4	6	0
31	F1	1	43	33	4	6	0
31	H1	1	43	33	4	6	0
31	I1	1	43	33	4	6	0
31	J1	1	43	33	4	6	0
31	K1	1	43	33	4	6	0
31	L1	1	43	33	4	6	0
31	M1	1	43	33	4	6	0
31	N1	1	43	33	4	6	0
31	C7	1	43	33	4	6	0
31	D7	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	E7	1	Total 43	C 33	N 4	O 6	0
31	F7	1	Total 43	C 33	N 4	O 6	0
31	G7	1	Total 43	C 33	N 4	O 6	0
31	H7	1	Total 43	C 33	N 4	O 6	0
31	I7	1	Total 43	C 33	N 4	O 6	0
31	J7	1	Total 43	C 33	N 4	O 6	0
31	K7	1	Total 43	C 33	N 4	O 6	0
31	L7	1	Total 43	C 33	N 4	O 6	0
31	M7	1	Total 43	C 33	N 4	O 6	0
31	N7	1	Total 43	C 33	N 4	O 6	0
31	C9	1	Total 43	C 33	N 4	O 6	0
31	D9	1	Total 43	C 33	N 4	O 6	0
31	E9	1	Total 43	C 33	N 4	O 6	0
31	F9	1	Total 43	C 33	N 4	O 6	0
31	G9	1	Total 43	C 33	N 4	O 6	0
31	H9	1	Total 43	C 33	N 4	O 6	0
31	I9	1	Total 43	C 33	N 4	O 6	0
31	J9	1	Total 43	C 33	N 4	O 6	0
31	K9	1	Total 43	C 33	N 4	O 6	0
31	L9	1	Total 43	C 33	N 4	O 6	0
31	M9	1	Total 43	C 33	N 4	O 6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	N9	1	43	33	4	6	0
31	CF	1	43	33	4	6	0
31	DF	1	43	33	4	6	0
31	EF	1	43	33	4	6	0
31	FF	1	43	33	4	6	0
31	GF	1	43	33	4	6	0
31	HF	1	43	33	4	6	0
31	IF	1	43	33	4	6	0
31	JF	1	43	33	4	6	0
31	KF	1	43	33	4	6	0
31	LF	1	43	33	4	6	0
31	MF	1	43	33	4	6	0
31	NF	1	43	33	4	6	0
31	CI	1	43	33	4	6	0
31	DI	1	43	33	4	6	0
31	EI	1	43	33	4	6	0
31	FI	1	43	33	4	6	0
31	GI	1	43	33	4	6	0
31	HI	1	43	33	4	6	0
31	II	1	43	33	4	6	0
31	JI	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	KI	1	43	33	4	6	0
31	LI	1	43	33	4	6	0
31	MI	1	43	33	4	6	0
31	NI	1	43	33	4	6	0
31	CK	1	43	33	4	6	0
31	DK	1	43	33	4	6	0
31	EK	1	43	33	4	6	0
31	FK	1	43	33	4	6	0
31	GK	1	43	33	4	6	0
31	HK	1	43	33	4	6	0
31	IK	1	43	33	4	6	0
31	JK	1	43	33	4	6	0
31	KK	1	43	33	4	6	0
31	LK	1	43	33	4	6	0
31	MK	1	43	33	4	6	0
31	NK	1	43	33	4	6	0
31	AP	1	43	33	4	6	0
31	DP	1	43	33	4	6	0
31	CP	1	43	33	4	6	0
31	FP	1	43	33	4	6	0
31	EP	1	43	33	4	6	0

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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	BP	1	Total 43	C 33	N 4	O 6	0
31	GP	1	Total 43	C 33	N 4	O 6	0
31	HP	1	Total 43	C 33	N 4	O 6	0
31	IP	1	Total 43	C 33	N 4	O 6	0
31	JP	1	Total 43	C 33	N 4	O 6	0
31	KP	1	Total 43	C 33	N 4	O 6	0
31	MP	1	Total 43	C 33	N 4	O 6	0
31	NP	1	Total 43	C 33	N 4	O 6	0
31	OP	1	Total 43	C 33	N 4	O 6	0
31	PP	1	Total 43	C 33	N 4	O 6	0
31	QP	1	Total 43	C 33	N 4	O 6	0
31	RP	1	Total 43	C 33	N 4	O 6	0
31	SP	1	Total 43	C 33	N 4	O 6	0
31	TP	1	Total 43	C 33	N 4	O 6	0
31	UP	1	Total 43	C 33	N 4	O 6	0
31	VP	1	Total 43	C 33	N 4	O 6	0
31	WP	1	Total 43	C 33	N 4	O 6	0
31	XP	1	Total 43	C 33	N 4	O 6	0
31	YP	1	Total 43	C 33	N 4	O 6	0
31	cP	1	Total 43	C 33	N 4	O 6	0
31	eP	1	Total 43	C 33	N 4	O 6	0

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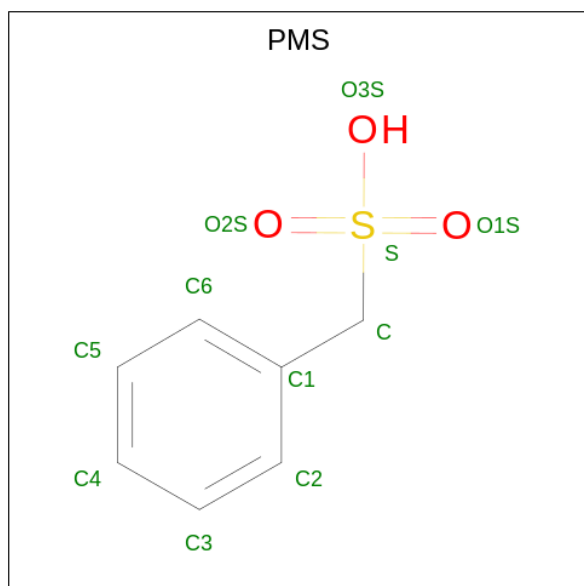
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	fP	1	Total 43	C 33	N 4	O 6	0
31	gP	1	Total 43	C 33	N 4	O 6	0
31	hP	1	Total 43	C 33	N 4	O 6	0
31	iP	1	Total 43	C 33	N 4	O 6	0
31	jP	1	Total 43	C 33	N 4	O 6	0
31	kP	1	Total 43	C 33	N 4	O 6	0
31	lP	1	Total 43	C 33	N 4	O 6	0
31	mP	1	Total 43	C 33	N 4	O 6	0
31	nP	1	Total 43	C 33	N 4	O 6	0
31	oP	1	Total 43	C 33	N 4	O 6	0
31	pP	1	Total 43	C 33	N 4	O 6	0
31	qP	1	Total 43	C 33	N 4	O 6	0
31	rP	1	Total 43	C 33	N 4	O 6	0
31	sP	1	Total 43	C 33	N 4	O 6	0
31	tP	1	Total 43	C 33	N 4	O 6	0
31	uP	1	Total 43	C 33	N 4	O 6	0
31	vP	1	Total 43	C 33	N 4	O 6	0
31	wP	1	Total 43	C 33	N 4	O 6	0
31	xP	1	Total 43	C 33	N 4	O 6	0
31	yP	1	Total 43	C 33	N 4	O 6	0
31	1P	1	Total 43	C 33	N 4	O 6	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
31	1P	1	43	33	4	6	0

- Molecule 32 is phenylmethanesulfonic acid (three-letter code: PMS) (formula: $C_7H_8O_3S$).

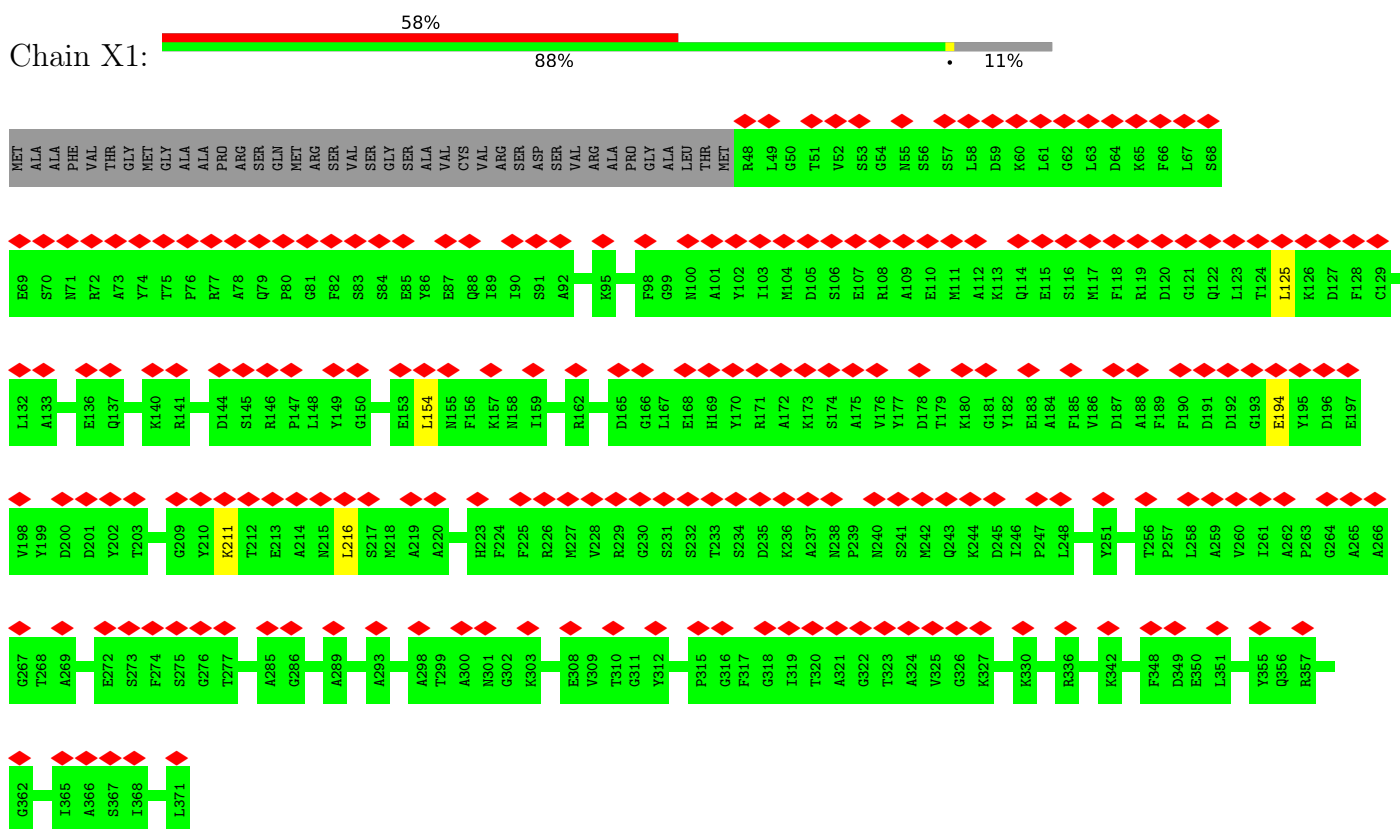


Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	S	
32	k6	1	11	7	3	1	0
32	k6	1	11	7	3	1	0
32	kH	1	11	7	3	1	0
32	kH	1	11	7	3	1	0

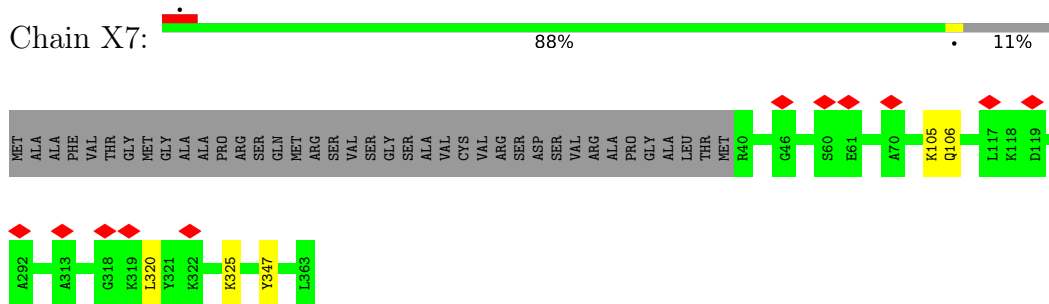
3 Residue-property plots

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

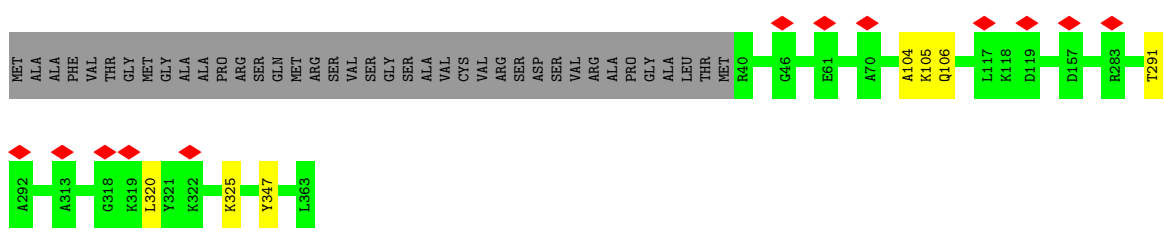
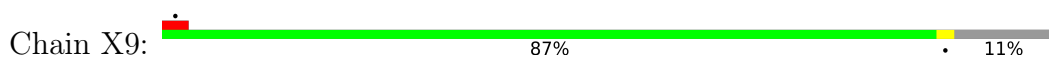
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



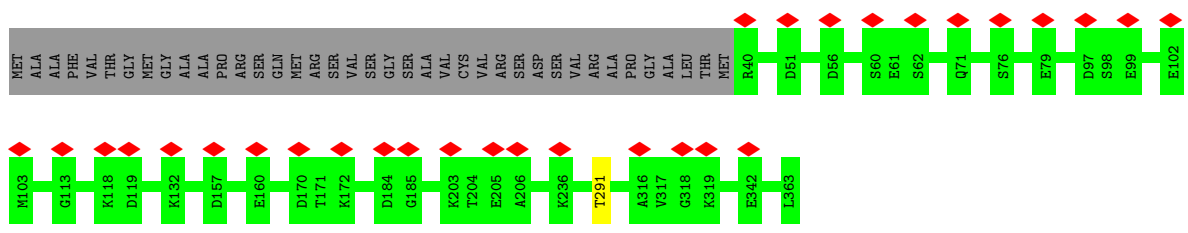
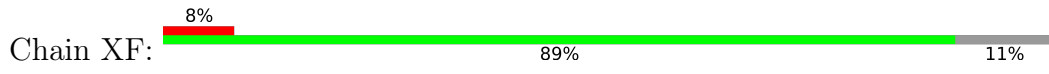
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



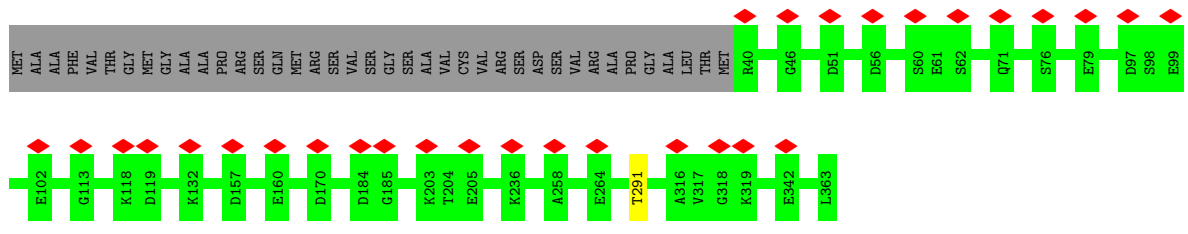
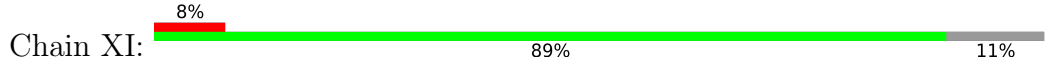
- Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



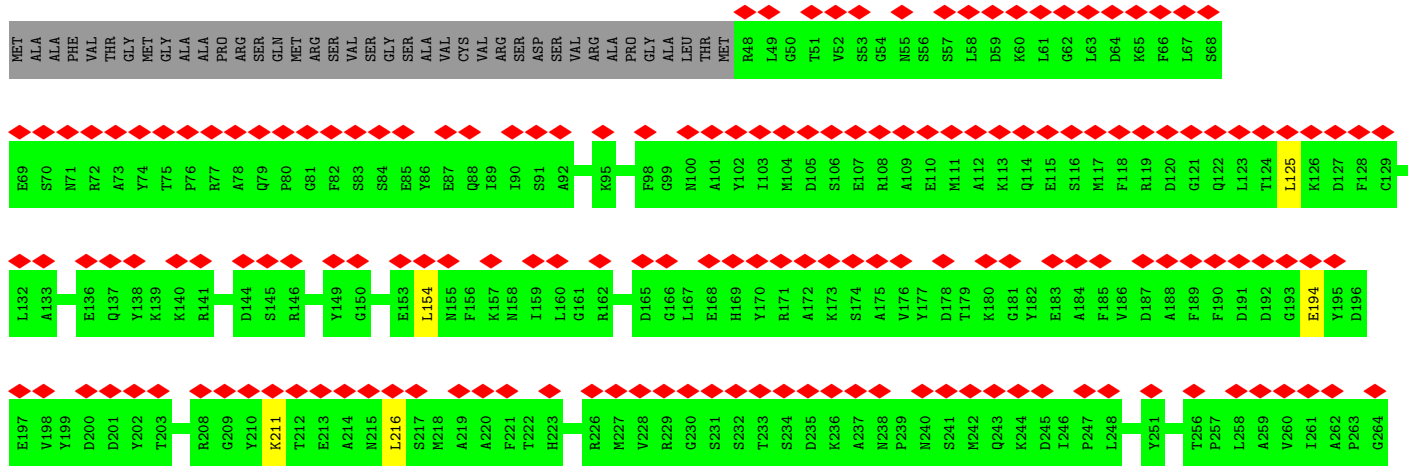
• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

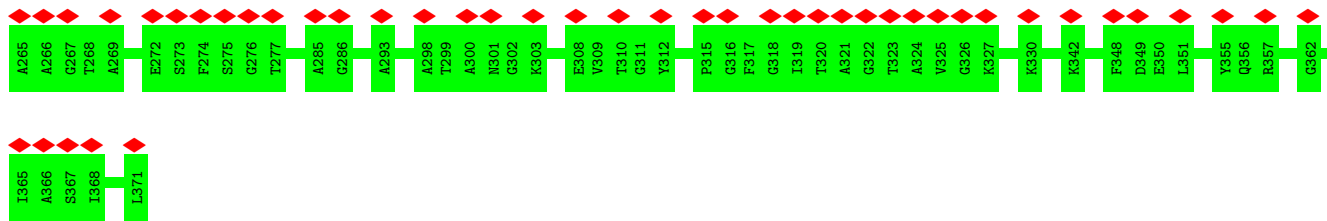


• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

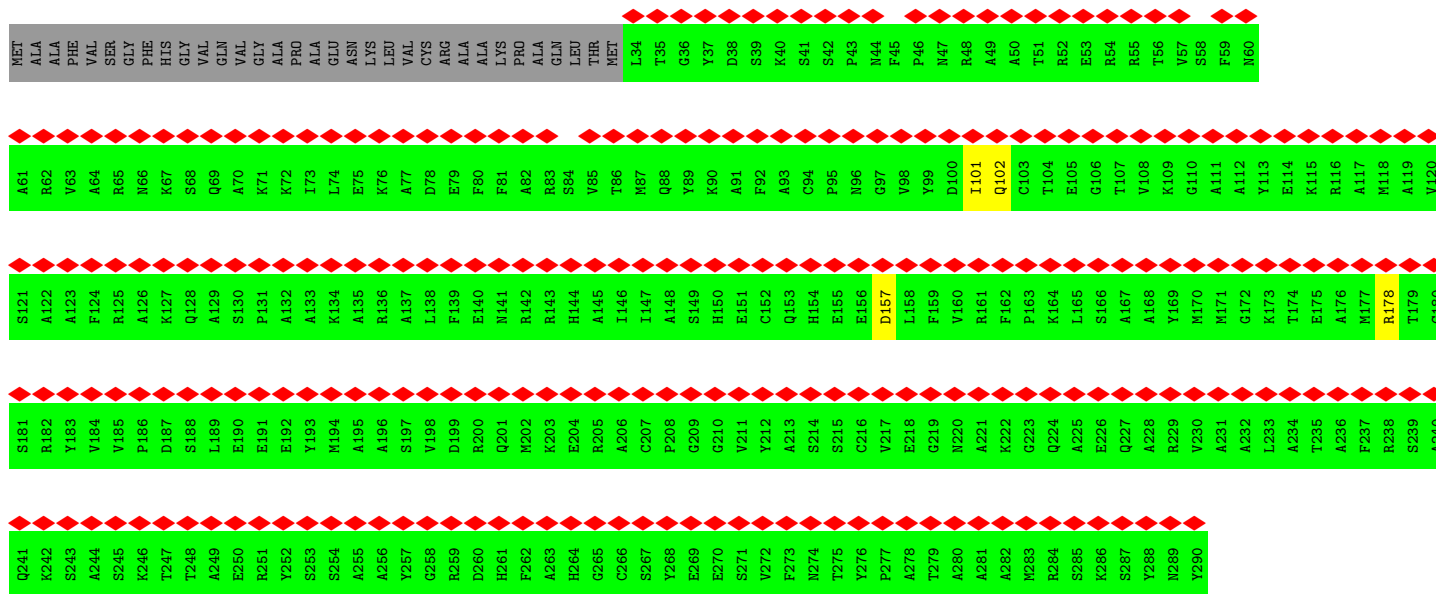
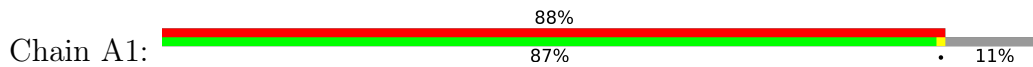


• Molecule 1: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

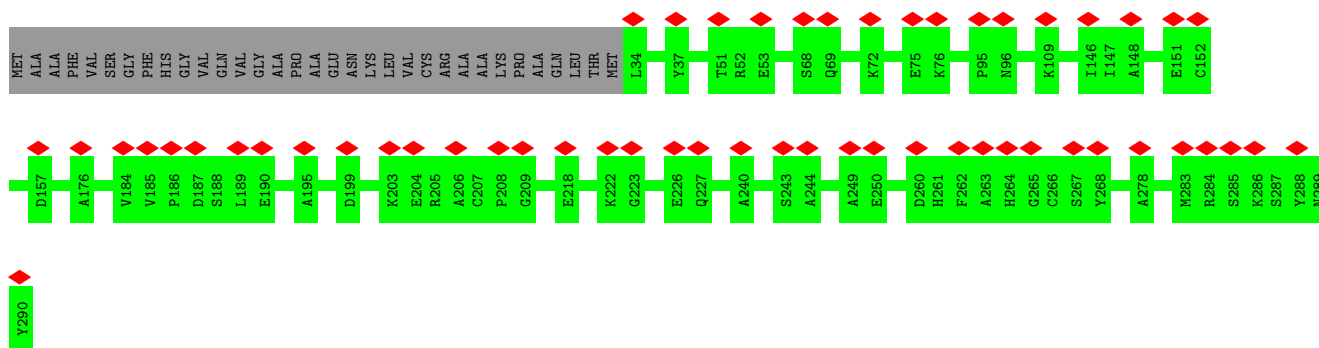
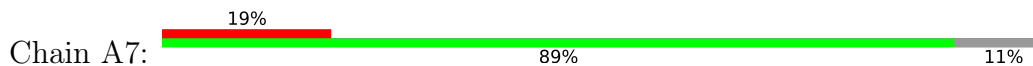




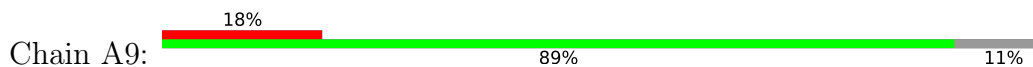
• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

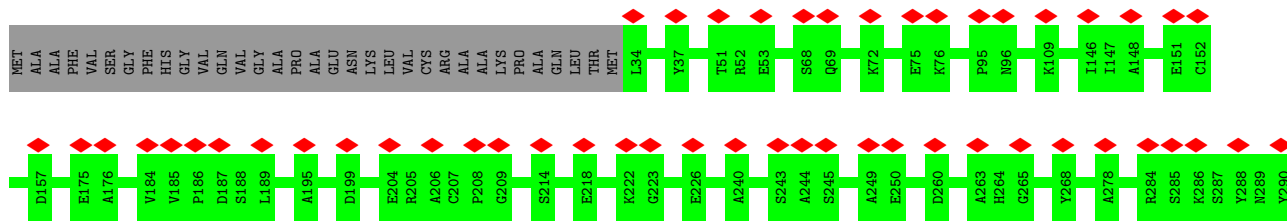


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

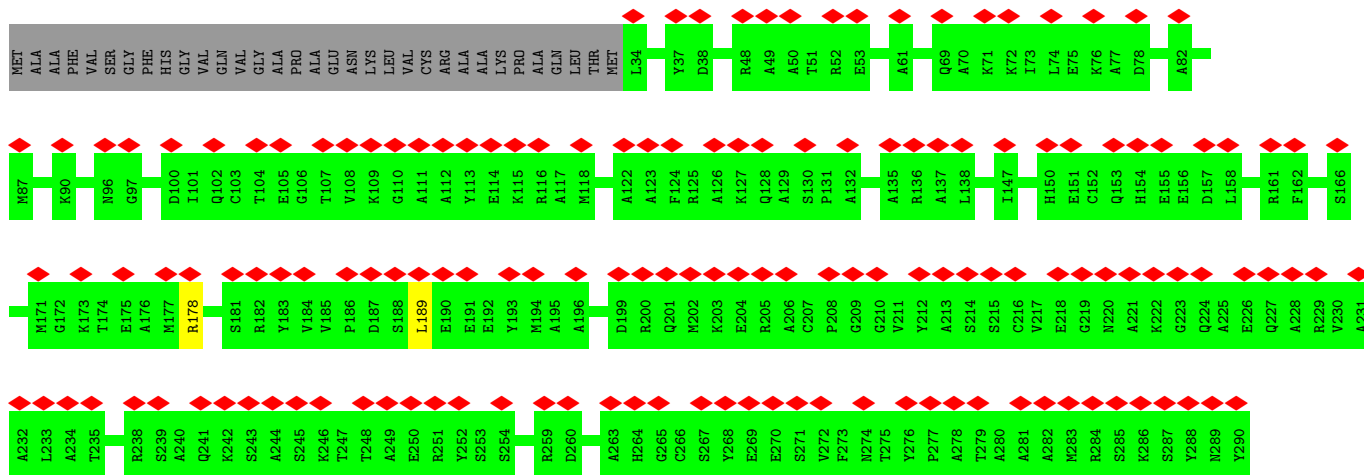
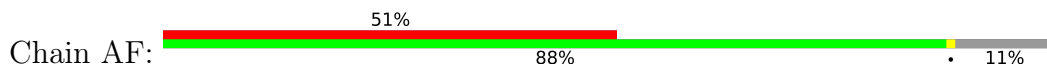


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

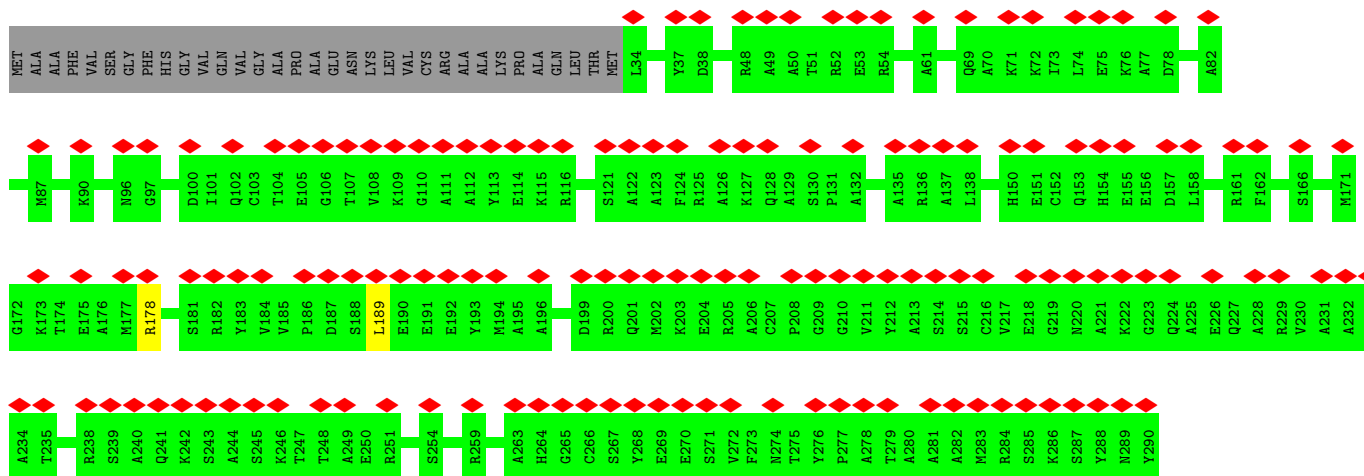
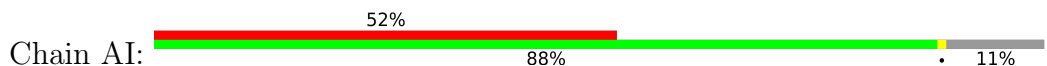




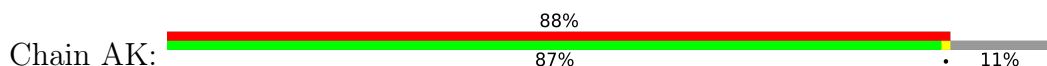
• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

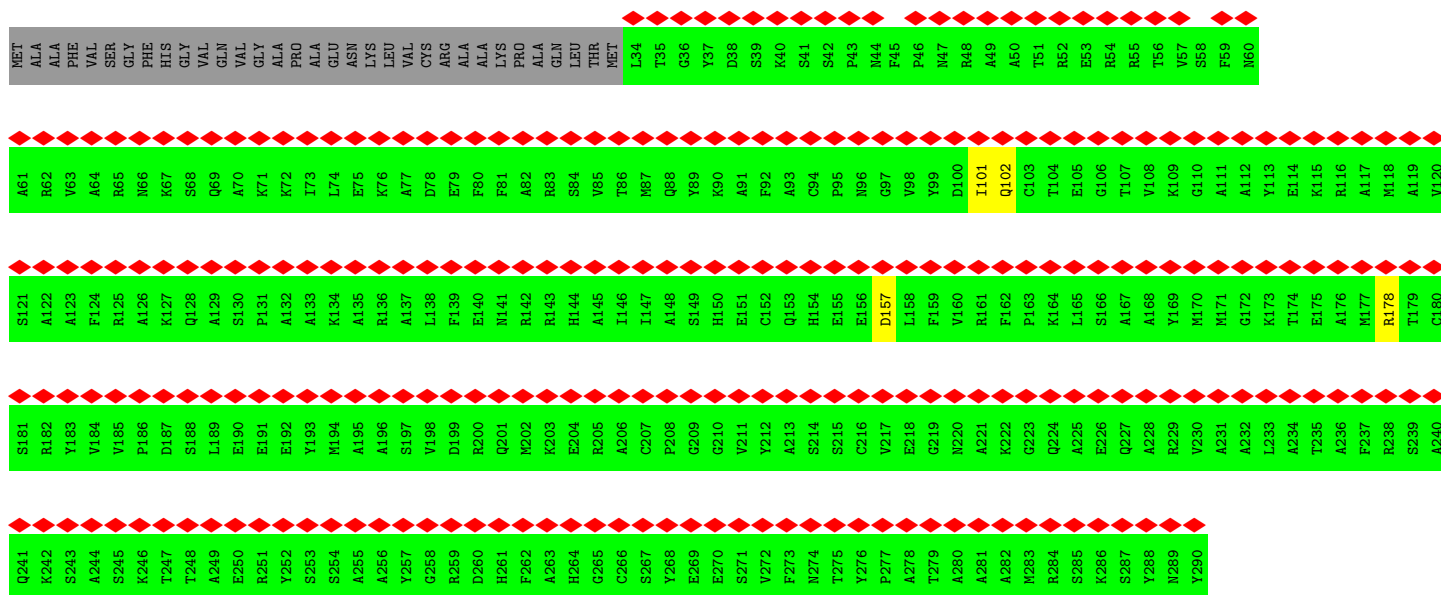


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

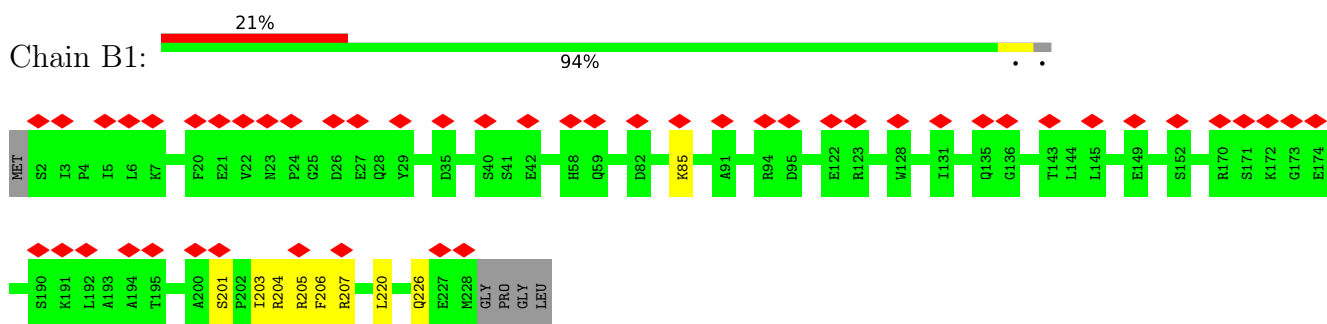


• Molecule 2: R-phycoerythrin gamma chain, chloroplastic

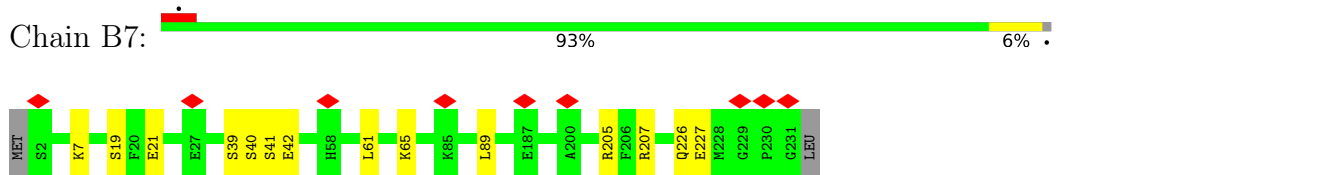




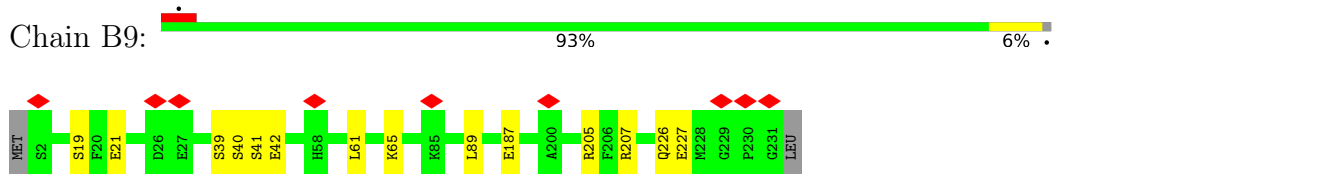
• Molecule 3: Phycobilisome rod-core linker polypeptide



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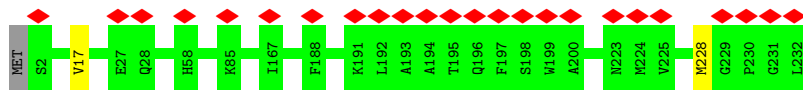


• Molecule 3: Phycobilisome rod-core linker polypeptide



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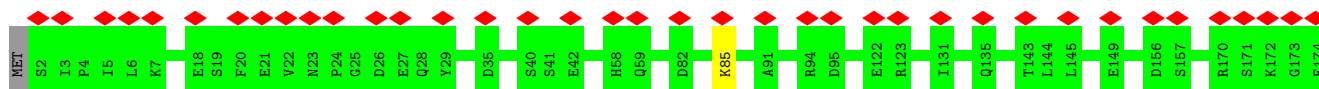




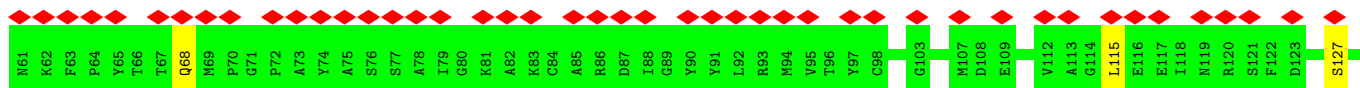
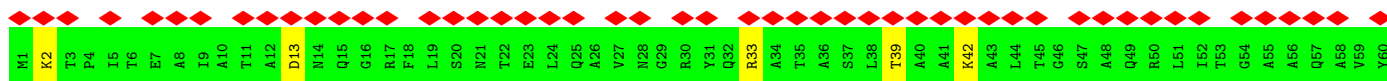
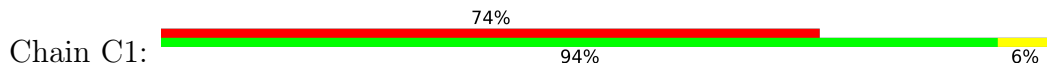
- Molecule 3: Phycobilisome rod-core linker polypeptide



- Molecule 3: Phycobilisome rod-core linker polypeptide



- Molecule 4: C-phycoerythrin alpha subunit

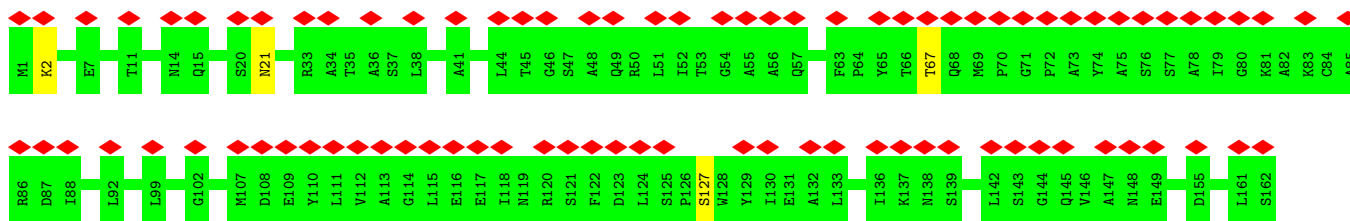


- Molecule 4: C-phycoerythrin alpha subunit

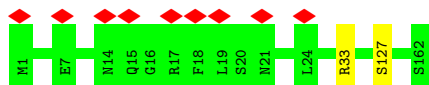


- Molecule 4: C-phycoerythrin alpha subunit

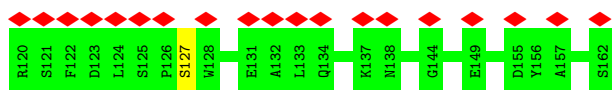
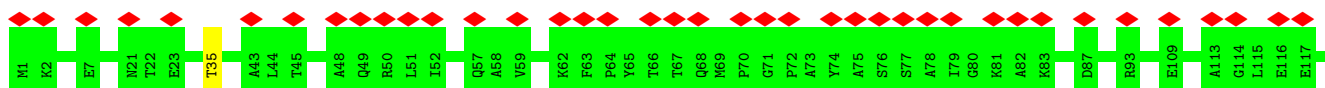




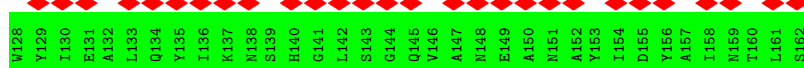
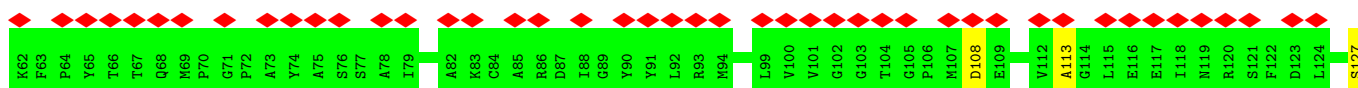
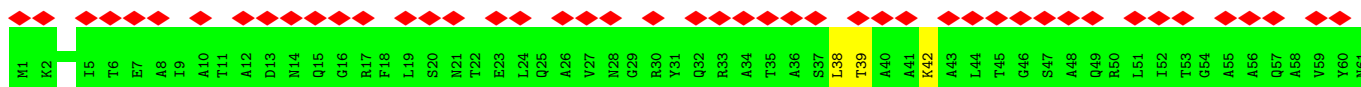
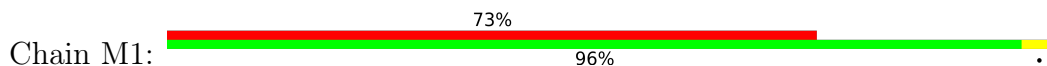
- Molecule 4: C-phycoerythrin alpha subunit



- Molecule 4: C-phycoerythrin alpha subunit



- Molecule 4: C-phycoerythrin alpha subunit



- Molecule 4: C-phycoerythrin alpha subunit



- Molecule 4: C-phycoerythrin alpha subunit

Chain E7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain G7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain I7:  93% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain K7:  93% 7%



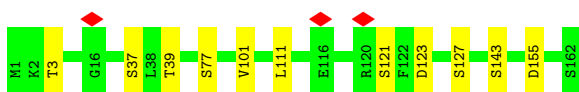
• Molecule 4: C-phyco cyanin alpha subunit

Chain M7:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain C9:  93% 7%



• Molecule 4: C-phyco cyanin alpha subunit

Chain E9:  94% 6%



• Molecule 4: C-phyco cyanin alpha subunit

Chain G9:  94% 6%



• Molecule 4: C-phycoerythrin alpha subunit

Chain I9:  93% 6%



• Molecule 4: C-phycoerythrin alpha subunit

Chain K9:  93% 7%



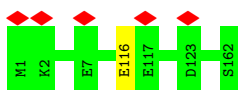
• Molecule 4: C-phycoerythrin alpha subunit

Chain M9:  94% 6%



• Molecule 4: C-phycoerythrin alpha subunit

Chain CF:  99%



• Molecule 4: C-phycoerythrin alpha subunit

Chain EF:  99%



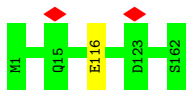
• Molecule 4: C-phycoerythrin alpha subunit

Chain GF:  99%



- Molecule 4: C-phycoerythrin alpha subunit

Chain IF:  99%



- Molecule 4: C-phycoerythrin alpha subunit

Chain KF:  99%



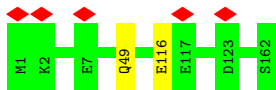
- Molecule 4: C-phycoerythrin alpha subunit

Chain MF:  99%



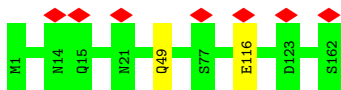
- Molecule 4: C-phycoerythrin alpha subunit

Chain CI:  99%



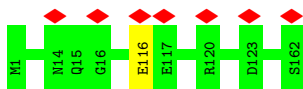
- Molecule 4: C-phycoerythrin alpha subunit

Chain EI:  99%



- Molecule 4: C-phycoerythrin alpha subunit

Chain GI:  99%

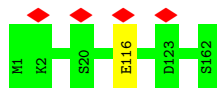


- Molecule 4: C-phycoerythrin alpha subunit

Chain II:  99%



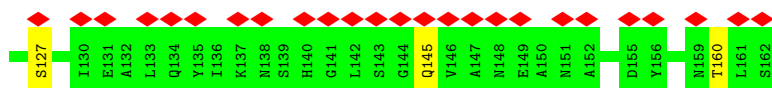
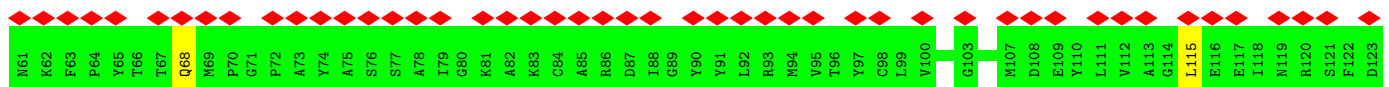
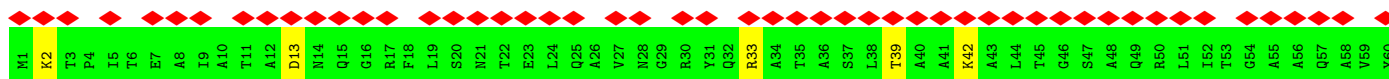
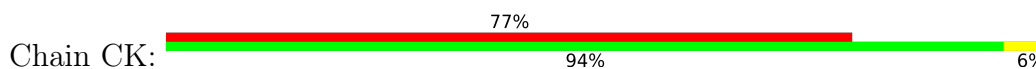
- Molecule 4: C-phycoerythrin alpha subunit



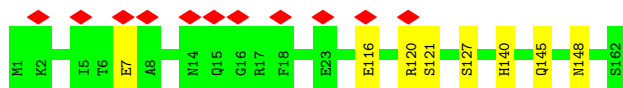
- Molecule 4: C-phycoerythrin alpha subunit



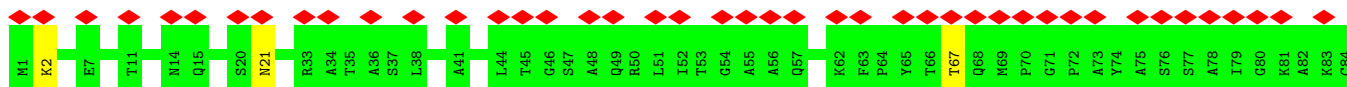
- Molecule 4: C-phycoerythrin alpha subunit

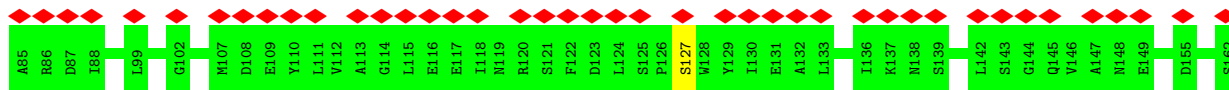


- Molecule 4: C-phycoerythrin alpha subunit

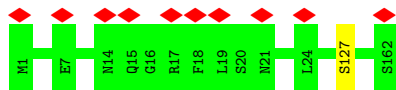


- Molecule 4: C-phycoerythrin alpha subunit

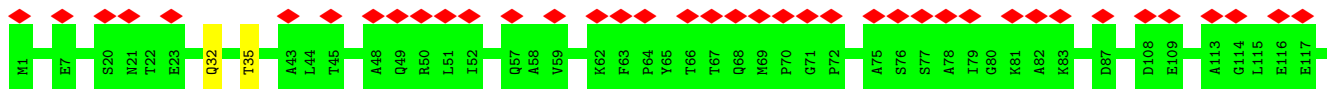




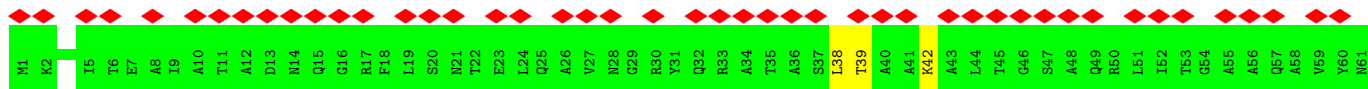
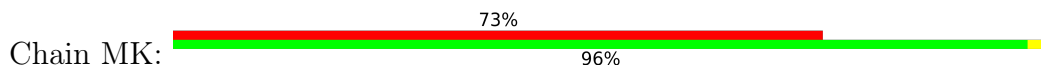
• Molecule 4: C-phycoerythrin alpha subunit



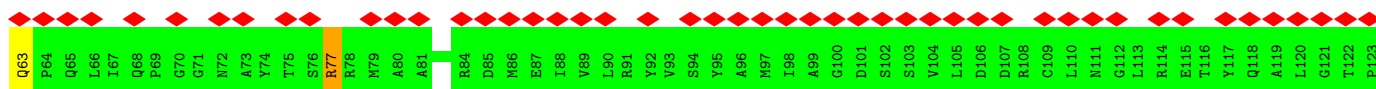
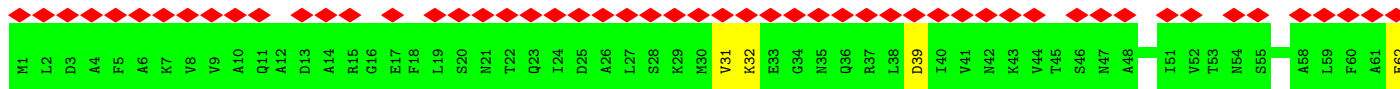
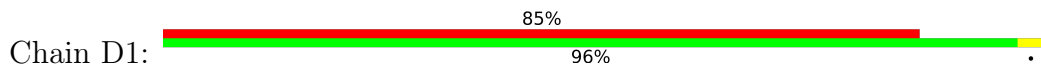
• Molecule 4: C-phycoerythrin alpha subunit

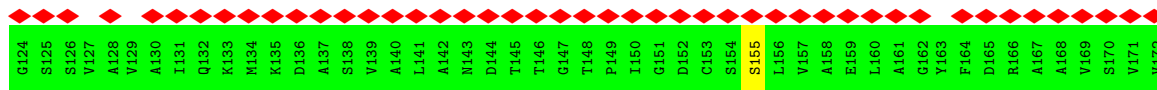


• Molecule 4: C-phycoerythrin alpha subunit

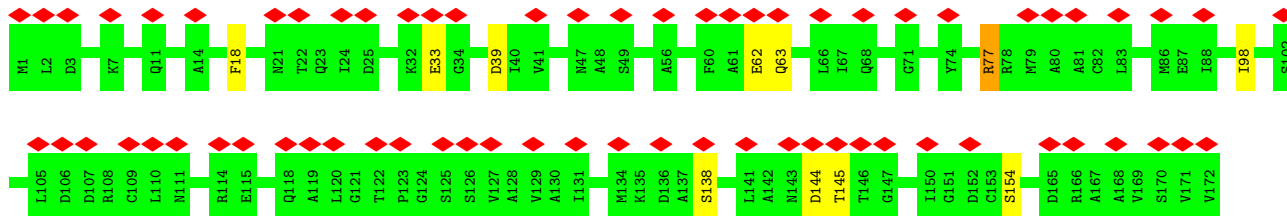
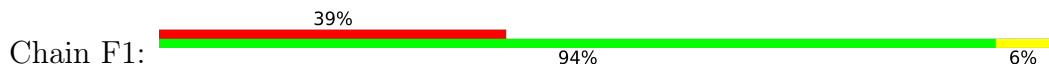


• Molecule 5: C-phycoerythrin beta subunit

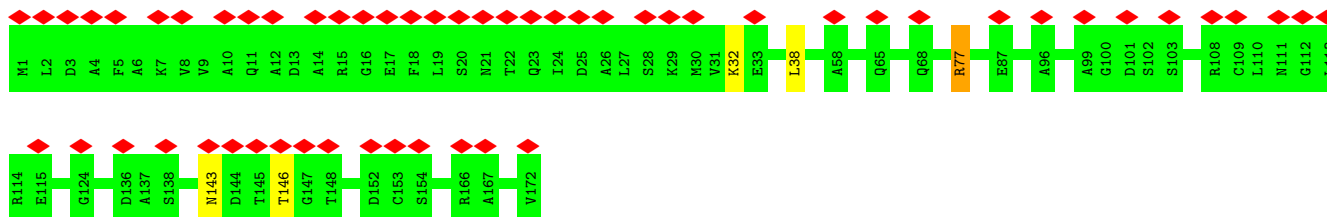




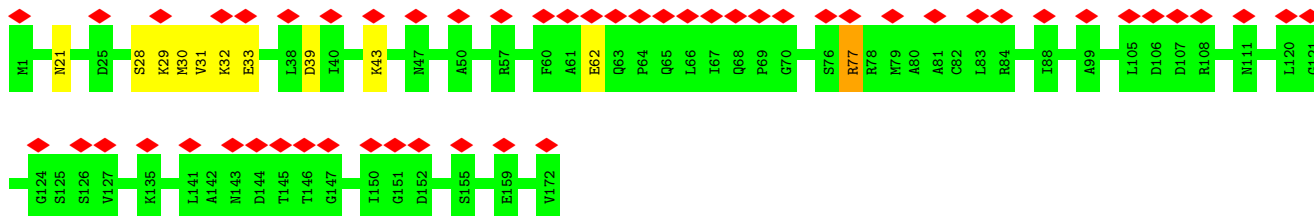
• Molecule 5: C-phyco cyanin beta subunit



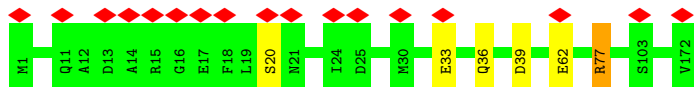
• Molecule 5: C-phyco cyanin beta subunit



• Molecule 5: C-phyco cyanin beta subunit

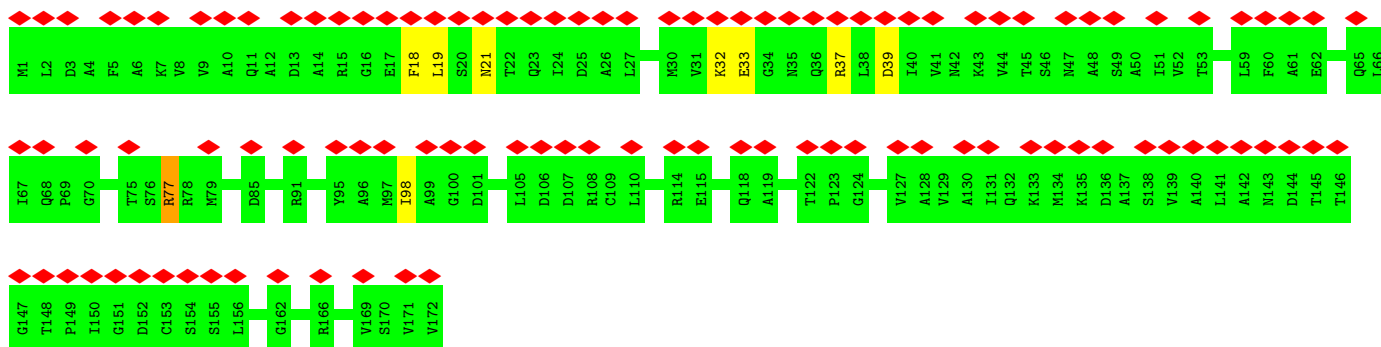


• Molecule 5: C-phyco cyanin beta subunit

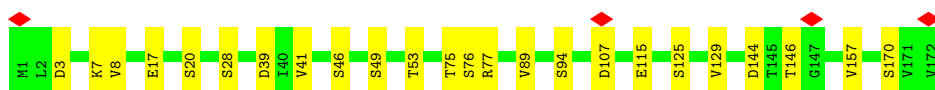


• Molecule 5: C-phyco cyanin beta subunit

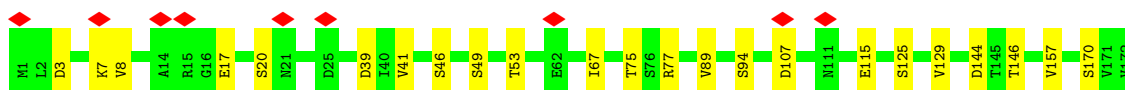
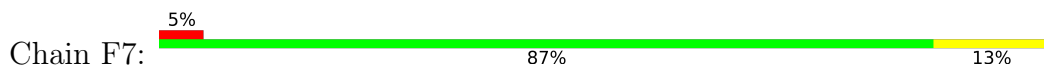




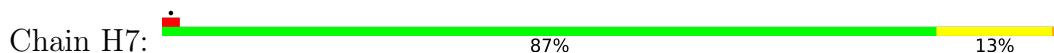
- Molecule 5: C-phycoerythrin beta subunit



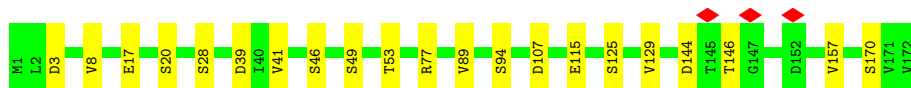
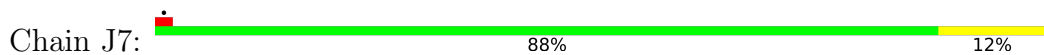
- Molecule 5: C-phycoerythrin beta subunit



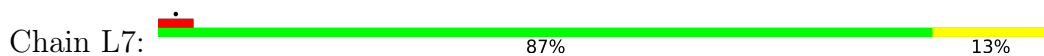
- Molecule 5: C-phycoerythrin beta subunit




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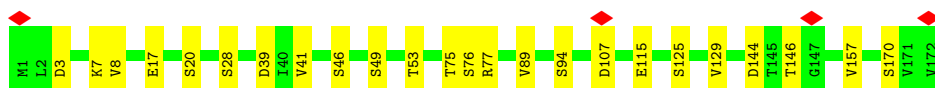
- Molecule 5: C-phycoerythrin beta subunit

Chain N7:  88% 12%




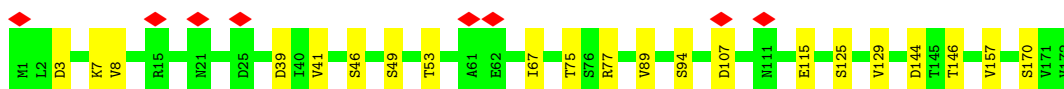
● Molecule 5: C-phycoyanin beta subunit

Chain D9:  86% 14%




● Molecule 5: C-phycoyanin beta subunit

Chain F9:  88% 12% 5%




● Molecule 5: C-phycoyanin beta subunit

Chain H9:  87% 13%




● Molecule 5: C-phycoyanin beta subunit

Chain J9:  88% 12%




● Molecule 5: C-phycoyanin beta subunit

Chain L9:  87% 13%

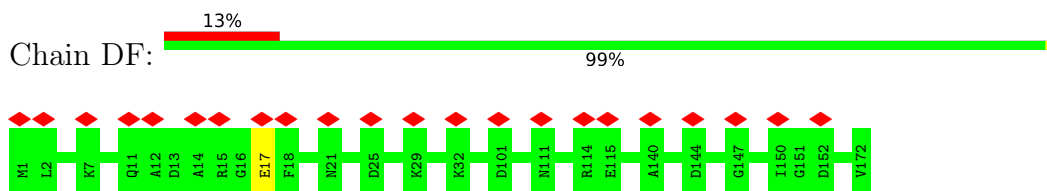


● Molecule 5: C-phycoyanin beta subunit

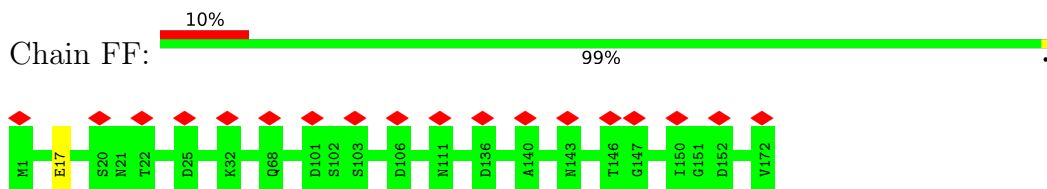
Chain N9:  88% 12%



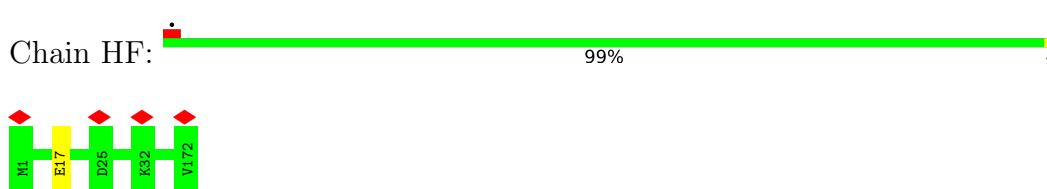
- Molecule 5: C-phycoerythrin beta subunit



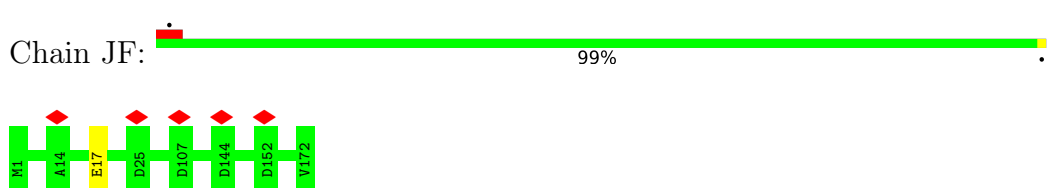
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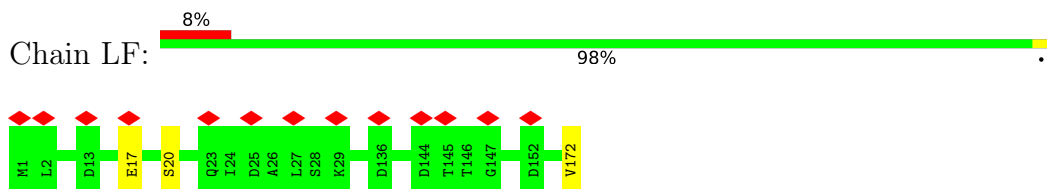
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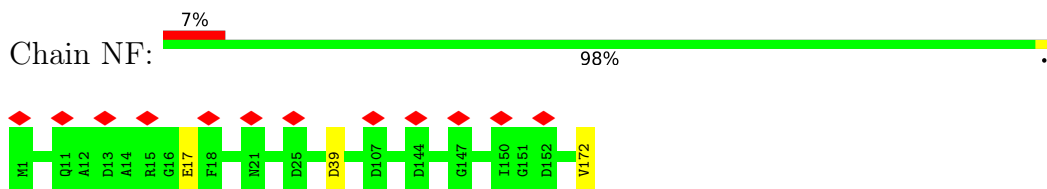
- Molecule 5: C-phycoerythrin beta subunit



- Molecule 5: C-phycoerythrin beta subunit

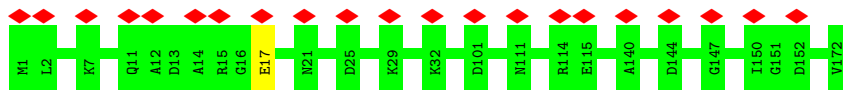


- Molecule 5: C-phycoerythrin beta subunit

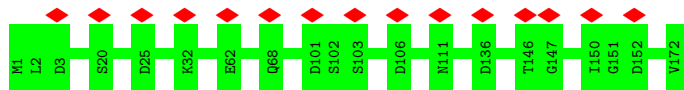


- Molecule 5: C-phycoerythrin beta subunit

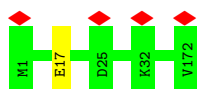




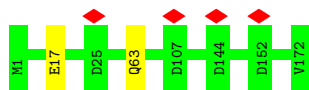
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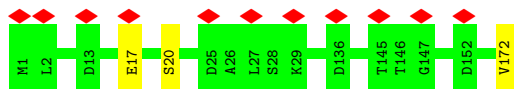
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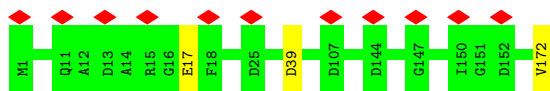
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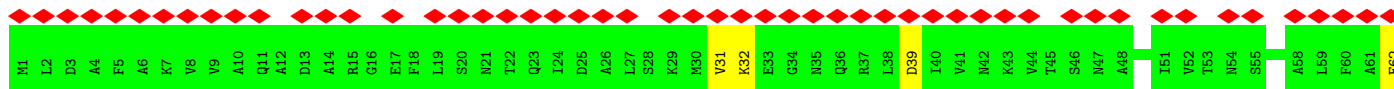
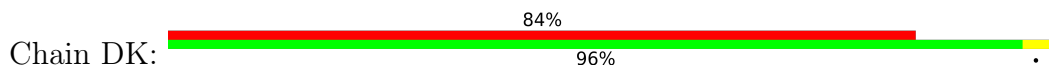
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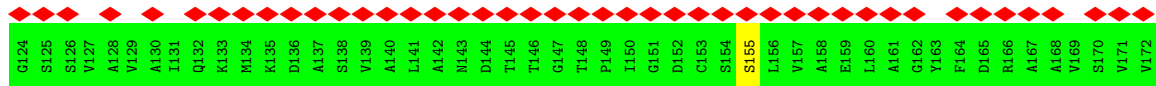
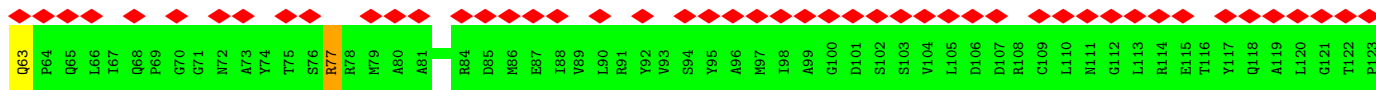


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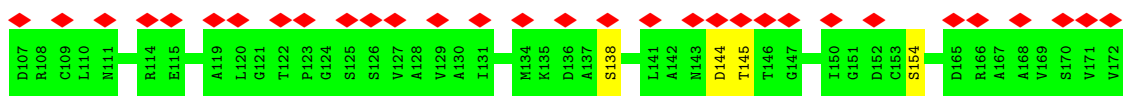
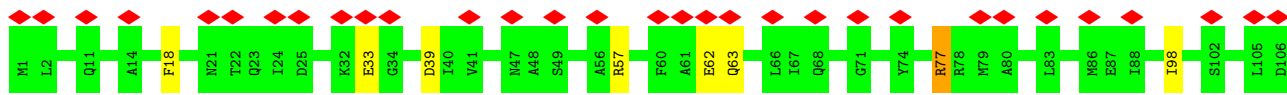
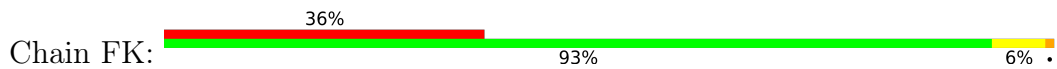


• Molecule 5: C-phycoerythrin beta subunit

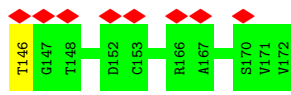
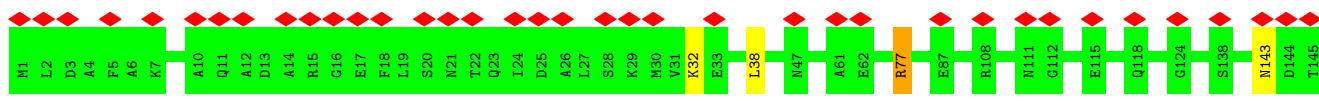




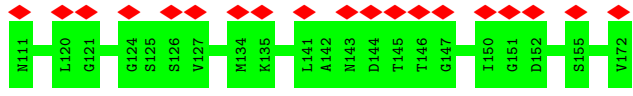
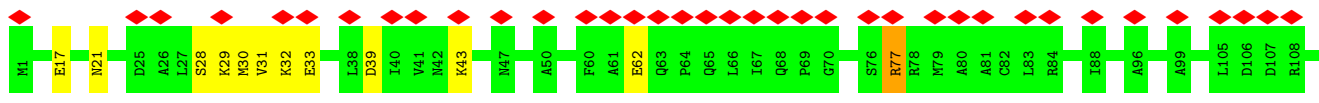
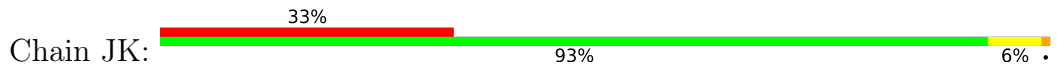
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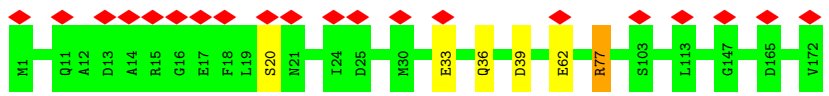
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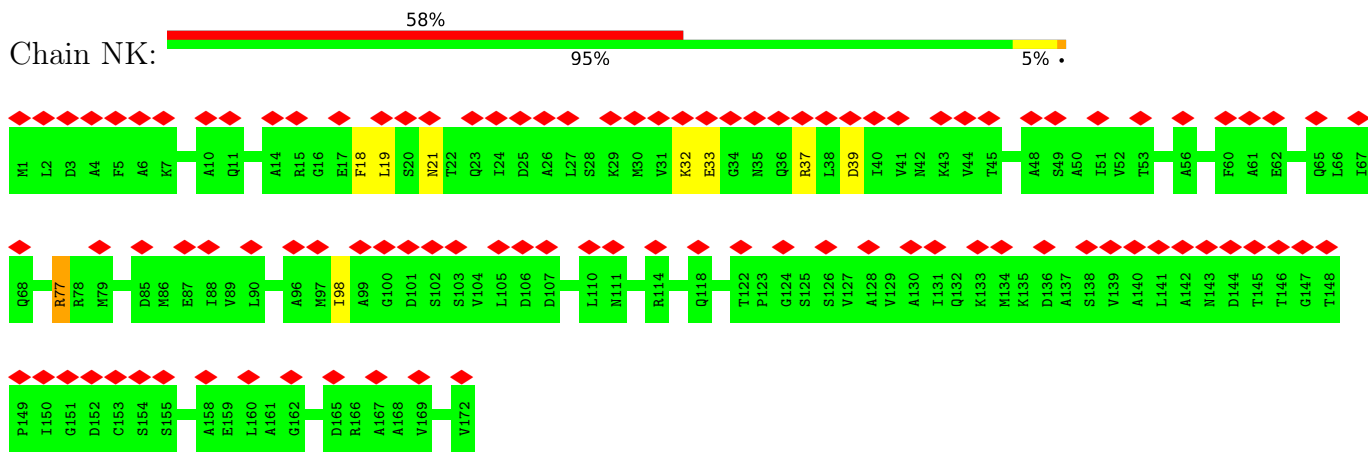
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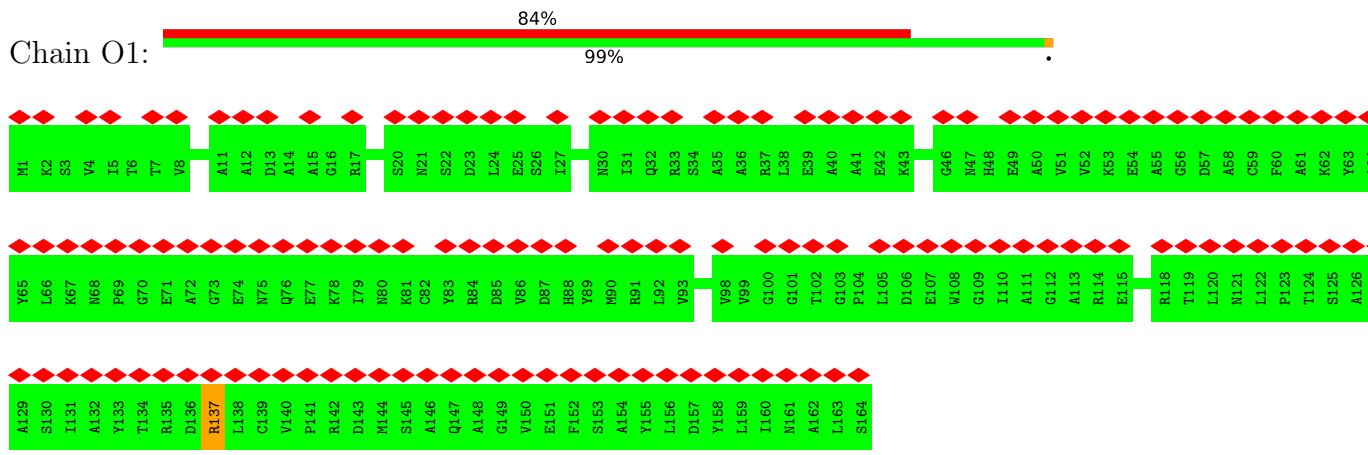
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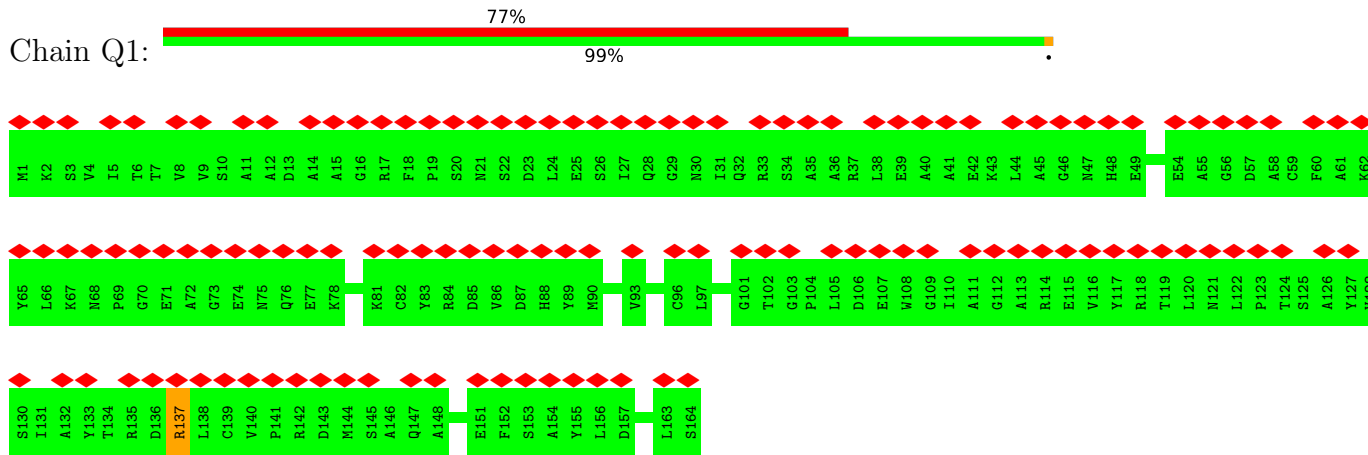
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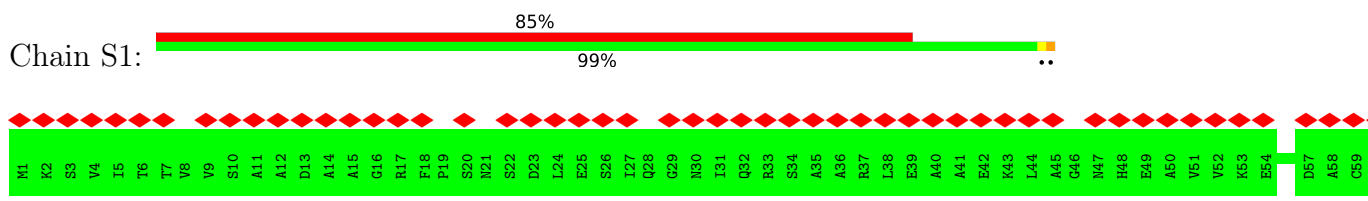
• Molecule 6: Phycoerythrin alpha subunit

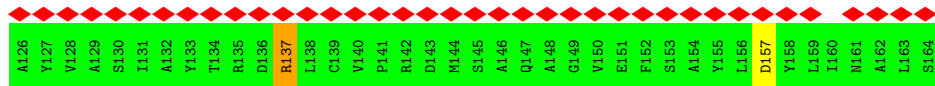
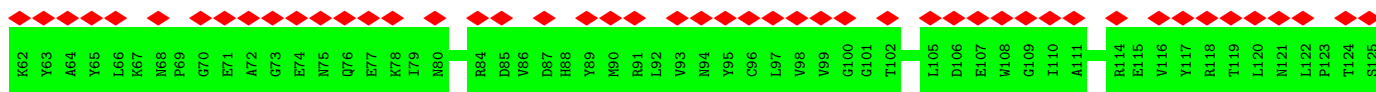


• Molecule 6: Phycoerythrin alpha subunit

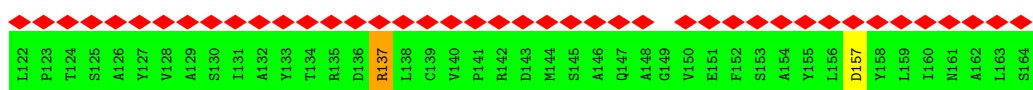
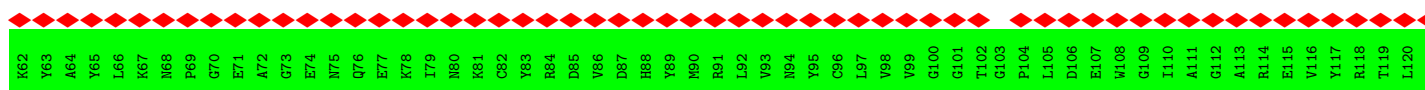


• Molecule 6: Phycoerythrin alpha subunit

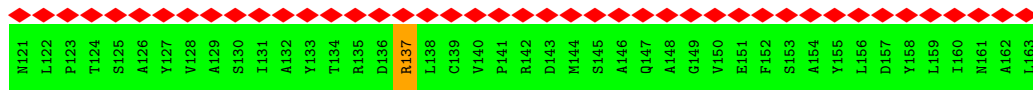
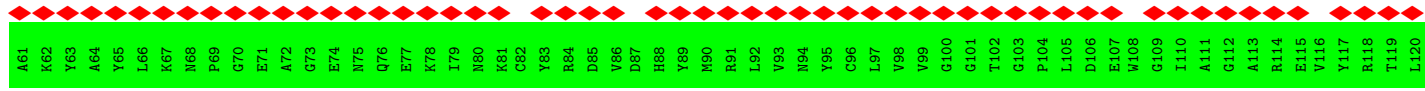
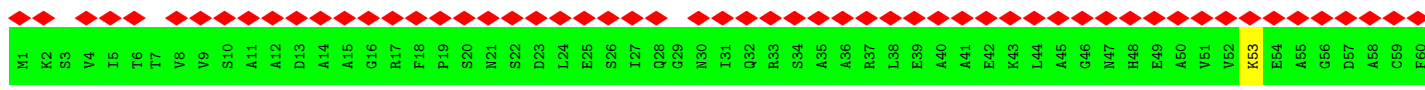




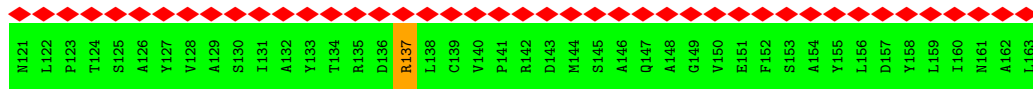
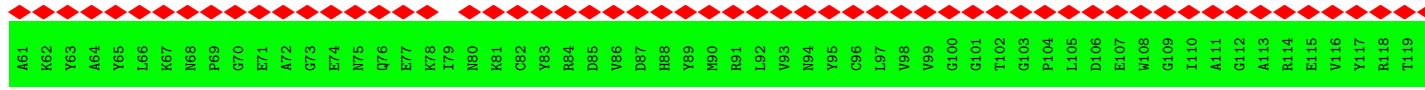
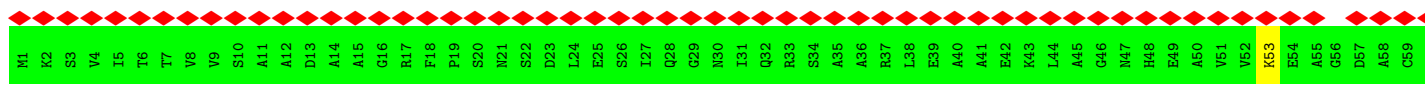
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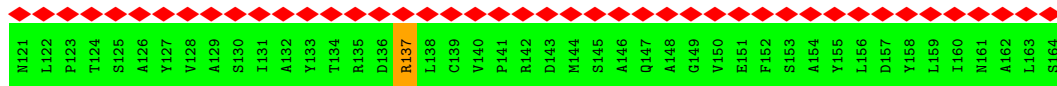
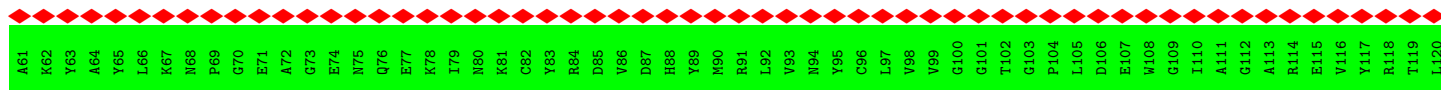


• Molecule 6: Phycoerythrin alpha subunit

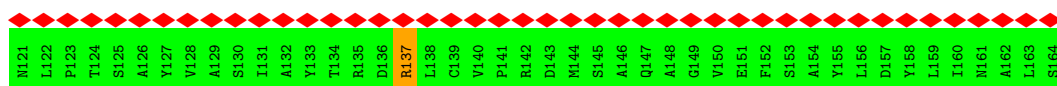
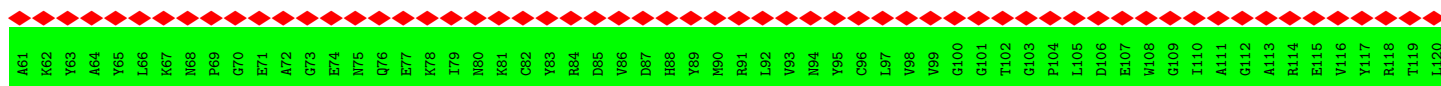
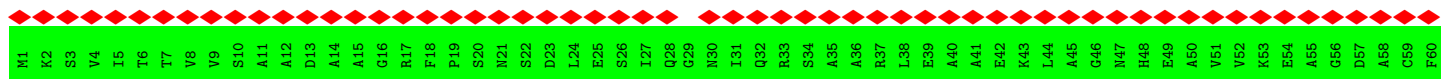


• Molecule 6: Phycoerythrin alpha subunit

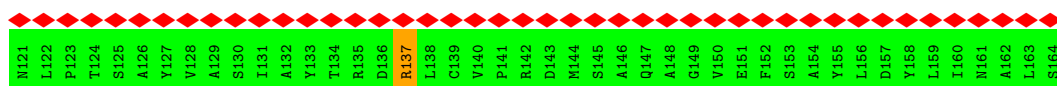
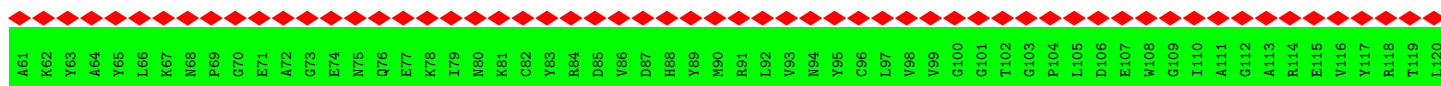
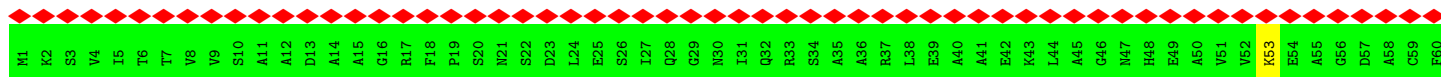




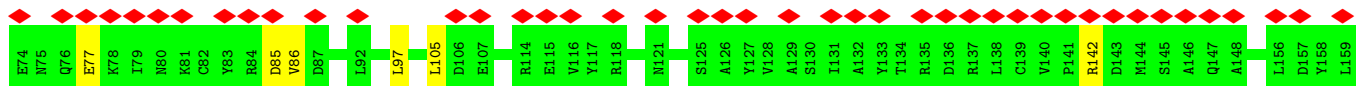
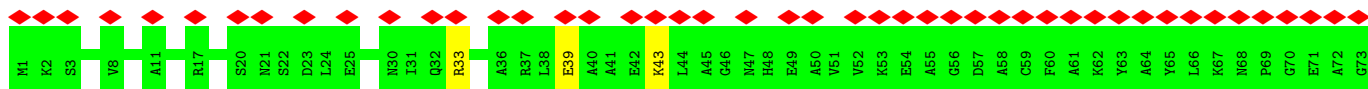
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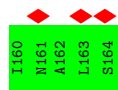


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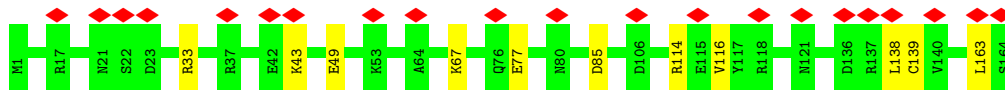


• Molecule 6: Phycoerythrin alpha subunit

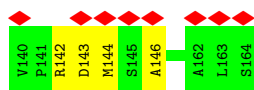
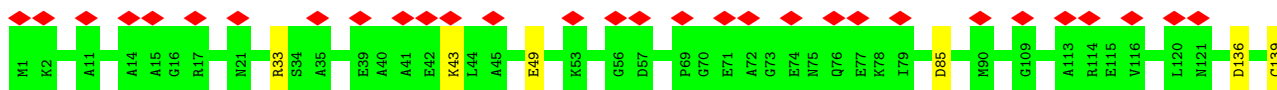




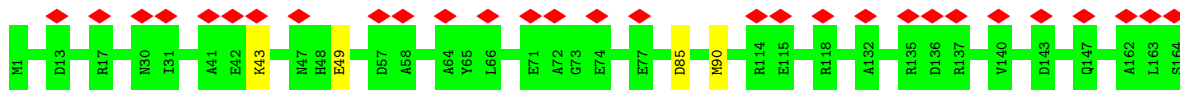
• Molecule 6: Phycoerythrin alpha subunit



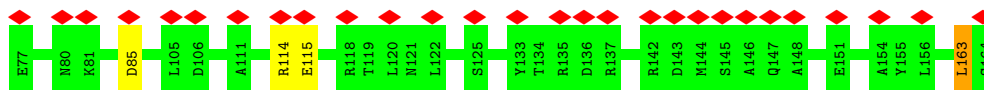
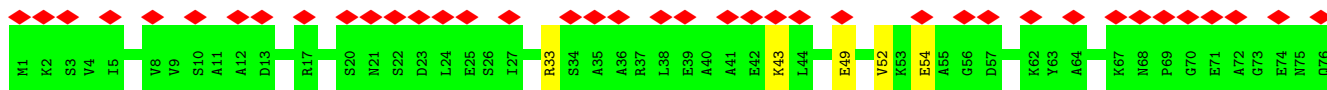
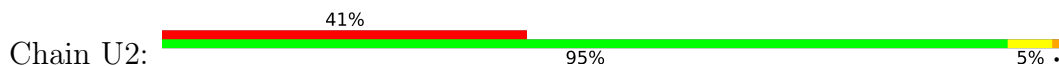
• Molecule 6: Phycoerythrin alpha subunit



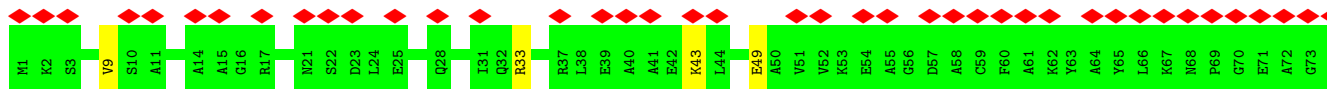
• Molecule 6: Phycoerythrin alpha subunit



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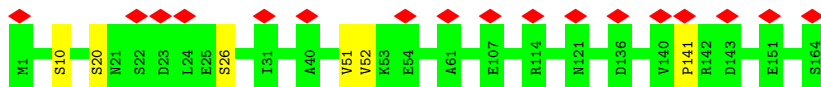


• Molecule 6: Phycoerythrin alpha subunit

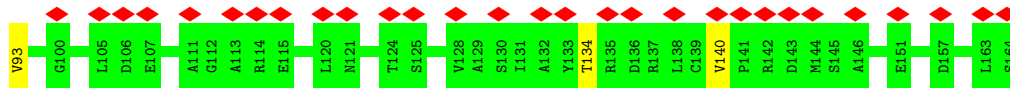
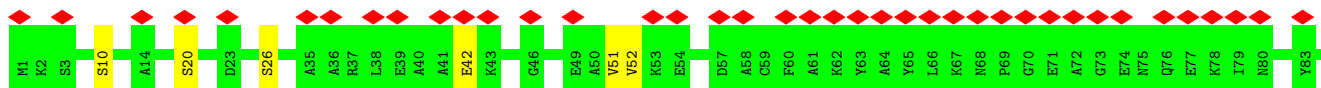
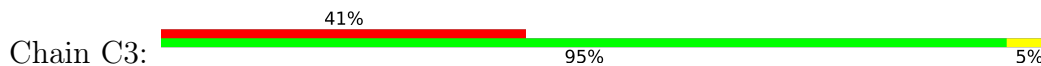




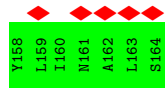
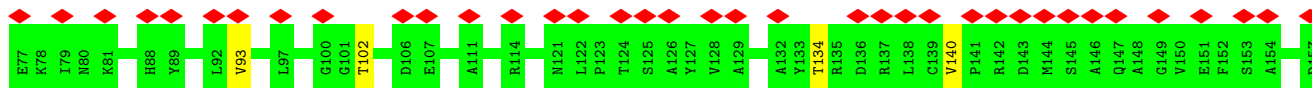
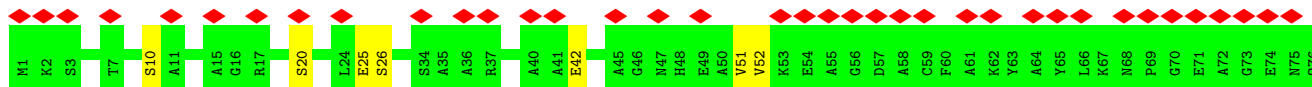
• Molecule 6: Phycoerythrin alpha subunit



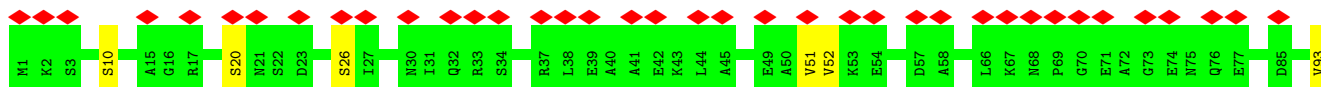
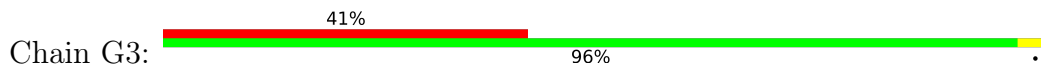
• Molecule 6: Phycoerythrin alpha subunit

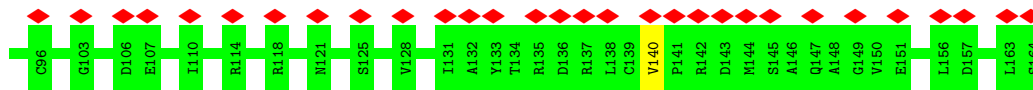


• Molecule 6: Phycoerythrin alpha subunit

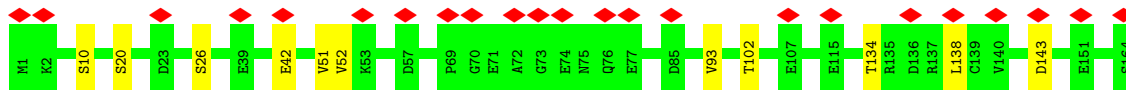
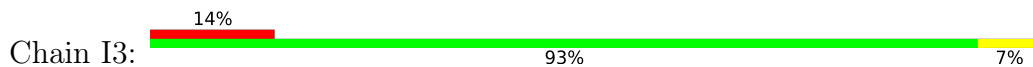


• Molecule 6: Phycoerythrin alpha subunit





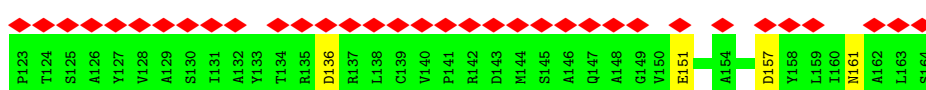
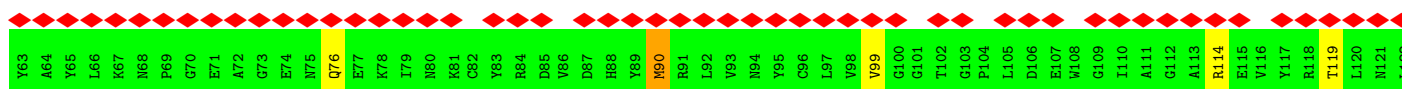
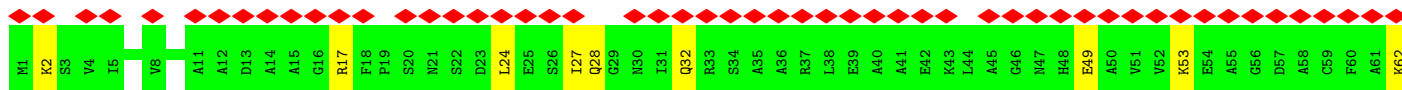
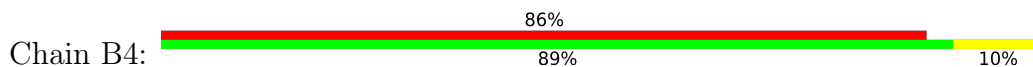
• Molecule 6: Phycoerythrin alpha subunit



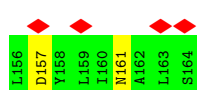
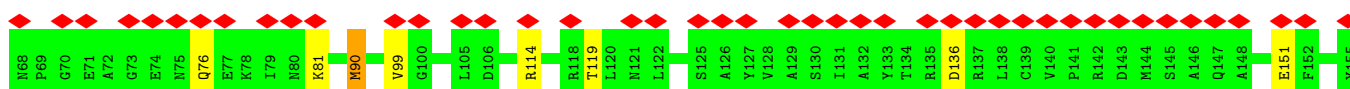
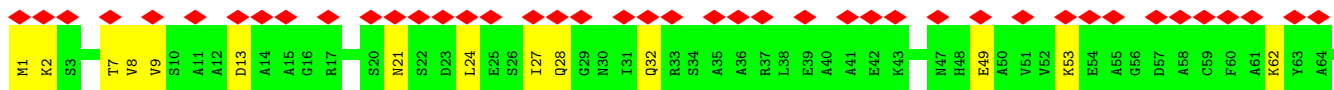
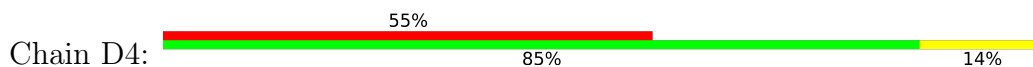
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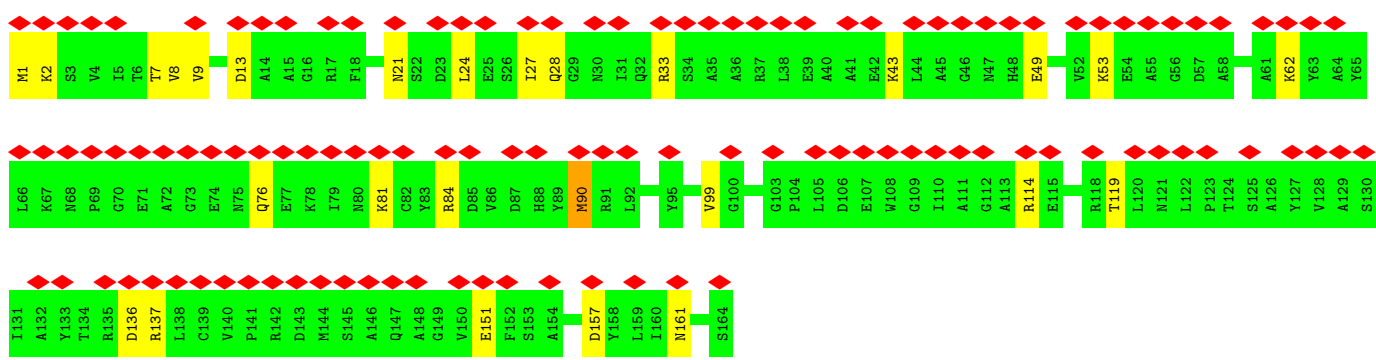
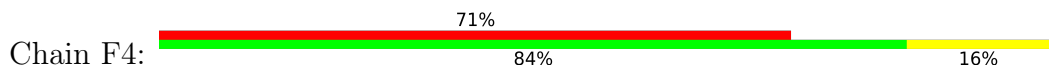
• Molecule 6: Phycoerythrin alpha subunit



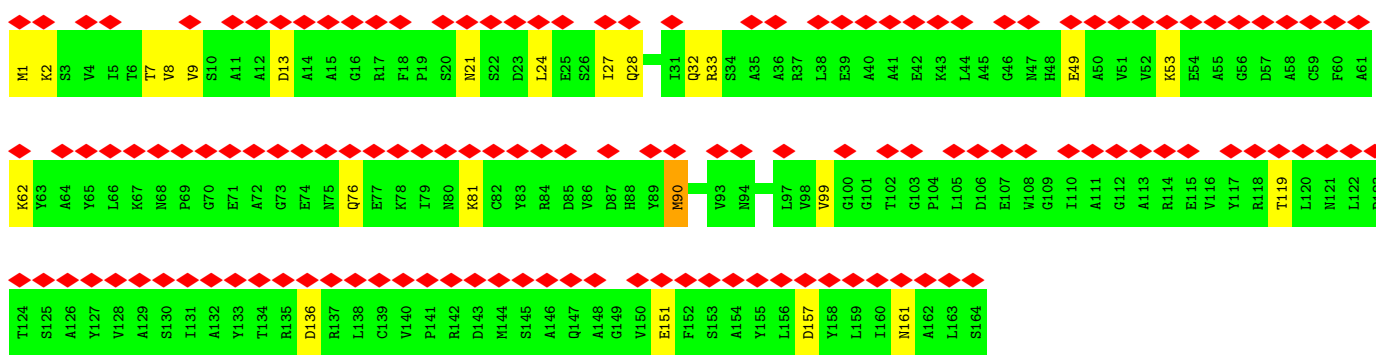
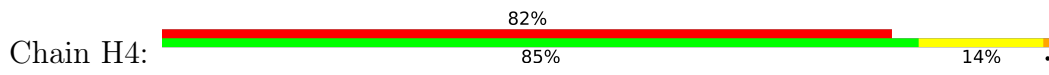
• Molecule 6: Phycoerythrin alpha subunit



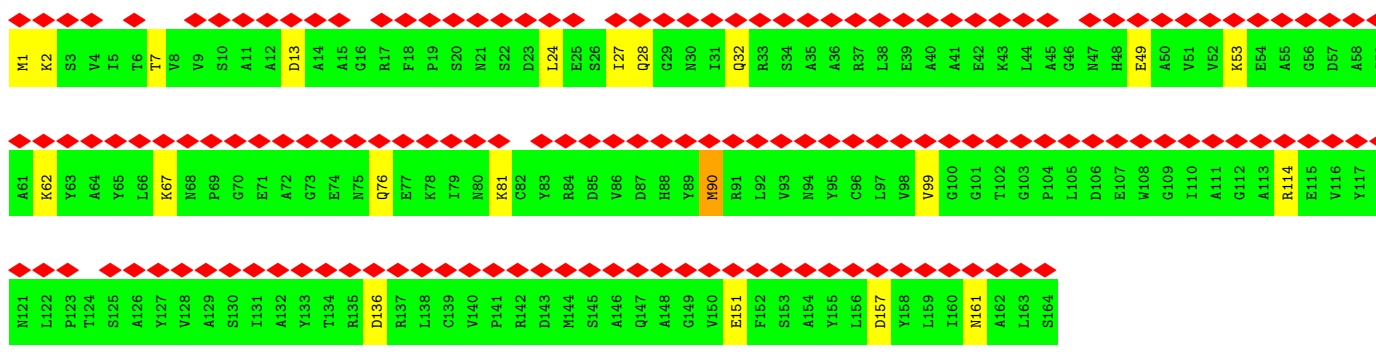
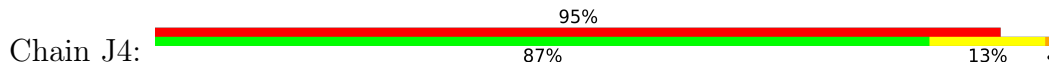
• Molecule 6: Phycoerythrin alpha subunit



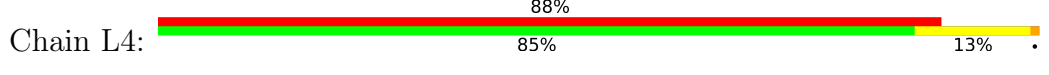
• Molecule 6: Phycoerythrin alpha subunit

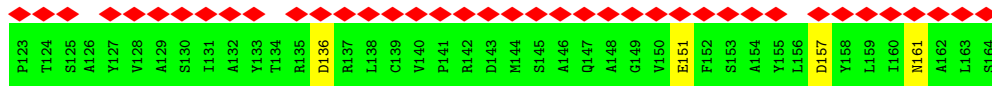
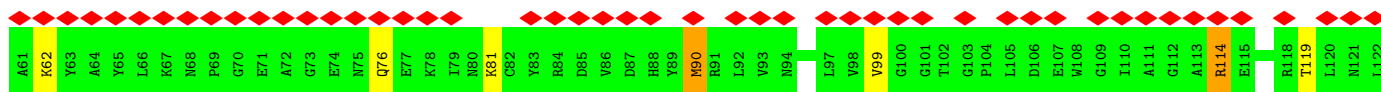


• Molecule 6: Phycoerythrin alpha subunit

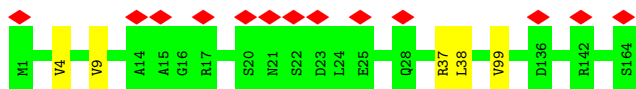


• Molecule 6: Phycoerythrin alpha subunit

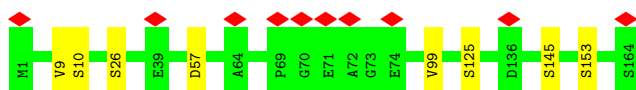




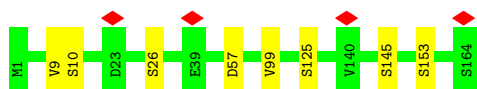
• Molecule 6: Phycoerythrin alpha subunit



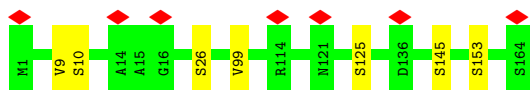
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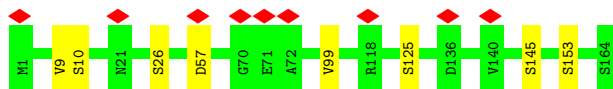
• Molecule 6: Phycoerythrin alpha subunit



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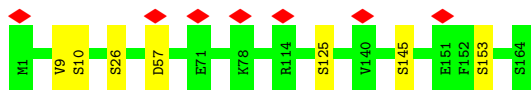


• Molecule 6: Phycoerythrin alpha subunit

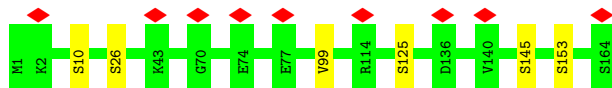


• Molecule 6: Phycoerythrin alpha subunit

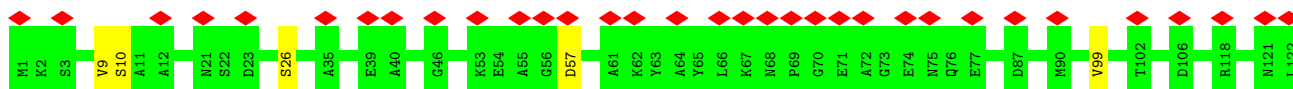




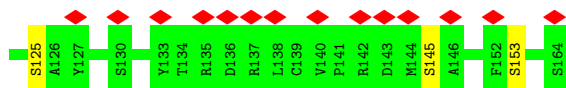
- Molecule 6: Phycoerythrin alpha subunit



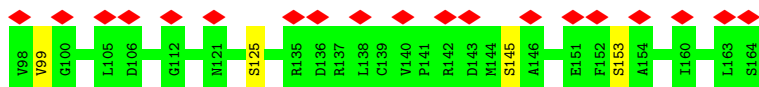
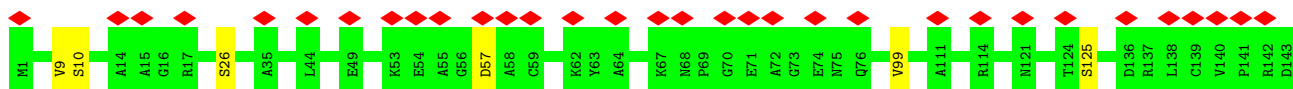
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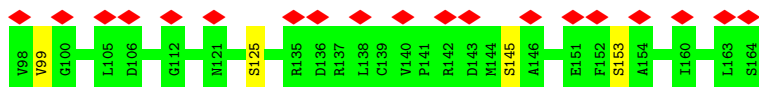
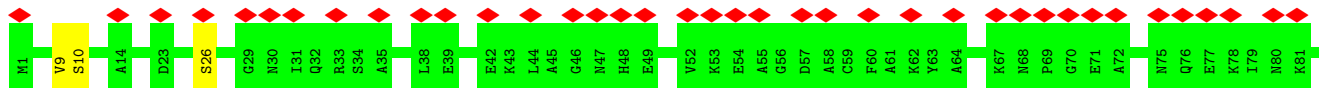
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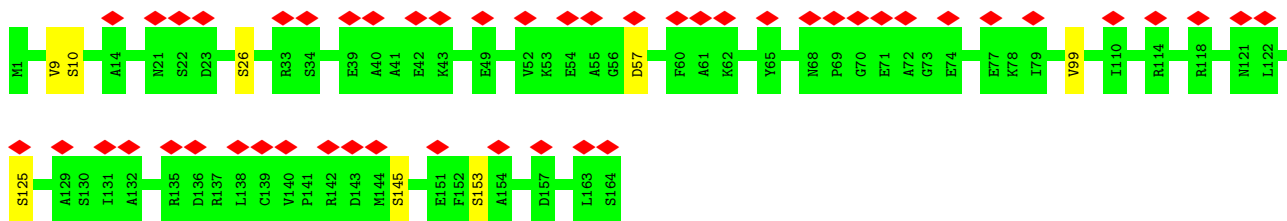


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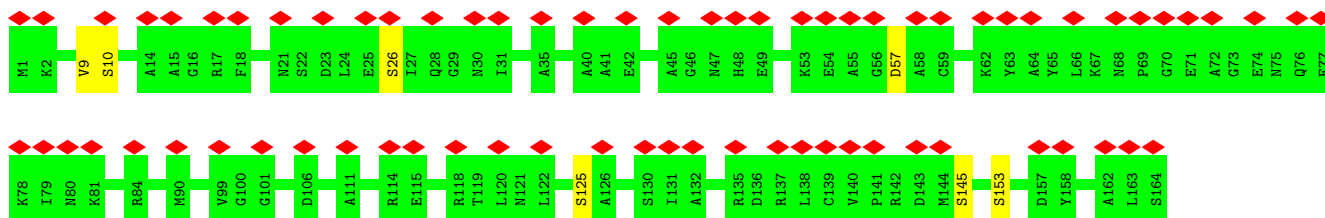
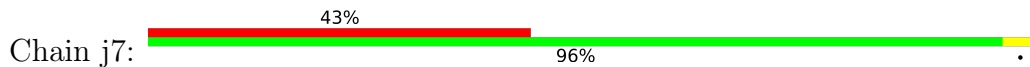


- Molecule 6: Phycoerythrin alpha subunit

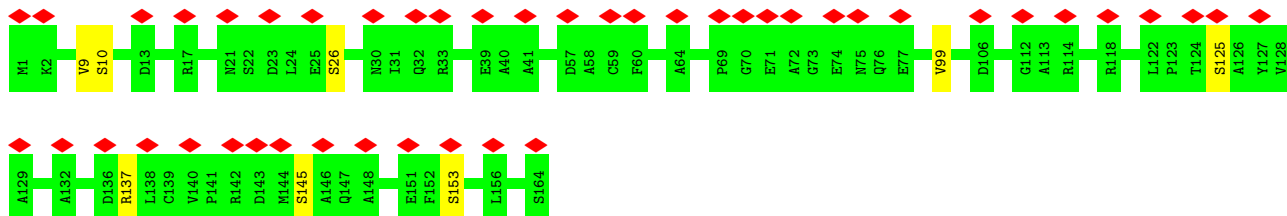




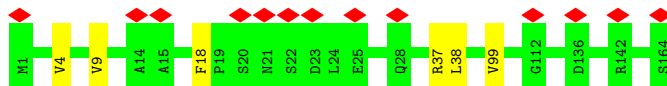
- Molecule 6: Phycoerythrin alpha subunit



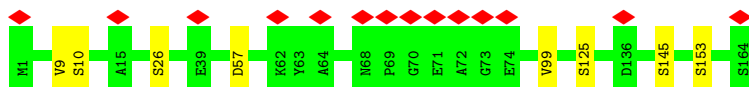
- Molecule 6: Phycoerythrin alpha subunit



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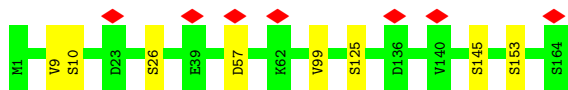


- Molecule 6: Phycoerythrin alpha subunit

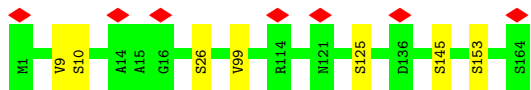


- Molecule 6: Phycoerythrin alpha subunit

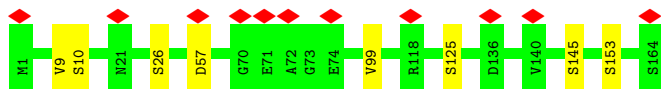




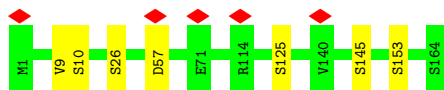
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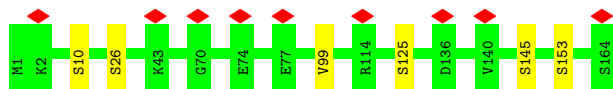
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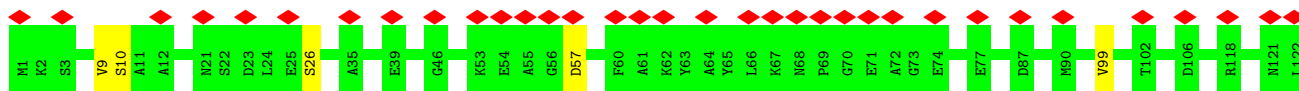
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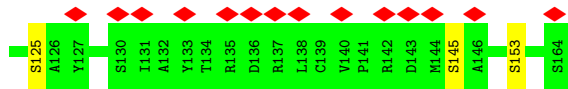
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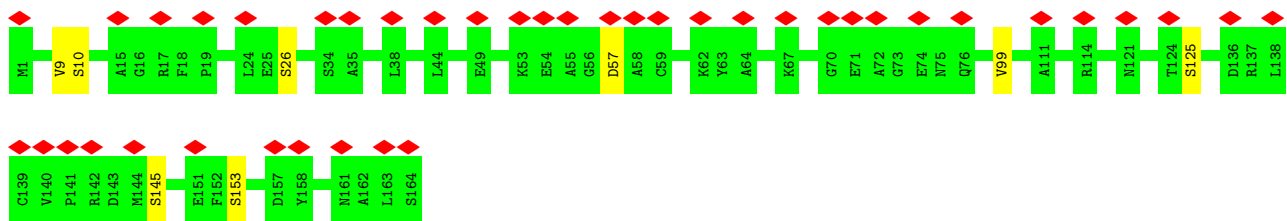


• Molecule 6: Phycoerythrin alpha subunit

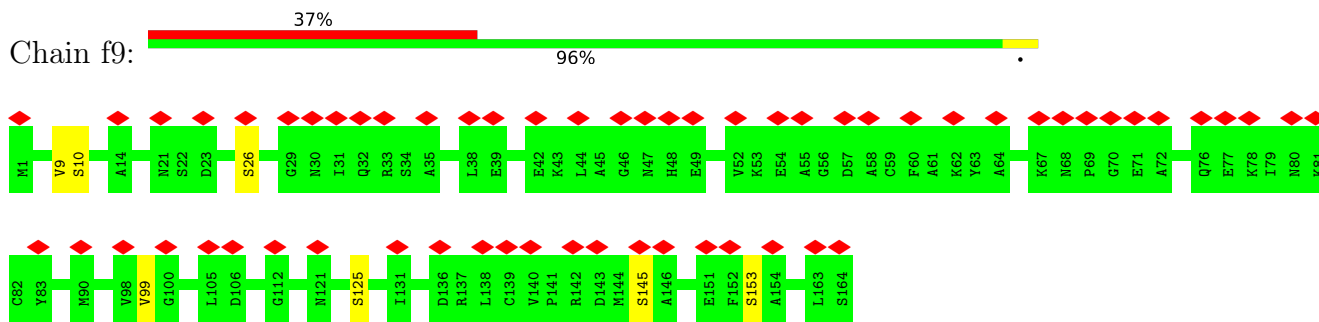


• Molecule 6: Phycoerythrin alpha subunit

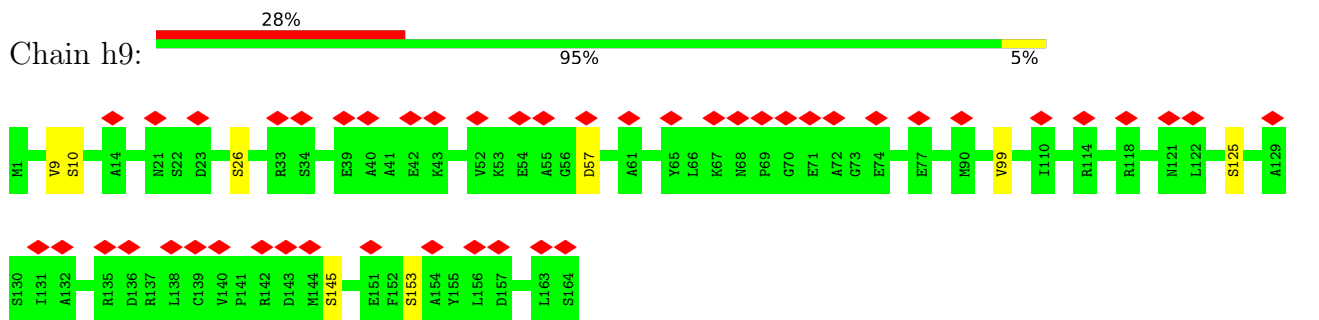




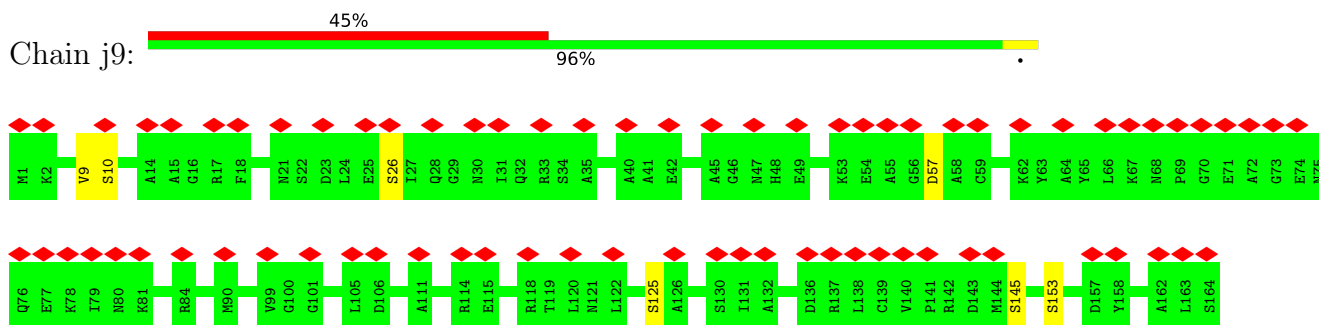
- Molecule 6: Phycoerythrin alpha subunit



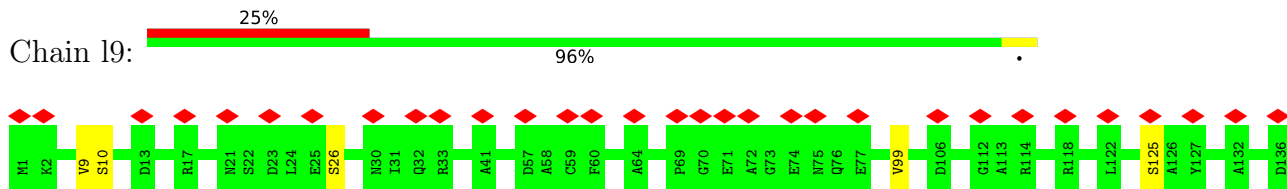
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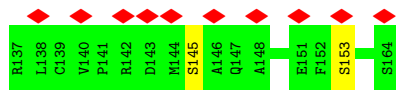


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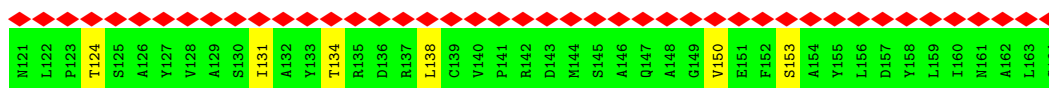
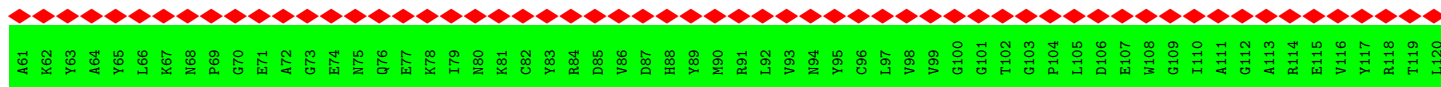
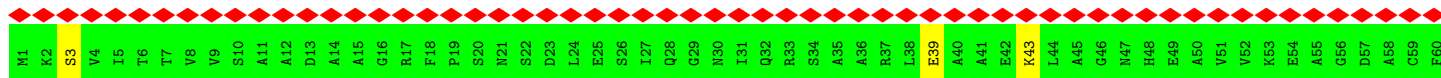


- Molecule 6: Phycoerythrin alpha subunit

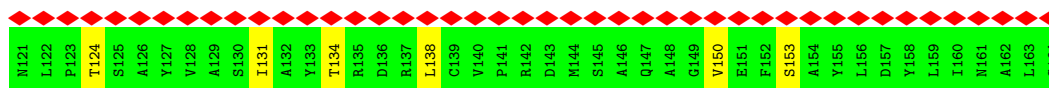
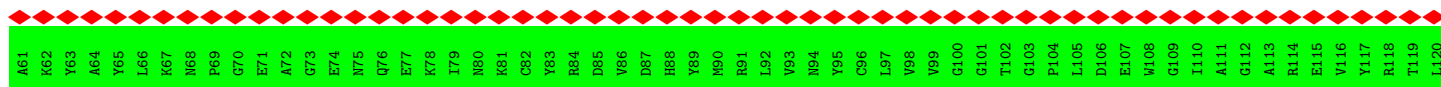
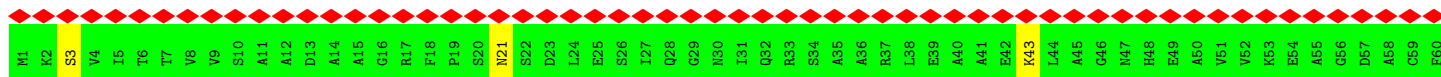




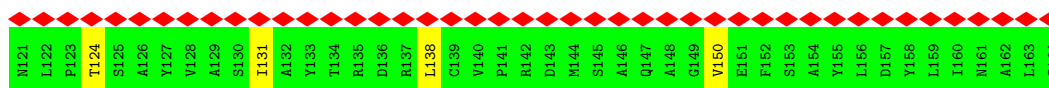
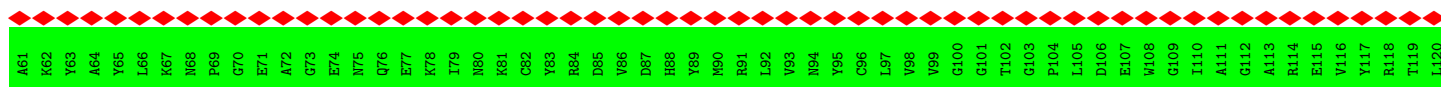
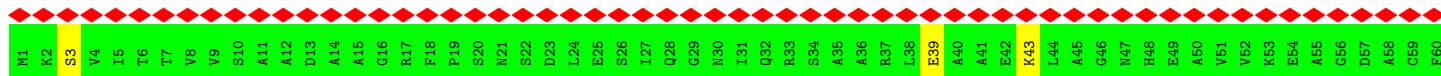
• Molecule 6: Phycoerythrin alpha subunit



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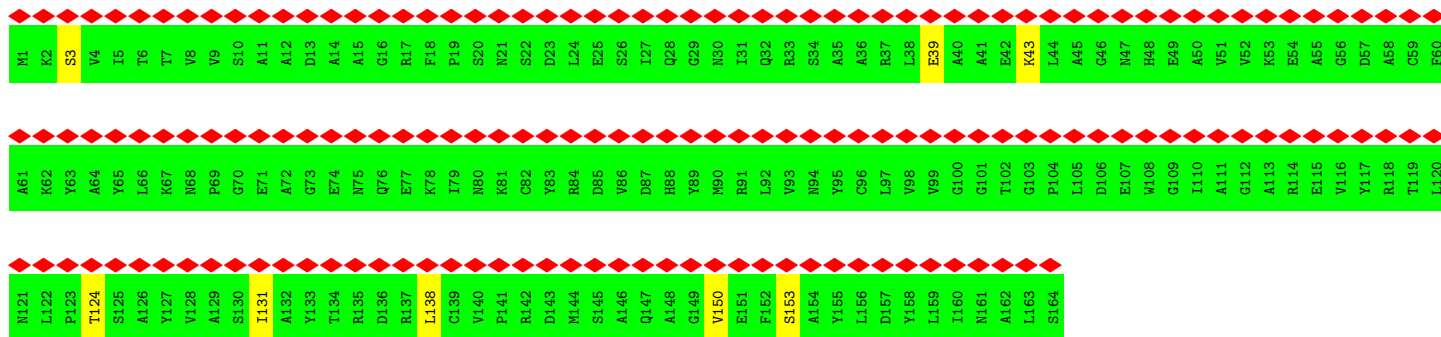


• Molecule 6: Phycoerythrin alpha subunit

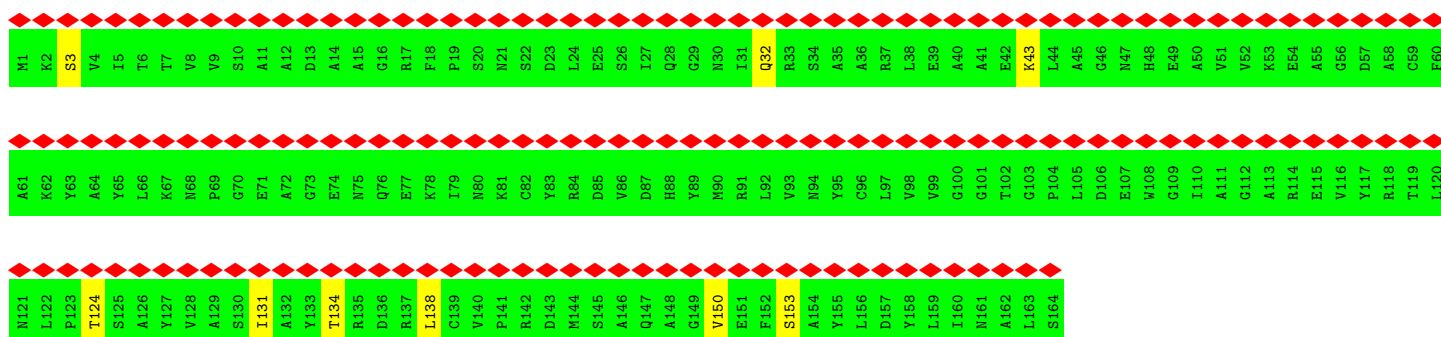


• Molecule 6: Phycoerythrin alpha subunit





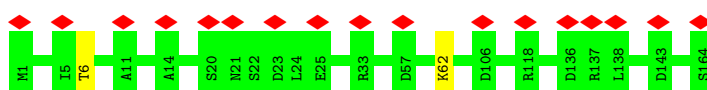
• Molecule 6: Phycoerythrin alpha subunit



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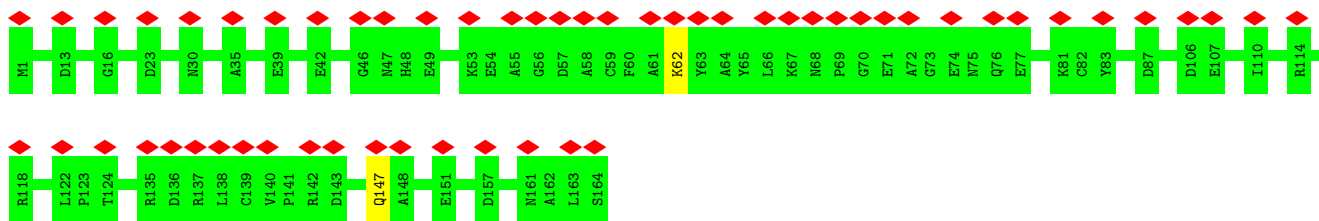


• Molecule 6: Phycoerythrin alpha subunit

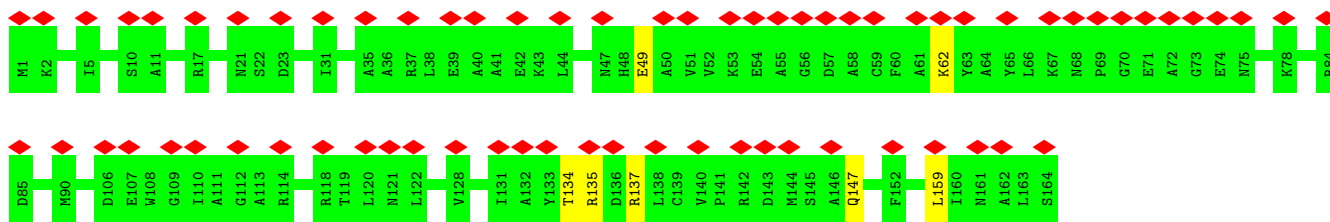
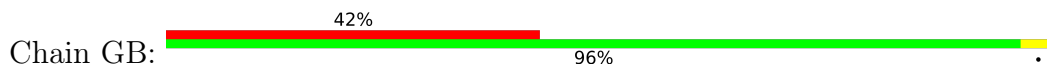


• Molecule 6: Phycoerythrin alpha subunit

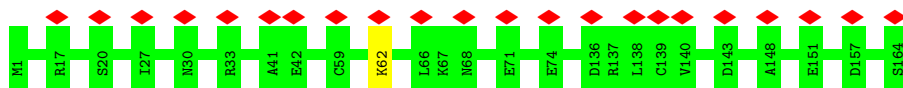




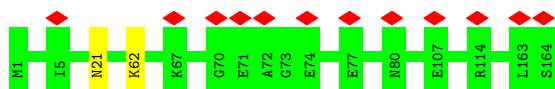
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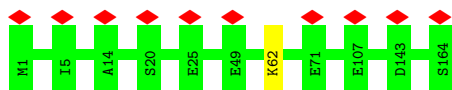
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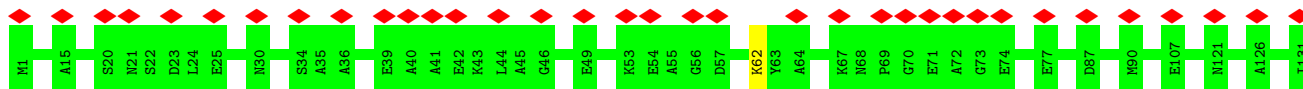
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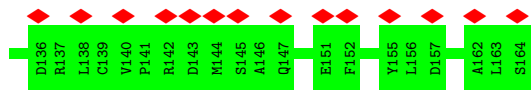


- Molecule 6: Phycoerythrin alpha subunit

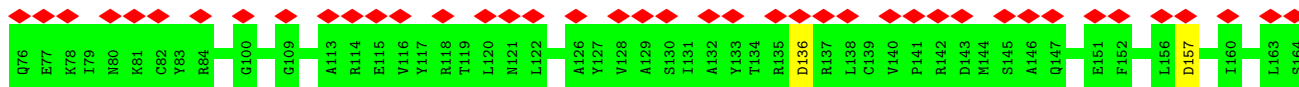
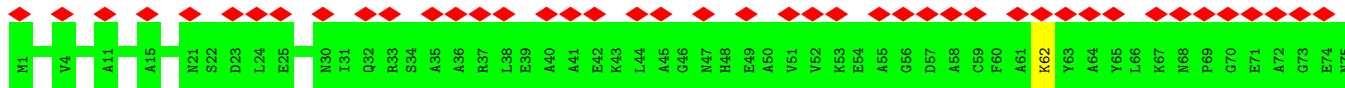


- Molecule 6: Phycoerythrin alpha subunit

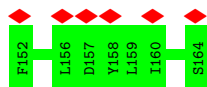
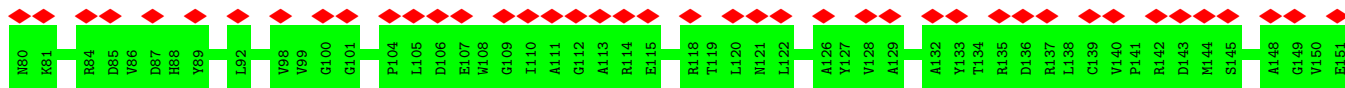




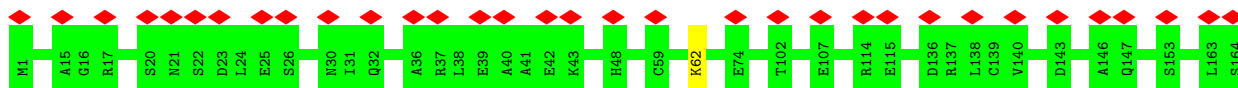
• Molecule 6: Phycoerythrin alpha subunit



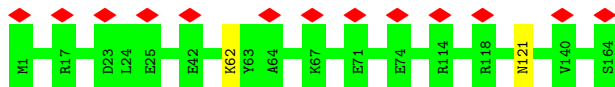
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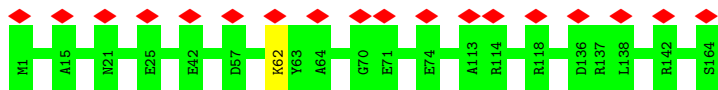


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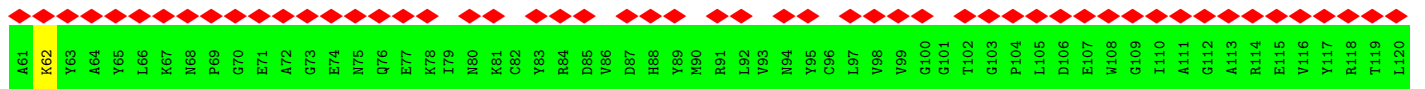
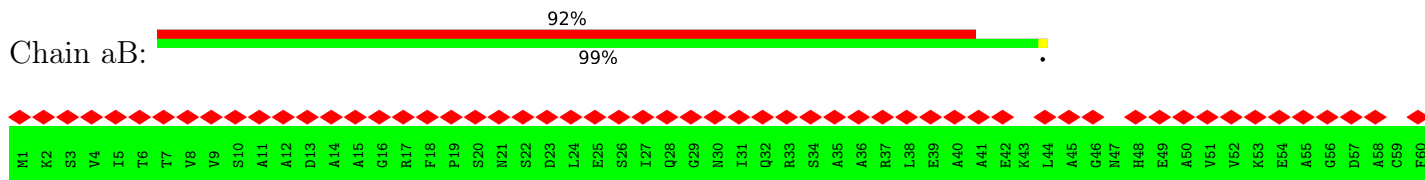


• Molecule 6: Phycoerythrin alpha subunit

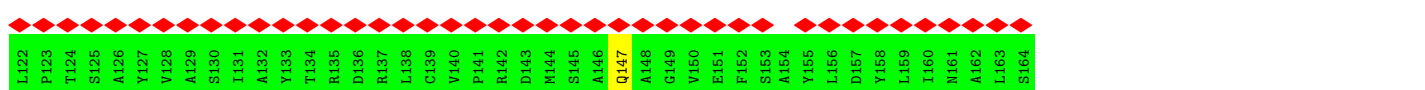
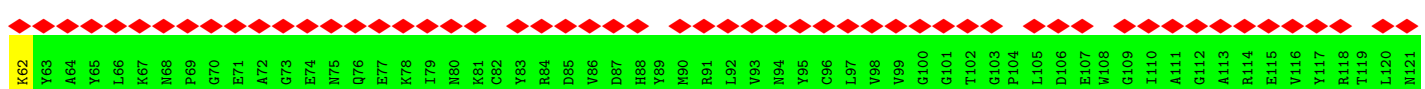
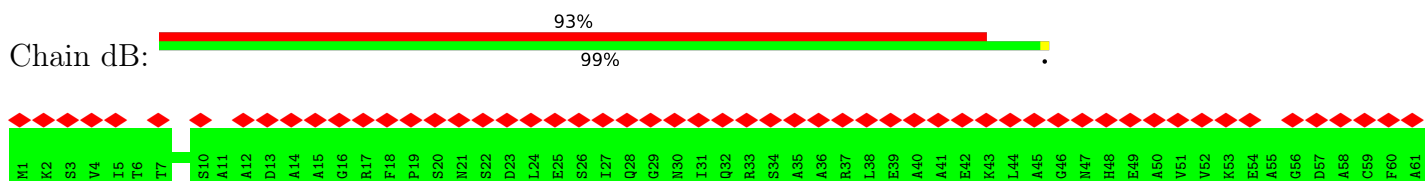




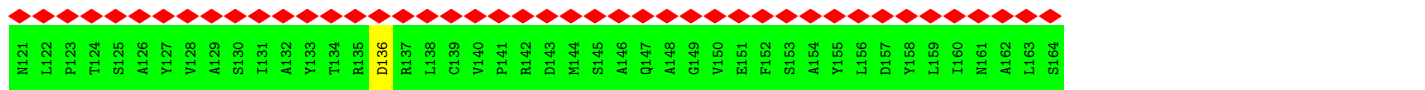
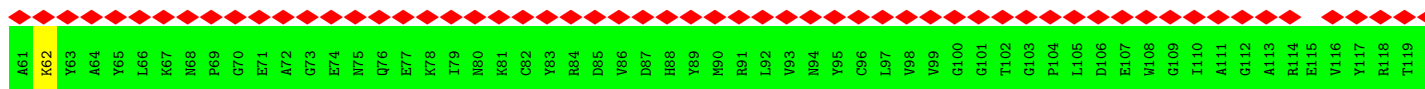
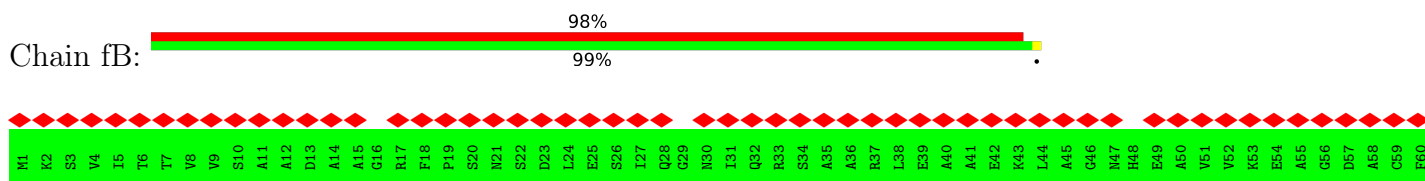
• Molecule 6: Phycoerythrin alpha subunit



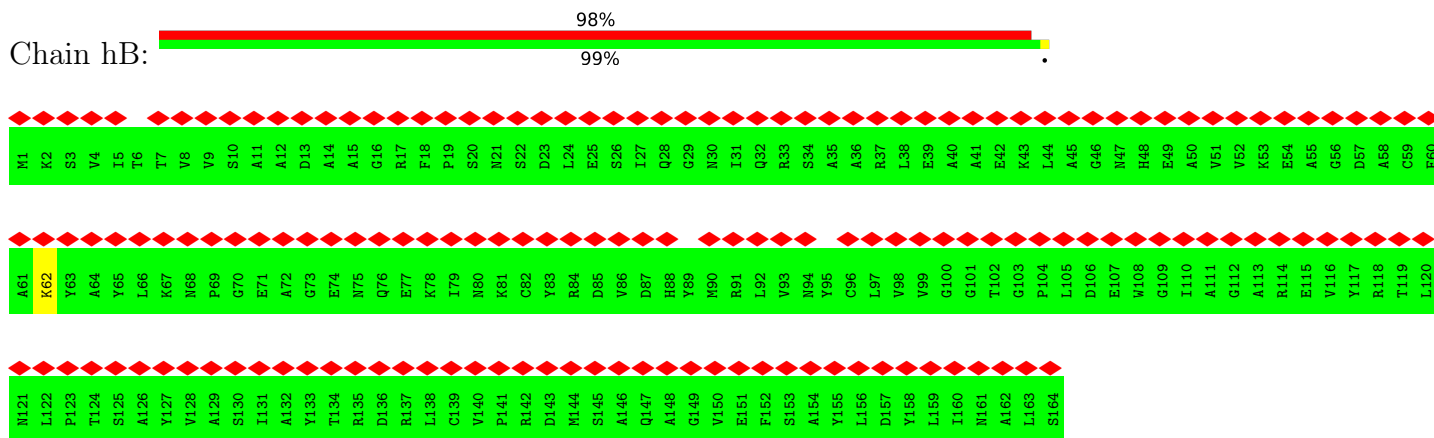
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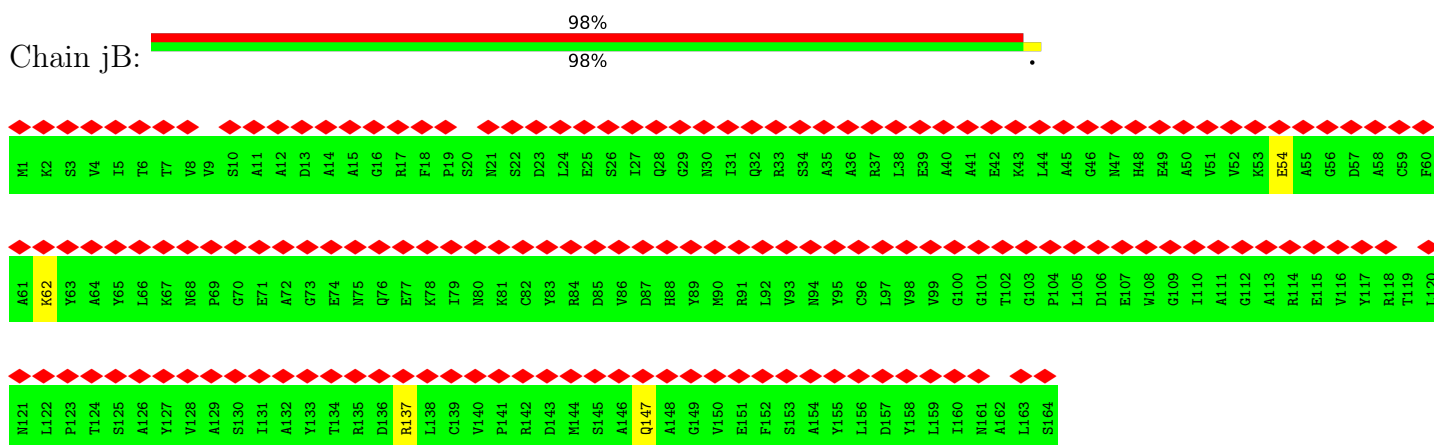
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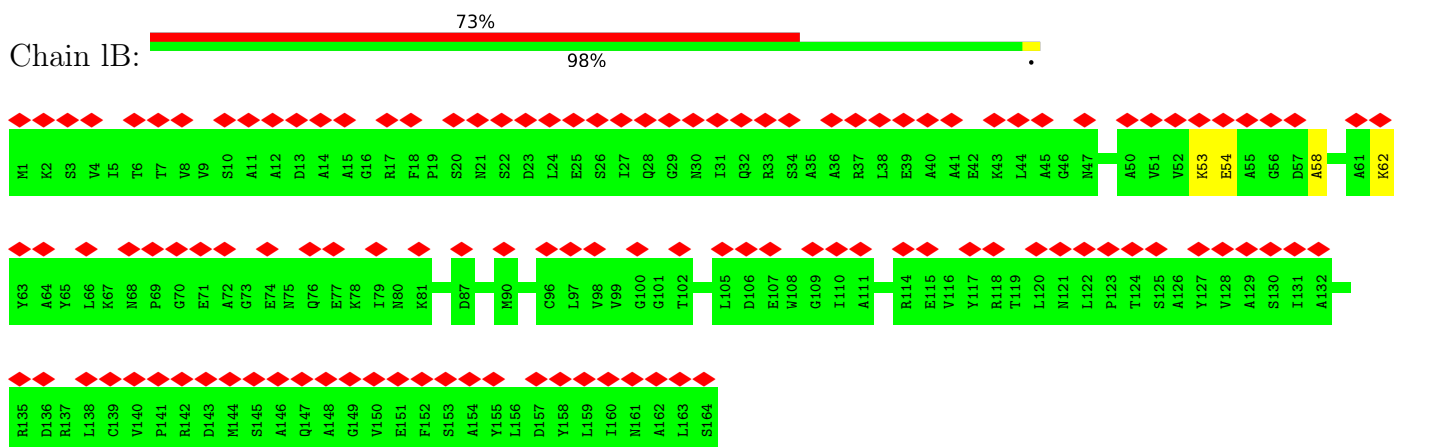
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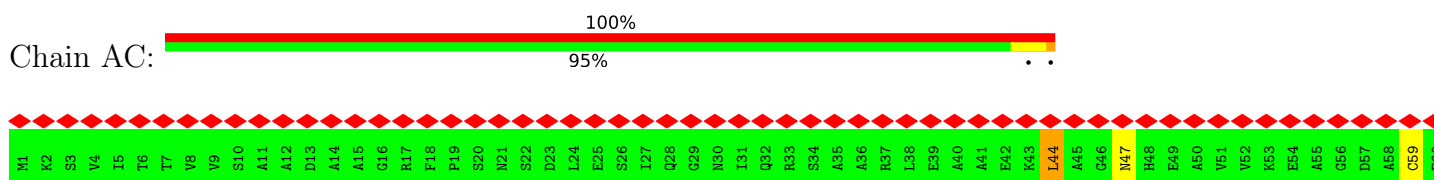
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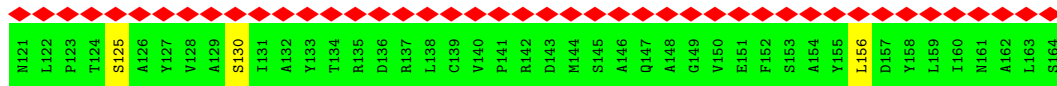
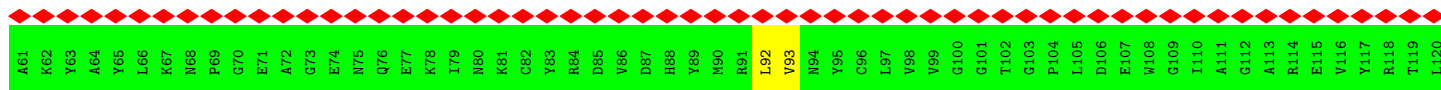


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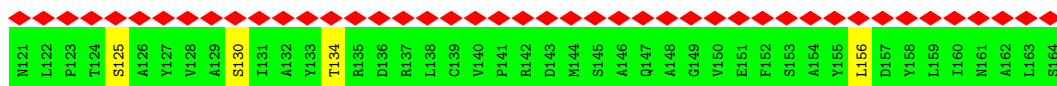
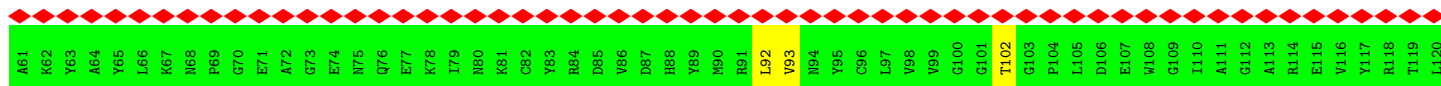
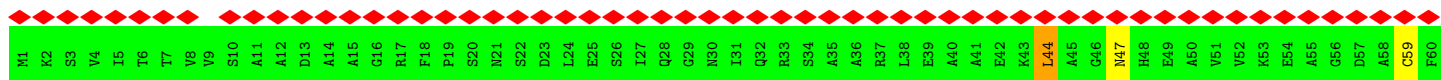


• Molecule 6: Phycoerythrin alpha subunit

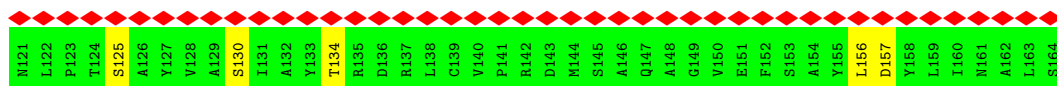
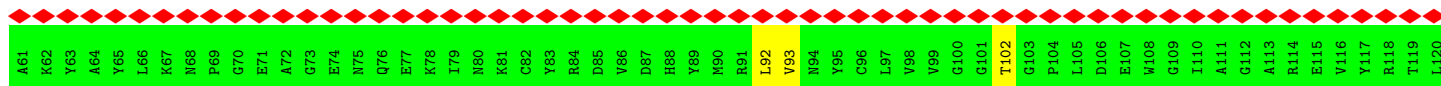
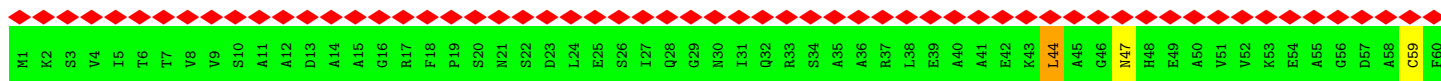
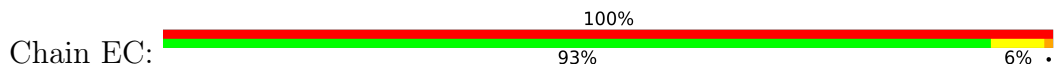




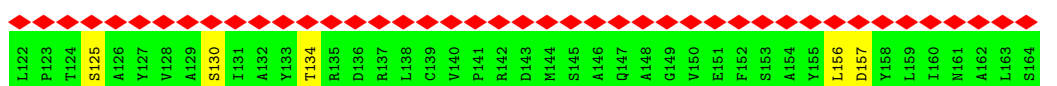
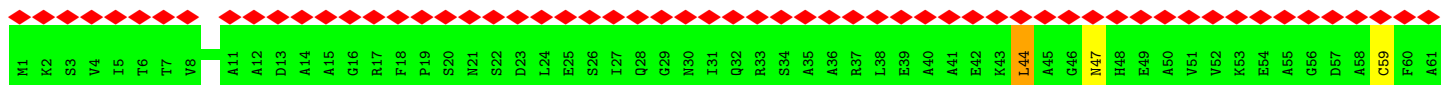
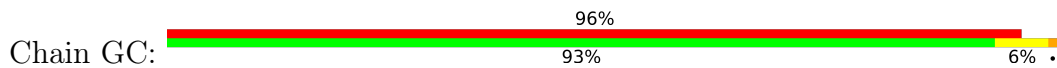
• Molecule 6: Phycoerythrin alpha subunit



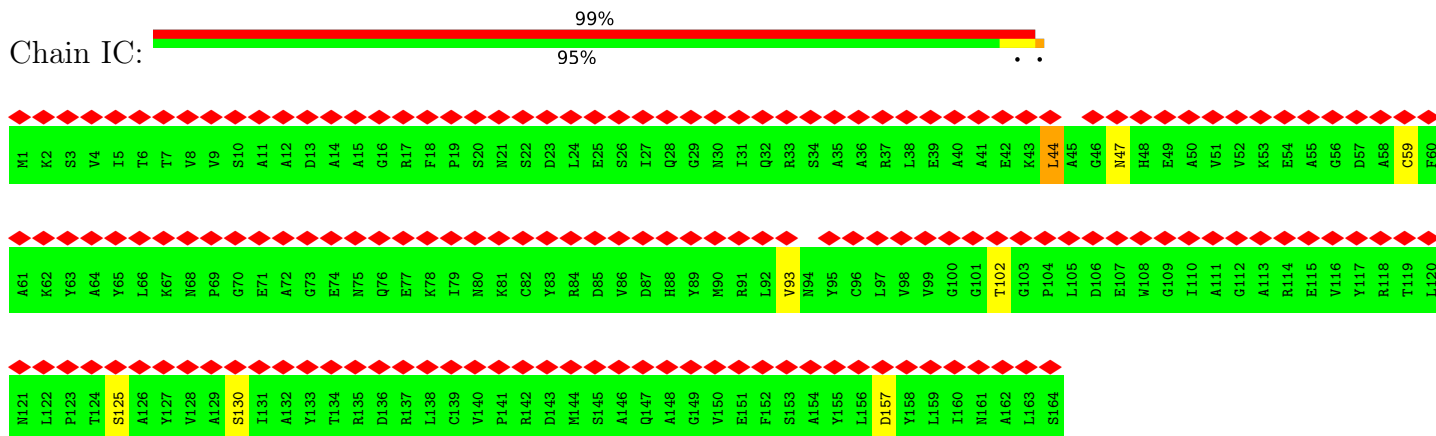
• Molecule 6: Phycoerythrin alpha subunit



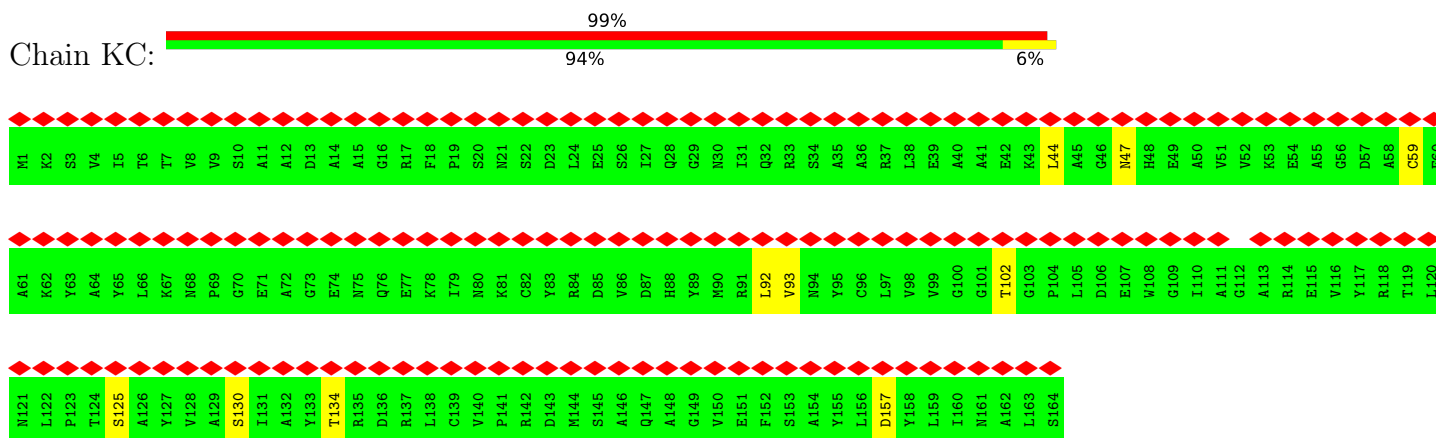
• Molecule 6: Phycoerythrin alpha subunit



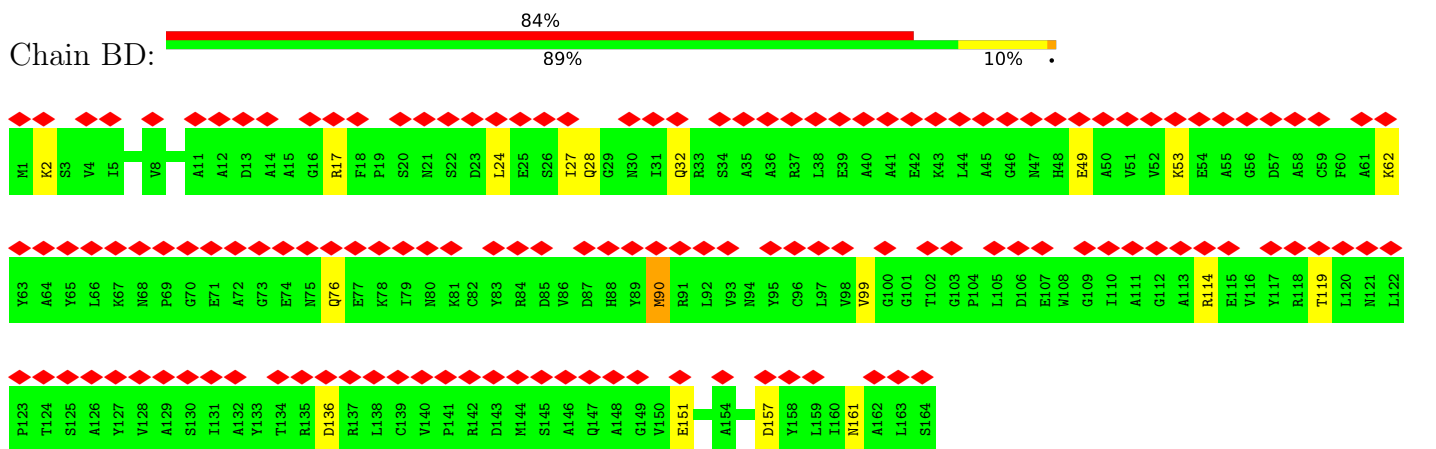
• Molecule 6: Phycoerythrin alpha subunit



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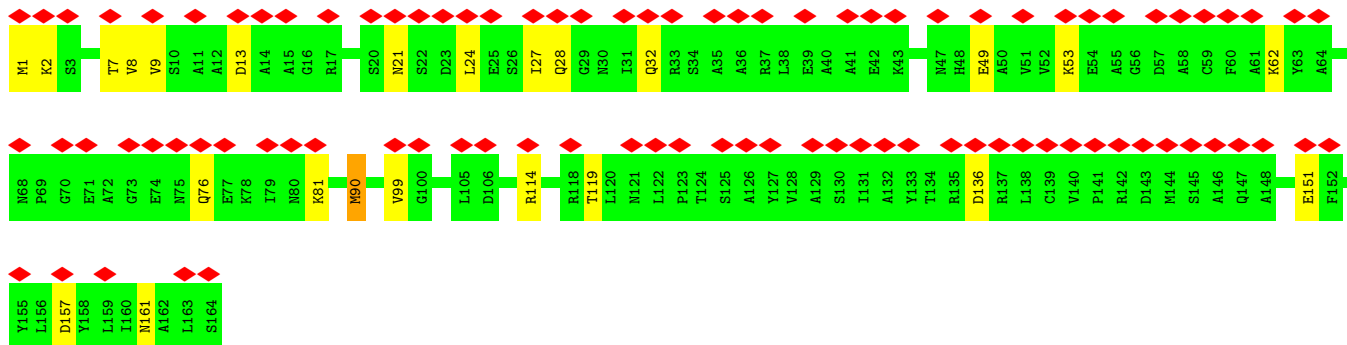


• Molecule 6: Phycoerythrin alpha subunit

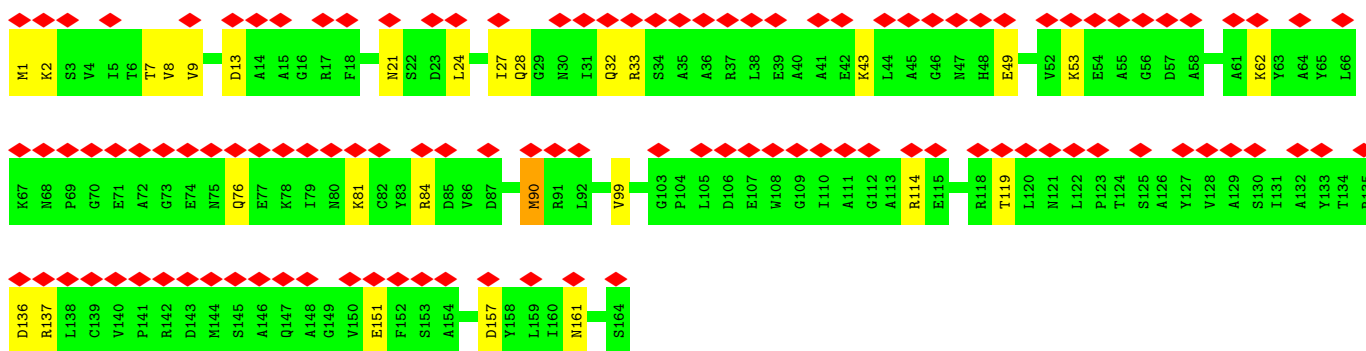
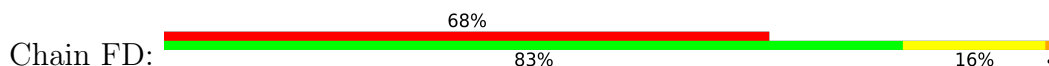


• Molecule 6: Phycoerythrin alpha subunit

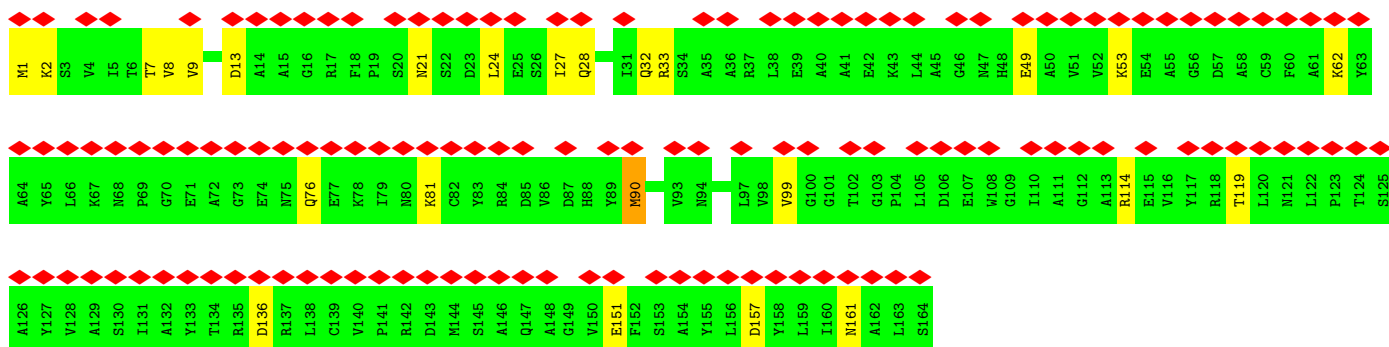
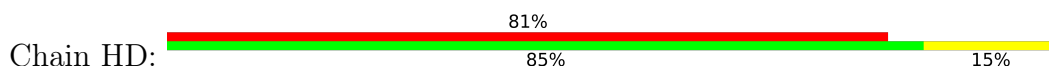




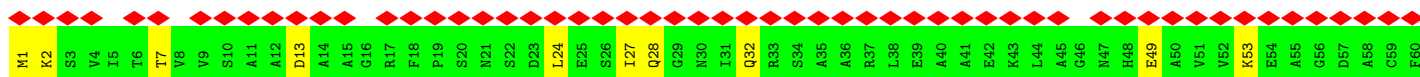
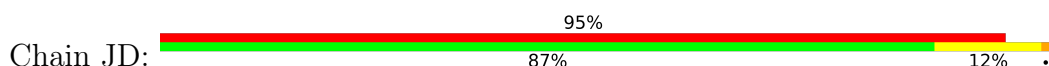
• Molecule 6: Phycoerythrin alpha subunit

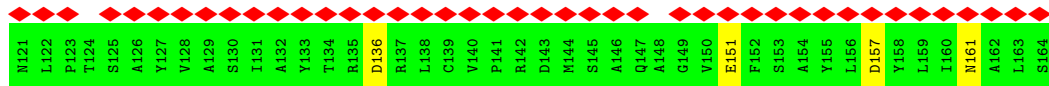
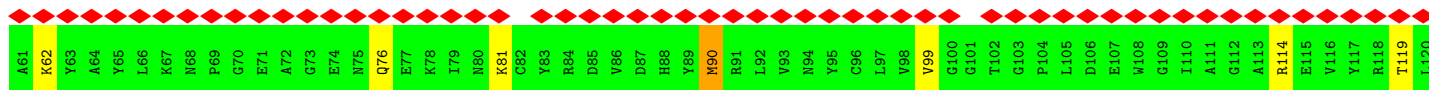


• Molecule 6: Phycoerythrin alpha subunit

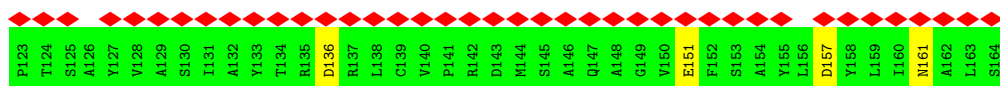
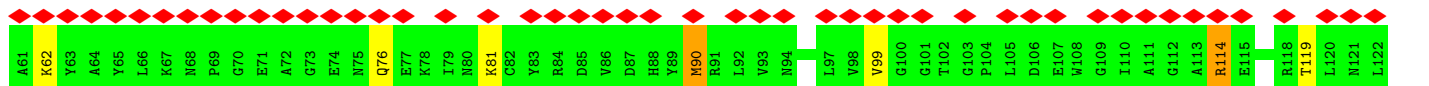
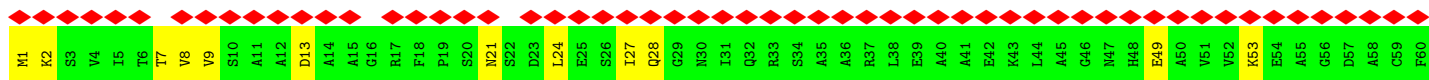
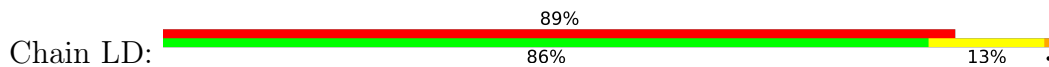


• Molecule 6: Phycoerythrin alpha subunit

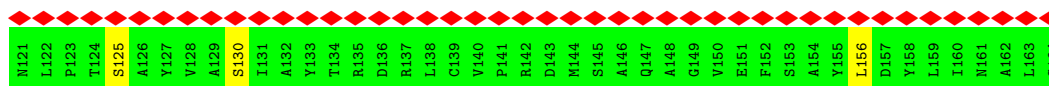
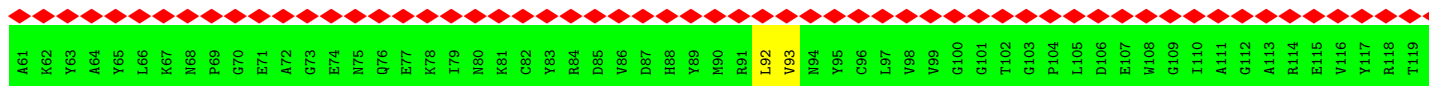
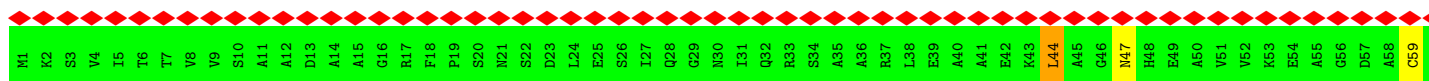




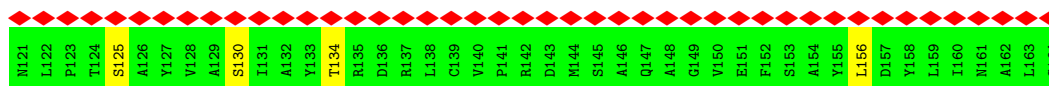
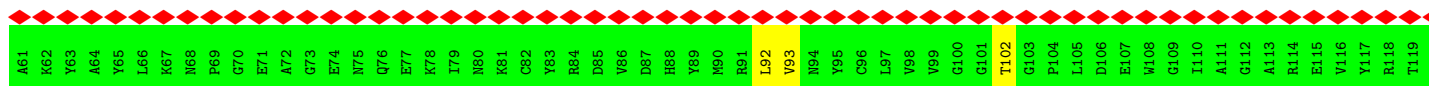
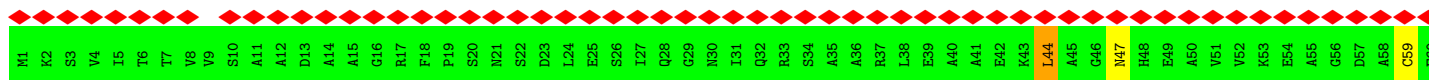
• Molecule 6: Phycoerythrin alpha subunit



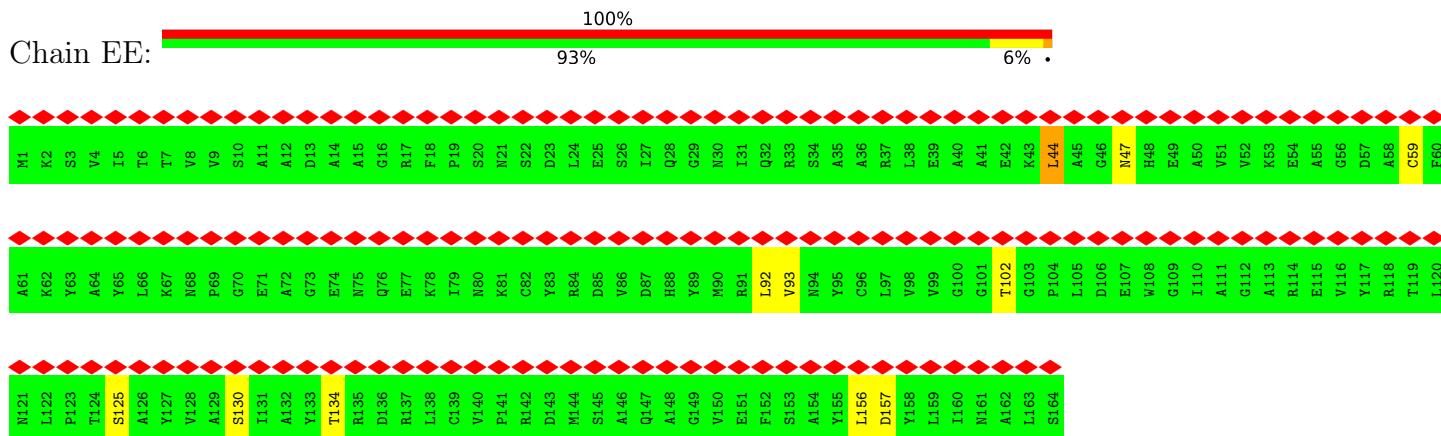
• Molecule 6: Phycoerythrin alpha subunit



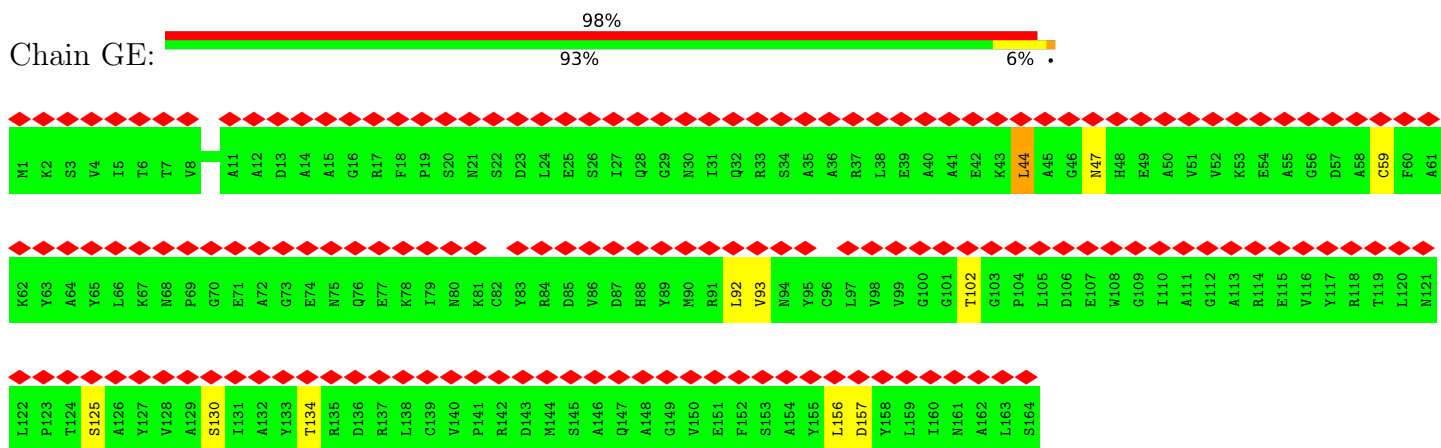
• Molecule 6: Phycoerythrin alpha subunit



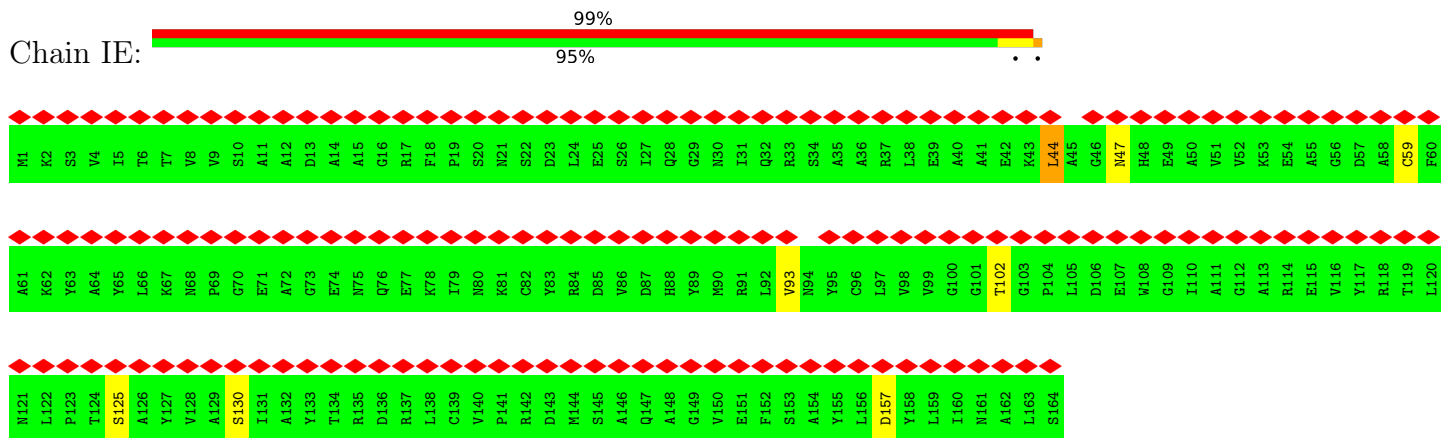
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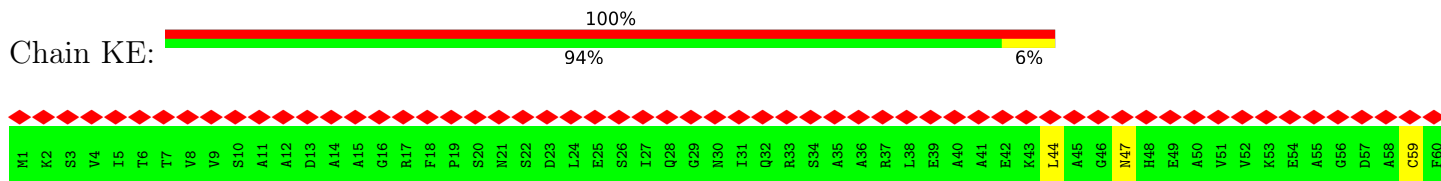
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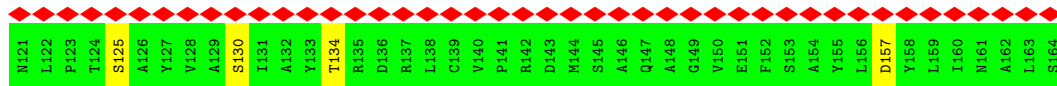
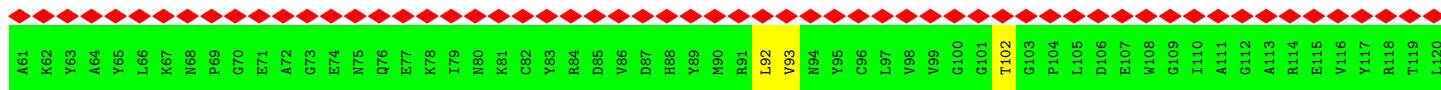


• Molecule 6: Phycoerythrin alpha subunit

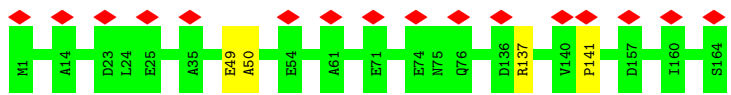


• Molecule 6: Phycoerythrin alpha subunit

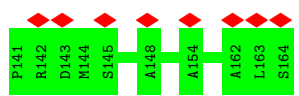
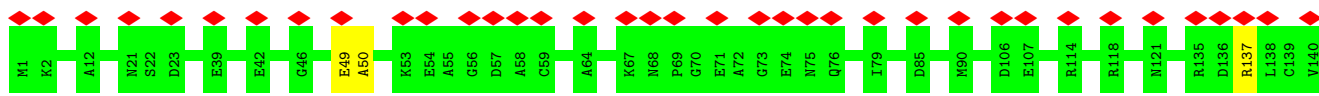




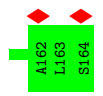
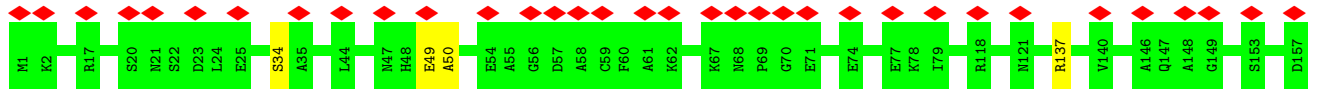
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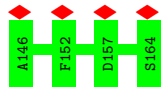
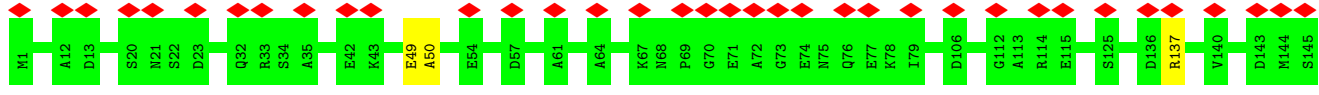
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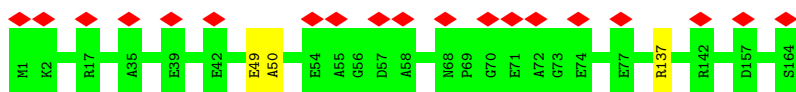
• Molecule 6: Phycoerythrin alpha subunit



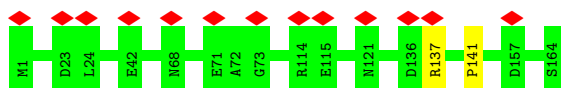
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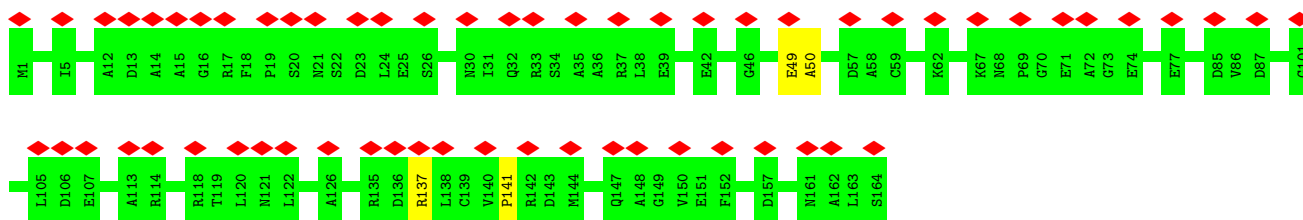
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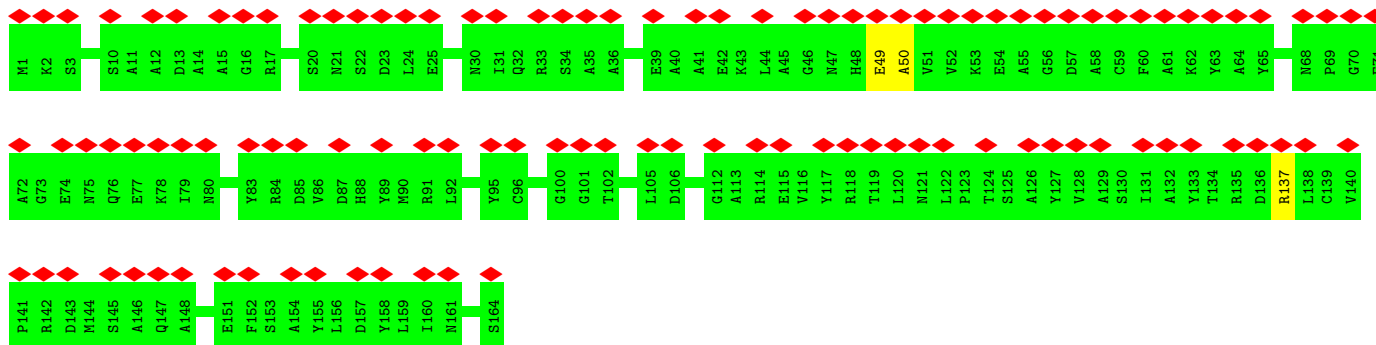
- Molecule 6: Phycoerythrin alpha subunit



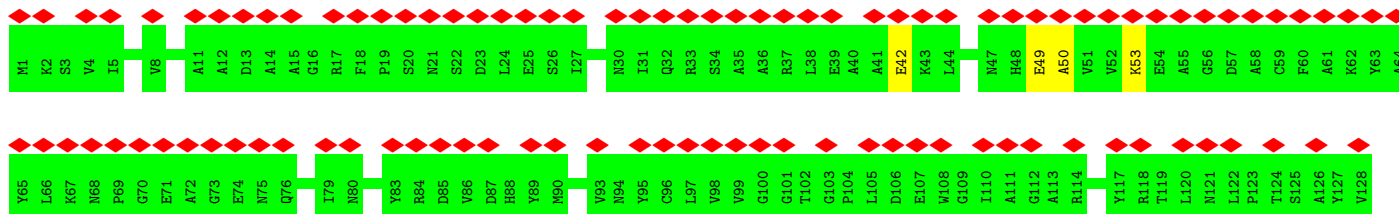
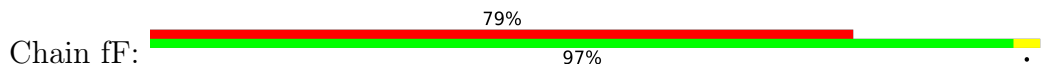
- Molecule 6: Phycoerythrin alpha subunit



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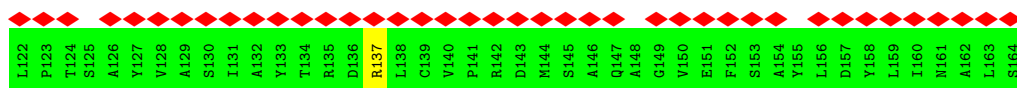
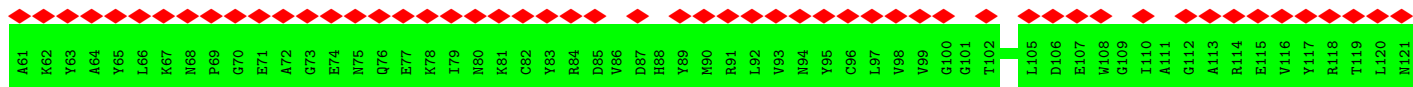
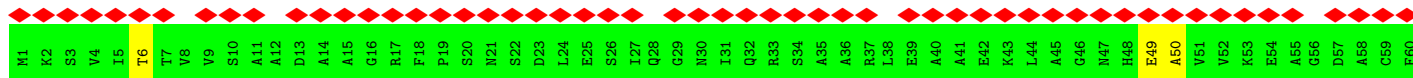


- Molecule 6: Phycoerythrin alpha subunit

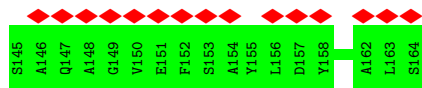
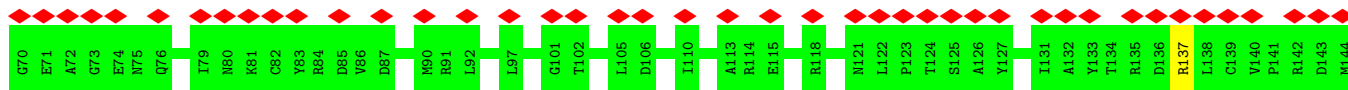
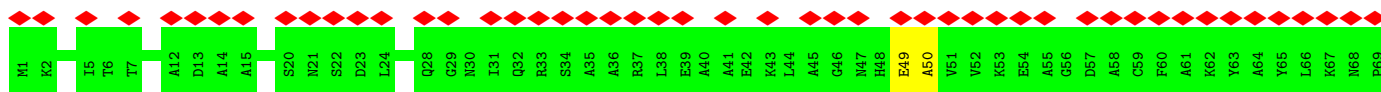




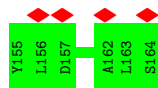
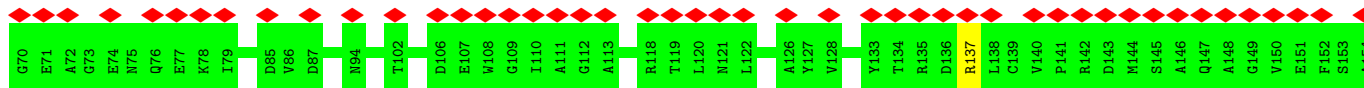
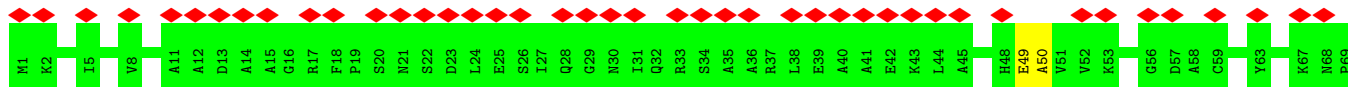
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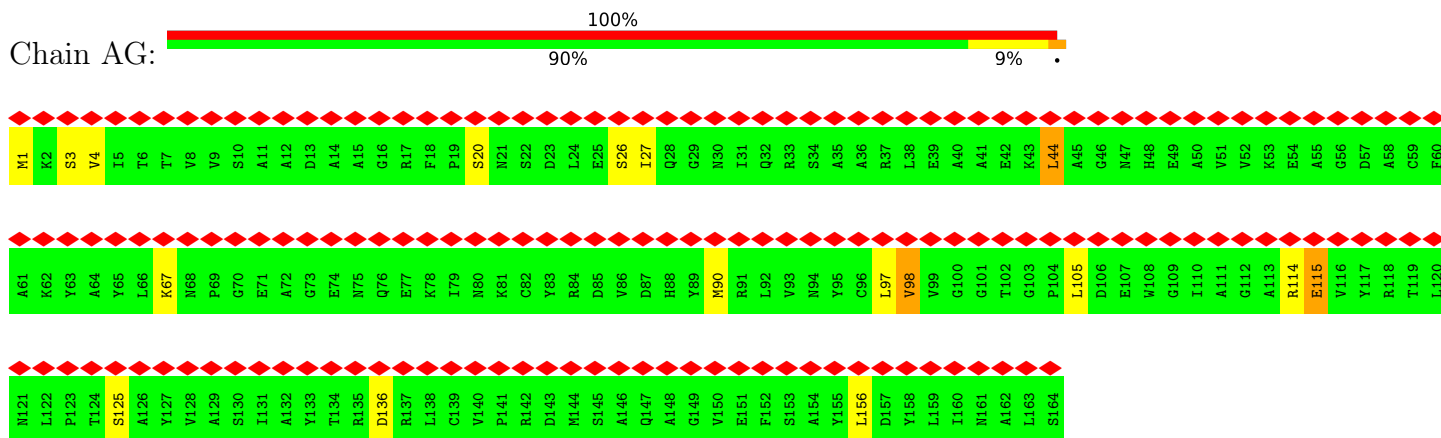
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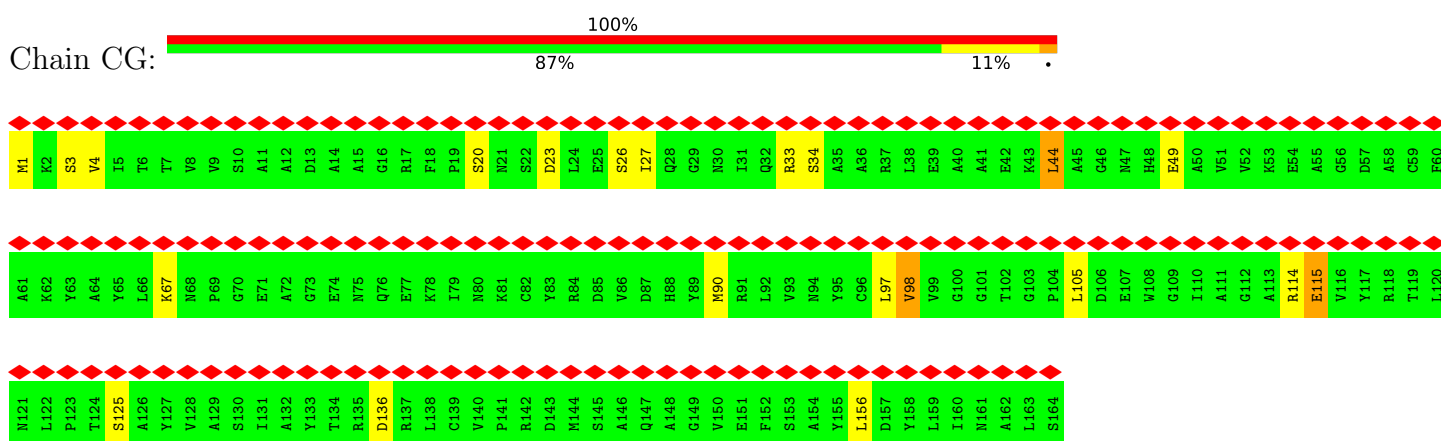
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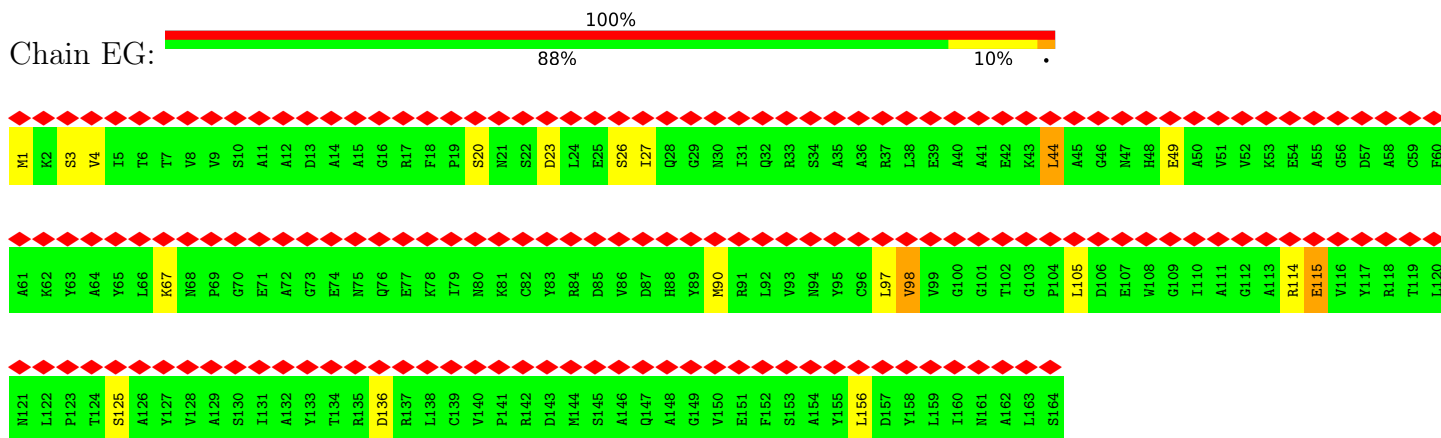
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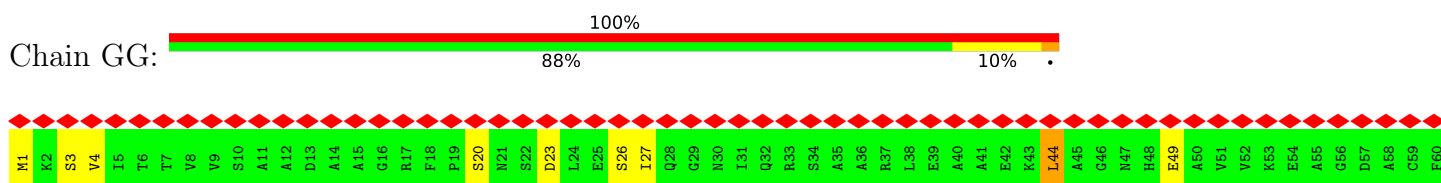
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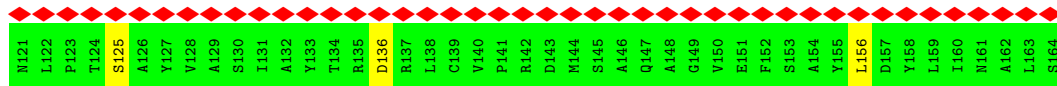
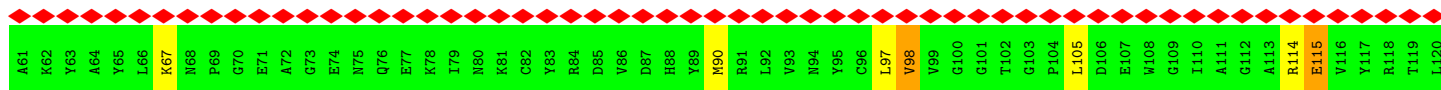


• Molecule 6: Phycoerythrin alpha subunit

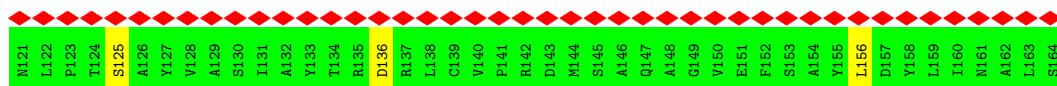
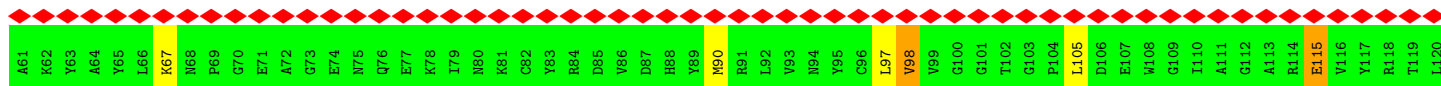
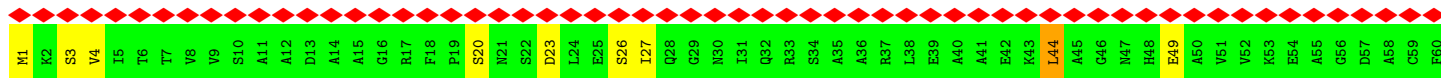
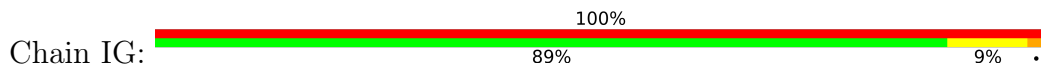


• Molecule 6: Phycoerythrin alpha subunit

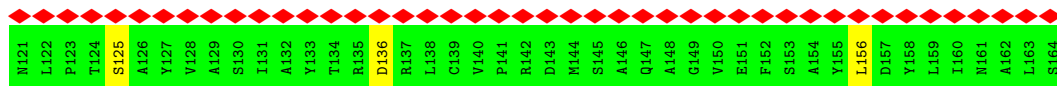
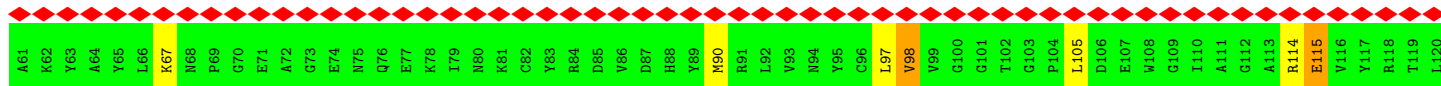
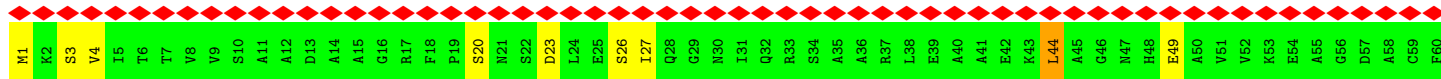
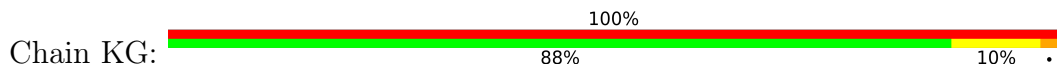




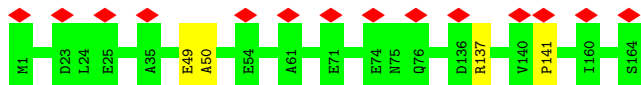
• Molecule 6: Phycoerythrin alpha subunit



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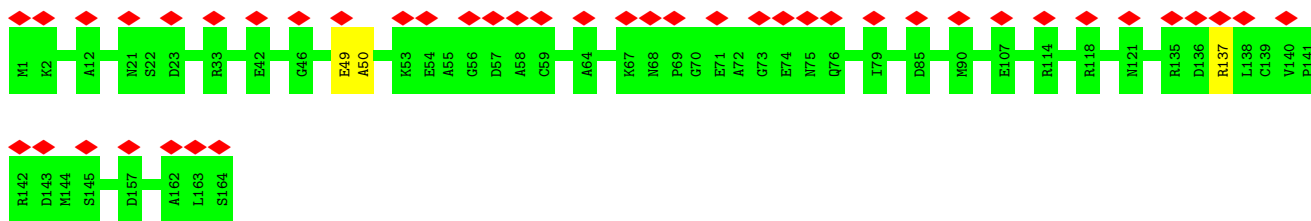


• Molecule 6: Phycoerythrin alpha subunit

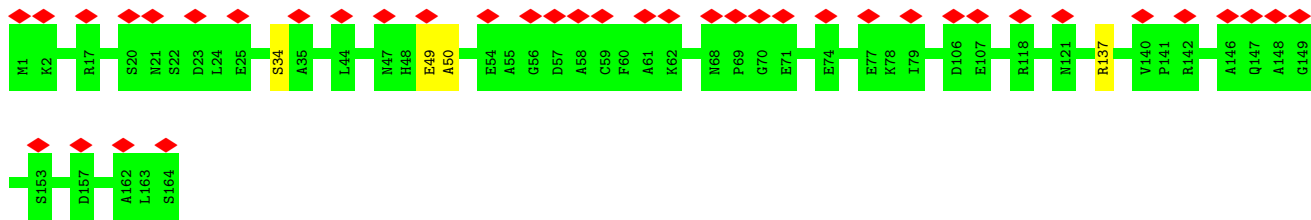


• Molecule 6: Phycoerythrin alpha subunit

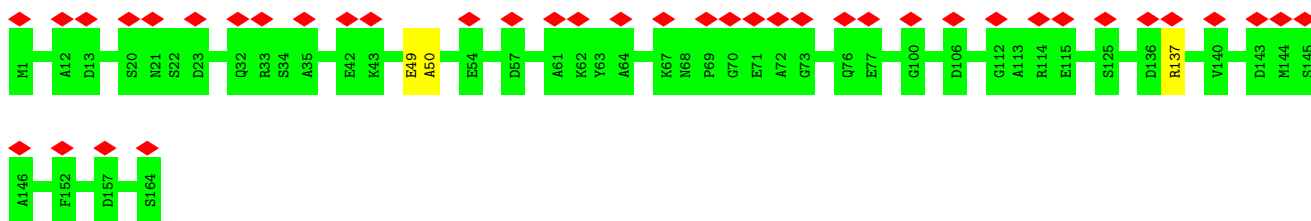




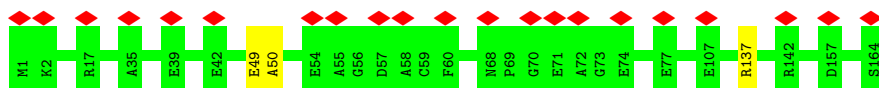
• Molecule 6: Phycoerythrin alpha subunit



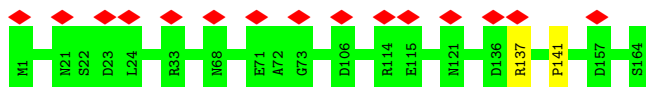
• Molecule 6: Phycoerythrin alpha subunit



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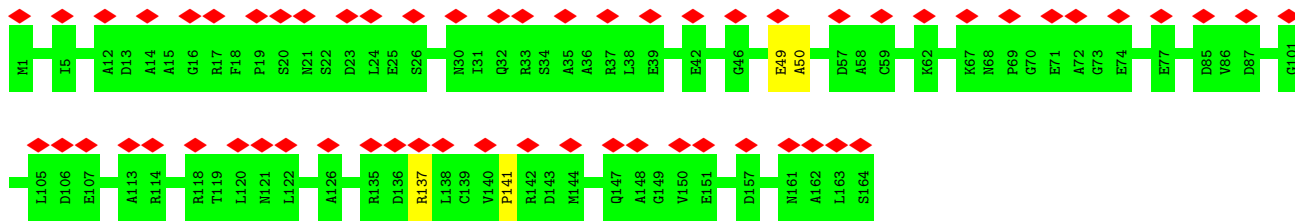


• Molecule 6: Phycoerythrin alpha subunit

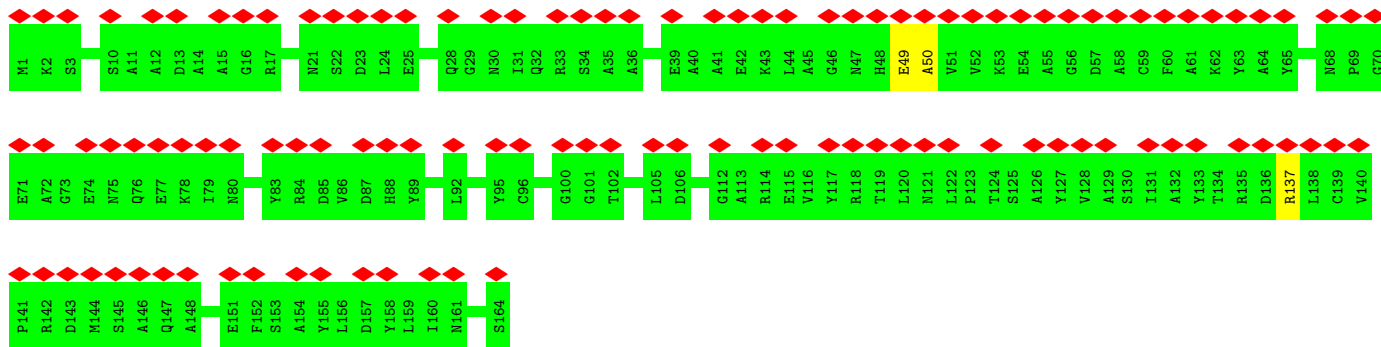


• Molecule 6: Phycoerythrin alpha subunit

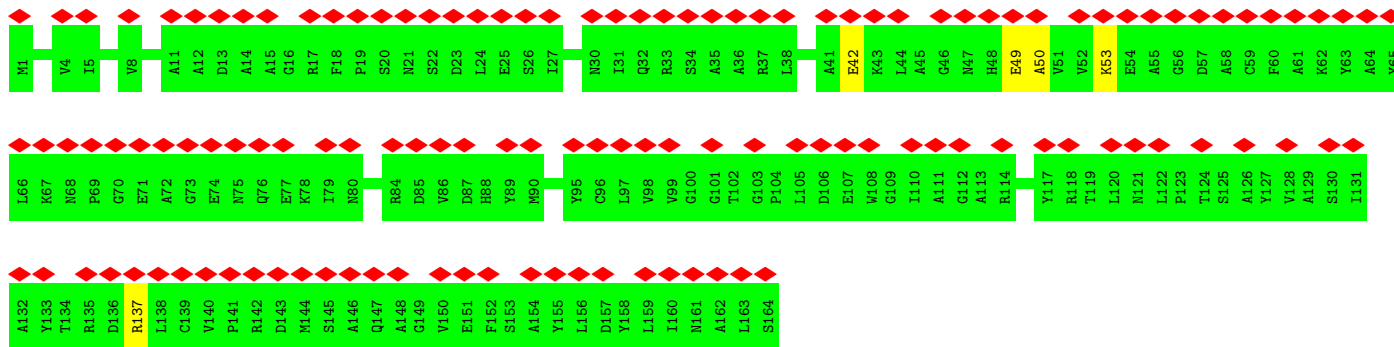
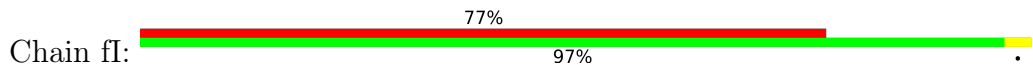




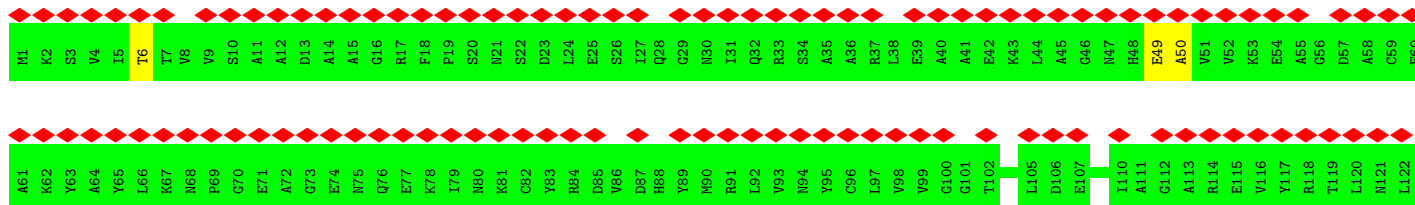
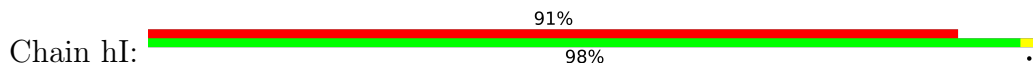
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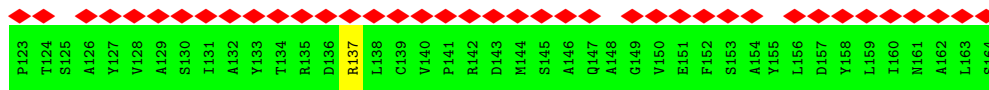


• Molecule 6: Phycoerythrin alpha subunit

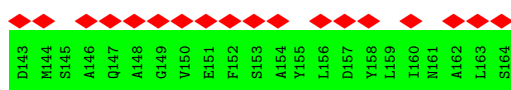
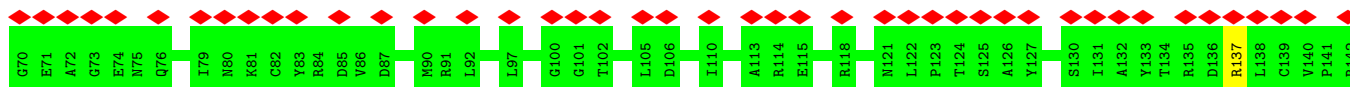
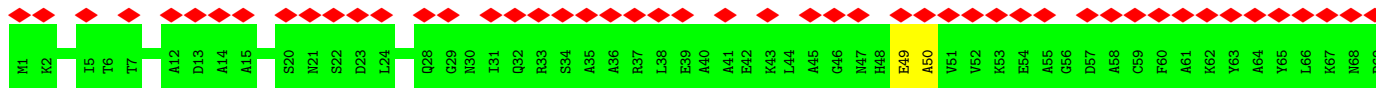


• Molecule 6: Phycoerythrin alpha subunit

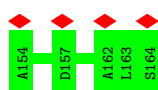
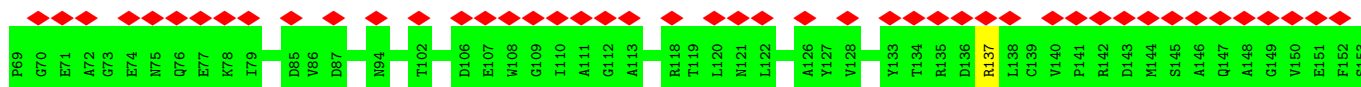
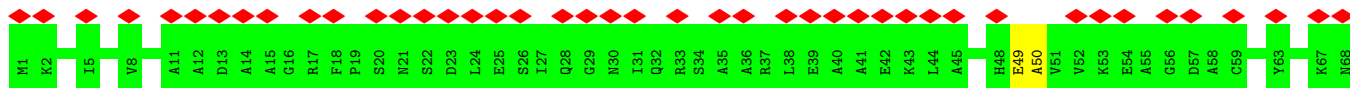




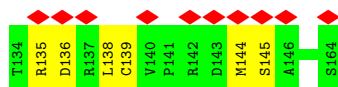
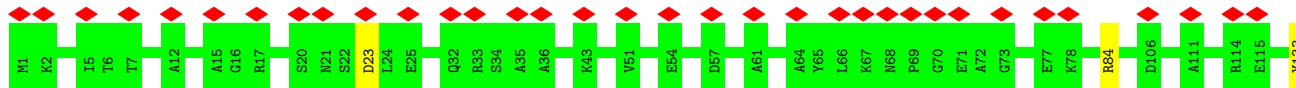
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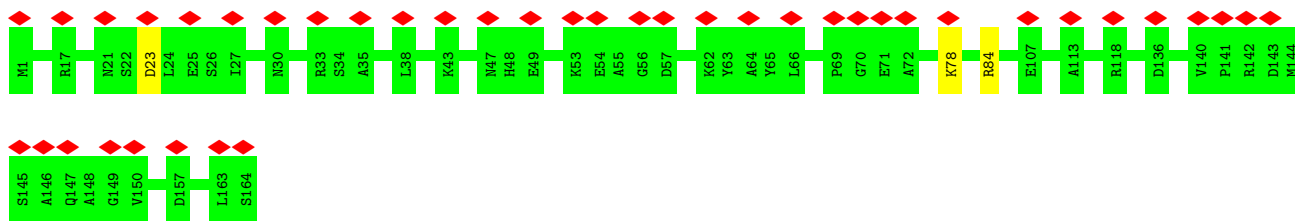


• Molecule 6: Phycoerythrin alpha subunit

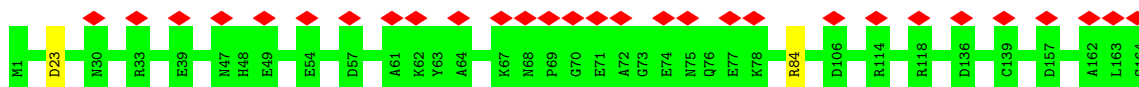


• Molecule 6: Phycoerythrin alpha subunit





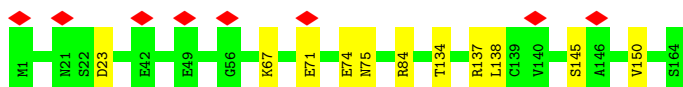
- Molecule 6: Phycoerythrin alpha subunit



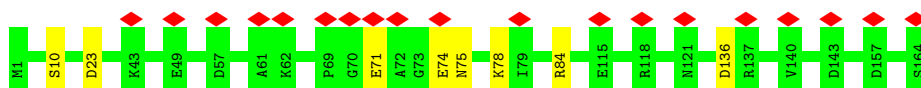
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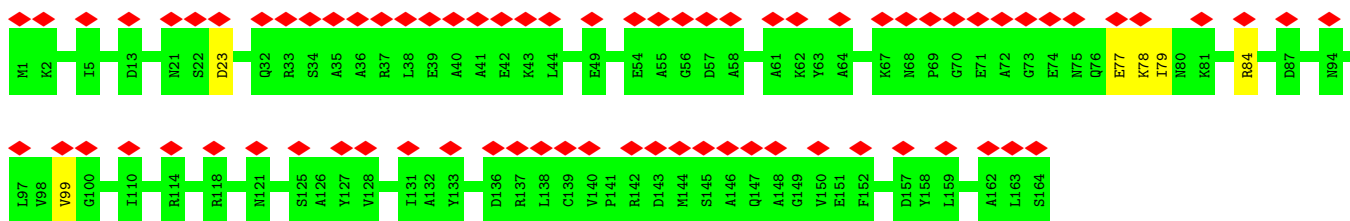
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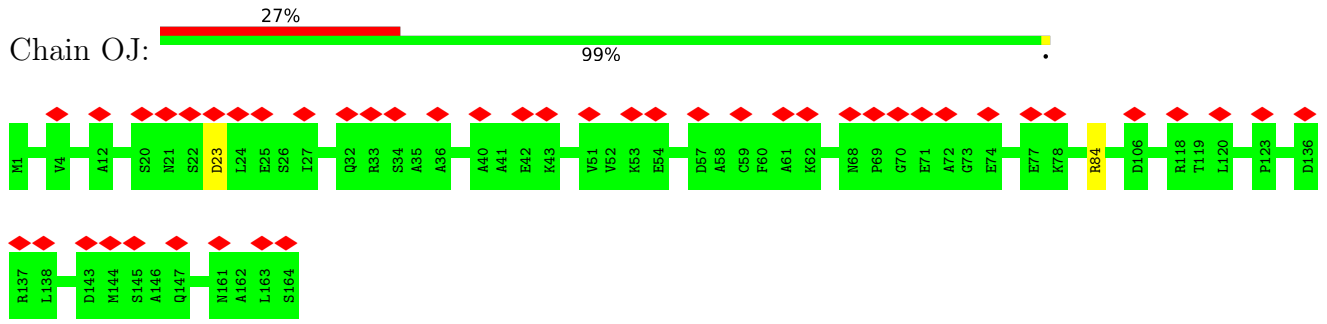
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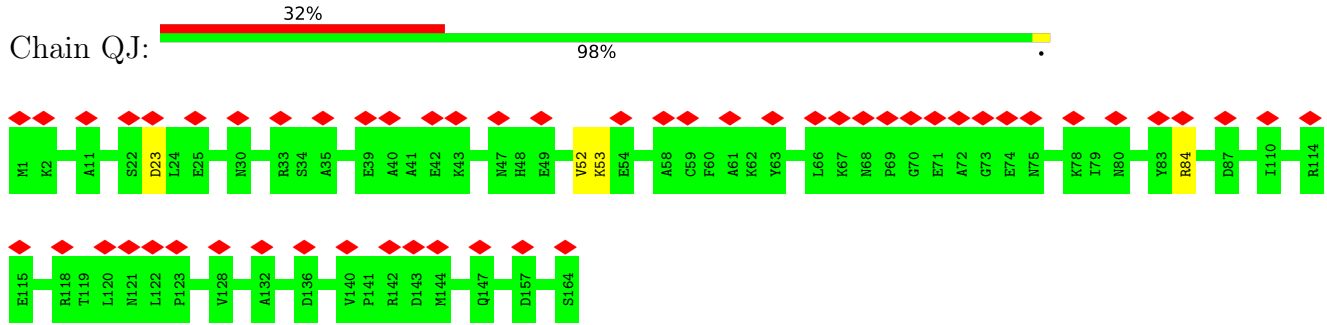
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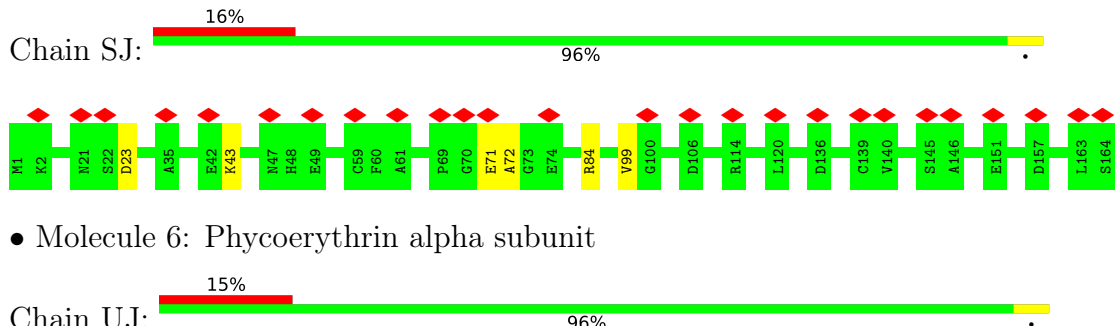
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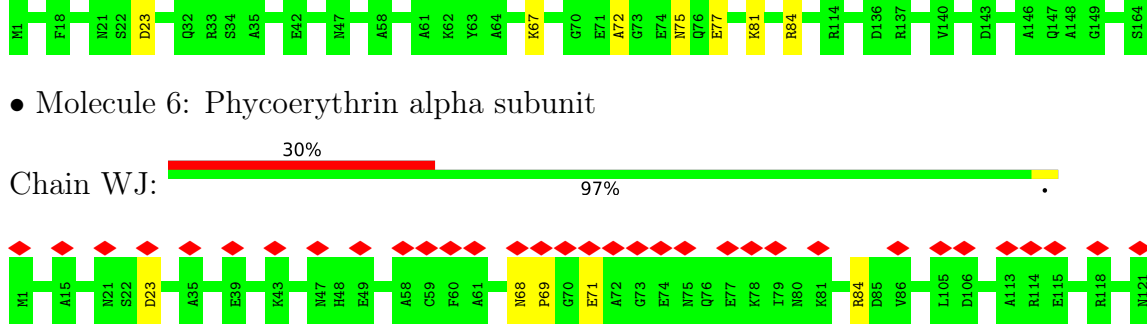
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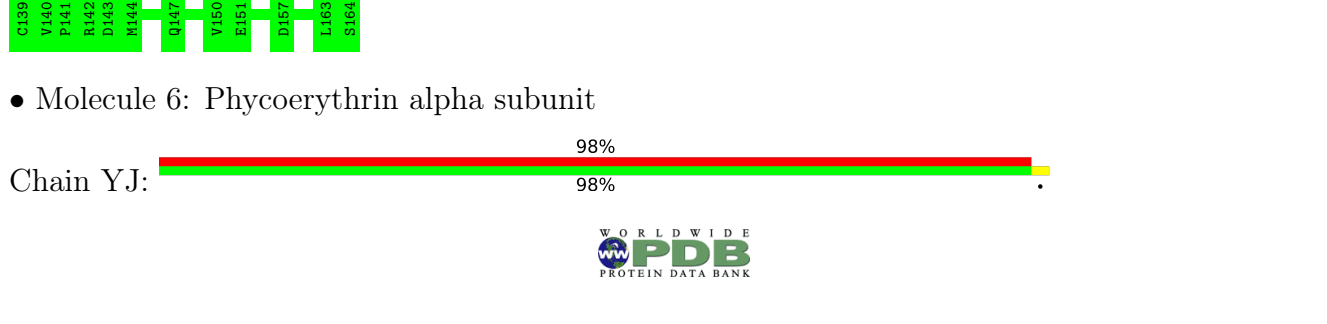
• Molecule 6: Phycoerythrin alpha subunit



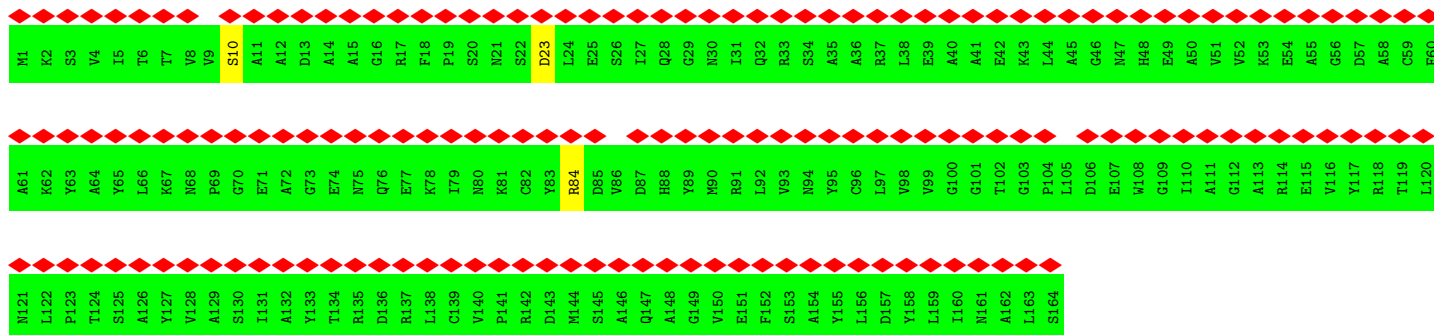
• Molecule 6: Phycoerythrin alpha subunit



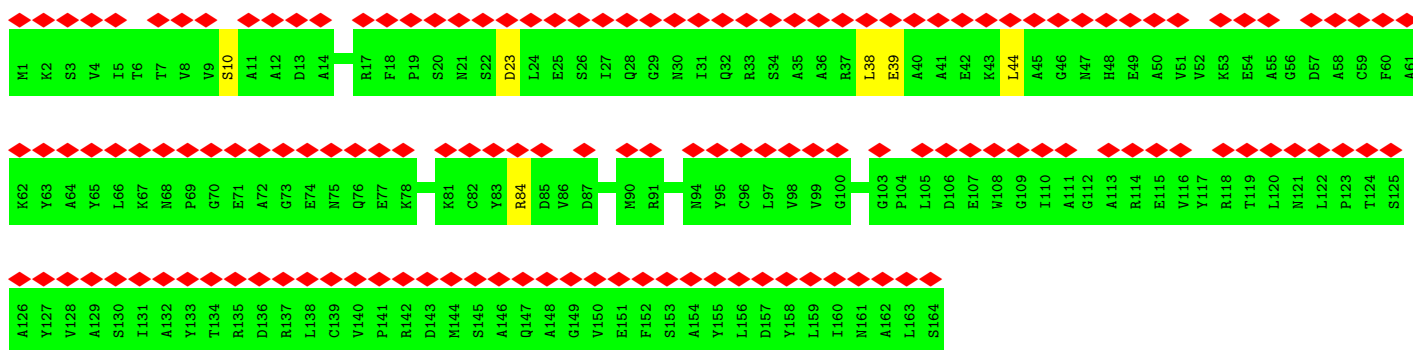
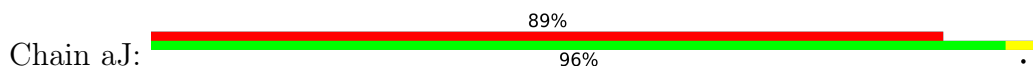
• Molecule 6: Phycoerythrin alpha subunit



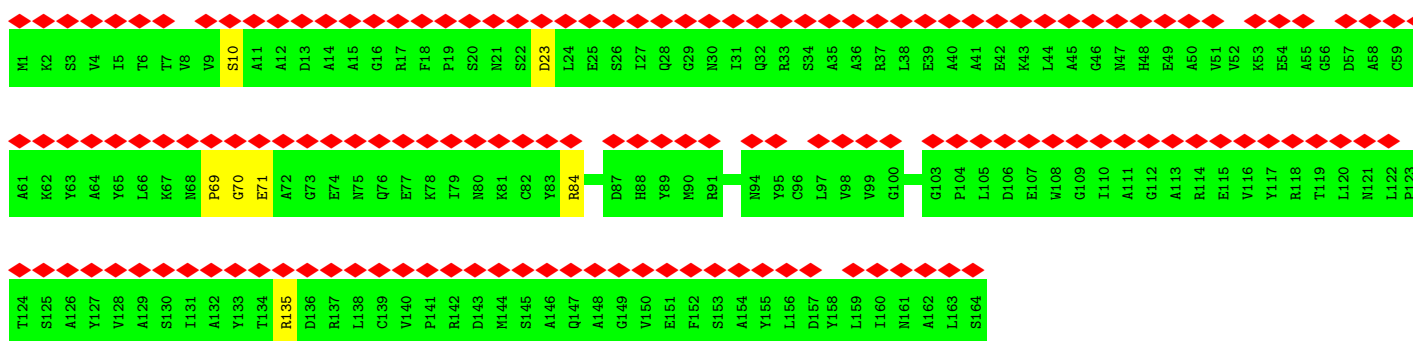
• Molecule 6: Phycoerythrin alpha subunit



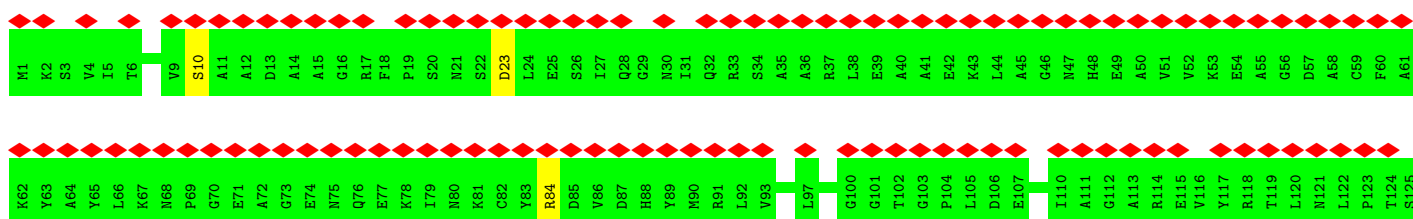
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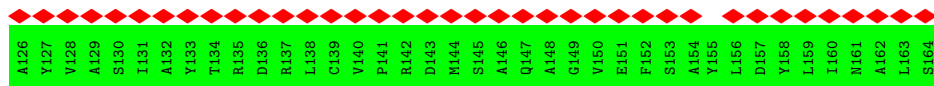


• Molecule 6: Phycoerythrin alpha subunit

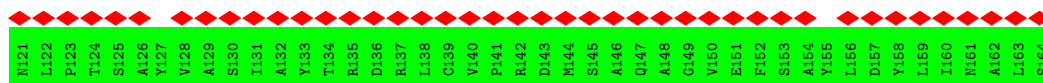
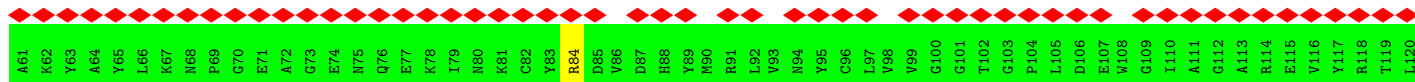
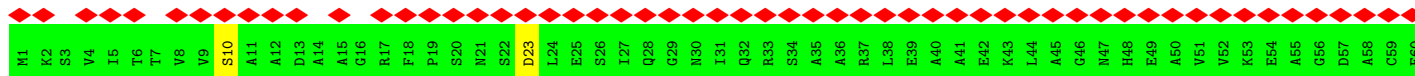


• Molecule 6: Phycoerythrin alpha subunit

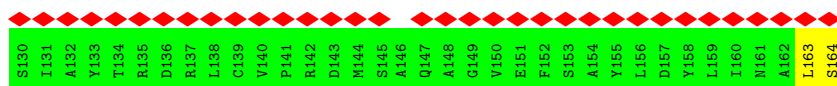
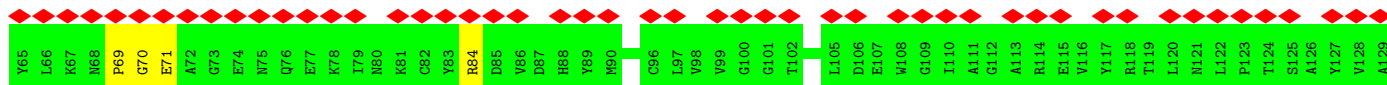
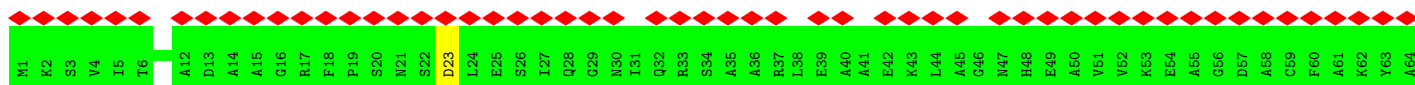
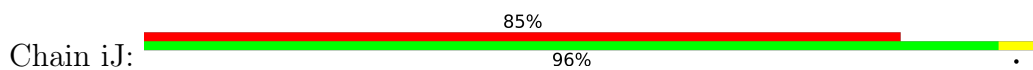




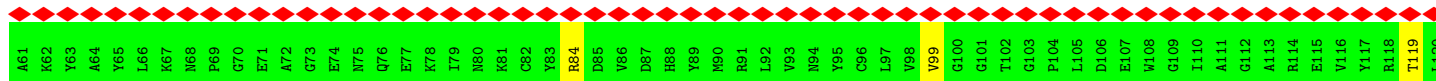
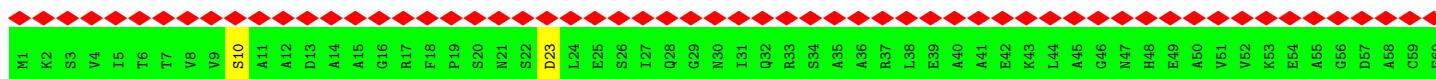
- Molecule 6: Phycoerythrin alpha subunit



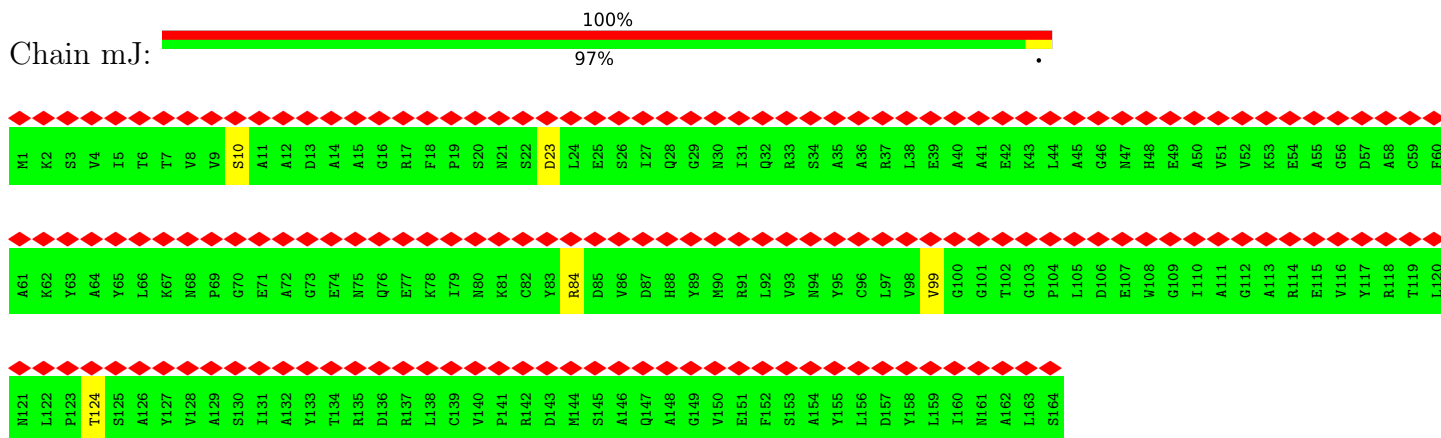
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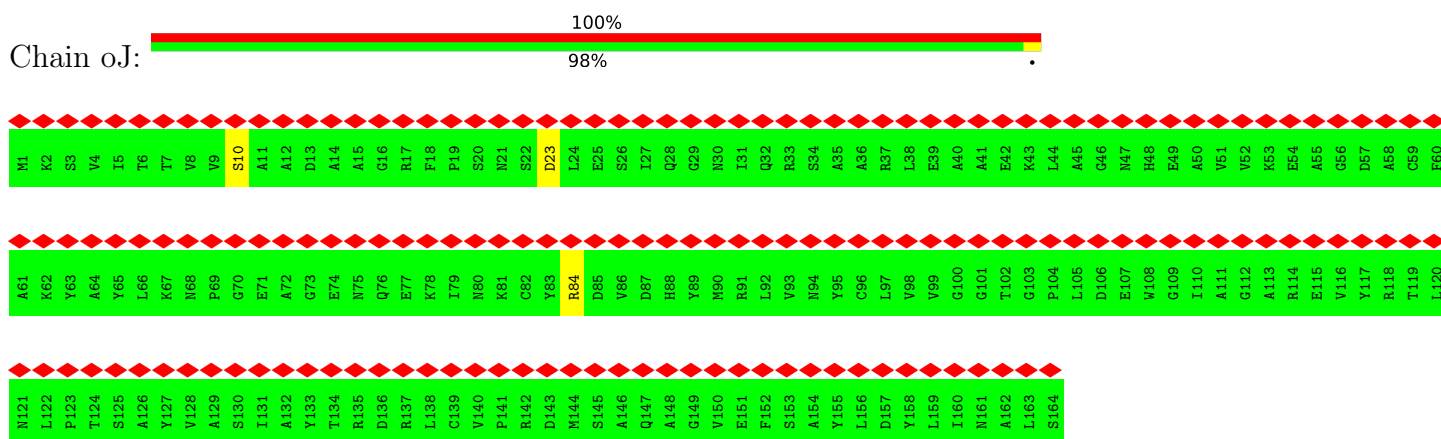
- Molecule 6: Phycoerythrin alpha subunit



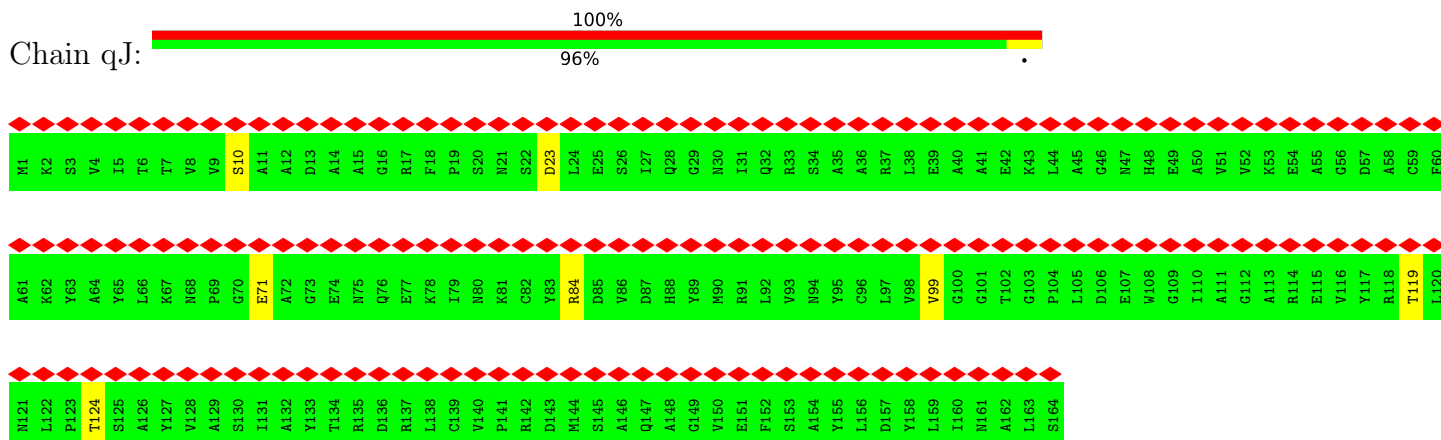
- Molecule 6: Phycoerythrin alpha subunit



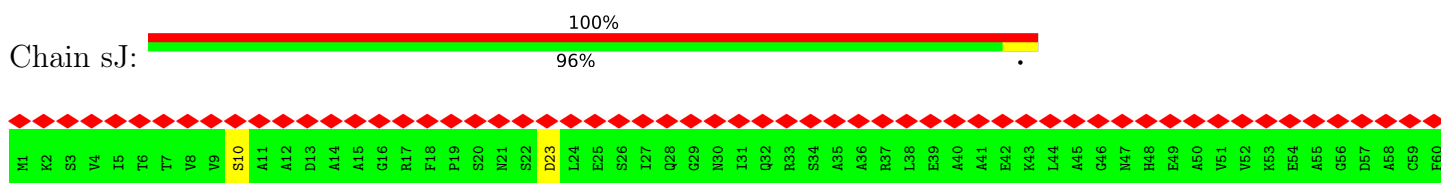
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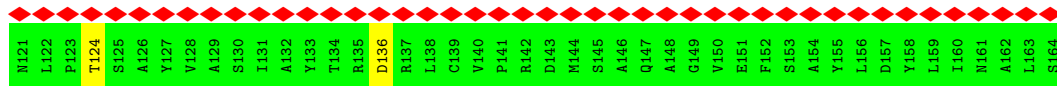
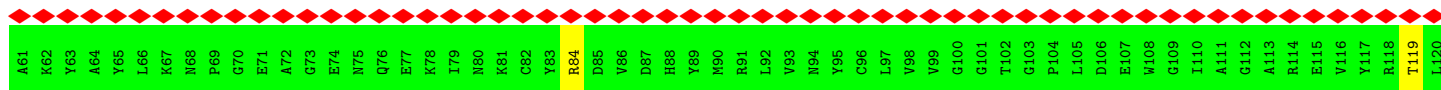


• Molecule 6: Phycoerythrin alpha subunit

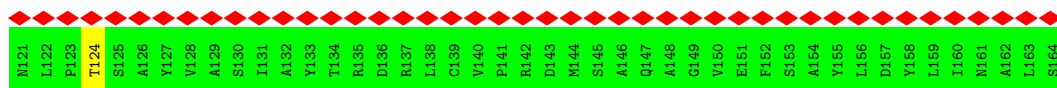
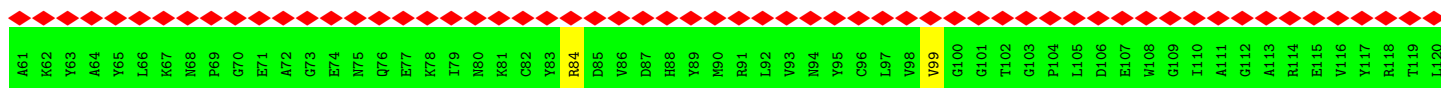
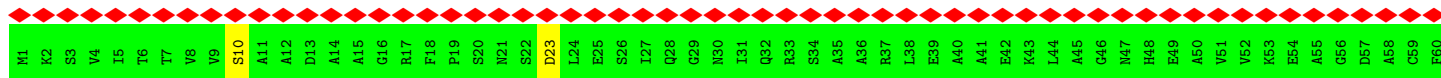


• Molecule 6: Phycoerythrin alpha subunit

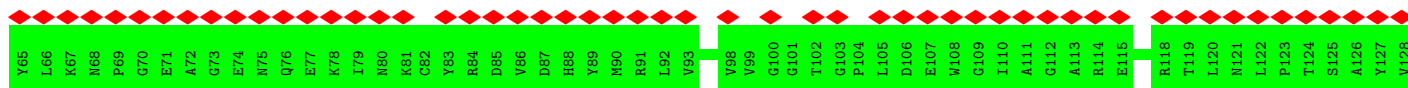
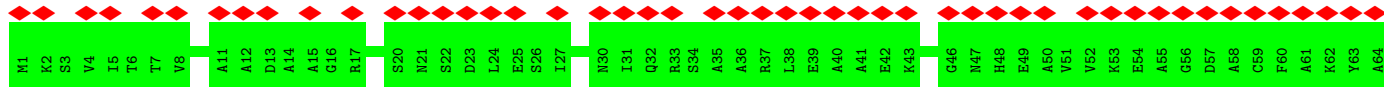
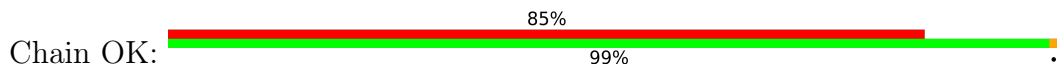




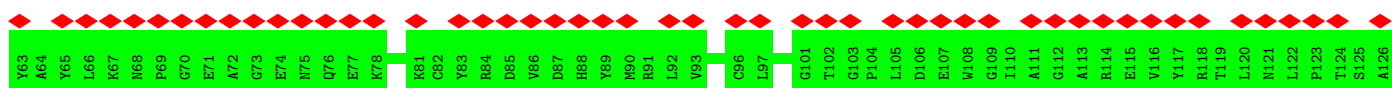
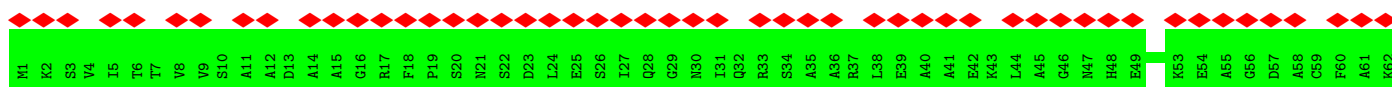
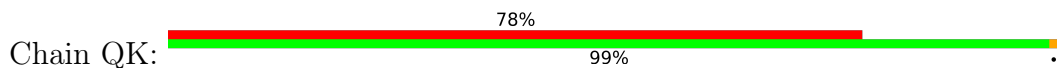
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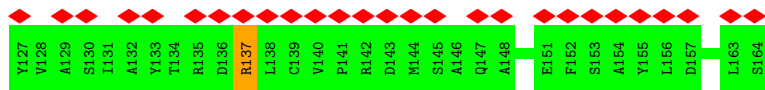


• Molecule 6: Phycoerythrin alpha subunit

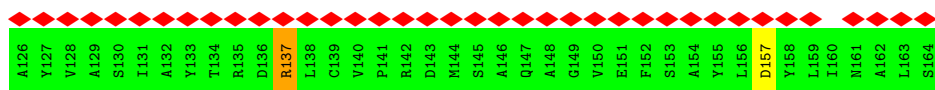
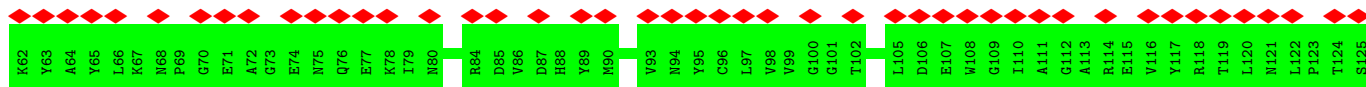
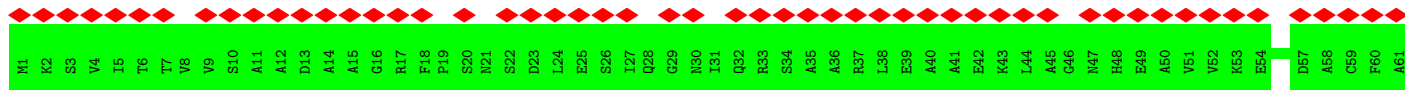
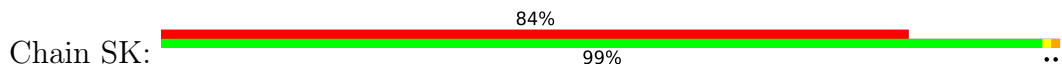


• Molecule 6: Phycoerythrin alpha subunit

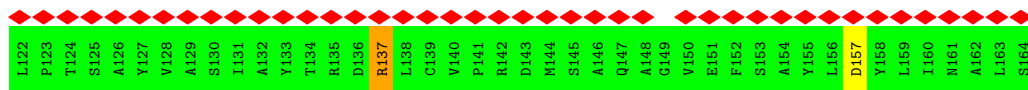
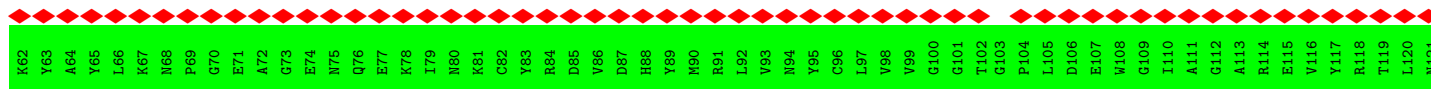
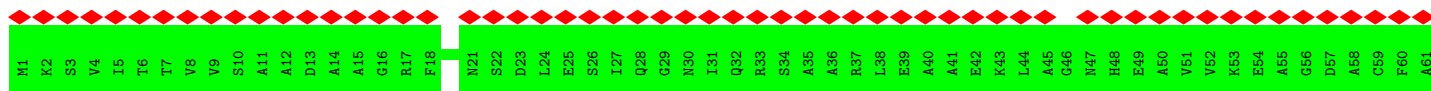




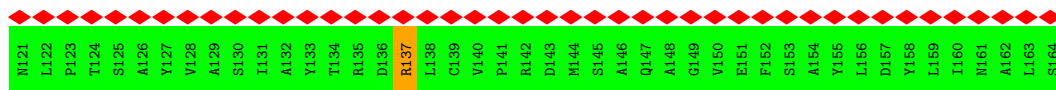
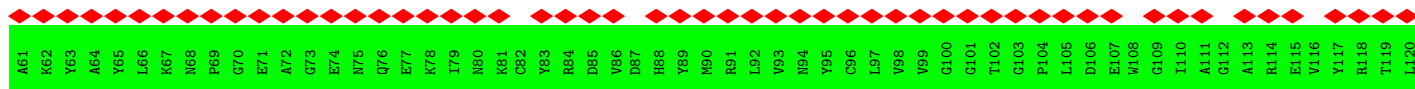
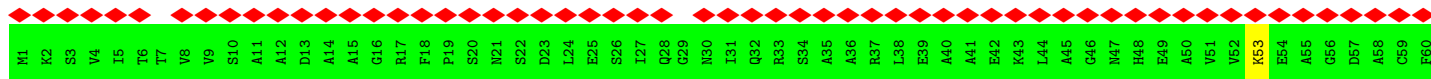
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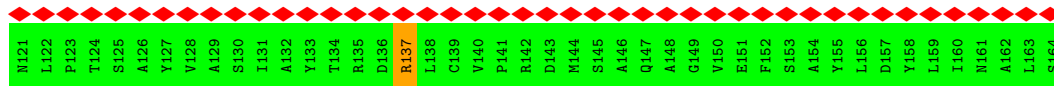
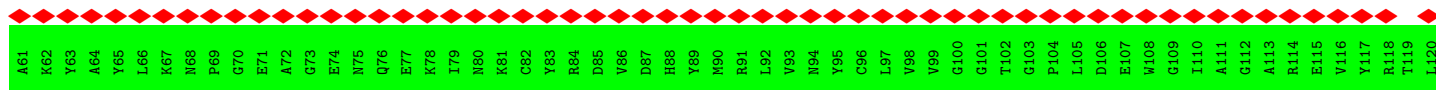
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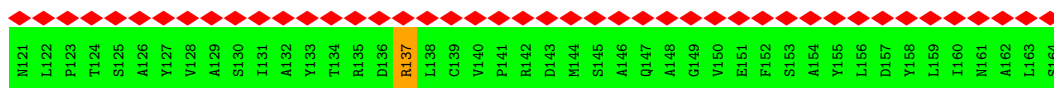
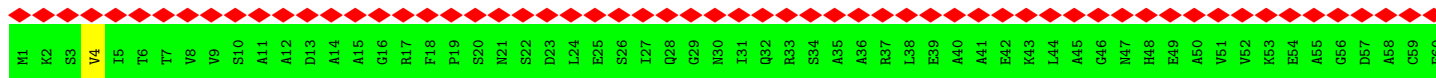
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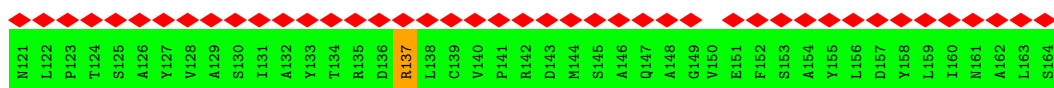
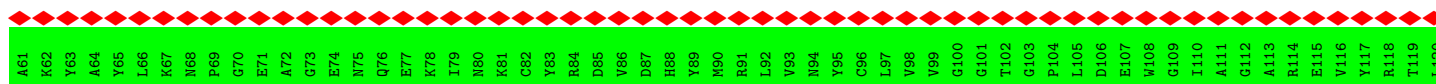
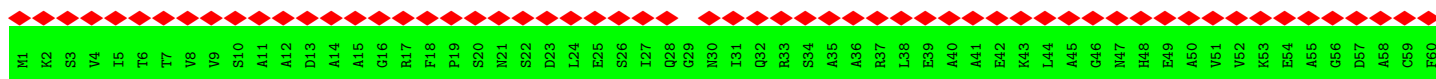
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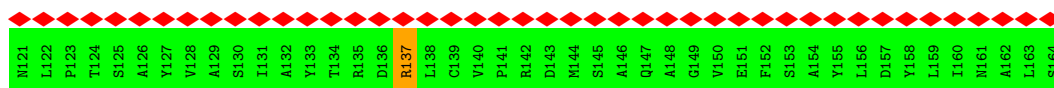
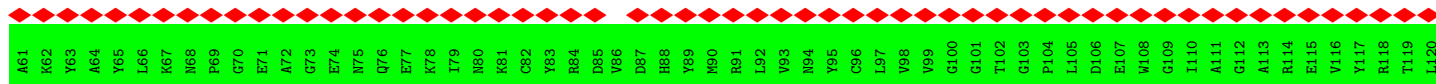
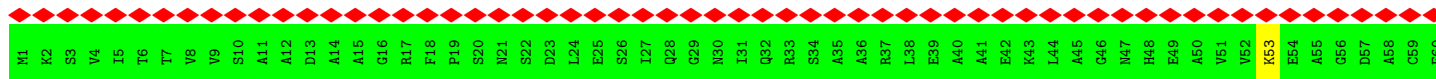
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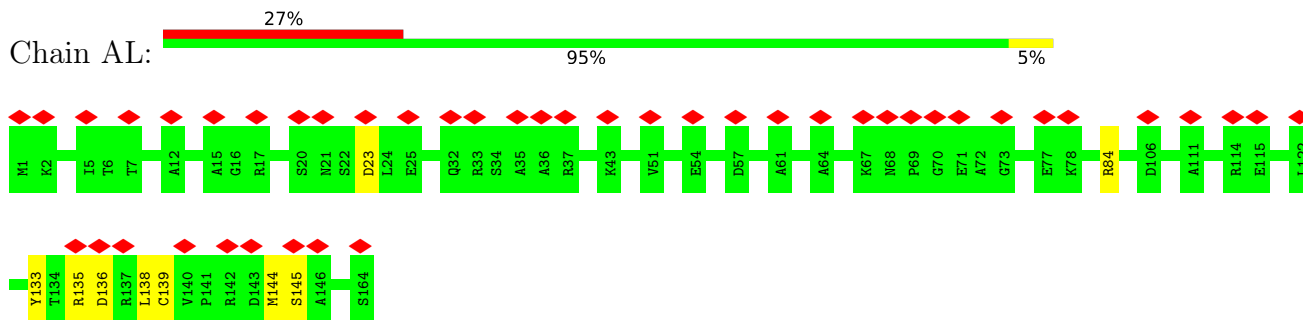
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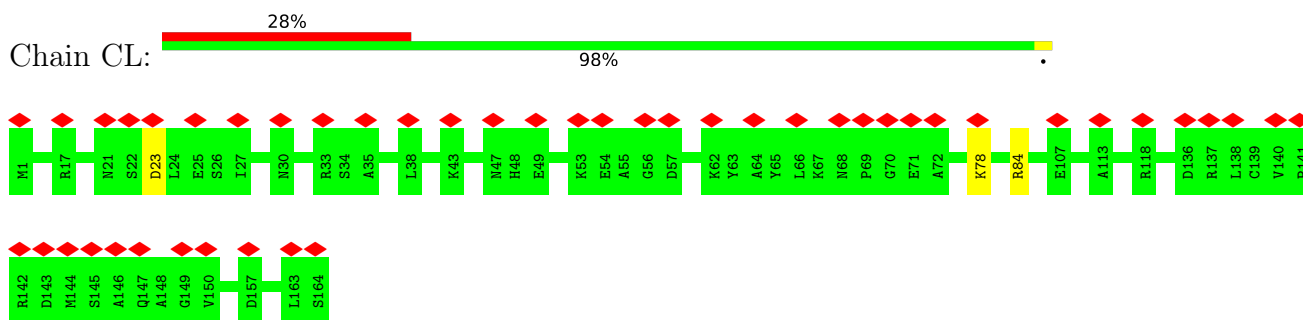
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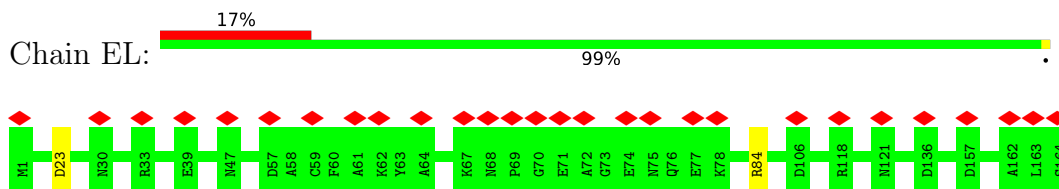
- Molecule 6: Phycoerythrin alpha subunit



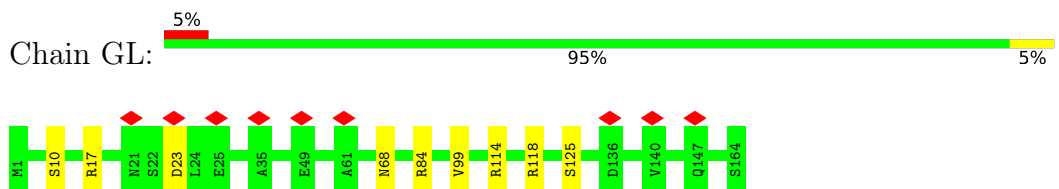
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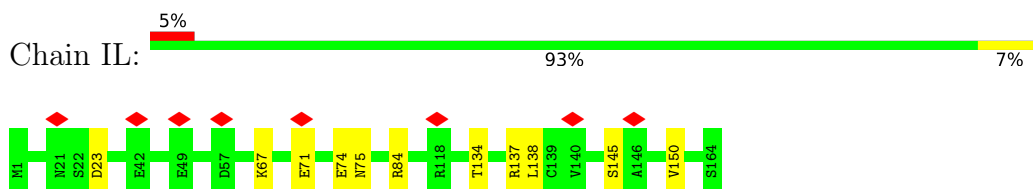
- Molecule 6: Phycoerythrin alpha subunit



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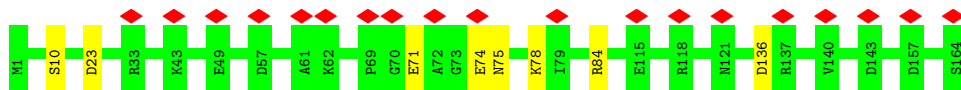


- Molecule 6: Phycoerythrin alpha subunit

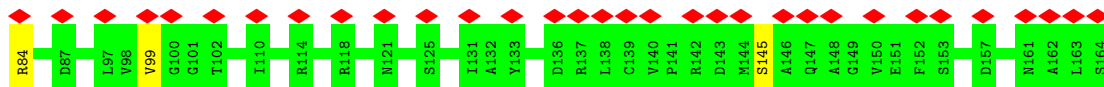
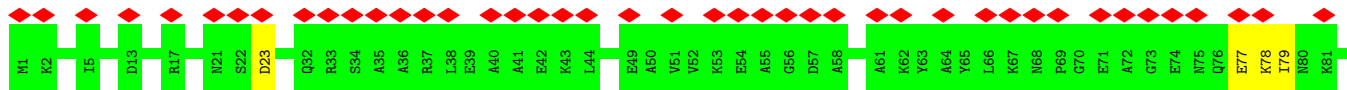


- Molecule 6: Phycoerythrin alpha subunit

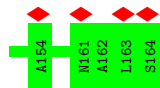
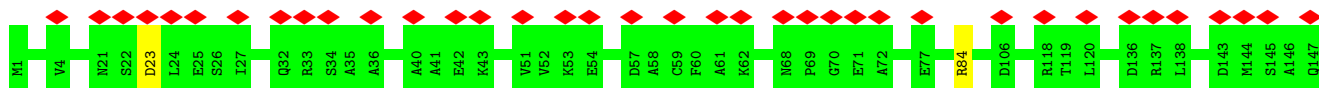




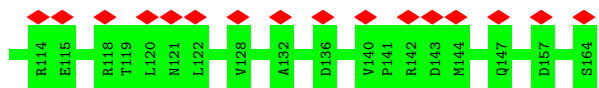
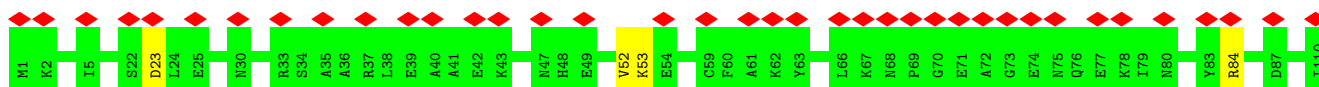
• Molecule 6: Phycoerythrin alpha subunit



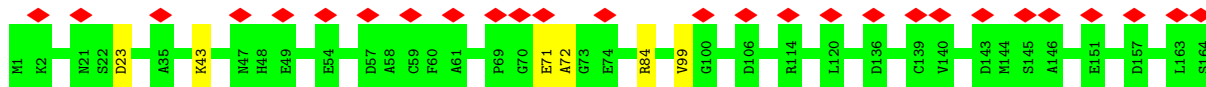
• Molecule 6: Phycoerythrin alpha subunit



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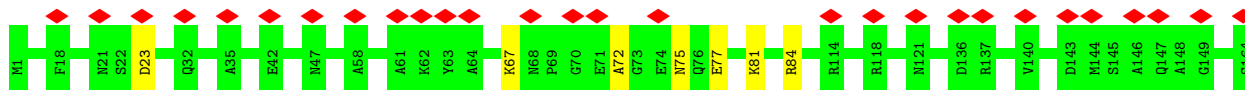


• Molecule 6: Phycoerythrin alpha subunit

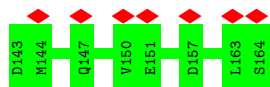
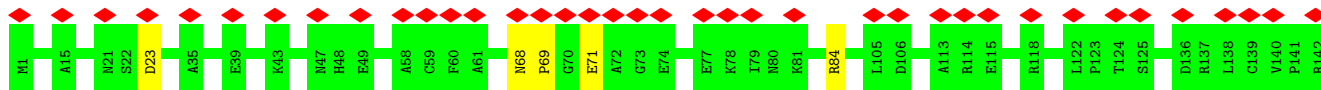


• Molecule 6: Phycoerythrin alpha subunit

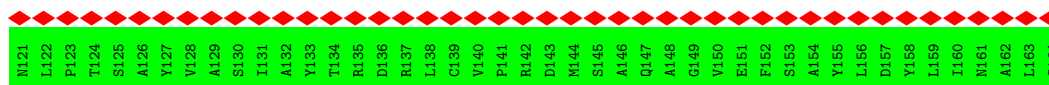
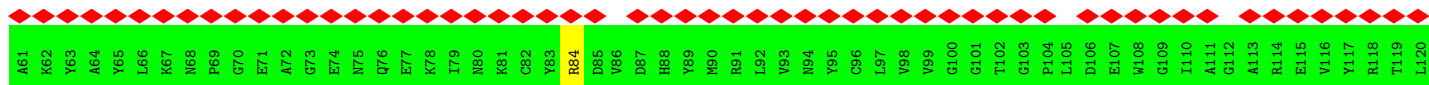
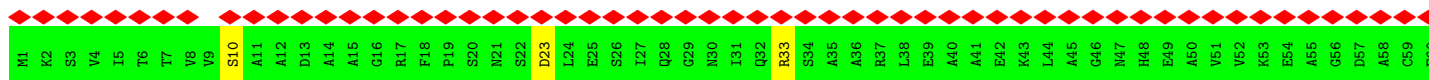




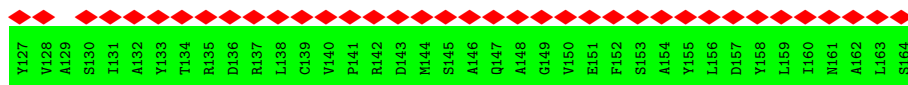
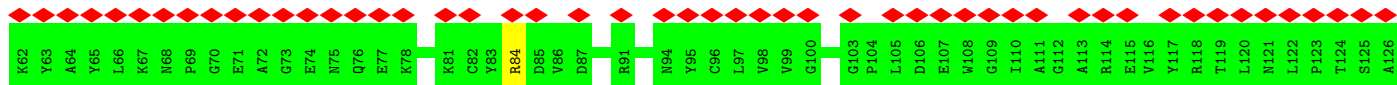
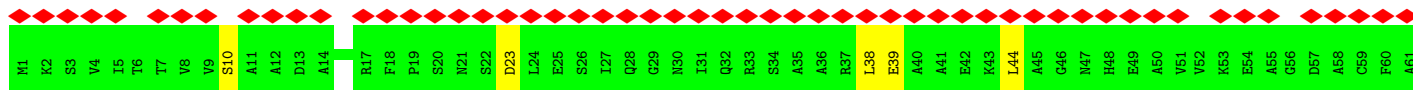
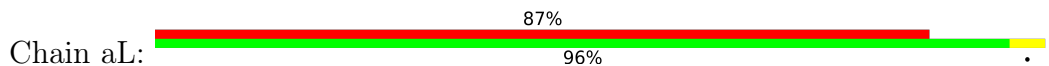
• Molecule 6: Phycoerythrin alpha subunit



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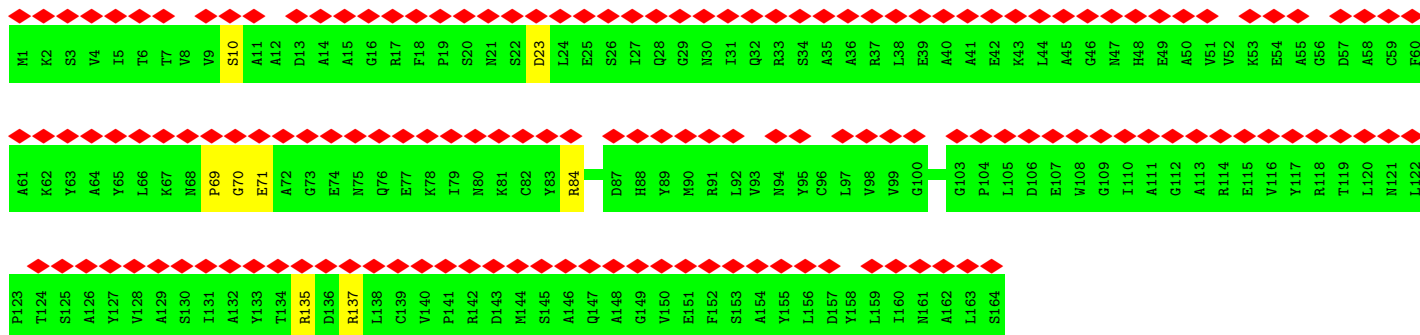


• Molecule 6: Phycoerythrin alpha subunit

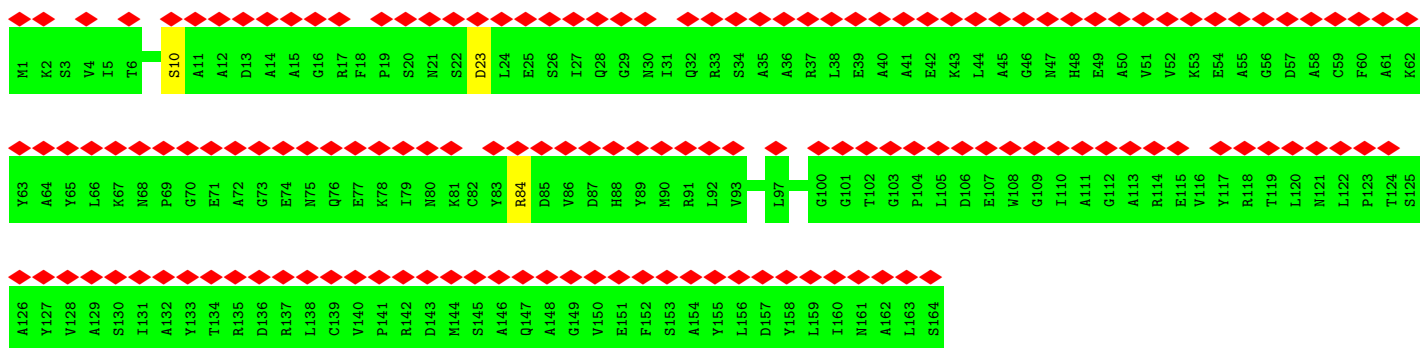


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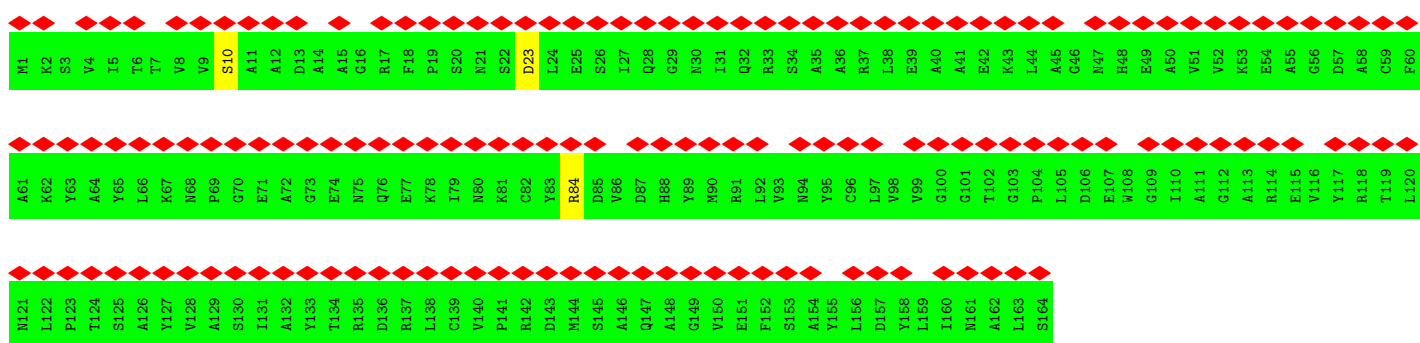




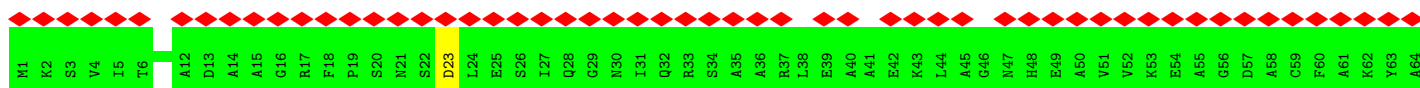
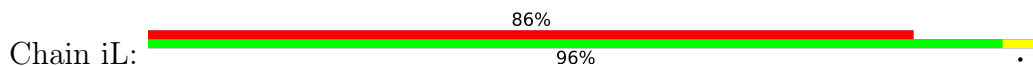
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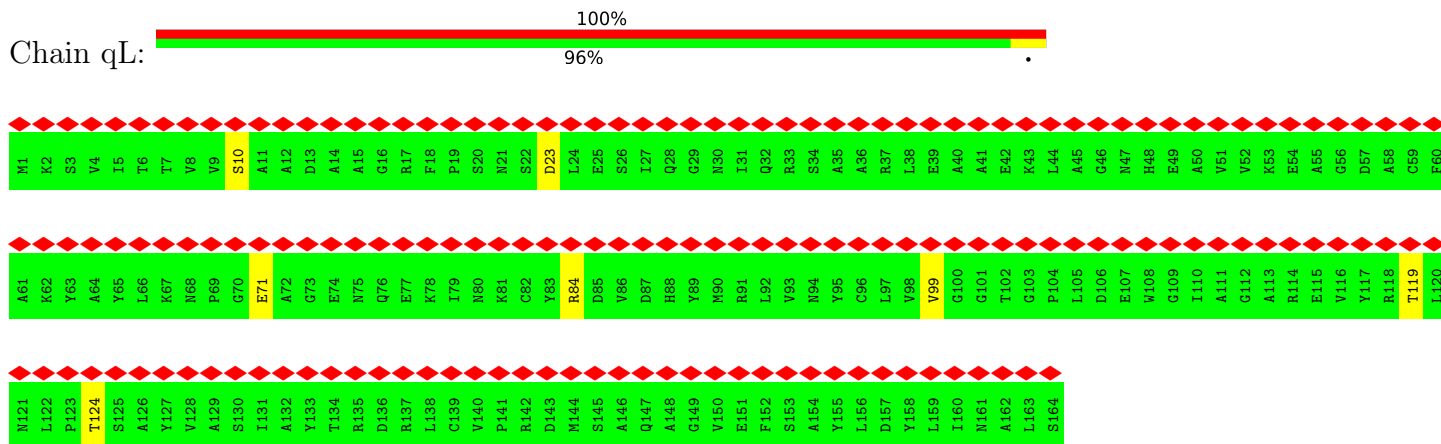
• Molecule 6: Phycoerythrin alpha subunit



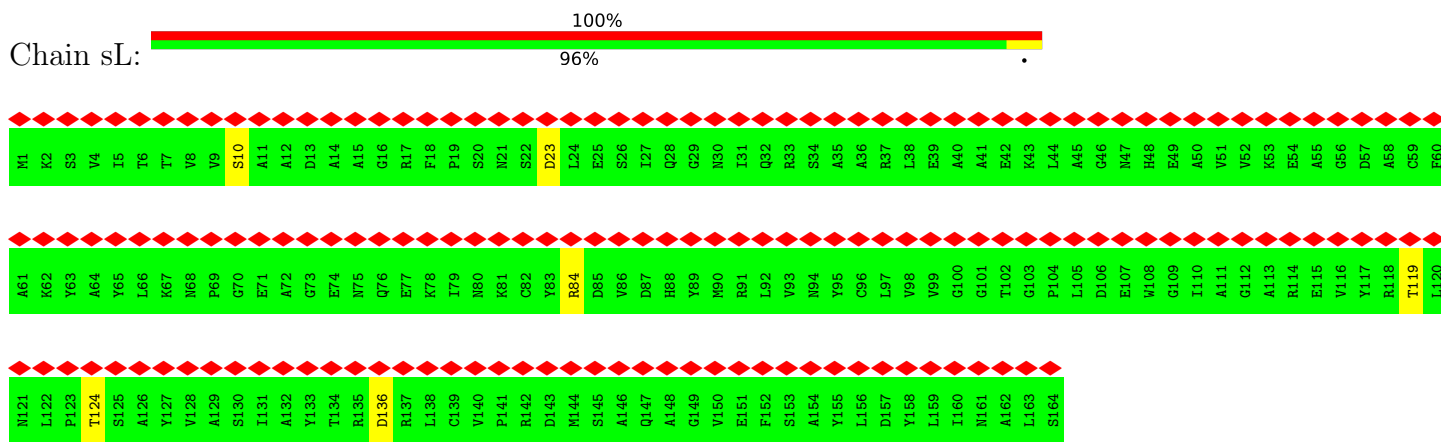
• Molecule 6: Phycoerythrin alpha subunit



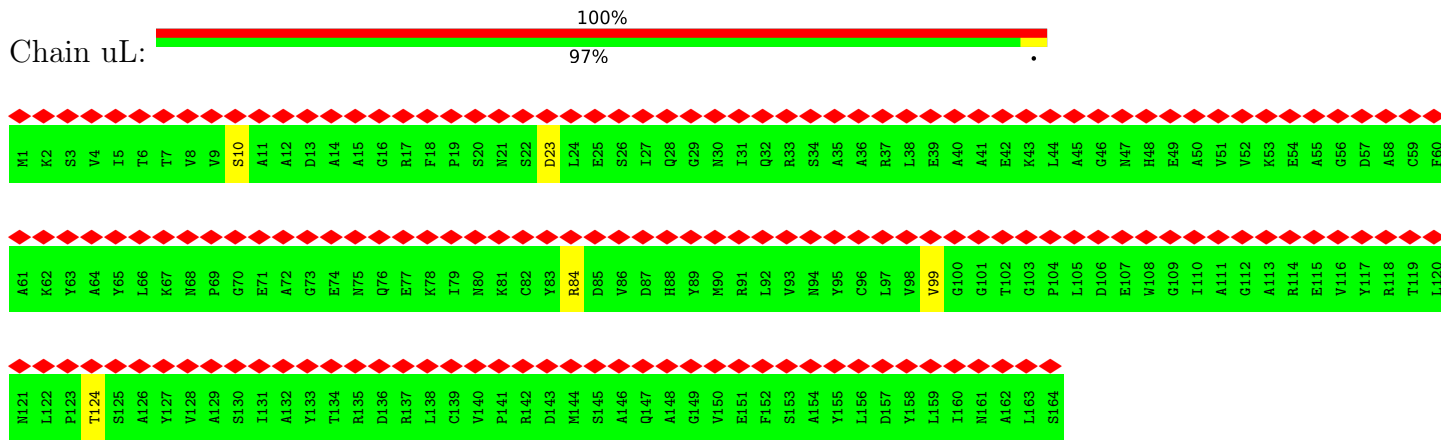
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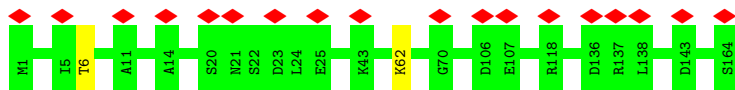


• Molecule 6: Phycoerythrin alpha subunit

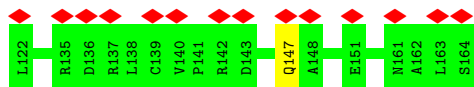
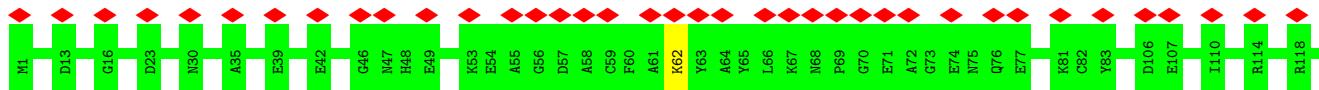


• Molecule 6: Phycoerythrin alpha subunit

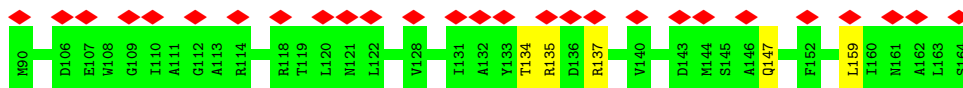
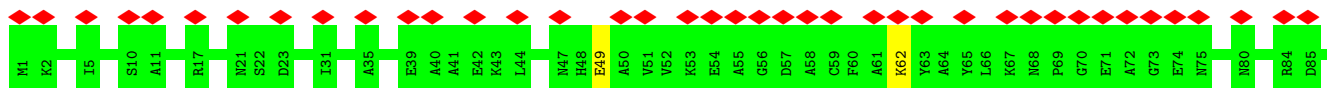
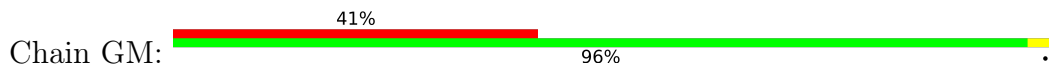




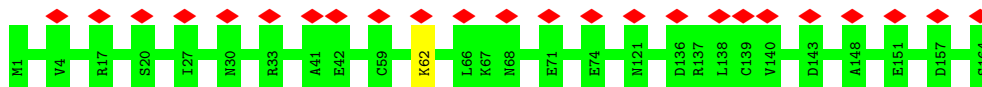
- Molecule 6: Phycoerythrin alpha subunit



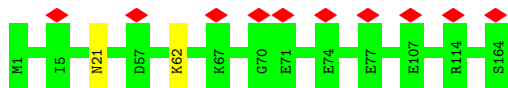
- Molecule 6: Phycoerythrin alpha subunit



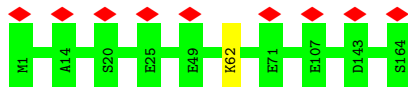
- Molecule 6: Phycoerythrin alpha subunit



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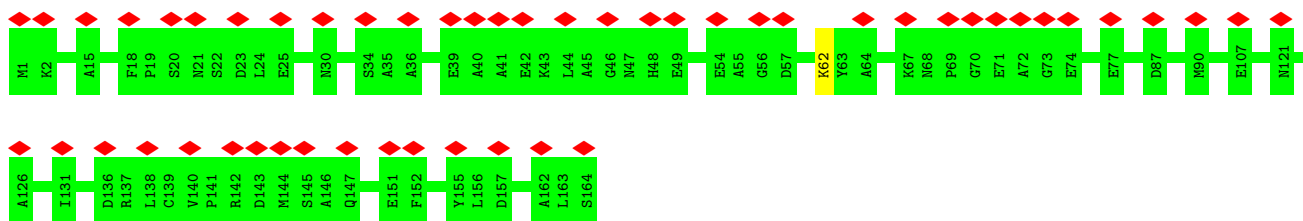


- Molecule 6: Phycoerythrin alpha subunit



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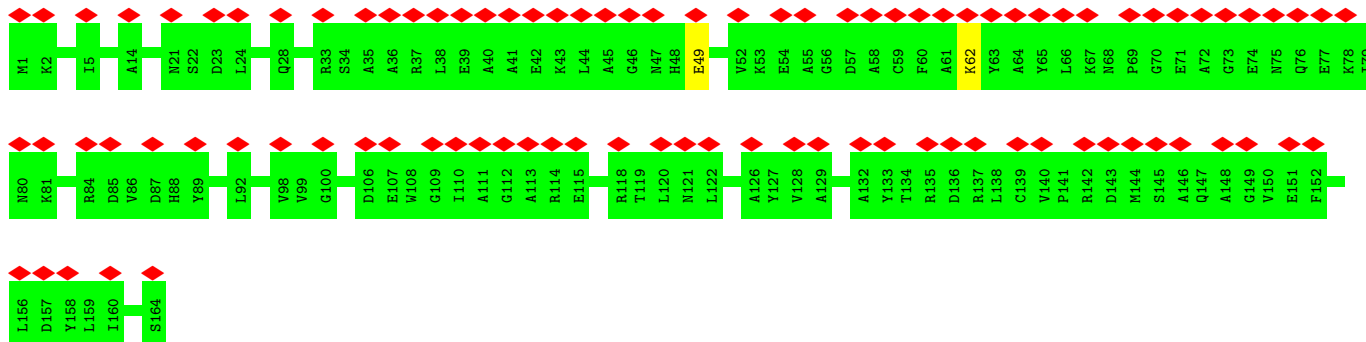
• Molecule 6: Phycoerythrin alpha subunit

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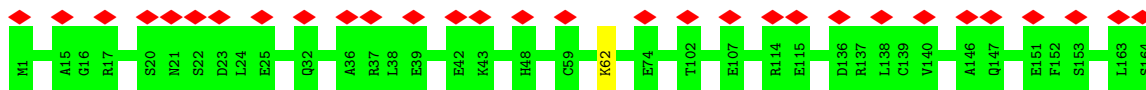
• Molecule 6: Phycoerythrin alpha subunit

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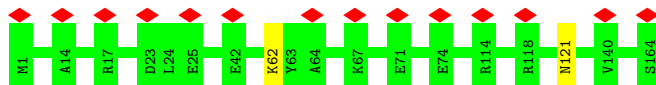
• Molecule 6: Phycoerythrin alpha subunit

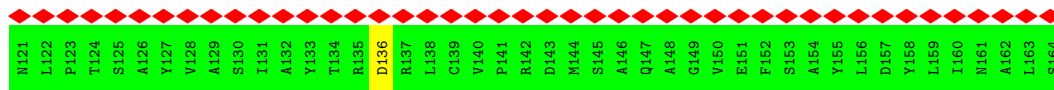
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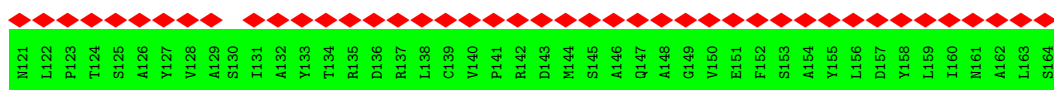
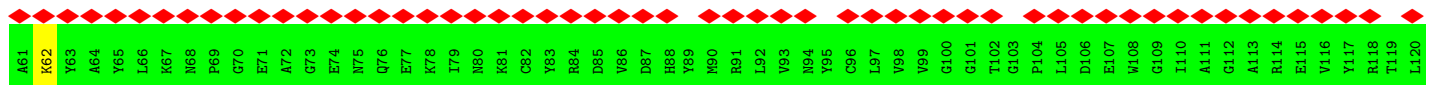
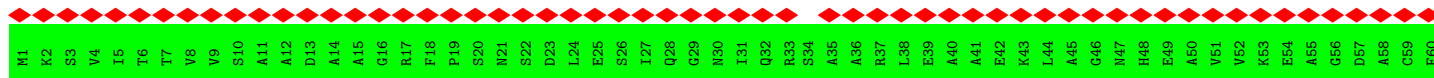
• Molecule 6: Phycoerythrin alpha subunit

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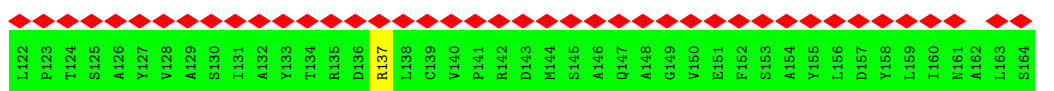
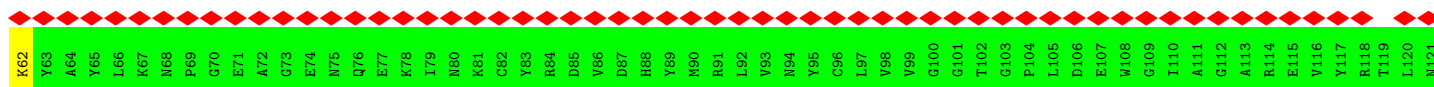
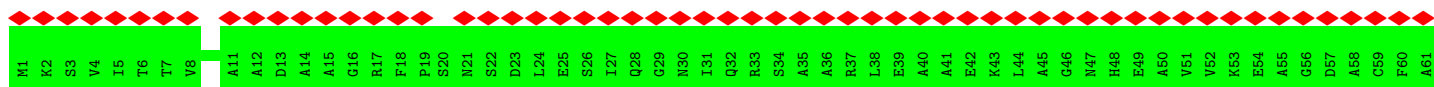




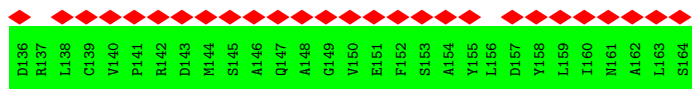
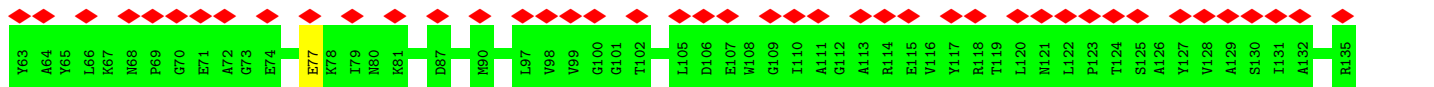
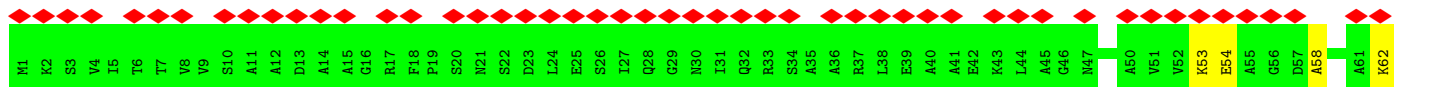
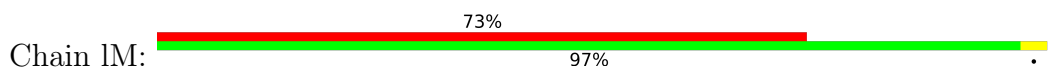
• Molecule 6: Phycoerythrin alpha subunit



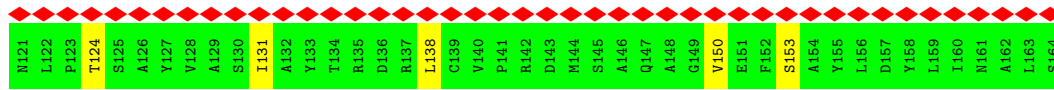
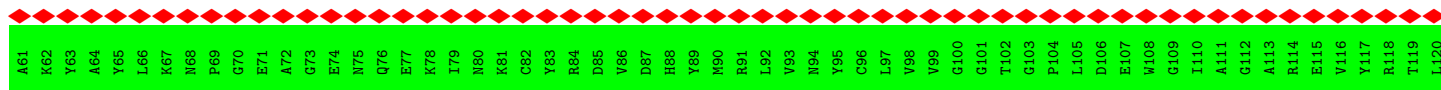
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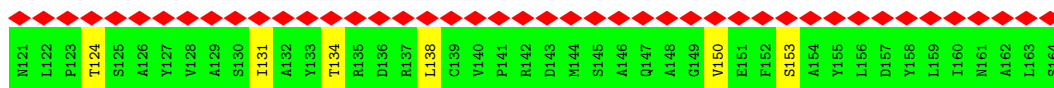
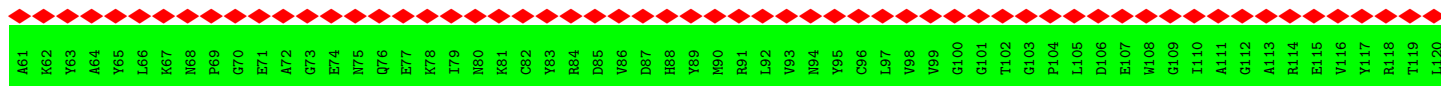
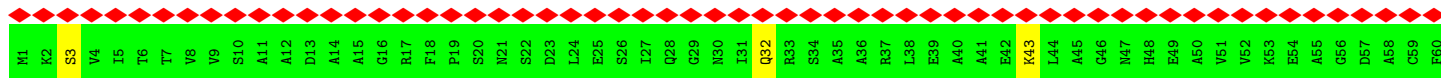
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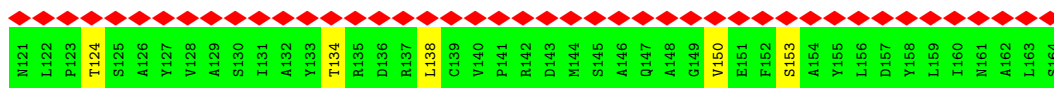
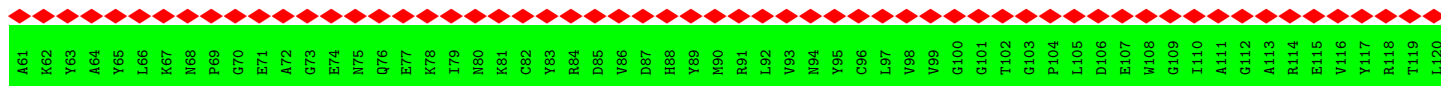
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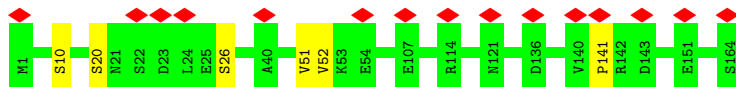
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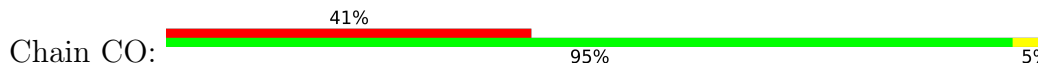
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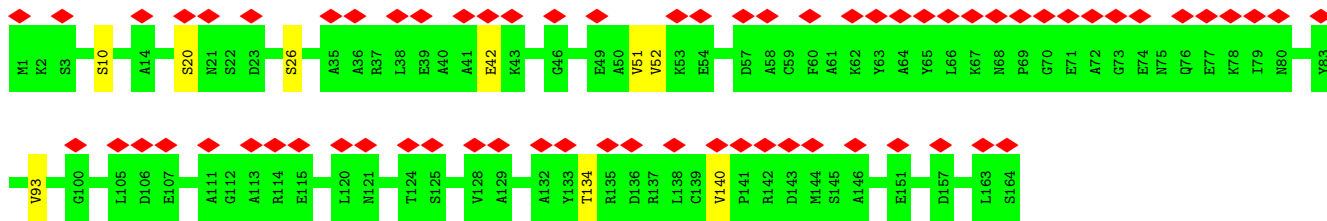


• Molecule 6: Phycoerythrin alpha subunit

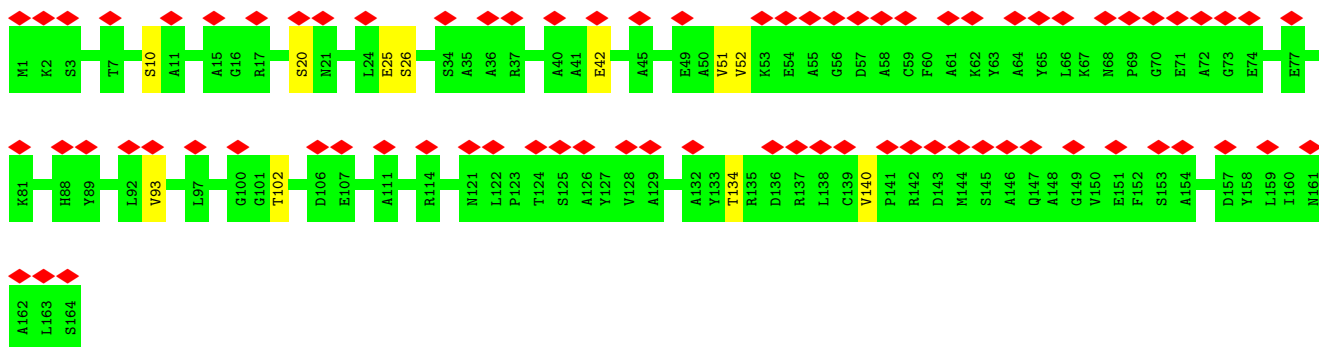


• Molecule 6: Phycoerythrin alpha subunit

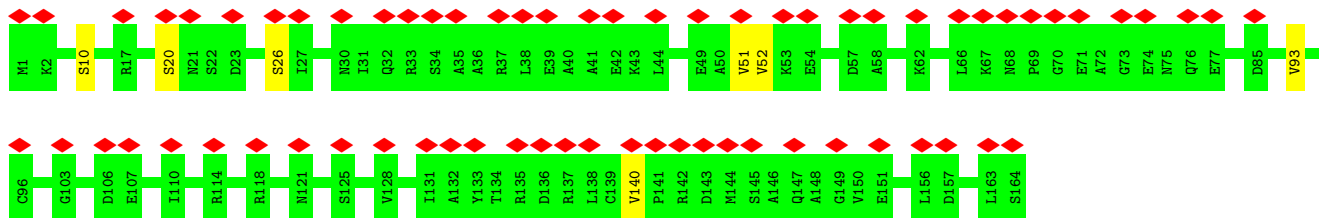
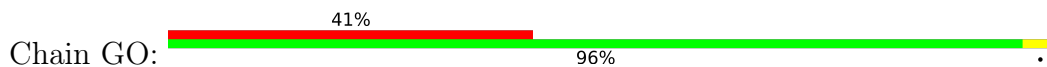




- Molecule 6: Phycoerythrin alpha subunit



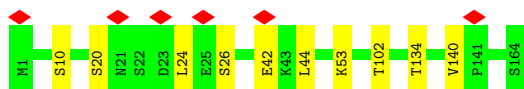
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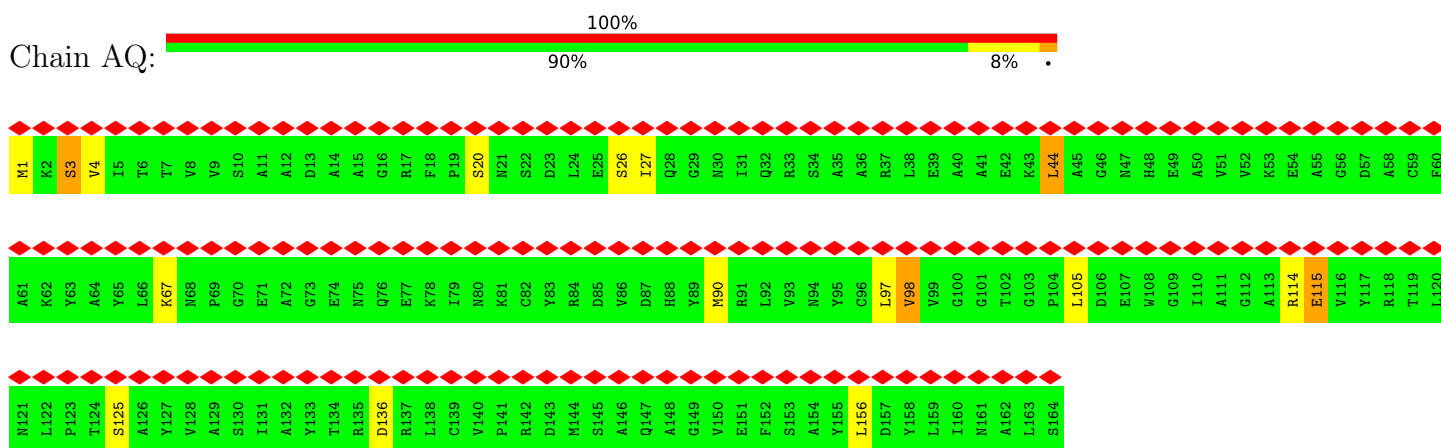
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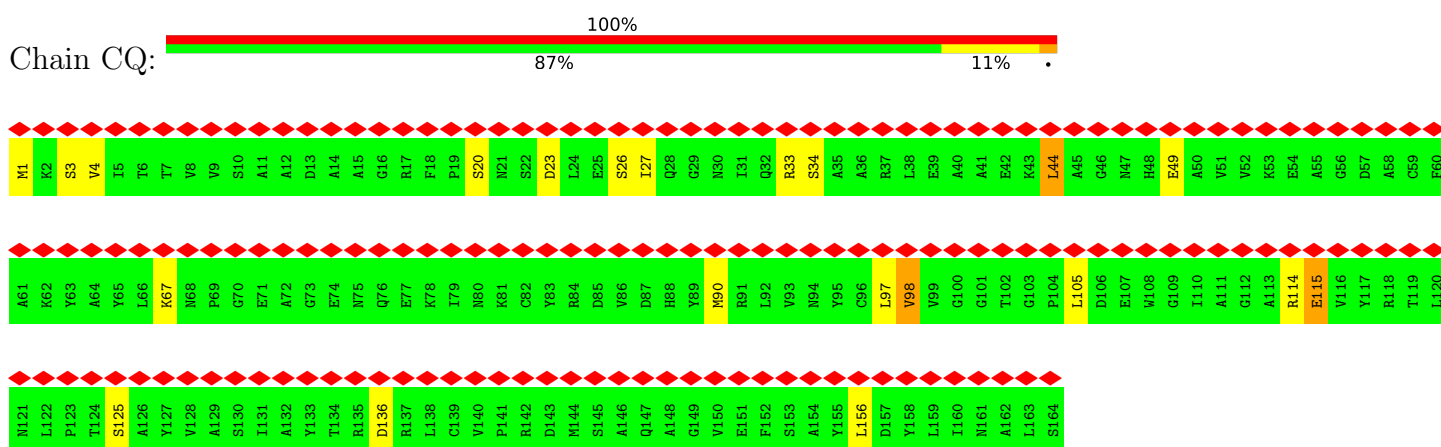
- Molecule 6: Phycoerythrin alpha subunit



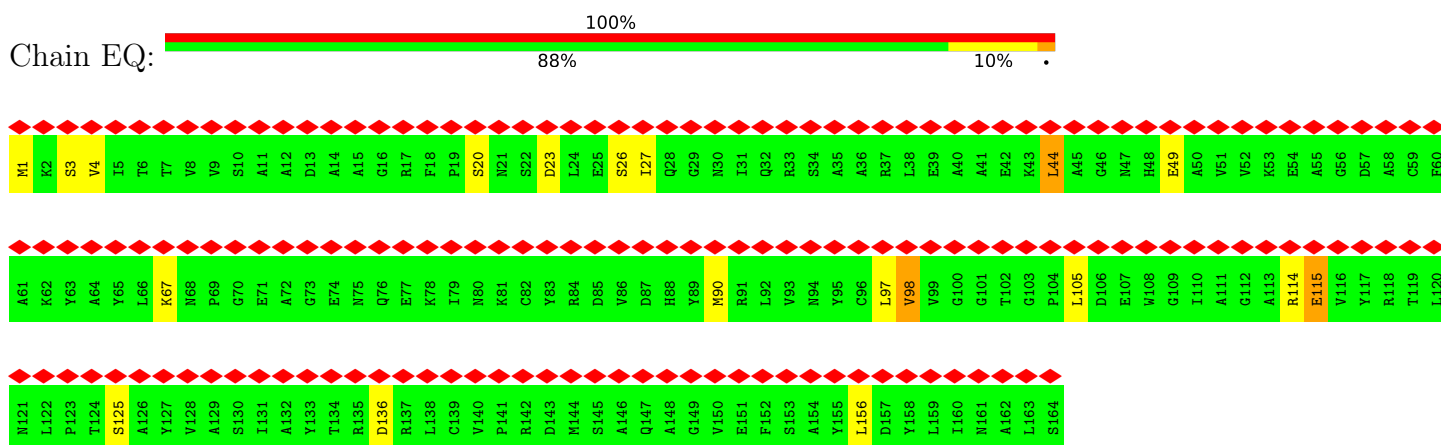
- Molecule 6: Phycoerythrin alpha subunit



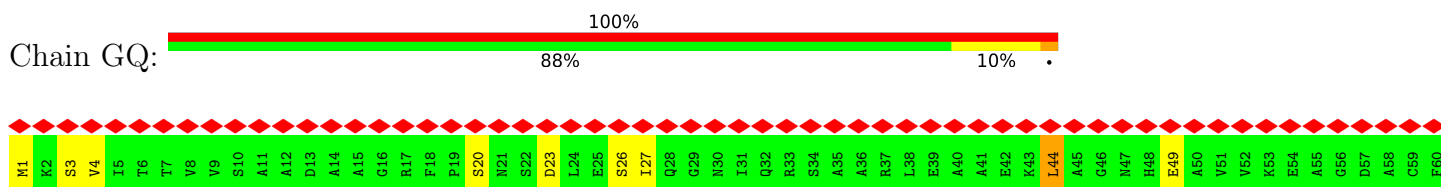
- Molecule 6: Phycoerythrin alpha subunit

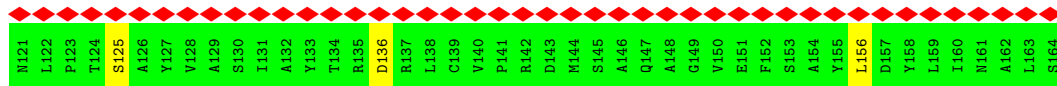
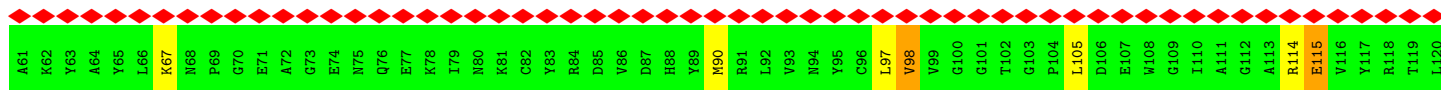


- Molecule 6: Phycoerythrin alpha subunit

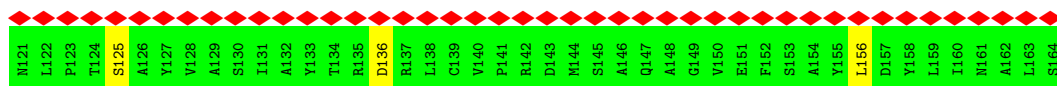
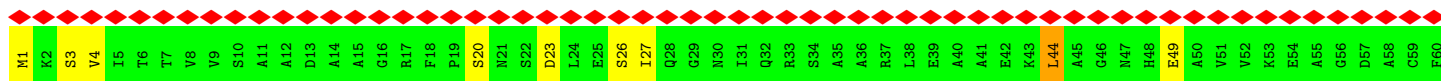
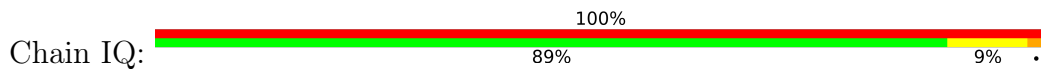


- Molecule 6: Phycoerythrin alpha subunit

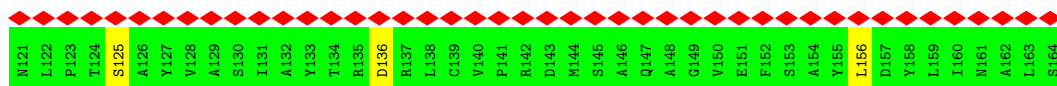
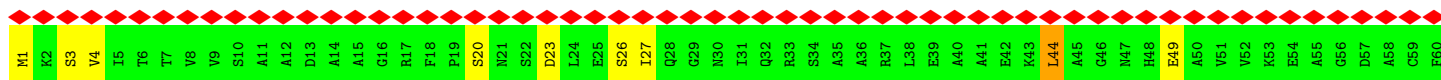
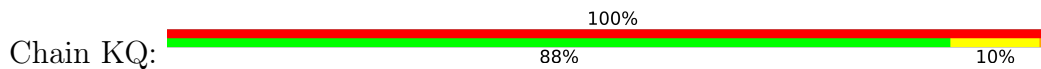




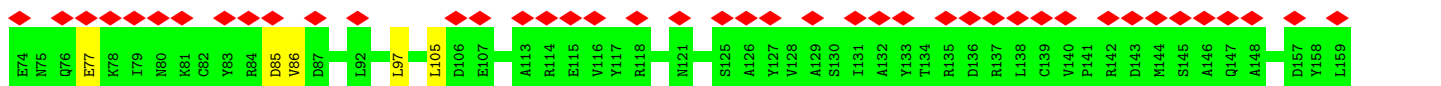
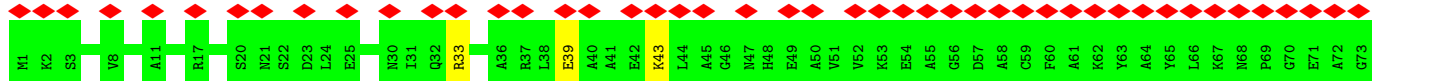
• Molecule 6: Phycoerythrin alpha subunit

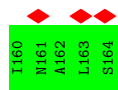


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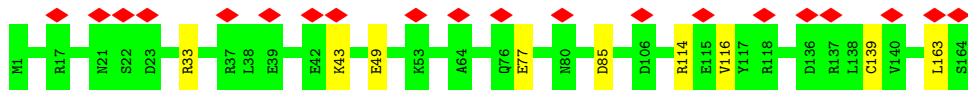


• Molecule 6: Phycoerythrin alpha subunit

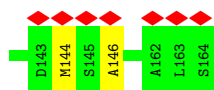
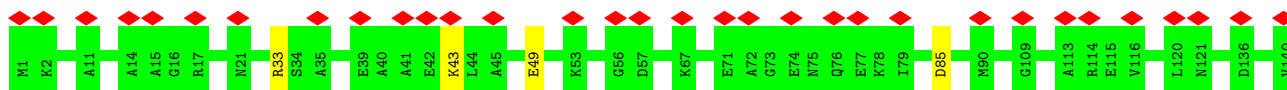




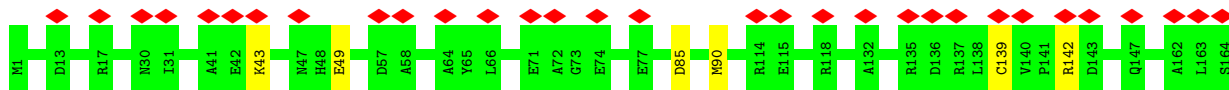
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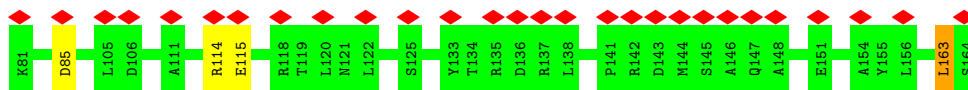
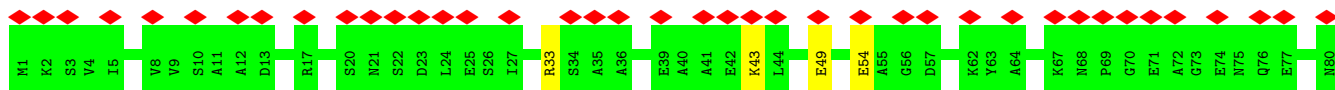
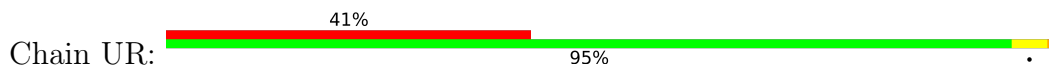
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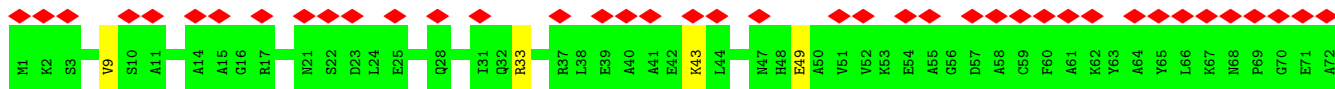
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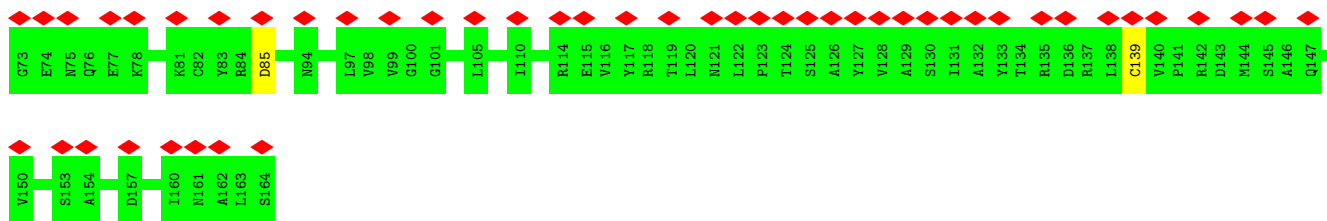


• Molecule 6: Phycoerythrin alpha subunit

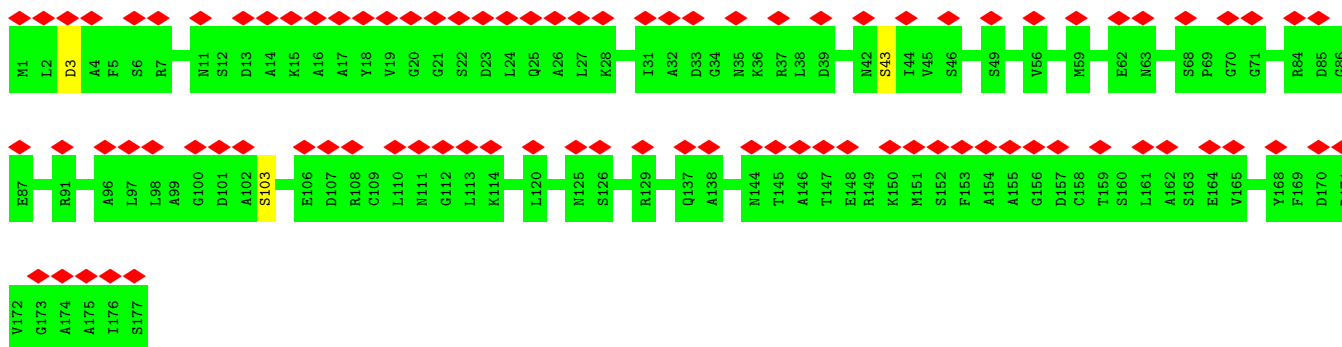


• Molecule 6: Phycoerythrin alpha subunit

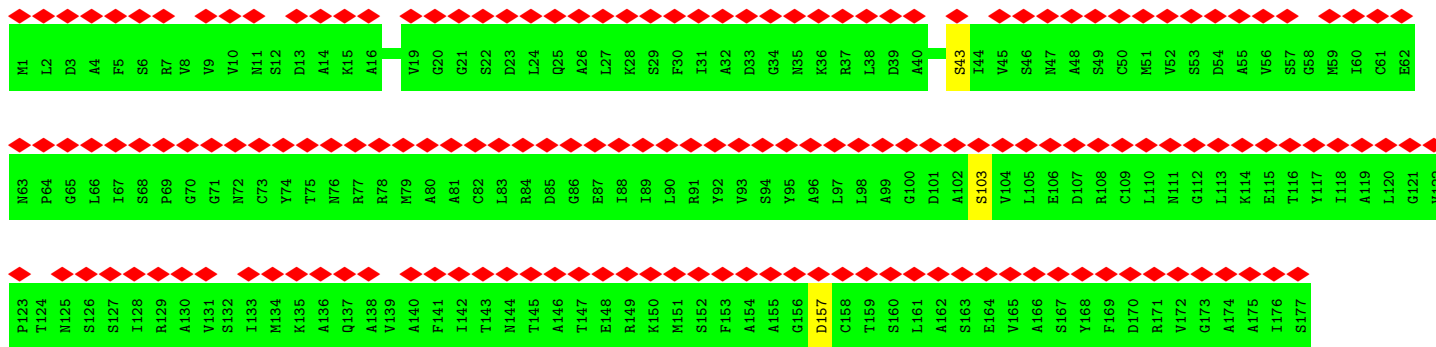




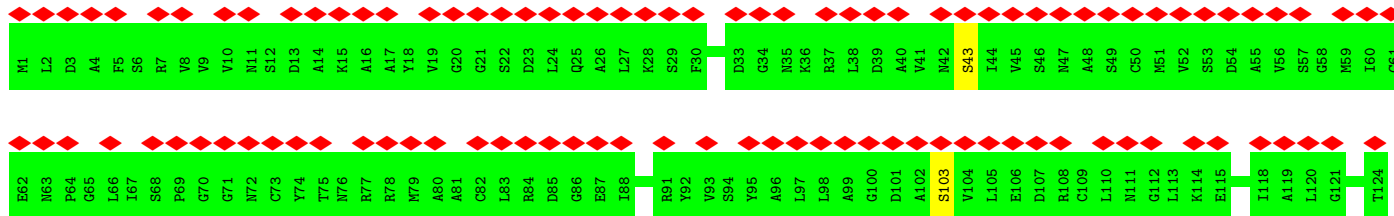
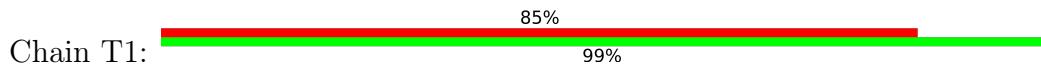
• Molecule 7: B-phycoerythrin beta chain

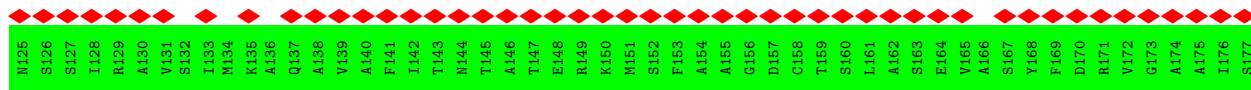


• Molecule 7: B-phycoerythrin beta chain

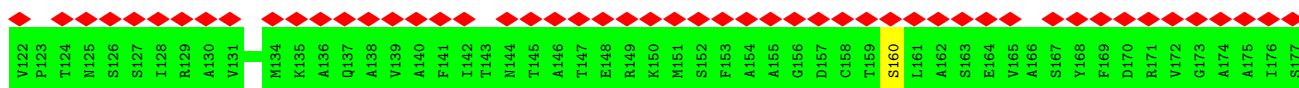
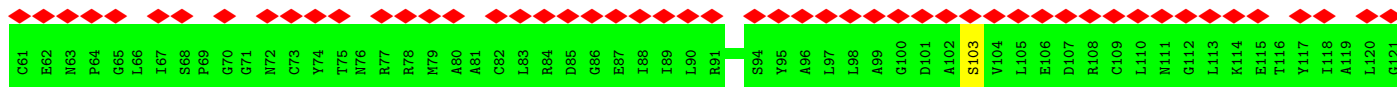
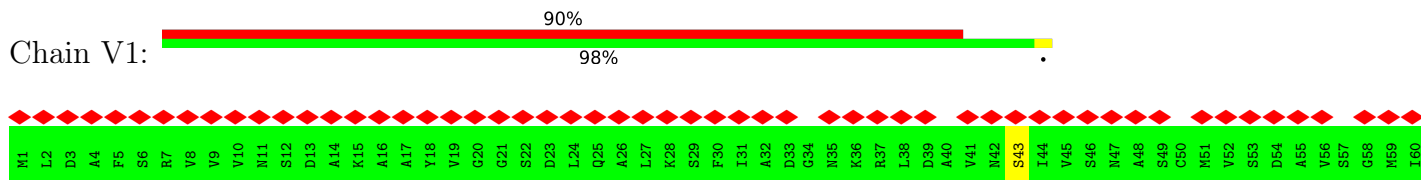


• Molecule 7: B-phycoerythrin beta chain

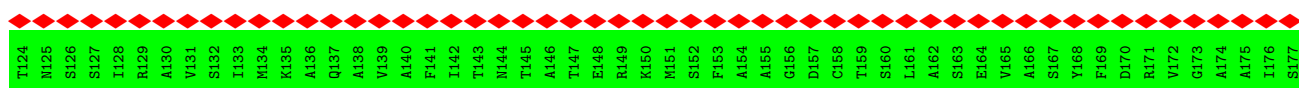
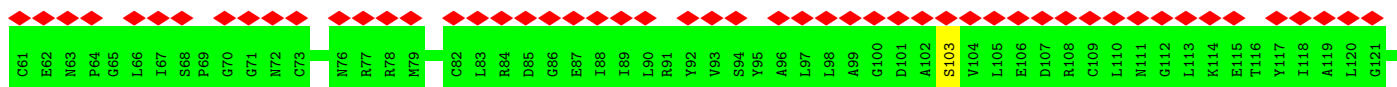
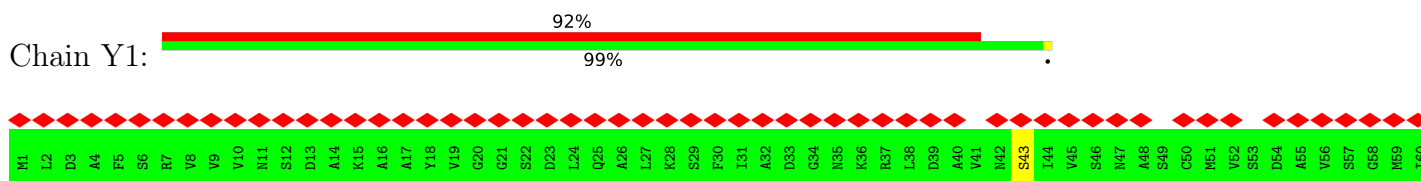




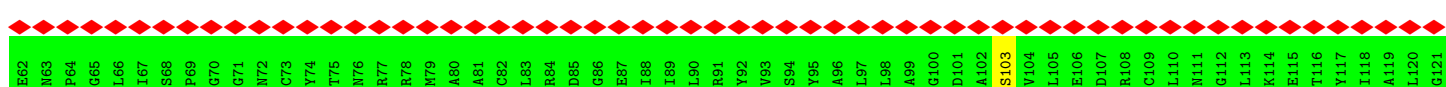
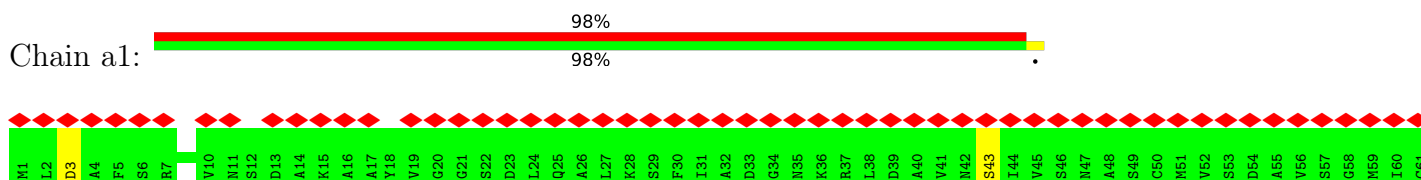
• Molecule 7: B-phycoerythrin beta chain



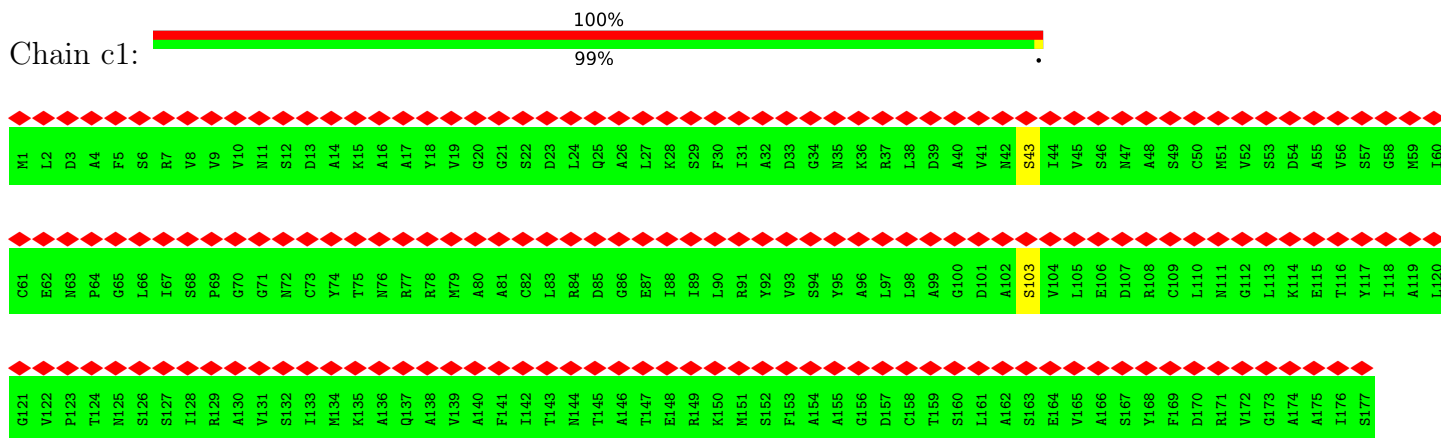
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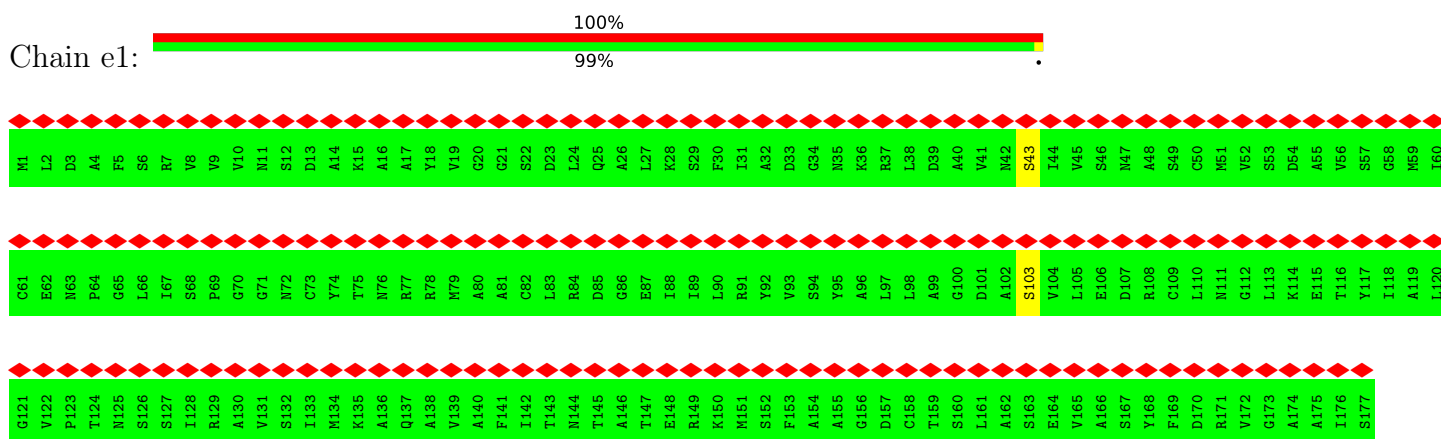
• Molecule 7: B-phycoerythrin beta chain



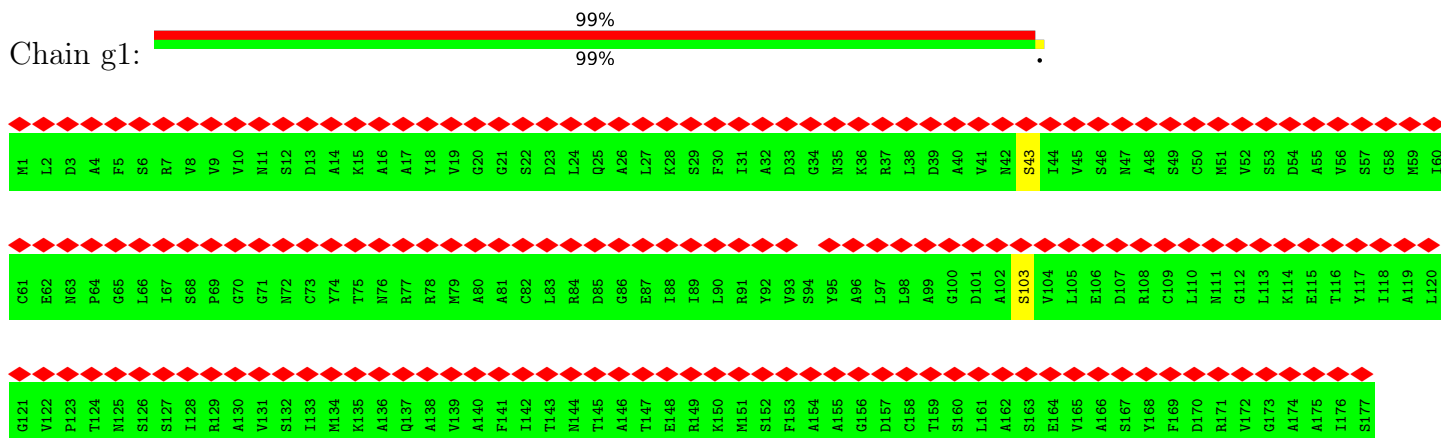
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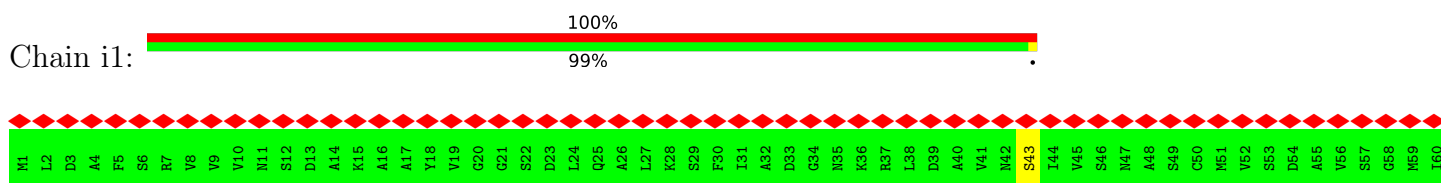
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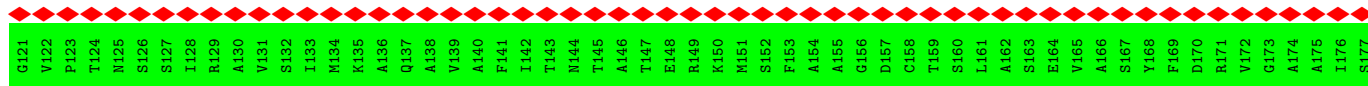
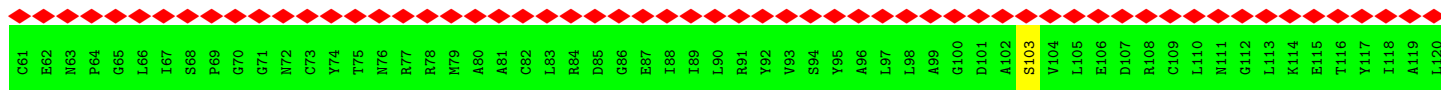


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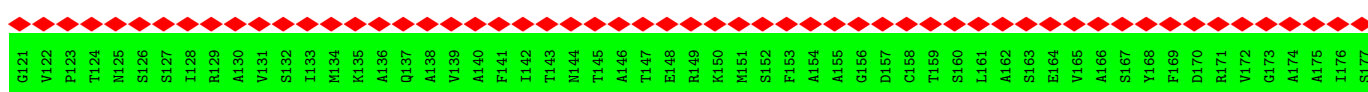
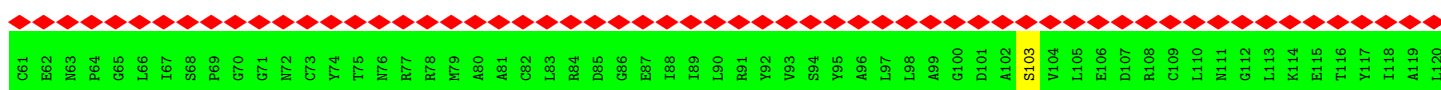


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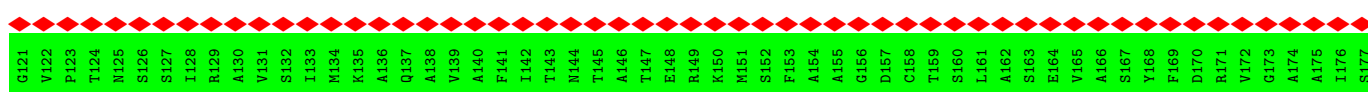
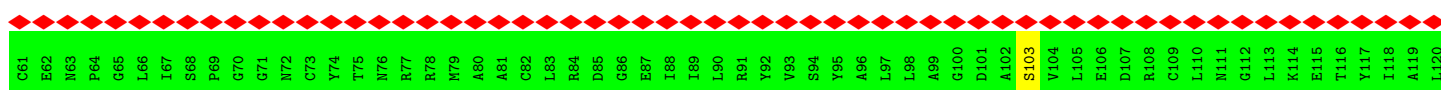




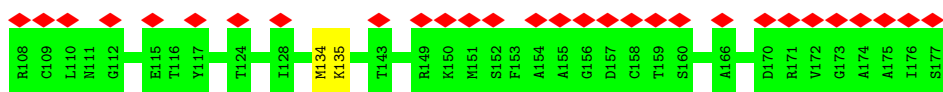
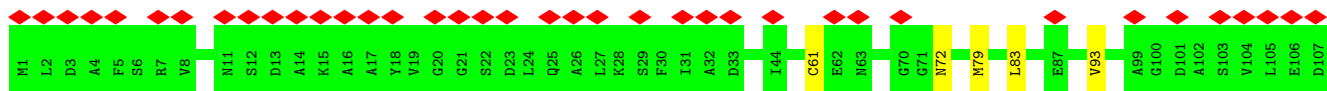
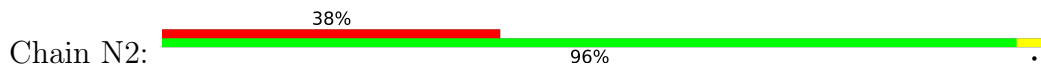
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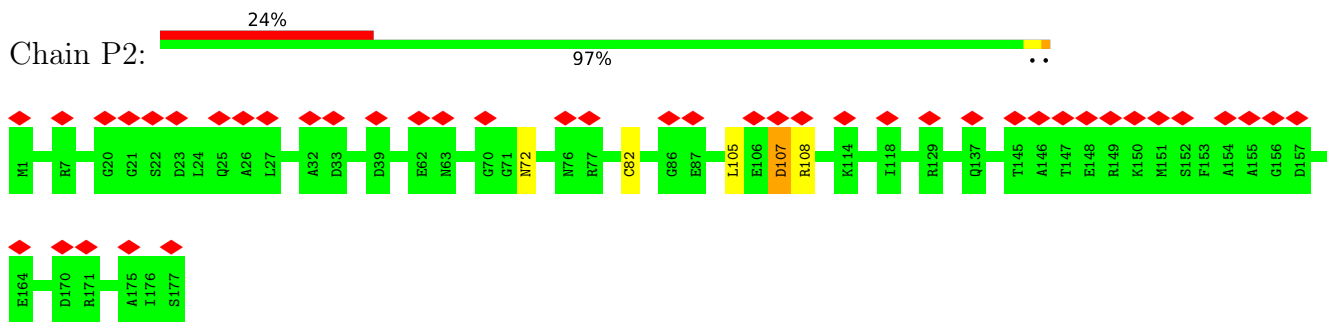
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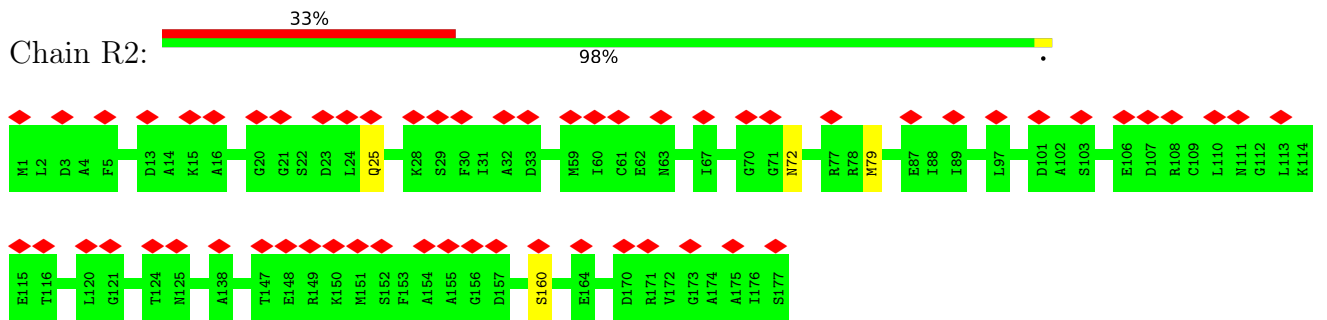
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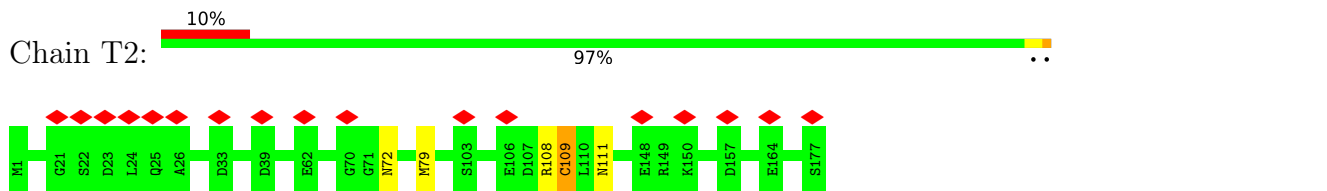
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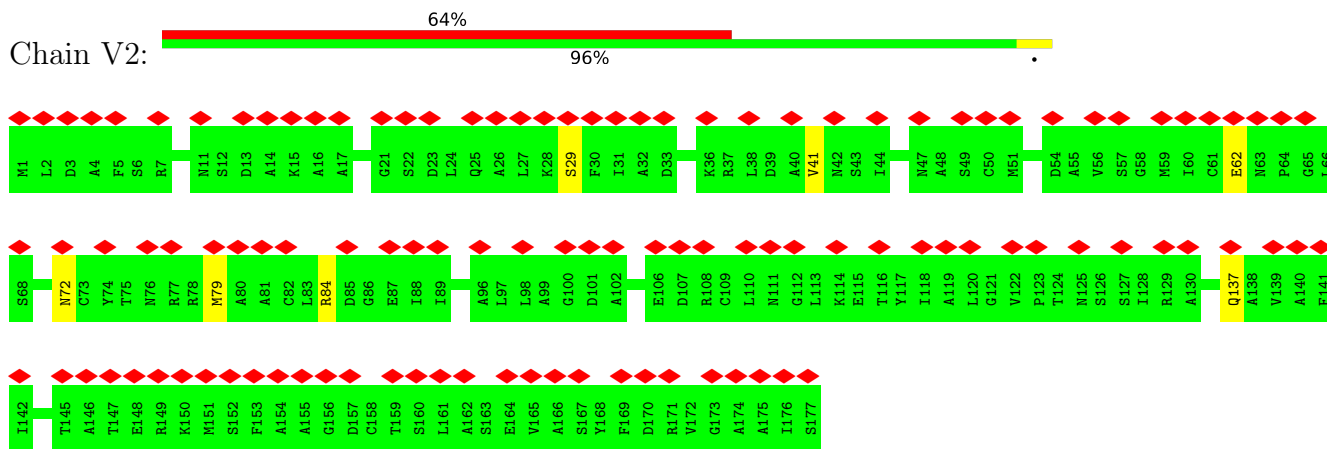
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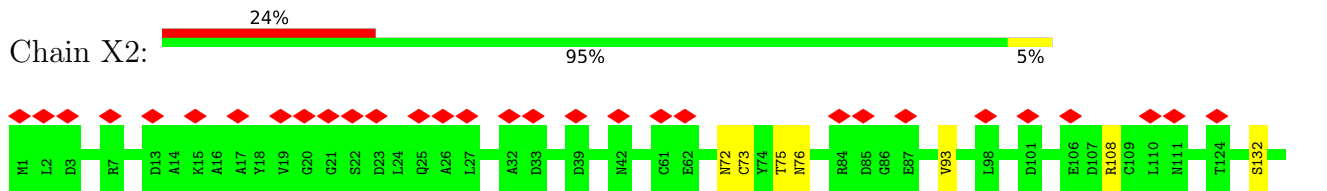
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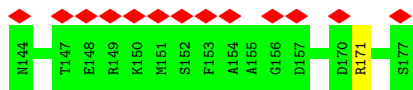


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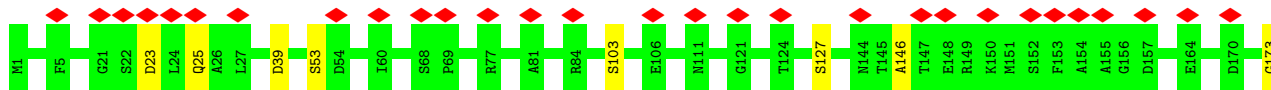


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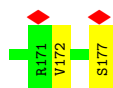
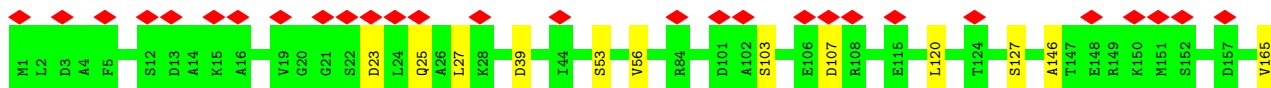




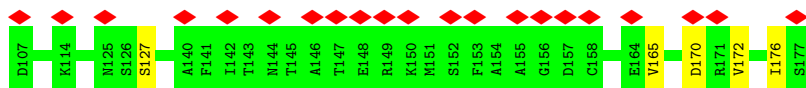
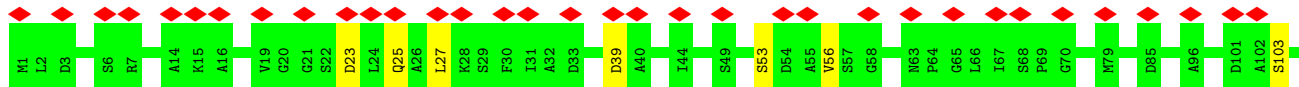
• Molecule 7: B-phycoerythrin beta chain



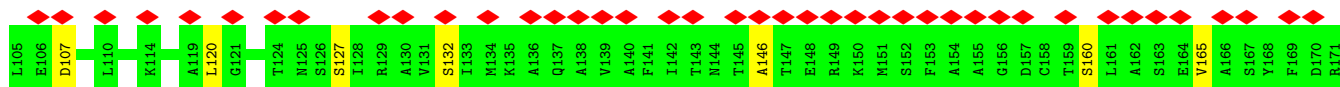
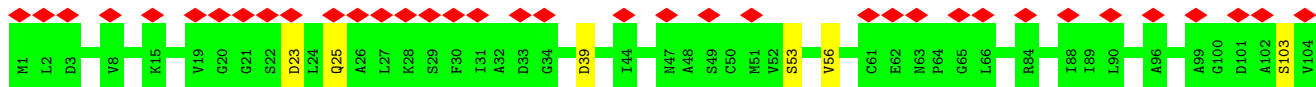
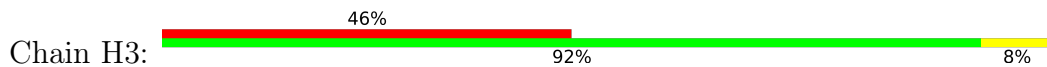
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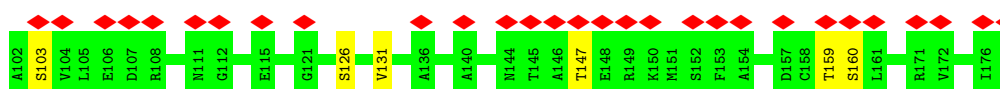
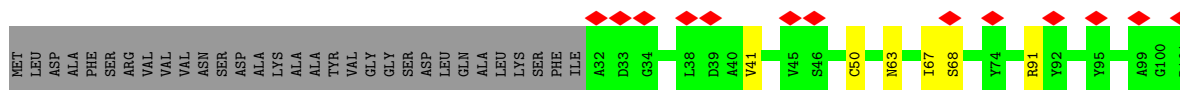
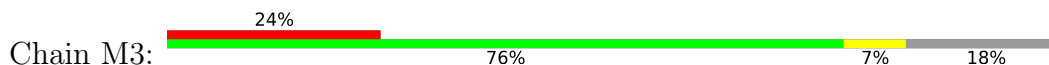
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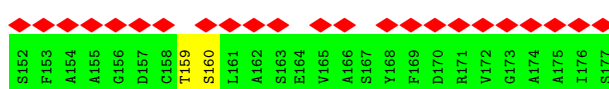
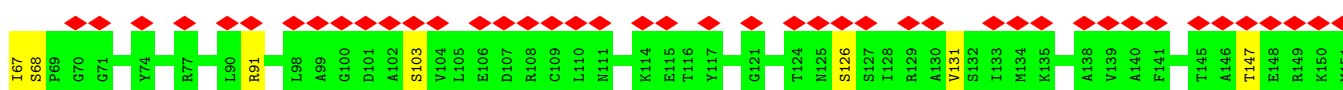
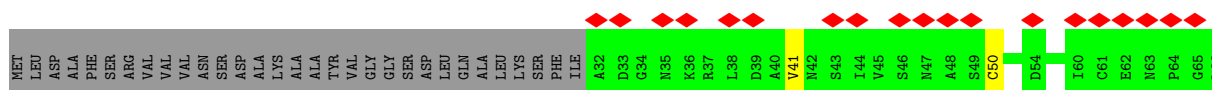
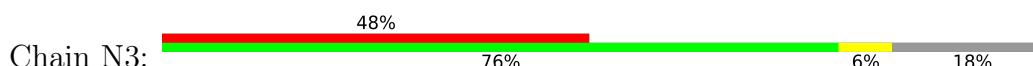
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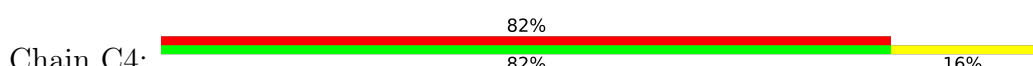
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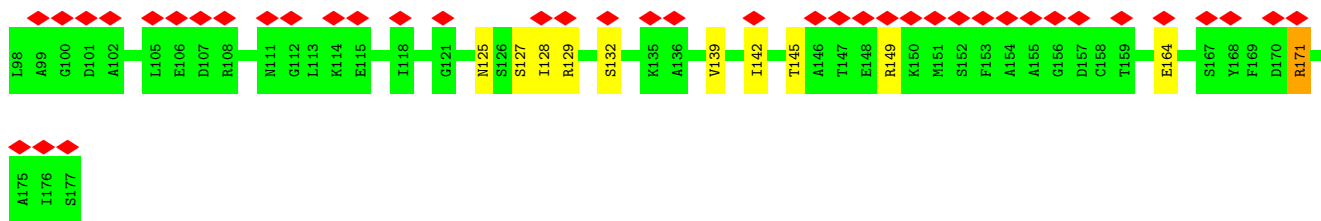


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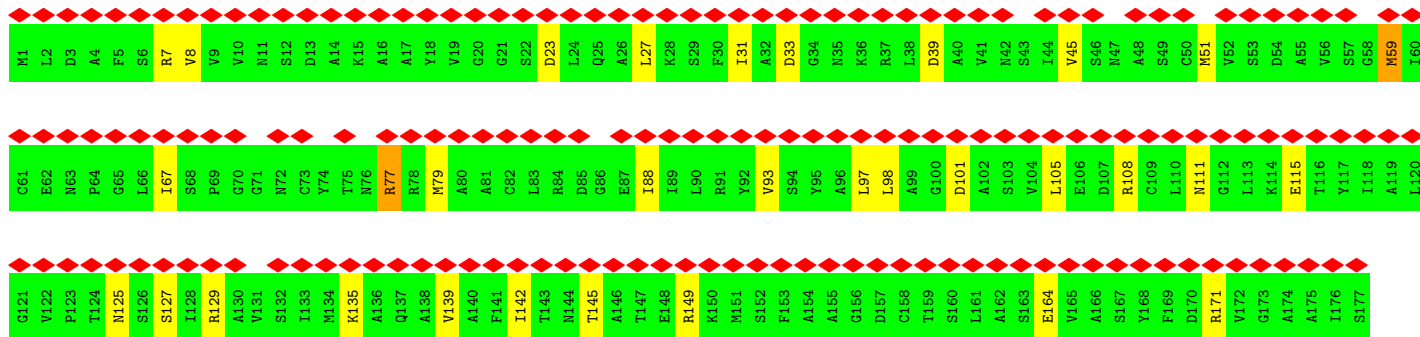
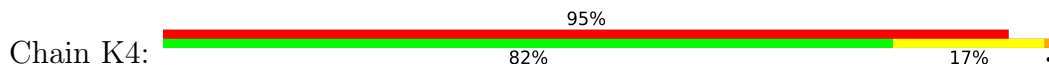


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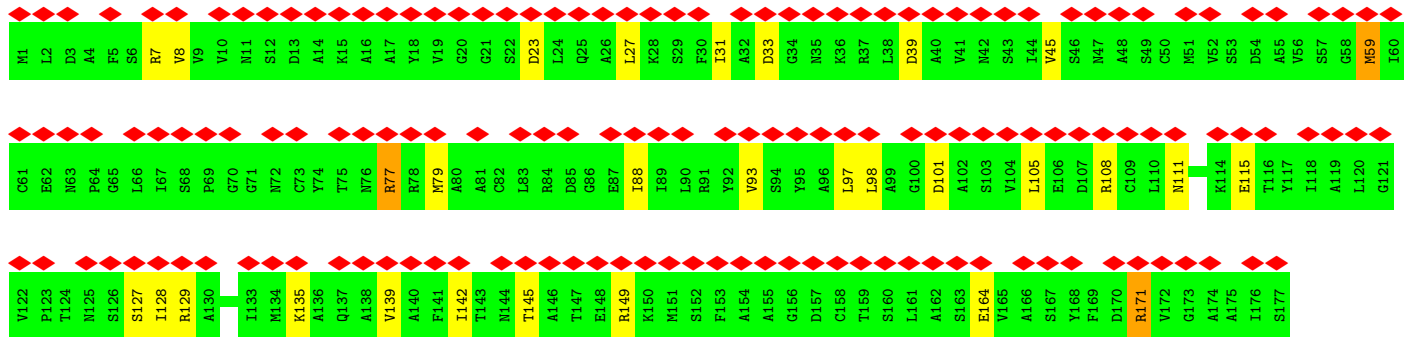
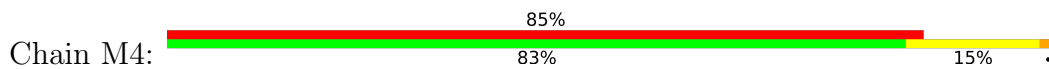




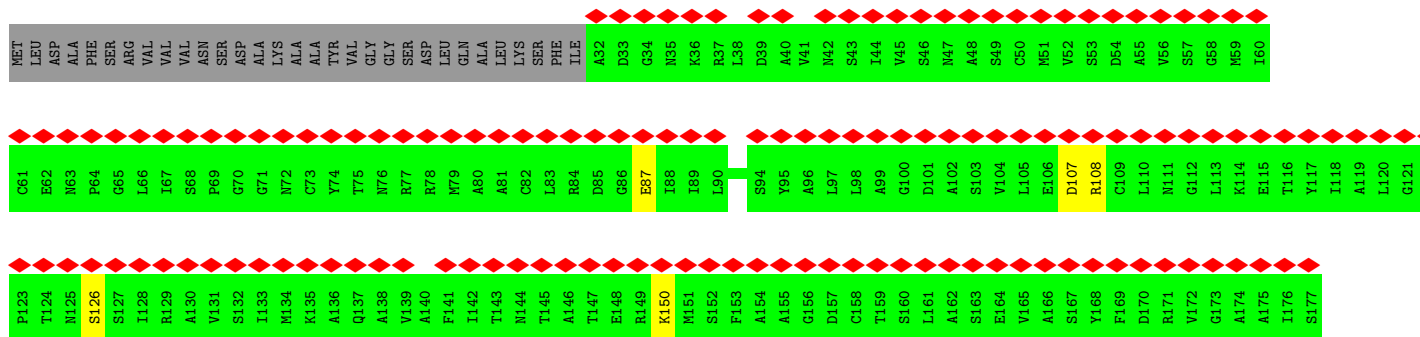
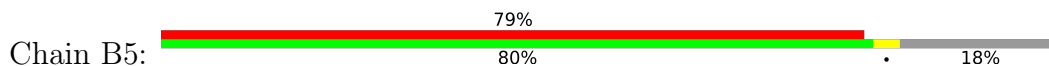
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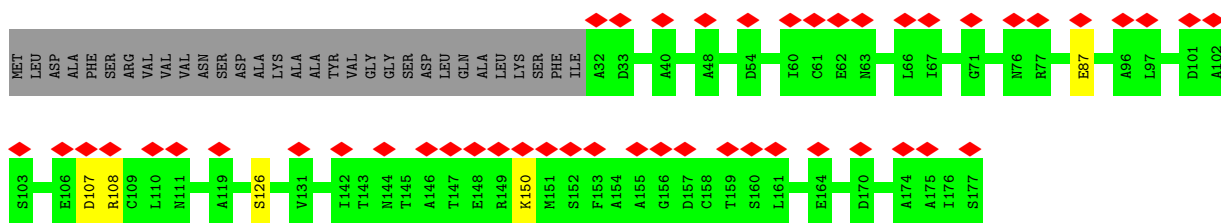
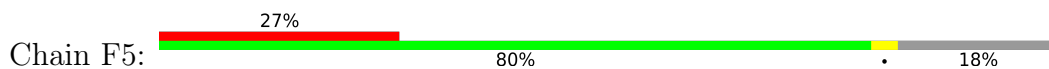
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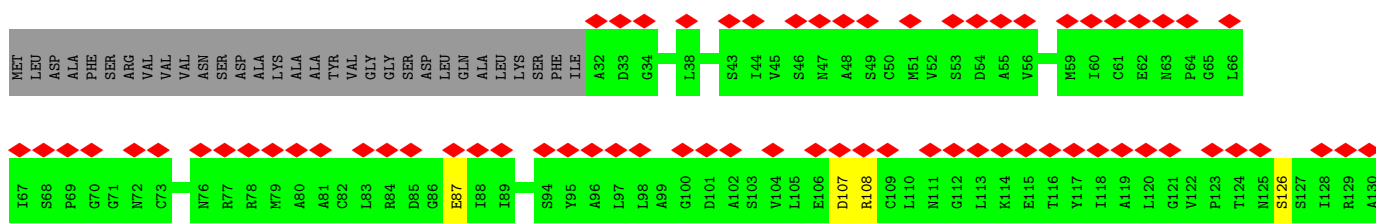
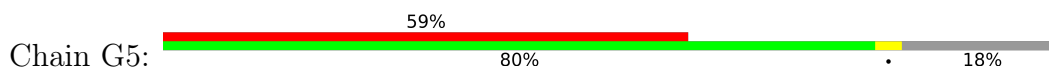
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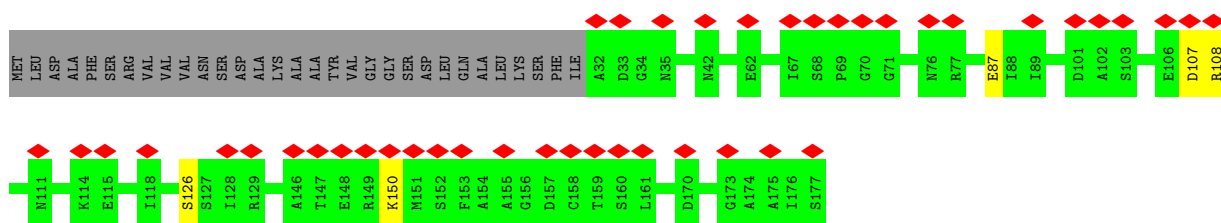
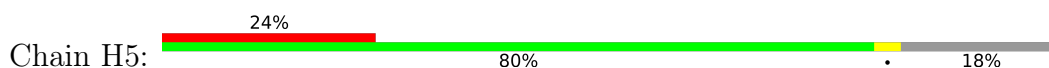
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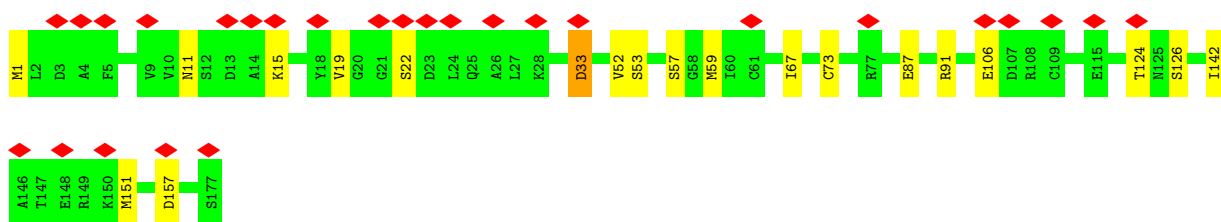
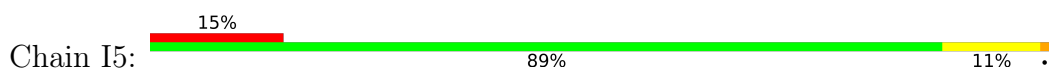
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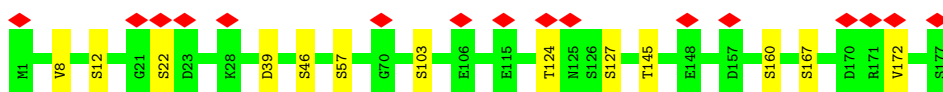


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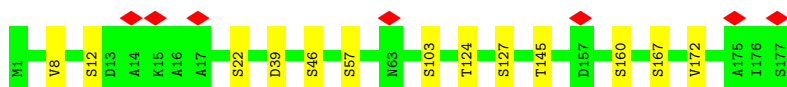


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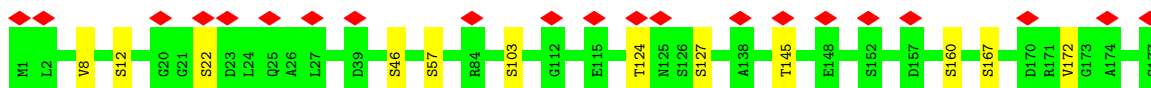
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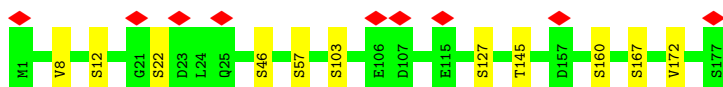
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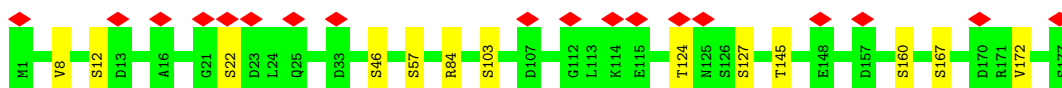
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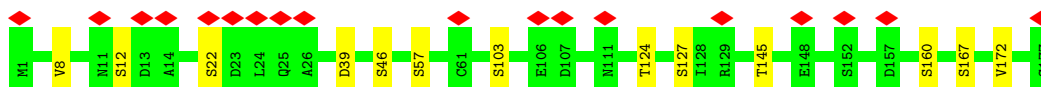
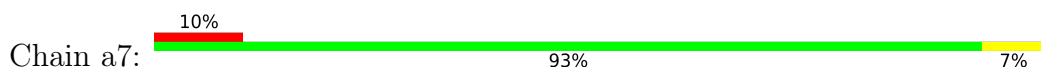
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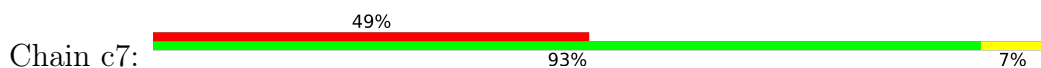
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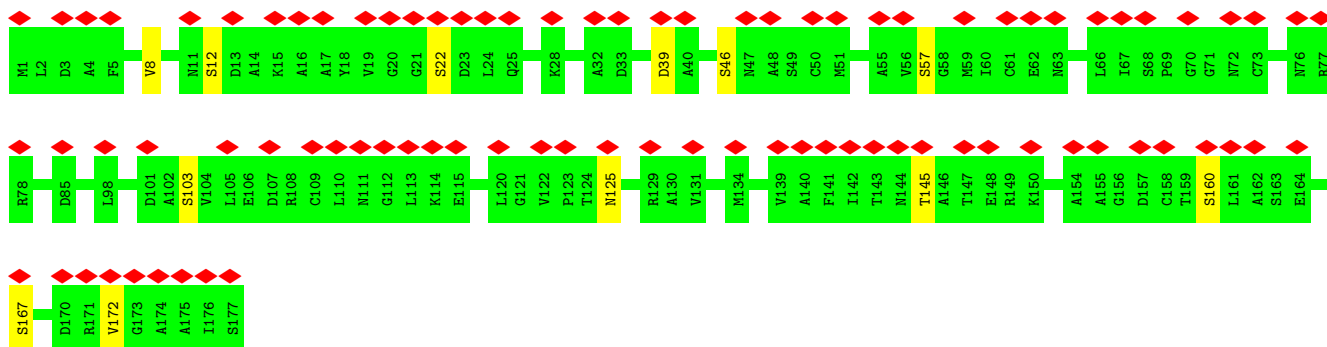


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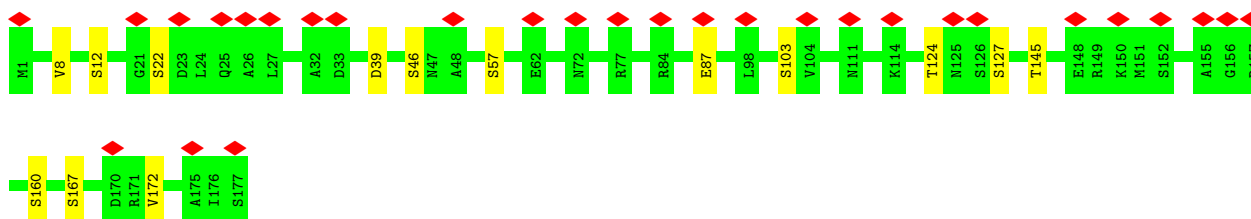
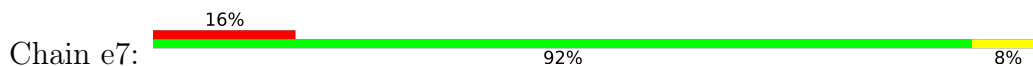


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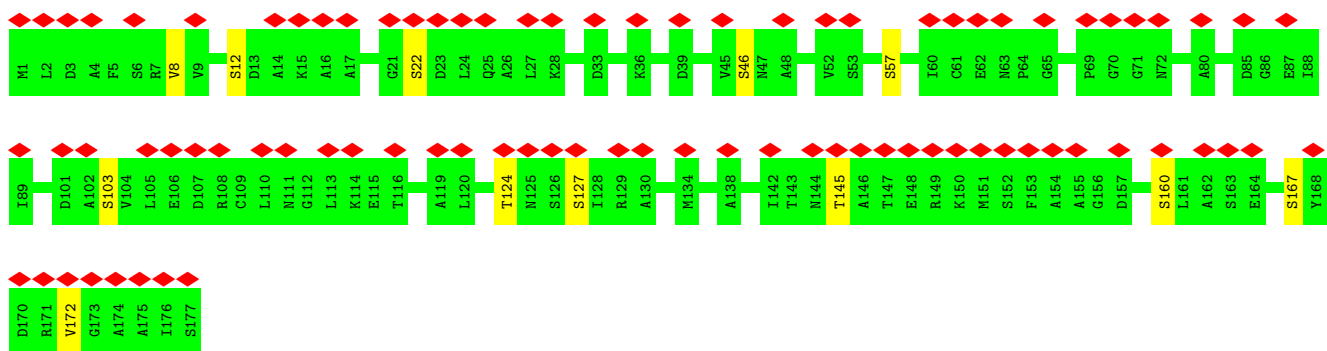




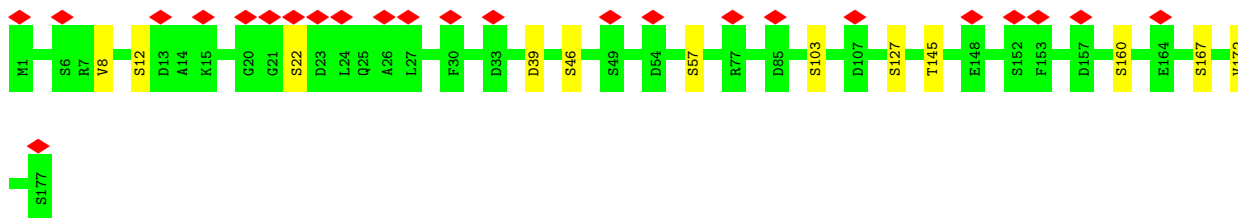
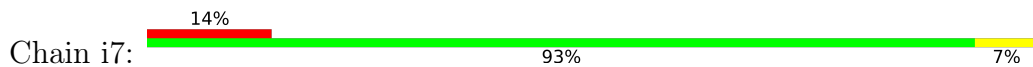
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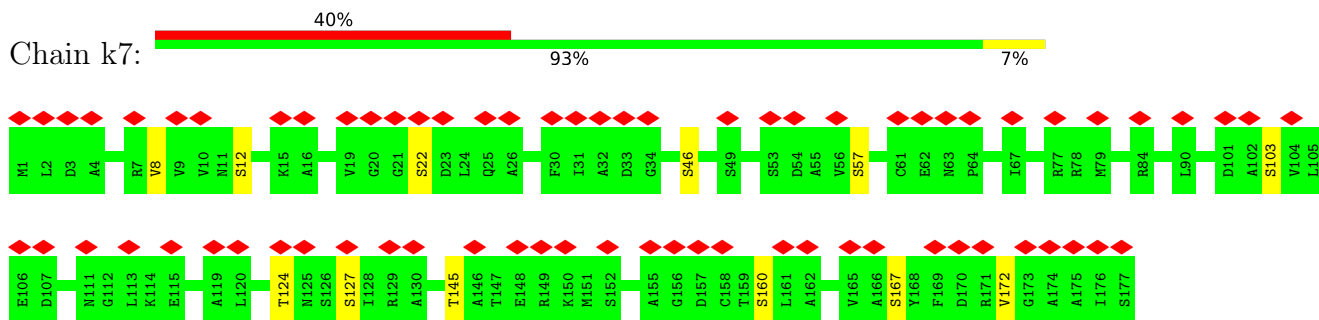
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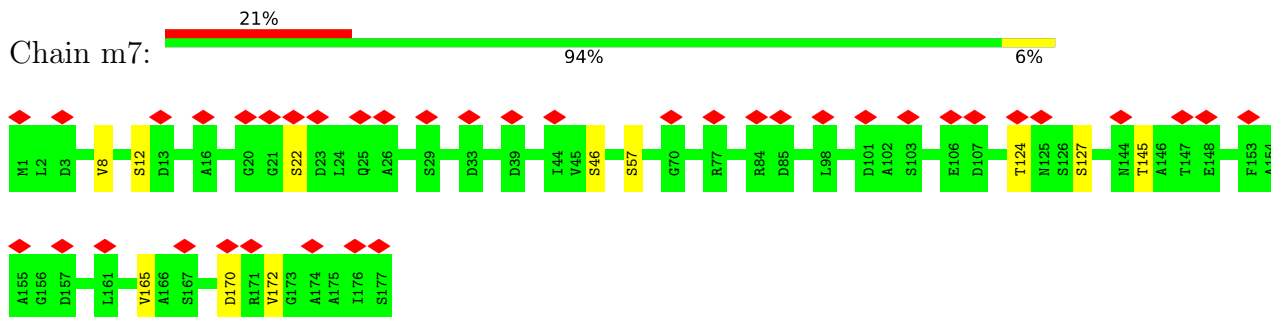
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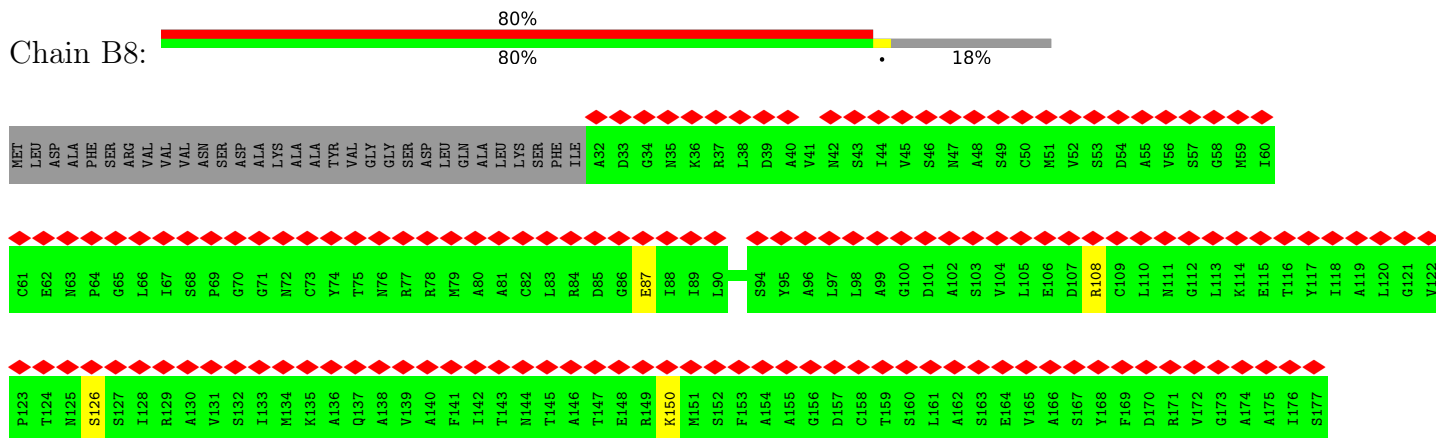
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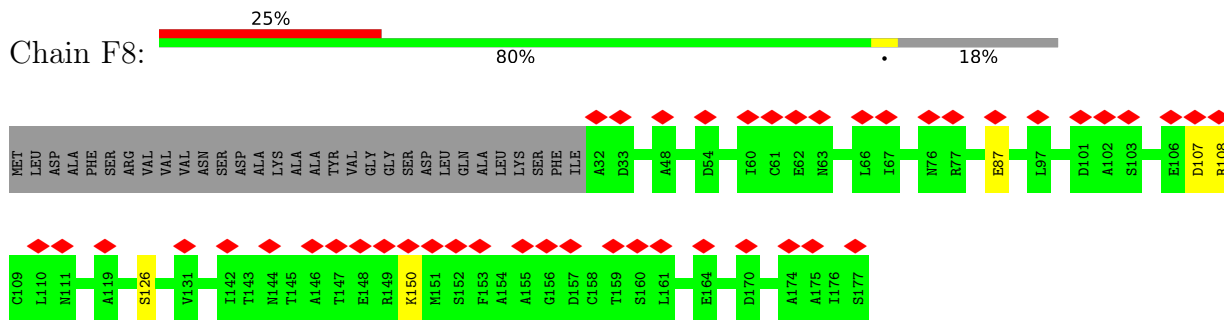
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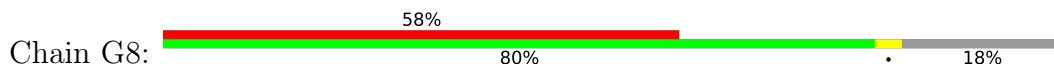
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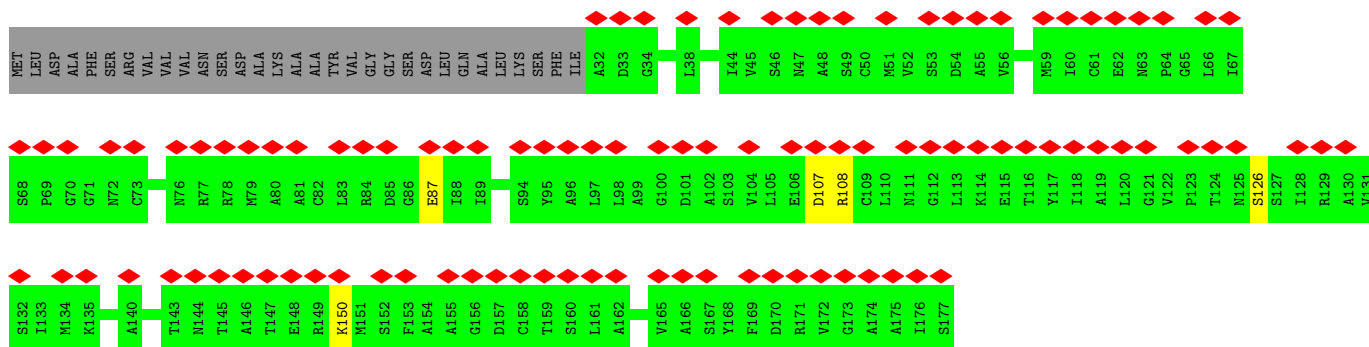


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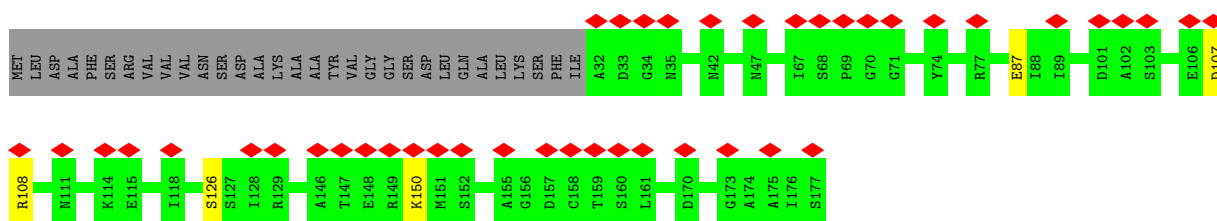
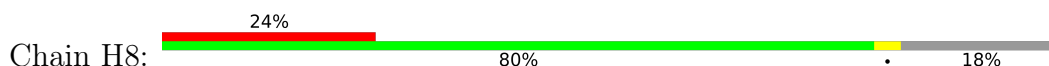


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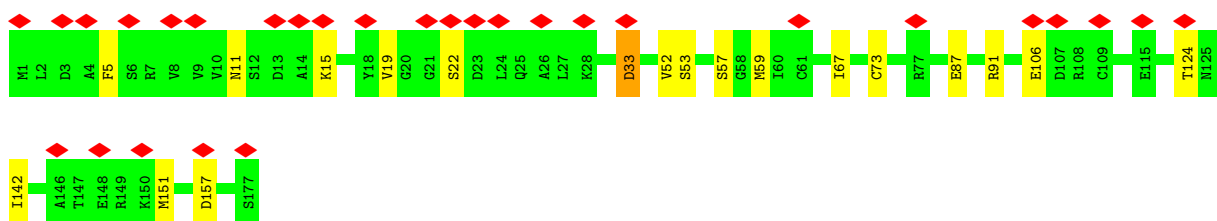
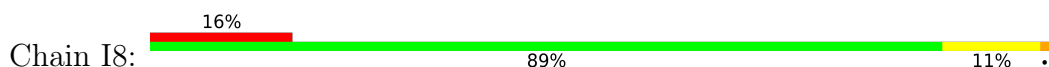




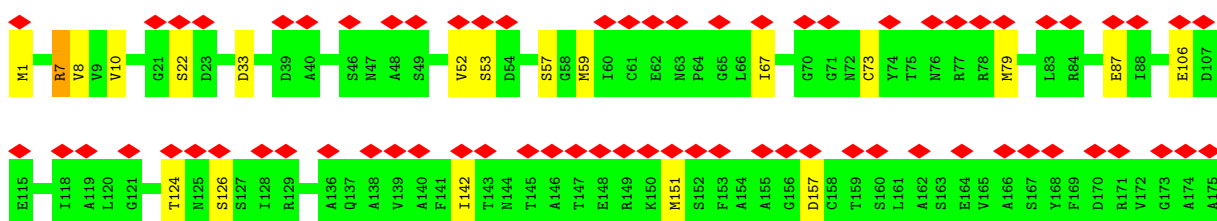
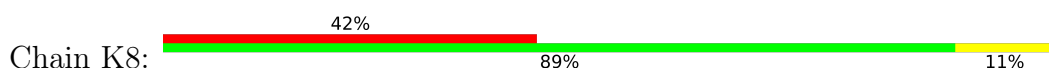
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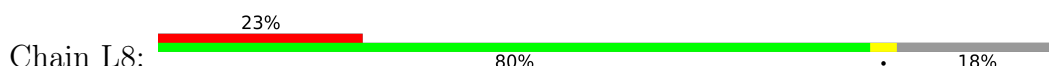
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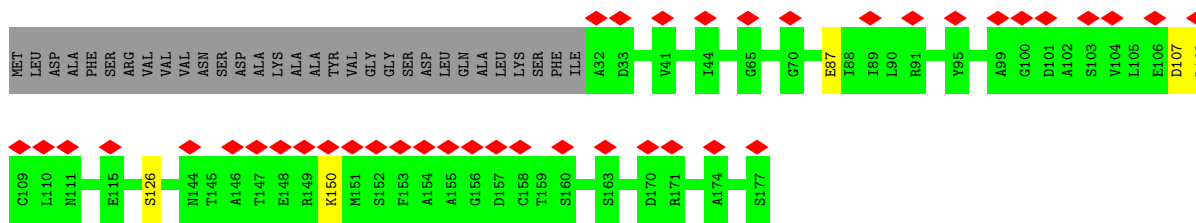


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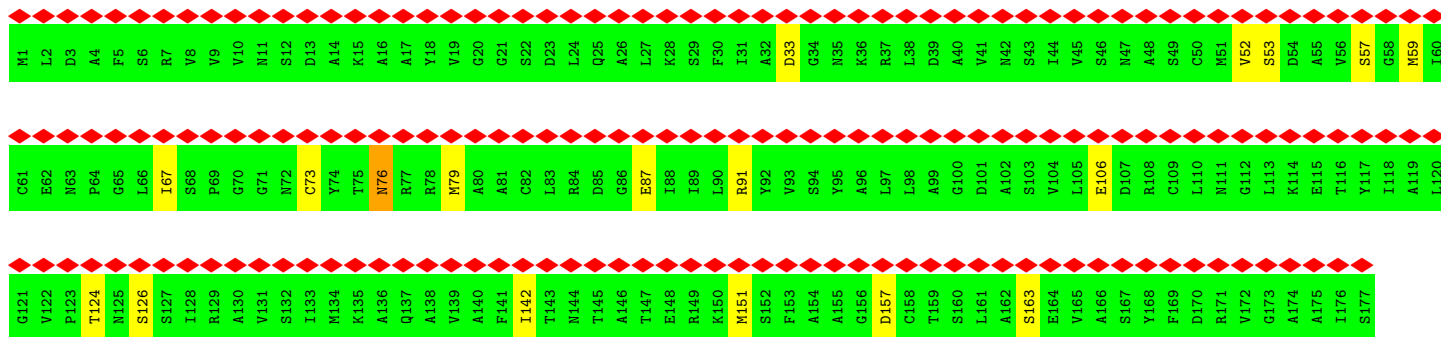
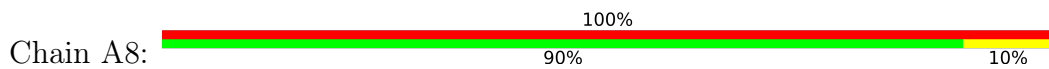


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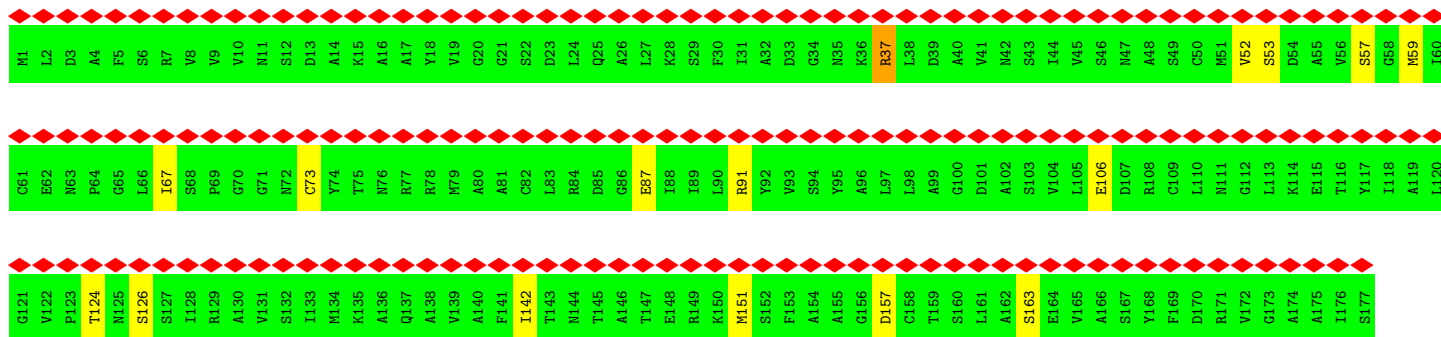
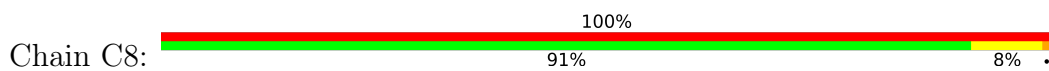




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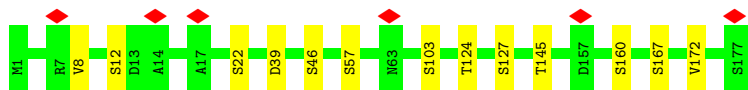


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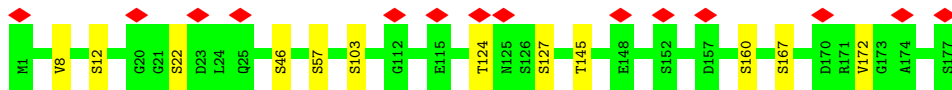


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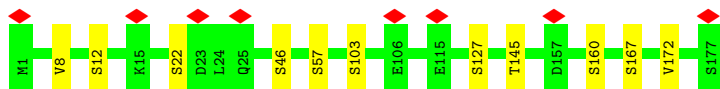




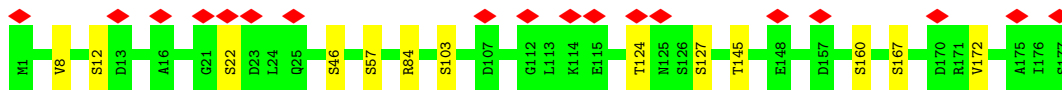
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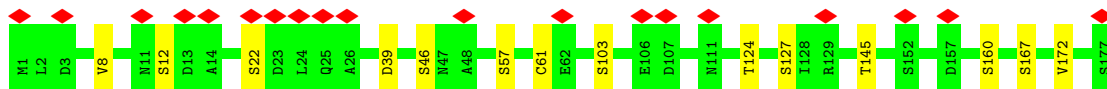
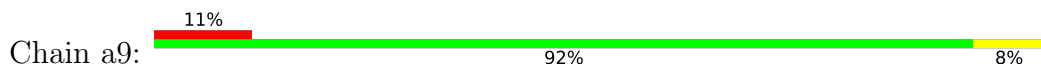
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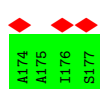
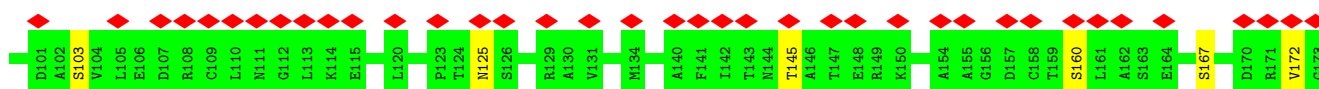
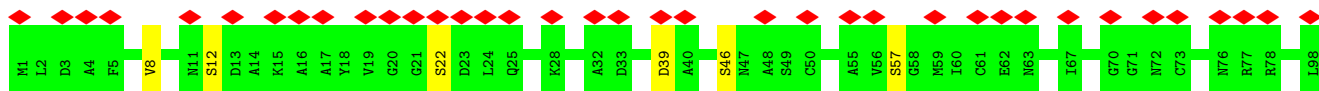
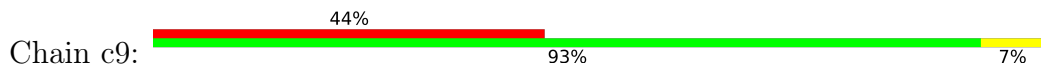
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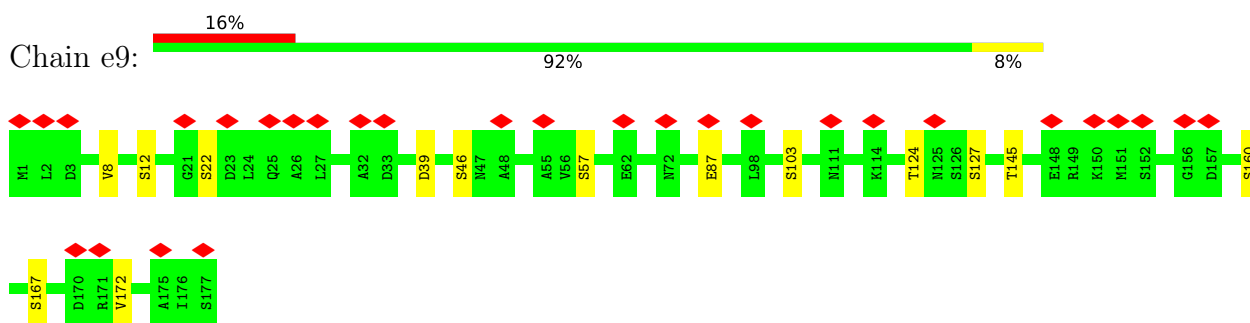
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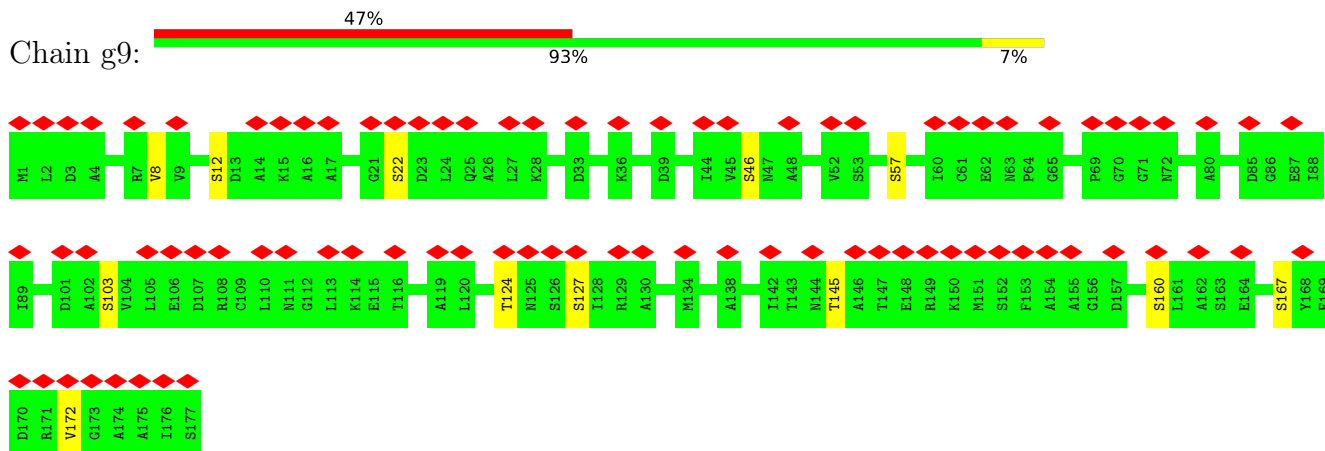
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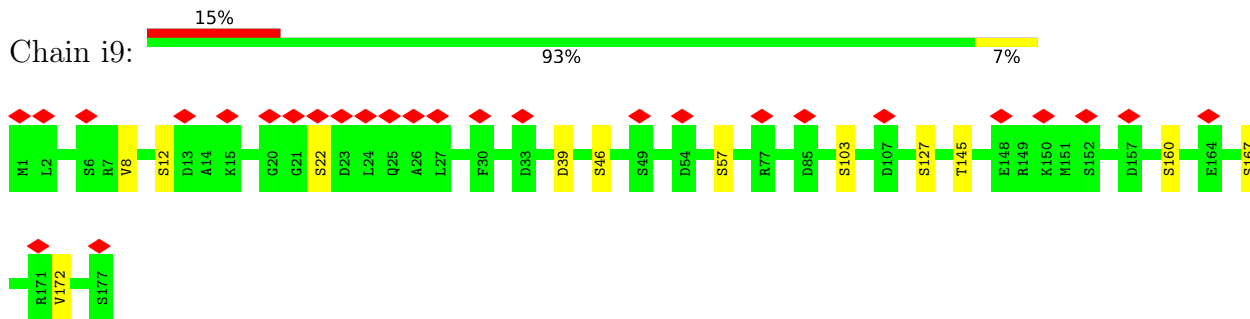
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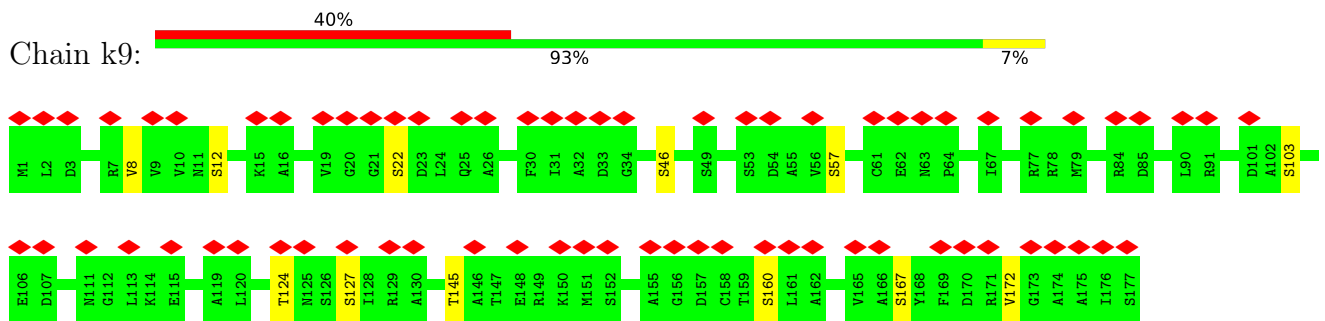
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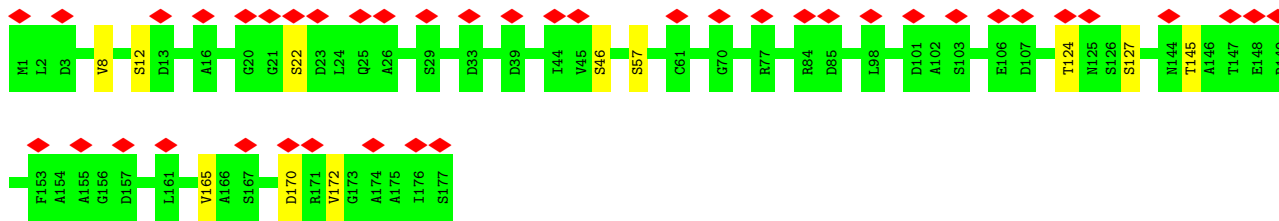


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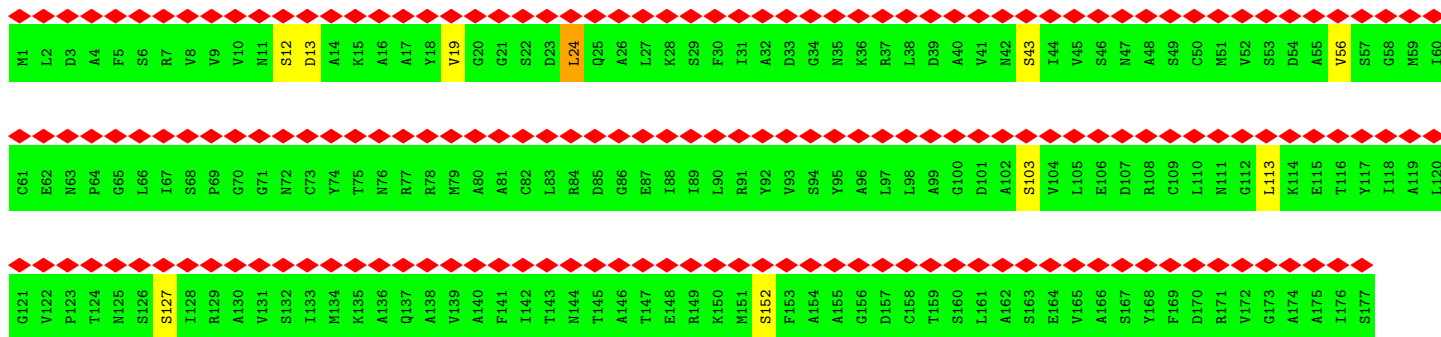


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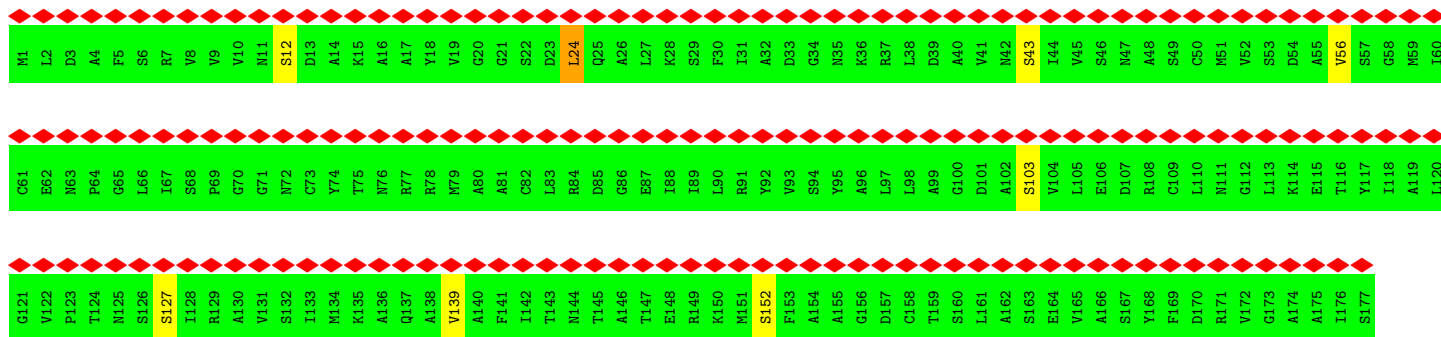




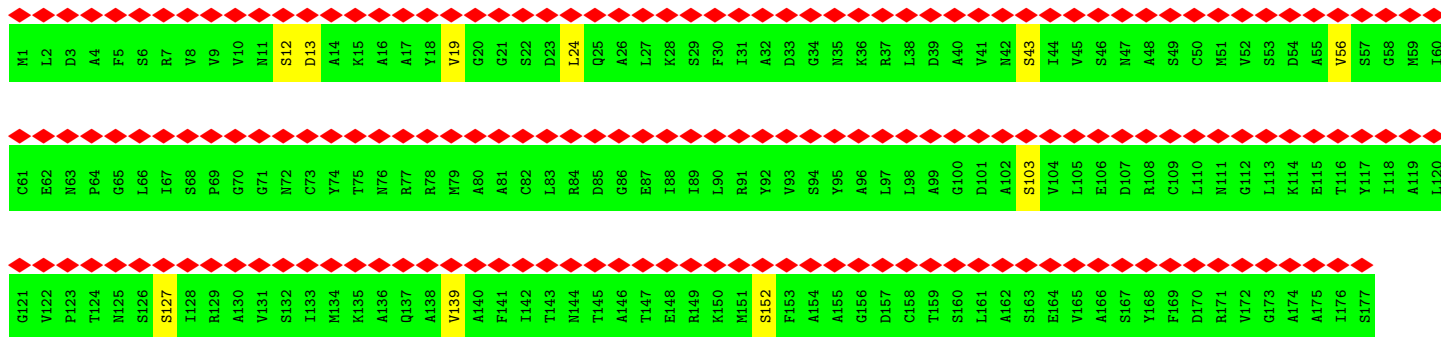
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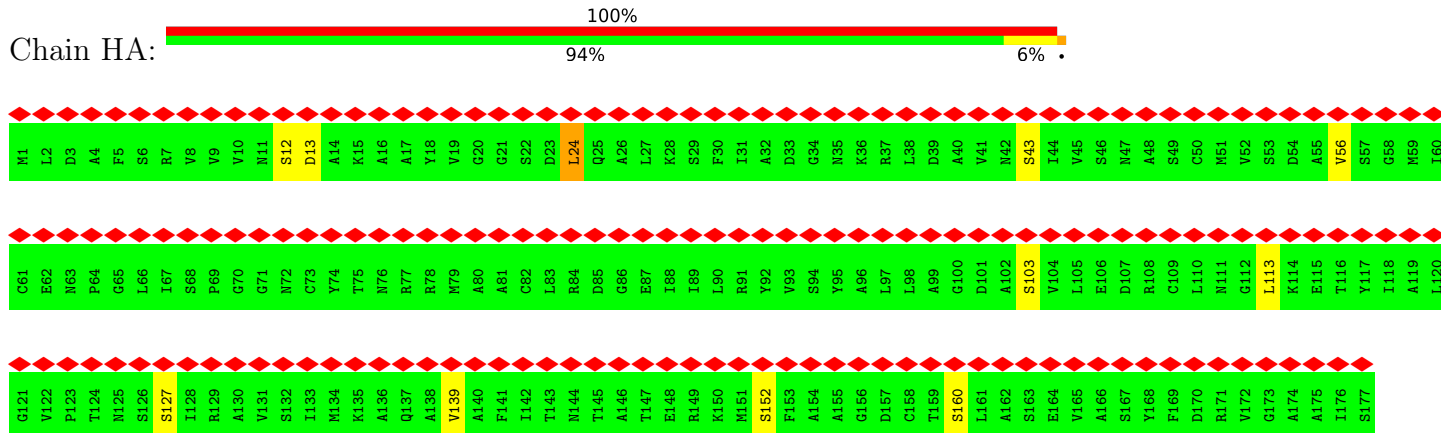
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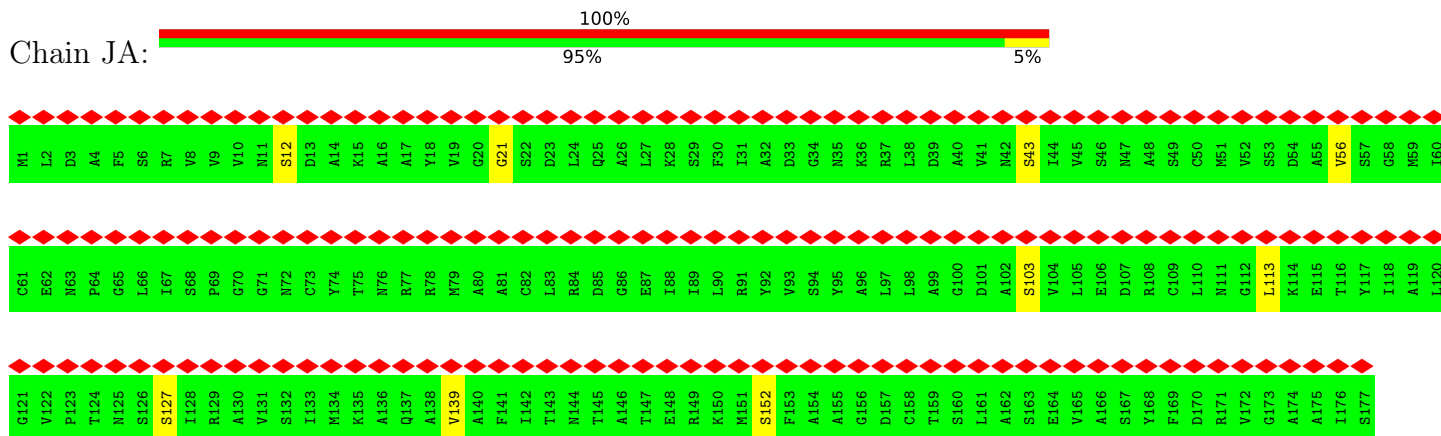
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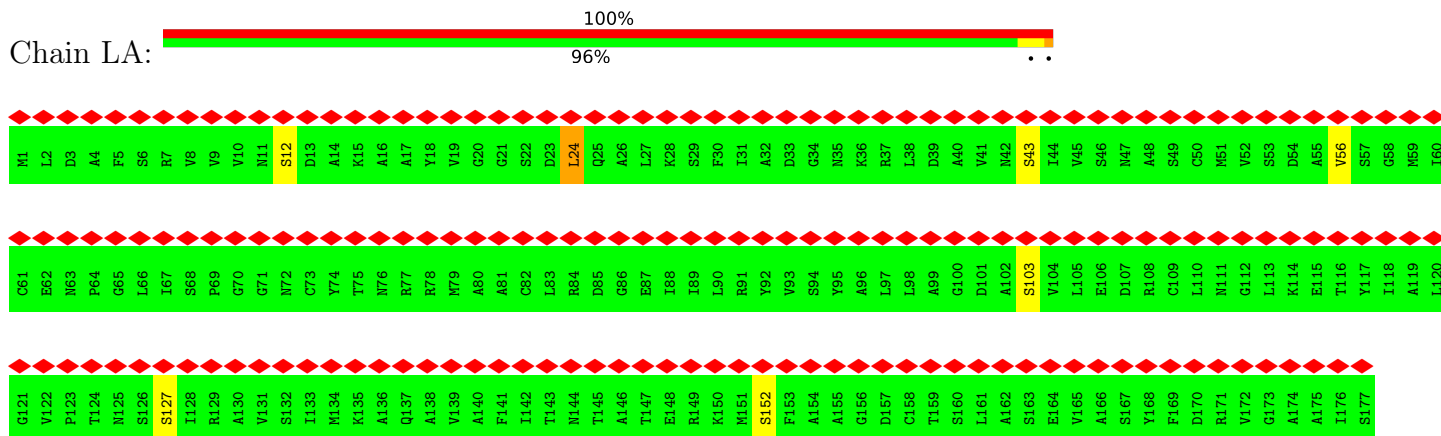
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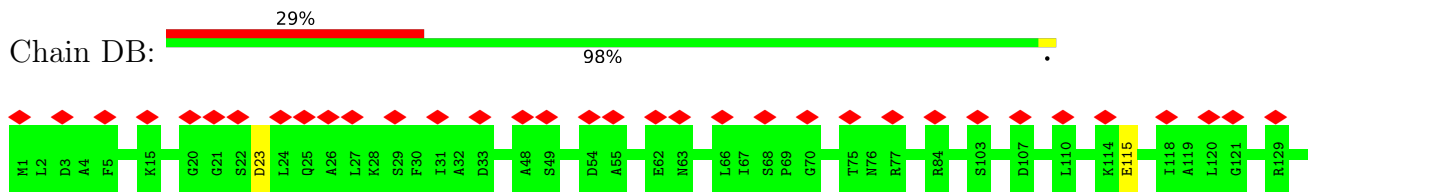
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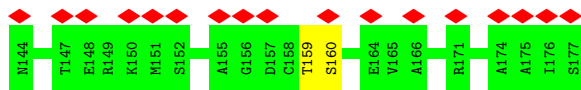


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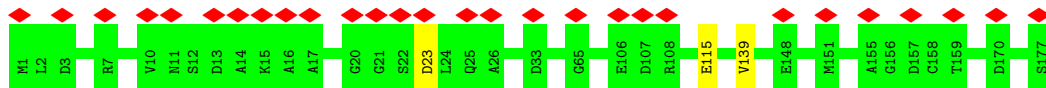


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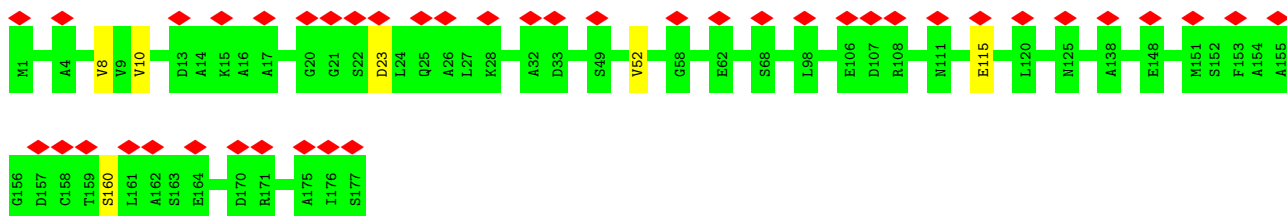




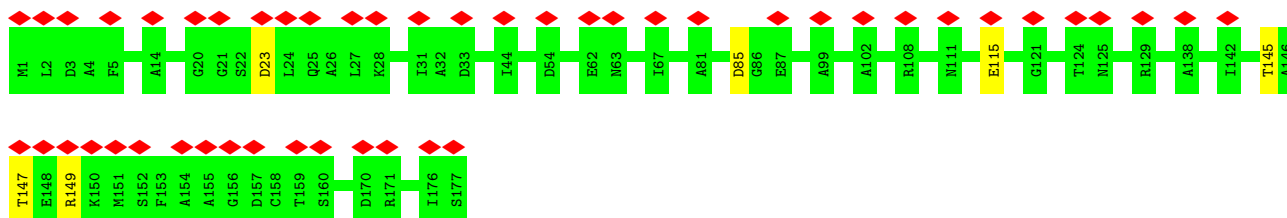
- Molecule 7: B-phycoerythrin beta chain



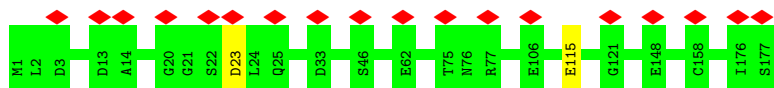
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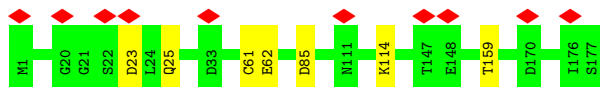
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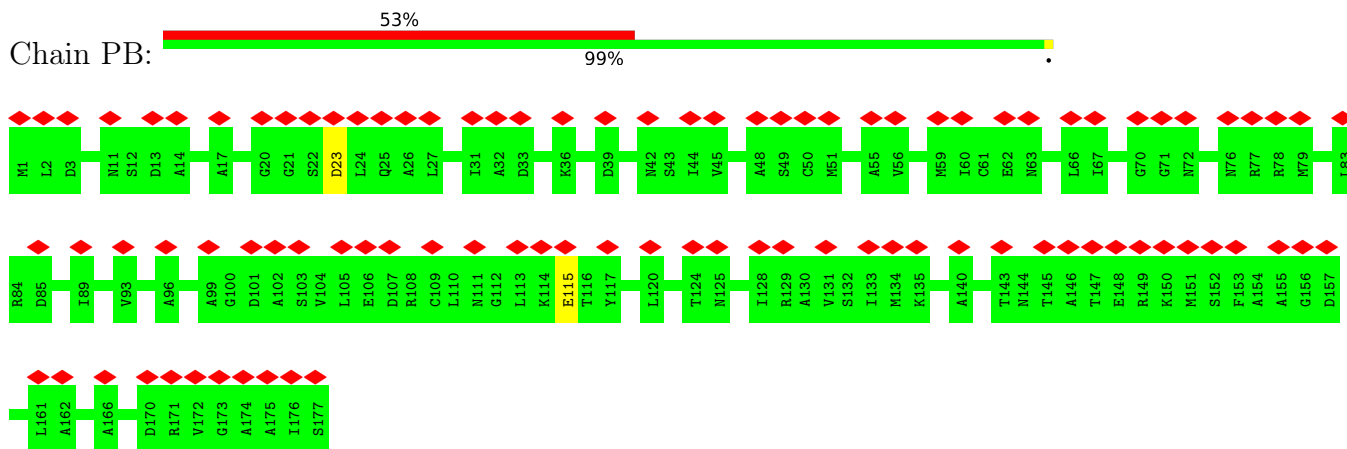
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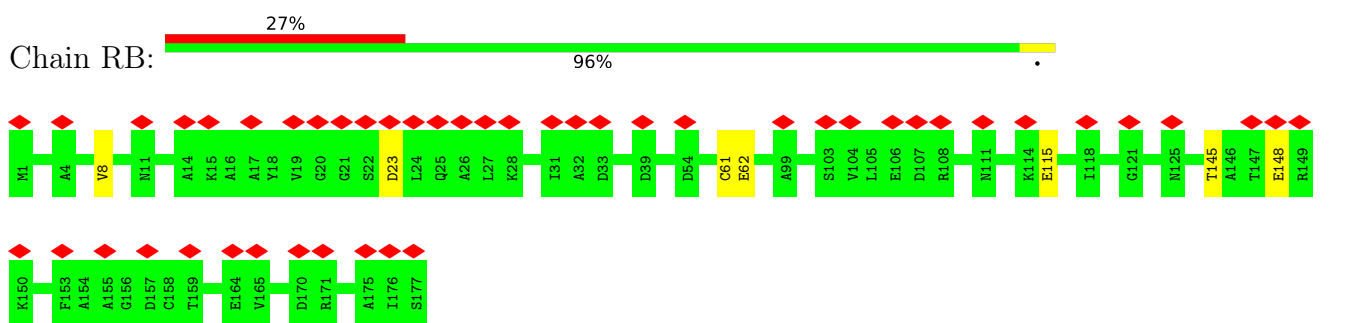
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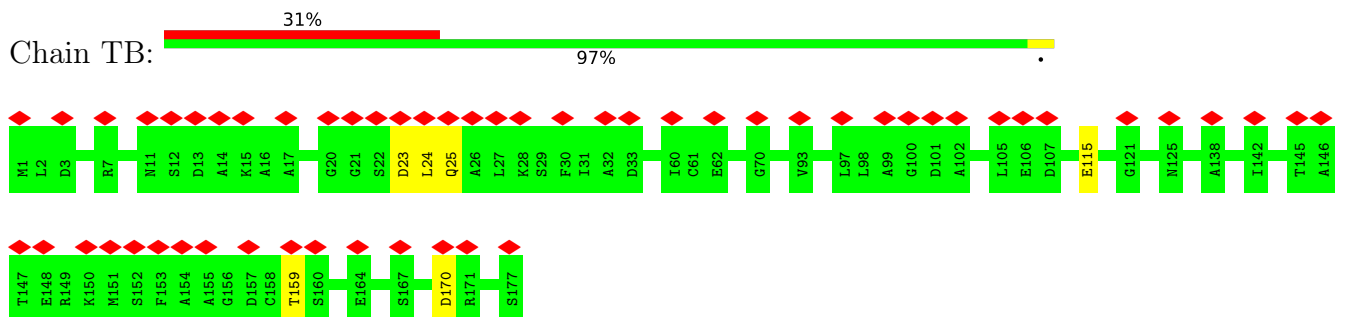
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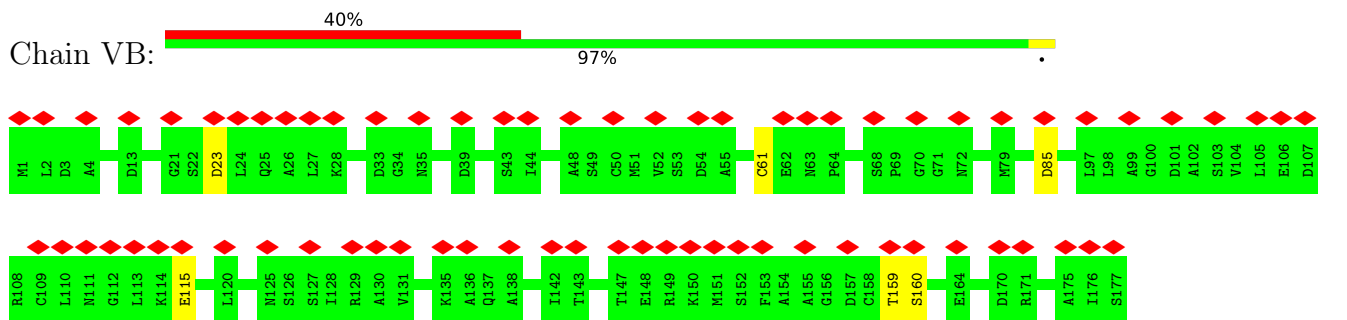
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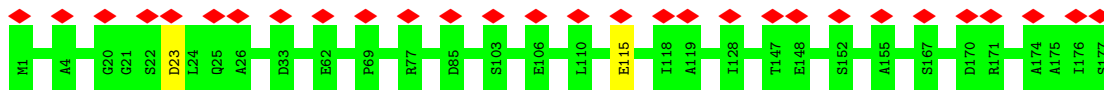


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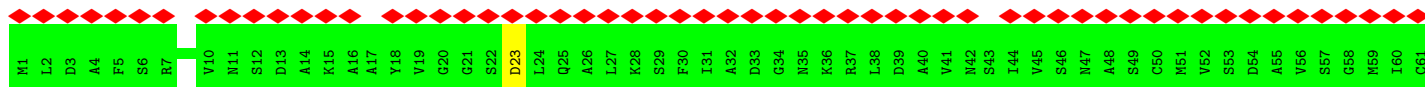




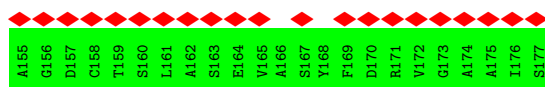
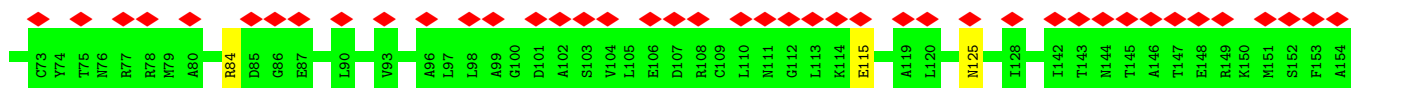
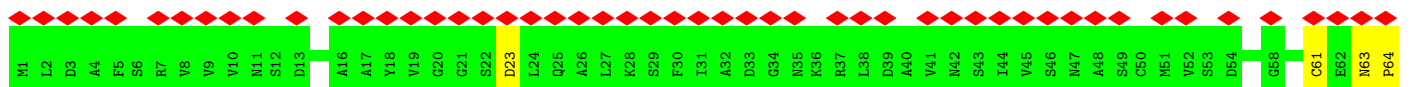
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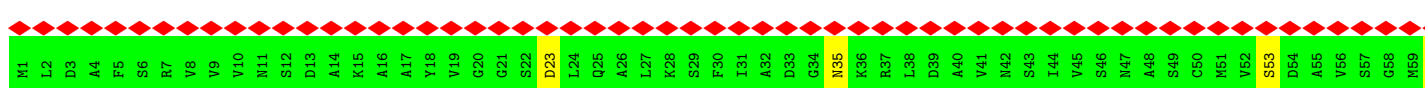
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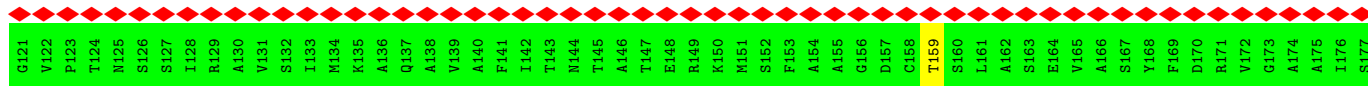
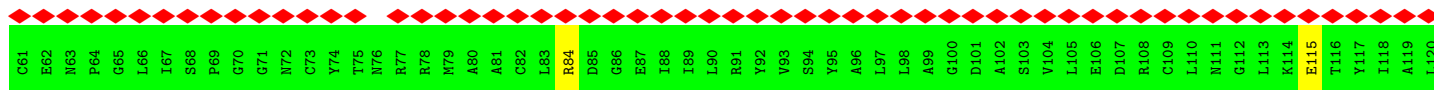


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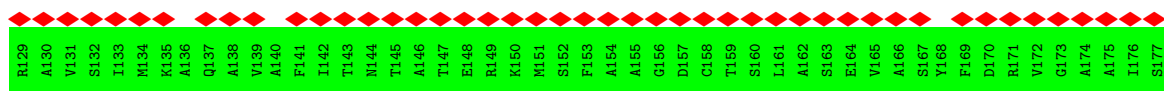
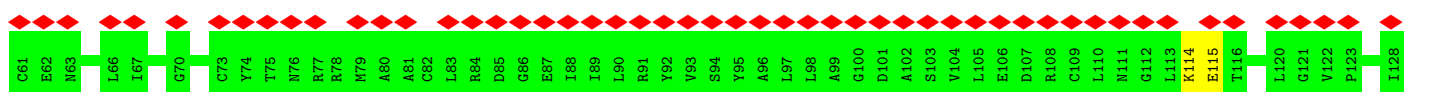
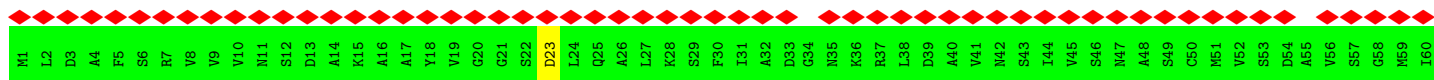
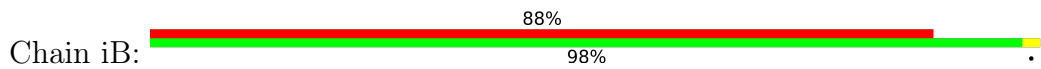


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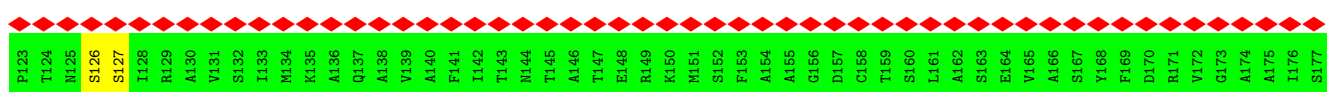
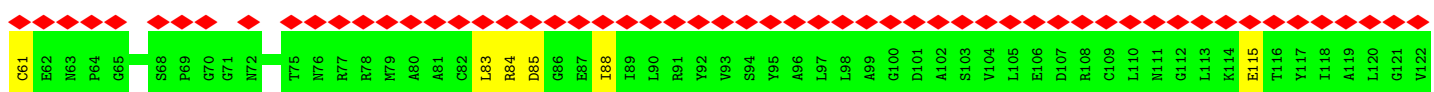
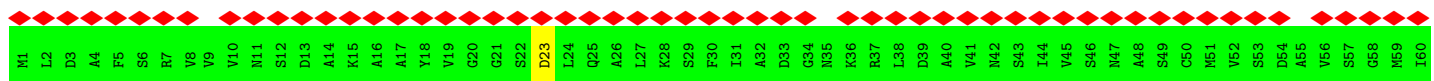




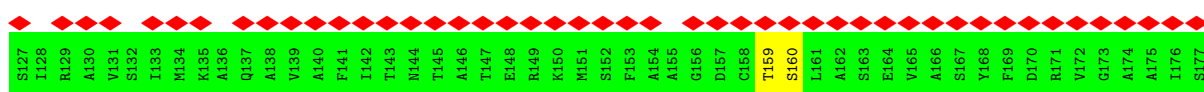
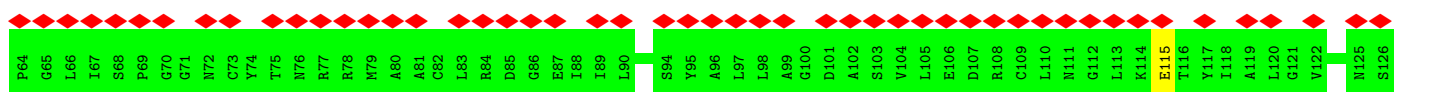
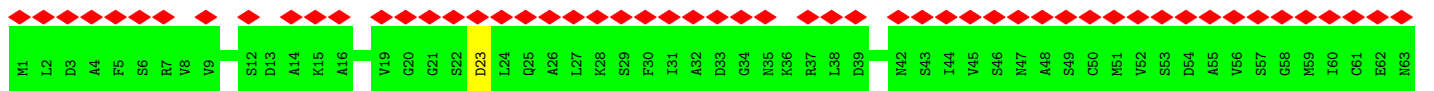
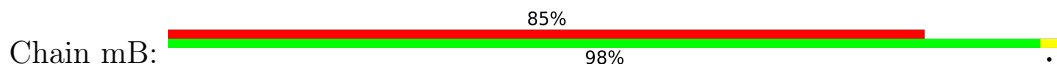
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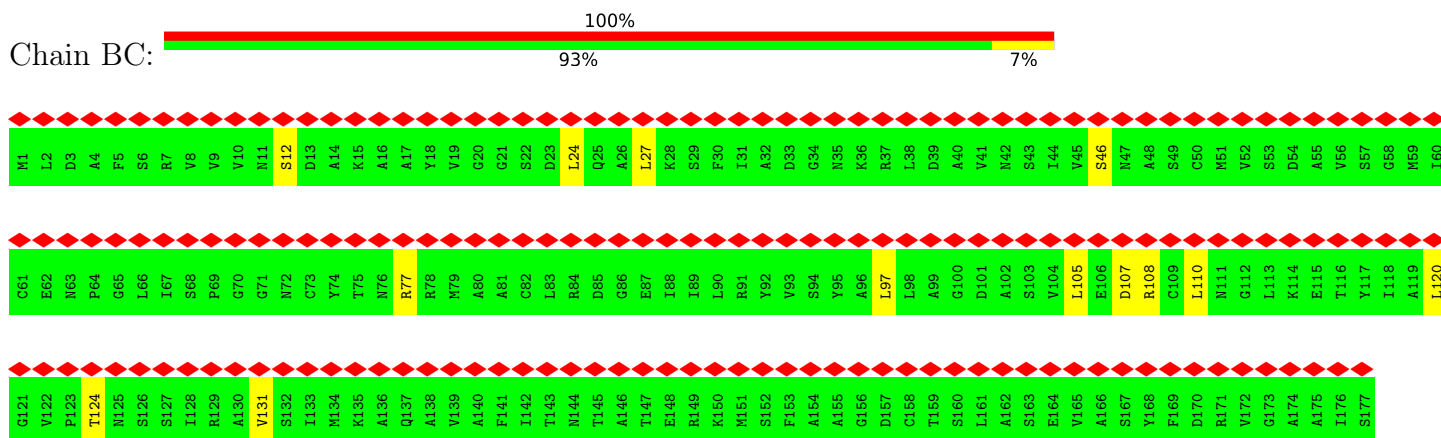
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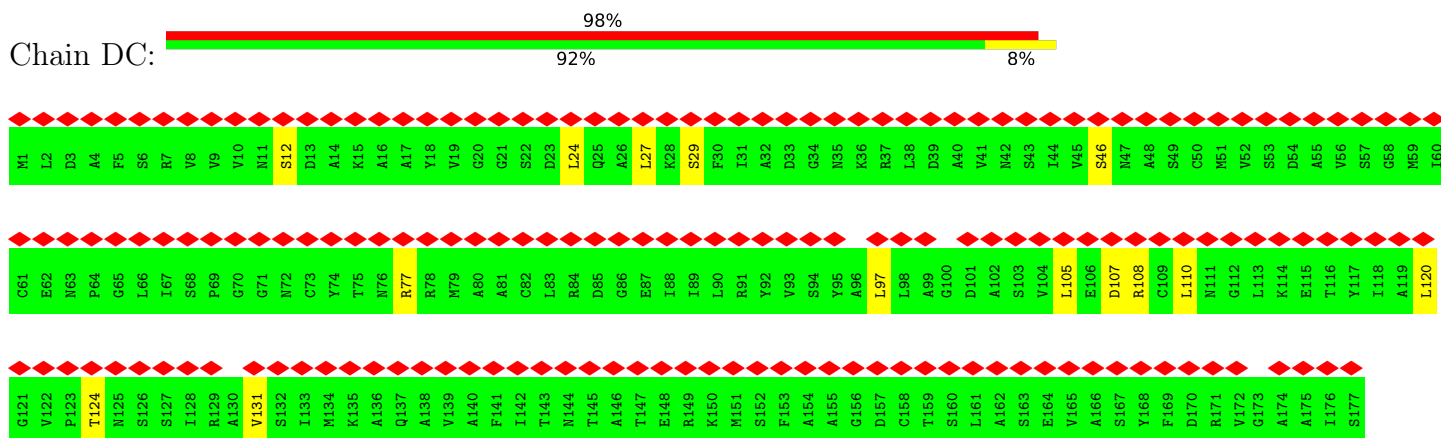
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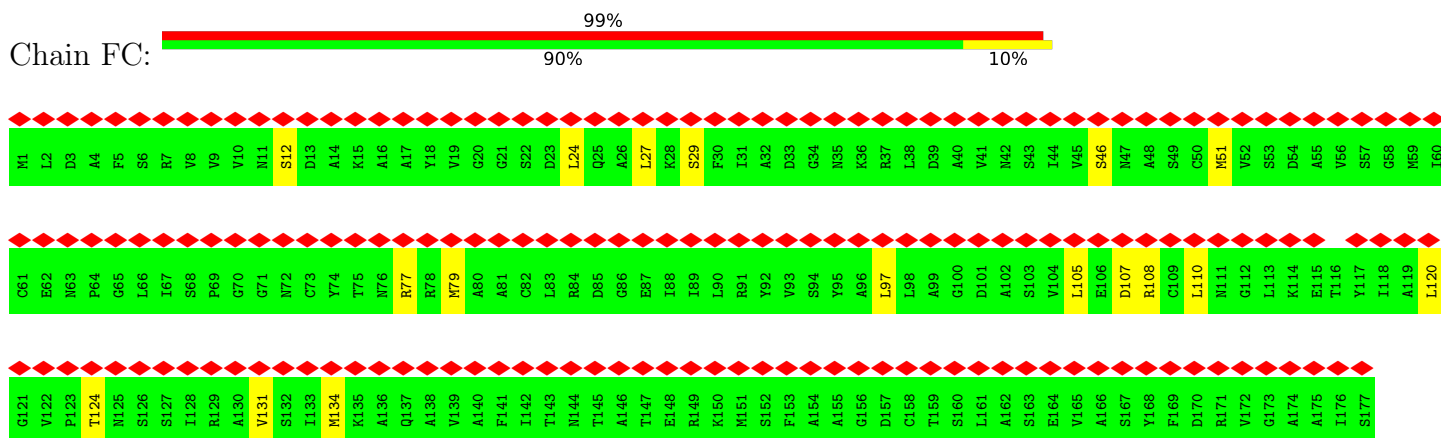
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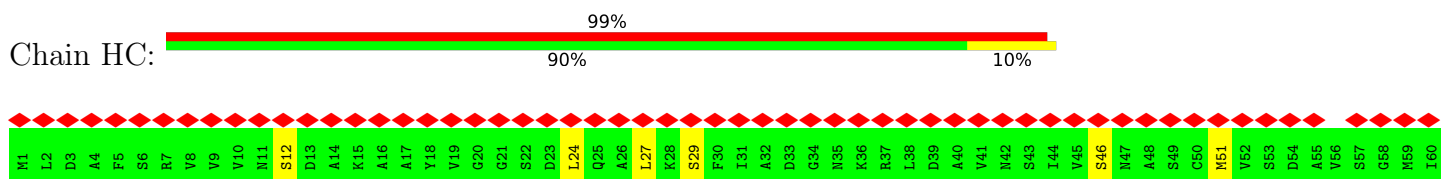
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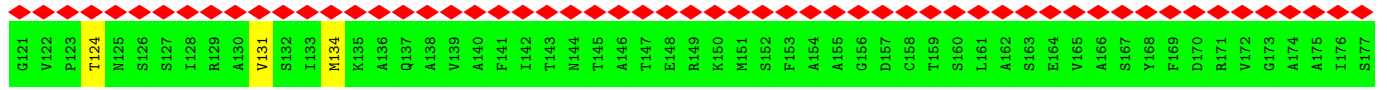
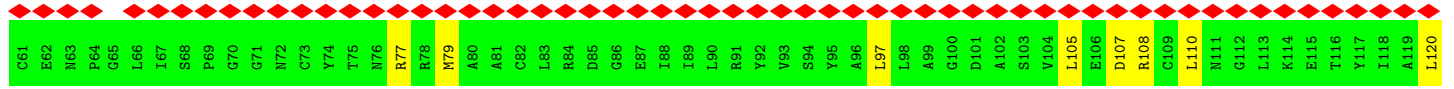


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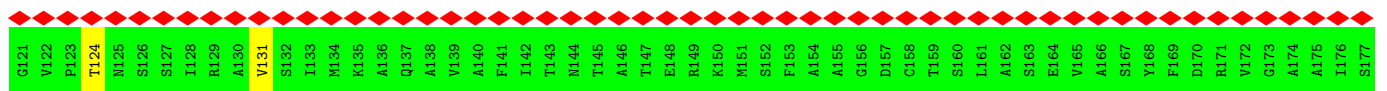
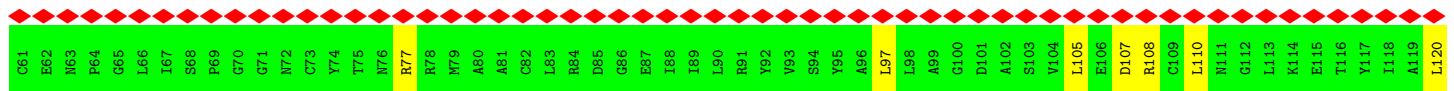
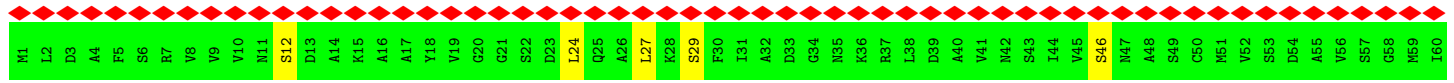
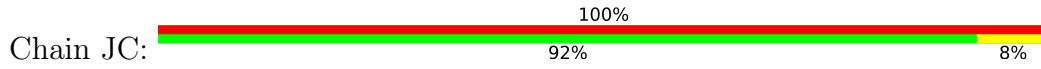


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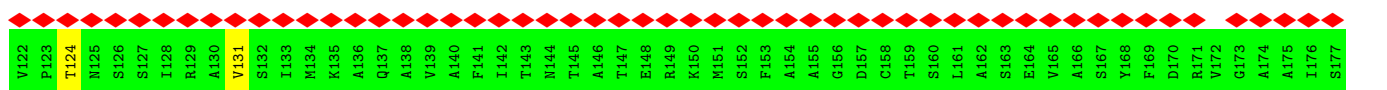
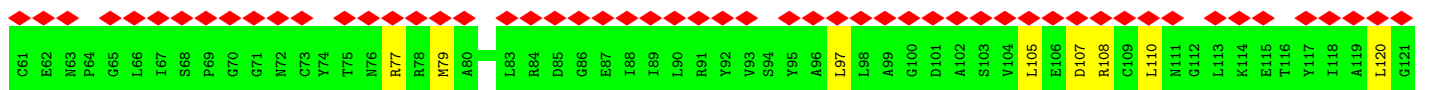
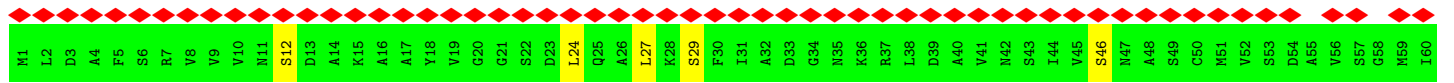
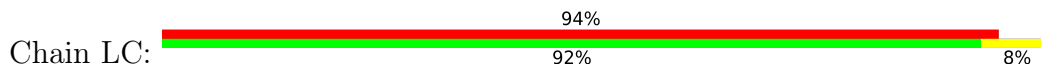




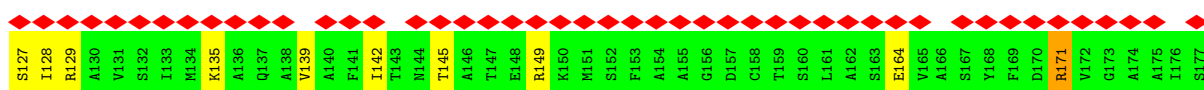
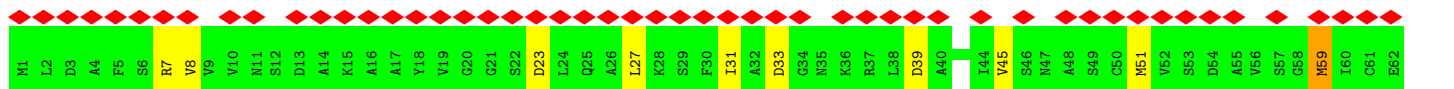
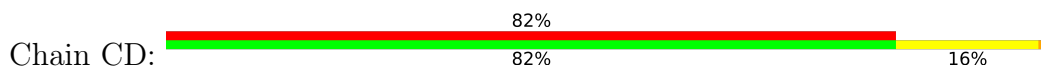
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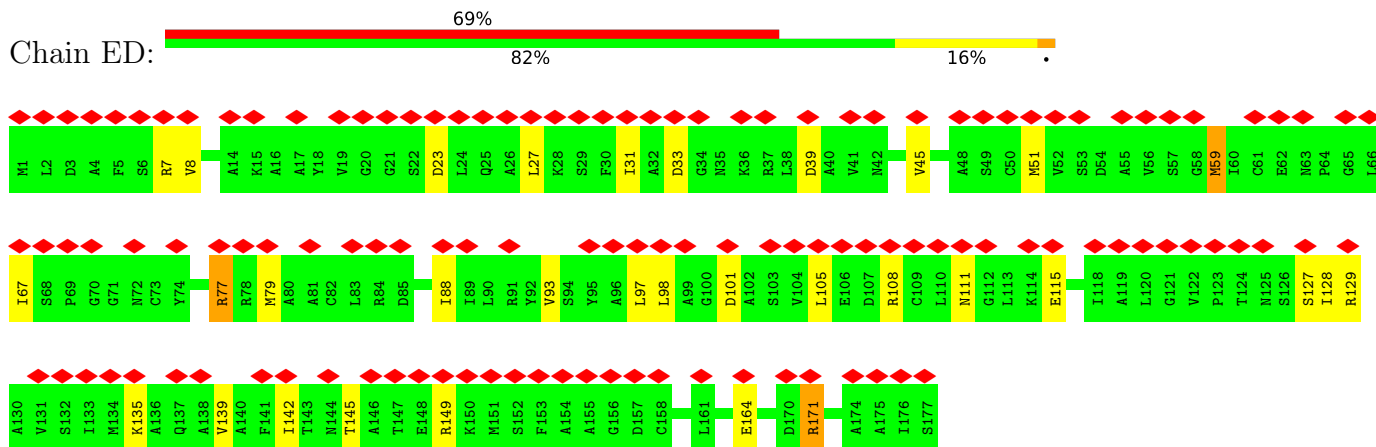
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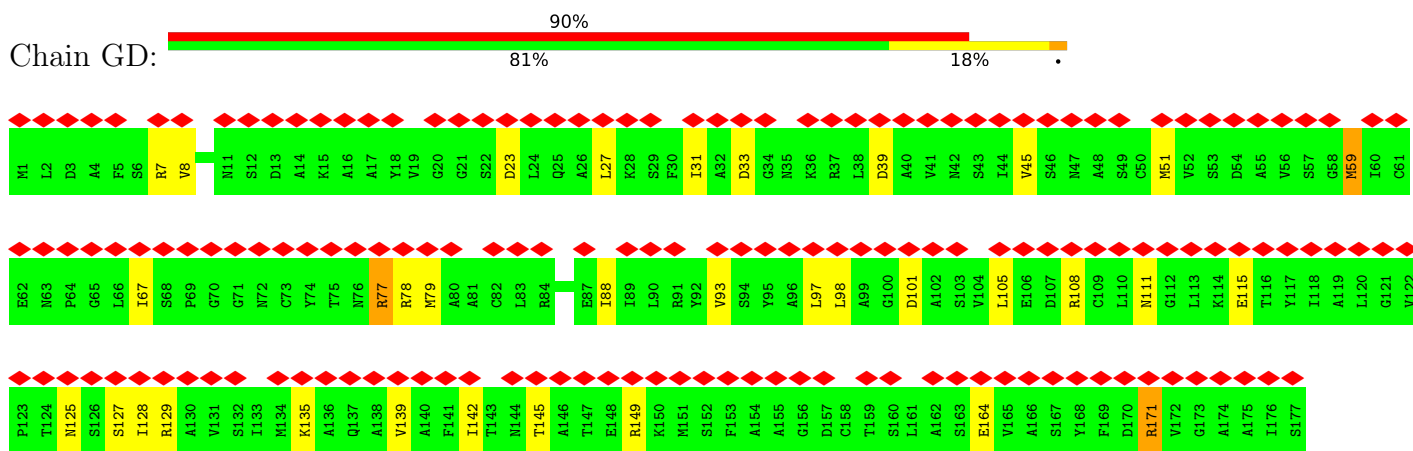
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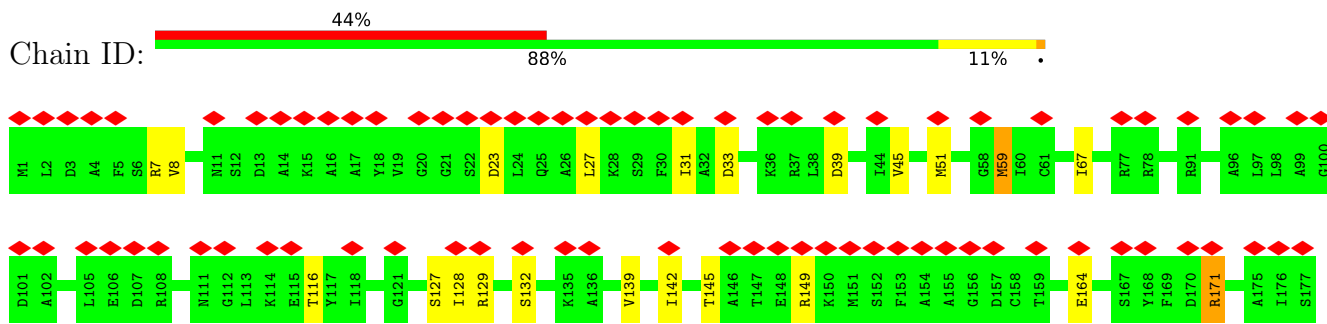
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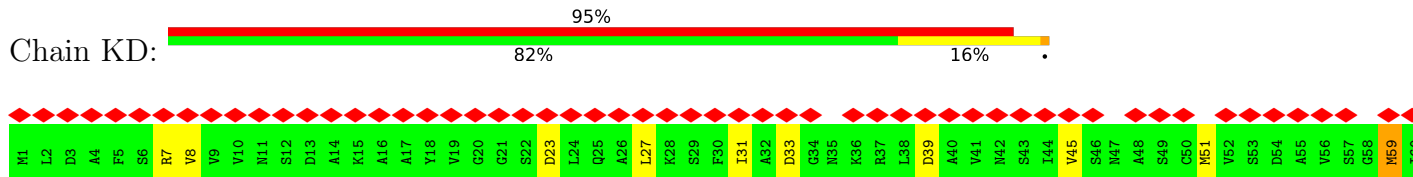
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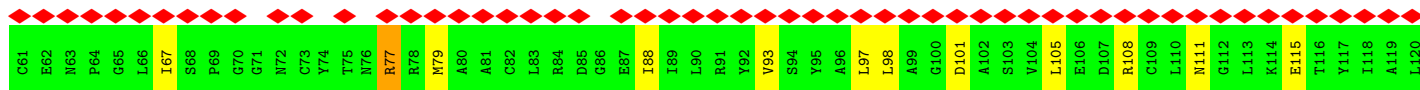


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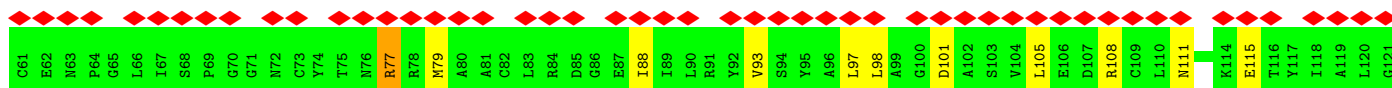
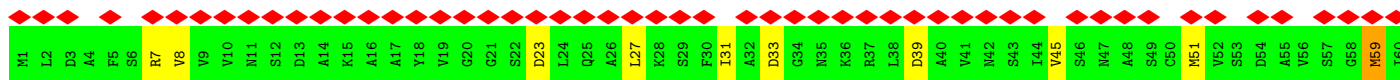
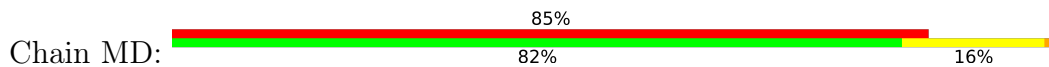


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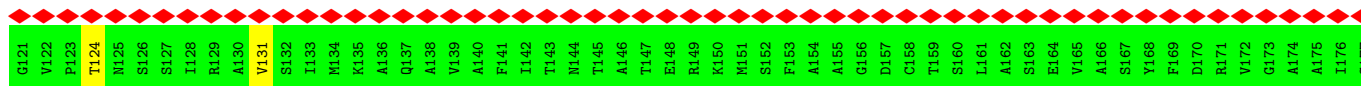
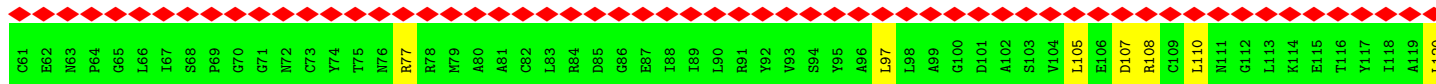




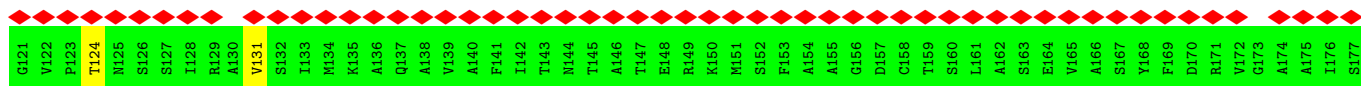
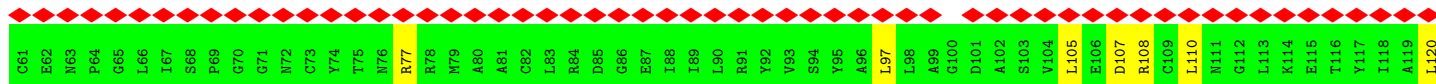
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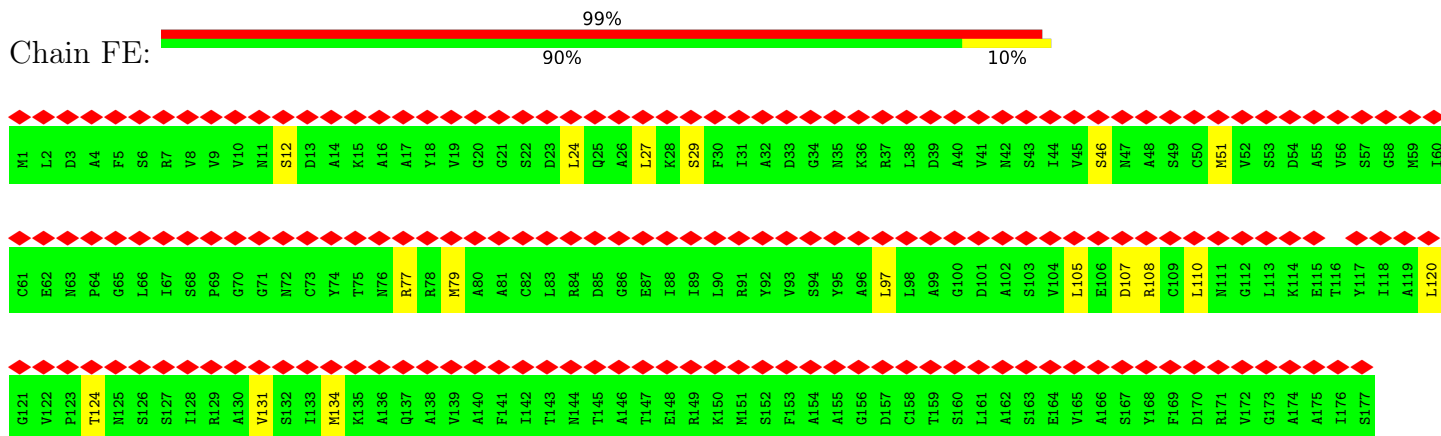
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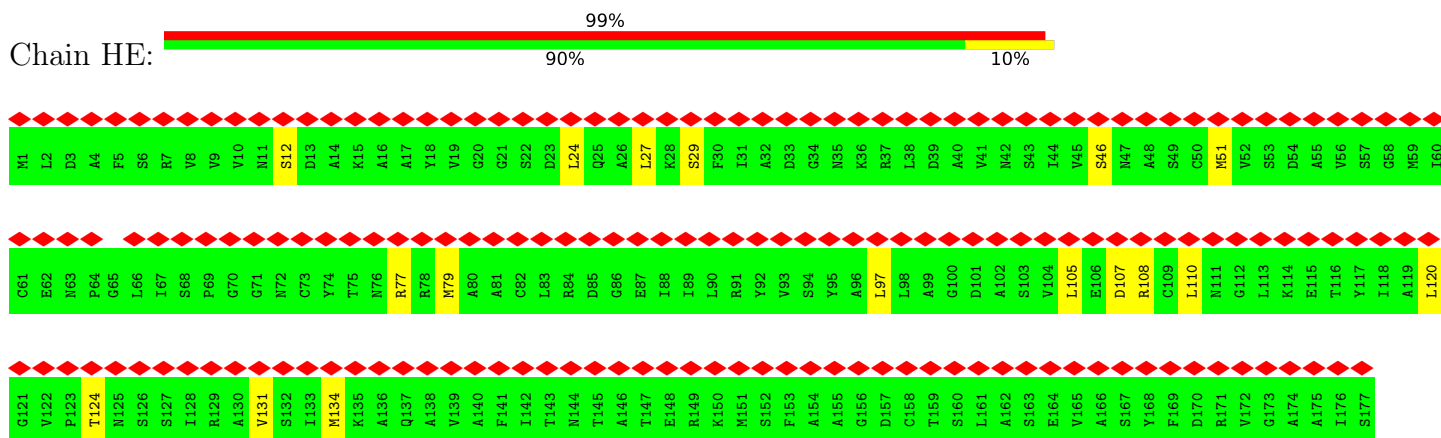
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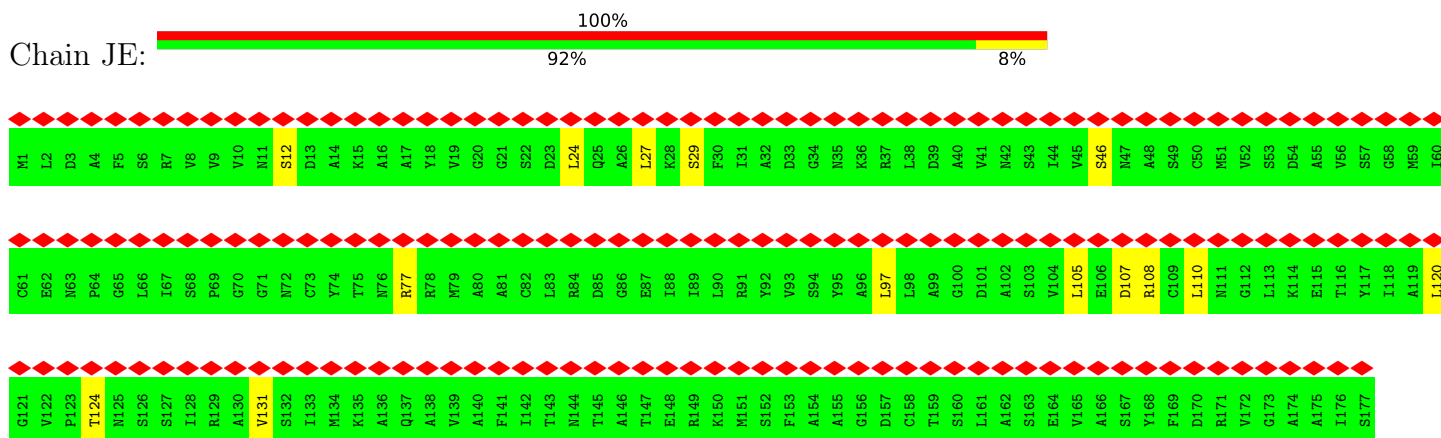
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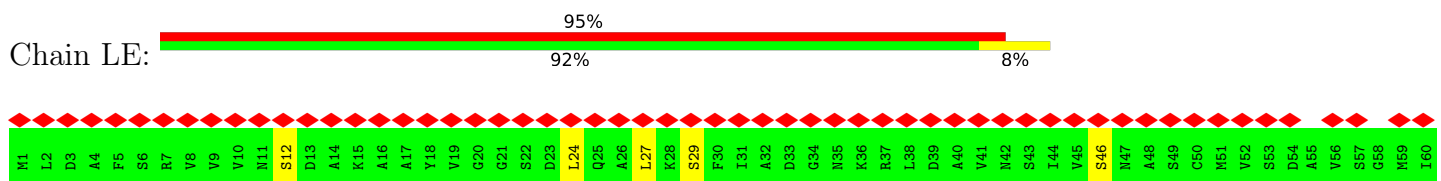
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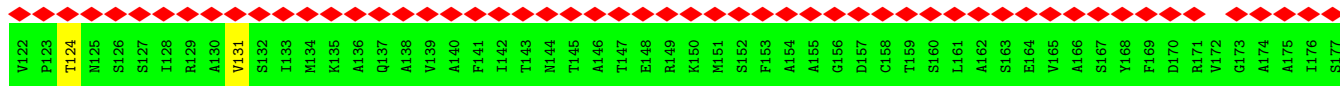
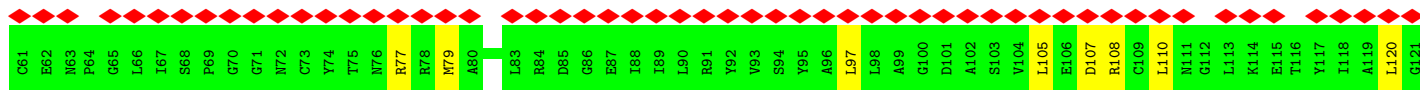


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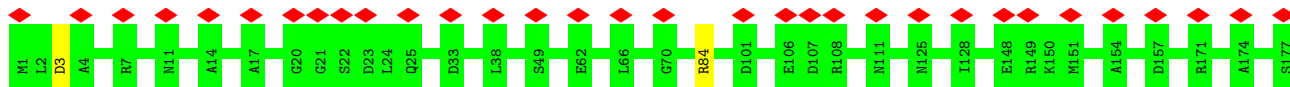


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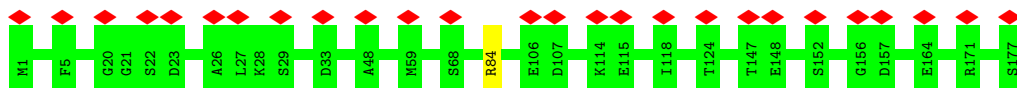




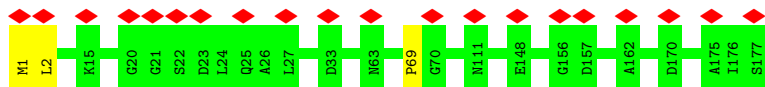
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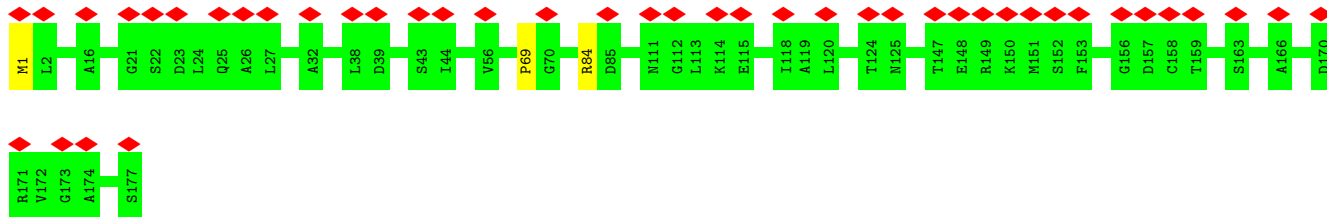
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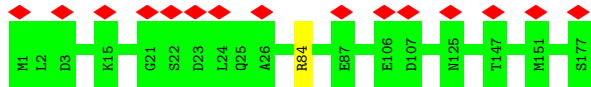
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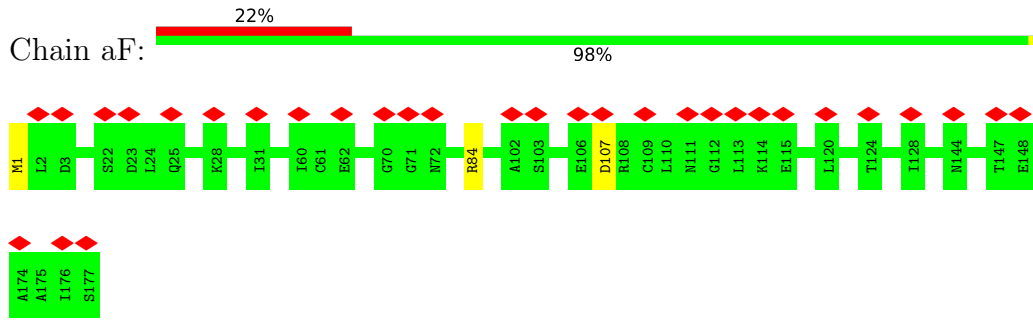
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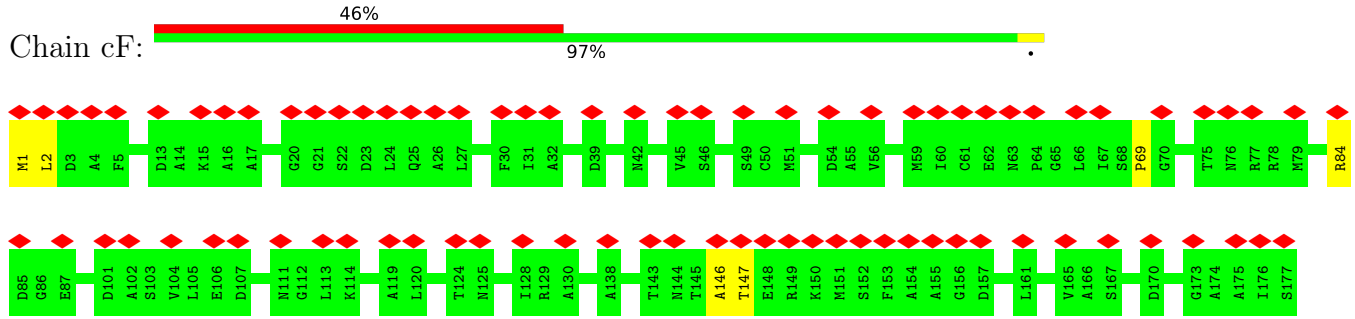
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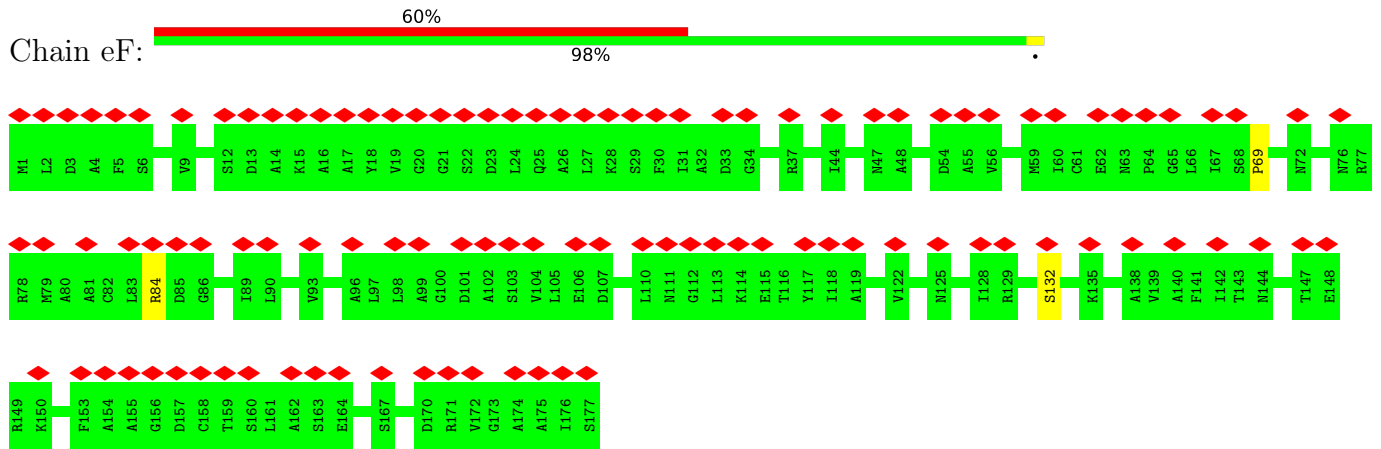
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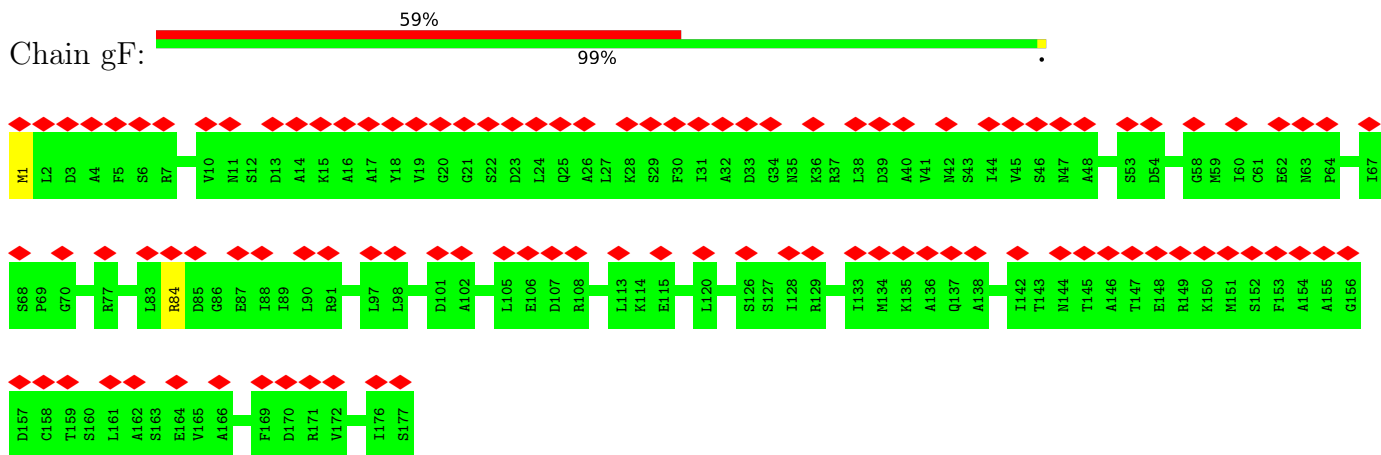
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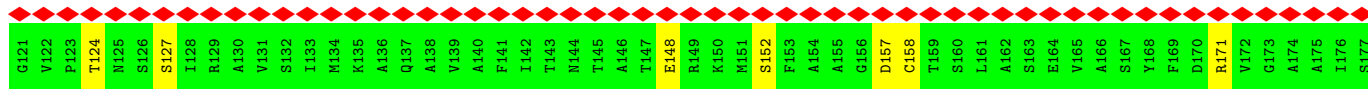
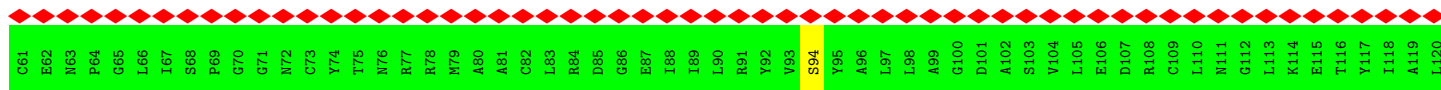


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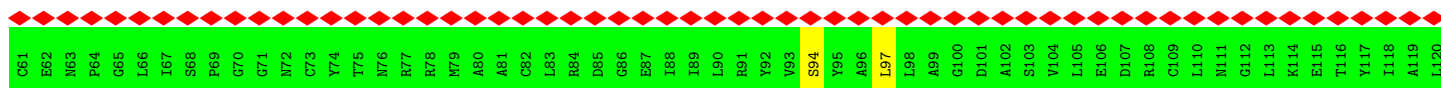


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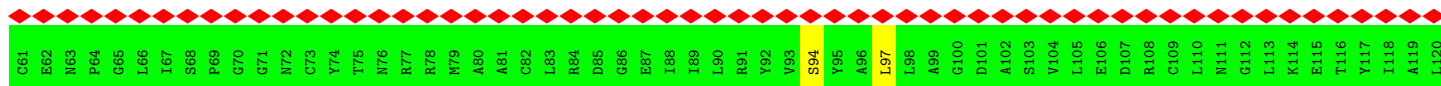




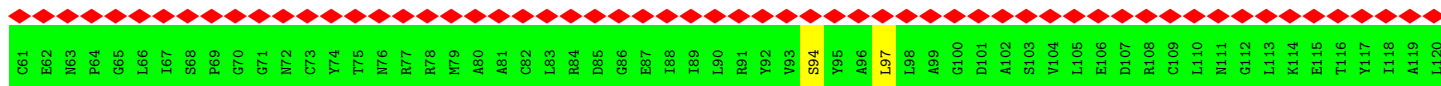
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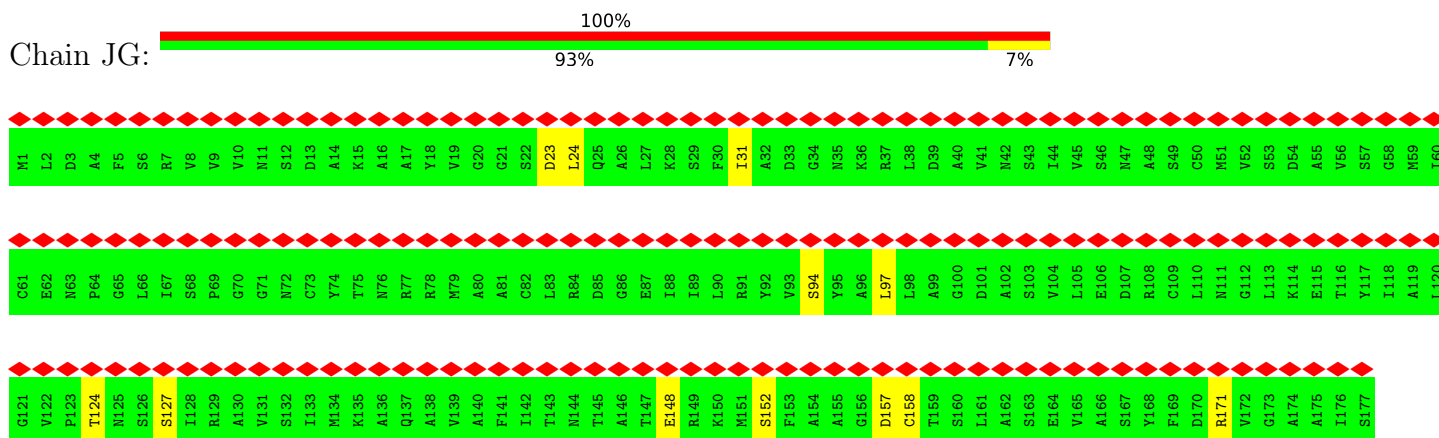
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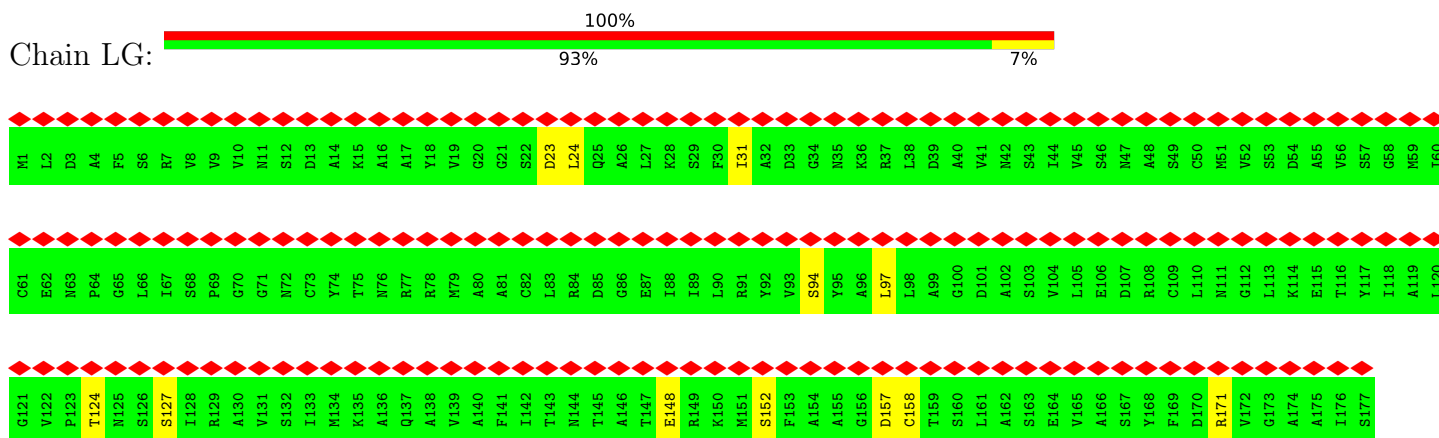
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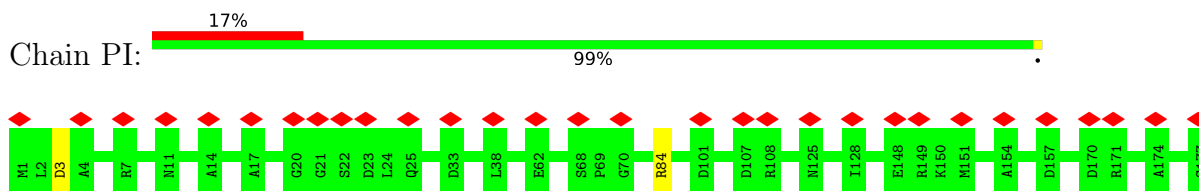
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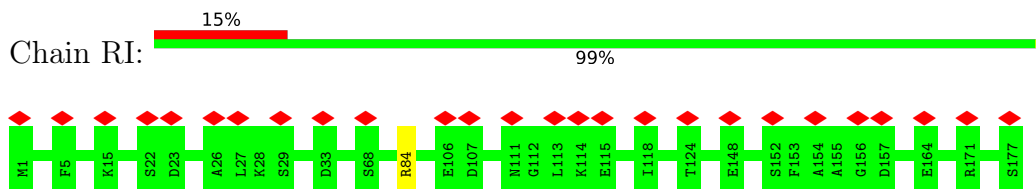
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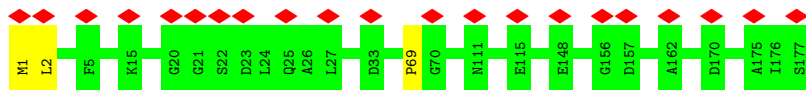


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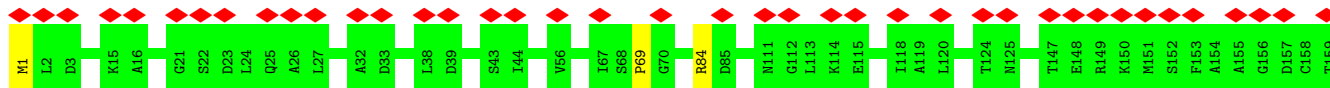


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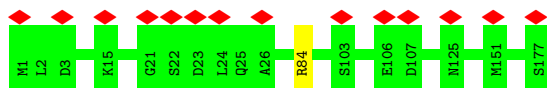




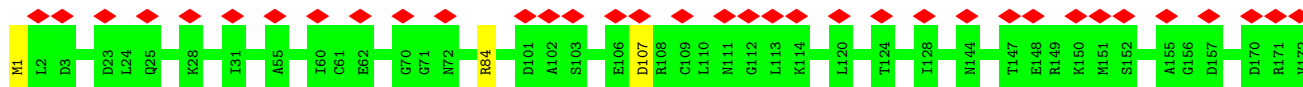
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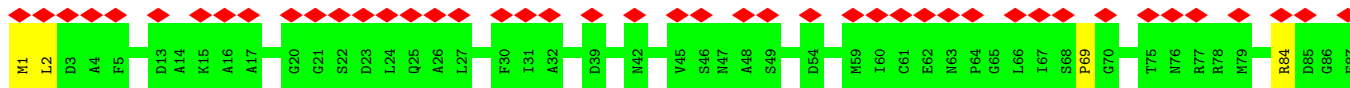
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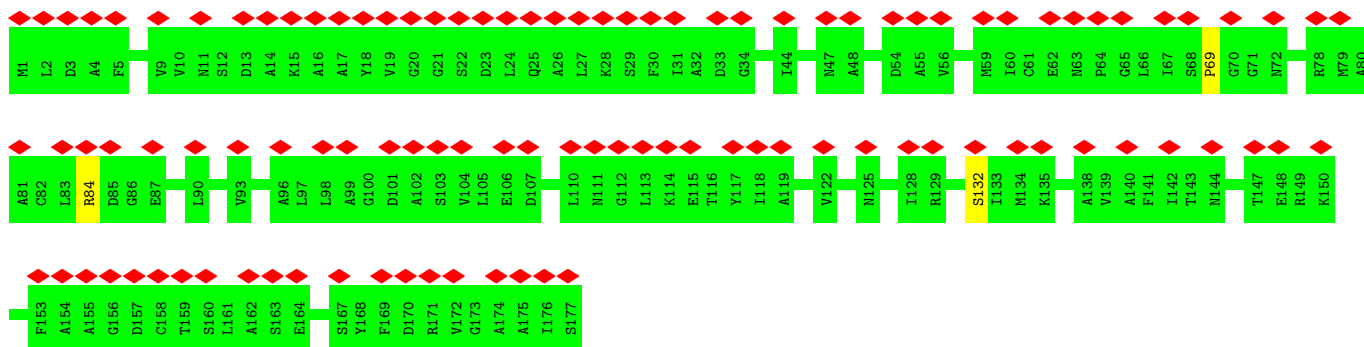


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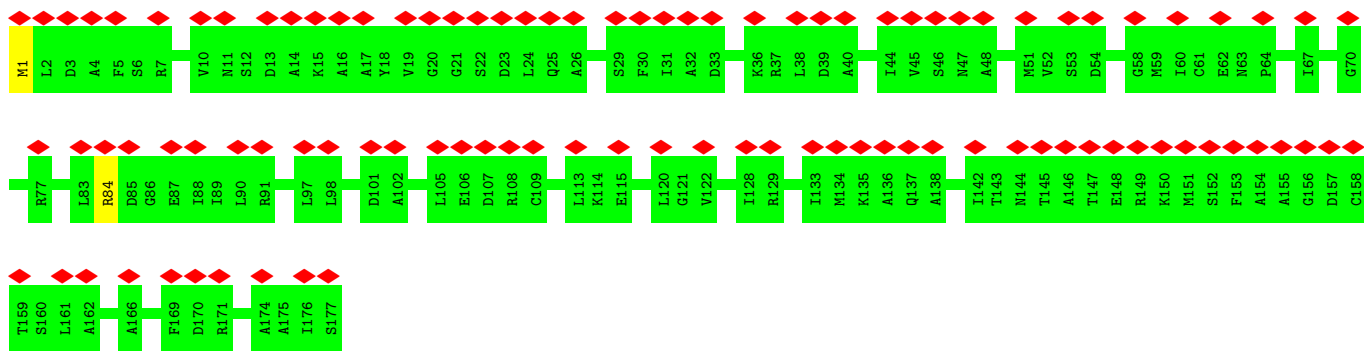


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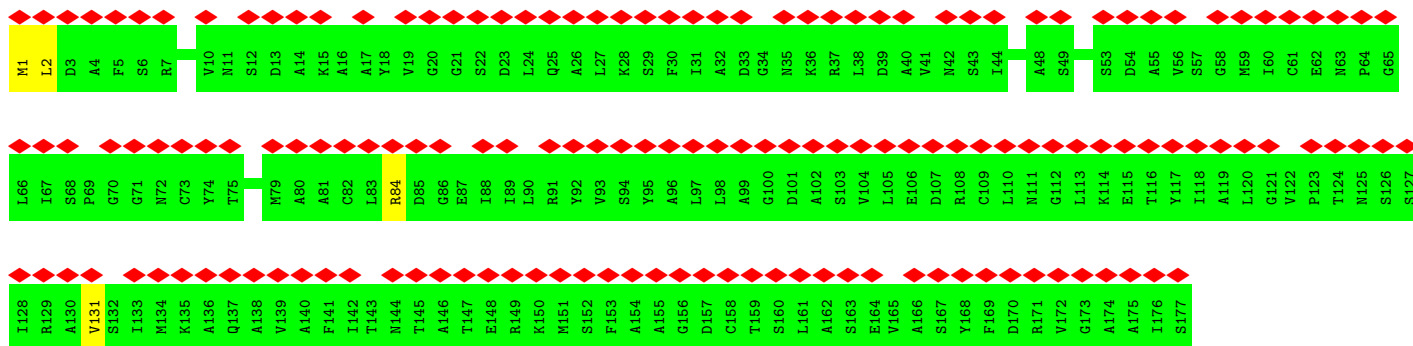
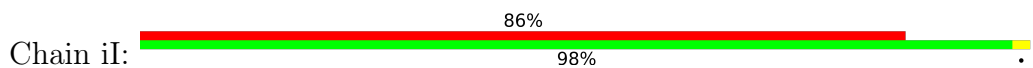




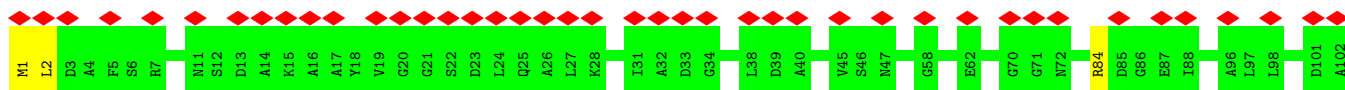
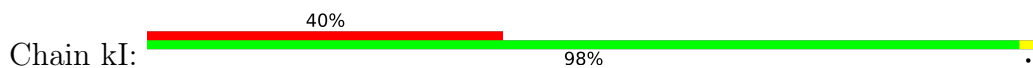
• Molecule 7: B-phycoerythrin beta chain

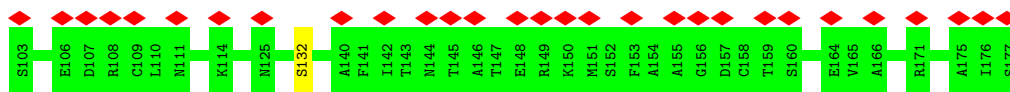


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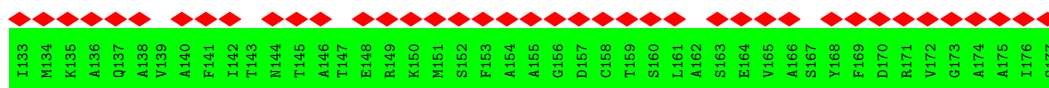
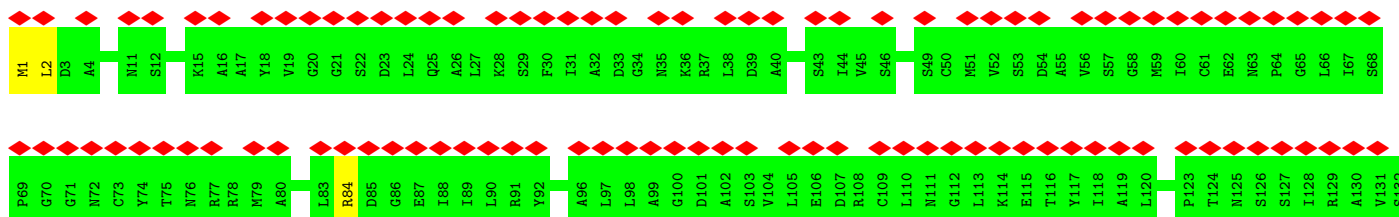
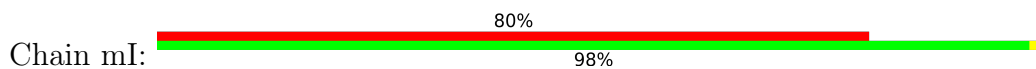


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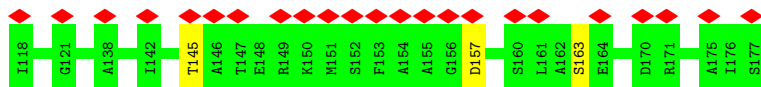
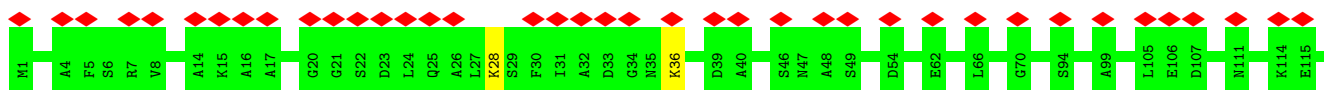




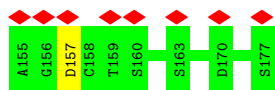
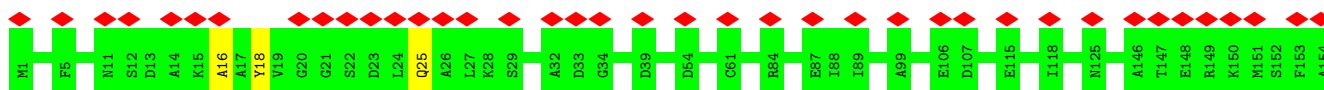
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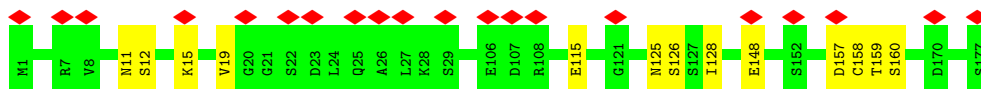
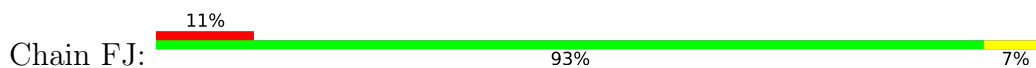
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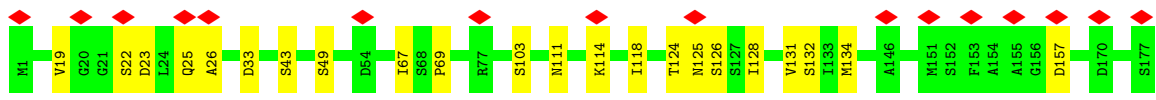
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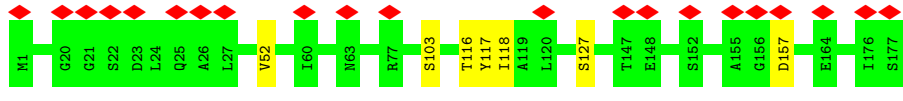
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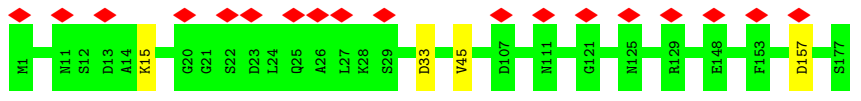
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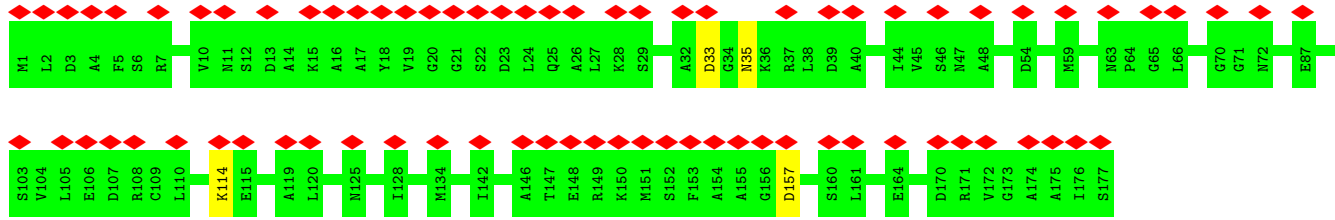
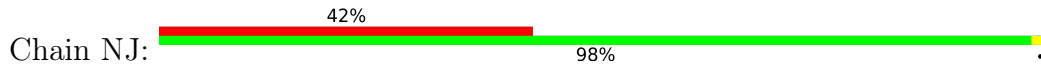
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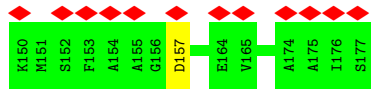
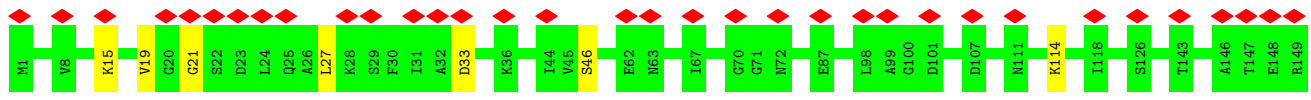
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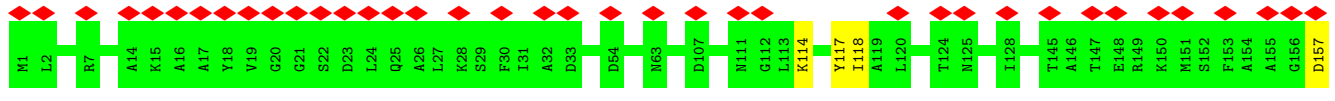
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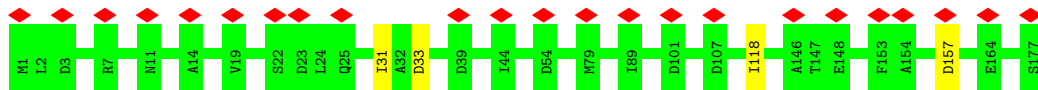


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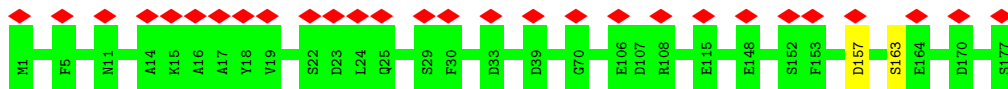
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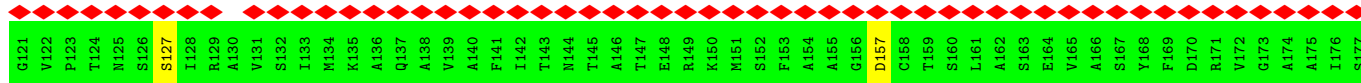
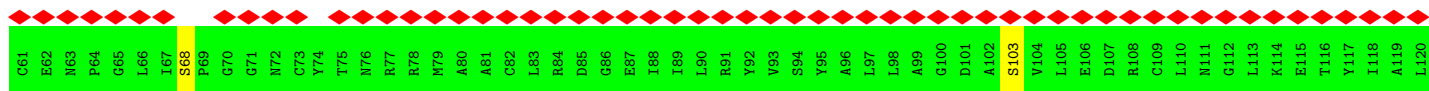
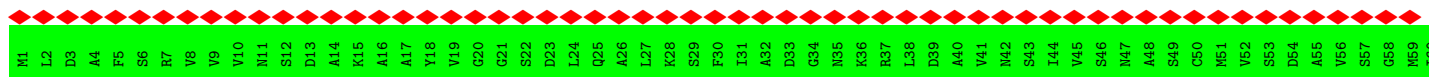
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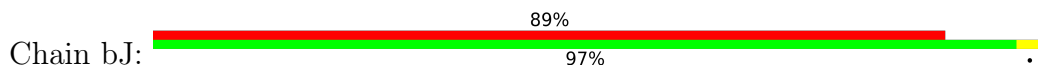
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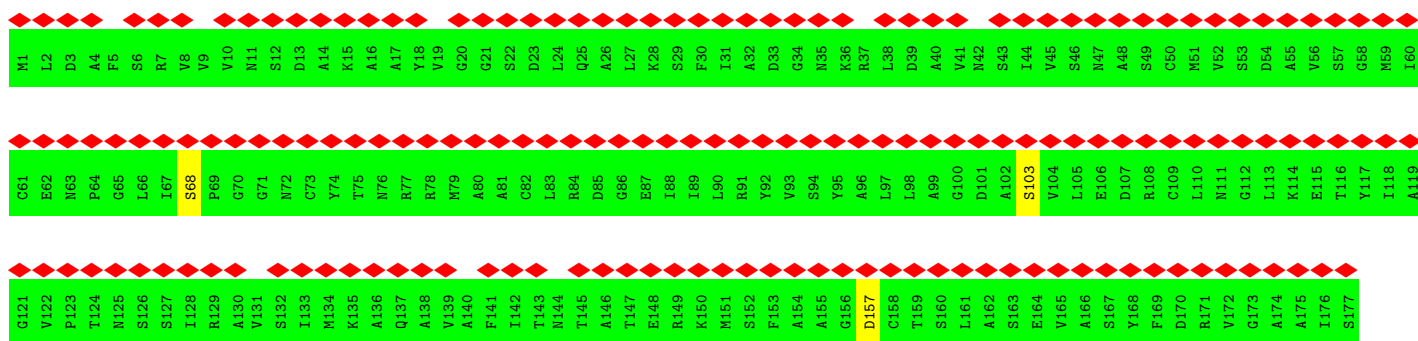


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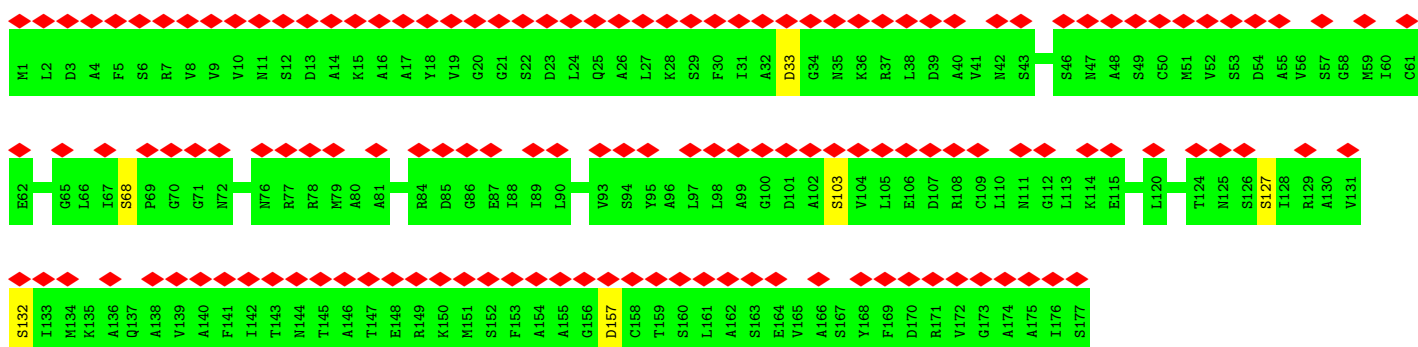
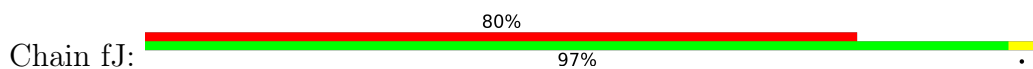




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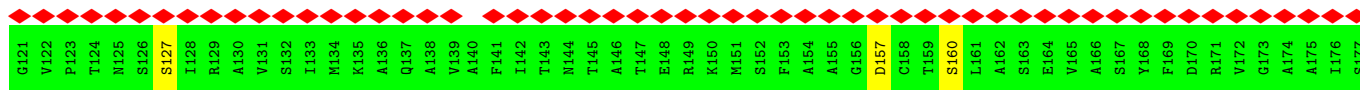


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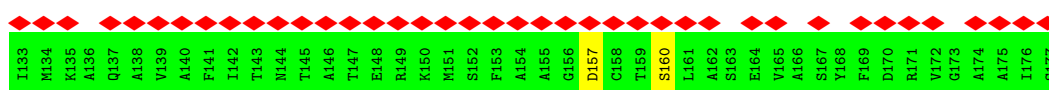
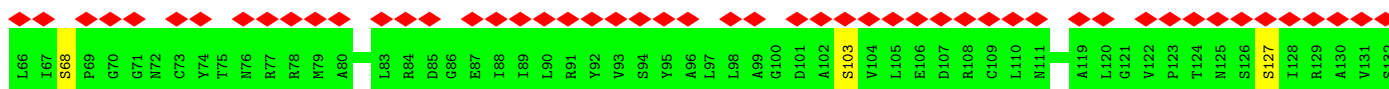
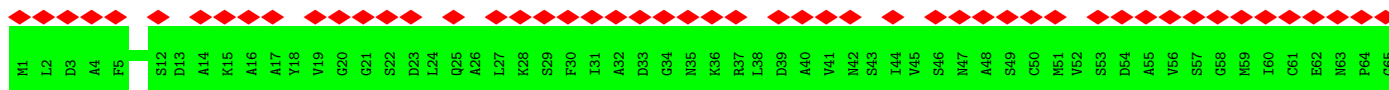
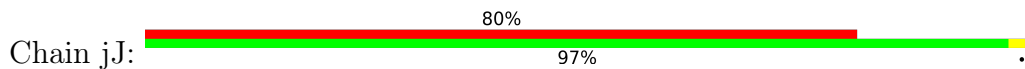


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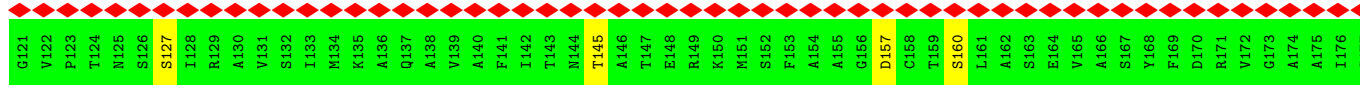
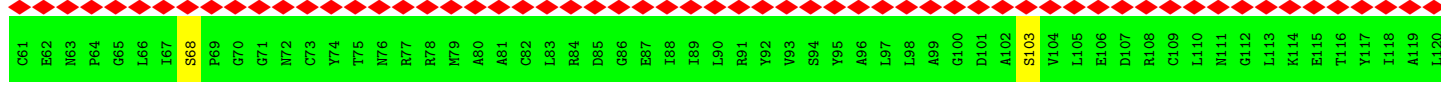
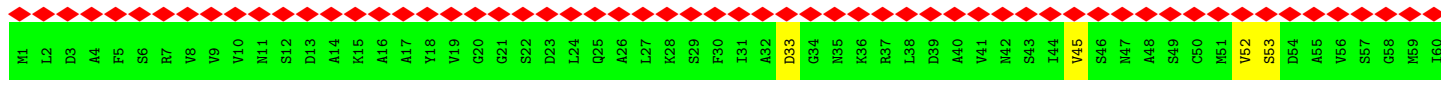




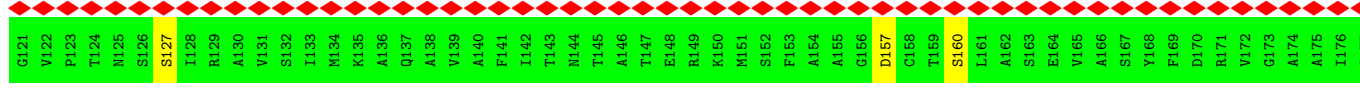
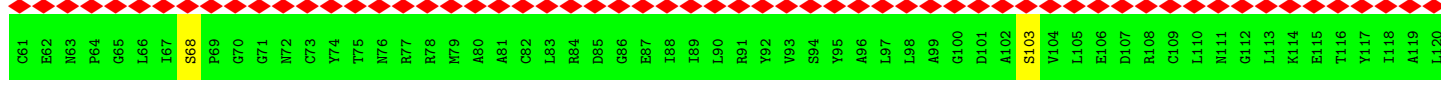
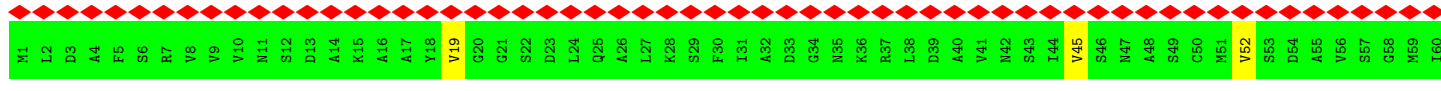
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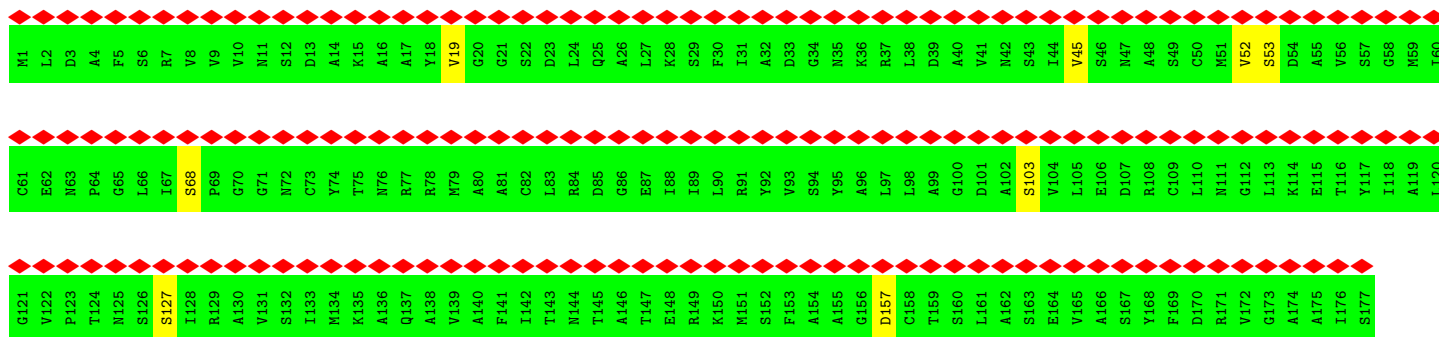
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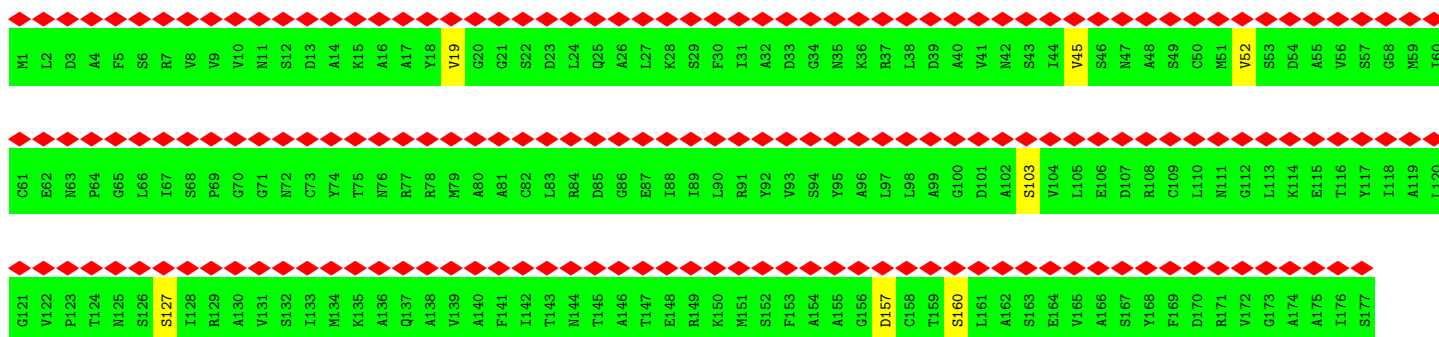
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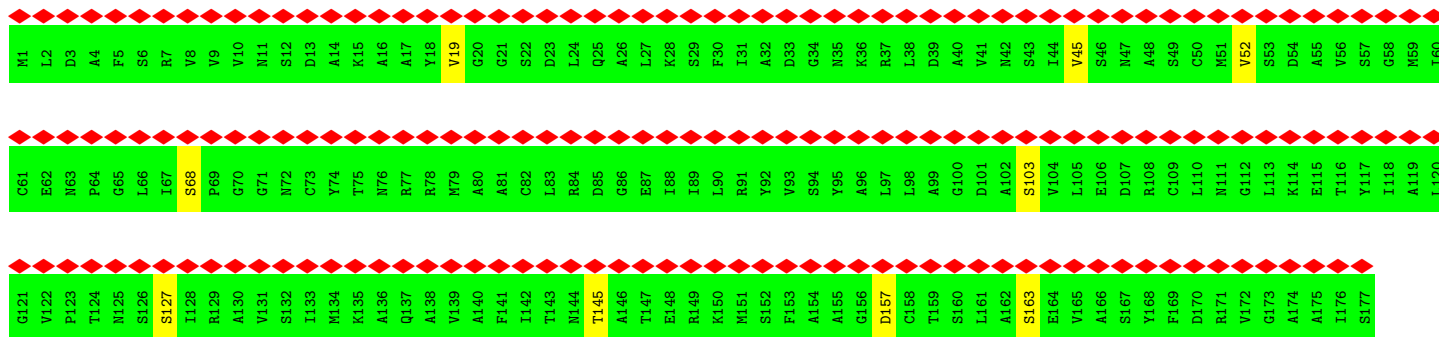
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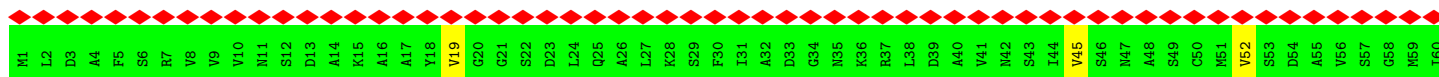
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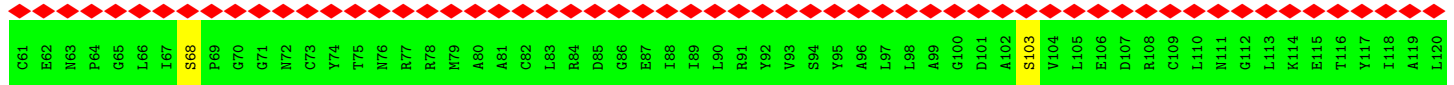


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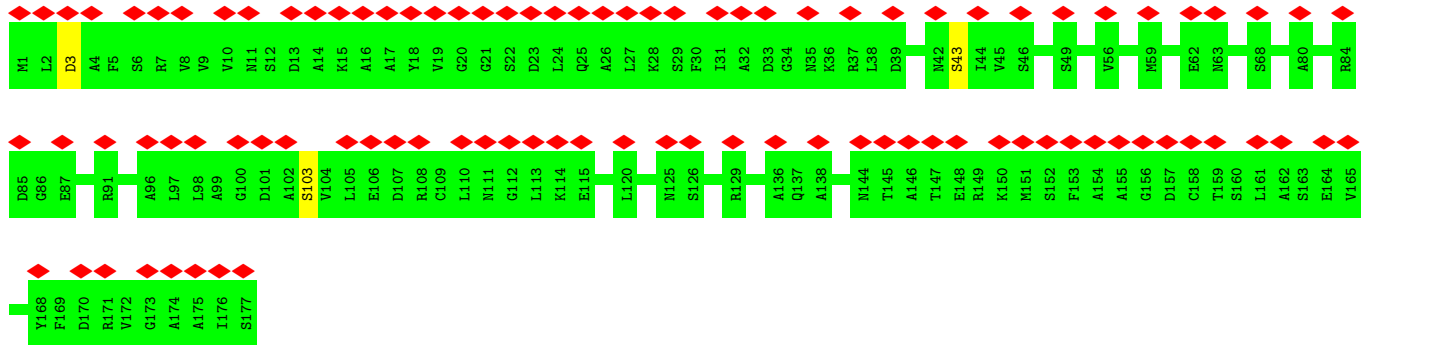


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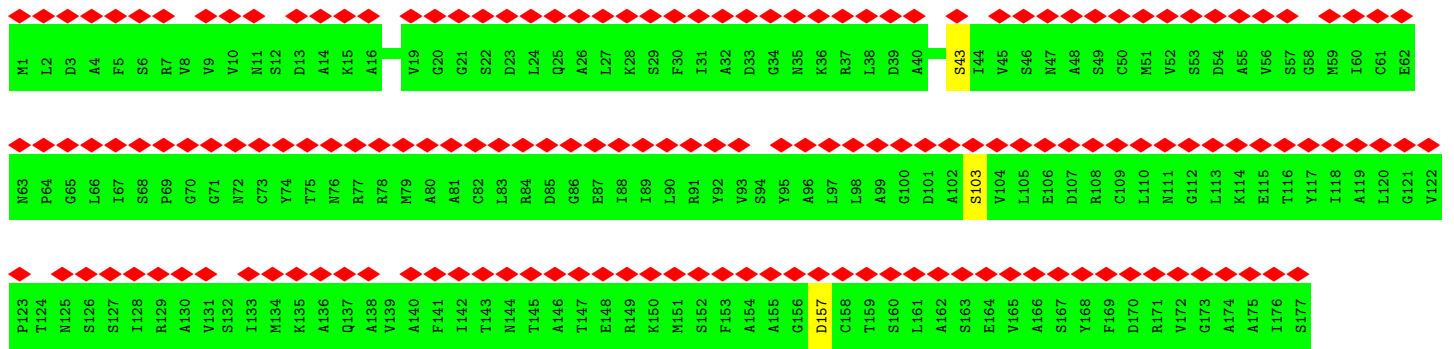




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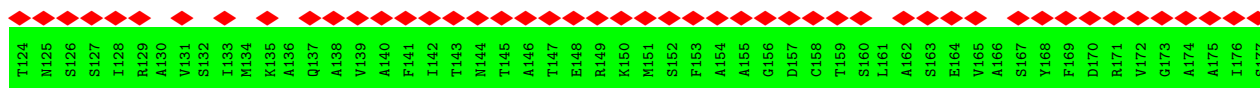


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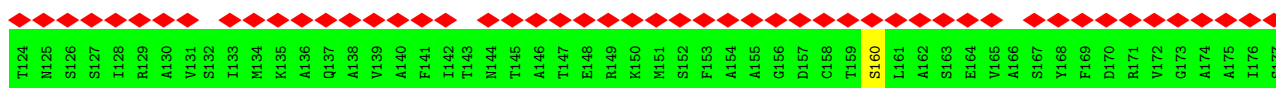
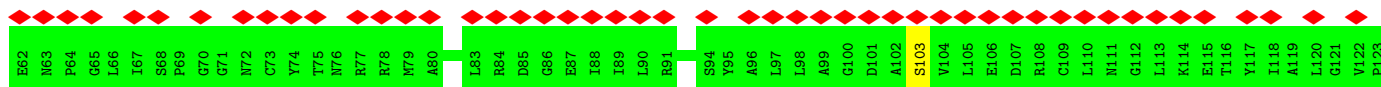
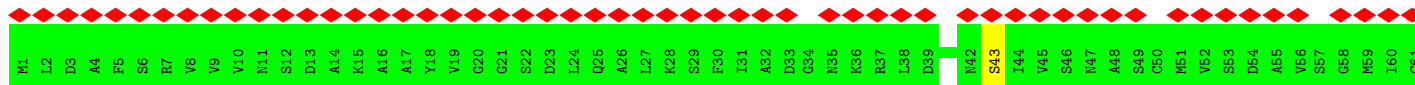


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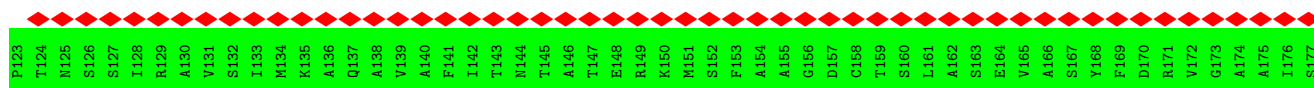
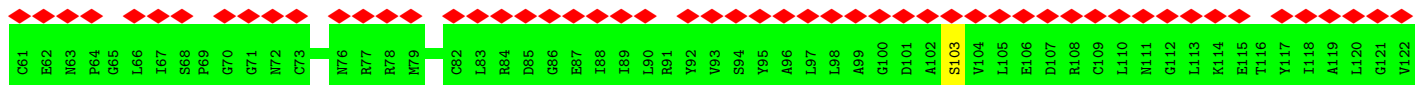




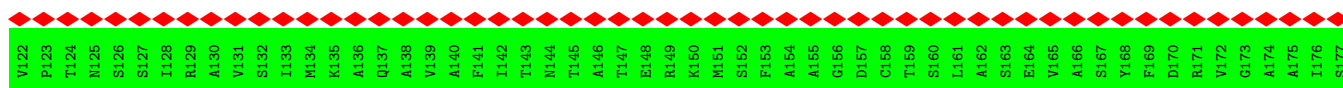
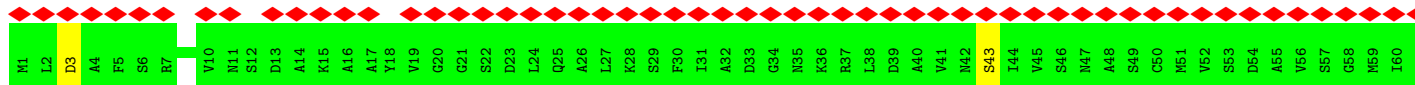
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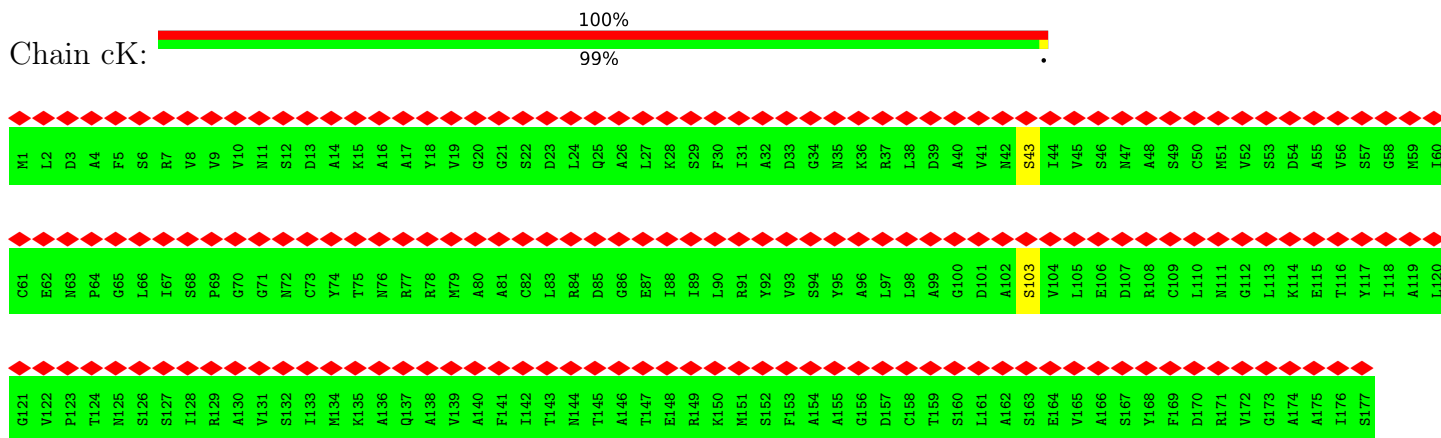
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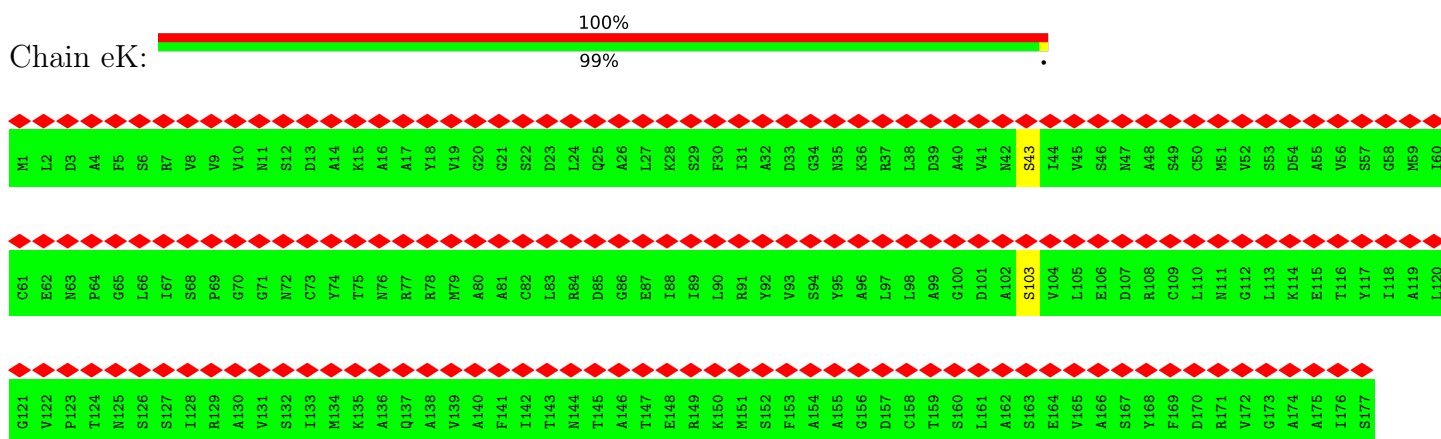
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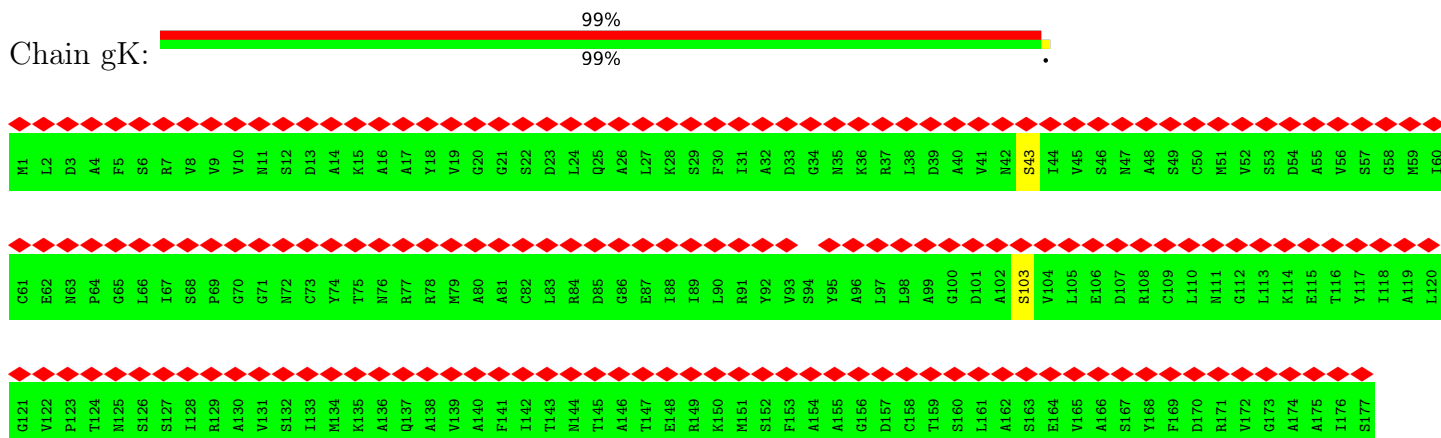
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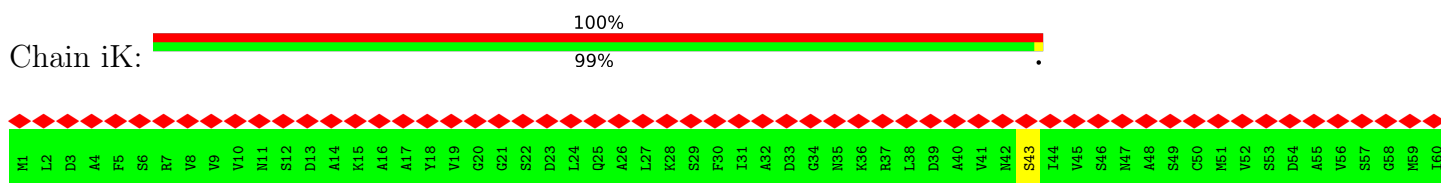
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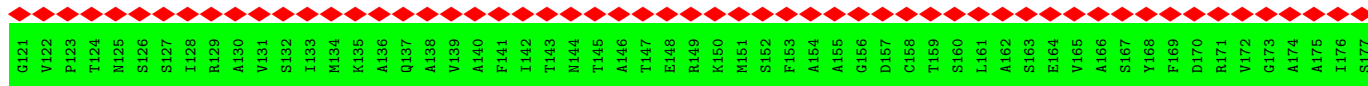
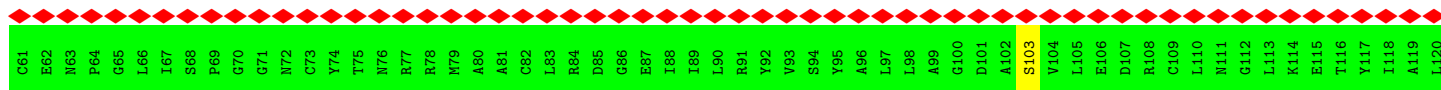


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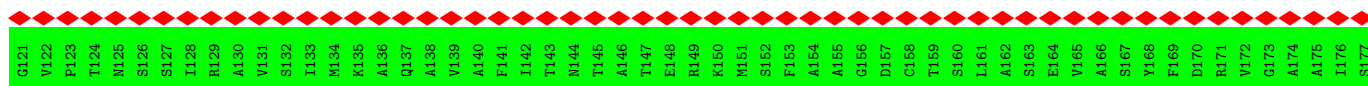
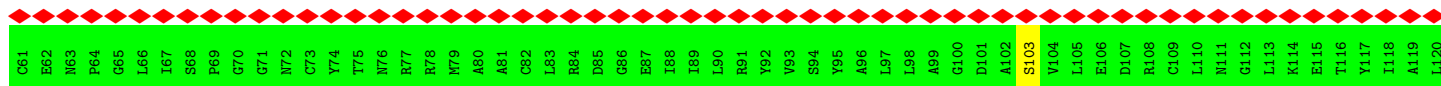
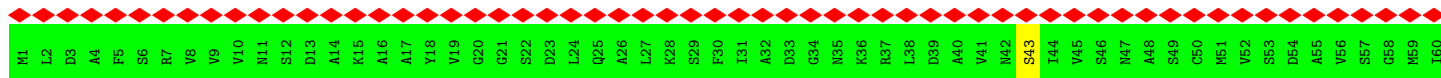


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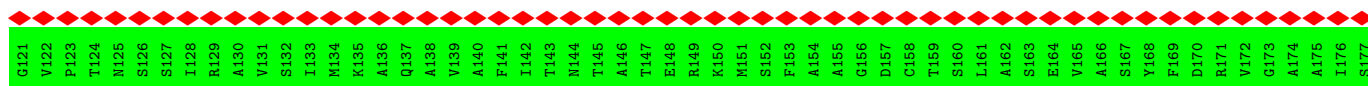
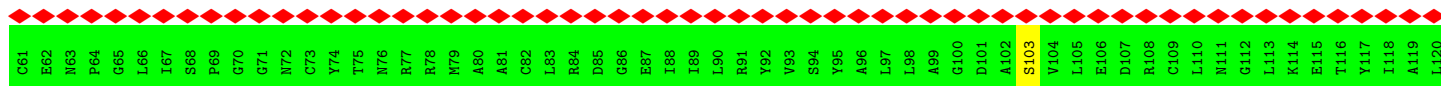




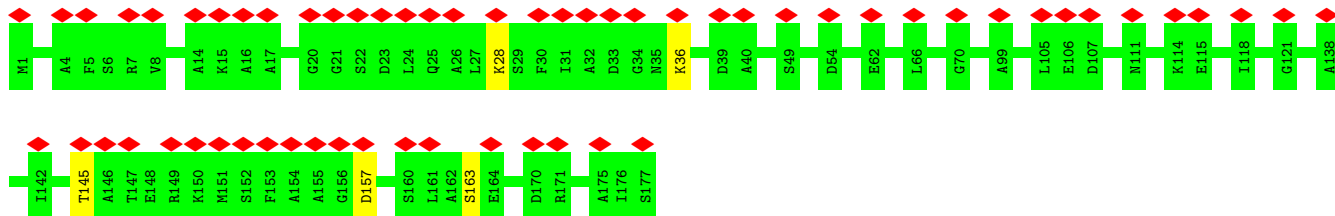
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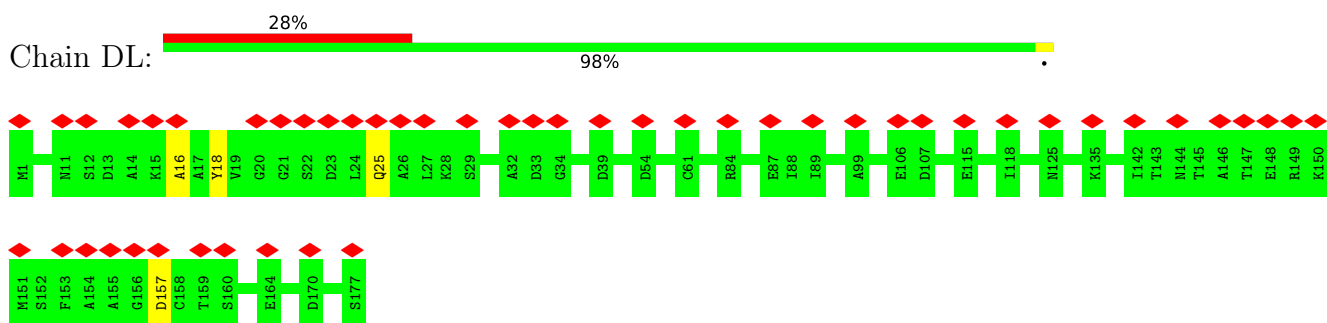
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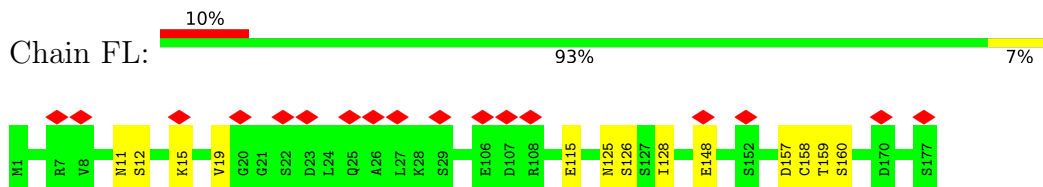
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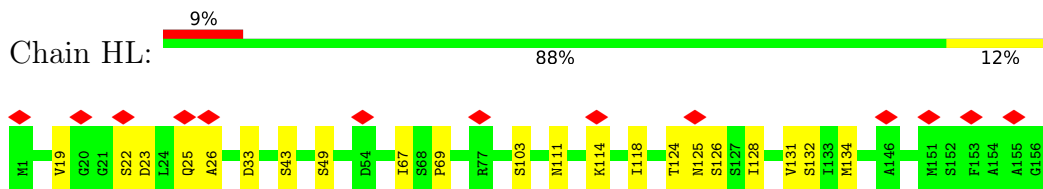
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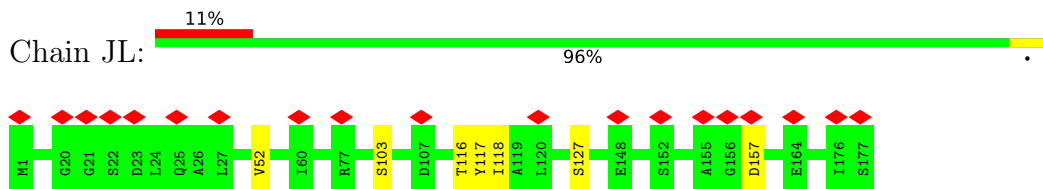
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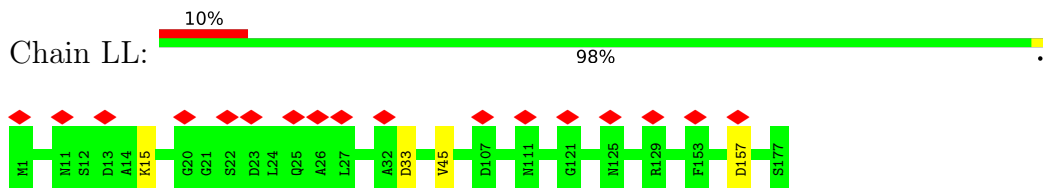
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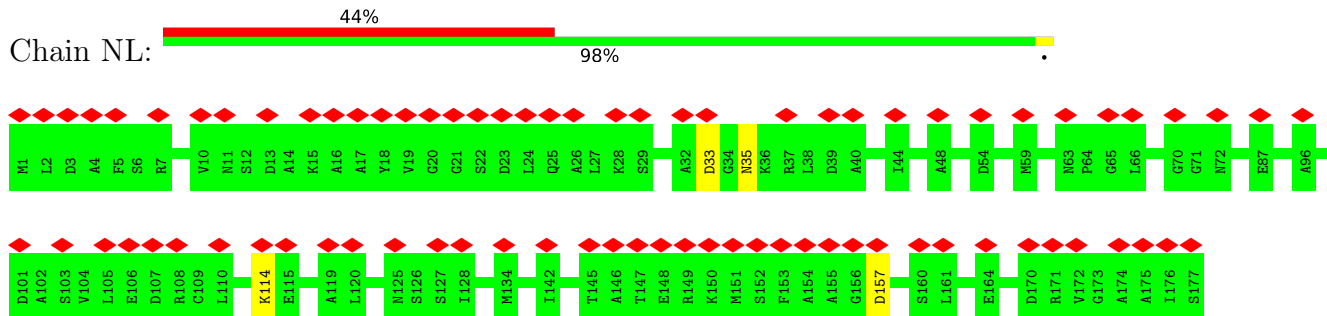
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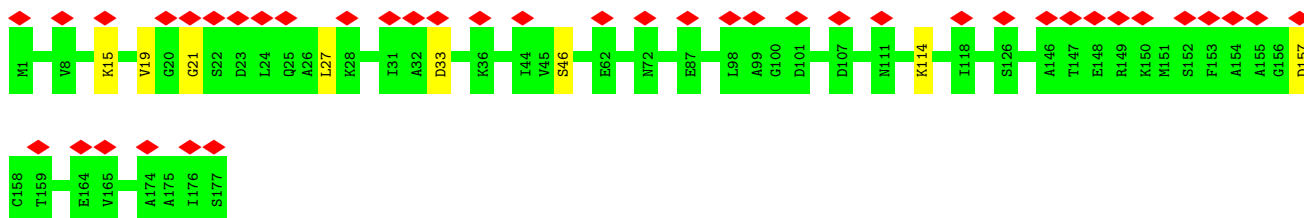
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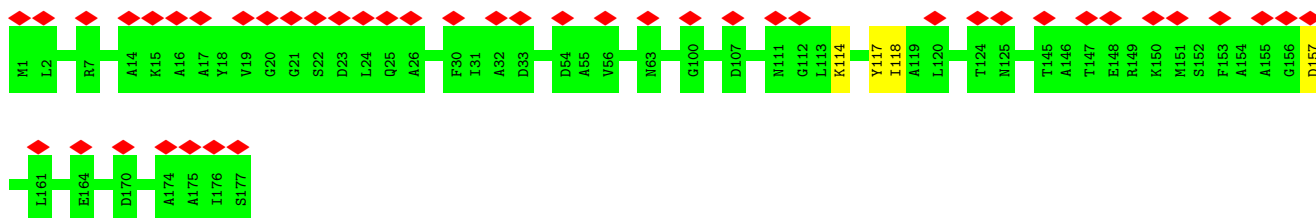
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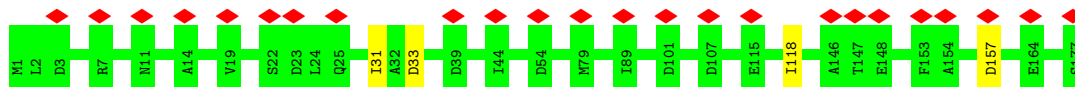
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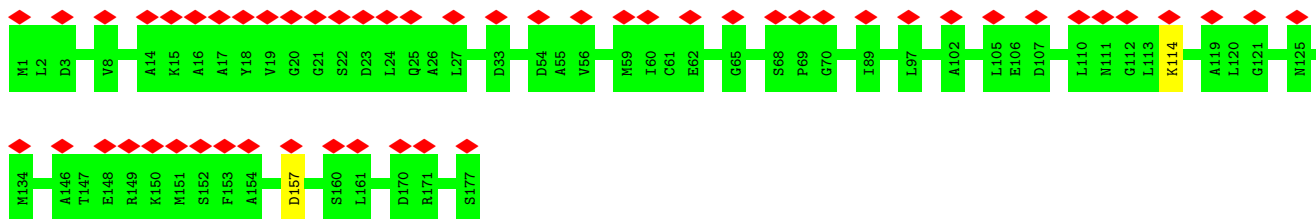
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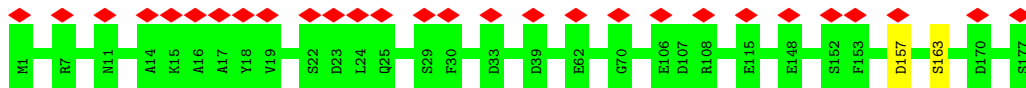
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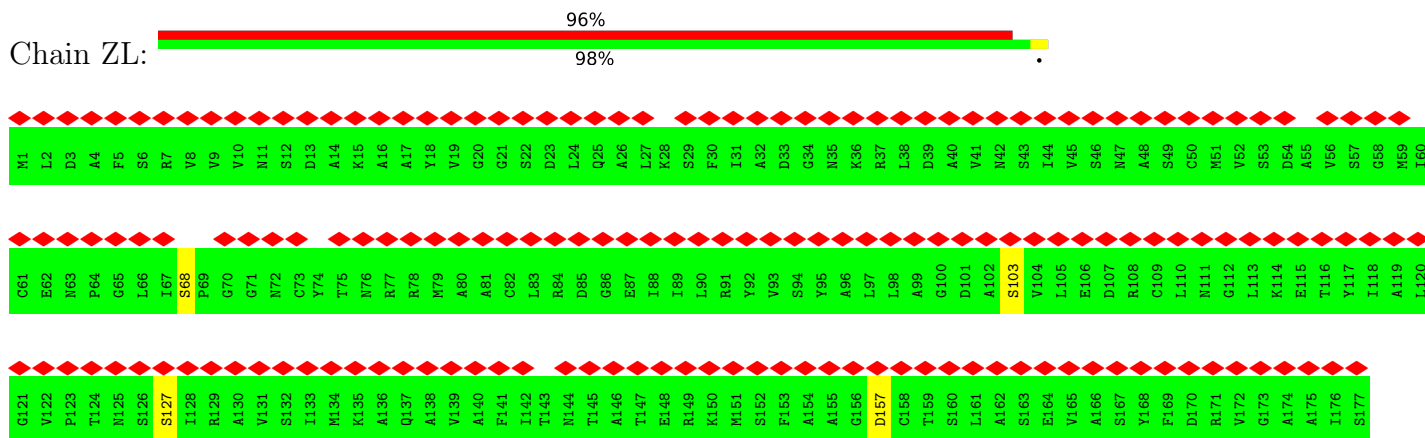
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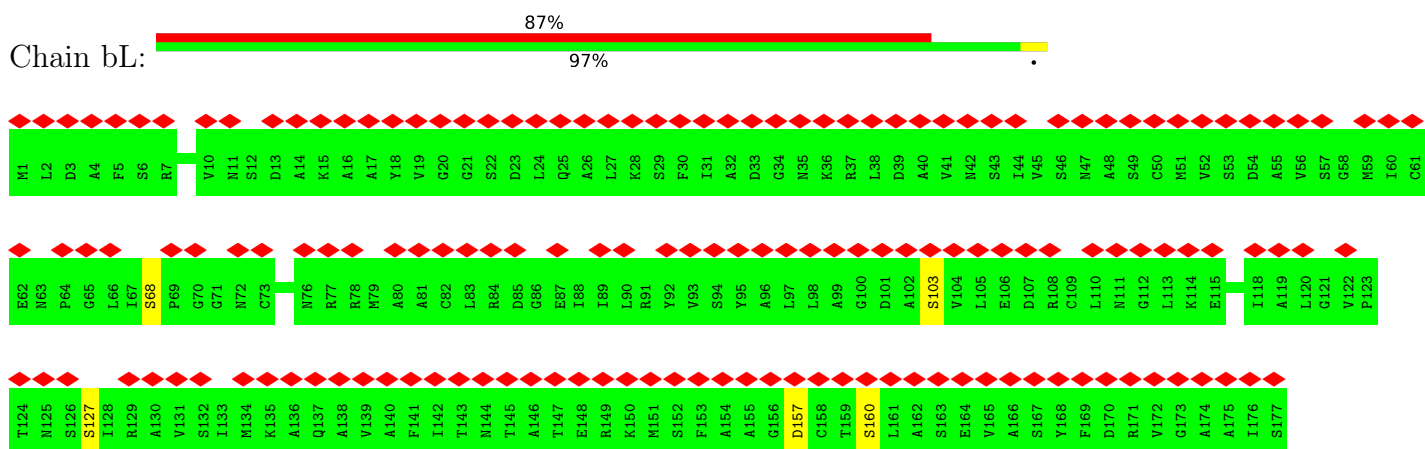
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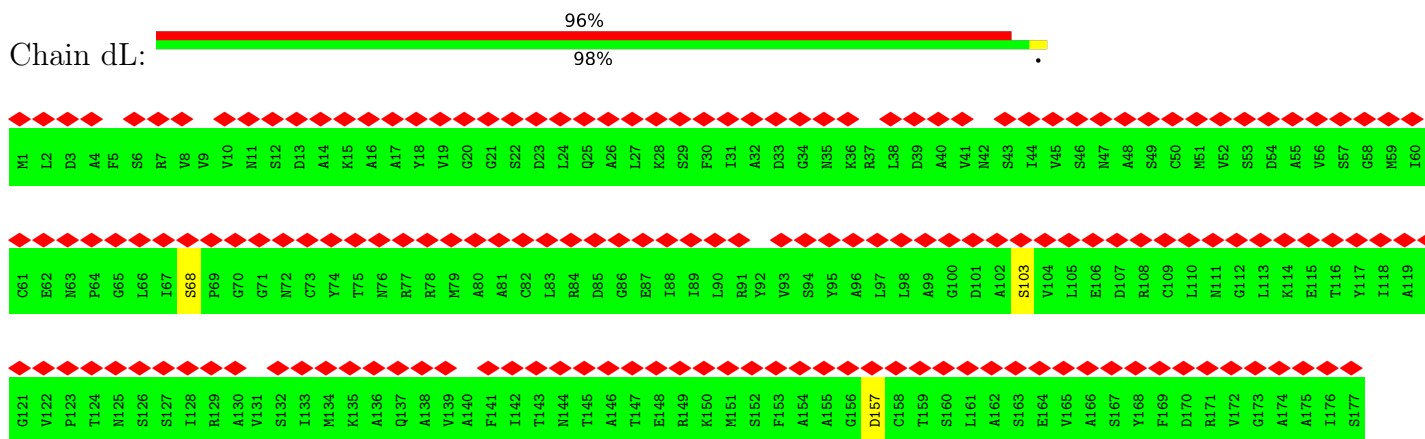
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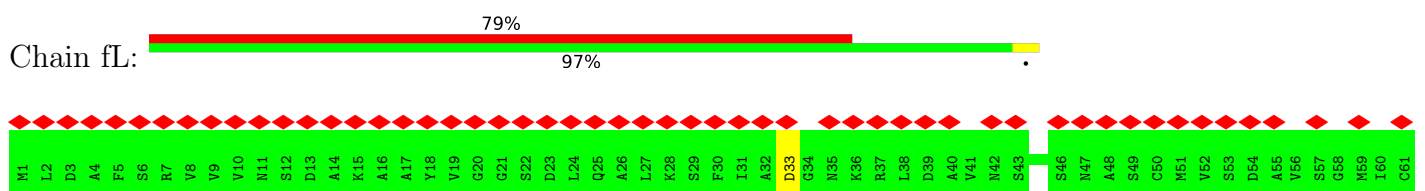
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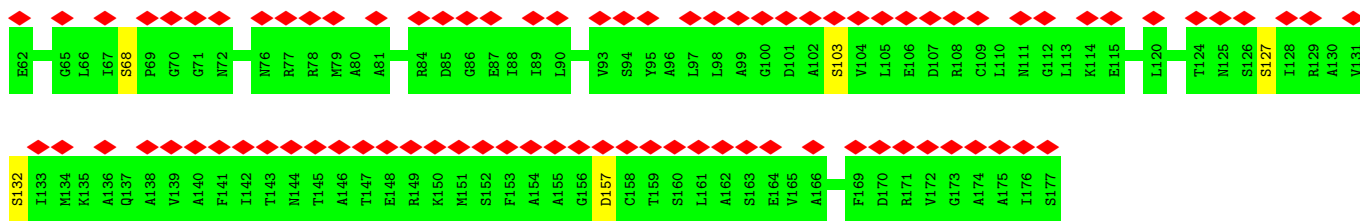


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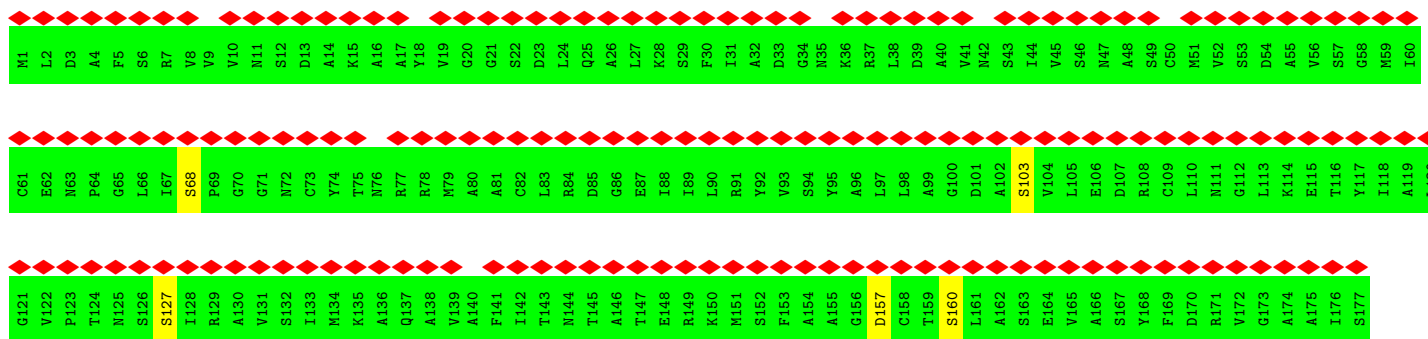


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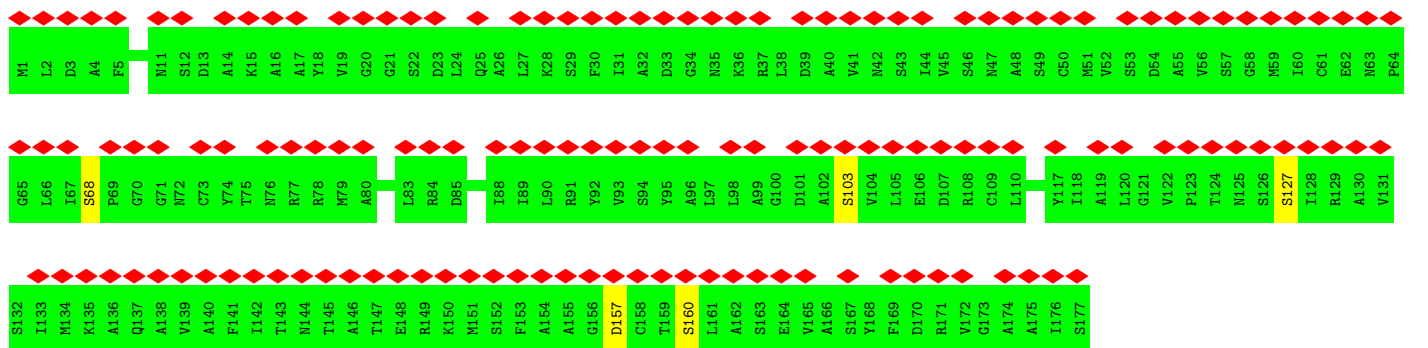
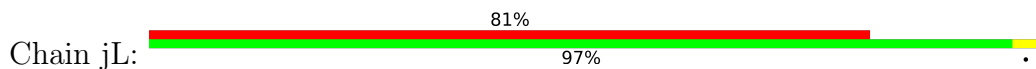




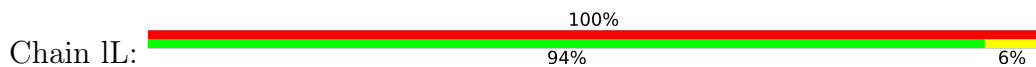
- Molecule 7: B-phycoerythrin beta chain

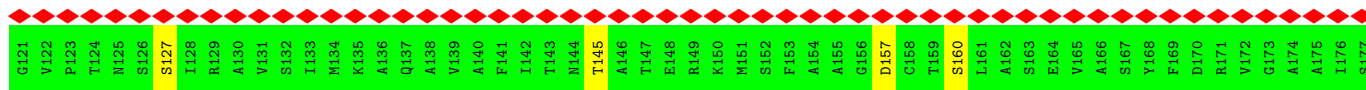


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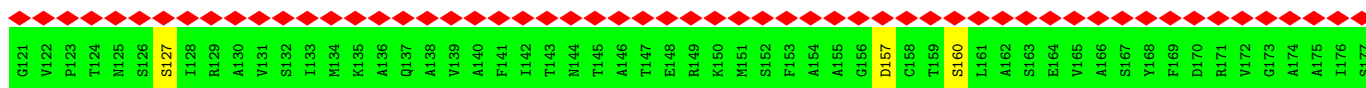
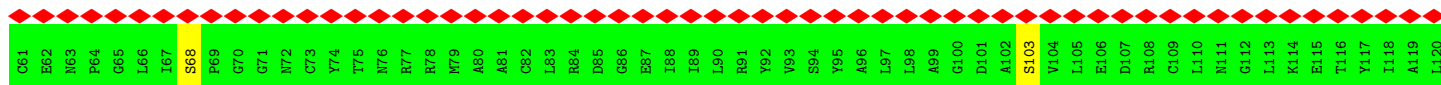


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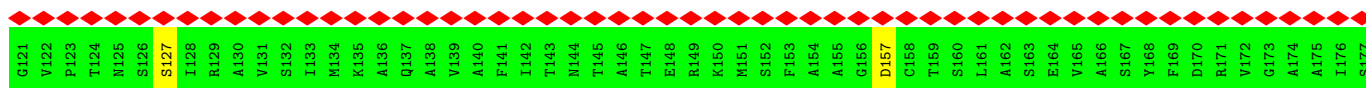
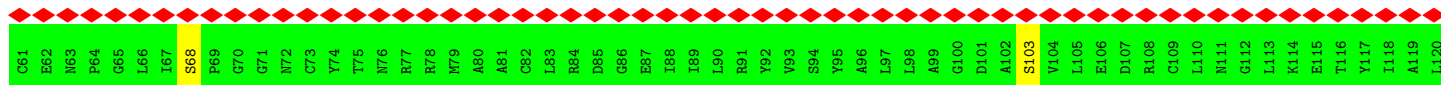
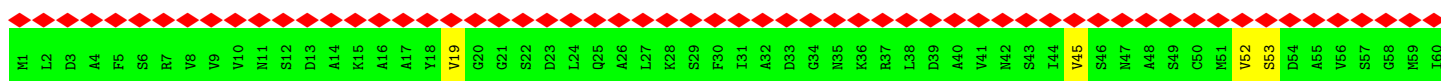




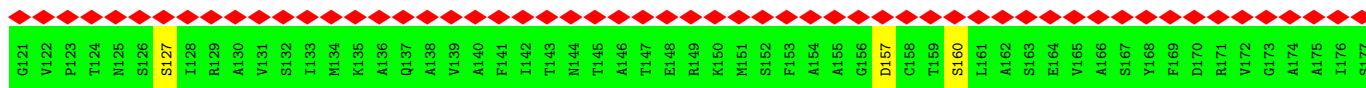
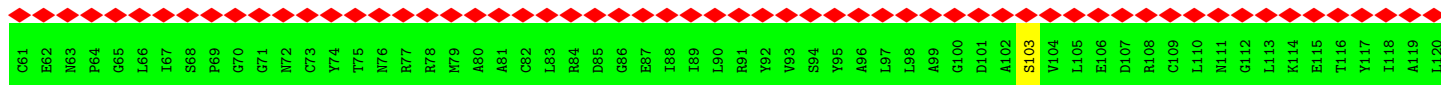
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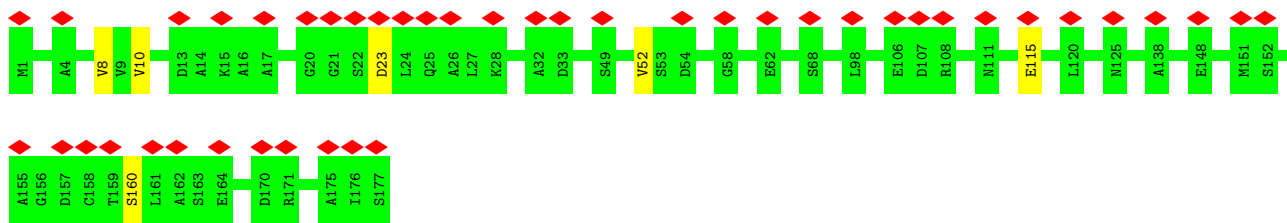
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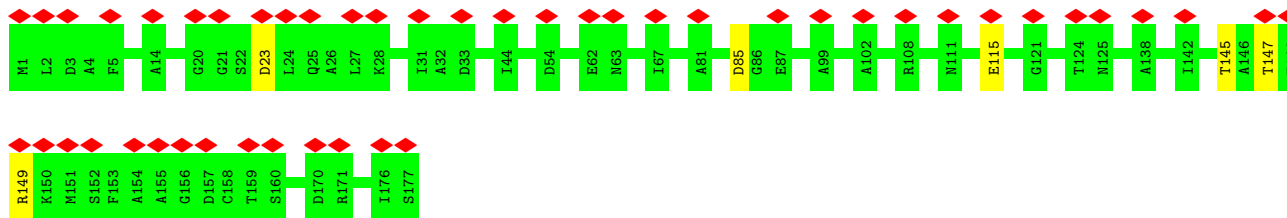
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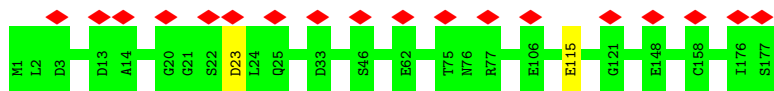
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain



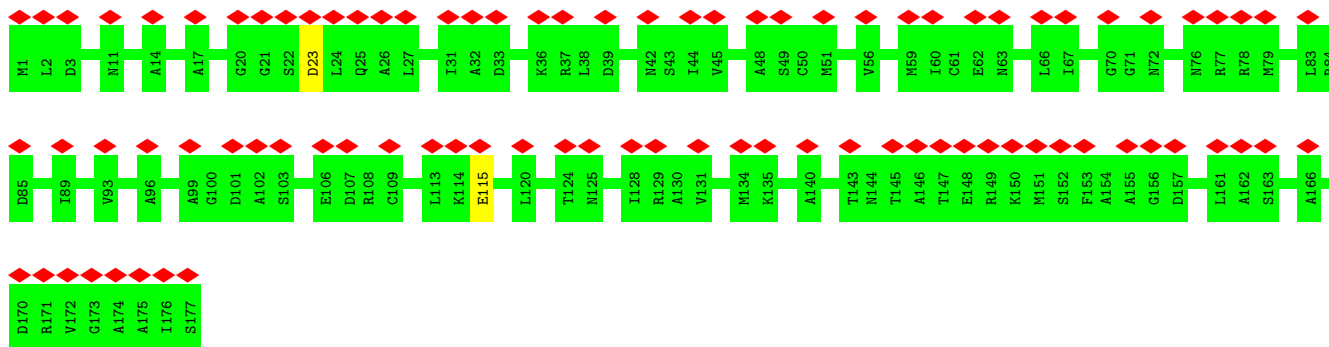
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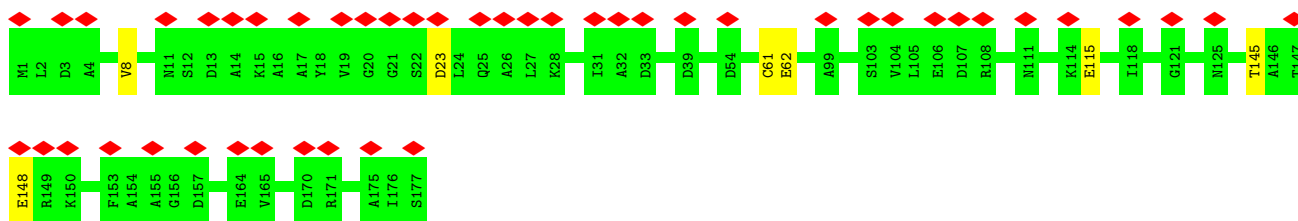
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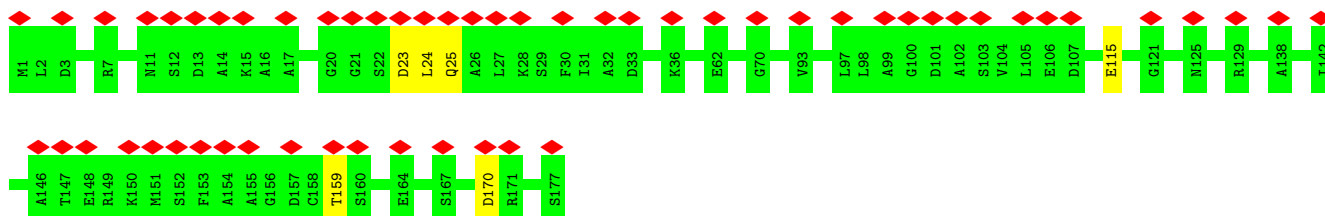
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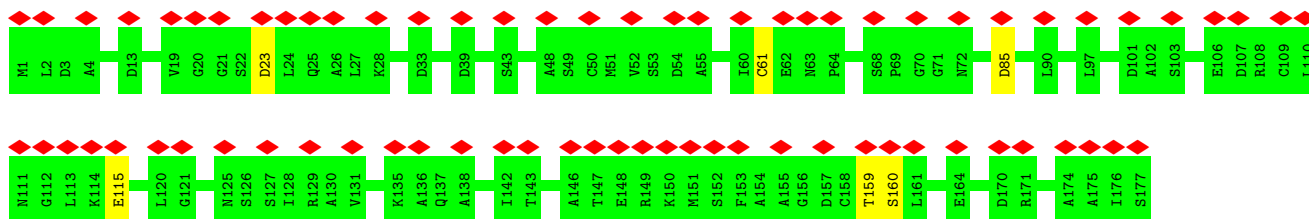
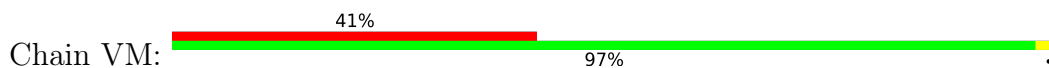
• Molecule 7: B-phycoerythrin beta chain



- Molecule 7: B-phycoerythrin beta chain



- Molecule 7: B-phycoerythrin beta chain



- Molecule 7: B-phycoerythrin beta chain

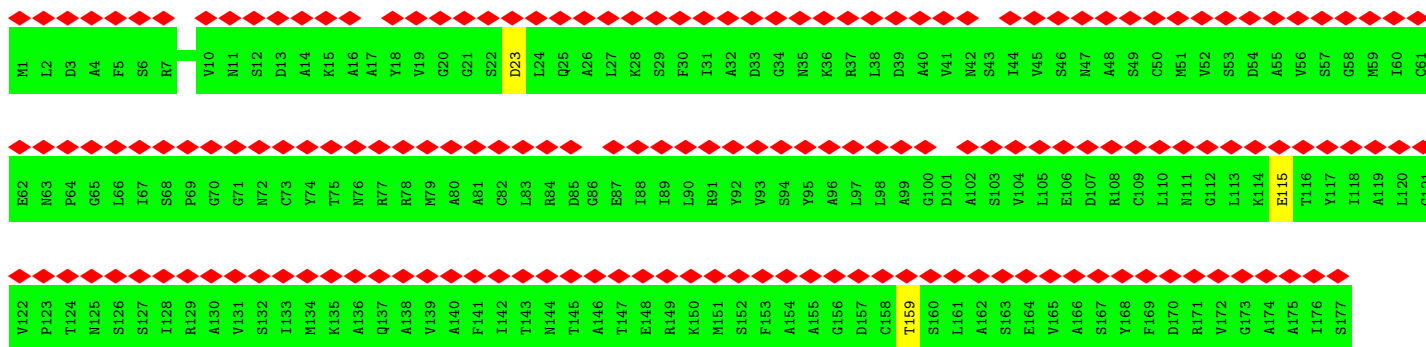


- Molecule 7: B-phycoerythrin beta chain

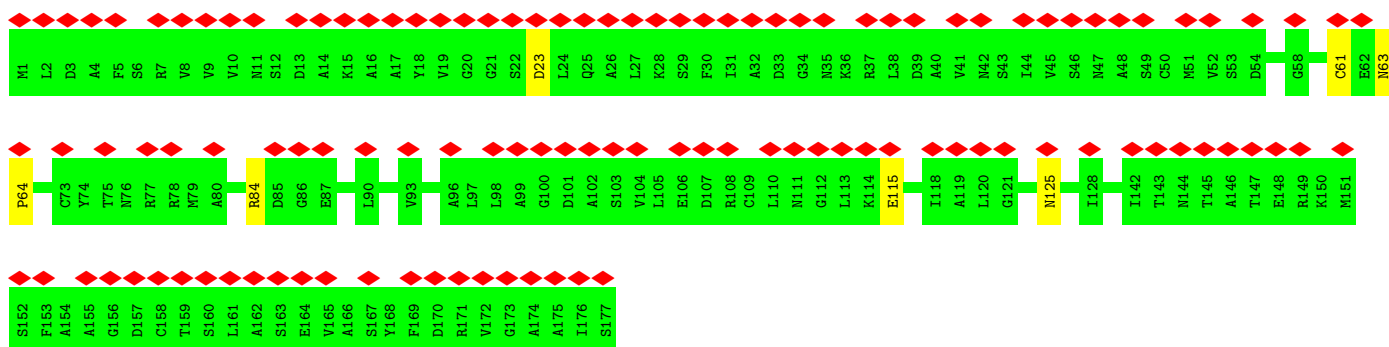


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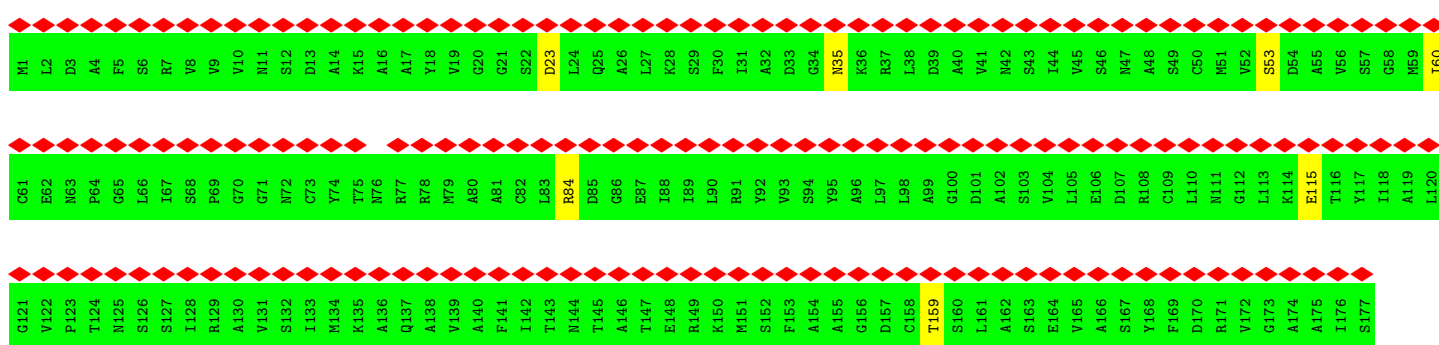




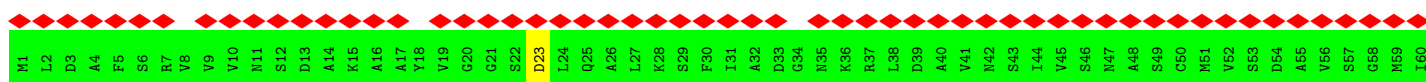
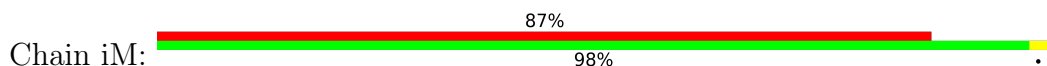
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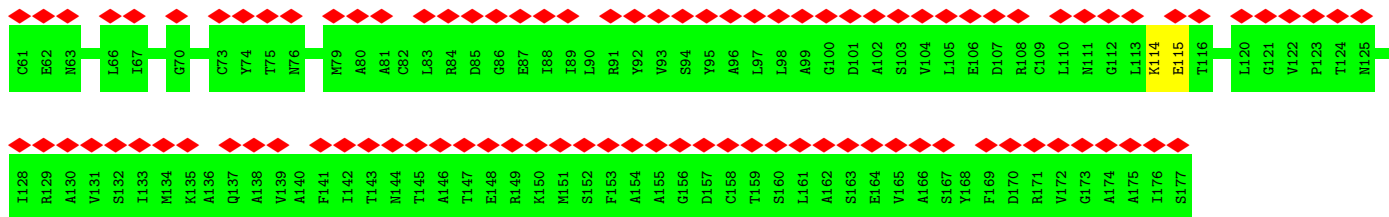


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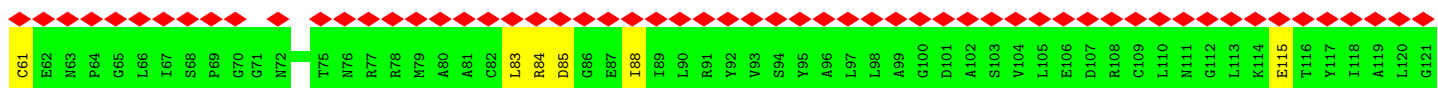
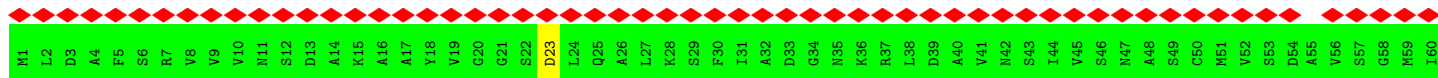


• Molecule 7: B-phycoerythrin beta chain

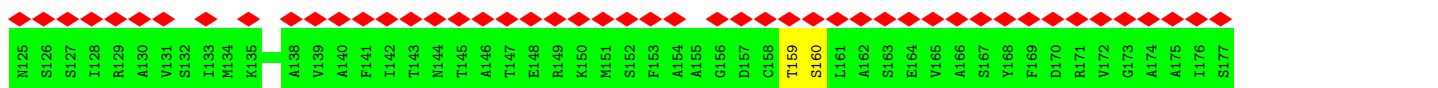
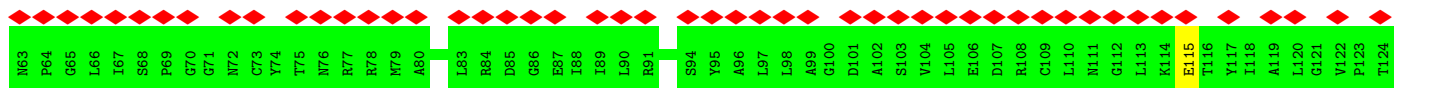
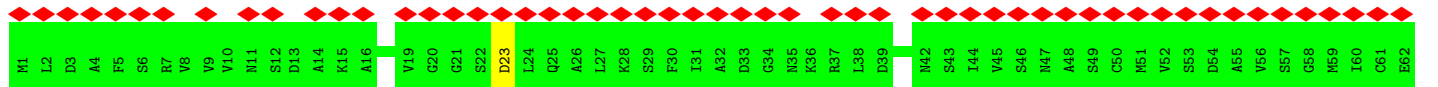




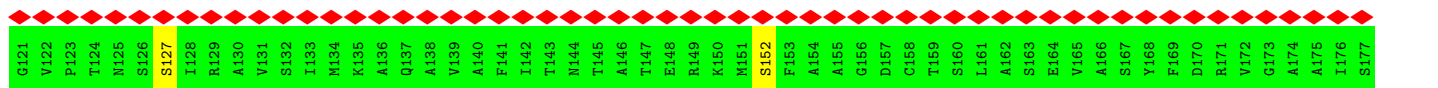
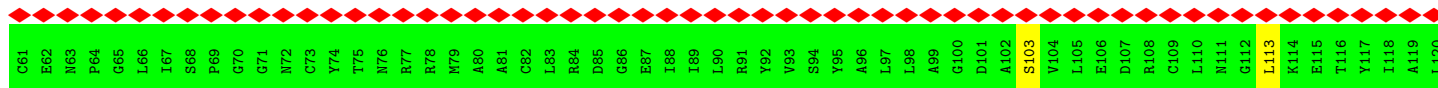
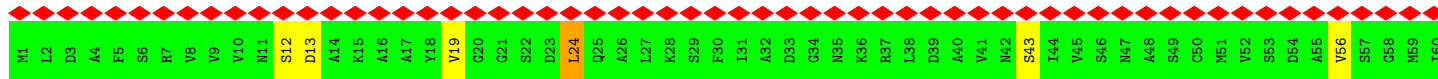
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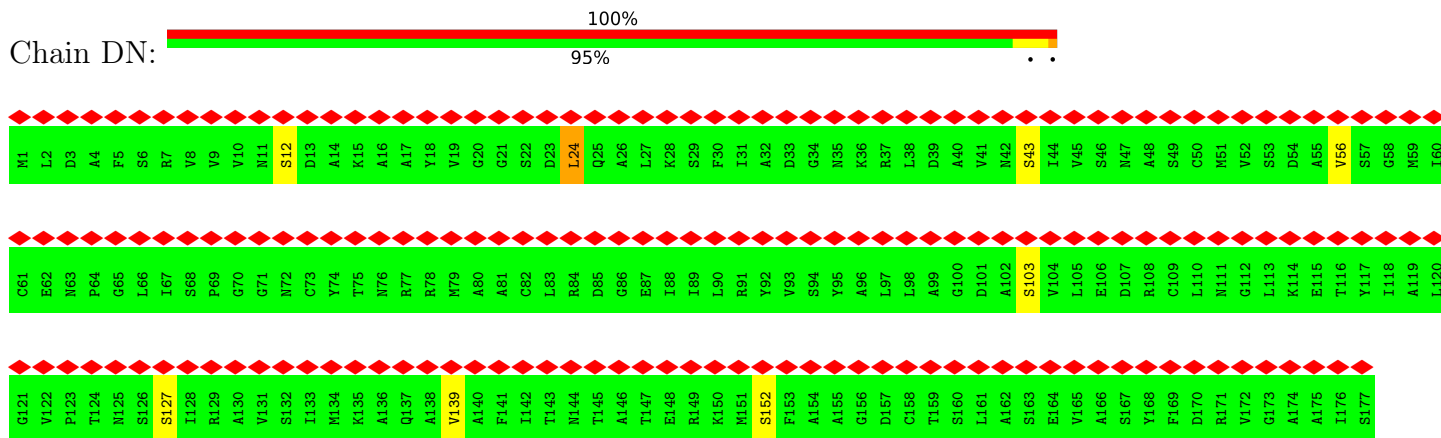
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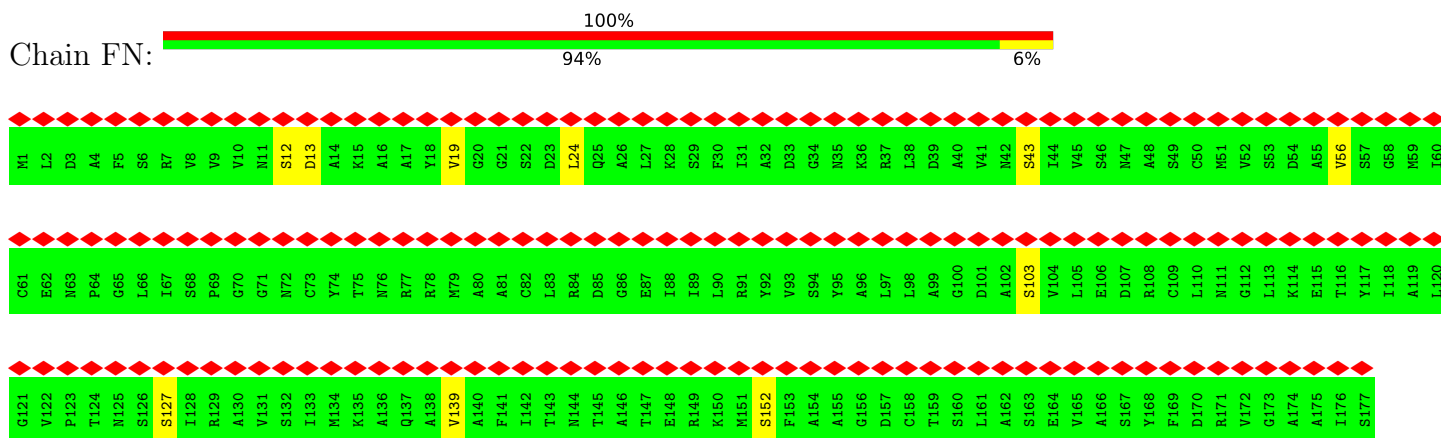
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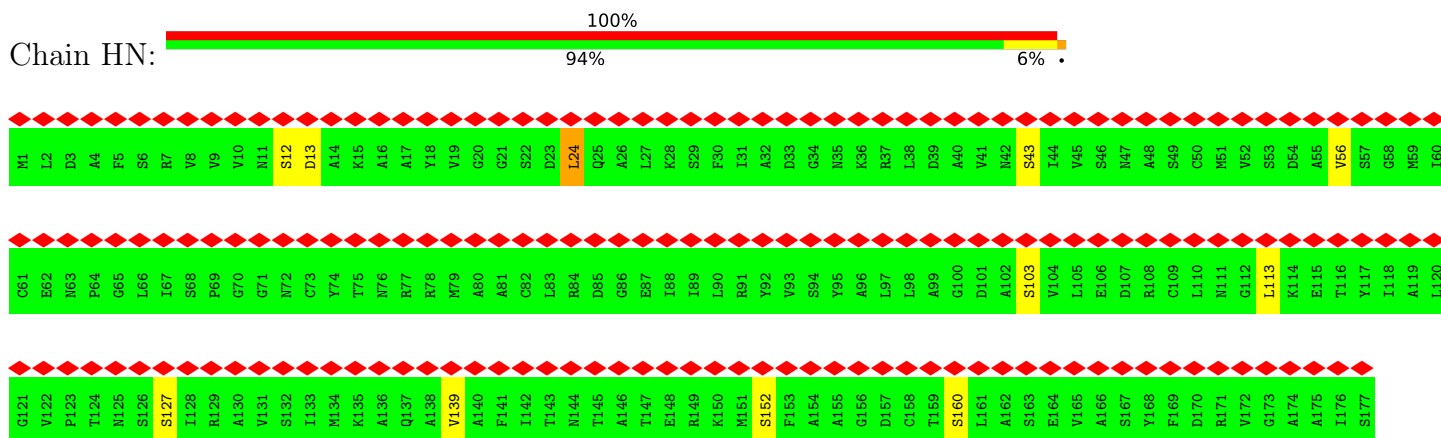
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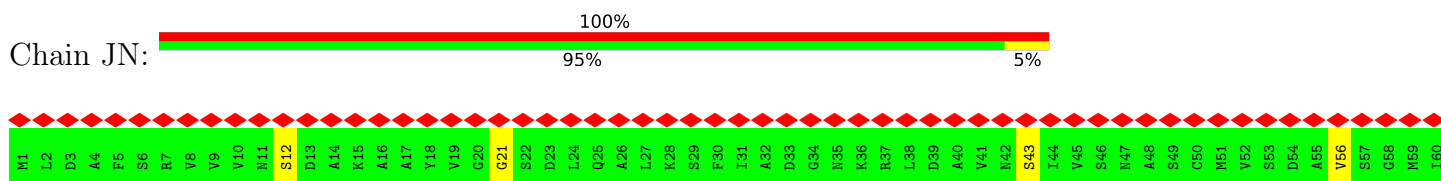
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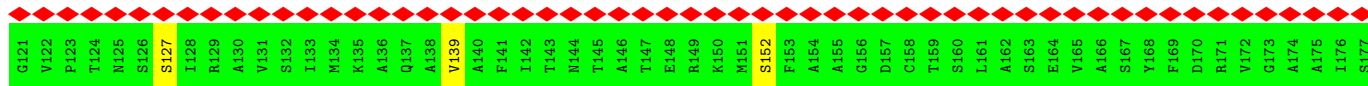
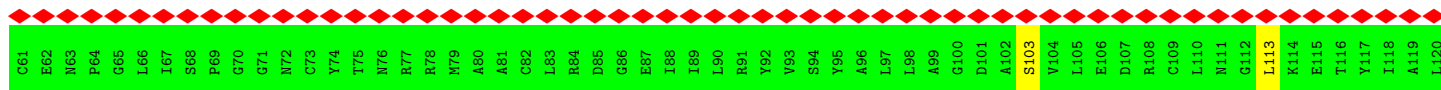


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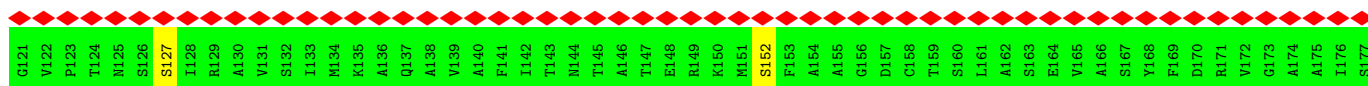
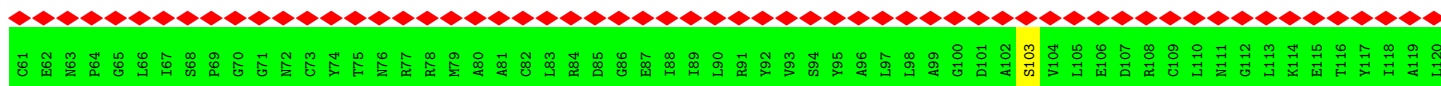


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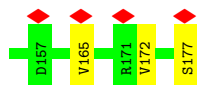
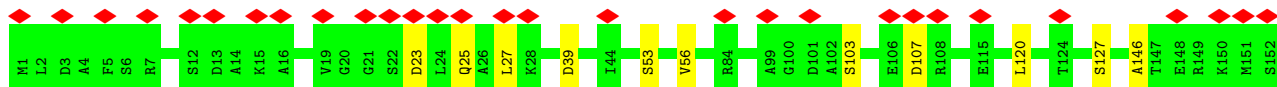
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain

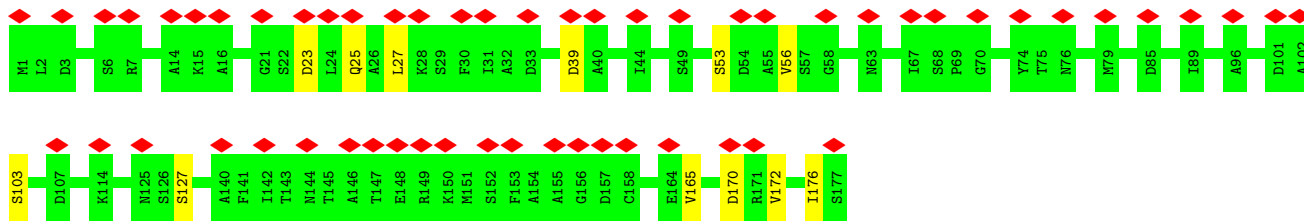


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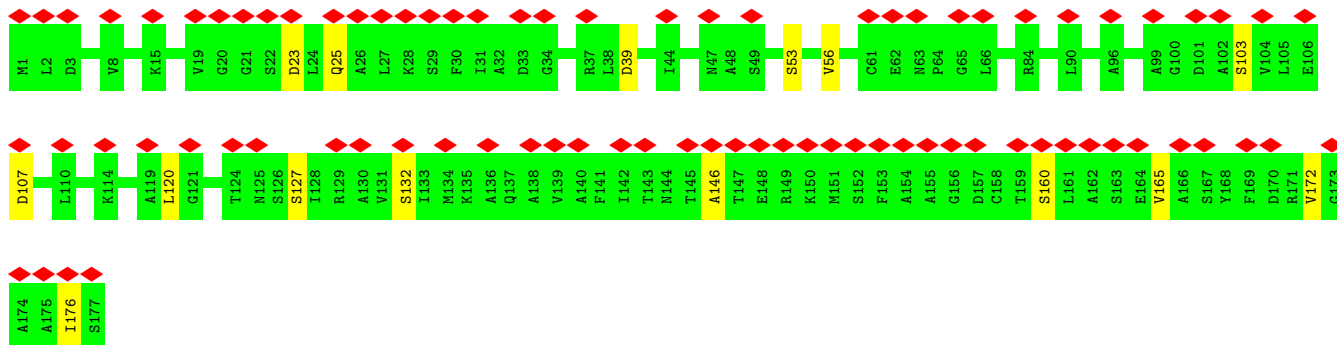


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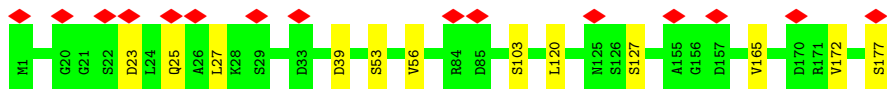




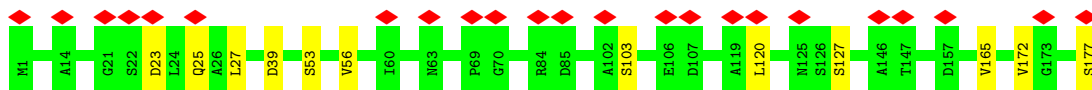
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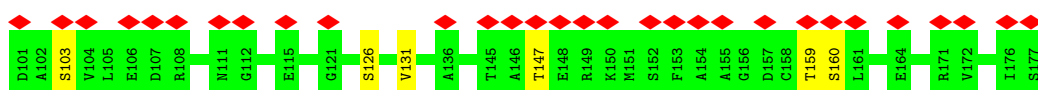
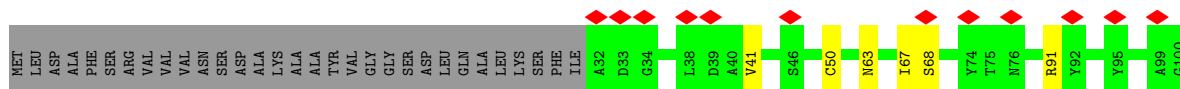
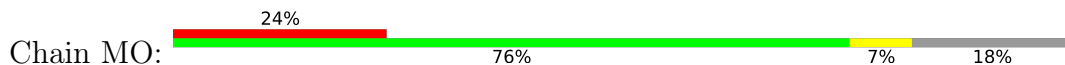
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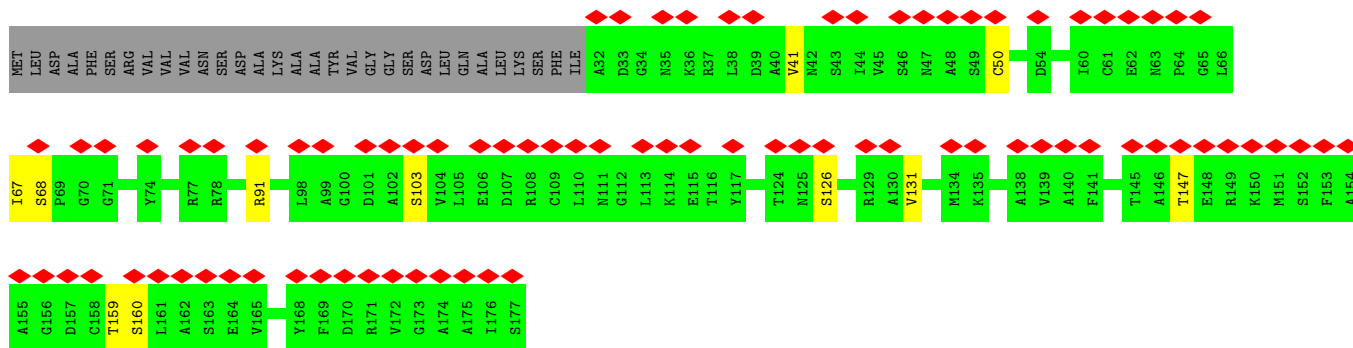
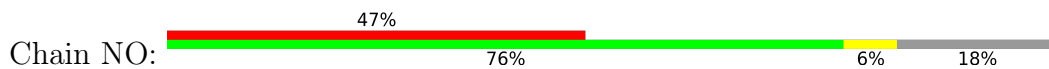
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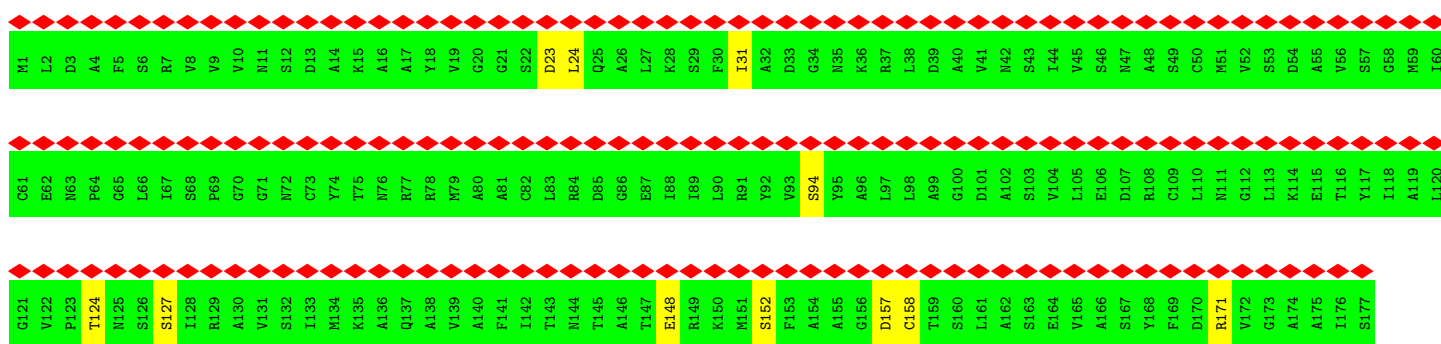
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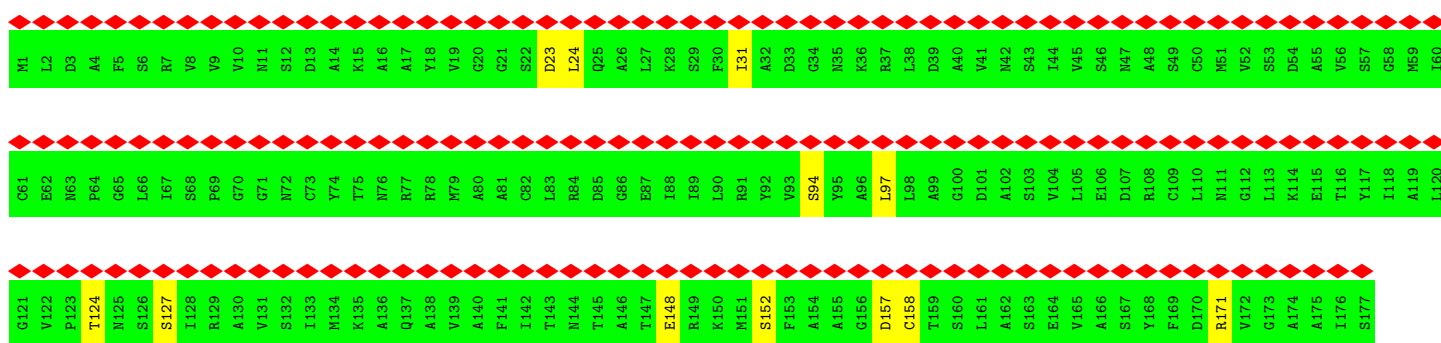
• Molecule 7: B-phycoerythrin beta chain



• Molecule 7: B-phycoerythrin beta chain

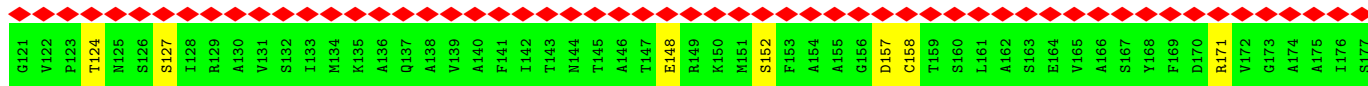
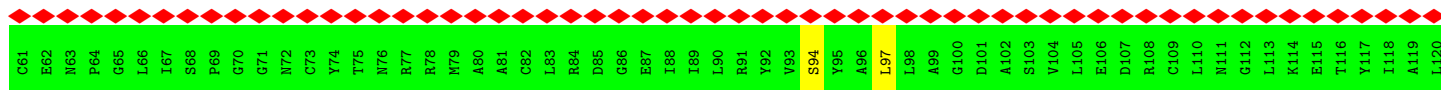


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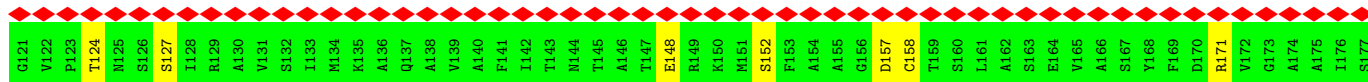
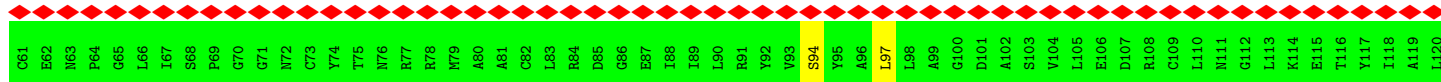
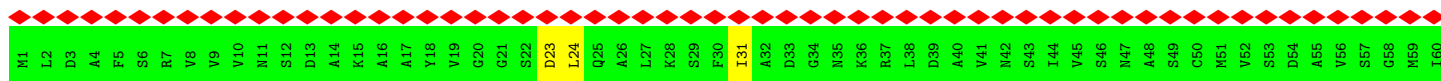


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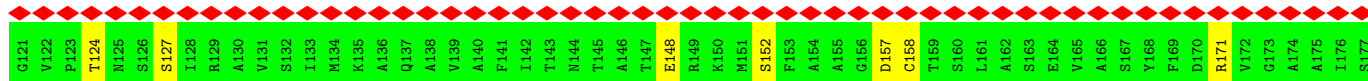
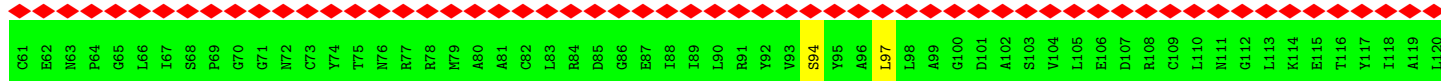
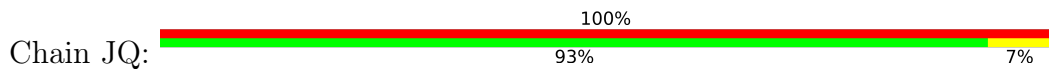




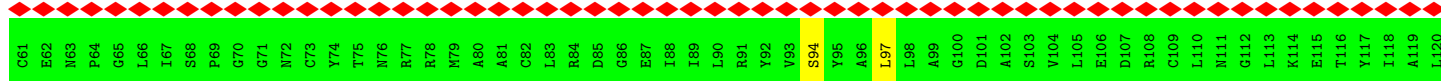
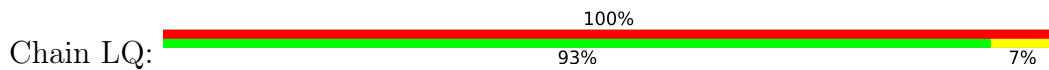
• Molecule 7: B-phycoerythrin beta chain



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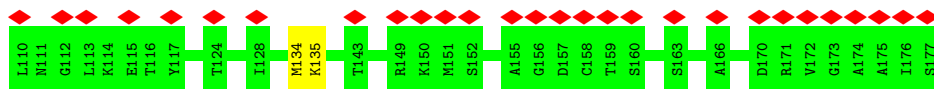
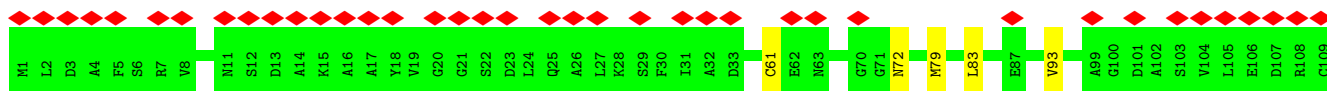
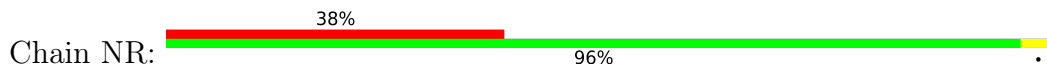


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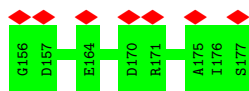
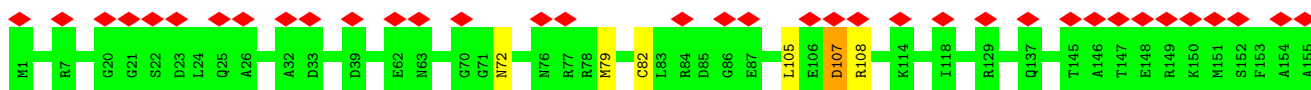




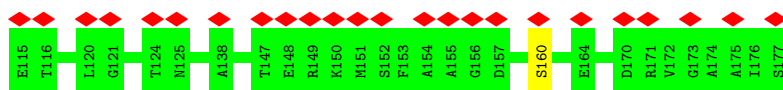
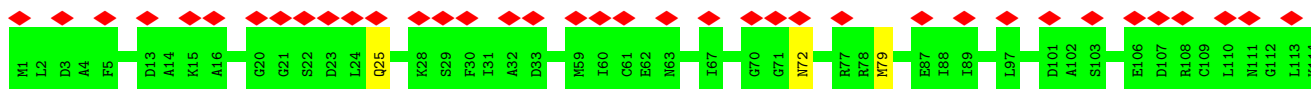
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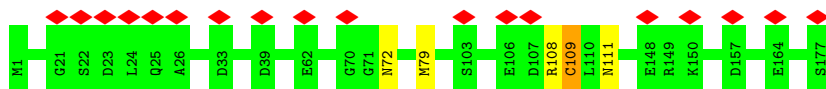
- Molecule 7: B-phycoerythrin beta chain



- Molecule 7: B-phycoerythrin beta chain

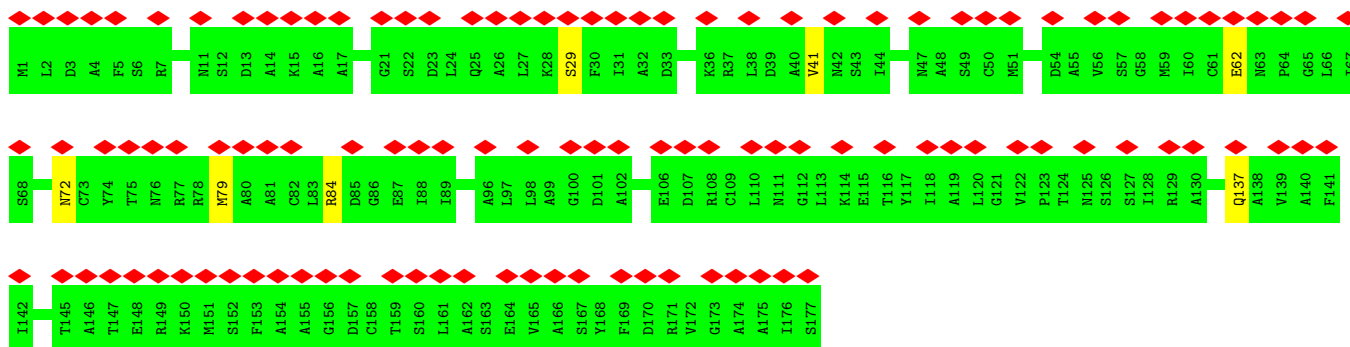


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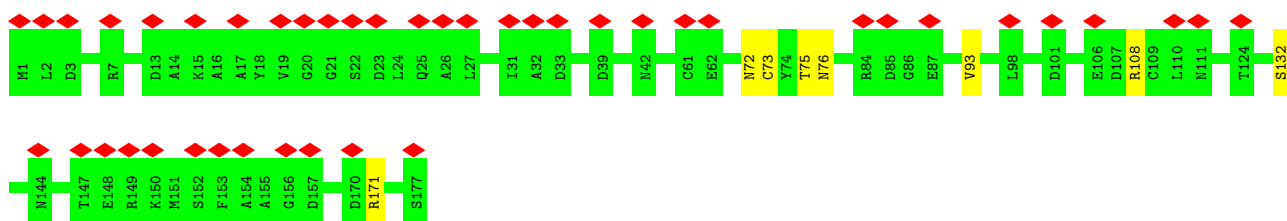


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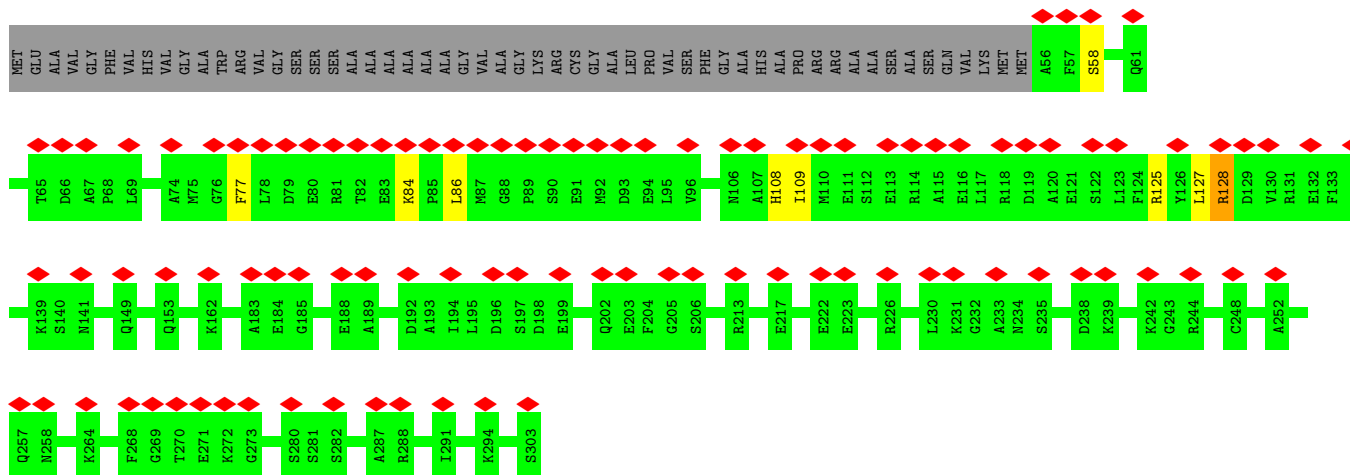
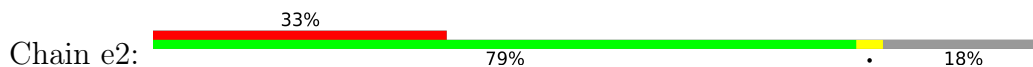




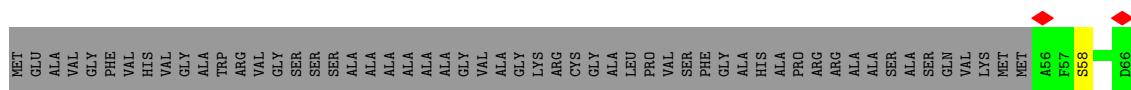
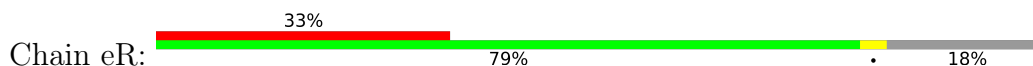
• Molecule 7: B-phycoerythrin beta chain

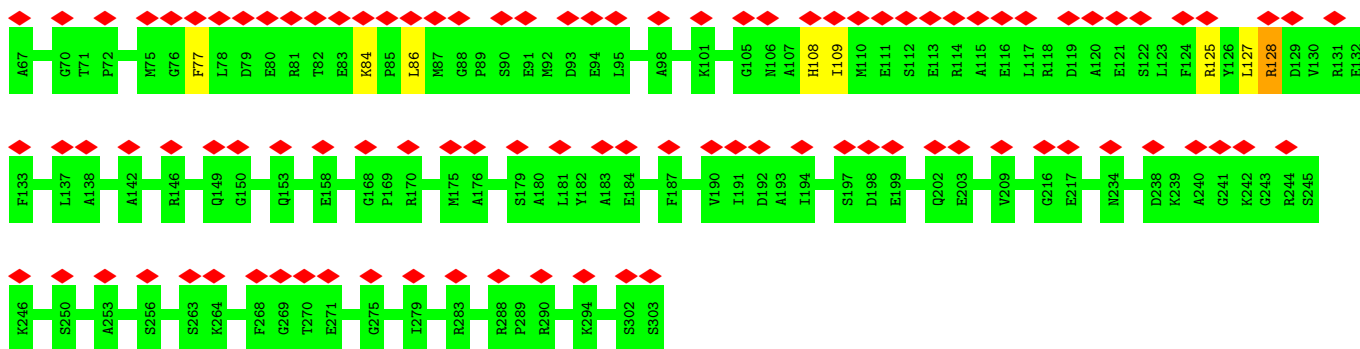


• Molecule 8: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

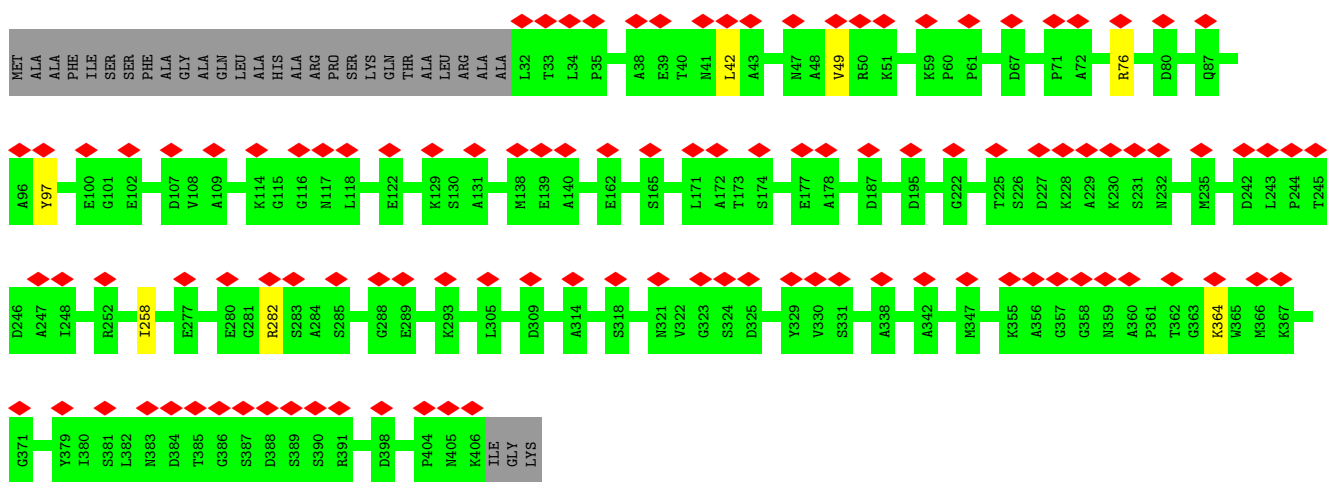


• Molecule 8: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod

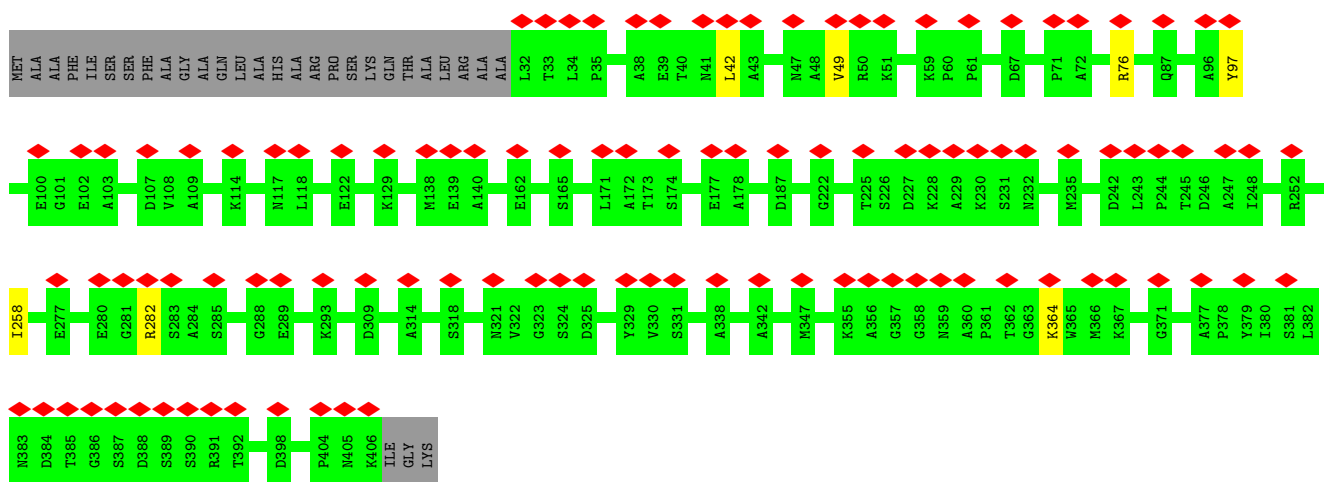




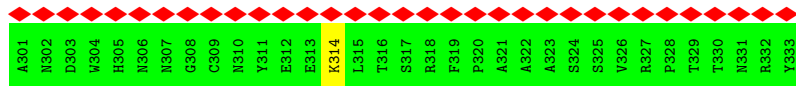
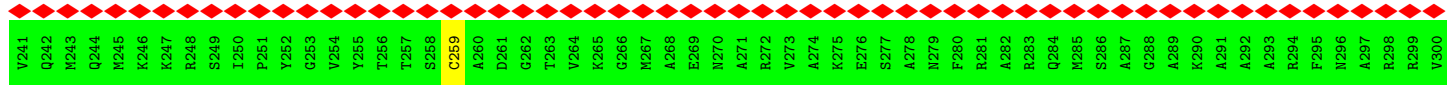
• Molecule 9: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



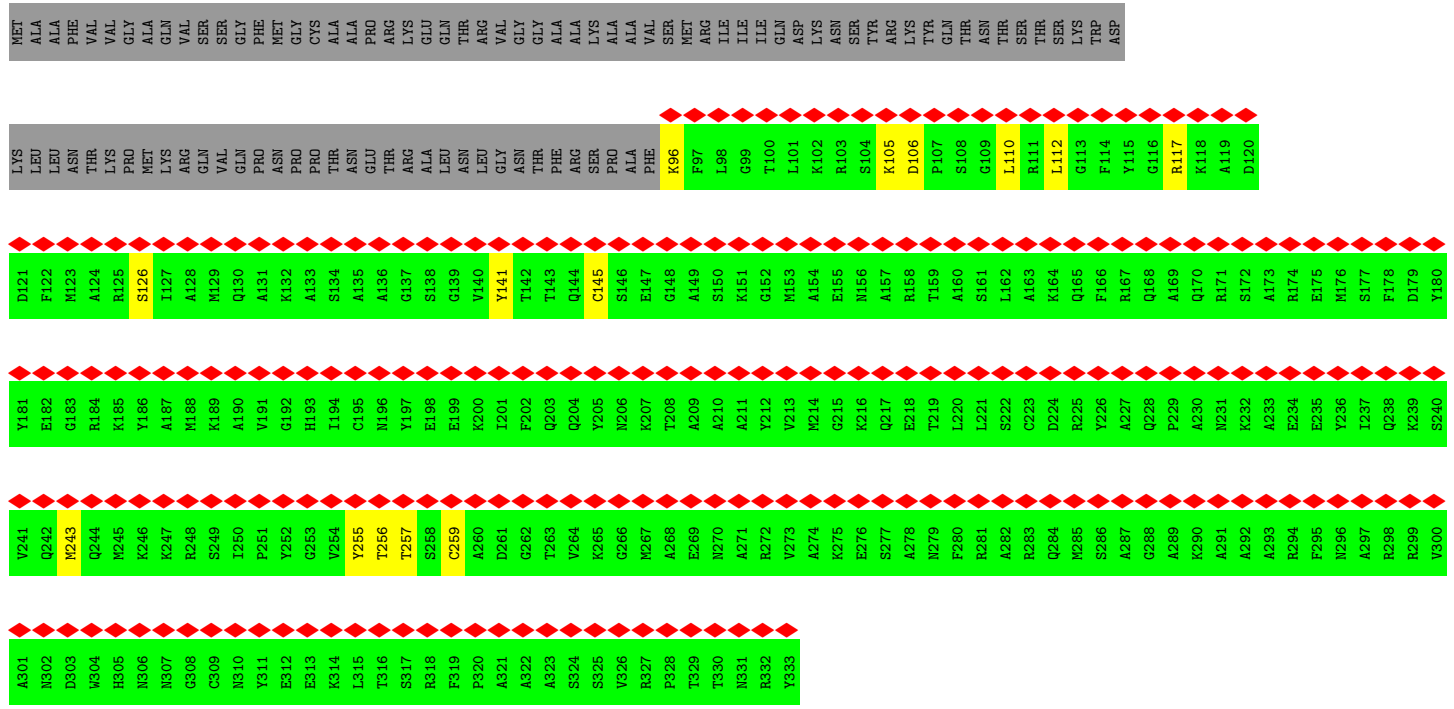
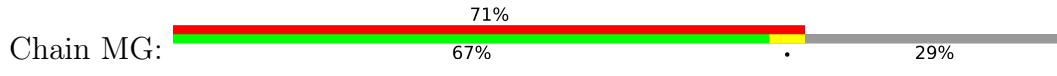
• Molecule 9: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod



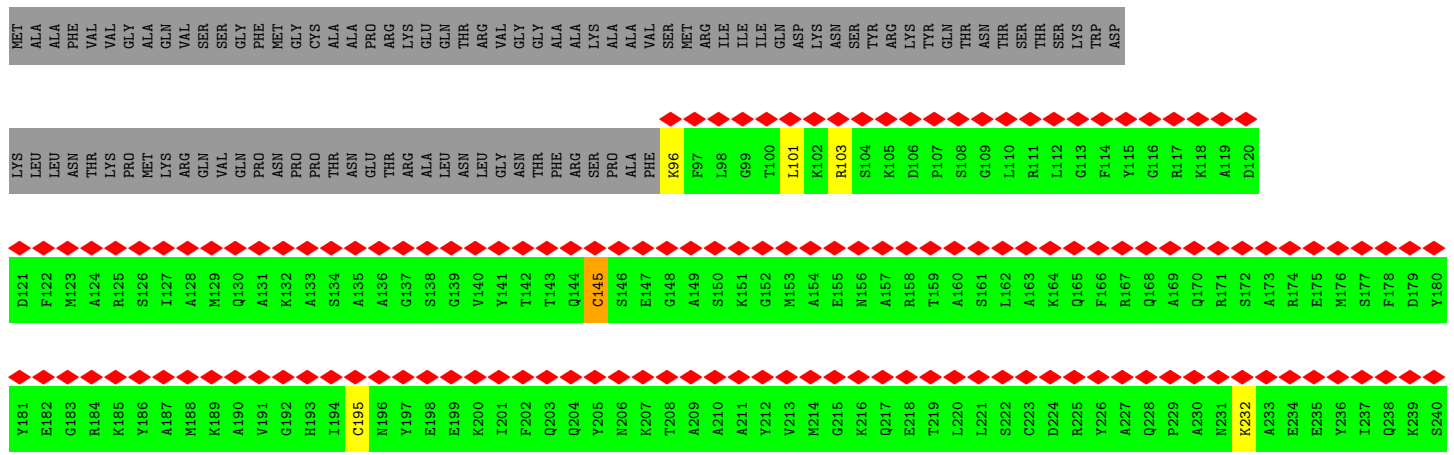
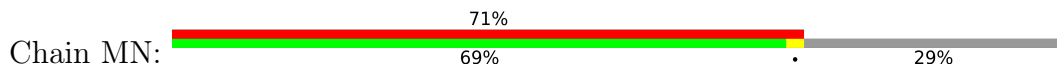
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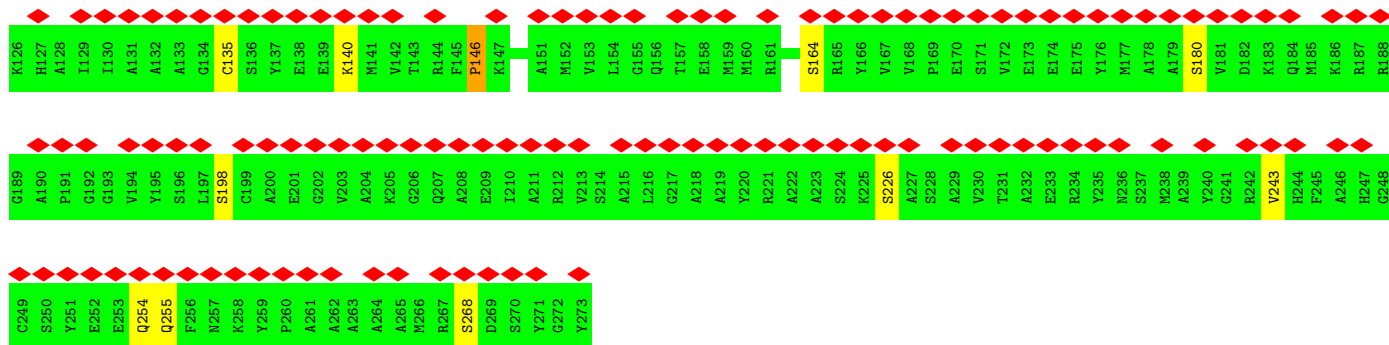


• Molecule 14: R-phycoerythrin gamma chain, chloroplastic

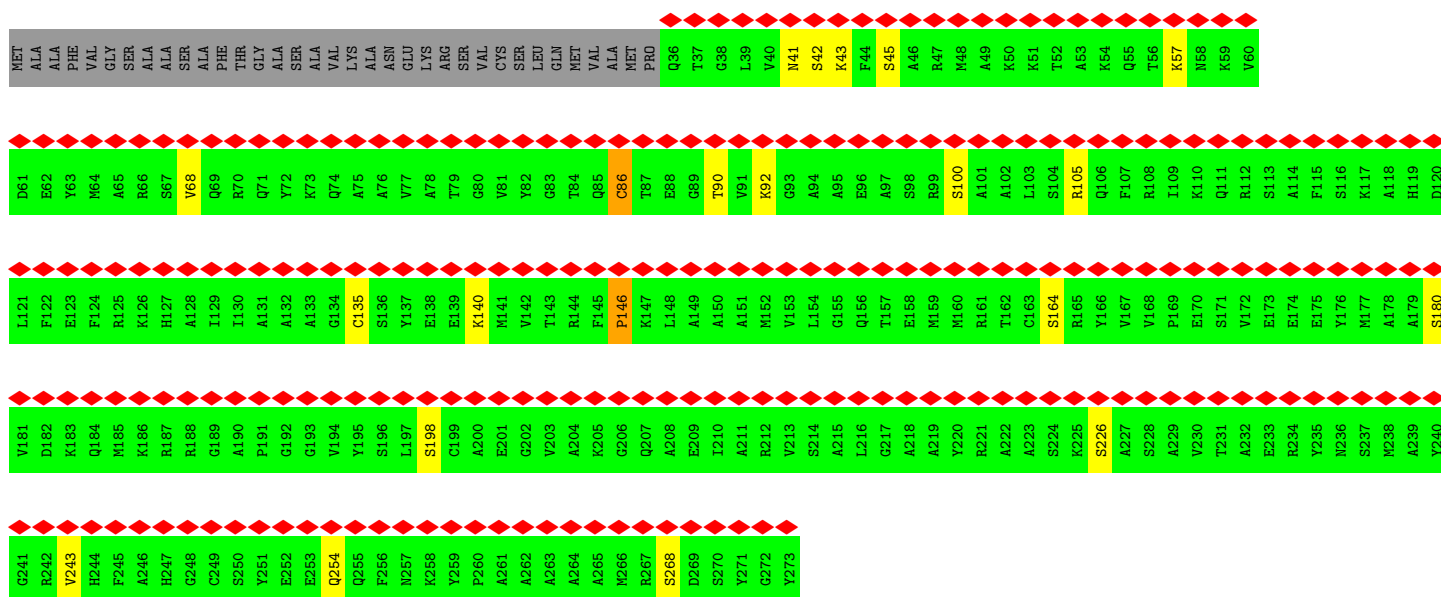
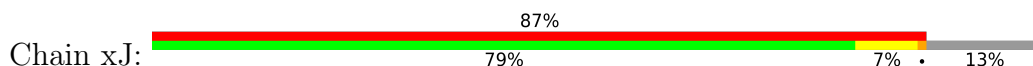


• Molecule 14: R-phycoerythrin gamma chain, chloroplastic

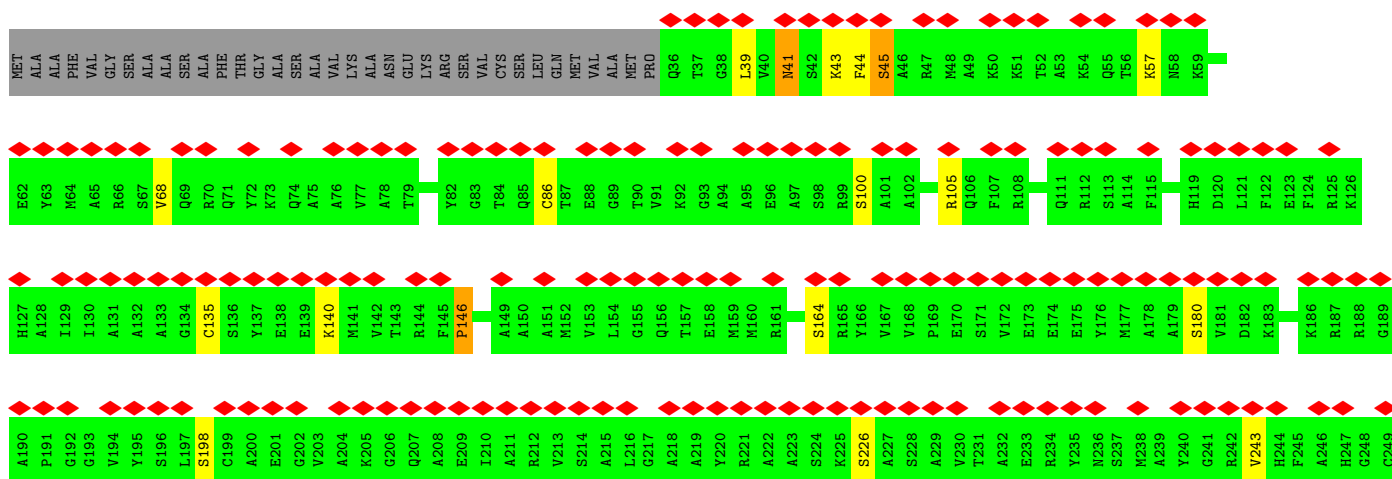
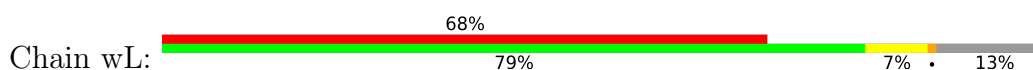


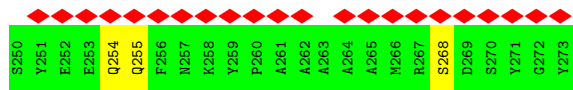


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

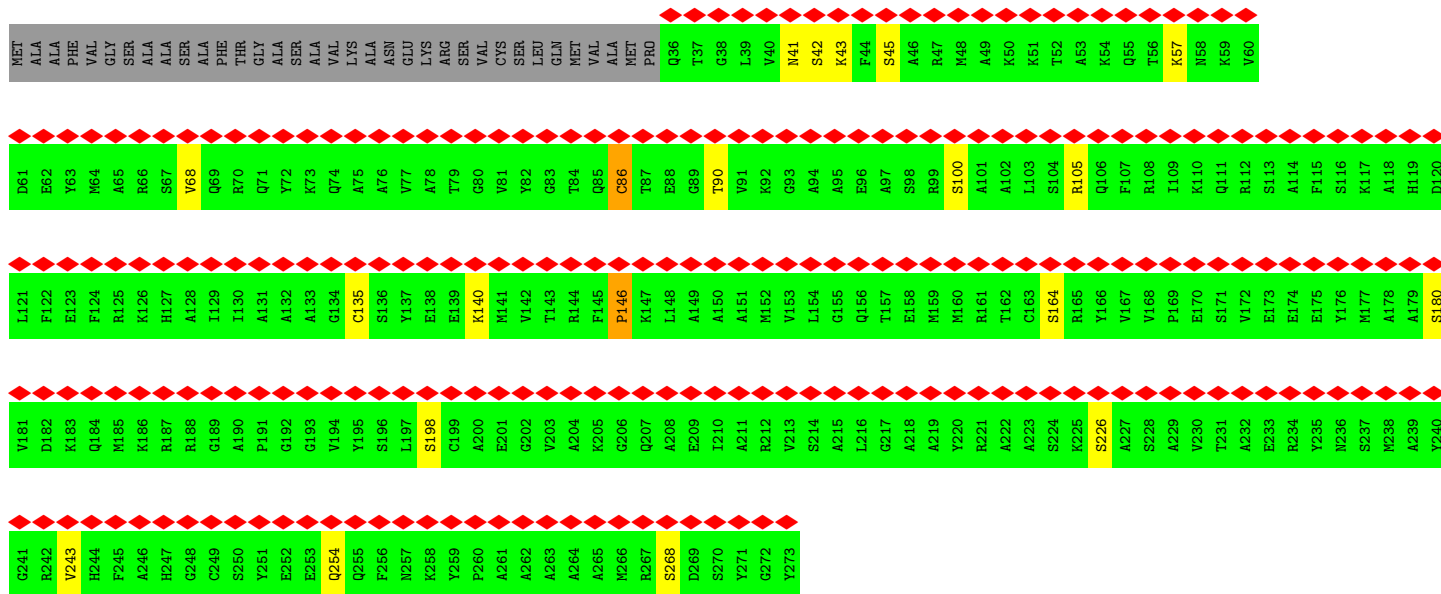
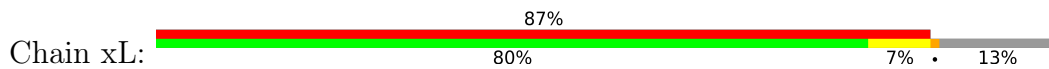


• Molecule 16: R-phycoerythrin gamma chain, chloroplastic

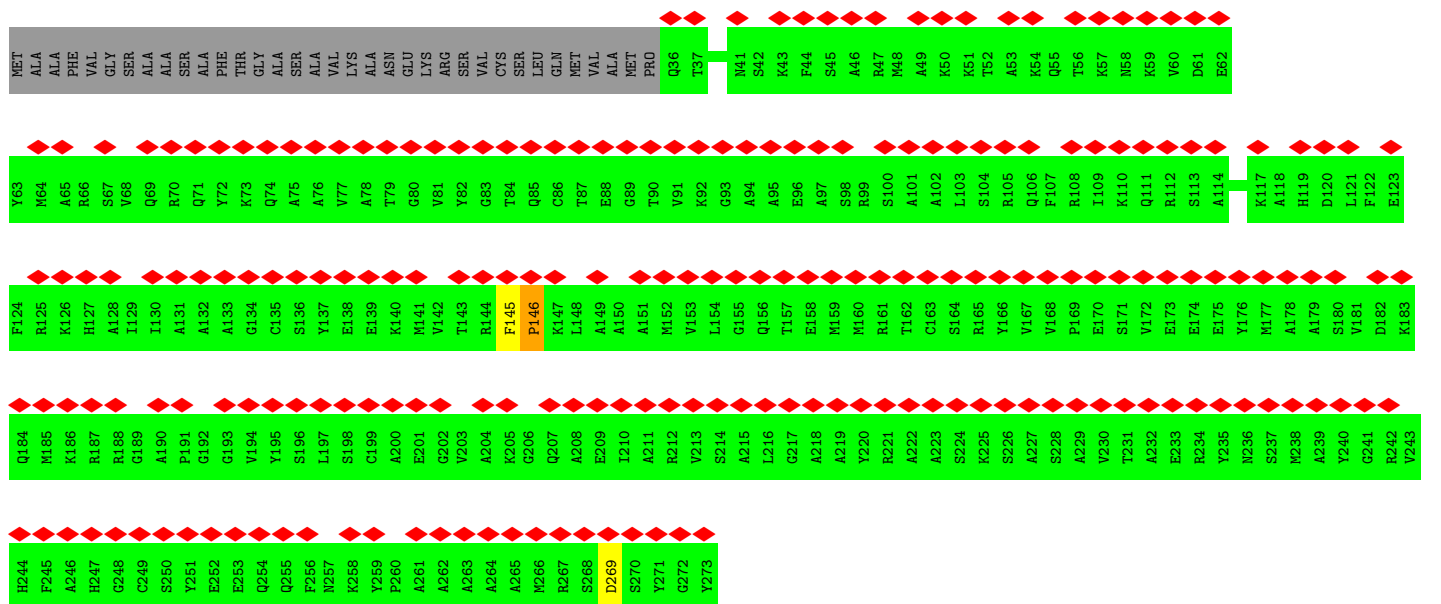
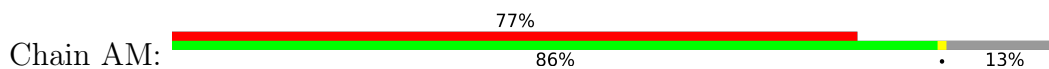




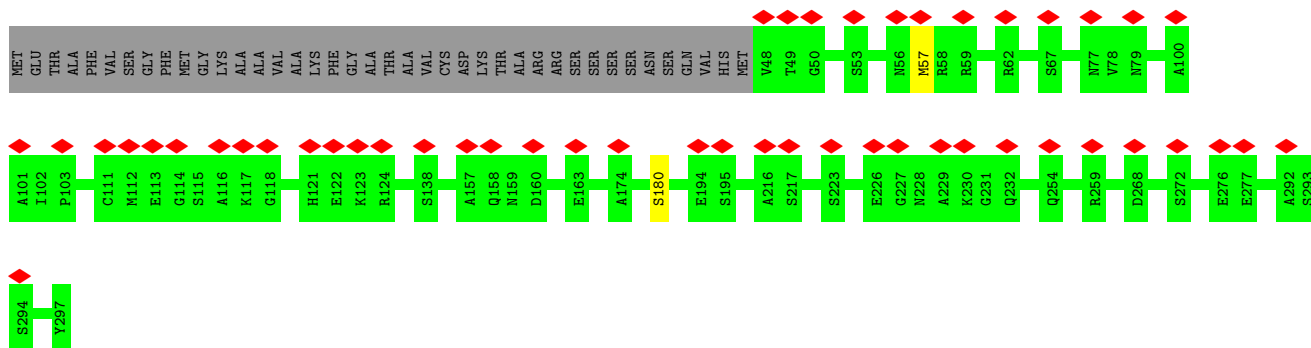
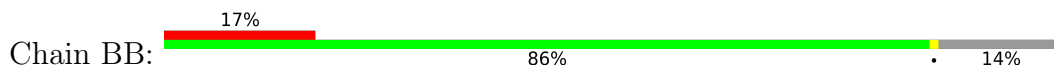
• Molecule 16: R-phycoerythrin gamma chain, chloroplastic



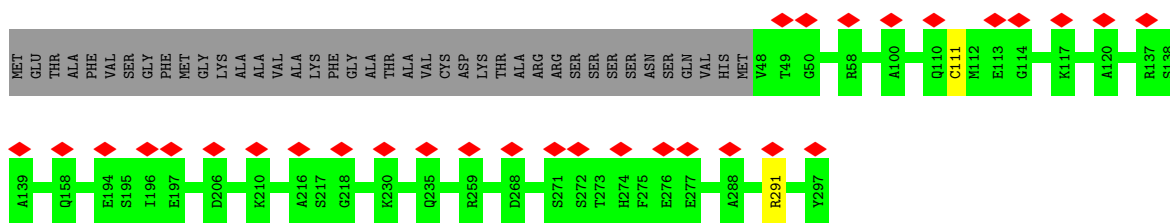
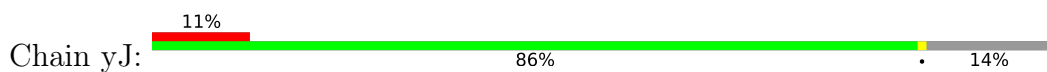
• Molecule 16: R-phycoerythrin gamma chain, chloroplastic



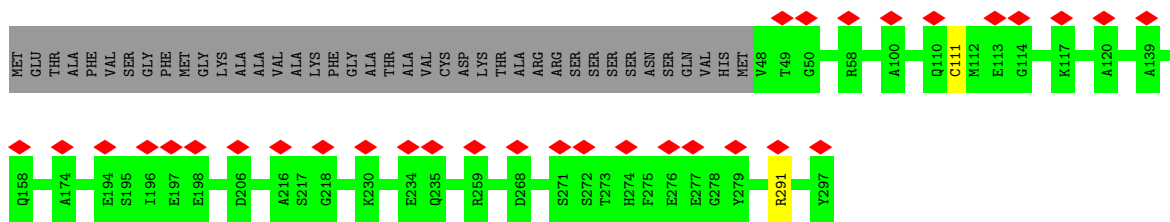
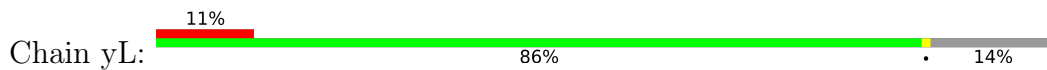
• Molecule 17: R-phycoerythrin gamma chain, chloroplastic



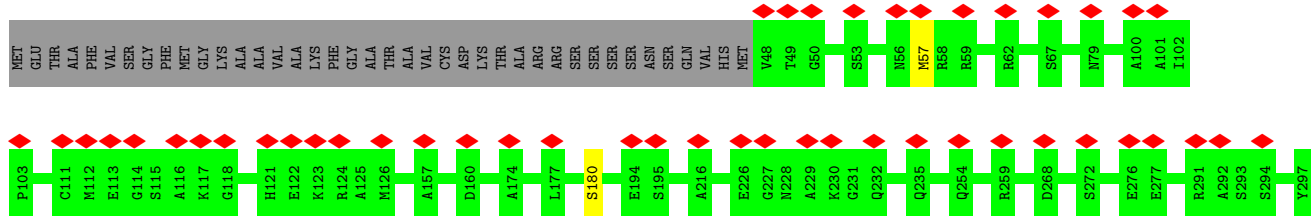
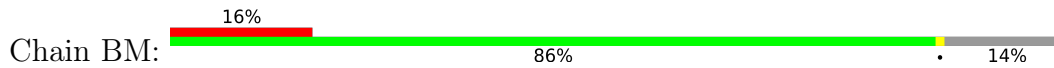
- Molecule 17: R-phycoerythrin gamma chain, chloroplastic



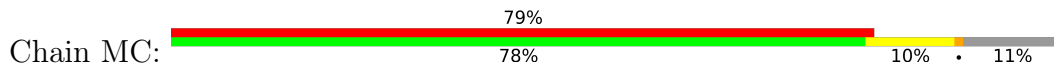
- Molecule 17: R-phycoerythrin gamma chain, chloroplastic

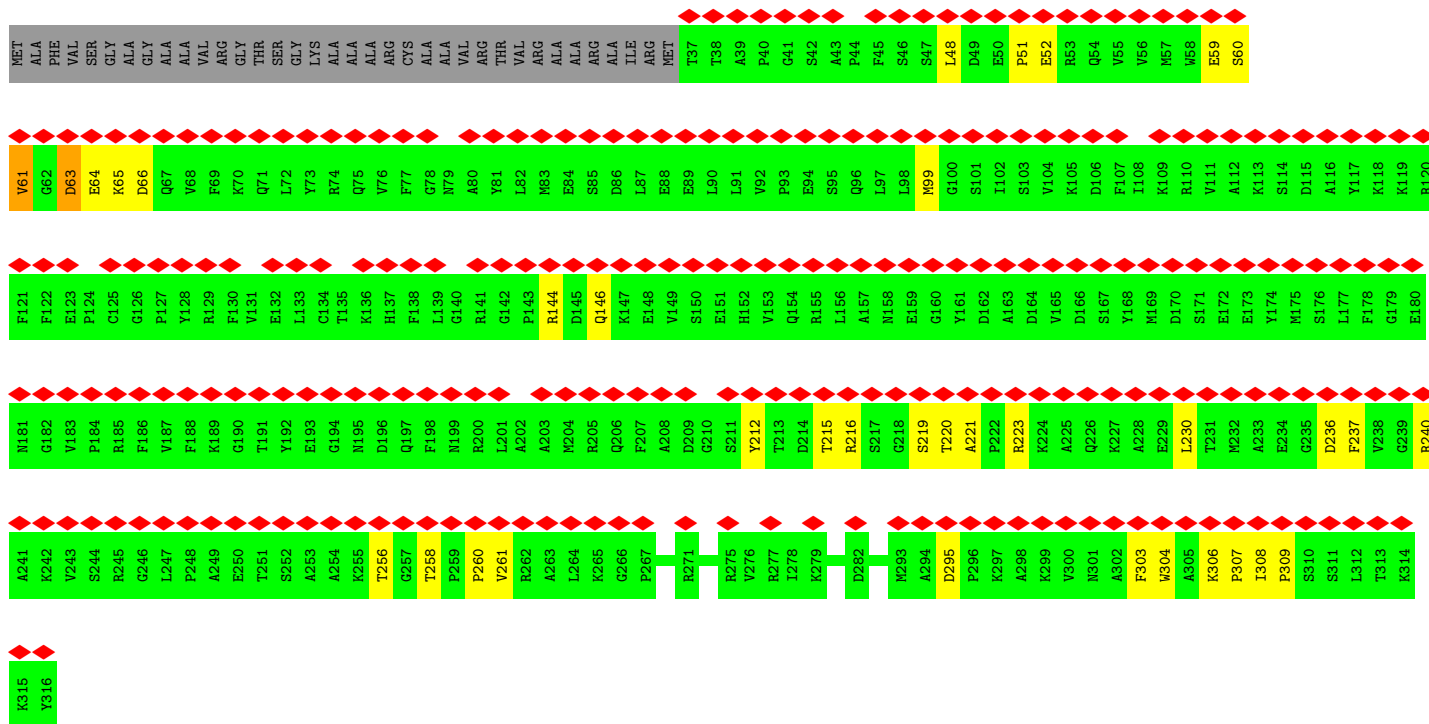


- Molecule 17: R-phycoerythrin gamma chain, chloroplastic

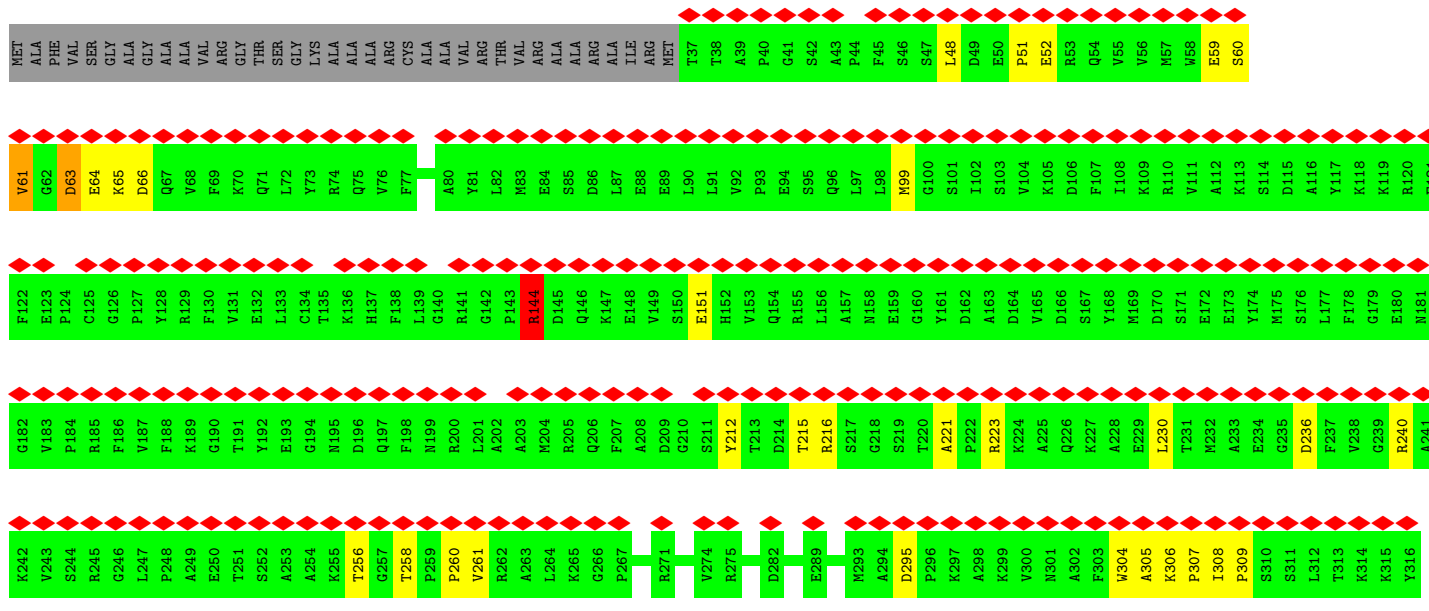
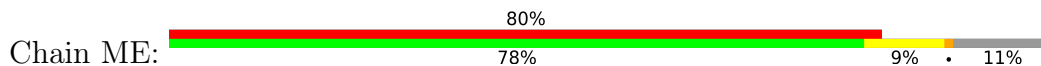


- Molecule 18: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

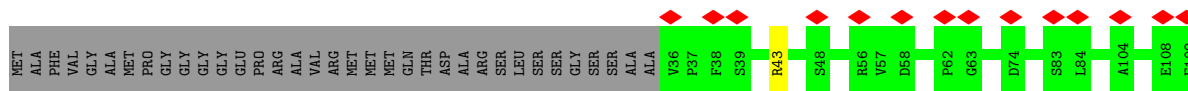
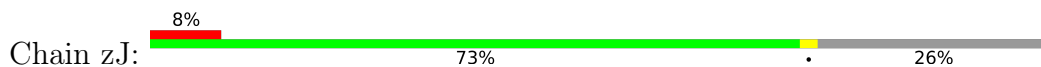


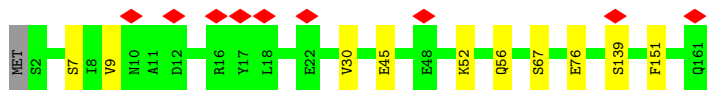


• Molecule 18: Phycobilisome 27.9 kDa linker polypeptide, phycoerythrin-associated, rod

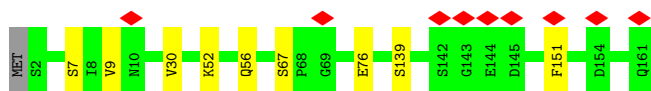
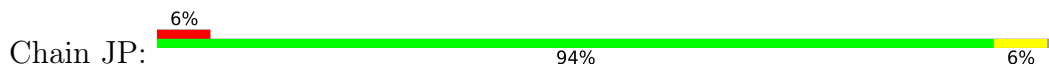


• Molecule 19: Phycobilisome 31.8 kDa linker polypeptide, phycoerythrin-associated, rod





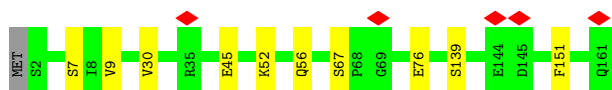
- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



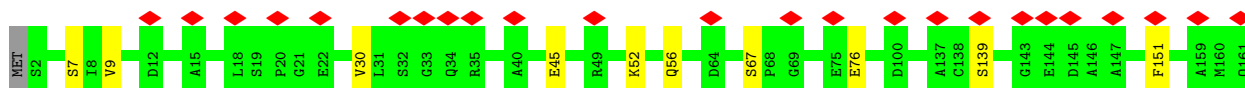
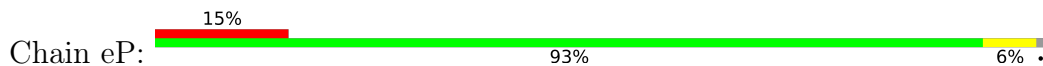
- Molecule 20: Allophycocyanin alpha subunit



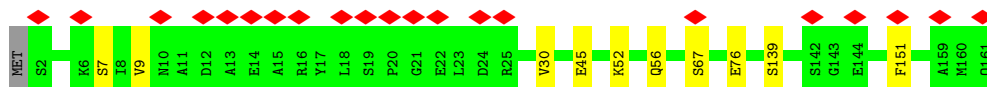
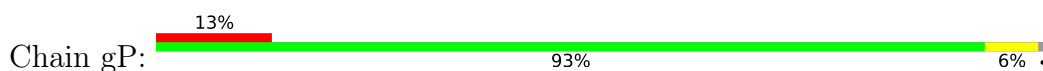
- Molecule 20: Allophycocyanin alpha subunit



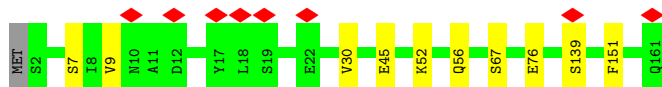
- Molecule 20: Allophycocyanin alpha subunit



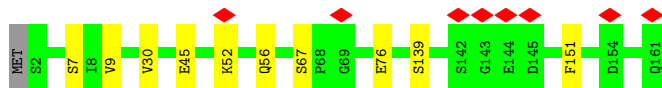
- Molecule 20: Allophycocyanin alpha subunit



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- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit

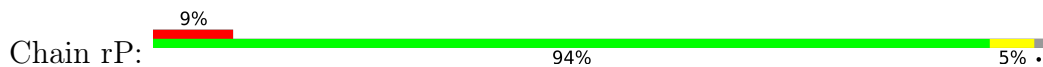


- Molecule 20: Allophycocyanin alpha subunit

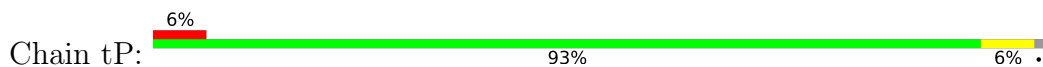




- Molecule 20: Allophycocyanin alpha subunit



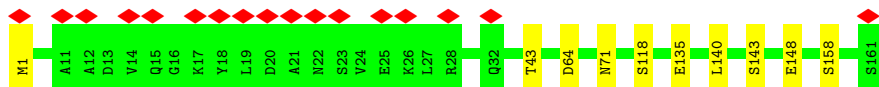
- Molecule 20: Allophycocyanin alpha subunit



- Molecule 20: Allophycocyanin alpha subunit



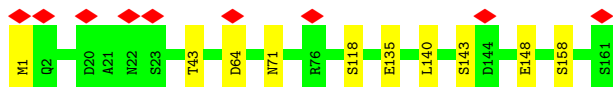
- Molecule 21: Allophycocyanin beta subunit



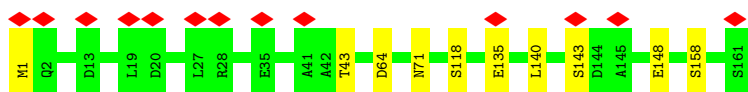
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



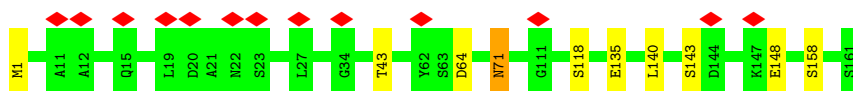
- Molecule 21: Allophycocyanin beta subunit



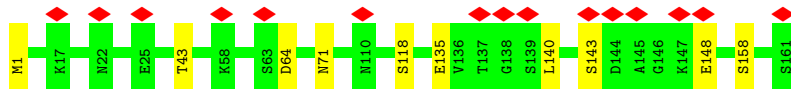
- Molecule 21: Allophycocyanin beta subunit



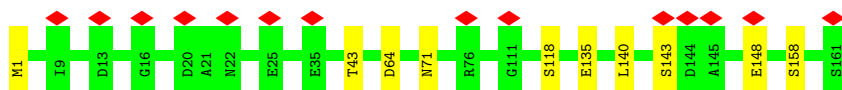
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



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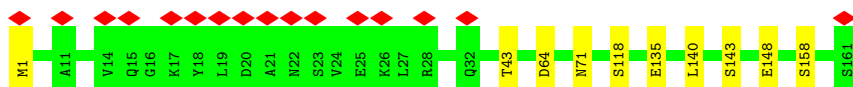
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



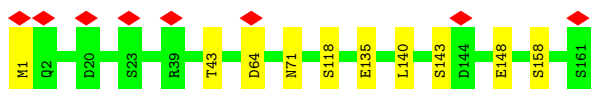
- Molecule 21: Allophycocyanin beta subunit



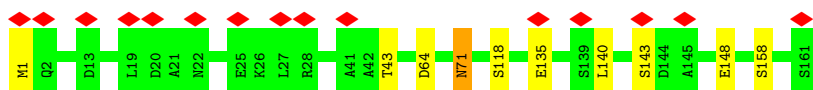
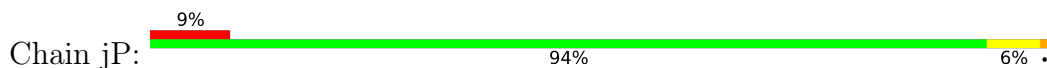
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit

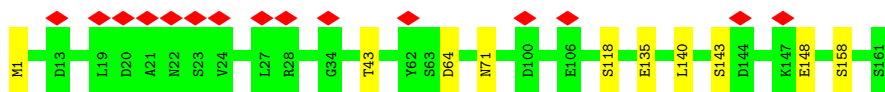


- Molecule 21: Allophycocyanin beta subunit

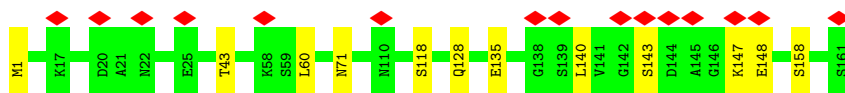


- Molecule 21: Allophycocyanin beta subunit

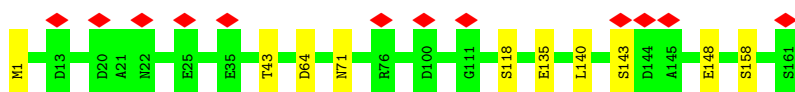




- Molecule 21: Allophycocyanin beta subunit



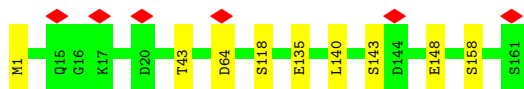
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit



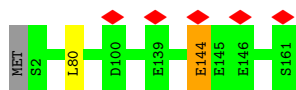
- Molecule 21: Allophycocyanin beta subunit



- Molecule 21: Allophycocyanin beta subunit

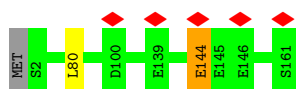


- Molecule 22: Allophycocyanin gamma subunit



- Molecule 22: Allophycocyanin gamma subunit

Chain xP:  98%



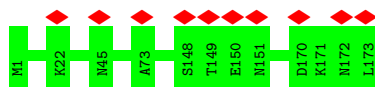
- Molecule 23: Allophycocyanin beta 18 subunit

Chain WP:  5% 100%



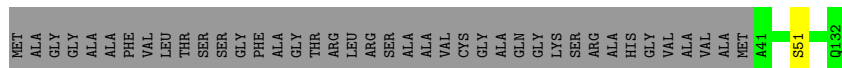
- Molecule 23: Allophycocyanin beta 18 subunit

Chain yP:  6% 100%



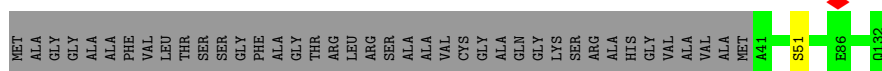
- Molecule 24: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain XP:  69% 30%



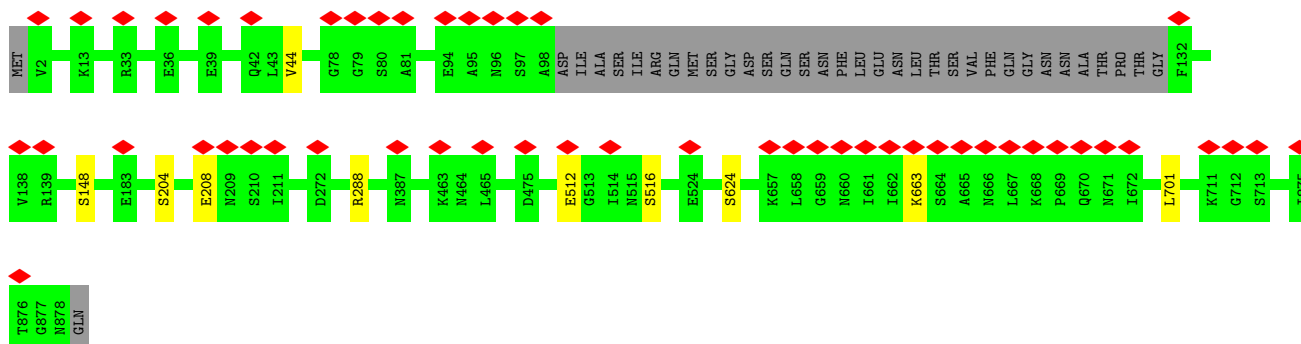
- Molecule 24: Phycobilisome 7.8 kDa linker polypeptide, allophycocyanin-associated, core

Chain zP:  69% 30%

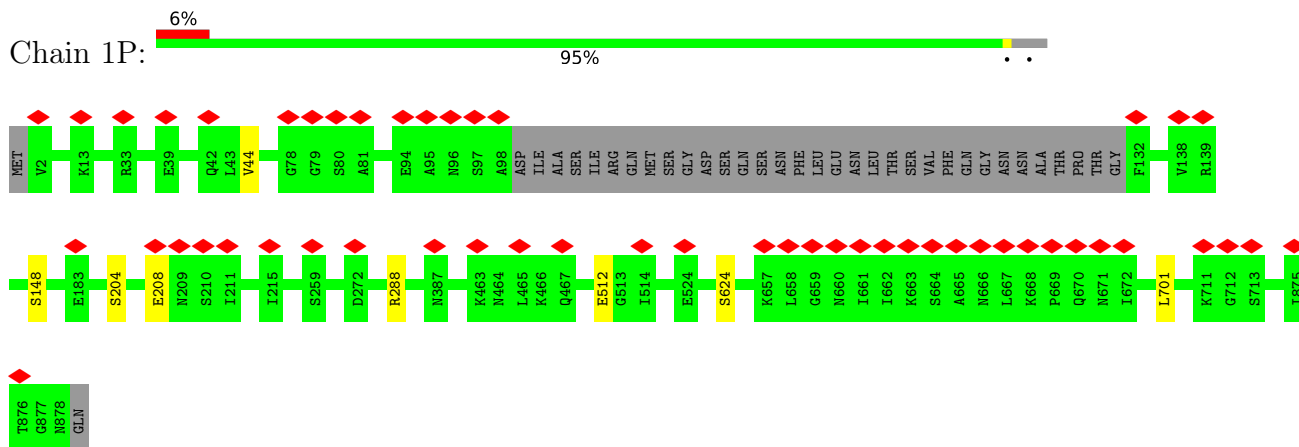


- Molecule 25: Phycobilisome linker polypeptide

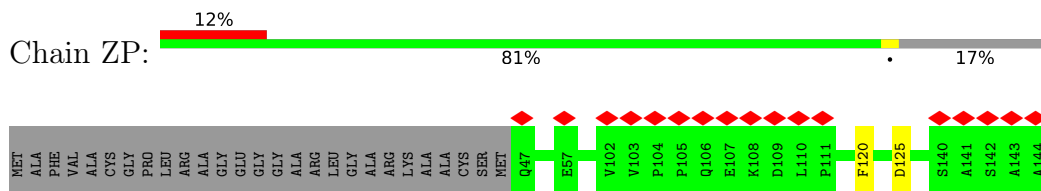
Chain yP:  6% 95%



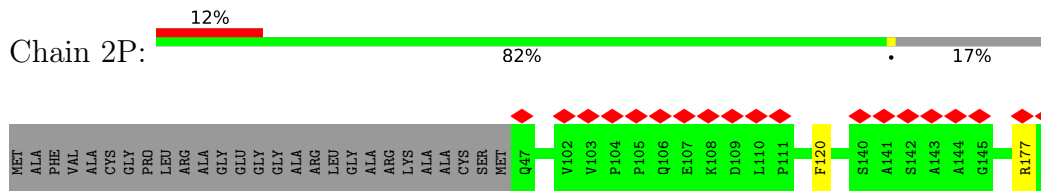
• Molecule 25: Phycobilisome linker polypeptide



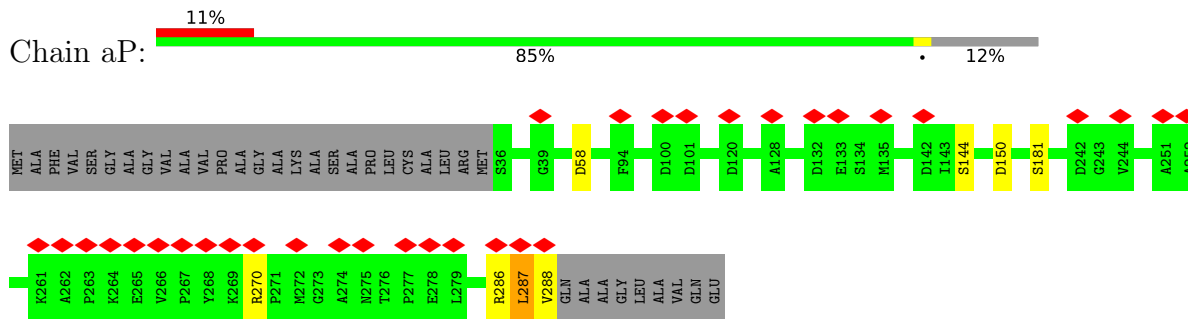
• Molecule 26: Lrc4



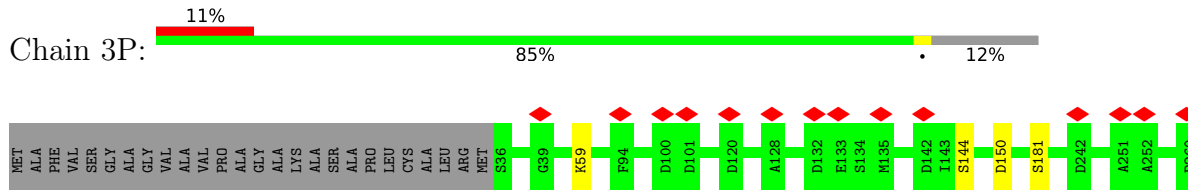
• Molecule 26: Lrc4

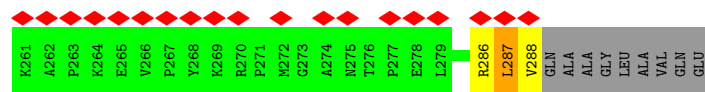


• Molecule 27: LRC5

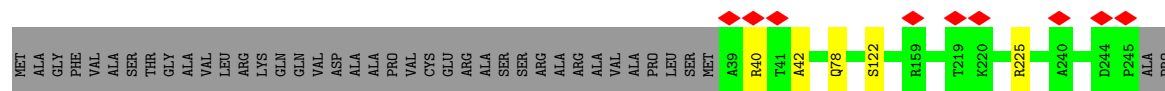
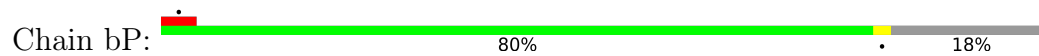


• Molecule 27: LRC5



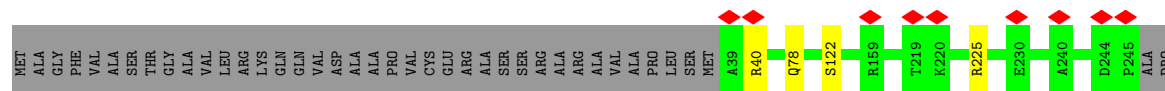
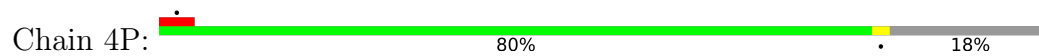


- Molecule 28: FAS1 domain-containing protein



SER
LYS
ILE
VAL
LYS
TYR

- Molecule 28: FAS1 domain-containing protein



SER
LYS
ILE
VAL
LYS
TYR

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	87399	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1300	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.065	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	618.2801, 618.2801, 618.2801	wwPDB
Map dimensions	580, 580, 580	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.0660001, 1.0660001, 1.0660001	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, PEB, PMS, PUB, 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	X1	0.50	0/2585	0.69	3/3492 (0.1%)
1	X7	0.48	1/2585 (0.0%)	0.66	0/3492
1	X9	0.48	1/2585 (0.0%)	0.66	0/3492
1	XF	0.54	0/2585	0.66	0/3492
1	XI	0.54	0/2581	0.66	0/3488
1	XK	0.50	0/2585	0.69	3/3492 (0.1%)
2	A1	0.44	0/2025	0.59	1/2722 (0.0%)
2	A7	0.42	0/2025	0.56	0/2722
2	A9	0.42	0/2025	0.56	0/2722
2	AF	0.44	0/2025	0.60	1/2722 (0.0%)
2	AI	0.44	0/2025	0.60	1/2722 (0.0%)
2	AK	0.44	0/2025	0.59	1/2722 (0.0%)
3	B1	0.48	0/1917	0.64	1/2592 (0.0%)
3	B7	0.44	0/1933	0.65	1/2614 (0.0%)
3	B9	0.44	0/1933	0.65	1/2614 (0.0%)
3	BF	0.56	1/1941 (0.1%)	0.63	0/2625
3	BI	0.56	1/1941 (0.1%)	0.64	0/2625
3	BK	0.49	0/1917	0.65	1/2592 (0.0%)
4	C1	0.37	0/1251	0.49	0/1699
4	C7	0.41	0/1251	0.53	0/1699
4	C9	0.41	0/1251	0.53	0/1699
4	CF	0.50	0/1251	0.56	1/1699 (0.1%)
4	CI	0.50	0/1251	0.56	1/1699 (0.1%)
4	CK	0.37	0/1251	0.48	0/1699
4	E1	0.36	0/1251	0.48	0/1699
4	E7	0.41	0/1251	0.53	0/1699
4	E9	0.41	0/1251	0.53	0/1699
4	EF	0.50	0/1251	0.56	1/1699 (0.1%)
4	EI	0.50	0/1251	0.56	1/1699 (0.1%)
4	EK	0.36	0/1251	0.48	0/1699
4	G1	0.38	0/1251	0.50	0/1699
4	G7	0.41	0/1251	0.53	0/1699

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
4	G9	0.41	0/1251	0.53	0/1699
4	GF	0.50	0/1251	0.56	1/1699 (0.1%)
4	GI	0.50	0/1251	0.56	1/1699 (0.1%)
4	GK	0.38	0/1251	0.50	0/1699
4	I1	0.40	0/1251	0.52	0/1699
4	I7	0.39	0/1251	0.54	0/1699
4	I9	0.39	0/1251	0.54	0/1699
4	IF	0.50	0/1251	0.56	1/1699 (0.1%)
4	II	0.50	0/1251	0.56	1/1699 (0.1%)
4	IK	0.40	0/1251	0.52	0/1699
4	K1	0.40	0/1251	0.52	0/1699
4	K7	0.41	0/1251	0.53	0/1699
4	K9	0.41	0/1251	0.53	0/1699
4	KF	0.49	0/1251	0.58	1/1699 (0.1%)
4	KI	0.50	0/1251	0.58	1/1699 (0.1%)
4	KK	0.40	0/1251	0.52	0/1699
4	M1	0.38	0/1251	0.51	0/1699
4	M7	0.41	0/1251	0.53	0/1699
4	M9	0.41	0/1251	0.53	0/1699
4	MF	0.50	0/1251	0.64	2/1699 (0.1%)
4	MI	0.50	0/1251	0.64	2/1699 (0.1%)
4	MK	0.38	0/1251	0.51	0/1699
5	D1	0.39	0/1274	0.64	1/1723 (0.1%)
5	D7	0.49	0/1274	0.70	4/1723 (0.2%)
5	D9	0.49	0/1274	0.70	4/1723 (0.2%)
5	DF	0.47	0/1274	0.59	0/1723
5	DI	0.47	0/1274	0.59	0/1723
5	DK	0.39	0/1274	0.64	1/1723 (0.1%)
5	F1	0.42	0/1274	0.68	2/1723 (0.1%)
5	F7	0.46	0/1274	0.61	1/1723 (0.1%)
5	F9	0.46	0/1274	0.61	1/1723 (0.1%)
5	FF	0.46	0/1274	0.60	0/1723
5	FI	0.47	0/1274	0.60	0/1723
5	FK	0.42	0/1274	0.68	2/1723 (0.1%)
5	H1	0.40	0/1274	0.65	1/1723 (0.1%)
5	H7	0.49	0/1274	0.66	2/1723 (0.1%)
5	H9	0.49	0/1274	0.66	2/1723 (0.1%)
5	HF	0.46	0/1274	0.59	0/1723
5	HI	0.46	0/1274	0.59	0/1723
5	HK	0.40	0/1274	0.65	1/1723 (0.1%)
5	J1	0.44	0/1274	0.70	3/1723 (0.2%)
5	J7	0.49	0/1274	0.67	2/1723 (0.1%)
5	J9	0.49	0/1274	0.67	2/1723 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
5	JF	0.47	0/1274	0.63	0/1723
5	JI	0.47	0/1274	0.63	0/1723
5	JK	0.44	0/1274	0.70	3/1723 (0.2%)
5	L1	0.45	0/1274	0.72	3/1723 (0.2%)
5	L7	0.49	0/1274	0.70	4/1723 (0.2%)
5	L9	0.49	0/1274	0.70	4/1723 (0.2%)
5	LF	0.46	0/1274	0.60	0/1723
5	LI	0.46	0/1274	0.60	0/1723
5	LK	0.45	0/1274	0.72	3/1723 (0.2%)
5	N1	0.41	0/1274	0.67	2/1723 (0.1%)
5	N7	0.49	0/1274	0.69	4/1723 (0.2%)
5	N9	0.49	0/1274	0.69	4/1723 (0.2%)
5	NF	0.46	0/1274	0.63	0/1723
5	NI	0.46	0/1274	0.63	0/1723
5	NK	0.41	0/1274	0.67	2/1723 (0.1%)
6	A3	0.42	1/1271 (0.1%)	0.63	3/1721 (0.2%)
6	AA	0.38	0/1271	0.58	0/1721
6	AC	0.28	0/1271	0.51	1/1721 (0.1%)
6	AE	0.28	0/1271	0.51	1/1721 (0.1%)
6	AG	0.46	0/1271	0.75	4/1721 (0.2%)
6	AJ	0.39	0/1271	0.57	2/1721 (0.1%)
6	AL	0.39	0/1271	0.57	2/1721 (0.1%)
6	AN	0.38	0/1271	0.58	0/1721
6	AO	0.42	1/1271 (0.1%)	0.63	3/1721 (0.2%)
6	AQ	0.46	0/1271	0.76	4/1721 (0.2%)
6	B4	0.61	0/1271	0.82	3/1721 (0.2%)
6	BD	0.61	0/1271	0.82	3/1721 (0.2%)
6	C3	0.40	0/1271	0.68	2/1721 (0.1%)
6	CA	0.38	0/1271	0.59	0/1721
6	CB	0.33	0/1271	0.50	0/1721
6	CC	0.28	0/1271	0.51	1/1721 (0.1%)
6	CE	0.28	0/1271	0.51	1/1721 (0.1%)
6	CG	0.45	0/1271	0.75	4/1721 (0.2%)
6	CJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	CL	0.39	0/1271	0.58	2/1721 (0.1%)
6	CM	0.33	0/1271	0.50	0/1721
6	CN	0.38	0/1271	0.59	0/1721
6	CO	0.40	0/1271	0.68	2/1721 (0.1%)
6	CQ	0.45	0/1271	0.75	4/1721 (0.2%)
6	D4	0.61	0/1271	0.82	3/1721 (0.2%)
6	DD	0.61	0/1271	0.83	3/1721 (0.2%)
6	E3	0.40	0/1271	0.70	2/1721 (0.1%)
6	EA	0.38	0/1271	0.58	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	EB	0.35	0/1271	0.52	0/1721
6	EC	0.28	0/1271	0.51	1/1721 (0.1%)
6	EE	0.28	0/1271	0.51	1/1721 (0.1%)
6	EG	0.46	0/1271	0.75	4/1721 (0.2%)
6	EJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	EL	0.40	0/1271	0.59	2/1721 (0.1%)
6	EM	0.35	0/1271	0.52	0/1721
6	EN	0.38	0/1271	0.58	0/1721
6	EO	0.40	0/1271	0.70	2/1721 (0.1%)
6	EQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	F4	0.61	0/1271	0.83	3/1721 (0.2%)
6	FD	0.61	0/1271	0.83	3/1721 (0.2%)
6	G3	0.39	0/1271	0.69	0/1721
6	GA	0.38	0/1271	0.58	0/1721
6	GB	0.34	0/1271	0.45	0/1721
6	GC	0.28	0/1271	0.51	1/1721 (0.1%)
6	GE	0.28	0/1271	0.51	1/1721 (0.1%)
6	GG	0.46	0/1271	0.75	4/1721 (0.2%)
6	GJ	0.35	0/1271	0.56	2/1721 (0.1%)
6	GL	0.35	0/1271	0.56	2/1721 (0.1%)
6	GM	0.34	0/1271	0.45	0/1721
6	GN	0.38	0/1271	0.58	0/1721
6	GO	0.39	0/1271	0.69	0/1721
6	GQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	H4	0.60	0/1271	0.81	3/1721 (0.2%)
6	HD	0.61	0/1271	0.82	3/1721 (0.2%)
6	I3	0.39	0/1271	0.69	2/1721 (0.1%)
6	IA	0.39	0/1271	0.60	0/1721
6	IB	0.35	0/1271	0.52	0/1721
6	IC	0.28	0/1271	0.51	1/1721 (0.1%)
6	IE	0.28	0/1271	0.51	1/1721 (0.1%)
6	IG	0.46	0/1271	0.75	4/1721 (0.2%)
6	IJ	0.39	0/1271	0.56	2/1721 (0.1%)
6	IL	0.39	0/1271	0.56	2/1721 (0.1%)
6	IM	0.35	0/1271	0.52	0/1721
6	IN	0.39	0/1271	0.60	0/1721
6	IO	0.39	0/1271	0.69	2/1721 (0.1%)
6	IQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	J4	0.63	0/1271	0.84	3/1721 (0.2%)
6	J5	0.95	6/1271 (0.5%)	0.70	1/1721 (0.1%)
6	J8	0.95	6/1271 (0.5%)	0.70	1/1721 (0.1%)
6	JD	0.63	0/1271	0.84	3/1721 (0.2%)
6	K3	0.40	0/1271	0.68	3/1721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	KA	0.38	0/1271	0.58	0/1721
6	KB	0.34	0/1271	0.49	0/1721
6	KC	0.28	0/1271	0.51	1/1721 (0.1%)
6	KE	0.28	0/1271	0.51	1/1721 (0.1%)
6	KG	0.46	0/1271	0.75	4/1721 (0.2%)
6	KJ	0.40	0/1271	0.57	2/1721 (0.1%)
6	KL	0.40	0/1271	0.57	2/1721 (0.1%)
6	KM	0.34	0/1271	0.49	0/1721
6	KN	0.38	0/1271	0.58	0/1721
6	KO	0.40	0/1271	0.68	3/1721 (0.2%)
6	KQ	0.46	0/1271	0.75	4/1721 (0.2%)
6	L4	0.61	0/1271	0.85	4/1721 (0.2%)
6	LD	0.62	0/1271	0.86	4/1721 (0.2%)
6	M2	0.49	0/1271	0.83	8/1721 (0.5%)
6	MB	0.34	0/1271	0.50	0/1721
6	MJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	ML	0.38	0/1271	0.57	2/1721 (0.1%)
6	MM	0.34	0/1271	0.50	0/1721
6	MR	0.48	0/1271	0.68	3/1721 (0.2%)
6	O1	0.37	0/1271	0.56	1/1721 (0.1%)
6	O2	0.46	0/1270	0.71	4/1721 (0.2%)
6	O7	0.39	0/1271	0.52	0/1721
6	O9	0.39	0/1271	0.52	0/1721
6	OB	0.36	0/1271	0.52	0/1721
6	OF	0.44	1/1271 (0.1%)	0.70	4/1721 (0.2%)
6	OI	0.44	1/1271 (0.1%)	0.70	4/1721 (0.2%)
6	OJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	OK	0.37	0/1271	0.56	1/1721 (0.1%)
6	OL	0.40	0/1271	0.59	2/1721 (0.1%)
6	OM	0.36	0/1271	0.52	0/1721
6	OR	0.46	0/1270	0.71	4/1721 (0.2%)
6	Q1	0.37	0/1271	0.56	1/1721 (0.1%)
6	Q2	0.47	0/1271	0.71	4/1721 (0.2%)
6	Q7	0.39	0/1271	0.52	0/1721
6	Q9	0.39	0/1271	0.52	0/1721
6	QB	0.35	0/1271	0.52	0/1721
6	QF	0.40	0/1271	0.63	2/1721 (0.1%)
6	QI	0.40	0/1271	0.63	2/1721 (0.1%)
6	QJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	QK	0.37	0/1271	0.56	1/1721 (0.1%)
6	QL	0.40	0/1271	0.58	2/1721 (0.1%)
6	QM	0.35	0/1271	0.52	0/1721
6	QR	0.47	0/1271	0.71	4/1721 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	S1	0.37	0/1271	0.56	1/1721 (0.1%)
6	S2	0.46	0/1270	0.73	3/1721 (0.2%)
6	S7	0.39	0/1271	0.51	0/1721
6	S9	0.39	0/1271	0.51	0/1721
6	SB	0.34	0/1271	0.50	0/1721
6	SF	0.40	0/1271	0.63	2/1721 (0.1%)
6	SI	0.40	0/1271	0.63	2/1721 (0.1%)
6	SJ	0.38	0/1271	0.57	2/1721 (0.1%)
6	SK	0.37	0/1271	0.56	1/1721 (0.1%)
6	SL	0.38	0/1271	0.57	2/1721 (0.1%)
6	SM	0.34	0/1271	0.50	0/1721
6	SR	0.47	0/1270	0.87	8/1721 (0.5%)
6	U1	0.37	0/1271	0.56	1/1721 (0.1%)
6	U2	0.46	0/1270	0.72	5/1721 (0.3%)
6	U7	0.39	0/1271	0.52	0/1721
6	U9	0.39	0/1271	0.52	0/1721
6	UB	0.35	0/1271	0.52	0/1721
6	UF	0.40	0/1271	0.65	2/1721 (0.1%)
6	UI	0.40	0/1271	0.65	2/1721 (0.1%)
6	UJ	0.39	0/1271	0.58	2/1721 (0.1%)
6	UK	0.37	0/1271	0.56	1/1721 (0.1%)
6	UL	0.39	0/1271	0.58	2/1721 (0.1%)
6	UM	0.35	0/1271	0.52	0/1721
6	UR	0.46	0/1270	0.71	5/1721 (0.3%)
6	W1	0.36	0/1271	0.54	1/1721 (0.1%)
6	W2	0.47	0/1271	0.73	4/1721 (0.2%)
6	W7	0.38	0/1271	0.52	0/1721
6	W9	0.38	0/1271	0.52	0/1721
6	WB	0.35	0/1271	0.52	0/1721
6	WF	0.40	0/1271	0.63	2/1721 (0.1%)
6	WI	0.40	0/1271	0.63	2/1721 (0.1%)
6	WJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	WK	0.36	0/1271	0.54	1/1721 (0.1%)
6	WL	0.40	0/1271	0.59	2/1721 (0.1%)
6	WM	0.35	0/1271	0.52	0/1721
6	WR	0.46	0/1271	0.74	4/1721 (0.2%)
6	YB	0.34	0/1271	0.50	0/1721
6	YJ	0.39	0/1271	0.59	2/1721 (0.1%)
6	YL	0.39	0/1271	0.58	2/1721 (0.1%)
6	YM	0.34	0/1271	0.51	0/1721
6	Z1	0.37	0/1271	0.55	1/1721 (0.1%)
6	Z7	0.39	0/1271	0.52	0/1721
6	Z9	0.39	0/1271	0.52	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	ZF	0.43	1/1271 (0.1%)	0.59	0/1721
6	ZI	0.43	1/1271 (0.1%)	0.61	0/1721
6	ZK	0.37	0/1271	0.55	1/1721 (0.1%)
6	aB	0.35	0/1271	0.52	0/1721
6	aJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	aL	0.40	0/1271	0.58	2/1721 (0.1%)
6	aM	0.35	0/1271	0.52	0/1721
6	b1	0.37	0/1271	0.56	1/1721 (0.1%)
6	b7	0.39	0/1271	0.52	0/1721
6	b9	0.39	0/1271	0.52	0/1721
6	bF	0.44	1/1271 (0.1%)	0.68	4/1721 (0.2%)
6	bI	0.44	1/1271 (0.1%)	0.68	4/1721 (0.2%)
6	bK	0.37	0/1271	0.56	1/1721 (0.1%)
6	cJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	cL	0.40	0/1271	0.58	2/1721 (0.1%)
6	d1	0.36	0/1271	0.56	1/1721 (0.1%)
6	d7	0.39	0/1271	0.52	0/1721
6	d9	0.39	0/1271	0.52	0/1721
6	dB	0.35	0/1271	0.52	0/1721
6	dF	0.41	0/1271	0.68	2/1721 (0.1%)
6	dI	0.41	0/1271	0.68	2/1721 (0.1%)
6	dK	0.36	0/1271	0.56	1/1721 (0.1%)
6	dM	0.35	0/1271	0.52	0/1721
6	eJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	eL	0.40	0/1271	0.59	2/1721 (0.1%)
6	f1	0.37	0/1271	0.56	1/1721 (0.1%)
6	f7	0.39	0/1271	0.52	0/1721
6	f9	0.39	0/1271	0.52	0/1721
6	fB	0.35	0/1271	0.53	0/1721
6	fF	0.40	0/1271	0.67	3/1721 (0.2%)
6	fI	0.40	0/1271	0.67	3/1721 (0.2%)
6	fK	0.37	0/1271	0.56	1/1721 (0.1%)
6	fM	0.35	0/1271	0.53	0/1721
6	gJ	0.40	0/1271	0.58	2/1721 (0.1%)
6	gL	0.40	0/1271	0.59	2/1721 (0.1%)
6	h1	0.36	0/1271	0.55	1/1721 (0.1%)
6	h7	0.39	0/1271	0.52	0/1721
6	h9	0.39	0/1271	0.52	0/1721
6	hB	0.35	0/1271	0.52	0/1721
6	hF	0.40	0/1271	0.64	2/1721 (0.1%)
6	hI	0.40	0/1271	0.64	2/1721 (0.1%)
6	hK	0.36	0/1271	0.56	1/1721 (0.1%)
6	hM	0.35	0/1271	0.52	0/1721

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
6	iJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	iL	0.40	0/1271	0.59	2/1721 (0.1%)
6	j1	0.37	0/1271	0.56	1/1721 (0.1%)
6	j7	0.39	0/1271	0.52	0/1721
6	j9	0.39	0/1271	0.52	0/1721
6	jB	0.35	0/1271	0.50	0/1721
6	jF	0.39	0/1271	0.59	1/1721 (0.1%)
6	jI	0.39	0/1271	0.59	1/1721 (0.1%)
6	jK	0.37	0/1271	0.56	1/1721 (0.1%)
6	jM	0.33	0/1271	0.49	0/1721
6	kJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	kL	0.40	0/1271	0.59	2/1721 (0.1%)
6	l1	0.37	0/1271	0.55	1/1721 (0.1%)
6	l7	0.39	0/1271	0.52	0/1721
6	l9	0.39	0/1271	0.52	0/1721
6	lB	0.34	0/1271	0.50	0/1721
6	lF	0.40	0/1271	0.66	2/1721 (0.1%)
6	lI	0.40	0/1271	0.66	2/1721 (0.1%)
6	lK	0.37	0/1271	0.55	1/1721 (0.1%)
6	lM	0.33	0/1271	0.51	0/1721
6	mJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	mL	0.40	0/1271	0.59	2/1721 (0.1%)
6	oJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	oL	0.40	0/1271	0.59	2/1721 (0.1%)
6	qJ	0.39	0/1271	0.59	2/1721 (0.1%)
6	qL	0.39	0/1271	0.59	2/1721 (0.1%)
6	sJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	sL	0.40	0/1271	0.59	2/1721 (0.1%)
6	uJ	0.40	0/1271	0.59	2/1721 (0.1%)
6	uL	0.40	0/1271	0.59	2/1721 (0.1%)
7	A5	0.42	0/1297	0.63	1/1750 (0.1%)
7	A8	0.42	0/1297	0.63	1/1750 (0.1%)
7	B3	0.40	0/1297	0.78	6/1750 (0.3%)
7	B5	0.33	0/1065	0.51	0/1437
7	B8	0.33	0/1065	0.52	0/1437
7	BA	0.37	0/1297	0.62	2/1750 (0.1%)
7	BC	0.30	0/1297	0.56	0/1750
7	BE	0.30	0/1297	0.56	0/1750
7	BG	0.37	0/1297	0.62	0/1750
7	BJ	0.40	0/1297	0.62	1/1750 (0.1%)
7	BL	0.40	0/1297	0.62	1/1750 (0.1%)
7	BN	0.37	0/1297	0.62	2/1750 (0.1%)
7	BO	0.40	0/1297	0.78	6/1750 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	BQ	0.37	0/1297	0.62	0/1750
7	C4	0.68	0/1297	1.09	10/1750 (0.6%)
7	C5	0.44	0/1297	0.66	2/1750 (0.1%)
7	C8	0.44	0/1297	0.66	2/1750 (0.1%)
7	CD	0.68	0/1297	1.09	10/1750 (0.6%)
7	D3	0.39	0/1297	0.74	6/1750 (0.3%)
7	DA	0.37	0/1297	0.62	2/1750 (0.1%)
7	DB	0.38	0/1309	0.61	1/1766 (0.1%)
7	DC	0.29	0/1297	0.56	0/1750
7	DE	0.29	0/1297	0.56	0/1750
7	DG	0.37	0/1297	0.62	0/1750
7	DJ	0.39	0/1297	0.60	1/1750 (0.1%)
7	DL	0.39	0/1297	0.60	1/1750 (0.1%)
7	DM	0.38	0/1309	0.61	1/1766 (0.1%)
7	DN	0.37	0/1297	0.62	2/1750 (0.1%)
7	DO	0.39	0/1297	0.74	6/1750 (0.3%)
7	DQ	0.37	0/1297	0.62	0/1750
7	E4	0.65	0/1297	1.00	8/1750 (0.5%)
7	ED	0.68	0/1297	1.09	10/1750 (0.6%)
7	F3	0.37	0/1297	0.64	3/1750 (0.2%)
7	F5	0.33	0/1065	0.51	0/1437
7	F8	0.33	0/1065	0.51	0/1437
7	FA	0.36	0/1297	0.62	2/1750 (0.1%)
7	FB	0.38	0/1303	0.62	1/1758 (0.1%)
7	FC	0.30	0/1297	0.56	0/1750
7	FE	0.30	0/1297	0.56	0/1750
7	FG	0.36	0/1297	0.62	0/1750
7	FJ	0.37	0/1297	0.57	1/1750 (0.1%)
7	FL	0.37	0/1297	0.57	1/1750 (0.1%)
7	FM	0.38	0/1303	0.62	1/1758 (0.1%)
7	FN	0.36	0/1297	0.62	2/1750 (0.1%)
7	FO	0.37	0/1297	0.64	3/1750 (0.2%)
7	FQ	0.37	0/1297	0.62	0/1750
7	G4	0.67	0/1297	1.09	10/1750 (0.6%)
7	G5	0.33	0/1065	0.51	0/1437
7	G8	0.33	0/1065	0.51	0/1437
7	GD	0.67	0/1297	1.09	10/1750 (0.6%)
7	H3	0.38	0/1297	0.71	5/1750 (0.3%)
7	H5	0.33	0/1065	0.51	0/1437
7	H8	0.33	0/1065	0.51	0/1437
7	HA	0.37	0/1303	0.62	2/1758 (0.1%)
7	HB	0.38	0/1309	0.62	1/1766 (0.1%)
7	HC	0.30	0/1297	0.56	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	HE	0.30	0/1297	0.56	0/1750
7	HG	0.37	0/1303	0.62	0/1758
7	HJ	0.33	0/1297	0.54	1/1750 (0.1%)
7	HL	0.33	0/1297	0.54	1/1750 (0.1%)
7	HM	0.38	0/1309	0.62	1/1766 (0.1%)
7	HN	0.37	0/1303	0.62	2/1758 (0.1%)
7	HO	0.38	0/1297	0.71	5/1750 (0.3%)
7	HQ	0.37	0/1303	0.62	0/1758
7	I4	0.67	0/1303	1.05	8/1758 (0.5%)
7	I5	0.33	0/1297	0.61	1/1750 (0.1%)
7	I8	0.33	0/1297	0.60	1/1750 (0.1%)
7	ID	0.66	0/1303	1.05	8/1758 (0.5%)
7	J3	0.37	0/1297	0.66	4/1750 (0.2%)
7	JA	0.36	0/1297	0.55	0/1750
7	JB	0.38	0/1309	0.60	1/1766 (0.1%)
7	JC	0.30	0/1297	0.56	0/1750
7	JE	0.30	0/1297	0.56	0/1750
7	JG	0.37	0/1297	0.62	0/1750
7	JJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	JL	0.40	0/1297	0.61	1/1750 (0.1%)
7	JM	0.38	0/1309	0.60	1/1766 (0.1%)
7	JN	0.36	0/1297	0.55	0/1750
7	JO	0.37	0/1297	0.66	4/1750 (0.2%)
7	JQ	0.37	0/1297	0.62	0/1750
7	K4	0.68	0/1297	1.09	10/1750 (0.6%)
7	K5	0.71	2/1297 (0.2%)	0.76	2/1750 (0.1%)
7	K8	0.71	2/1297 (0.2%)	0.76	2/1750 (0.1%)
7	KD	0.68	0/1297	1.09	10/1750 (0.6%)
7	L3	0.38	0/1297	0.68	4/1750 (0.2%)
7	L5	0.33	0/1065	0.52	0/1437
7	L8	0.33	0/1065	0.51	0/1437
7	LA	0.37	0/1297	0.62	2/1750 (0.1%)
7	LB	0.38	0/1309	0.62	1/1766 (0.1%)
7	LC	0.30	0/1297	0.56	0/1750
7	LE	0.30	0/1297	0.56	0/1750
7	LG	0.37	0/1297	0.62	0/1750
7	LJ	0.39	0/1297	0.60	1/1750 (0.1%)
7	LL	0.39	0/1297	0.60	1/1750 (0.1%)
7	LM	0.38	0/1309	0.62	1/1766 (0.1%)
7	LN	0.37	0/1297	0.62	2/1750 (0.1%)
7	LO	0.38	0/1297	0.68	4/1750 (0.2%)
7	LQ	0.36	0/1297	0.62	0/1750
7	M3	0.33	0/1065	0.69	1/1437 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	M4	0.67	0/1297	1.07	8/1750 (0.5%)
7	MD	0.68	0/1297	1.09	10/1750 (0.6%)
7	MO	0.33	0/1065	0.69	1/1437 (0.1%)
7	N2	0.42	0/1297	0.62	0/1750
7	N3	0.32	0/1065	0.63	0/1437
7	NB	0.35	0/1309	0.55	0/1766
7	NJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	NL	0.40	0/1297	0.61	1/1750 (0.1%)
7	NM	0.35	0/1309	0.55	0/1766
7	NO	0.32	0/1065	0.63	0/1437
7	NR	0.42	0/1297	0.62	0/1750
7	P1	0.37	0/1297	0.57	0/1750
7	P2	0.43	0/1303	0.58	0/1758
7	P7	0.37	0/1297	0.51	0/1750
7	P9	0.37	0/1297	0.51	0/1750
7	PB	0.37	0/1297	0.60	1/1750 (0.1%)
7	PF	0.41	0/1297	0.66	2/1750 (0.1%)
7	PI	0.41	0/1297	0.66	2/1750 (0.1%)
7	PJ	0.38	0/1303	0.59	1/1758 (0.1%)
7	PK	0.37	0/1297	0.57	0/1750
7	PL	0.38	0/1303	0.59	1/1758 (0.1%)
7	PM	0.37	0/1297	0.60	1/1750 (0.1%)
7	PR	0.43	0/1303	0.63	1/1758 (0.1%)
7	R1	0.37	0/1297	0.56	0/1750
7	R2	0.41	0/1297	0.63	1/1750 (0.1%)
7	R7	0.38	0/1297	0.53	0/1750
7	R9	0.38	0/1297	0.53	0/1750
7	RB	0.38	0/1303	0.59	1/1758 (0.1%)
7	RF	0.41	0/1297	0.65	2/1750 (0.1%)
7	RI	0.41	0/1297	0.65	2/1750 (0.1%)
7	RJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	RK	0.37	0/1297	0.56	0/1750
7	RL	0.40	0/1297	0.61	1/1750 (0.1%)
7	RM	0.38	0/1303	0.59	1/1758 (0.1%)
7	RR	0.41	0/1297	0.63	1/1750 (0.1%)
7	T1	0.37	0/1297	0.57	0/1750
7	T2	0.43	0/1297	0.62	1/1750 (0.1%)
7	T7	0.37	0/1297	0.52	0/1750
7	T9	0.37	0/1297	0.52	0/1750
7	TB	0.37	0/1303	0.59	1/1758 (0.1%)
7	TF	0.48	1/1297 (0.1%)	0.59	0/1750
7	TI	0.48	1/1297 (0.1%)	0.59	0/1750
7	TJ	0.40	0/1297	0.61	1/1750 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	TK	0.37	0/1297	0.57	0/1750
7	TL	0.40	0/1297	0.61	1/1750 (0.1%)
7	TM	0.37	0/1303	0.59	1/1758 (0.1%)
7	TR	0.43	0/1297	0.62	1/1750 (0.1%)
7	V1	0.37	0/1309	0.56	0/1766
7	V2	0.46	0/1297	0.64	2/1750 (0.1%)
7	V7	0.37	0/1297	0.53	0/1750
7	V9	0.37	0/1297	0.53	0/1750
7	VB	0.37	0/1309	0.59	1/1766 (0.1%)
7	VF	0.44	1/1309 (0.1%)	0.68	2/1766 (0.1%)
7	VI	0.44	1/1309 (0.1%)	0.68	2/1766 (0.1%)
7	VJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	VK	0.37	0/1309	0.56	0/1766
7	VL	0.40	0/1297	0.61	1/1750 (0.1%)
7	VM	0.37	0/1309	0.59	1/1766 (0.1%)
7	VR	0.46	0/1297	0.64	2/1750 (0.1%)
7	X2	0.42	0/1297	0.62	0/1750
7	XB	0.38	0/1309	0.62	1/1766 (0.1%)
7	XJ	0.41	0/1303	0.62	1/1758 (0.1%)
7	XL	0.41	0/1303	0.62	1/1758 (0.1%)
7	XM	0.38	0/1309	0.62	1/1766 (0.1%)
7	XR	0.42	0/1297	0.62	0/1750
7	Y1	0.37	0/1297	0.57	0/1750
7	Y7	0.38	0/1297	0.53	0/1750
7	Y9	0.38	0/1297	0.53	0/1750
7	YF	0.41	0/1297	0.67	2/1750 (0.1%)
7	YI	0.41	0/1297	0.67	2/1750 (0.1%)
7	YK	0.37	0/1297	0.57	0/1750
7	ZB	0.37	0/1309	0.59	1/1766 (0.1%)
7	ZJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	ZL	0.41	0/1297	0.62	1/1750 (0.1%)
7	ZM	0.37	0/1309	0.59	1/1766 (0.1%)
7	a1	0.37	0/1297	0.57	0/1750
7	a7	0.36	0/1297	0.55	0/1750
7	a9	0.36	0/1297	0.55	0/1750
7	aF	0.41	0/1297	0.69	3/1750 (0.2%)
7	aI	0.41	0/1297	0.69	3/1750 (0.2%)
7	aK	0.37	0/1297	0.57	0/1750
7	bJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	bL	0.41	0/1297	0.62	1/1750 (0.1%)
7	c1	0.37	0/1297	0.57	0/1750
7	c7	0.38	0/1297	0.53	0/1750
7	c9	0.38	0/1297	0.53	0/1750

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	cB	0.38	0/1303	0.62	1/1758 (0.1%)
7	cF	0.43	1/1297 (0.1%)	0.70	2/1750 (0.1%)
7	cI	0.43	1/1297 (0.1%)	0.70	2/1750 (0.1%)
7	cK	0.37	0/1297	0.57	0/1750
7	cM	0.38	0/1303	0.62	1/1758 (0.1%)
7	dJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	dL	0.41	0/1297	0.62	1/1750 (0.1%)
7	e1	0.37	0/1297	0.57	0/1750
7	e7	0.38	0/1297	0.53	0/1750
7	e9	0.38	0/1297	0.53	0/1750
7	eB	0.37	0/1309	0.59	1/1766 (0.1%)
7	eF	0.49	1/1297 (0.1%)	0.73	3/1750 (0.2%)
7	eI	0.49	1/1297 (0.1%)	0.73	3/1750 (0.2%)
7	eK	0.37	0/1297	0.57	0/1750
7	eM	0.37	0/1309	0.59	1/1766 (0.1%)
7	fJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	fL	0.41	0/1297	0.62	1/1750 (0.1%)
7	g1	0.37	0/1297	0.57	0/1750
7	g7	0.38	0/1297	0.53	0/1750
7	g9	0.38	0/1297	0.53	0/1750
7	gB	0.37	0/1309	0.59	1/1766 (0.1%)
7	gF	0.42	0/1297	0.70	2/1750 (0.1%)
7	gI	0.42	0/1297	0.70	2/1750 (0.1%)
7	gK	0.37	0/1297	0.57	0/1750
7	gM	0.37	0/1309	0.59	1/1766 (0.1%)
7	hJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	hL	0.41	0/1297	0.62	1/1750 (0.1%)
7	i1	0.37	0/1303	0.57	0/1758
7	i7	0.37	0/1303	0.52	0/1758
7	i9	0.37	0/1303	0.52	0/1758
7	iB	0.36	0/1309	0.59	0/1766
7	iF	0.42	0/1303	0.68	2/1758 (0.1%)
7	iI	0.42	0/1303	0.68	2/1758 (0.1%)
7	iK	0.37	0/1303	0.57	0/1758
7	iM	0.36	0/1309	0.59	0/1766
7	jJ	0.41	0/1303	0.62	1/1758 (0.1%)
7	jL	0.41	0/1303	0.62	1/1758 (0.1%)
7	k1	0.37	0/1297	0.58	0/1750
7	k7	0.38	0/1297	0.53	0/1750
7	k9	0.38	0/1297	0.53	0/1750
7	kB	0.37	0/1309	0.59	1/1766 (0.1%)
7	kF	0.42	0/1297	0.69	3/1750 (0.2%)
7	kI	0.42	0/1297	0.69	3/1750 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
7	kK	0.37	0/1297	0.58	0/1750
7	kM	0.37	0/1309	0.59	1/1766 (0.1%)
7	lJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	lL	0.41	0/1297	0.62	1/1750 (0.1%)
7	m1	0.37	0/1297	0.59	0/1750
7	m7	0.37	0/1297	0.53	0/1750
7	m9	0.37	0/1297	0.53	0/1750
7	mB	0.38	0/1309	0.61	1/1766 (0.1%)
7	mF	0.42	0/1297	0.67	2/1750 (0.1%)
7	mI	0.42	0/1297	0.67	2/1750 (0.1%)
7	mK	0.37	0/1297	0.59	0/1750
7	mM	0.38	0/1309	0.61	1/1766 (0.1%)
7	nJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	nL	0.41	0/1297	0.62	1/1750 (0.1%)
7	pJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	pL	0.41	0/1297	0.62	1/1750 (0.1%)
7	rJ	0.40	0/1297	0.62	1/1750 (0.1%)
7	rL	0.40	0/1297	0.62	1/1750 (0.1%)
7	tJ	0.41	0/1297	0.62	1/1750 (0.1%)
7	tL	0.41	0/1297	0.62	1/1750 (0.1%)
7	vJ	0.40	0/1297	0.61	1/1750 (0.1%)
7	vL	0.40	0/1297	0.62	1/1750 (0.1%)
8	e2	0.59	0/1973	0.64	2/2657 (0.1%)
8	eR	0.61	0/1973	0.64	2/2657 (0.1%)
9	O3	0.40	1/2936 (0.0%)	0.61	2/3989 (0.1%)
9	OO	0.40	1/2936 (0.0%)	0.61	2/3989 (0.1%)
10	d4	0.79	0/2332	0.71	1/3145 (0.0%)
10	dD	0.80	0/2332	0.71	1/3145 (0.0%)
11	D5	0.34	0/670	0.58	0/904
11	D8	0.35	0/670	0.58	0/904
12	E5	0.33	0/1612	0.51	0/2179
12	E8	0.34	0/1612	0.50	0/2179
13	k6	0.38	0/2233	0.49	0/3024
13	kH	0.37	0/2233	0.50	0/3024
14	MA	0.43	0/1882	0.64	1/2518 (0.0%)
14	MG	0.51	2/1882 (0.1%)	0.70	5/2518 (0.2%)
14	MN	0.43	0/1882	0.65	2/2518 (0.1%)
14	MQ	0.51	1/1882 (0.1%)	0.70	5/2518 (0.2%)
15	bB	0.44	0/3022	0.60	0/4084
15	bM	0.44	1/3022 (0.0%)	0.60	0/4084
16	AB	0.40	0/1843	0.62	3/2469 (0.1%)
16	AM	0.40	0/1843	0.62	3/2469 (0.1%)
16	wJ	0.47	0/1843	0.85	8/2469 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
16	wL	0.47	0/1843	0.85	8/2469 (0.3%)
16	xJ	0.47	0/1843	0.85	8/2469 (0.3%)
16	xL	0.48	0/1843	0.86	8/2469 (0.3%)
17	BB	0.42	0/1932	0.60	1/2590 (0.0%)
17	BM	0.42	0/1932	0.60	1/2590 (0.0%)
17	yJ	0.45	0/1932	0.59	1/2590 (0.0%)
17	yL	0.45	0/1932	0.59	1/2590 (0.0%)
18	MC	0.36	0/2247	0.73	6/3036 (0.2%)
18	ME	0.36	0/2247	0.74	7/3036 (0.2%)
19	zJ	0.45	1/2964 (0.0%)	0.60	0/4003
19	zL	0.45	1/2964 (0.0%)	0.59	0/4003
20	AP	0.34	0/1241	0.48	0/1676
20	CP	0.34	0/1241	0.48	0/1676
20	EP	0.34	0/1241	0.48	0/1676
20	GP	0.34	0/1241	0.48	0/1676
20	JP	0.34	0/1241	0.47	0/1676
20	KP	0.34	0/1241	0.48	0/1676
20	NP	0.34	0/1241	0.48	0/1676
20	PP	0.33	0/1241	0.48	0/1676
20	RP	0.34	0/1241	0.48	0/1676
20	TP	0.34	0/1241	0.48	0/1676
20	cP	0.34	0/1241	0.48	0/1676
20	eP	0.34	0/1241	0.48	0/1676
20	gP	0.34	0/1241	0.48	0/1676
20	iP	0.34	0/1241	0.48	0/1676
20	lP	0.34	0/1241	0.48	0/1676
20	mP	0.34	0/1241	0.48	0/1676
20	pP	0.34	0/1241	0.48	0/1676
20	rP	0.33	0/1241	0.47	0/1676
20	tP	0.34	0/1241	0.49	0/1676
20	vP	0.34	0/1241	0.48	0/1676
21	BP	0.33	0/1226	0.46	0/1655
21	DP	0.34	0/1226	0.47	0/1655
21	FP	0.33	0/1226	0.47	0/1655
21	HP	0.34	0/1226	0.47	0/1655
21	IP	0.34	0/1226	0.47	0/1655
21	LP	0.34	0/1226	0.47	0/1655
21	MP	0.33	0/1226	0.46	0/1655
21	OP	0.34	0/1226	0.47	0/1655
21	QP	0.34	0/1226	0.47	0/1655
21	SP	0.34	0/1226	0.47	0/1655
21	UP	0.34	0/1226	0.47	0/1655
21	dP	0.34	0/1226	0.47	0/1655

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
21	fP	0.34	0/1226	0.47	0/1655
21	hP	0.33	0/1226	0.46	0/1655
21	jP	0.34	0/1226	0.47	0/1655
21	kP	0.34	0/1226	0.47	0/1655
21	nP	0.34	0/1226	0.47	0/1655
21	oP	0.33	0/1226	0.47	0/1655
21	qP	0.34	0/1226	0.47	0/1655
21	sP	0.34	0/1226	0.47	0/1655
21	uP	0.34	0/1226	0.46	0/1655
21	wP	0.34	0/1226	0.47	0/1655
22	VP	0.34	0/1281	0.50	2/1731 (0.1%)
22	xP	0.34	0/1281	0.50	2/1731 (0.1%)
23	WP	0.31	0/1396	0.44	0/1886
23	yP	0.31	0/1396	0.44	0/1886
24	XP	0.39	0/732	0.52	0/981
24	zP	0.39	0/732	0.52	0/981
25	1P	0.31	0/6891	0.47	0/9305
25	YP	0.31	0/6891	0.47	0/9305
26	2P	0.33	0/1027	0.54	0/1399
26	ZP	0.33	0/1027	0.54	0/1399
27	3P	0.30	0/1940	0.51	0/2637
27	aP	0.30	0/1940	0.51	0/2637
28	4P	0.29	0/1574	0.48	0/2154
28	bP	0.29	0/1574	0.47	0/2154
All	All	0.41	44/891758 (0.0%)	0.61	861/1205190 (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
6	U2	0	1
6	UR	0	1
7	A5	0	1
7	A8	0	1
7	C5	0	1
7	C8	0	1
12	E5	0	1
12	E8	0	1
21	LP	0	1
21	jP	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
21	kP	0	1
All	All	0	11

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	eF	69	PRO	N-CD	-9.95	1.33	1.47
7	eI	69	PRO	N-CD	-9.95	1.33	1.47
7	TF	69	PRO	N-CD	-9.94	1.33	1.47
7	TI	69	PRO	N-CD	-9.94	1.33	1.47
6	J5	4	VAL	CB-CG2	-8.97	1.34	1.52

The worst 5 of 861 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I4	59	MET	CG-SD-CE	-14.92	76.33	100.20
7	K4	59	MET	CG-SD-CE	-14.91	76.34	100.20
7	ED	59	MET	CG-SD-CE	-14.91	76.34	100.20
7	G4	59	MET	CG-SD-CE	-14.91	76.35	100.20
7	GD	59	MET	CG-SD-CE	-14.90	76.36	100.20

There are no chirality outliers.

5 of 11 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	A5	33	ASP	Mainchain
7	A8	33	ASP	Mainchain
7	C5	37	ARG	Mainchain
12	E5	161	SER	Peptide
6	U2	163	LEU	Mainchain

5.2 Too-close contacts

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	X1	322/363 (89%)	296 (92%)	26 (8%)	0	100	100
1	X7	322/363 (89%)	283 (88%)	38 (12%)	1 (0%)	41	76
1	X9	322/363 (89%)	283 (88%)	37 (12%)	2 (1%)	25	64
1	XF	322/363 (89%)	283 (88%)	39 (12%)	0	100	100
1	XI	322/363 (89%)	283 (88%)	39 (12%)	0	100	100
1	XK	322/363 (89%)	296 (92%)	26 (8%)	0	100	100
2	A1	255/290 (88%)	241 (94%)	14 (6%)	0	100	100
2	A7	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
2	A9	255/290 (88%)	237 (93%)	18 (7%)	0	100	100
2	AF	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
2	AI	255/290 (88%)	239 (94%)	16 (6%)	0	100	100
2	AK	255/290 (88%)	241 (94%)	14 (6%)	0	100	100
3	B1	225/232 (97%)	207 (92%)	17 (8%)	1 (0%)	34	72
3	B7	228/232 (98%)	206 (90%)	21 (9%)	1 (0%)	34	72
3	B9	228/232 (98%)	205 (90%)	22 (10%)	1 (0%)	34	72
3	BF	229/232 (99%)	207 (90%)	22 (10%)	0	100	100
3	BI	229/232 (99%)	208 (91%)	21 (9%)	0	100	100
3	BK	225/232 (97%)	207 (92%)	17 (8%)	1 (0%)	34	72
4	C1	160/162 (99%)	146 (91%)	12 (8%)	2 (1%)	12	45
4	C7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	C9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	CF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	CI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	CK	160/162 (99%)	146 (91%)	12 (8%)	2 (1%)	12	45
4	E1	160/162 (99%)	153 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	E9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	EF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	EI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	EK	160/162 (99%)	153 (96%)	7 (4%)	0	100	100
4	G1	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	G7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	G9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	GF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	GI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	GK	160/162 (99%)	155 (97%)	5 (3%)	0	100	100
4	I1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	I7	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	64
4	I9	160/162 (99%)	158 (99%)	1 (1%)	1 (1%)	25	64
4	IF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	II	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	IK	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	K1	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	K7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	K9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	KF	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	KI	160/162 (99%)	157 (98%)	3 (2%)	0	100	100
4	KK	160/162 (99%)	158 (99%)	2 (1%)	0	100	100
4	M1	160/162 (99%)	152 (95%)	7 (4%)	1 (1%)	25	64
4	M7	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	M9	160/162 (99%)	159 (99%)	1 (1%)	0	100	100
4	MF	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	MI	160/162 (99%)	156 (98%)	4 (2%)	0	100	100
4	MK	160/162 (99%)	152 (95%)	7 (4%)	1 (1%)	25	64
5	D1	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
5	D7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	D9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	DK	169/172 (98%)	165 (98%)	4 (2%)	0	100	100
5	F1	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	F7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	F9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	FK	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	H1	169/172 (98%)	164 (97%)	4 (2%)	1 (1%)	25	64
5	H7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	H9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	HK	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	J1	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
5	J7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	J9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	JF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	JI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	JK	169/172 (98%)	163 (96%)	6 (4%)	0	100	100
5	L1	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	L7	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	L9	169/172 (98%)	163 (96%)	5 (3%)	1 (1%)	25	64
5	LF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	LI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	LK	169/172 (98%)	162 (96%)	7 (4%)	0	100	100
5	N1	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
5	N7	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	N9	169/172 (98%)	164 (97%)	5 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	NF	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	NI	169/172 (98%)	164 (97%)	5 (3%)	0	100	100
5	NK	169/172 (98%)	162 (96%)	6 (4%)	1 (1%)	25	64
6	A3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	AA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	AC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	AJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AL	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	AN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	AO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	AQ	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	B4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	BD	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	C3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	CA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	CB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	CC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CG	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	CJ	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CL	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	CM	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	CN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	CO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	CQ	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	D4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	DD	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	E3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	EA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	EB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	EC	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	EE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	EG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	EJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	EL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	EM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	EN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	EO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	EQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	F4	162/164 (99%)	147 (91%)	14 (9%)	1 (1%)	25	64
6	FD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	G3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	GA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	GB	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	GC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	GE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	GG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	GJ	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	GL	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	GM	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	GN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	GO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	GQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	H4	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	HD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	I3	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	IA	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	IB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	IE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	IG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	IJ	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IL	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	IN	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	IO	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	IQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	J4	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	J5	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	J8	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	JD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	K3	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	KA	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	KB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	KC	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	KE	162/164 (99%)	151 (93%)	11 (7%)	0	100	100
6	KG	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	KJ	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	KL	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	KM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	KN	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	KO	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	KQ	162/164 (99%)	149 (92%)	13 (8%)	0	100	100
6	L4	162/164 (99%)	148 (91%)	13 (8%)	1 (1%)	25	64
6	LD	162/164 (99%)	146 (90%)	15 (9%)	1 (1%)	25	64
6	M2	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	MB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	ML	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	MR	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	O1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	O2	162/164 (99%)	156 (96%)	5 (3%)	1 (1%)	25	64
6	O7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	O9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	OB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	OF	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	OI	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	OJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	OK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	OL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	OM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	OR	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
6	Q1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	Q2	162/164 (99%)	155 (96%)	5 (3%)	2 (1%)	13	48
6	Q7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	Q9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	QB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	QF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	QI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	QJ	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	QK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	QL	162/164 (99%)	150 (93%)	12 (7%)	0	100	100
6	QM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	QR	162/164 (99%)	155 (96%)	6 (4%)	1 (1%)	25	64
6	S1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	S2	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
6	S7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	S9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	SB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	SJ	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	SK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	SL	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	SM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	SR	162/164 (99%)	158 (98%)	4 (2%)	0	100	100
6	U1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	U2	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	U7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	U9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	UB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	UF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	UI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	UJ	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	UK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	UL	162/164 (99%)	154 (95%)	7 (4%)	1 (1%)	25	64
6	UM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	UR	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	W1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	W2	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	W7	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	W9	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	WB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WJ	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	WK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	WL	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	WM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	WR	162/164 (99%)	157 (97%)	5 (3%)	0	100	100
6	YB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	YJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	YL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	YM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	Z1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	Z7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	Z9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	ZF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	ZI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	ZK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	aB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	aJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	aL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	aM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	b1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	b7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	b9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bF	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bI	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	bK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	cJ	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	48
6	cL	162/164 (99%)	152 (94%)	8 (5%)	2 (1%)	13	48
6	d1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	d7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	d9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	dB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	dF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	dI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	dK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	dM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	eJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	eL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	f1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	f9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	fB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	fF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	fI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	fK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	fM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	gJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	gL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	h1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	h7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	h9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	hB	162/164 (99%)	154 (95%)	8 (5%)	0	100	100
6	hF	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	hI	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	hK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	hM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	iJ	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	48
6	iL	162/164 (99%)	151 (93%)	9 (6%)	2 (1%)	13	48
6	j1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	j7	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	j9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	jB	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	jF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	jI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	jK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	jM	162/164 (99%)	153 (94%)	9 (6%)	0	100	100
6	kJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	kL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	l1	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	l7	162/164 (99%)	156 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	l9	162/164 (99%)	155 (96%)	7 (4%)	0	100	100
6	lB	162/164 (99%)	151 (93%)	10 (6%)	1 (1%)	25	64
6	lF	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	lI	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	lK	162/164 (99%)	156 (96%)	6 (4%)	0	100	100
6	lM	162/164 (99%)	150 (93%)	11 (7%)	1 (1%)	25	64
6	mJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	mL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	oJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	oL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	qJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	qL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	sJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	sL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	uJ	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
6	uL	162/164 (99%)	152 (94%)	10 (6%)	0	100	100
7	A5	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	A8	174/177 (98%)	170 (98%)	3 (2%)	1 (1%)	25	64
7	B3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	B5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	B8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	BA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	BC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	BE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	BG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	BJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	BL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	BN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	BO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	BQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	C4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	C5	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	C8	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	CD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	D3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	DA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	DB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	DC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	DE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	DG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	DJ	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	DL	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	DM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	DN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	DO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	DQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	E4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	ED	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	F3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	F5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	F8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	FA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	FB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	FC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	FE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	FG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	FJ	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
7	FL	174/177 (98%)	164 (94%)	10 (6%)	0	100	100
7	FM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	FN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	FO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	FQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G4	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
7	G5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	G8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	GD	174/177 (98%)	158 (91%)	16 (9%)	0	100	100
7	H3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	H5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	H8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	HA	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
7	HB	176/177 (99%)	176 (100%)	0	0	100	100
7	HC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	HE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	HG	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
7	HJ	174/177 (98%)	160 (92%)	11 (6%)	3 (2%)	9	39
7	HL	174/177 (98%)	160 (92%)	11 (6%)	3 (2%)	9	39
7	HM	176/177 (99%)	176 (100%)	0	0	100	100
7	HN	175/177 (99%)	163 (93%)	12 (7%)	0	100	100
7	HO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	HQ	175/177 (99%)	167 (95%)	8 (5%)	0	100	100
7	I4	175/177 (99%)	159 (91%)	16 (9%)	0	100	100
7	I5	174/177 (98%)	167 (96%)	4 (2%)	3 (2%)	9	39
7	I8	174/177 (98%)	168 (97%)	3 (2%)	3 (2%)	9	39
7	ID	175/177 (99%)	161 (92%)	14 (8%)	0	100	100
7	J3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	JA	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	25	64
7	JB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	JC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	JJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JL	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	JM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	JN	174/177 (98%)	161 (92%)	12 (7%)	1 (1%)	25	64
7	JO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	JQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	K4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	K5	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	K8	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	KD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	L3	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	L5	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	L8	143/177 (81%)	136 (95%)	7 (5%)	0	100	100
7	LA	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	LB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	LC	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LE	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LG	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	LJ	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LL	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	LM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	LN	174/177 (98%)	163 (94%)	11 (6%)	0	100	100
7	LO	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	LQ	174/177 (98%)	166 (95%)	8 (5%)	0	100	100
7	M3	143/177 (81%)	128 (90%)	15 (10%)	0	100	100
7	M4	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	MD	174/177 (98%)	159 (91%)	15 (9%)	0	100	100
7	MO	143/177 (81%)	128 (90%)	15 (10%)	0	100	100
7	N2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	N3	143/177 (81%)	130 (91%)	13 (9%)	0	100	100
7	NB	176/177 (99%)	173 (98%)	2 (1%)	1 (1%)	25	64
7	NJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	NL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	NM	176/177 (99%)	173 (98%)	2 (1%)	1 (1%)	25	64

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	NO	143/177 (81%)	130 (91%)	13 (9%)	0	100	100
7	NR	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	P1	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	P2	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	P7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	P9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	PB	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
7	PF	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	PI	174/177 (98%)	169 (97%)	4 (2%)	1 (1%)	25	64
7	PJ	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	PK	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	PL	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	PM	174/177 (98%)	172 (99%)	2 (1%)	0	100	100
7	PR	175/177 (99%)	167 (95%)	7 (4%)	1 (1%)	25	64
7	R1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	R2	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	R7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	R9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	RB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	RF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	RK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	RL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	RM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	RR	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	T1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	T2	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	T7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	T9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	TF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	TJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	TK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	TL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	TM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	TR	174/177 (98%)	168 (97%)	4 (2%)	2 (1%)	14	50
7	V1	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
7	V2	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	V7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	V9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	VB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	VF	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
7	VI	176/177 (99%)	171 (97%)	5 (3%)	0	100	100
7	VJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	VK	176/177 (99%)	172 (98%)	4 (2%)	0	100	100
7	VL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	VM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	VR	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	X2	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	XB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	XJ	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	XL	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	XM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	XR	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	Y1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	Y7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	Y9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	YF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	YI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	YK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	ZB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	ZJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	ZL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	ZM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	a1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	a7	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	a9	174/177 (98%)	168 (97%)	6 (3%)	0	100	100
7	aF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	aI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	aK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	bJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	bL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	c1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	c7	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	25	64
7	c9	174/177 (98%)	167 (96%)	6 (3%)	1 (1%)	25	64
7	cB	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	cF	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
7	cI	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
7	cK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	cM	175/177 (99%)	174 (99%)	1 (1%)	0	100	100
7	dJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	dL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	e1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	e7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	e9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	eB	176/177 (99%)	172 (98%)	2 (1%)	2 (1%)	14	50
7	eF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	eM	176/177 (99%)	172 (98%)	2 (1%)	2 (1%)	14	50
7	fJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	fL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	g1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	g7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	g9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gB	176/177 (99%)	176 (100%)	0	0	100	100
7	gF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	gK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	gM	176/177 (99%)	176 (100%)	0	0	100	100
7	hJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	hL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	i1	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
7	i7	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	i9	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	iF	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iI	175/177 (99%)	170 (97%)	5 (3%)	0	100	100
7	iK	175/177 (99%)	171 (98%)	4 (2%)	0	100	100
7	iM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	jJ	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	jL	175/177 (99%)	172 (98%)	3 (2%)	0	100	100
7	k1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	k7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	k9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kB	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	kF	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kI	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	kK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	kM	176/177 (99%)	174 (99%)	2 (1%)	0	100	100
7	lJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	lL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	m1	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	m7	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	m9	174/177 (98%)	169 (97%)	5 (3%)	0	100	100
7	mB	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	mF	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mI	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mK	174/177 (98%)	170 (98%)	4 (2%)	0	100	100
7	mM	176/177 (99%)	175 (99%)	1 (1%)	0	100	100
7	nJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	nL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	pJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	pL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	rJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	rL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	tJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	tL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	vJ	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
7	vL	174/177 (98%)	171 (98%)	3 (2%)	0	100	100
8	e2	246/303 (81%)	223 (91%)	21 (8%)	2 (1%)	19	57
8	eR	246/303 (81%)	224 (91%)	20 (8%)	2 (1%)	19	57
9	O3	373/405 (92%)	344 (92%)	29 (8%)	0	100	100
9	OO	373/405 (92%)	344 (92%)	29 (8%)	0	100	100
10	d4	295/342 (86%)	260 (88%)	33 (11%)	2 (1%)	22	60
10	dD	295/342 (86%)	260 (88%)	34 (12%)	1 (0%)	41	76
11	D5	79/327 (24%)	73 (92%)	6 (8%)	0	100	100
11	D8	79/327 (24%)	73 (92%)	6 (8%)	0	100	100
12	E5	199/288 (69%)	192 (96%)	7 (4%)	0	100	100
12	E8	199/288 (69%)	192 (96%)	7 (4%)	0	100	100
13	k6	283/288 (98%)	257 (91%)	26 (9%)	0	100	100
13	kH	283/288 (98%)	257 (91%)	25 (9%)	1 (0%)	34	72
14	MA	236/333 (71%)	221 (94%)	14 (6%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	MG	236/333 (71%)	208 (88%)	24 (10%)	4 (2%)	9	39
14	MN	236/333 (71%)	220 (93%)	16 (7%)	0	100	100
14	MQ	236/333 (71%)	209 (89%)	25 (11%)	2 (1%)	19	57
15	bB	378/490 (77%)	352 (93%)	23 (6%)	3 (1%)	19	57
15	bM	378/490 (77%)	351 (93%)	24 (6%)	3 (1%)	19	57
16	AB	236/273 (86%)	229 (97%)	6 (2%)	1 (0%)	34	72
16	AM	236/273 (86%)	229 (97%)	6 (2%)	1 (0%)	34	72
16	wJ	236/273 (86%)	221 (94%)	12 (5%)	3 (1%)	12	45
16	wL	236/273 (86%)	221 (94%)	12 (5%)	3 (1%)	12	45
16	xJ	236/273 (86%)	221 (94%)	13 (6%)	2 (1%)	19	57
16	xL	236/273 (86%)	221 (94%)	13 (6%)	2 (1%)	19	57
17	BB	248/290 (86%)	241 (97%)	7 (3%)	0	100	100
17	BM	248/290 (86%)	241 (97%)	7 (3%)	0	100	100
17	yJ	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
17	yL	248/290 (86%)	239 (96%)	9 (4%)	0	100	100
18	MC	278/316 (88%)	214 (77%)	50 (18%)	14 (5%)	2	12
18	ME	278/316 (88%)	210 (76%)	51 (18%)	17 (6%)	1	8
19	zJ	368/498 (74%)	339 (92%)	26 (7%)	3 (1%)	19	57
19	zL	368/498 (74%)	339 (92%)	26 (7%)	3 (1%)	19	57
20	AP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	CP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	EP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	GP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	JP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
20	KP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	NP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	PP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	RP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	TP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	cP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	eP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	gP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	iP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	lP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	mP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	pP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	rP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	tP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
20	vP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	BP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	DP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	FP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	HP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	IP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	LP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	MP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	OP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	QP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	SP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	UP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	dP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	fP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	hP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	jP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	kP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	nP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	oP	158/161 (98%)	153 (97%)	5 (3%)	0	100	100
21	qP	158/161 (98%)	155 (98%)	3 (2%)	0	100	100
21	sP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	uP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
21	wP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
22	VP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	xP	158/161 (98%)	154 (98%)	4 (2%)	0	100	100
23	WP	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
23	yP	171/173 (99%)	164 (96%)	7 (4%)	0	100	100
24	XP	90/132 (68%)	87 (97%)	3 (3%)	0	100	100
24	zP	90/132 (68%)	87 (97%)	3 (3%)	0	100	100
25	1P	840/879 (96%)	787 (94%)	53 (6%)	0	100	100
25	YP	840/879 (96%)	788 (94%)	50 (6%)	2 (0%)	47	82
26	2P	130/159 (82%)	119 (92%)	11 (8%)	0	100	100
26	ZP	130/159 (82%)	117 (90%)	13 (10%)	0	100	100
27	3P	251/288 (87%)	228 (91%)	22 (9%)	1 (0%)	34	72
27	aP	251/288 (87%)	229 (91%)	21 (8%)	1 (0%)	34	72
28	4P	205/253 (81%)	191 (93%)	14 (7%)	0	100	100
28	bP	205/253 (81%)	191 (93%)	13 (6%)	1 (0%)	29	68
All	All	115760/120800 (96%)	110526 (96%)	5057 (4%)	177 (0%)	50	82

5 of 177 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C1	13	ASP
5	N1	18	PHE
6	Q2	146	ALA
6	I3	143	ASP
10	d4	284	LEU

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	X1	261/290 (90%)	259 (99%)	2 (1%)	81	93
1	X7	261/290 (90%)	257 (98%)	4 (2%)	65	87
1	X9	261/290 (90%)	257 (98%)	4 (2%)	65	87

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	XF	261/290 (90%)	260 (100%)	1 (0%)	91	97
1	XI	260/290 (90%)	259 (100%)	1 (0%)	91	97
1	XK	261/290 (90%)	259 (99%)	2 (1%)	81	93
2	A1	199/222 (90%)	196 (98%)	3 (2%)	65	87
2	A7	199/222 (90%)	199 (100%)	0	100	100
2	A9	199/222 (90%)	199 (100%)	0	100	100
2	AF	199/222 (90%)	198 (100%)	1 (0%)	88	96
2	AI	199/222 (90%)	198 (100%)	1 (0%)	88	96
2	AK	199/222 (90%)	196 (98%)	3 (2%)	65	87
3	B1	208/211 (99%)	201 (97%)	7 (3%)	37	72
3	B7	209/211 (99%)	197 (94%)	12 (6%)	20	56
3	B9	209/211 (99%)	197 (94%)	12 (6%)	20	56
3	BF	210/211 (100%)	209 (100%)	1 (0%)	88	96
3	BI	210/211 (100%)	207 (99%)	3 (1%)	67	88
3	BK	208/211 (99%)	200 (96%)	8 (4%)	33	69
4	C1	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	C7	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	C9	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	CF	125/125 (100%)	125 (100%)	0	100	100
4	CI	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	CK	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	E1	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	E7	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	E9	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	EF	125/125 (100%)	125 (100%)	0	100	100
4	EI	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	EK	125/125 (100%)	117 (94%)	8 (6%)	17	51
4	G1	125/125 (100%)	121 (97%)	4 (3%)	39	74
4	G7	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	G9	125/125 (100%)	115 (92%)	10 (8%)	12	40
4	GF	125/125 (100%)	125 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	GI	125/125 (100%)	125 (100%)	0	100	100
4	GK	125/125 (100%)	121 (97%)	4 (3%)	39	74
4	I1	125/125 (100%)	123 (98%)	2 (2%)	62	86
4	I7	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	I9	125/125 (100%)	114 (91%)	11 (9%)	10	36
4	IF	125/125 (100%)	125 (100%)	0	100	100
4	II	125/125 (100%)	125 (100%)	0	100	100
4	IK	125/125 (100%)	124 (99%)	1 (1%)	81	93
4	K1	125/125 (100%)	123 (98%)	2 (2%)	62	86
4	K7	125/125 (100%)	113 (90%)	12 (10%)	8	32
4	K9	125/125 (100%)	113 (90%)	12 (10%)	8	32
4	KF	125/125 (100%)	125 (100%)	0	100	100
4	KI	125/125 (100%)	125 (100%)	0	100	100
4	KK	125/125 (100%)	122 (98%)	3 (2%)	49	79
4	M1	125/125 (100%)	120 (96%)	5 (4%)	31	68
4	M7	125/125 (100%)	116 (93%)	9 (7%)	14	45
4	M9	125/125 (100%)	116 (93%)	9 (7%)	14	45
4	MF	125/125 (100%)	125 (100%)	0	100	100
4	MI	125/125 (100%)	125 (100%)	0	100	100
4	MK	125/125 (100%)	120 (96%)	5 (4%)	31	68
5	D1	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	D7	134/134 (100%)	113 (84%)	21 (16%)	2	13
5	D9	134/134 (100%)	113 (84%)	21 (16%)	2	13
5	DF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	DI	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	DK	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	F1	134/134 (100%)	125 (93%)	9 (7%)	16	49
5	F7	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	F9	134/134 (100%)	114 (85%)	20 (15%)	3	14
5	FF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	FI	134/134 (100%)	134 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	FK	134/134 (100%)	124 (92%)	10 (8%)	13	43
5	H1	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	H7	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	H9	134/134 (100%)	112 (84%)	22 (16%)	2	11
5	HF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	HI	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	HK	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	J1	134/134 (100%)	125 (93%)	9 (7%)	16	49
5	J7	134/134 (100%)	115 (86%)	19 (14%)	3	16
5	J9	134/134 (100%)	115 (86%)	19 (14%)	3	16
5	JF	134/134 (100%)	133 (99%)	1 (1%)	84	94
5	JI	134/134 (100%)	132 (98%)	2 (2%)	65	87
5	JK	134/134 (100%)	124 (92%)	10 (8%)	13	43
5	L1	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	L7	134/134 (100%)	116 (87%)	18 (13%)	4	17
5	L9	134/134 (100%)	116 (87%)	18 (13%)	4	17
5	LF	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	LI	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	LK	134/134 (100%)	130 (97%)	4 (3%)	41	75
5	N1	134/134 (100%)	127 (95%)	7 (5%)	23	59
5	N7	134/134 (100%)	117 (87%)	17 (13%)	4	19
5	N9	134/134 (100%)	117 (87%)	17 (13%)	4	19
5	NF	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	NI	134/134 (100%)	131 (98%)	3 (2%)	52	81
5	NK	134/134 (100%)	127 (95%)	7 (5%)	23	59
6	A3	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	AA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	AC	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AE	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AG	128/128 (100%)	112 (88%)	16 (12%)	4	20
6	AJ	128/128 (100%)	120 (94%)	8 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	AL	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	AN	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	AO	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	AQ	128/128 (100%)	112 (88%)	16 (12%)	4	20
6	B4	128/128 (100%)	113 (88%)	15 (12%)	5	22
6	BD	128/128 (100%)	113 (88%)	15 (12%)	5	22
6	C3	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	CA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	CB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CC	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	CE	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	CG	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	CJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	CN	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	CO	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	CQ	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	D4	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	DD	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	E3	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	EA	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	EB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	EC	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	EE	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	EG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	EJ	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	EL	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	EM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	EN	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	EO	128/128 (100%)	119 (93%)	9 (7%)	15	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	EQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	F4	128/128 (100%)	104 (81%)	24 (19%)	1	8
6	FD	128/128 (100%)	103 (80%)	25 (20%)	1	7
6	G3	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GA	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GB	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GC	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	GE	128/128 (100%)	117 (91%)	11 (9%)	10	37
6	GG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	GJ	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GL	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GM	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GN	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	GO	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	GQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	H4	128/128 (100%)	106 (83%)	22 (17%)	2	10
6	HD	128/128 (100%)	106 (83%)	22 (17%)	2	10
6	I3	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IA	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	IC	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	IE	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	IG	128/128 (100%)	111 (87%)	17 (13%)	4	17
6	IJ	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	IL	128/128 (100%)	118 (92%)	10 (8%)	12	42
6	IM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	IN	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IO	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	IQ	128/128 (100%)	111 (87%)	17 (13%)	4	17
6	J4	128/128 (100%)	109 (85%)	19 (15%)	3	14
6	J5	128/128 (100%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J8	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	JD	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	K3	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KA	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	KC	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	KE	128/128 (100%)	119 (93%)	9 (7%)	15	47
6	KG	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	KJ	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	KL	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	KM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	KN	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KO	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	KQ	128/128 (100%)	110 (86%)	18 (14%)	3	16
6	L4	128/128 (100%)	107 (84%)	21 (16%)	2	11
6	LD	128/128 (100%)	108 (84%)	20 (16%)	2	13
6	M2	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	MB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	MJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	ML	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	MM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	MR	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	O1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	O2	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	O7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	O9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	OB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OJ	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OK	128/128 (100%)	127 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	OL	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	OR	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	Q1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	Q2	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	Q7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	Q9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	QB	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QJ	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	QL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QM	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	QR	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	S1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	S2	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	S7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	S9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	SB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	SK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	SM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	SR	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	U1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	U2	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	U7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	U9	128/128 (100%)	120 (94%)	8 (6%)	18	51

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	UB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	UK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	UL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	UM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	UR	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	W1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	W2	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	W7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	W9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	WB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	WI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	WJ	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	WK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	WM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	WR	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	YB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	YJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	YL	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	YM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	Z1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	Z7	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	Z9	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	ZF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	ZI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	ZK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	aB	128/128 (100%)	127 (99%)	1 (1%)	81	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	aJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	aL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	aM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	b1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	b7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	b9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	bF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	bI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	bK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	cJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	cL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	d1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	d7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	d9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	dB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	dF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	dI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	dK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	dM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	eJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	eL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	f1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	f7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	f9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	fB	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	fK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	fM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	gJ	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	gL	128/128 (100%)	126 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	h1	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	h7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	h9	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	hB	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	hF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	hM	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	iJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	iL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	j1	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	j7	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	j9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	jB	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	jF	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	jI	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	jK	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	jM	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	kJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	kL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	l1	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	l7	128/128 (100%)	120 (94%)	8 (6%)	18	51
6	l9	128/128 (100%)	121 (94%)	7 (6%)	21	57
6	lB	128/128 (100%)	125 (98%)	3 (2%)	50	80
6	lF	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	lI	128/128 (100%)	127 (99%)	1 (1%)	81	93
6	lK	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	lM	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	mJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	mL	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	oJ	128/128 (100%)	126 (98%)	2 (2%)	62	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	oL	128/128 (100%)	126 (98%)	2 (2%)	62	86
6	qJ	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	qL	128/128 (100%)	122 (95%)	6 (5%)	26	63
6	sJ	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	sL	128/128 (100%)	123 (96%)	5 (4%)	32	69
6	uJ	128/128 (100%)	124 (97%)	4 (3%)	40	75
6	uL	128/128 (100%)	124 (97%)	4 (3%)	40	75
7	A5	137/137 (100%)	121 (88%)	16 (12%)	5	22
7	A8	137/137 (100%)	121 (88%)	16 (12%)	5	22
7	B3	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	B5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	B8	113/137 (82%)	109 (96%)	4 (4%)	36	71
7	BA	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	BC	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	BE	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	BG	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	BJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BN	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	BO	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	BQ	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	C4	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	C5	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	C8	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	CD	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	D3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	DA	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	DB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	DC	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	DE	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	DG	137/137 (100%)	125 (91%)	12 (9%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	DJ	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	DL	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	DM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	DN	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	DO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	DQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	E4	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	ED	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	F3	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	F5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	F8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	FA	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	FB	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	FC	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	FE	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	FG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	FJ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	FL	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	FM	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	FN	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	FO	137/137 (100%)	127 (93%)	10 (7%)	14	44
7	FQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	G4	137/137 (100%)	104 (76%)	33 (24%)	0	3
7	G5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	G8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	GD	137/137 (100%)	105 (77%)	32 (23%)	1	4
7	H3	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	H5	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	H8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	HA	138/137 (101%)	127 (92%)	11 (8%)	12	40
7	HB	139/137 (102%)	134 (96%)	5 (4%)	35	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	HC	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	HE	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	HG	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	HJ	137/137 (100%)	119 (87%)	18 (13%)	4	18
7	HL	137/137 (100%)	119 (87%)	18 (13%)	4	18
7	HM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	HN	138/137 (101%)	127 (92%)	11 (8%)	12	40
7	HO	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	HQ	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	I4	138/137 (101%)	118 (86%)	20 (14%)	3	15
7	I5	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	I8	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	ID	138/137 (101%)	118 (86%)	20 (14%)	3	15
7	J3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	JA	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	JB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	JC	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	JE	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	JG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	JJ	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	JL	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	JM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	JN	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	JO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	JQ	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	K4	137/137 (100%)	108 (79%)	29 (21%)	1	5
7	K5	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	K8	137/137 (100%)	120 (88%)	17 (12%)	4	20
7	KD	137/137 (100%)	109 (80%)	28 (20%)	1	6
7	L3	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	L5	113/137 (82%)	109 (96%)	4 (4%)	36	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	L8	113/137 (82%)	108 (96%)	5 (4%)	28	65
7	LA	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	LB	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	LC	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	LE	137/137 (100%)	122 (89%)	15 (11%)	6	25
7	LG	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	LJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	LL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	LM	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	LN	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	LO	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	LQ	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	M3	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	M4	137/137 (100%)	108 (79%)	29 (21%)	1	5
7	MD	137/137 (100%)	107 (78%)	30 (22%)	1	5
7	MO	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	N2	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	N3	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	NB	139/137 (102%)	133 (96%)	6 (4%)	29	66
7	NJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	NL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	NM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	NO	113/137 (82%)	102 (90%)	11 (10%)	8	31
7	NR	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	P1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	P2	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	P7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	P9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	PB	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	PF	137/137 (100%)	137 (100%)	0	100	100
7	PI	137/137 (100%)	137 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	PJ	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	PK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	PL	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	PM	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	PR	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	R1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	R2	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	R7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	R9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	RB	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	RF	137/137 (100%)	137 (100%)	0	100	100
7	RI	137/137 (100%)	137 (100%)	0	100	100
7	RJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	RM	138/137 (101%)	132 (96%)	6 (4%)	29	66
7	RR	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T2	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	T7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	T9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	TB	138/137 (101%)	133 (96%)	5 (4%)	35	70
7	TF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	TK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	TL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	TM	138/137 (101%)	133 (96%)	5 (4%)	35	70
7	TR	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	V1	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	V2	137/137 (100%)	133 (97%)	4 (3%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	V7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	V9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	VB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	VF	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	VI	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	VJ	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	VK	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	VL	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	VM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	VR	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	X2	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	XB	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	XJ	138/137 (101%)	137 (99%)	1 (1%)	84	94
7	XL	138/137 (101%)	137 (99%)	1 (1%)	84	94
7	XM	139/137 (102%)	138 (99%)	1 (1%)	84	94
7	XR	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	Y1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	Y7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	Y9	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	YF	137/137 (100%)	137 (100%)	0	100	100
7	YI	137/137 (100%)	137 (100%)	0	100	100
7	YK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	ZB	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	ZJ	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	ZL	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	ZM	139/137 (102%)	134 (96%)	5 (4%)	35	70
7	a1	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	a7	137/137 (100%)	124 (90%)	13 (10%)	8	32
7	a9	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	aF	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	aI	137/137 (100%)	136 (99%)	1 (1%)	84	94

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	aK	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	bJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	bL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	c1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	c7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	c9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	cB	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	cF	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	cI	137/137 (100%)	134 (98%)	3 (2%)	52	81
7	cK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	cM	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	dJ	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	dL	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	e1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	e7	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	e9	137/137 (100%)	123 (90%)	14 (10%)	7	28
7	eB	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	eF	137/137 (100%)	137 (100%)	0	100	100
7	eI	137/137 (100%)	137 (100%)	0	100	100
7	eK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	eM	139/137 (102%)	135 (97%)	4 (3%)	42	76
7	fJ	137/137 (100%)	132 (96%)	5 (4%)	35	70
7	fL	137/137 (100%)	132 (96%)	5 (4%)	35	70
7	g1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	g7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	g9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	gB	139/137 (102%)	132 (95%)	7 (5%)	24	60
7	gF	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	gI	137/137 (100%)	136 (99%)	1 (1%)	84	94
7	gK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	gM	139/137 (102%)	132 (95%)	7 (5%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	hJ	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	hL	137/137 (100%)	133 (97%)	4 (3%)	42	76
7	i1	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	i7	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	i9	138/137 (101%)	126 (91%)	12 (9%)	10	37
7	iB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	iF	138/137 (101%)	135 (98%)	3 (2%)	52	81
7	iI	138/137 (101%)	135 (98%)	3 (2%)	52	81
7	iK	138/137 (101%)	136 (99%)	2 (1%)	67	88
7	iM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	jJ	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	jL	138/137 (101%)	134 (97%)	4 (3%)	42	76
7	k1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	k7	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	k9	137/137 (100%)	125 (91%)	12 (9%)	10	36
7	kB	139/137 (102%)	131 (94%)	8 (6%)	20	55
7	kF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	kM	139/137 (102%)	131 (94%)	8 (6%)	20	55
7	lJ	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	lL	137/137 (100%)	128 (93%)	9 (7%)	16	49
7	m1	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	m7	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	m9	137/137 (100%)	126 (92%)	11 (8%)	12	40
7	mB	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	mF	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mI	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mK	137/137 (100%)	135 (98%)	2 (2%)	65	87
7	mM	139/137 (102%)	136 (98%)	3 (2%)	52	81
7	nJ	137/137 (100%)	130 (95%)	7 (5%)	24	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	nL	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	pJ	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	pL	137/137 (100%)	130 (95%)	7 (5%)	24	60
7	rJ	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	rL	137/137 (100%)	131 (96%)	6 (4%)	28	65
7	tJ	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	tL	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	vJ	137/137 (100%)	129 (94%)	8 (6%)	20	55
7	vL	137/137 (100%)	129 (94%)	8 (6%)	20	55
8	e2	204/237 (86%)	197 (97%)	7 (3%)	37	72
8	eR	204/237 (86%)	197 (97%)	7 (3%)	37	72
9	O3	312/331 (94%)	308 (99%)	4 (1%)	69	89
9	OO	312/331 (94%)	308 (99%)	4 (1%)	69	89
10	d4	247/278 (89%)	244 (99%)	3 (1%)	71	90
10	dD	247/278 (89%)	243 (98%)	4 (2%)	62	86
11	D5	72/268 (27%)	72 (100%)	0	100	100
11	D8	72/268 (27%)	72 (100%)	0	100	100
12	E5	164/223 (74%)	164 (100%)	0	100	100
12	E8	164/223 (74%)	164 (100%)	0	100	100
13	k6	227/229 (99%)	211 (93%)	16 (7%)	15	47
13	kH	227/229 (99%)	211 (93%)	16 (7%)	15	47
14	MA	184/262 (70%)	178 (97%)	6 (3%)	38	73
14	MG	184/262 (70%)	180 (98%)	4 (2%)	52	81
14	MN	184/262 (70%)	177 (96%)	7 (4%)	33	69
14	MQ	184/262 (70%)	179 (97%)	5 (3%)	44	77
15	bB	304/389 (78%)	295 (97%)	9 (3%)	41	75
15	bM	304/389 (78%)	294 (97%)	10 (3%)	38	73
16	AB	179/203 (88%)	179 (100%)	0	100	100
16	AM	179/203 (88%)	179 (100%)	0	100	100
16	wJ	179/203 (88%)	165 (92%)	14 (8%)	12	42
16	wL	179/203 (88%)	165 (92%)	14 (8%)	12	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	xJ	179/203 (88%)	165 (92%)	14 (8%)	12	42
16	xL	179/203 (88%)	166 (93%)	13 (7%)	14	44
17	BB	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	BM	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	yJ	188/218 (86%)	187 (100%)	1 (0%)	88	96
17	yL	188/218 (86%)	187 (100%)	1 (0%)	88	96
18	MC	231/256 (90%)	213 (92%)	18 (8%)	12	42
18	ME	231/256 (90%)	218 (94%)	13 (6%)	21	56
19	zJ	303/406 (75%)	299 (99%)	4 (1%)	69	89
19	zL	303/406 (75%)	298 (98%)	5 (2%)	60	85
20	AP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	CP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	EP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	GP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	JP	130/131 (99%)	121 (93%)	9 (7%)	15	48
20	KP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	NP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	PP	130/131 (99%)	121 (93%)	9 (7%)	15	48
20	RP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	TP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	cP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	eP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	gP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	iP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	lP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	mP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	pP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	rP	130/131 (99%)	122 (94%)	8 (6%)	18	52
20	tP	130/131 (99%)	120 (92%)	10 (8%)	13	42
20	vP	130/131 (99%)	120 (92%)	10 (8%)	13	42
21	BP	124/124 (100%)	115 (93%)	9 (7%)	14	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	DP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	FP	124/124 (100%)	113 (91%)	11 (9%)	9	35
21	HP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	IP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	LP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	MP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	OP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	QP	124/124 (100%)	114 (92%)	10 (8%)	11	40
21	SP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	UP	124/124 (100%)	114 (92%)	10 (8%)	11	40
21	dP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	fP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	hP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	jP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	kP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	nP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	oP	124/124 (100%)	113 (91%)	11 (9%)	9	35
21	qP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	sP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	uP	124/124 (100%)	115 (93%)	9 (7%)	14	44
21	wP	124/124 (100%)	114 (92%)	10 (8%)	11	40
22	VP	133/136 (98%)	132 (99%)	1 (1%)	81	93
22	xP	133/136 (98%)	132 (99%)	1 (1%)	81	93
23	WP	147/153 (96%)	147 (100%)	0	100	100
23	yP	147/153 (96%)	147 (100%)	0	100	100
24	XP	78/101 (77%)	77 (99%)	1 (1%)	69	89
24	zP	78/101 (77%)	77 (99%)	1 (1%)	69	89
25	1P	742/772 (96%)	734 (99%)	8 (1%)	73	90
25	YP	742/772 (96%)	734 (99%)	8 (1%)	73	90
26	2P	106/121 (88%)	104 (98%)	2 (2%)	57	84
26	ZP	106/121 (88%)	103 (97%)	3 (3%)	43	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
27	3P	194/214 (91%)	187 (96%)	7 (4%)	35	70
27	aP	194/214 (91%)	186 (96%)	8 (4%)	30	67
28	4P	165/199 (83%)	161 (98%)	4 (2%)	49	79
28	bP	165/199 (83%)	161 (98%)	4 (2%)	49	79
All	All	91927/94464 (97%)	87419 (95%)	4508 (5%)	29	61

5 of 4508 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
7	BO	127	SER
7	NO	147	THR
6	AO	52	VAL
21	nP	158	SER
6	b9	10	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 1080 such sidechains are listed below:

Mol	Chain	Res	Type
21	SP	15	GLN
25	YP	849	ASN
20	RP	71	ASN
7	FQ	35	ASN
4	EF	145	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

308 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
7	MEN	VJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	RJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	a9	72	7	7,8,9	0.70	0	6,9,11	0.80	0
7	MEN	DO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	PI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
21	MEN	oP	71	21	7,8,9	1.13	1 (14%)	6,9,11	0.94	0
7	MEN	rL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	V1	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	Y9	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	L3	72	7	7,8,9	0.72	0	6,9,11	0.66	0
7	MEN	e9	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	kK	72	7	7,8,9	0.70	0	6,9,11	0.91	0
7	MEN	i1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	V9	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	iM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	mF	72	7	7,8,9	0.77	0	6,9,11	0.81	0
7	MEN	FB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	cB	72	7	7,8,9	0.68	0	6,9,11	0.87	0
7	MEN	iK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	NR	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
7	MEN	FL	72	7,29	7,8,9	0.75	0	6,9,11	0.89	0
7	MEN	kI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	eI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	vJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	kB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	H5	72	7	7,8,9	0.72	0	6,9,11	0.65	0
7	MEN	gM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	XB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	PM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
5	MEN	HK	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	HM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	ZB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
5	MEN	HI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	LJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
5	MEN	L7	72	5	7,8,9	0.62	0	6,9,11	0.71	0
7	MEN	iI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	PJ	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	BO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	NJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	F5	72	7	7,8,9	0.72	0	6,9,11	0.64	0
7	MEN	fL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	aK	72	7	7,8,9	0.71	0	6,9,11	0.92	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	DA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	FG	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	jJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	mB	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	BJ	72	7,29	7,8,9	0.75	0	6,9,11	0.91	0
7	MEN	TM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	L8	72	7	7,8,9	0.72	0	6,9,11	0.63	0
7	MEN	HC	72	7	7,8,9	0.66	0	6,9,11	0.75	0
5	MEN	L9	72	5	7,8,9	0.62	0	6,9,11	0.72	0
7	MEN	HL	72	7	7,8,9	0.62	0	6,9,11	1.08	0
5	MEN	JF	72	5	7,8,9	0.70	0	6,9,11	0.90	0
7	MEN	aF	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	Y1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	VK	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	LE	72	7	7,8,9	0.67	0	6,9,11	0.74	0
7	MEN	iB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	VF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	cM	72	7	7,8,9	0.68	0	6,9,11	0.87	0
7	MEN	TI	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	dL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	m1	72	7	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	YK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	fJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	C4	72	7	7,8,9	0.64	0	6,9,11	0.51	0
7	MEN	E4	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	nL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	BC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	k9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	J3	72	7	7,8,9	0.74	0	6,9,11	0.67	0
21	MEN	LP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.38	5 (83%)
7	MEN	k1	72	7	7,8,9	0.70	0	6,9,11	0.91	0
7	MEN	C8	72	7	7,8,9	0.67	0	6,9,11	0.79	0
7	MEN	NB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	PR	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
7	MEN	tJ	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	HO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	GD	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	CD	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	DL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
5	MEN	DI	72	5,1	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	LG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	bL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	gB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	VR	72	7	7,8,9	0.74	0	6,9,11	1.16	1 (16%)
21	MEN	OP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.97	0
7	MEN	vL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	IJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	HG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	HA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	ED	72	7	7,8,9	0.63	0	6,9,11	0.53	0
5	MEN	H9	72	5	7,8,9	0.67	0	6,9,11	0.83	0
7	MEN	TF	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	ID	72	7	7,8,9	0.63	0	6,9,11	0.52	0
7	MEN	HE	72	7	7,8,9	0.66	0	6,9,11	0.75	0
7	MEN	Y7	72	7	7,8,9	0.72	0	6,9,11	0.77	0
5	MEN	FK	72	5	7,8,9	0.71	0	6,9,11	0.88	0
7	MEN	gF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	cF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	G8	72	7	7,8,9	0.72	0	6,9,11	0.64	0
7	MEN	F8	72	7	7,8,9	0.72	0	6,9,11	0.64	0
5	MEN	H7	72	5	7,8,9	0.67	0	6,9,11	0.83	0
7	MEN	TB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	LL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
21	MEN	qP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.99	0
7	MEN	V7	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	eM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	KD	72	7	7,8,9	0.62	0	6,9,11	0.52	0
7	MEN	m7	72	7	7,8,9	0.71	0	6,9,11	0.77	0
7	MEN	FO	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	NL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	H3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	g1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
5	MEN	L1	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	HN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
5	MEN	JK	72	5	7,8,9	0.71	0	6,9,11	0.87	0
21	MEN	fP	71	21	7,8,9	1.16	1 (14%)	6,9,11	1.10	0
7	MEN	B5	72	7	7,8,9	0.73	0	6,9,11	0.65	0
7	MEN	DJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
21	MEN	UP	71	21	7,8,9	0.80	0	6,9,11	0.61	0
7	MEN	JC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	I4	72	7	7,8,9	0.63	0	6,9,11	0.53	0
7	MEN	FQ	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	LN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	hL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	BG	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	PK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	FJ	72	7,29	7,8,9	0.75	0	6,9,11	0.89	0
7	MEN	XM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	MO	72	7	7,8,9	0.69	0	6,9,11	0.75	0
5	MEN	F7	72	5	7,8,9	0.65	0	6,9,11	0.79	0
7	MEN	FM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	e1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	RI	72	7	7,8,9	0.76	0	6,9,11	0.81	0
5	MEN	N1	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	R7	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	JB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	rJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	A5	72	7	7,8,9	0.68	0	6,9,11	0.78	0
7	MEN	DQ	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	c9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	C5	72	7	7,8,9	0.67	0	6,9,11	0.79	0
5	MEN	N9	72	5	7,8,9	0.63	0	6,9,11	0.70	0
7	MEN	JE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	HQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	tL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
5	MEN	J7	72	5	7,8,9	0.66	0	6,9,11	0.84	0
7	MEN	VB	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	LB	72	7	7,8,9	0.67	0	6,9,11	0.87	0
21	MEN	DP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.95	0
7	MEN	VI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	LC	72	7	7,8,9	0.67	0	6,9,11	0.74	0
7	MEN	T1	72	7	7,8,9	0.72	0	6,9,11	0.92	0
7	MEN	e7	72	7	7,8,9	0.71	0	6,9,11	0.78	0
7	MEN	aI	72	7	7,8,9	0.75	0	6,9,11	0.81	0
7	MEN	FN	72	7	7,8,9	0.74	0	6,9,11	0.82	0
7	MEN	DC	72	7	7,8,9	0.67	0	6,9,11	0.73	0
21	MEN	IP	71	21	7,8,9	1.17	1 (14%)	6,9,11	0.86	0
7	MEN	BL	72	7,29	7,8,9	0.75	0	6,9,11	0.91	0
7	MEN	DM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	DG	72	7	7,8,9	0.66	0	6,9,11	0.97	0
7	MEN	eB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	G4	72	7	7,8,9	0.63	0	6,9,11	0.53	0
7	MEN	JA	72	7	7,8,9	0.73	0	6,9,11	0.82	0
21	MEN	kP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.37	5 (83%)
7	MEN	HJ	72	7	7,8,9	0.61	0	6,9,11	1.13	0
7	MEN	L5	72	7	7,8,9	0.72	0	6,9,11	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	NM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	TJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	k7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	JO	72	7	7,8,9	0.74	0	6,9,11	0.67	0
7	MEN	ZJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	cK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
5	MEN	FF	72	5	7,8,9	0.71	0	6,9,11	0.89	0
7	MEN	RB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	gK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	c1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	JL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	i7	72	7	7,8,9	0.70	0	6,9,11	0.78	0
5	MEN	D1	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	JJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	NO	72	7	7,8,9	0.70	0	6,9,11	0.75	0
5	MEN	H1	72	5	7,8,9	0.71	0	6,9,11	0.85	0
7	MEN	V2	72	7	7,8,9	0.75	0	6,9,11	1.15	1 (16%)
21	MEN	BP	71	21	7,8,9	1.16	1 (14%)	6,9,11	1.29	1 (16%)
7	MEN	B3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	nJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	PB	72	7	7,8,9	0.68	0	6,9,11	0.86	0
7	MEN	G5	72	7	7,8,9	0.73	0	6,9,11	0.63	0
7	MEN	gI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	bJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	T9	72	7	7,8,9	0.71	0	6,9,11	0.79	0
7	MEN	LO	72	7	7,8,9	0.72	0	6,9,11	0.66	0
7	MEN	RK	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	I8	72	7	7,8,9	0.69	0	6,9,11	0.76	0
7	MEN	M4	72	7	7,8,9	0.61	0	6,9,11	0.53	0
7	MEN	A8	72	7	7,8,9	0.68	0	6,9,11	0.77	0
7	MEN	g7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	T7	72	7	7,8,9	0.71	0	6,9,11	0.79	0
5	MEN	F1	72	5	7,8,9	0.71	0	6,9,11	0.88	0
7	MEN	K5	72	7	7,8,9	0.68	0	6,9,11	0.78	0
5	MEN	JI	72	5	7,8,9	0.70	0	6,9,11	0.90	0
5	MEN	LF	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	PL	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	YI	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	VM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
5	MEN	LI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	dJ	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	PF	72	7	7,8,9	0.75	0	6,9,11	0.82	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	kF	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	g9	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	P2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
21	MEN	MP	71	21	7,8,9	1.13	1 (14%)	6,9,11	0.96	0
7	MEN	DB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	XJ	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	K8	72	7	7,8,9	0.68	0	6,9,11	0.78	0
21	MEN	uP	71	21	7,8,9	0.64	0	6,9,11	0.96	0
7	MEN	i9	72	7	7,8,9	0.70	0	6,9,11	0.78	0
7	MEN	BE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
5	MEN	LK	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	TK	72	7	7,8,9	0.72	0	6,9,11	0.92	0
7	MEN	BQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	BA	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	FA	72	7	7,8,9	0.74	0	6,9,11	0.82	0
7	MEN	DN	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	jL	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
5	MEN	NI	72	5	7,8,9	0.71	0	6,9,11	0.90	0
7	MEN	pL	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	c7	72	7	7,8,9	0.72	0	6,9,11	0.78	0
7	MEN	ZM	72	7	7,8,9	0.68	0	6,9,11	0.86	0
5	MEN	D7	72	5	7,8,9	0.65	0	6,9,11	0.87	0
7	MEN	YF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	K4	72	7	7,8,9	0.62	0	6,9,11	0.52	0
5	MEN	DK	72	5	7,8,9	0.71	0	6,9,11	0.86	0
7	MEN	cI	72	7	7,8,9	0.75	0	6,9,11	0.82	0
7	MEN	mI	72	7	7,8,9	0.77	0	6,9,11	0.81	0
7	MEN	R2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
7	MEN	FC	72	7	7,8,9	0.66	0	6,9,11	0.74	0
7	MEN	MD	72	7	7,8,9	0.62	0	6,9,11	0.54	0
7	MEN	HB	72	7	7,8,9	0.67	0	6,9,11	0.86	0
21	MEN	jP	71	21	7,8,9	8.57	4 (57%)	6,9,11	12.38	5 (83%)
7	MEN	I5	72	7	7,8,9	0.69	0	6,9,11	0.76	0
7	MEN	H8	72	7	7,8,9	0.74	0	6,9,11	0.64	0
5	MEN	J1	72	5	7,8,9	0.71	0	6,9,11	0.87	0
7	MEN	mM	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	D3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
7	MEN	N3	72	7	7,8,9	0.69	0	6,9,11	0.73	0
7	MEN	XR	72	7	7,8,9	0.76	0	6,9,11	1.14	1 (16%)
7	MEN	eK	72	7	7,8,9	0.71	0	6,9,11	0.92	0
7	MEN	F3	72	7	7,8,9	0.73	0	6,9,11	0.66	0
5	MEN	HF	72	5	7,8,9	0.71	0	6,9,11	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	MEN	NK	72	5	7,8,9	0.70	0	6,9,11	0.87	0
7	MEN	VL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	LQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
5	MEN	NF	72	5	7,8,9	0.71	0	6,9,11	0.90	0
5	MEN	FI	72	5	7,8,9	0.71	0	6,9,11	0.89	0
7	MEN	P9	72	7	7,8,9	0.72	0	6,9,11	0.79	0
5	MEN	D9	72	5	7,8,9	0.65	0	6,9,11	0.87	0
7	MEN	kM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	P1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
7	MEN	RM	72	7	7,8,9	0.67	0	6,9,11	0.86	0
7	MEN	XL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	TL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	M3	72	7	7,8,9	0.69	0	6,9,11	0.75	0
7	MEN	TR	72	7	7,8,9	0.74	0	6,9,11	1.16	1 (16%)
21	MEN	HP	71	21	7,8,9	1.18	1 (14%)	6,9,11	0.97	0
7	MEN	a7	72	7	7,8,9	0.70	0	6,9,11	0.80	0
7	MEN	JQ	72	7	7,8,9	0.67	0	6,9,11	0.97	0
7	MEN	DE	72	7	7,8,9	0.67	0	6,9,11	0.73	0
21	MEN	sP	71	21	7,8,9	0.63	0	6,9,11	0.78	0
7	MEN	hJ	72	7,29	7,8,9	0.75	0	6,9,11	0.90	0
7	MEN	N2	72	7	7,8,9	0.74	0	6,9,11	1.15	1 (16%)
7	MEN	iF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
7	MEN	BN	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	T2	72	7	7,8,9	0.75	0	6,9,11	1.14	1 (16%)
21	MEN	nP	71	21	7,8,9	1.15	1 (14%)	6,9,11	0.91	0
7	MEN	m9	72	7	7,8,9	0.71	0	6,9,11	0.77	0
7	MEN	P7	72	7	7,8,9	0.72	0	6,9,11	0.79	0
7	MEN	B8	72	7	7,8,9	0.73	0	6,9,11	0.65	0
7	MEN	RL	72	7,29	7,8,9	0.76	0	6,9,11	0.90	0
7	MEN	IL	72	7,29	7,8,9	0.77	0	6,9,11	0.89	0
7	MEN	R9	72	7	7,8,9	0.72	0	6,9,11	0.77	0
7	MEN	LA	72	7	7,8,9	0.74	0	6,9,11	0.83	0
7	MEN	pJ	72	7,29	7,8,9	0.77	0	6,9,11	0.90	0
7	MEN	a1	72	7	7,8,9	0.71	0	6,9,11	0.92	0
21	MEN	dP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.93	0
5	MEN	N7	72	5	7,8,9	0.63	0	6,9,11	0.70	0
5	MEN	J9	72	5	7,8,9	0.65	0	6,9,11	0.84	0
7	MEN	R1	72	7	7,8,9	0.70	0	6,9,11	0.92	0
21	MEN	wP	71	21	7,8,9	0.79	0	6,9,11	0.63	0
7	MEN	JN	72	7	7,8,9	0.73	0	6,9,11	0.82	0
7	MEN	RF	72	7	7,8,9	0.76	0	6,9,11	0.81	0
7	MEN	JG	72	7	7,8,9	0.67	0	6,9,11	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MEN	JM	72	7	7,8,9	0.68	0	6,9,11	0.85	0
7	MEN	mK	72	7	7,8,9	0.71	0	6,9,11	0.91	0
21	MEN	FP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.86	0
5	MEN	DF	72	5,1	7,8,9	0.71	0	6,9,11	0.91	0
7	MEN	X2	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
21	MEN	hP	71	21	7,8,9	1.14	1 (14%)	6,9,11	0.96	0
7	MEN	eF	72	7	7,8,9	0.76	0	6,9,11	0.82	0
21	MEN	SP	71	21	7,8,9	0.63	0	6,9,11	0.99	0
7	MEN	RR	72	7	7,8,9	0.76	0	6,9,11	1.15	1 (16%)
7	MEN	ZL	72	7,29	7,8,9	0.76	0	6,9,11	0.89	0
7	MEN	LM	72	7	7,8,9	0.67	0	6,9,11	0.87	0
7	MEN	FE	72	7	7,8,9	0.66	0	6,9,11	0.74	0
5	MEN	F9	72	5	7,8,9	0.65	0	6,9,11	0.78	0
21	MEN	QP	71	21	7,8,9	0.63	0	6,9,11	0.76	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	VJ	72	7,29	-	4/7/8/10	-
7	MEN	RJ	72	7,29	-	4/7/8/10	-
7	MEN	a9	72	7	-	6/7/8/10	-
7	MEN	DO	72	7	-	4/7/8/10	-
7	MEN	PI	72	7	-	6/7/8/10	-
21	MEN	oP	71	21	-	6/7/8/10	-
7	MEN	rL	72	7,29	-	4/7/8/10	-
7	MEN	V1	72	7	-	6/7/8/10	-
7	MEN	Y9	72	7	-	6/7/8/10	-
7	MEN	L3	72	7	-	4/7/8/10	-
7	MEN	e9	72	7	-	6/7/8/10	-
7	MEN	kK	72	7	-	6/7/8/10	-
7	MEN	i1	72	7	-	6/7/8/10	-
7	MEN	V9	72	7	-	6/7/8/10	-
7	MEN	iM	72	7	-	6/7/8/10	-
7	MEN	mF	72	7	-	6/7/8/10	-
7	MEN	FB	72	7	-	6/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	cB	72	7	-	6/7/8/10	-
7	MEN	iK	72	7	-	6/7/8/10	-
7	MEN	NR	72	7	-	3/7/8/10	-
7	MEN	FL	72	7,29	-	4/7/8/10	-
7	MEN	kI	72	7	-	6/7/8/10	-
7	MEN	eI	72	7	-	6/7/8/10	-
7	MEN	vJ	72	7,29	-	4/7/8/10	-
7	MEN	kB	72	7	-	6/7/8/10	-
7	MEN	H5	72	7	-	2/7/8/10	-
7	MEN	gM	72	7	-	6/7/8/10	-
7	MEN	XB	72	7	-	6/7/8/10	-
7	MEN	PM	72	7	-	6/7/8/10	-
5	MEN	HK	72	5	-	2/7/8/10	-
7	MEN	HM	72	7	-	6/7/8/10	-
7	MEN	ZB	72	7	-	6/7/8/10	-
5	MEN	HI	72	5	-	4/7/8/10	-
7	MEN	LJ	72	7,29	-	4/7/8/10	-
5	MEN	L7	72	5	-	2/7/8/10	-
7	MEN	iI	72	7	-	6/7/8/10	-
7	MEN	PJ	72	7,29	-	4/7/8/10	-
7	MEN	BO	72	7	-	4/7/8/10	-
7	MEN	NJ	72	7,29	-	4/7/8/10	-
7	MEN	F5	72	7	-	2/7/8/10	-
7	MEN	fL	72	7,29	-	4/7/8/10	-
7	MEN	aK	72	7	-	6/7/8/10	-
7	MEN	DA	72	7	-	2/7/8/10	-
7	MEN	FG	72	7	-	4/7/8/10	-
7	MEN	jJ	72	7,29	-	4/7/8/10	-
7	MEN	mB	72	7	-	6/7/8/10	-
7	MEN	BJ	72	7,29	-	4/7/8/10	-
7	MEN	TM	72	7	-	6/7/8/10	-
7	MEN	L8	72	7	-	2/7/8/10	-
7	MEN	HC	72	7	-	2/7/8/10	-
5	MEN	L9	72	5	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	HL	72	7	-	5/7/8/10	-
5	MEN	JF	72	5	-	4/7/8/10	-
7	MEN	aF	72	7	-	6/7/8/10	-
7	MEN	Y1	72	7	-	6/7/8/10	-
7	MEN	VK	72	7	-	6/7/8/10	-
7	MEN	LE	72	7	-	2/7/8/10	-
7	MEN	iB	72	7	-	6/7/8/10	-
7	MEN	VF	72	7	-	6/7/8/10	-
7	MEN	cM	72	7	-	6/7/8/10	-
7	MEN	TI	72	7	-	6/7/8/10	-
7	MEN	dL	72	7,29	-	4/7/8/10	-
7	MEN	m1	72	7	-	6/7/8/10	-
7	MEN	YK	72	7	-	6/7/8/10	-
7	MEN	fJ	72	7,29	-	4/7/8/10	-
7	MEN	C4	72	7	-	5/7/8/10	-
7	MEN	E4	72	7	-	5/7/8/10	-
7	MEN	nL	72	7,29	-	4/7/8/10	-
7	MEN	BC	72	7	-	2/7/8/10	-
7	MEN	k9	72	7	-	6/7/8/10	-
7	MEN	J3	72	7	-	4/7/8/10	-
21	MEN	LP	71	21	-	6/7/8/10	-
7	MEN	k1	72	7	-	6/7/8/10	-
7	MEN	C8	72	7	-	6/7/8/10	-
7	MEN	NB	72	7	-	6/7/8/10	-
7	MEN	PR	72	7	-	3/7/8/10	-
7	MEN	tJ	72	7,29	-	4/7/8/10	-
7	MEN	HO	72	7	-	4/7/8/10	-
7	MEN	GD	72	7	-	5/7/8/10	-
7	MEN	CD	72	7	-	5/7/8/10	-
7	MEN	DL	72	7,29	-	4/7/8/10	-
5	MEN	DI	72	5,1	-	5/7/8/10	-
7	MEN	LG	72	7	-	4/7/8/10	-
7	MEN	bL	72	7,29	-	4/7/8/10	-
7	MEN	gB	72	7	-	6/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	VR	72	7	-	3/7/8/10	-
21	MEN	OP	71	21	-	4/7/8/10	-
7	MEN	vL	72	7,29	-	4/7/8/10	-
7	MEN	IJ	72	7,29	-	4/7/8/10	-
7	MEN	HG	72	7	-	4/7/8/10	-
7	MEN	HA	72	7	-	2/7/8/10	-
7	MEN	ED	72	7	-	5/7/8/10	-
5	MEN	H9	72	5	-	6/7/8/10	-
7	MEN	TF	72	7	-	6/7/8/10	-
7	MEN	ID	72	7	-	5/7/8/10	-
7	MEN	HE	72	7	-	2/7/8/10	-
7	MEN	Y7	72	7	-	6/7/8/10	-
5	MEN	FK	72	5	-	2/7/8/10	-
7	MEN	gF	72	7	-	6/7/8/10	-
7	MEN	cF	72	7	-	6/7/8/10	-
7	MEN	G8	72	7	-	2/7/8/10	-
7	MEN	F8	72	7	-	2/7/8/10	-
5	MEN	H7	72	5	-	6/7/8/10	-
7	MEN	TB	72	7	-	6/7/8/10	-
7	MEN	LL	72	7,29	-	4/7/8/10	-
21	MEN	qP	71	21	-	4/7/8/10	-
7	MEN	V7	72	7	-	6/7/8/10	-
7	MEN	eM	72	7	-	6/7/8/10	-
7	MEN	KD	72	7	-	5/7/8/10	-
7	MEN	m7	72	7	-	6/7/8/10	-
7	MEN	FO	72	7	-	4/7/8/10	-
7	MEN	NL	72	7,29	-	4/7/8/10	-
7	MEN	H3	72	7	-	4/7/8/10	-
7	MEN	g1	72	7	-	6/7/8/10	-
5	MEN	L1	72	5	-	2/7/8/10	-
7	MEN	HN	72	7	-	2/7/8/10	-
5	MEN	JK	72	5	-	2/7/8/10	-
21	MEN	fP	71	21	-	4/7/8/10	-
7	MEN	B5	72	7	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	DJ	72	7,29	-	4/7/8/10	-
21	MEN	UP	71	21	-	4/7/8/10	-
7	MEN	JC	72	7	-	2/7/8/10	-
7	MEN	I4	72	7	-	5/7/8/10	-
7	MEN	FQ	72	7	-	4/7/8/10	-
7	MEN	LN	72	7	-	2/7/8/10	-
7	MEN	hL	72	7,29	-	4/7/8/10	-
7	MEN	BG	72	7	-	4/7/8/10	-
7	MEN	PK	72	7	-	6/7/8/10	-
7	MEN	FJ	72	7,29	-	4/7/8/10	-
7	MEN	XM	72	7	-	6/7/8/10	-
7	MEN	MO	72	7	-	2/7/8/10	-
5	MEN	F7	72	5	-	4/7/8/10	-
7	MEN	FM	72	7	-	6/7/8/10	-
7	MEN	e1	72	7	-	6/7/8/10	-
7	MEN	RI	72	7	-	6/7/8/10	-
5	MEN	N1	72	5	-	2/7/8/10	-
7	MEN	R7	72	7	-	6/7/8/10	-
7	MEN	JB	72	7	-	6/7/8/10	-
7	MEN	rJ	72	7,29	-	4/7/8/10	-
7	MEN	A5	72	7	-	6/7/8/10	-
7	MEN	DQ	72	7	-	4/7/8/10	-
7	MEN	c9	72	7	-	6/7/8/10	-
7	MEN	C5	72	7	-	6/7/8/10	-
5	MEN	N9	72	5	-	4/7/8/10	-
7	MEN	JE	72	7	-	2/7/8/10	-
7	MEN	HQ	72	7	-	4/7/8/10	-
7	MEN	tL	72	7,29	-	4/7/8/10	-
5	MEN	J7	72	5	-	4/7/8/10	-
7	MEN	VB	72	7	-	6/7/8/10	-
7	MEN	LB	72	7	-	6/7/8/10	-
21	MEN	DP	71	21	-	2/7/8/10	-
7	MEN	VI	72	7	-	6/7/8/10	-
7	MEN	LC	72	7	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	T1	72	7	-	6/7/8/10	-
7	MEN	e7	72	7	-	6/7/8/10	-
7	MEN	aI	72	7	-	6/7/8/10	-
7	MEN	FN	72	7	-	2/7/8/10	-
7	MEN	DC	72	7	-	2/7/8/10	-
21	MEN	IP	71	21	-	2/7/8/10	-
7	MEN	BL	72	7,29	-	4/7/8/10	-
7	MEN	DM	72	7	-	6/7/8/10	-
7	MEN	DG	72	7	-	4/7/8/10	-
7	MEN	eB	72	7	-	6/7/8/10	-
7	MEN	G4	72	7	-	5/7/8/10	-
7	MEN	JA	72	7	-	2/7/8/10	-
21	MEN	kP	71	21	-	6/7/8/10	-
7	MEN	HJ	72	7	-	4/7/8/10	-
7	MEN	L5	72	7	-	2/7/8/10	-
7	MEN	NM	72	7	-	6/7/8/10	-
7	MEN	TJ	72	7,29	-	4/7/8/10	-
7	MEN	k7	72	7	-	6/7/8/10	-
7	MEN	JO	72	7	-	4/7/8/10	-
7	MEN	ZJ	72	7,29	-	4/7/8/10	-
7	MEN	cK	72	7	-	6/7/8/10	-
5	MEN	FF	72	5	-	4/7/8/10	-
7	MEN	RB	72	7	-	6/7/8/10	-
7	MEN	gK	72	7	-	6/7/8/10	-
7	MEN	c1	72	7	-	6/7/8/10	-
7	MEN	JL	72	7,29	-	4/7/8/10	-
7	MEN	i7	72	7	-	6/7/8/10	-
5	MEN	D1	72	5	-	2/7/8/10	-
7	MEN	JJ	72	7,29	-	4/7/8/10	-
7	MEN	NO	72	7	-	2/7/8/10	-
5	MEN	H1	72	5	-	2/7/8/10	-
7	MEN	V2	72	7	-	3/7/8/10	-
21	MEN	BP	71	21	-	4/7/8/10	-
7	MEN	B3	72	7	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	nJ	72	7,29	-	4/7/8/10	-
7	MEN	PB	72	7	-	6/7/8/10	-
7	MEN	G5	72	7	-	2/7/8/10	-
7	MEN	gI	72	7	-	6/7/8/10	-
7	MEN	bJ	72	7,29	-	4/7/8/10	-
7	MEN	T9	72	7	-	6/7/8/10	-
7	MEN	LO	72	7	-	4/7/8/10	-
7	MEN	RK	72	7	-	6/7/8/10	-
7	MEN	I8	72	7	-	6/7/8/10	-
7	MEN	M4	72	7	-	5/7/8/10	-
7	MEN	A8	72	7	-	6/7/8/10	-
7	MEN	g7	72	7	-	6/7/8/10	-
7	MEN	T7	72	7	-	6/7/8/10	-
5	MEN	F1	72	5	-	2/7/8/10	-
7	MEN	K5	72	7	-	6/7/8/10	-
5	MEN	JI	72	5	-	4/7/8/10	-
5	MEN	LF	72	5	-	4/7/8/10	-
7	MEN	PL	72	7,29	-	4/7/8/10	-
7	MEN	YI	72	7	-	6/7/8/10	-
7	MEN	VM	72	7	-	6/7/8/10	-
5	MEN	LI	72	5	-	4/7/8/10	-
7	MEN	dJ	72	7,29	-	4/7/8/10	-
7	MEN	PF	72	7	-	6/7/8/10	-
7	MEN	kF	72	7	-	6/7/8/10	-
7	MEN	g9	72	7	-	6/7/8/10	-
7	MEN	P2	72	7	-	3/7/8/10	-
21	MEN	MP	71	21	-	6/7/8/10	-
7	MEN	DB	72	7	-	6/7/8/10	-
7	MEN	XJ	72	7,29	-	4/7/8/10	-
7	MEN	K8	72	7	-	6/7/8/10	-
21	MEN	uP	71	21	-	5/7/8/10	-
7	MEN	i9	72	7	-	6/7/8/10	-
7	MEN	BE	72	7	-	2/7/8/10	-
5	MEN	LK	72	5	-	2/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	TK	72	7	-	6/7/8/10	-
7	MEN	BQ	72	7	-	4/7/8/10	-
7	MEN	BA	72	7	-	2/7/8/10	-
7	MEN	FA	72	7	-	2/7/8/10	-
7	MEN	DN	72	7	-	2/7/8/10	-
7	MEN	jL	72	7,29	-	4/7/8/10	-
5	MEN	NI	72	5	-	4/7/8/10	-
7	MEN	pL	72	7,29	-	4/7/8/10	-
7	MEN	c7	72	7	-	6/7/8/10	-
7	MEN	ZM	72	7	-	6/7/8/10	-
5	MEN	D7	72	5	-	2/7/8/10	-
7	MEN	YF	72	7	-	6/7/8/10	-
7	MEN	K4	72	7	-	5/7/8/10	-
5	MEN	DK	72	5	-	2/7/8/10	-
7	MEN	cI	72	7	-	6/7/8/10	-
7	MEN	mI	72	7	-	6/7/8/10	-
7	MEN	R2	72	7	-	3/7/8/10	-
7	MEN	FC	72	7	-	2/7/8/10	-
7	MEN	MD	72	7	-	5/7/8/10	-
7	MEN	HB	72	7	-	6/7/8/10	-
21	MEN	jP	71	21	-	6/7/8/10	-
7	MEN	I5	72	7	-	6/7/8/10	-
7	MEN	H8	72	7	-	2/7/8/10	-
5	MEN	J1	72	5	-	2/7/8/10	-
7	MEN	mM	72	7	-	6/7/8/10	-
7	MEN	D3	72	7	-	4/7/8/10	-
7	MEN	N3	72	7	-	2/7/8/10	-
7	MEN	XR	72	7	-	3/7/8/10	-
7	MEN	eK	72	7	-	6/7/8/10	-
7	MEN	F3	72	7	-	4/7/8/10	-
5	MEN	HF	72	5	-	4/7/8/10	-
5	MEN	NK	72	5	-	2/7/8/10	-
7	MEN	VL	72	7,29	-	4/7/8/10	-
7	MEN	LQ	72	7	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	MEN	NF	72	5	-	4/7/8/10	-
5	MEN	FI	72	5	-	4/7/8/10	-
7	MEN	P9	72	7	-	6/7/8/10	-
5	MEN	D9	72	5	-	2/7/8/10	-
7	MEN	kM	72	7	-	6/7/8/10	-
7	MEN	P1	72	7	-	6/7/8/10	-
7	MEN	RM	72	7	-	6/7/8/10	-
7	MEN	XL	72	7,29	-	4/7/8/10	-
7	MEN	TL	72	7,29	-	4/7/8/10	-
7	MEN	M3	72	7	-	2/7/8/10	-
7	MEN	TR	72	7	-	3/7/8/10	-
21	MEN	HP	71	21	-	4/7/8/10	-
7	MEN	a7	72	7	-	6/7/8/10	-
7	MEN	JQ	72	7	-	4/7/8/10	-
7	MEN	DE	72	7	-	2/7/8/10	-
21	MEN	sP	71	21	-	2/7/8/10	-
7	MEN	hJ	72	7,29	-	4/7/8/10	-
7	MEN	N2	72	7	-	3/7/8/10	-
7	MEN	iF	72	7	-	6/7/8/10	-
7	MEN	BN	72	7	-	2/7/8/10	-
7	MEN	T2	72	7	-	3/7/8/10	-
21	MEN	nP	71	21	-	4/7/8/10	-
7	MEN	m9	72	7	-	6/7/8/10	-
7	MEN	P7	72	7	-	6/7/8/10	-
7	MEN	B8	72	7	-	2/7/8/10	-
7	MEN	RL	72	7,29	-	4/7/8/10	-
7	MEN	IL	72	7,29	-	4/7/8/10	-
7	MEN	R9	72	7	-	6/7/8/10	-
7	MEN	LA	72	7	-	2/7/8/10	-
7	MEN	pJ	72	7,29	-	4/7/8/10	-
7	MEN	a1	72	7	-	6/7/8/10	-
21	MEN	dP	71	21	-	2/7/8/10	-
5	MEN	N7	72	5	-	4/7/8/10	-
5	MEN	J9	72	5	-	4/7/8/10	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MEN	R1	72	7	-	6/7/8/10	-
21	MEN	wP	71	21	-	4/7/8/10	-
7	MEN	JN	72	7	-	2/7/8/10	-
7	MEN	RF	72	7	-	6/7/8/10	-
7	MEN	JG	72	7	-	4/7/8/10	-
7	MEN	JM	72	7	-	6/7/8/10	-
7	MEN	mK	72	7	-	6/7/8/10	-
21	MEN	FP	71	21	-	6/7/8/10	-
5	MEN	DF	72	5,1	-	5/7/8/10	-
7	MEN	X2	72	7	-	3/7/8/10	-
21	MEN	hP	71	21	-	5/7/8/10	-
7	MEN	eF	72	7	-	6/7/8/10	-
21	MEN	SP	71	21	-	5/7/8/10	-
7	MEN	RR	72	7	-	3/7/8/10	-
7	MEN	ZL	72	7,29	-	4/7/8/10	-
7	MEN	LM	72	7	-	6/7/8/10	-
7	MEN	FE	72	7	-	2/7/8/10	-
5	MEN	F9	72	5	-	4/7/8/10	-
21	MEN	QP	71	21	-	2/7/8/10	-

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	LP	71	MEN	O-C	21.59	2.06	1.19
21	kP	71	MEN	O-C	21.59	2.06	1.19
21	jP	71	MEN	O-C	21.58	2.06	1.19
21	jP	71	MEN	CB-CA	-5.16	1.42	1.53
21	kP	71	MEN	CB-CA	-5.16	1.42	1.53

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	jP	71	MEN	CB-CA-C	-19.45	75.00	111.47
21	LP	71	MEN	CB-CA-C	-19.45	75.00	111.47
21	kP	71	MEN	CB-CA-C	-19.44	75.03	111.47
21	LP	71	MEN	CB-CG-ND2	14.88	135.50	115.48
21	kP	71	MEN	CB-CG-ND2	14.88	135.50	115.48

There are no chirality outliers.

5 of 1368 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	P1	72	MEN	C-CA-CB-CG
7	R1	72	MEN	C-CA-CB-CG
7	T1	72	MEN	C-CA-CB-CG
7	V1	72	MEN	C-CA-CB-CG
7	Y1	72	MEN	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

1462 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	CYC	GI	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	fB	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	PB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	c7	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	S9	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	FN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	A1	303	2	43,46,46	3.24	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	T7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	AL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	QK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
31	CYC	M7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	DA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	mF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	RM	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	FB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	a7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	qL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	eK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	S1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	MP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	e9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	NL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	16 (35%)
29	PEB	aI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	aK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	Q1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	dB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	E4	203	-	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	LL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	J5	201	6	43,46,46	3.37	11 (25%)	45,67,67	2.77	16 (35%)
29	PEB	NO	202	7	43,46,46	3.36	10 (23%)	45,67,67	2.25	13 (28%)
29	PEB	iL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	C9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)
29	PEB	CA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	JC	202	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
31	CYC	I9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	IN	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
31	CYC	E1	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	LN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	B3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	f9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	A1	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.13	15 (33%)
29	PEB	iJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	VM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	gL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
32	PMS	kH	301	-	11,11,11	0.83	1 (9%)	14,15,15	0.65	0
29	PEB	VL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	H8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	dK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	RB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
31	CYC	CF	1001	4,5	42,46,46	3.08	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	RI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	AM	303	16	43,46,46	3.34	10 (23%)	45,67,67	2.18	14 (31%)
29	PEB	R1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	R7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	IM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	AF	304	2	43,46,46	3.29	10 (23%)	45,67,67	2.25	15 (33%)
29	PEB	L7	1002	-	43,46,46	3.24	11 (25%)	45,67,67	2.21	17 (37%)
29	PEB	W7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	k9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	c1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	LK	1002	-	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	kM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	bL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	RL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	mI	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	OR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.55	18 (40%)
29	PEB	UJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	tL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	EG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	kF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	rL	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	mM	201	7,16	43,46,46	3.36	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	cF	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	MG	405	14	43,46,46	3.11	10 (23%)	45,67,67	2.98	17 (37%)
29	PEB	VM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	UK	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
32	PMS	kH	302	-	11,11,11	1.23	1 (9%)	14,15,15	1.08	1 (7%)
31	CYC	sP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	SL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
30	PUB	QB	201	6,17	42,46,46	3.60	8 (19%)	37,67,67	3.06	14 (37%)
29	PEB	B8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	BE	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	PL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	S7	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	g1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	ZK	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	I4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	bK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	MN	404	14	43,46,46	3.15	12 (27%)	45,67,67	2.49	13 (28%)
29	PEB	HA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	mI	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
31	CYC	tP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	hJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	A9	303	-	42,46,46	3.34	7 (16%)	37,67,67	3.09	14 (37%)
29	PEB	H5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	IG	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	M3	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.14	14 (31%)
29	PEB	P1	201	7,1	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	cF	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	dJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	CO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	TL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	gF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	WF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	NR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.36	14 (31%)
31	CYC	I1	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	C4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	K3	202	6	43,46,46	3.61	12 (27%)	45,67,67	1.97	15 (33%)
29	PEB	KB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	A7	305	-	43,46,46	3.31	10 (23%)	45,67,67	2.24	17 (37%)
31	CYC	EF	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	UF	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	M9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	IE	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	N7	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	H3	203	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	L5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	AE	201	6	43,46,46	3.45	9 (20%)	45,67,67	2.08	15 (33%)
29	PEB	B4	201	6	43,46,46	3.12	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	nL	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
31	CYC	eP	1001	20	42,46,46	3.37	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	KB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	U7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	DO	201	7	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	eM	202	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
30	PUB	AI	303	2	42,46,46	3.29	7 (16%)	37,67,67	3.30	14 (37%)
29	PEB	dI	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	sJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	DL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	E7	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	JD	201	6	43,46,46	3.11	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	i1	202	6,7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	RR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.47	17 (37%)
31	CYC	CP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	D1	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	WK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	A1	302	-	43,46,46	3.36	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	l9	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
31	CYC	oP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
30	PUB	A1	305	-	42,46,46	3.40	8 (19%)	37,67,67	4.48	16 (43%)
29	PEB	FA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.27	16 (35%)
29	PEB	LI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	LG	203	-	43,46,46	3.44	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	M2	202	6	43,46,46	3.63	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	JA	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	kI	202	7,6	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
31	CYC	PP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.12	22 (44%)
29	PEB	ED	202	7	43,46,46	3.31	10 (23%)	45,67,67	2.62	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	hJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	U2	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.55	18 (40%)
29	PEB	hF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	FF	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	e1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	l7	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	LJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	A9	302	2	42,46,46	3.35	7 (16%)	37,67,67	3.17	18 (48%)
29	PEB	iI	202	6,7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	R9	201	7,1	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	HG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	SK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	k1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	cJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	FE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	HQ	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	DA	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.25	16 (35%)
29	PEB	YL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	mF	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	SR	202	6	43,46,46	3.59	12 (27%)	45,67,67	2.04	15 (33%)
29	PEB	LF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	J1	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	K8	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	DG	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.07	16 (35%)
29	PEB	eK	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
31	CYC	EP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	dF	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	f1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	YK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	MR	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.55	18 (40%)
29	PEB	g7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	dB	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	YF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	UR	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.55	18 (40%)
30	PUB	yJ	303	-	42,46,46	3.50	7 (16%)	37,67,67	3.28	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	WR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	sL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	Y1	202	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	FO	202	7,6	43,46,46	3.53	12 (27%)	45,67,67	2.12	15 (33%)
30	PUB	MQ	404	14	42,46,46	3.70	9 (21%)	37,67,67	4.02	21 (56%)
29	PEB	DN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	H3	202	6,7	43,46,46	3.53	13 (30%)	45,67,67	2.12	15 (33%)
30	PUB	AK	305	-	42,46,46	3.40	8 (19%)	37,67,67	4.48	16 (43%)
29	PEB	B5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	TF	202	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
31	CYC	XP	1001	24,21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
30	PUB	BB	302	17	42,46,46	3.40	7 (16%)	37,67,67	3.33	12 (32%)
29	PEB	BJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LG	201	7,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	lB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	oL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	h7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	SJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	17 (37%)
29	PEB	K5	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.10	15 (33%)
29	PEB	VR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
30	PUB	MG	403	14	42,46,46	3.55	8 (19%)	37,67,67	3.60	19 (51%)
29	PEB	JF	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.12	16 (35%)
31	CYC	DF	1001	5	42,46,46	3.20	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	PR	202	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
31	CYC	M1	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	R2	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	VK	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	L4	201	6	43,46,46	3.13	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	PJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	N2	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.36	14 (31%)
29	PEB	fl	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	WM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	MQ	401	6,14	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	PB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	QI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	JP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	Q9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	sJ	203	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
30	PUB	xL	305	16	42,46,46	3.29	8 (19%)	37,67,67	3.75	15 (40%)
31	CYC	JK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	SM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	kI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	JN	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	UI	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	Z1	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	hJ	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	bJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	O9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	QI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	RP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	A5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	DB	201	7,17	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	W2	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	JL	203	7	43,46,46	3.41	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	AQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
31	CYC	BP	1001	25,21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	wL	303	16	43,46,46	3.43	12 (27%)	45,67,67	2.28	18 (40%)
29	PEB	LL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	CB	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	CN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	LA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	H4	201	6	43,46,46	3.14	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	vL	201	7	43,46,46	3.33	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	IC	201	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	g1	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	g7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	jM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	PI	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	aL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	iL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	CM	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	NJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	16 (35%)
29	PEB	kK	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	jL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	R7	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	DE	201	7,18	43,46,46	3.55	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	h1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	SF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	fP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	GA	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	21 (46%)
29	PEB	XJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	EA	201	6	43,46,46	3.04	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	Q7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	fB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
30	PUB	AI	302	2	42,46,46	3.54	8 (19%)	37,67,67	3.18	15 (40%)
29	PEB	IC	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	IF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
29	PEB	KD	202	7,6	43,46,46	3.05	11 (25%)	45,67,67	2.59	16 (35%)
29	PEB	WM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	WJ	202	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	DC	201	7	43,46,46	3.55	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	jL	202	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	F5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	GD	202	7	43,46,46	3.05	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	G3	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	I3	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	JK	203	6,7	43,46,46	3.10	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	lB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	XJ	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	G8	203	7	43,46,46	3.33	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	GN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	B4	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	GF	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	HO	203	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	hM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	VF	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	lF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	PR	201	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	18 (40%)
29	PEB	BE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.42	15 (33%)
29	PEB	hB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	m7	203	7	43,46,46	3.50	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	N2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	VR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	KA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	FC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	16 (35%)
31	CYC	KI	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
31	CYC	IK	1001	4,5	42,46,46	3.10	14 (33%)	50,67,67	2.78	18 (36%)
29	PEB	VB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	d9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
32	PMS	k6	301	-	11,11,11	0.83	1 (9%)	14,15,15	0.65	0
29	PEB	F8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	FG	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.17	16 (35%)
29	PEB	wL	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
30	PUB	yJ	302	-	42,46,46	3.35	7 (16%)	37,67,67	3.26	15 (40%)
29	PEB	uJ	203	6	43,46,46	3.29	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	iK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	CG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.06	14 (31%)
29	PEB	m7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	BL	201	7,19	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	FQ	203	-	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	eR	401	-	43,46,46	1.07	2 (4%)	45,67,67	1.02	2 (4%)
29	PEB	A8	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	JB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	GA	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	c9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	KJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	OM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.42	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	I8	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	KG	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
29	PEB	DB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	NL	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	m1	202	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	aI	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	DG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	KD	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	V7	203	7	43,46,46	3.47	12 (27%)	45,67,67	2.10	14 (31%)
31	CYC	J9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	25 (50%)
30	PUB	xJ	304	-	42,46,46	3.35	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	EJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	iM	201	7,16	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	CA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	AK	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.13	15 (33%)
29	PEB	HN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
30	PUB	xL	304	-	42,46,46	3.36	7 (16%)	37,67,67	3.30	16 (43%)
31	CYC	H7	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	YB	203	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	Y9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	c1	202	7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	T7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	hM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	WB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	HO	201	7,9	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	YK	202	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
31	CYC	1P	1001	25,21	42,46,46	3.28	14 (33%)	50,67,67	3.10	21 (42%)
29	PEB	C5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	15 (33%)
30	PUB	MQ	405	14	42,46,46	3.56	8 (19%)	37,67,67	3.60	19 (51%)
29	PEB	EB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	lM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	SI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	sJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	WI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	IA	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.90	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	BA	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	Q9	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	EL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	i1	203	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	IJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	jB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	OI	203	6,7	43,46,46	3.15	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	G3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	17 (37%)
29	PEB	BN	203	-	43,46,46	3.29	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	ZJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	hK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	MM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	IB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	W1	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	ZF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	L4	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	GQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	OM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	H1	1002	-	43,46,46	3.44	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	AA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.89	20 (44%)
29	PEB	mL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	mB	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	gB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	QM	204	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	L8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	IB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	HG	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
31	CYC	F7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	f9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	tJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	R9	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	iB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	BL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	LN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	DF	1002	-	43,46,46	3.33	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
29	PEB	eK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	uL	201	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	DB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	C3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	16 (35%)
30	PUB	yL	303	-	42,46,46	3.51	7 (16%)	37,67,67	3.28	16 (43%)
29	PEB	K8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	W2	202	6	43,46,46	3.62	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	H4	202	6	43,46,46	3.11	10 (23%)	45,67,67	2.39	19 (42%)
29	PEB	OL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	KG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	KD	203	-	43,46,46	3.30	10 (23%)	45,67,67	2.62	18 (40%)
30	PUB	AM	305	16	42,46,46	3.40	7 (16%)	37,67,67	3.00	15 (40%)
31	CYC	pP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	HJ	201	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	QB	204	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	LB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	d1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	VI	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	EO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
31	CYC	L1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	Y9	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	kJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
30	PUB	MA	402	14	42,46,46	3.43	7 (16%)	37,67,67	3.77	19 (51%)
29	PEB	U1	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	e1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	j7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
30	PUB	wJ	305	16	42,46,46	3.29	8 (19%)	37,67,67	3.74	15 (40%)
29	PEB	JC	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	D3	203	-	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	EA	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	20 (44%)
29	PEB	kL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	bI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	WP	1001	-	42,46,46	3.50	15 (35%)	50,67,67	2.92	20 (40%)
29	PEB	qJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	LB	202	7,6	43,46,46	3.18	10 (23%)	45,67,67	2.47	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	OI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
29	PEB	DO	202	-	43,46,46	3.41	11 (25%)	45,67,67	2.10	13 (28%)
29	PEB	hL	201	7	43,46,46	3.31	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	c7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	S7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	JM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	T7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	F3	202	7,6	43,46,46	3.53	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	DN	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.25	16 (35%)
29	PEB	YJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	XR	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	c1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	CE	202	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	UM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	GM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	fM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
31	CYC	NI	1001	5,3	42,46,46	3.21	15 (35%)	50,67,67	3.03	21 (42%)
31	CYC	D1	1003	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
31	CYC	D7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	JG	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	WF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	HL	201	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	NB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	eL	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.12	13 (28%)
29	PEB	J5	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.17	16 (35%)
29	PEB	TR	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	17 (37%)
29	PEB	kJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	J3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	iB	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	SK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	mK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	tL	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	HP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	D3	201	7	43,46,46	3.43	11 (25%)	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	CYC	LI	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.03	21 (42%)
29	PEB	MQ	407	14	43,46,46	3.13	9 (20%)	45,67,67	2.99	17 (37%)
29	PEB	iK	202	6,7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	YL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	F3	201	7,9	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
31	CYC	NF	1001	5,3	42,46,46	3.21	15 (35%)	50,67,67	3.03	21 (42%)
29	PEB	HC	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	eM	201	7,16	43,46,46	3.35	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	pJ	202	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	a1	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	cK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	TL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	OB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	NR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	WL	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	IN	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.90	20 (44%)
29	PEB	bJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	FA	201	7	43,46,46	3.23	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	M2	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.55	18 (40%)
31	CYC	OP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	FJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	mI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	eF	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	e9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	rJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	F5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	SB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	AC	201	6	43,46,46	3.45	9 (20%)	45,67,67	2.08	15 (33%)
29	PEB	WL	202	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	K3	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.16	16 (35%)
30	PUB	BM	302	17	42,46,46	3.40	7 (16%)	37,67,67	3.33	12 (32%)
29	PEB	fJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
31	CYC	QP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	LB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	pL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	dI	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	HI	1001	5	42,46,46	3.20	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	a9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	FG	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	eL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	J9	1002	-	43,46,46	3.25	10 (23%)	45,67,67	2.22	16 (35%)
29	PEB	N3	203	7	43,46,46	3.23	10 (23%)	45,67,67	2.14	14 (31%)
29	PEB	nJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	XR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	N2	202	7	43,46,46	3.02	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	FQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	IJ	202	7	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
31	CYC	AP	1001	20	42,46,46	3.37	15 (35%)	50,67,67	3.12	22 (44%)
29	PEB	b7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	dL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	BO	201	7,9	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
31	CYC	K1	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	MA	401	14	43,46,46	3.16	9 (20%)	45,67,67	2.86	14 (31%)
29	PEB	b9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	J3	202	7,6	43,46,46	3.55	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	oJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	A7	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.15	14 (31%)
29	PEB	QL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	eJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	gB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	EM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	aJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	HM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	JI	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.12	16 (35%)
29	PEB	CQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	l1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	PM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	OF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	xJ	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.55	17 (37%)
29	PEB	PJ	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	M4	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	AE	203	6,7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	NO	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.13	14 (31%)
29	PEB	C3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	bL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	D3	202	-	43,46,46	3.41	9 (20%)	45,67,67	2.10	13 (28%)
29	PEB	CM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	FB	201	7,15	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
31	CYC	EI	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	e7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	DO	203	-	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	m9	203	7	43,46,46	3.50	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	F7	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.22	17 (37%)
29	PEB	g9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	GJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	DN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	IO	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	G4	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.61	18 (40%)
29	PEB	L3	202	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
31	CYC	jP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	JJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	N1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	bF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	HI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.10	16 (35%)
29	PEB	HA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	k1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	MN	401	14	43,46,46	3.16	9 (20%)	45,67,67	2.86	14 (31%)
29	PEB	J4	201	6	43,46,46	3.11	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	EL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	D1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.01	24 (48%)
29	PEB	I5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	JJ	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	K4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	R2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	dD	401	7,10	43,46,46	3.17	10 (23%)	45,67,67	2.23	20 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	DL	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	TJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	cB	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	GC	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	YB	201	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	g7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	NF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	aF	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	H8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	kK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	S9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	BC	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	mF	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	BD	202	6	43,46,46	3.15	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	Z9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	AL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	FL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	cM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
30	PUB	AM	304	16	42,46,46	3.14	9 (21%)	37,67,67	3.65	18 (48%)
31	CYC	FI	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	IJ	203	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	JB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	OL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	c9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	iF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	AE	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	GB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	wL	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.54	17 (37%)
29	PEB	IA	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	J8	201	6	43,46,46	3.37	11 (25%)	45,67,67	2.77	16 (35%)
29	PEB	bL	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JE	202	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	L3	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.07	14 (31%)
29	PEB	Z7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	eJ	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.12	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	U1	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.61	14 (31%)
29	PEB	IJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
30	PUB	wJ	304	-	42,46,46	3.35	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	G5	203	7	43,46,46	3.34	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	LJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	HB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	cB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	LQ	201	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	iI	201	7	43,46,46	3.32	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	WR	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	U7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	HG	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	HE	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	C8	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	N1	1002	5	43,46,46	3.41	13 (30%)	45,67,67	2.33	18 (40%)
29	PEB	uJ	202	6	43,46,46	2.93	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	SL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	O1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	W1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	I4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	IK	202	6	43,46,46	3.25	10 (23%)	45,67,67	2.61	15 (33%)
29	PEB	aB	203	6,7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	cL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	RR	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	FD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
31	CYC	GP	1001	20	42,46,46	3.38	15 (35%)	50,67,67	3.10	22 (44%)
29	PEB	TK	202	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	G8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	F9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	ZL	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.00	12 (26%)
29	PEB	IL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	ZI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	QK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	P2	202	7	43,46,46	3.42	10 (23%)	45,67,67	2.20	16 (35%)
31	CYC	vP	1001	20	42,46,46	3.40	15 (35%)	50,67,67	3.11	22 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	fK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	JO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	XL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	XM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	MA	404	14	43,46,46	3.14	12 (27%)	45,67,67	2.49	13 (28%)
29	PEB	WJ	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	mB	201	7,16	43,46,46	3.36	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	gJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
30	PUB	A7	302	2	42,46,46	3.35	7 (16%)	37,67,67	3.17	18 (48%)
29	PEB	k7	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	aF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	l7	202	6	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)
29	PEB	A7	304	-	43,46,46	3.30	9 (20%)	45,67,67	2.23	14 (31%)
31	CYC	G9	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	QF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	VK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	gJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	P7	203	7	43,46,46	3.47	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	Z9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	MQ	402	7,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	AK	303	2	43,46,46	3.24	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	iK	203	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	MQ	406	29,14	43,46,46	3.22	10 (23%)	45,67,67	2.48	20 (44%)
29	PEB	IJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	R1	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	VI	202	6,7	43,46,46	3.14	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	kP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	LC	202	6,7	43,46,46	3.26	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	kB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	jK	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	pJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	aB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	G8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	MJ	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	aM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	BQ	201	7,29,14	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	MR	202	6	43,46,46	3.44	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	KM	203	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	e7	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	CB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	SI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	KN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	OF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
31	CYC	DP	1001	25,21	42,46,46	3.29	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	I8	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	Q2	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	O2	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	A3	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.16	17 (37%)
29	PEB	UI	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	CO	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.16	16 (35%)
29	PEB	CL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	IF	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	gM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	JA	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.26	16 (35%)
31	CYC	HK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	RF	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	F4	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	I3	203	6,7	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	D4	201	6	43,46,46	3.12	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	JQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	iM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	HN	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	NM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	C8	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.21	12 (26%)
31	CYC	nP	1001	24,21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	HQ	201	7,14	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
31	CYC	gP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	YI	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	UB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	AC	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	I4	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.39	15 (33%)
29	PEB	IL	202	7	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JL	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	KQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
30	PUB	yL	302	-	42,46,46	3.35	7 (16%)	37,67,67	3.26	15 (40%)
29	PEB	PI	201	7,1	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	zJ	501	7	43,46,46	3.38	9 (20%)	45,67,67	2.03	14 (31%)
29	PEB	qJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	iP	1001	20	42,46,46	3.39	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	H5	203	7	43,46,46	3.33	10 (23%)	45,67,67	1.90	12 (26%)
30	PUB	MN	403	14	42,46,46	3.46	10 (23%)	37,67,67	3.90	16 (43%)
29	PEB	V2	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	MJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	mM	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	nJ	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	EN	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	20 (44%)
31	CYC	LF	1001	5	42,46,46	3.19	15 (35%)	50,67,67	3.03	21 (42%)
31	CYC	N7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	k1	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
31	CYC	GK	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	GL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	YF	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	BO	202	7,6	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	FJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	CJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	nL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	c9	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	TI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
30	PUB	A7	303	-	42,46,46	3.34	7 (16%)	37,67,67	3.09	14 (37%)
29	PEB	CD	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	H8	202	-	43,46,46	3.25	10 (23%)	45,67,67	2.05	13 (28%)
31	CYC	FP	1001	21	42,46,46	3.29	13 (30%)	50,67,67	3.10	21 (42%)
29	PEB	EQ	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.05	13 (28%)
29	PEB	KE	203	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	BL	202	7,6	43,46,46	3.07	11 (25%)	45,67,67	2.85	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	pJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	EM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
31	CYC	CK	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	UL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	LC	203	-	43,46,46	3.45	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	FJ	202	7,6	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	T9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	uL	203	6	43,46,46	3.29	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	T2	202	7	43,46,46	3.04	8 (18%)	45,67,67	2.47	17 (37%)
29	PEB	Z7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
30	PUB	AF	303	2	42,46,46	3.29	7 (16%)	37,67,67	3.30	14 (37%)
29	PEB	PJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
31	CYC	xP	1001	21	42,46,46	3.95	18 (42%)	50,67,67	3.57	28 (56%)
29	PEB	ED	201	7	43,46,46	3.07	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	V1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	FB	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	HE	201	7	43,46,46	3.56	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	eF	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	YJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	kL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	KC	202	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	OB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.42	16 (35%)
31	CYC	EK	1001	4,5	42,46,46	3.09	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	J8	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.17	16 (35%)
29	PEB	hL	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	qL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	R2	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.46	17 (37%)
29	PEB	TK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
30	PUB	MA	403	14	42,46,46	3.46	10 (23%)	37,67,67	3.89	16 (43%)
29	PEB	TR	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.36	14 (31%)
29	PEB	LD	202	6	43,46,46	3.14	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	l1	202	6	43,46,46	3.25	10 (23%)	45,67,67	2.61	15 (33%)
29	PEB	bJ	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	GD	203	7	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	j1	201	6	43,46,46	3.20	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
29	PEB	LE	202	6,7	43,46,46	3.26	11 (25%)	45,67,67	2.43	16 (35%)
29	PEB	i7	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	II	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	vL	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	K4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	AK	302	-	43,46,46	3.36	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	VB	202	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	LA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	K8	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	hL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	BG	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	AN	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	FG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	L8	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.89	12 (26%)
29	PEB	cI	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	i9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	QL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	FD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	RI	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
31	CYC	YP	1000	25	42,46,46	3.41	13 (30%)	50,67,67	2.92	19 (38%)
29	PEB	WB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	QR	202	6	43,46,46	3.60	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	FL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	gI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	xJ	303	16	43,46,46	3.43	11 (25%)	45,67,67	2.27	18 (40%)
29	PEB	BM	301	17	43,46,46	3.38	11 (25%)	45,67,67	2.41	17 (37%)
29	PEB	PF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	d7	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	S2	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	JG	203	7	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	e2	401	-	43,46,46	1.07	2 (4%)	45,67,67	1.01	2 (4%)
31	CYC	HF	1001	5	42,46,46	3.20	15 (35%)	50,67,67	3.02	22 (44%)
29	PEB	QB	203	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	HJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	GM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	O7	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	C1	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	DM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	RM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	MG	401	14	43,46,46	3.11	11 (25%)	45,67,67	2.44	14 (31%)
29	PEB	RJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	nL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	rL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	TI	202	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	TJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	NI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	O1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	a9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	A9	305	-	43,46,46	3.31	10 (23%)	45,67,67	2.24	17 (37%)
29	PEB	aM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	BQ	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	AG	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	LQ	202	-	43,46,46	3.44	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	gF	202	7,6	43,46,46	3.15	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	J4	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	fJ	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	FQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
31	CYC	SP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.10	21 (42%)
31	CYC	D9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	FA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	FM	201	7,15	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	AG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	dF	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	E4	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.23	20 (44%)
29	PEB	KC	201	7,6	43,46,46	3.26	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	bF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	17 (37%)
29	PEB	IM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	UB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	iF	201	7	43,46,46	3.32	11 (25%)	45,67,67	2.42	21 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	cK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	GL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	GC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	pL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
31	CYC	N9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	RL	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	LM	202	7,6	43,46,46	3.18	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	LE	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	BJ	202	7,6	43,46,46	3.07	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	DK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	B3	201	7,9	43,46,46	3.43	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	U1	201	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	hI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	gI	202	7,6	43,46,46	3.15	10 (23%)	45,67,67	2.59	14 (31%)
31	CYC	hP	1001	25,21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
31	CYC	LK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	FC	201	7,18	43,46,46	3.57	12 (27%)	45,67,67	2.18	16 (35%)
29	PEB	V1	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	RK	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	DM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	eB	202	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	FN	201	7	43,46,46	3.23	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	a1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	g9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	N3	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	mJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	fJ	201	7,16	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	ZL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	E3	201	6	43,46,46	3.27	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	dJ	202	7,6	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	fL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	KN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	I5	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	FO	201	7,9	43,46,46	3.44	11 (25%)	45,67,67	2.08	16 (35%)
30	PUB	A1	304	2	42,46,46	3.54	8 (19%)	37,67,67	3.22	16 (43%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	BN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	P9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	j7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	gM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
31	CYC	KK	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.78	18 (36%)
29	PEB	ZB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	T2	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	UF	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	NK	1001	5,3	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	Y7	203	7	43,46,46	3.49	12 (27%)	45,67,67	2.11	14 (31%)
29	PEB	k7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	iB	201	7,16	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	HQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
31	CYC	1P	1002	25	42,46,46	3.42	13 (30%)	50,67,67	2.93	19 (38%)
29	PEB	VK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	NM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	dK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	bI	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	17 (37%)
29	PEB	DD	201	6	43,46,46	3.11	13 (30%)	45,67,67	2.72	21 (46%)
29	PEB	BD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.73	21 (46%)
29	PEB	AO	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.16	17 (37%)
29	PEB	YM	201	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	MA	405	14	43,46,46	3.20	12 (27%)	45,67,67	2.60	16 (35%)
29	PEB	GQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	O2	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.05	15 (33%)
29	PEB	h9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
30	PUB	AF	302	2	42,46,46	3.54	8 (19%)	37,67,67	3.18	15 (40%)
29	PEB	AJ	203	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
30	PUB	xJ	305	16	42,46,46	3.28	8 (19%)	37,67,67	3.74	15 (40%)
29	PEB	CN	201	6	43,46,46	3.06	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	m9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	U2	202	-	43,46,46	3.60	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	oJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
31	CYC	K7	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	K4	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	18 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PUB	MN	402	14	42,46,46	3.43	7 (16%)	37,67,67	3.76	19 (51%)
29	PEB	QJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	L1	1002	-	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	j9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	mP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	d1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	C7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)
29	PEB	HD	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.40	20 (44%)
29	PEB	HB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	GE	202	6	43,46,46	3.42	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	JM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	IO	203	6,7	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	AL	203	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	VL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	ZM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	V2	201	7,8	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	mL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	h1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.38	17 (37%)
29	PEB	lK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	JM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	YI	202	7	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	CQ	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.06	14 (31%)
29	PEB	OI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	cL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	HA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	DA	203	-	43,46,46	3.30	9 (20%)	45,67,67	2.07	15 (33%)
31	CYC	H1	1001	5	42,46,46	3.20	13 (30%)	50,67,67	2.98	24 (48%)
29	PEB	NK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	L5	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	M3	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	J3	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	XM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	SB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	UK	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.61	14 (31%)
29	PEB	oL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	ZB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	aK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	bK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	V7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	d7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	V9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	QJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	KE	201	7,6	43,46,46	3.26	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	RF	202	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	HC	201	7	43,46,46	3.56	12 (27%)	45,67,67	2.17	16 (35%)
29	PEB	jF	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	cP	1001	20	42,46,46	3.39	15 (35%)	50,67,67	3.10	22 (44%)
29	PEB	GG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	fM	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	gL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	PL	202	7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	JN	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	KQ	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	14 (31%)
29	PEB	mK	202	7	43,46,46	3.38	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	X2	202	7	43,46,46	3.42	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	E4	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	YF	201	7	43,46,46	3.34	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	i9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	FL	202	7,6	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
31	CYC	MI	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	GG	202	6	43,46,46	3.34	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	WJ	203	6	43,46,46	3.29	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	dM	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	TL	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	BA	203	-	43,46,46	3.29	9 (20%)	45,67,67	2.07	15 (33%)
29	PEB	kM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	NR	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	A8	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	lJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
31	CYC	I7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	MD	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	DQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.07	16 (35%)
29	PEB	jK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	MO	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	F4	201	6	43,46,46	3.14	13 (30%)	45,67,67	2.73	21 (46%)
29	PEB	CJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	rJ	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
32	PMS	k6	302	-	11,11,11	1.23	1 (9%)	14,15,15	1.08	1 (7%)
29	PEB	ZM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
31	CYC	MF	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	U9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	b1	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	CC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	B8	203	7	43,46,46	3.35	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	RK	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	A9	304	-	43,46,46	3.30	10 (23%)	45,67,67	2.23	14 (31%)
29	PEB	UL	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)
29	PEB	dI	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	IL	201	7	43,46,46	3.32	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	GO	202	6	43,46,46	3.62	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	iJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	dL	201	7	43,46,46	3.32	9 (20%)	45,67,67	2.99	15 (33%)
29	PEB	kI	201	7,2	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	aM	203	6,7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	N3	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	vJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	3.00	15 (33%)
29	PEB	V9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
31	CYC	FK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	F8	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	OF	203	6,7	43,46,46	3.15	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	Q7	201	6	43,46,46	3.24	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	gM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	EC	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	cI	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	ZB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	PUB	MG	402	14	42,46,46	3.70	9 (21%)	37,67,67	4.02	21 (56%)
29	PEB	aK	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	P1	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	HM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	a7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	CL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	YI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	L5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.89	12 (26%)
29	PEB	P7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	AB	303	16	43,46,46	3.35	10 (23%)	45,67,67	2.18	14 (31%)
30	PUB	AK	304	2	42,46,46	3.54	8 (19%)	37,67,67	3.22	16 (43%)
29	PEB	jM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	QM	203	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	JQ	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	VI	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	PI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	rL	201	7,16	43,46,46	3.30	9 (20%)	45,67,67	2.98	15 (33%)
29	PEB	gK	202	7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
31	CYC	JI	1001	5,3	42,46,46	3.19	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	e7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	F5	203	7	43,46,46	3.32	10 (23%)	45,67,67	1.90	12 (26%)
29	PEB	aF	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	HK	1002	-	43,46,46	3.44	13 (30%)	45,67,67	2.34	17 (37%)
29	PEB	AN	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.89	20 (44%)
29	PEB	JJ	203	7	43,46,46	3.41	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	RJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	C5	202	-	43,46,46	3.28	10 (23%)	45,67,67	2.21	12 (26%)
29	PEB	BA	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	TB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	EC	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	VF	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	G5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	I3	201	6	43,46,46	3.28	11 (25%)	45,67,67	2.17	17 (37%)
29	PEB	GJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	m9	202	7	43,46,46	3.18	10 (23%)	45,67,67	2.37	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	I8	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.21	12 (26%)
29	PEB	FF	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	PK	201	7,1	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	T1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	AC	203	6,7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	mJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	ZL	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	E3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	CD	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.60	18 (40%)
29	PEB	JA	203	-	43,46,46	3.29	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	i7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	MM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	T1	202	7	43,46,46	3.39	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	FK	1002	5	43,46,46	3.43	13 (30%)	45,67,67	2.35	17 (37%)
29	PEB	BG	201	7	43,46,46	3.28	10 (23%)	45,67,67	2.08	16 (35%)
29	PEB	T9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	eI	201	7	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	IQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	m1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	P2	201	7	43,46,46	3.04	9 (20%)	45,67,67	2.48	17 (37%)
29	PEB	cJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	VM	202	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	UK	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	VB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	LO	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.07	14 (31%)
30	PUB	wL	304	-	42,46,46	3.33	7 (16%)	37,67,67	3.30	16 (43%)
29	PEB	DC	202	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	H7	1002	-	43,46,46	3.22	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	R9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
31	CYC	J7	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	26 (52%)
29	PEB	HE	203	-	43,46,46	3.44	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	kF	202	7,6	43,46,46	3.14	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	PM	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
31	CYC	H9	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.24	26 (52%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	eI	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	c7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	P1	202	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	yJ	301	-	43,46,46	3.29	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	cM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	TJ	202	6,7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	OK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	AB	302	6,16	43,46,46	3.34	8 (18%)	45,67,67	2.01	13 (28%)
29	PEB	ID	203	7	43,46,46	3.29	10 (23%)	45,67,67	2.62	18 (40%)
29	PEB	C4	202	7,6	43,46,46	3.06	11 (25%)	45,67,67	2.58	15 (33%)
29	PEB	gK	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	jJ	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	QM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	a7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	fL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	sL	203	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	TR	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.19	16 (35%)
29	PEB	QF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	iF	202	6,7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	j1	203	6,7	43,46,46	3.10	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	M4	203	7	43,46,46	3.41	9 (20%)	45,67,67	2.28	14 (31%)
29	PEB	jF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	OJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.31	15 (33%)
31	CYC	E9	1001	-	42,46,46	3.14	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	fF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	V1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	i9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	JK	1002	5	43,46,46	3.42	13 (30%)	45,67,67	2.34	17 (37%)
31	CYC	TP	1001	20	42,46,46	3.39	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	f7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	G5	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
31	CYC	CI	1001	4,5	42,46,46	3.08	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	LN	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	AA	201	6	43,46,46	3.05	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	SM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	QB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	JO	201	7	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	DQ	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.38	16 (35%)
29	PEB	XL	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	A5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	EN	201	6	43,46,46	3.04	10 (23%)	45,67,67	2.23	16 (35%)
29	PEB	QR	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.54	18 (40%)
29	PEB	RB	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	uJ	201	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	D7	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	g1	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	N9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	i7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	XL	202	6,7	43,46,46	3.07	10 (23%)	45,67,67	2.84	14 (31%)
29	PEB	BC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.42	15 (33%)
29	PEB	k9	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	DD	202	6	43,46,46	3.13	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	M3	202	7	43,46,46	3.35	10 (23%)	45,67,67	2.24	13 (28%)
29	PEB	e1	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	J7	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.22	17 (37%)
29	PEB	P9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	U9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	KO	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	ID	201	7	43,46,46	3.15	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	CC	202	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	RL	201	7	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	DJ	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	wL	305	16	42,46,46	3.28	7 (16%)	37,67,67	3.74	15 (40%)
29	PEB	kK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	14 (31%)
29	PEB	k7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	HF	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.10	16 (35%)
29	PEB	PF	201	7,1	43,46,46	3.34	11 (25%)	45,67,67	2.41	21 (46%)
29	PEB	kF	201	7,2	43,46,46	3.33	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	ID	202	7	43,46,46	3.07	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	cM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	HC	202	7	43,46,46	3.25	11 (25%)	45,67,67	2.43	15 (33%)
29	PEB	KM	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	h9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	AI	305	6,2	43,46,46	3.26	8 (18%)	45,67,67	1.98	13 (28%)
29	PEB	C4	203	7	43,46,46	3.28	10 (23%)	45,67,67	2.61	18 (40%)
29	PEB	FM	203	7	43,46,46	3.37	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	BE	201	7	43,46,46	3.56	11 (25%)	45,67,67	2.18	16 (35%)
29	PEB	DM	201	7,17	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	EQ	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	LG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	R1	202	6,7	43,46,46	3.08	10 (23%)	45,67,67	2.58	15 (33%)
29	PEB	ZK	201	7,6	43,46,46	3.08	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	cK	202	7	43,46,46	3.10	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	eB	201	7,16	43,46,46	3.35	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	A5	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	YM	202	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	JE	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
31	CYC	IP	1001	20	42,46,46	3.37	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	j1	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	TM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	wJ	303	16	43,46,46	3.44	12 (27%)	45,67,67	2.28	18 (40%)
29	PEB	XB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.34	15 (33%)
29	PEB	EE	202	6	43,46,46	3.41	11 (25%)	45,67,67	2.13	13 (28%)
29	PEB	JG	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	16 (35%)
29	PEB	ZI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	pL	202	7	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	mM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	GE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	XJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.98	15 (33%)
29	PEB	TB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	dJ	201	7	43,46,46	3.32	9 (20%)	45,67,67	2.99	15 (33%)
29	PEB	OK	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	gK	203	7	43,46,46	3.39	9 (20%)	45,67,67	2.01	15 (33%)
29	PEB	KE	202	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	UJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.12	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	WK	201	6	43,46,46	3.20	10 (23%)	45,67,67	2.39	17 (37%)
31	CYC	DK	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	CD	202	7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	K5	202	-	43,46,46	3.27	10 (23%)	45,67,67	2.20	12 (26%)
29	PEB	EG	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.05	13 (28%)
29	PEB	iI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	HN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	OR	202	6	43,46,46	3.39	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	ML	202	6	43,46,46	3.28	9 (20%)	45,67,67	2.13	13 (28%)
29	PEB	UF	201	7,6	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
29	PEB	RJ	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	FC	203	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	MD	203	7	43,46,46	3.30	10 (23%)	45,67,67	2.63	18 (40%)
29	PEB	H3	201	7,9	43,46,46	3.42	11 (25%)	45,67,67	2.08	15 (33%)
29	PEB	e2	402	7,8	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	A9	301	2	43,46,46	3.25	10 (23%)	45,67,67	2.15	14 (31%)
29	PEB	RK	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	SR	201	6	43,46,46	3.43	11 (25%)	45,67,67	2.52	14 (31%)
29	PEB	xL	301	-	43,46,46	3.18	10 (23%)	45,67,67	2.56	17 (37%)
29	PEB	g9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	D9	1002	-	43,46,46	3.23	10 (23%)	45,67,67	2.21	17 (37%)
29	PEB	IM	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
31	CYC	KF	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.81	18 (36%)
29	PEB	H5	202	-	43,46,46	3.25	10 (23%)	45,67,67	2.06	13 (28%)
29	PEB	dL	202	7,6	43,46,46	3.10	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	A8	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	KA	202	6	43,46,46	3.29	11 (25%)	45,67,67	2.90	20 (44%)
29	PEB	JL	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	I5	203	7	43,46,46	3.38	10 (23%)	45,67,67	2.09	17 (37%)
29	PEB	FO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	MB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	B5	202	-	43,46,46	3.26	10 (23%)	45,67,67	2.06	13 (28%)
31	CYC	UP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	P9	203	7	43,46,46	3.47	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	NL	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	aI	203	7	43,46,46	3.39	10 (23%)	45,67,67	2.13	17 (37%)
29	PEB	DG	203	-	43,46,46	3.47	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	F1	1002	5	43,46,46	3.43	13 (30%)	45,67,67	2.35	17 (37%)
29	PEB	hK	202	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
31	CYC	J1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	2.99	24 (48%)
29	PEB	TF	201	7	43,46,46	3.41	11 (25%)	45,67,67	2.10	15 (33%)
29	PEB	hI	201	6	43,46,46	3.24	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	BB	301	17	43,46,46	3.38	11 (25%)	45,67,67	2.41	17 (37%)
29	PEB	KC	203	6	43,46,46	3.41	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	FN	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.27	16 (35%)
29	PEB	HM	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	EE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	jI	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	MD	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.22	20 (44%)
29	PEB	Y9	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	aJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)
29	PEB	FM	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	NJ	202	7,6	43,46,46	3.08	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	SF	202	6	43,46,46	3.36	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	T9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	JN	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.26	16 (35%)
29	PEB	jB	201	6	43,46,46	3.27	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	YM	203	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	EB	201	6	43,46,46	3.28	10 (23%)	45,67,67	2.25	14 (31%)
29	PEB	TM	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	VR	203	7	43,46,46	3.41	10 (23%)	45,67,67	2.20	16 (35%)
29	PEB	CG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	FE	203	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	WI	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	NP	1001	20,19	42,46,46	3.39	15 (35%)	50,67,67	3.11	22 (44%)
29	PEB	AM	301	16	43,46,46	3.29	11 (25%)	45,67,67	2.34	19 (42%)
29	PEB	l9	202	6	43,46,46	3.21	9 (20%)	45,67,67	2.07	13 (28%)
31	CYC	JF	1001	5,3	42,46,46	3.19	14 (33%)	50,67,67	3.02	21 (42%)
31	CYC	II	1001	4	42,46,46	3.09	13 (30%)	50,67,67	2.80	18 (36%)
29	PEB	G4	202	7	43,46,46	3.05	11 (25%)	45,67,67	2.58	16 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	Q1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
30	PUB	AB	305	16	42,46,46	3.41	7 (16%)	37,67,67	3.01	15 (40%)
29	PEB	T2	201	7	43,46,46	3.37	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	dM	202	6	43,46,46	3.33	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	Y7	201	7	43,46,46	3.25	10 (23%)	45,67,67	2.15	16 (35%)
31	CYC	DI	1001	5	42,46,46	3.20	14 (33%)	50,67,67	3.02	21 (42%)
29	PEB	OJ	202	6	43,46,46	3.28	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	GN	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.89	21 (46%)
29	PEB	yL	301	-	43,46,46	3.29	10 (23%)	45,67,67	2.21	16 (35%)
31	CYC	yP	1001	-	42,46,46	3.49	15 (35%)	50,67,67	2.92	20 (40%)
29	PEB	Z1	201	7,6	43,46,46	3.08	9 (20%)	45,67,67	2.59	15 (33%)
29	PEB	ZJ	203	7	43,46,46	3.42	10 (23%)	45,67,67	2.00	12 (26%)
29	PEB	O9	202	6	43,46,46	3.20	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	IE	201	6	43,46,46	3.44	11 (25%)	45,67,67	2.07	15 (33%)
29	PEB	KL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	B5	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.15	16 (35%)
31	CYC	IP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	L9	1002	-	43,46,46	3.24	10 (23%)	45,67,67	2.21	16 (35%)
29	PEB	mB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	HB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	IG	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	IL	203	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	BJ	201	7,19	43,46,46	3.32	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	L8	201	7	43,46,46	3.27	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	HL	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	fl	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	NB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	cB	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	D4	202	6	43,46,46	3.12	10 (23%)	45,67,67	2.39	20 (44%)
29	PEB	GD	201	7	43,46,46	3.17	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	K5	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.13	14 (31%)
31	CYC	MK	1001	4	42,46,46	3.10	13 (30%)	50,67,67	2.79	18 (36%)
29	PEB	tJ	201	7	43,46,46	3.33	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	KL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	gB	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	JO	202	7,6	43,46,46	3.55	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	b9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	RB	202	7	43,46,46	3.20	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	AM	302	6,16	43,46,46	3.35	8 (18%)	45,67,67	2.01	13 (28%)
29	PEB	dF	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.25	19 (42%)
31	CYC	F9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.24	25 (50%)
29	PEB	VF	201	7	43,46,46	3.35	11 (25%)	45,67,67	2.42	21 (46%)
29	PEB	vJ	202	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	IL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	xJ	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.25	19 (42%)
29	PEB	W7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	jJ	202	6,7	43,46,46	3.09	11 (25%)	45,67,67	2.85	14 (31%)
29	PEB	AI	301	2	43,46,46	3.23	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	zL	501	7	43,46,46	3.36	9 (20%)	45,67,67	2.02	14 (31%)
29	PEB	sL	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	BQ	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.18	16 (35%)
31	CYC	F1	1001	5	42,46,46	3.21	13 (30%)	50,67,67	3.00	24 (48%)
29	PEB	k9	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	xL	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
29	PEB	MO	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	AF	305	6,2	43,46,46	3.26	8 (18%)	45,67,67	1.98	13 (28%)
29	PEB	UI	203	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
31	CYC	rP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.10	22 (44%)
29	PEB	S1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	TB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	wJ	302	-	43,46,46	3.42	12 (27%)	45,67,67	2.26	19 (42%)
29	PEB	C5	201	7	43,46,46	3.32	10 (23%)	45,67,67	2.12	14 (31%)
29	PEB	NJ	203	7	43,46,46	3.44	10 (23%)	45,67,67	1.99	12 (26%)
30	PUB	QM	201	6,17	42,46,46	3.60	8 (19%)	37,67,67	3.06	14 (37%)
31	CYC	G7	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.82	21 (42%)
29	PEB	P7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	PF	202	7	43,46,46	3.13	10 (23%)	45,67,67	2.59	14 (31%)
30	PUB	AB	304	16	42,46,46	3.14	9 (21%)	37,67,67	3.65	18 (48%)
29	PEB	m7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	fF	201	6	43,46,46	3.23	10 (23%)	45,67,67	2.25	19 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	rJ	201	7	43,46,46	3.30	9 (20%)	45,67,67	2.98	15 (33%)
29	PEB	kB	202	7,6	43,46,46	3.19	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	jJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	ZM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	NO	201	-	43,46,46	3.31	9 (20%)	45,67,67	2.29	15 (33%)
29	PEB	O7	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	FE	201	7,18	43,46,46	3.57	12 (27%)	45,67,67	2.18	16 (35%)
29	PEB	MG	404	14	43,46,46	3.22	10 (23%)	45,67,67	2.49	20 (44%)
29	PEB	KJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	II	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.24	19 (42%)
31	CYC	qP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	HO	202	6,7	43,46,46	3.53	13 (30%)	45,67,67	2.12	15 (33%)
29	PEB	LA	201	7	43,46,46	3.25	11 (25%)	45,67,67	2.34	20 (44%)
29	PEB	b1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	wJ	301	-	43,46,46	3.17	10 (23%)	45,67,67	2.54	17 (37%)
29	PEB	IO	201	6	43,46,46	3.28	11 (25%)	45,67,67	2.17	17 (37%)
29	PEB	H9	1002	-	43,46,46	3.22	10 (23%)	45,67,67	2.21	17 (37%)
31	CYC	uP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	ZK	202	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	DI	1002	-	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)
29	PEB	f1	201	6	43,46,46	3.19	10 (23%)	45,67,67	2.39	17 (37%)
29	PEB	XR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	aB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	G4	201	7	43,46,46	3.16	10 (23%)	45,67,67	2.21	20 (44%)
29	PEB	Y1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	X2	201	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	17 (37%)
29	PEB	DQ	203	-	43,46,46	3.45	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	Q2	201	6	43,46,46	3.25	10 (23%)	45,67,67	2.54	18 (40%)
31	CYC	KP	1001	20	42,46,46	3.38	14 (33%)	50,67,67	3.11	22 (44%)
29	PEB	PK	202	7,6	43,46,46	3.09	10 (23%)	45,67,67	2.59	15 (33%)
29	PEB	IL	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	V7	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	ZF	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	16 (35%)
29	PEB	UR	202	6	43,46,46	3.61	12 (27%)	45,67,67	2.06	15 (33%)
29	PEB	aL	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.31	15 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	jL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.98	12 (26%)
29	PEB	W9	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.66	19 (42%)
29	PEB	V2	202	7	43,46,46	3.03	8 (18%)	45,67,67	2.48	18 (40%)
29	PEB	kM	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	KB	203	6,7	43,46,46	3.20	10 (23%)	45,67,67	2.47	15 (33%)
29	PEB	Z1	203	6	43,46,46	3.24	10 (23%)	45,67,67	2.60	14 (31%)
29	PEB	KO	202	6	43,46,46	3.61	12 (27%)	45,67,67	1.97	15 (33%)
29	PEB	j9	201	6	43,46,46	3.25	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	W9	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	BC	201	7	43,46,46	3.56	11 (25%)	45,67,67	2.18	16 (35%)
29	PEB	V9	203	7	43,46,46	3.47	12 (27%)	45,67,67	2.10	14 (31%)
29	PEB	AF	301	2	43,46,46	3.23	10 (23%)	45,67,67	2.14	13 (28%)
29	PEB	HD	201	6	43,46,46	3.13	14 (32%)	45,67,67	2.72	21 (46%)
29	PEB	LO	202	-	43,46,46	3.41	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	AI	304	2	43,46,46	3.29	10 (23%)	45,67,67	2.25	15 (33%)
29	PEB	RR	201	7	43,46,46	3.38	12 (27%)	45,67,67	2.35	14 (31%)
29	PEB	a1	201	7	43,46,46	3.24	10 (23%)	45,67,67	2.18	17 (37%)
29	PEB	M4	202	6,7	43,46,46	3.06	11 (25%)	45,67,67	2.58	16 (35%)
29	PEB	A3	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	DE	202	-	43,46,46	3.43	9 (20%)	45,67,67	1.97	13 (28%)
29	PEB	YB	202	6	43,46,46	3.27	10 (23%)	45,67,67	2.24	14 (31%)
29	PEB	TM	201	7	43,46,46	3.33	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	B8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.15	16 (35%)
29	PEB	ML	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	xL	303	16	43,46,46	3.43	10 (23%)	45,67,67	2.28	18 (40%)
29	PEB	XB	202	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
29	PEB	F8	201	7	43,46,46	3.29	10 (23%)	45,67,67	2.16	16 (35%)
29	PEB	LC	201	7	43,46,46	3.55	11 (25%)	45,67,67	2.17	16 (35%)
29	PEB	F3	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	fK	202	6	43,46,46	3.23	10 (23%)	45,67,67	2.60	15 (33%)
29	PEB	AO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	eF	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
29	PEB	hF	201	6	43,46,46	3.24	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	RM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	17 (37%)
29	PEB	WL	203	6	43,46,46	3.29	10 (23%)	45,67,67	2.12	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
31	CYC	L7	1001	5	42,46,46	3.03	15 (35%)	50,67,67	3.23	26 (52%)
29	PEB	EJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	EO	202	6	43,46,46	3.63	12 (27%)	45,67,67	1.98	15 (33%)
29	PEB	fL	202	6,7	43,46,46	3.09	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	AQ	201	6	43,46,46	3.26	10 (23%)	45,67,67	2.06	15 (33%)
29	PEB	b7	201	6	43,46,46	3.26	11 (25%)	45,67,67	2.65	19 (42%)
29	PEB	JQ	203	7	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	uL	202	6	43,46,46	2.93	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	MO	203	7	43,46,46	3.23	11 (25%)	45,67,67	2.14	14 (31%)
29	PEB	AB	301	16	43,46,46	3.29	11 (25%)	45,67,67	2.34	19 (42%)
29	PEB	MQ	403	14	43,46,46	3.10	12 (27%)	45,67,67	2.44	14 (31%)
31	CYC	K9	1001	-	42,46,46	3.15	14 (33%)	50,67,67	2.81	21 (42%)
29	PEB	e9	203	7	43,46,46	3.49	13 (30%)	45,67,67	2.11	14 (31%)
29	PEB	ZJ	202	7	43,46,46	3.08	10 (23%)	45,67,67	2.85	14 (31%)
29	PEB	hB	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	a9	203	7	43,46,46	3.48	13 (30%)	45,67,67	2.10	14 (31%)
29	PEB	C8	201	7	43,46,46	3.32	10 (23%)	45,67,67	2.13	14 (31%)
29	PEB	LM	203	7	43,46,46	3.38	11 (25%)	45,67,67	2.40	16 (35%)
31	CYC	L9	1001	5	42,46,46	3.04	15 (35%)	50,67,67	3.23	26 (52%)
29	PEB	kB	201	7	43,46,46	3.34	10 (23%)	45,67,67	2.33	15 (33%)
29	PEB	S2	201	6	43,46,46	3.45	11 (25%)	45,67,67	2.17	14 (31%)
29	PEB	PL	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	d9	202	6	43,46,46	3.22	10 (23%)	45,67,67	2.07	13 (28%)
31	CYC	VP	1001	21	42,46,46	3.95	18 (42%)	50,67,67	3.57	28 (56%)
29	PEB	MN	405	14	43,46,46	3.19	12 (27%)	45,67,67	2.60	16 (35%)
29	PEB	R7	201	7,1	43,46,46	3.24	10 (23%)	45,67,67	2.15	17 (37%)
29	PEB	f7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)
29	PEB	B3	202	7,6	43,46,46	3.54	12 (27%)	45,67,67	2.12	15 (33%)
29	PEB	nJ	203	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	IQ	202	6	43,46,46	3.35	10 (23%)	45,67,67	2.05	13 (28%)
29	PEB	AJ	201	6	43,46,46	2.91	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	Y7	202	7	43,46,46	3.19	10 (23%)	45,67,67	2.37	15 (33%)
29	PEB	jI	201	6	43,46,46	3.22	10 (23%)	45,67,67	2.25	19 (42%)
29	PEB	PK	203	7	43,46,46	3.40	9 (20%)	45,67,67	2.02	15 (33%)
29	PEB	h7	202	6	43,46,46	3.21	10 (23%)	45,67,67	2.07	13 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	PEB	VJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	i1	201	7	43,46,46	3.23	10 (23%)	45,67,67	2.17	17 (37%)
29	PEB	BO	203	-	43,46,46	3.40	10 (23%)	45,67,67	2.09	15 (33%)
29	PEB	AJ	202	6	43,46,46	3.29	10 (23%)	45,67,67	2.13	13 (28%)
29	PEB	DJ	201	7	43,46,46	3.31	8 (18%)	45,67,67	2.99	15 (33%)
29	PEB	LE	203	-	43,46,46	3.45	9 (20%)	45,67,67	1.98	13 (28%)
29	PEB	MB	202	6	43,46,46	3.35	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	KM	202	6	43,46,46	3.34	11 (25%)	45,67,67	2.41	16 (35%)
29	PEB	BN	201	7	43,46,46	3.24	11 (25%)	45,67,67	2.35	20 (44%)
29	PEB	SJ	201	6	43,46,46	2.92	9 (20%)	45,67,67	2.32	15 (33%)
29	PEB	BG	203	-	43,46,46	3.46	9 (20%)	45,67,67	2.18	16 (35%)
29	PEB	eI	203	7	43,46,46	3.40	10 (23%)	45,67,67	2.14	17 (37%)
31	CYC	wP	1001	21	42,46,46	3.28	13 (30%)	50,67,67	3.09	21 (42%)
29	PEB	iM	202	6,7	43,46,46	3.18	10 (23%)	45,67,67	2.48	15 (33%)
29	PEB	VJ	202	7	43,46,46	3.43	10 (23%)	45,67,67	1.99	12 (26%)
29	PEB	CE	201	6	43,46,46	3.44	10 (23%)	45,67,67	2.08	15 (33%)
29	PEB	FI	1002	4	43,46,46	3.33	10 (23%)	45,67,67	2.11	16 (35%)

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	CYC	GI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	fB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	PB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	c7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	S9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	FN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	A1	303	2	-	9/24/74/74	0/4/4/4
29	PEB	T7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	AL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	QK	201	6	-	8/24/74/74	0/4/4/4
31	CYC	M7	1001	-	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	DA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	mF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	RM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	a7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	qL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	eK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S1	202	6	-	9/24/74/74	0/4/4/4
31	CYC	MP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	e9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	NL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	aI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	aK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	Q1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	dB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	E4	203	-	-	11/24/74/74	0/4/4/4
29	PEB	LL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	J5	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NO	202	7	-	10/24/74/74	0/4/4/4
29	PEB	iL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	C9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	CA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	JC	202	-	-	9/24/74/74	0/4/4/4
31	CYC	I9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	IN	201	6	-	10/24/74/74	0/4/4/4
31	CYC	E1	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	LN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	B3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	f9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	A1	301	2	-	10/24/74/74	0/4/4/4
29	PEB	iJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	VM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	gL	202	6	-	10/24/74/74	0/4/4/4
32	PMS	kH	301	-	-	2/5/5/5	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	VL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	H8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	RB	203	7	-	13/24/74/74	0/4/4/4
31	CYC	CF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	RI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	AM	303	16	-	13/24/74/74	0/4/4/4
29	PEB	R1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	R7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	IM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	JB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	AF	304	2	-	9/24/74/74	0/4/4/4
29	PEB	L7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	W7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	k9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	c1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LK	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	kM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	bL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	RL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	mI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	OR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	UJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	tL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	EG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	kF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	rL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	mM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	cF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	MG	405	14	-	11/24/74/74	0/4/4/4
29	PEB	VM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	UK	201	7,6	-	6/24/74/74	0/4/4/4
32	PMS	kH	302	-	-	2/5/5/5	0/1/1/1
31	CYC	sP	1001	21	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	SL	201	6	-	9/24/74/74	0/4/4/4
30	PUB	QB	201	6,17	-	6/24/74/74	0/4/4/4
29	PEB	B8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	BE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	PL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	S7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	g1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	ZK	203	6	-	9/24/74/74	0/4/4/4
29	PEB	I4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	bK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	MN	404	14	-	11/24/74/74	0/4/4/4
29	PEB	HA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	mI	203	7	-	14/24/74/74	0/4/4/4
31	CYC	tP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	hJ	203	7	-	13/24/74/74	0/4/4/4
30	PUB	A9	303	-	-	8/24/74/74	0/4/4/4
29	PEB	H5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	IG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	M3	203	7	-	10/24/74/74	0/4/4/4
29	PEB	P1	201	7,1	-	6/24/74/74	0/4/4/4
29	PEB	cF	202	7	-	14/24/74/74	0/4/4/4
29	PEB	dJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	CO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	TL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	gF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	WF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	NR	201	7	-	9/24/74/74	0/4/4/4
31	CYC	I1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	C4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	K3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	KB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	A7	305	-	-	10/24/74/74	0/4/4/4
31	CYC	EF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	UF	203	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	M9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	IE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	N7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	H3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	L5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	AE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	B4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	nL	202	6,7	-	9/24/74/74	0/4/4/4
31	CYC	eP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	KB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	DO	201	7	-	5/24/74/74	0/4/4/4
29	PEB	eM	202	7	-	13/24/74/74	0/4/4/4
30	PUB	AI	303	2	-	6/24/74/74	0/4/4/4
29	PEB	dI	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	sJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	DL	201	7	-	7/24/74/74	0/4/4/4
31	CYC	E7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	JD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	iI	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	RR	202	7	-	7/24/74/74	0/4/4/4
31	CYC	CP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	D1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	WK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	A1	302	-	-	9/24/74/74	0/4/4/4
29	PEB	l9	201	6	-	8/24/74/74	0/4/4/4
31	CYC	oP	1001	21	-	8/25/74/74	0/4/4/4
30	PUB	A1	305	-	-	13/24/74/74	0/4/4/4
29	PEB	FA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	LI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	LG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	M2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	JA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	kI	202	7,6	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	PP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	ED	202	7	-	11/24/74/74	0/4/4/4
29	PEB	hJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	U2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	hF	202	6	-	8/24/74/74	0/4/4/4
31	CYC	FF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	e1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	l7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	LJ	202	7	-	13/24/74/74	0/4/4/4
30	PUB	A9	302	2	-	5/24/74/74	0/4/4/4
29	PEB	iI	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	R9	201	7,1	-	4/24/74/74	0/4/4/4
29	PEB	HG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	SK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	k1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	cJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	HQ	203	7	-	12/24/74/74	0/4/4/4
29	PEB	DA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	YL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mF	202	7	-	7/24/74/74	0/4/4/4
29	PEB	SR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	LF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	J1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	K8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	eK	202	6,7	-	6/24/74/74	0/4/4/4
31	CYC	EP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	dF	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	f1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	YK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	g7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dB	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	YF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	UR	201	6	-	7/24/74/74	0/4/4/4
30	PUB	yJ	303	-	-	5/24/74/74	0/4/4/4
29	PEB	WR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	sL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	Y1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FO	202	7,6	-	9/24/74/74	0/4/4/4
30	PUB	MQ	404	14	-	15/24/74/74	0/4/4/4
29	PEB	DN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	H3	202	6,7	-	9/24/74/74	0/4/4/4
30	PUB	AK	305	-	-	13/24/74/74	0/4/4/4
29	PEB	B5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	TF	202	7	-	14/24/74/74	0/4/4/4
31	CYC	XP	1001	24,21	-	8/25/74/74	0/4/4/4
30	PUB	BB	302	17	-	7/24/74/74	0/4/4/4
29	PEB	BJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	lB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	oL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	h7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	SJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	GO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	K5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	VR	201	7	-	9/24/74/74	0/4/4/4
30	PUB	MG	403	14	-	10/24/74/74	0/4/4/4
29	PEB	JF	1002	4	-	13/24/74/74	0/4/4/4
31	CYC	DF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	PR	202	7	-	12/24/74/74	0/4/4/4
31	CYC	M1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	R2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	VK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	L4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	PJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LM	201	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	N2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	fI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	WM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	MQ	401	6,14	-	10/24/74/74	0/4/4/4
29	PEB	PB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	QI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	JP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	Q9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	sJ	203	6,7	-	9/24/74/74	0/4/4/4
30	PUB	xL	305	16	-	5/24/74/74	0/4/4/4
31	CYC	JK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	SM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	kI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	JN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	UI	202	6	-	6/24/74/74	0/4/4/4
29	PEB	Z1	202	6	-	8/24/74/74	0/4/4/4
29	PEB	hJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	bJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	O9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	QI	202	6	-	8/24/74/74	0/4/4/4
31	CYC	RP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	A5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	DB	201	7,17	-	6/24/74/74	0/4/4/4
29	PEB	W2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	JL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	AQ	202	6	-	12/24/74/74	0/4/4/4
31	CYC	BP	1001	25,21	-	8/25/74/74	0/4/4/4
29	PEB	wL	303	16	-	14/24/74/74	0/4/4/4
29	PEB	LL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	LD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	CB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	CN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	LA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	H4	201	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	vL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	IC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	g1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	g7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	jM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	PI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	aL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	iL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	CM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	jL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	R7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	DE	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	h1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	SF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	fP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	GA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	XJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	EA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	Q7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	fB	201	6	-	5/24/74/74	0/4/4/4
30	PUB	AI	302	2	-	9/24/74/74	0/4/4/4
29	PEB	IC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KD	202	7,6	-	12/24/74/74	0/4/4/4
29	PEB	WM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	WJ	202	6	-	9/24/74/74	0/4/4/4
29	PEB	DC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	F5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	GD	202	7	-	12/24/74/74	0/4/4/4
29	PEB	G3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	I3	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	jK	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	lB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	XJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	G8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	GN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	B4	202	6	-	11/24/74/74	0/4/4/4
31	CYC	GF	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	HO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	hM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	VF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	lF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	PR	201	7	-	7/24/74/74	0/4/4/4
29	PEB	BE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	hB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	m7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	N2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	VR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	KA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	FC	202	7	-	8/24/74/74	0/4/4/4
31	CYC	KI	1001	4	-	8/25/74/74	0/4/4/4
31	CYC	IK	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	VB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	d9	201	6	-	8/24/74/74	0/4/4/4
32	PMS	k6	301	-	-	2/5/5/5	0/1/1/1
29	PEB	F8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	FG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	wL	302	-	-	7/24/74/74	0/4/4/4
30	PUB	yJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	uJ	203	6	-	10/24/74/74	0/4/4/4
29	PEB	iK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	CG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	m7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	BL	201	7,19	-	7/24/74/74	0/4/4/4
29	PEB	FQ	203	-	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	eR	401	-	-	9/24/74/74	0/4/4/4
29	PEB	A8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	JB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	c9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	KJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	OM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	I8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	KG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	DB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	NL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	m1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	aI	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	DG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	KD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	V7	203	7	-	12/24/74/74	0/4/4/4
31	CYC	J9	1001	5	-	9/25/74/74	0/4/4/4
30	PUB	xJ	304	-	-	9/24/74/74	0/4/4/4
29	PEB	EJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	iM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	CA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	AK	301	2	-	10/24/74/74	0/4/4/4
29	PEB	HN	201	7	-	12/24/74/74	0/4/4/4
30	PUB	xL	304	-	-	9/24/74/74	0/4/4/4
31	CYC	H7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	YB	203	6	-	10/24/74/74	0/4/4/4
29	PEB	Y9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	c1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	T7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	hM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	WB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	HO	201	7,9	-	5/24/74/74	0/4/4/4
29	PEB	YK	202	7	-	6/24/74/74	0/4/4/4
31	CYC	1P	1001	25,21	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	C5	203	7	-	9/24/74/74	0/4/4/4
30	PUB	MQ	405	14	-	10/24/74/74	0/4/4/4
29	PEB	EB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	IM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	SI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	sJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	WI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	BA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	Q9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	EL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	i1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	lJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	jB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	OI	203	6,7	-	7/24/74/74	0/4/4/4
29	PEB	G3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	BN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	ZJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	hK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	MM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	IB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	W1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	ZF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	L4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	GQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	OM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	H1	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	AA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	mL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	gB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	QM	204	6	-	10/24/74/74	0/4/4/4
29	PEB	L8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	IB	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	HG	203	7	-	12/24/74/74	0/4/4/4
31	CYC	F7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	f9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	tJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	R9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	iB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	LN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	DF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	eK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	uL	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	C3	201	6	-	4/24/74/74	0/4/4/4
30	PUB	yL	303	-	-	5/24/74/74	0/4/4/4
29	PEB	K8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	W2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	H4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	OL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	KG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	KD	203	-	-	11/24/74/74	0/4/4/4
30	PUB	AM	305	16	-	7/24/74/74	0/4/4/4
31	CYC	pP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	HJ	201	7	-	9/24/74/74	0/4/4/4
29	PEB	QB	204	6	-	10/24/74/74	0/4/4/4
29	PEB	LB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	d1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	VI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	EO	201	6	-	4/24/74/74	0/4/4/4
31	CYC	L1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	Y9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	kJ	202	6	-	10/24/74/74	0/4/4/4
30	PUB	MA	402	14	-	8/24/74/74	0/4/4/4
29	PEB	U1	202	6	-	8/24/74/74	0/4/4/4
29	PEB	e1	201	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	j7	201	6	-	8/24/74/74	0/4/4/4
30	PUB	wJ	305	16	-	5/24/74/74	0/4/4/4
29	PEB	JC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	D3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	EA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	kL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	bI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	WP	1001	-	-	8/25/74/74	0/4/4/4
29	PEB	qJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	OI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	DO	202	-	-	12/24/74/74	0/4/4/4
29	PEB	hL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	c7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	S7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	T7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	F3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	YJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	XR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	c1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	CE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	UM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	GM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	fM	201	6	-	5/24/74/74	0/4/4/4
31	CYC	NI	1001	5,3	-	7/25/74/74	0/4/4/4
31	CYC	D1	1003	4,5	-	9/25/74/74	0/4/4/4
31	CYC	D7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	JG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	WF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	HL	201	7	-	9/24/74/74	0/4/4/4
29	PEB	NB	201	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	eL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	J5	202	6	-	8/24/74/74	0/4/4/4
29	PEB	TR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	kJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	J3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	iB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	SK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	mK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	tL	201	7	-	7/24/74/74	0/4/4/4
31	CYC	HP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	D3	201	7	-	5/24/74/74	0/4/4/4
31	CYC	LI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	MQ	407	14	-	11/24/74/74	0/4/4/4
29	PEB	iK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	YL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	F3	201	7,9	-	5/24/74/74	0/4/4/4
31	CYC	NF	1001	5,3	-	7/25/74/74	0/4/4/4
29	PEB	HC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	eM	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	pJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	a1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	cK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	TL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	OB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	NR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	WL	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	IN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	bJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	FA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	M2	201	6	-	7/24/74/74	0/4/4/4
31	CYC	OP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	FJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	mI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	eF	202	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	e9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	rJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	F5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	SB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	AC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	WL	202	6	-	9/24/74/74	0/4/4/4
29	PEB	K3	201	6	-	4/24/74/74	0/4/4/4
30	PUB	BM	302	17	-	7/24/74/74	0/4/4/4
29	PEB	fJ	203	7	-	13/24/74/74	0/4/4/4
31	CYC	QP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	LB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	pL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	dI	203	6	-	8/24/74/74	0/4/4/4
31	CYC	HI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	a9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	eL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	J9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	N3	203	7	-	10/24/74/74	0/4/4/4
29	PEB	nJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	XR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	N2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	FQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	IJ	202	7	-	9/24/74/74	0/4/4/4
31	CYC	AP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	b7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	dL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BO	201	7,9	-	5/24/74/74	0/4/4/4
31	CYC	K1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	MA	401	14	-	12/24/74/74	0/4/4/4
29	PEB	b9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	J3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	oJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	A7	301	2	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	QL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	eJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	gB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	EM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	aJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	HM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	JI	1002	4	-	13/24/74/74	0/4/4/4
29	PEB	CQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	l1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	PM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	OF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	xJ	301	-	-	12/24/74/74	0/4/4/4
29	PEB	PJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	M4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	AE	203	6,7	-	8/24/74/74	0/4/4/4
29	PEB	NO	203	7	-	10/24/74/74	0/4/4/4
29	PEB	C3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	D3	202	-	-	12/24/74/74	0/4/4/4
29	PEB	CM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FB	201	7,15	-	6/24/74/74	0/4/4/4
31	CYC	EI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	e7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	DO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	m9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	F7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	g9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	GJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	DN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	IO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	G4	203	7	-	11/24/74/74	0/4/4/4
29	PEB	L3	202	-	-	10/24/74/74	0/4/4/4
31	CYC	jP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	JJ	201	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	N1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	bF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	HI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	HA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	k1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MN	401	14	-	12/24/74/74	0/4/4/4
29	PEB	J4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	EL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	D1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	I5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	JJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	K4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	R2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	dD	401	7,10	-	9/24/74/74	0/4/4/4
29	PEB	DL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	TJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	cB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	GC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	YB	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	g7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	NF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	aF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	H8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	BC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	mF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	BD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	Z9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	AL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	cM	201	7	-	6/24/74/74	0/4/4/4
30	PUB	AM	304	16	-	13/24/74/74	0/4/4/4
31	CYC	FI	1001	5	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	IJ	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	JB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	OL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	c9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	iF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	AE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	GB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	wL	301	-	-	12/24/74/74	0/4/4/4
29	PEB	IA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	J8	201	6	-	5/24/74/74	0/4/4/4
29	PEB	bL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JE	202	-	-	9/24/74/74	0/4/4/4
29	PEB	L3	201	7	-	5/24/74/74	0/4/4/4
29	PEB	Z7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	eJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U1	203	6	-	9/24/74/74	0/4/4/4
29	PEB	IJ	202	6	-	10/24/74/74	0/4/4/4
30	PUB	wJ	304	-	-	9/24/74/74	0/4/4/4
29	PEB	G5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	LJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	HB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	cB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LQ	201	7	-	6/24/74/74	0/4/4/4
29	PEB	iI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	WR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	U7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	HG	201	7,14	-	10/24/74/74	0/4/4/4
29	PEB	HE	202	7	-	8/24/74/74	0/4/4/4
29	PEB	C8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	N1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	uJ	202	6	-	9/24/74/74	0/4/4/4
29	PEB	SL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	O1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	W1	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	I4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	IK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	aB	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	cL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	RR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	FD	201	6	-	9/24/74/74	0/4/4/4
31	CYC	GP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	TK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	G8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	F9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	ZL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	IL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	ZI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	QK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	P2	202	7	-	12/24/74/74	0/4/4/4
31	CYC	vP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	fK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	XL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	XM	202	7	-	13/24/74/74	0/4/4/4
29	PEB	MA	404	14	-	11/24/74/74	0/4/4/4
29	PEB	WJ	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	mB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	gJ	201	6	-	9/24/74/74	0/4/4/4
30	PUB	A7	302	2	-	5/24/74/74	0/4/4/4
29	PEB	k7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	aF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	l7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	A7	304	-	-	10/24/74/74	0/4/4/4
31	CYC	G9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	QF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	VK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	gJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	P7	203	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	Z9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	MQ	402	7,14	-	10/24/74/74	0/4/4/4
29	PEB	AK	303	2	-	9/24/74/74	0/4/4/4
29	PEB	iK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	MQ	406	29,14	-	10/24/74/74	0/4/4/4
29	PEB	IJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	R1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	VI	202	6,7	-	7/24/74/74	0/4/4/4
31	CYC	kP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	LC	202	6,7	-	8/24/74/74	0/4/4/4
29	PEB	kB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	jK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	pJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	aB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	G8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	MJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	aM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	BQ	201	7,29,14	-	10/24/74/74	0/4/4/4
29	PEB	MR	202	6	-	5/24/74/74	0/4/4/4
29	PEB	KM	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	e7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	CB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	SI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	OF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	DP	1001	25,21	-	8/25/74/74	0/4/4/4
29	PEB	I8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	Q2	202	6	-	11/24/74/74	0/4/4/4
29	PEB	O2	201	6	-	7/24/74/74	0/4/4/4
29	PEB	A3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	UI	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	CO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	CL	202	6	-	10/24/74/74	0/4/4/4
31	CYC	IF	1001	4	-	8/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	gM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	JA	202	7	-	11/24/74/74	0/4/4/4
31	CYC	HK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	RF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	F4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	I3	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	D4	201	6	-	9/24/74/74	0/4/4/4
29	PEB	JQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	iM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HN	203	-	-	9/24/74/74	0/4/4/4
29	PEB	NM	202	7	-	13/24/74/74	0/4/4/4
29	PEB	C8	202	-	-	9/24/74/74	0/4/4/4
31	CYC	nP	1001	24,21	-	8/25/74/74	0/4/4/4
29	PEB	HQ	201	7,14	-	10/24/74/74	0/4/4/4
31	CYC	gP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	YI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	UB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	AC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	I4	203	7	-	8/24/74/74	0/4/4/4
29	PEB	IL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	KQ	201	6	-	7/24/74/74	0/4/4/4
30	PUB	yL	302	-	-	7/24/74/74	0/4/4/4
29	PEB	PI	201	7,1	-	11/24/74/74	0/4/4/4
29	PEB	zJ	501	7	-	8/24/74/74	0/4/4/4
29	PEB	qJ	202	6	-	10/24/74/74	0/4/4/4
31	CYC	iP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	H5	203	7	-	12/24/74/74	0/4/4/4
30	PUB	MN	403	14	-	10/24/74/74	0/4/4/4
29	PEB	V2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	MJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	mM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	nJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	EN	202	6	-	16/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CYC	LF	1001	5	-	7/25/74/74	0/4/4/4
31	CYC	N7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	k1	202	7	-	6/24/74/74	0/4/4/4
31	CYC	GK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	GL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	YF	202	7	-	7/24/74/74	0/4/4/4
29	PEB	BO	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	FJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	CJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	nL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	c9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	TI	201	7	-	11/24/74/74	0/4/4/4
30	PUB	A7	303	-	-	8/24/74/74	0/4/4/4
29	PEB	CD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	H8	202	-	-	10/24/74/74	0/4/4/4
31	CYC	FP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	EQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	KE	203	6	-	8/24/74/74	0/4/4/4
29	PEB	BL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	pJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	EM	202	6	-	10/24/74/74	0/4/4/4
31	CYC	CK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	UL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	FJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	T9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	uL	203	6	-	10/24/74/74	0/4/4/4
29	PEB	T2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	Z7	202	6	-	8/24/74/74	0/4/4/4
30	PUB	AF	303	2	-	6/24/74/74	0/4/4/4
29	PEB	PJ	201	7	-	7/24/74/74	0/4/4/4
31	CYC	xP	1001	21	-	10/25/74/74	0/4/4/4
29	PEB	ED	201	7	-	12/24/74/74	0/4/4/4
29	PEB	V1	203	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	FB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	HE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	eF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	YJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	kL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	KC	202	6	-	6/24/74/74	0/4/4/4
29	PEB	OB	202	6	-	10/24/74/74	0/4/4/4
31	CYC	EK	1001	4,5	-	9/25/74/74	0/4/4/4
29	PEB	J8	202	6	-	8/24/74/74	0/4/4/4
29	PEB	hL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	qL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	R2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	TK	201	7	-	6/24/74/74	0/4/4/4
30	PUB	MA	403	14	-	10/24/74/74	0/4/4/4
29	PEB	TR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	LD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	l1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	GD	203	7	-	11/24/74/74	0/4/4/4
29	PEB	j1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	LE	202	6,7	-	8/24/74/74	0/4/4/4
29	PEB	i7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	lI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	vL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	K4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	AK	302	-	-	9/24/74/74	0/4/4/4
29	PEB	VB	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	LA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	K8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	hL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	FG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	L8	203	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	cI	202	7	-	14/24/74/74	0/4/4/4
29	PEB	i9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	QL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	RI	202	7	-	14/24/74/74	0/4/4/4
31	CYC	YP	1000	25	-	7/25/74/74	0/4/4/4
29	PEB	WB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QR	202	6	-	10/24/74/74	0/4/4/4
29	PEB	FL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	gI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	xJ	303	16	-	14/24/74/74	0/4/4/4
29	PEB	BM	301	17	-	13/24/74/74	0/4/4/4
29	PEB	PF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	d7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	S2	202	6	-	10/24/74/74	0/4/4/4
29	PEB	JG	203	7	-	12/24/74/74	0/4/4/4
29	PEB	e2	401	-	-	9/24/74/74	0/4/4/4
31	CYC	HF	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	QB	203	6	-	5/24/74/74	0/4/4/4
29	PEB	JD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	HJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	GM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	O7	202	6	-	8/24/74/74	0/4/4/4
31	CYC	C1	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	DM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	RM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	MG	401	14	-	9/24/74/74	0/4/4/4
29	PEB	RJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	nL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	rL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	TI	202	7	-	14/24/74/74	0/4/4/4
29	PEB	TJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	NI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	O1	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	a9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	A9	305	-	-	10/24/74/74	0/4/4/4
29	PEB	aM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	LQ	202	-	-	12/24/74/74	0/4/4/4
29	PEB	gF	202	7,6	-	7/24/74/74	0/4/4/4
29	PEB	J4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	fJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	FQ	201	7	-	10/24/74/74	0/4/4/4
31	CYC	SP	1001	21	-	8/25/74/74	0/4/4/4
31	CYC	D9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	FA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	FM	201	7,15	-	6/24/74/74	0/4/4/4
29	PEB	AG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	dF	203	6	-	8/24/74/74	0/4/4/4
29	PEB	E4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	KC	201	7,6	-	8/24/74/74	0/4/4/4
29	PEB	bF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	iF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	cK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	GC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	pL	203	7	-	13/24/74/74	0/4/4/4
31	CYC	N9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	RL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	LM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	LE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	BJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	DK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	B3	201	7,9	-	5/24/74/74	0/4/4/4
29	PEB	U1	201	7,6	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	hI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	gI	202	7,6	-	7/24/74/74	0/4/4/4
31	CYC	hP	1001	25,21	-	8/25/74/74	0/4/4/4
31	CYC	LK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	FC	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	V1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	RK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	eB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	FN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	a1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	g9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	N3	201	-	-	6/24/74/74	0/4/4/4
29	PEB	mJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	fJ	201	7,16	-	7/24/74/74	0/4/4/4
29	PEB	ZL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	E3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	dJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	fL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	KN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	I5	201	7	-	6/24/74/74	0/4/4/4
29	PEB	FO	201	7,9	-	5/24/74/74	0/4/4/4
30	PUB	A1	304	2	-	4/24/74/74	0/4/4/4
29	PEB	BN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	P9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	j7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	gM	202	7	-	6/24/74/74	0/4/4/4
31	CYC	KK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	ZB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	T2	203	7	-	12/24/74/74	0/4/4/4
29	PEB	UF	202	6	-	6/24/74/74	0/4/4/4
31	CYC	NK	1001	5,3	-	7/25/74/74	0/4/4/4
29	PEB	Y7	203	7	-	12/24/74/74	0/4/4/4
29	PEB	k7	201	7	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	iB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	HQ	202	7	-	6/24/74/74	0/4/4/4
31	CYC	1P	1002	25	-	7/25/74/74	0/4/4/4
29	PEB	VK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	dK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	bI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	DD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	BD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	AO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	YM	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	MA	405	14	-	9/24/74/74	0/4/4/4
29	PEB	GQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	O2	202	6	-	11/24/74/74	0/4/4/4
29	PEB	h9	202	6	-	8/24/74/74	0/4/4/4
30	PUB	AF	302	2	-	9/24/74/74	0/4/4/4
29	PEB	AJ	203	6,7	-	9/24/74/74	0/4/4/4
30	PUB	xJ	305	16	-	5/24/74/74	0/4/4/4
29	PEB	CN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	m9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	U2	202	-	-	10/24/74/74	0/4/4/4
29	PEB	oJ	202	6	-	10/24/74/74	0/4/4/4
31	CYC	K7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	K4	203	7	-	11/24/74/74	0/4/4/4
30	PUB	MN	402	14	-	8/24/74/74	0/4/4/4
29	PEB	QJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	L1	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	j9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	mP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	d1	202	6	-	9/24/74/74	0/4/4/4
31	CYC	C7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	HD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	HB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	GE	202	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	JM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	IO	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	VL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	ZM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	V2	201	7,8	-	9/24/74/74	0/4/4/4
29	PEB	mL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	h1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	lK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	YI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	CQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	OI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	cL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	HA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	DA	203	-	-	9/24/74/74	0/4/4/4
31	CYC	H1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	NK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	L5	201	7	-	7/24/74/74	0/4/4/4
29	PEB	M3	201	-	-	6/24/74/74	0/4/4/4
29	PEB	J3	201	7	-	5/24/74/74	0/4/4/4
29	PEB	XM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	SB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UK	203	6	-	9/24/74/74	0/4/4/4
29	PEB	oL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	ZB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	aK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	bK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	d7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	QJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	KE	201	7,6	-	8/24/74/74	0/4/4/4
29	PEB	RF	202	7	-	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	HC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jF	201	6	-	6/24/74/74	0/4/4/4
31	CYC	cP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	GG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	fM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	gL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	PL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	KQ	202	6	-	12/24/74/74	0/4/4/4
29	PEB	mK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	X2	202	7	-	12/24/74/74	0/4/4/4
29	PEB	E4	202	7	-	12/24/74/74	0/4/4/4
29	PEB	YF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	i9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FL	202	7,6	-	9/24/74/74	0/4/4/4
31	CYC	MI	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	GG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	WJ	203	6	-	10/24/74/74	0/4/4/4
29	PEB	dM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	TL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	kM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	NR	202	7	-	7/24/74/74	0/4/4/4
29	PEB	A8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	IJ	203	7	-	13/24/74/74	0/4/4/4
31	CYC	I7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	MD	202	6,7	-	12/24/74/74	0/4/4/4
29	PEB	DQ	201	7	-	10/24/74/74	0/4/4/4
29	PEB	jK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	MO	202	7	-	10/24/74/74	0/4/4/4
29	PEB	F4	201	6	-	8/24/74/74	0/4/4/4
29	PEB	CJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	rJ	202	6,7	-	9/24/74/74	0/4/4/4
32	PMS	k6	302	-	-	2/5/5/5	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	ZM	202	7	-	6/24/74/74	0/4/4/4
31	CYC	MF	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	U9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	b1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	CC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	B8	203	7	-	12/24/74/74	0/4/4/4
29	PEB	RK	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	A9	304	-	-	10/24/74/74	0/4/4/4
29	PEB	UL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	dI	202	6	-	6/24/74/74	0/4/4/4
29	PEB	lL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	GO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	iJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	dL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kI	201	7,2	-	11/24/74/74	0/4/4/4
29	PEB	aM	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	N3	202	7	-	10/24/74/74	0/4/4/4
29	PEB	vJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	V9	201	7	-	4/24/74/74	0/4/4/4
31	CYC	FK	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	F8	202	-	-	10/24/74/74	0/4/4/4
29	PEB	OF	203	6,7	-	7/24/74/74	0/4/4/4
29	PEB	Q7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	gM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	EC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	cI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	ZB	203	7	-	13/24/74/74	0/4/4/4
30	PUB	MG	402	14	-	15/24/74/74	0/4/4/4
29	PEB	aK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	P1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	HM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	a7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	CL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	YI	203	7	-	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	L5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	P7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	AB	303	16	-	13/24/74/74	0/4/4/4
30	PUB	AK	304	2	-	4/24/74/74	0/4/4/4
29	PEB	jM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QM	203	6	-	5/24/74/74	0/4/4/4
29	PEB	JQ	201	7	-	10/24/74/74	0/4/4/4
29	PEB	VI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	PI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	rL	201	7,16	-	7/24/74/74	0/4/4/4
29	PEB	gK	202	7	-	6/24/74/74	0/4/4/4
31	CYC	JI	1001	5,3	-	7/25/74/74	0/4/4/4
29	PEB	e7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	F5	203	7	-	12/24/74/74	0/4/4/4
29	PEB	aF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	HK	1002	-	-	8/24/74/74	0/4/4/4
29	PEB	AN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	JJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	RJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	C5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	BA	202	7	-	11/24/74/74	0/4/4/4
29	PEB	TB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	EC	201	6	-	6/24/74/74	0/4/4/4
29	PEB	VF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	G5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	I3	201	6	-	4/24/74/74	0/4/4/4
29	PEB	GJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	m9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	I8	202	-	-	9/24/74/74	0/4/4/4
29	PEB	FF	1002	4	-	13/24/74/74	0/4/4/4
29	PEB	PK	201	7,1	-	6/24/74/74	0/4/4/4
29	PEB	T1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	AC	203	6,7	-	8/24/74/74	0/4/4/4
29	PEB	mJ	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	GB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	ZL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	E3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	CD	203	-	-	11/24/74/74	0/4/4/4
29	PEB	JA	203	-	-	9/24/74/74	0/4/4/4
29	PEB	i7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	MM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	T1	202	7	-	6/24/74/74	0/4/4/4
29	PEB	FK	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	BG	201	7	-	10/24/74/74	0/4/4/4
29	PEB	T9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	eI	201	7	-	11/24/74/74	0/4/4/4
29	PEB	IQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	m1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	P2	201	7	-	7/24/74/74	0/4/4/4
29	PEB	cJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	VM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	UK	202	6	-	8/24/74/74	0/4/4/4
29	PEB	VB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LO	201	7	-	5/24/74/74	0/4/4/4
30	PUB	wL	304	-	-	9/24/74/74	0/4/4/4
29	PEB	DC	202	-	-	9/24/74/74	0/4/4/4
29	PEB	H7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	R9	203	7	-	12/24/74/74	0/4/4/4
31	CYC	J7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	HE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	kF	202	7,6	-	7/24/74/74	0/4/4/4
29	PEB	PM	202	7	-	13/24/74/74	0/4/4/4
31	CYC	H9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	eI	202	7	-	7/24/74/74	0/4/4/4
29	PEB	c7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	P1	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	yJ	301	-	-	9/24/74/74	0/4/4/4
29	PEB	cM	202	7	-	6/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	TJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	OK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	AB	302	6,16	-	8/24/74/74	0/4/4/4
29	PEB	ID	203	7	-	11/24/74/74	0/4/4/4
29	PEB	C4	202	7,6	-	12/24/74/74	0/4/4/4
29	PEB	gK	201	7	-	6/24/74/74	0/4/4/4
29	PEB	jJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	QM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	a7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	fL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	sL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	TR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	QF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	iF	202	6,7	-	7/24/74/74	0/4/4/4
29	PEB	j1	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	M4	203	7	-	12/24/74/74	0/4/4/4
29	PEB	jF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	OJ	201	6	-	9/24/74/74	0/4/4/4
31	CYC	E9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	fF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	V1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	i9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	JK	1002	5	-	8/24/74/74	0/4/4/4
31	CYC	TP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	f7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	G5	201	7	-	7/24/74/74	0/4/4/4
31	CYC	CI	1001	4,5	-	8/25/74/74	0/4/4/4
29	PEB	LN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	AA	201	6	-	10/24/74/74	0/4/4/4
29	PEB	SM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	QB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	JO	201	7	-	5/24/74/74	0/4/4/4
29	PEB	DQ	202	7	-	6/24/74/74	0/4/4/4
29	PEB	XL	201	7	-	7/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	A5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	EN	201	6	-	10/24/74/74	0/4/4/4
29	PEB	QR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	RB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	uJ	201	7,6	-	9/24/74/74	0/4/4/4
29	PEB	D7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	g1	203	7	-	6/24/74/74	0/4/4/4
29	PEB	N9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	i7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	XL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BC	202	7	-	8/24/74/74	0/4/4/4
29	PEB	k9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	DD	202	6	-	11/24/74/74	0/4/4/4
29	PEB	M3	202	7	-	10/24/74/74	0/4/4/4
29	PEB	e1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	J7	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	P9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	U9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	KO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	ID	201	7	-	9/24/74/74	0/4/4/4
29	PEB	CC	202	6	-	8/24/74/74	0/4/4/4
29	PEB	RL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	DJ	202	7	-	13/24/74/74	0/4/4/4
30	PUB	wL	305	16	-	5/24/74/74	0/4/4/4
29	PEB	kK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	k7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	HF	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	PF	201	7,1	-	11/24/74/74	0/4/4/4
29	PEB	kF	201	7,2	-	11/24/74/74	0/4/4/4
29	PEB	ID	202	7	-	12/24/74/74	0/4/4/4
29	PEB	cM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HC	202	7	-	8/24/74/74	0/4/4/4
29	PEB	KM	201	6	-	5/24/74/74	0/4/4/4
29	PEB	h9	201	6	-	8/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	AI	305	6,2	-	7/24/74/74	0/4/4/4
29	PEB	C4	203	7	-	11/24/74/74	0/4/4/4
29	PEB	FM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	BE	201	7	-	6/24/74/74	0/4/4/4
29	PEB	DM	201	7,17	-	6/24/74/74	0/4/4/4
29	PEB	EQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	LG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	R1	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	ZK	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	cK	202	7	-	6/24/74/74	0/4/4/4
29	PEB	eB	201	7,16	-	6/24/74/74	0/4/4/4
29	PEB	A5	201	7	-	6/24/74/74	0/4/4/4
29	PEB	YM	202	6	-	5/24/74/74	0/4/4/4
29	PEB	JE	201	7	-	6/24/74/74	0/4/4/4
31	CYC	IP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	j1	202	6	-	9/24/74/74	0/4/4/4
29	PEB	TM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	wJ	303	16	-	14/24/74/74	0/4/4/4
29	PEB	XB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	EE	202	6	-	8/24/74/74	0/4/4/4
29	PEB	JG	202	7	-	6/24/74/74	0/4/4/4
29	PEB	ZI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	pL	202	7	-	9/24/74/74	0/4/4/4
29	PEB	mM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	GE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	XJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	TB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	dJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	OK	201	6	-	8/24/74/74	0/4/4/4
29	PEB	gK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	KE	202	6	-	6/24/74/74	0/4/4/4
29	PEB	UJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	WK	201	6	-	8/24/74/74	0/4/4/4
31	CYC	DK	1001	5	-	7/25/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	CD	202	7	-	12/24/74/74	0/4/4/4
29	PEB	K5	202	-	-	9/24/74/74	0/4/4/4
29	PEB	EG	202	6	-	12/24/74/74	0/4/4/4
29	PEB	iI	203	7	-	14/24/74/74	0/4/4/4
29	PEB	HN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	OR	202	6	-	8/24/74/74	0/4/4/4
29	PEB	ML	202	6	-	10/24/74/74	0/4/4/4
29	PEB	UF	201	7,6	-	7/24/74/74	0/4/4/4
29	PEB	RJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	FC	203	-	-	9/24/74/74	0/4/4/4
29	PEB	MD	203	7	-	11/24/74/74	0/4/4/4
29	PEB	H3	201	7,9	-	5/24/74/74	0/4/4/4
29	PEB	e2	402	7,8	-	9/24/74/74	0/4/4/4
29	PEB	A9	301	2	-	9/24/74/74	0/4/4/4
29	PEB	RK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	SR	201	6	-	7/24/74/74	0/4/4/4
29	PEB	xL	301	-	-	12/24/74/74	0/4/4/4
29	PEB	g9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	D9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	IM	202	6	-	10/24/74/74	0/4/4/4
31	CYC	KF	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	H5	202	-	-	10/24/74/74	0/4/4/4
29	PEB	dL	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	A8	203	7	-	9/24/74/74	0/4/4/4
29	PEB	KA	202	6	-	16/24/74/74	0/4/4/4
29	PEB	JL	201	7	-	7/24/74/74	0/4/4/4
29	PEB	I5	203	7	-	9/24/74/74	0/4/4/4
29	PEB	FO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	MB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	B5	202	-	-	10/24/74/74	0/4/4/4
31	CYC	UP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	P9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	NL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	aI	203	7	-	14/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	DG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	F1	1002	5	-	8/24/74/74	0/4/4/4
29	PEB	hK	202	6	-	9/24/74/74	0/4/4/4
31	CYC	J1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	TF	201	7	-	6/24/74/74	0/4/4/4
29	PEB	hI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	BB	301	17	-	13/24/74/74	0/4/4/4
29	PEB	KC	203	6	-	8/24/74/74	0/4/4/4
29	PEB	FN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	HM	202	7	-	6/24/74/74	0/4/4/4
29	PEB	EE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	jI	202	6	-	8/24/74/74	0/4/4/4
29	PEB	MD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	Y9	201	7	-	4/24/74/74	0/4/4/4
29	PEB	aJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	FM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	NJ	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	SF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	T9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	JN	202	7	-	11/24/74/74	0/4/4/4
29	PEB	jB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	YM	203	6	-	10/24/74/74	0/4/4/4
29	PEB	EB	201	6	-	5/24/74/74	0/4/4/4
29	PEB	TM	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	VR	203	7	-	12/24/74/74	0/4/4/4
29	PEB	CG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	FE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	WI	201	6	-	6/24/74/74	0/4/4/4
31	CYC	NP	1001	20,19	-	8/25/74/74	0/4/4/4
29	PEB	AM	301	16	-	10/24/74/74	0/4/4/4
29	PEB	l9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	JF	1001	5,3	-	7/25/74/74	0/4/4/4
31	CYC	II	1001	4	-	8/25/74/74	0/4/4/4
29	PEB	G4	202	7	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	Q1	201	6	-	8/24/74/74	0/4/4/4
30	PUB	AB	305	16	-	7/24/74/74	0/4/4/4
29	PEB	T2	201	7	-	9/24/74/74	0/4/4/4
29	PEB	dM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	Y7	201	7	-	4/24/74/74	0/4/4/4
31	CYC	DI	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	OJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	GN	202	6	-	16/24/74/74	0/4/4/4
29	PEB	yL	301	-	-	9/24/74/74	0/4/4/4
31	CYC	yP	1001	-	-	8/25/74/74	0/4/4/4
29	PEB	Z1	201	7,6	-	6/24/74/74	0/4/4/4
29	PEB	ZJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	O9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	IE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	KL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	B5	201	7	-	7/24/74/74	0/4/4/4
31	CYC	IP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	L9	1002	-	-	12/24/74/74	0/4/4/4
29	PEB	mB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	HB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	IG	201	6	-	7/24/74/74	0/4/4/4
29	PEB	IL	203	6,7	-	9/24/74/74	0/4/4/4
29	PEB	BJ	201	7,19	-	7/24/74/74	0/4/4/4
29	PEB	L8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	HL	202	7	-	13/24/74/74	0/4/4/4
29	PEB	fl	202	6	-	8/24/74/74	0/4/4/4
29	PEB	NB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	cB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	D4	202	6	-	11/24/74/74	0/4/4/4
29	PEB	GD	201	7	-	9/24/74/74	0/4/4/4
29	PEB	K5	201	7	-	6/24/74/74	0/4/4/4
31	CYC	MK	1001	4	-	9/25/74/74	0/4/4/4
29	PEB	tJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	KL	202	6	-	10/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	gB	203	7	-	13/24/74/74	0/4/4/4
29	PEB	JO	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	b9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	RB	202	7	-	6/24/74/74	0/4/4/4
29	PEB	AM	302	6,16	-	8/24/74/74	0/4/4/4
29	PEB	dF	202	6	-	6/24/74/74	0/4/4/4
31	CYC	F9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	VF	201	7	-	11/24/74/74	0/4/4/4
29	PEB	vJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	IL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	xJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	W7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	jJ	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AI	301	2	-	12/24/74/74	0/4/4/4
29	PEB	zL	501	7	-	8/24/74/74	0/4/4/4
29	PEB	sL	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BQ	203	-	-	12/24/74/74	0/4/4/4
31	CYC	F1	1001	5	-	7/25/74/74	0/4/4/4
29	PEB	k9	202	7	-	9/24/74/74	0/4/4/4
29	PEB	xL	302	-	-	7/24/74/74	0/4/4/4
29	PEB	MO	201	-	-	6/24/74/74	0/4/4/4
29	PEB	AF	305	6,2	-	7/24/74/74	0/4/4/4
29	PEB	UI	203	6	-	8/24/74/74	0/4/4/4
31	CYC	rP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	S1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	TB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	wJ	302	-	-	7/24/74/74	0/4/4/4
29	PEB	C5	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NJ	203	7	-	13/24/74/74	0/4/4/4
30	PUB	QM	201	6,17	-	6/24/74/74	0/4/4/4
31	CYC	G7	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	P7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	PF	202	7	-	7/24/74/74	0/4/4/4
30	PUB	AB	304	16	-	13/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	m7	201	7	-	4/24/74/74	0/4/4/4
29	PEB	fF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	rJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	kB	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	jJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	ZM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	NO	201	-	-	6/24/74/74	0/4/4/4
29	PEB	O7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	FE	201	7,18	-	6/24/74/74	0/4/4/4
29	PEB	MG	404	14	-	10/24/74/74	0/4/4/4
29	PEB	KJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	II	201	6	-	6/24/74/74	0/4/4/4
31	CYC	qP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	HO	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	LA	201	7	-	12/24/74/74	0/4/4/4
29	PEB	b1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	wJ	301	-	-	12/24/74/74	0/4/4/4
29	PEB	IO	201	6	-	4/24/74/74	0/4/4/4
29	PEB	H9	1002	-	-	12/24/74/74	0/4/4/4
31	CYC	uP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	ZK	202	6	-	8/24/74/74	0/4/4/4
29	PEB	DI	1002	-	-	13/24/74/74	0/4/4/4
29	PEB	f1	201	6	-	8/24/74/74	0/4/4/4
29	PEB	XR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	aB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	G4	201	7	-	9/24/74/74	0/4/4/4
29	PEB	Y1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	X2	201	7	-	7/24/74/74	0/4/4/4
29	PEB	DQ	203	-	-	12/24/74/74	0/4/4/4
29	PEB	Q2	201	6	-	7/24/74/74	0/4/4/4
31	CYC	KP	1001	20	-	8/25/74/74	0/4/4/4
29	PEB	PK	202	7,6	-	6/24/74/74	0/4/4/4
29	PEB	IL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	V7	201	7	-	4/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	ZF	202	6	-	8/24/74/74	0/4/4/4
29	PEB	UR	202	6	-	11/24/74/74	0/4/4/4
29	PEB	aL	201	6	-	9/24/74/74	0/4/4/4
29	PEB	jL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	W9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	V2	202	7	-	7/24/74/74	0/4/4/4
29	PEB	kM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	KB	203	6,7	-	6/24/74/74	0/4/4/4
29	PEB	Z1	203	6	-	9/24/74/74	0/4/4/4
29	PEB	KO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	j9	201	6	-	8/24/74/74	0/4/4/4
29	PEB	W9	202	6	-	8/24/74/74	0/4/4/4
29	PEB	BC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	V9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	AF	301	2	-	12/24/74/74	0/4/4/4
29	PEB	HD	201	6	-	9/24/74/74	0/4/4/4
29	PEB	LO	202	-	-	10/24/74/74	0/4/4/4
29	PEB	AI	304	2	-	9/24/74/74	0/4/4/4
29	PEB	RR	201	7	-	9/24/74/74	0/4/4/4
29	PEB	a1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	M4	202	6,7	-	12/24/74/74	0/4/4/4
29	PEB	A3	202	6	-	9/24/74/74	0/4/4/4
29	PEB	DE	202	-	-	9/24/74/74	0/4/4/4
29	PEB	YB	202	6	-	5/24/74/74	0/4/4/4
29	PEB	TM	201	7	-	6/24/74/74	0/4/4/4
29	PEB	B8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	ML	201	6	-	9/24/74/74	0/4/4/4
29	PEB	xL	303	16	-	14/24/74/74	0/4/4/4
29	PEB	XB	202	7	-	13/24/74/74	0/4/4/4
29	PEB	F8	201	7	-	7/24/74/74	0/4/4/4
29	PEB	LC	201	7	-	6/24/74/74	0/4/4/4
29	PEB	F3	203	-	-	10/24/74/74	0/4/4/4
29	PEB	fK	202	6	-	9/24/74/74	0/4/4/4
29	PEB	AO	202	6	-	9/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	eF	203	7	-	14/24/74/74	0/4/4/4
29	PEB	hF	201	6	-	6/24/74/74	0/4/4/4
29	PEB	RM	203	7	-	13/24/74/74	0/4/4/4
29	PEB	WL	203	6	-	10/24/74/74	0/4/4/4
31	CYC	L7	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	EJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	EO	202	6	-	9/24/74/74	0/4/4/4
29	PEB	fL	202	6,7	-	9/24/74/74	0/4/4/4
29	PEB	AQ	201	6	-	7/24/74/74	0/4/4/4
29	PEB	b7	201	6	-	8/24/74/74	0/4/4/4
29	PEB	JQ	203	7	-	12/24/74/74	0/4/4/4
29	PEB	uL	202	6	-	9/24/74/74	0/4/4/4
29	PEB	MO	203	7	-	10/24/74/74	0/4/4/4
29	PEB	AB	301	16	-	10/24/74/74	0/4/4/4
29	PEB	MQ	403	14	-	9/24/74/74	0/4/4/4
31	CYC	K9	1001	-	-	7/25/74/74	0/4/4/4
29	PEB	e9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	ZJ	202	7	-	9/24/74/74	0/4/4/4
29	PEB	hB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	a9	203	7	-	12/24/74/74	0/4/4/4
29	PEB	C8	201	7	-	6/24/74/74	0/4/4/4
29	PEB	LM	203	7	-	13/24/74/74	0/4/4/4
31	CYC	L9	1001	5	-	9/25/74/74	0/4/4/4
29	PEB	kB	201	7	-	6/24/74/74	0/4/4/4
29	PEB	S2	201	6	-	4/24/74/74	0/4/4/4
29	PEB	PL	203	7	-	13/24/74/74	0/4/4/4
29	PEB	d9	202	6	-	8/24/74/74	0/4/4/4
31	CYC	VP	1001	21	-	10/25/74/74	0/4/4/4
29	PEB	MN	405	14	-	9/24/74/74	0/4/4/4
29	PEB	R7	201	7,1	-	4/24/74/74	0/4/4/4
29	PEB	f7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	B3	202	7,6	-	9/24/74/74	0/4/4/4
29	PEB	nJ	203	7	-	13/24/74/74	0/4/4/4
29	PEB	IQ	202	6	-	12/24/74/74	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	PEB	AJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	Y7	202	7	-	9/24/74/74	0/4/4/4
29	PEB	jI	201	6	-	6/24/74/74	0/4/4/4
29	PEB	PK	203	7	-	6/24/74/74	0/4/4/4
29	PEB	h7	202	6	-	8/24/74/74	0/4/4/4
29	PEB	VJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	i1	201	7	-	6/24/74/74	0/4/4/4
29	PEB	BO	203	-	-	10/24/74/74	0/4/4/4
29	PEB	AJ	202	6	-	10/24/74/74	0/4/4/4
29	PEB	DJ	201	7	-	7/24/74/74	0/4/4/4
29	PEB	LE	203	-	-	9/24/74/74	0/4/4/4
29	PEB	MB	202	6	-	10/24/74/74	0/4/4/4
29	PEB	KM	202	6	-	10/24/74/74	0/4/4/4
29	PEB	BN	201	7	-	12/24/74/74	0/4/4/4
29	PEB	SJ	201	6	-	9/24/74/74	0/4/4/4
29	PEB	BG	203	-	-	12/24/74/74	0/4/4/4
29	PEB	eI	203	7	-	14/24/74/74	0/4/4/4
31	CYC	wP	1001	21	-	8/25/74/74	0/4/4/4
29	PEB	iM	202	6,7	-	6/24/74/74	0/4/4/4
29	PEB	VJ	202	7	-	13/24/74/74	0/4/4/4
29	PEB	CE	201	6	-	6/24/74/74	0/4/4/4
29	PEB	FI	1002	4	-	13/24/74/74	0/4/4/4

The worst 5 of 15197 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	VP	1001	CYC	CHA-C1A	19.85	1.51	1.35
31	xP	1001	CYC	CHA-C1A	19.80	1.51	1.35
29	C3	202	PEB	CHB-C4B	18.15	1.50	1.35
29	CO	202	PEB	CHB-C4B	18.15	1.50	1.35
29	A3	202	PEB	CHB-C4B	18.14	1.50	1.35

The worst 5 of 23317 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A1	305	PUB	CBA-CAA-C3A	-16.33	88.22	112.98
30	AK	305	PUB	CBA-CAA-C3A	-16.33	88.22	112.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A1	305	PUB	C2A-C1A-NA	14.04	119.67	107.21
30	AK	305	PUB	C2A-C1A-NA	14.04	119.67	107.21
30	wL	305	PUB	C2A-C1A-NA	12.40	118.21	107.21

There are no chirality outliers.

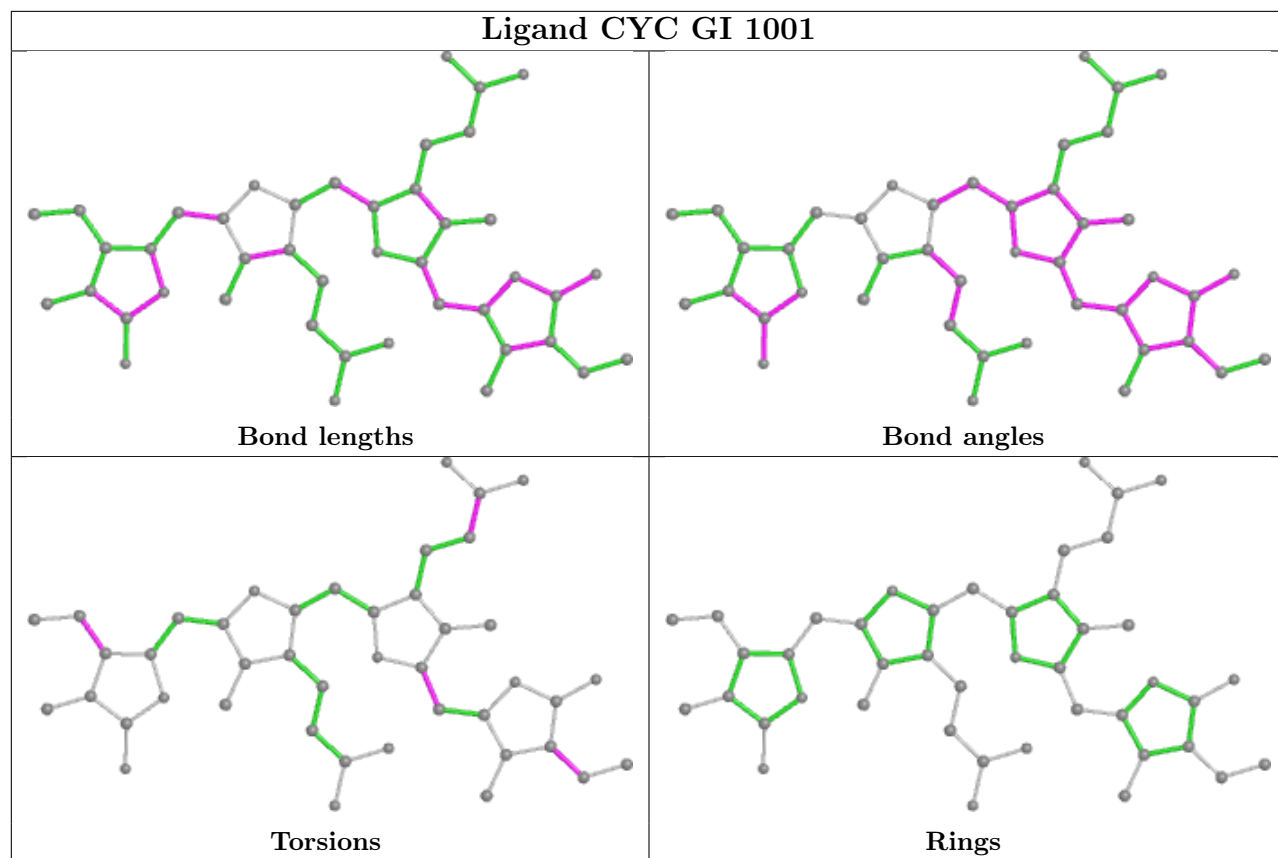
5 of 12797 torsion outliers are listed below:

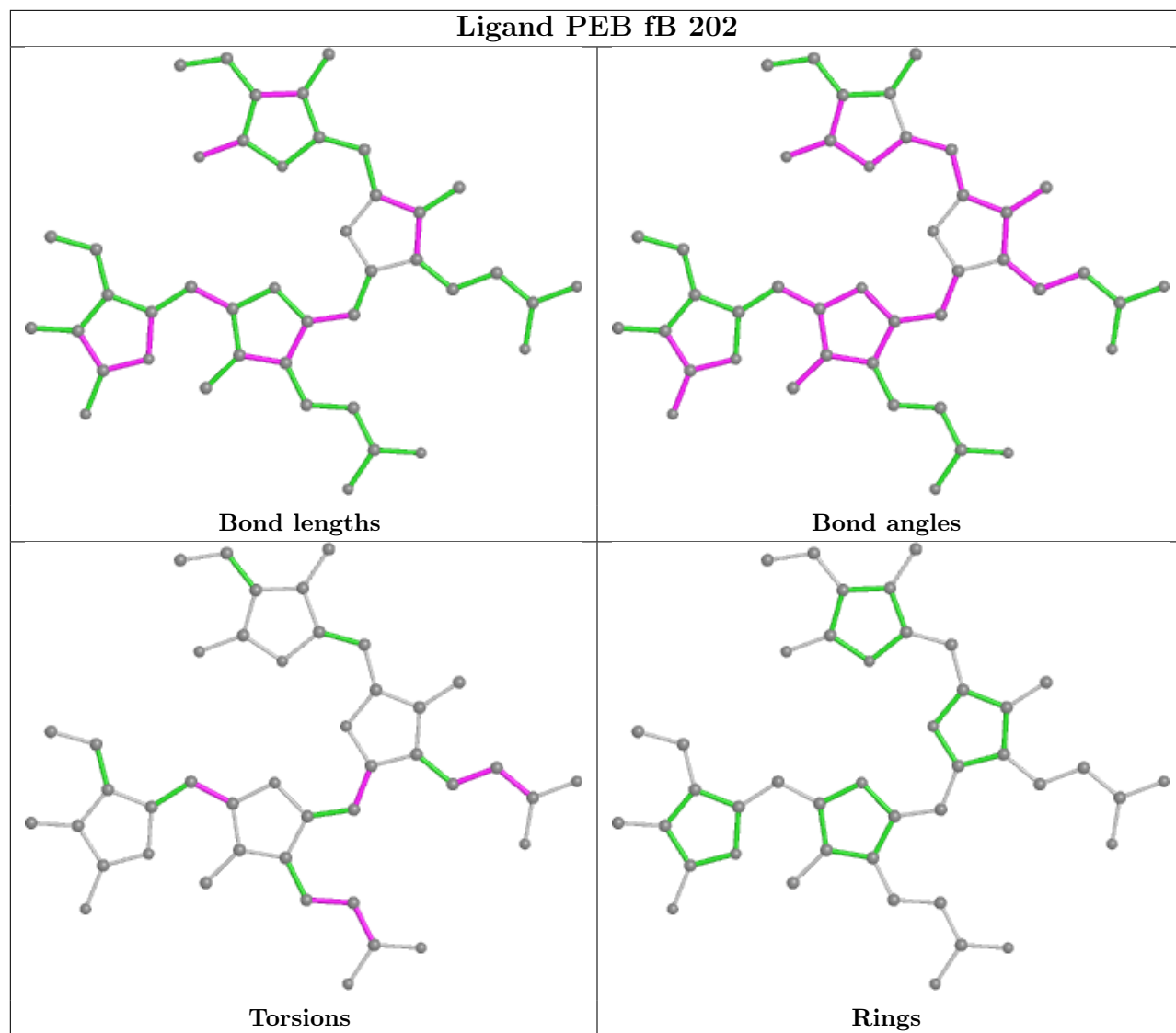
Mol	Chain	Res	Type	Atoms
29	A1	301	PEB	NB-C1B-CHA-C4A
29	A1	301	PEB	C2B-C1B-CHA-C4A
29	A1	302	PEB	ND-C1D-CHC-C4C
29	A1	302	PEB	NB-C1B-CHA-C4A
29	A1	302	PEB	C2B-C1B-CHA-C4A

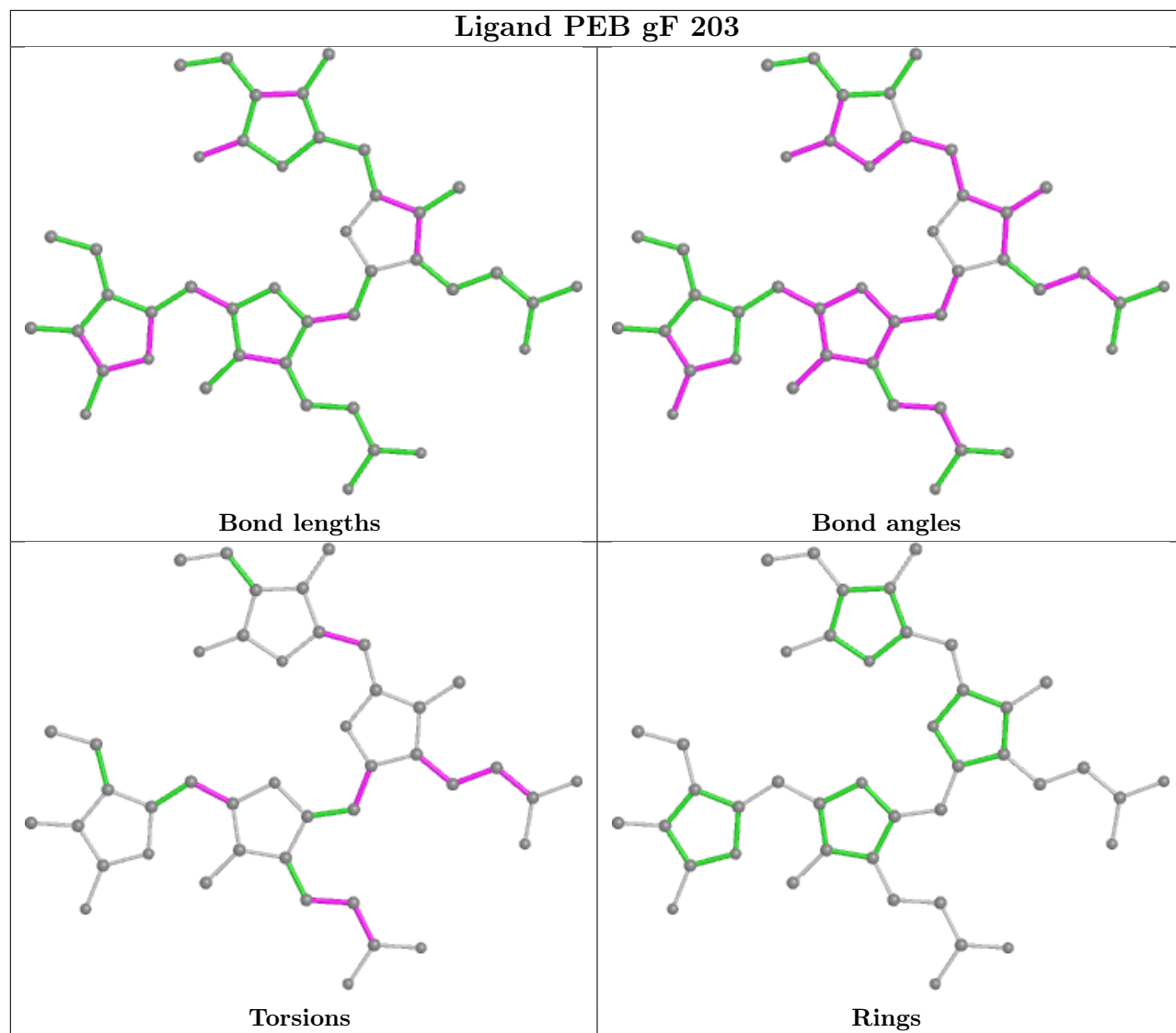
There are no ring outliers.

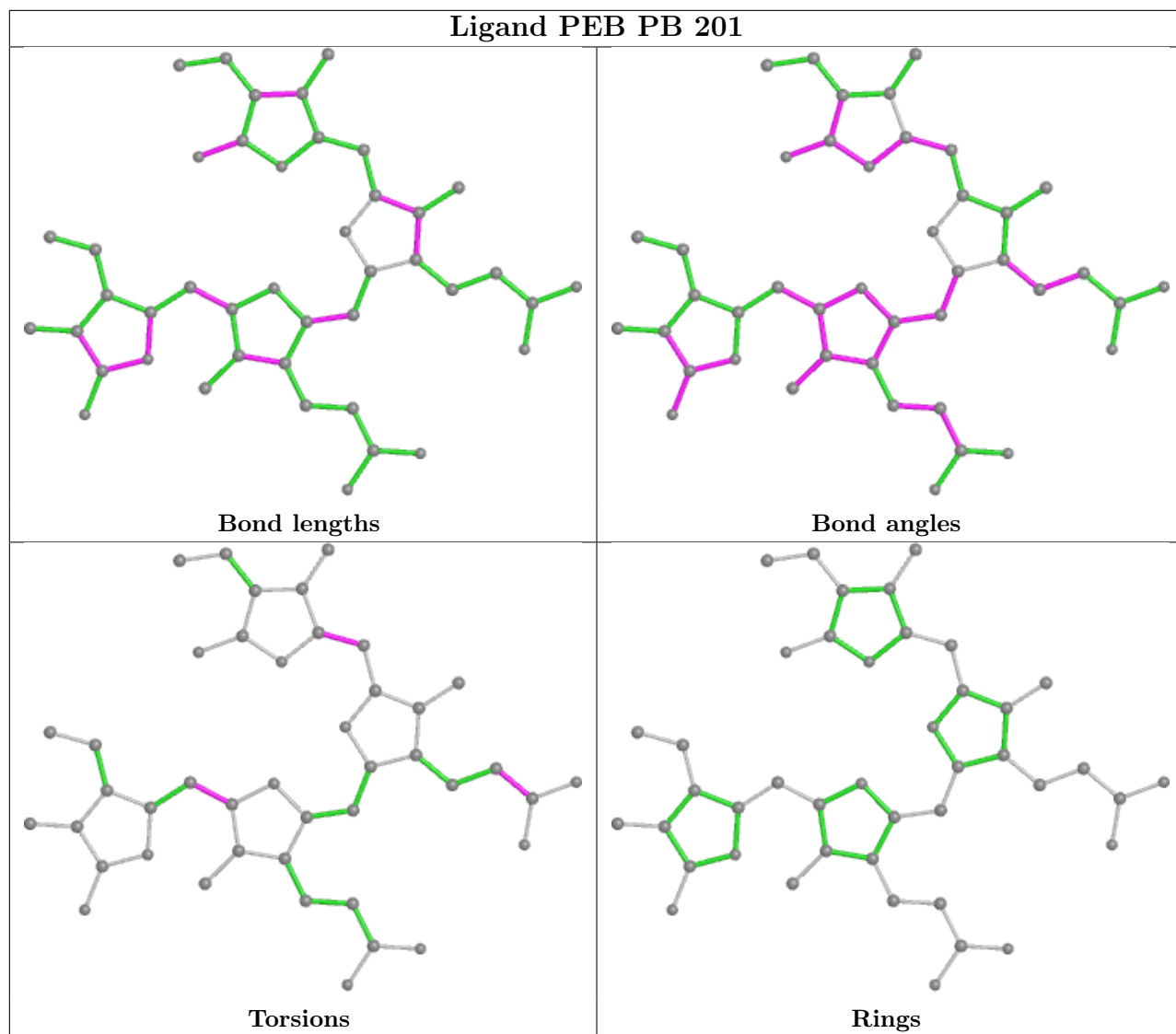
No monomer is involved in short contacts.

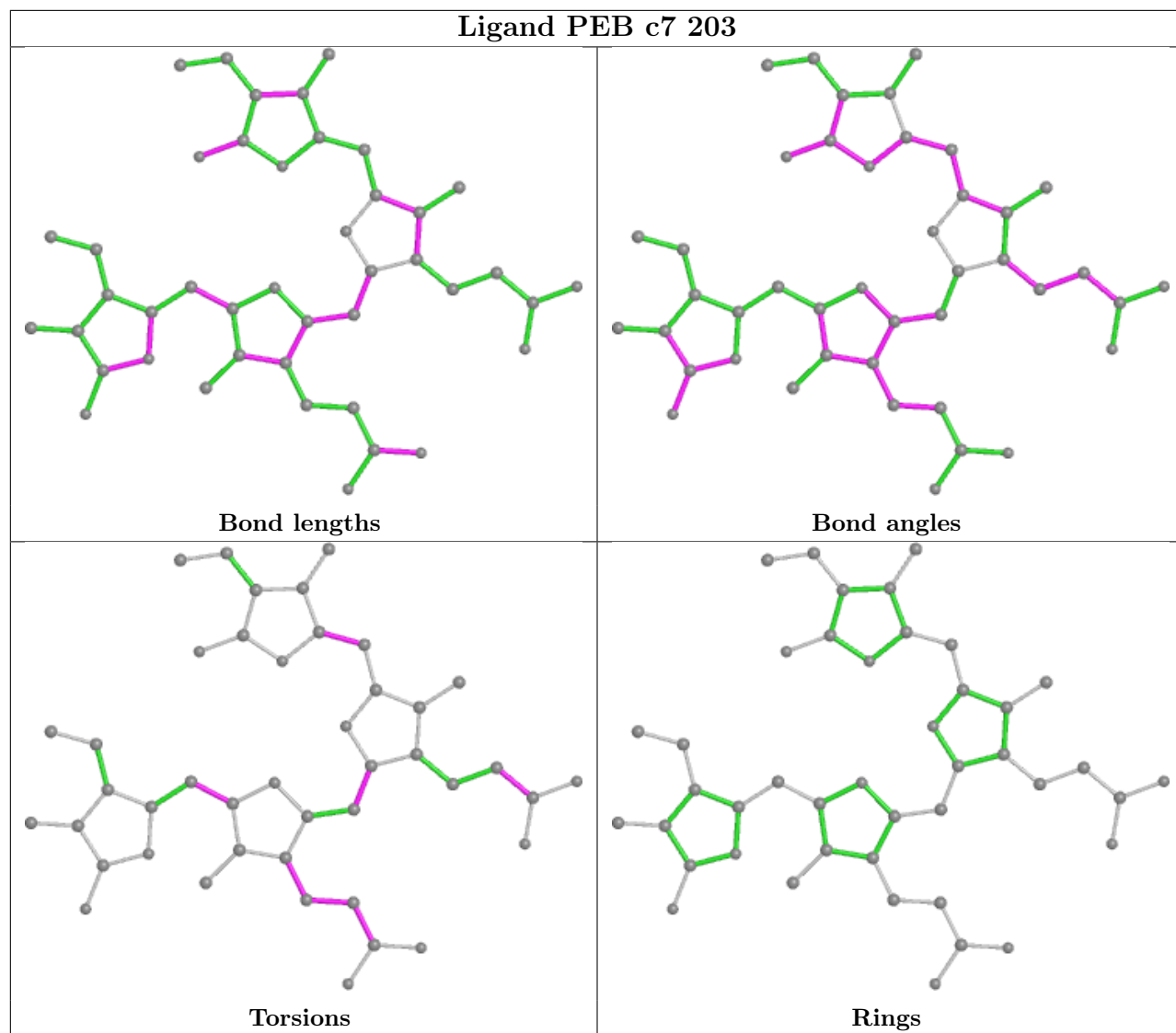
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

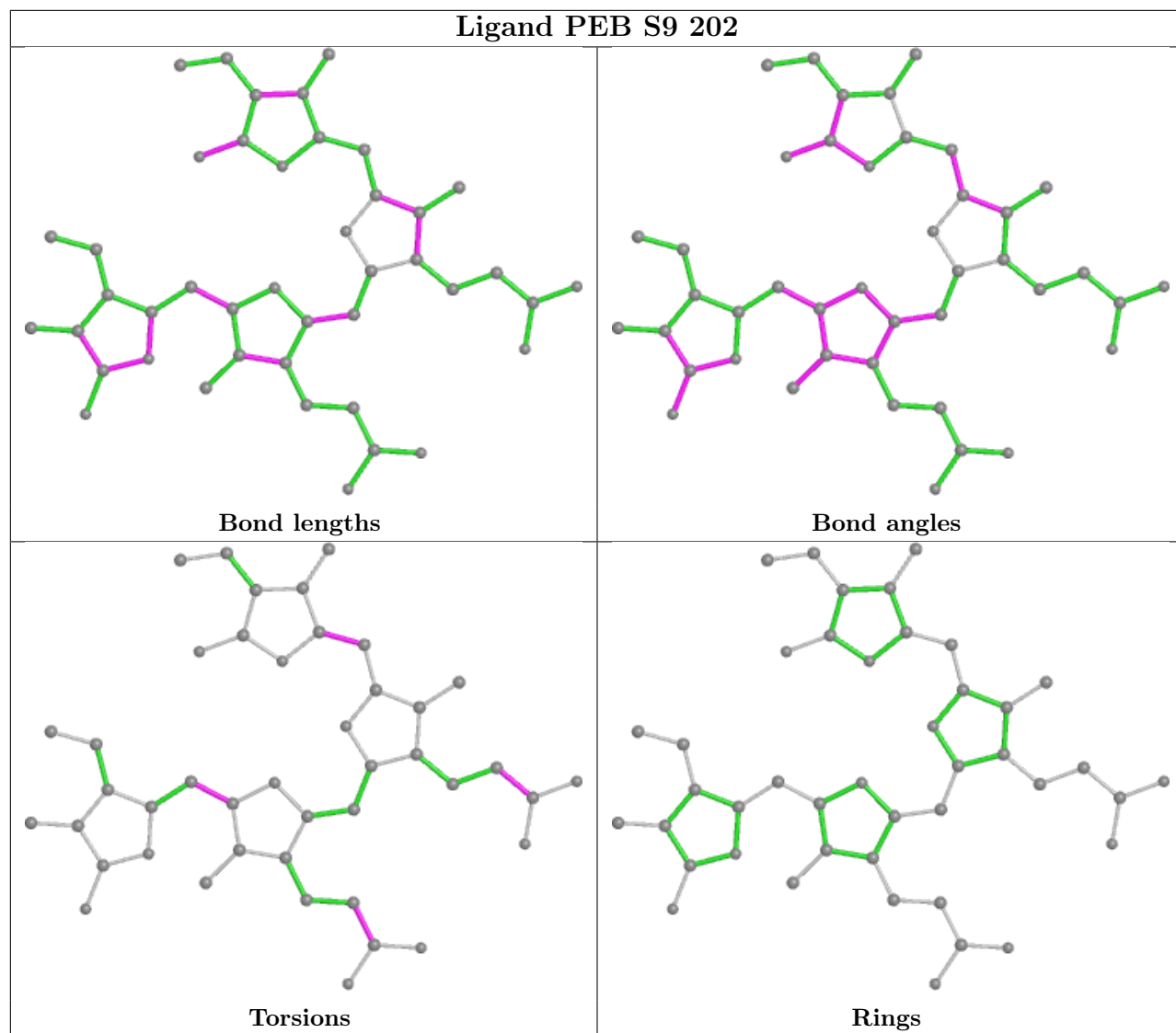


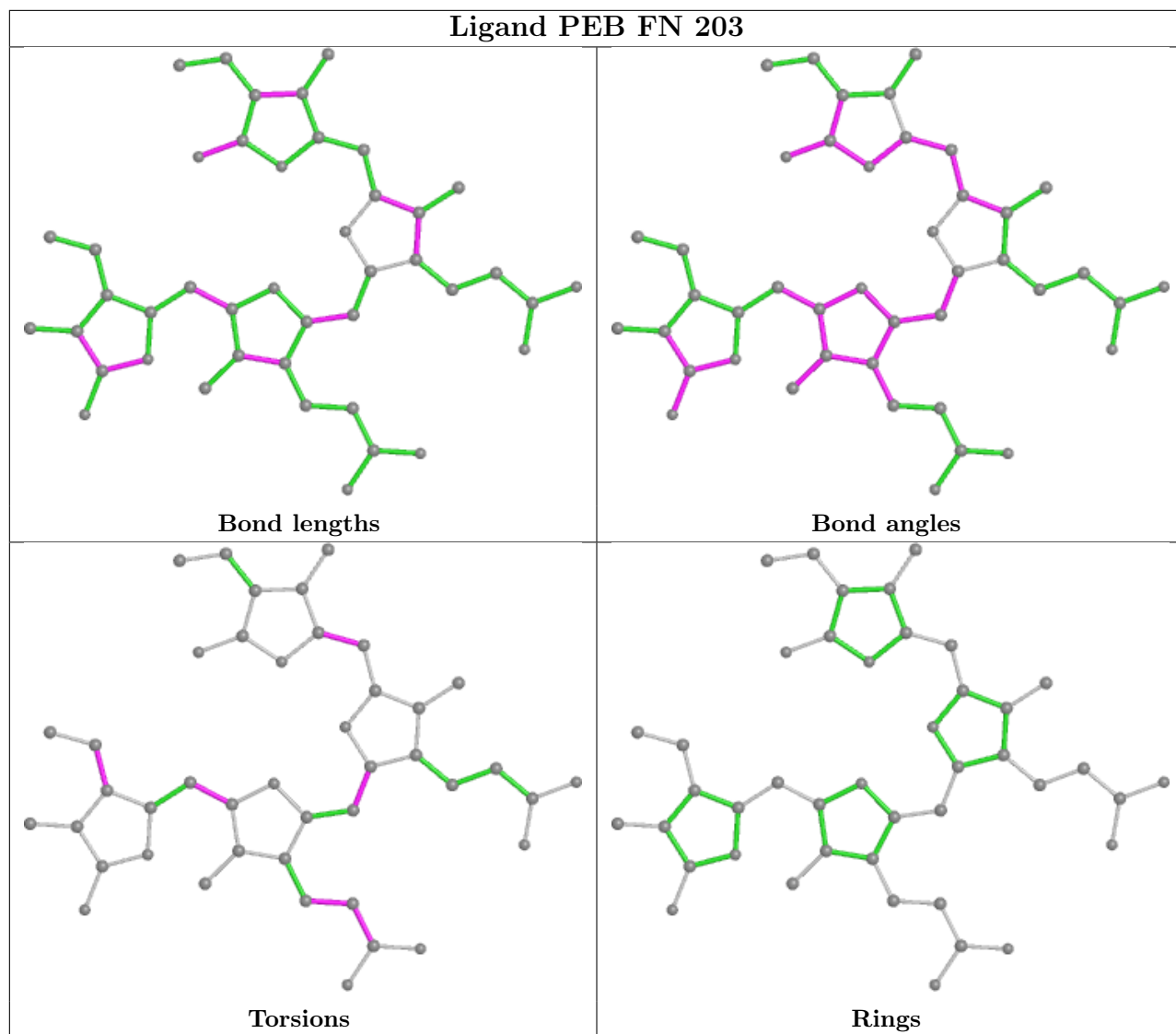


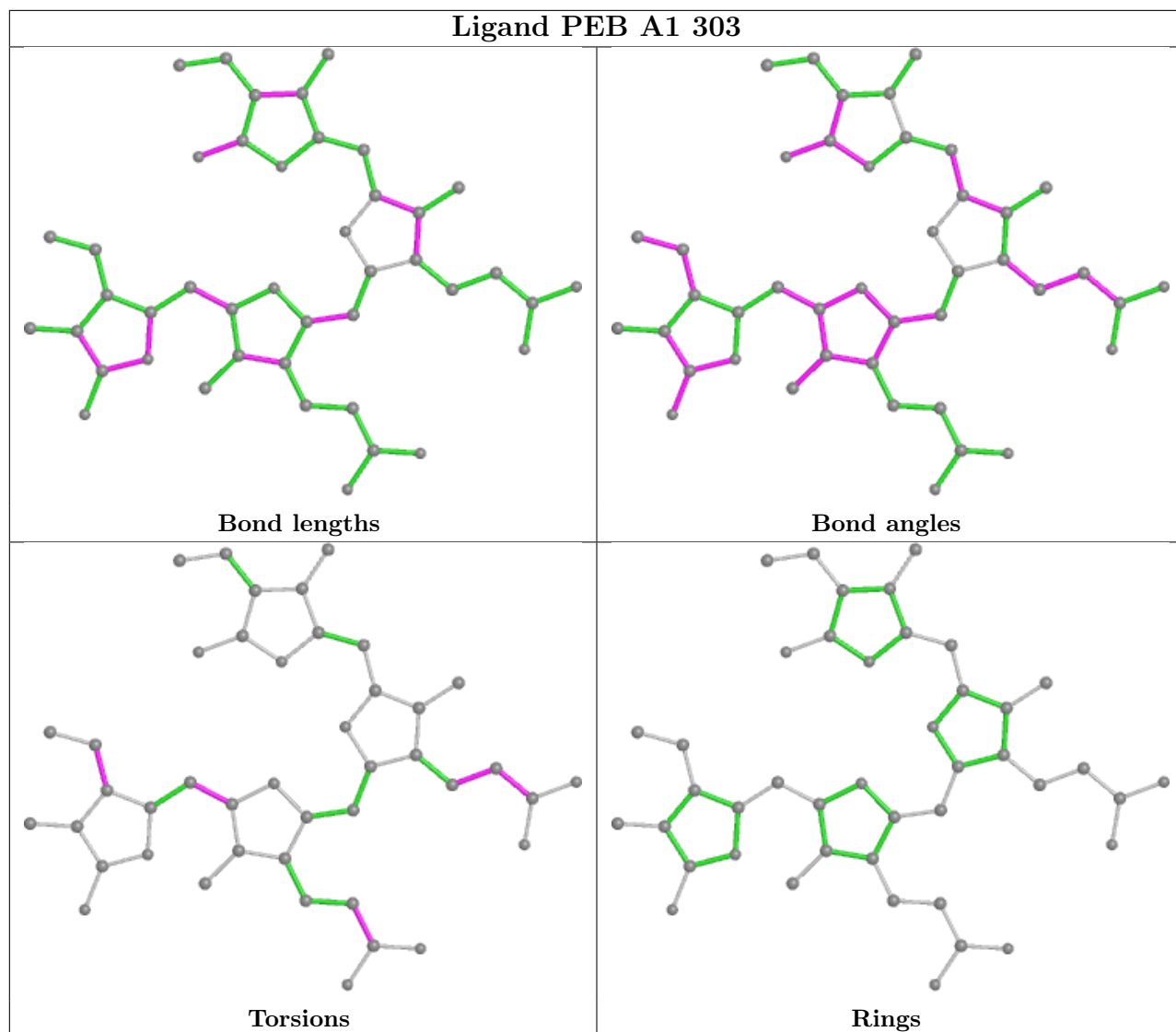


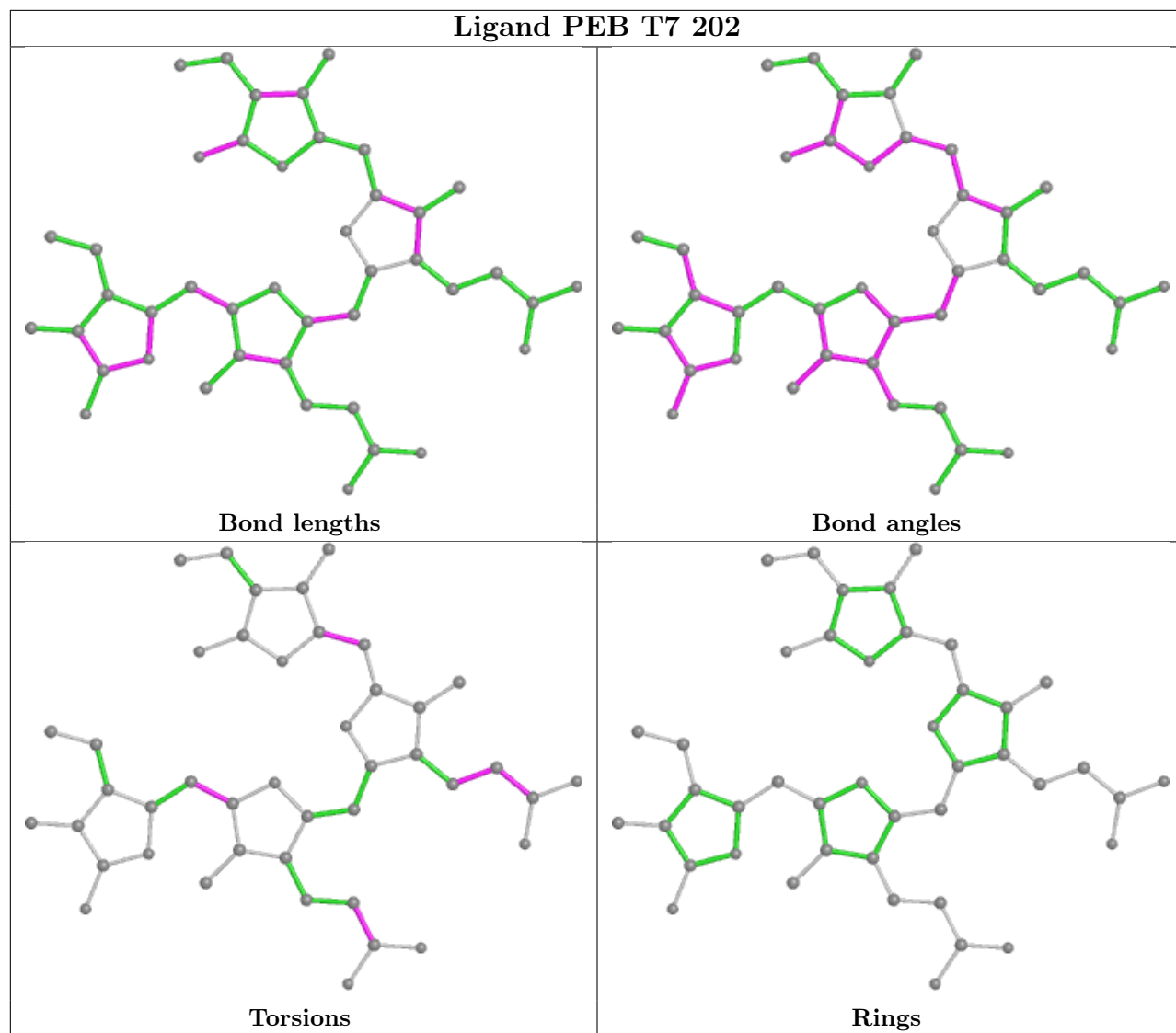


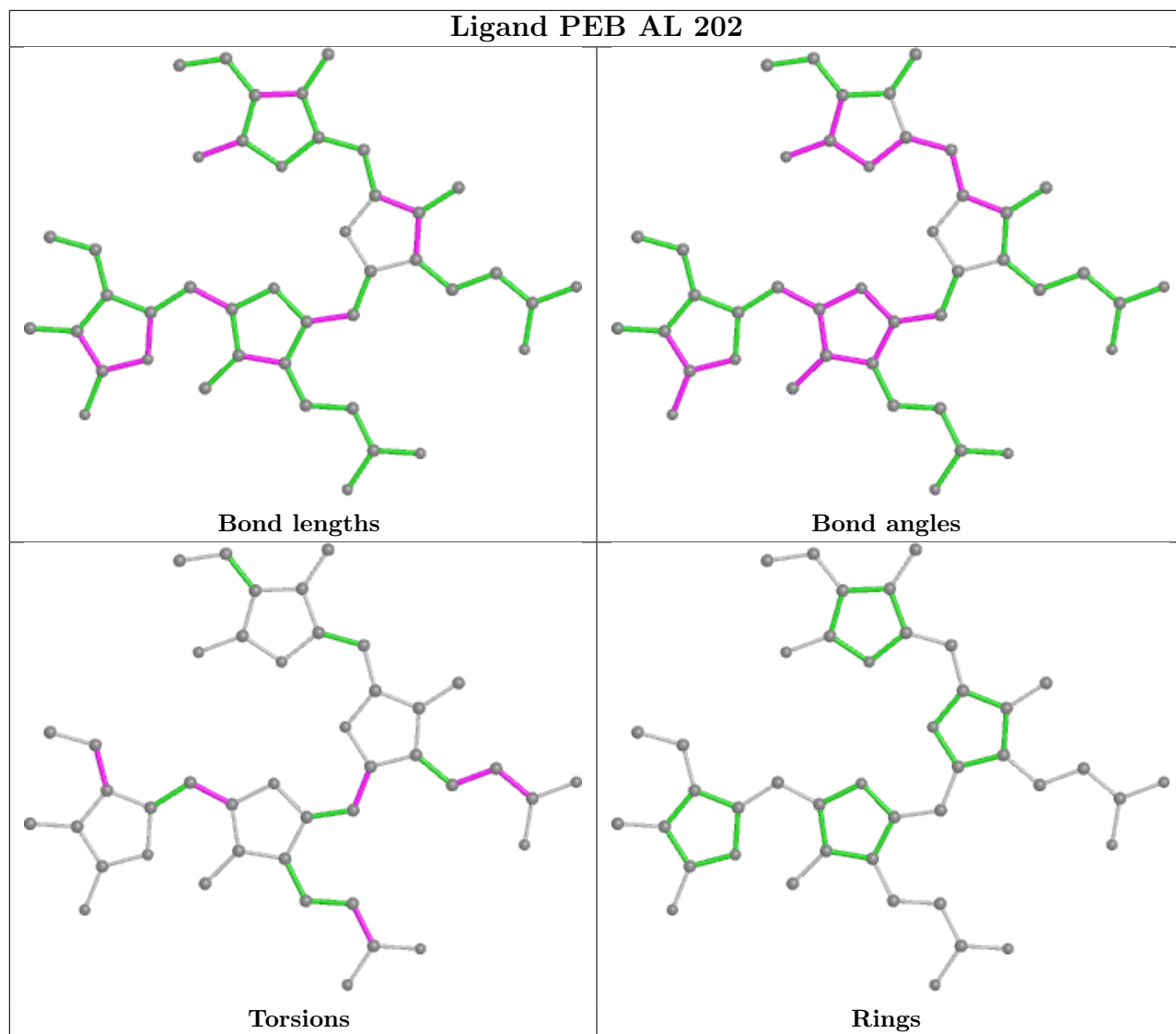


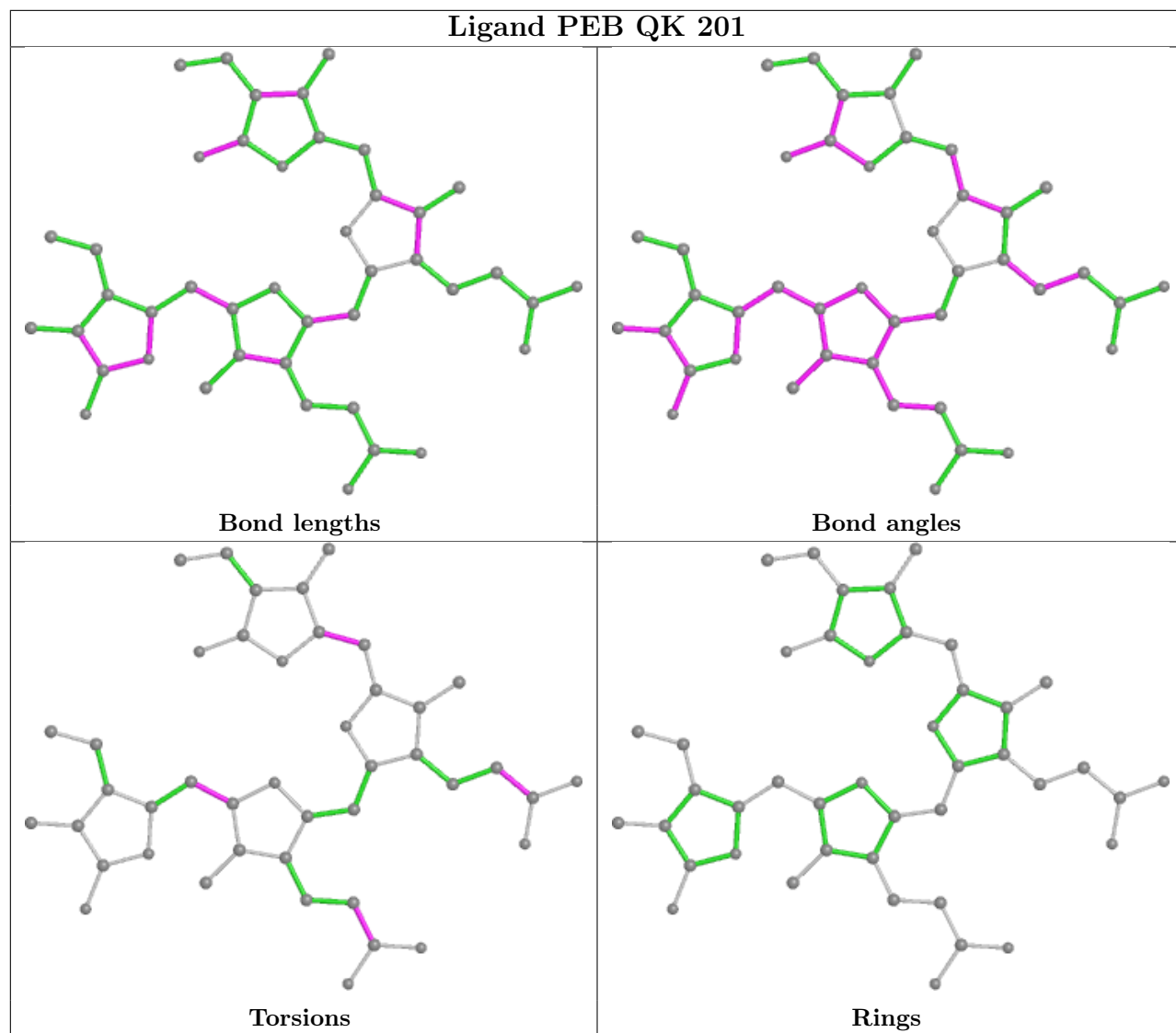


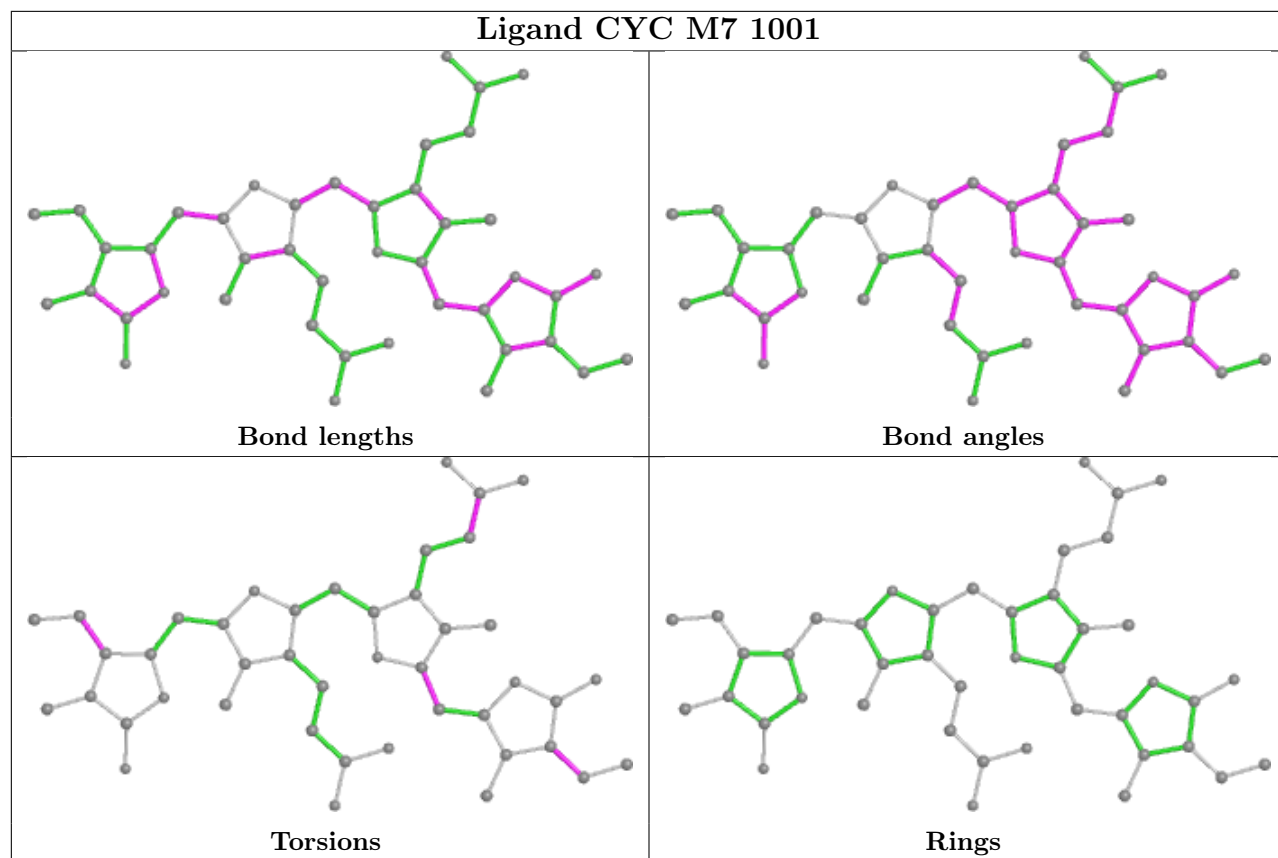


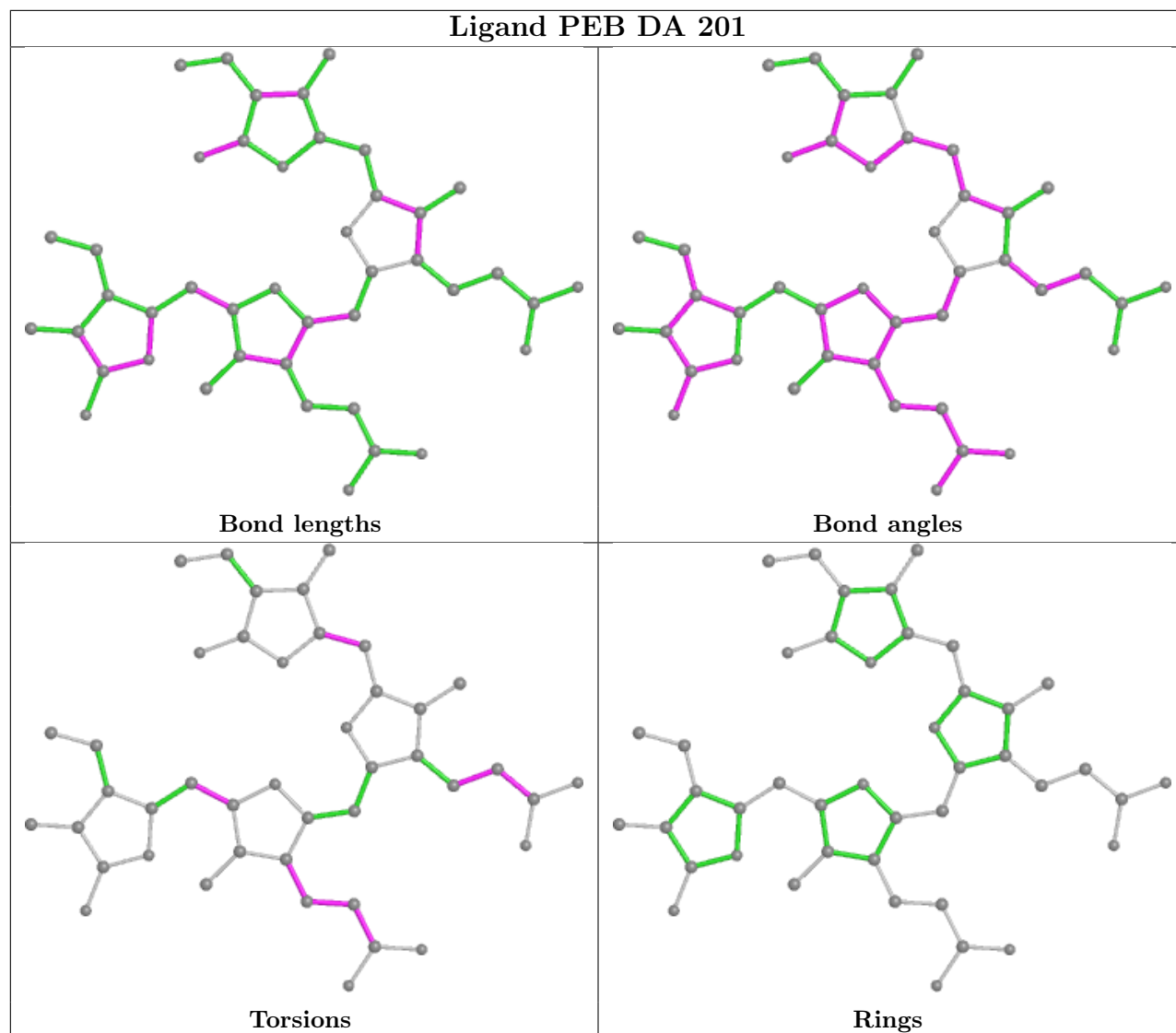


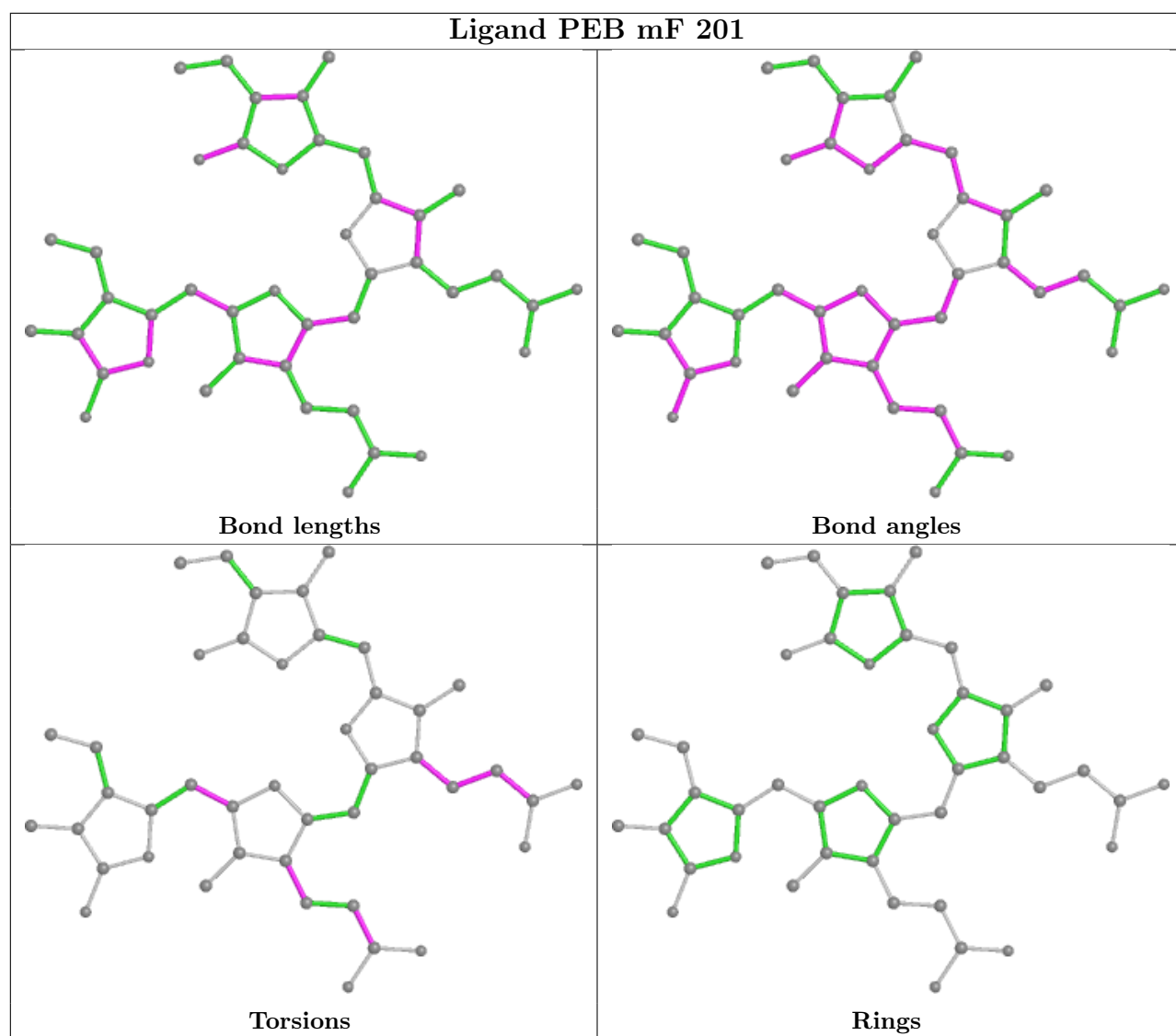


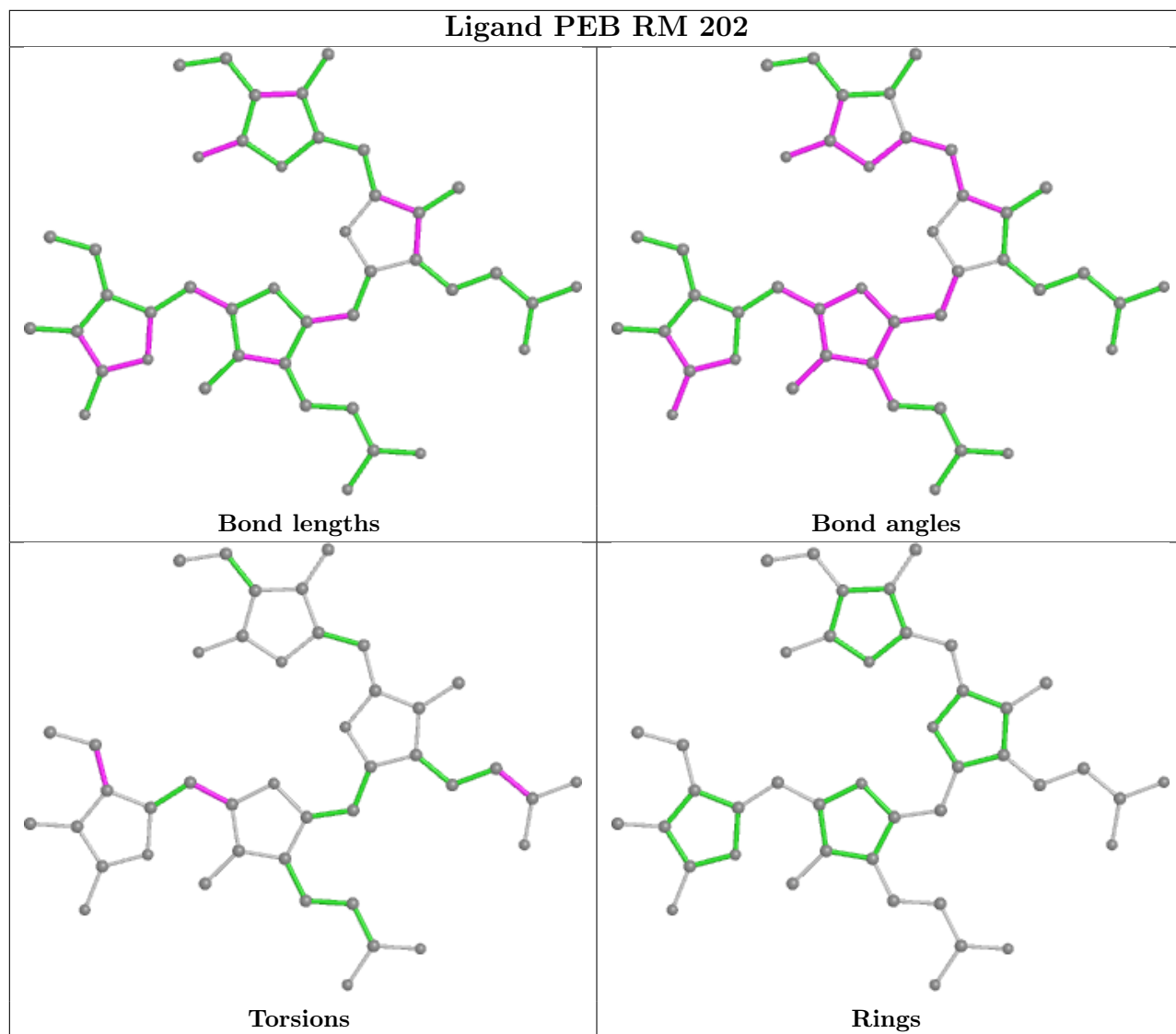


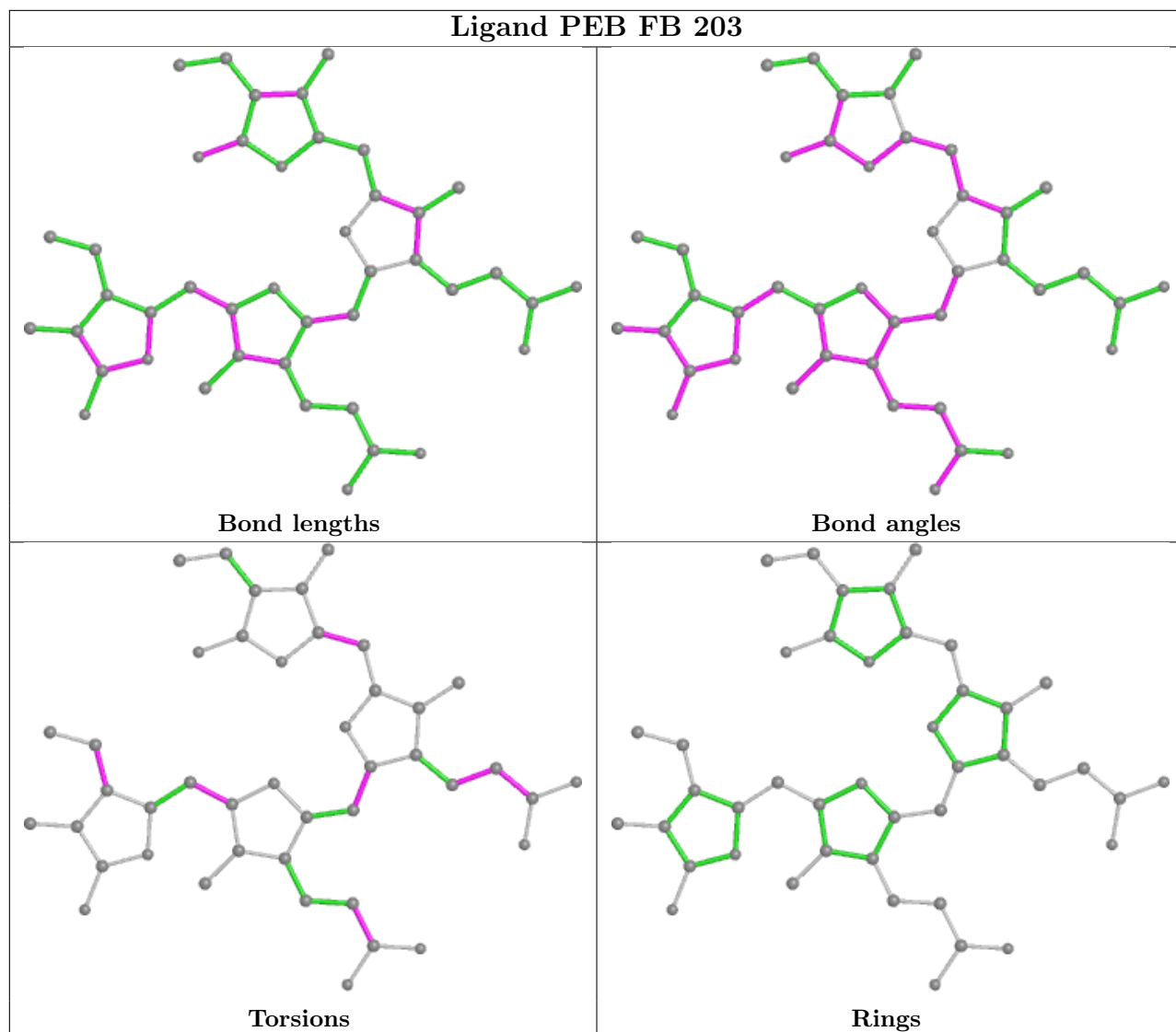


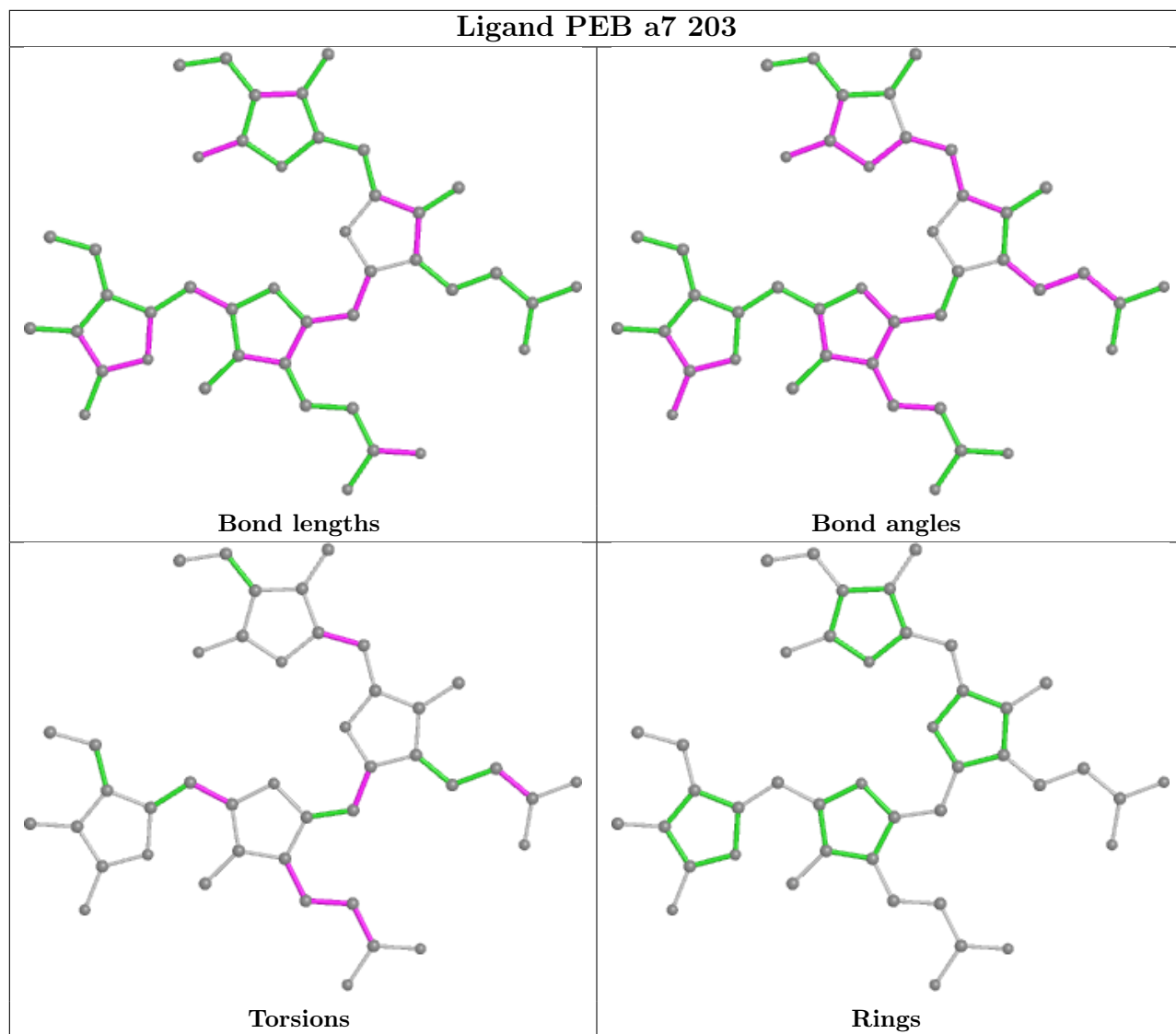


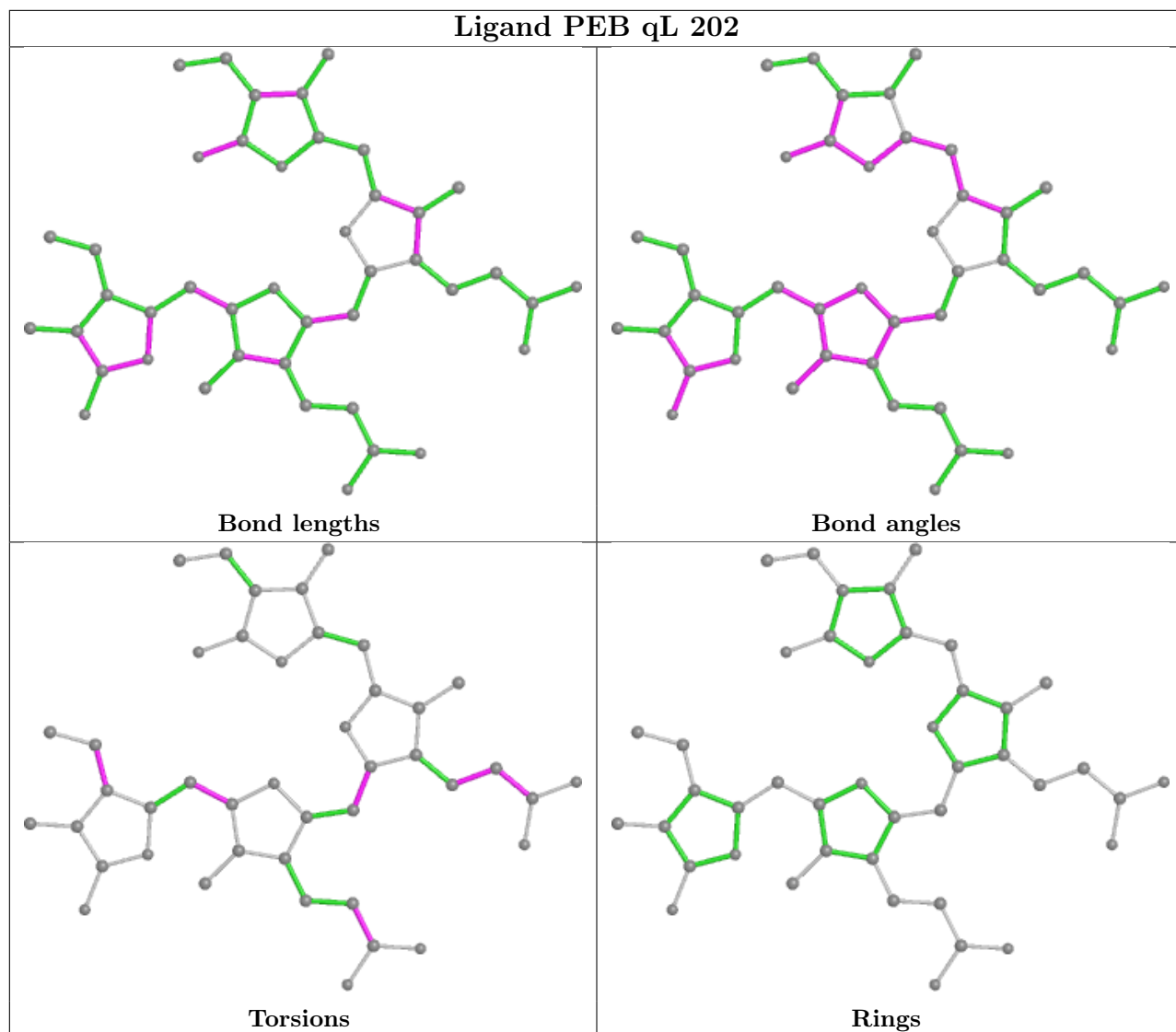


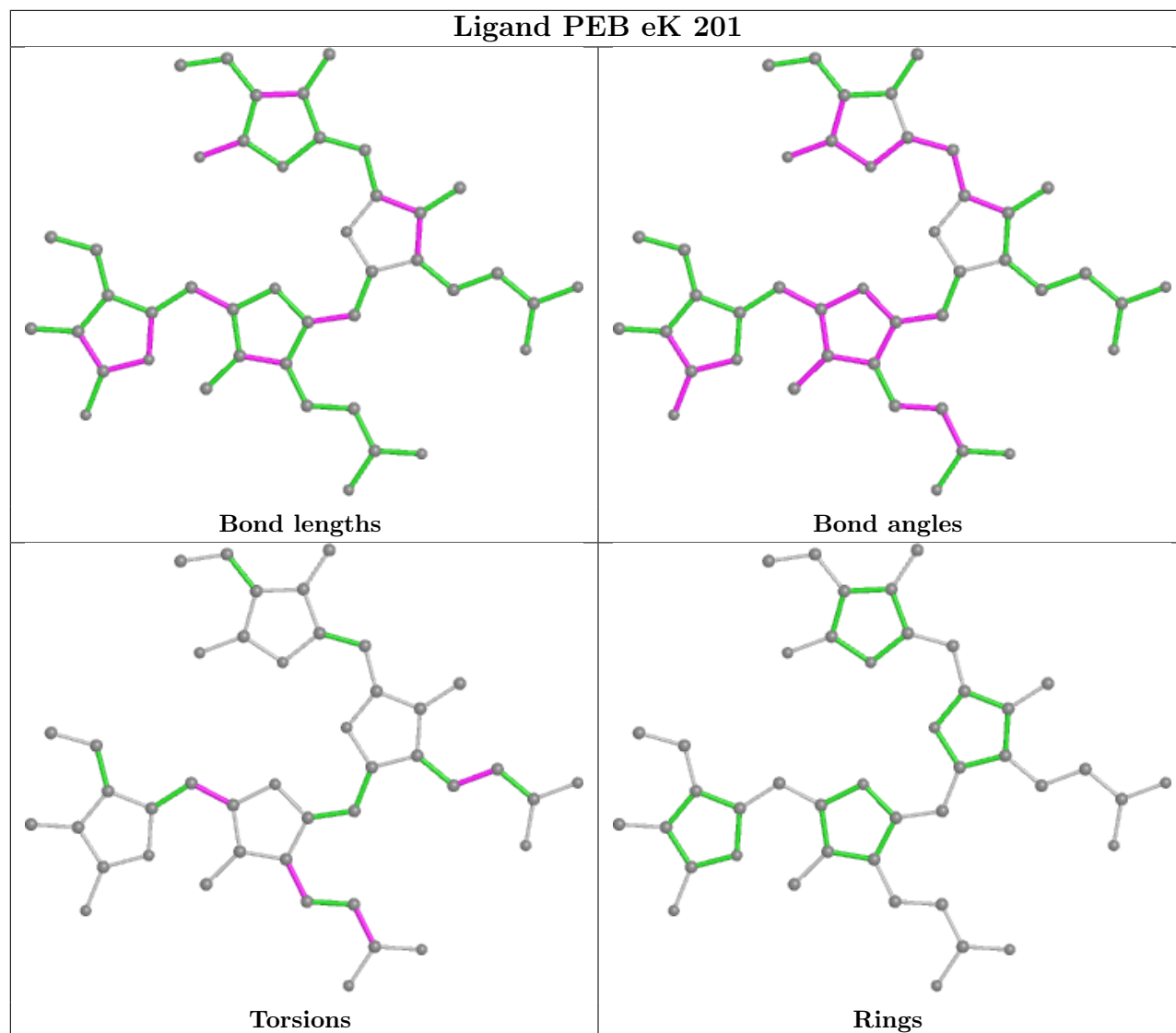


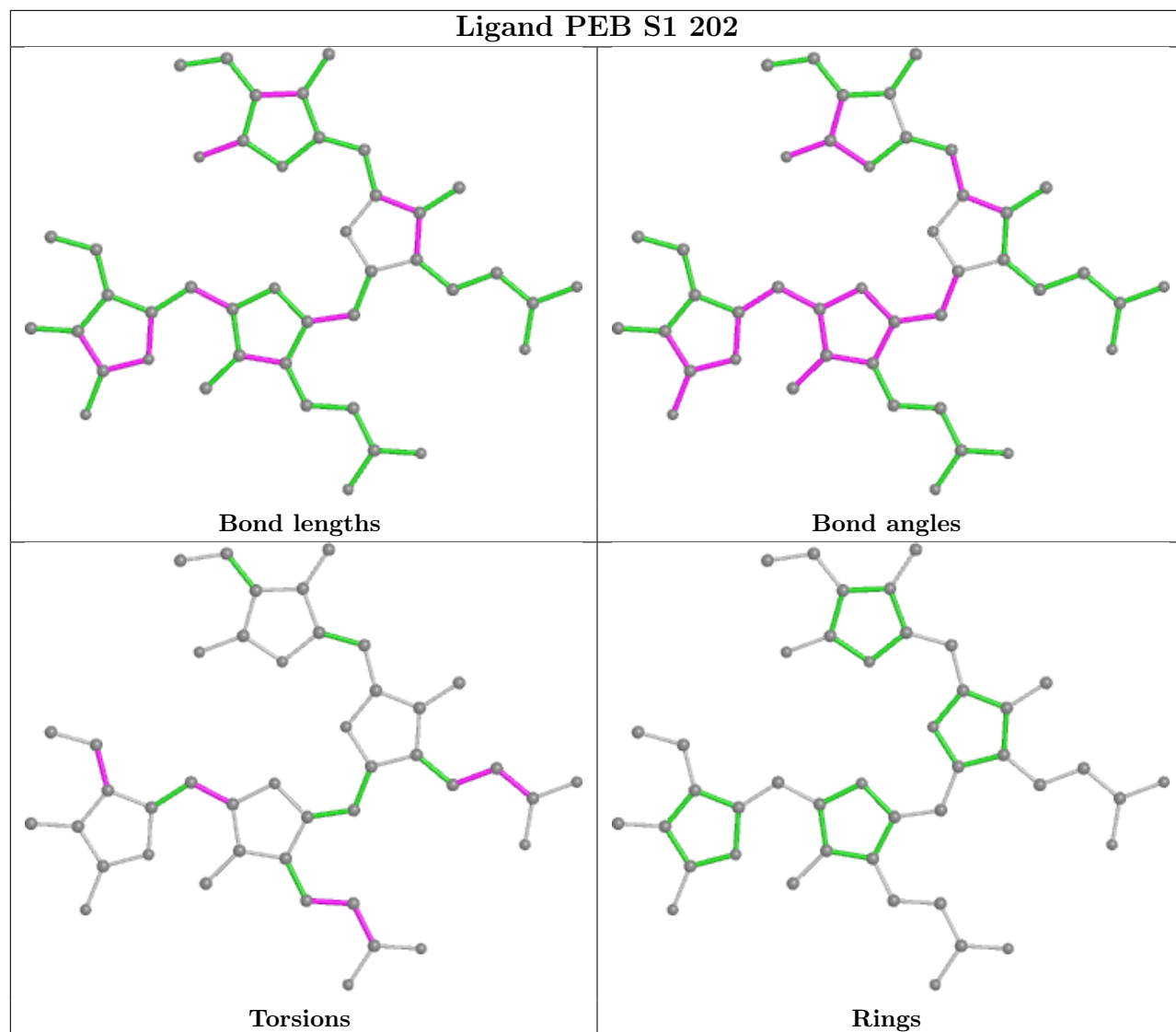


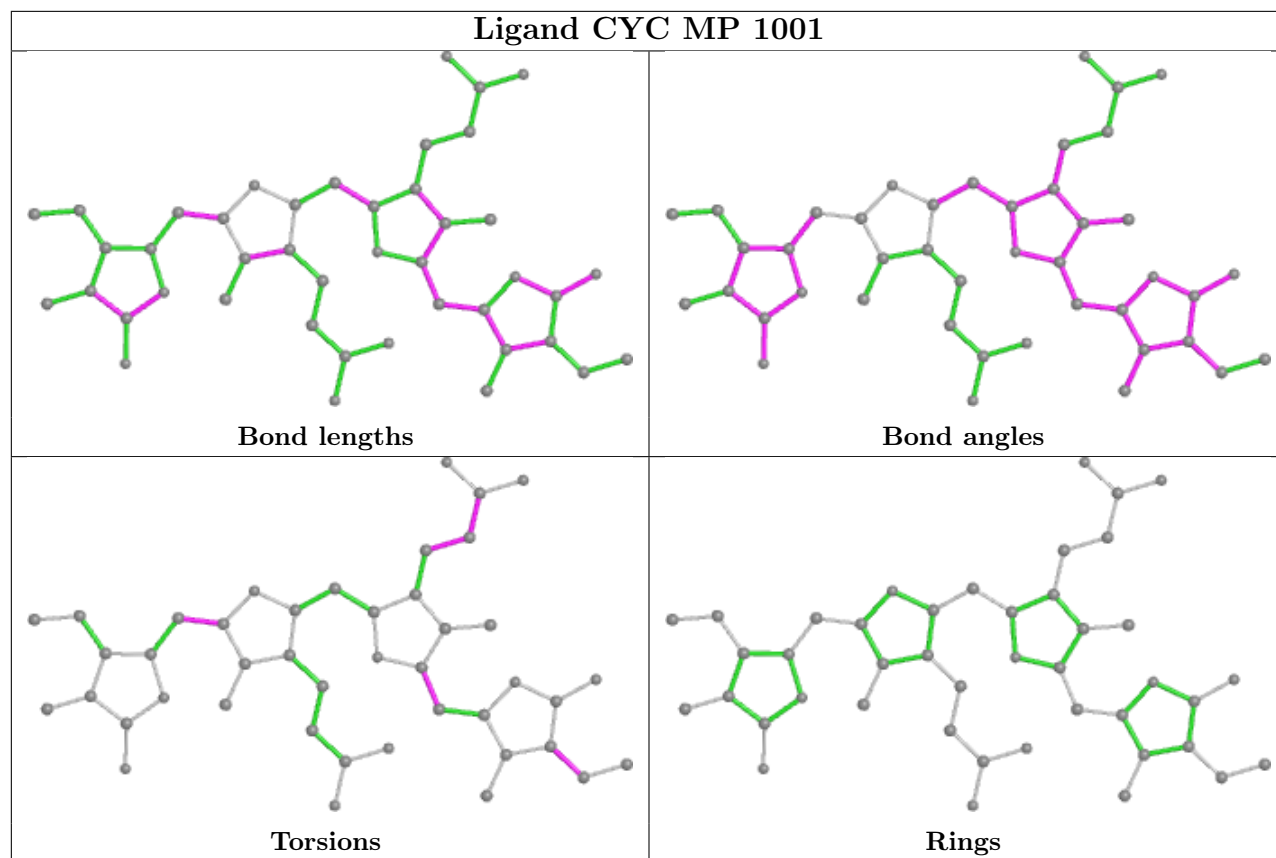


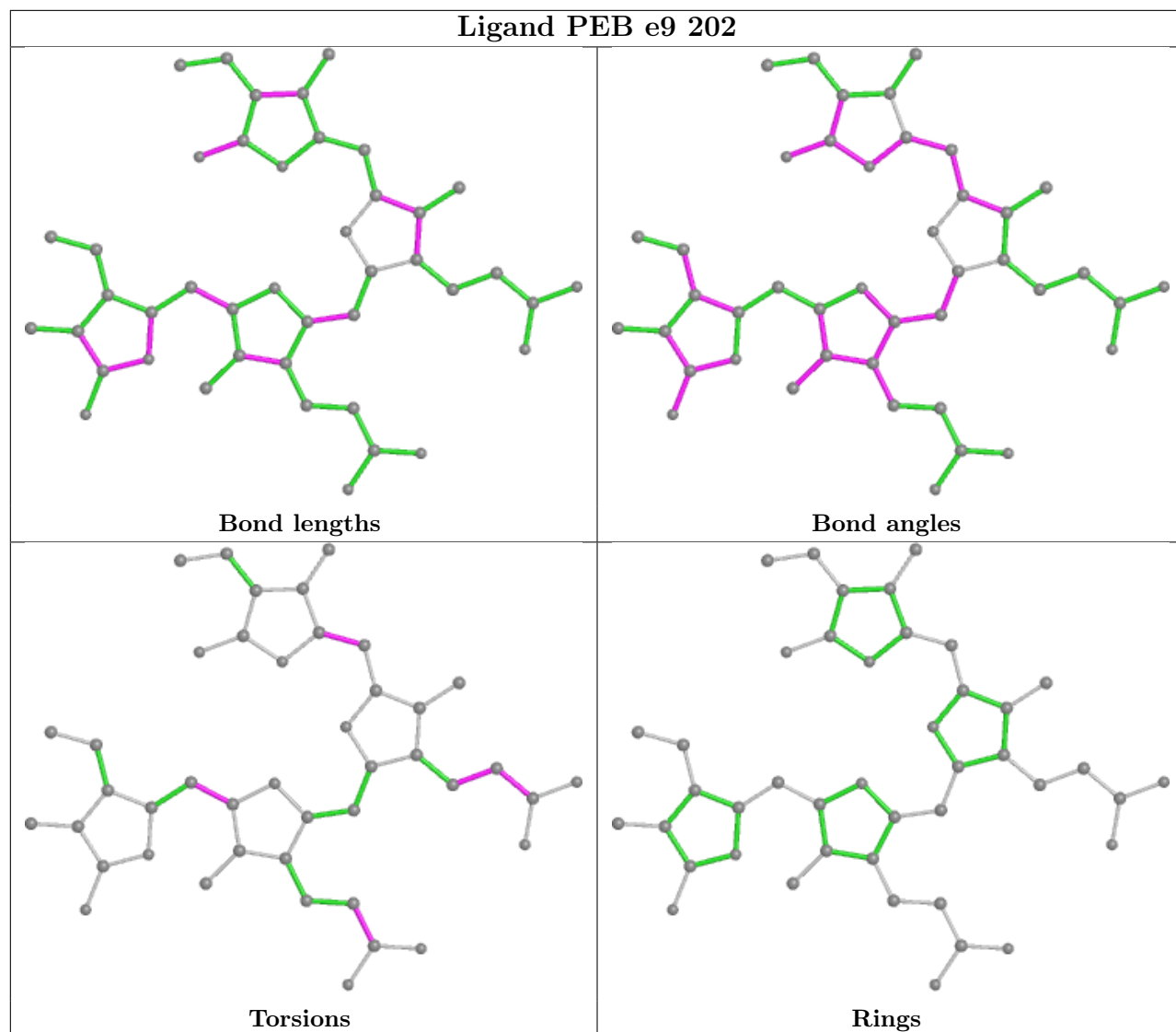


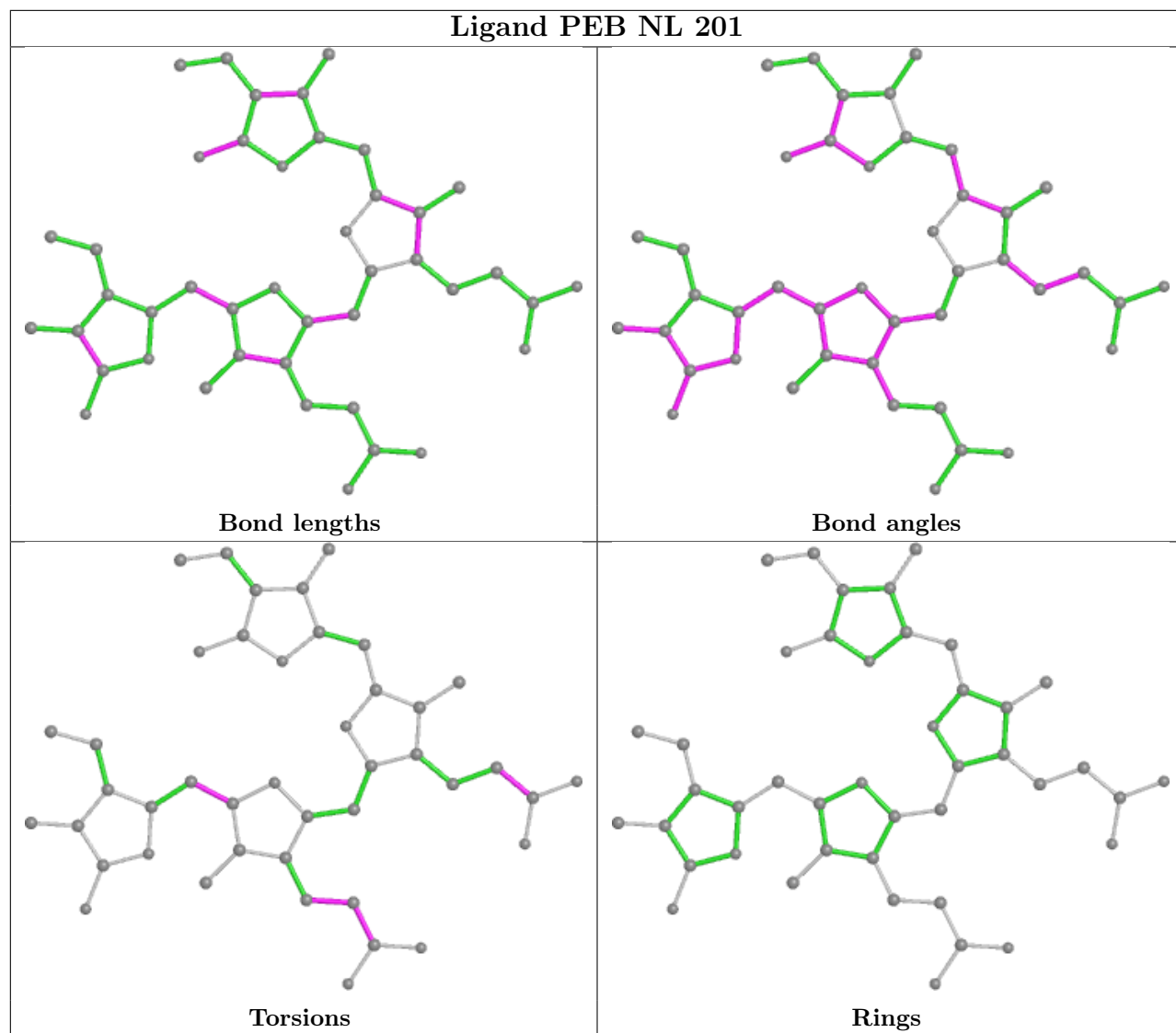


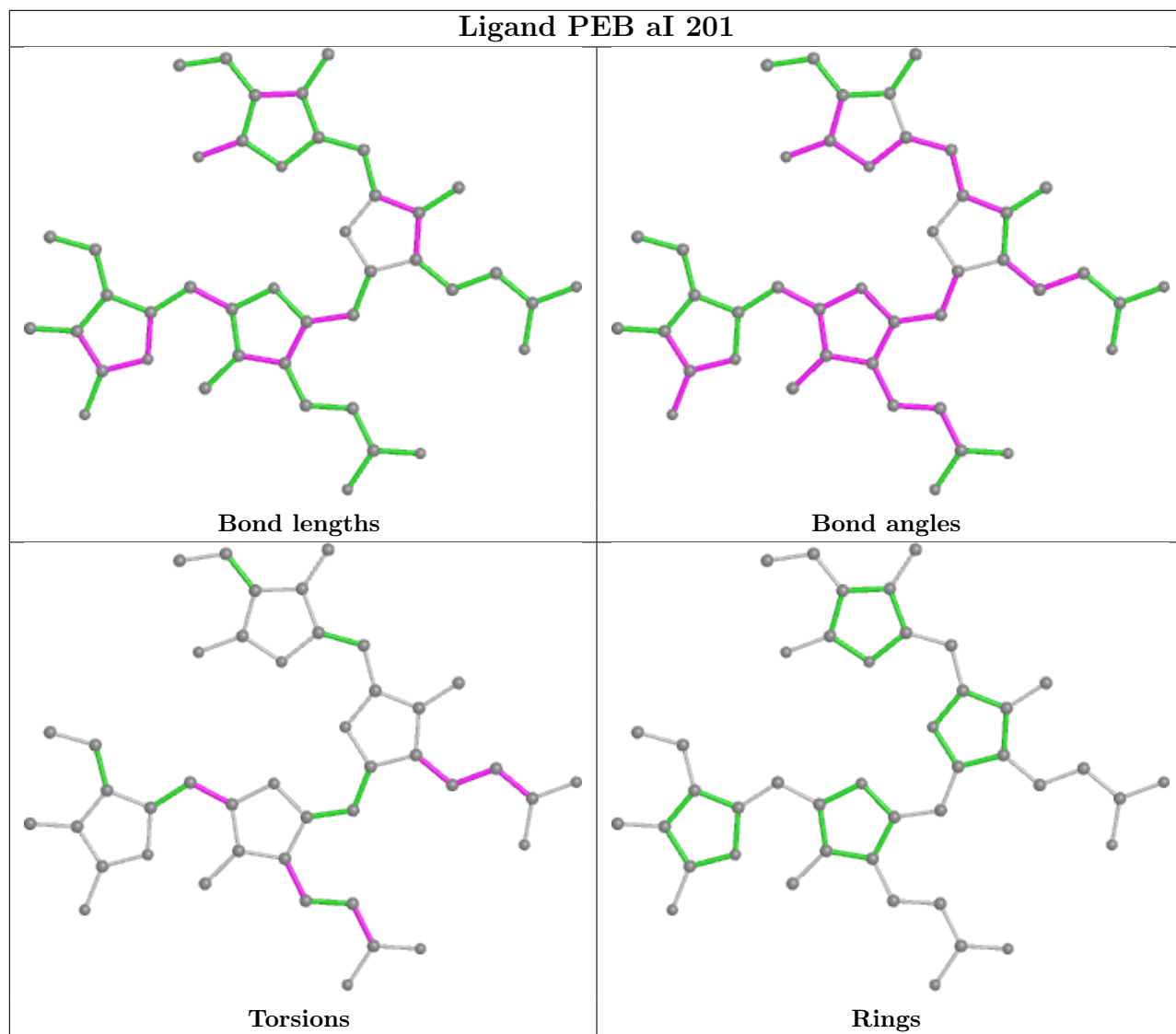


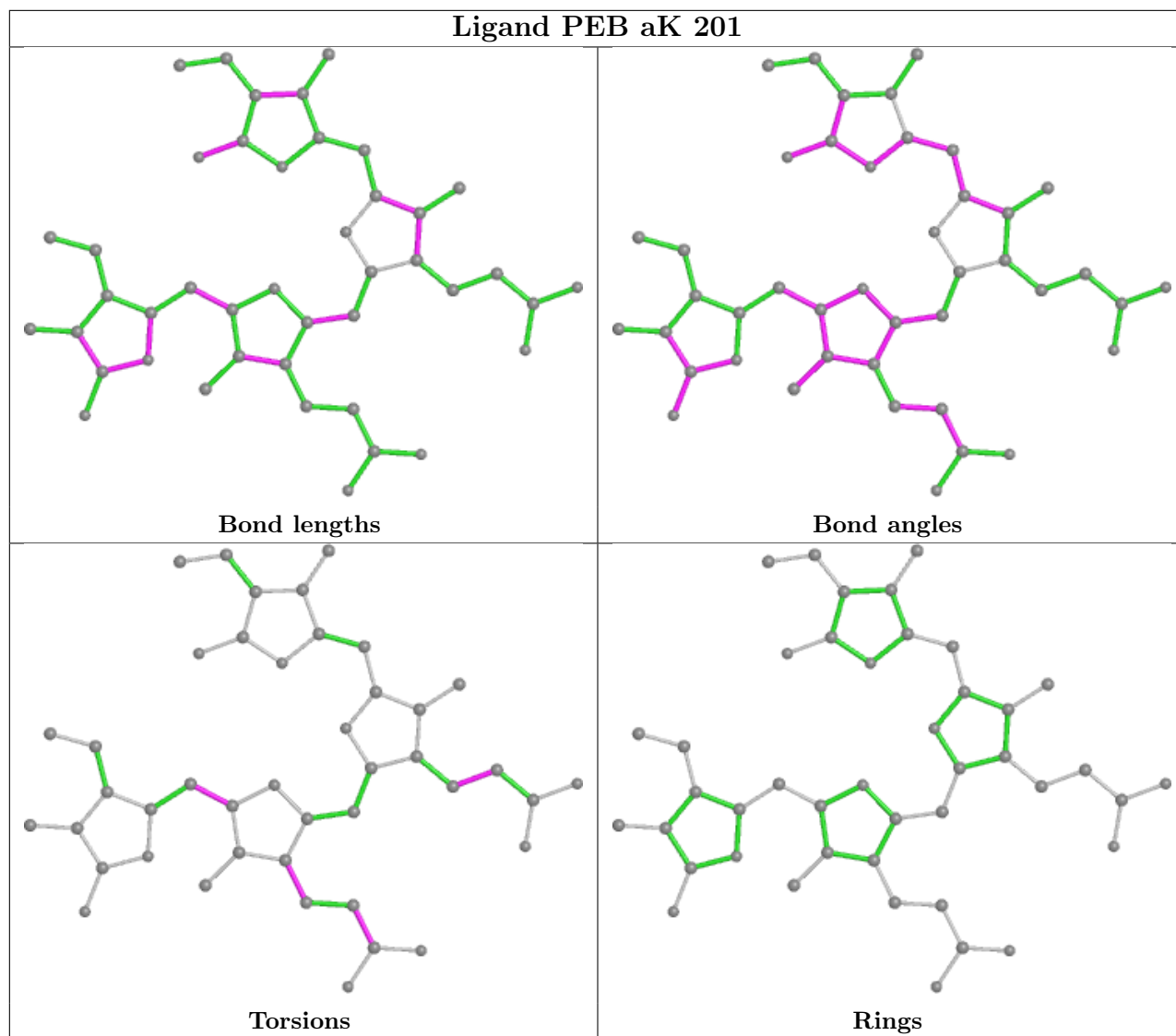


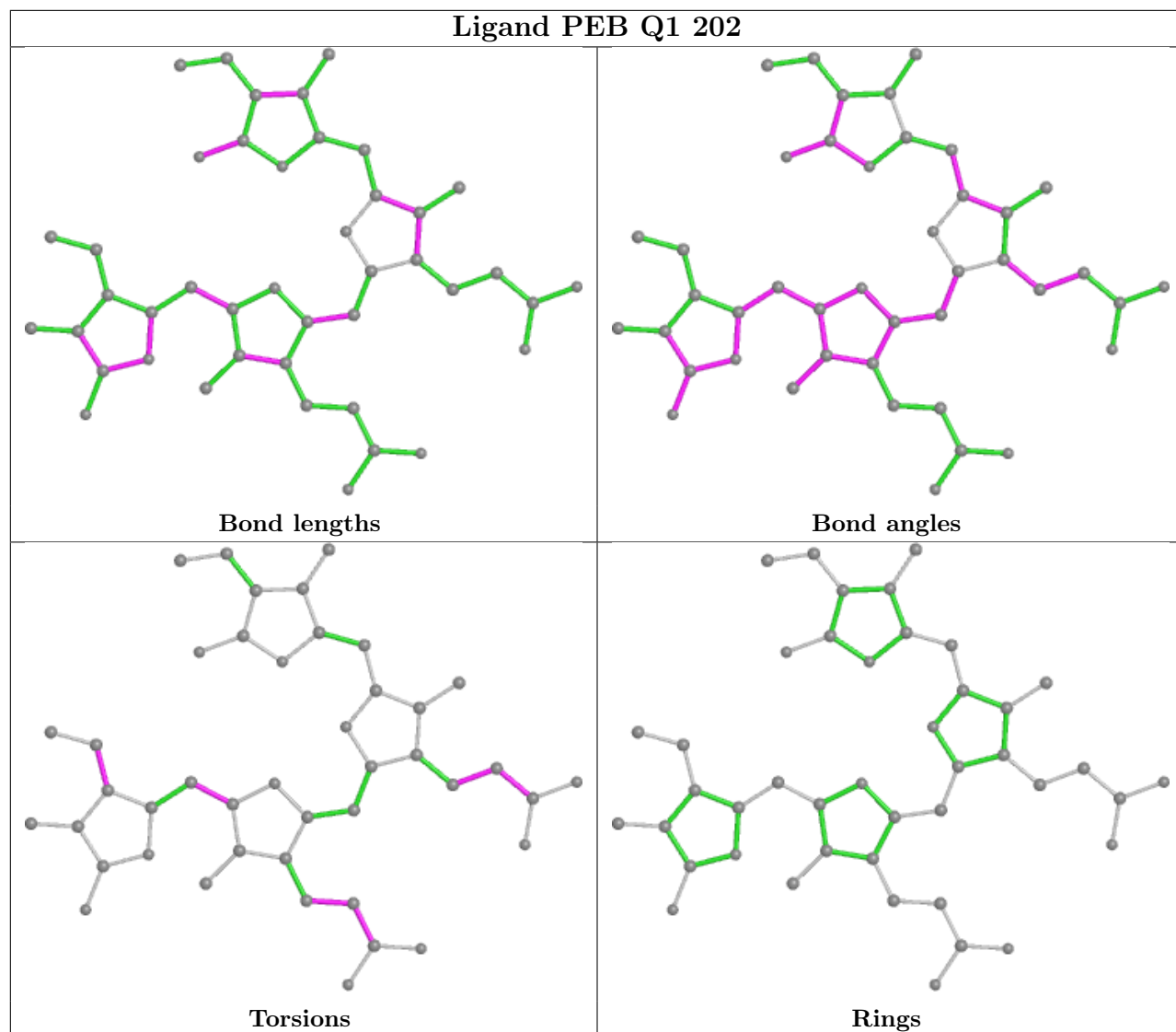


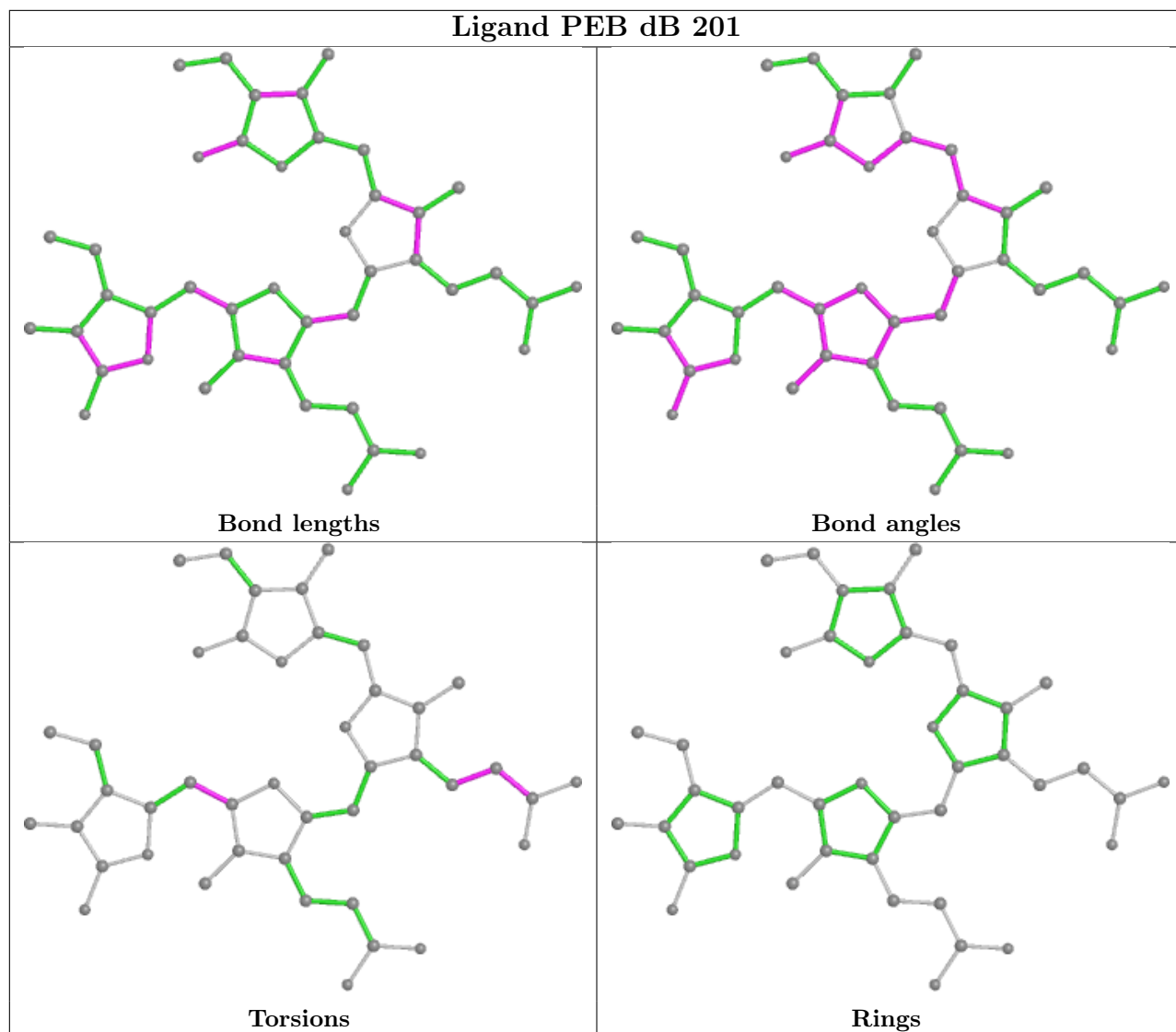


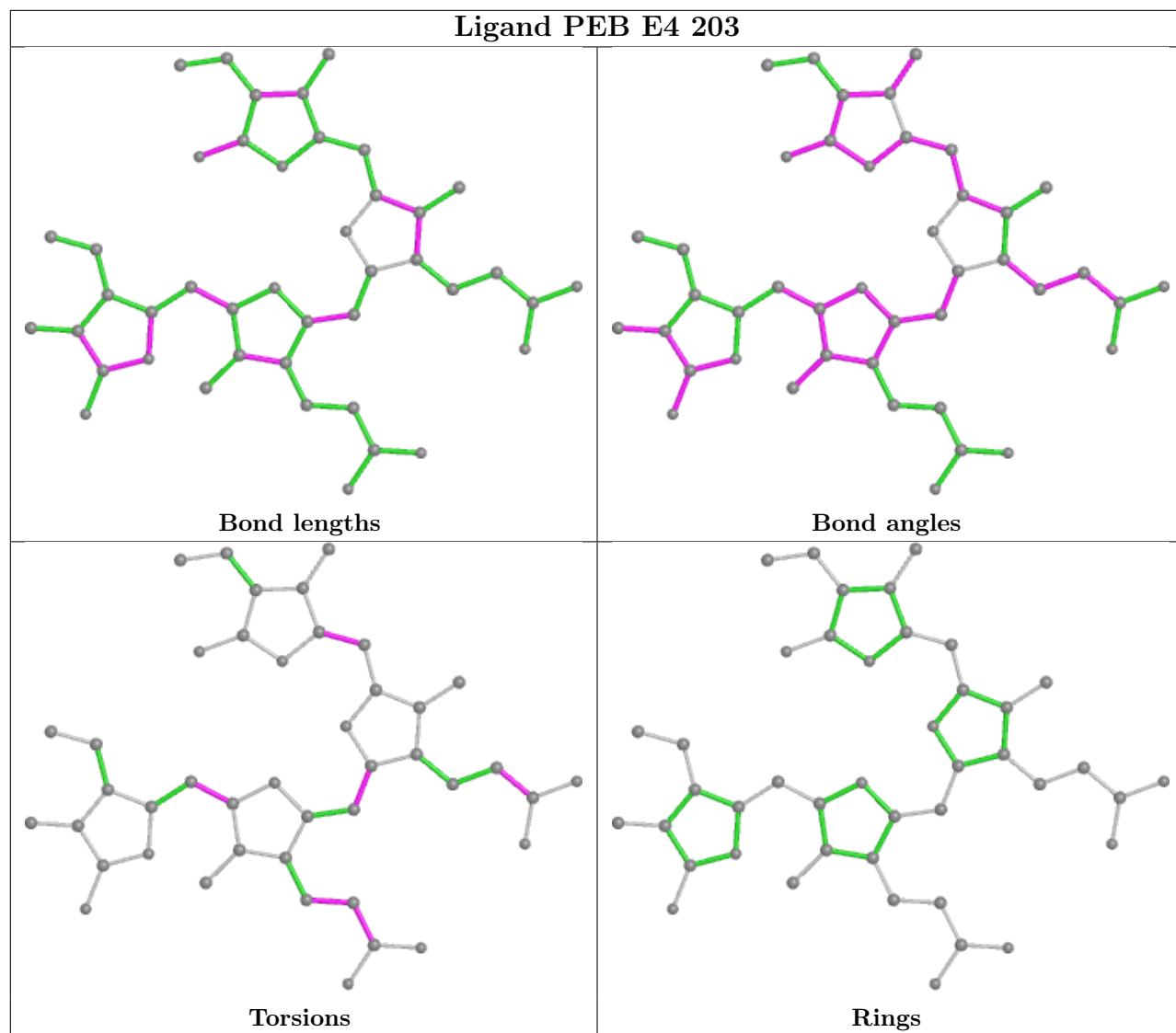


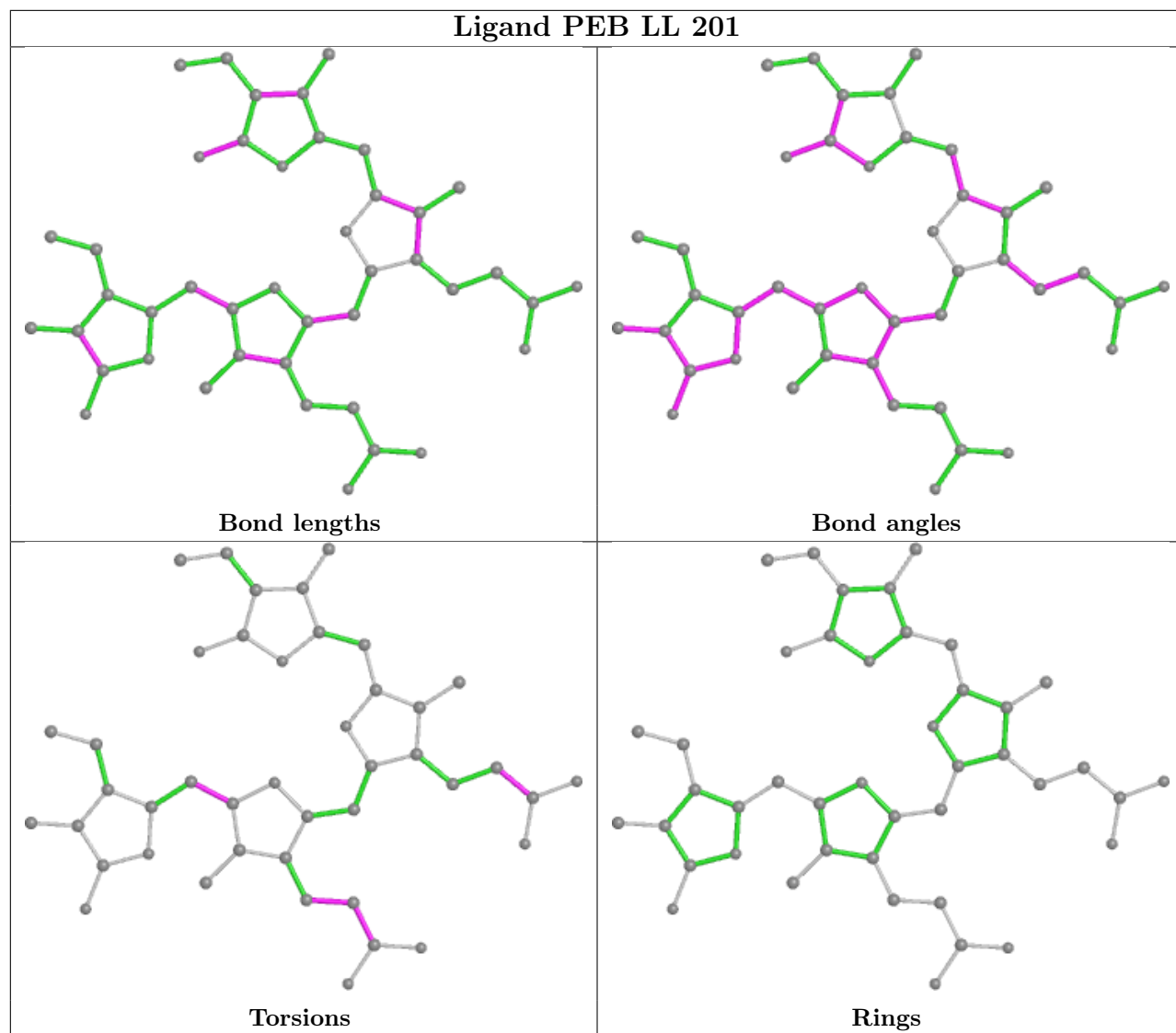


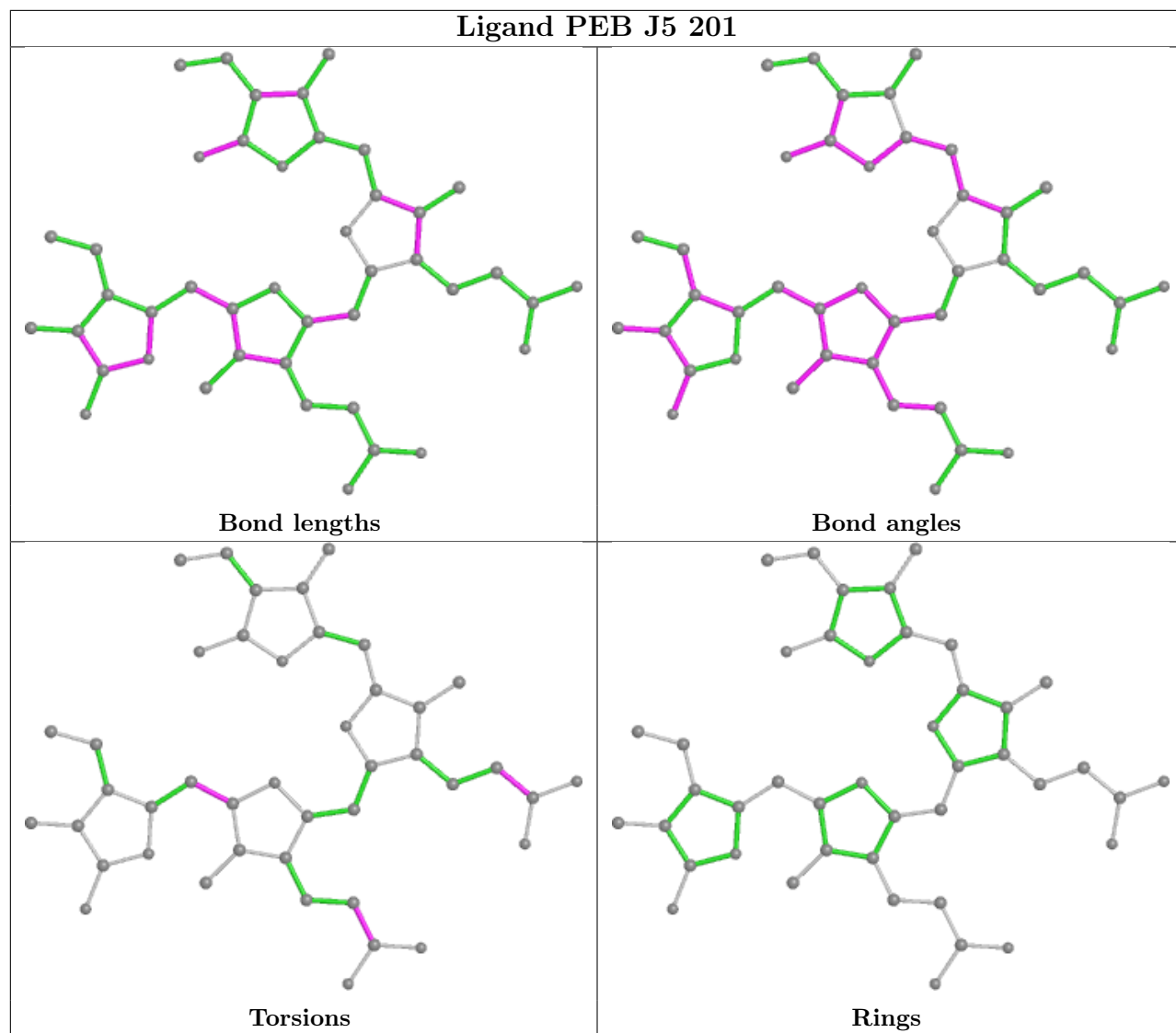


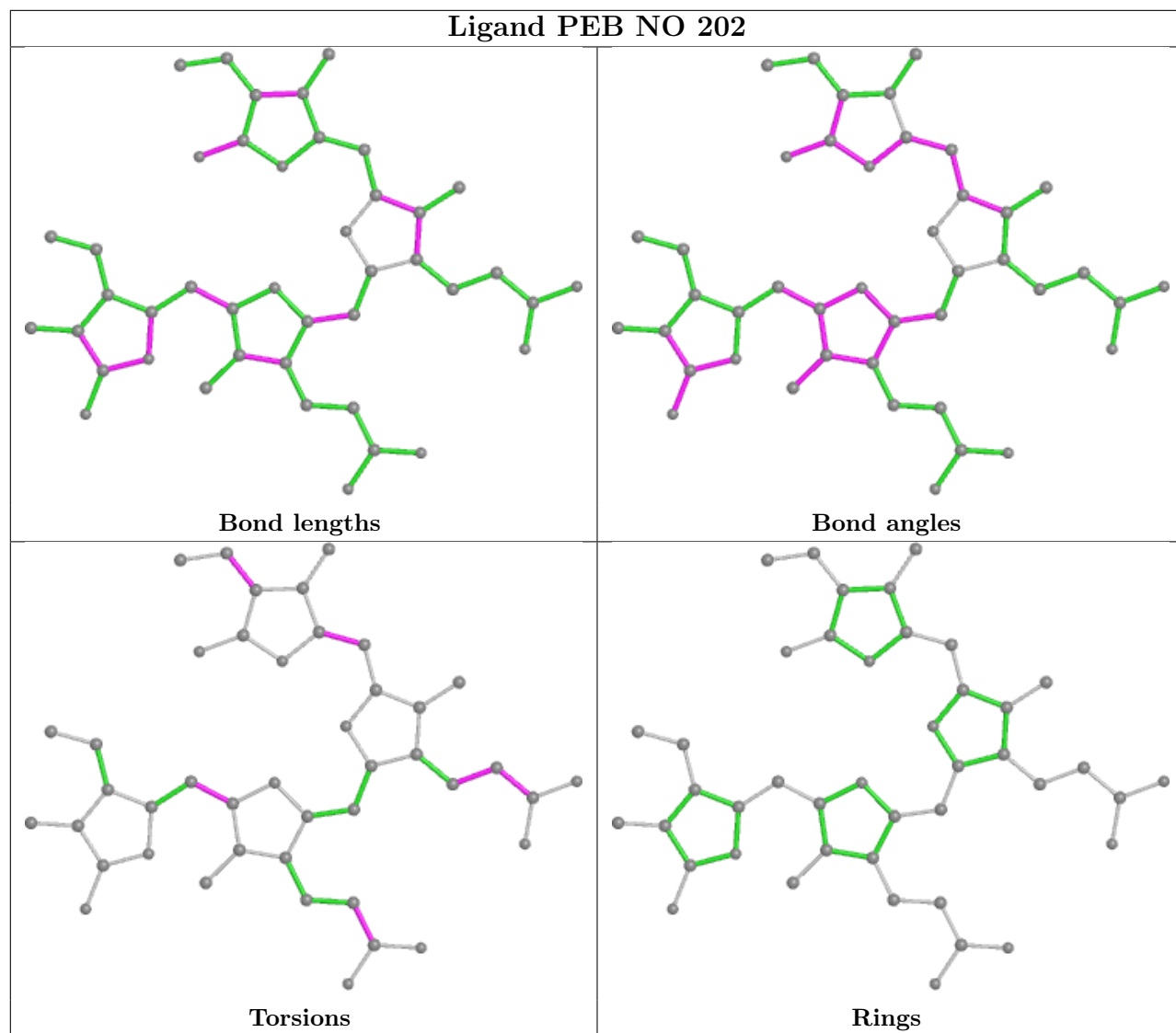


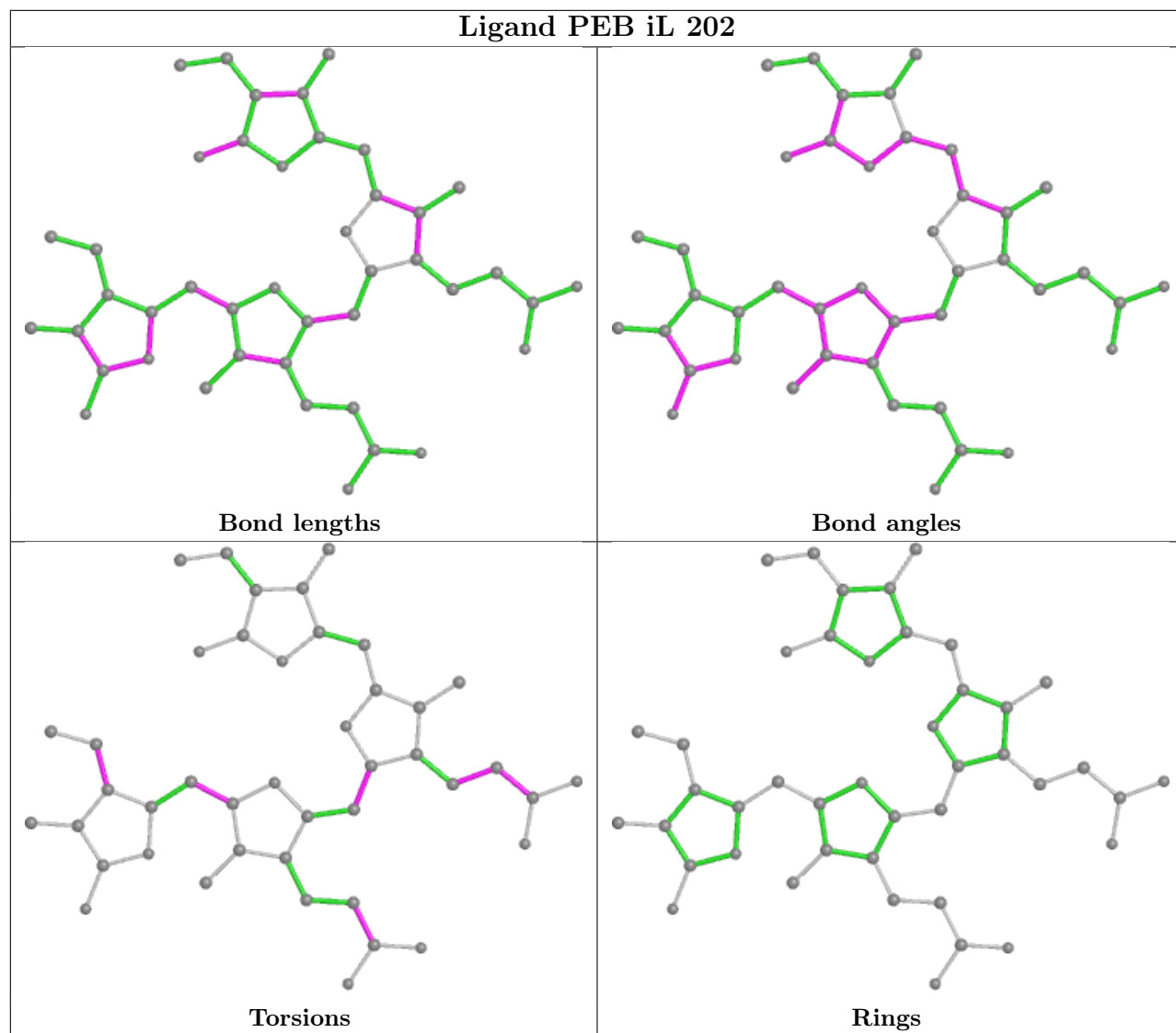


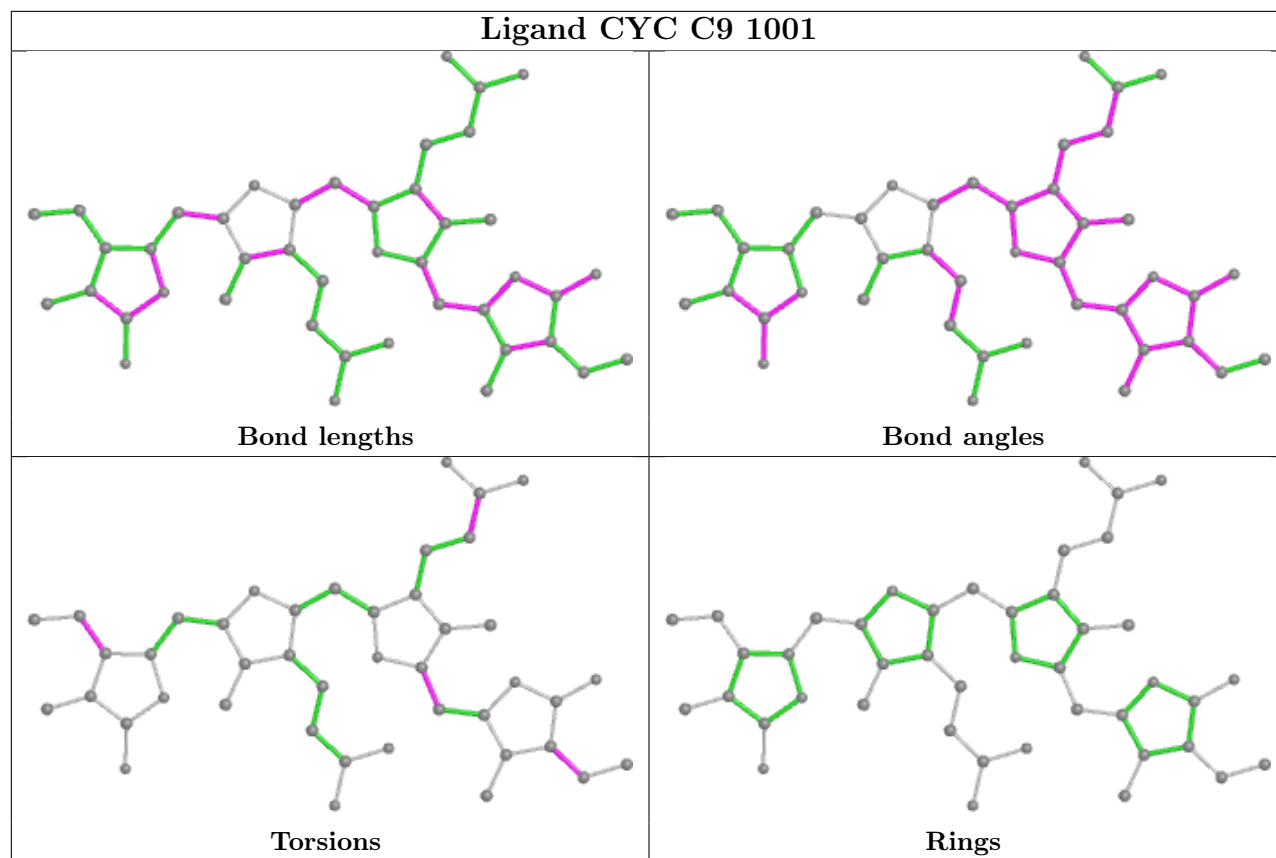


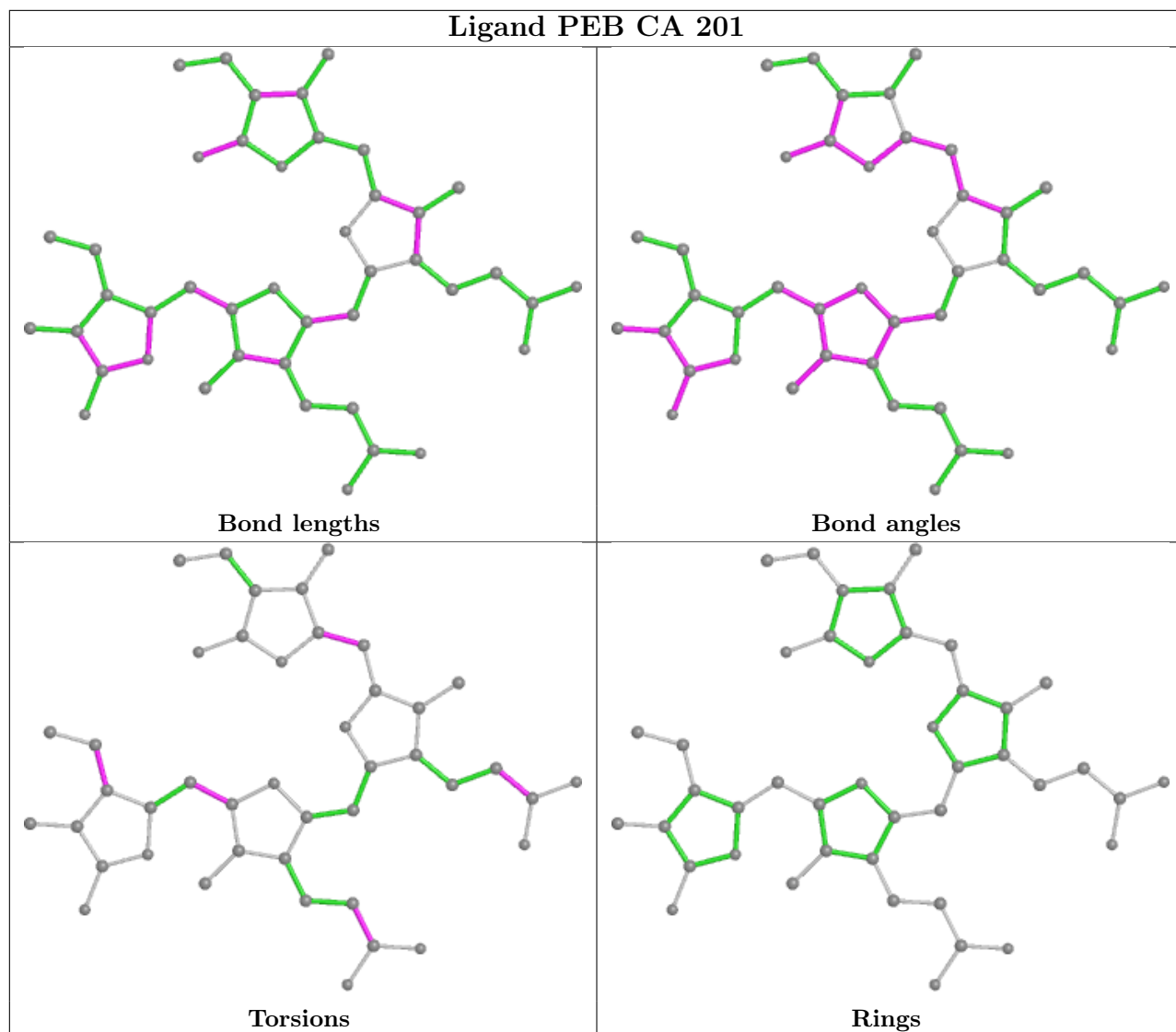


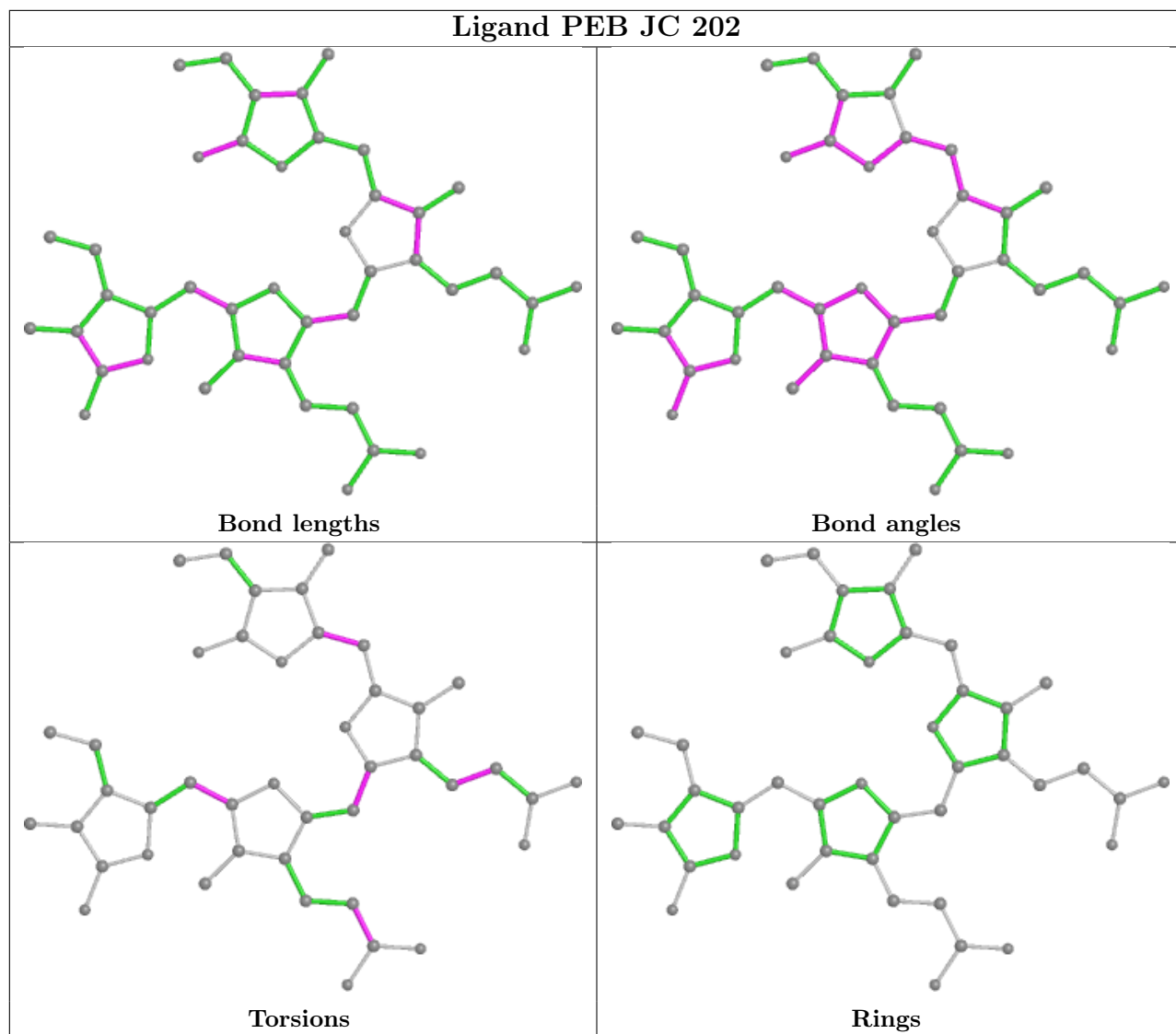


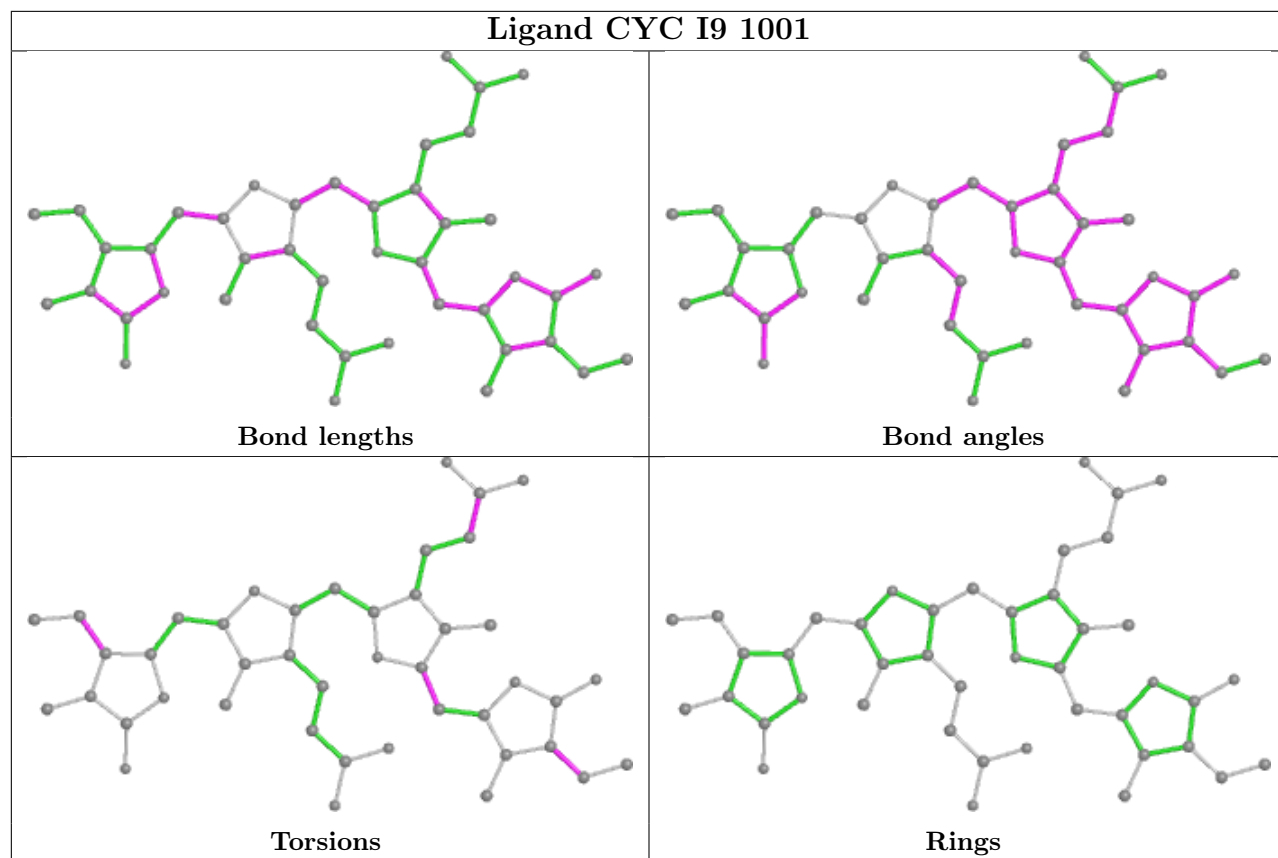


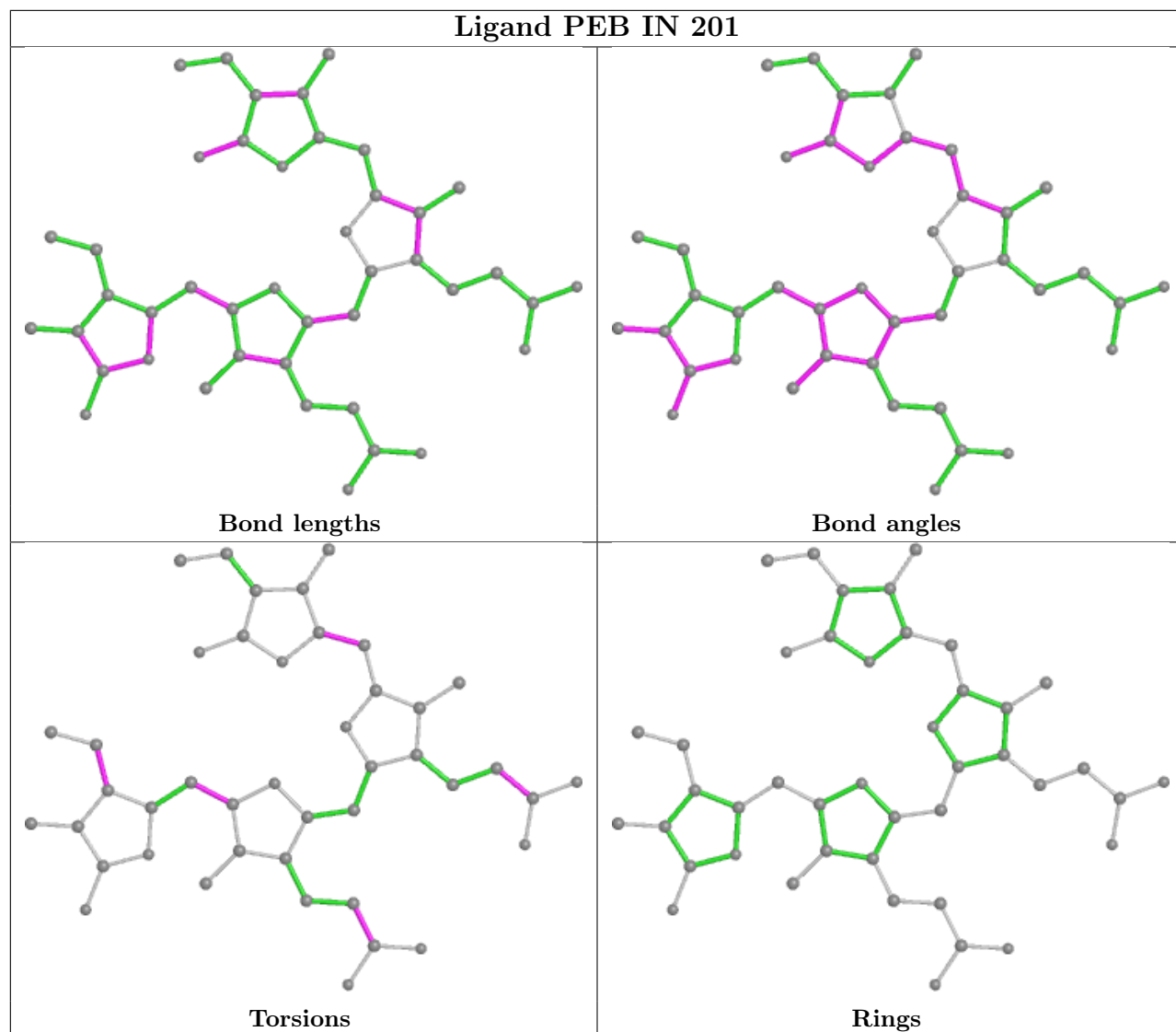


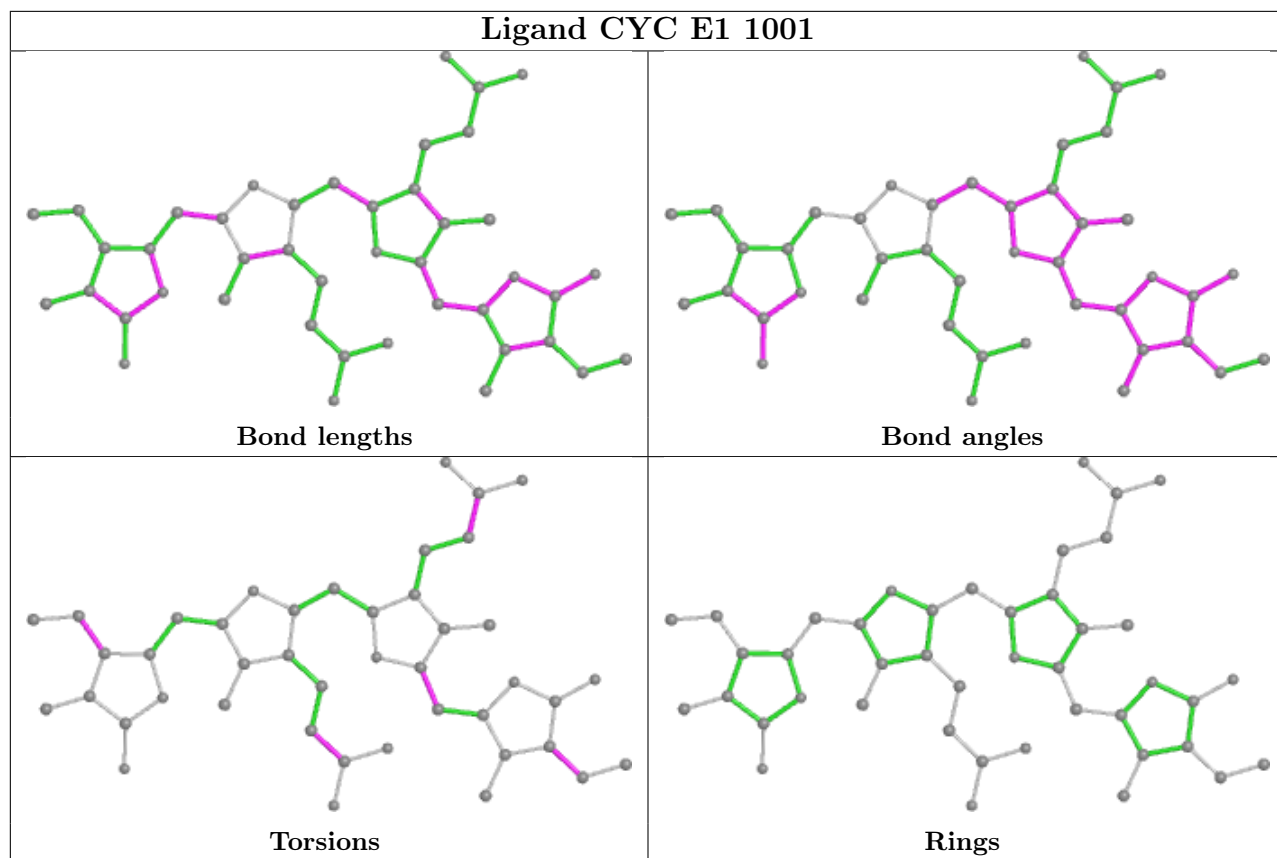


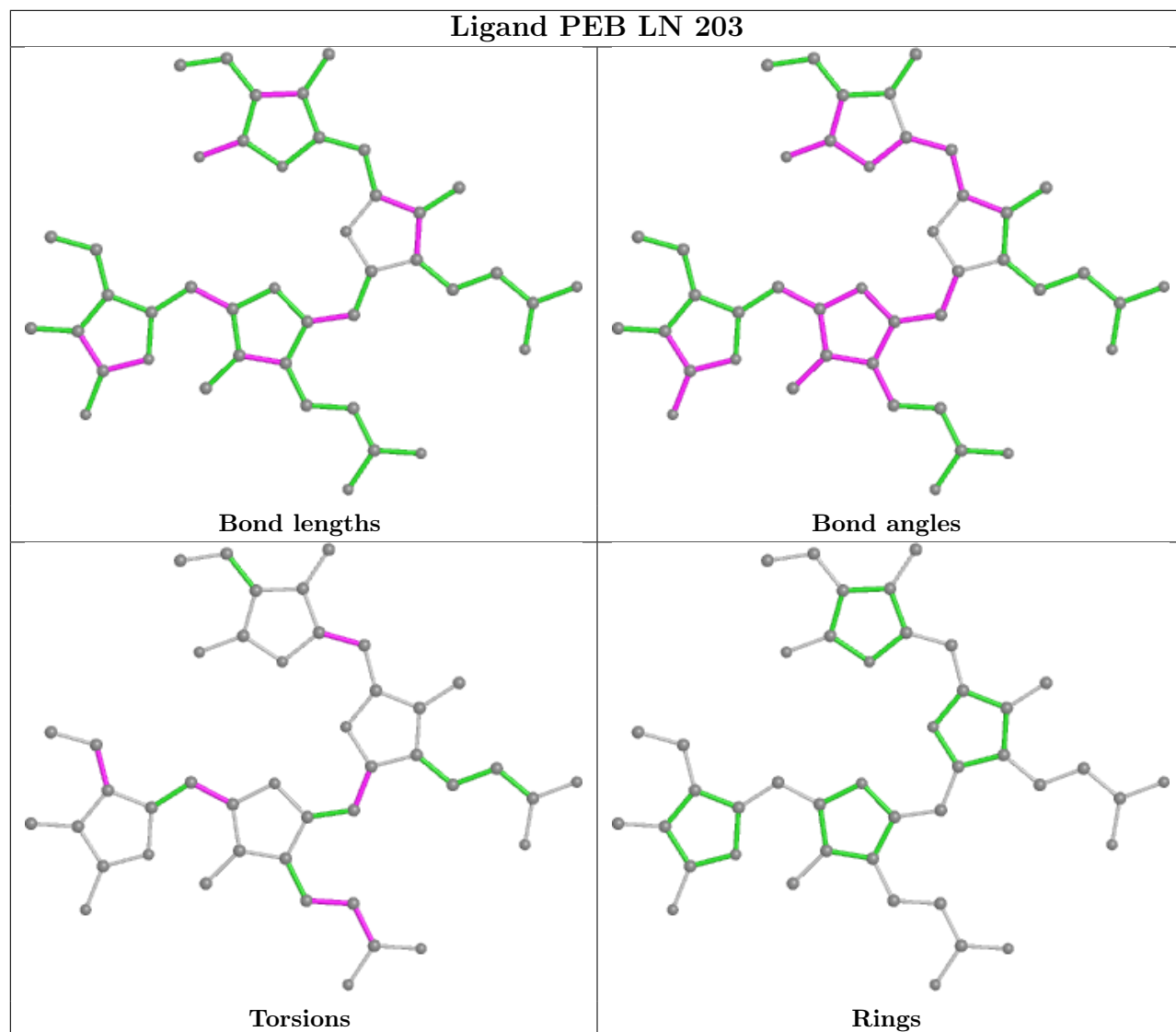


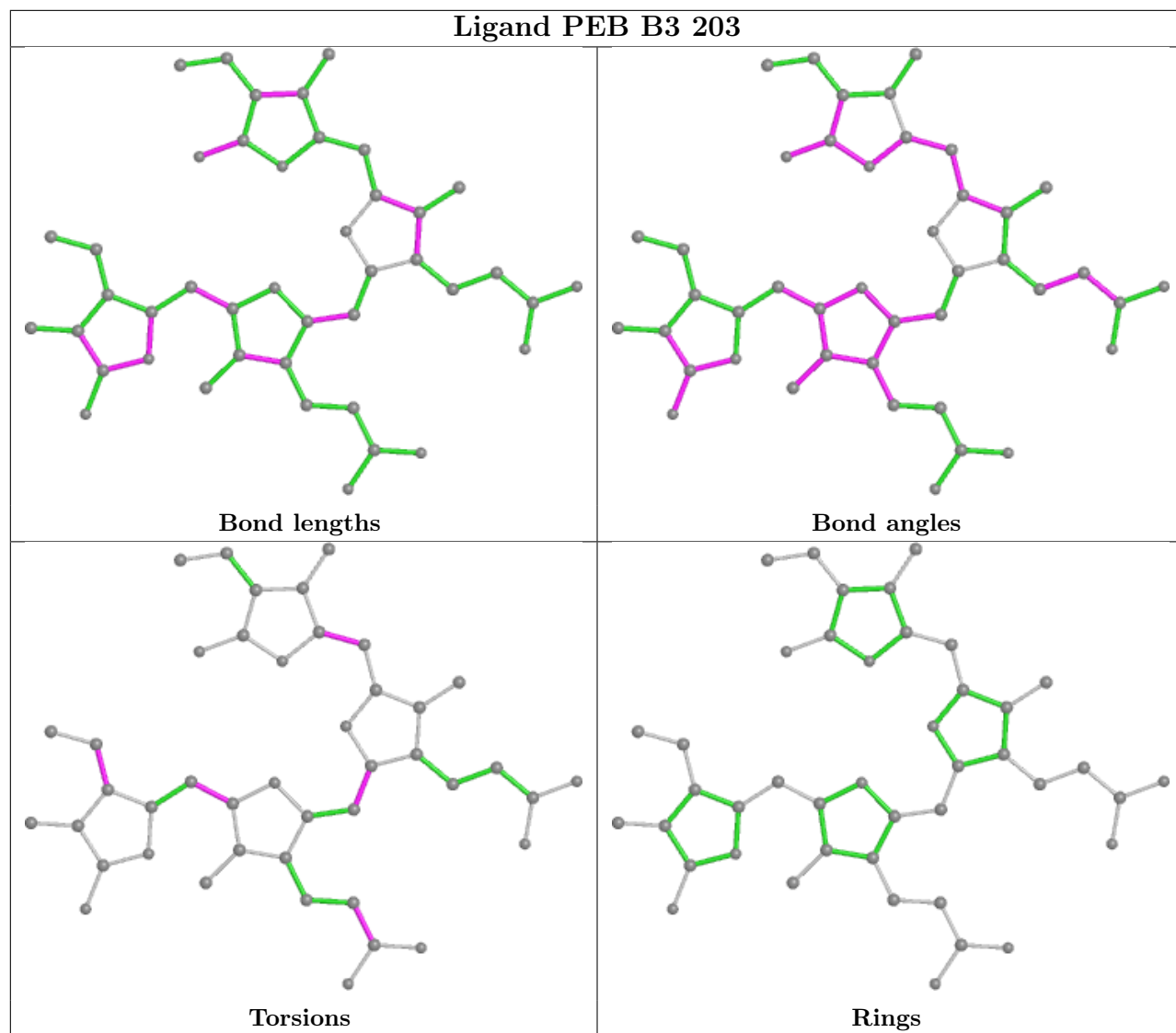


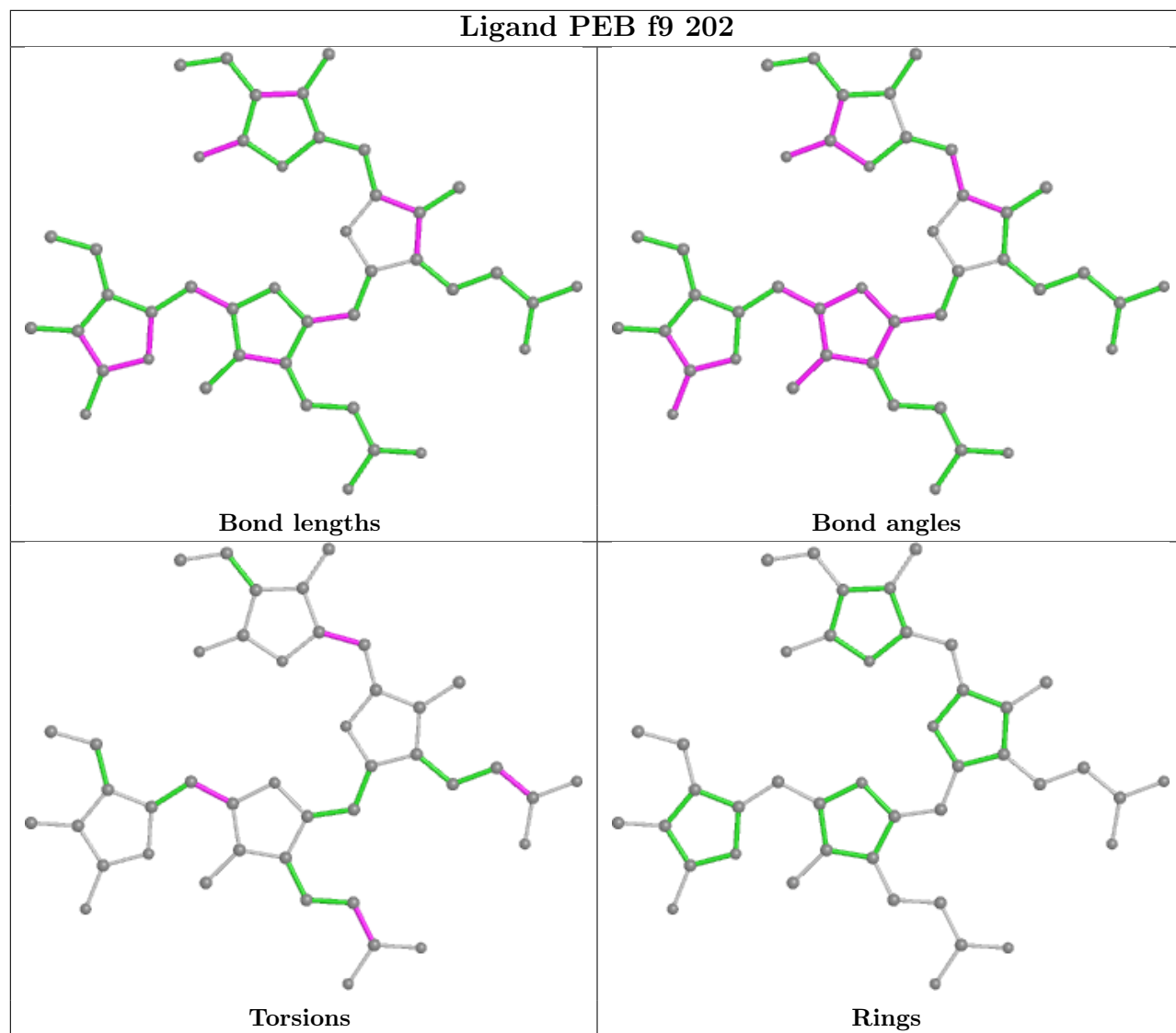


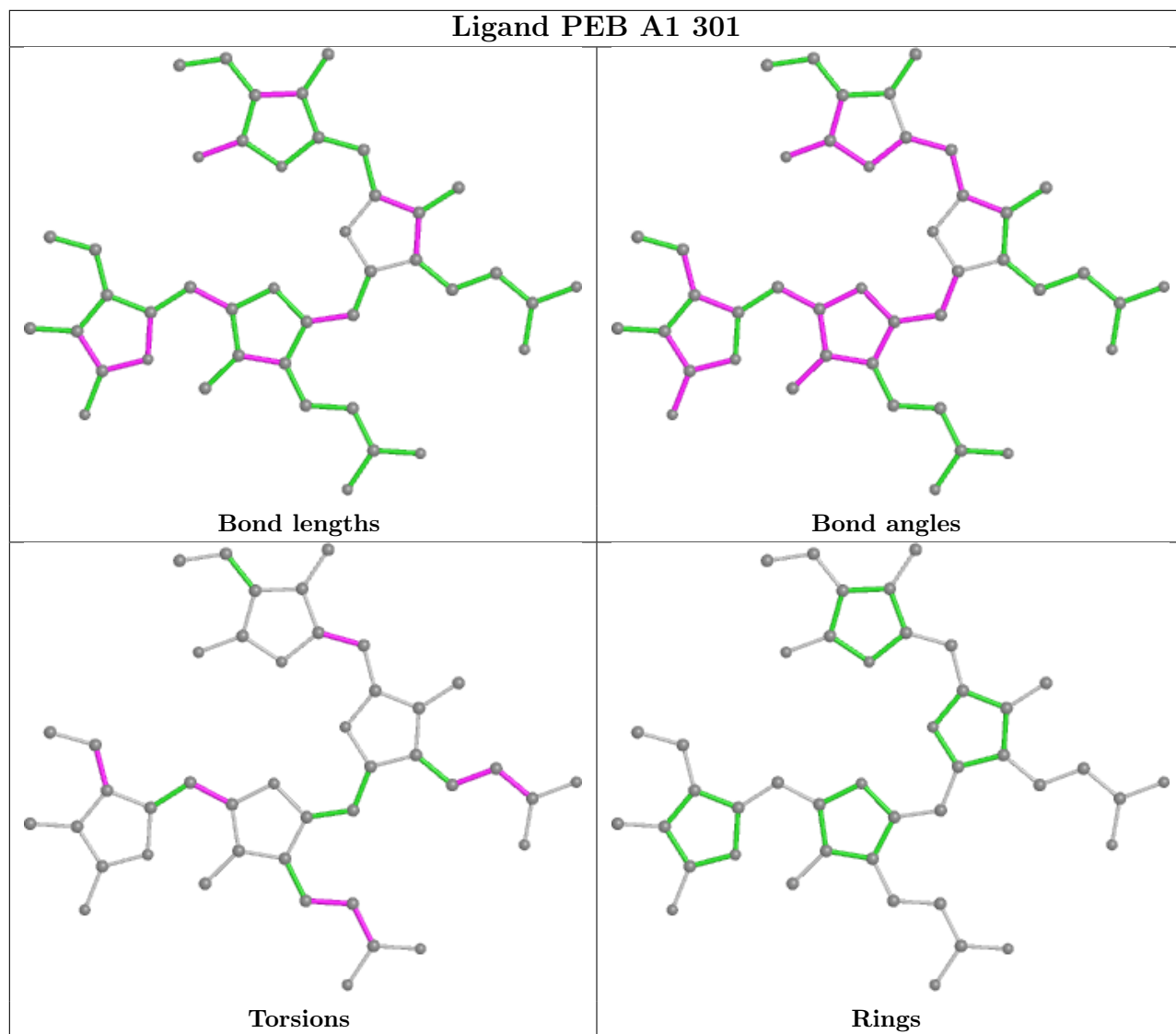


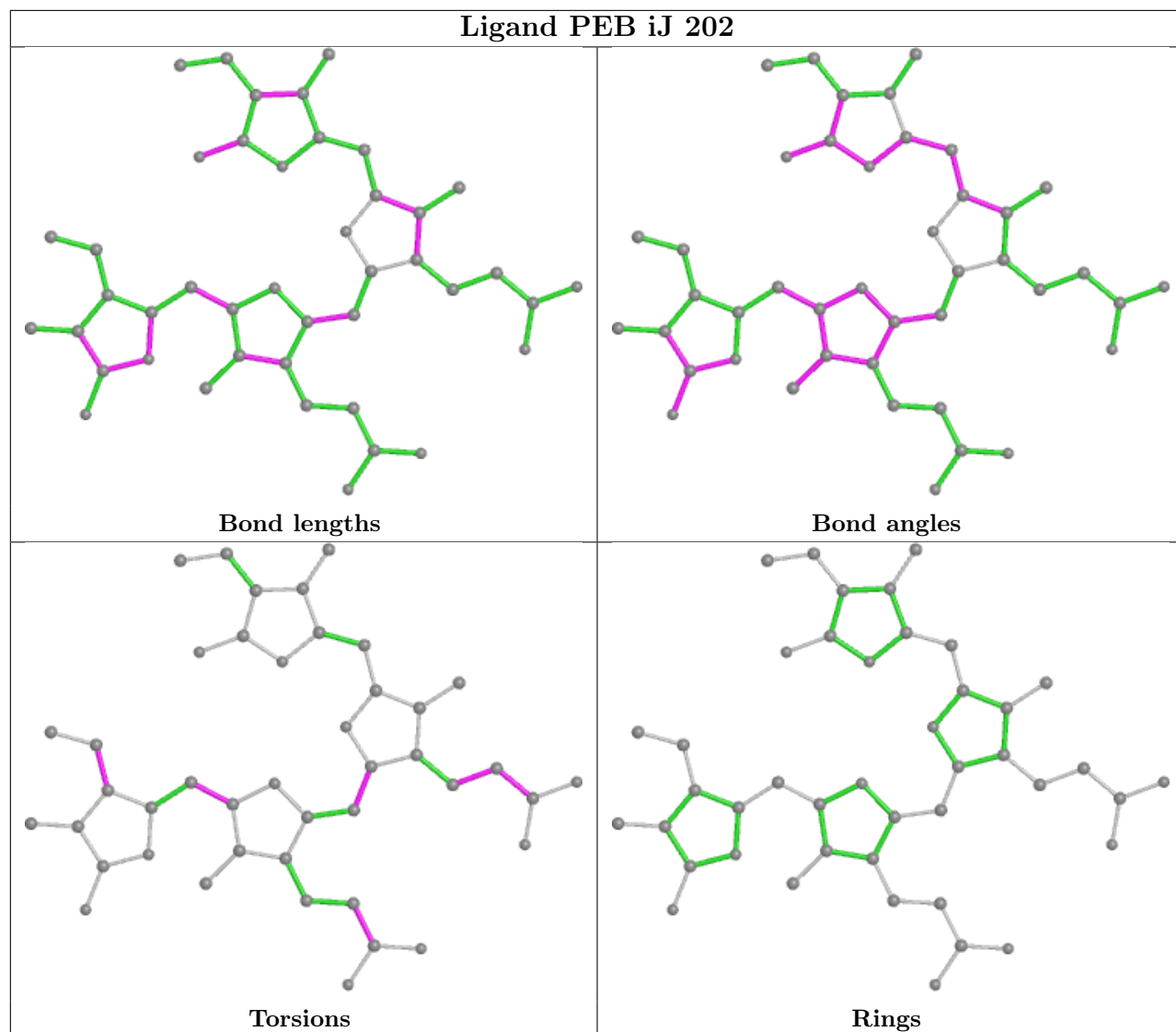


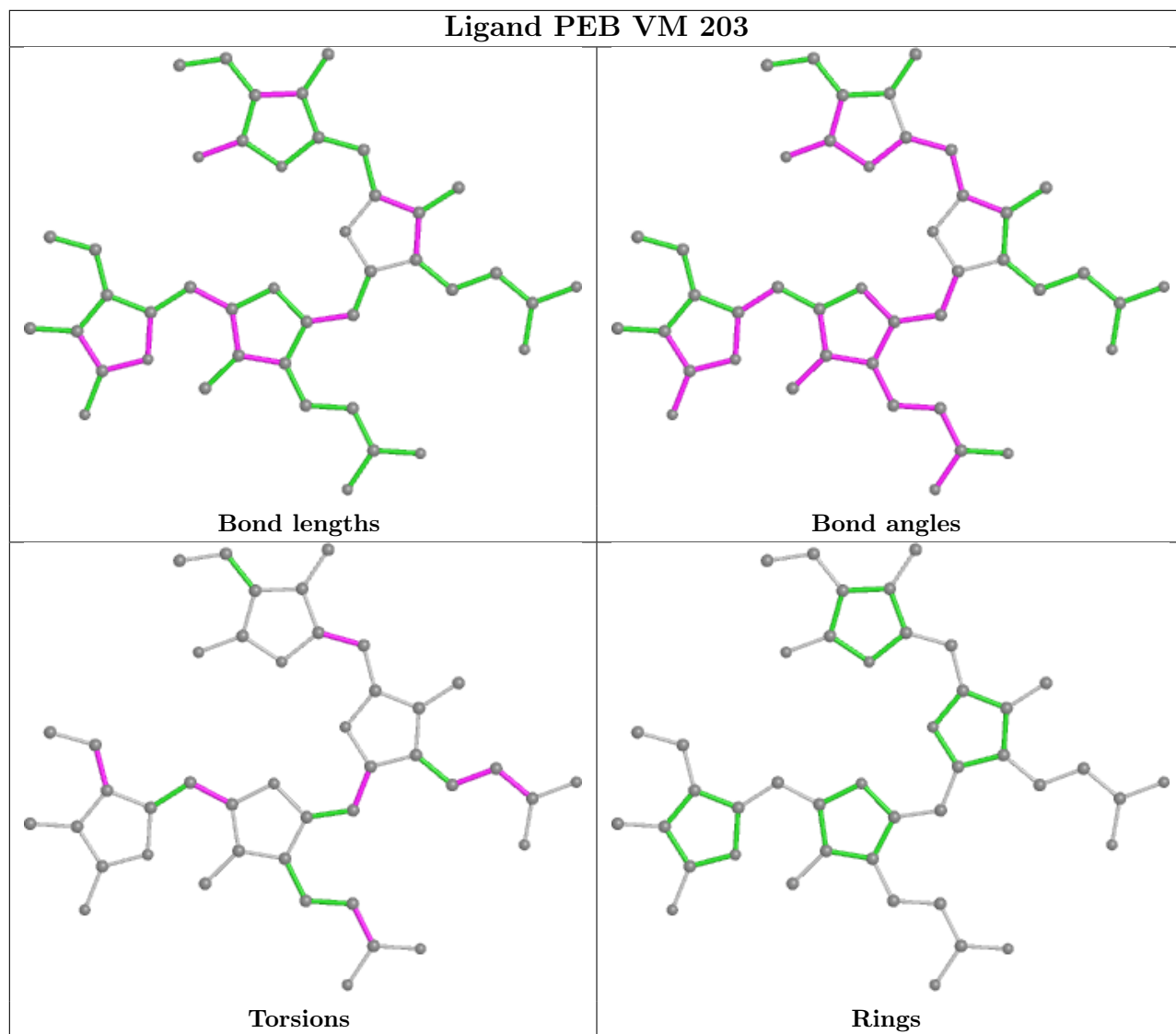


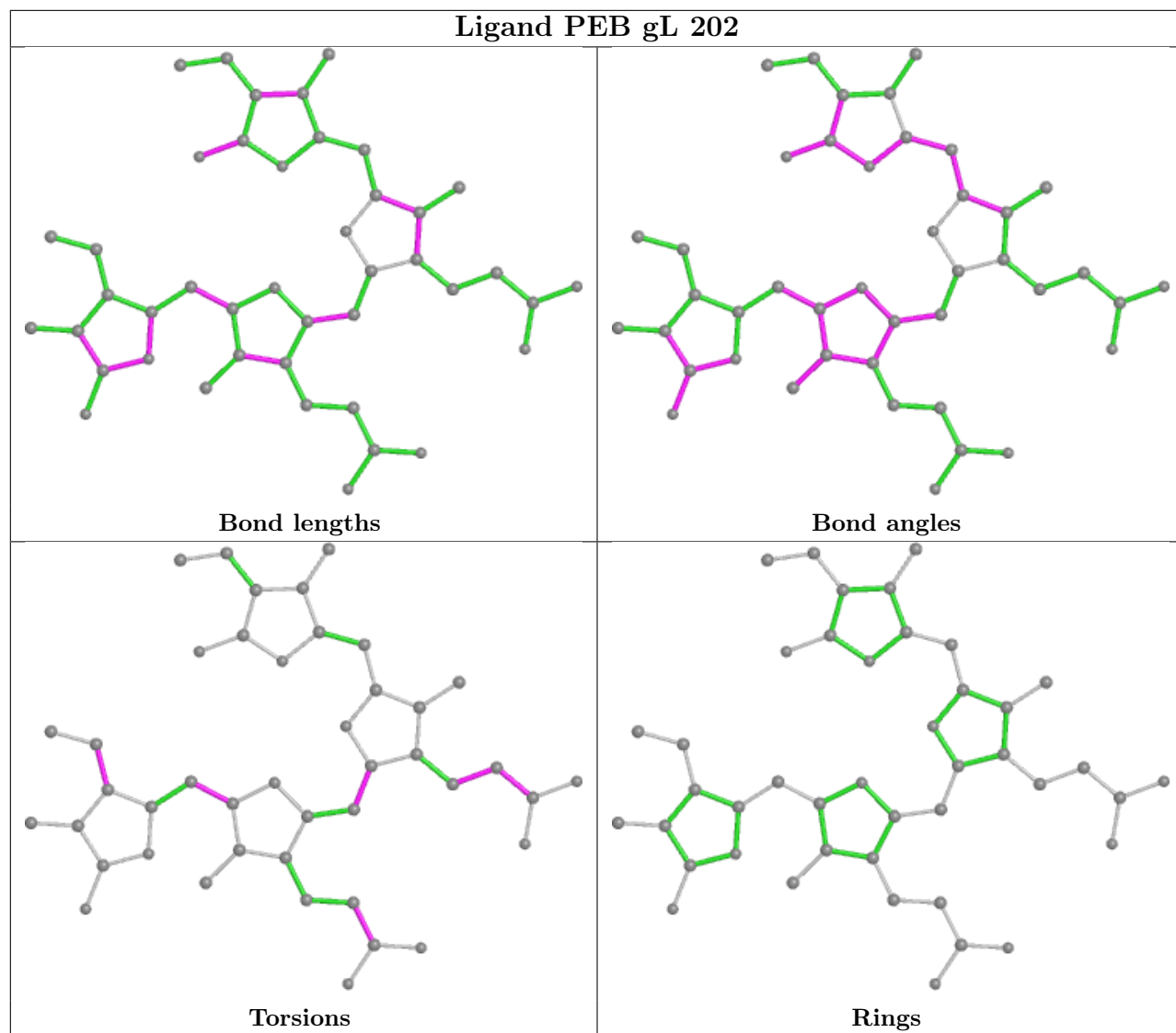


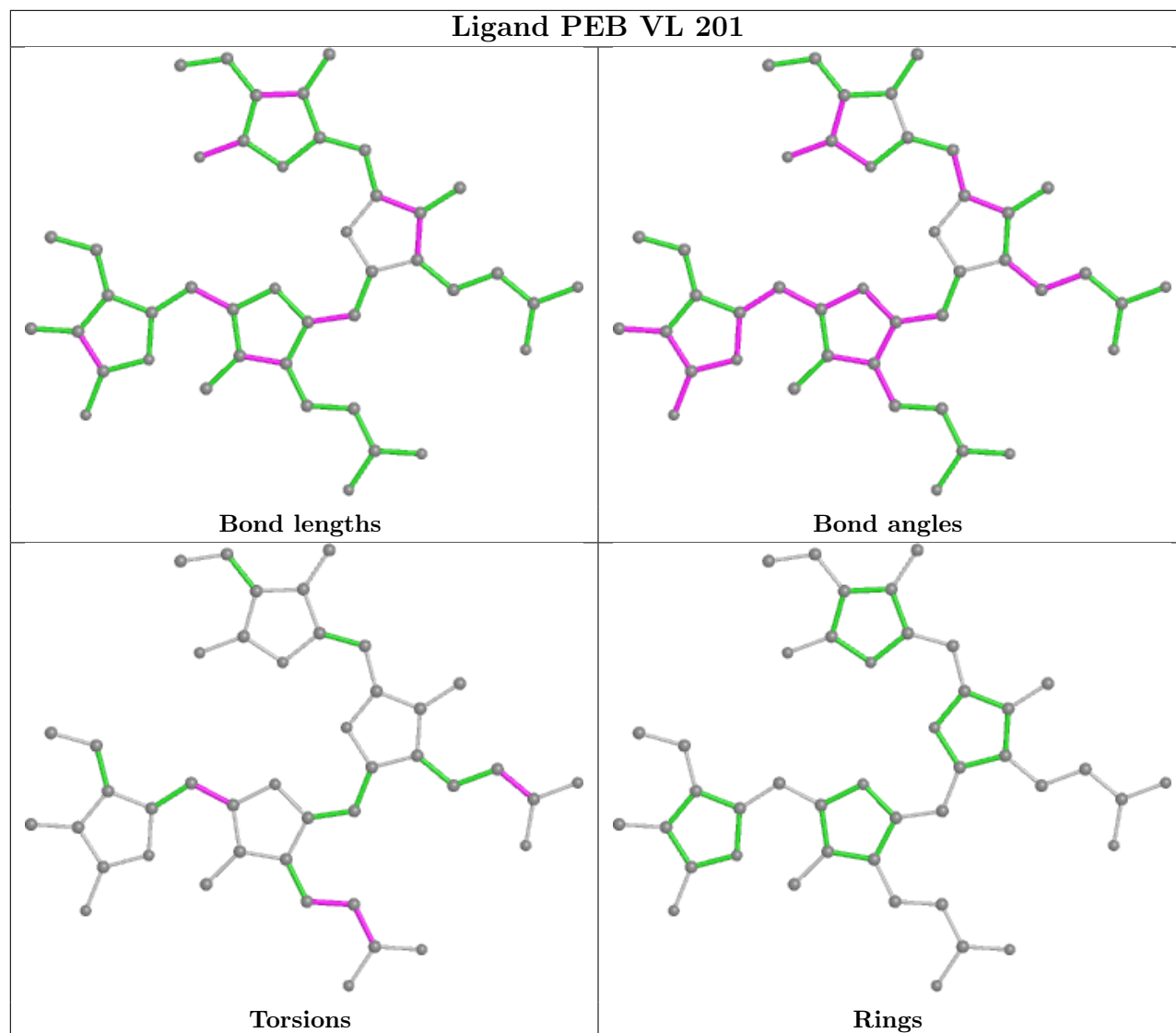


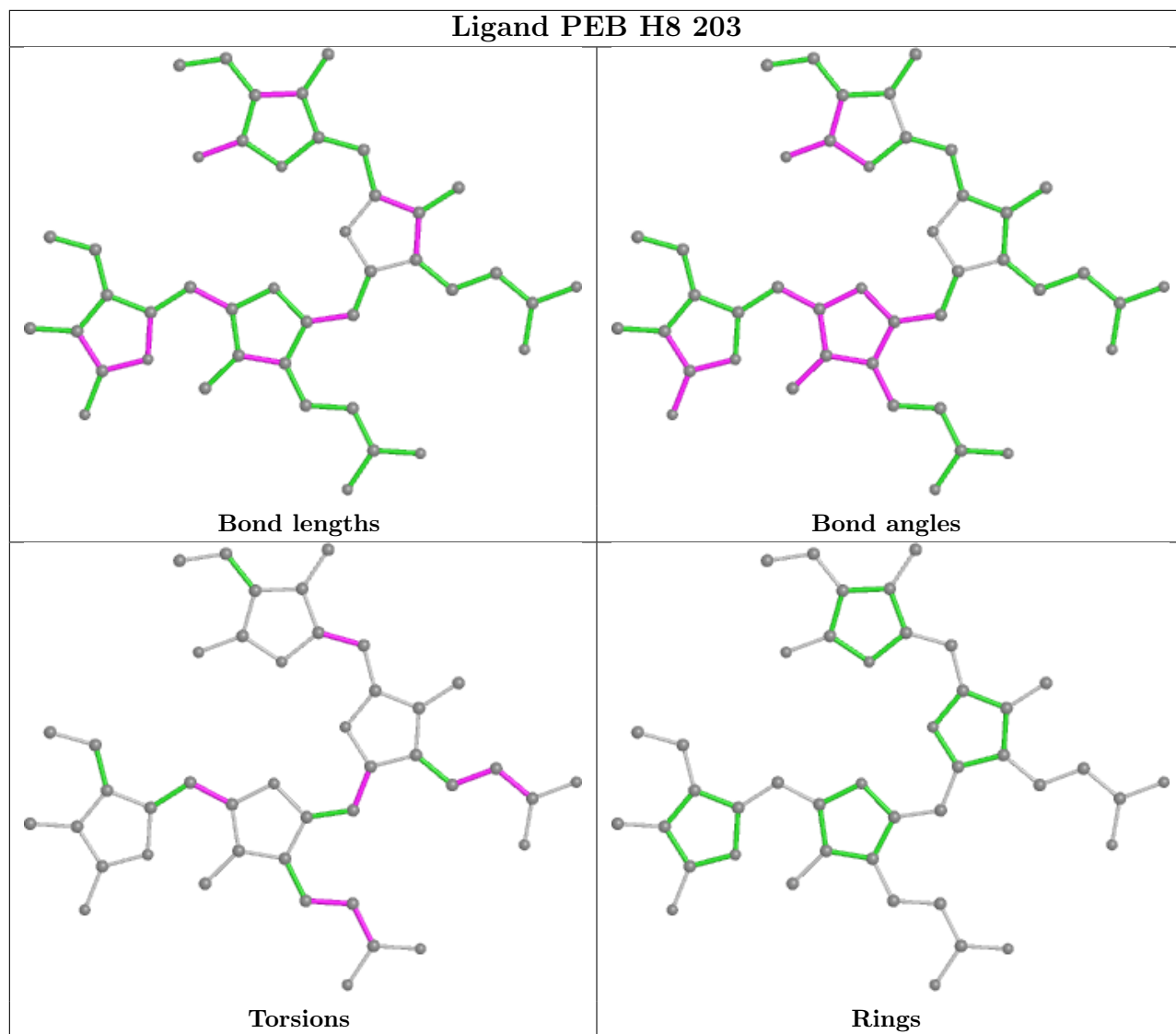


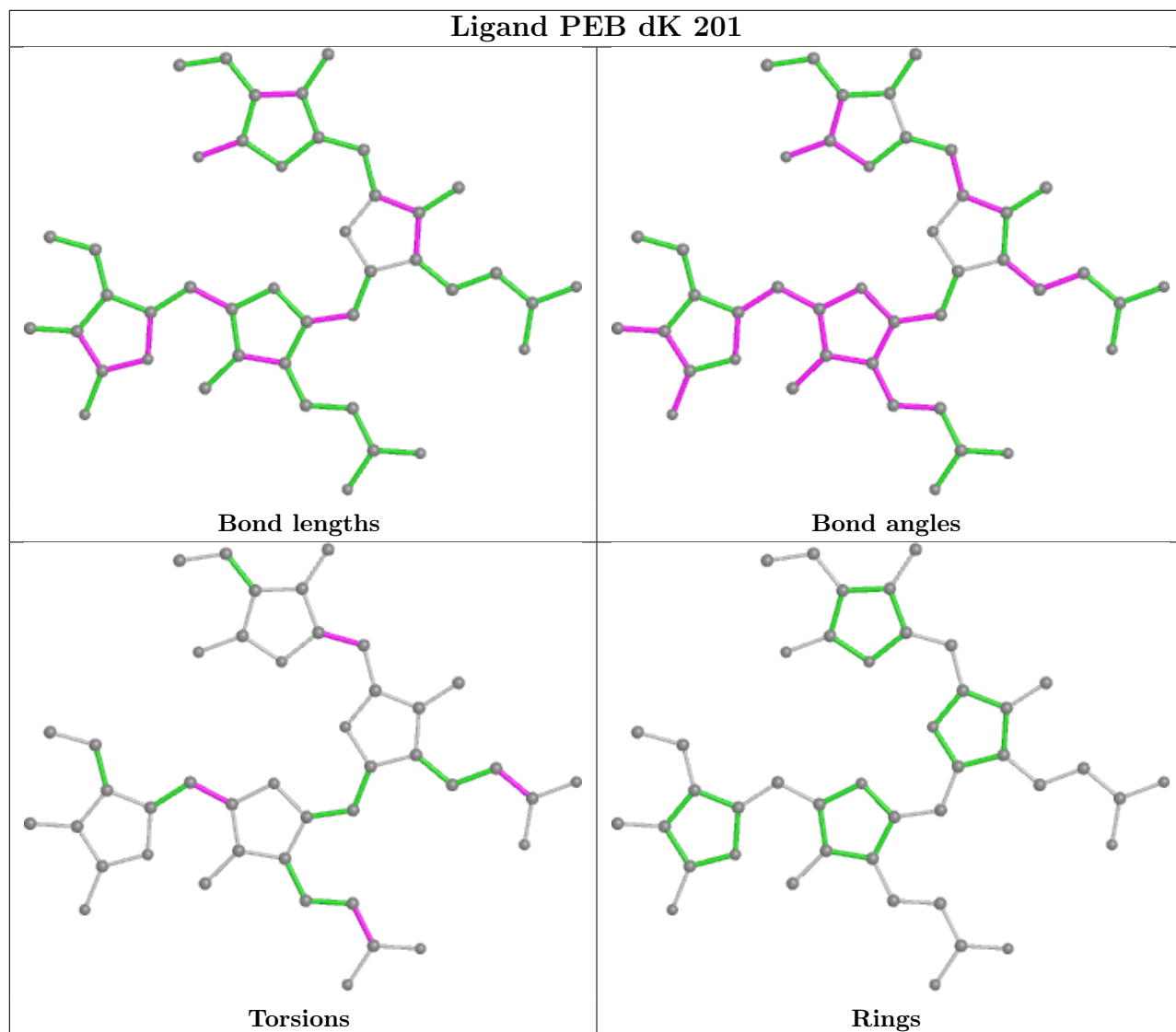


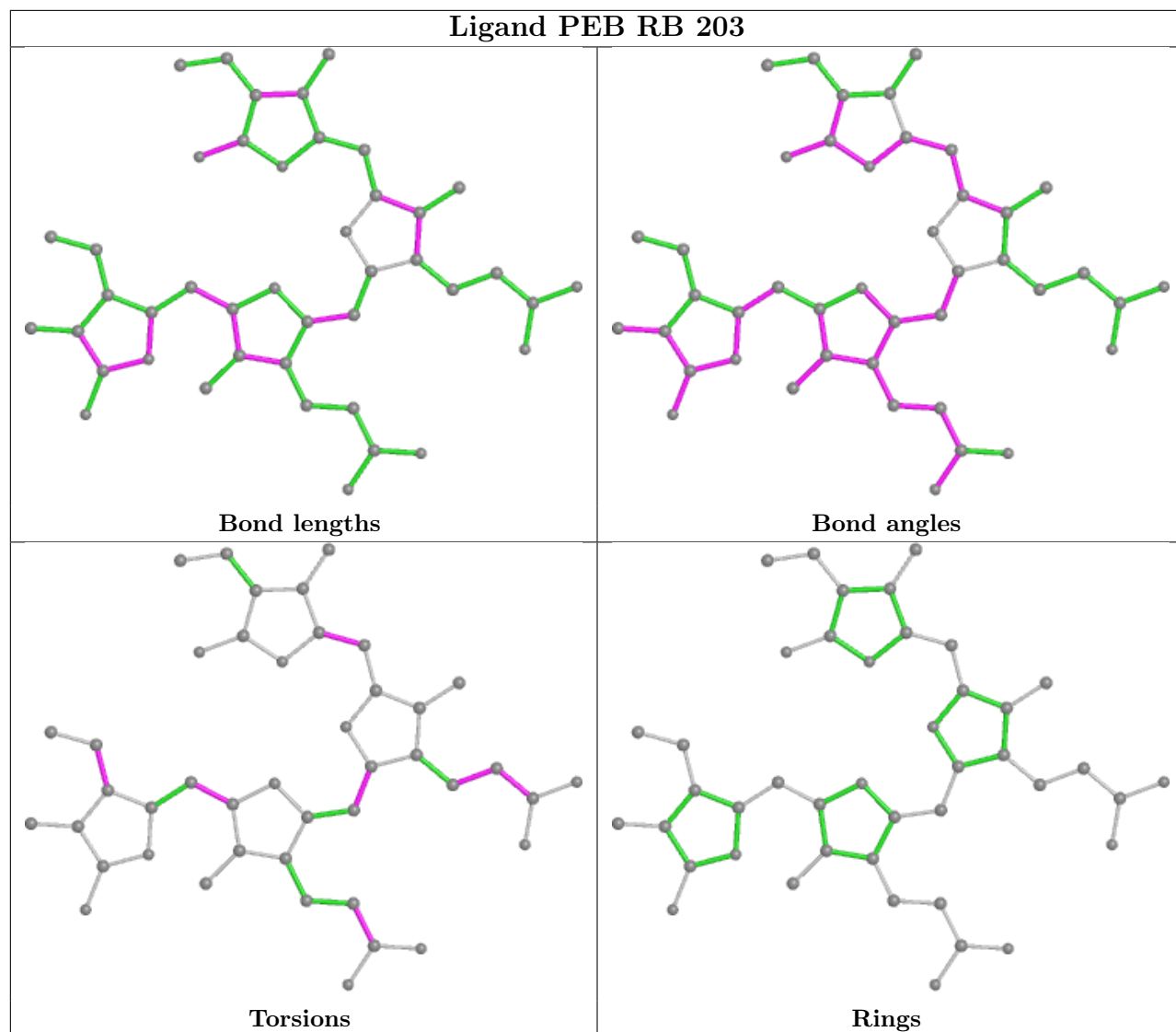


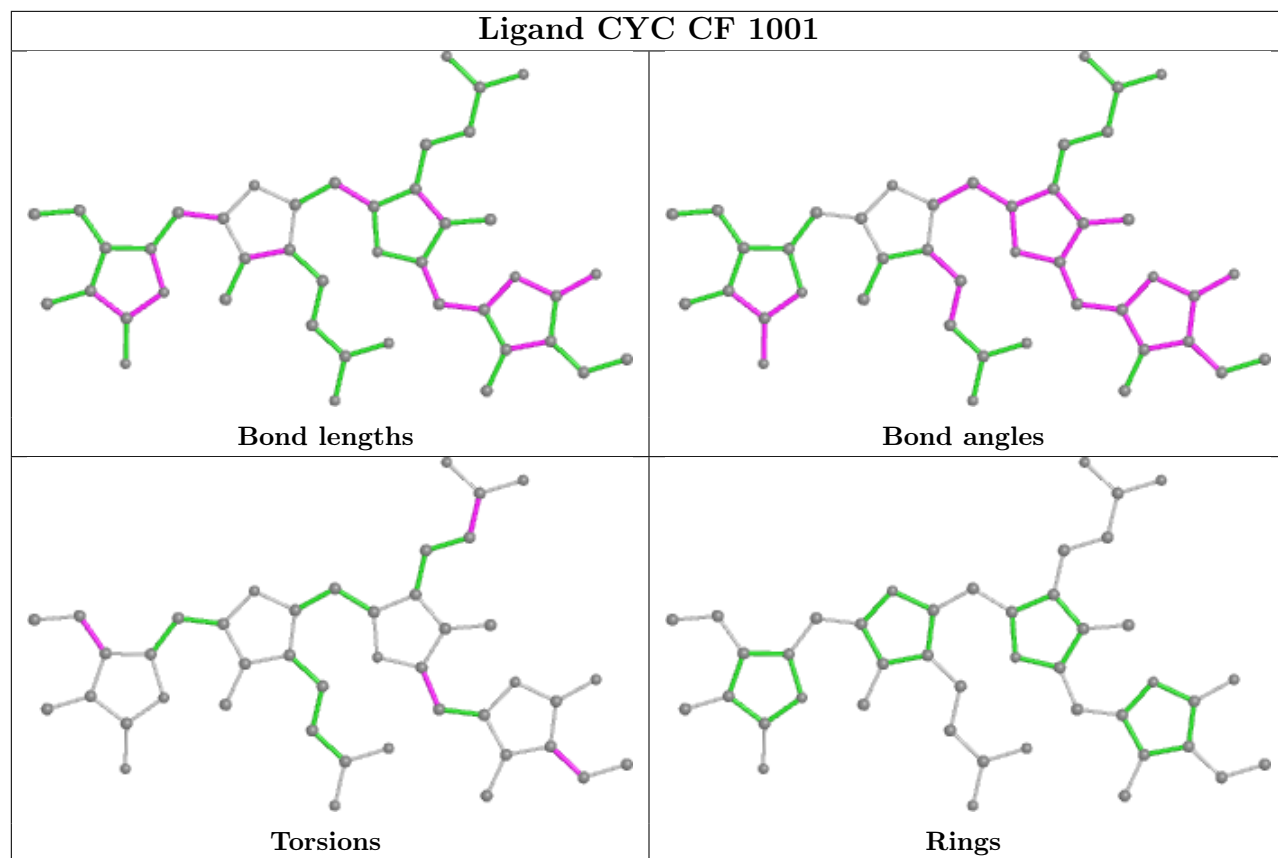


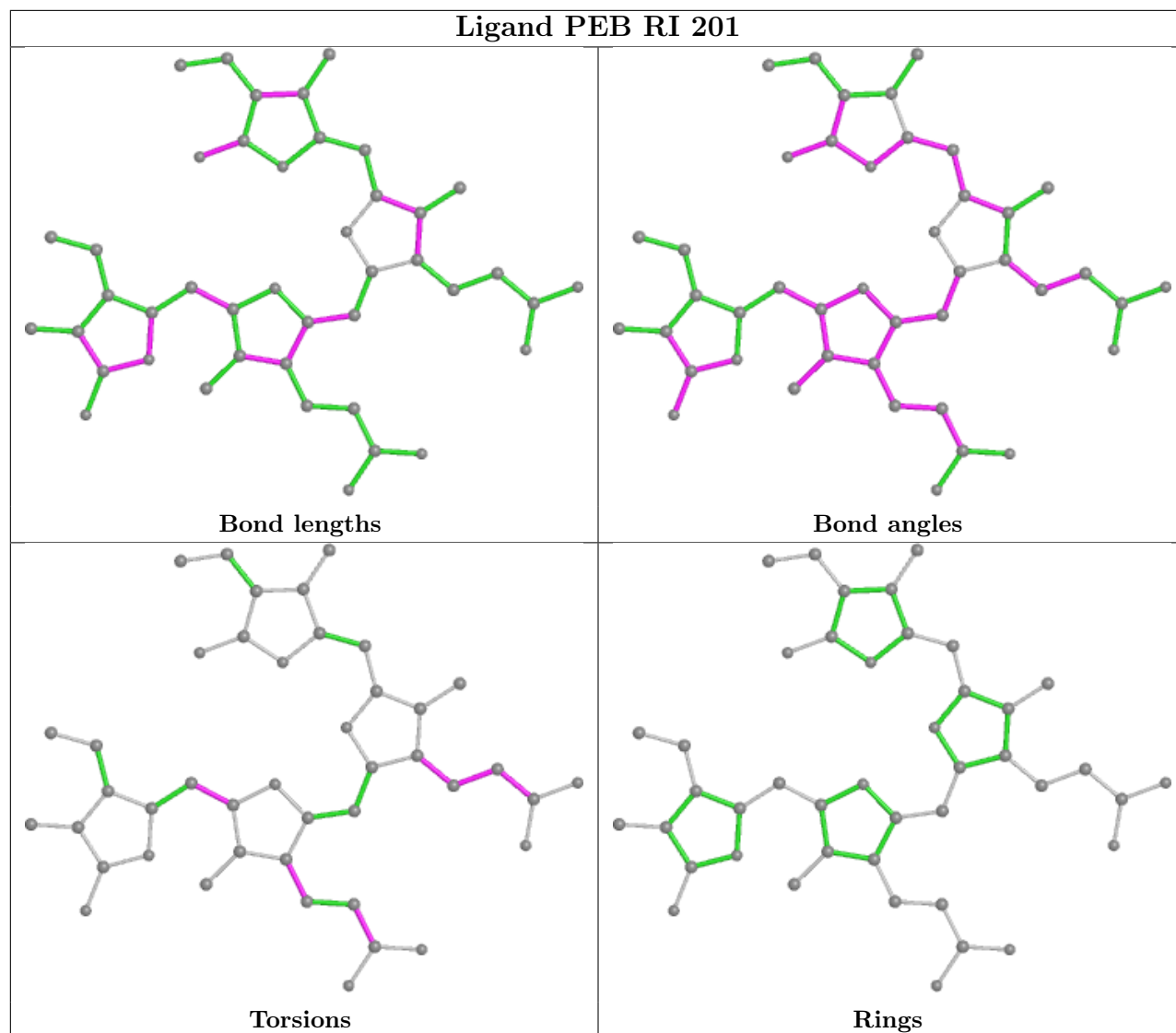


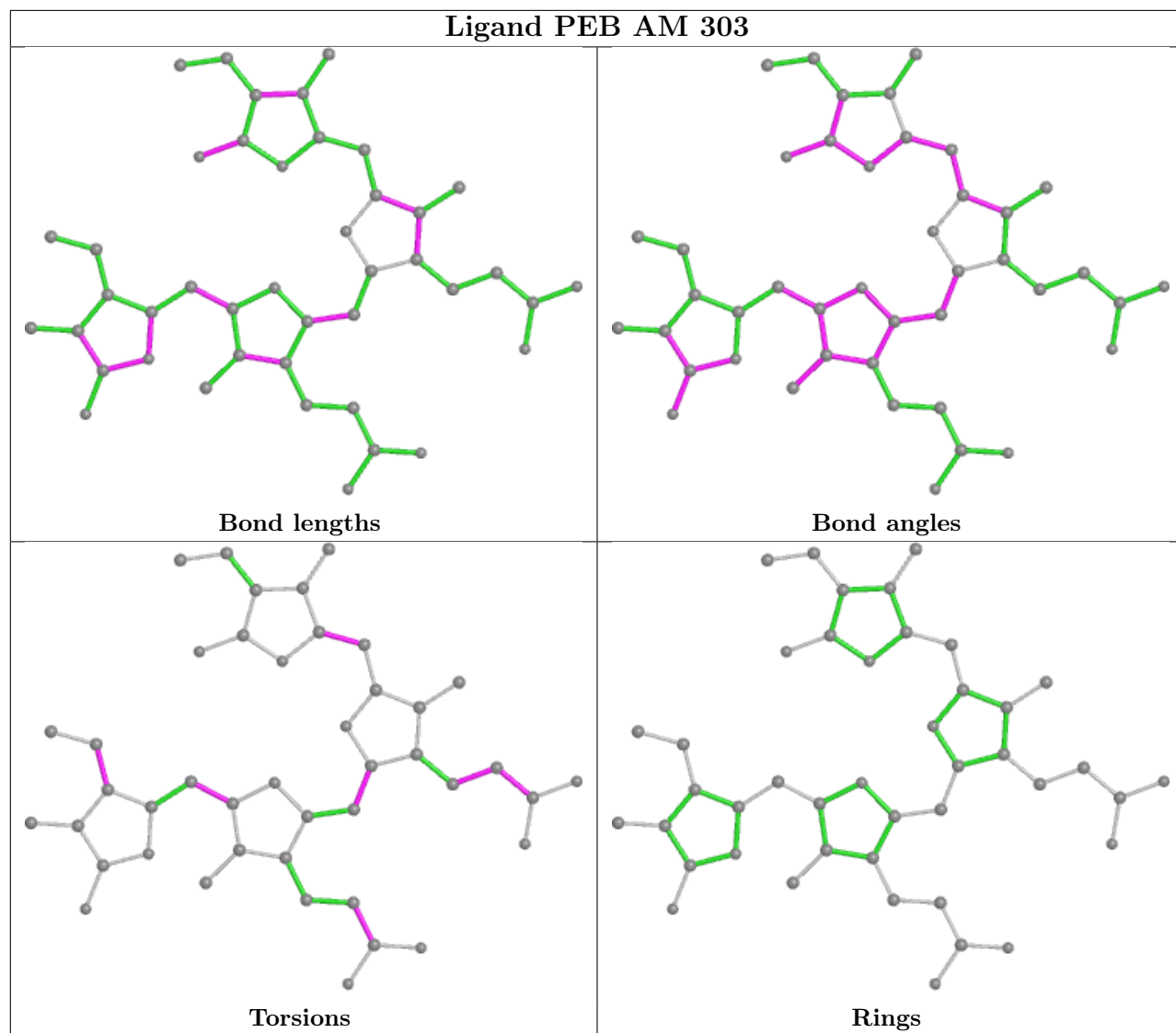


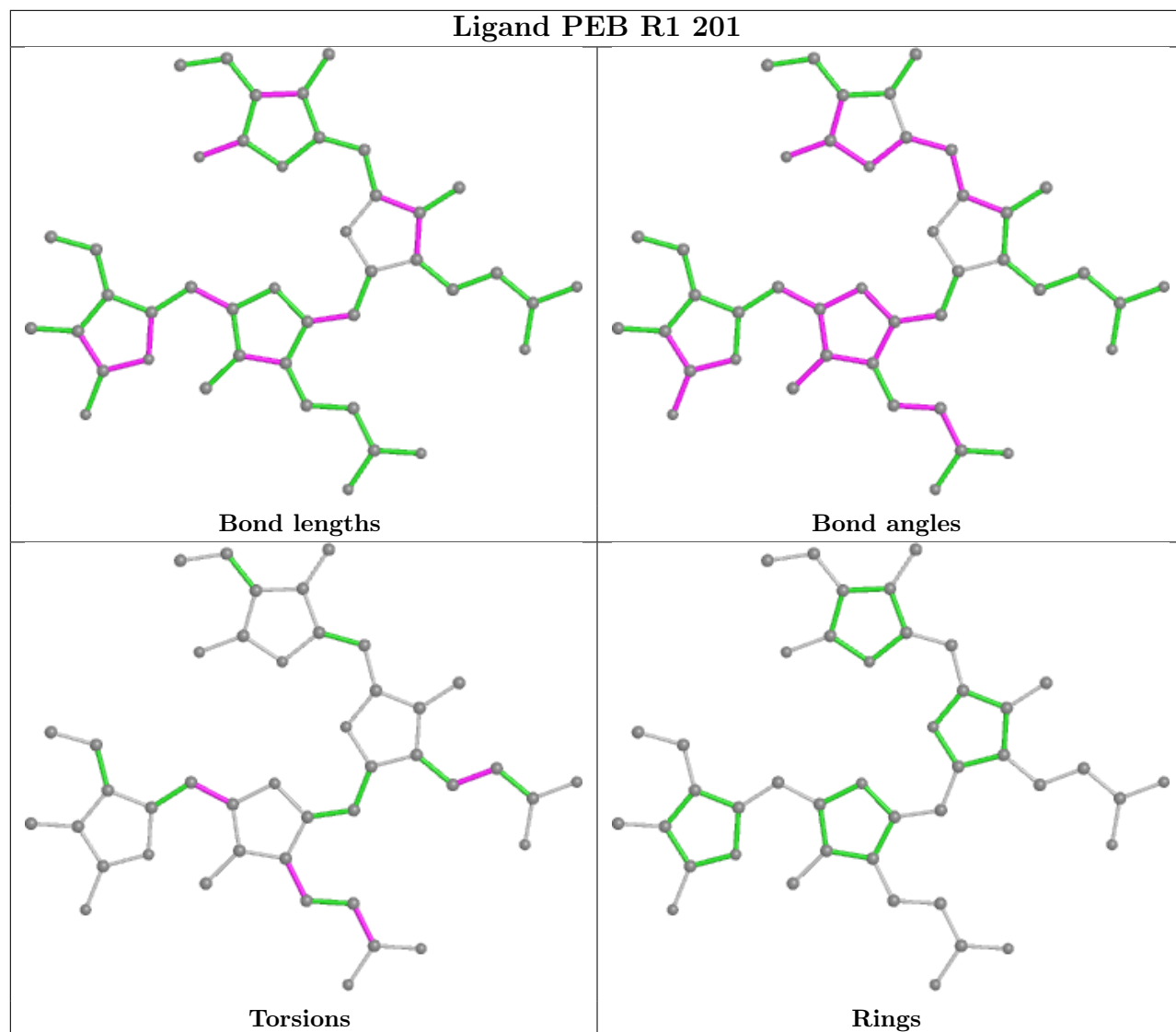


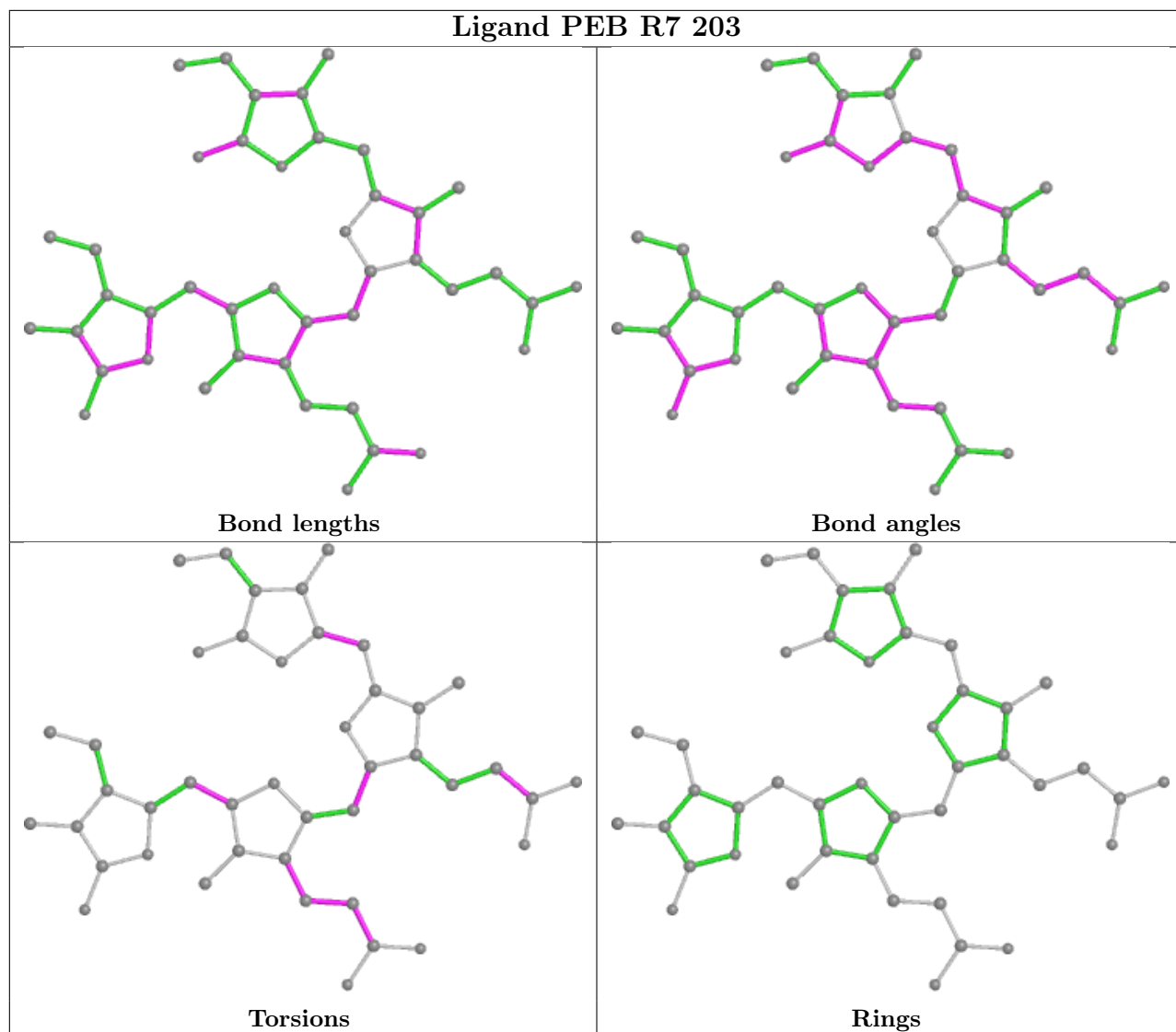


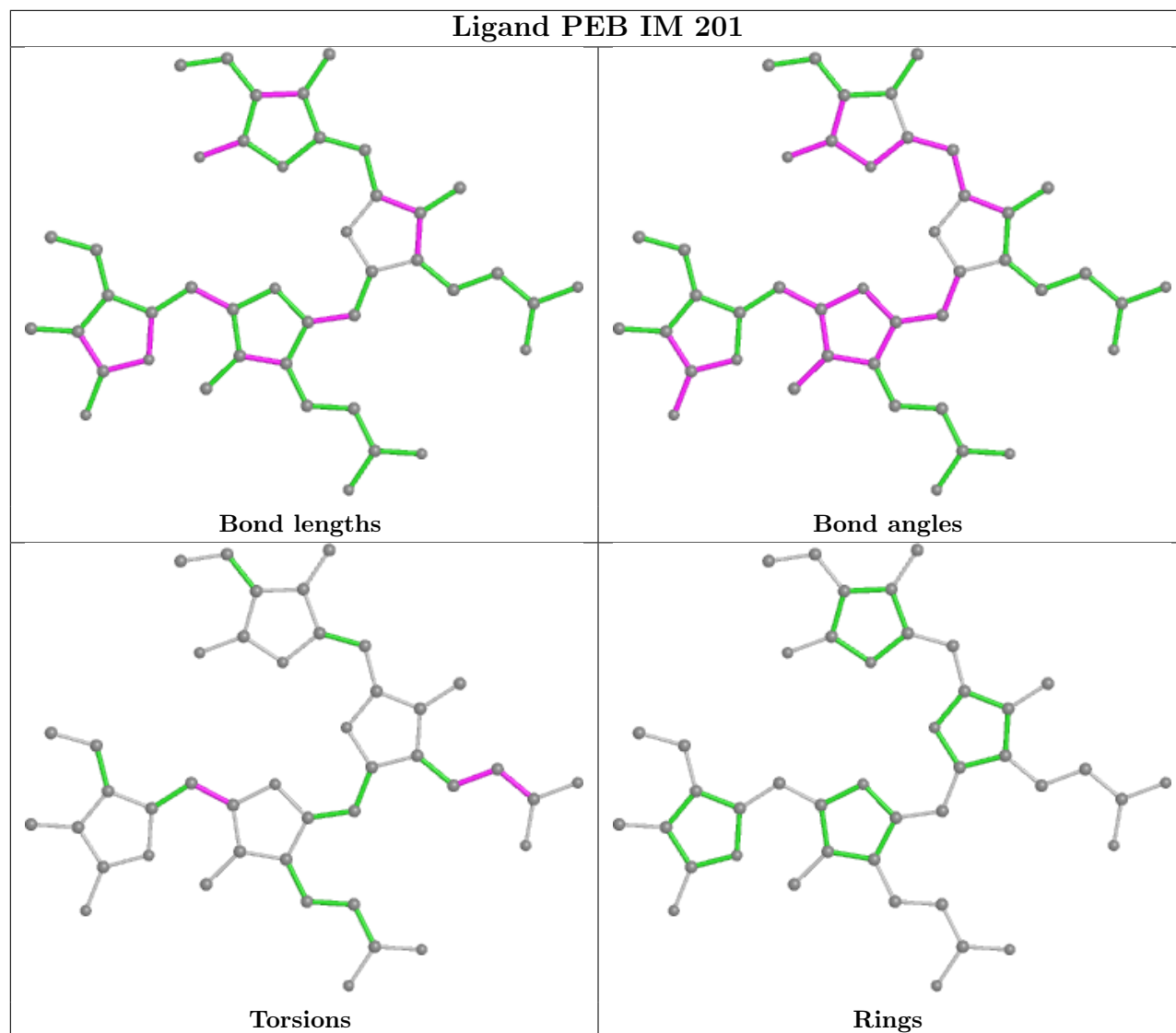


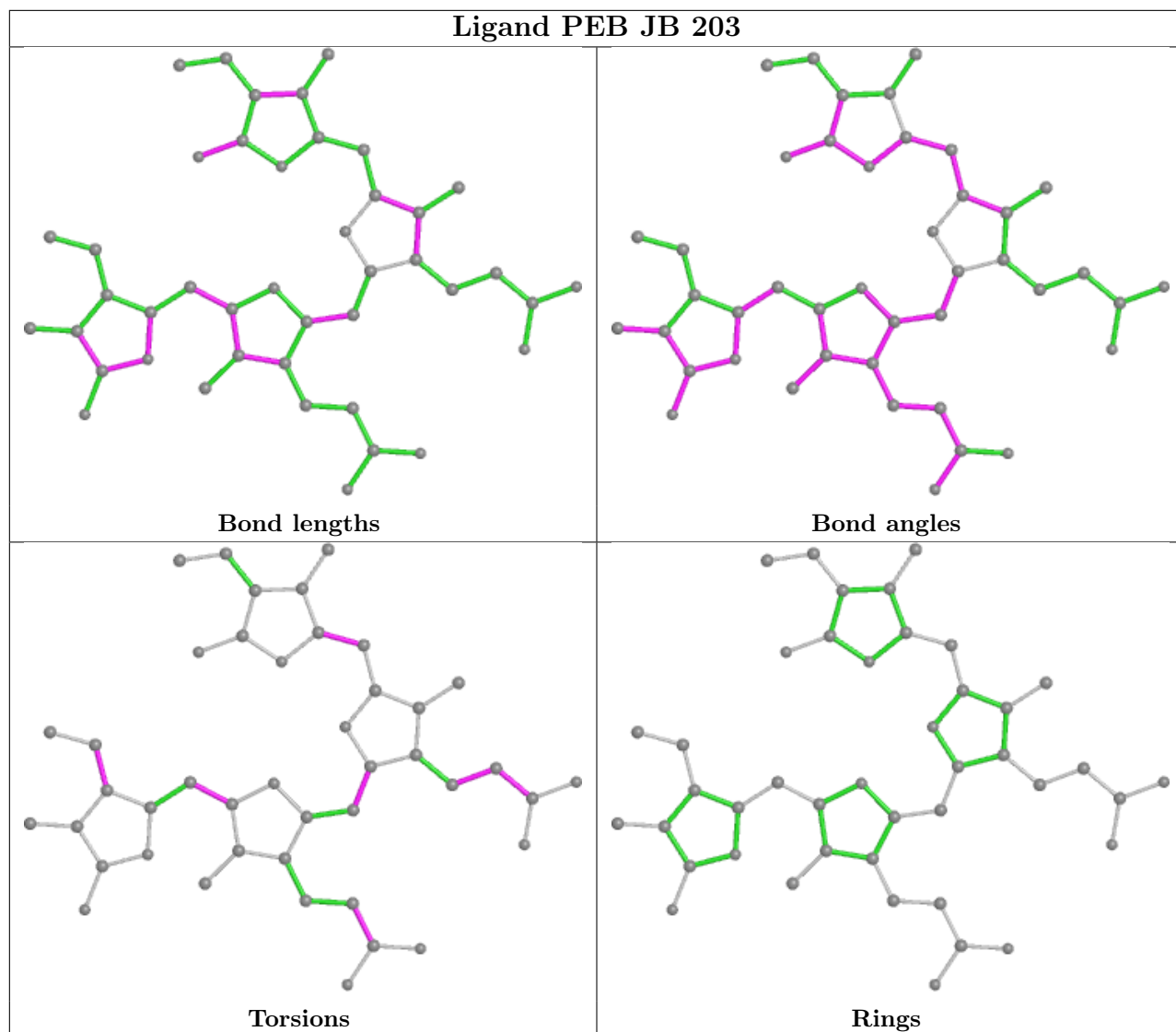


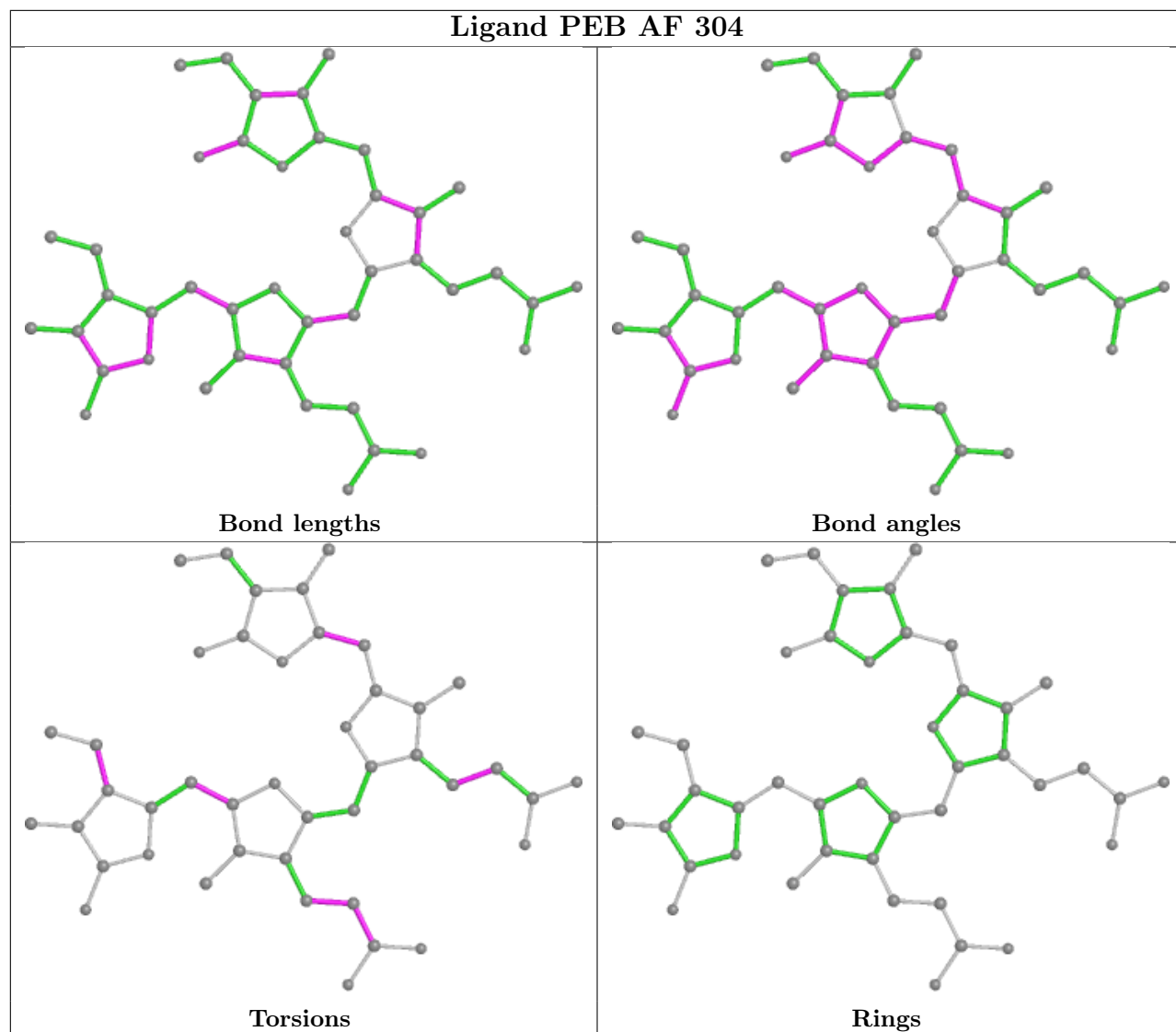


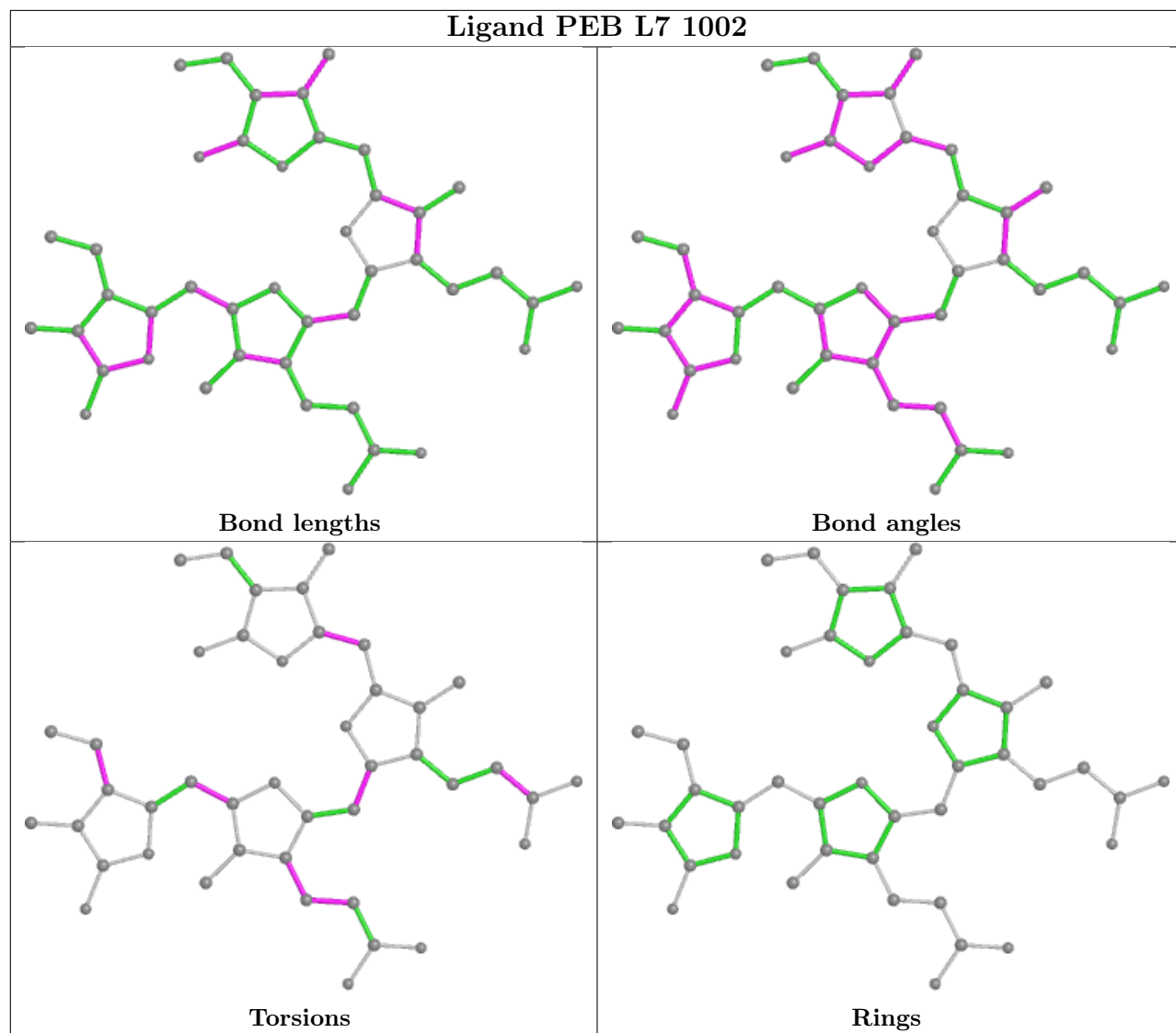


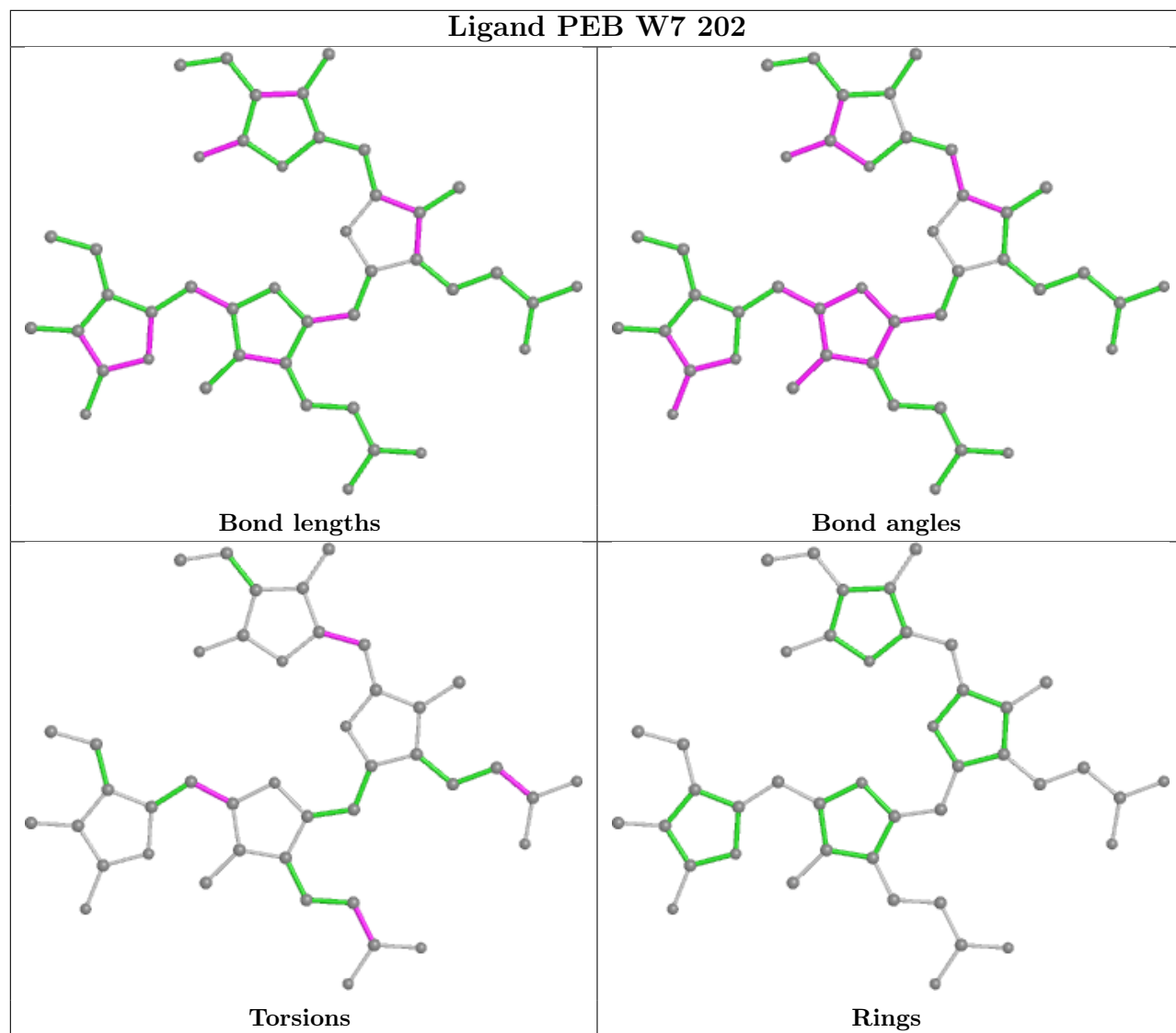


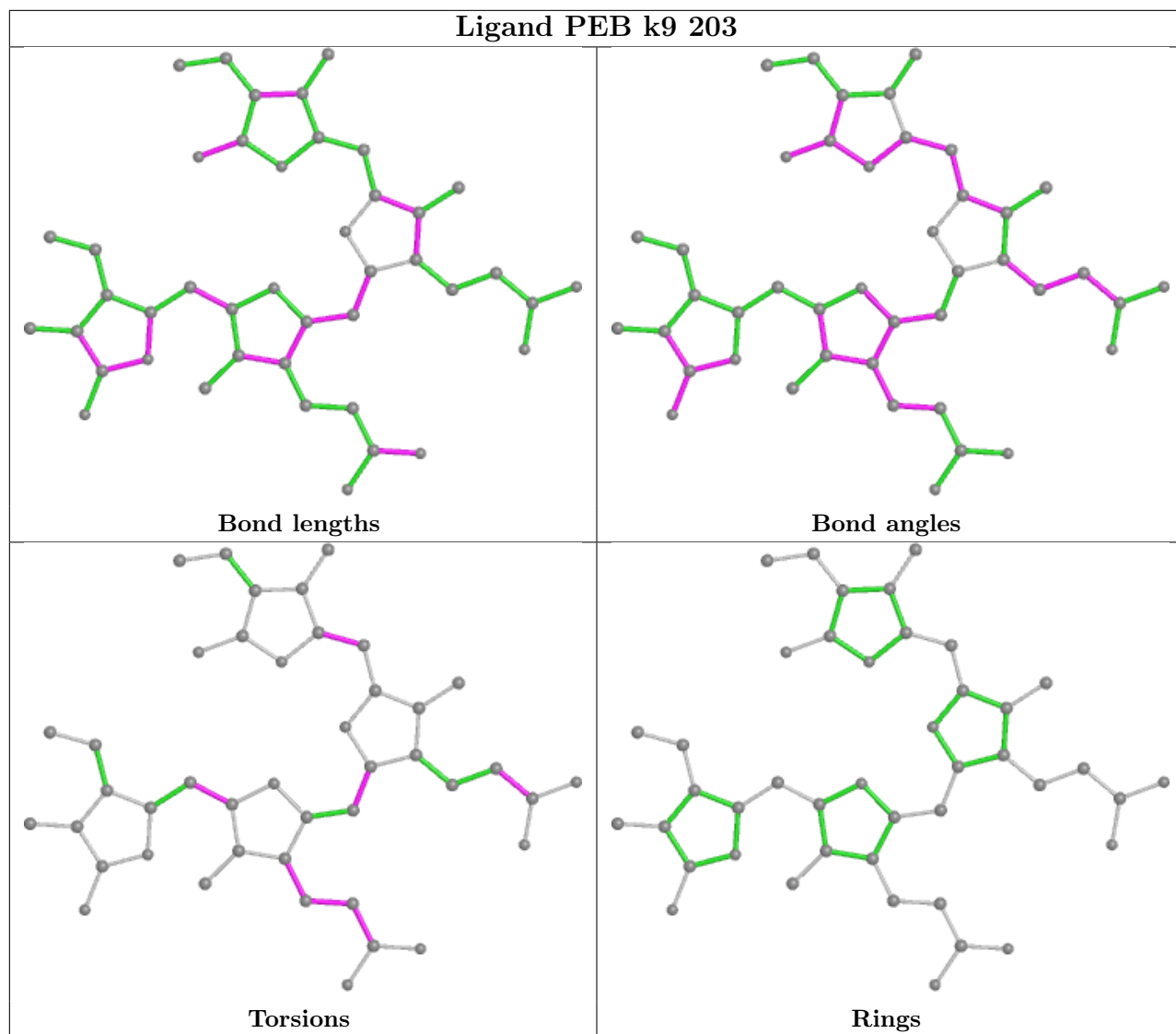


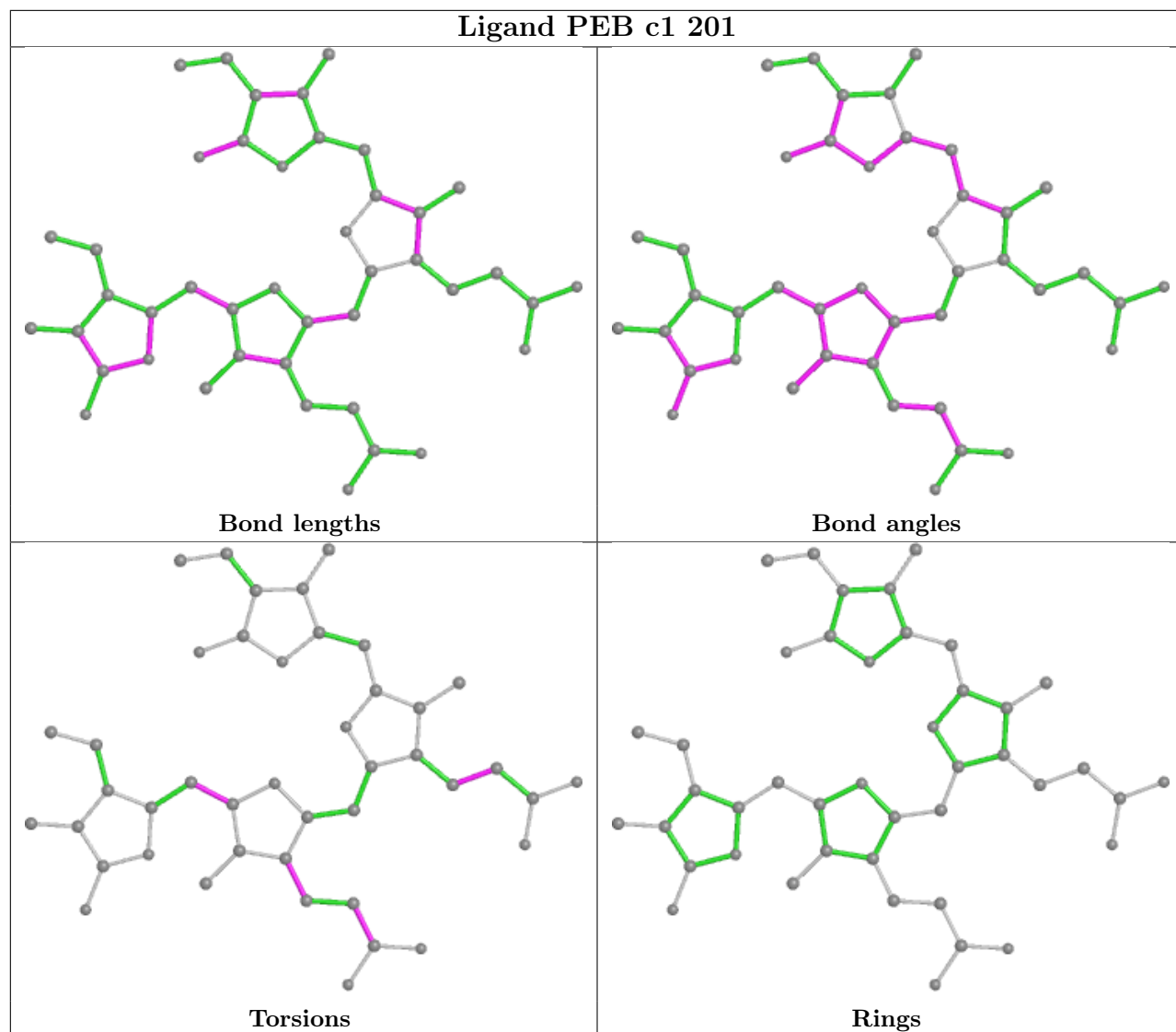


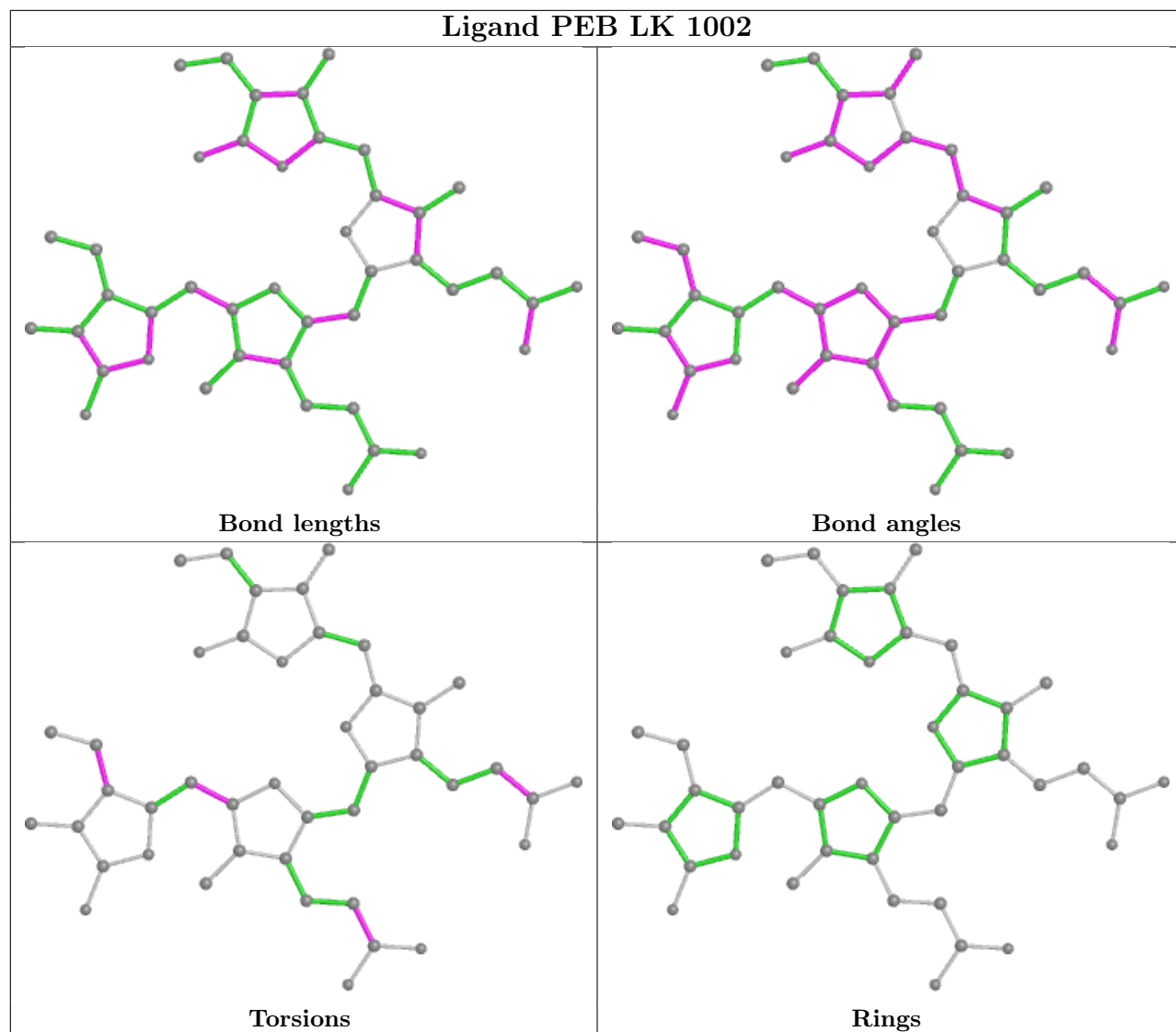


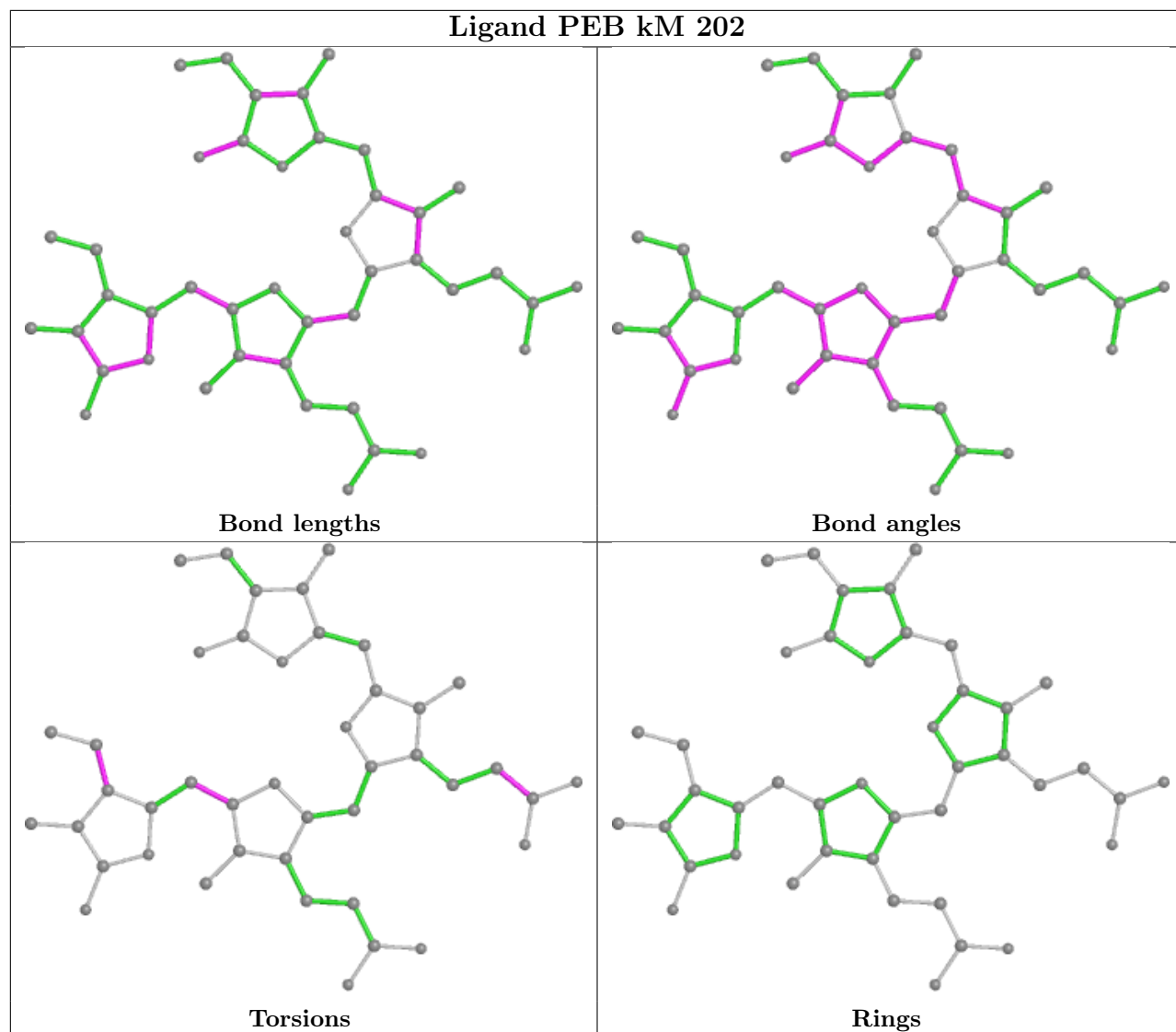


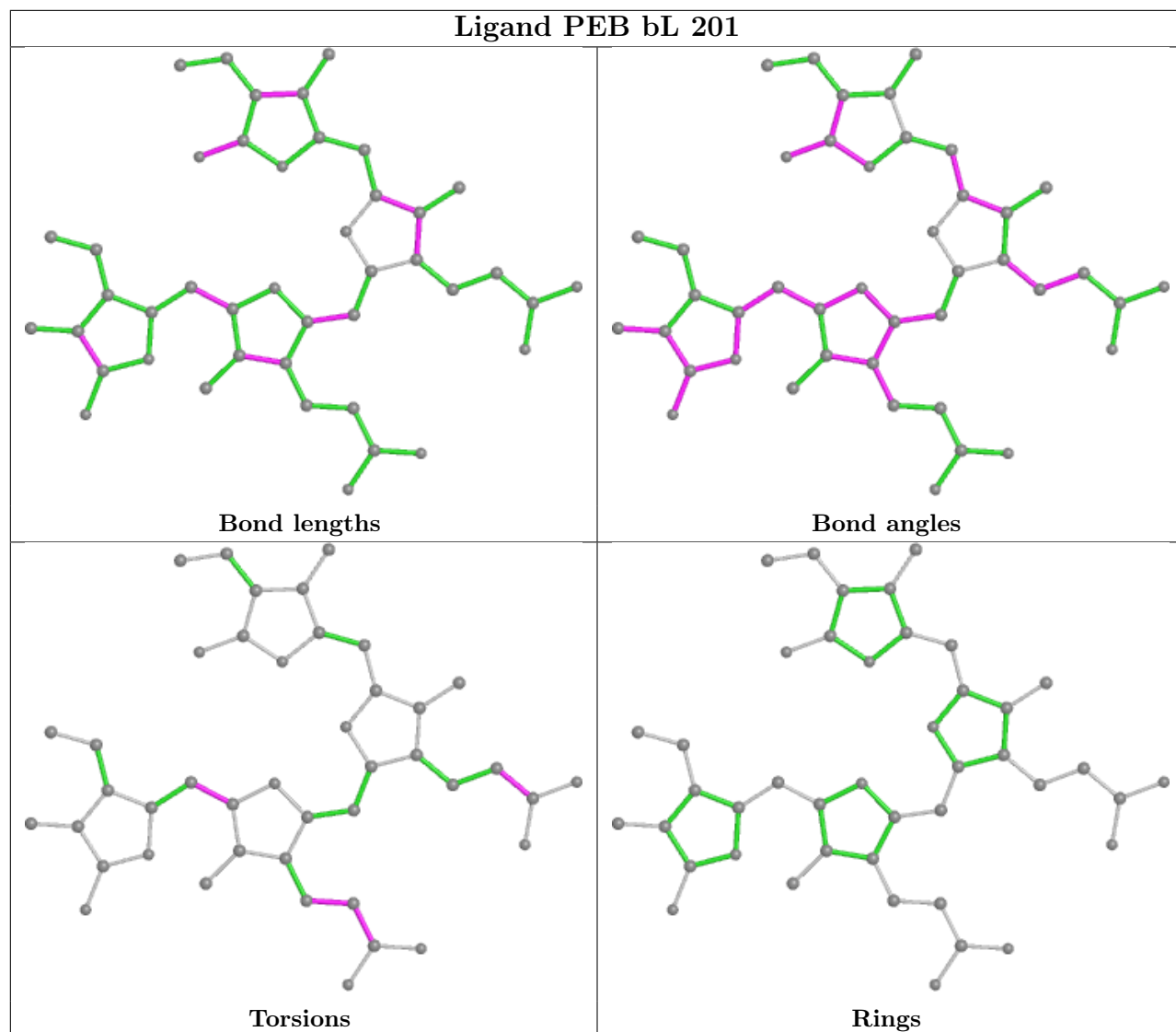


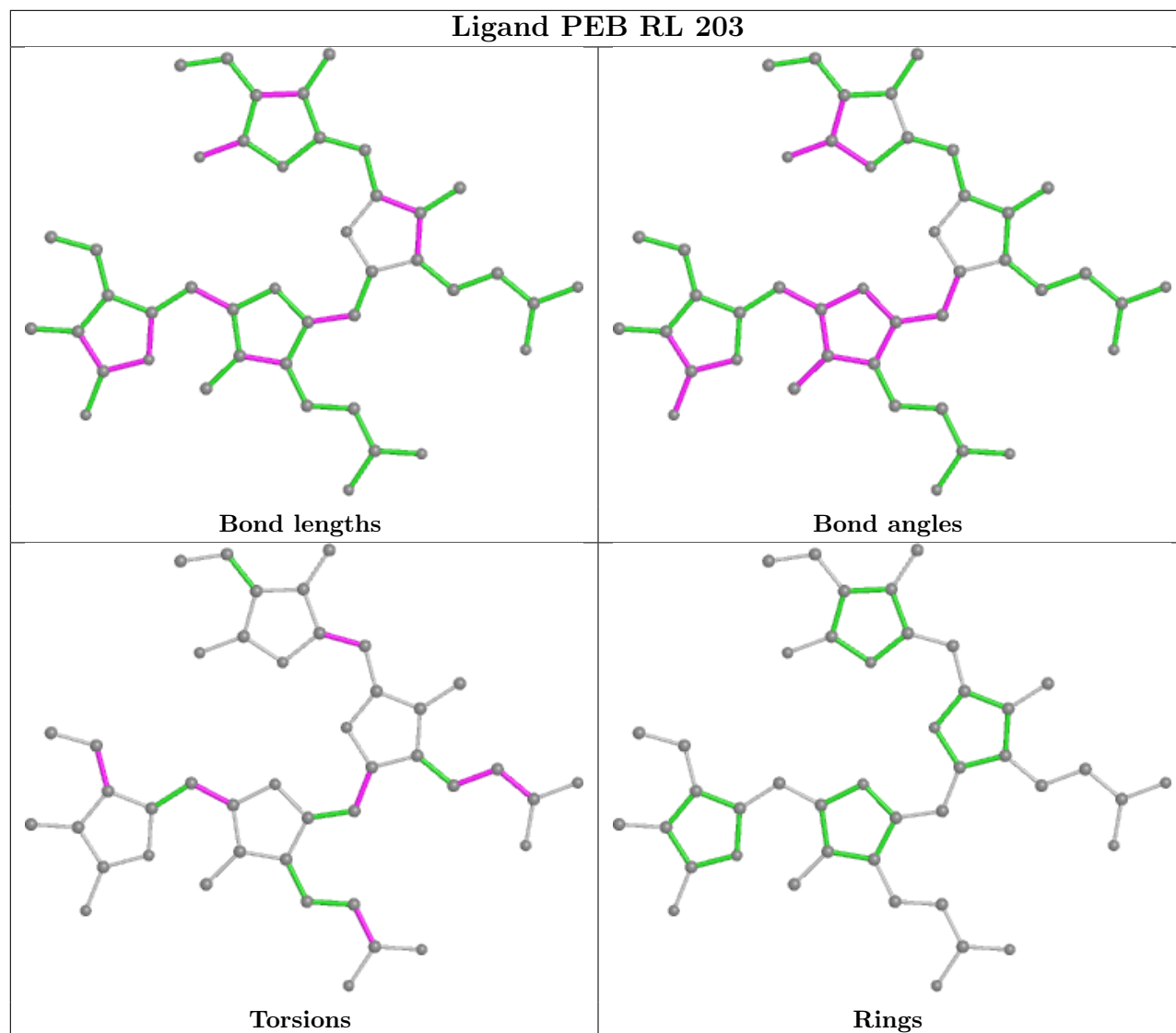


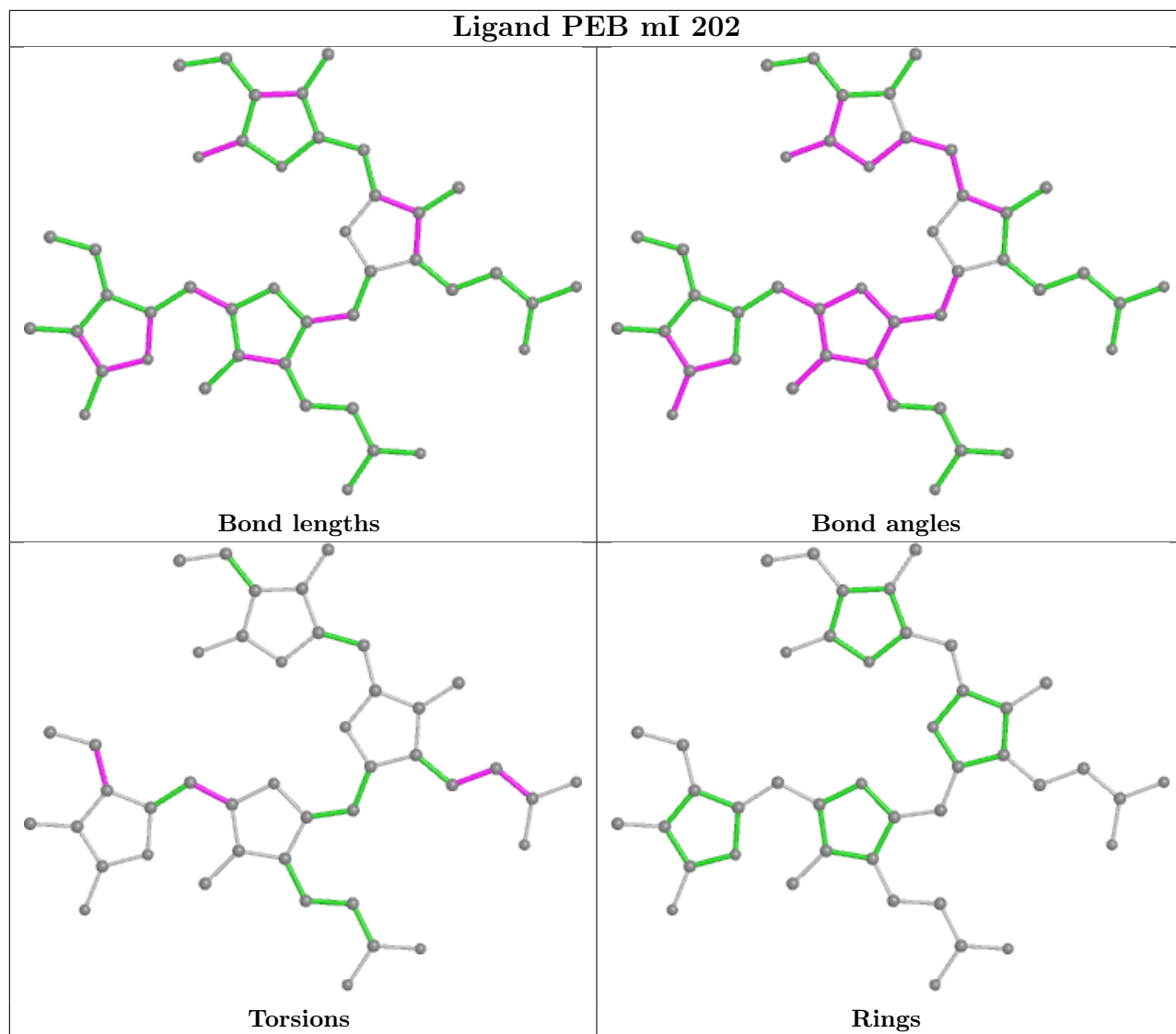


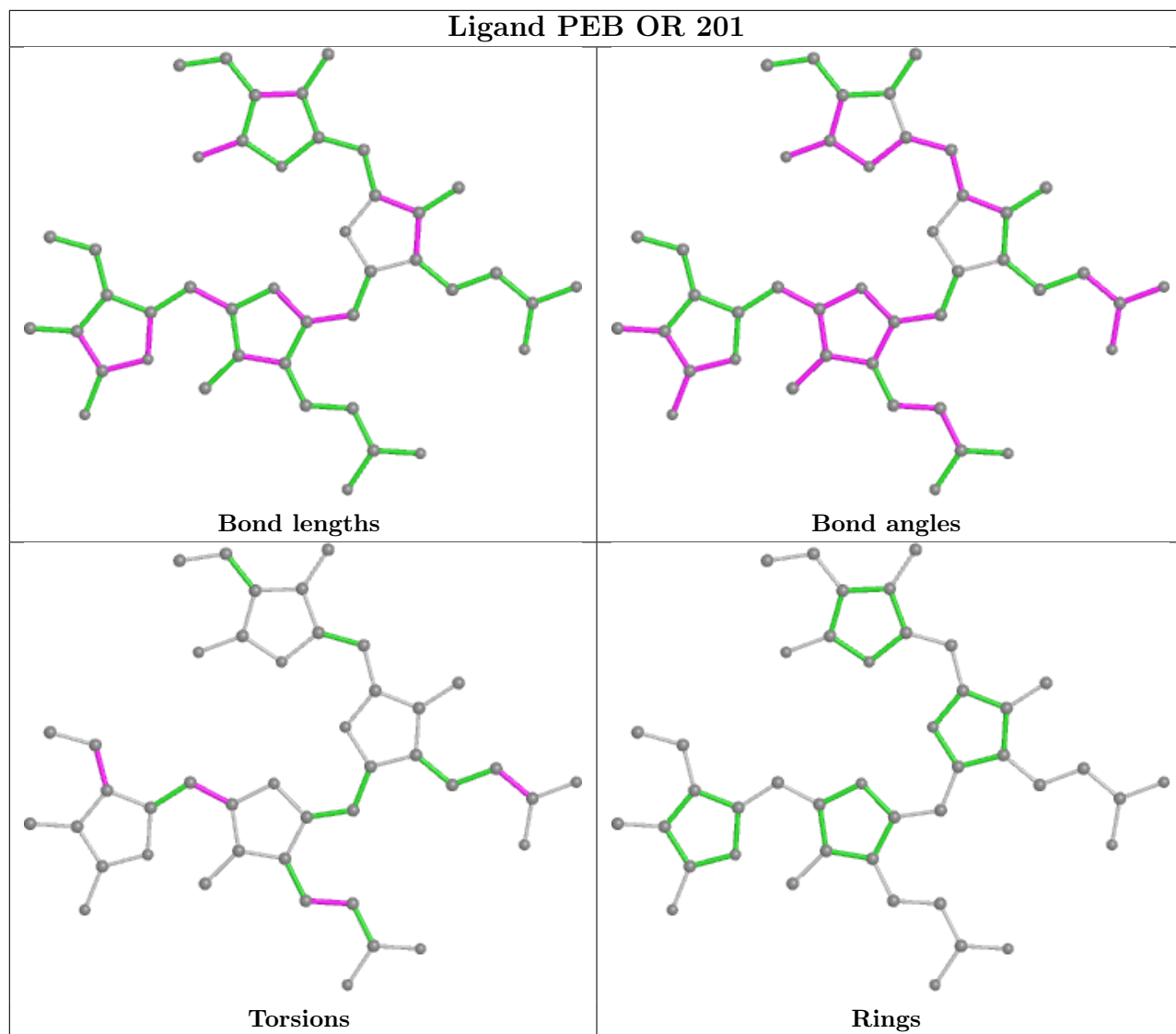


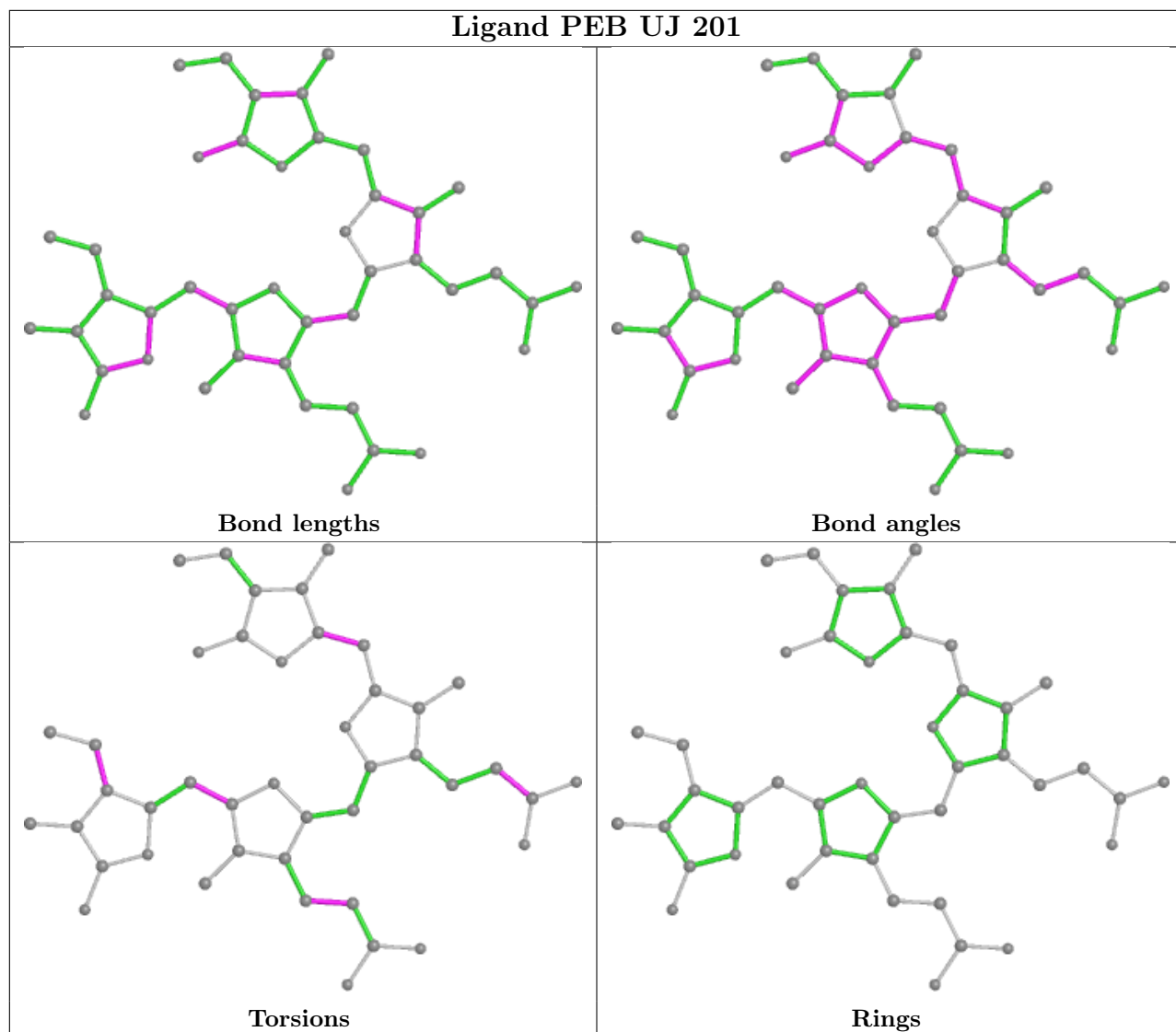


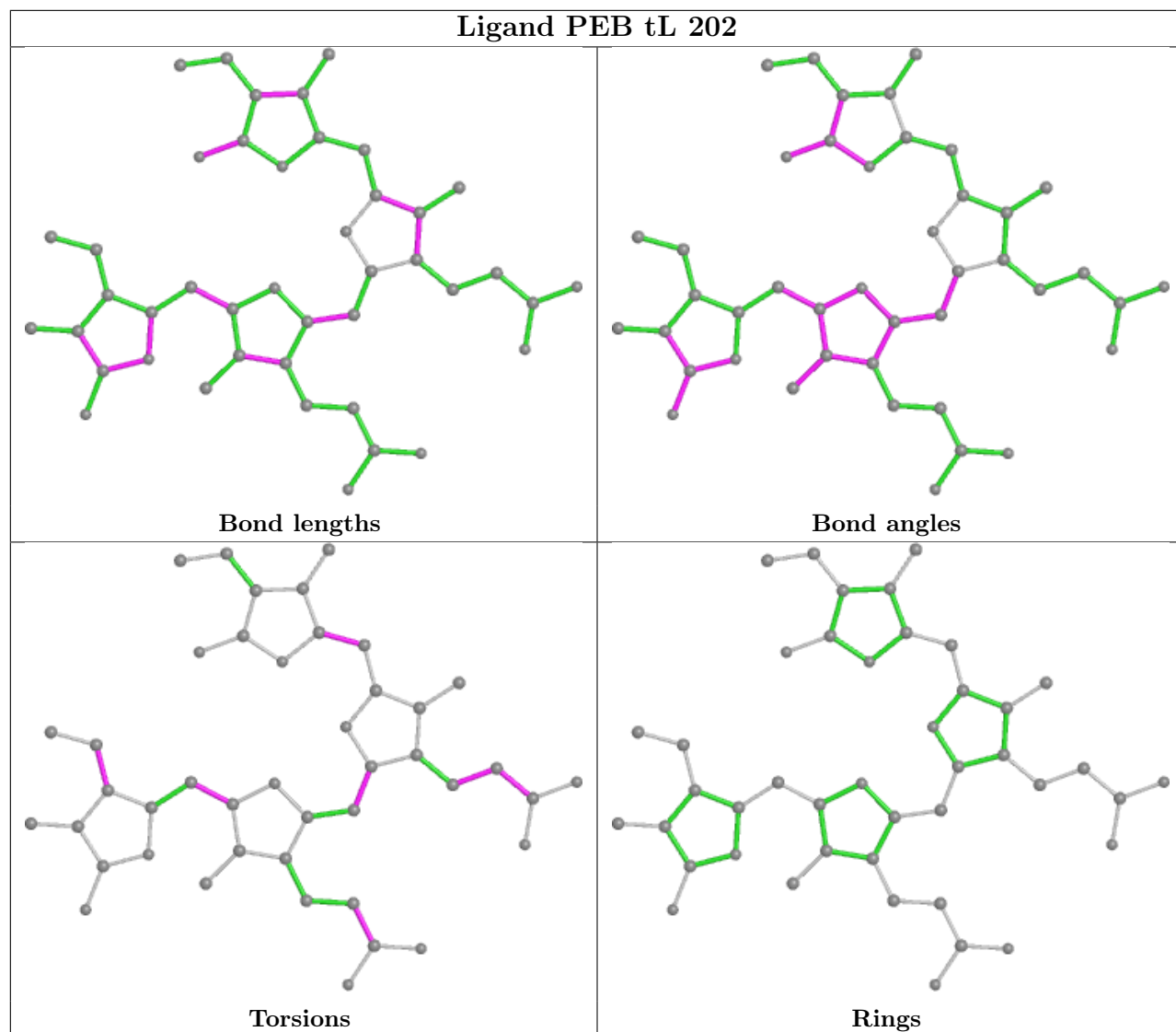


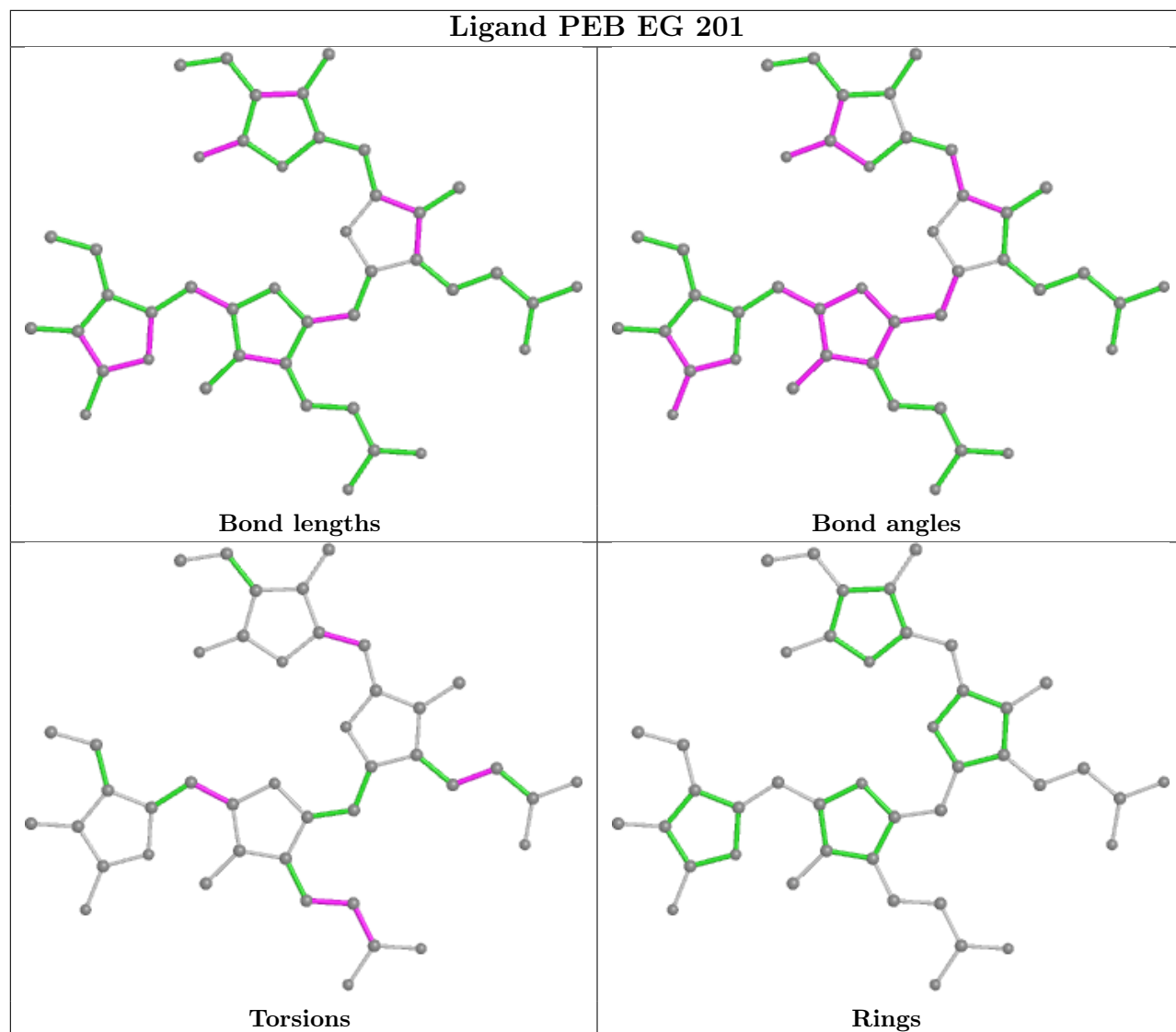


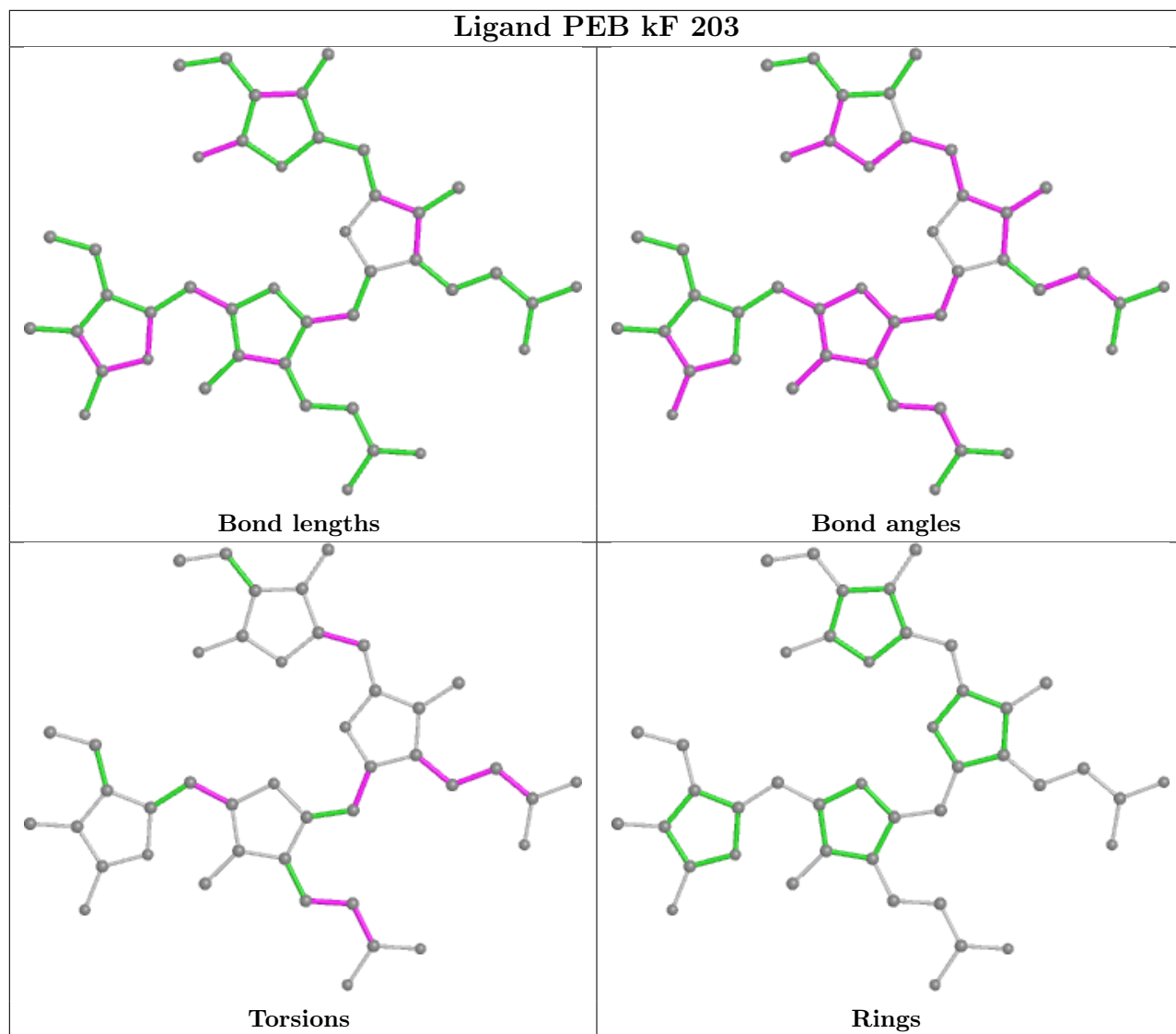


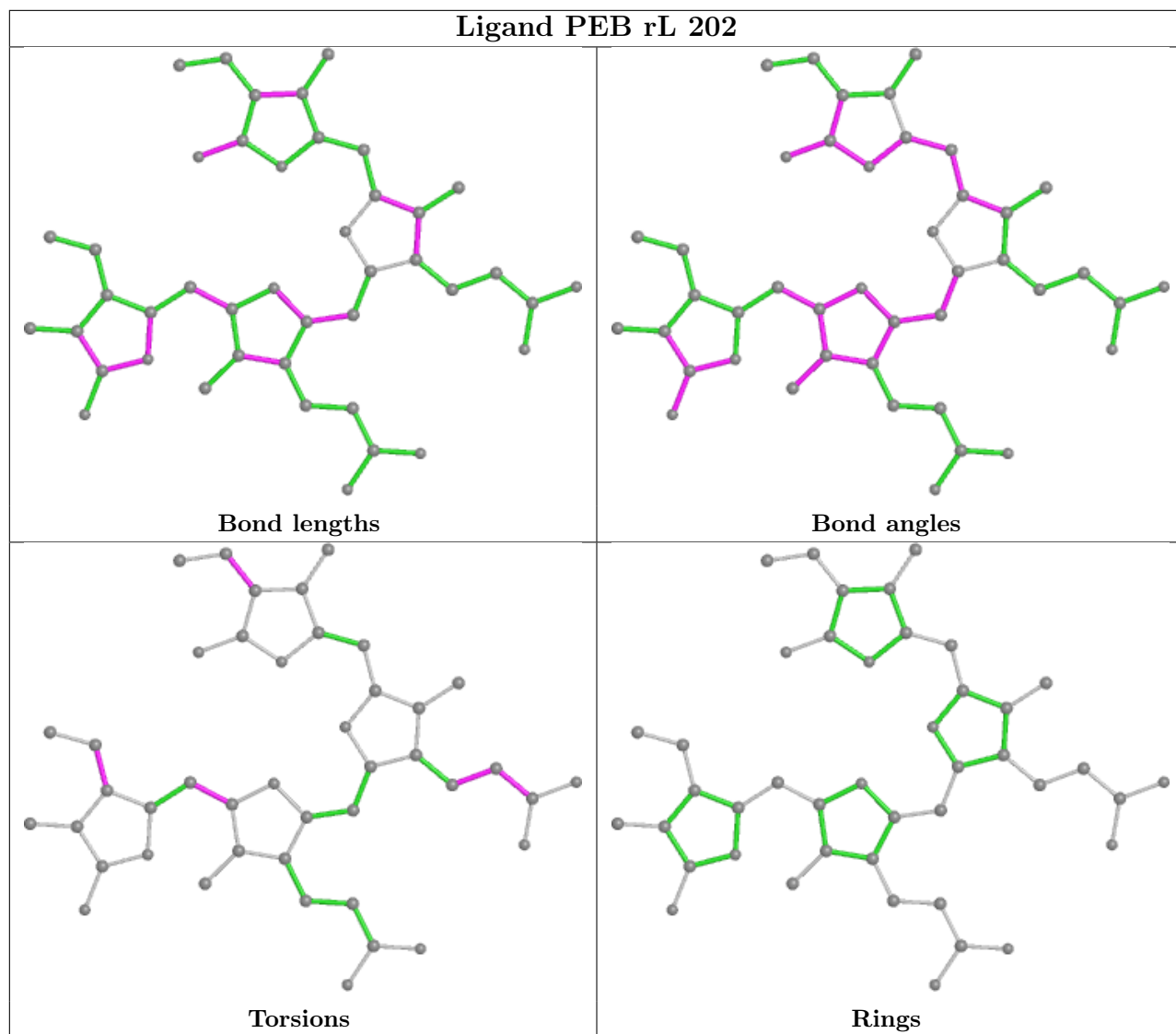


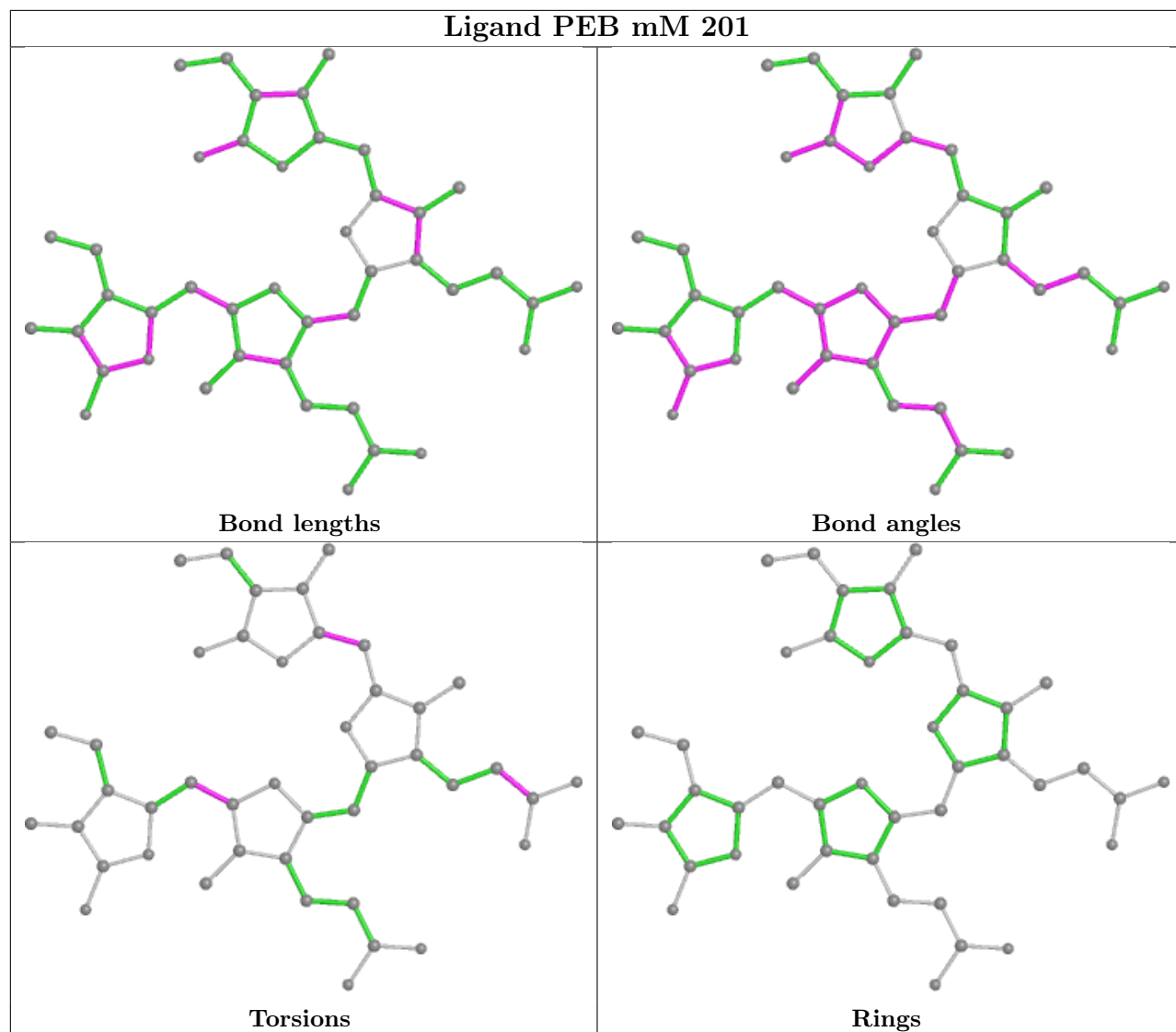


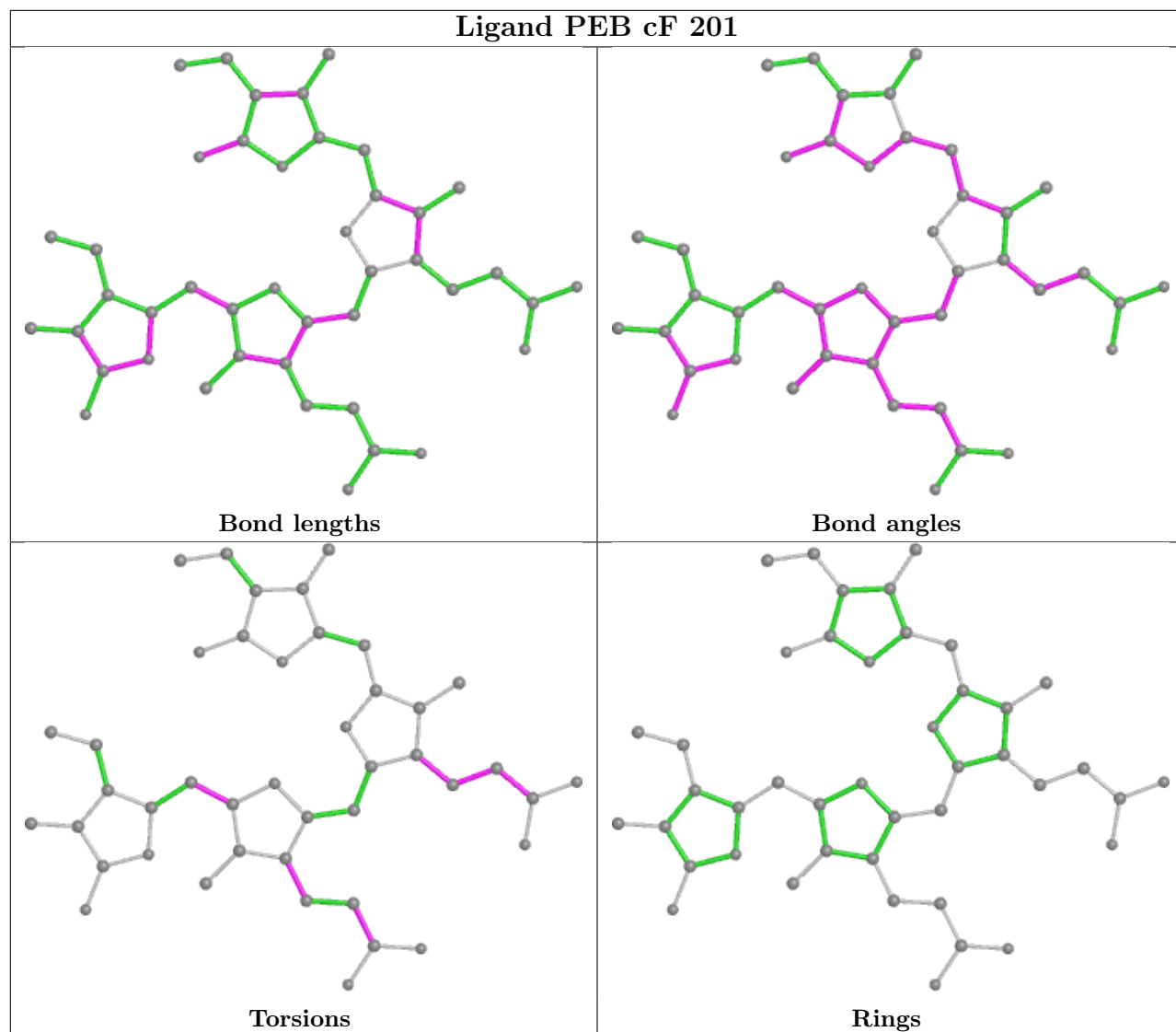


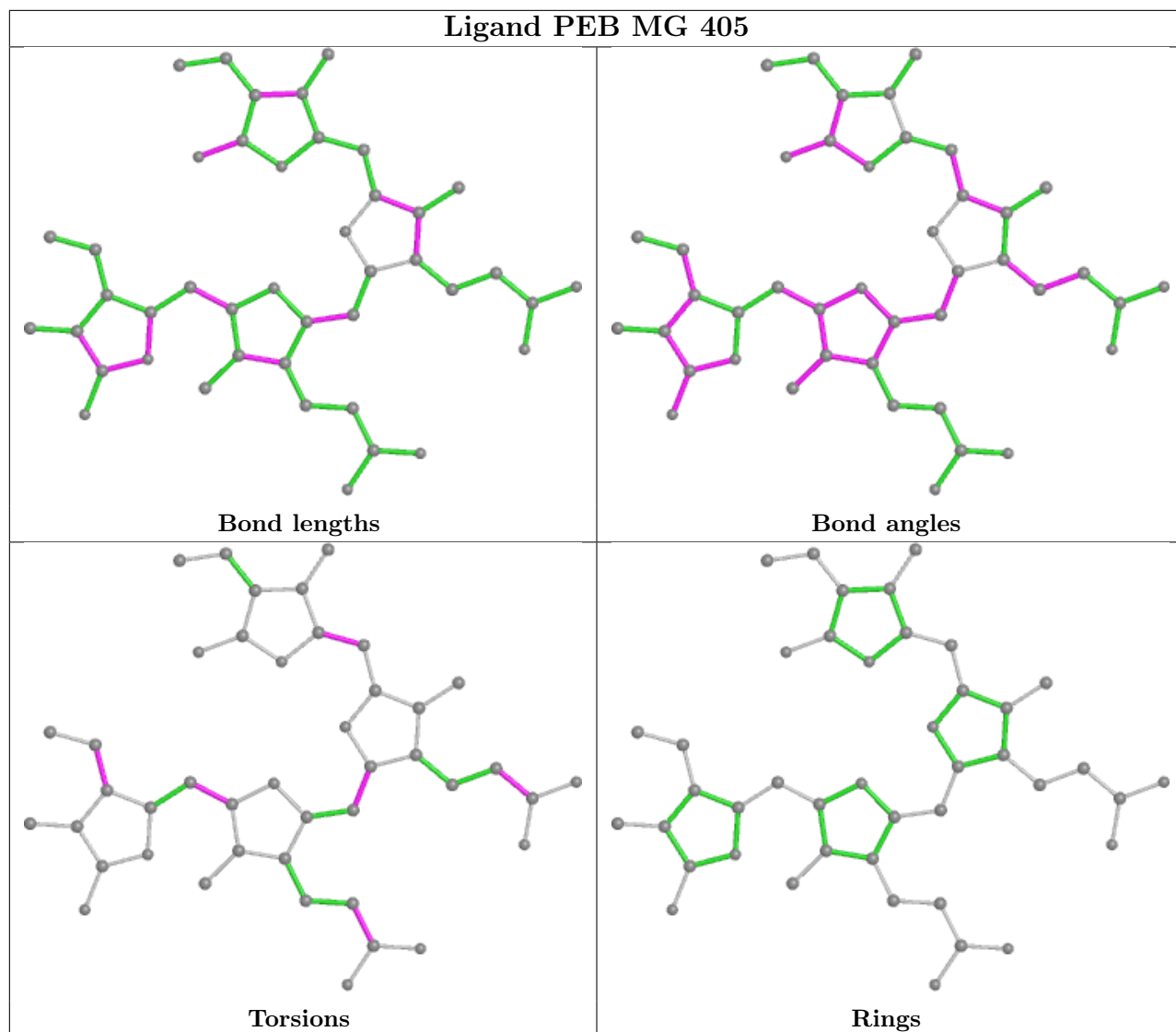


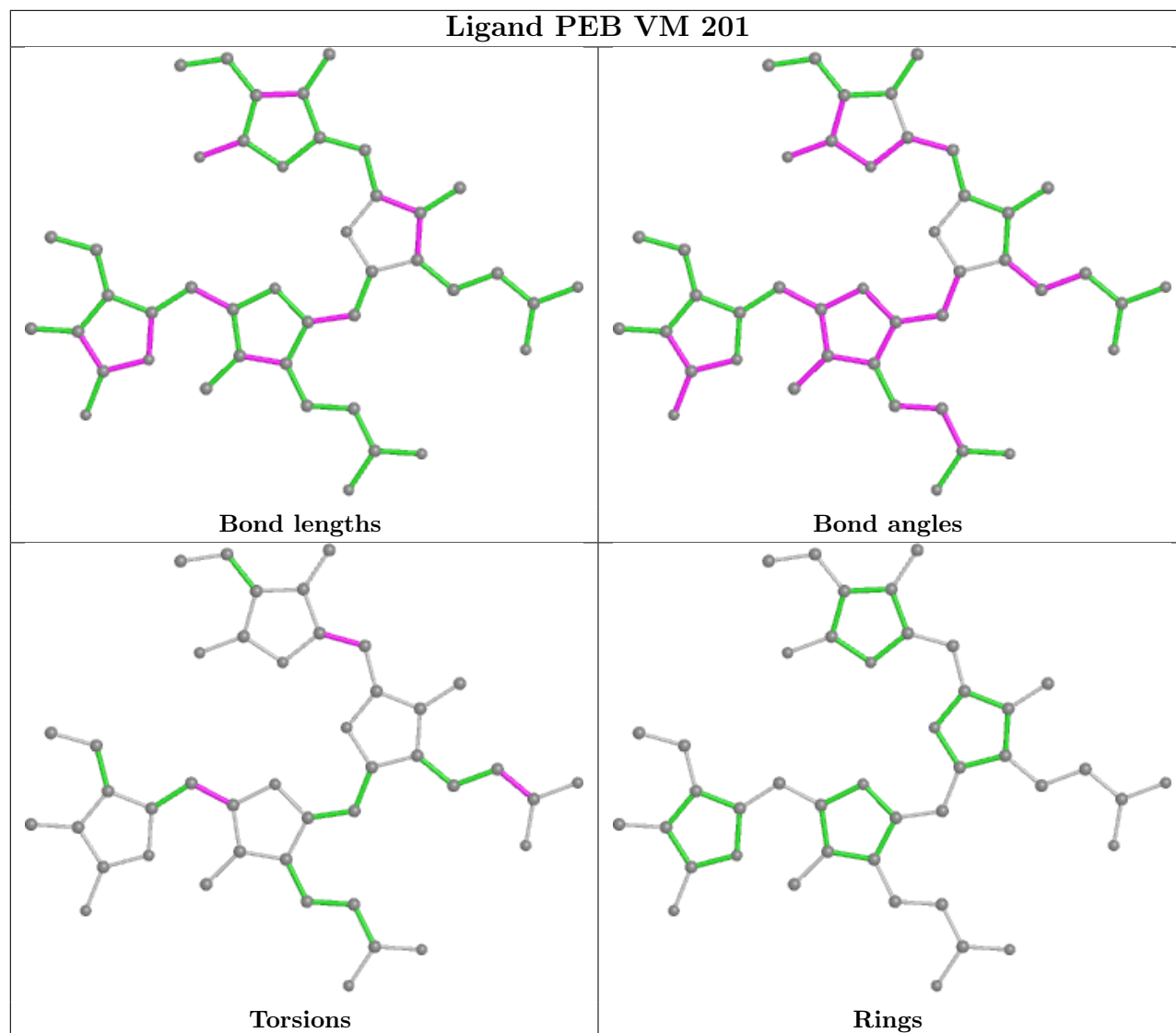


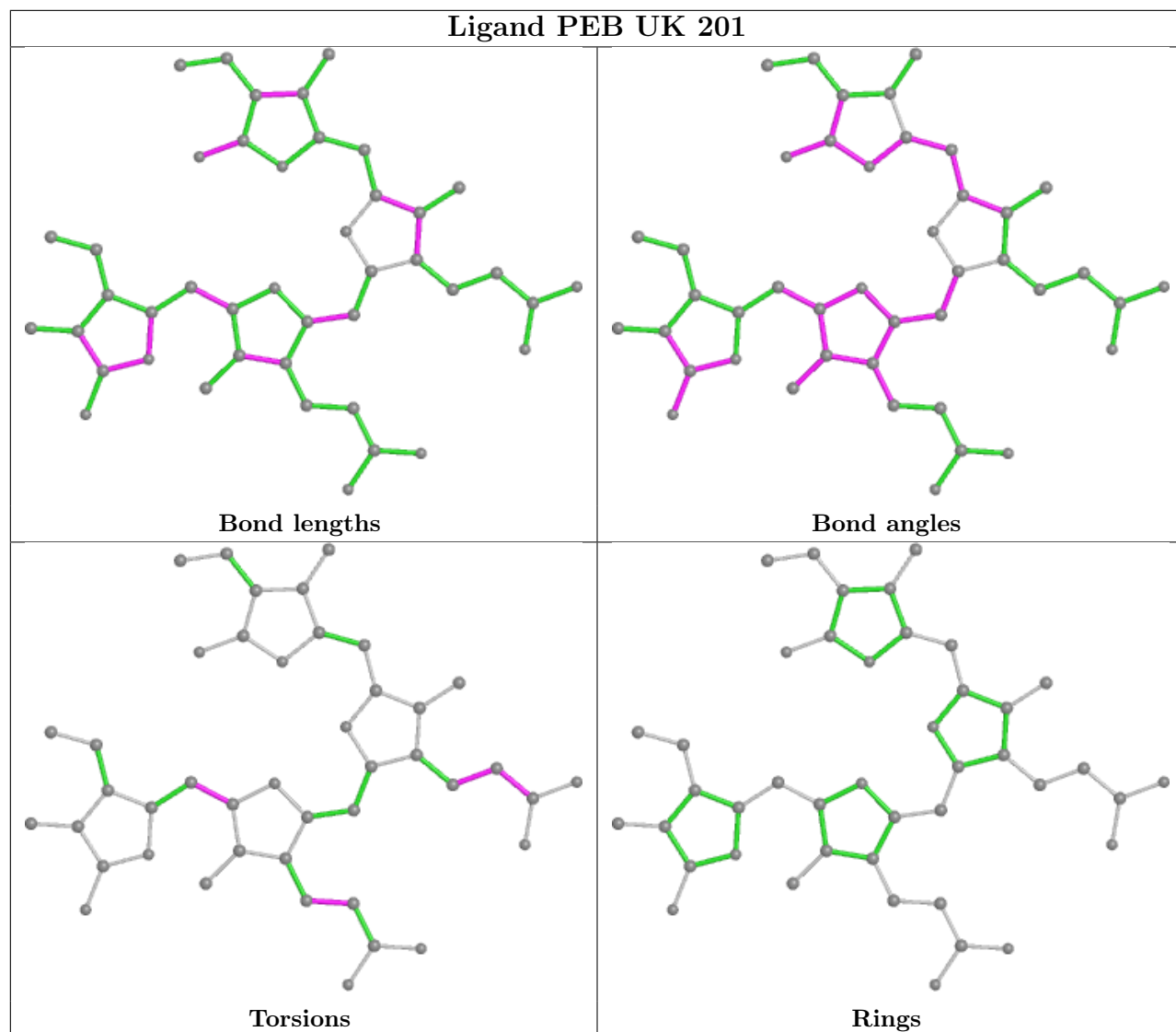


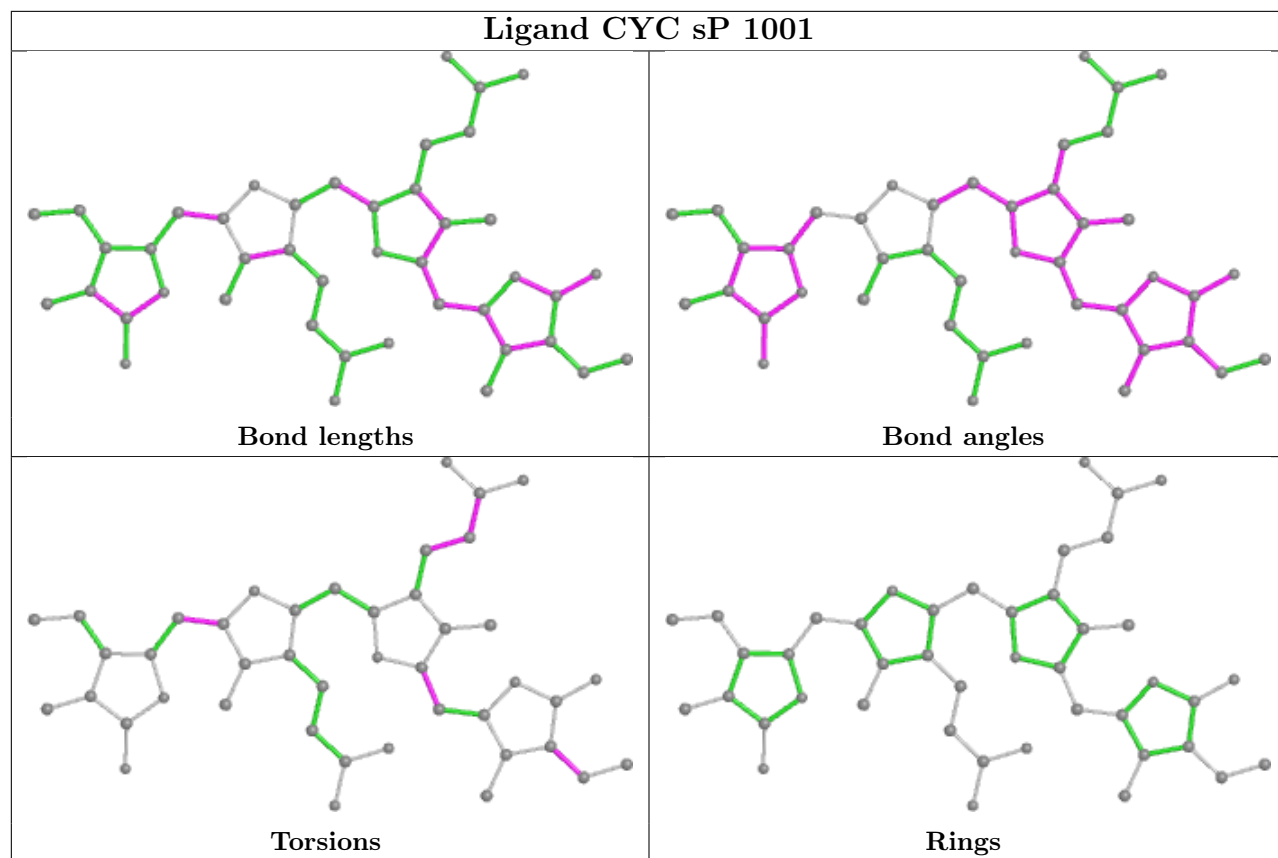


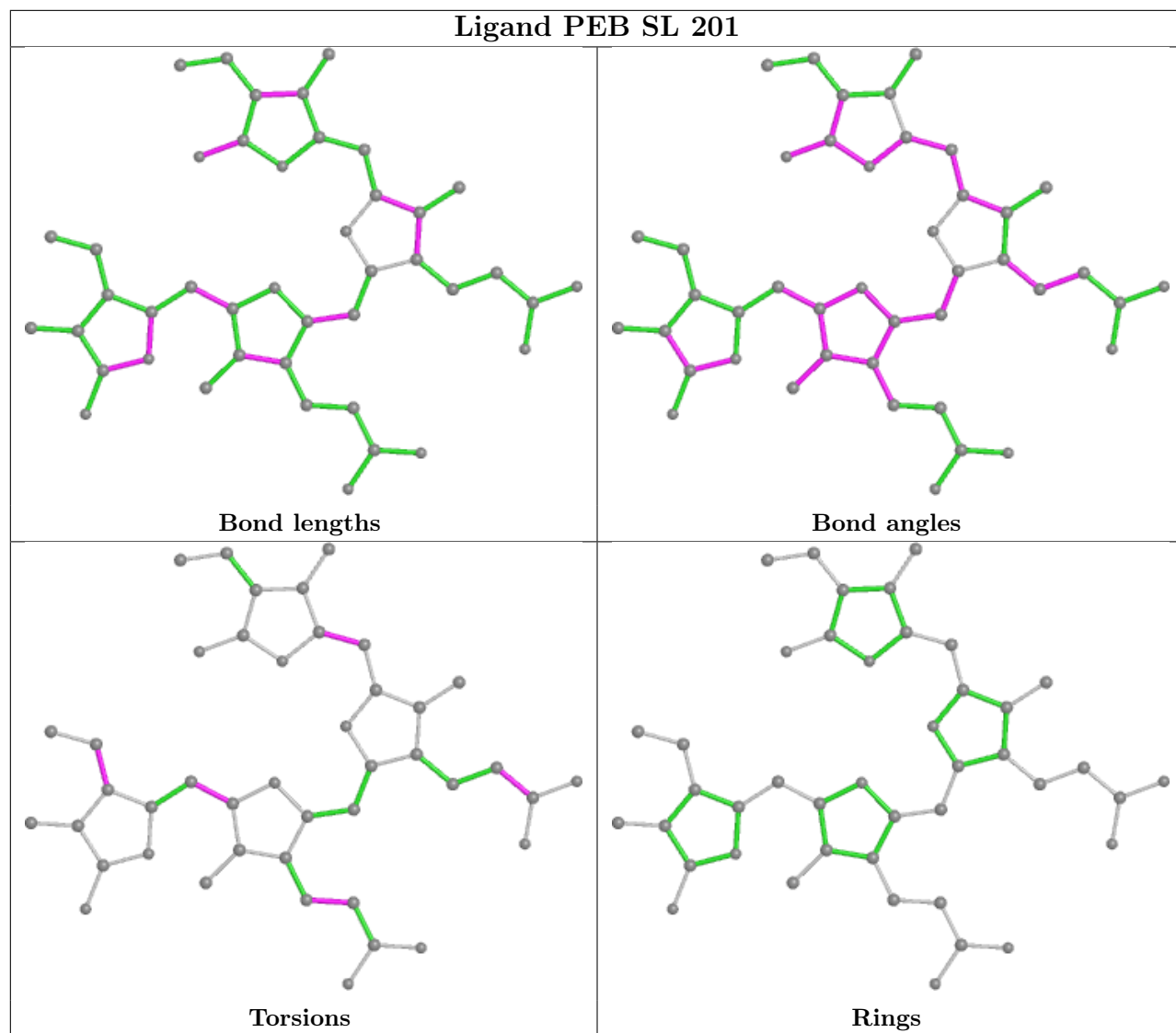


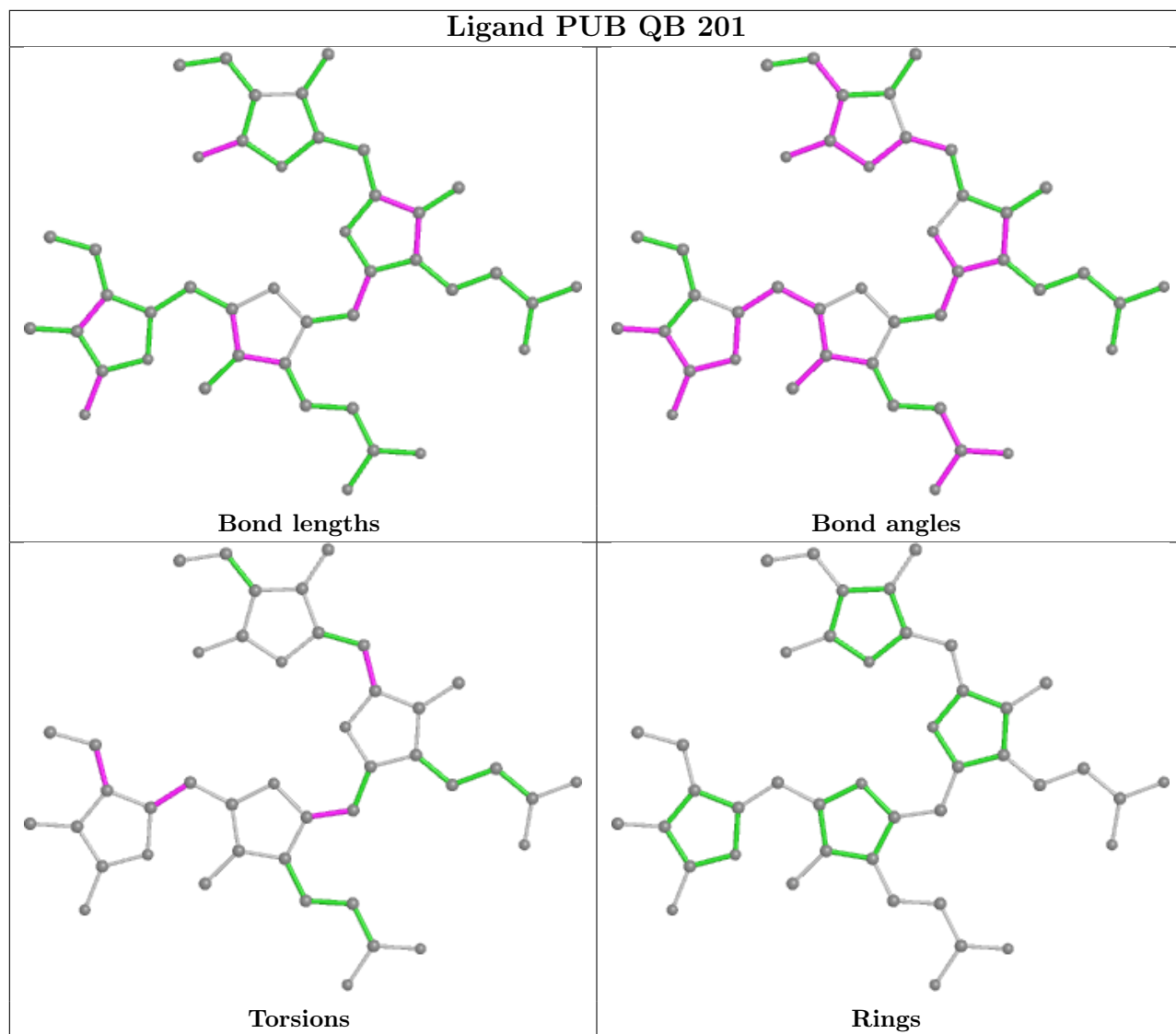


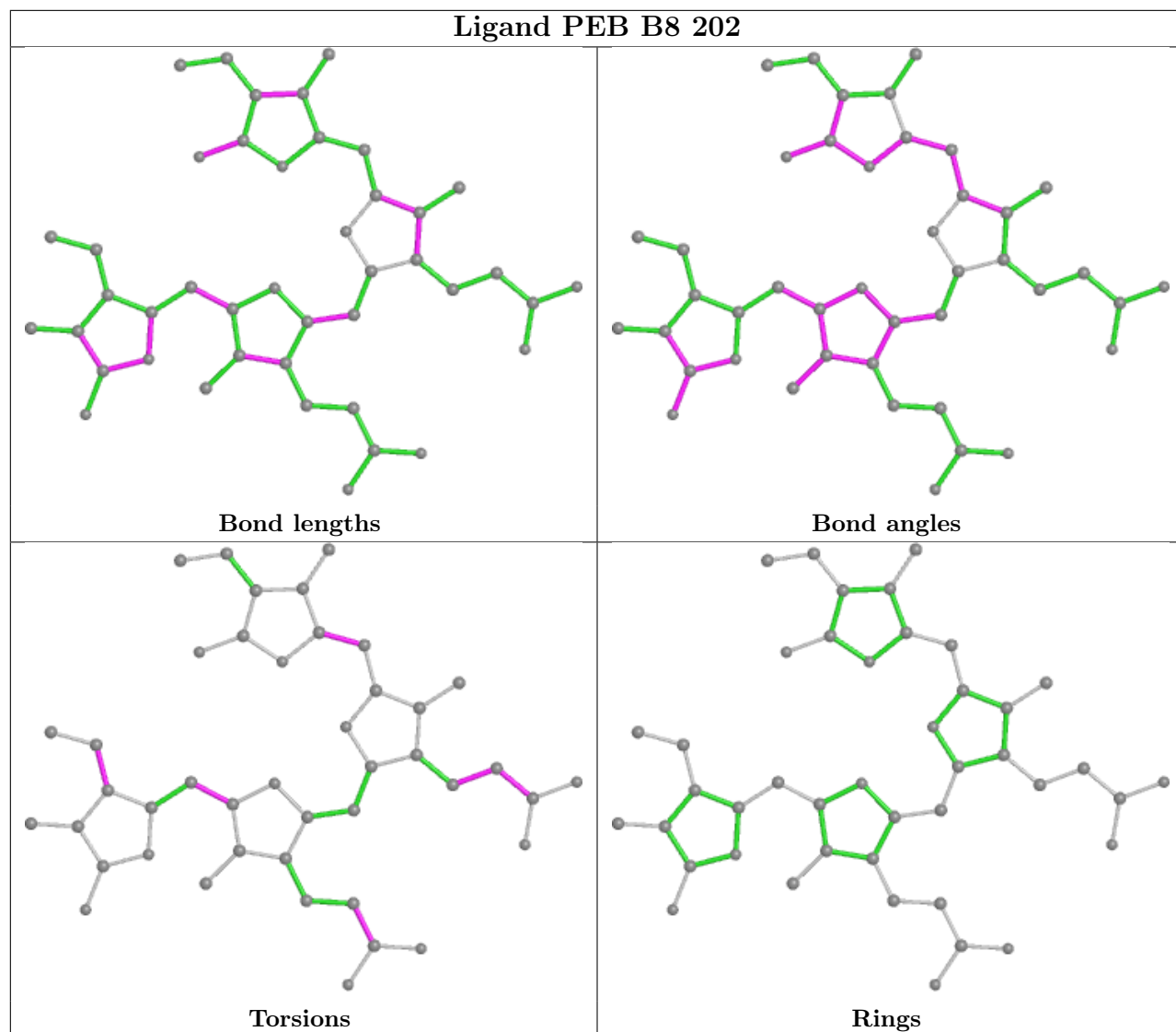


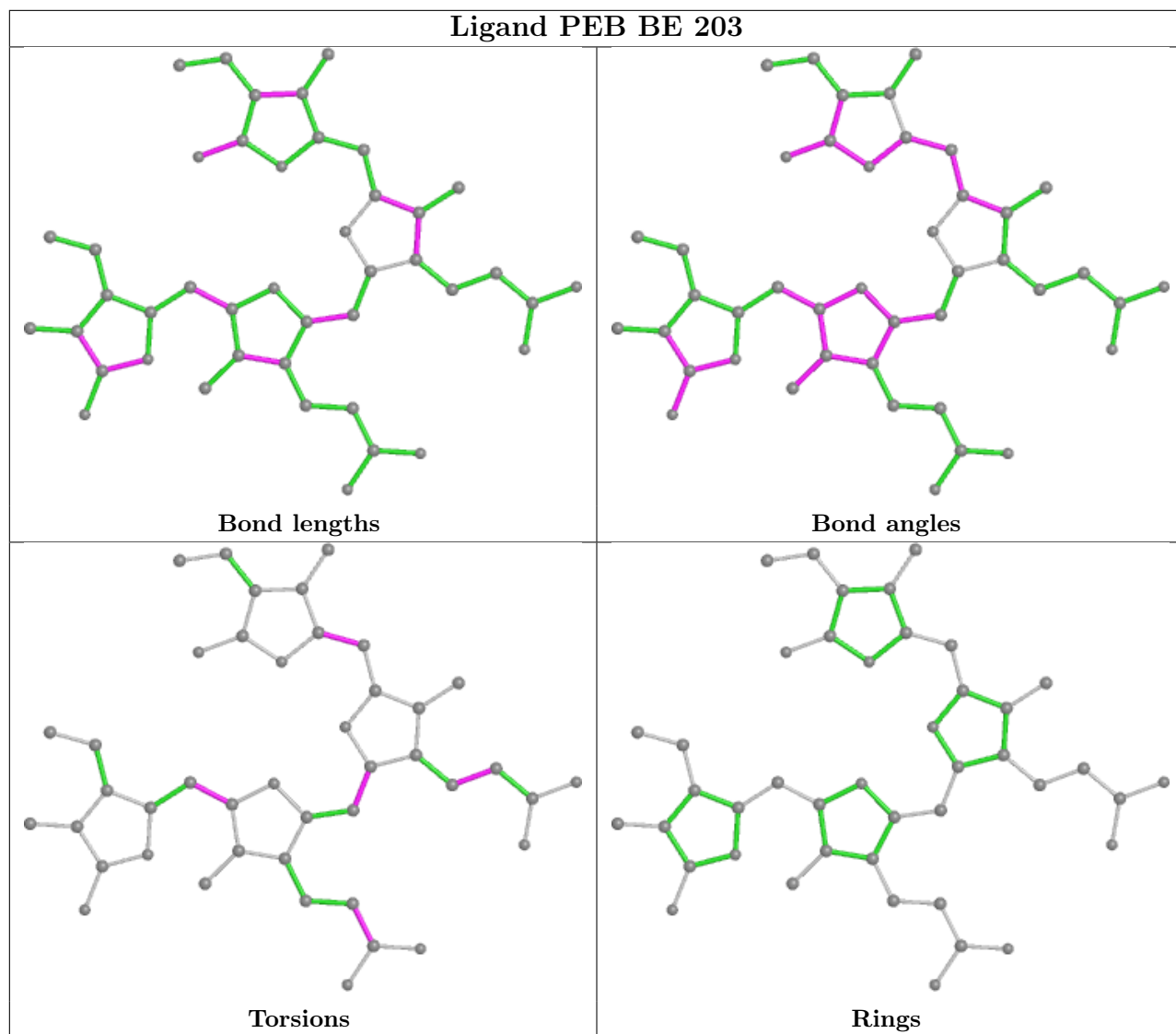


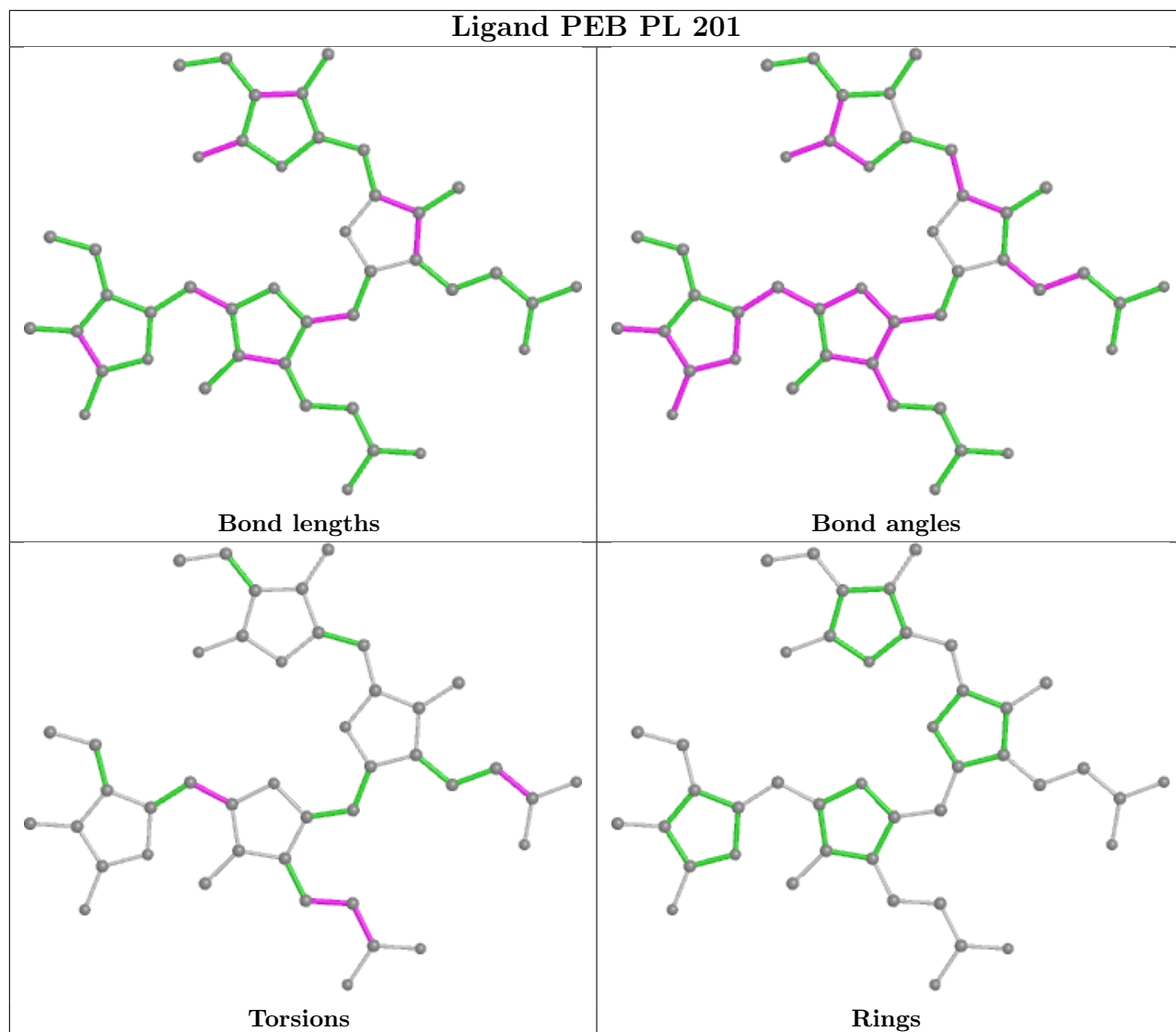


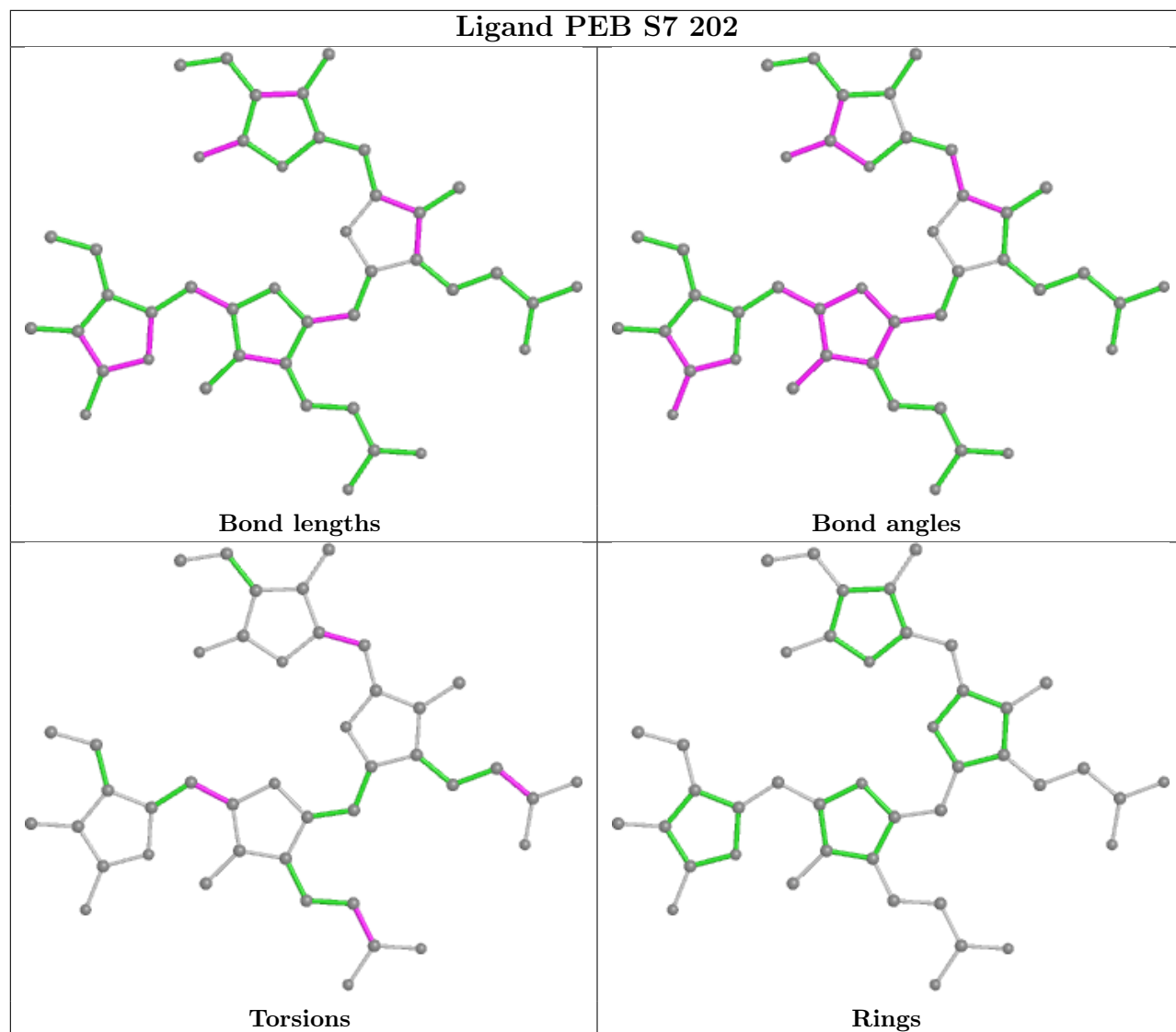


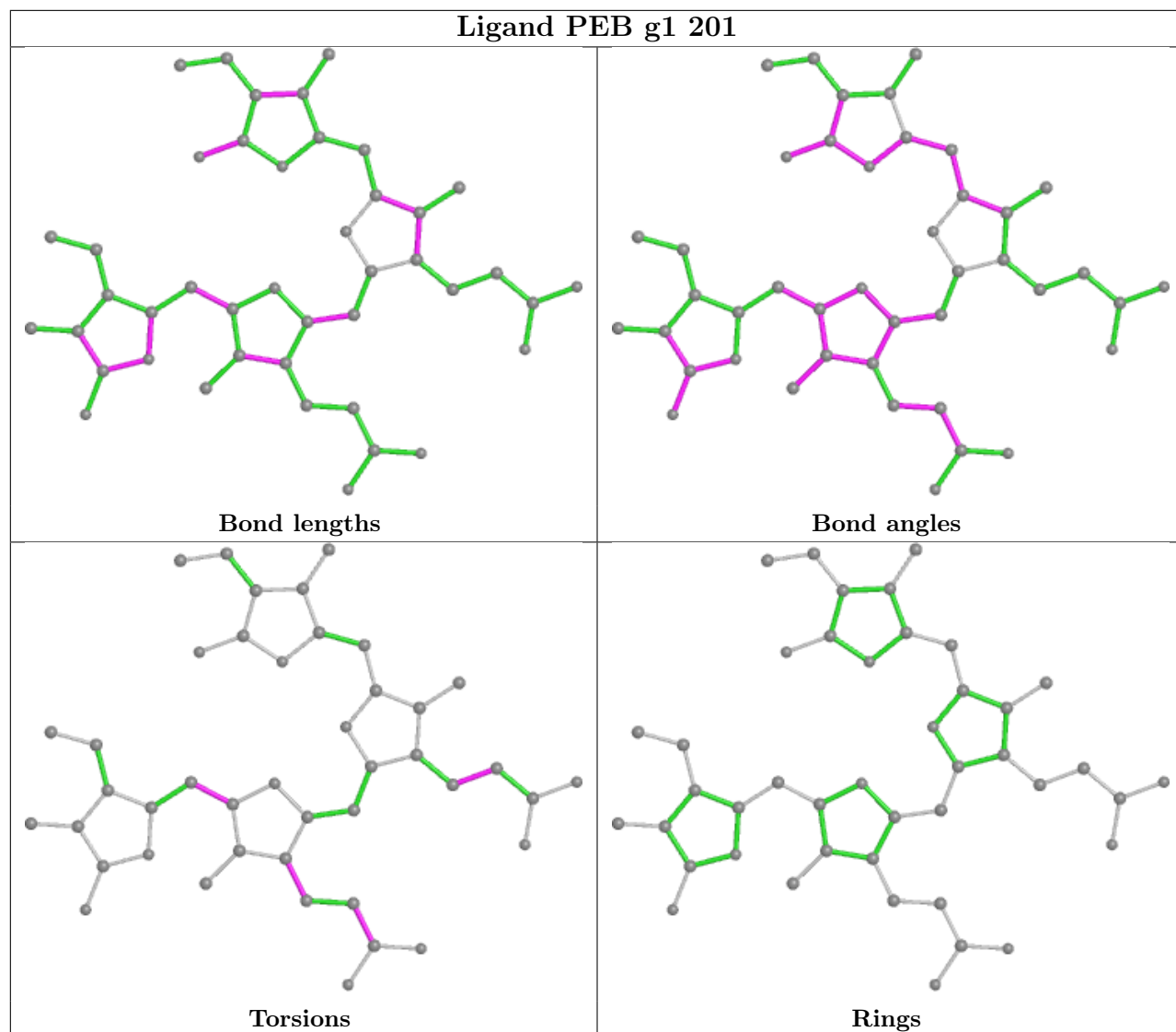


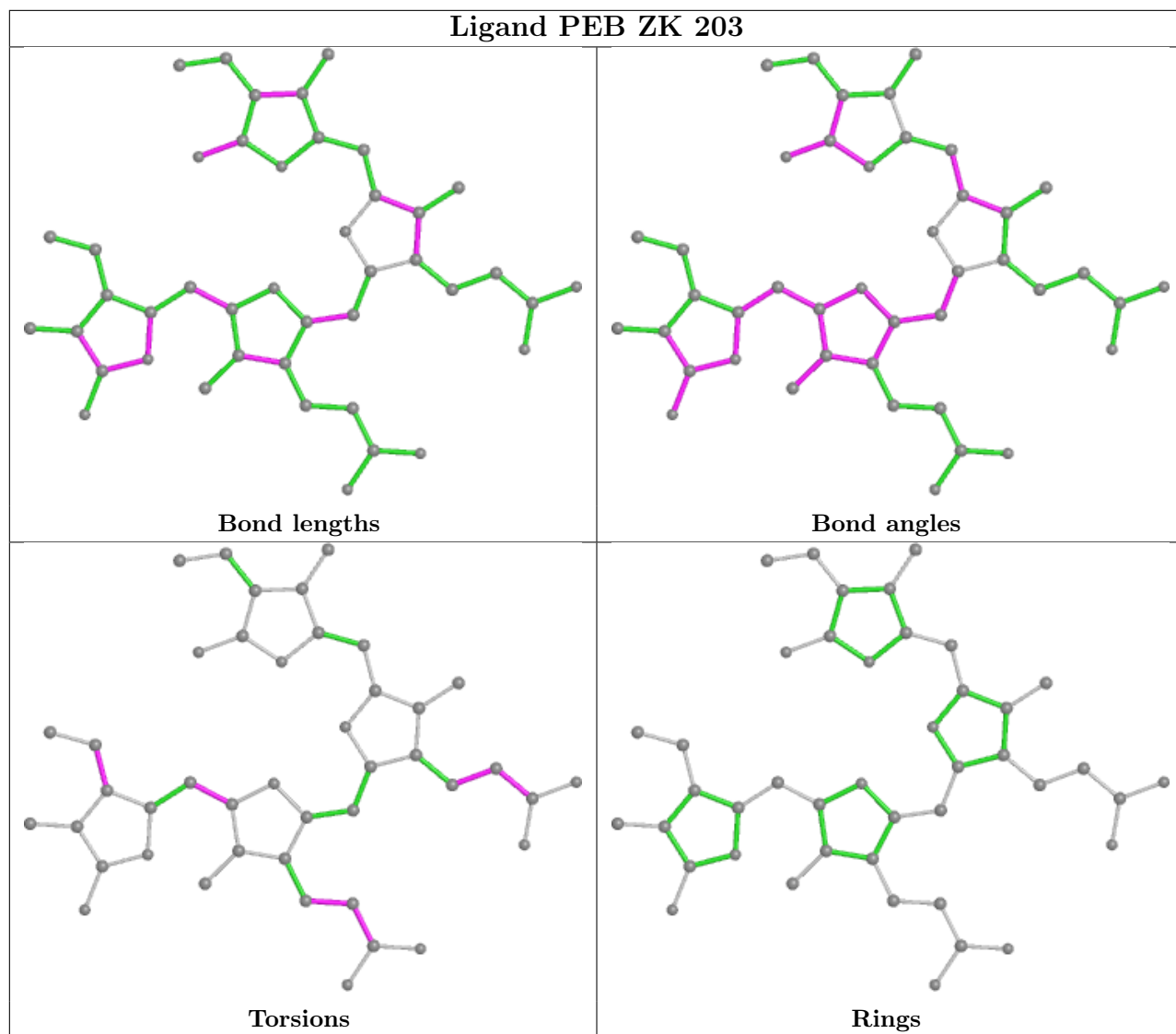


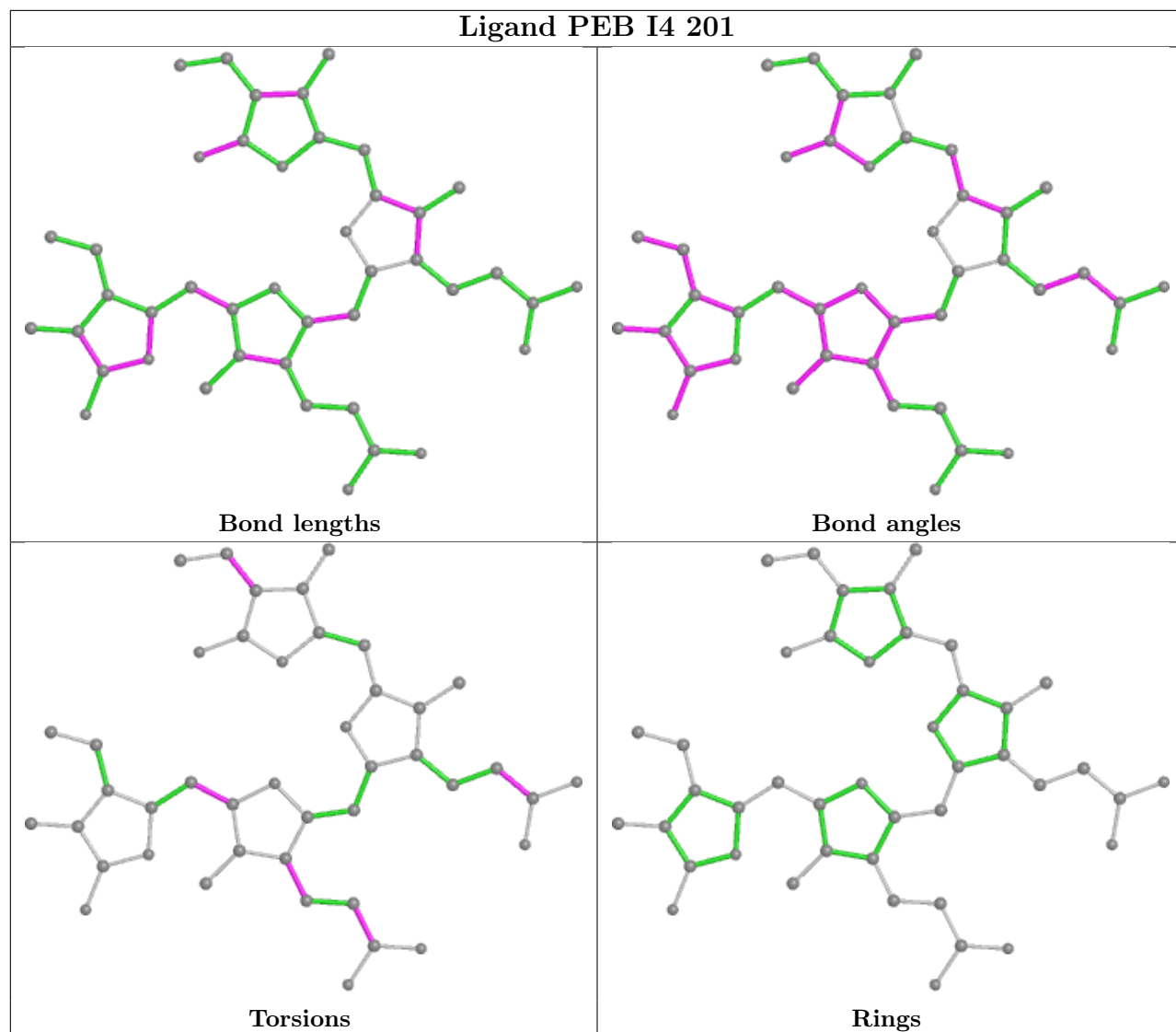


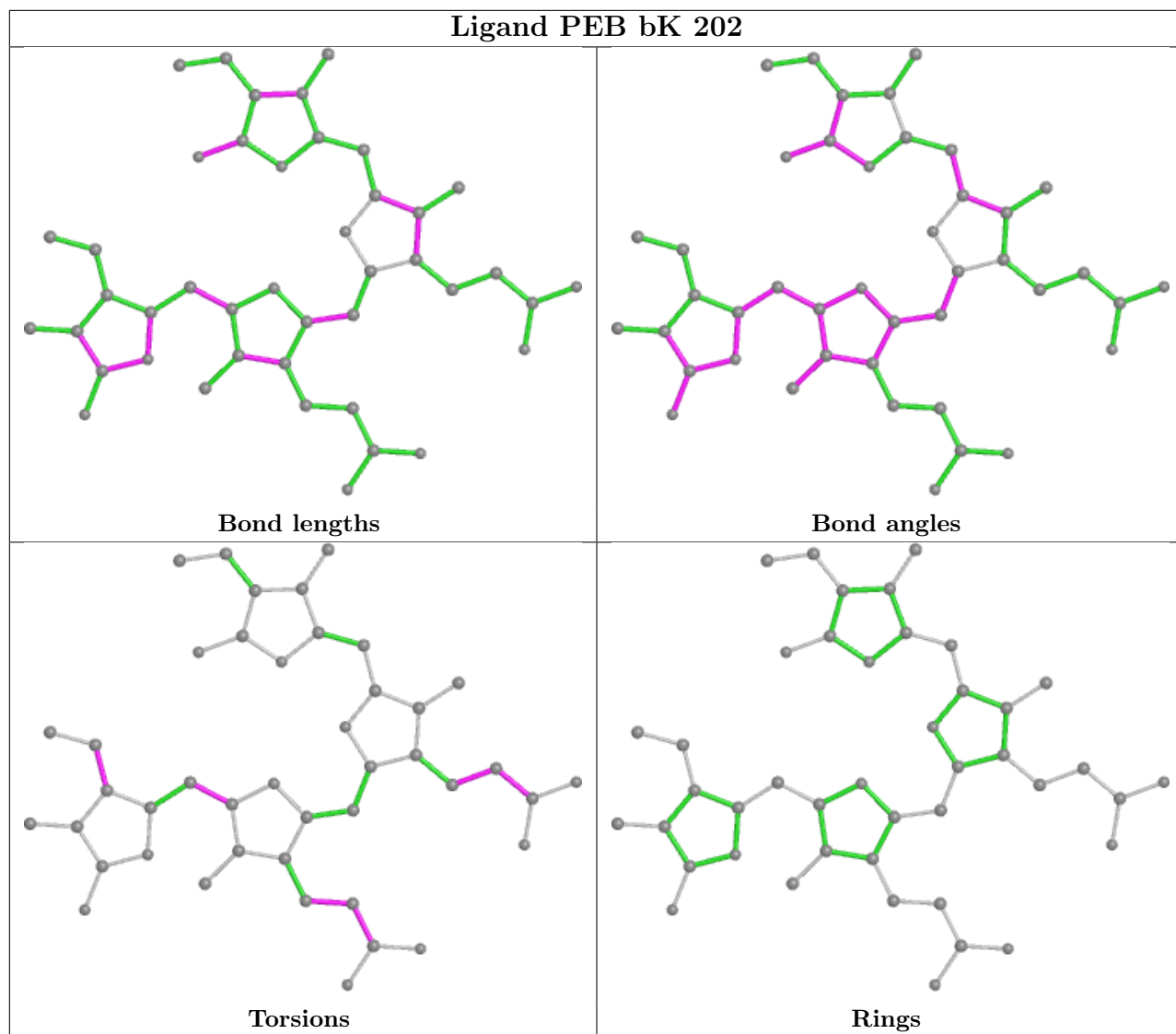


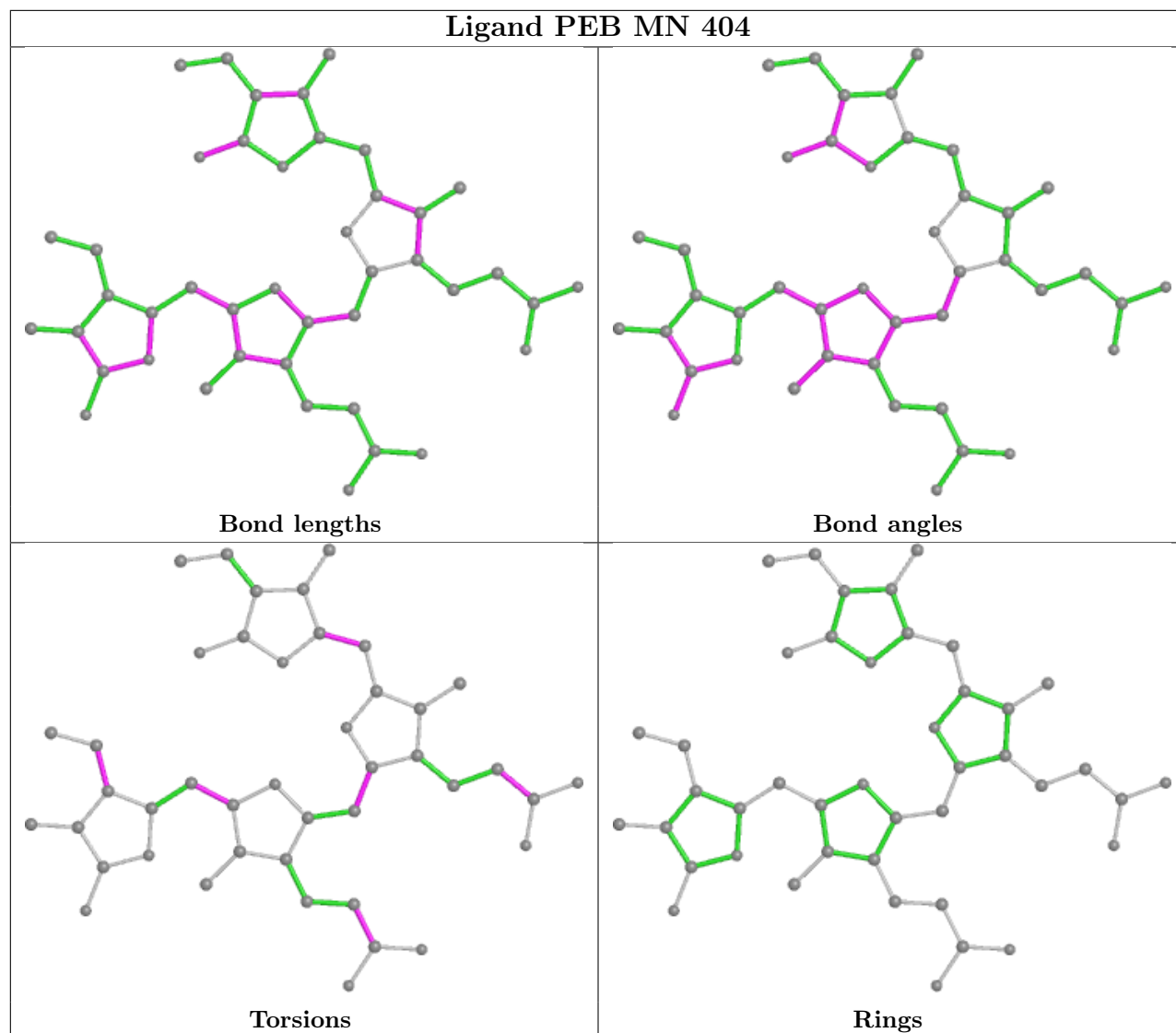


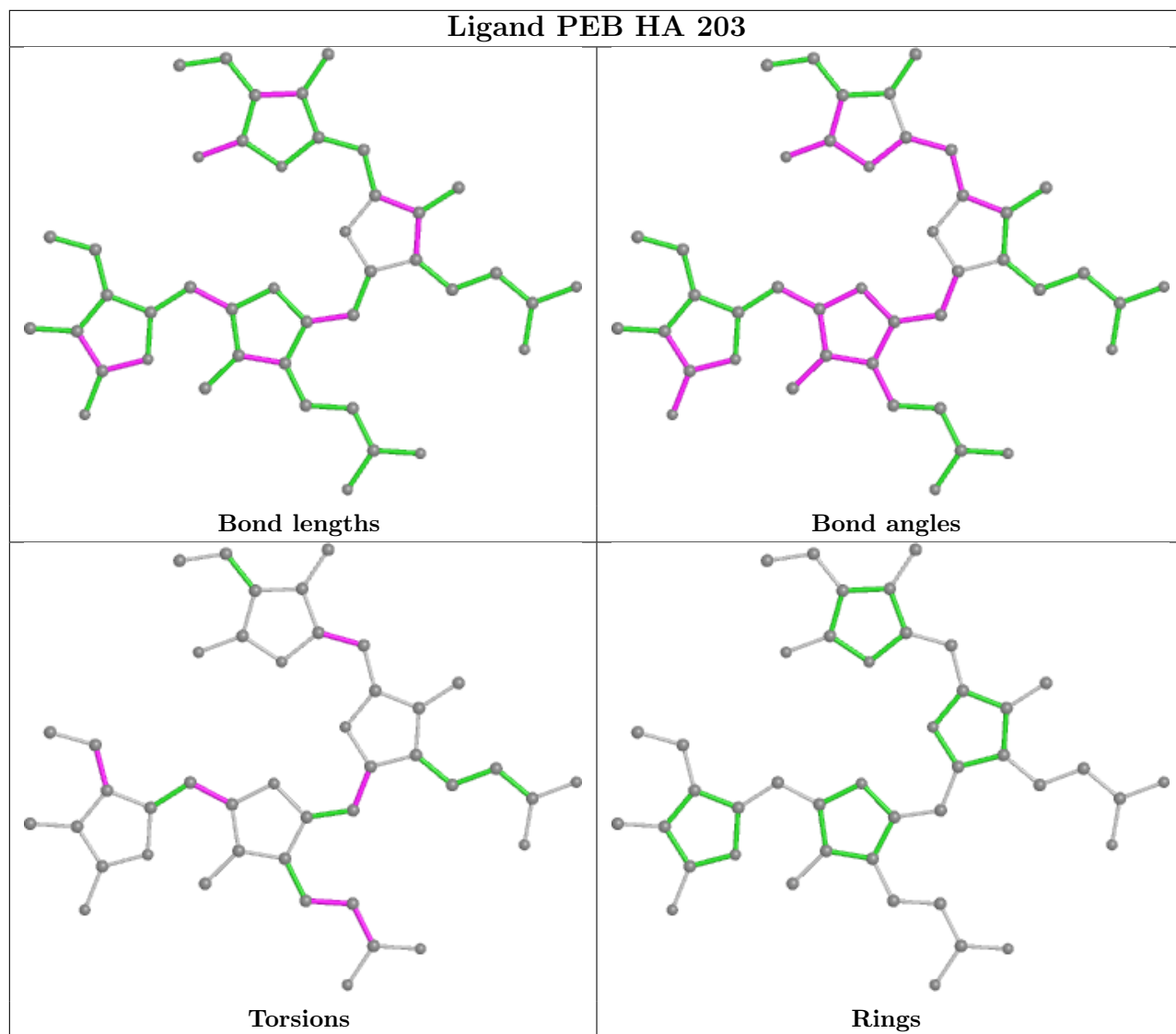


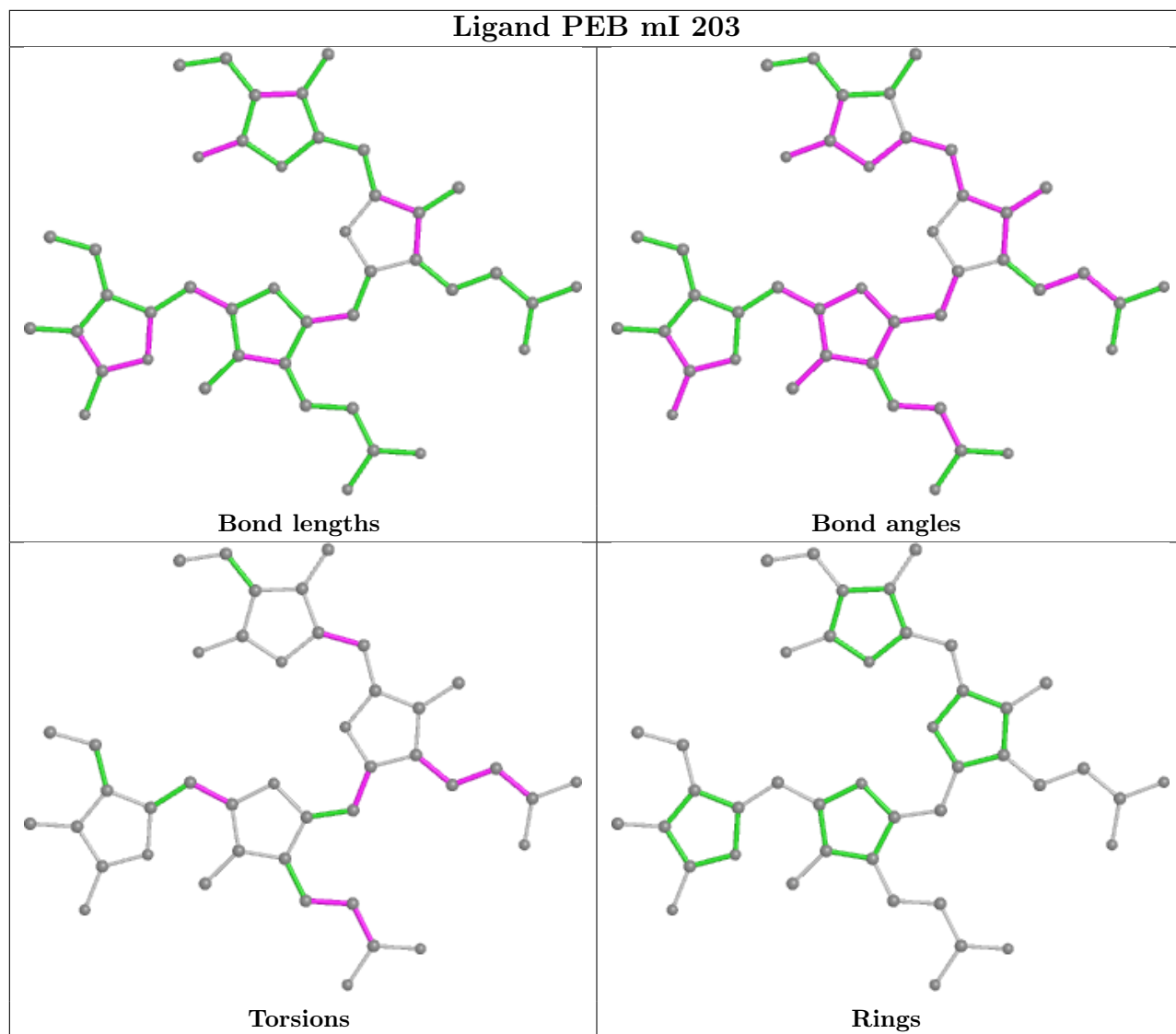


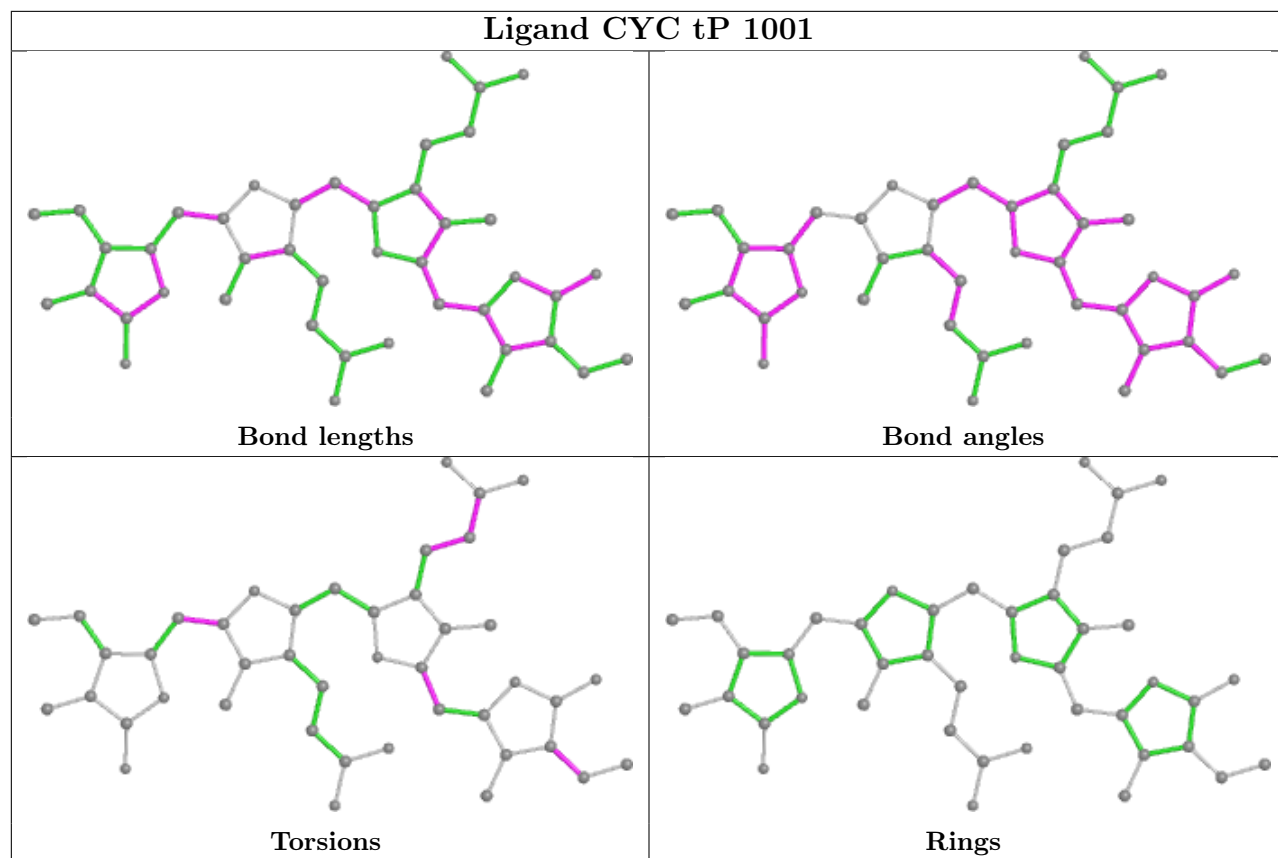


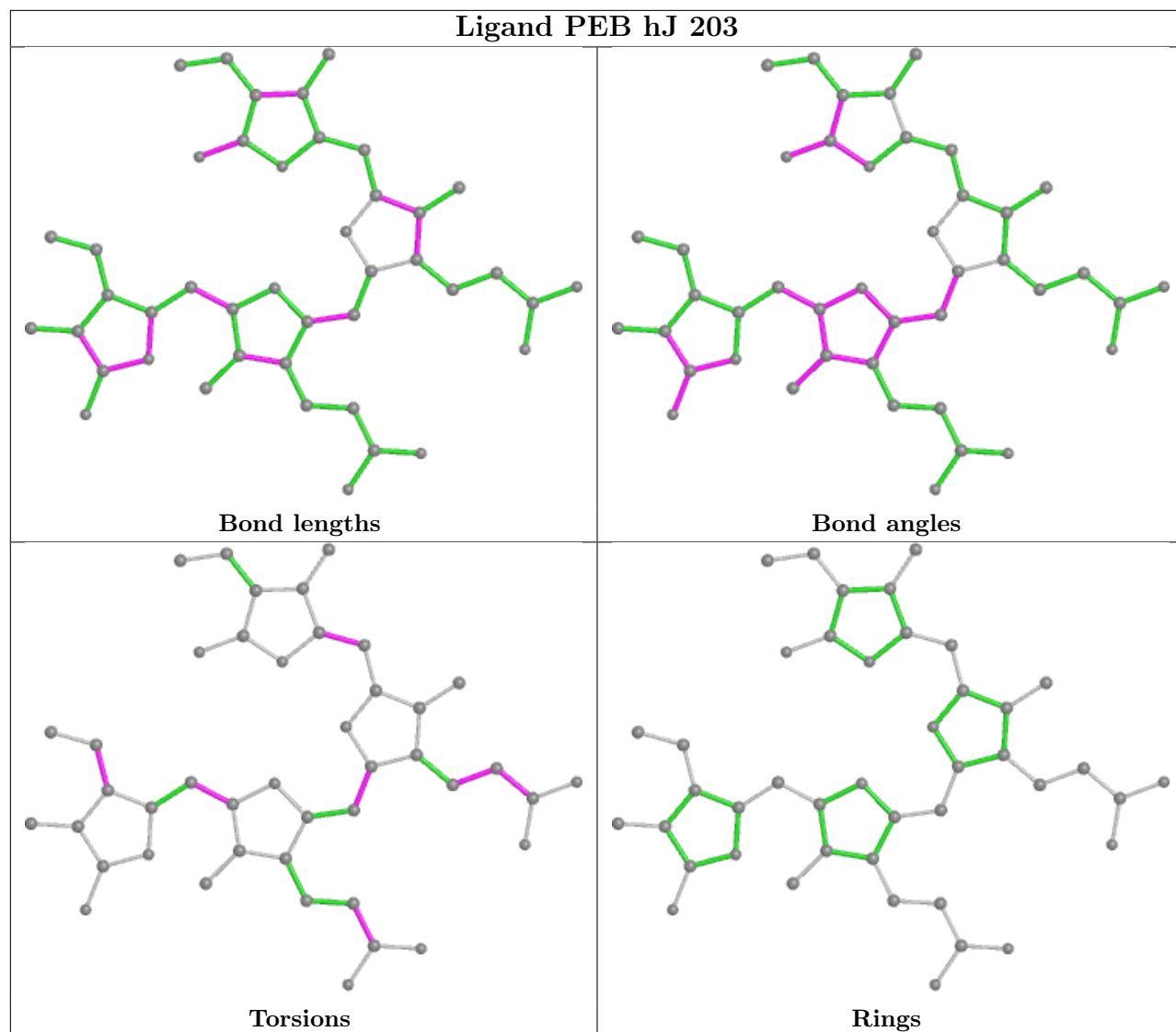


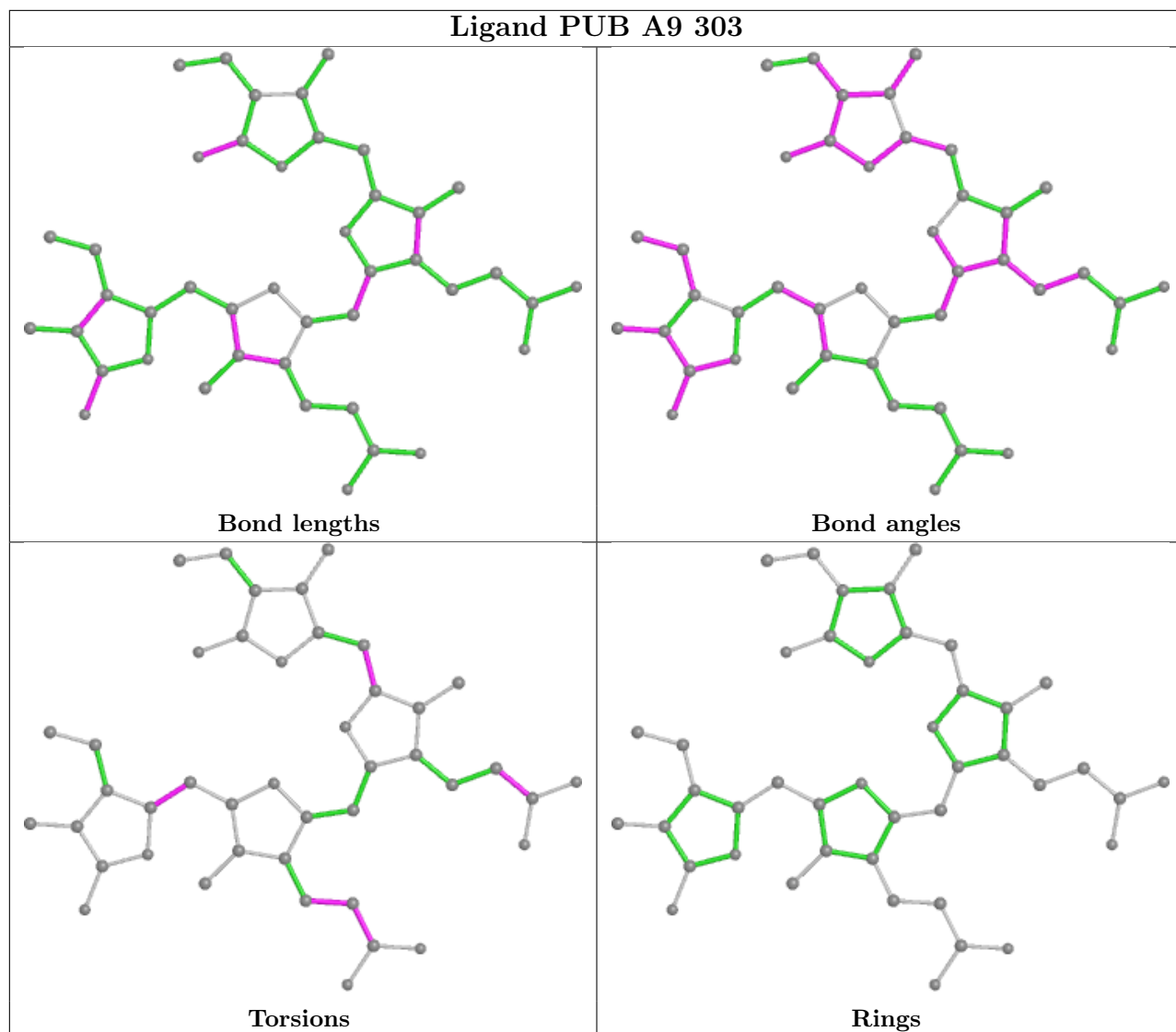


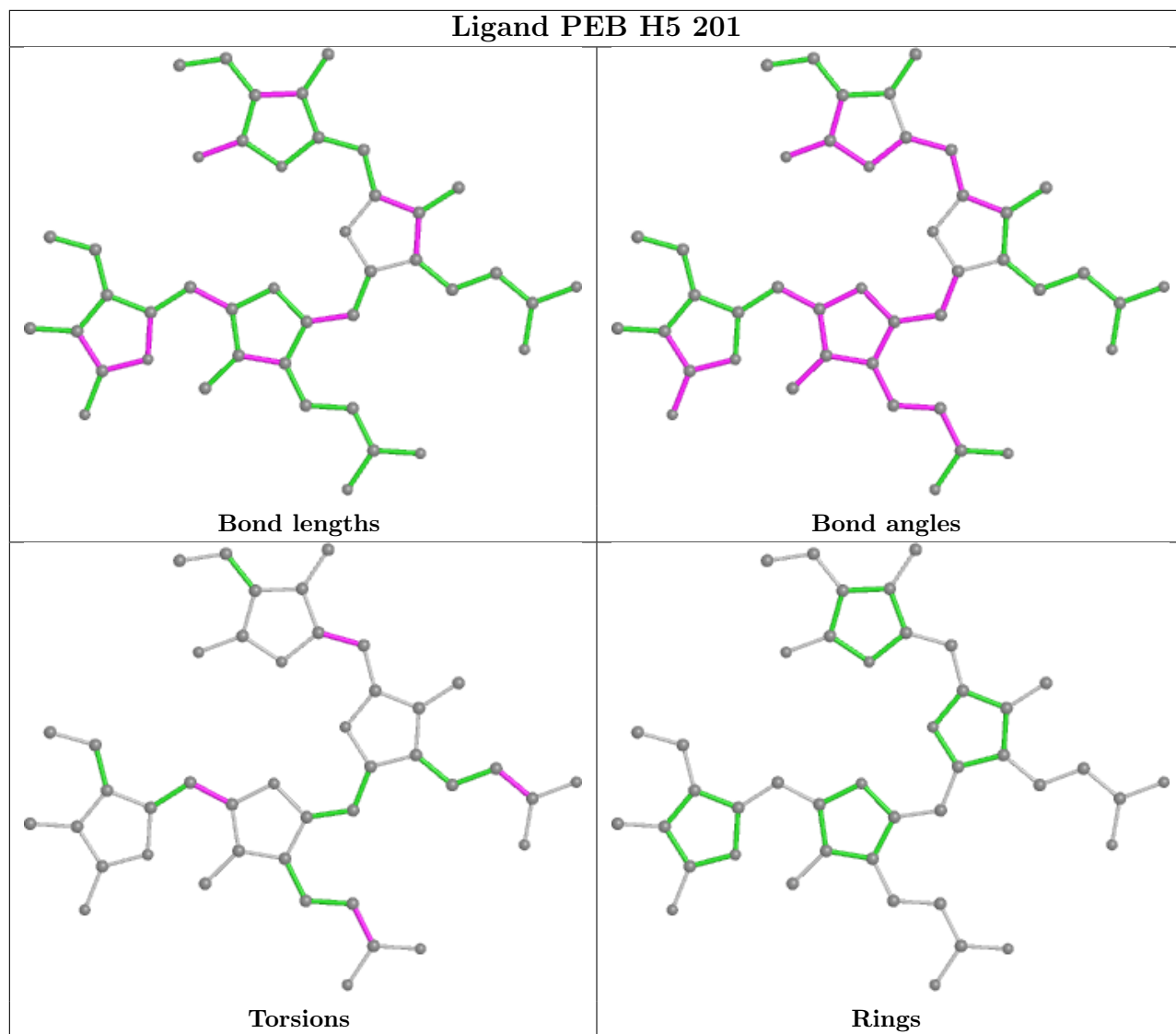


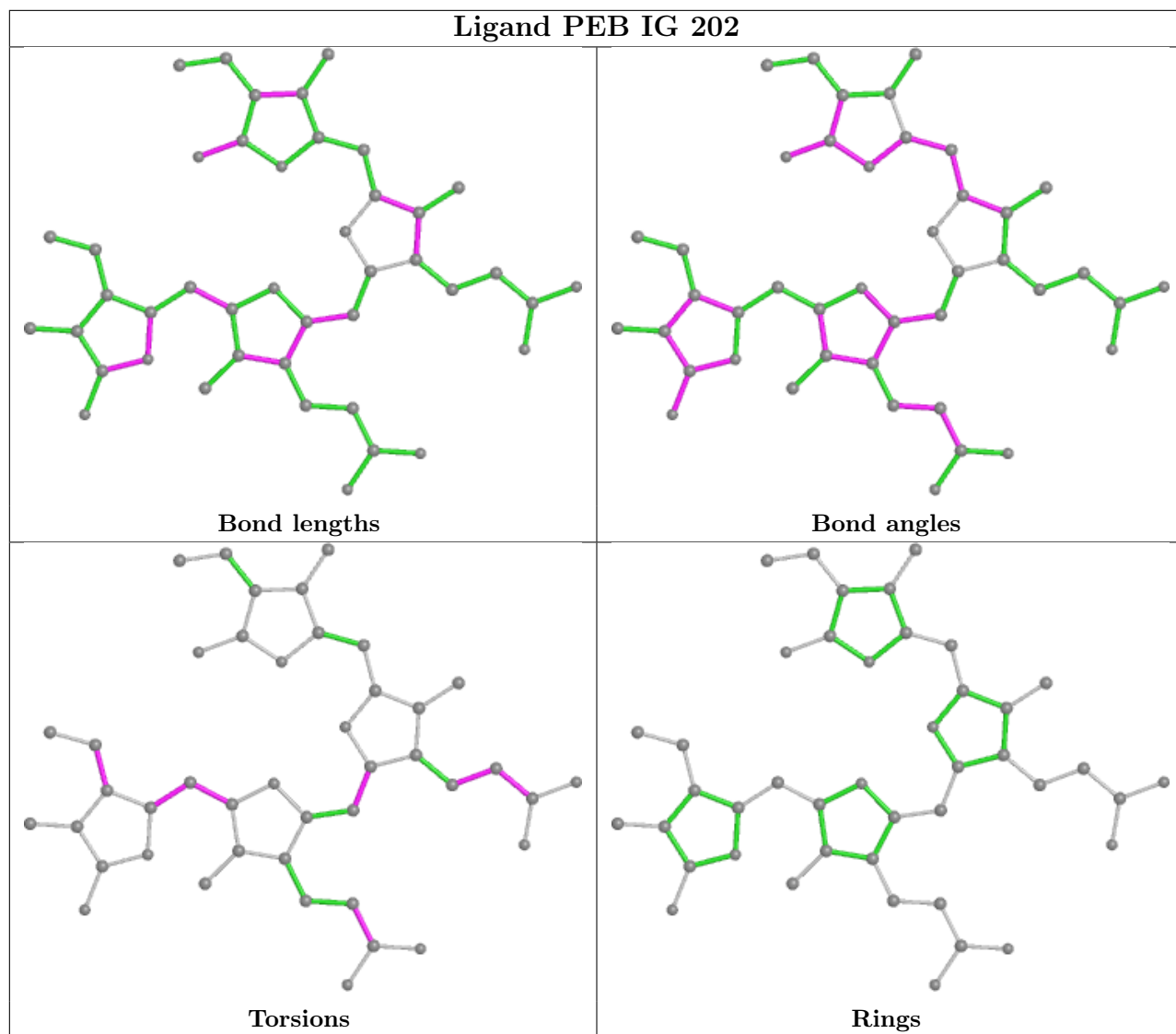


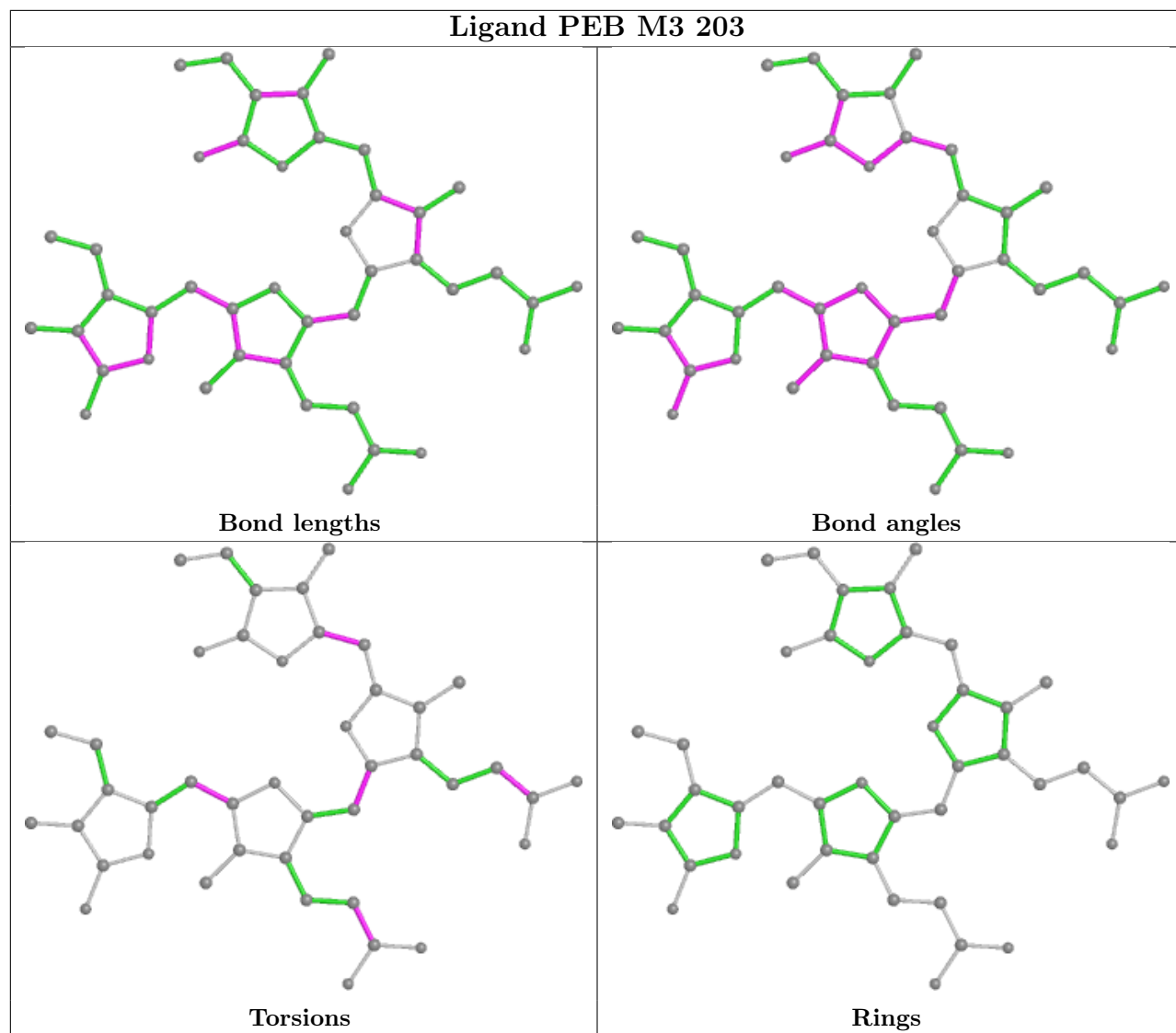


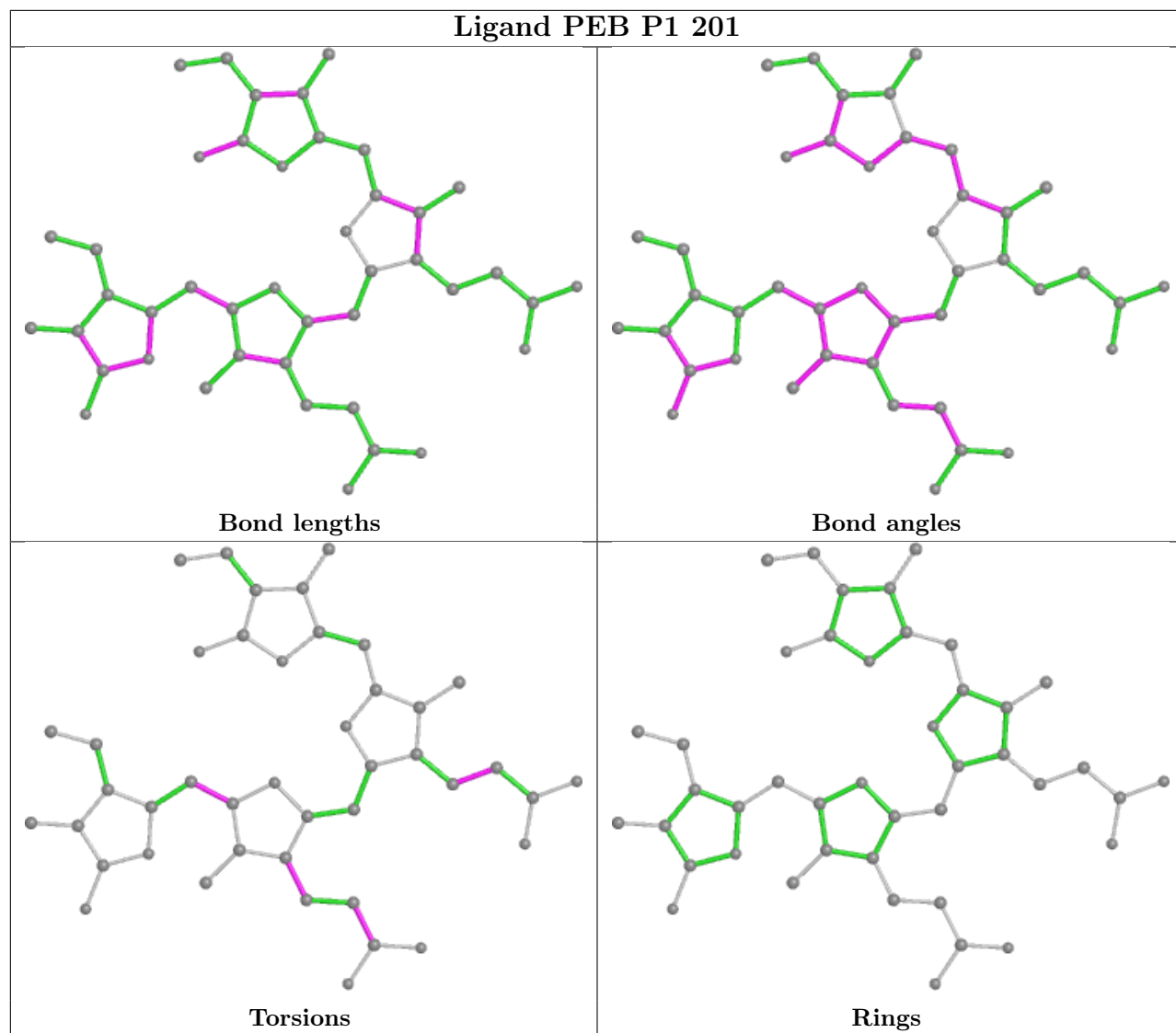


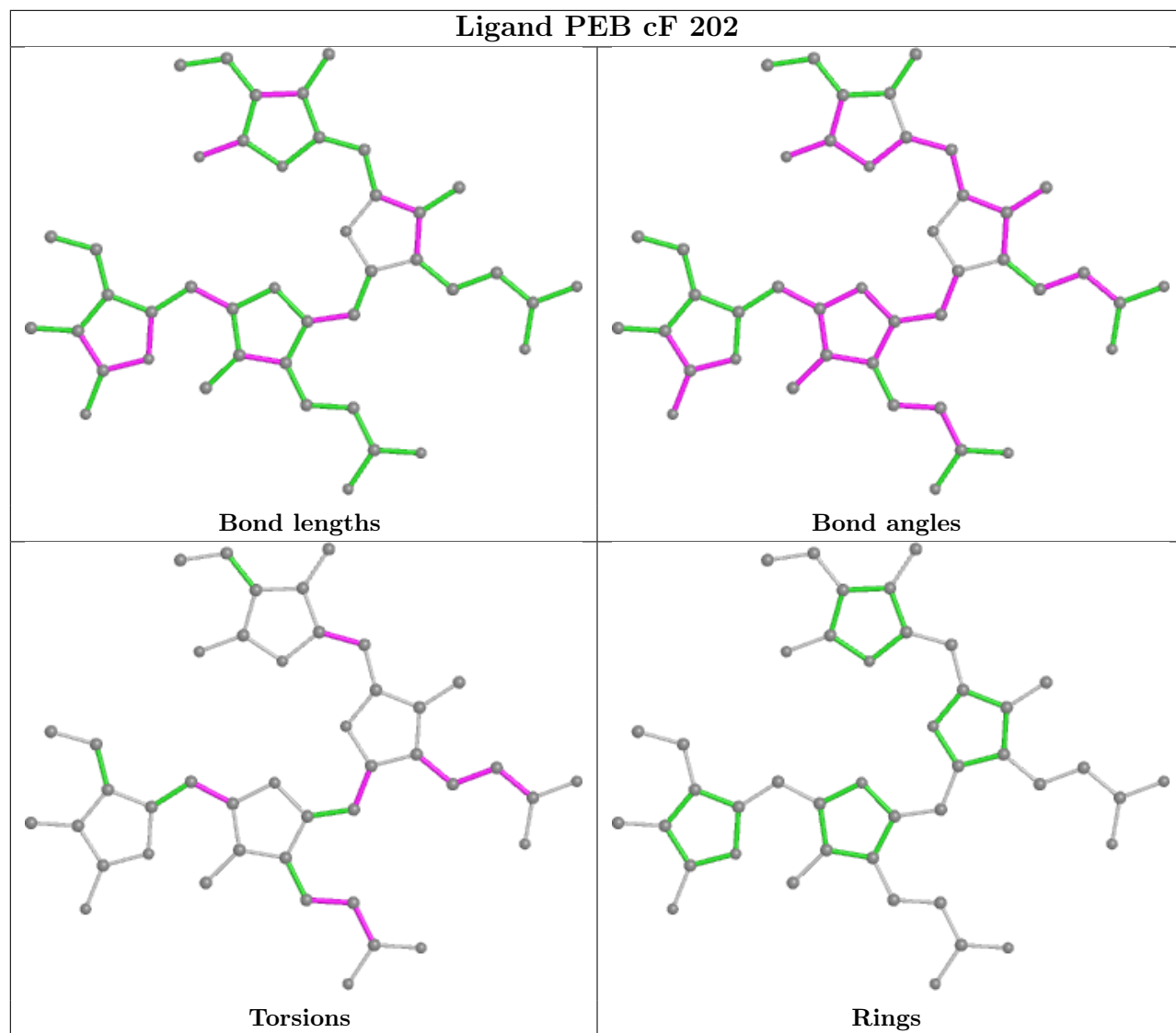


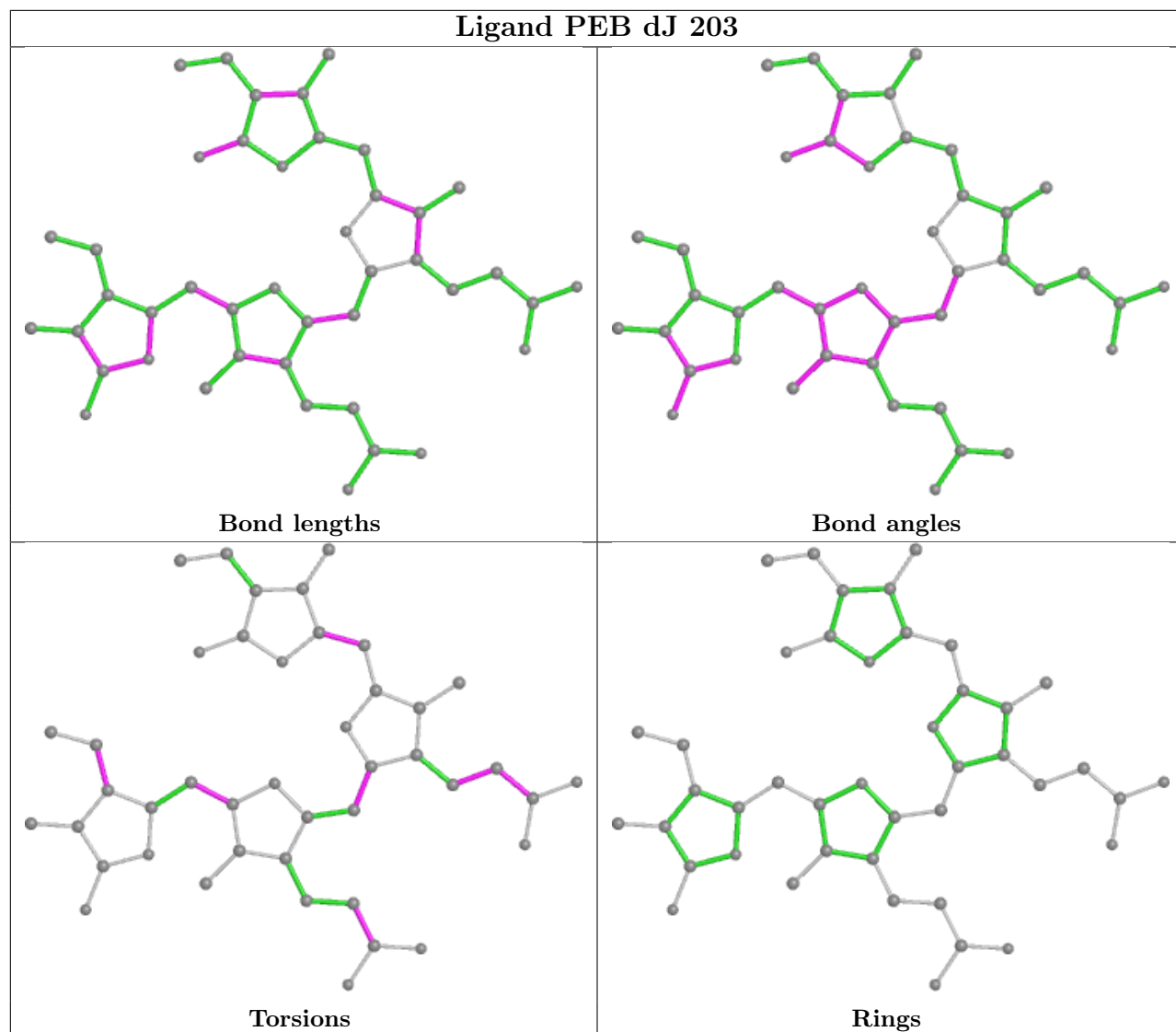


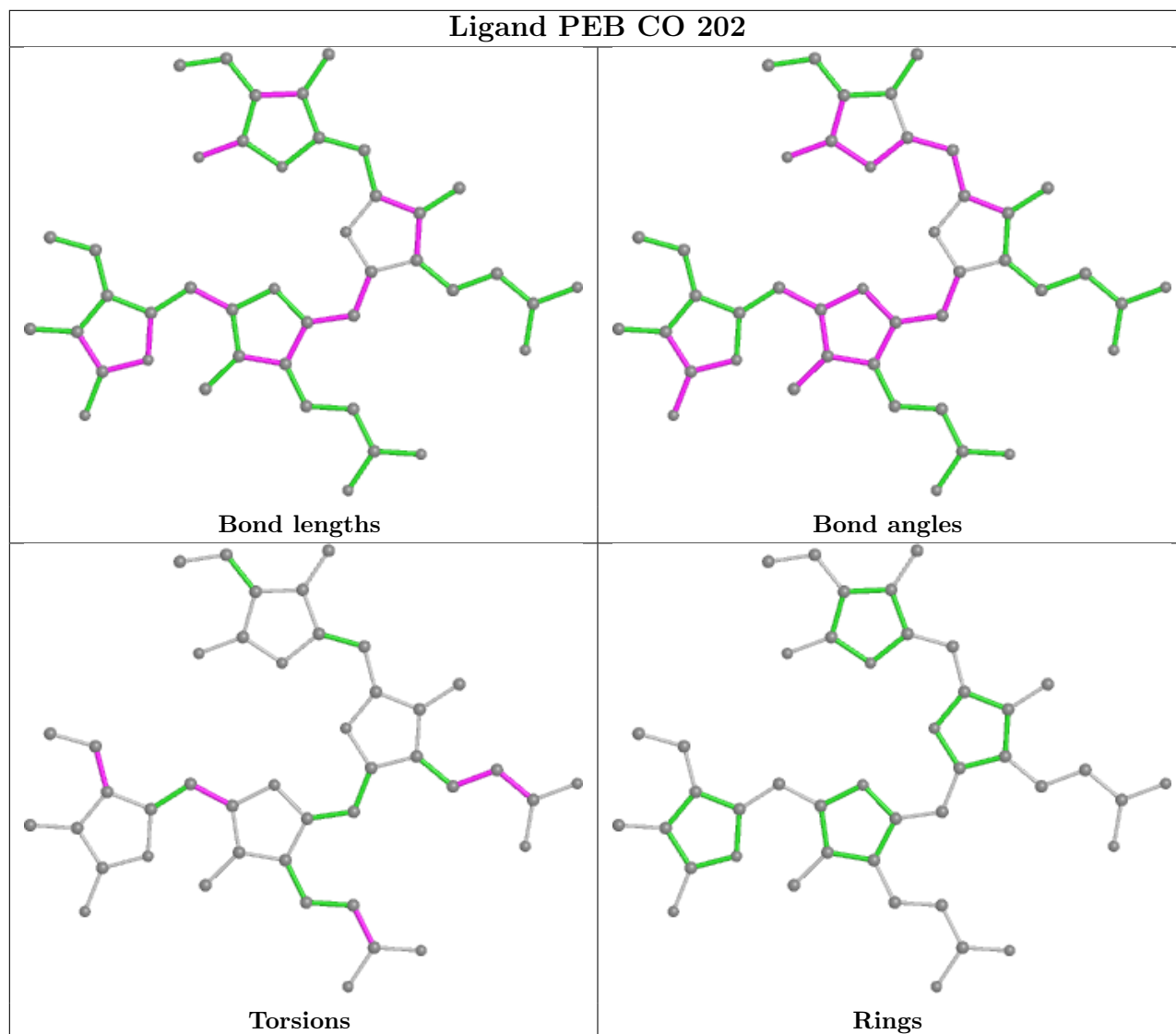


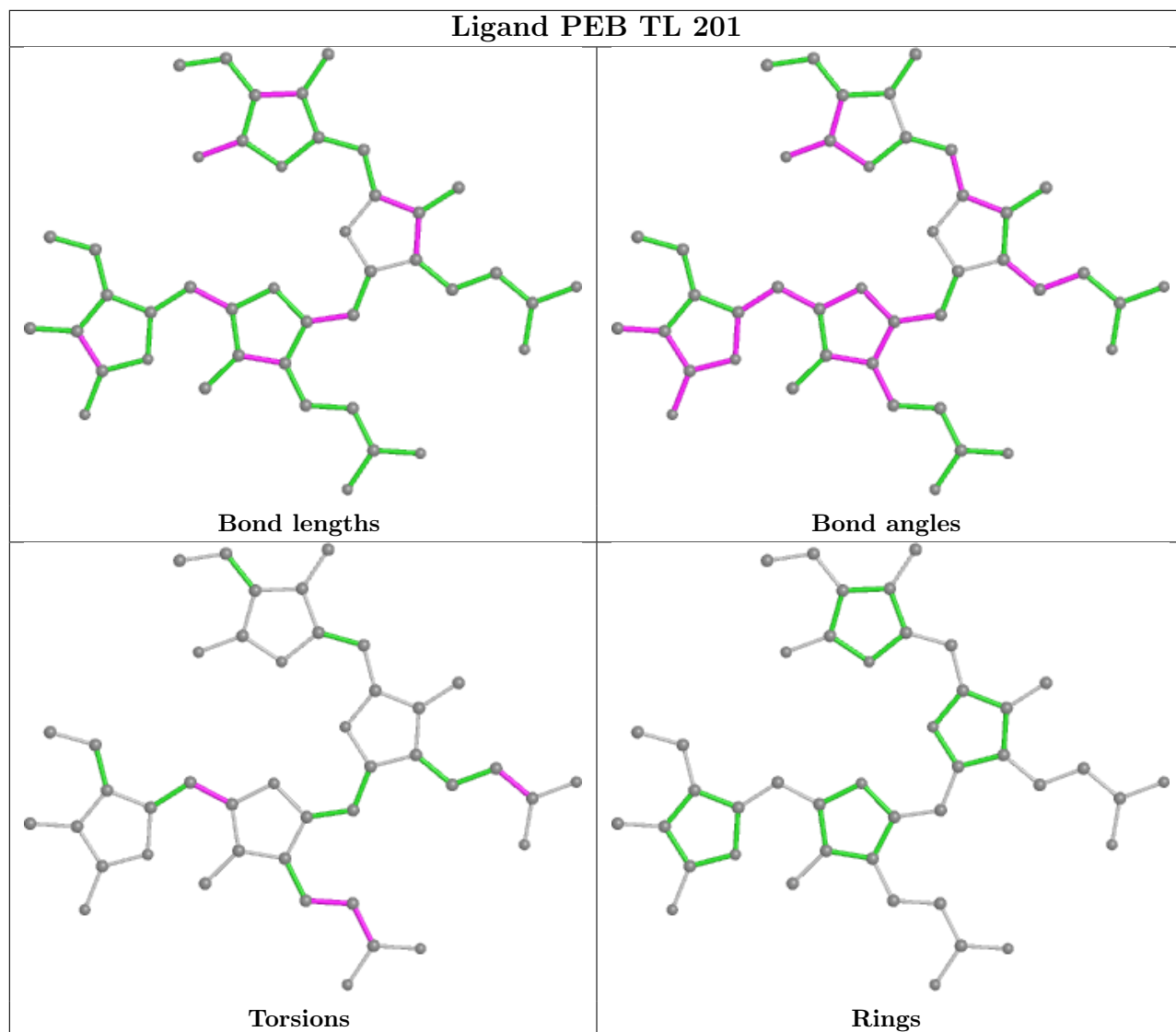


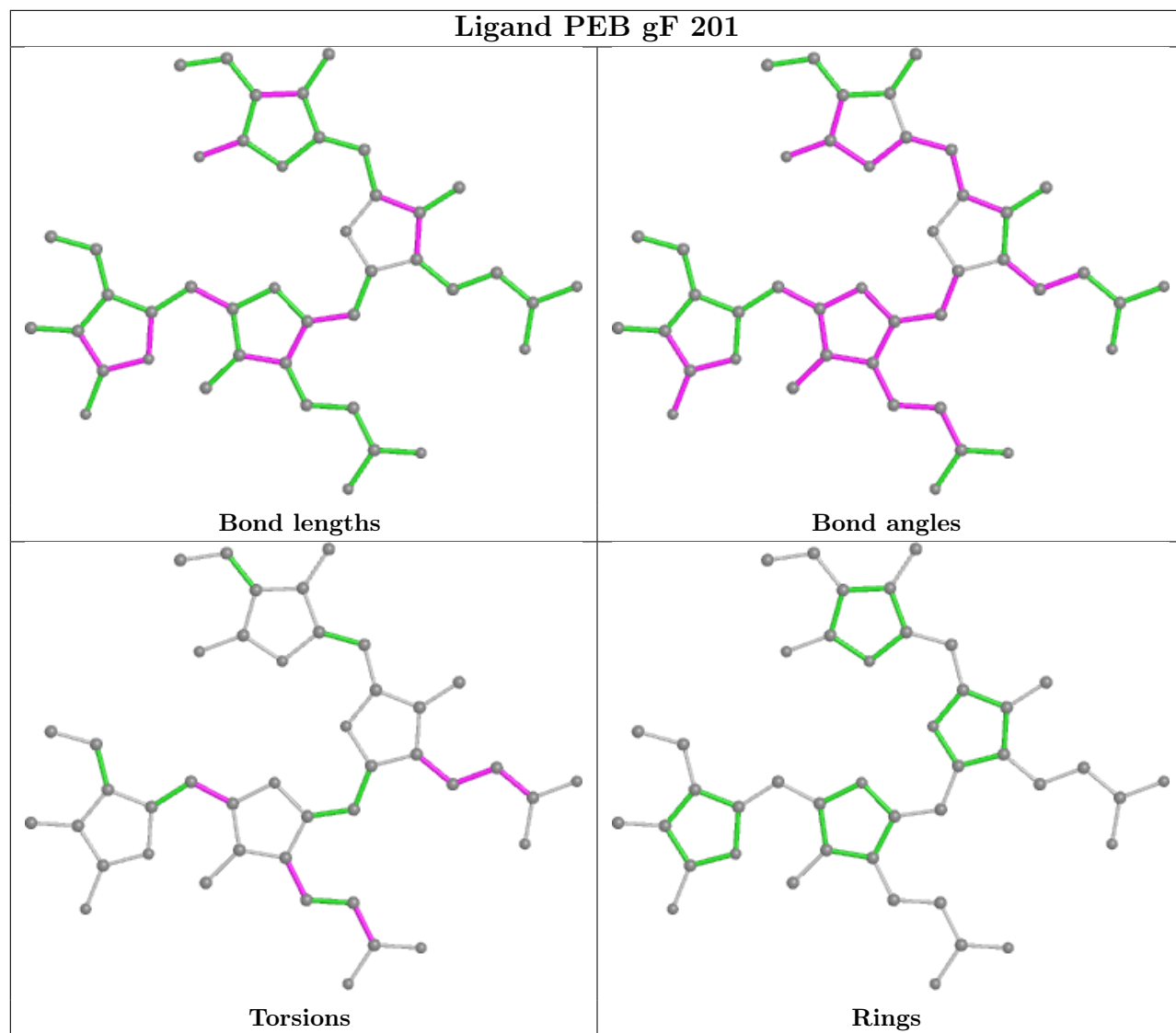


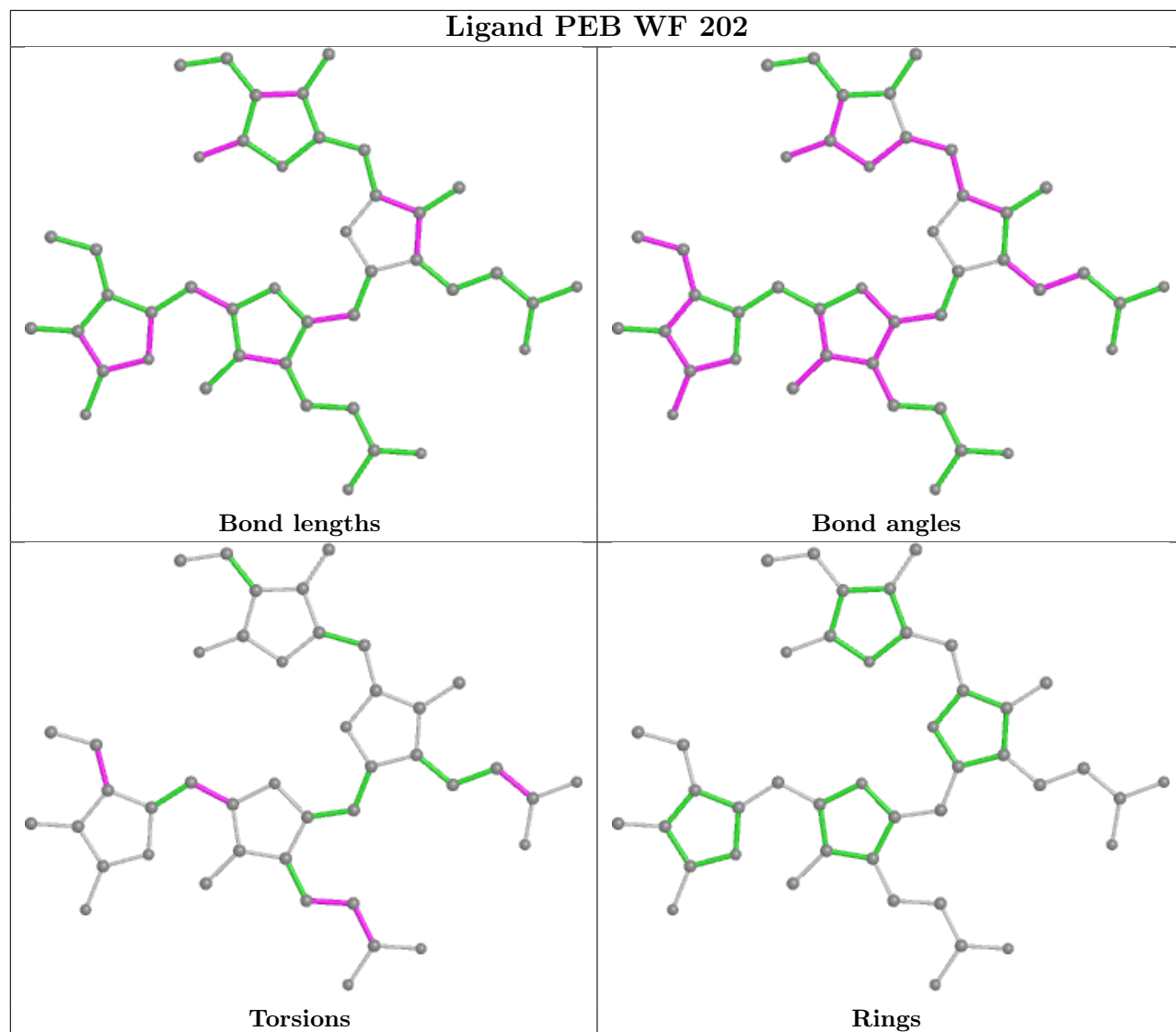


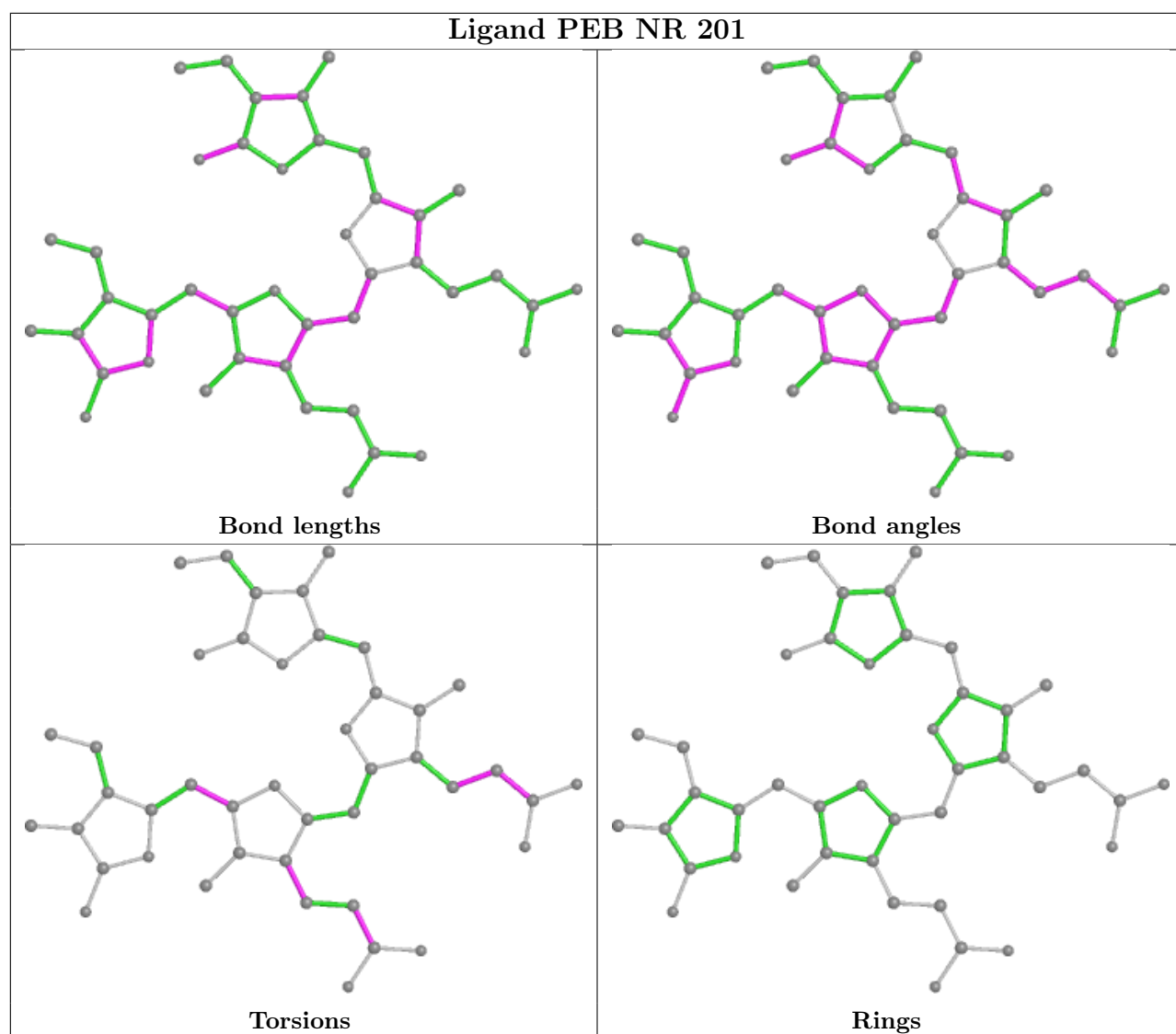


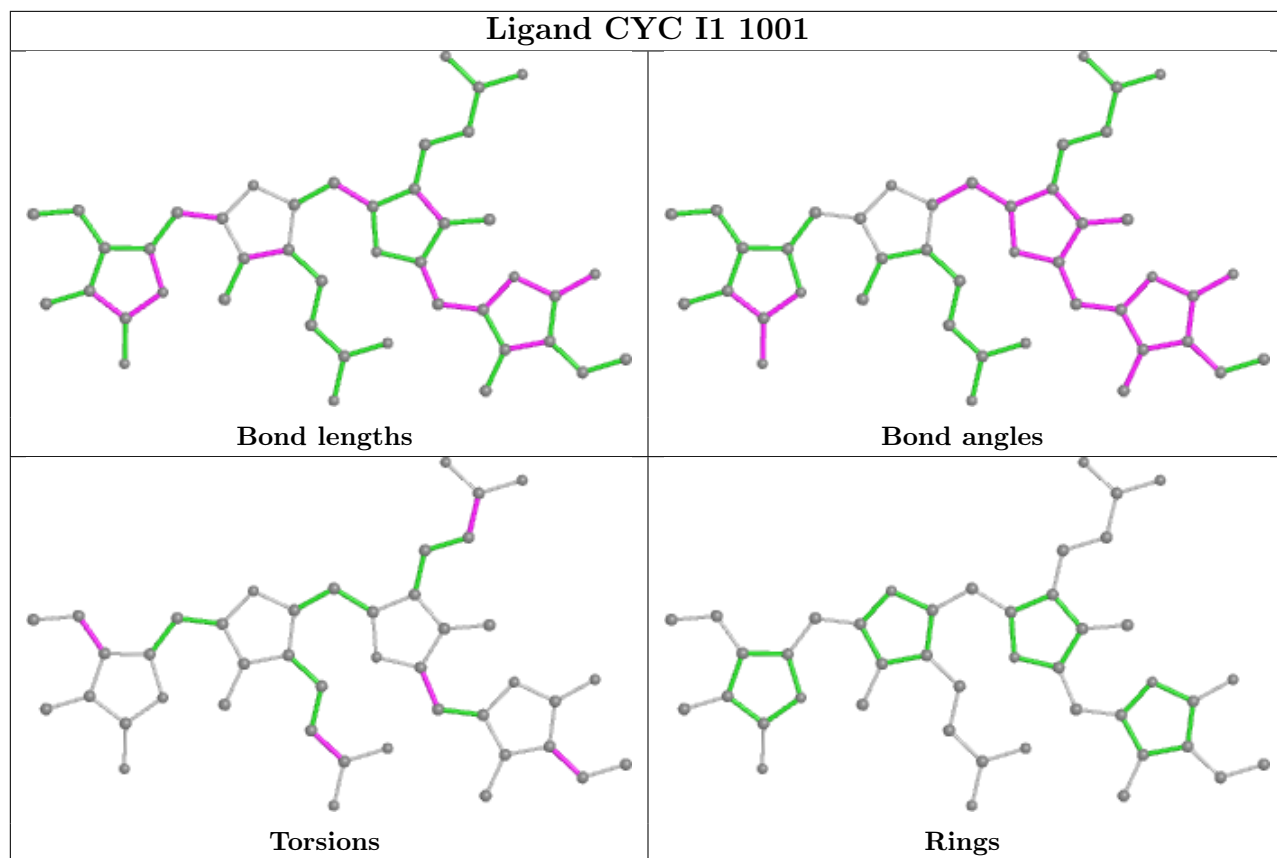


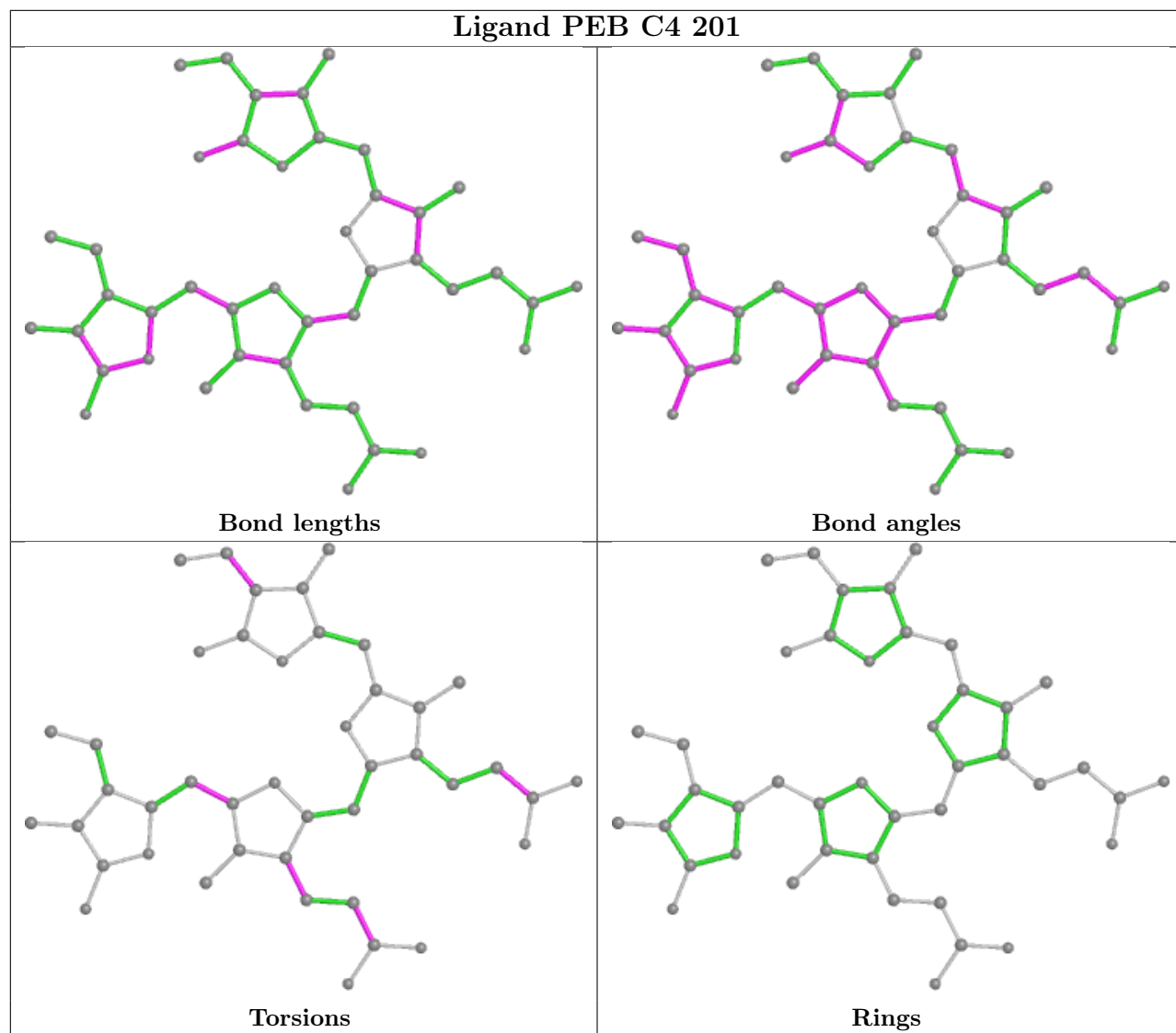


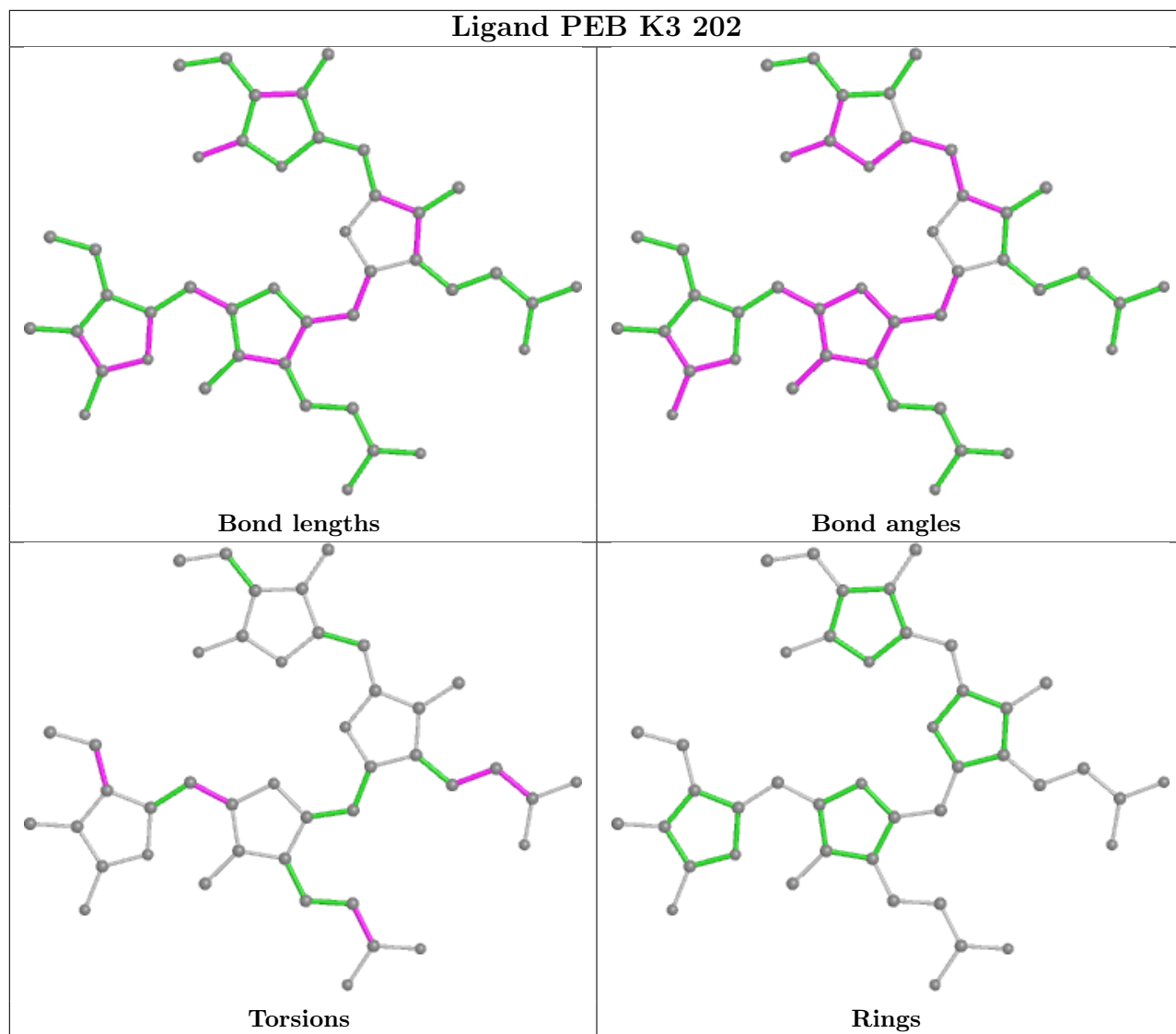


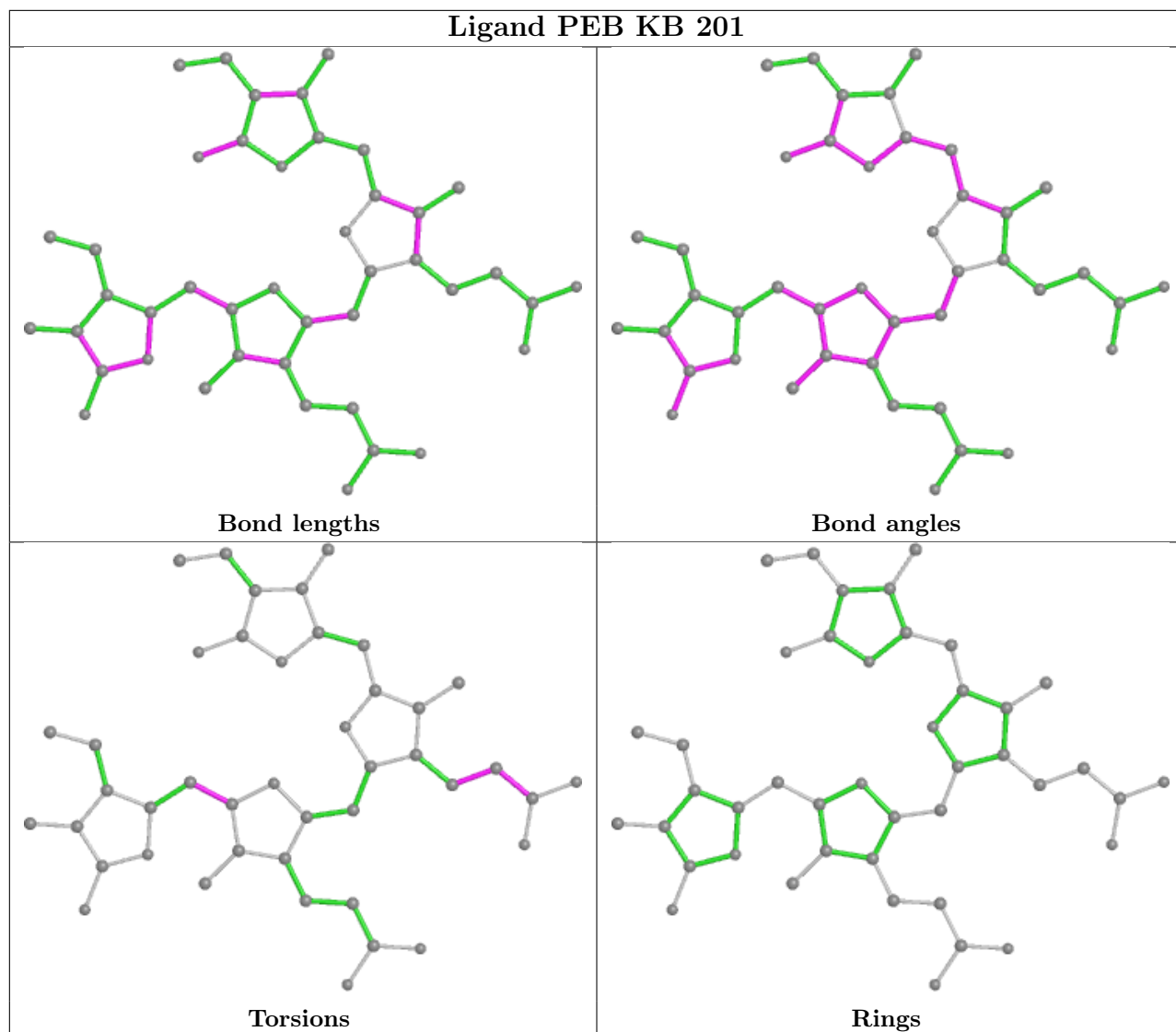


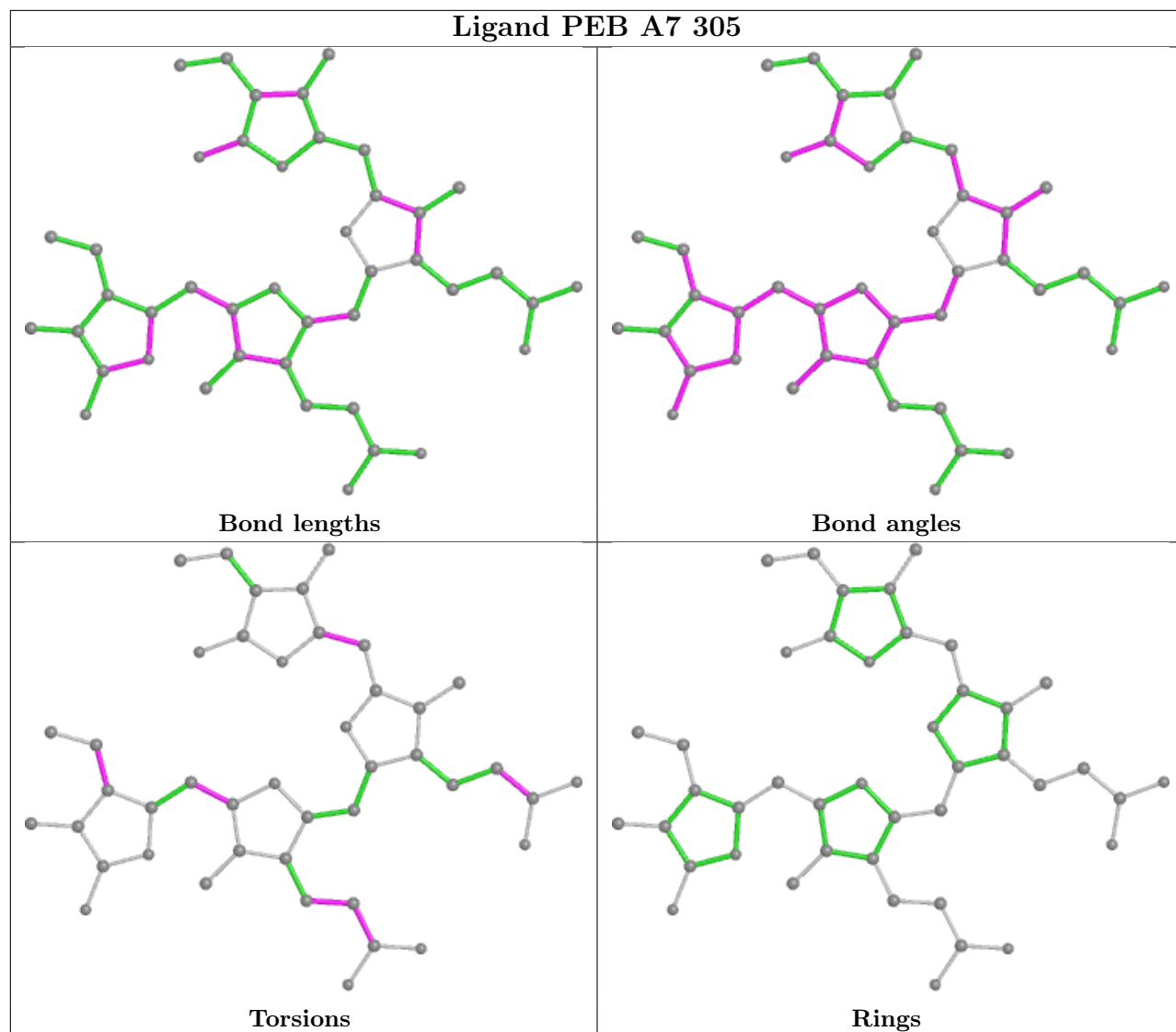


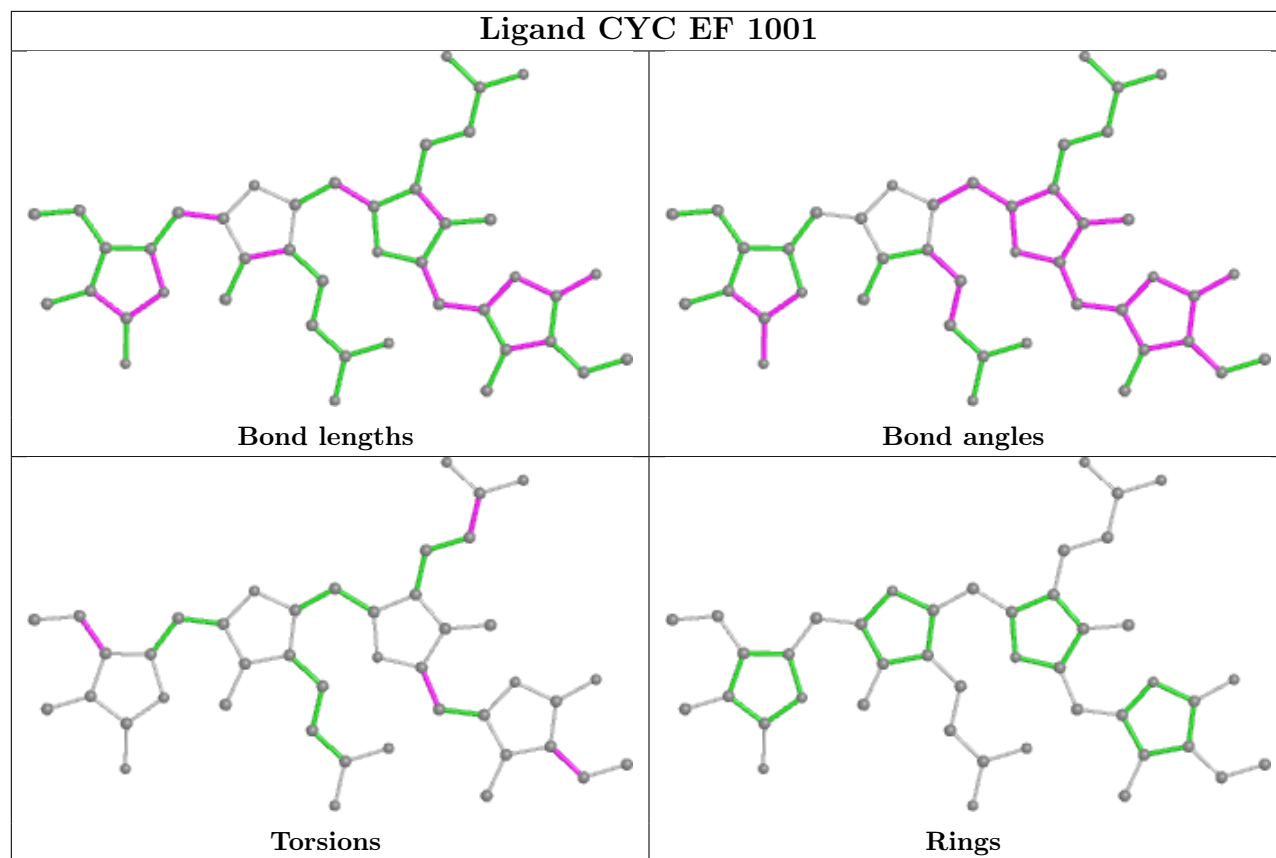


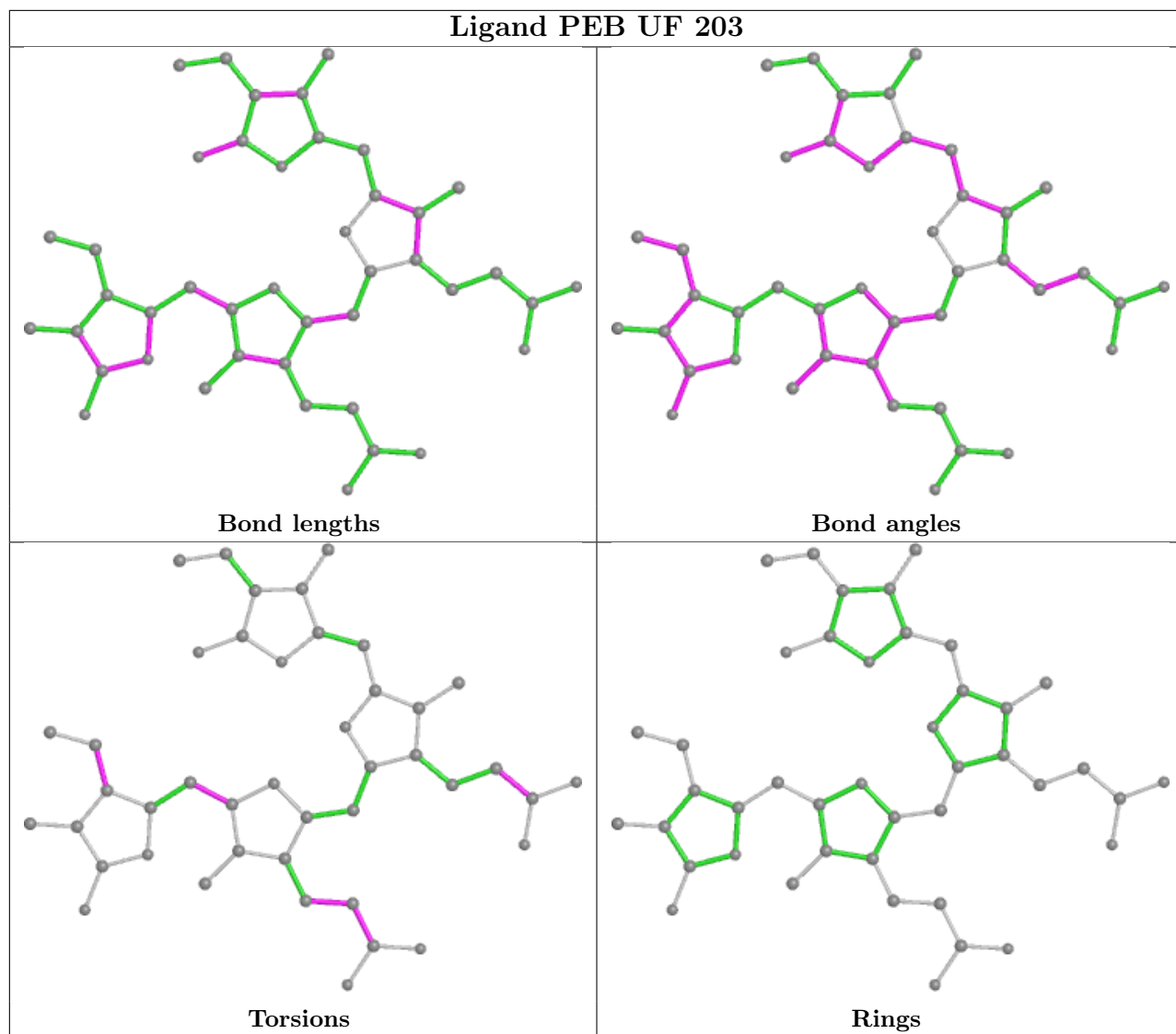


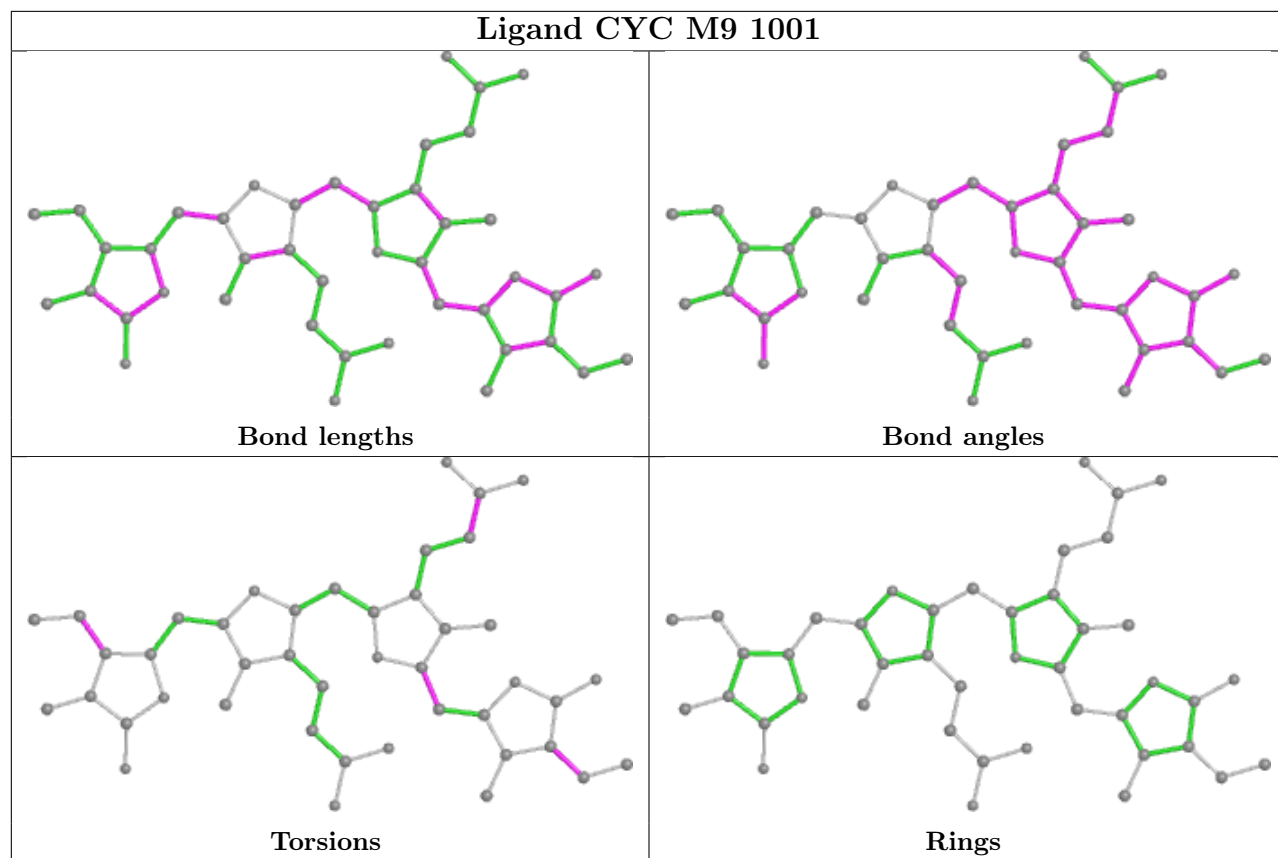


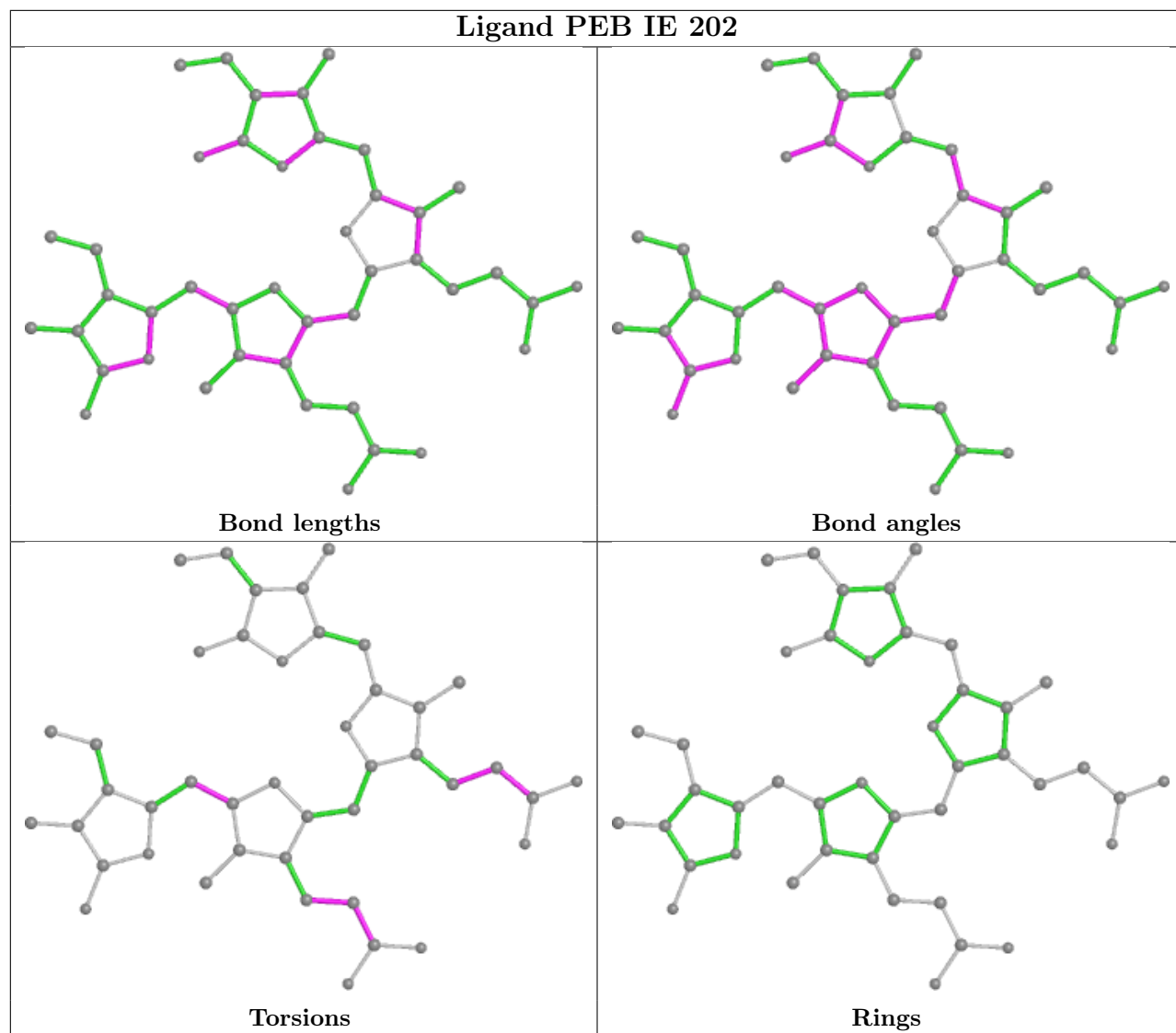


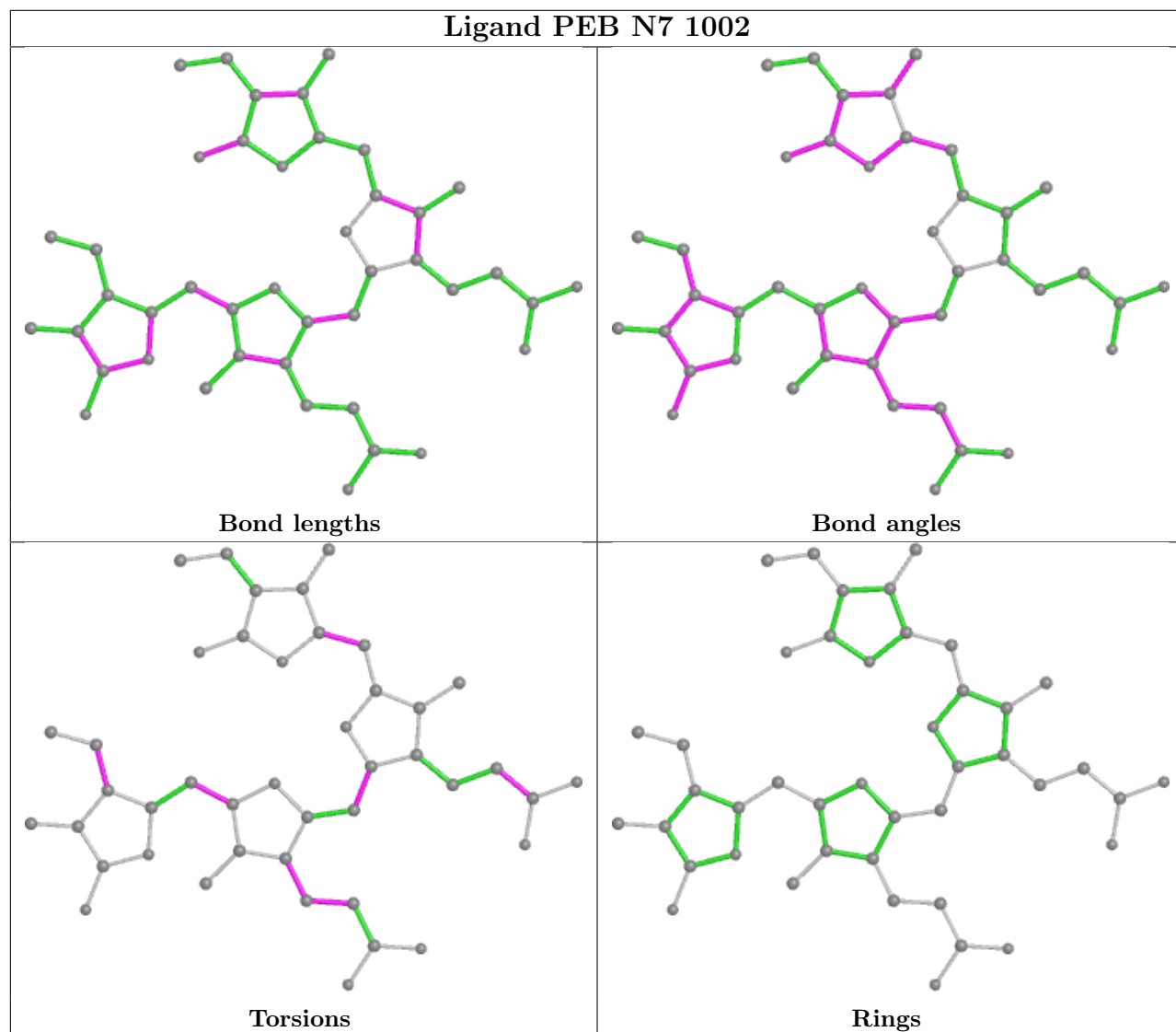


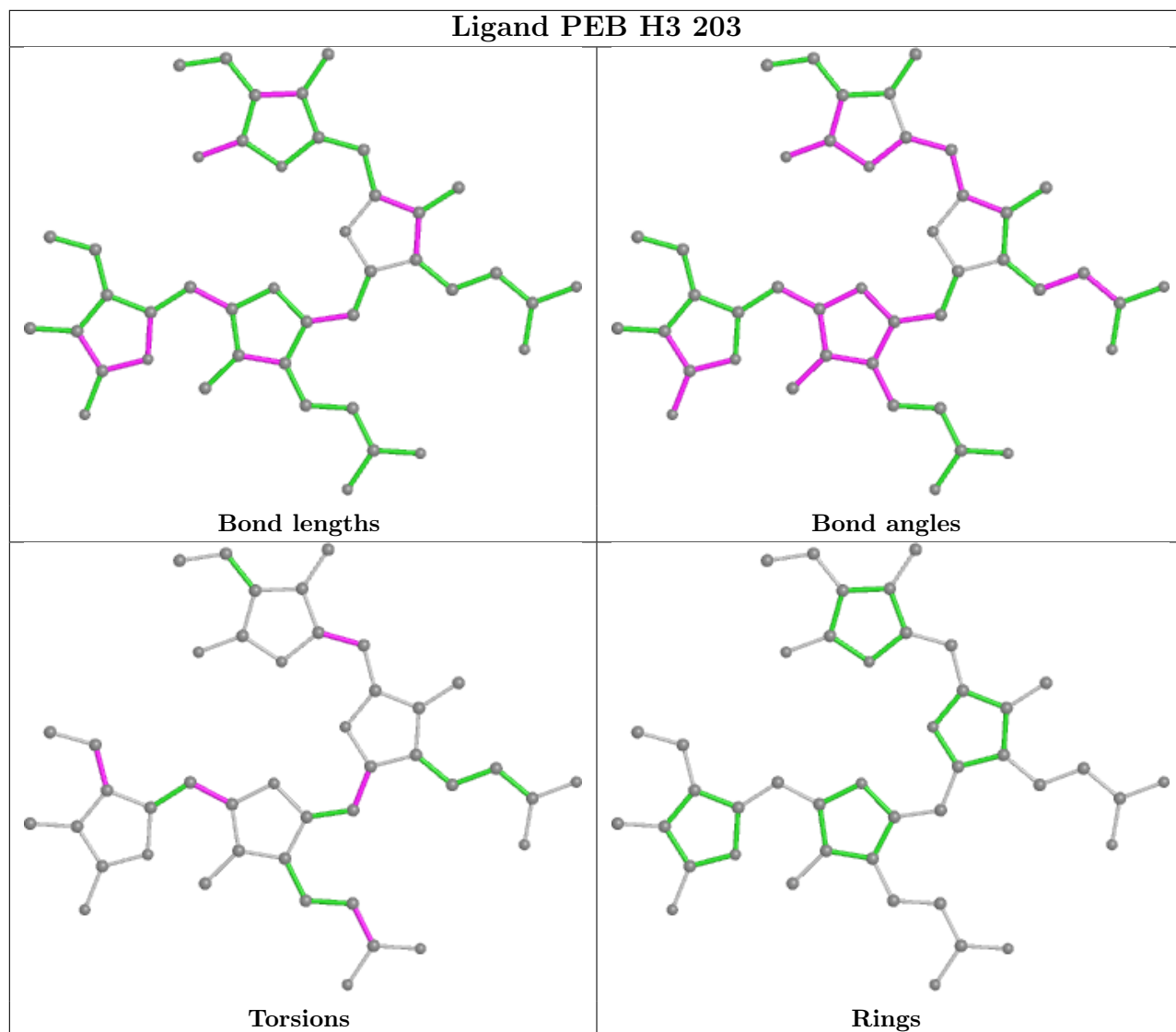


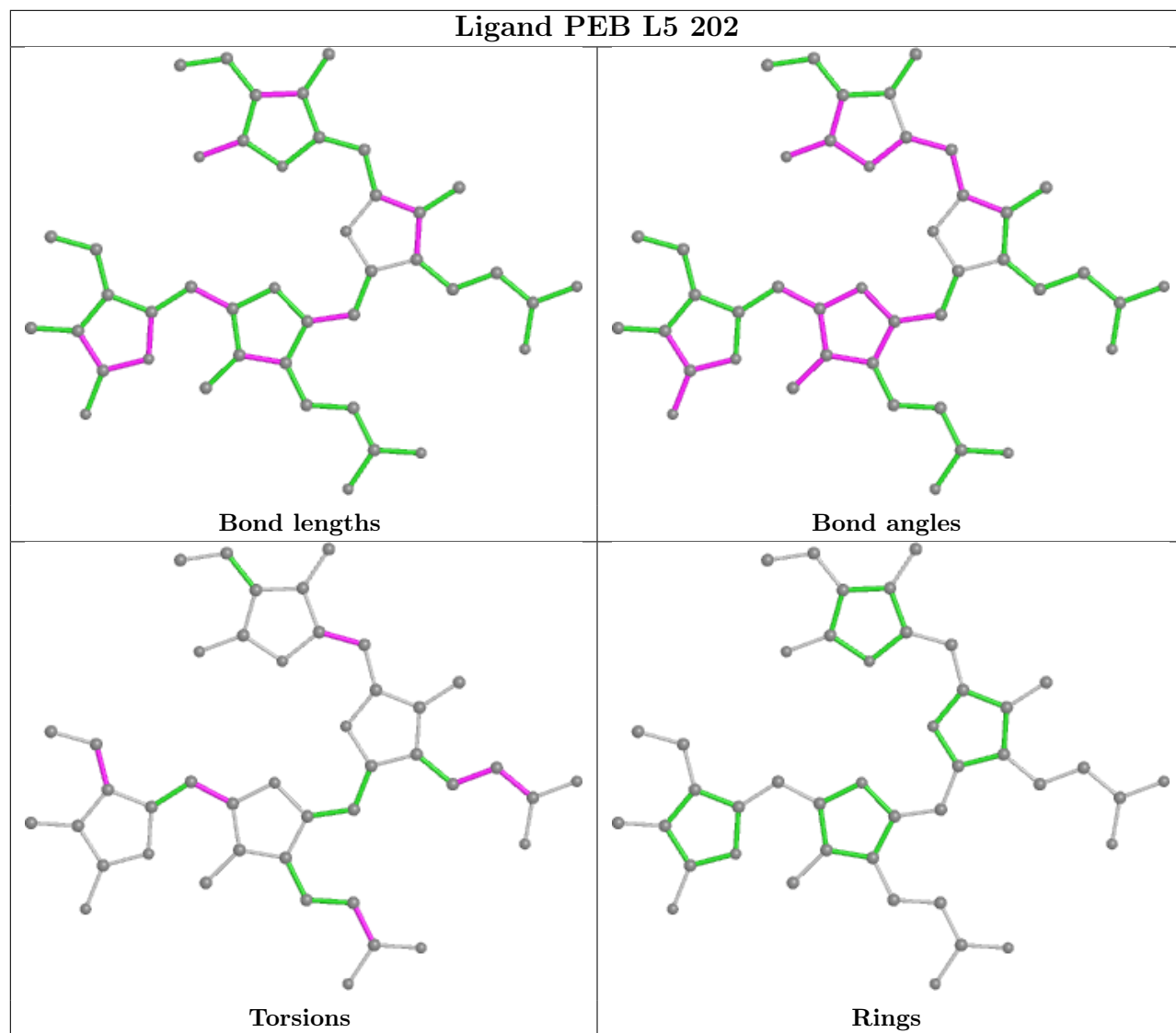


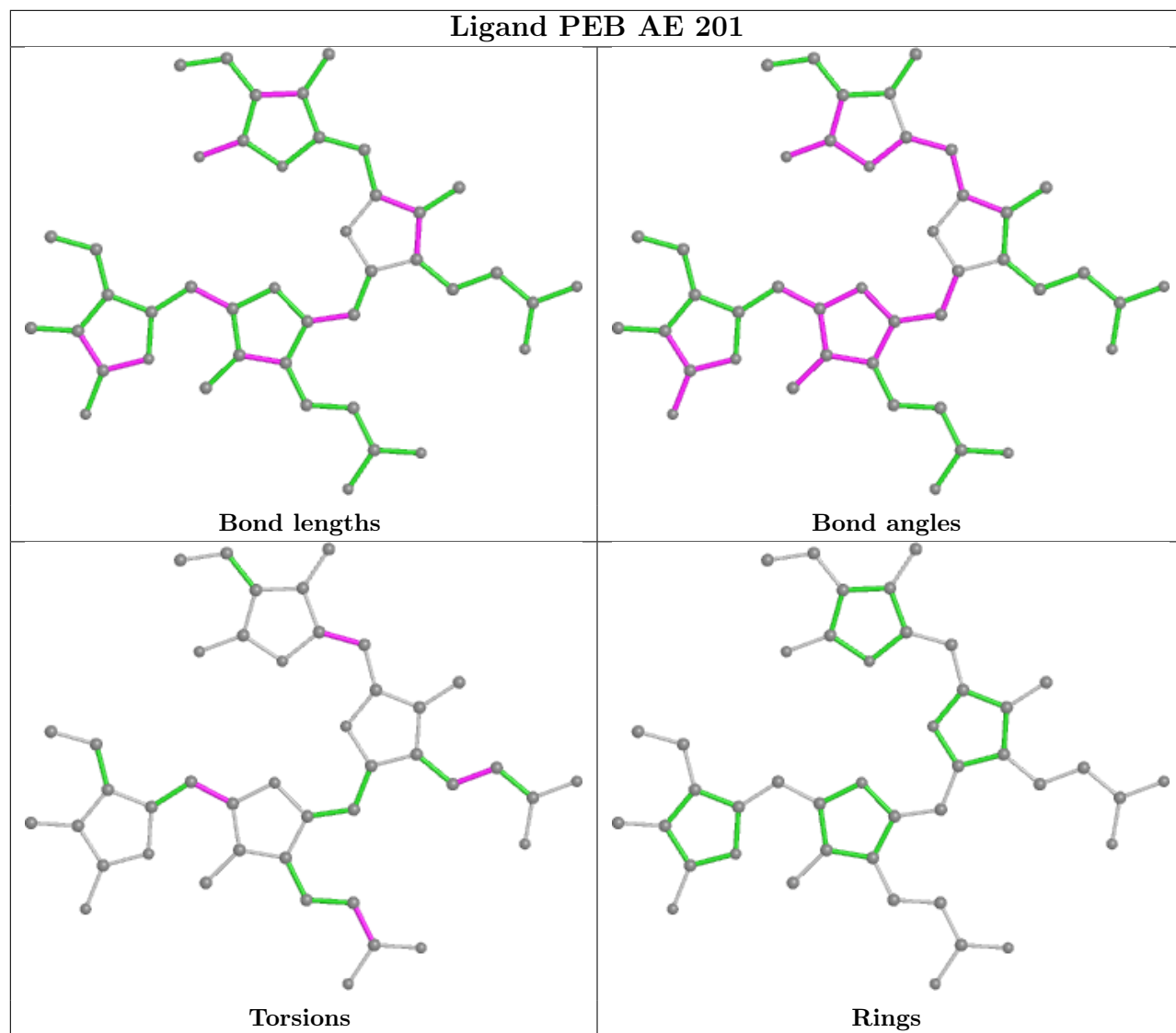


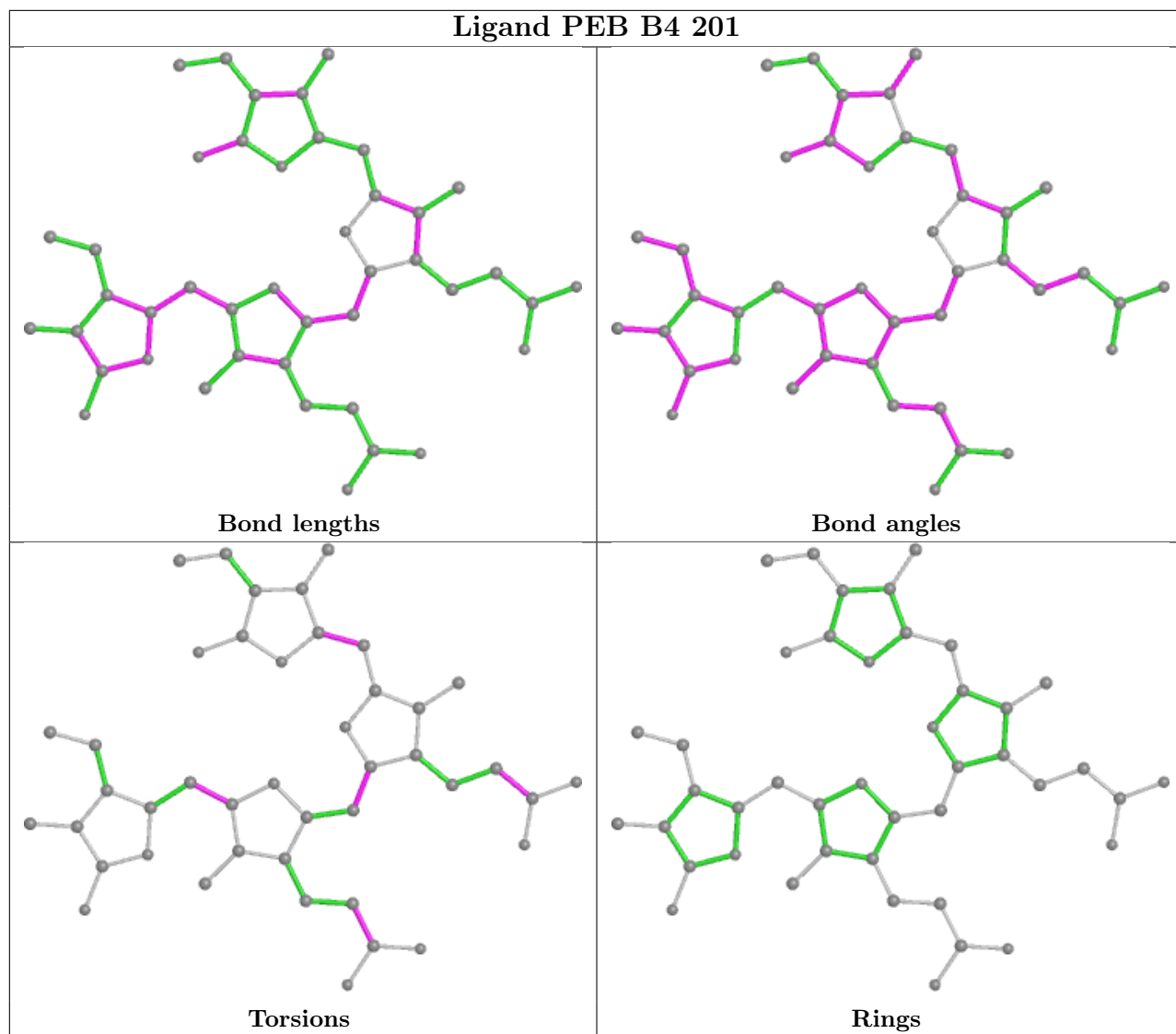


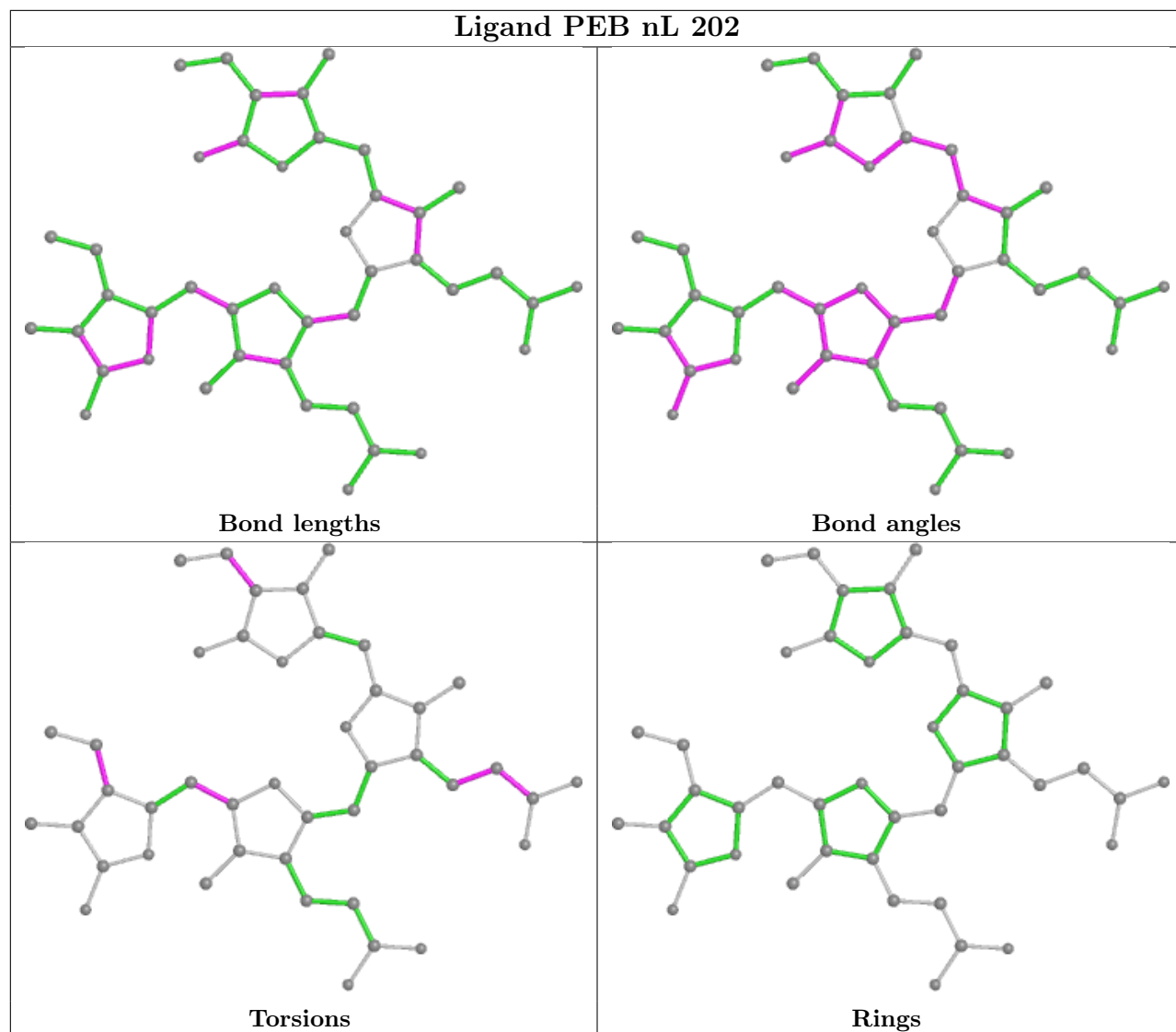


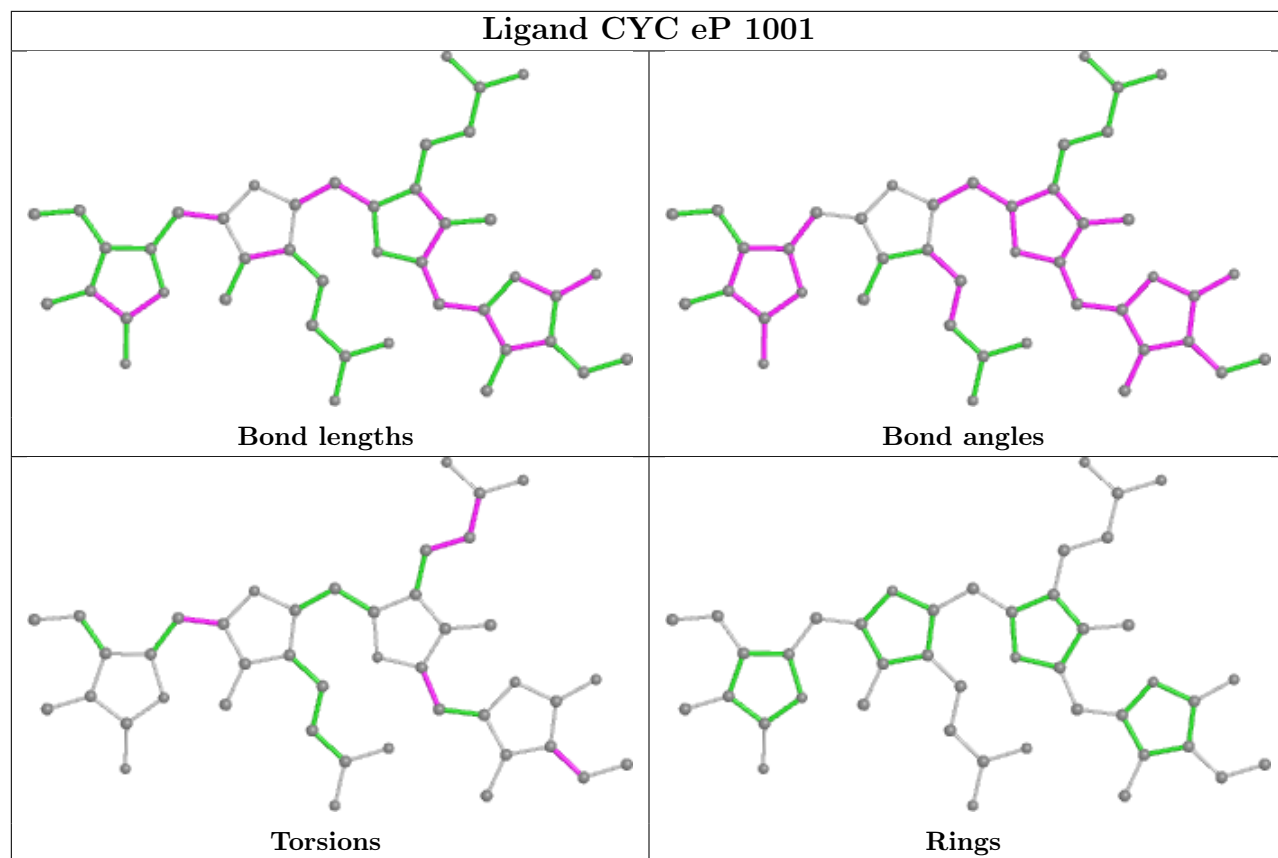


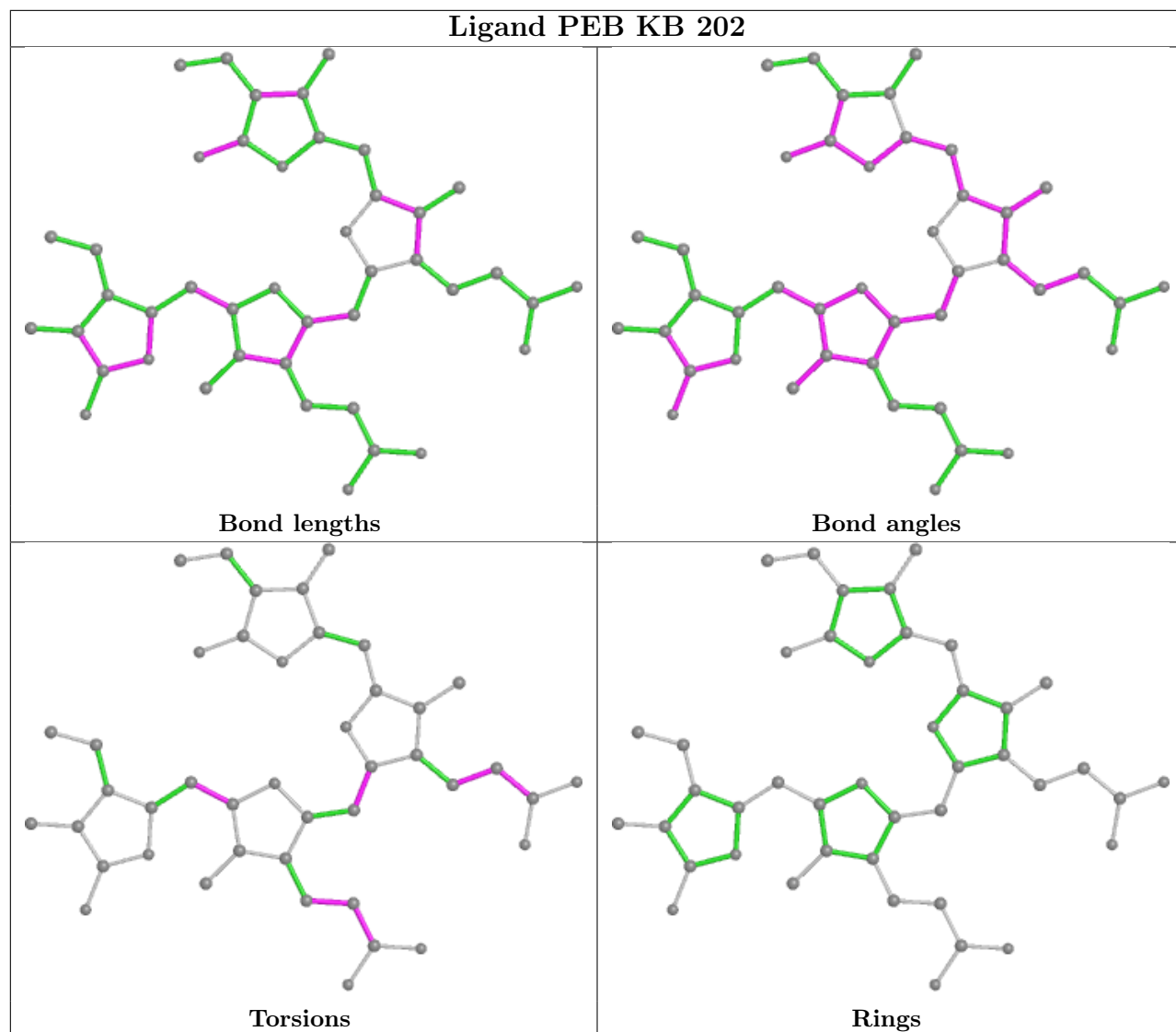


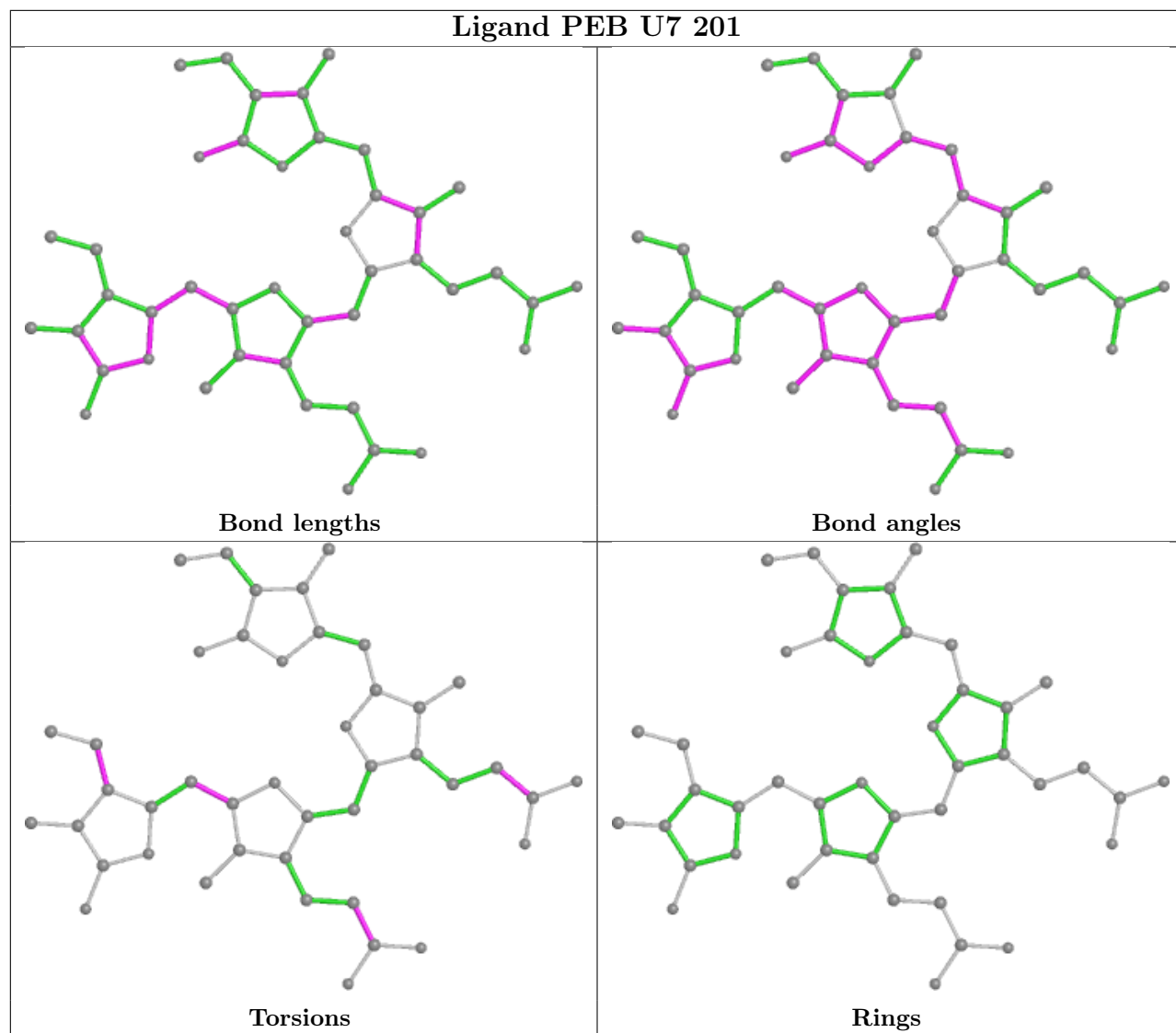


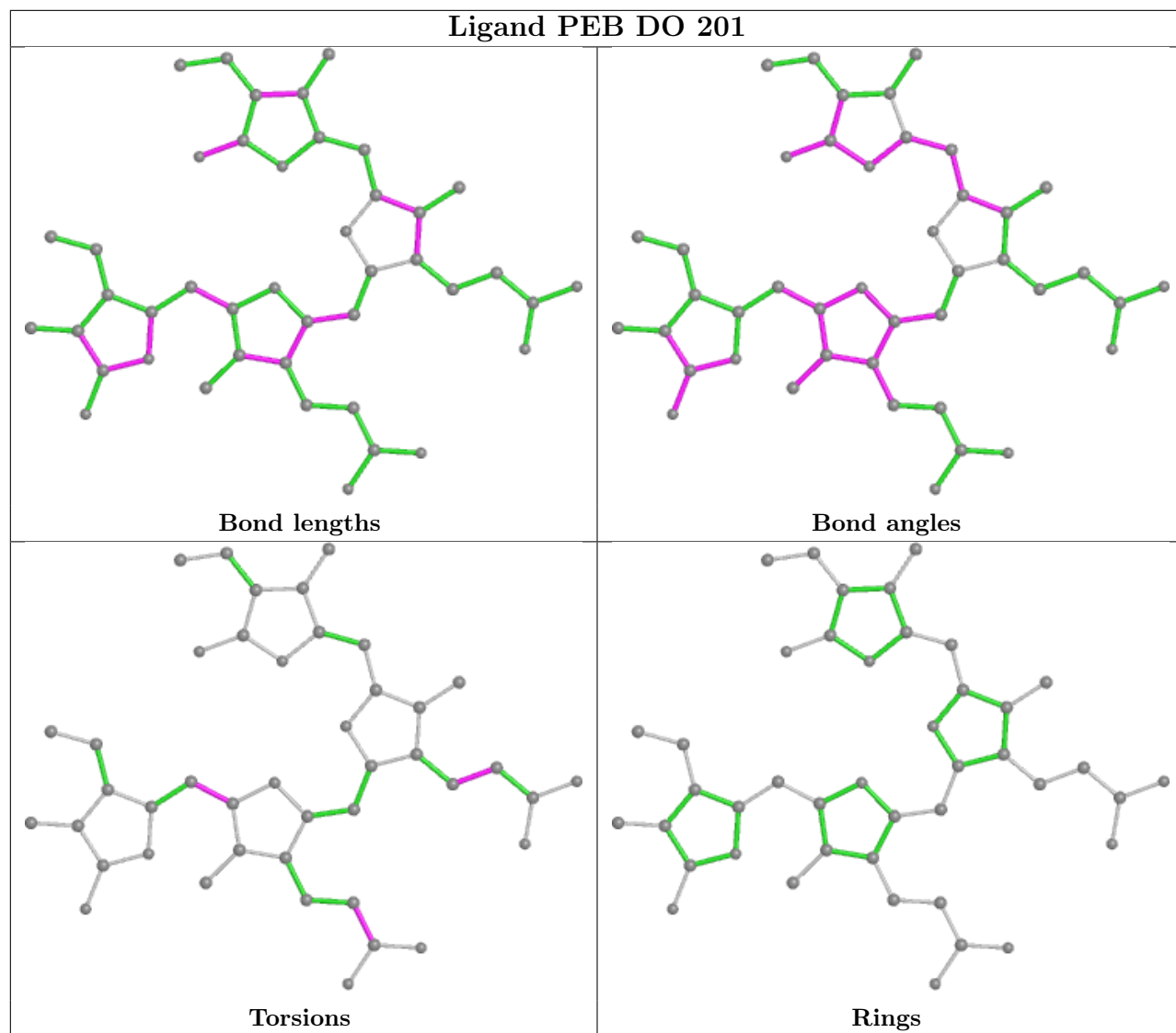


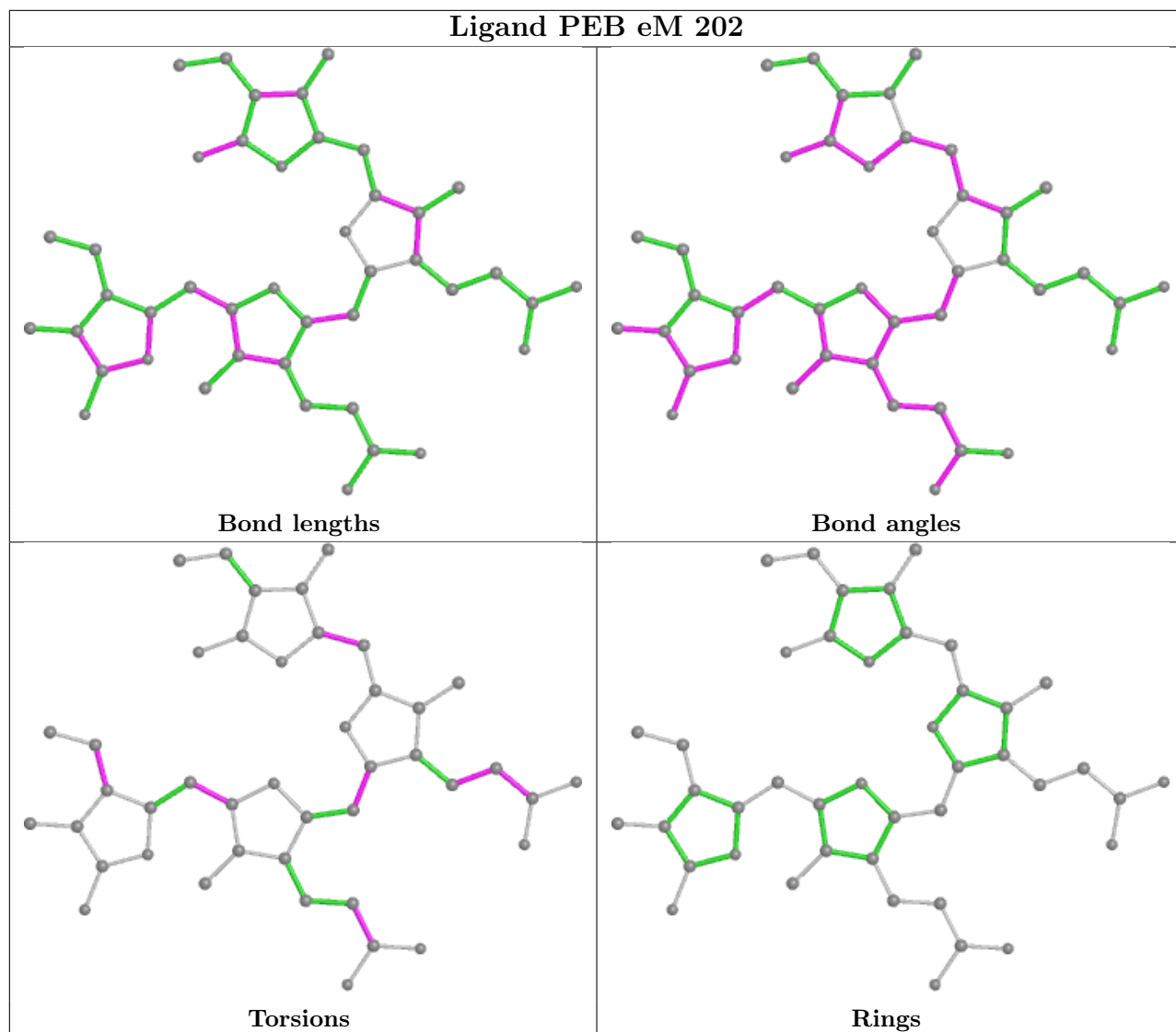


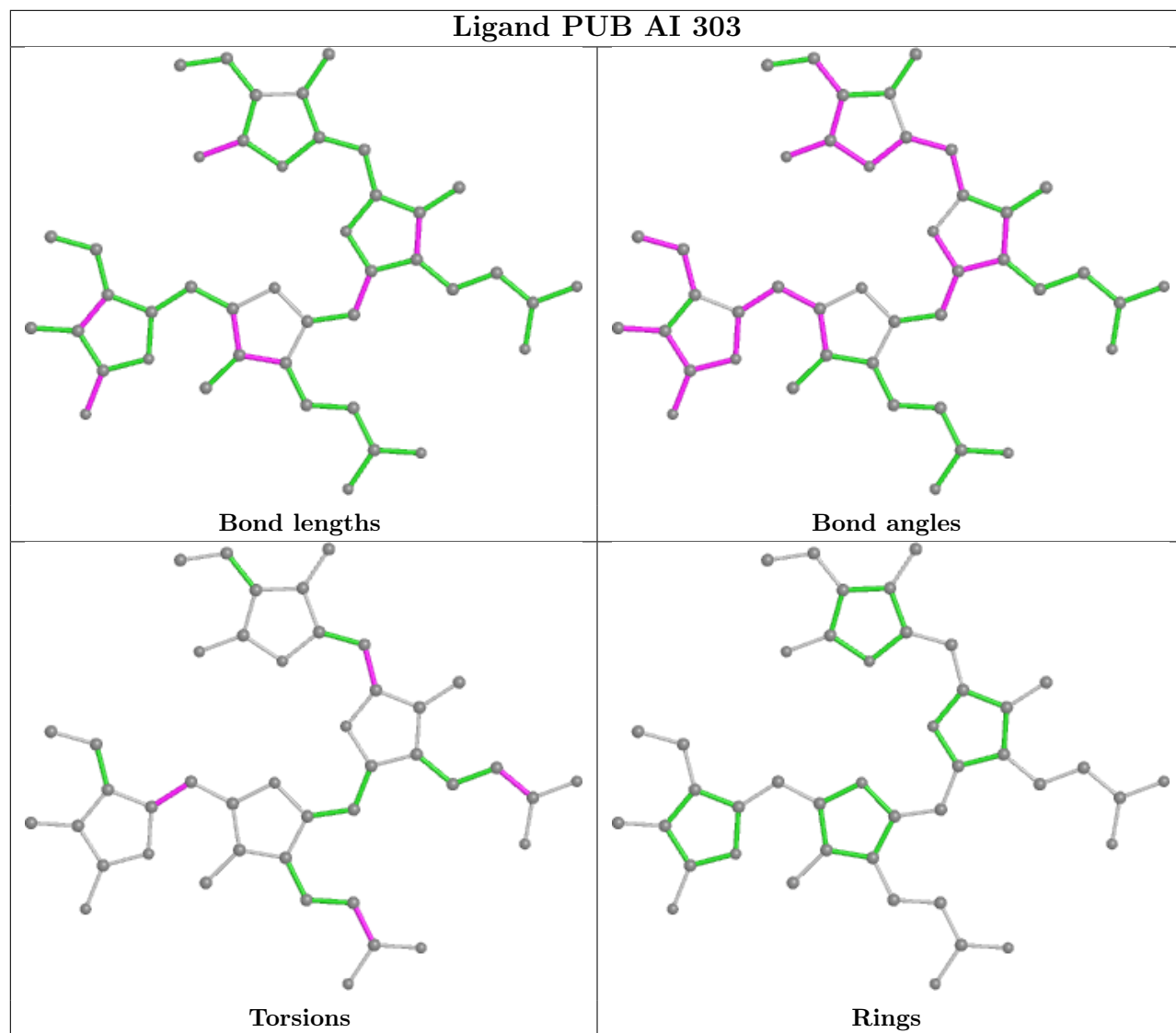


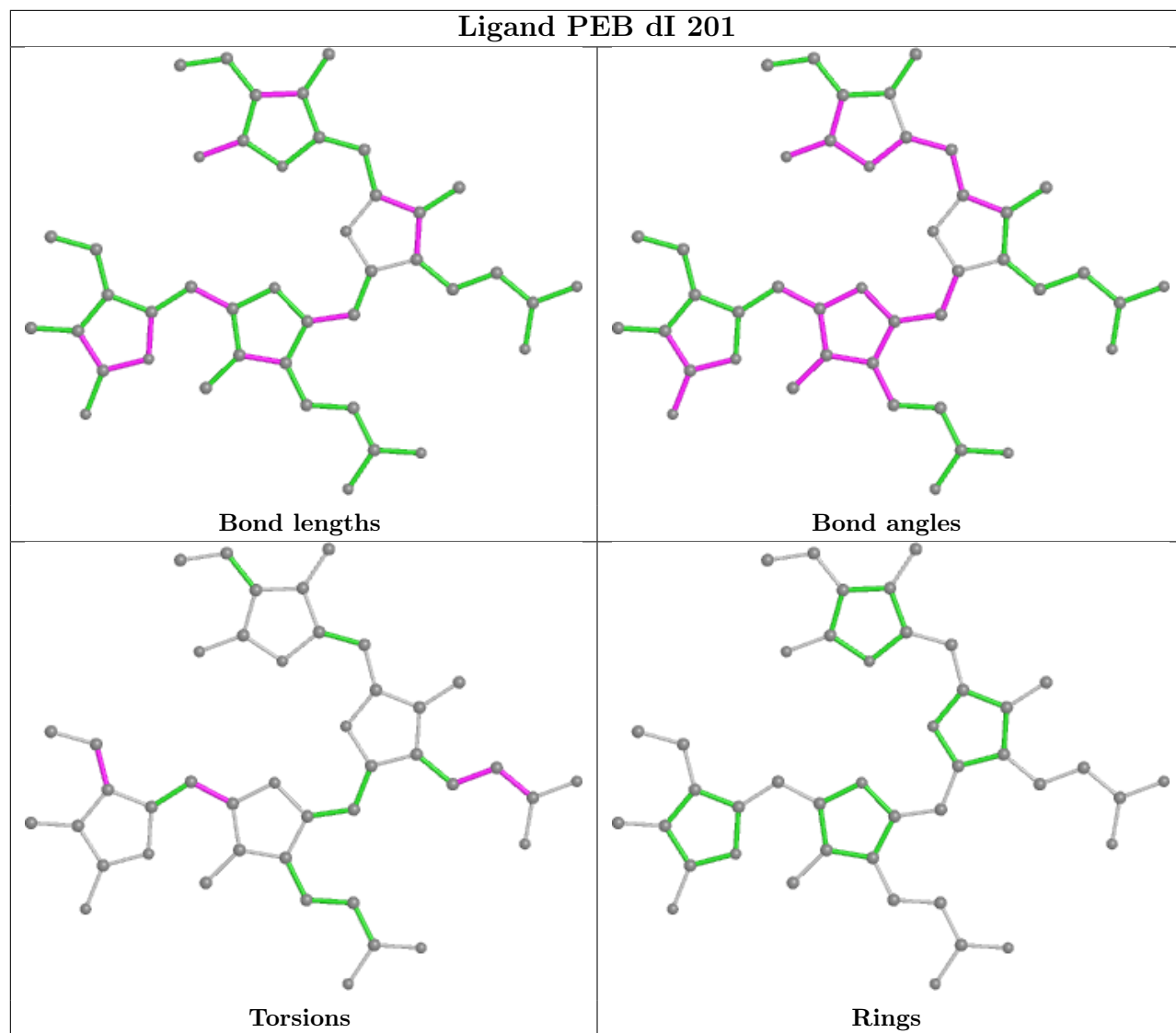


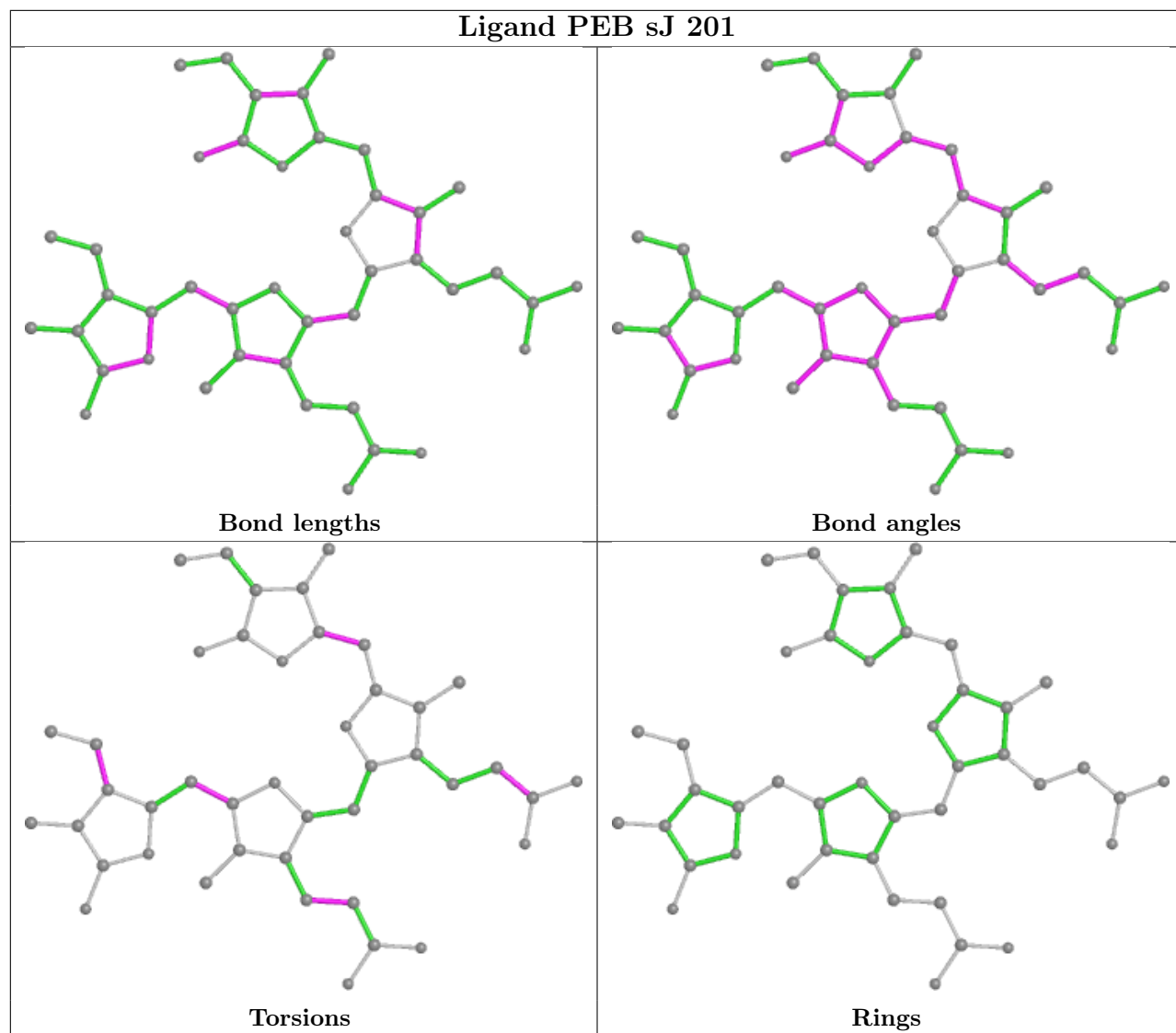


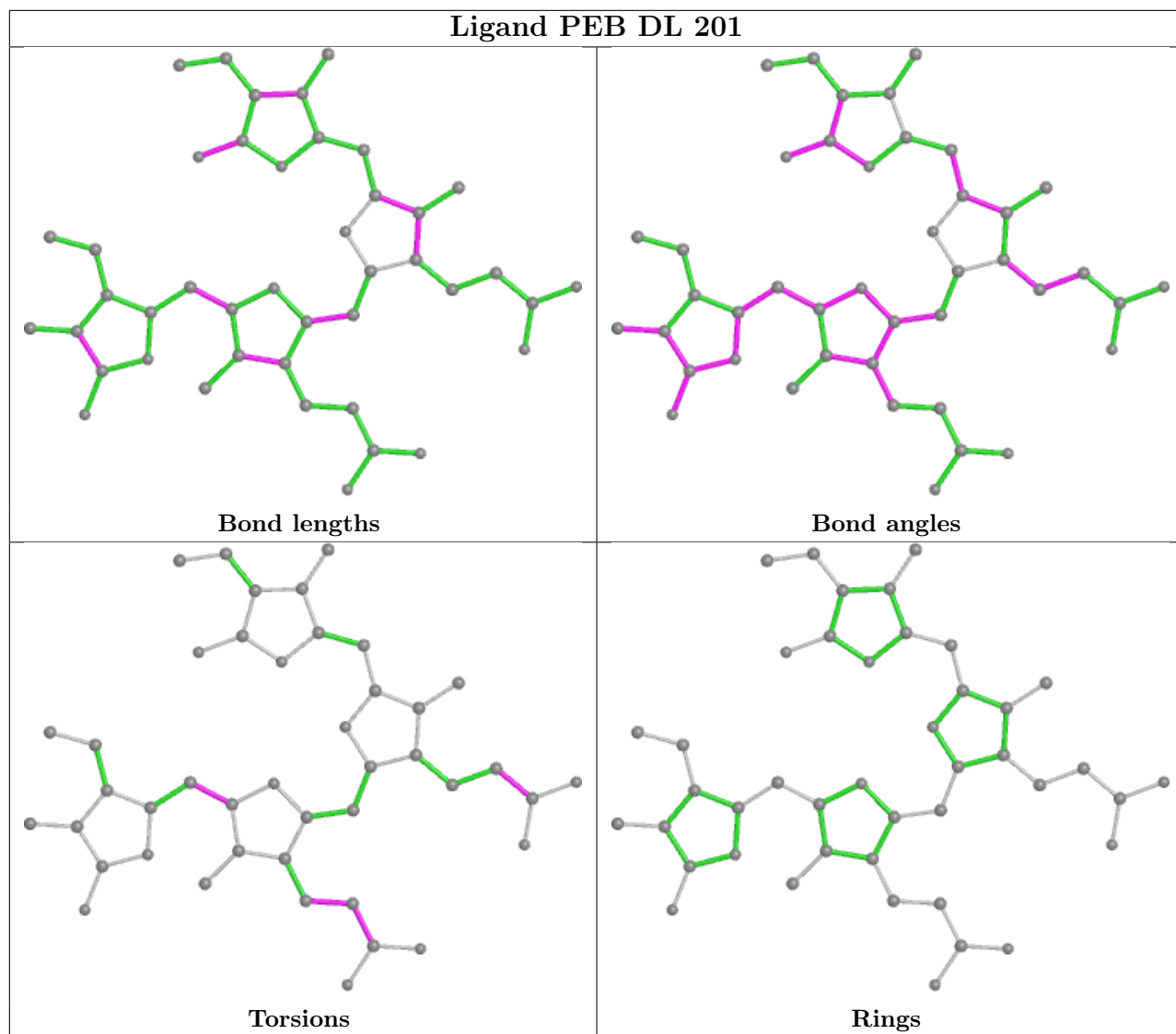


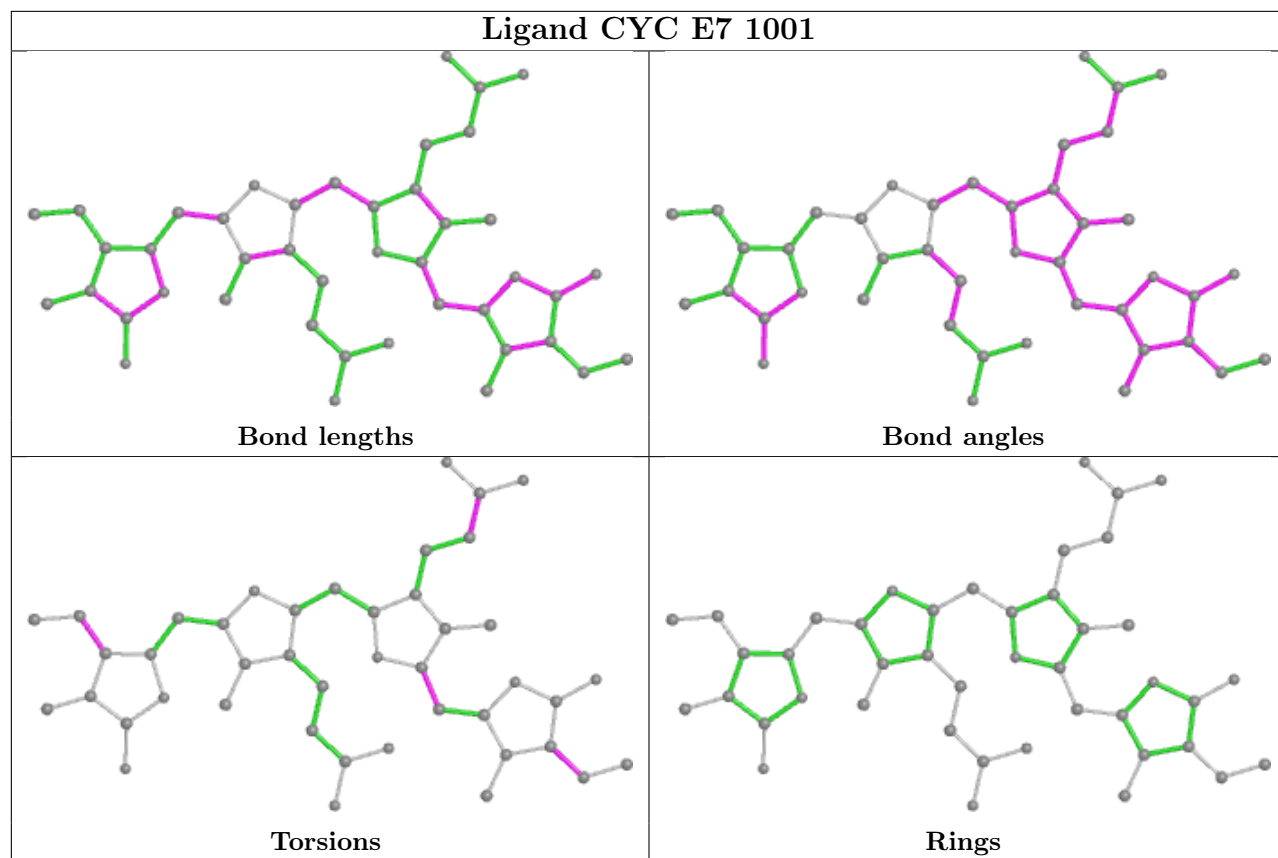


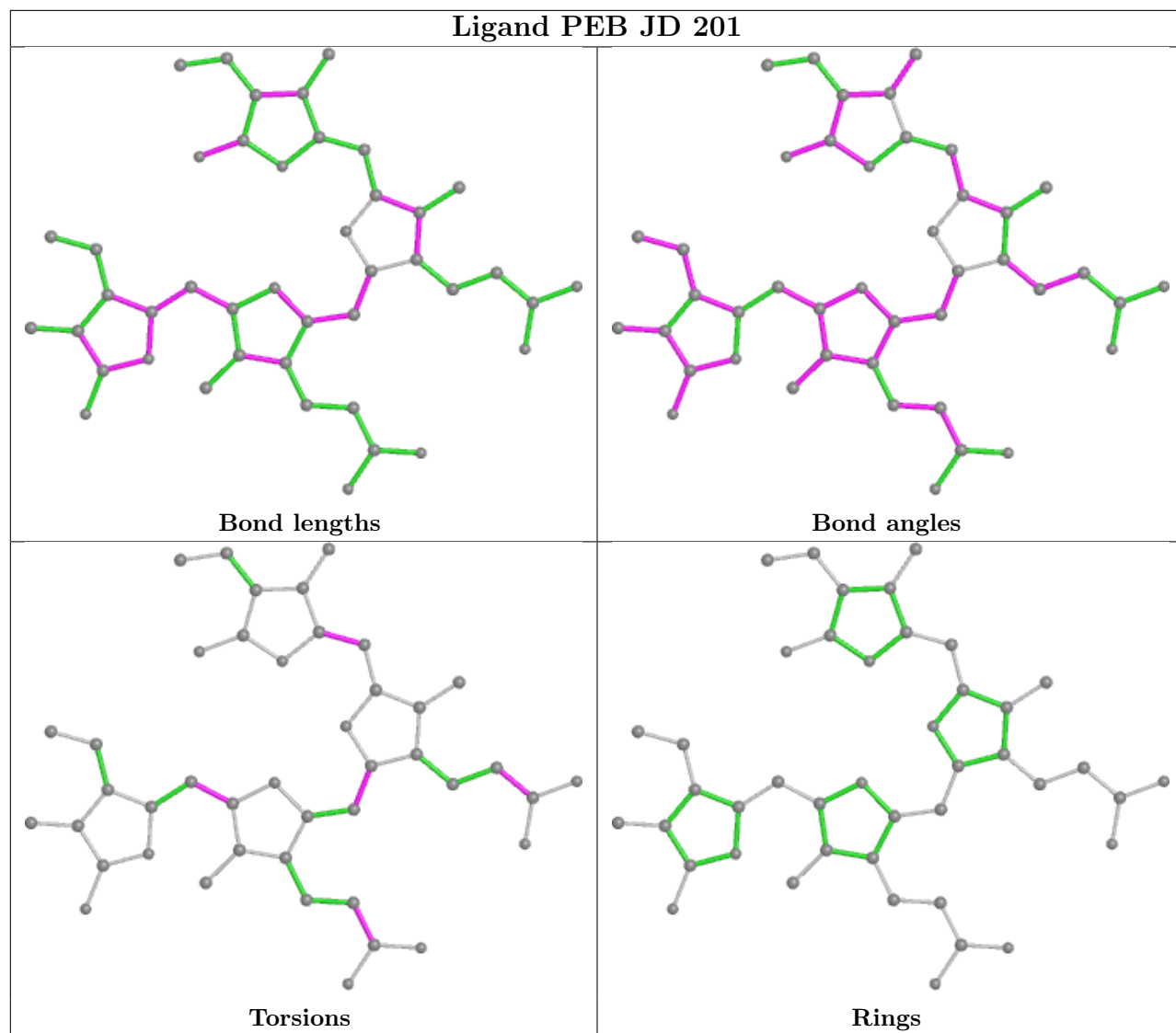


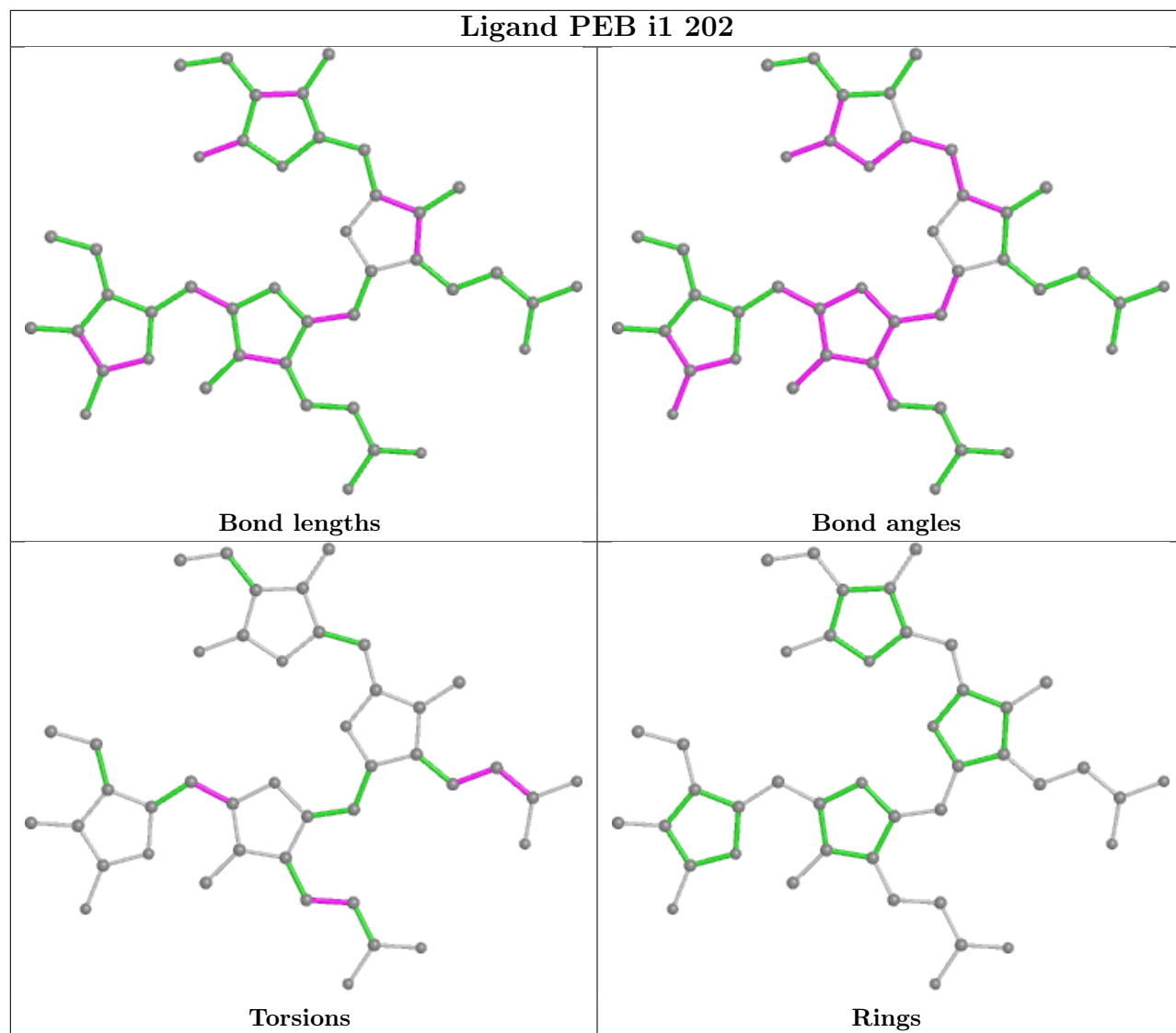


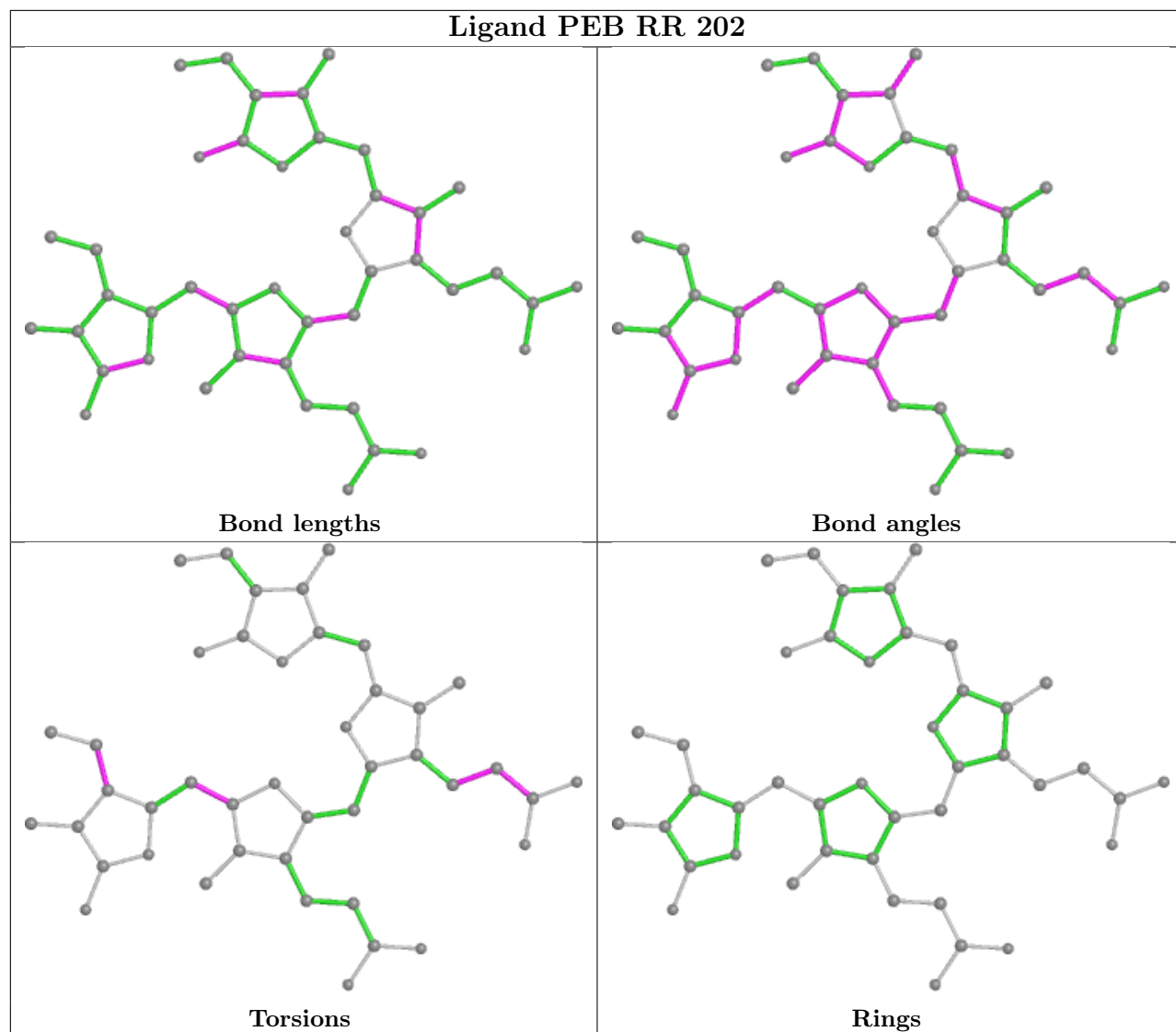


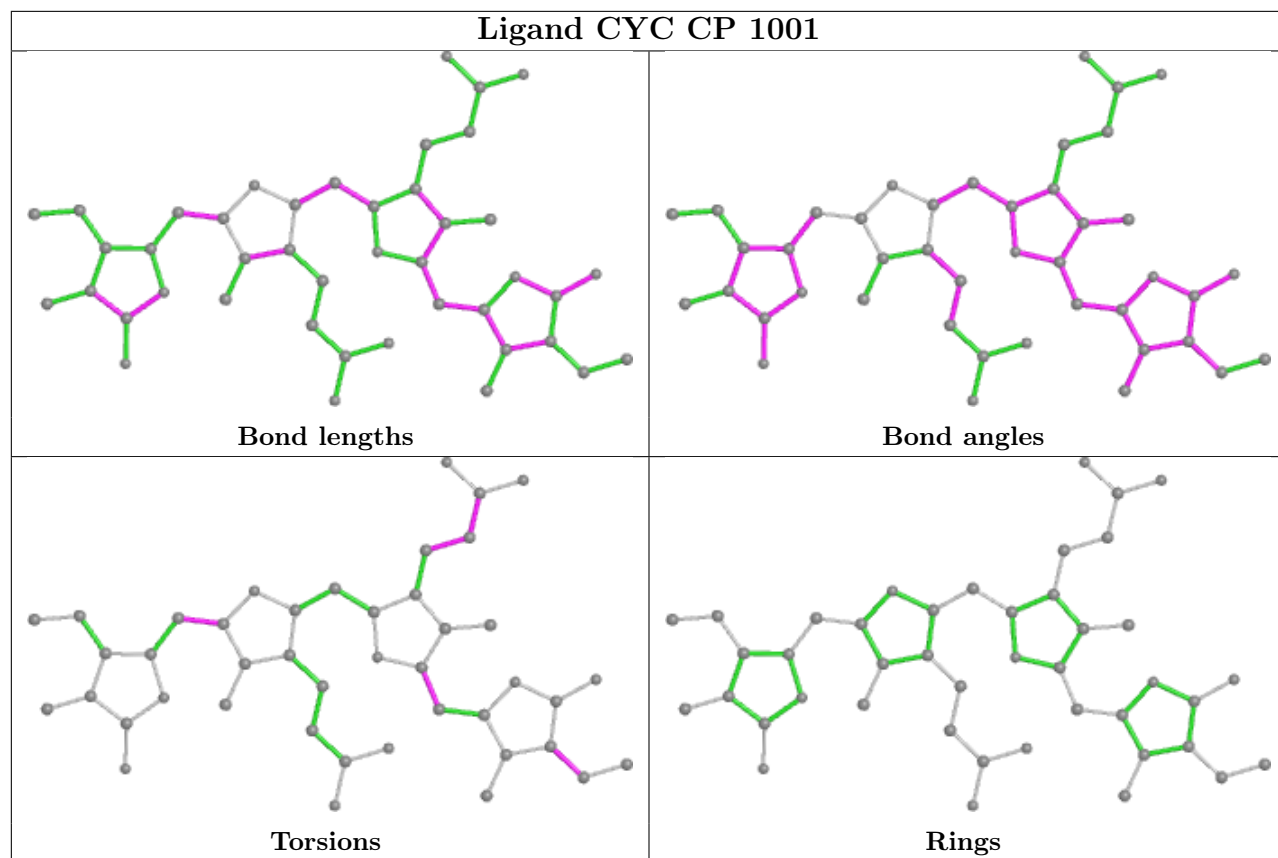


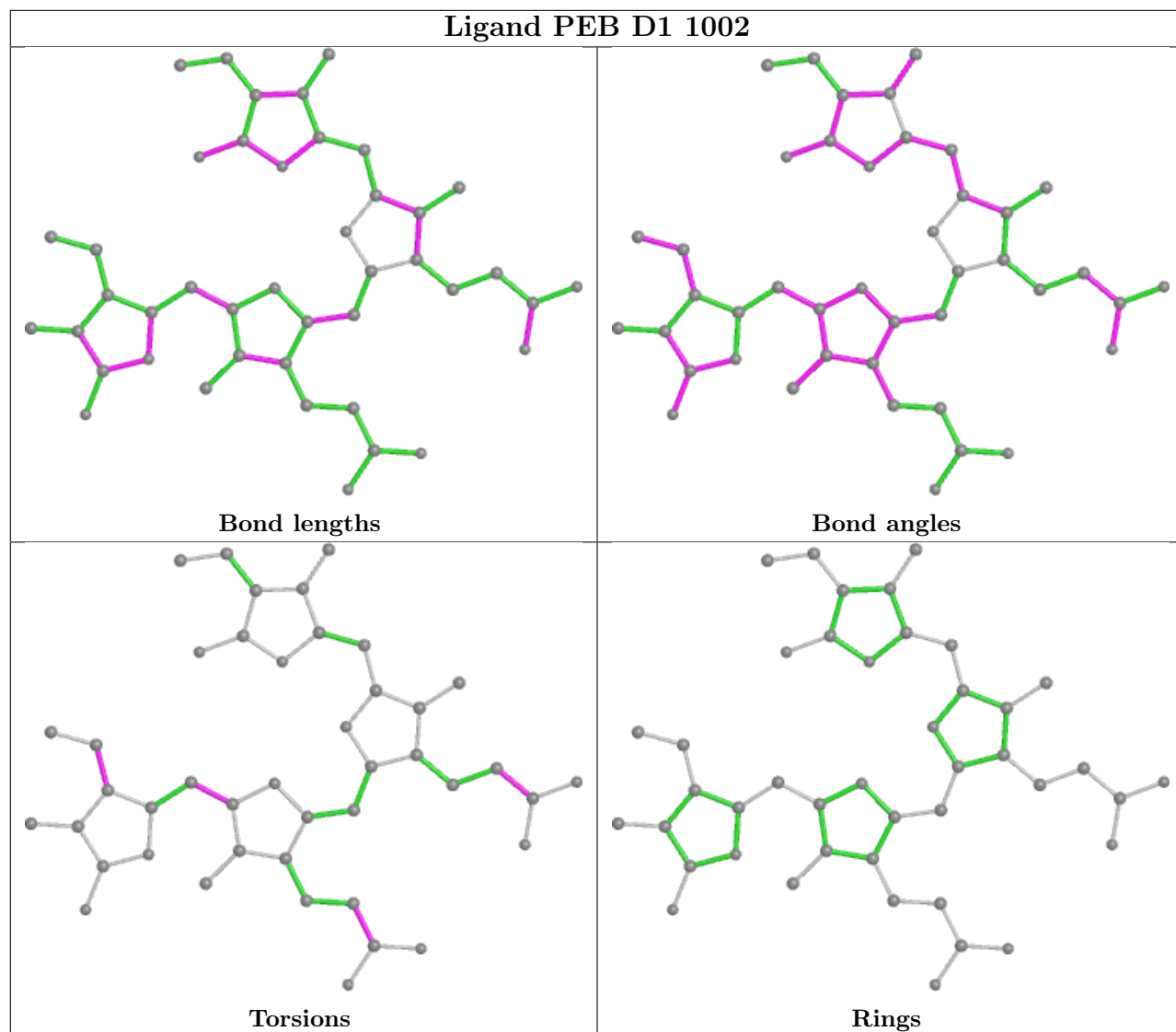


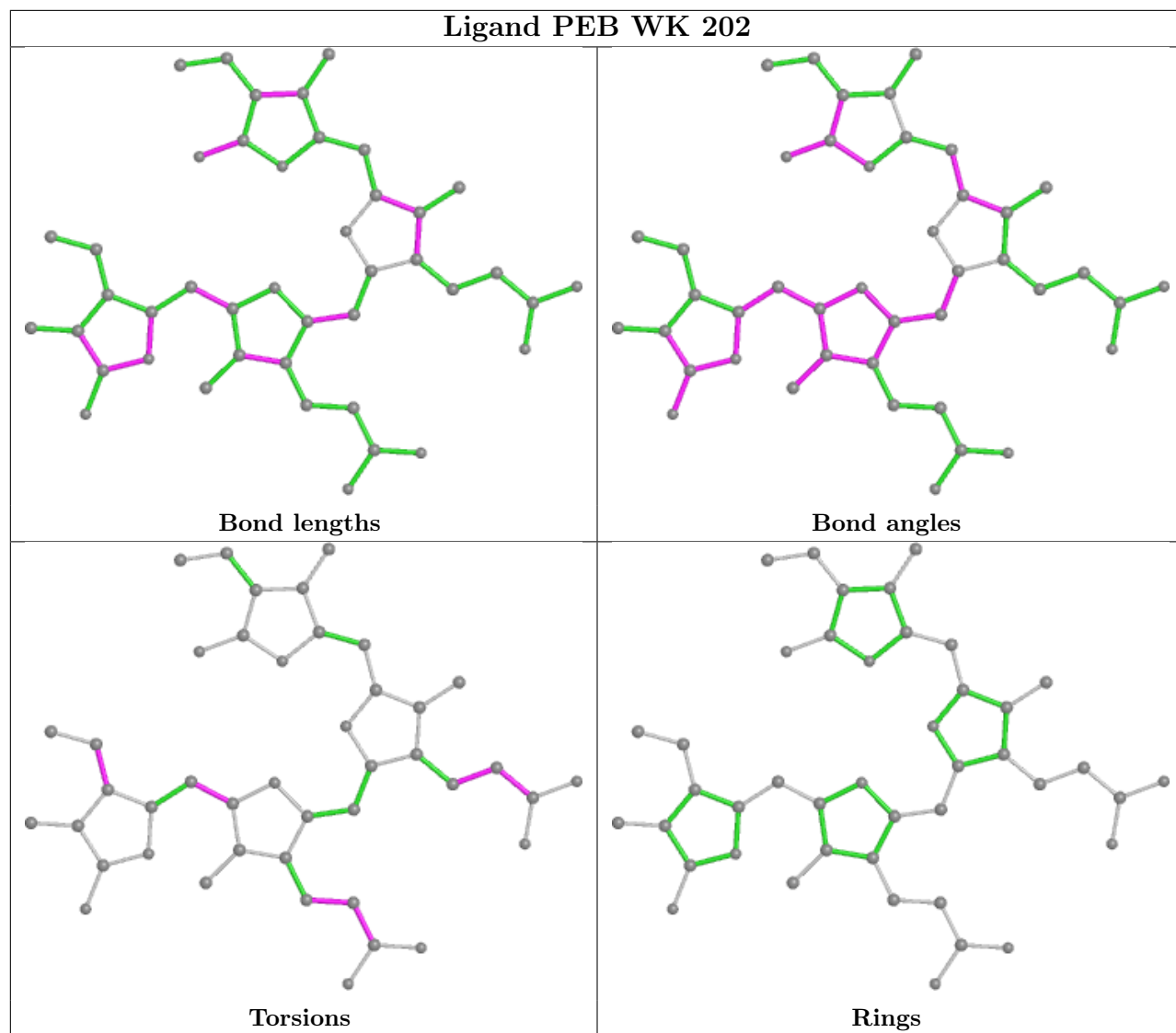


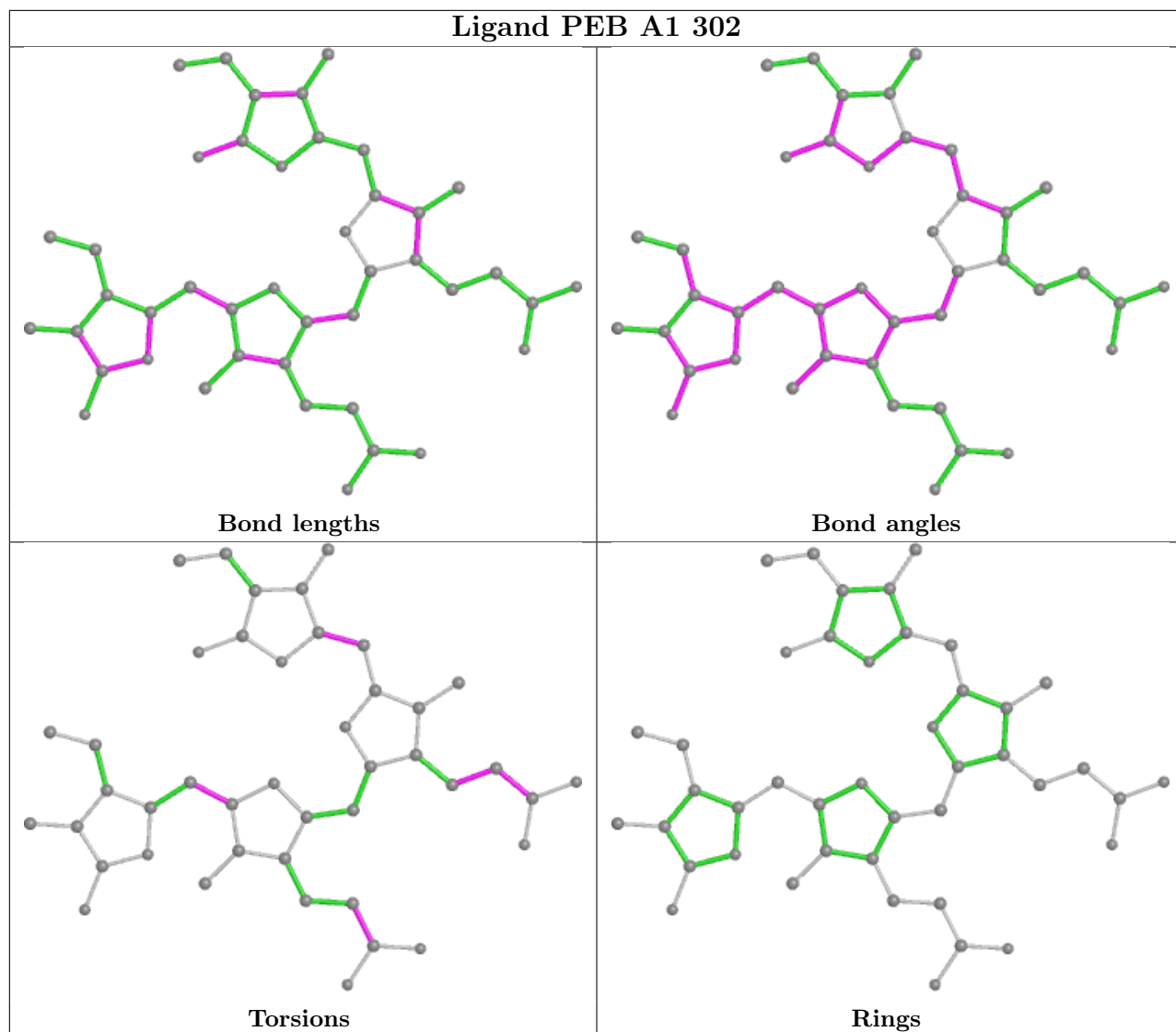


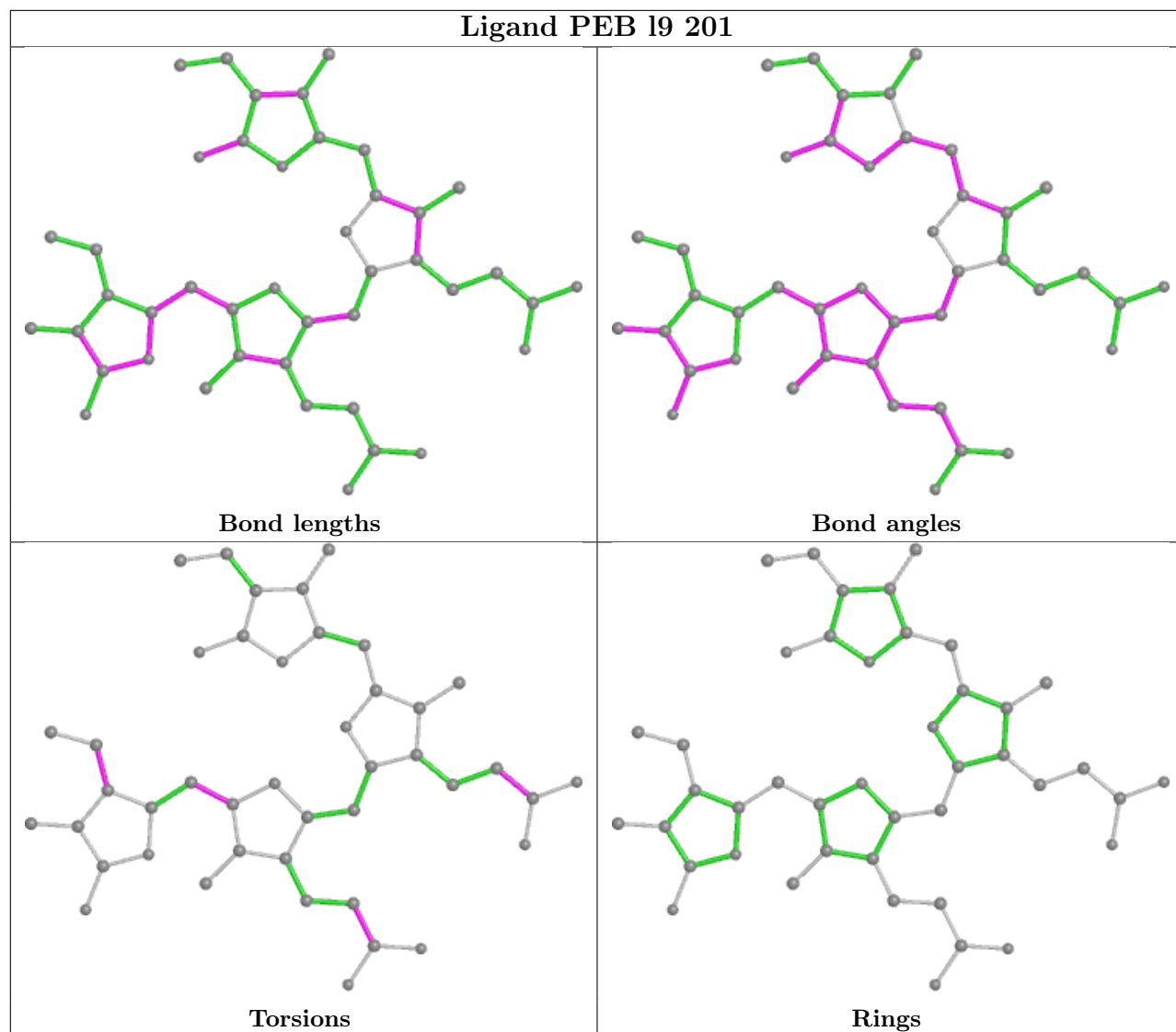


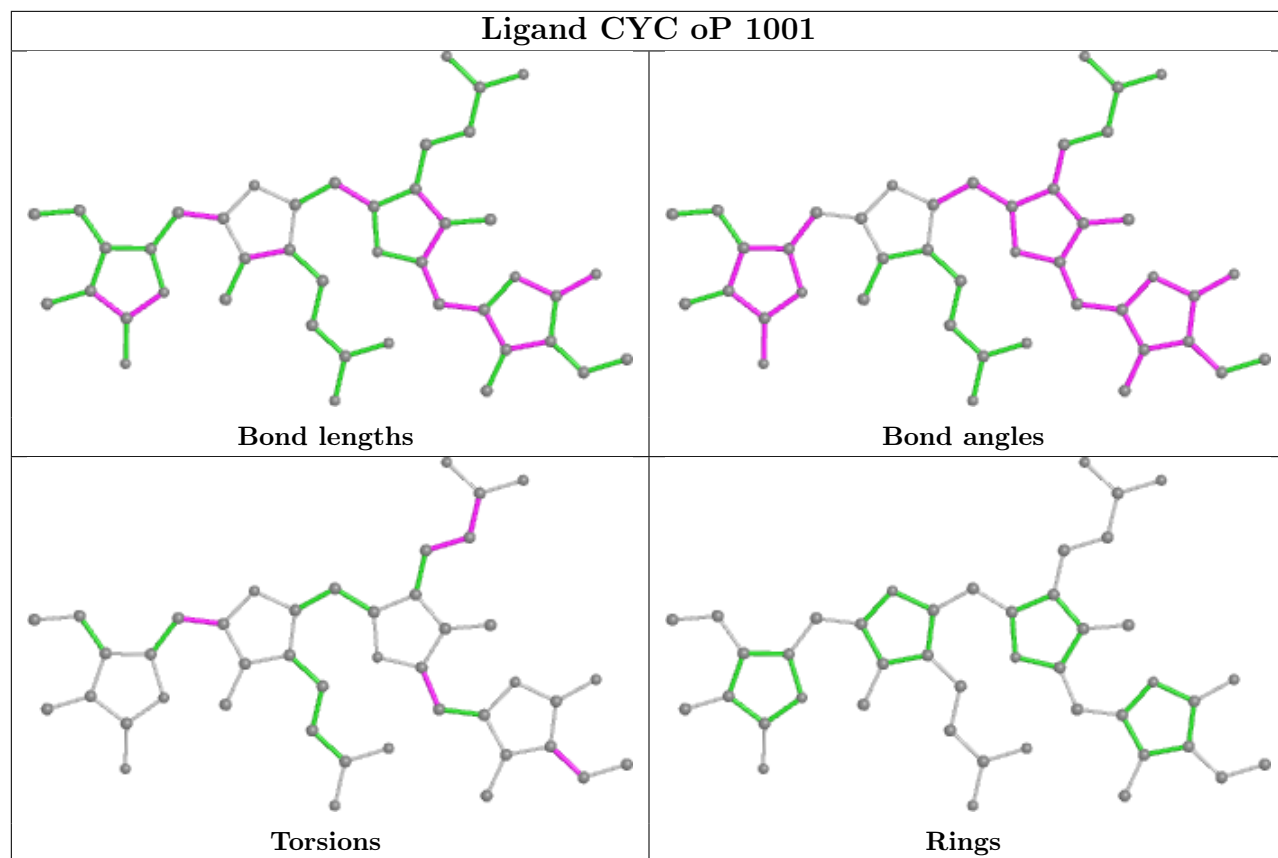


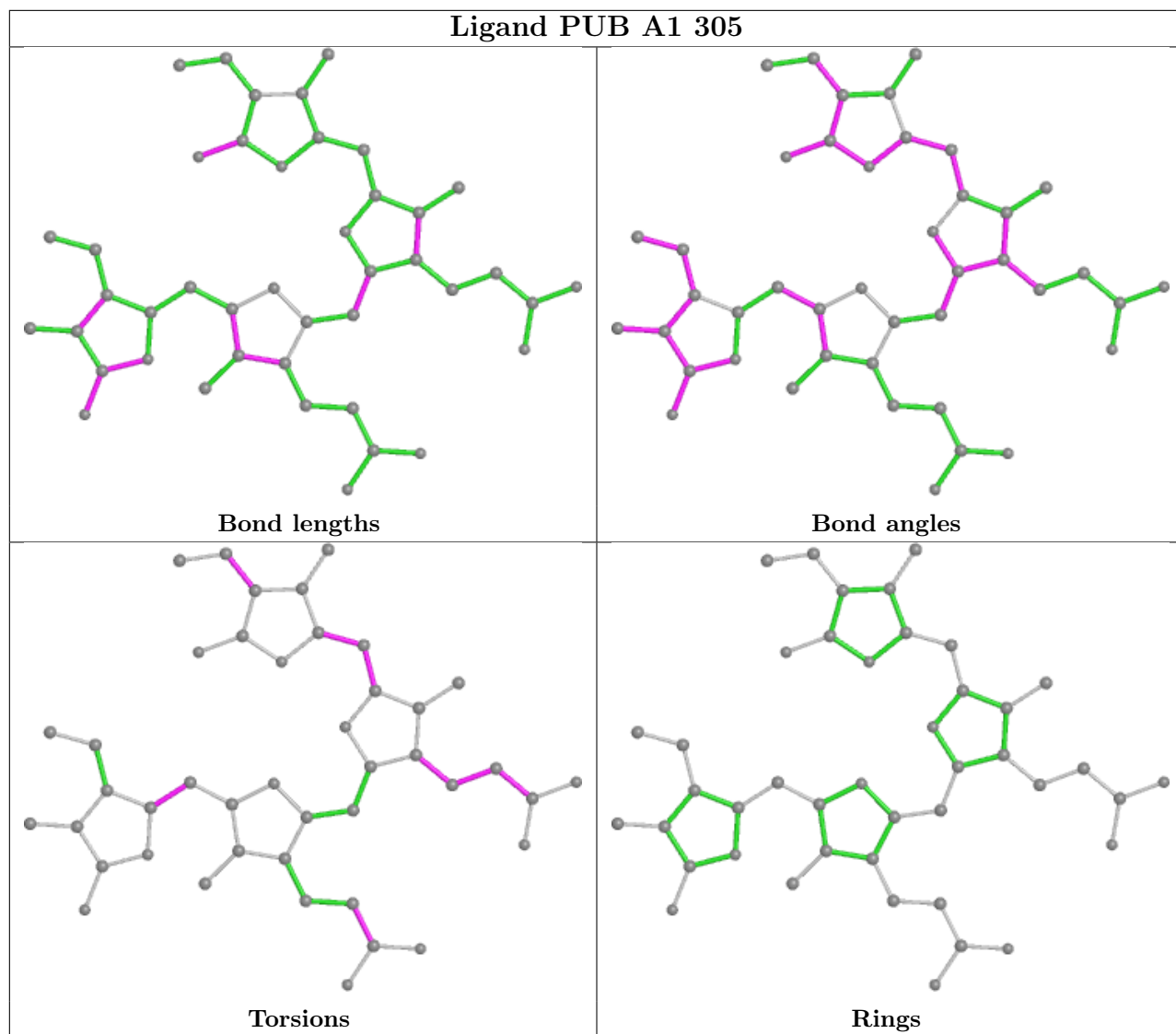


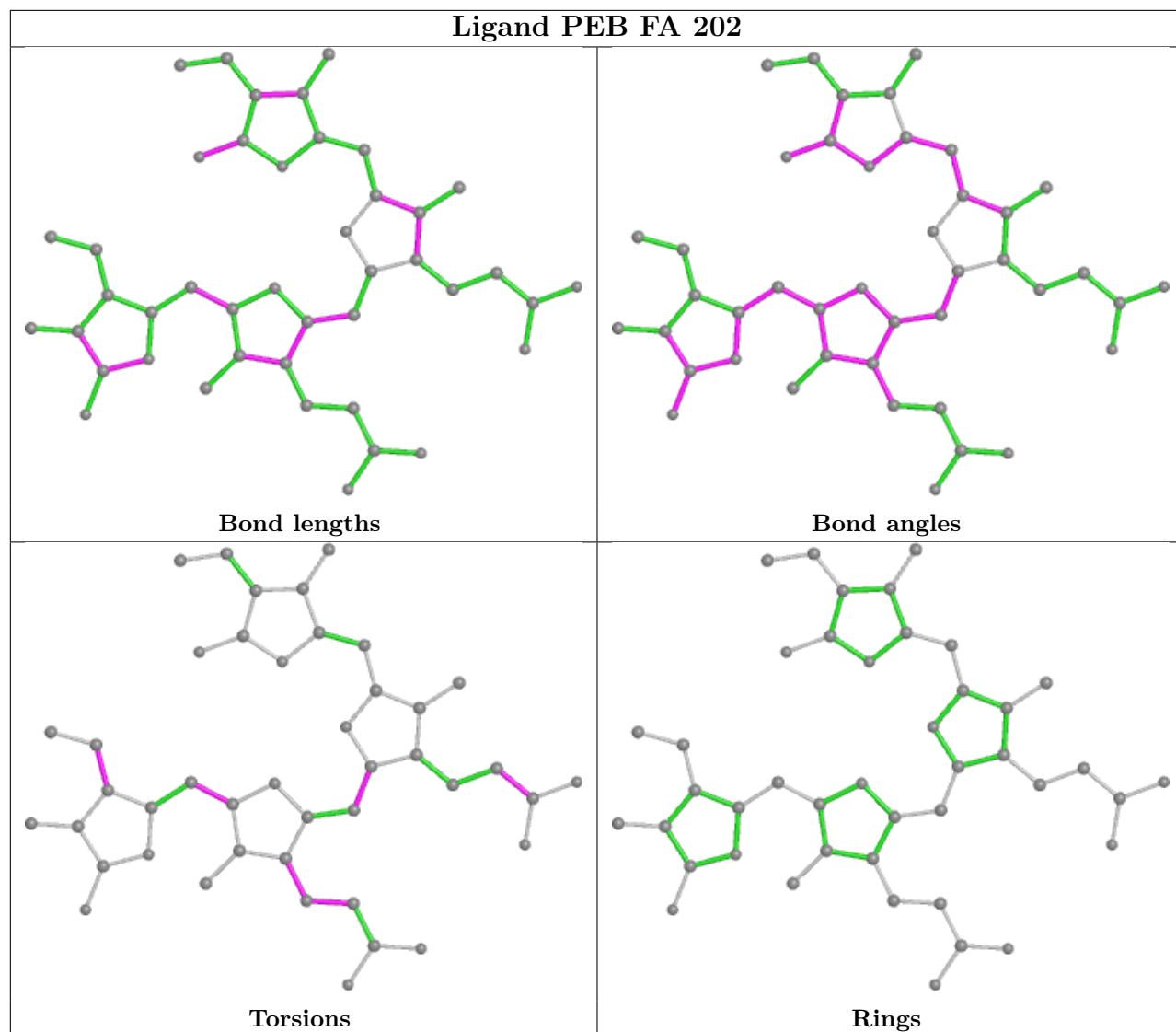


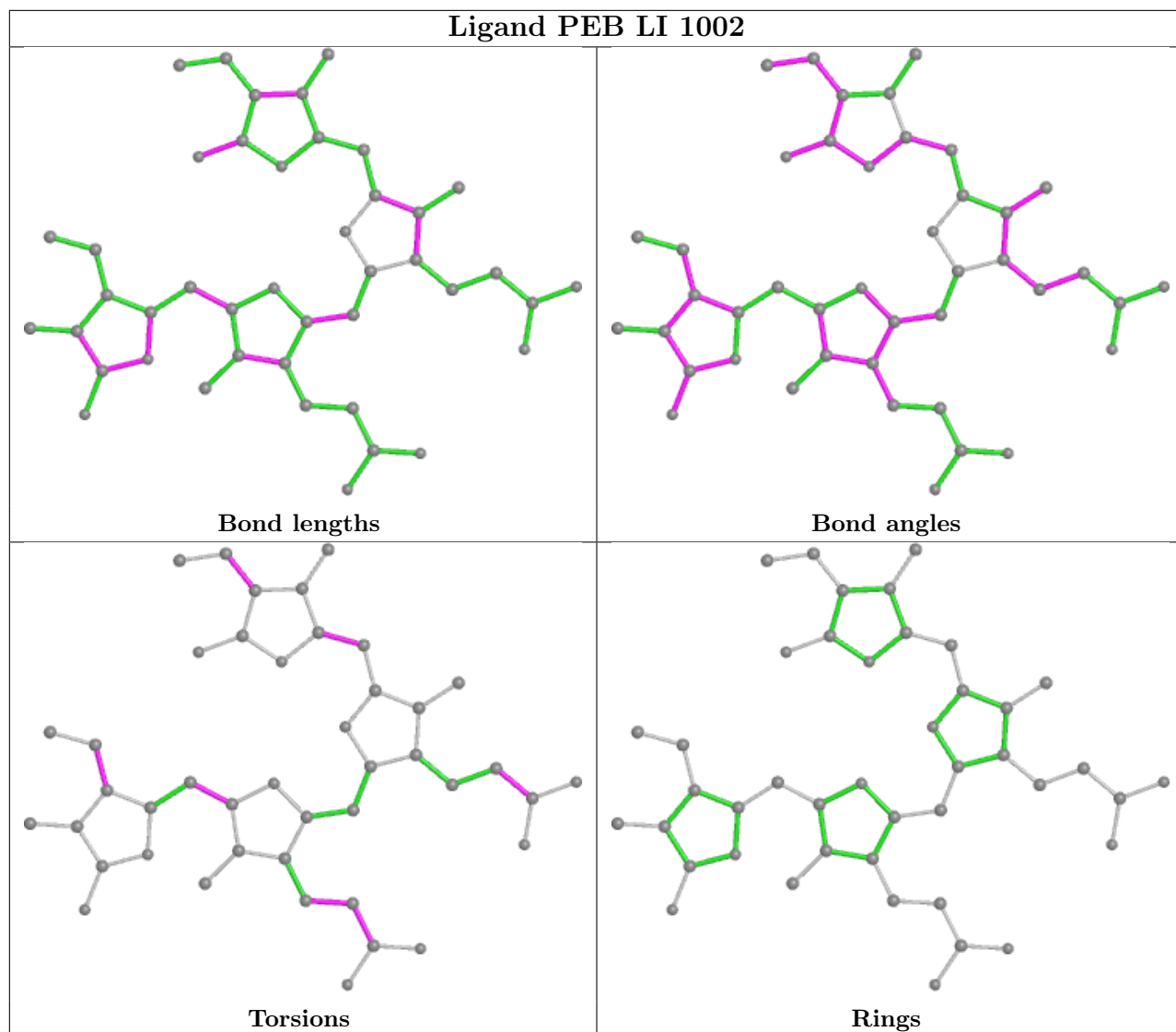


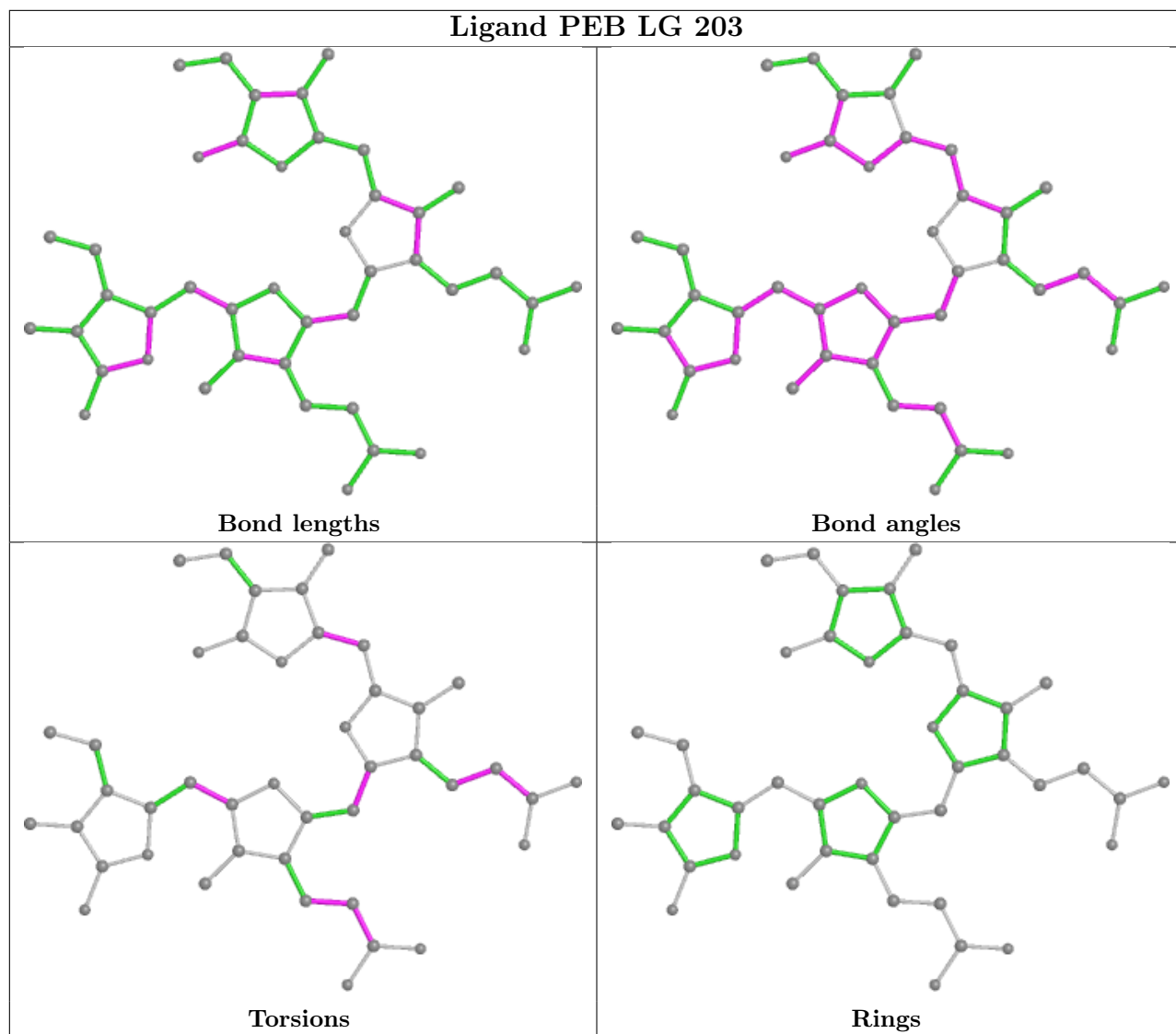


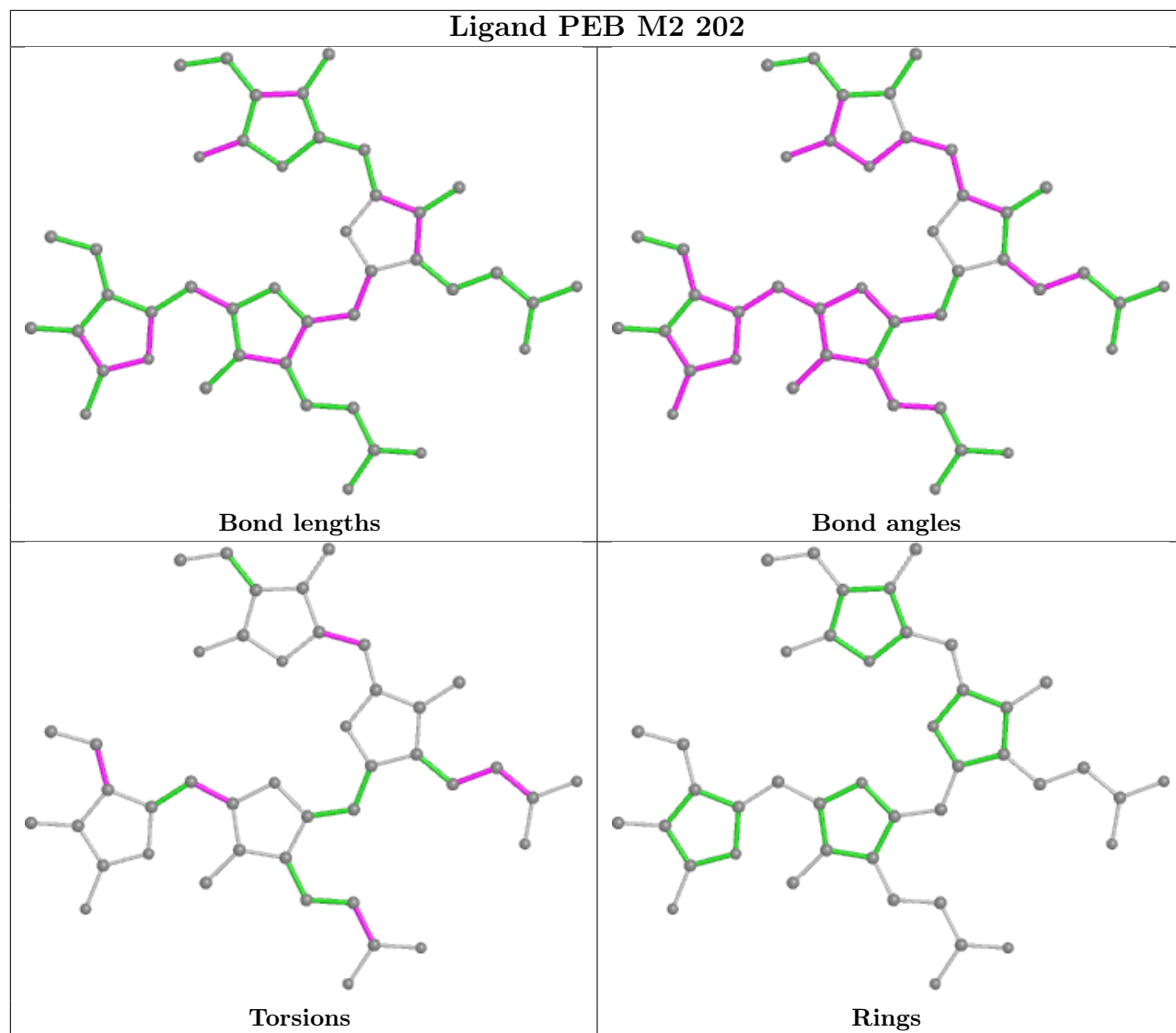


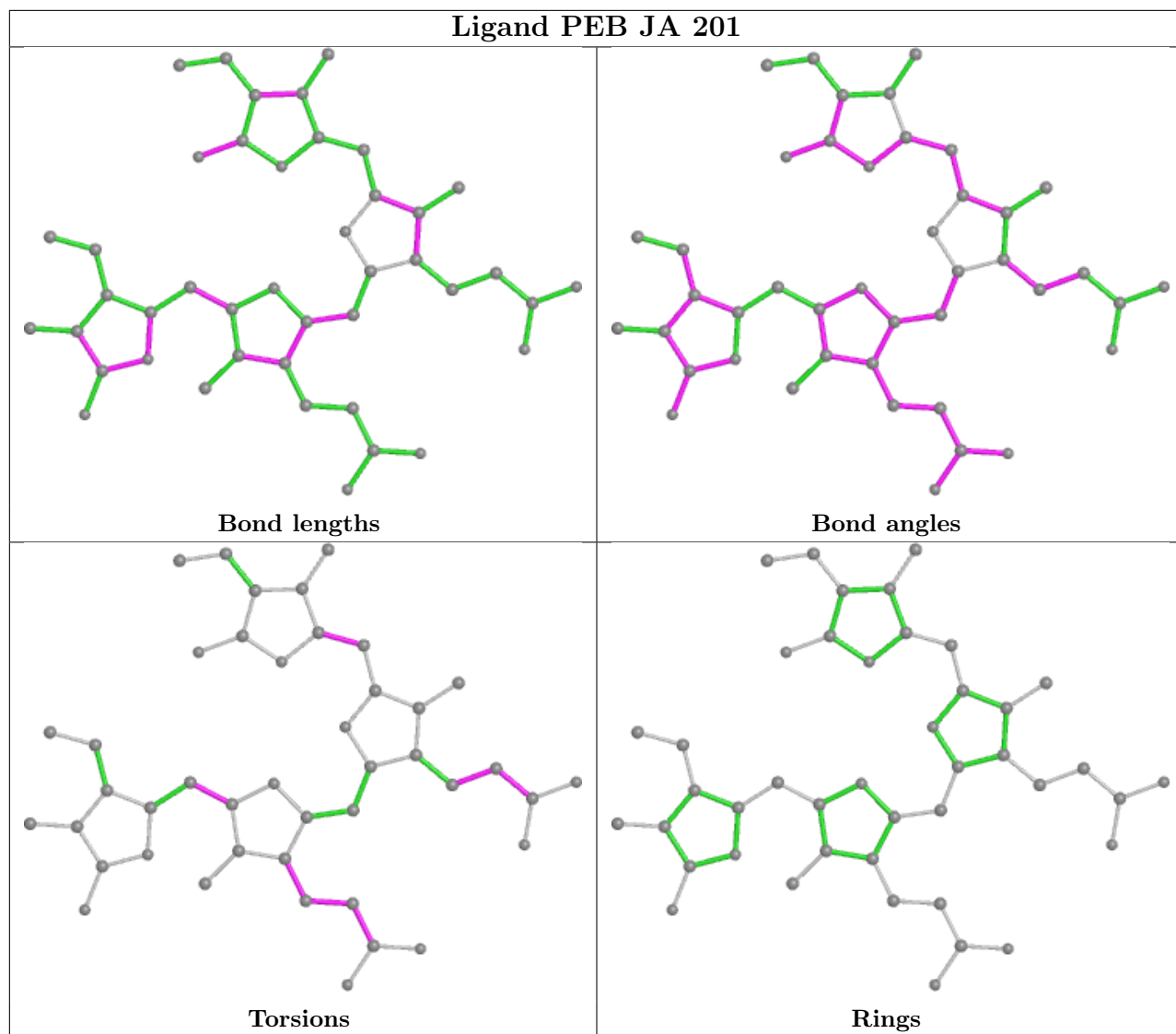


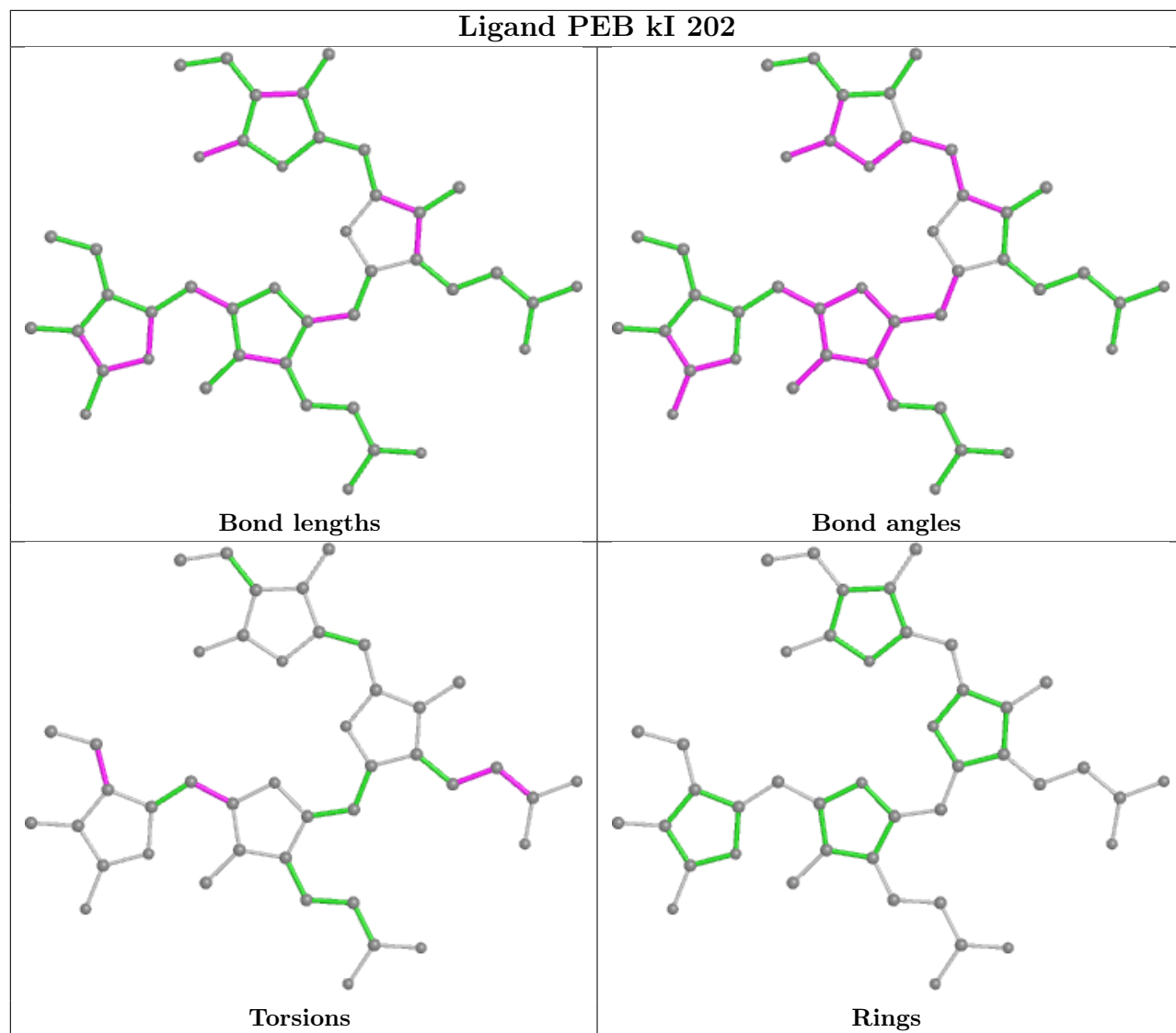


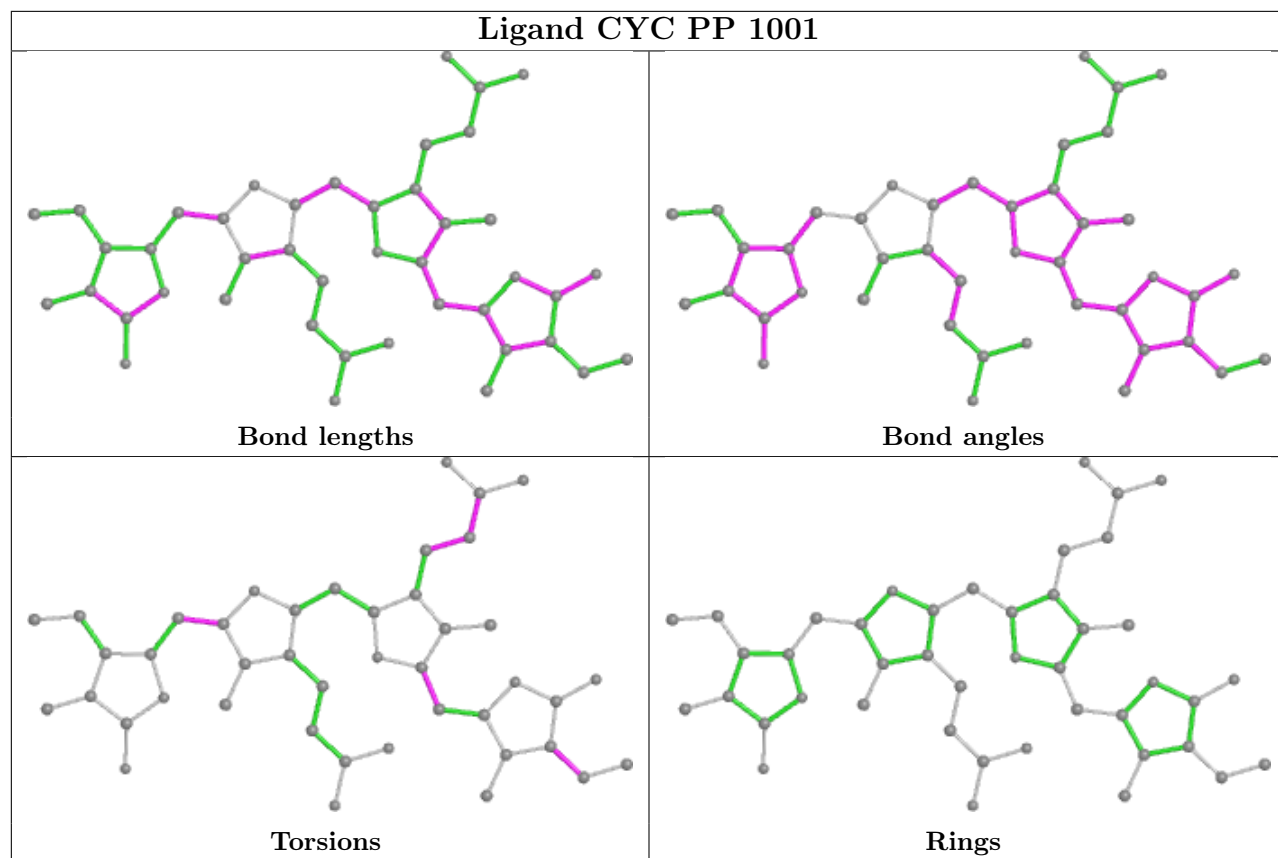


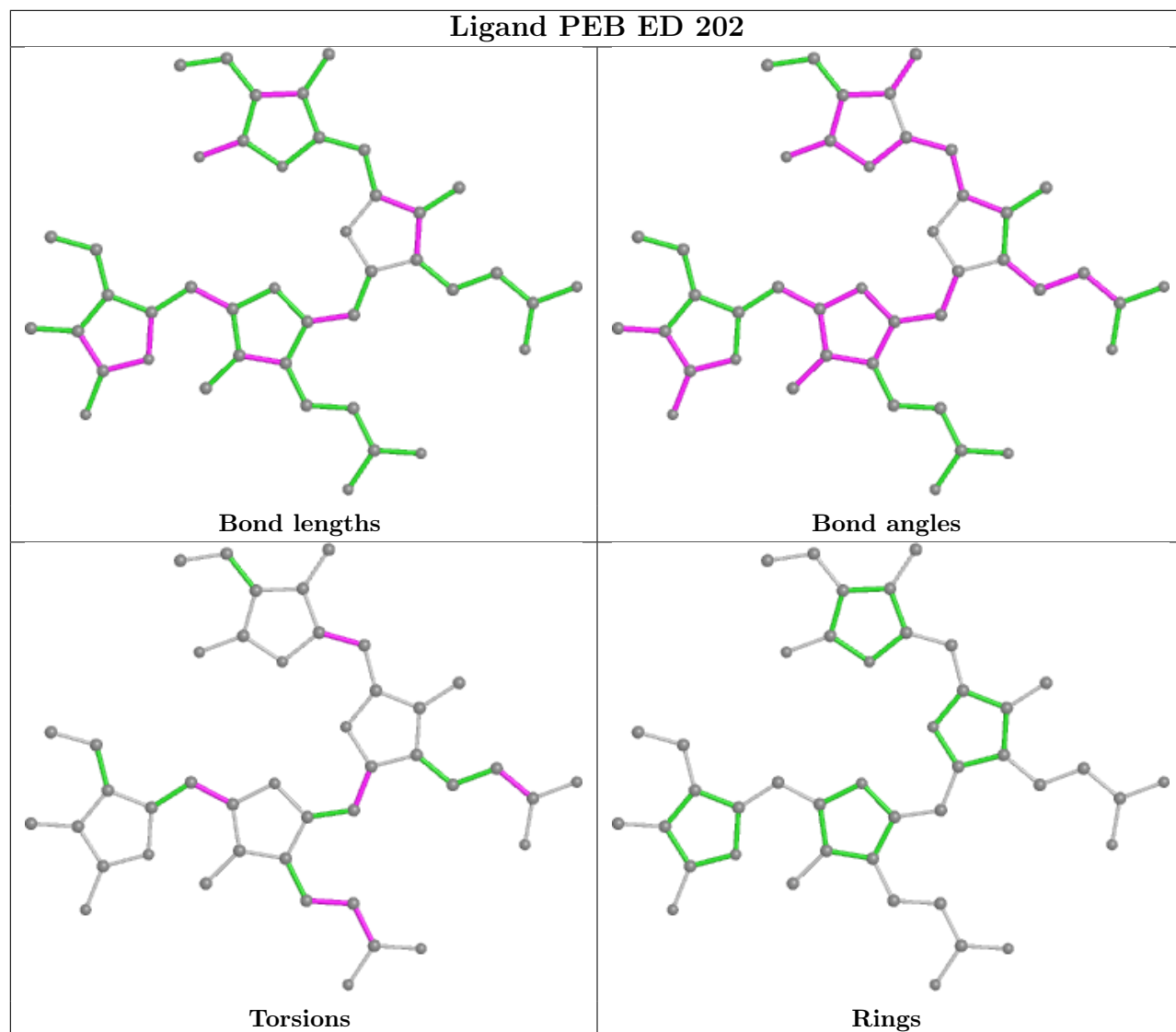


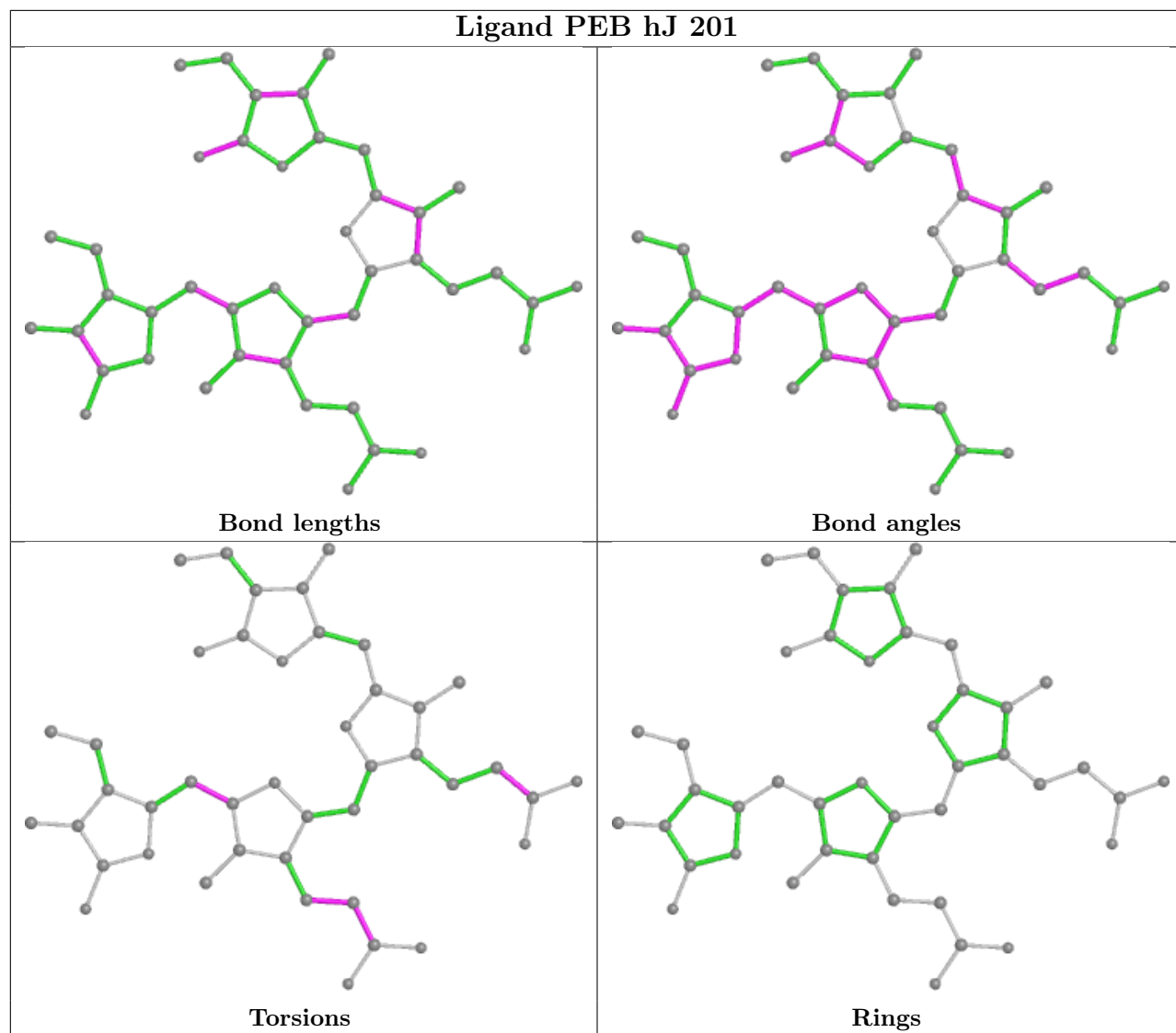


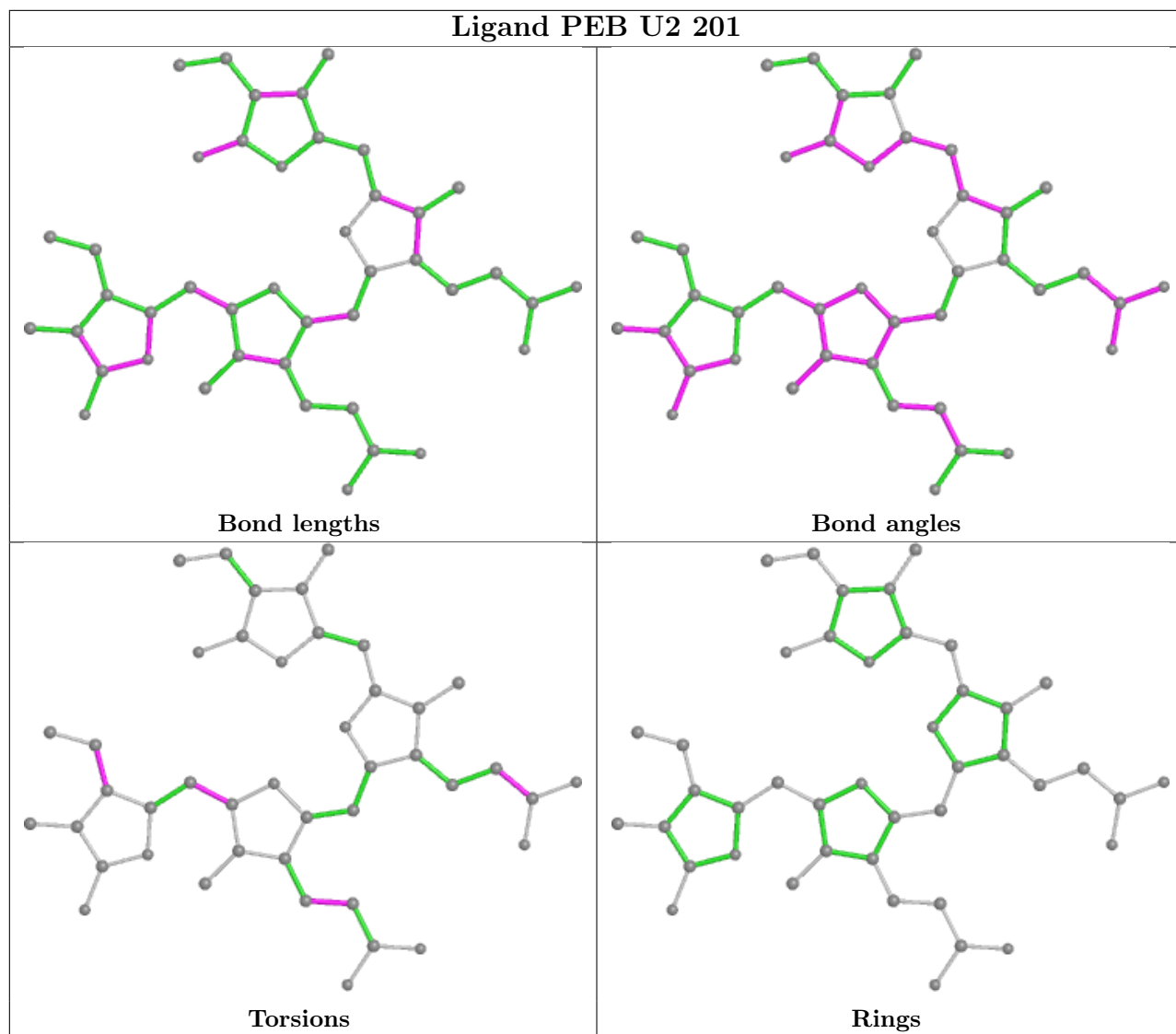


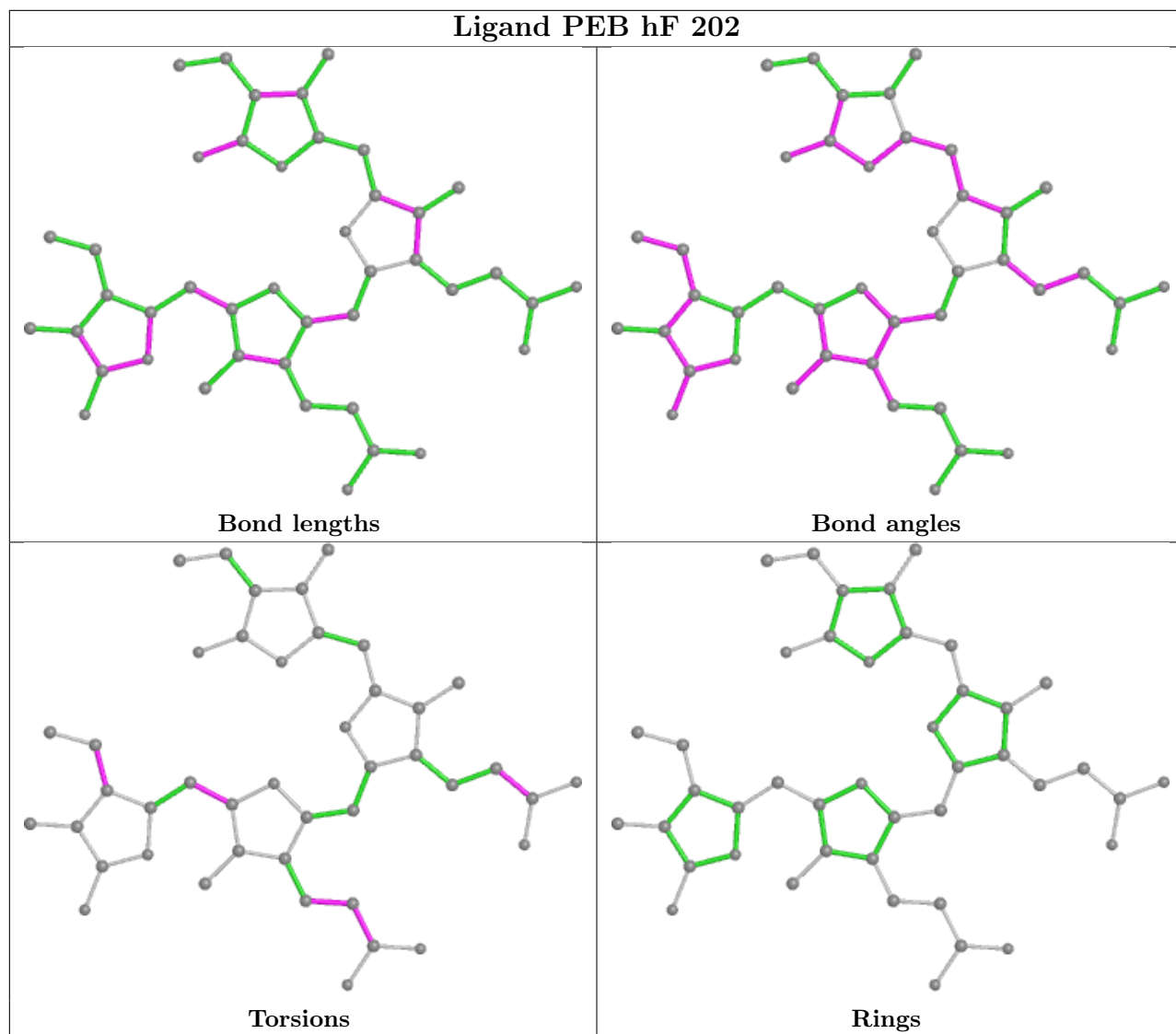


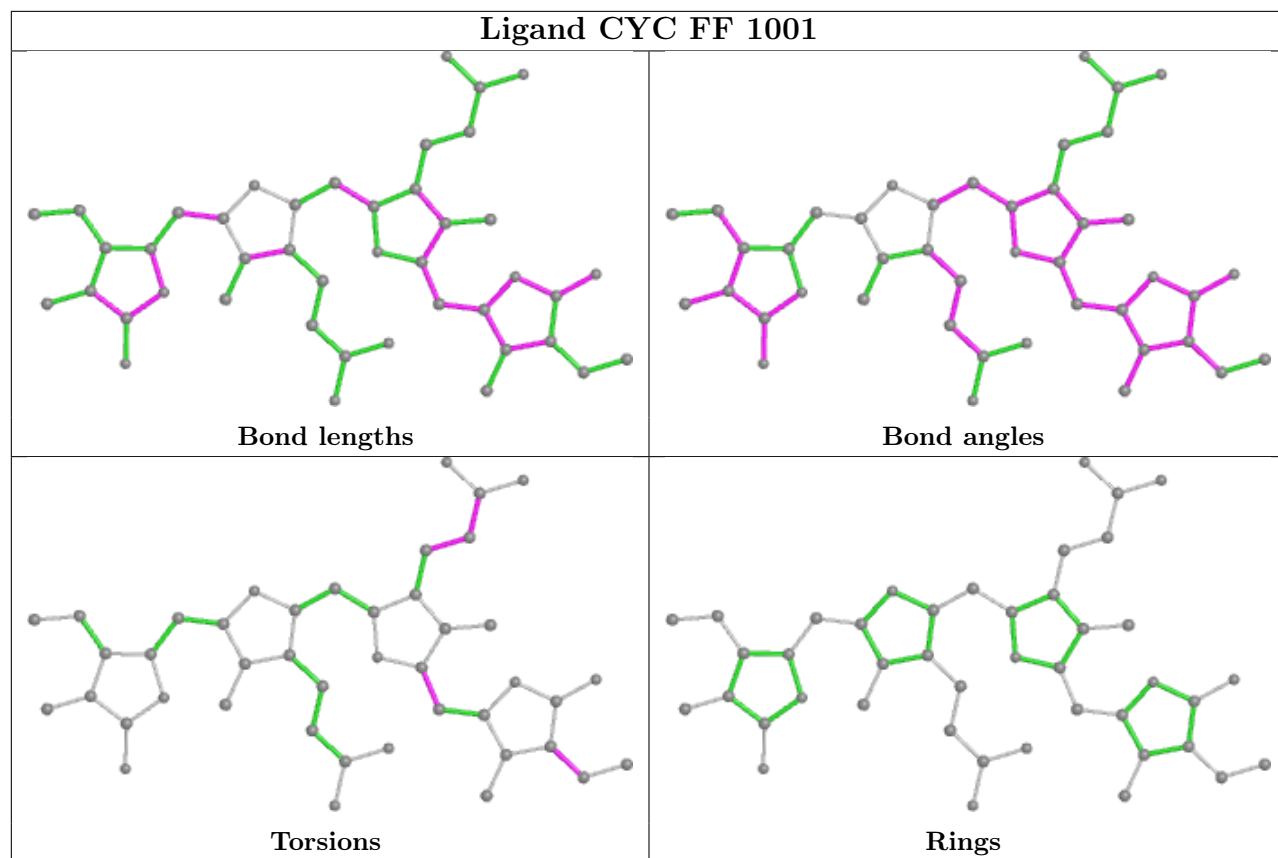


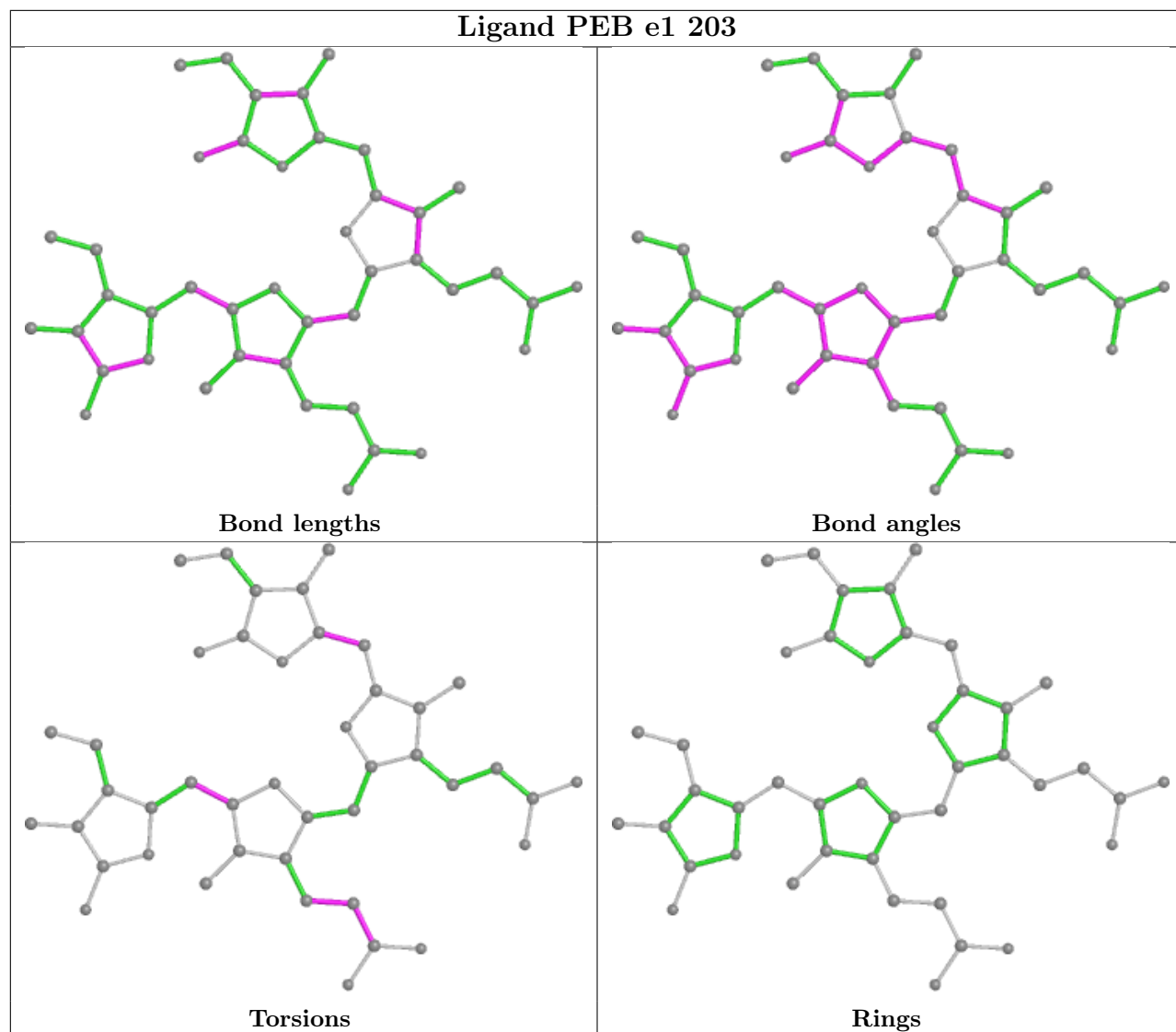


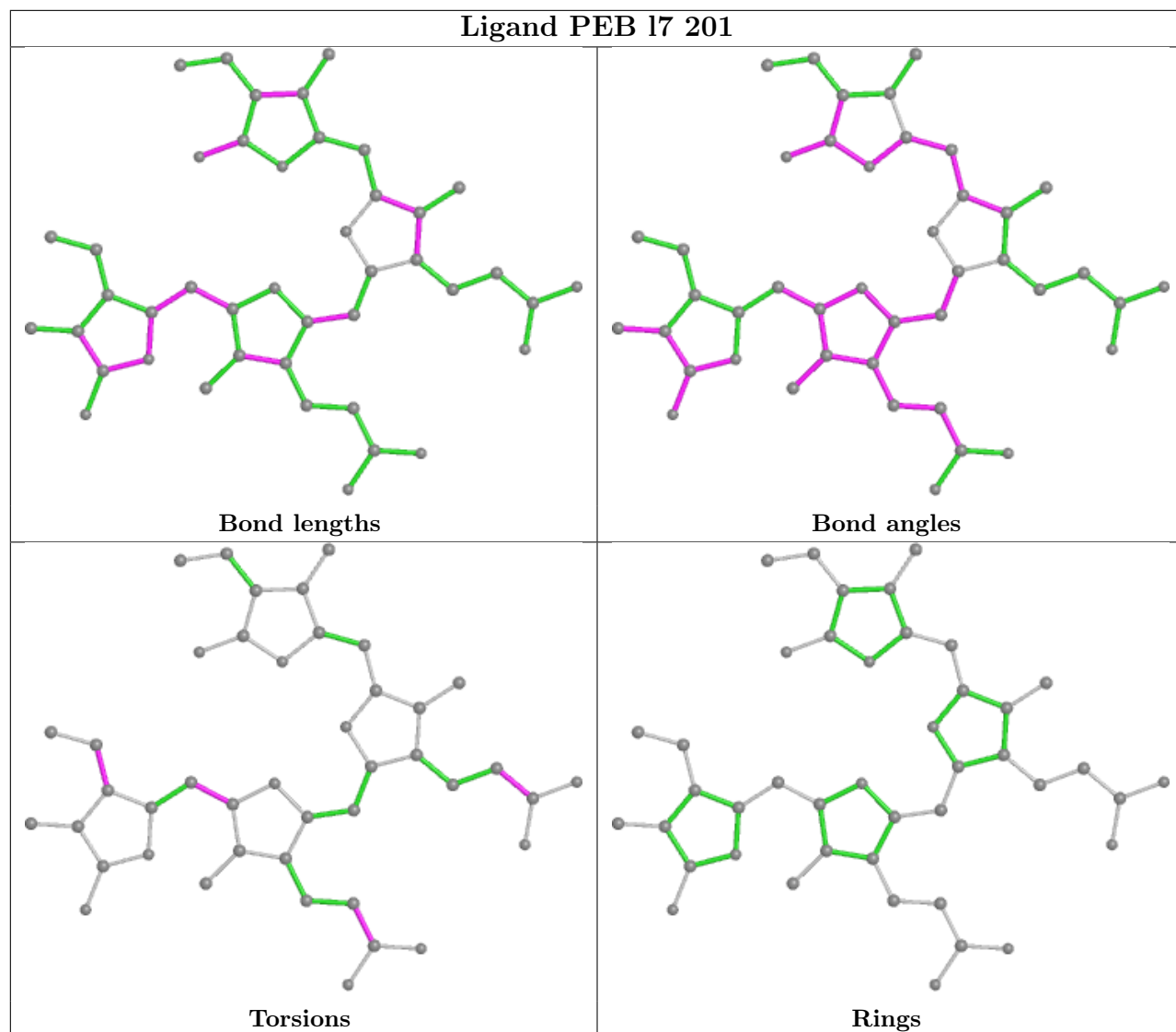


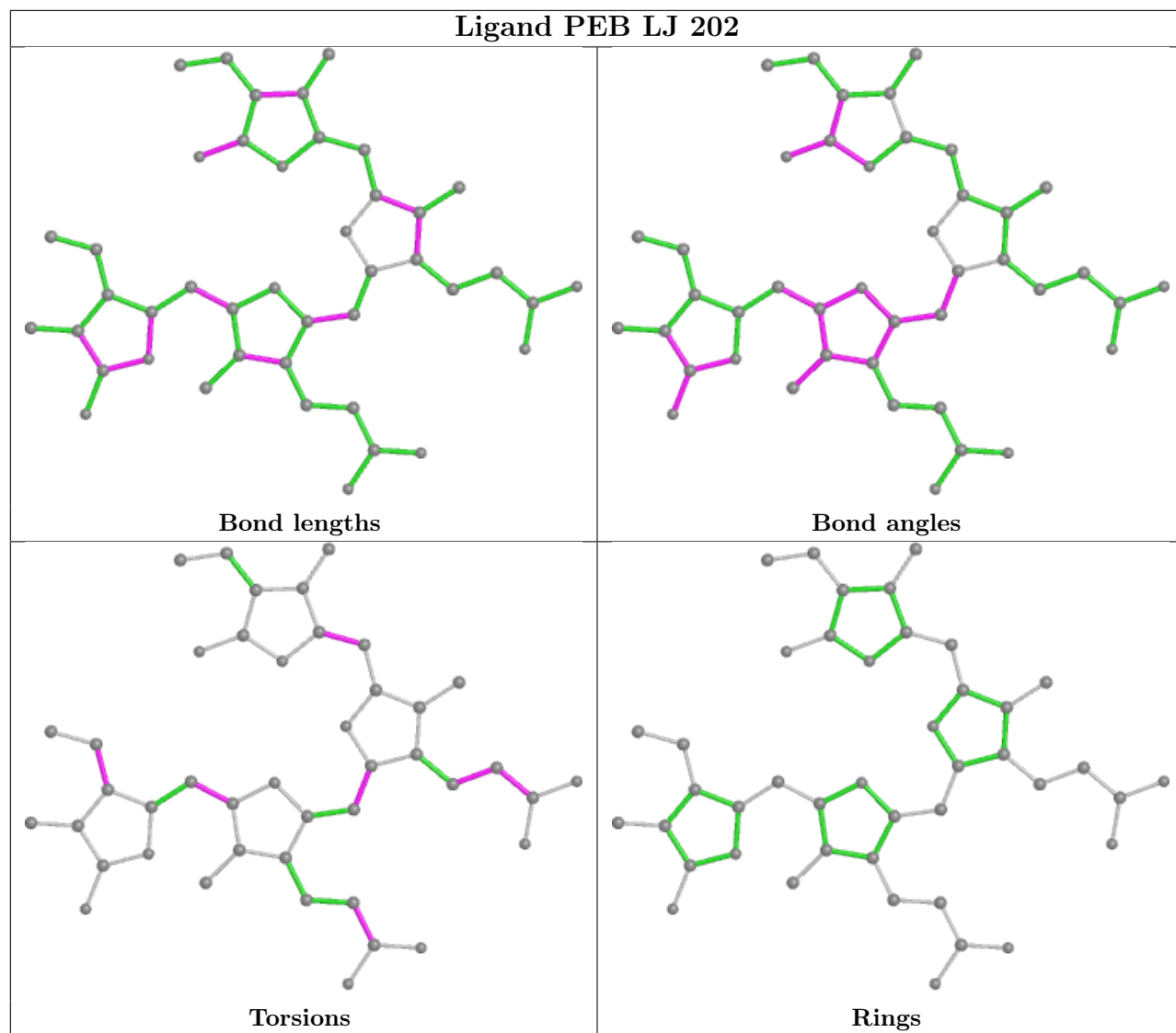


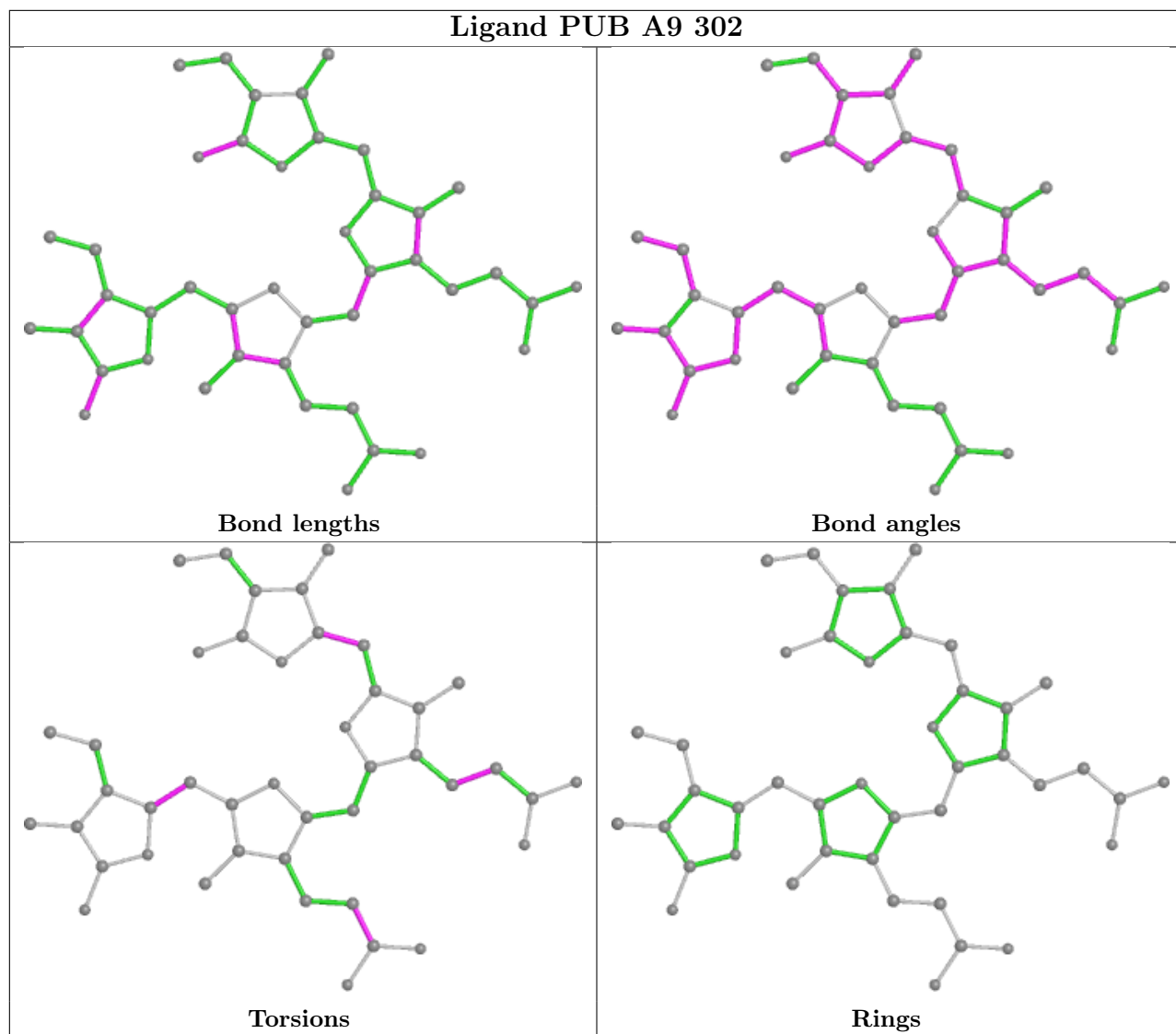


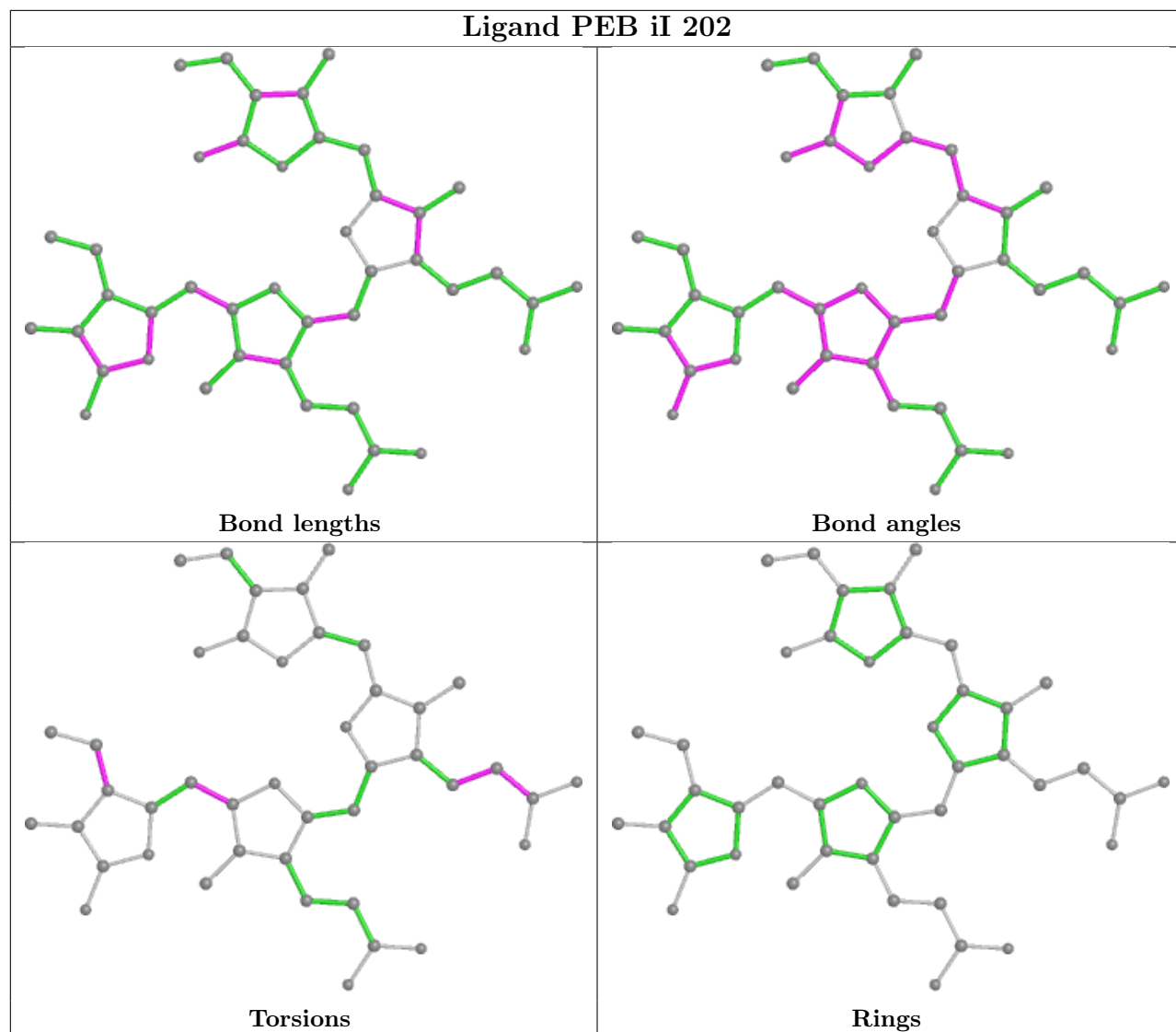


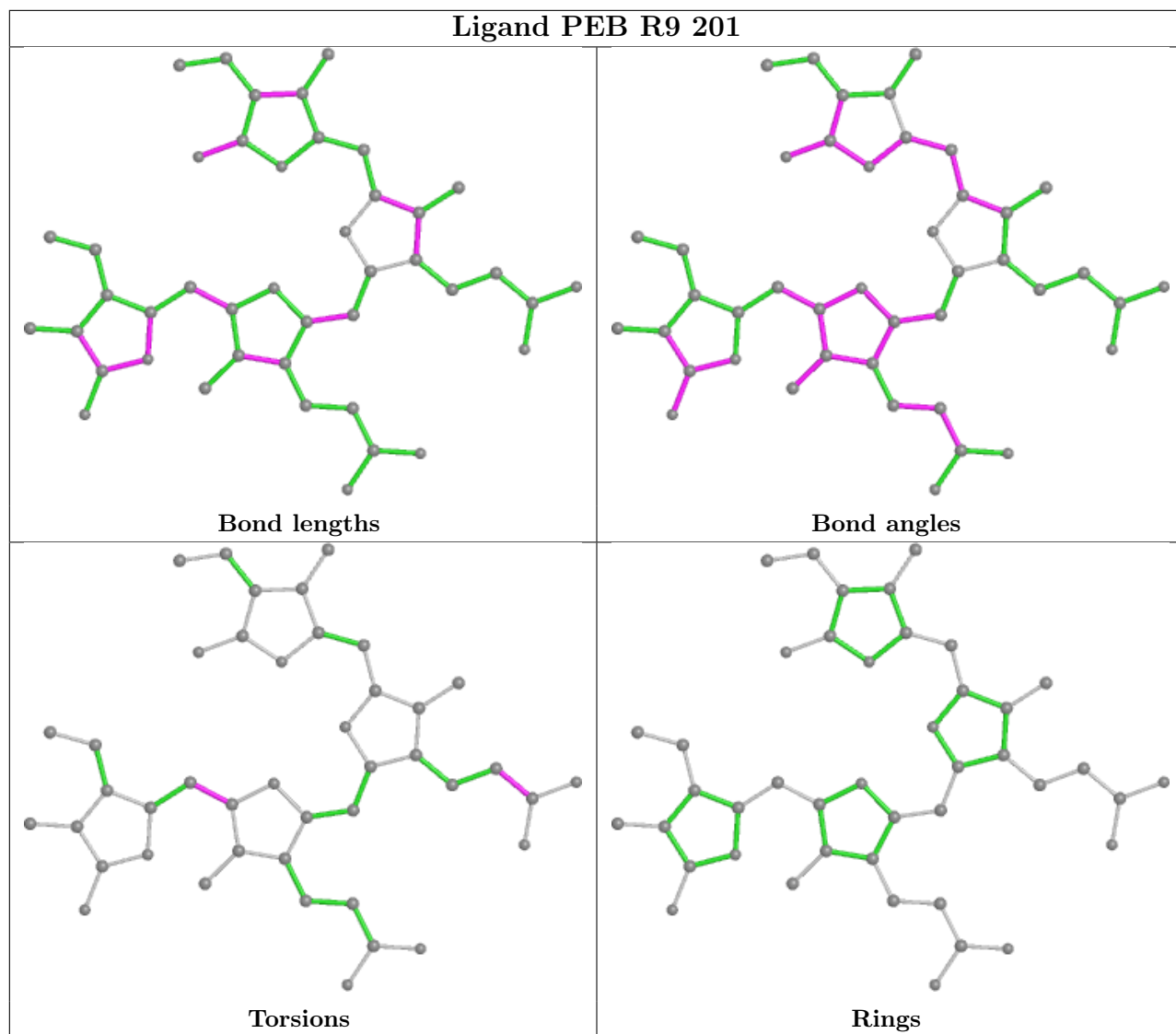


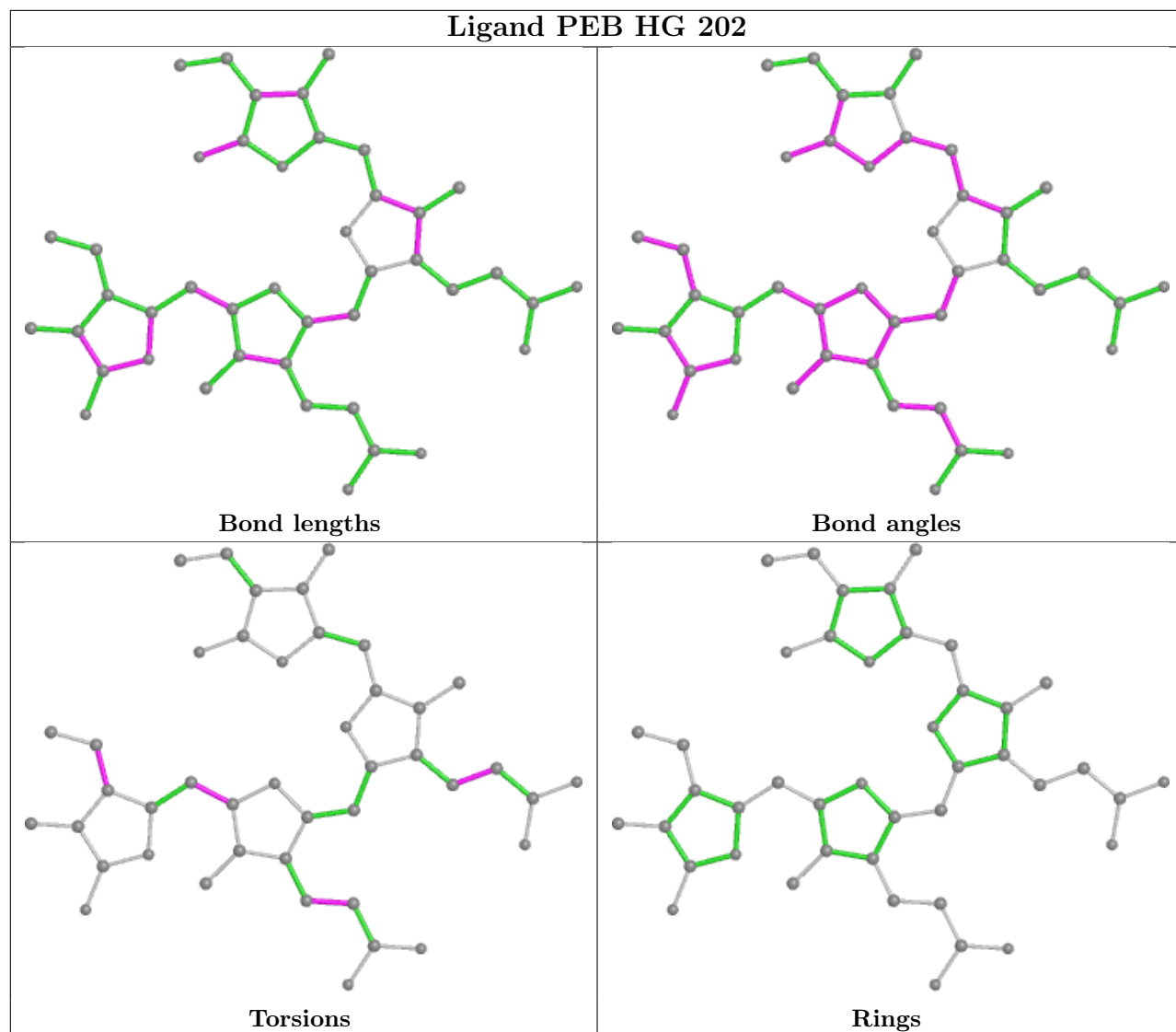


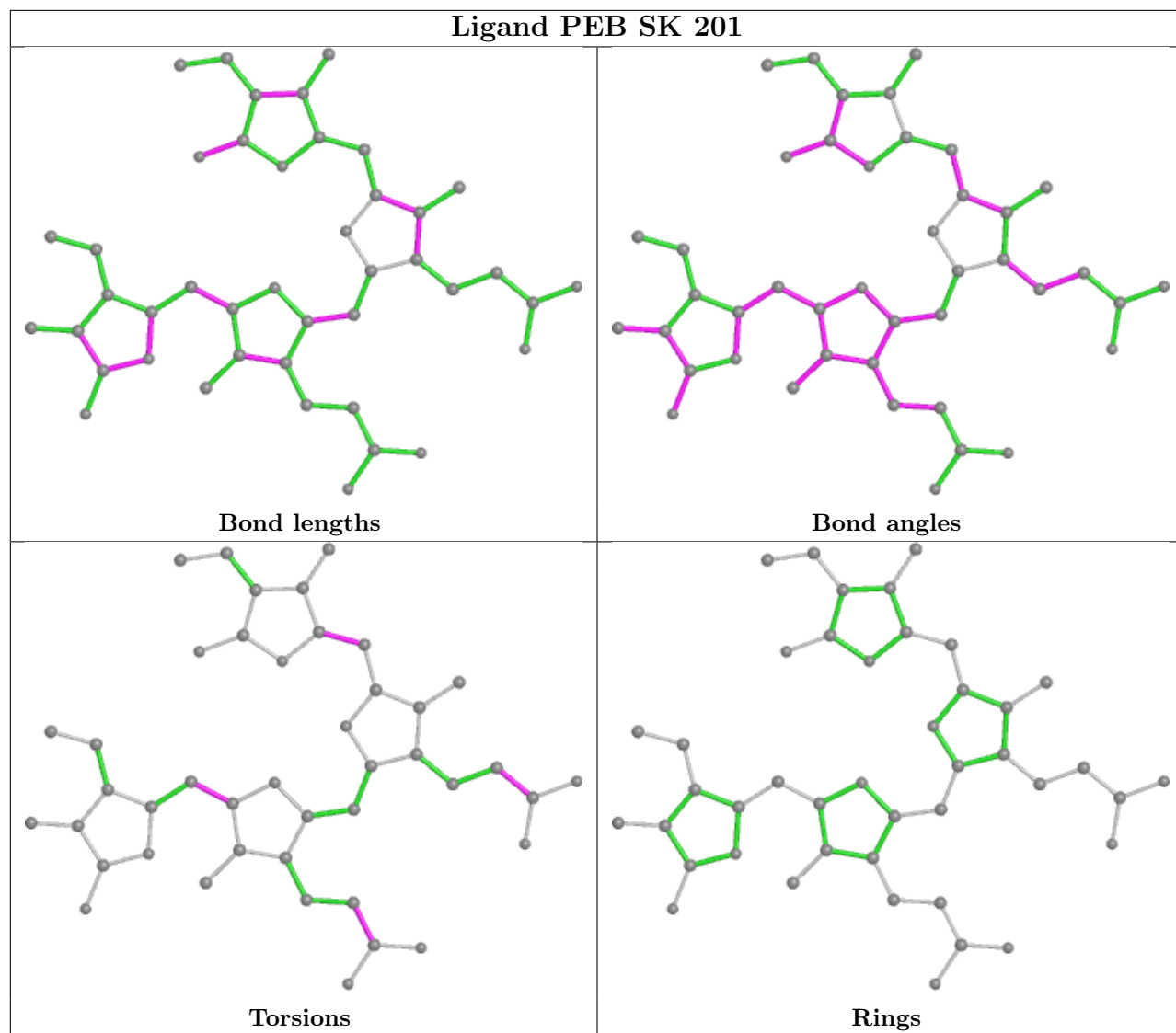


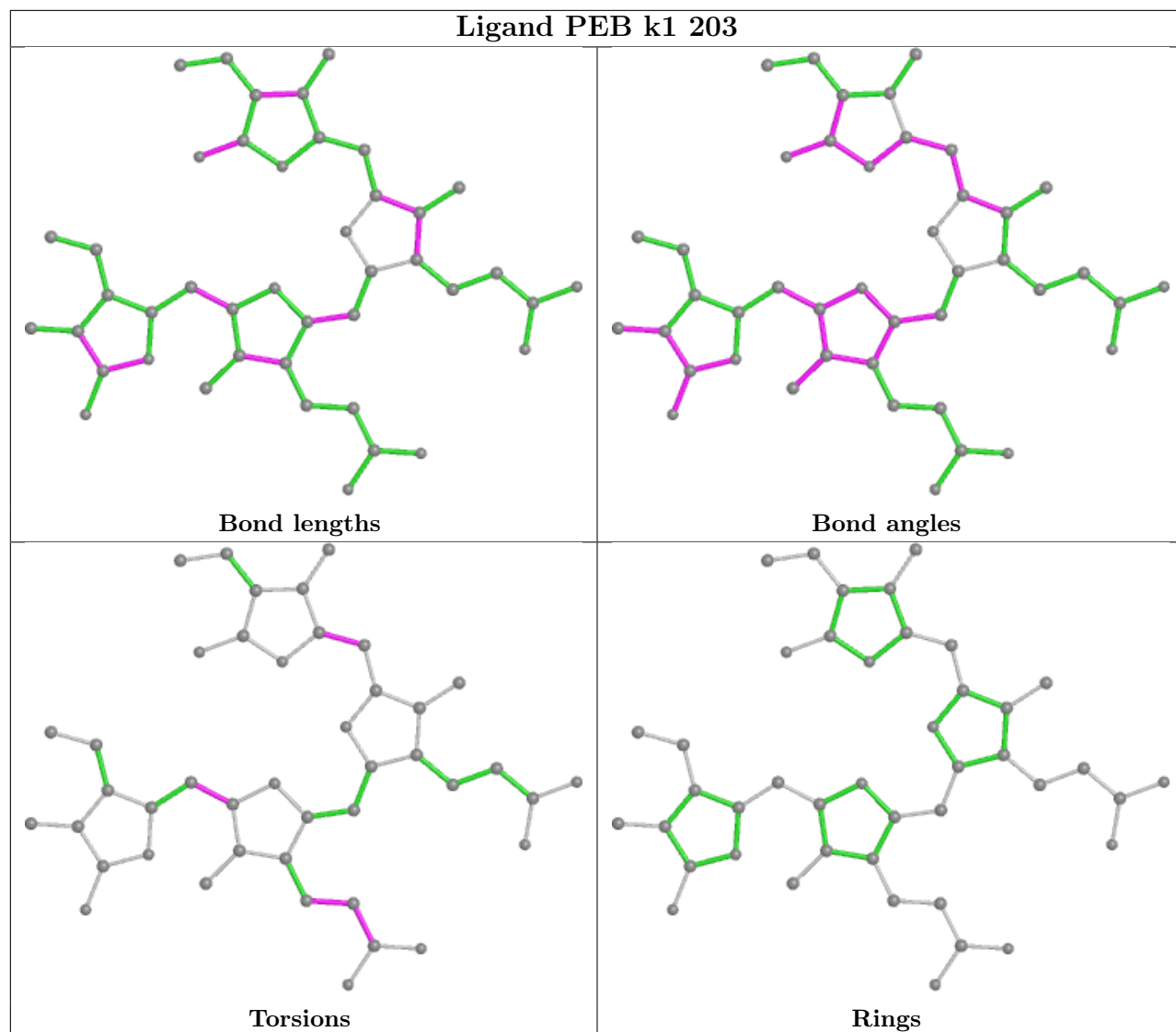


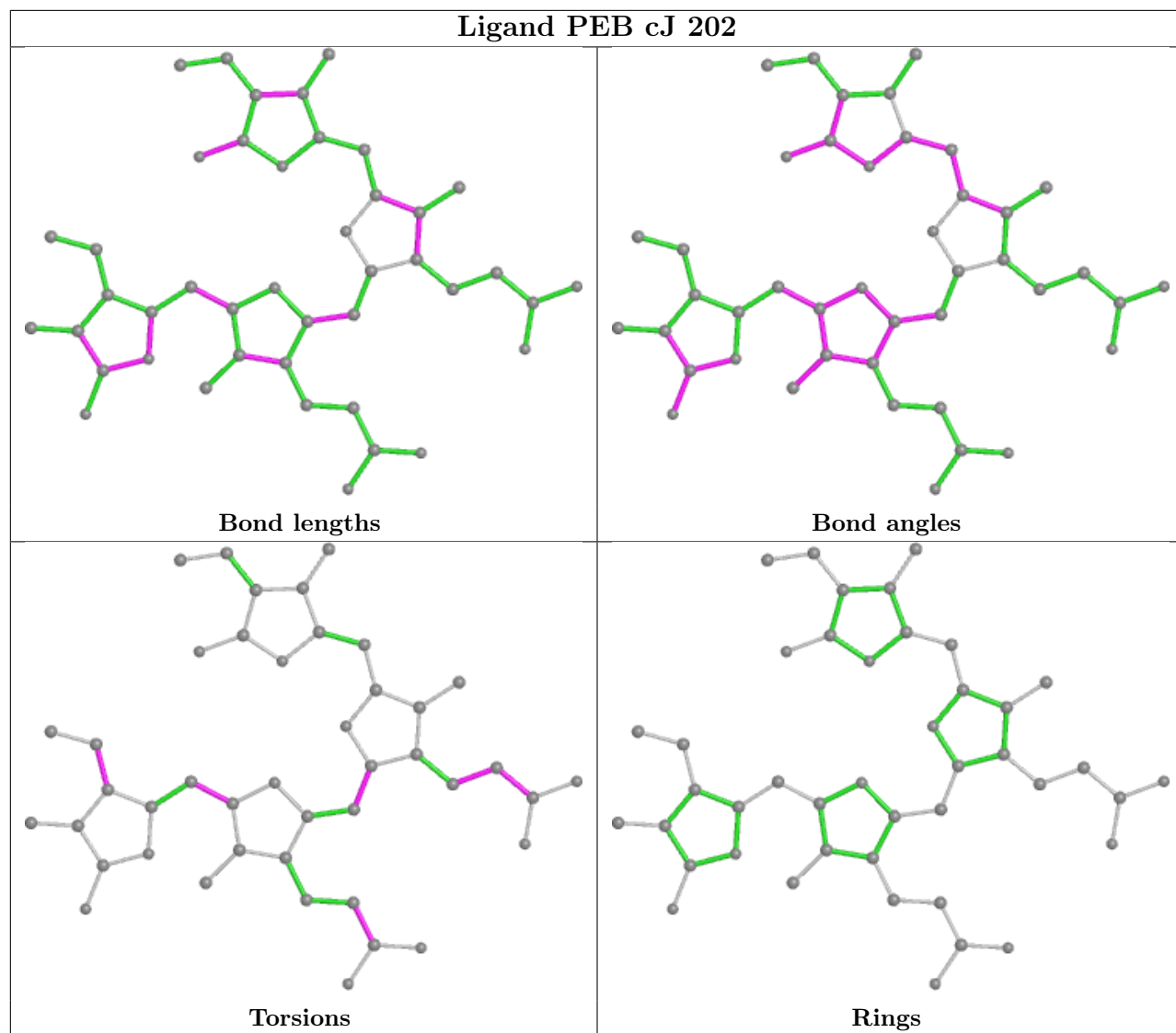


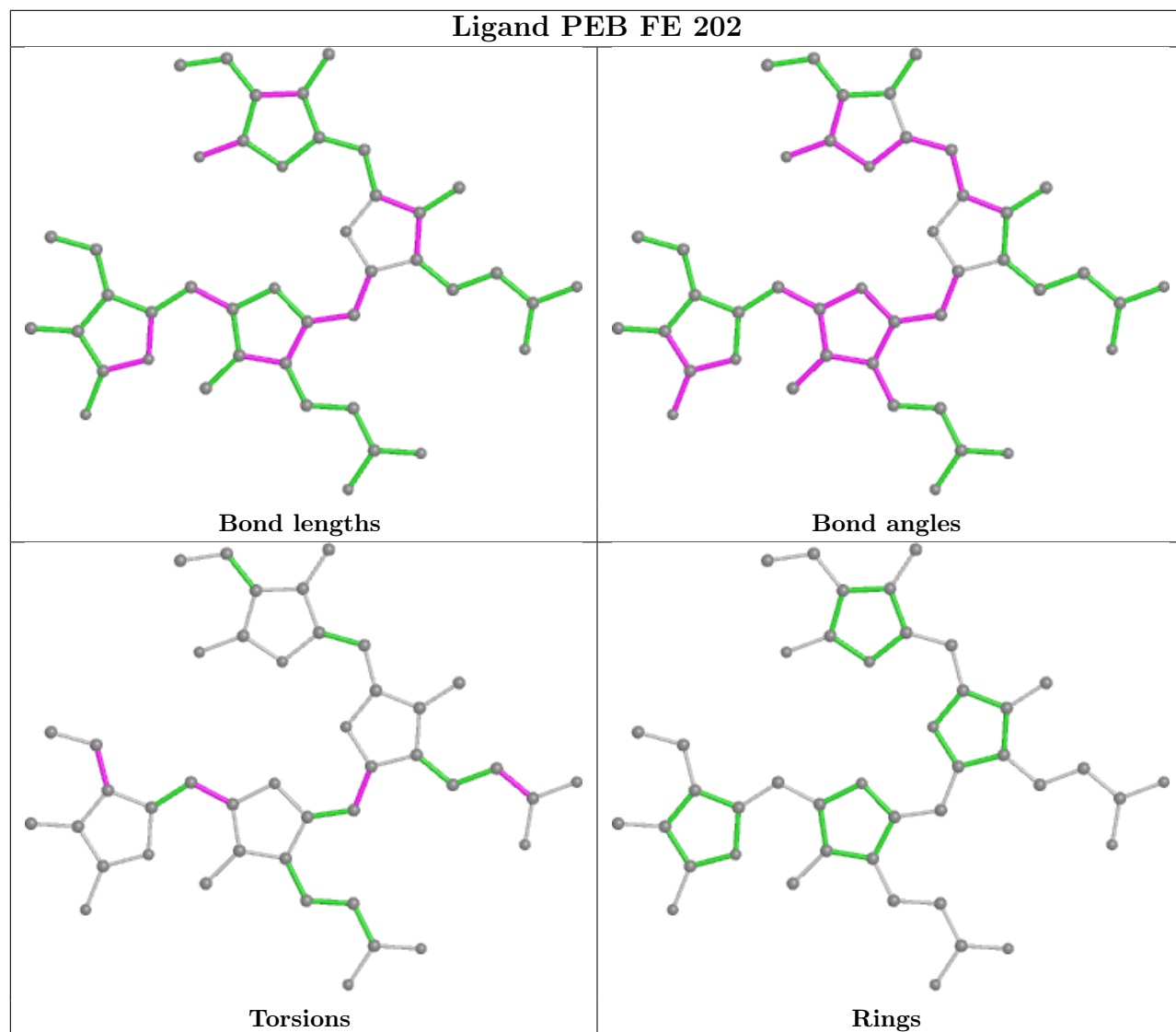


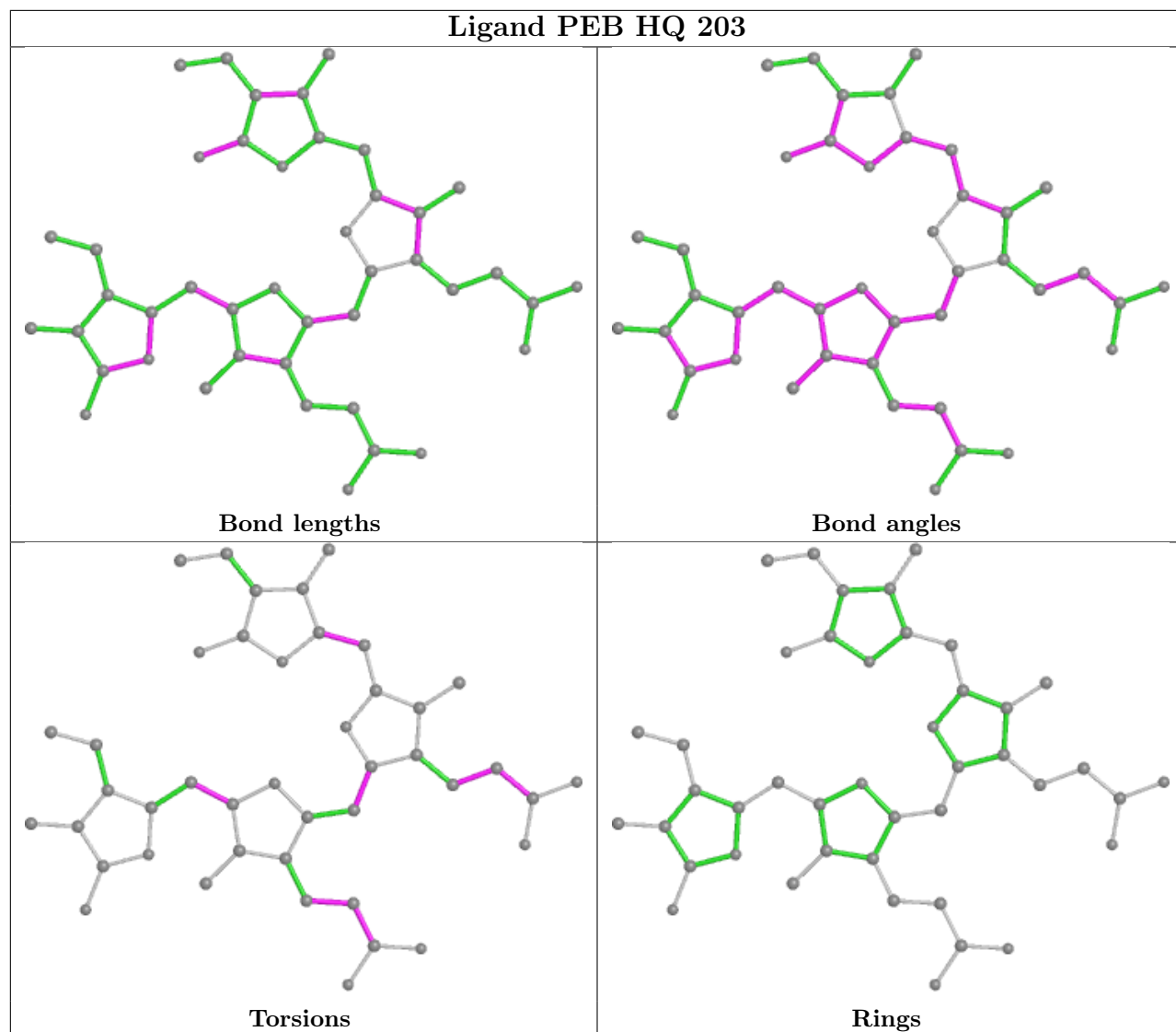


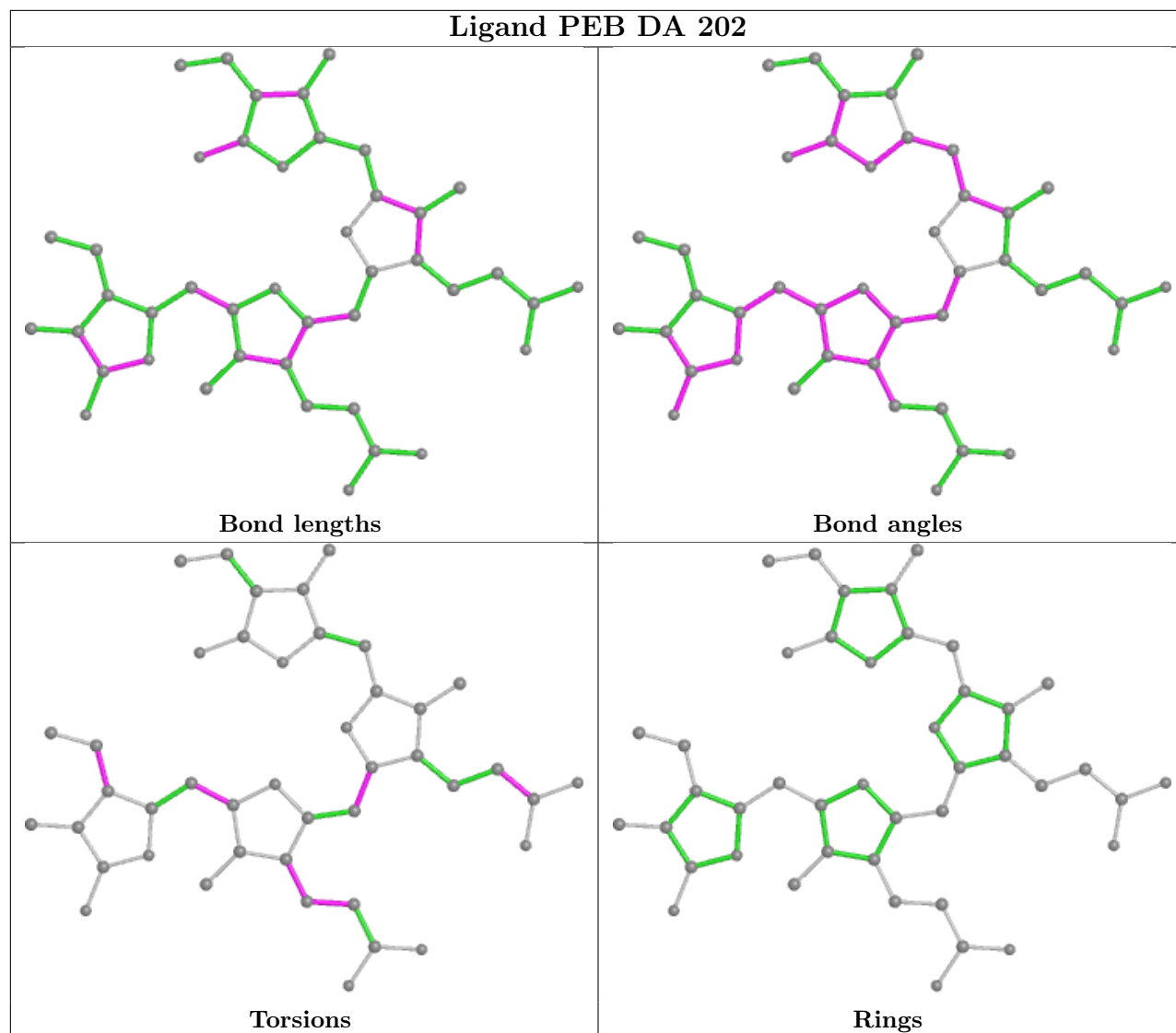


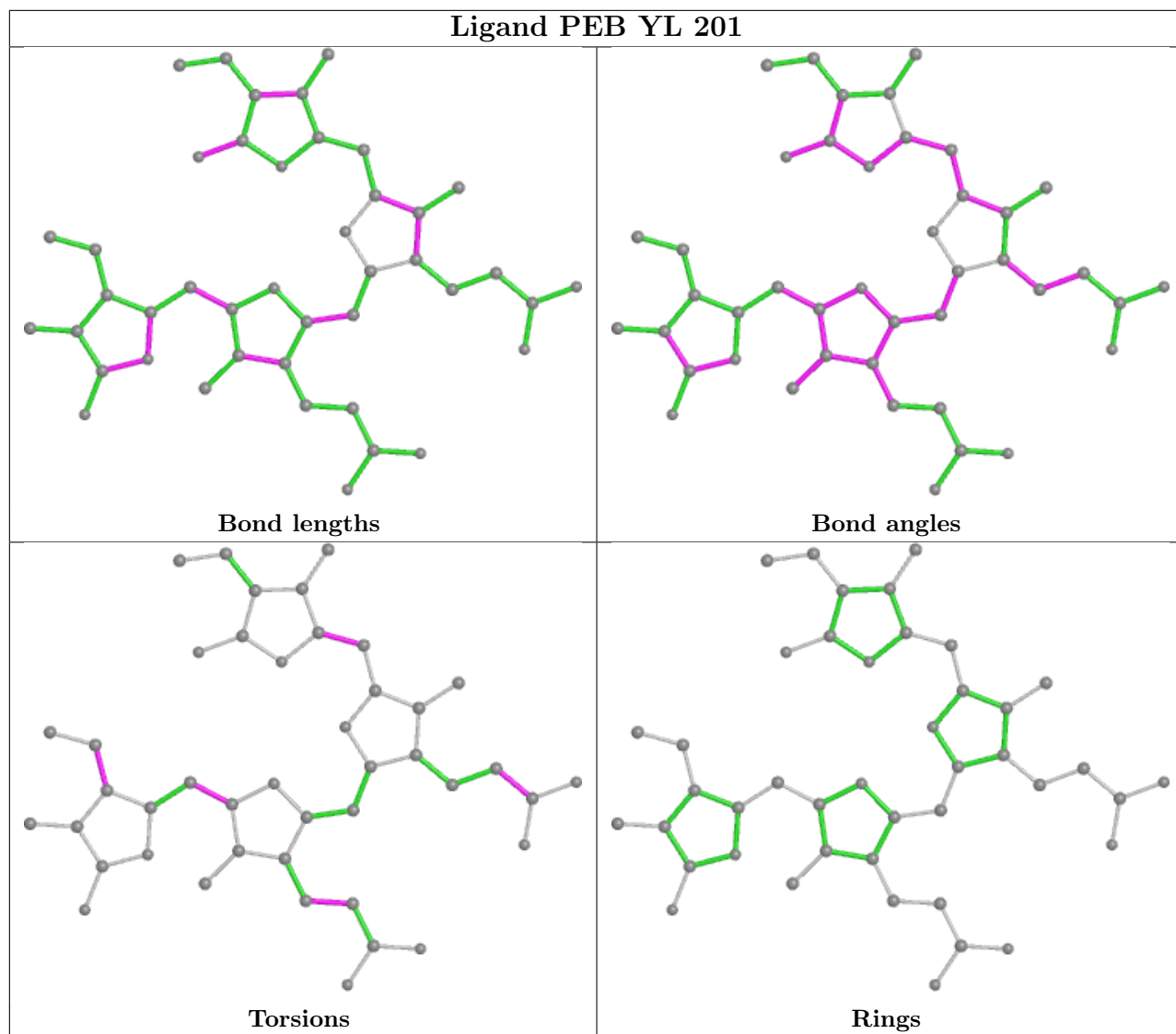


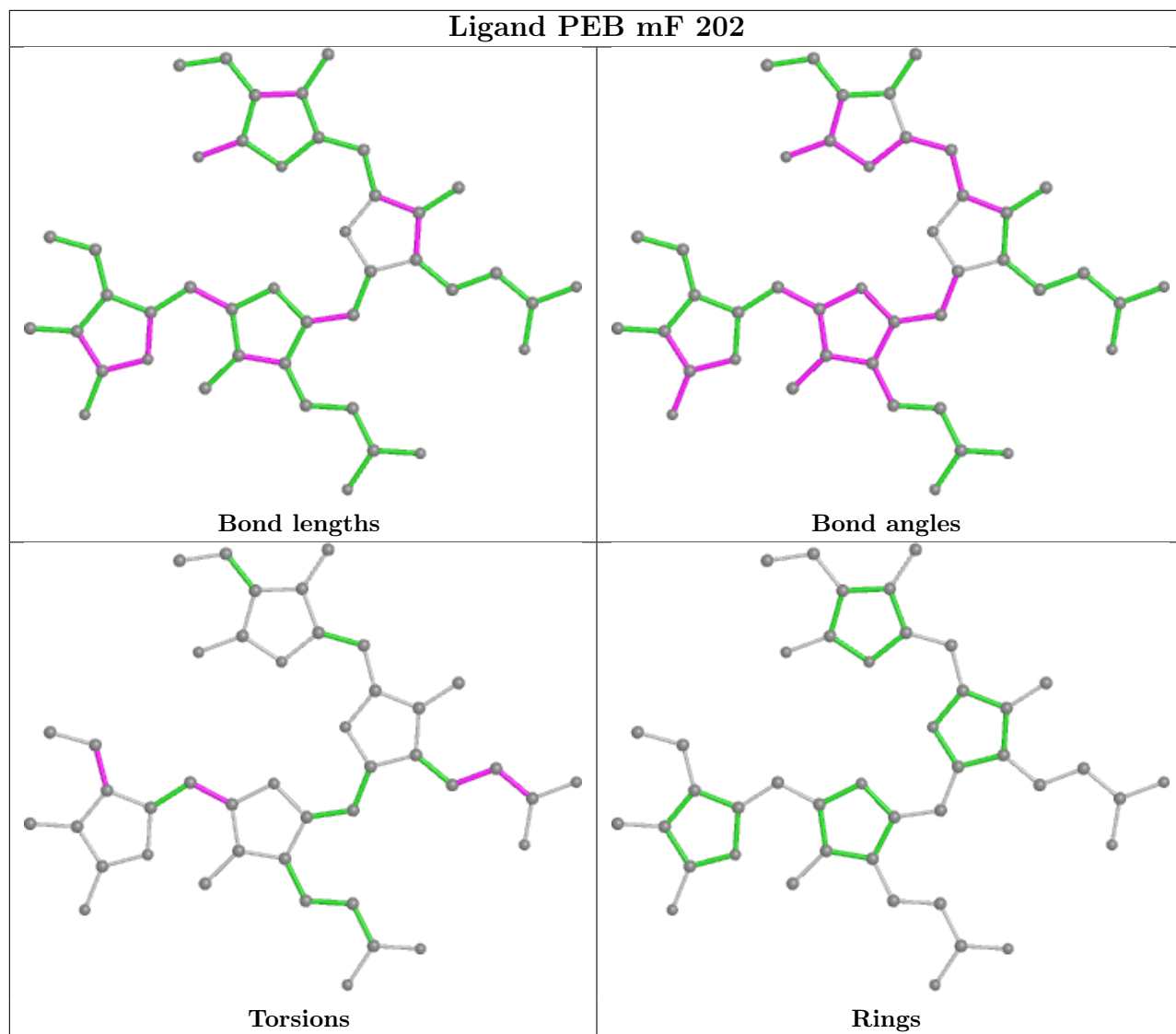


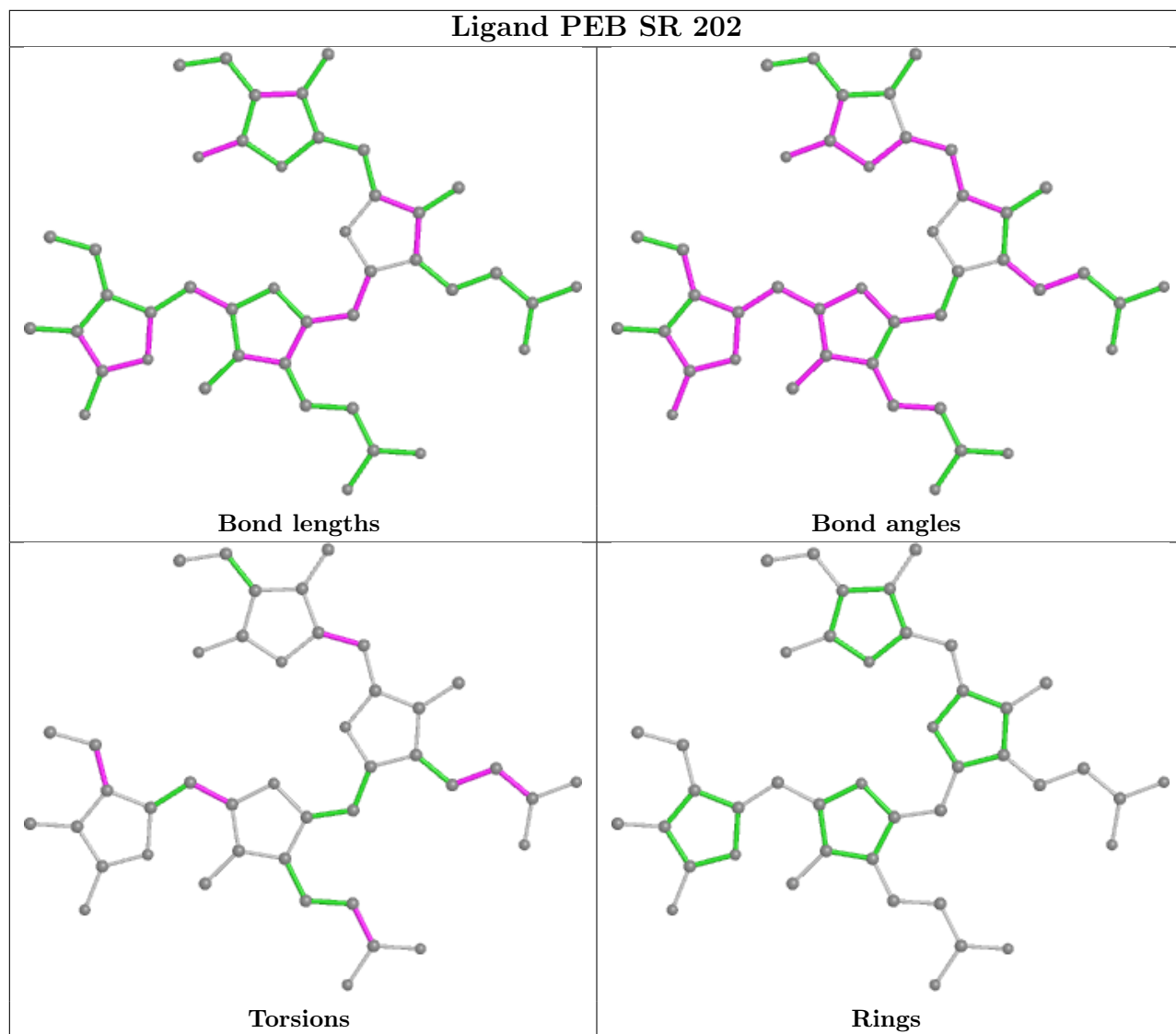


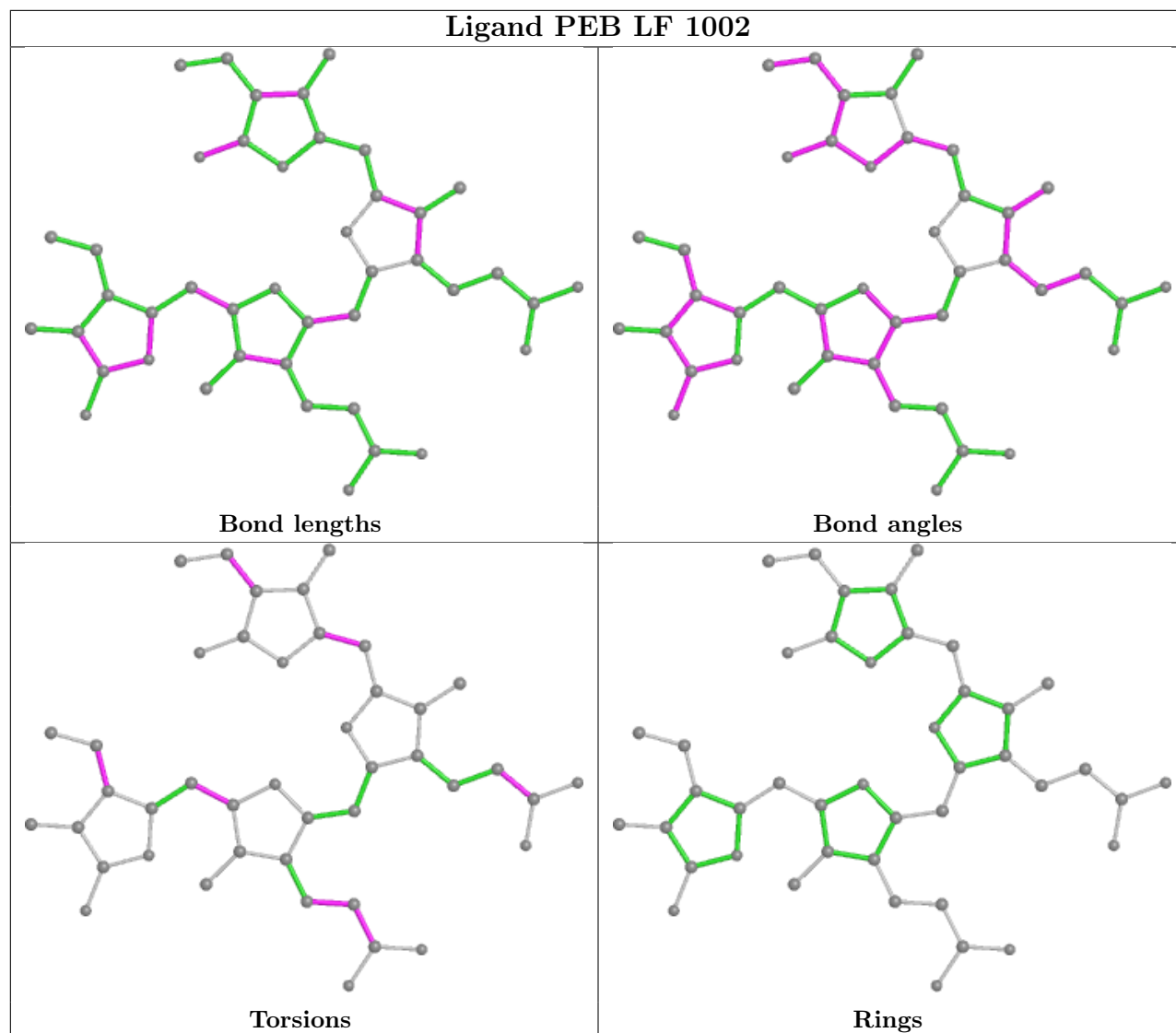


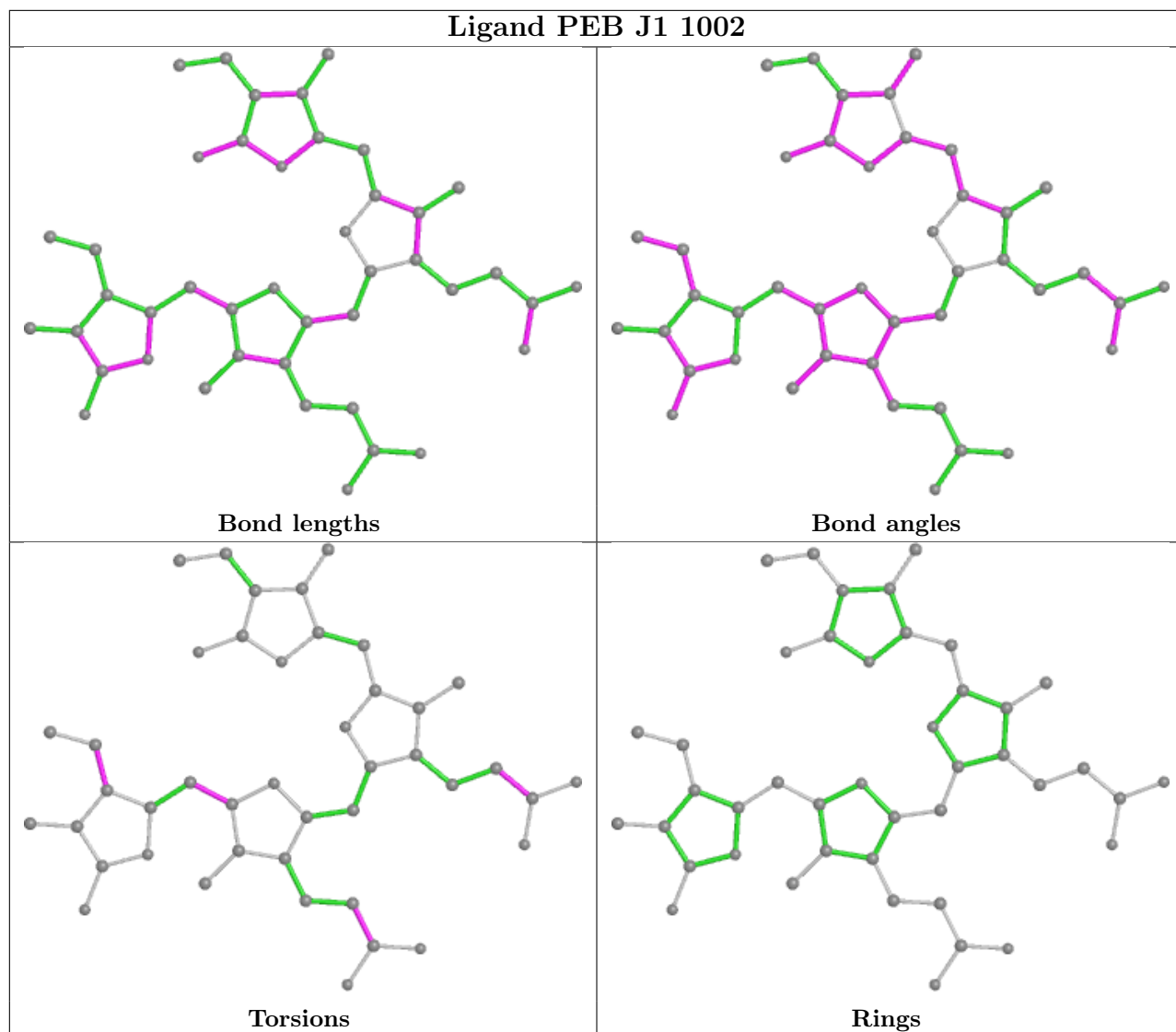


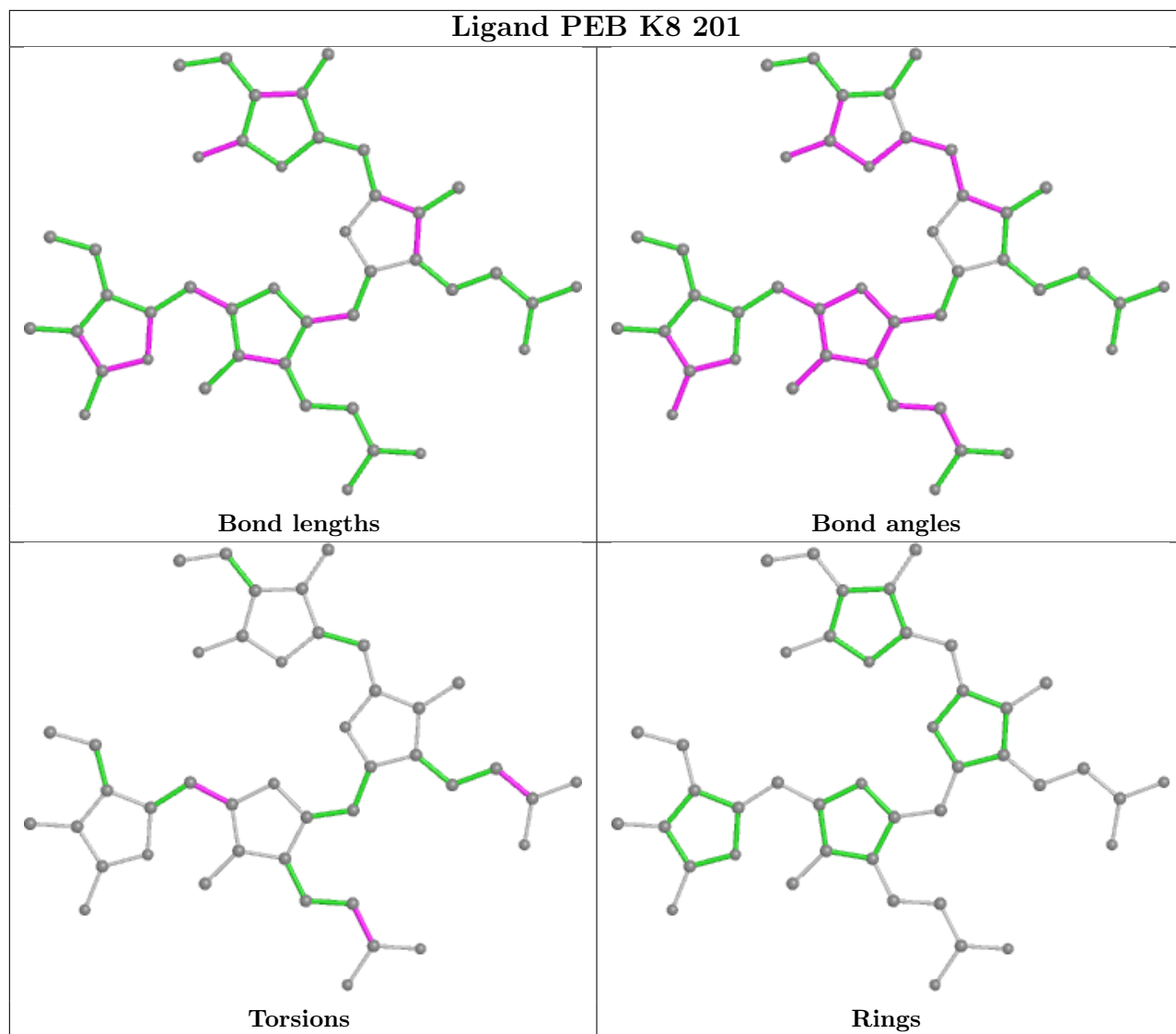


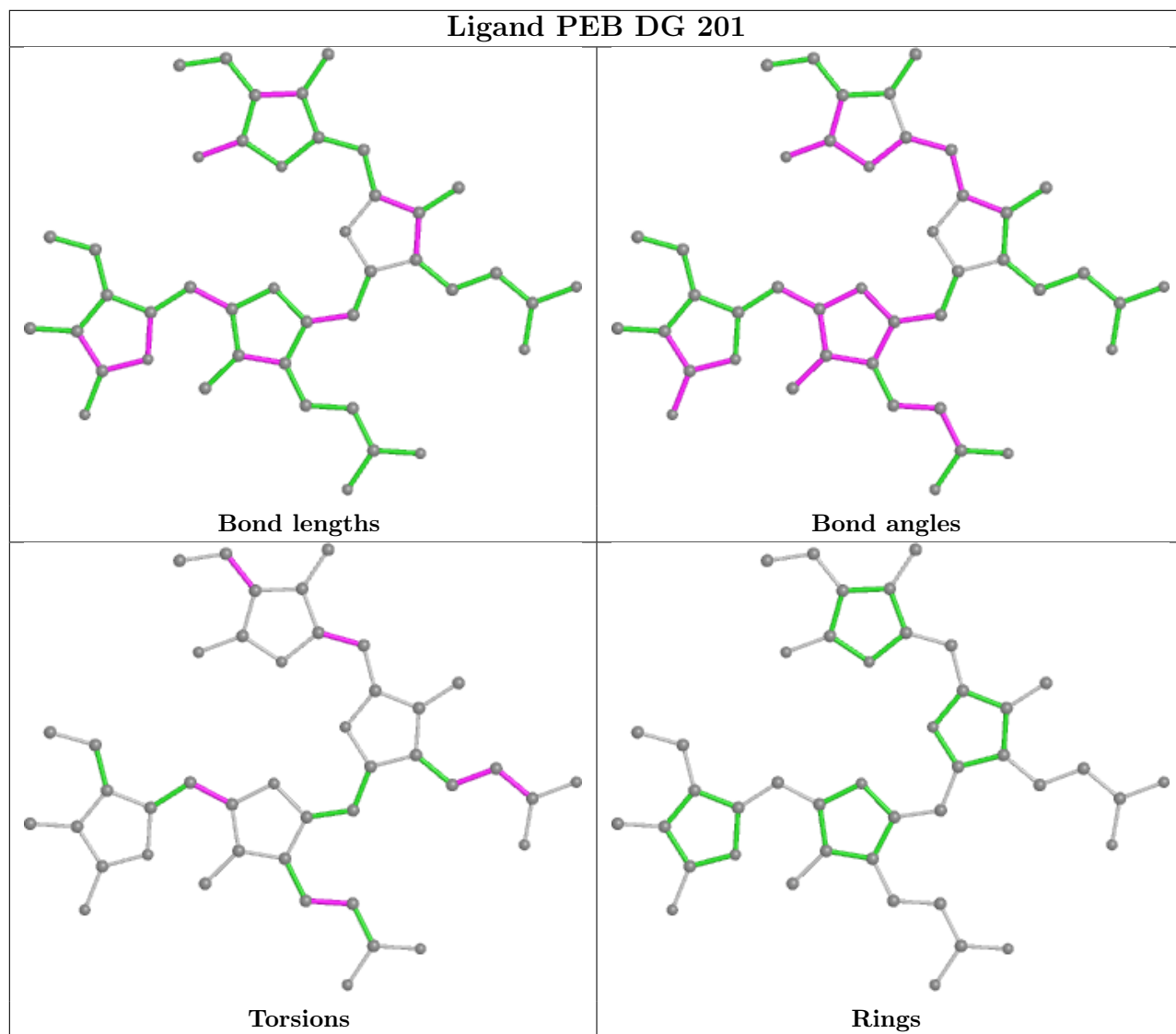


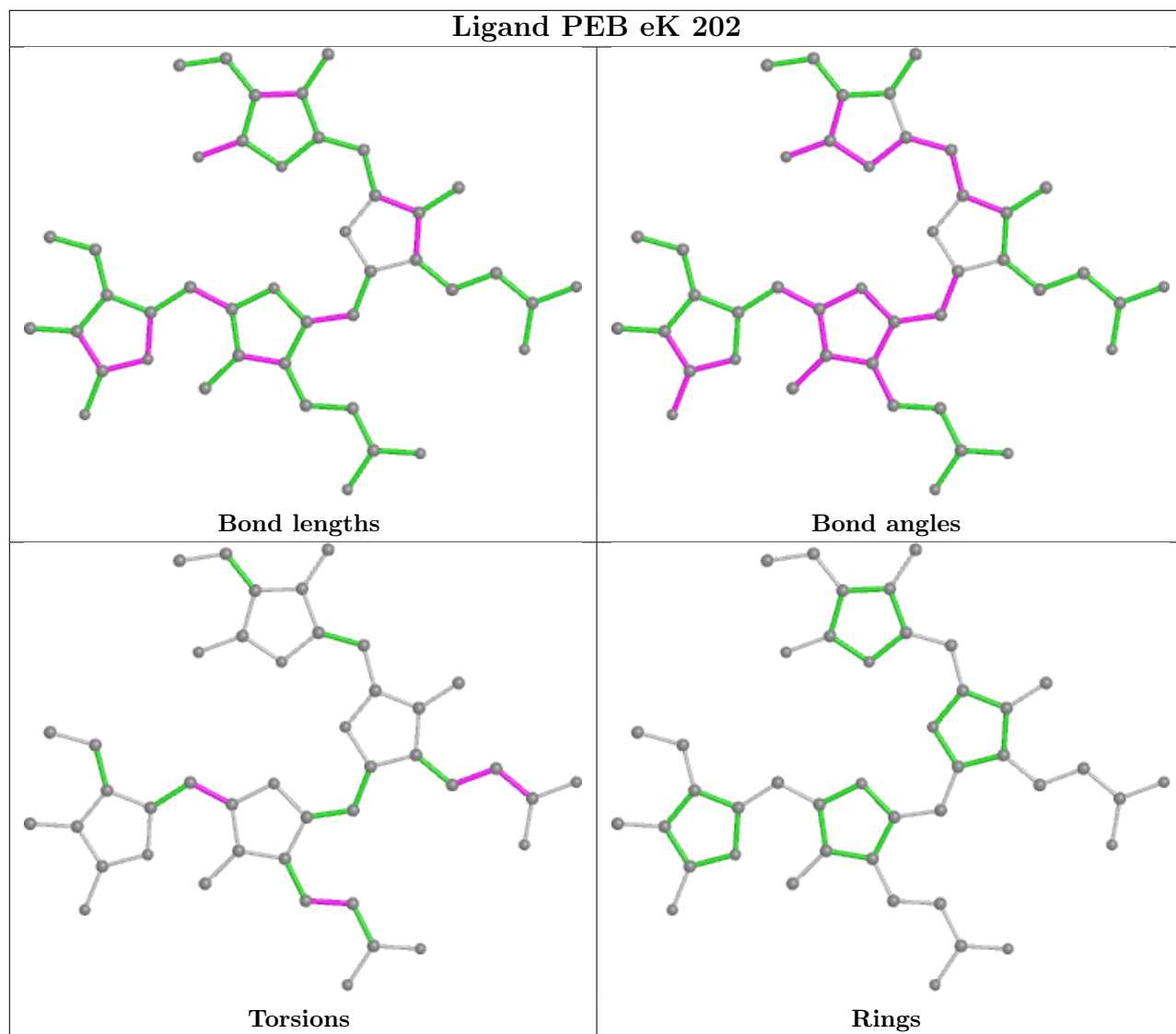


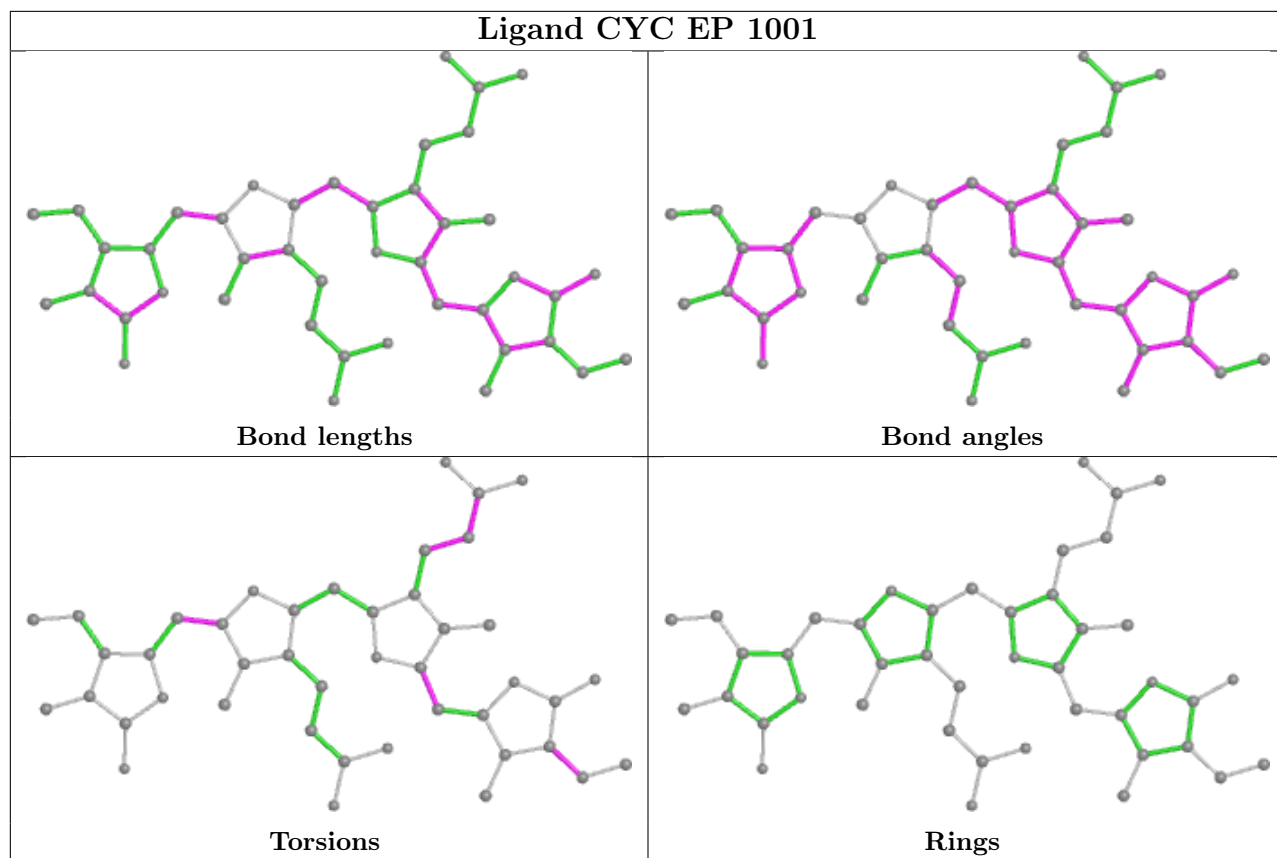


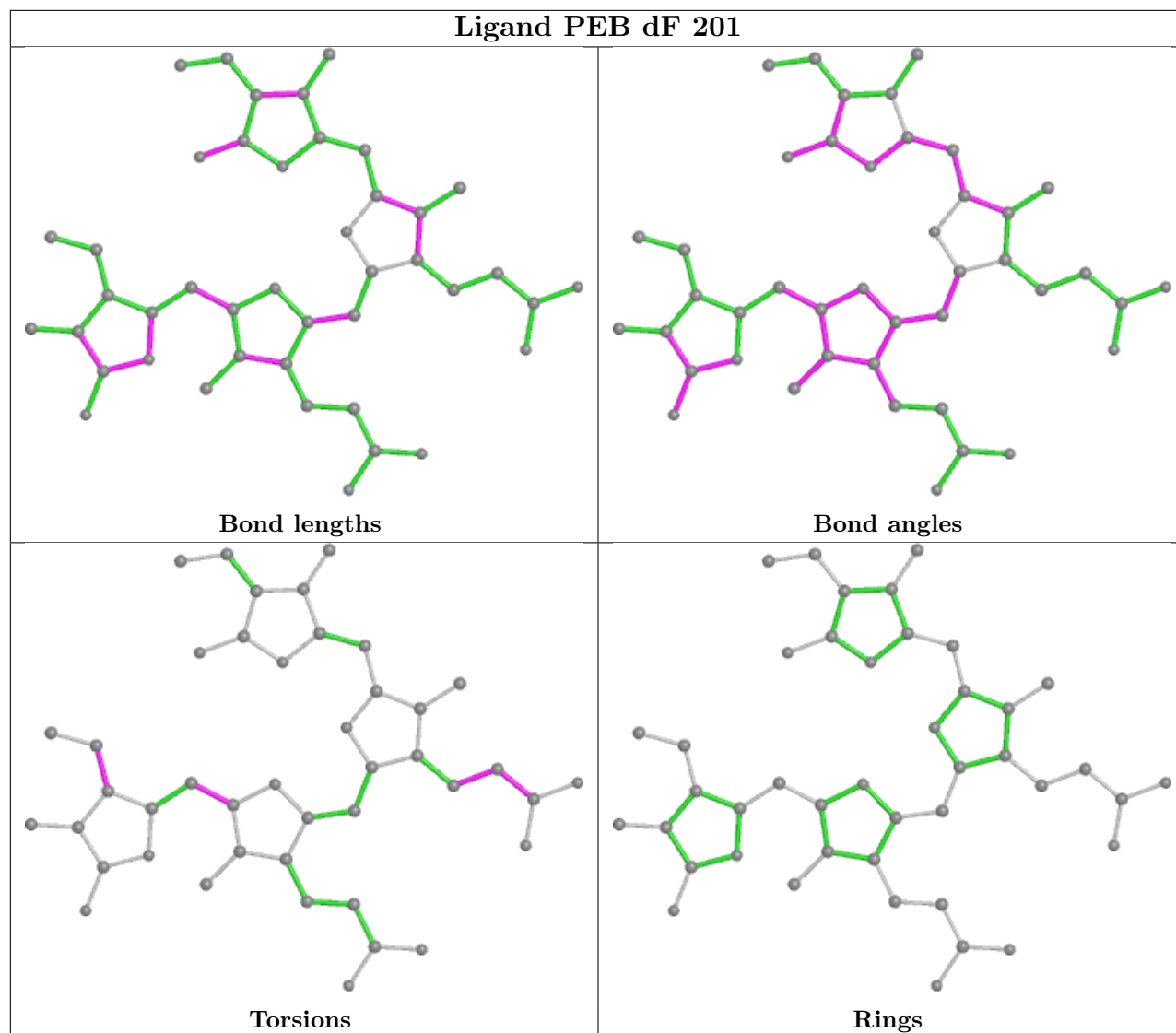


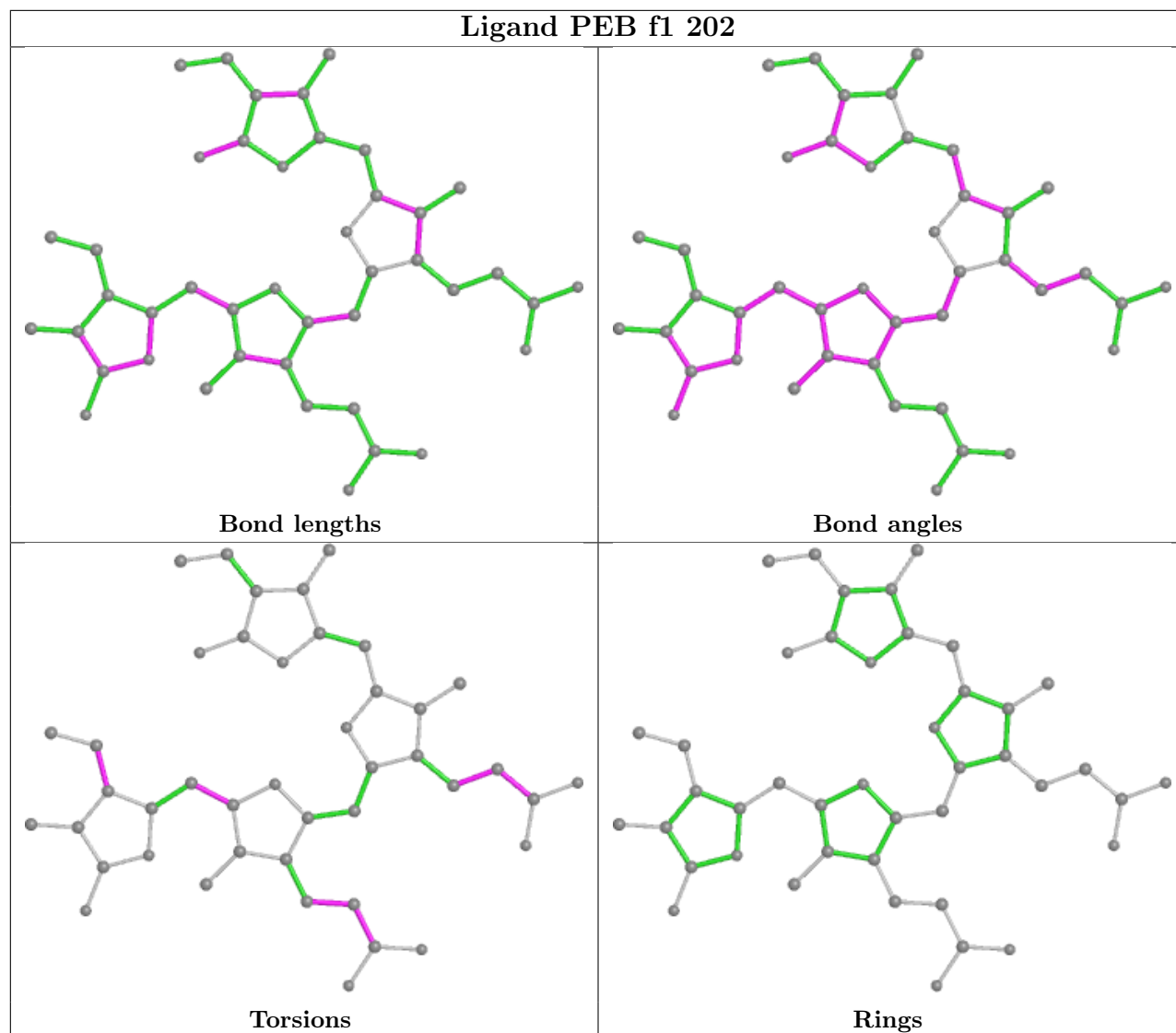


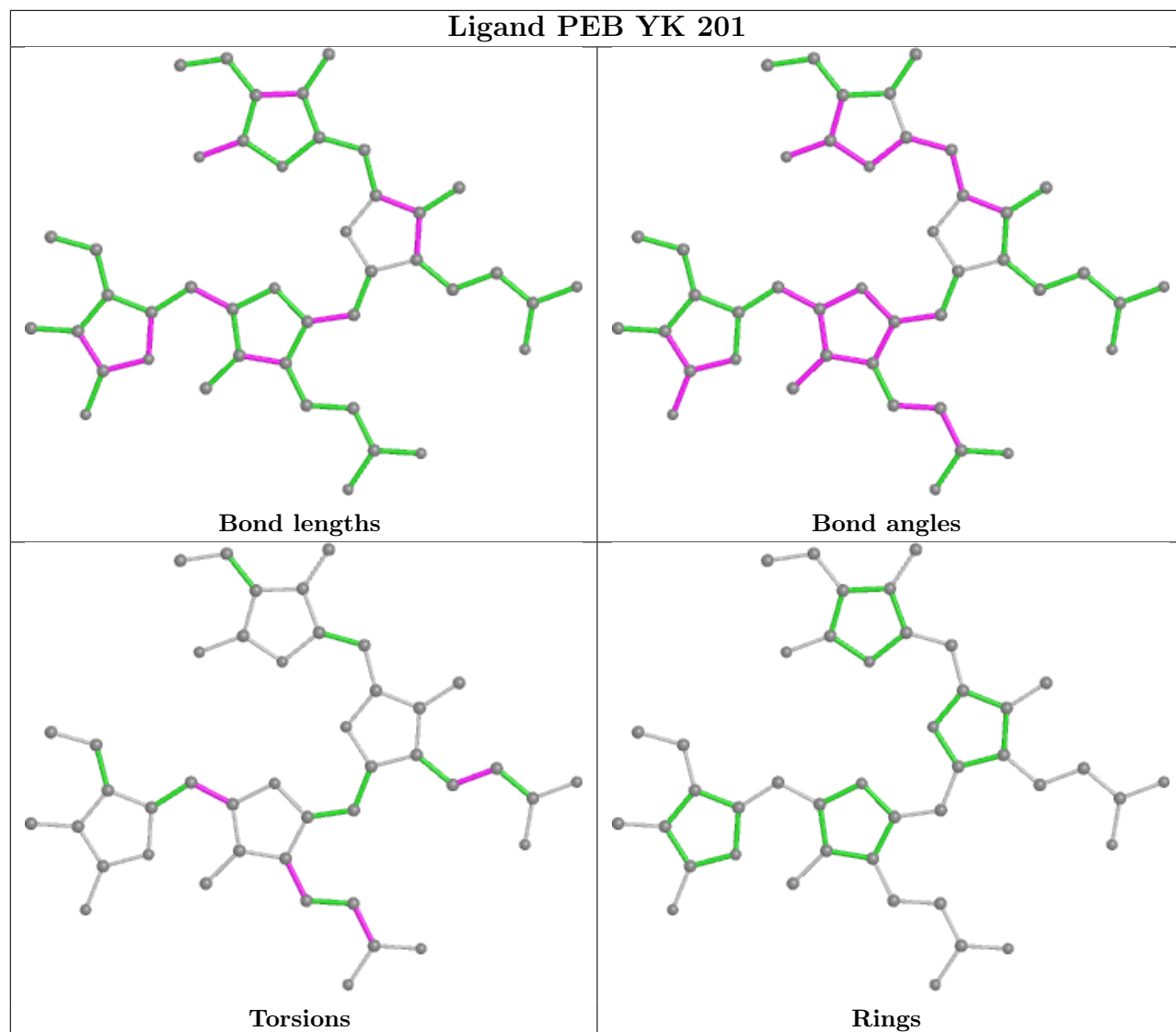


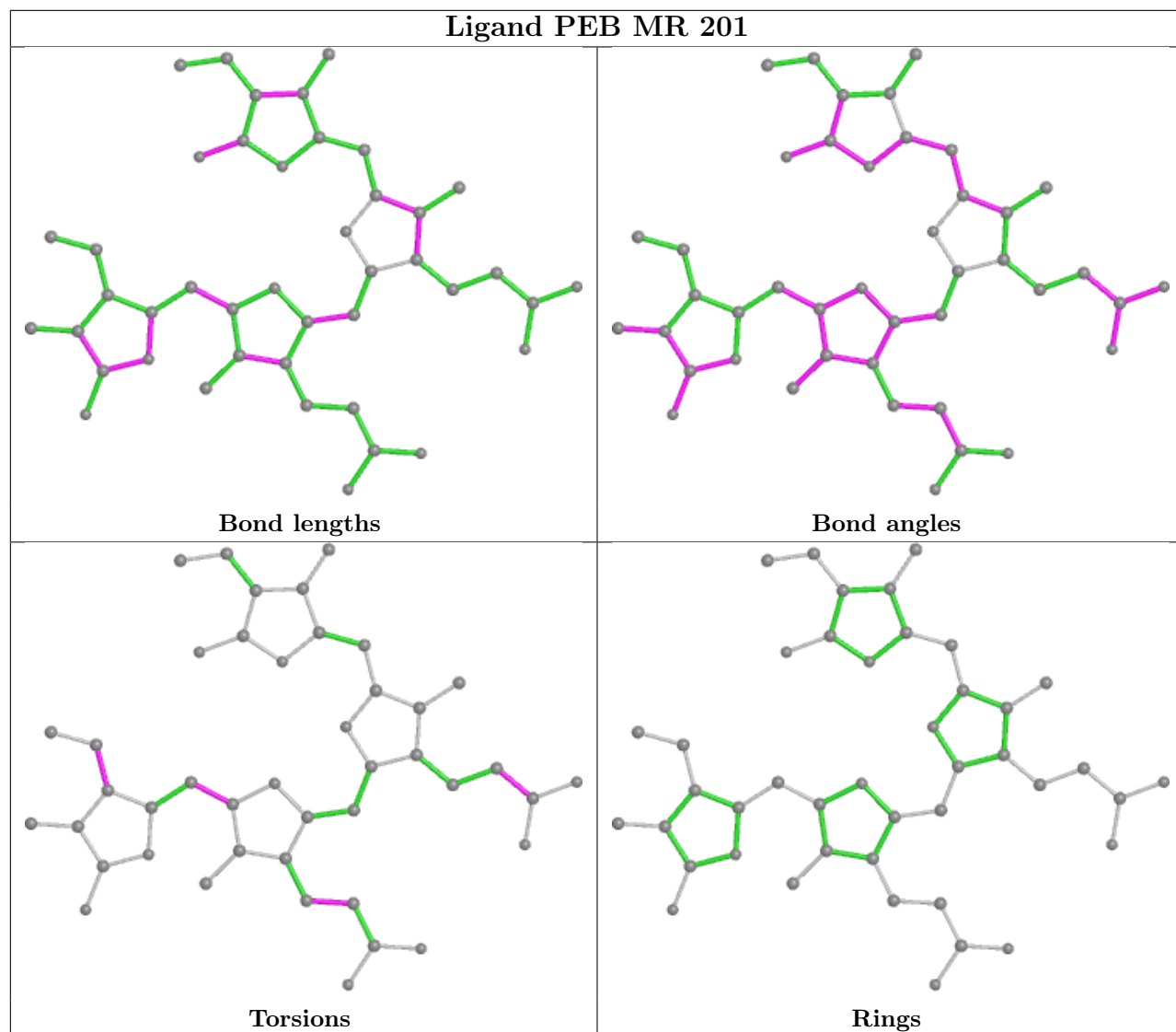


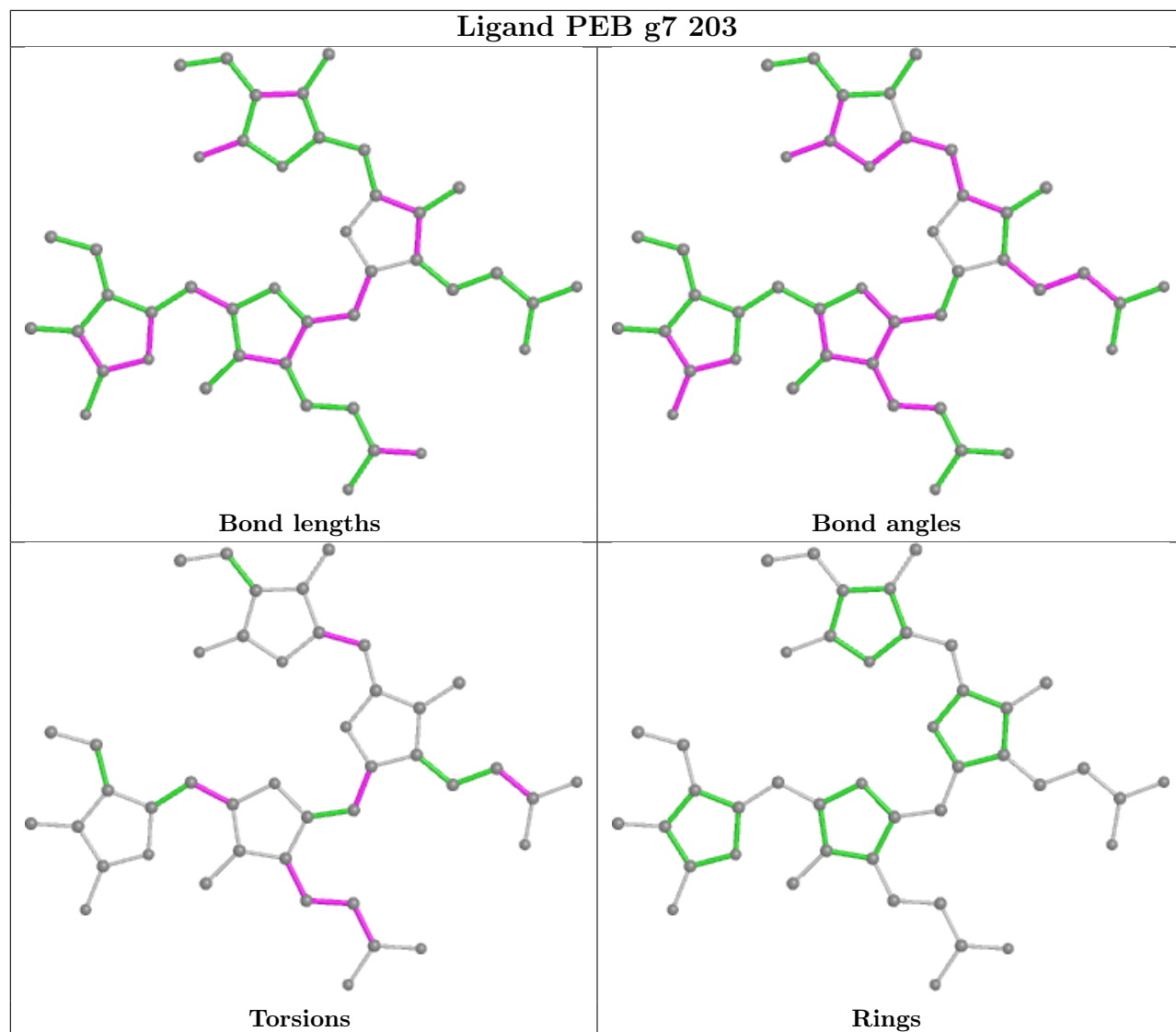


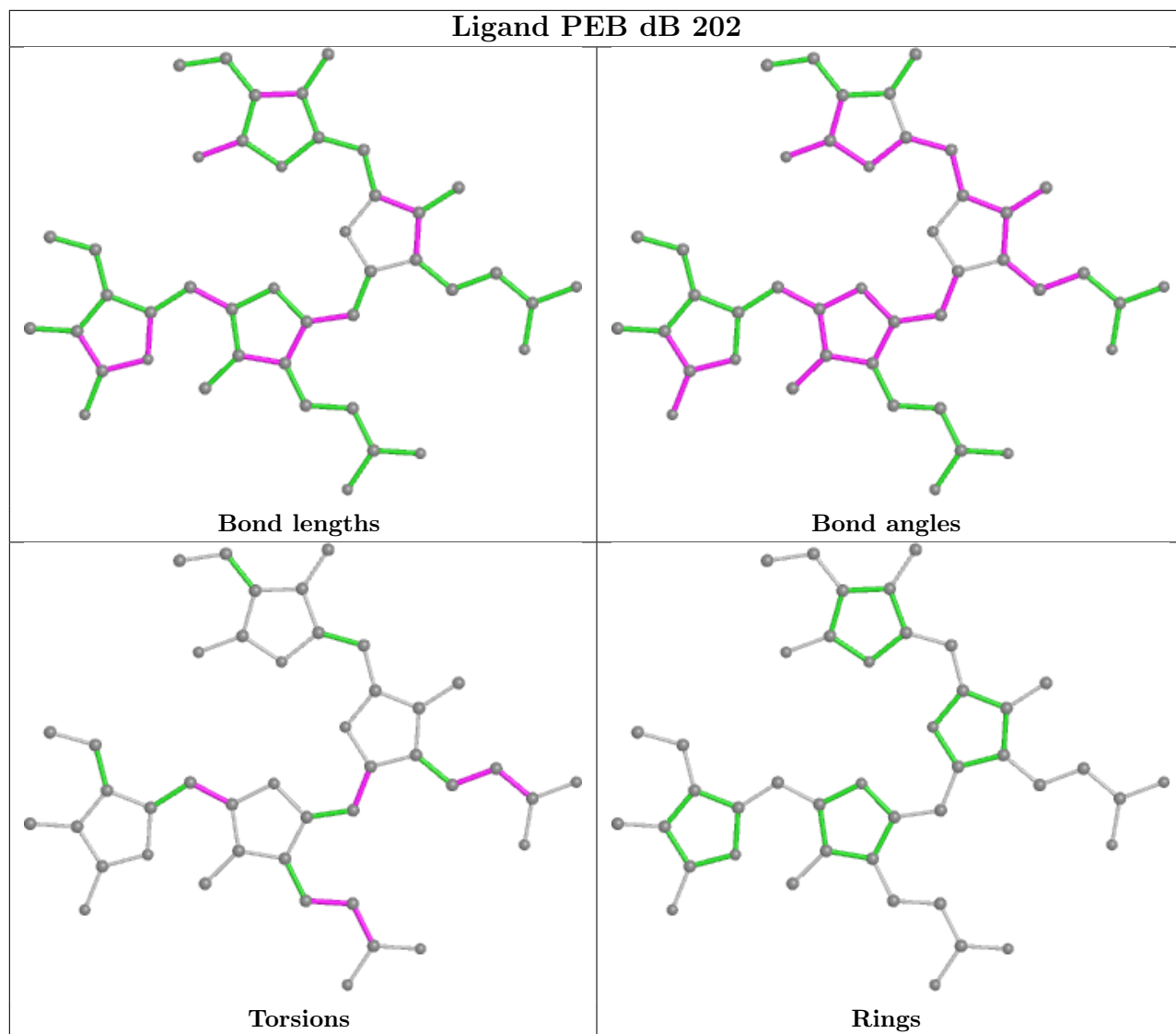


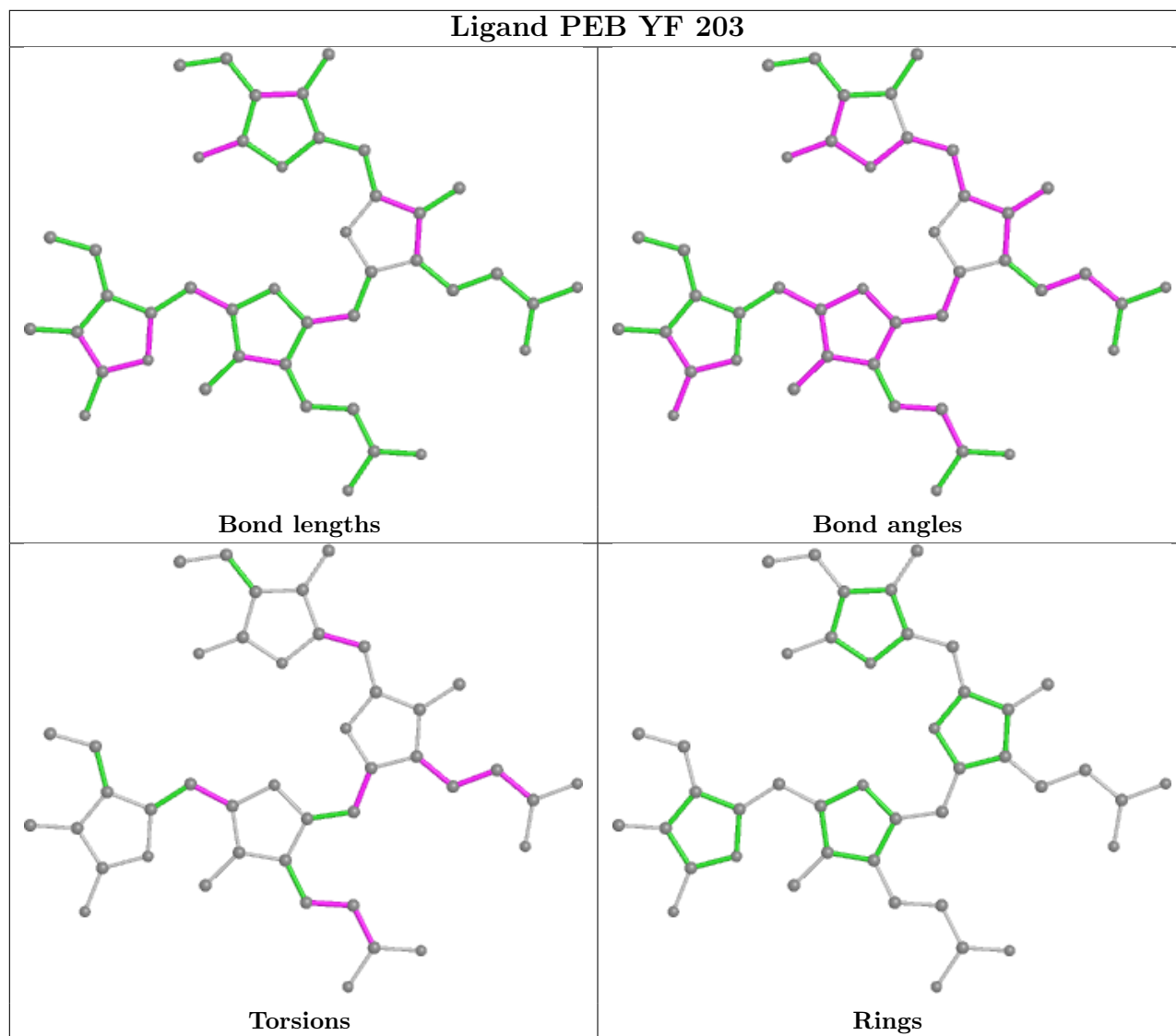


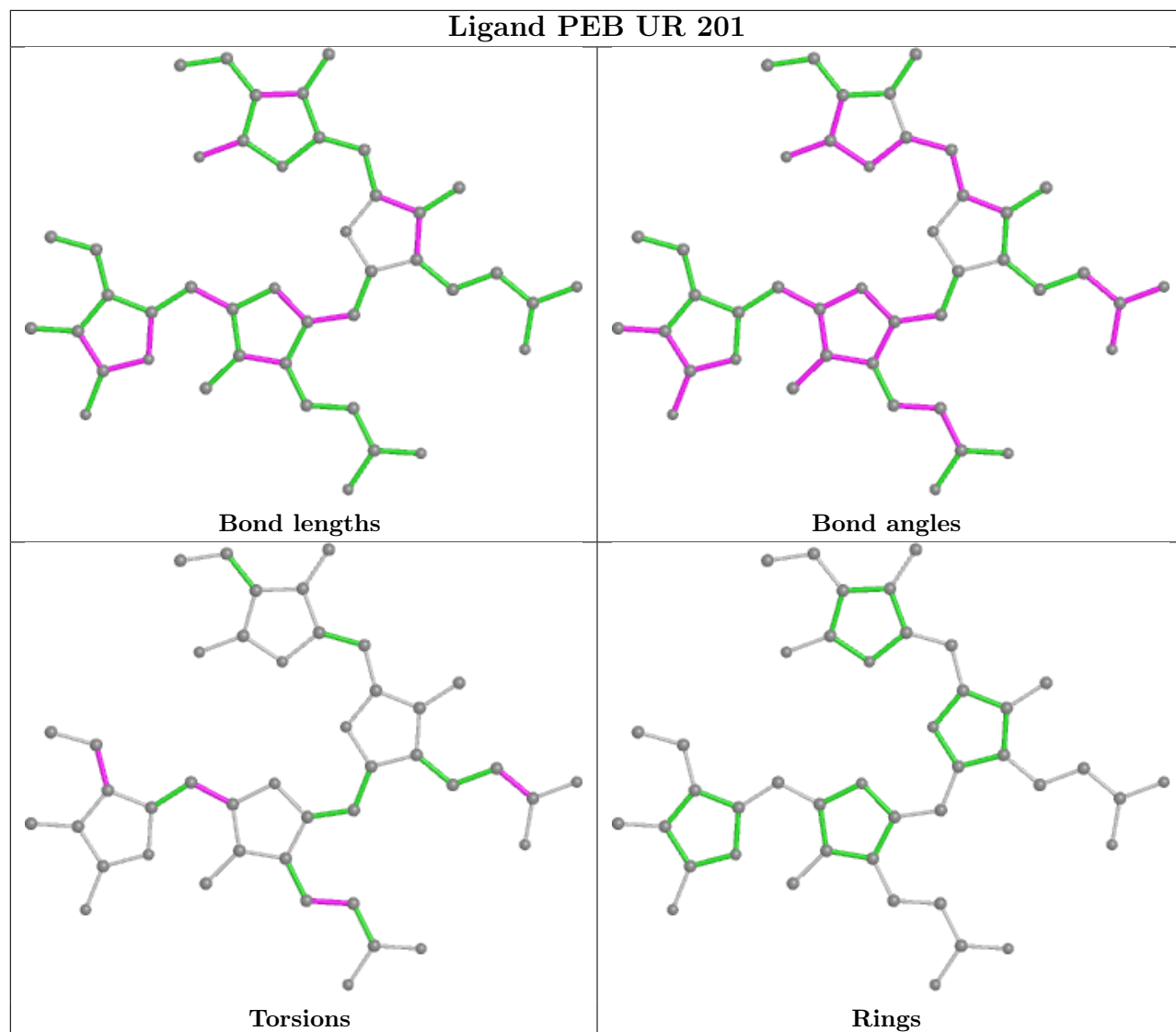


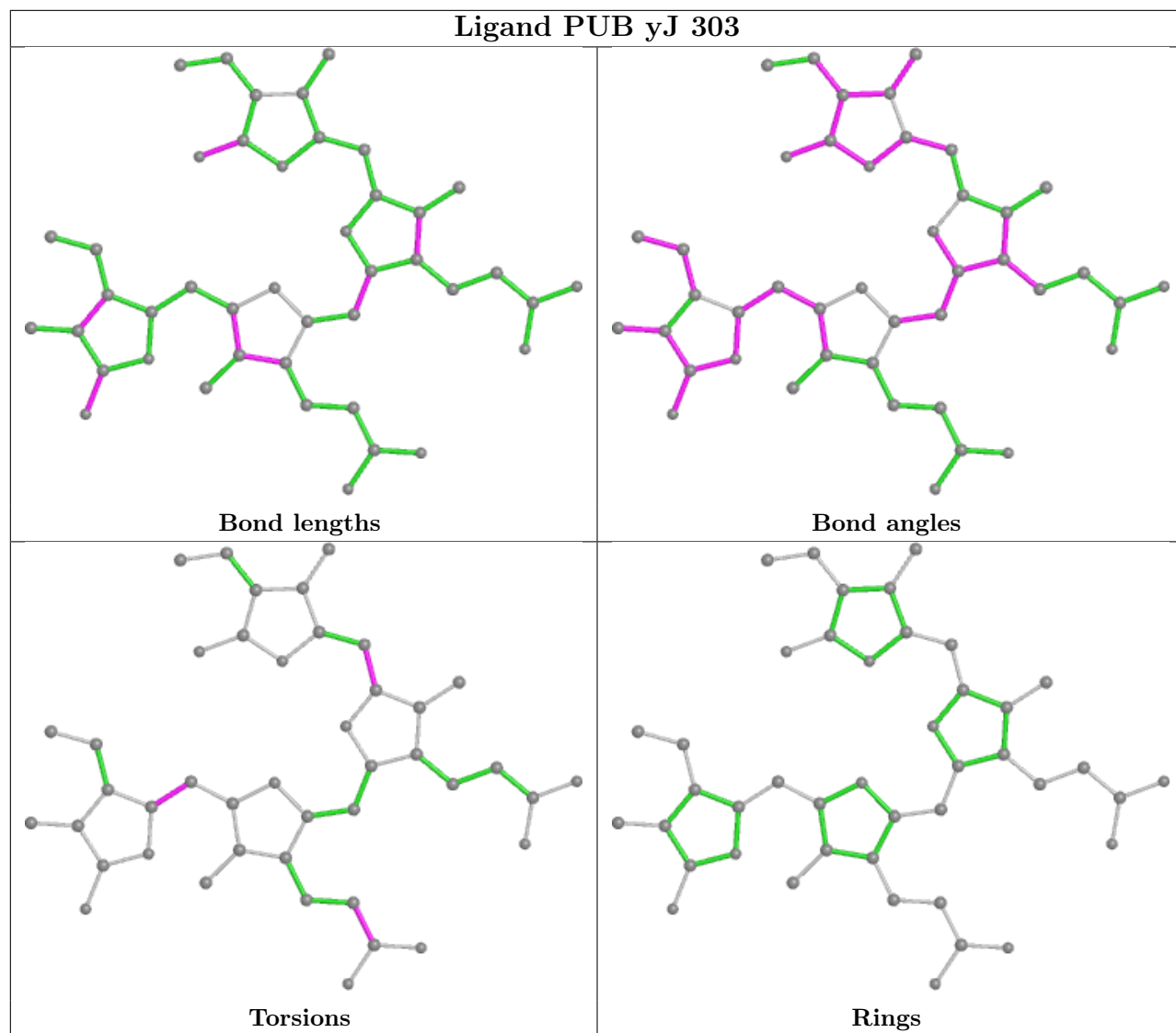


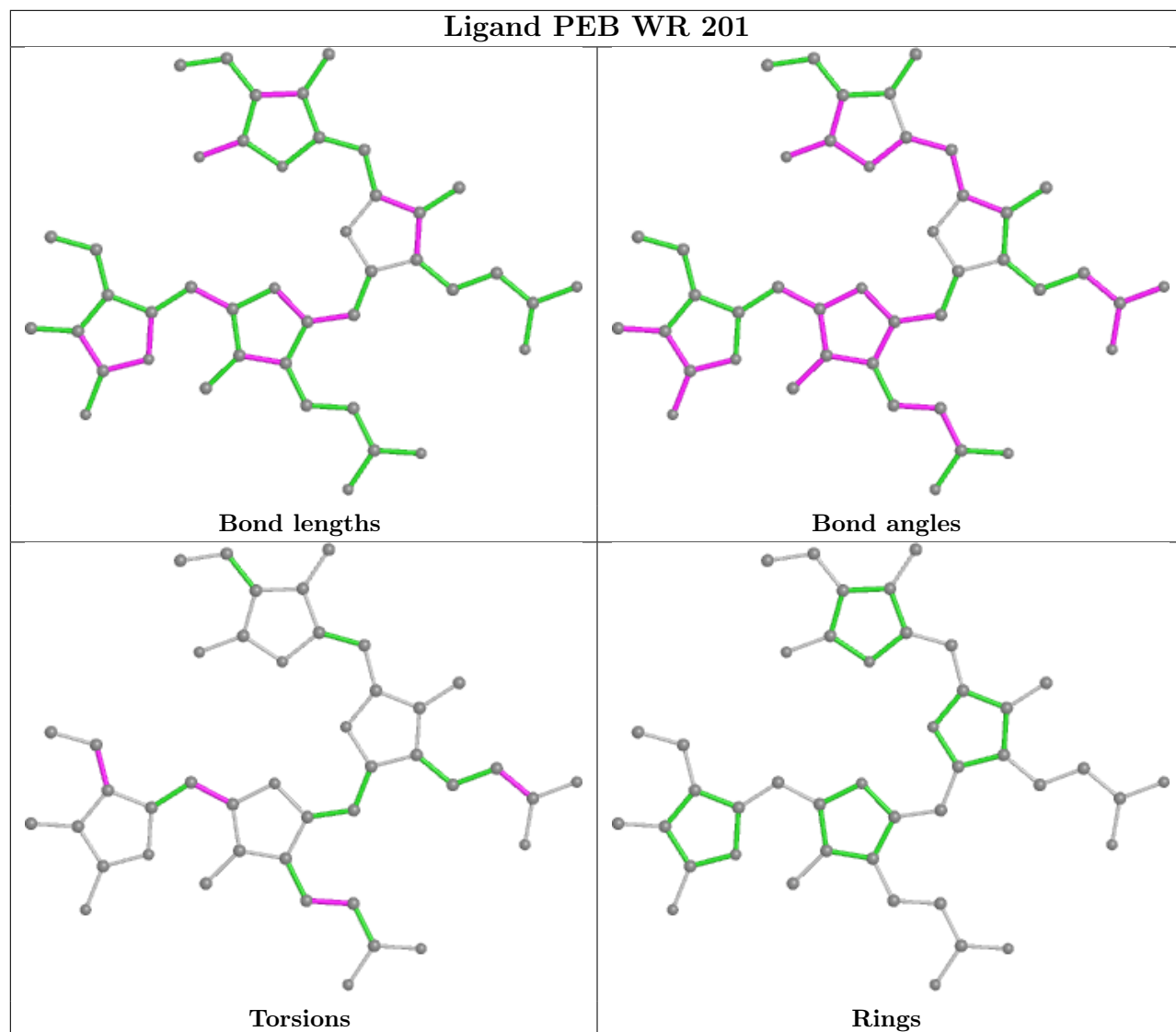


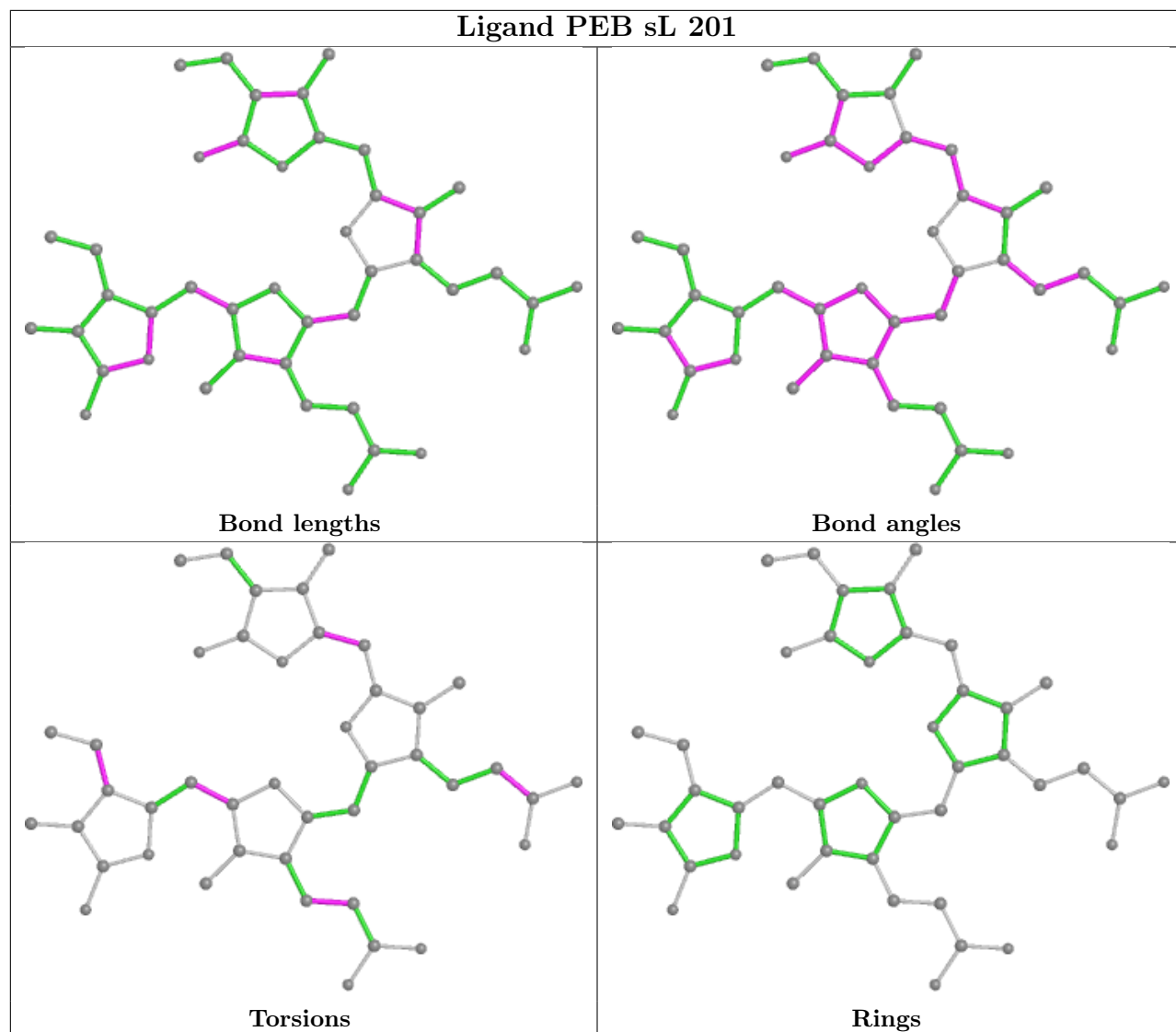


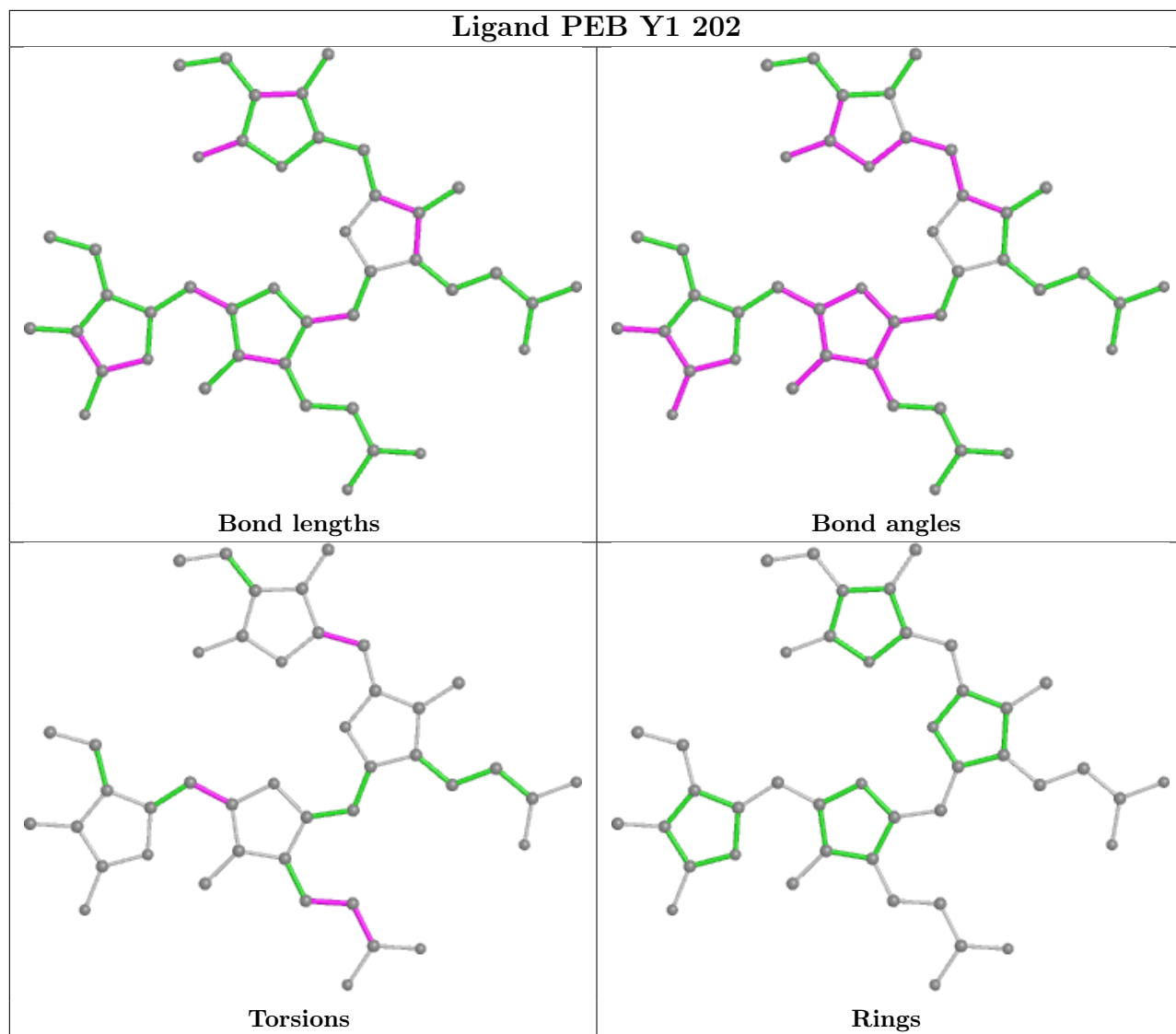


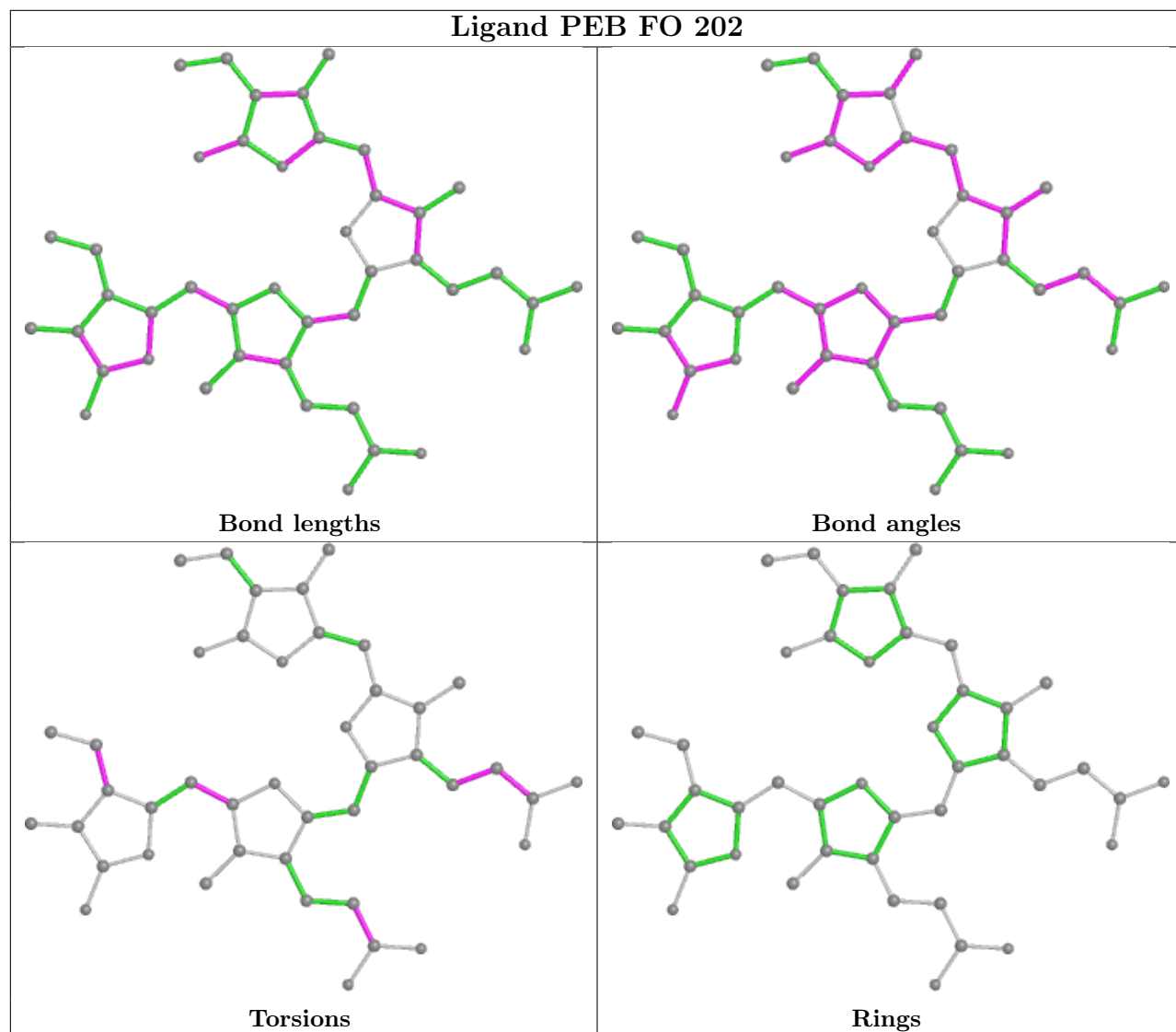


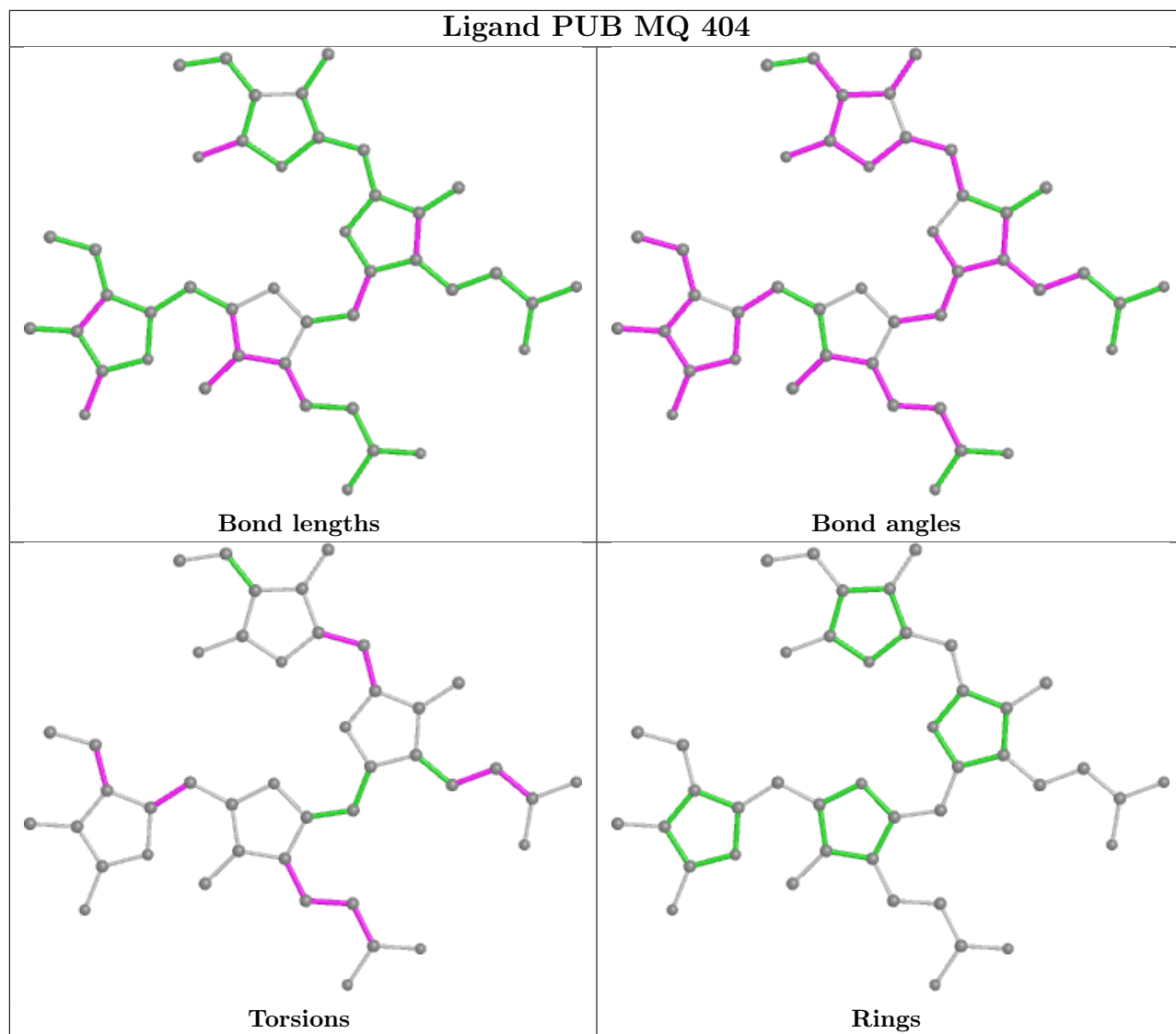


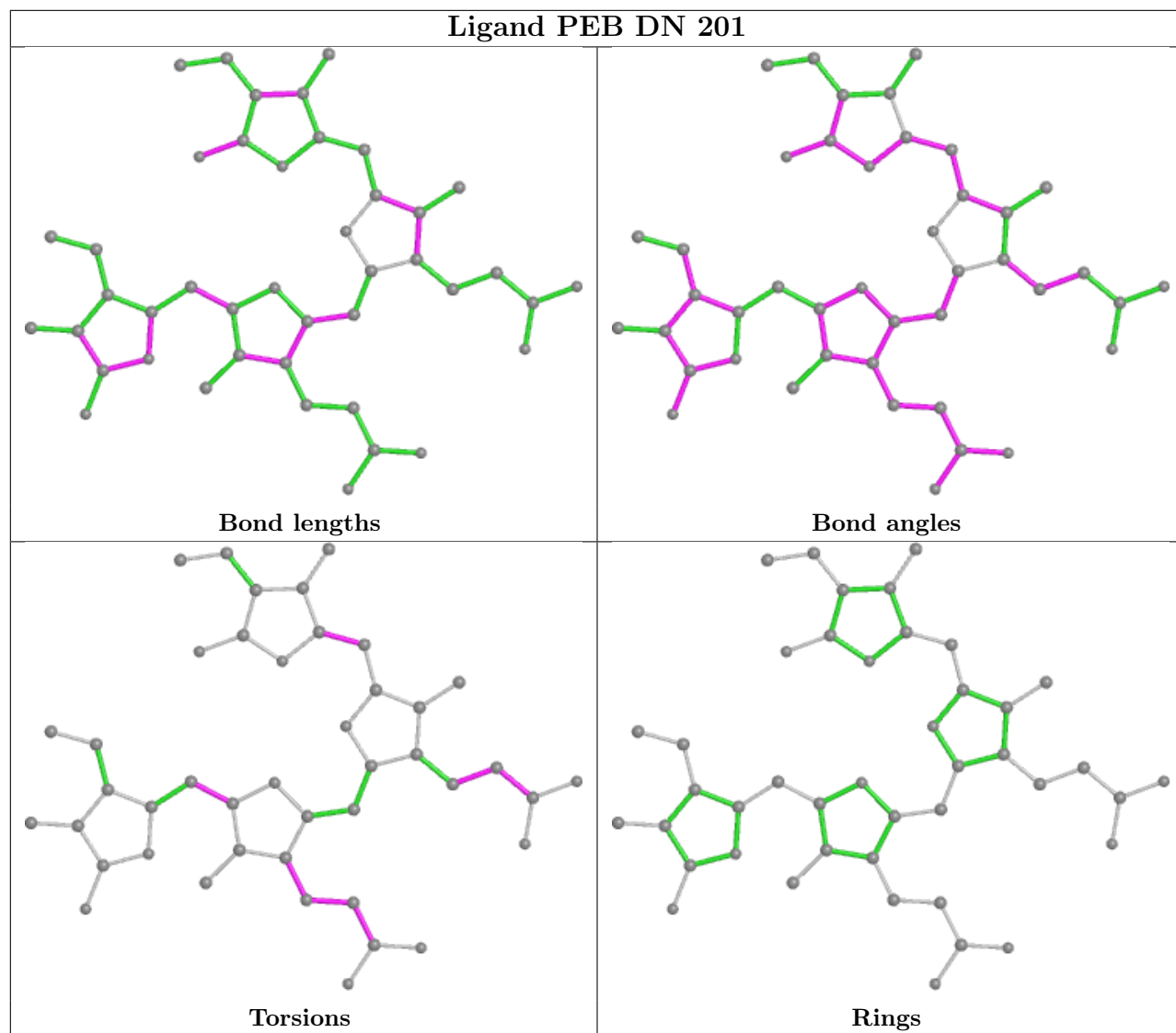


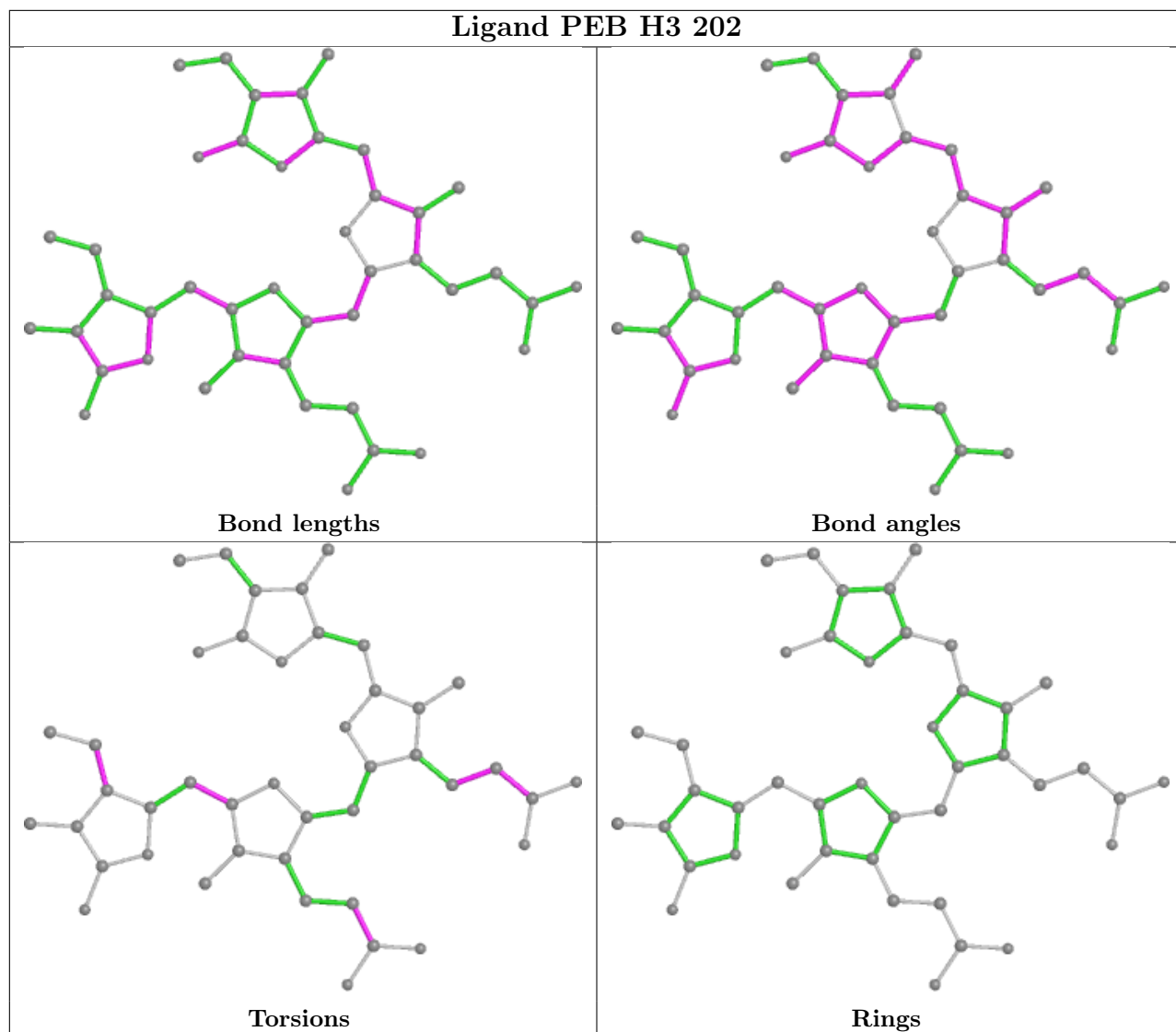


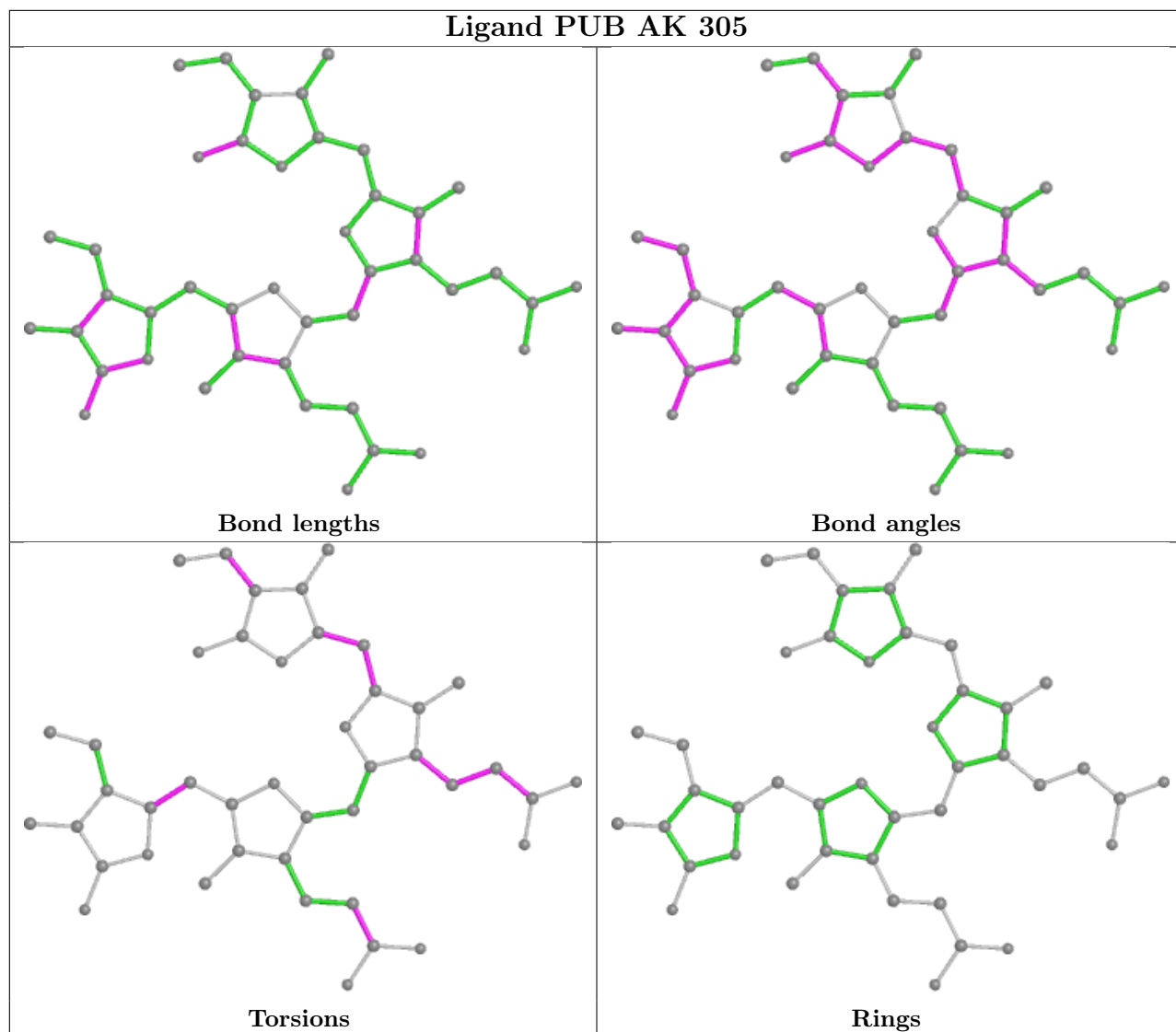


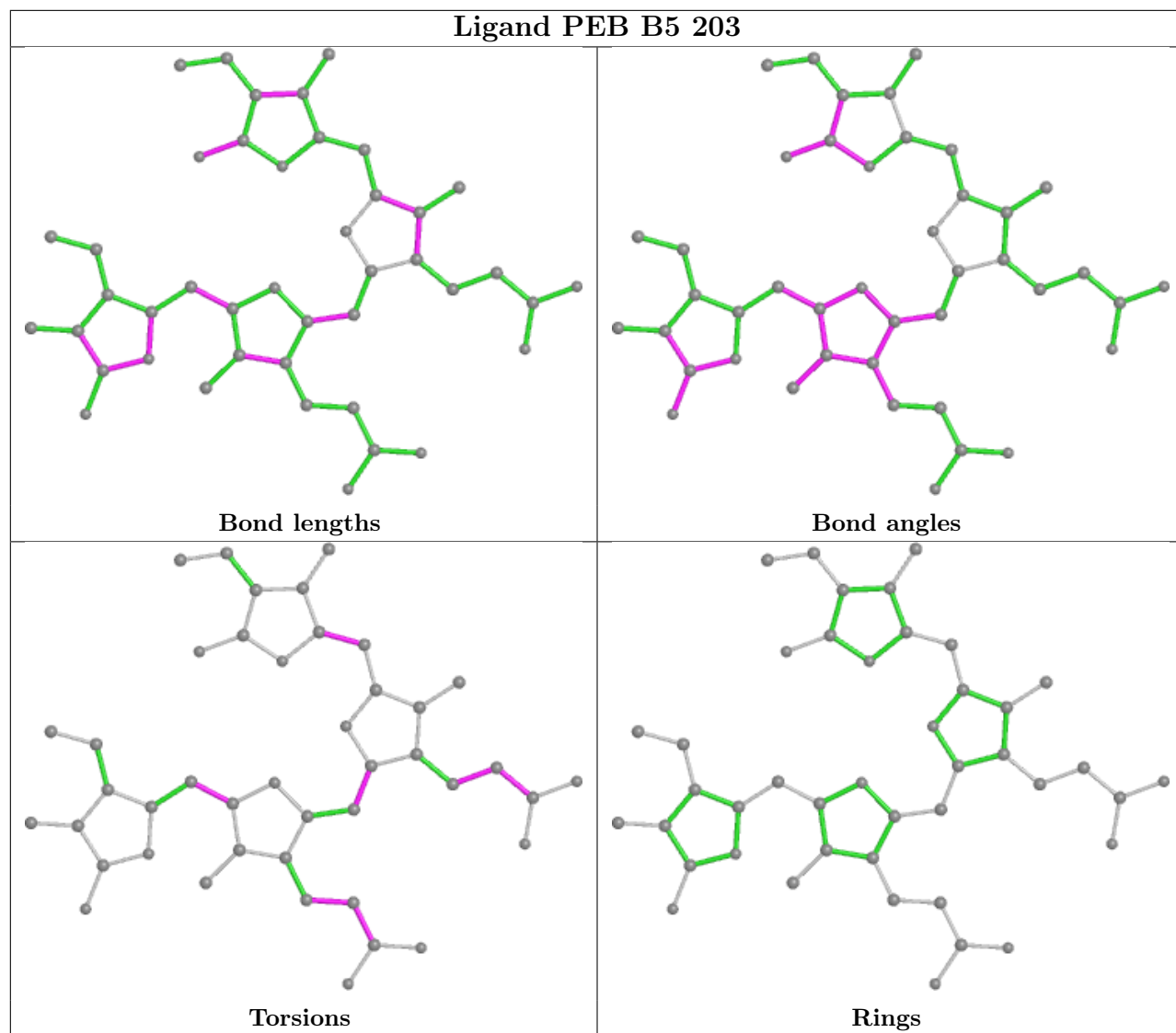


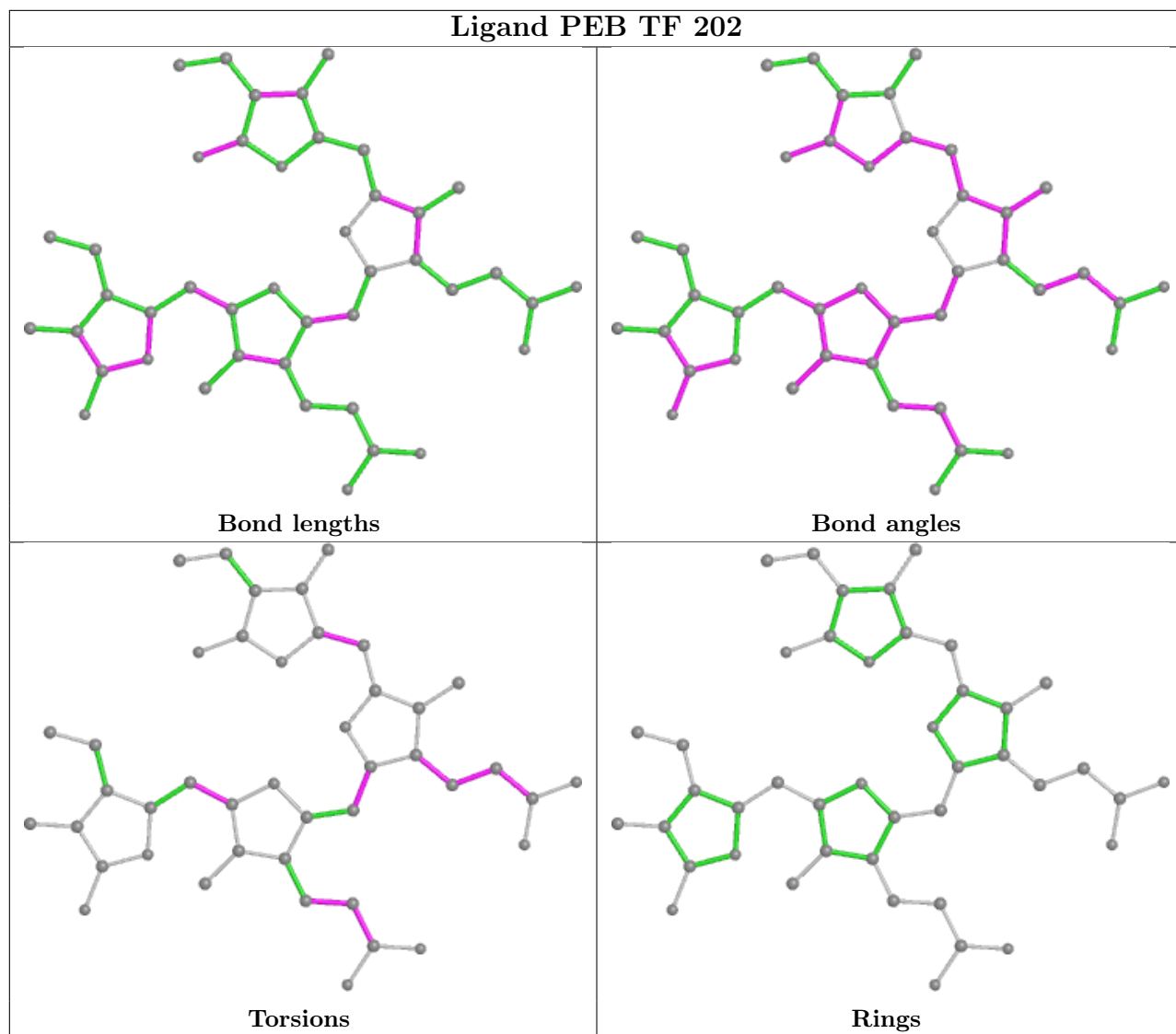


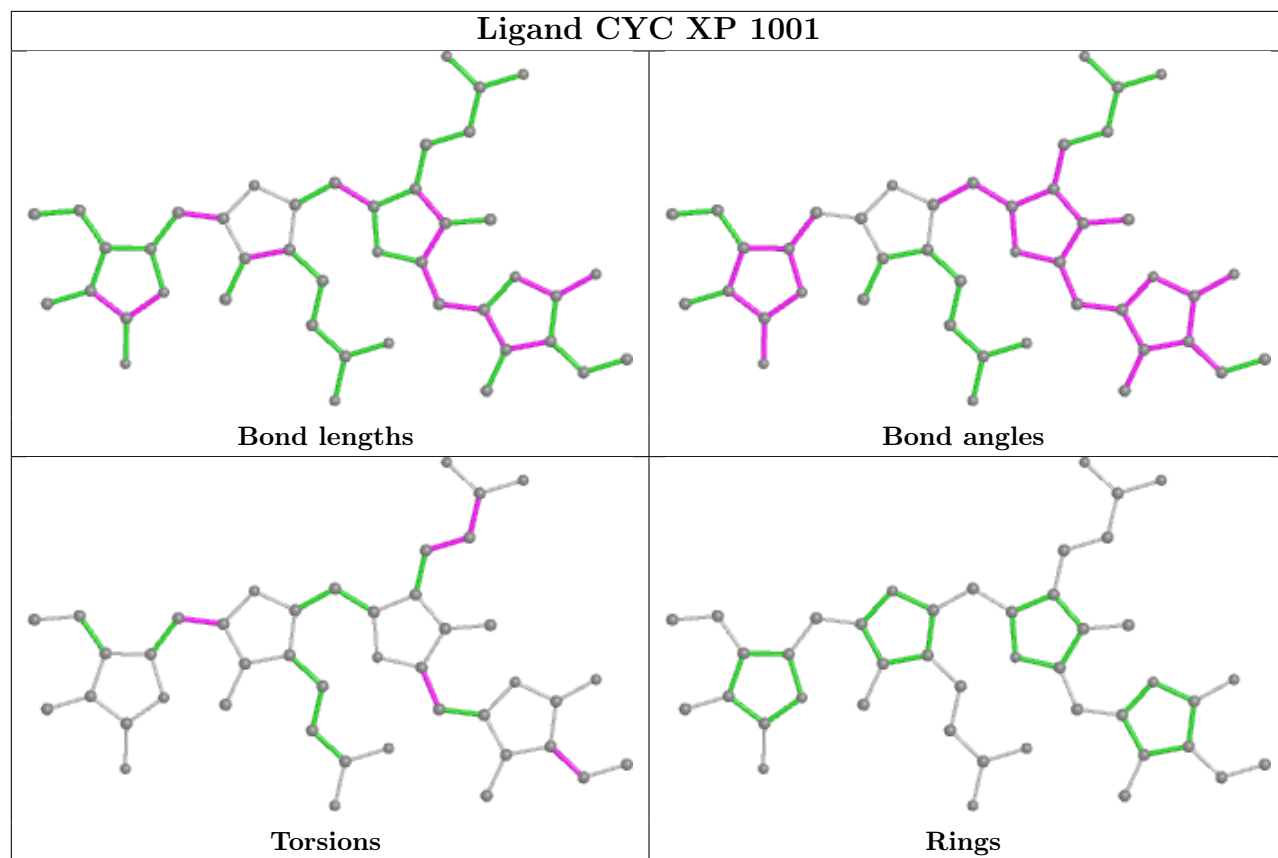


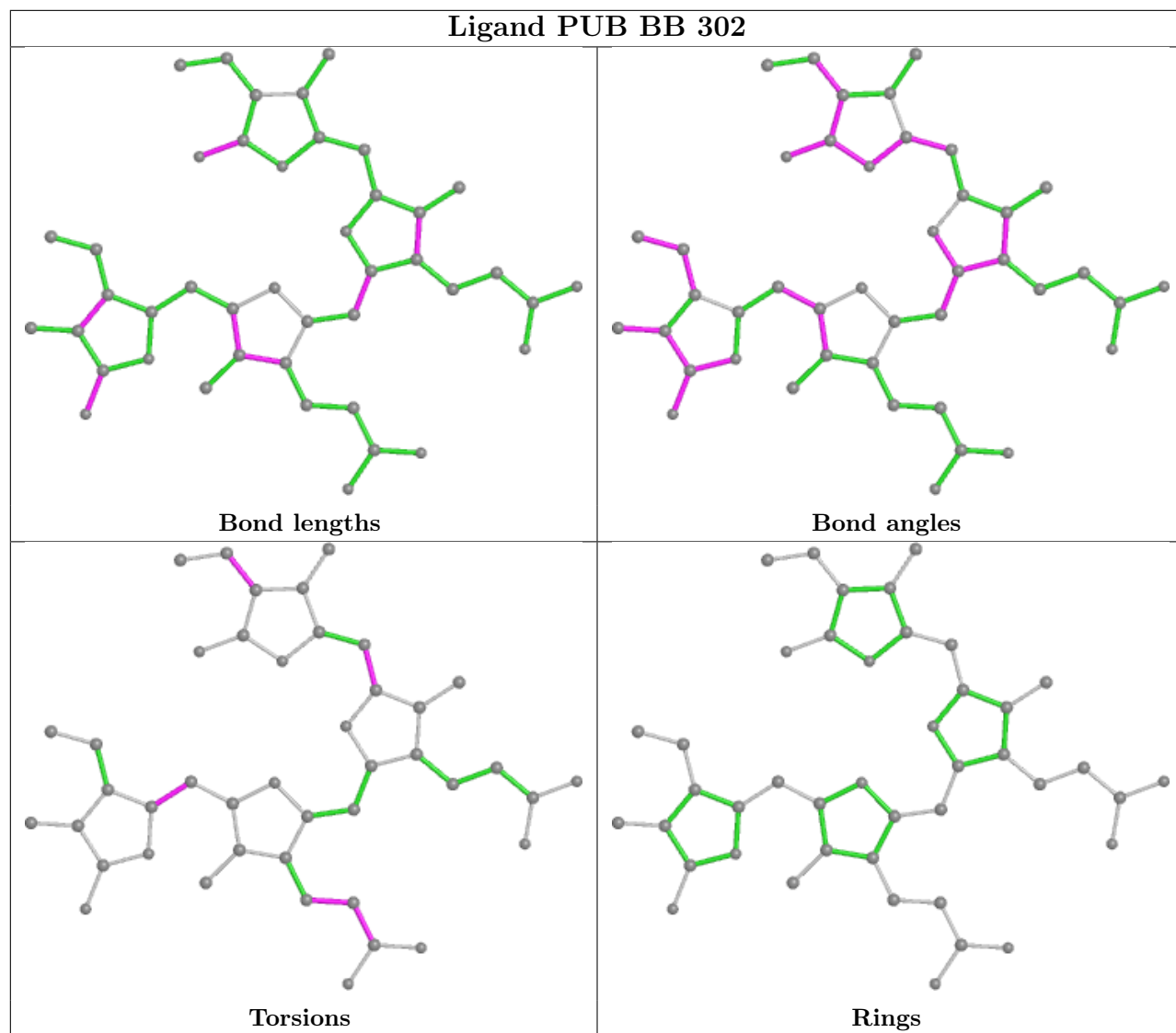


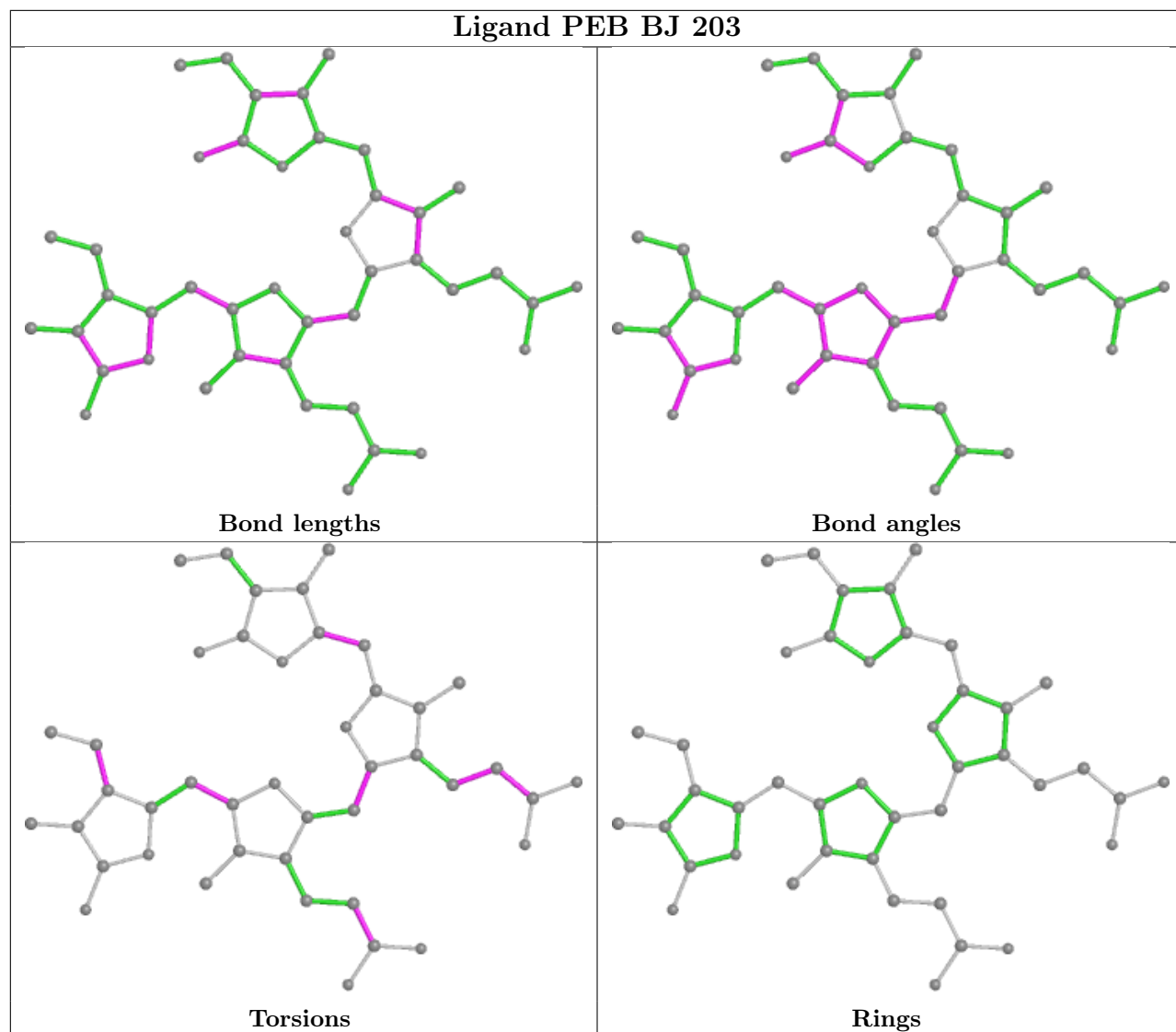


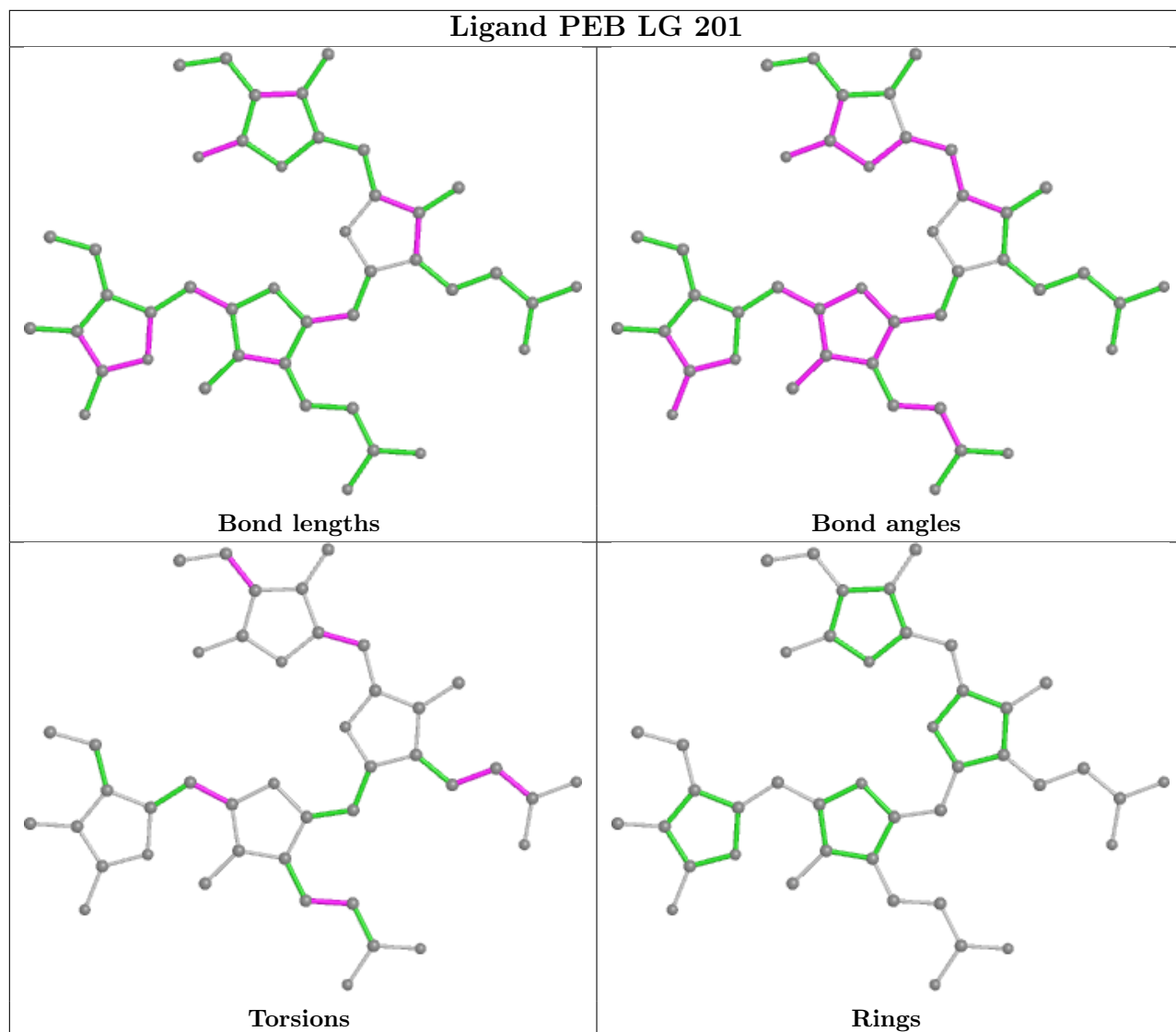


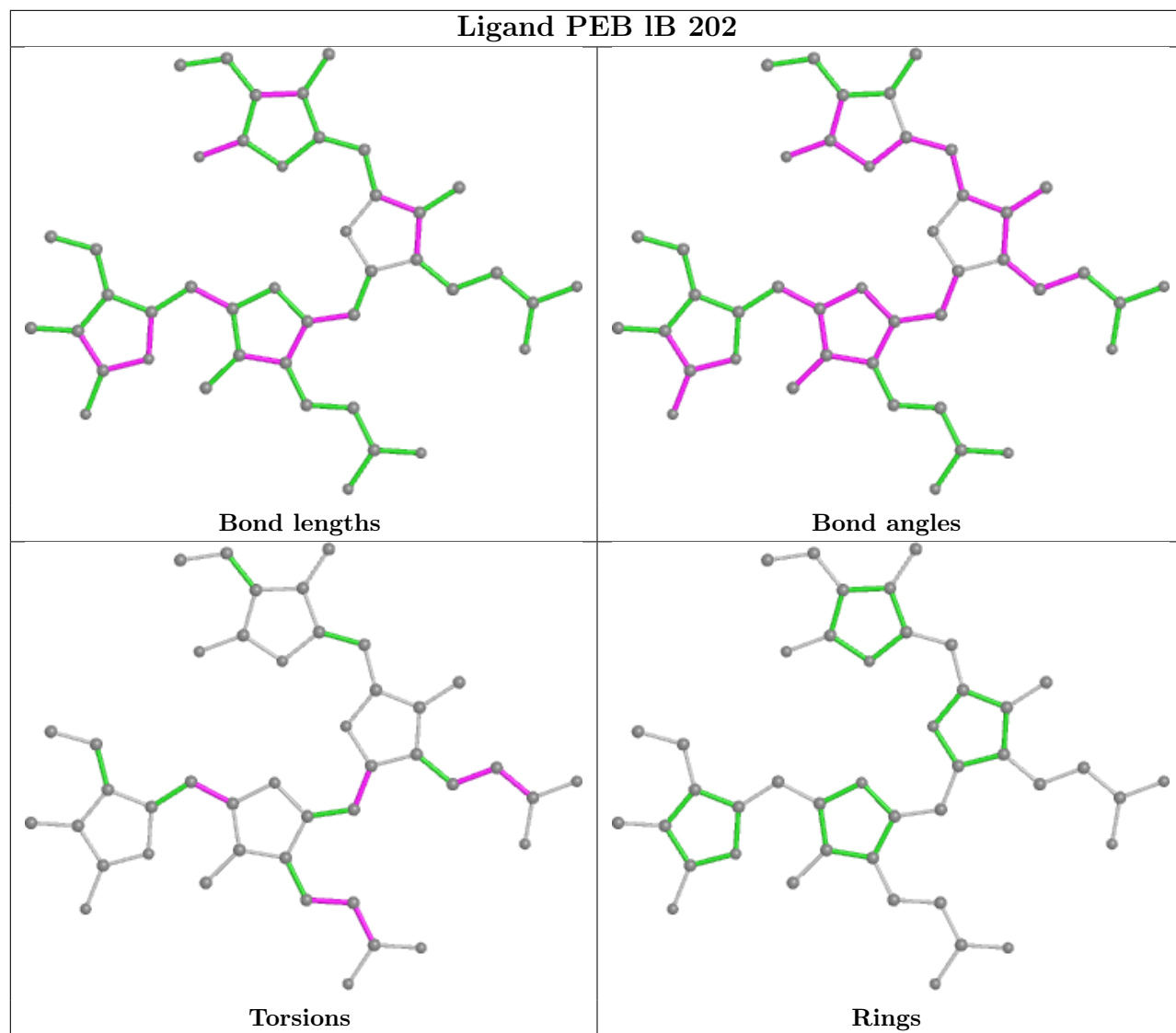


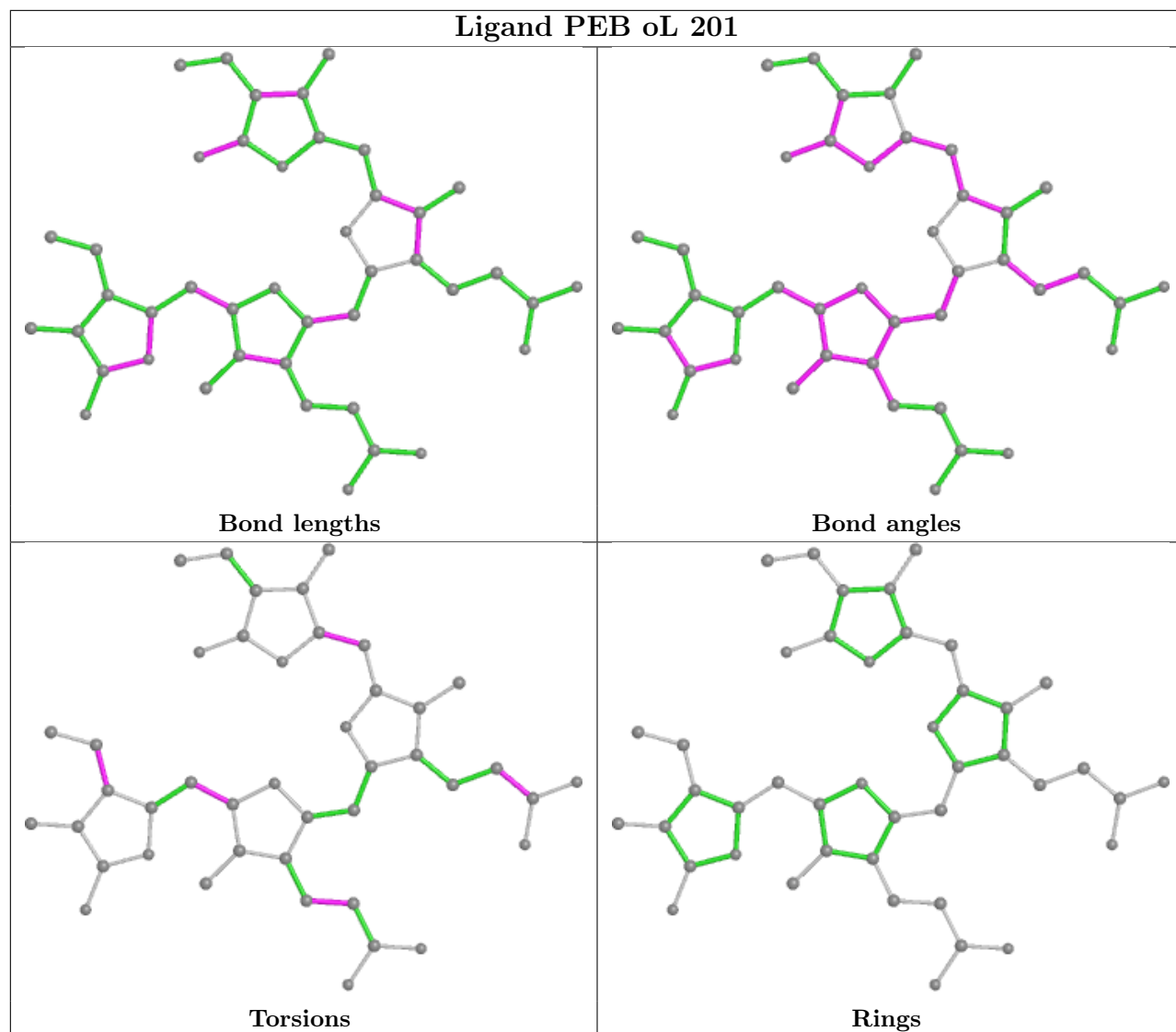


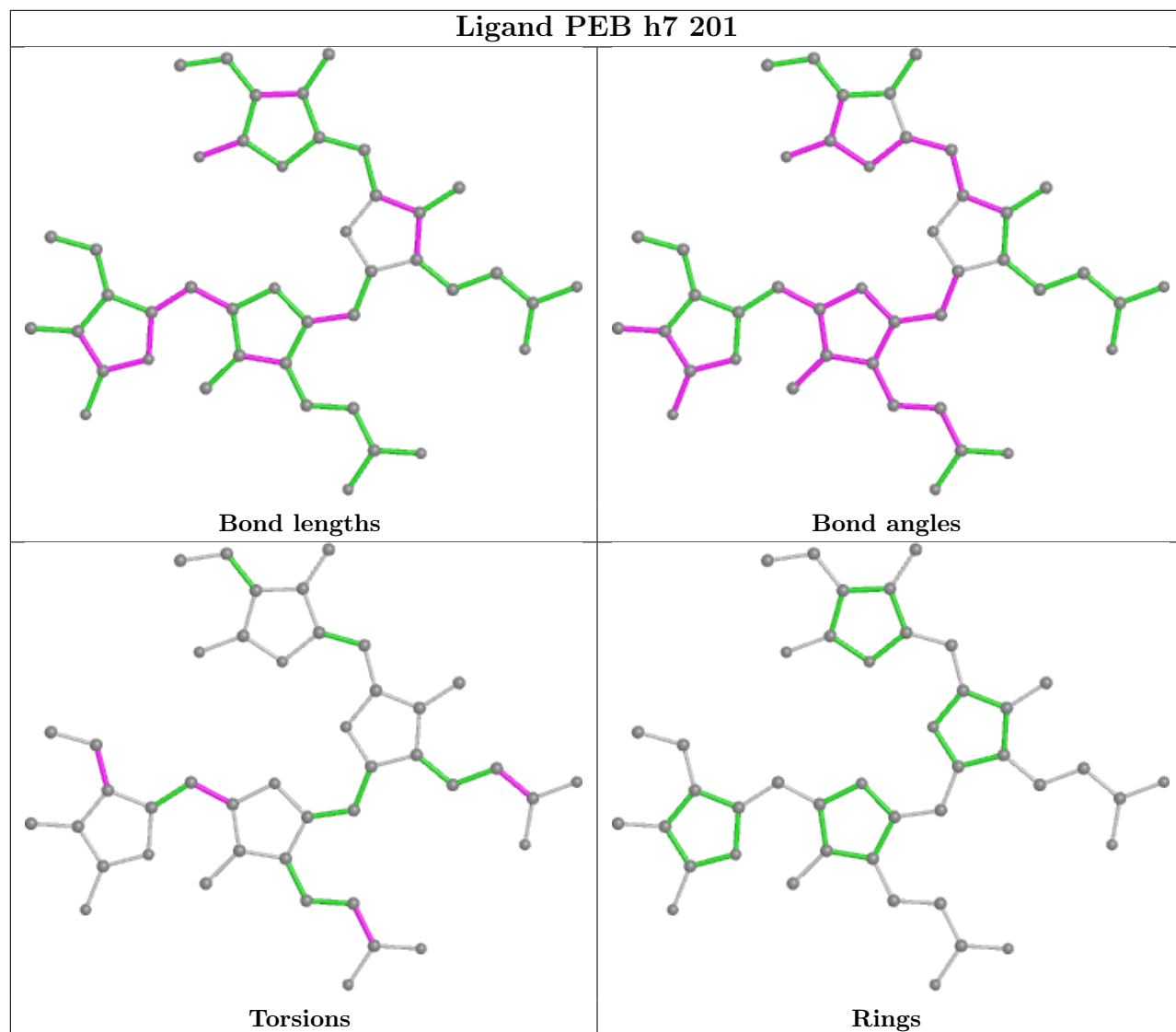


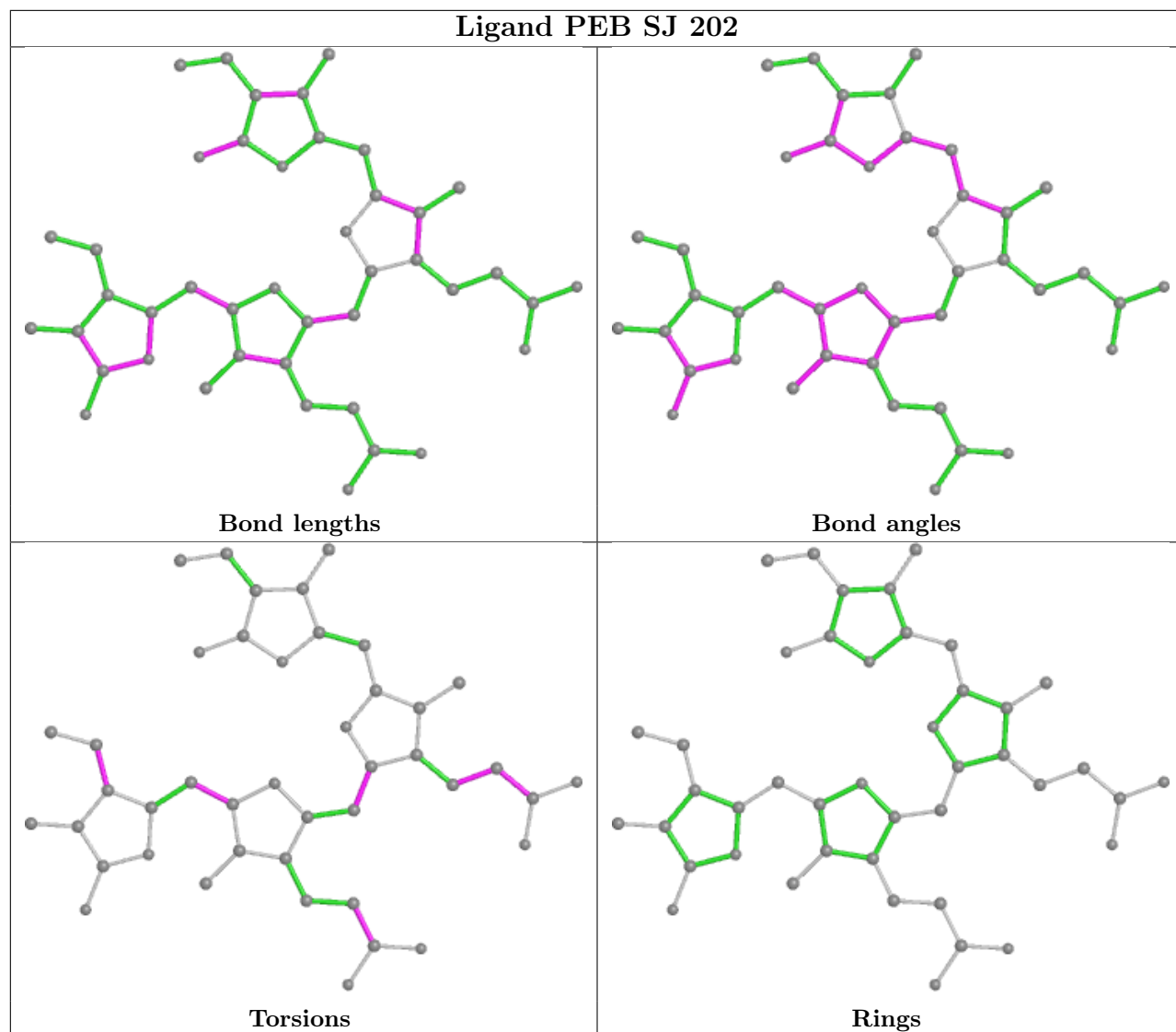


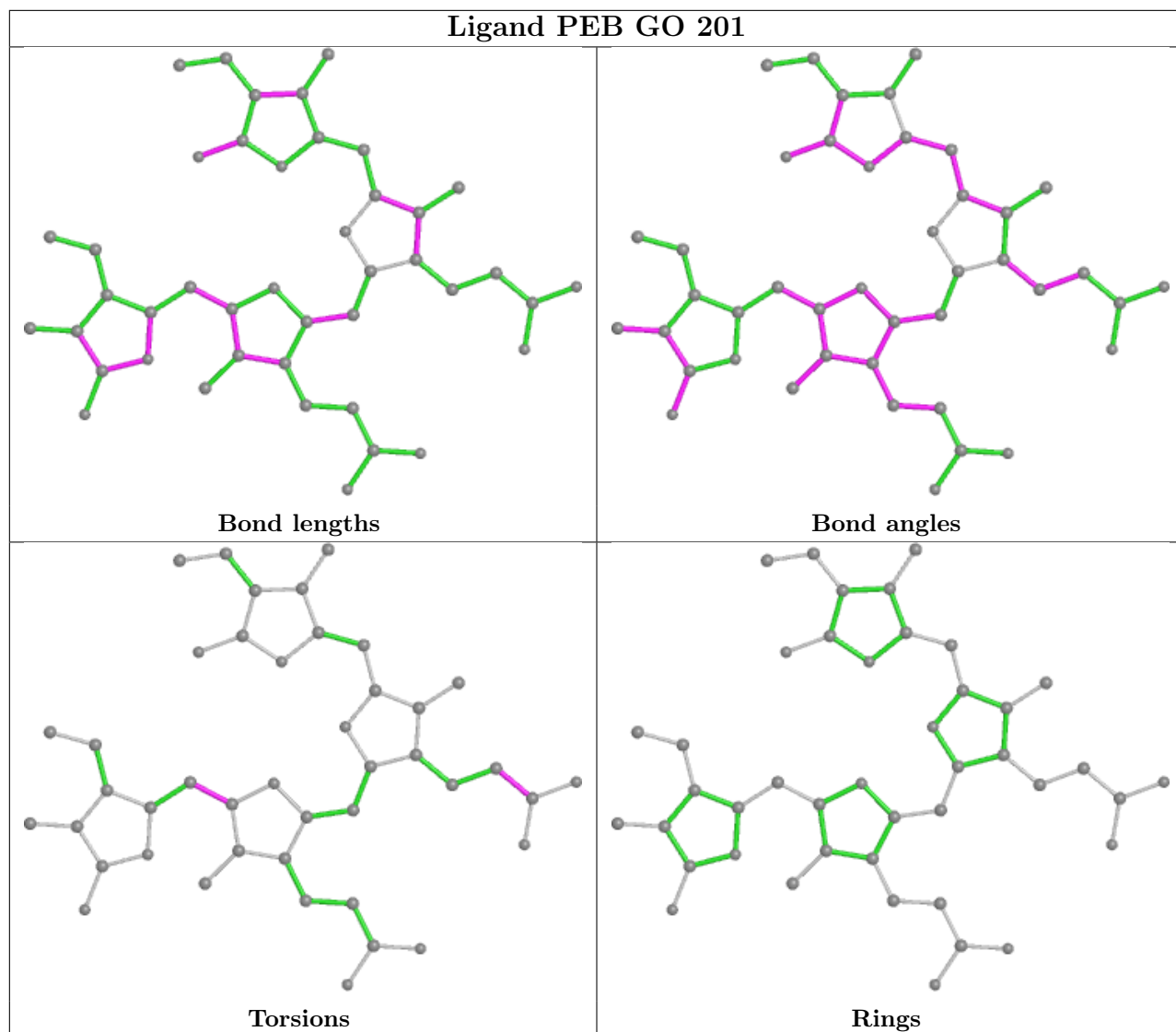


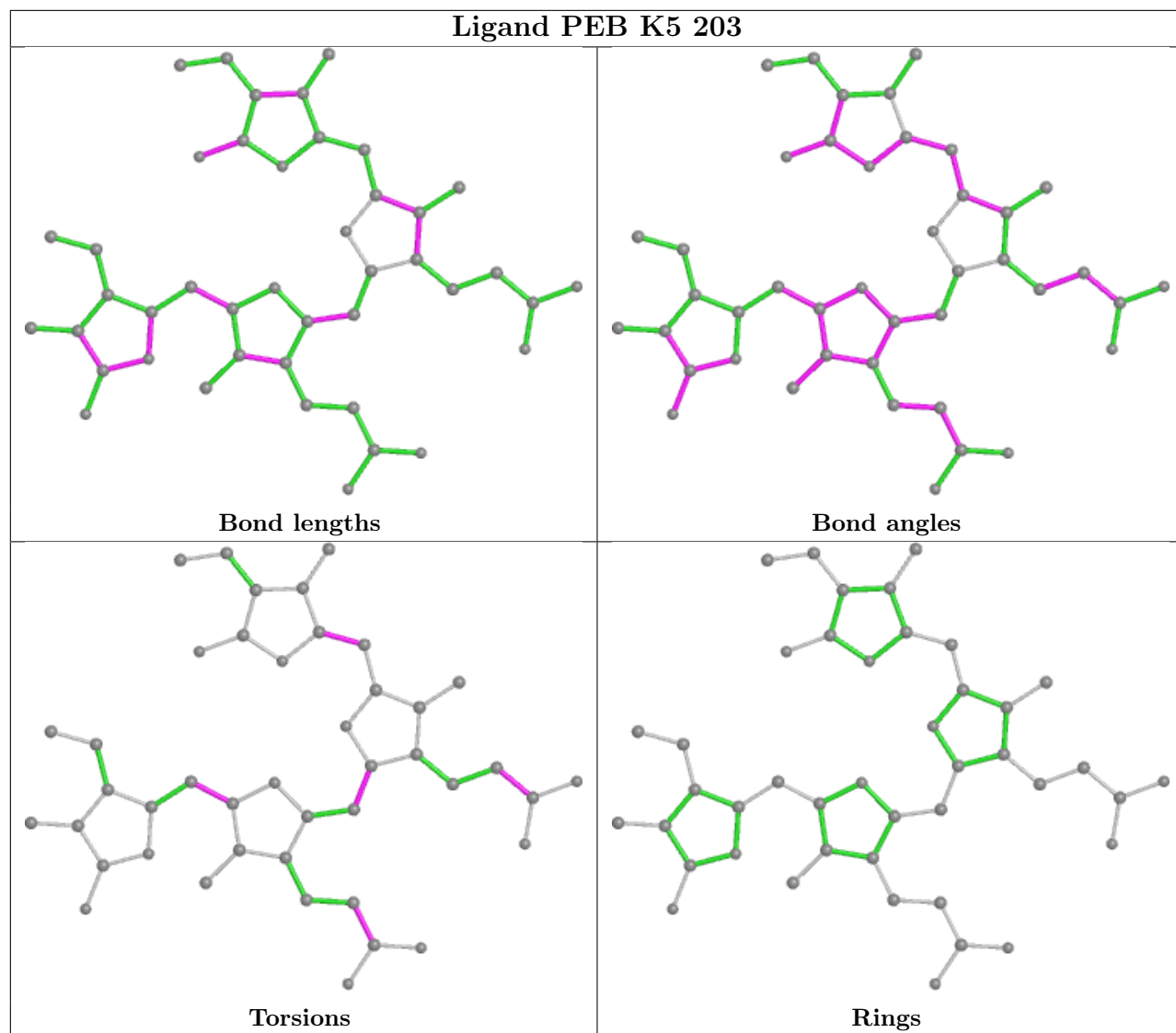


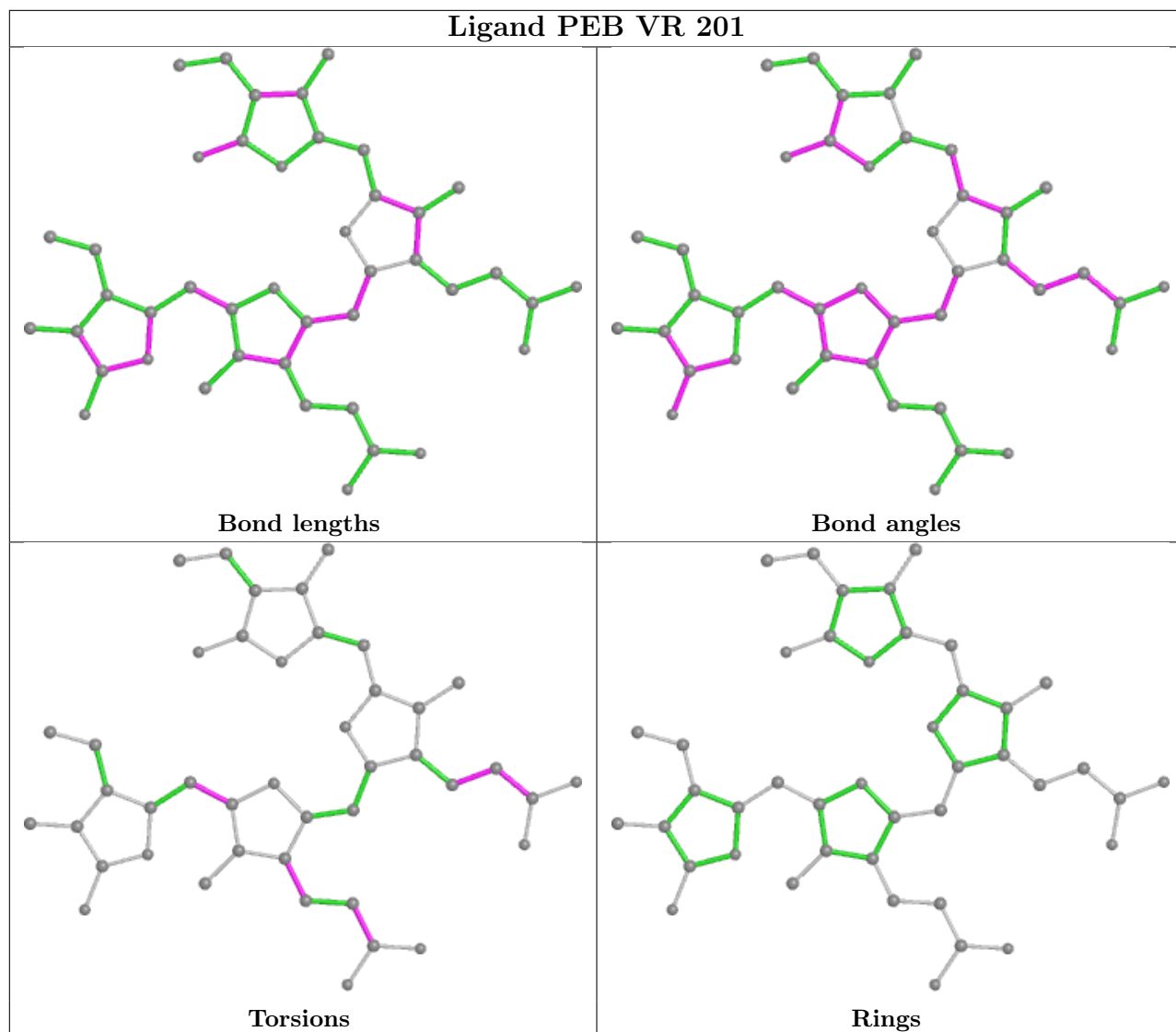


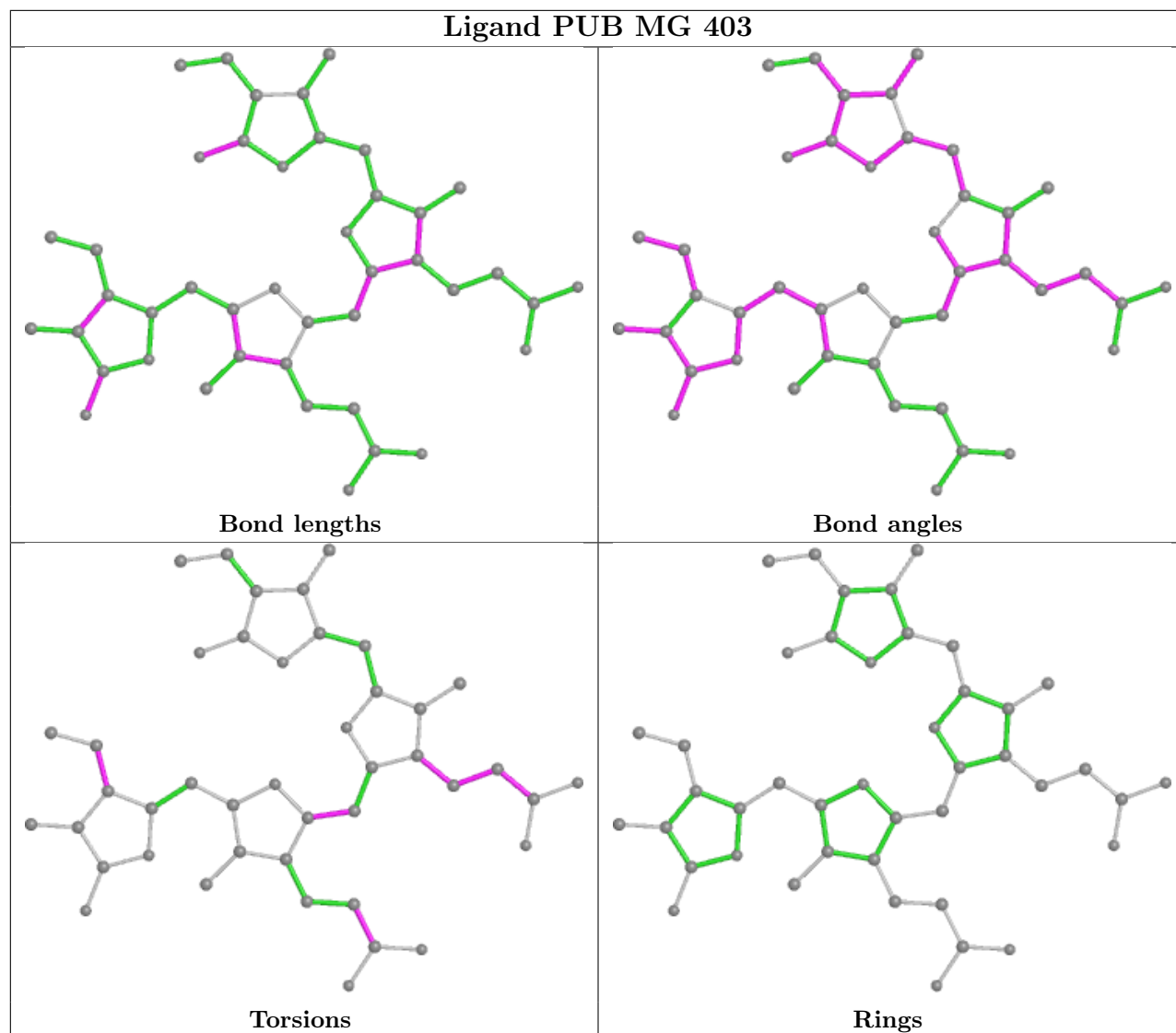


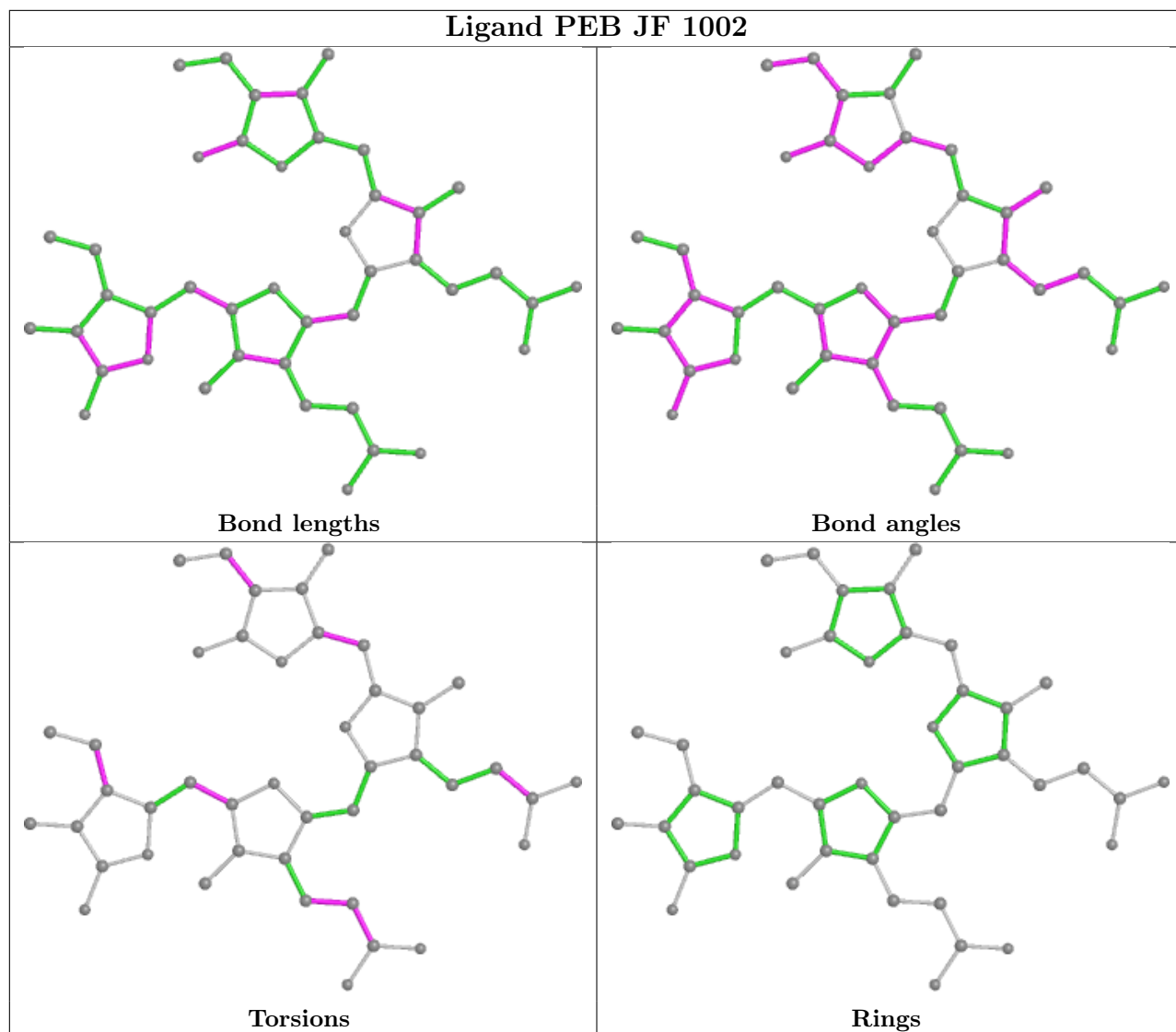


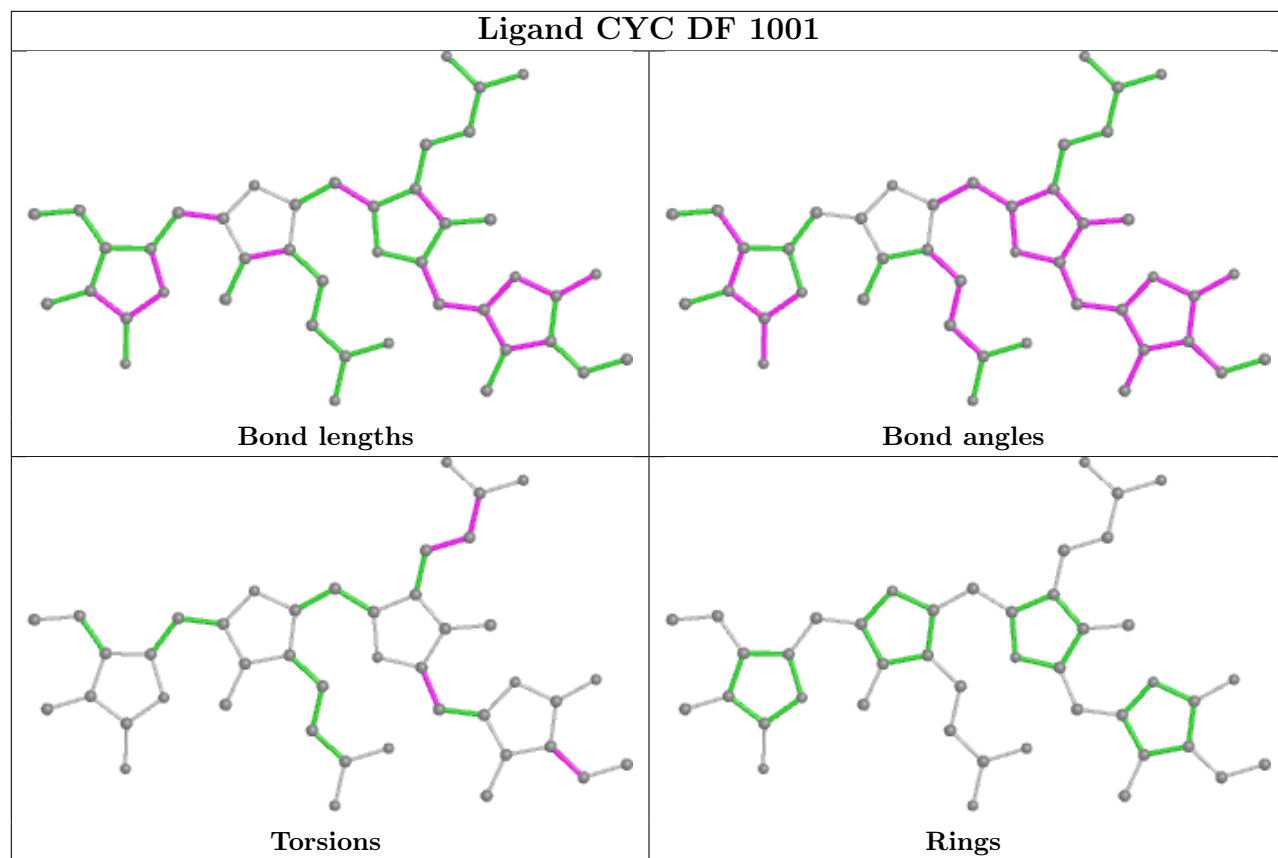


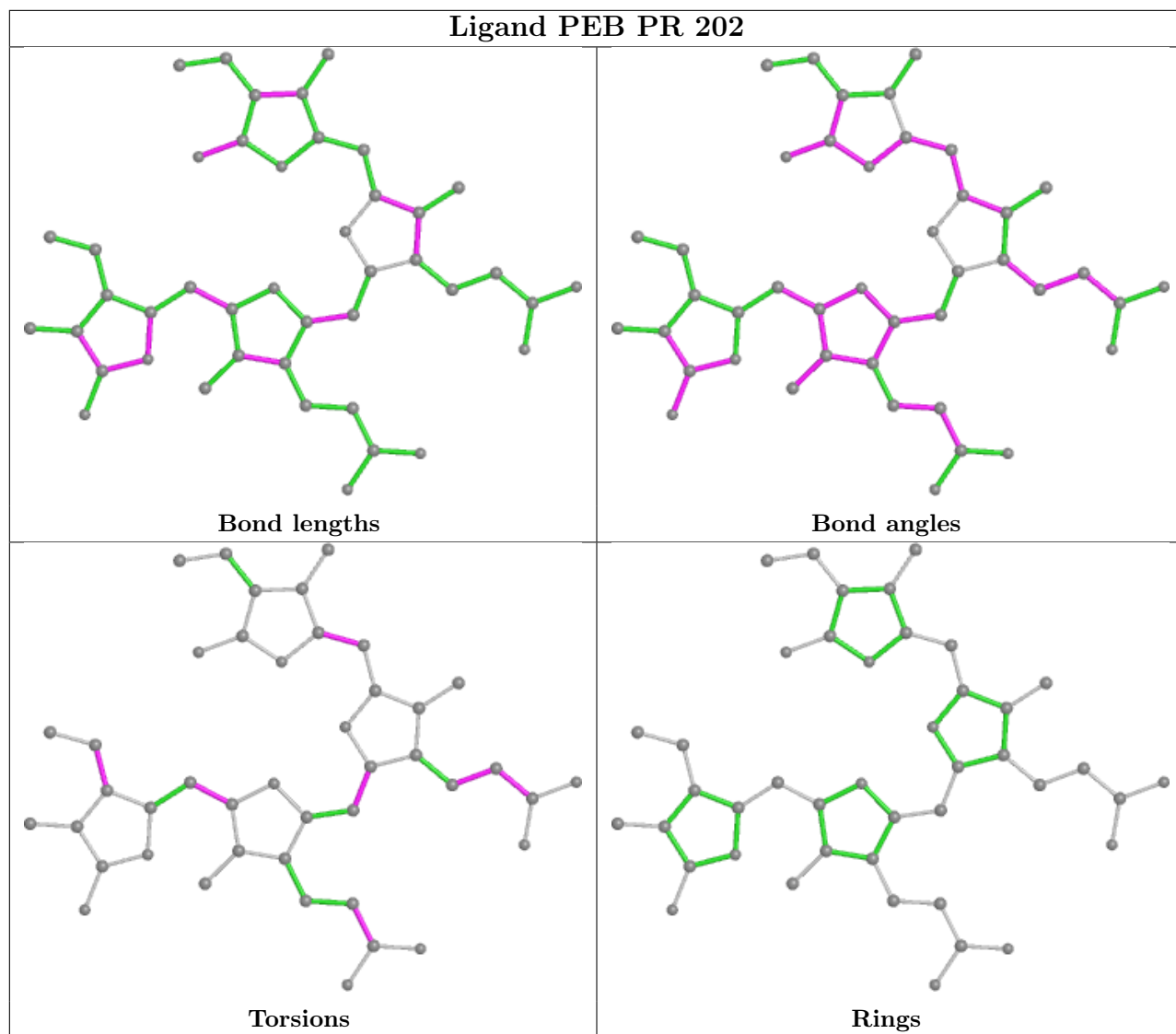


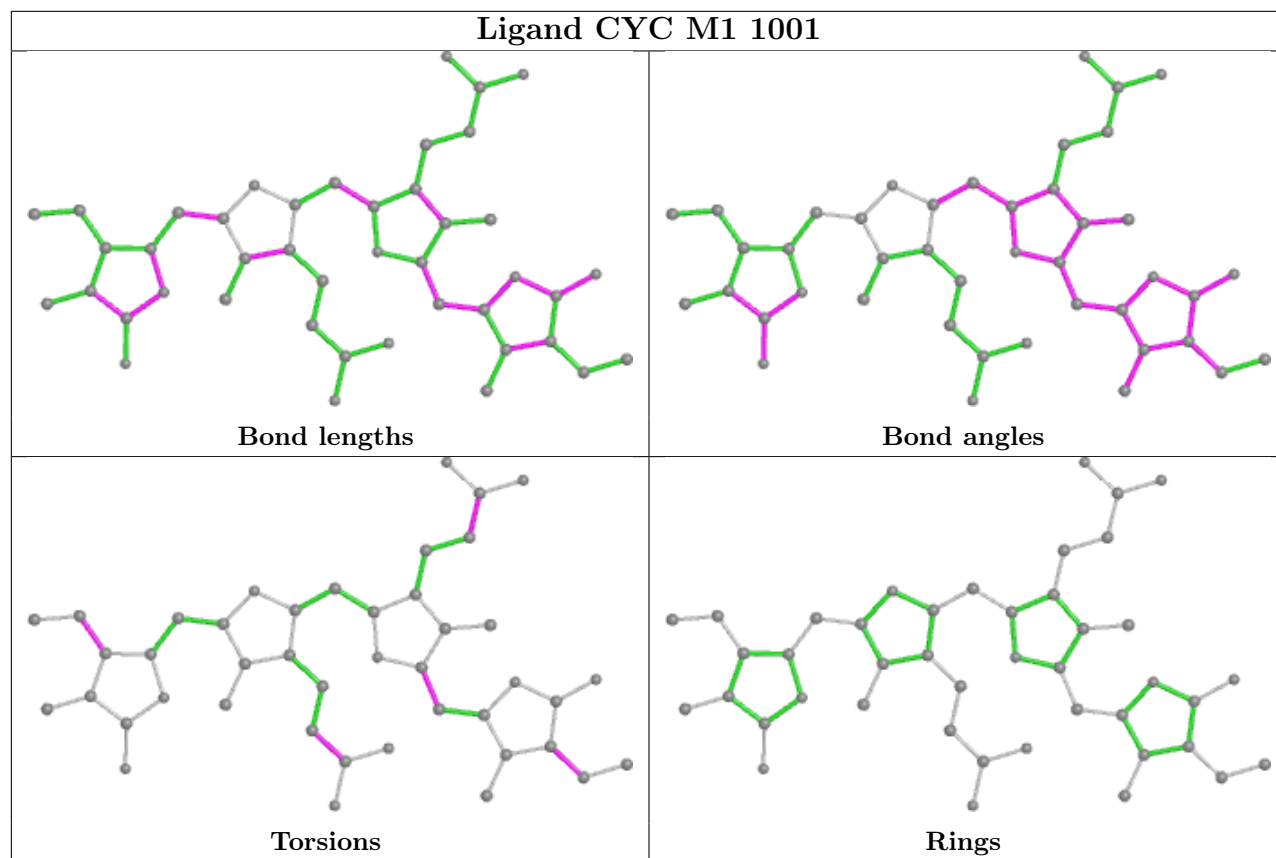


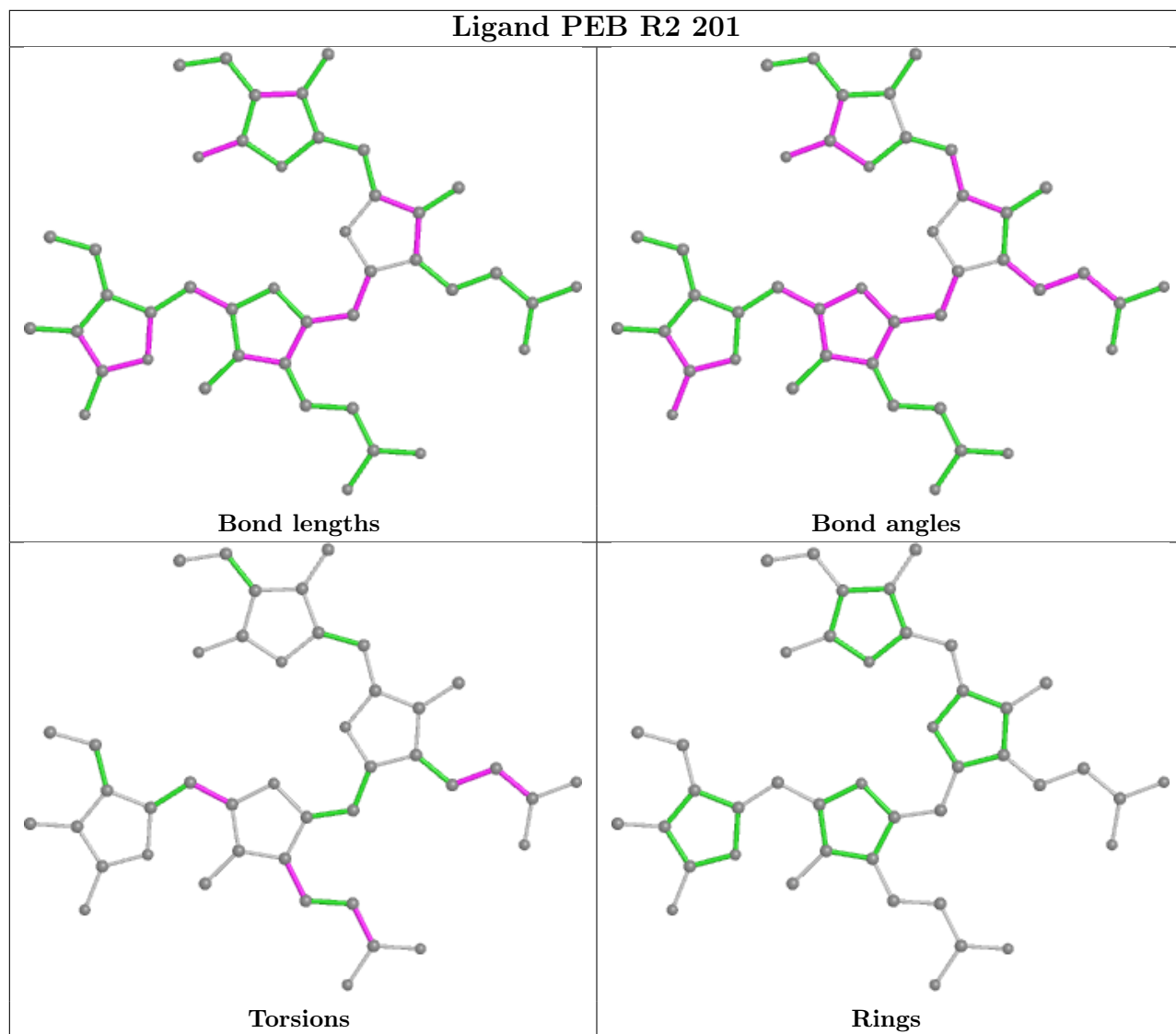


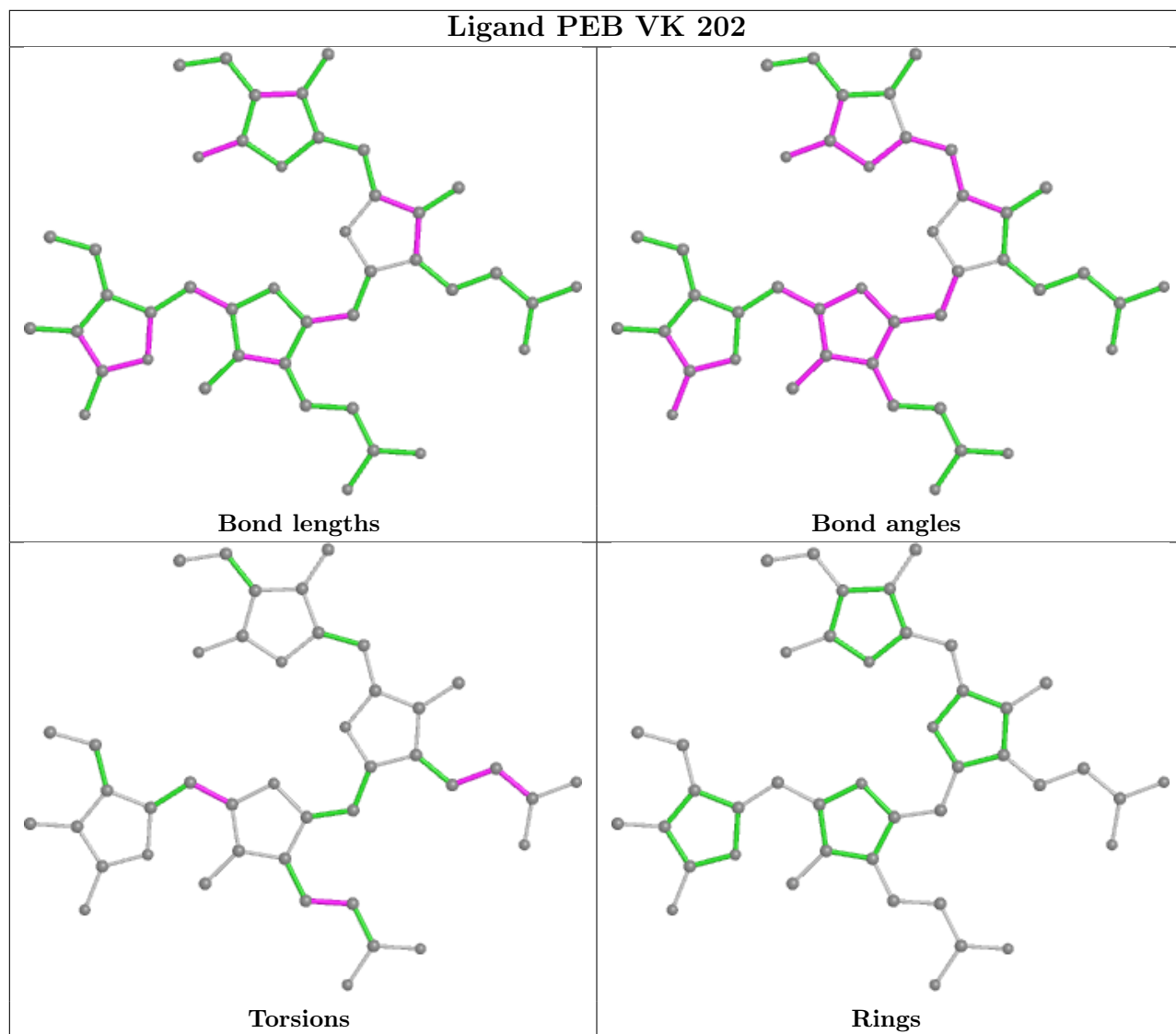


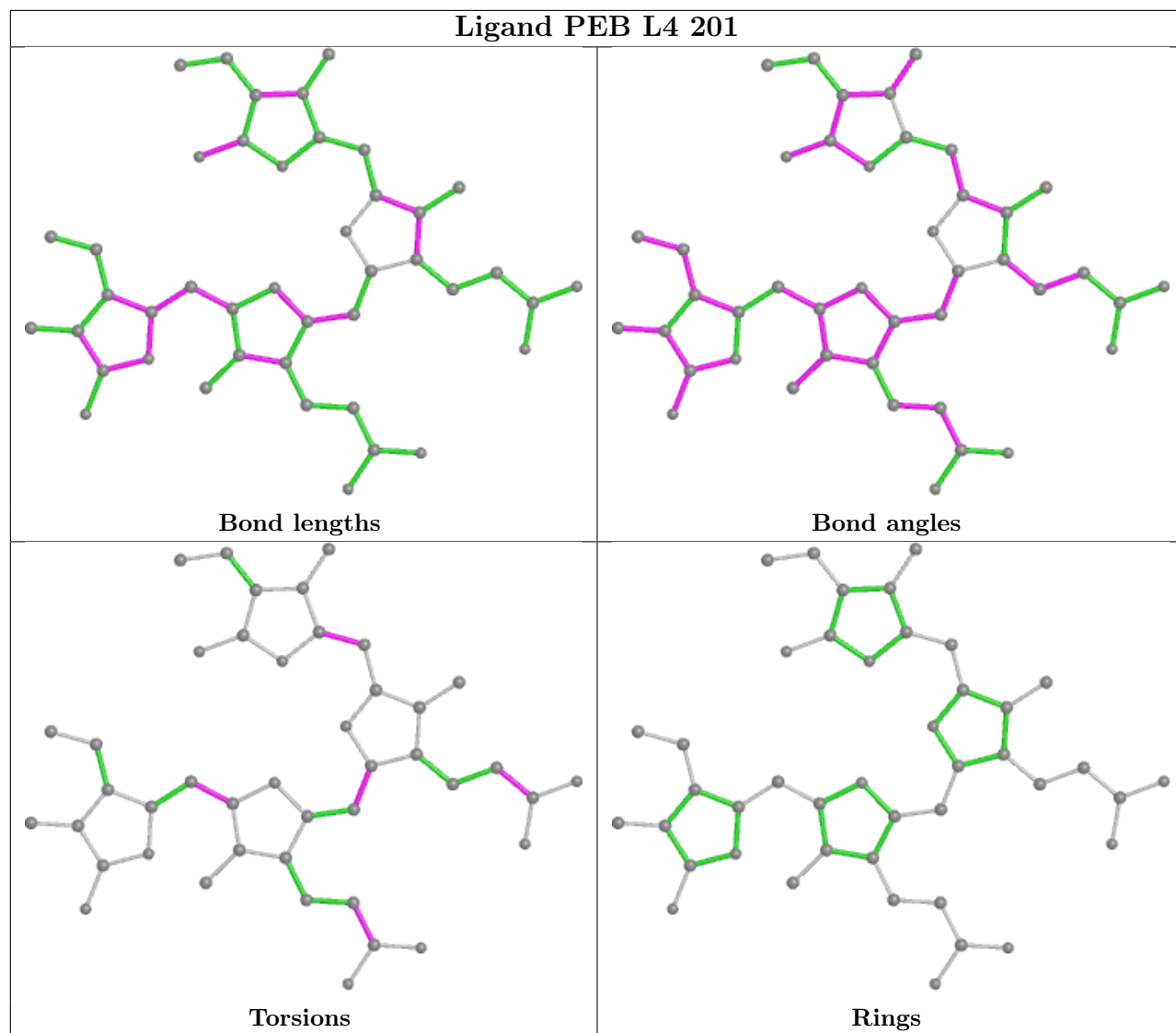


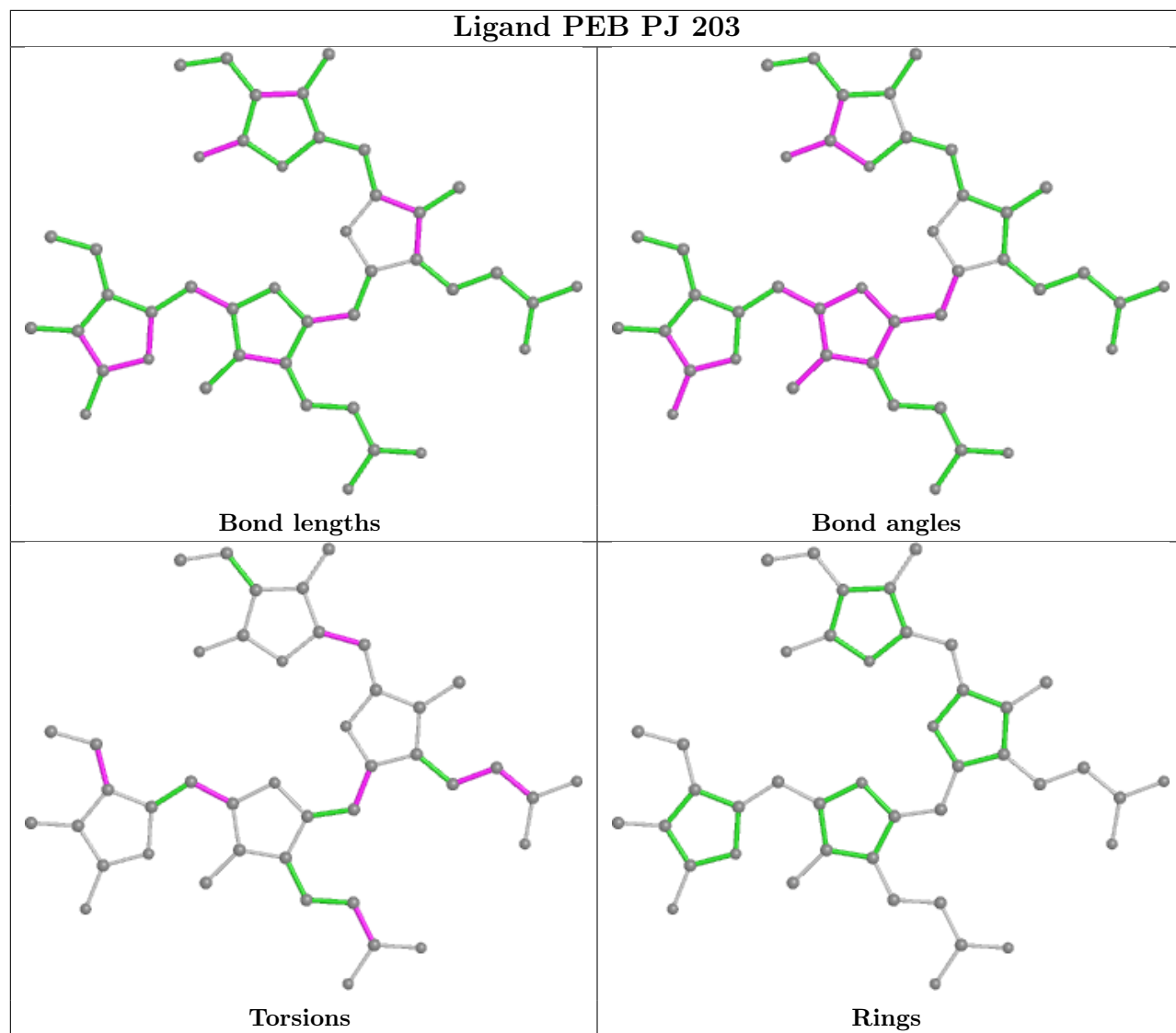


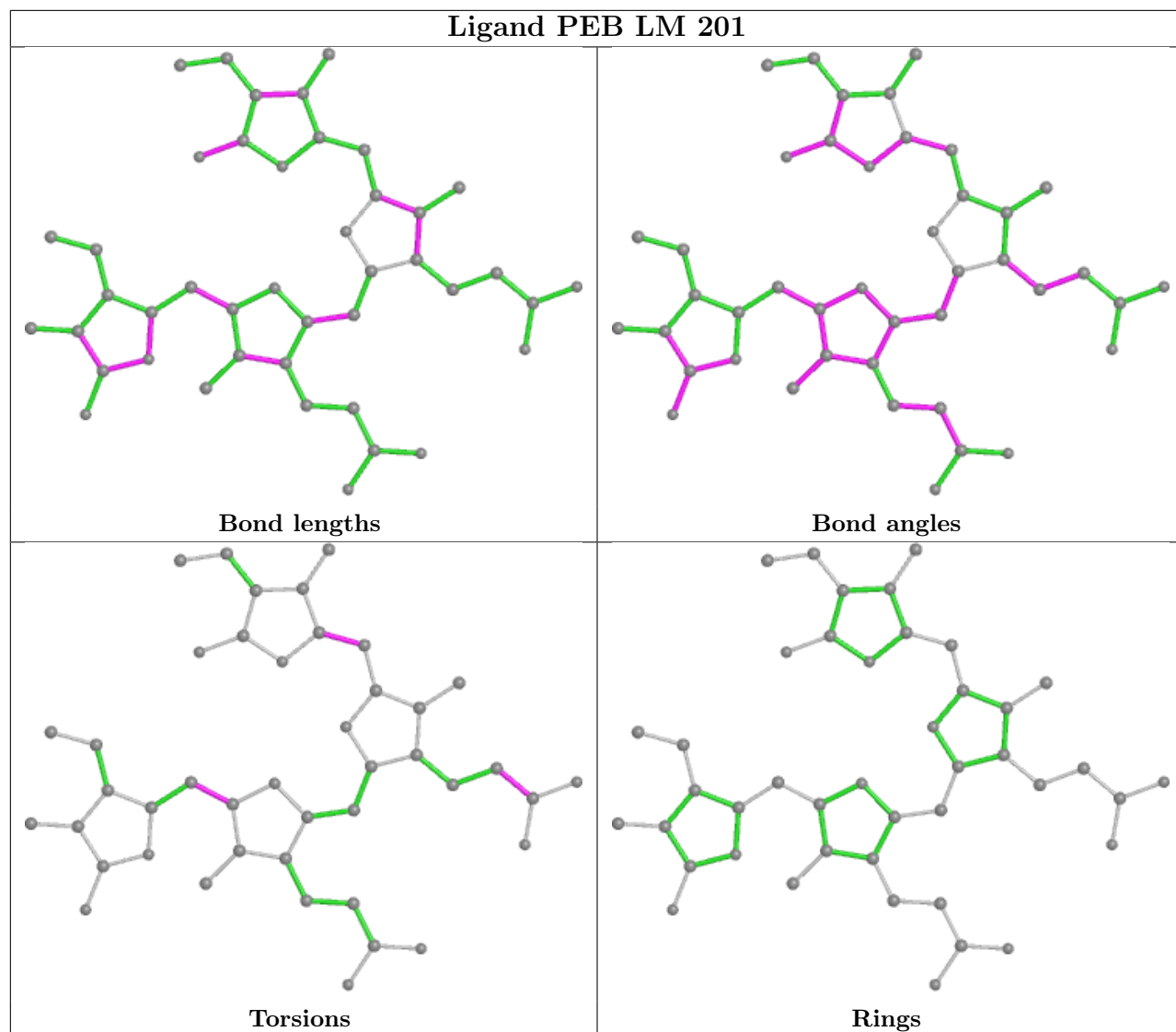


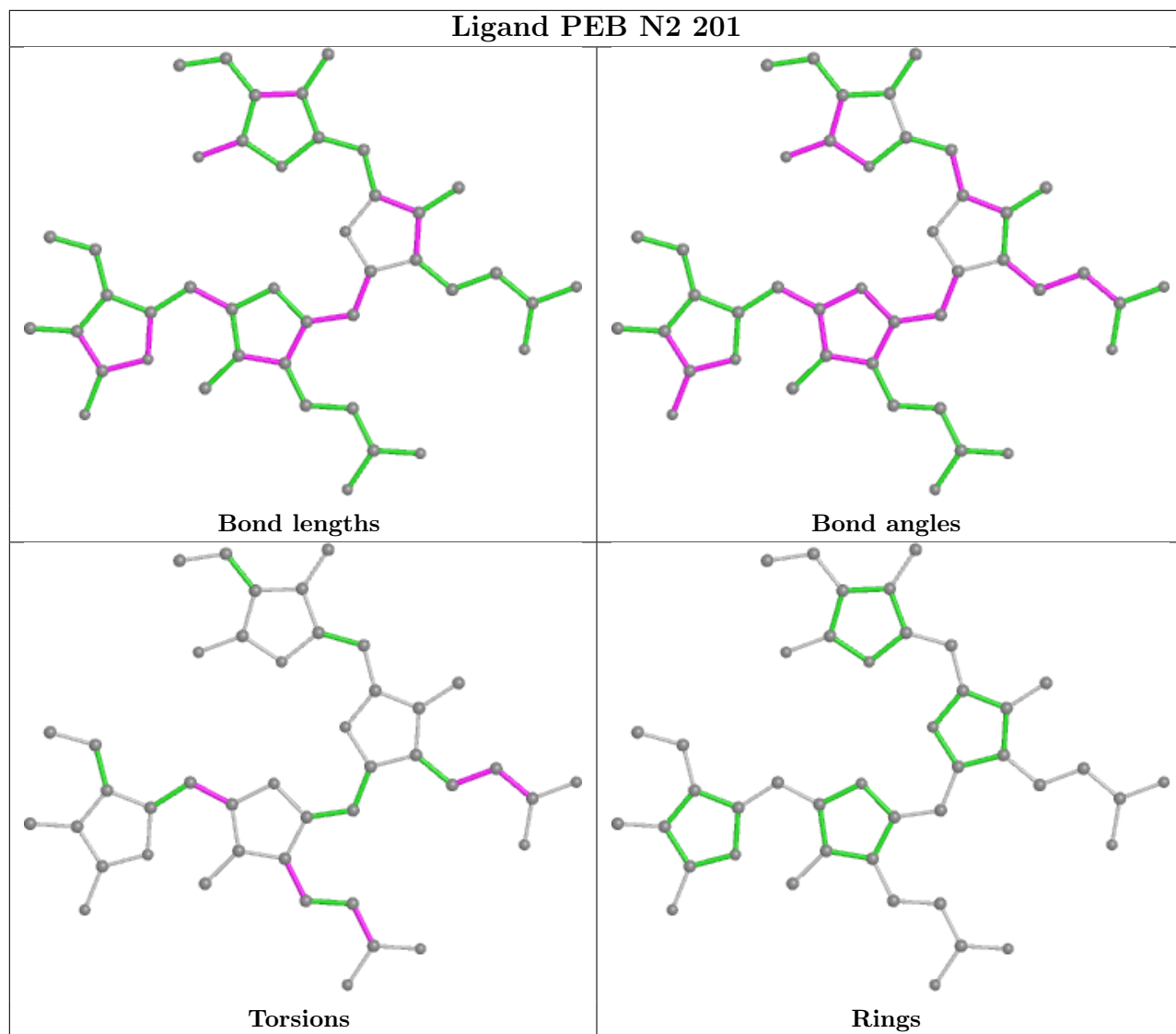


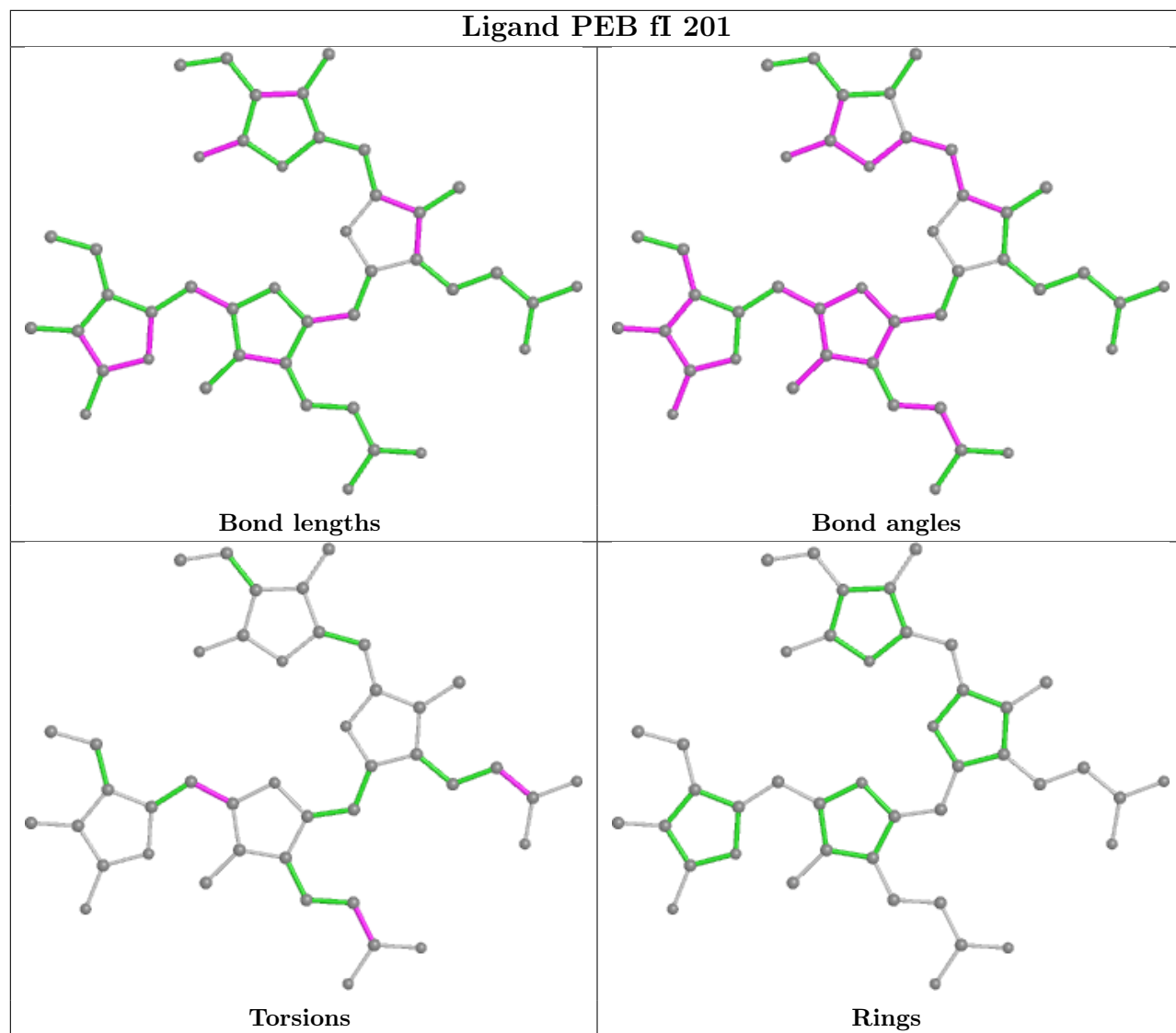


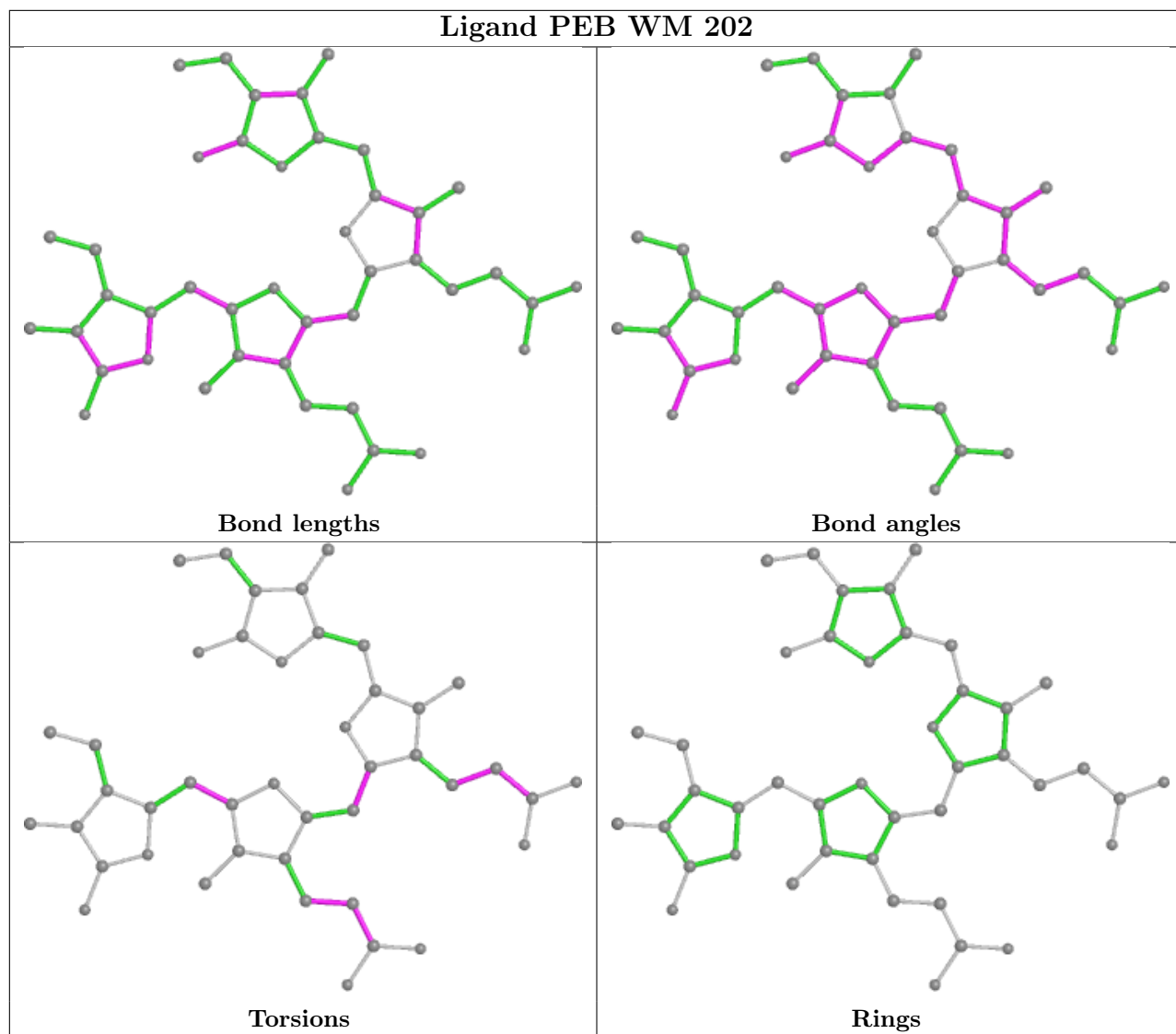


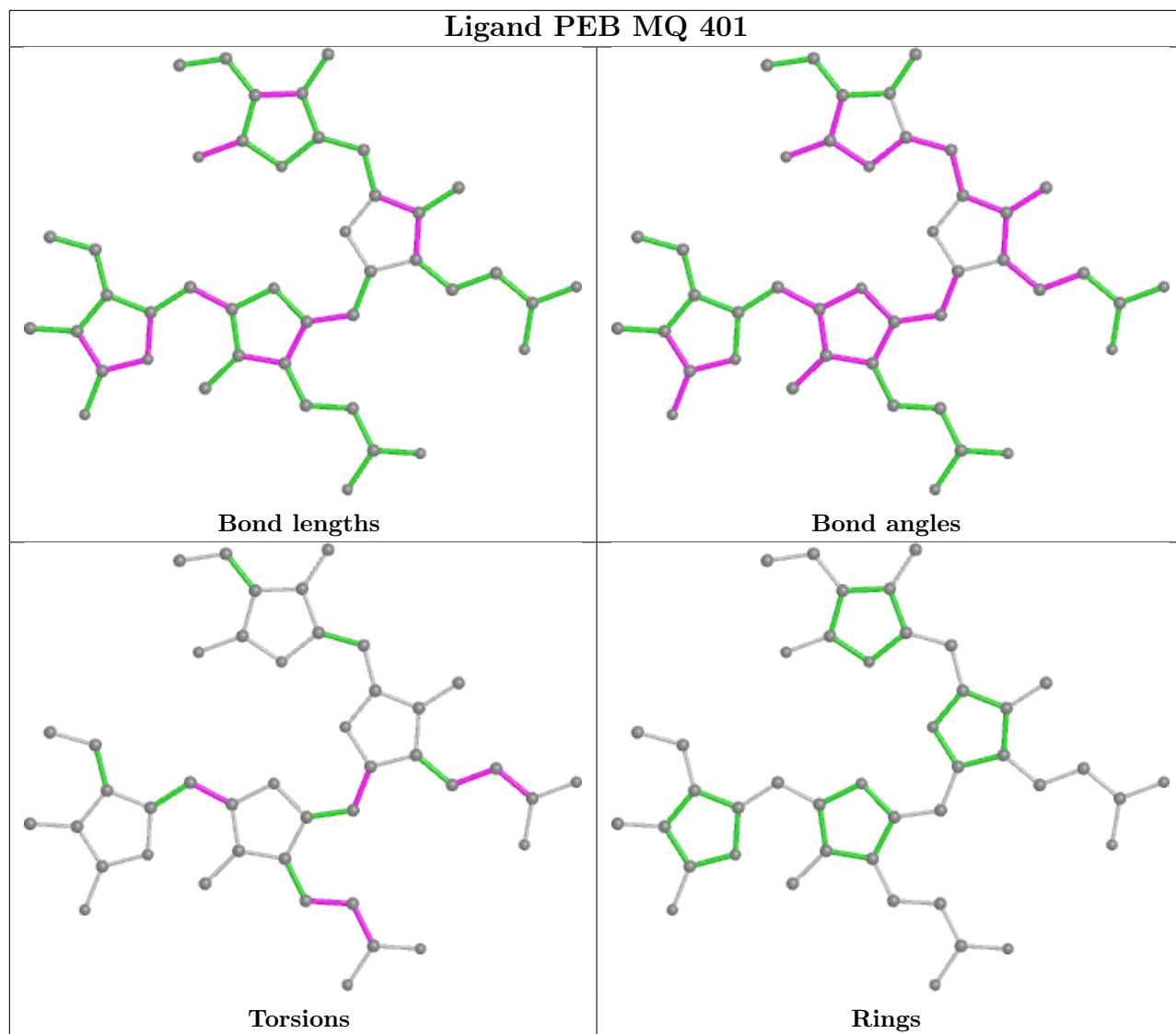


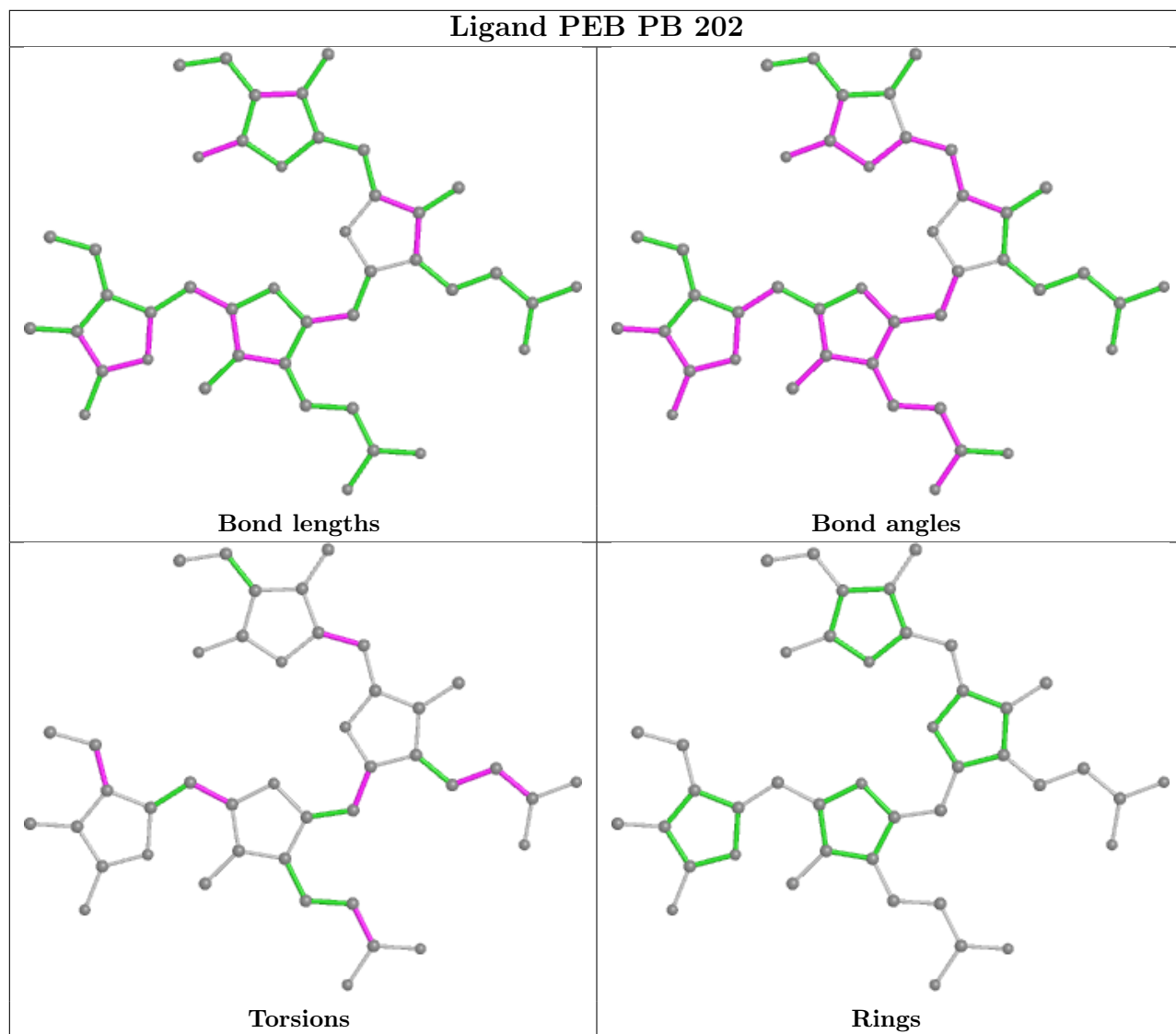


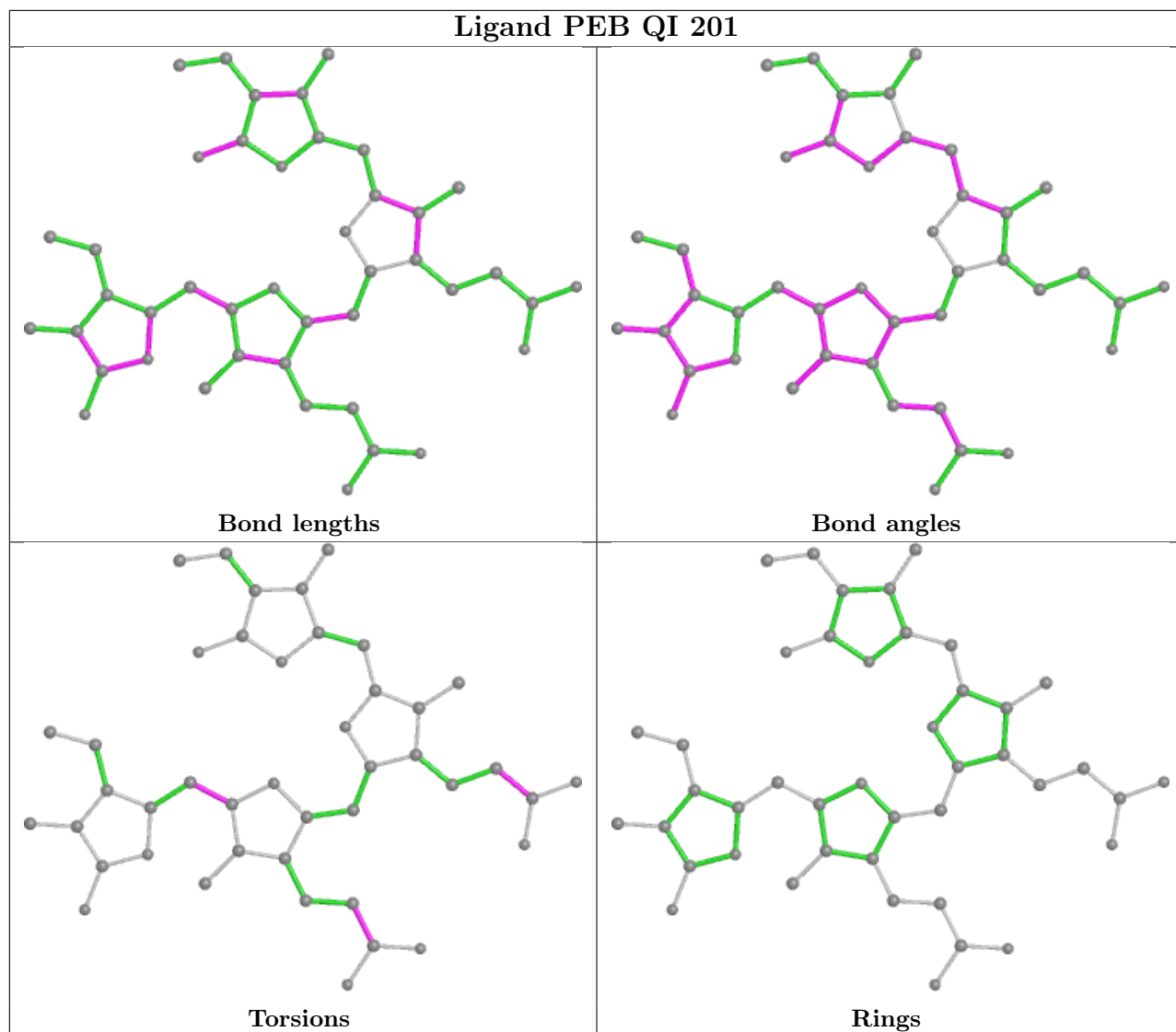


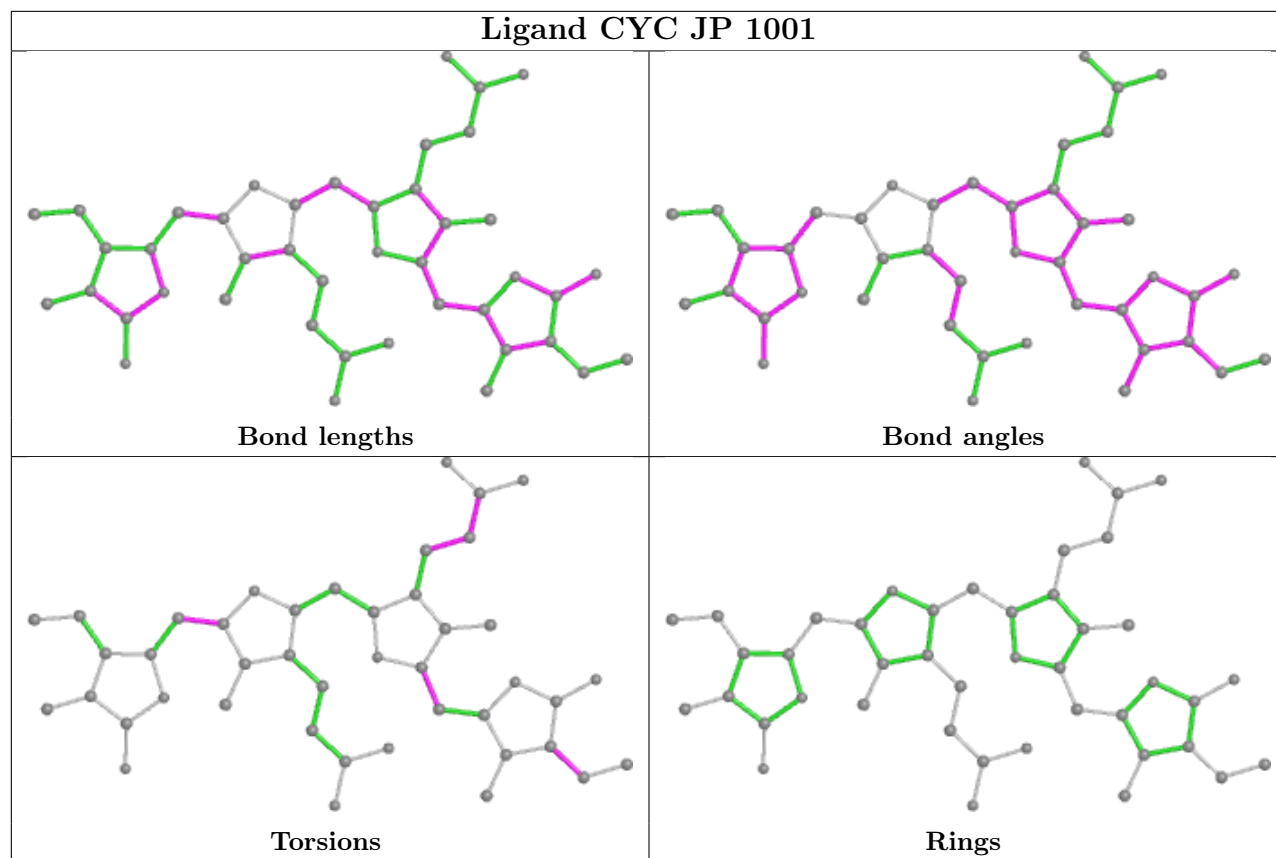


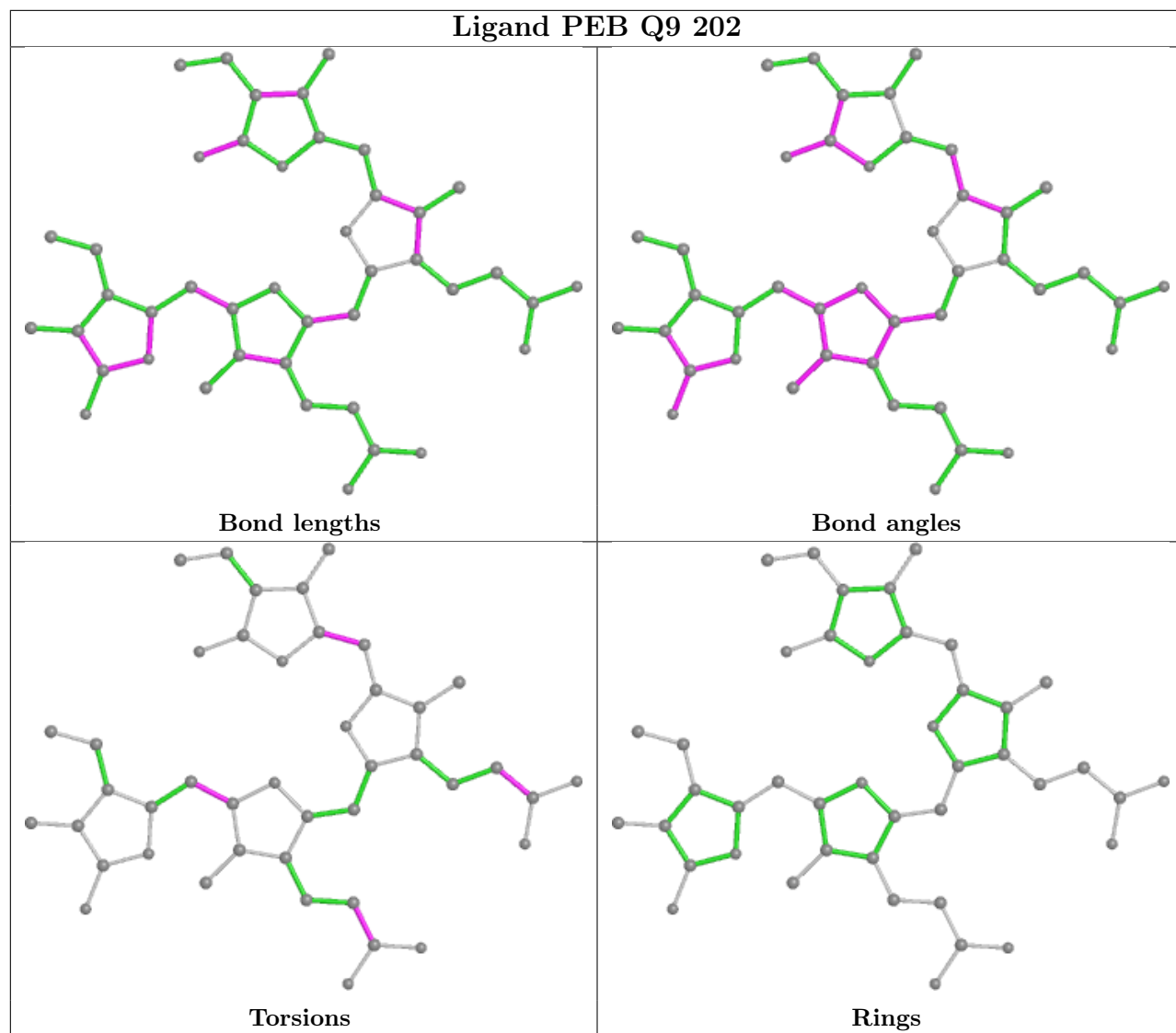


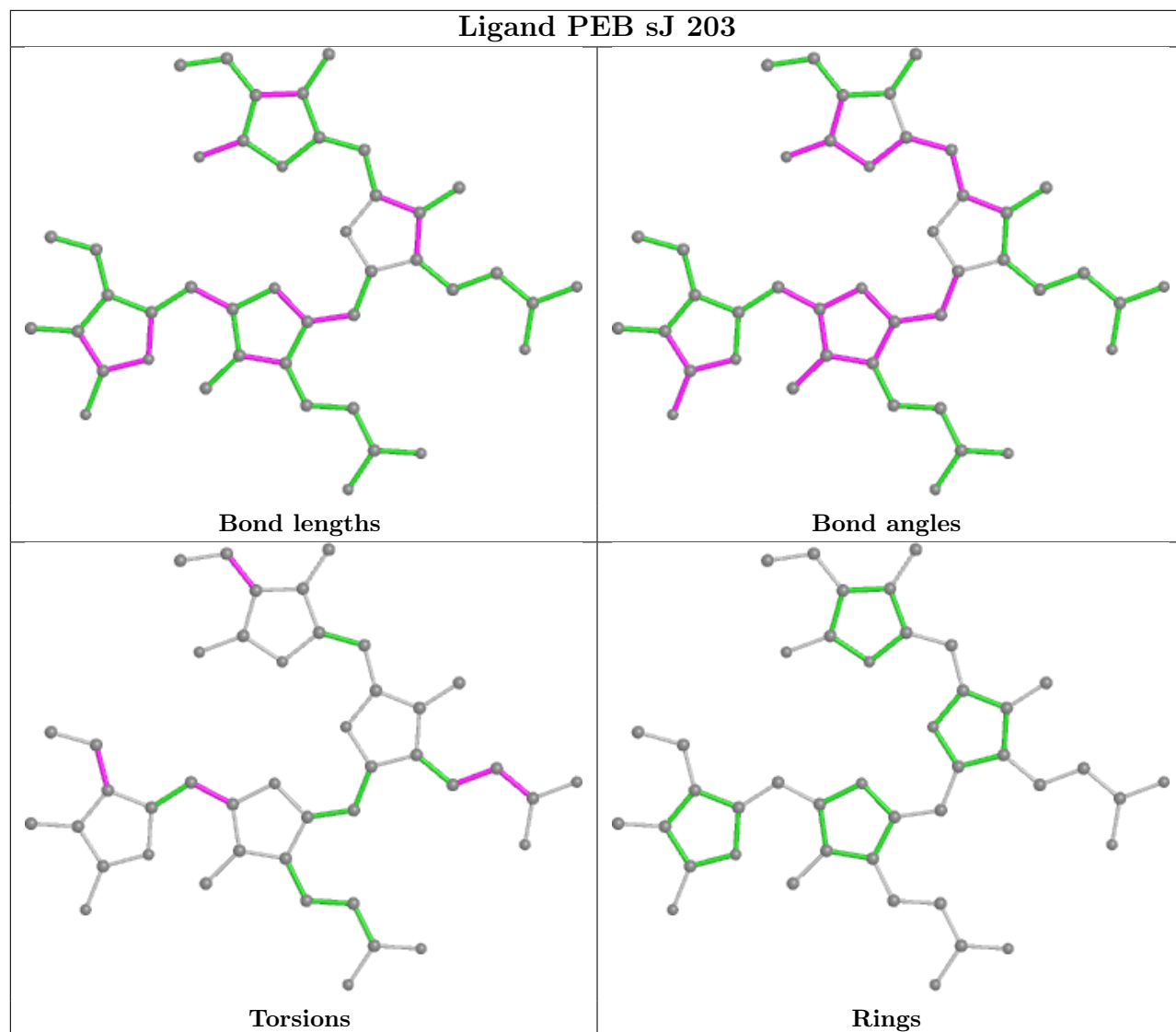


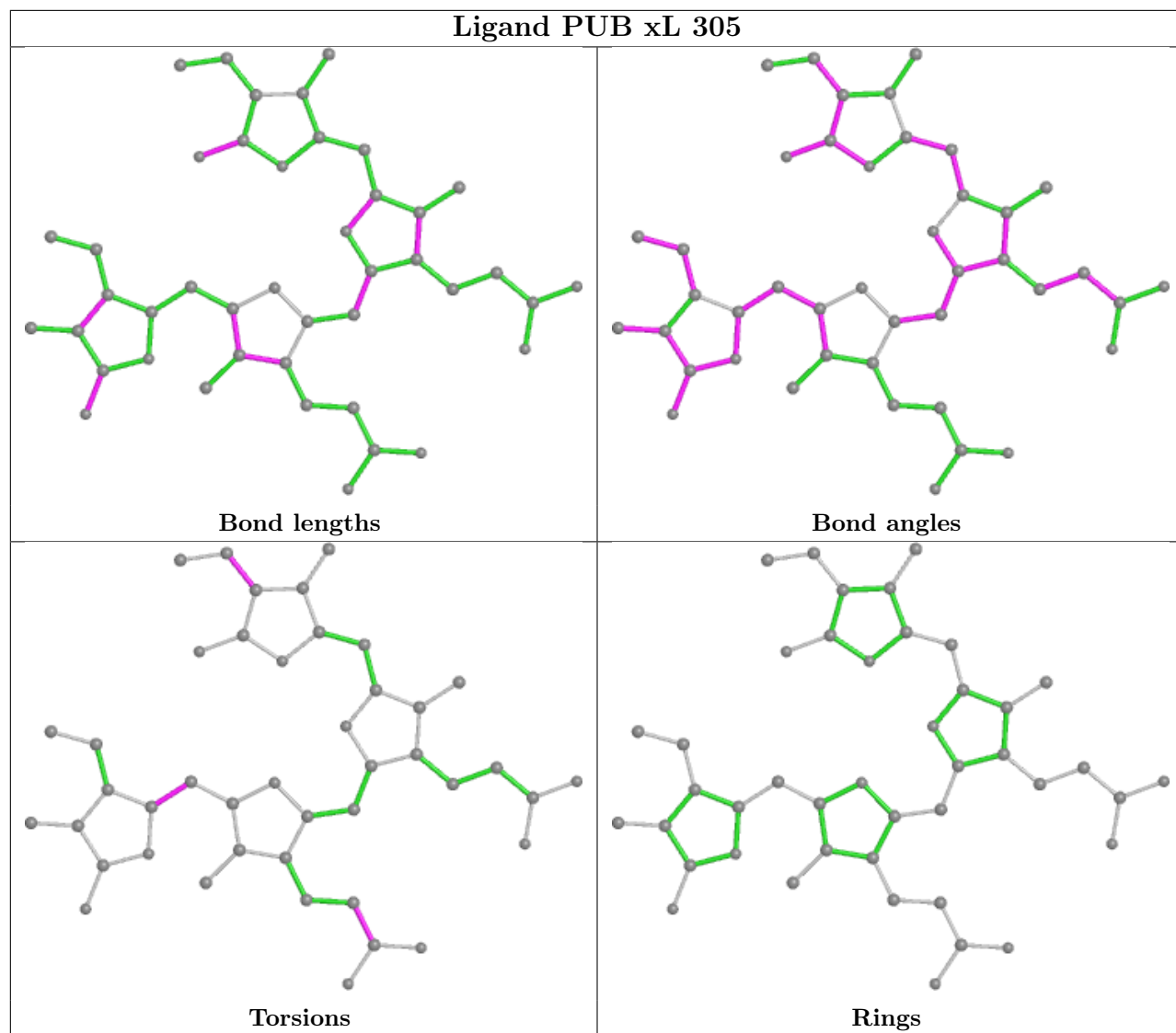


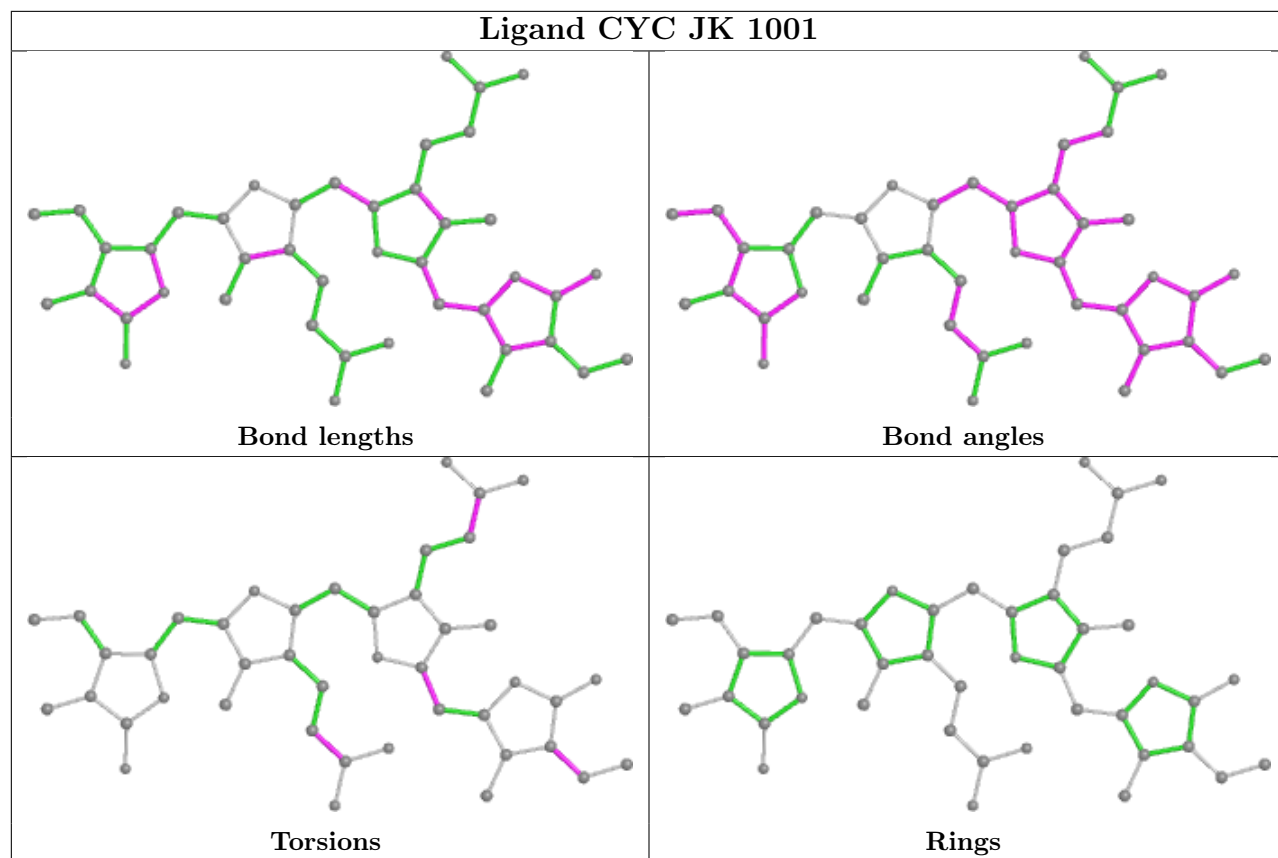


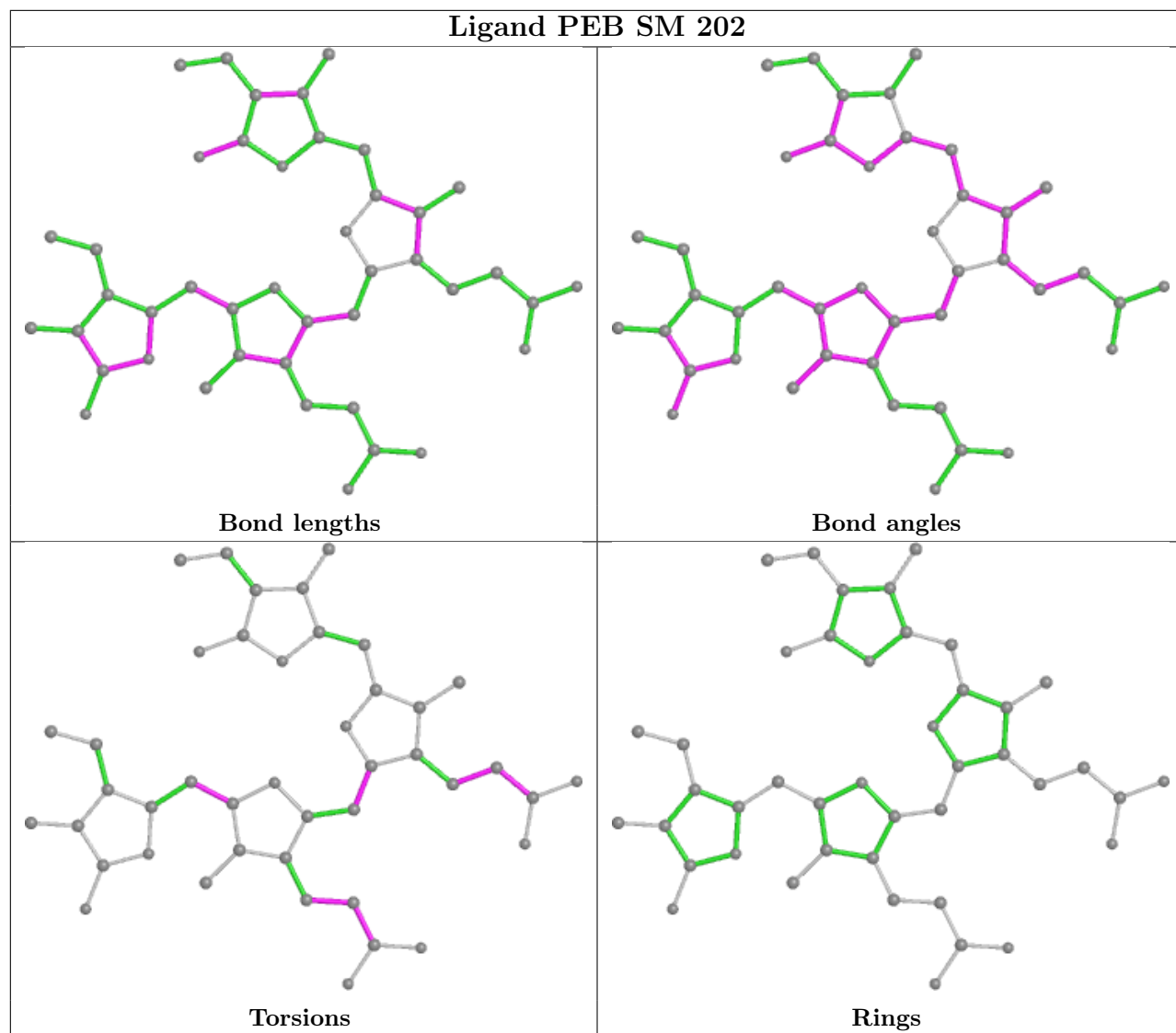


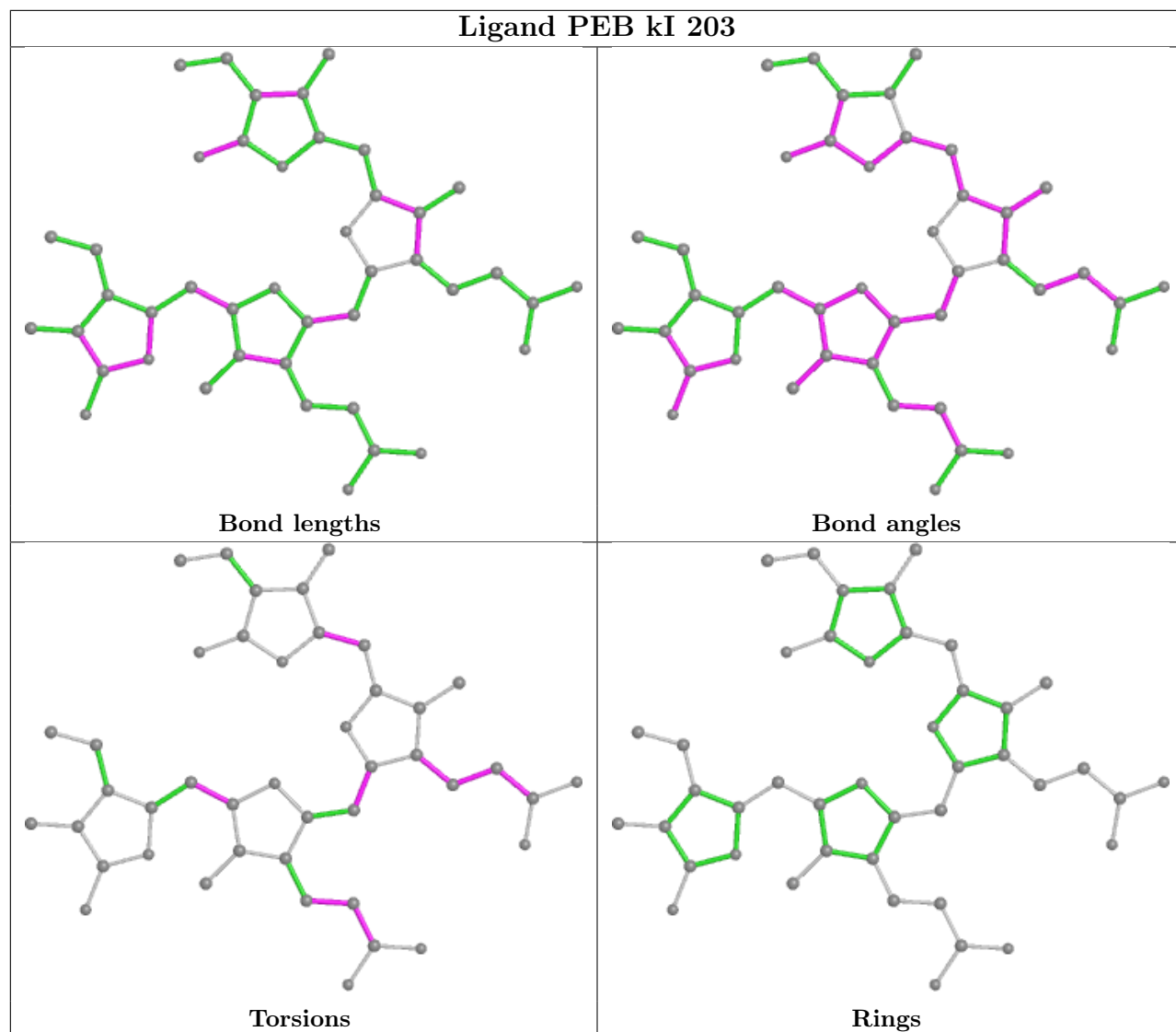


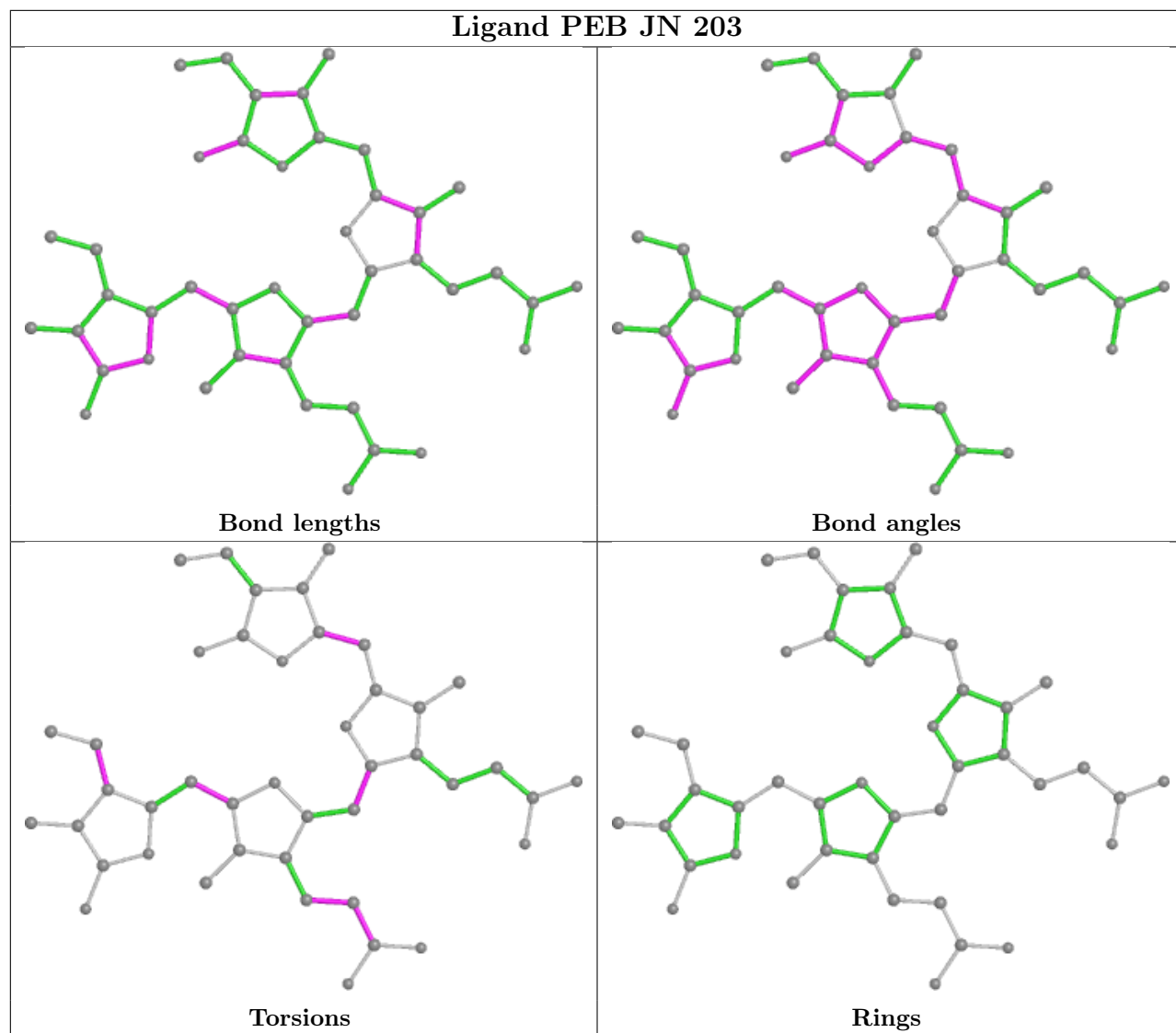


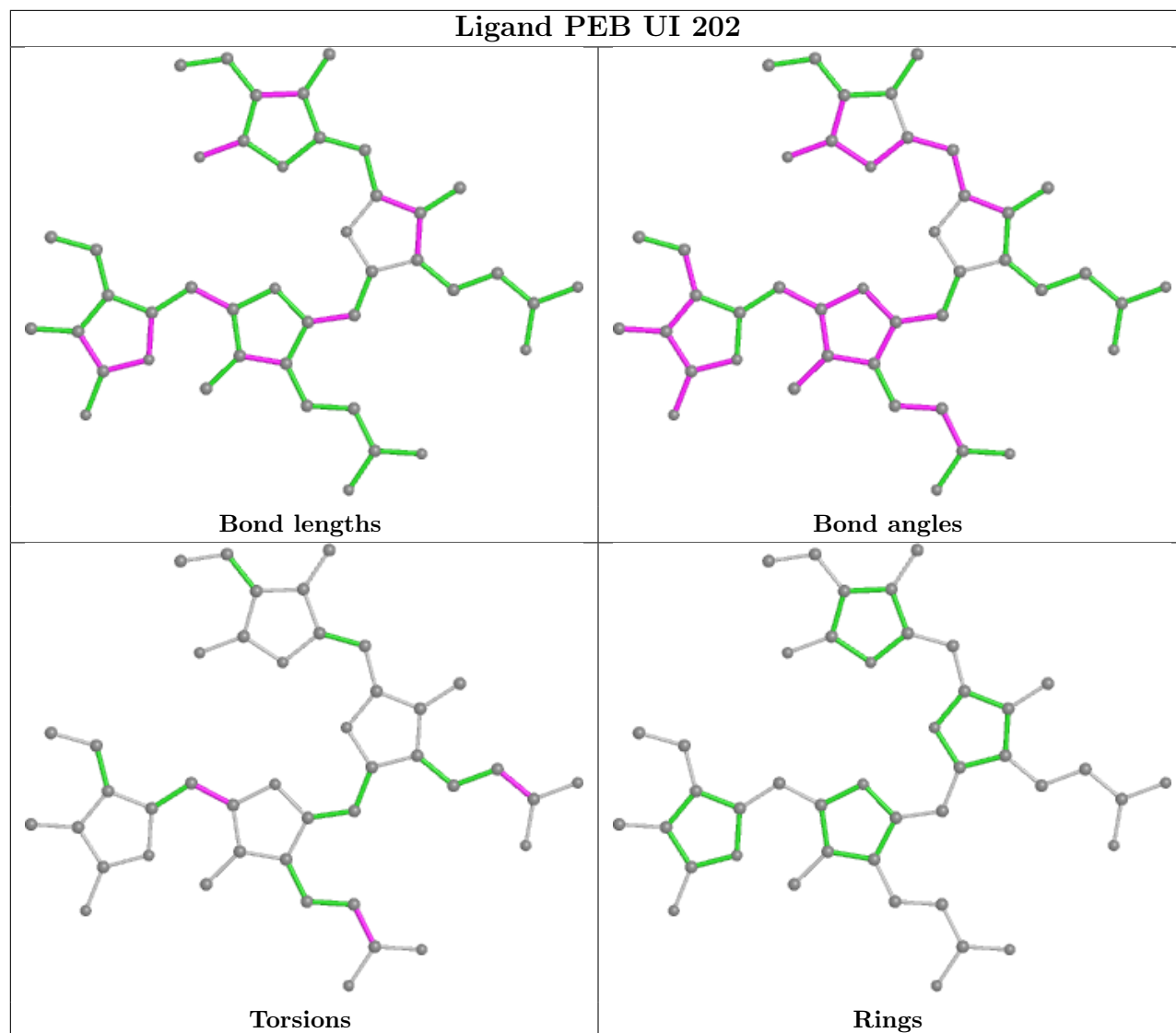


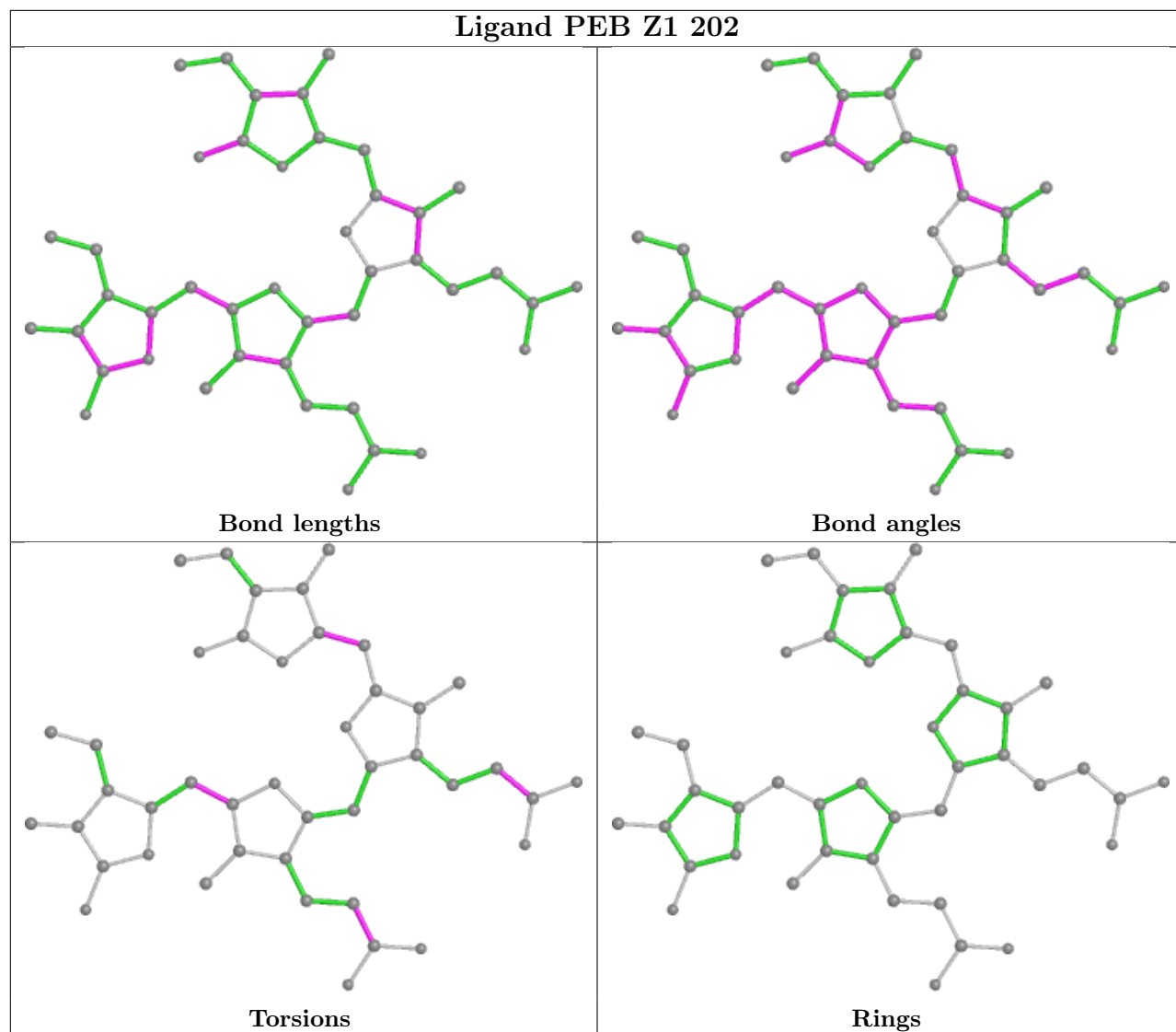


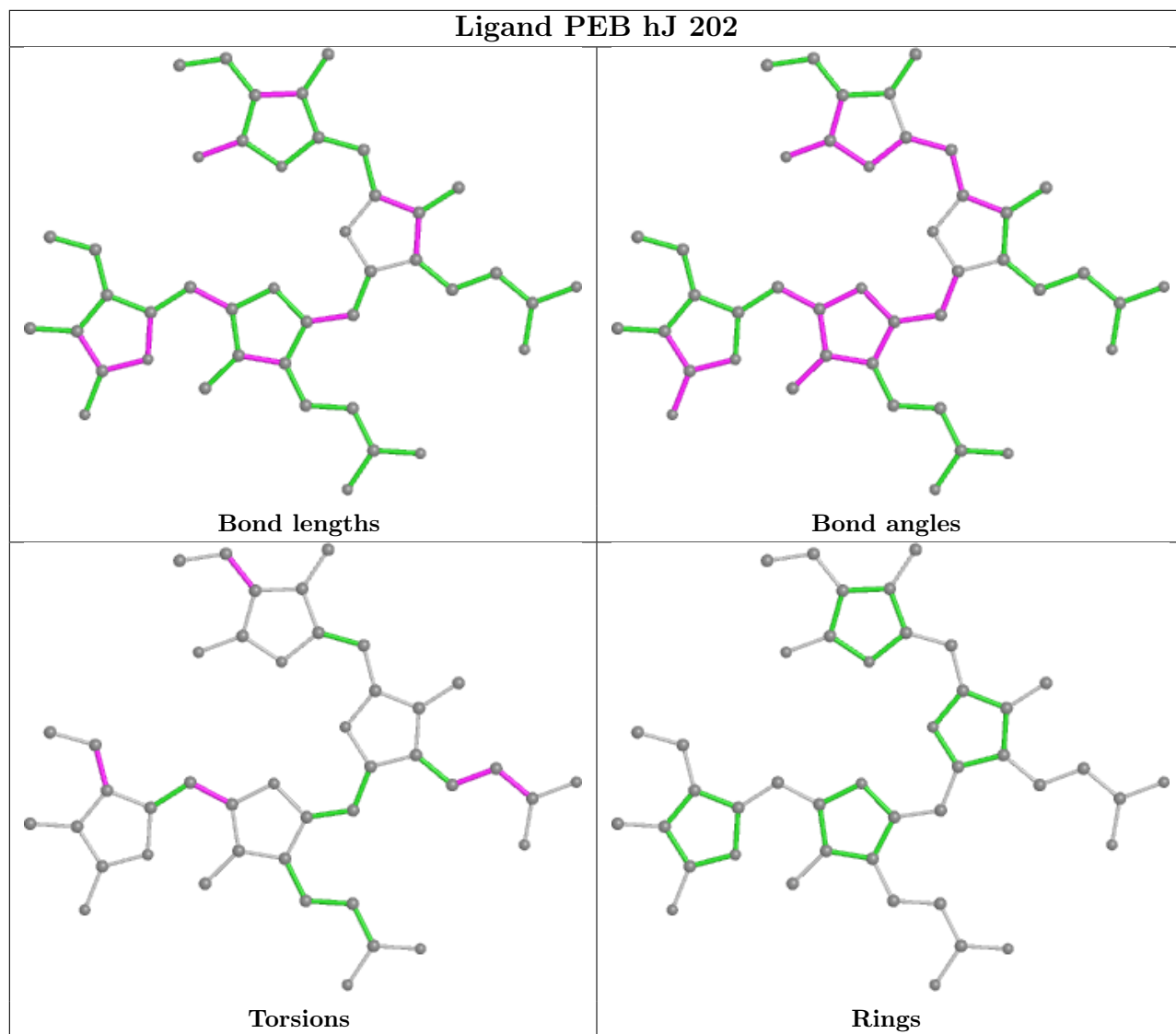


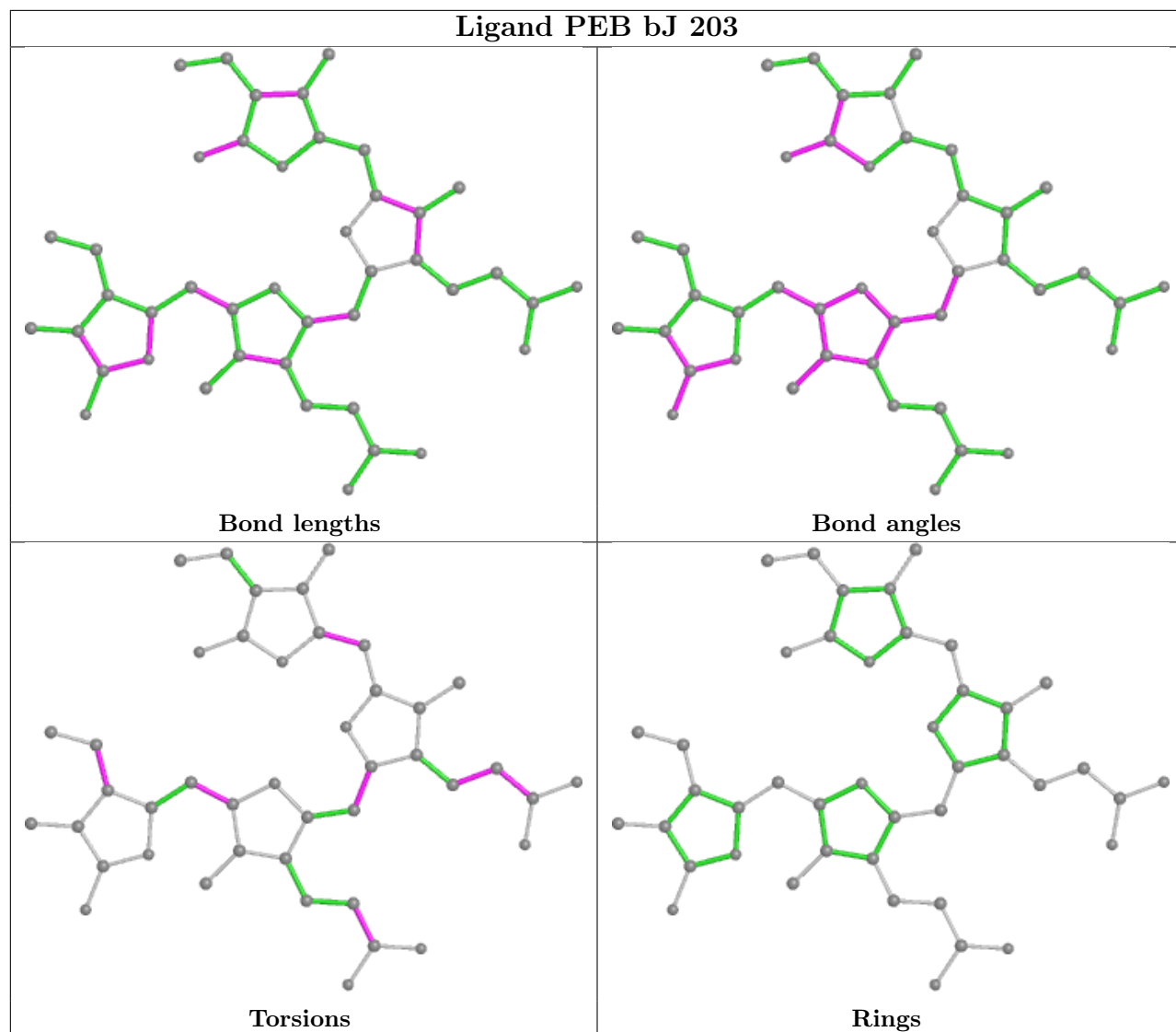


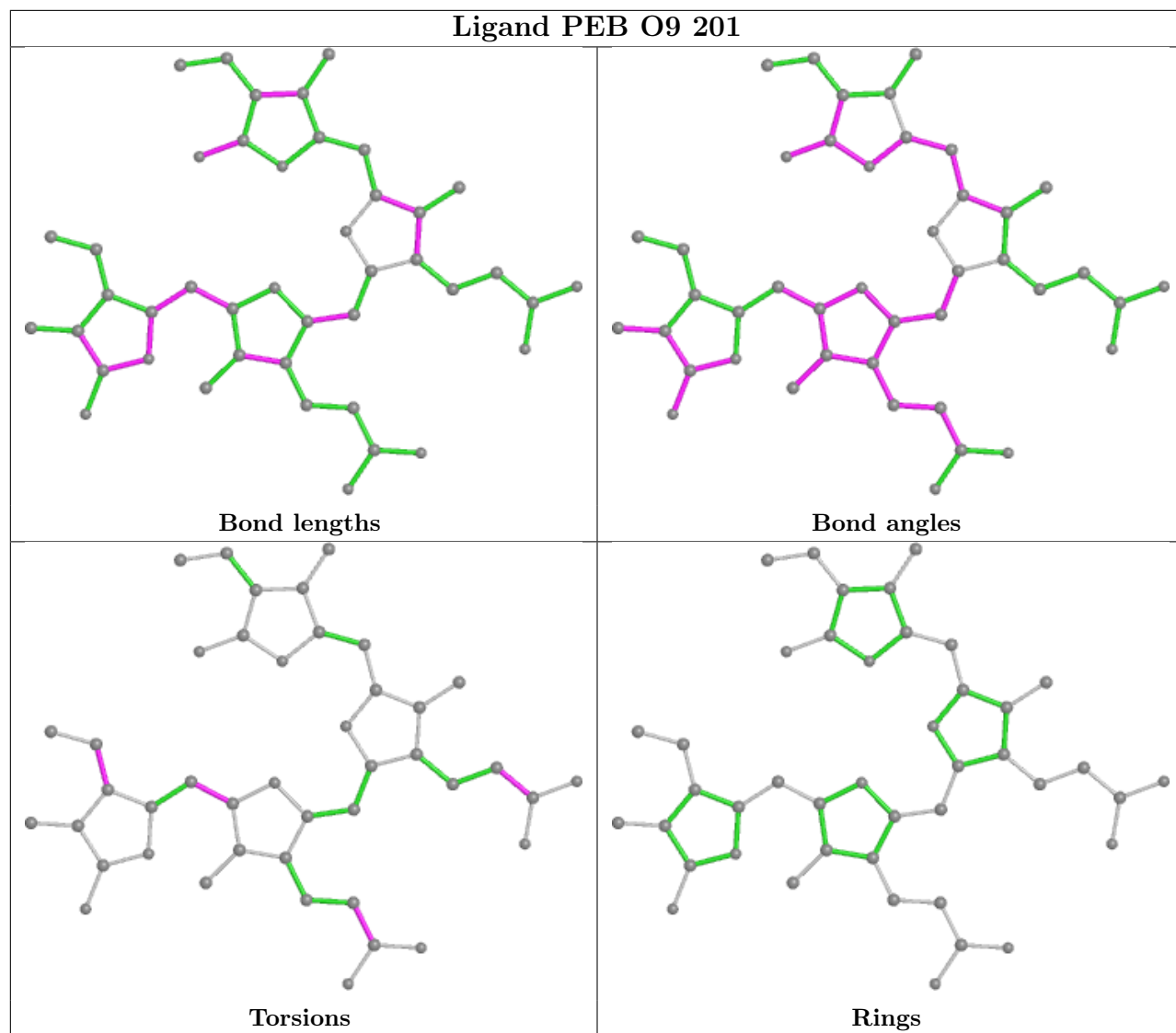


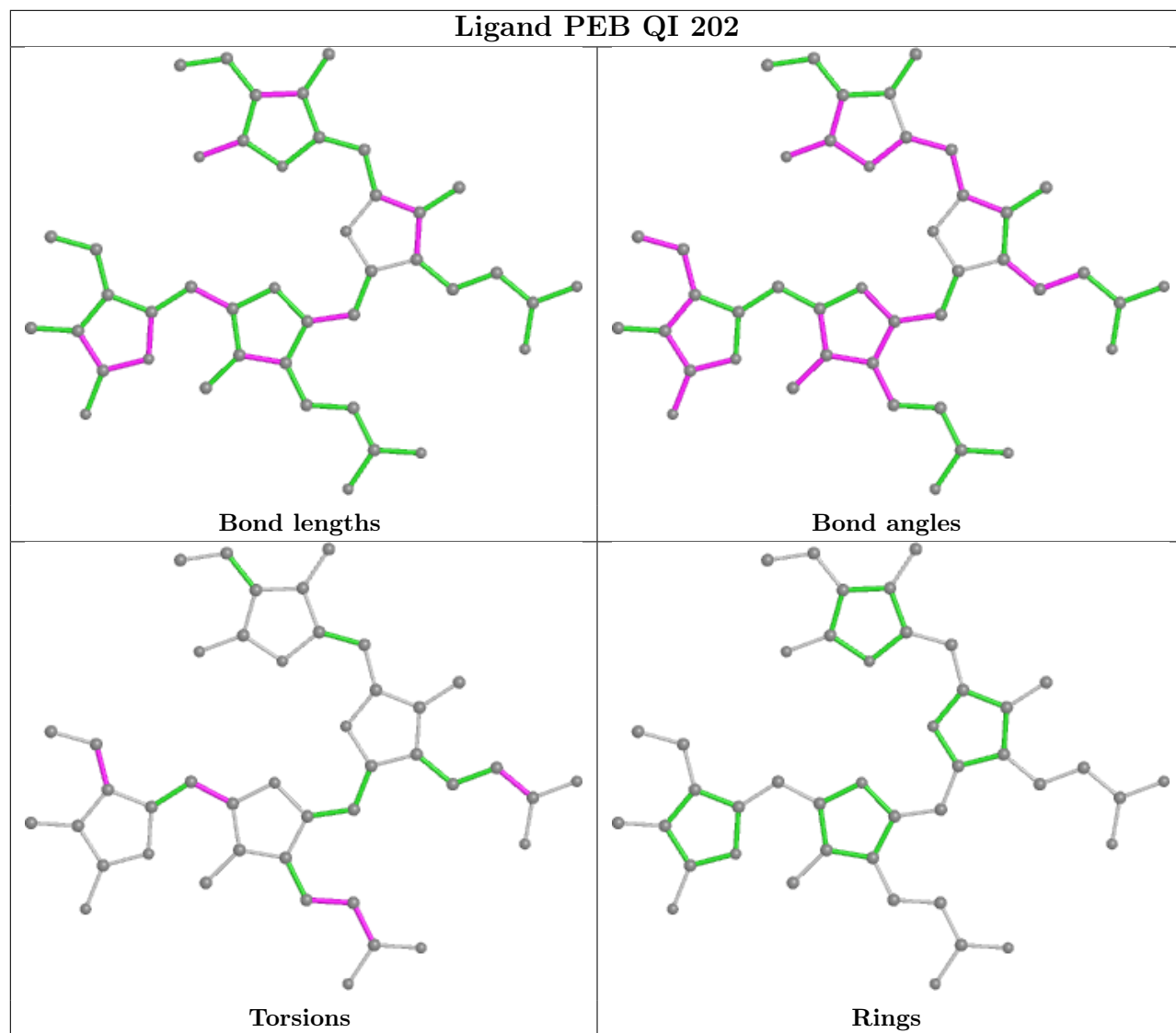


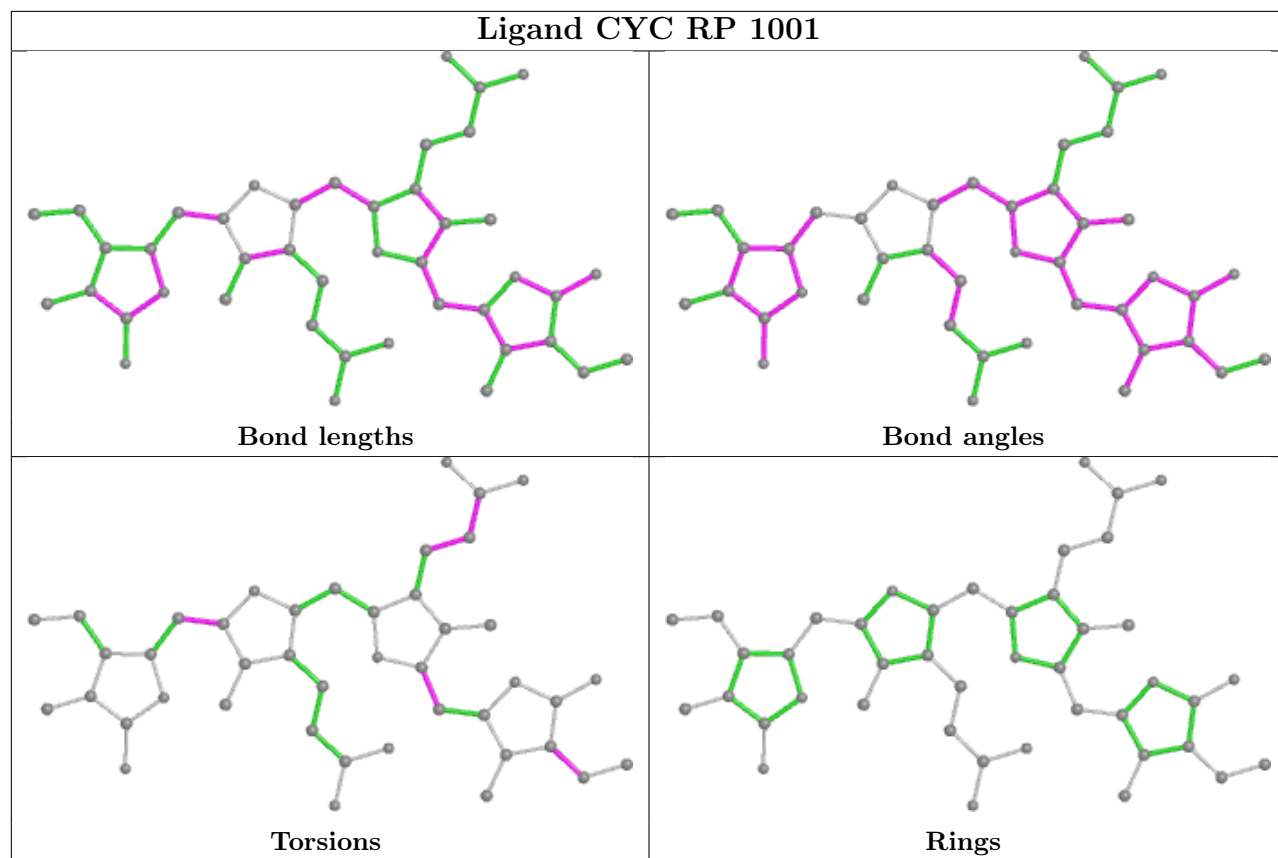


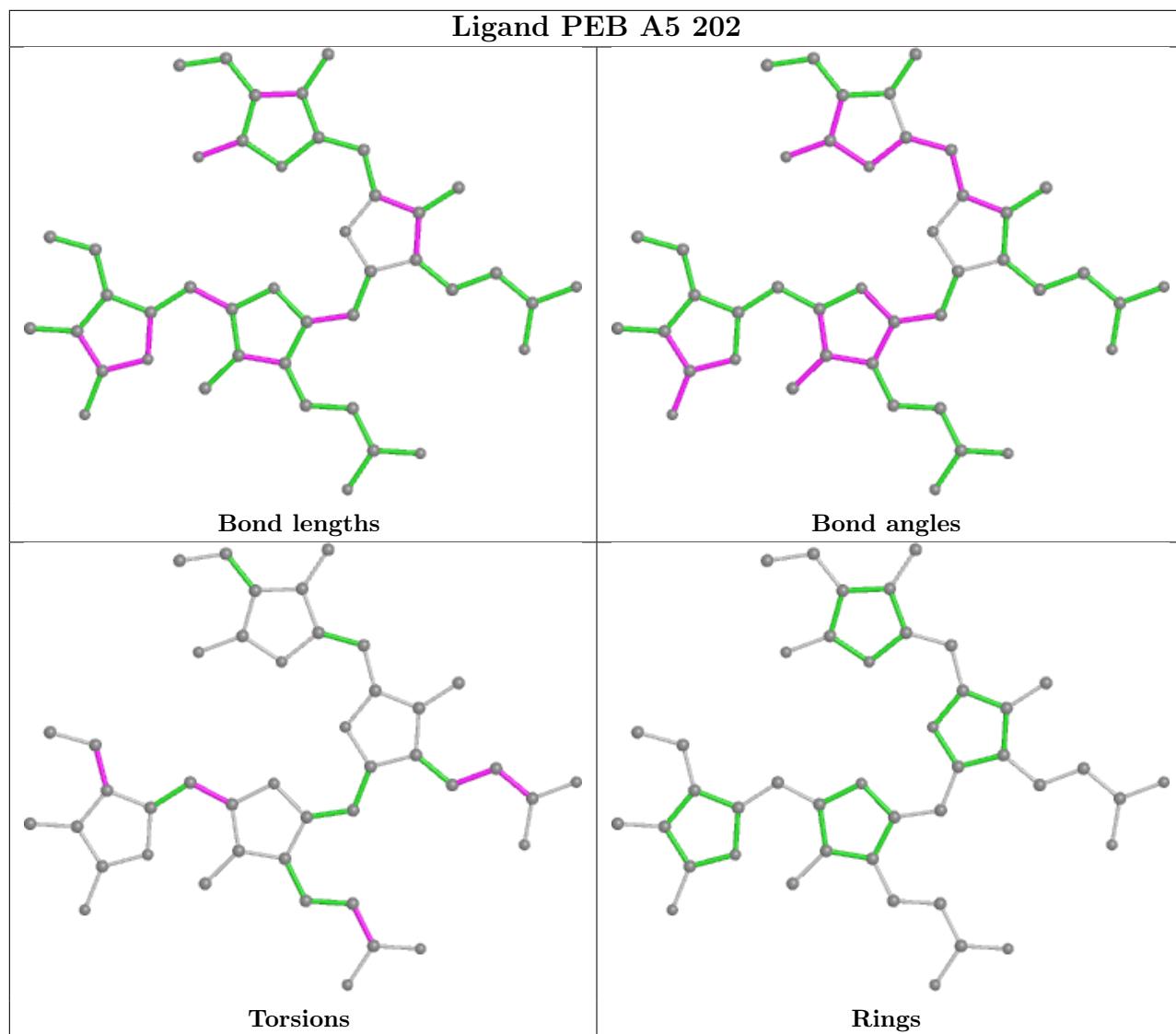


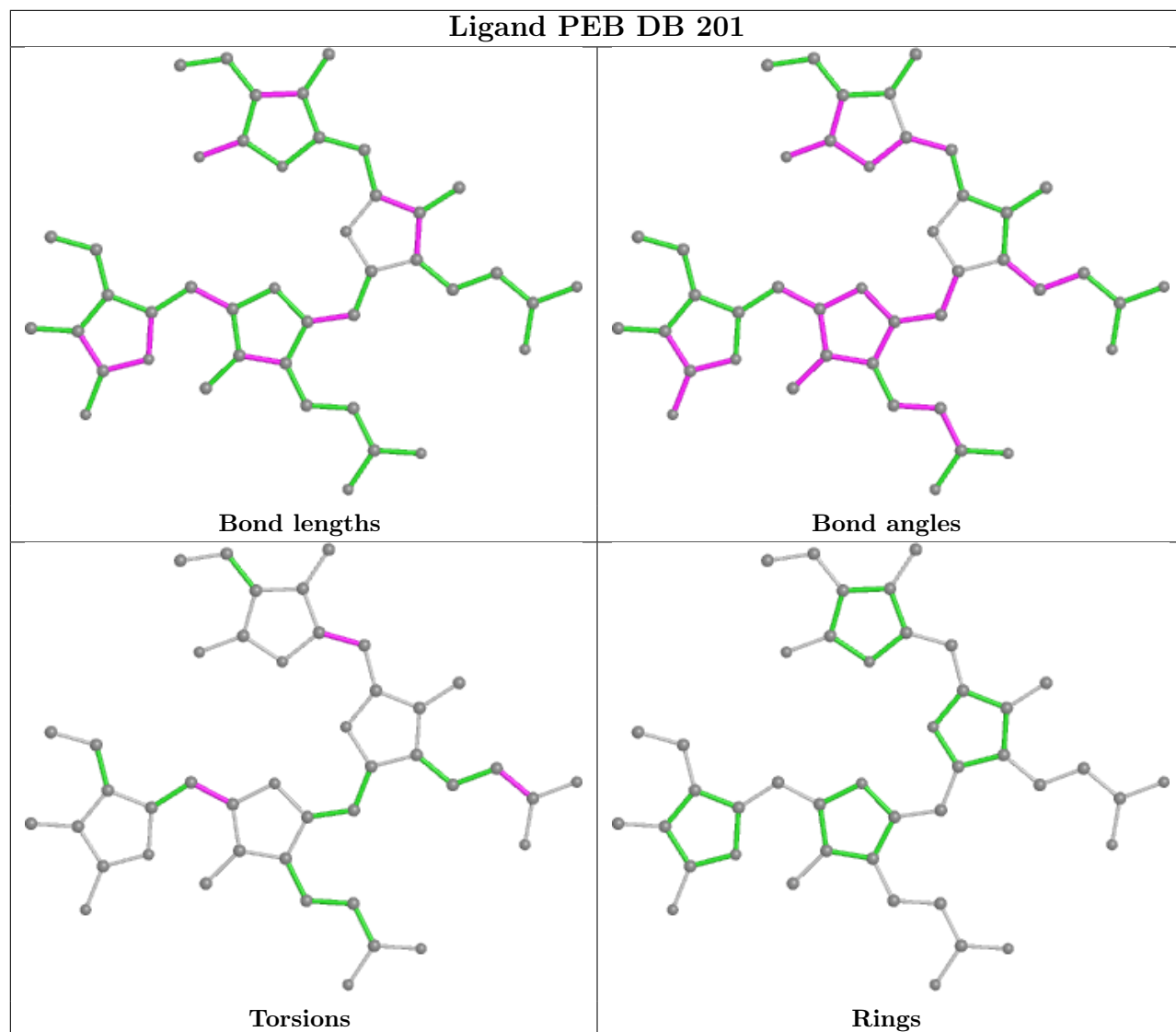


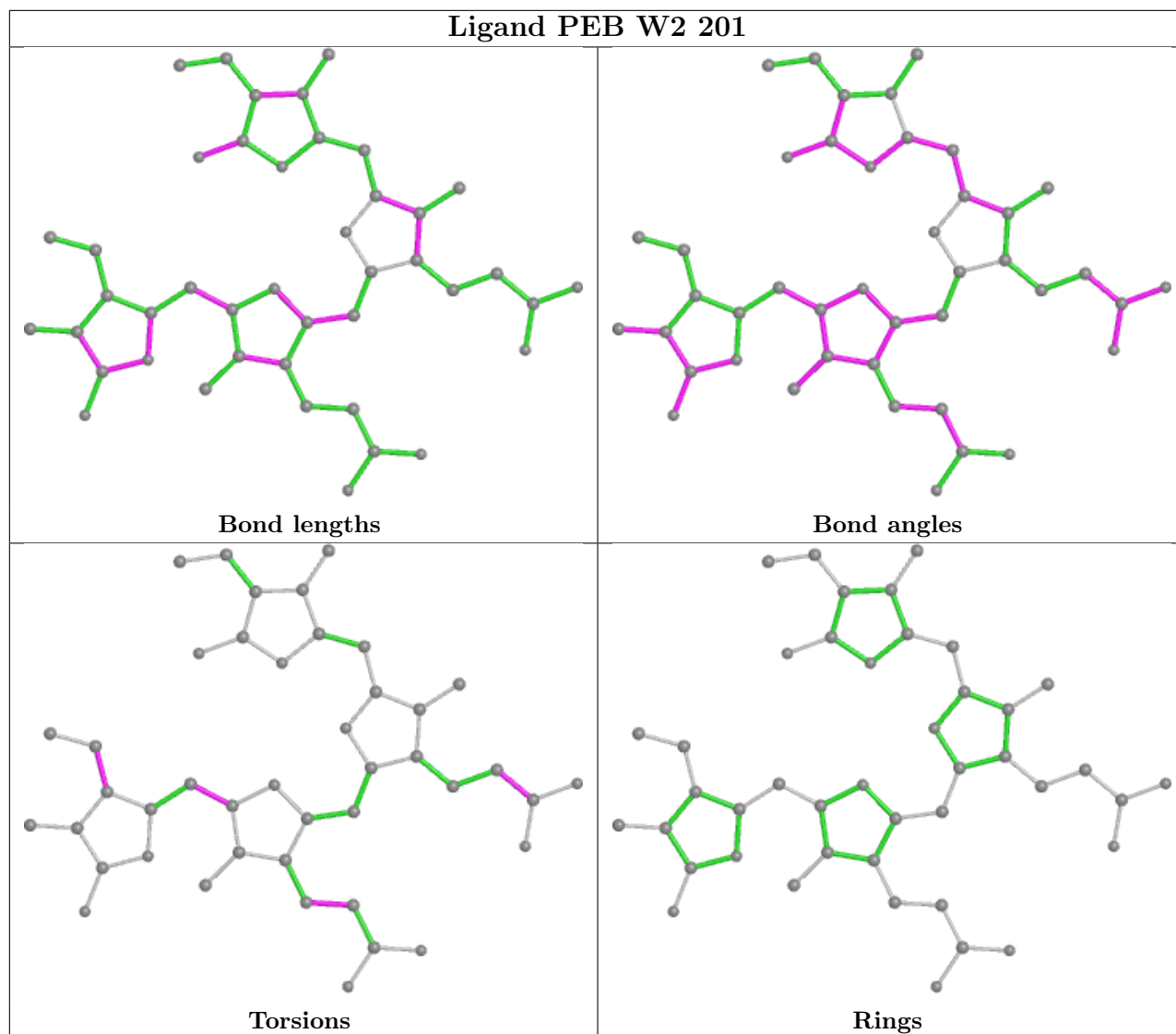


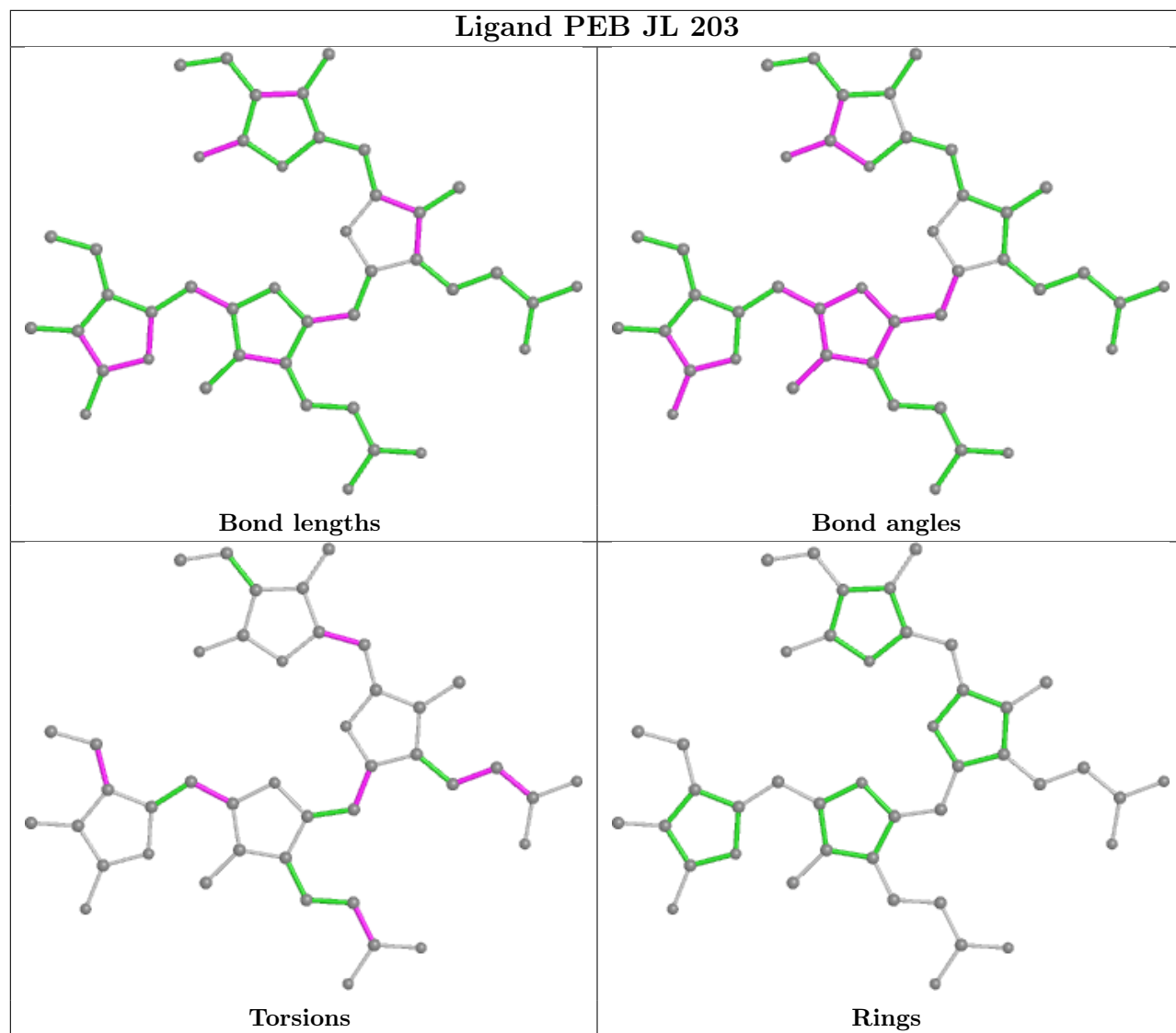


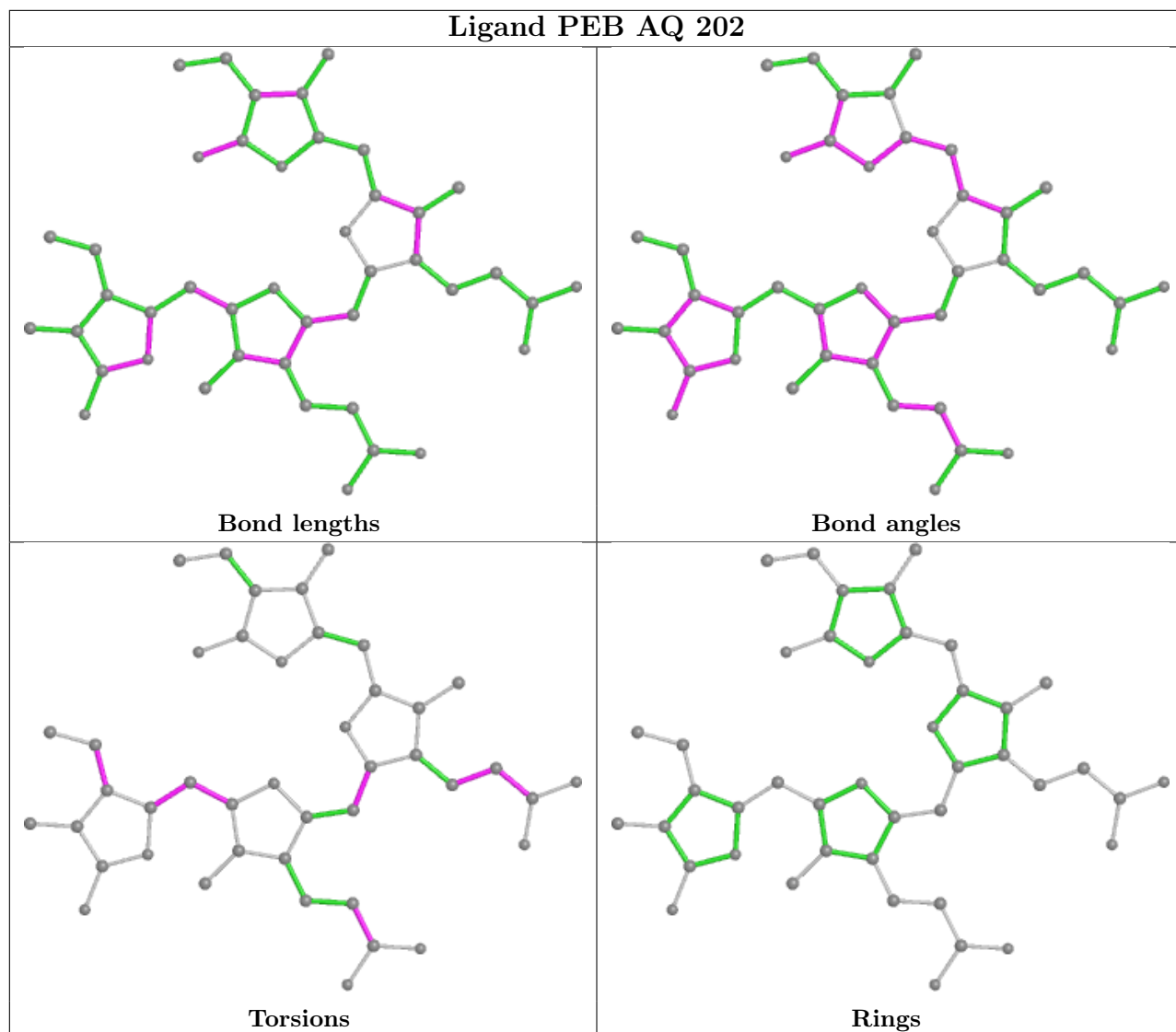


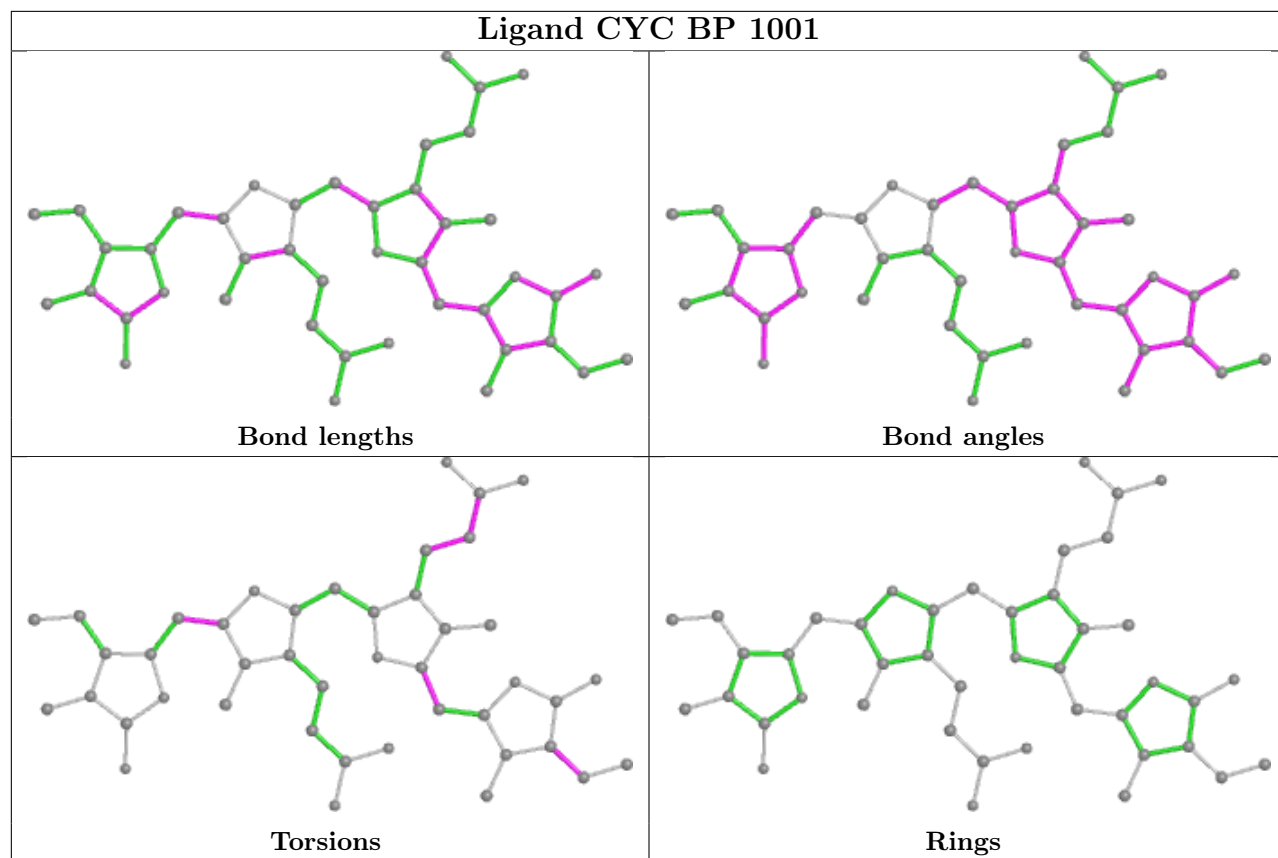


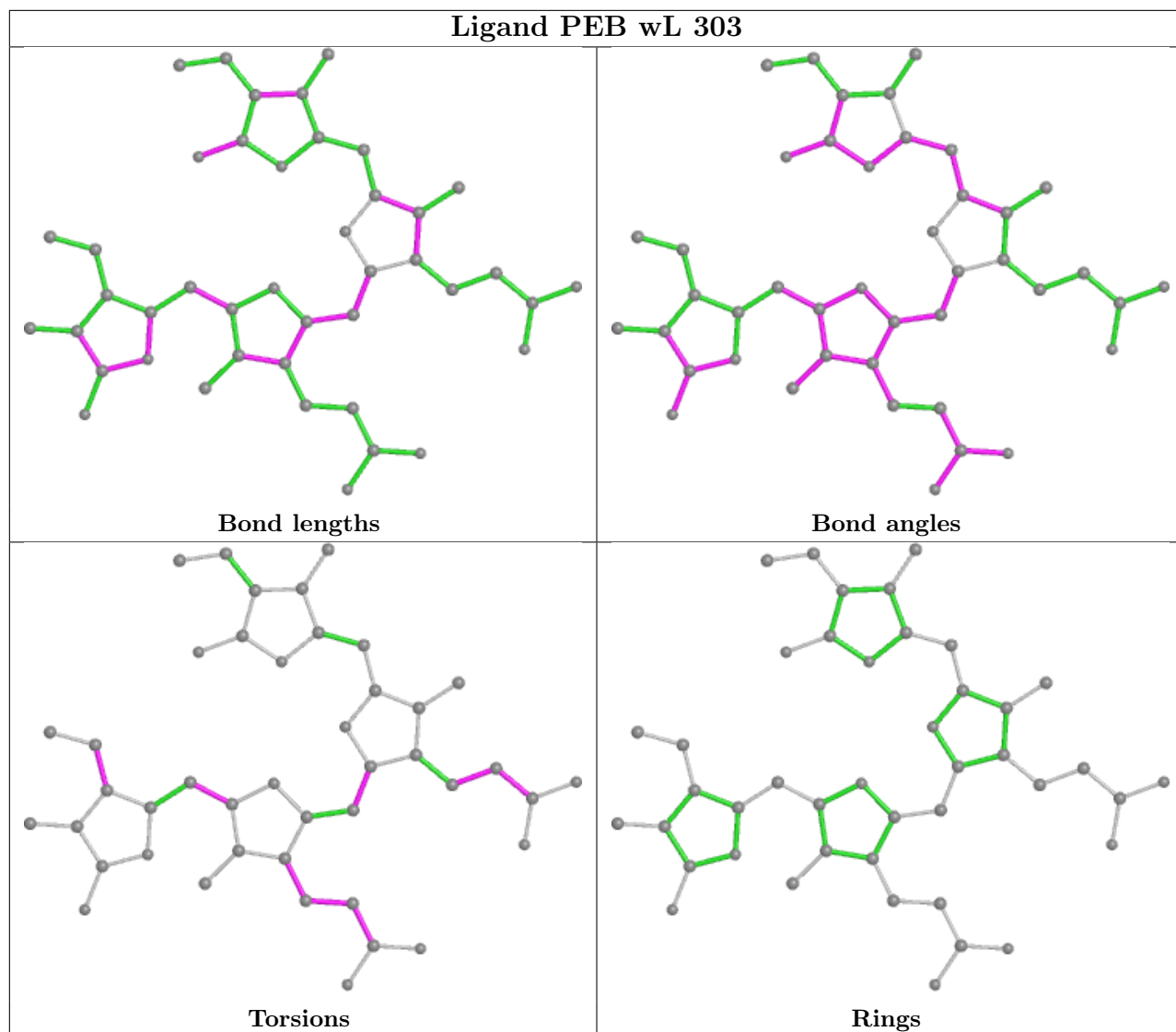


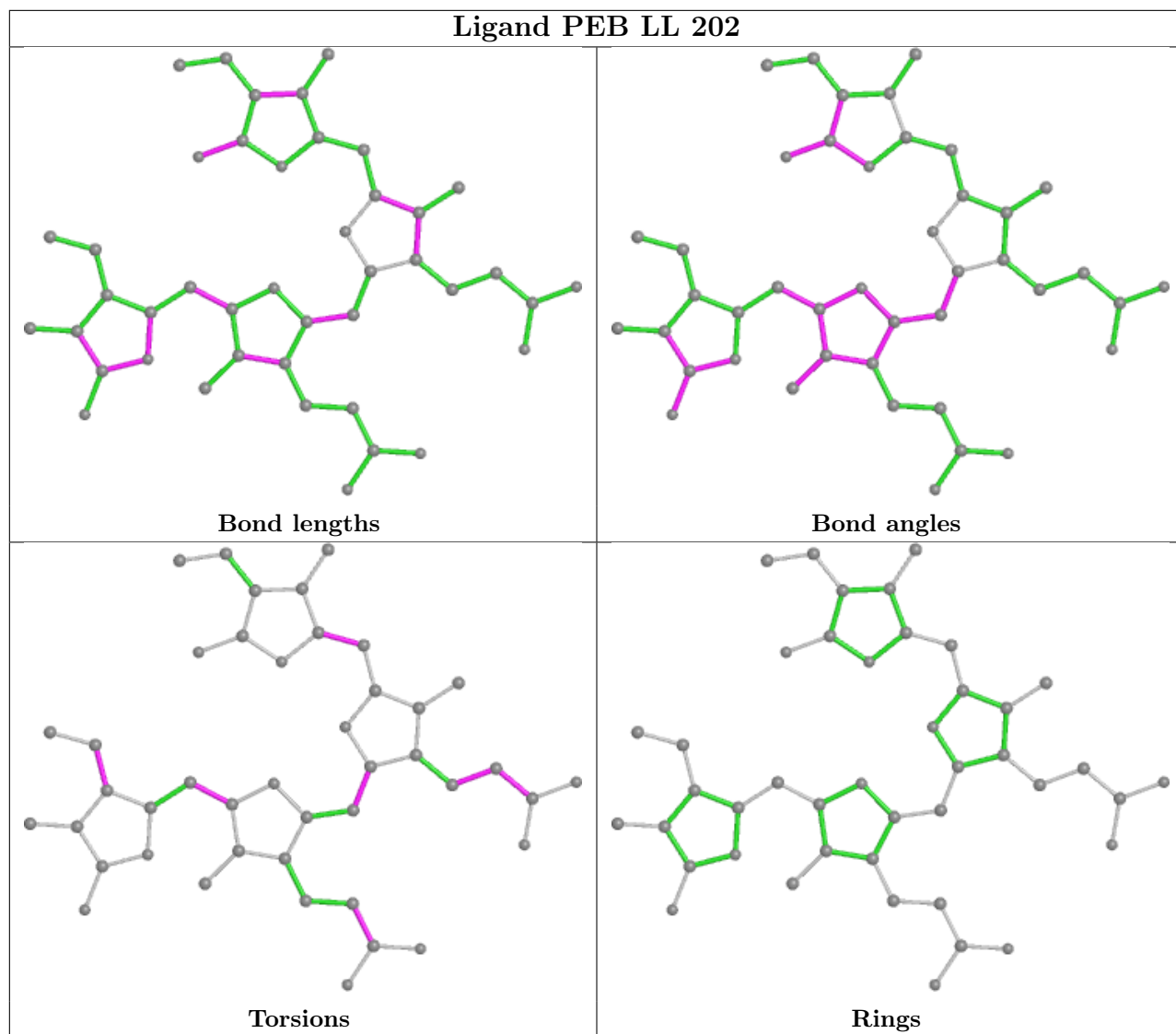


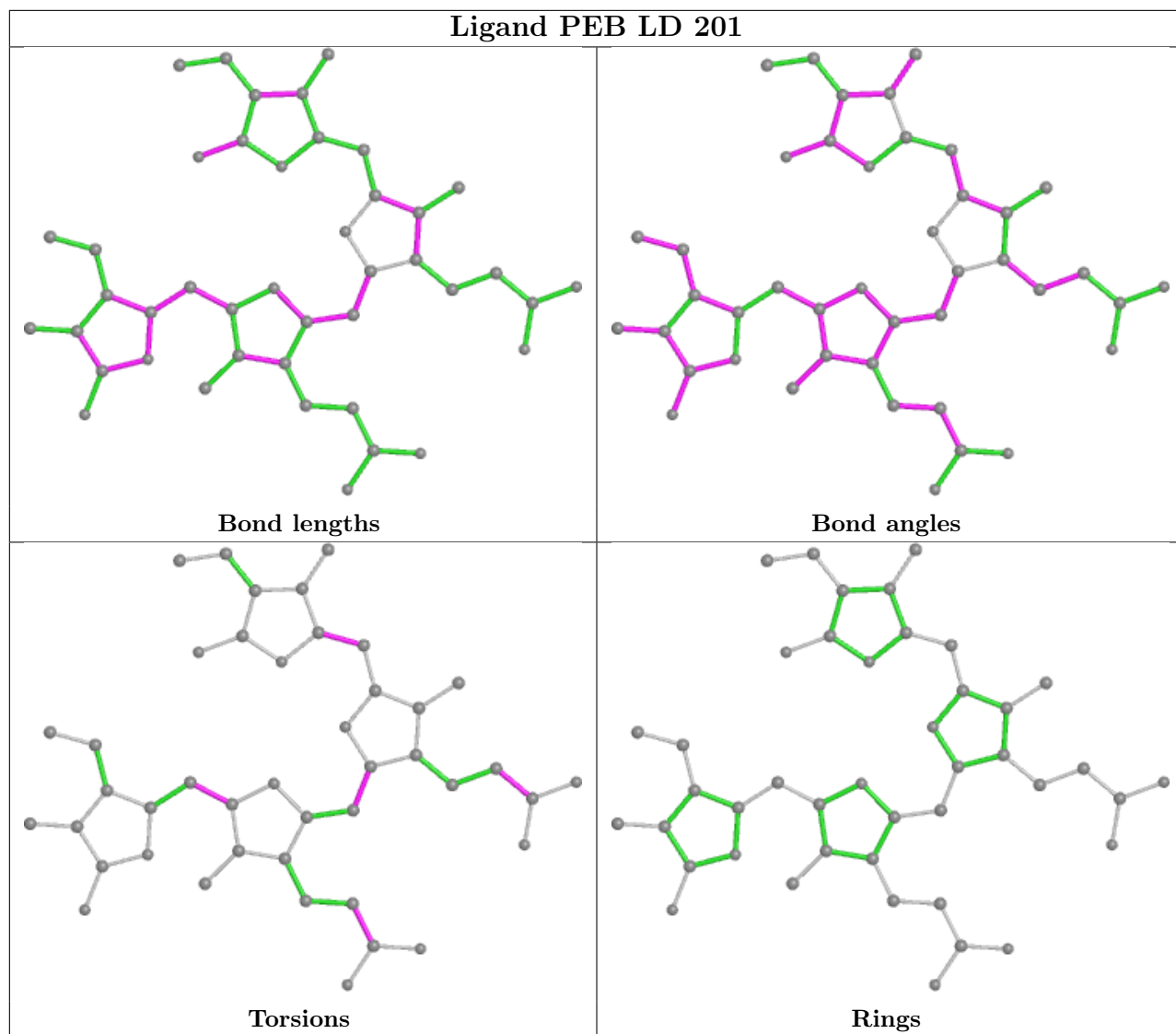


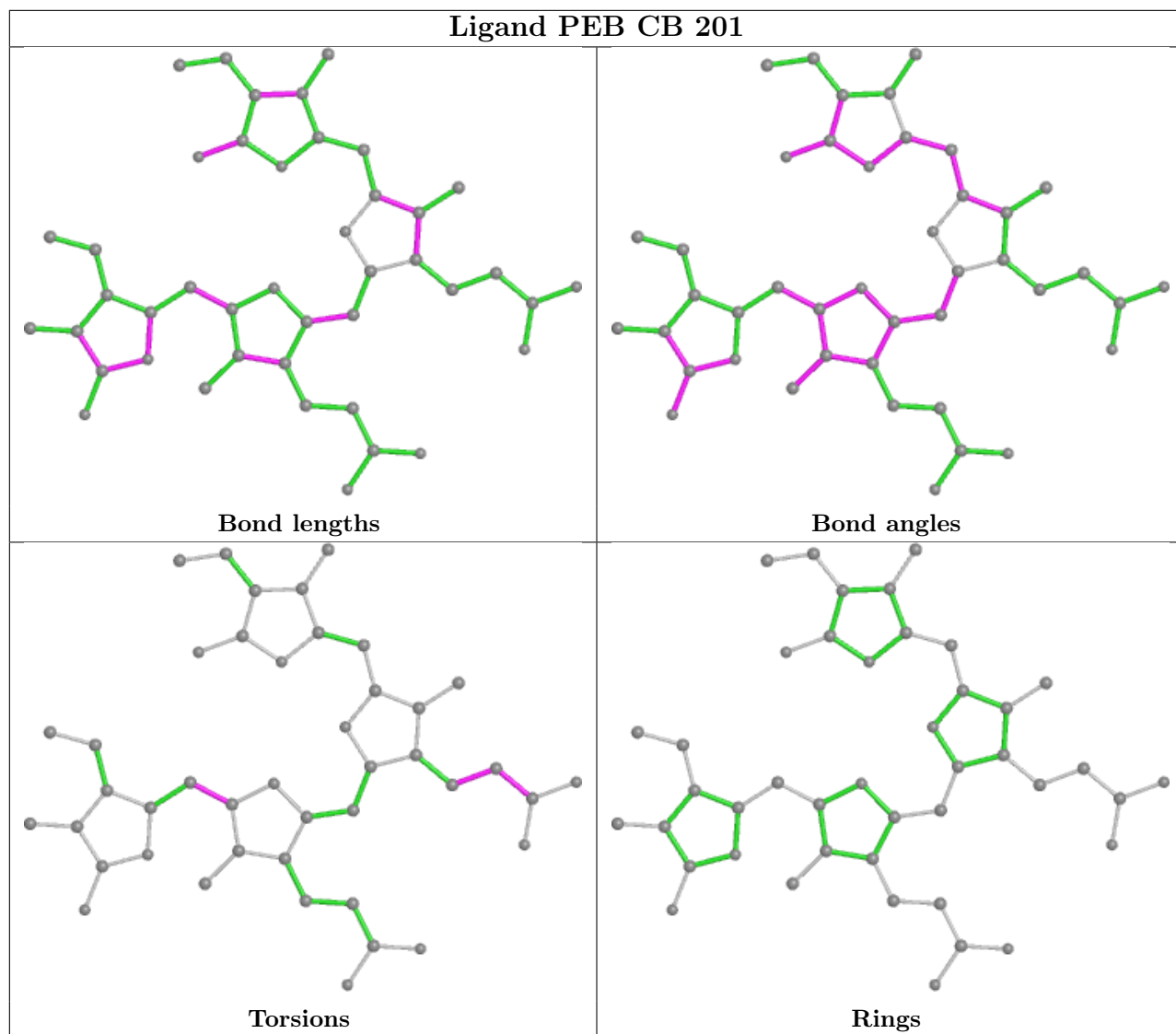


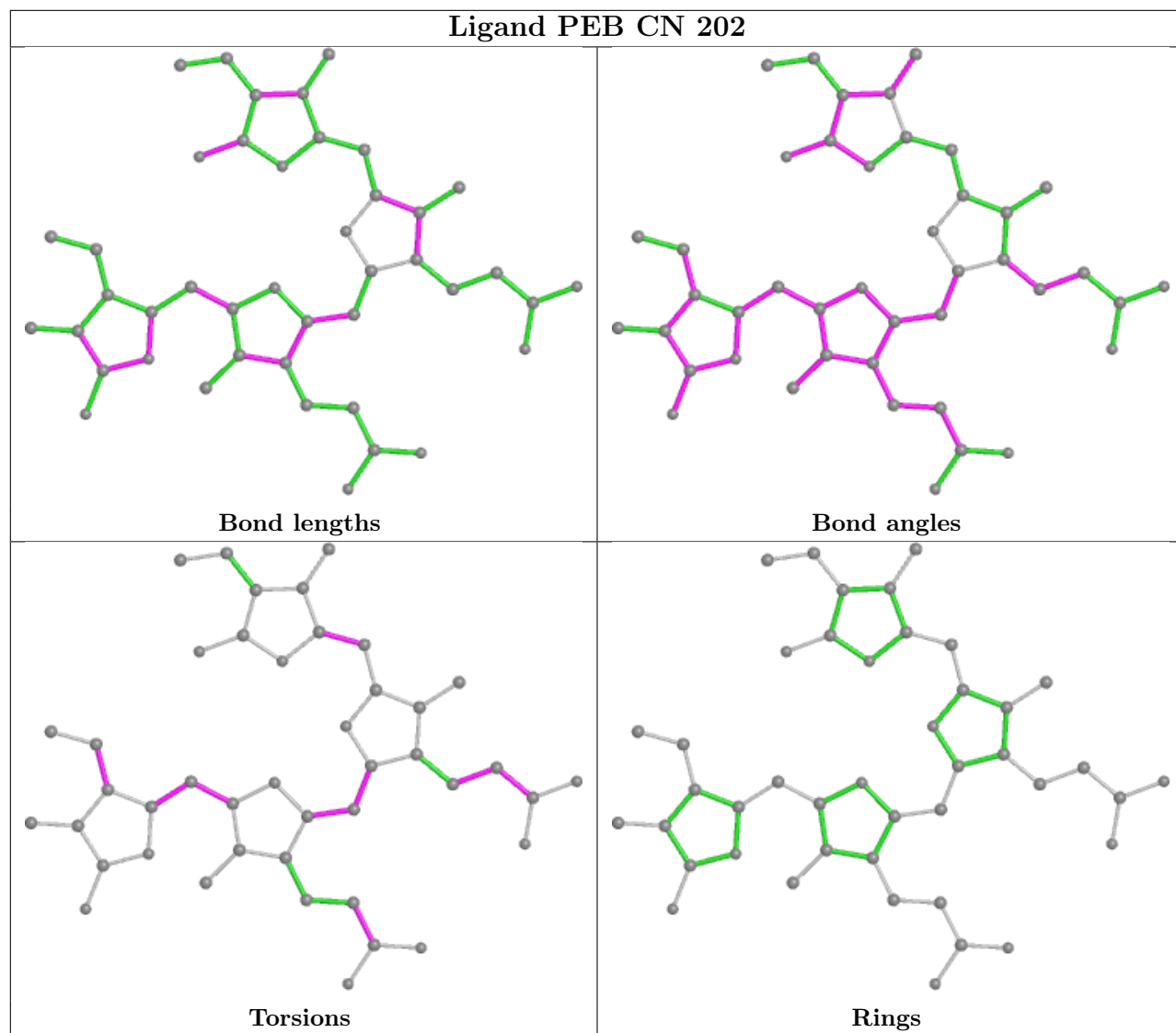


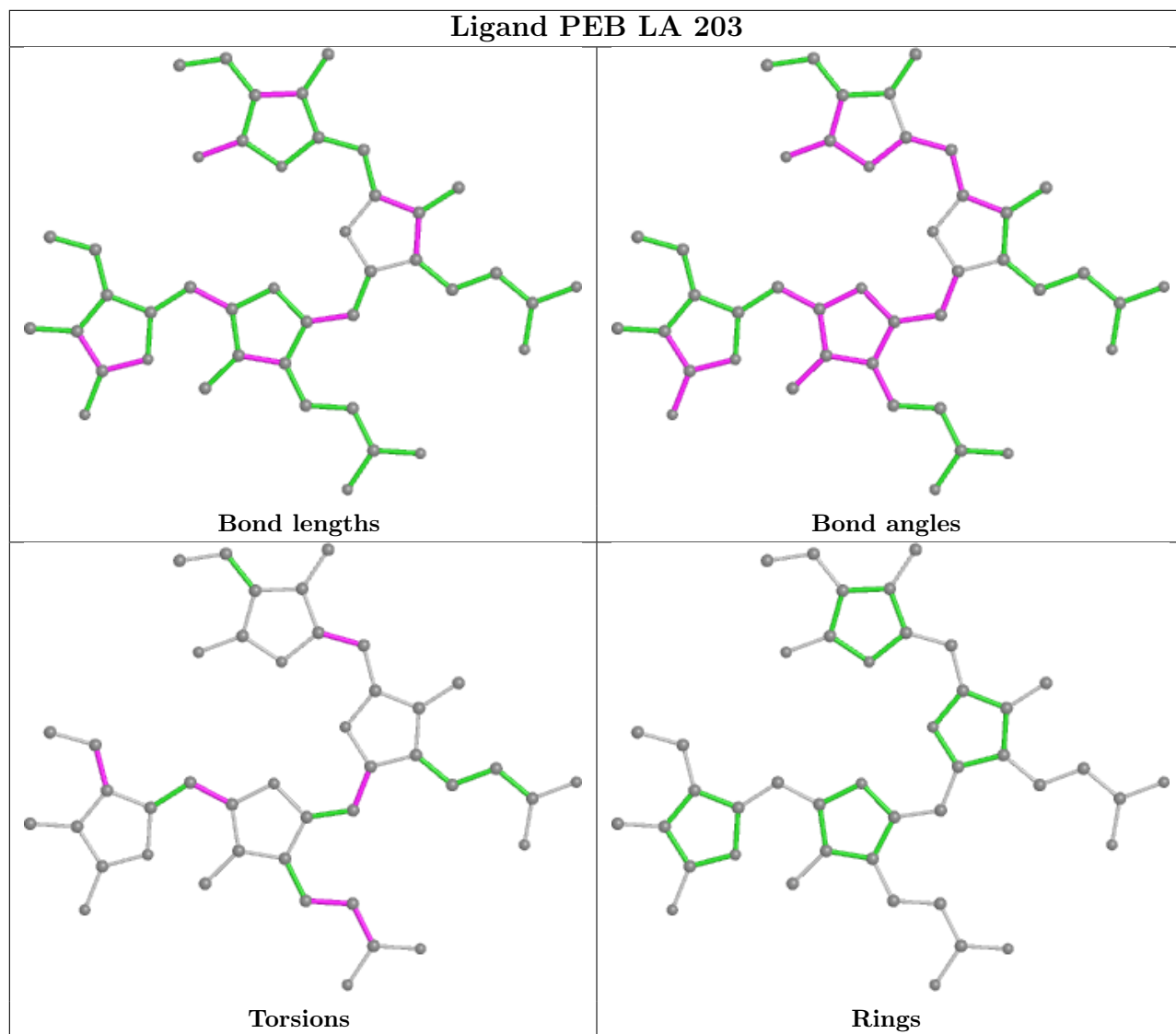


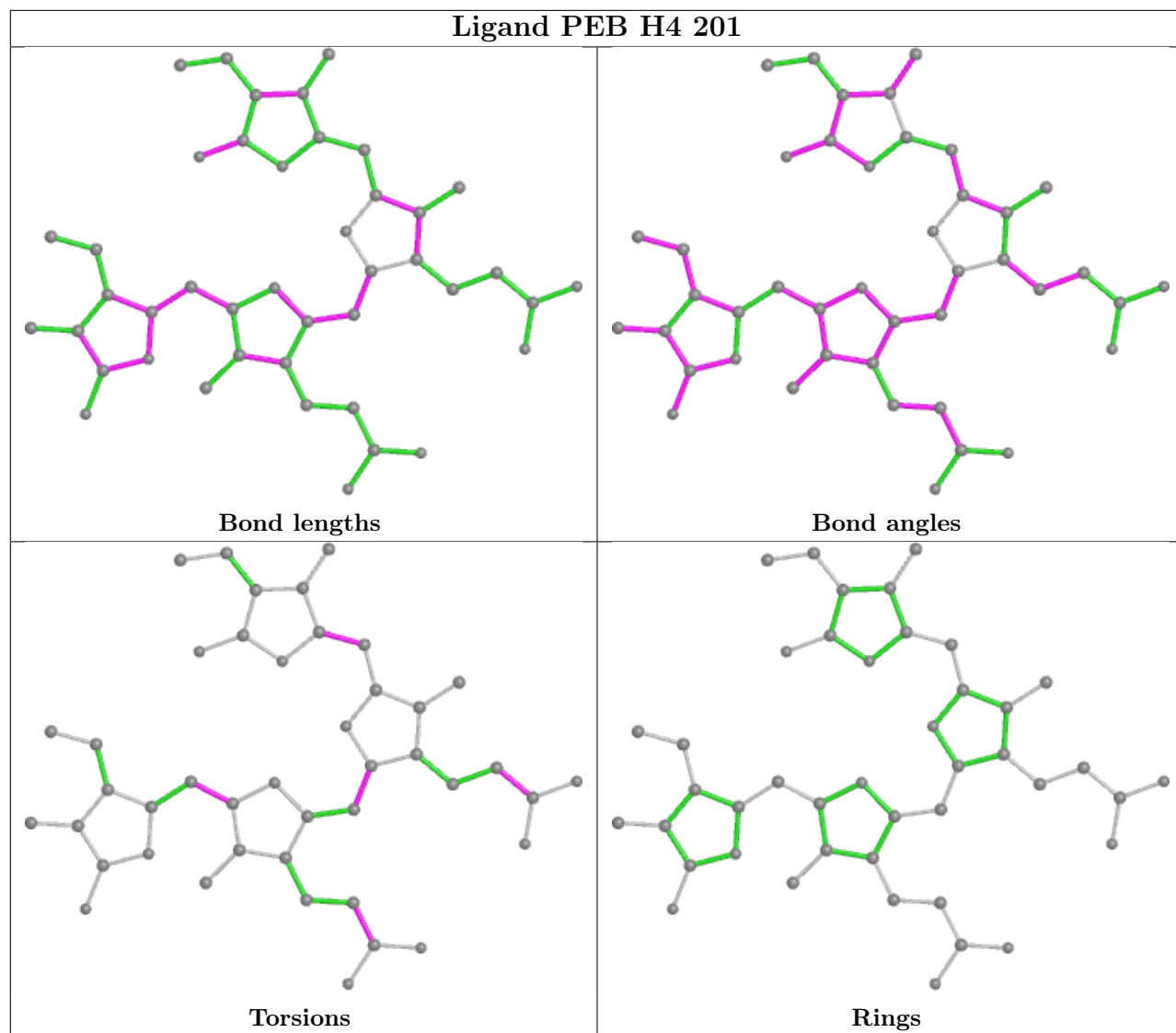


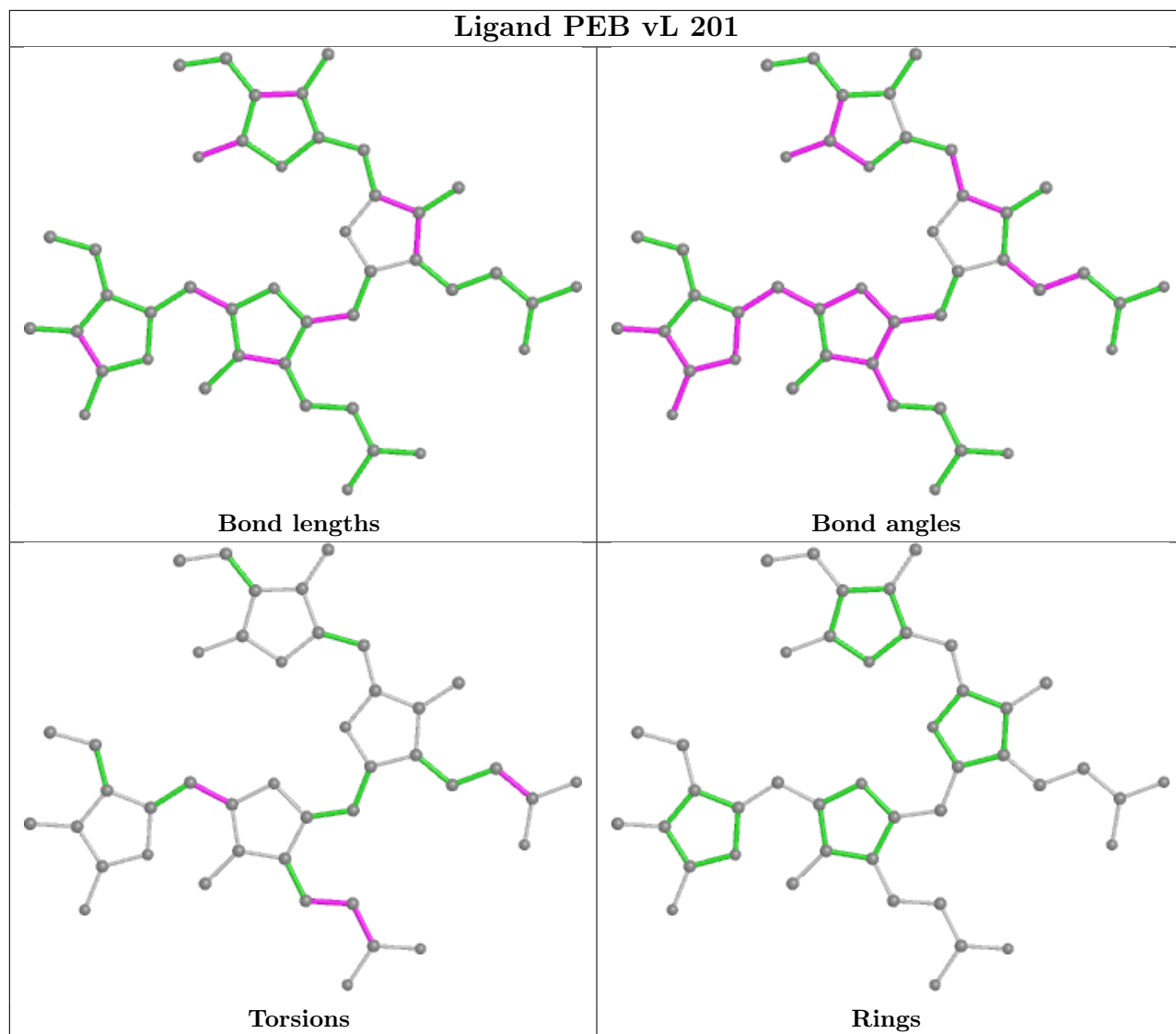


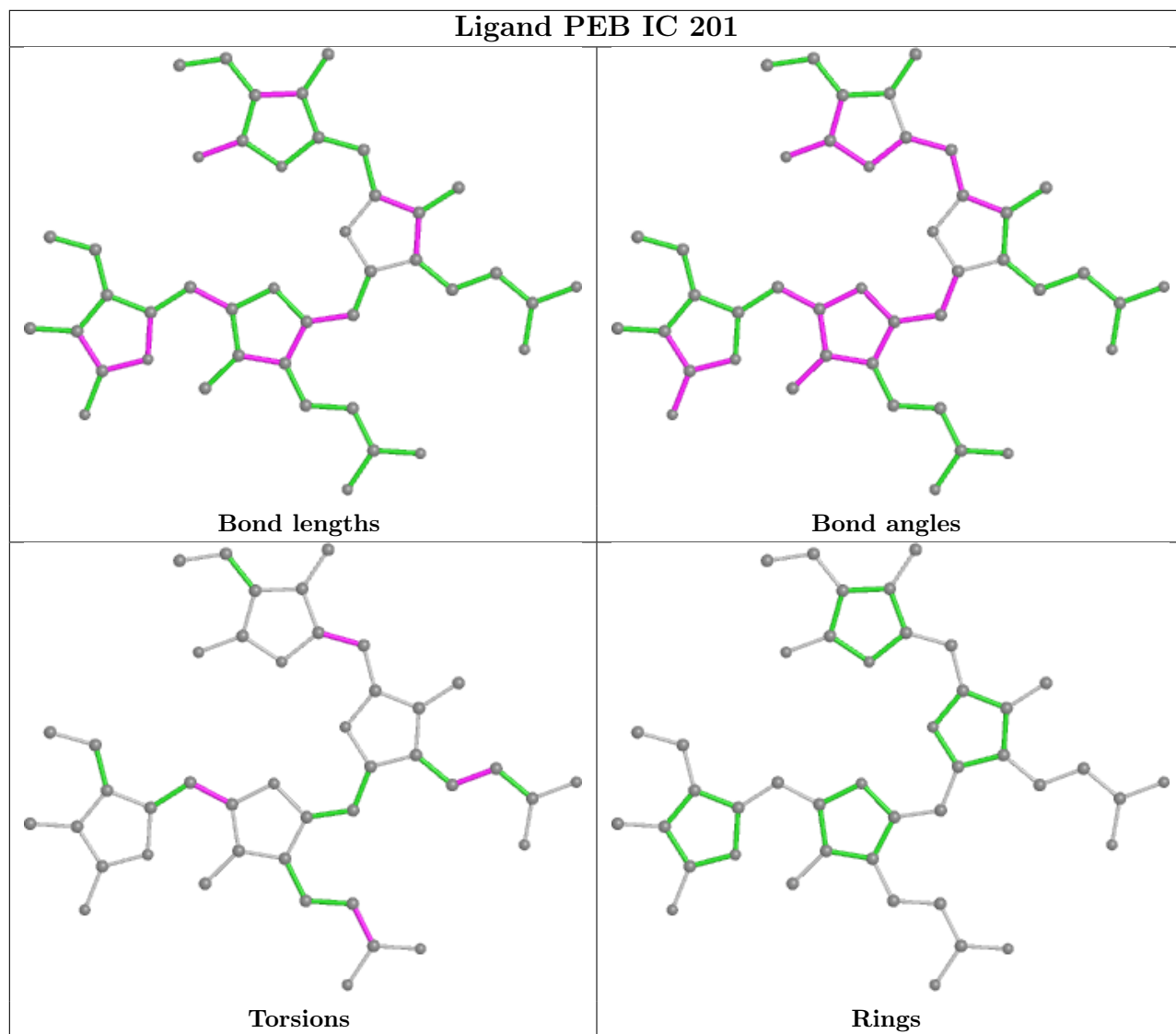


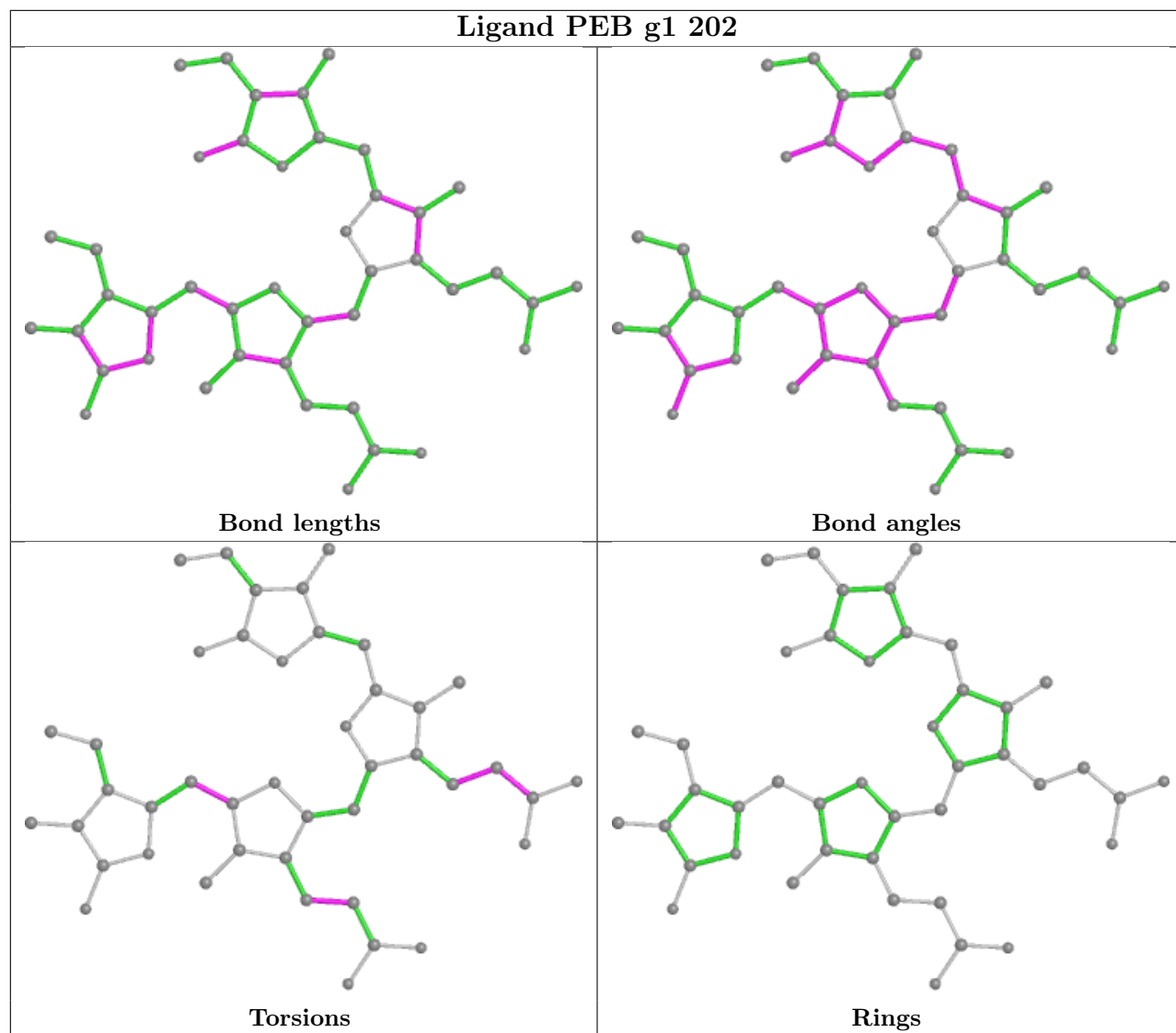


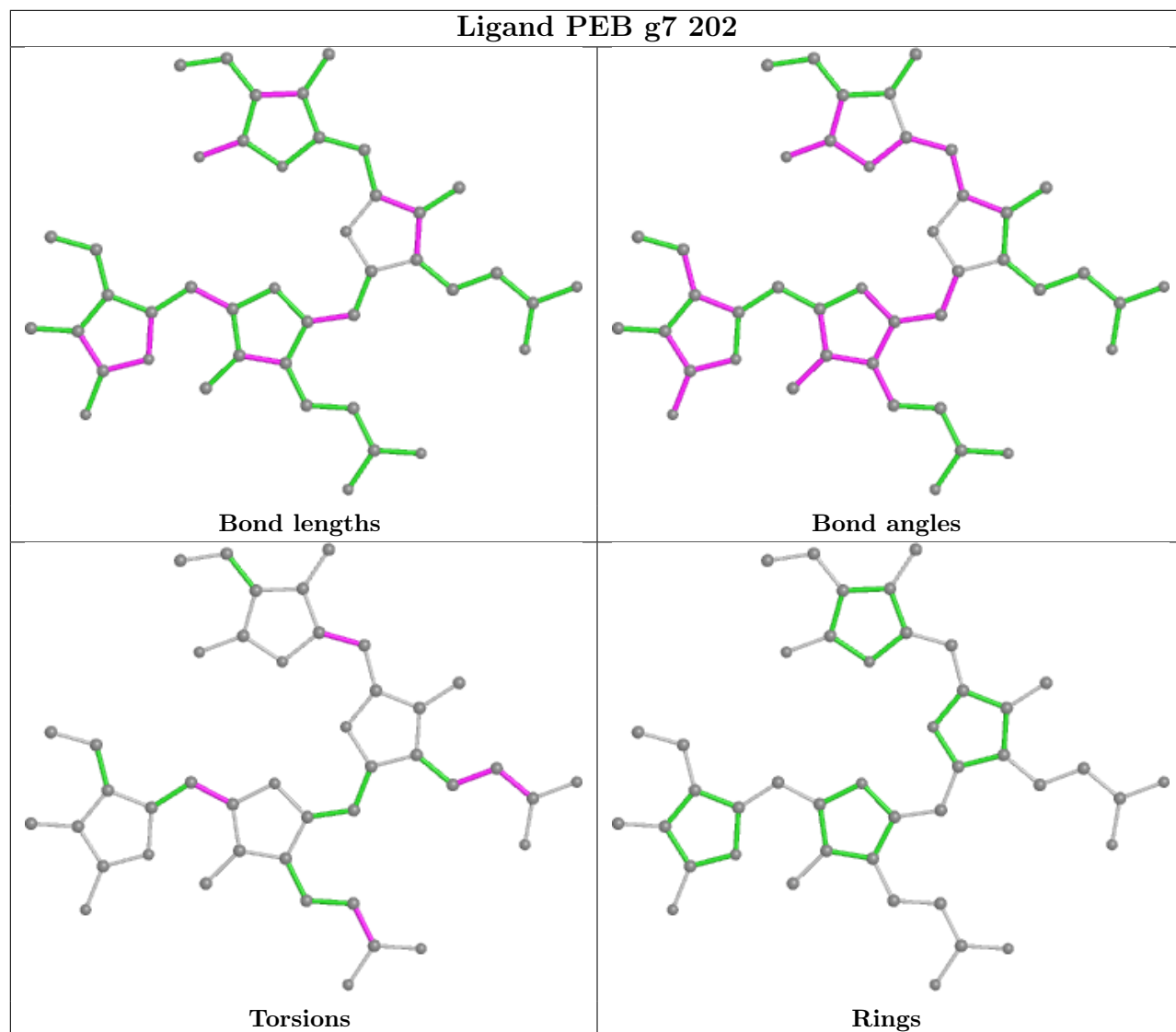


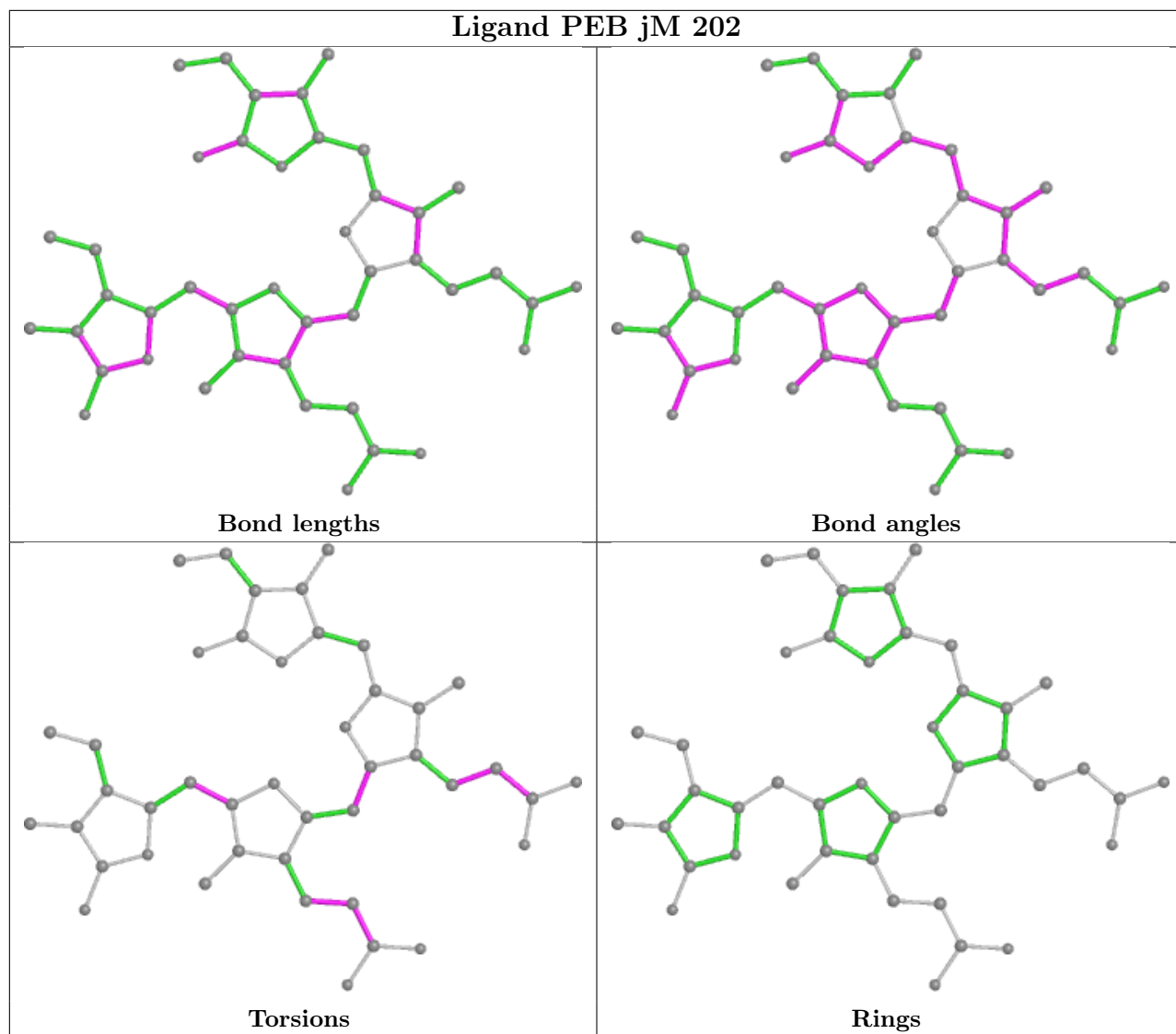


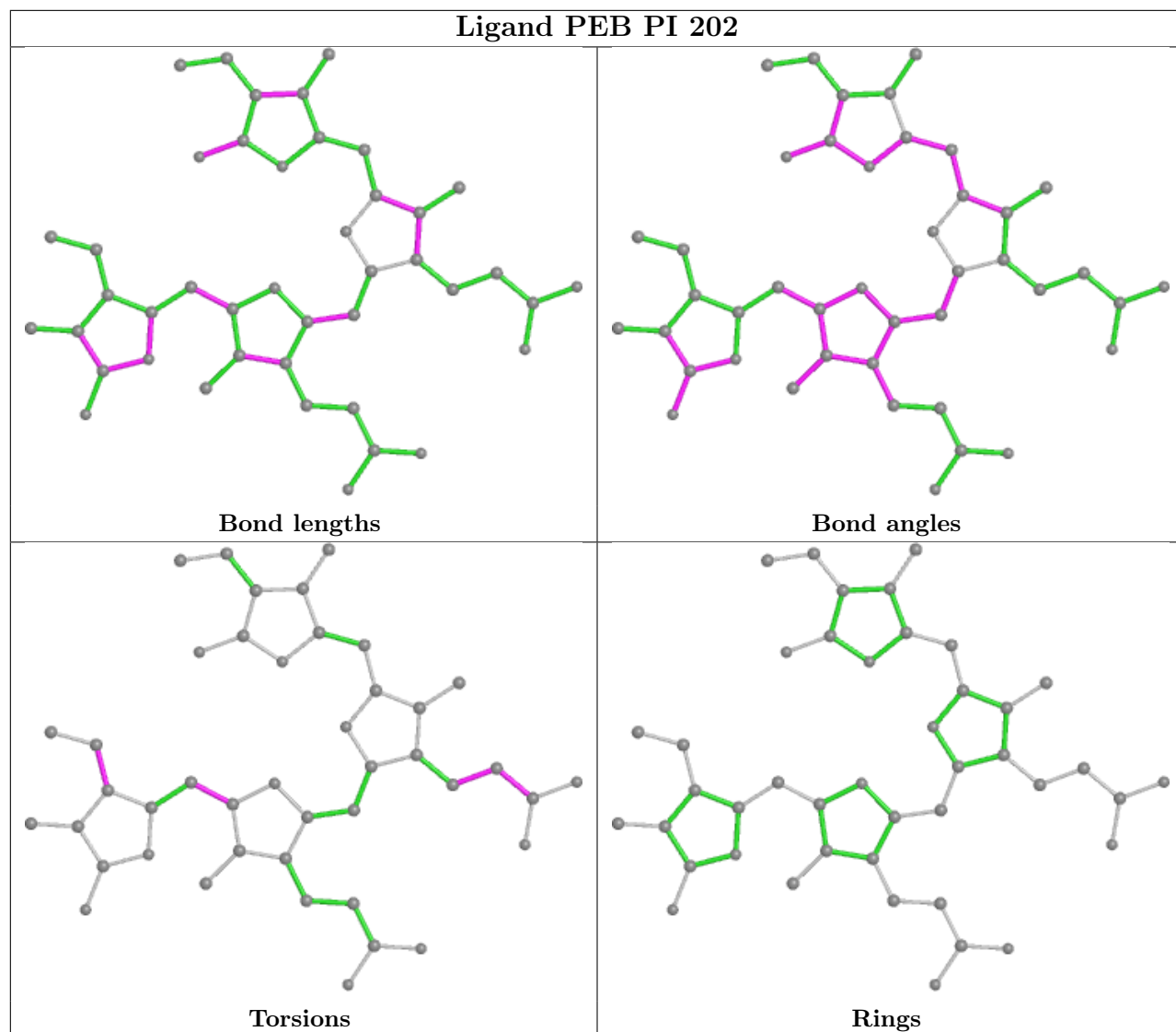


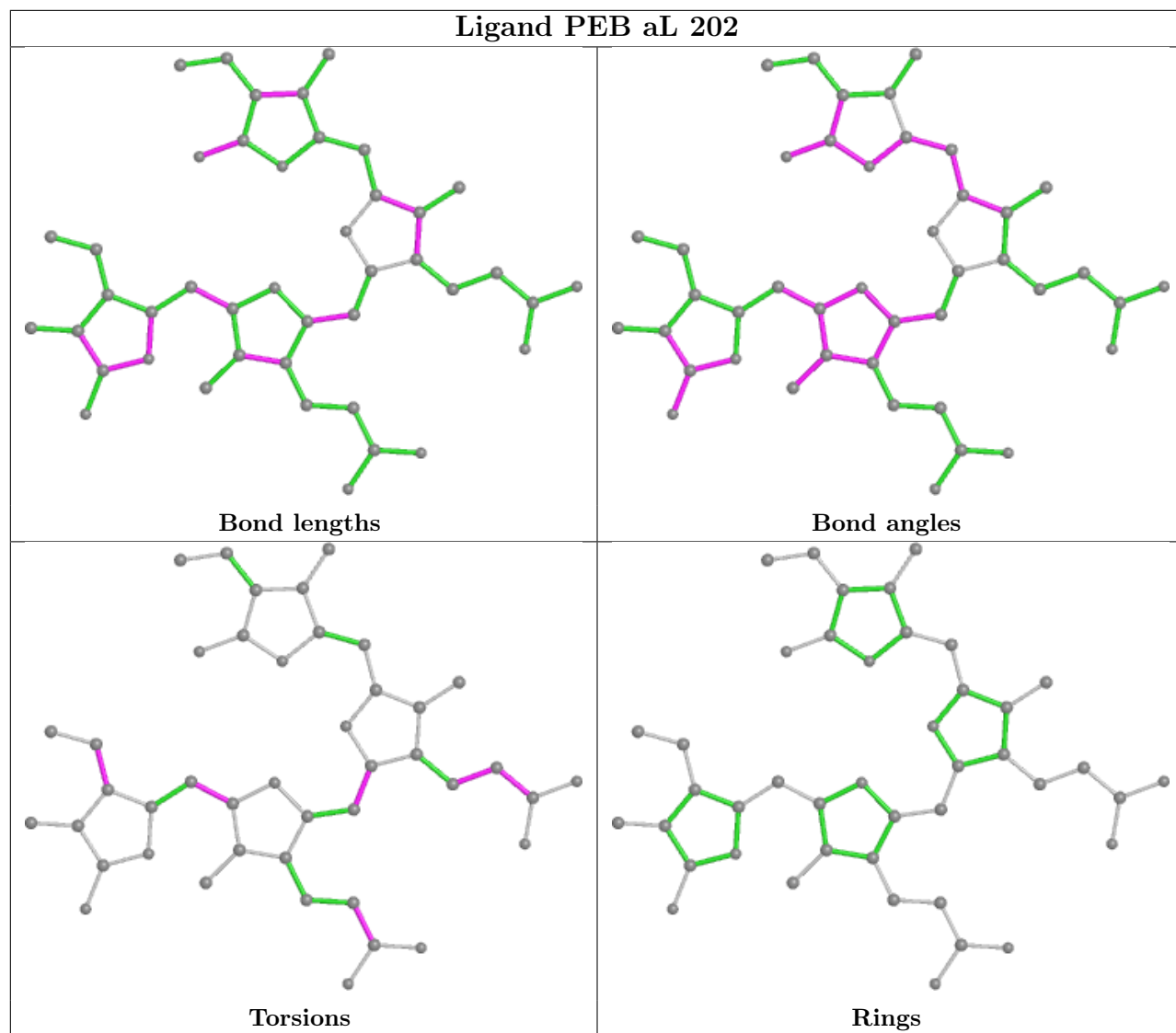


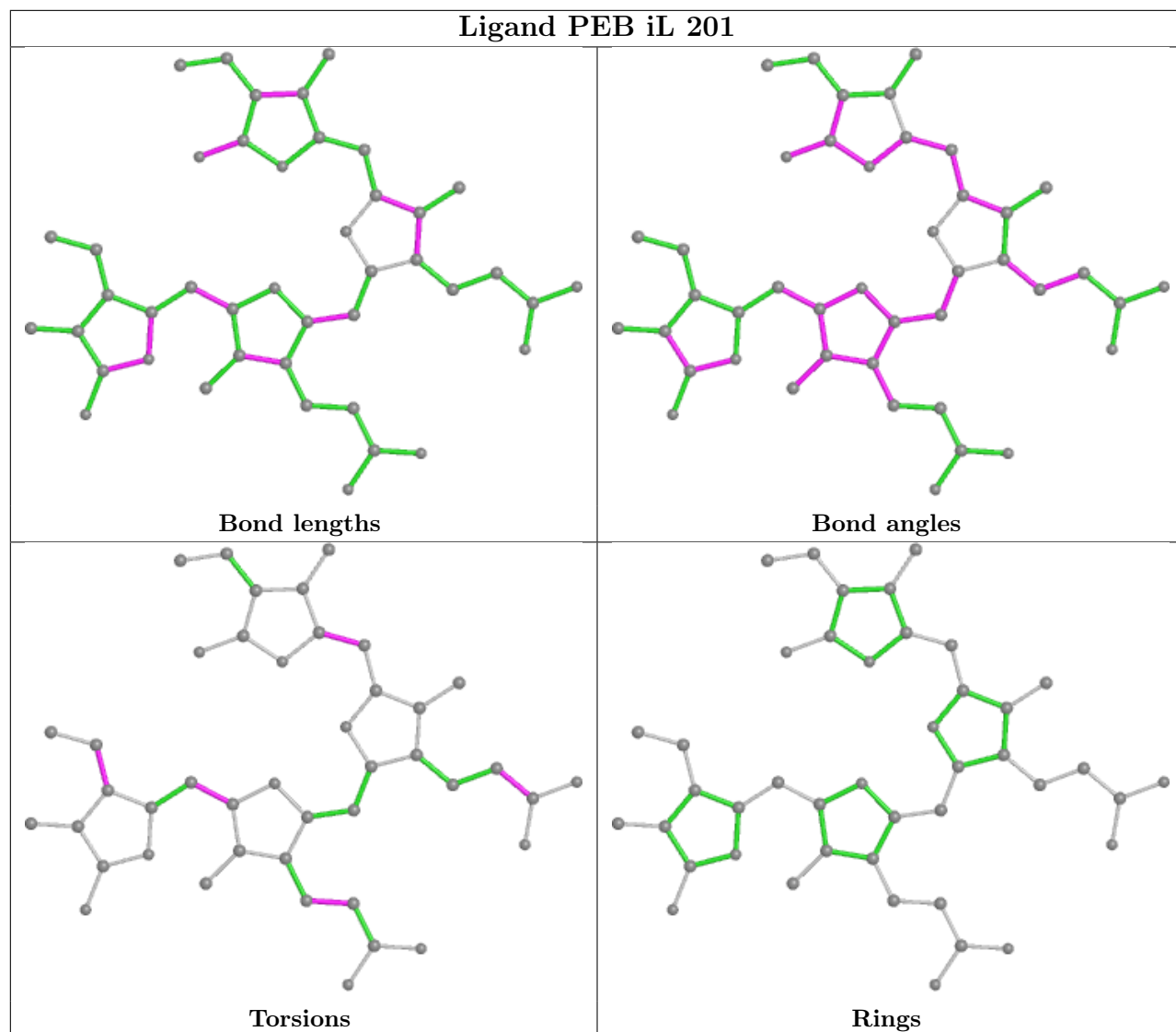


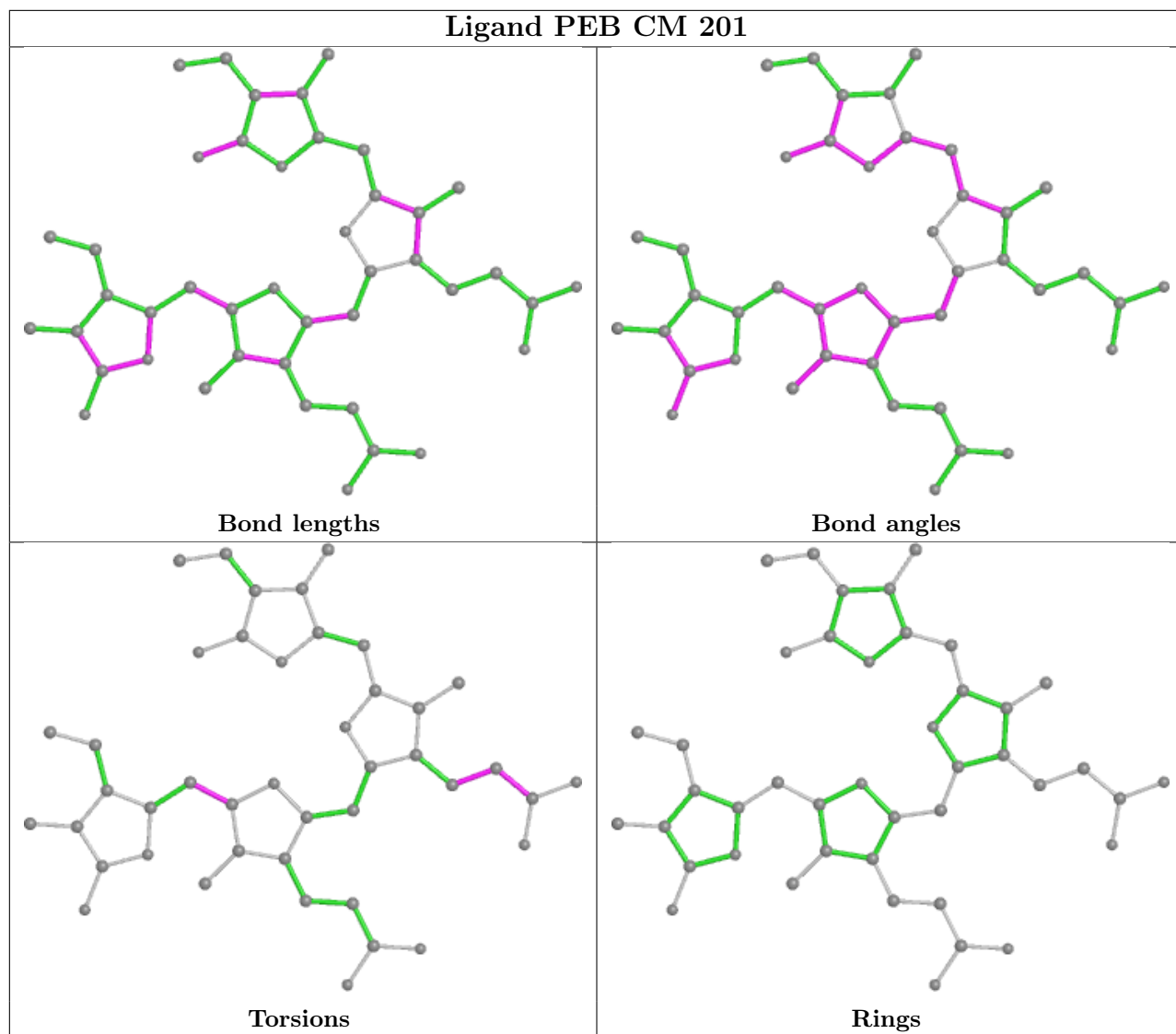


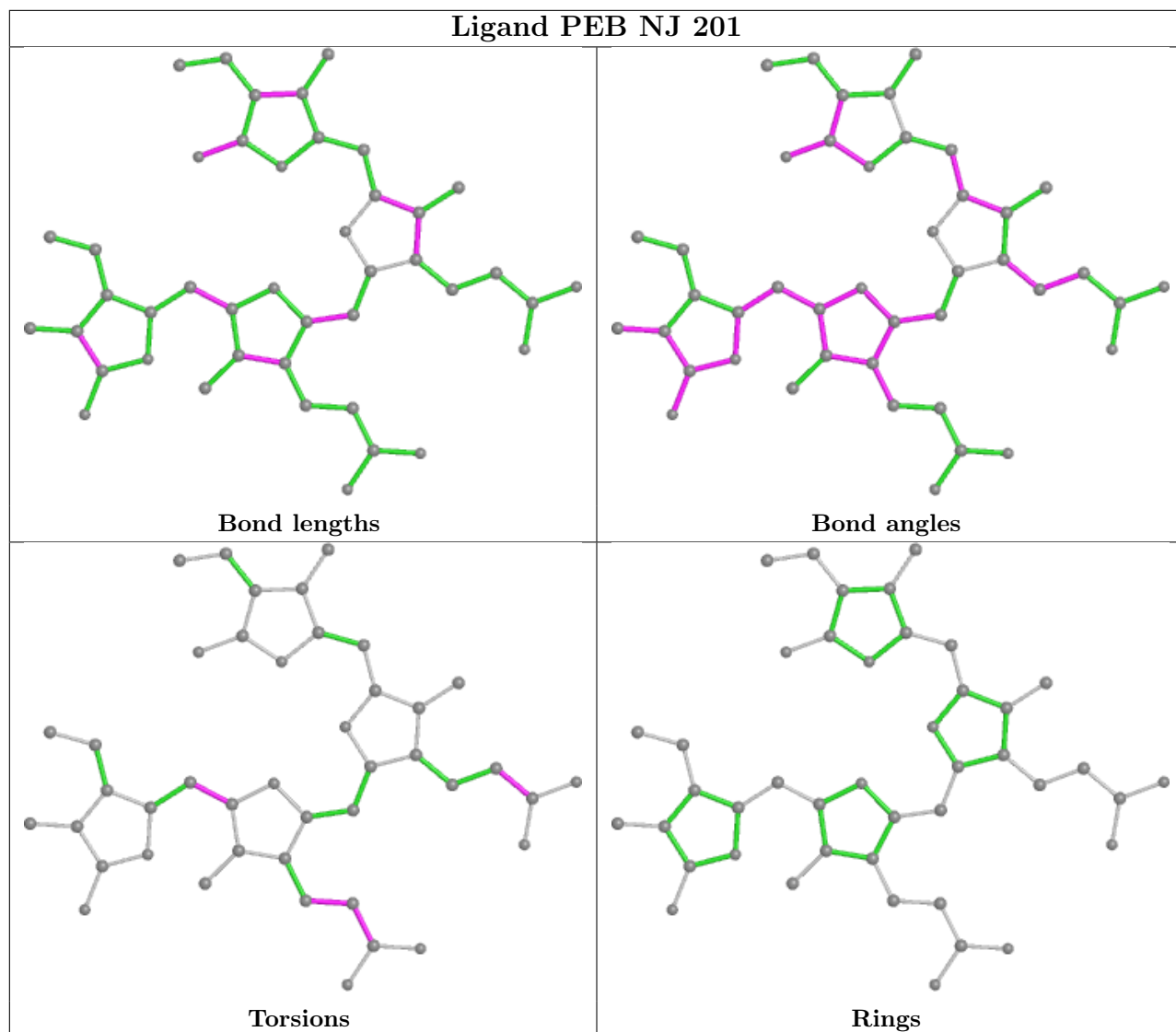


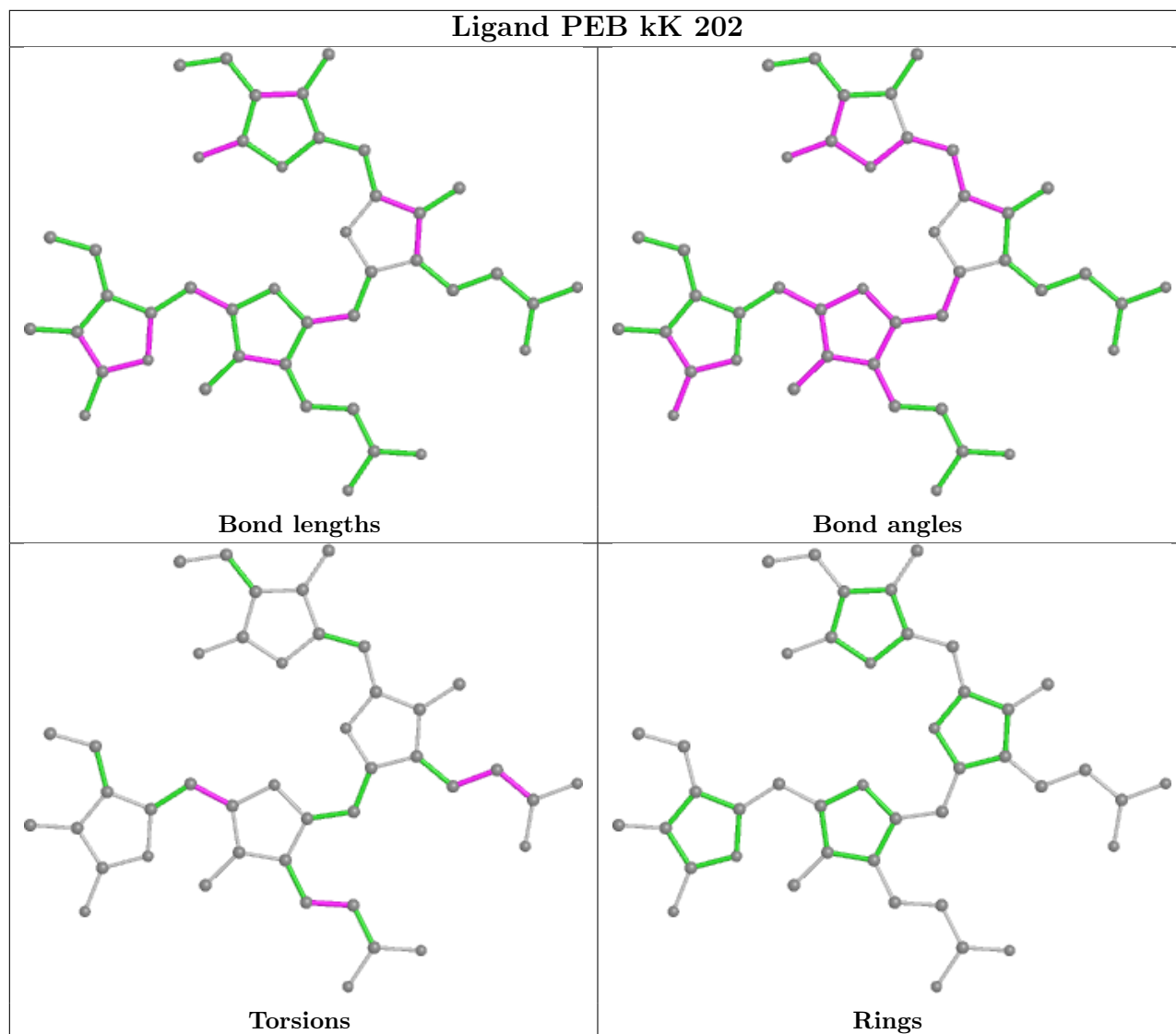


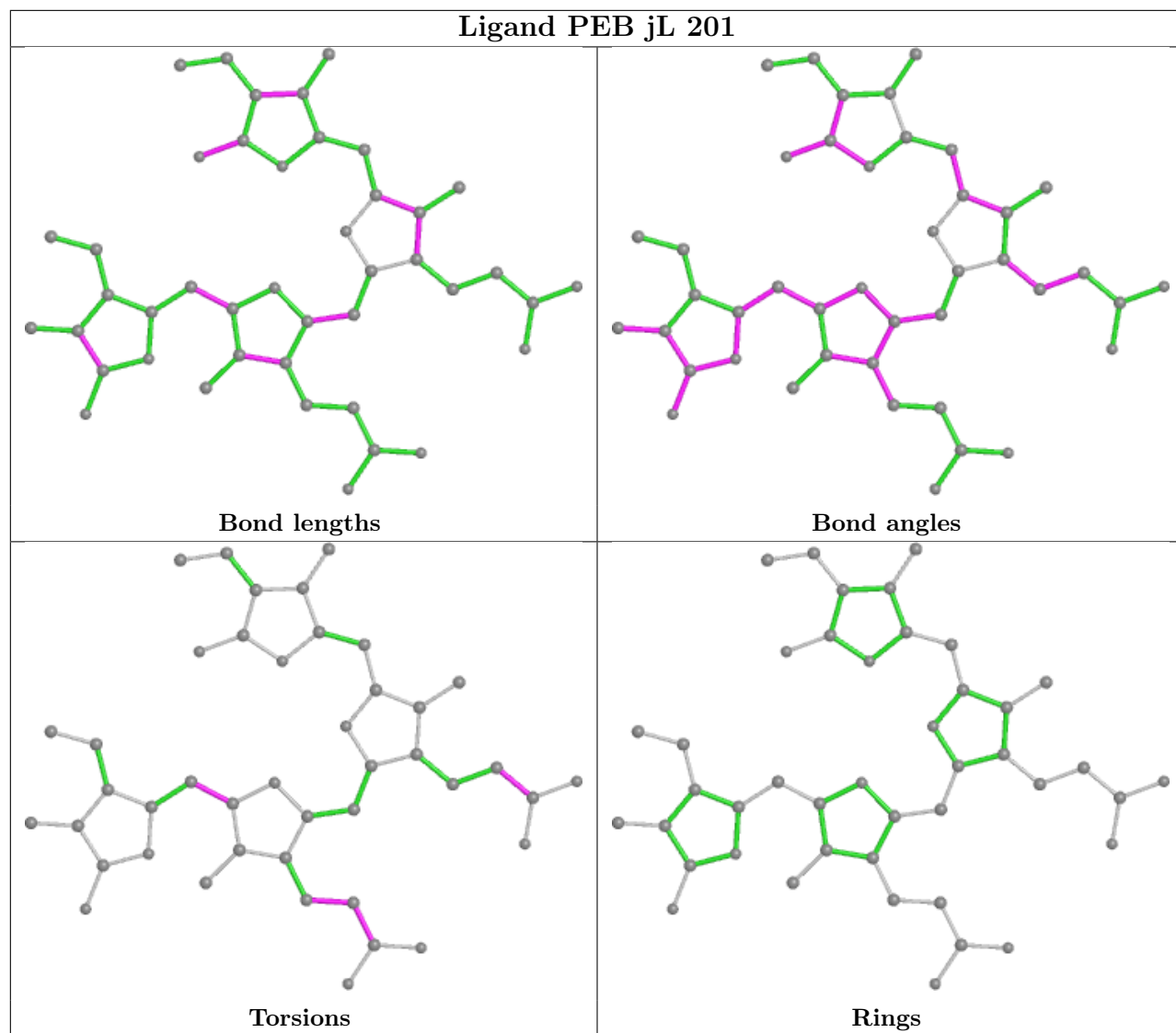


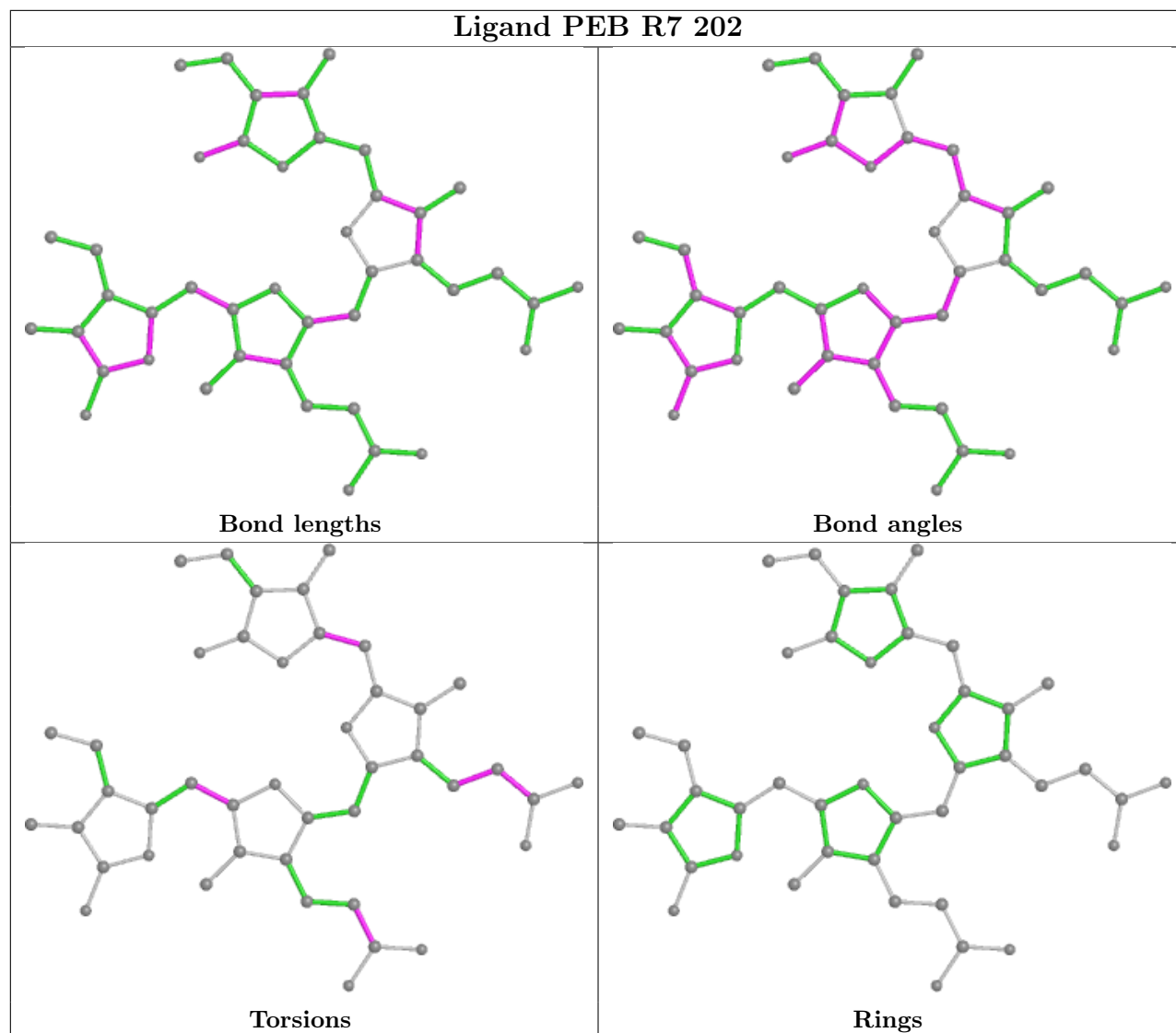


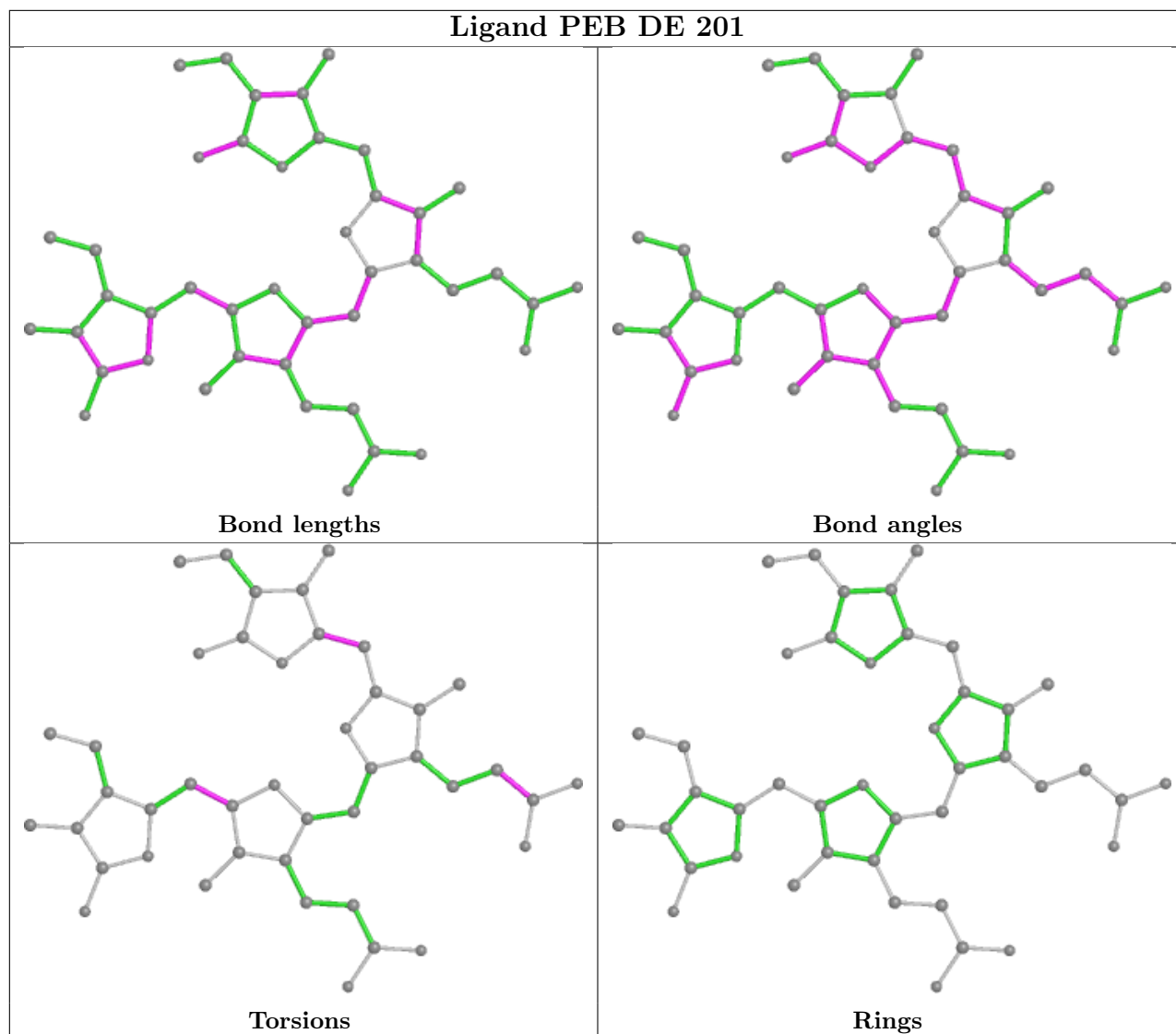


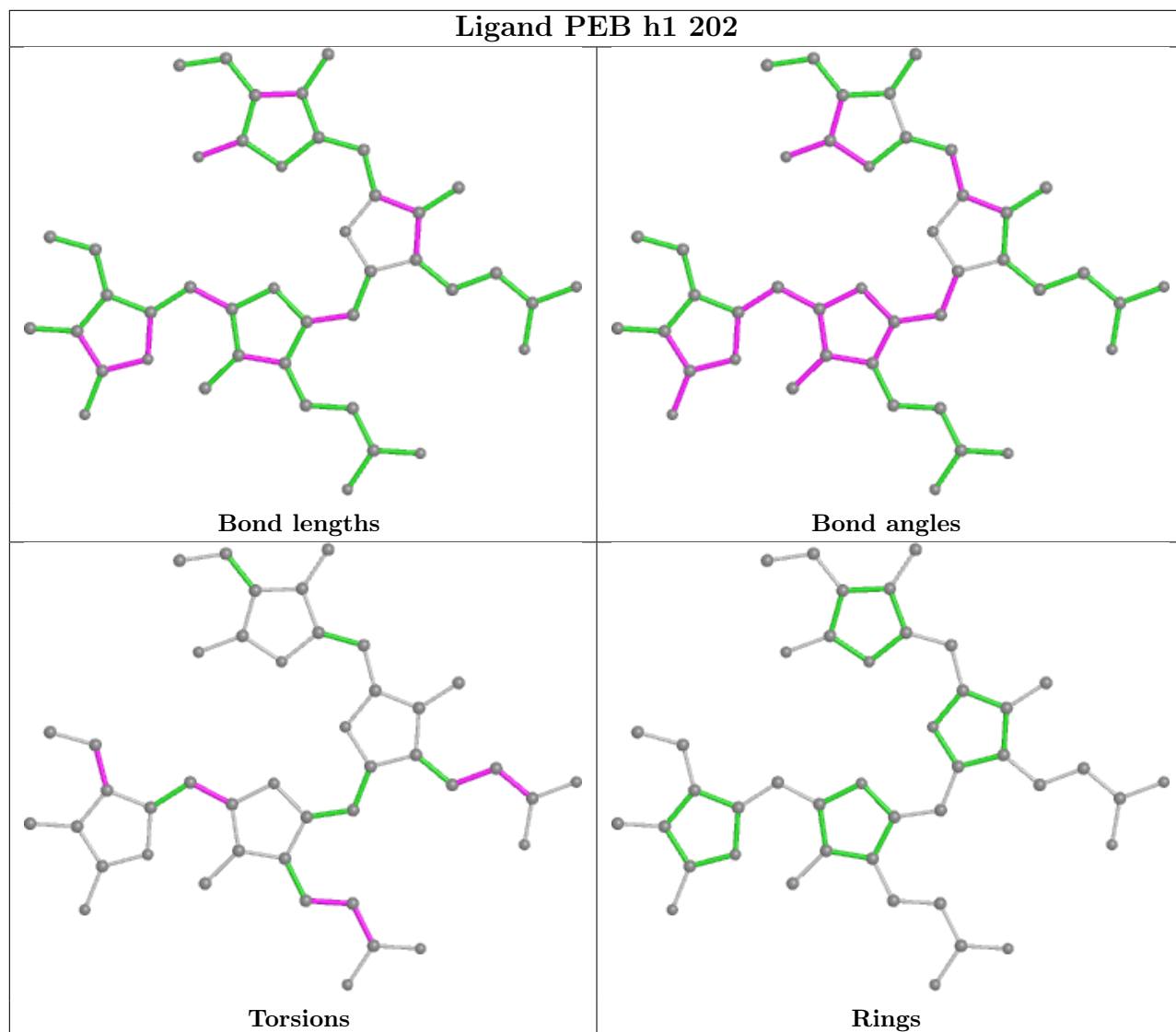


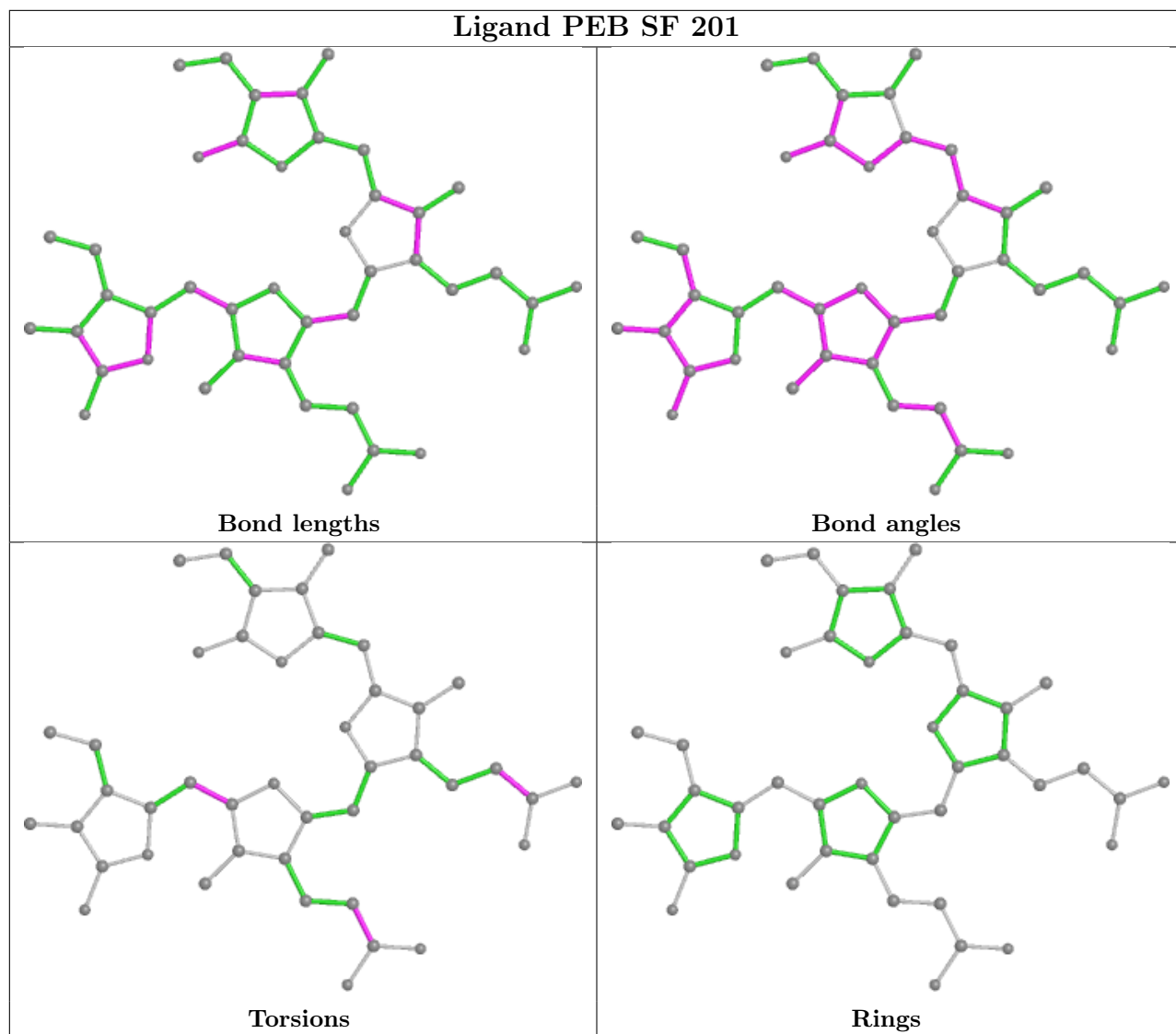


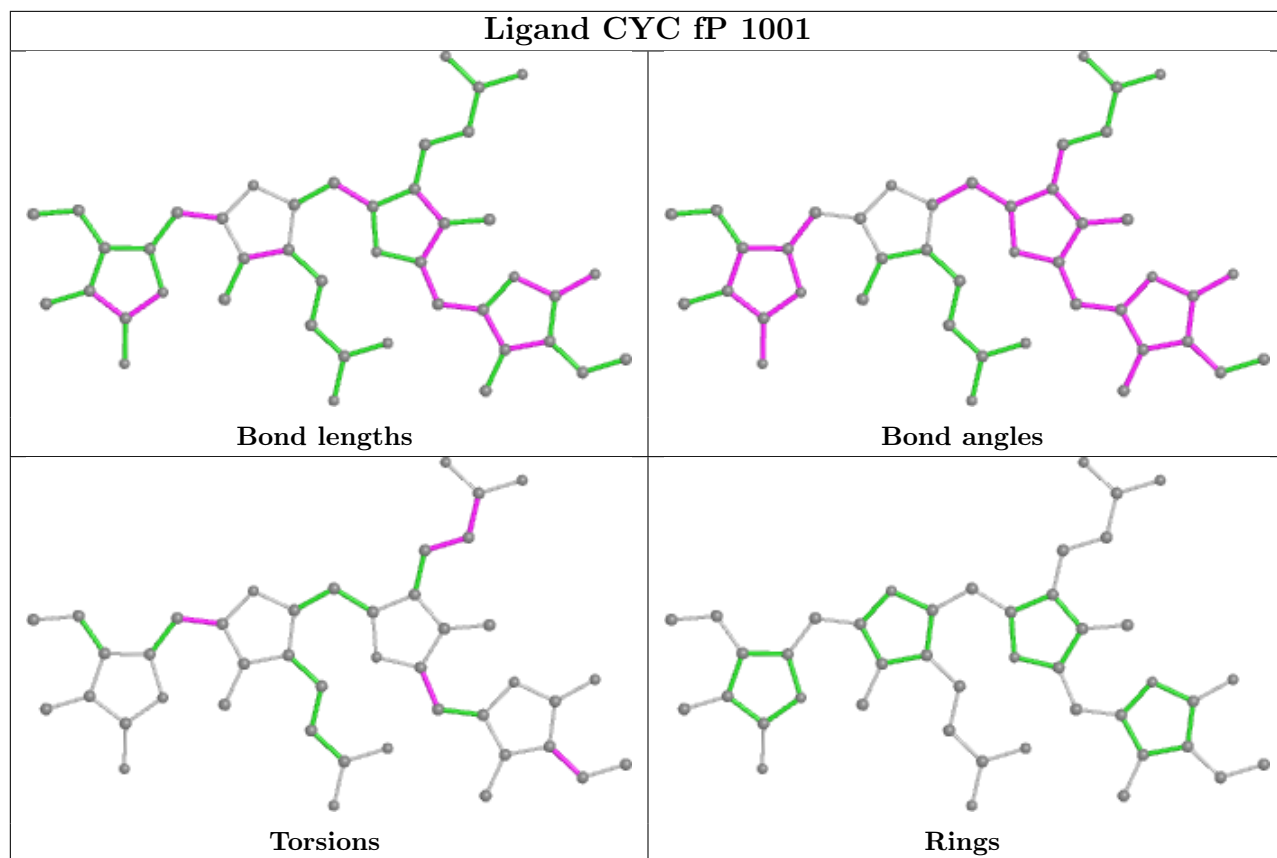


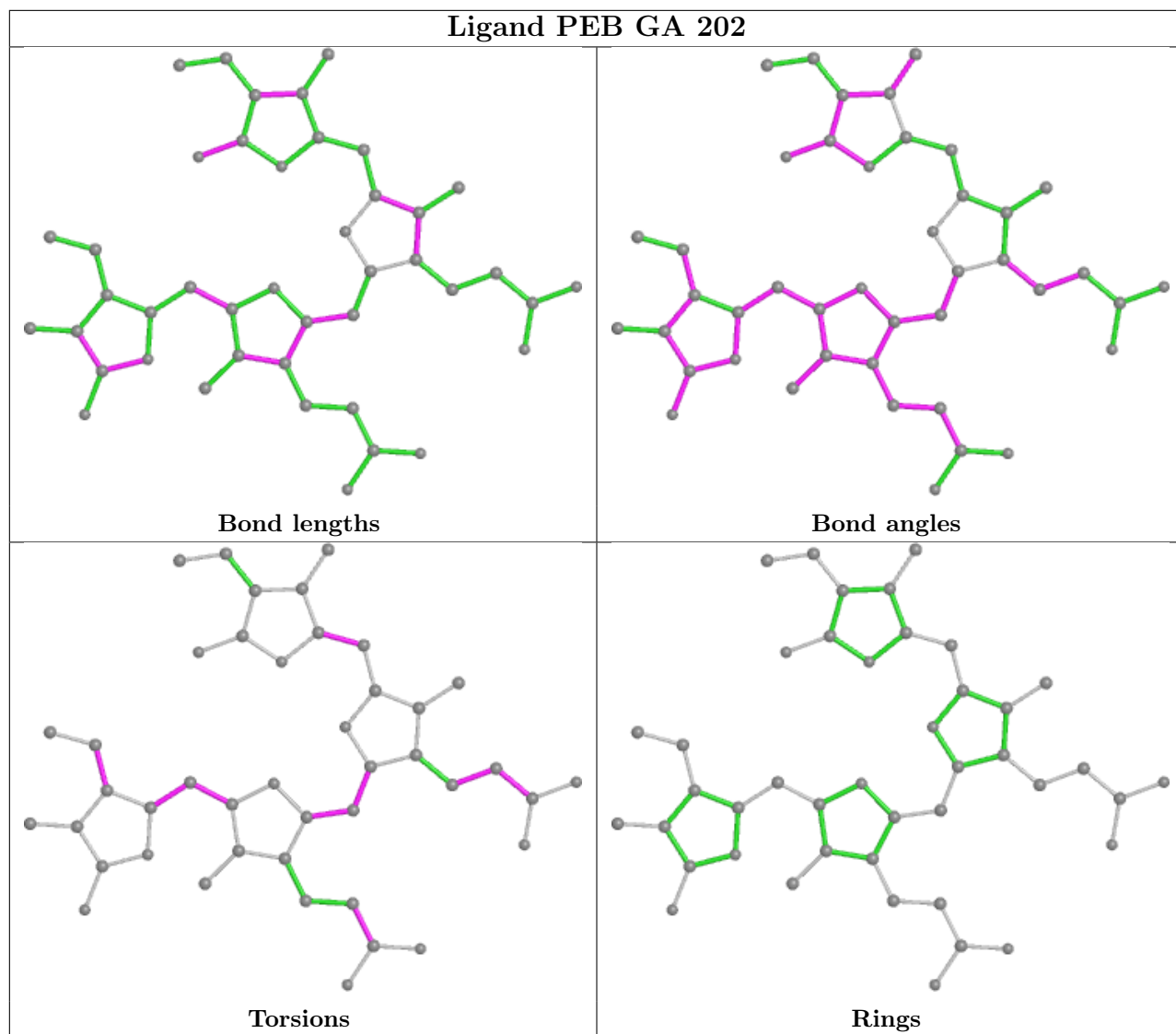


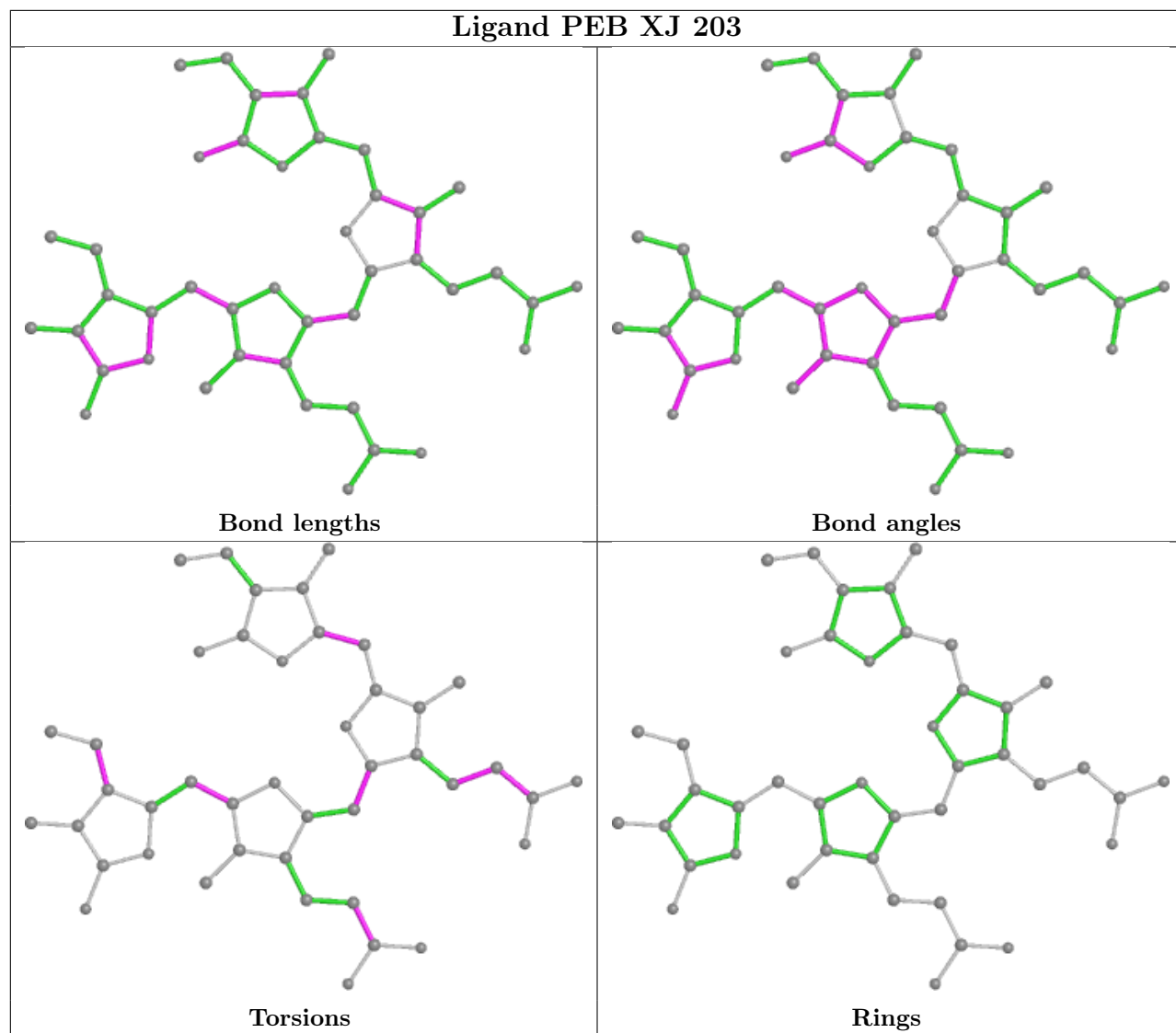


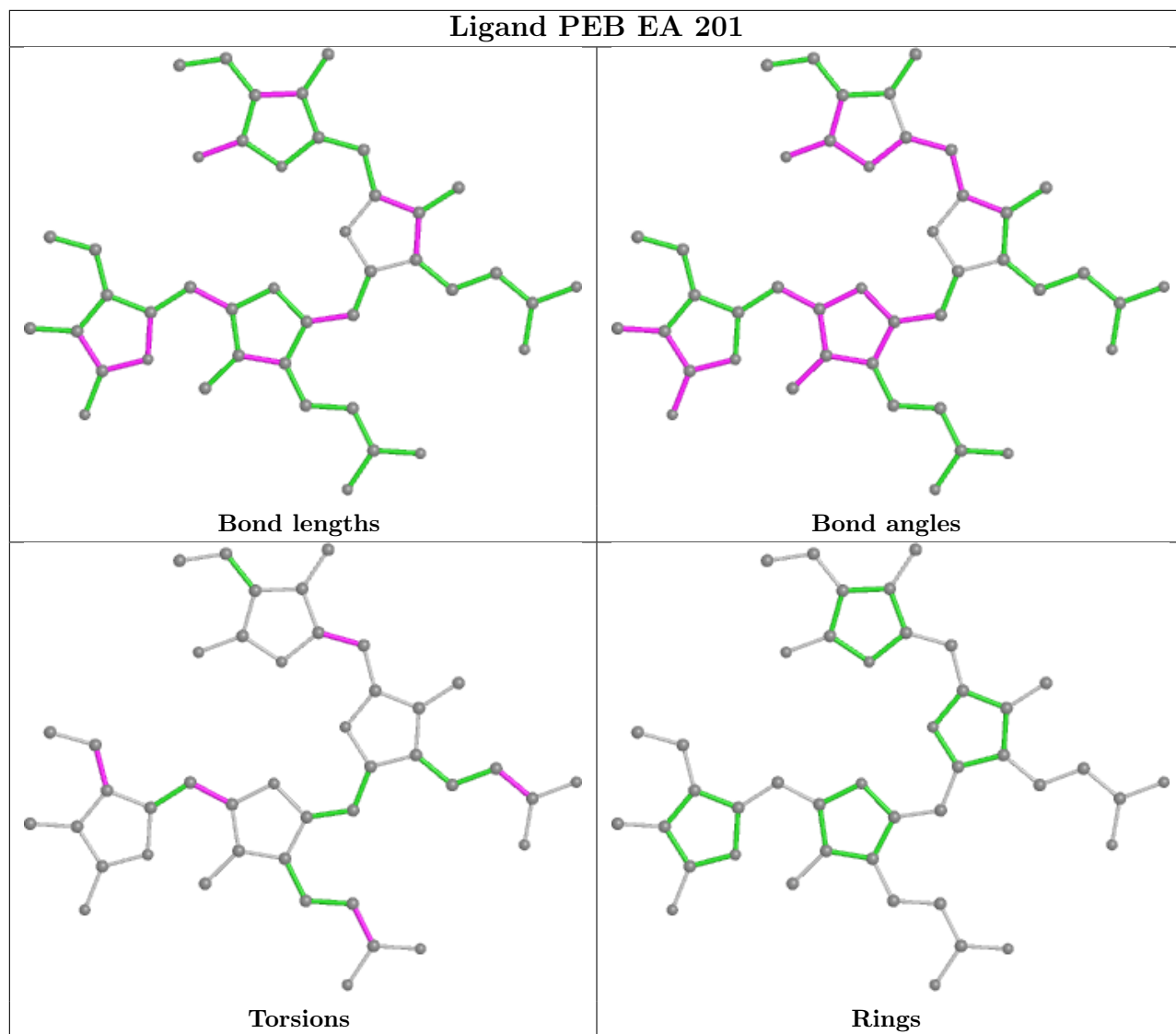


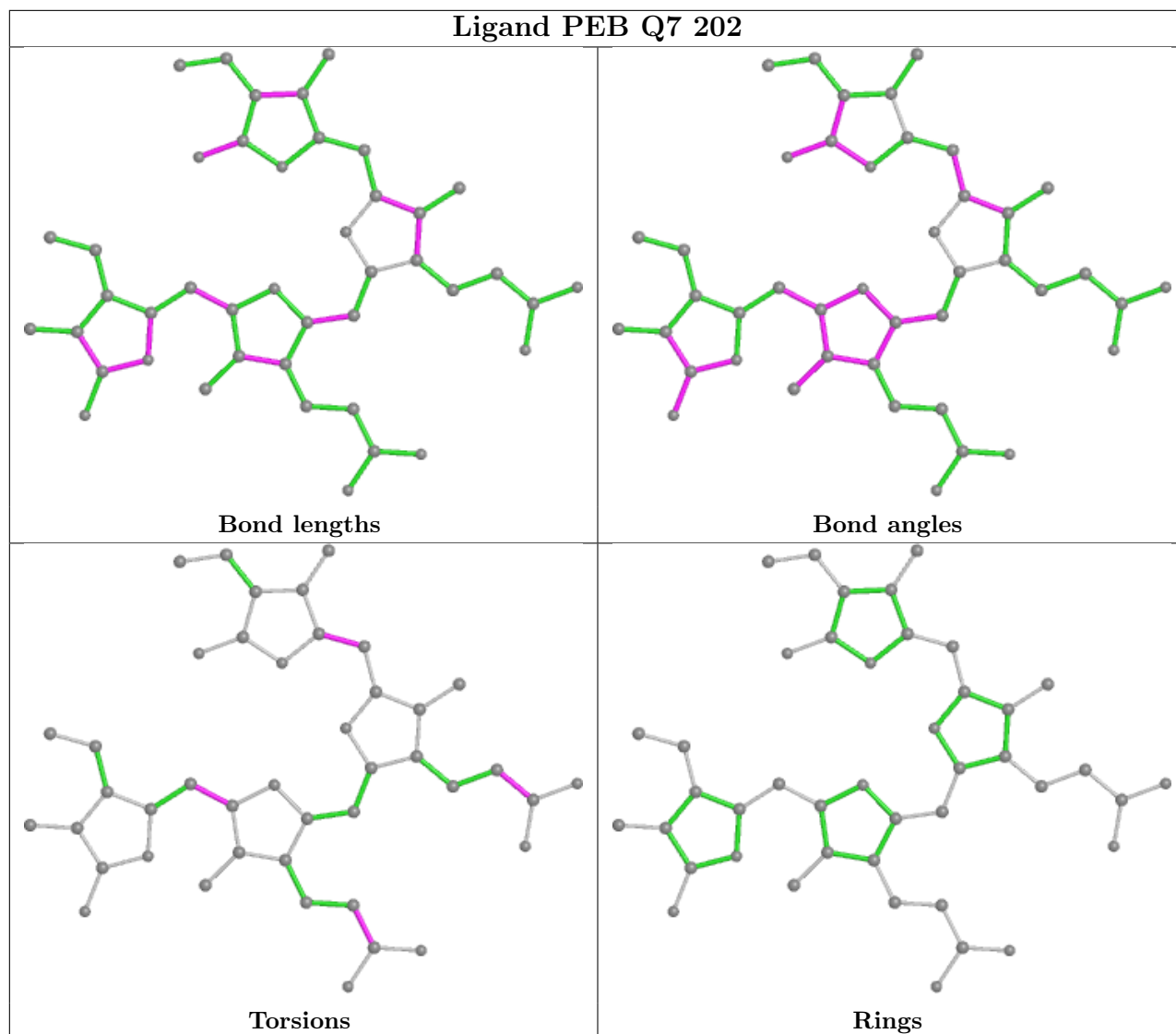


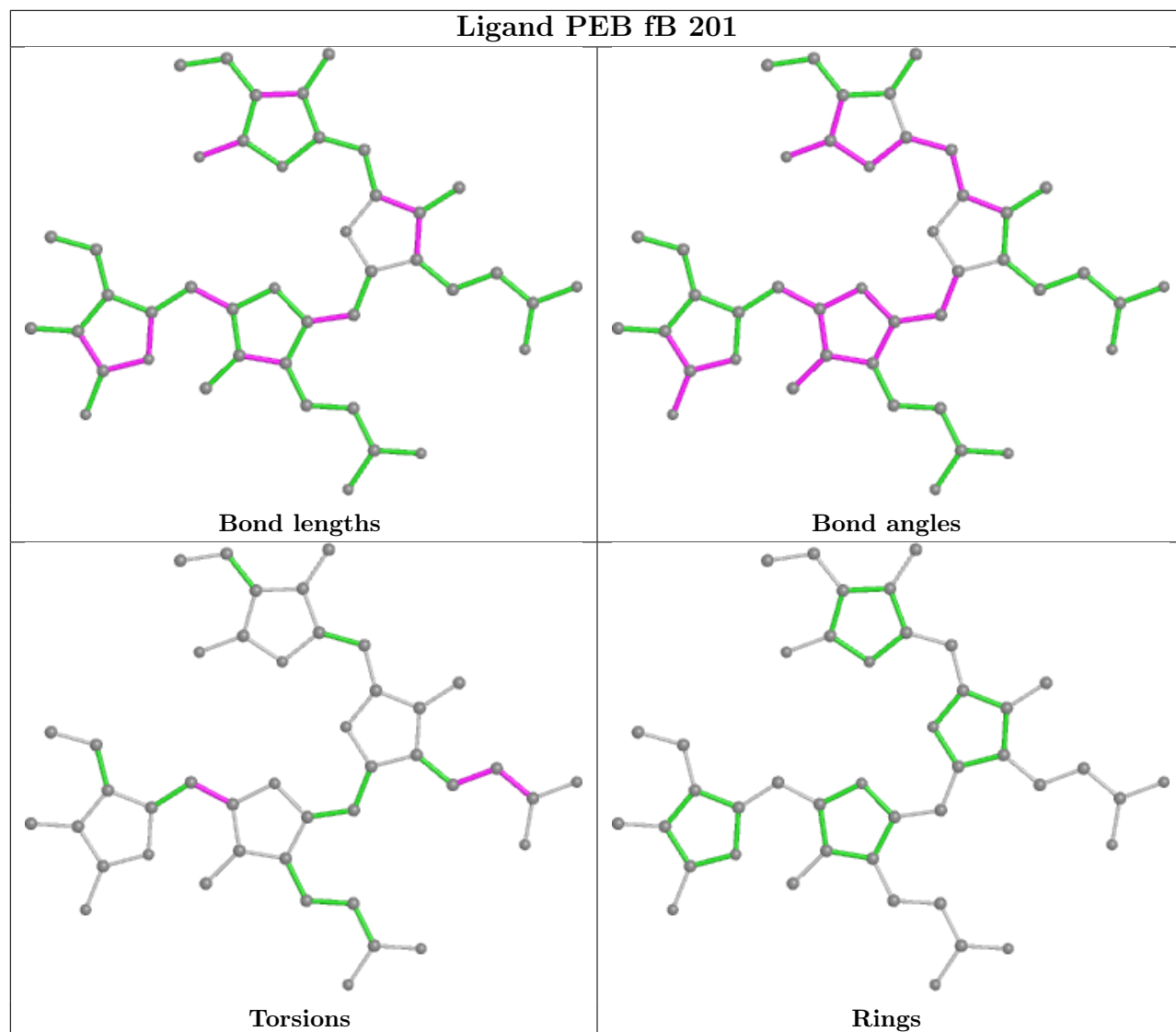


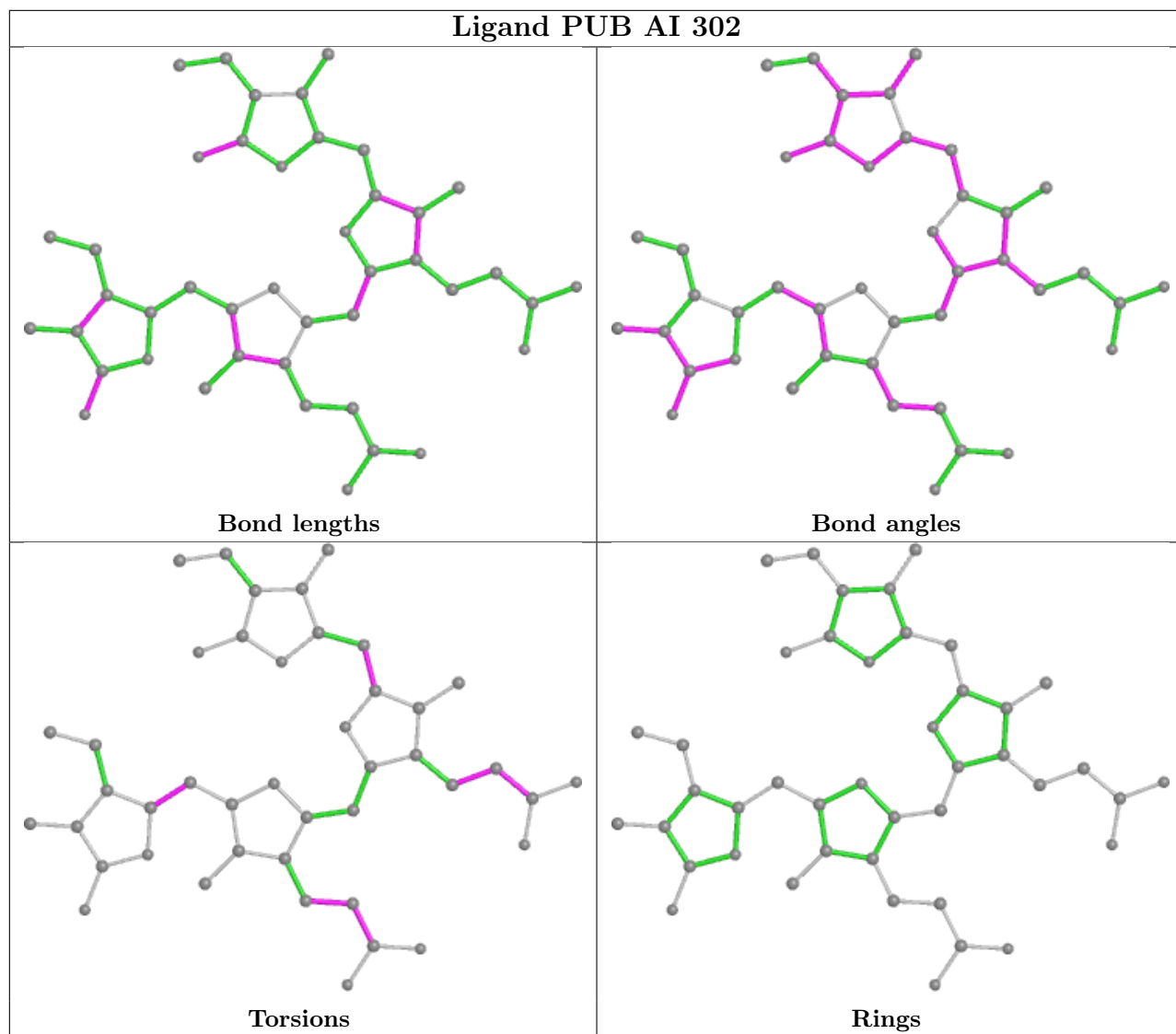


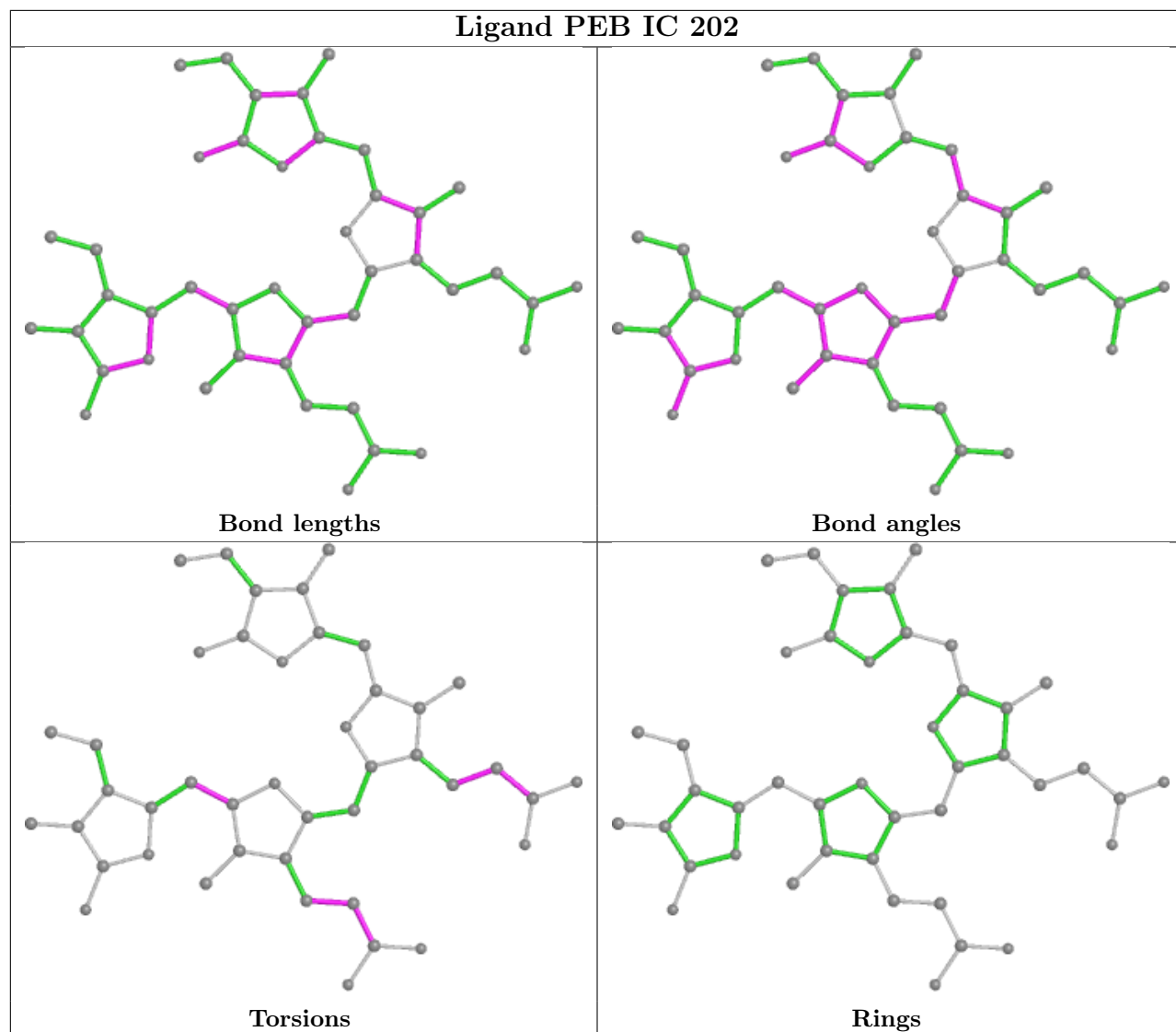


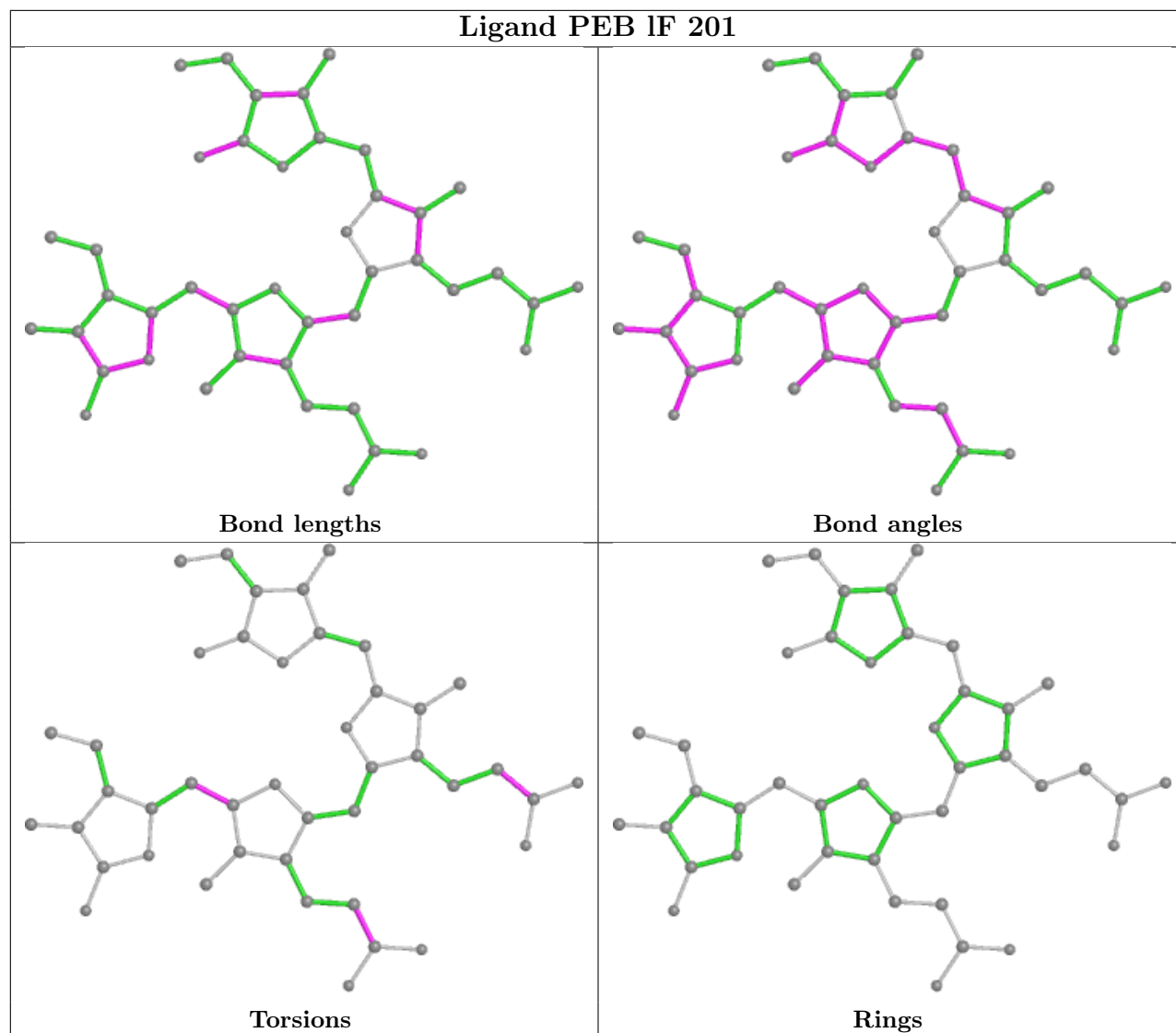


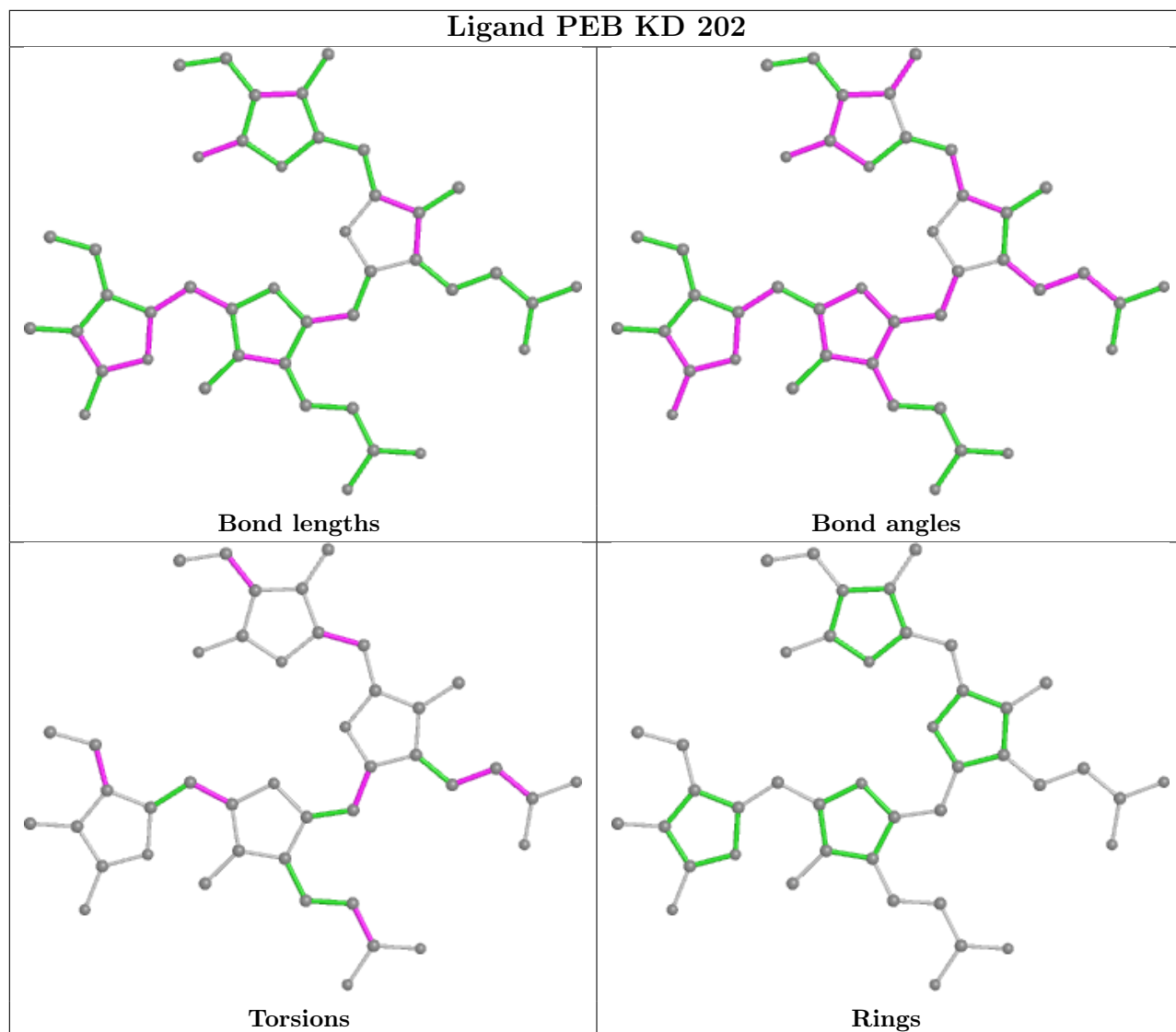


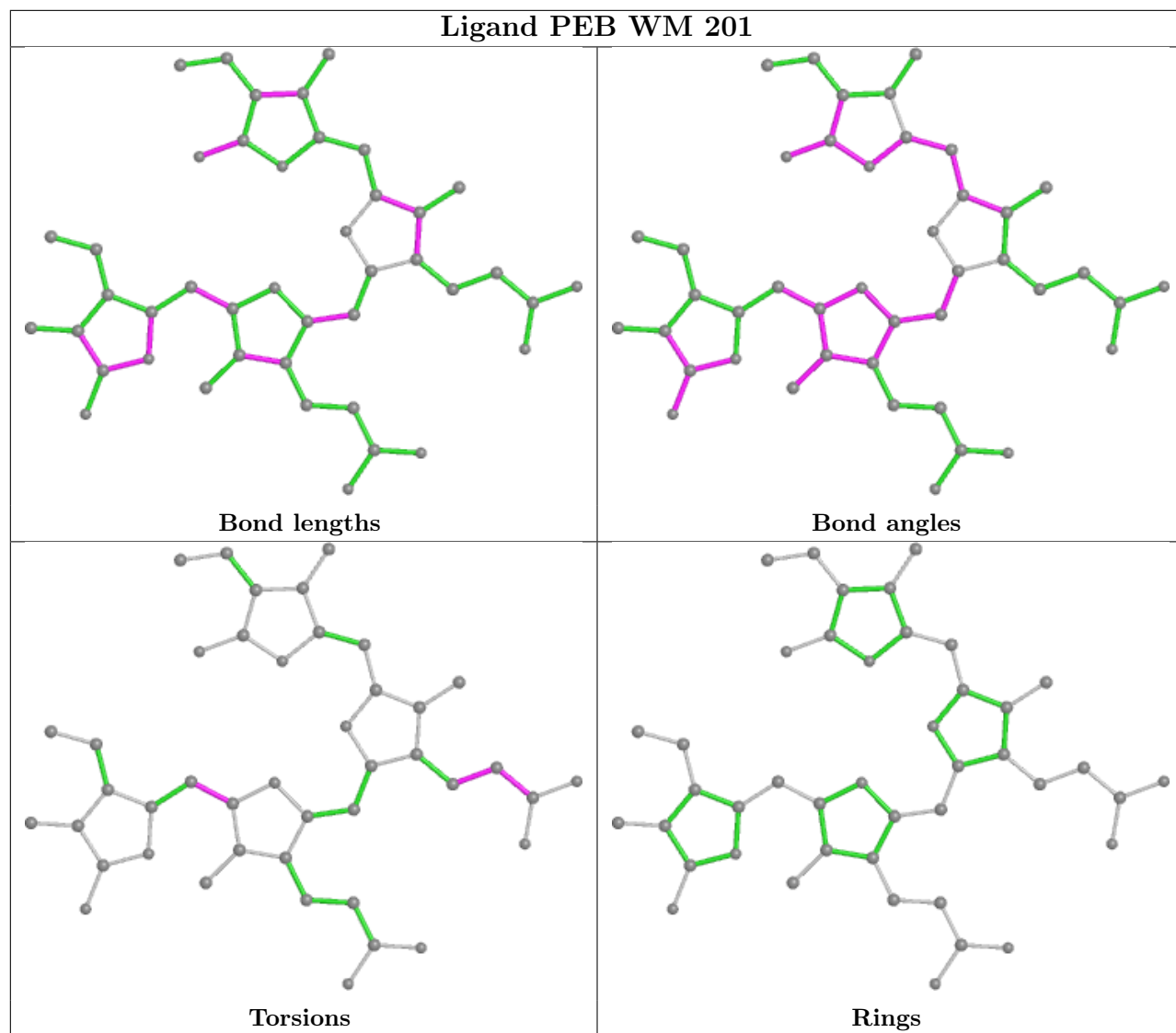


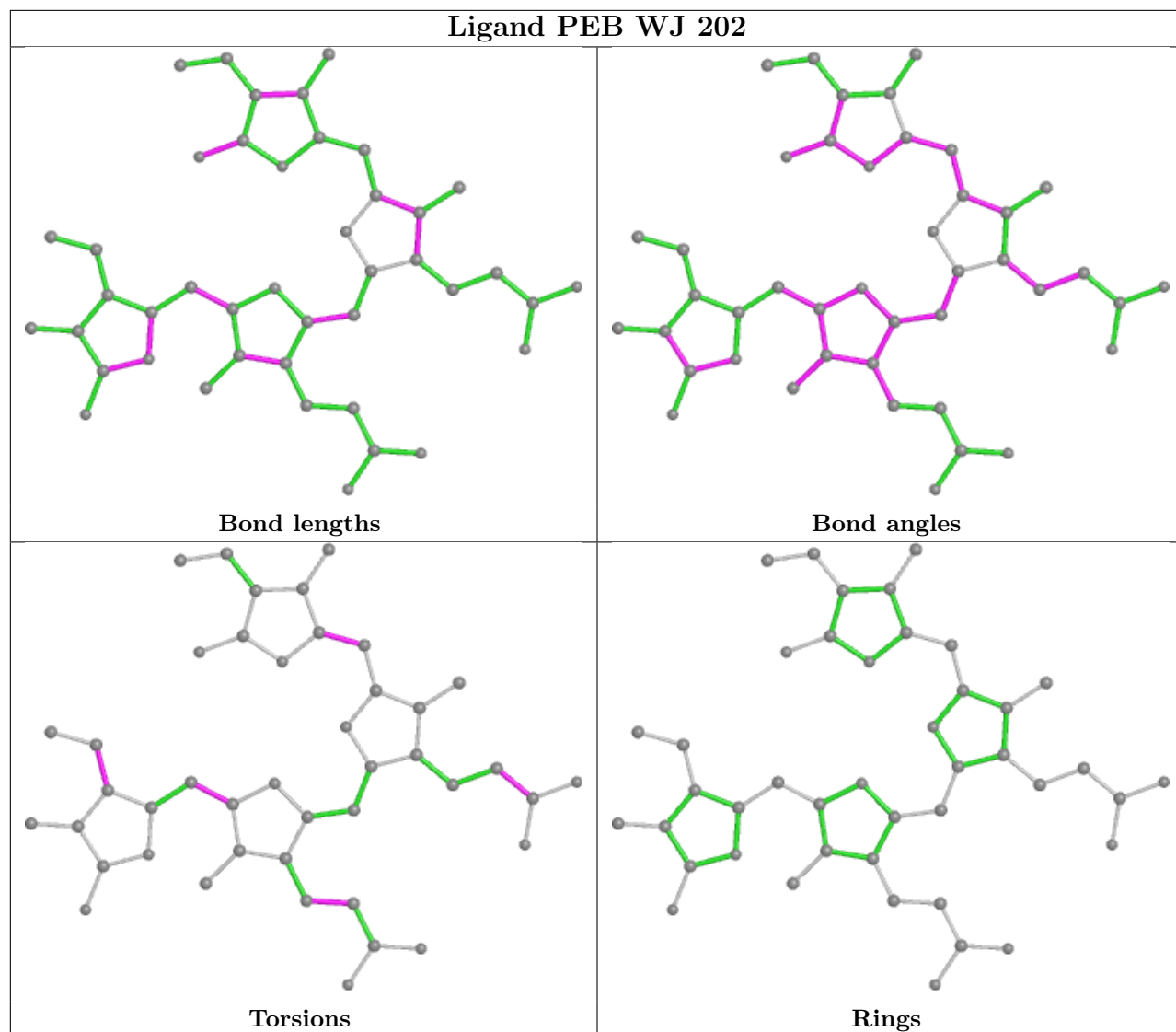


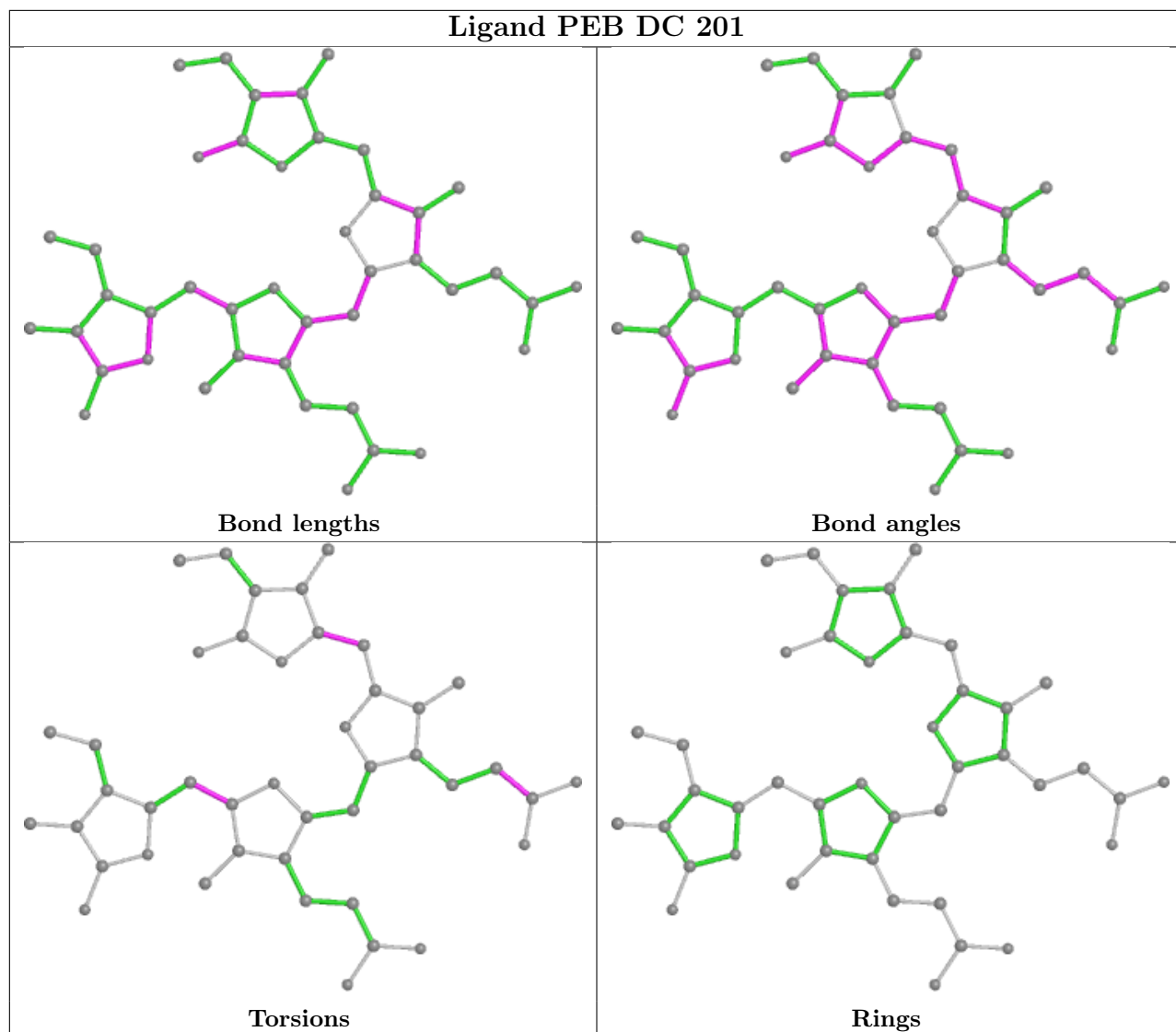


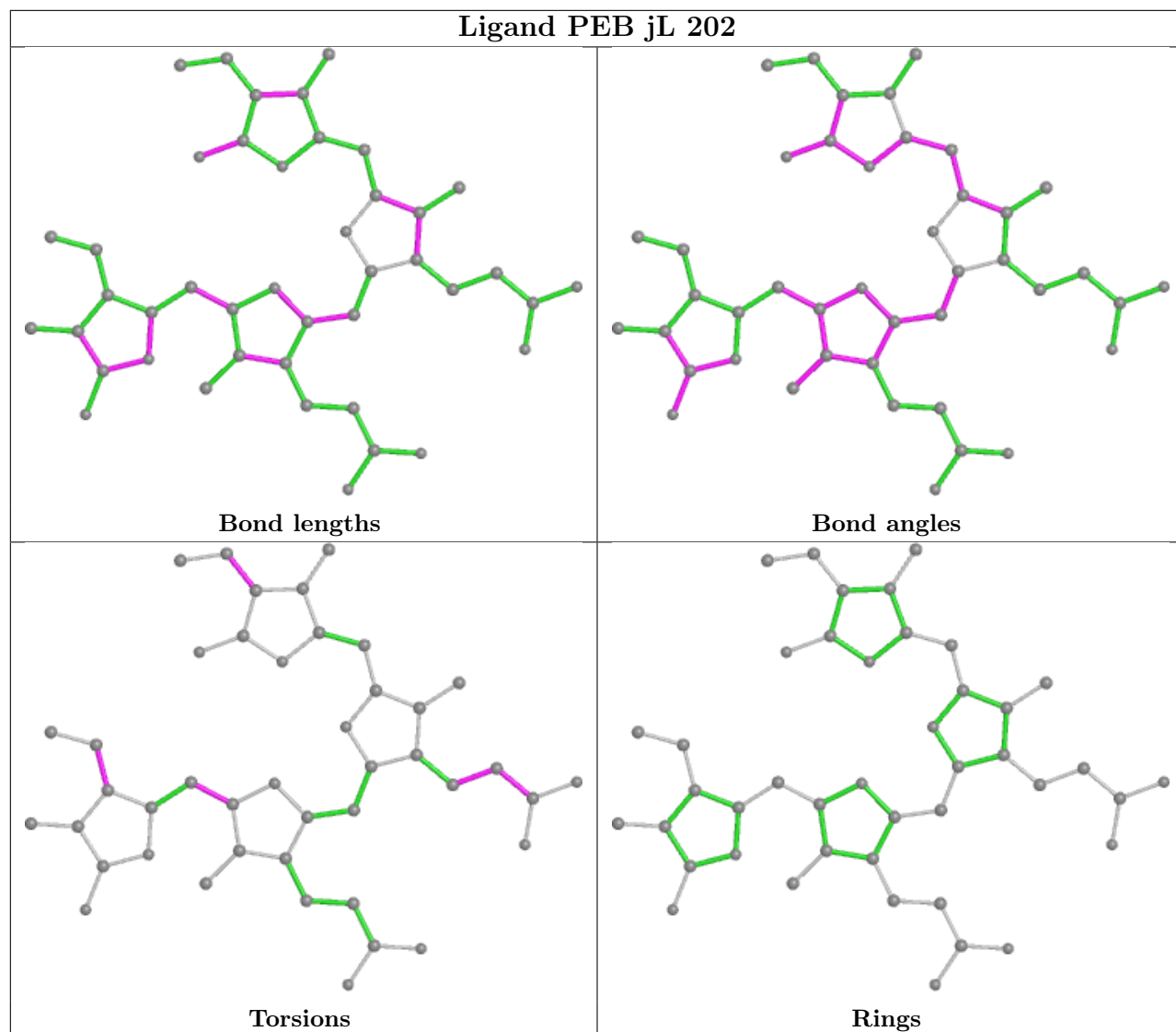


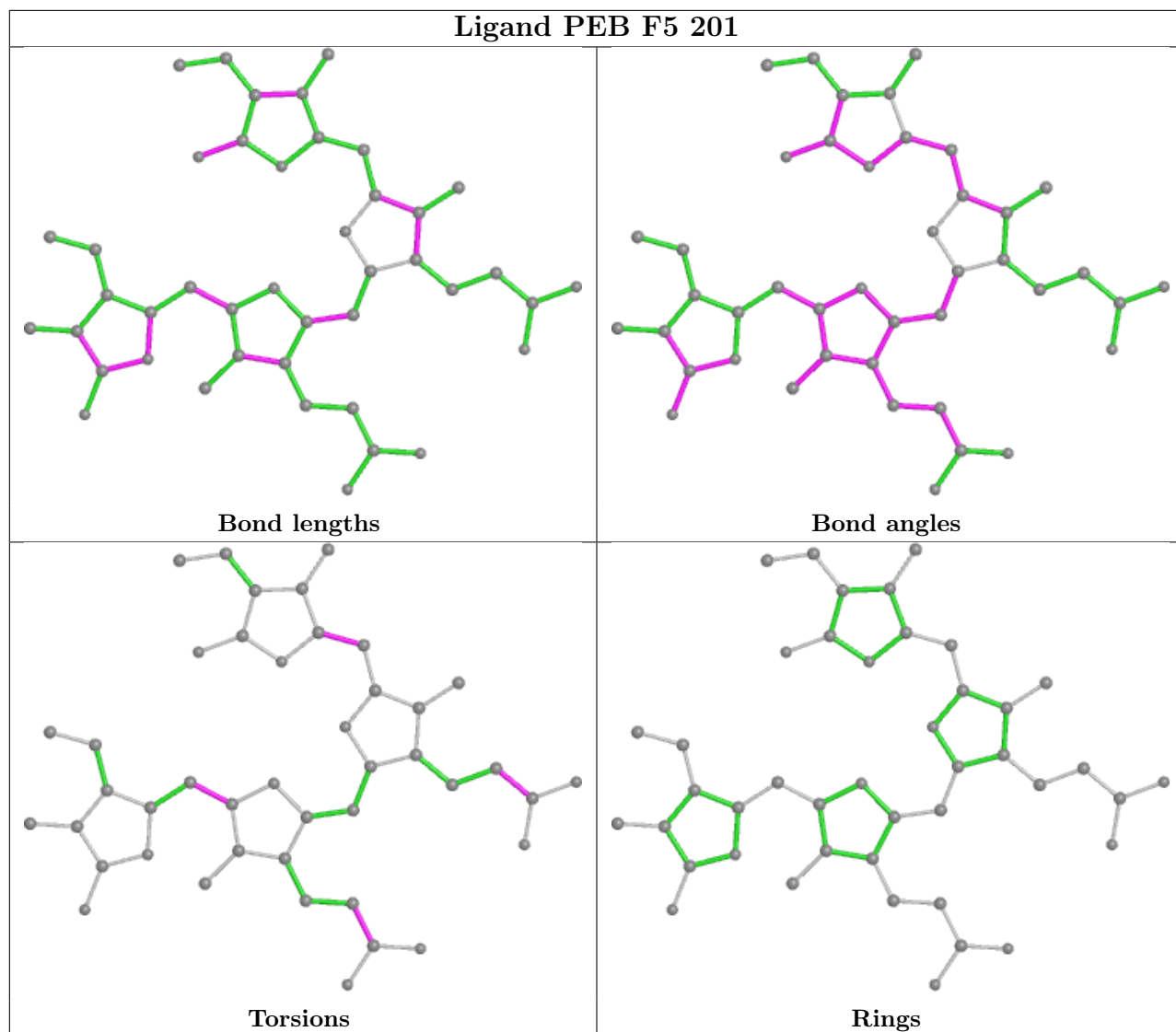


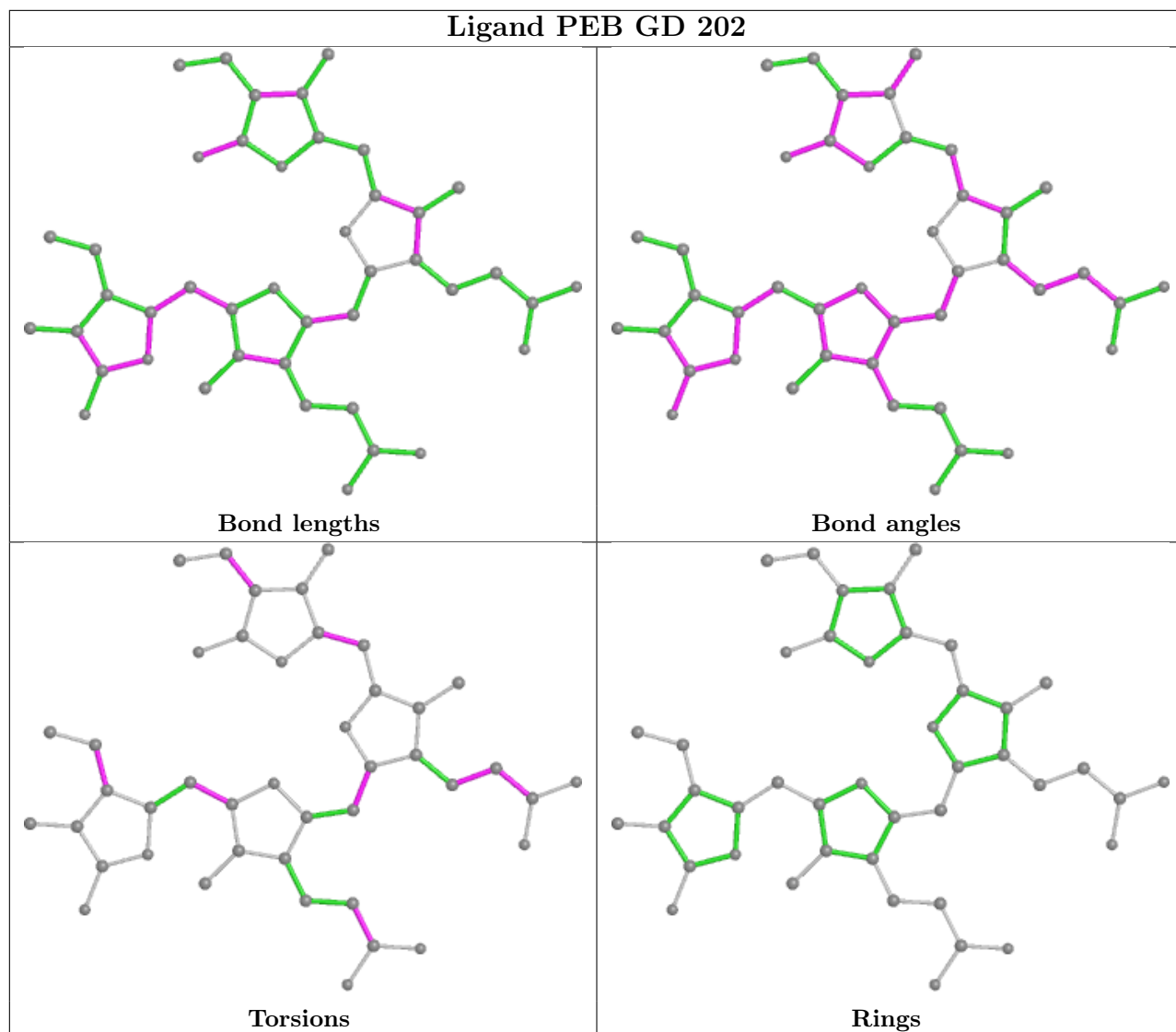


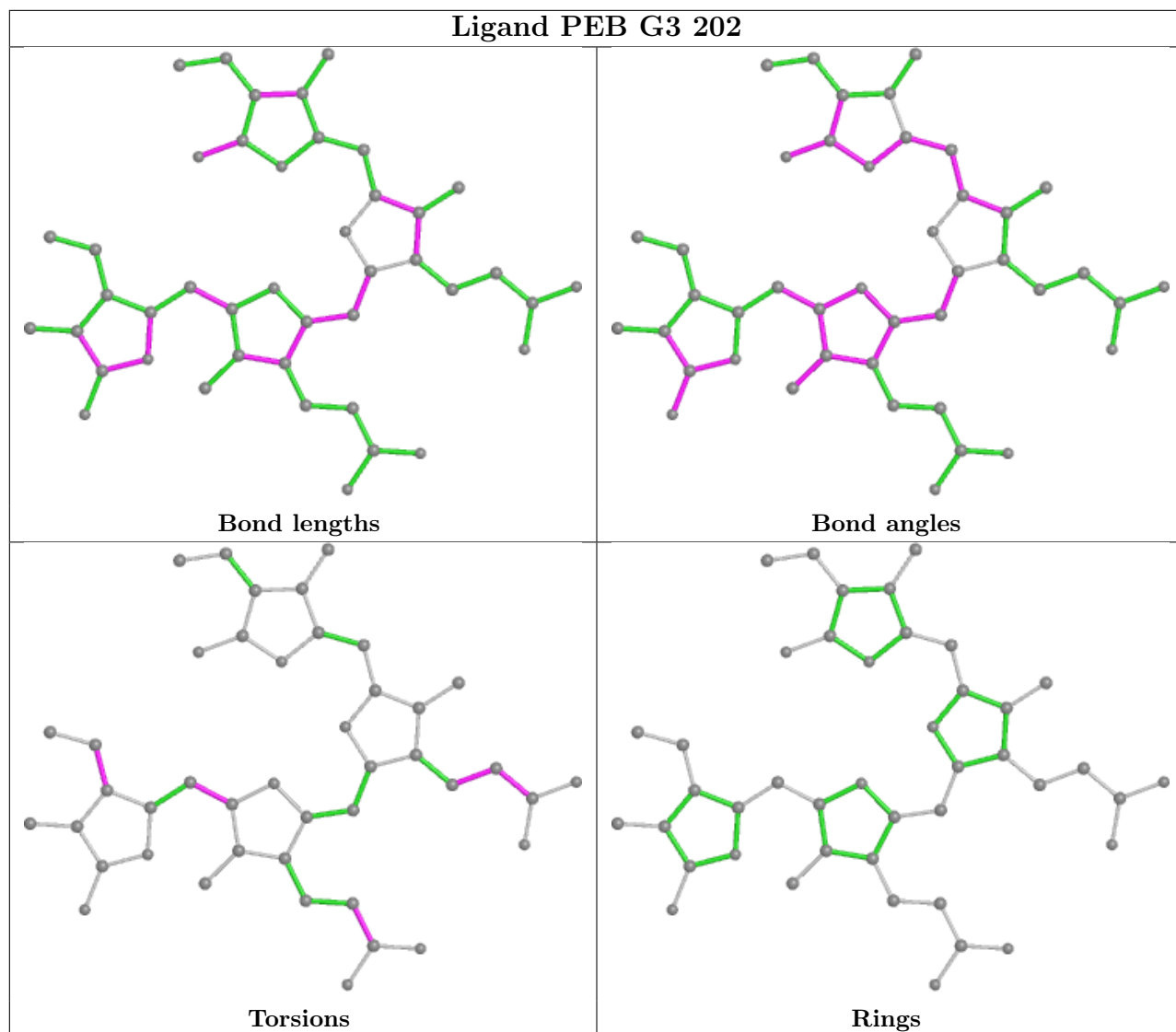


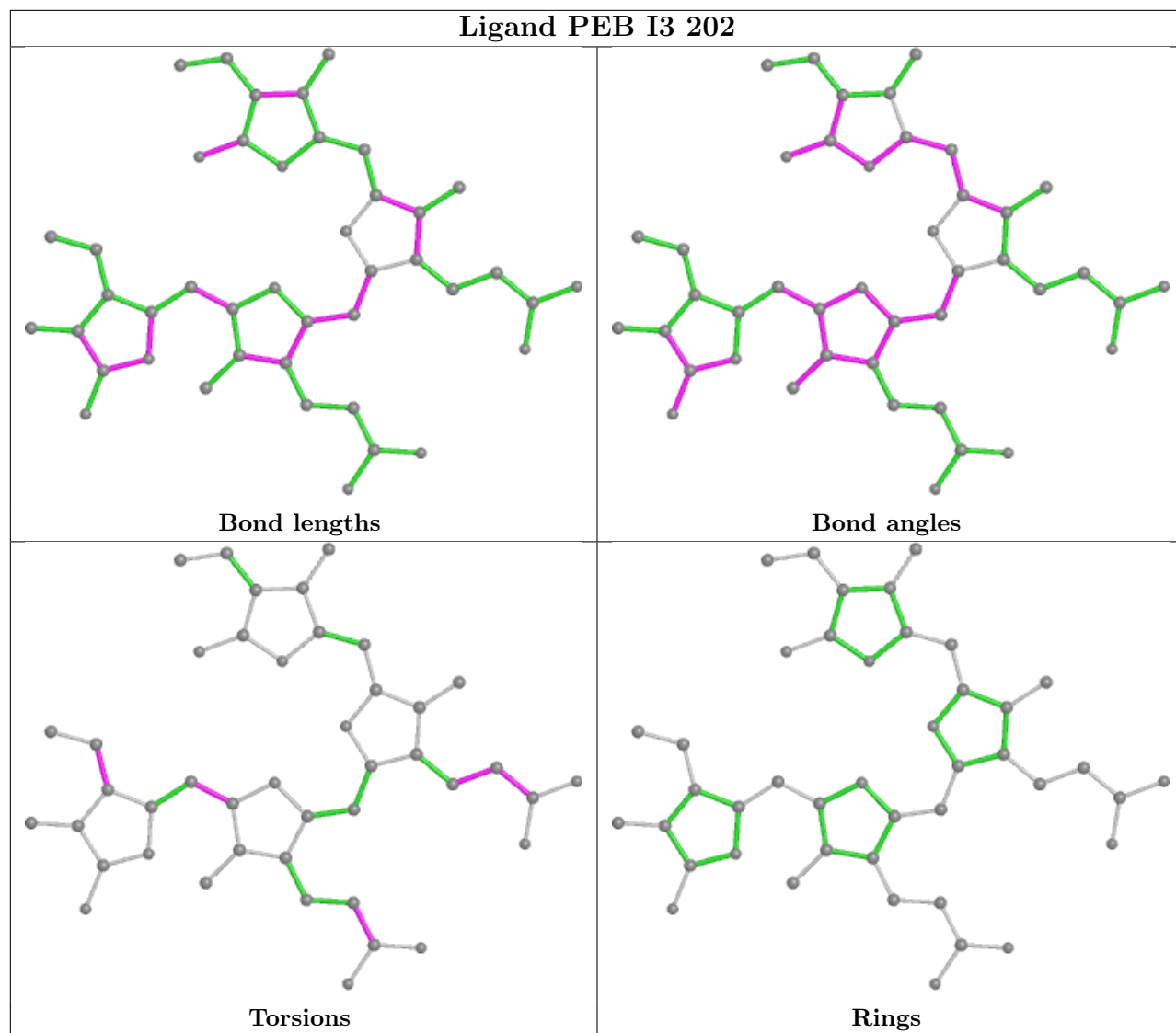


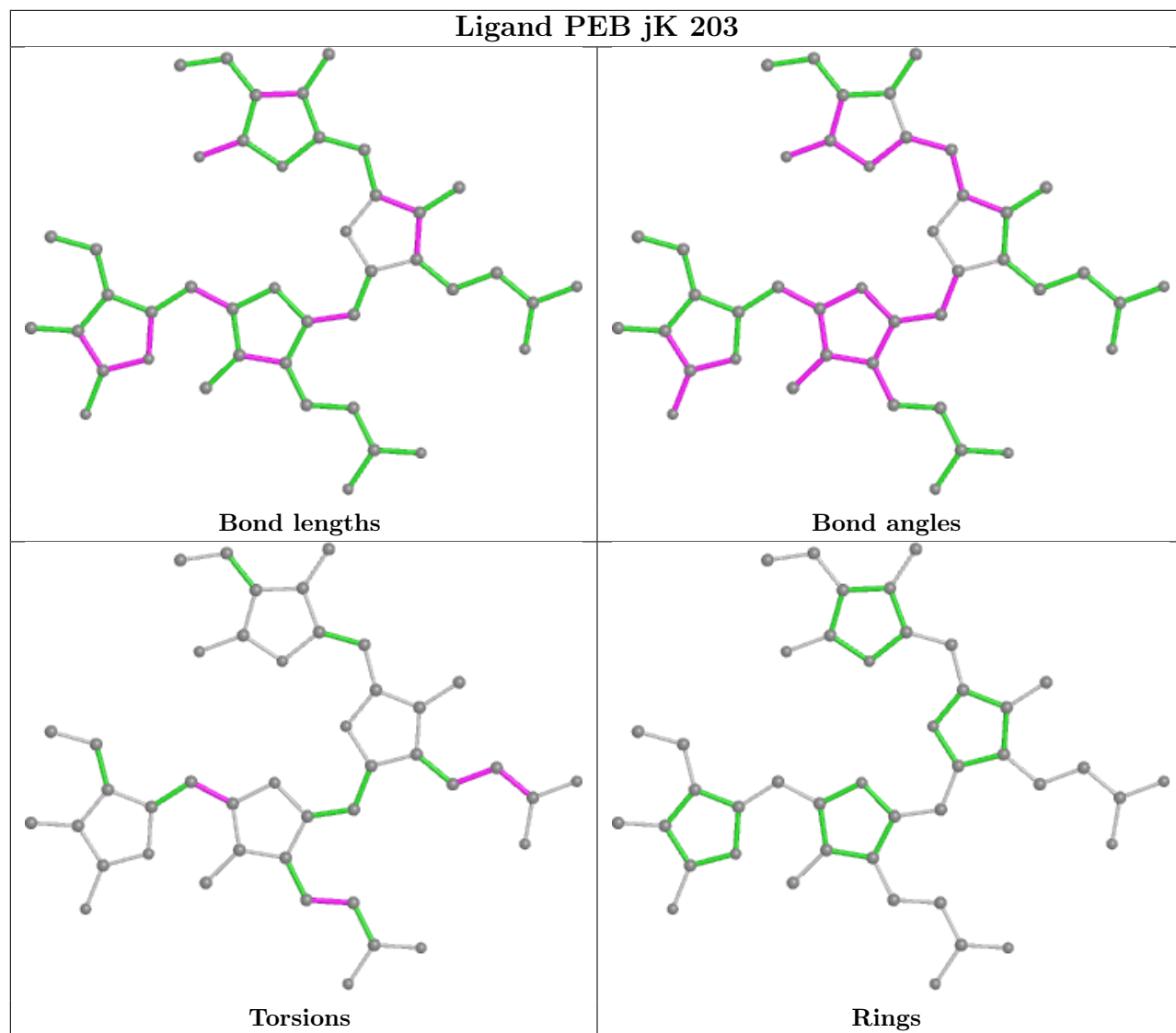


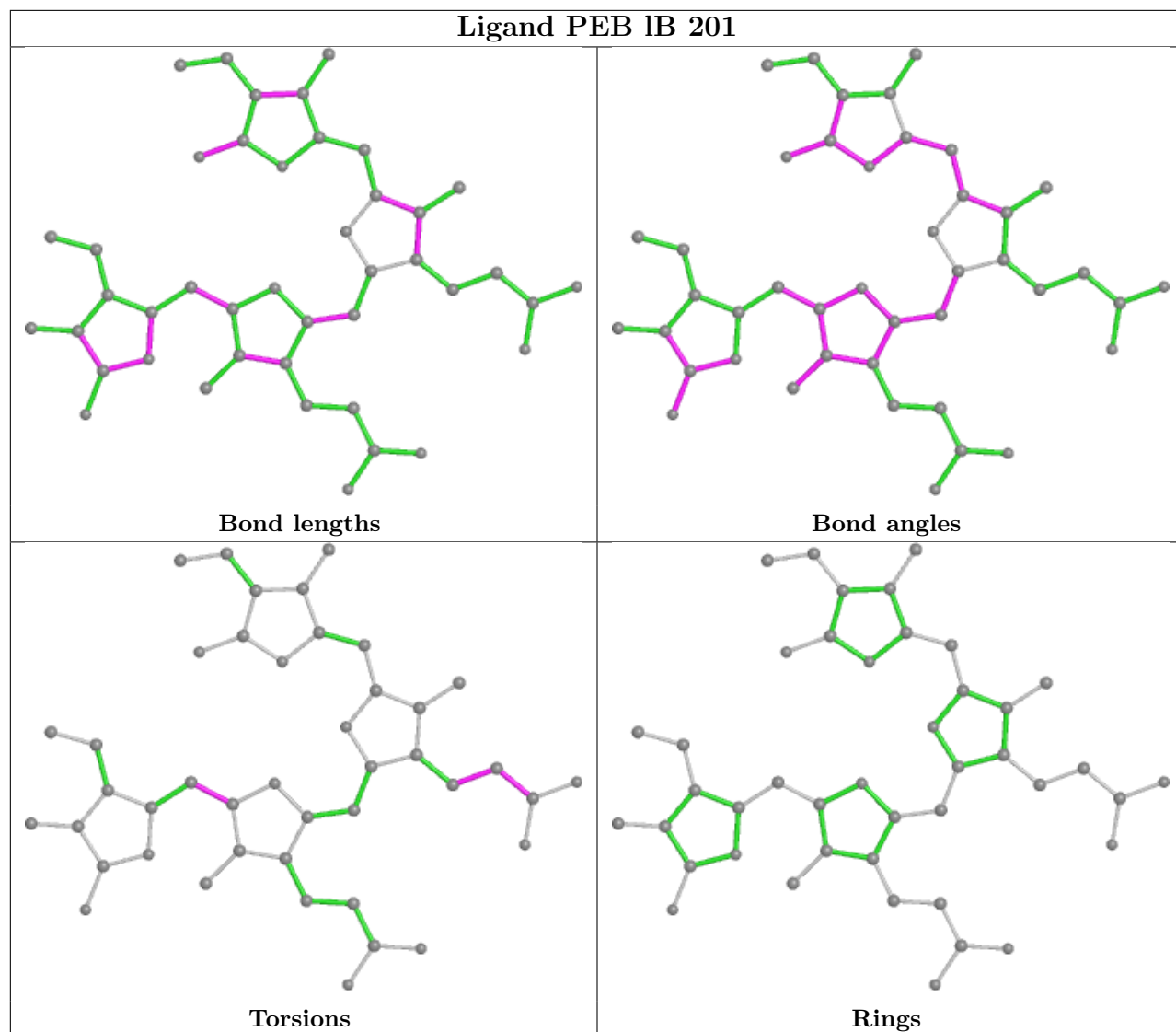


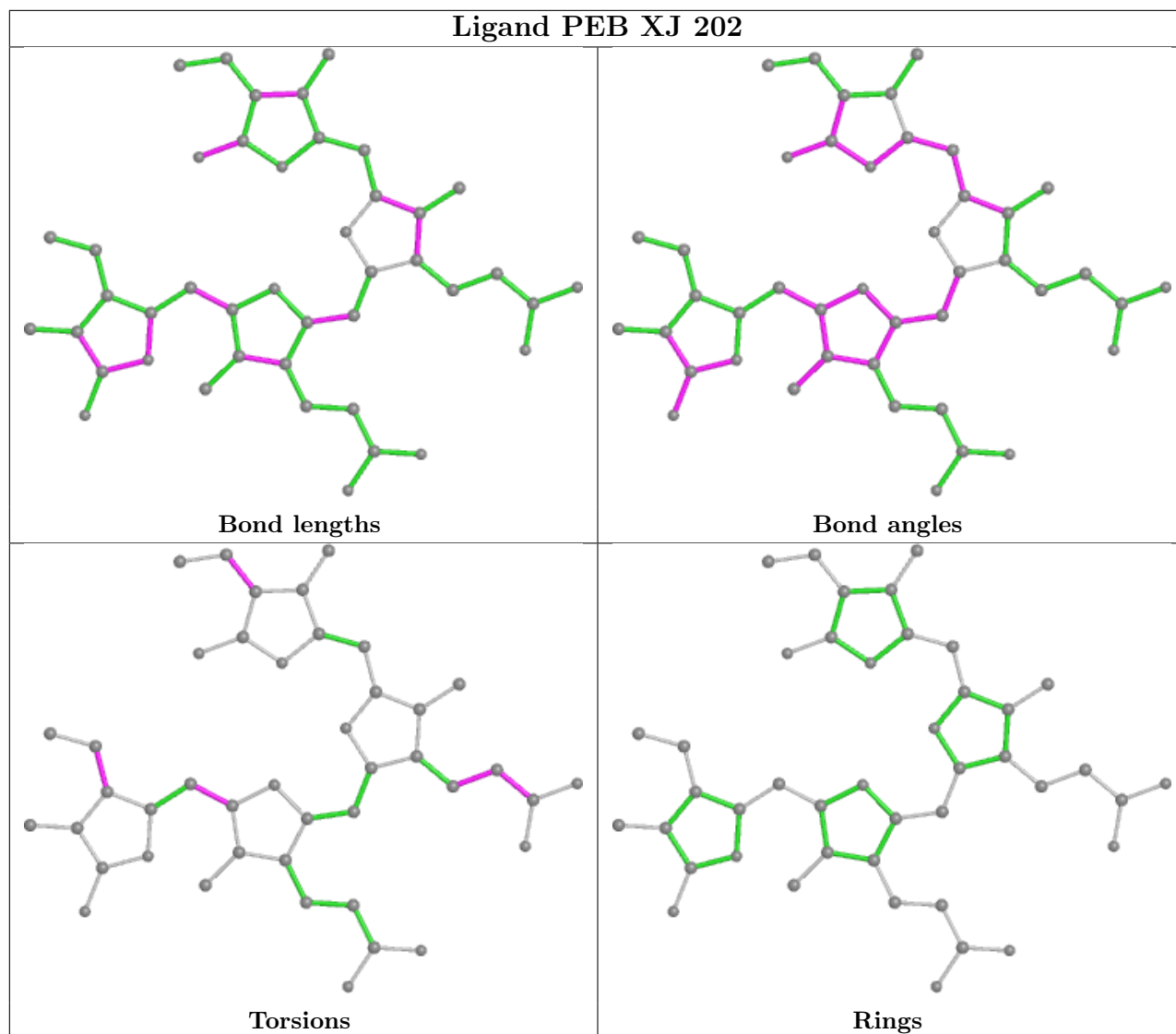


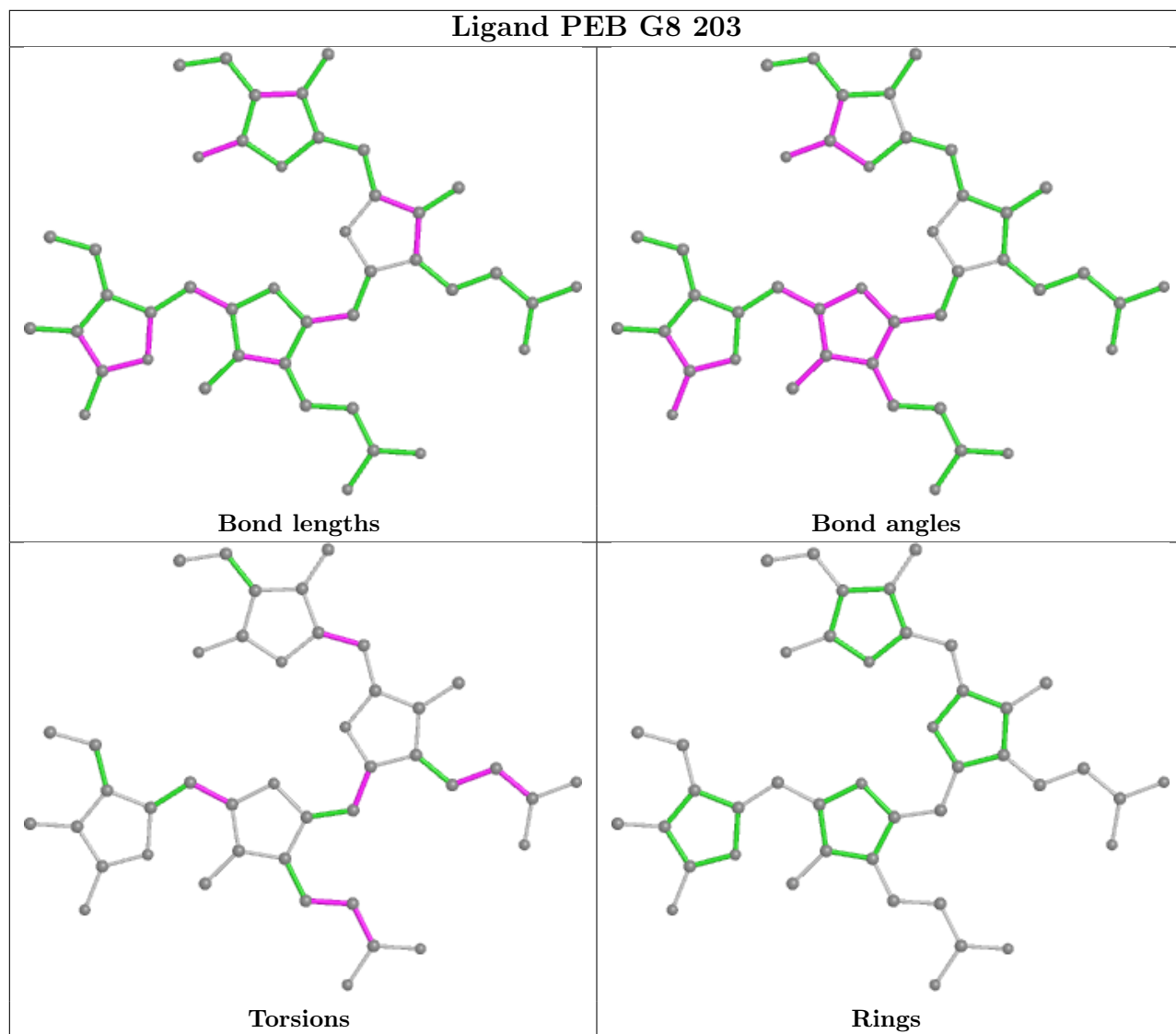


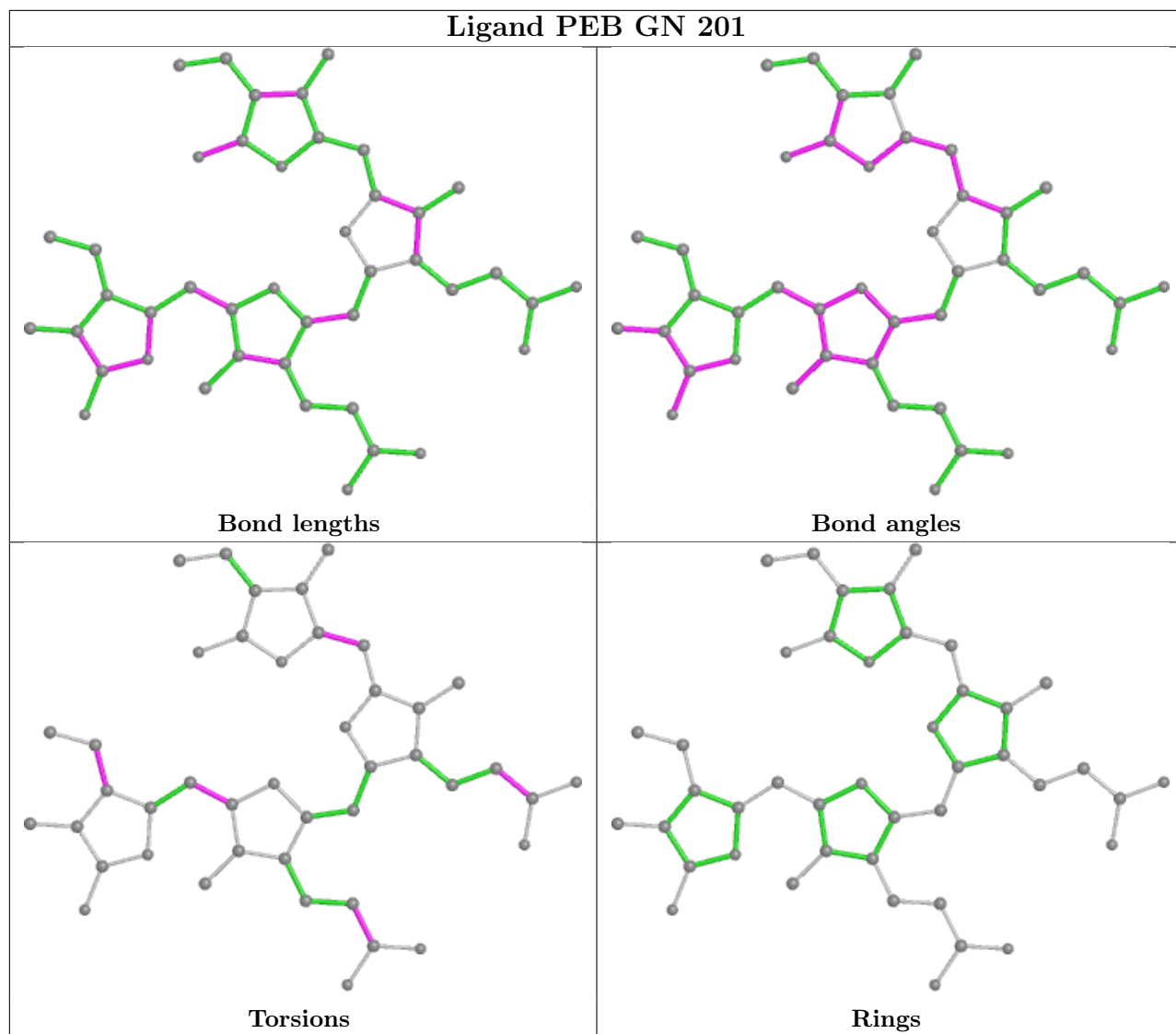


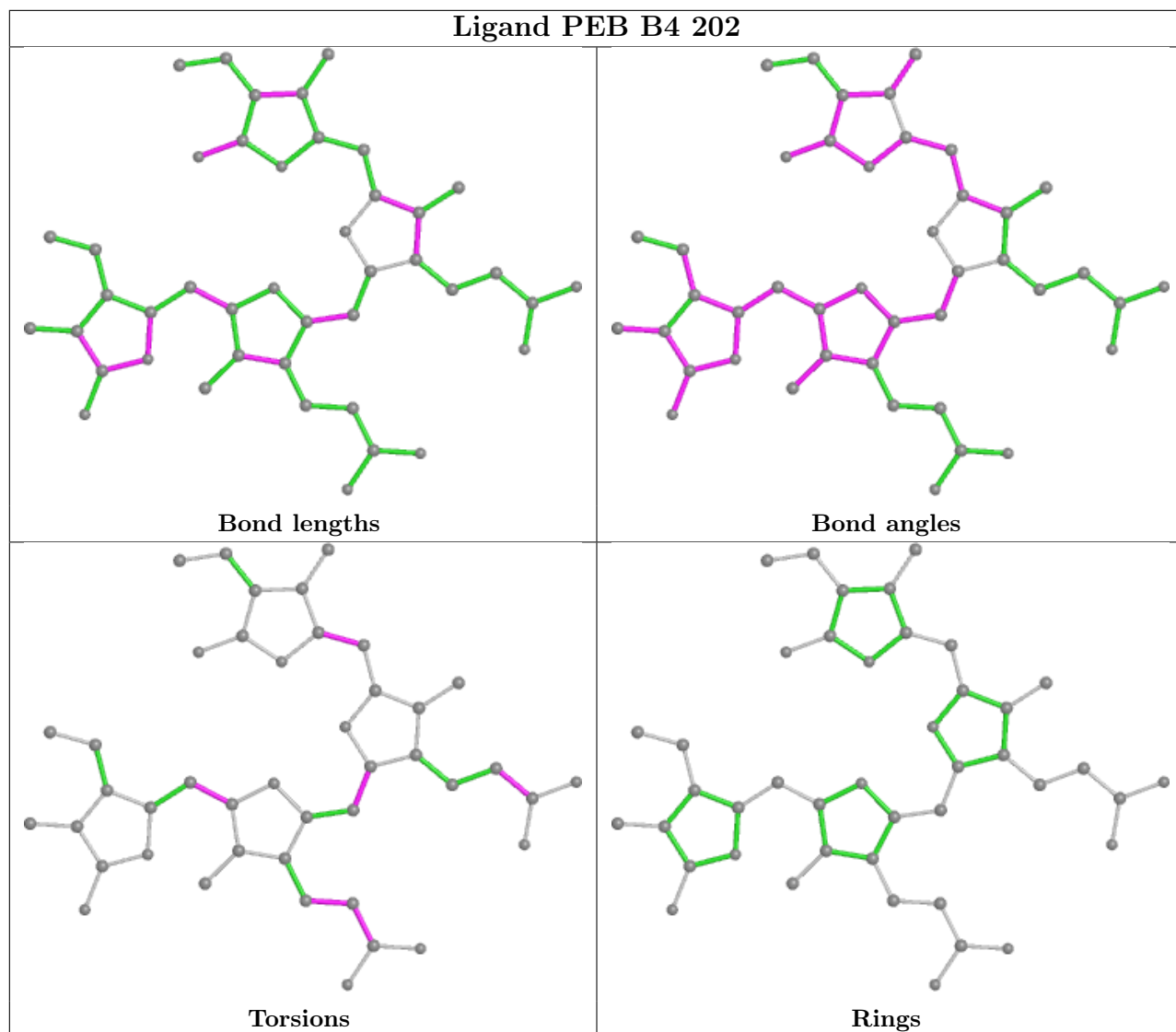


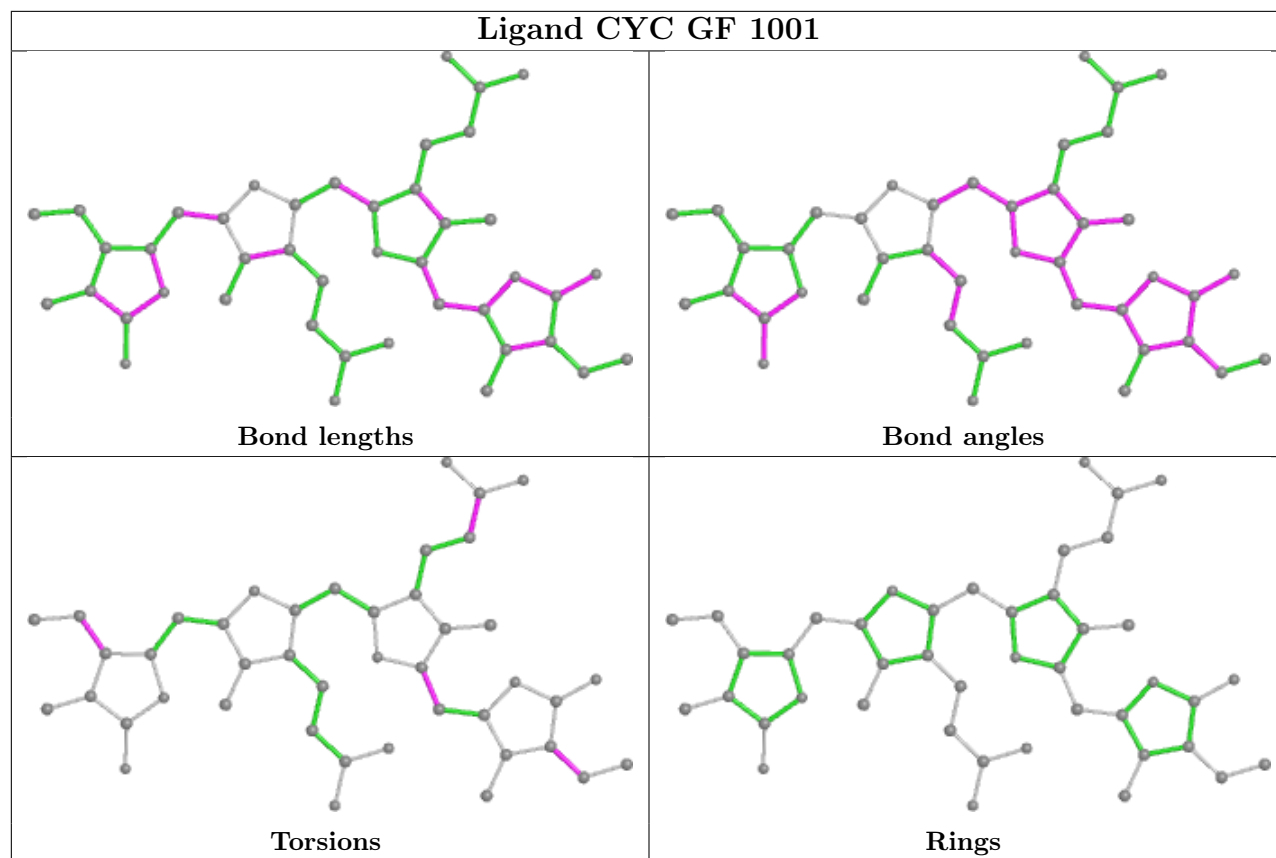


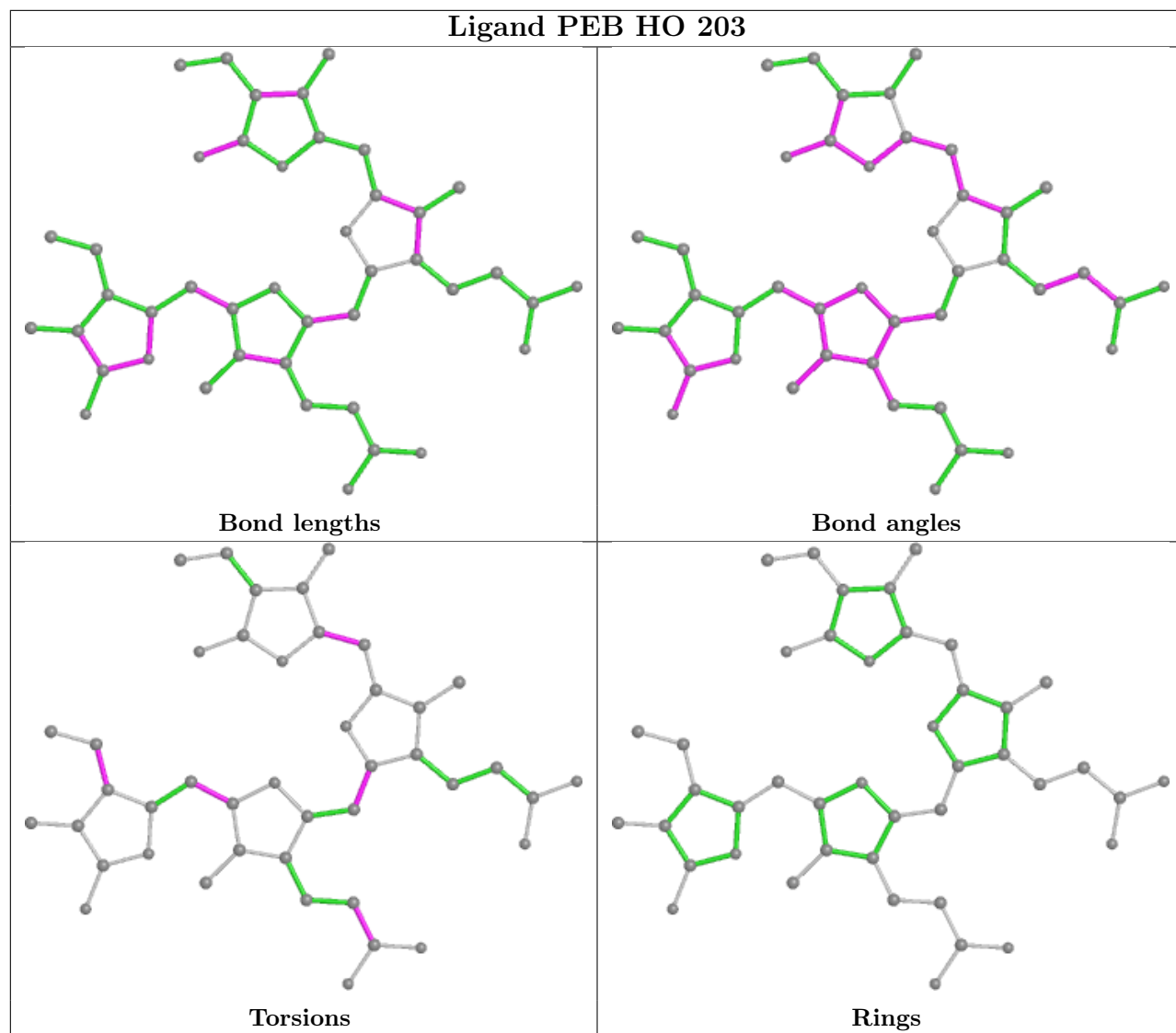


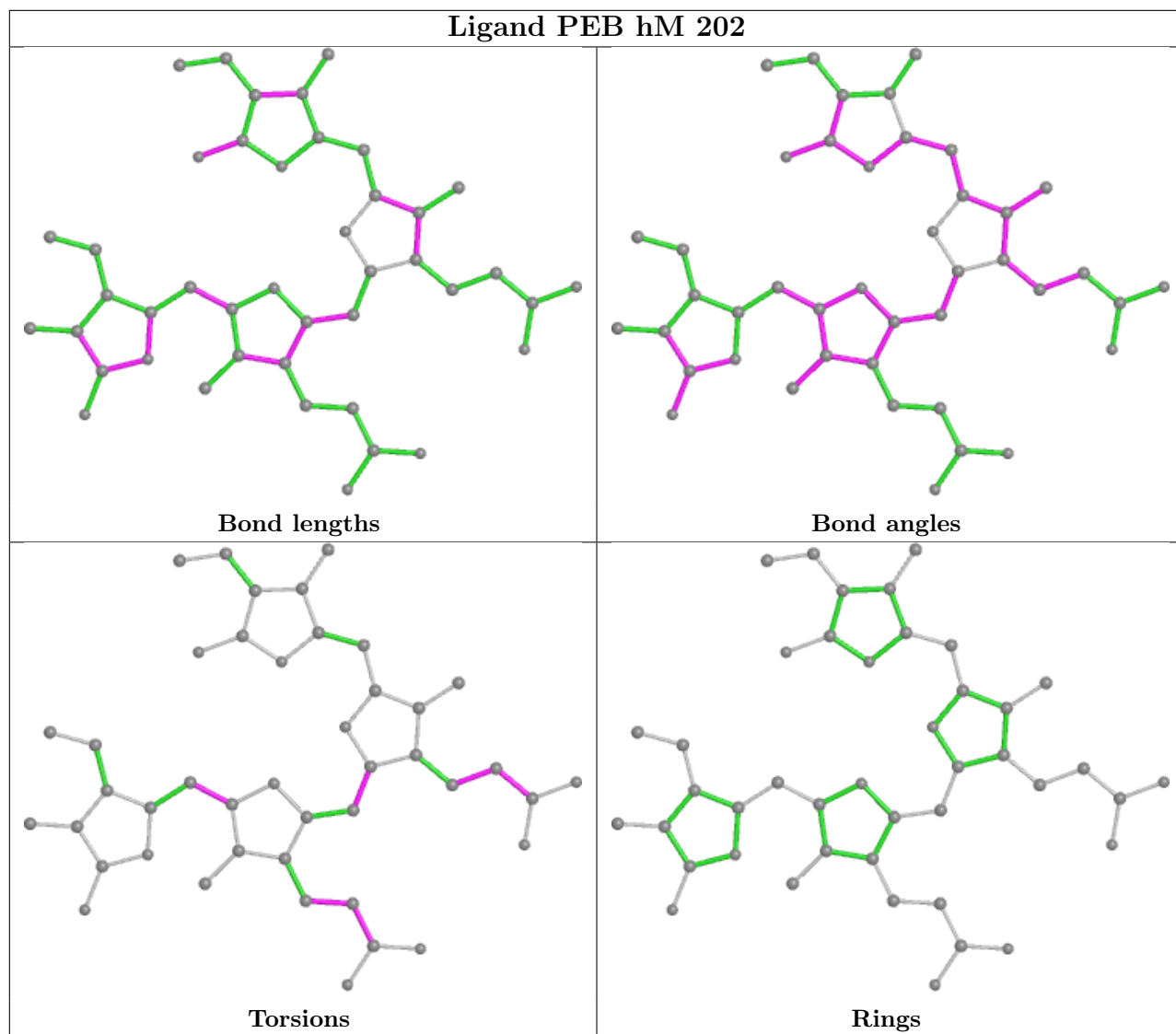


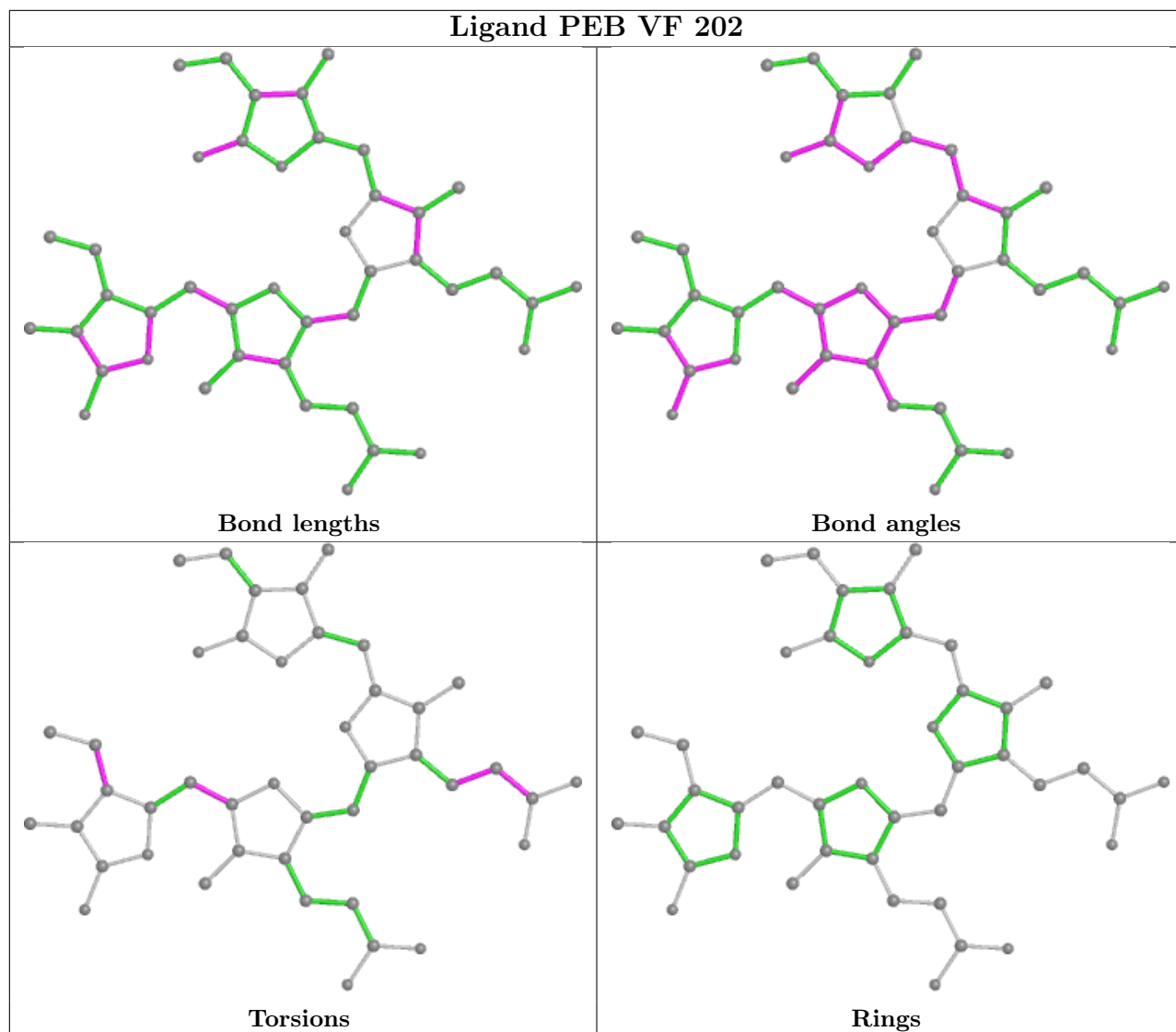


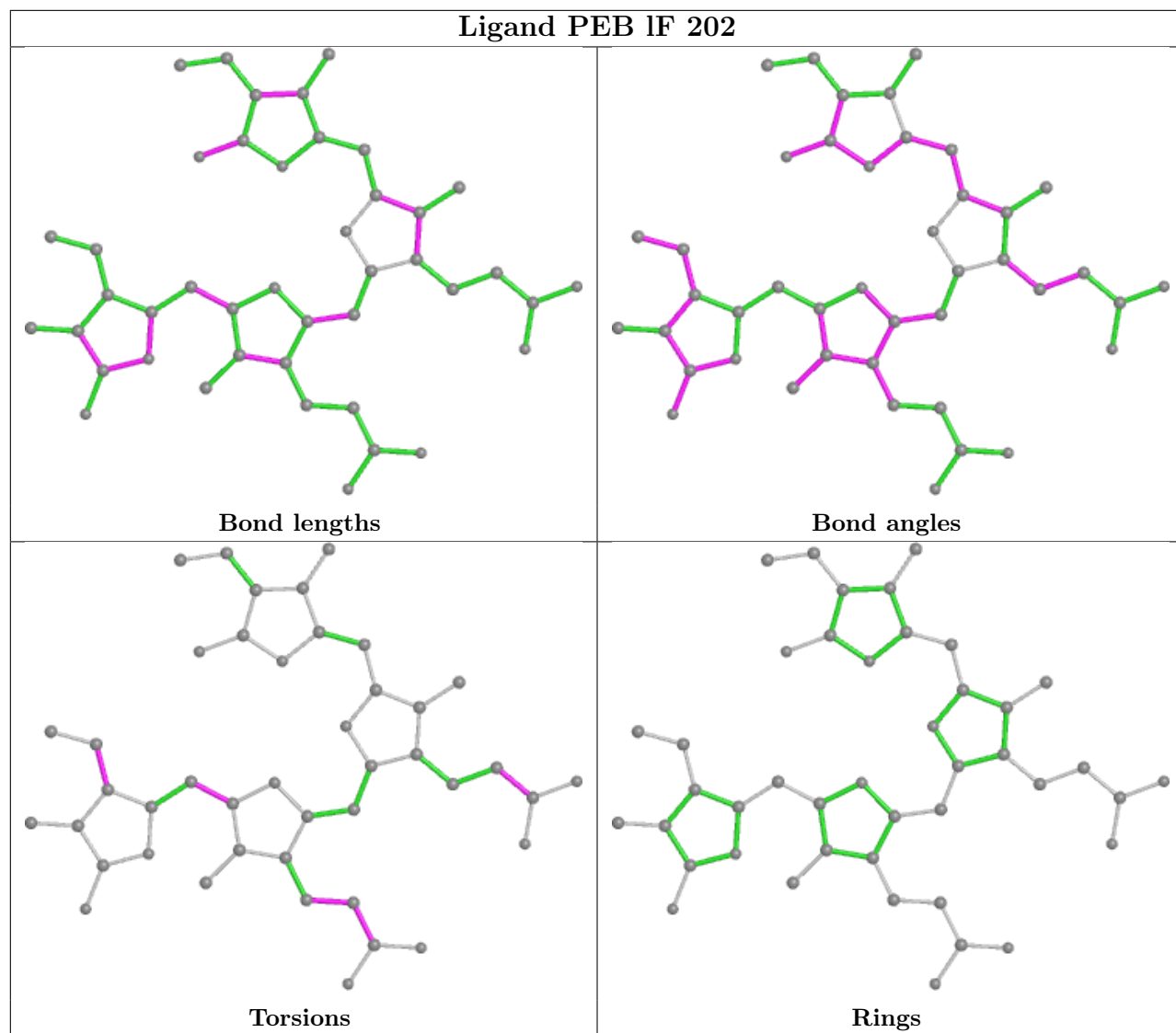


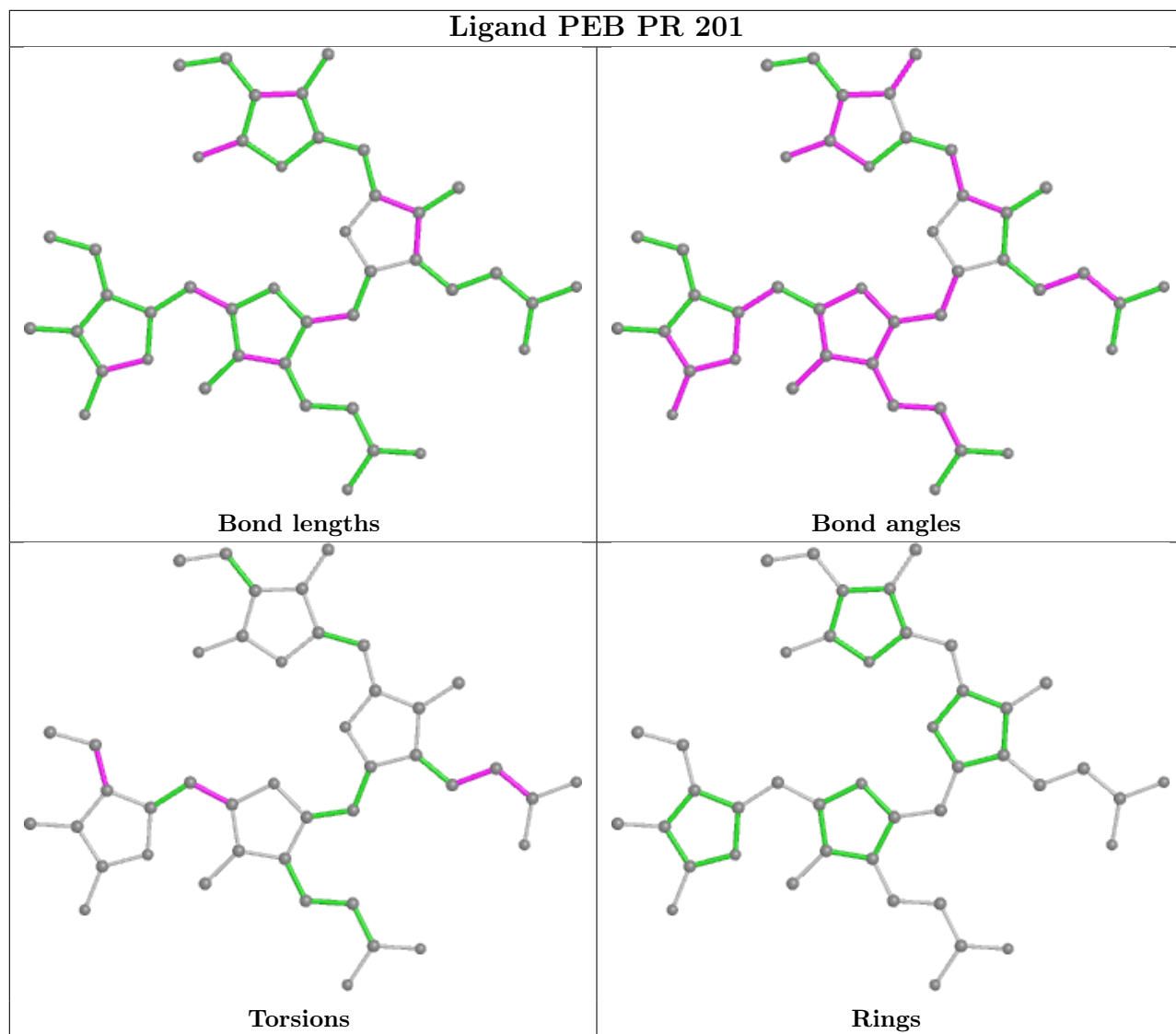


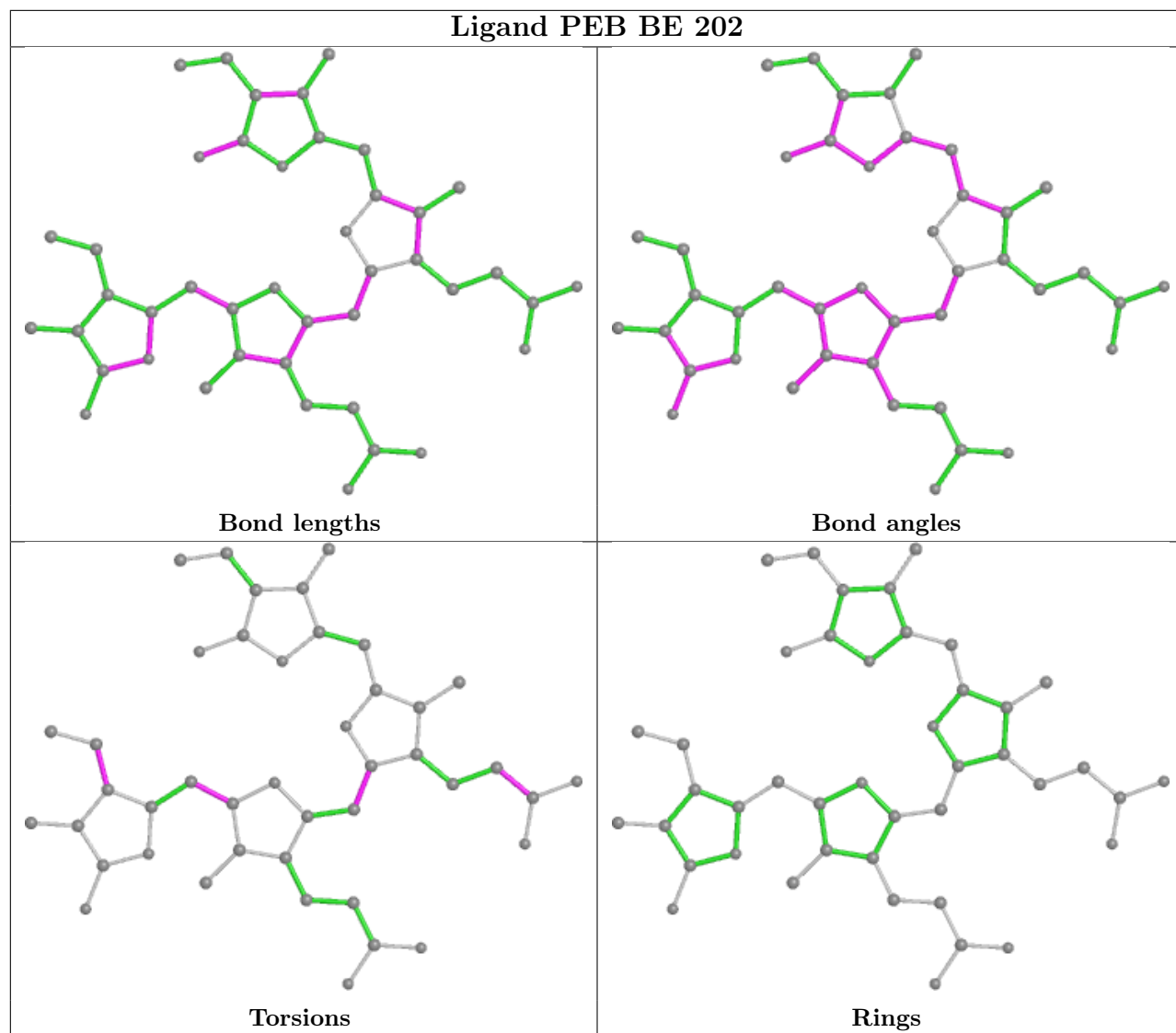


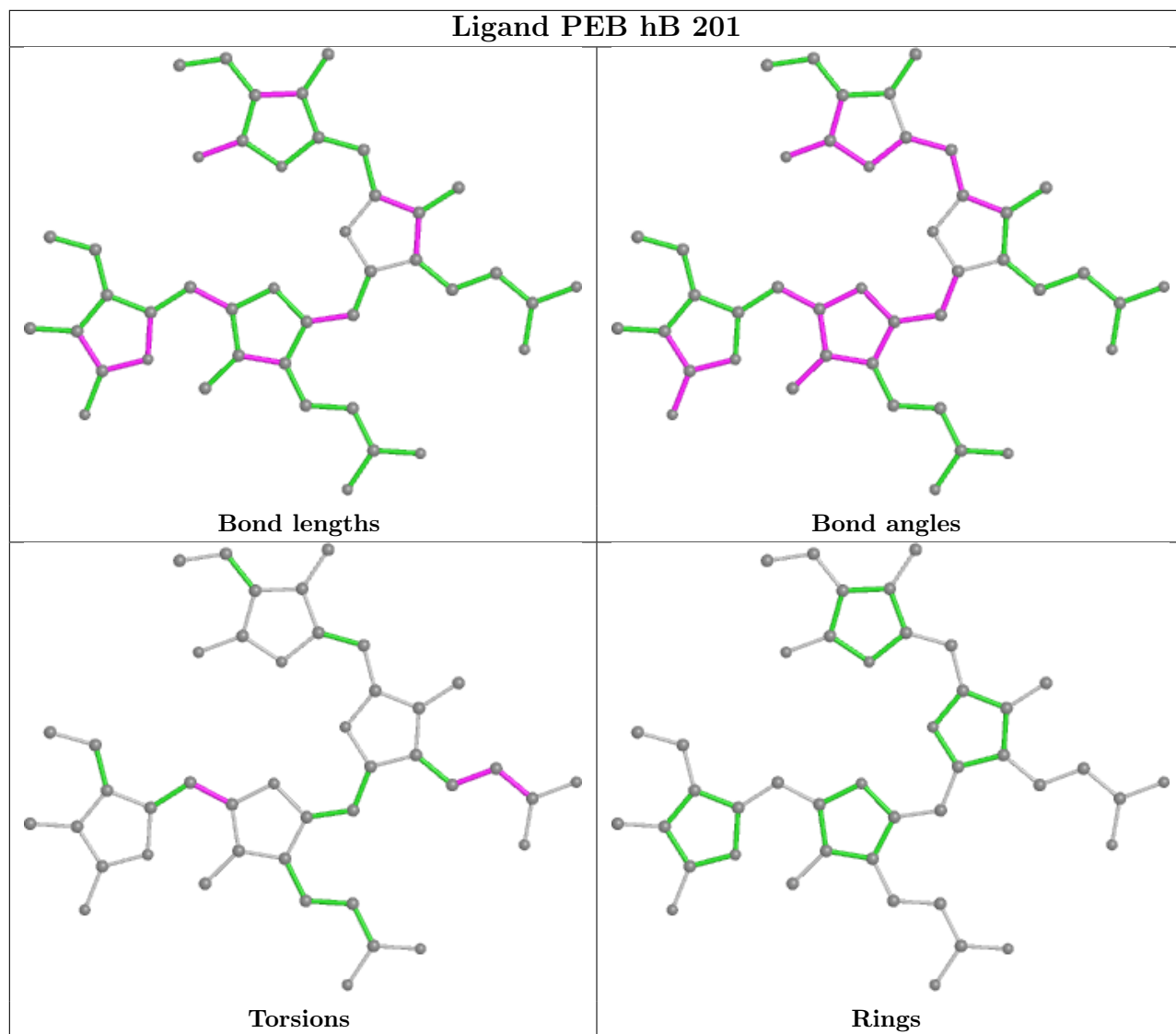


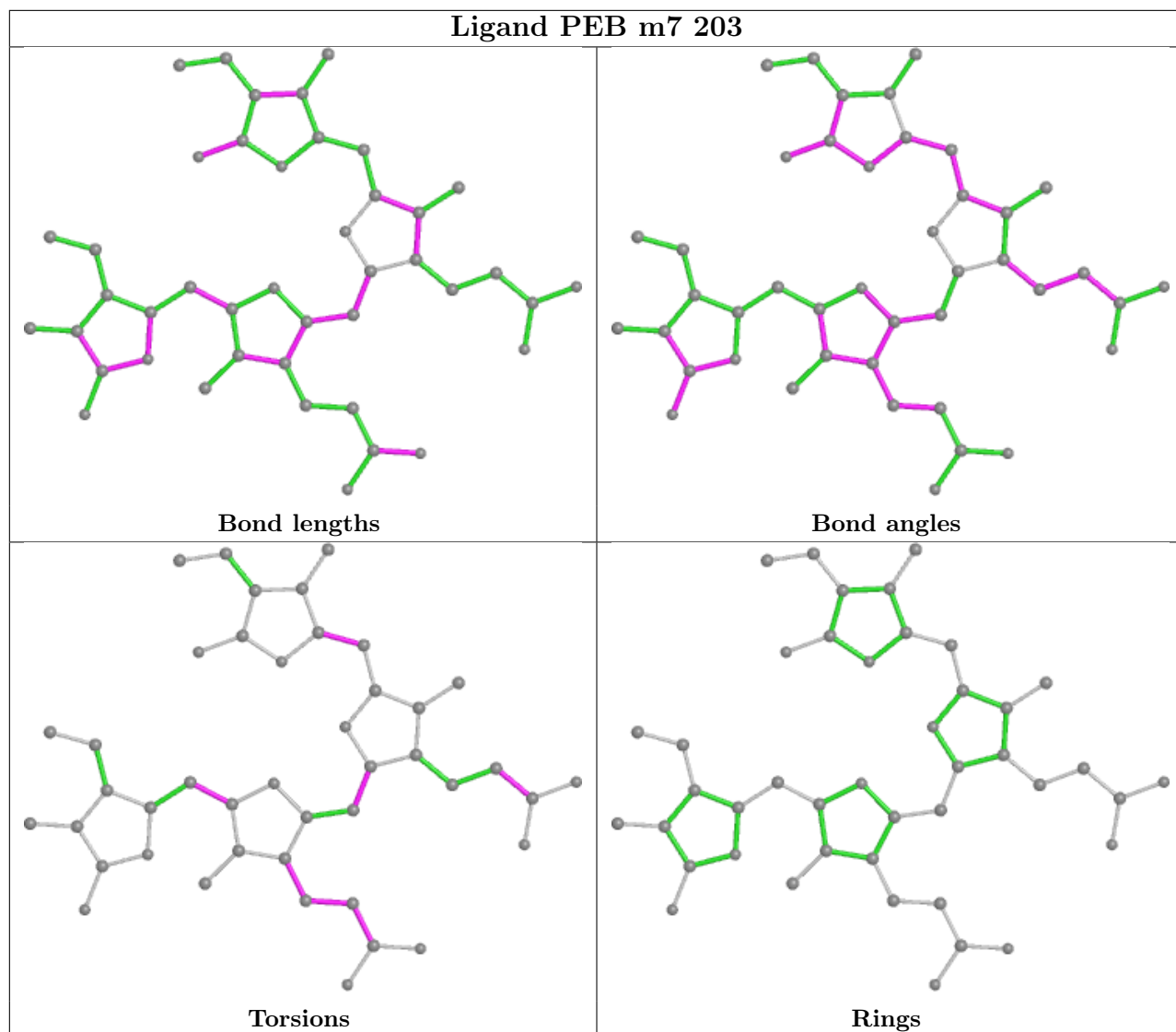


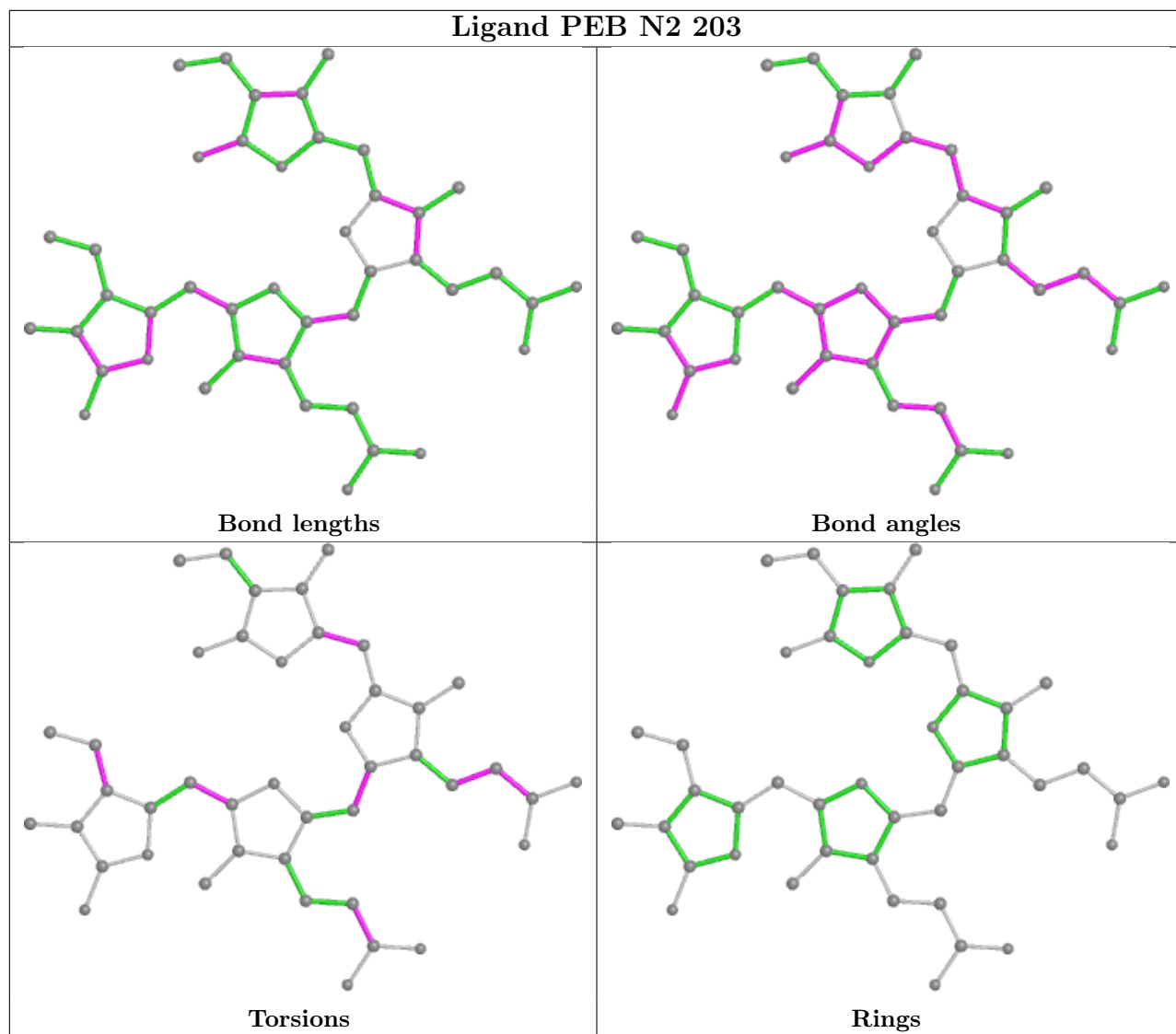


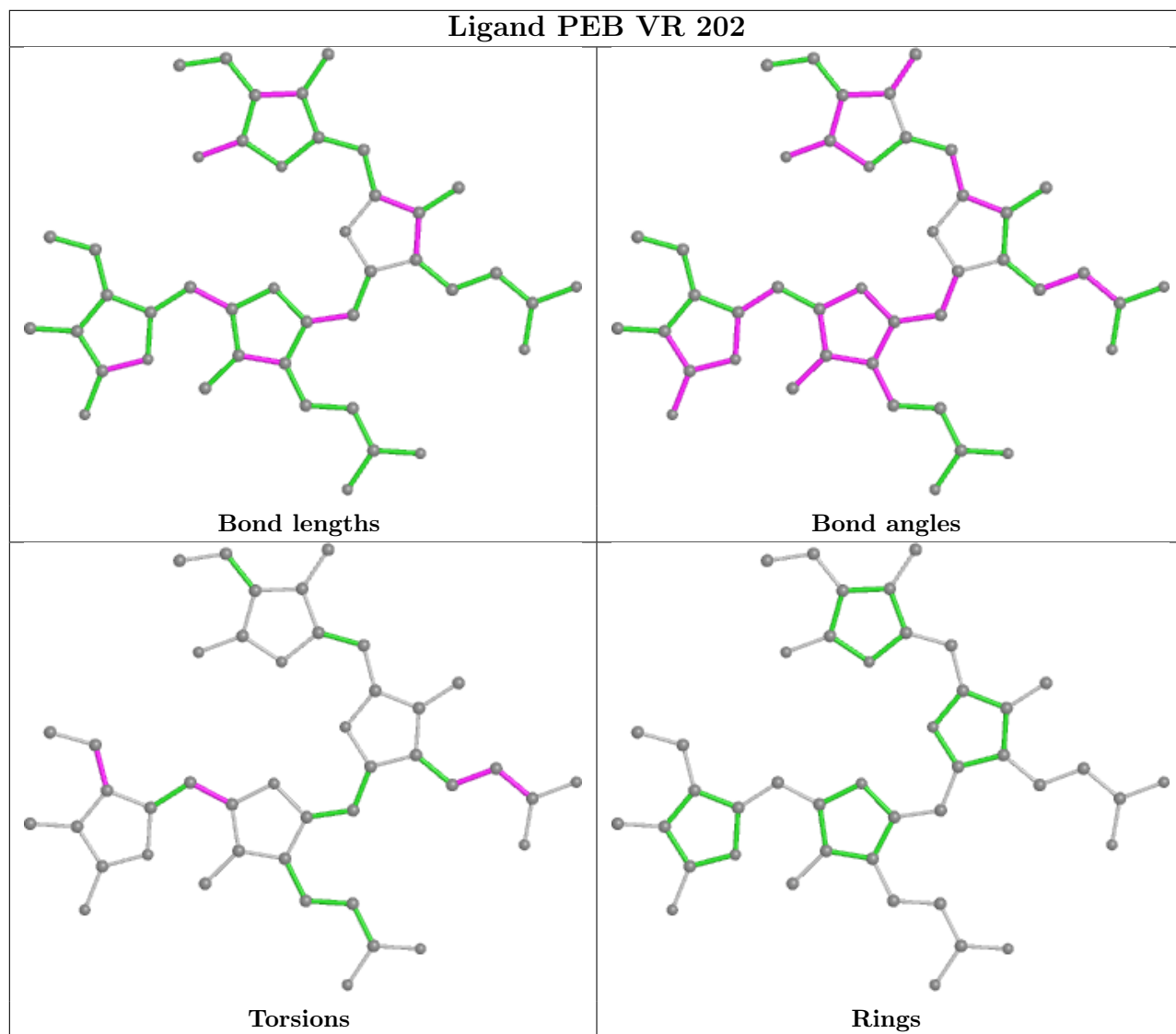


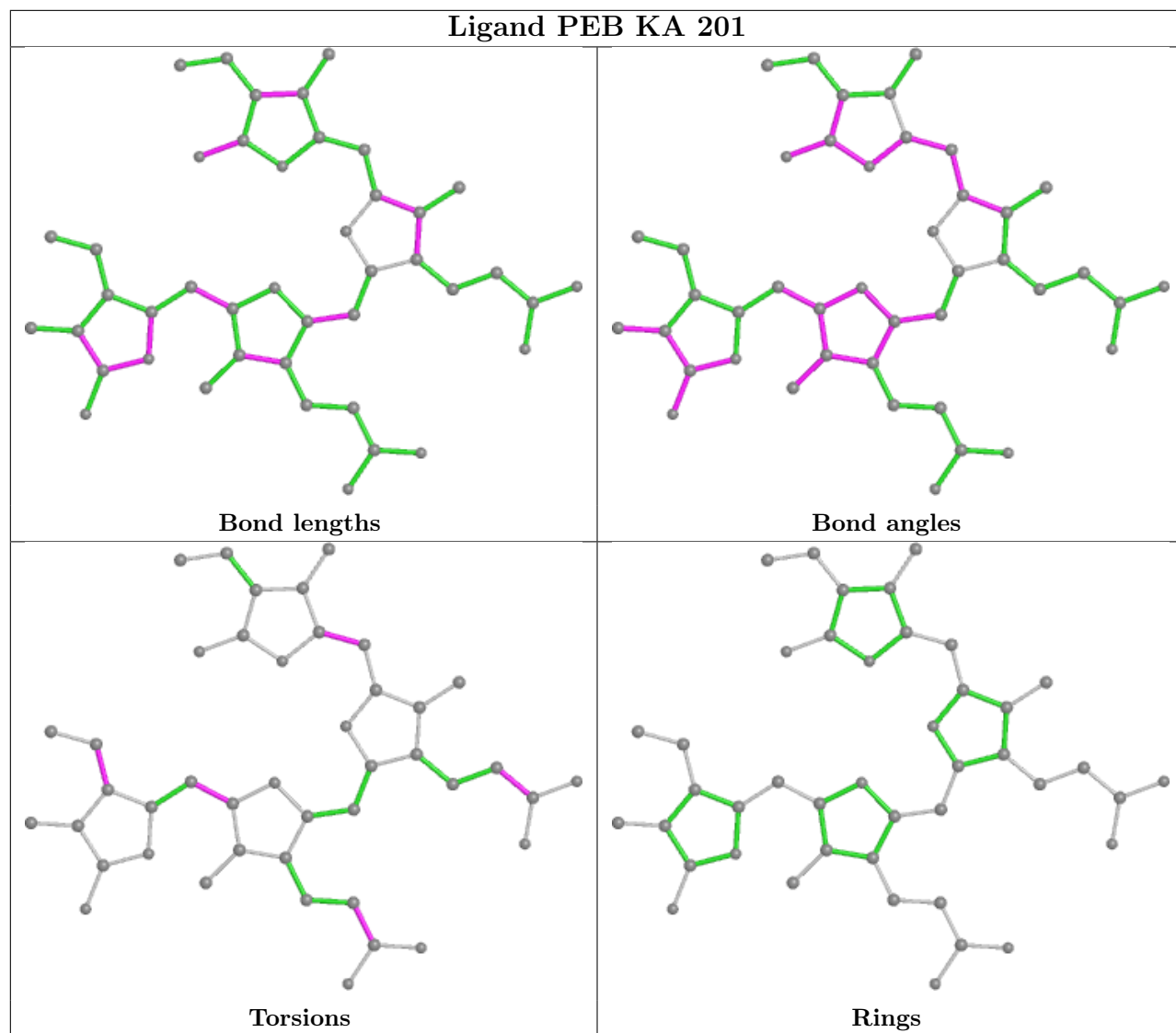


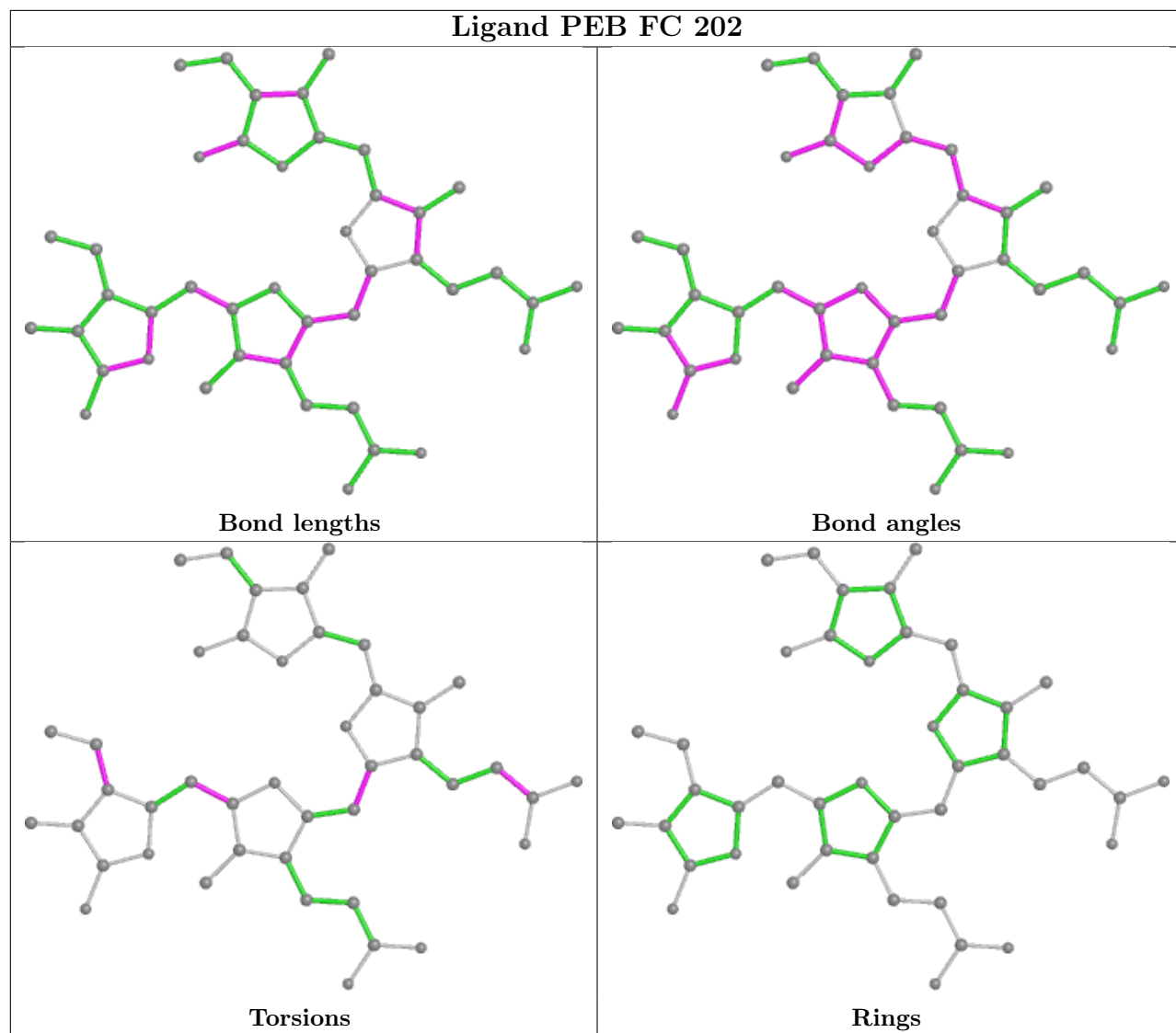


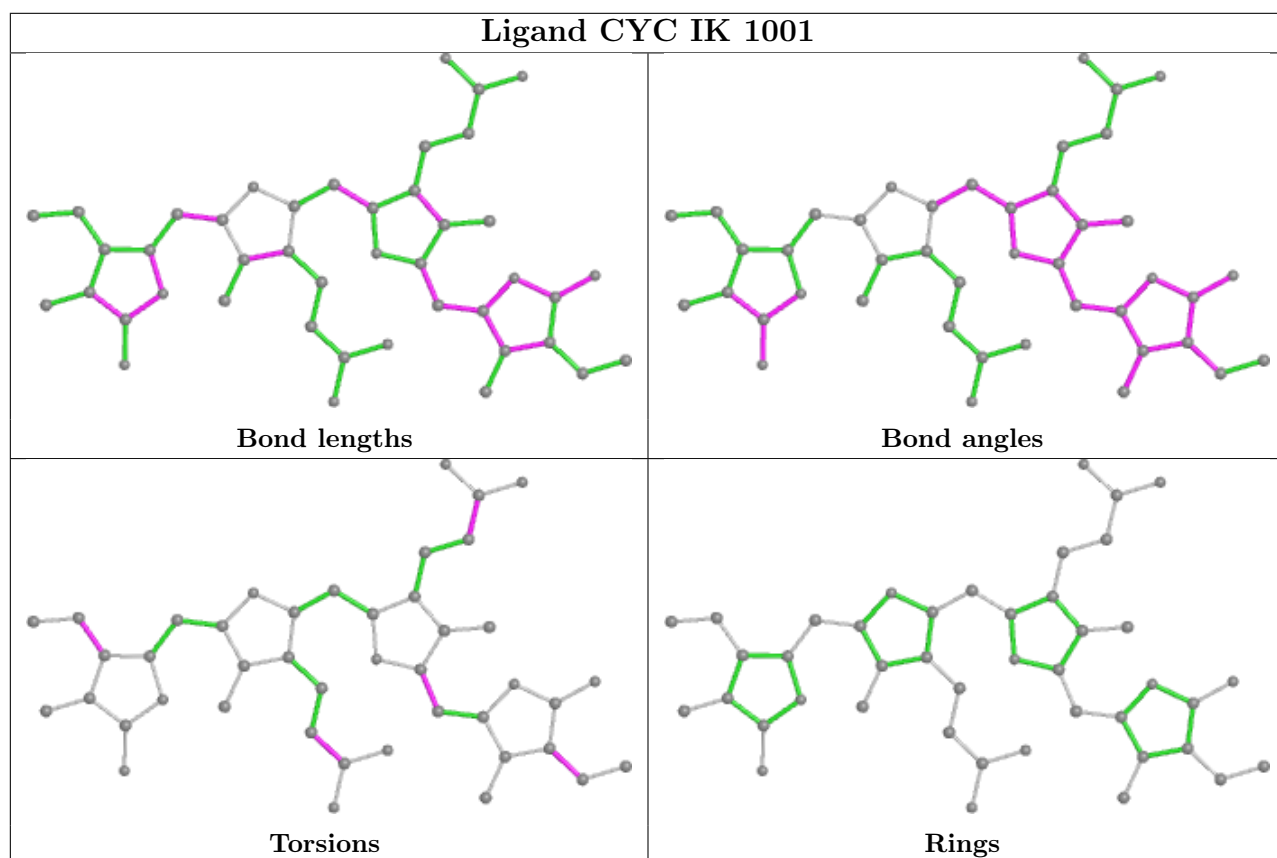
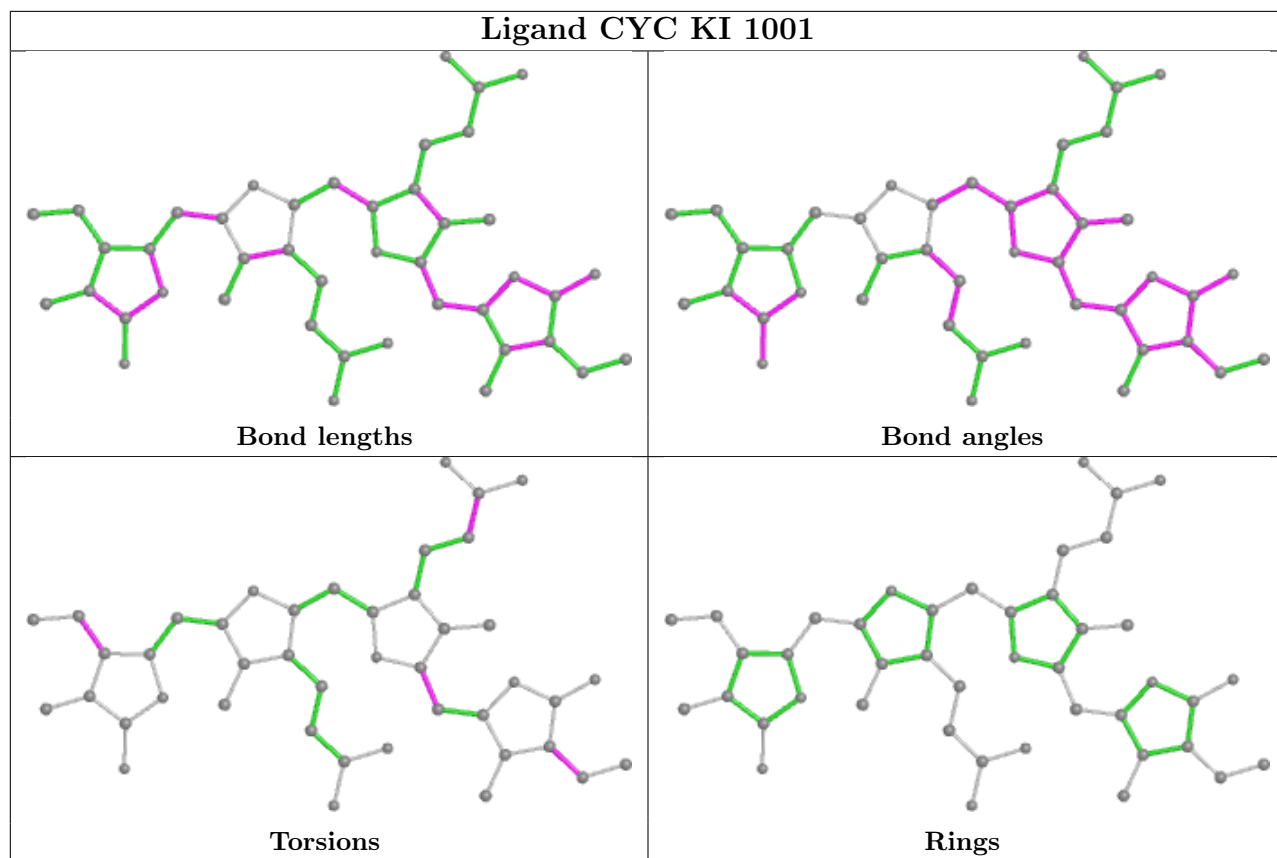


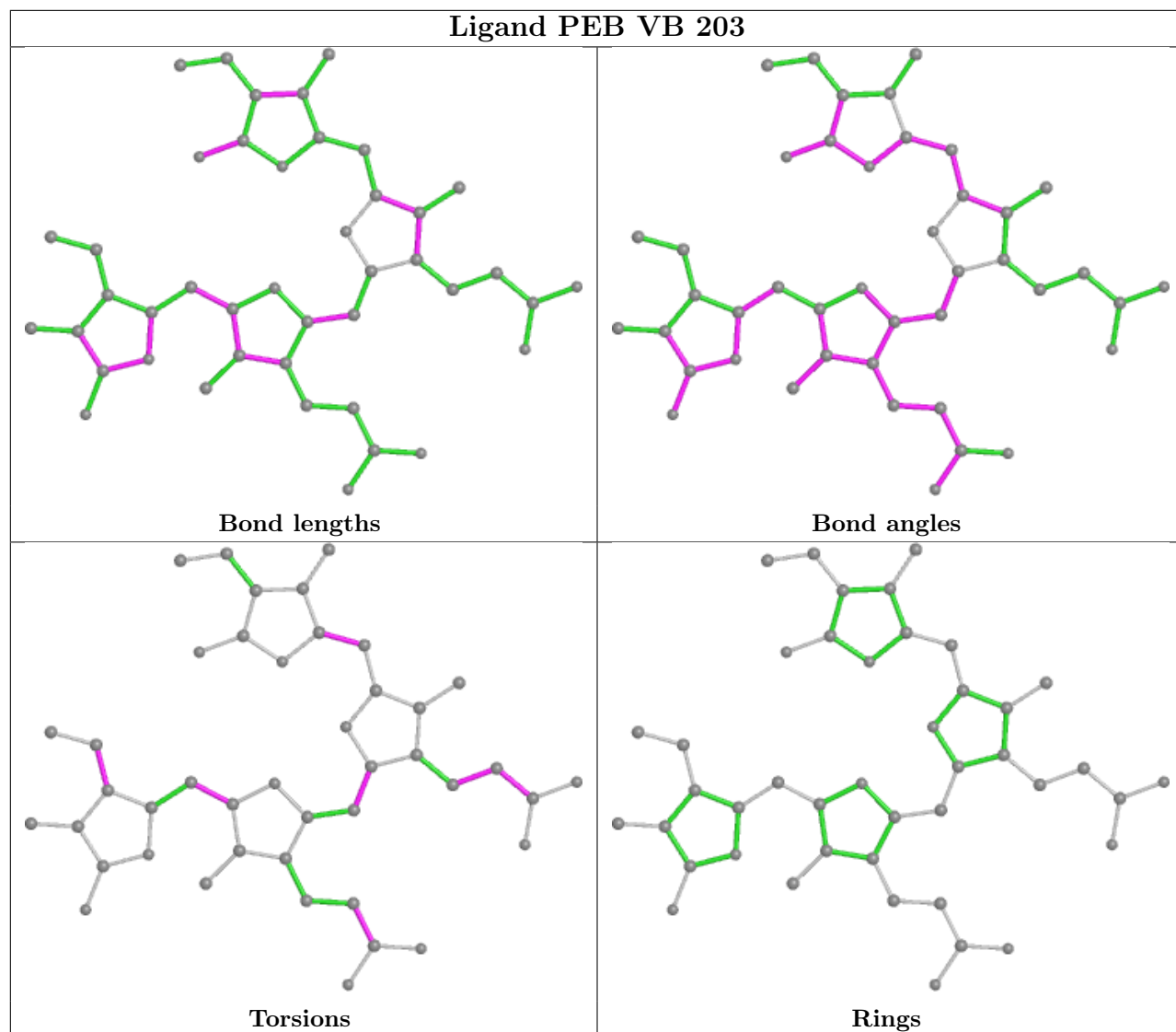


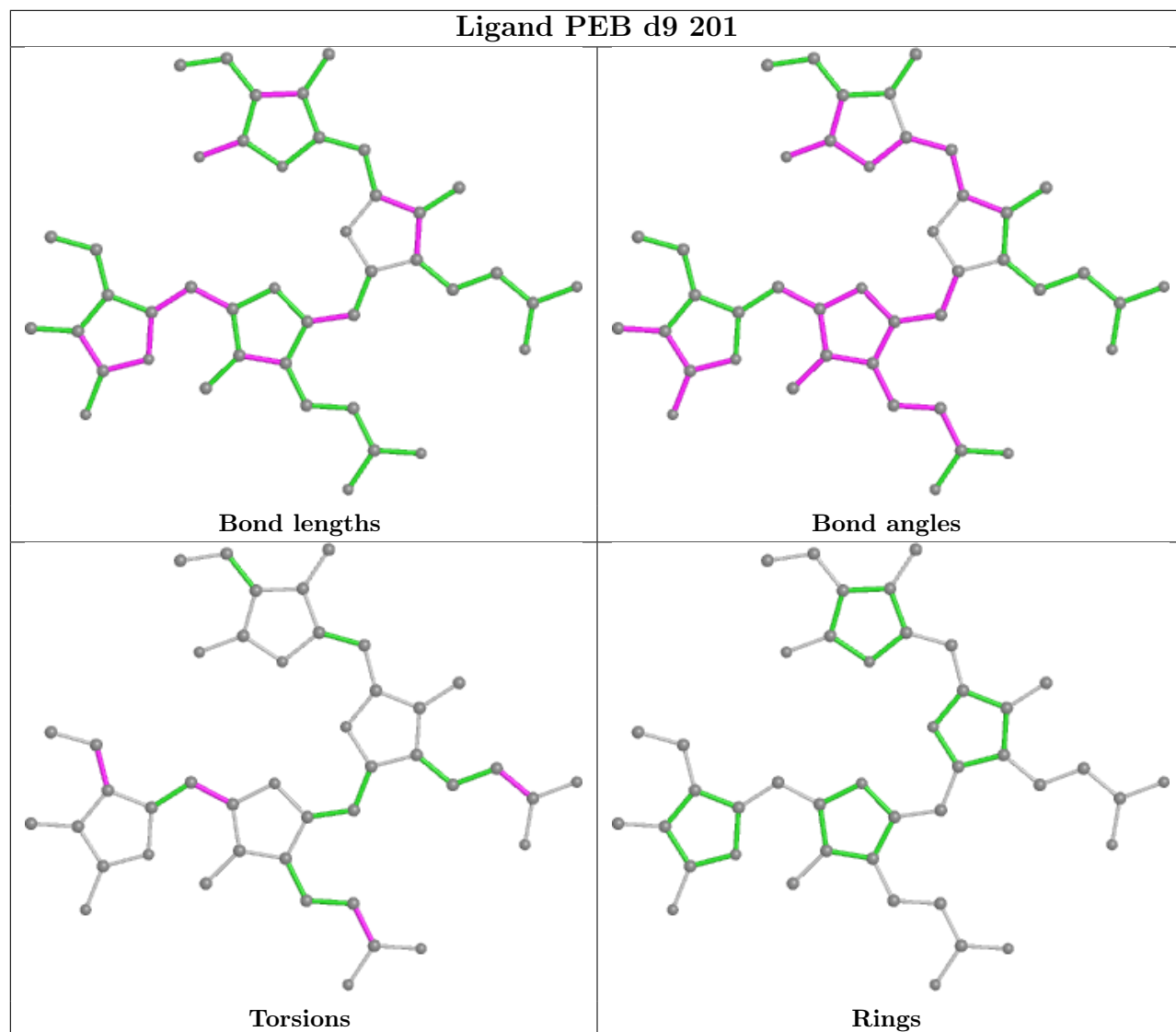


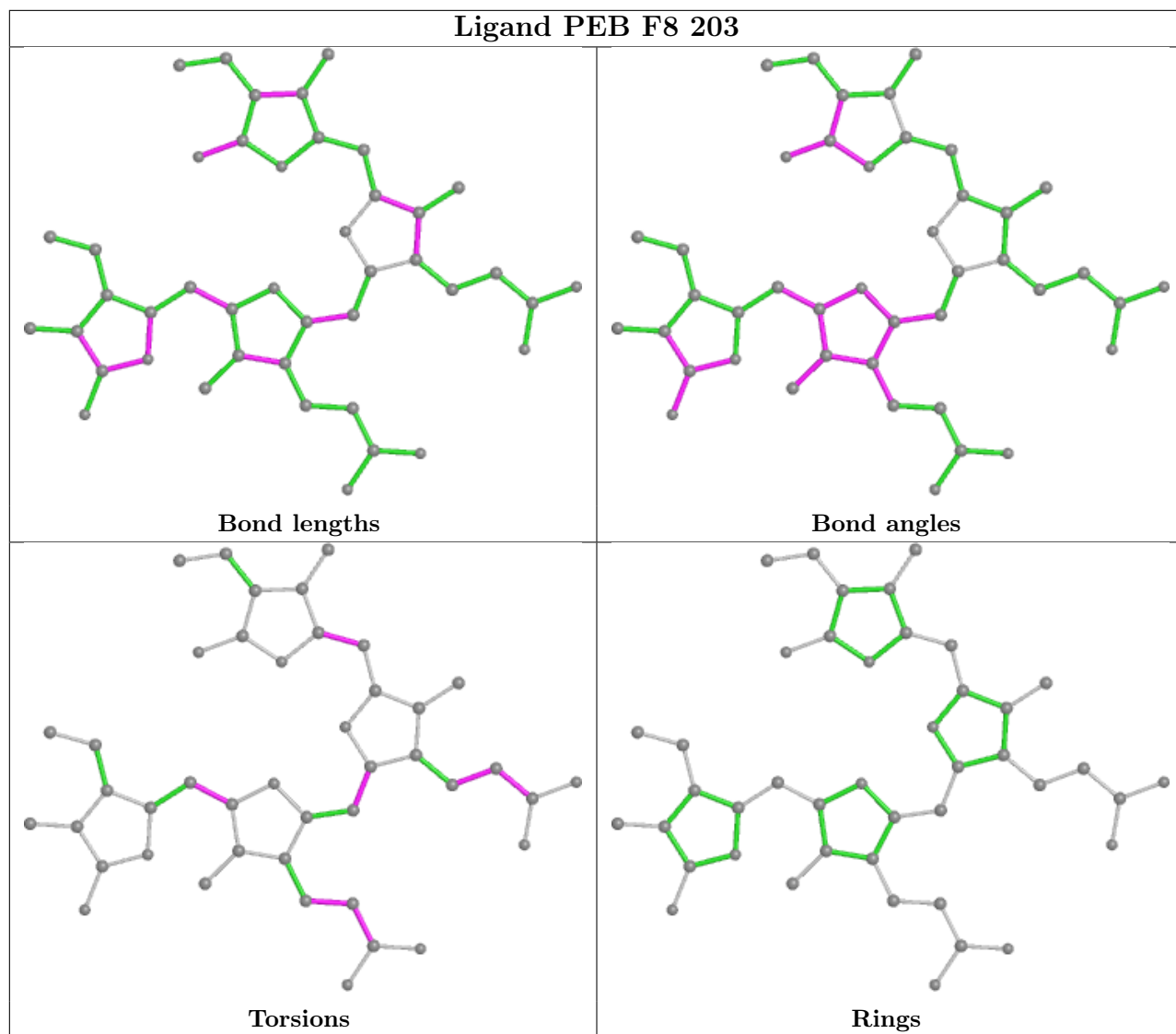


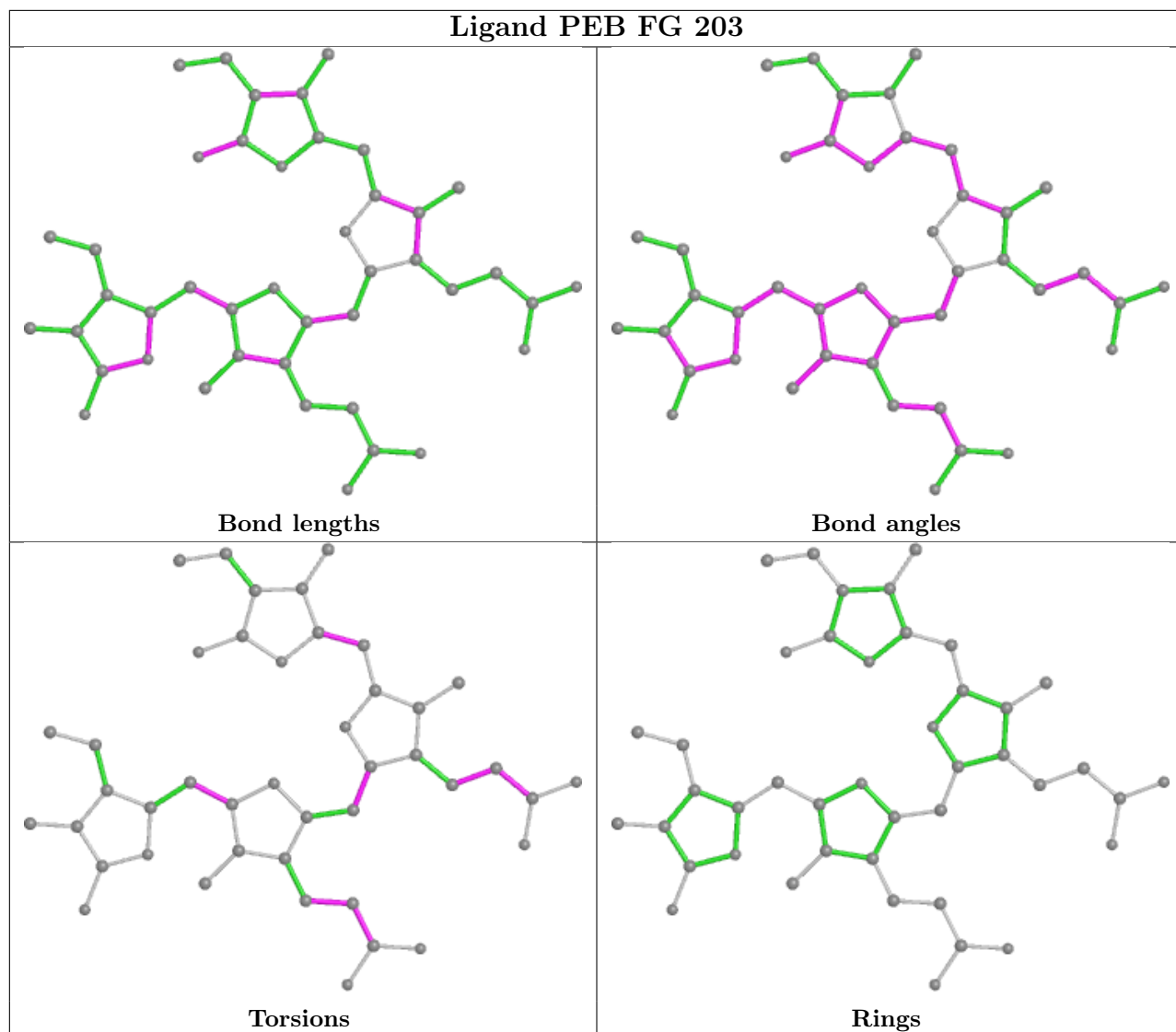


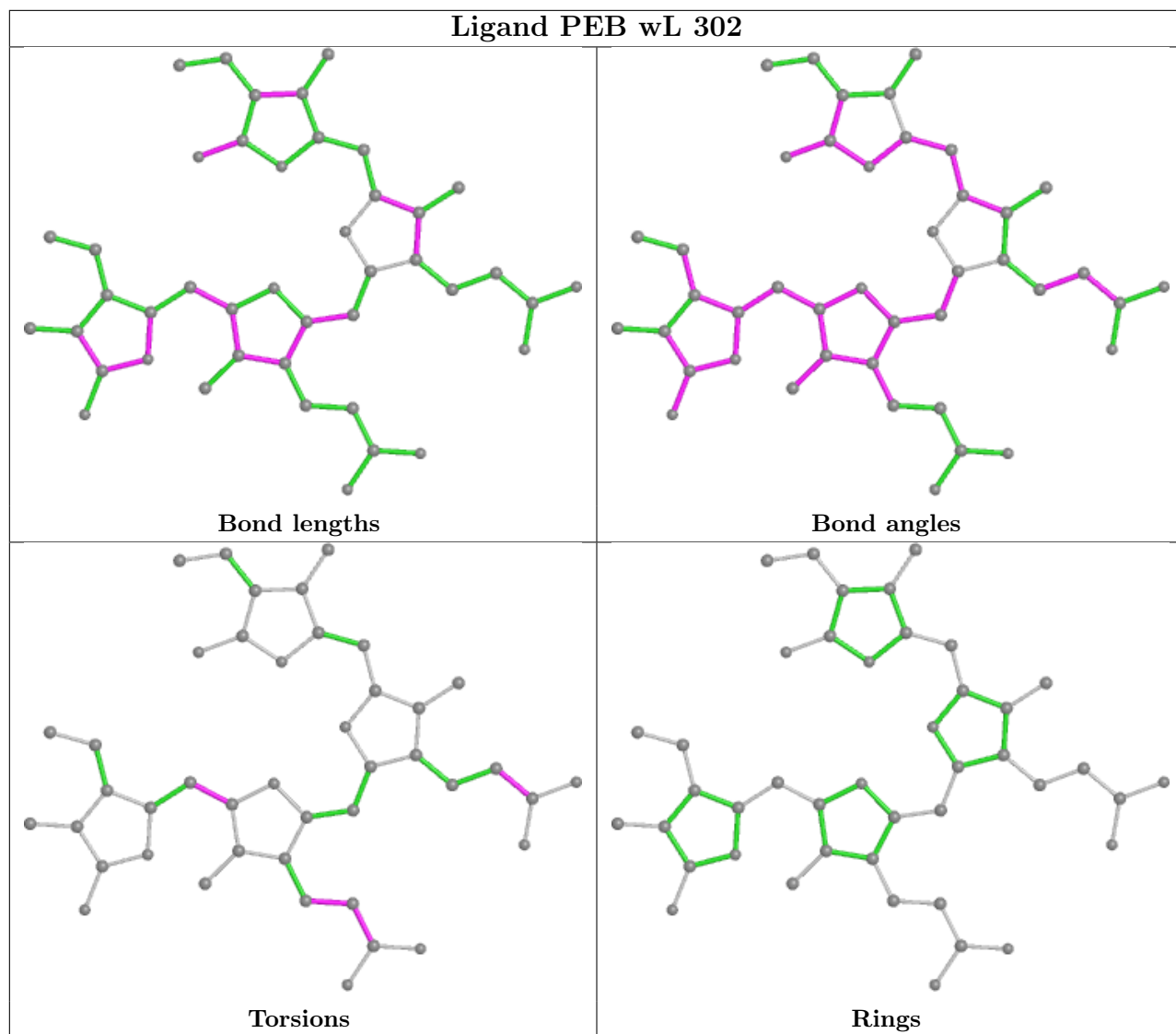


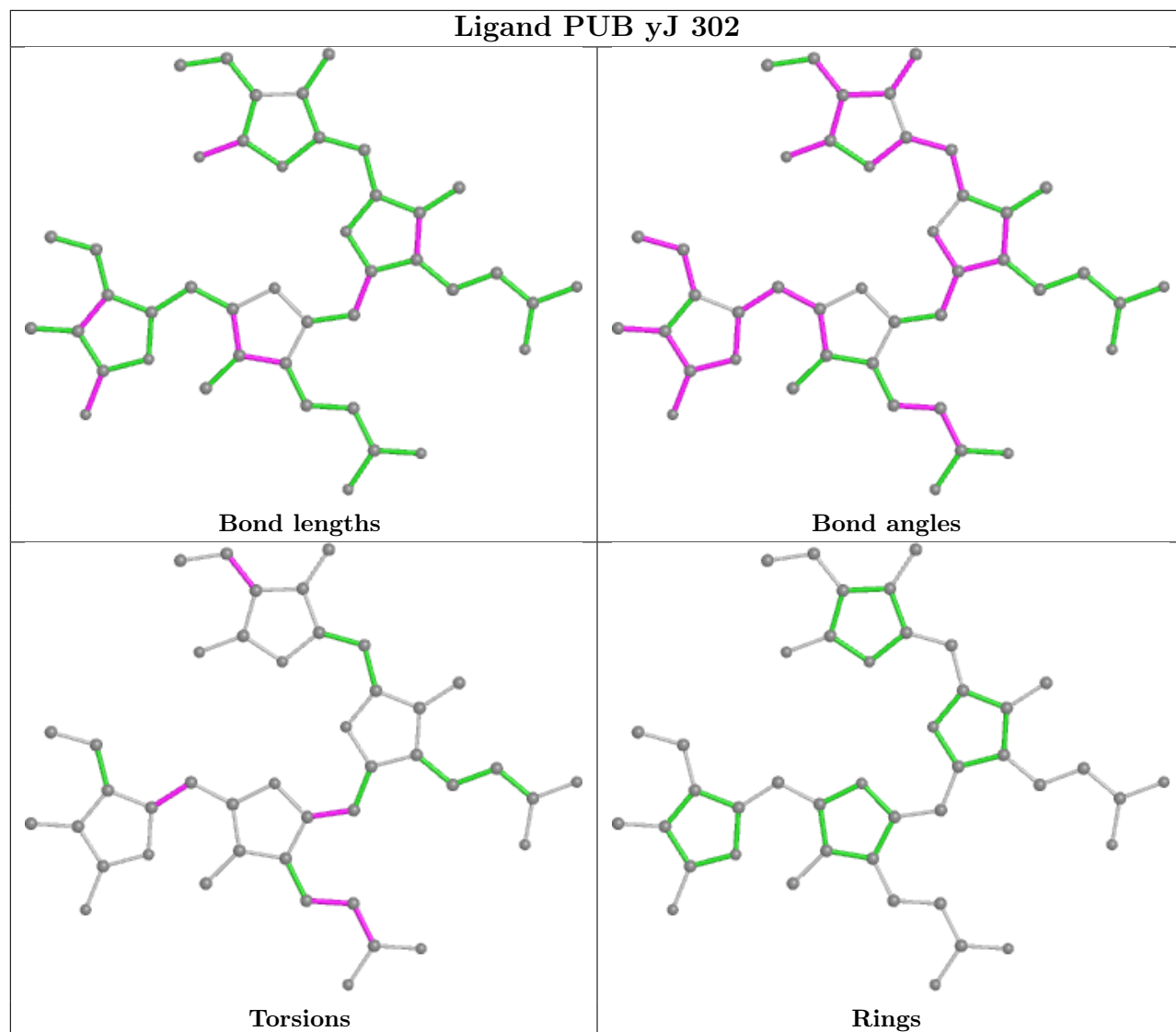


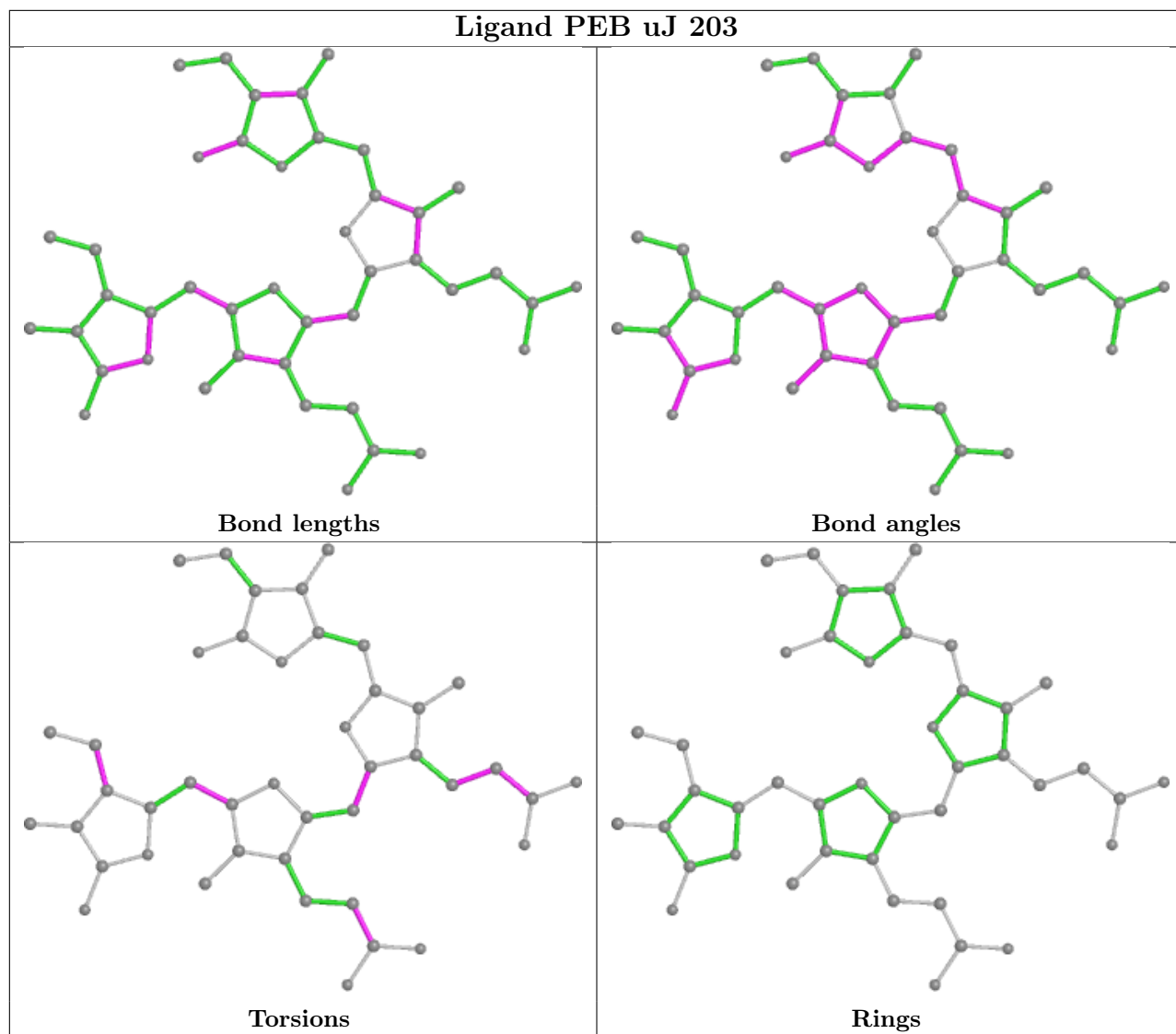


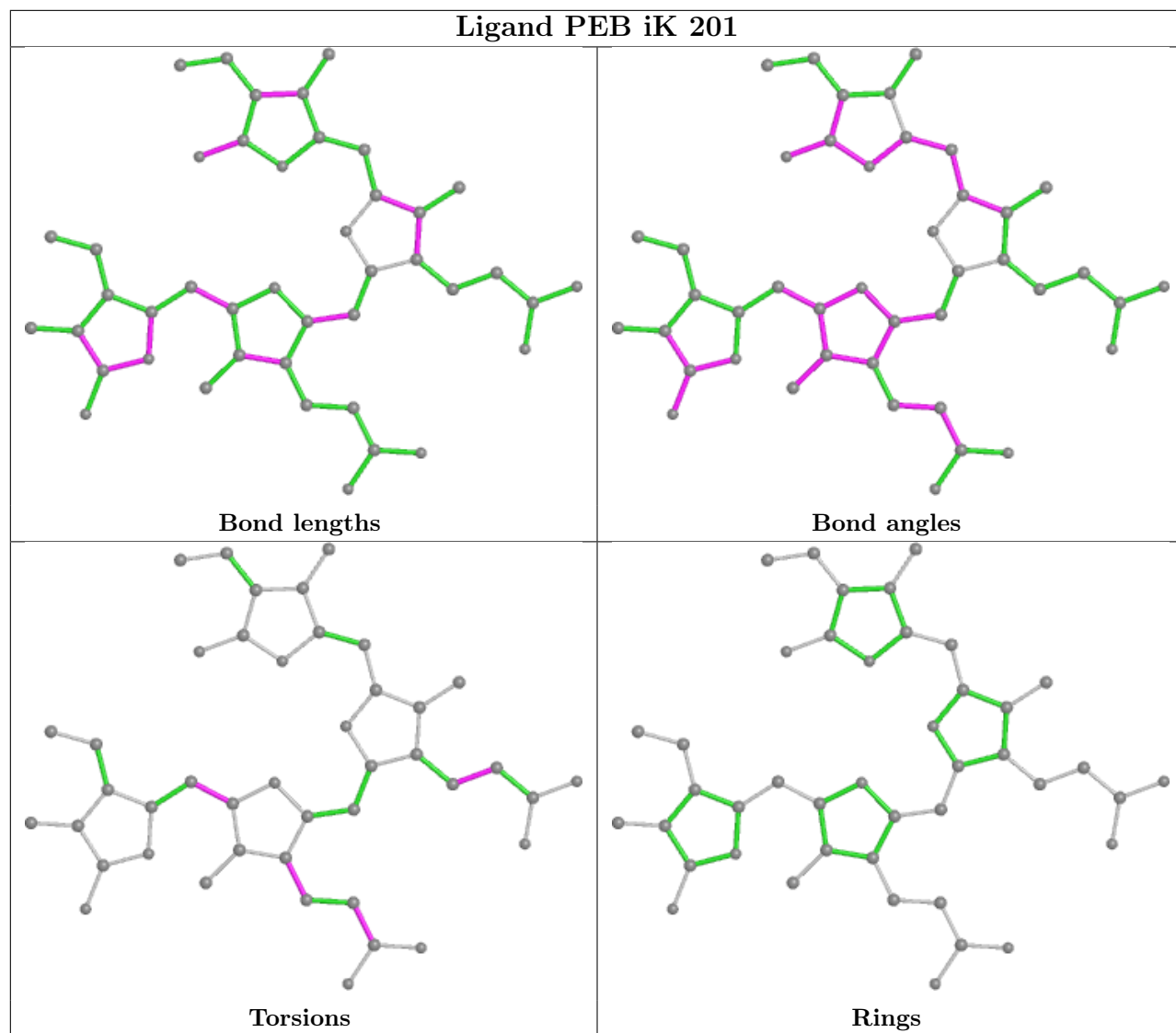


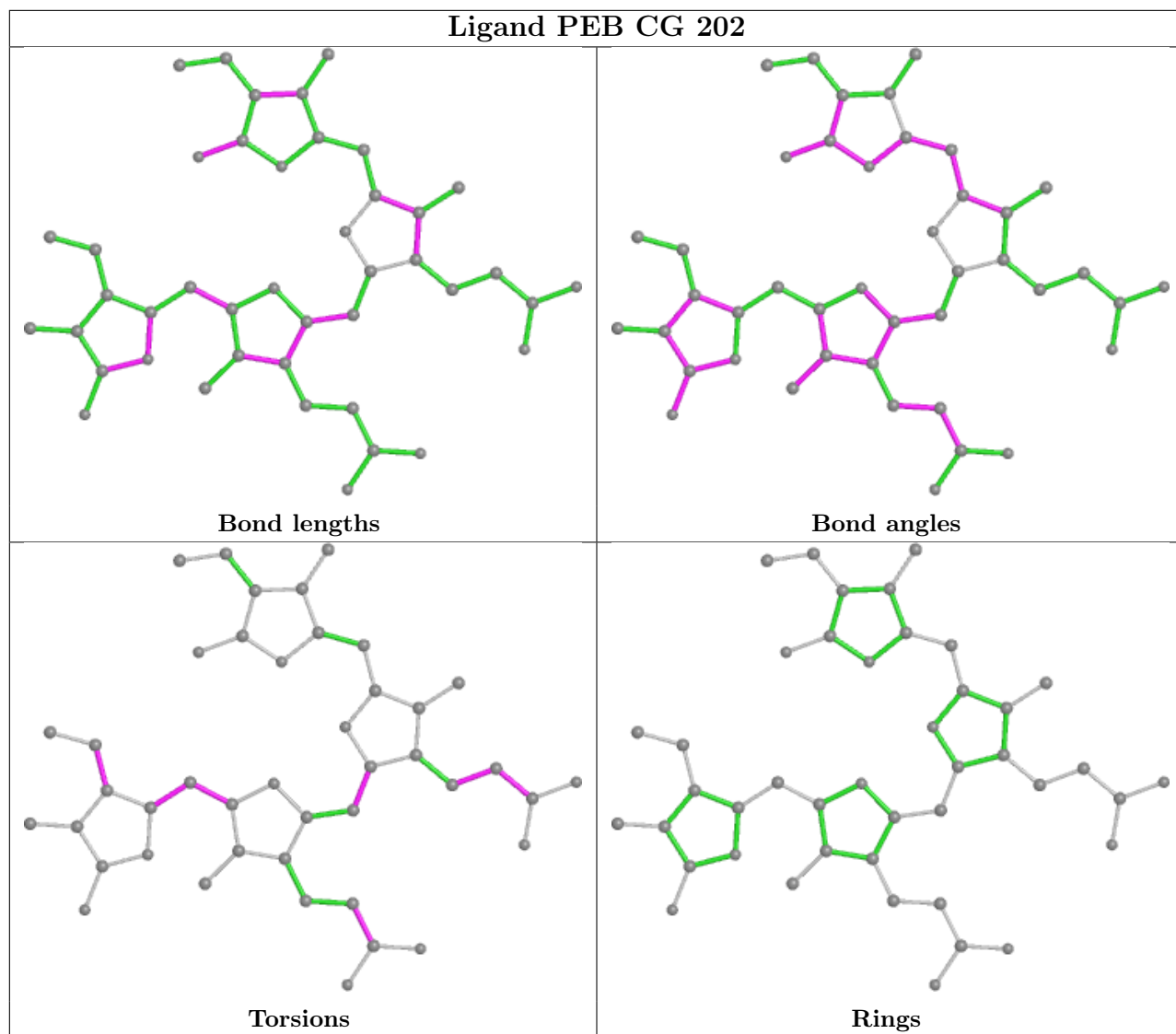


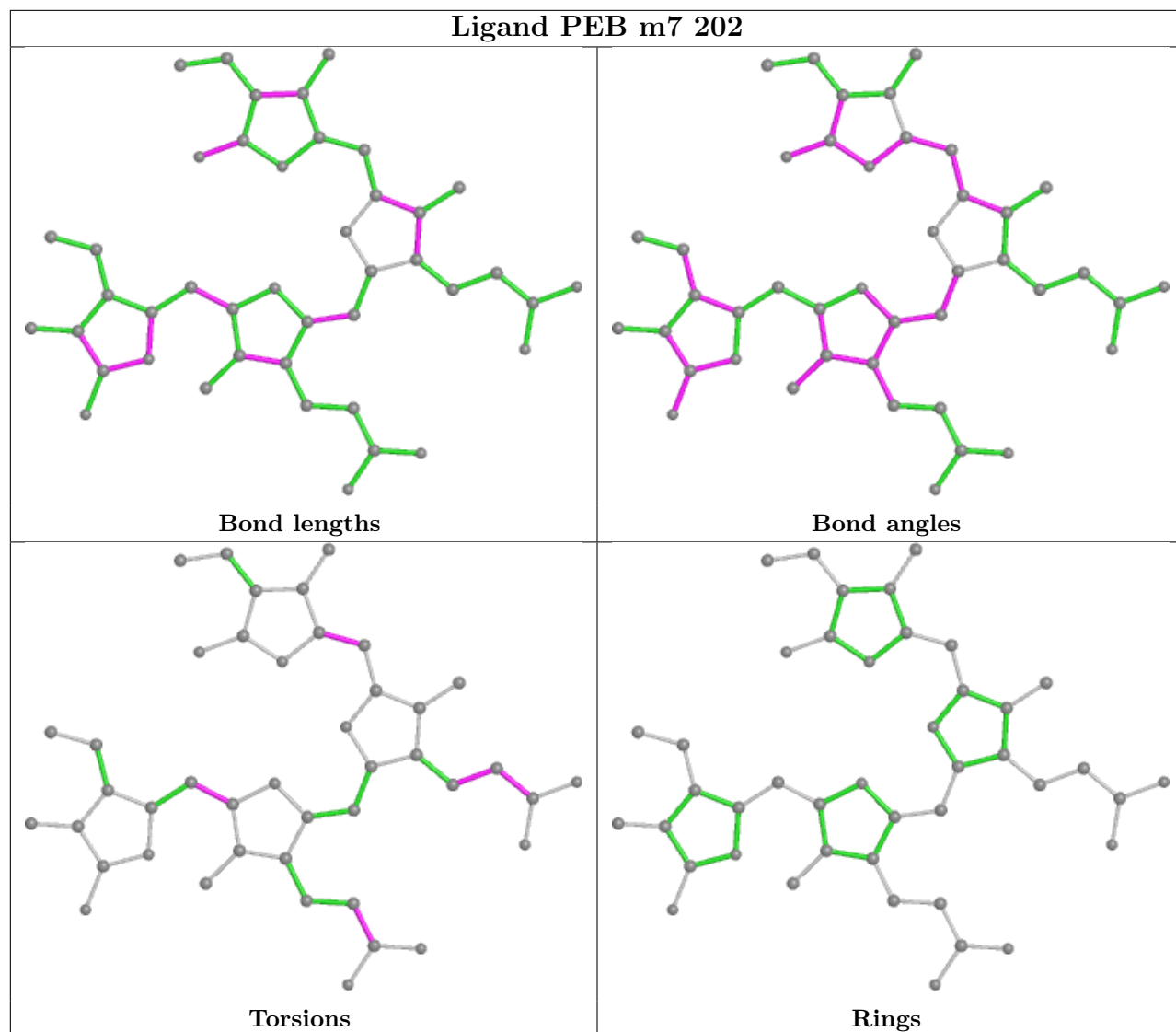


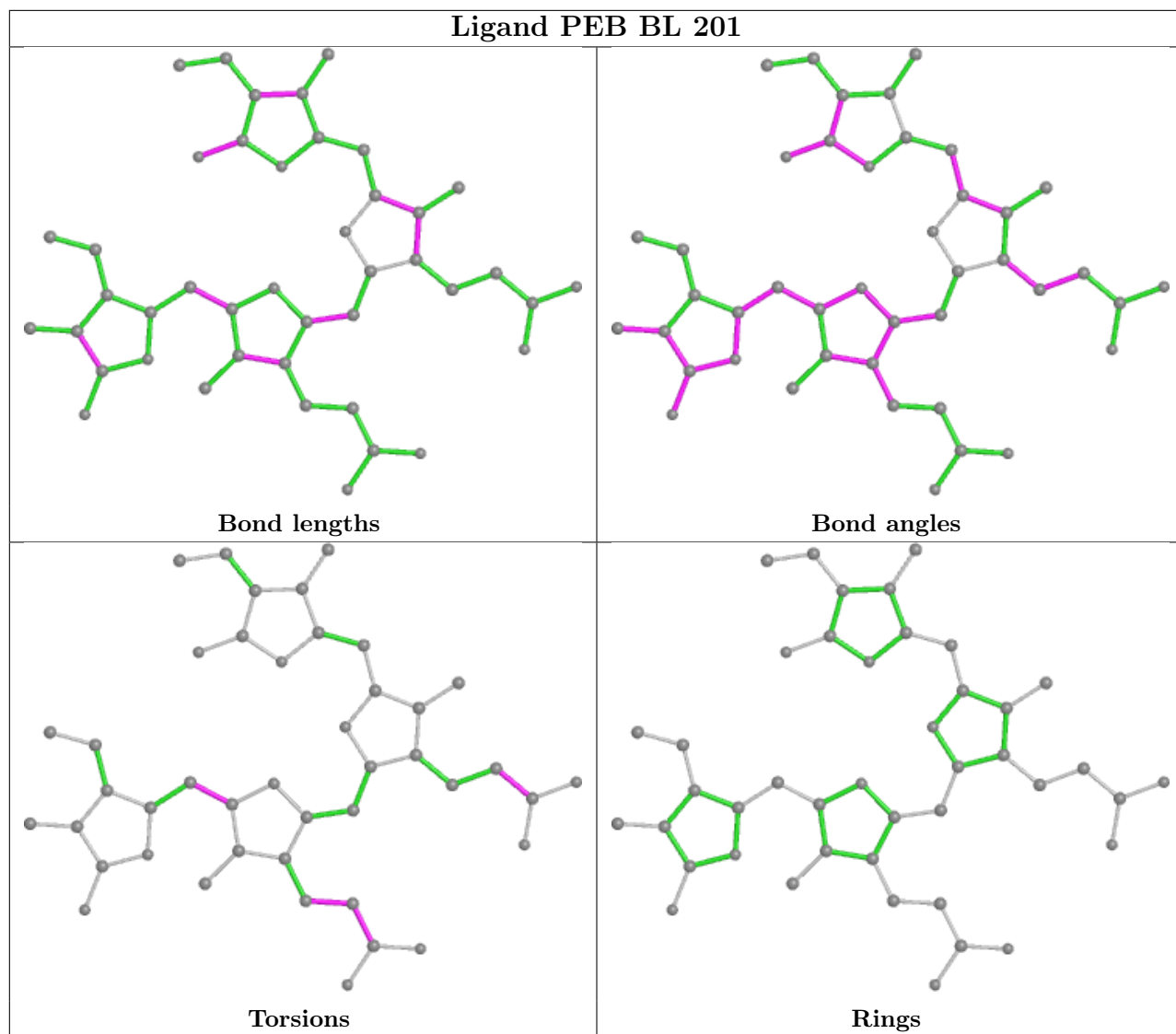


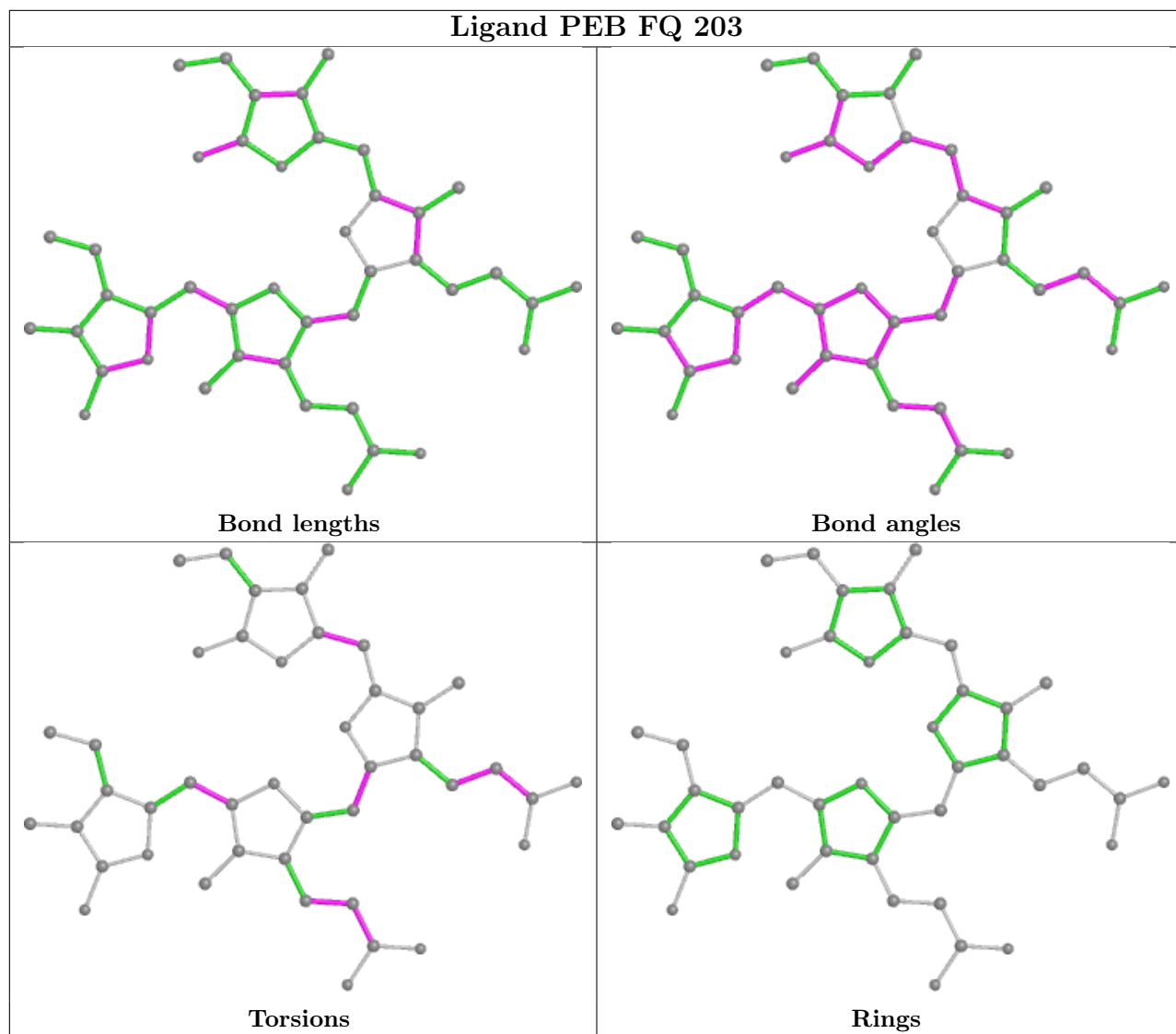


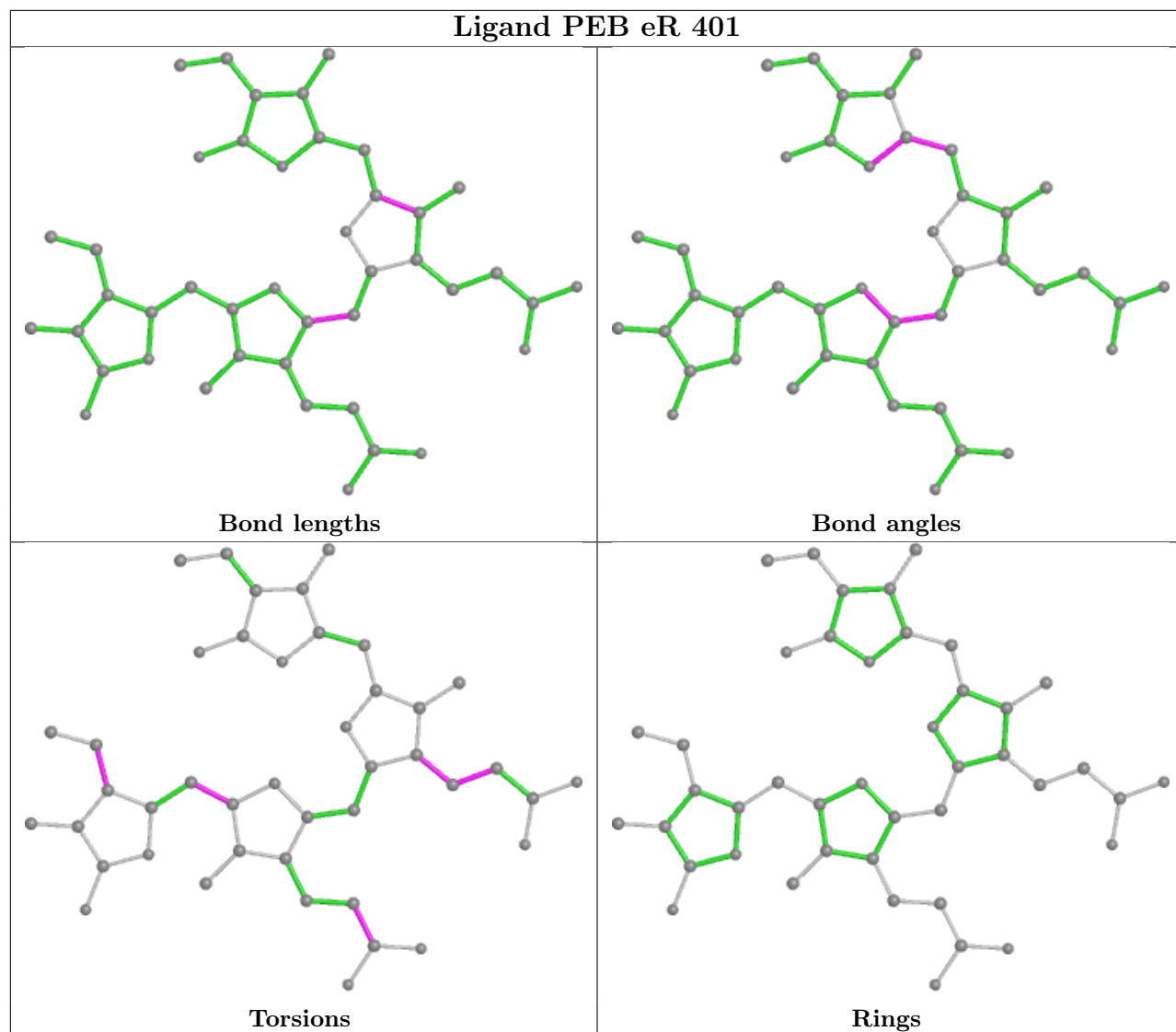


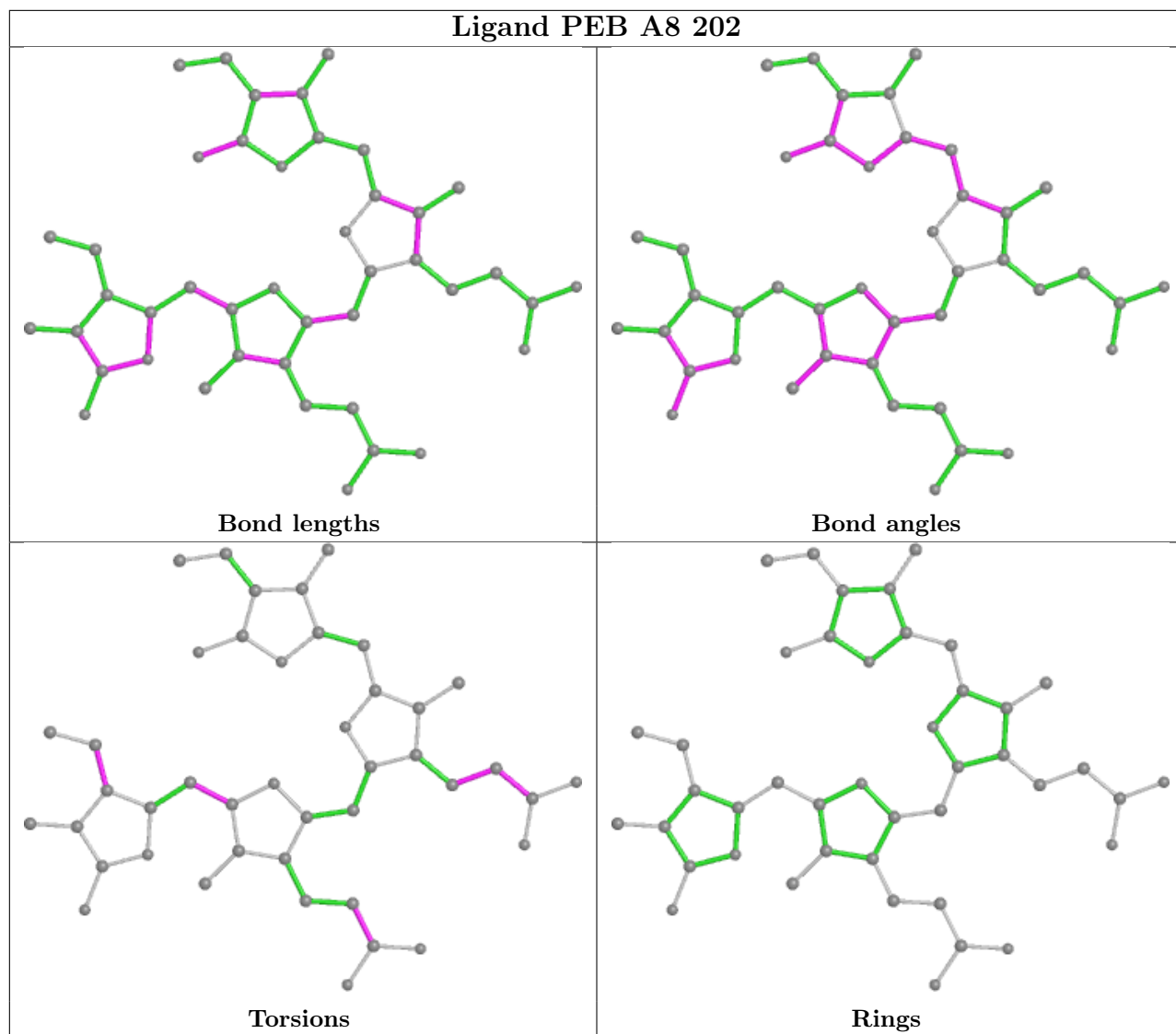


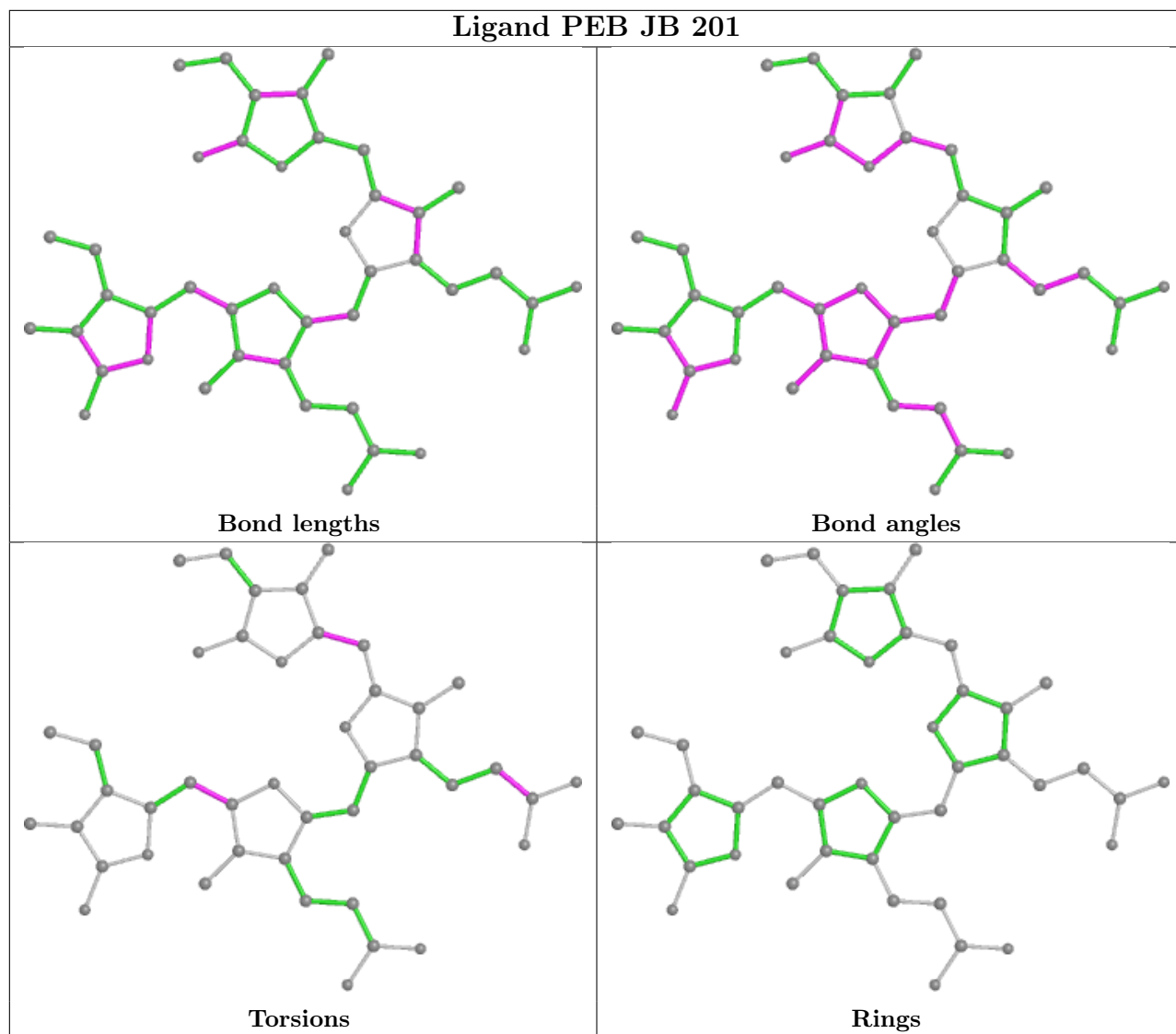


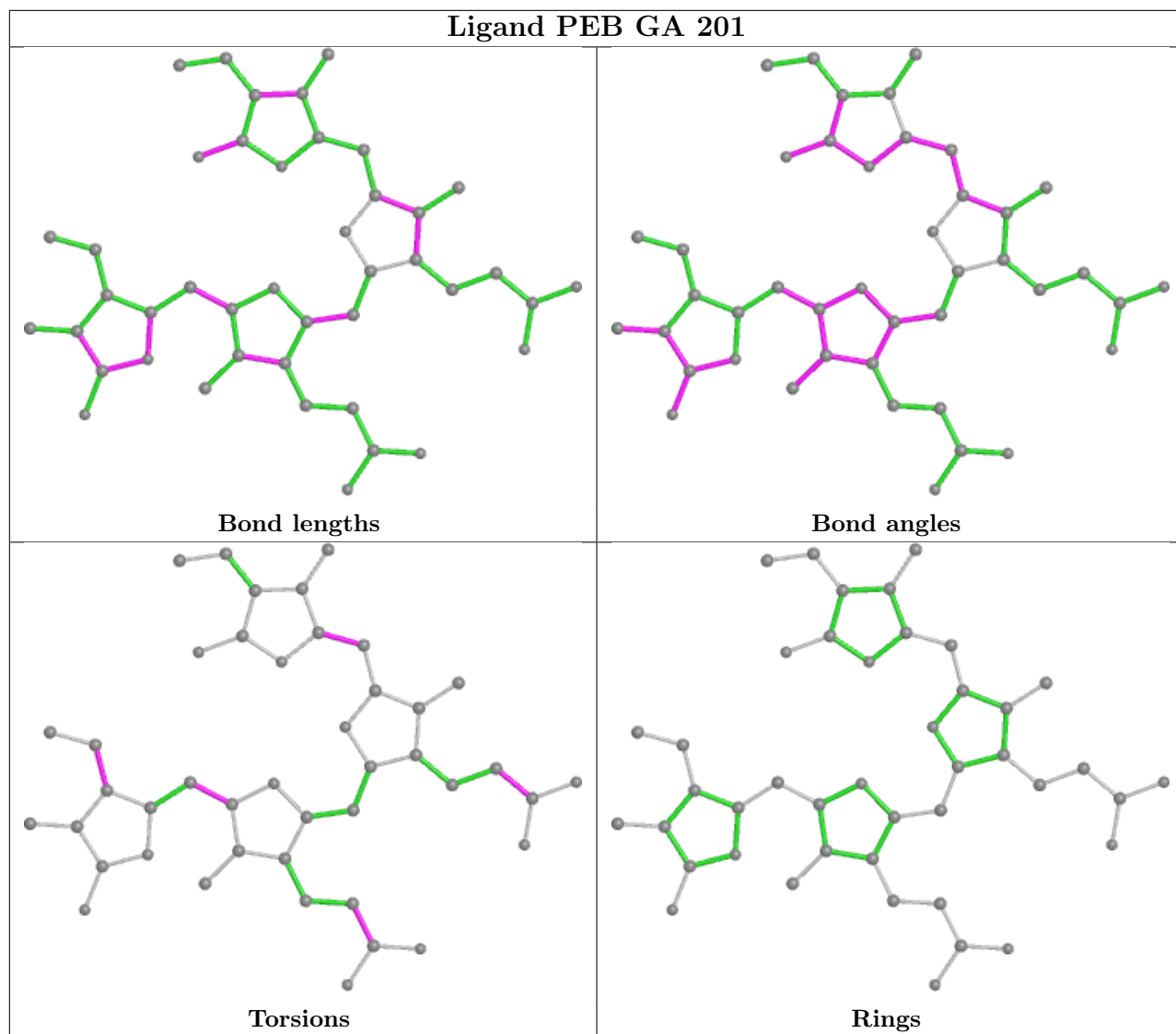


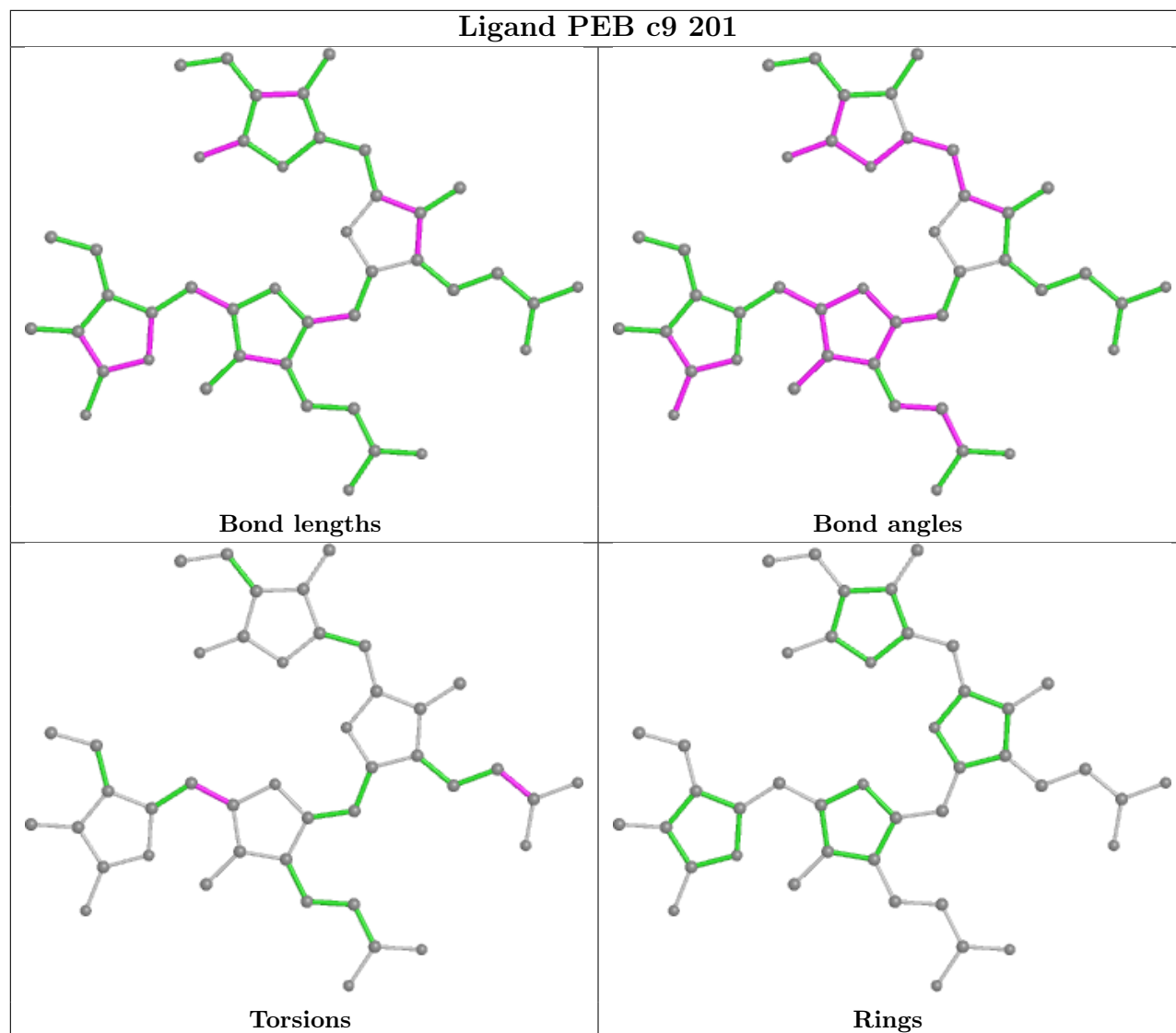


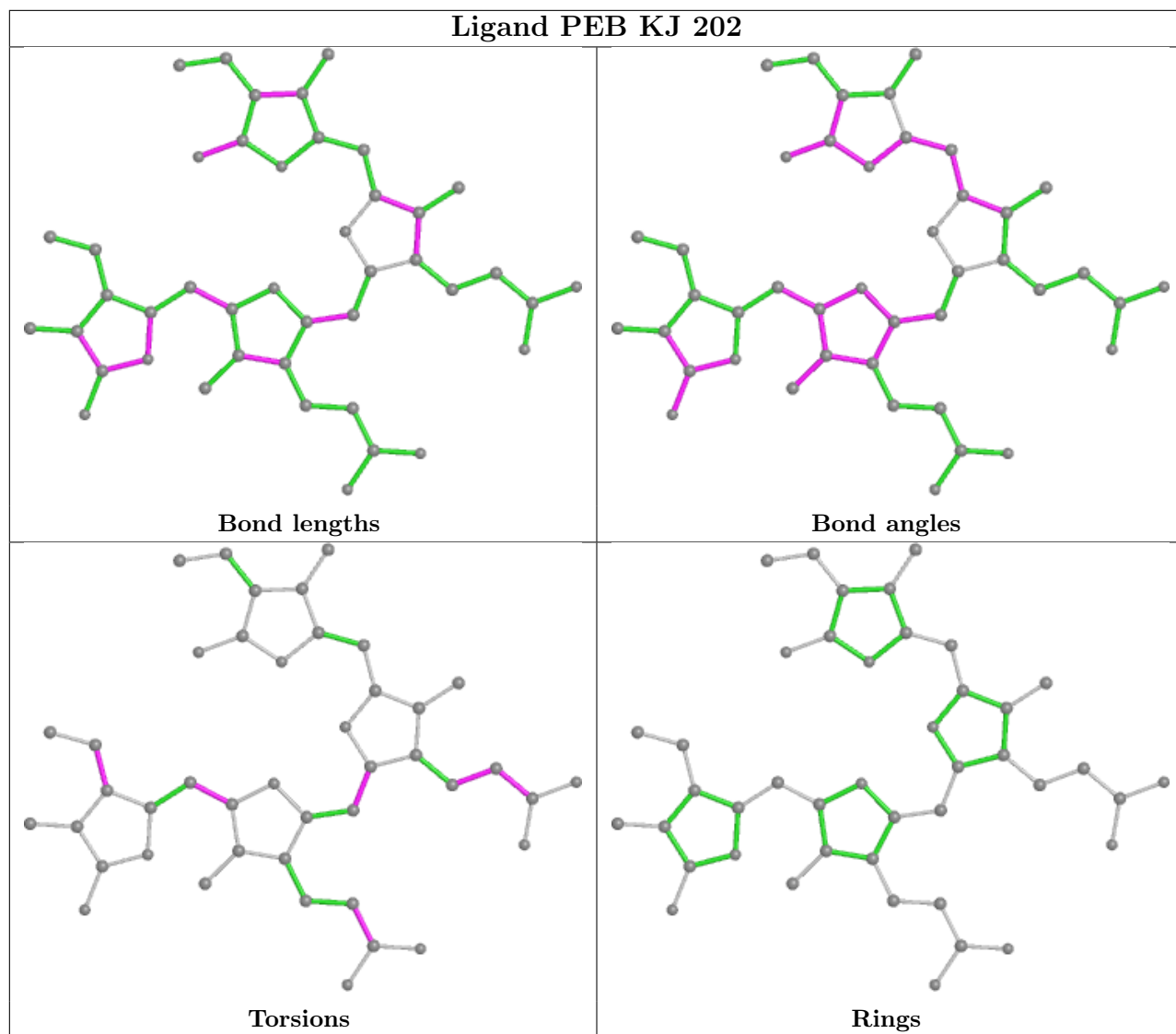


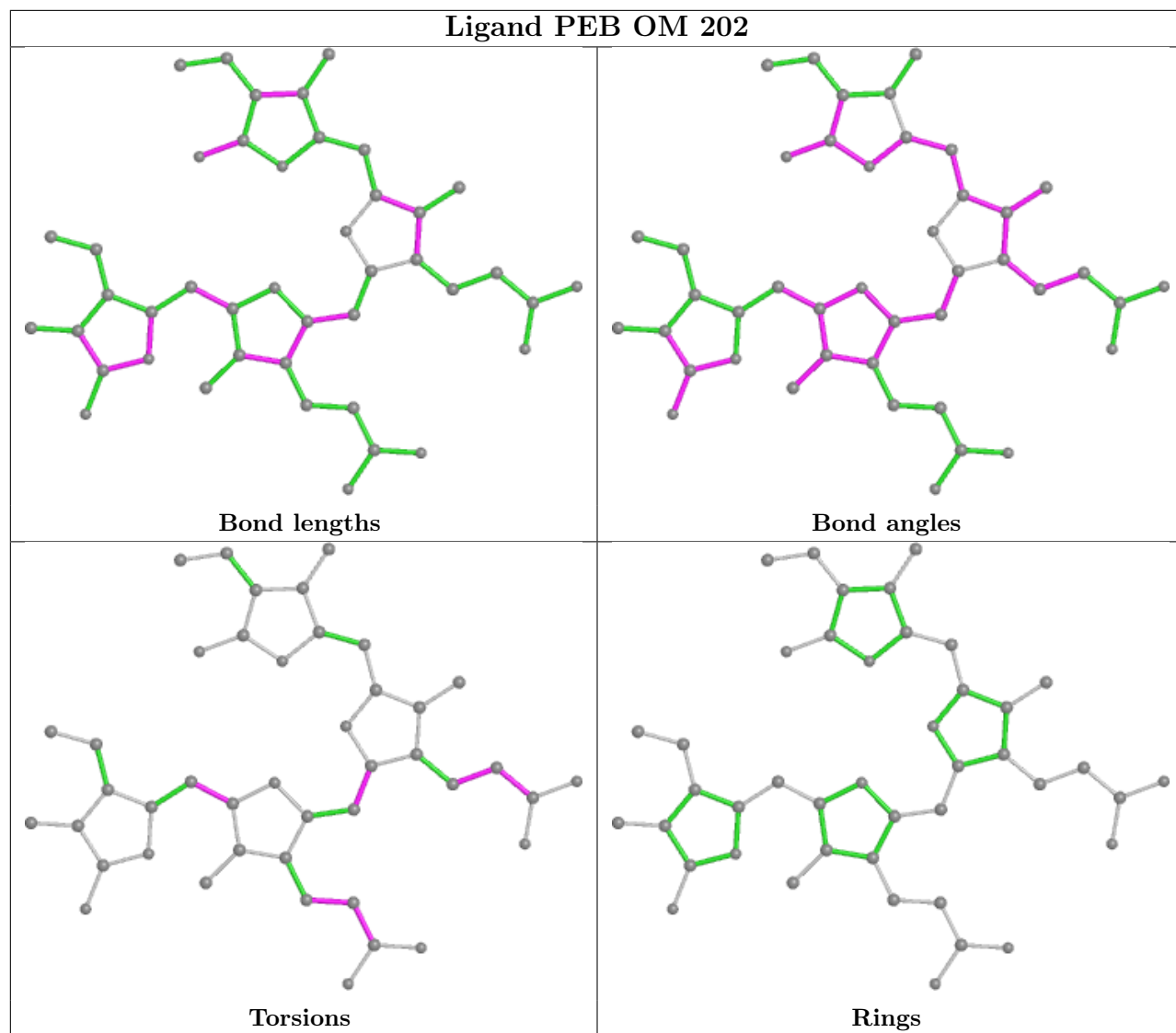


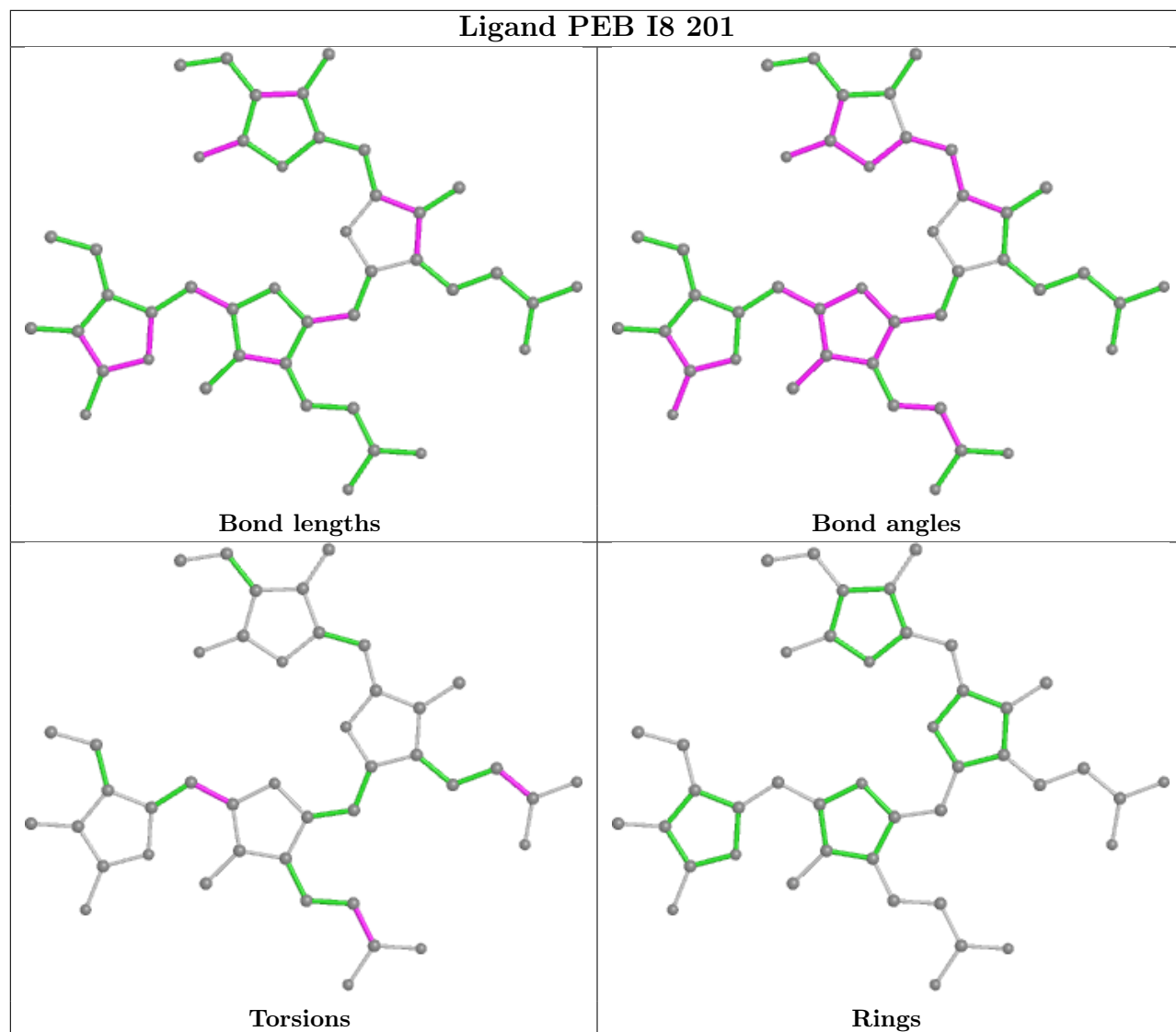


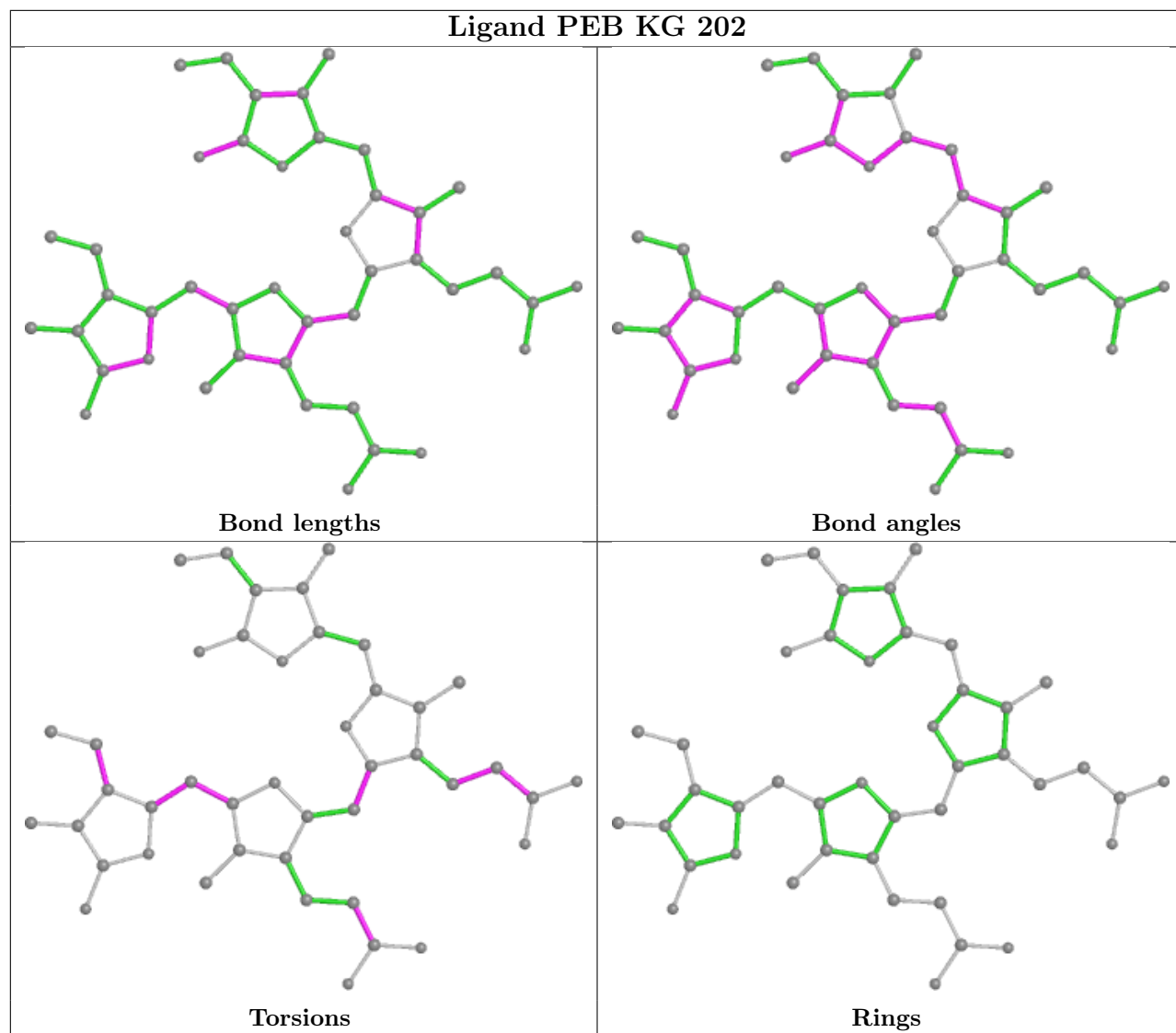


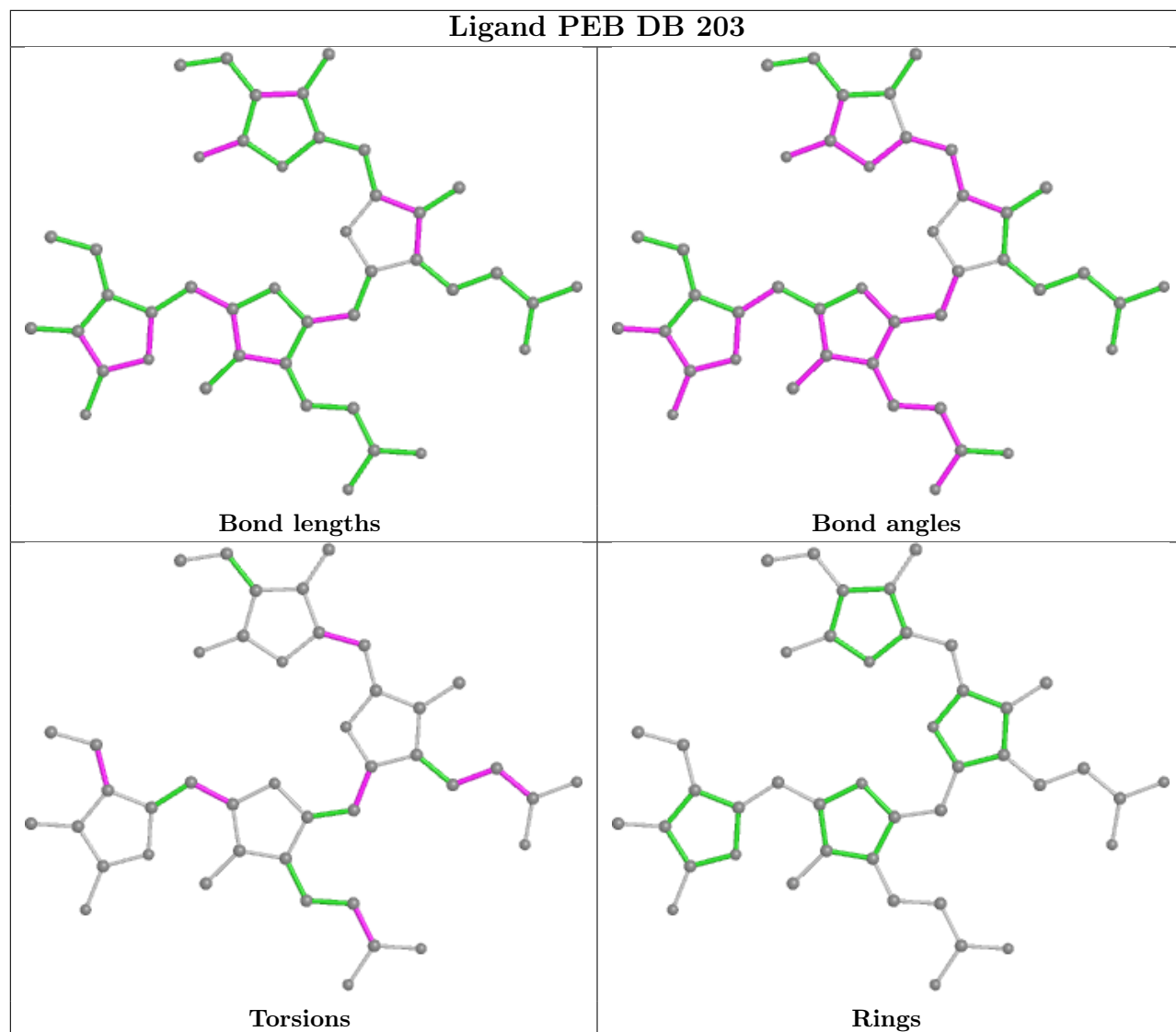


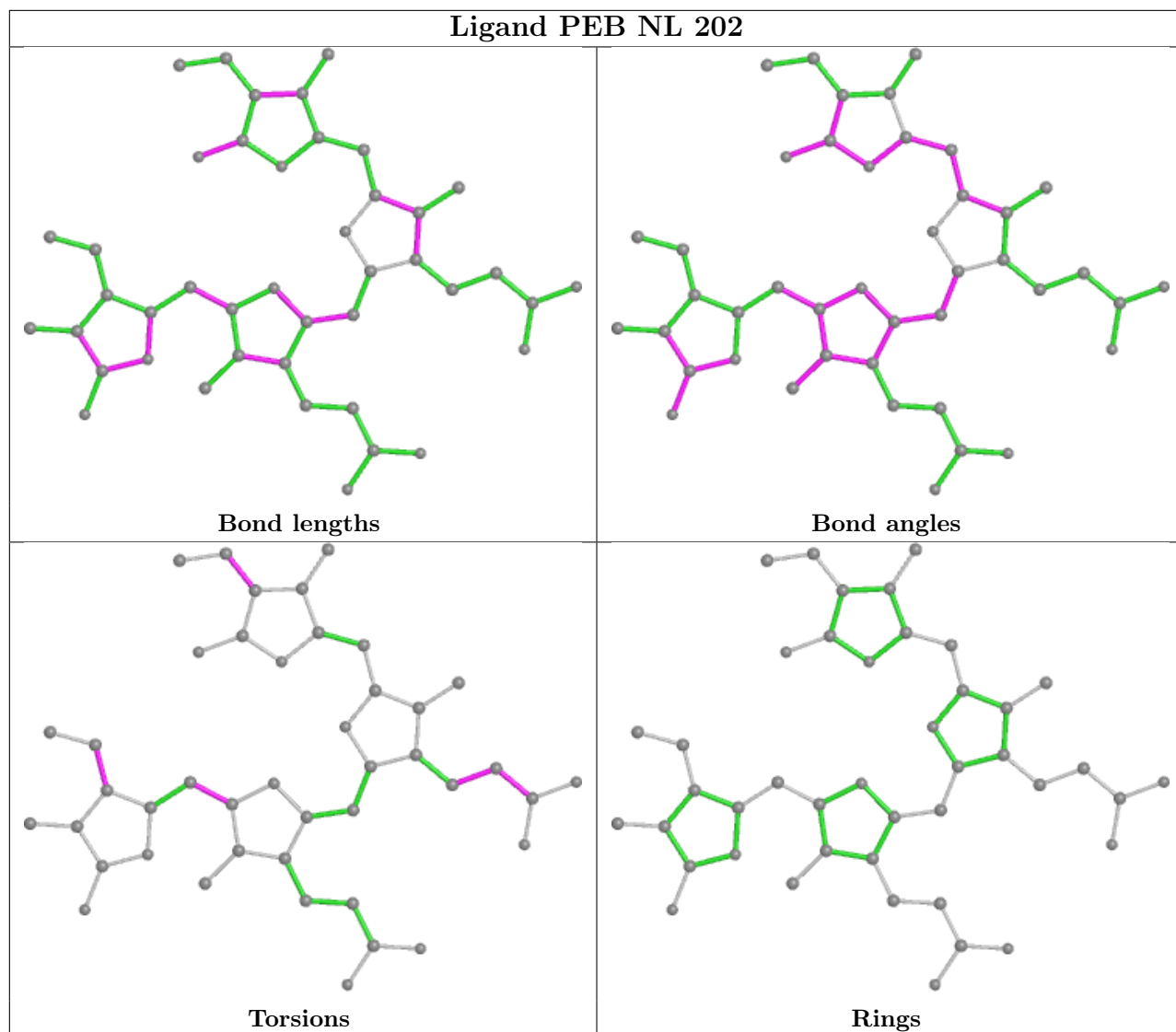


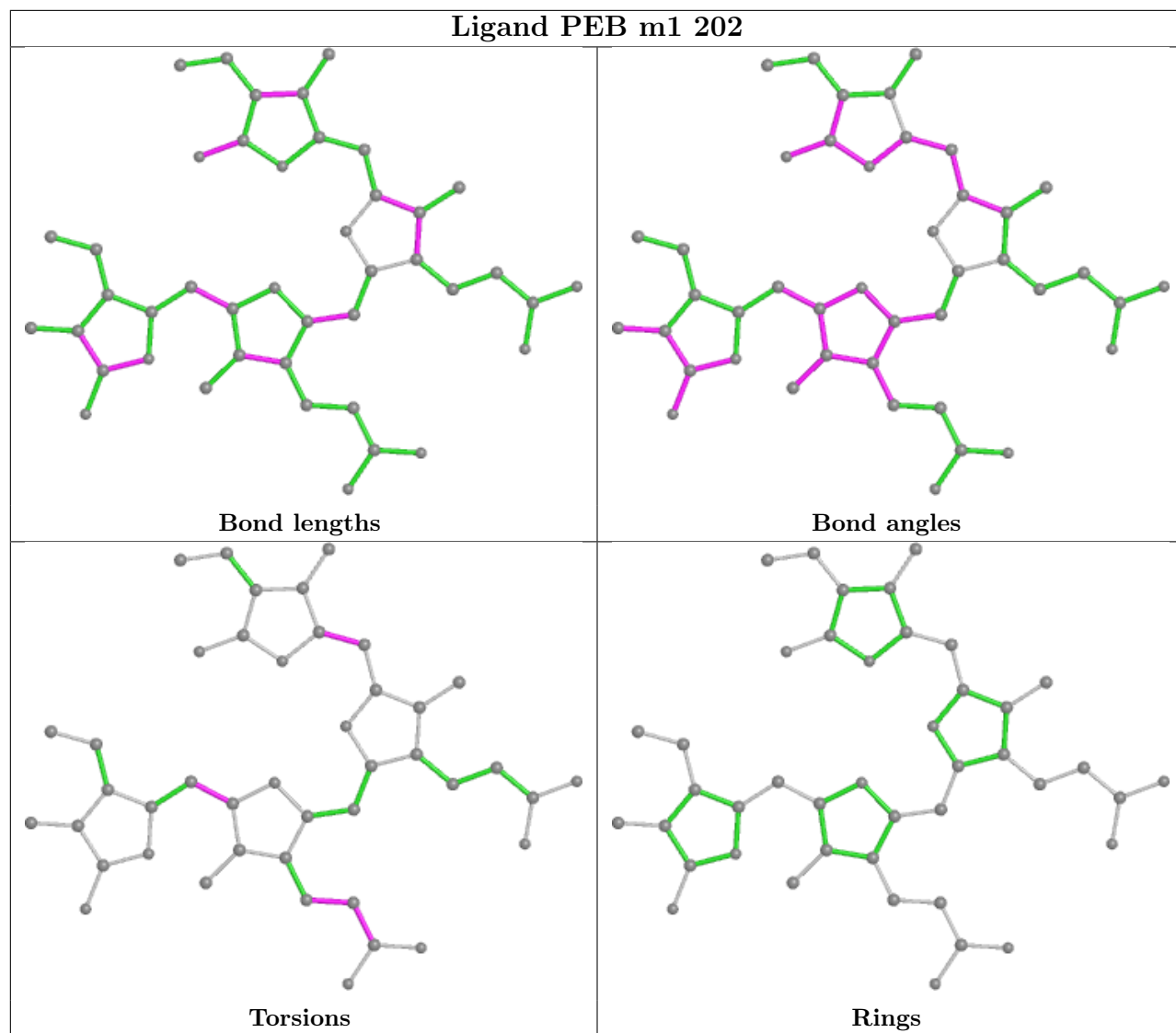


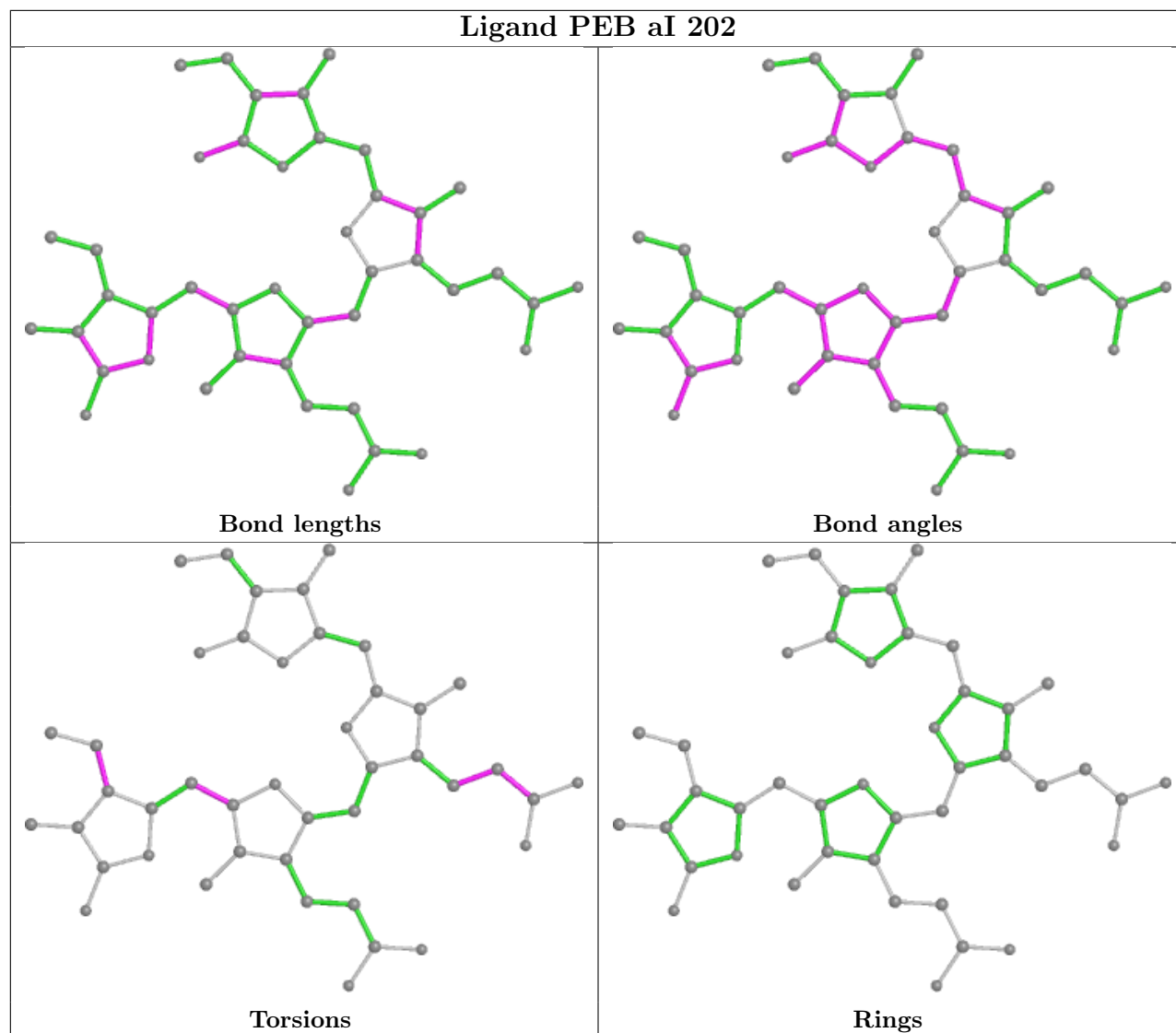


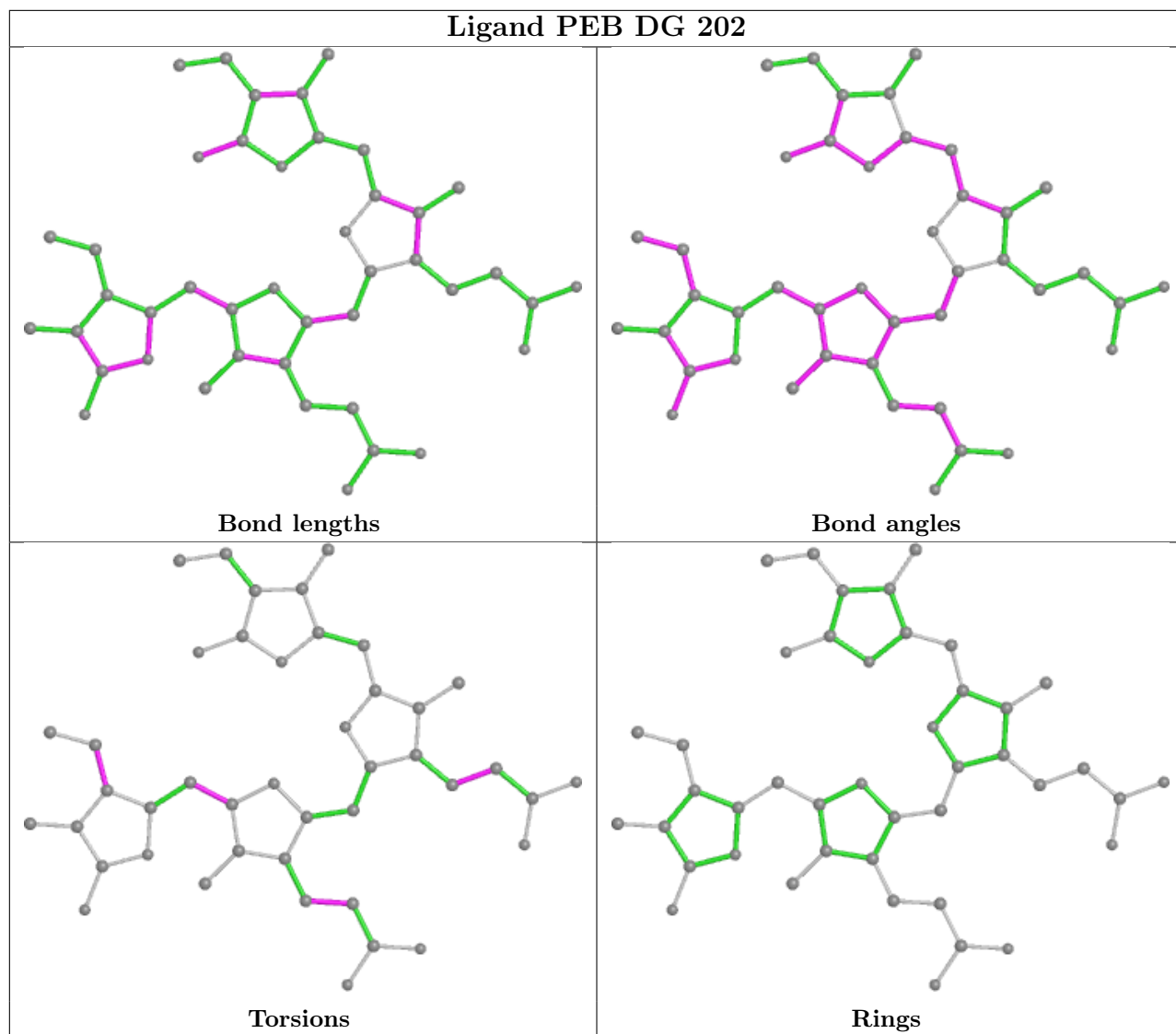


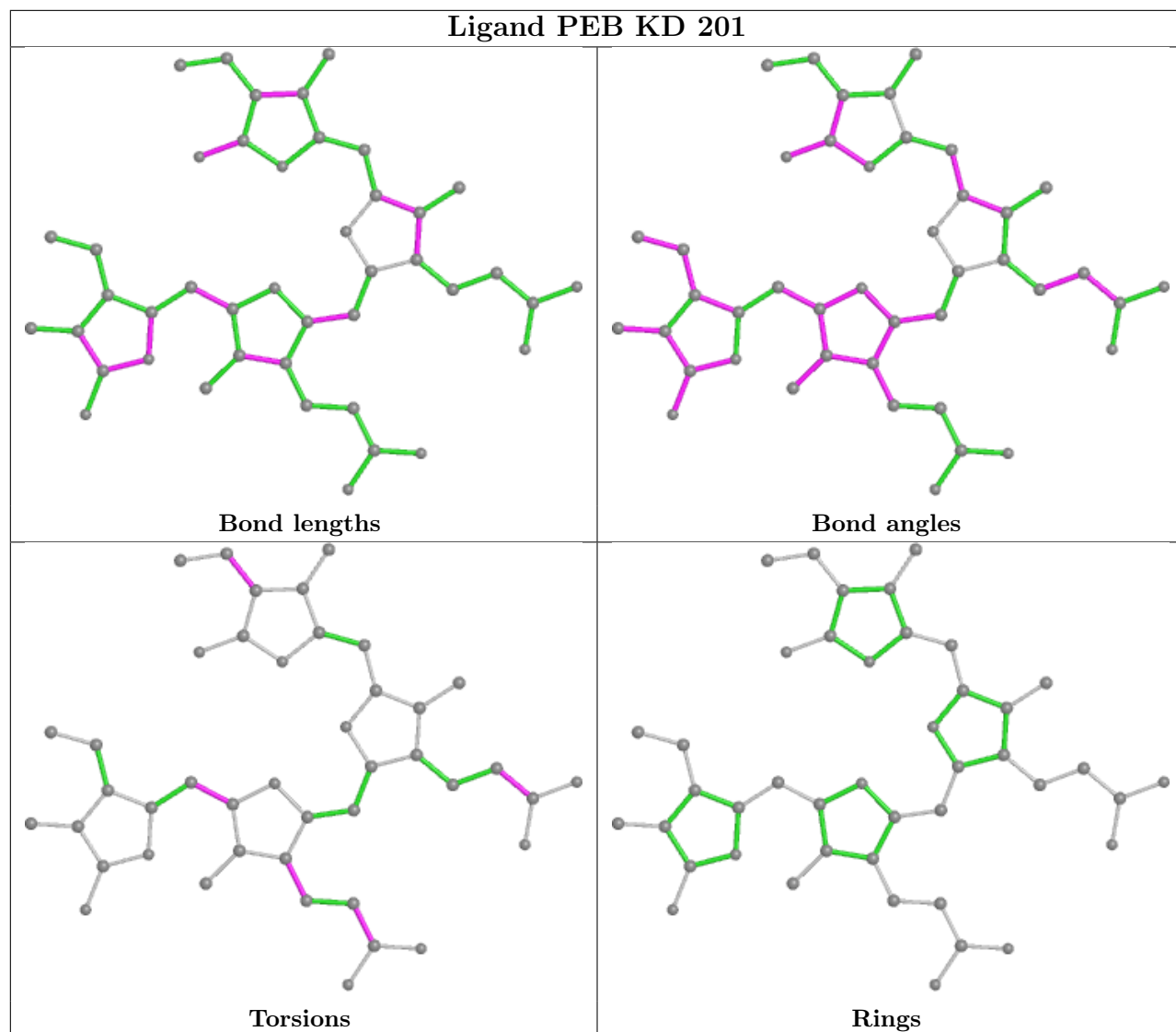


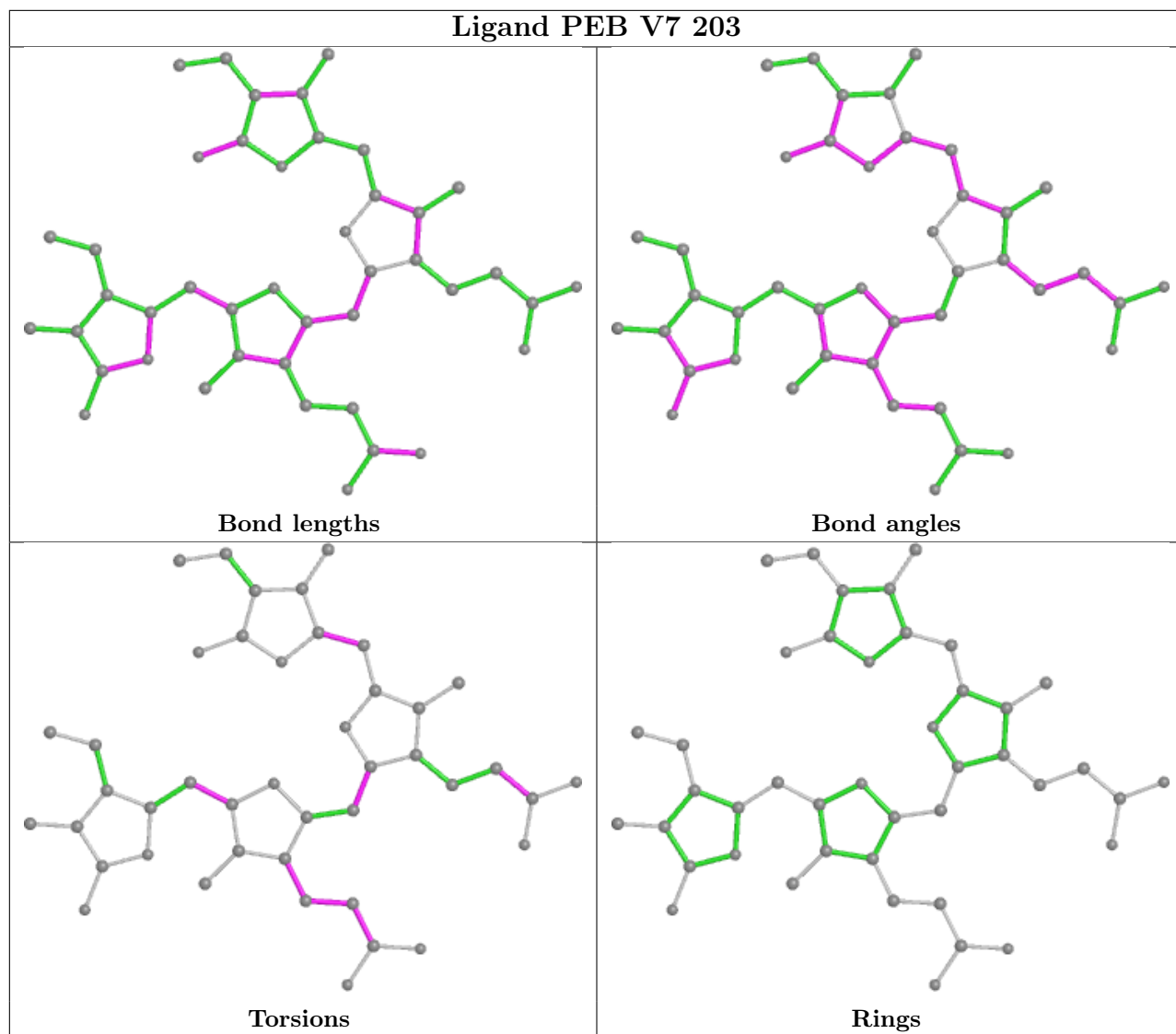


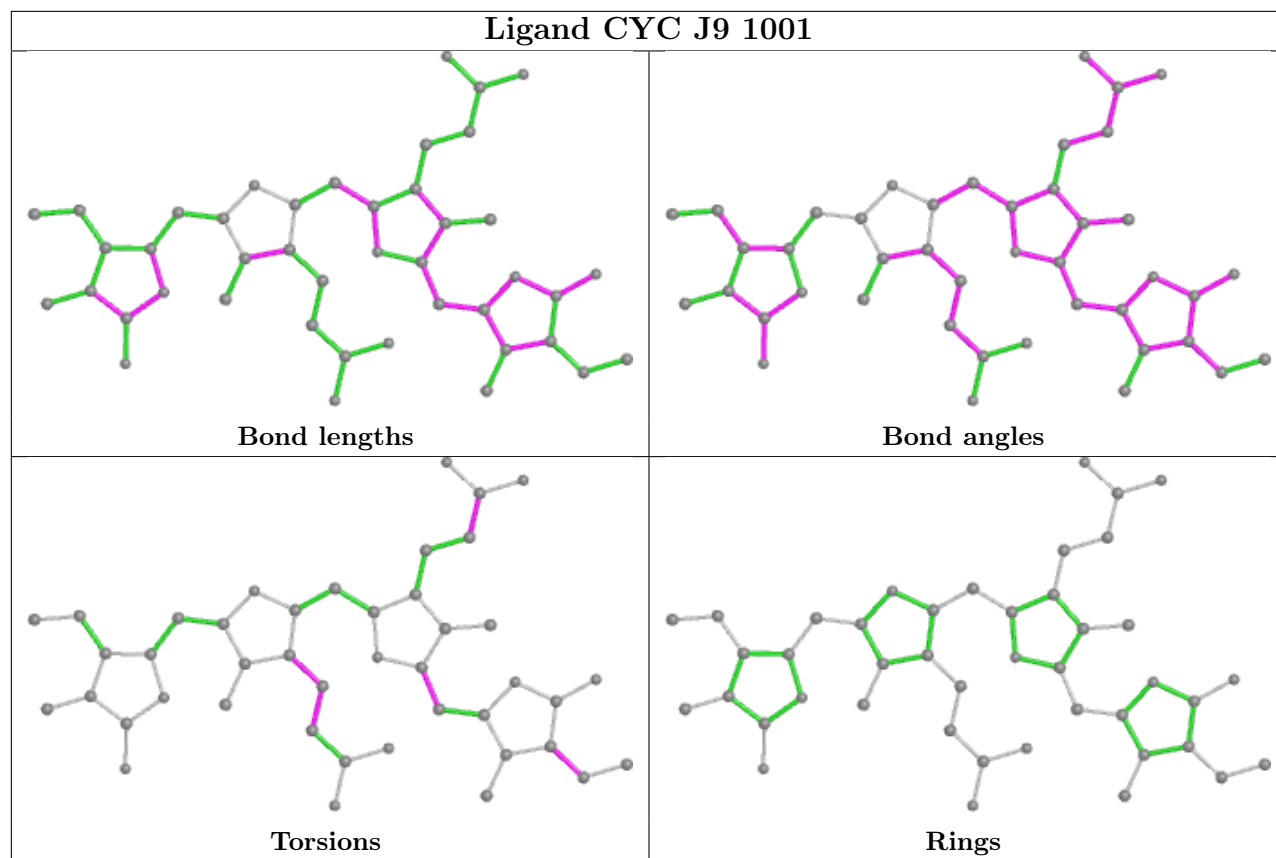


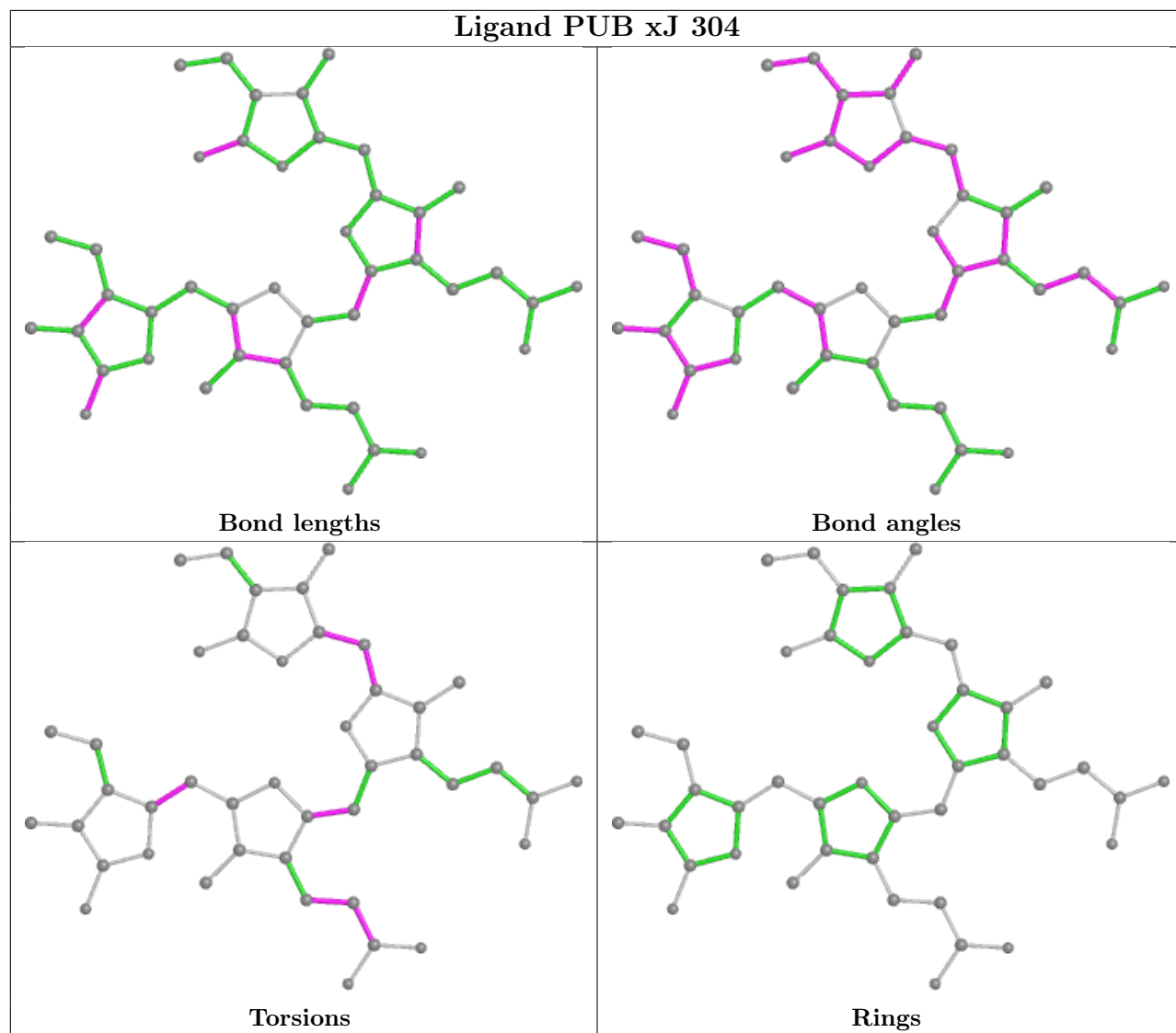


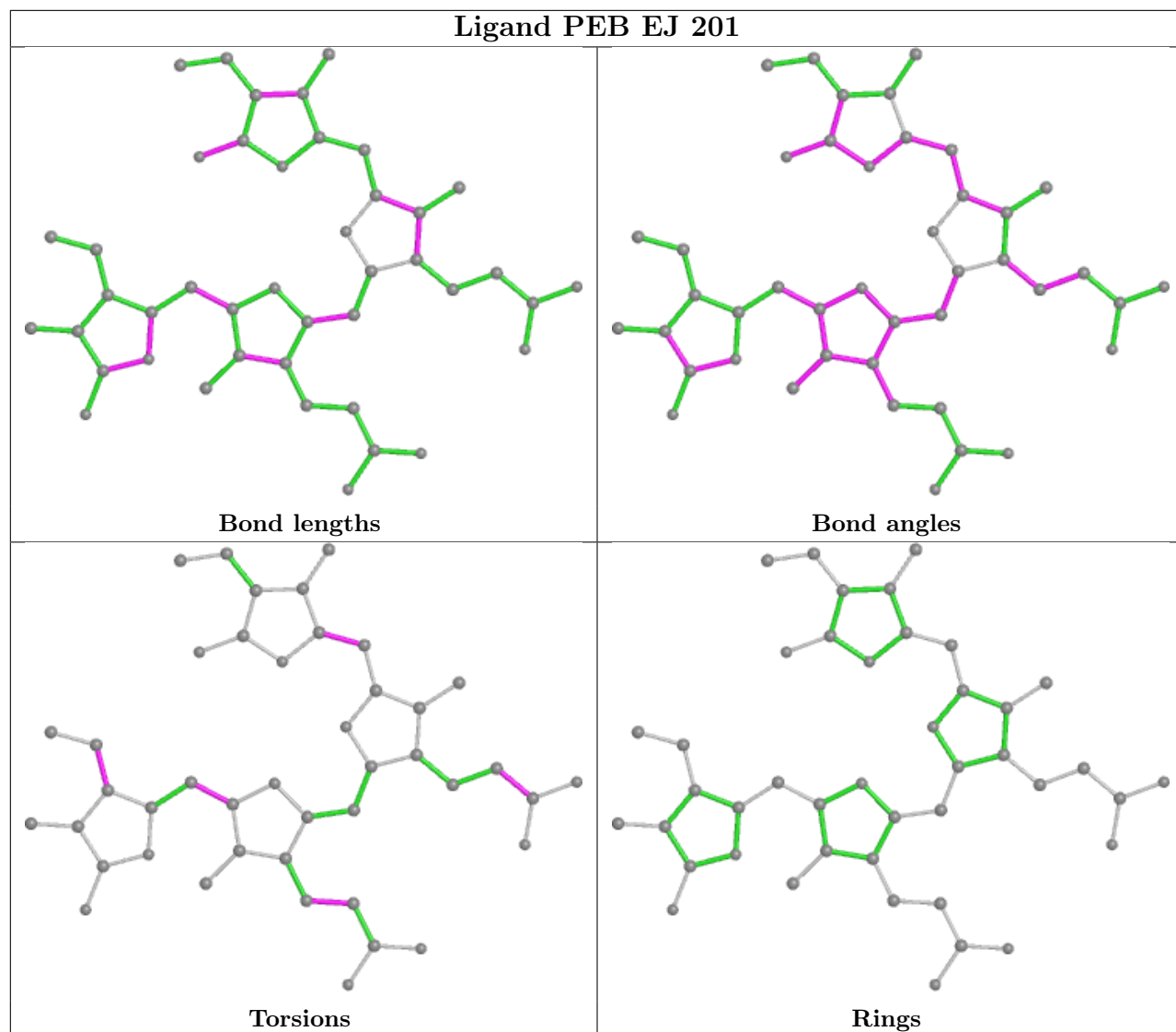


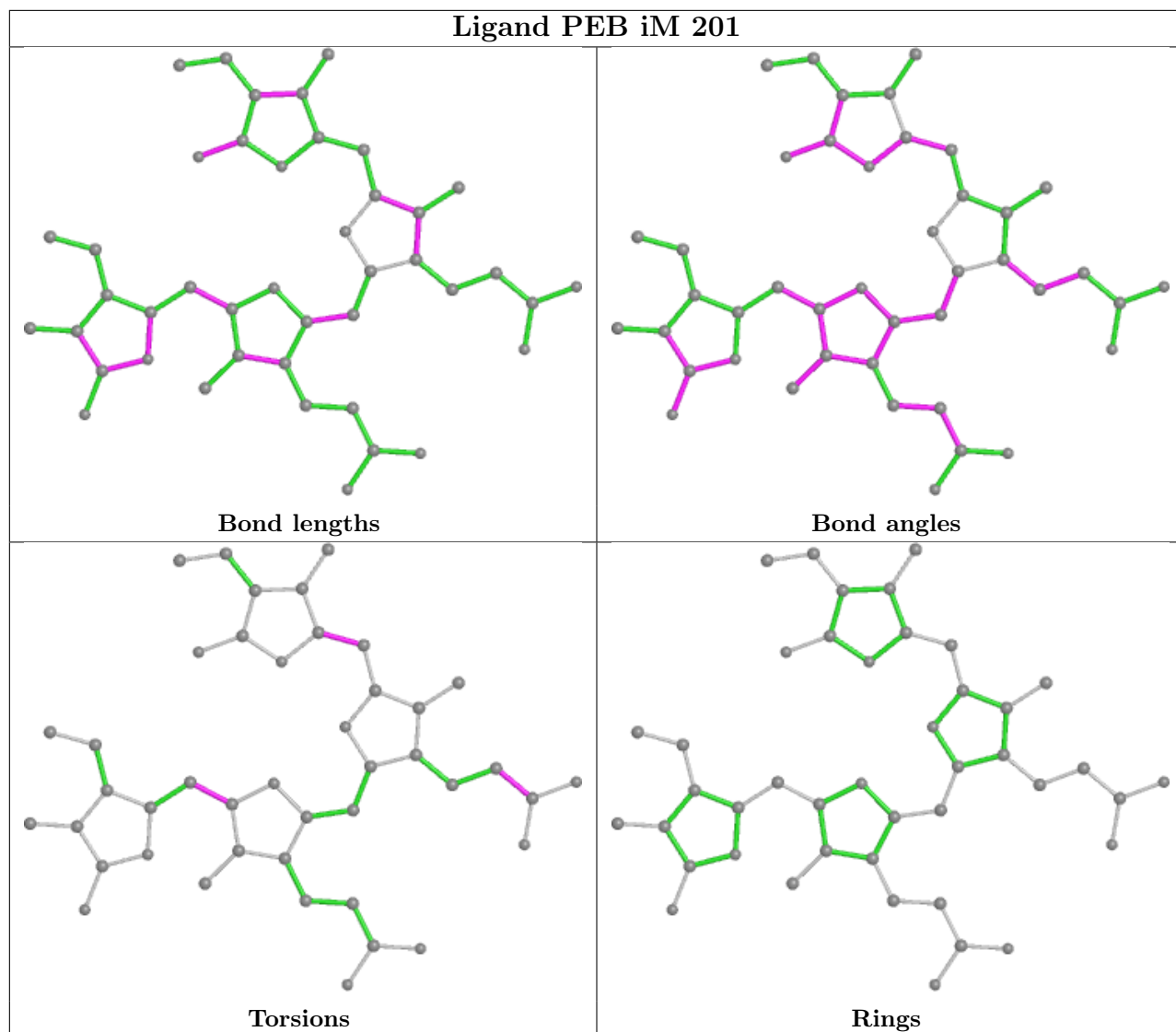


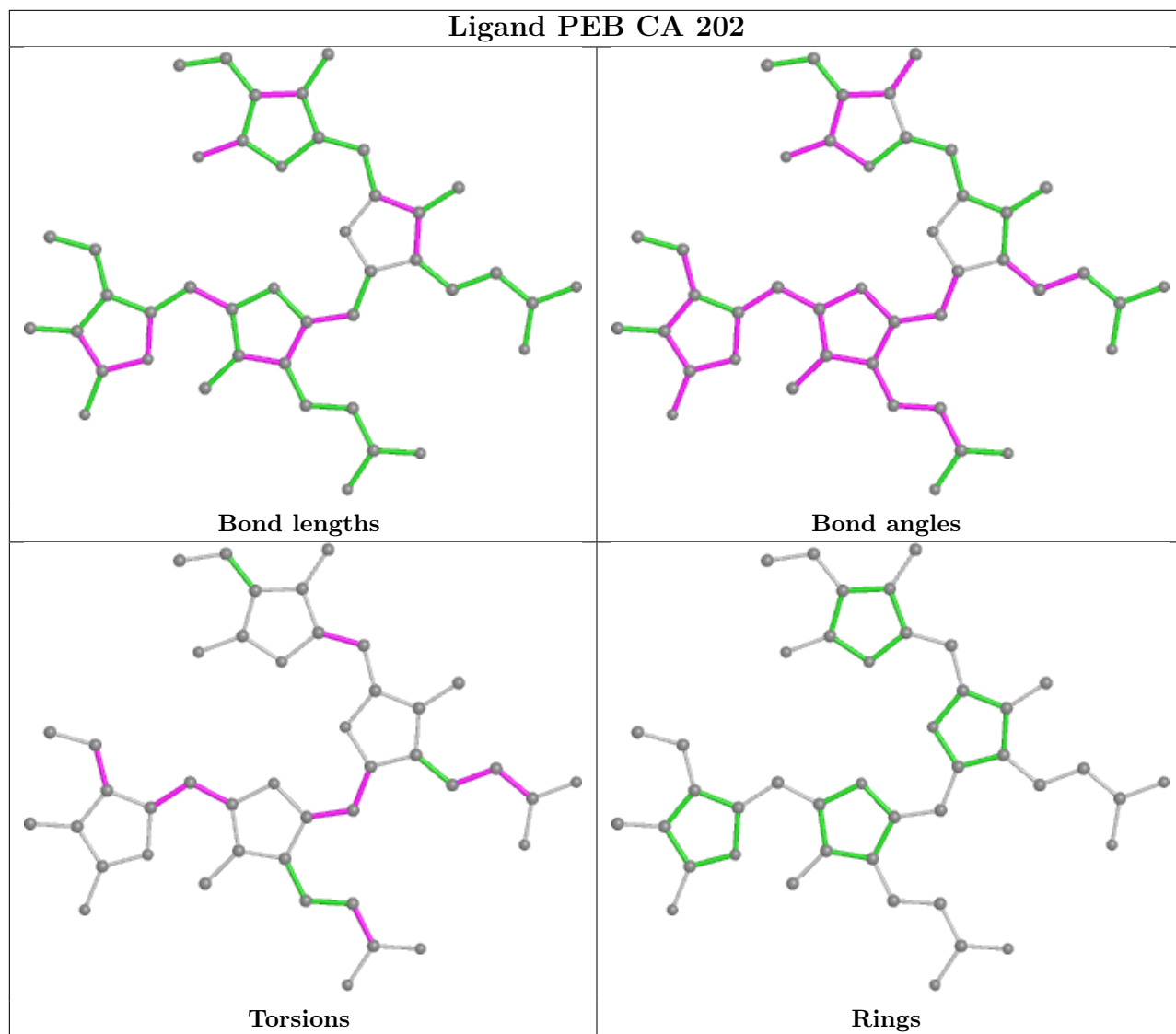


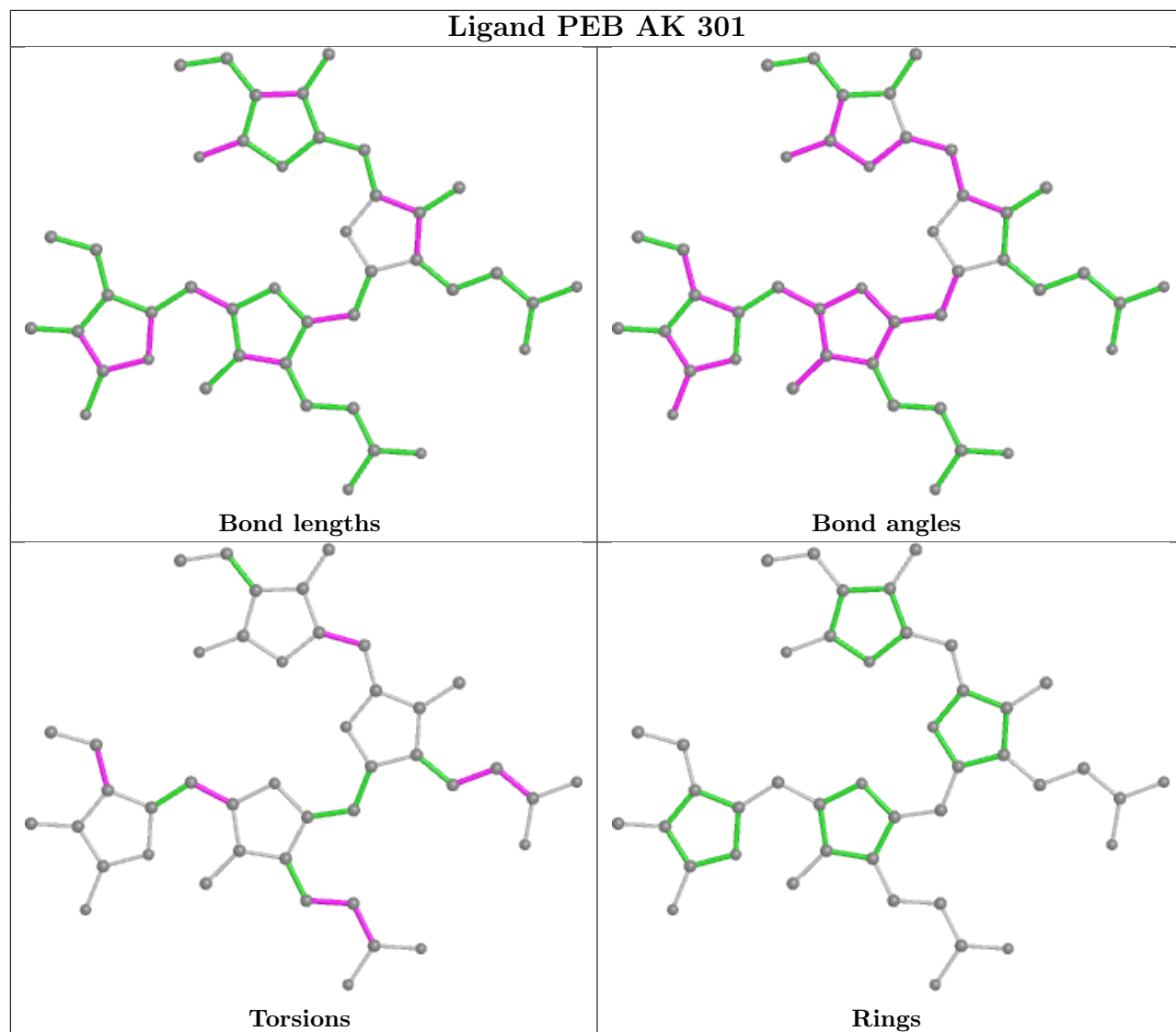


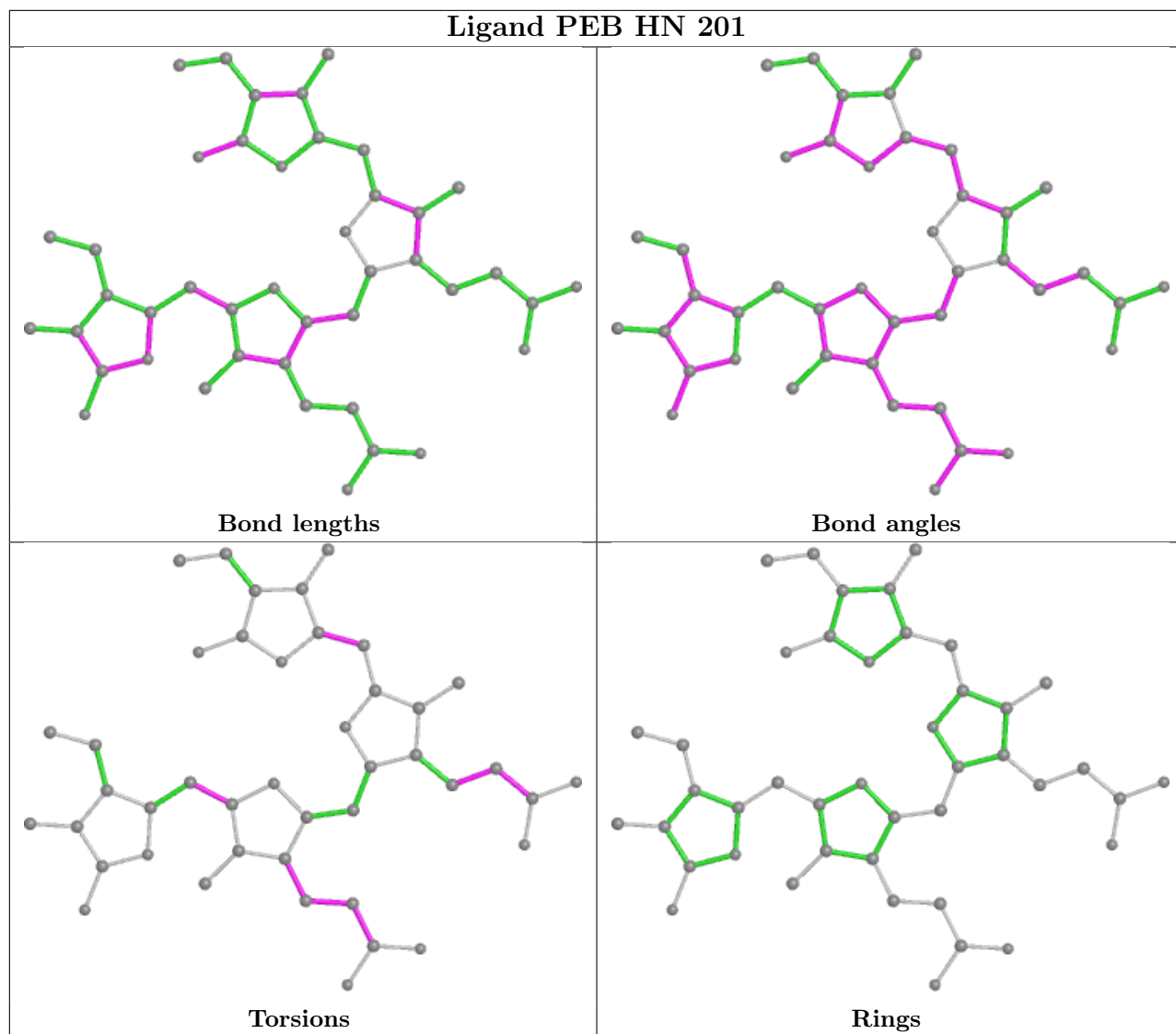


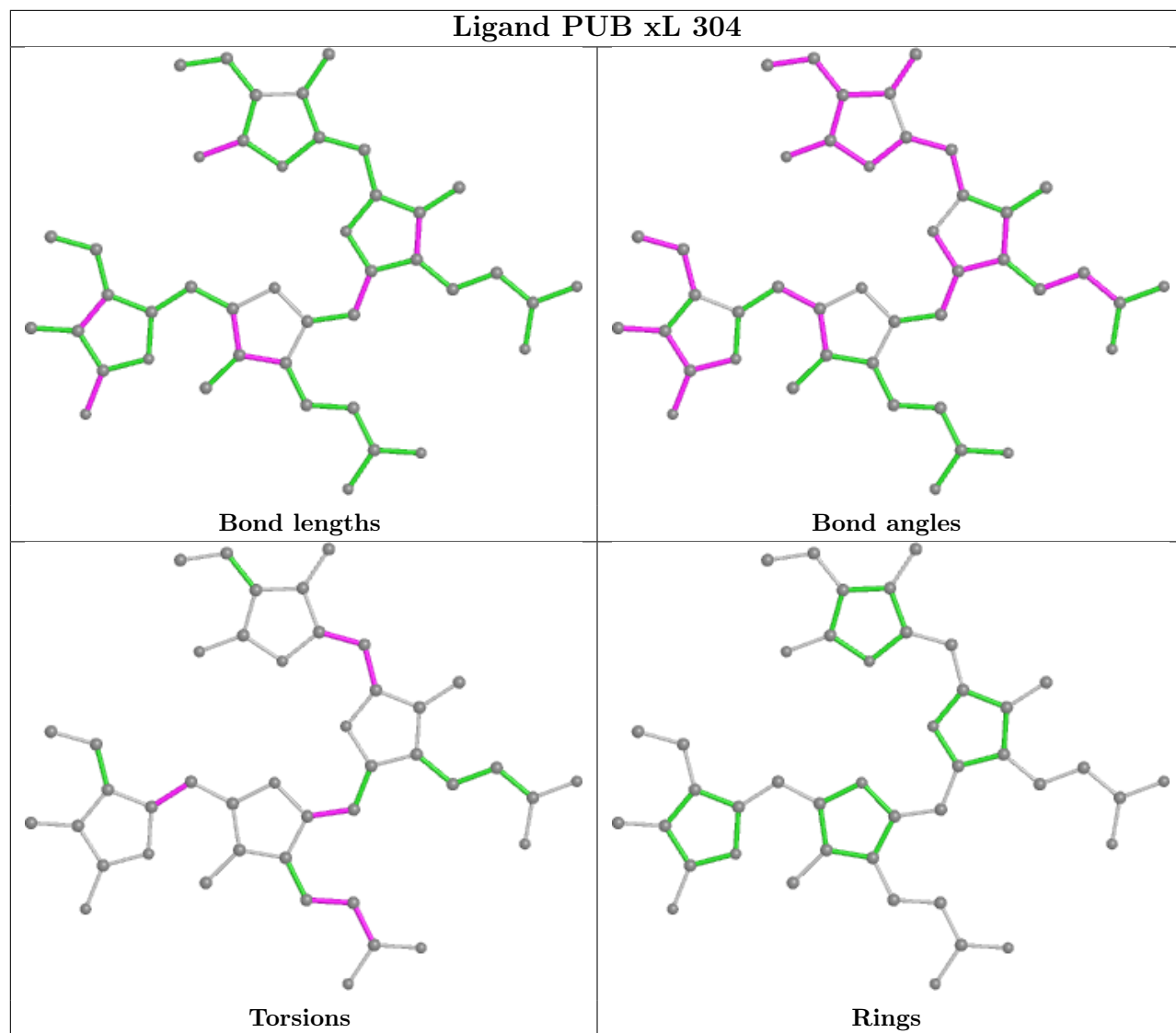


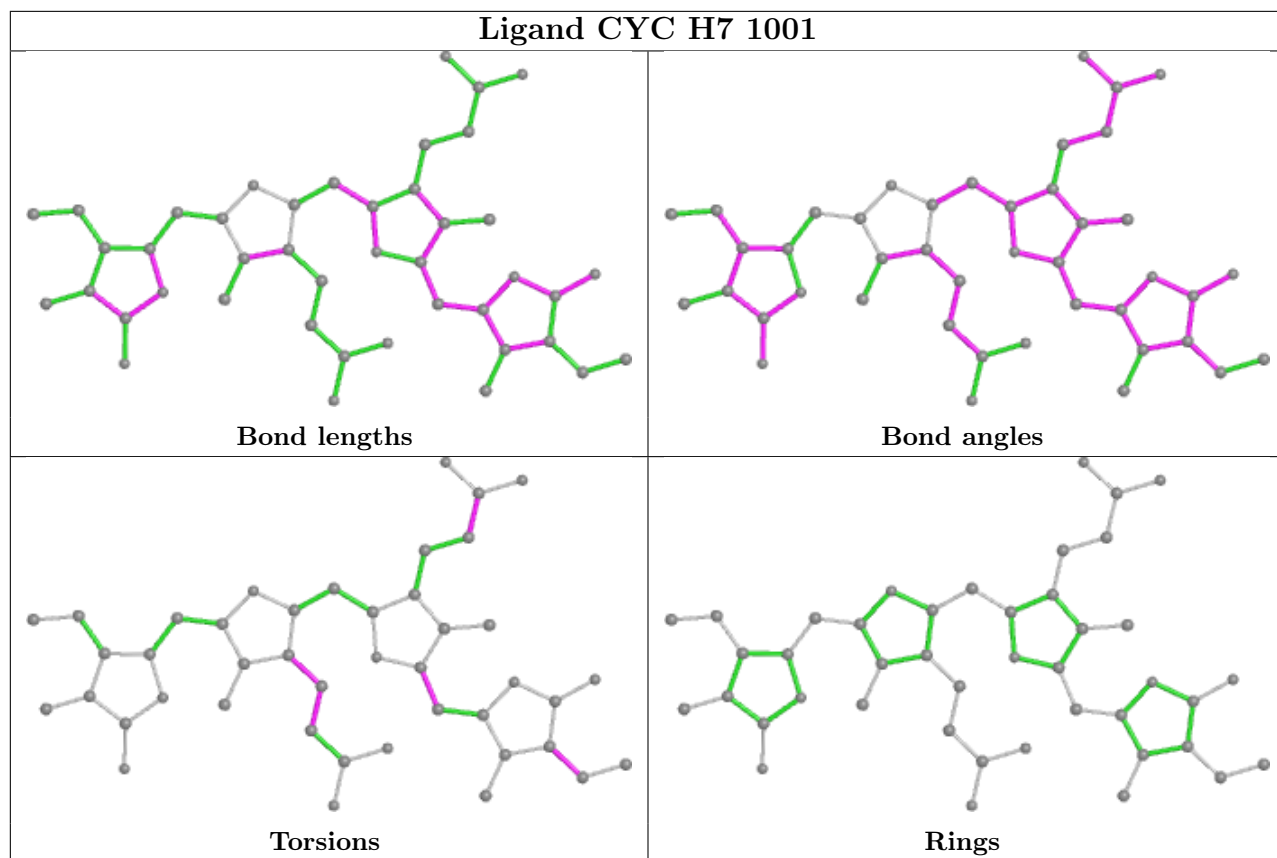


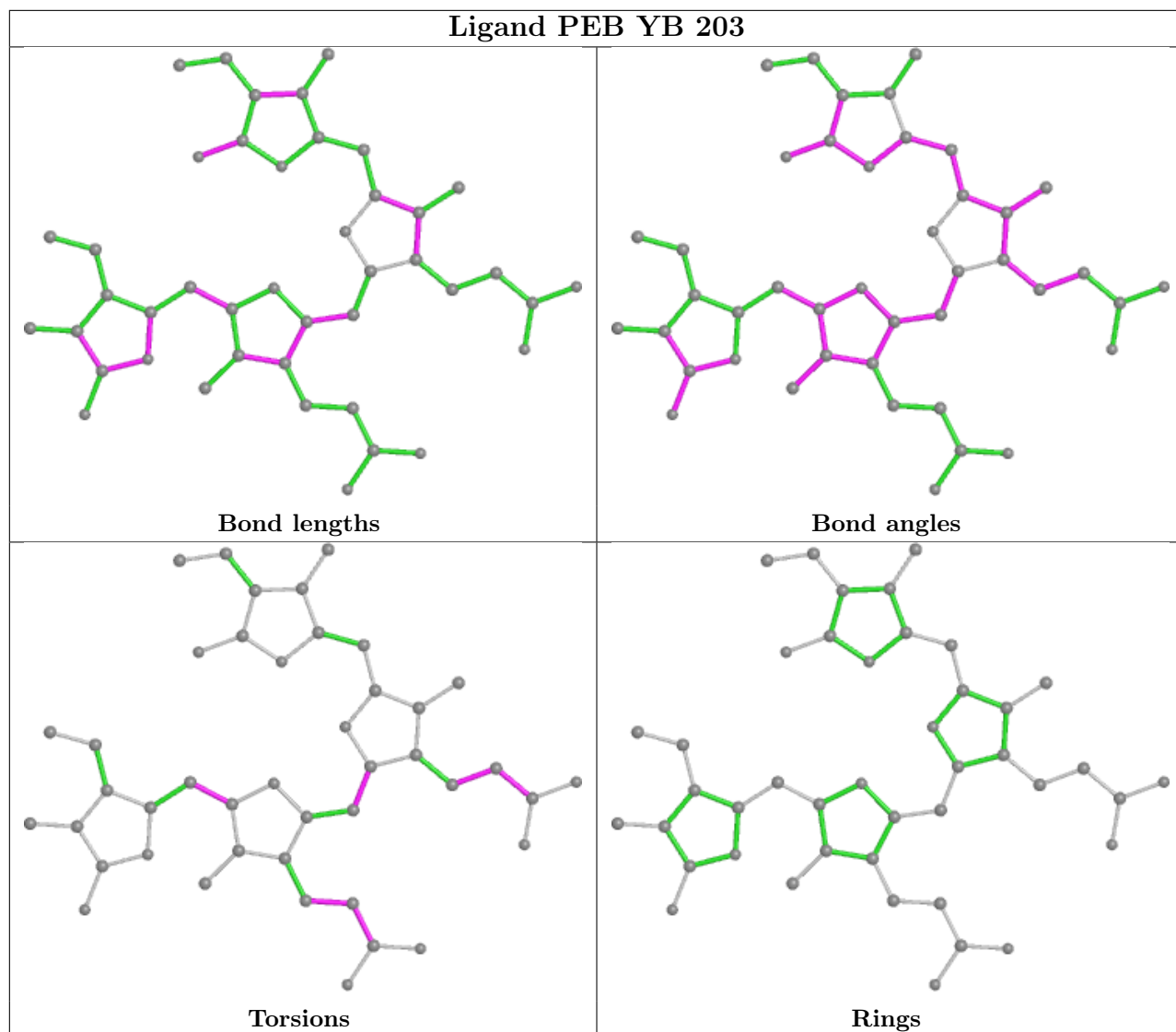


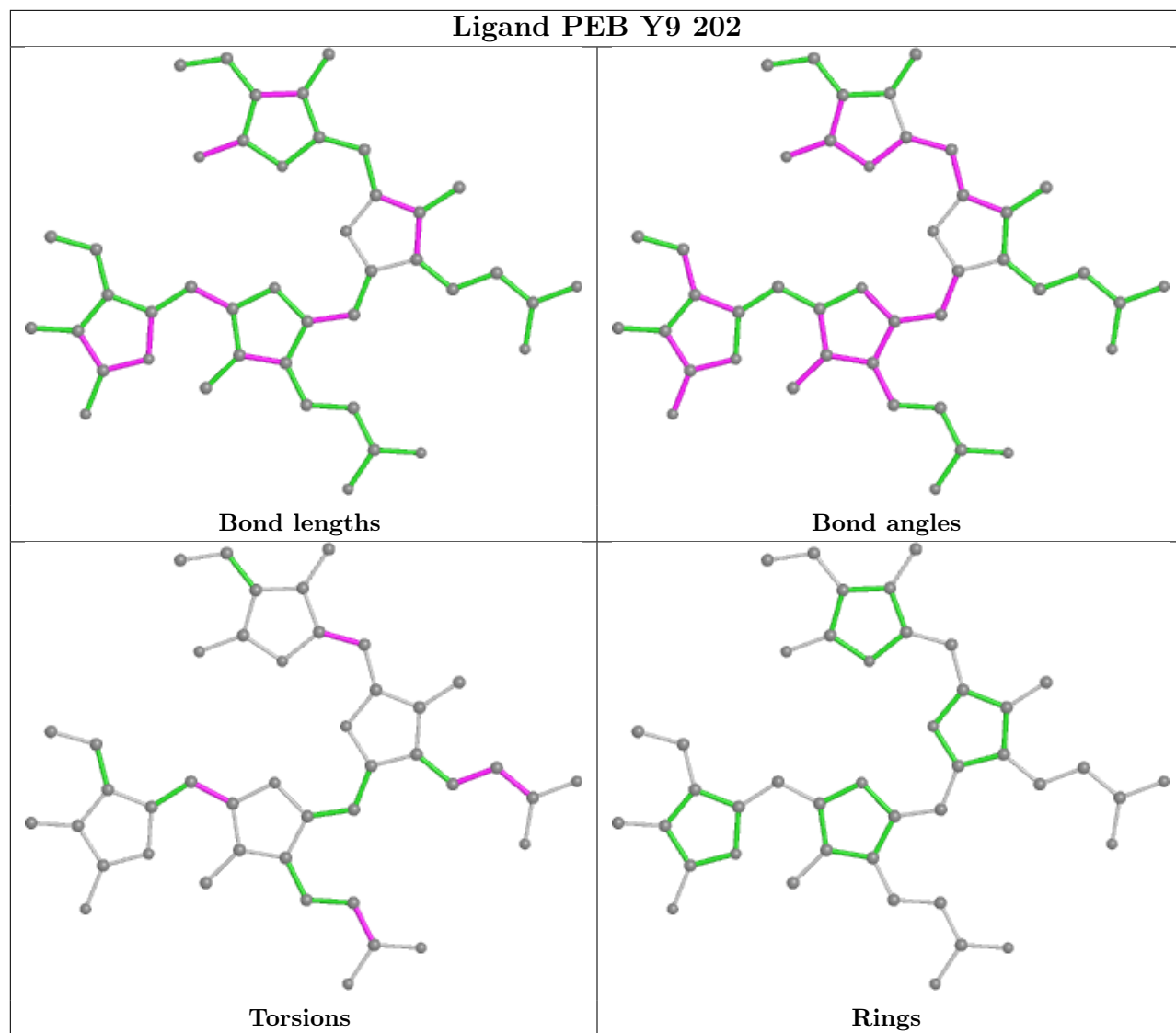


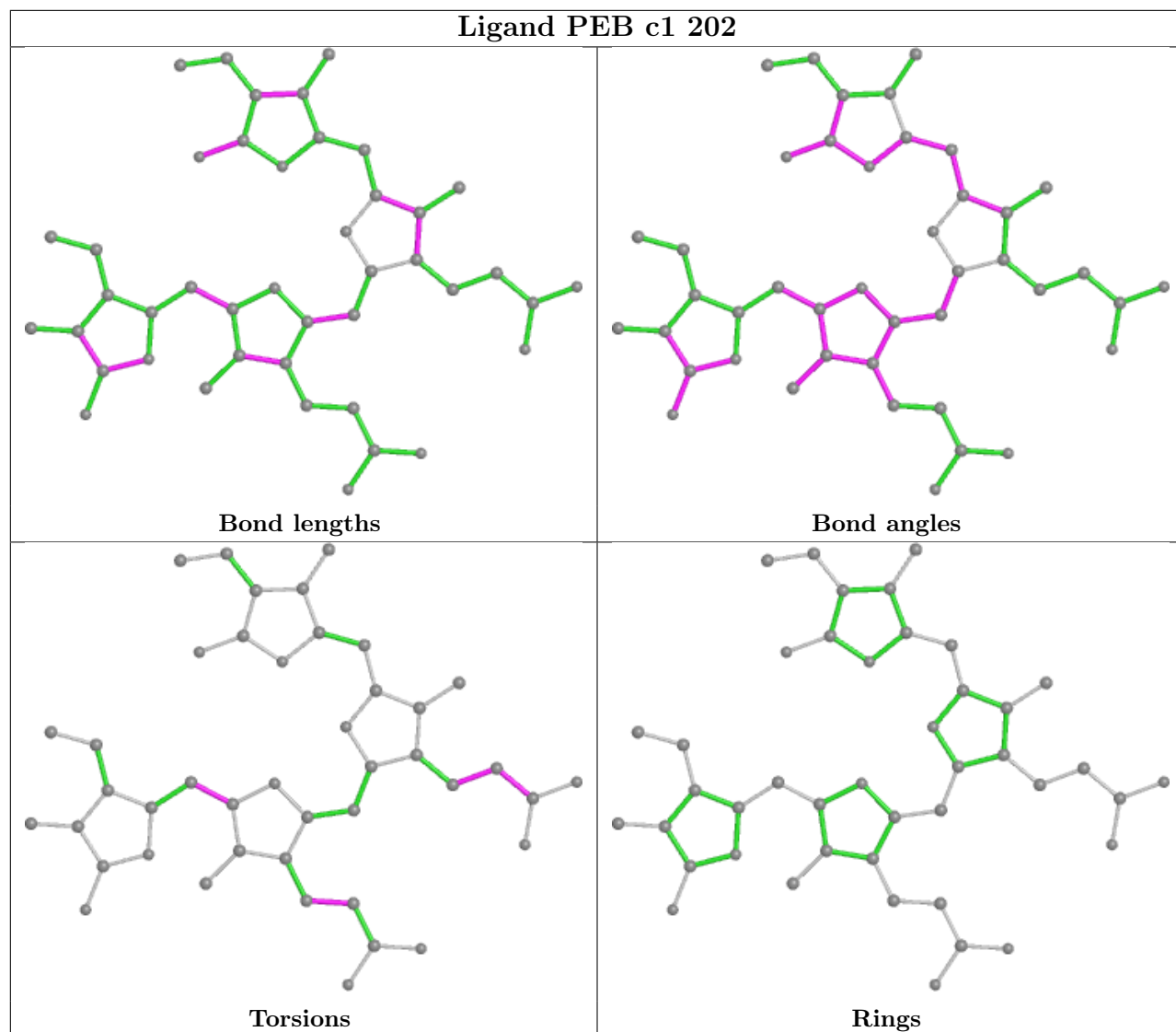


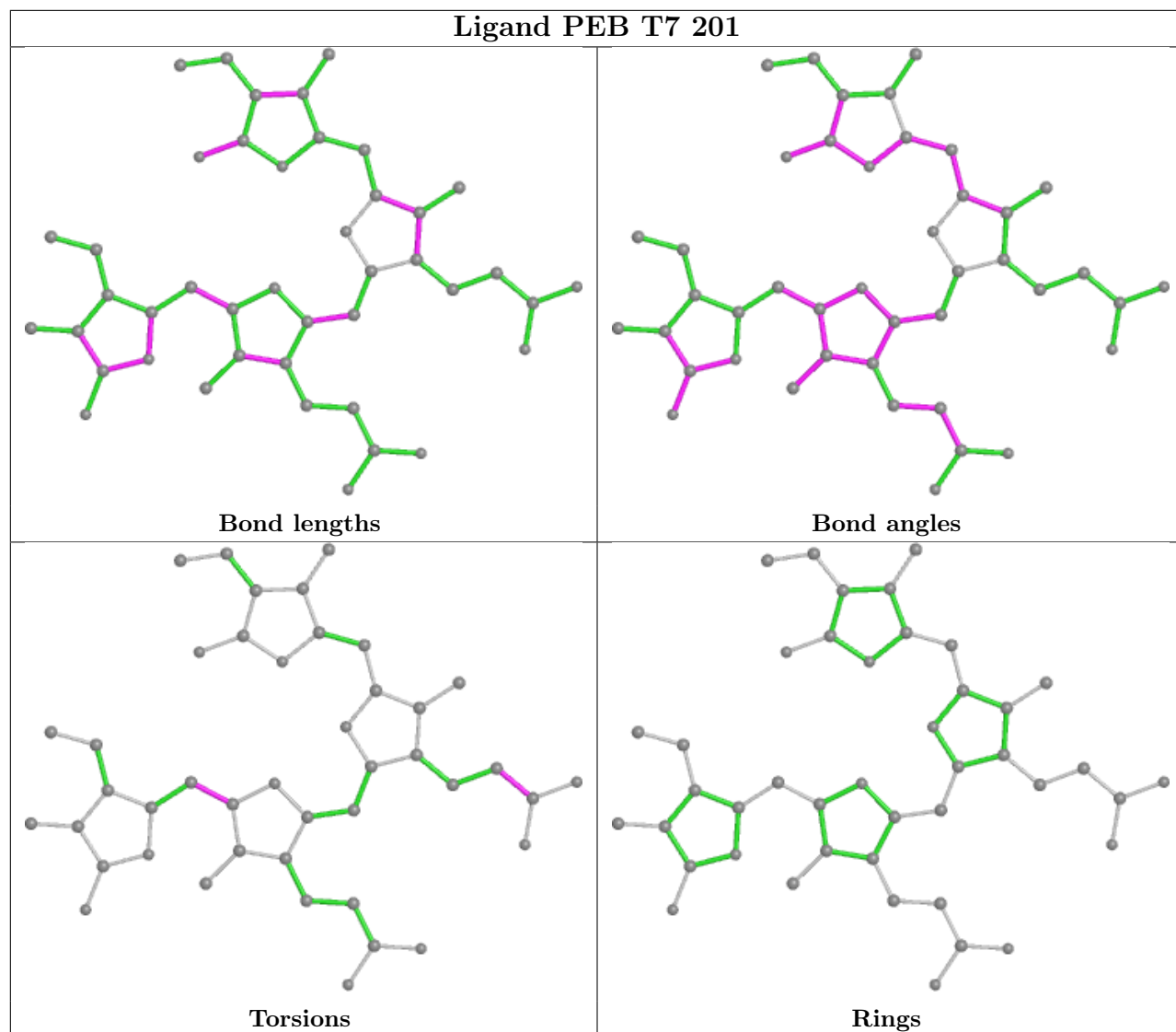


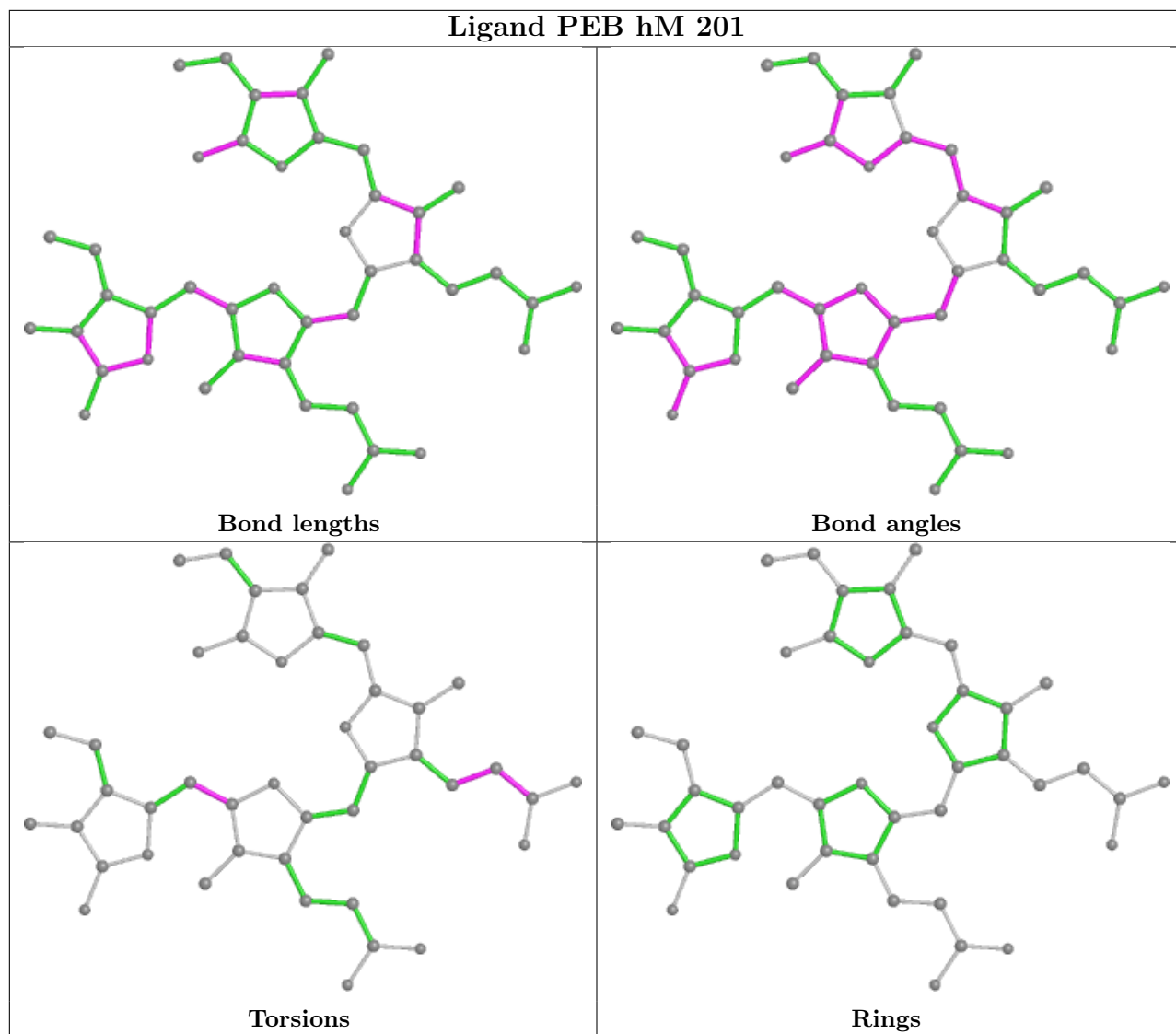


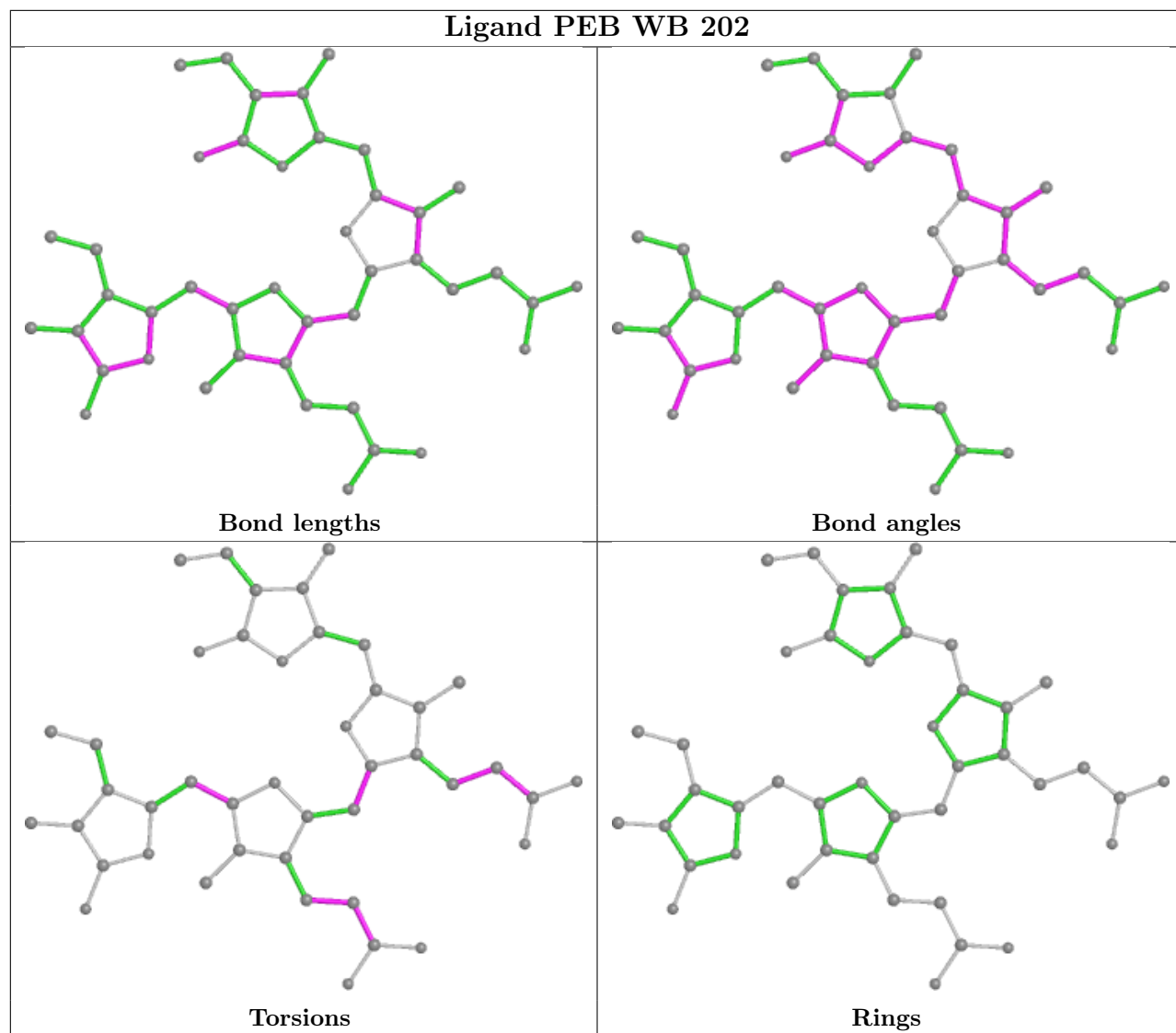


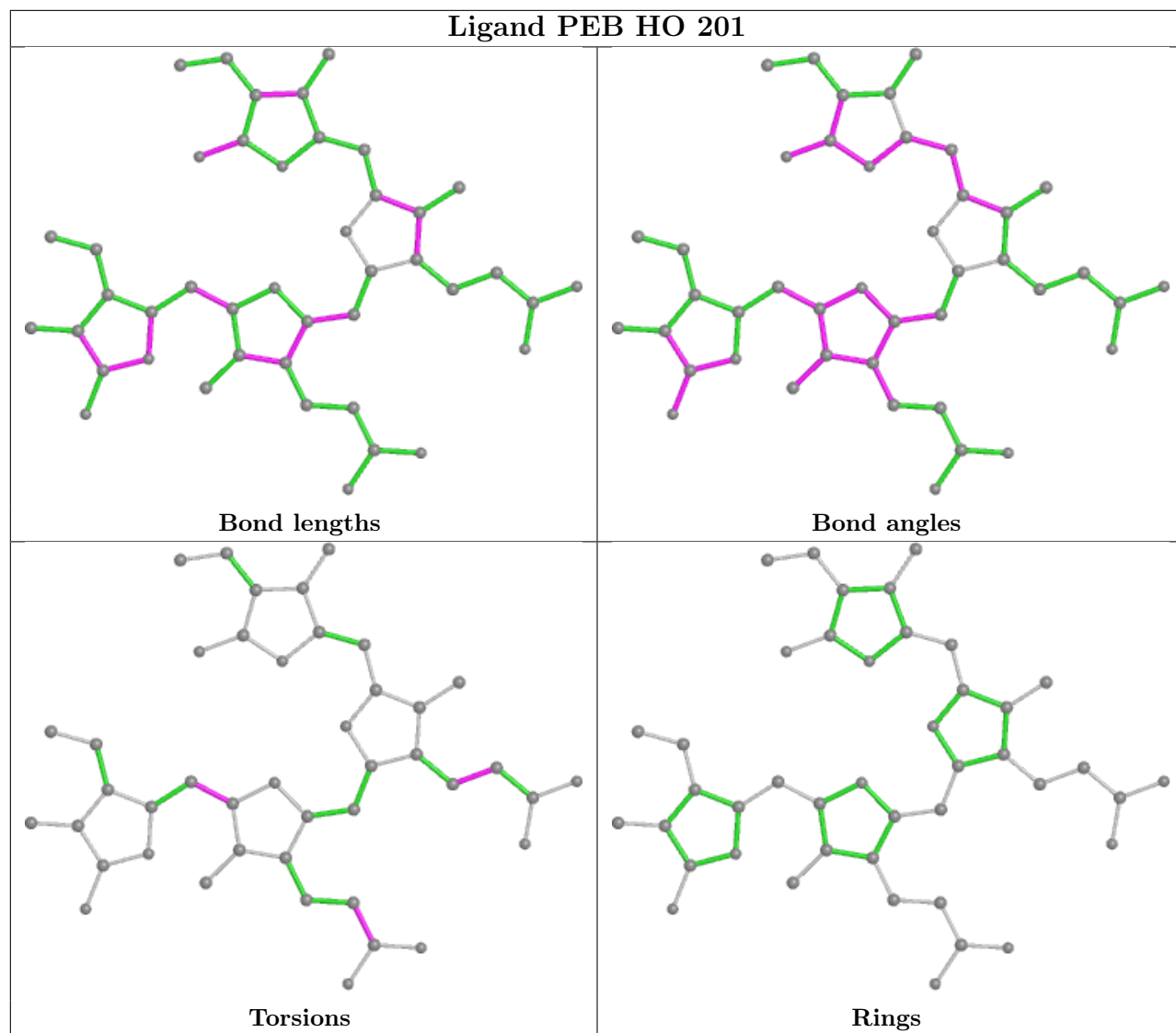


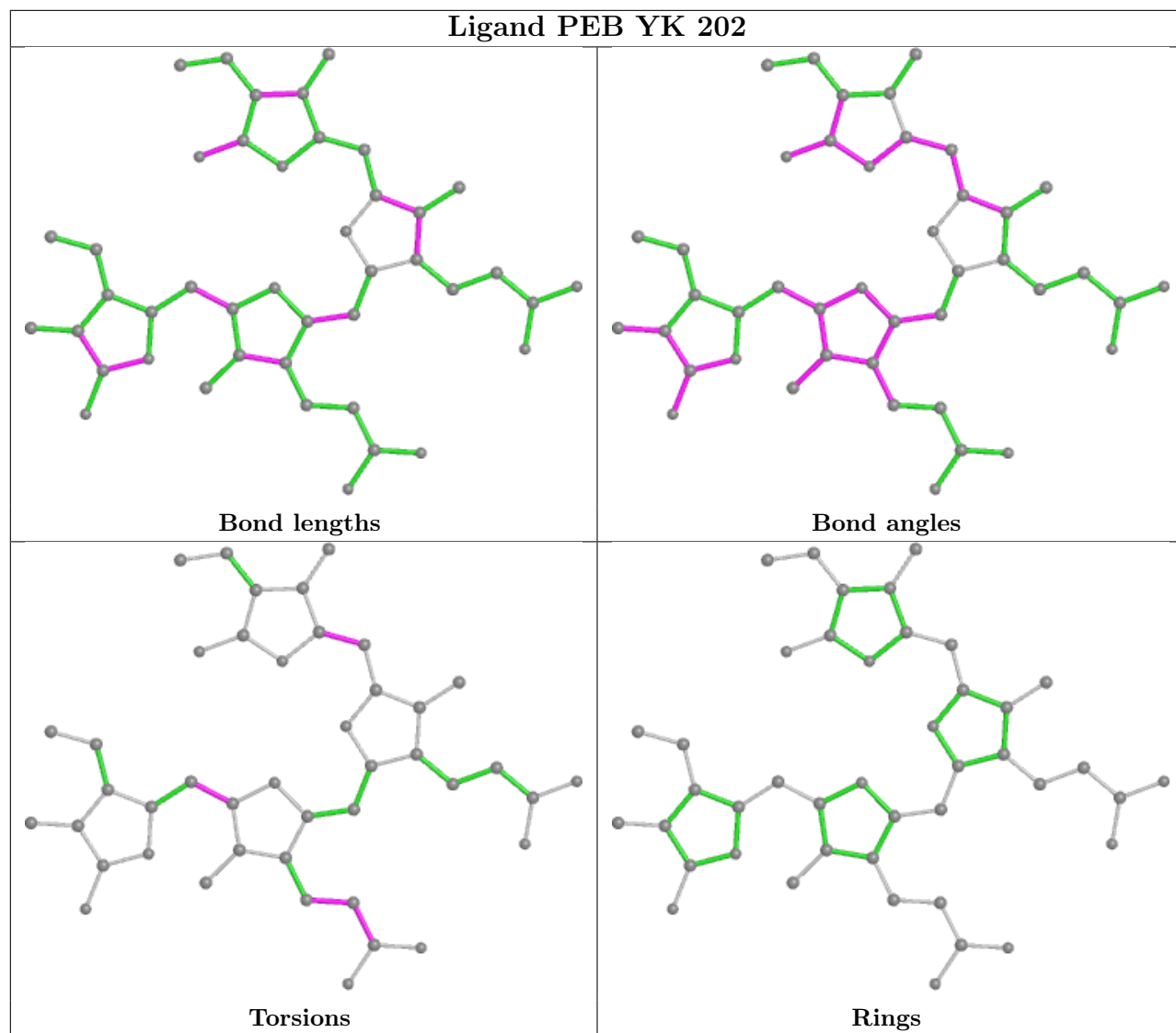


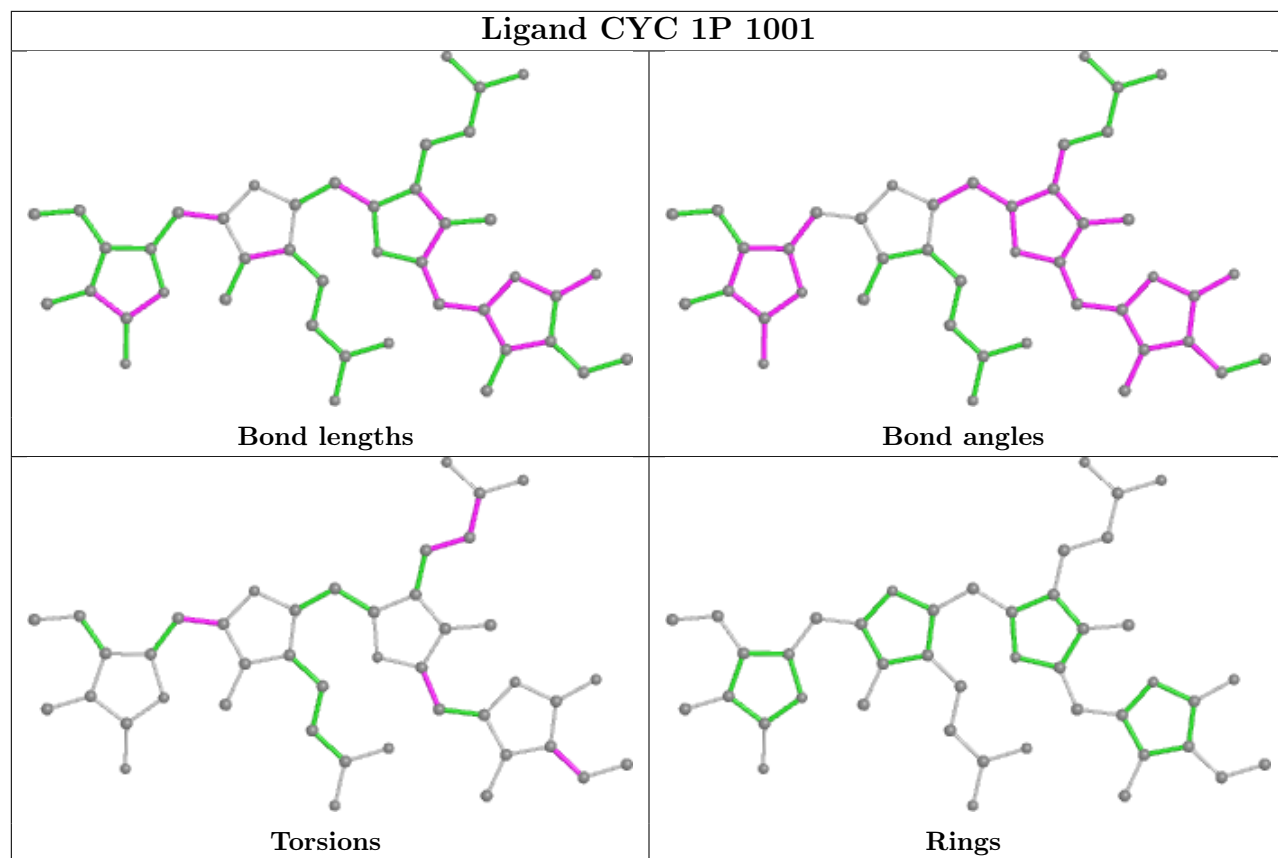


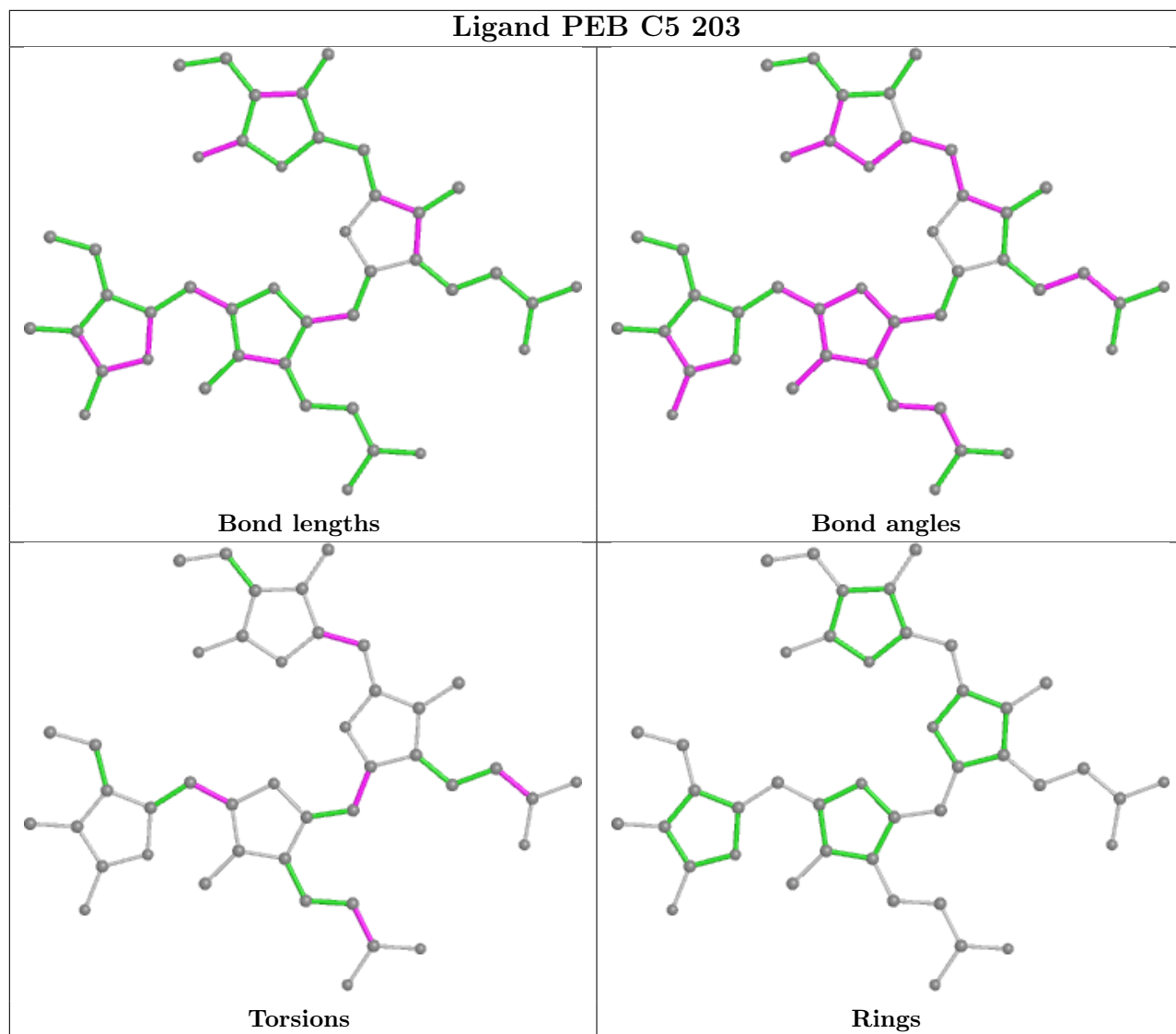


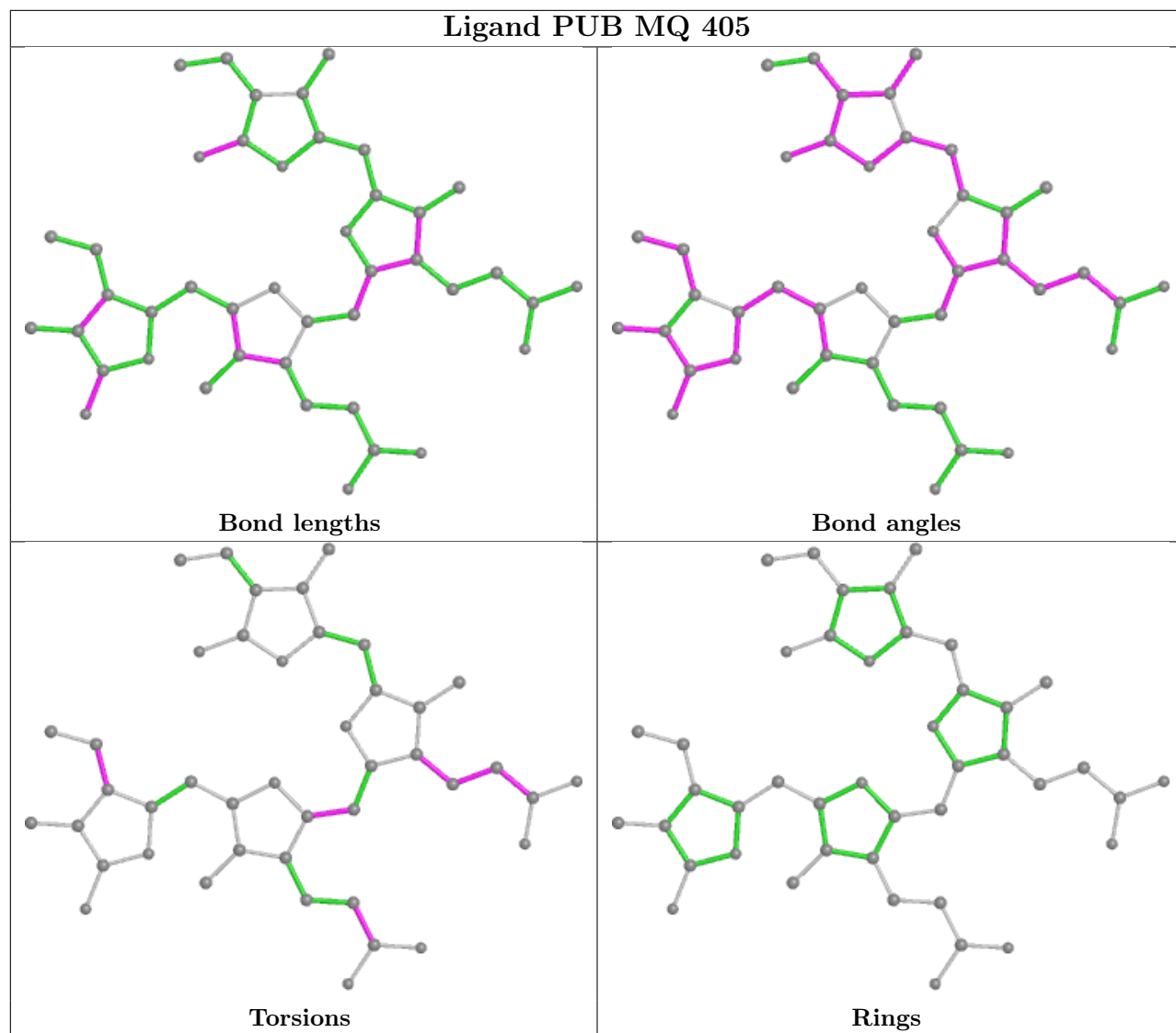


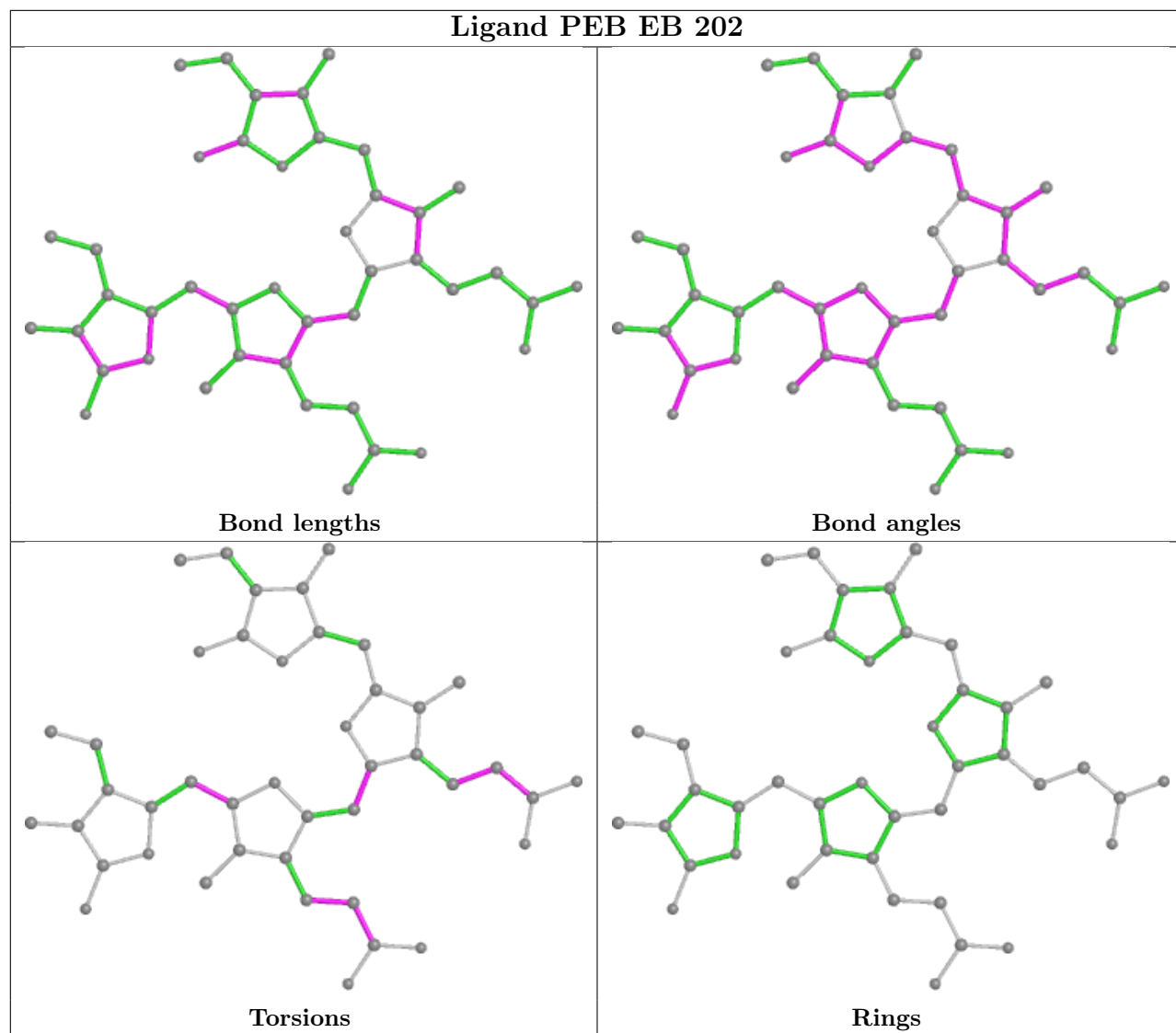


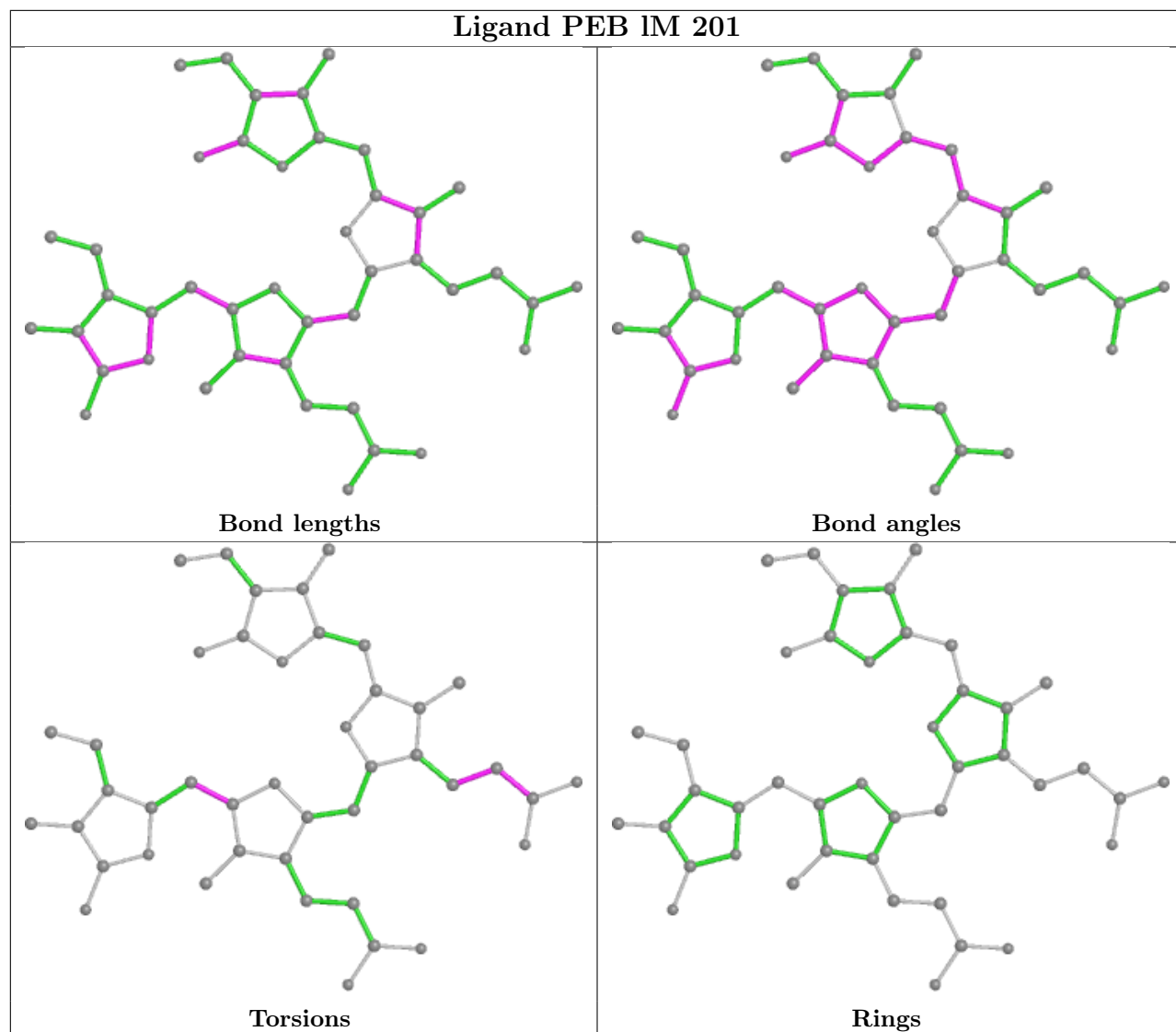


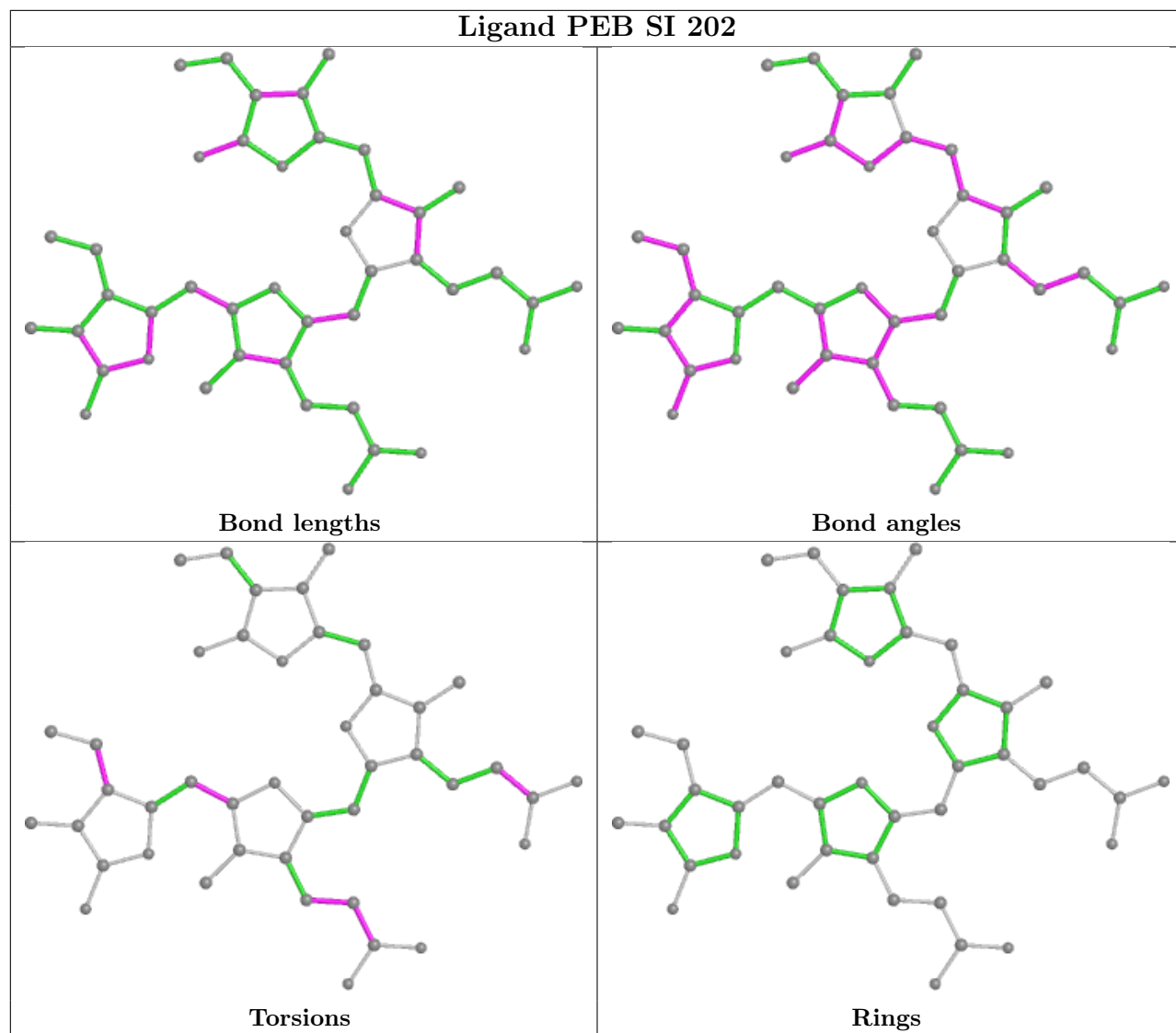


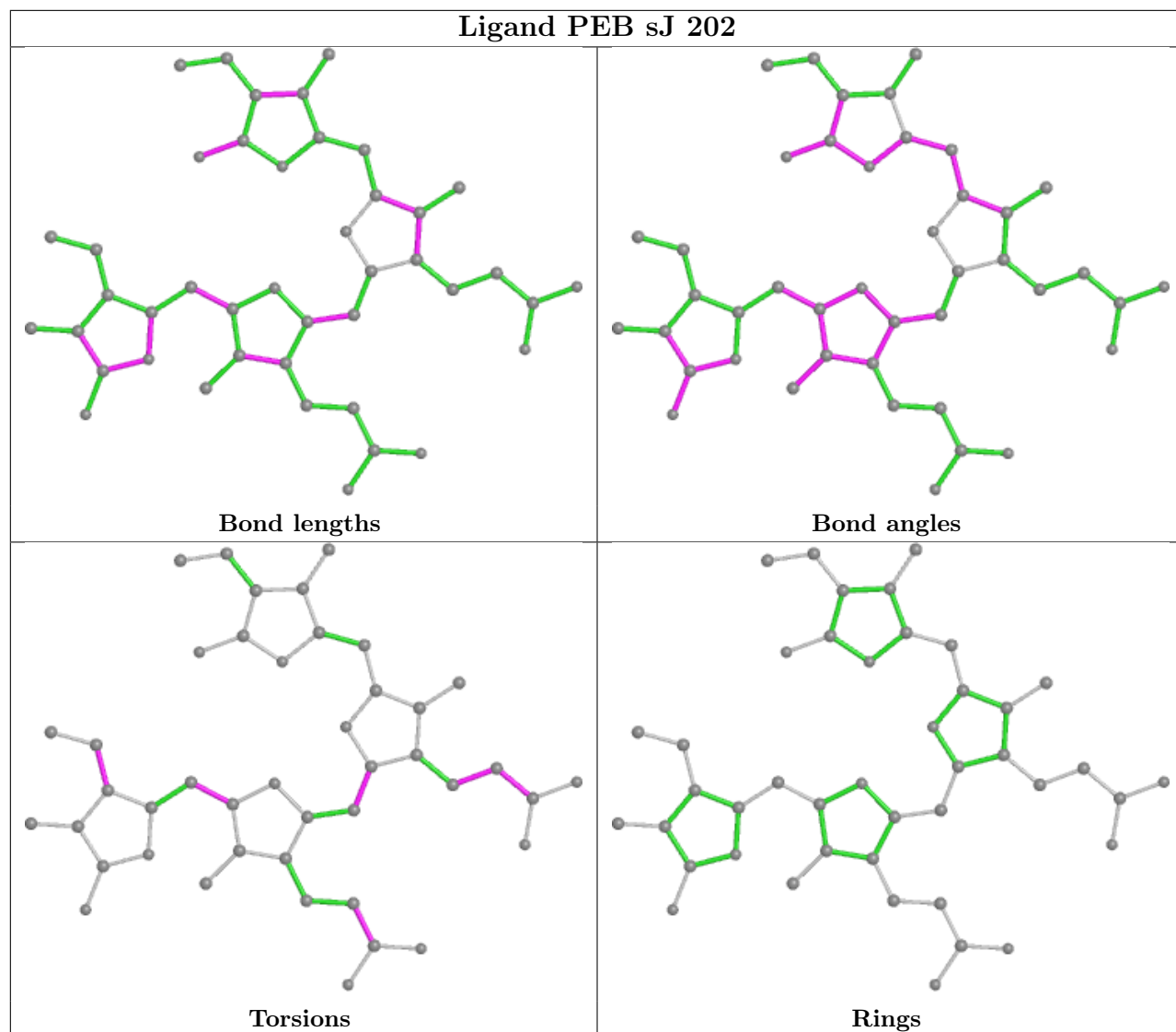


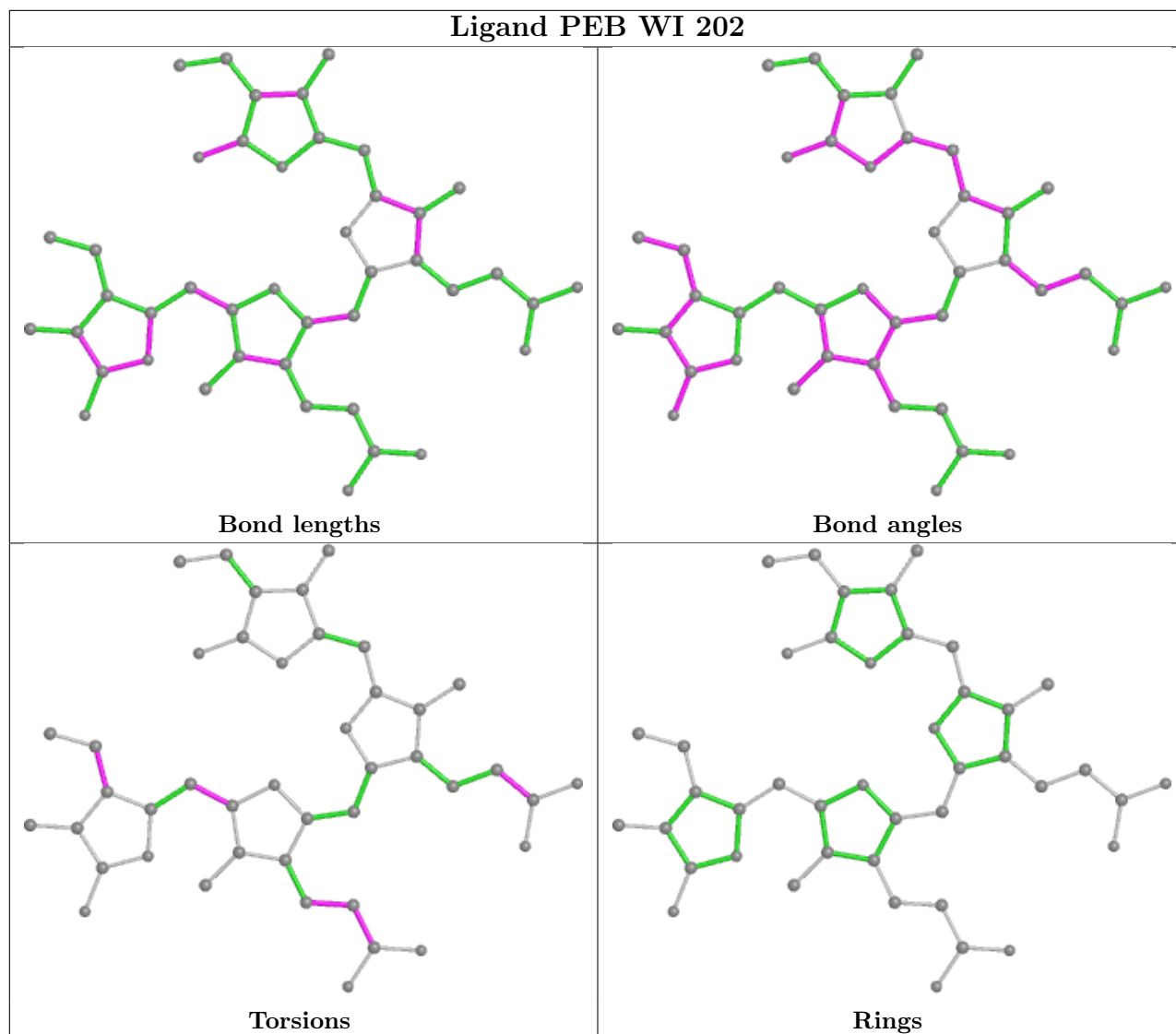


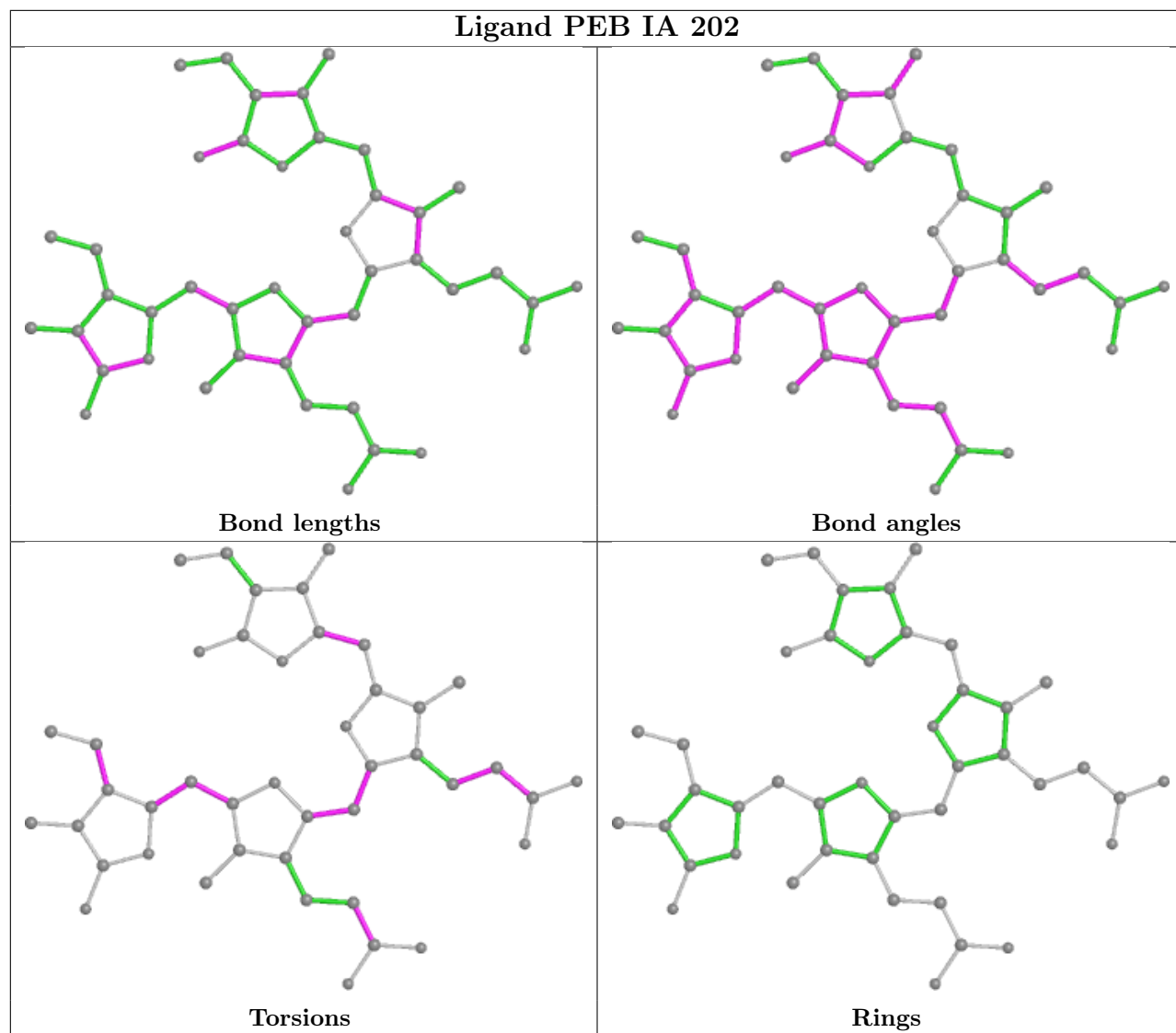


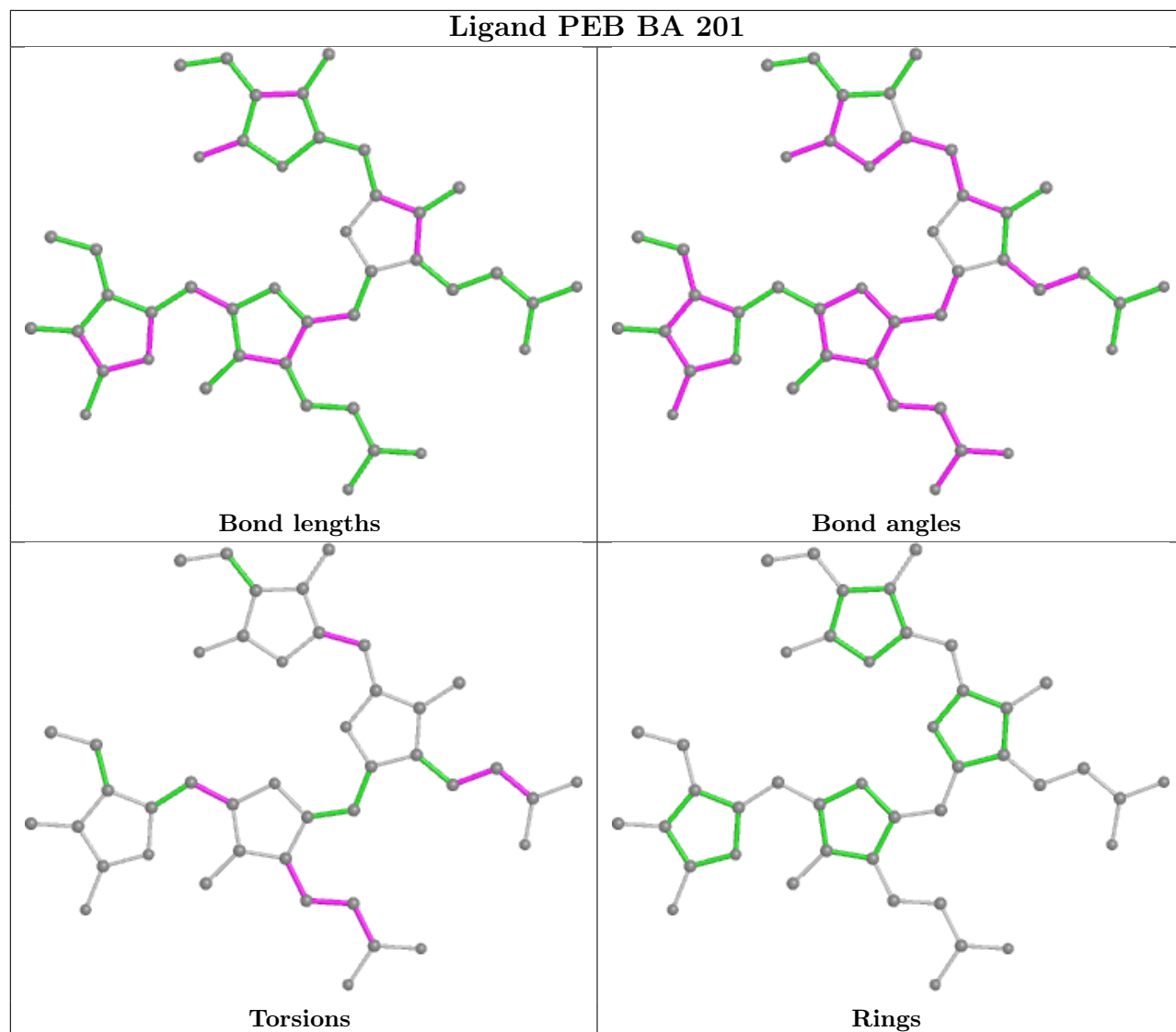


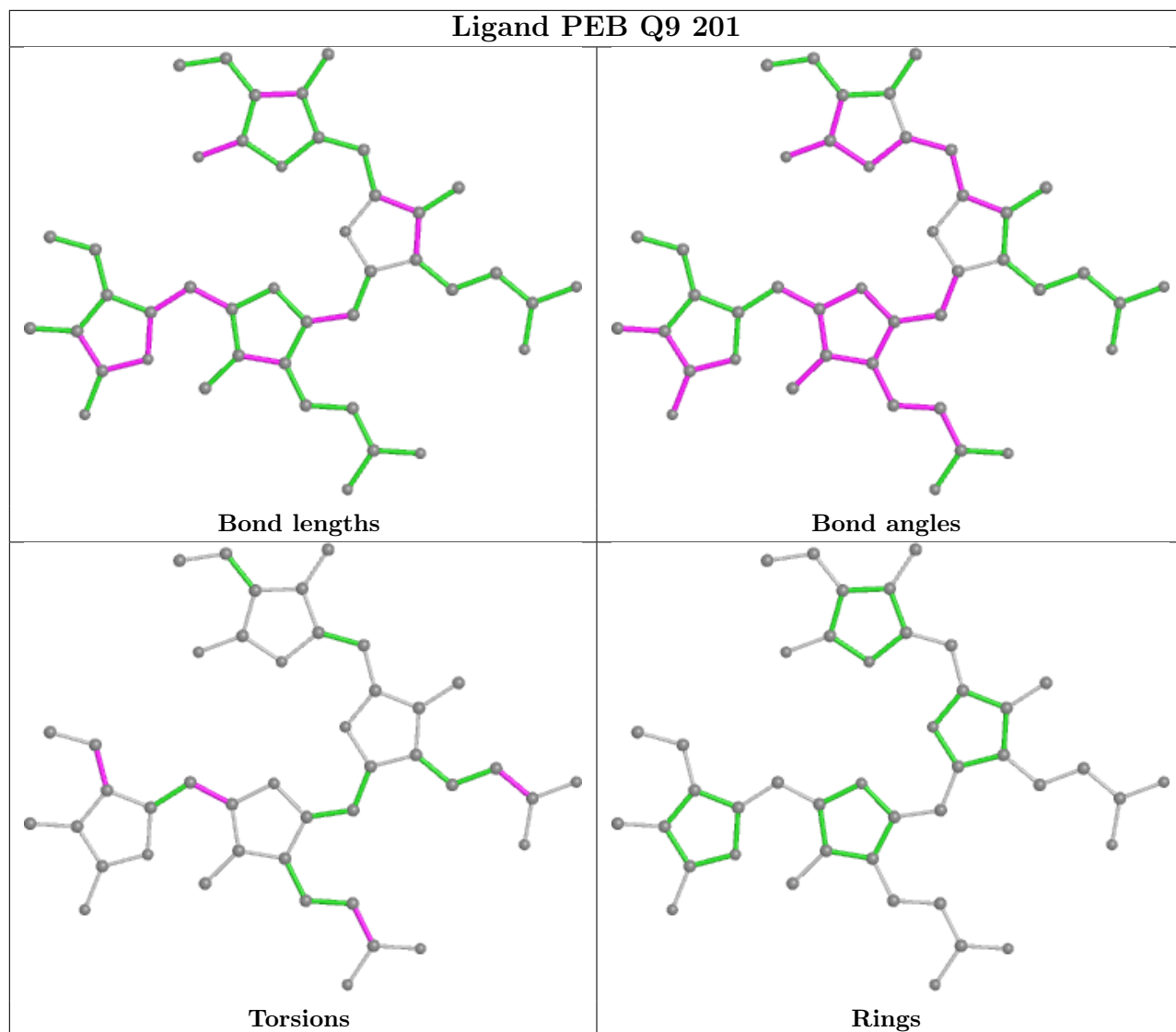


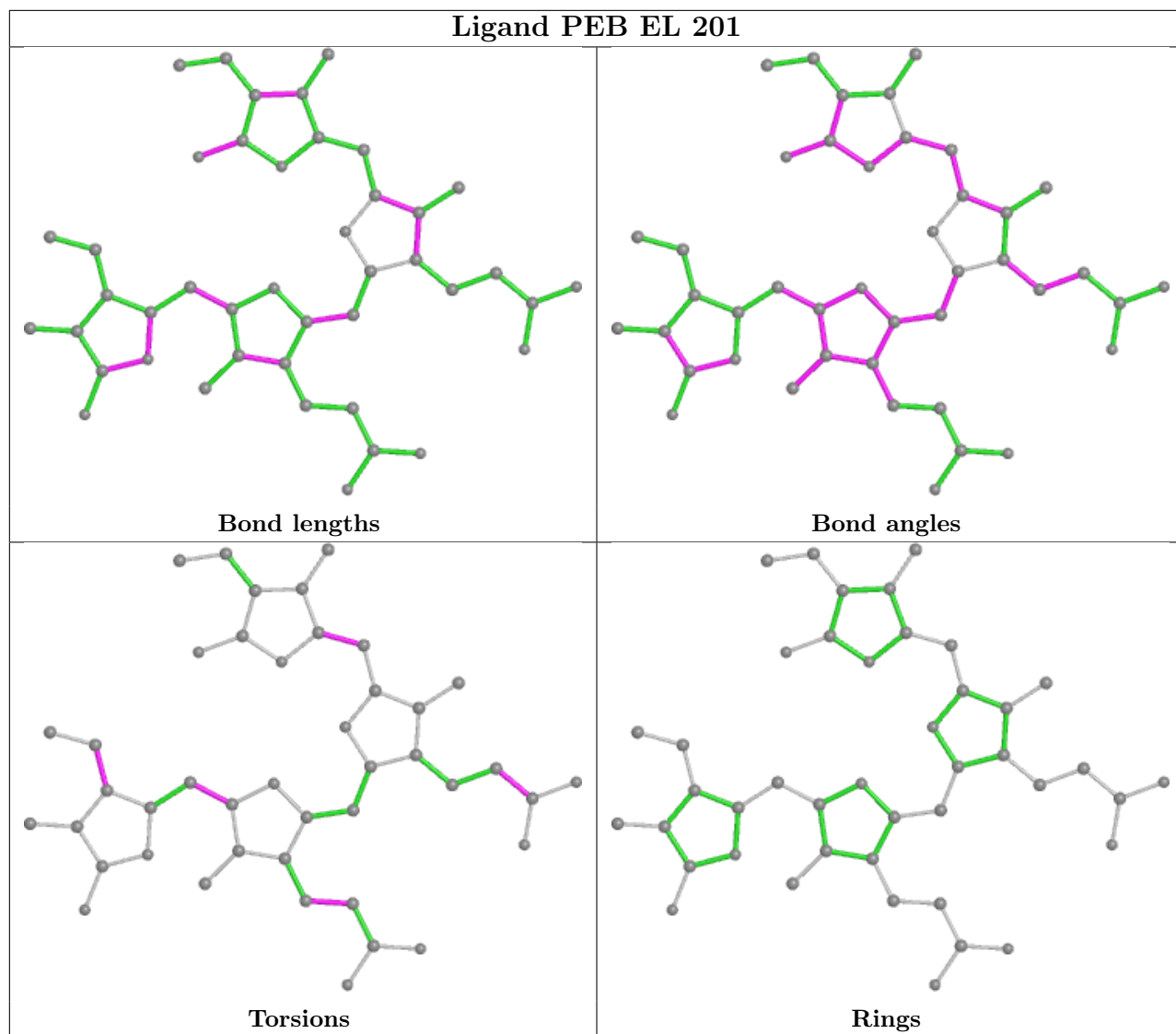


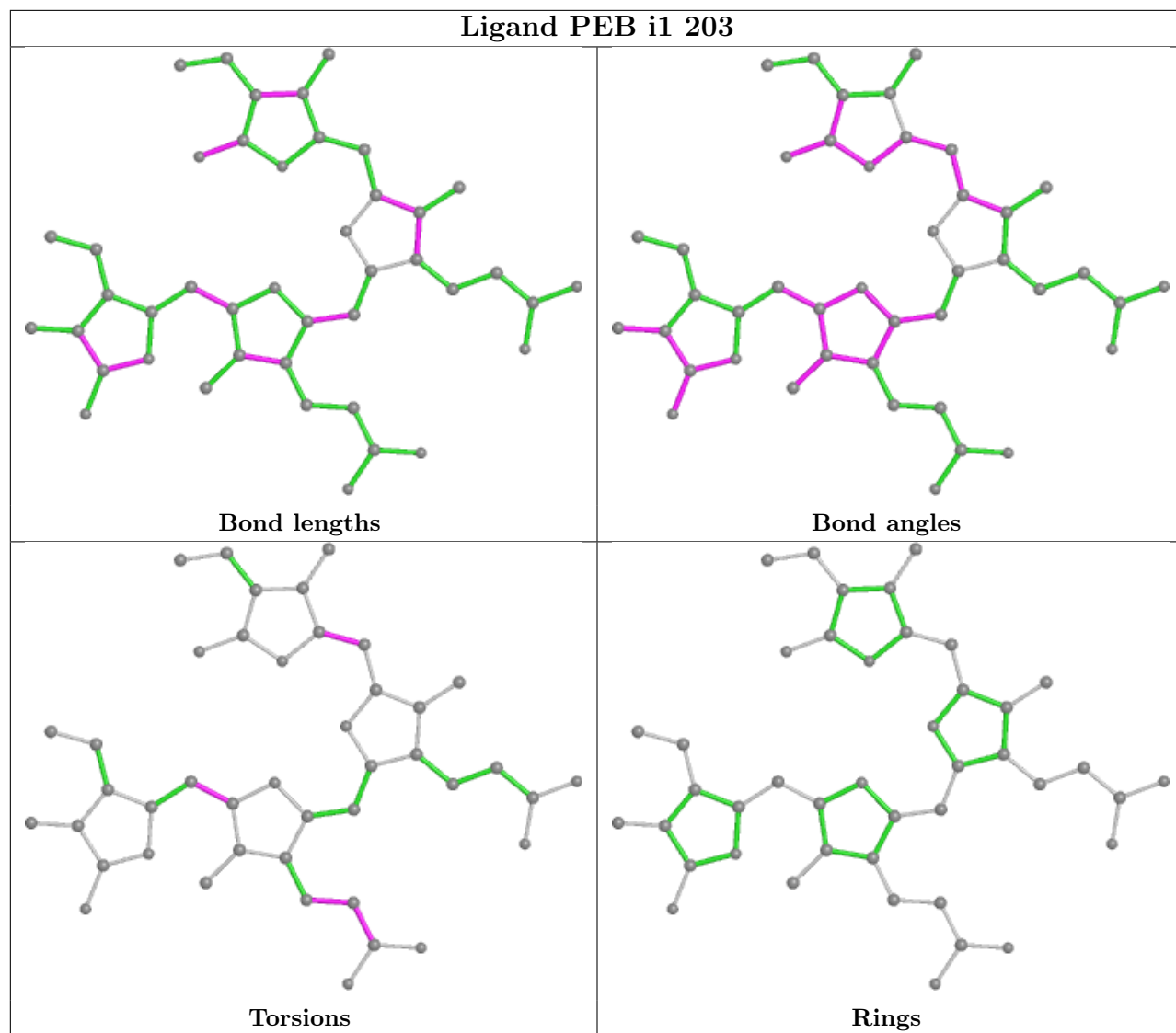


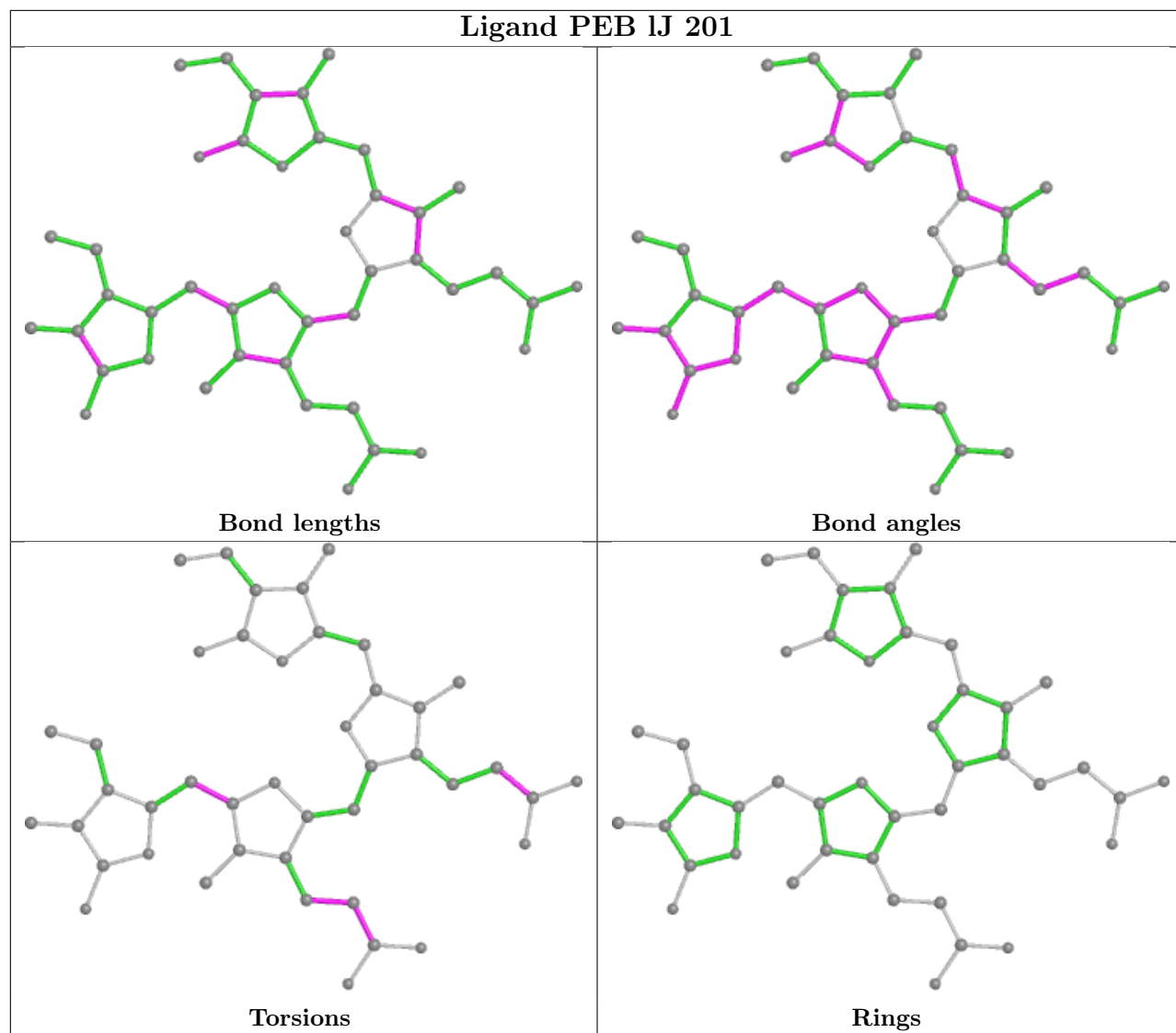


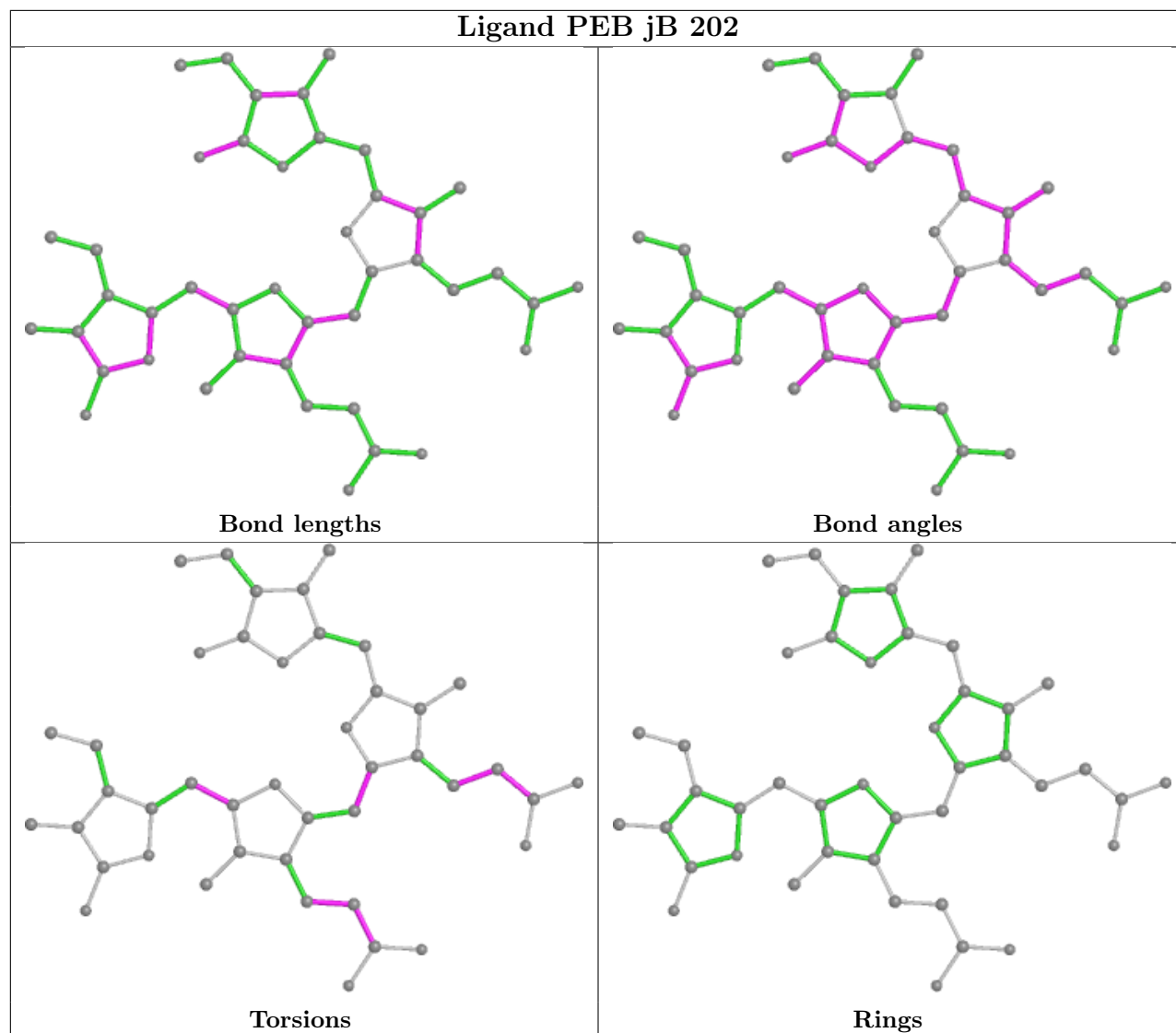


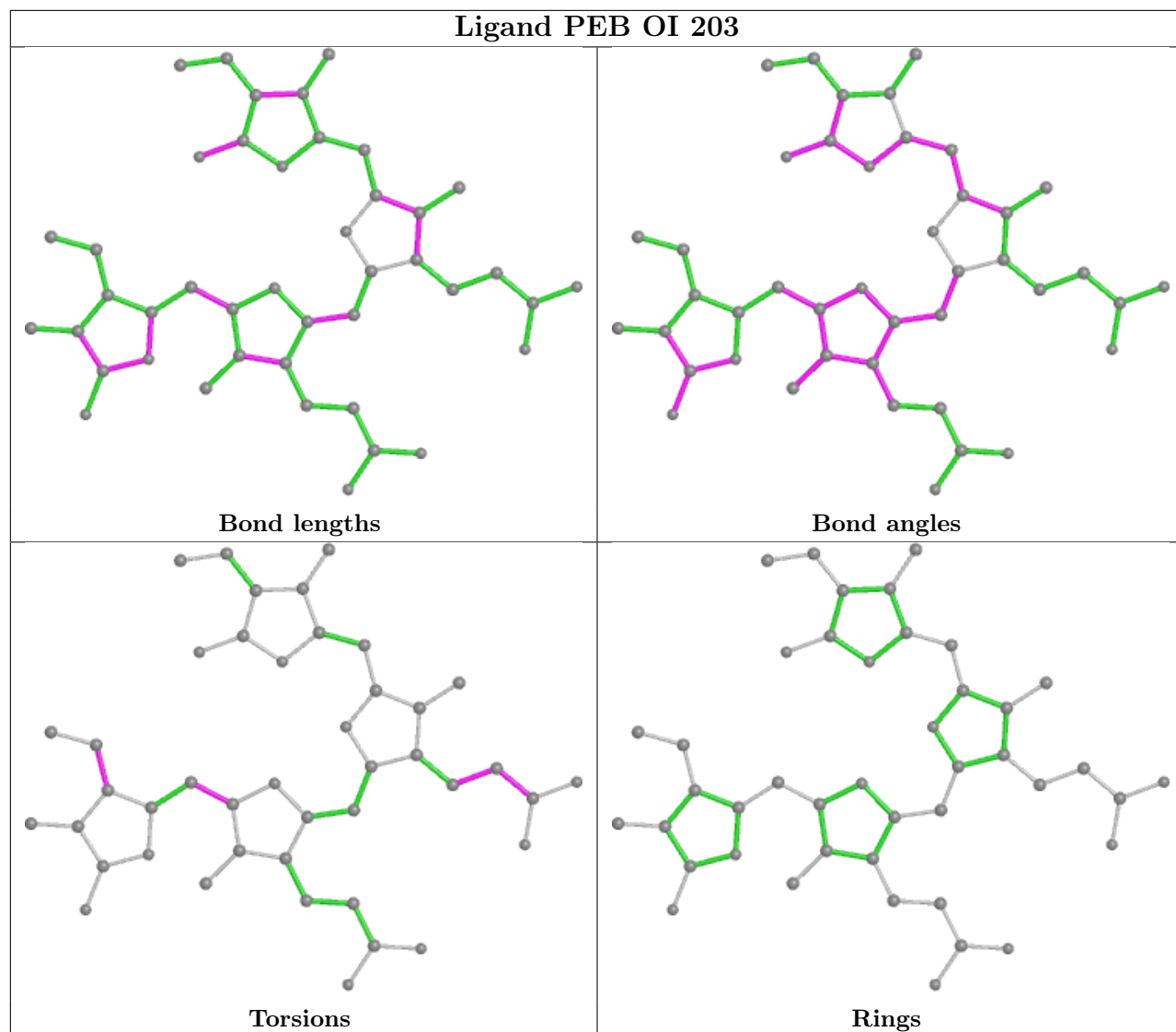


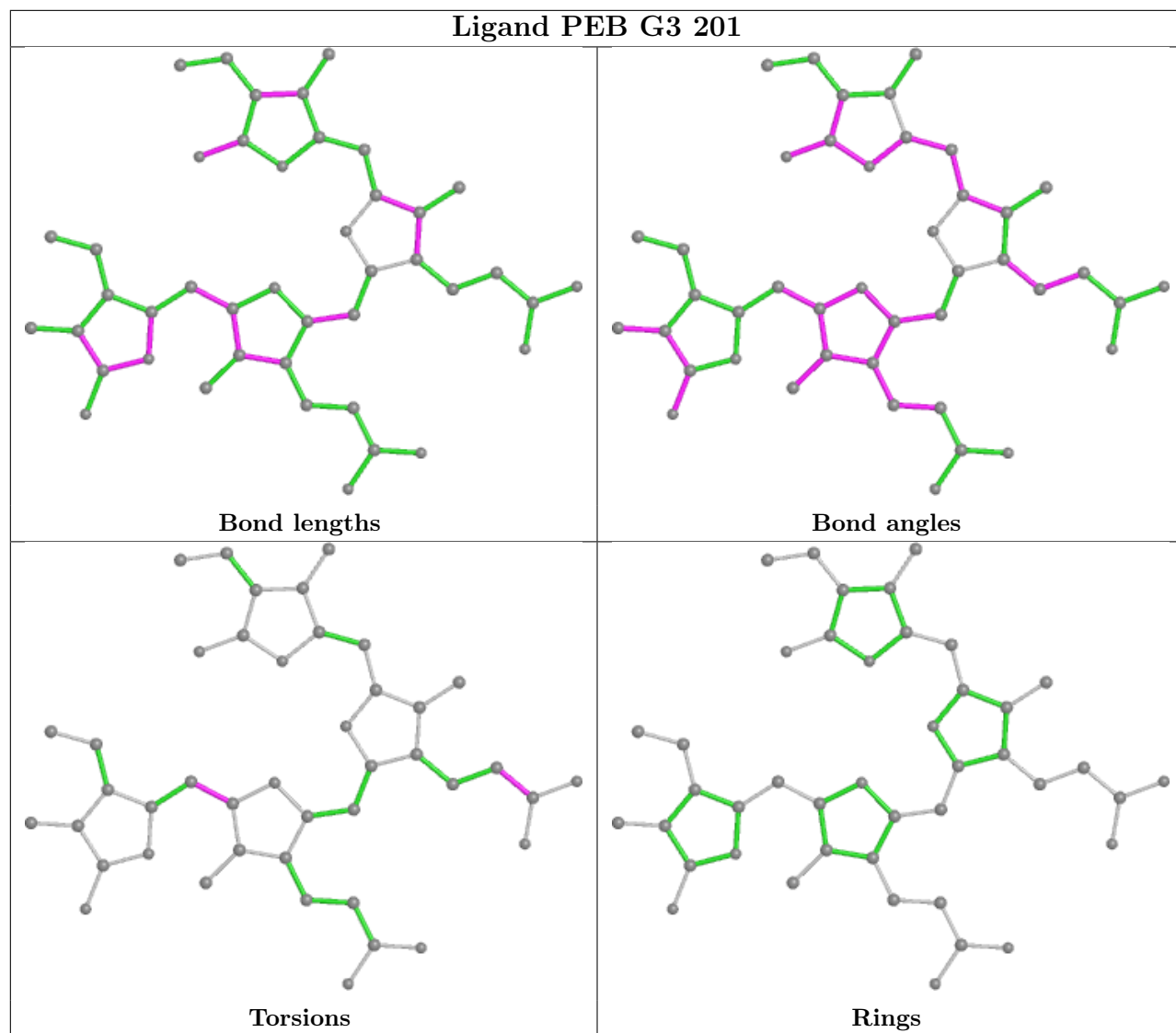


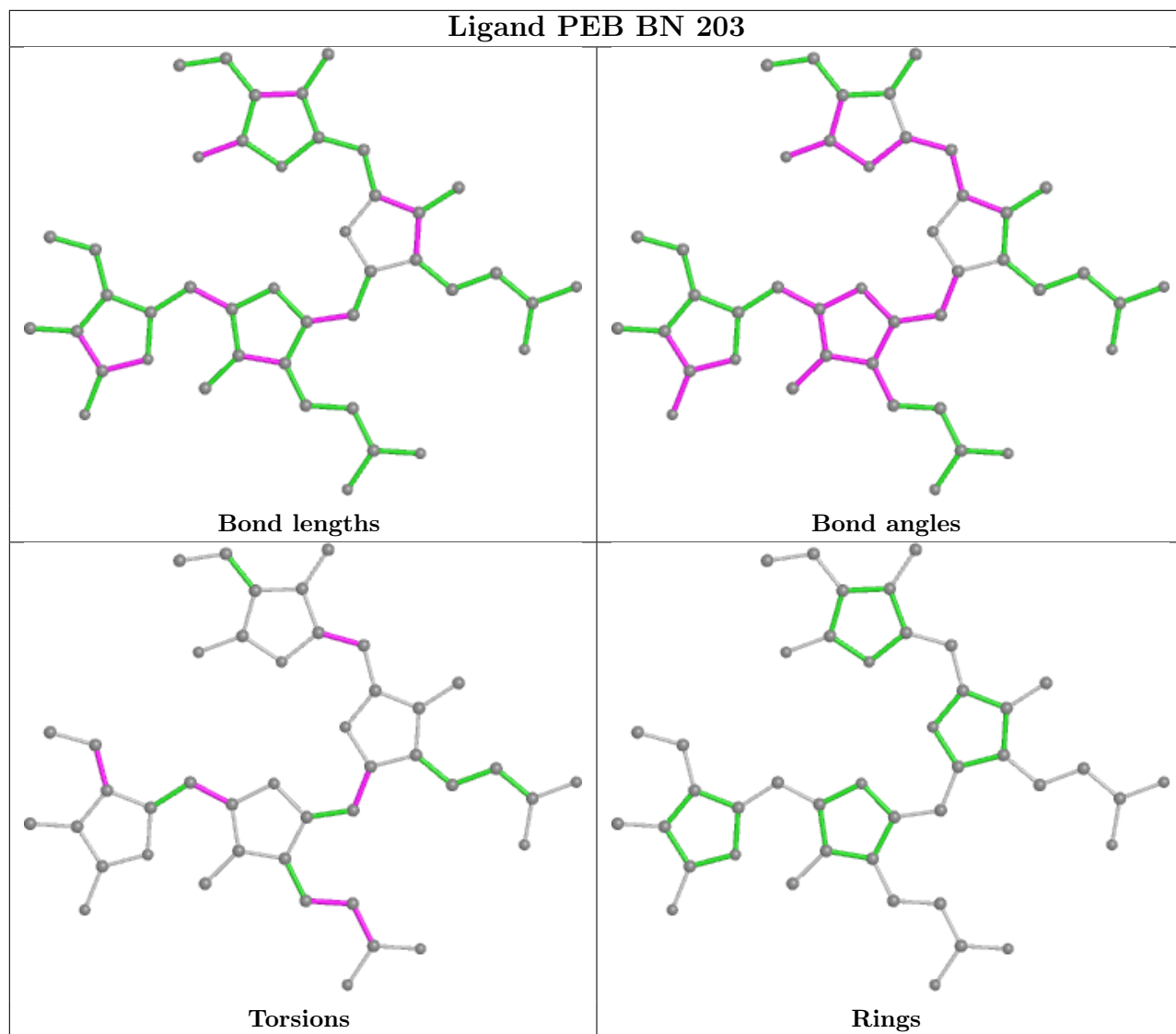


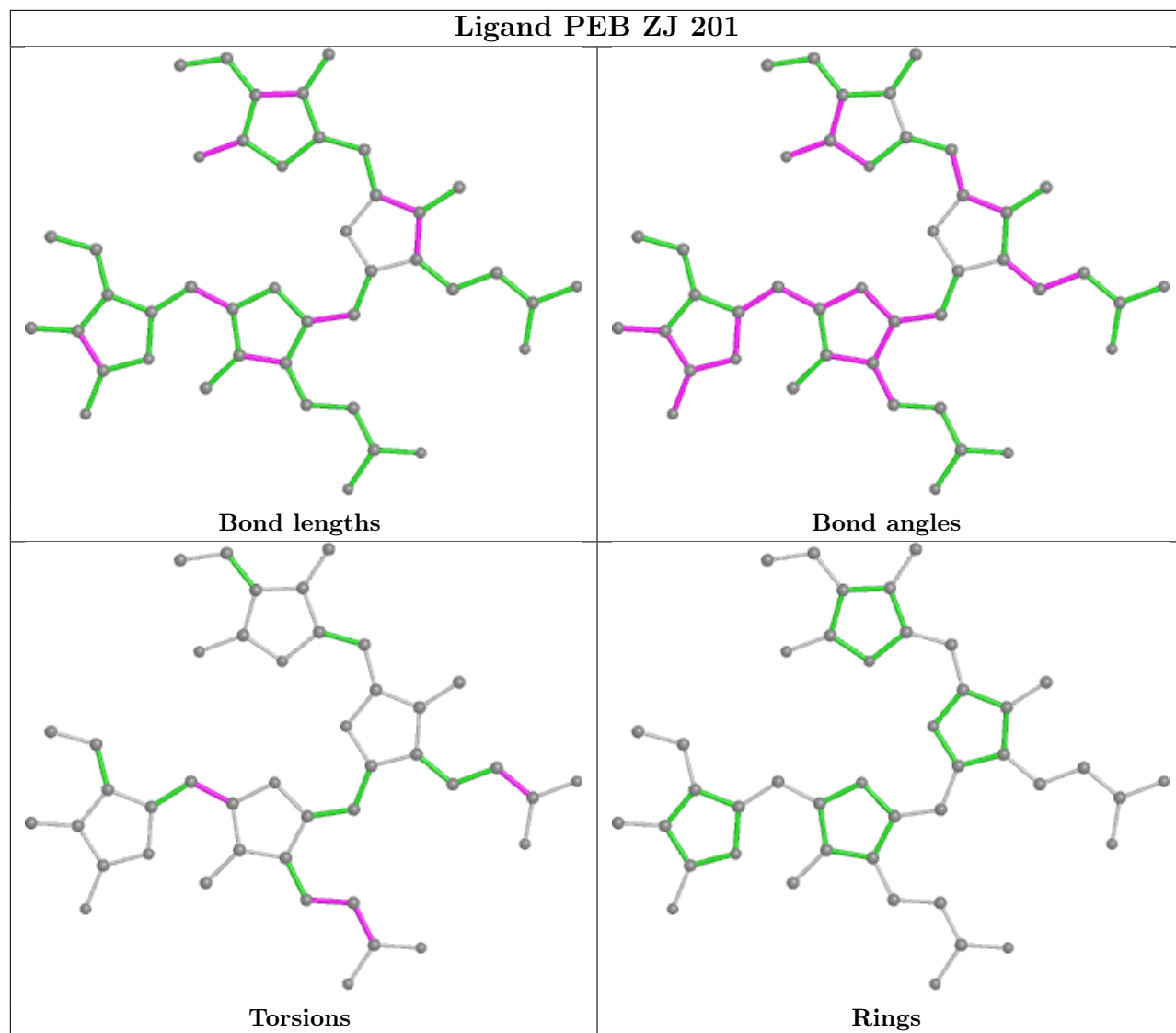


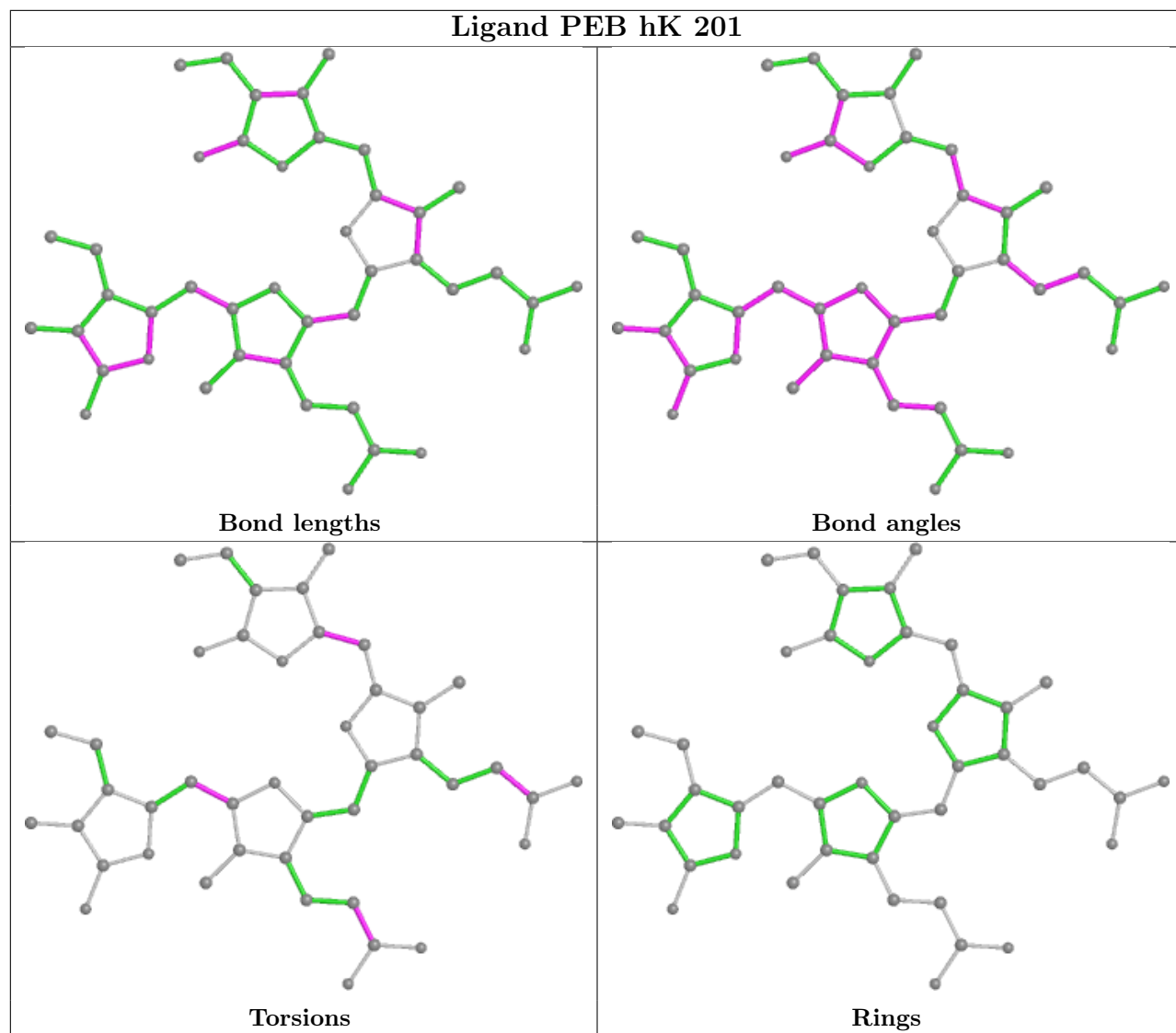


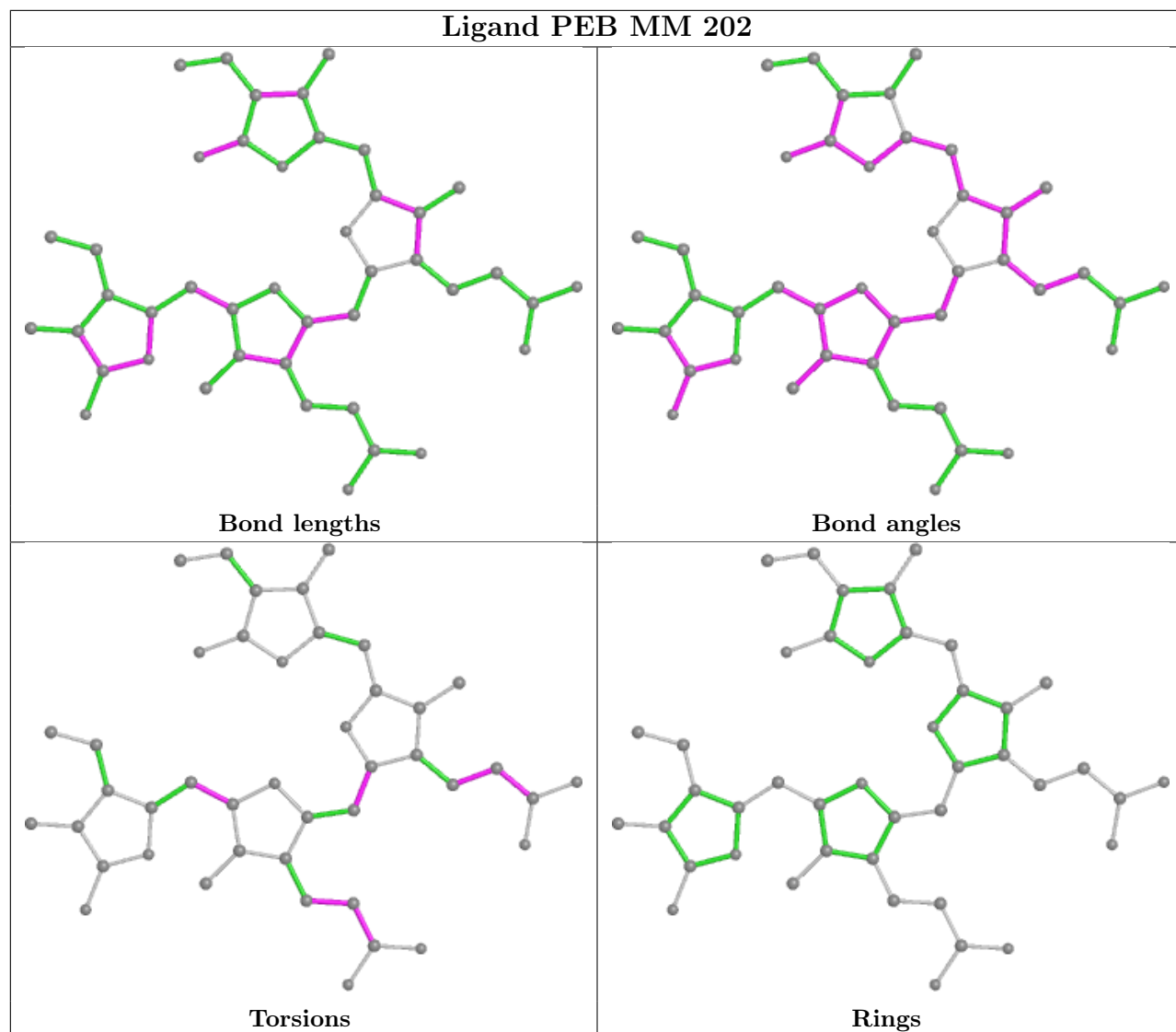


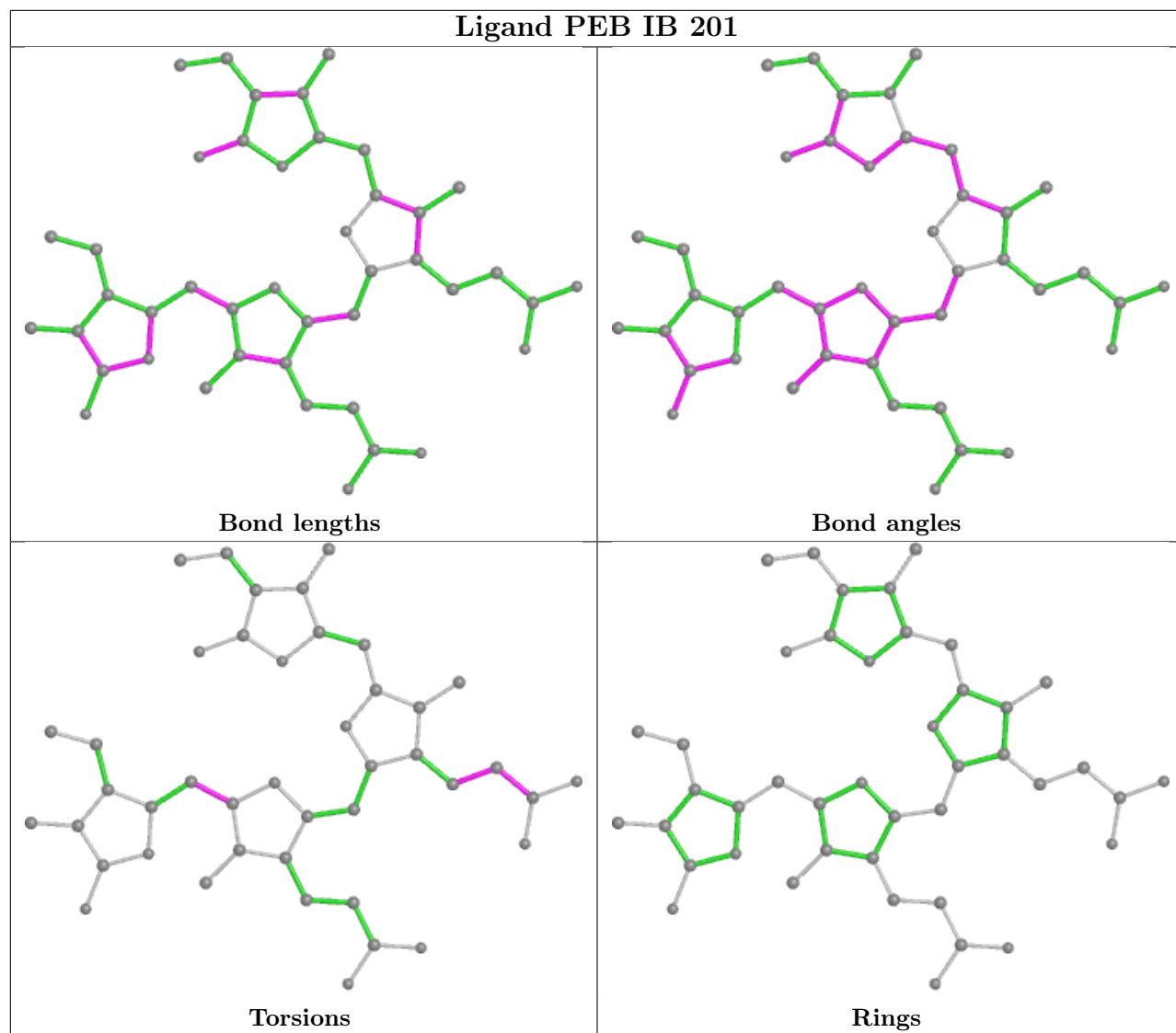


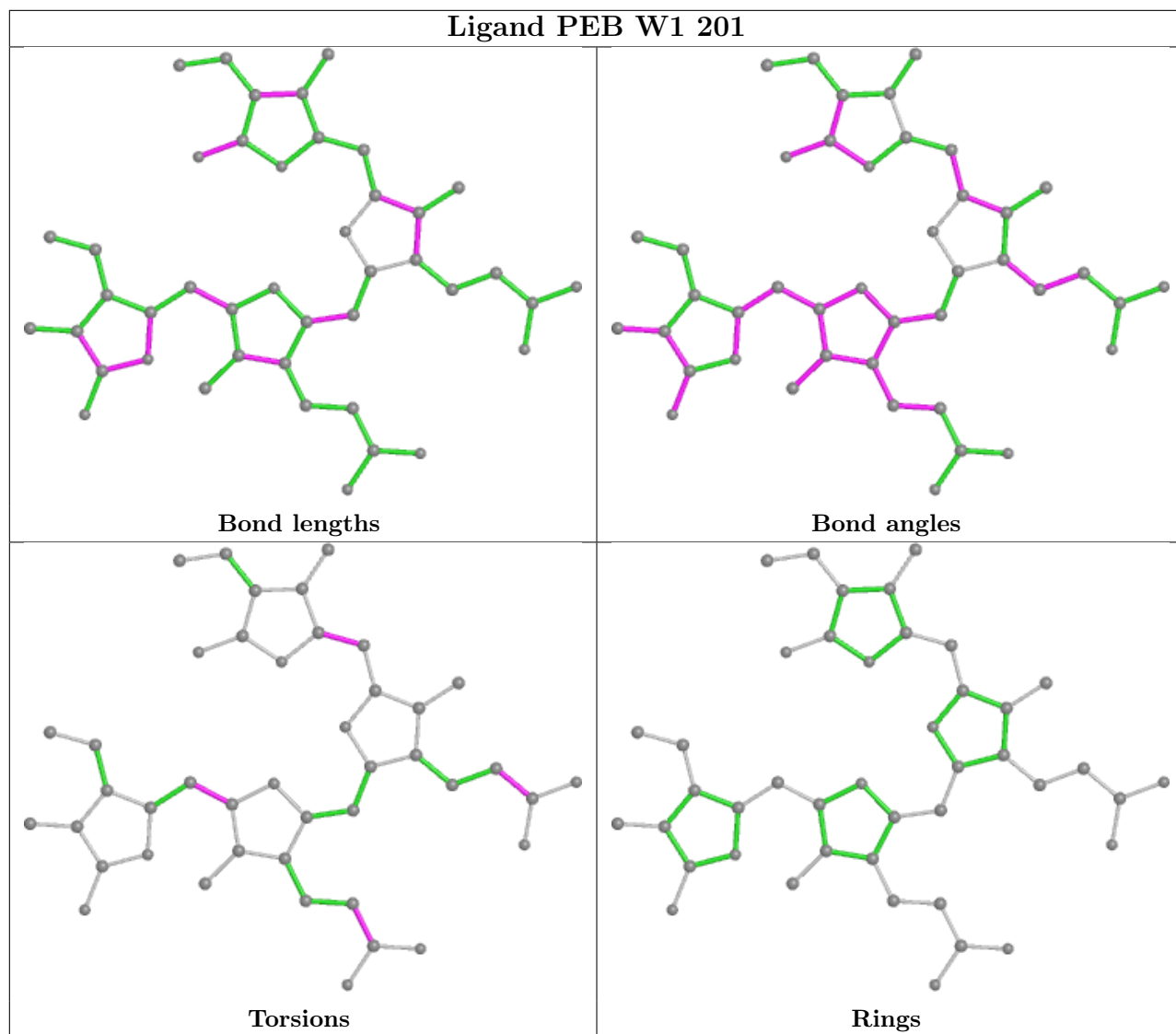


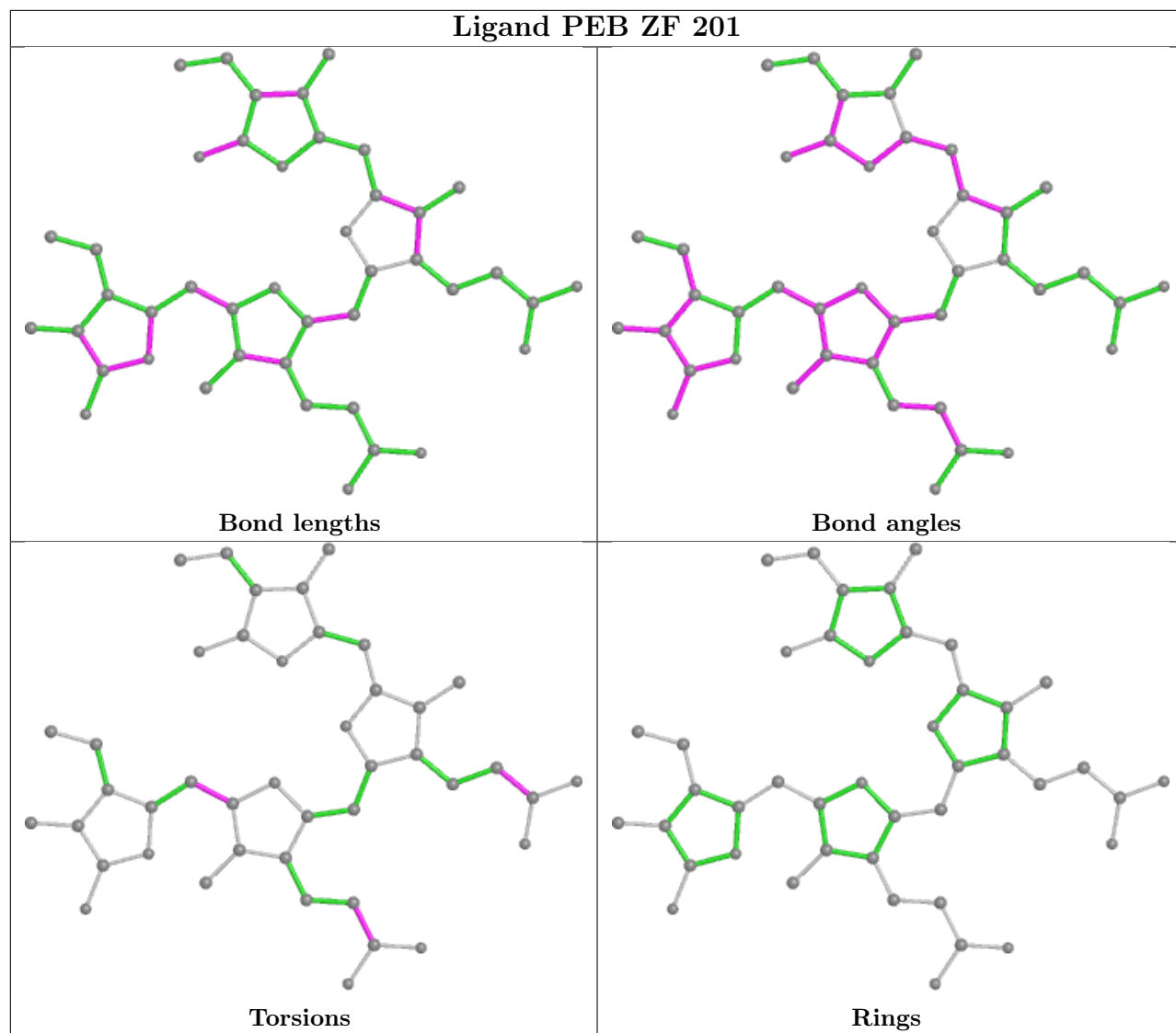


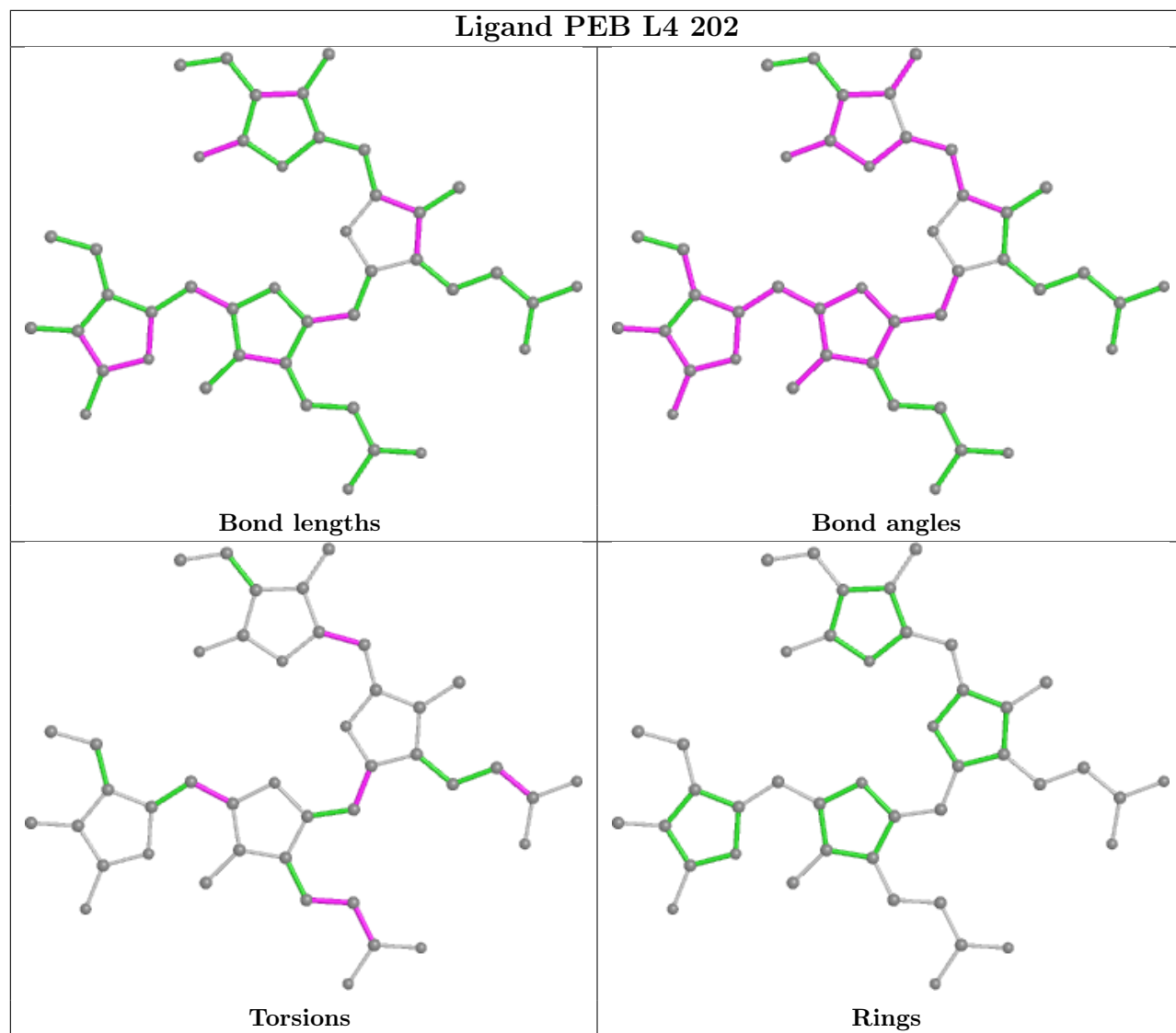


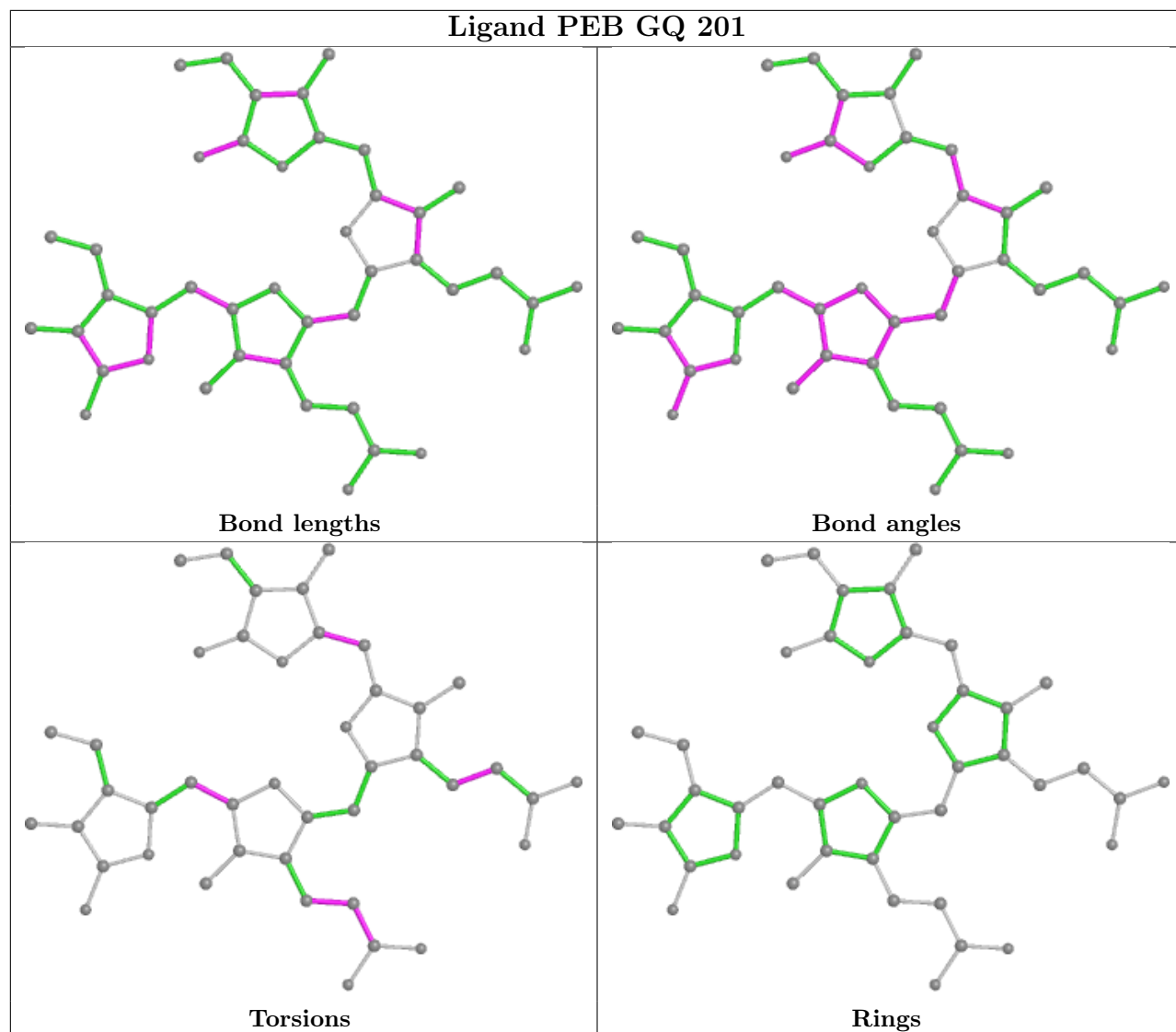


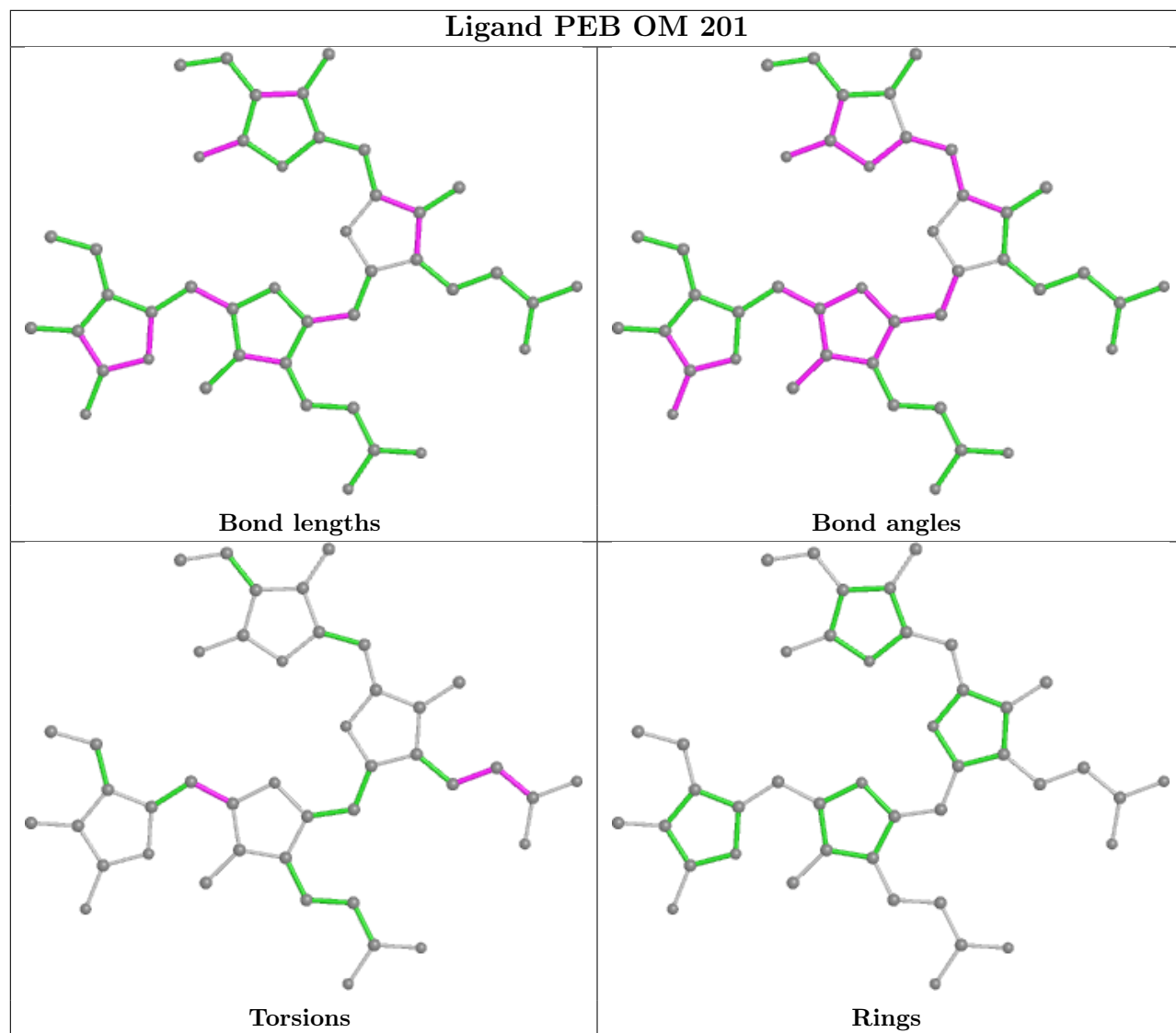


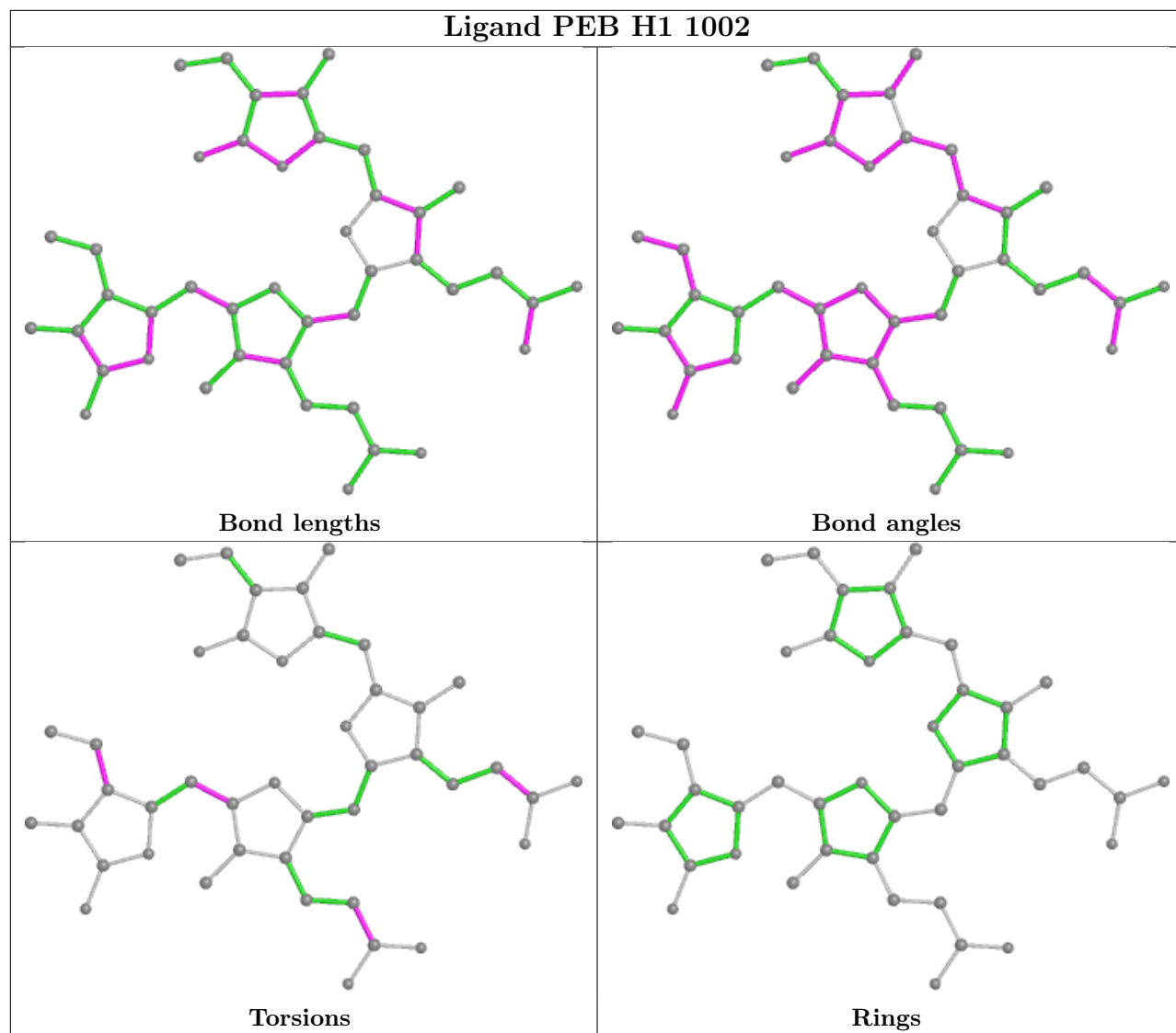


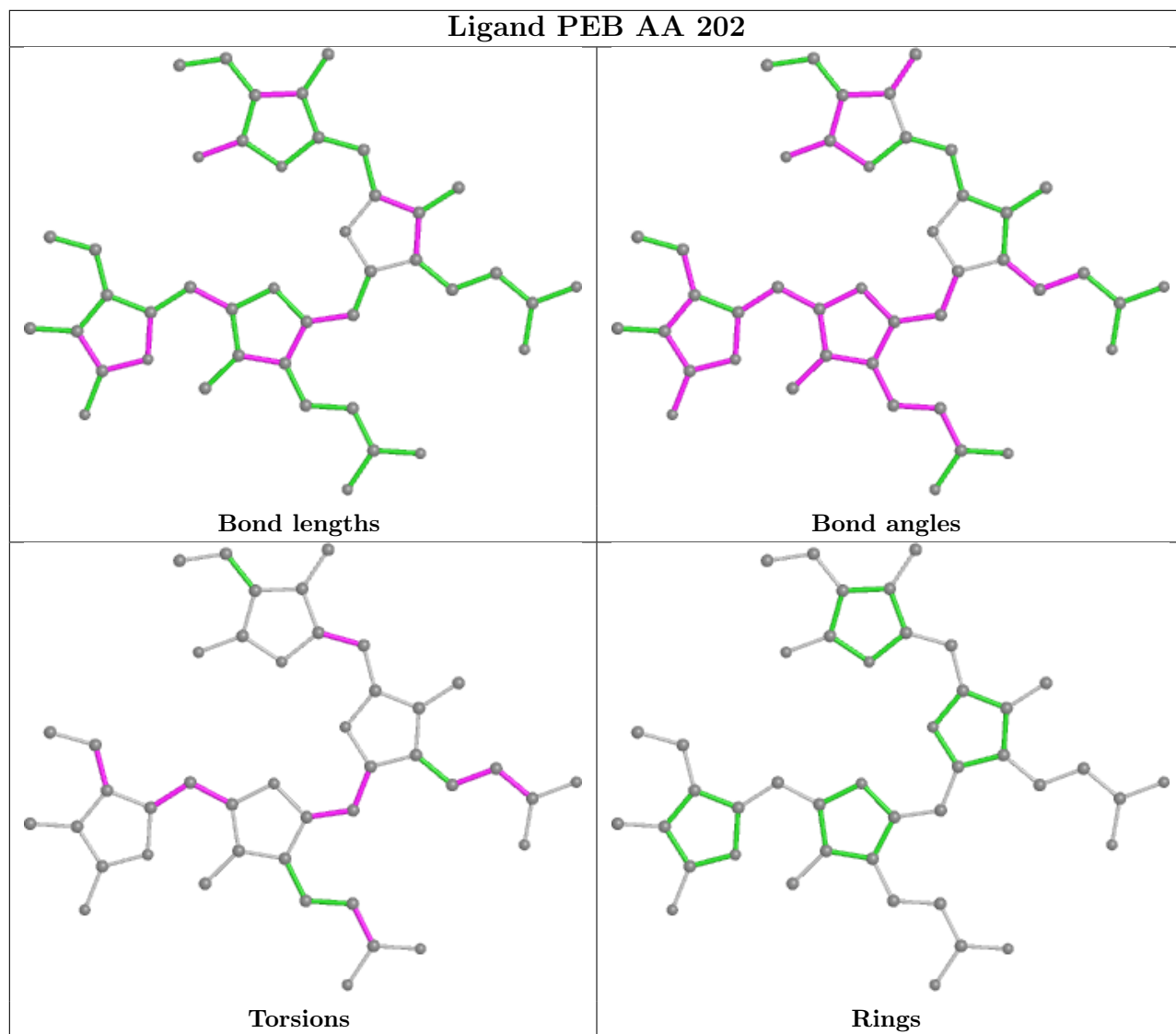


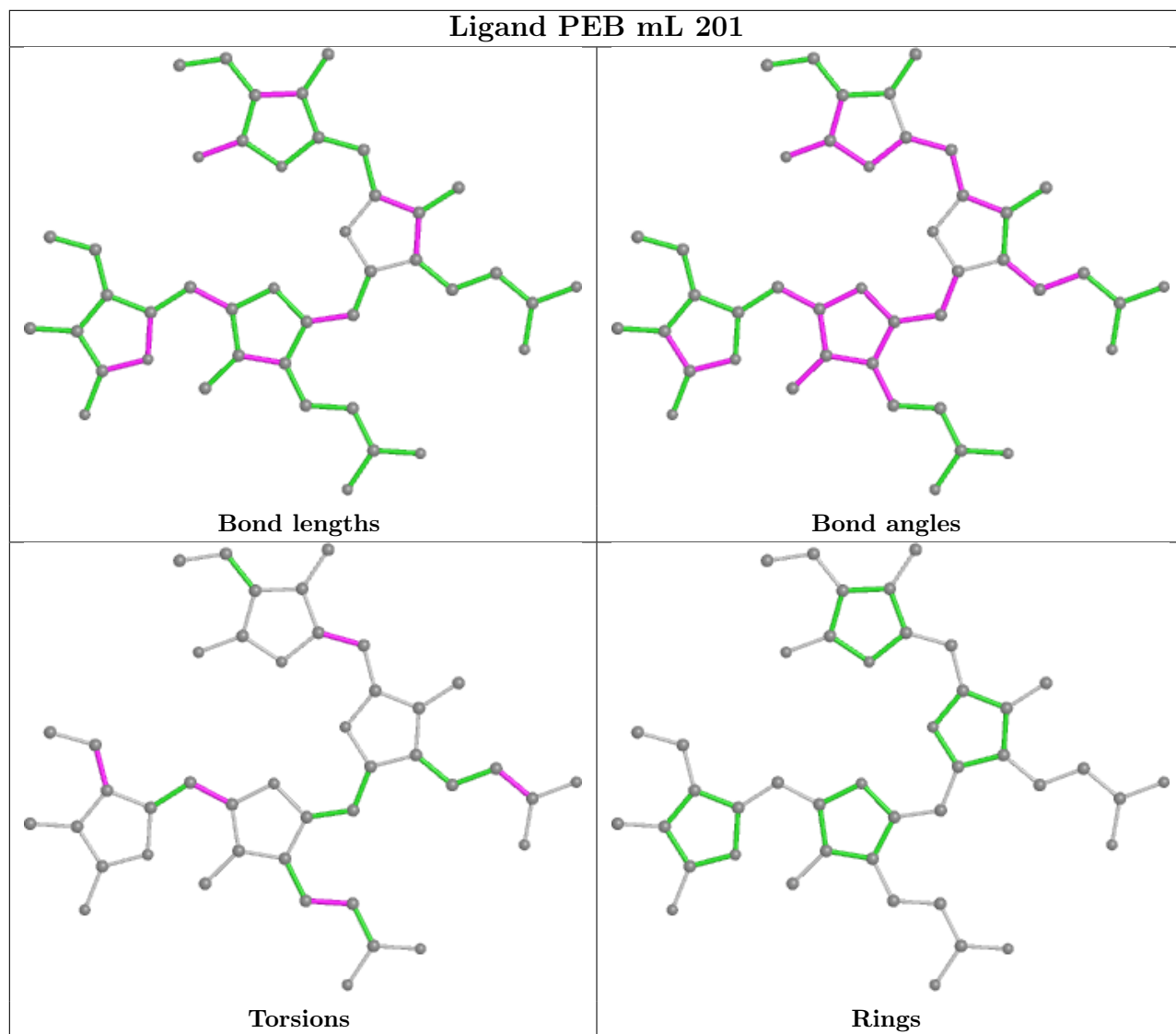


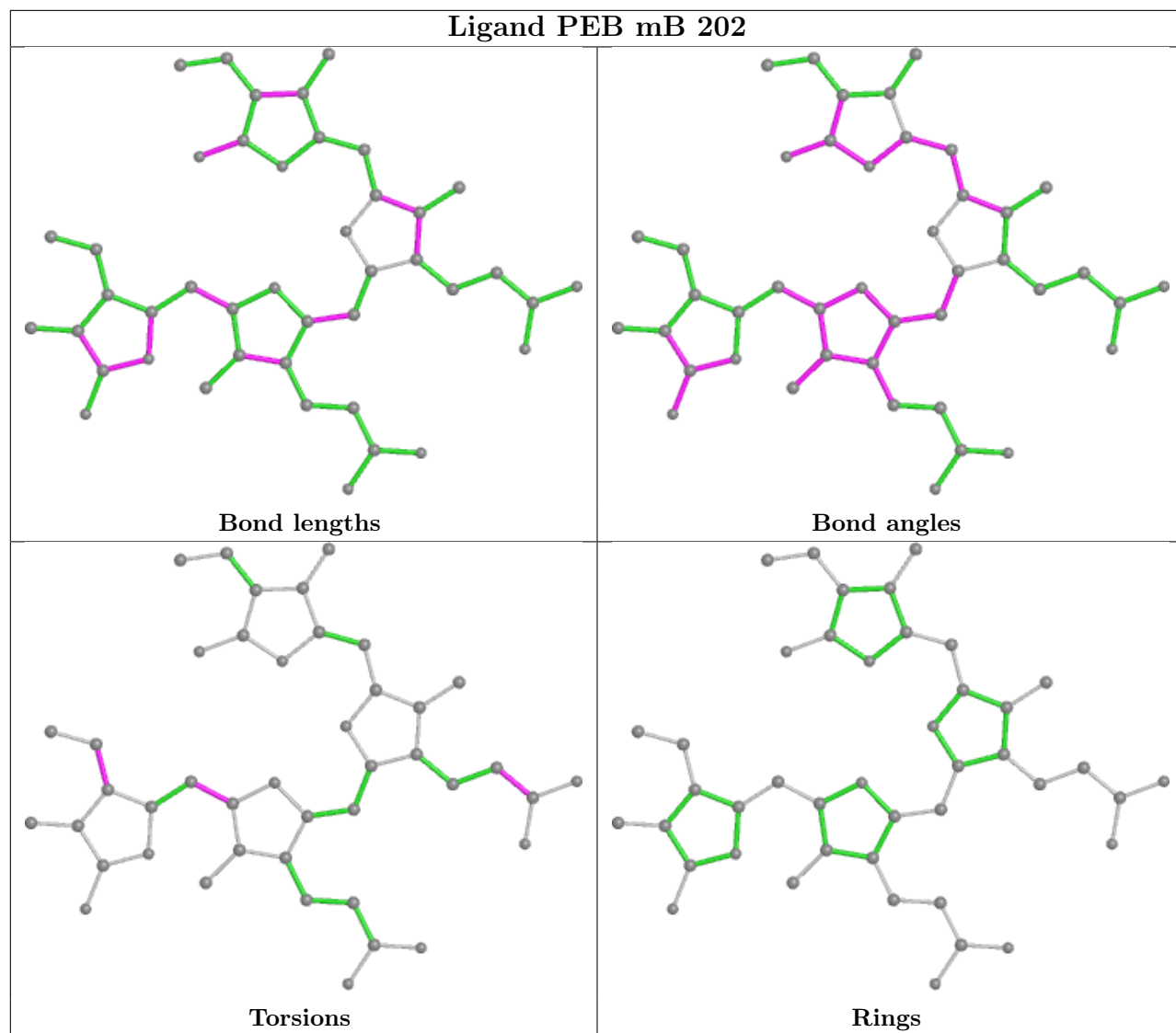


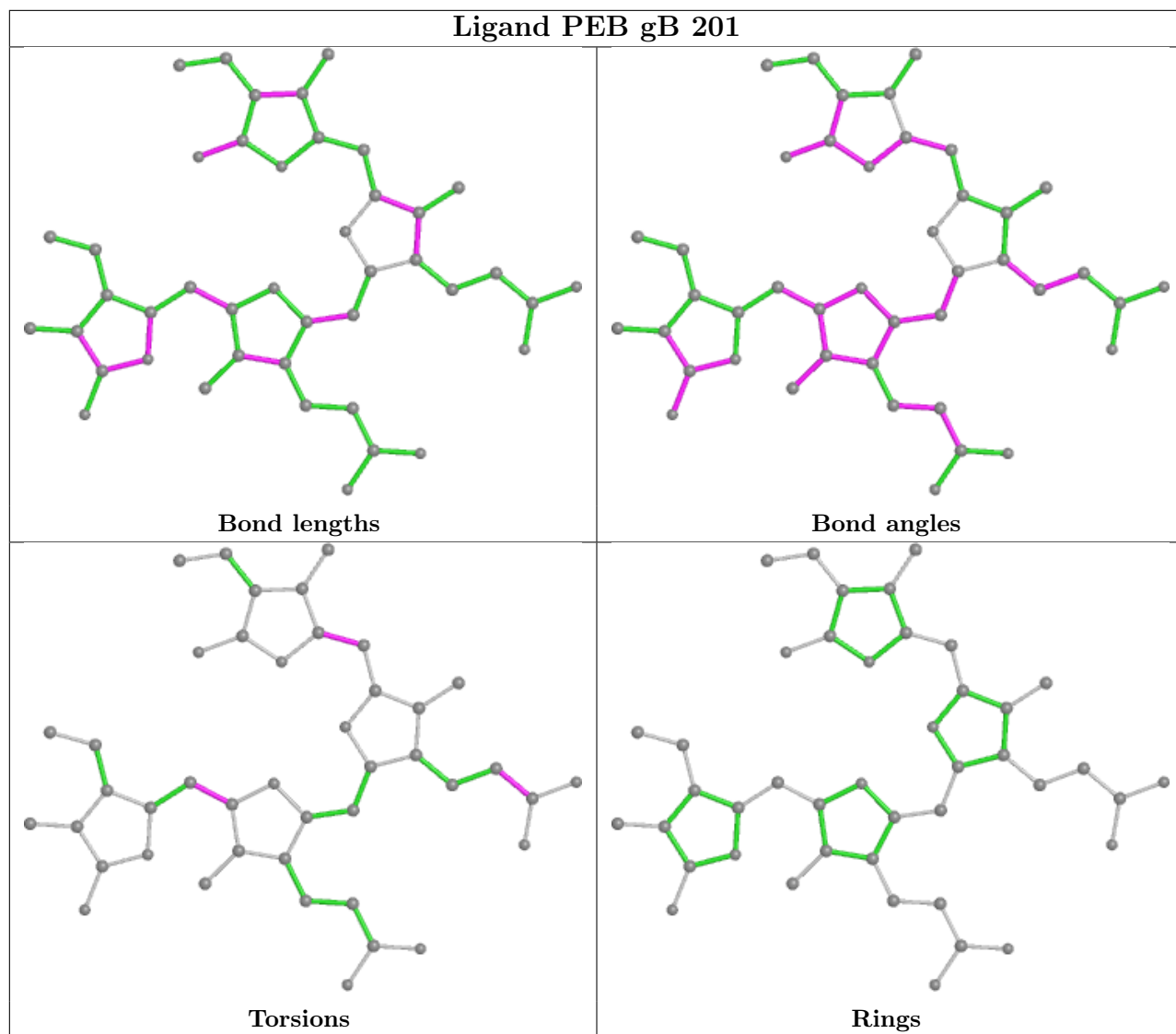


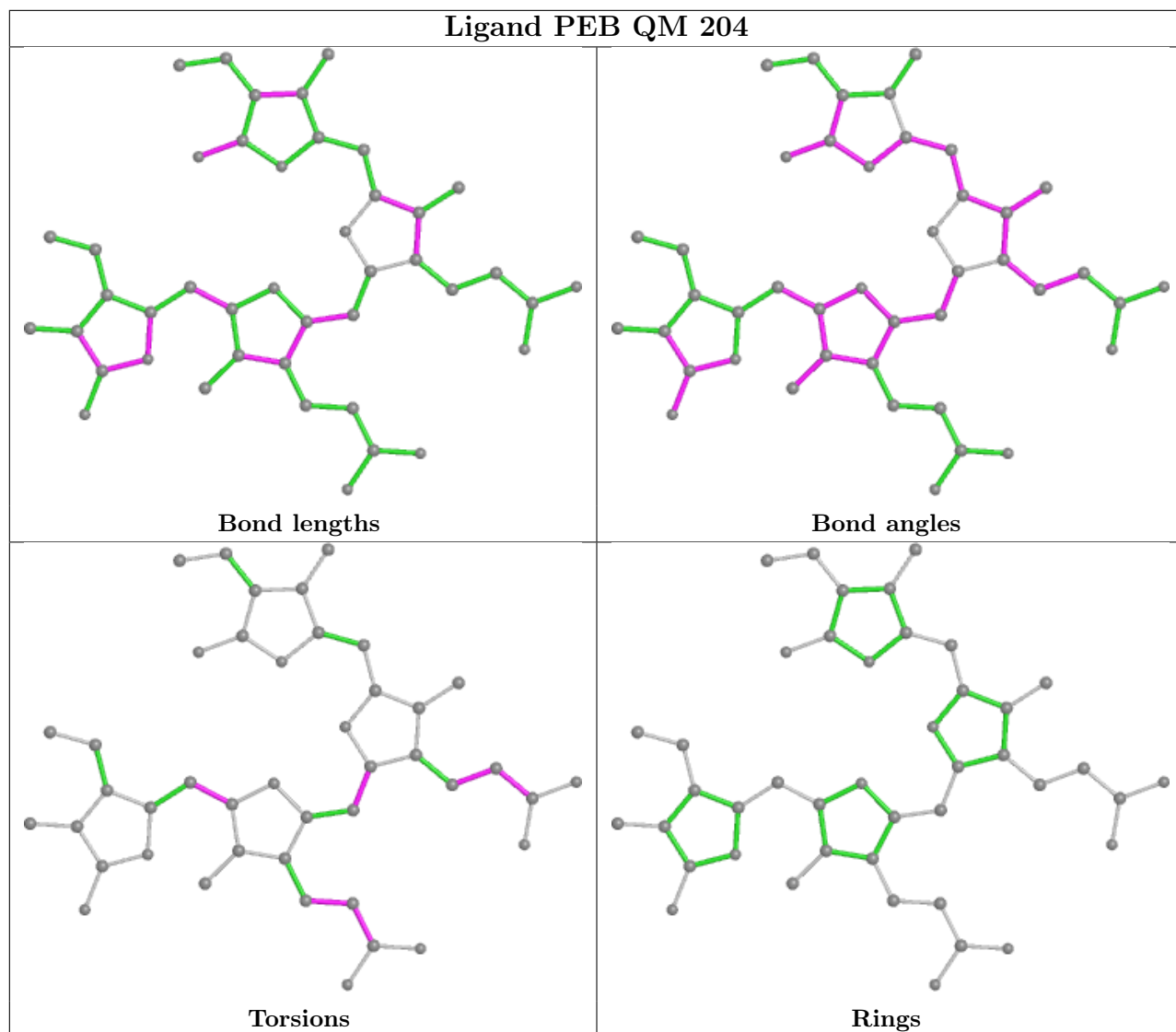


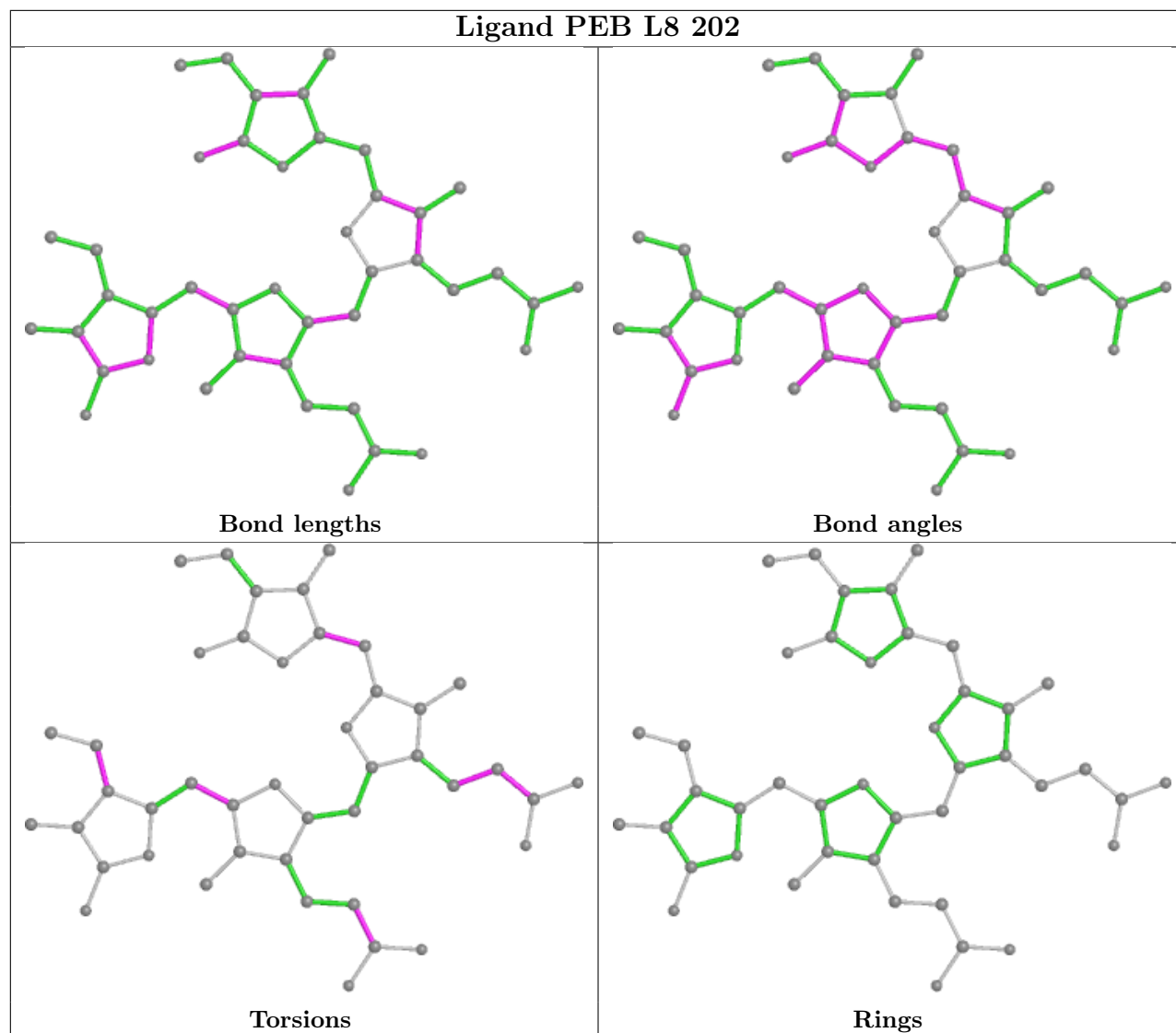


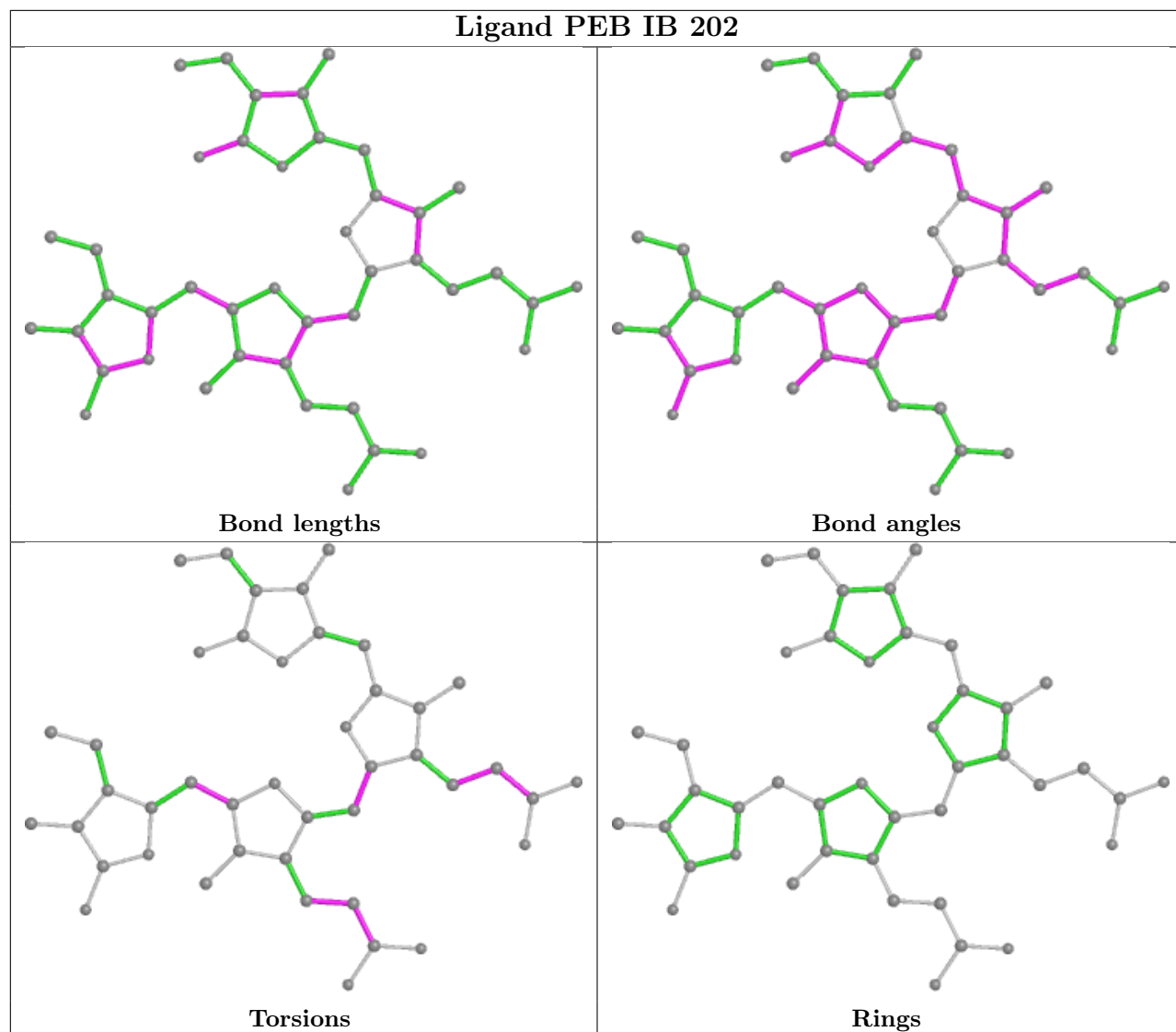


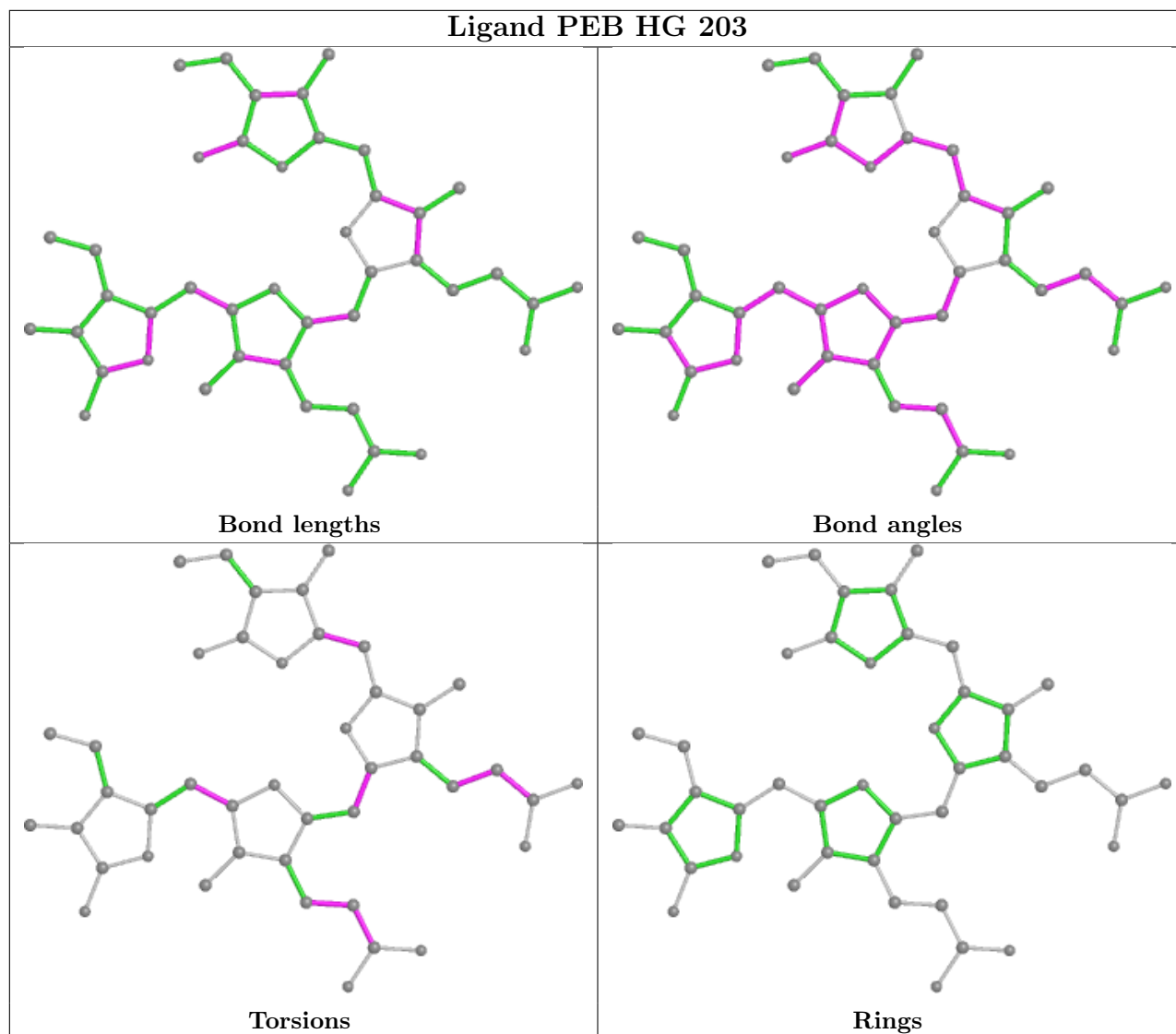


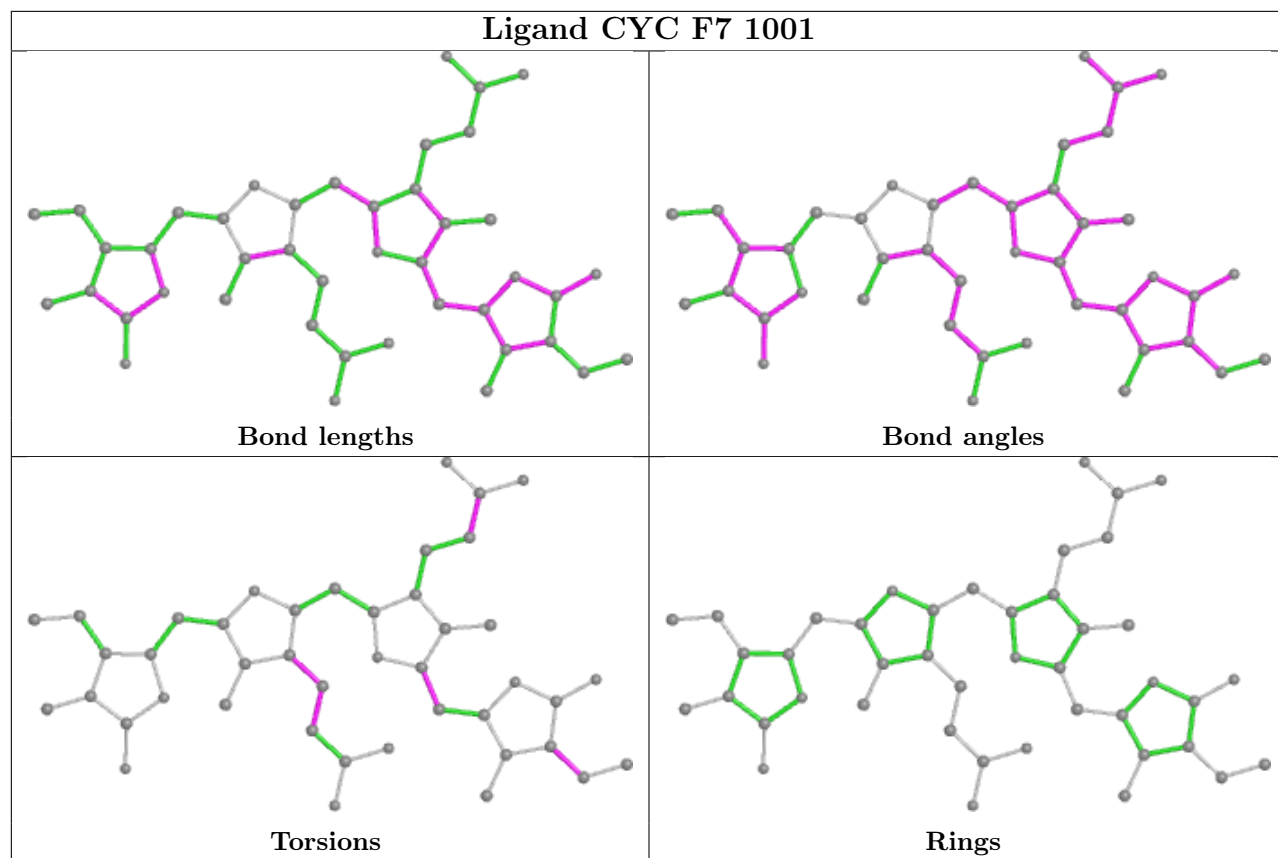


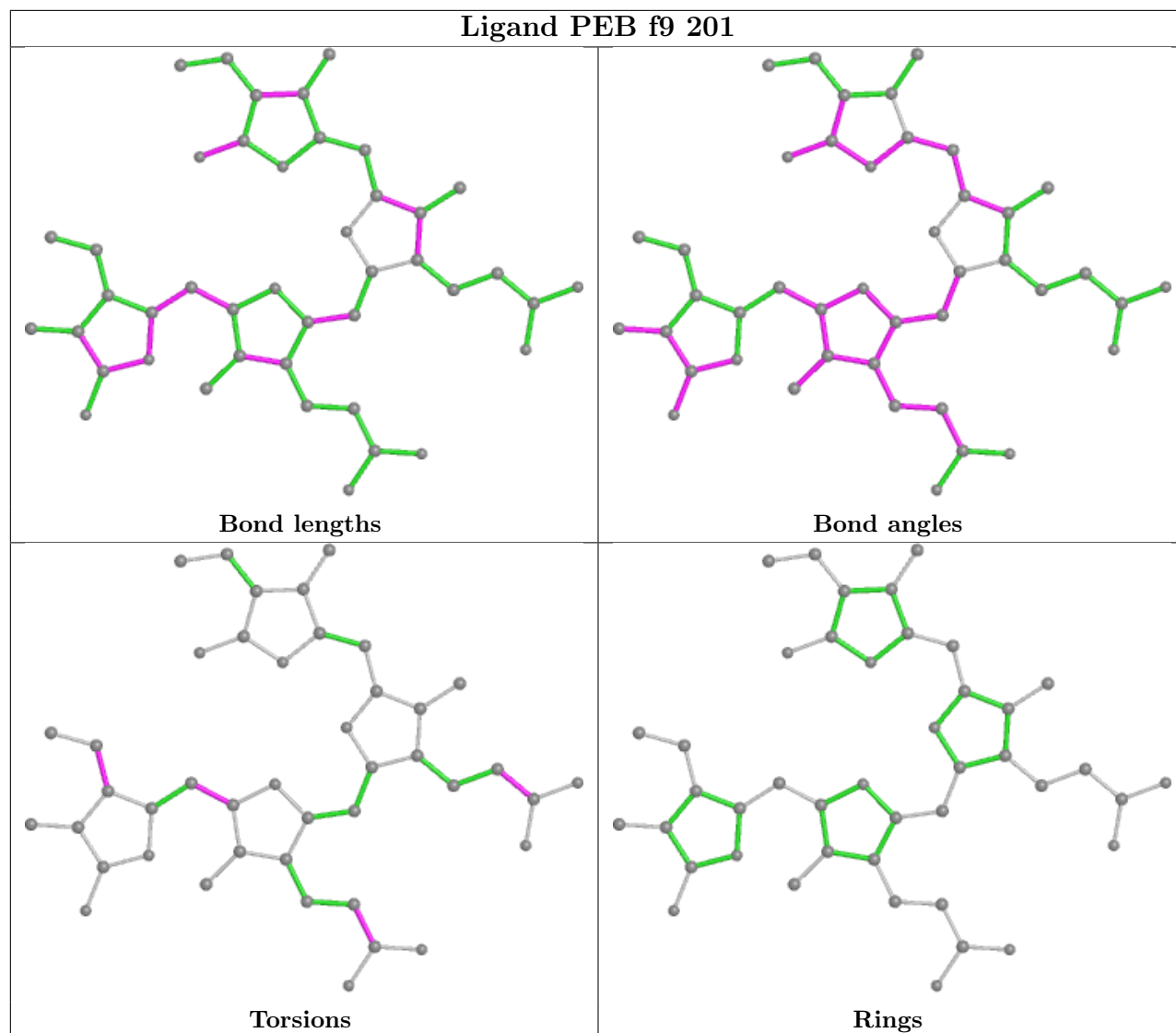


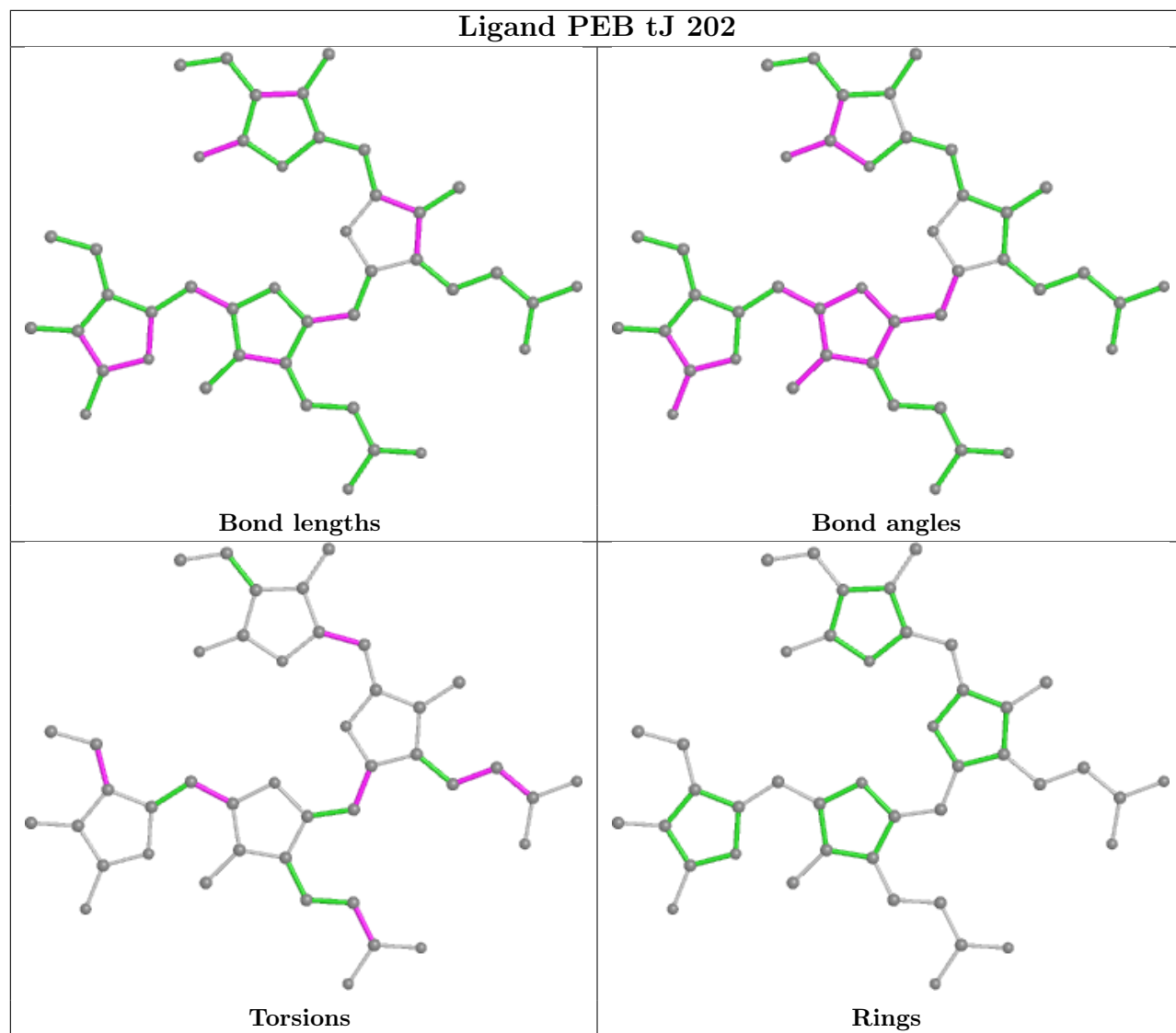


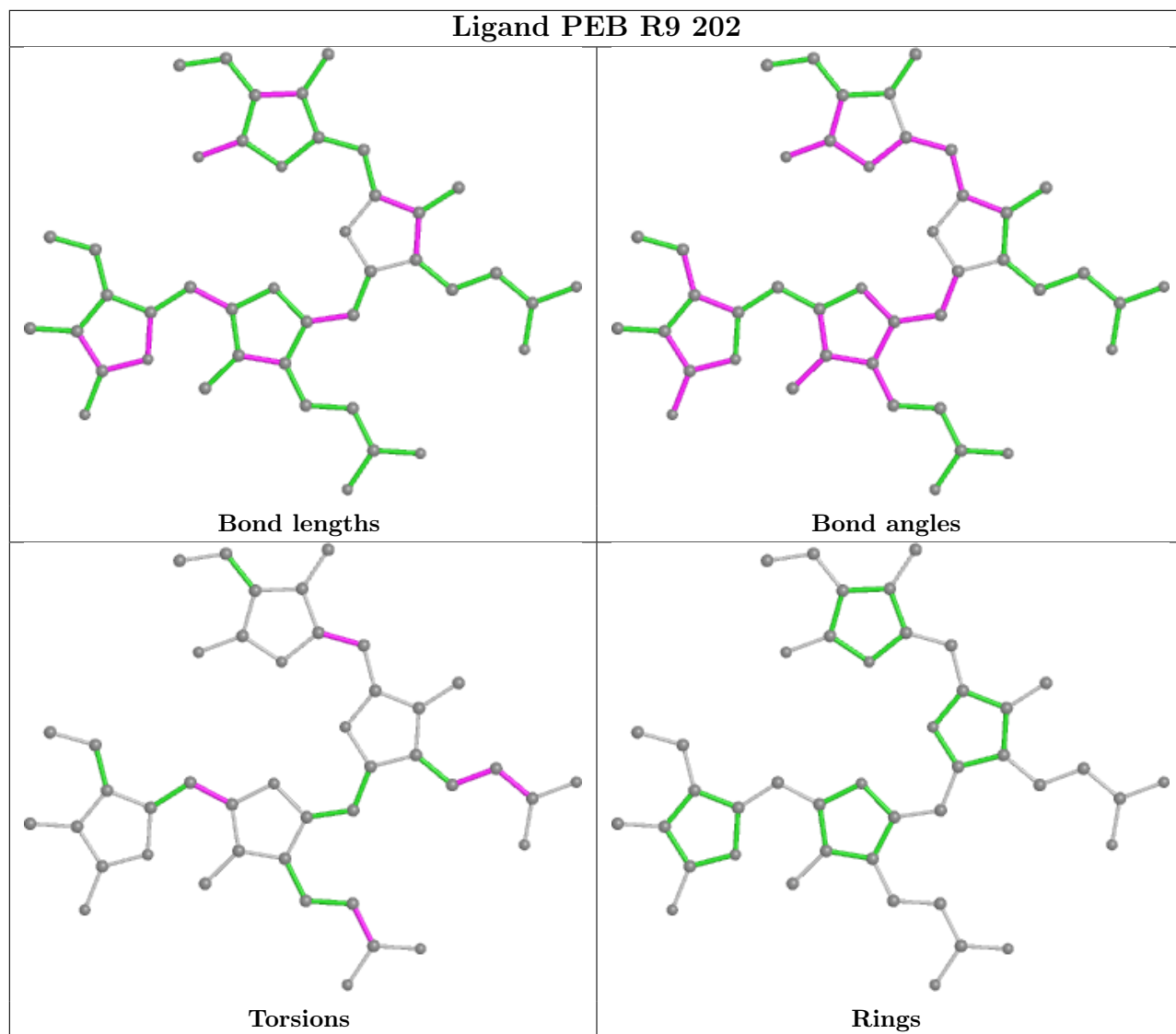


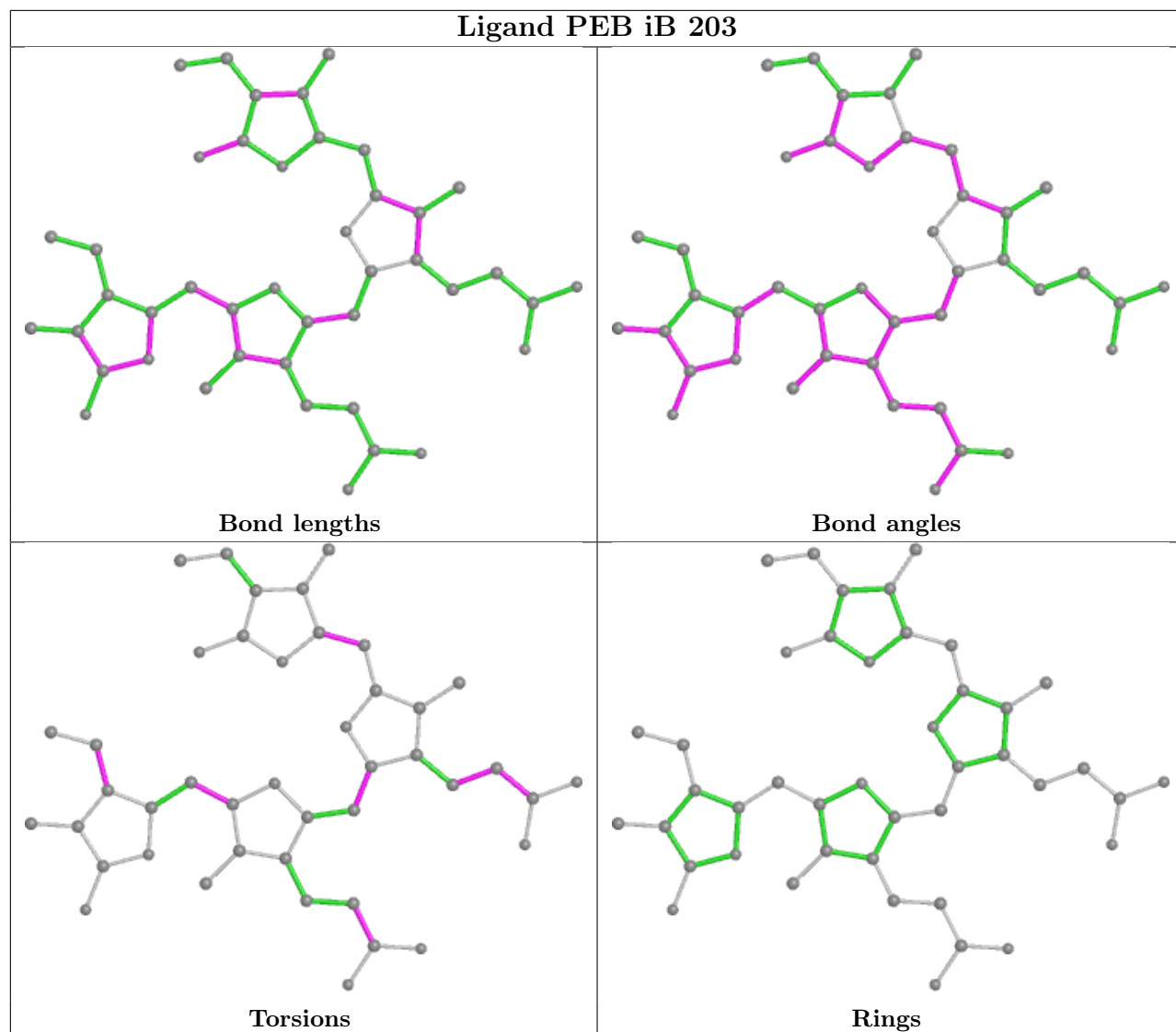


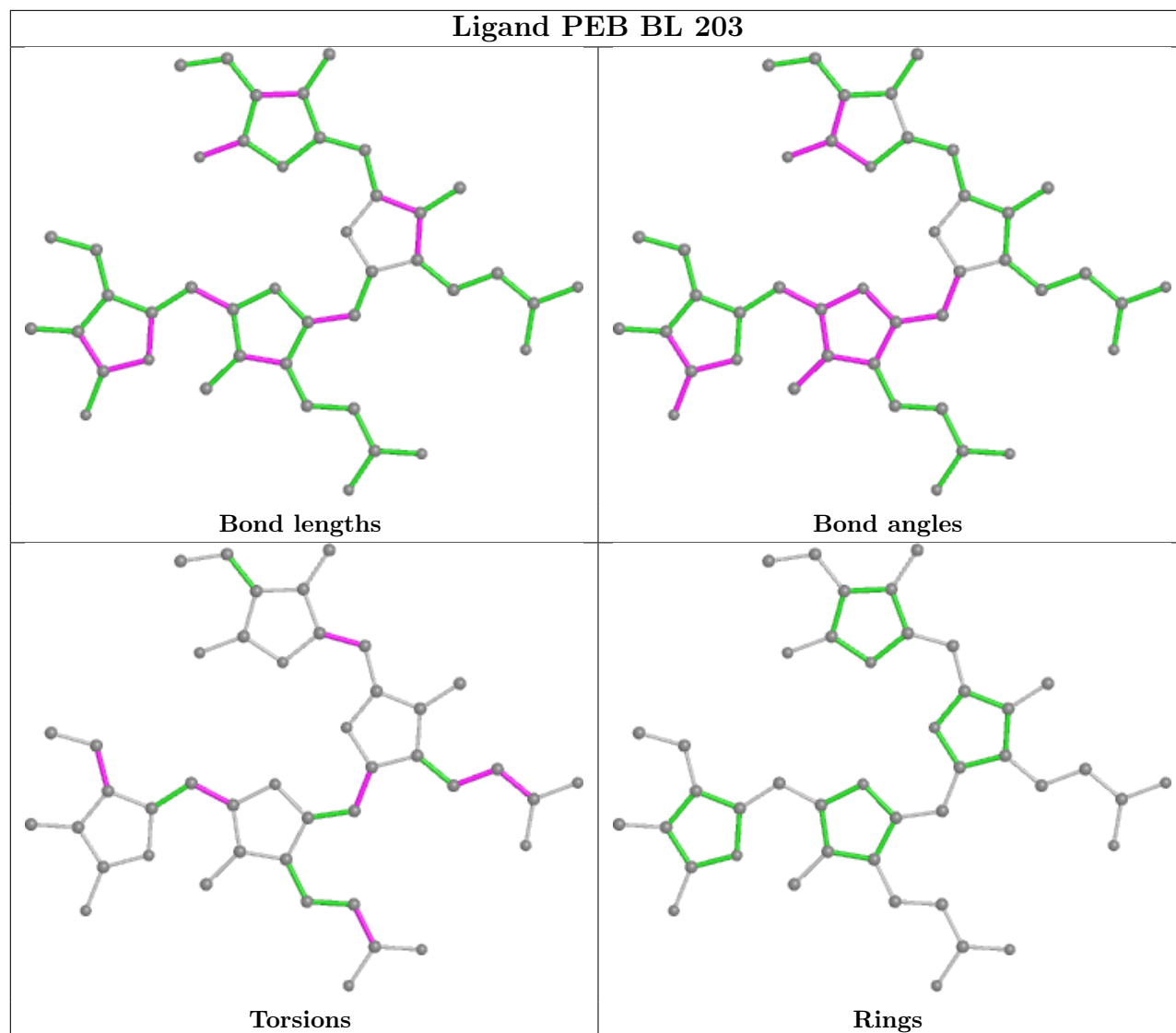


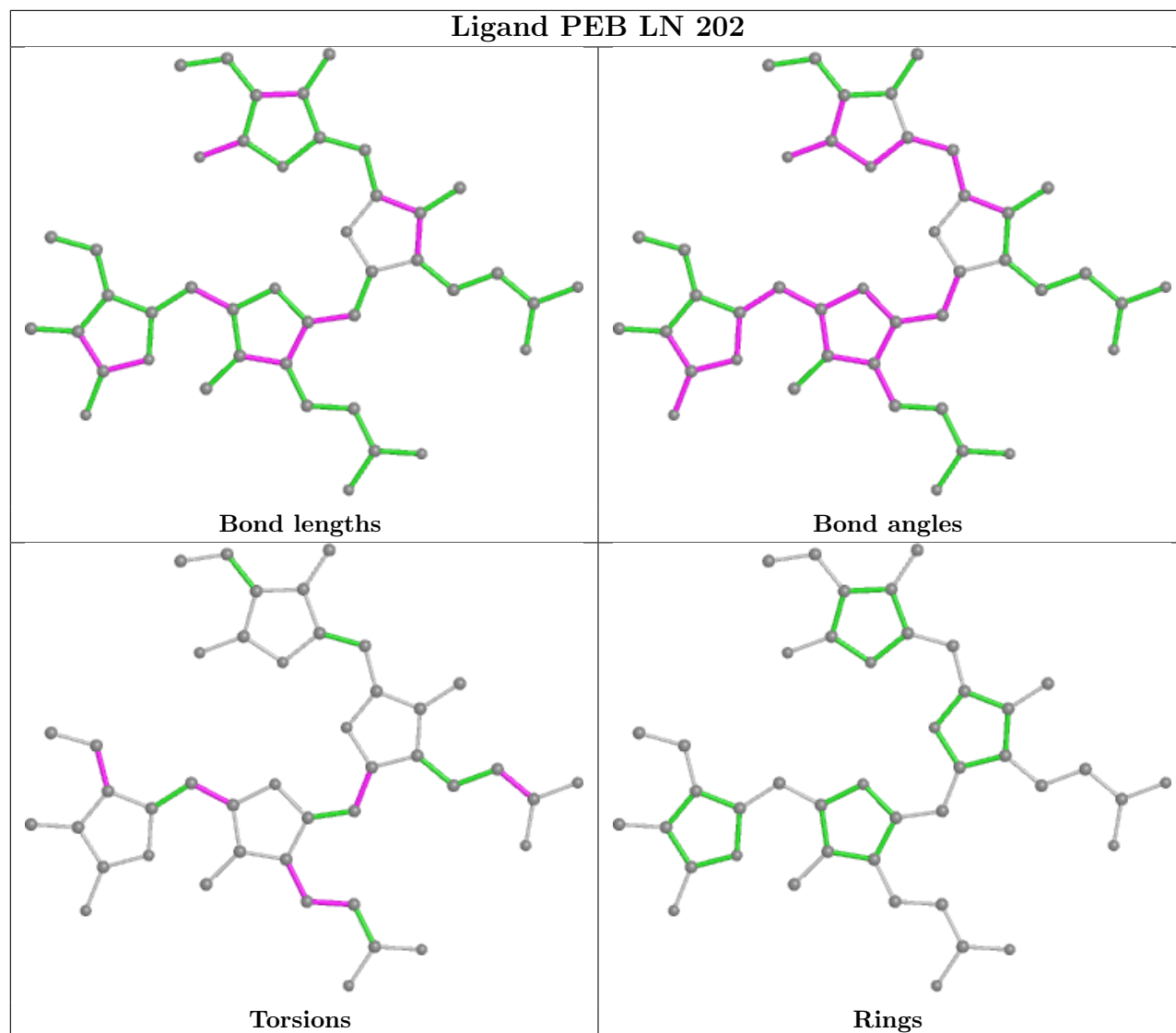


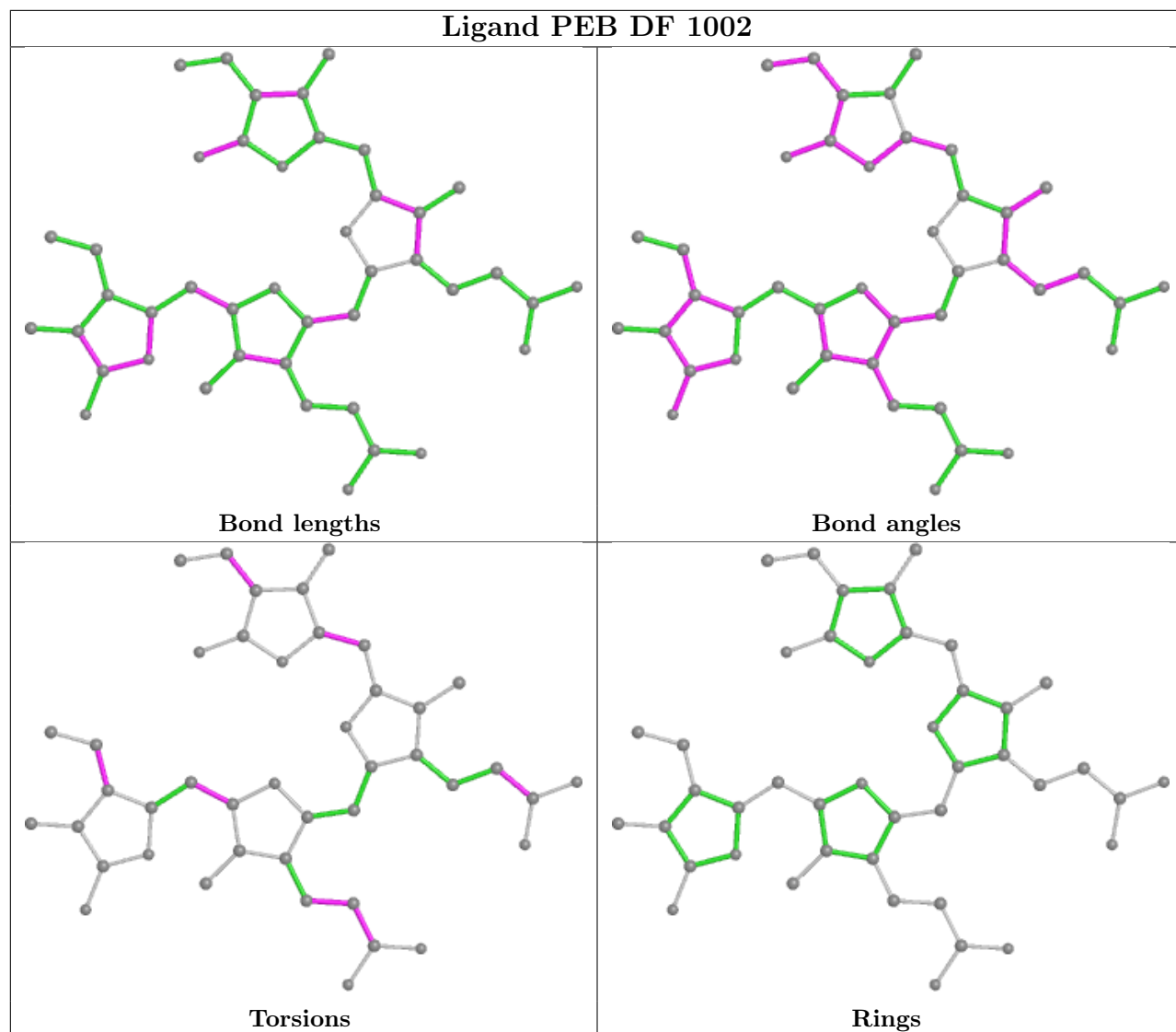


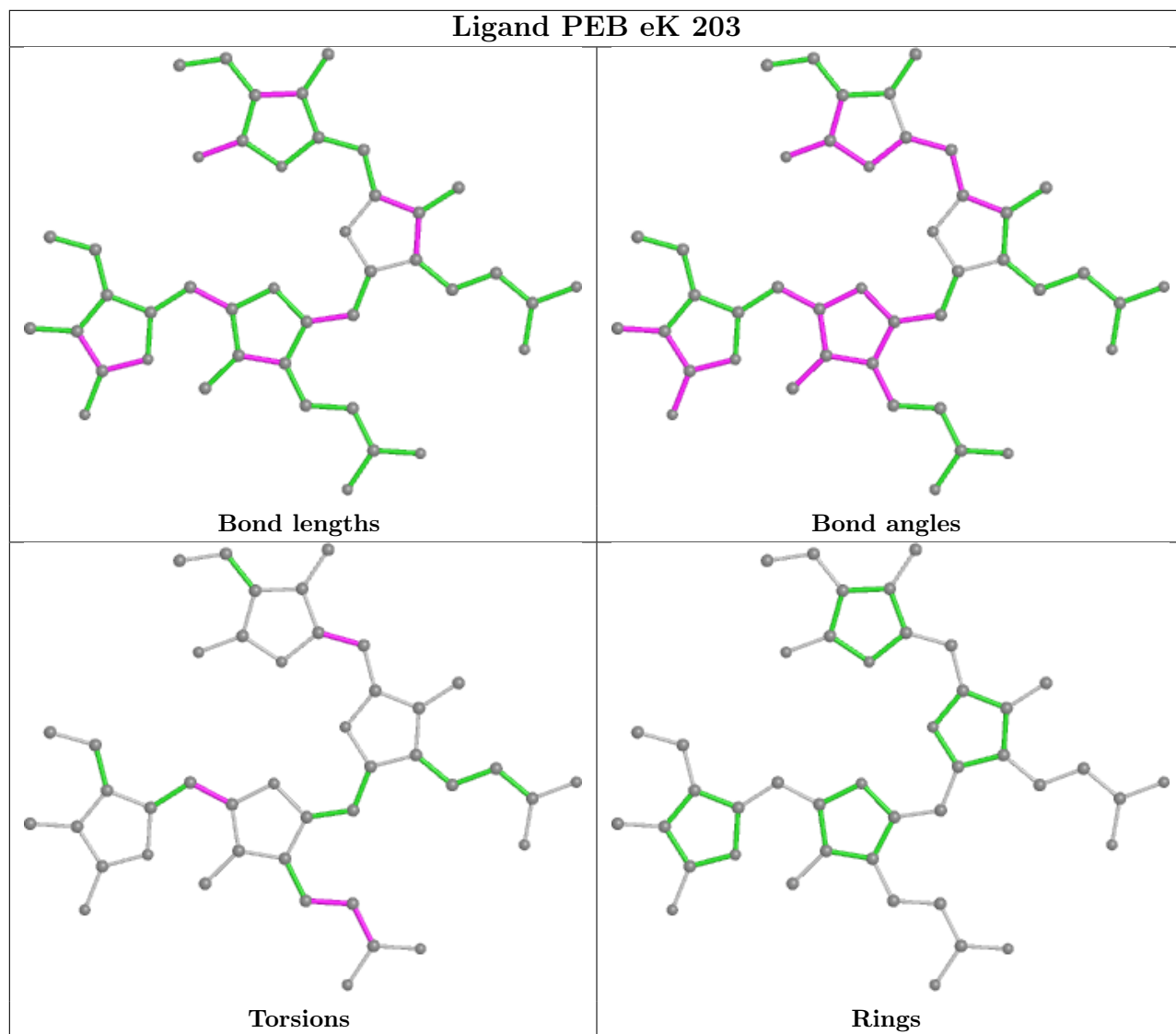


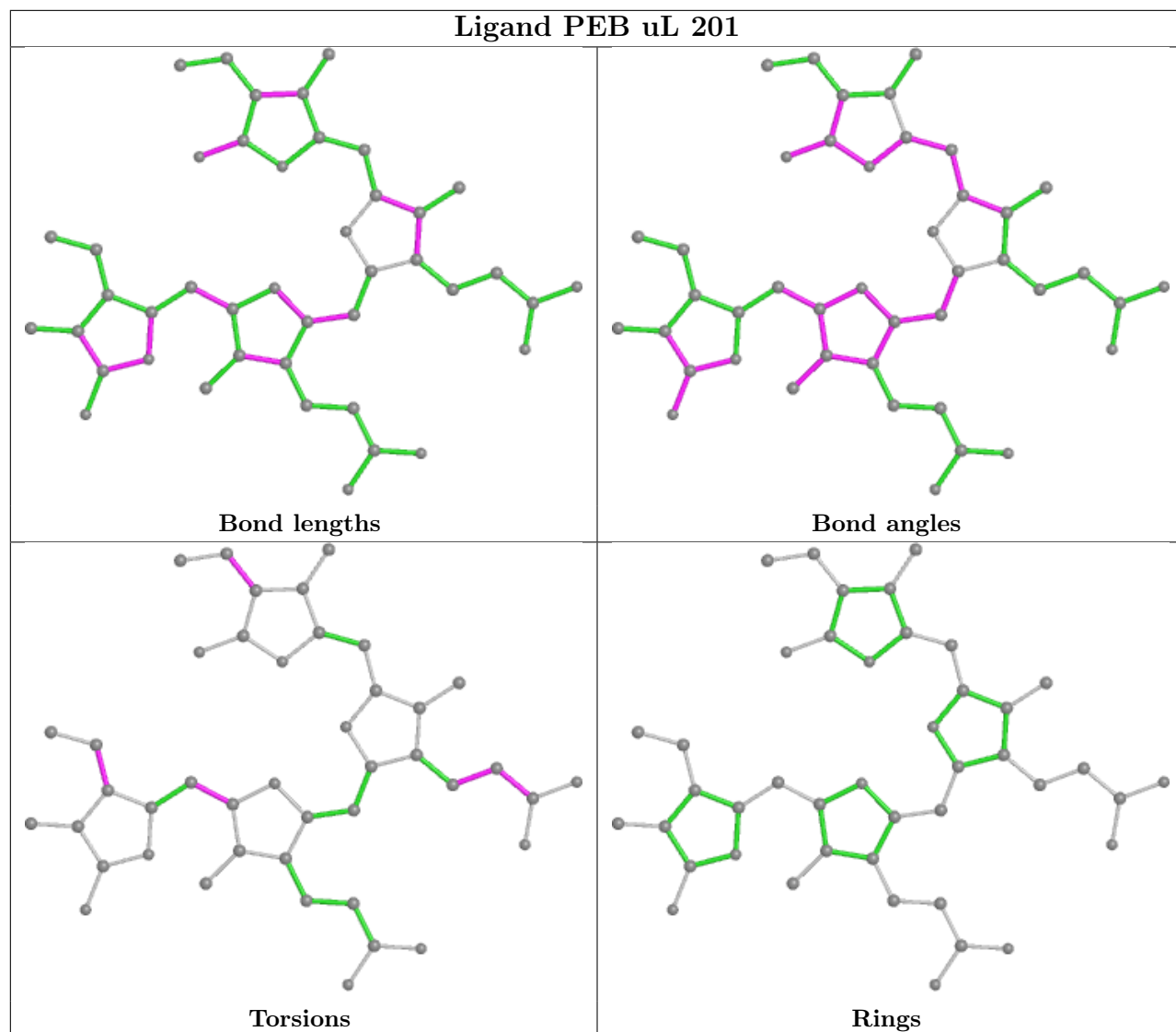


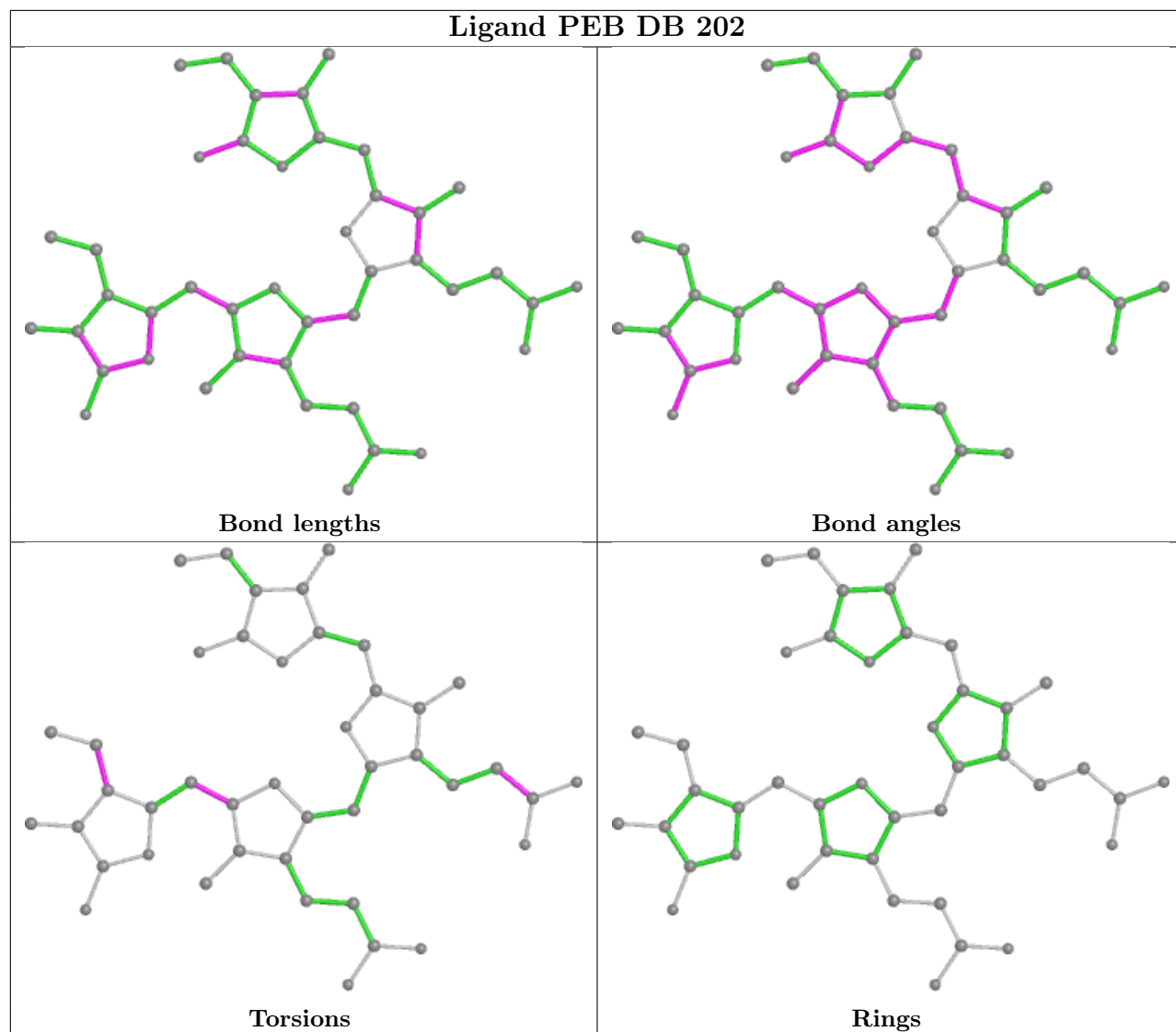


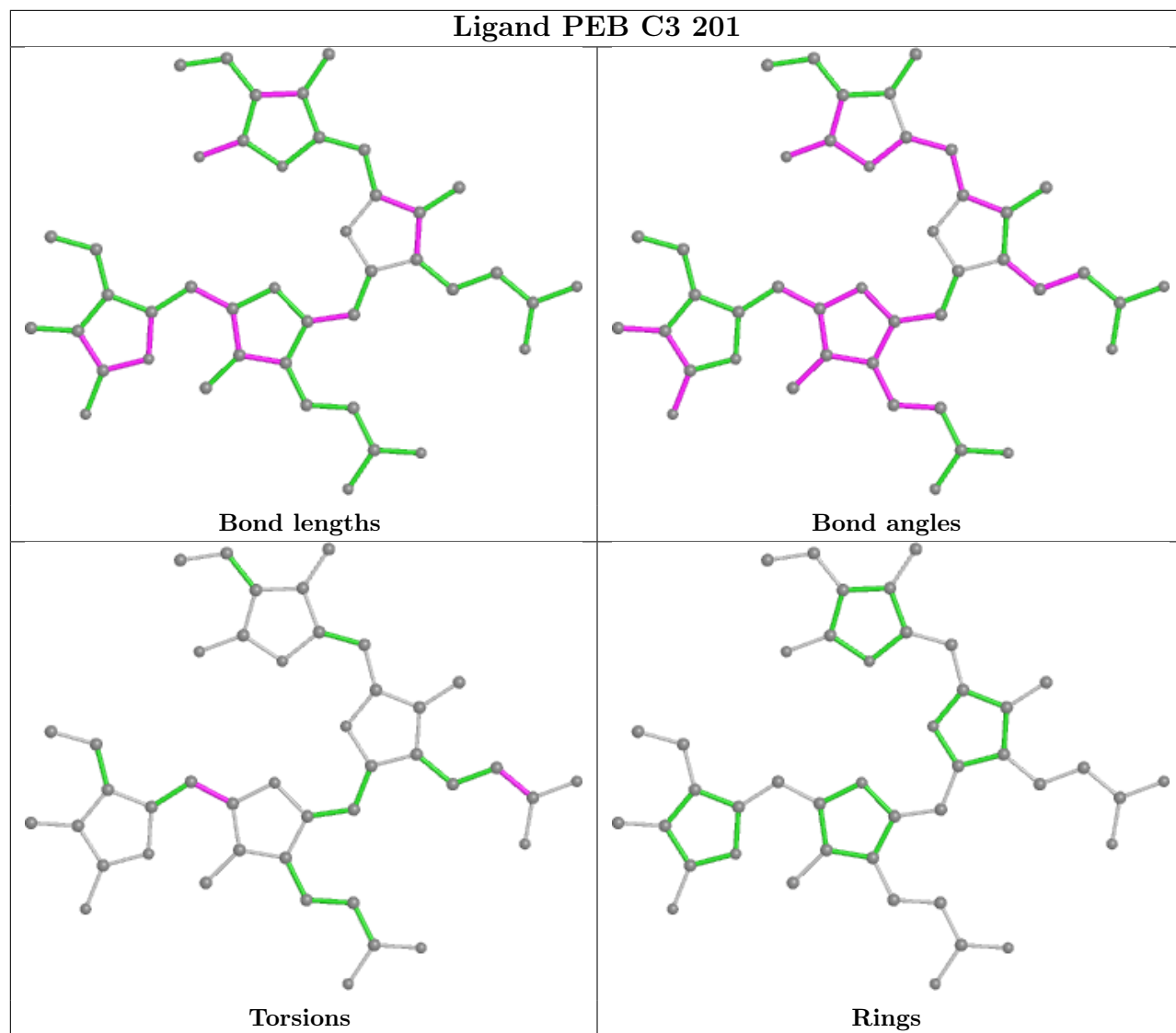


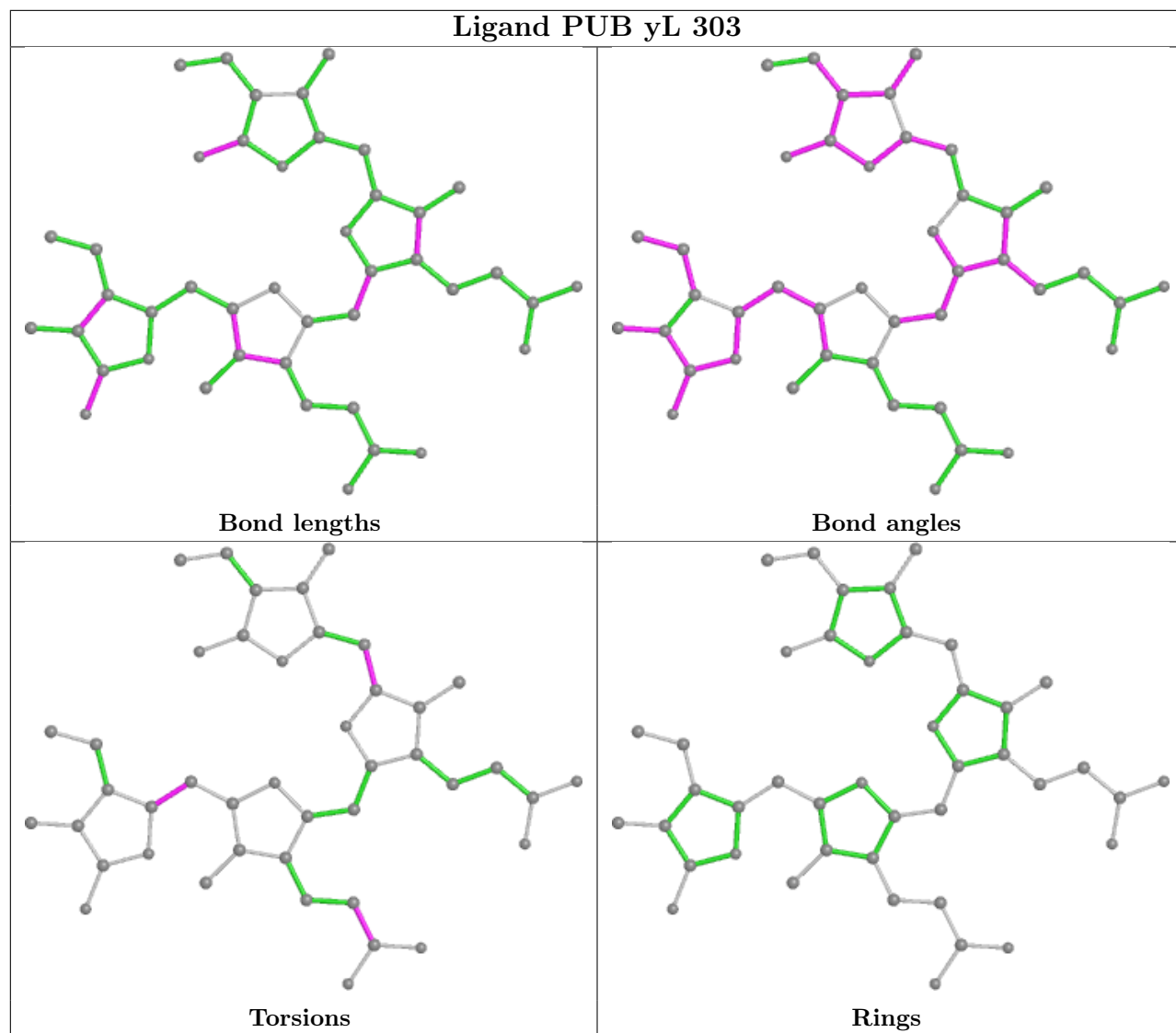


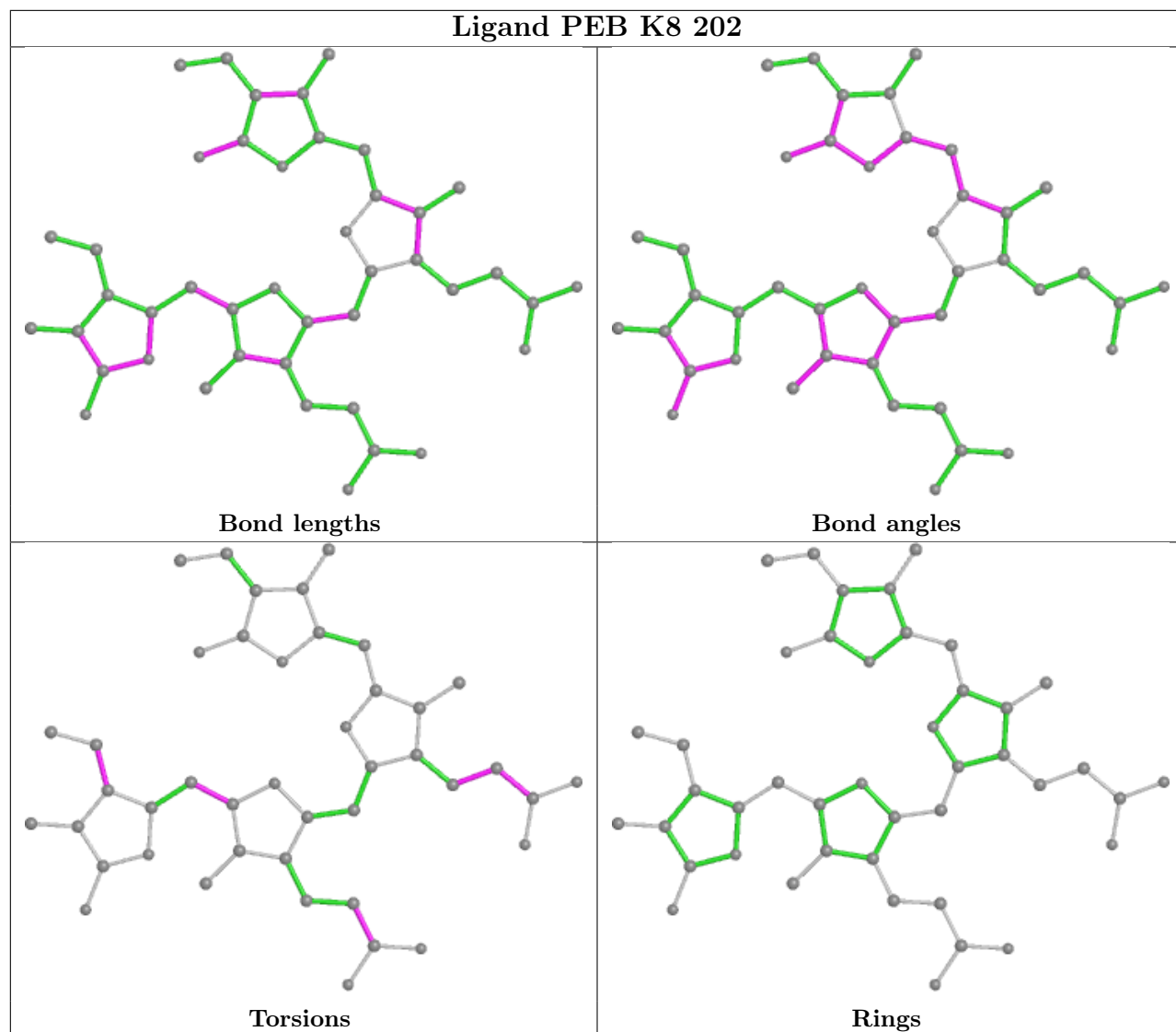


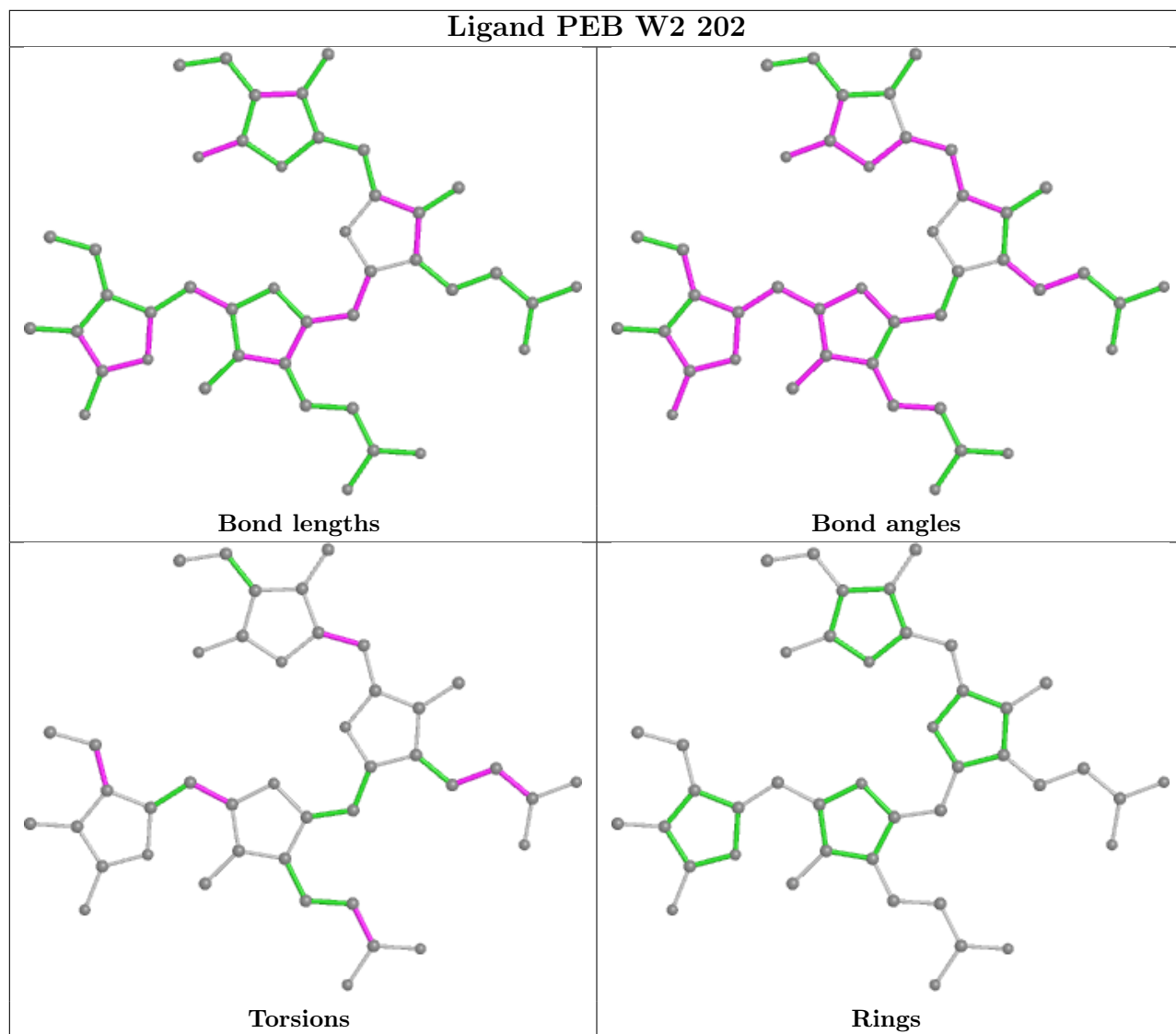


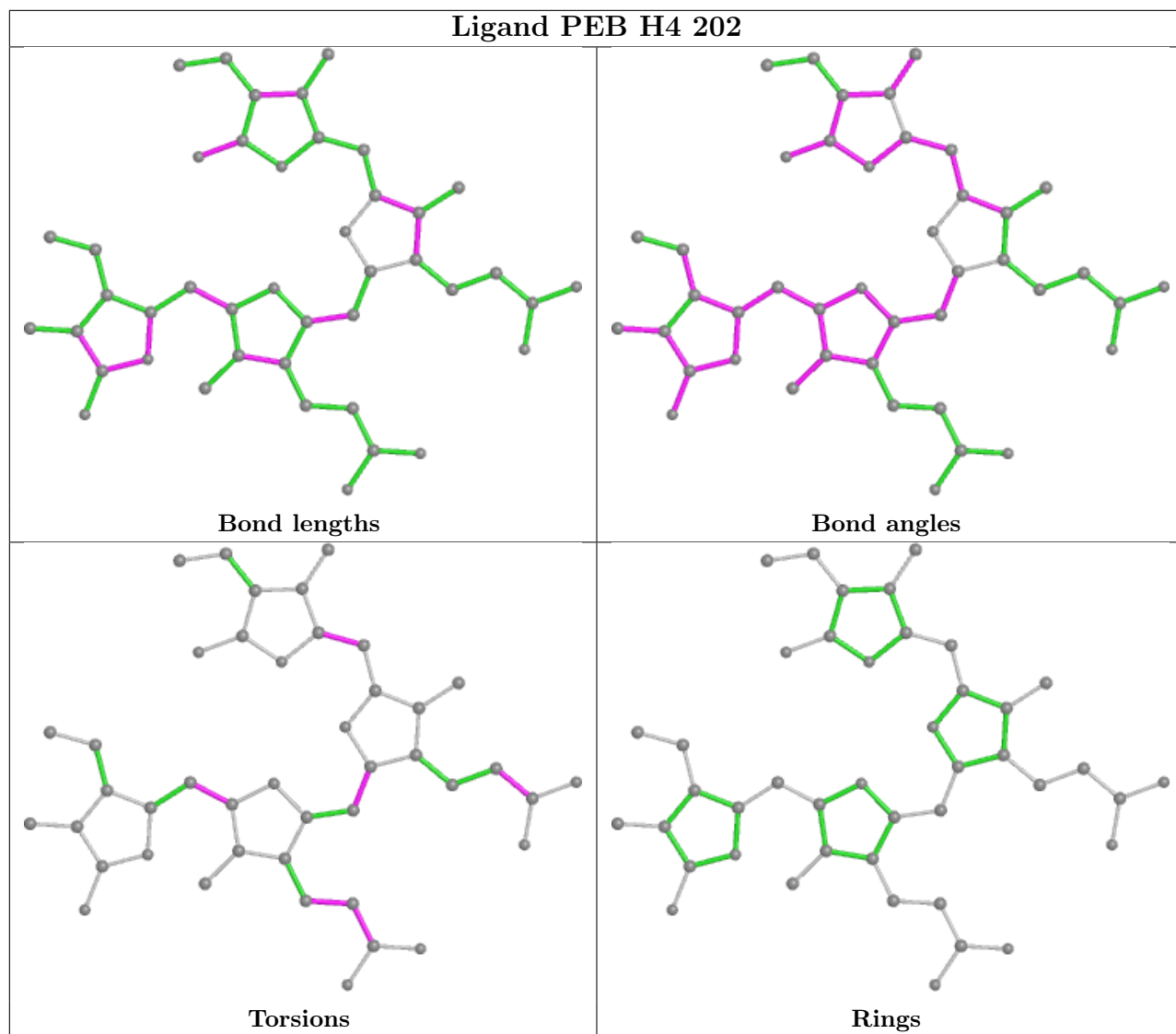


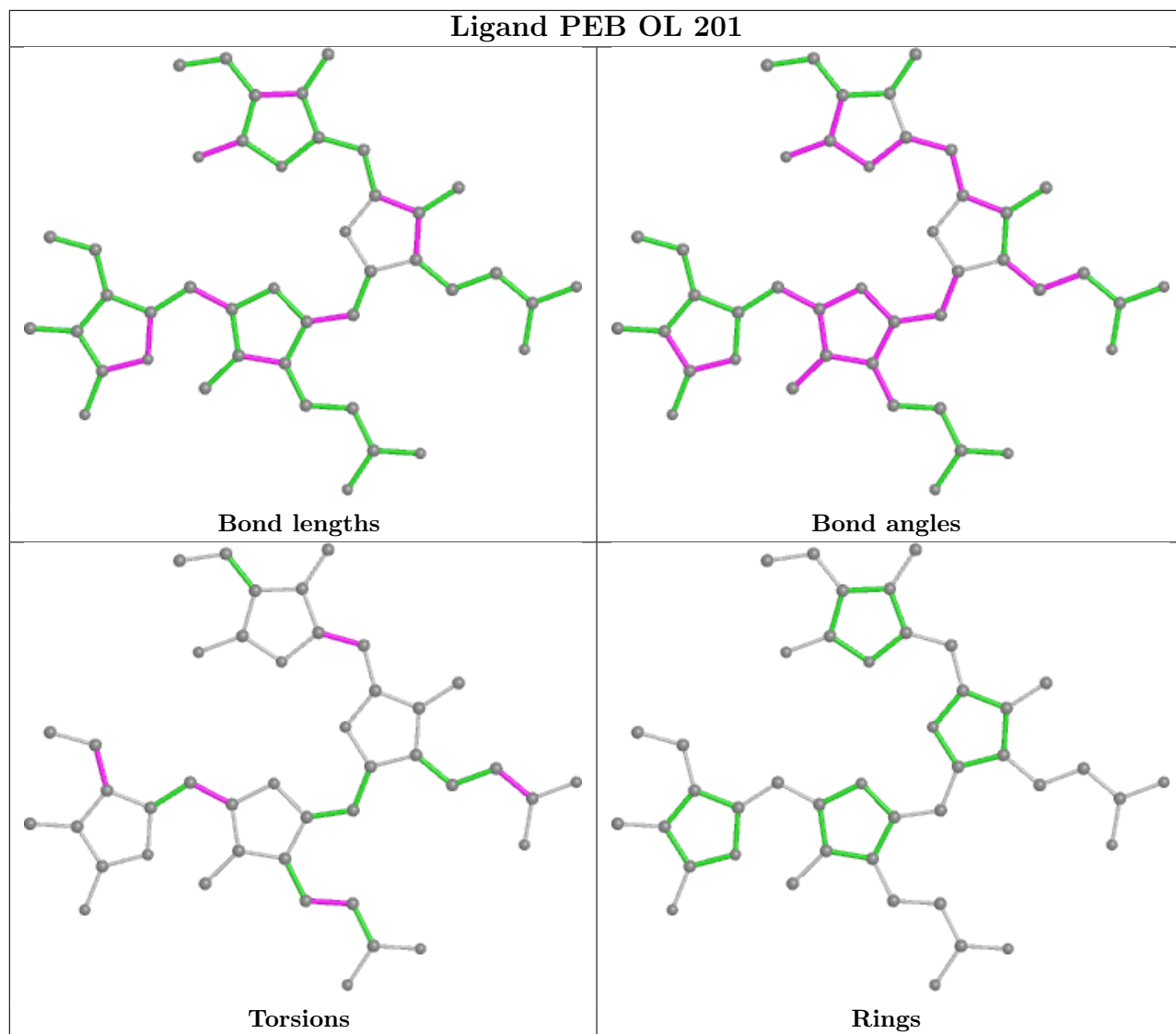


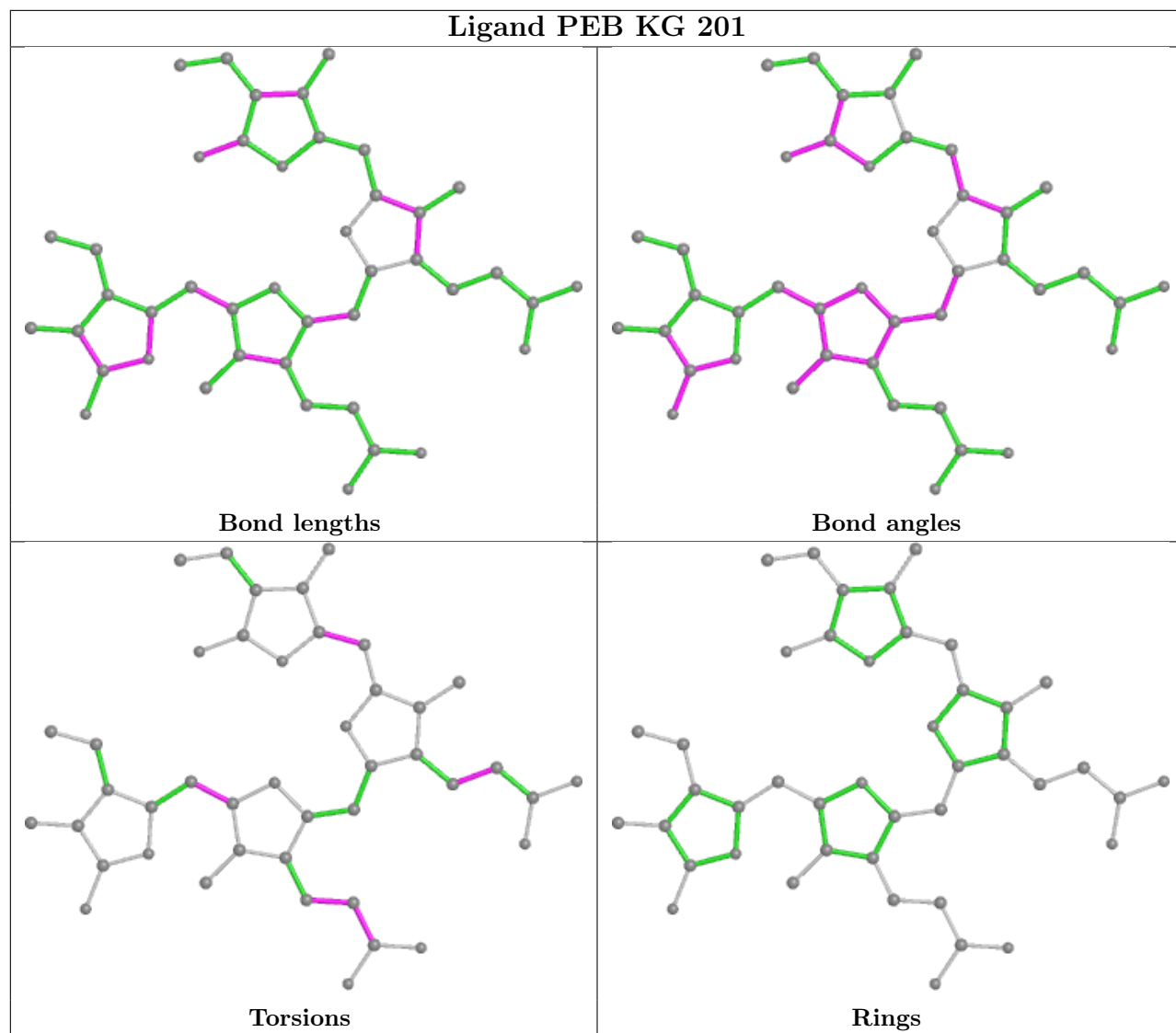


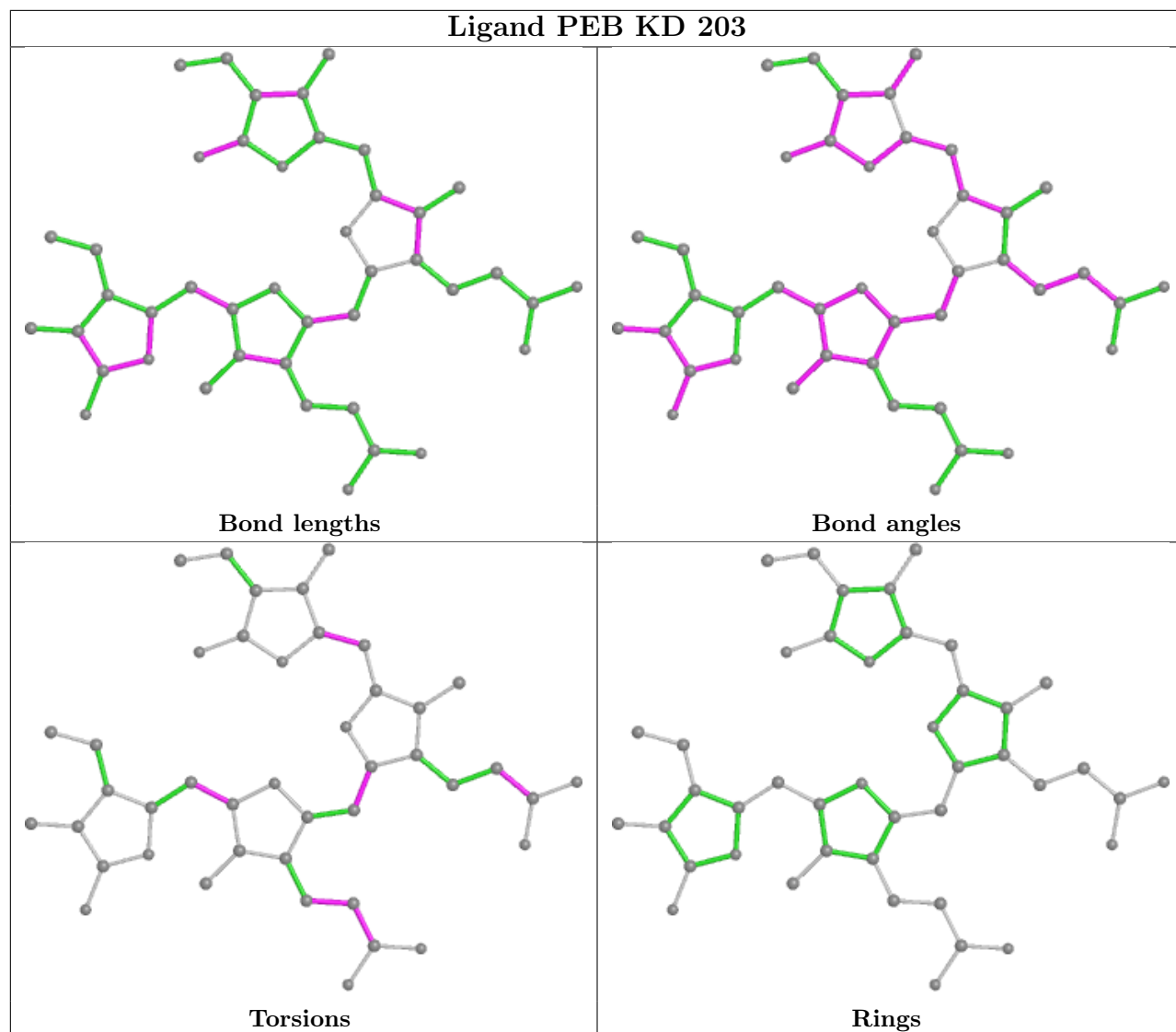


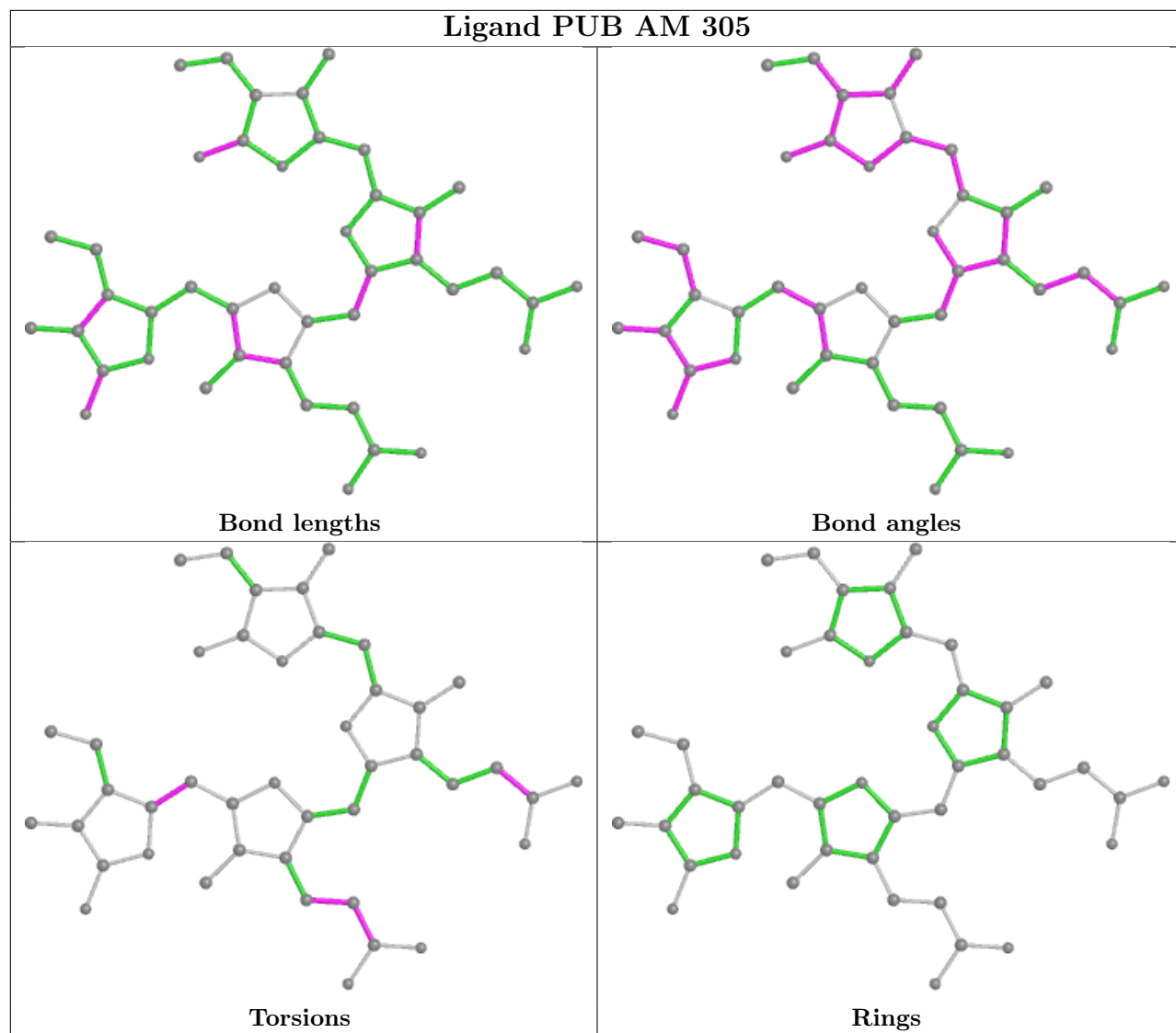


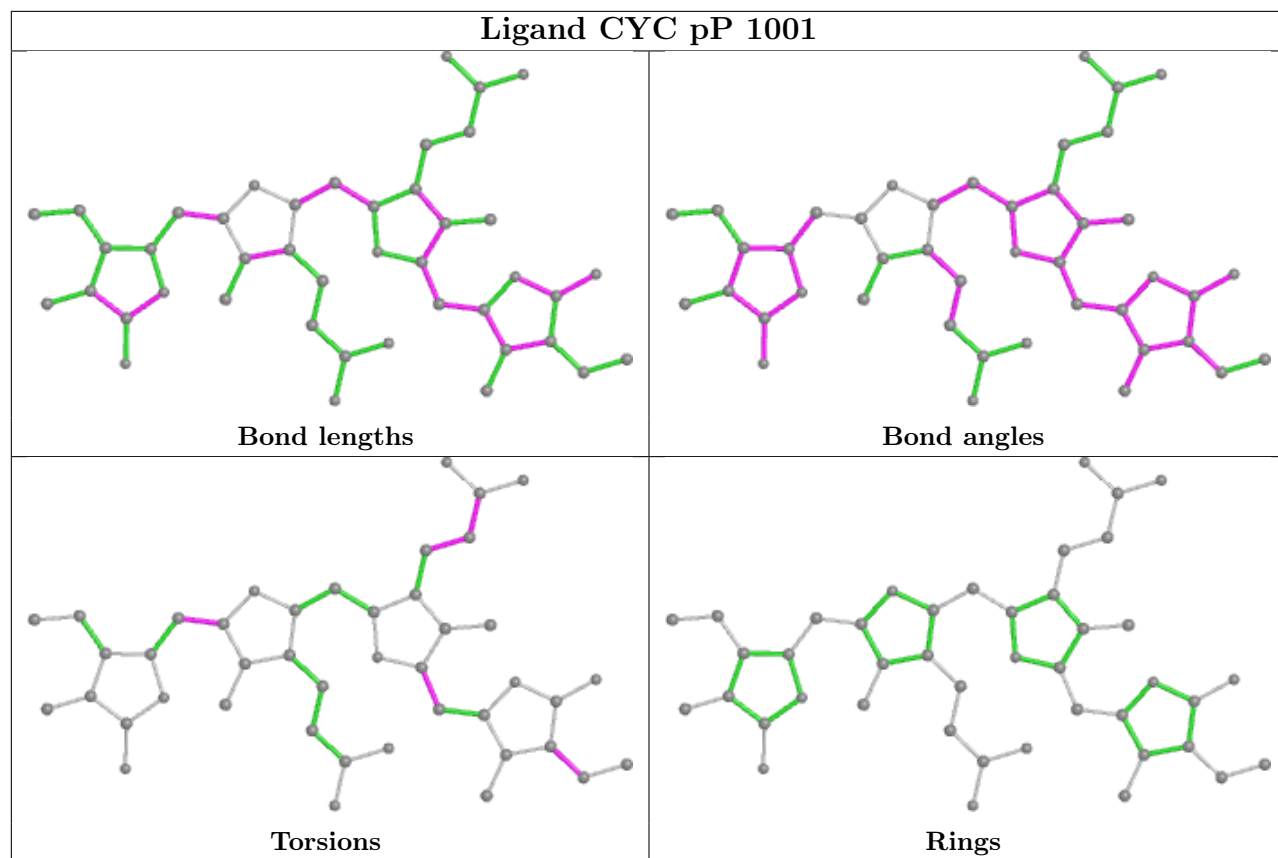


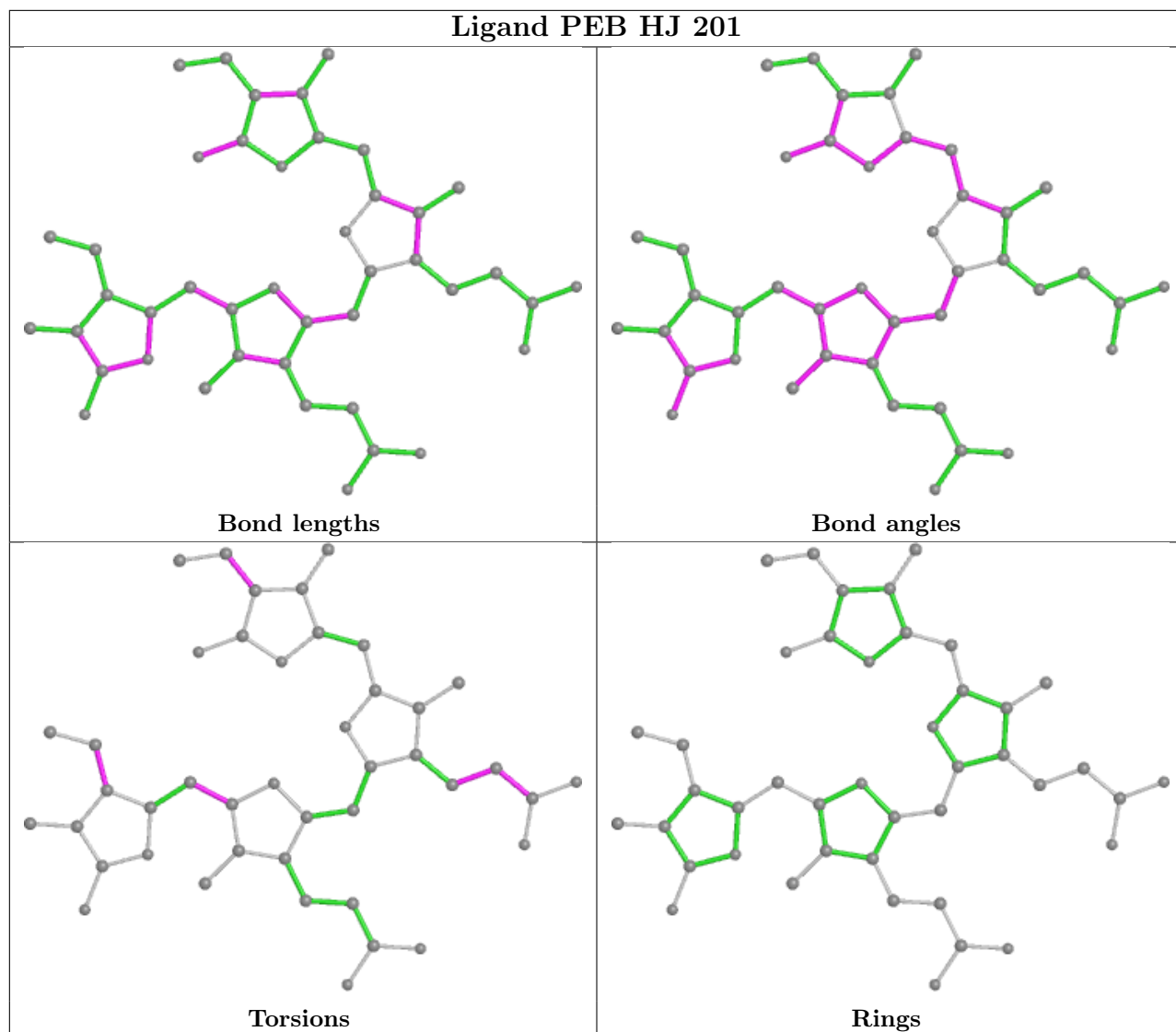


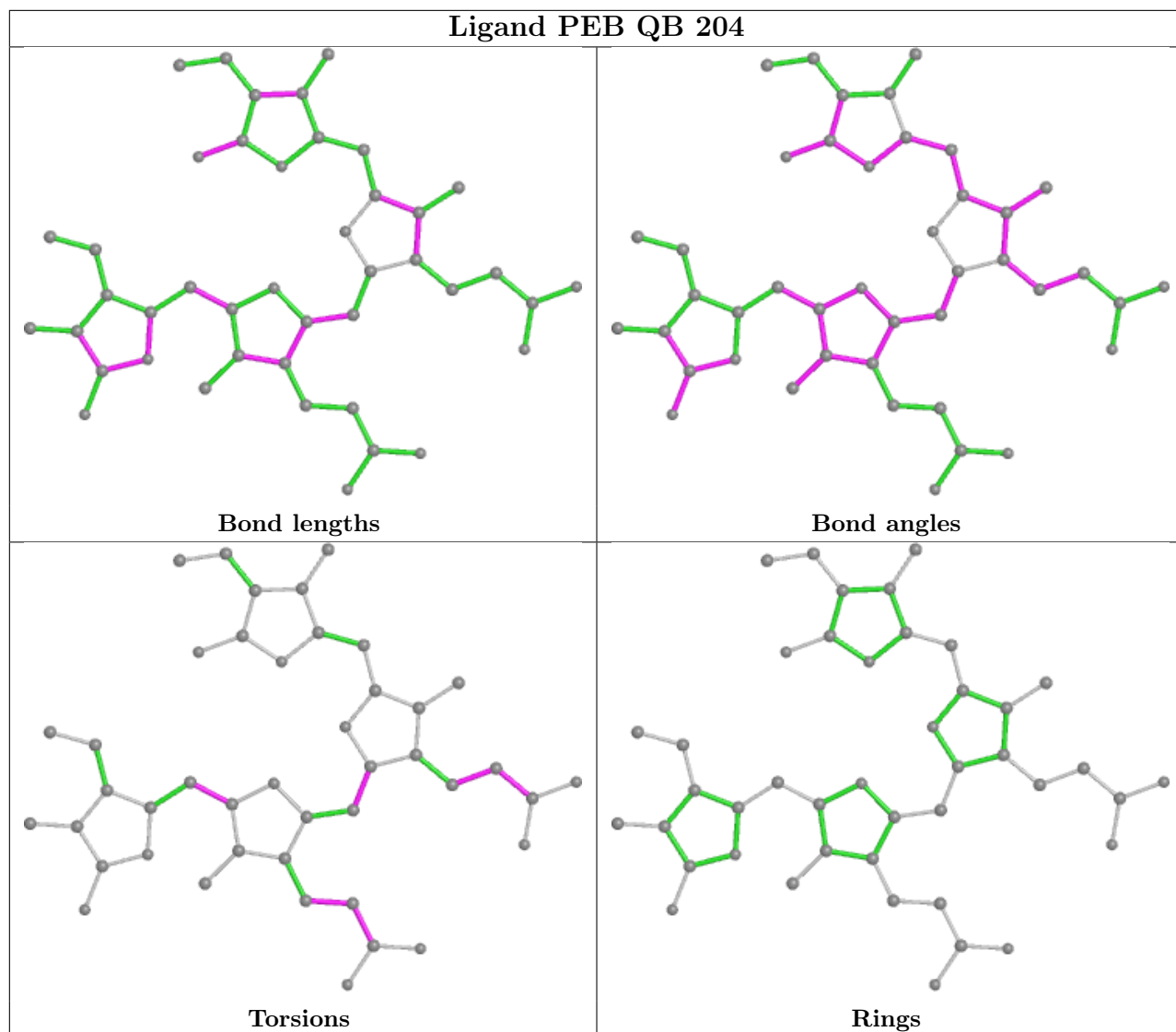


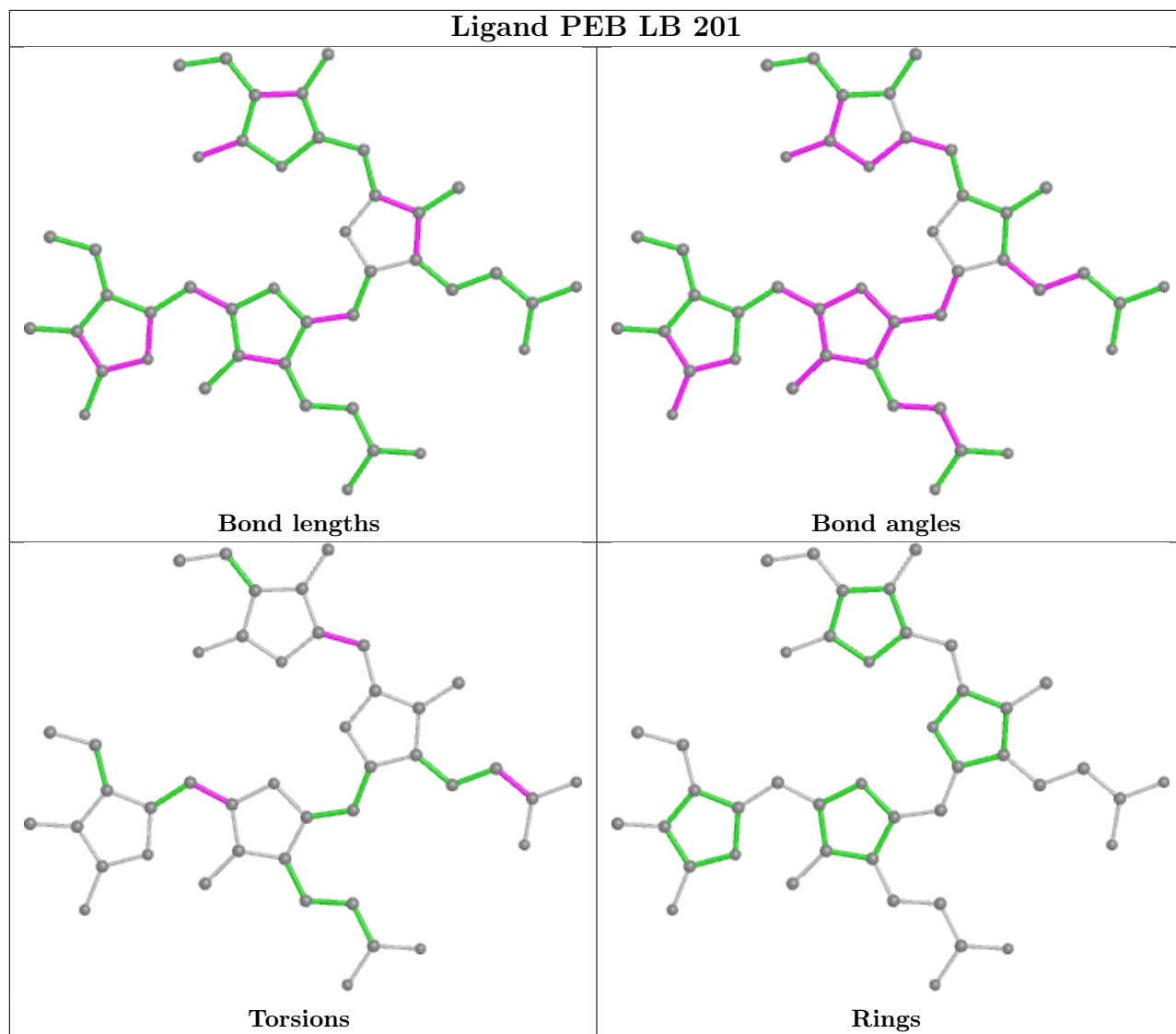


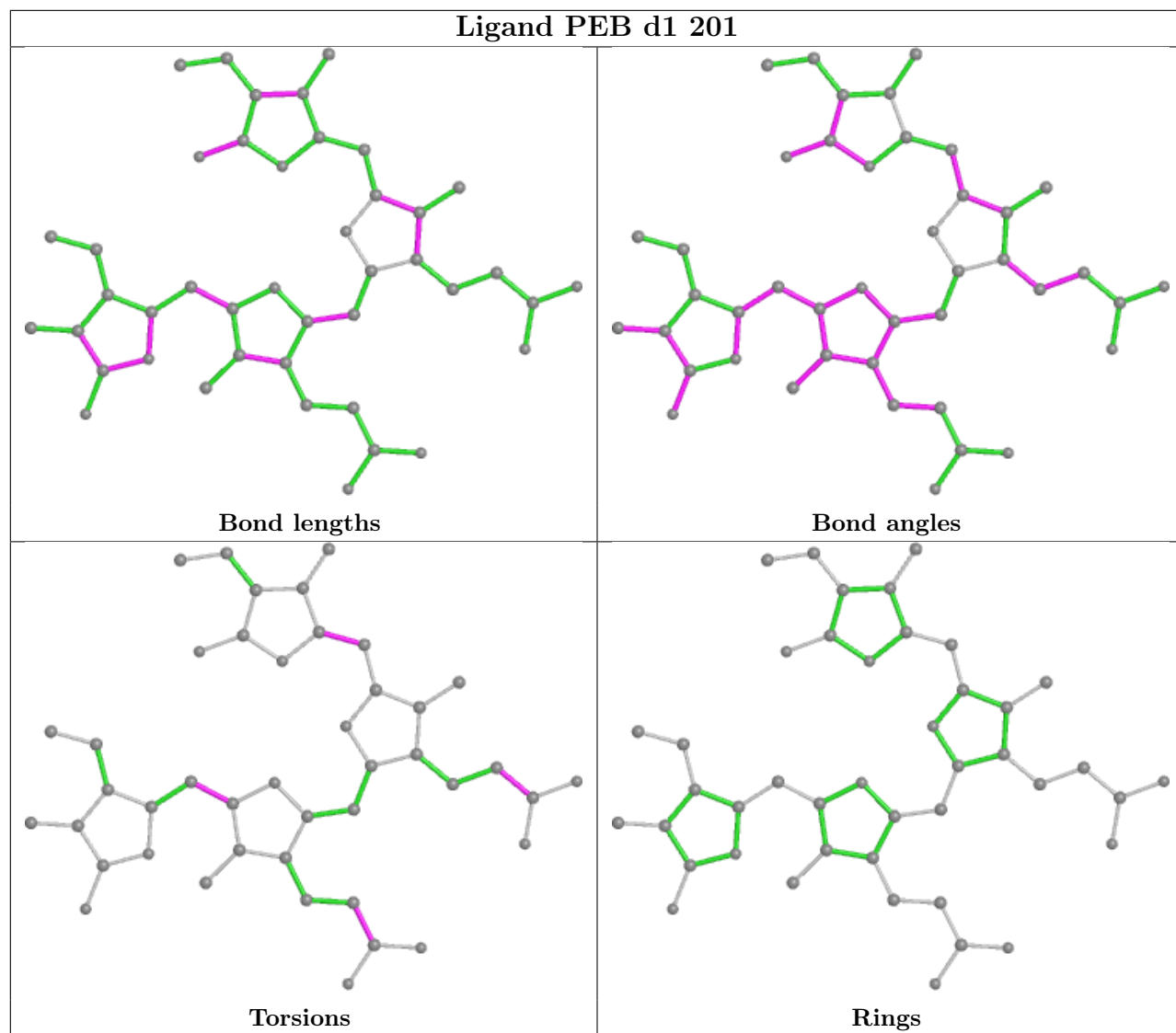


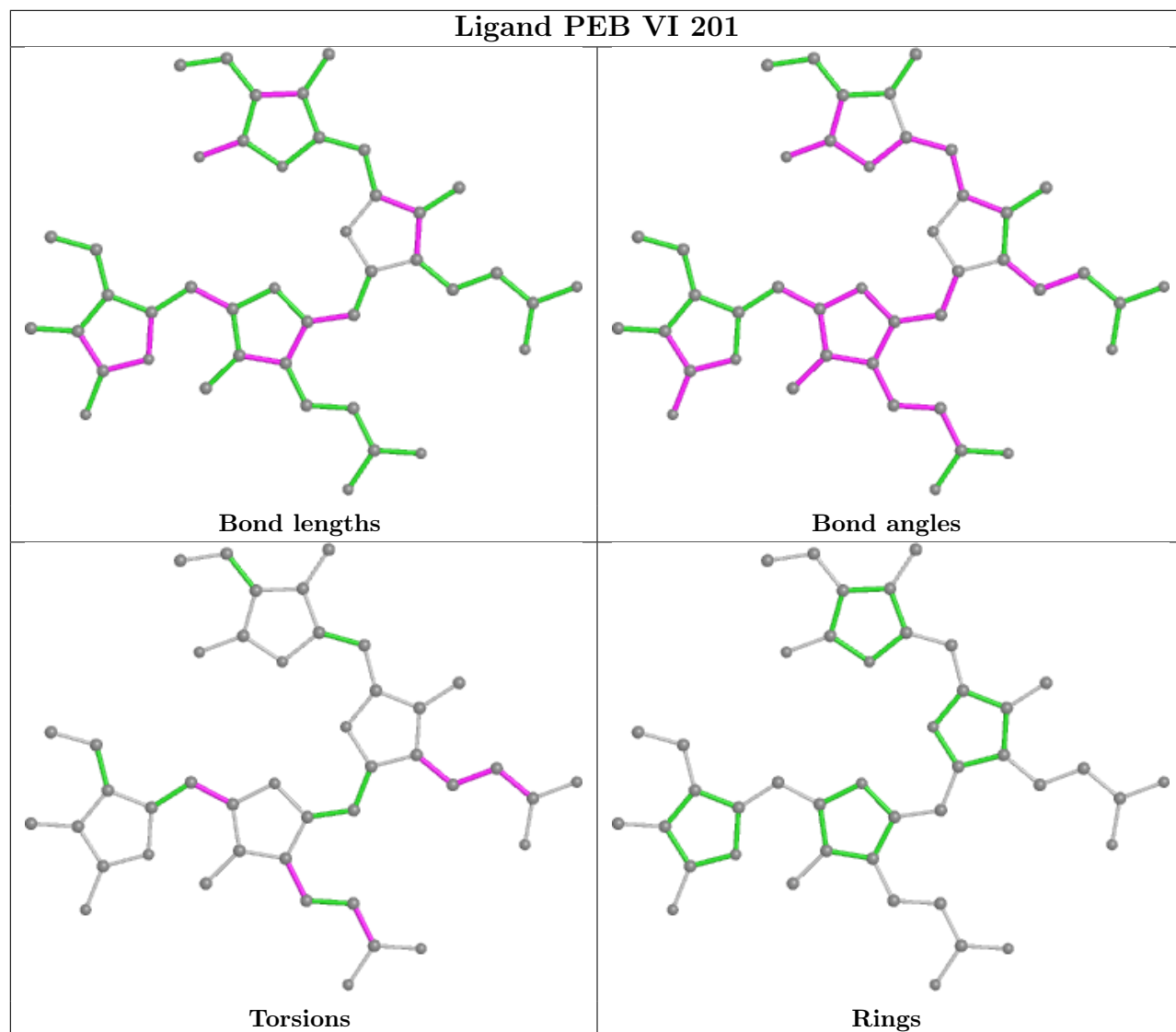


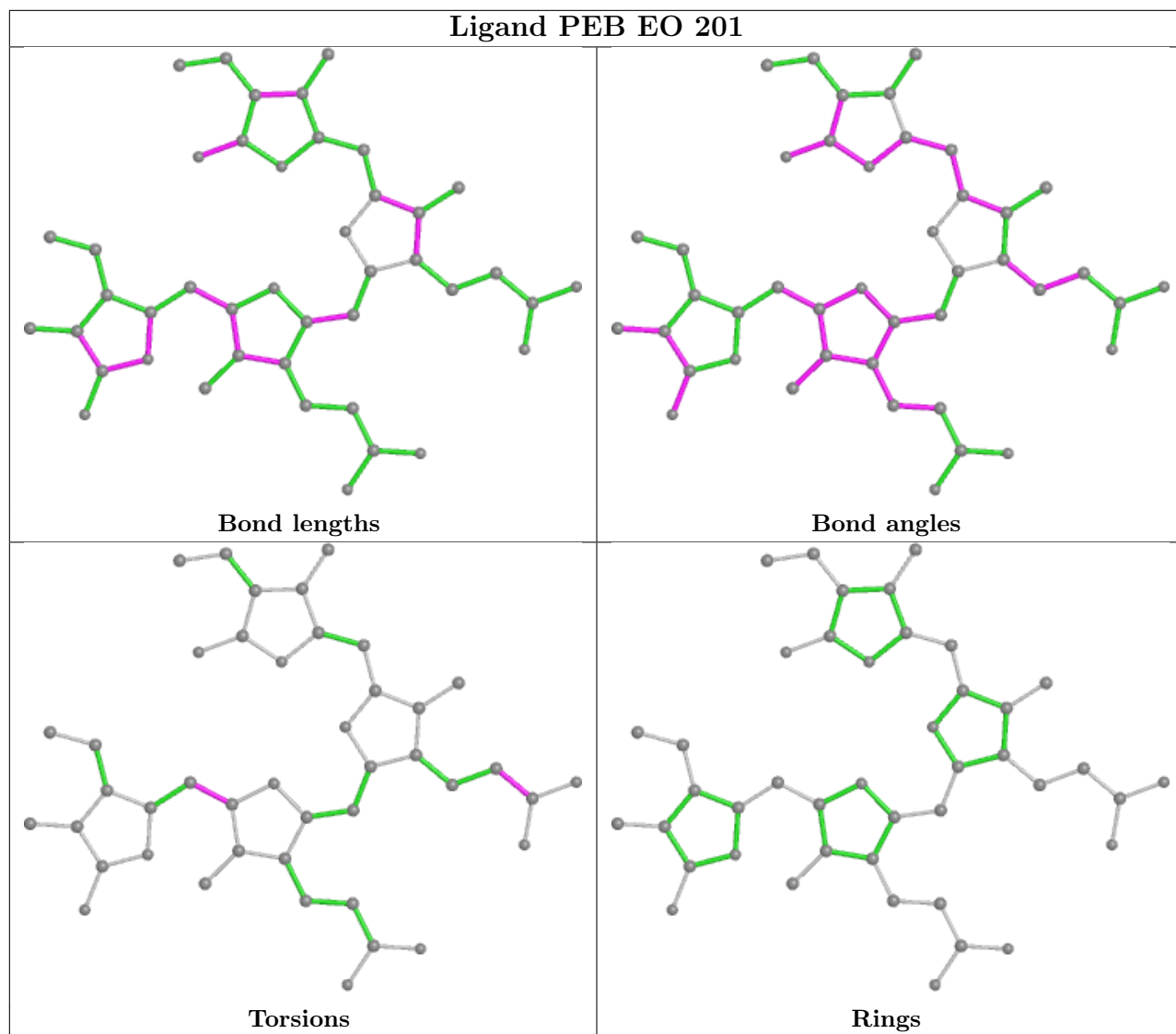


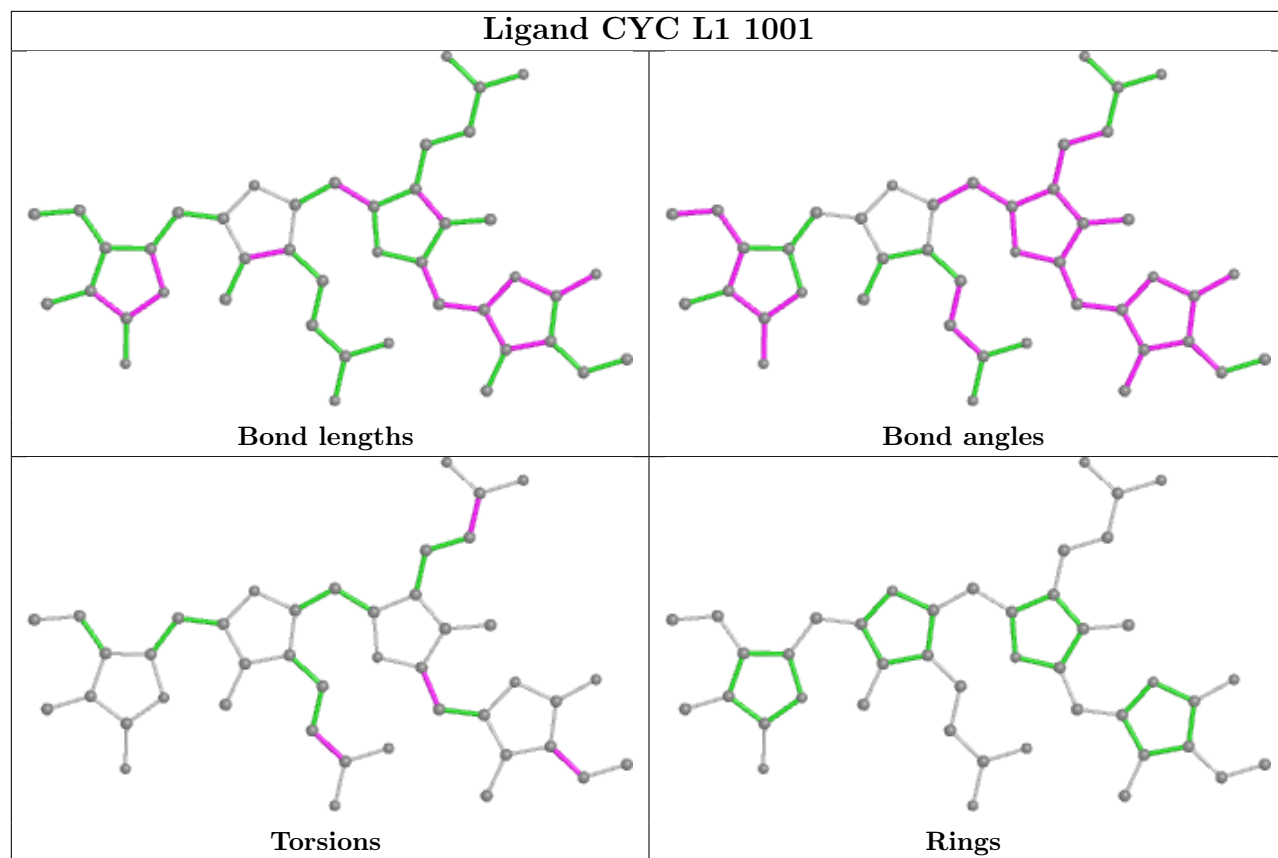


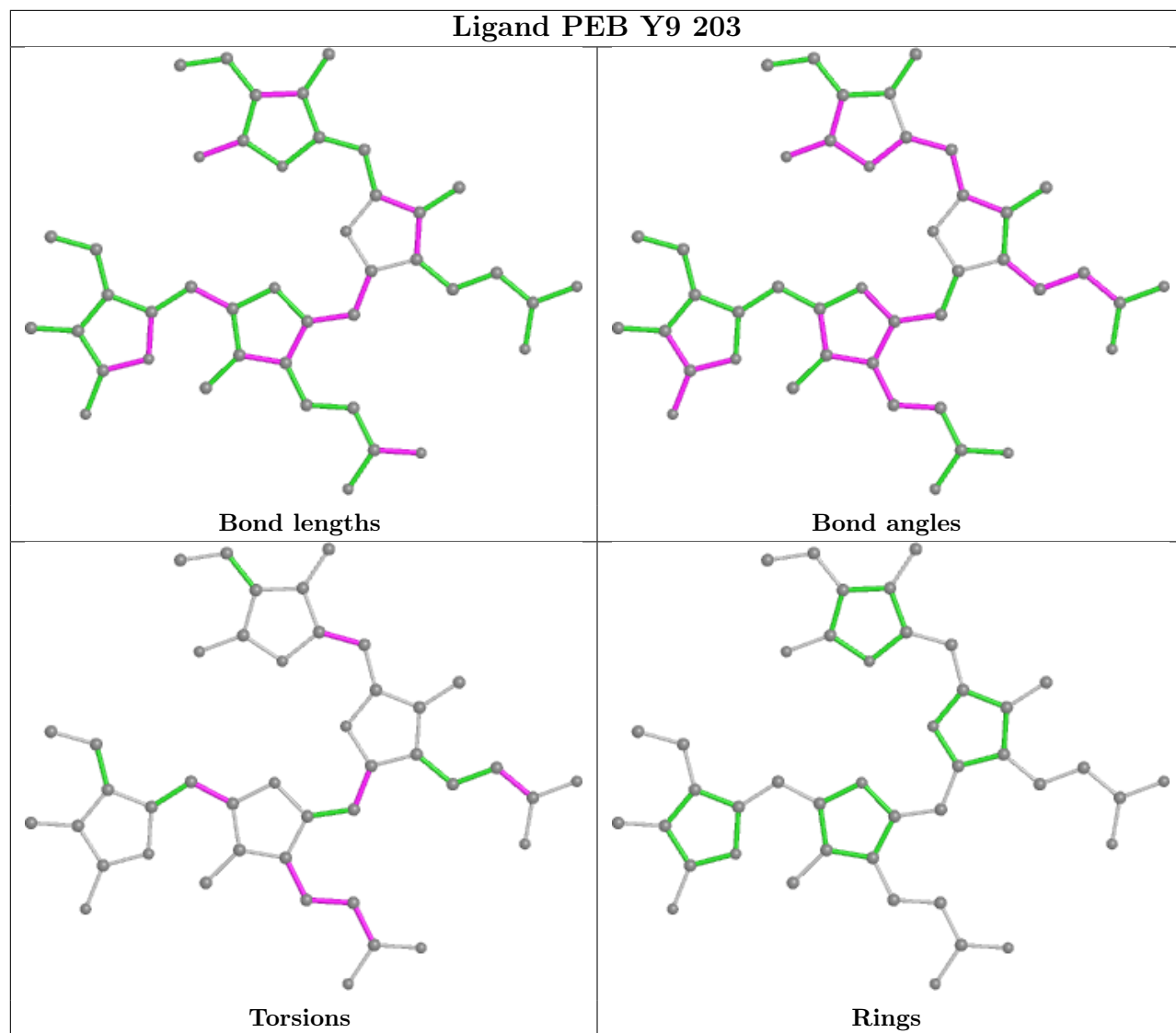


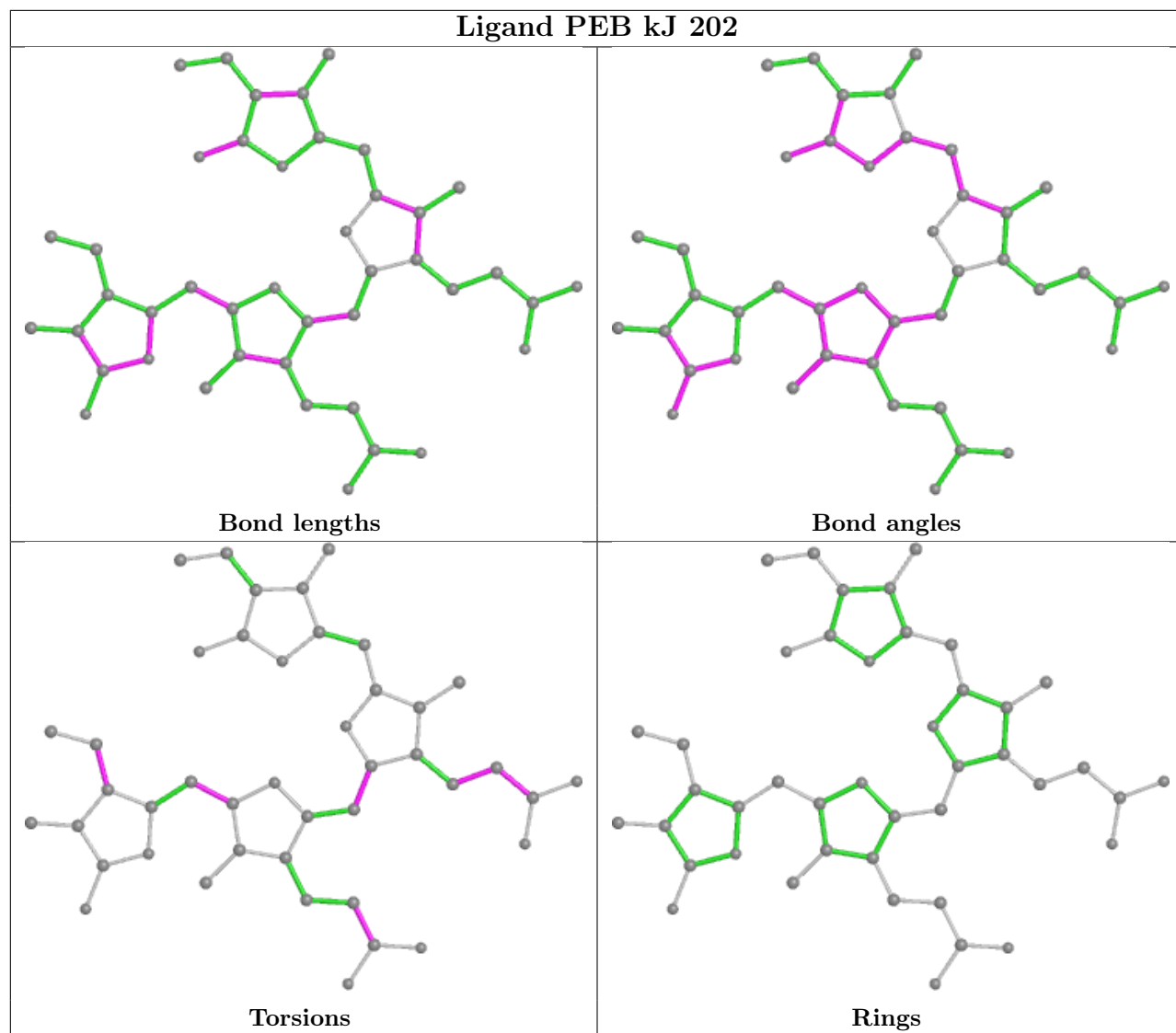


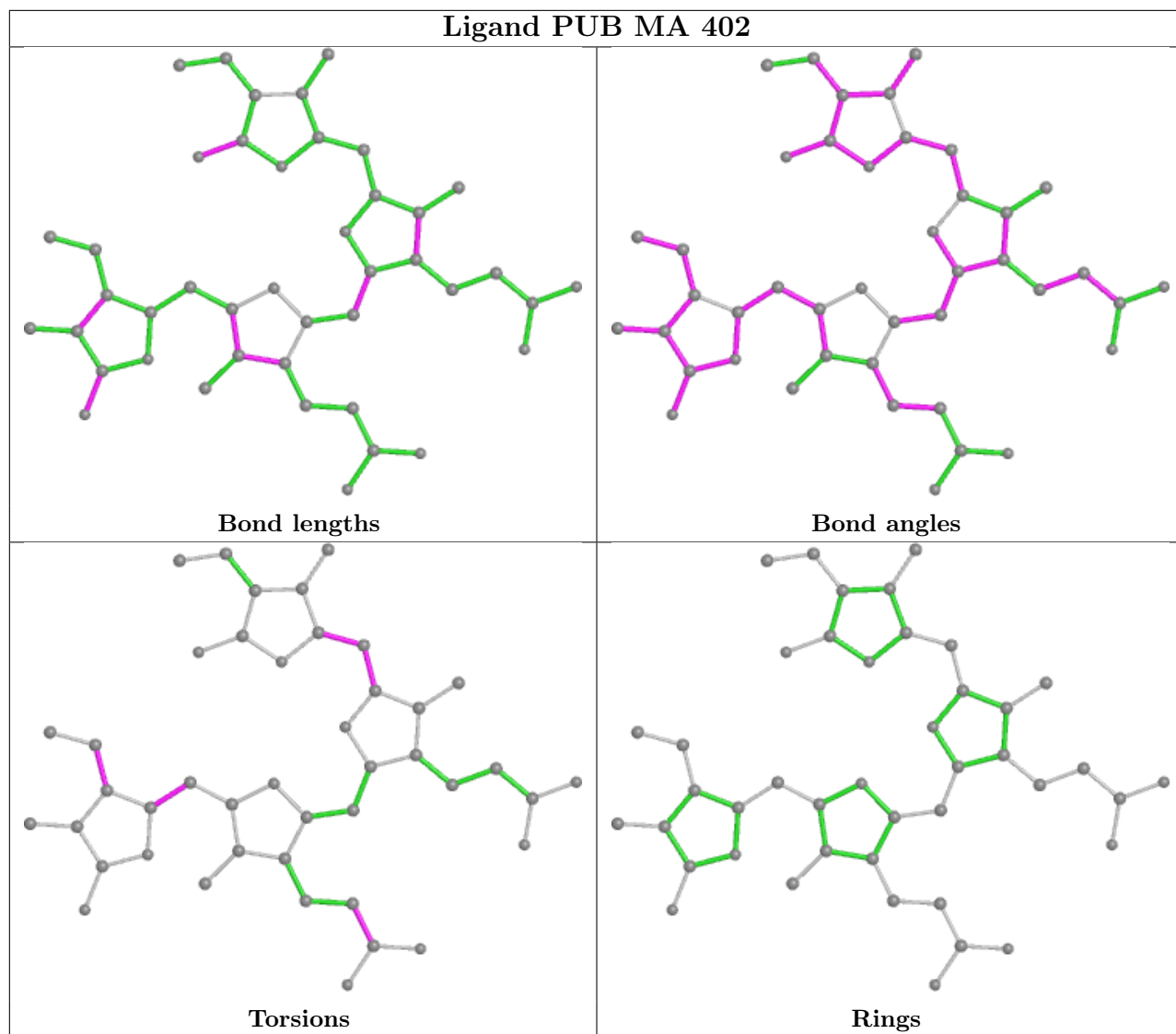


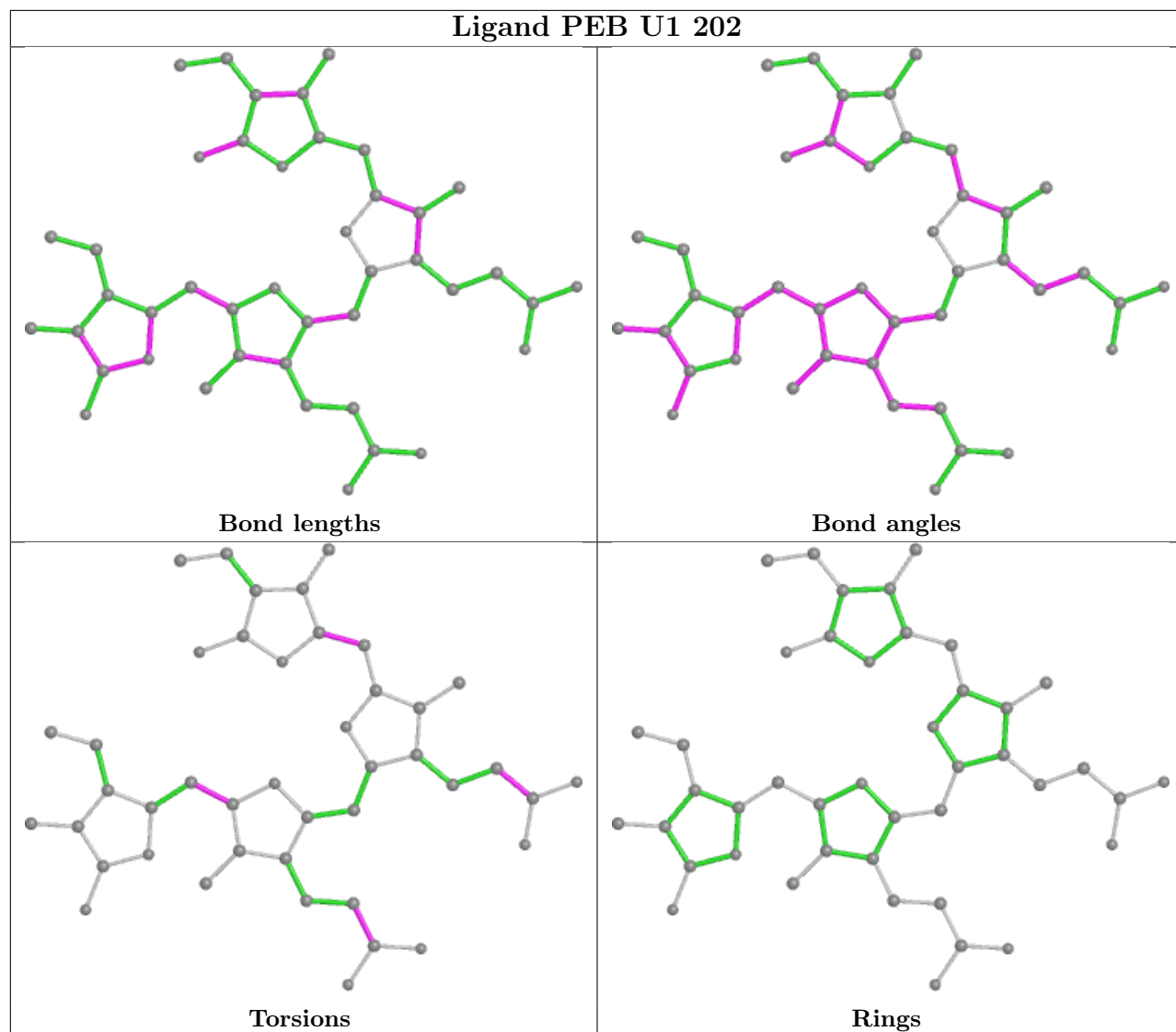


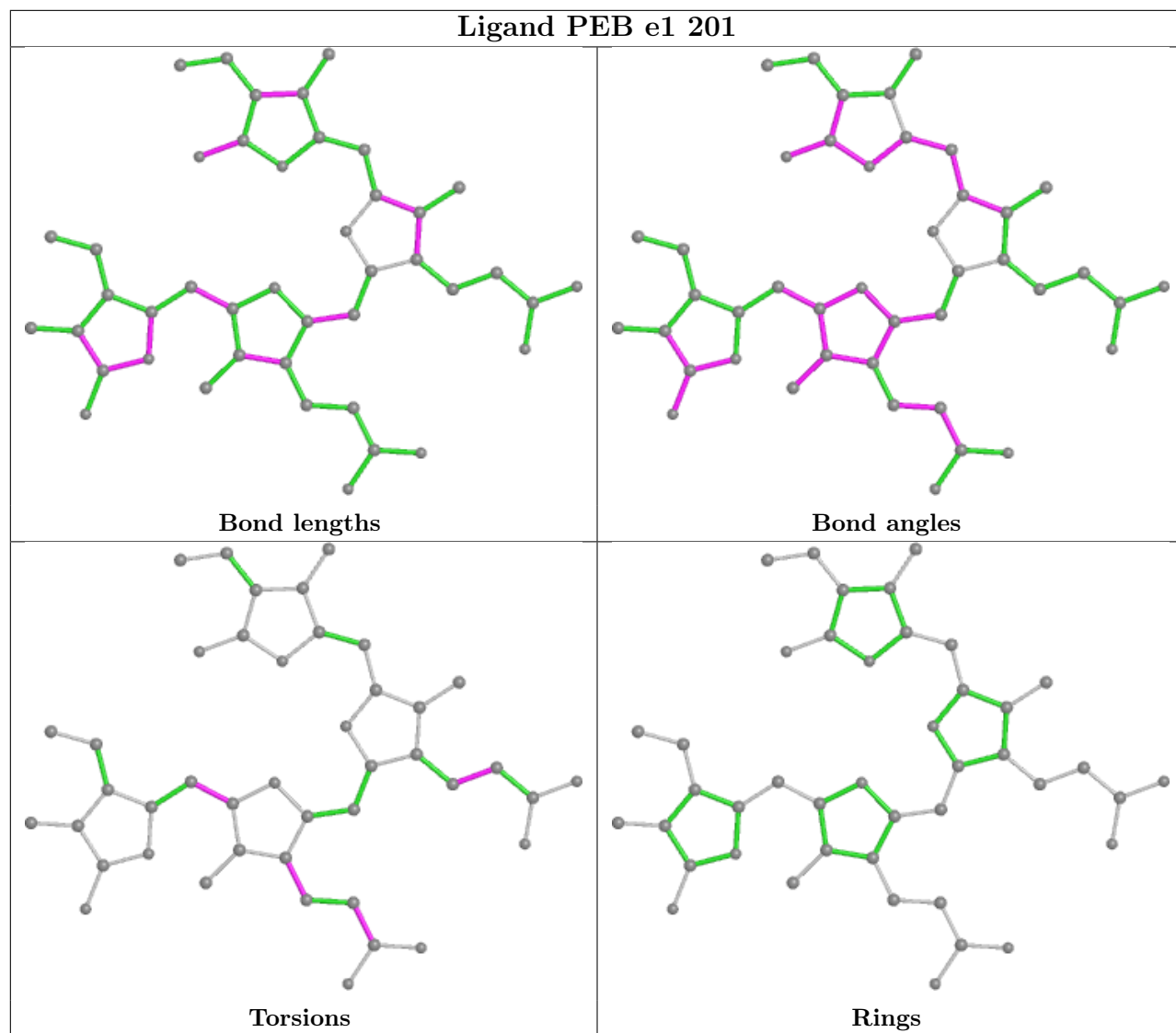


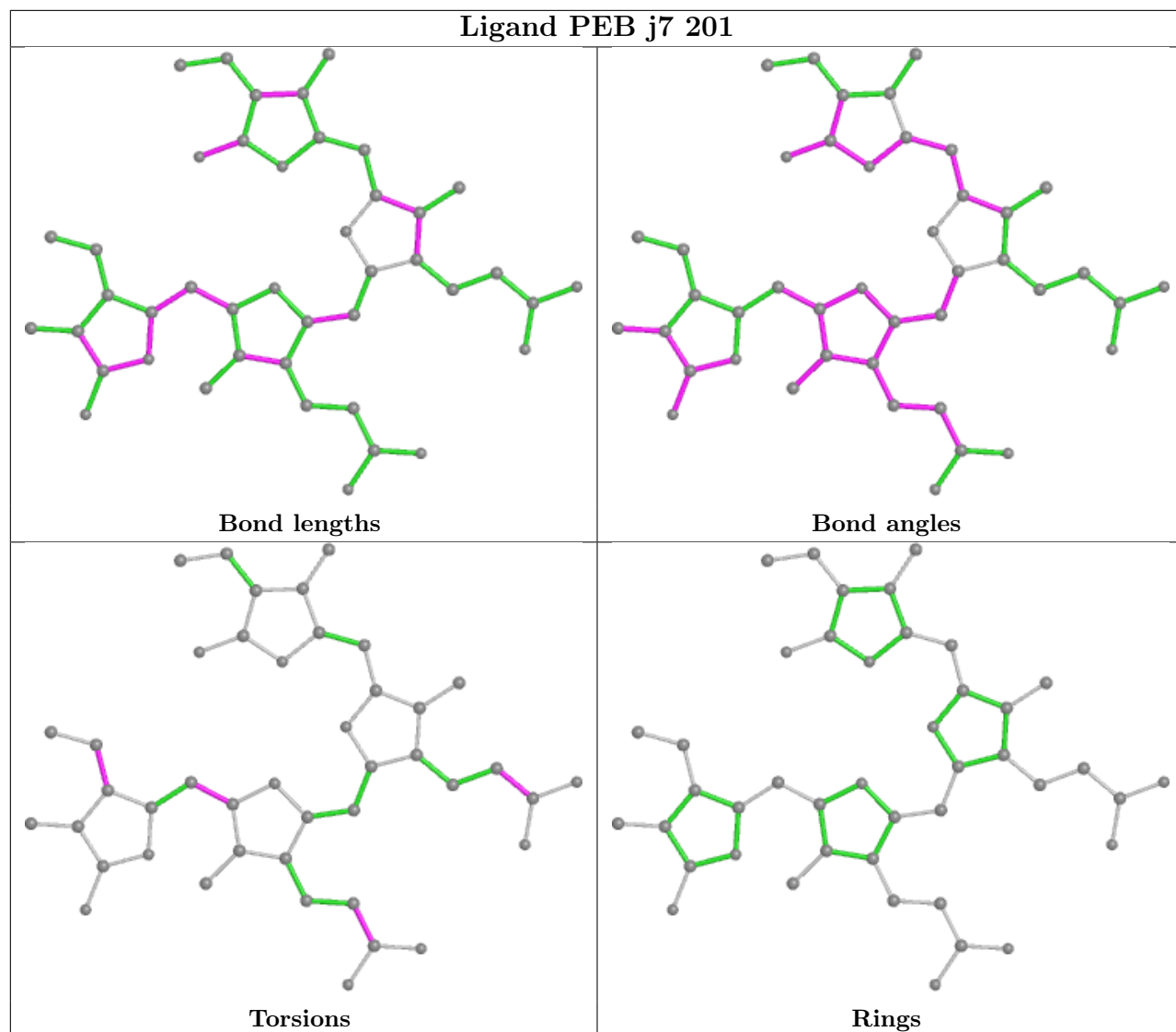


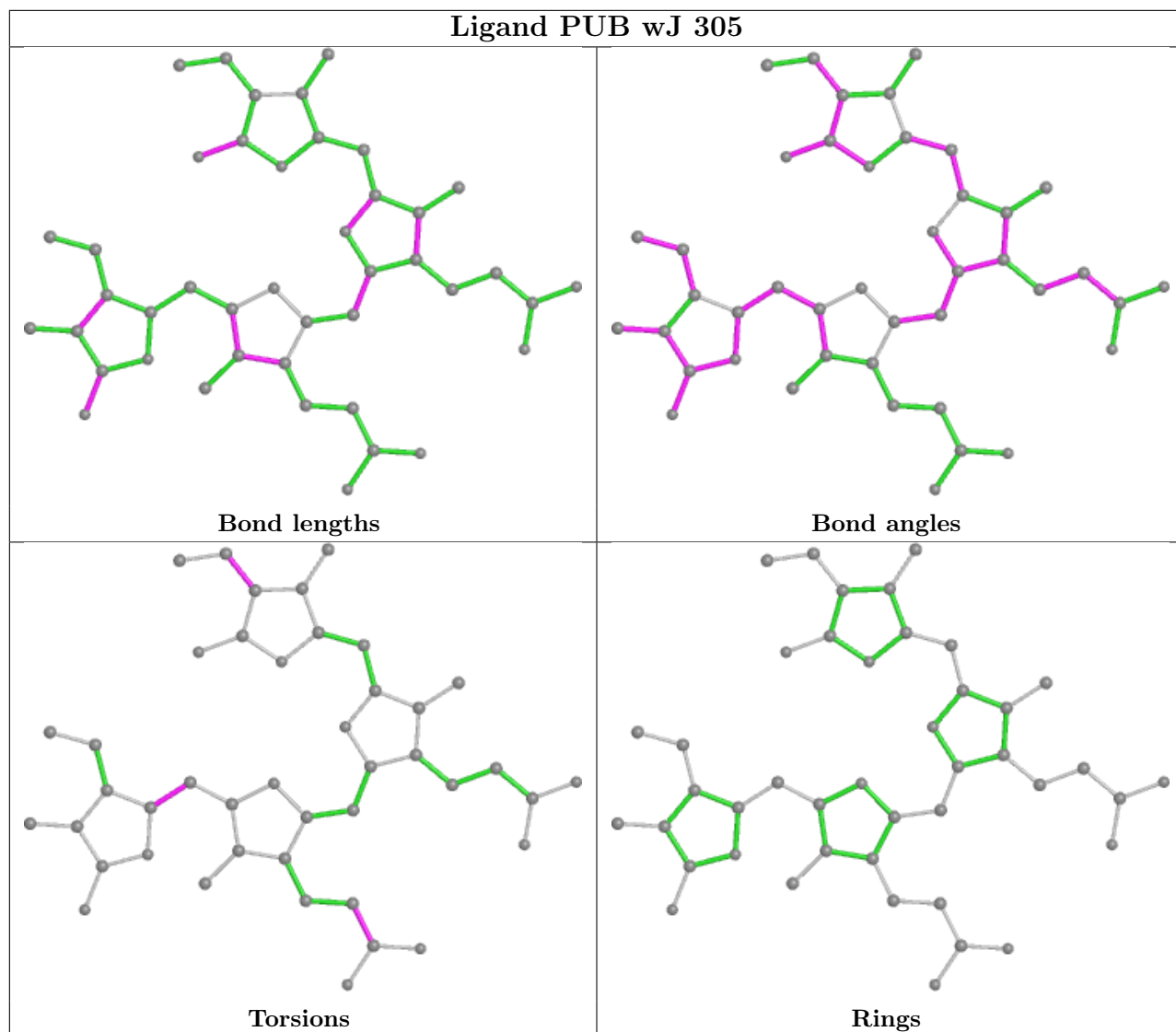


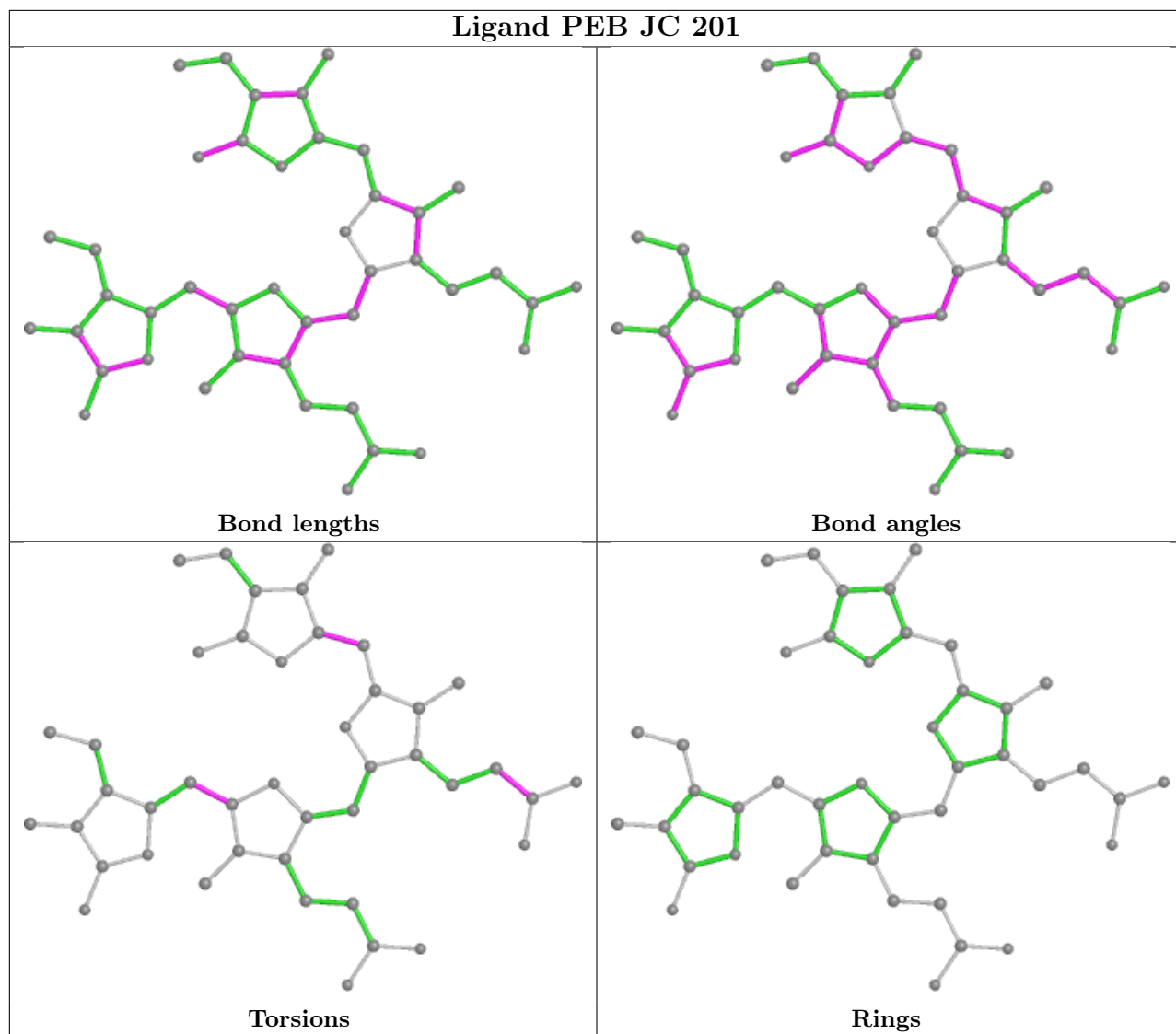


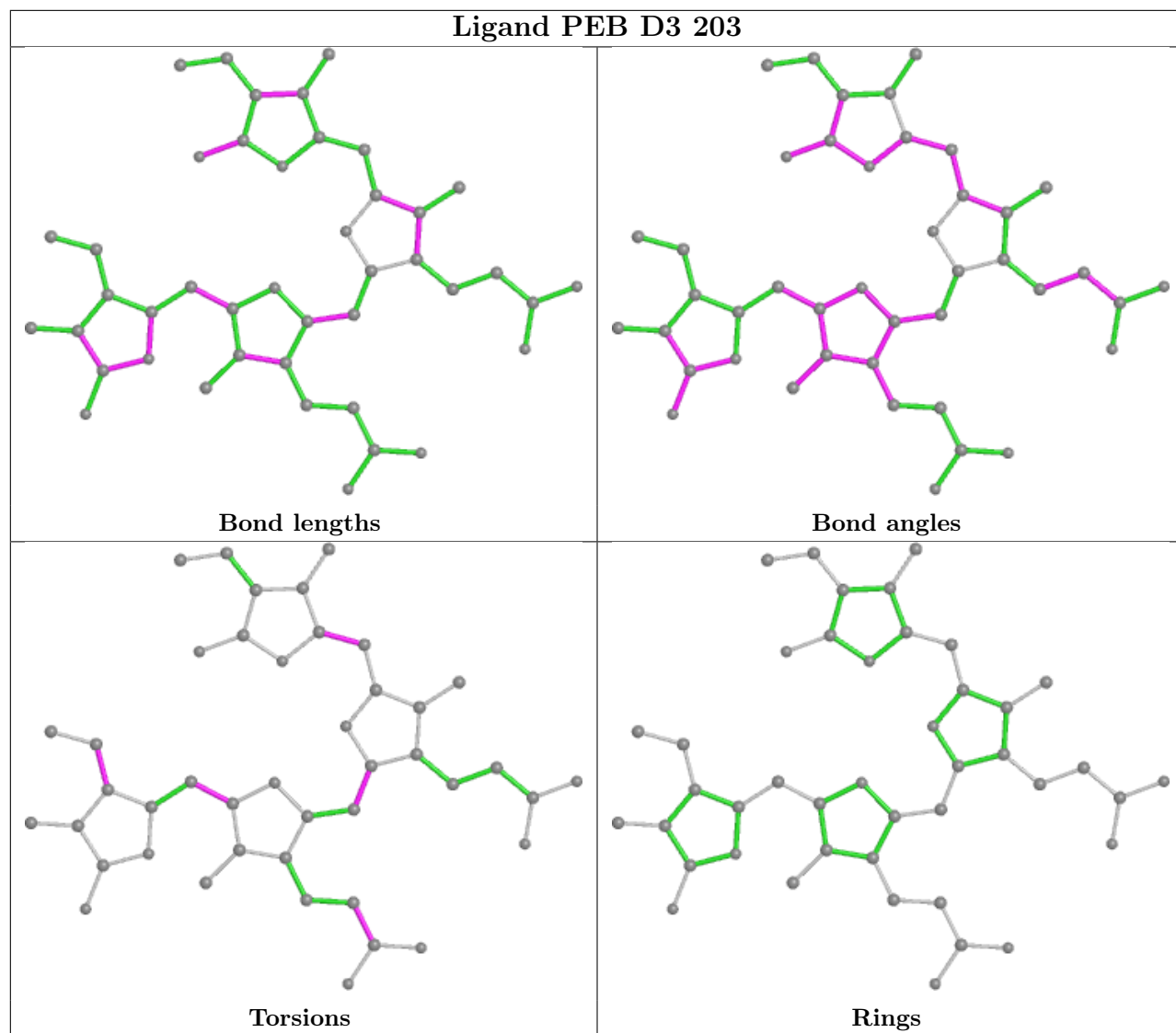


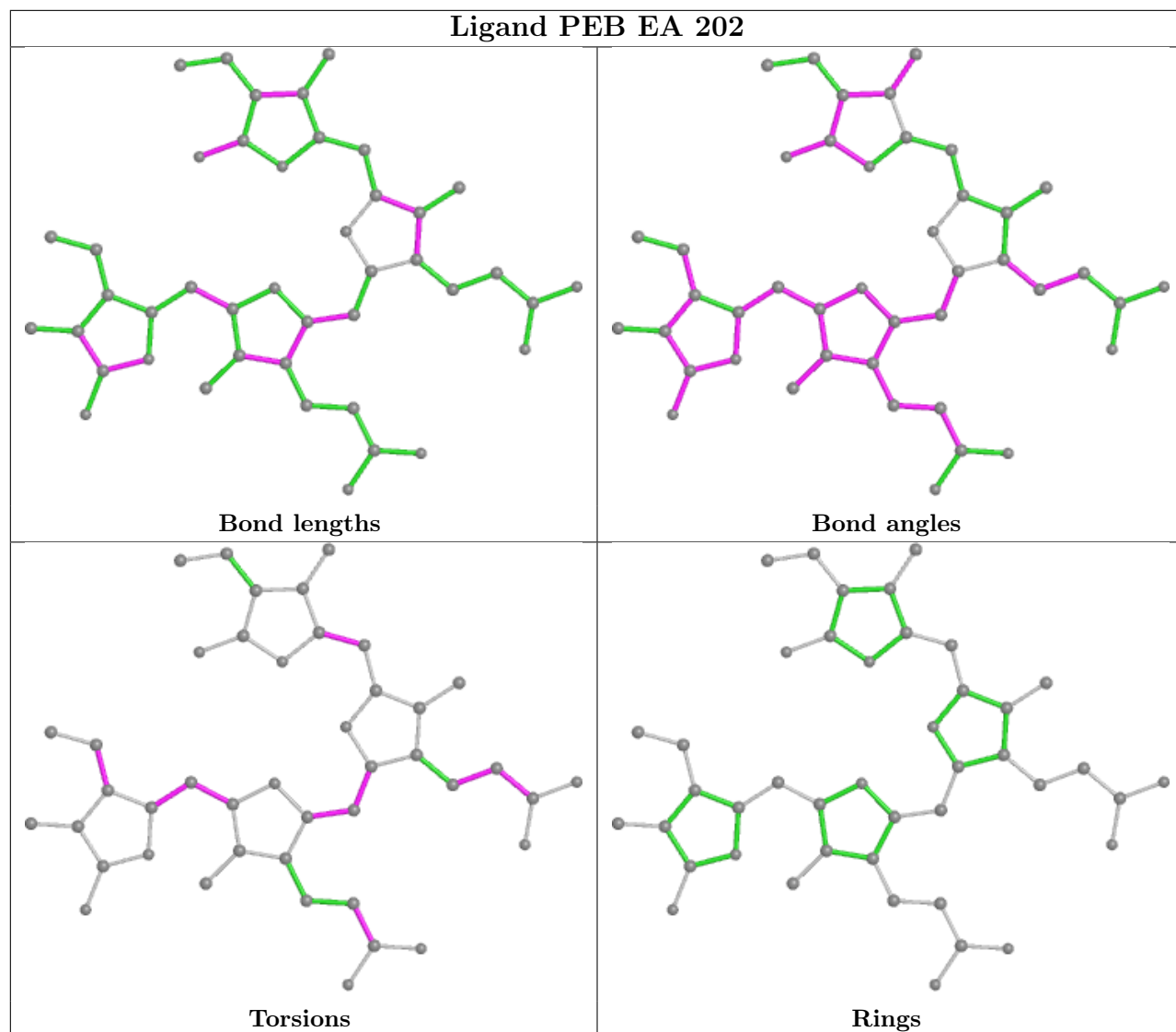


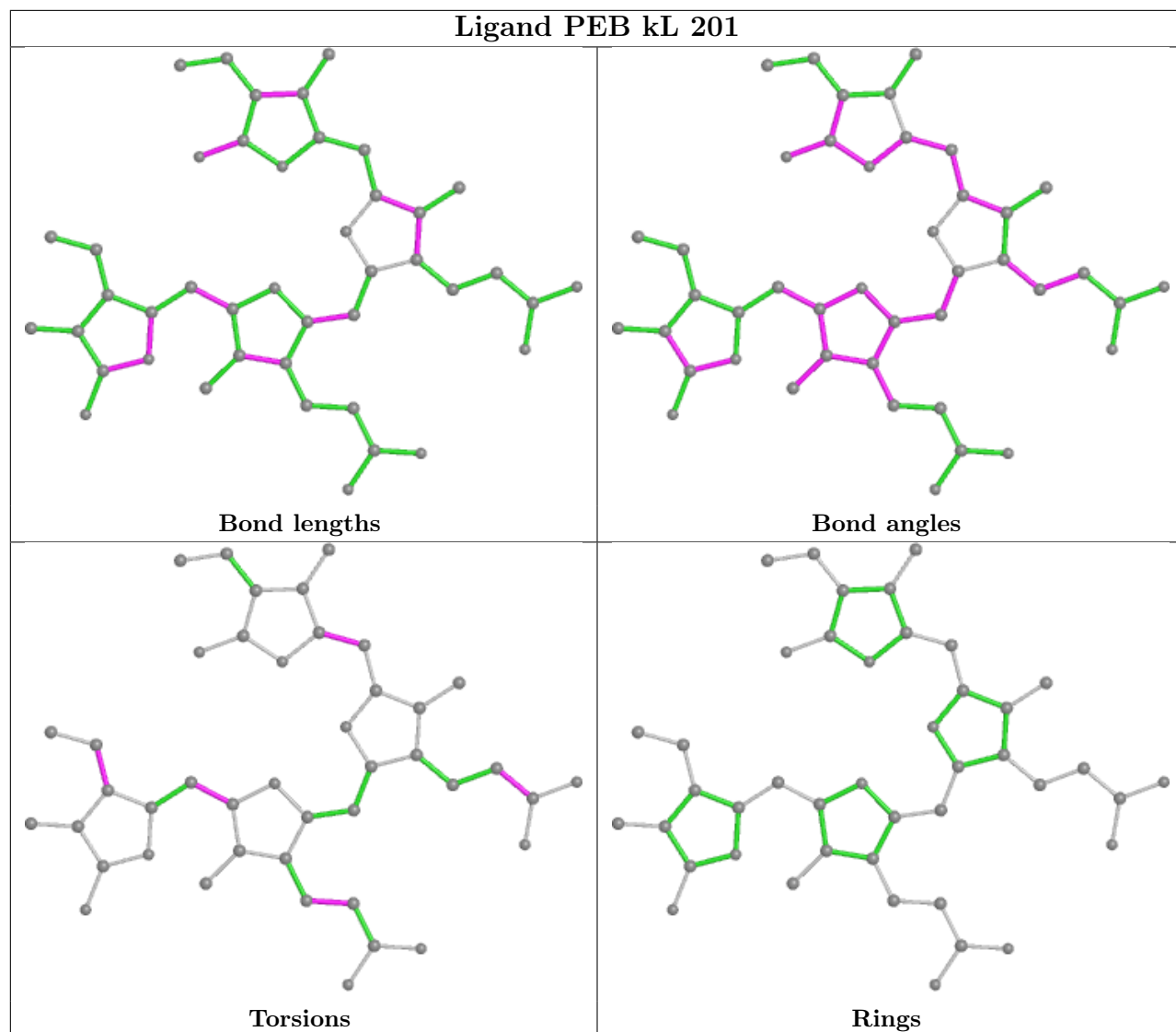


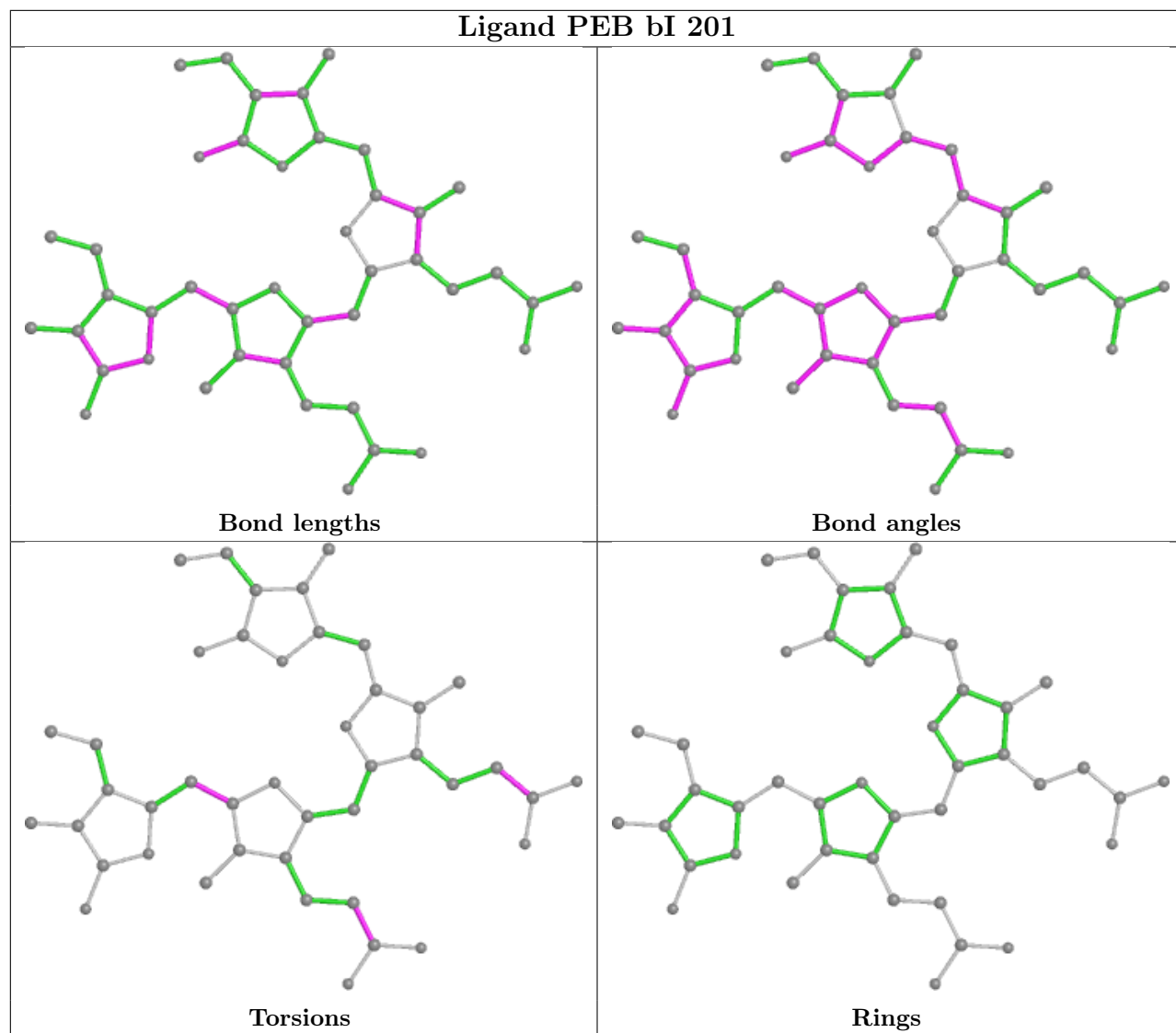


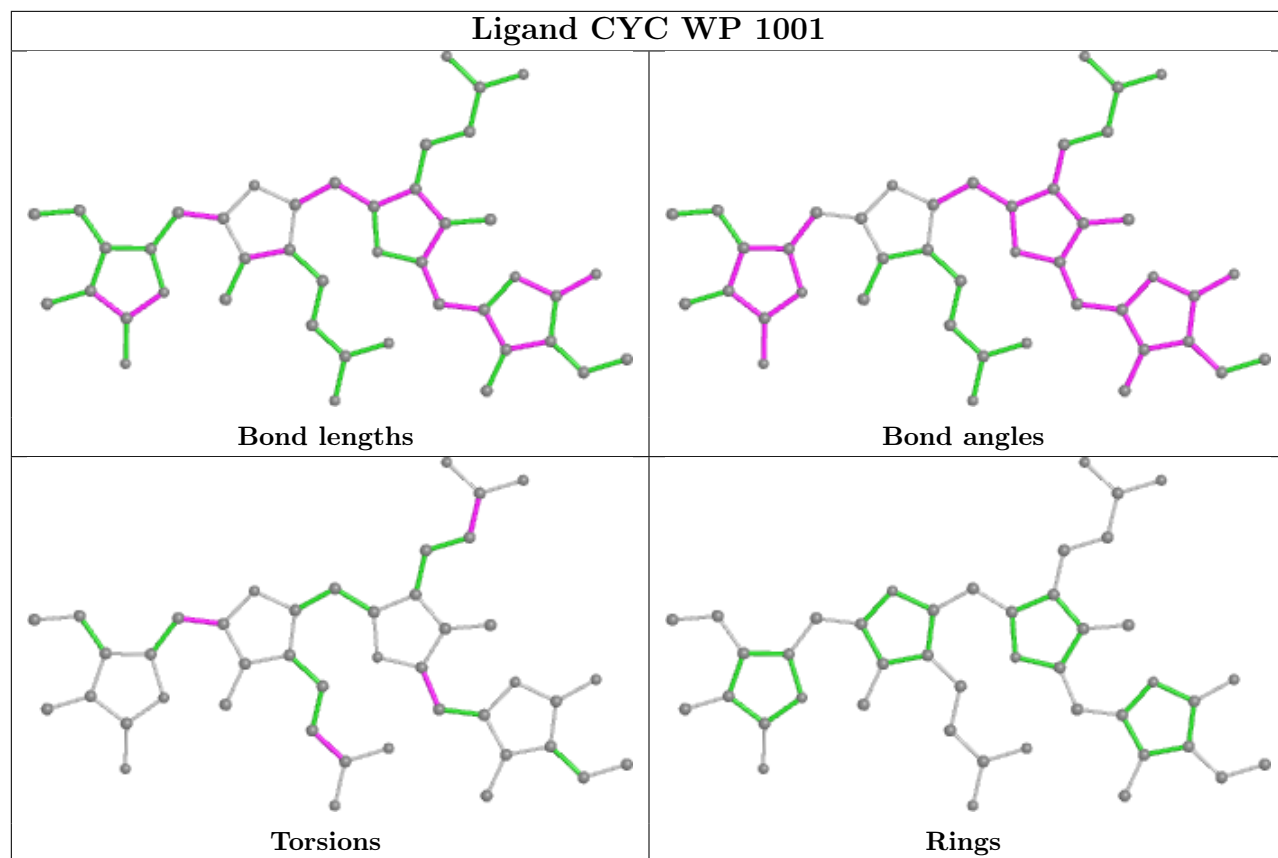


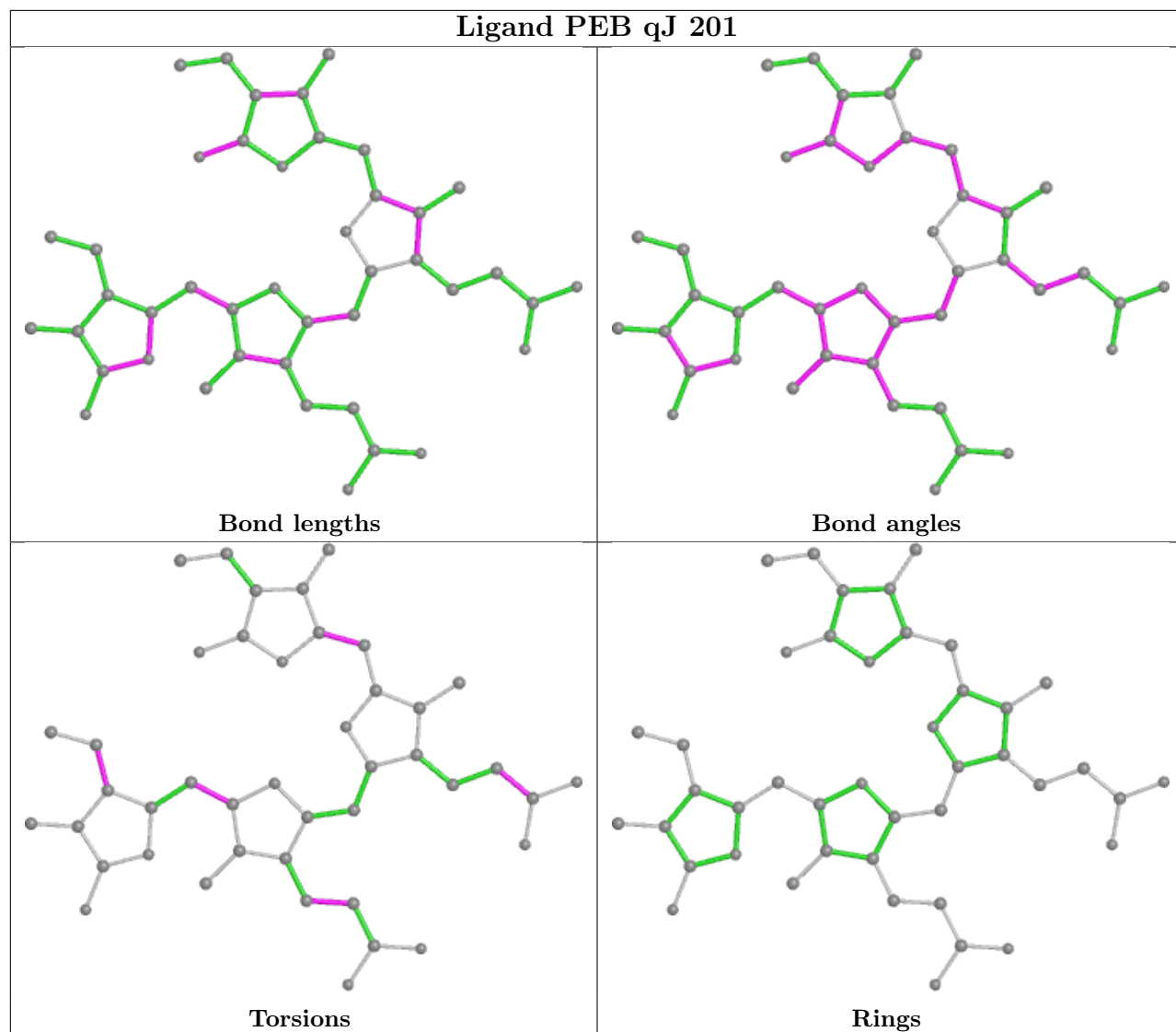


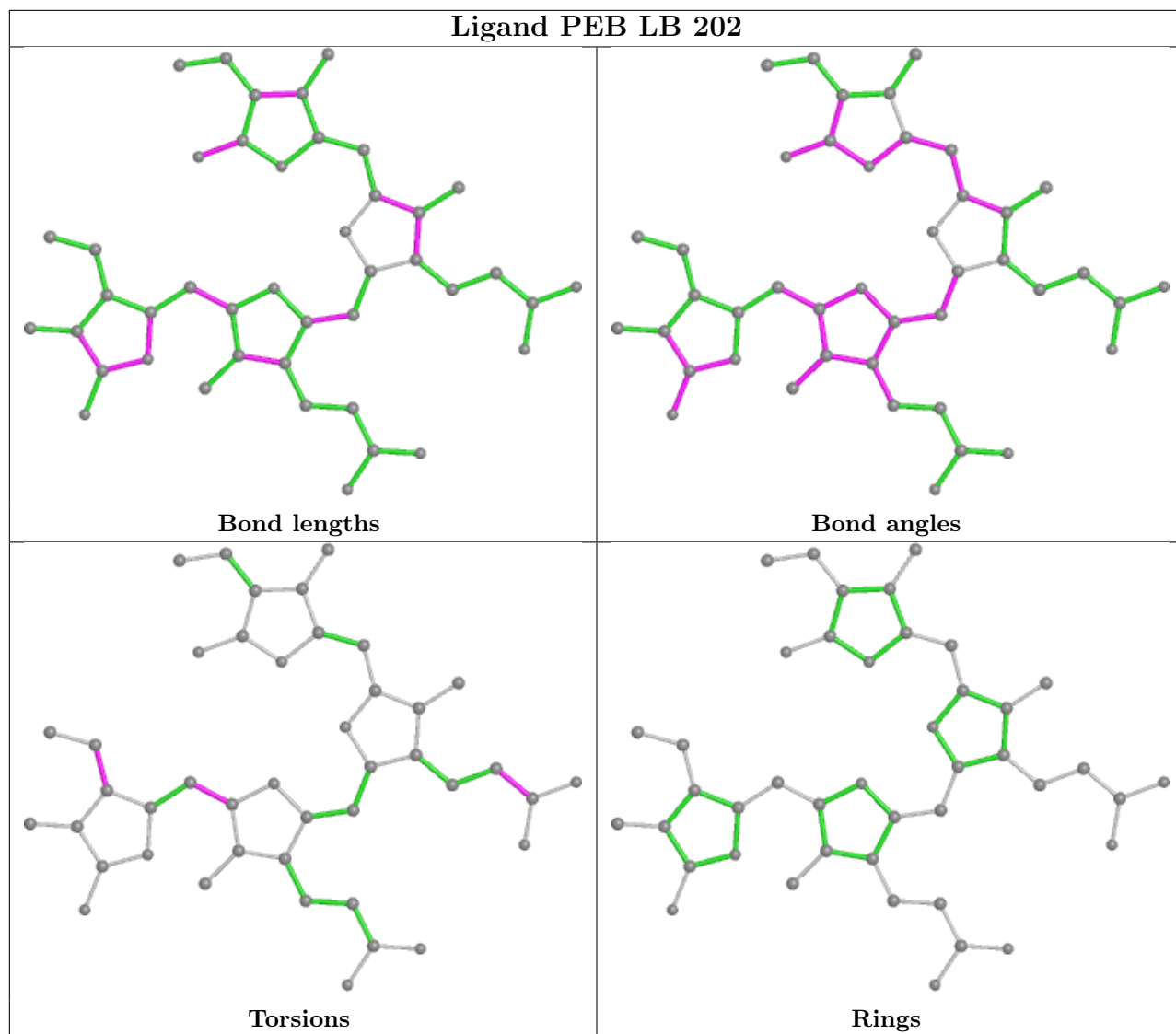


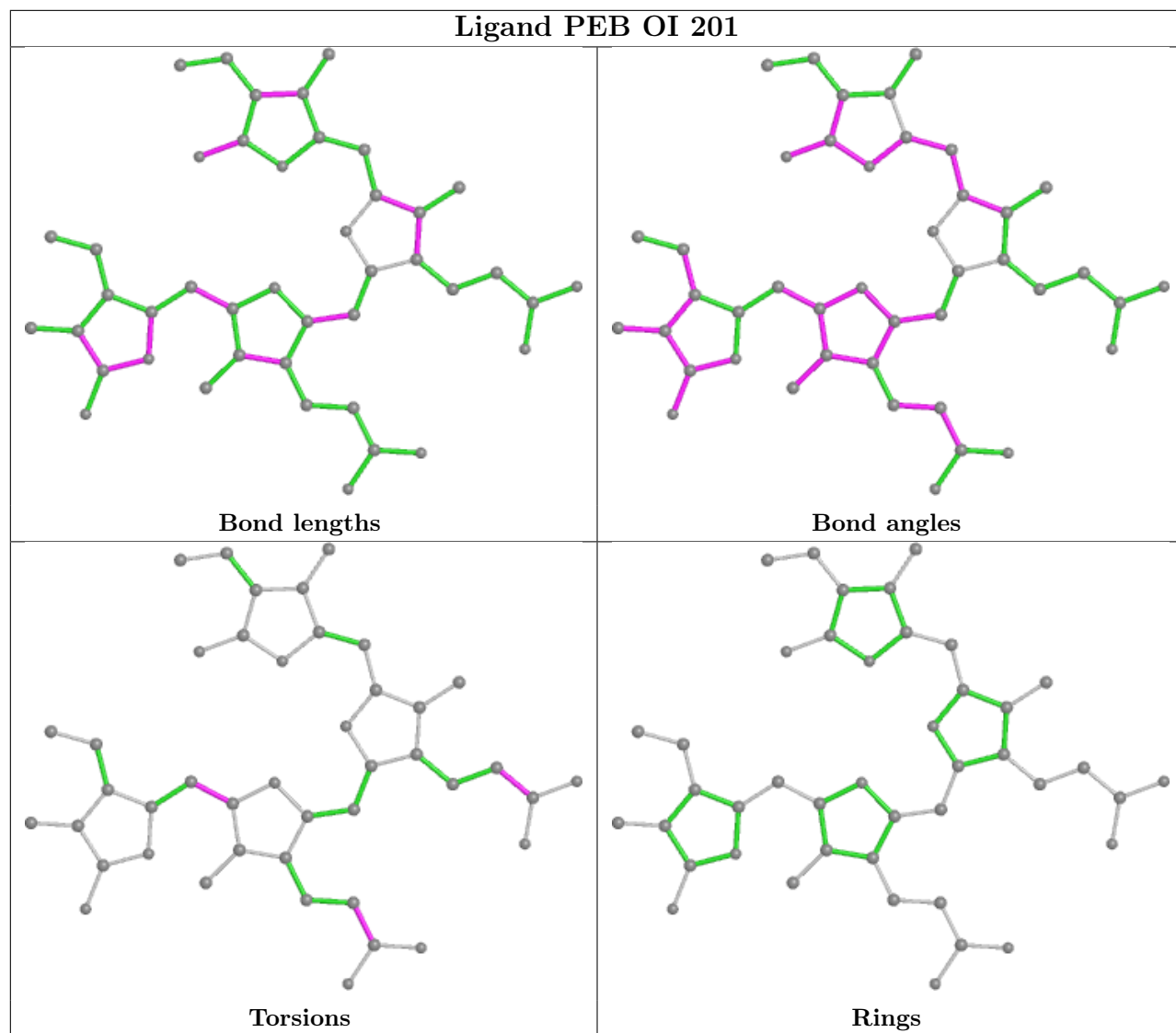


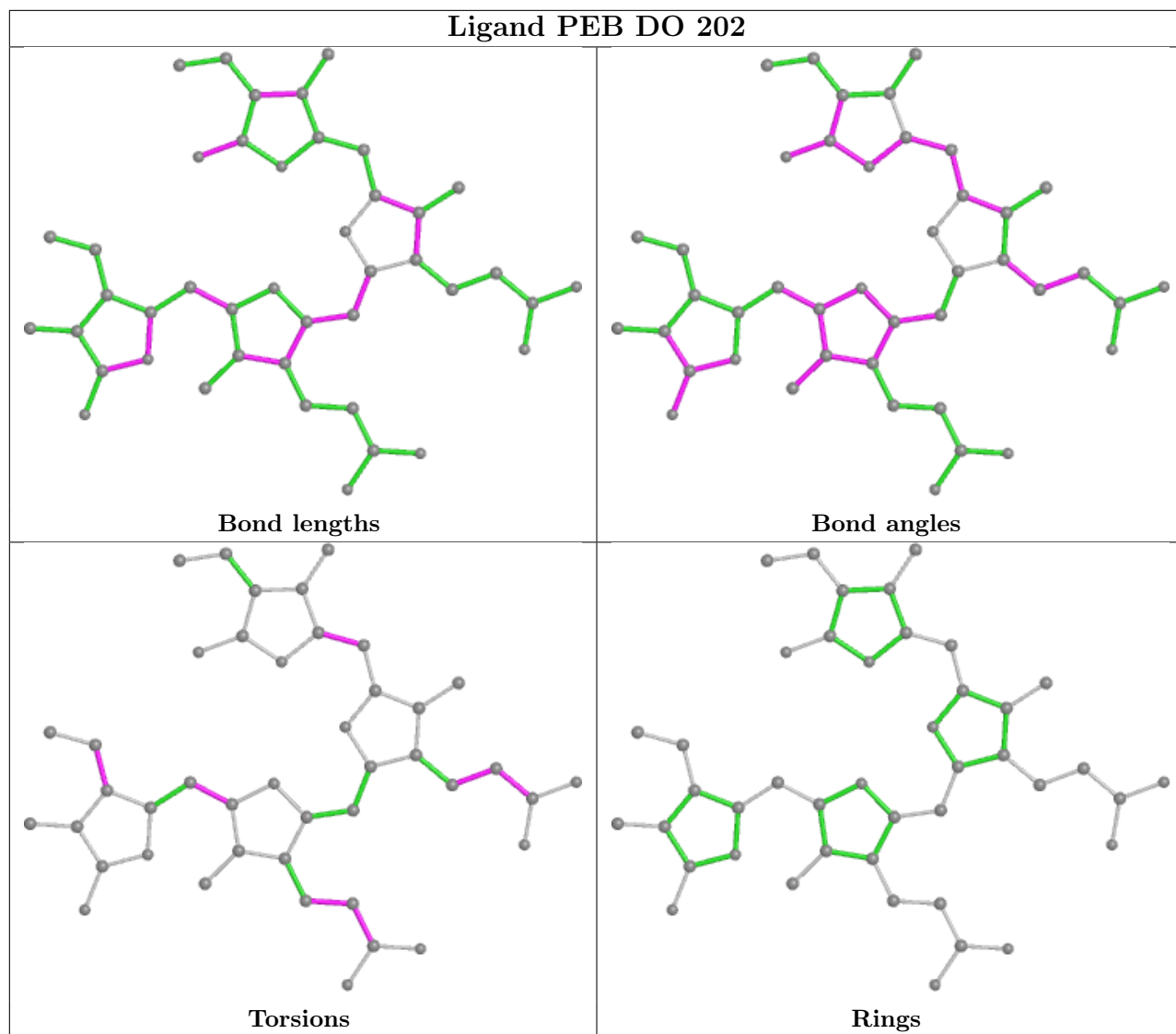


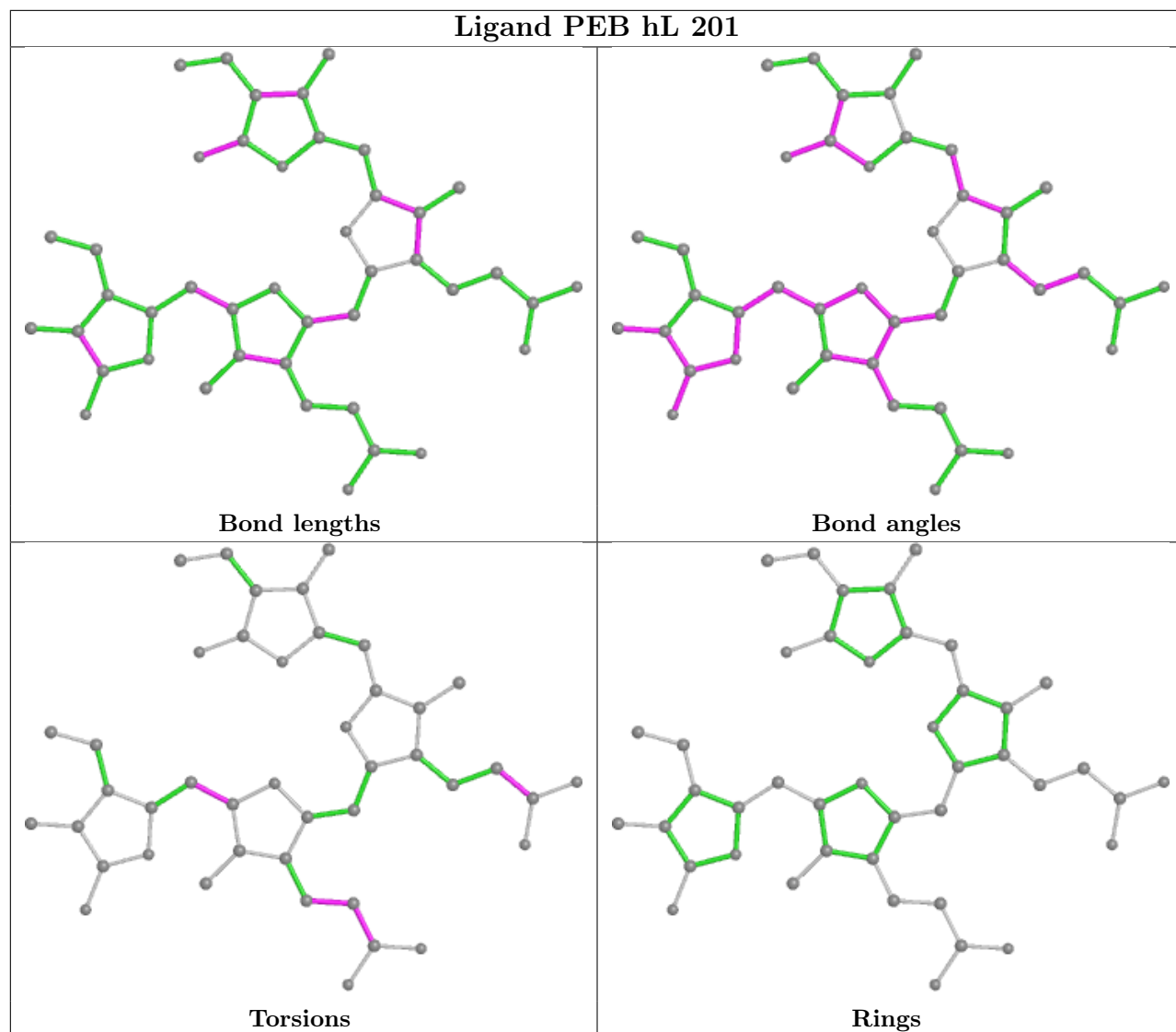


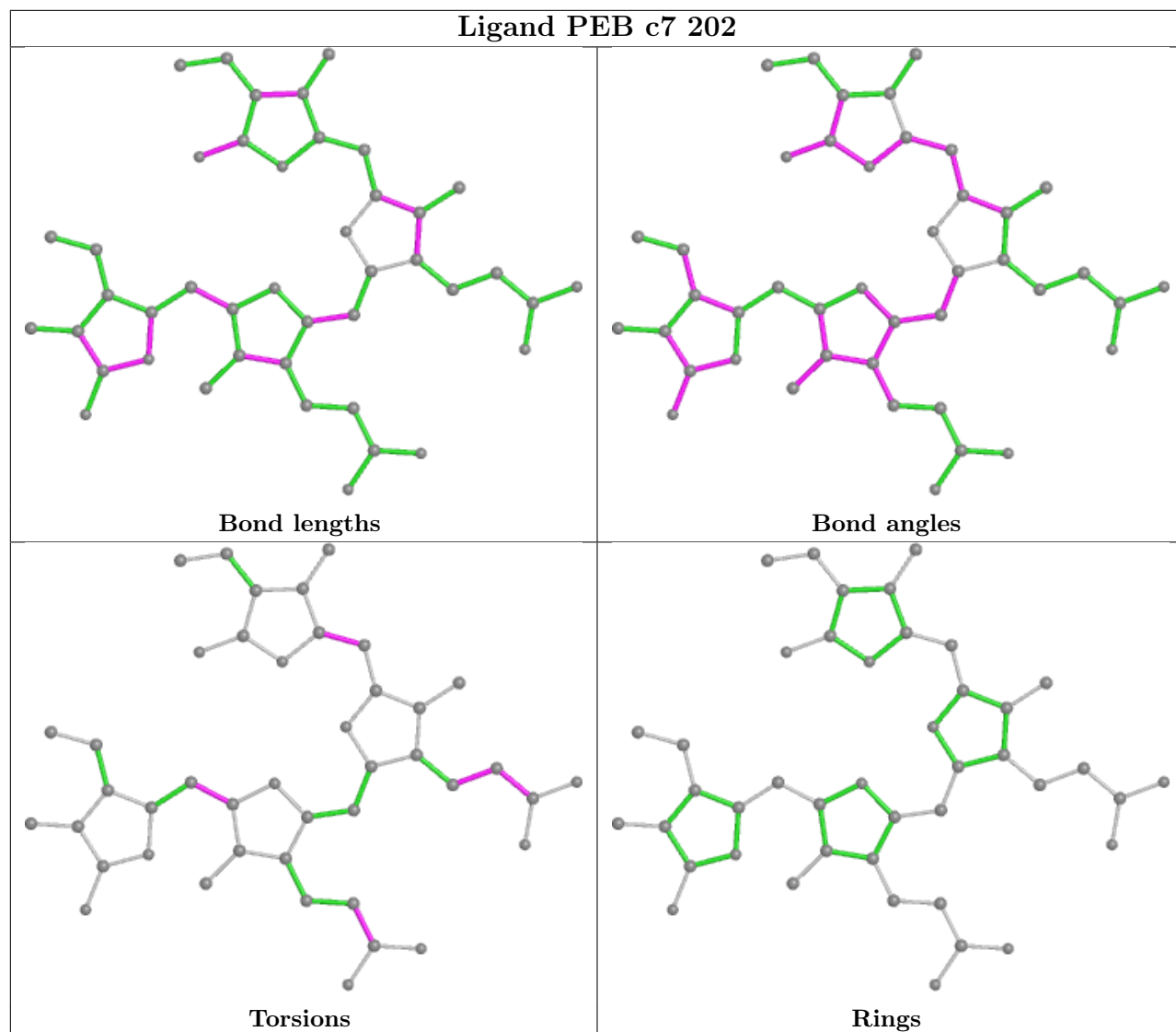


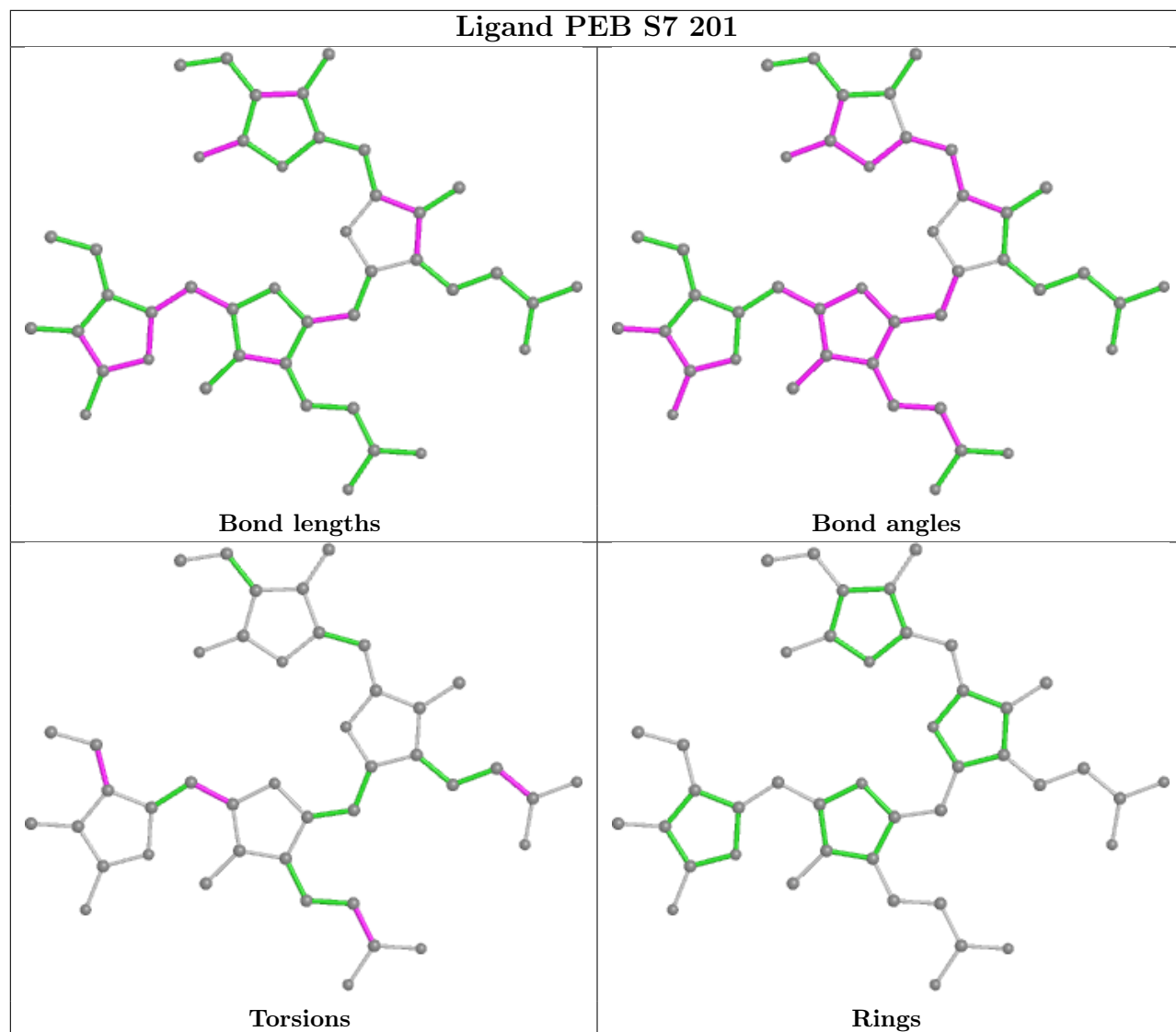


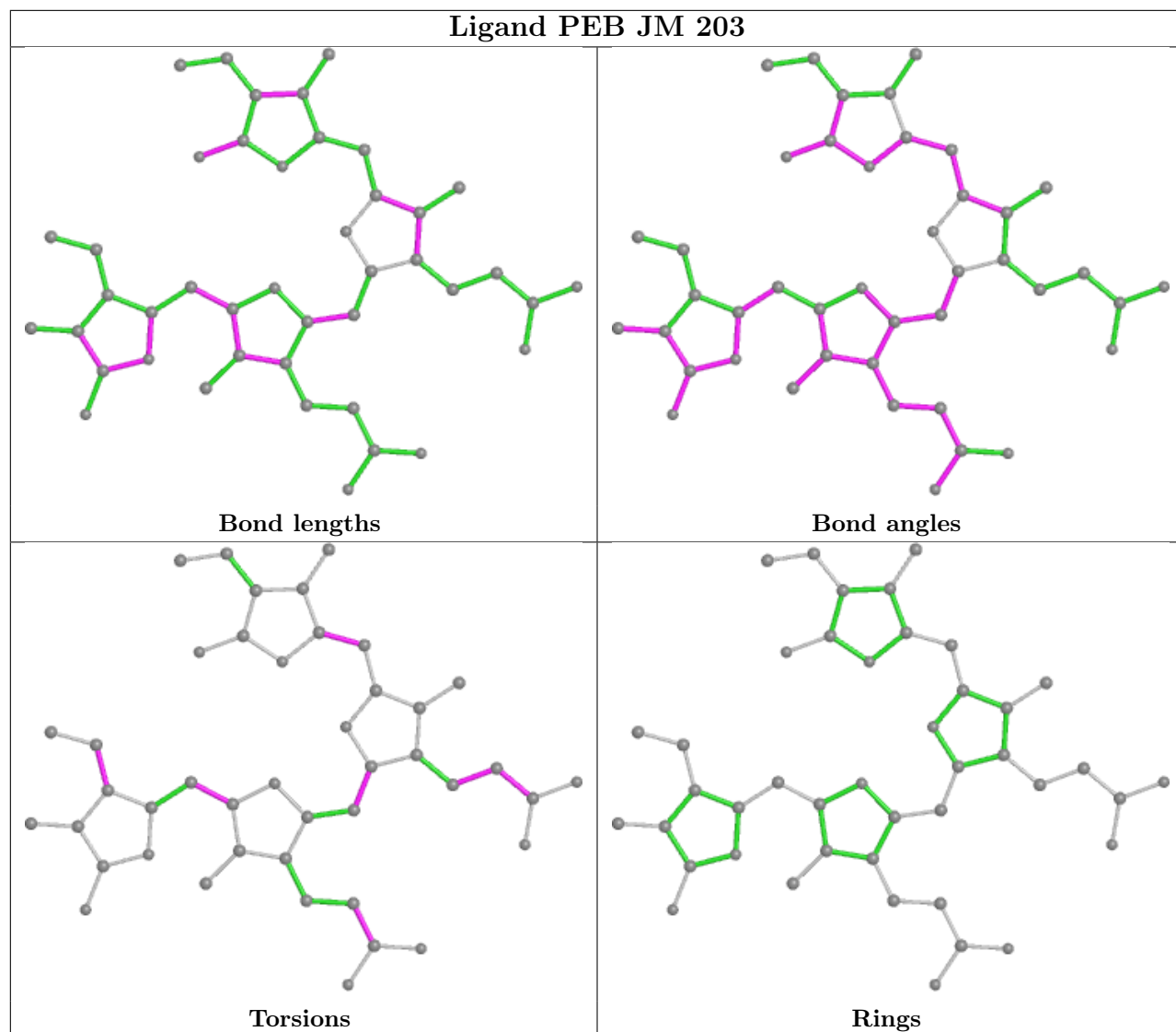


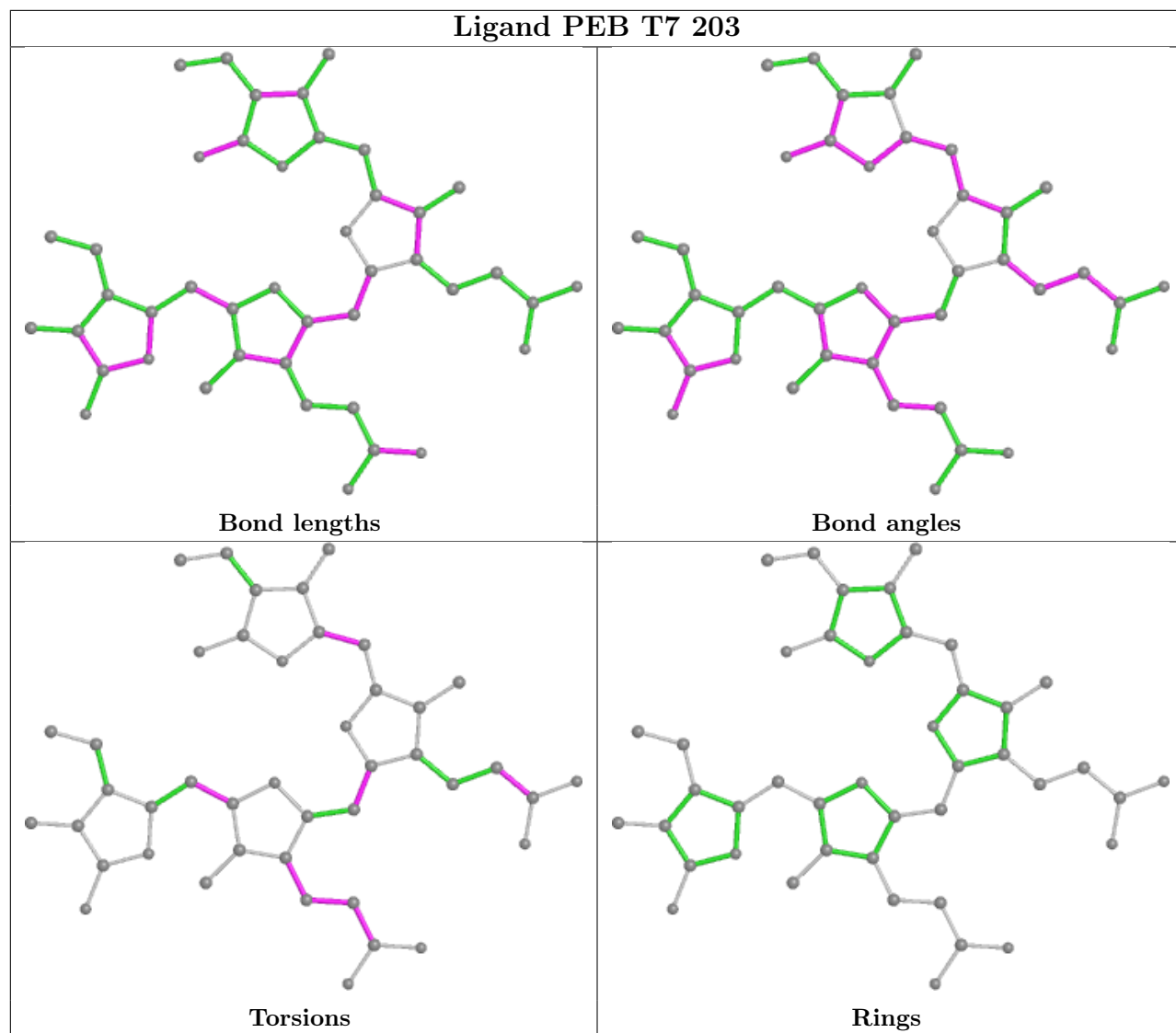


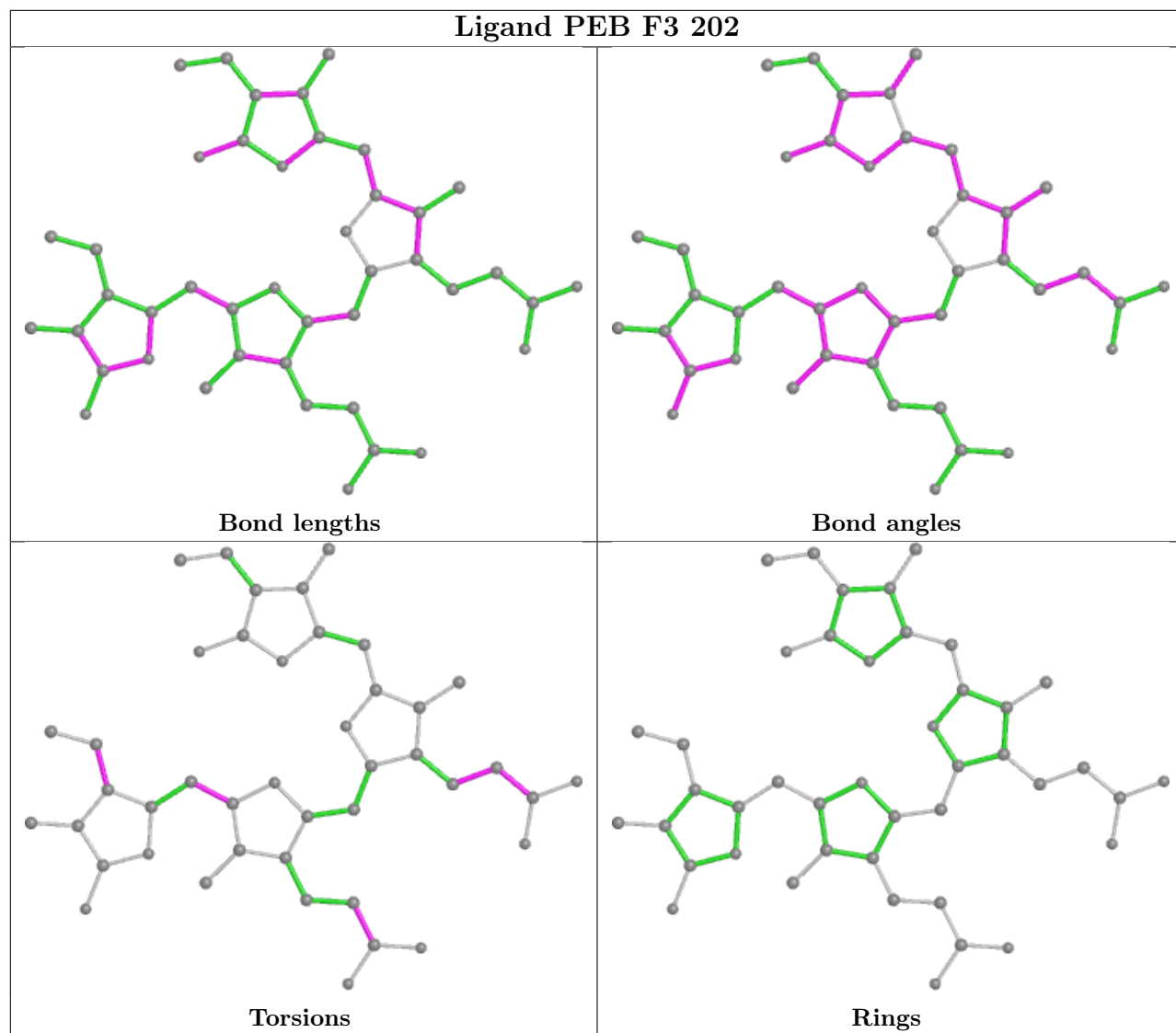


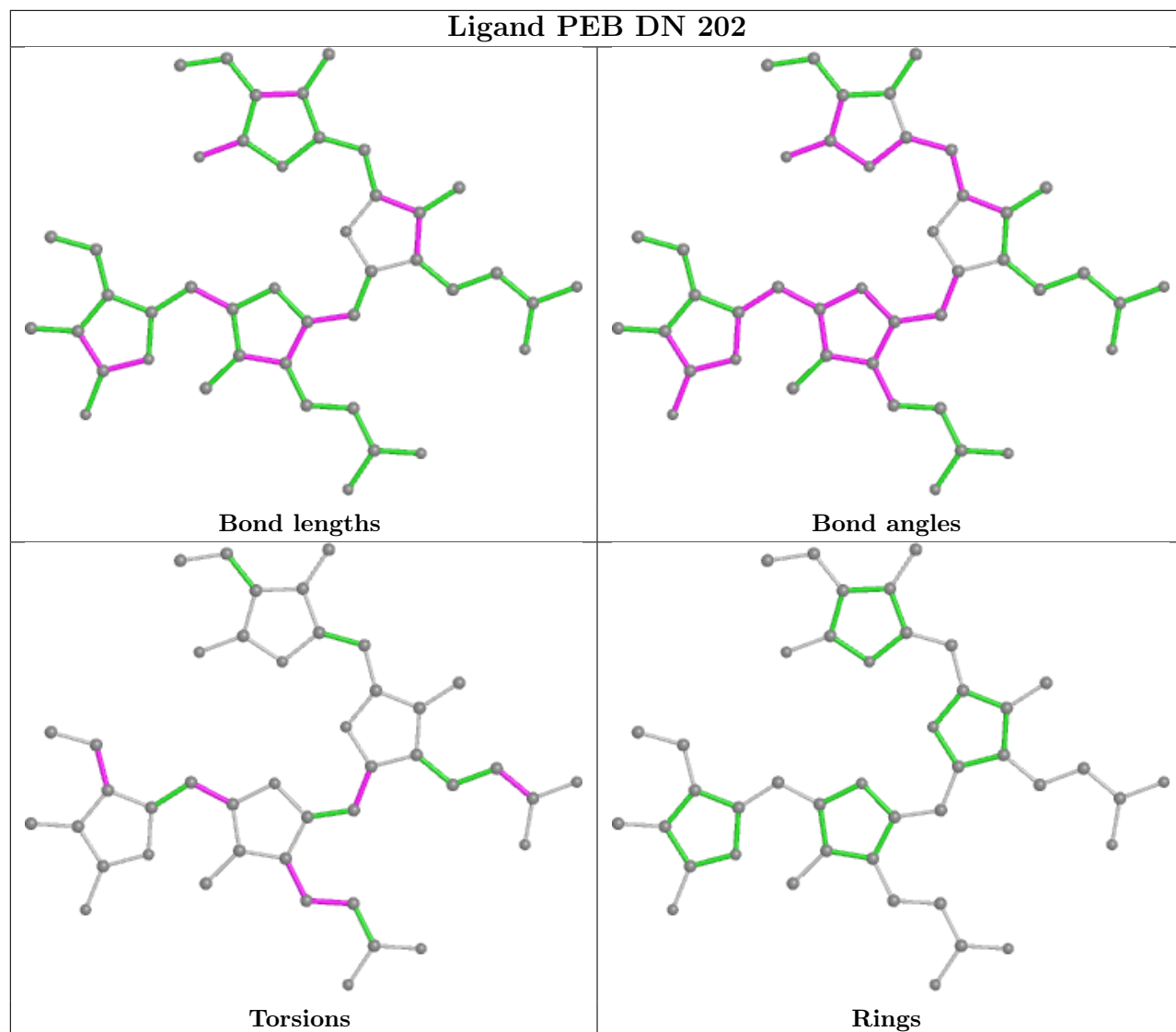


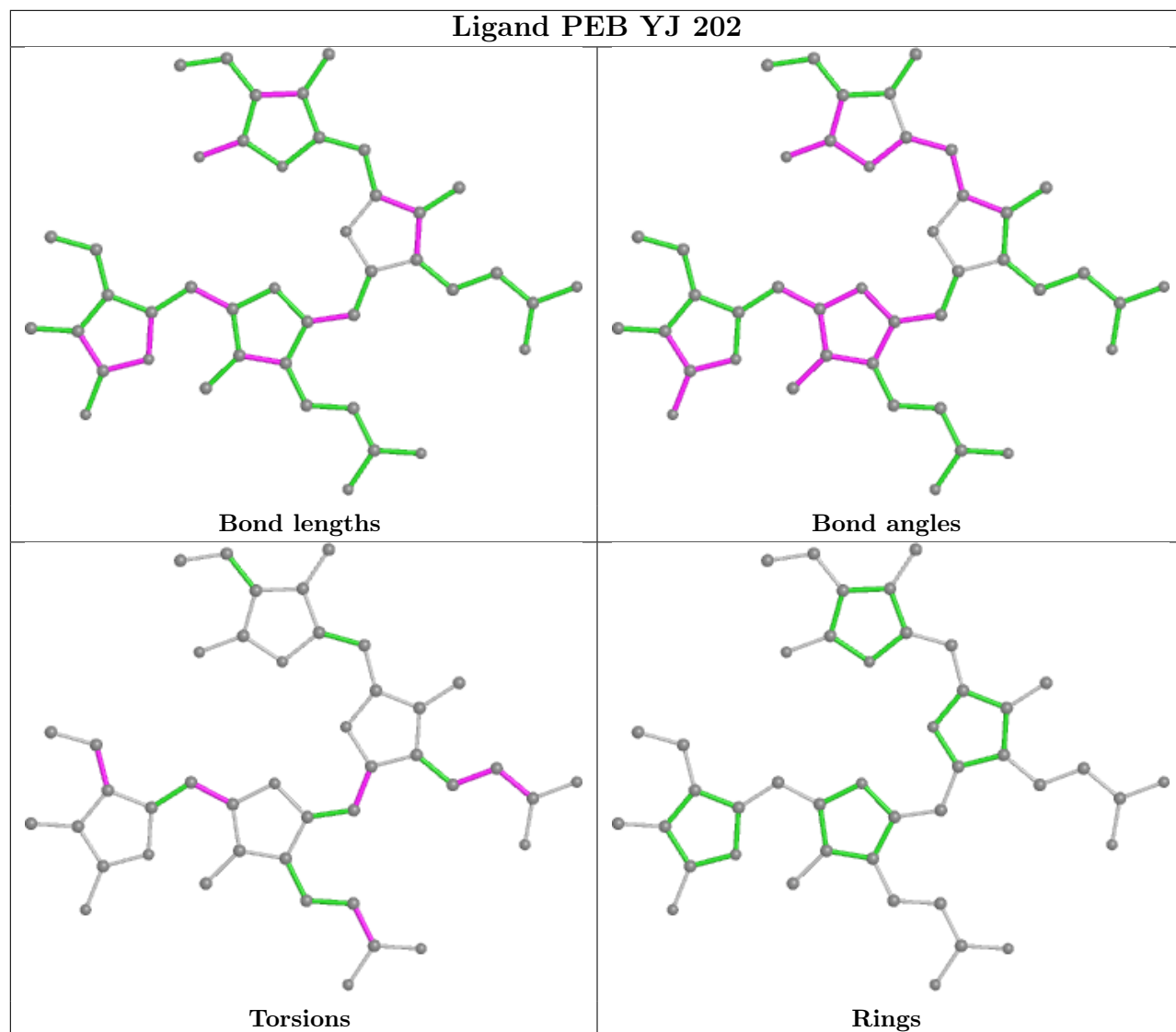


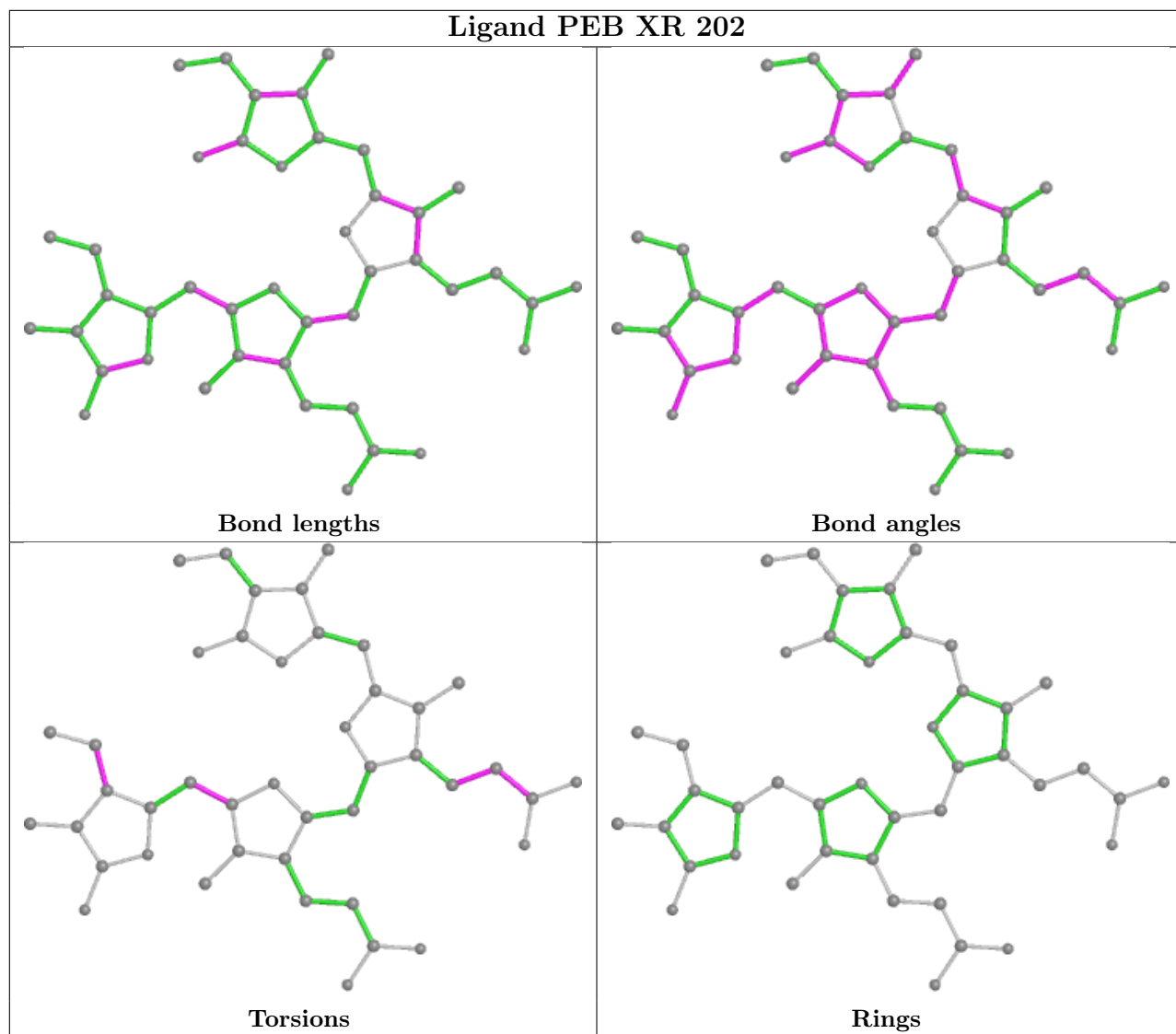


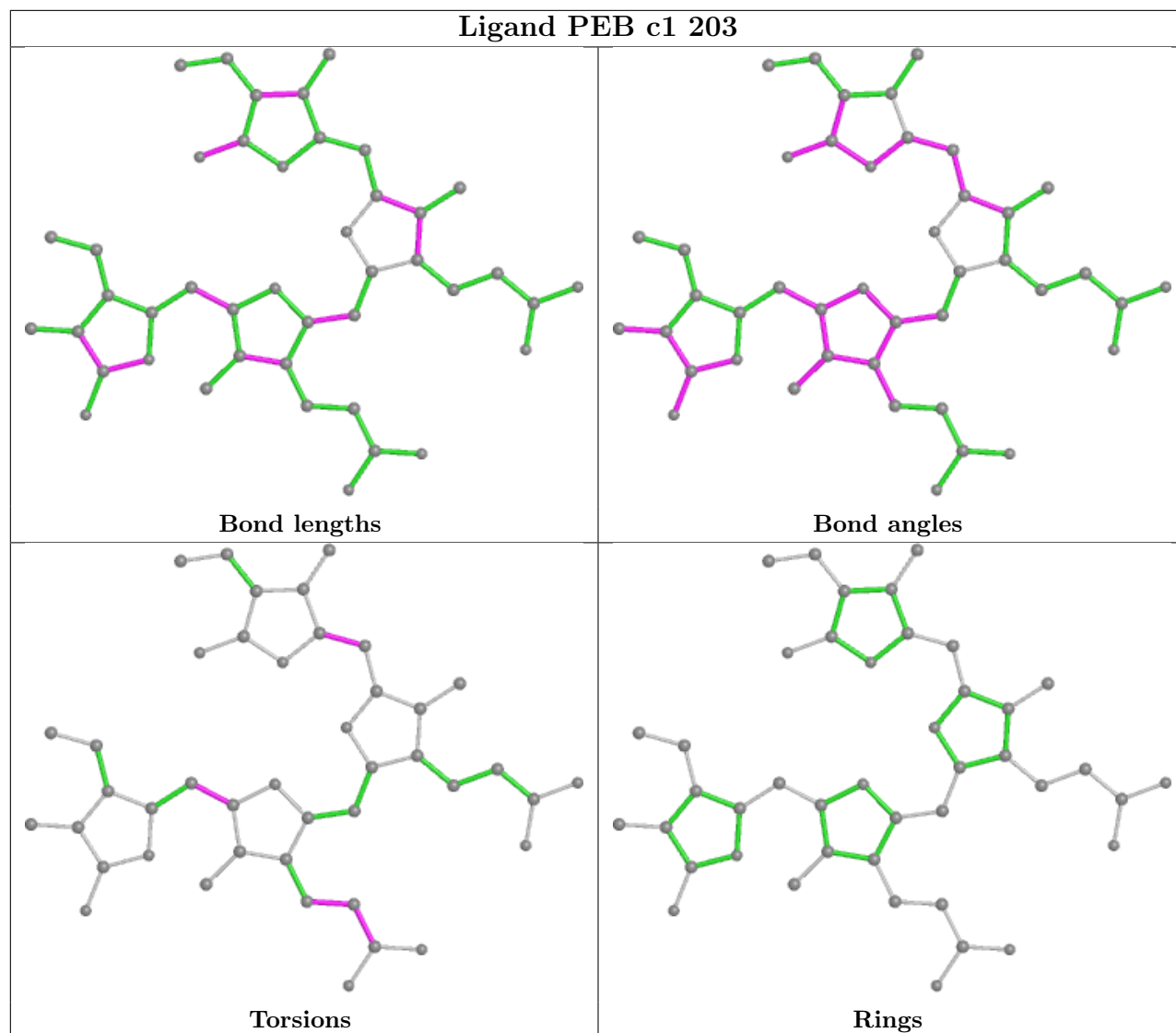


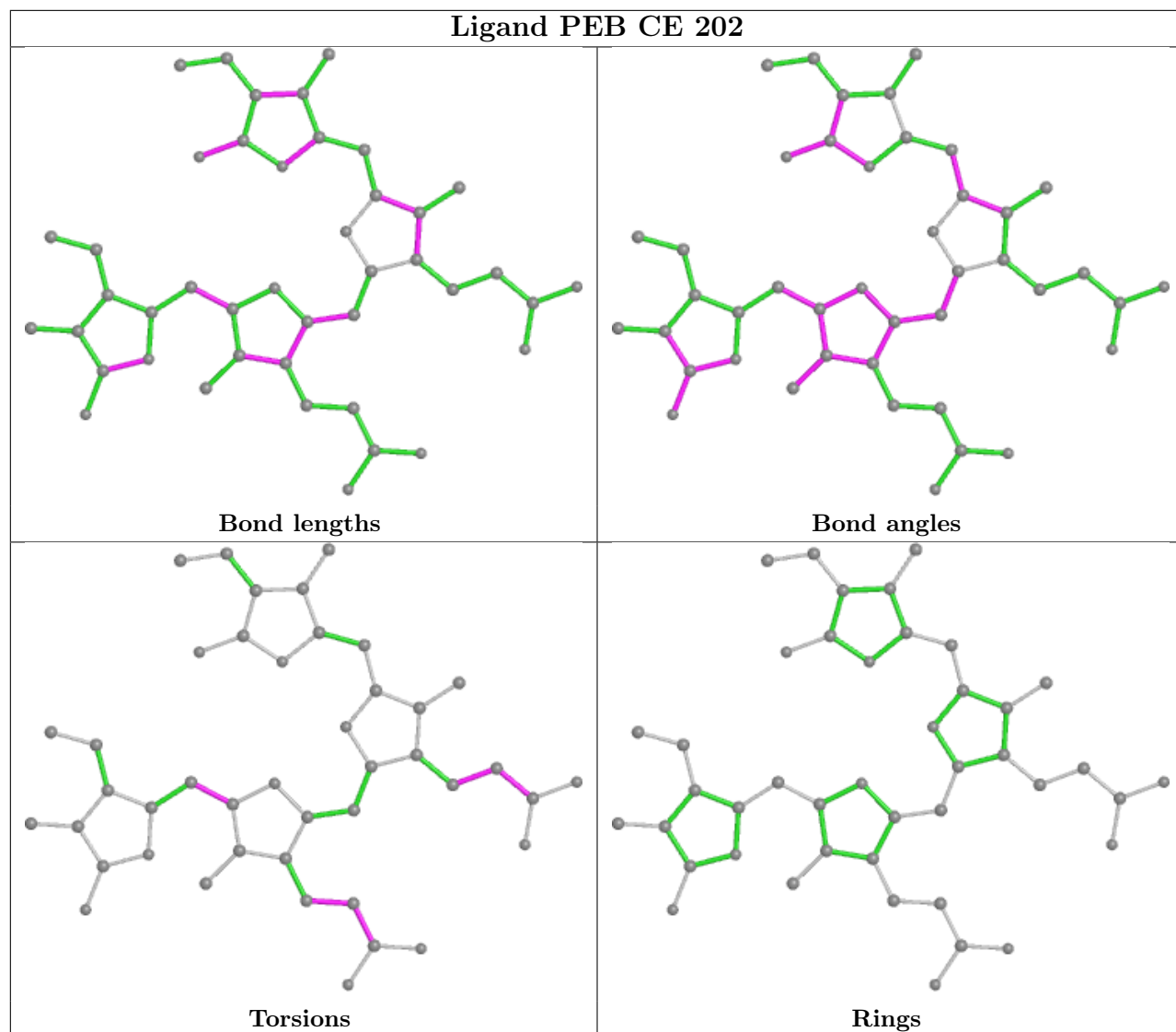


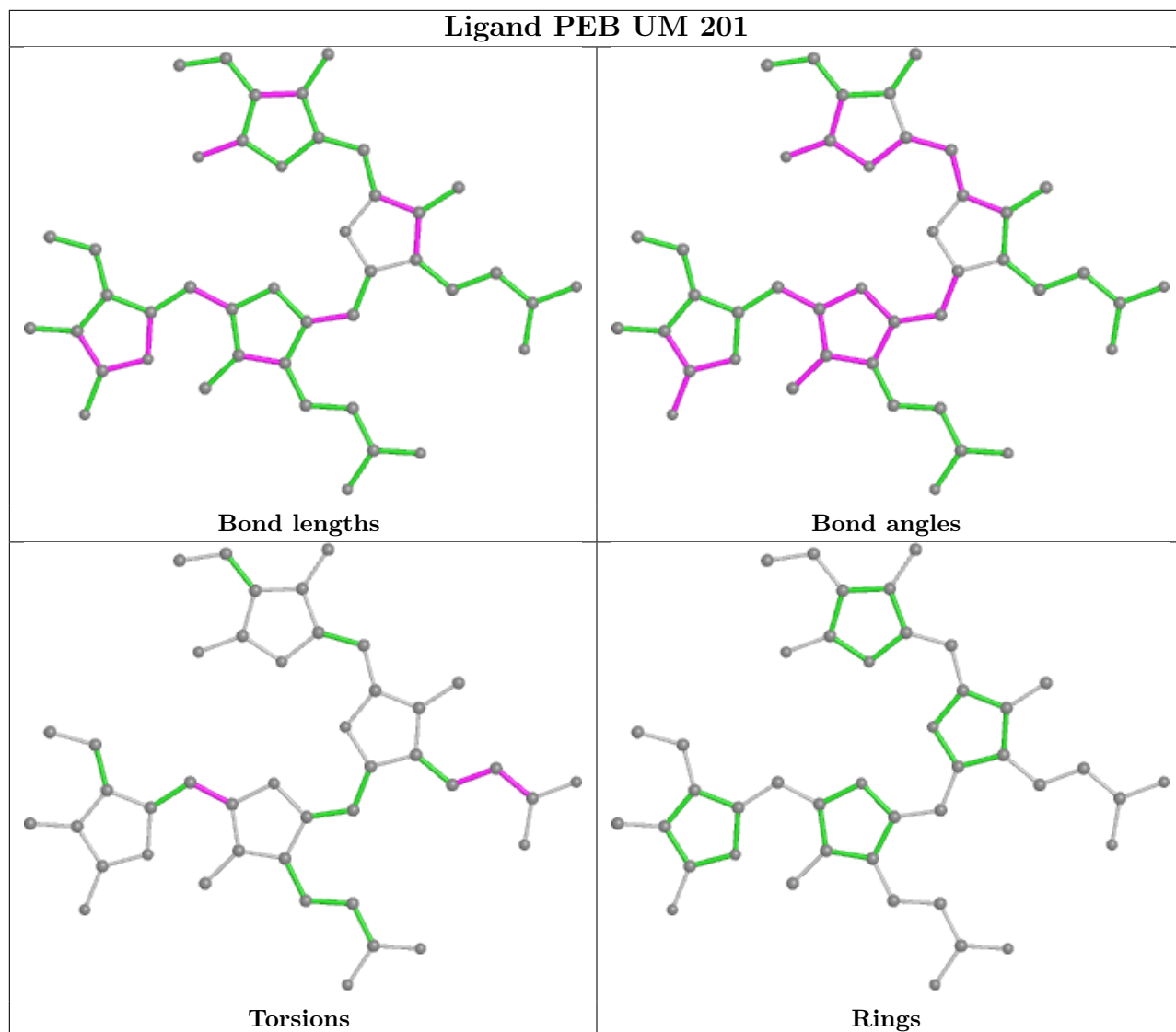


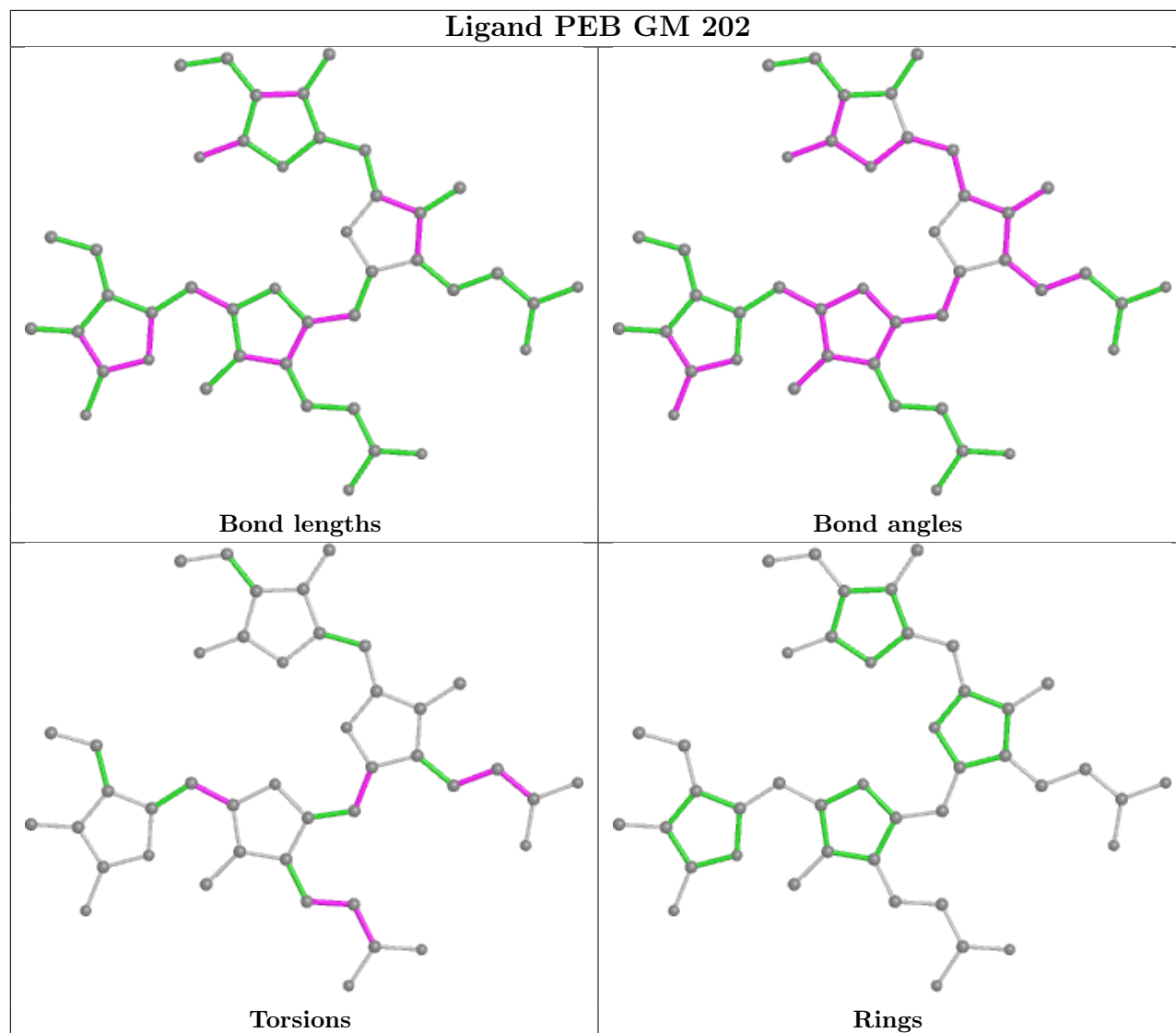


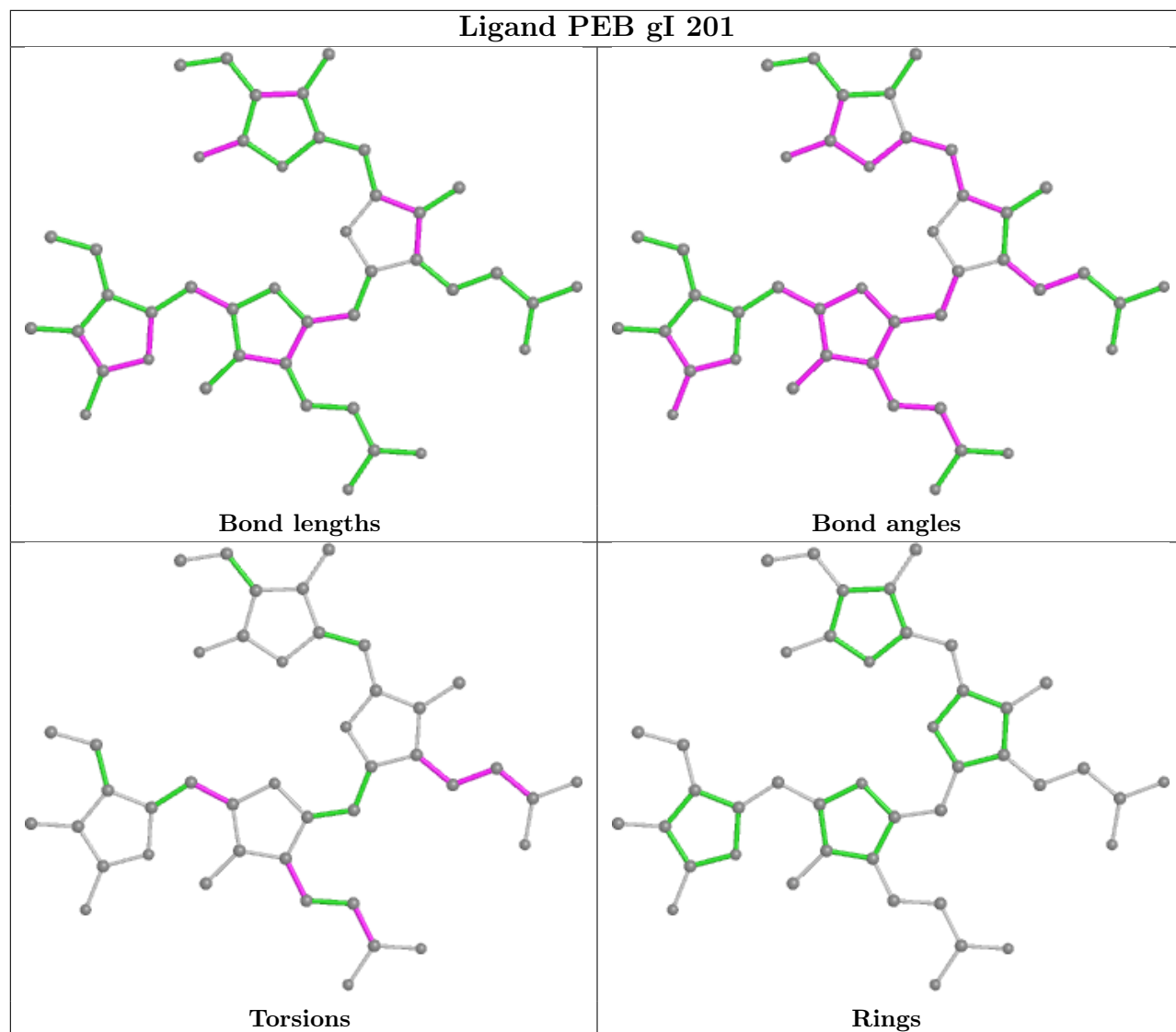


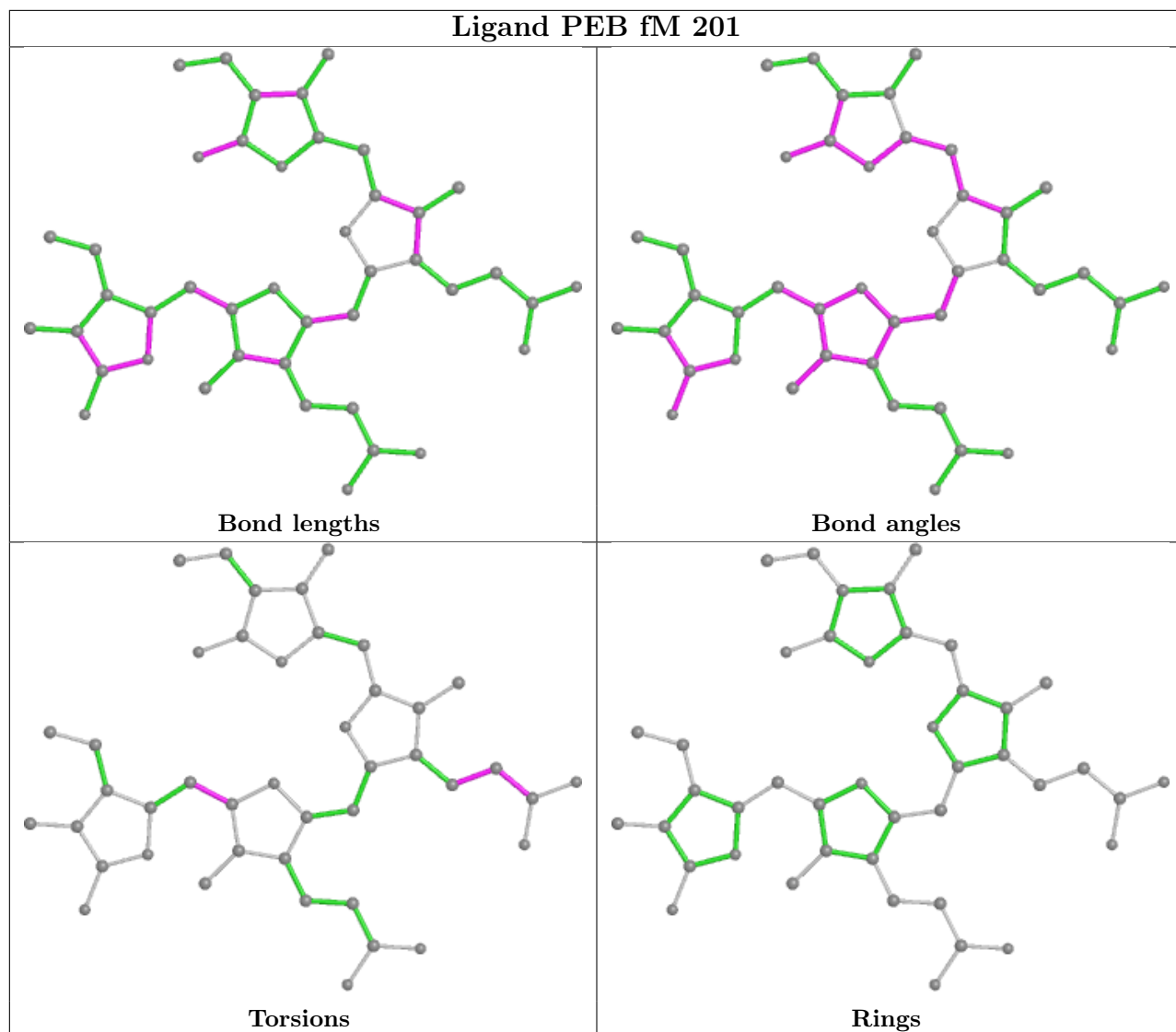


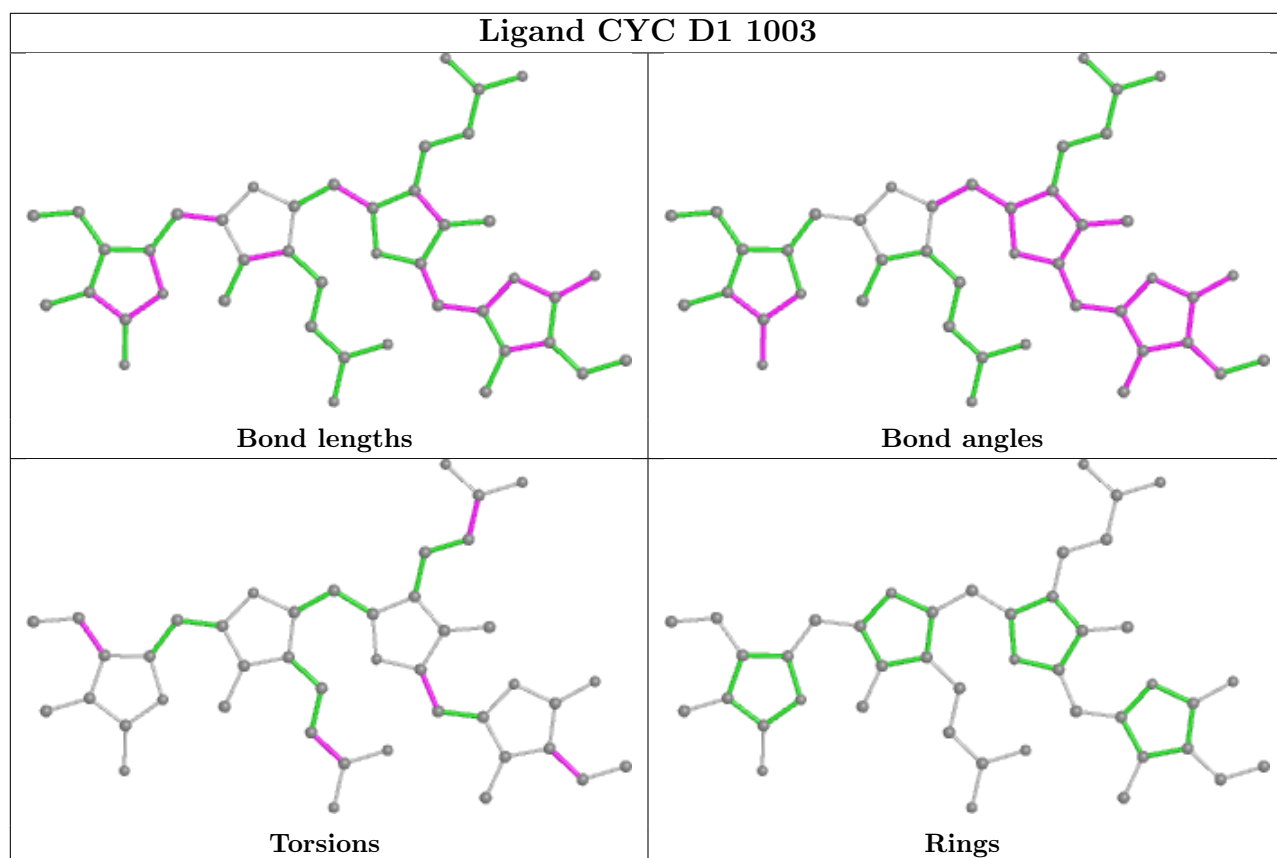
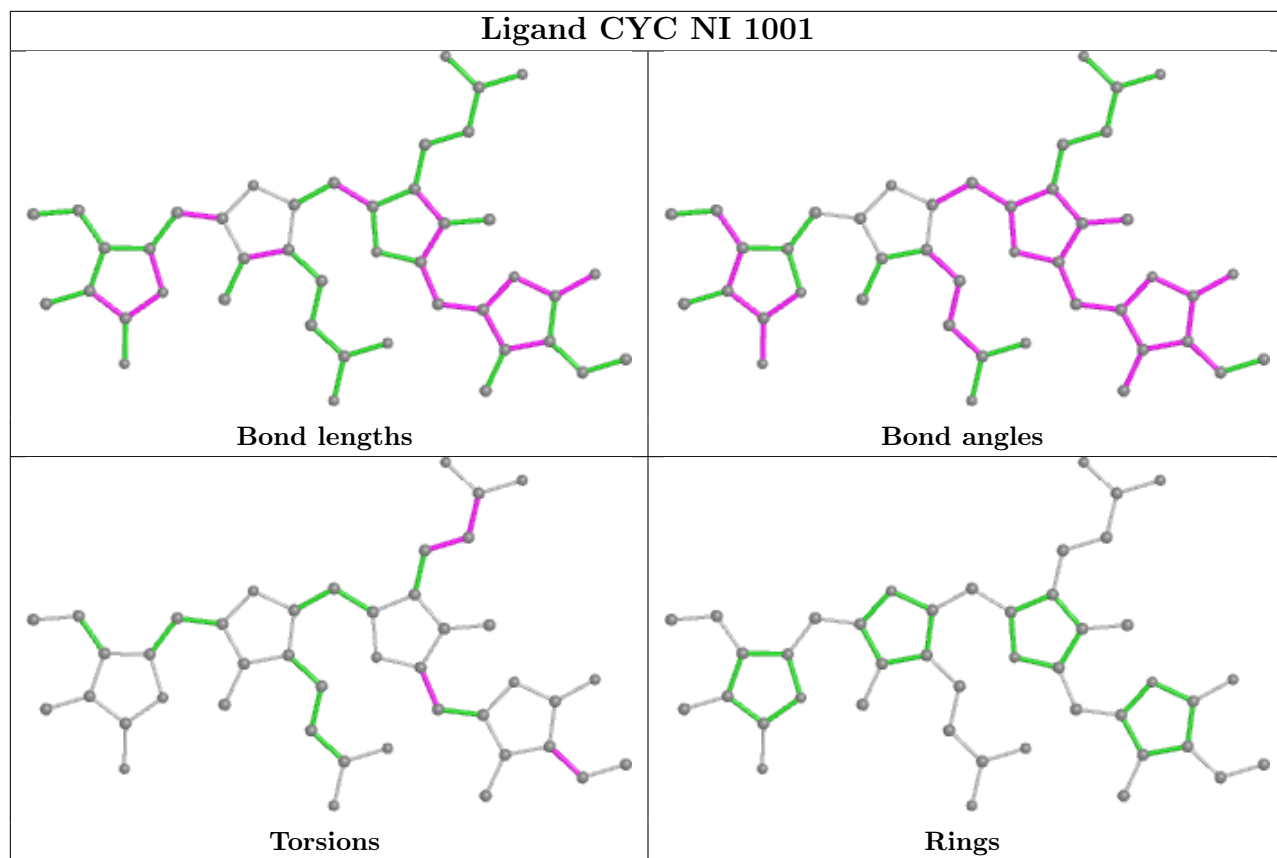


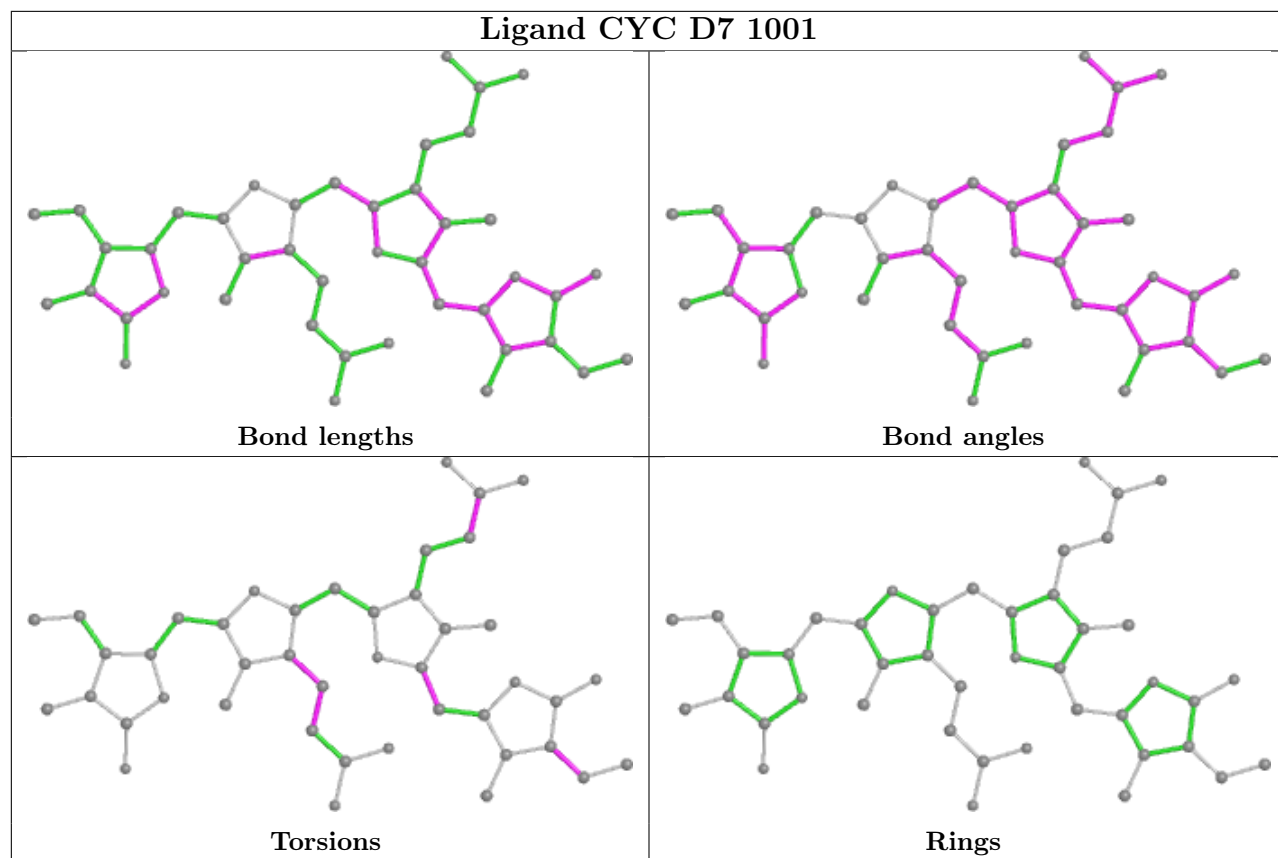


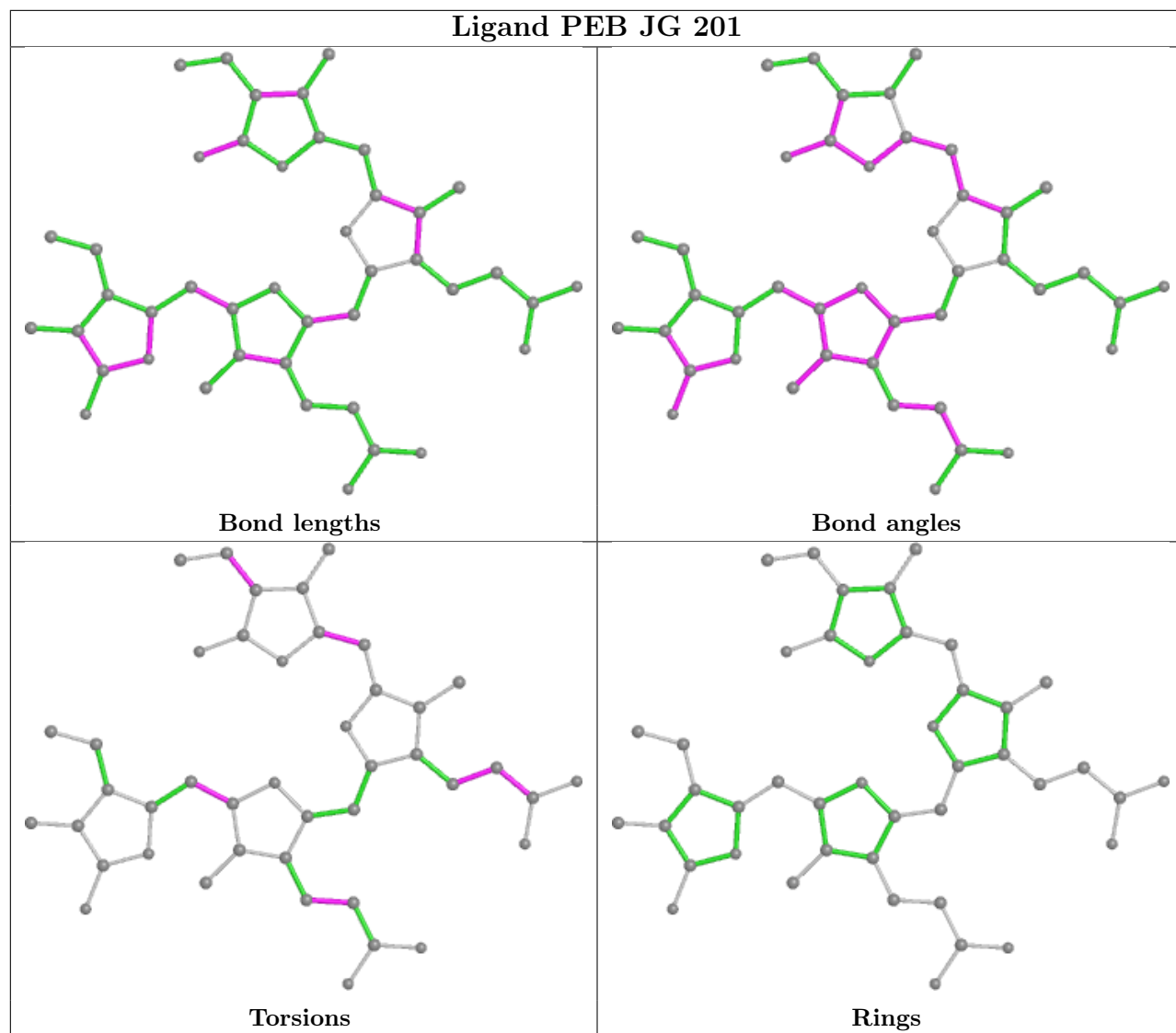


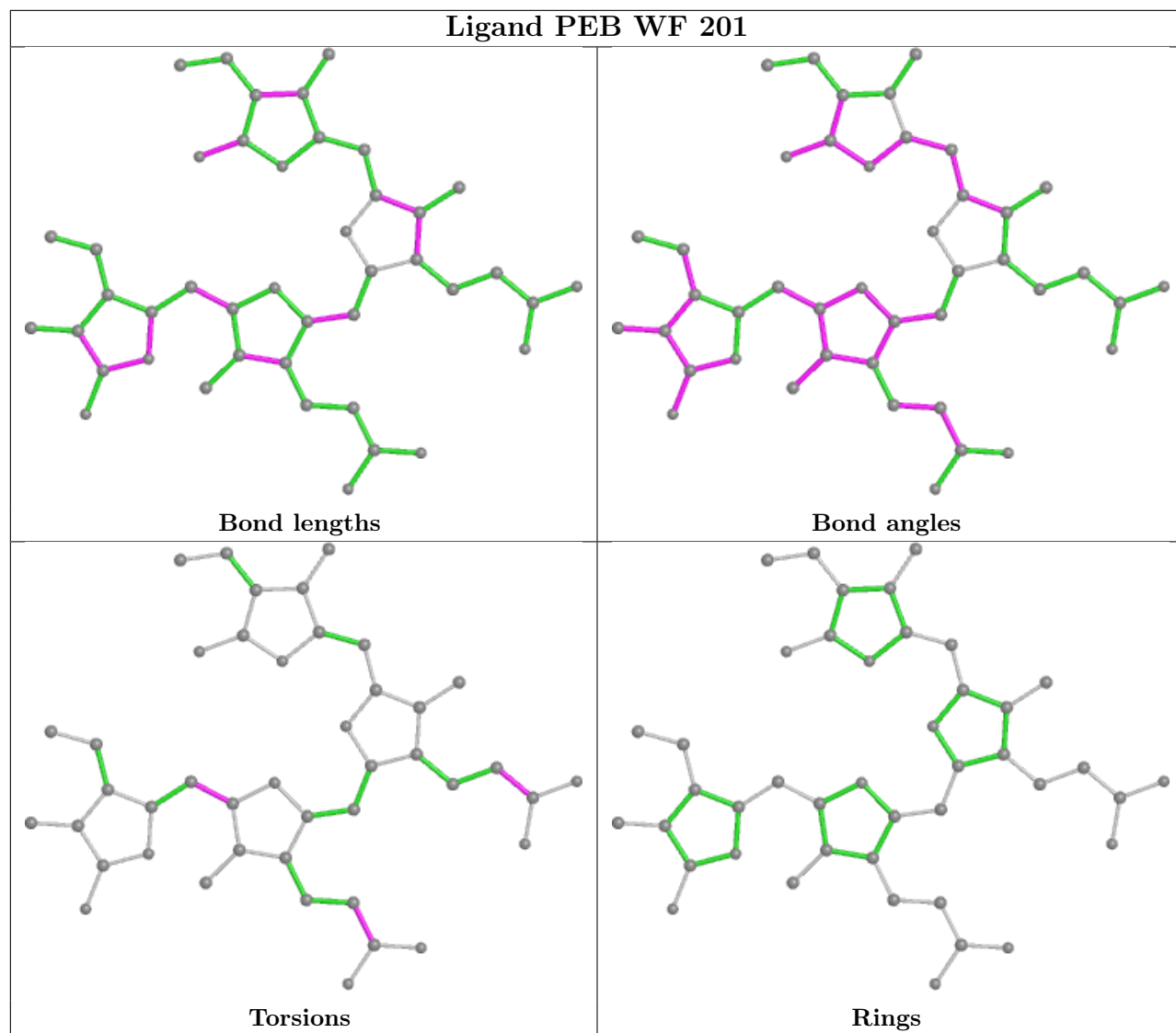


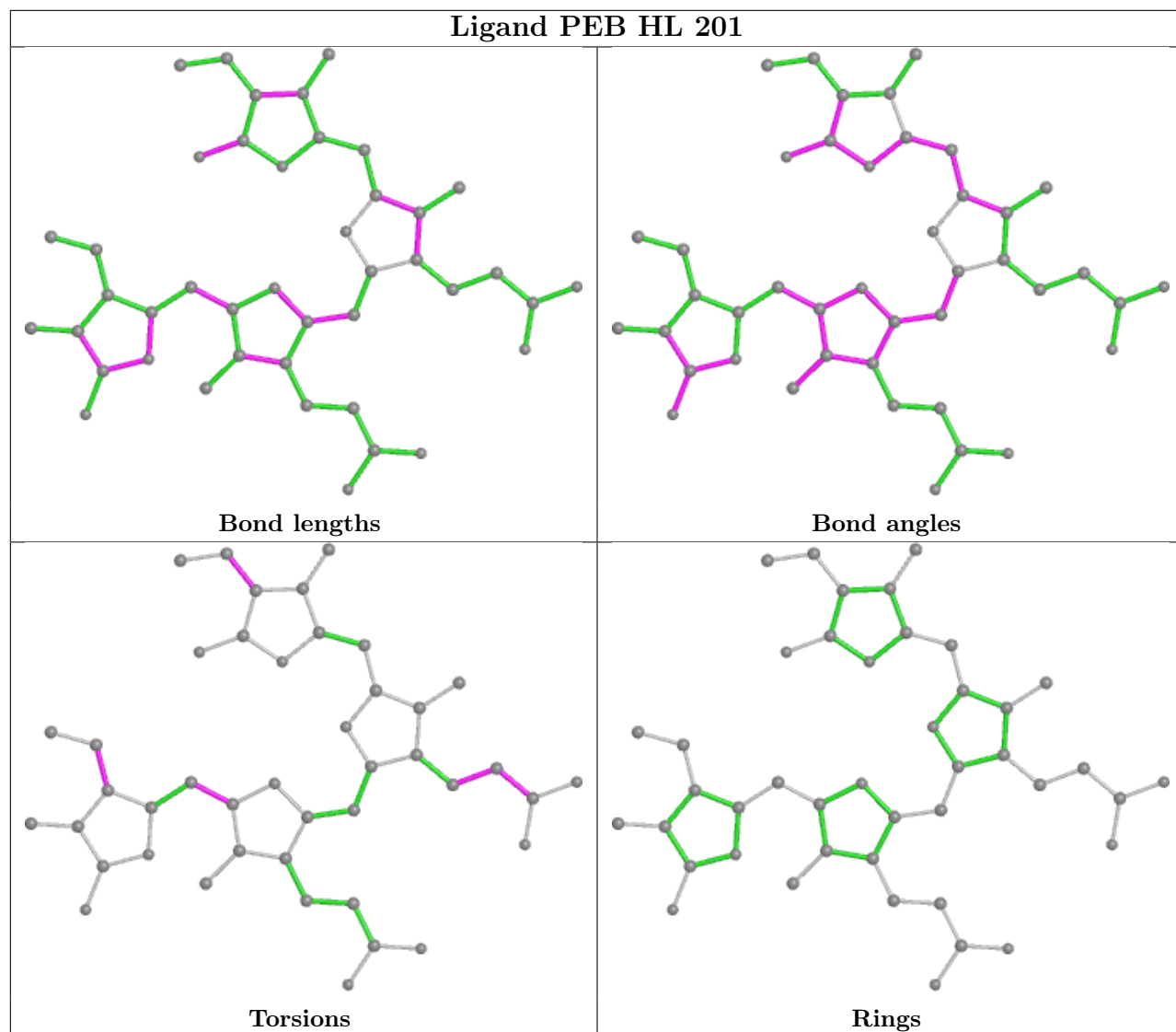


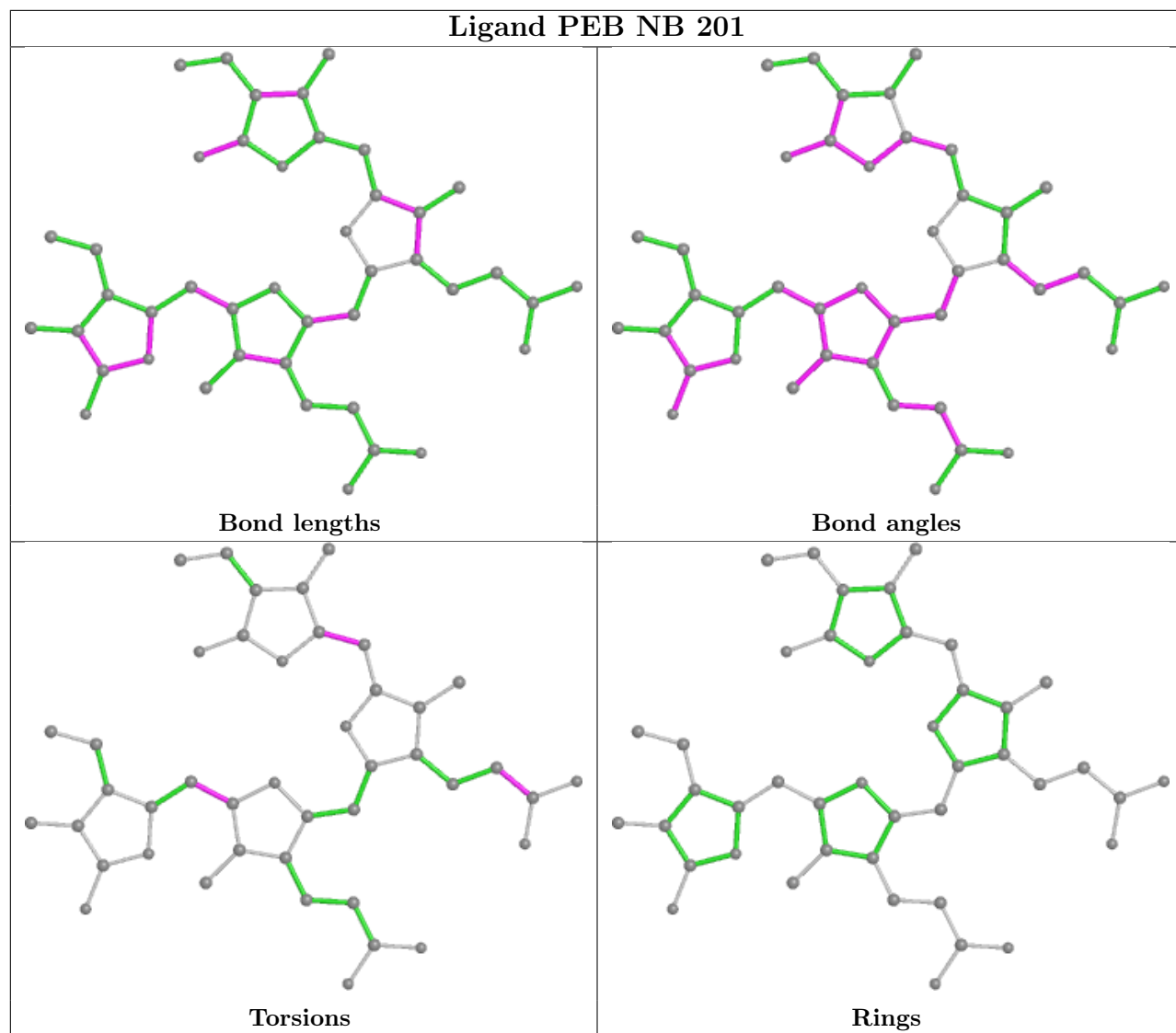


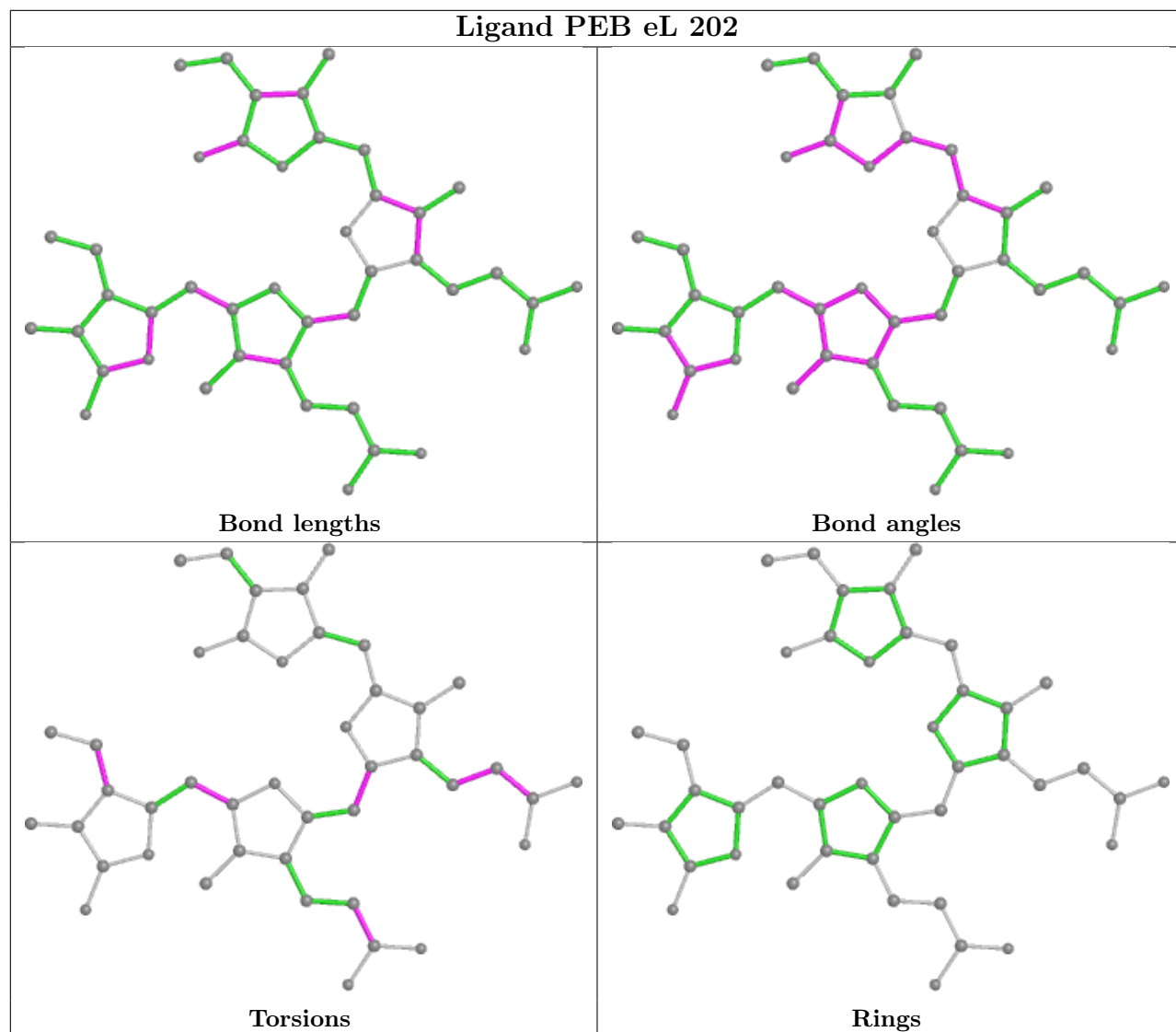


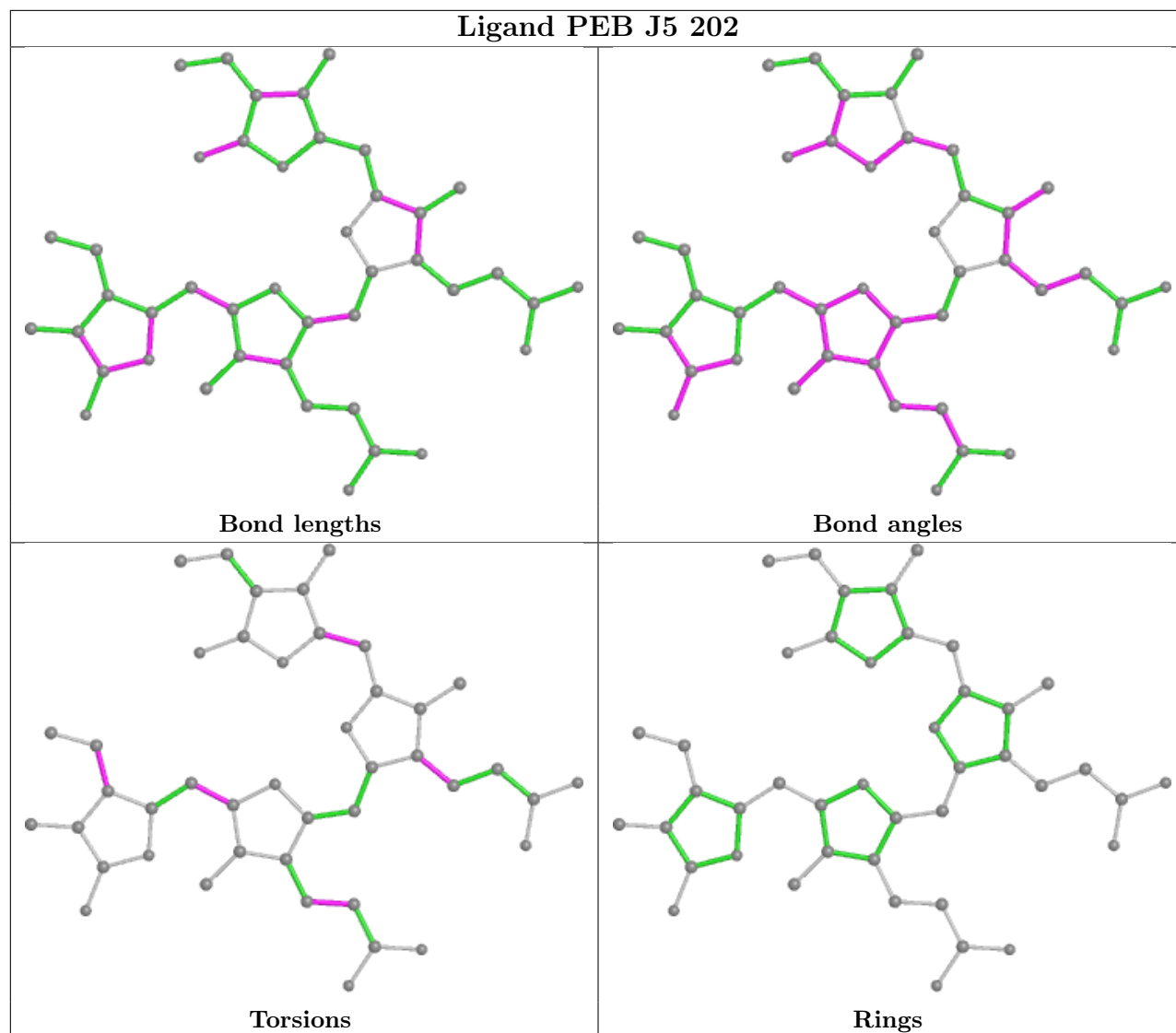


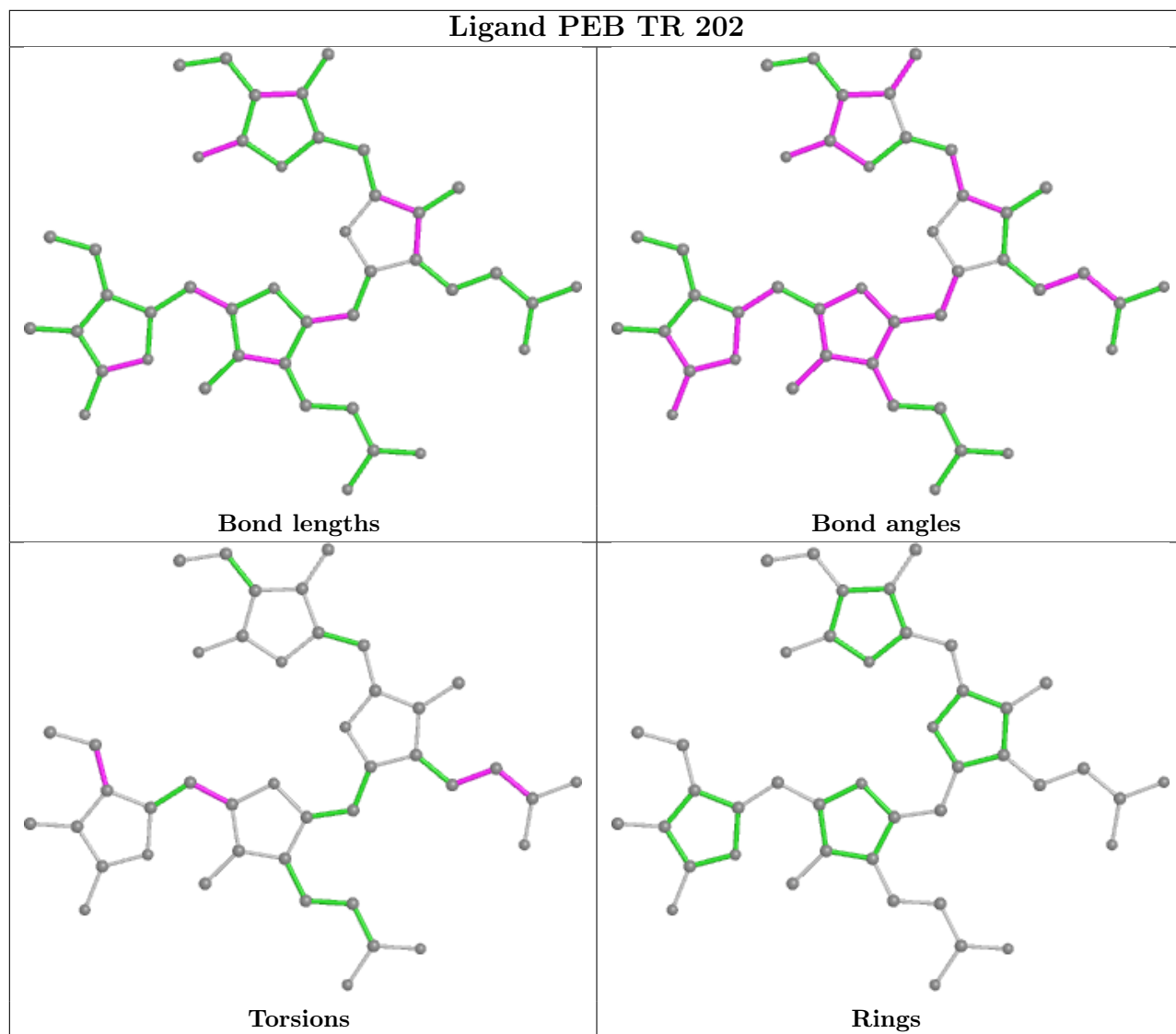


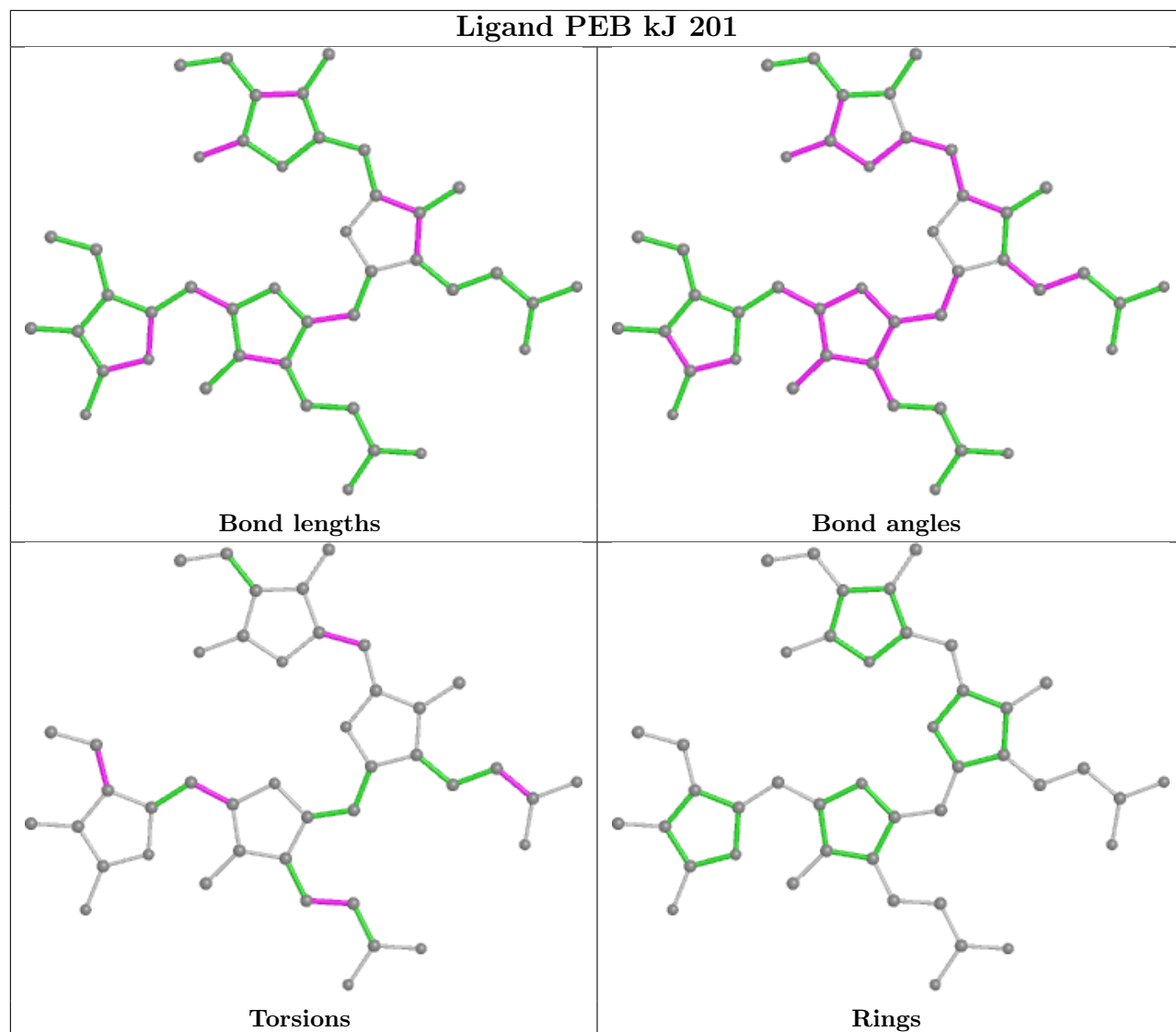


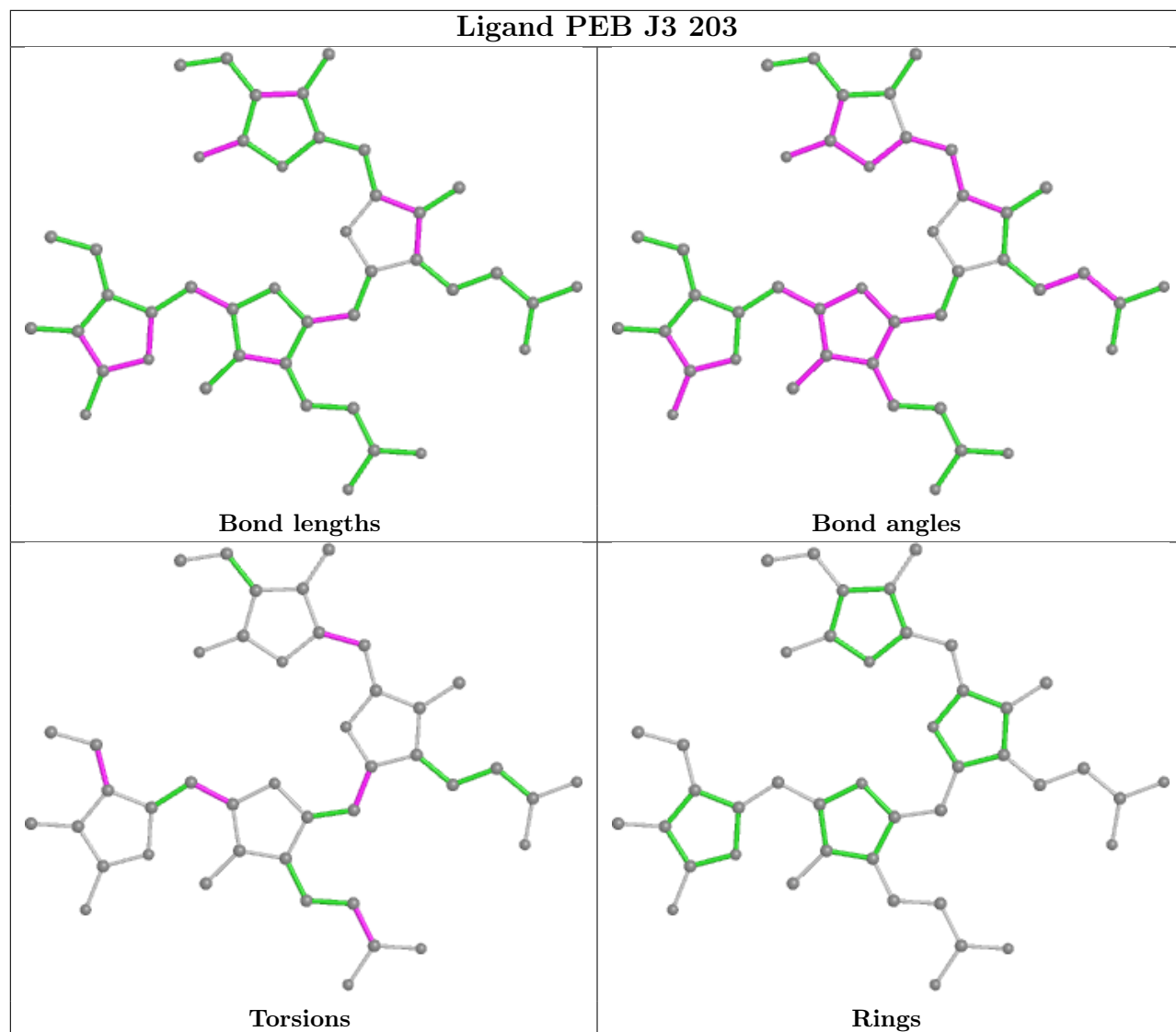


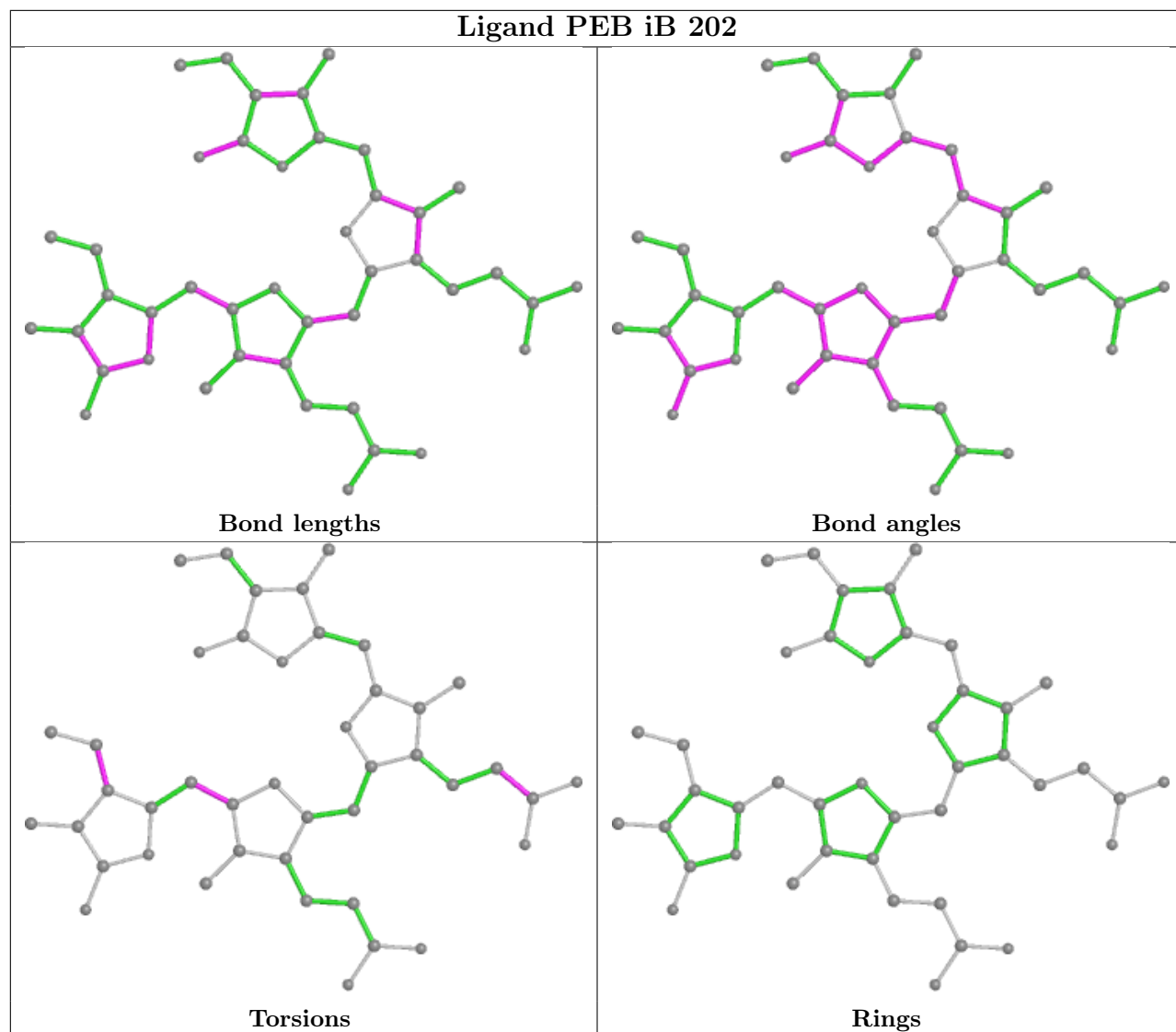


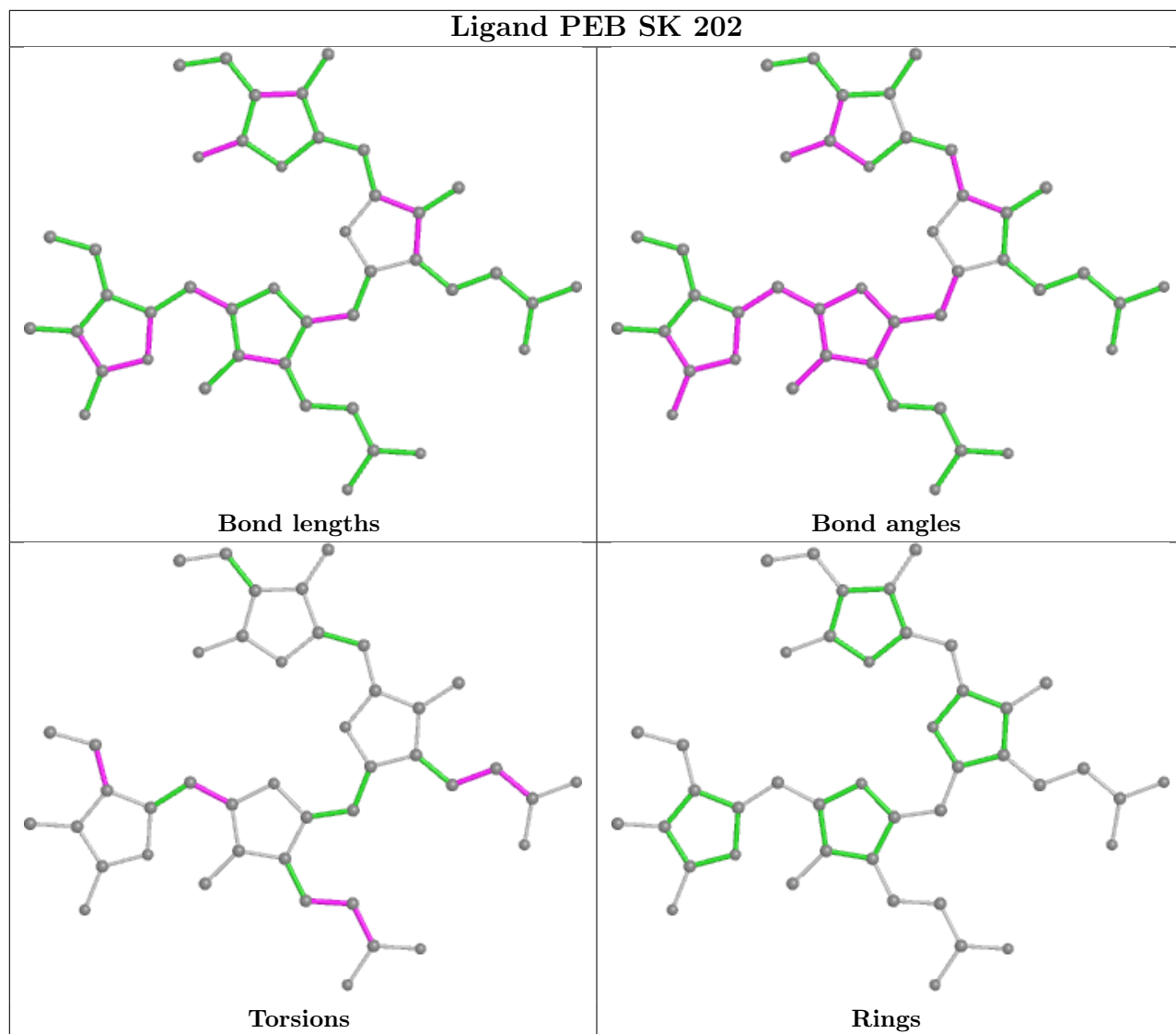


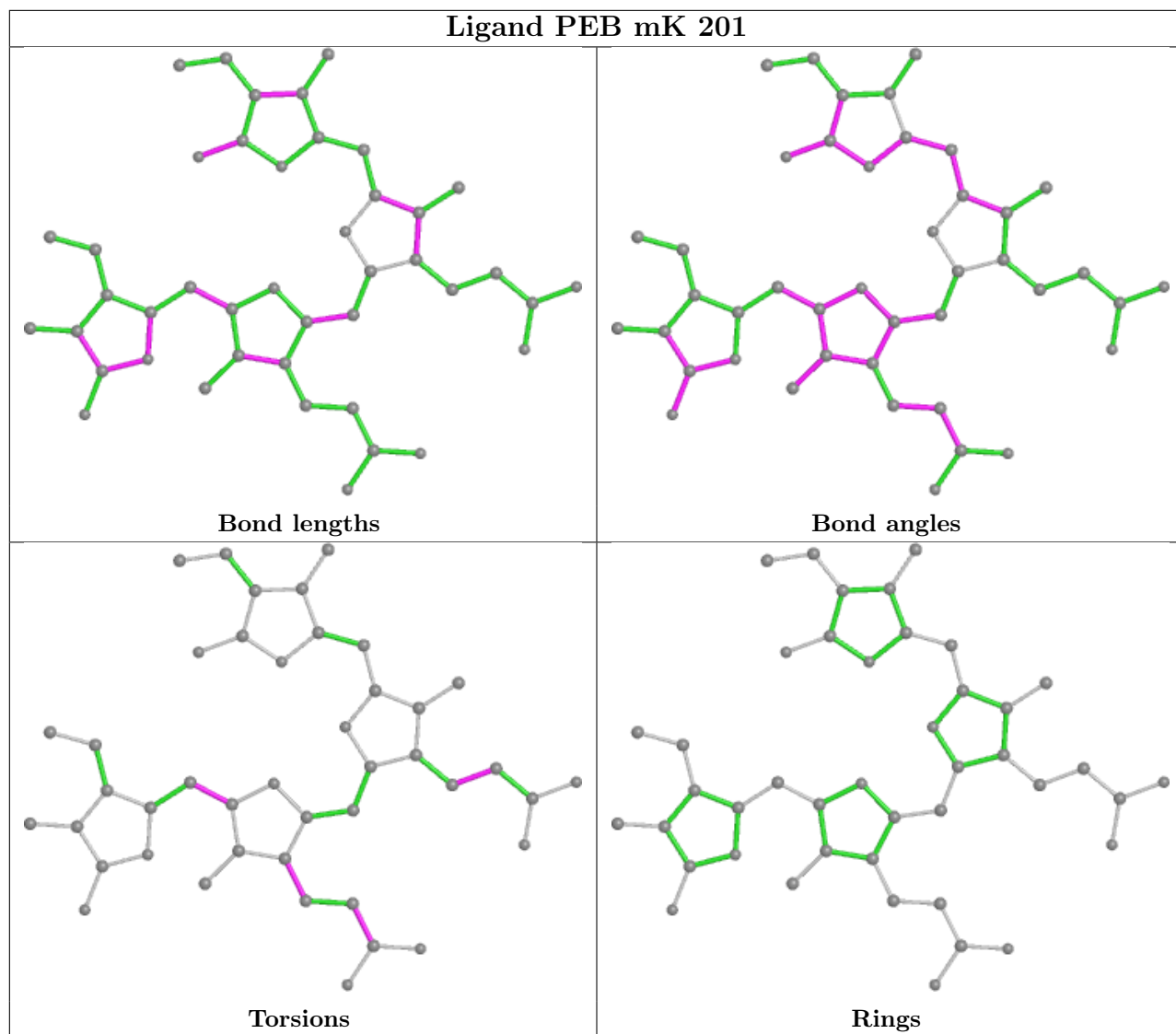


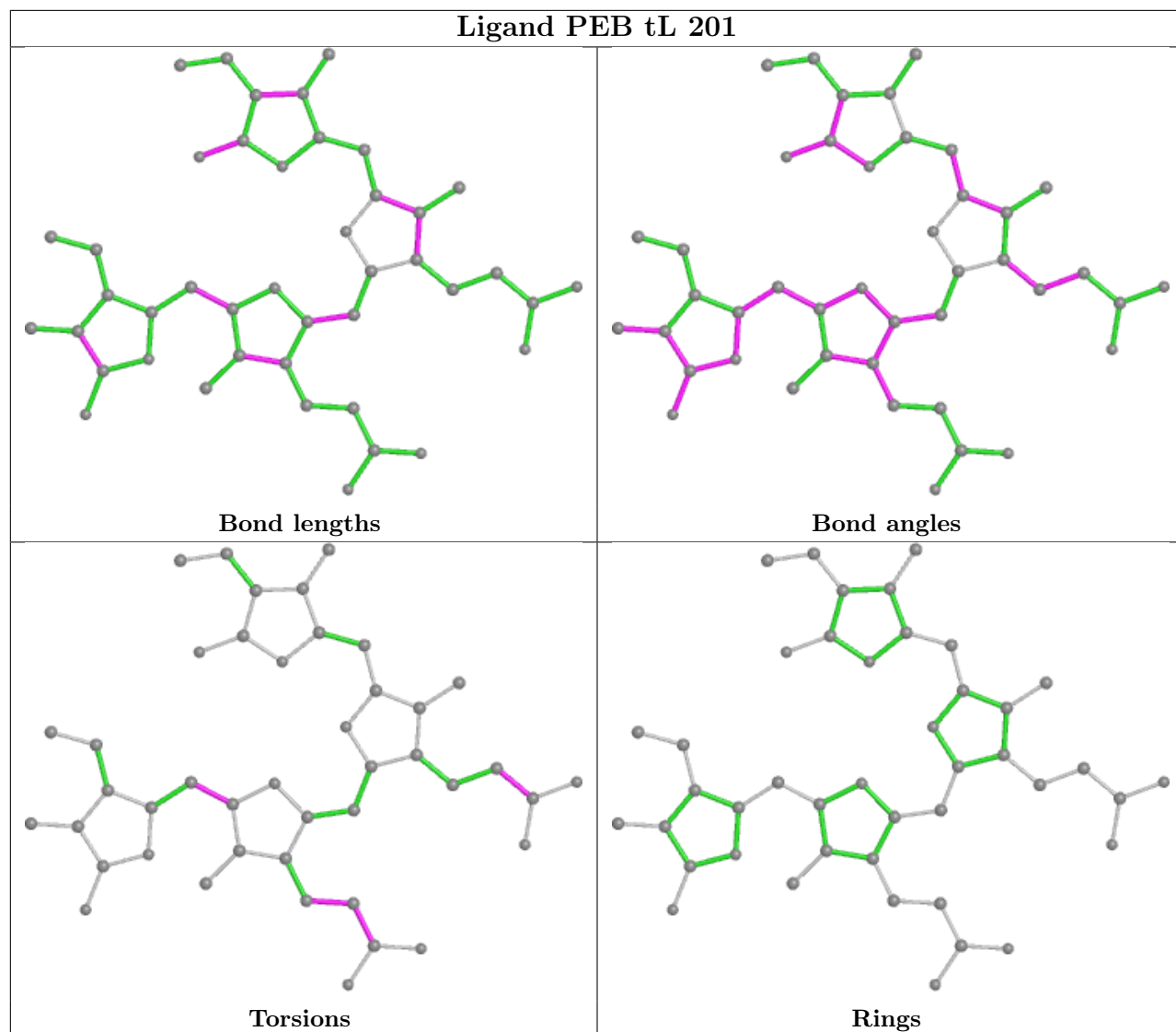


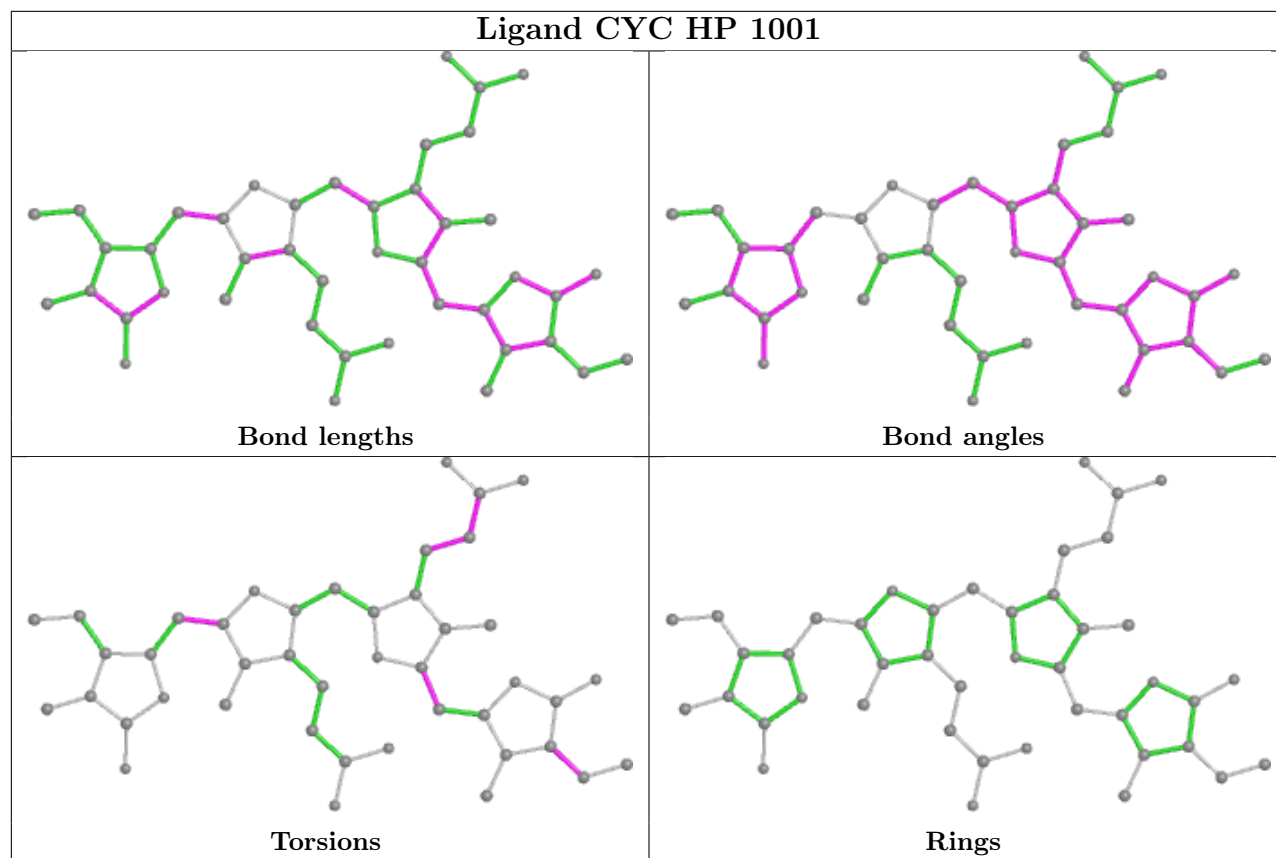


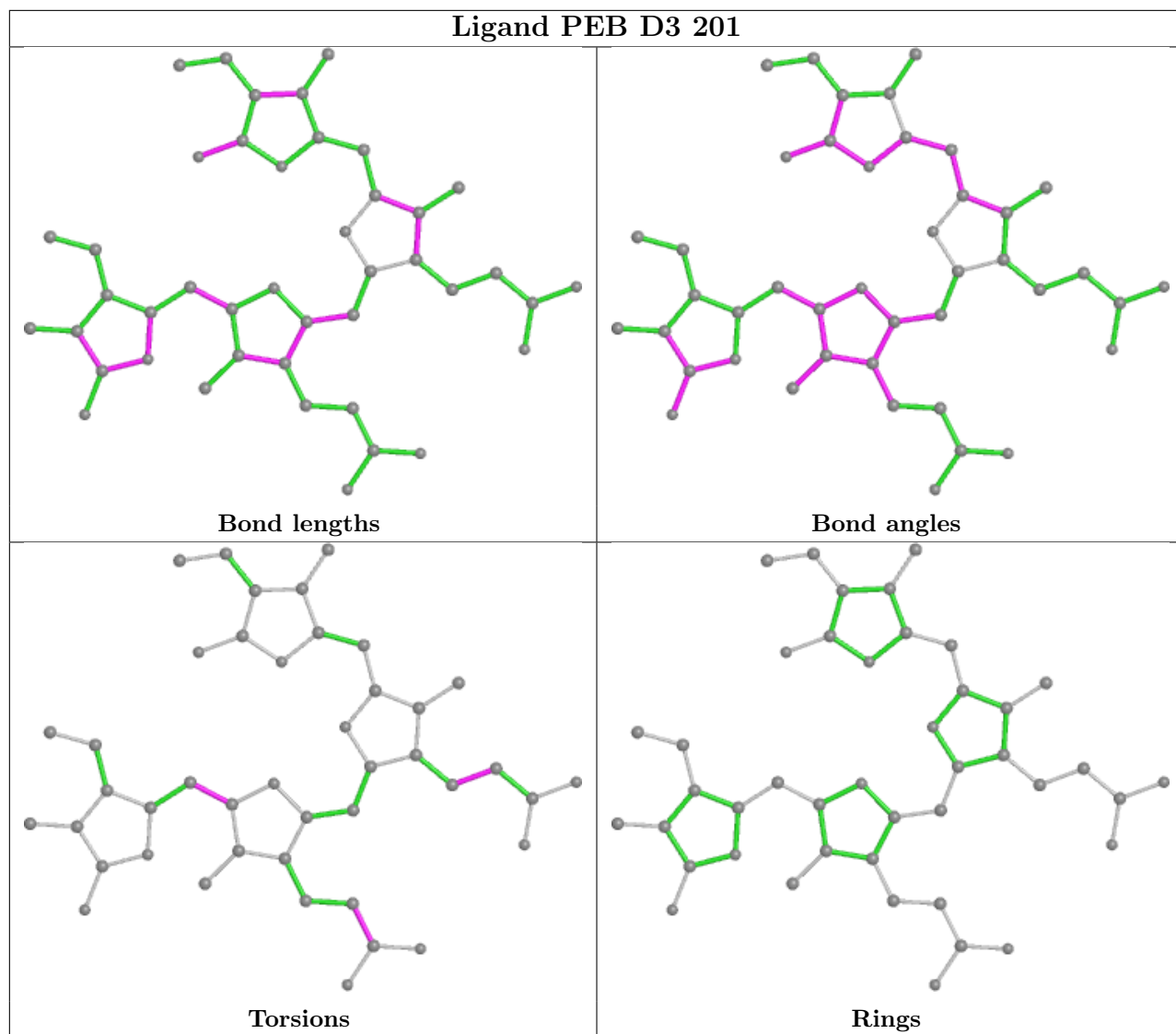


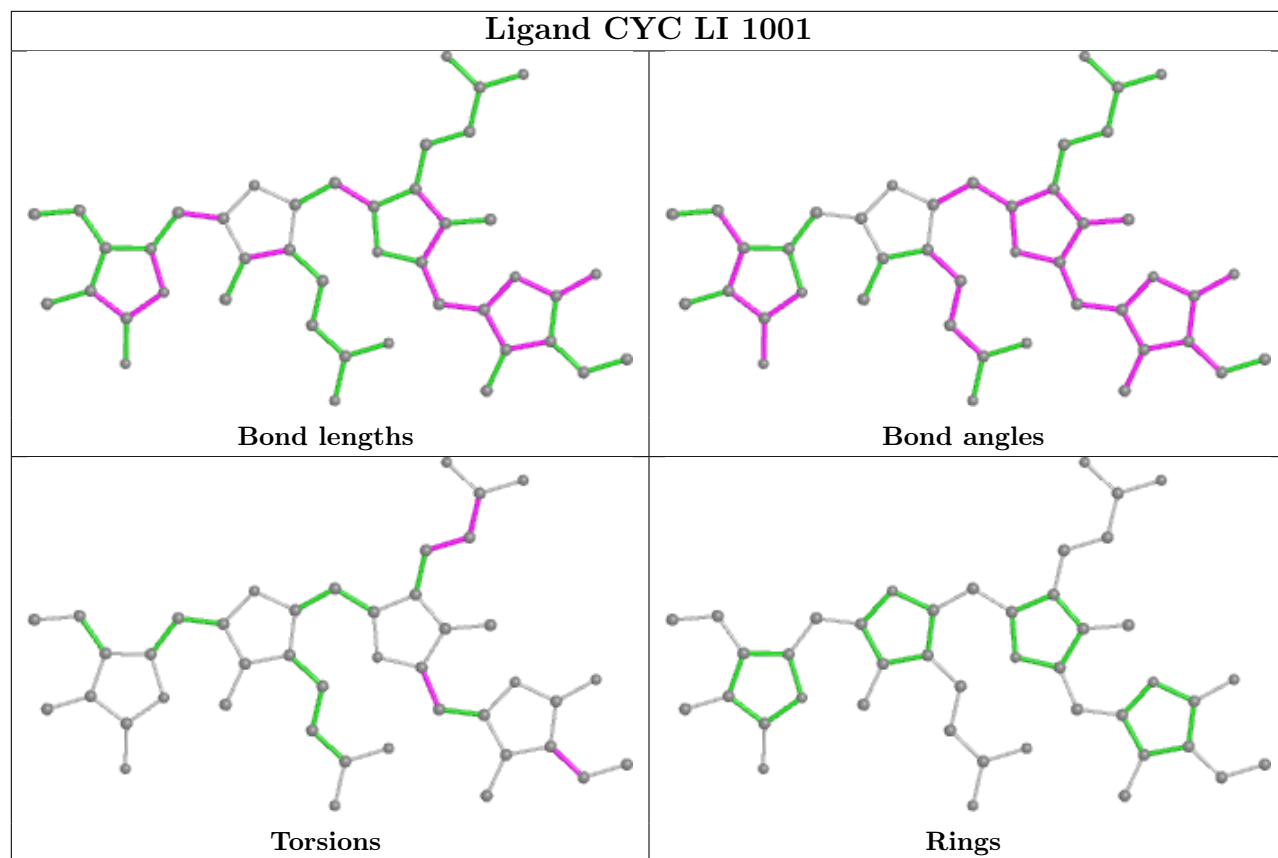


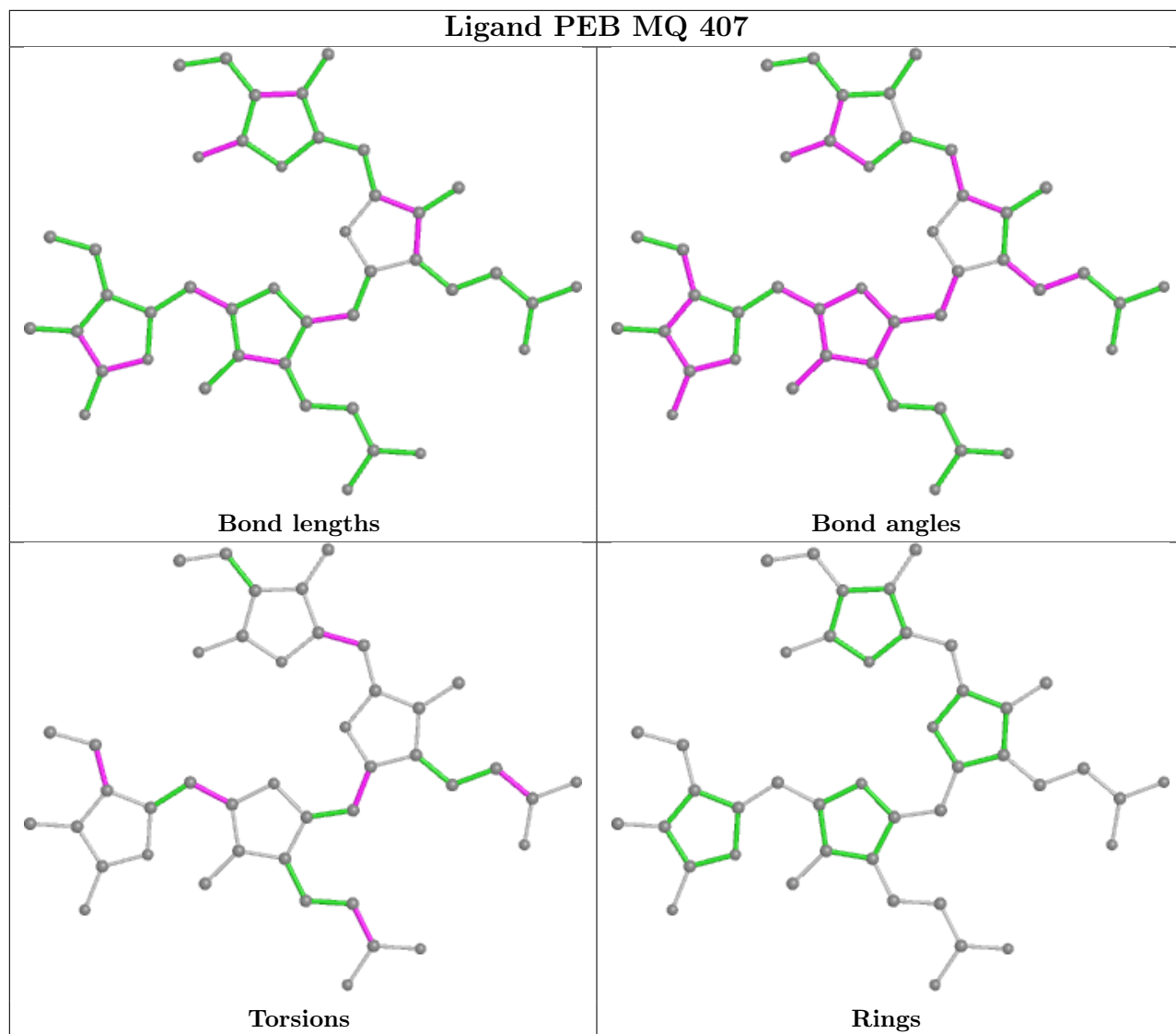


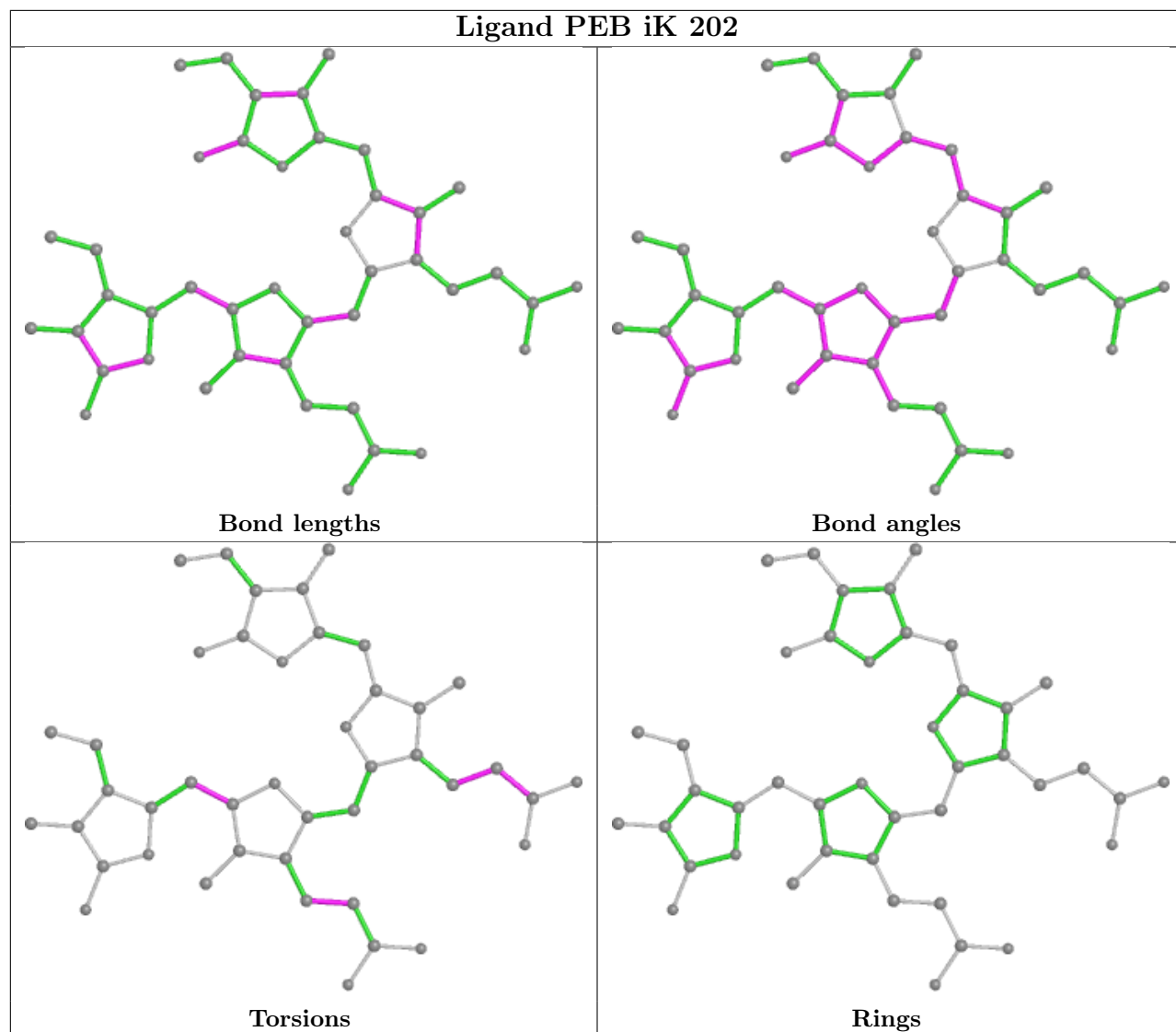


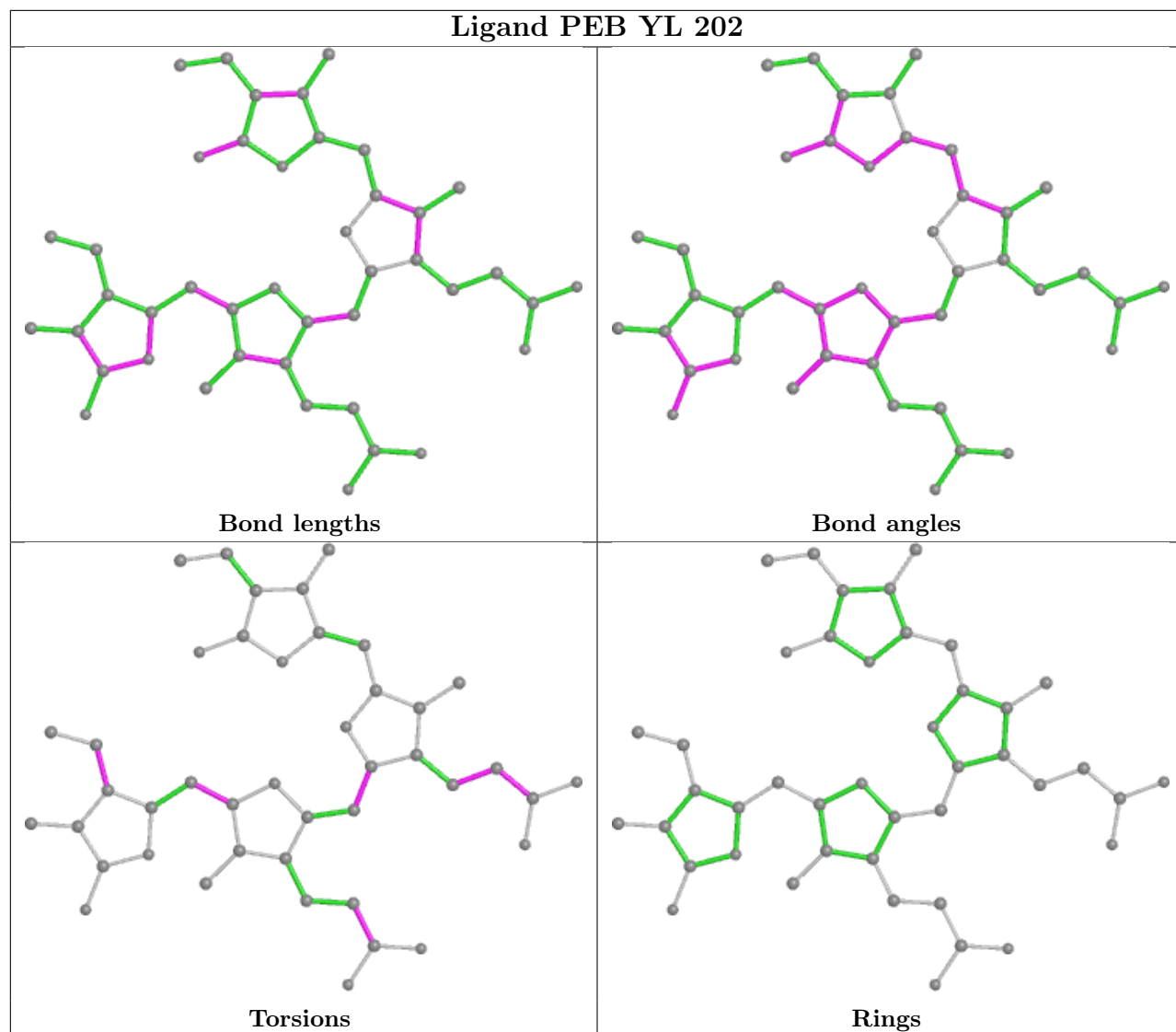


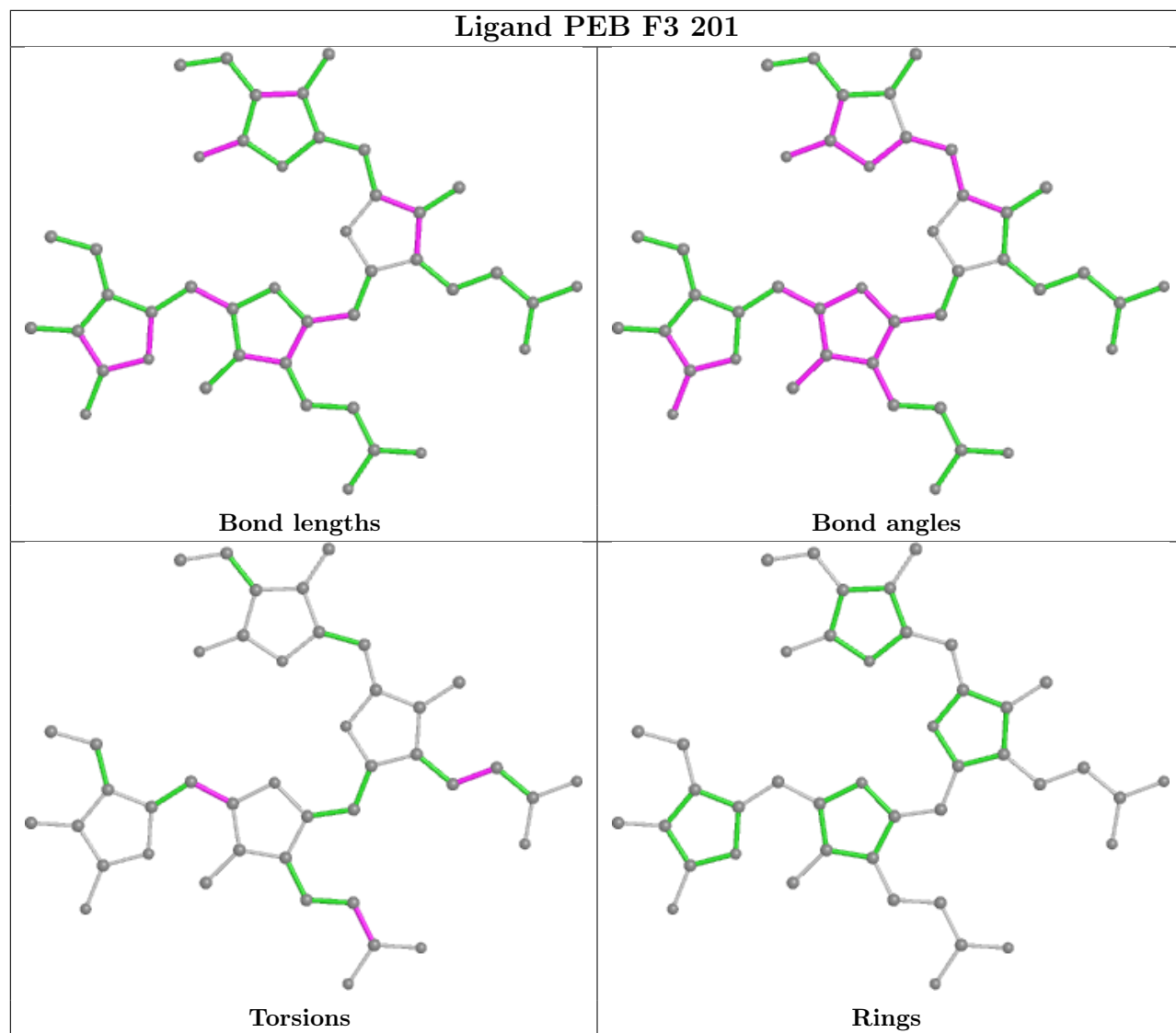


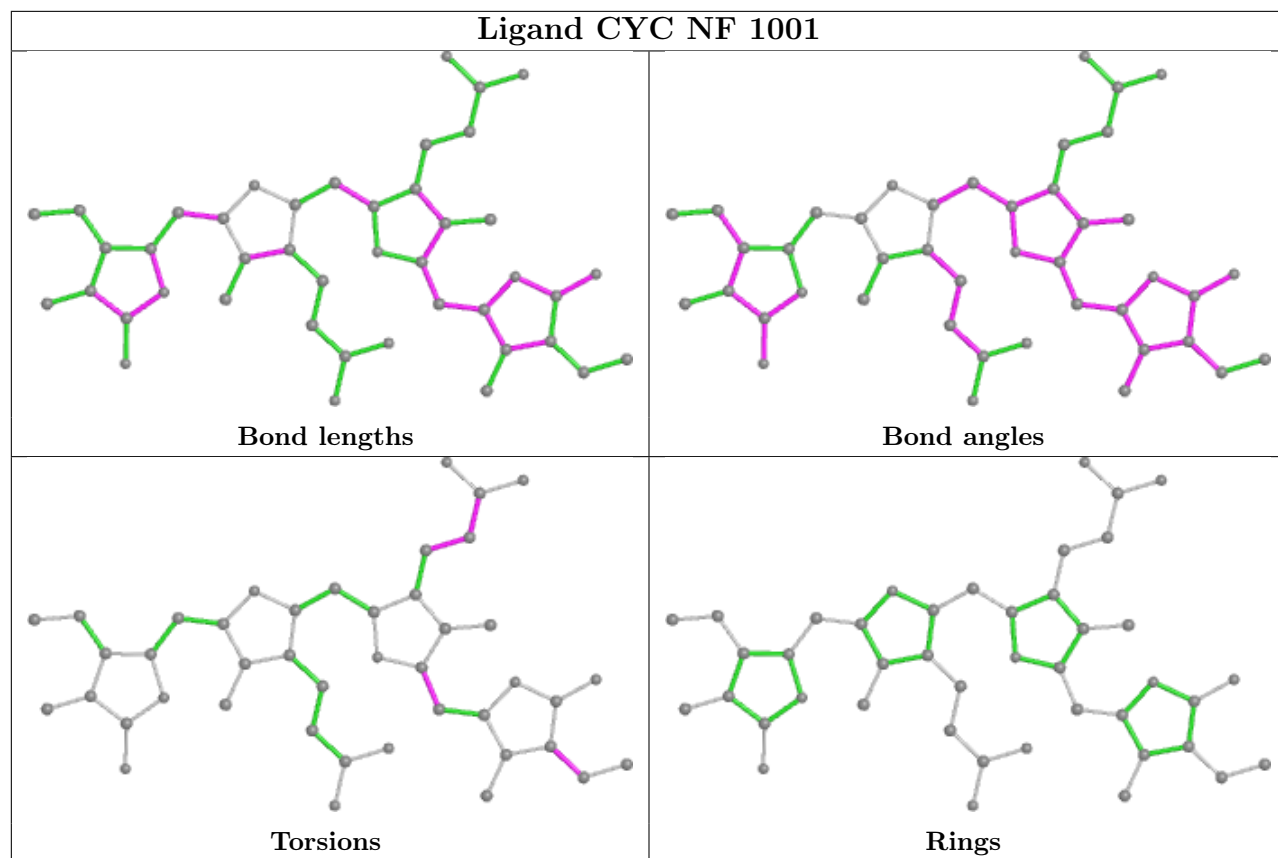


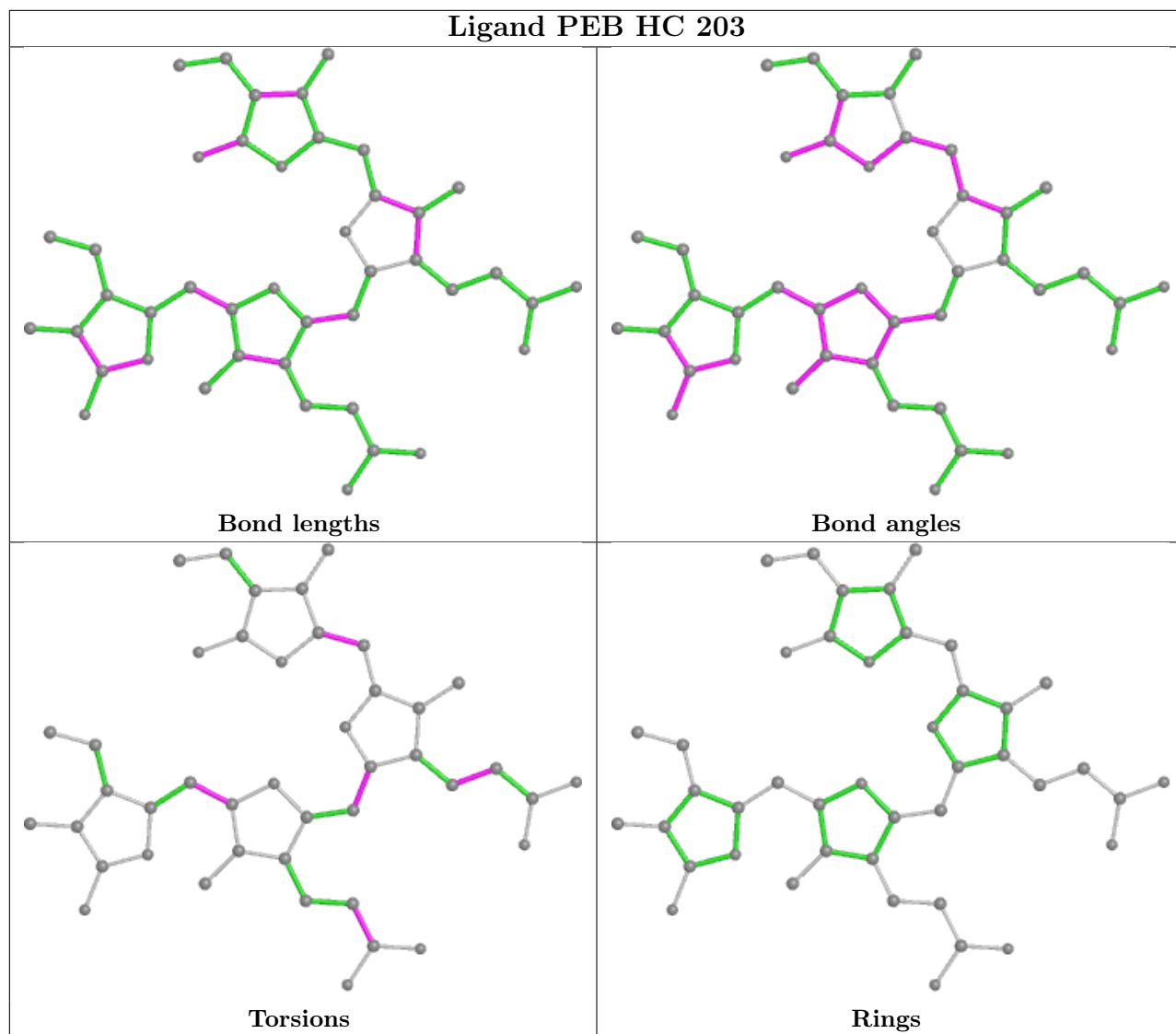


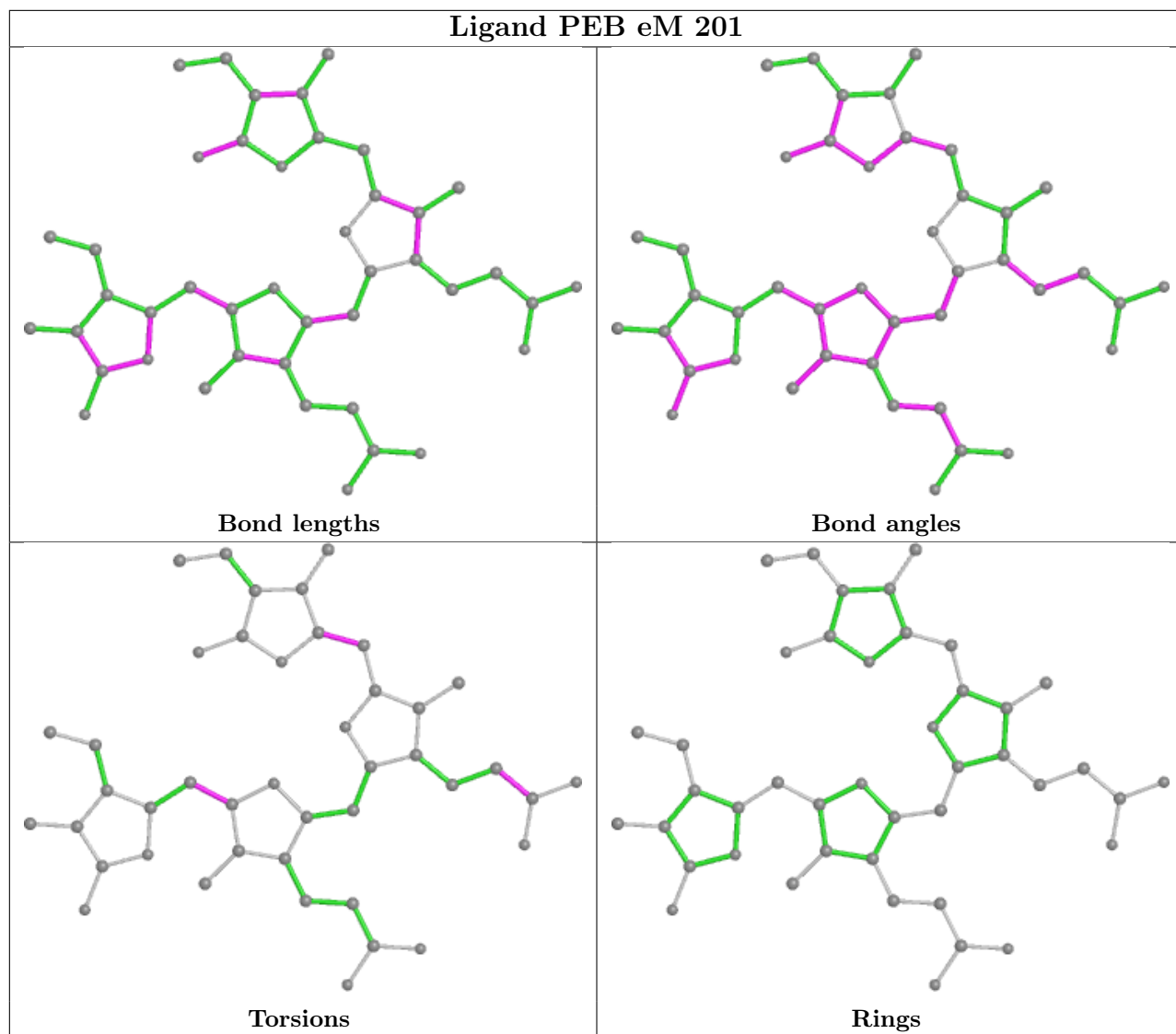


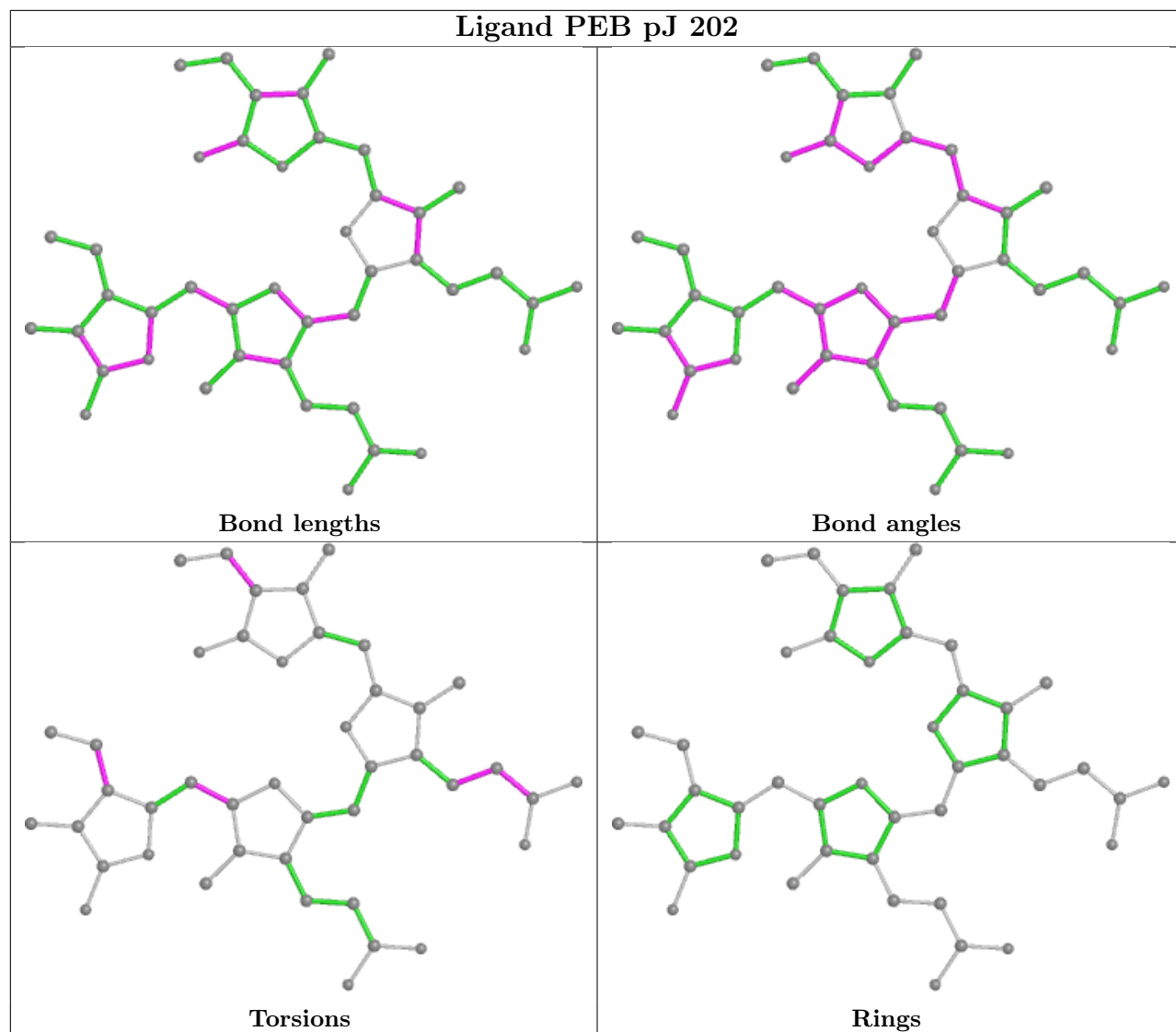


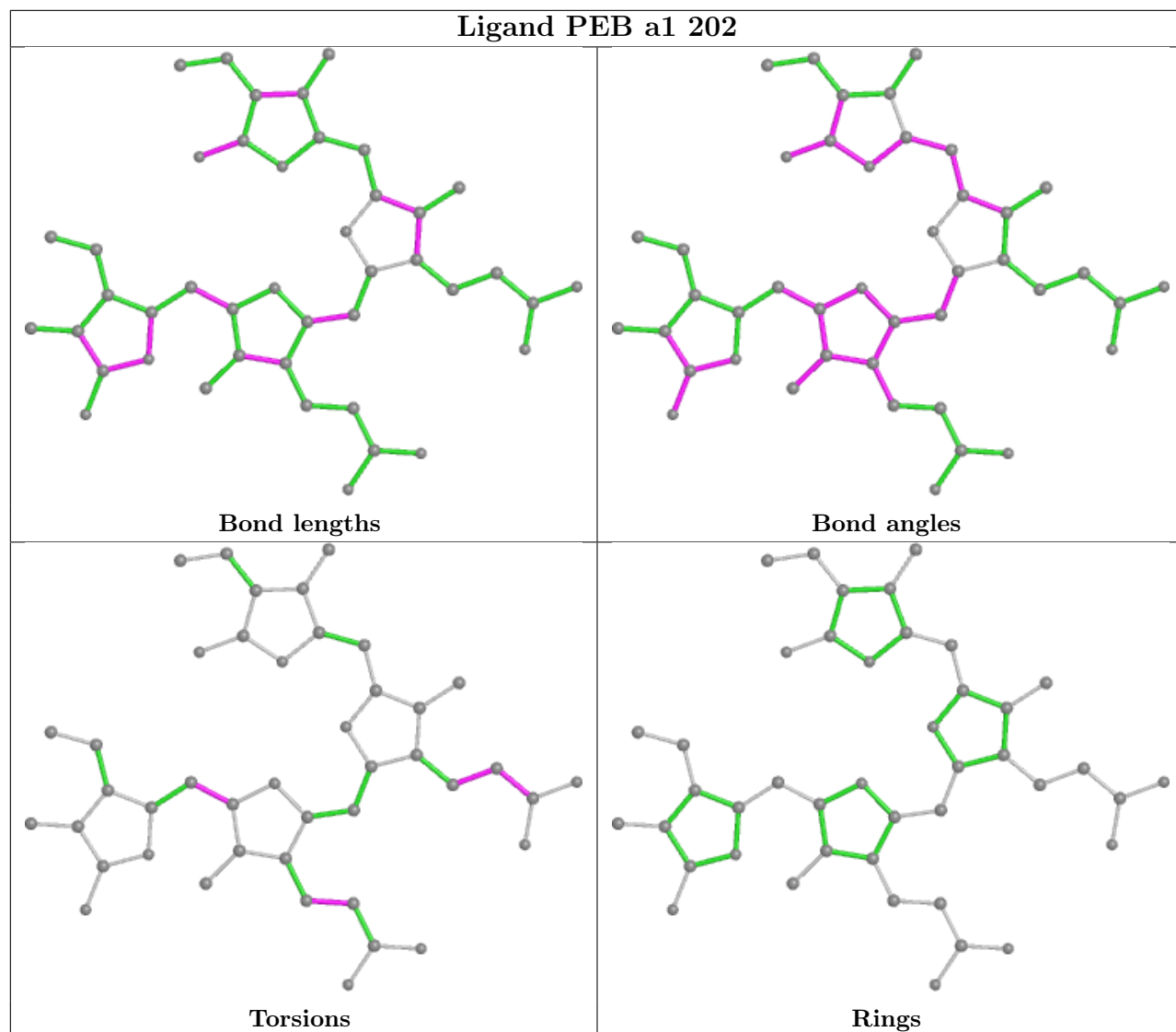


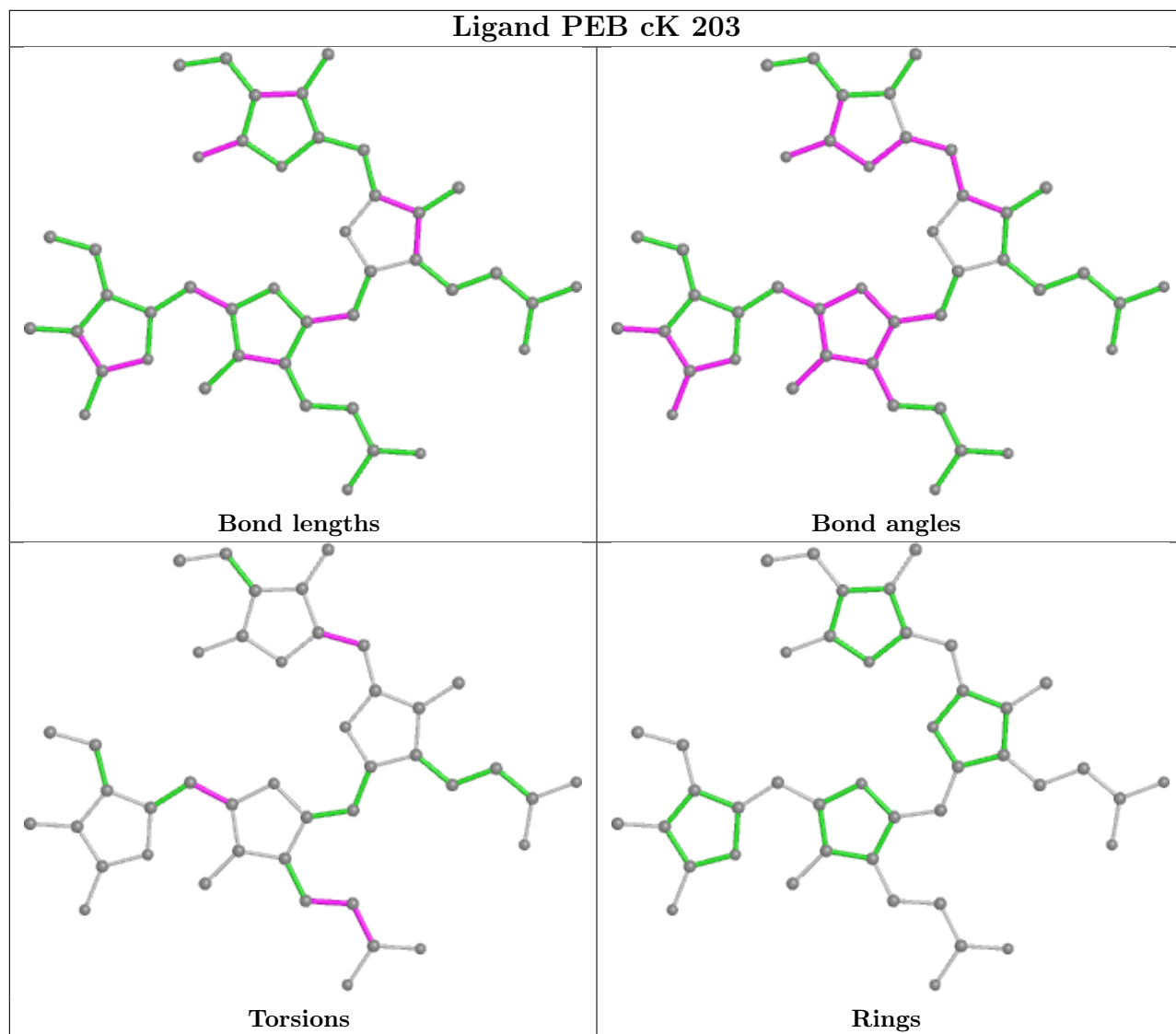


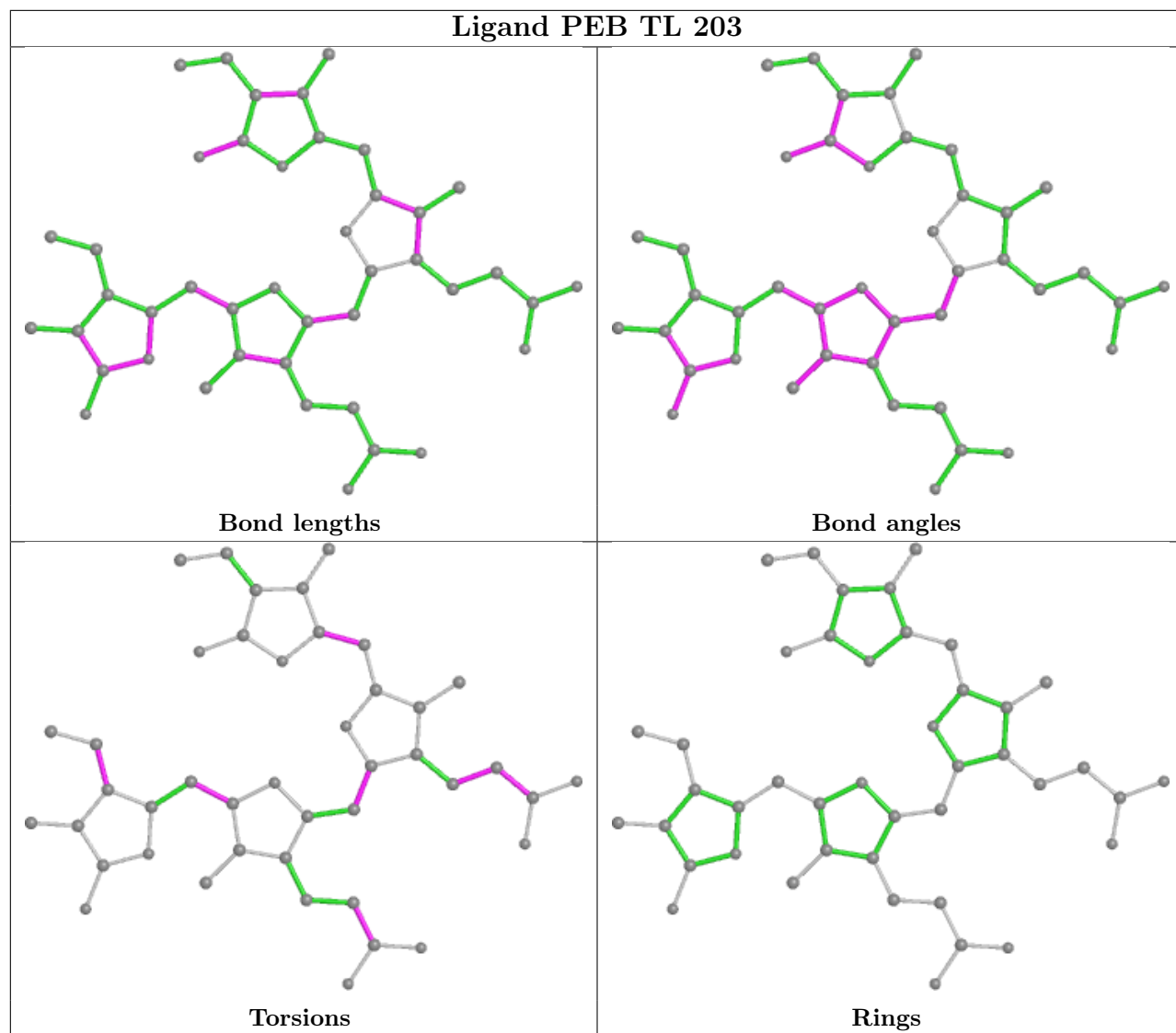


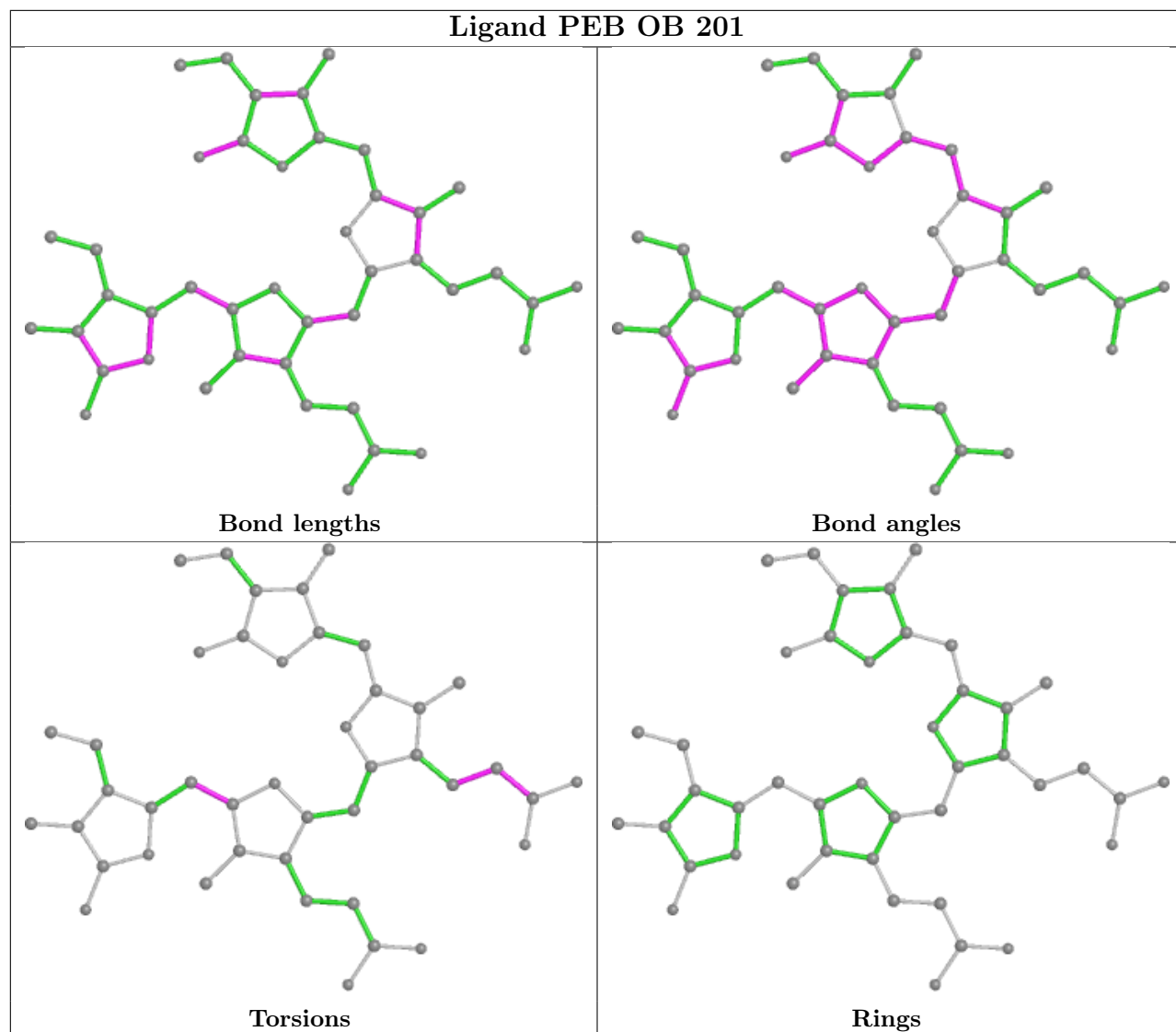


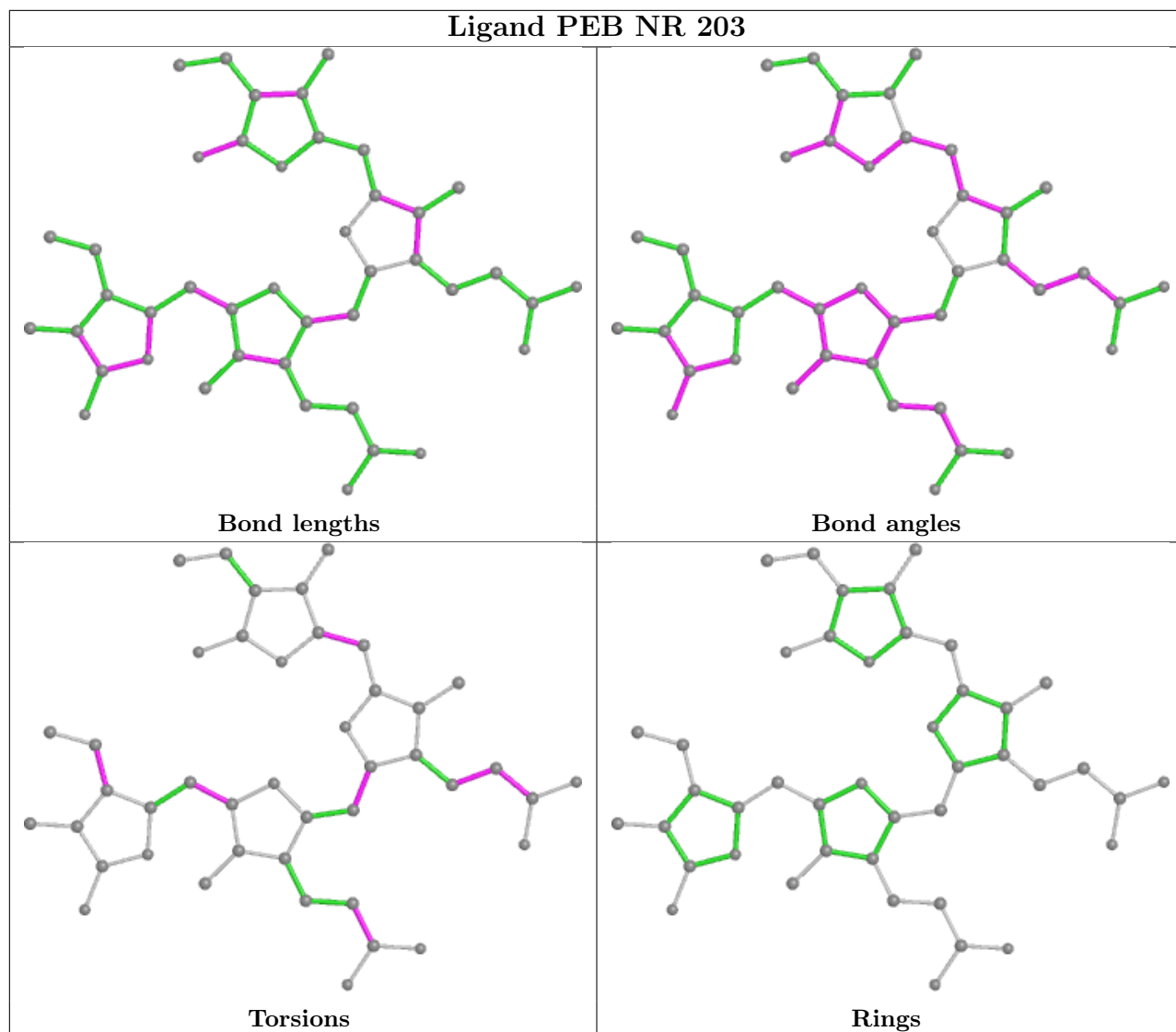


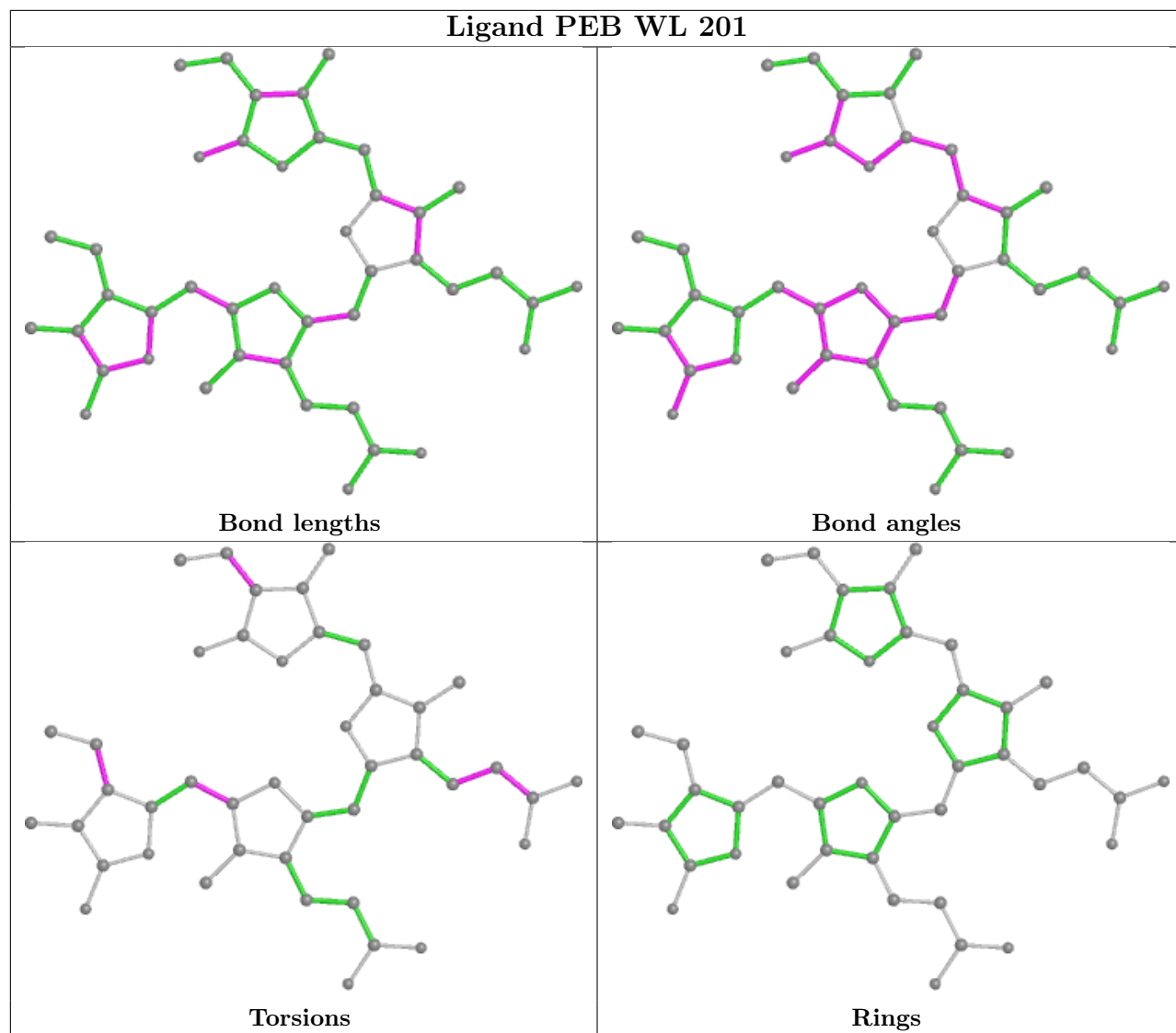


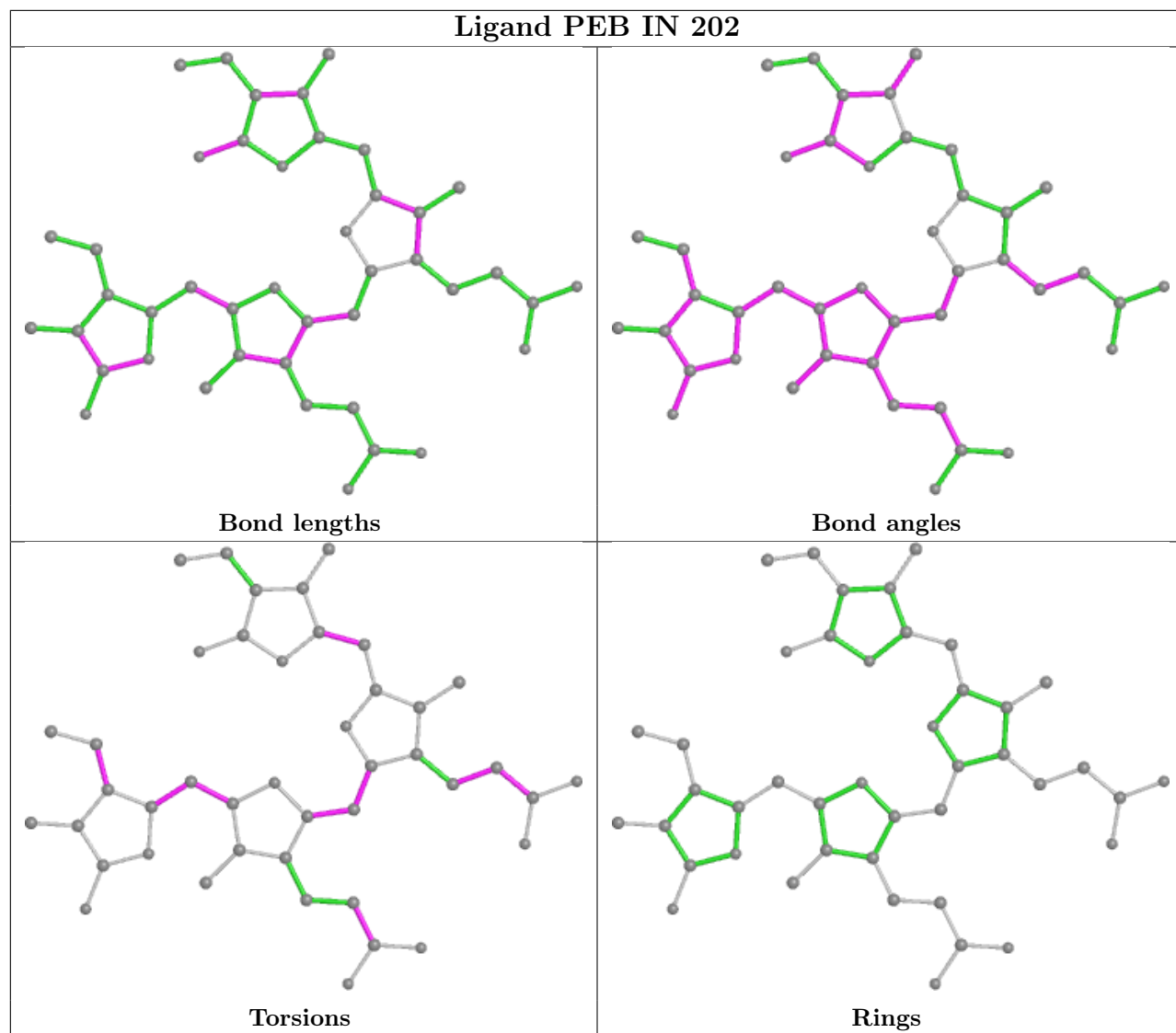


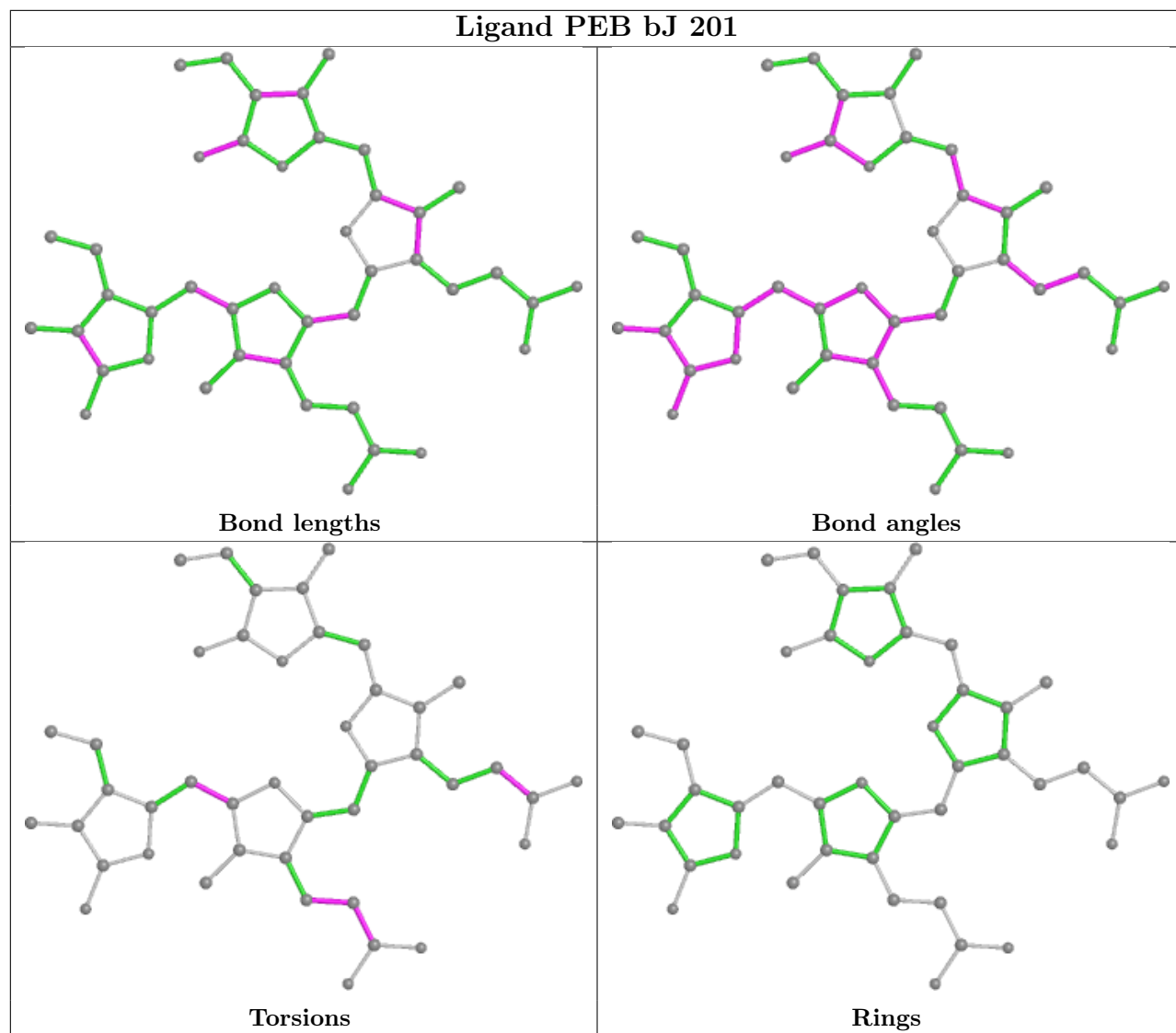


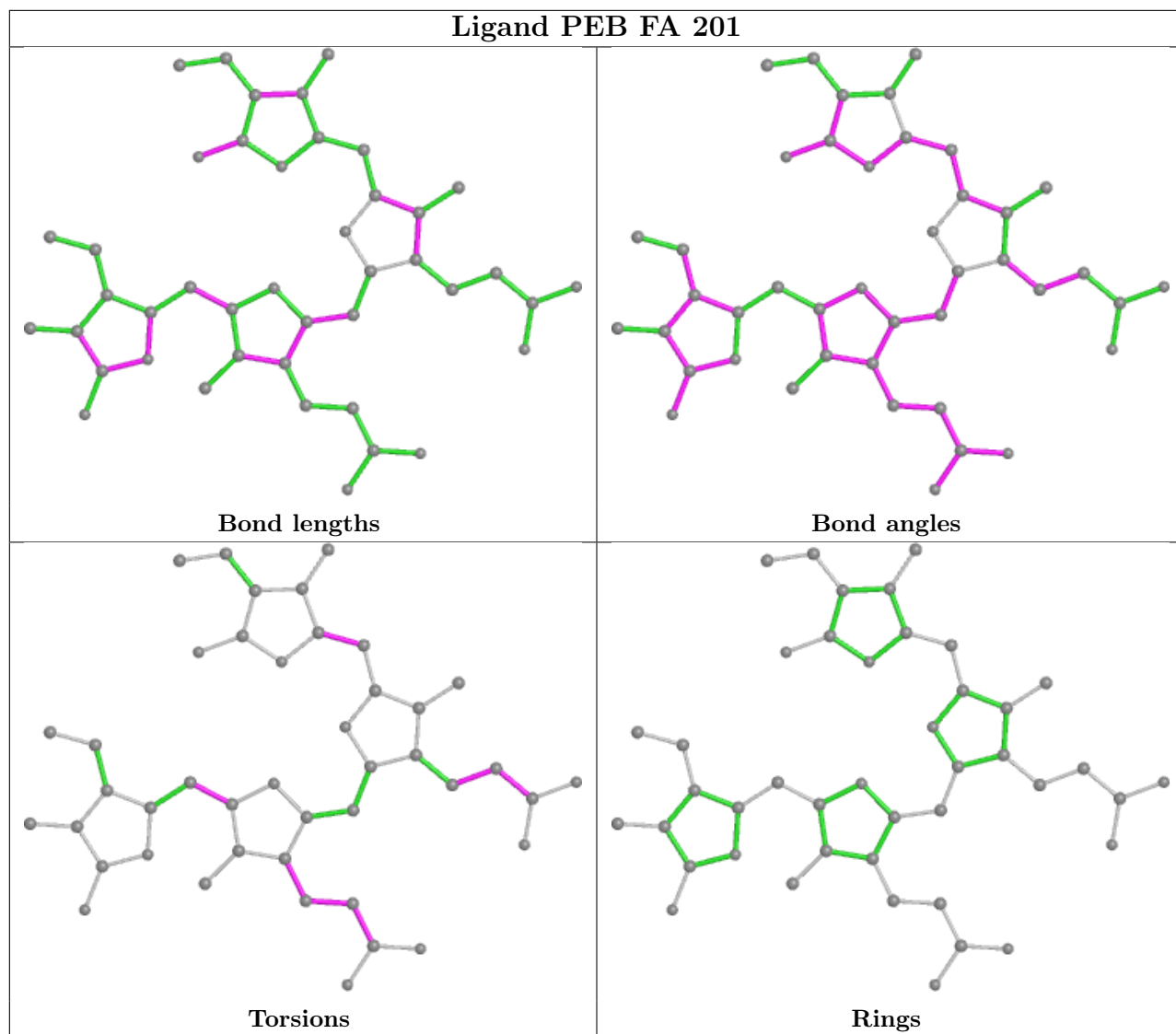


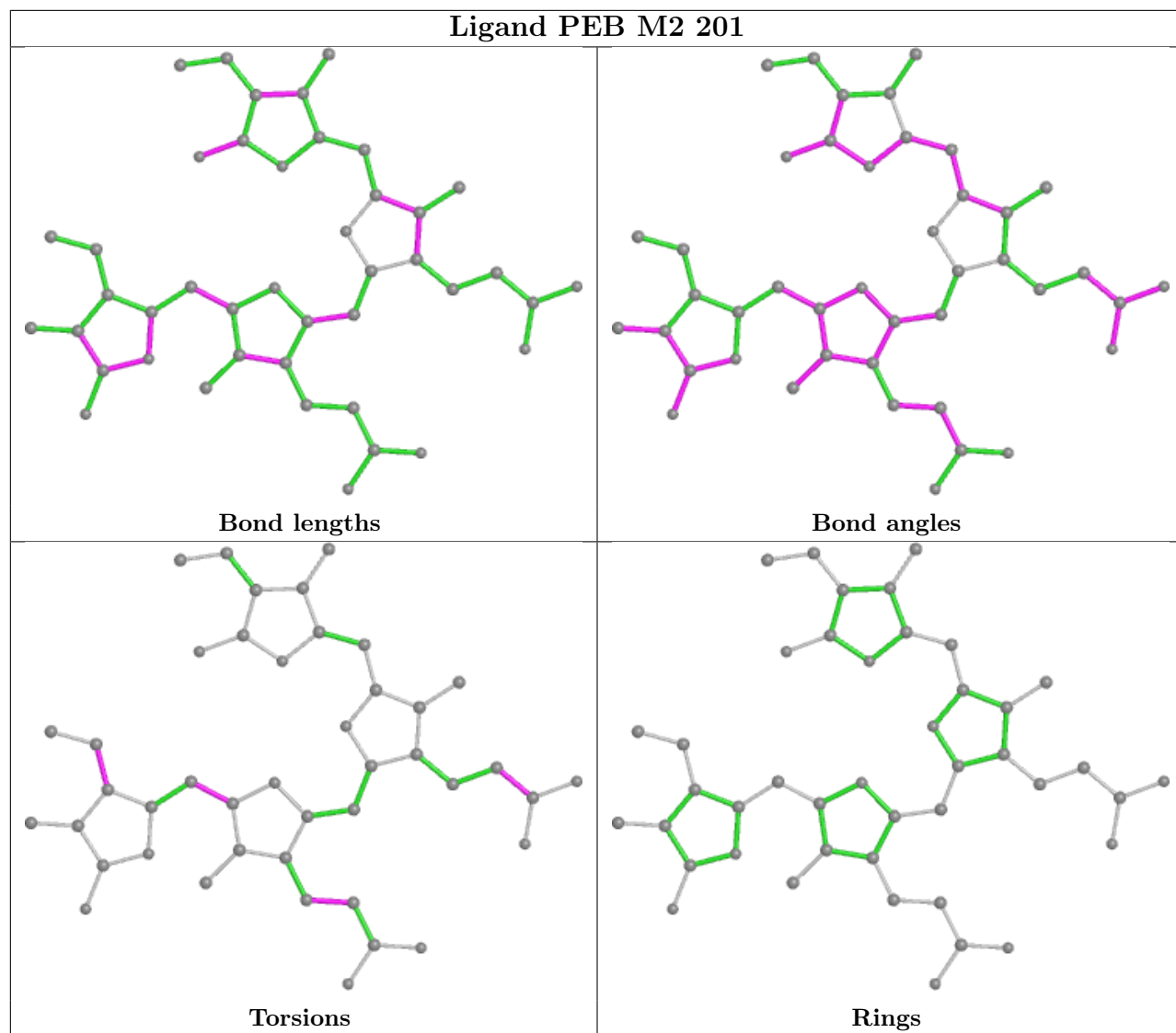


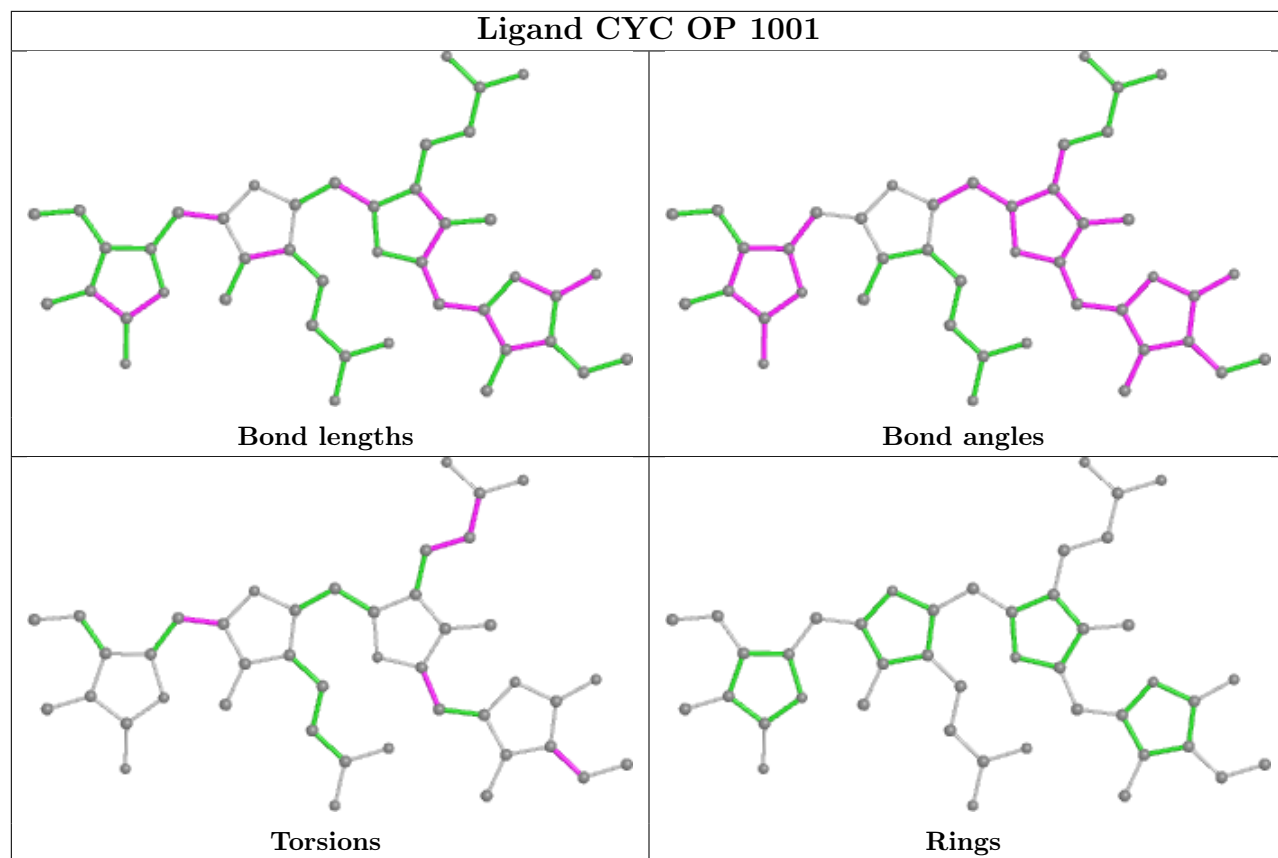


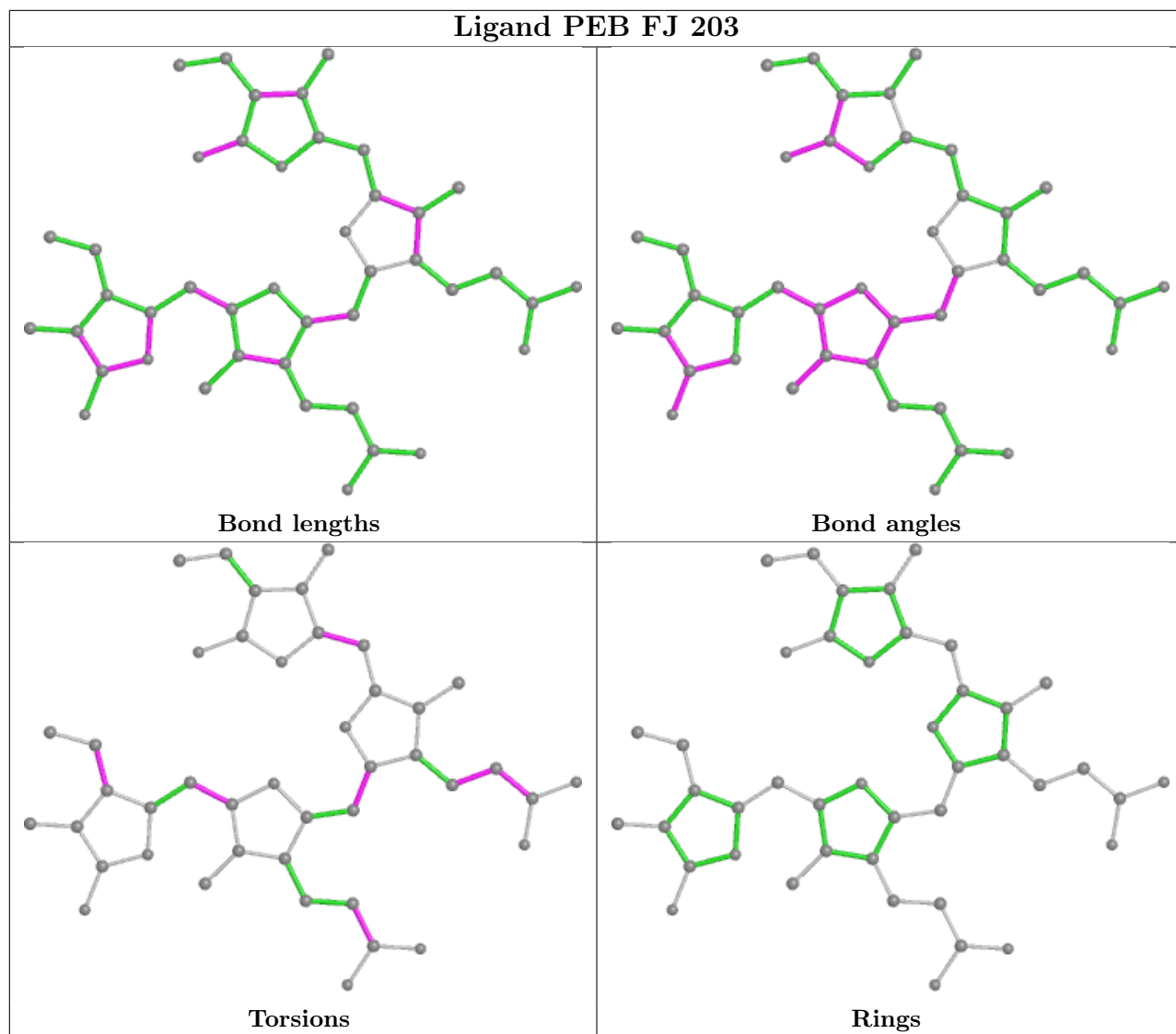


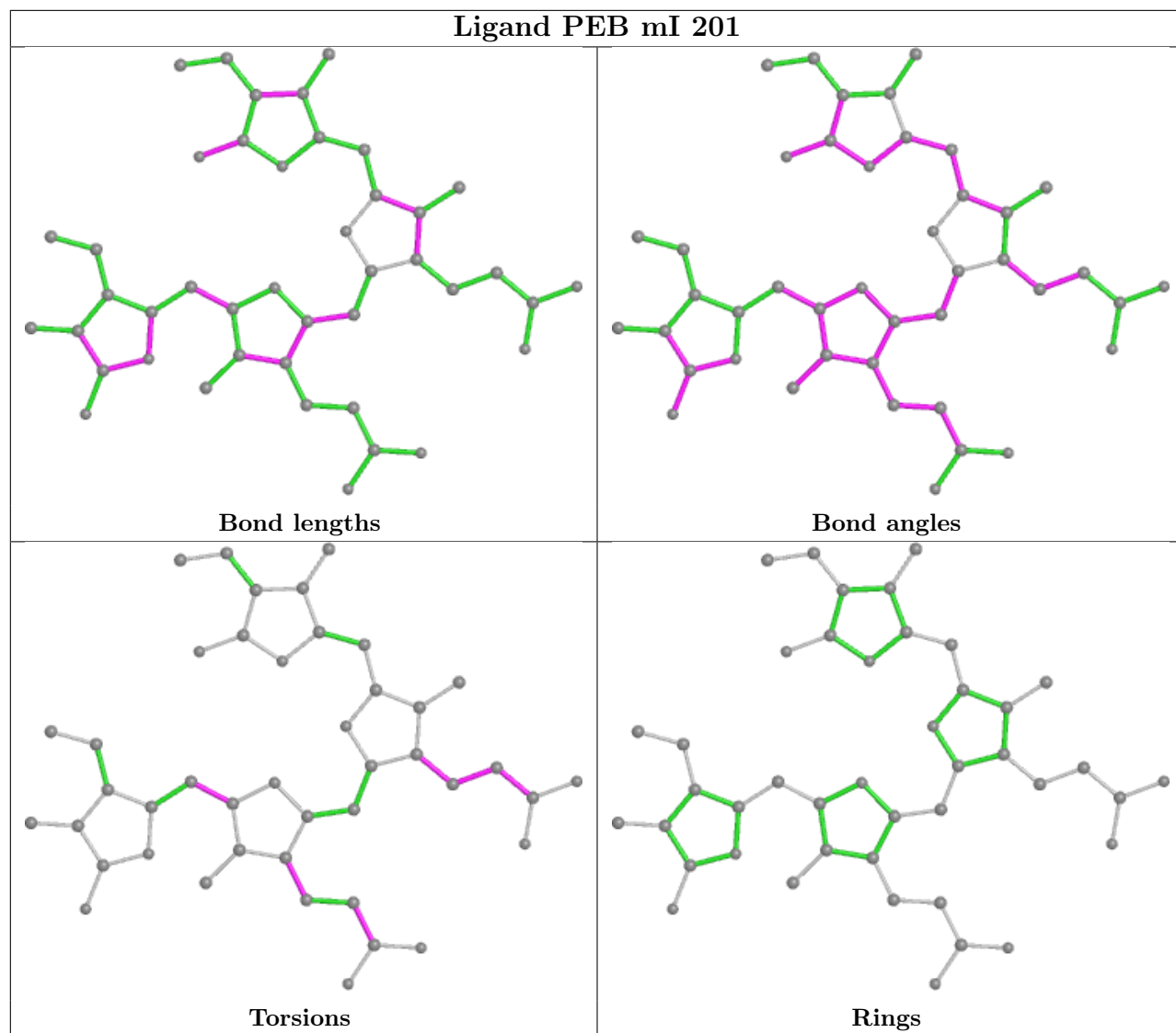


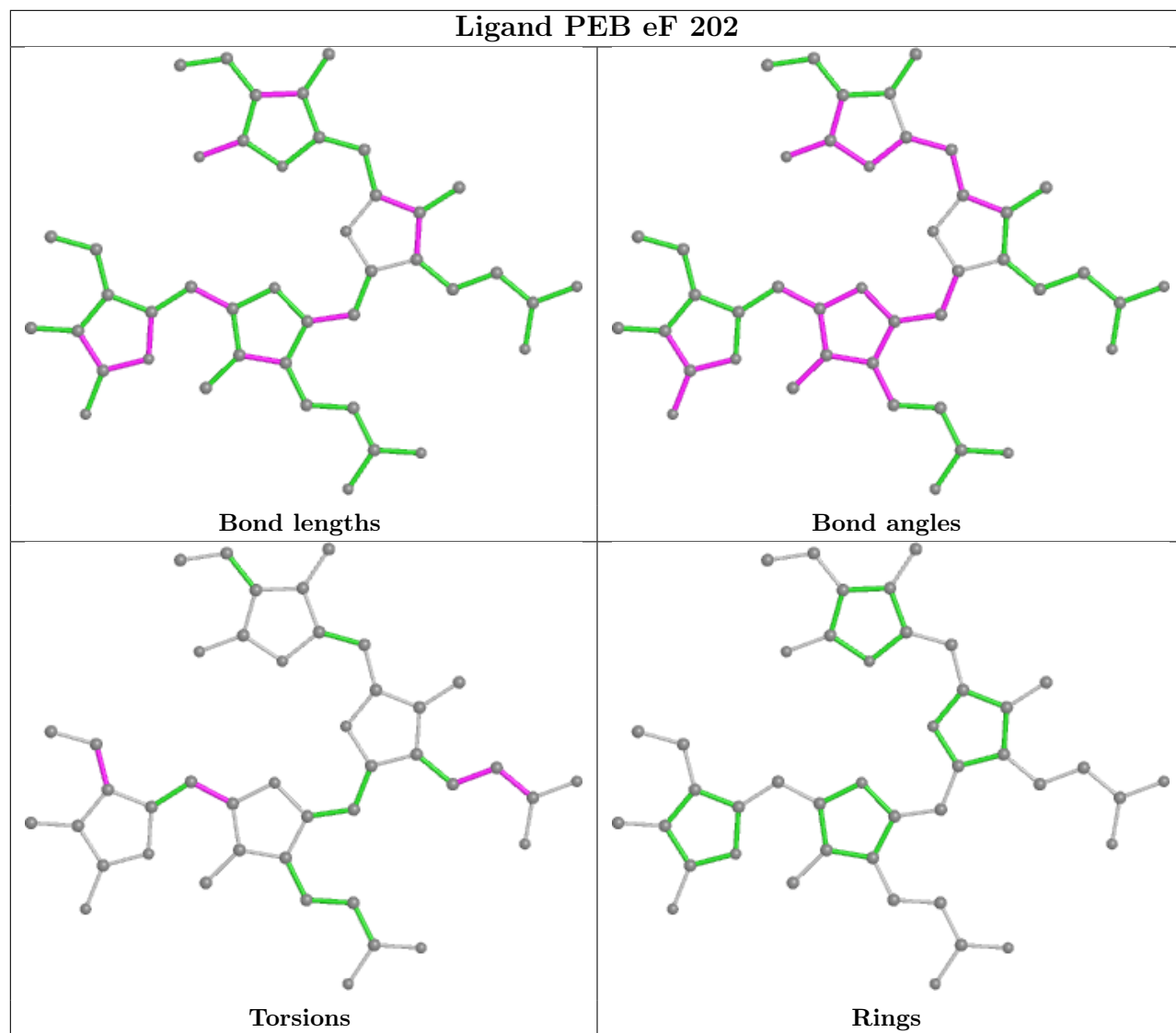


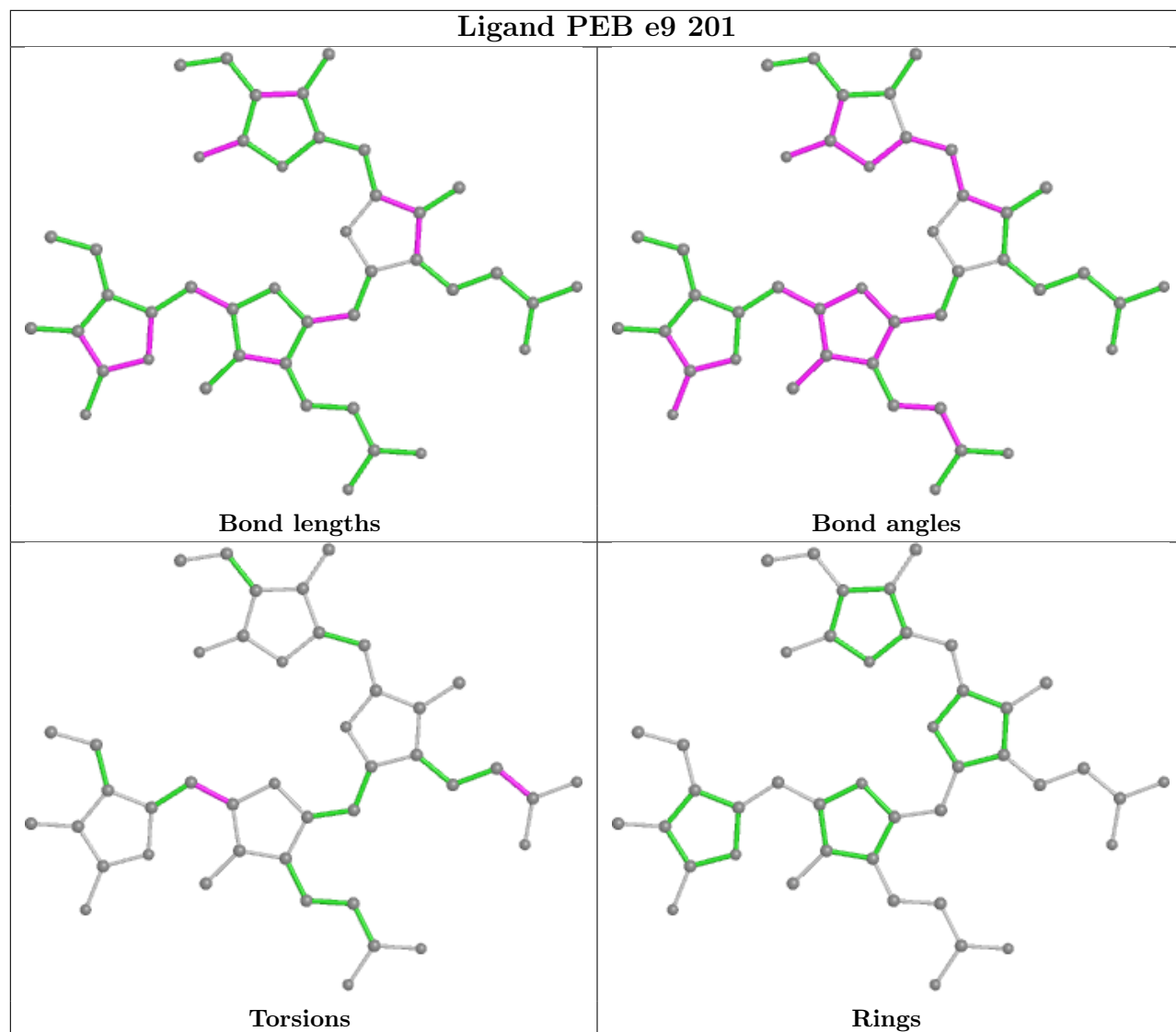


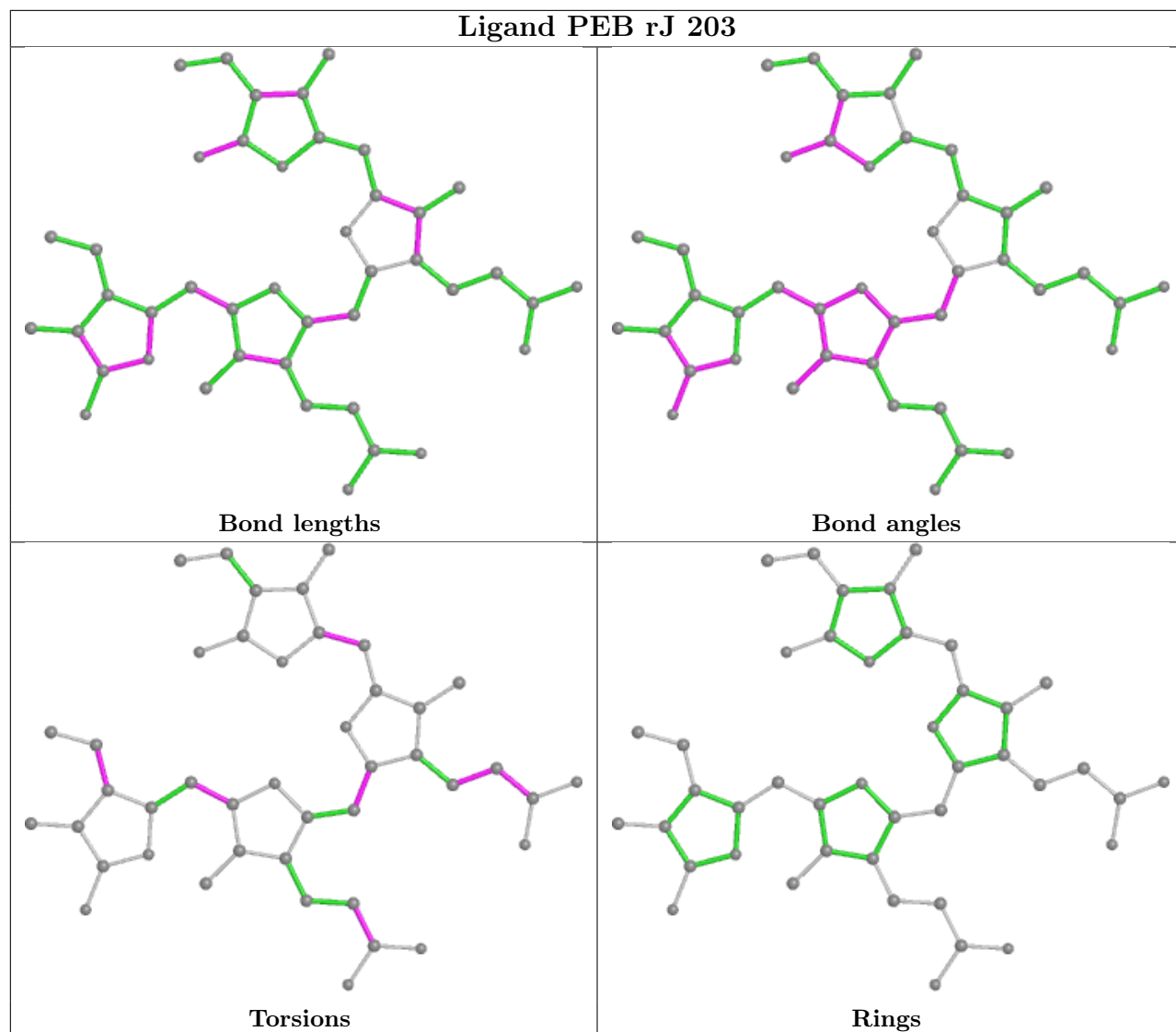


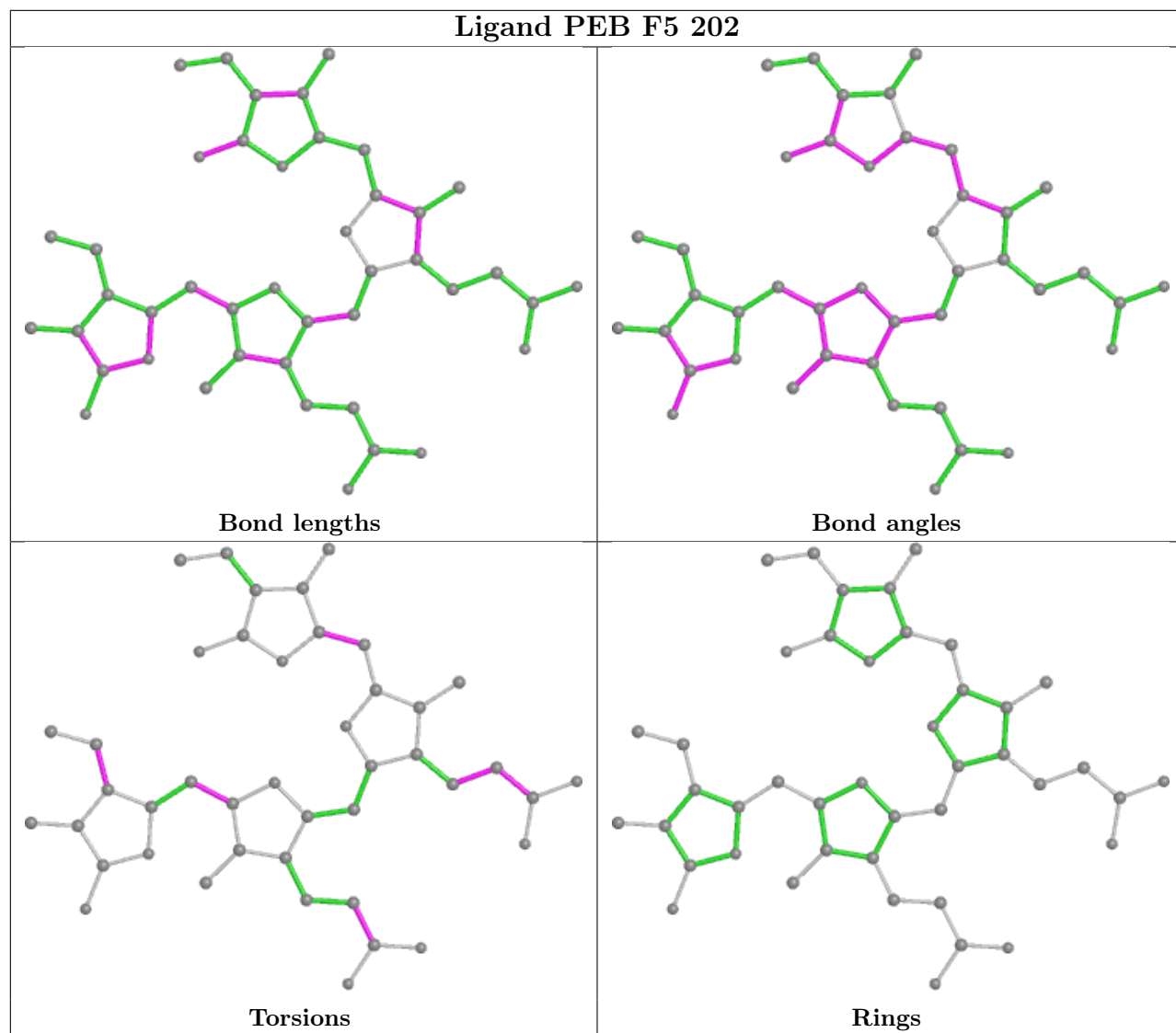


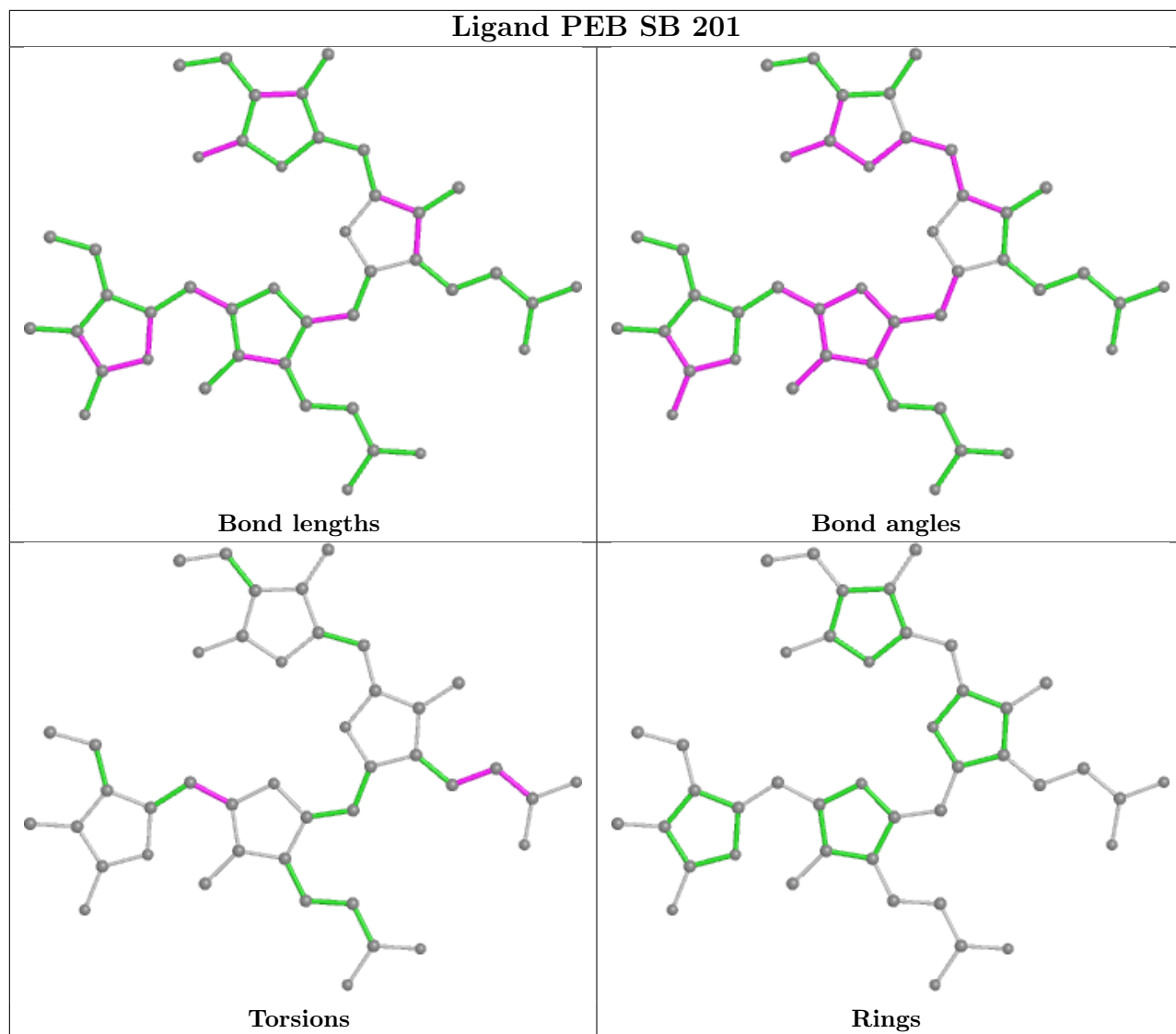


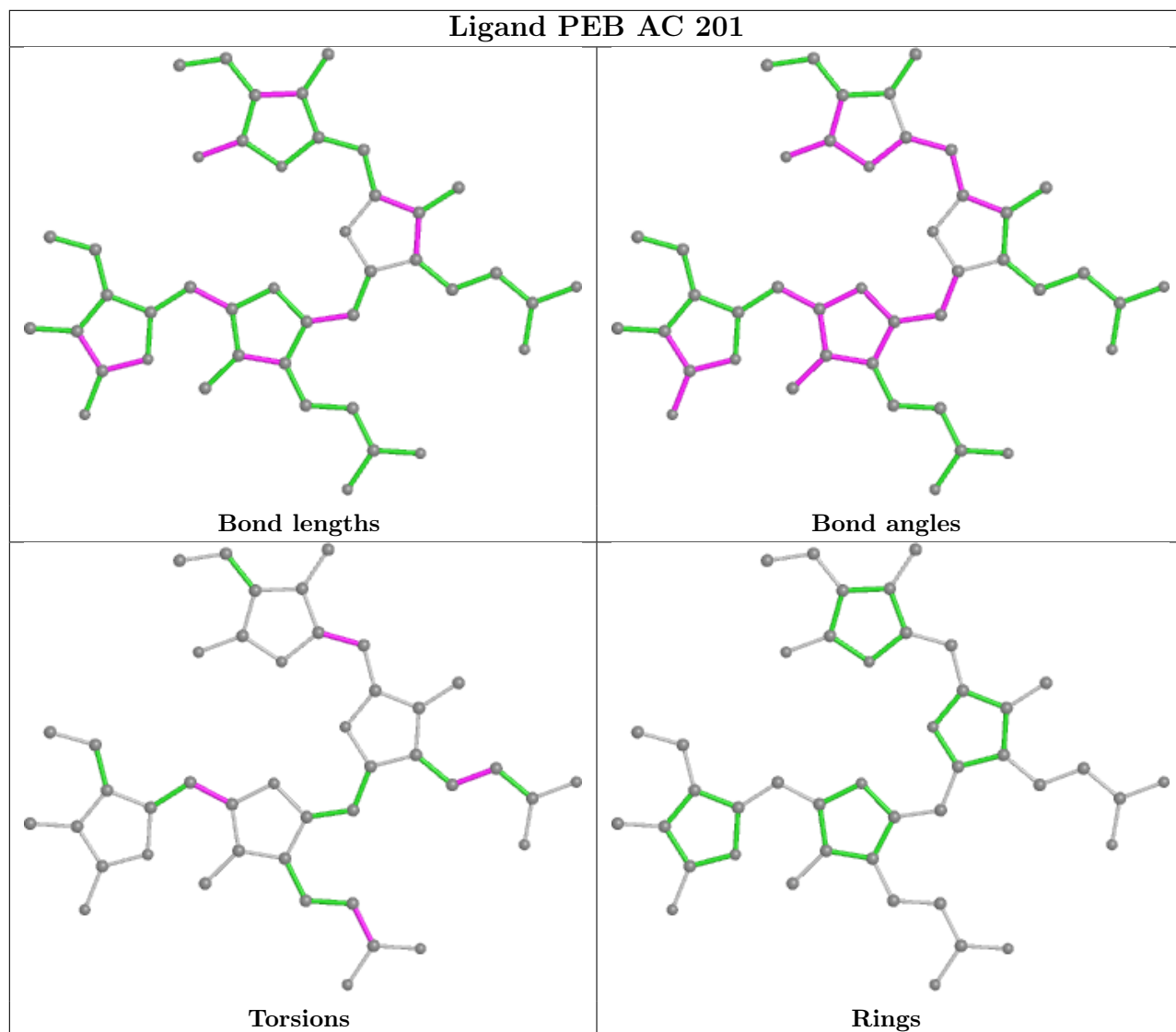


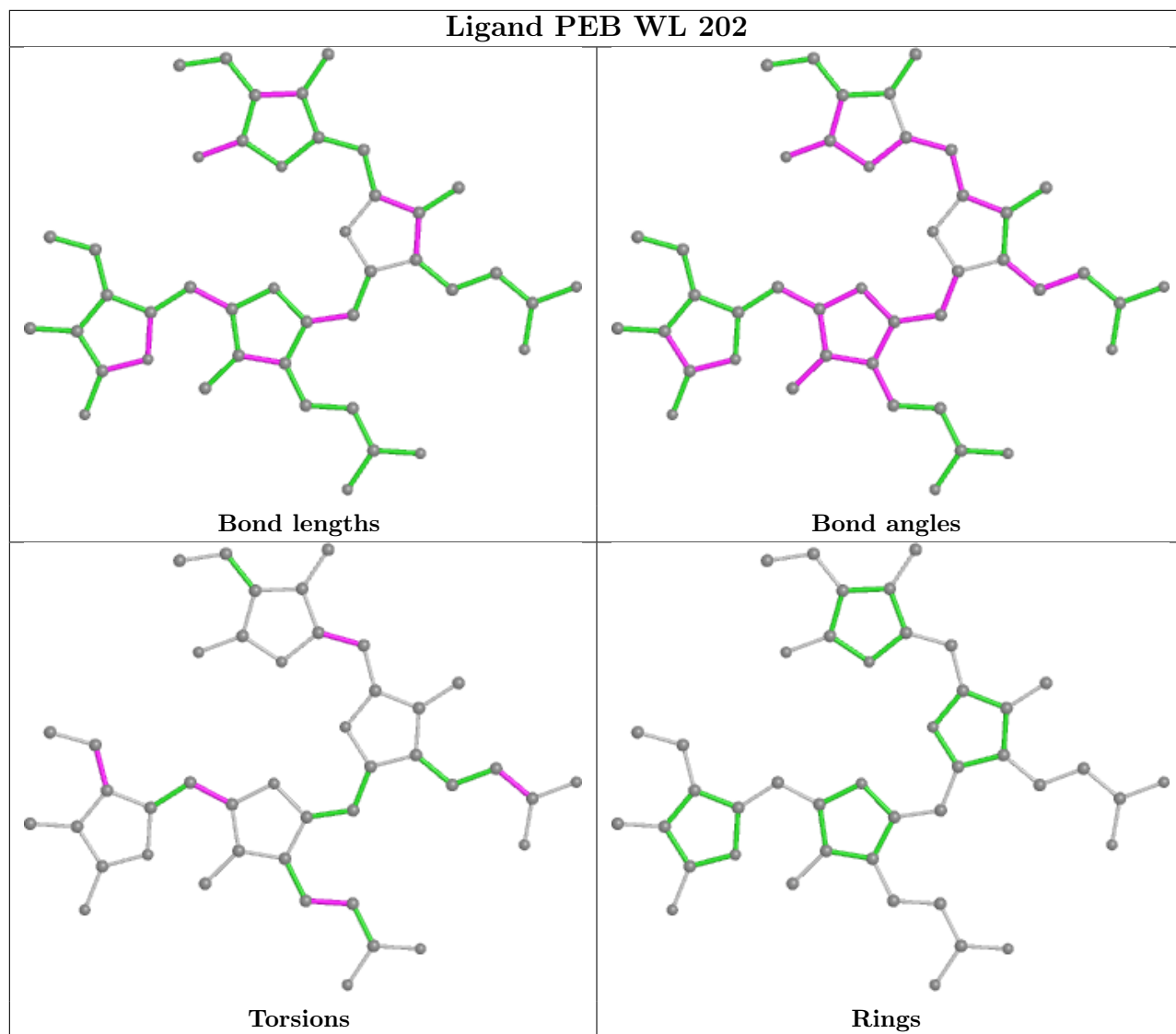


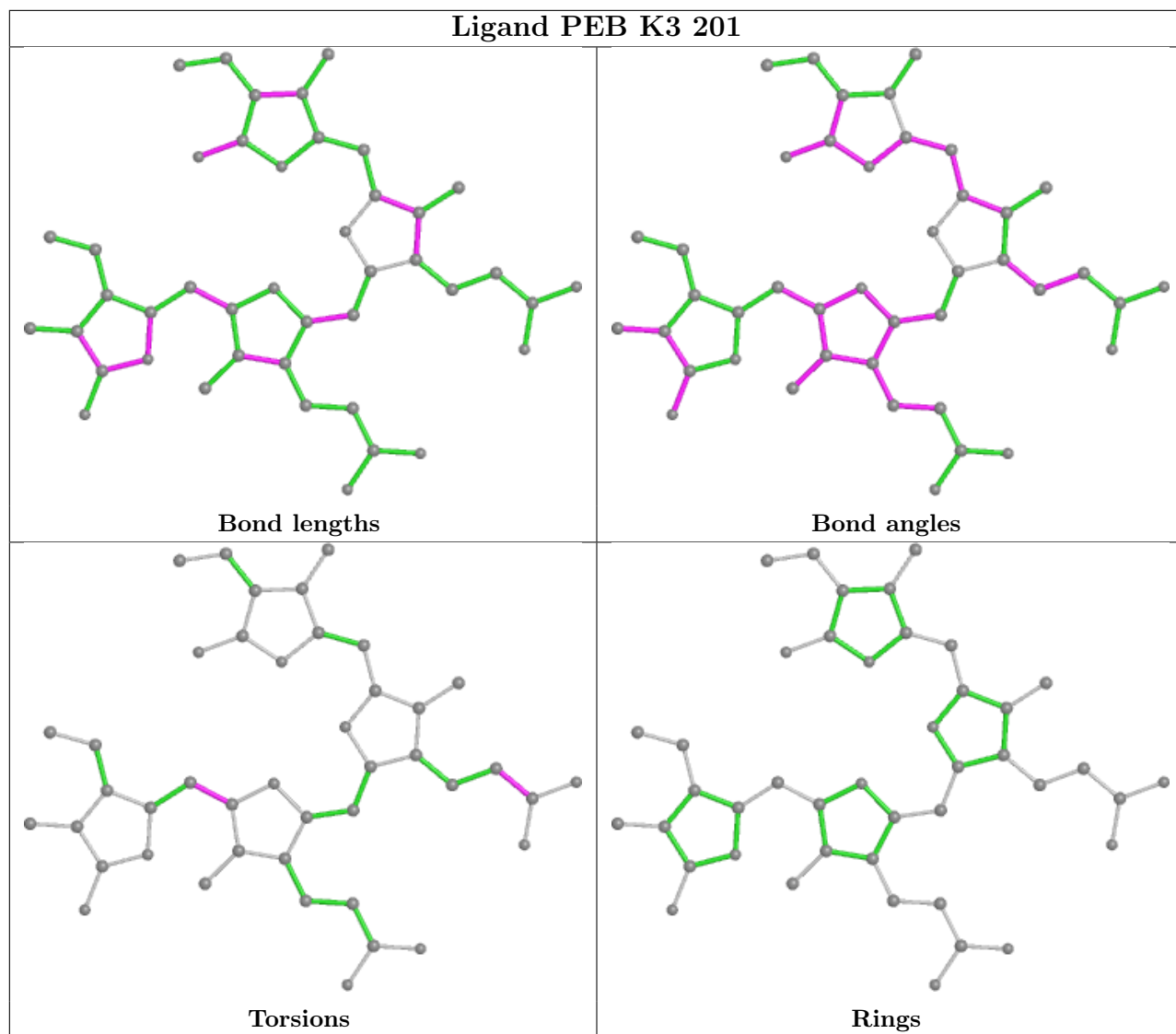


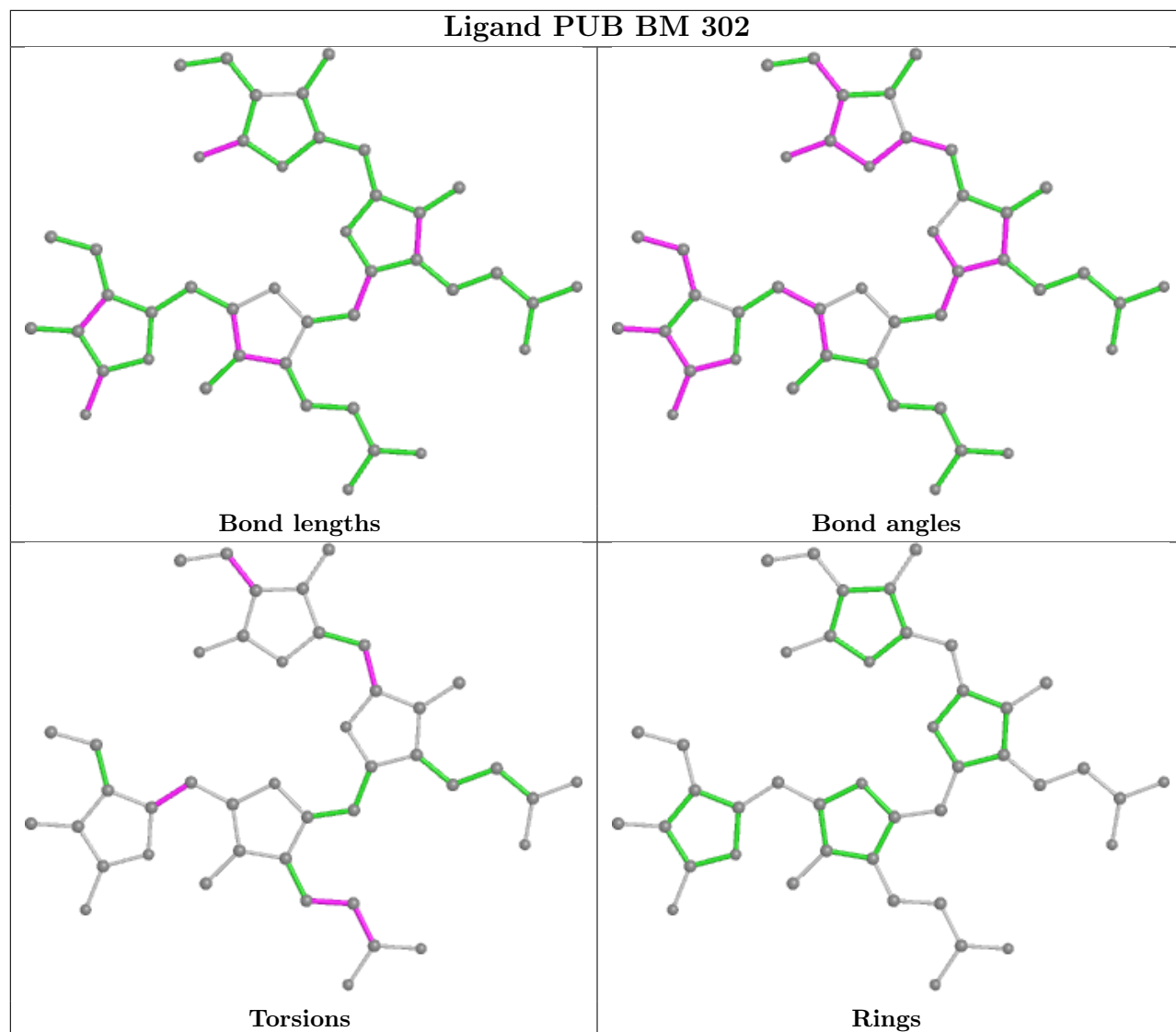


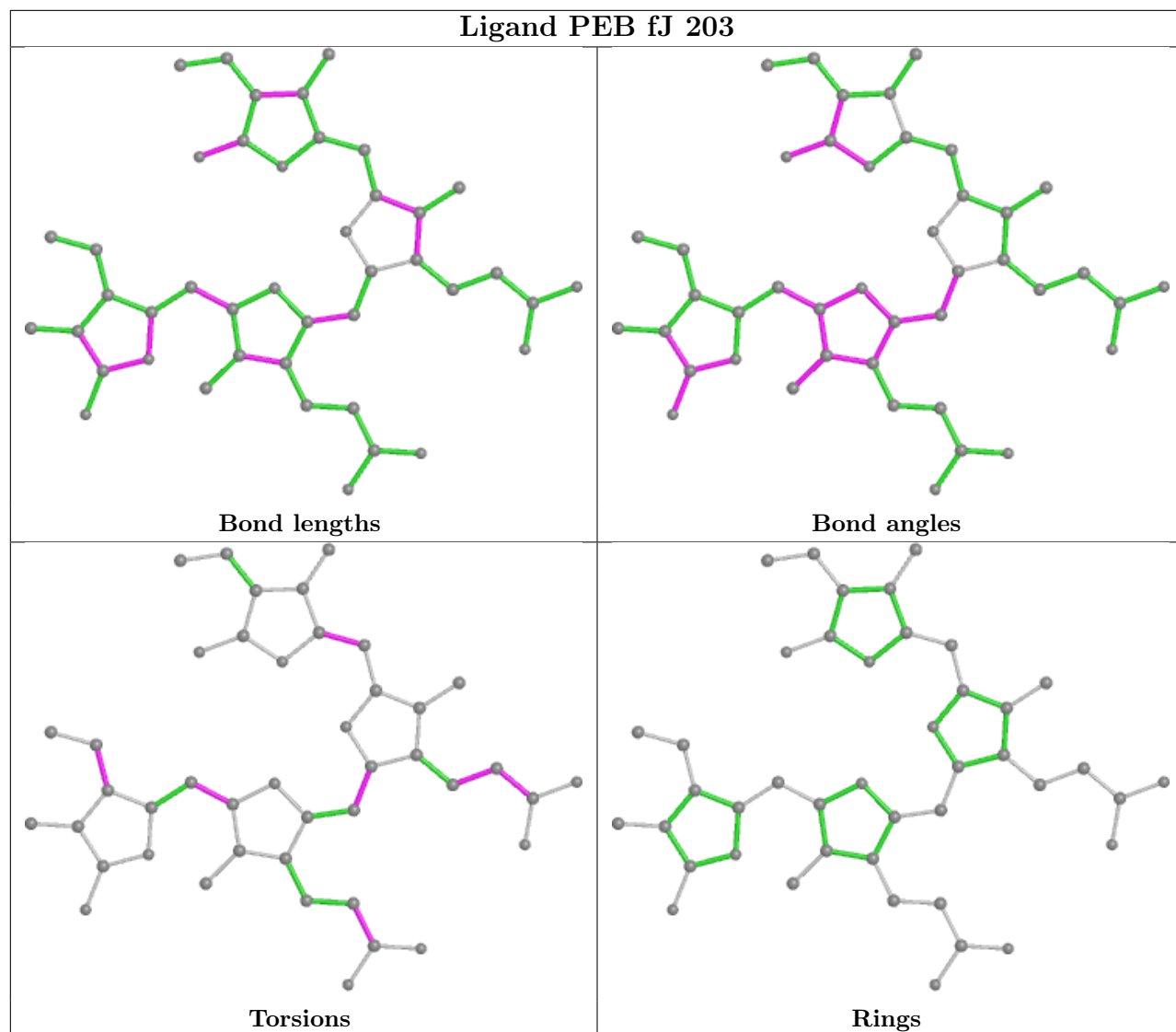


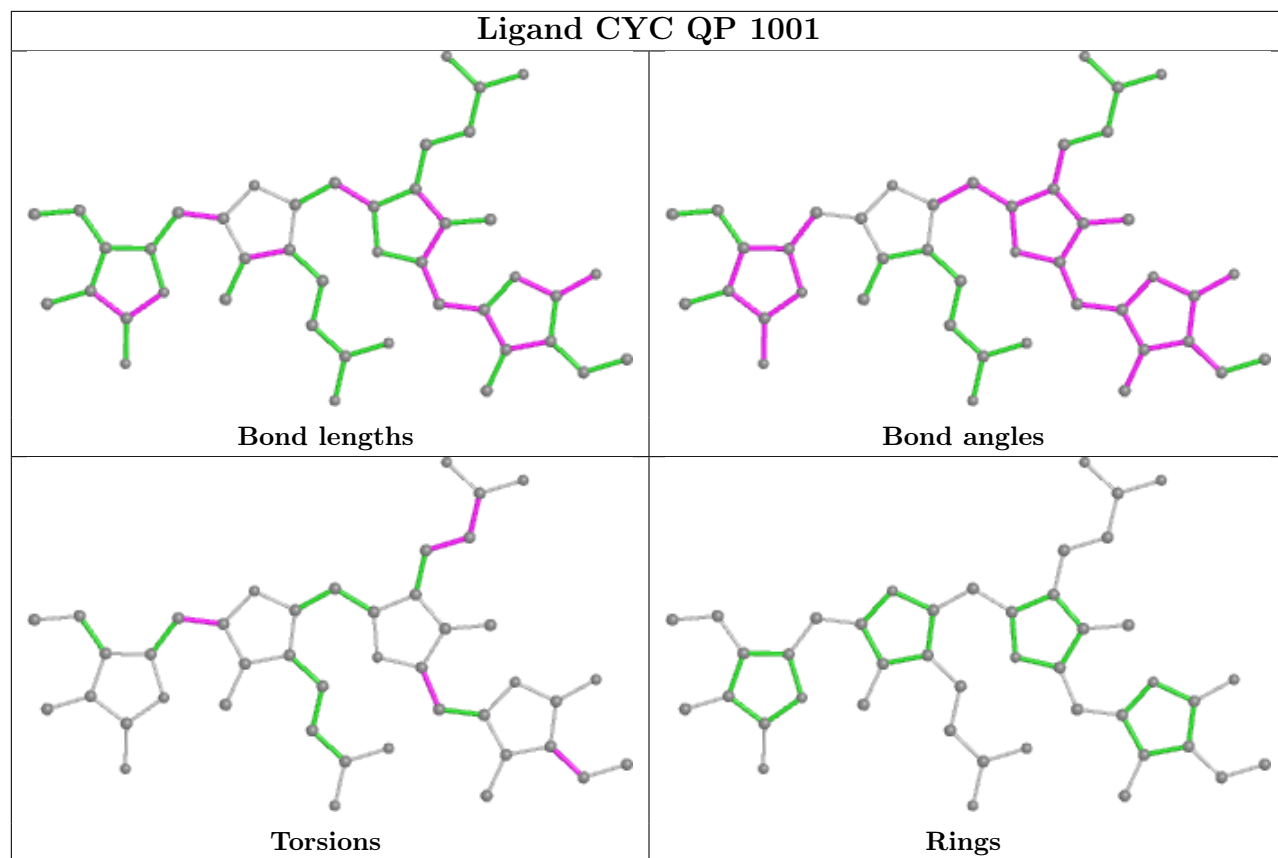


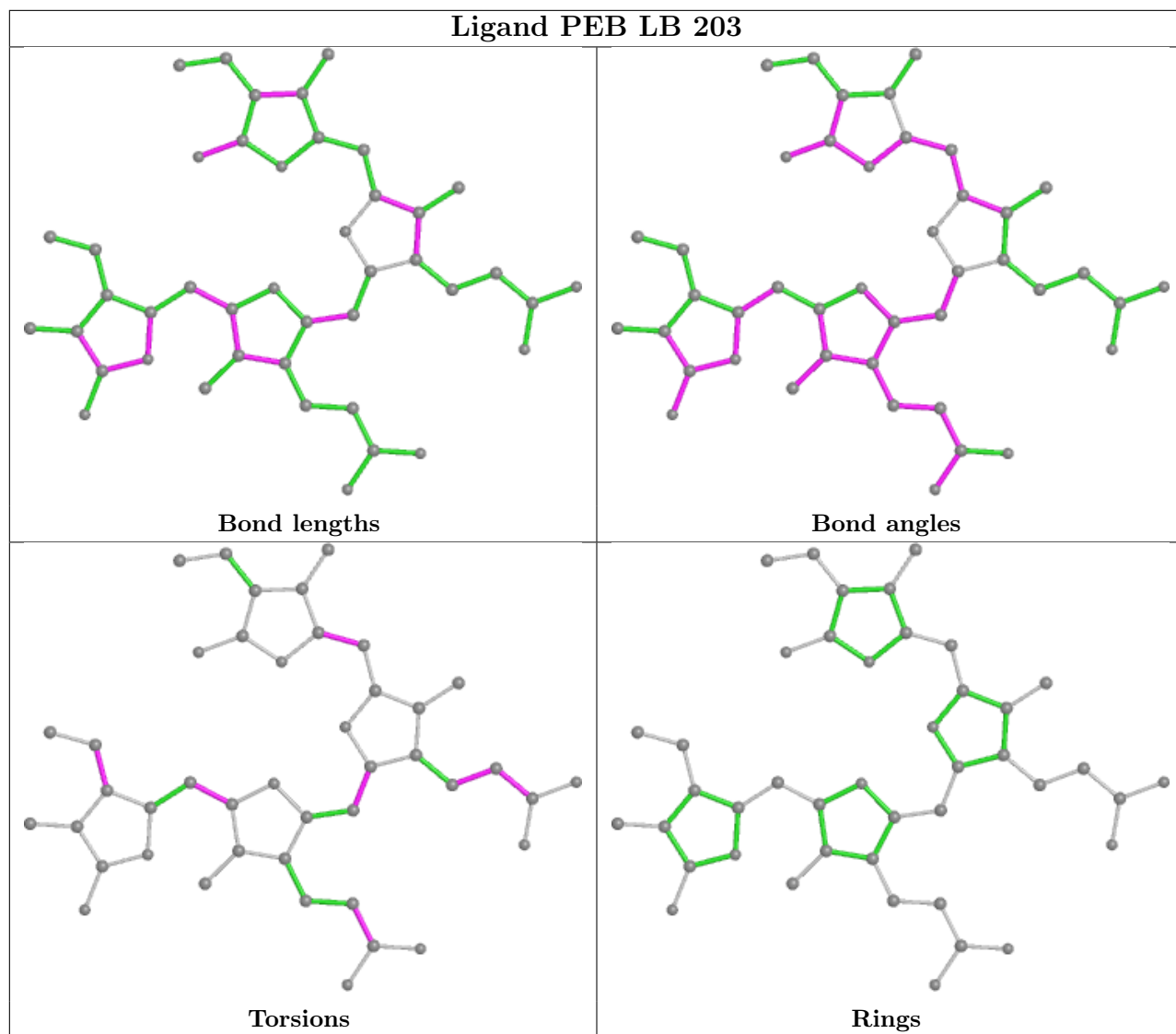


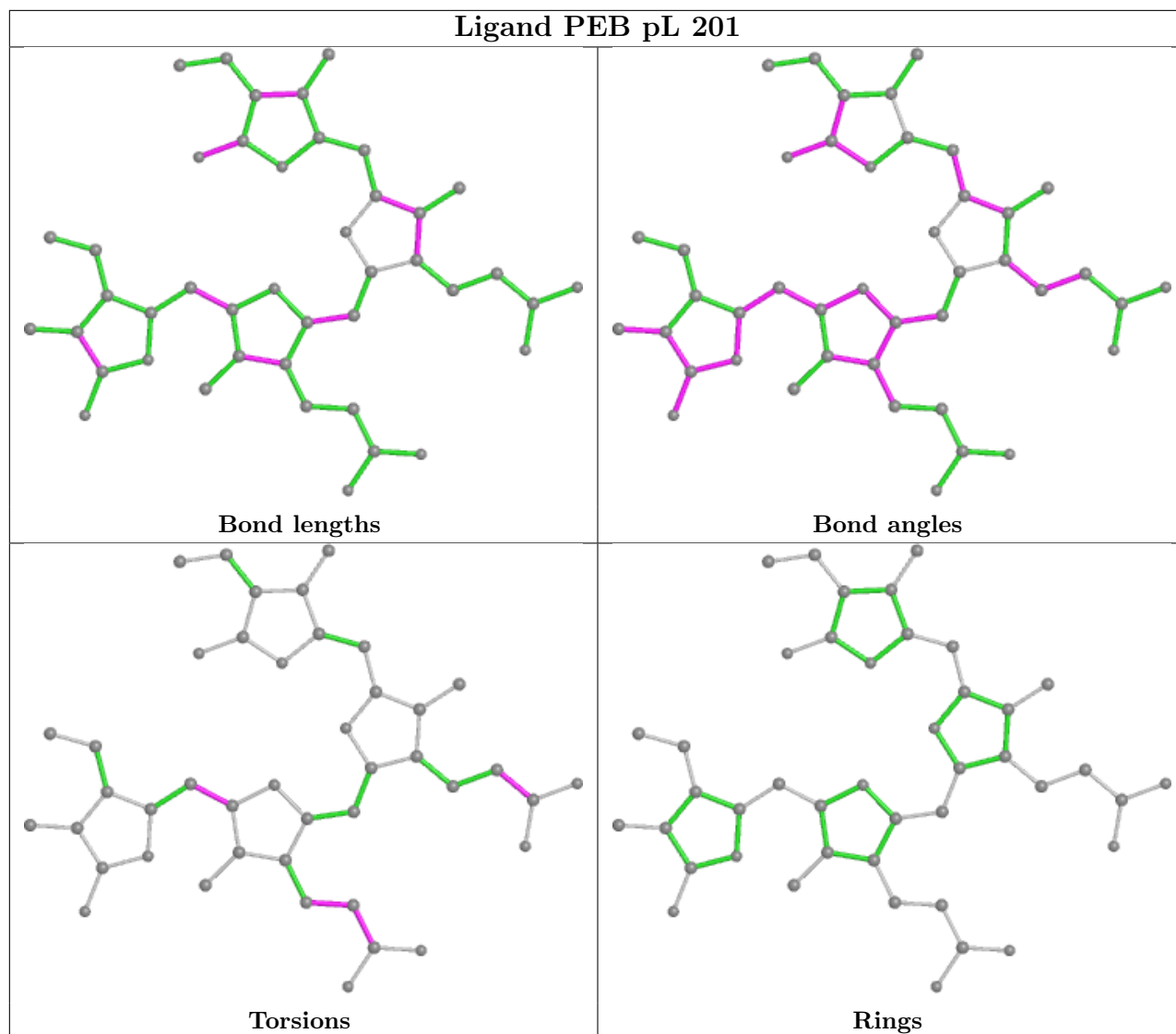


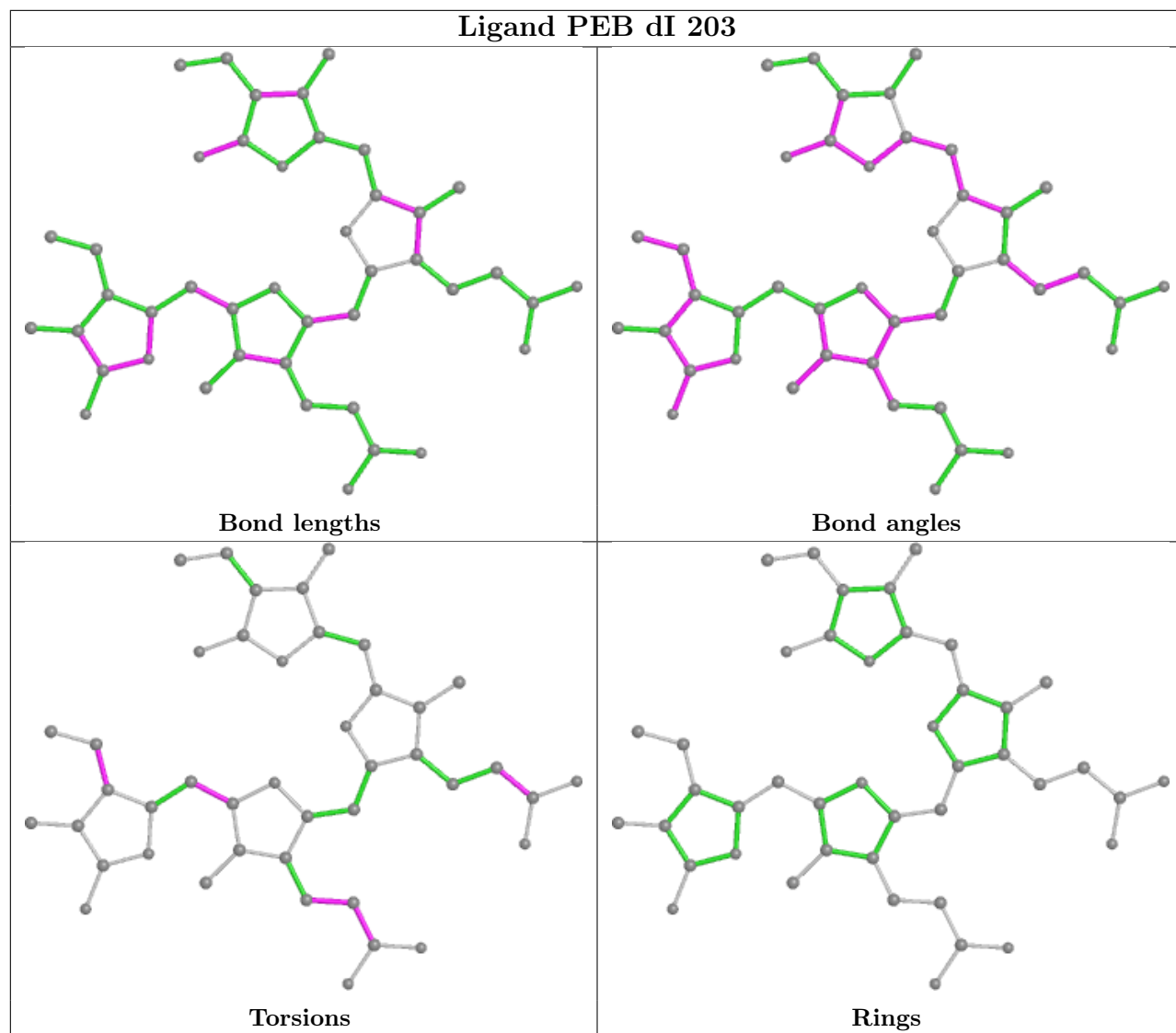


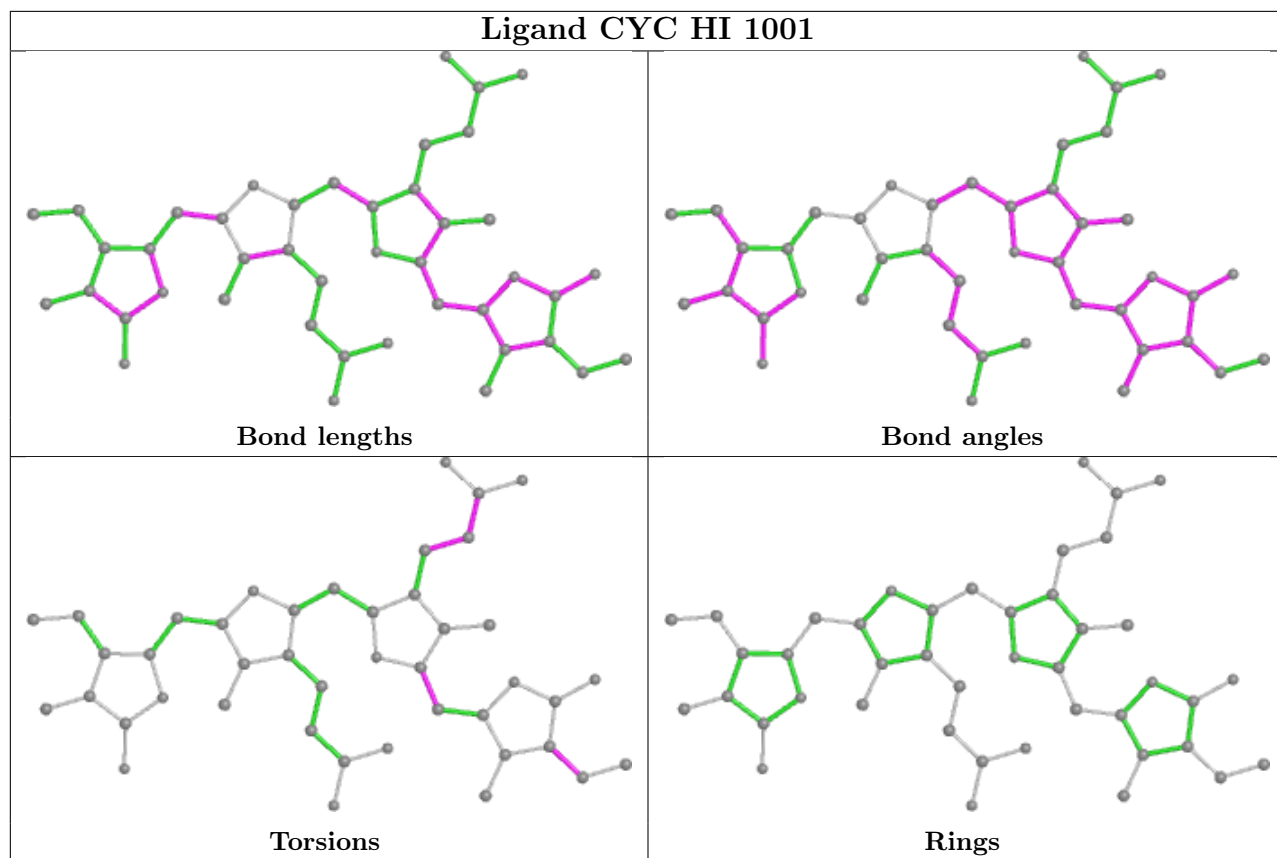


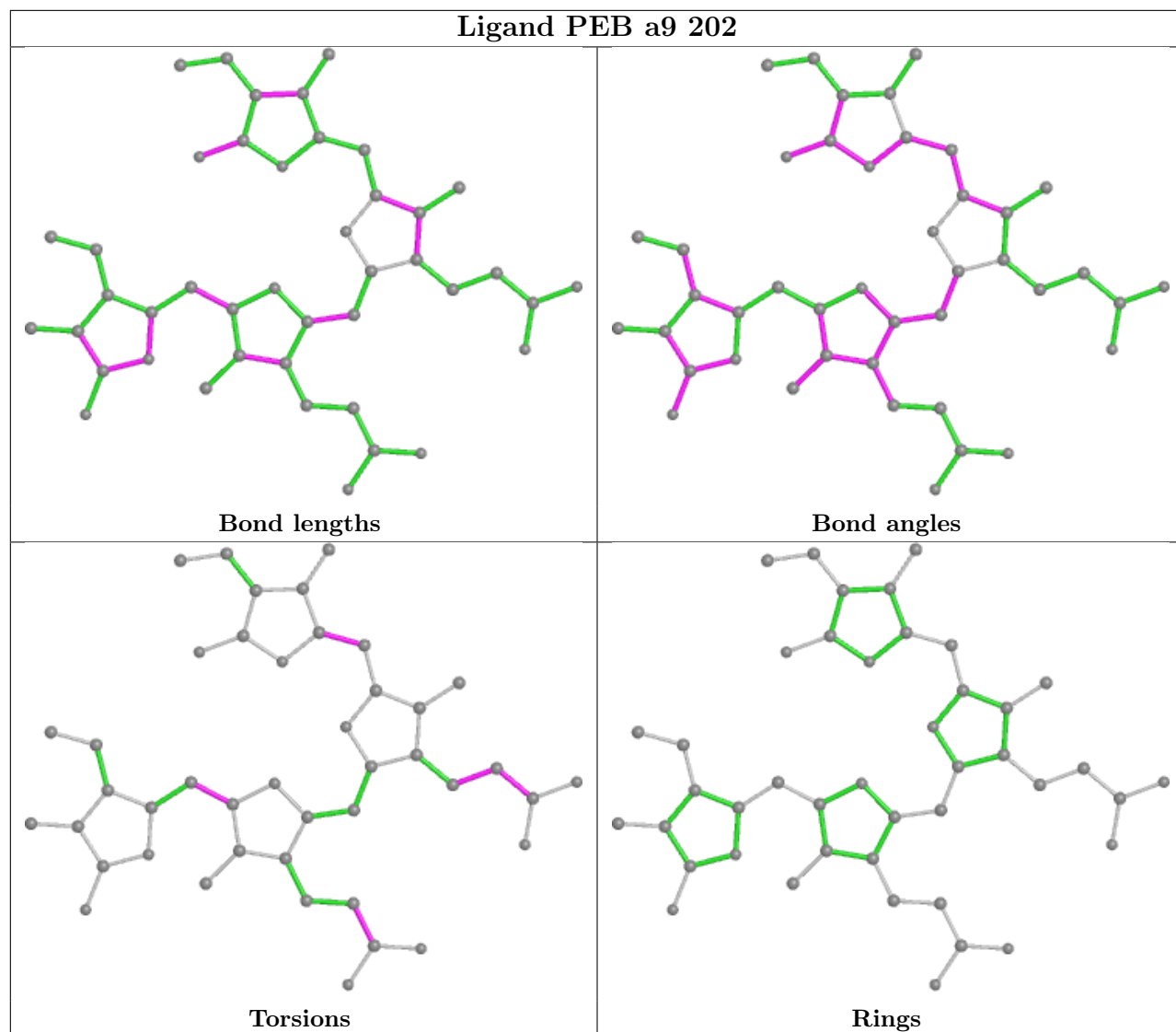


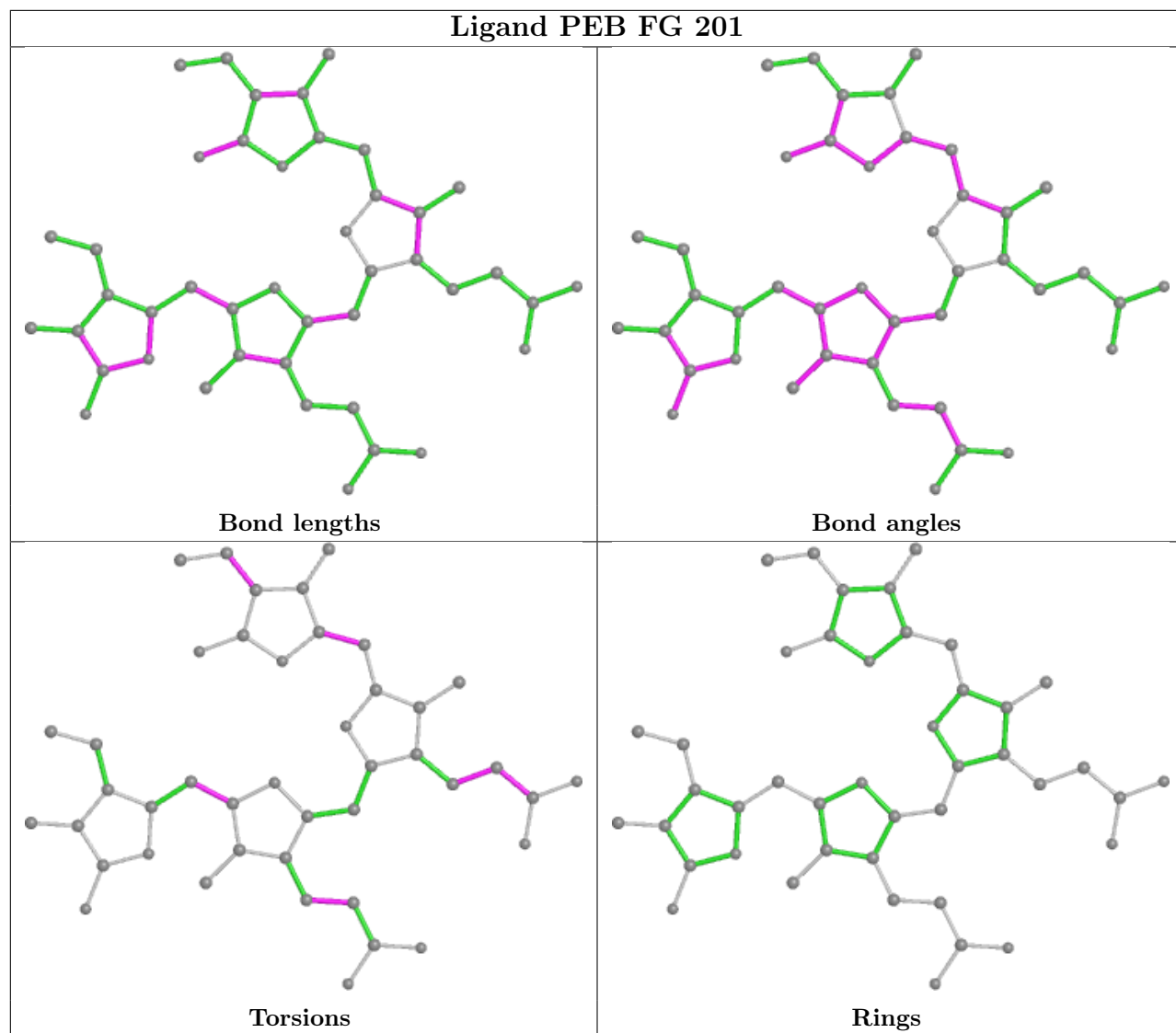


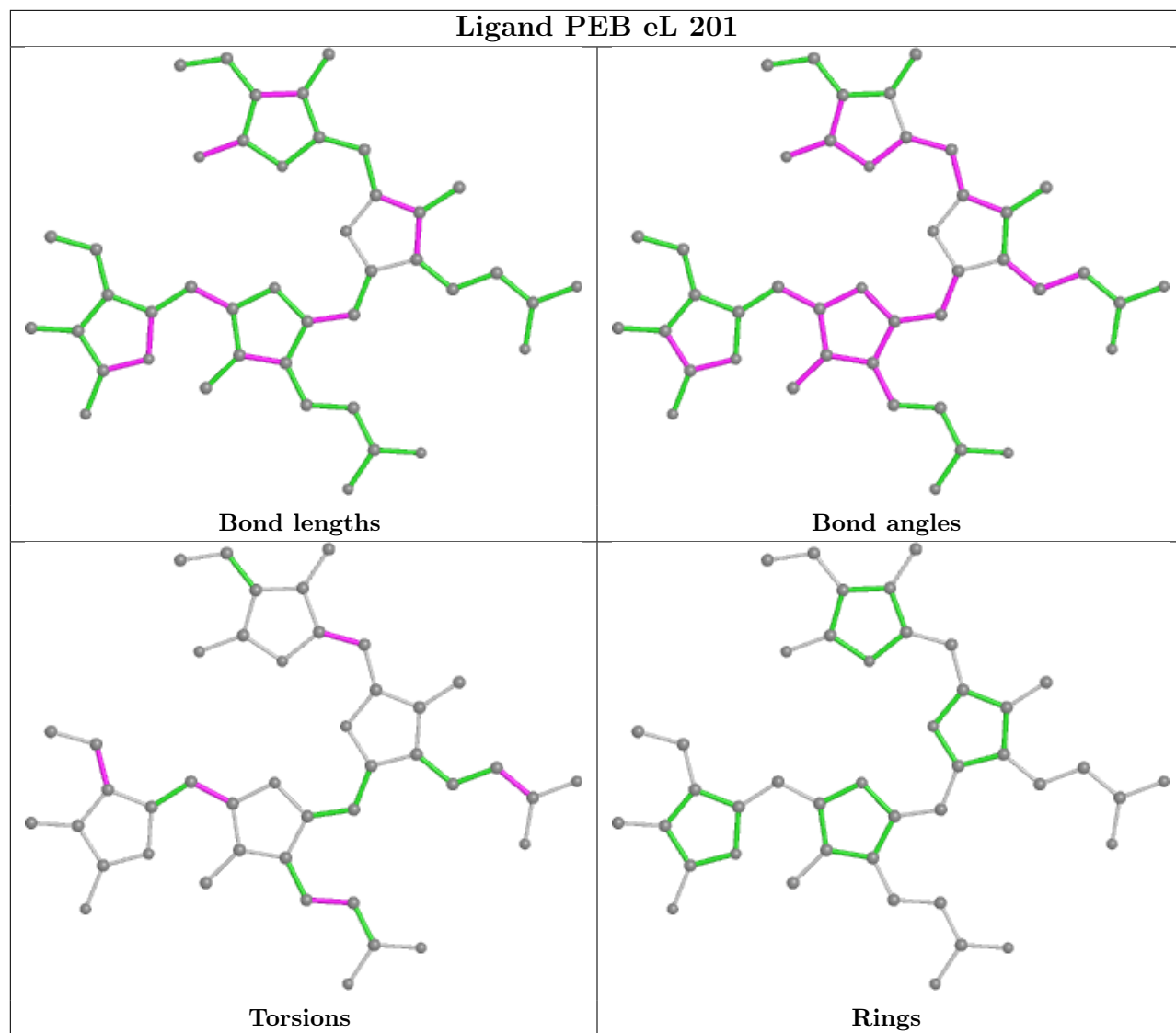


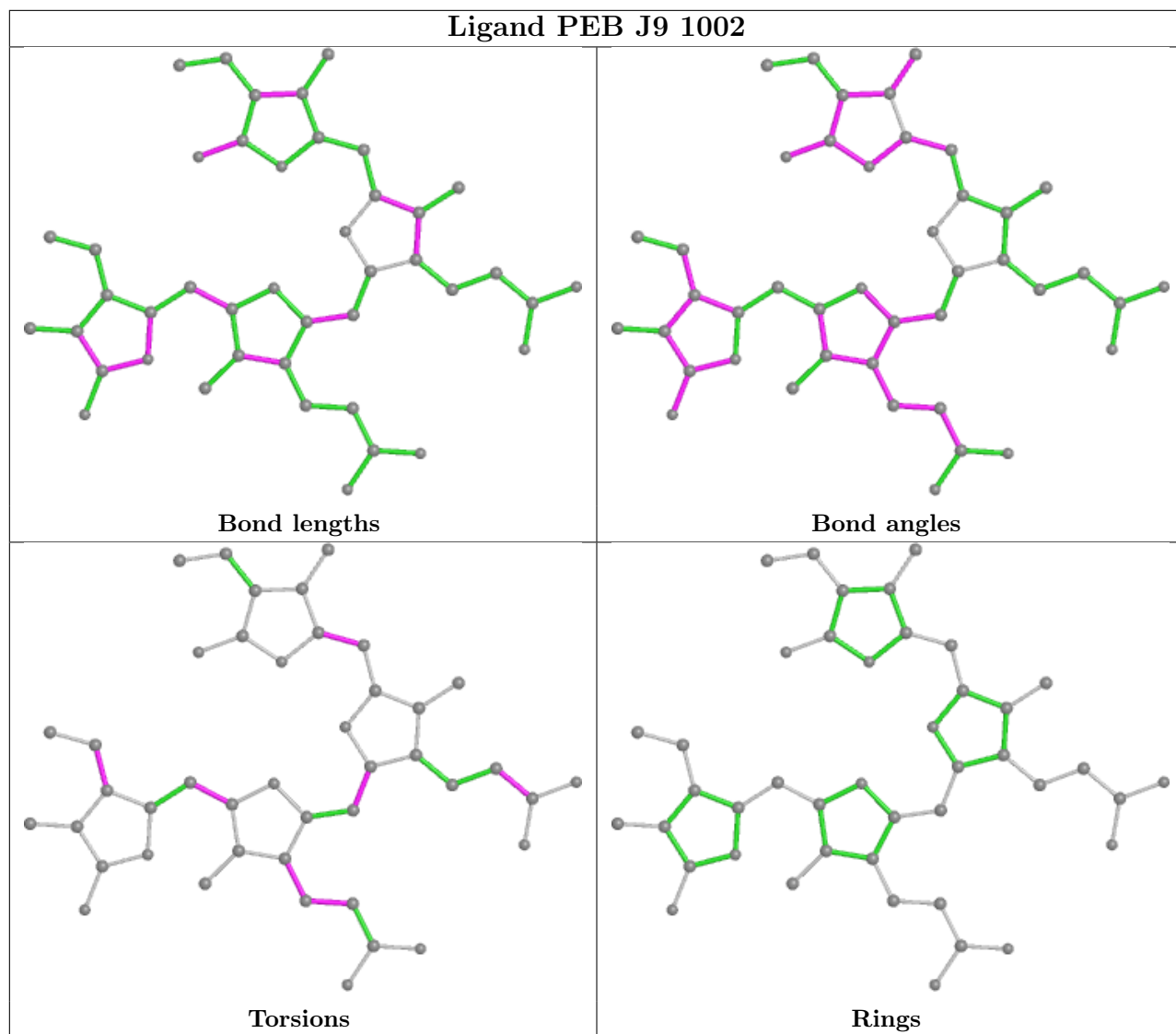


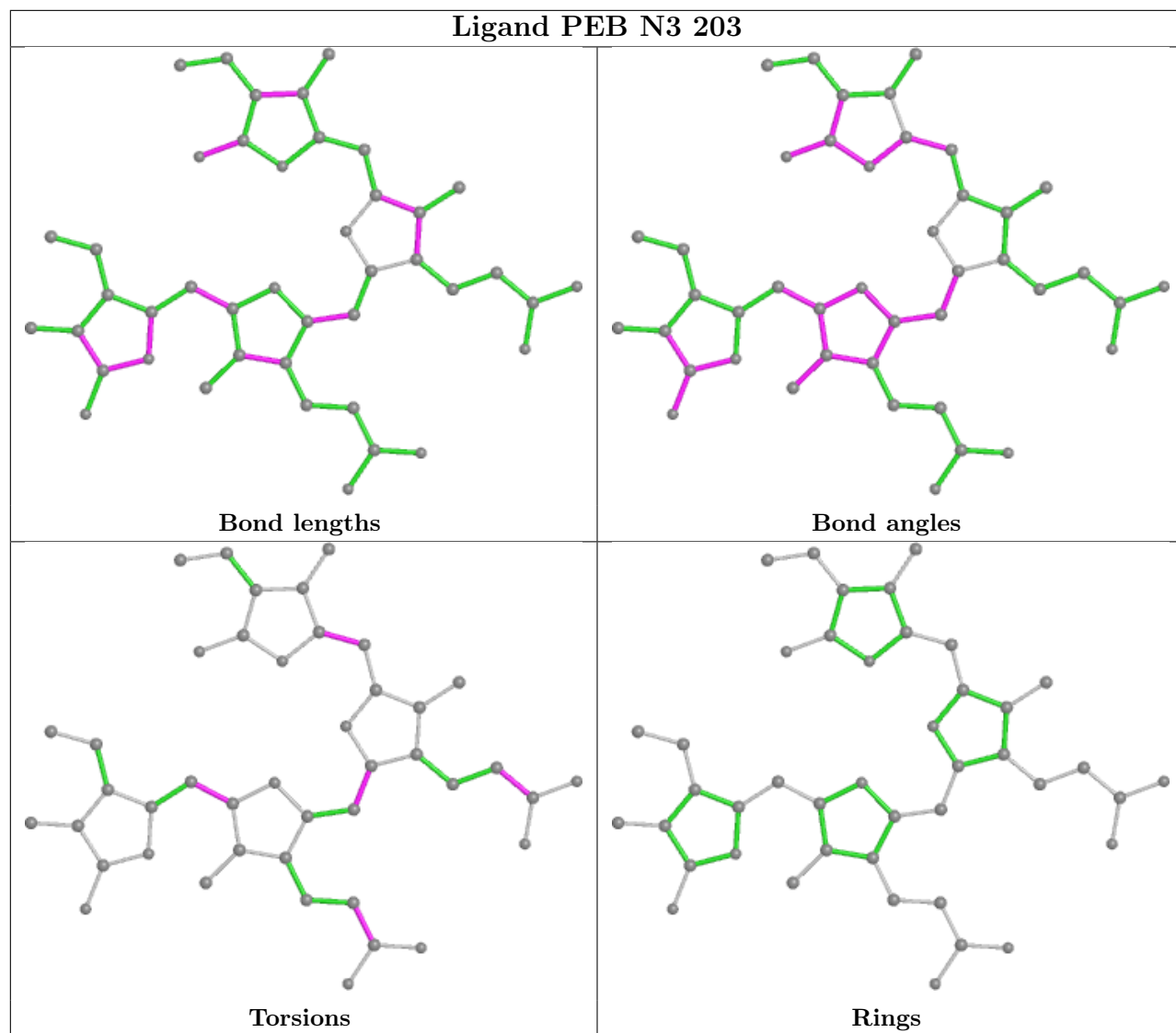


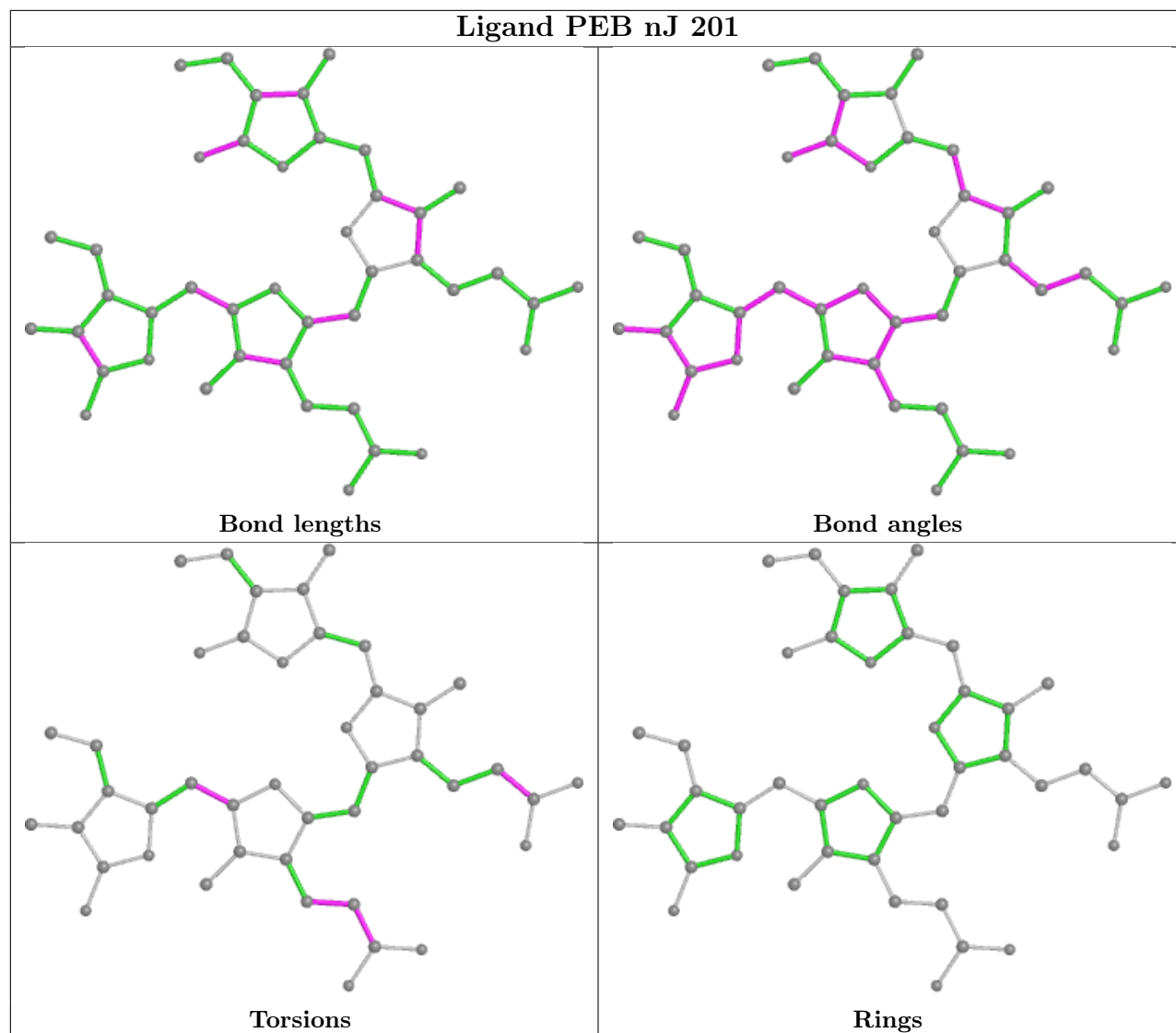


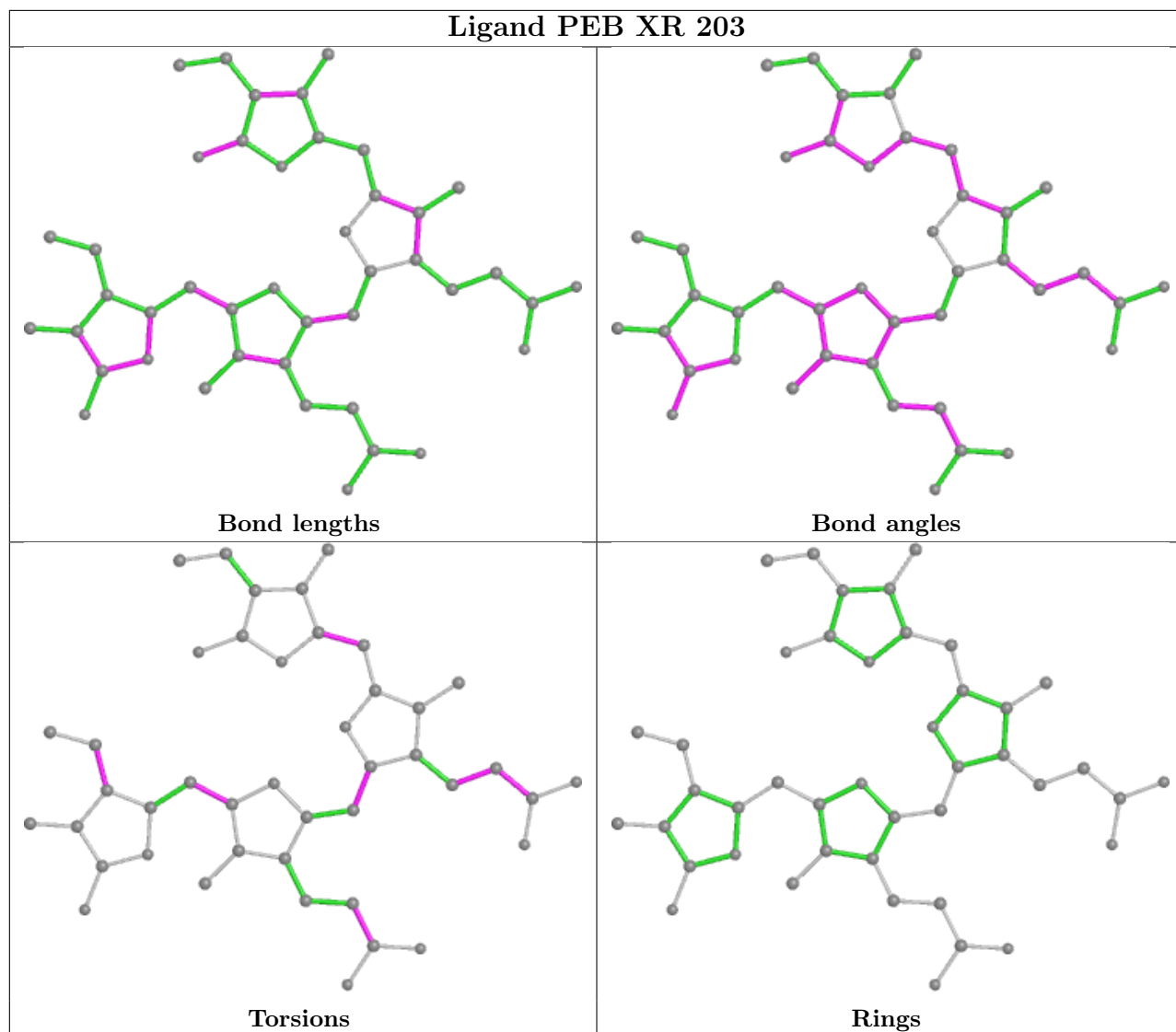


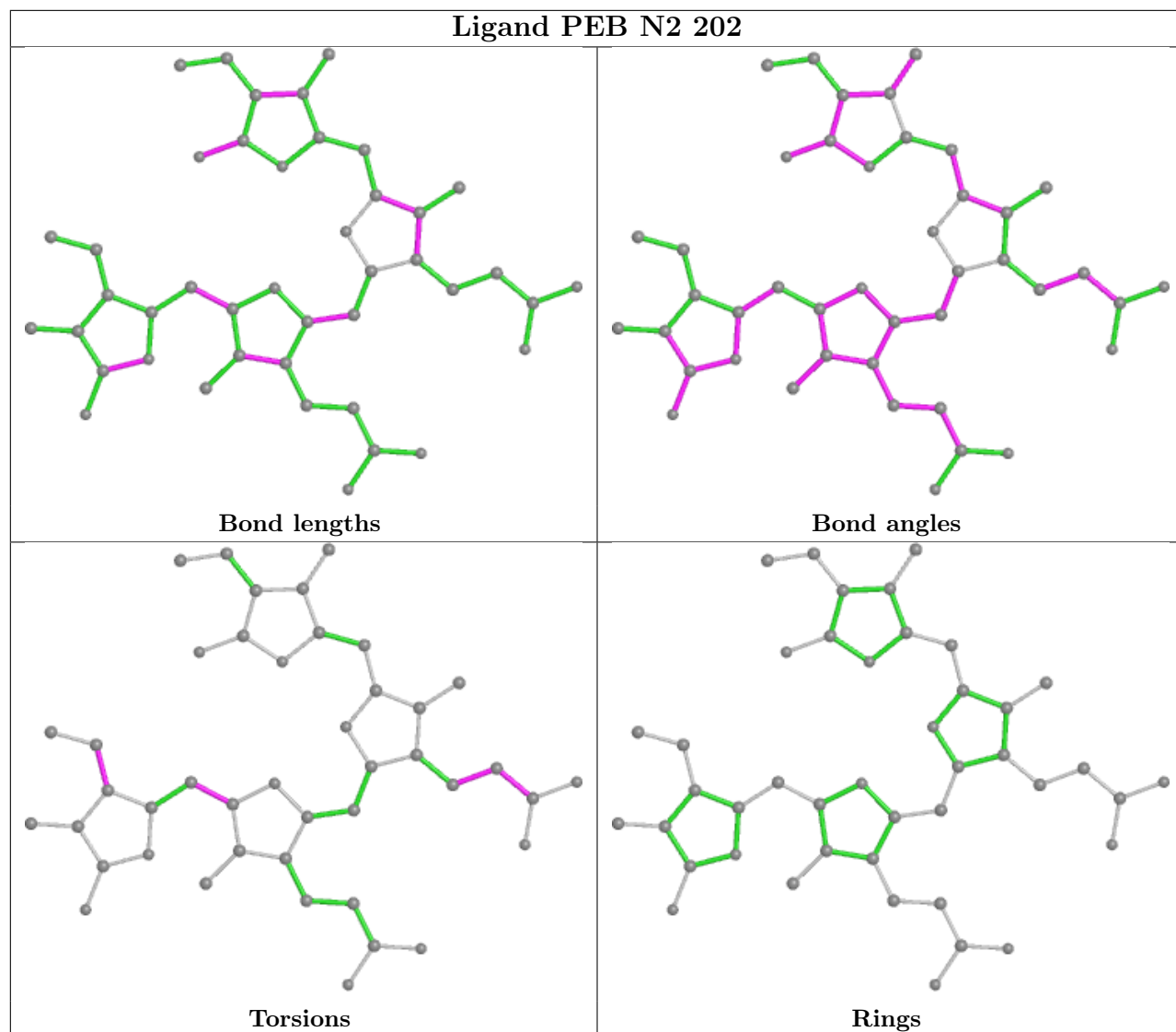


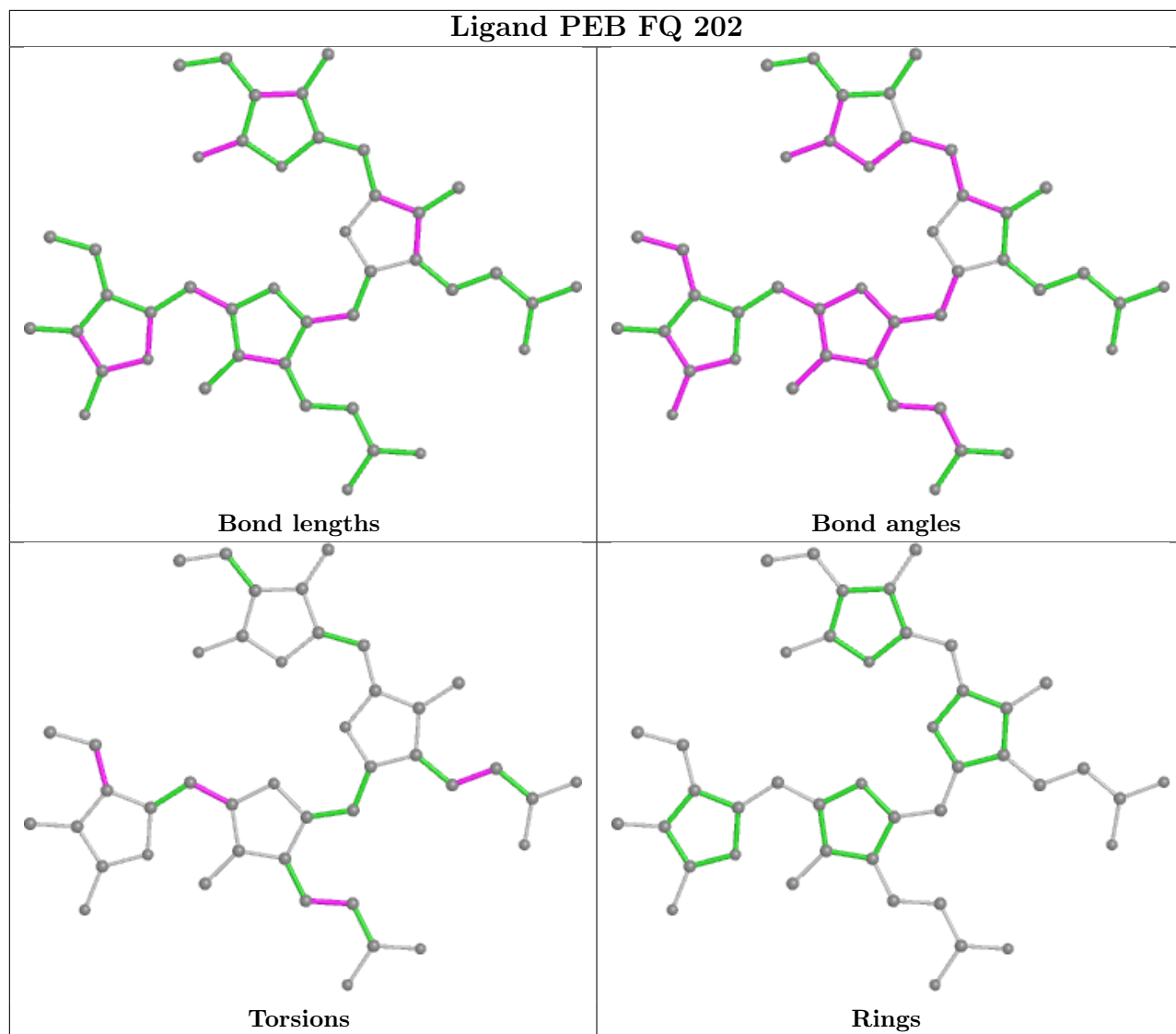


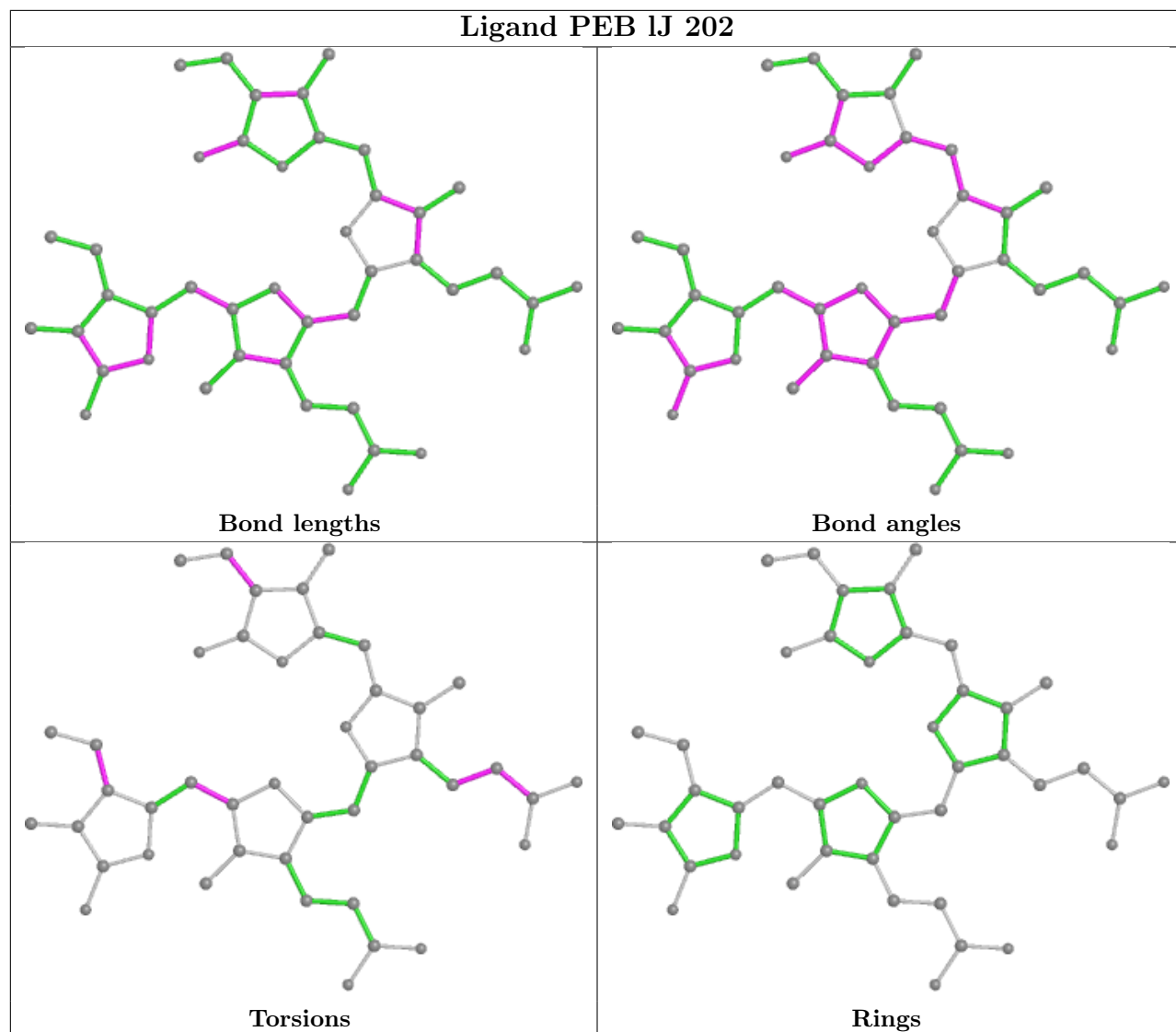


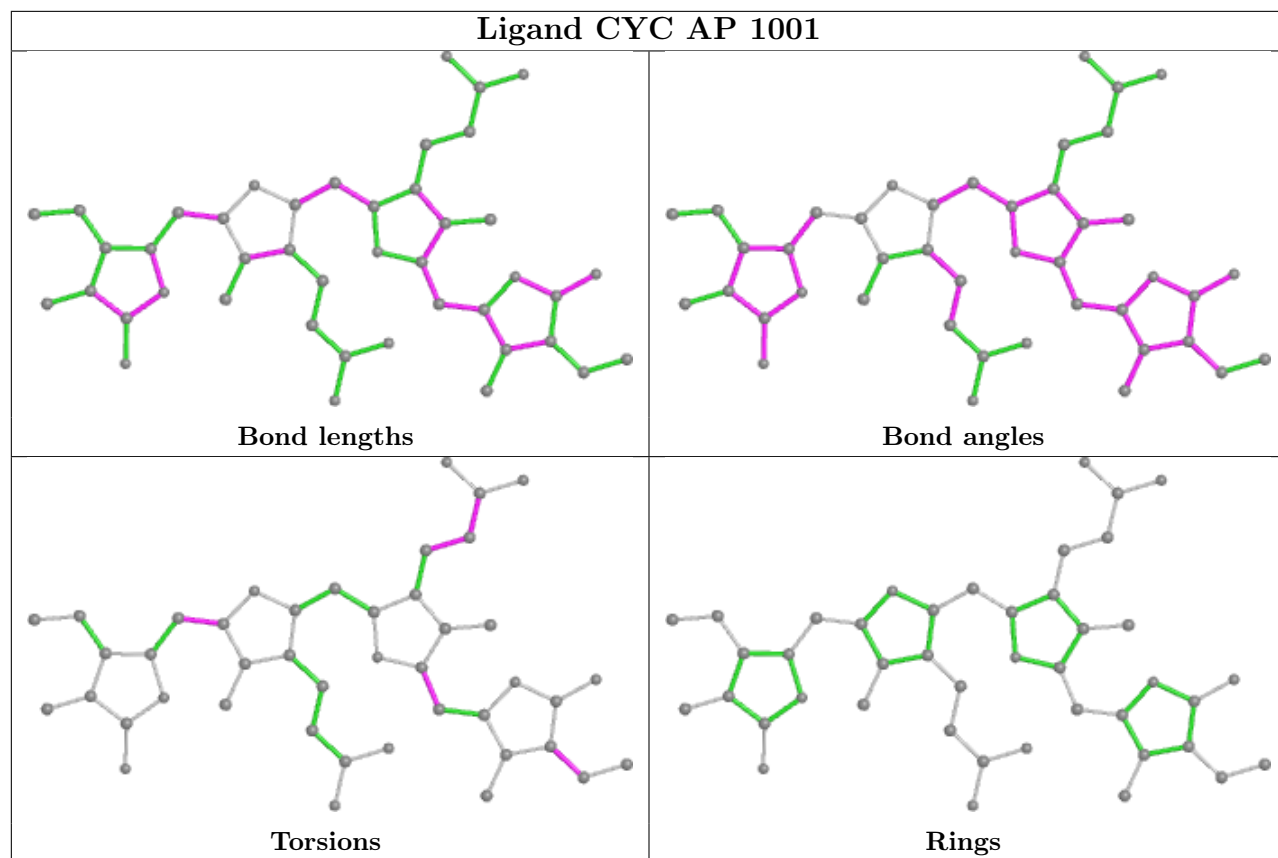


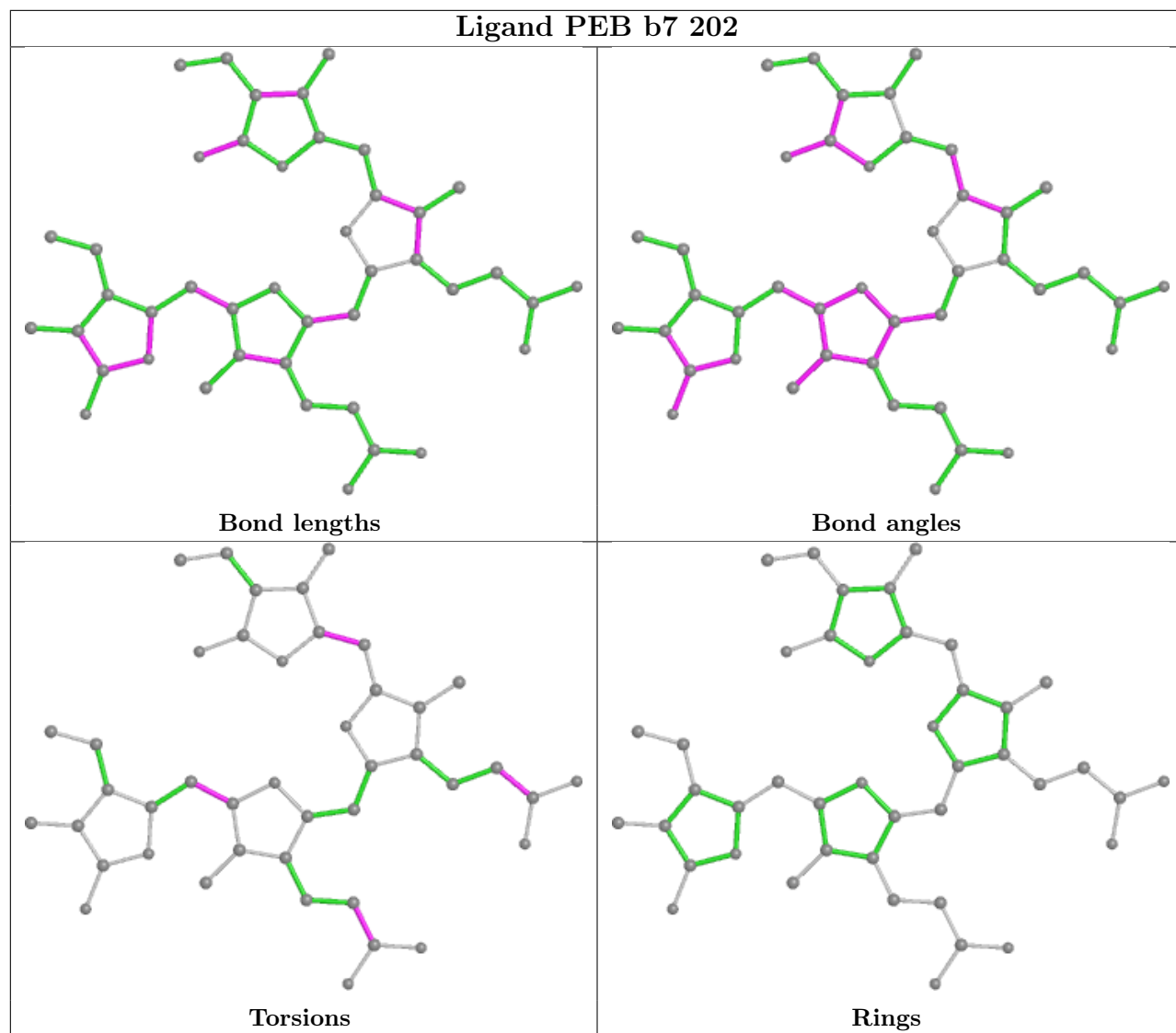


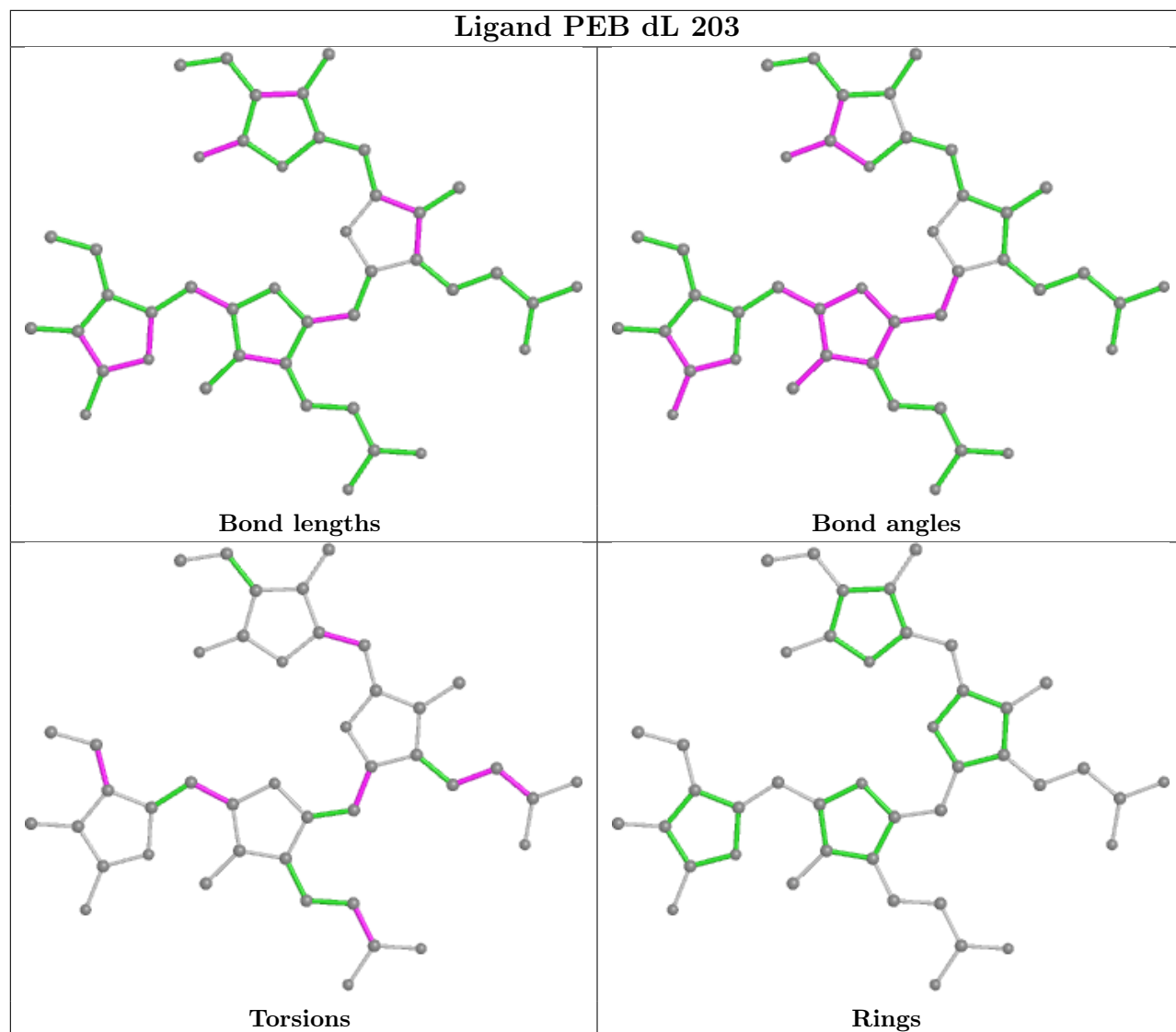


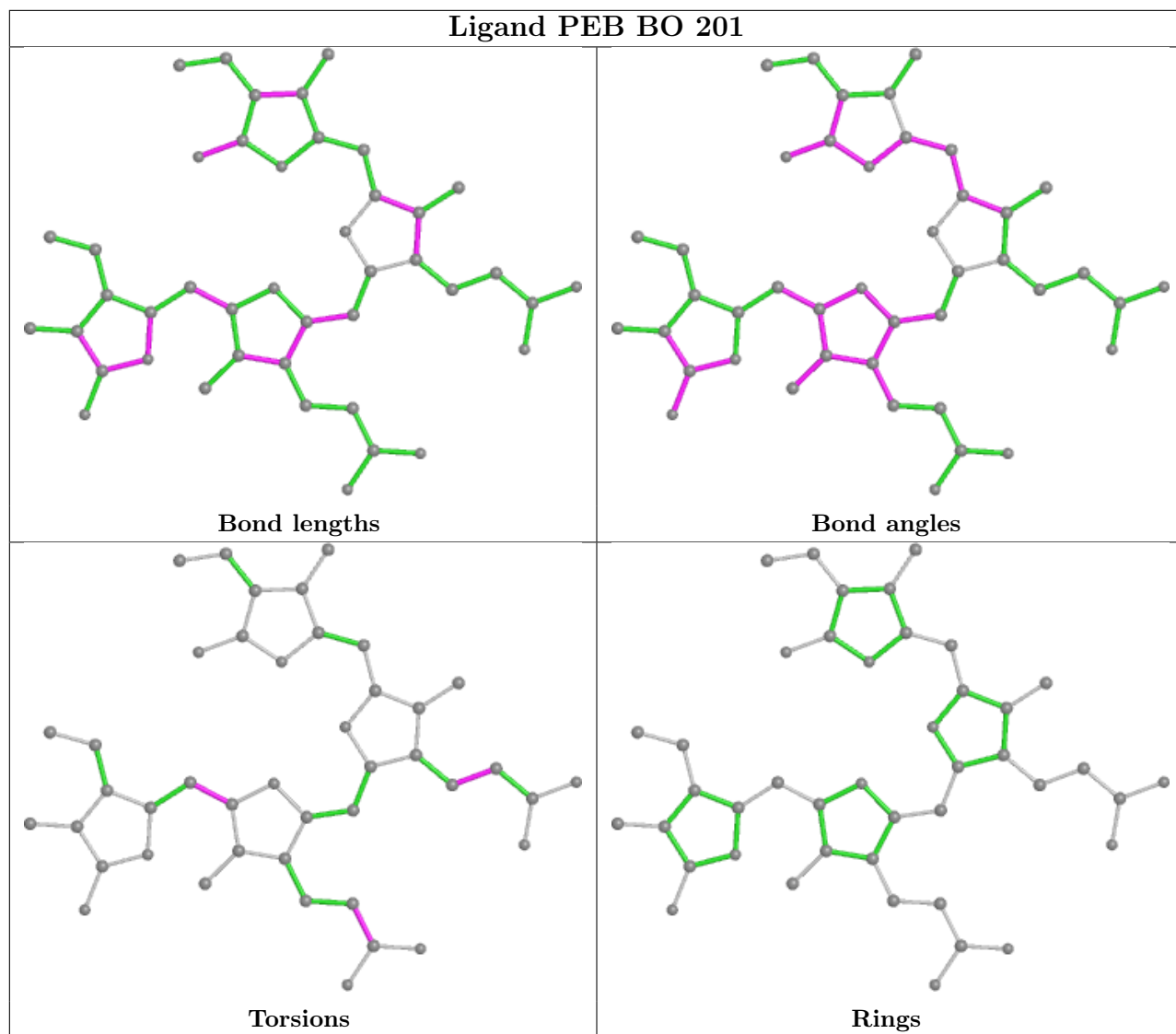


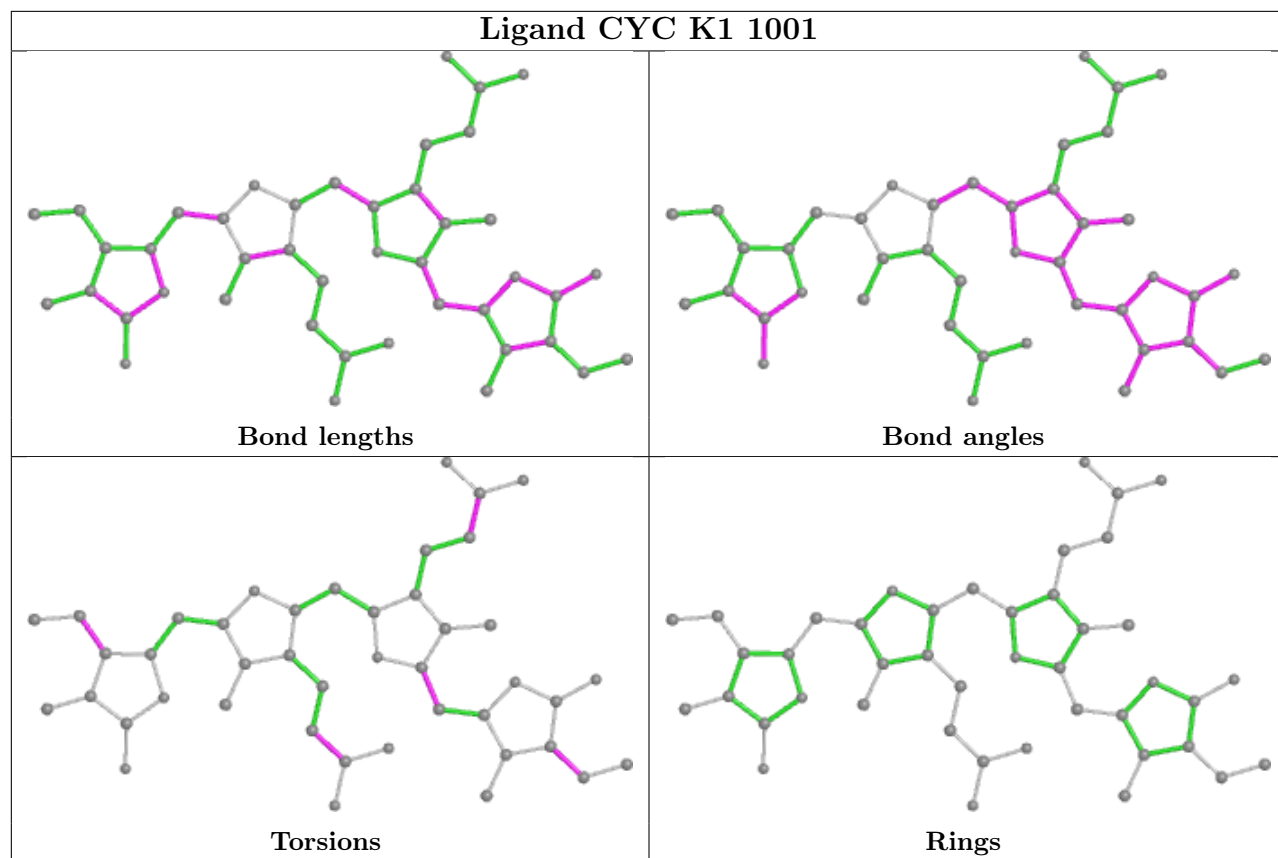


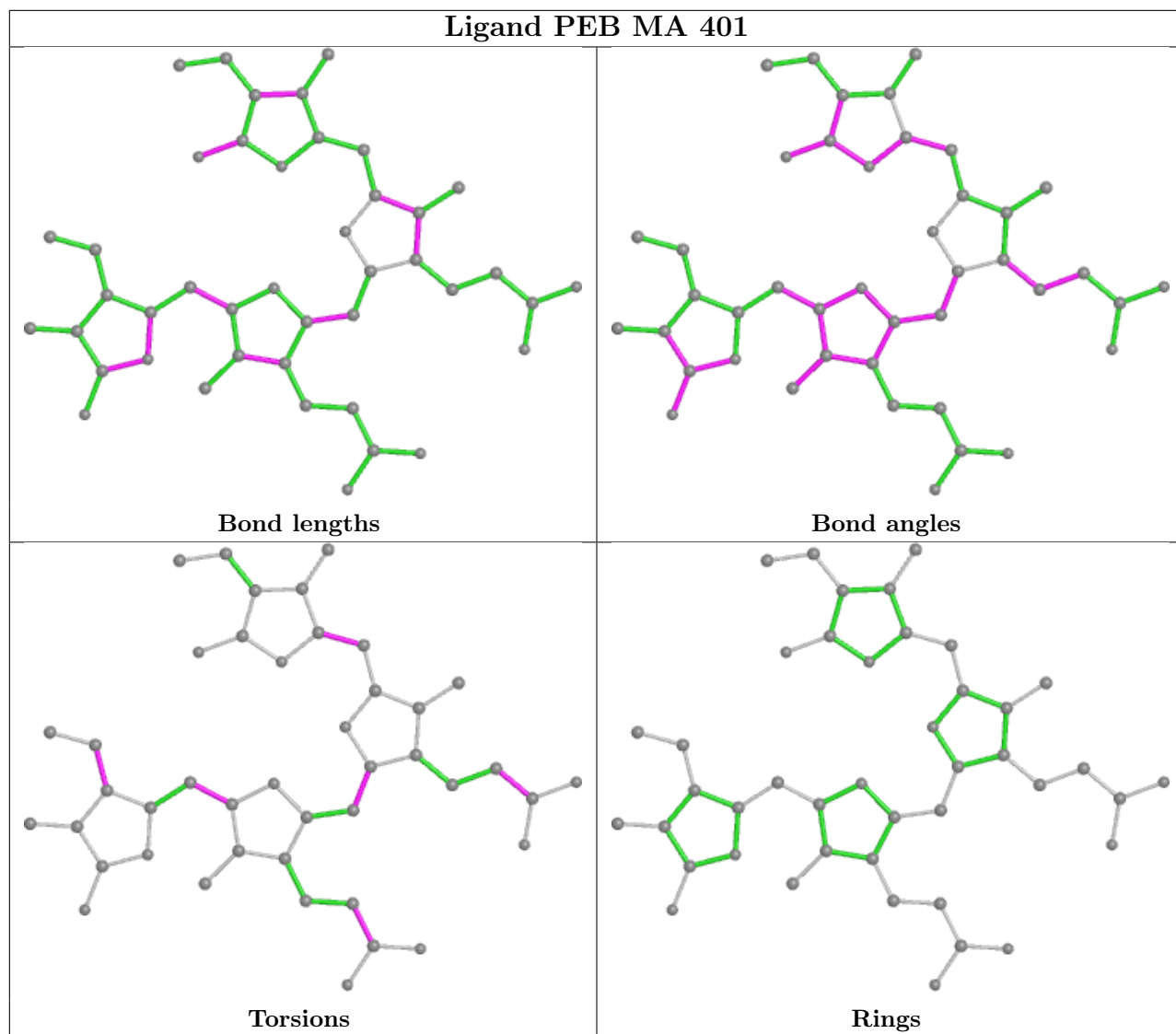


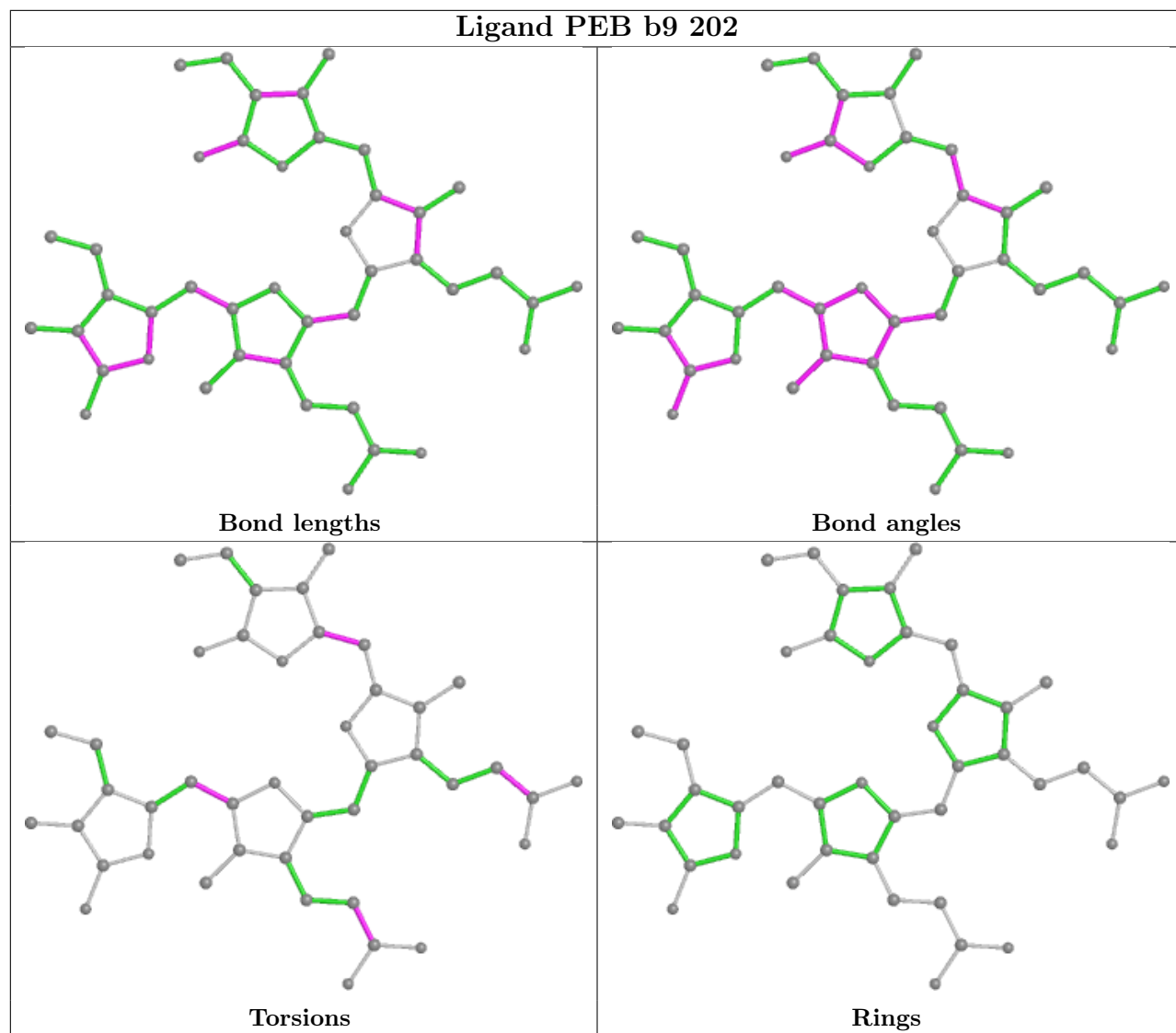


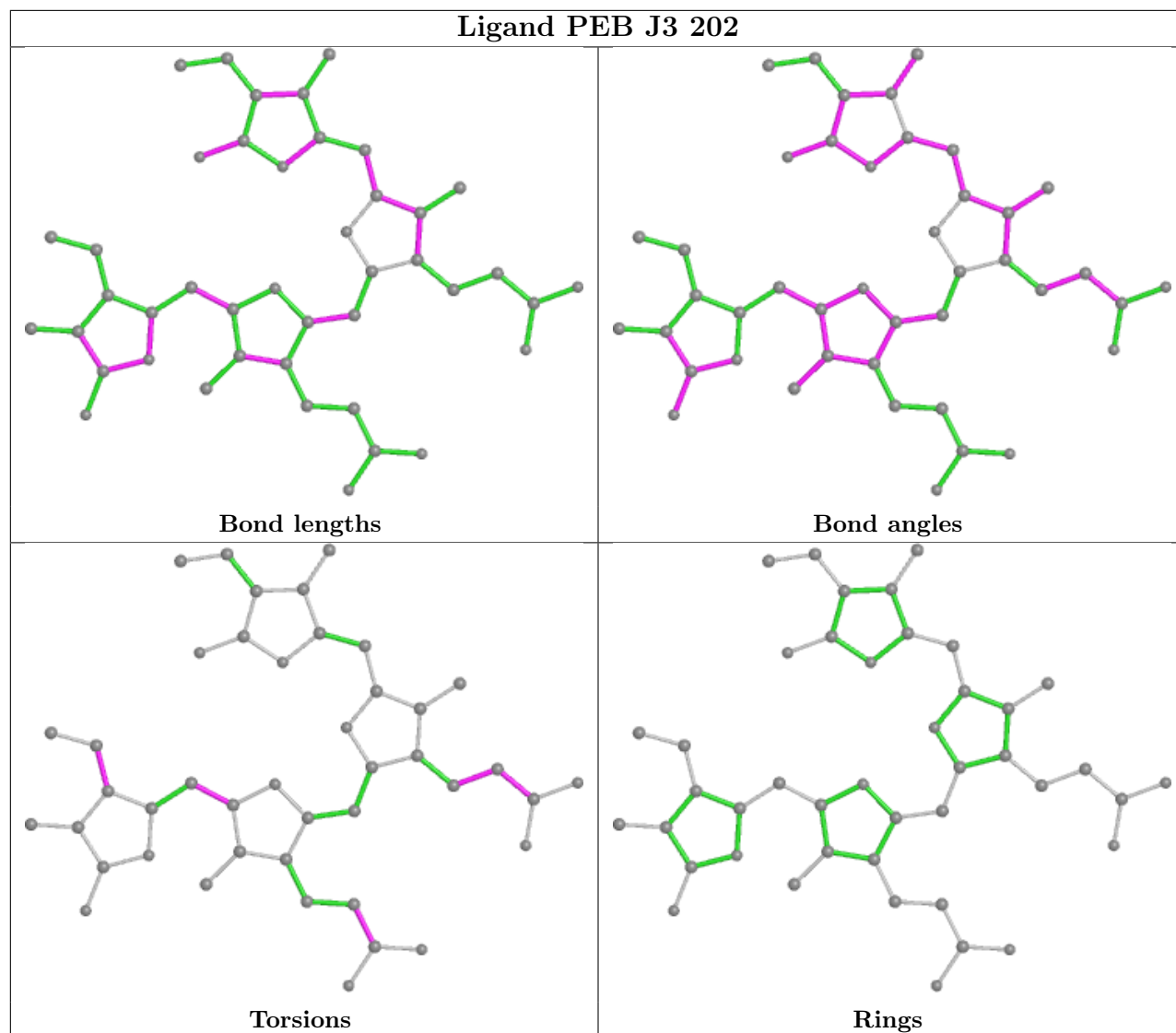


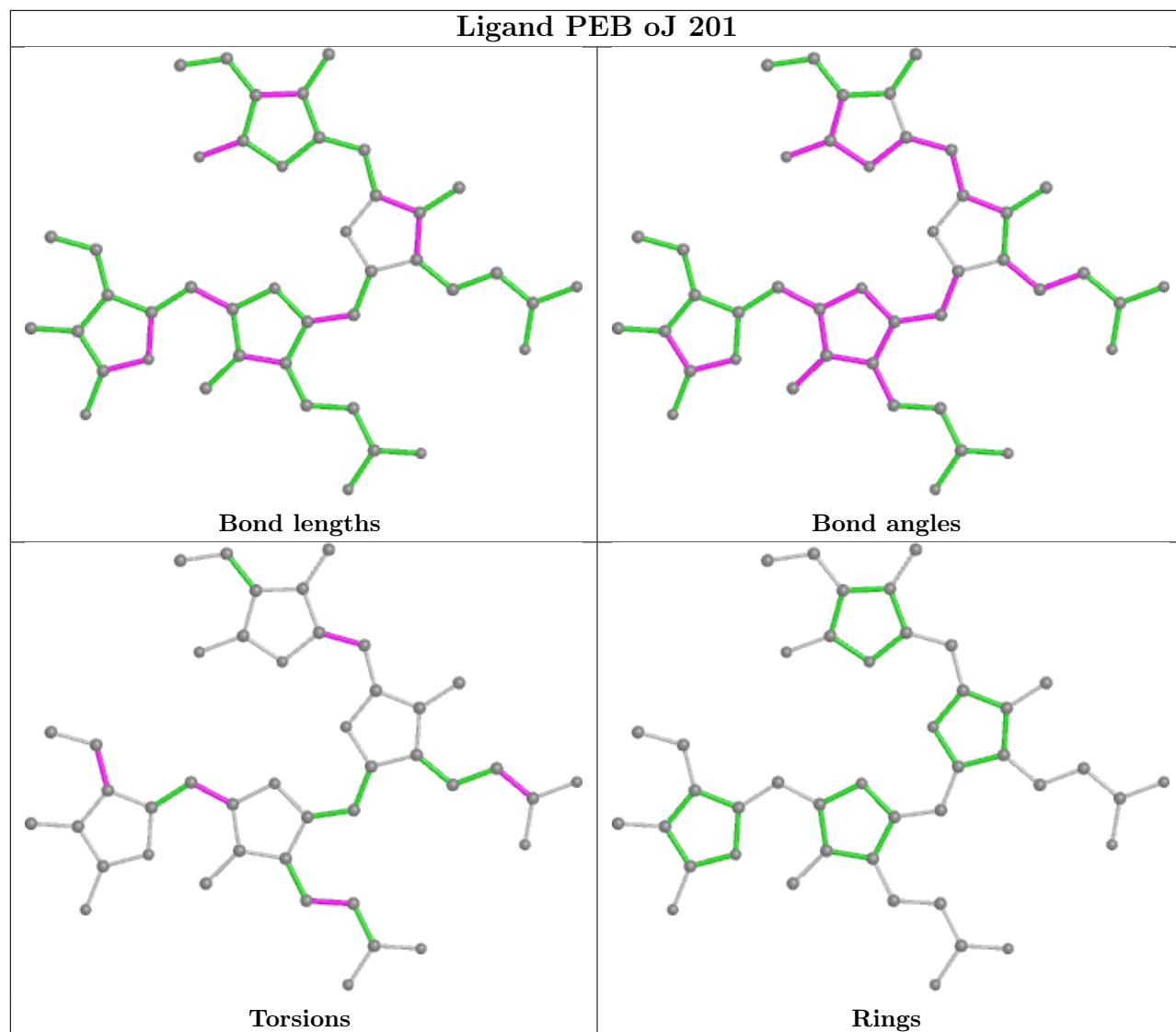


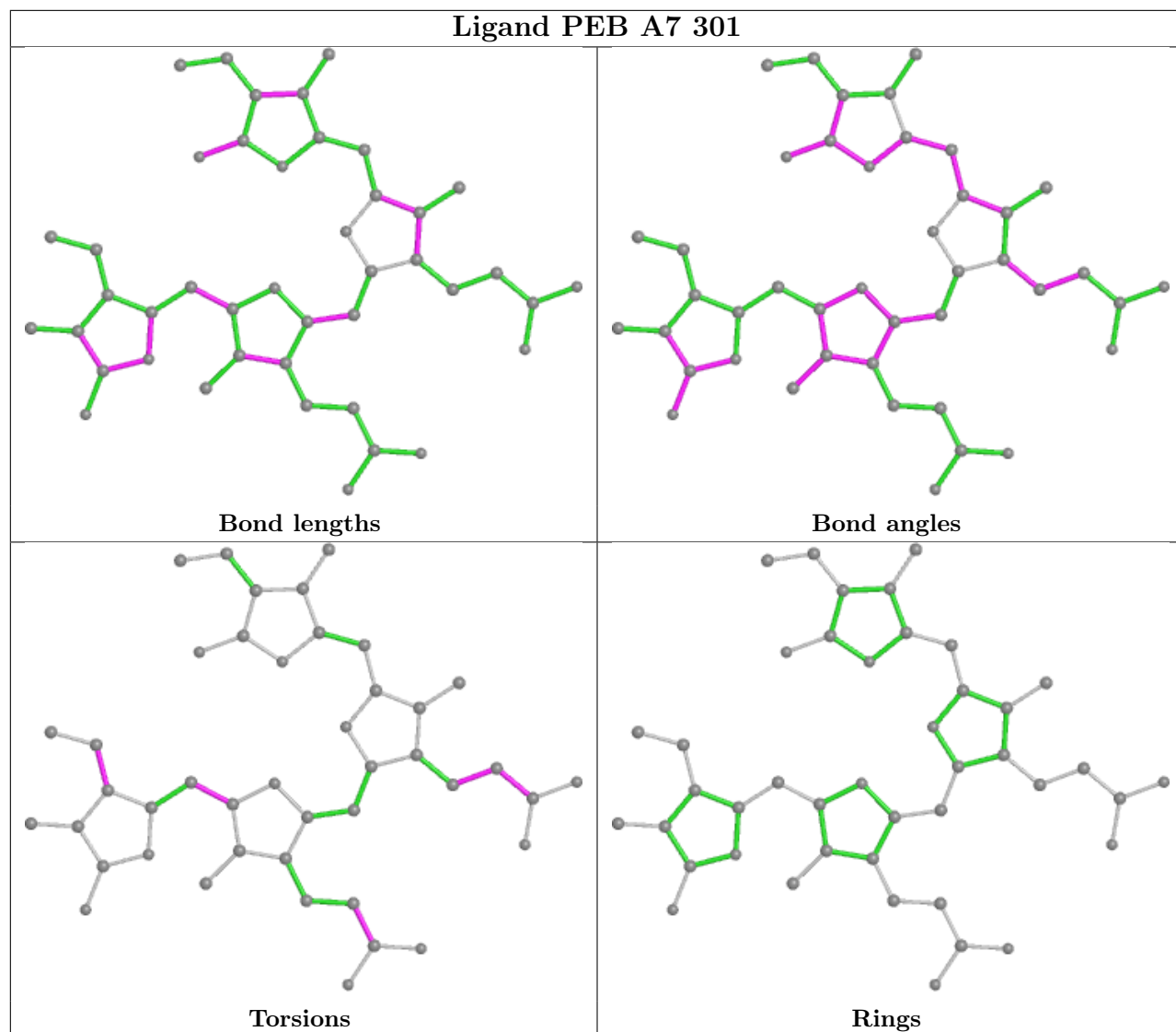


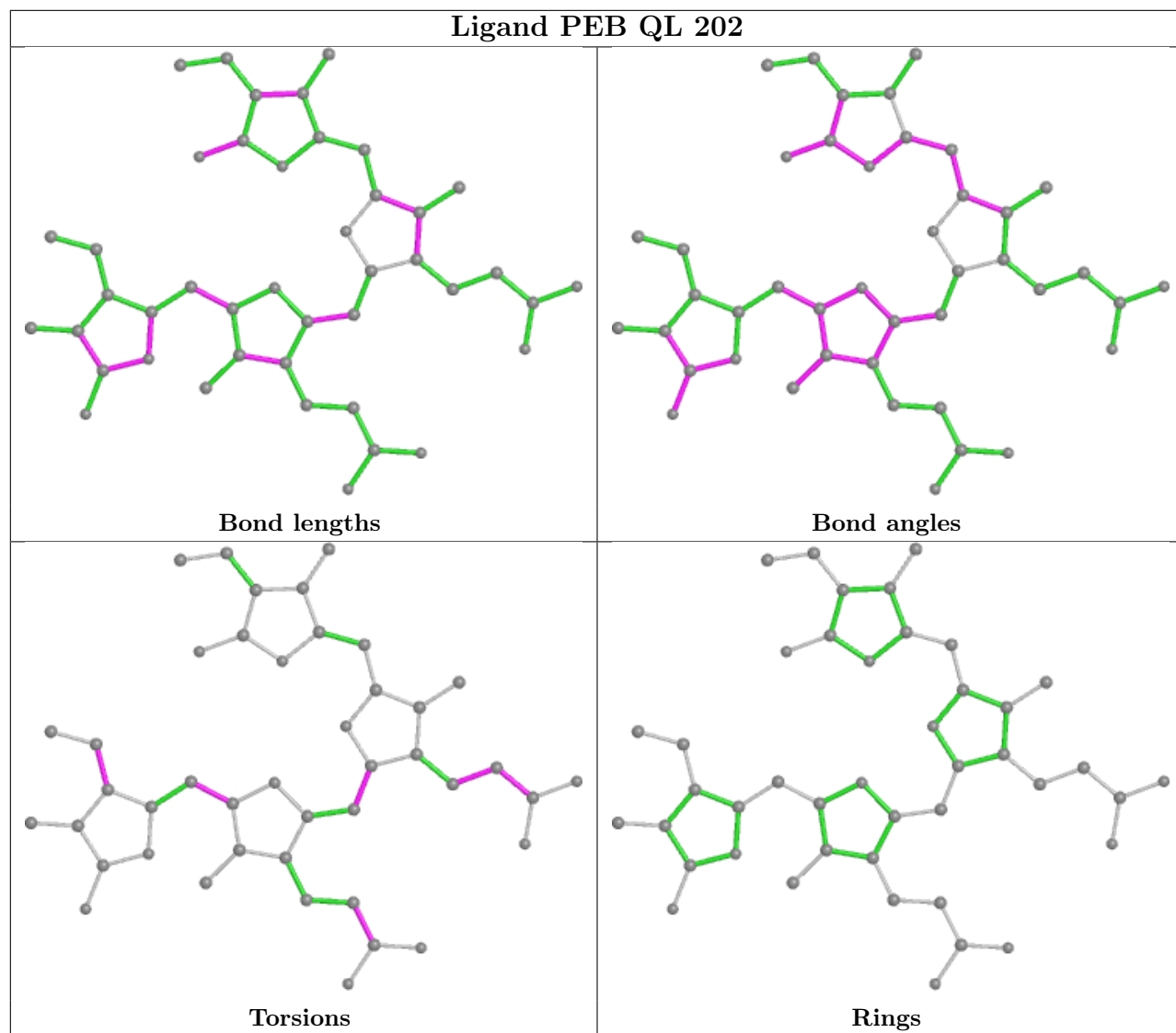


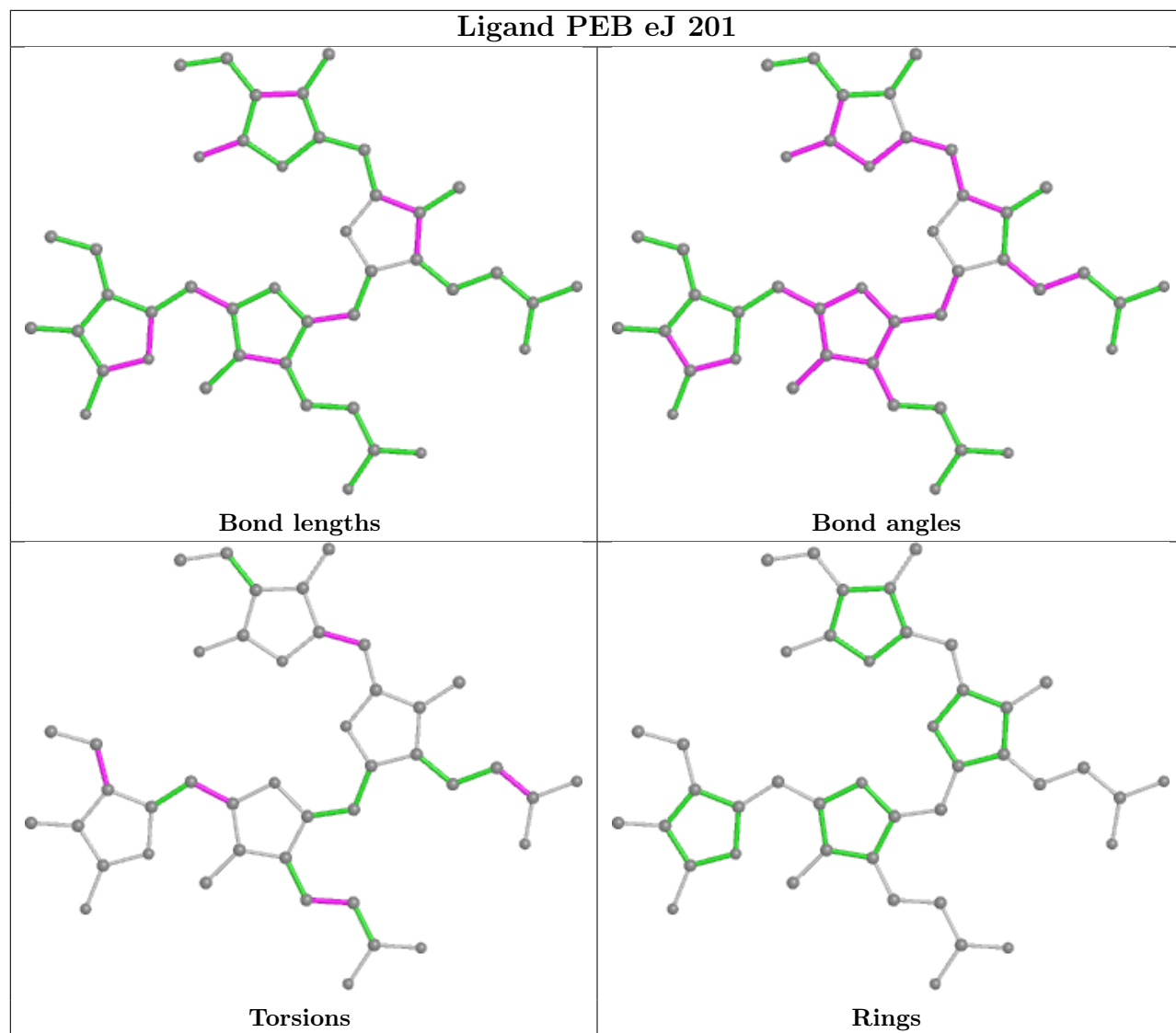


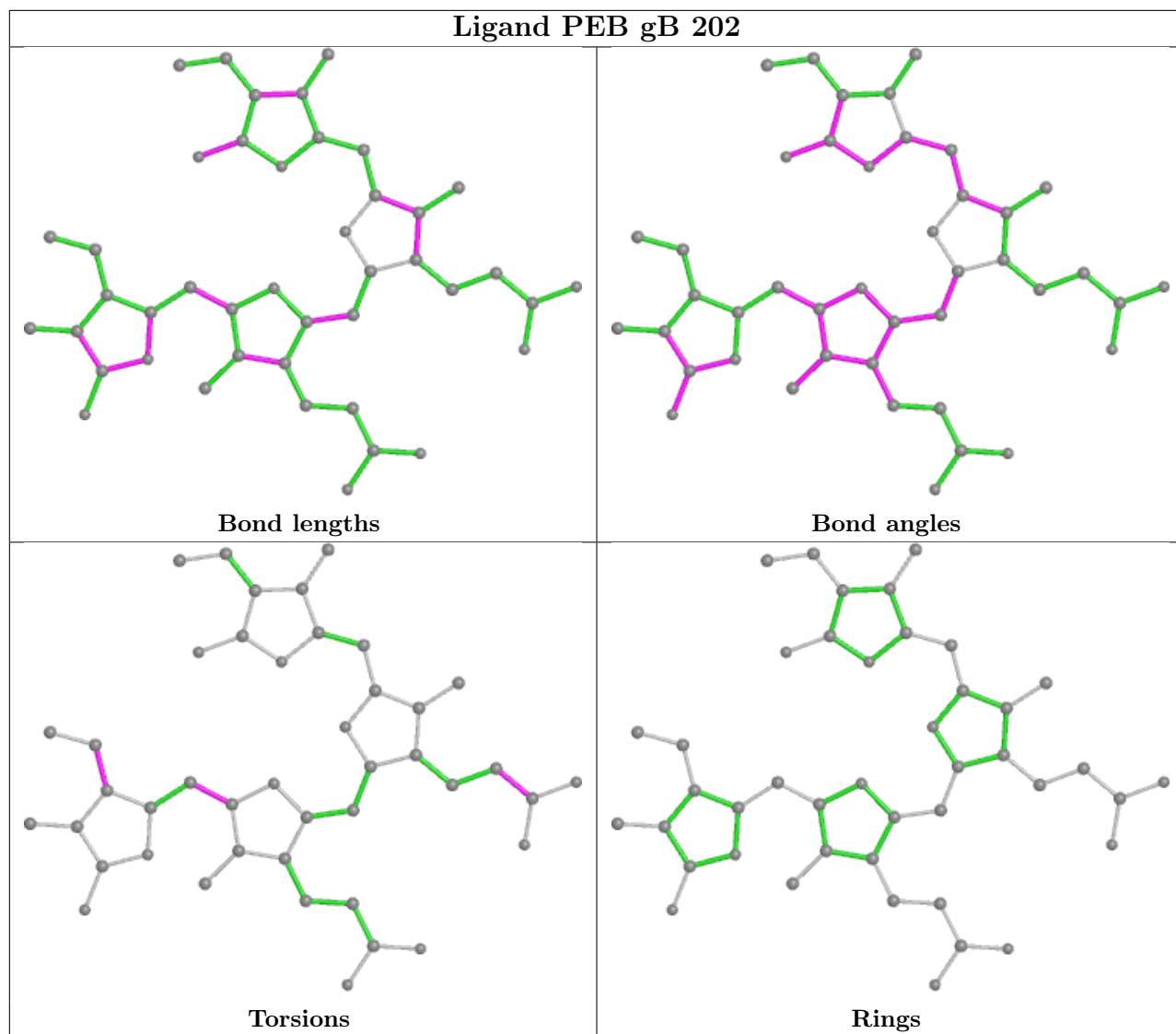


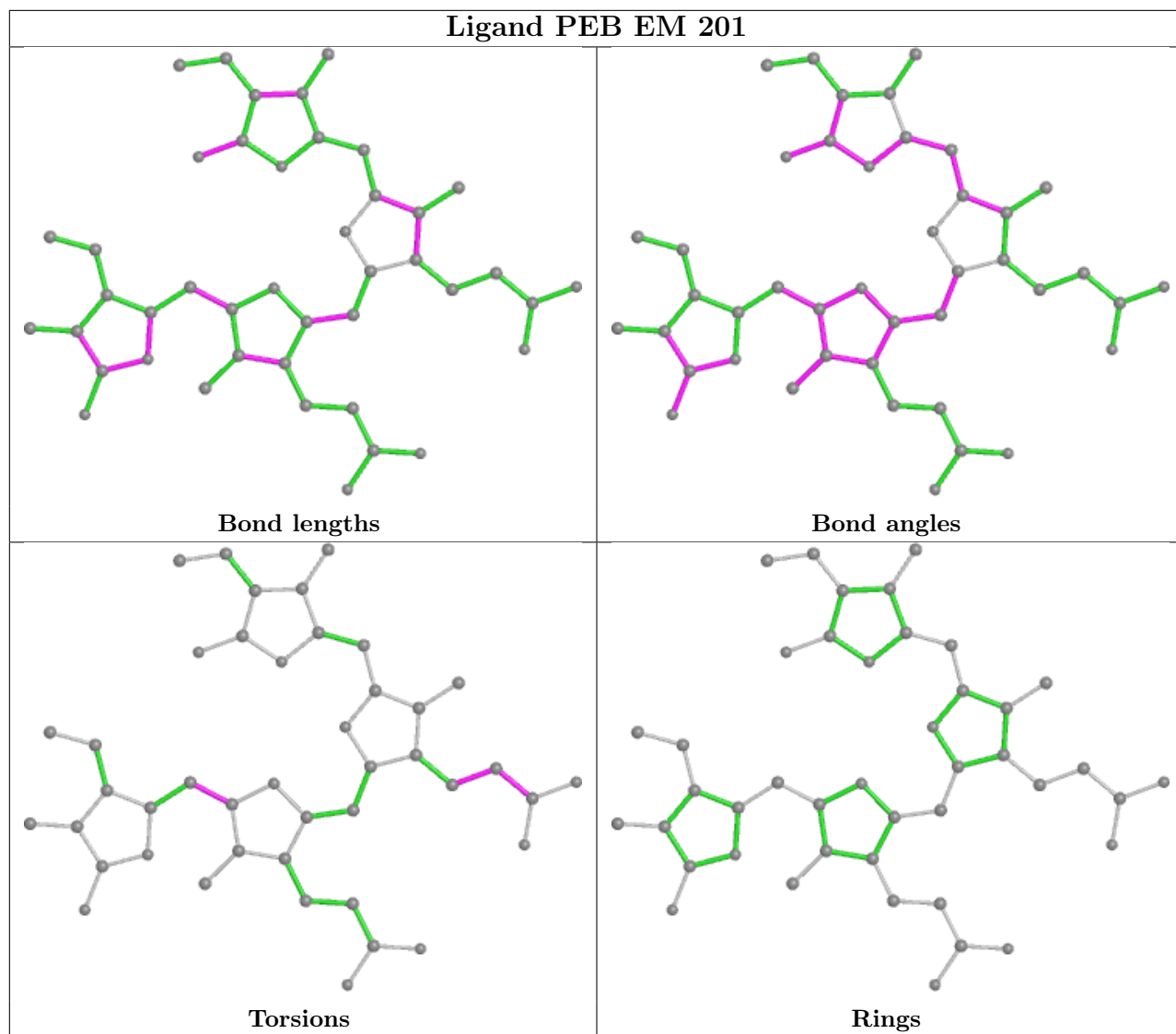


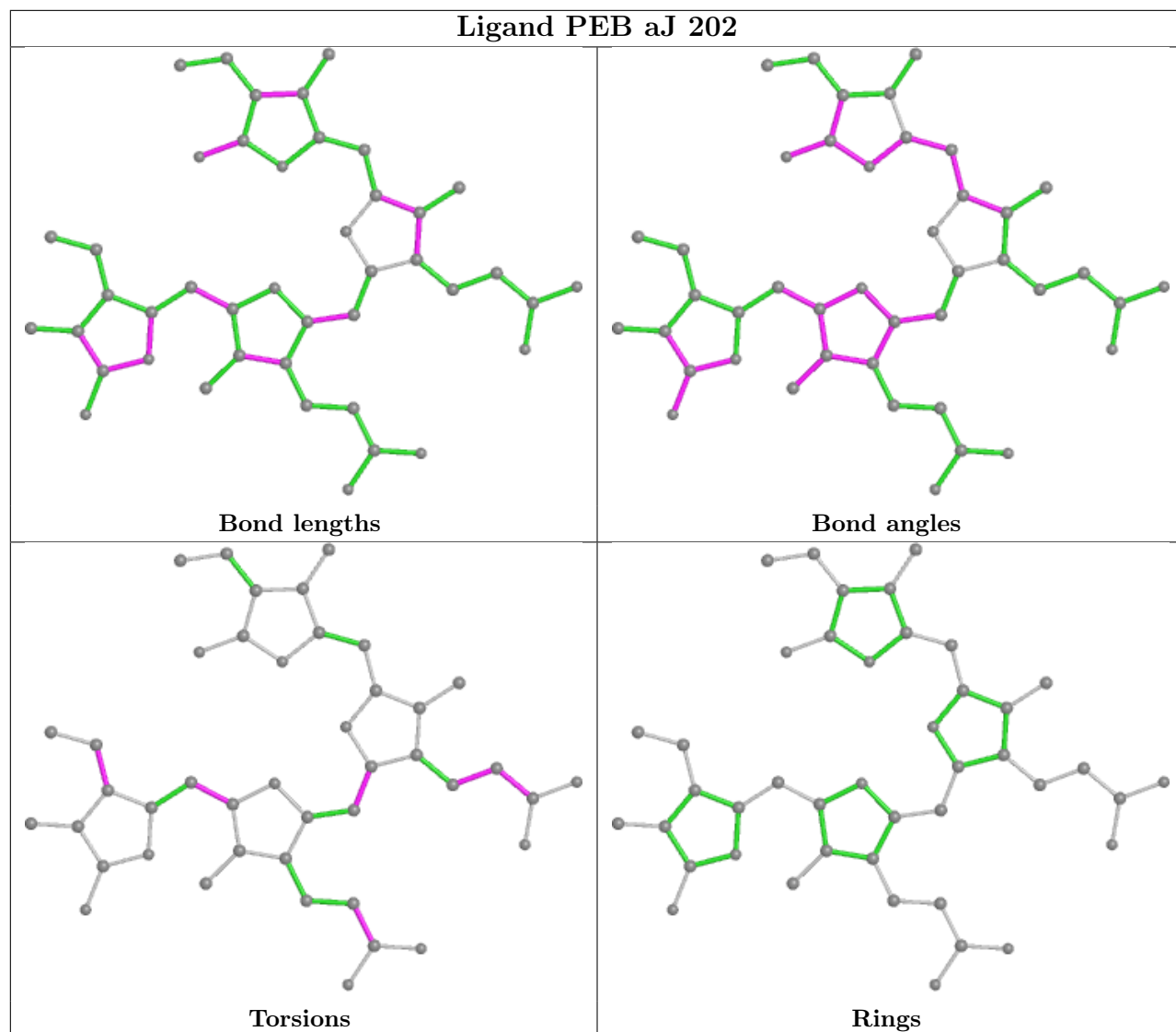


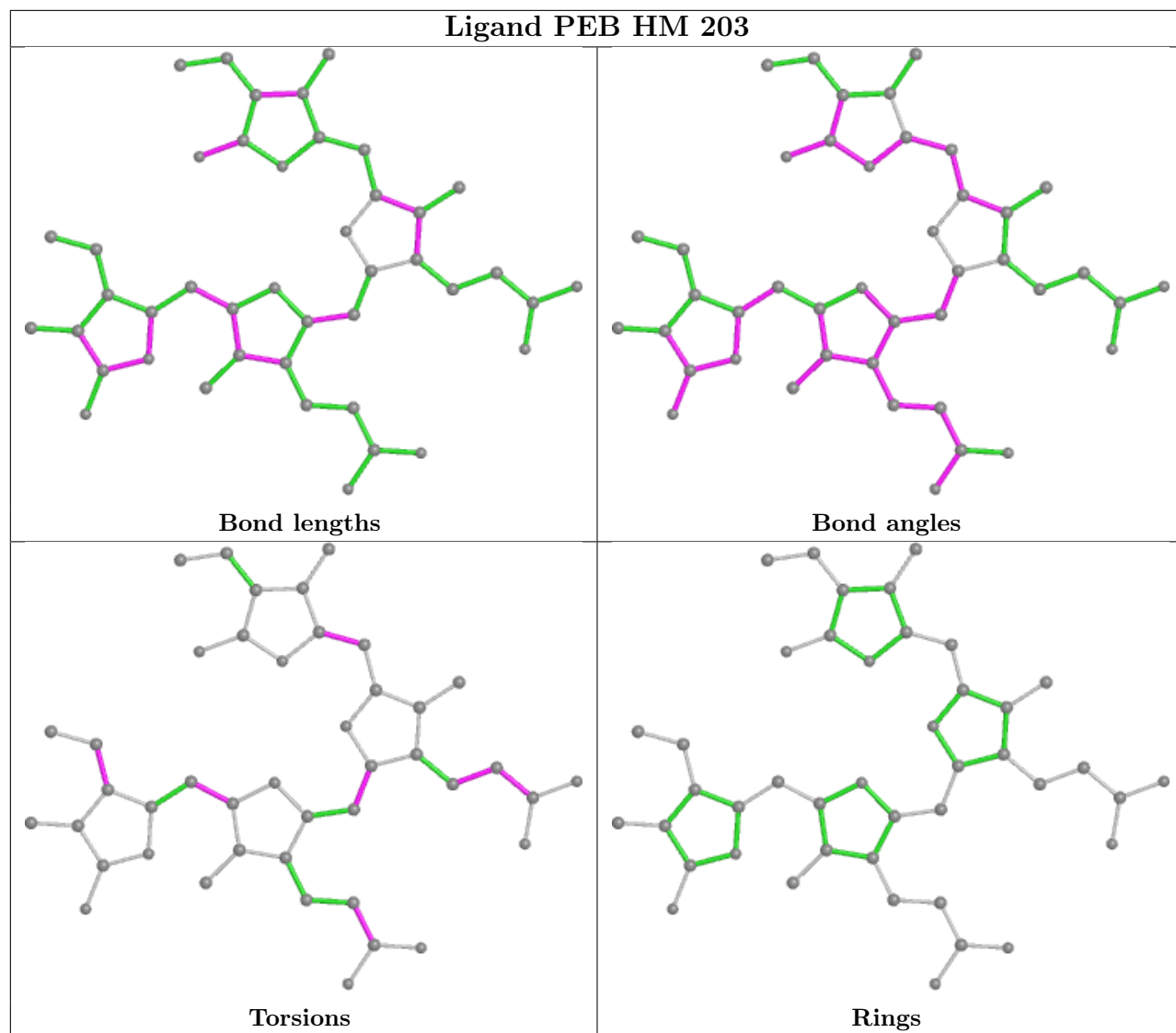


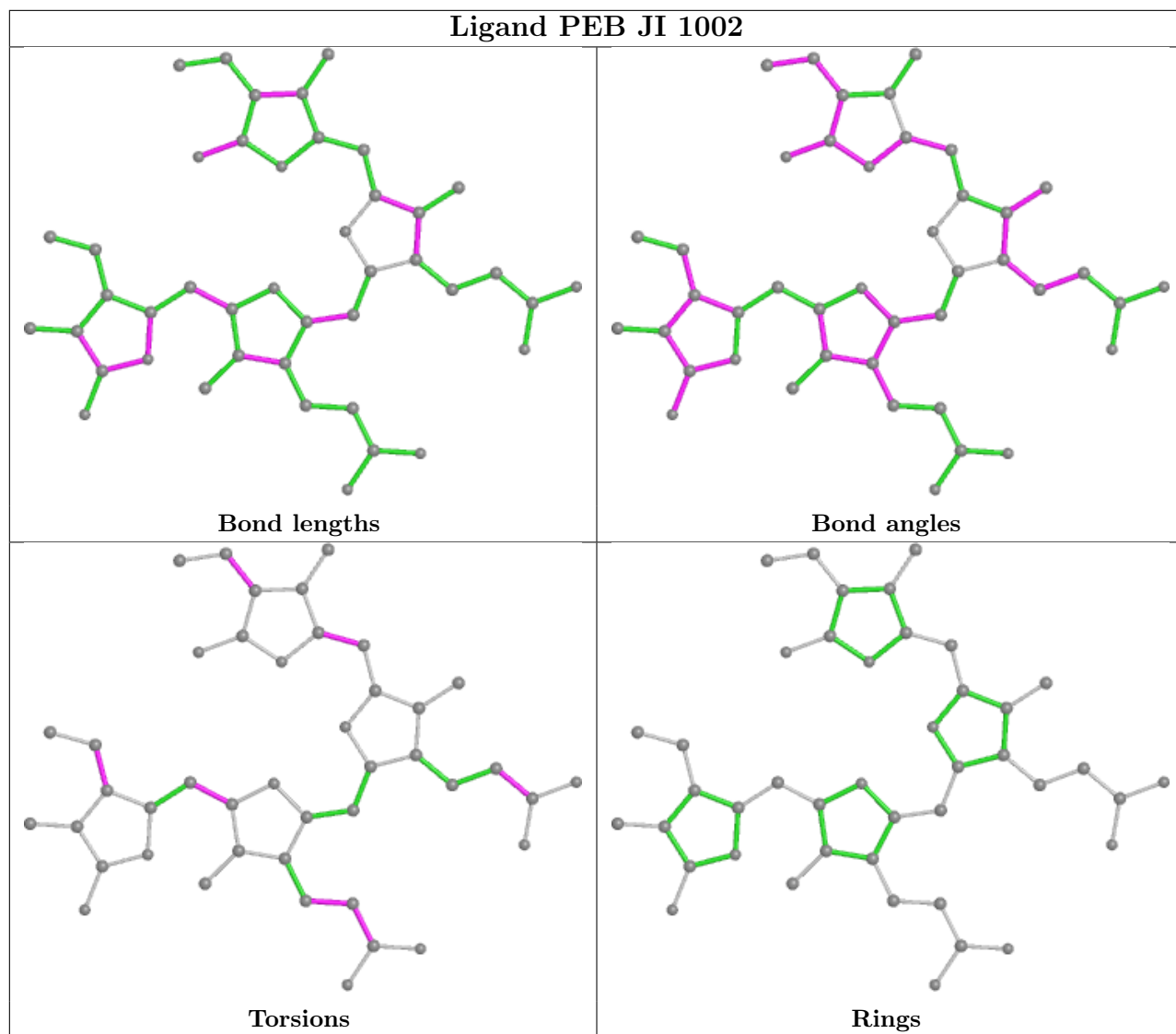


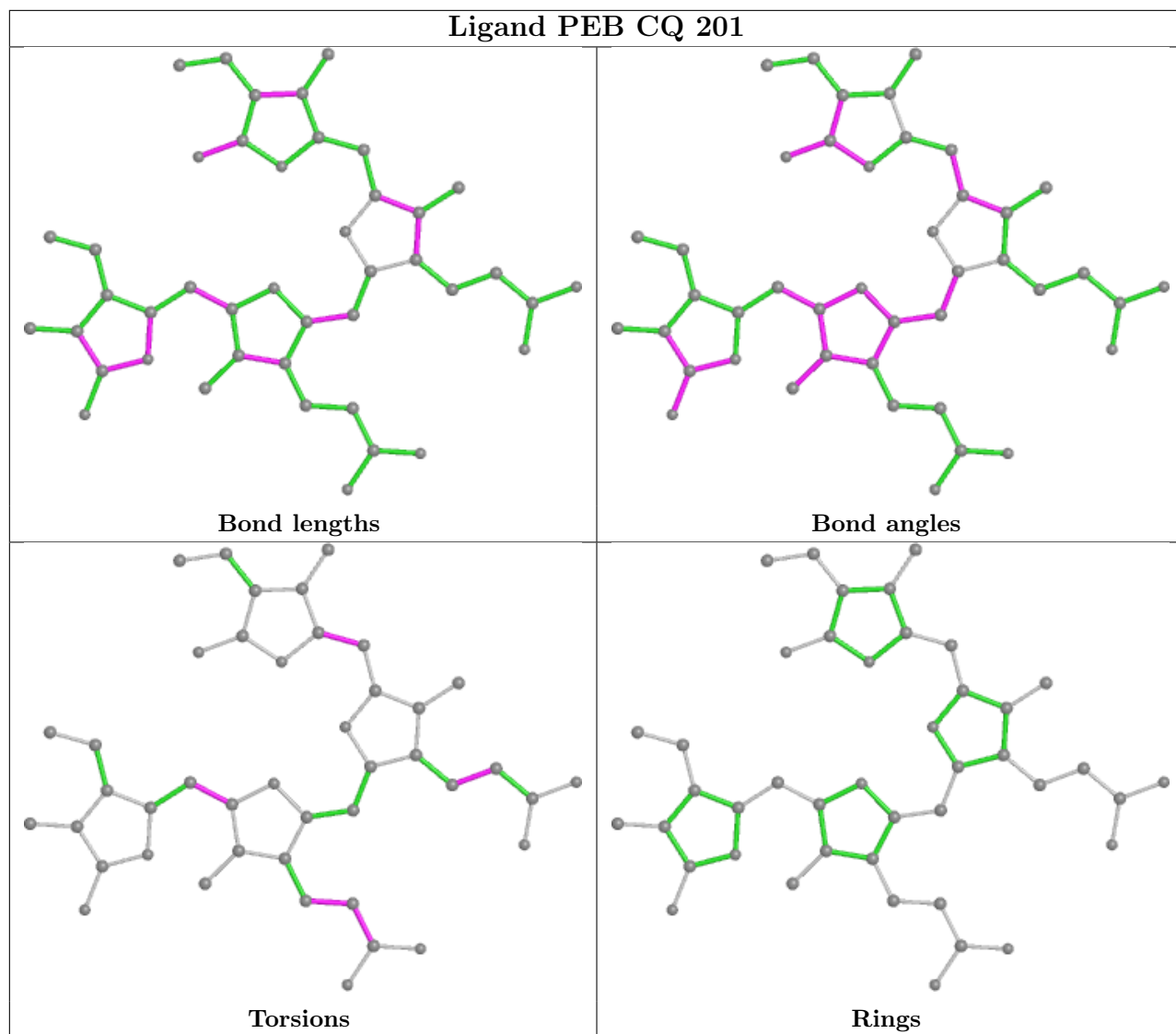


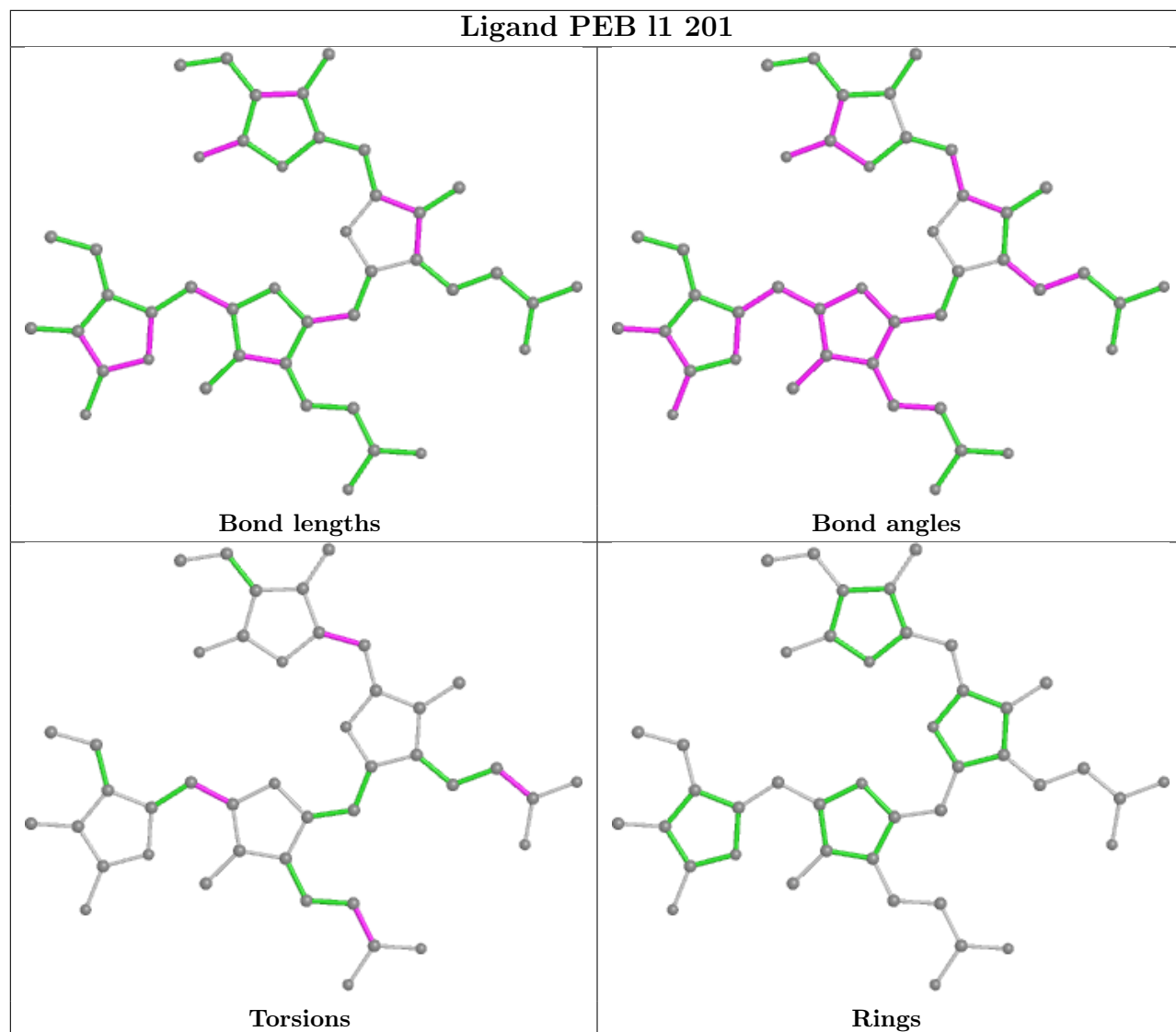


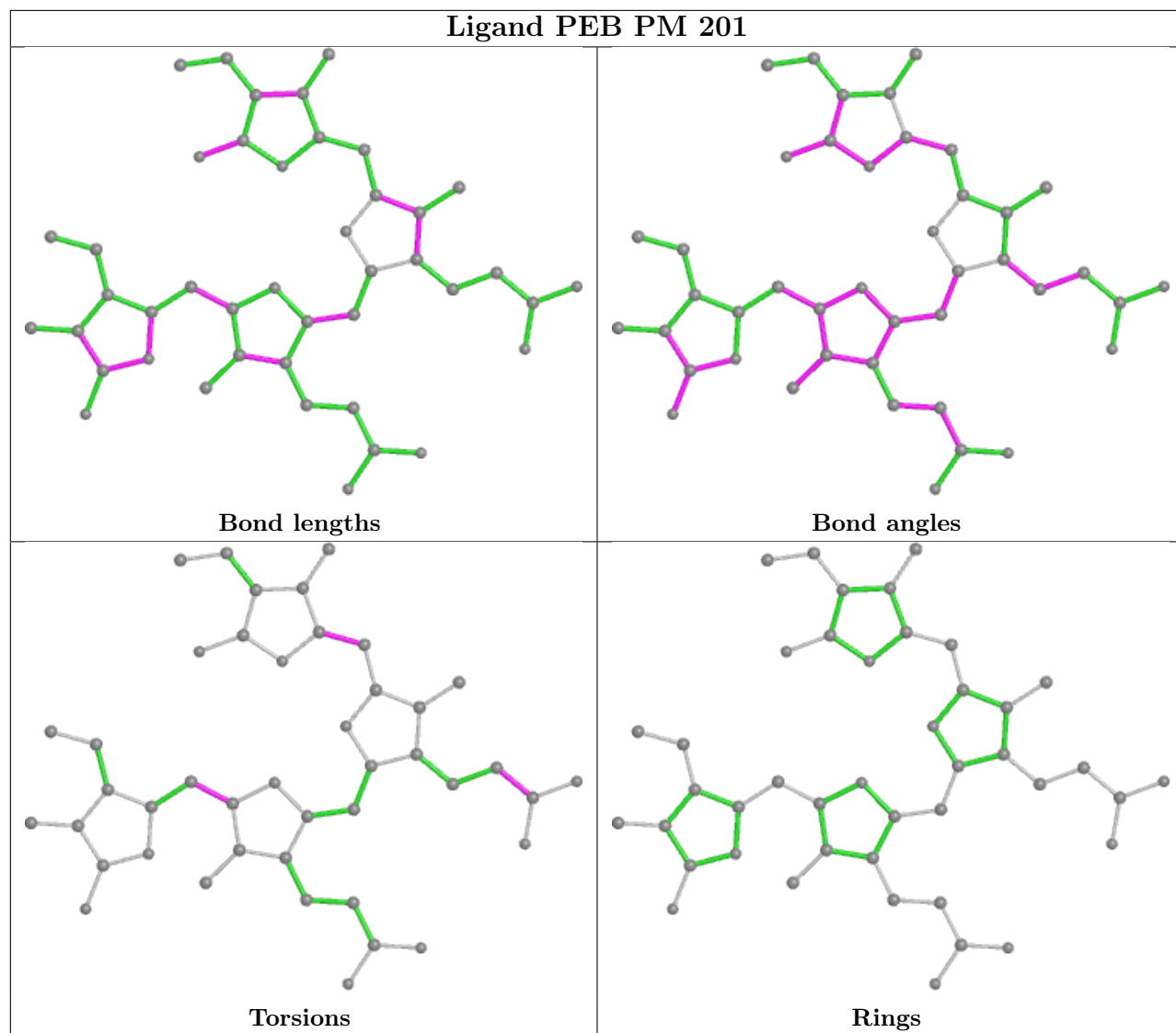


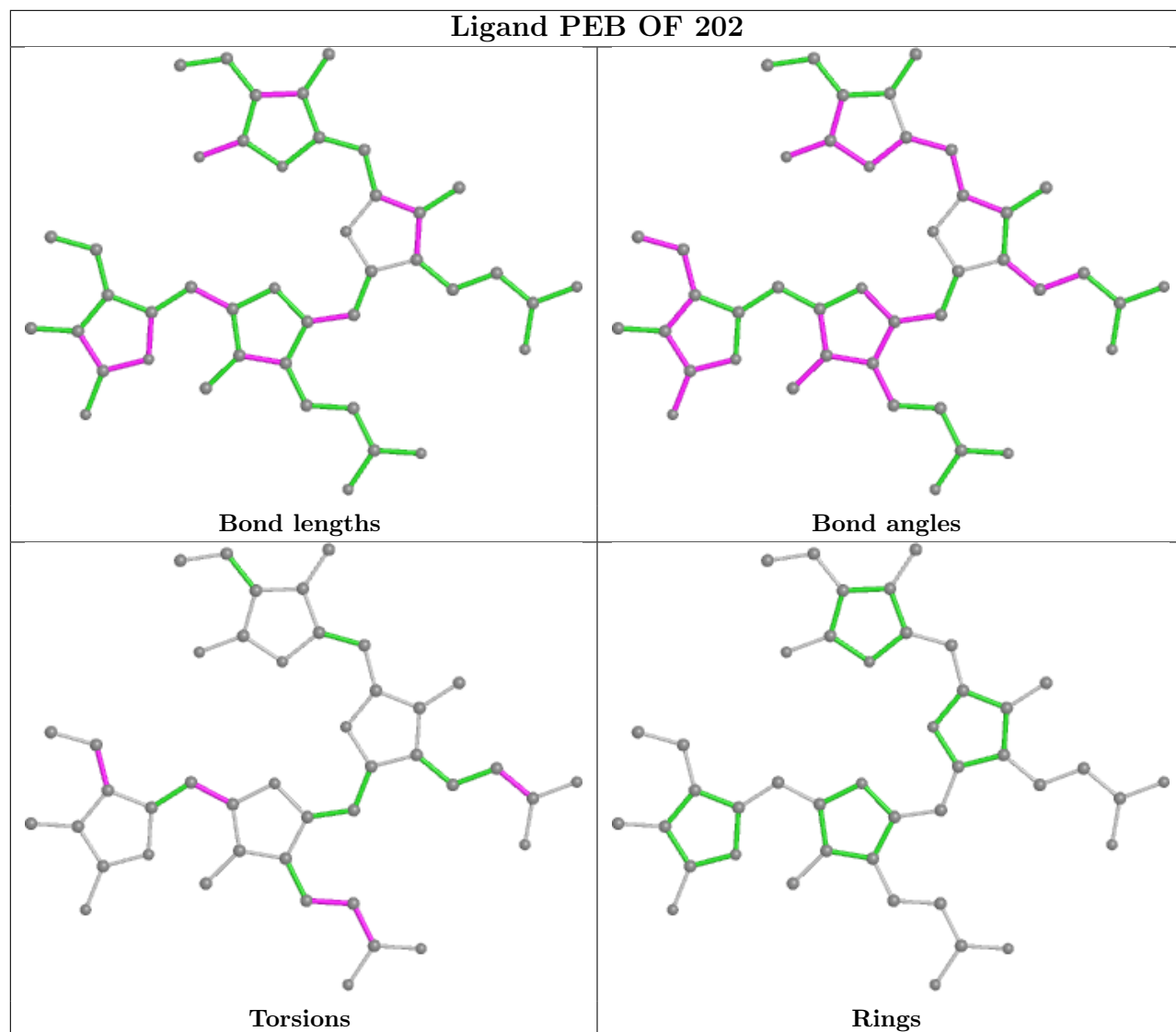


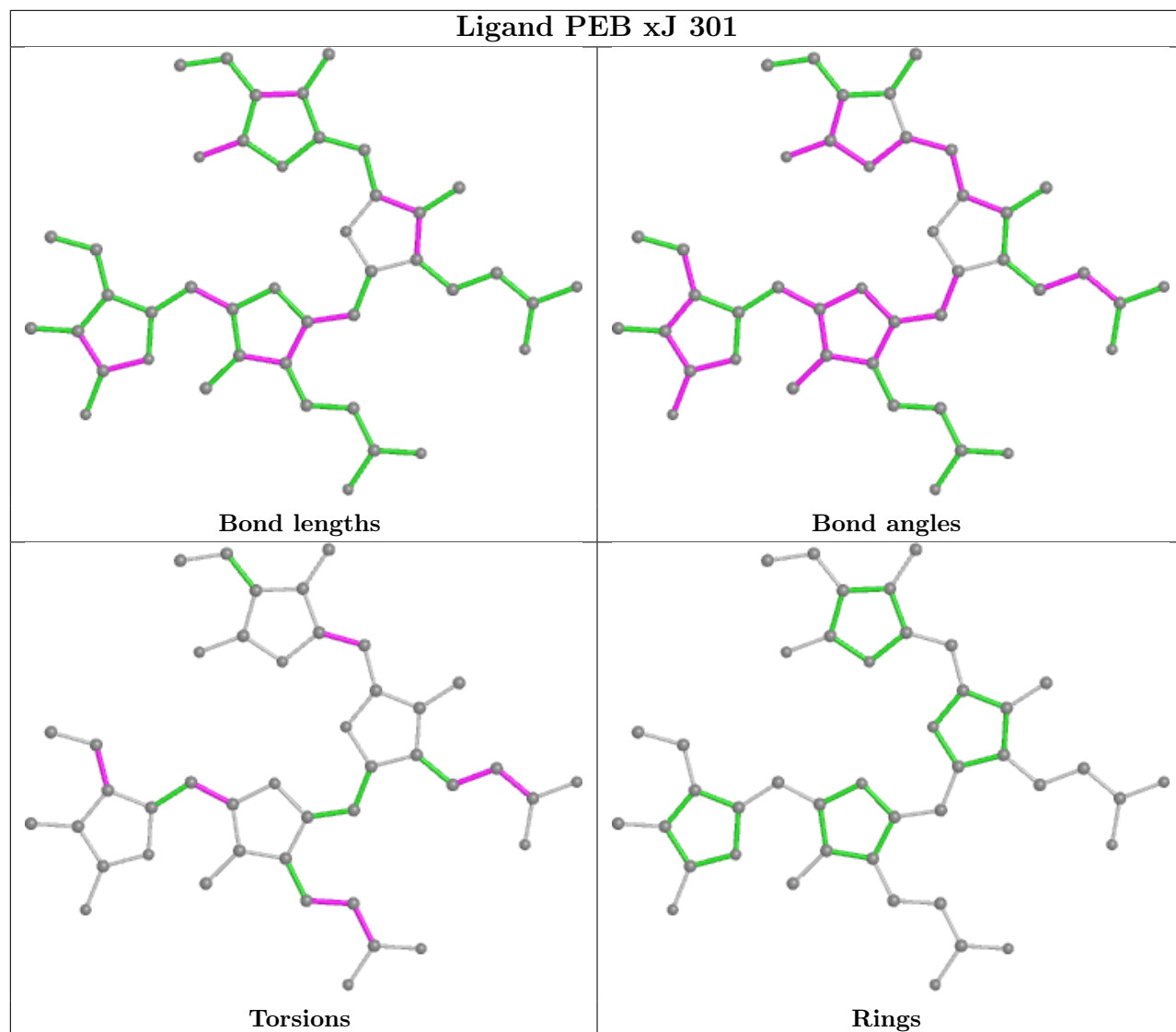


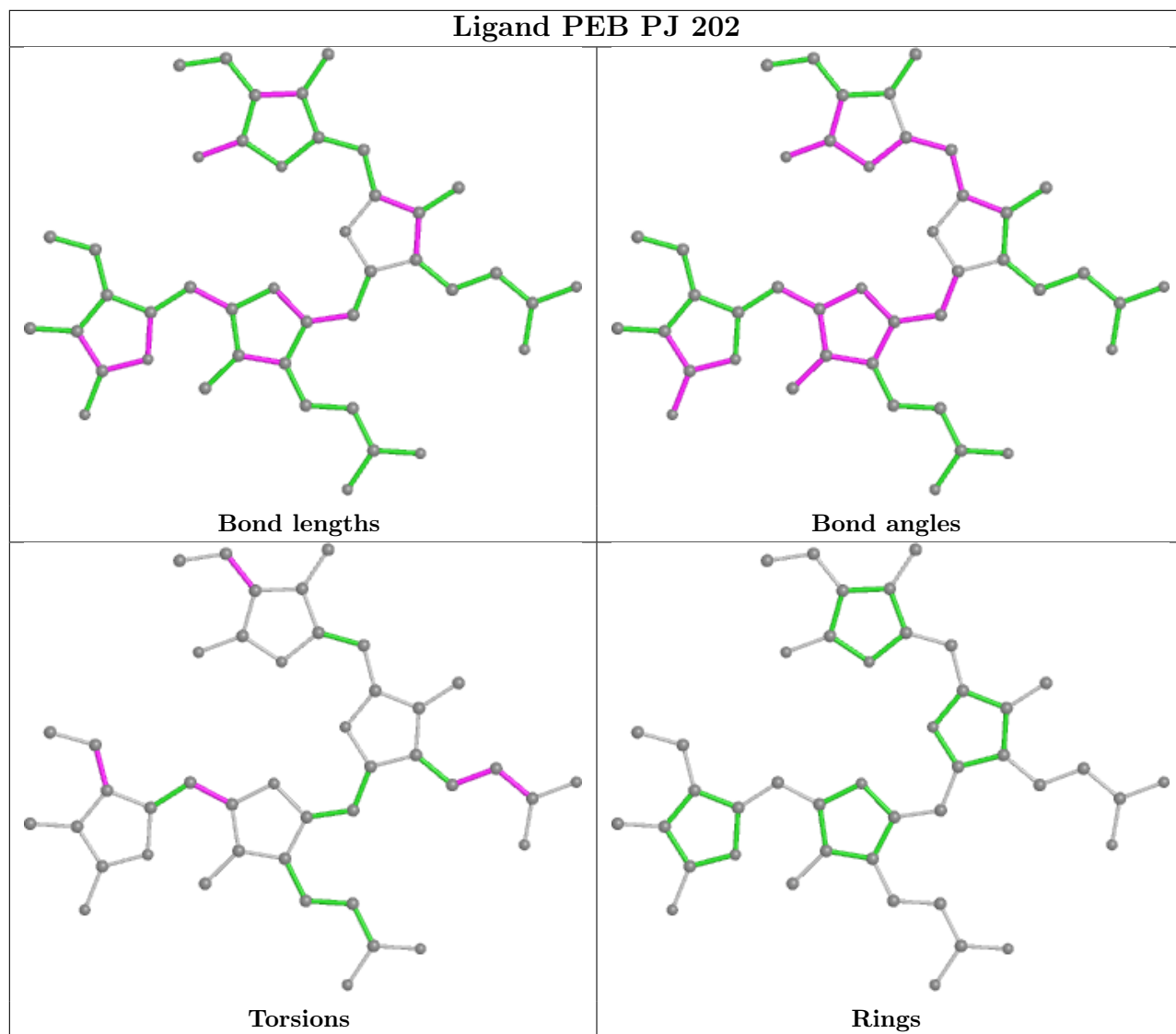


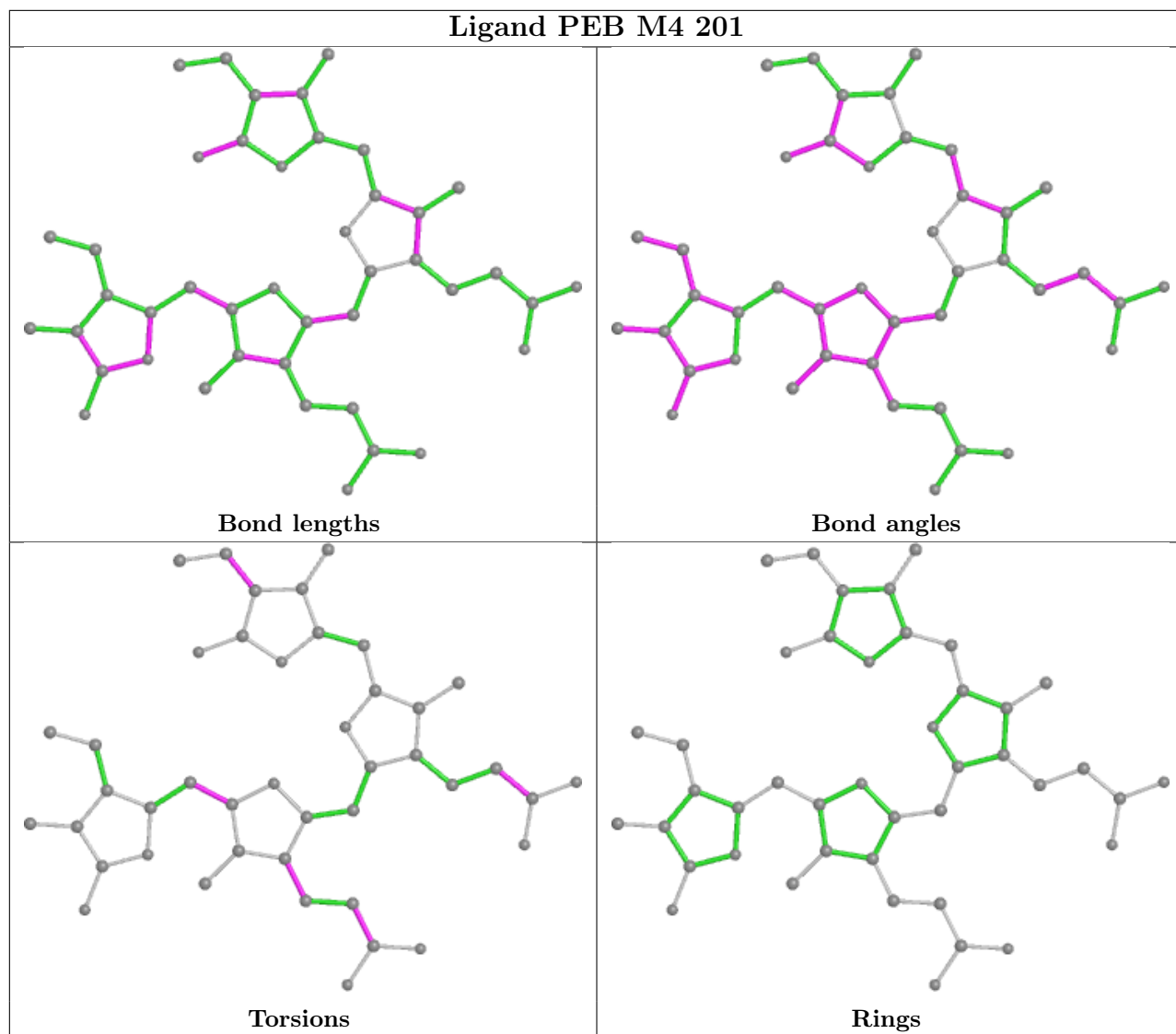


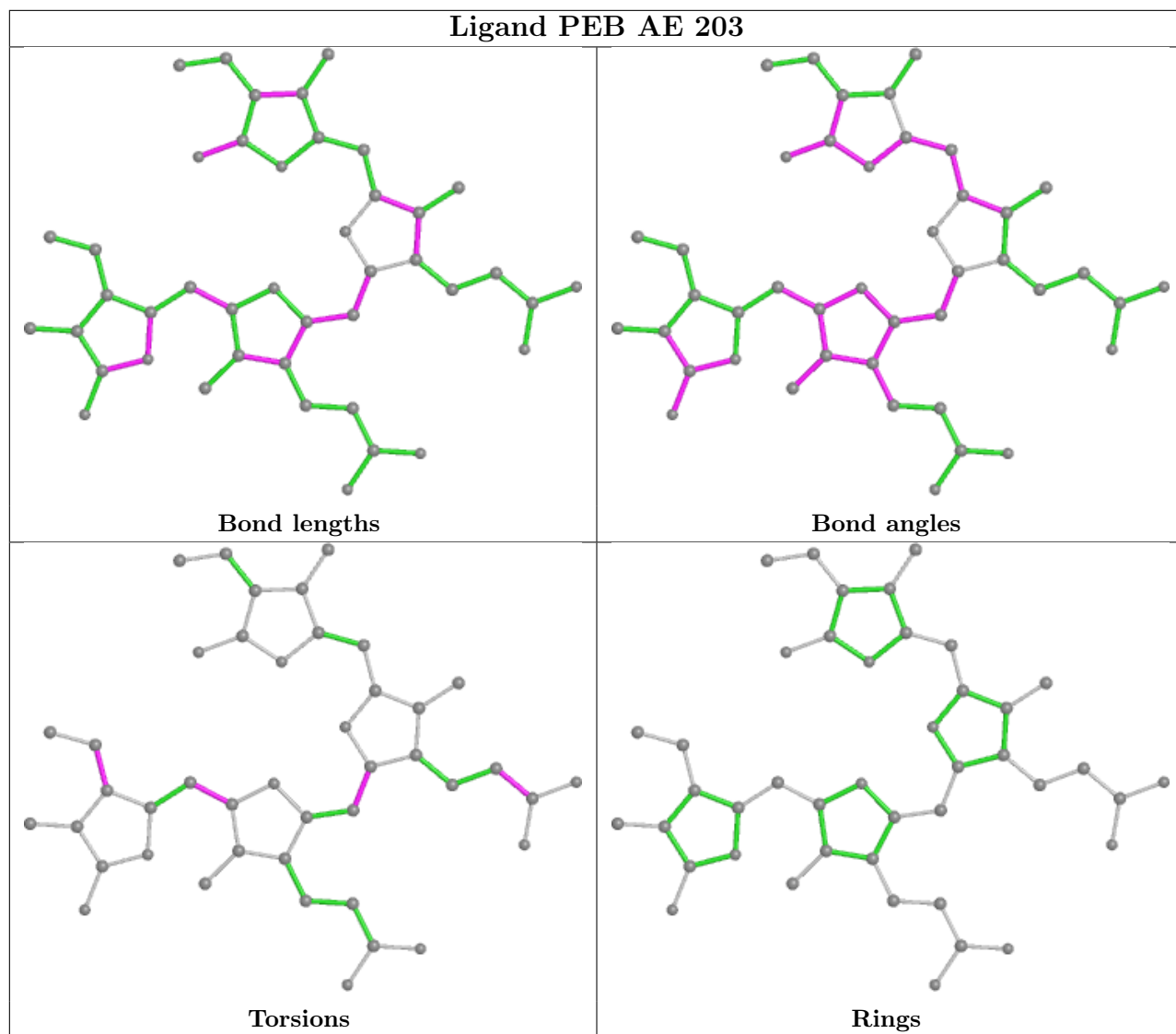


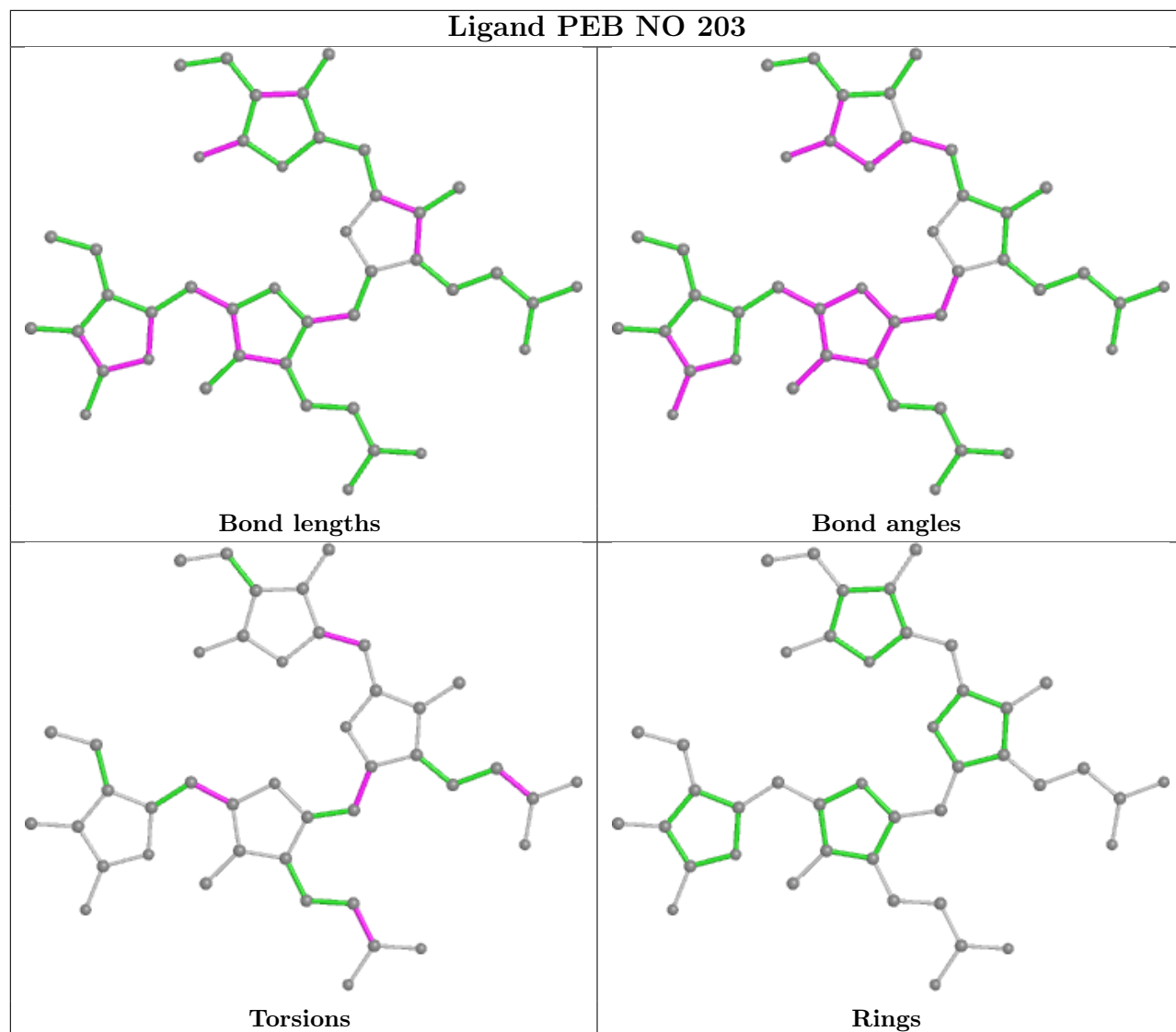


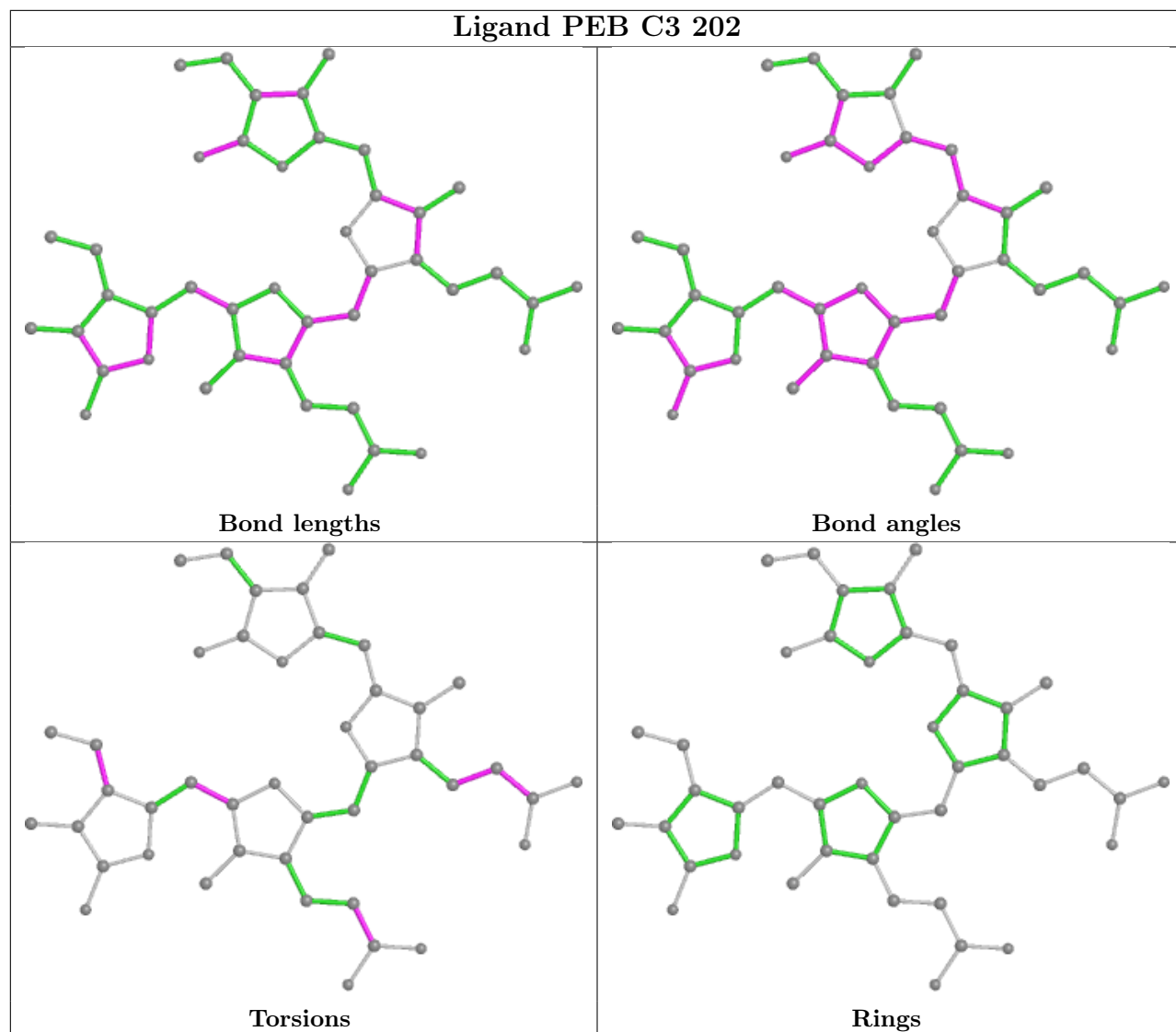


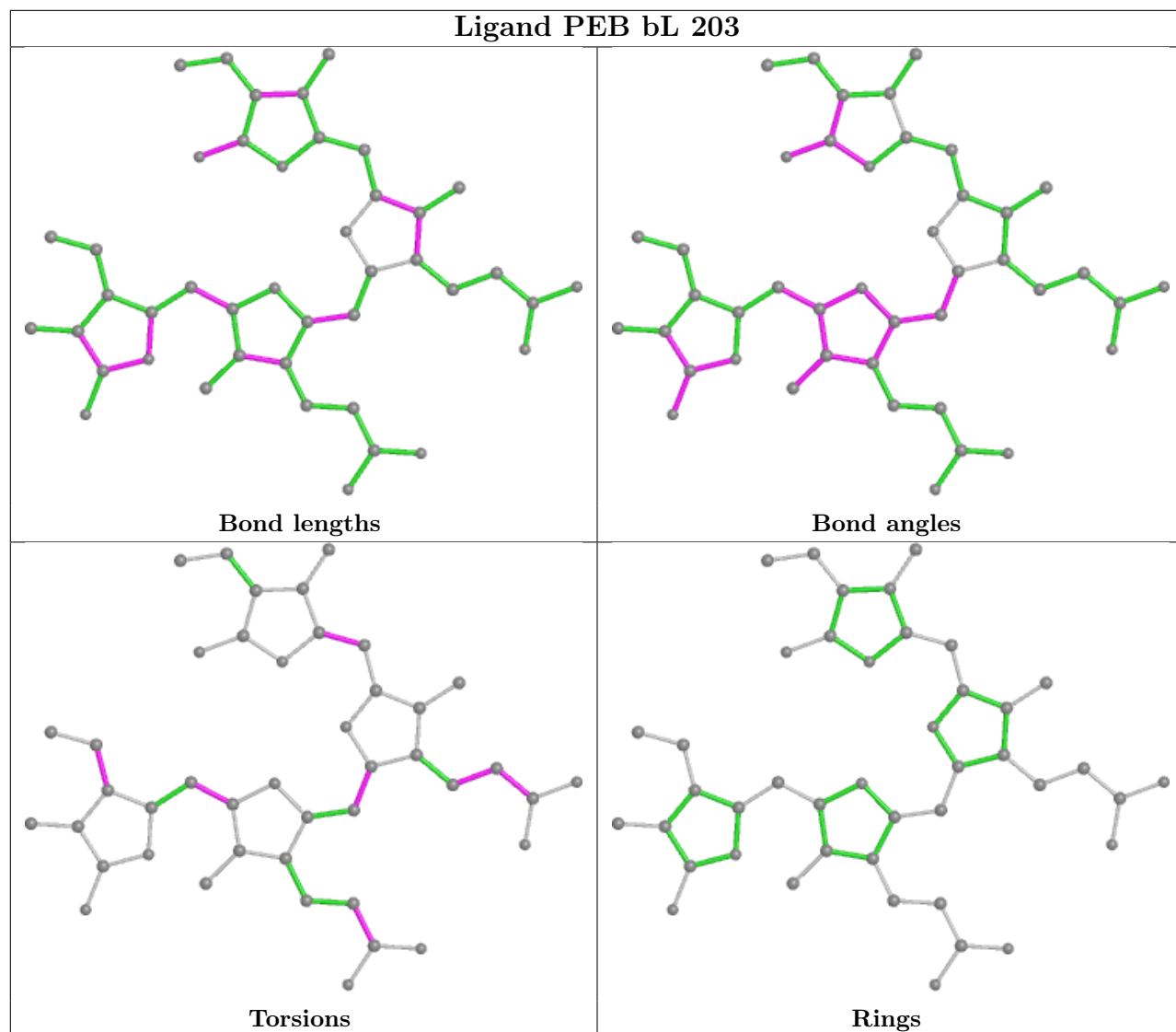


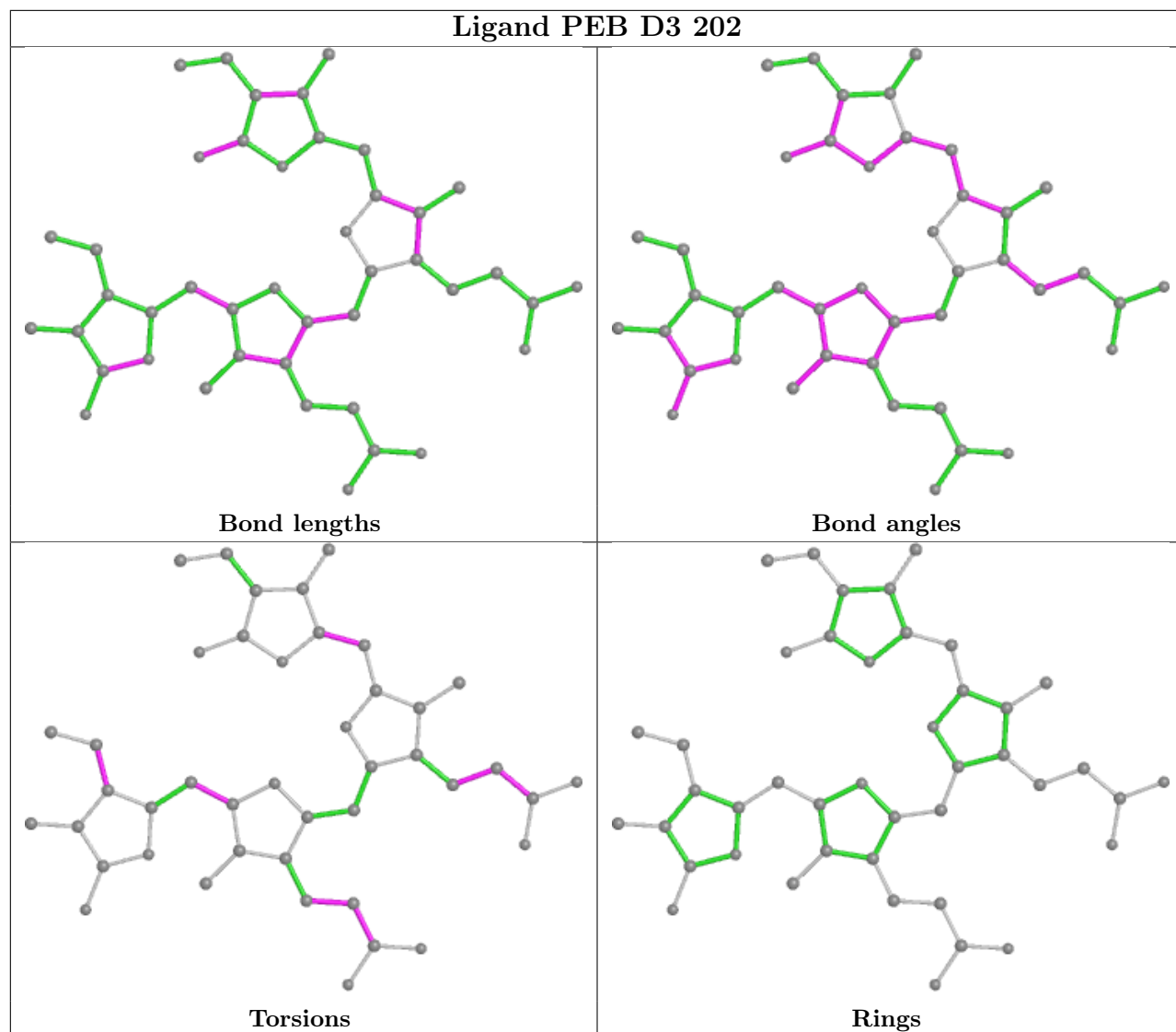


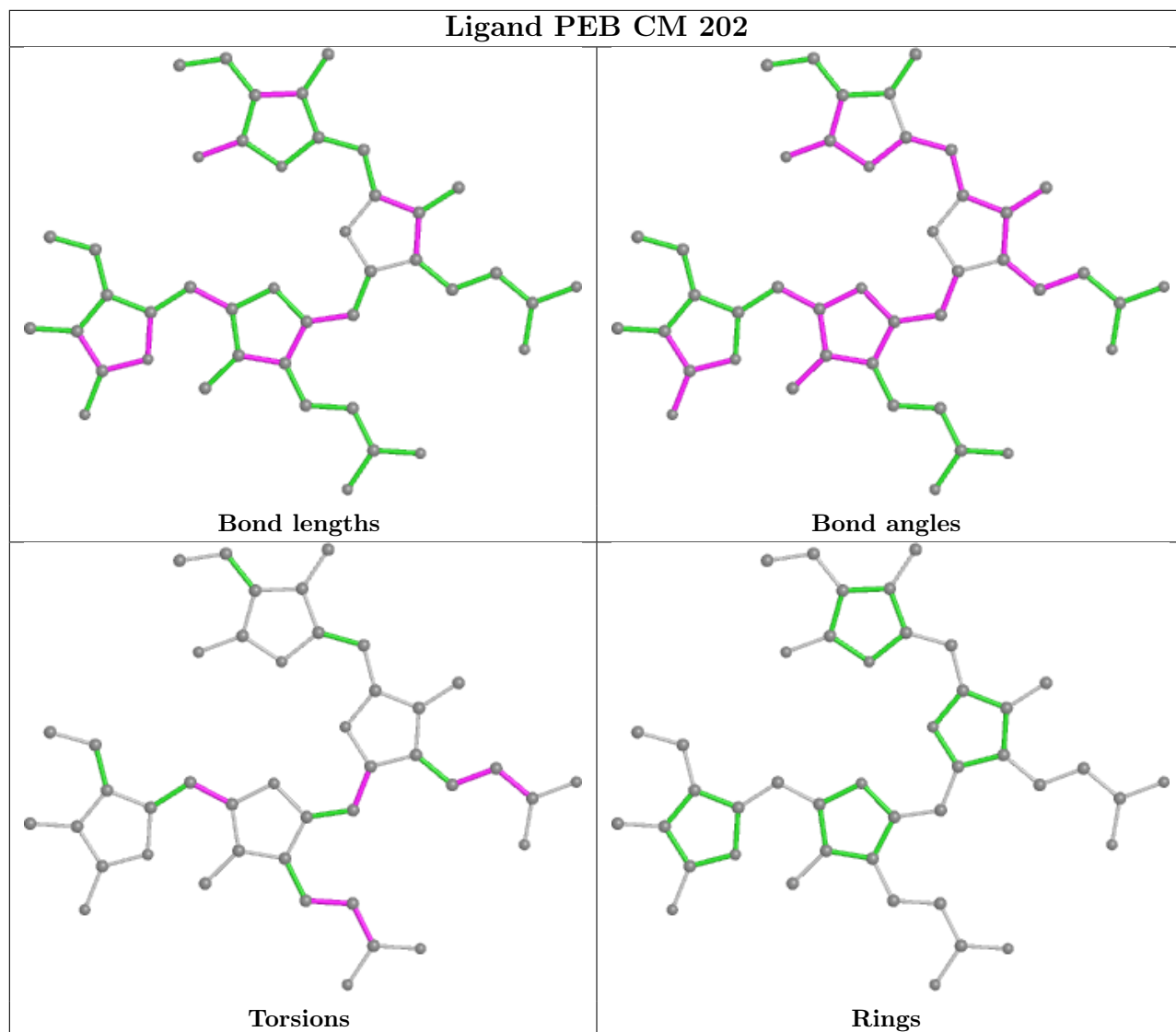


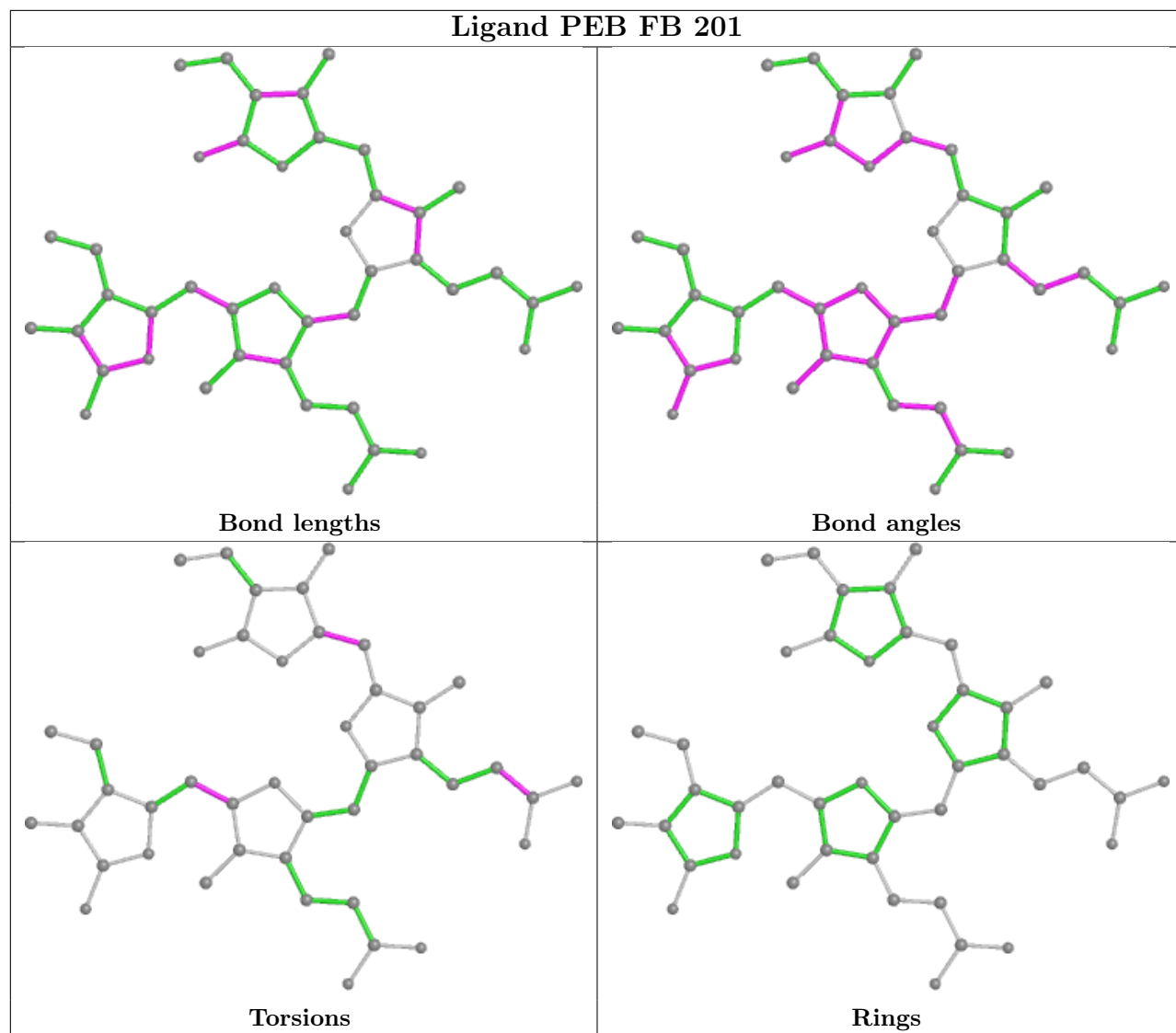


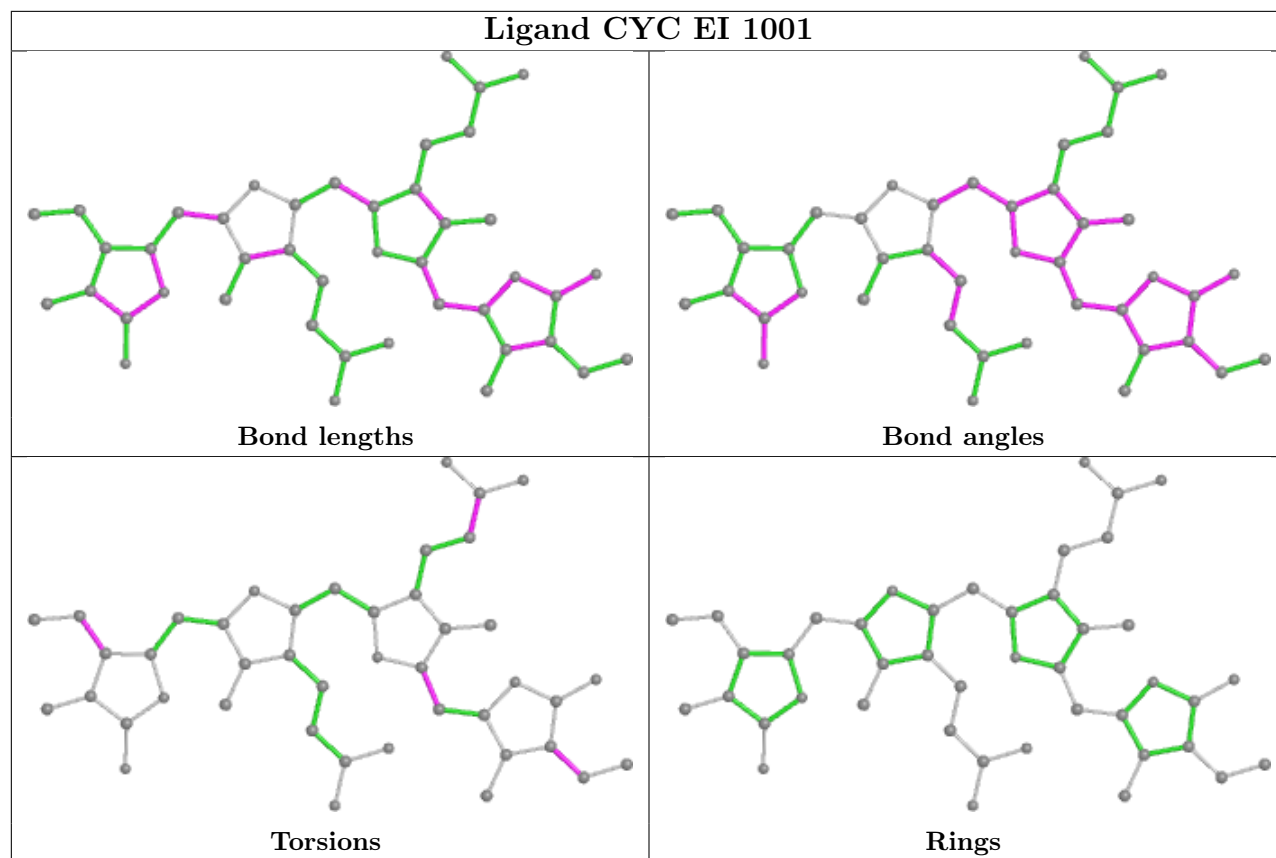


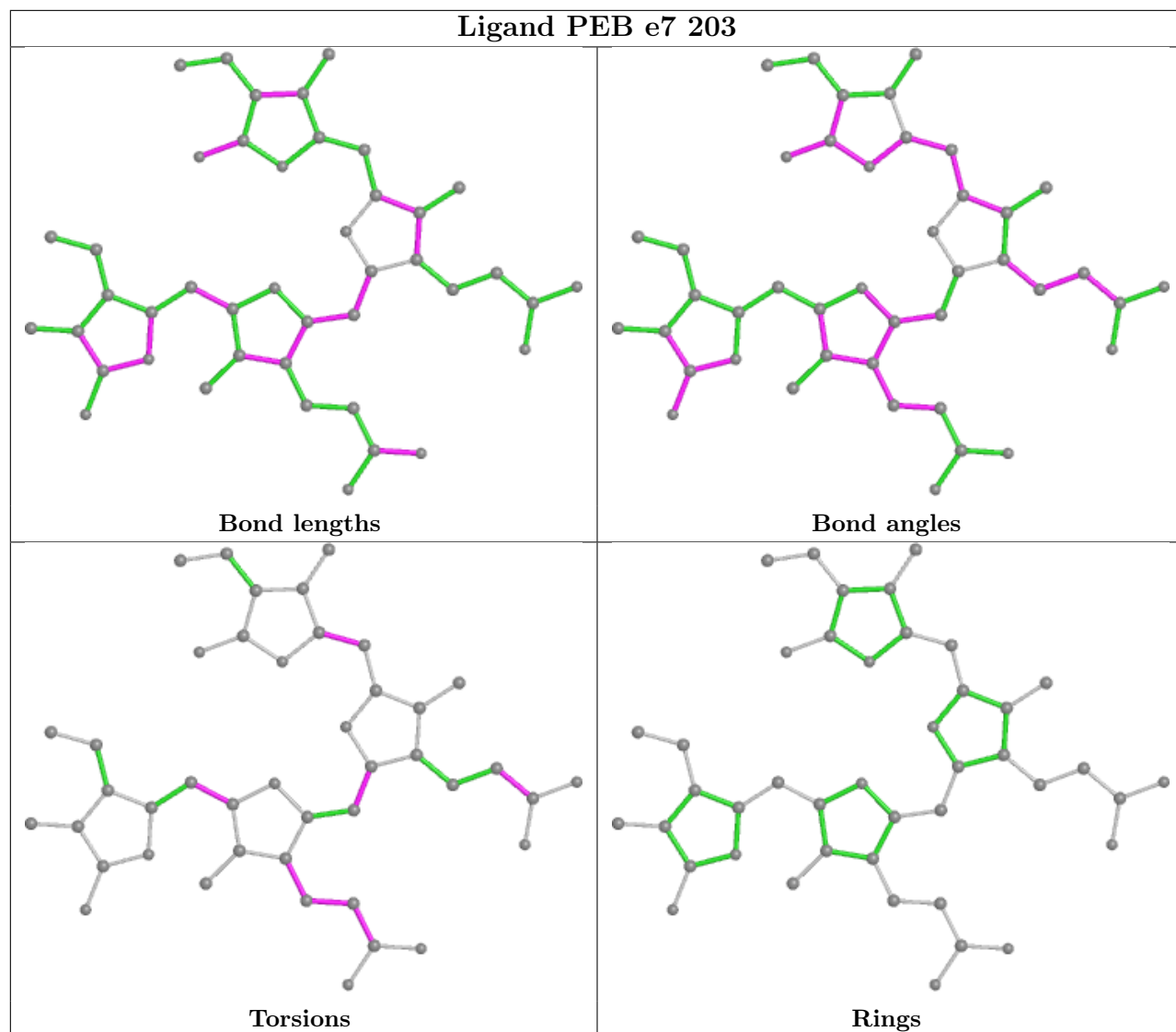


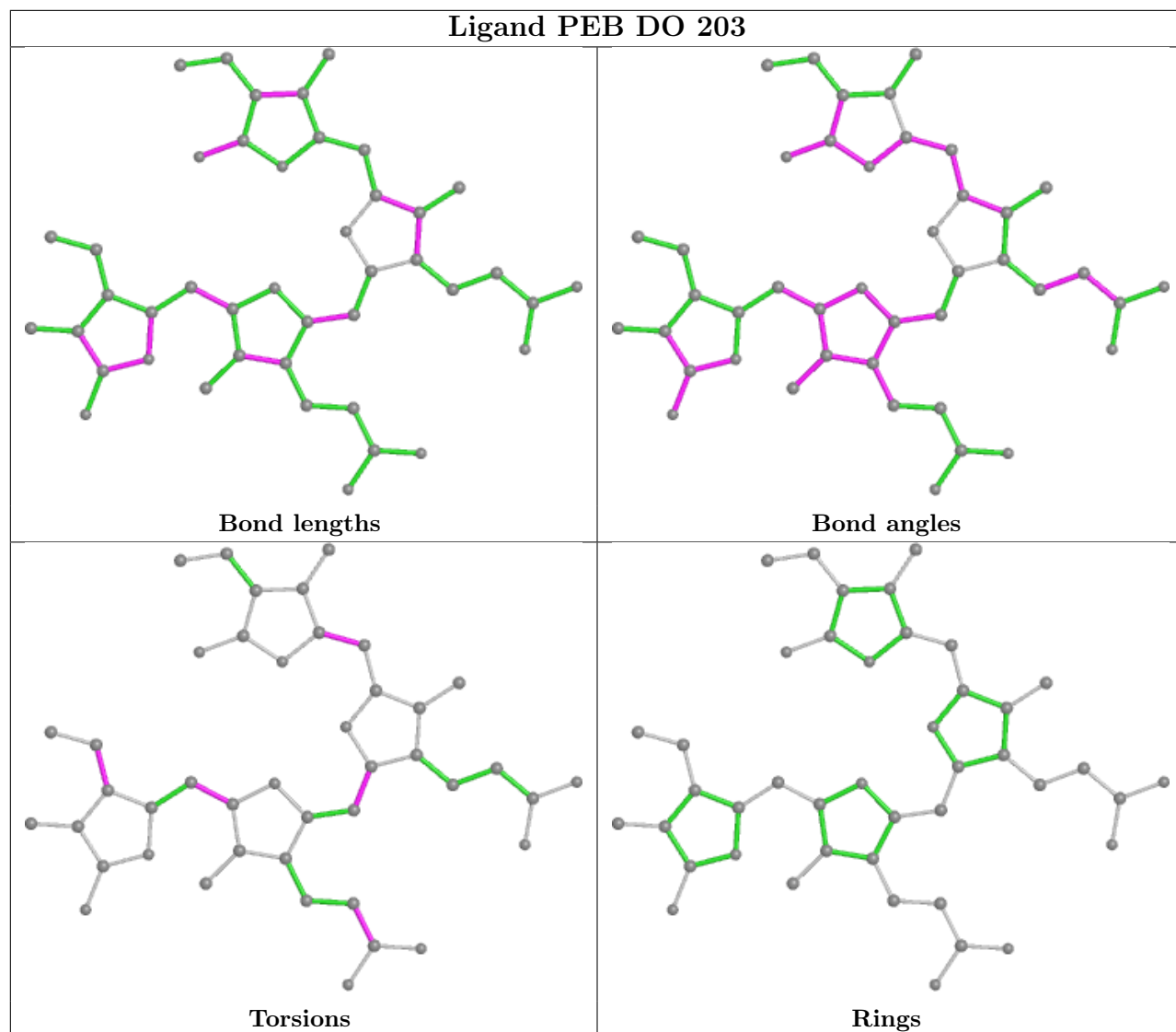


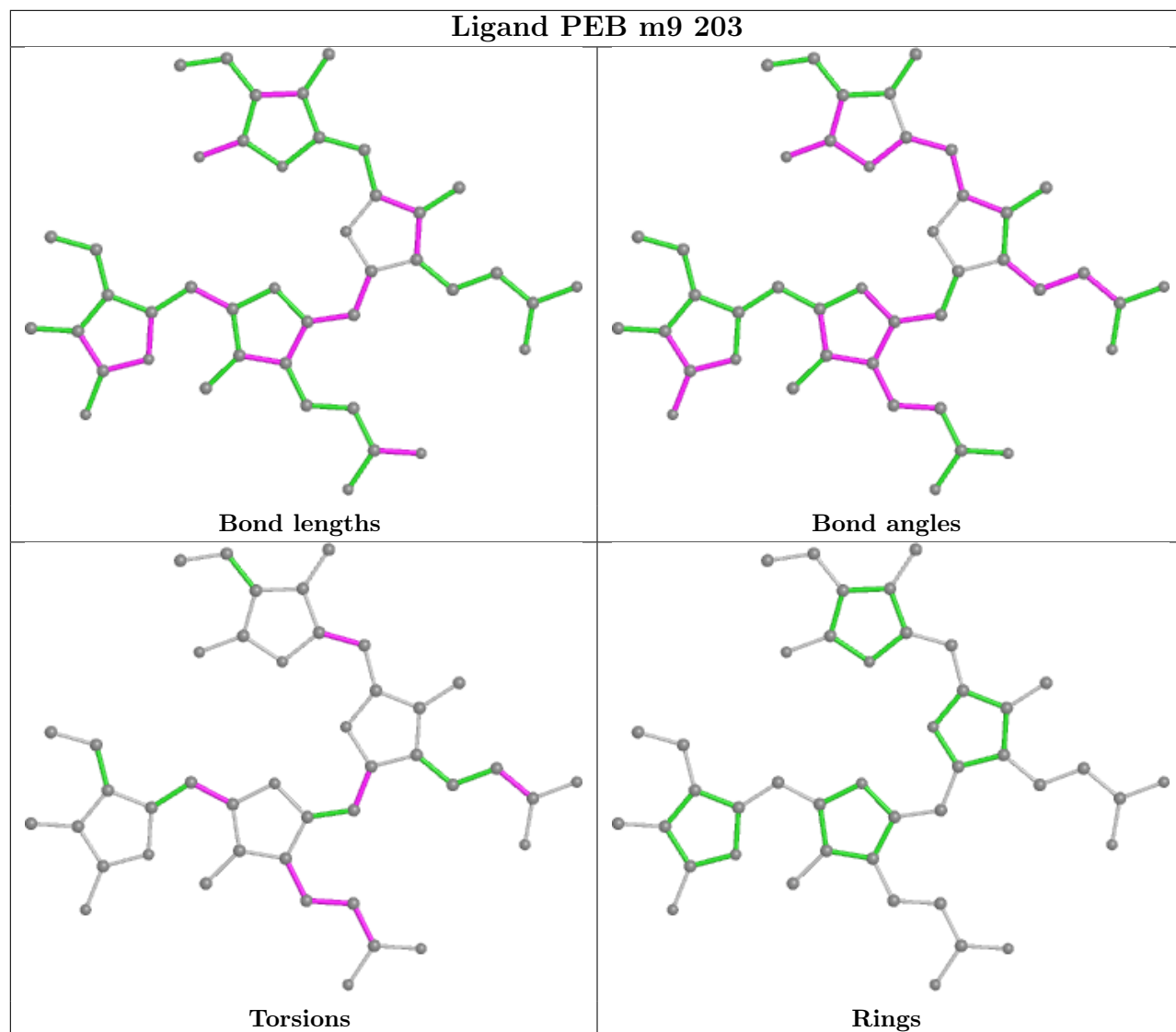


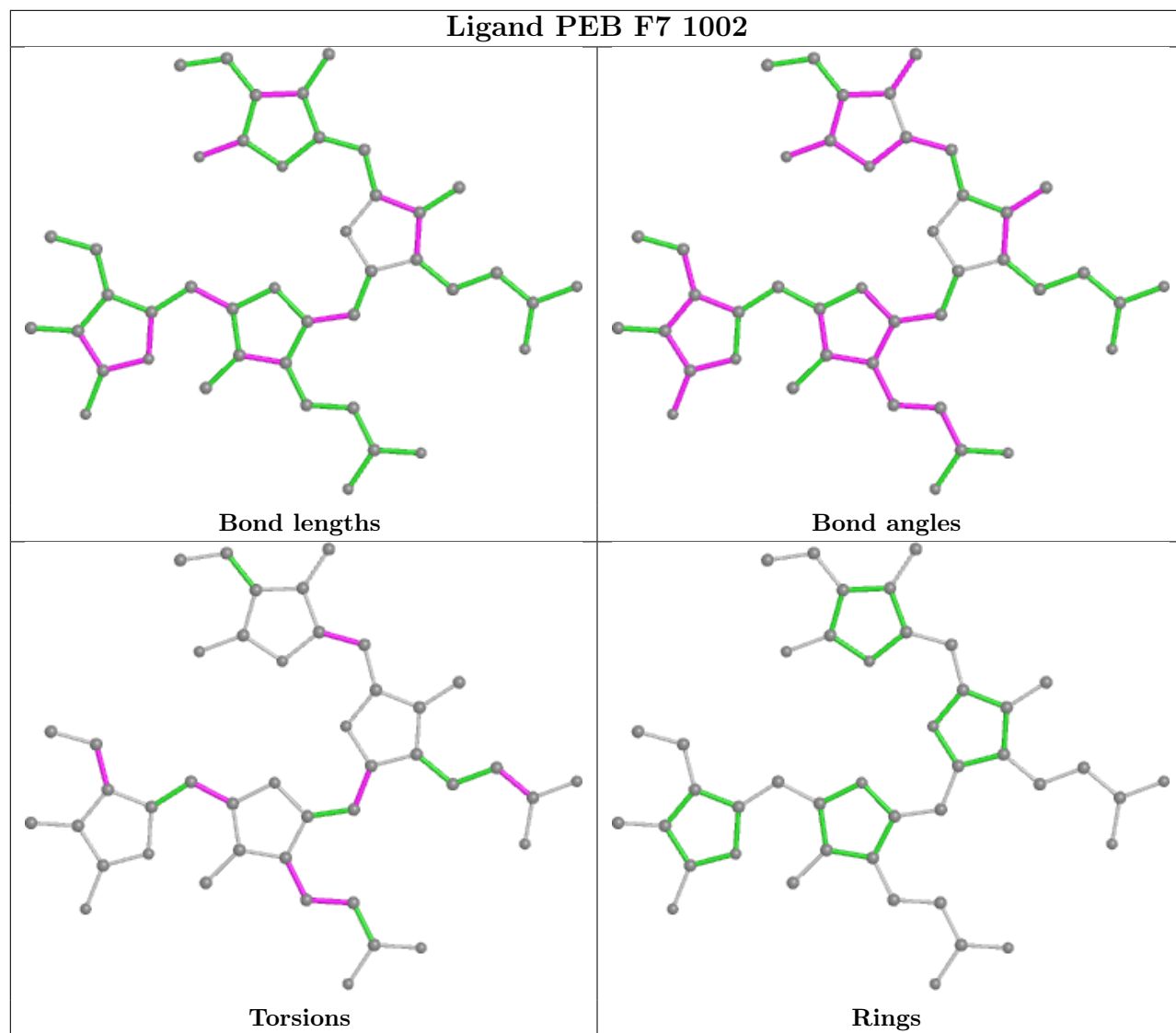


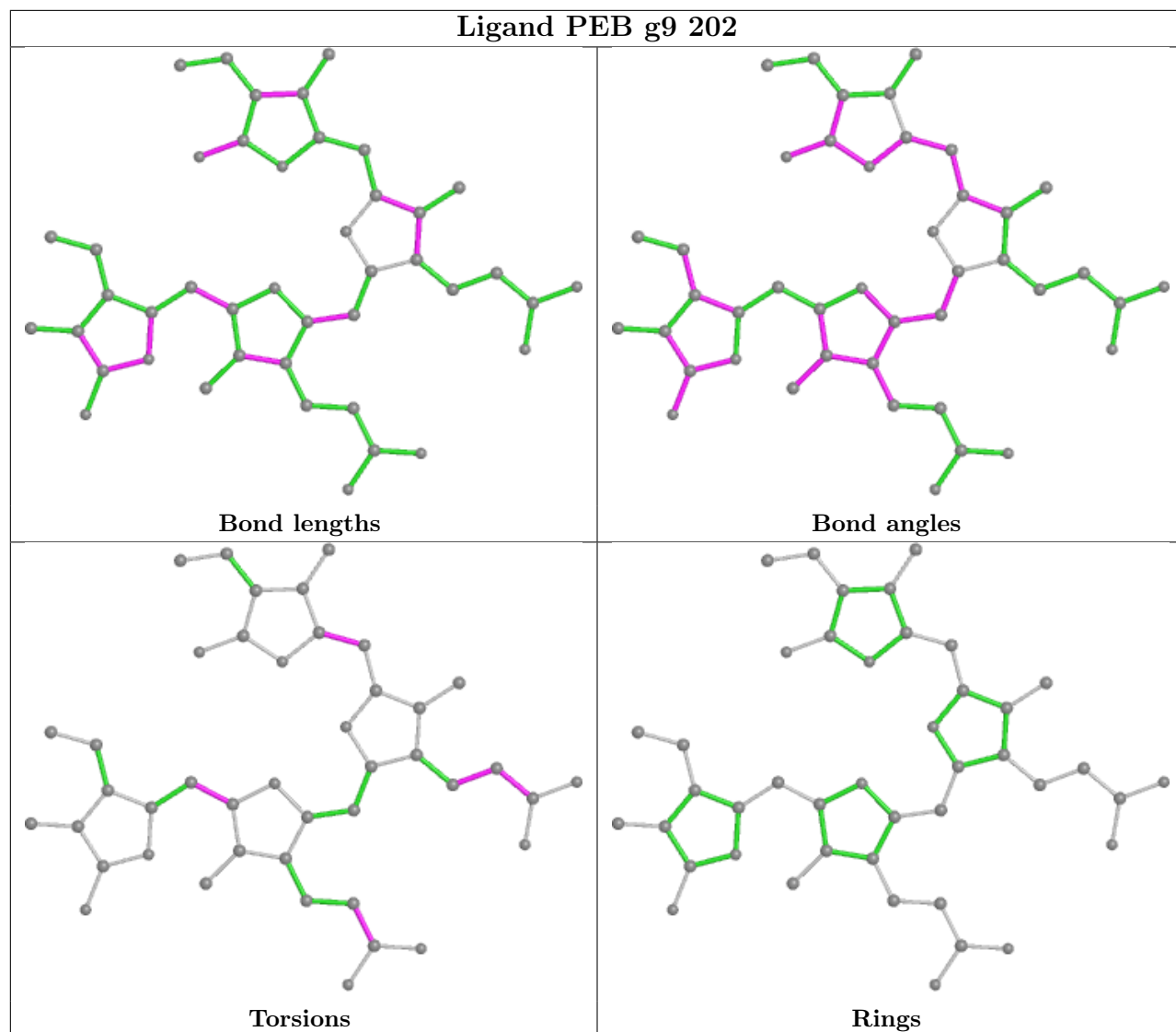


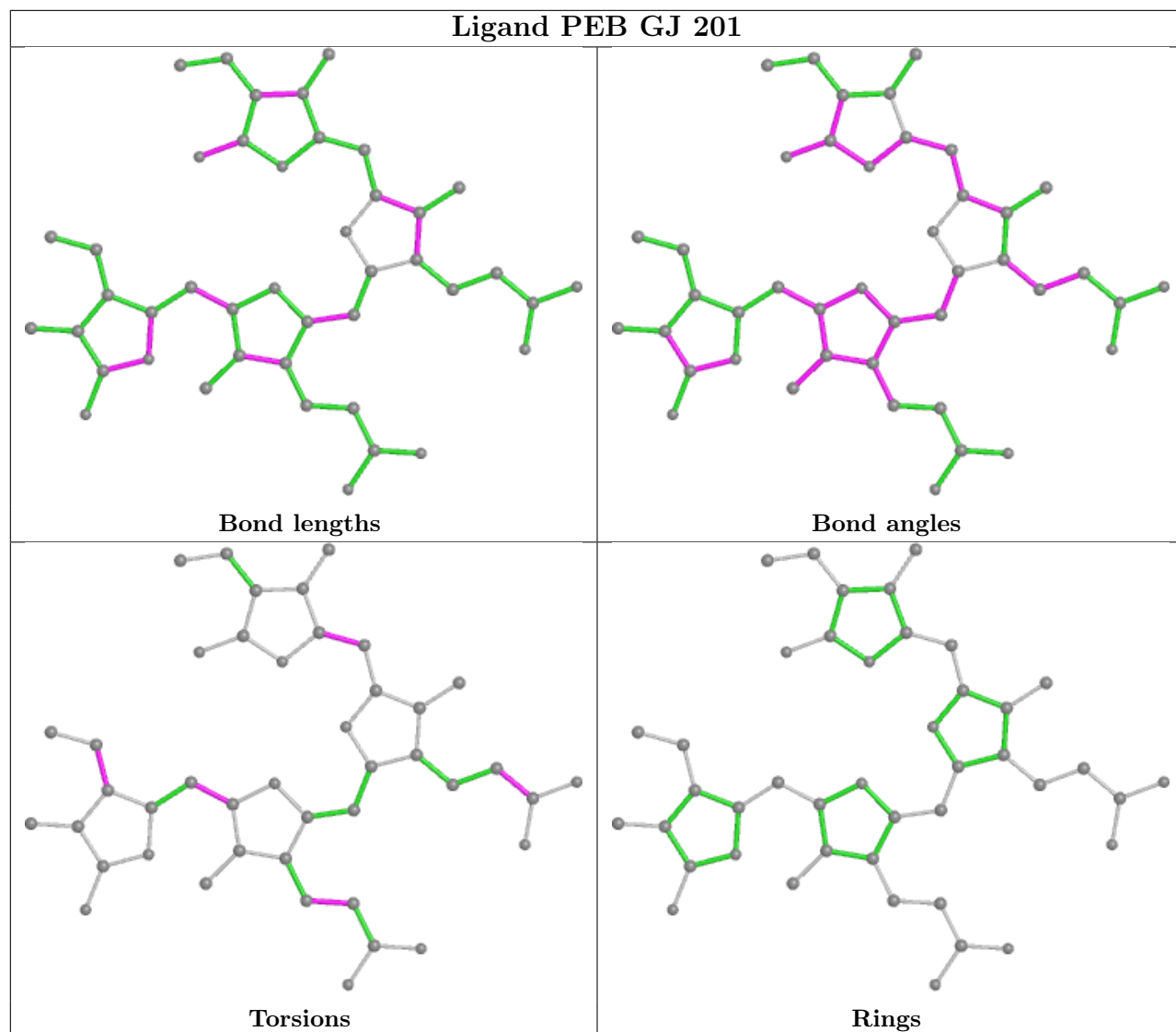


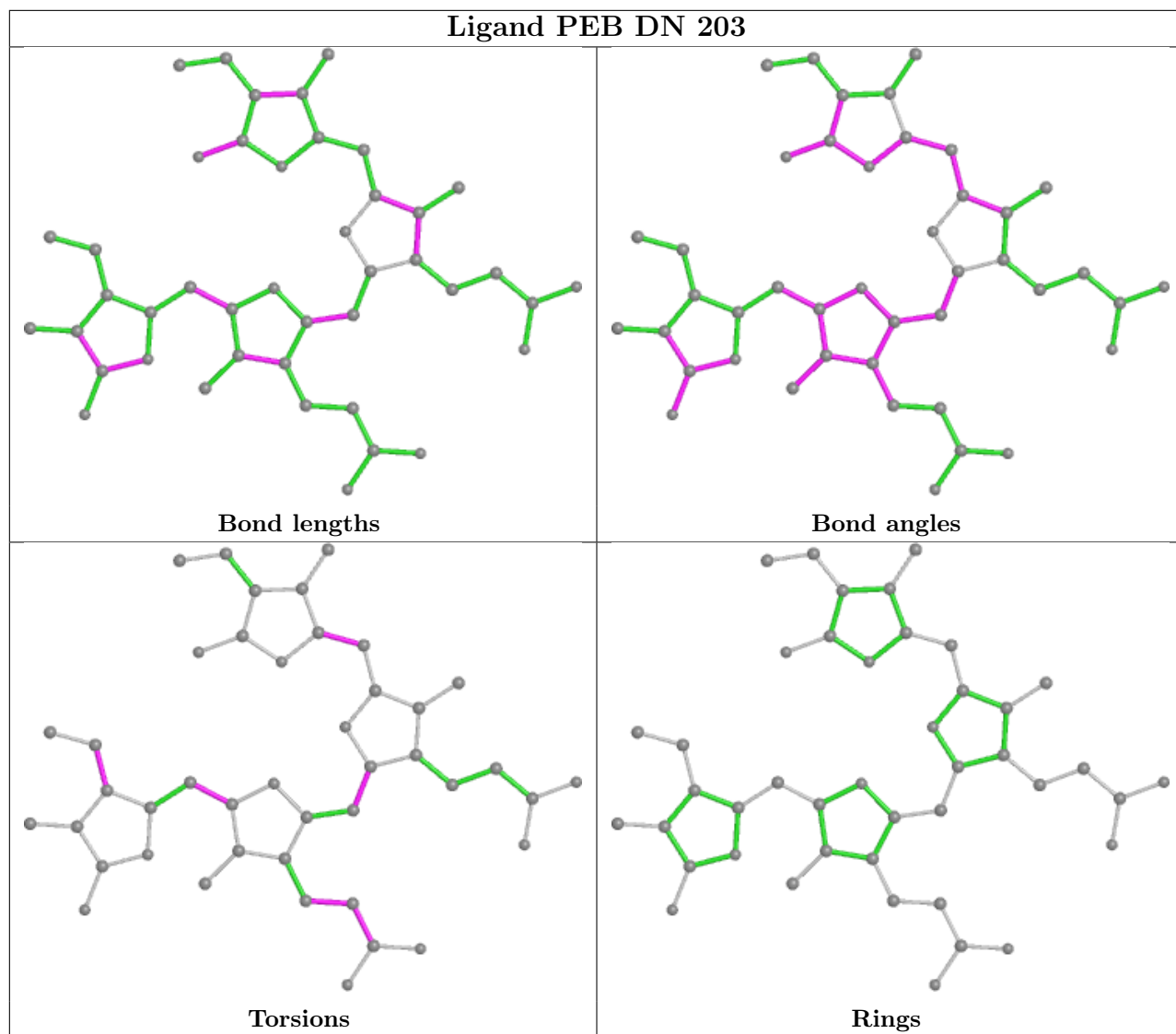


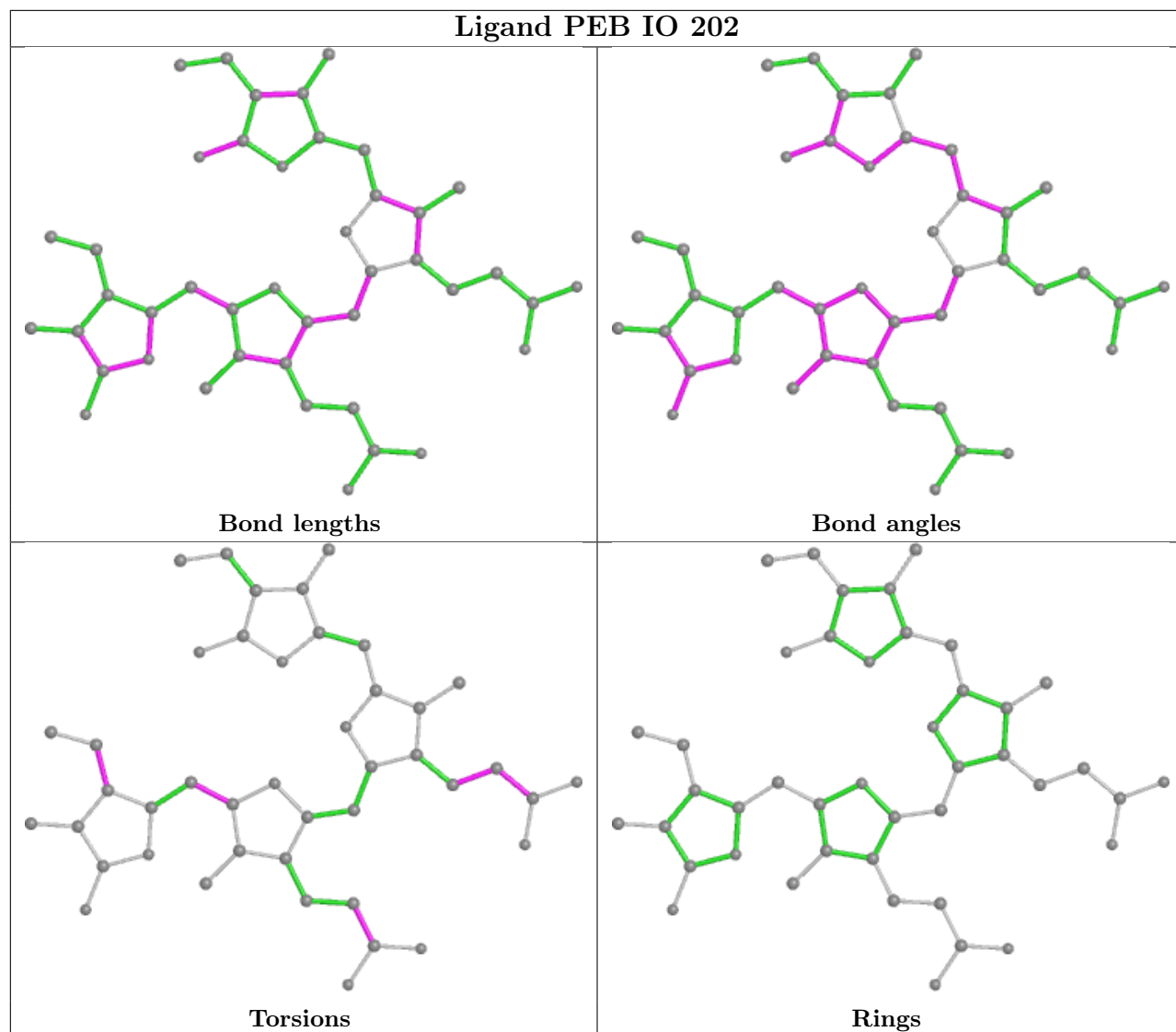


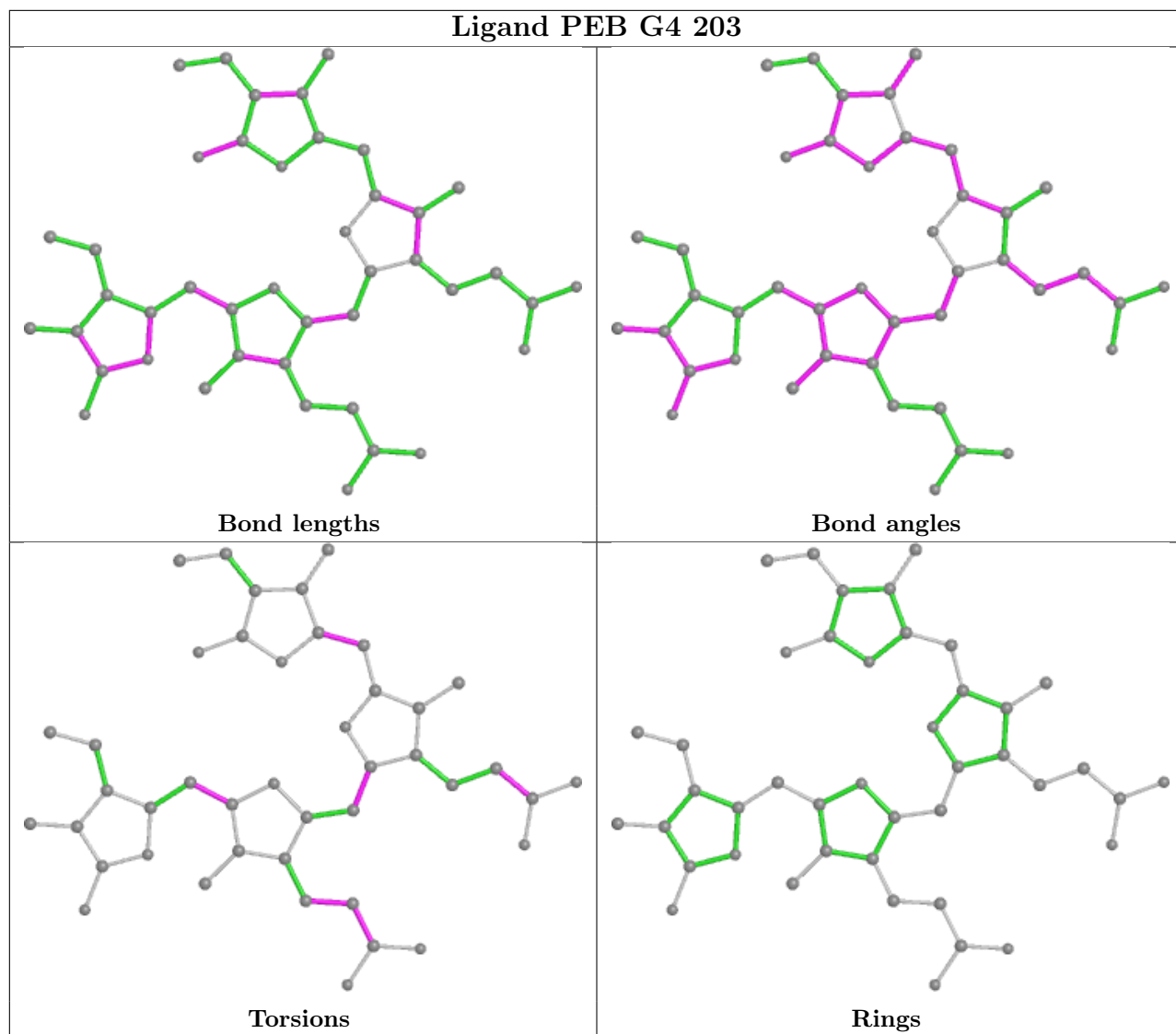


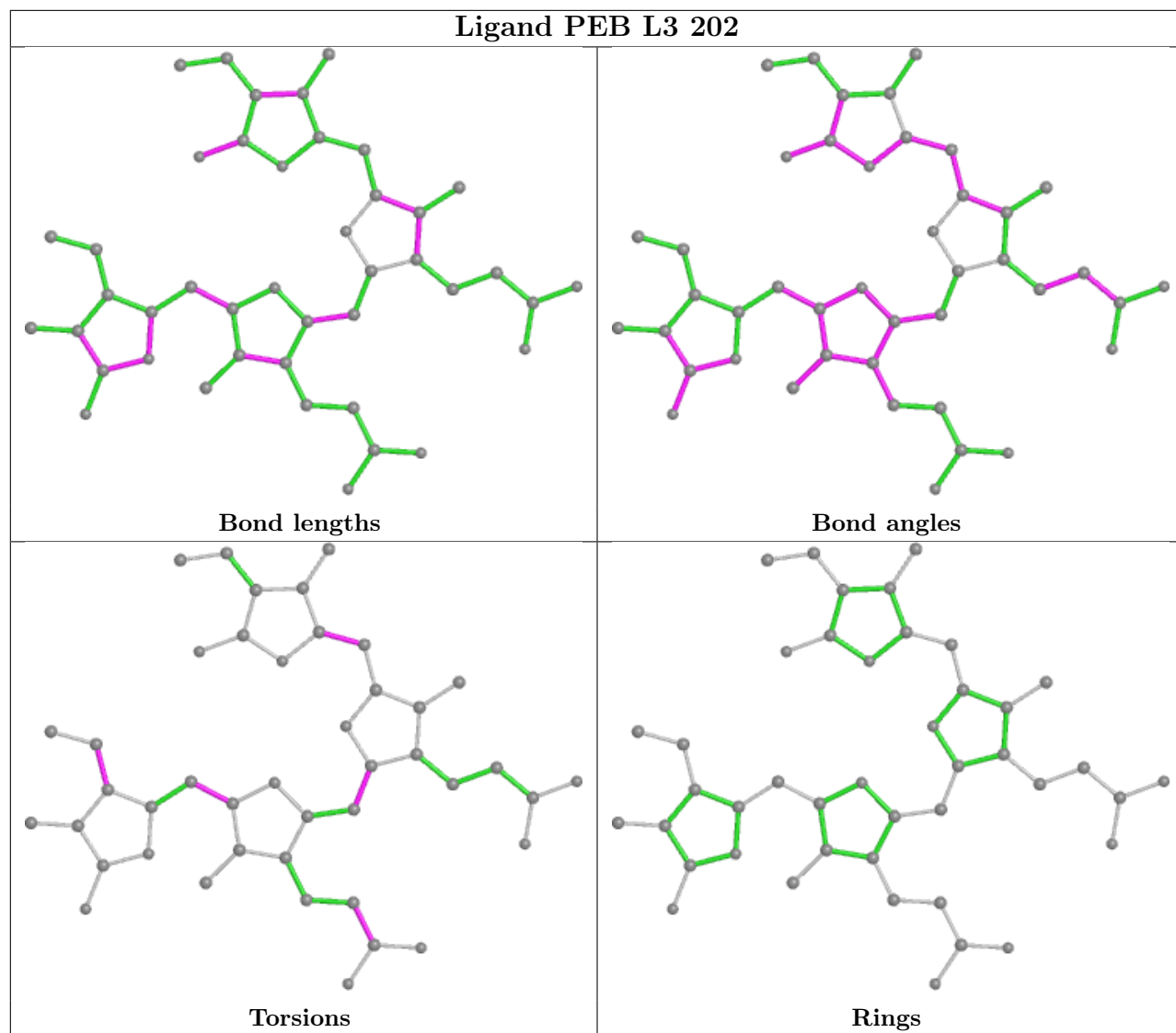


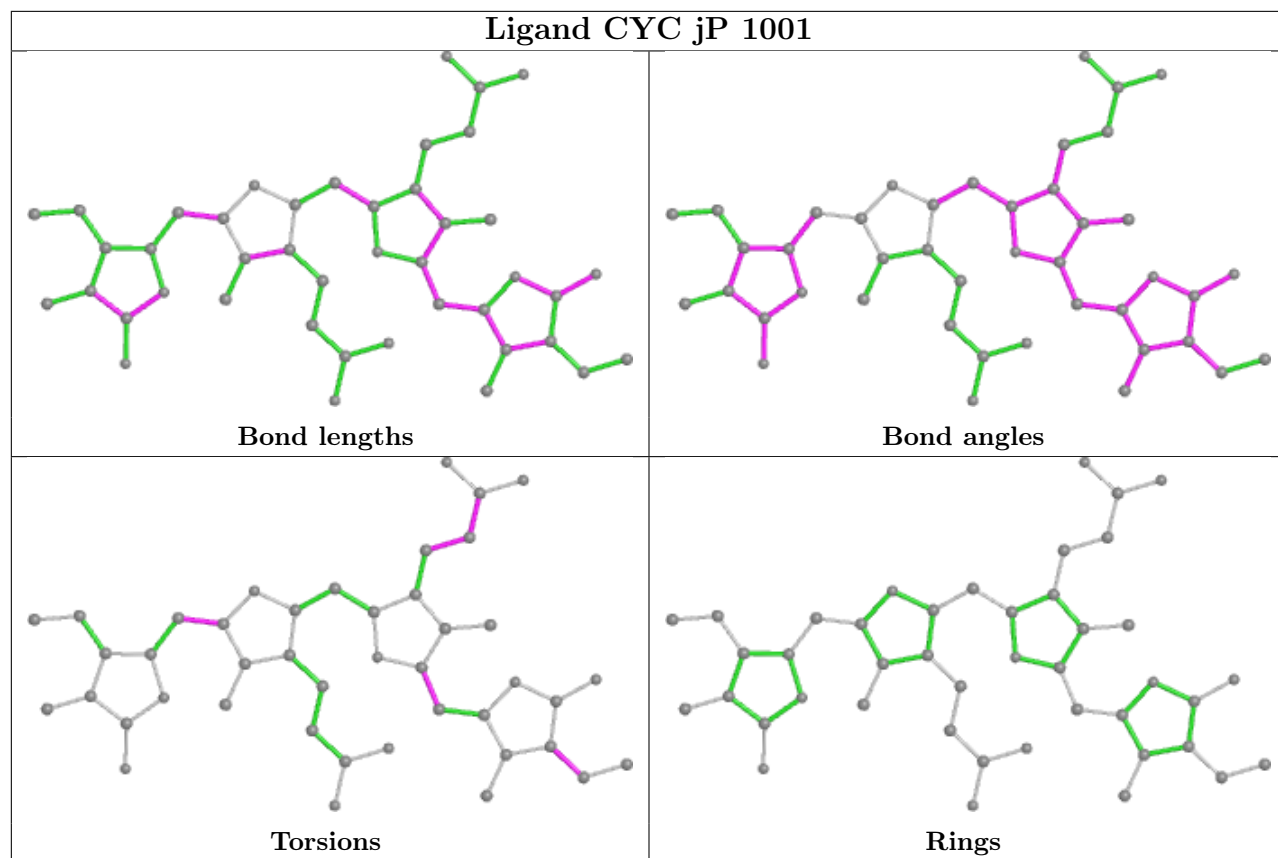


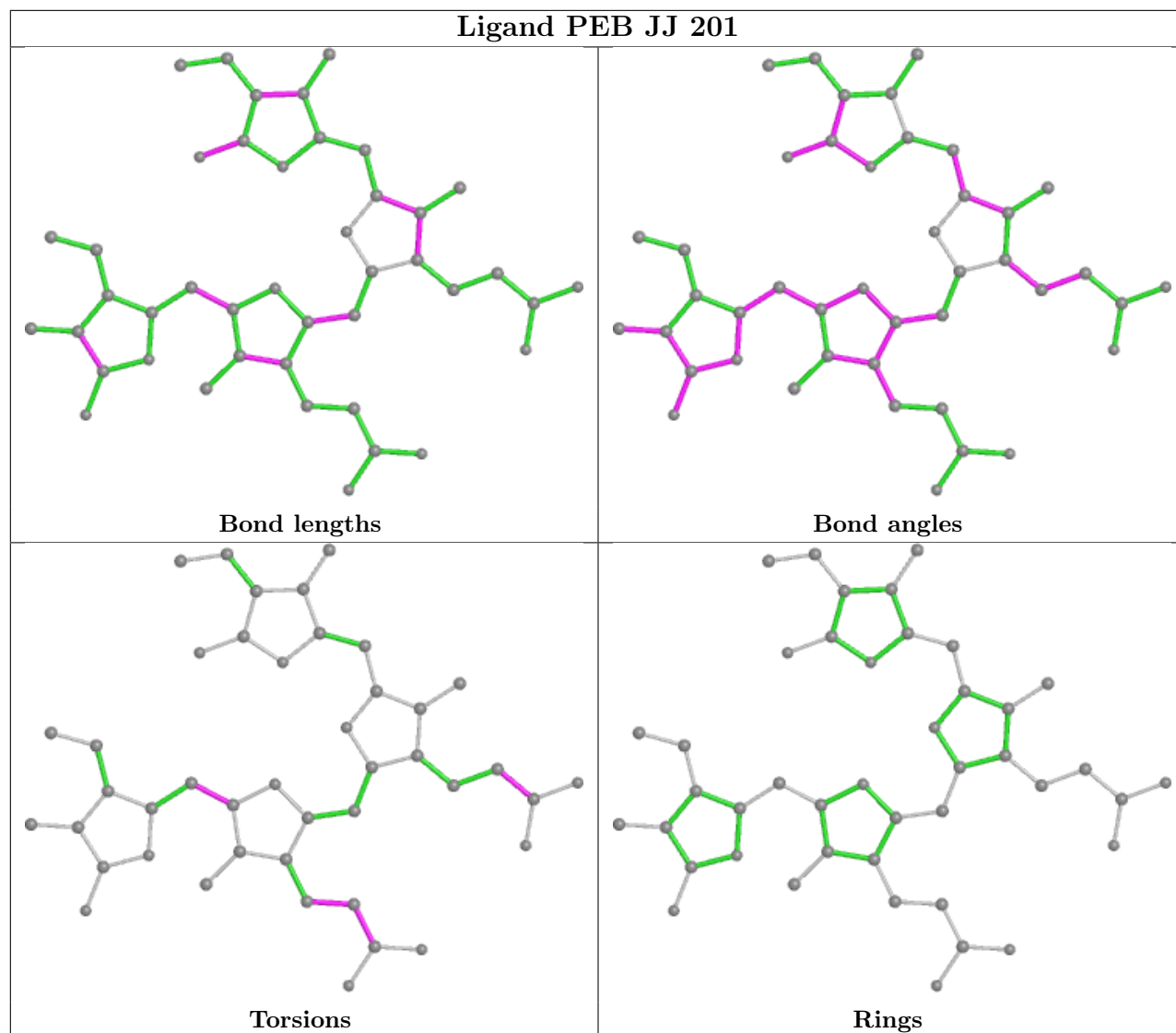


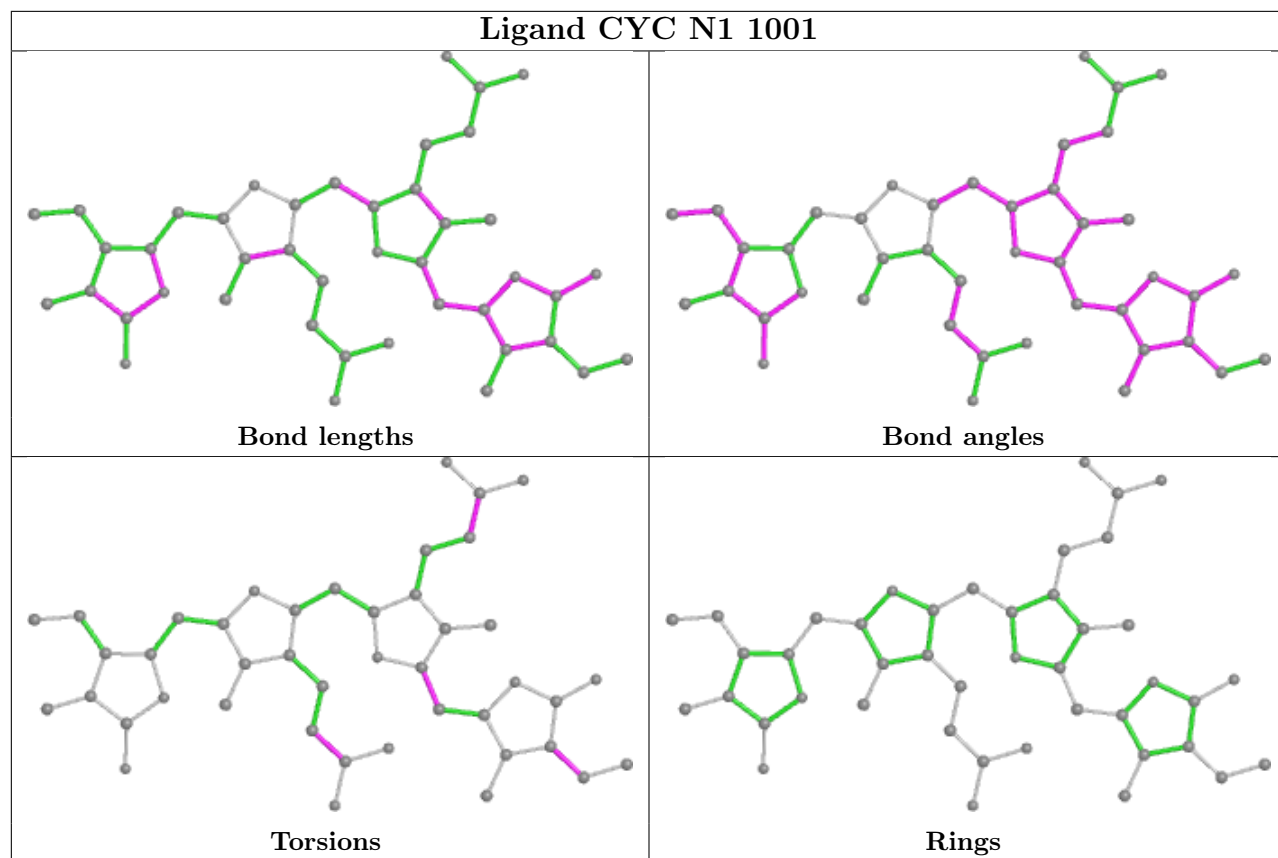


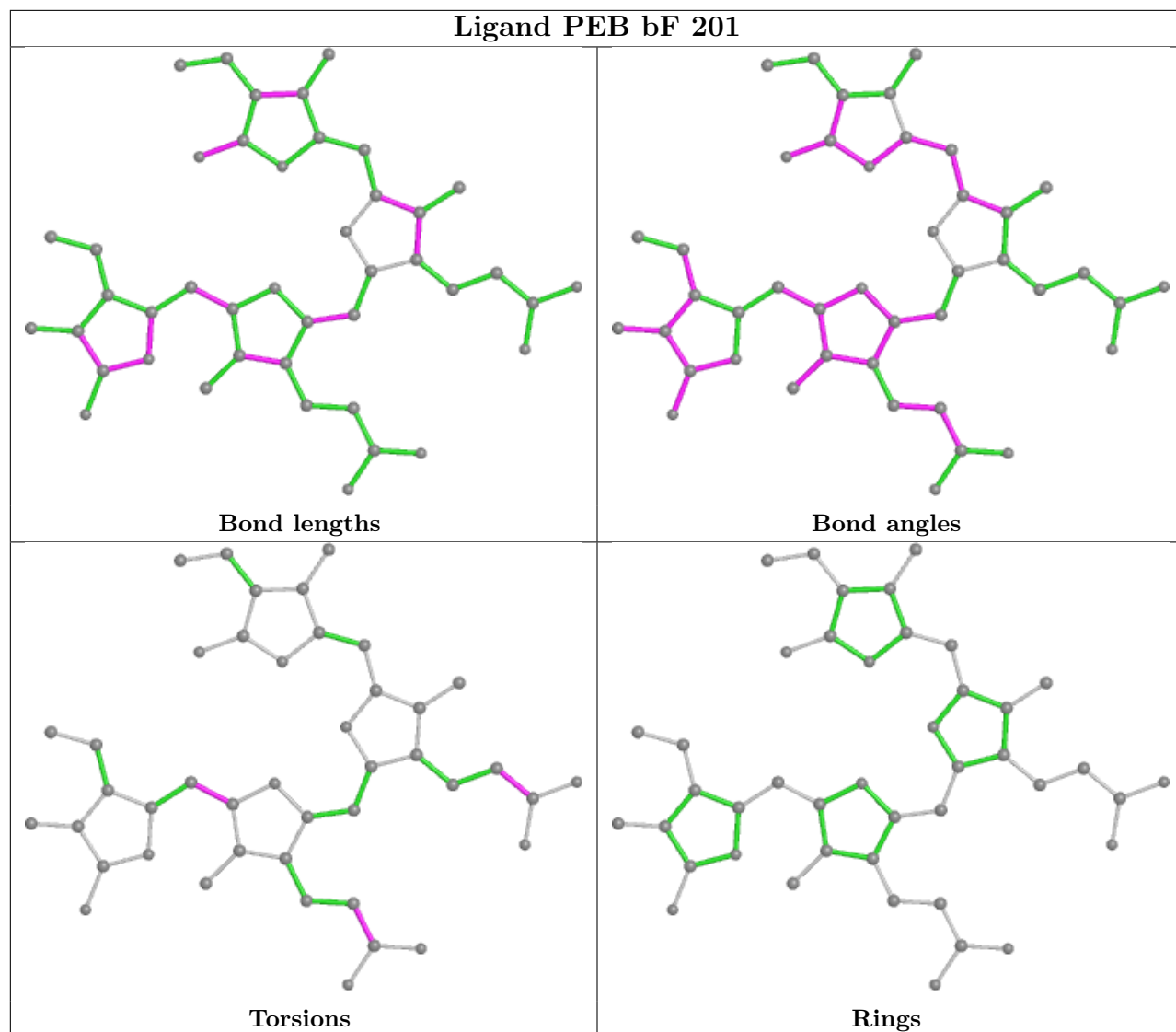


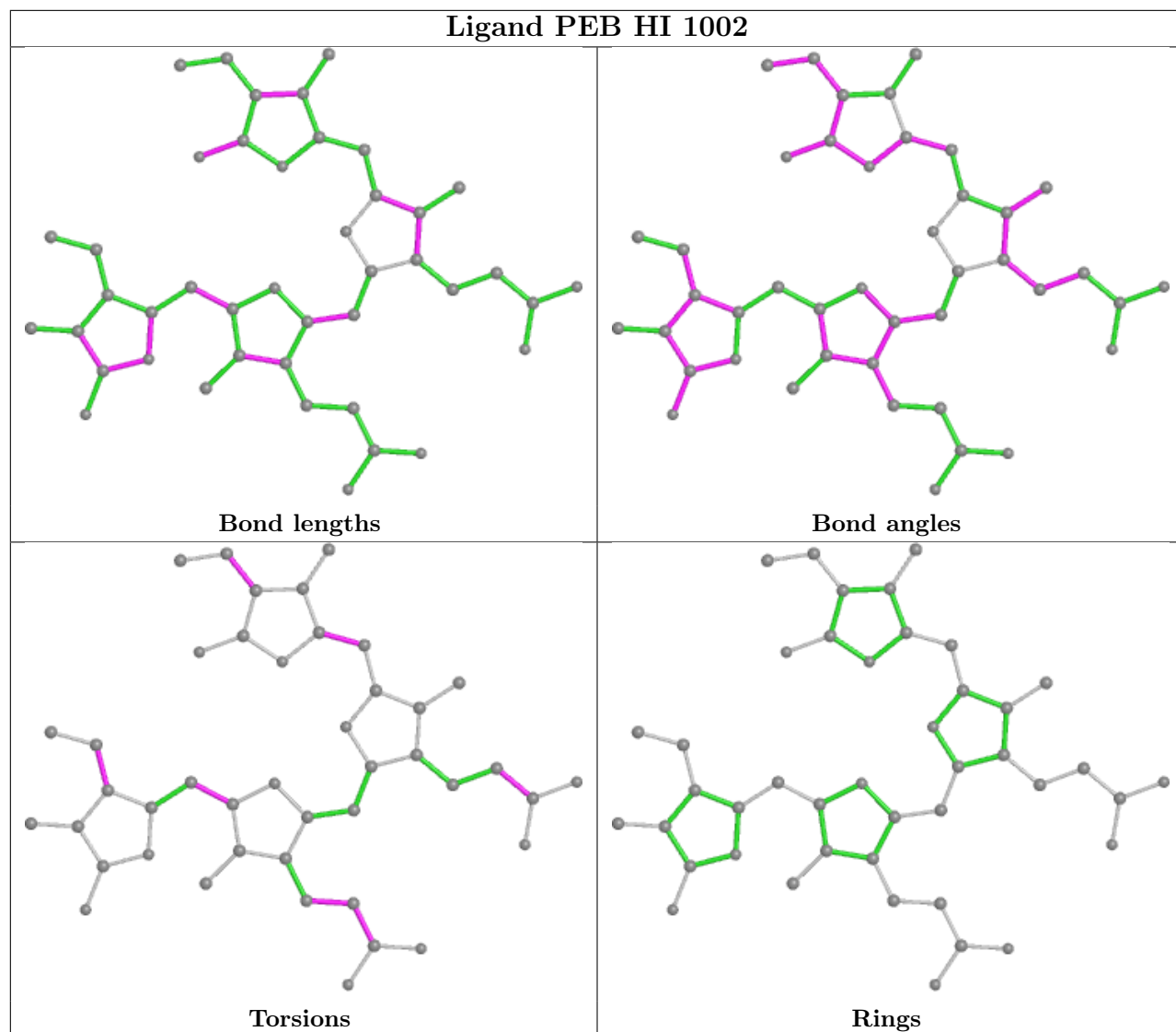


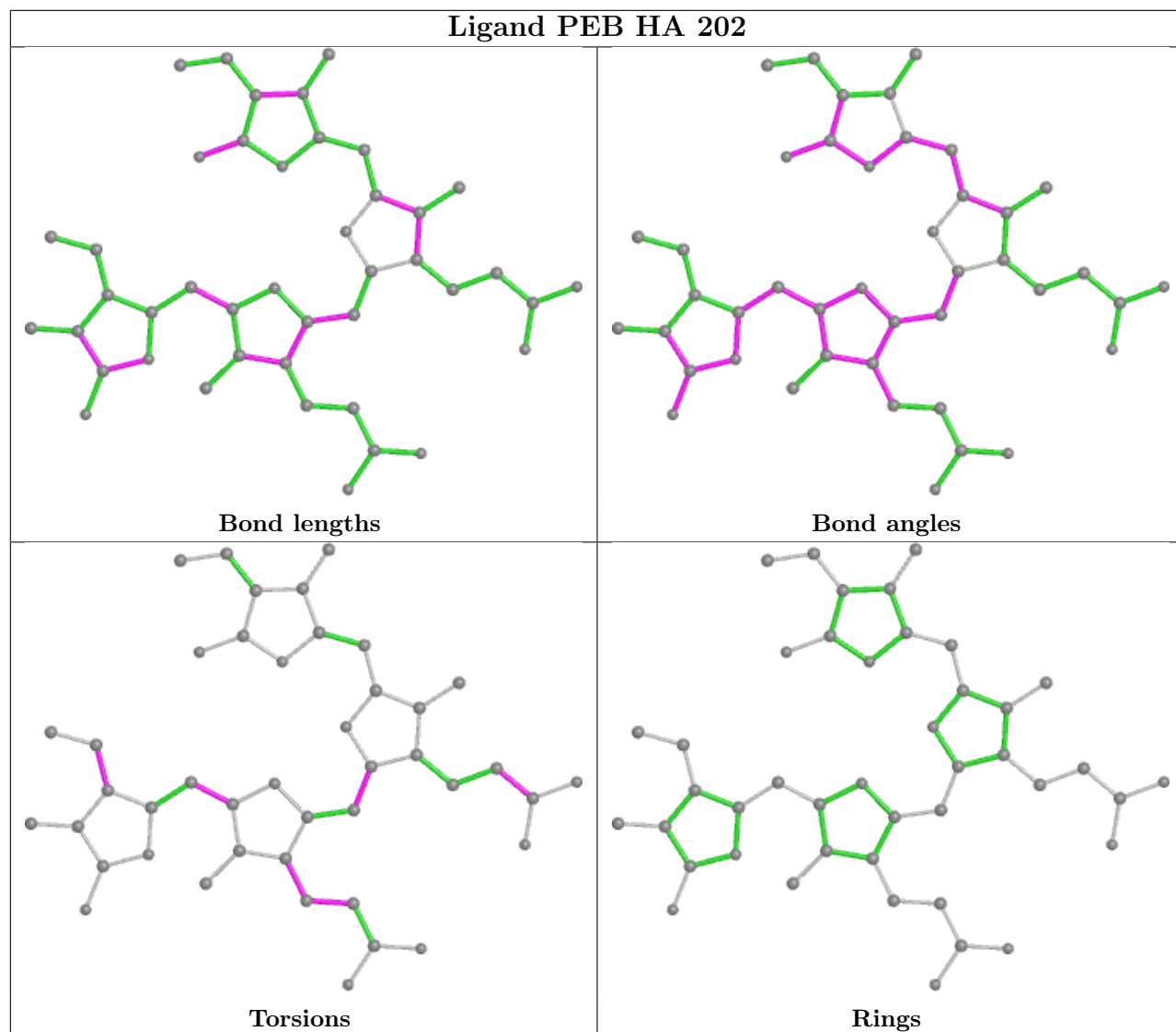


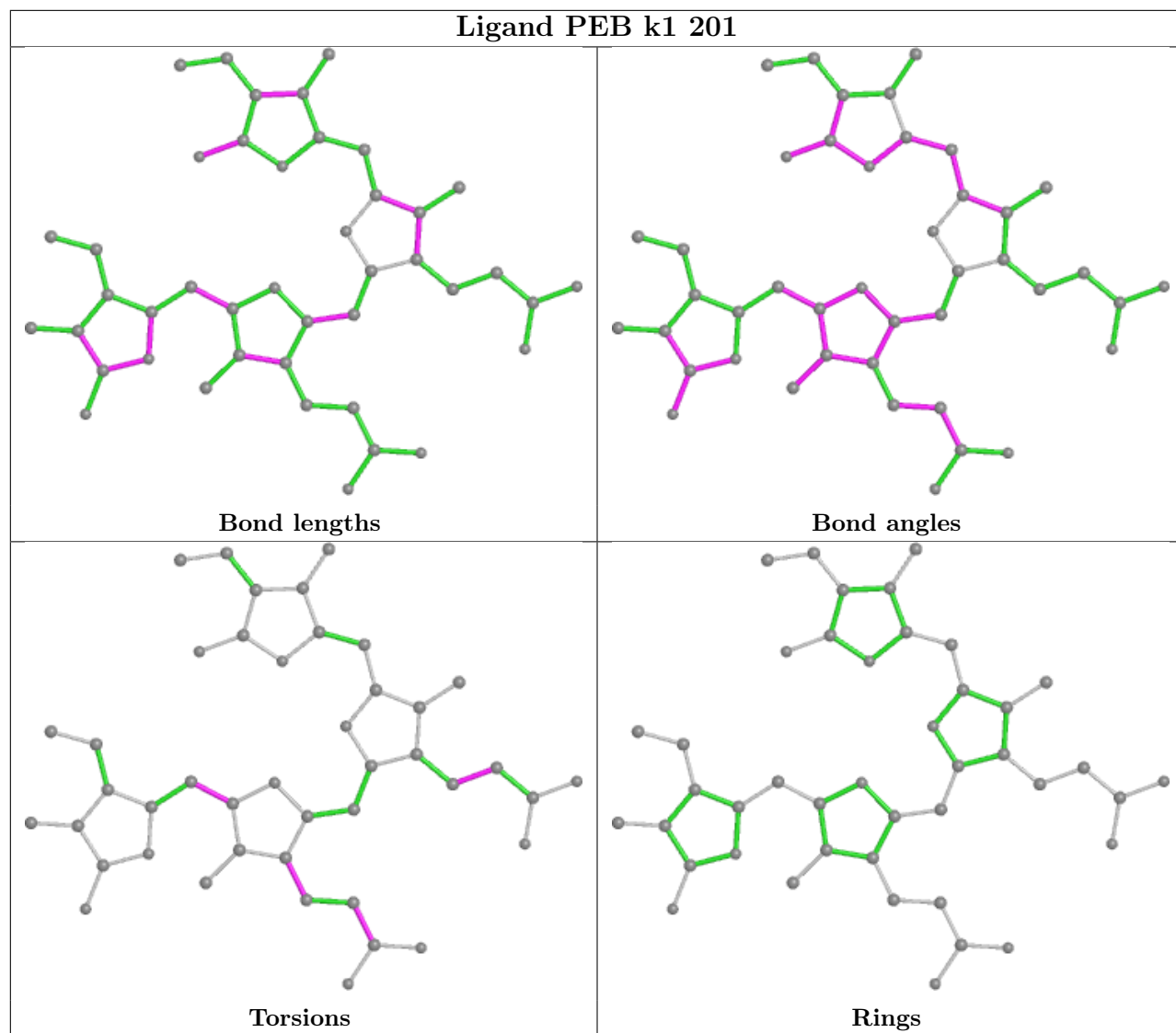


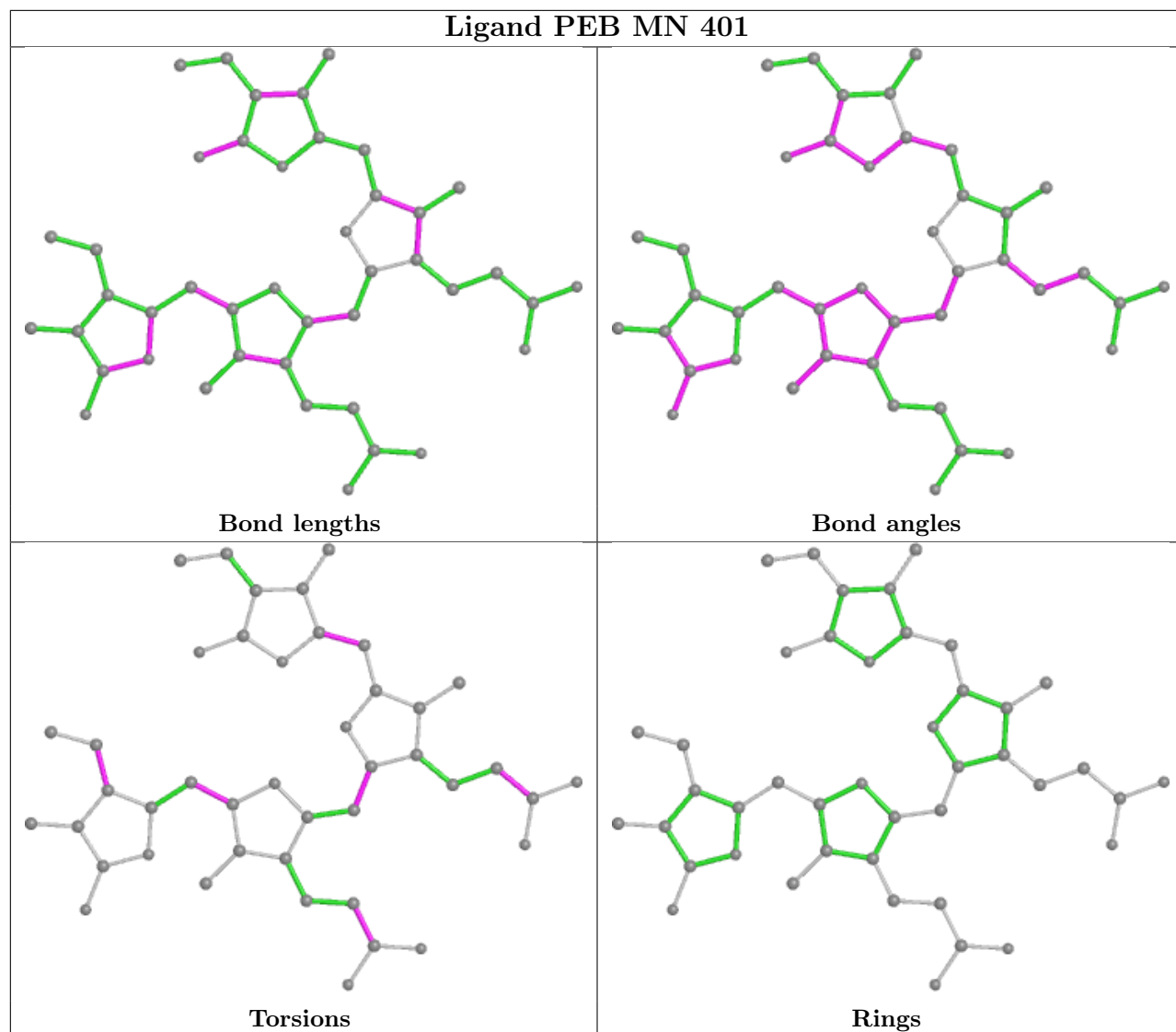


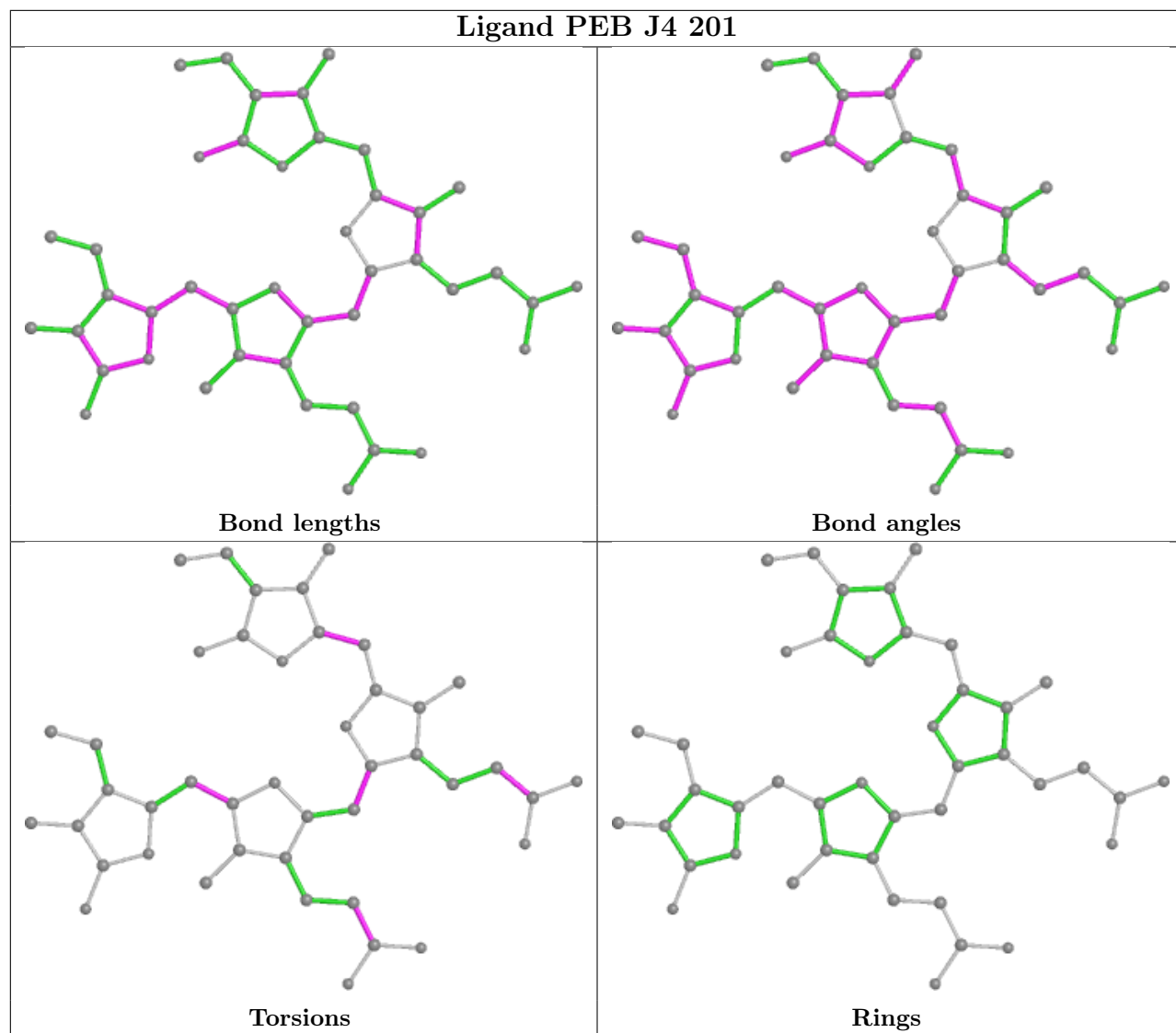


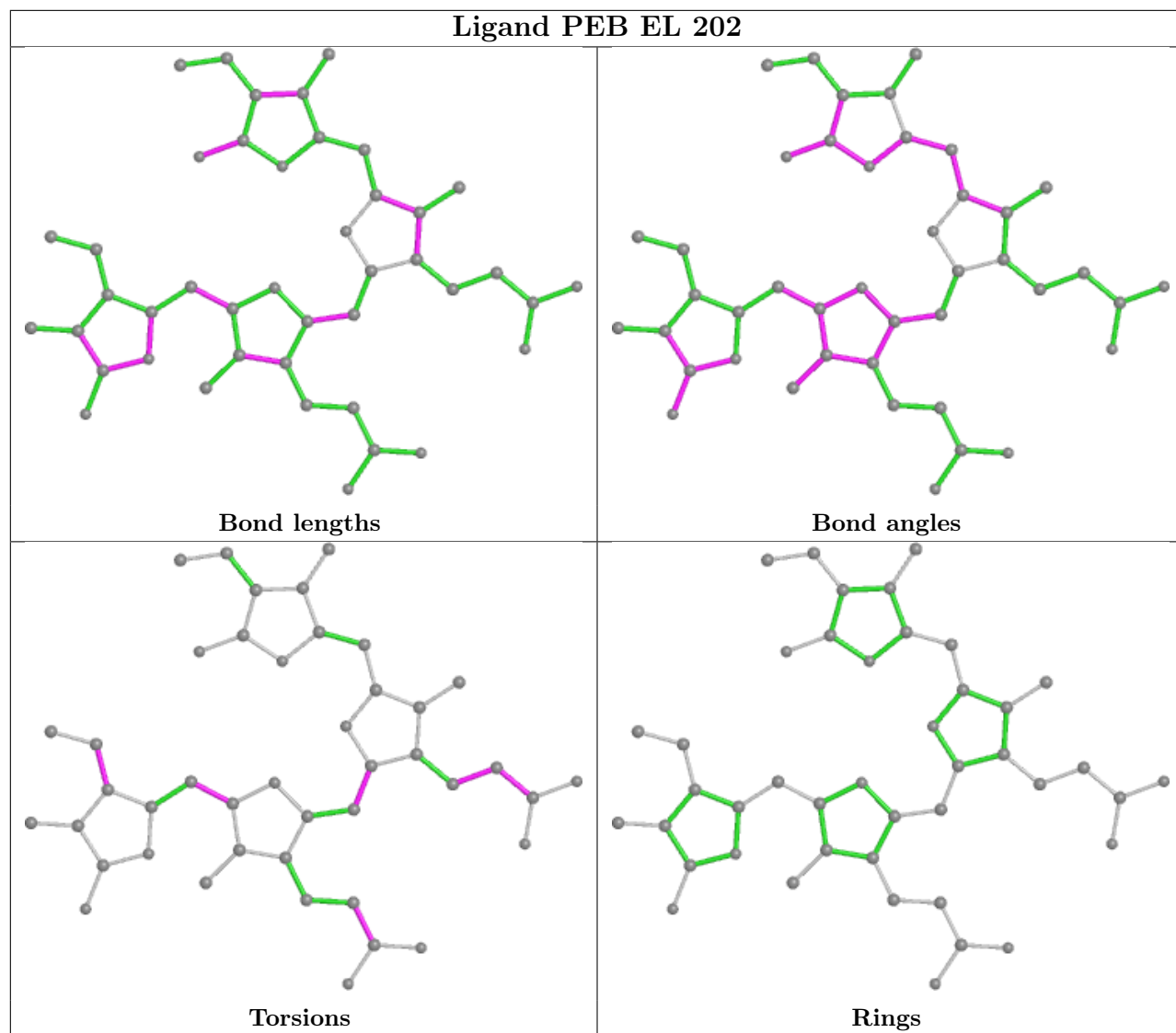


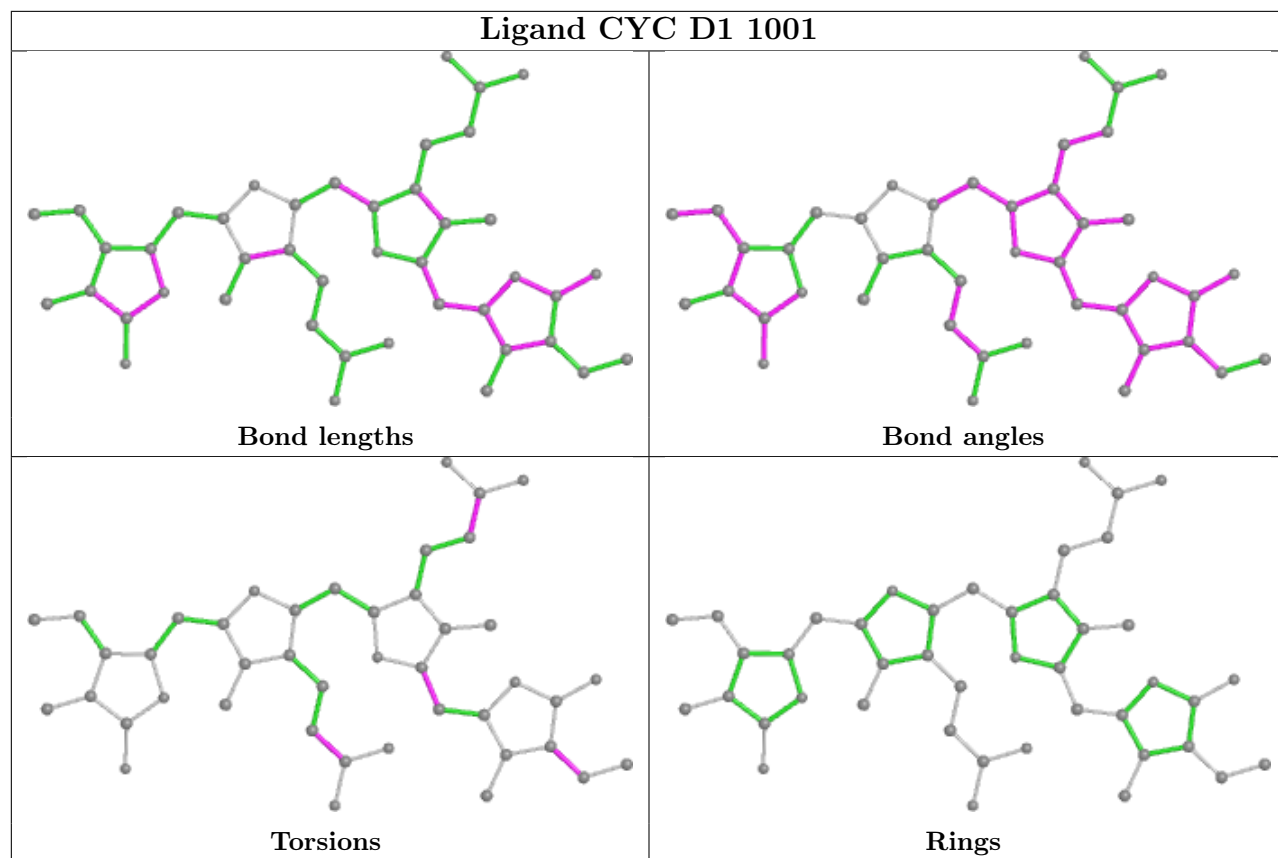


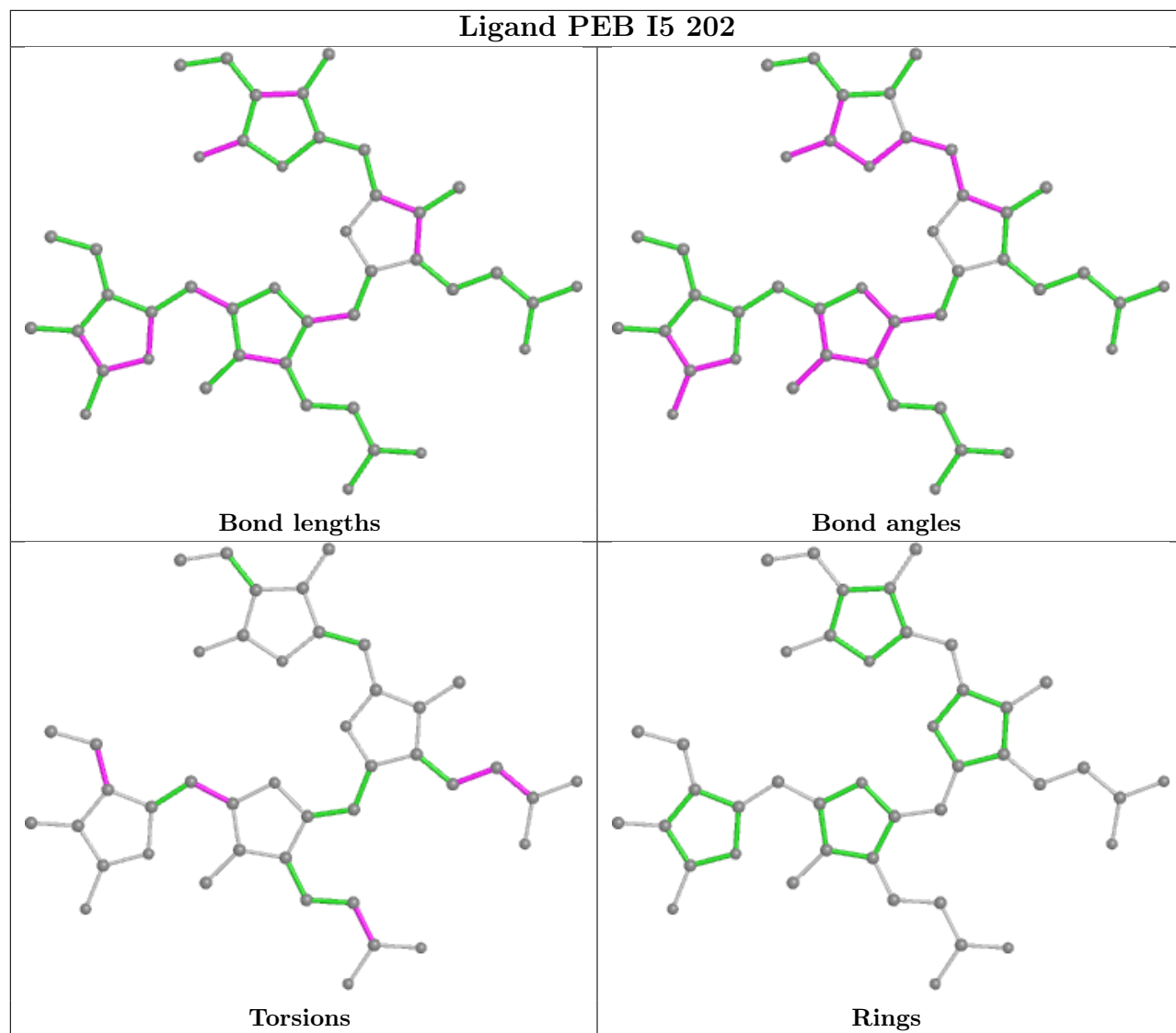


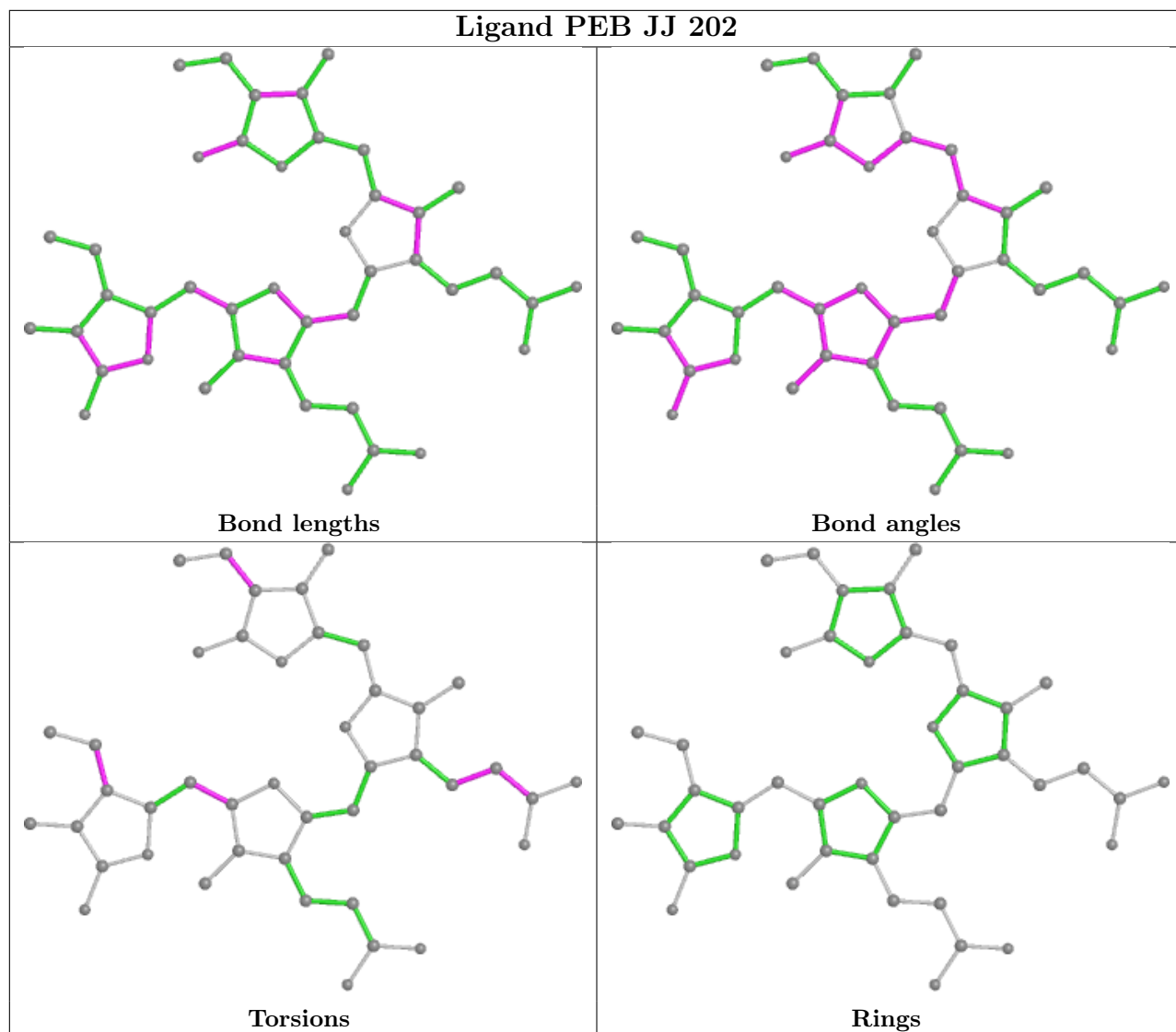


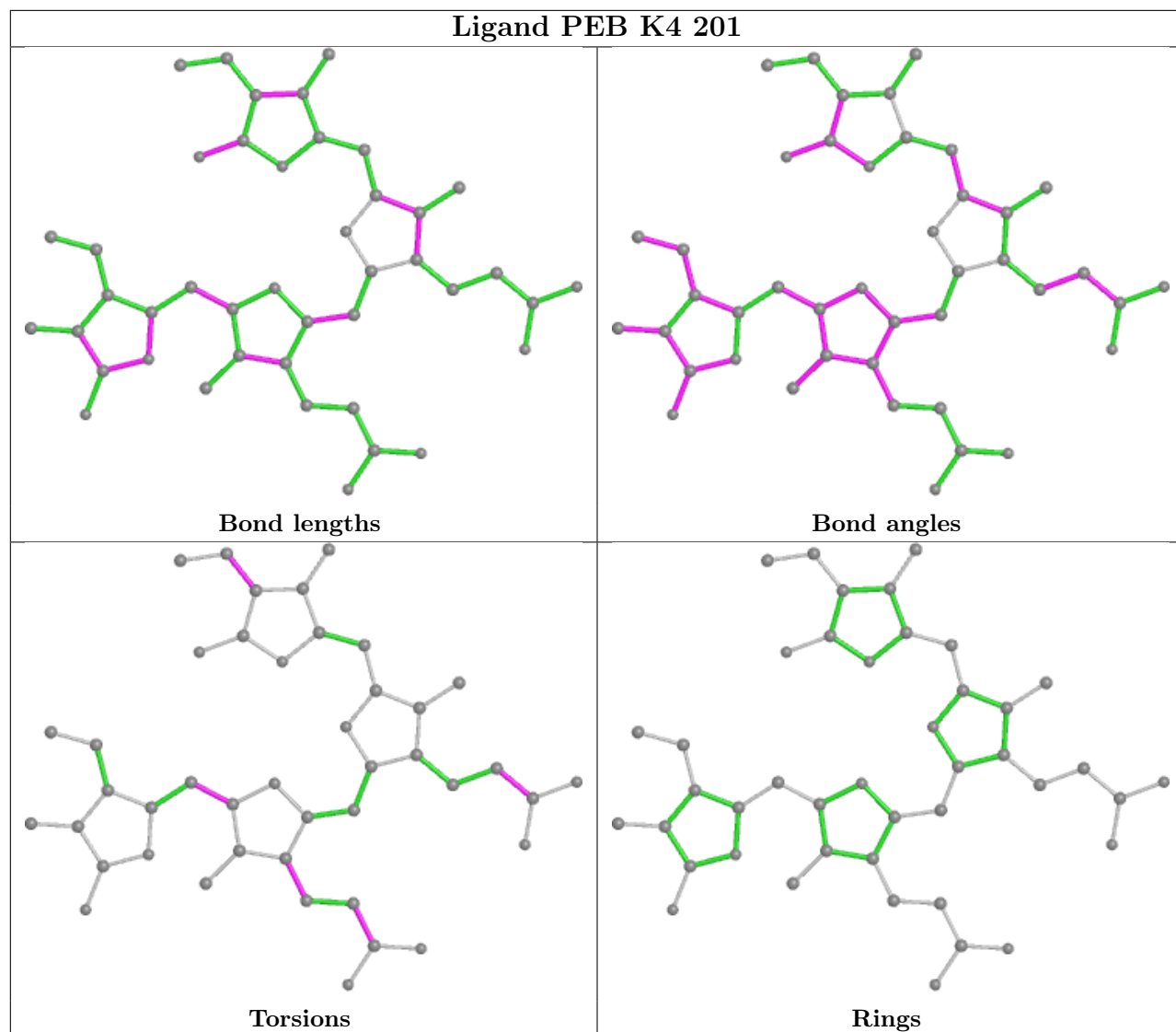


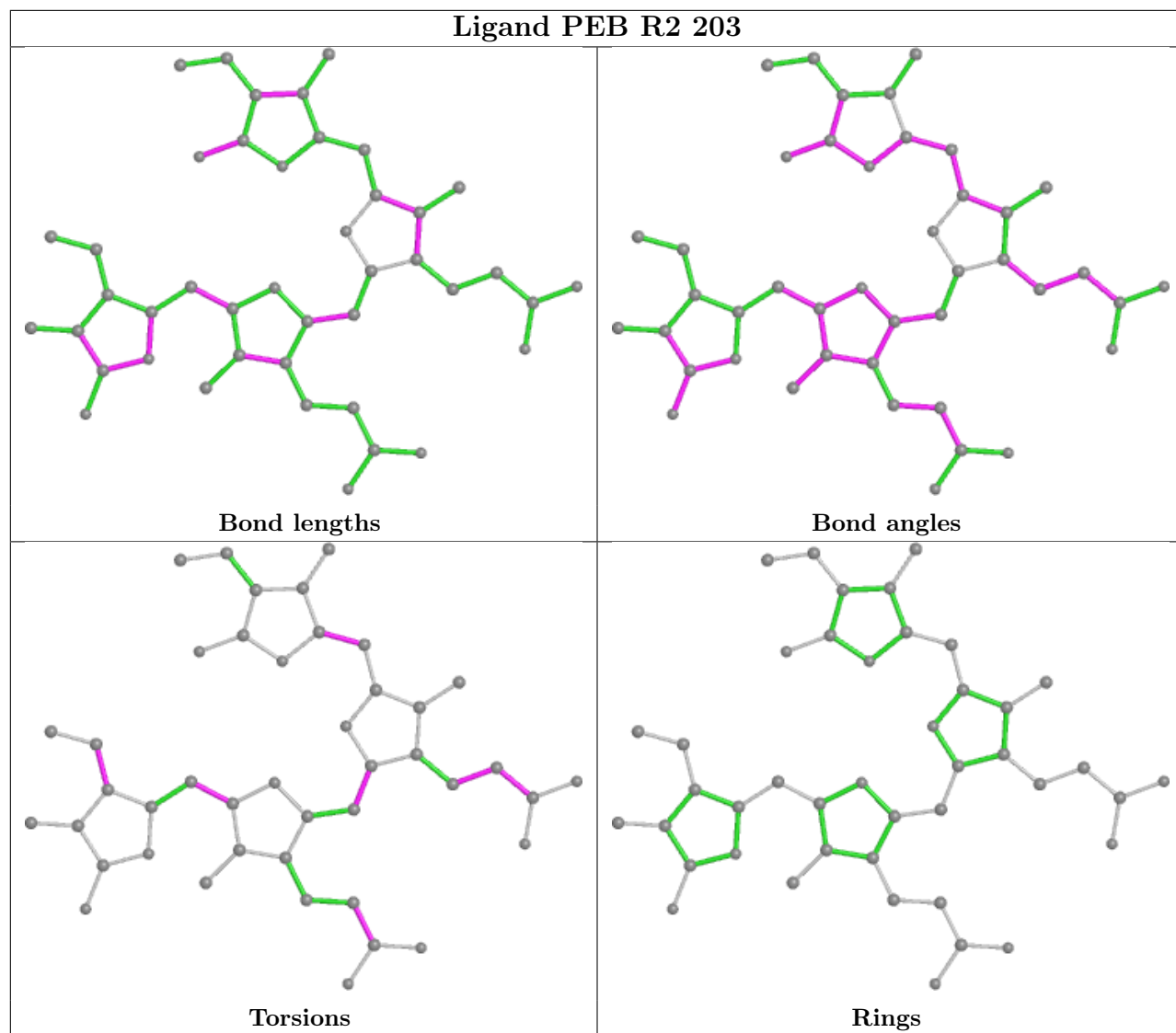


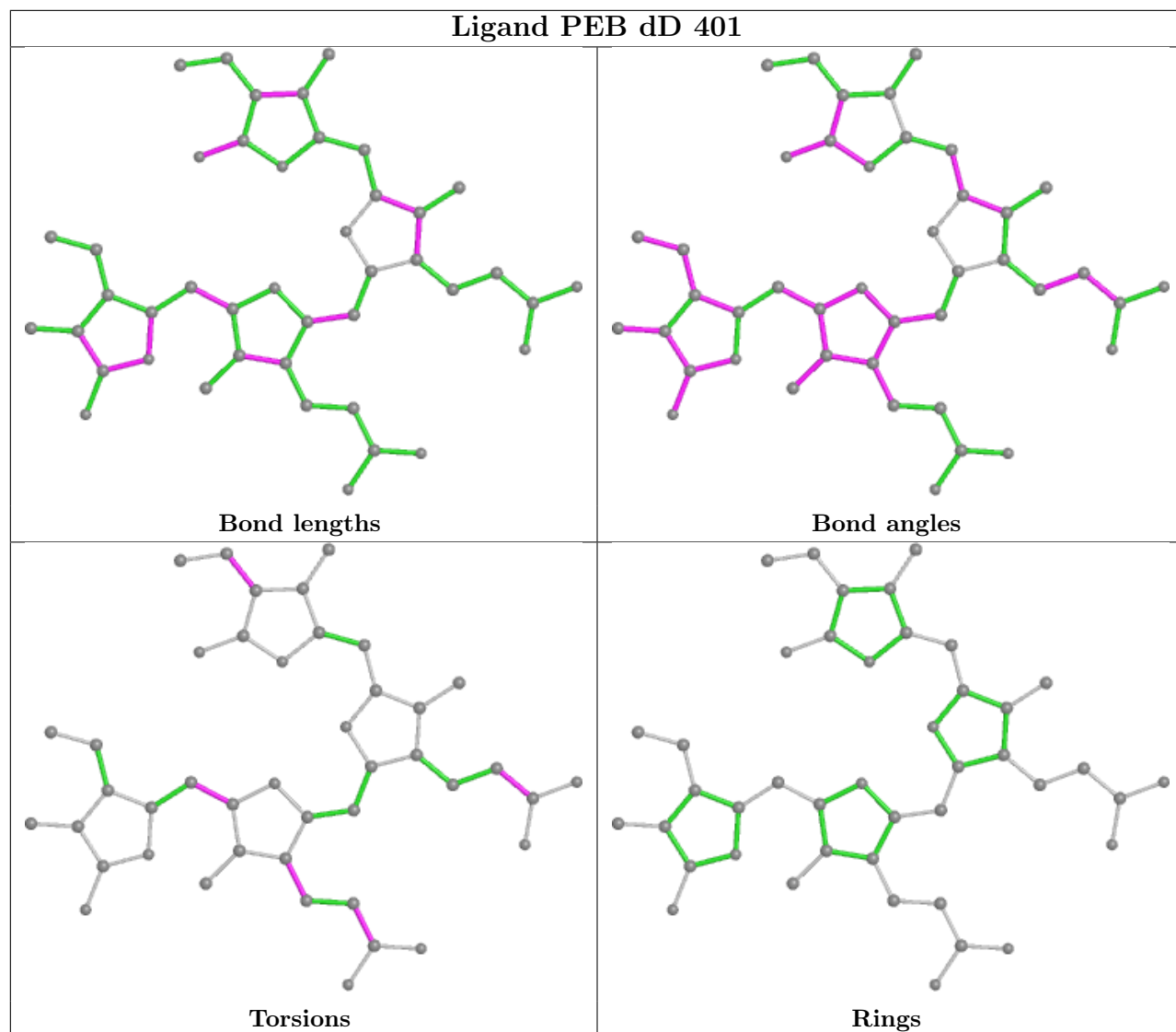


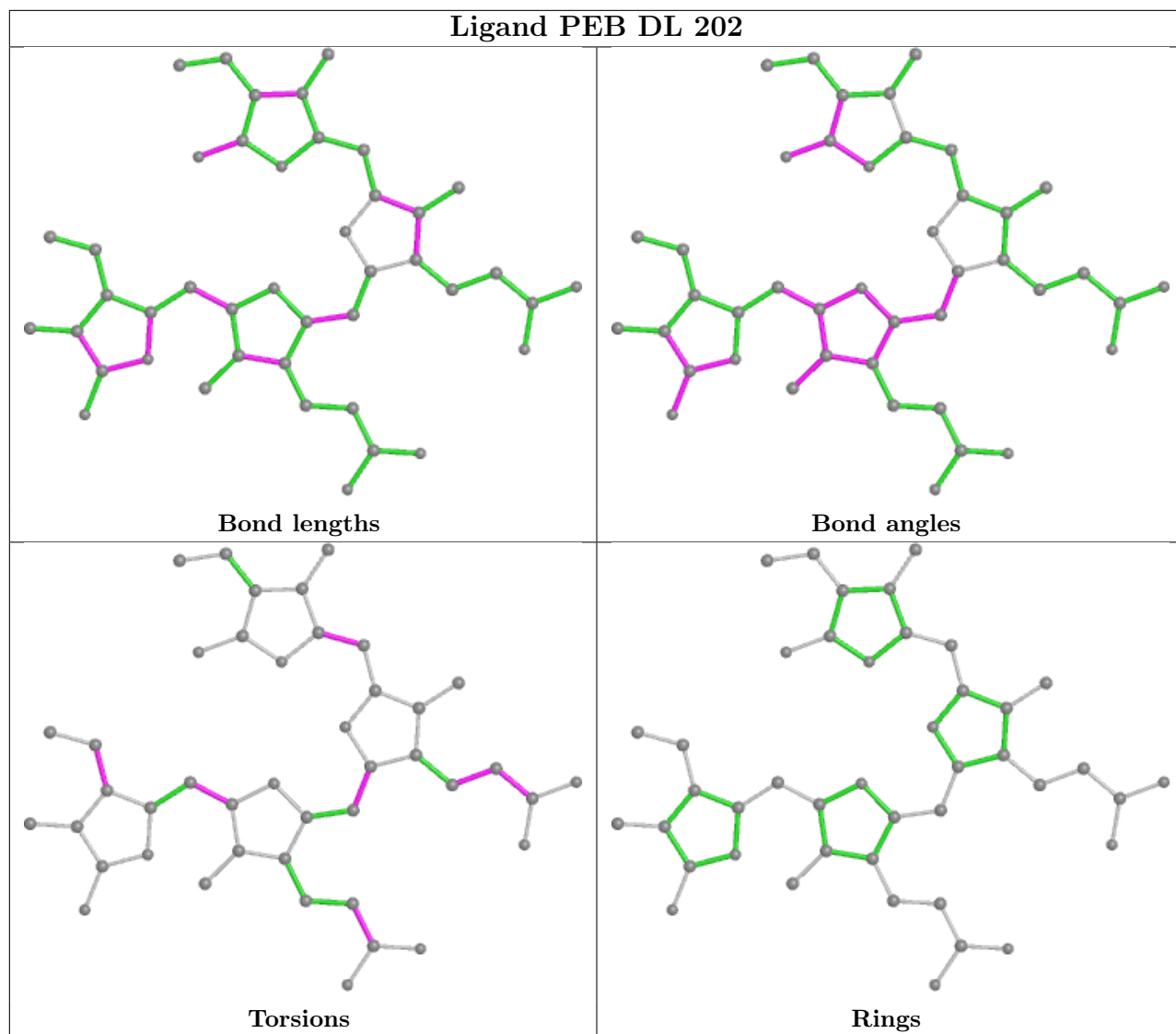


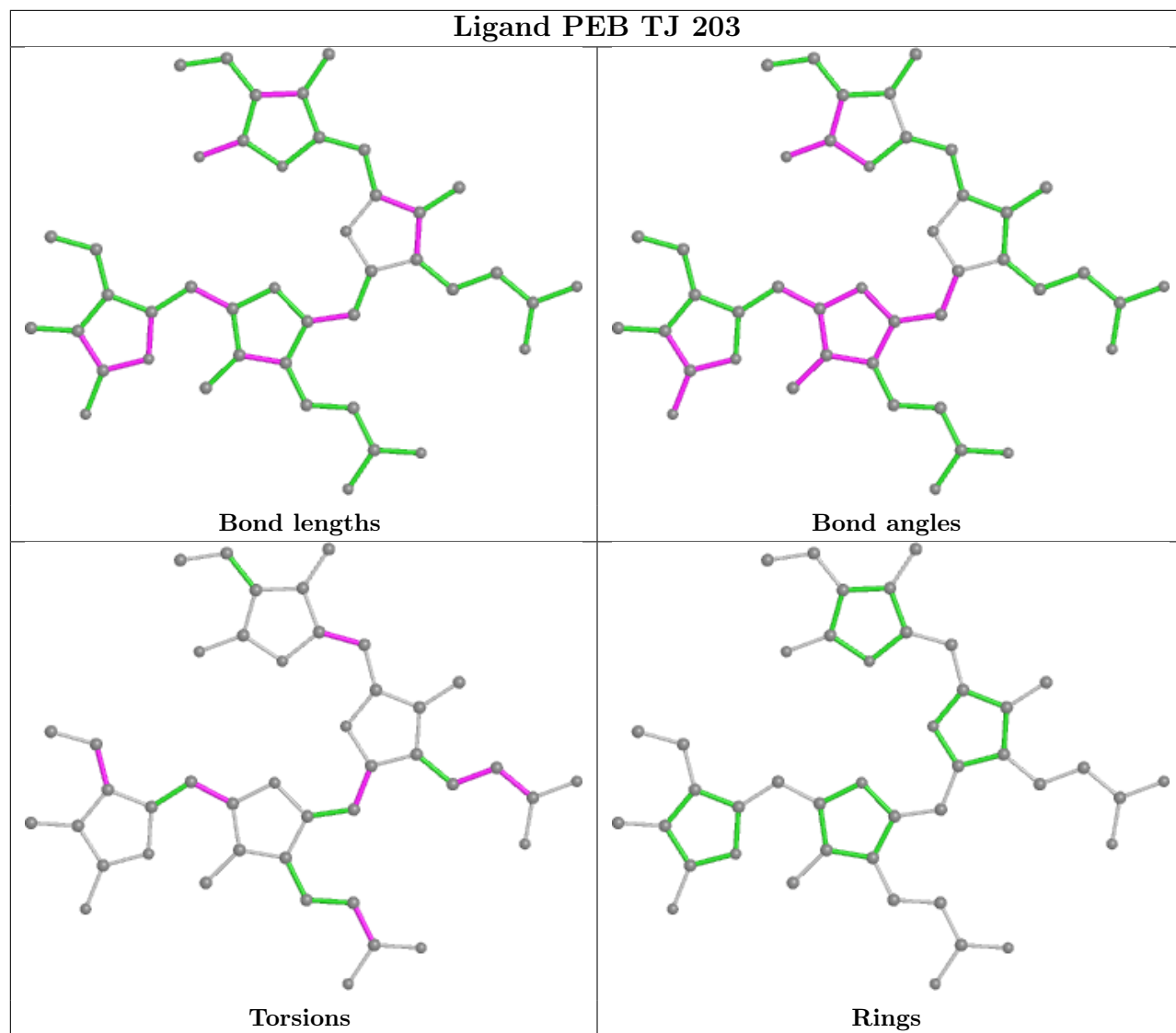


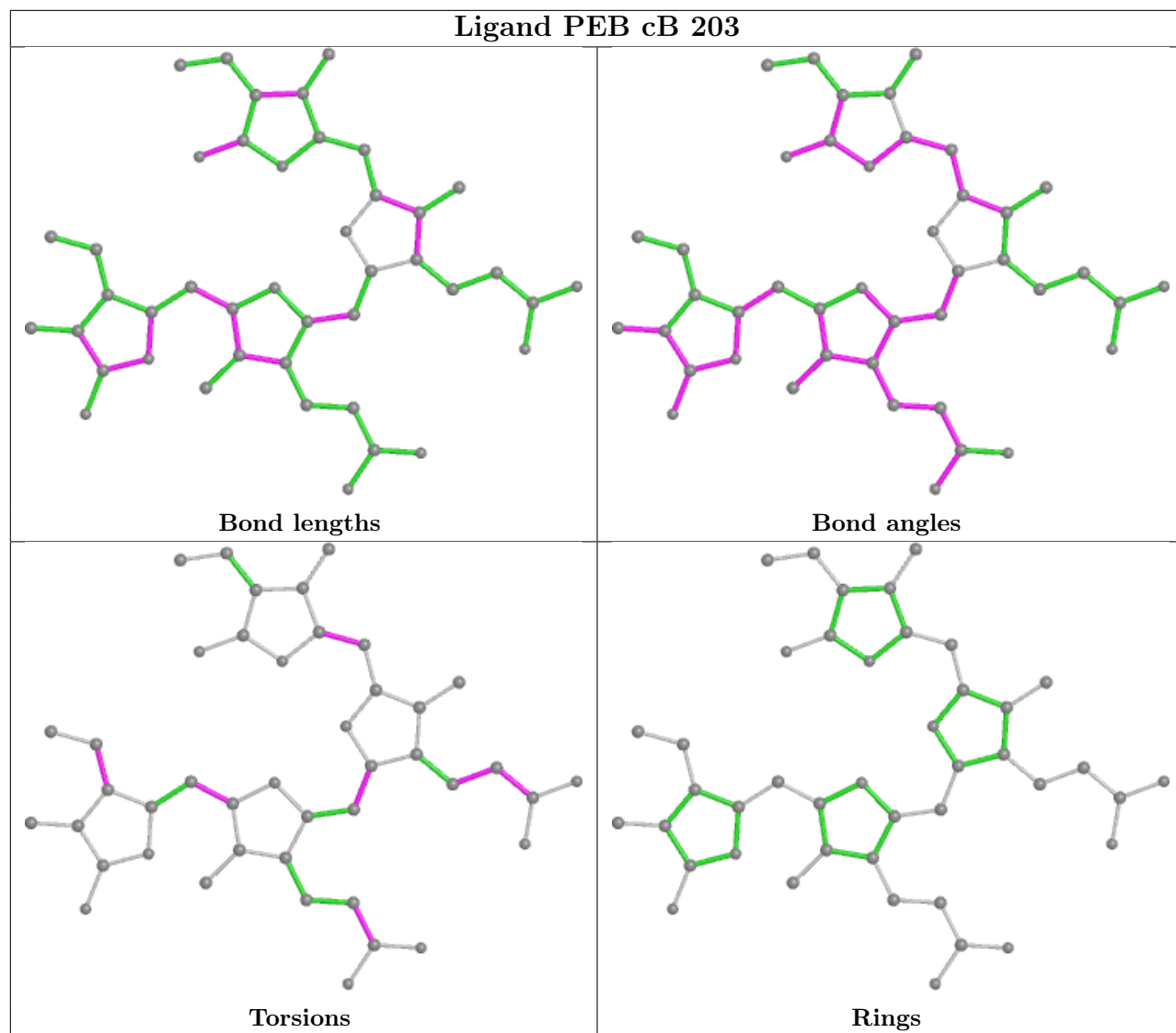


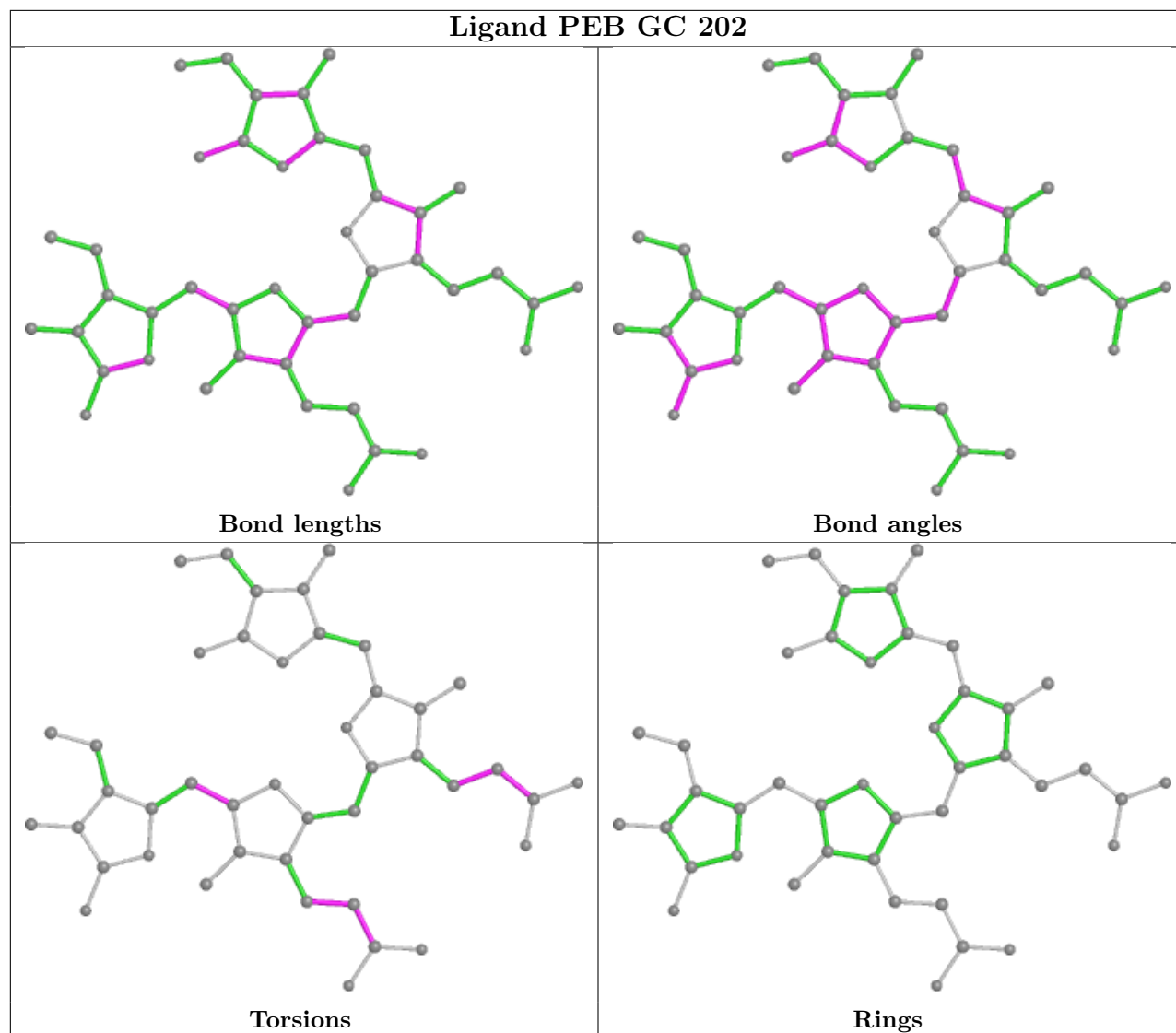


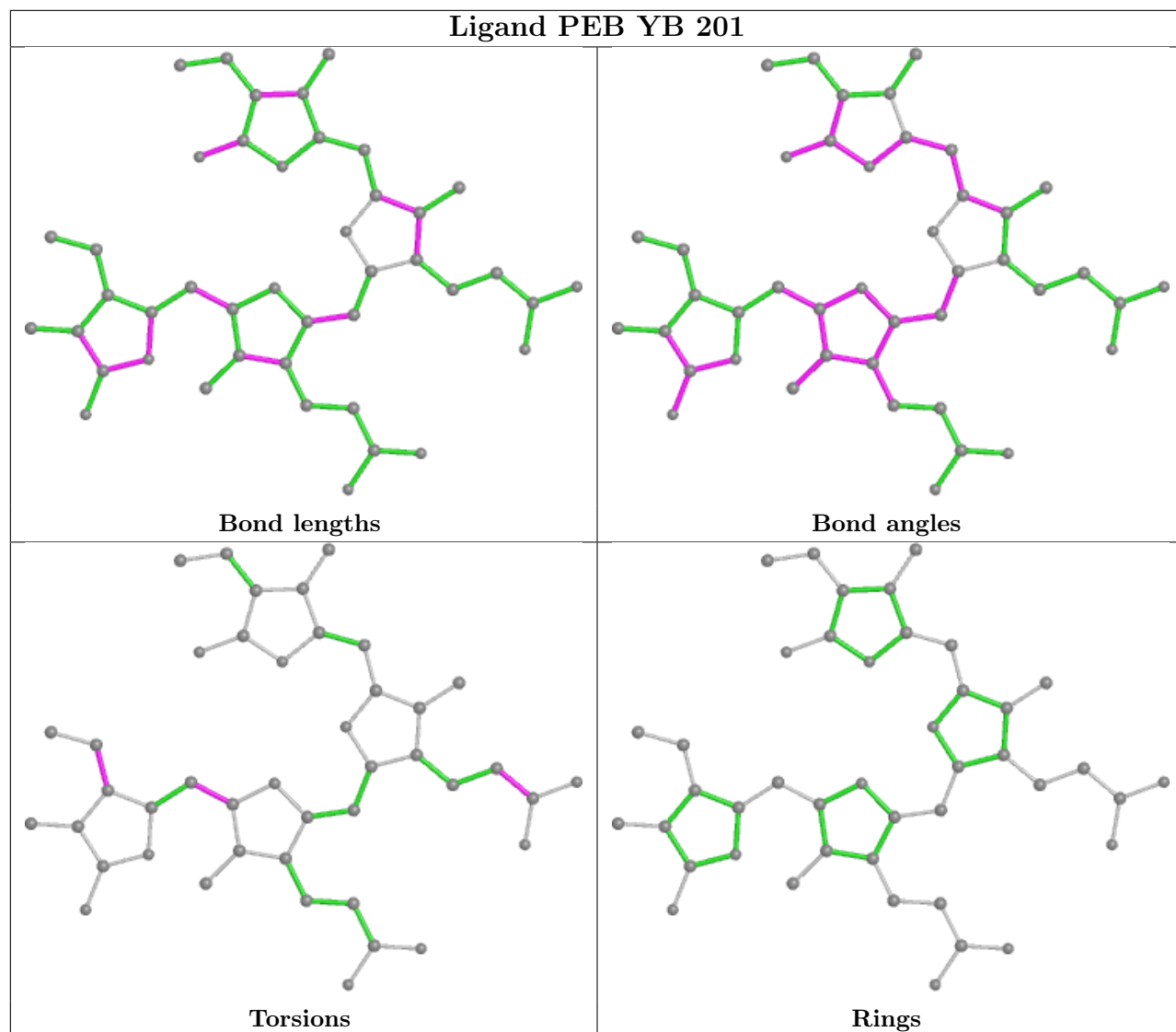


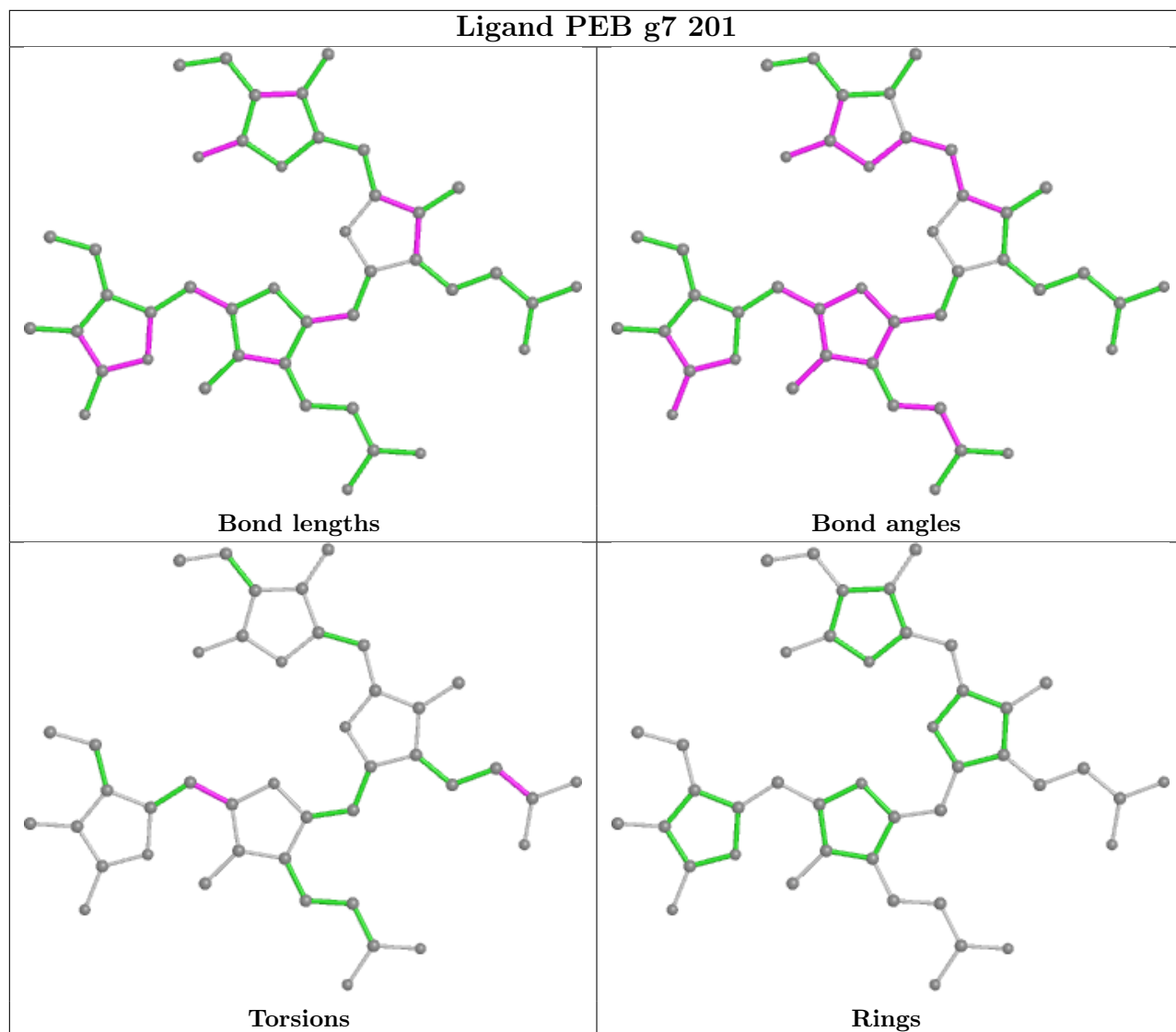


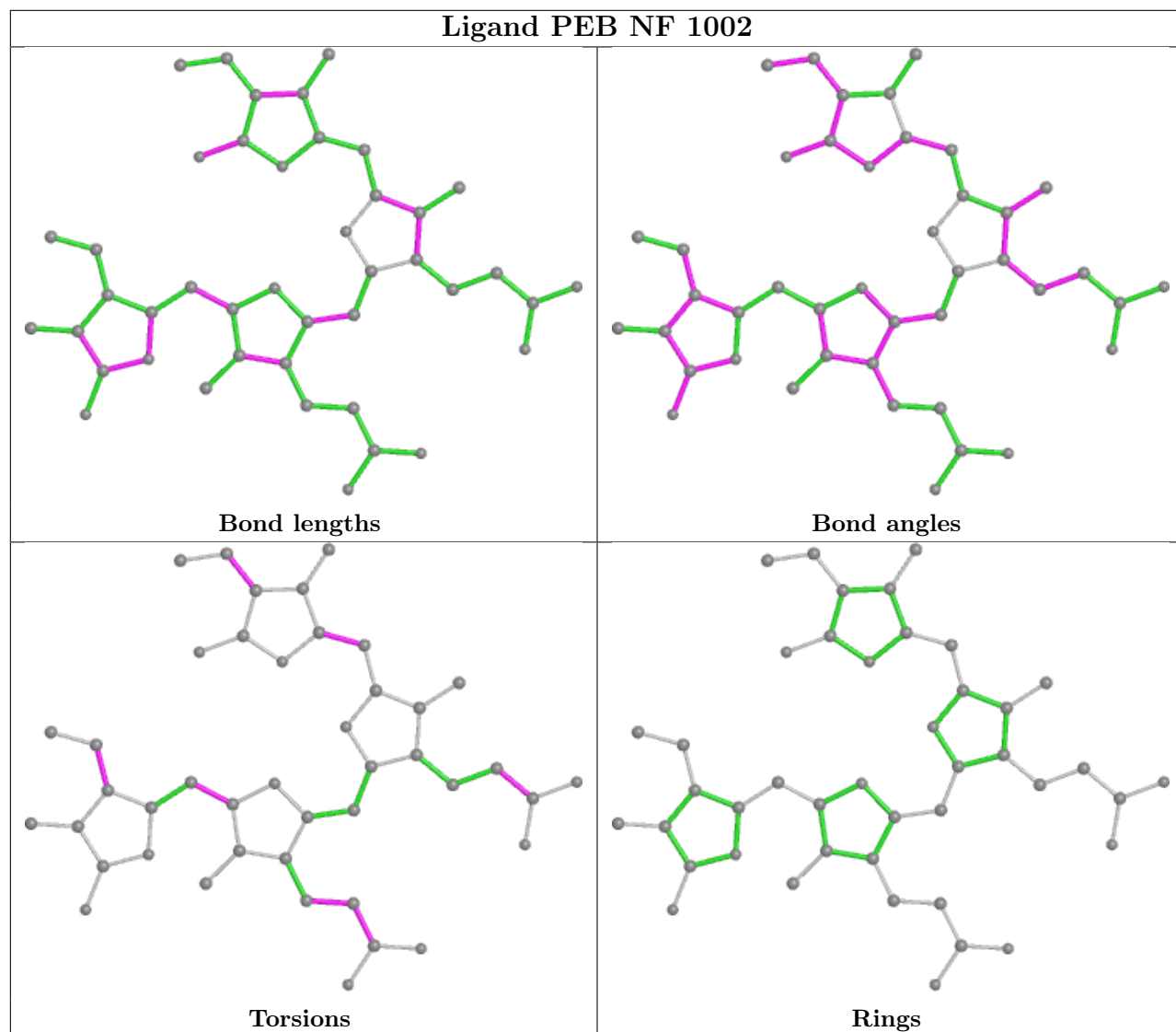


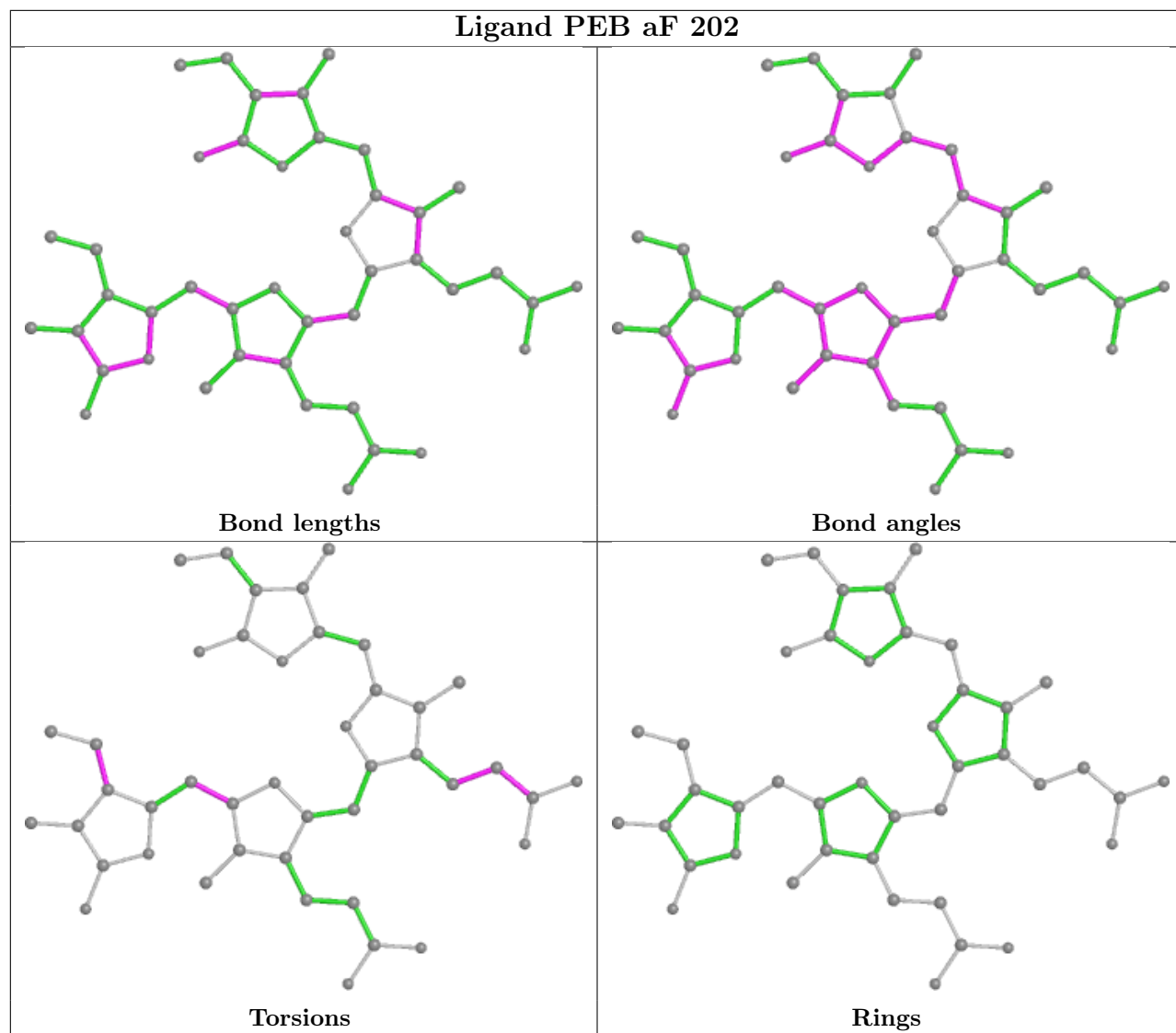


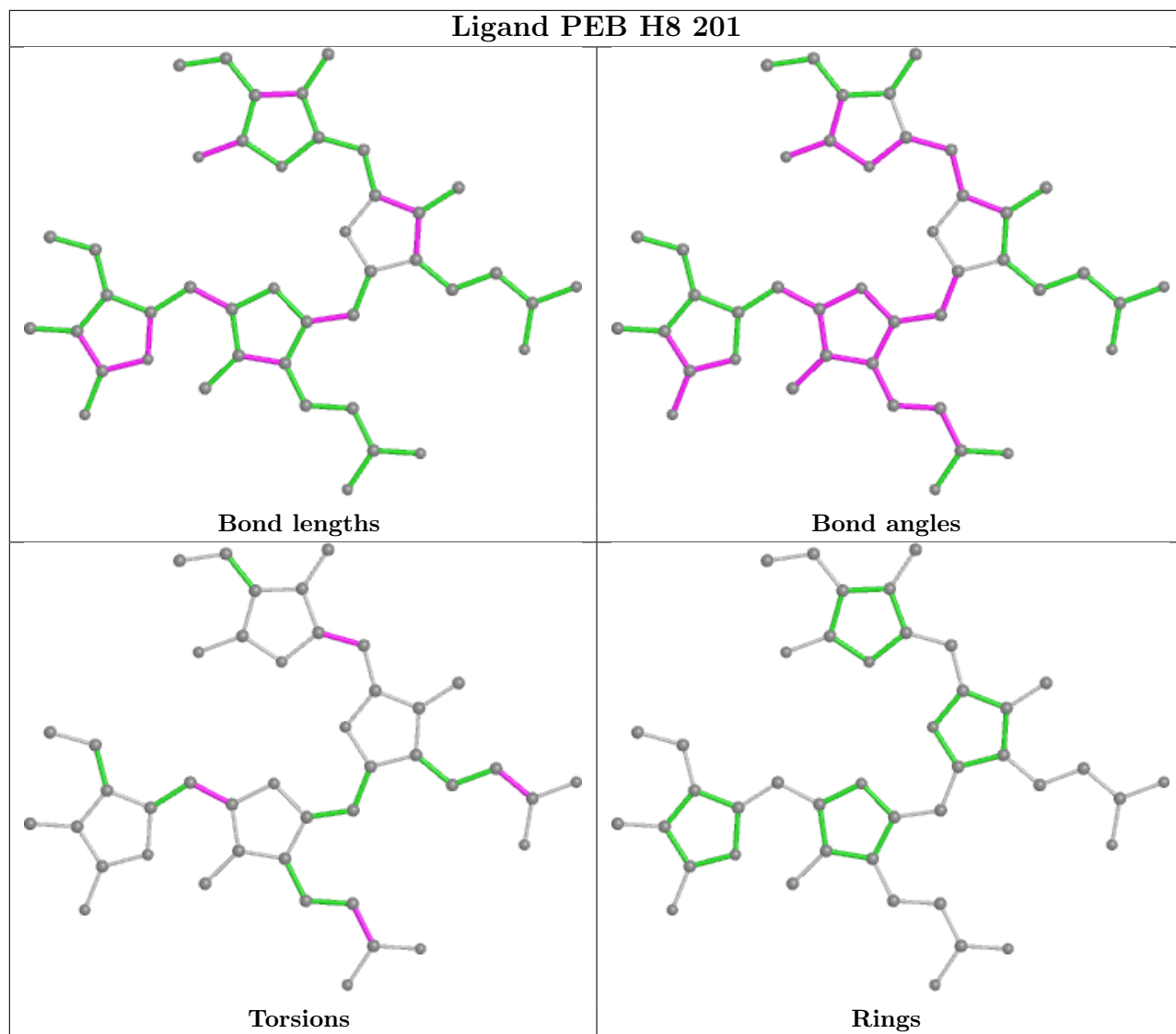


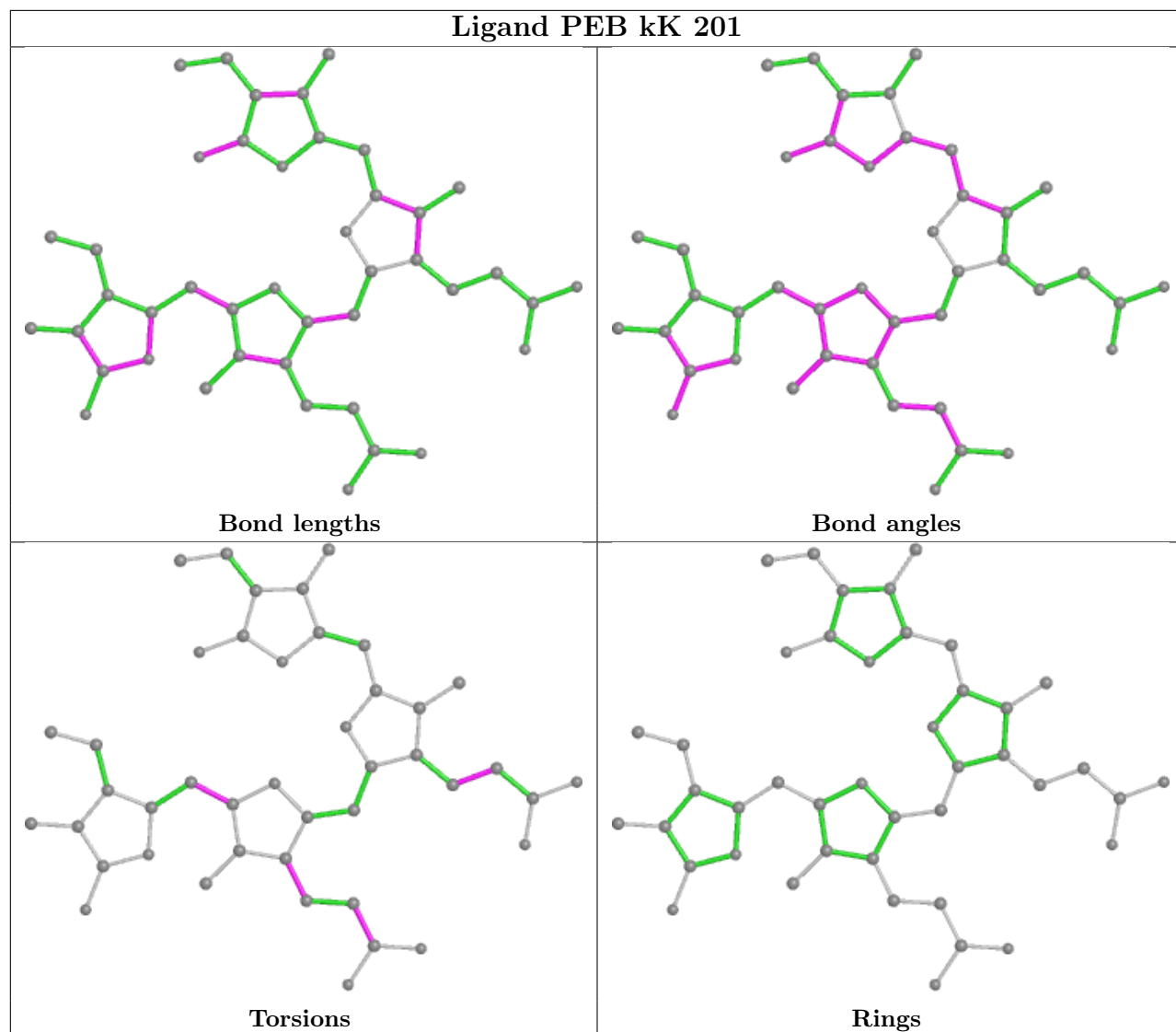


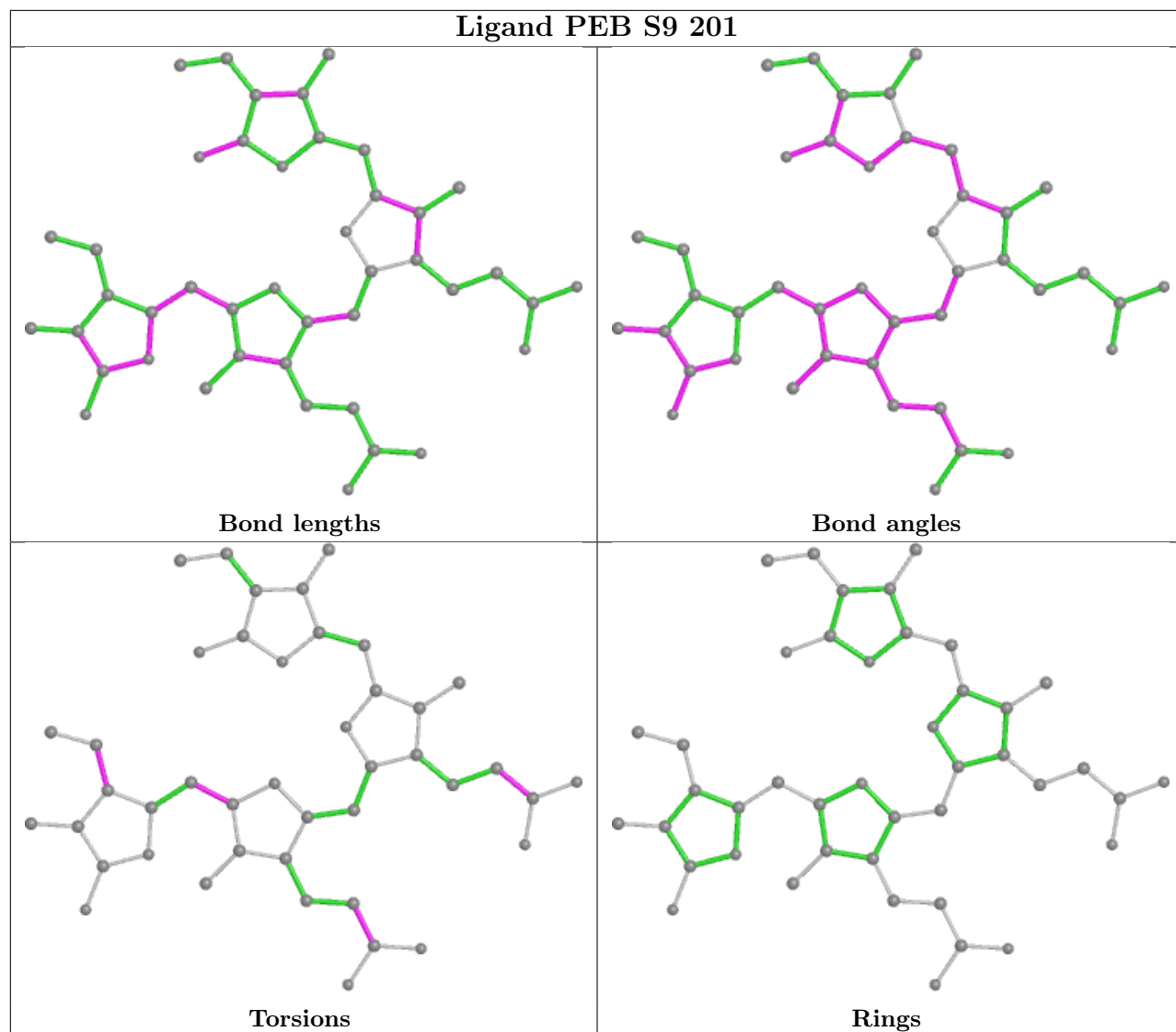


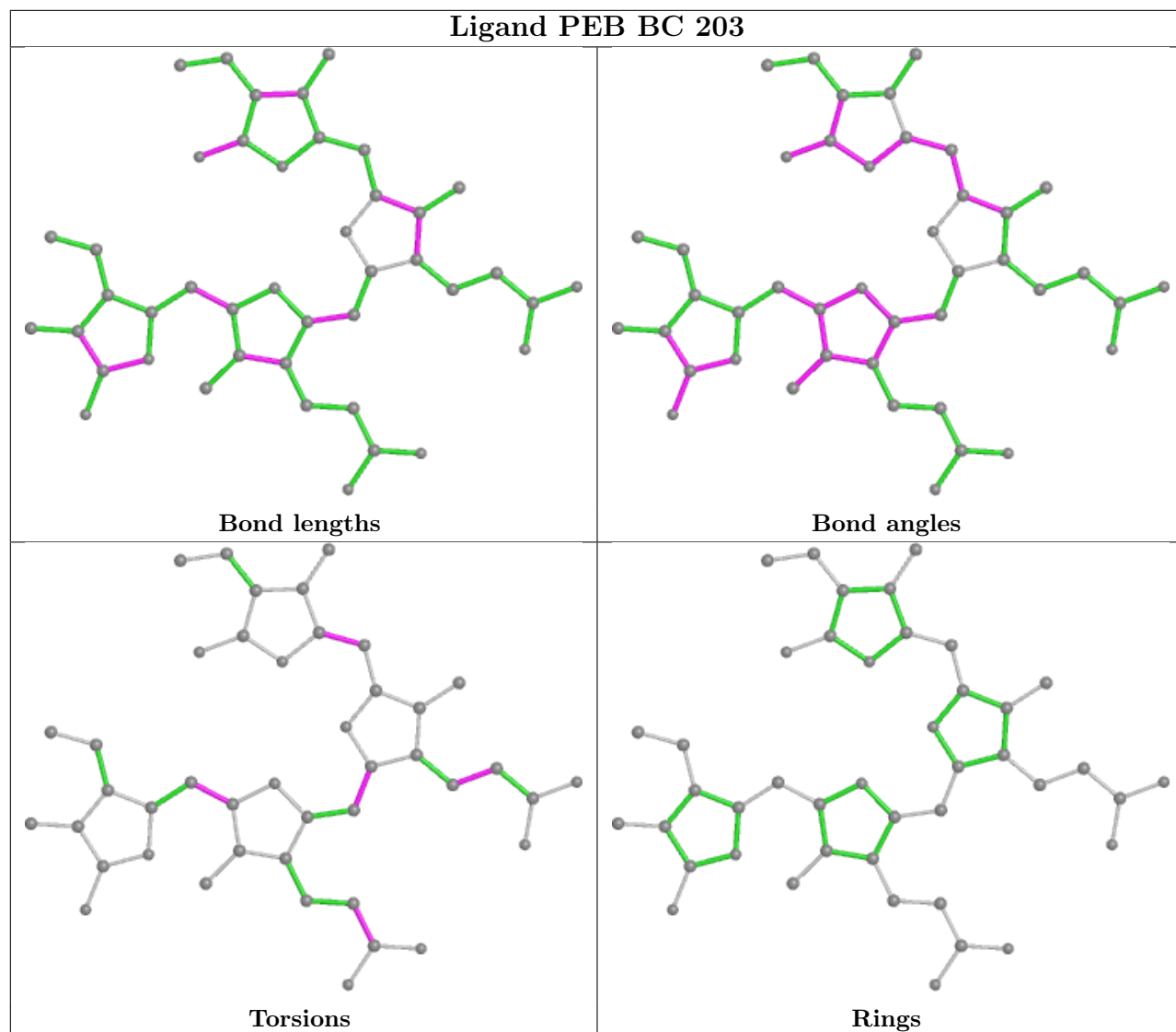


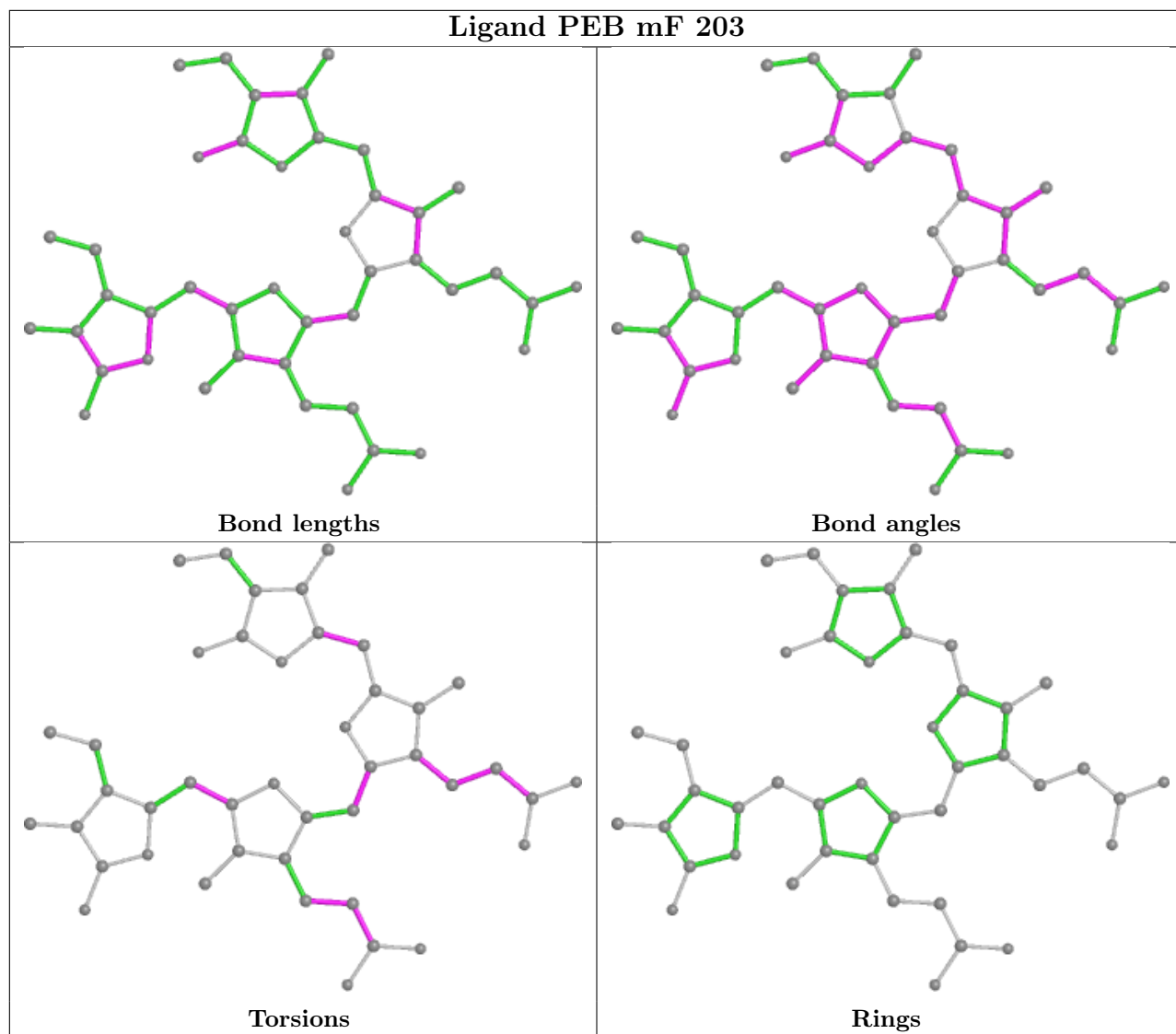


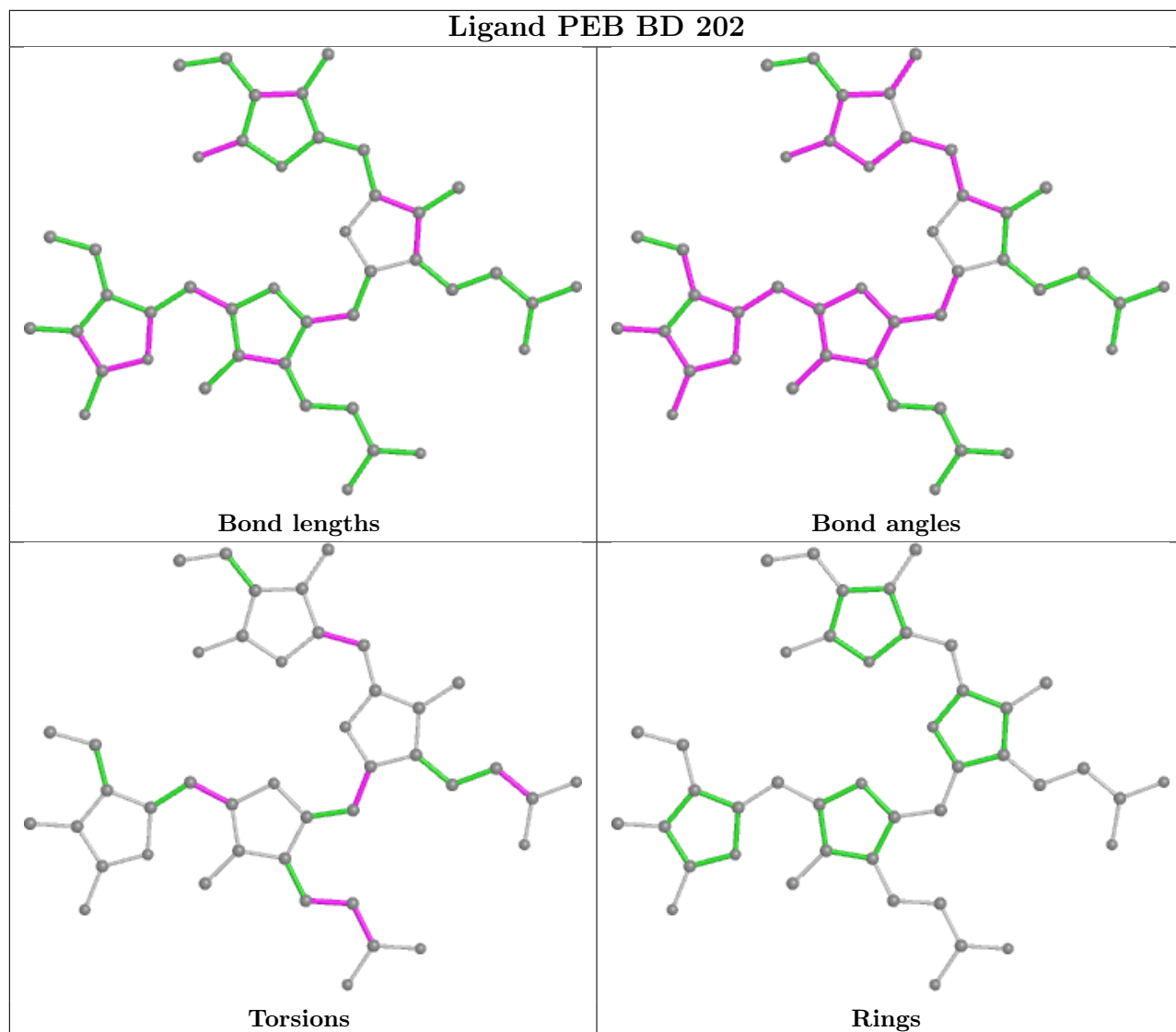


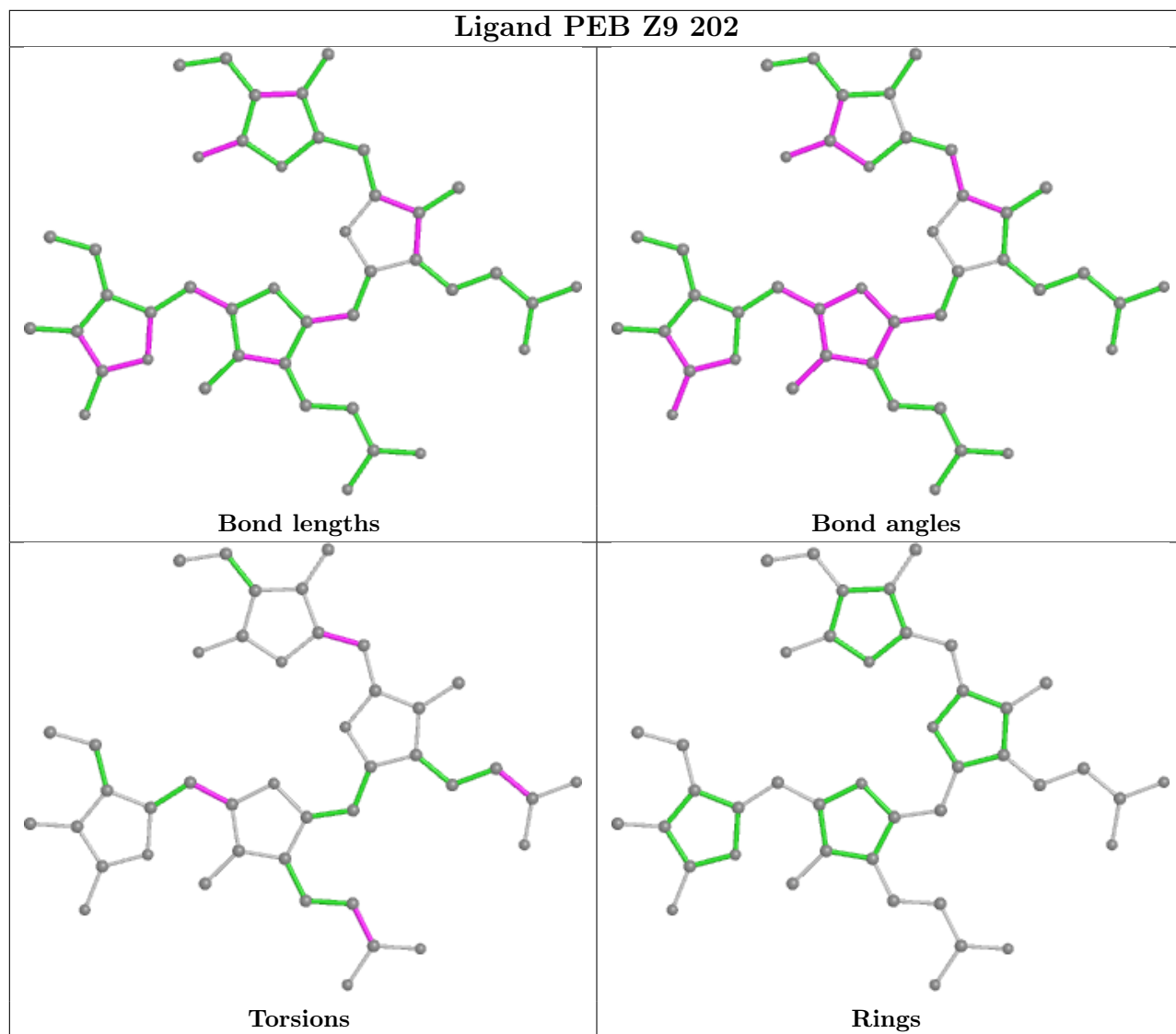


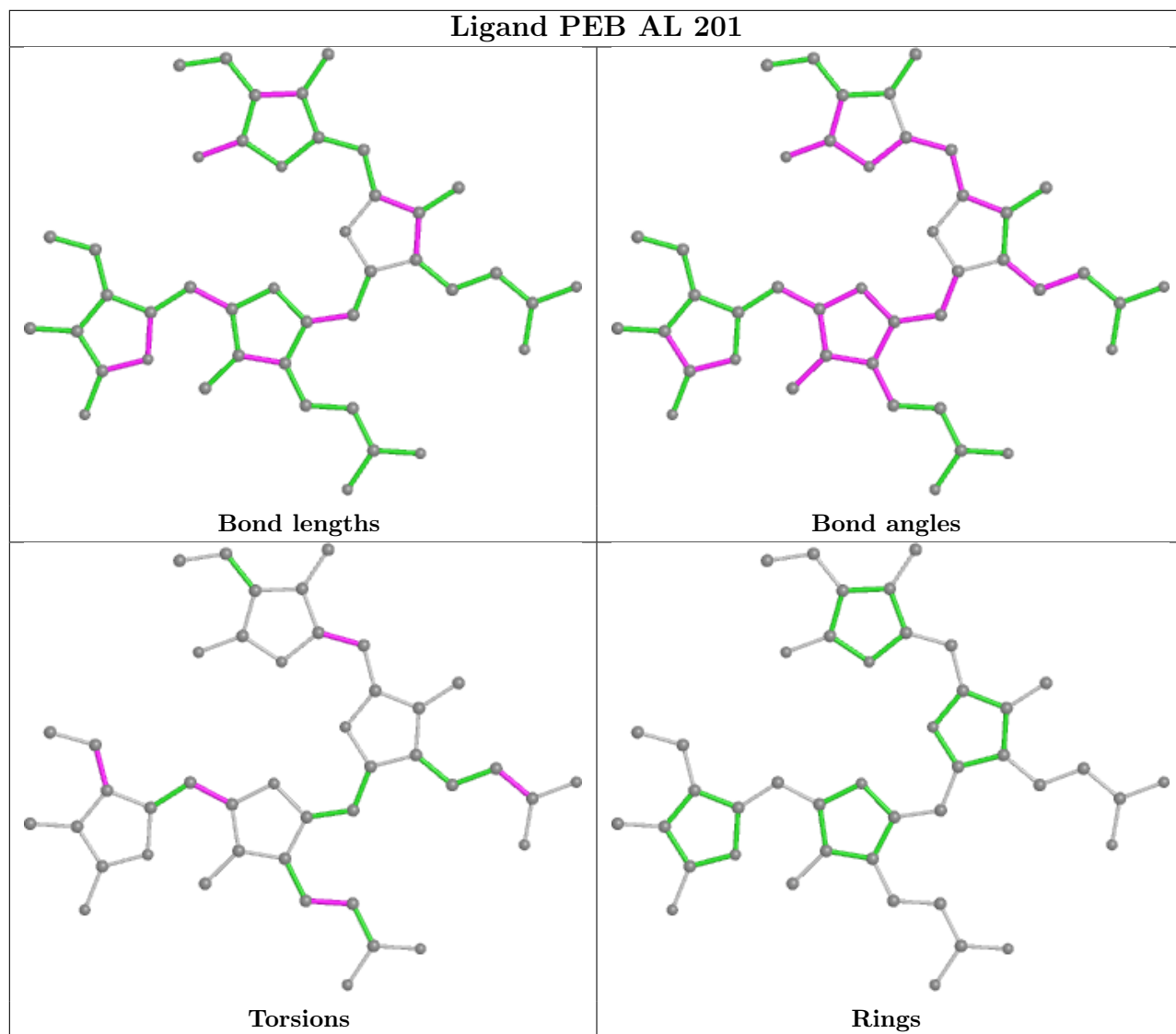


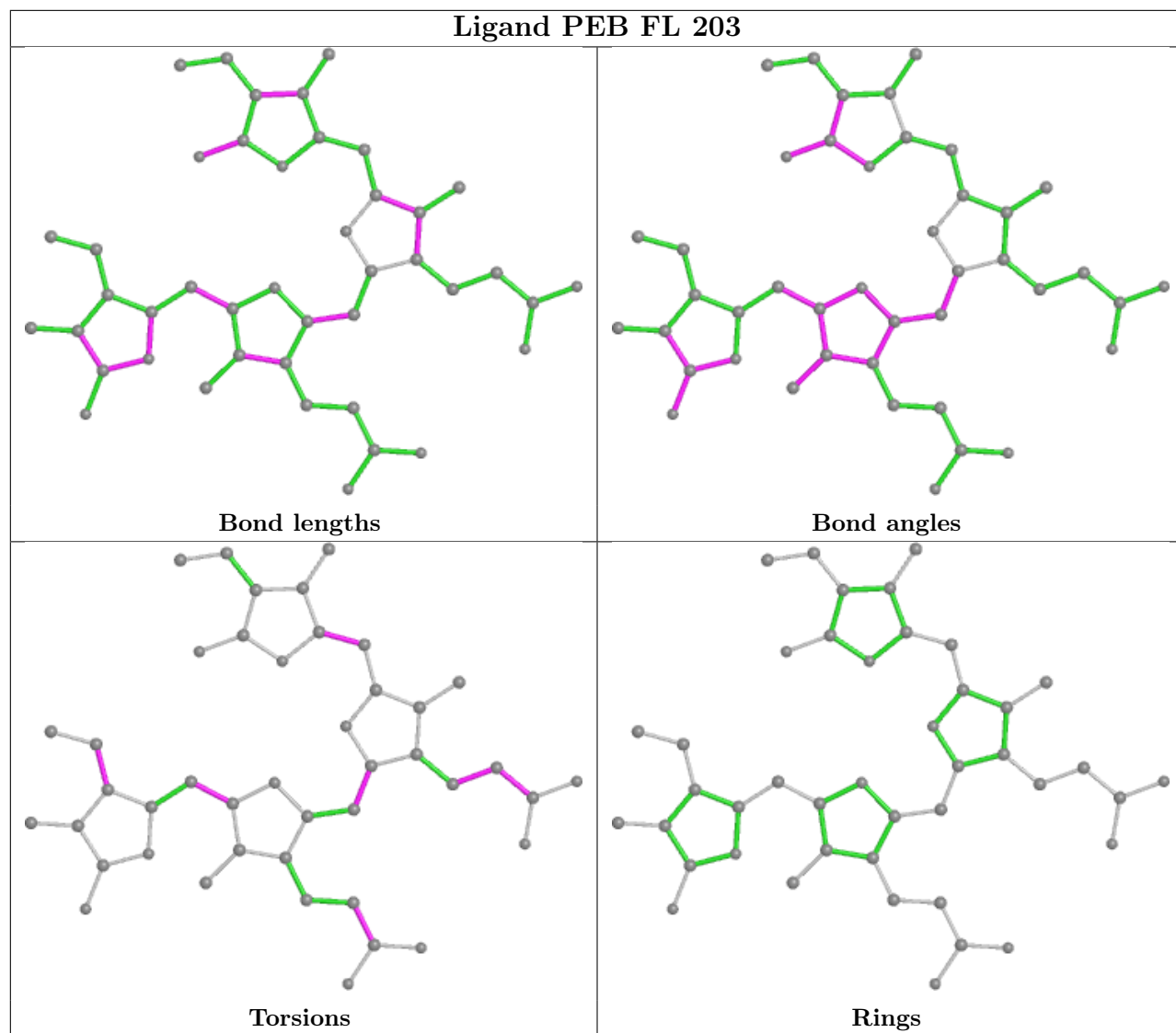


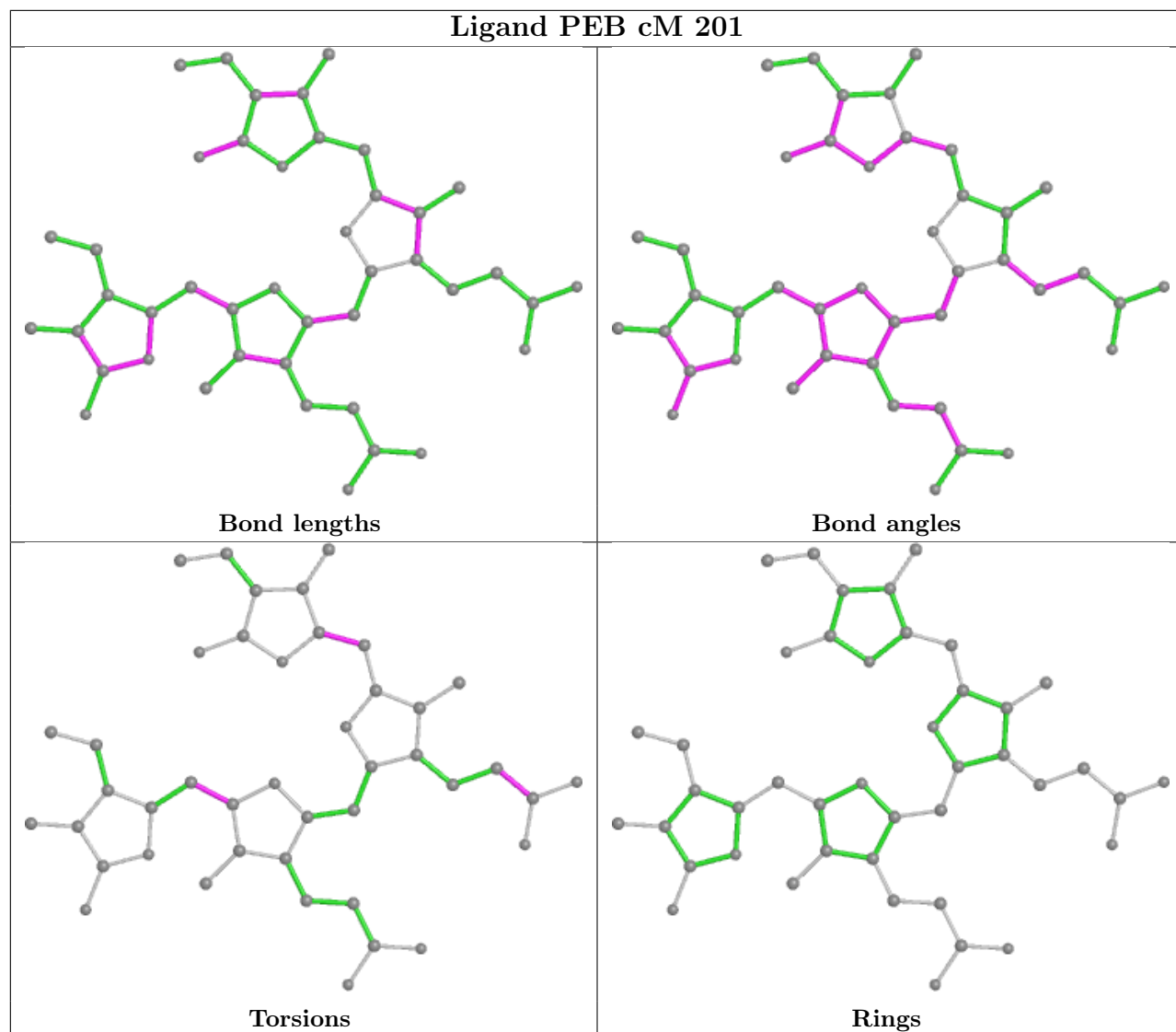


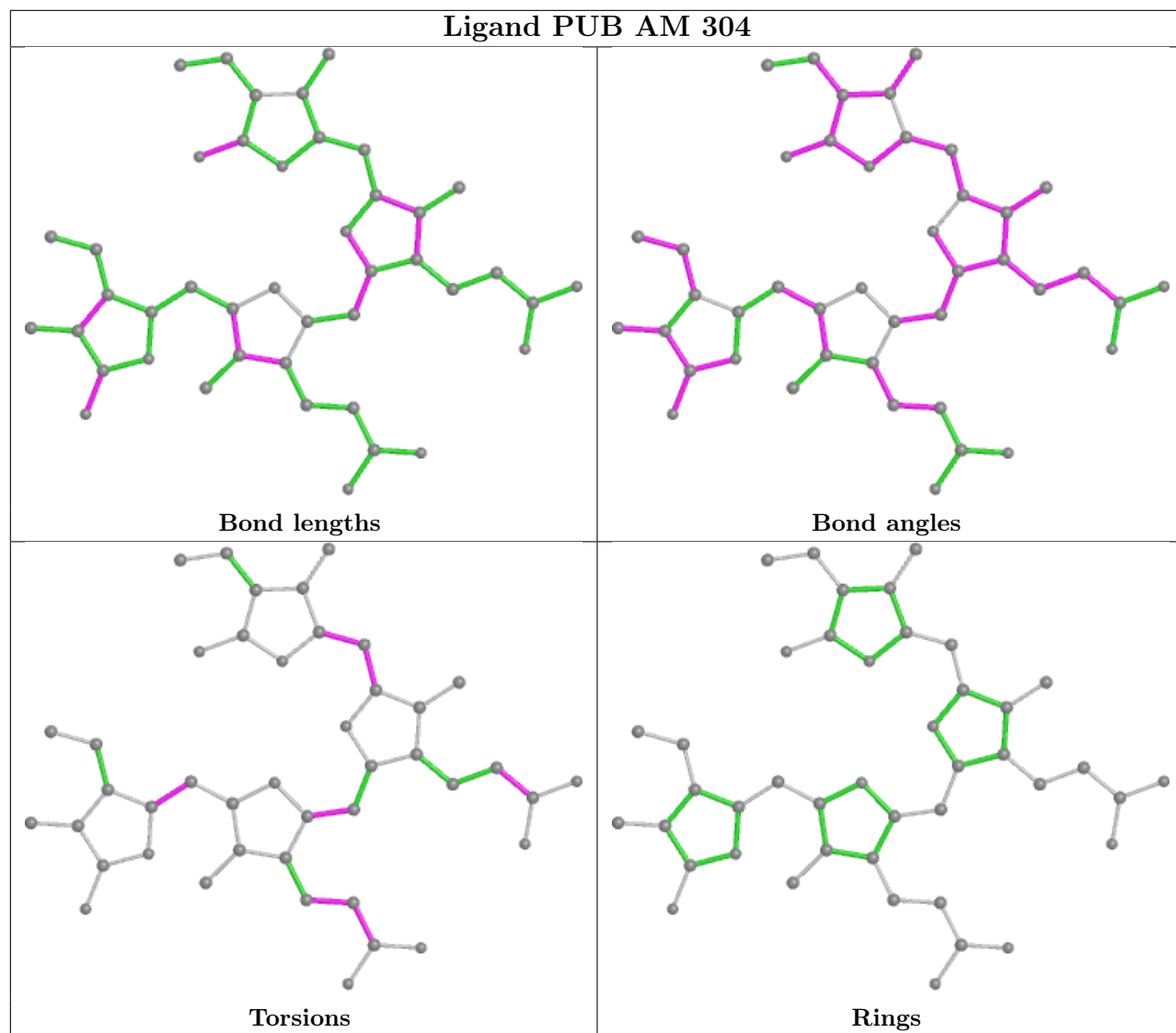


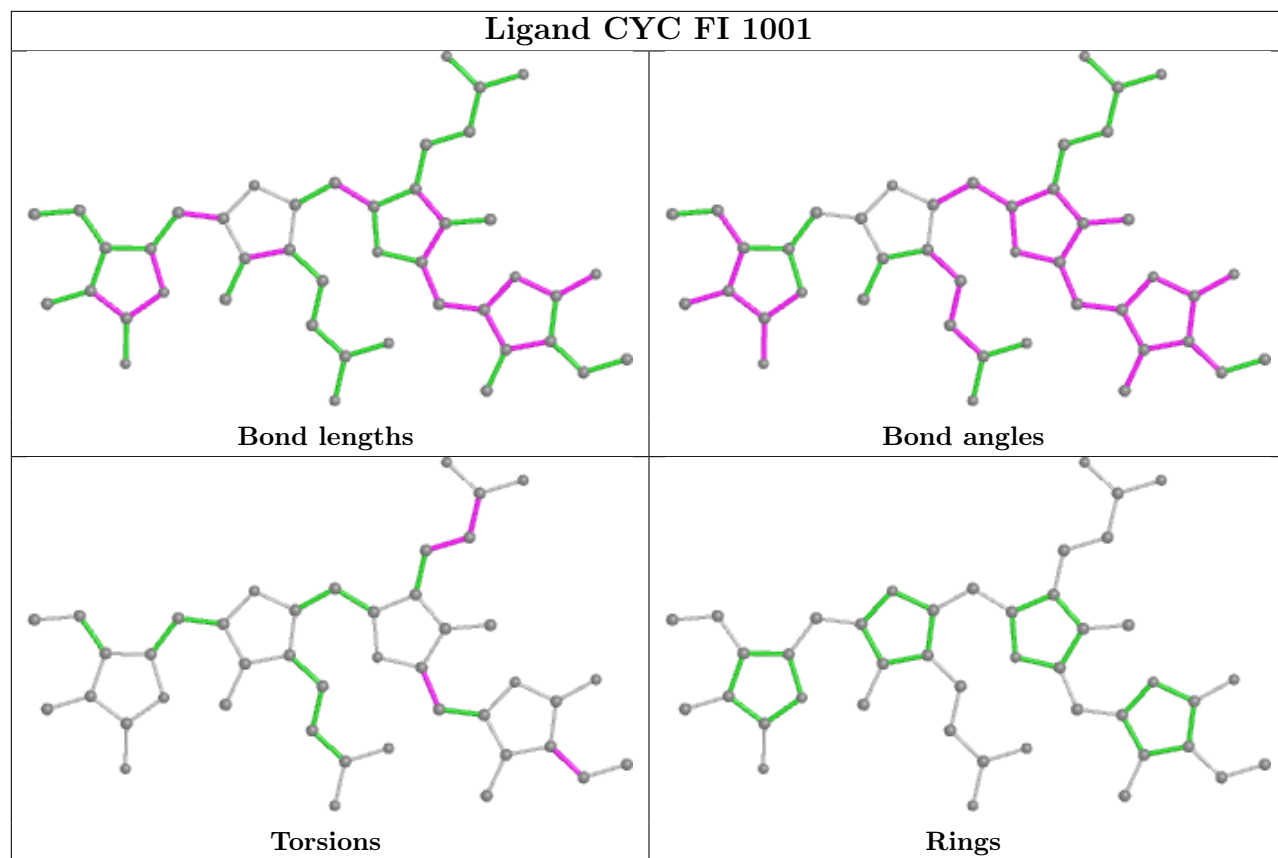


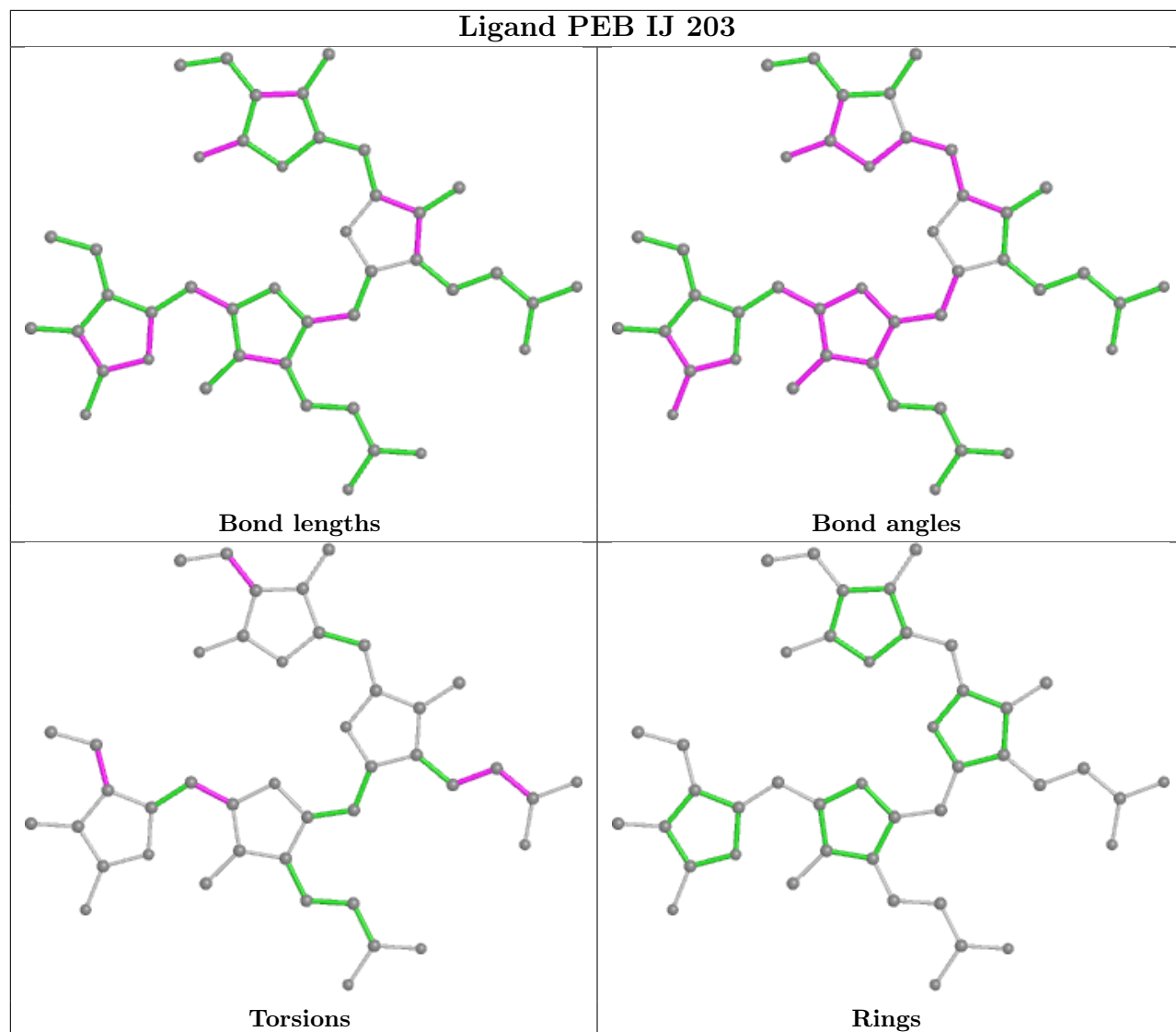


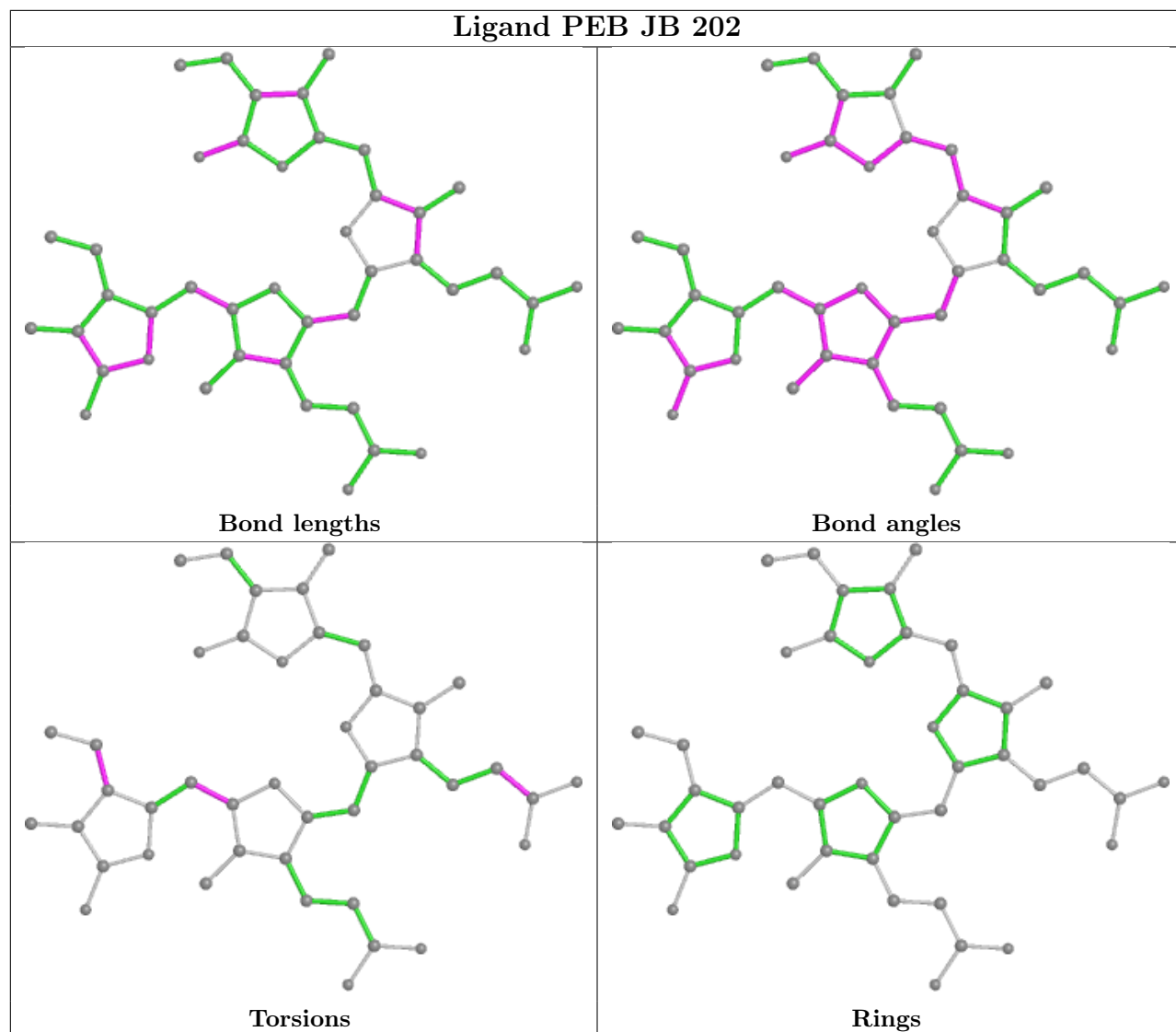


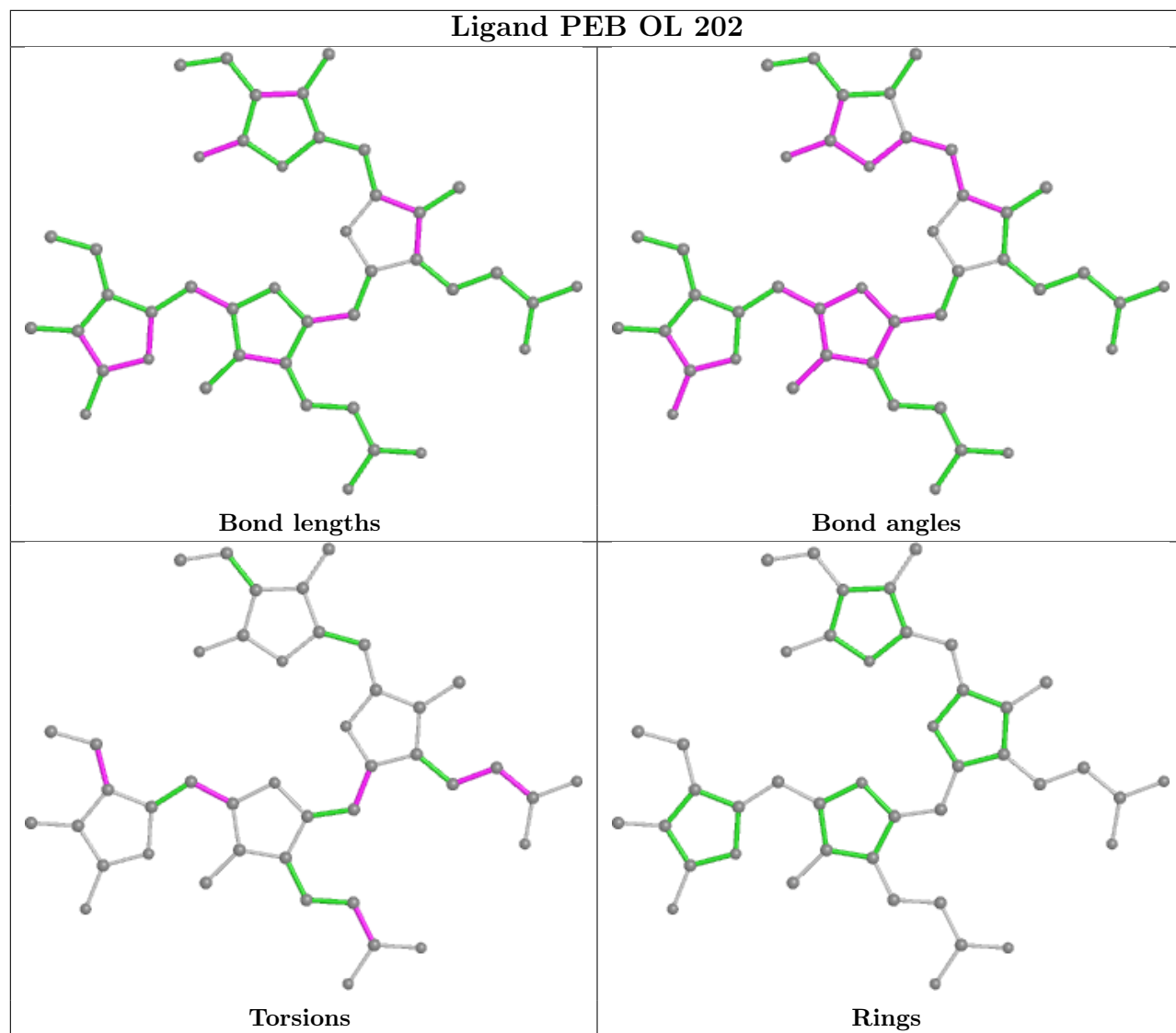


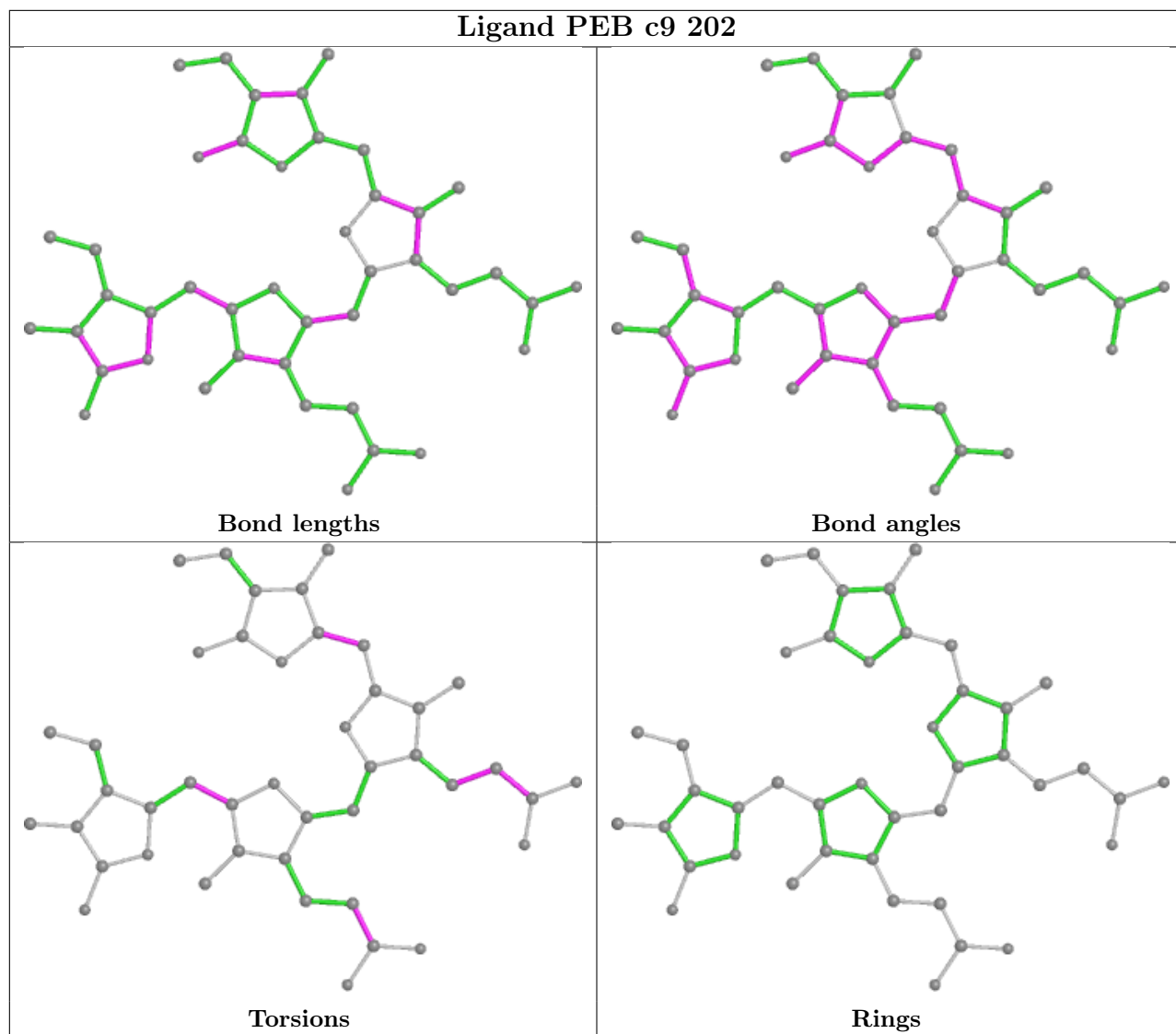


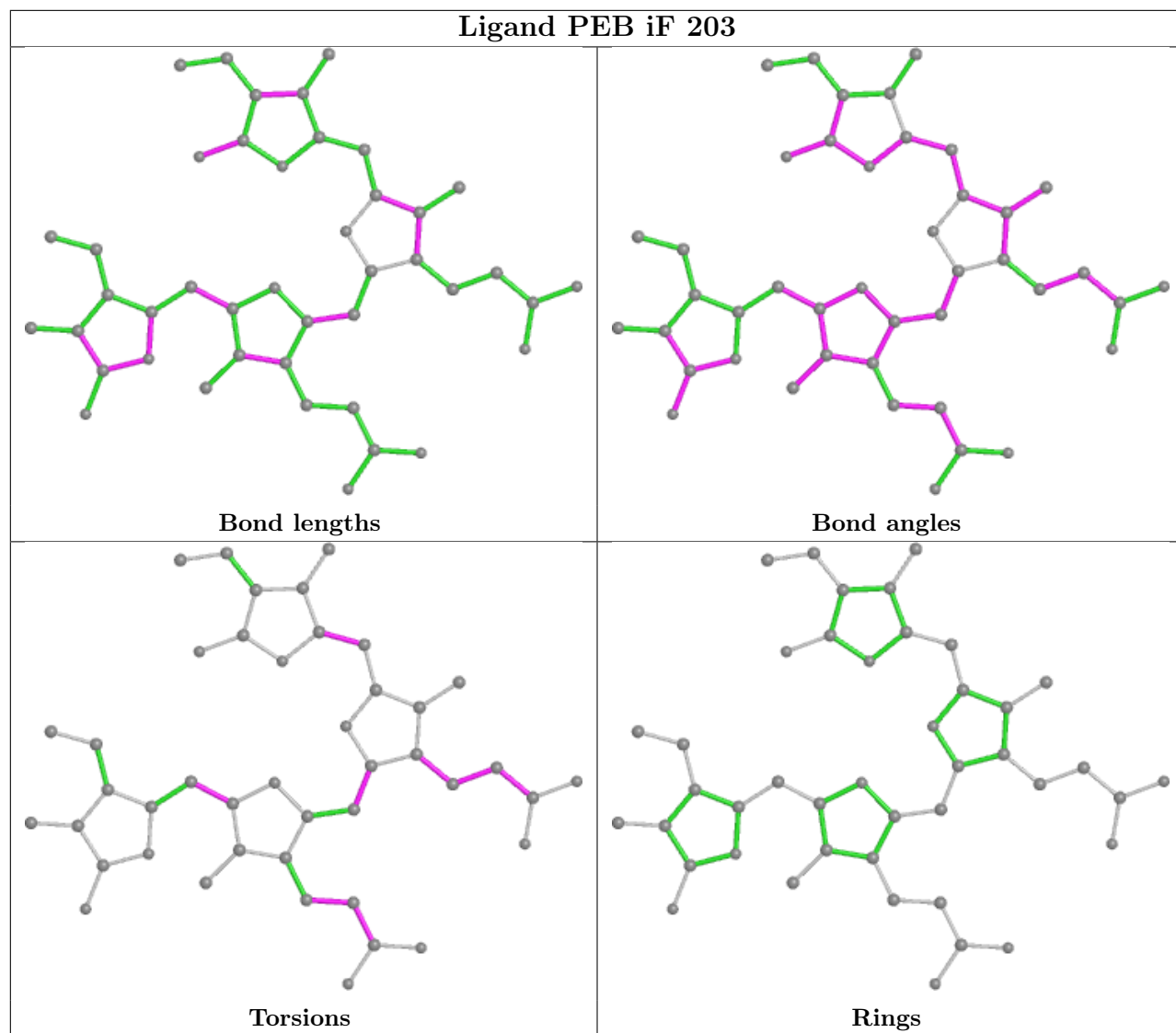


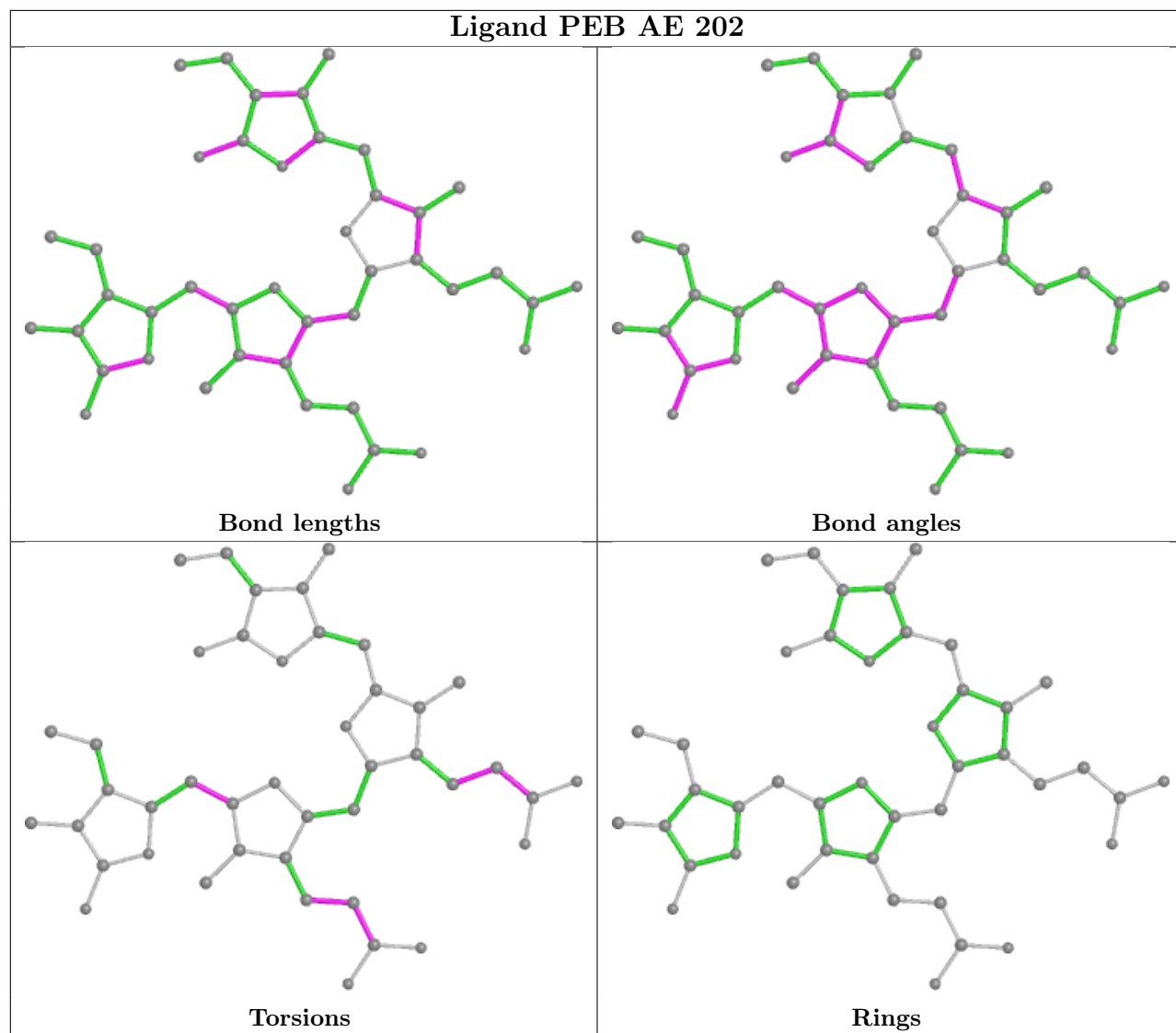


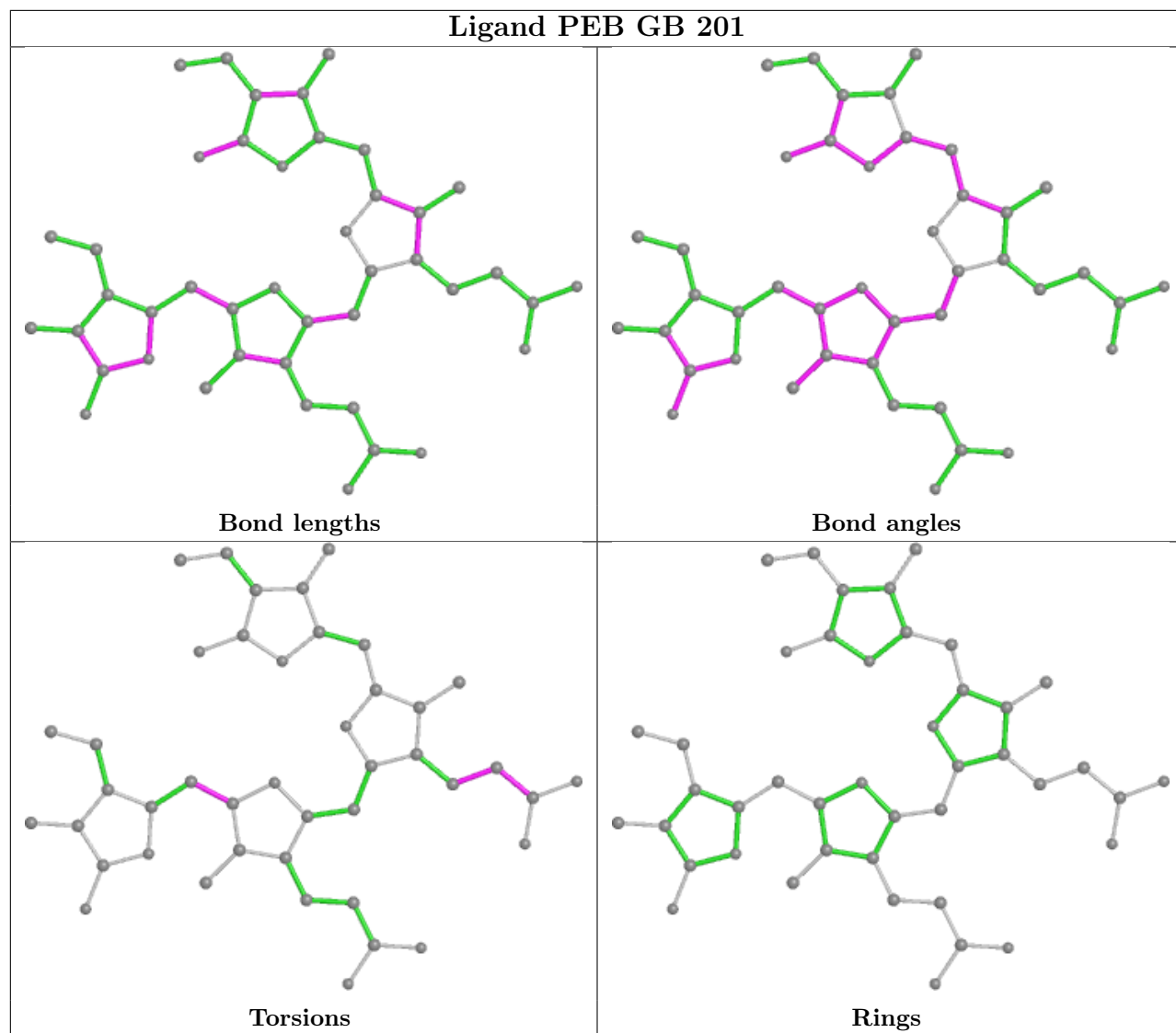


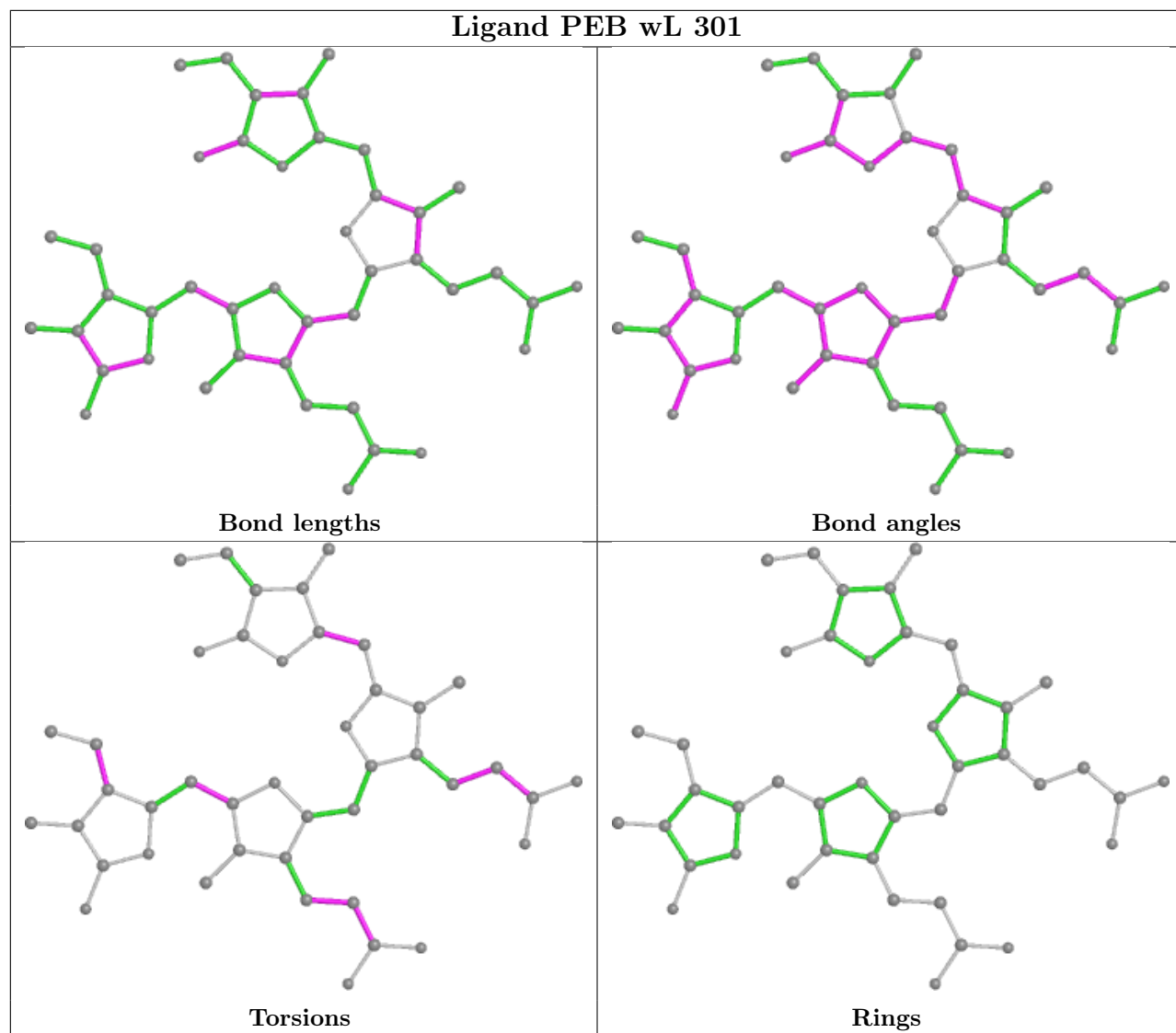


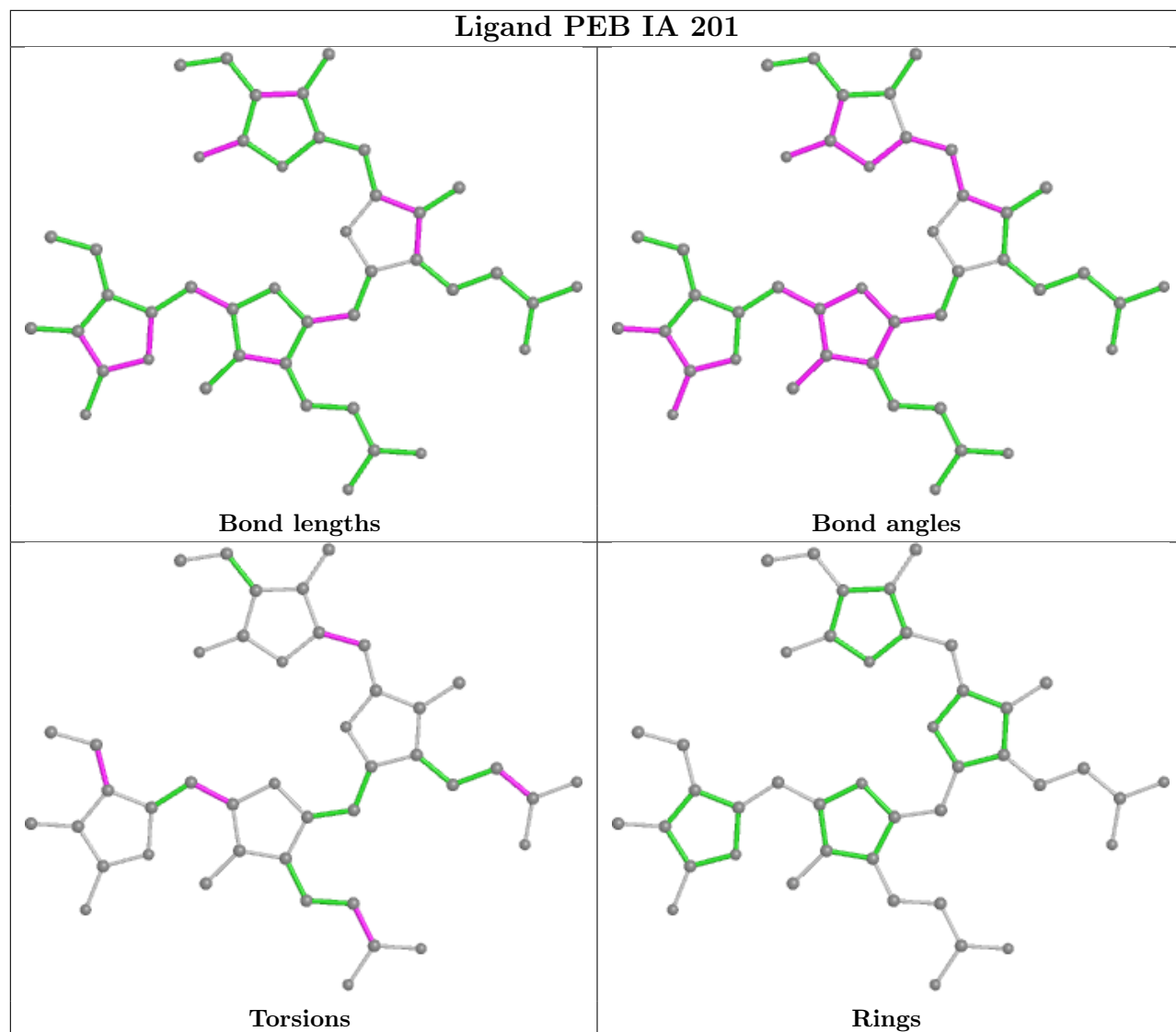


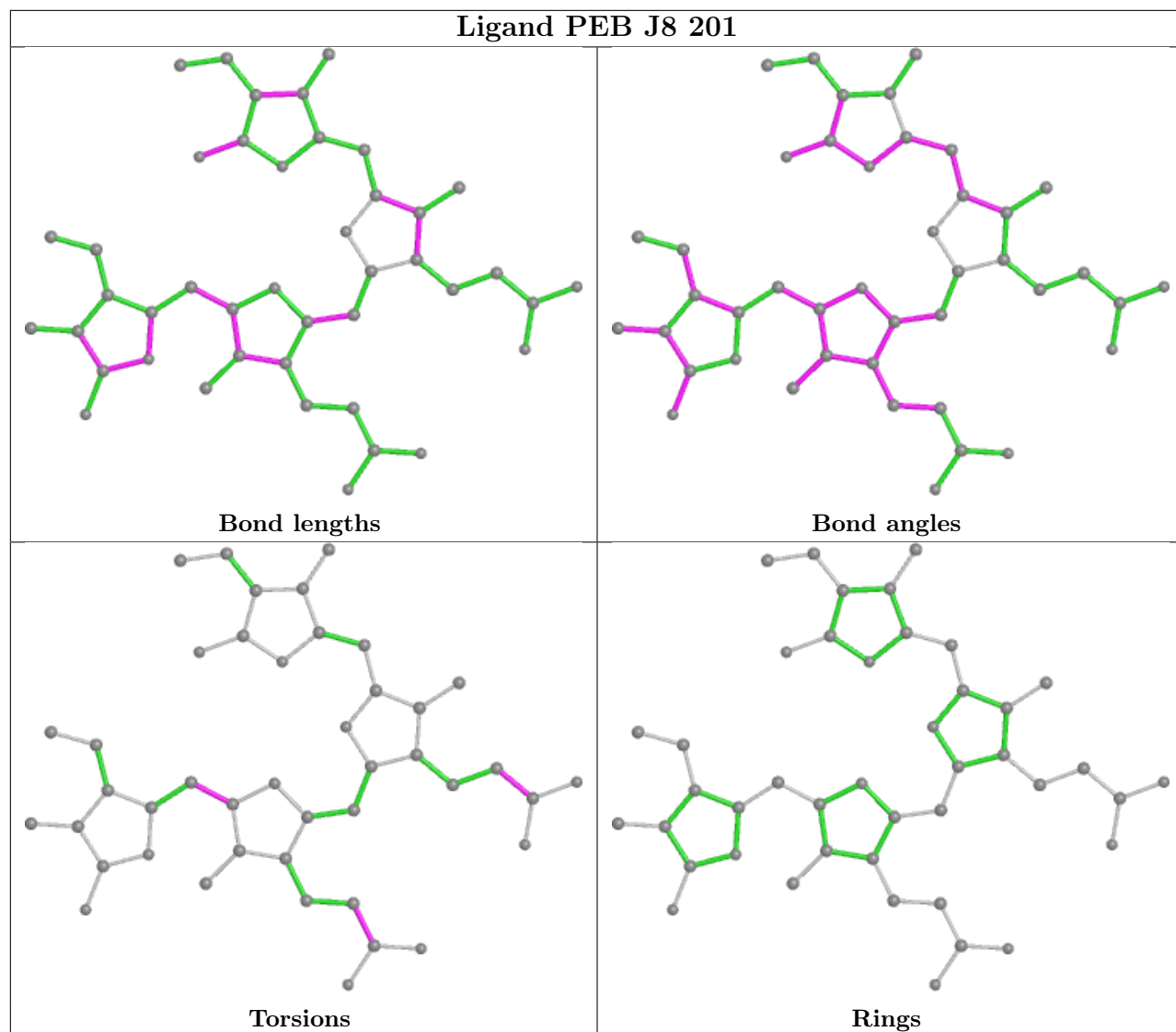


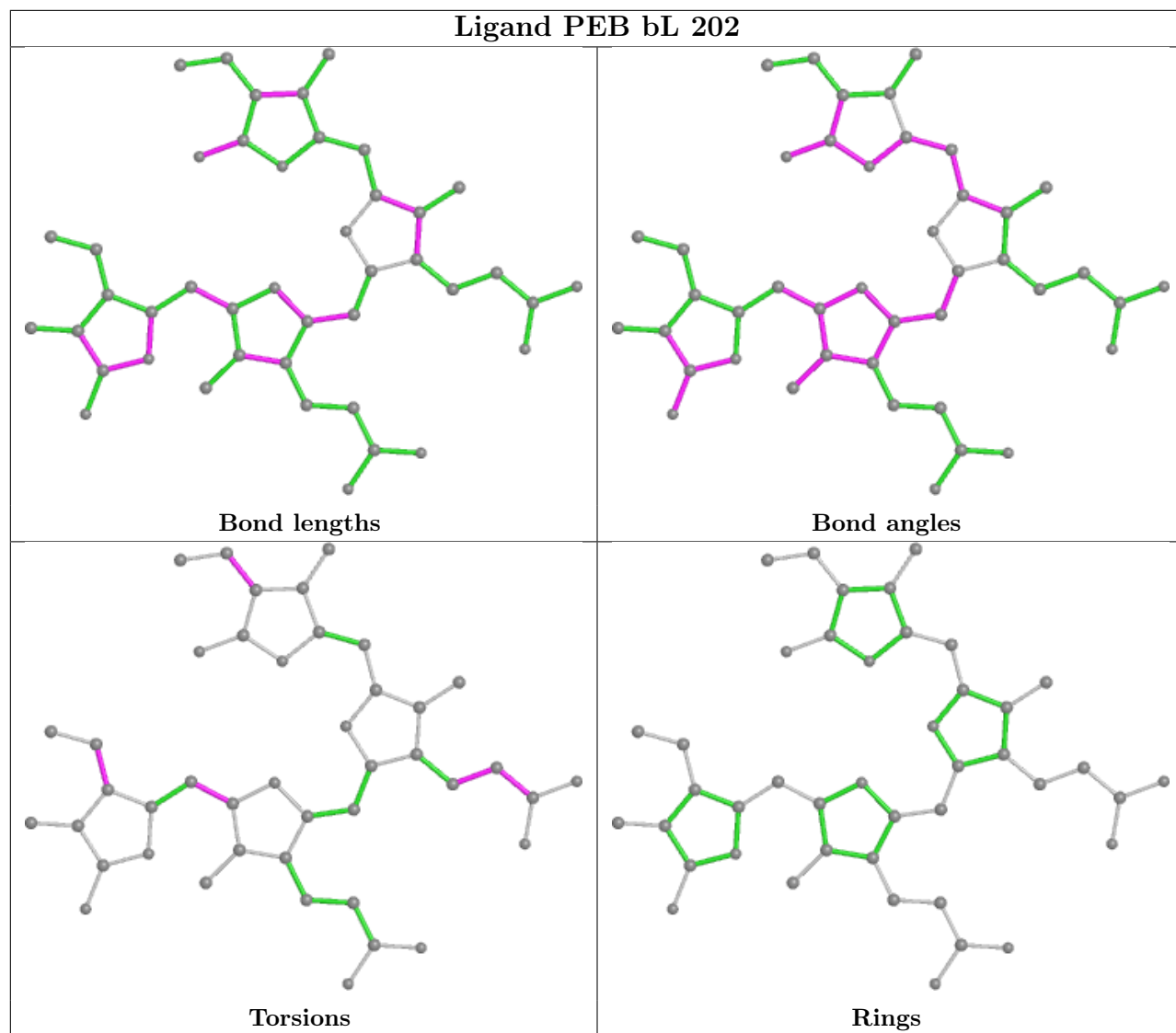


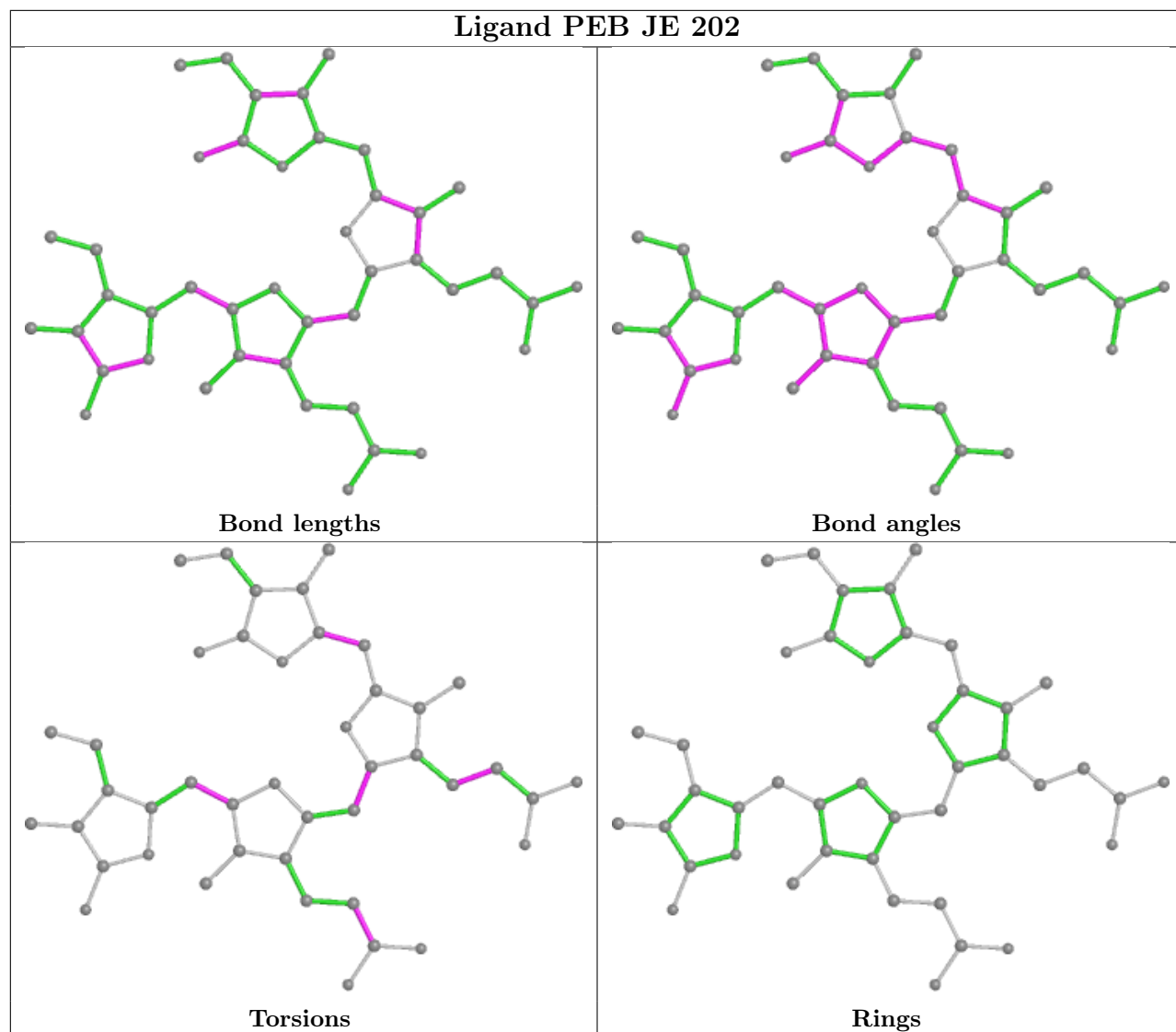


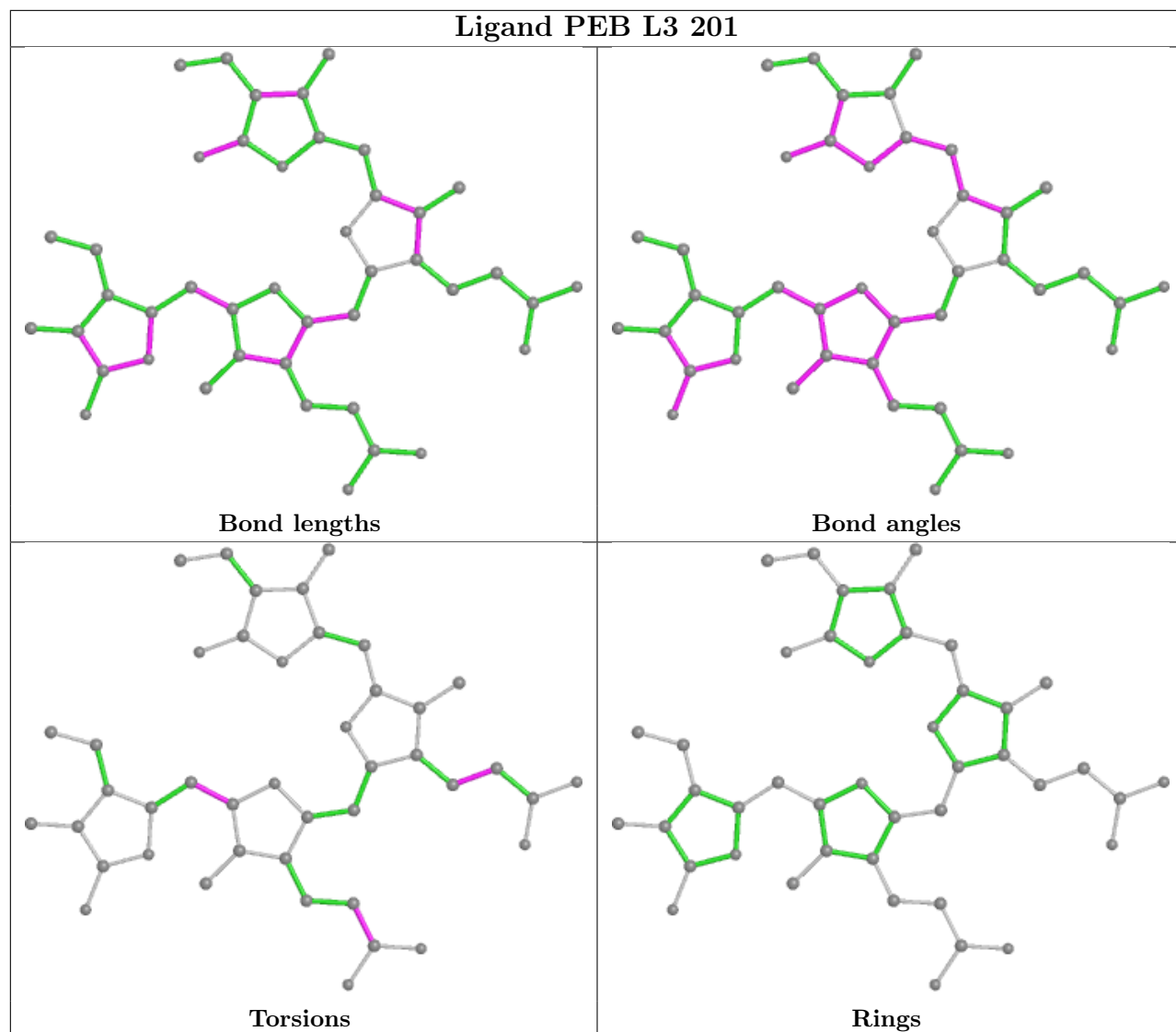


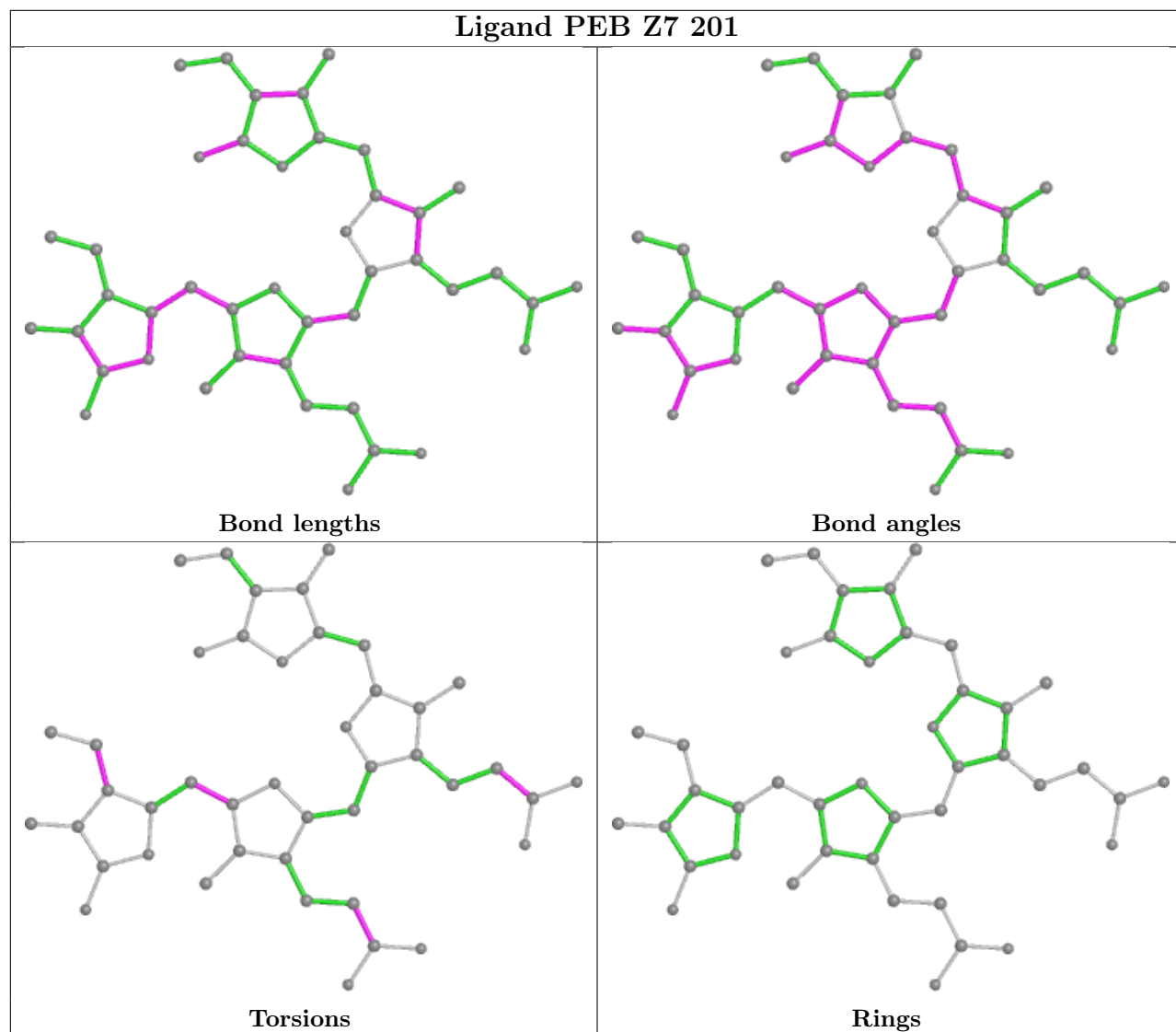


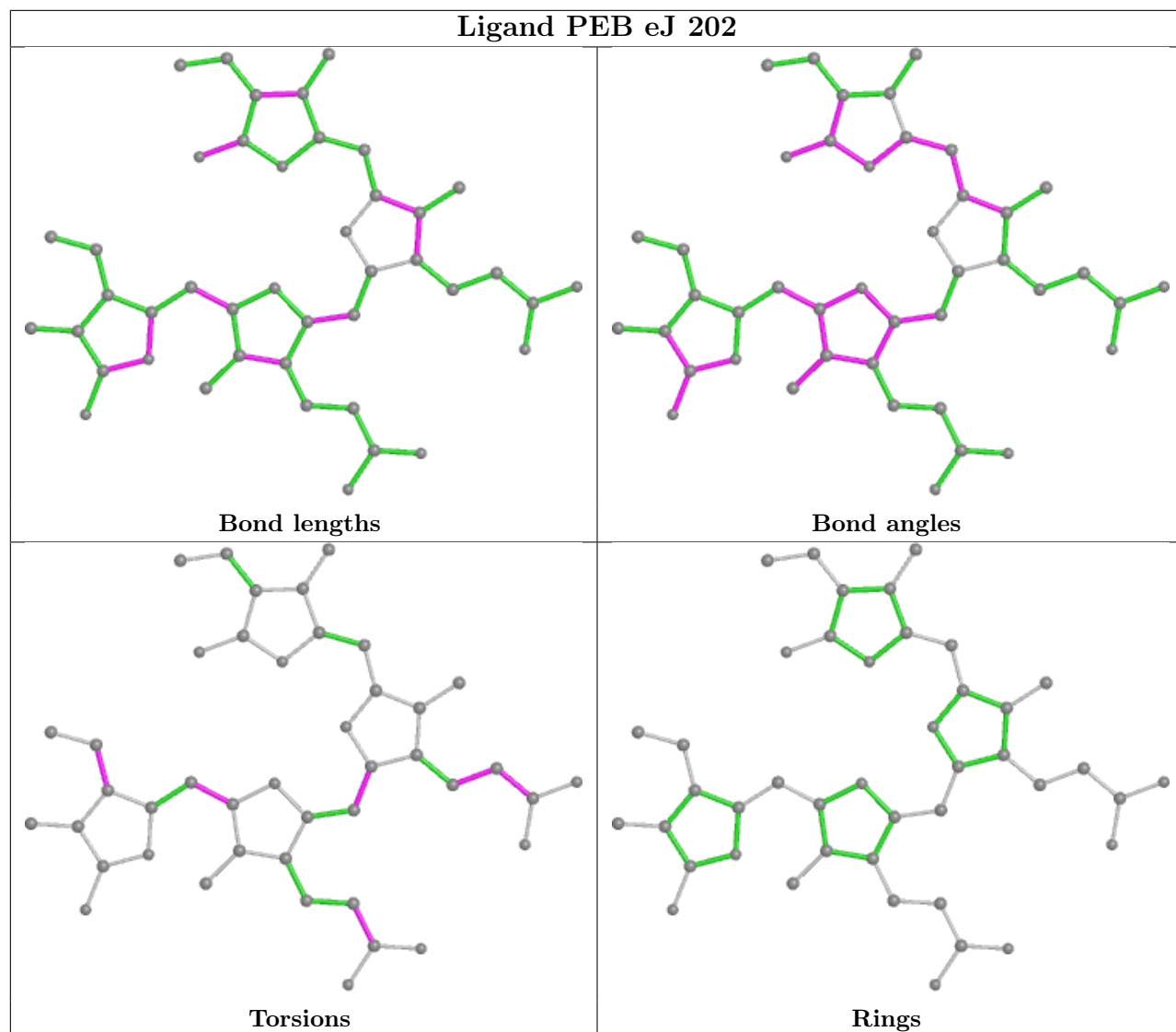


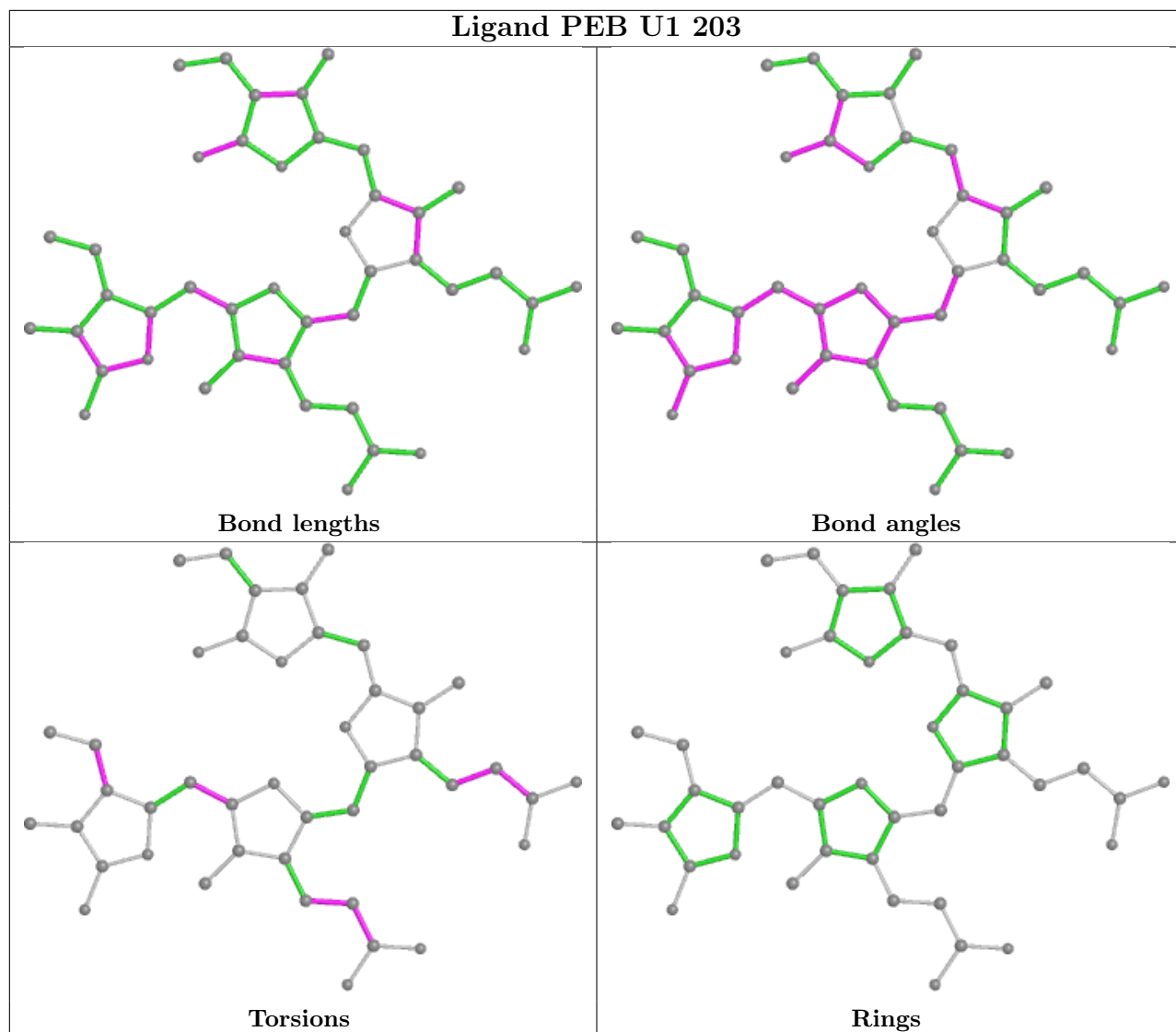


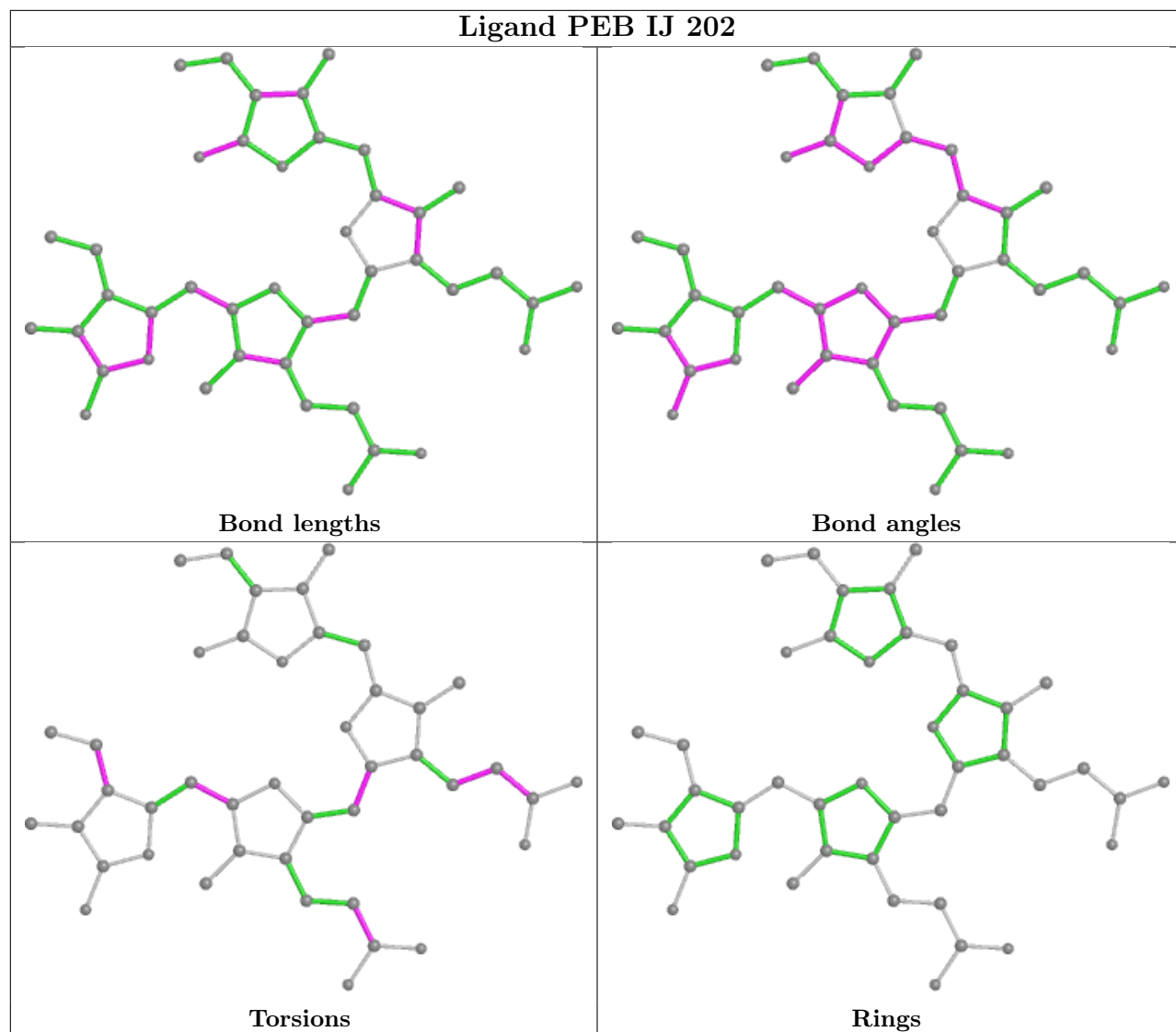


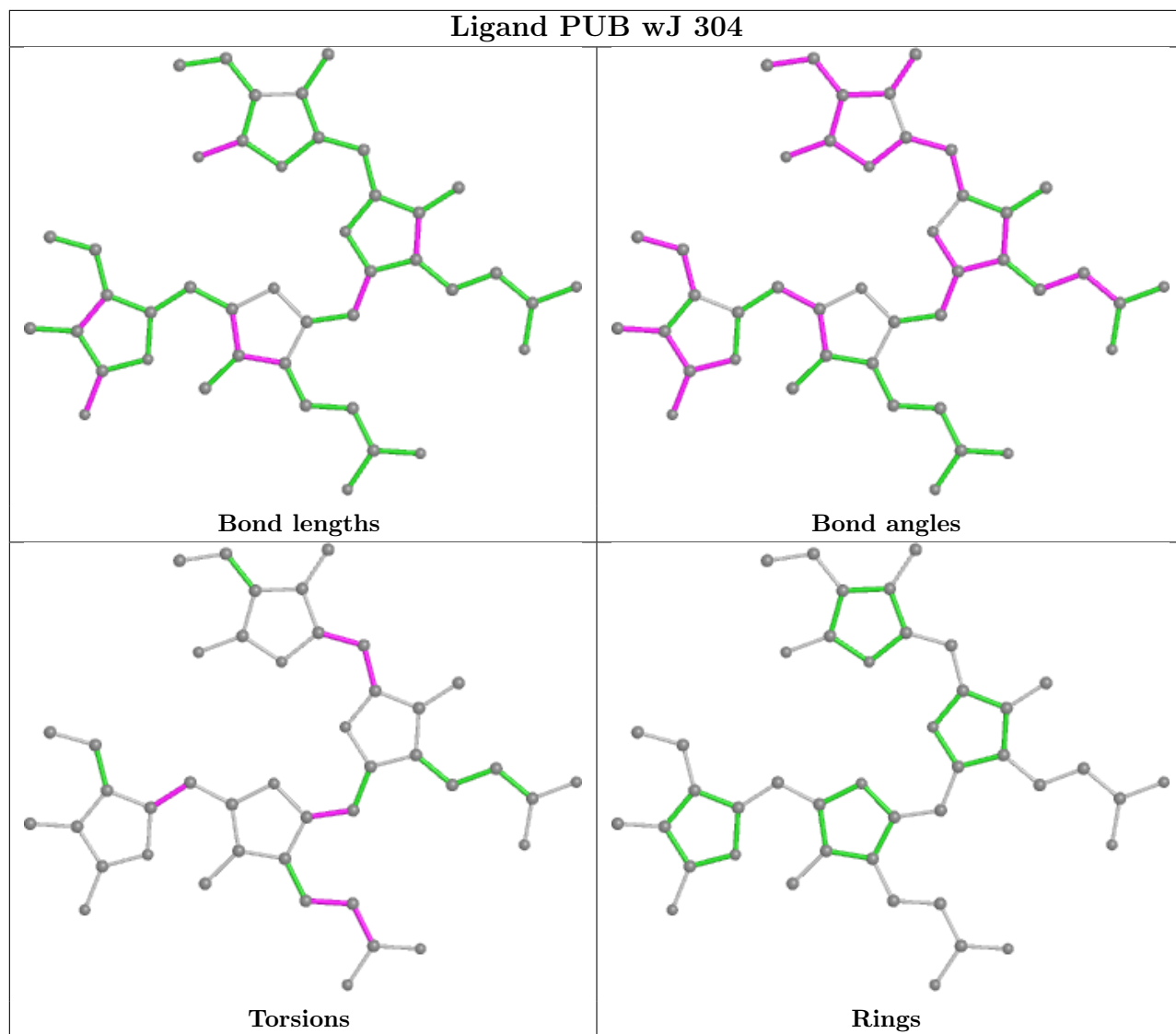


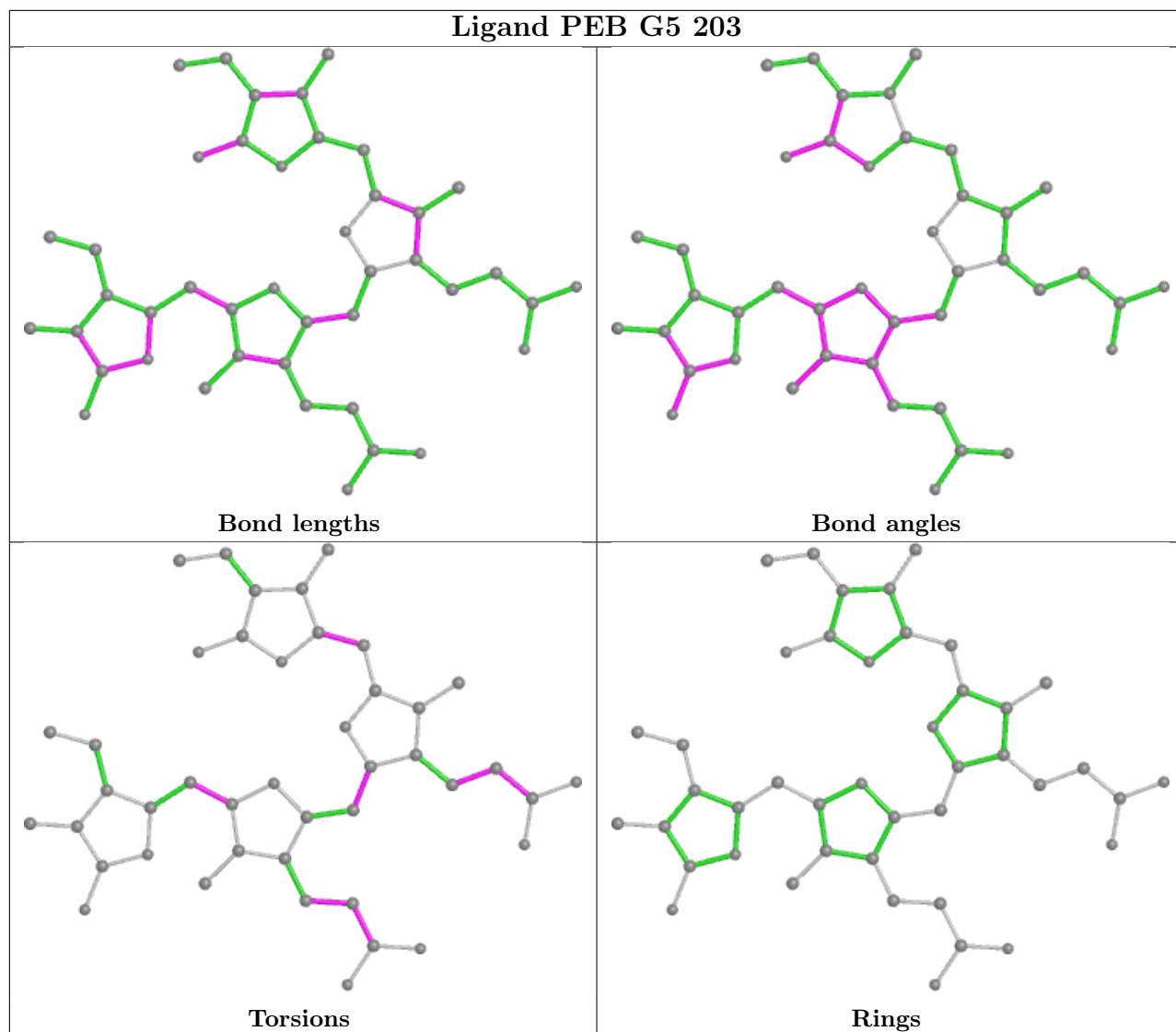


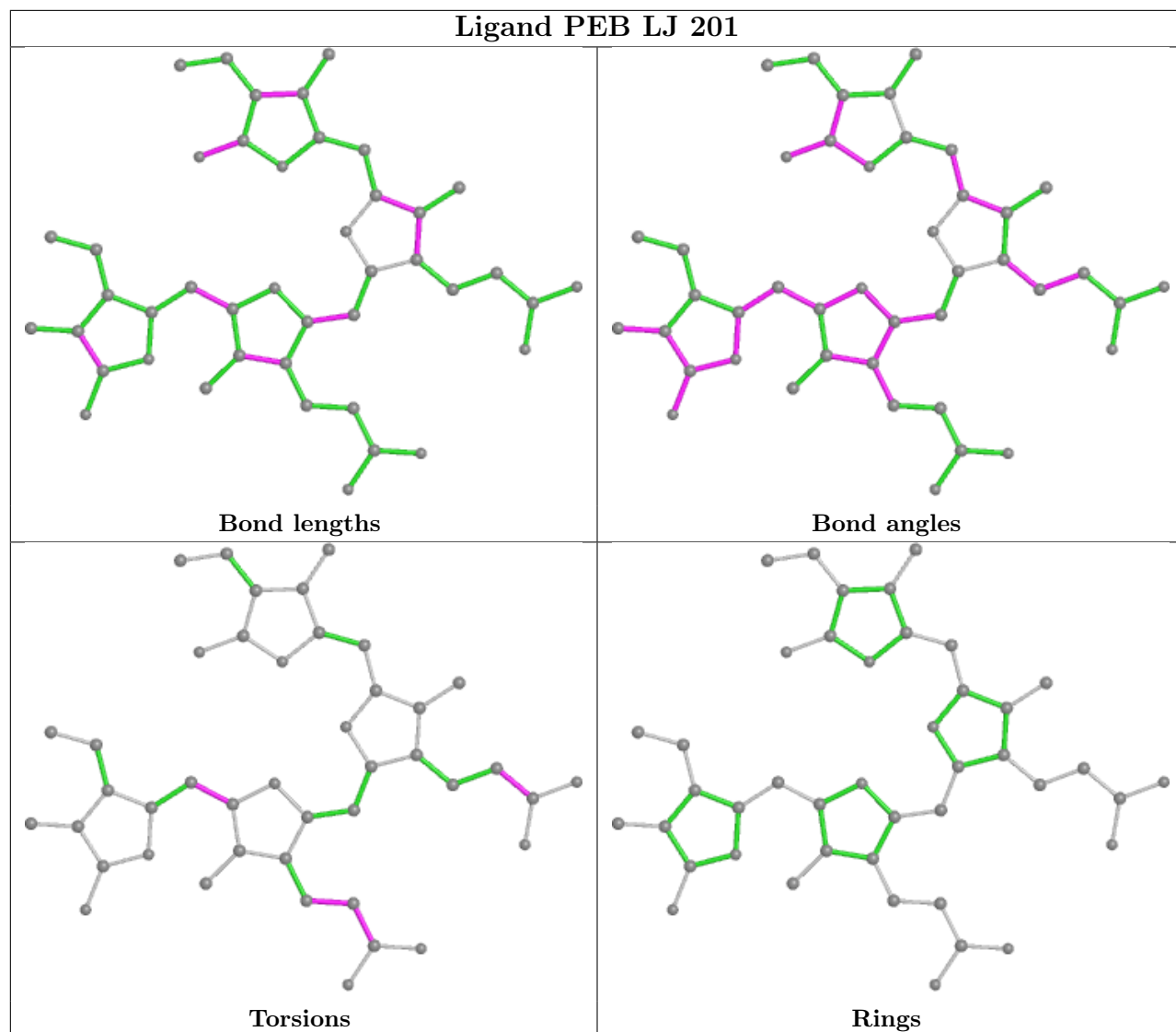


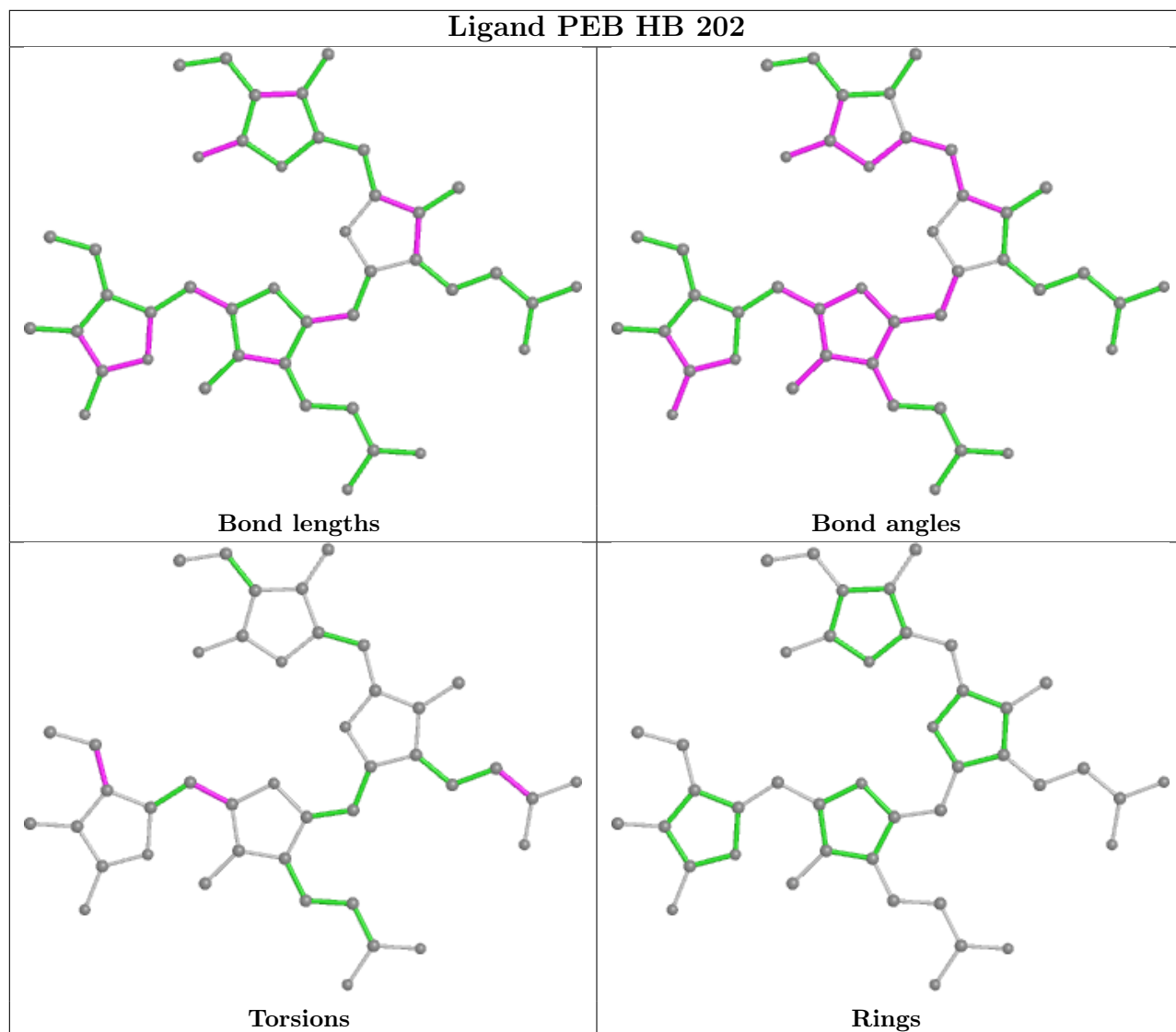


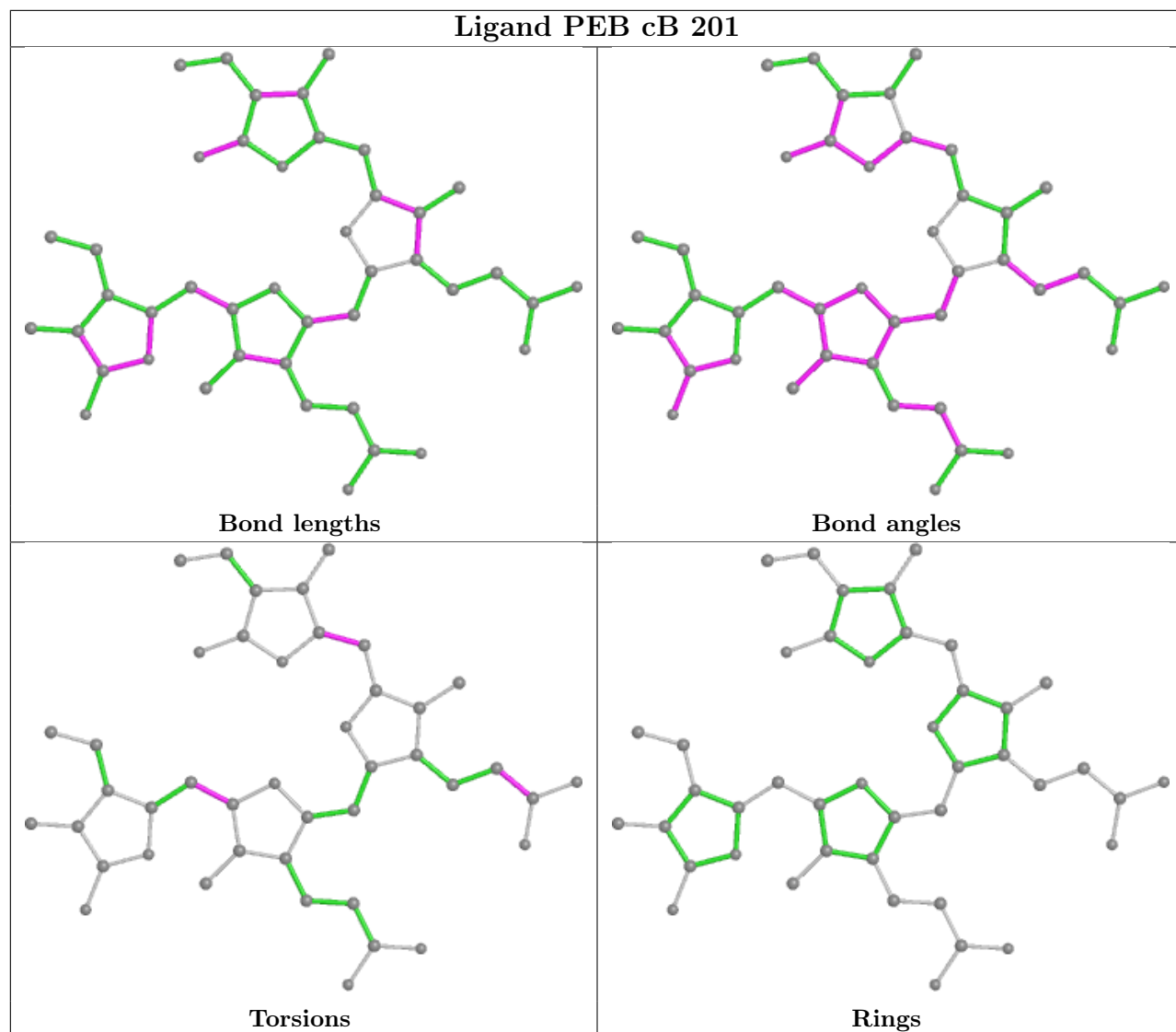


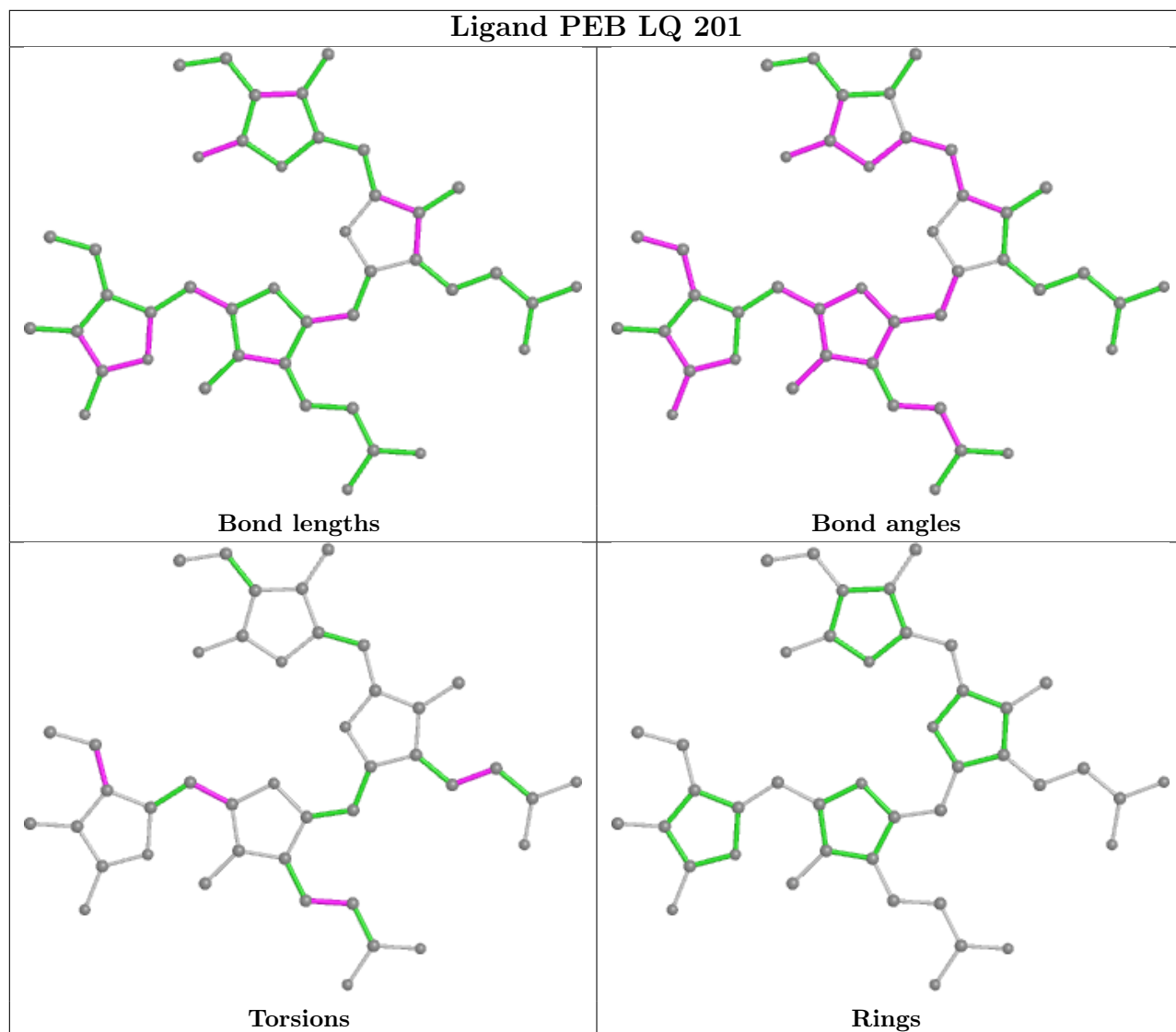


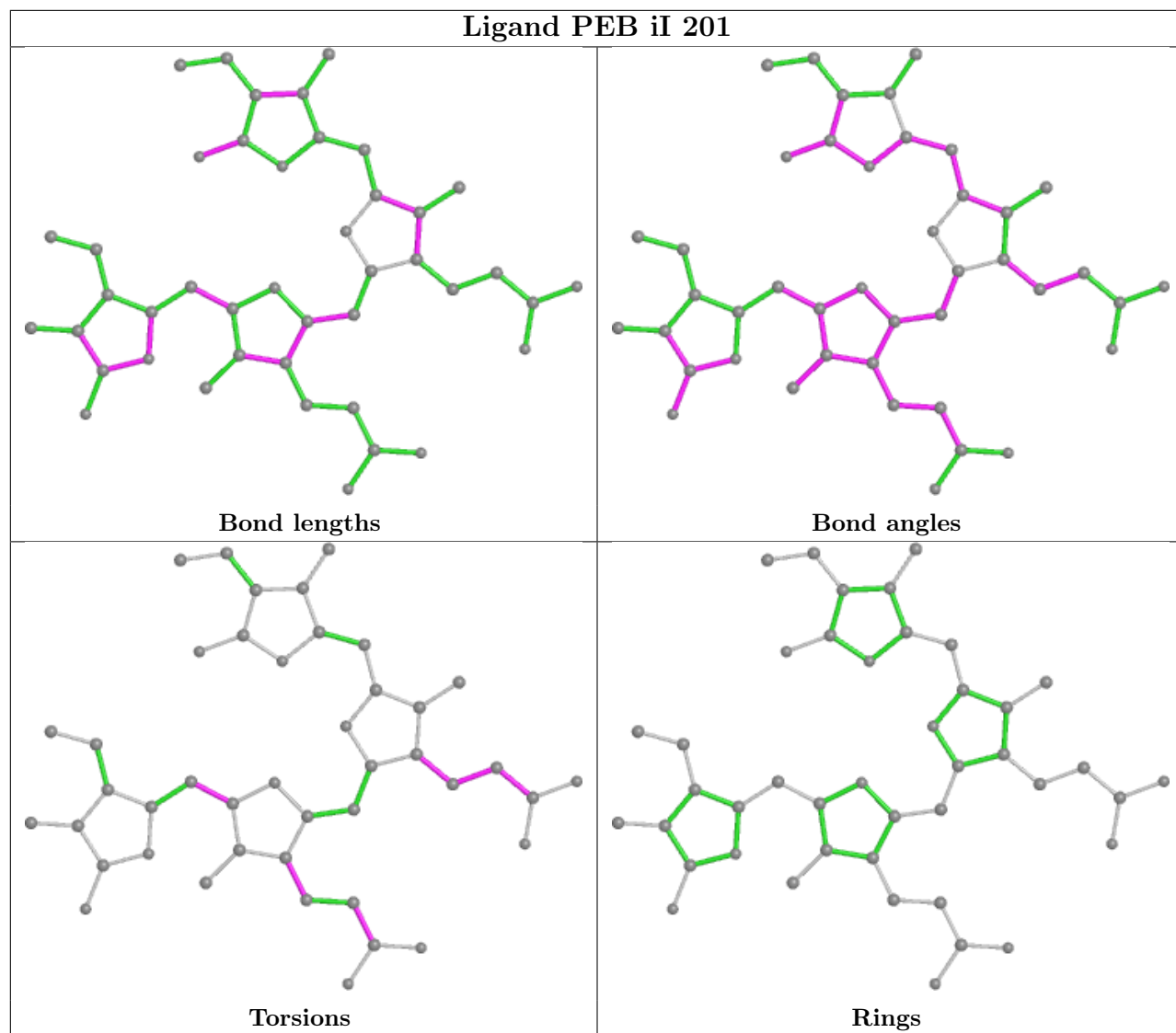


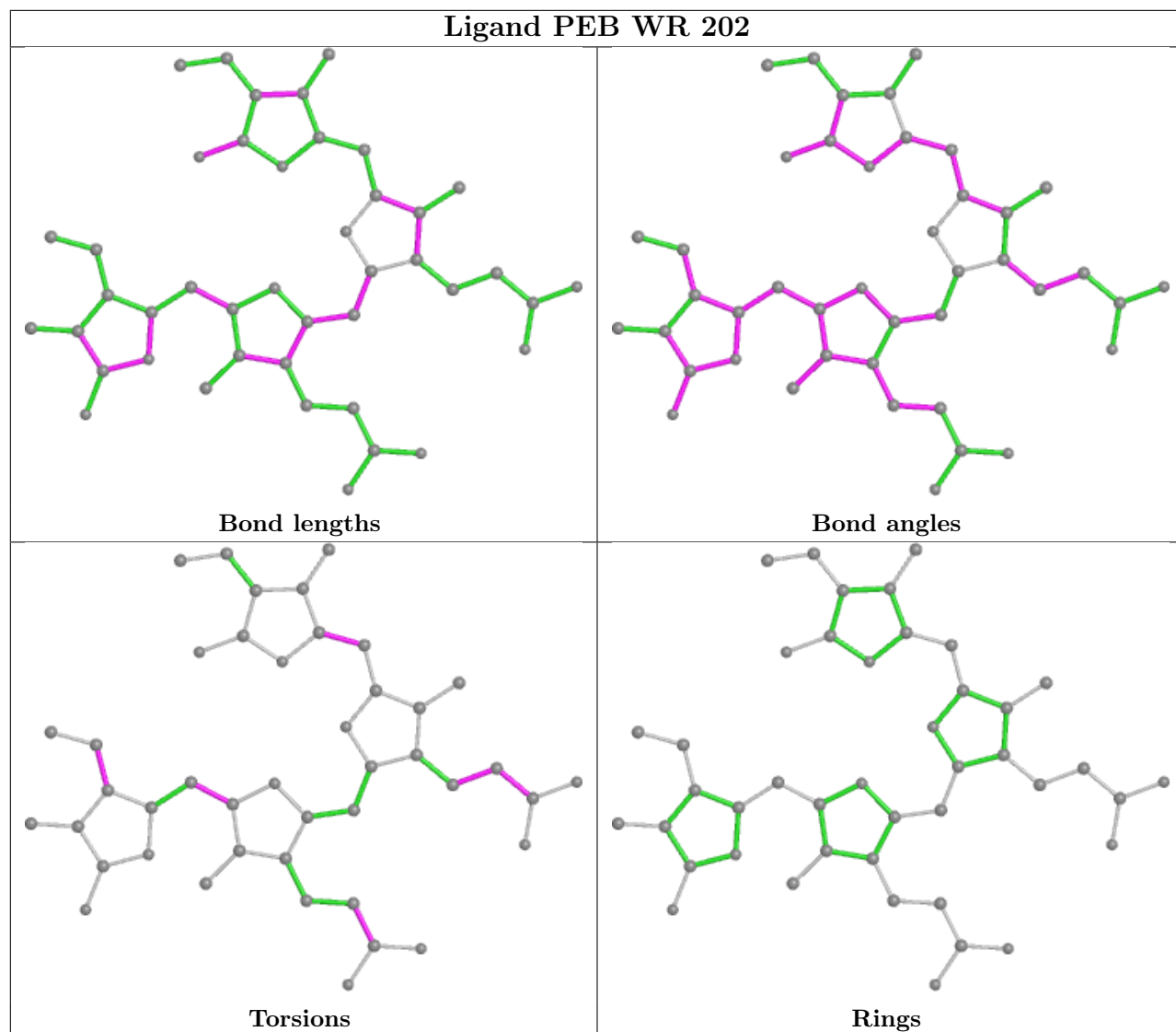


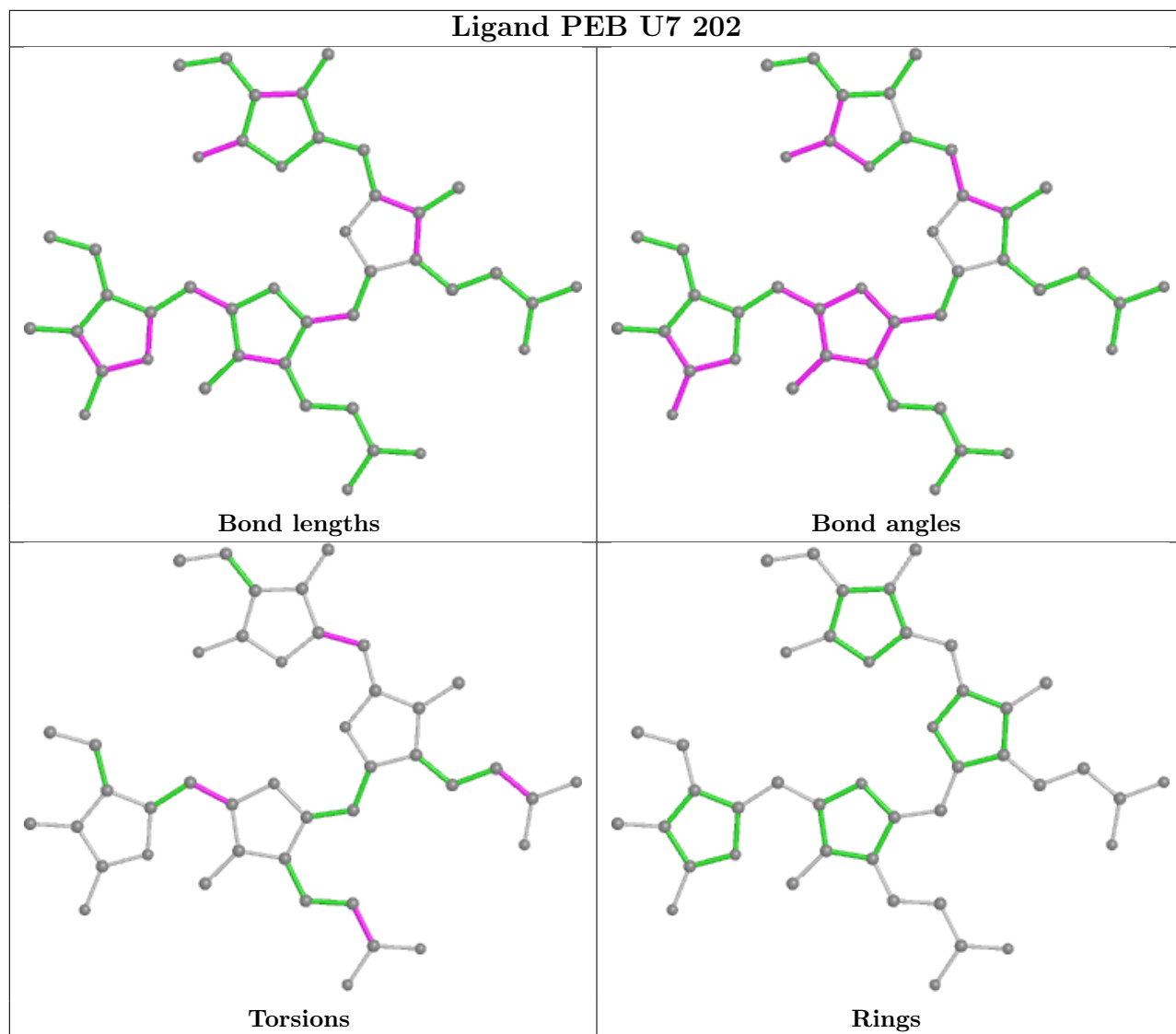


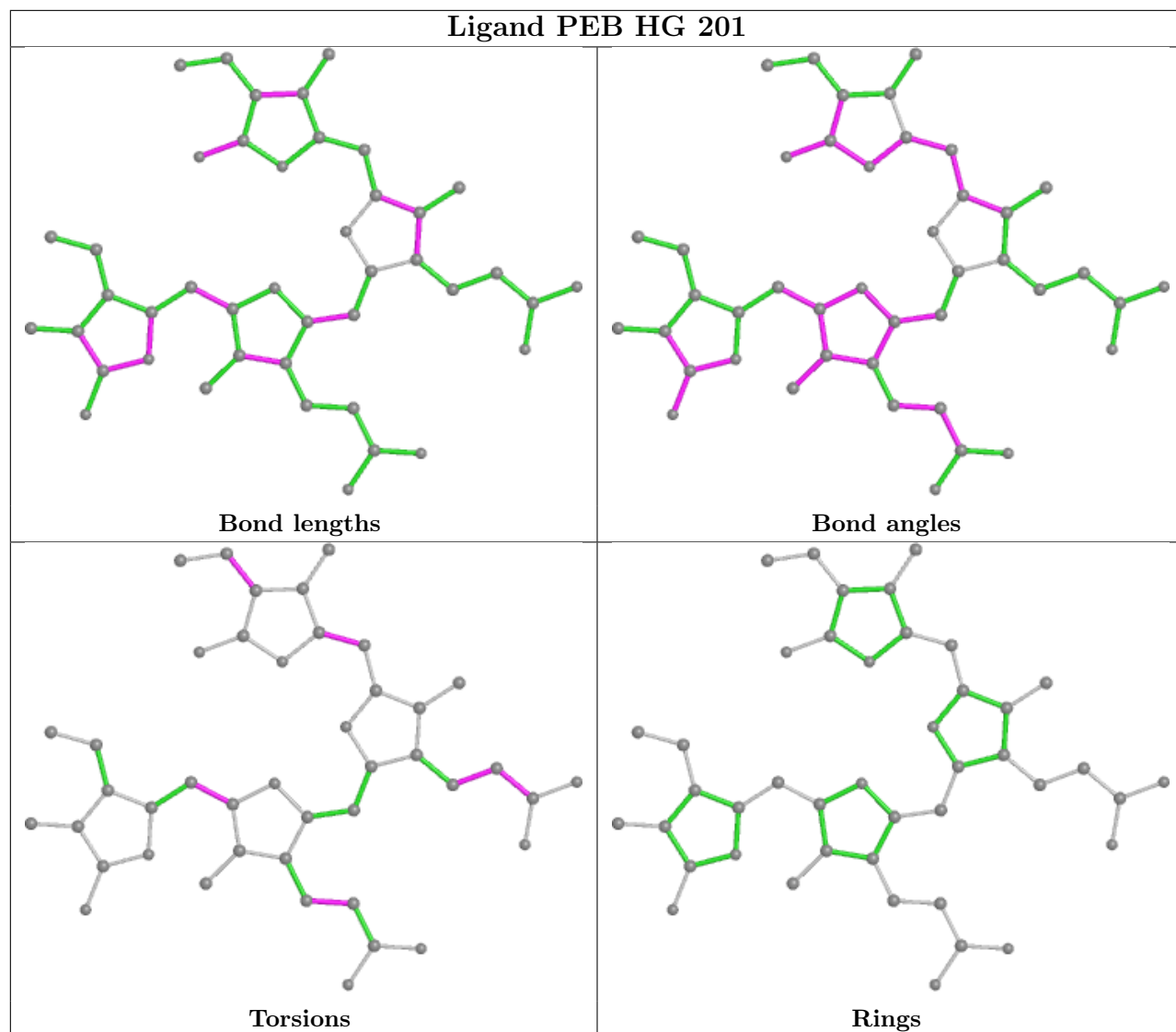


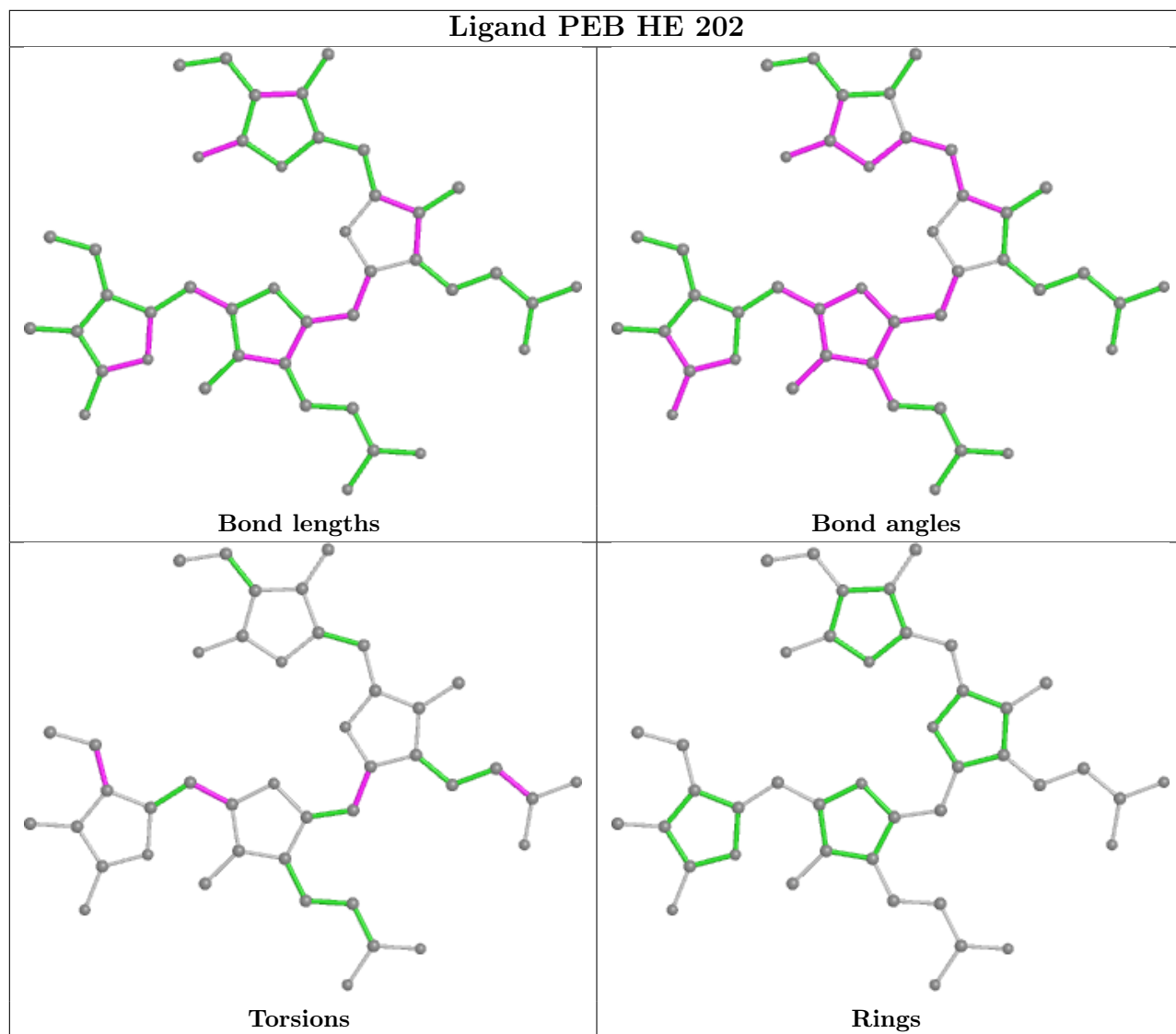


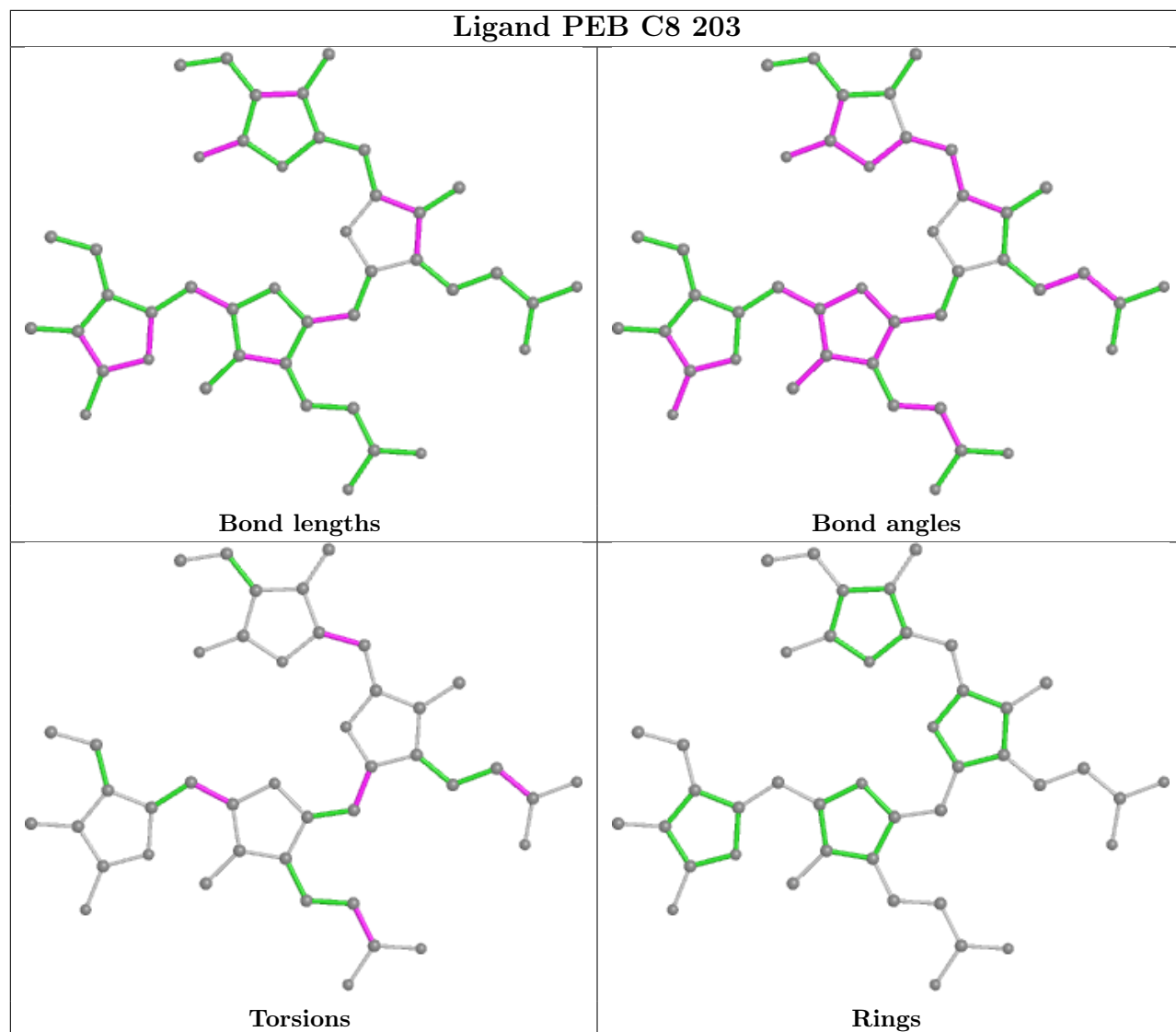


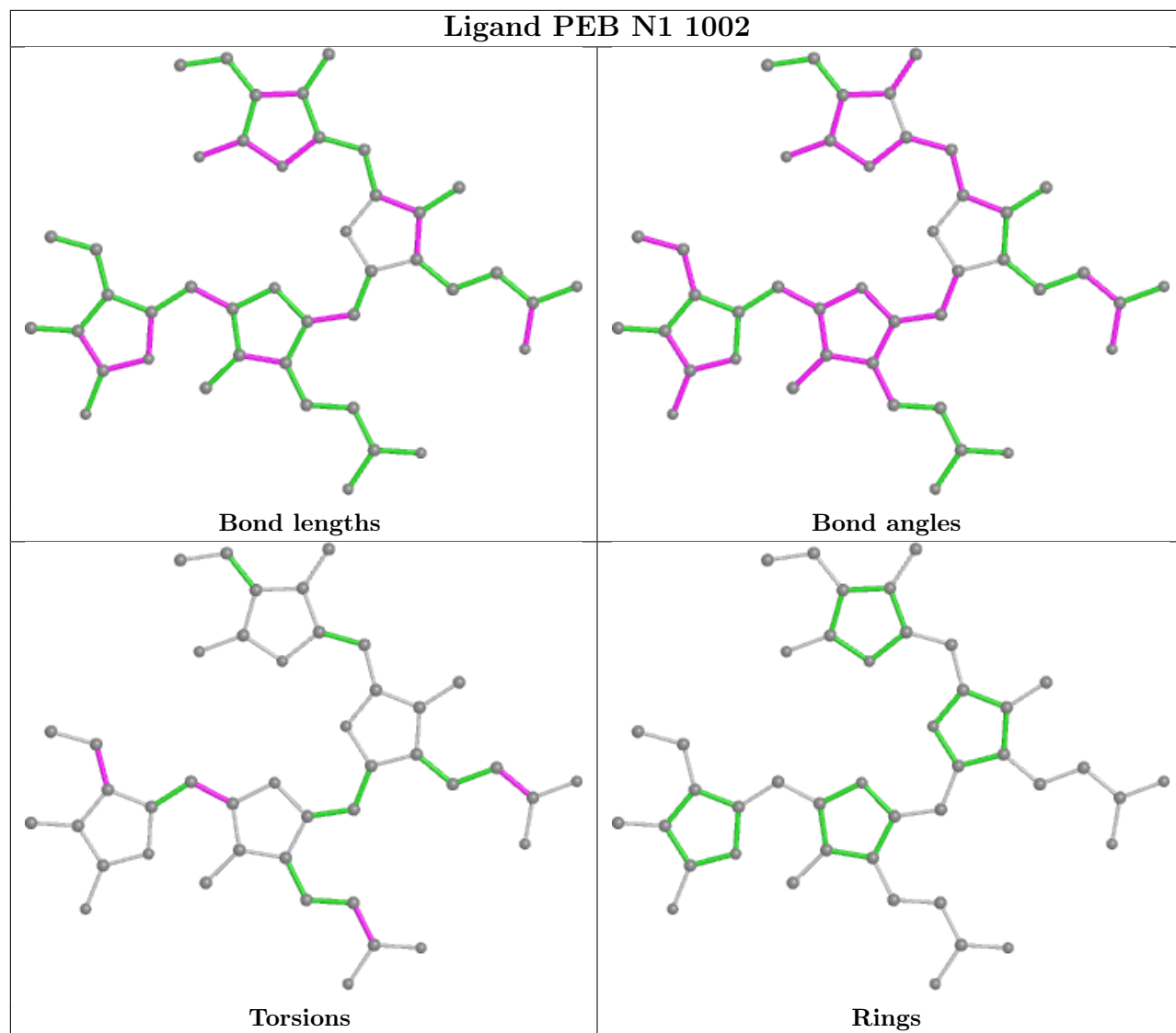


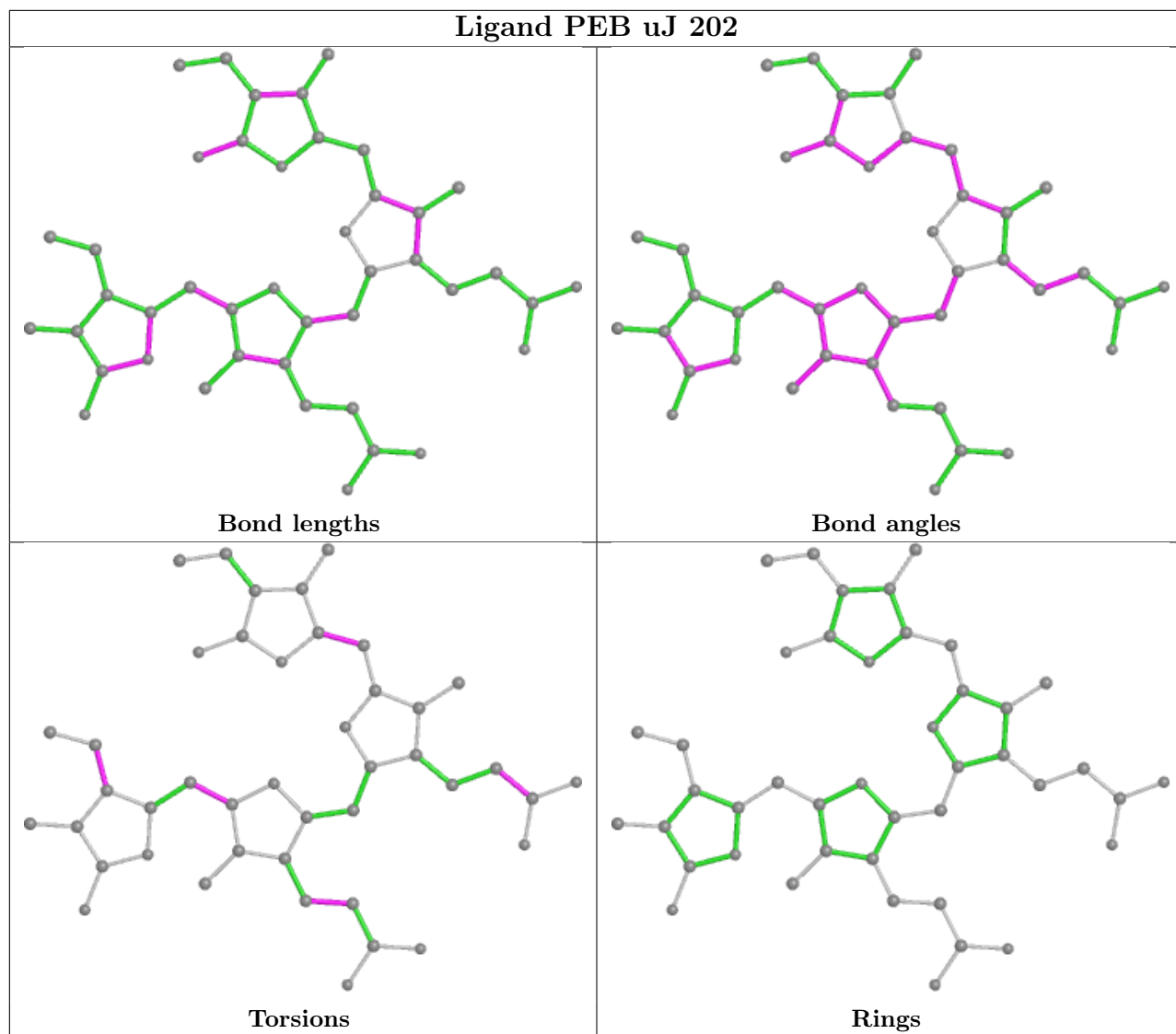


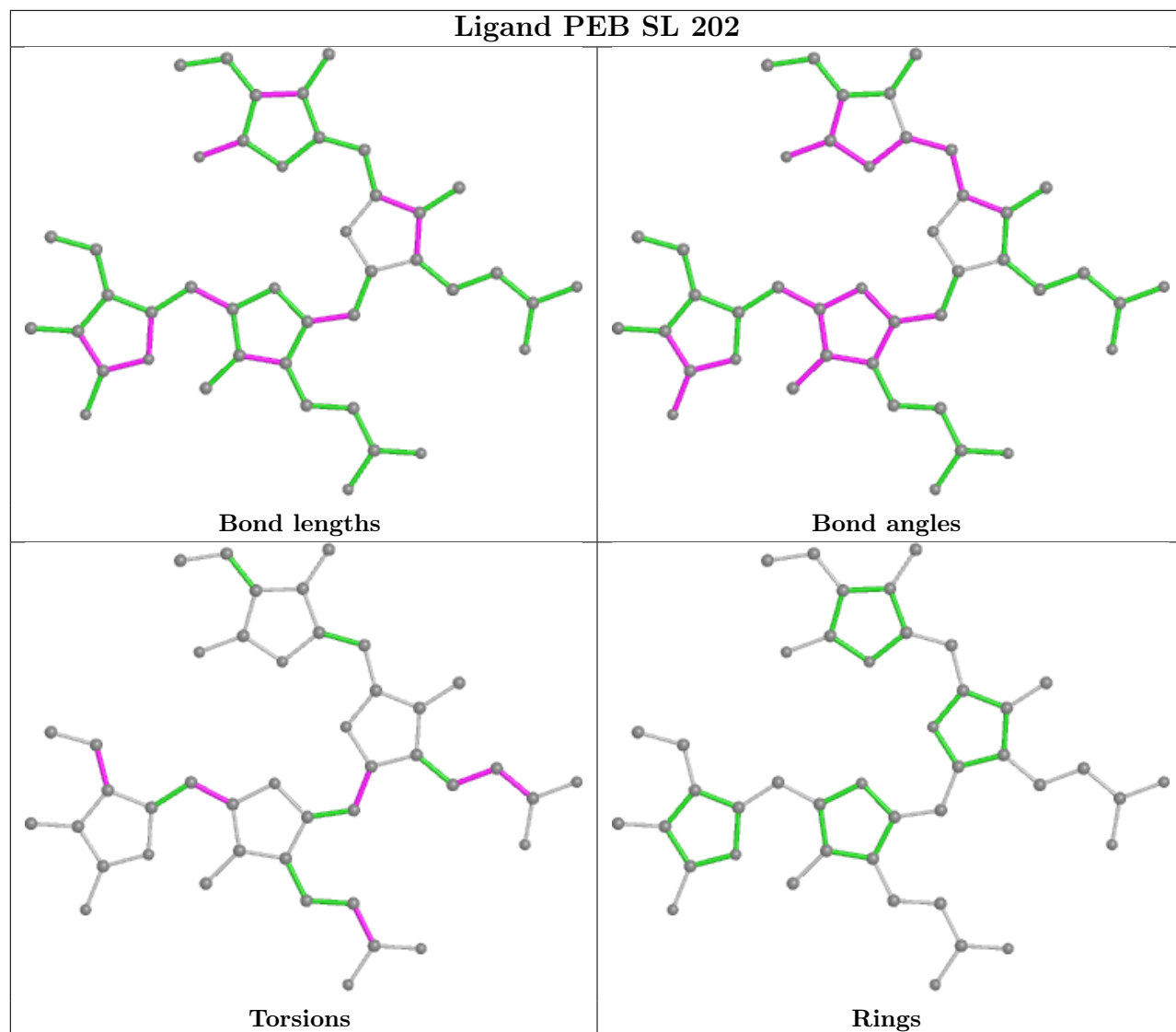


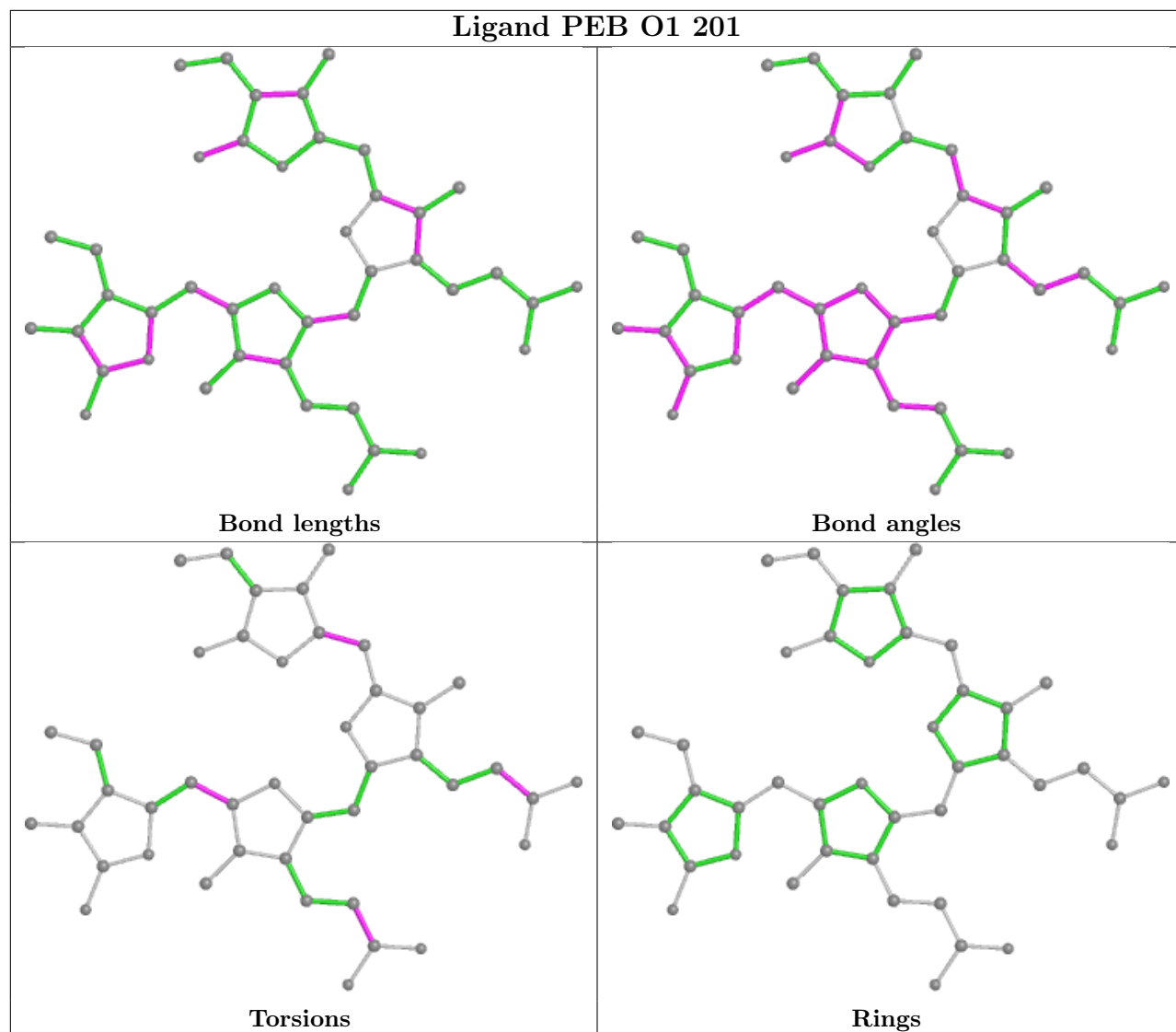


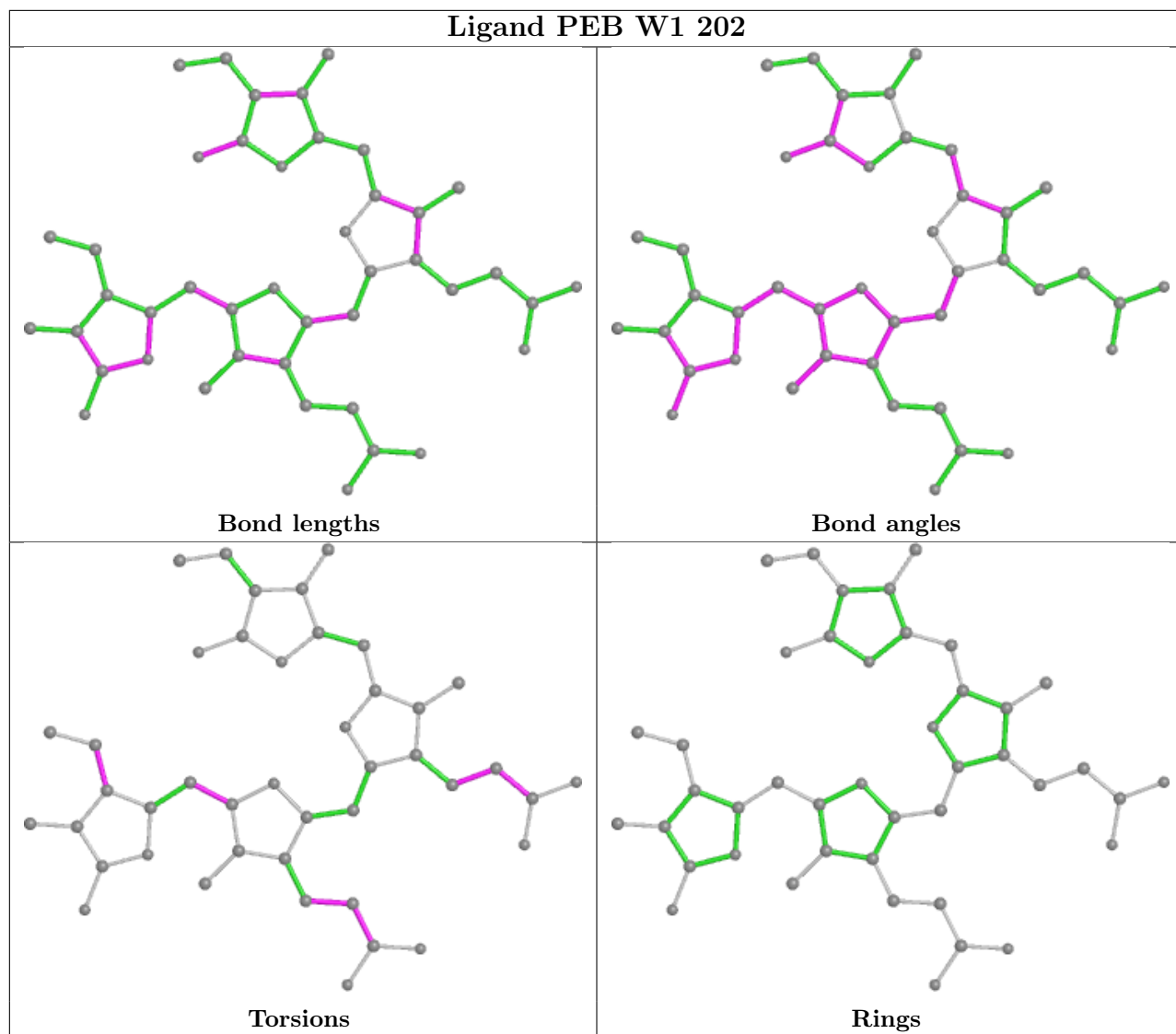


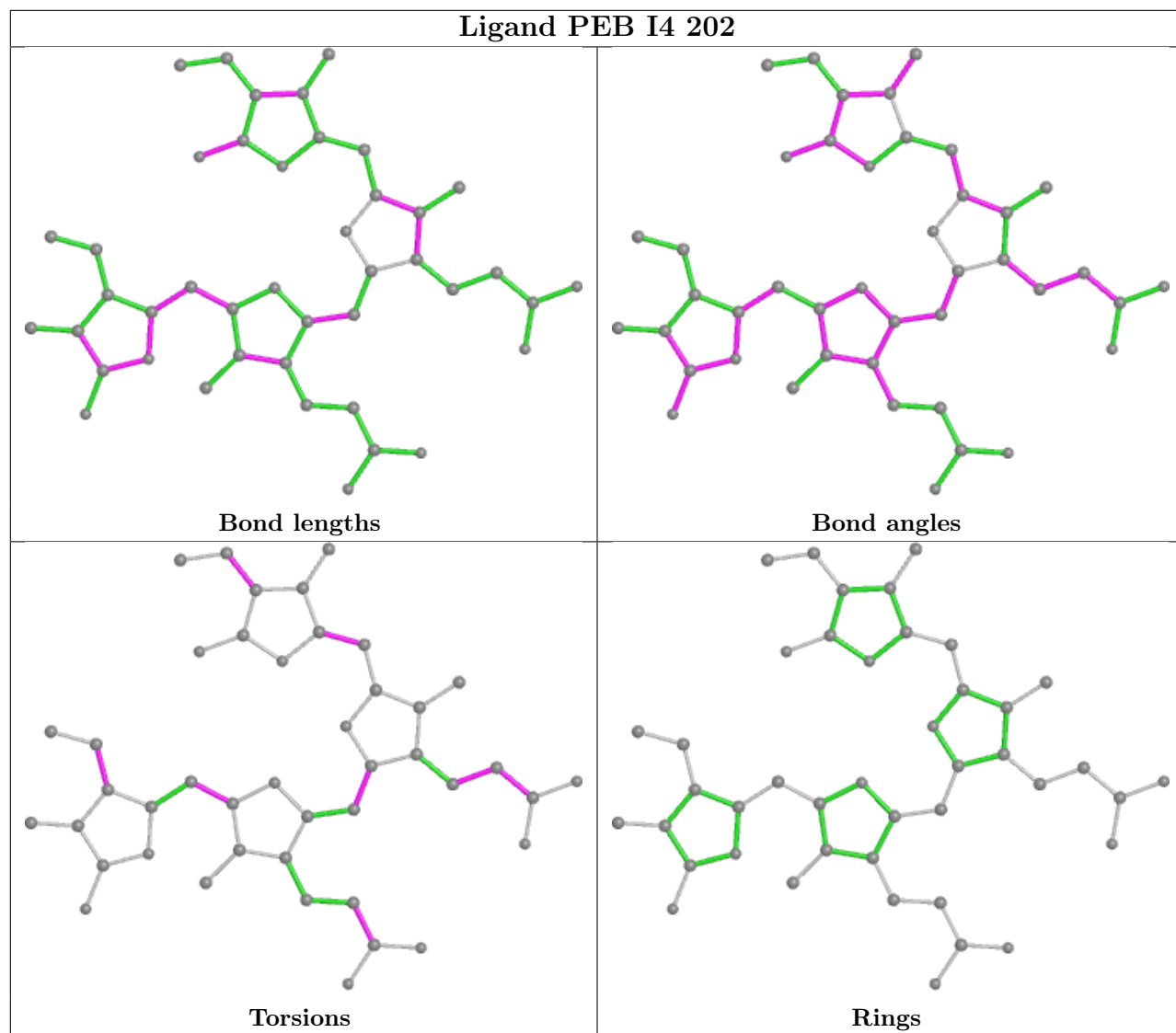


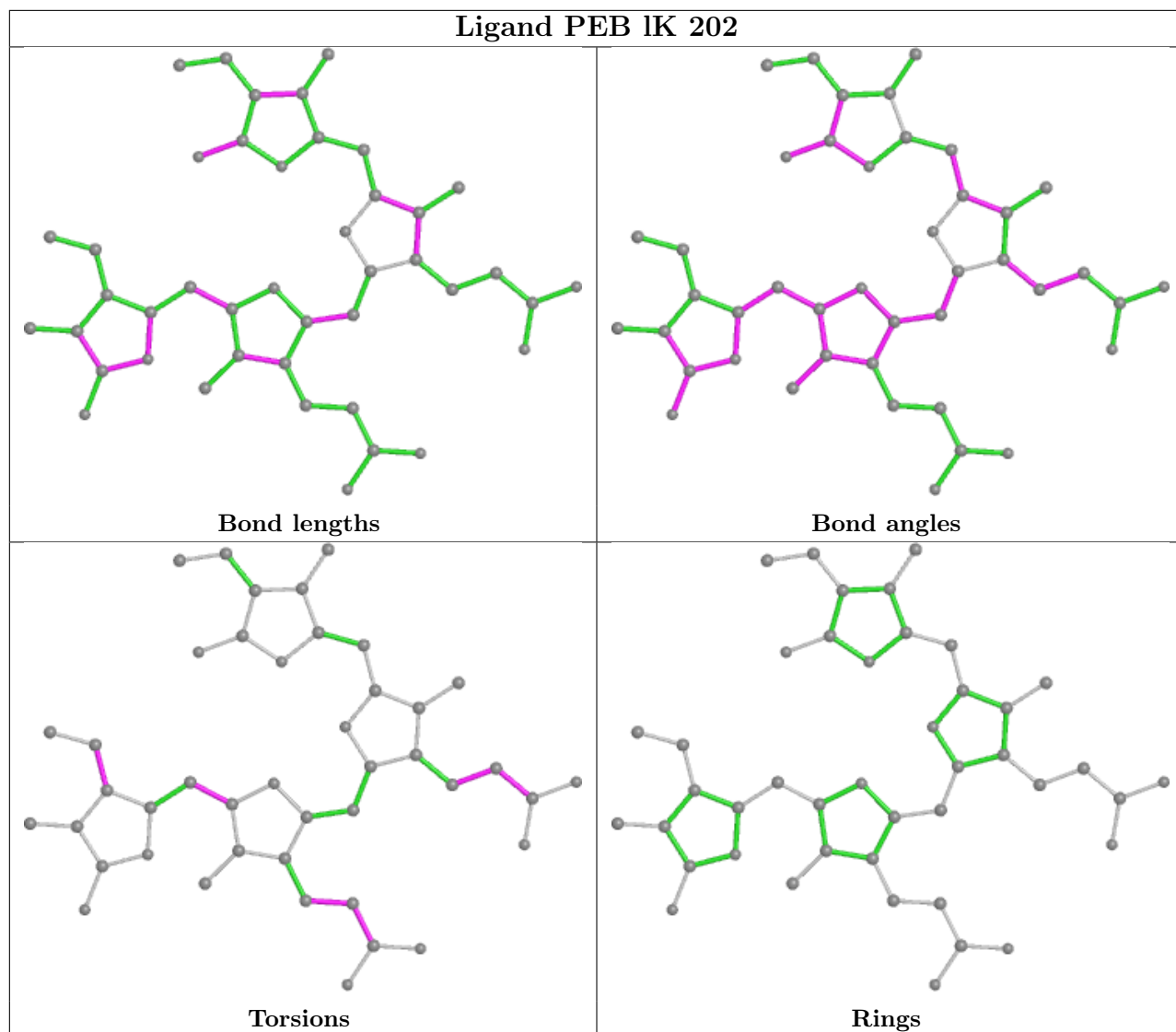


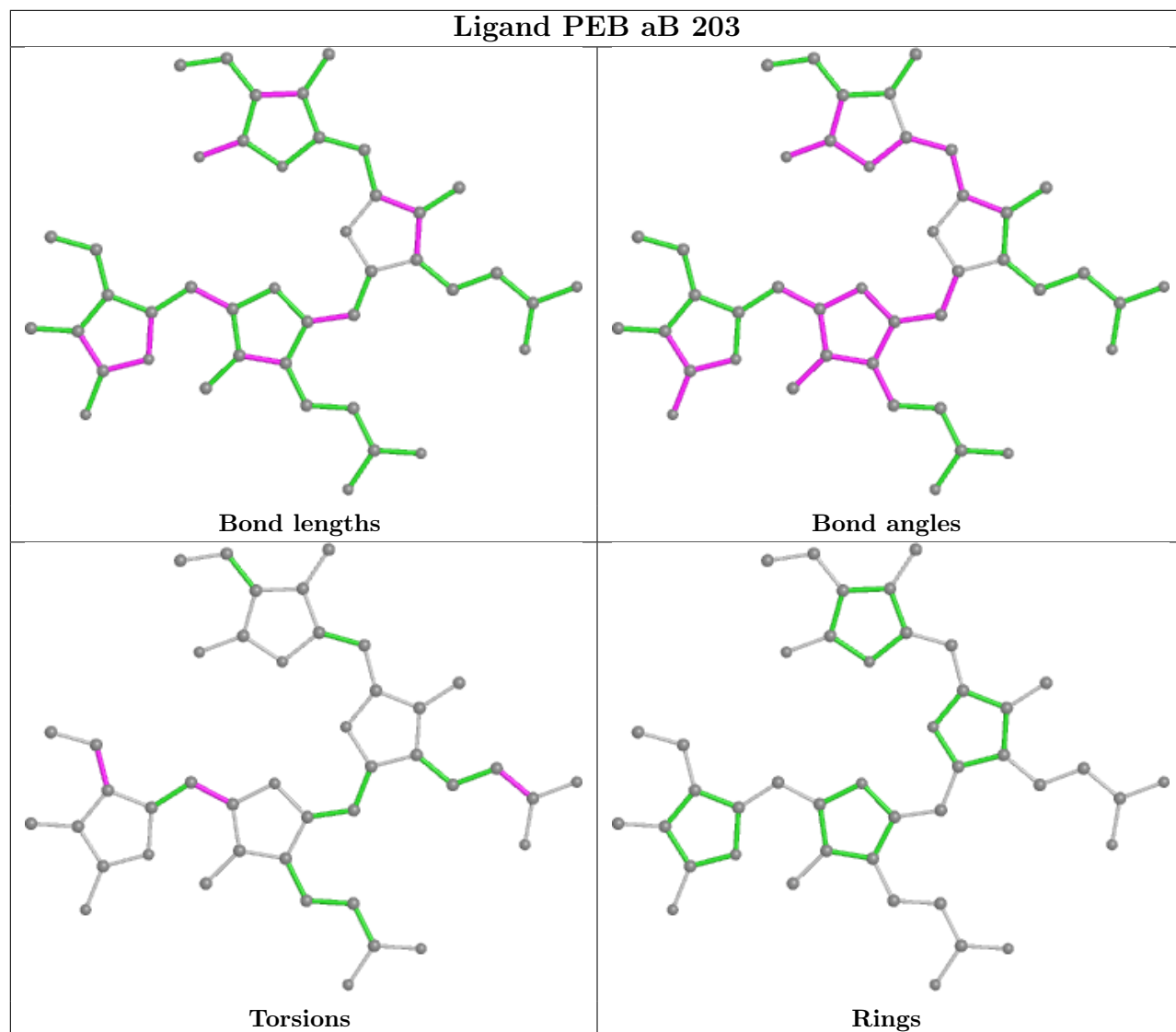


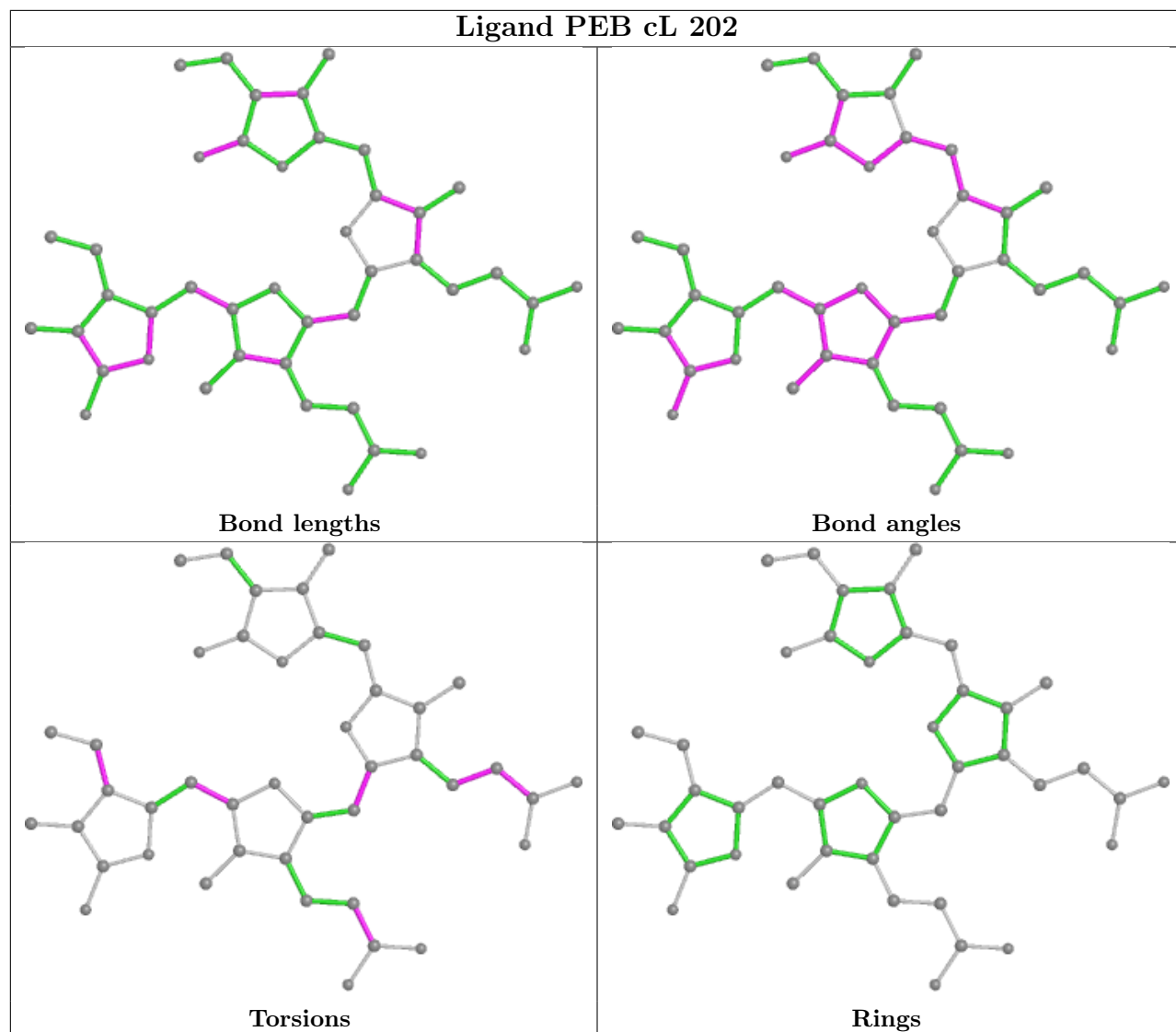


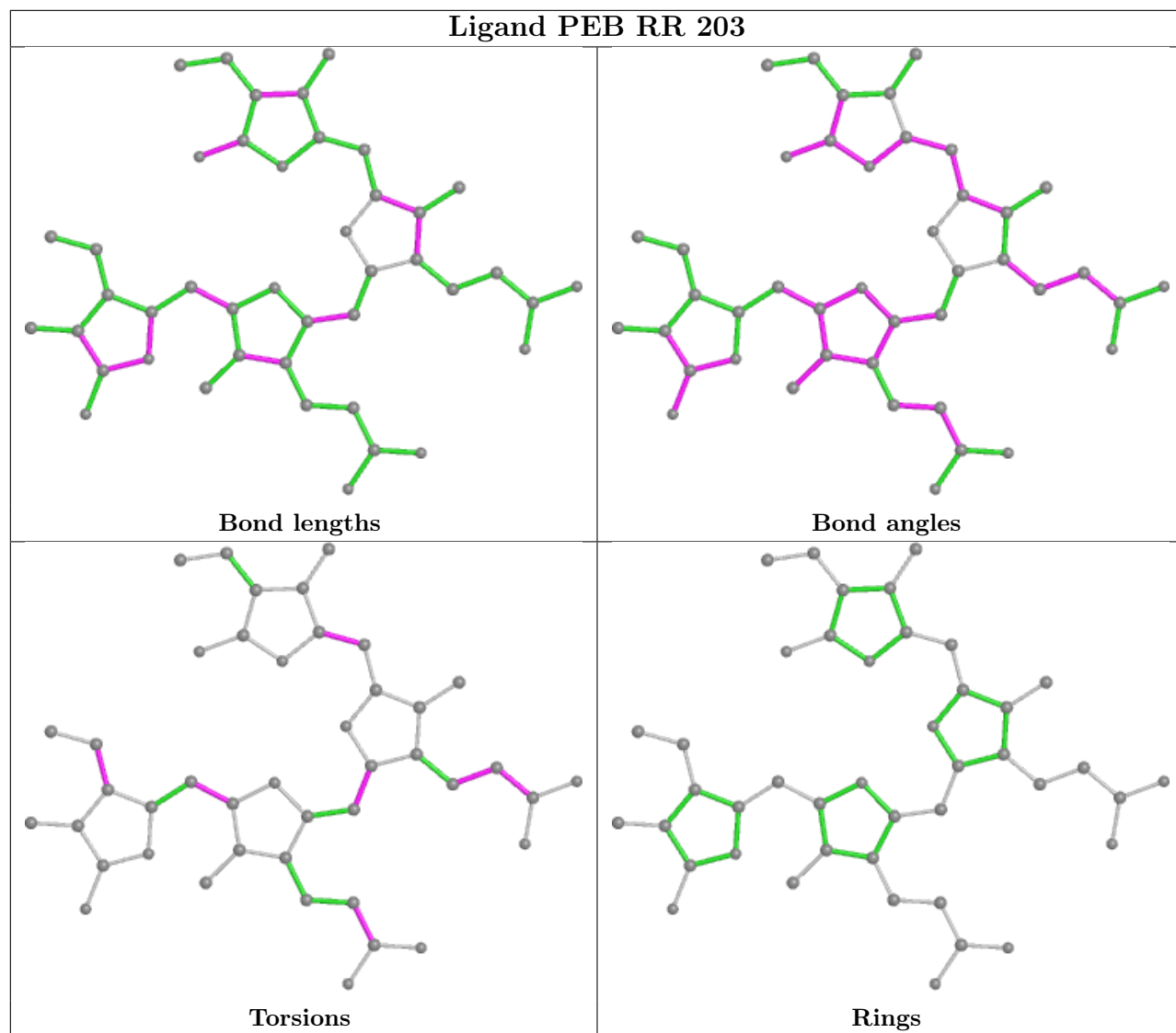


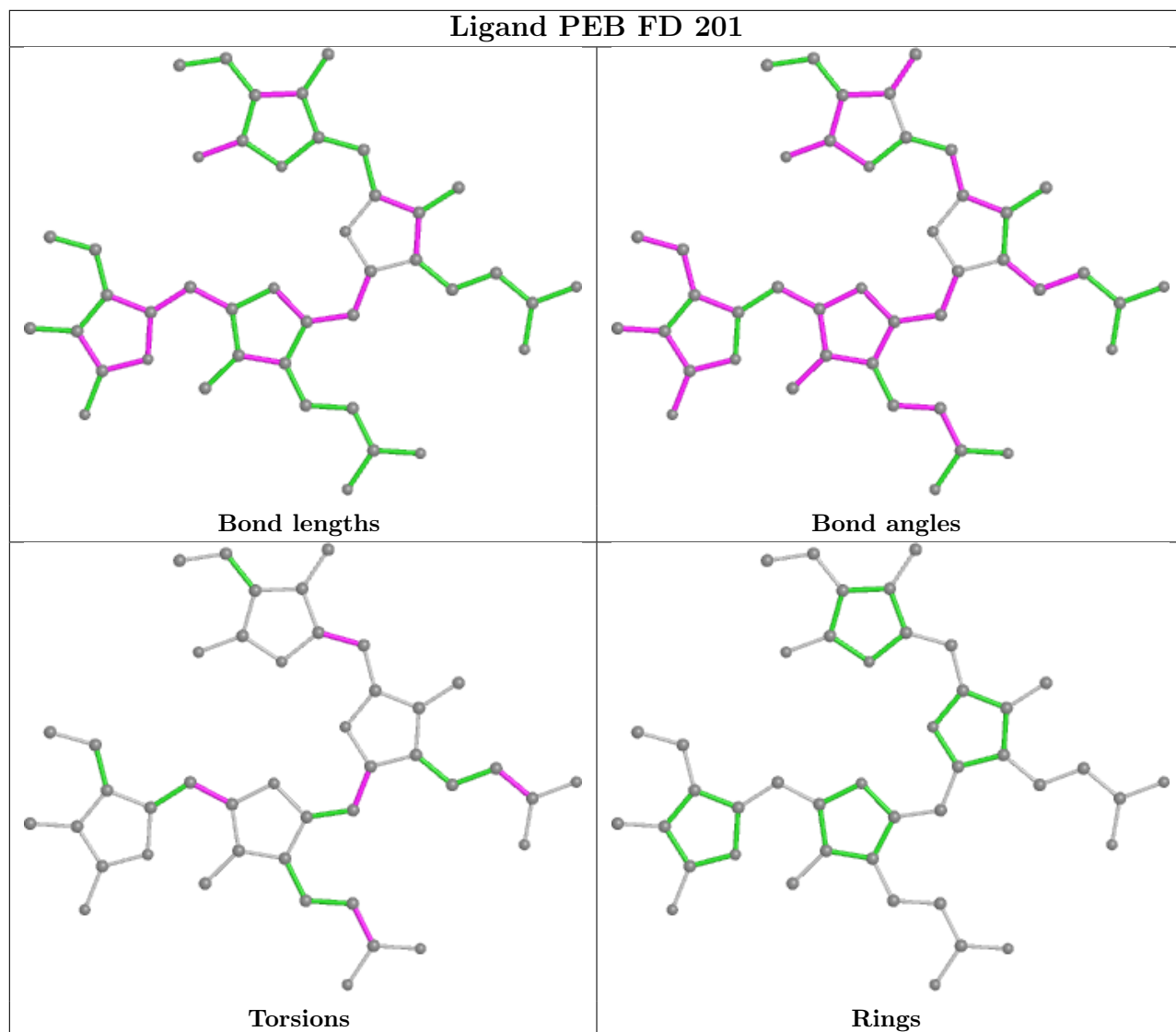


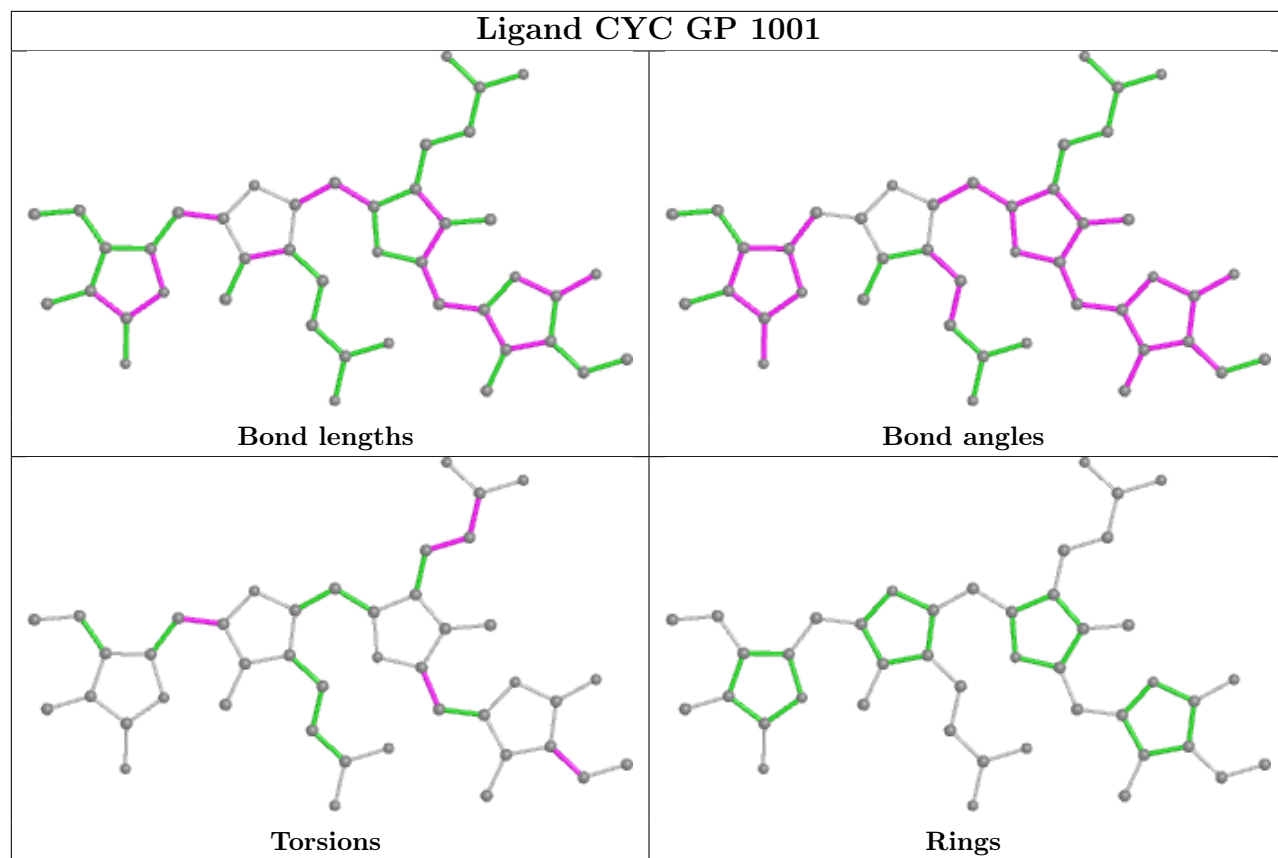


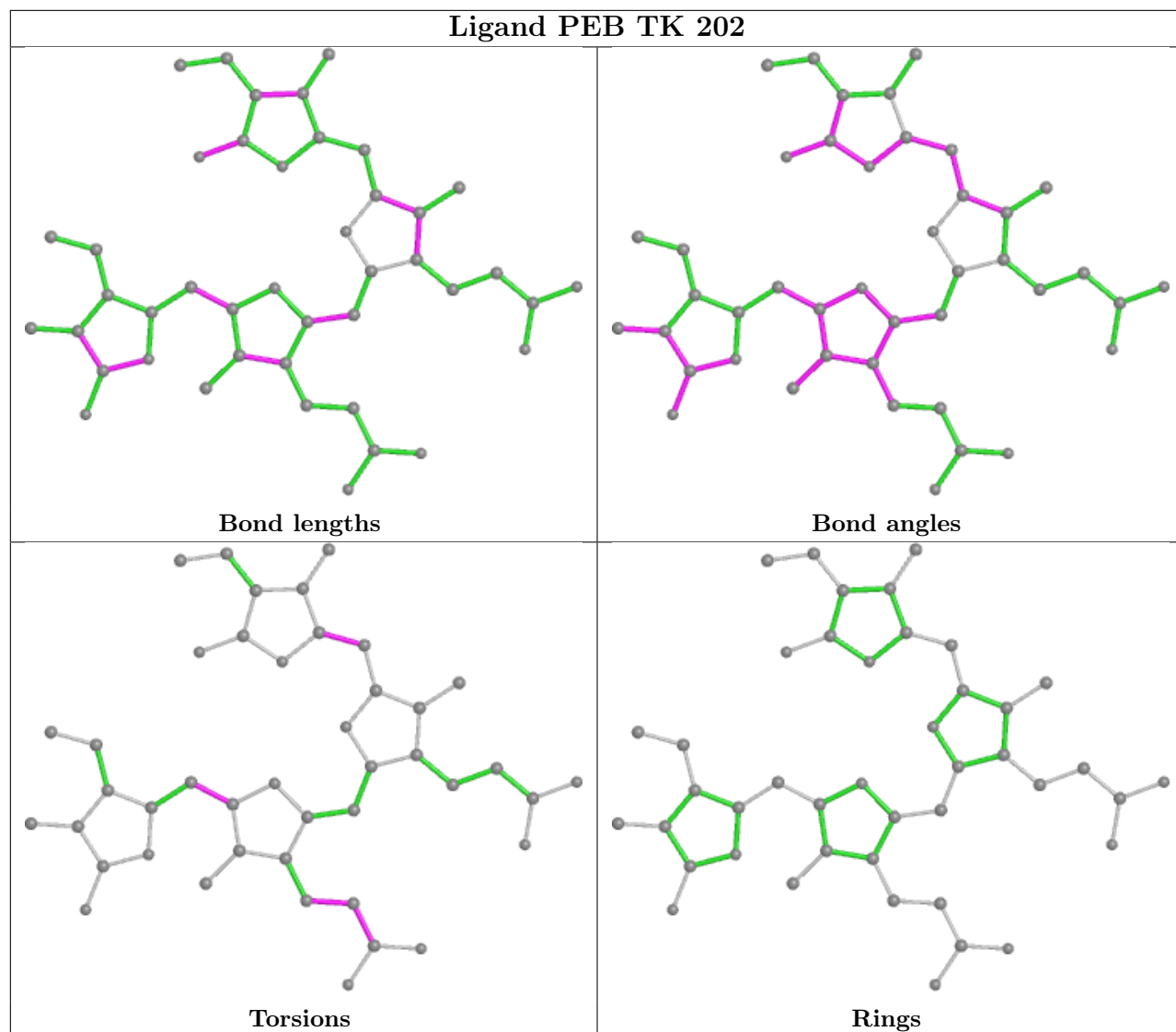


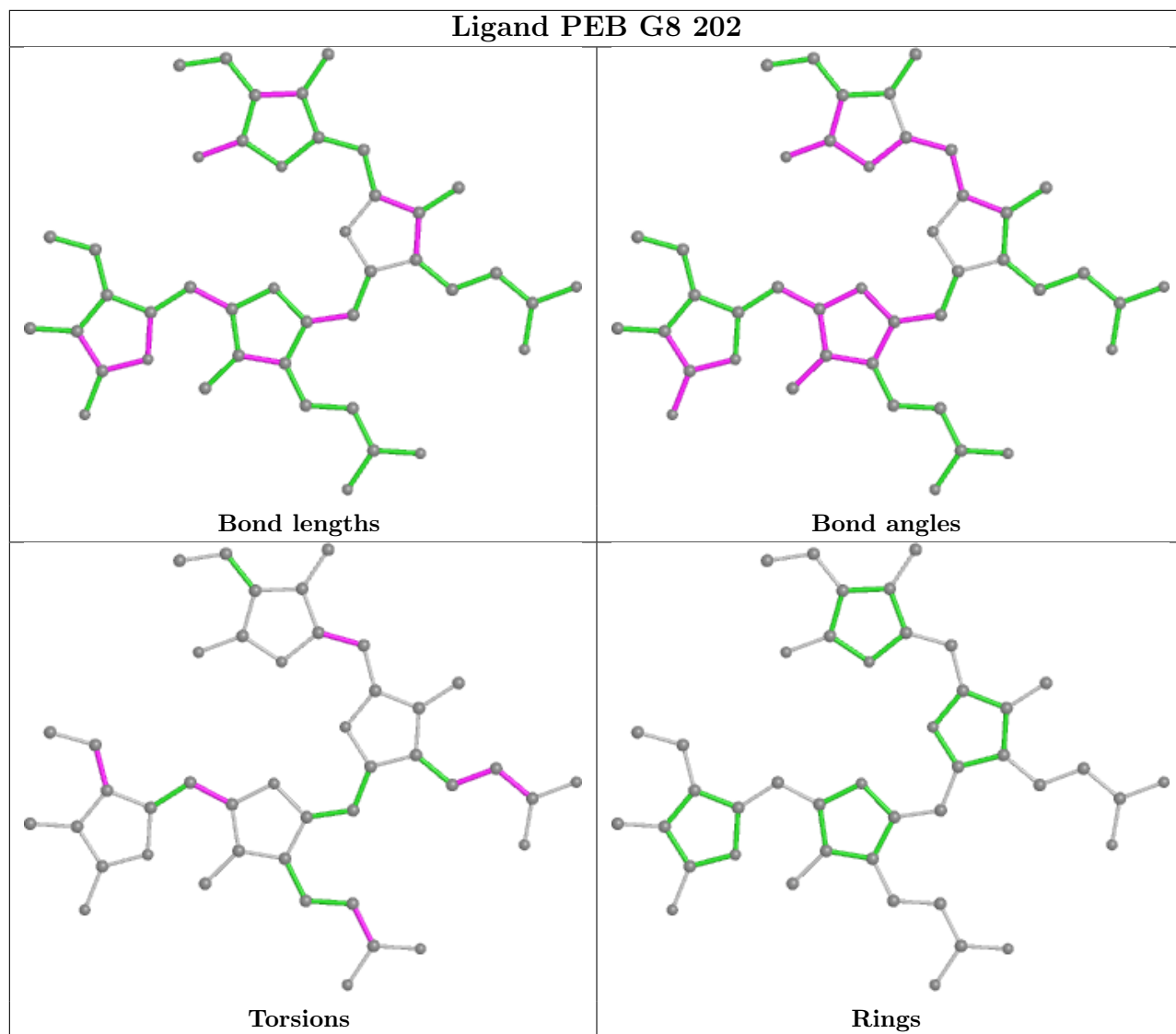


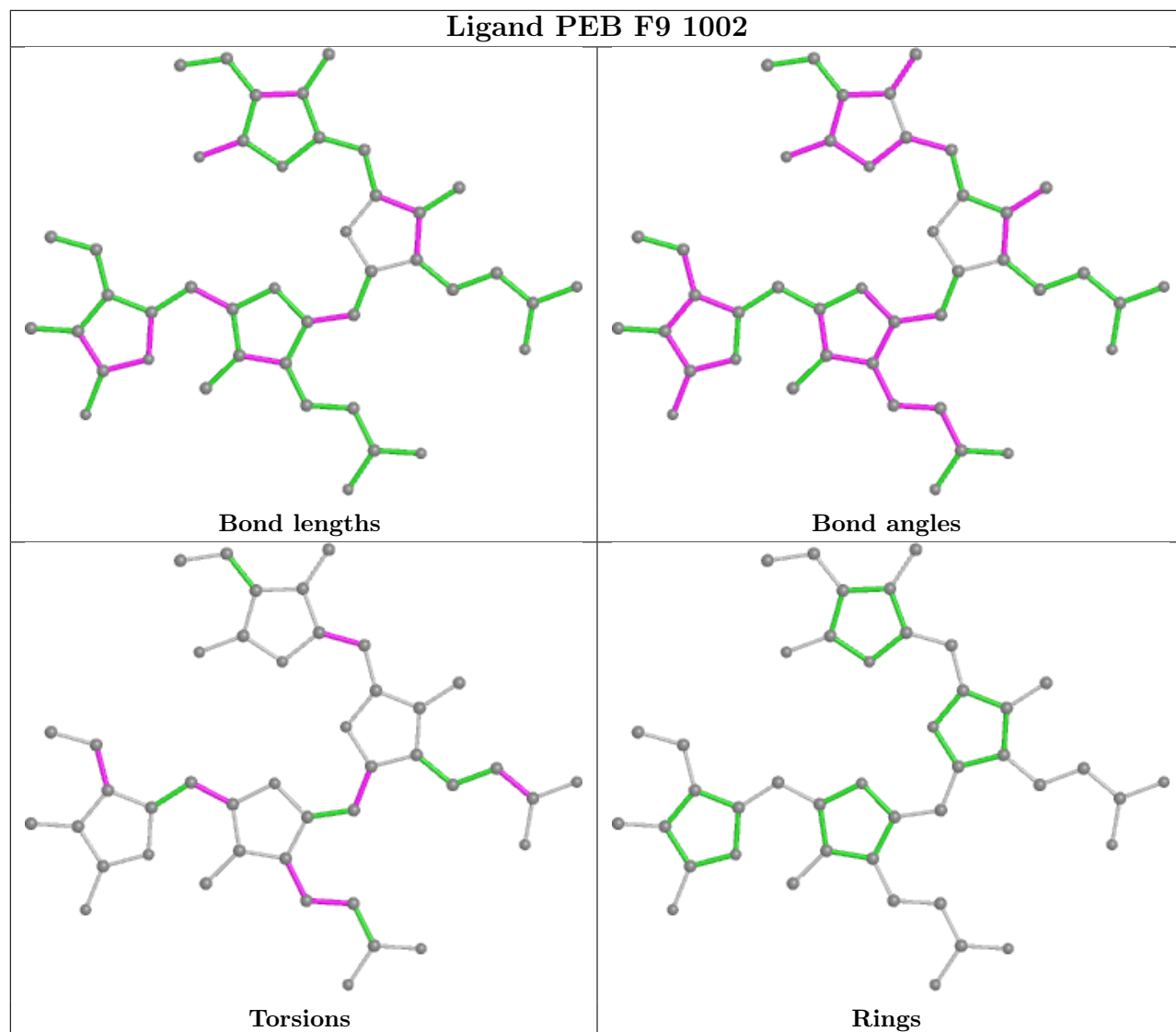


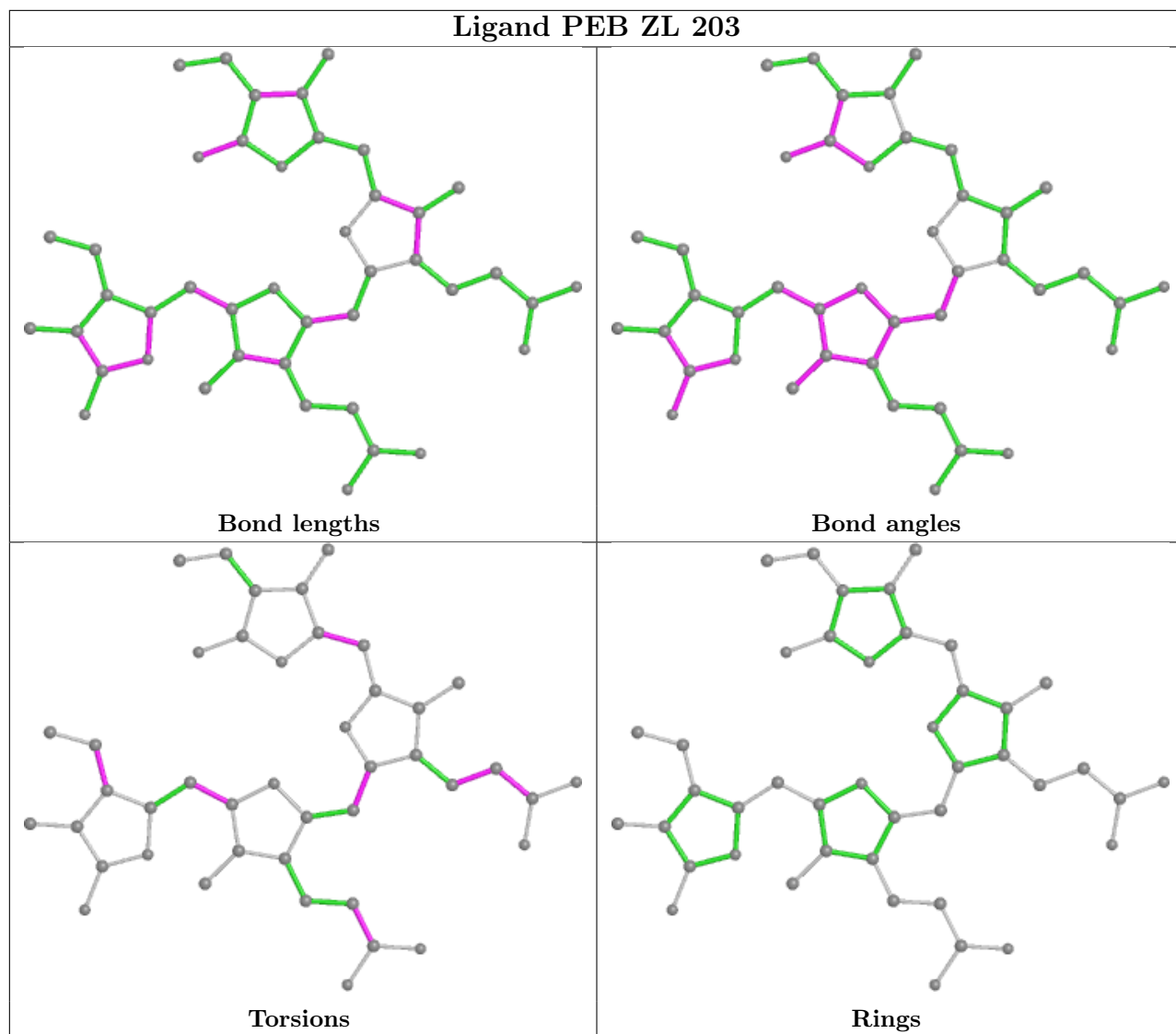


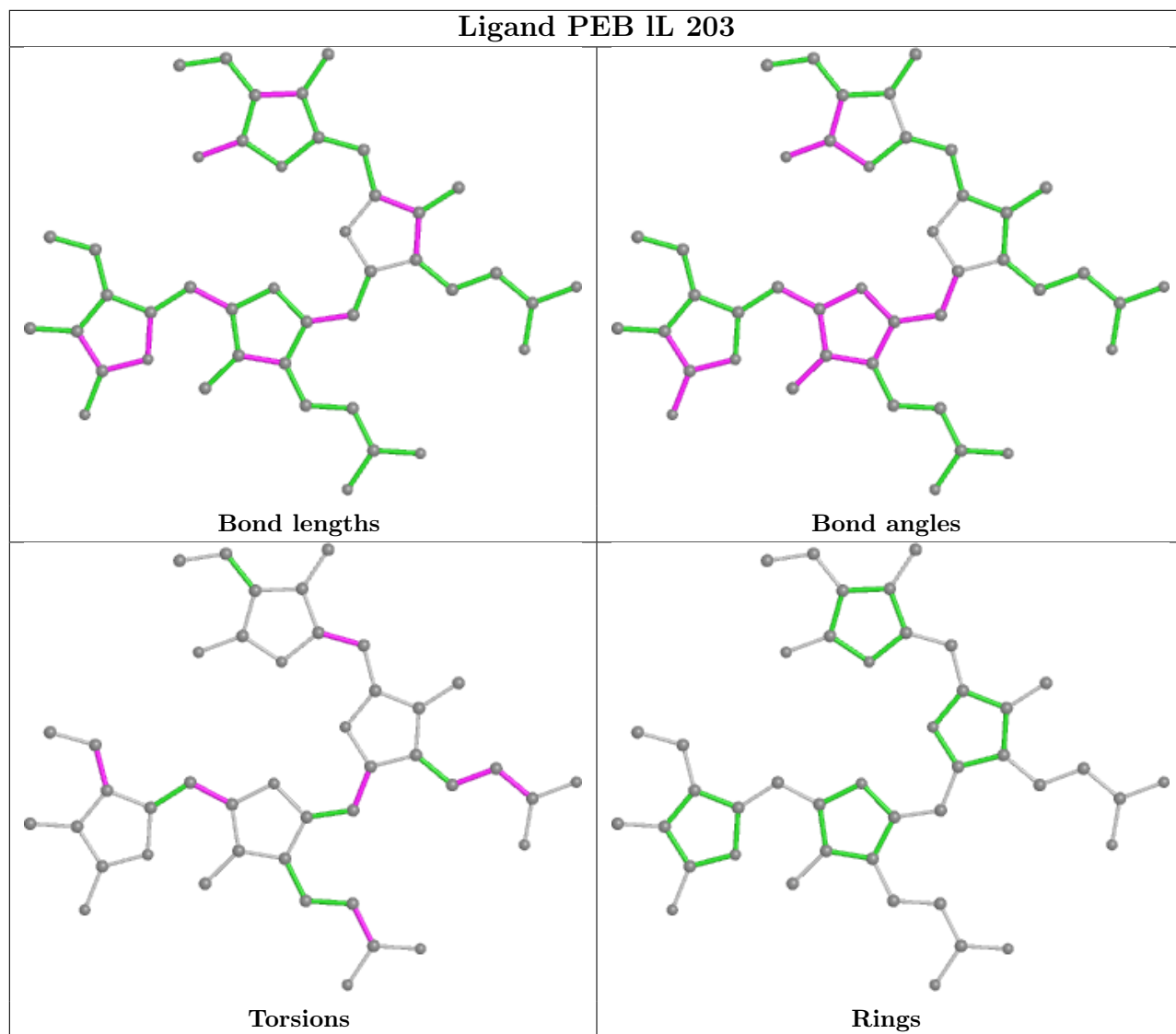


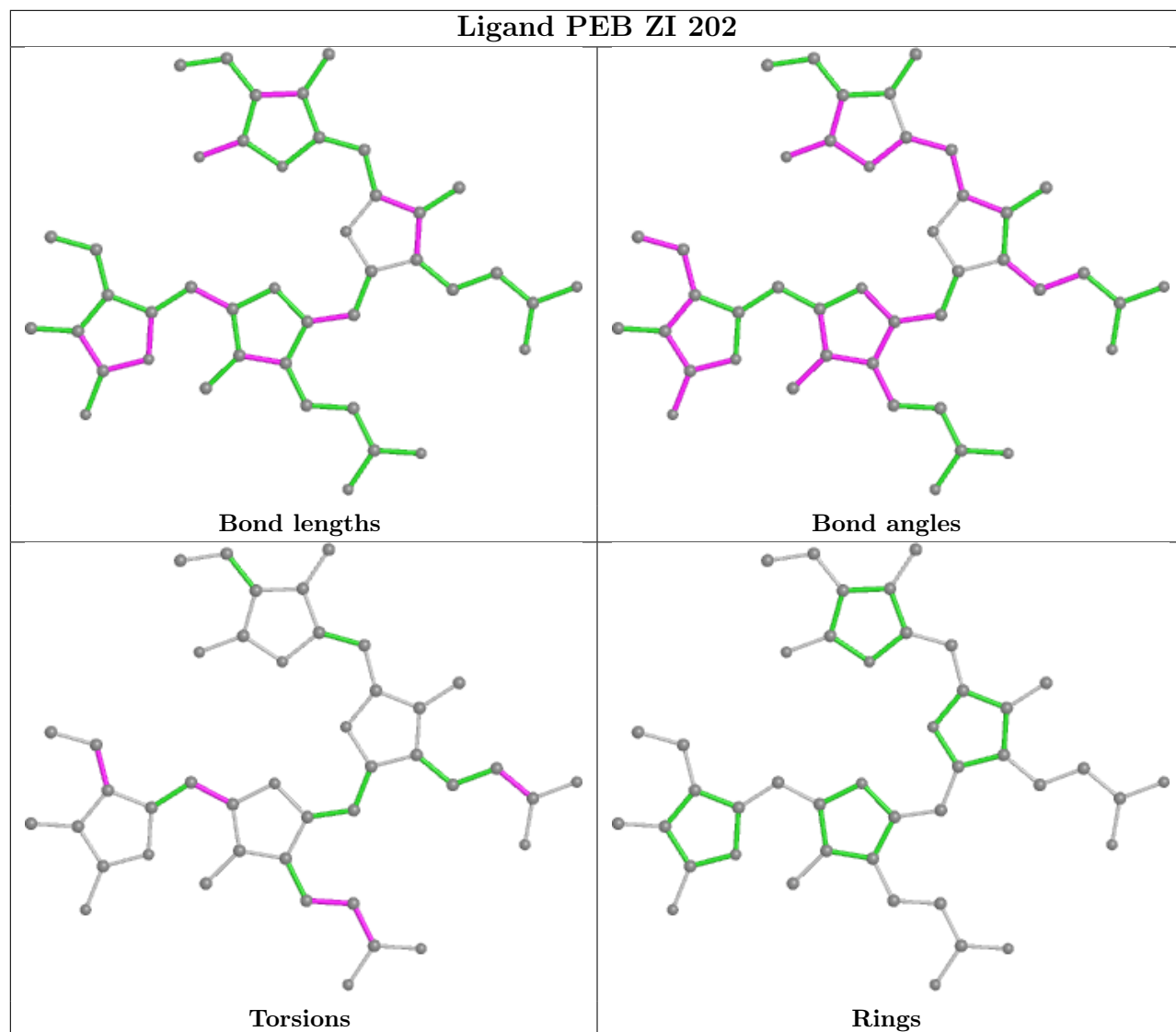


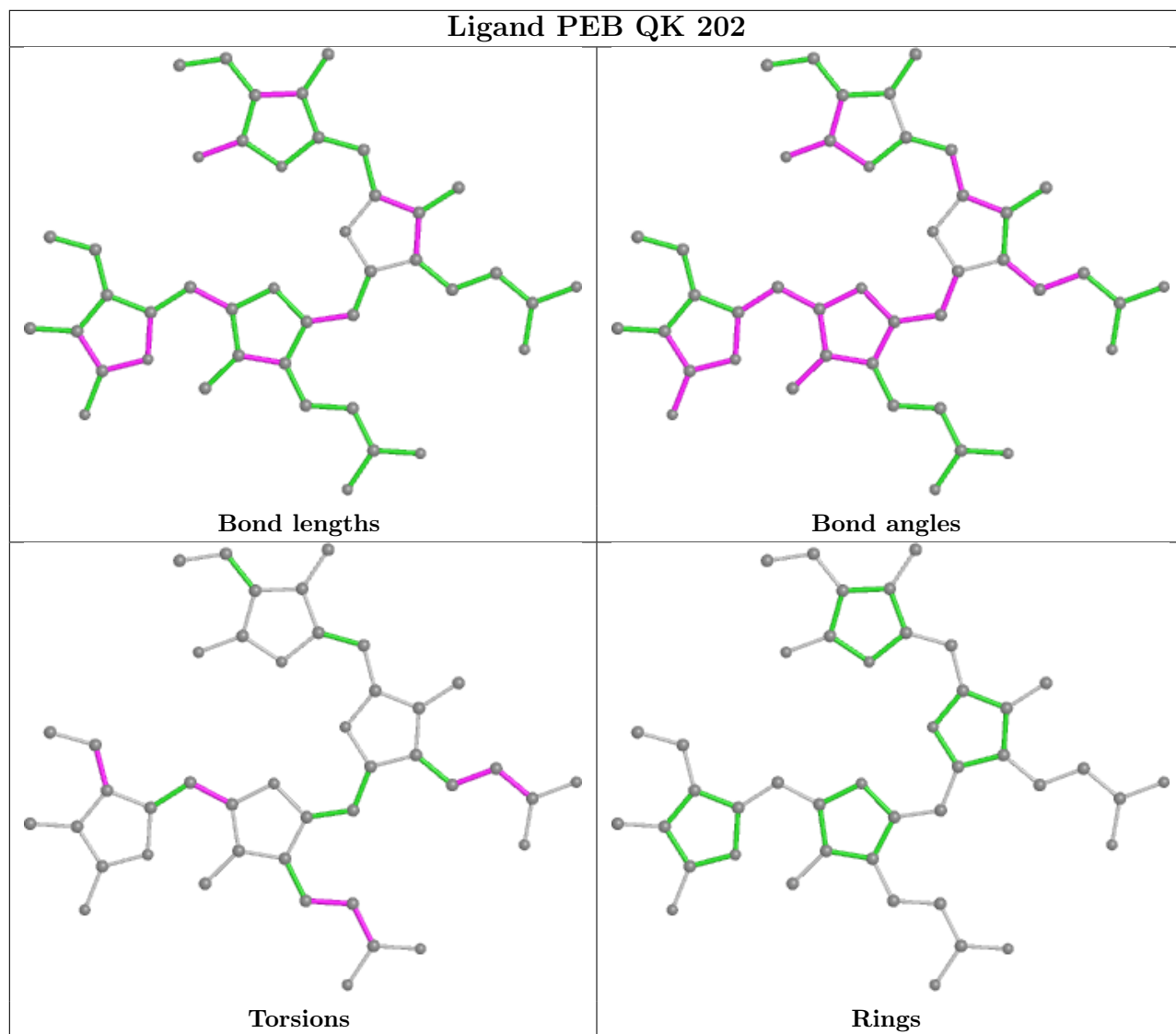


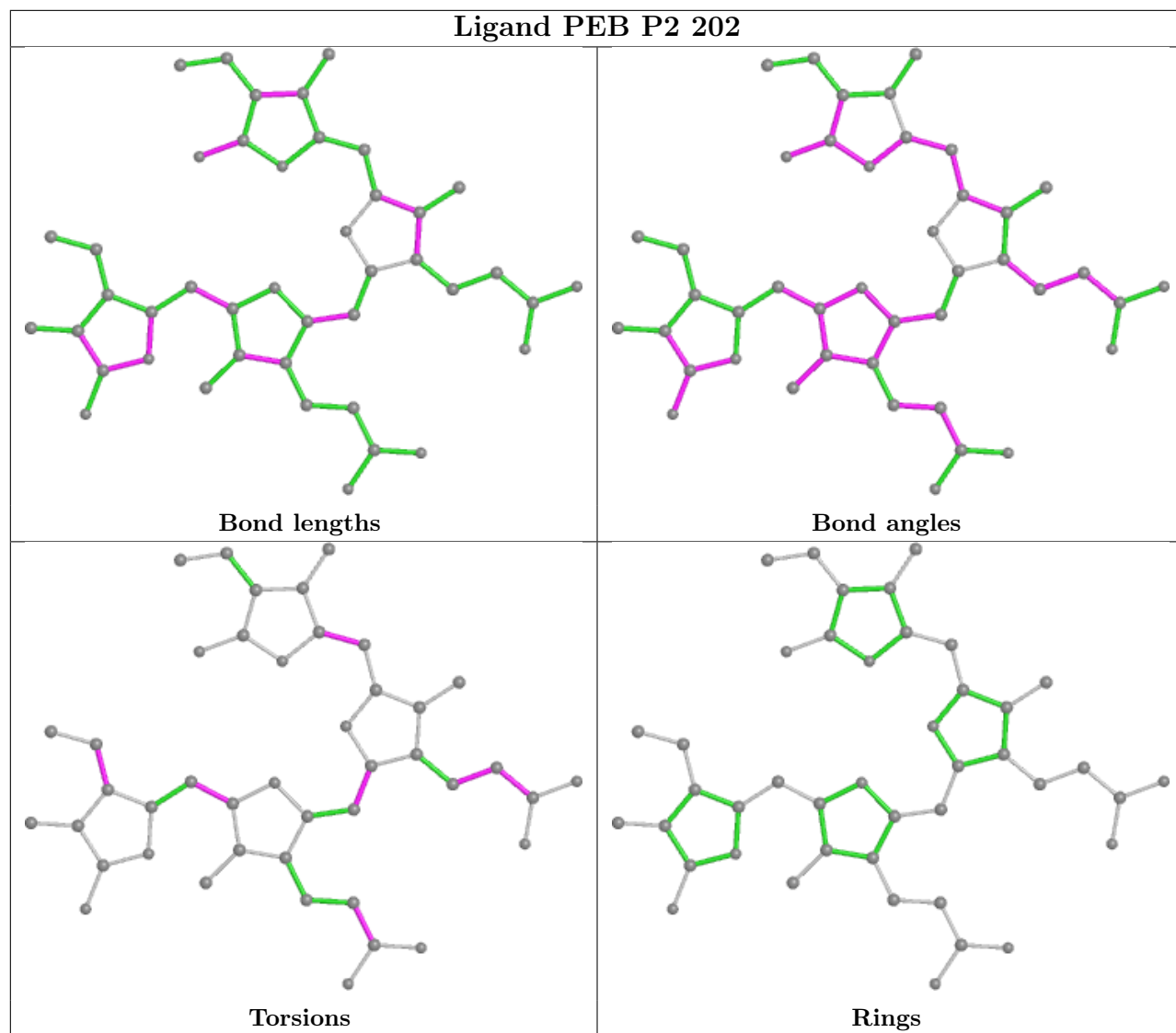


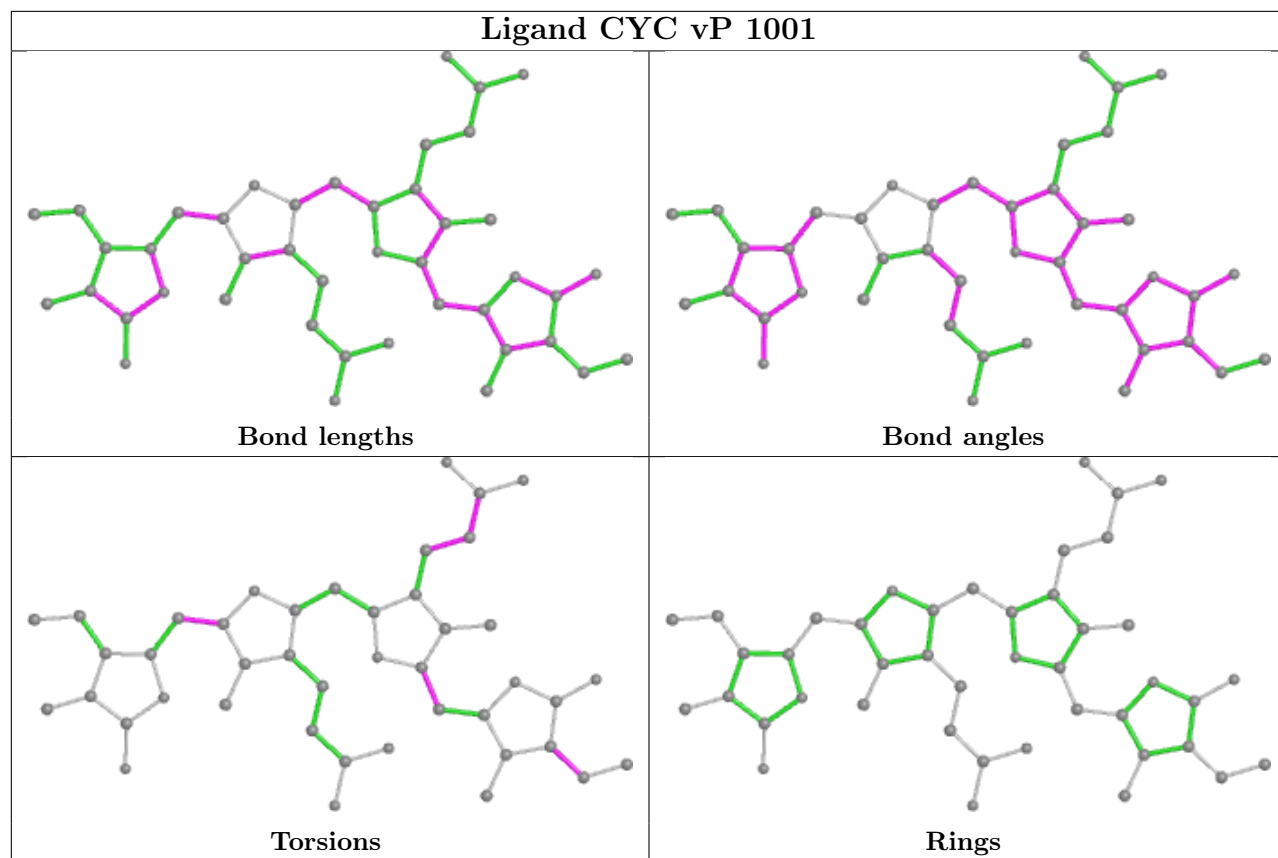


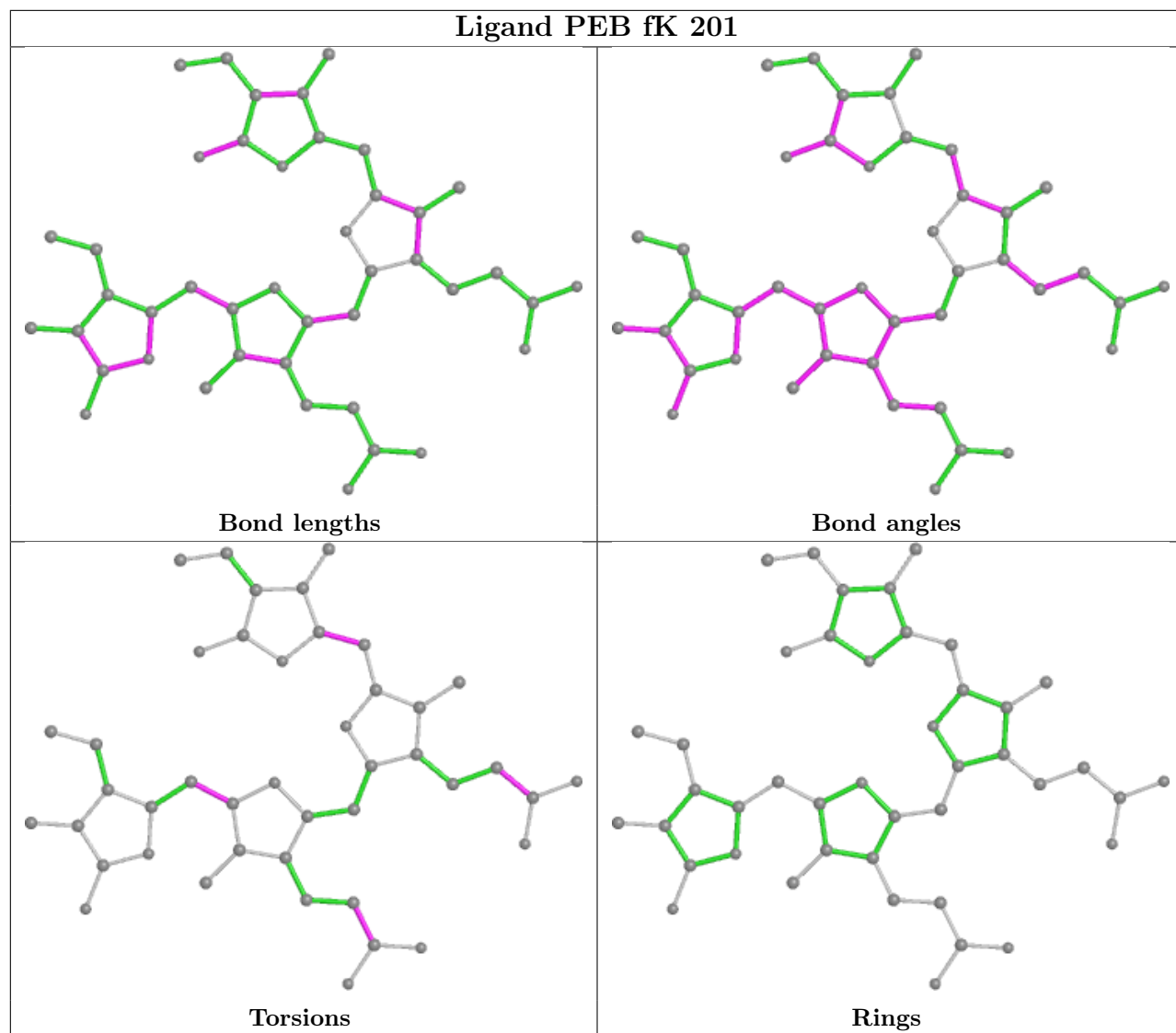


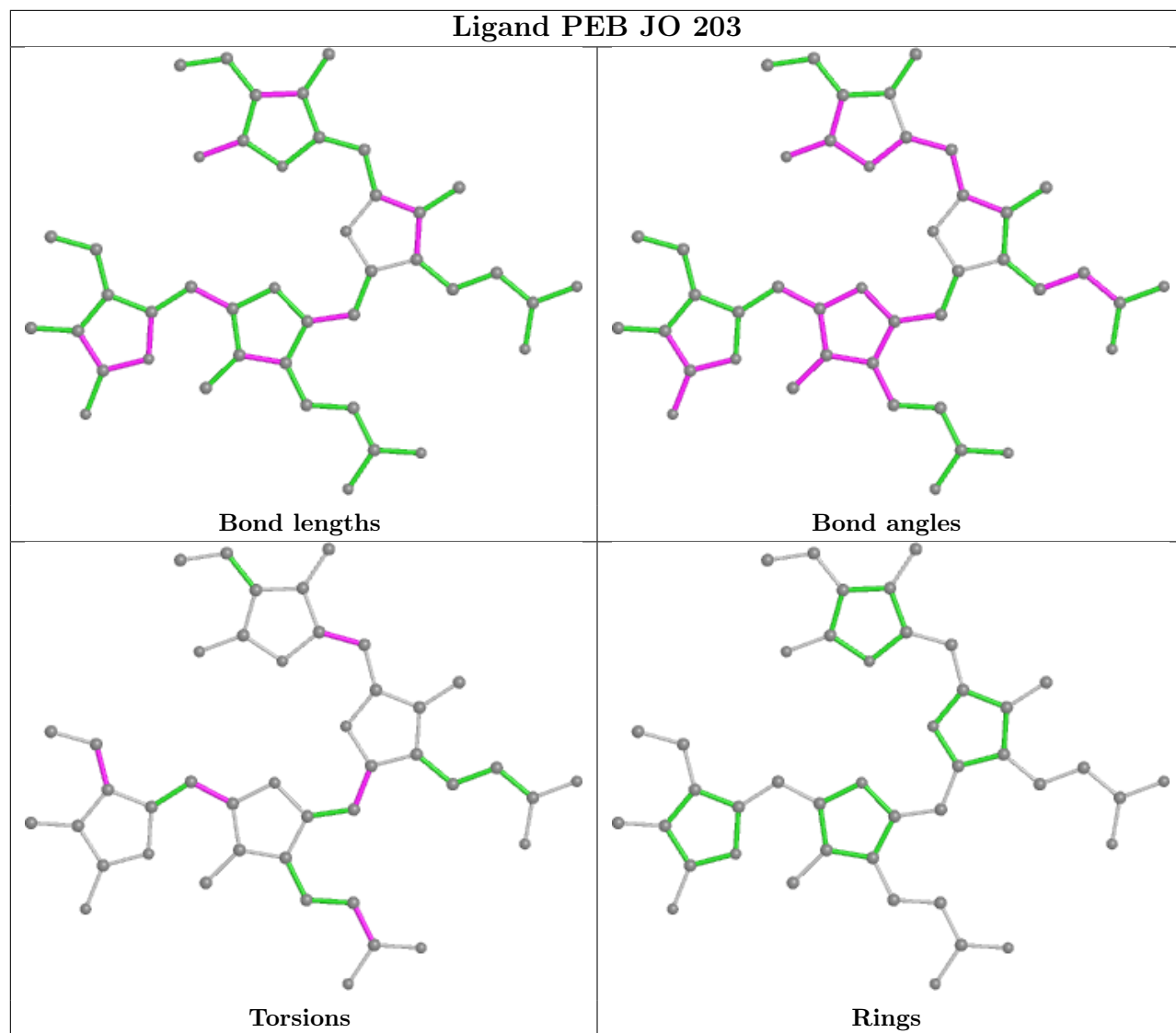


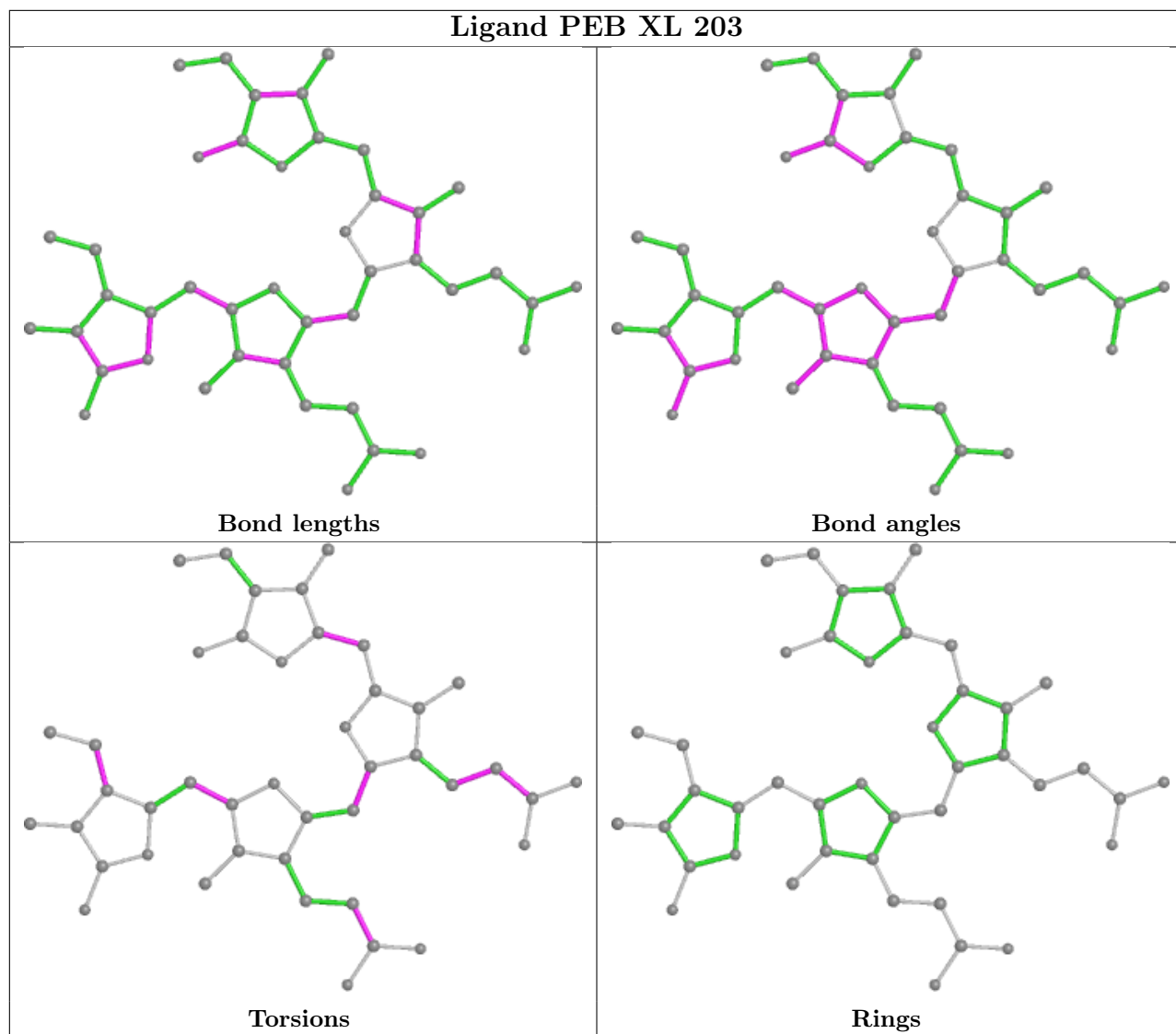


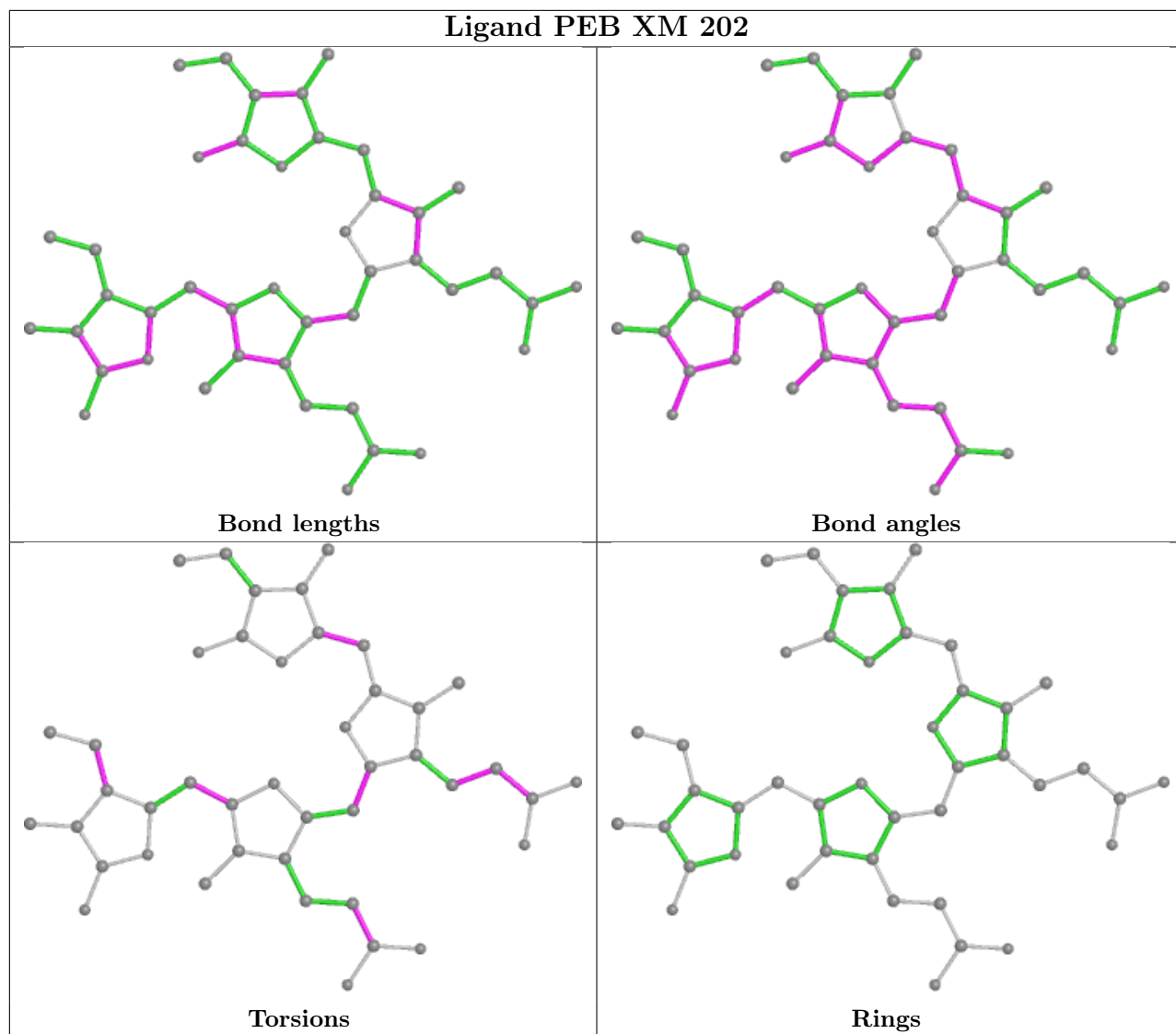


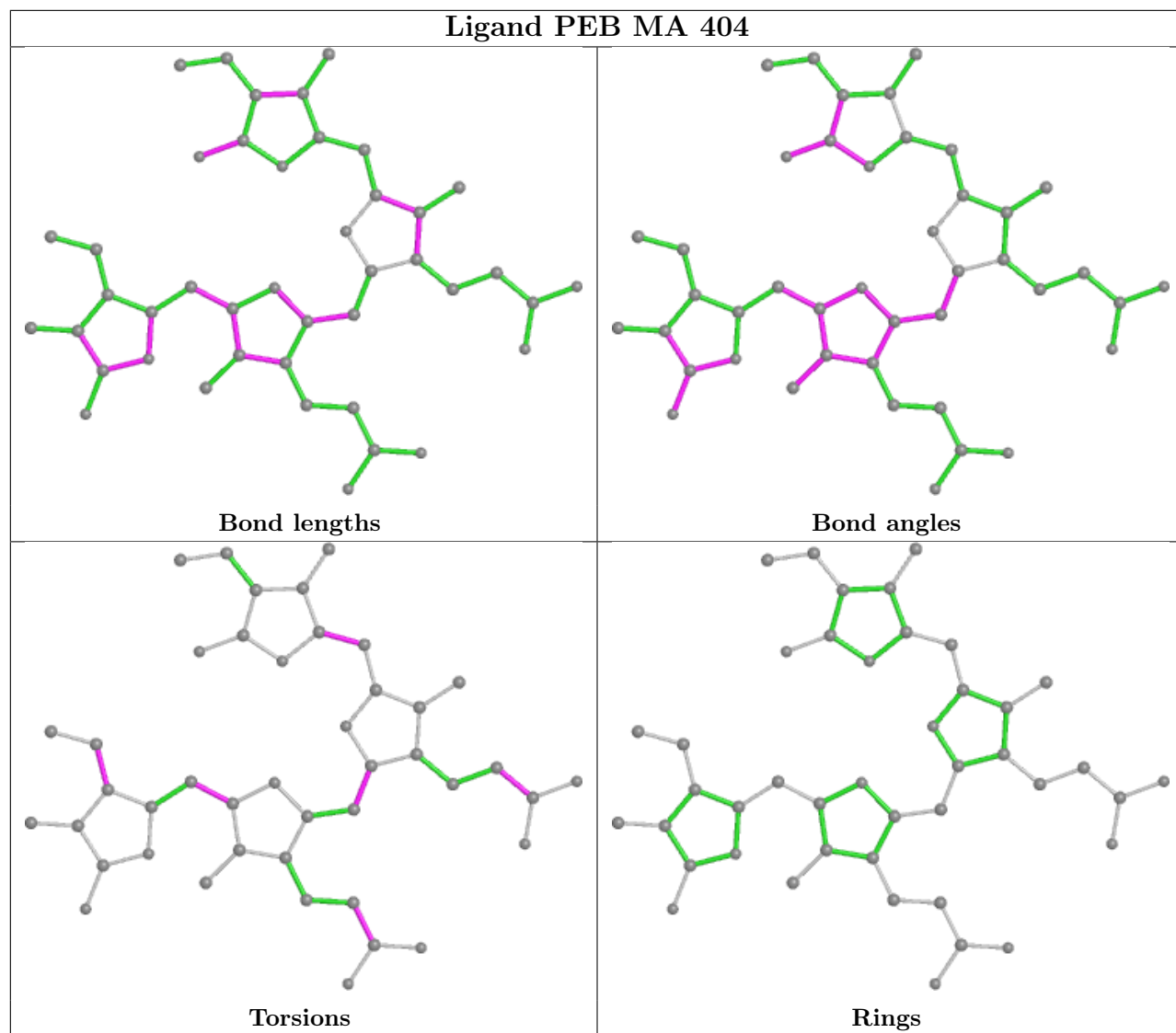


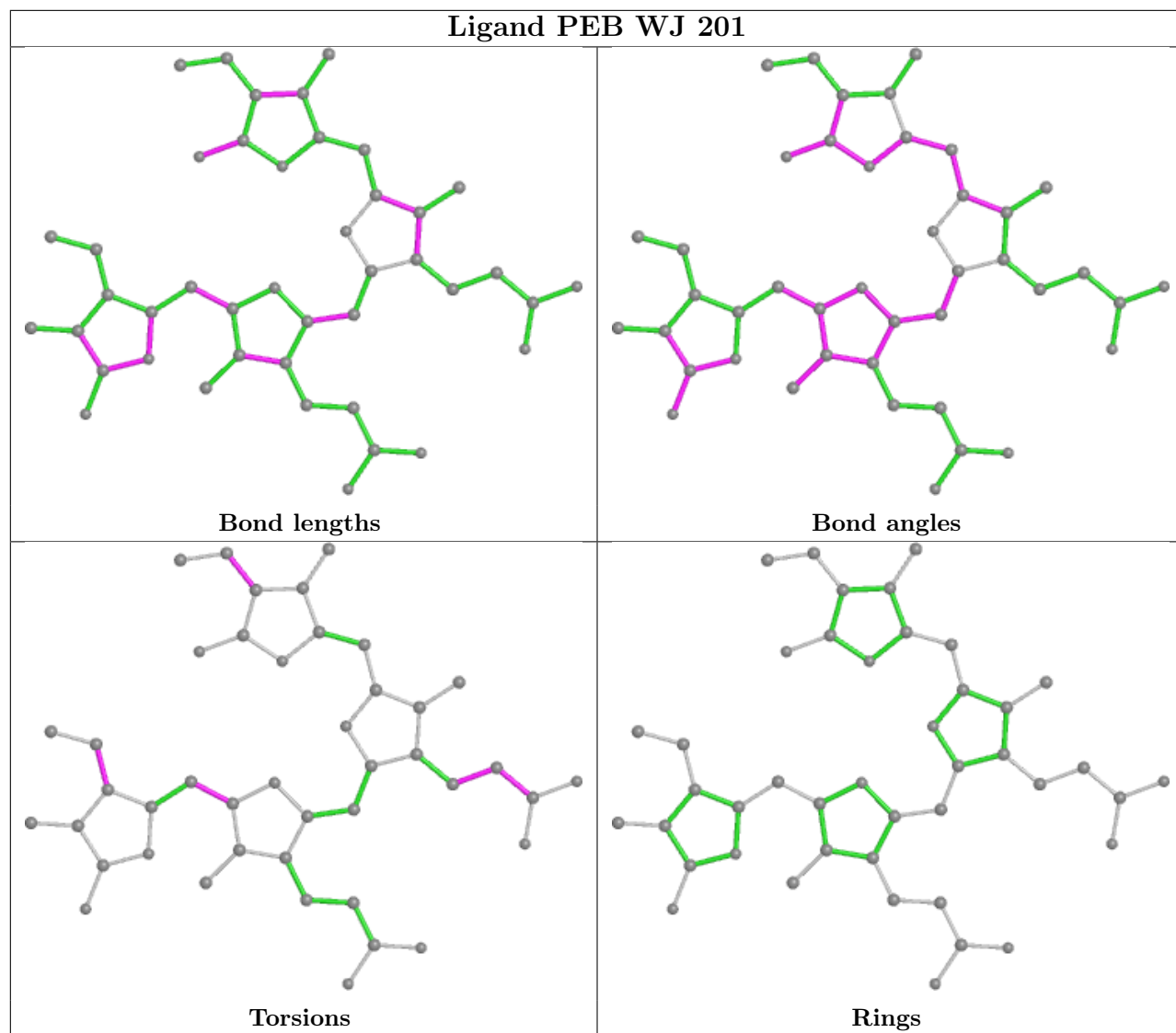


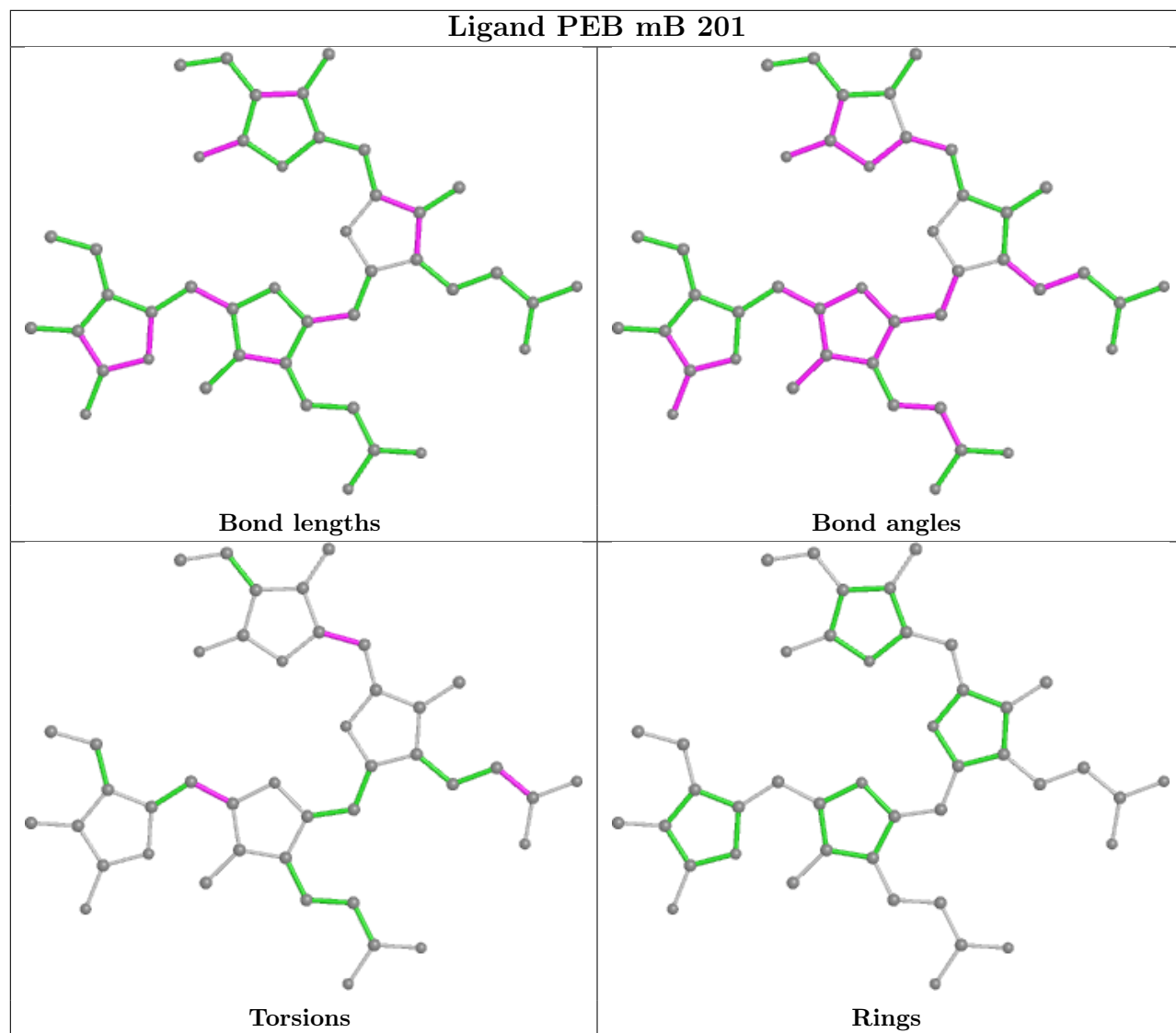


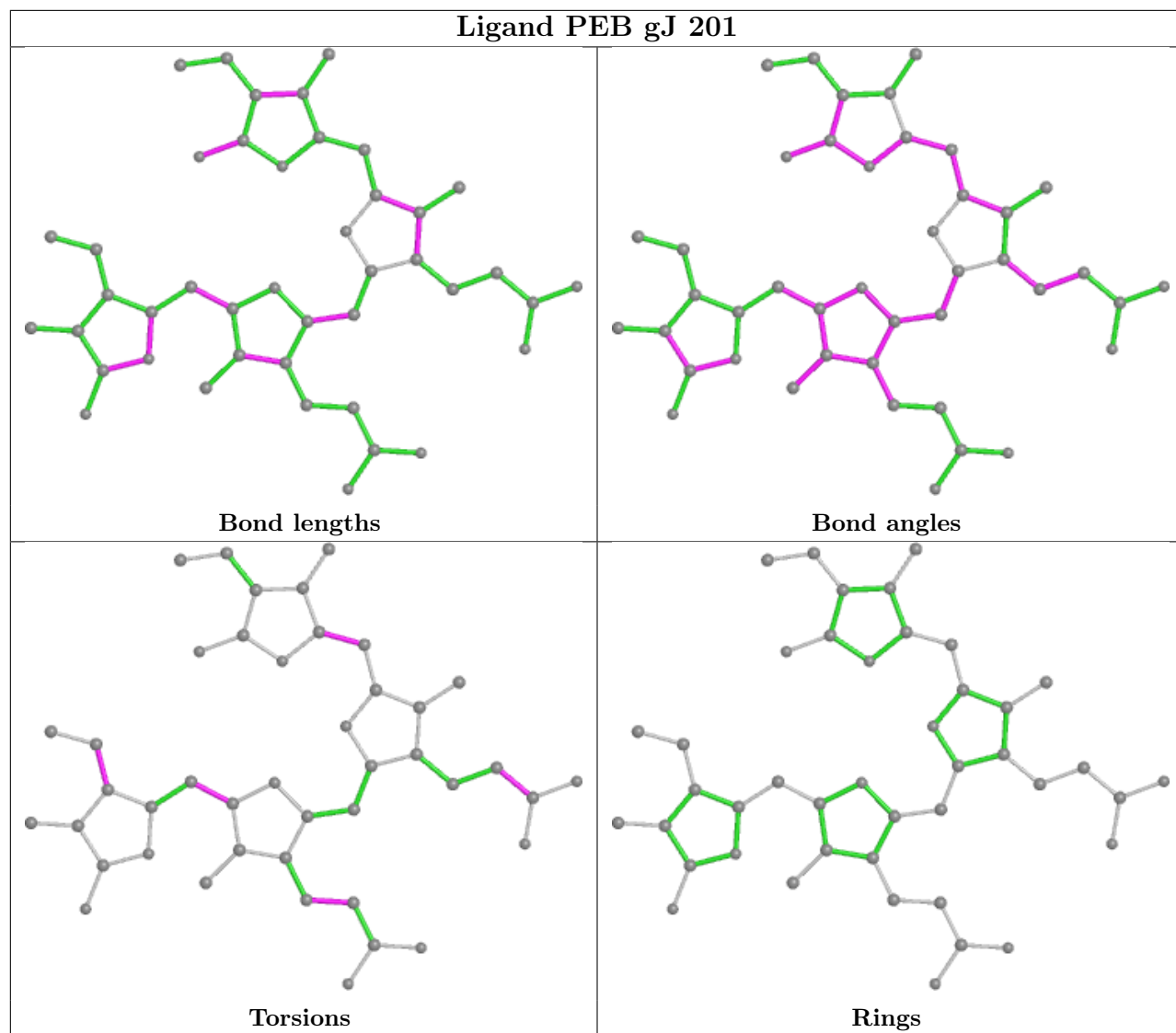


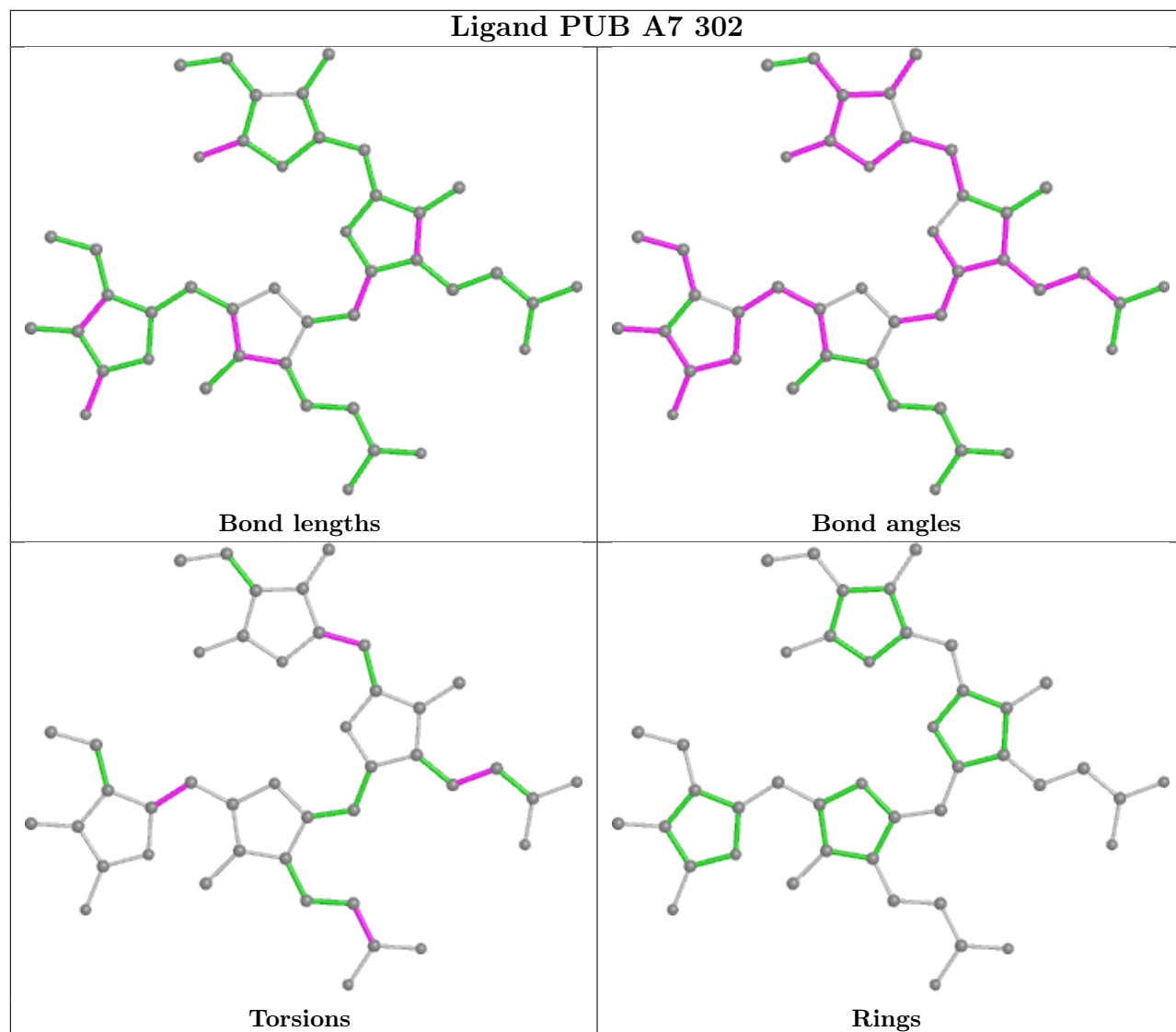


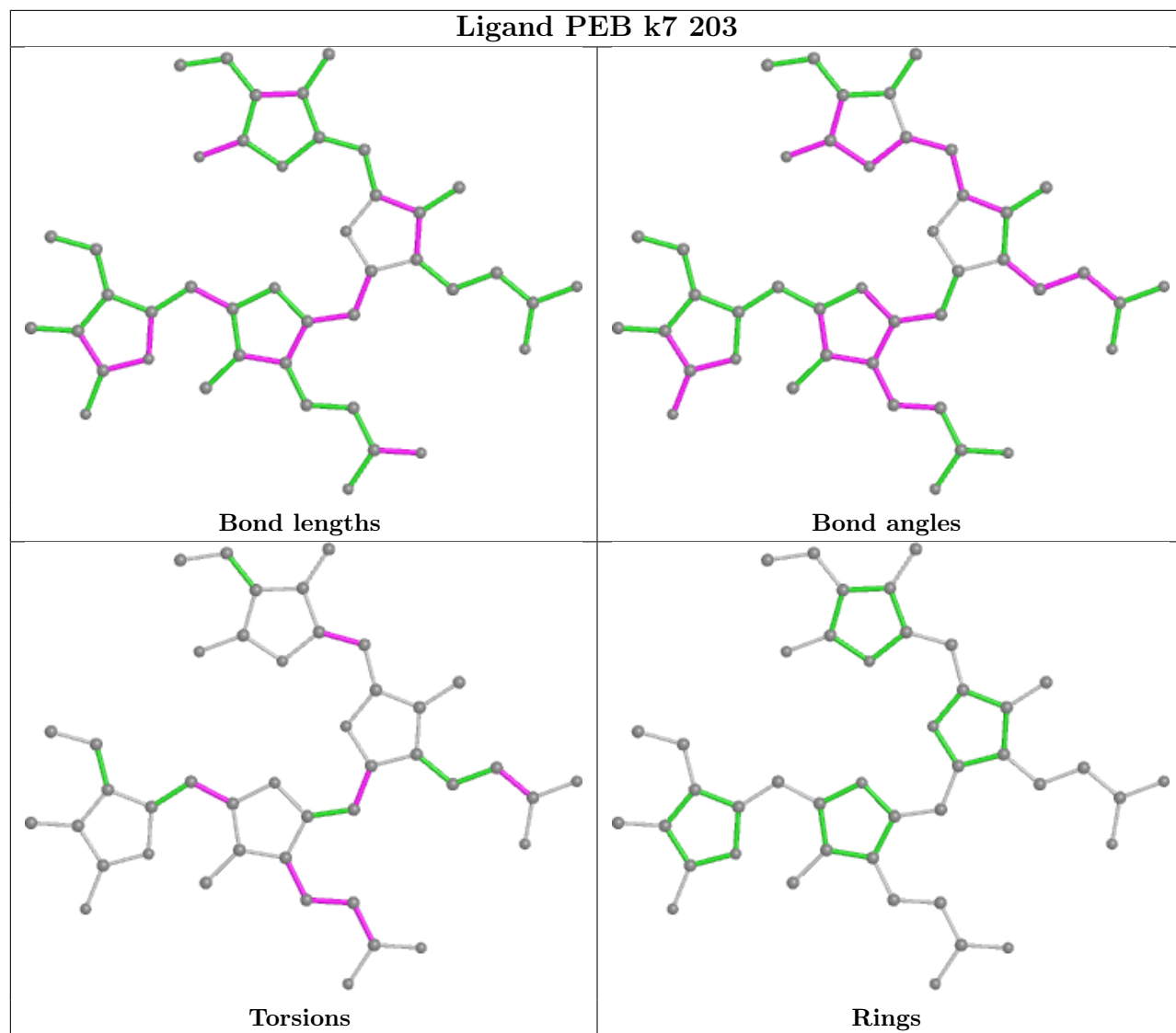


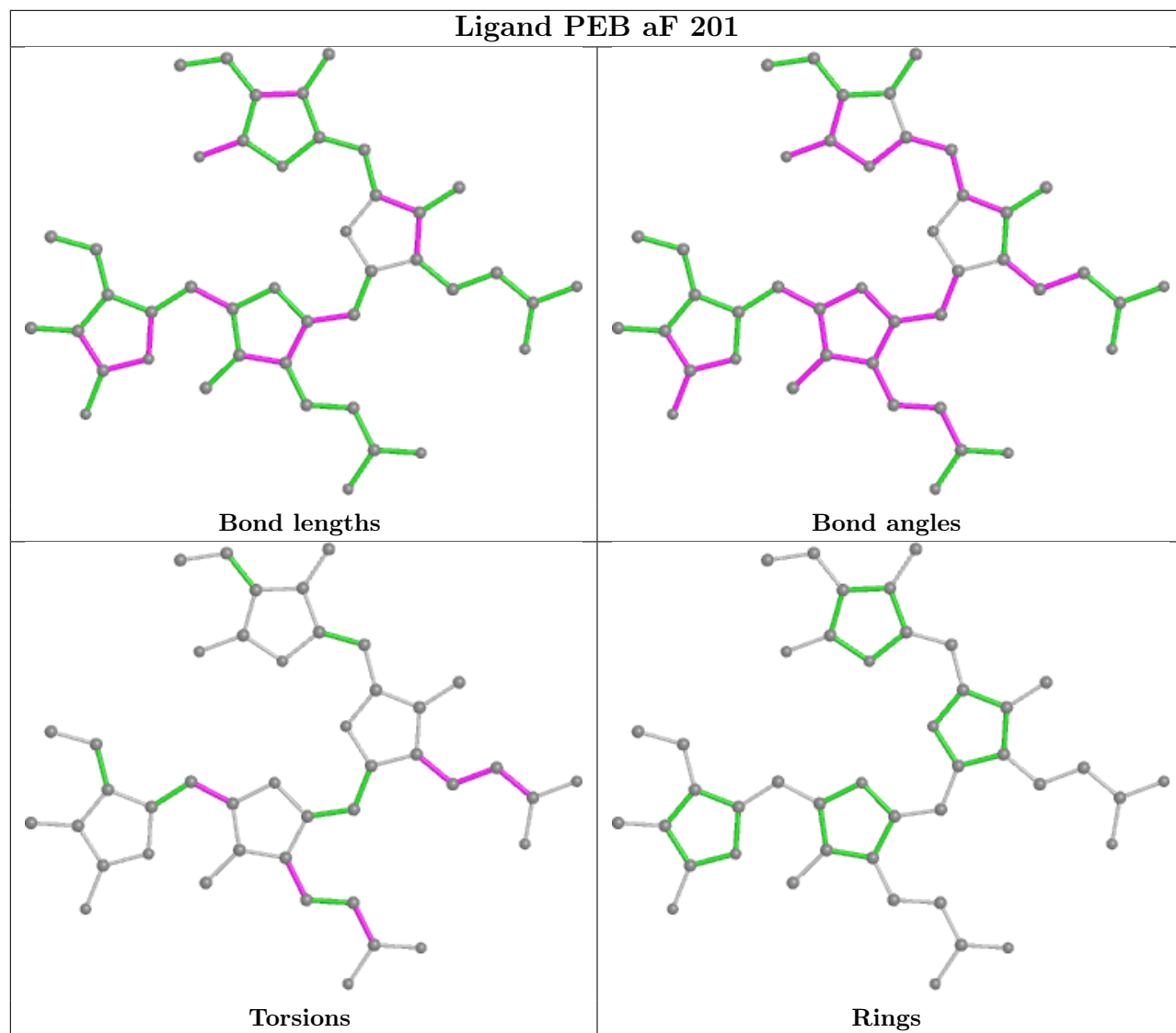


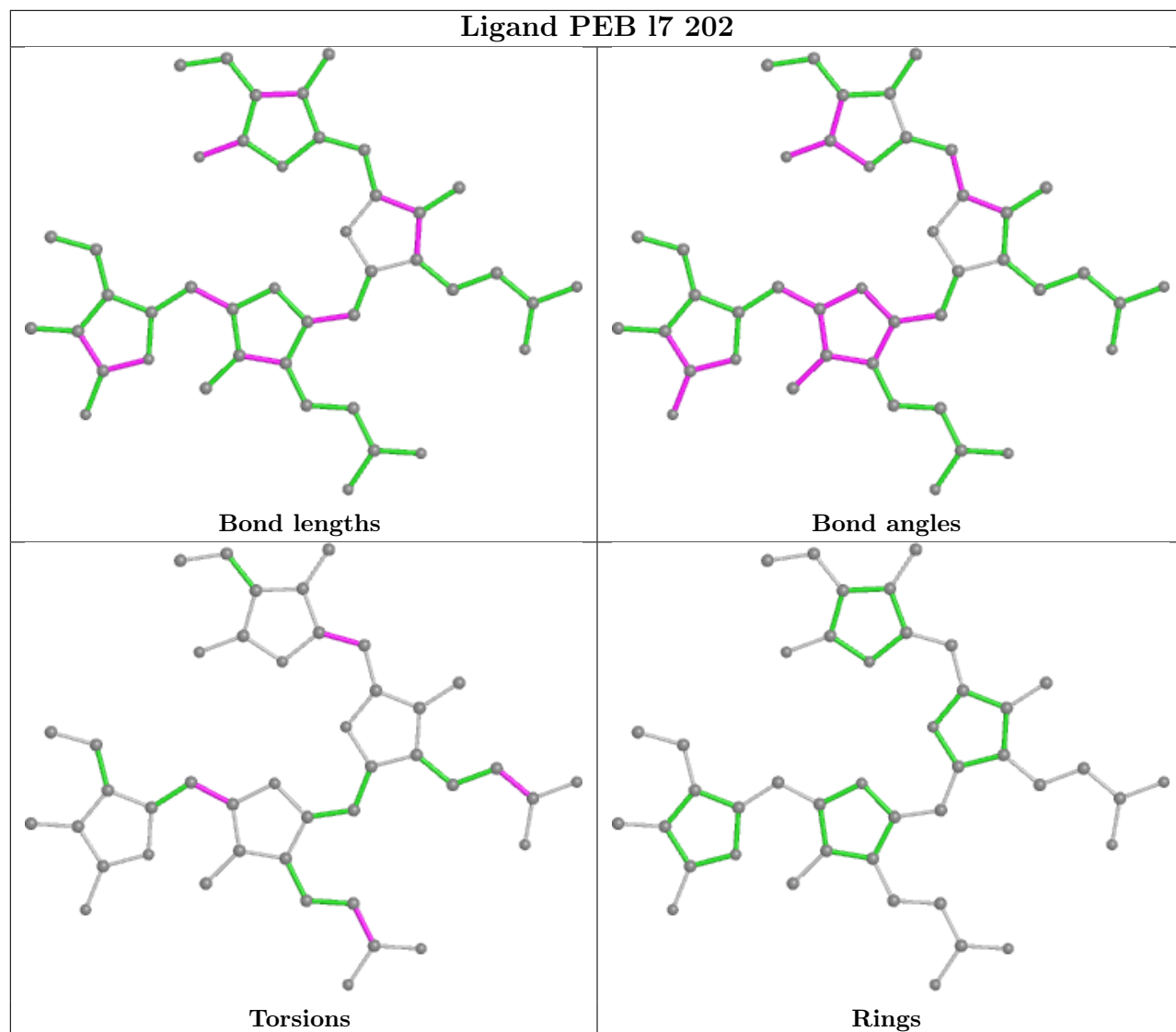


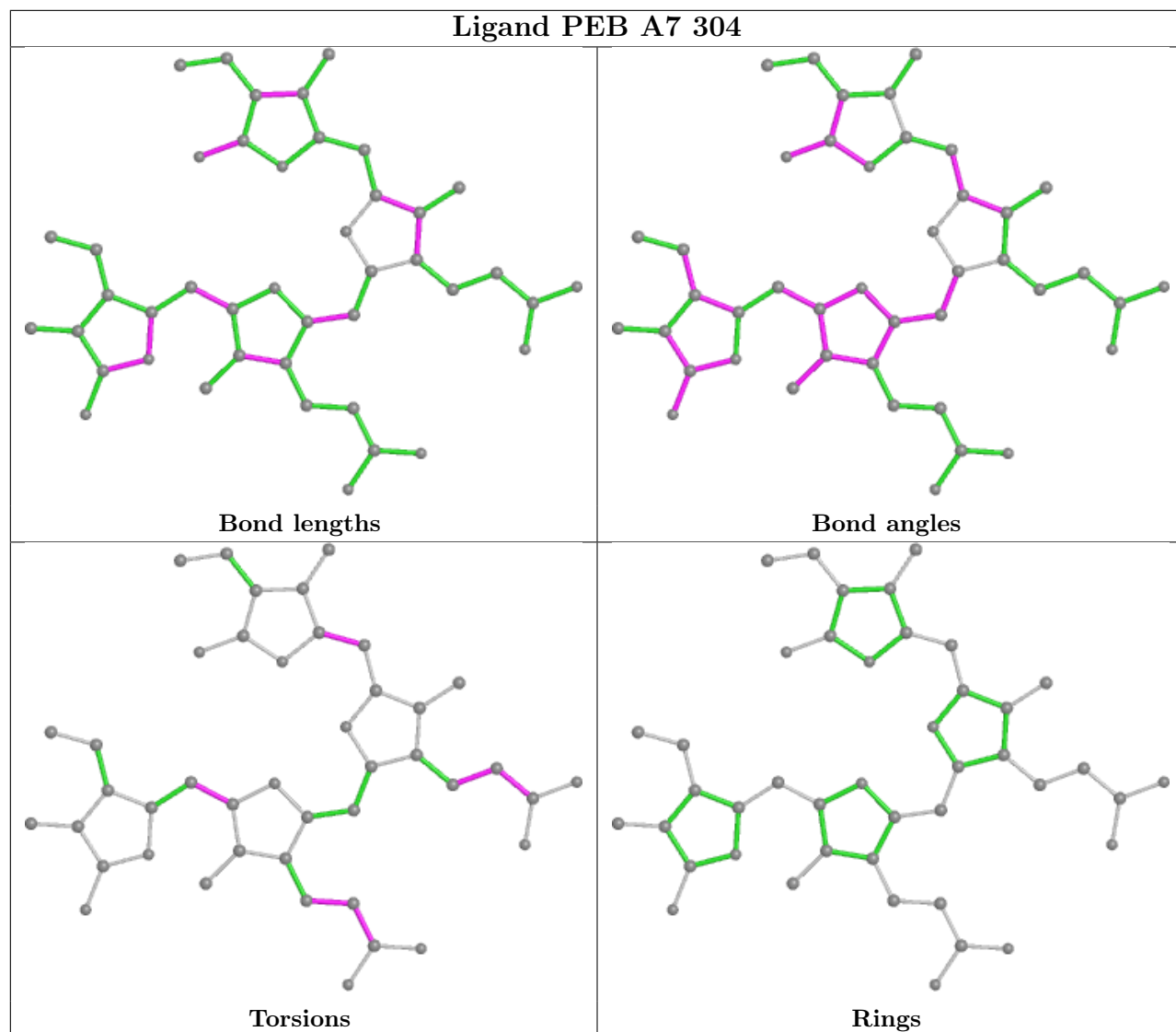


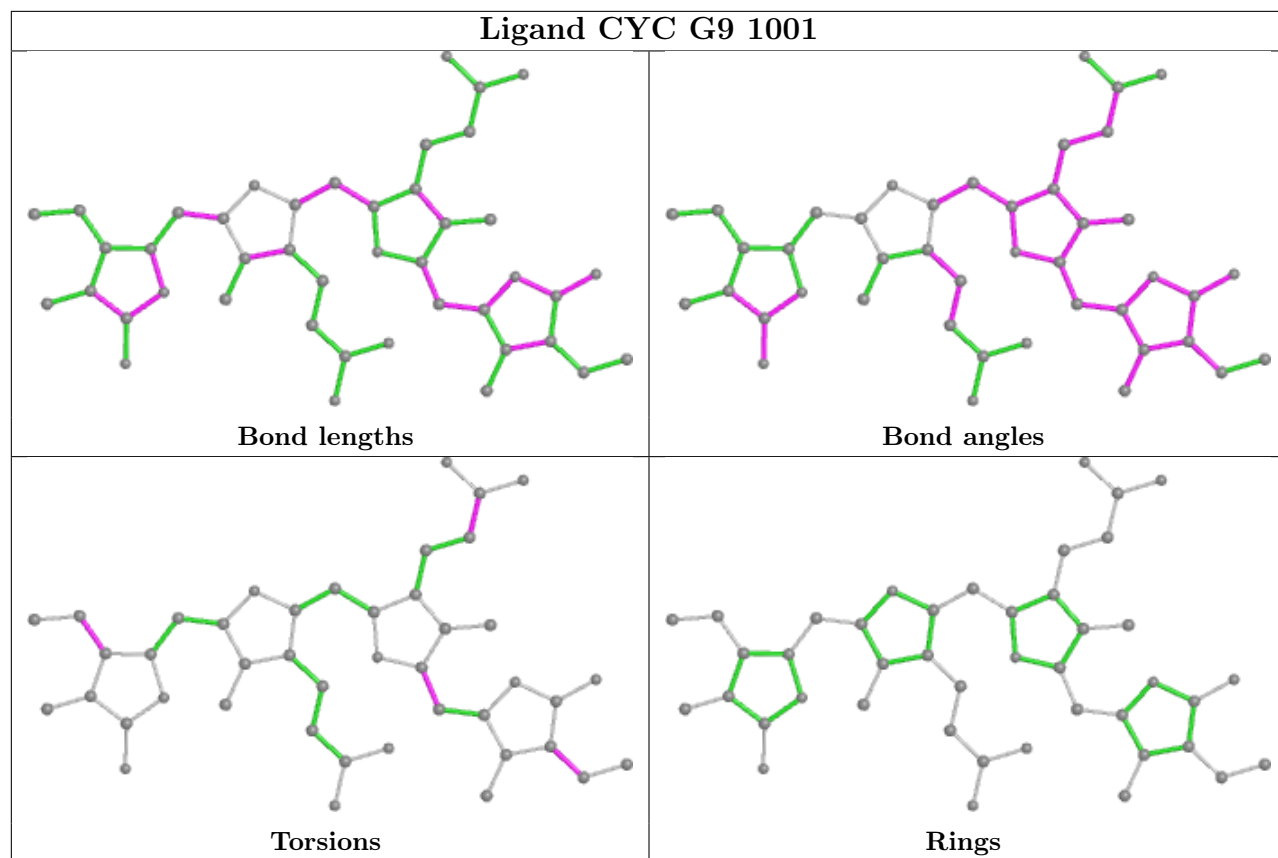


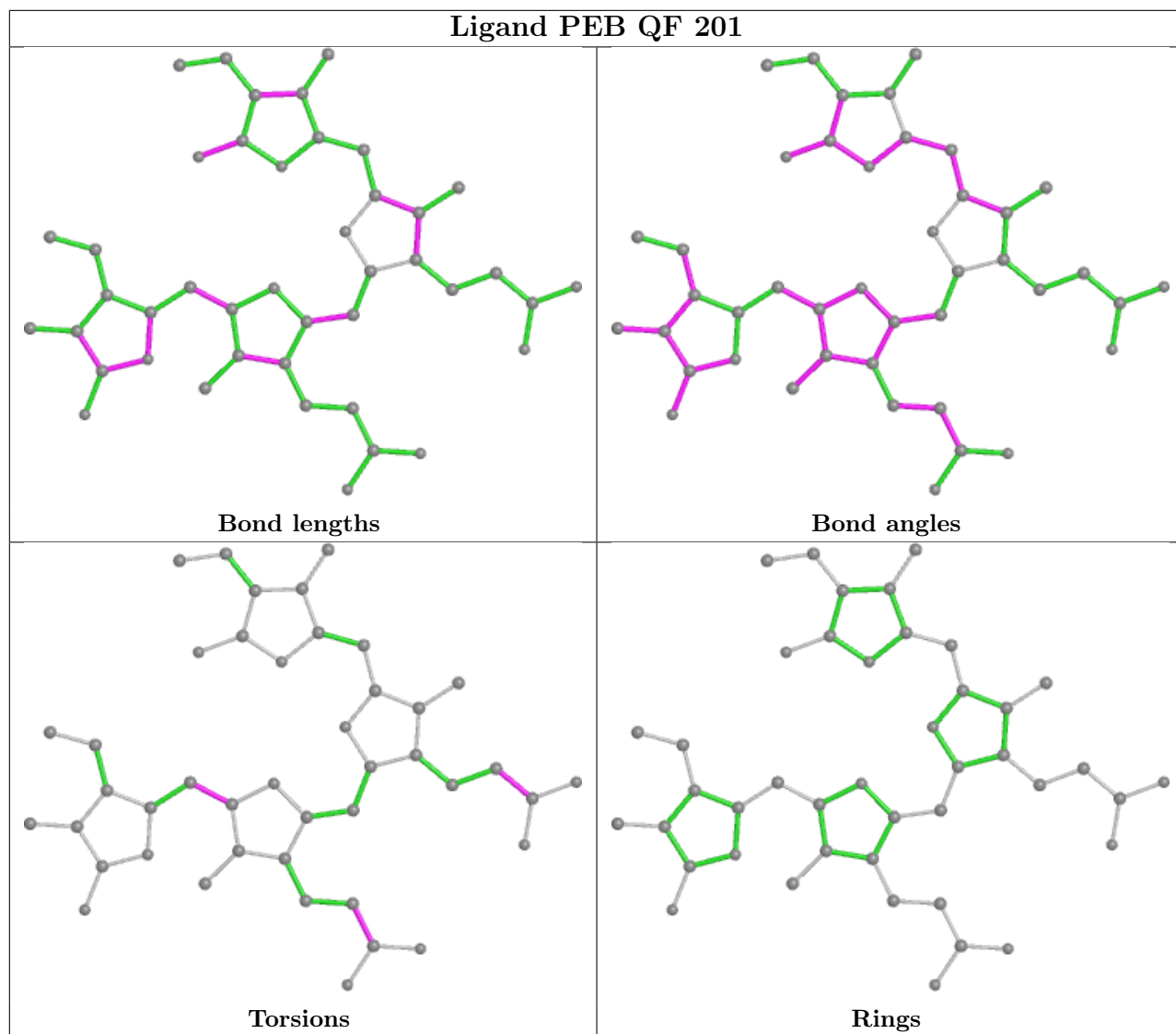


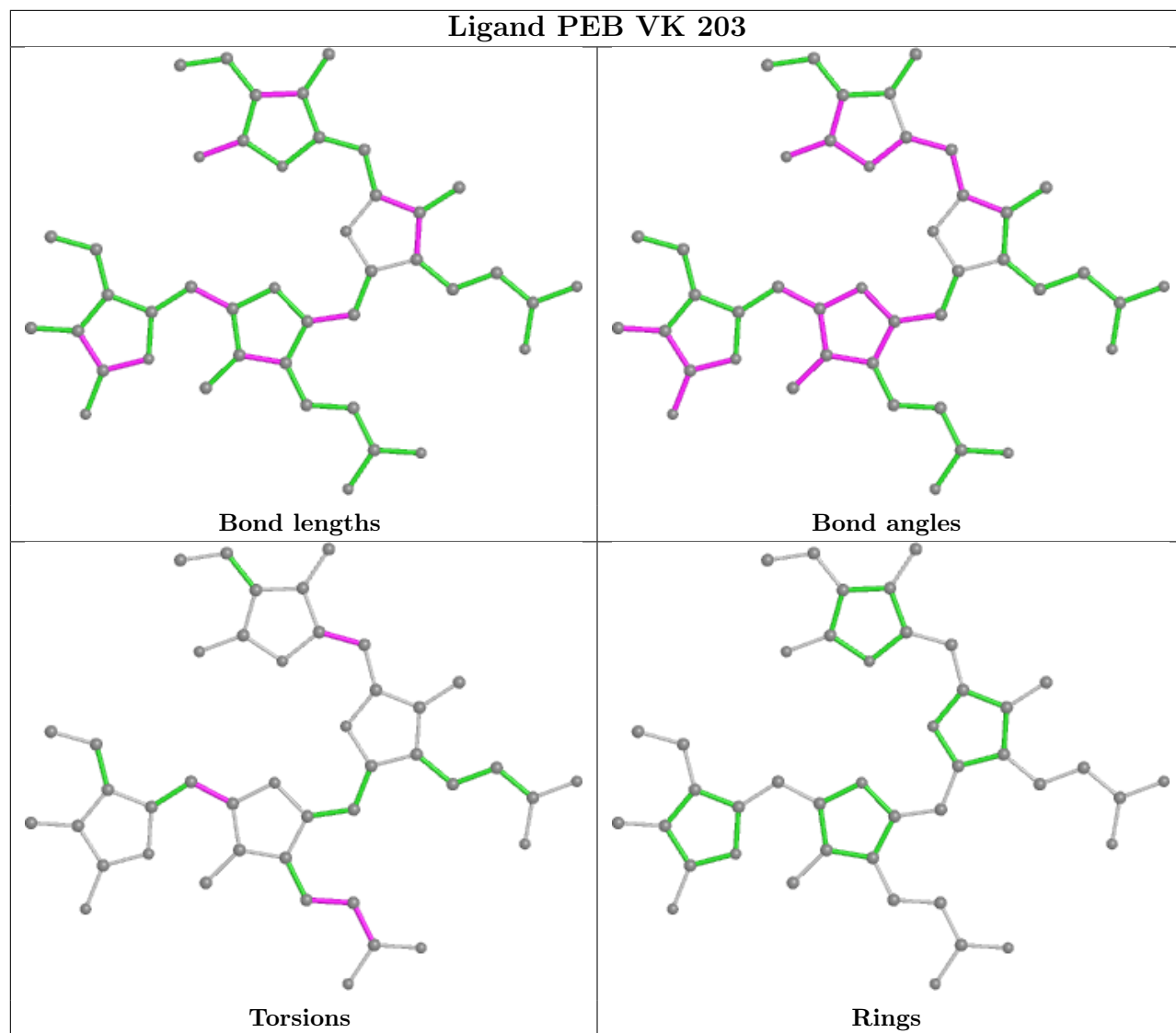


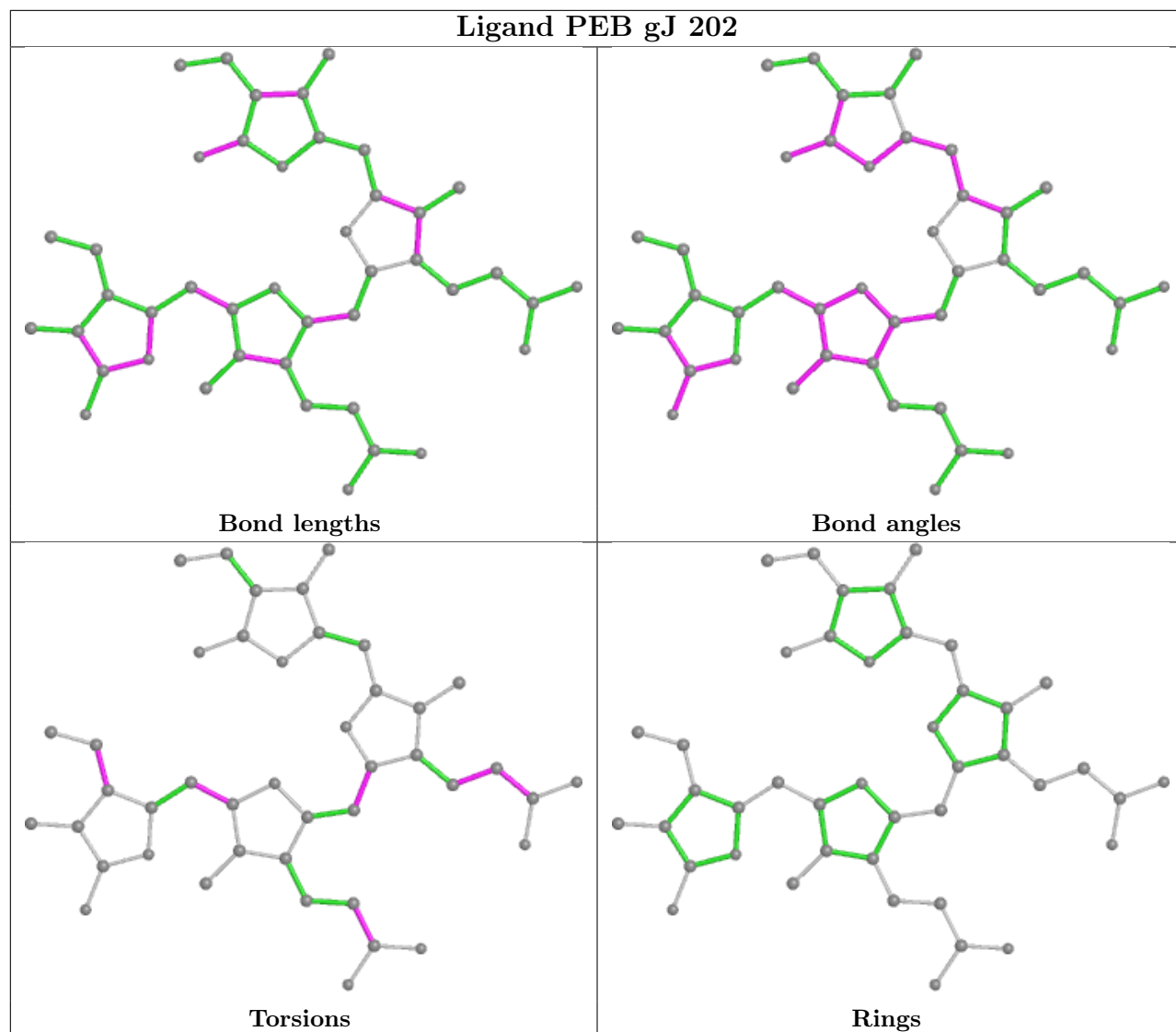


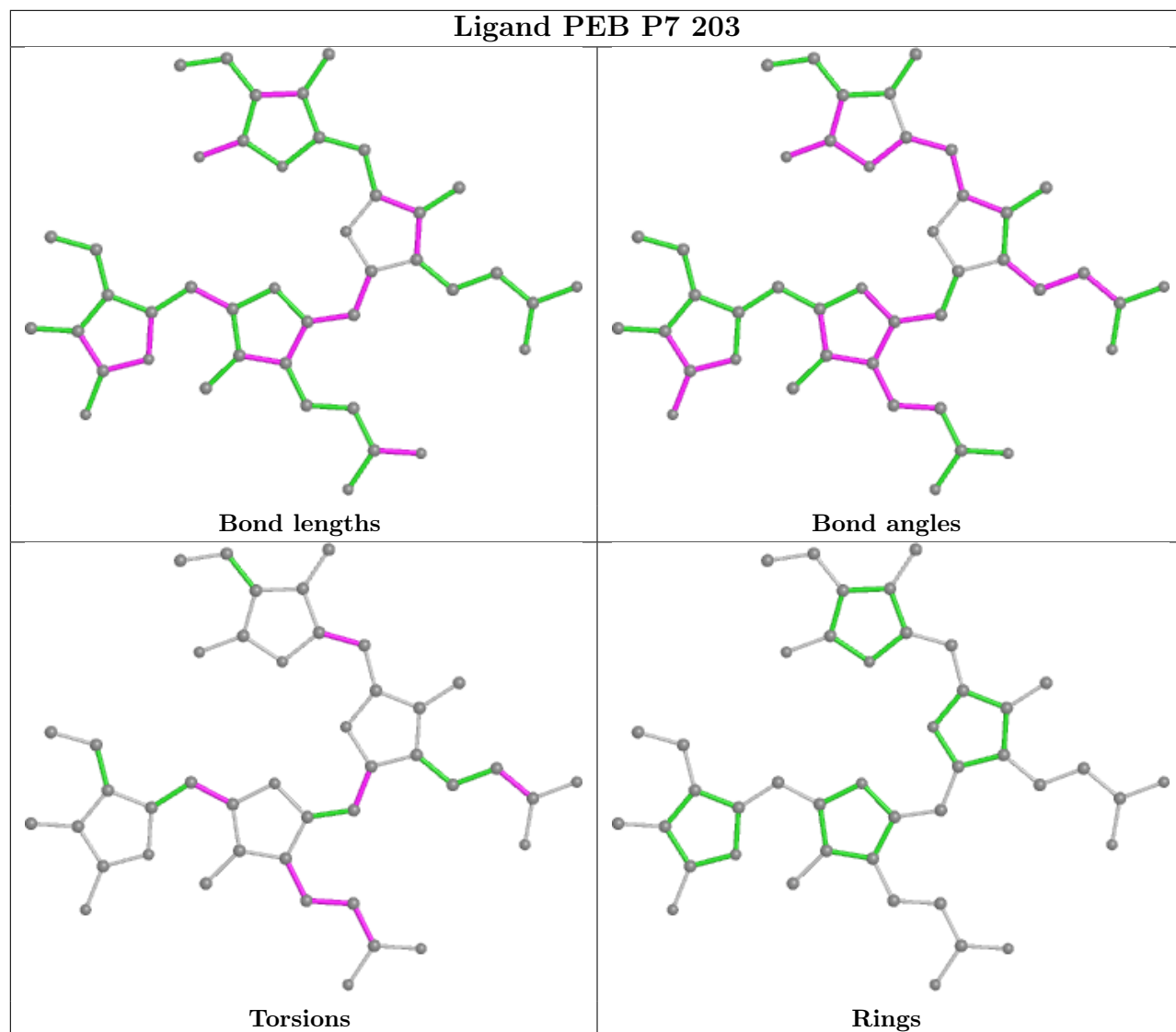


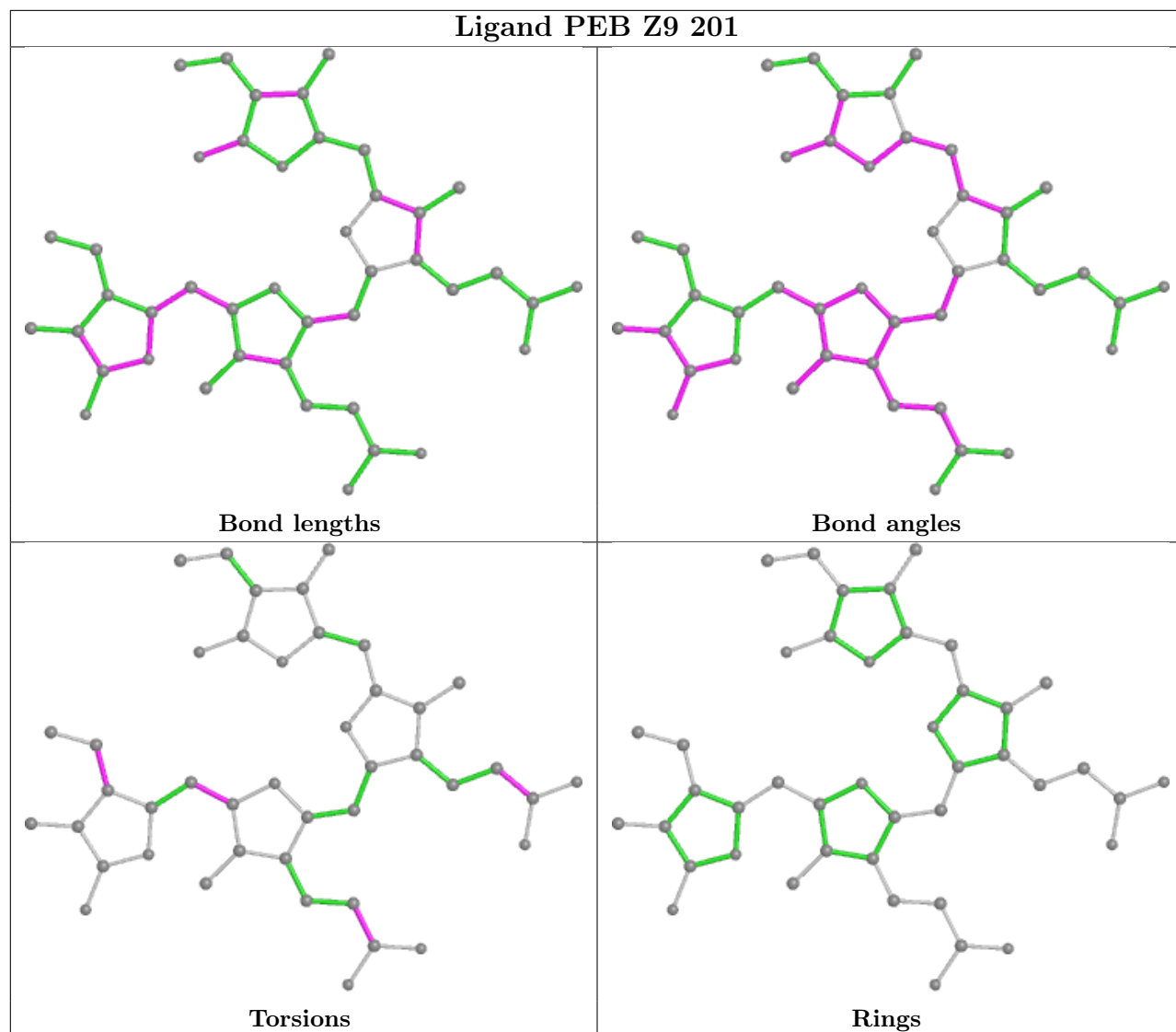


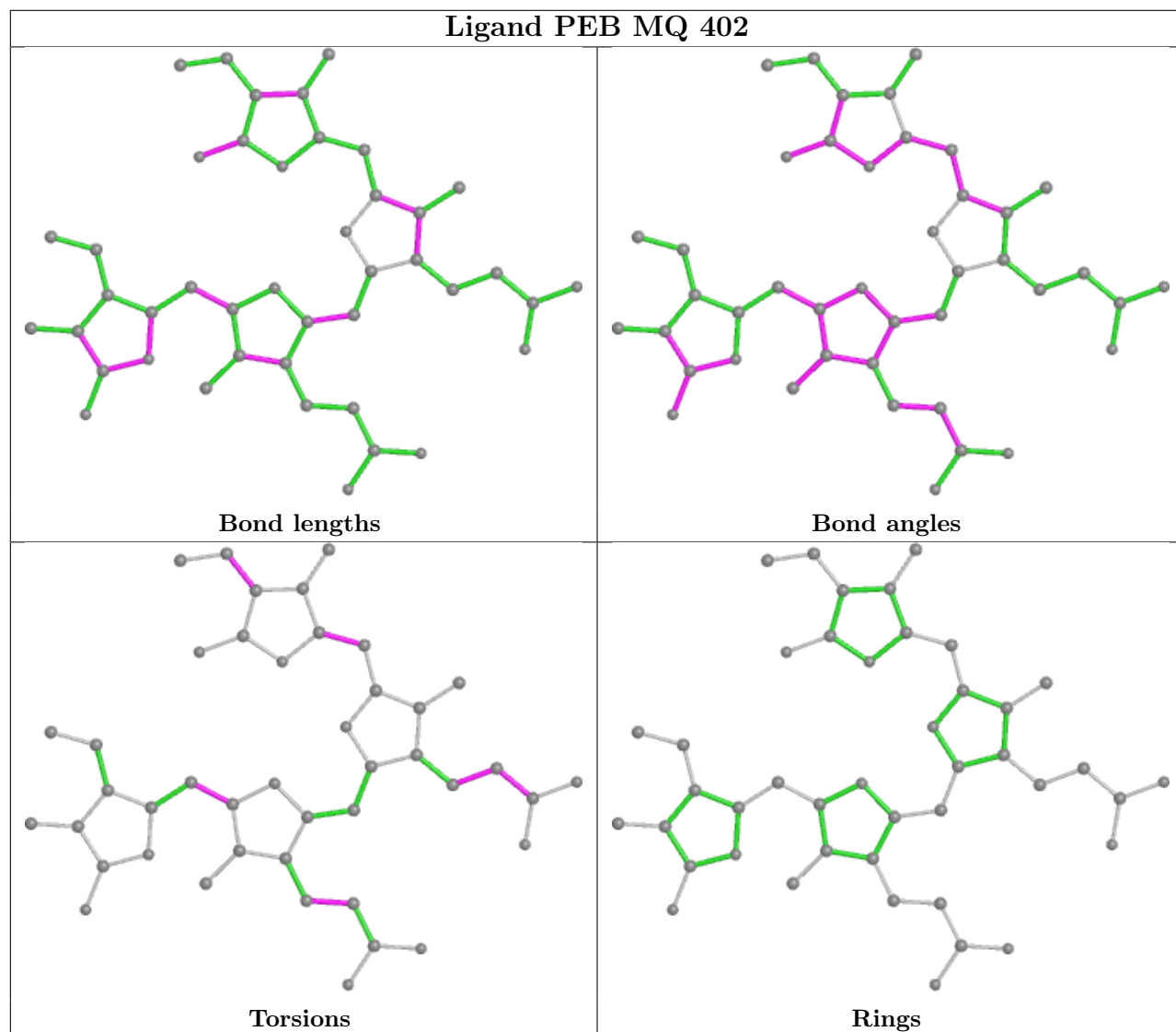


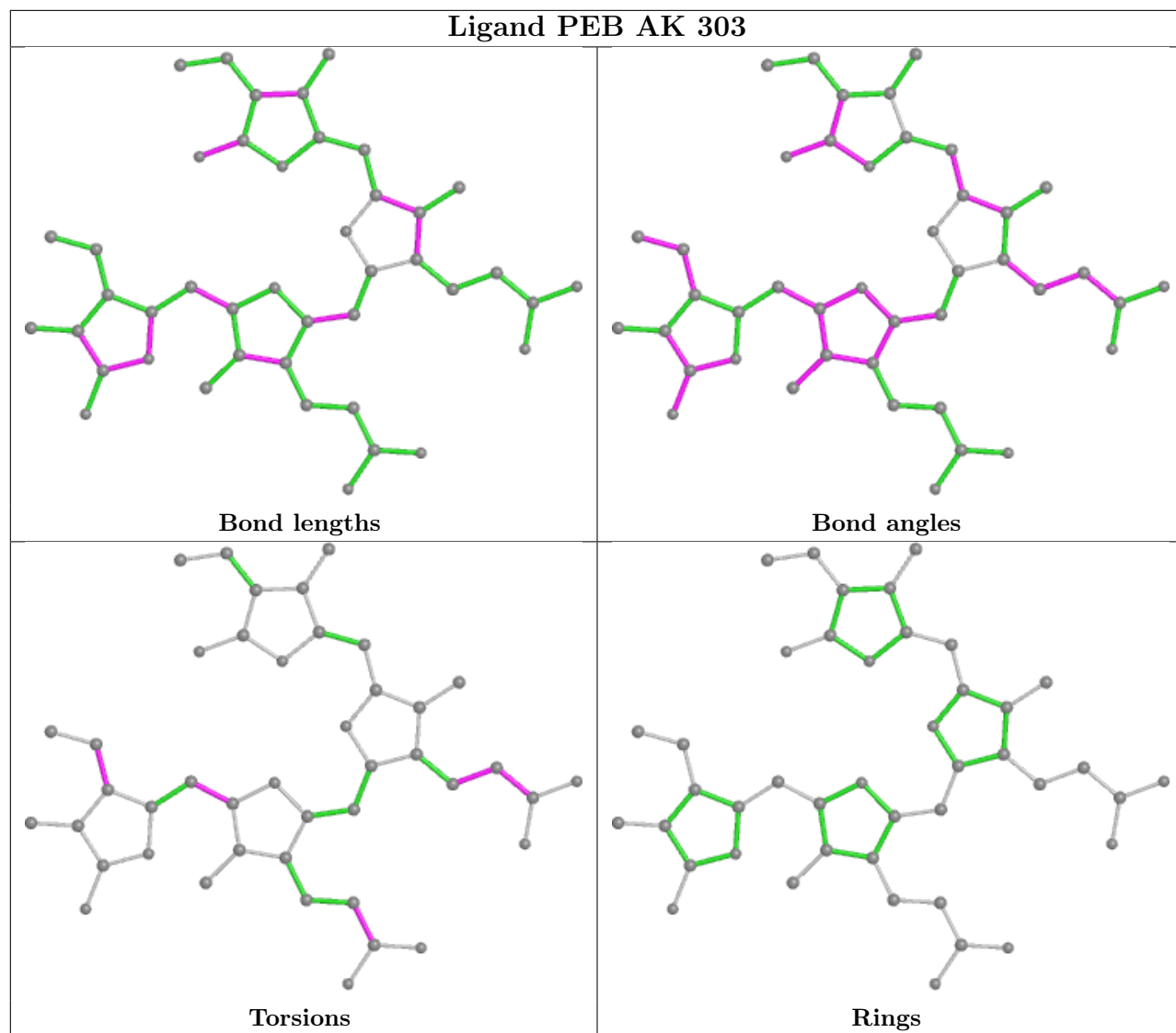


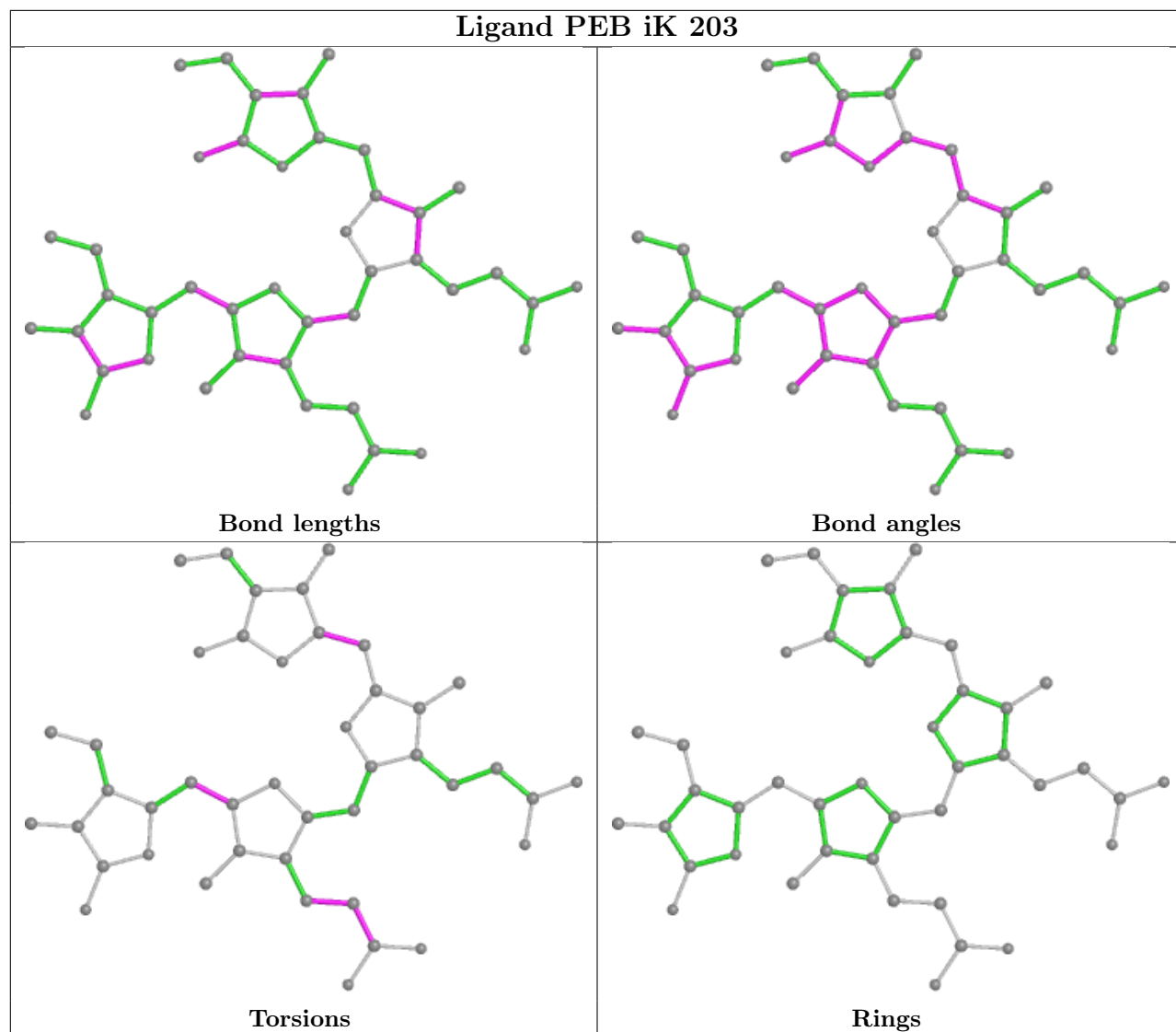


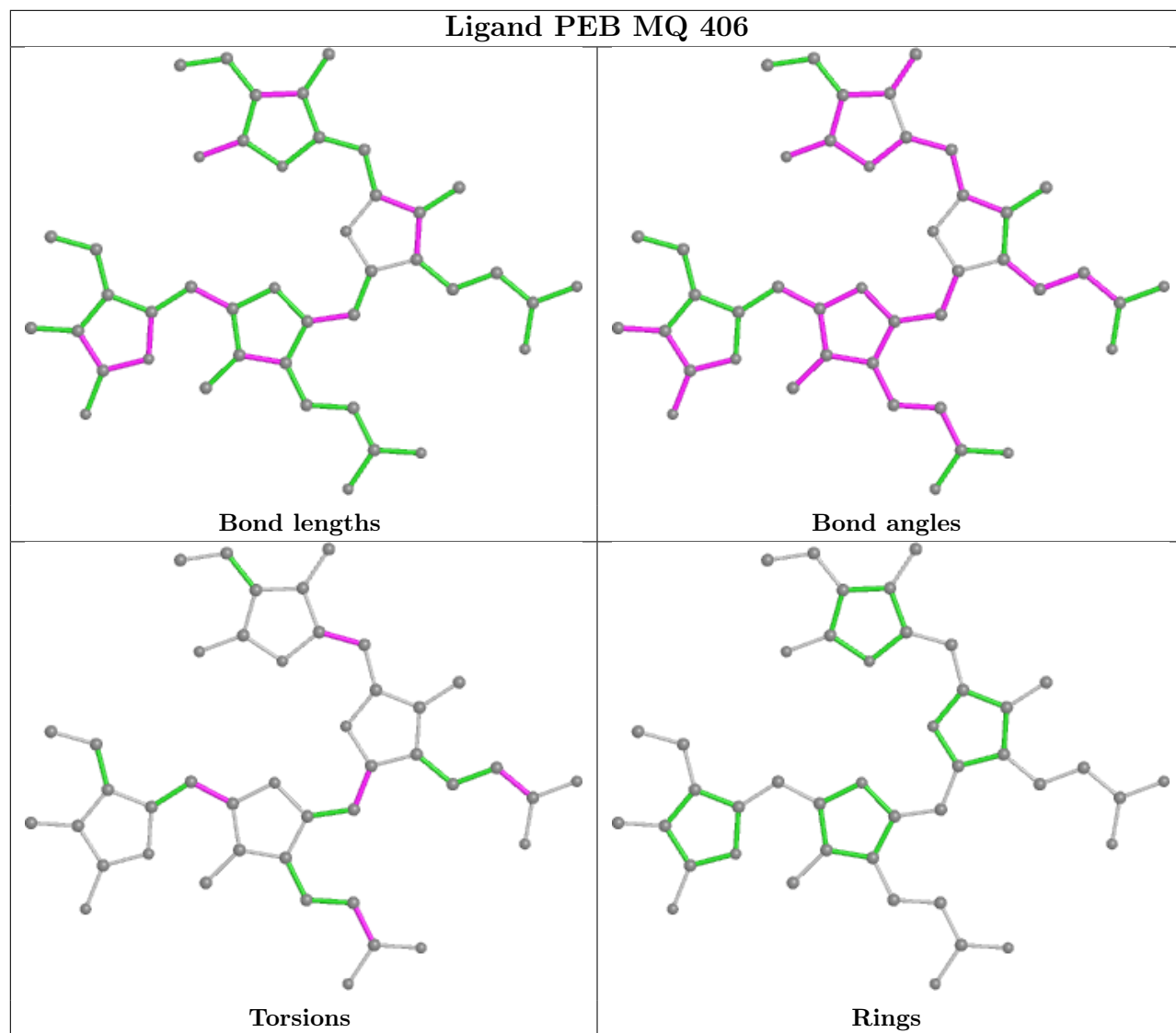


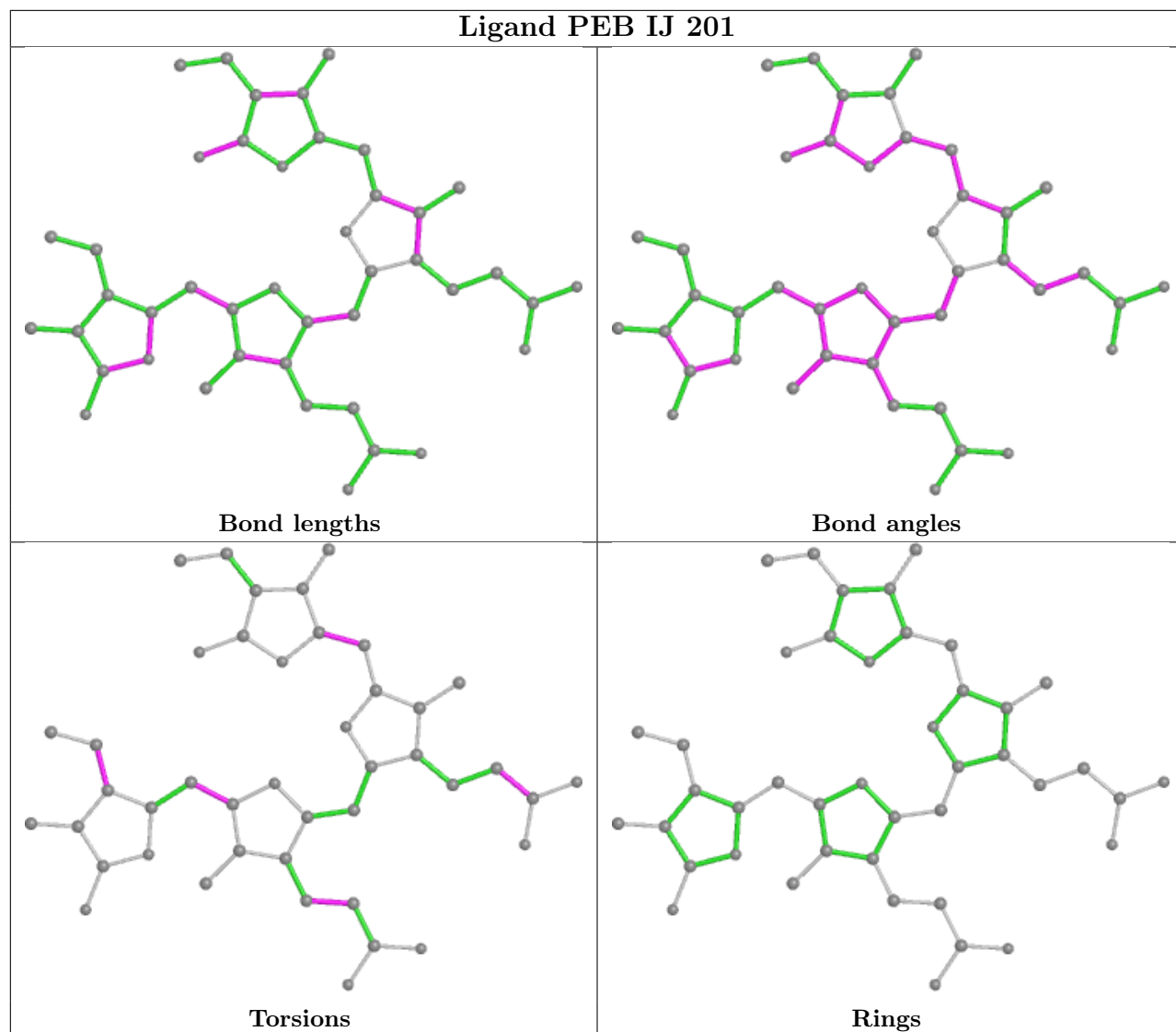


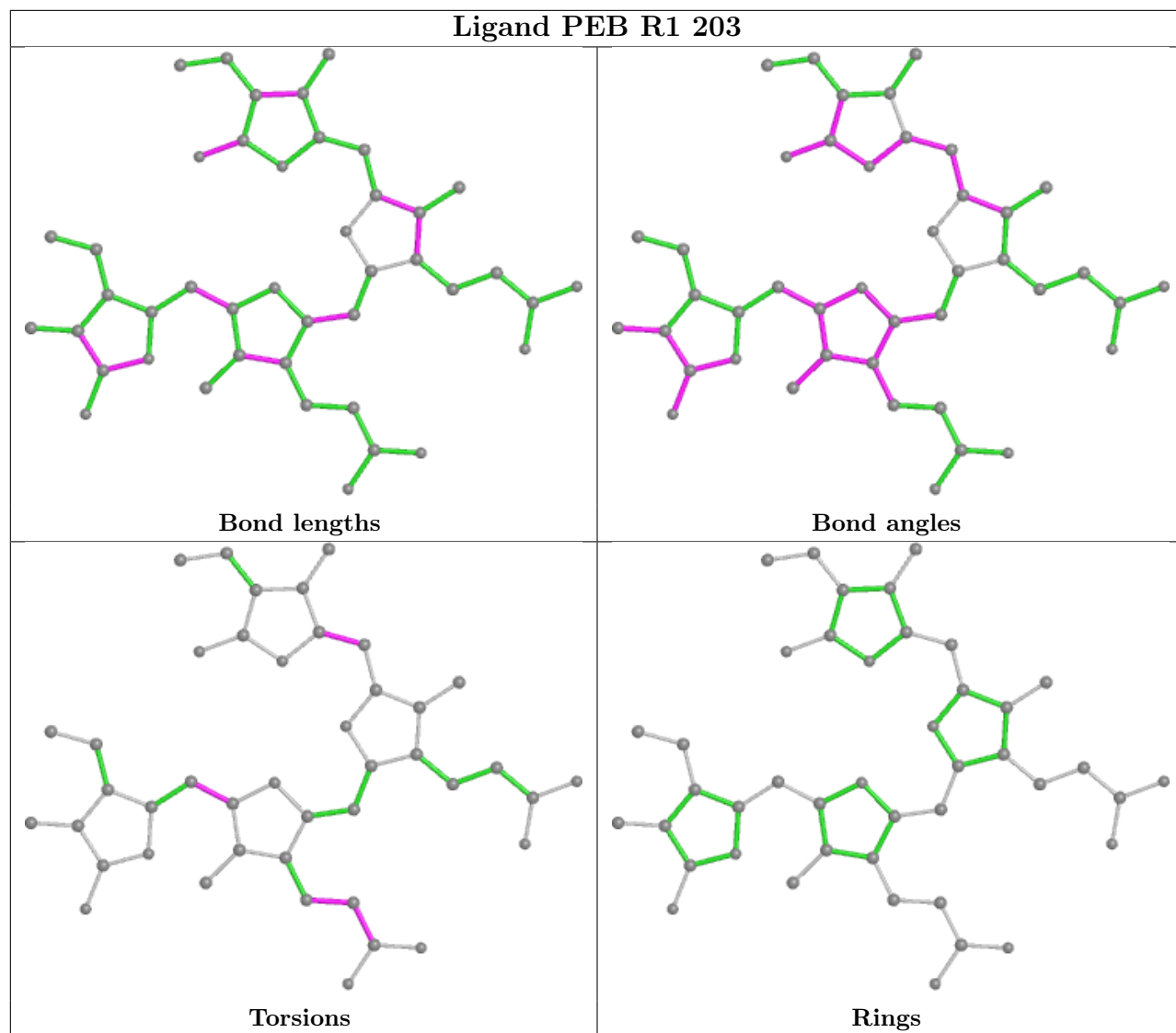


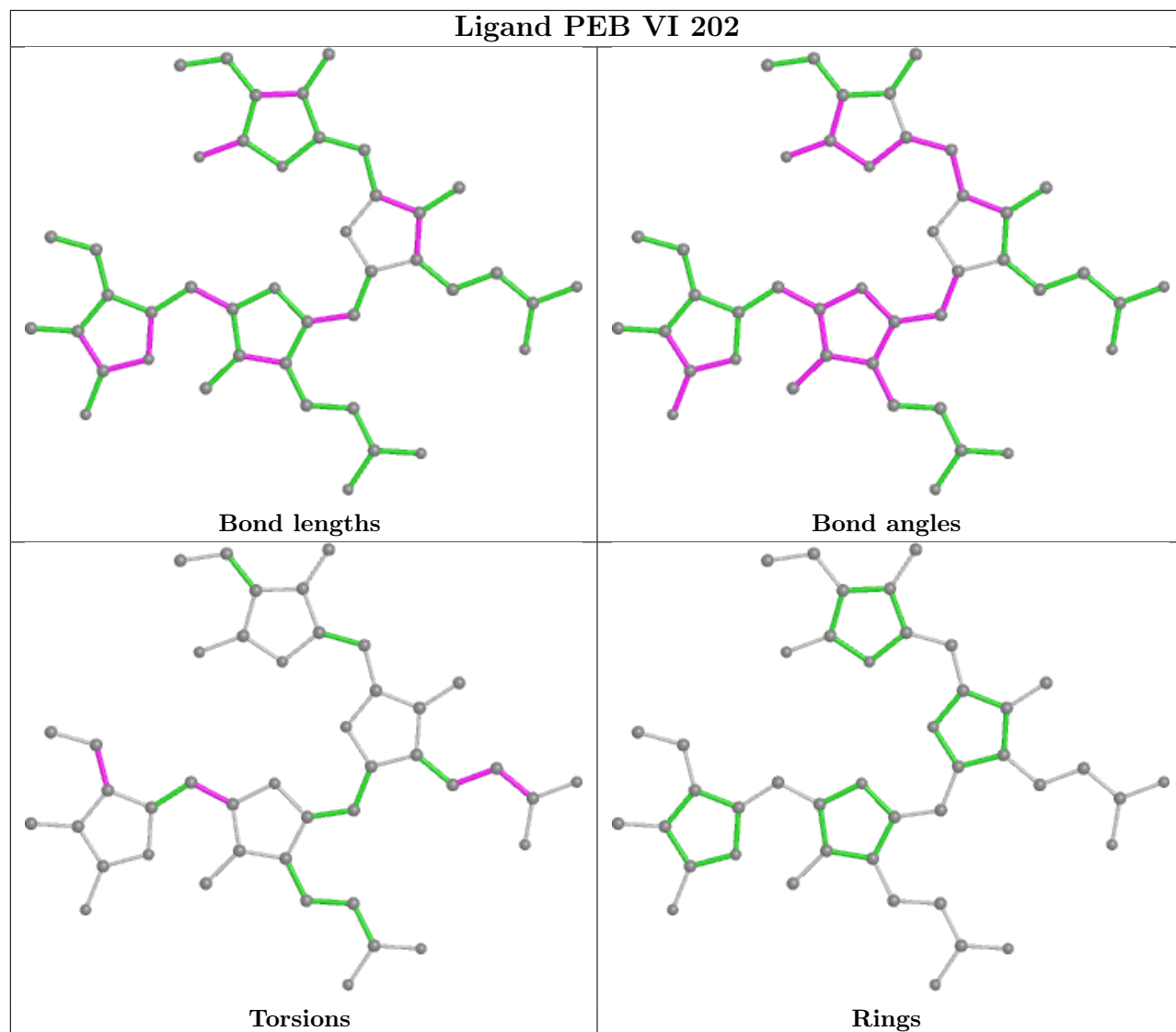


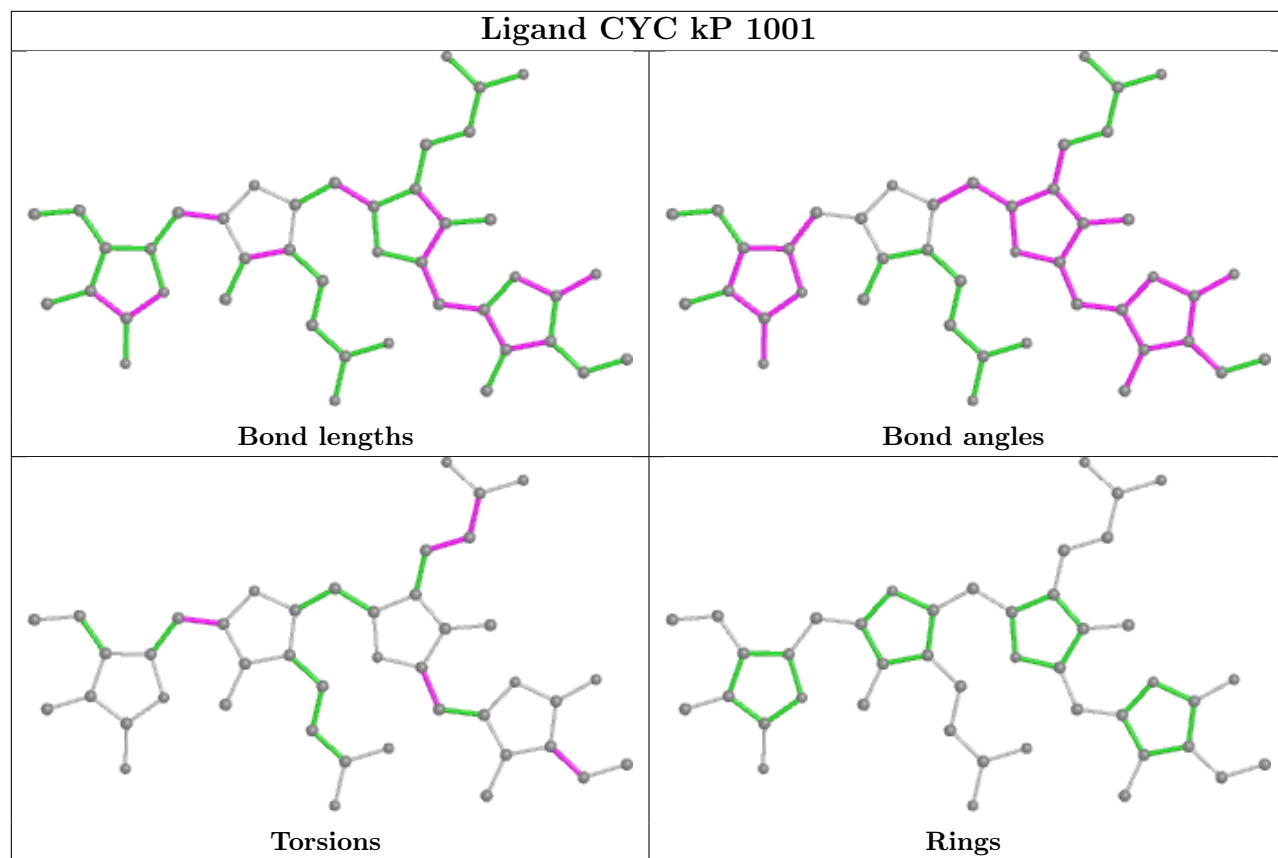


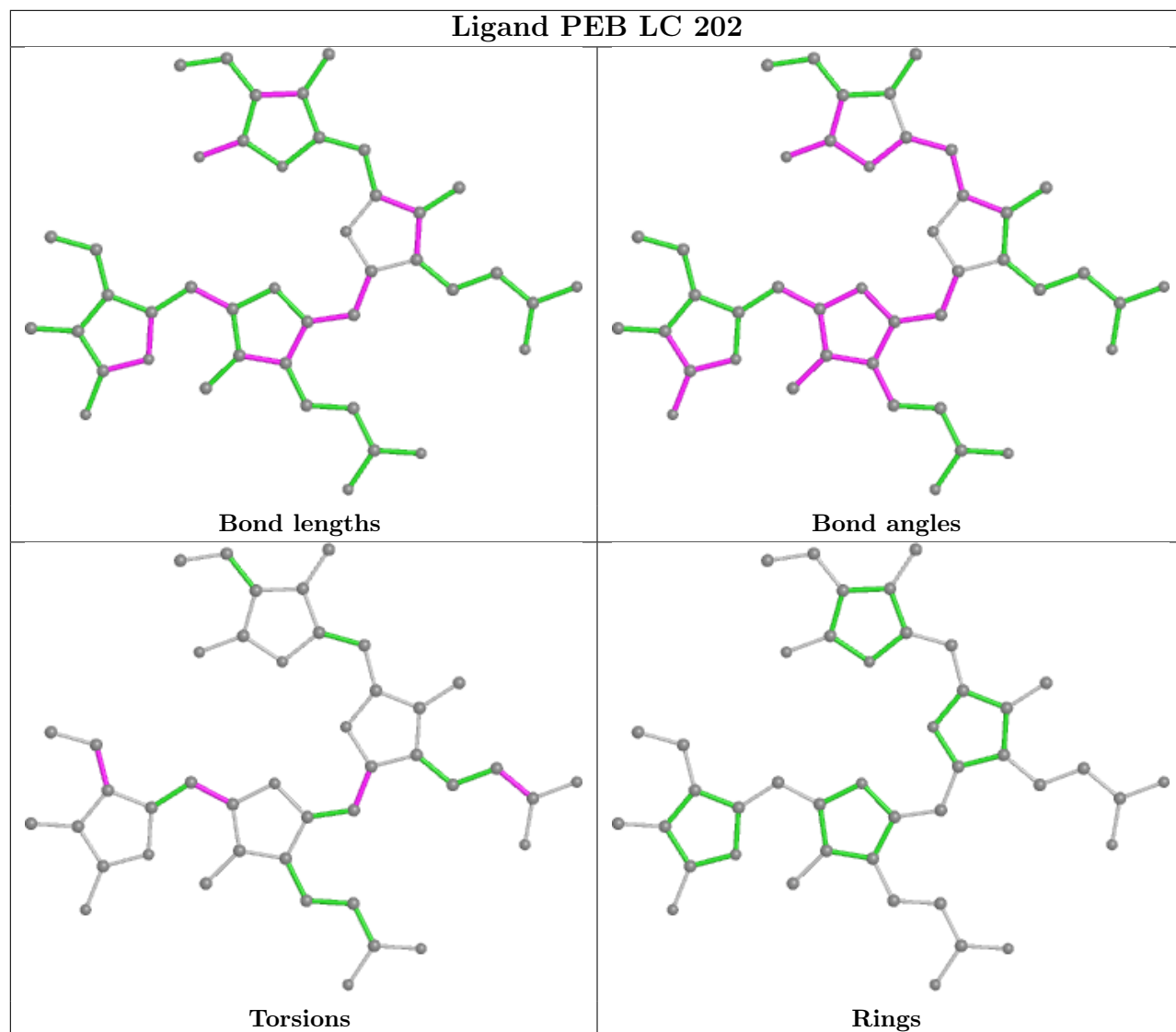


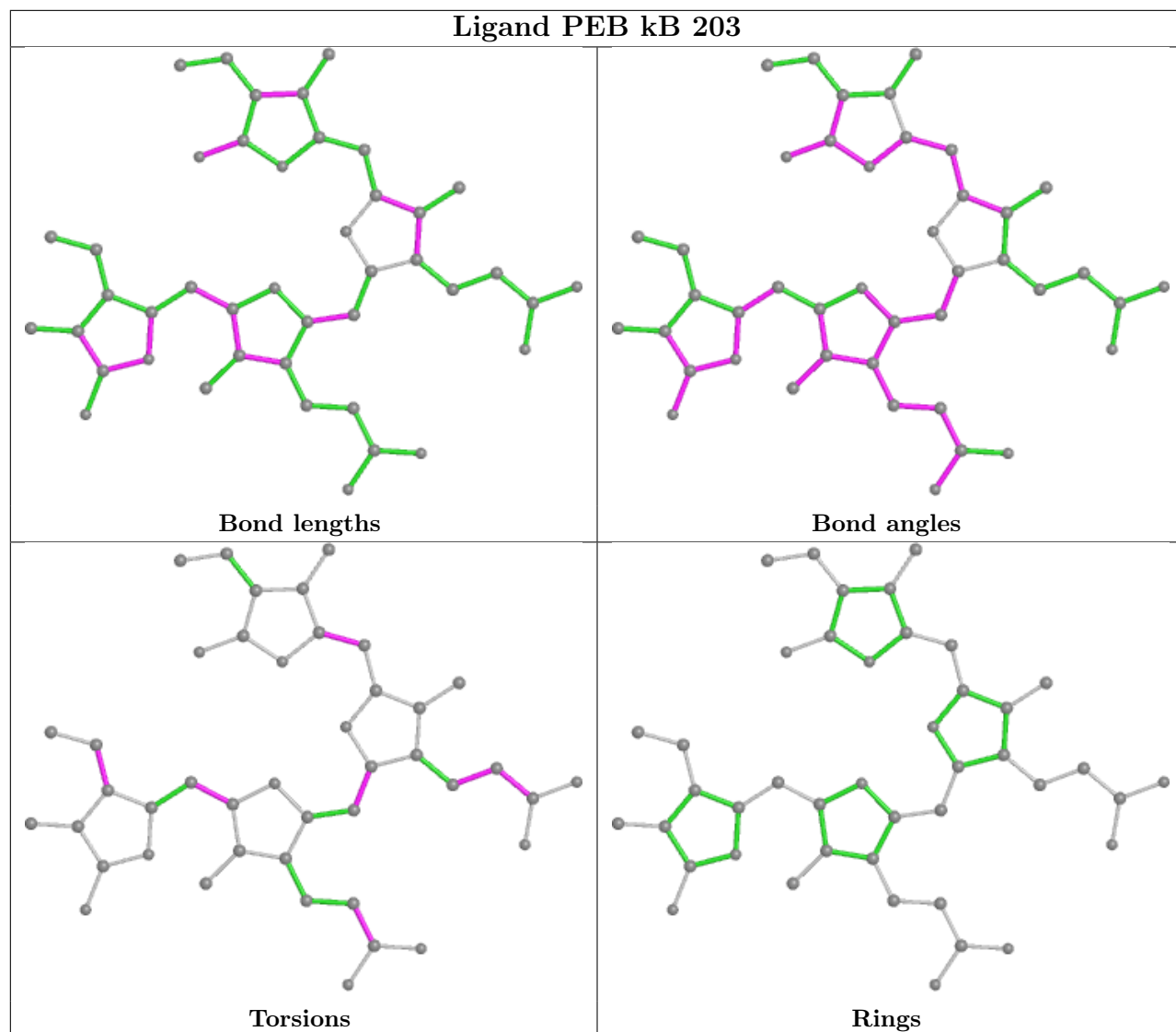


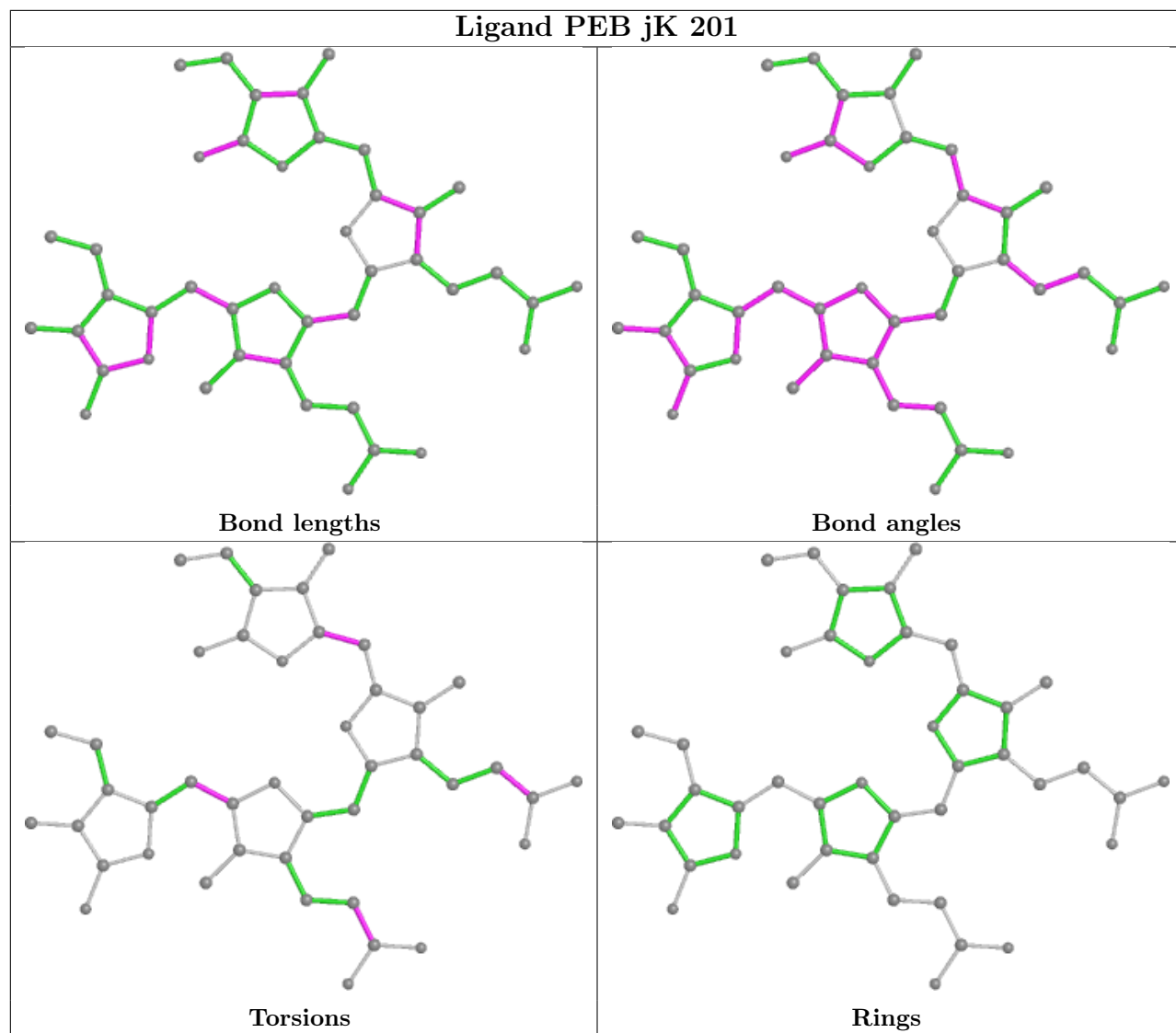


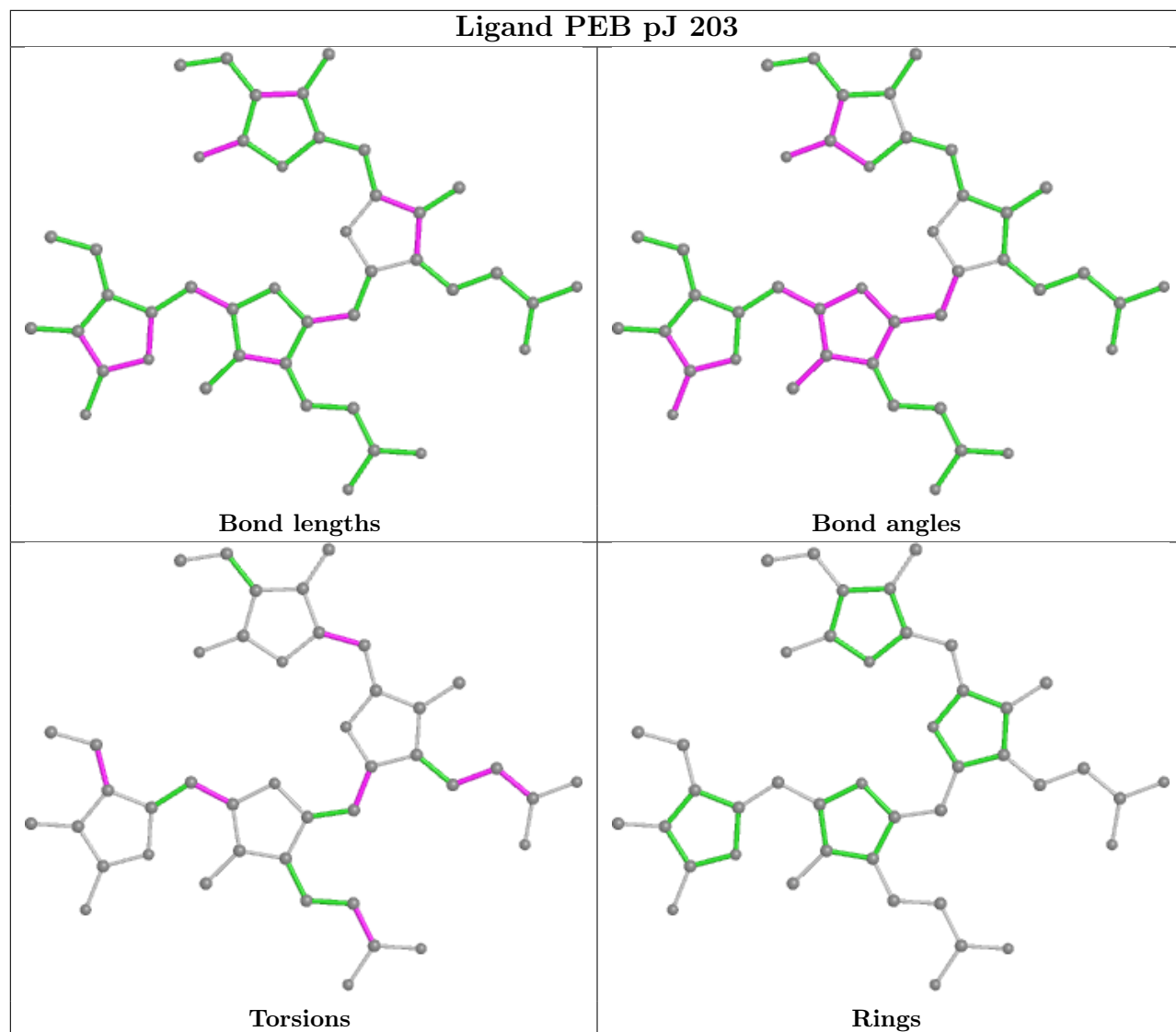


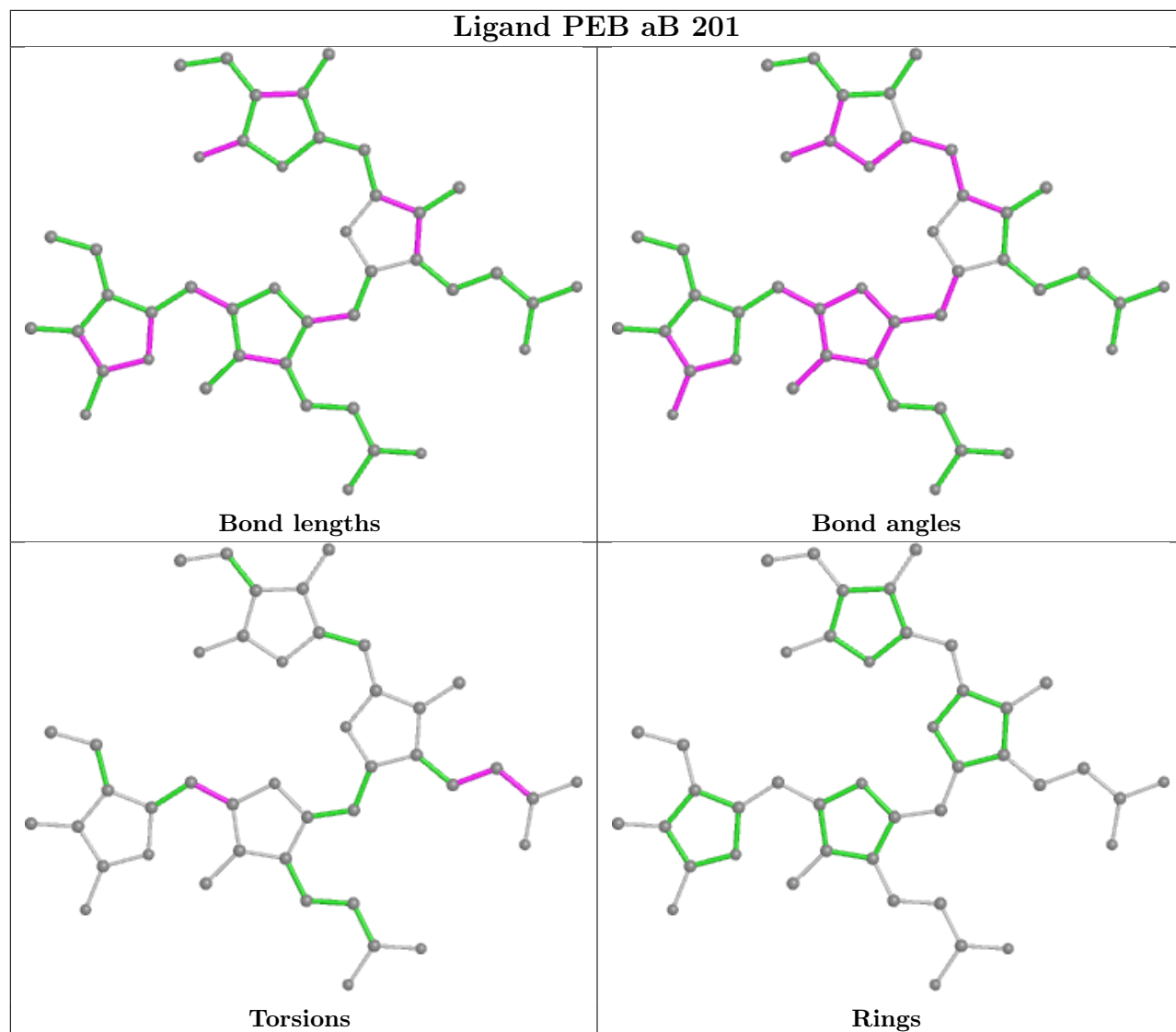


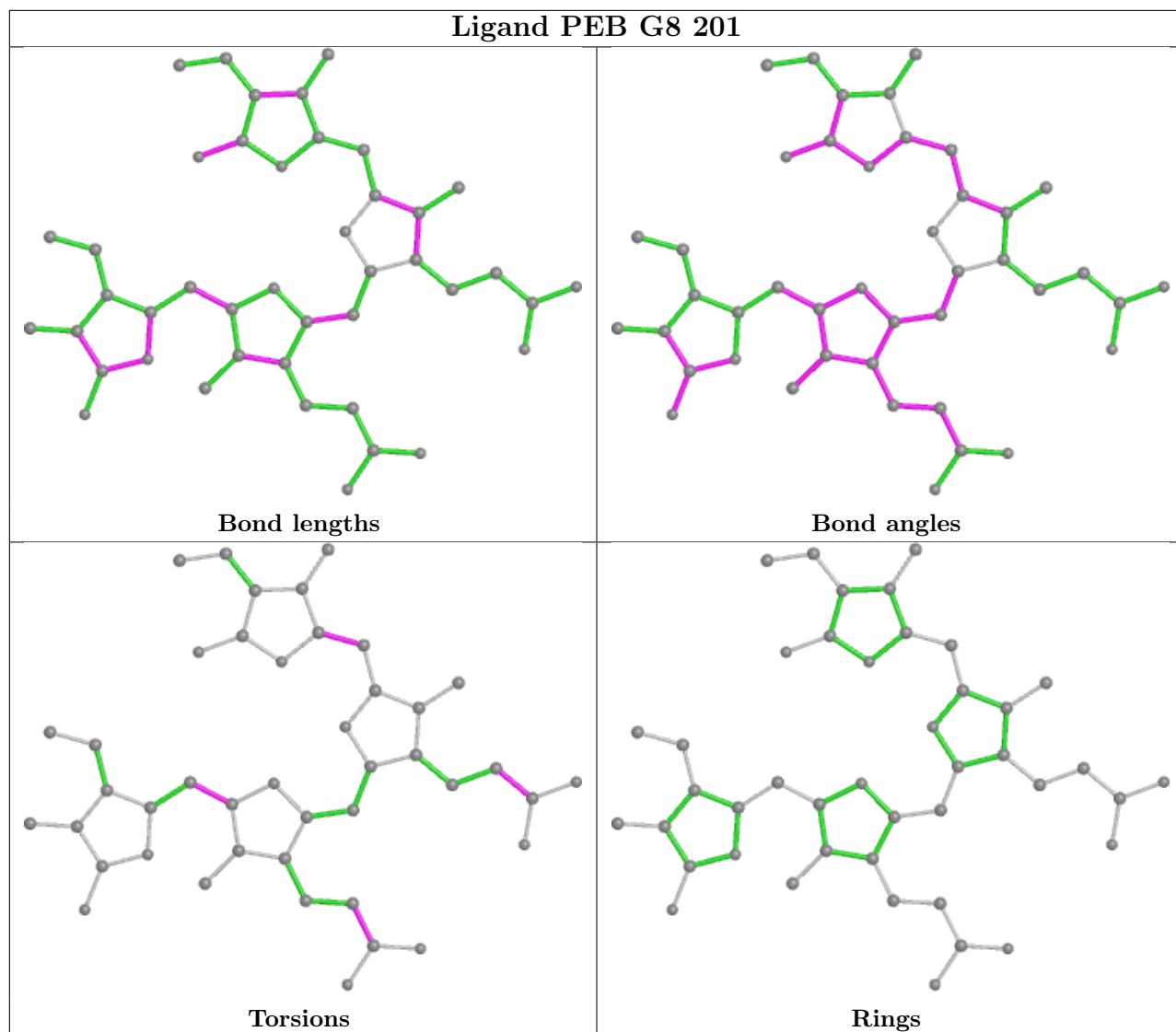


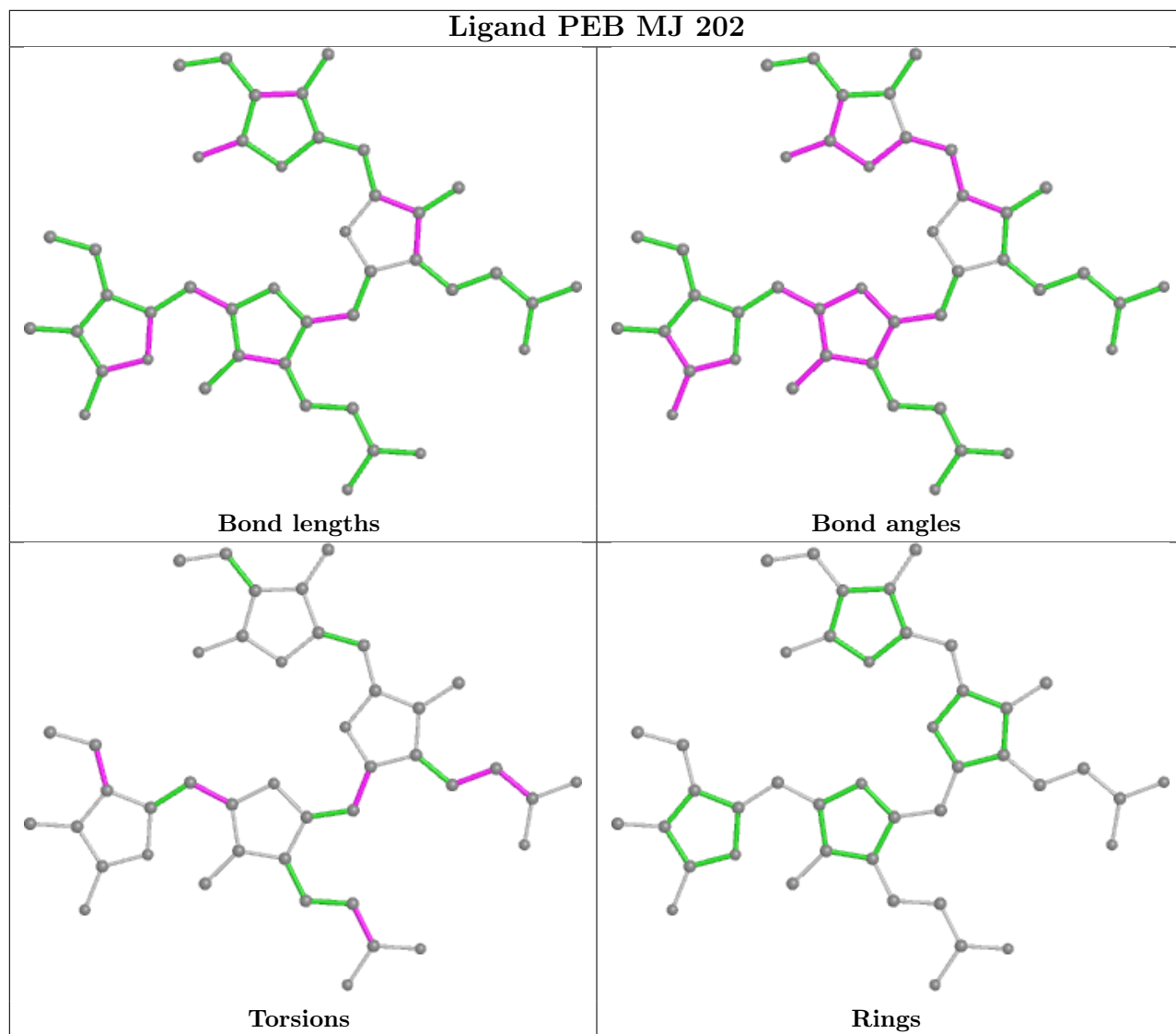


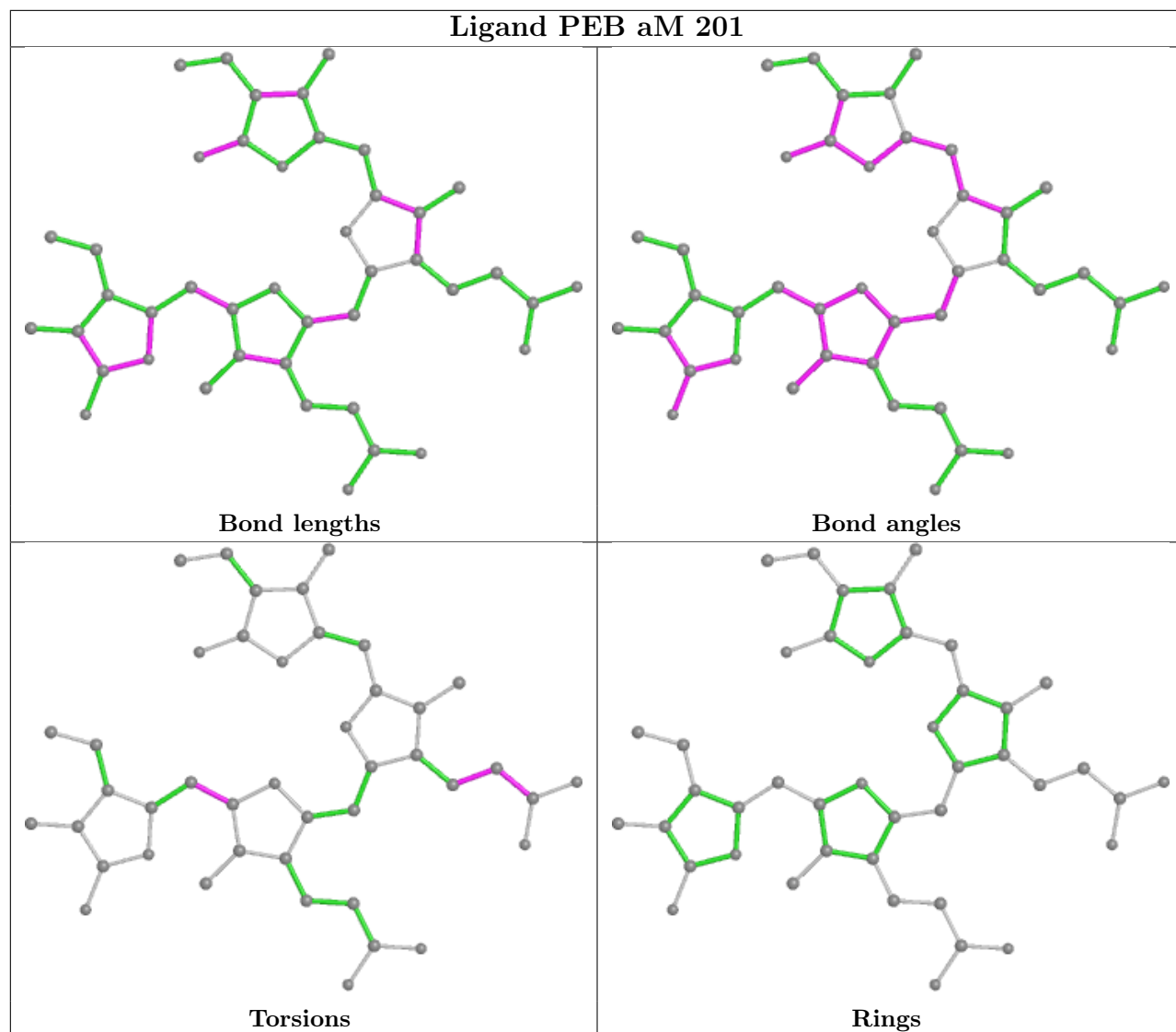


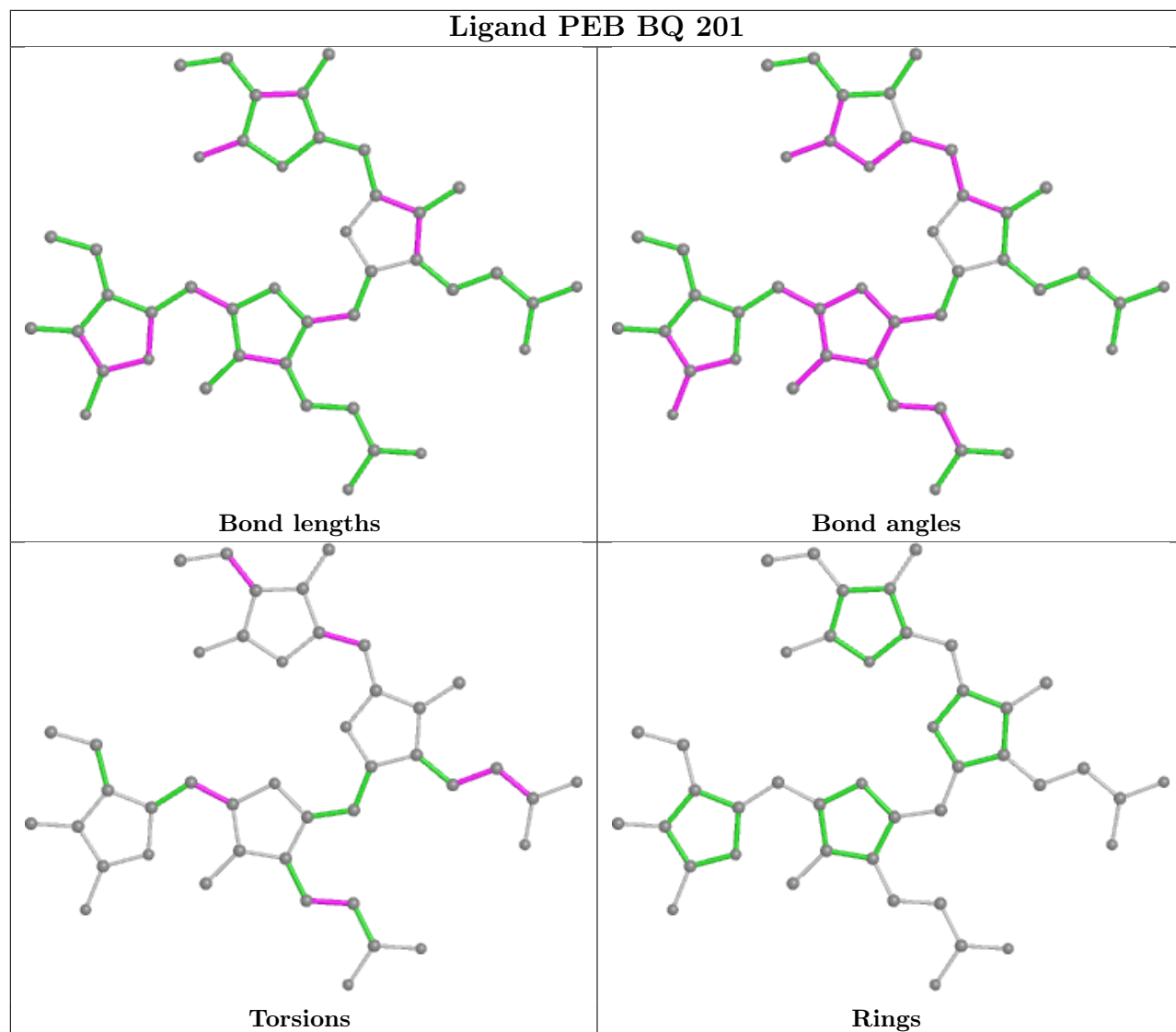


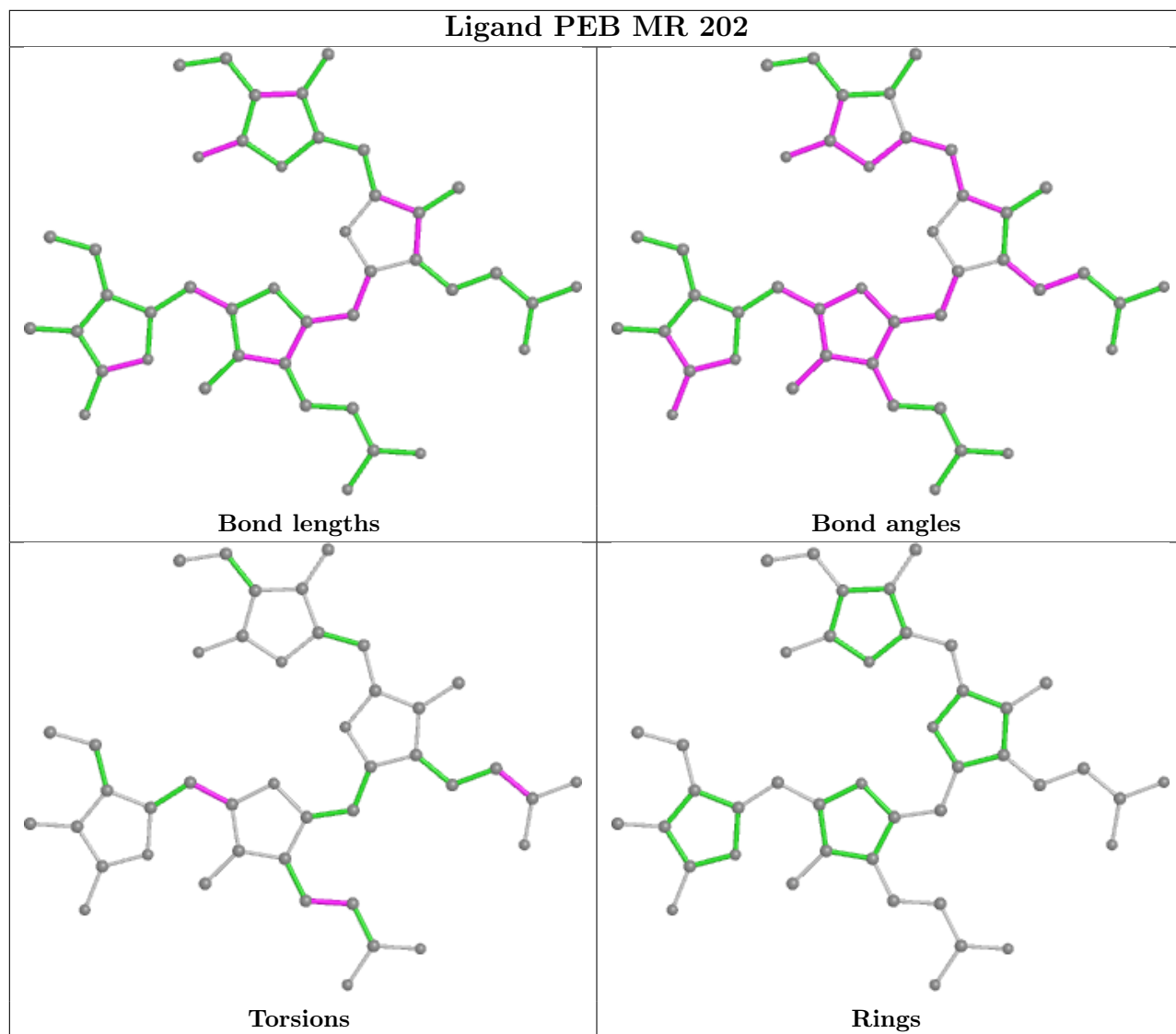


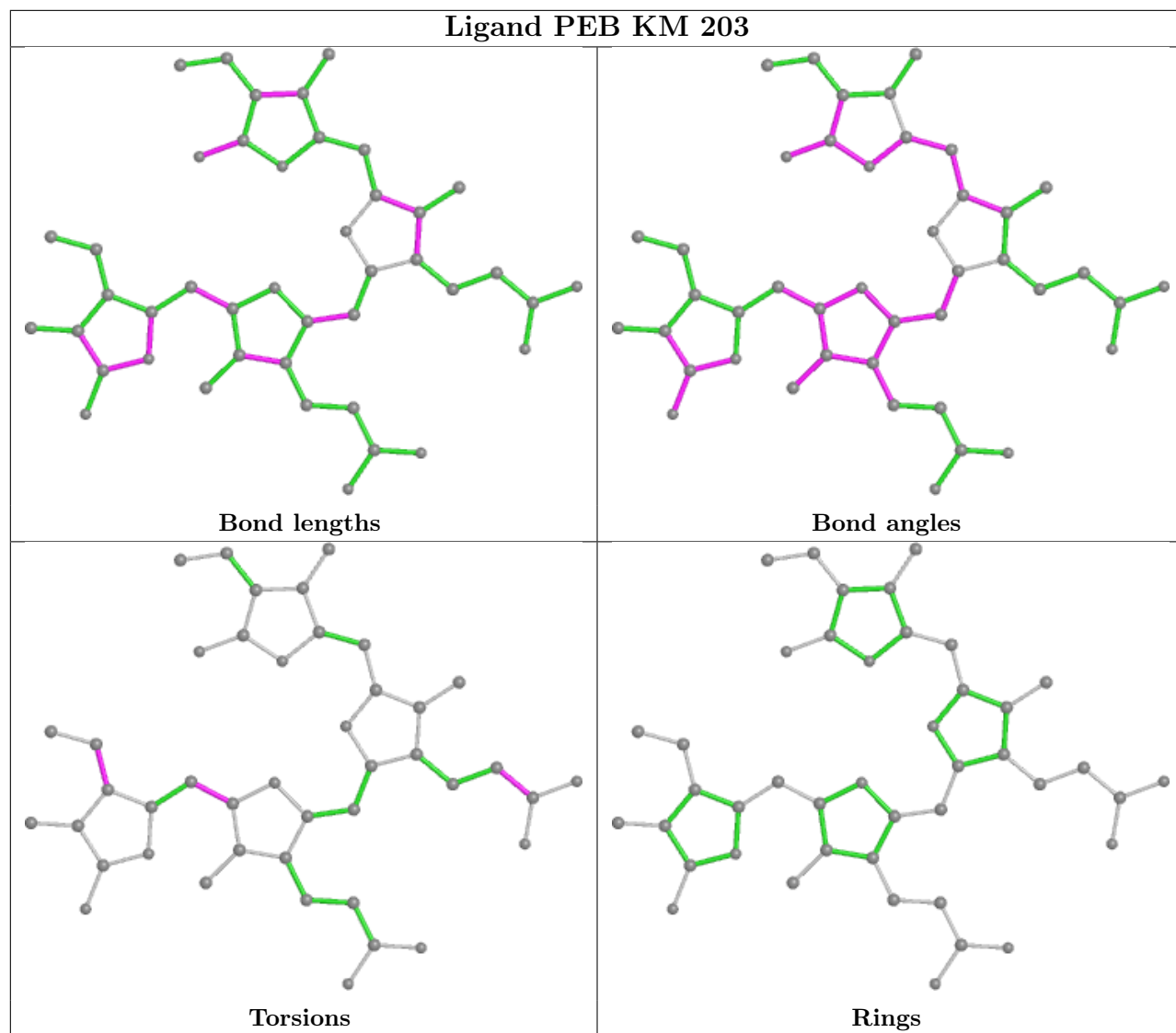


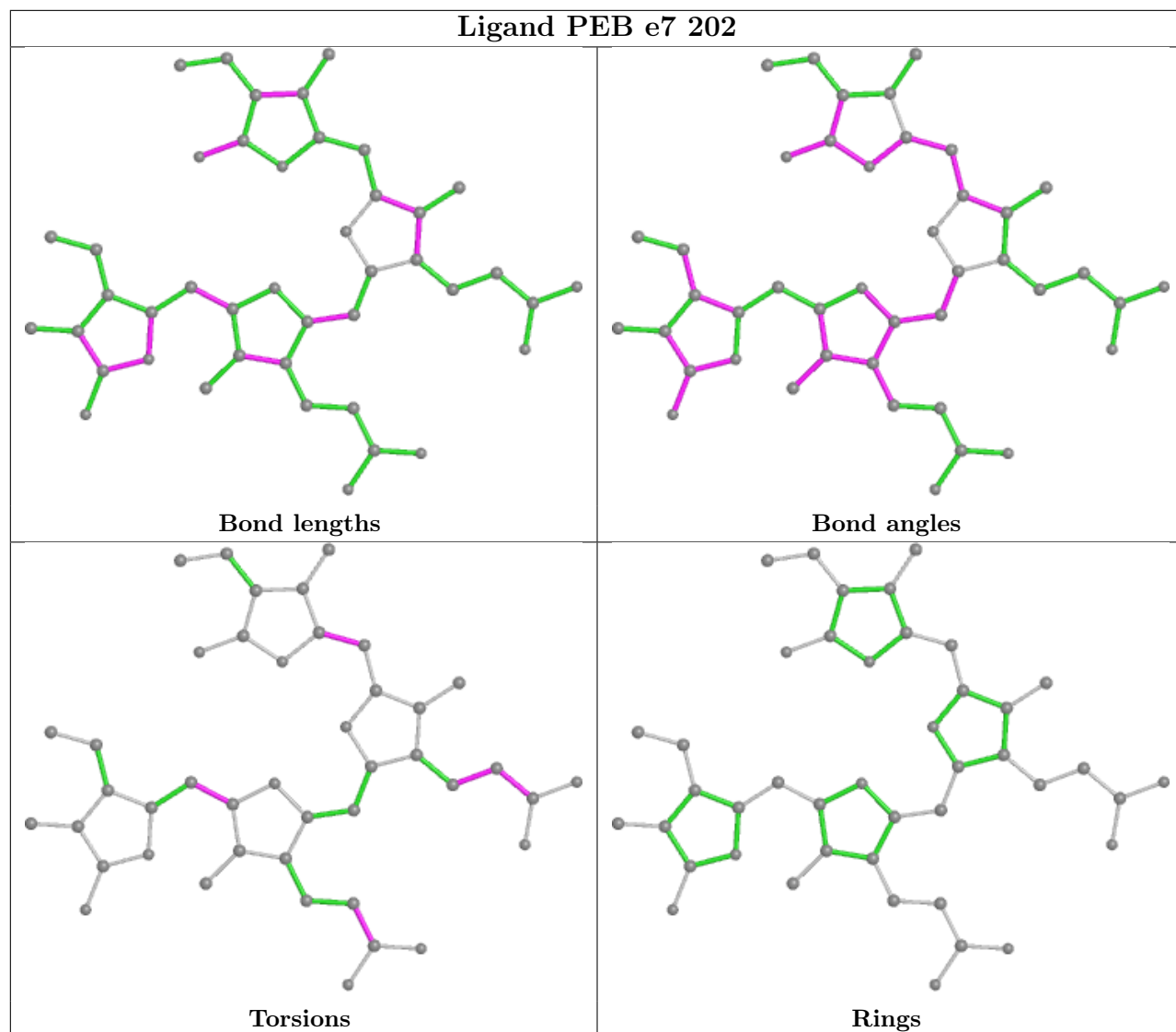


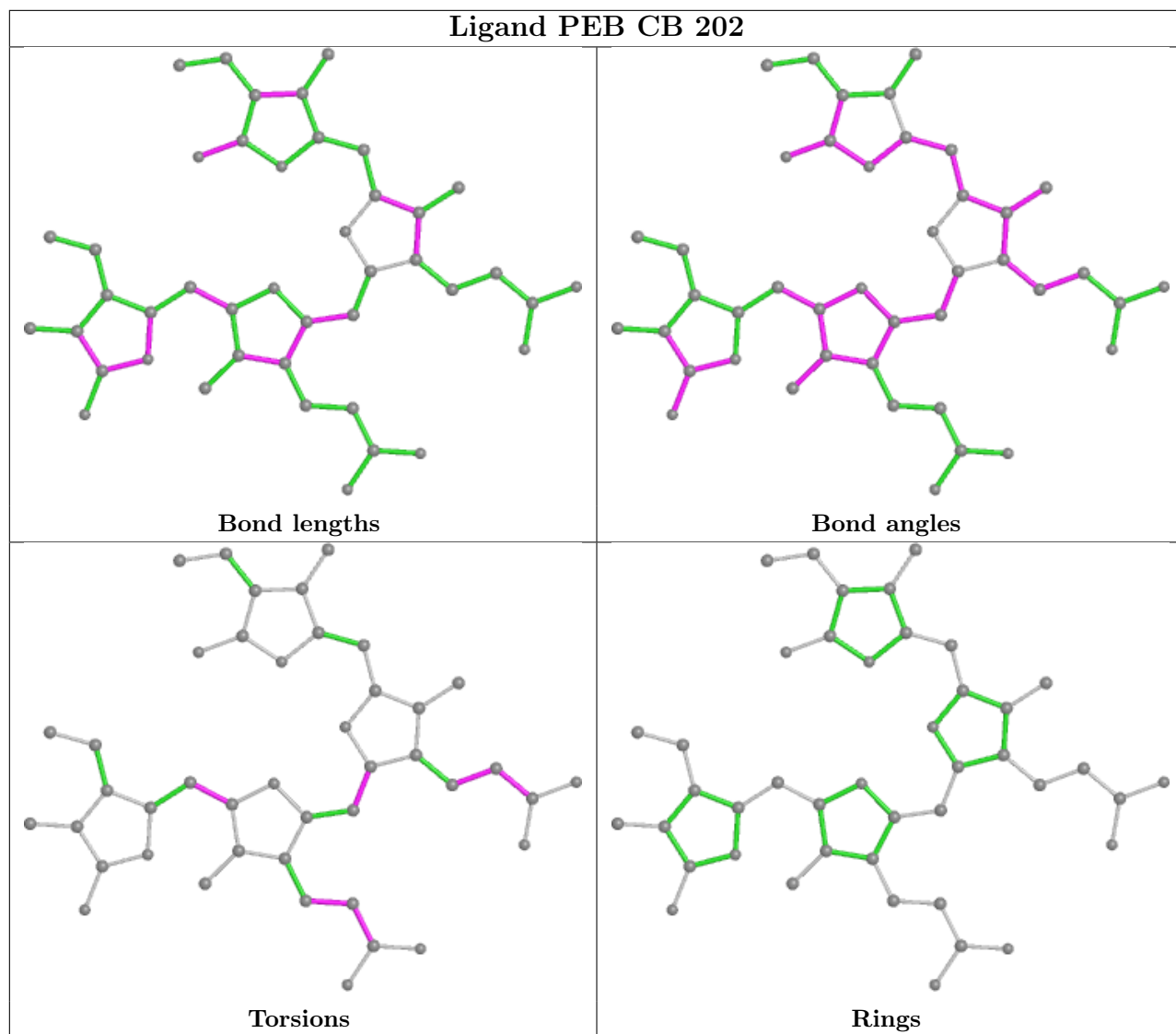


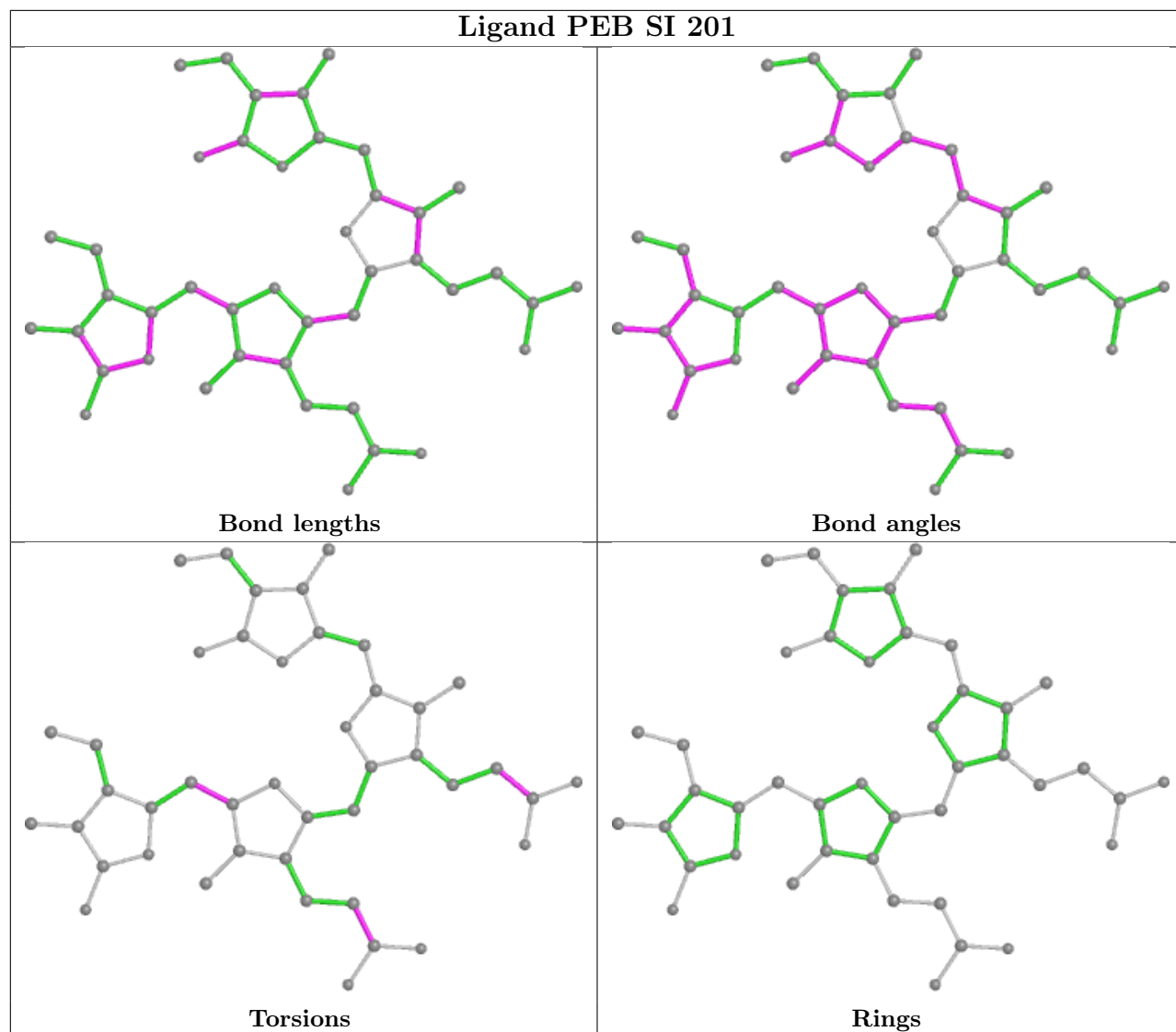


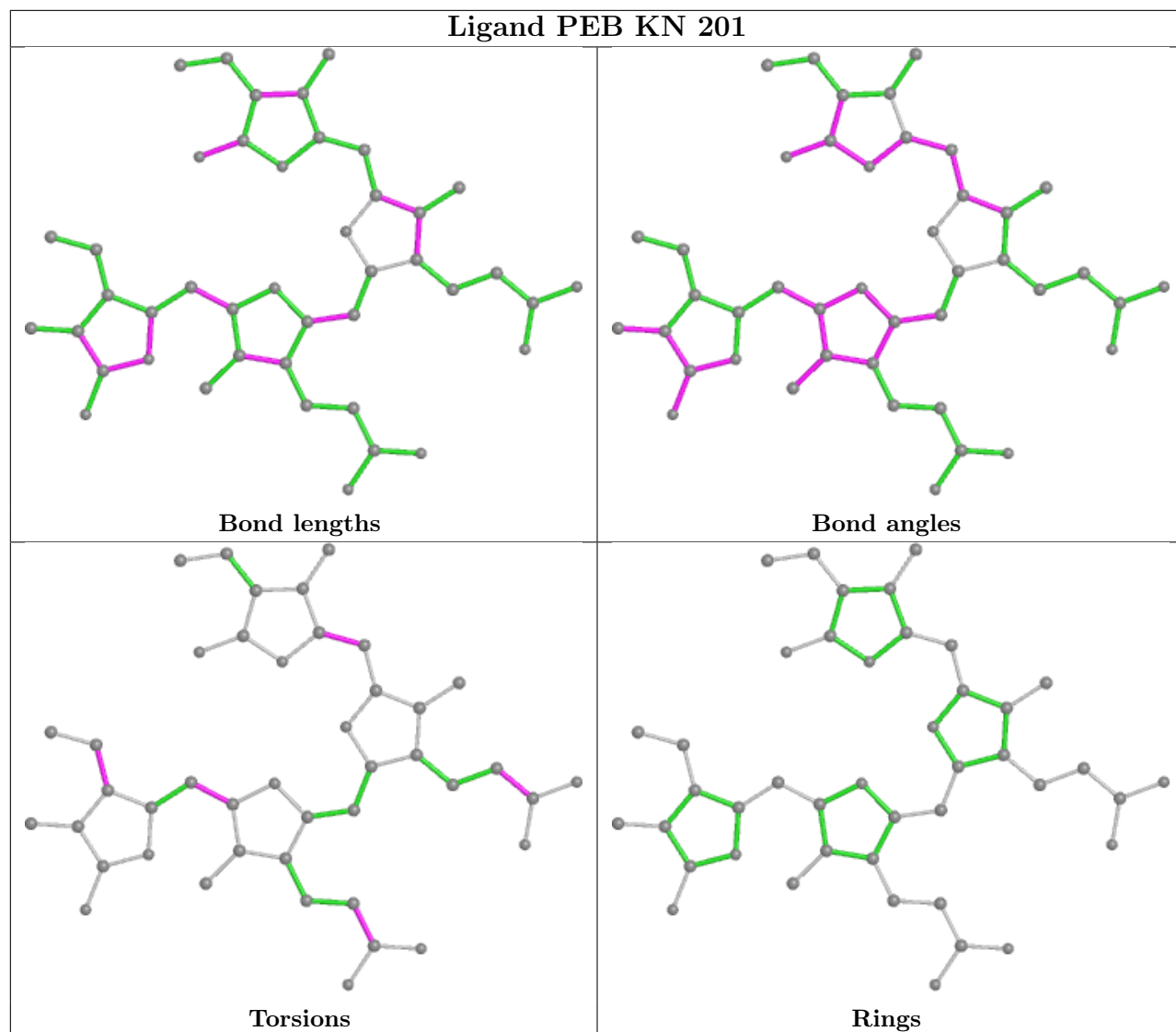


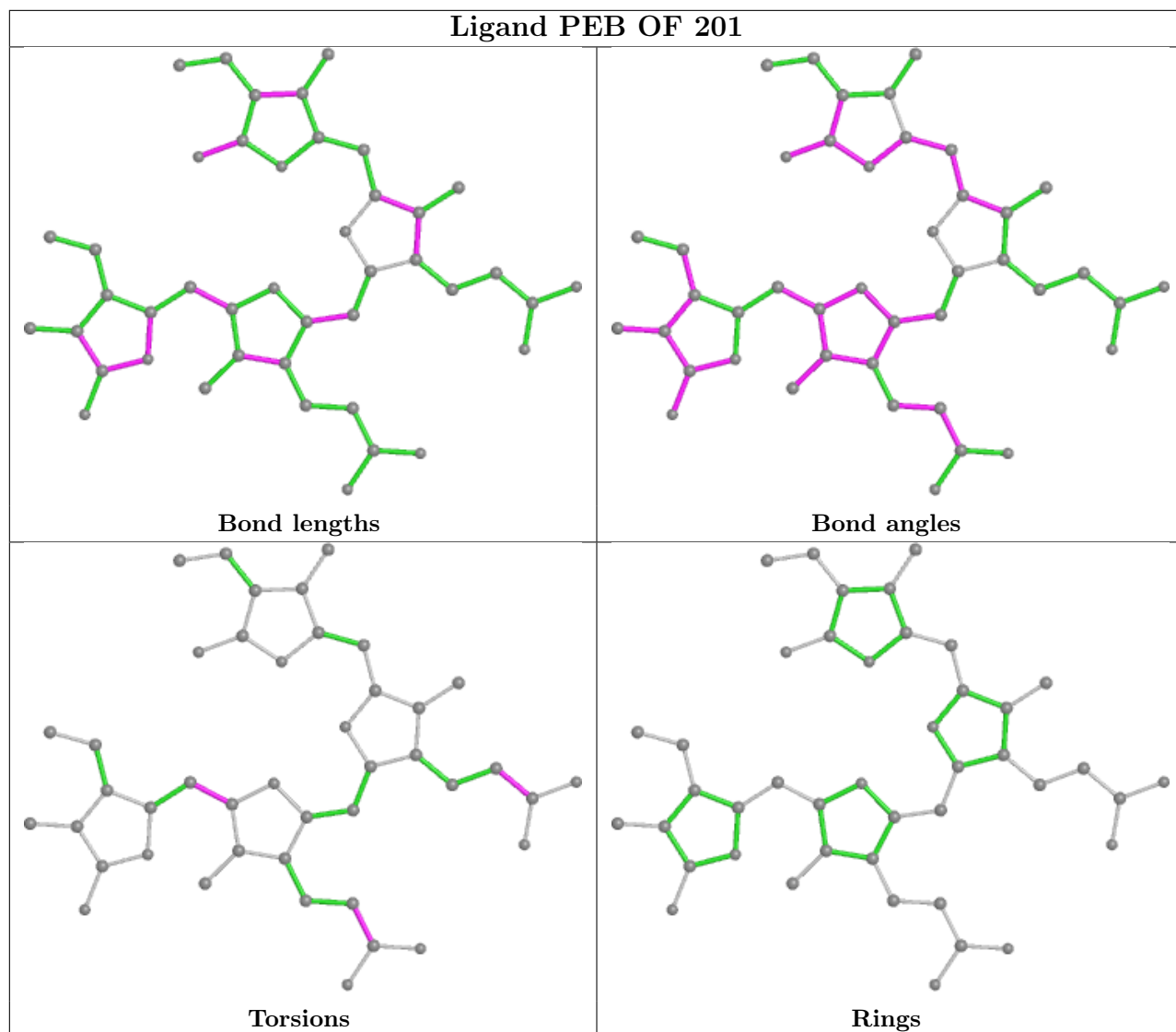


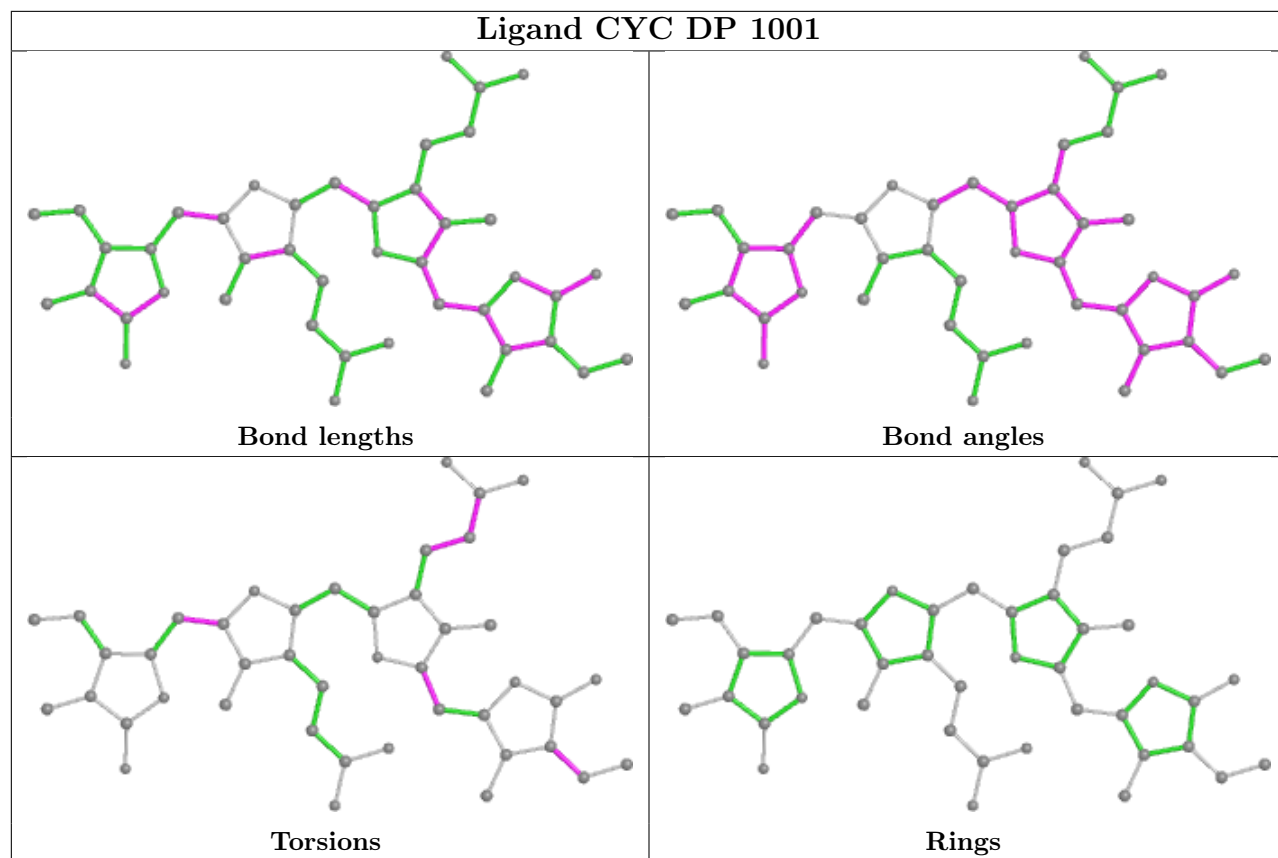


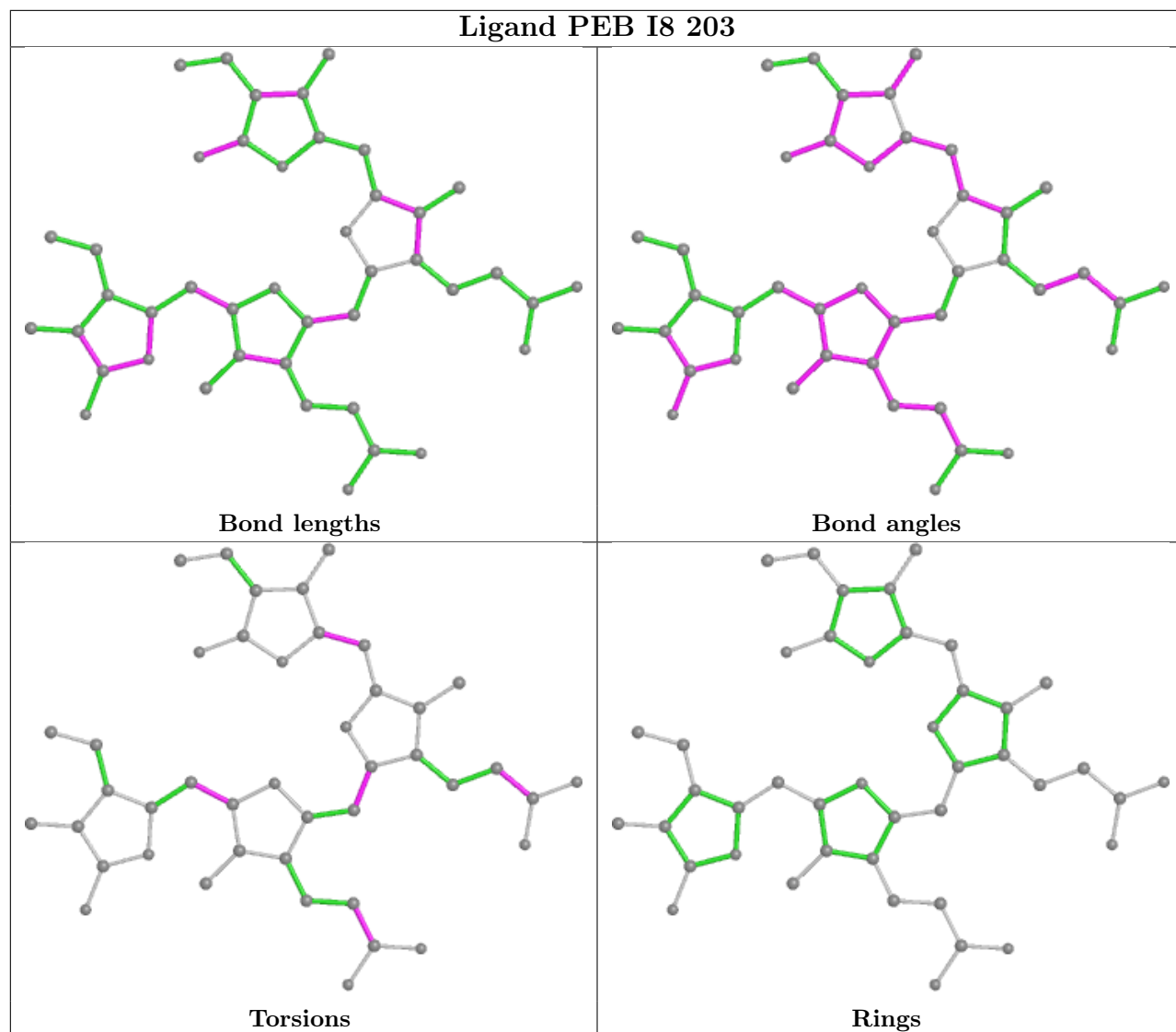


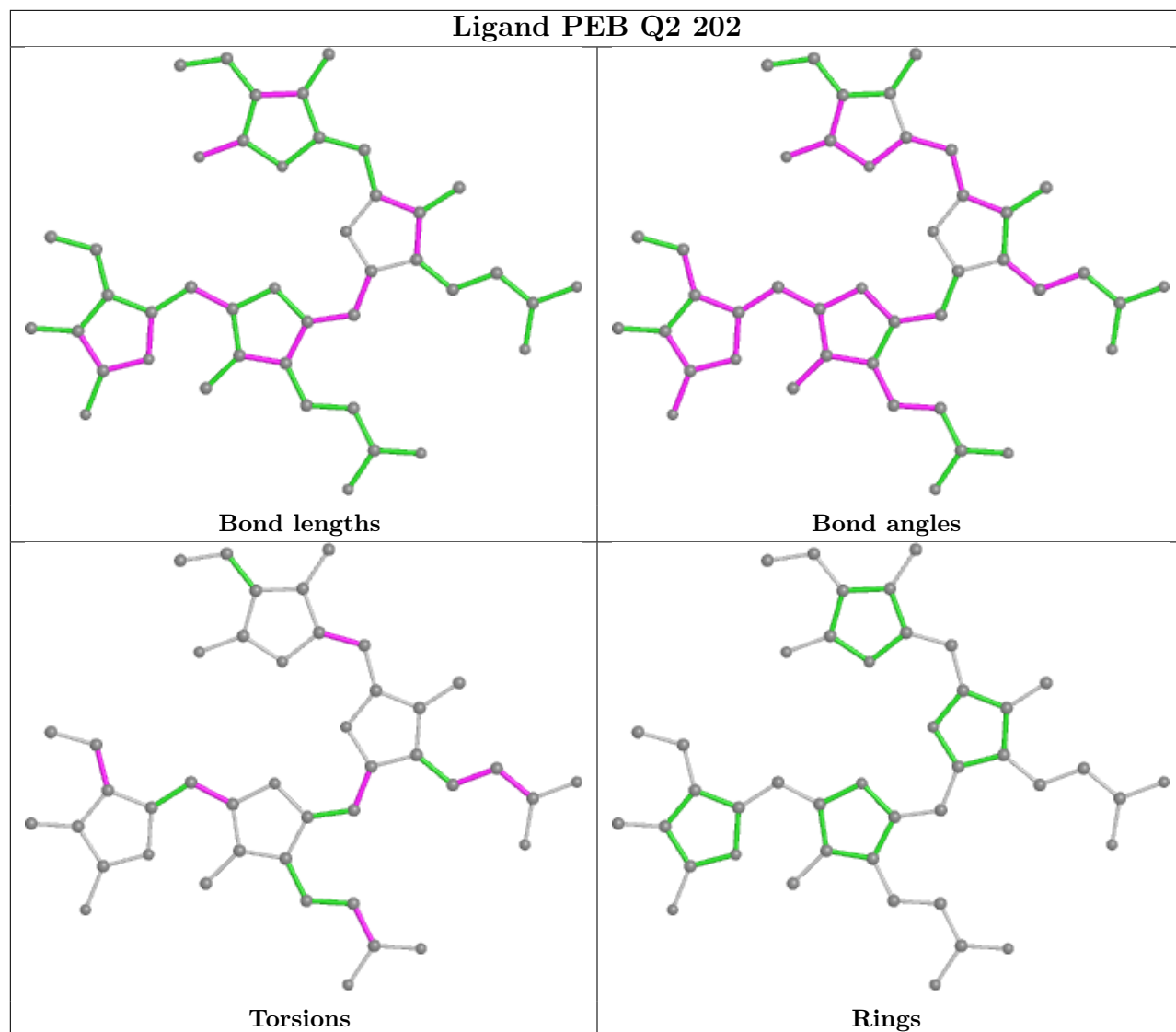


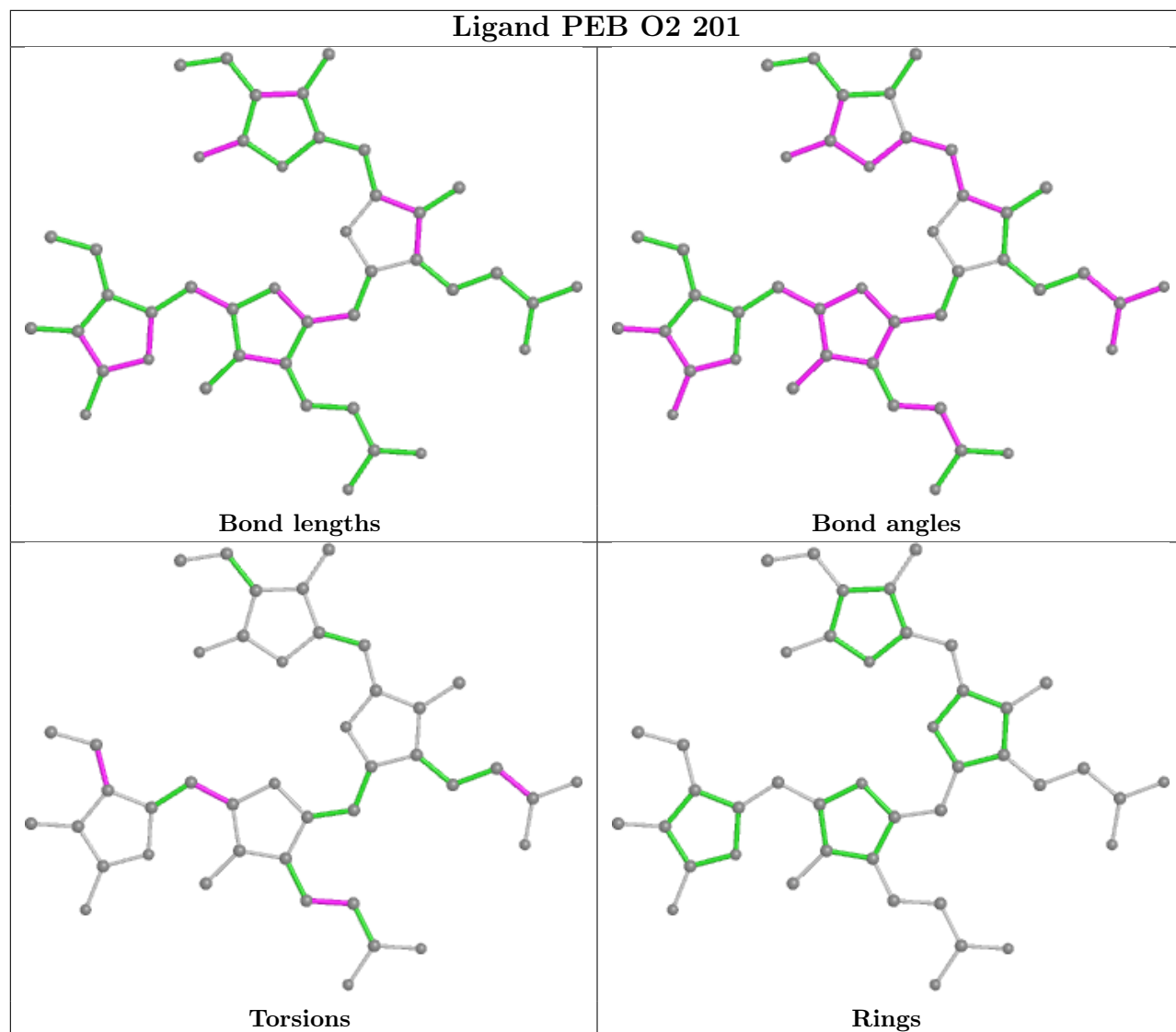


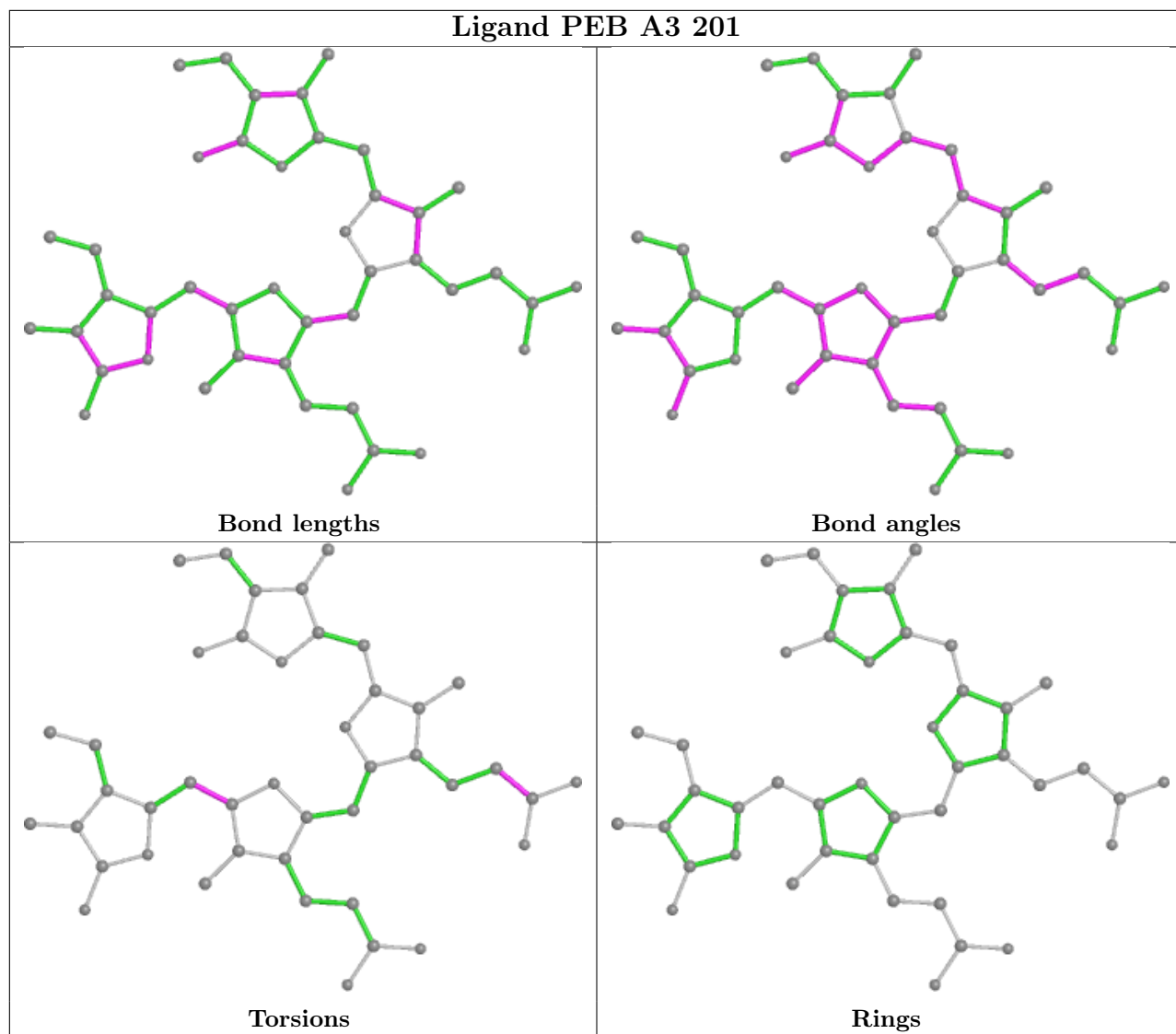


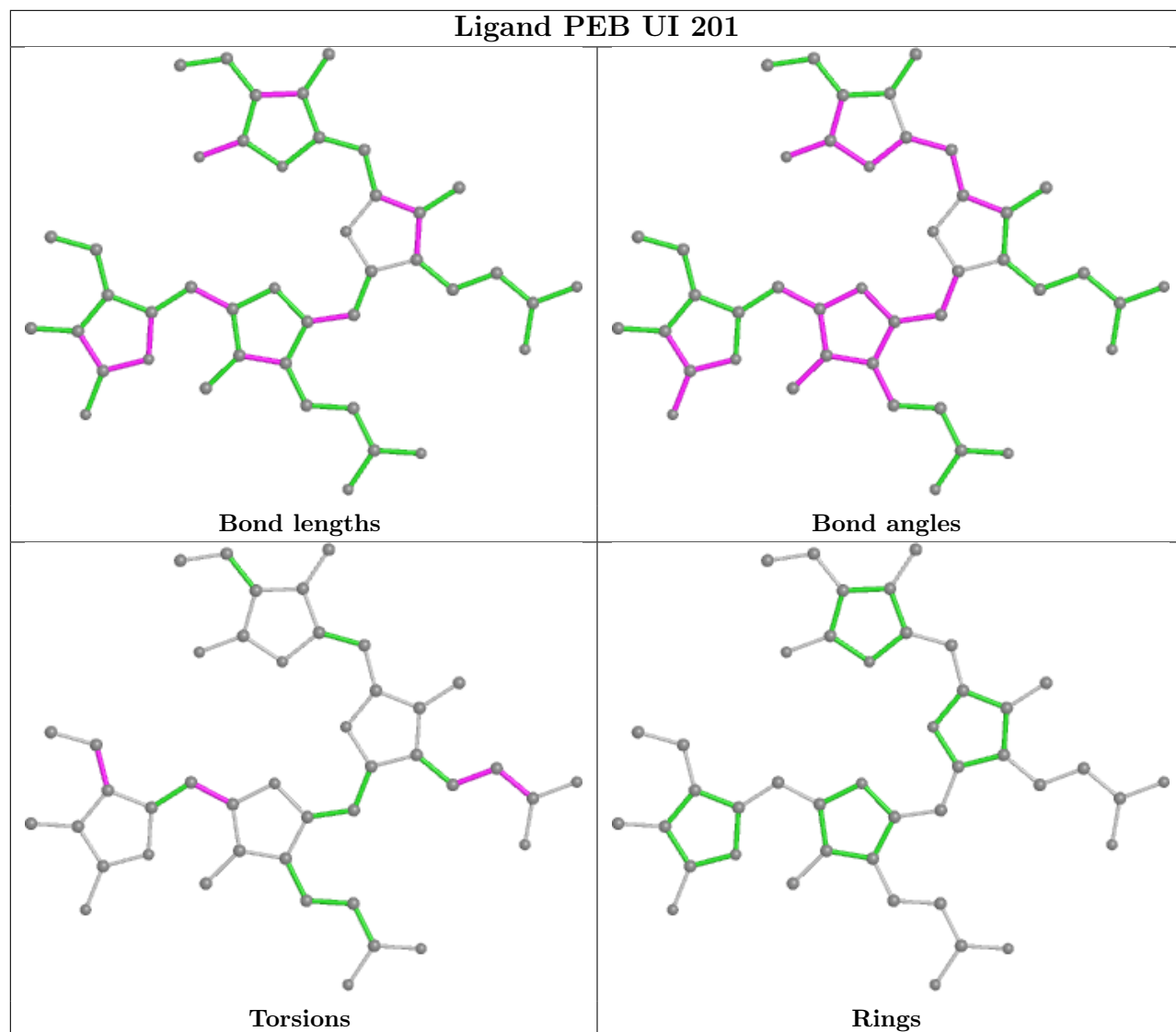


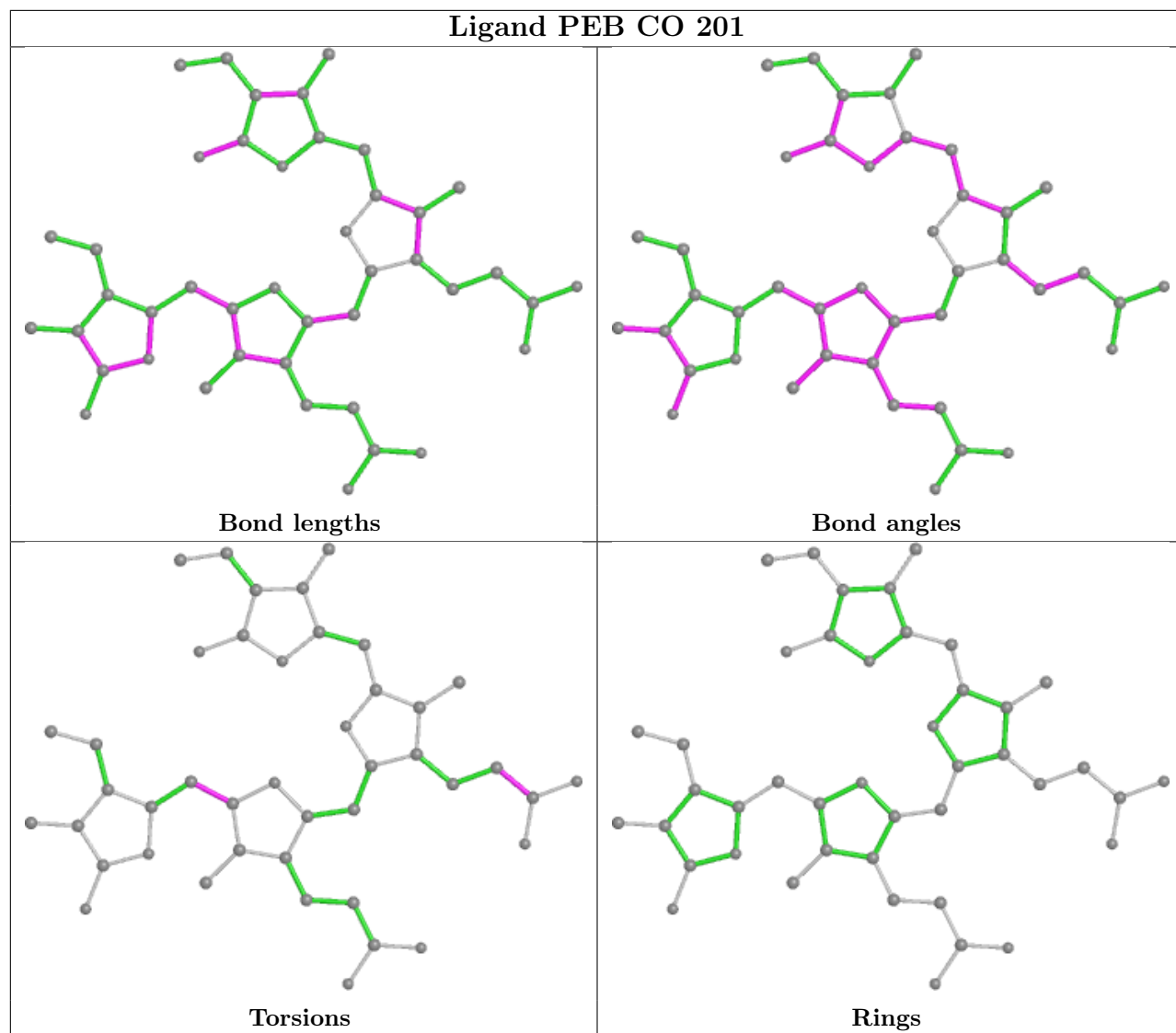


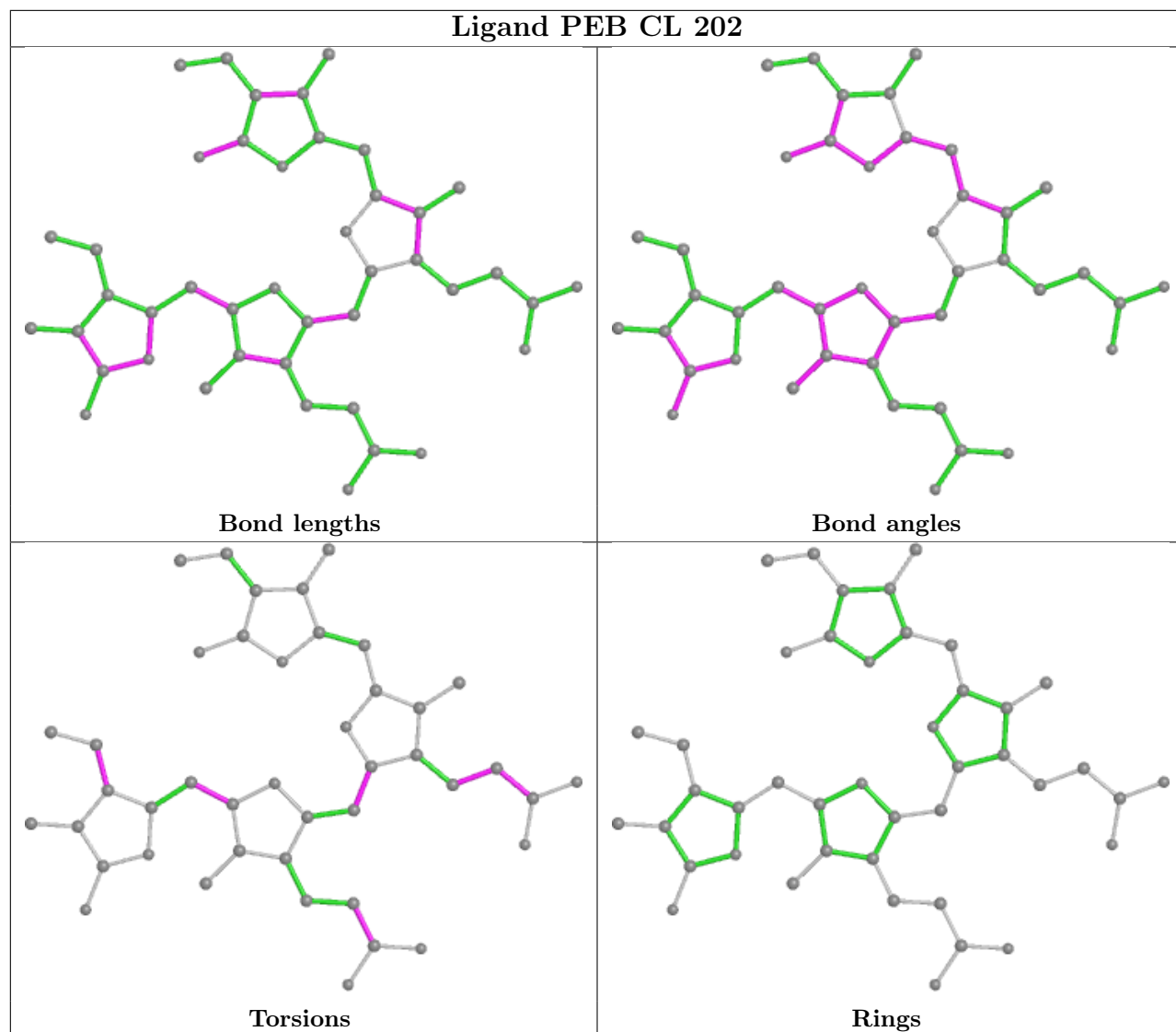


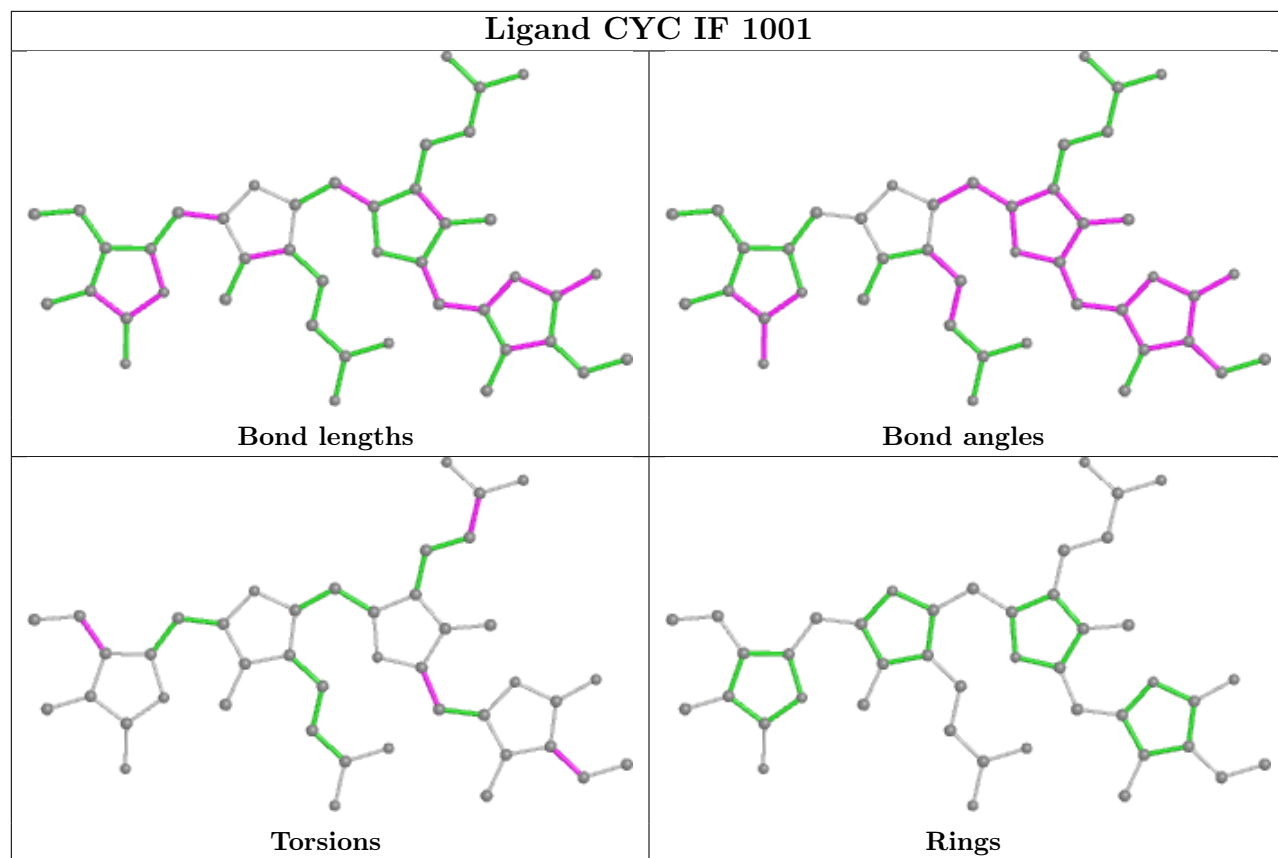


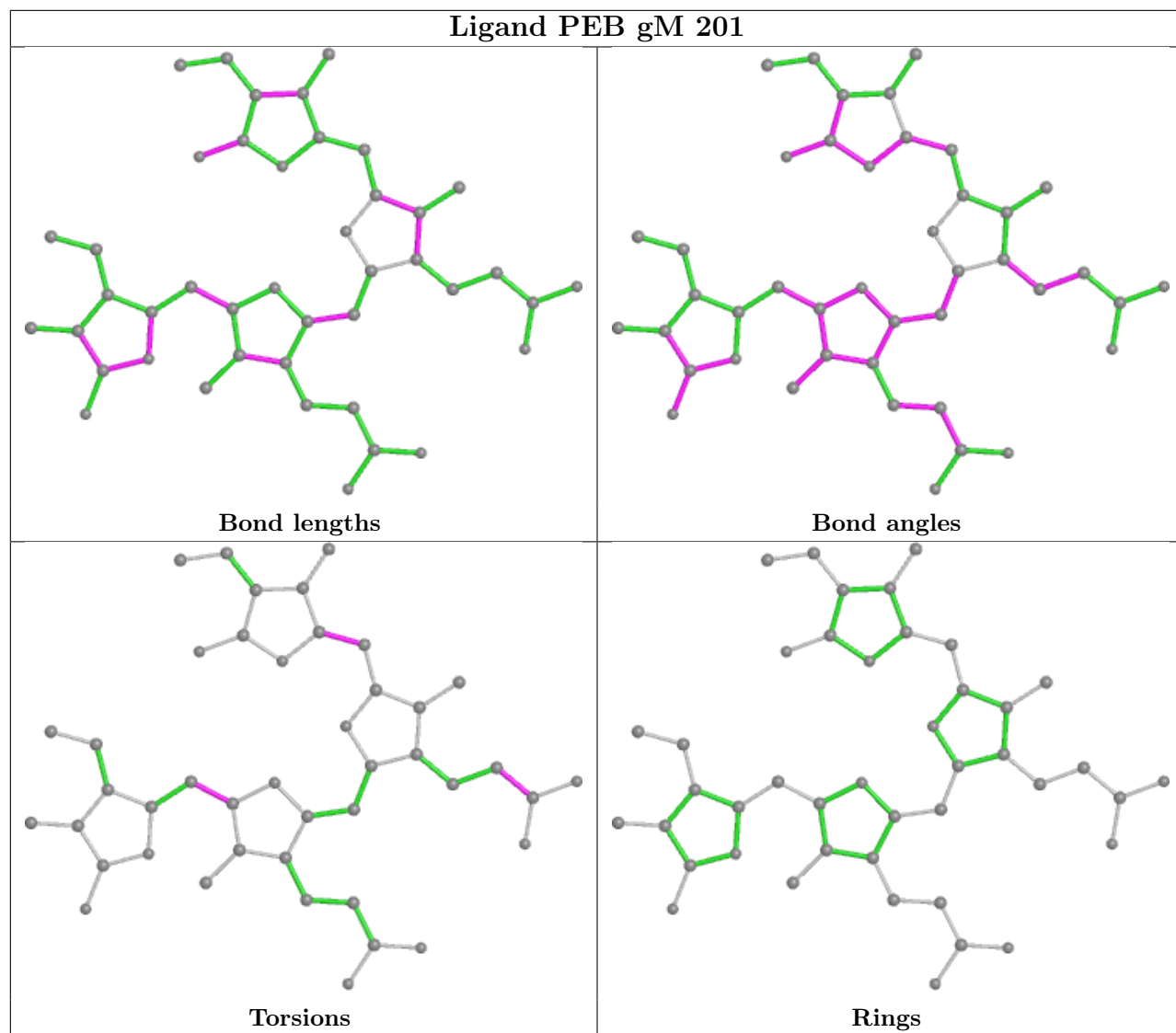


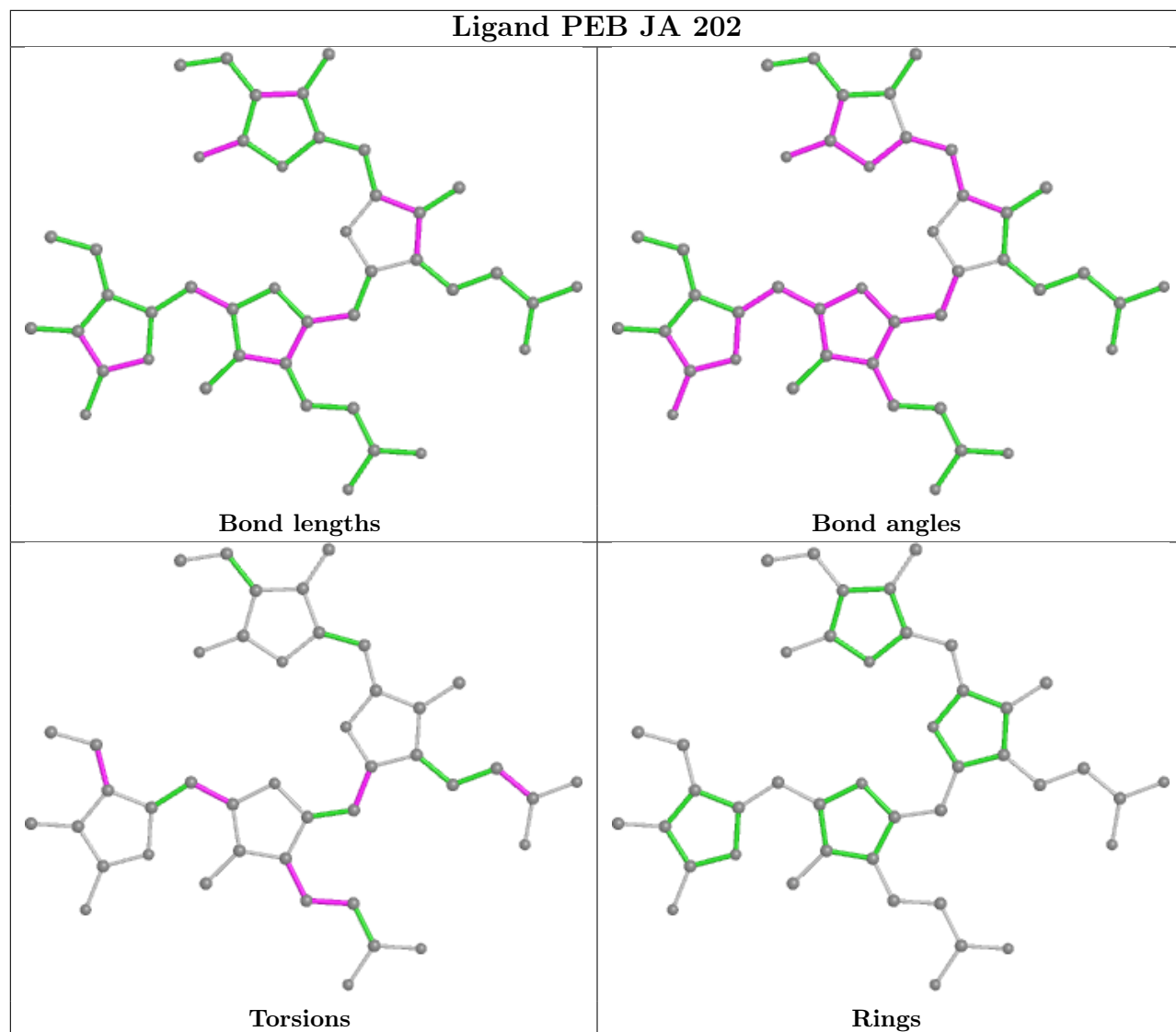


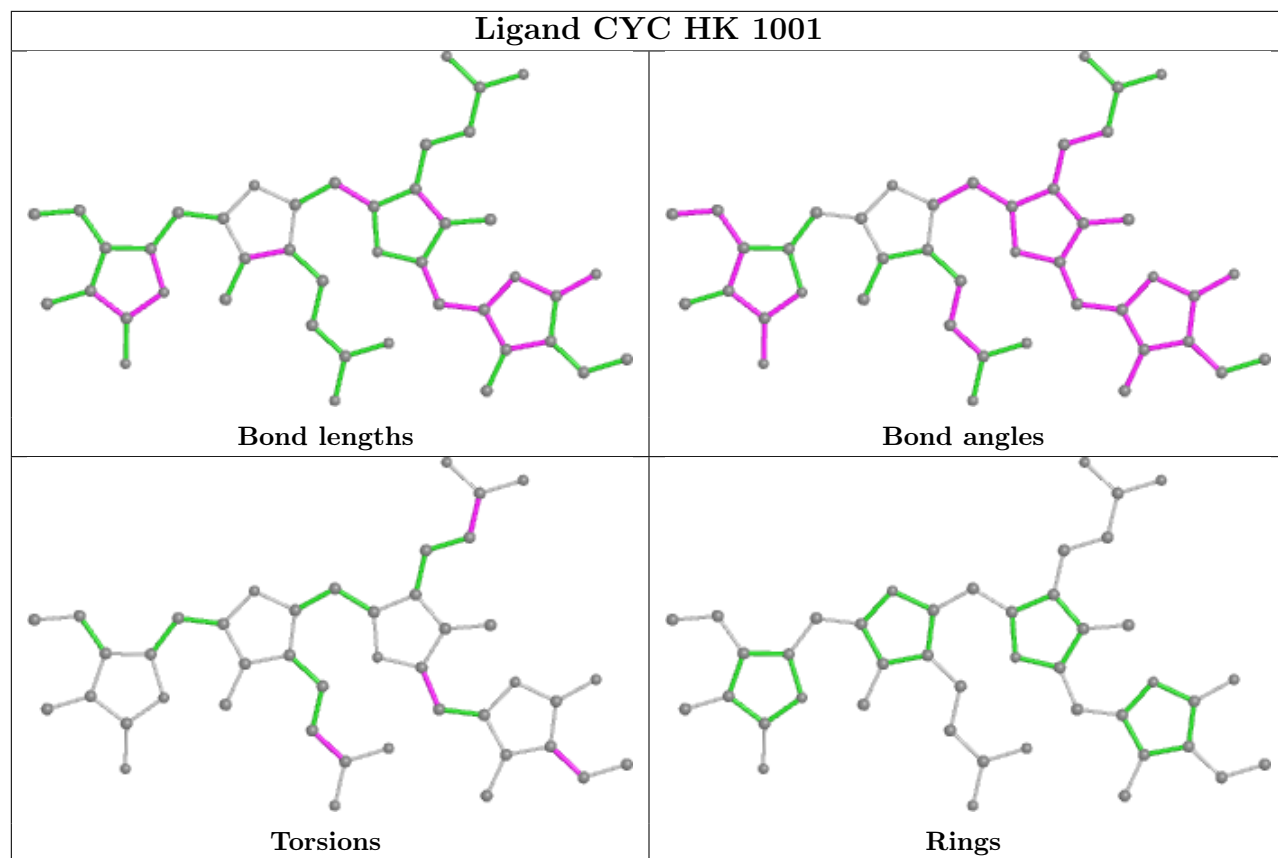


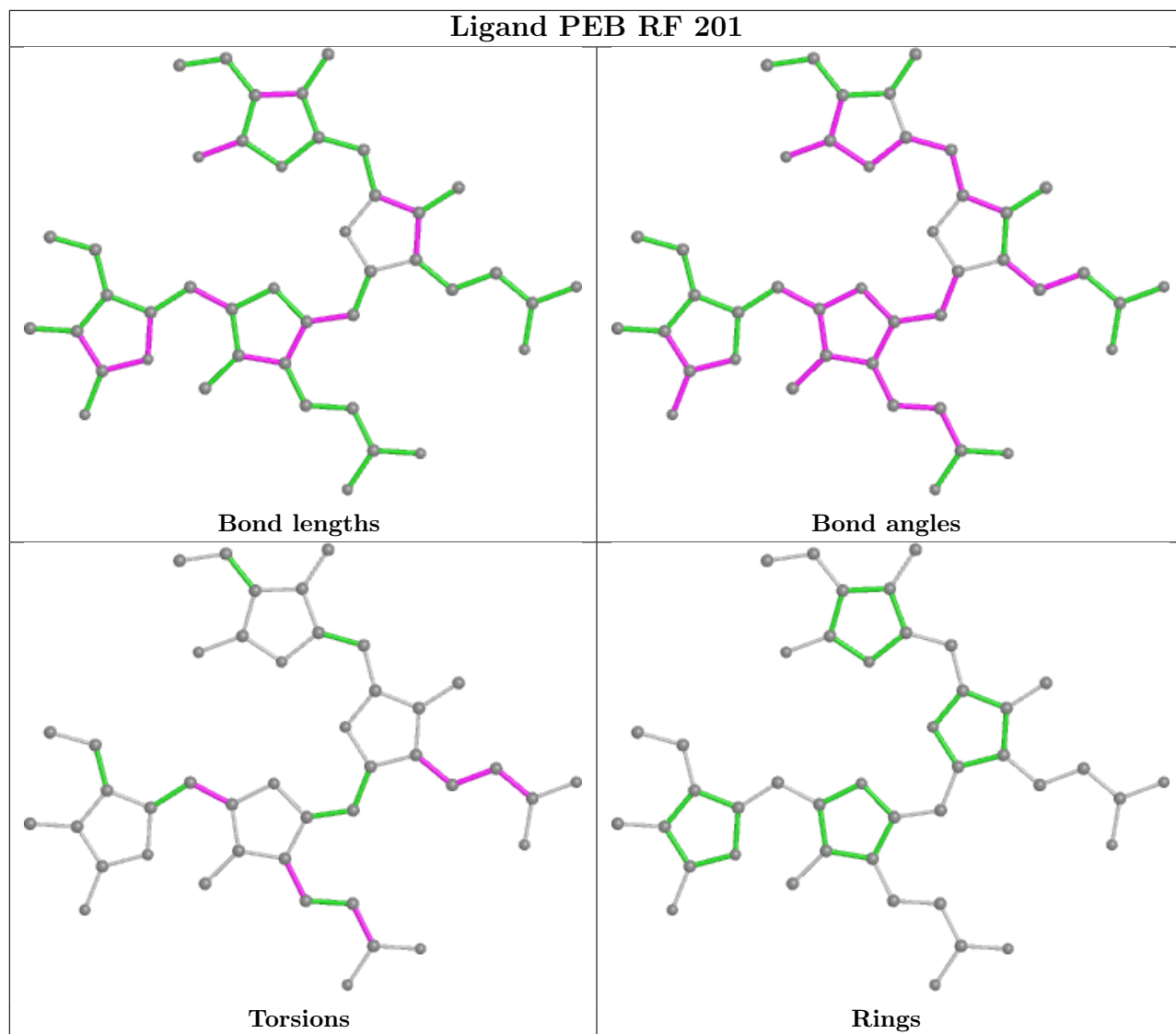


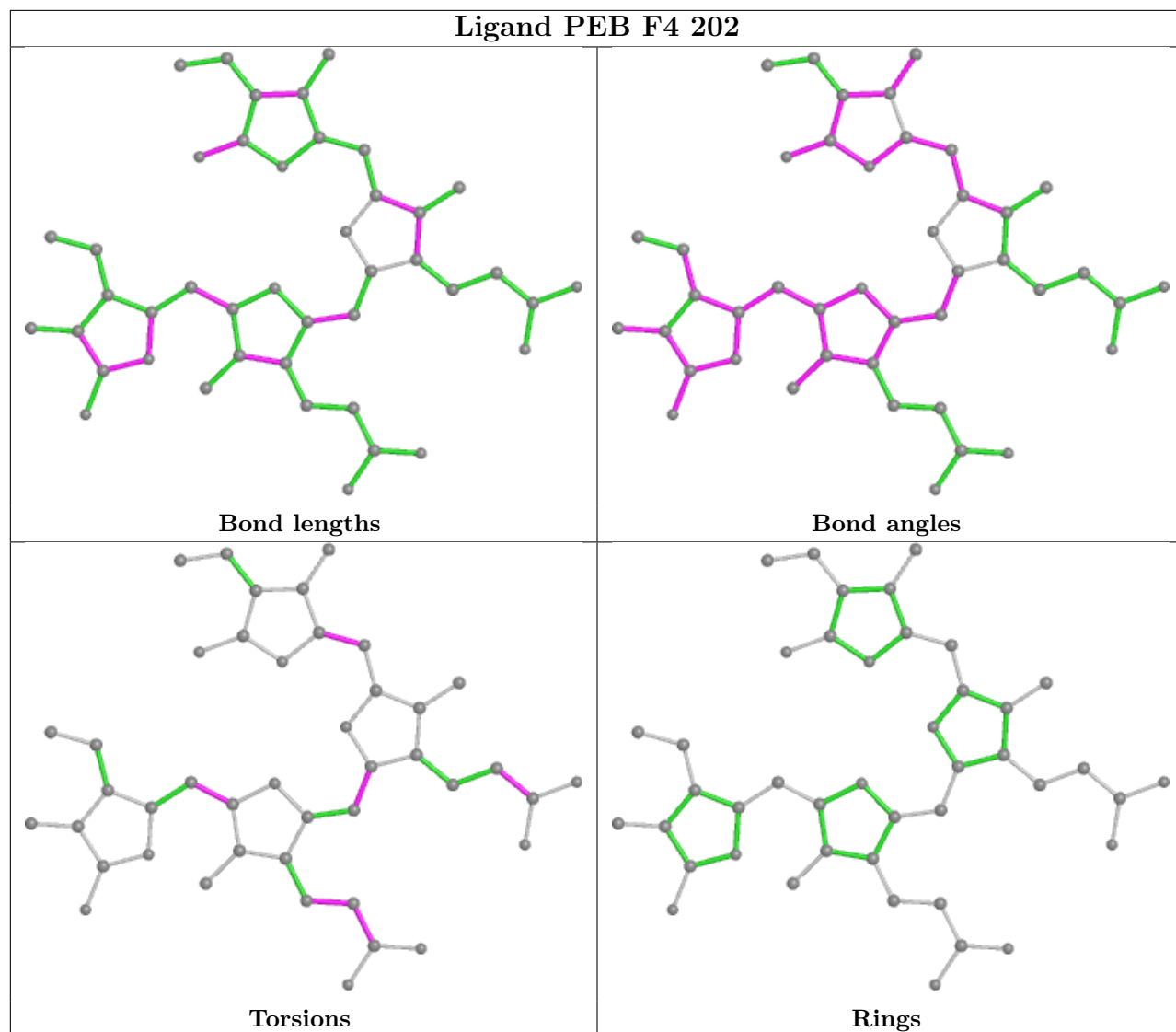


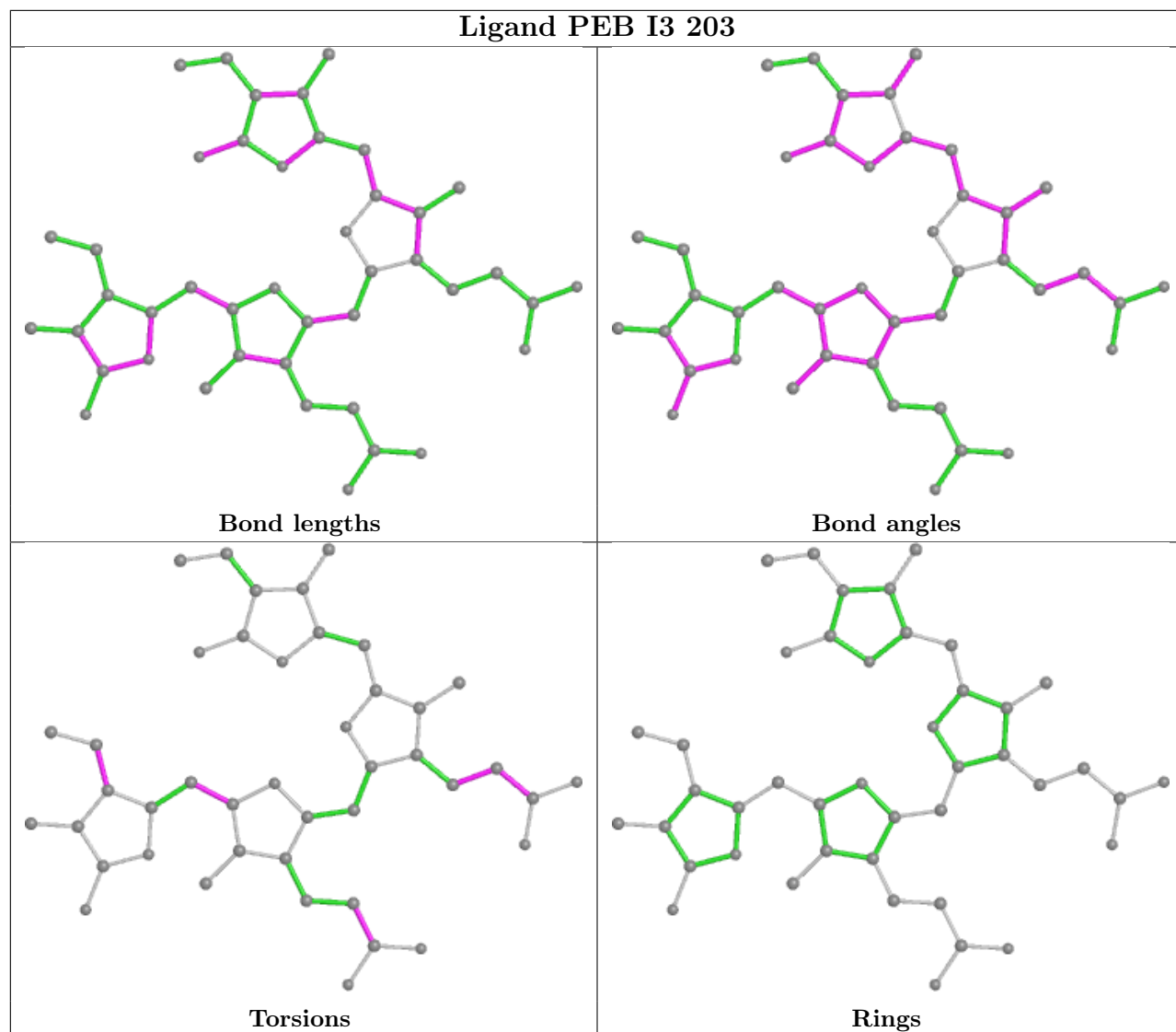


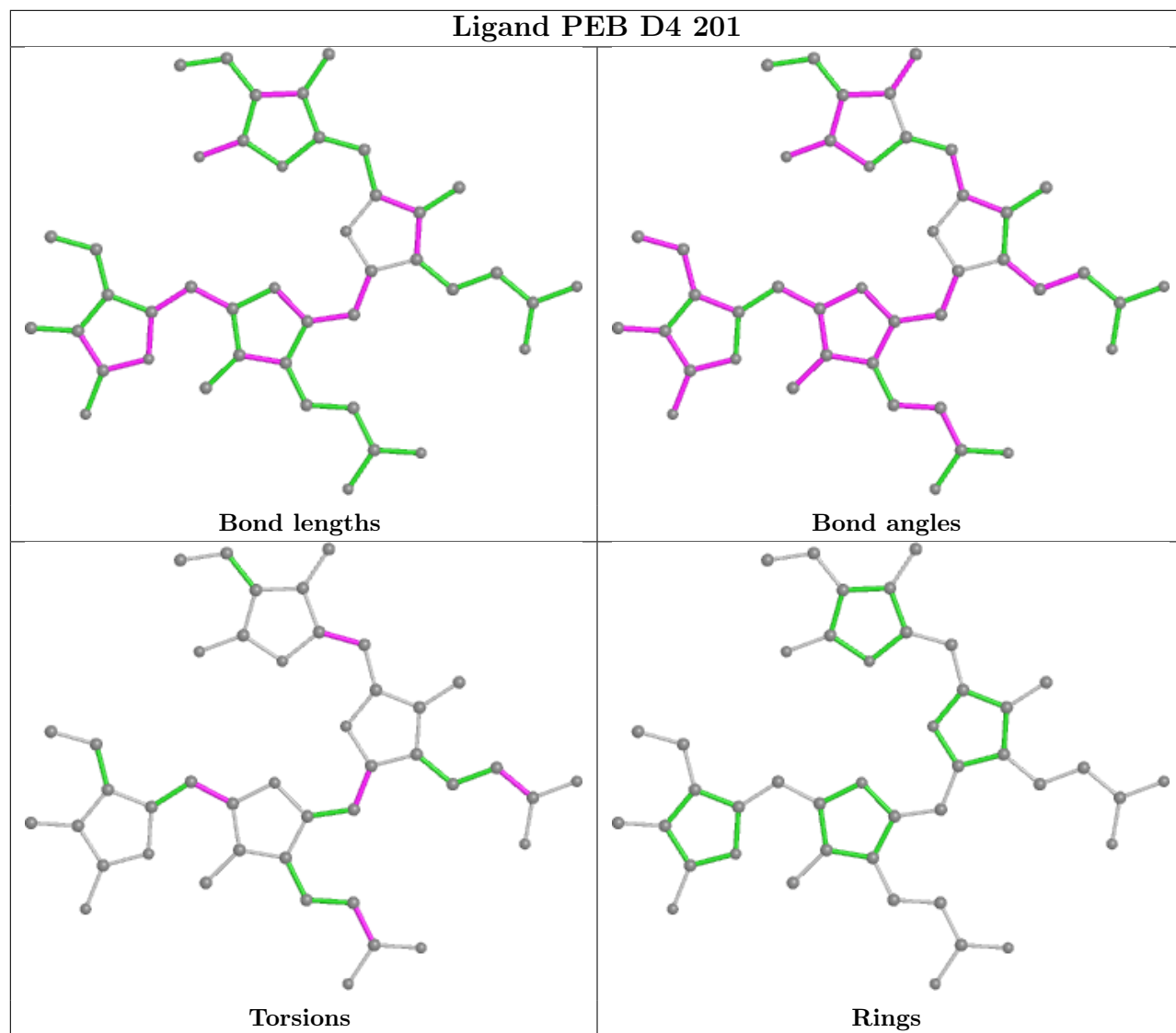


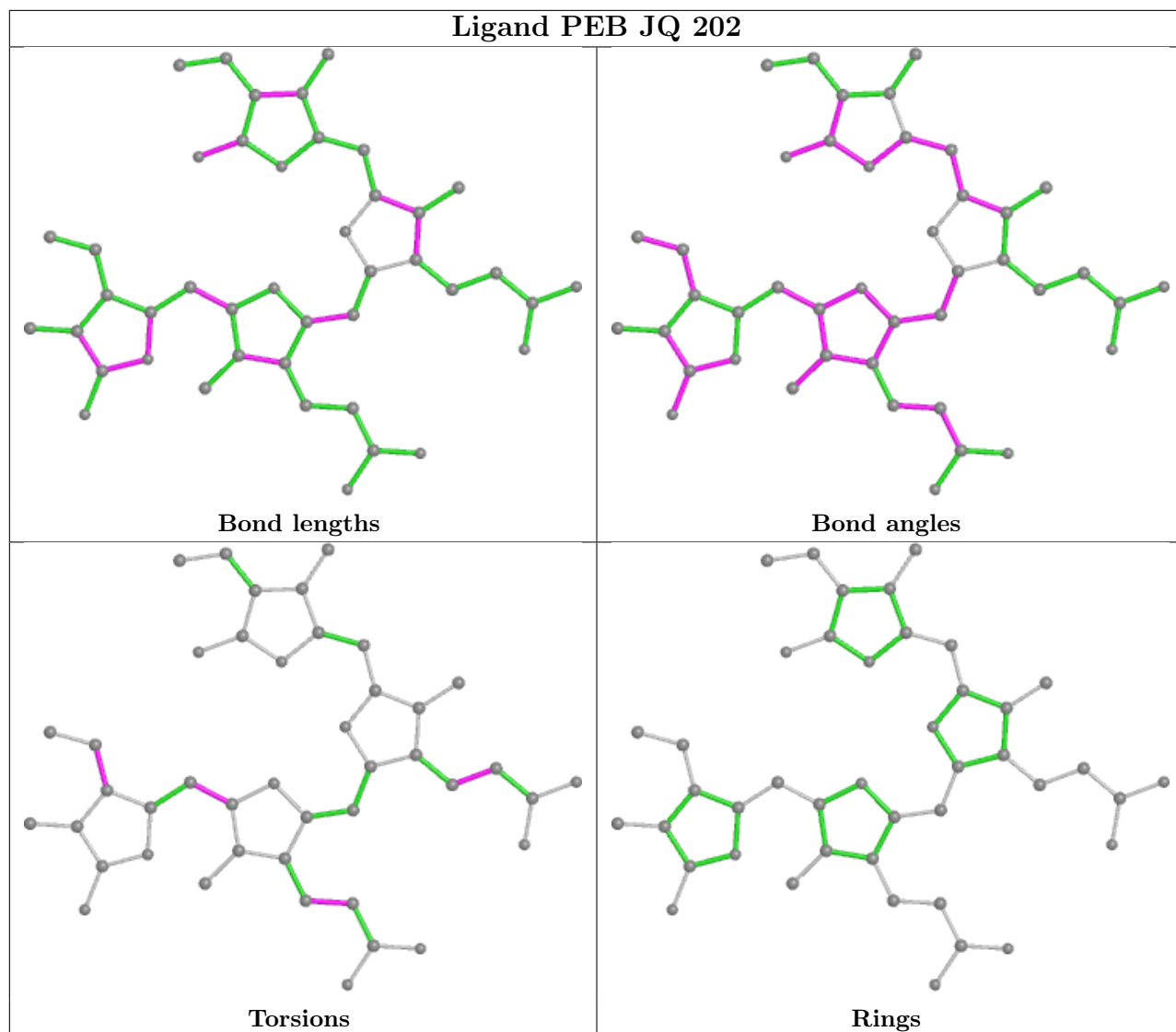


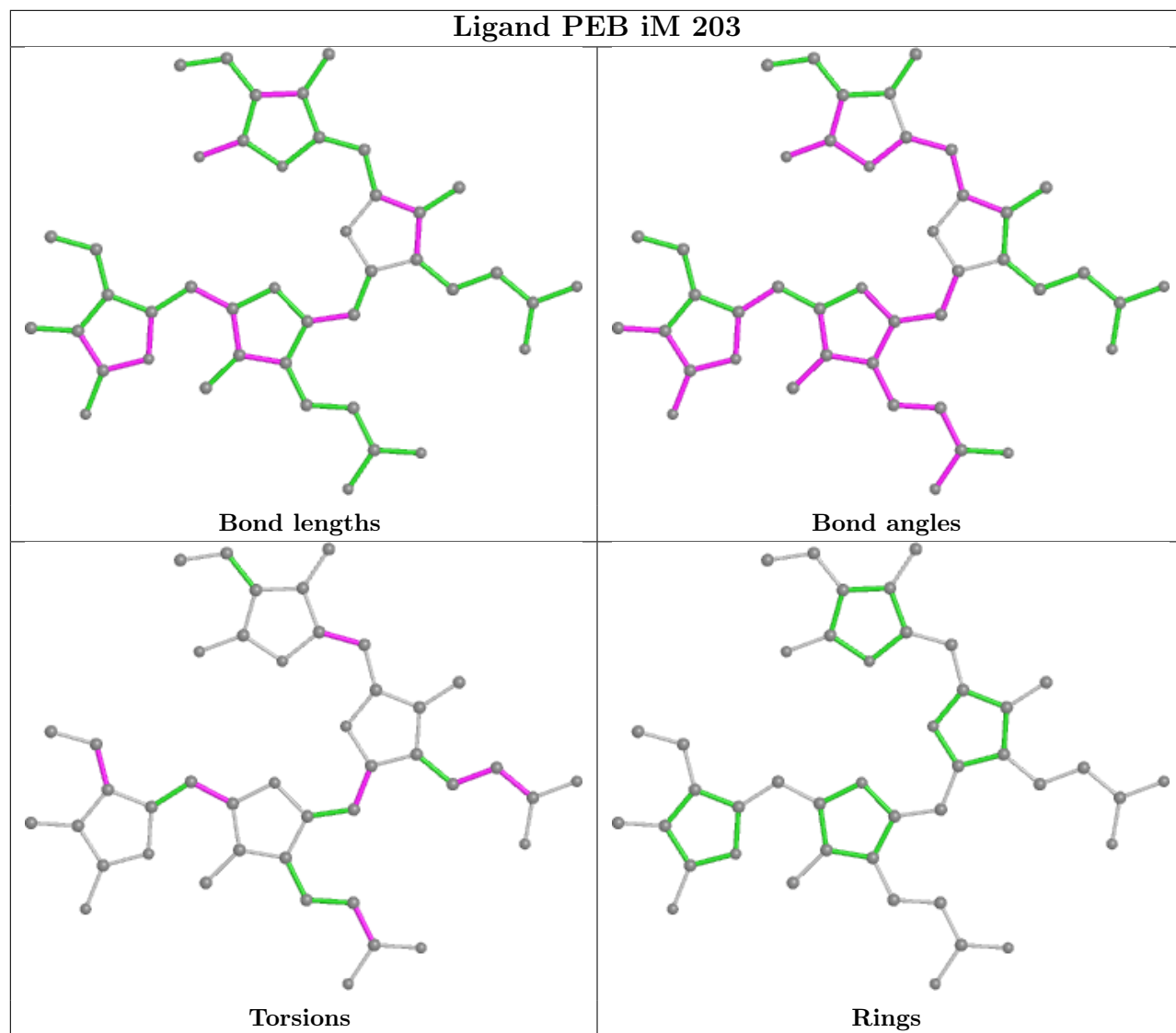


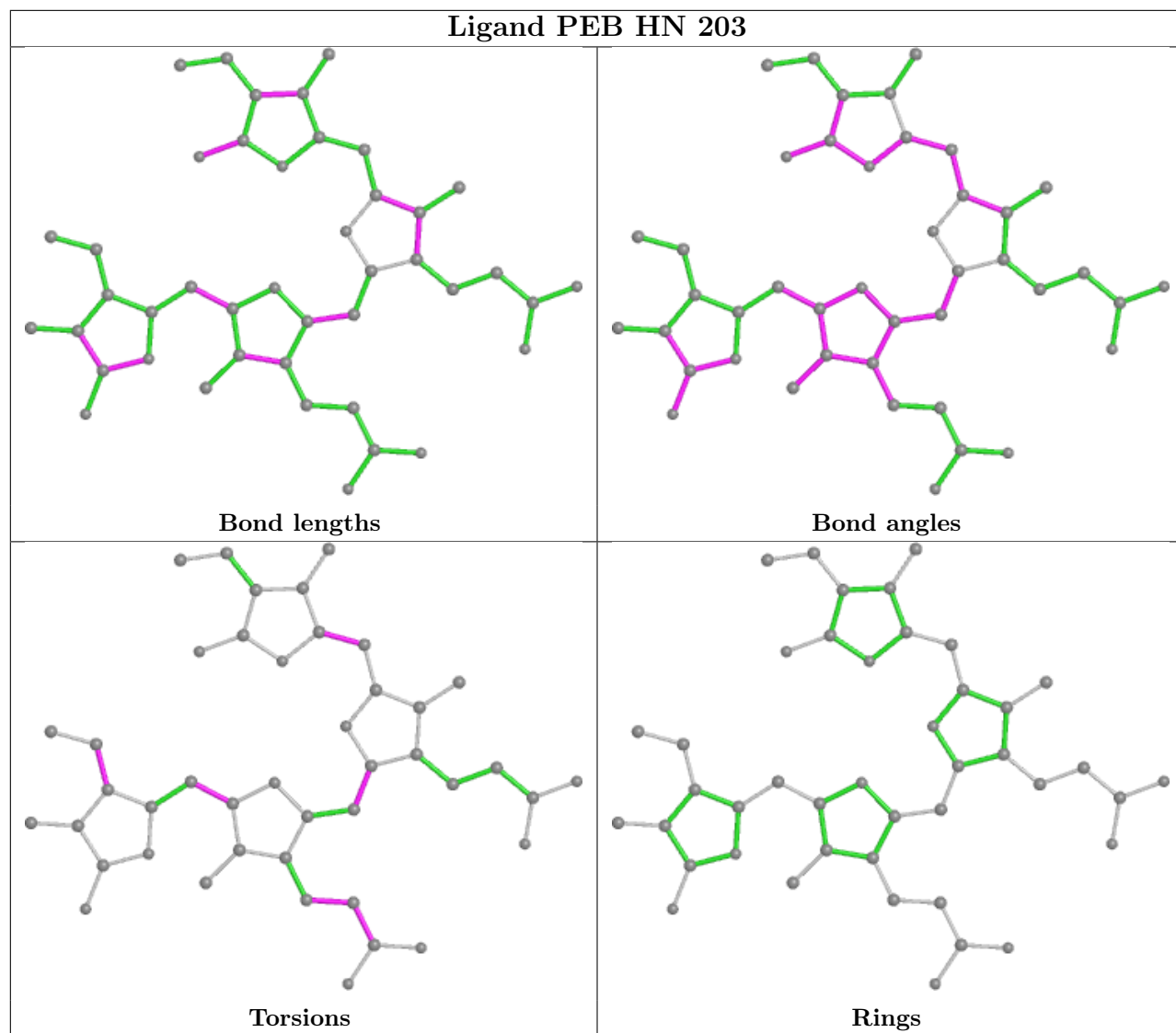


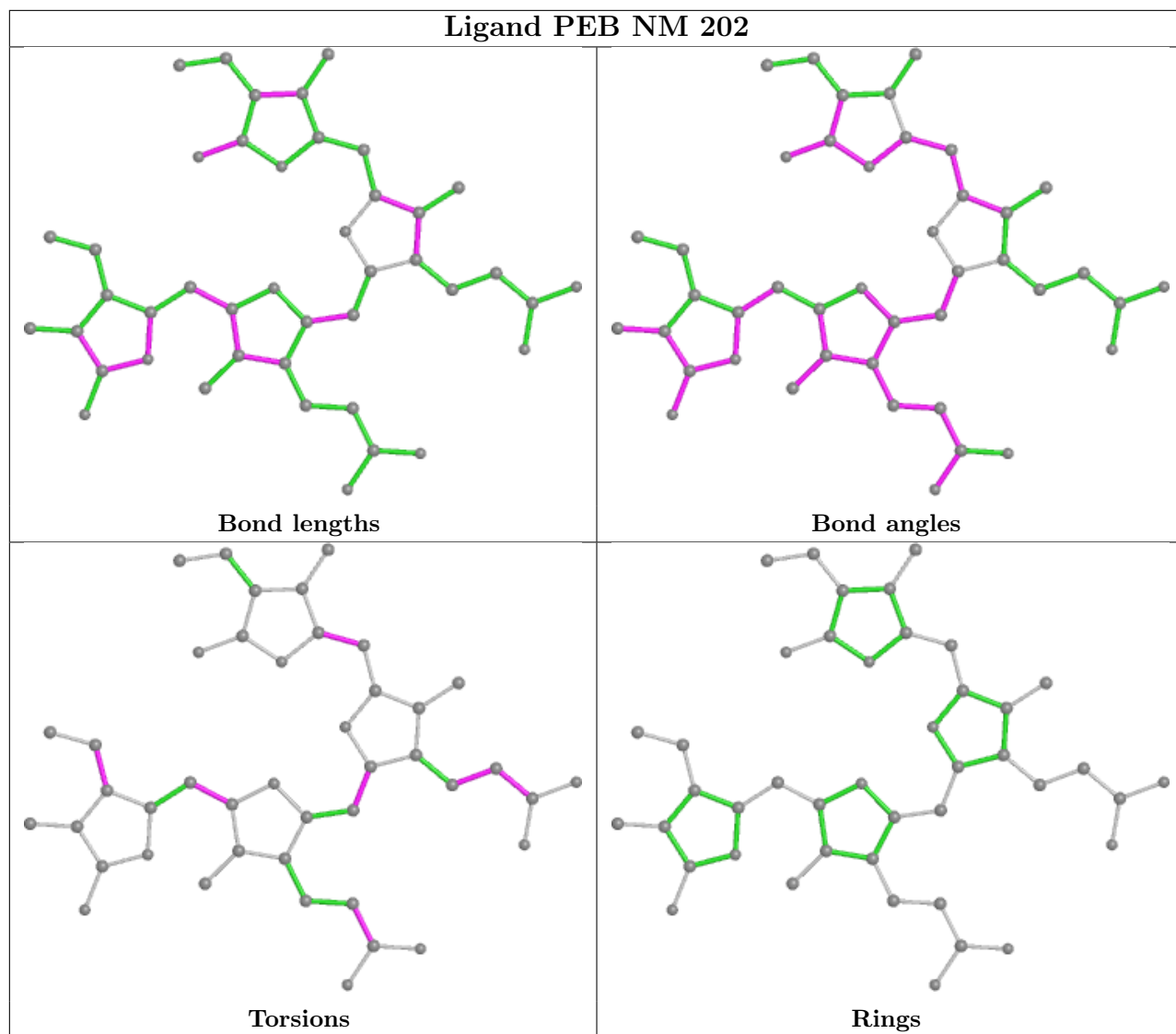


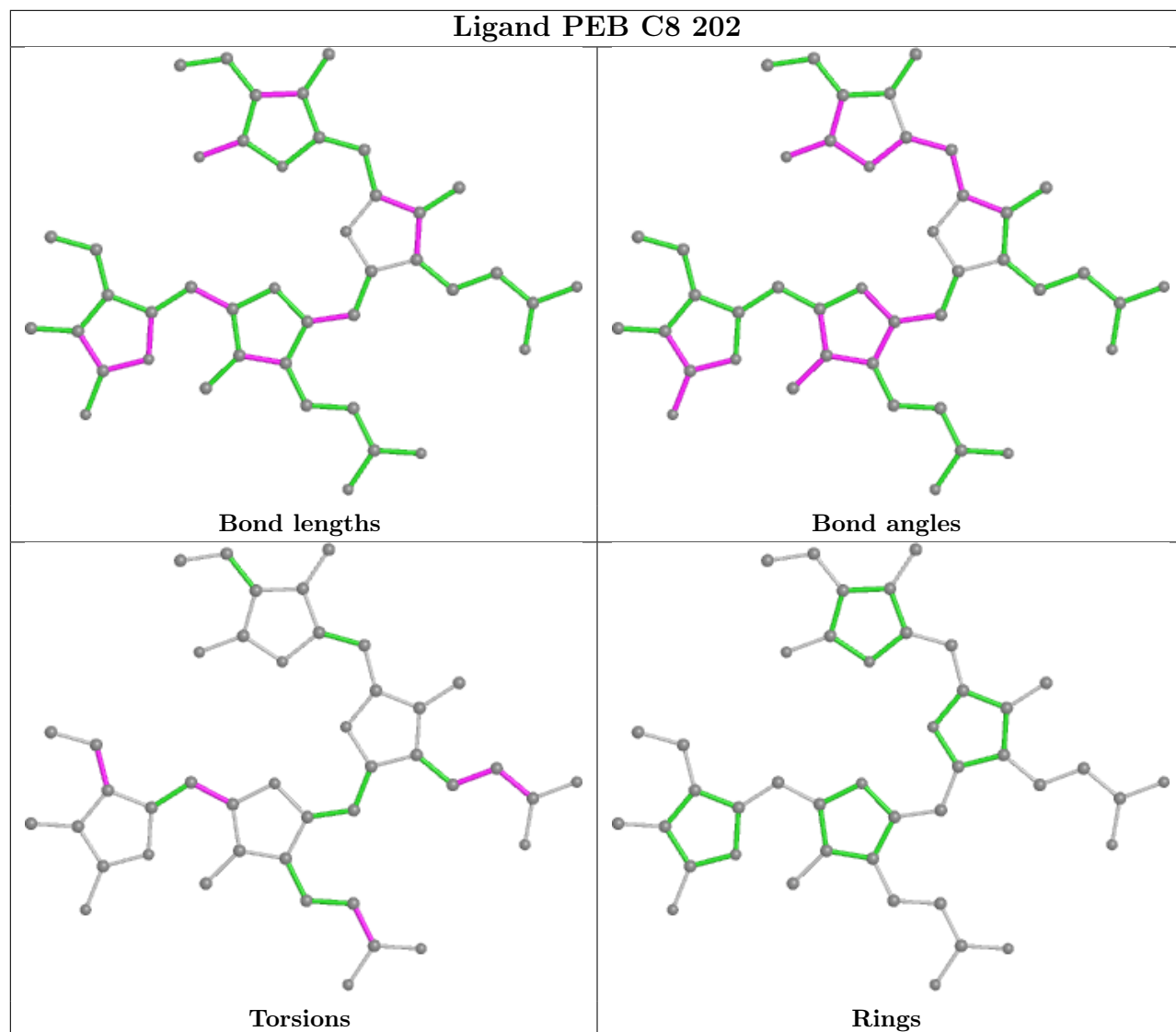


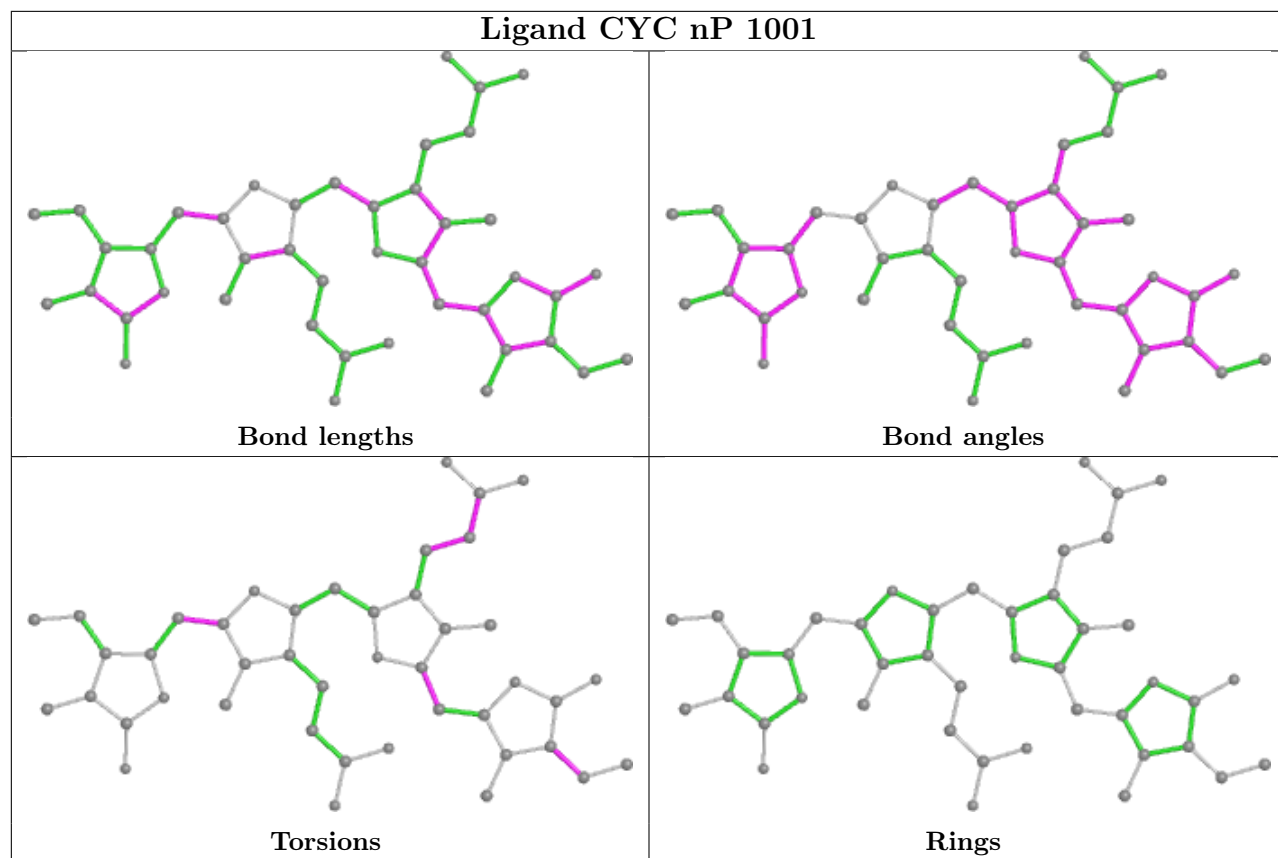


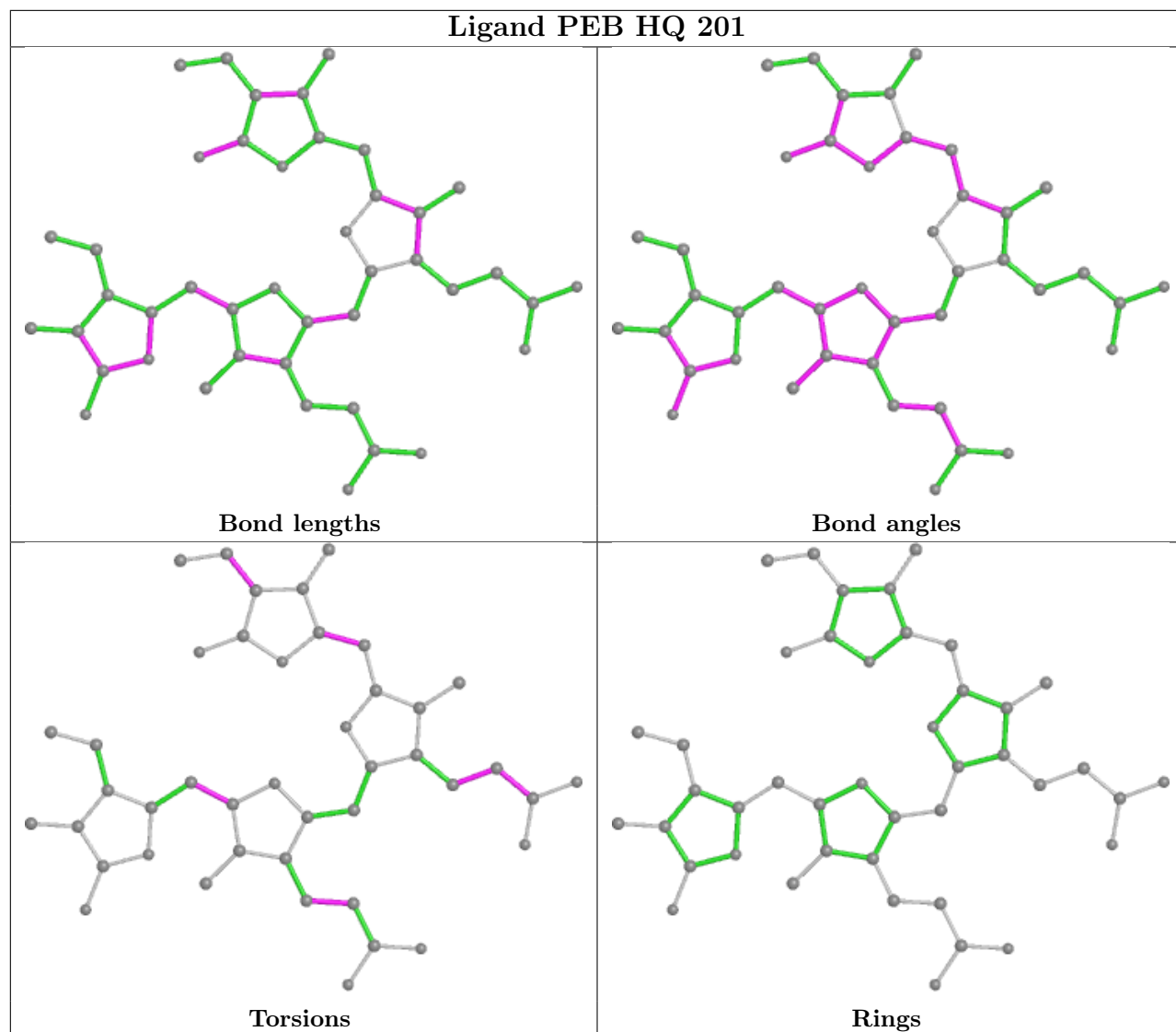


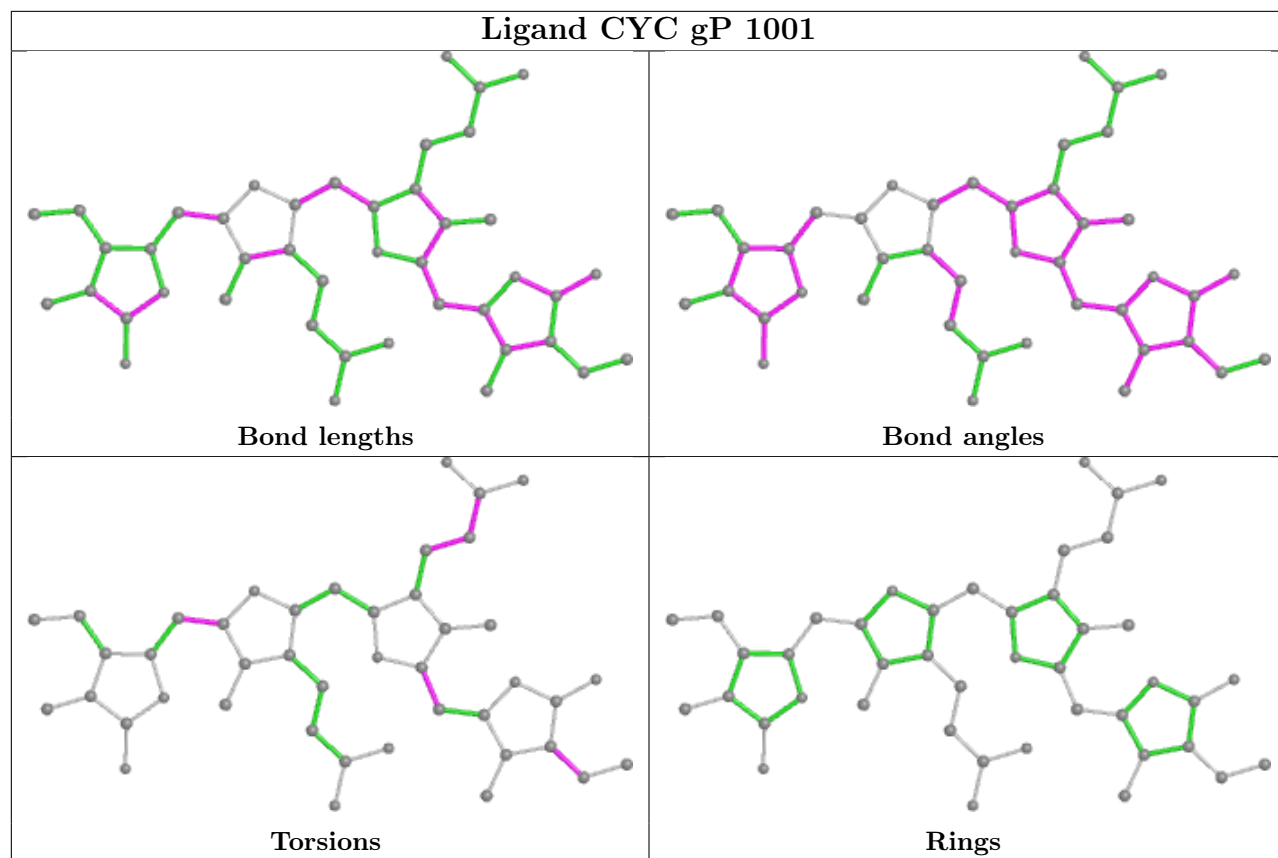


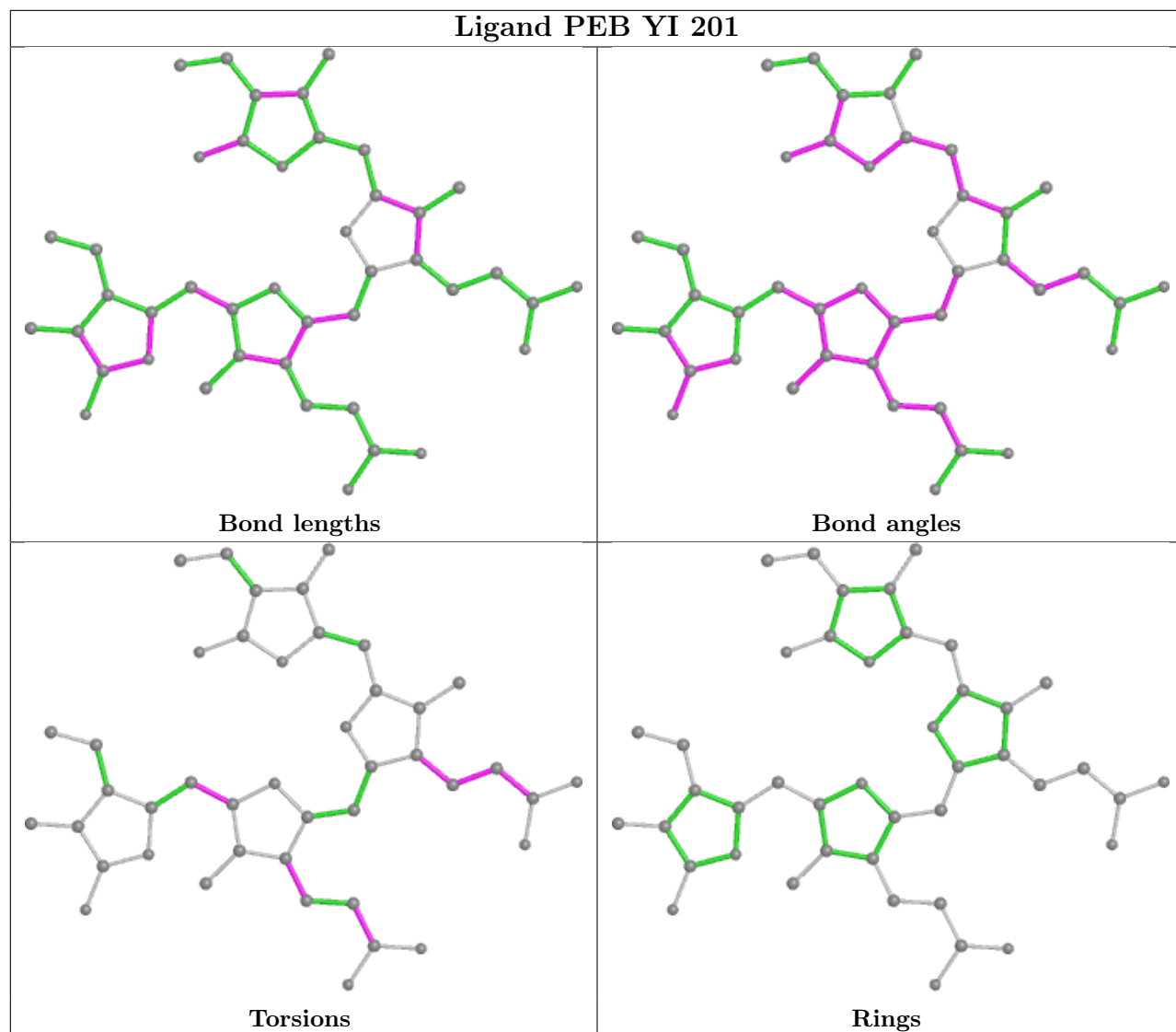


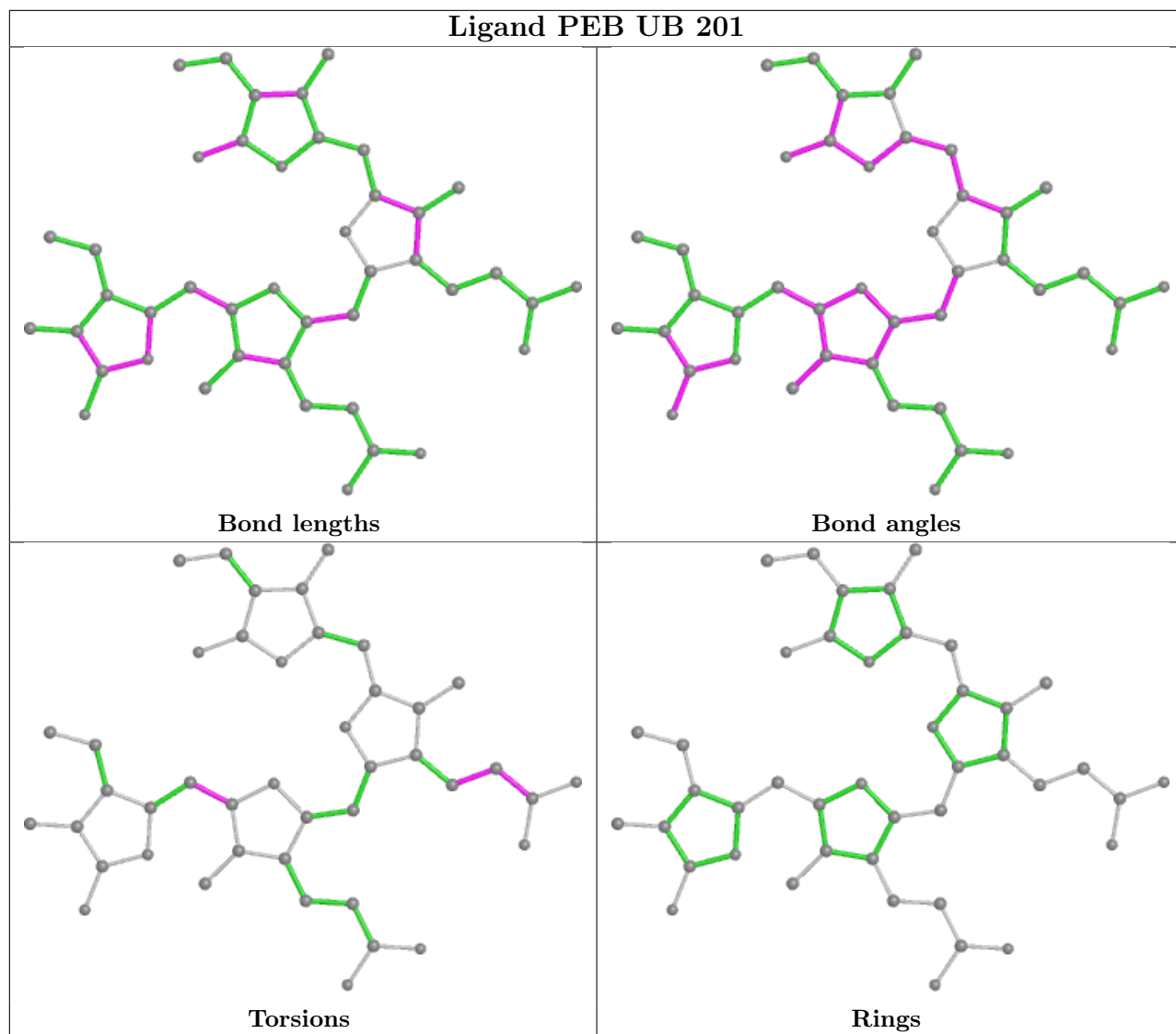


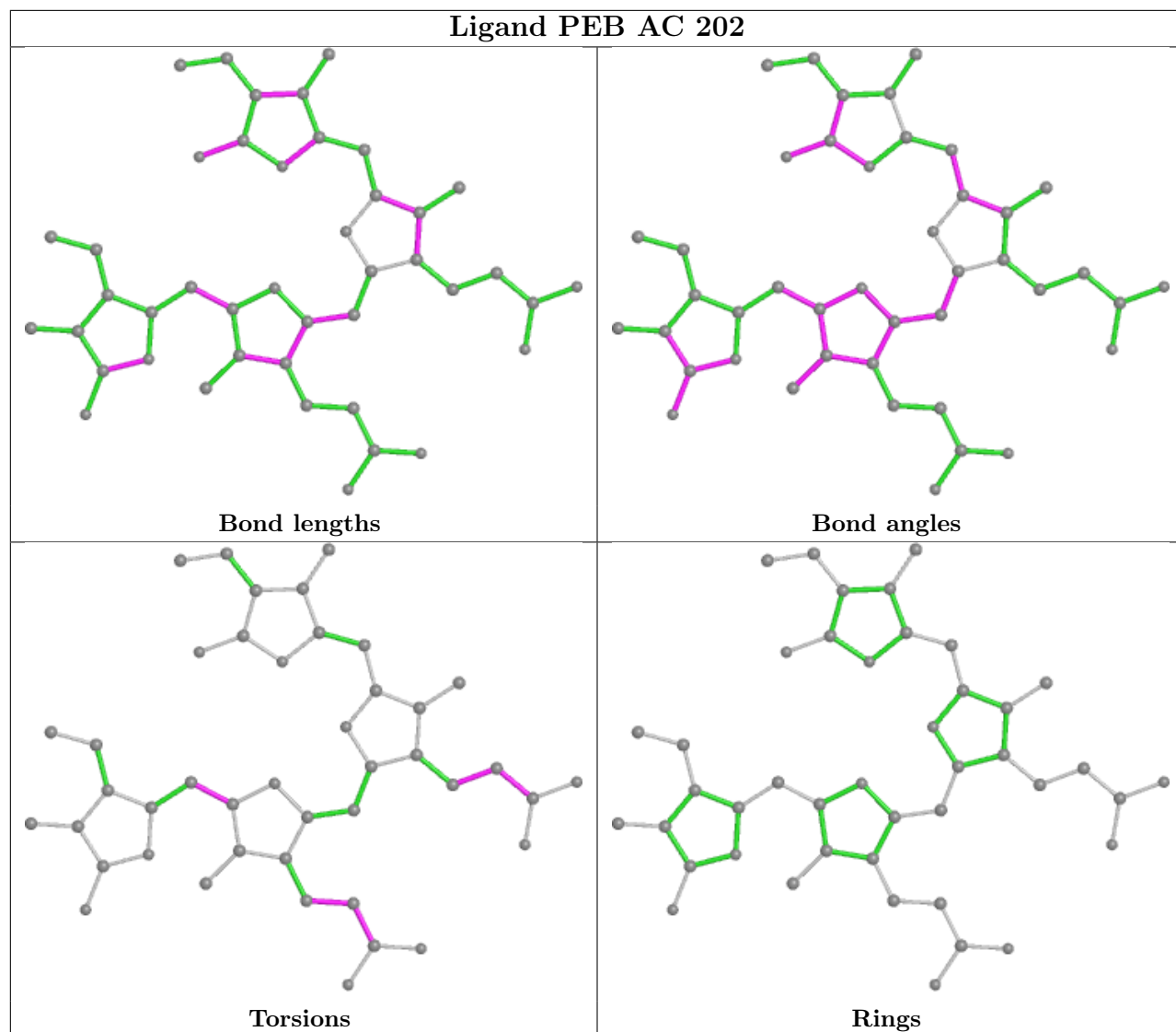


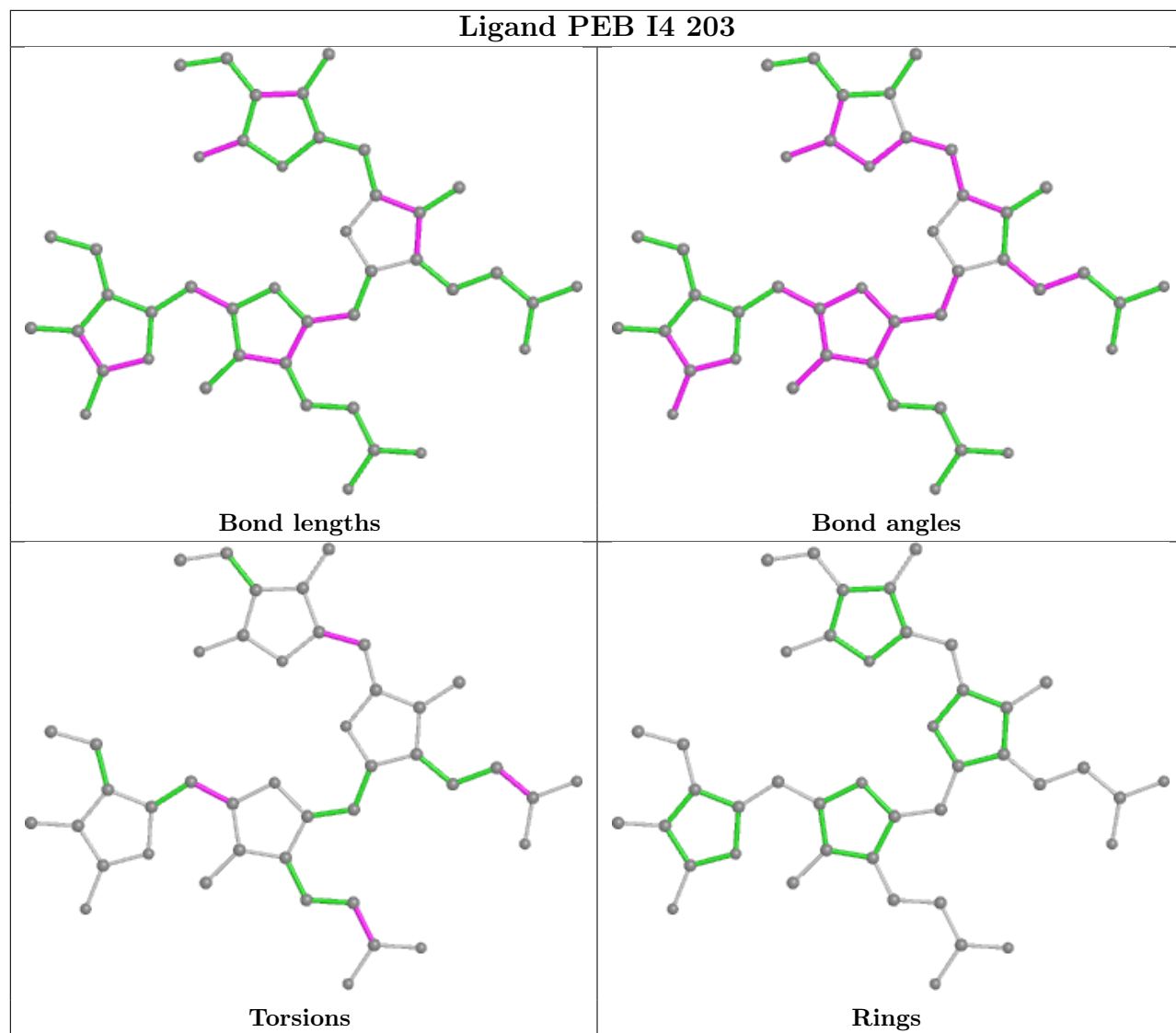


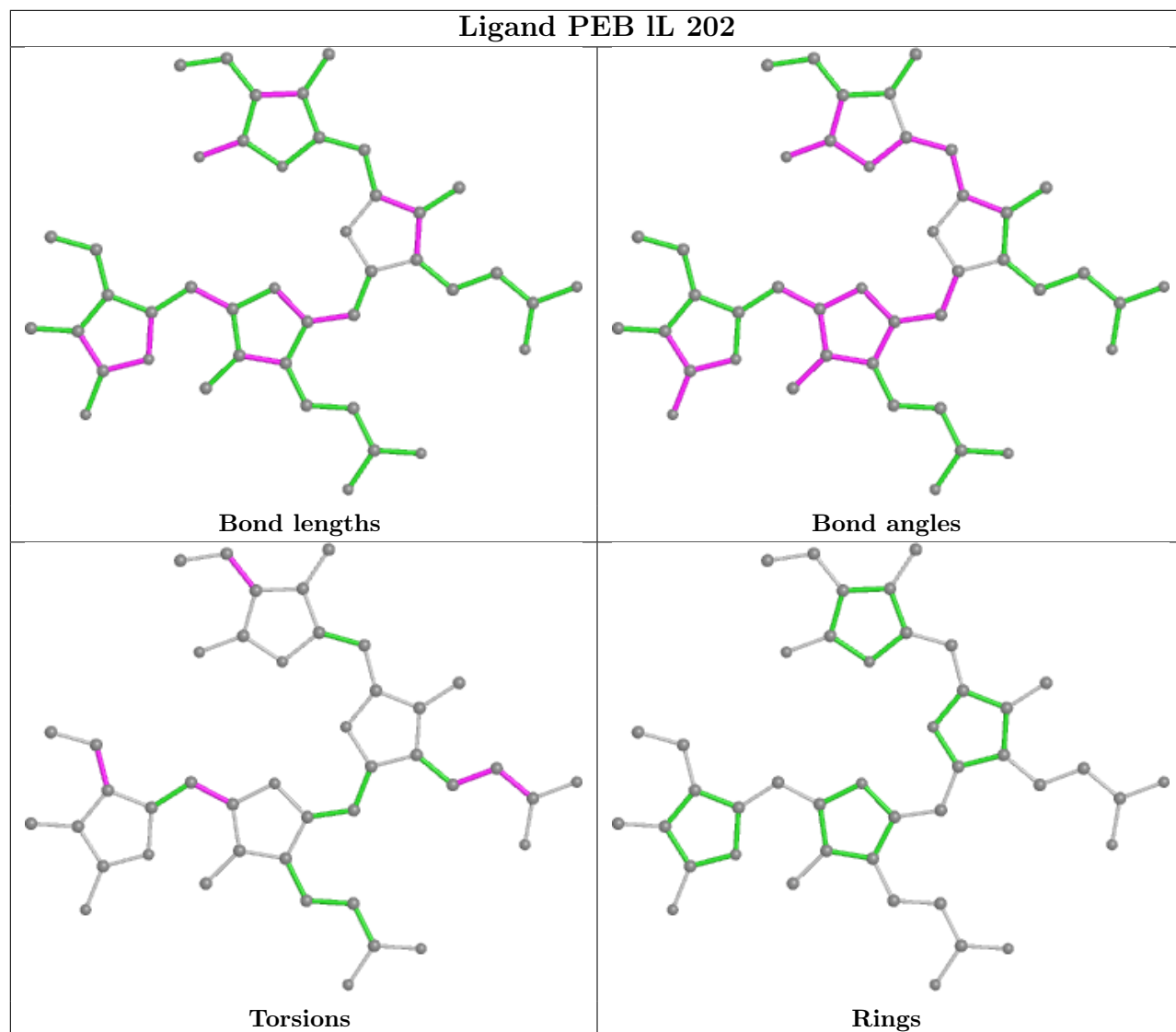


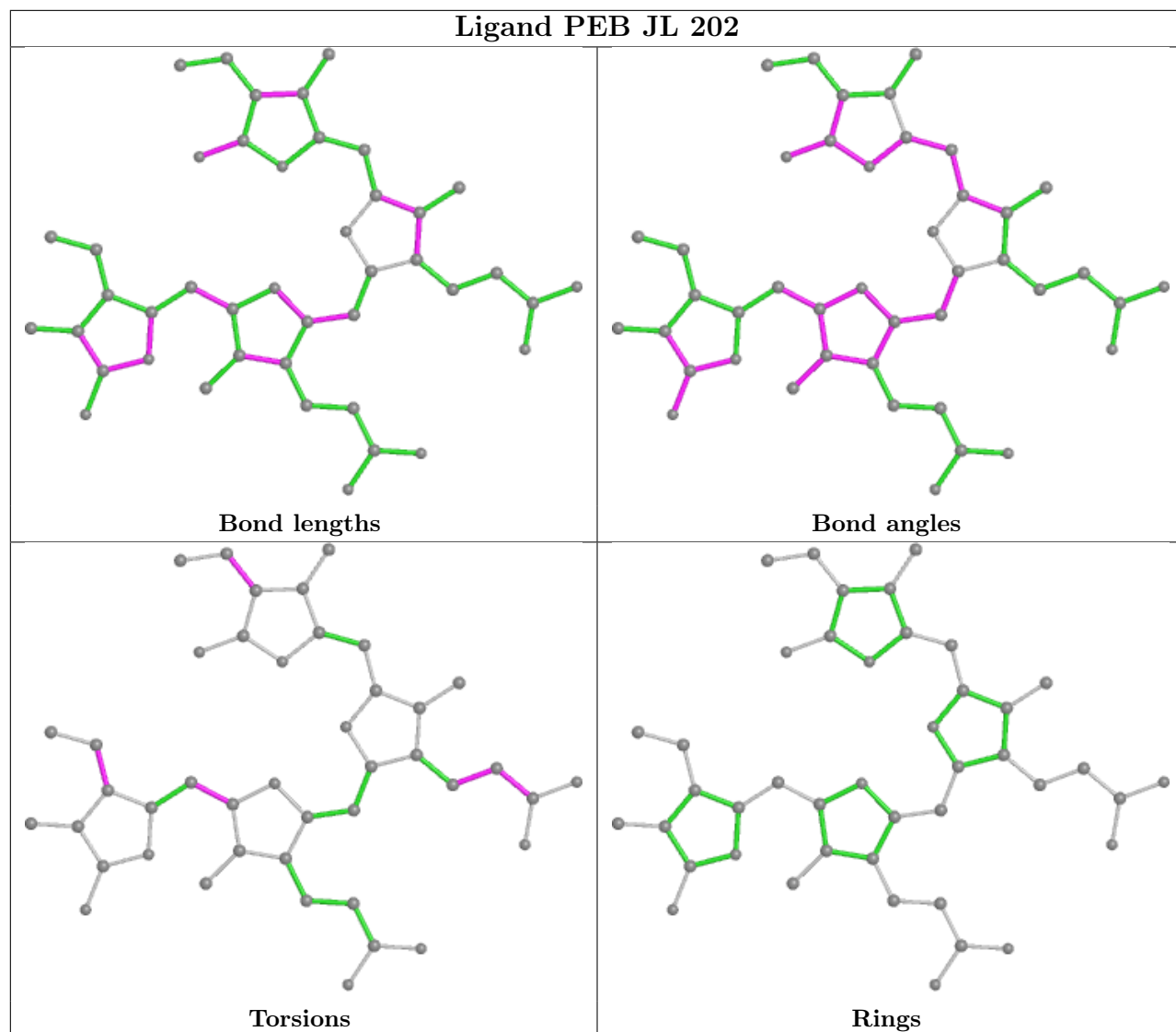


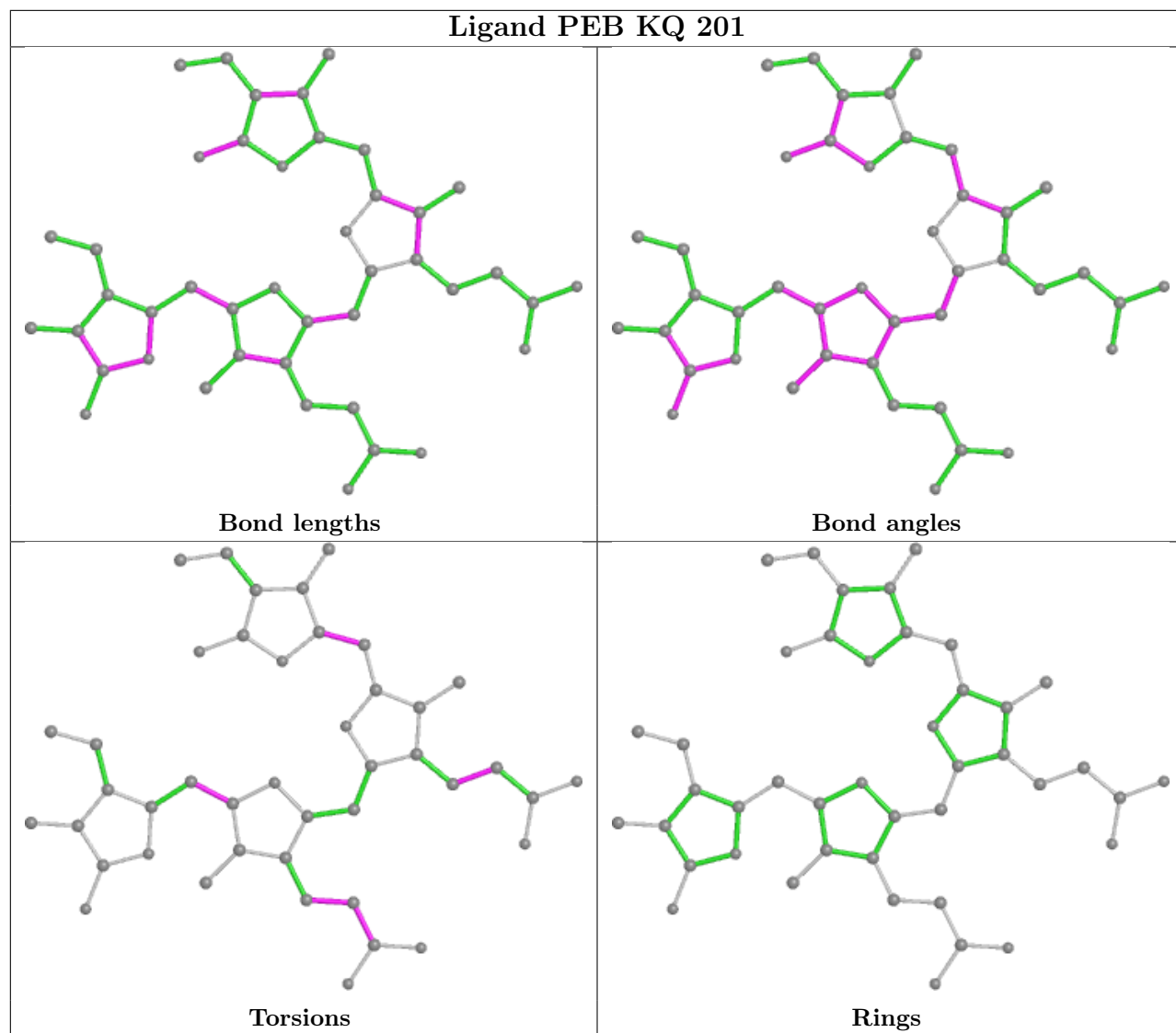


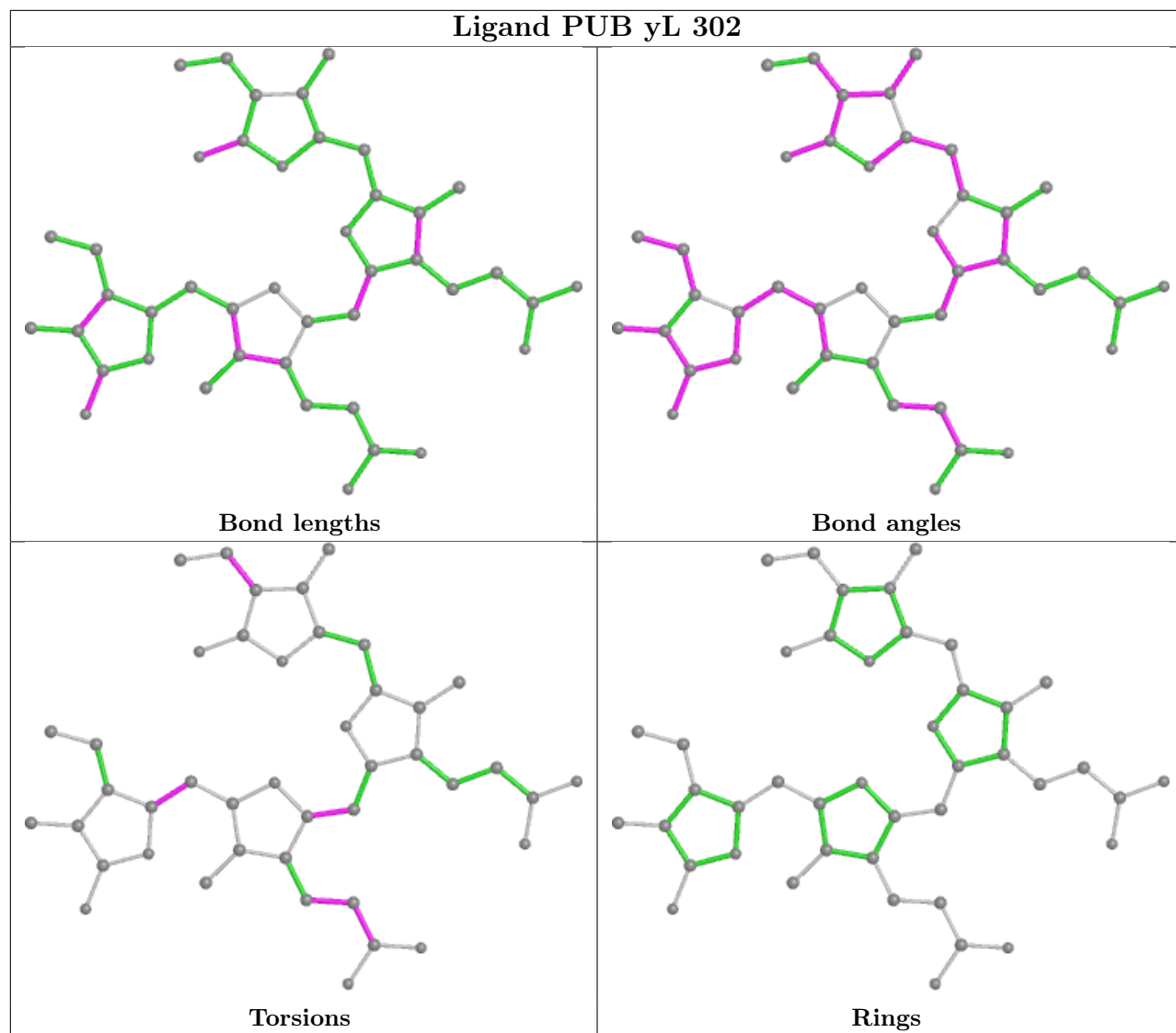


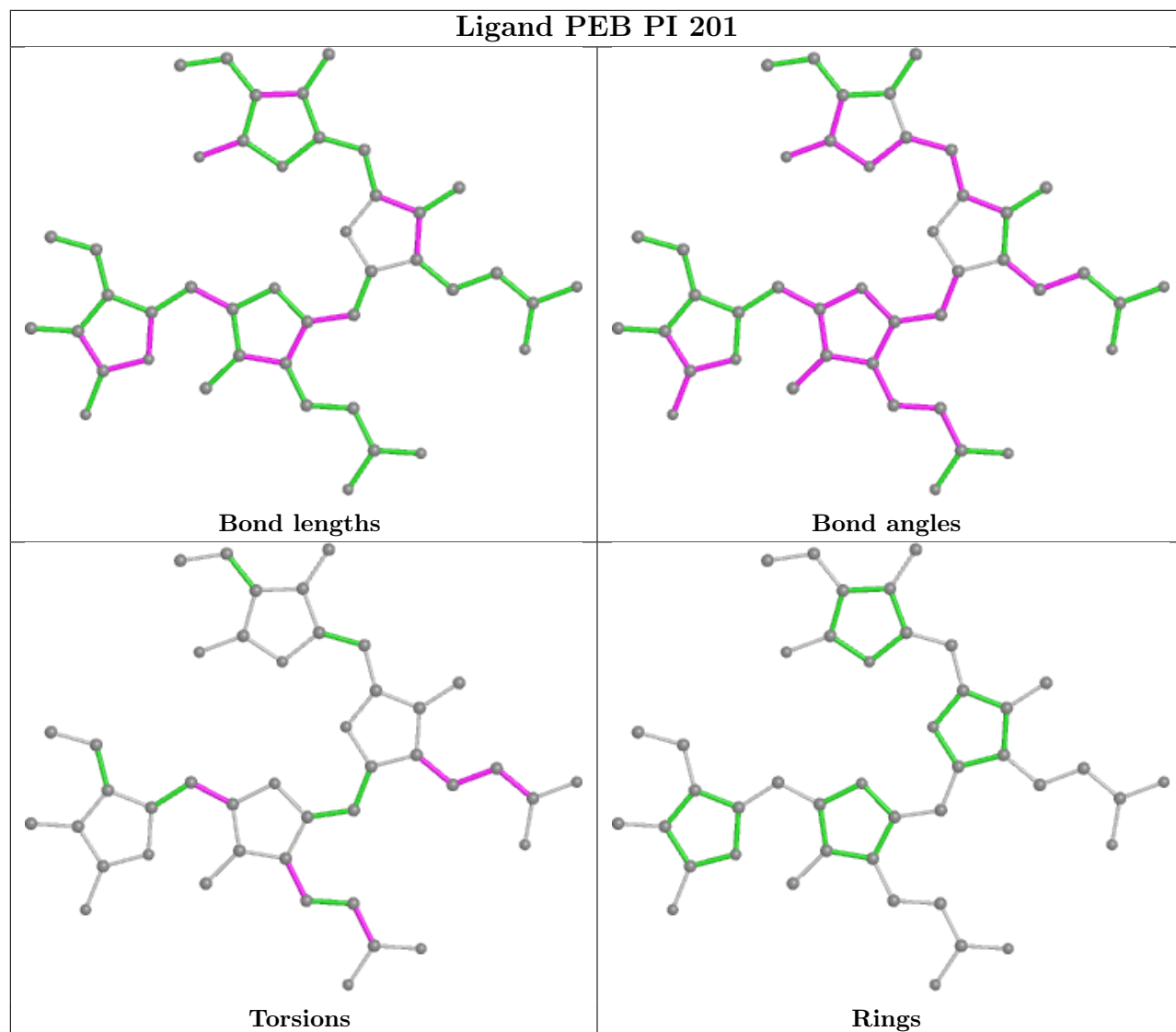


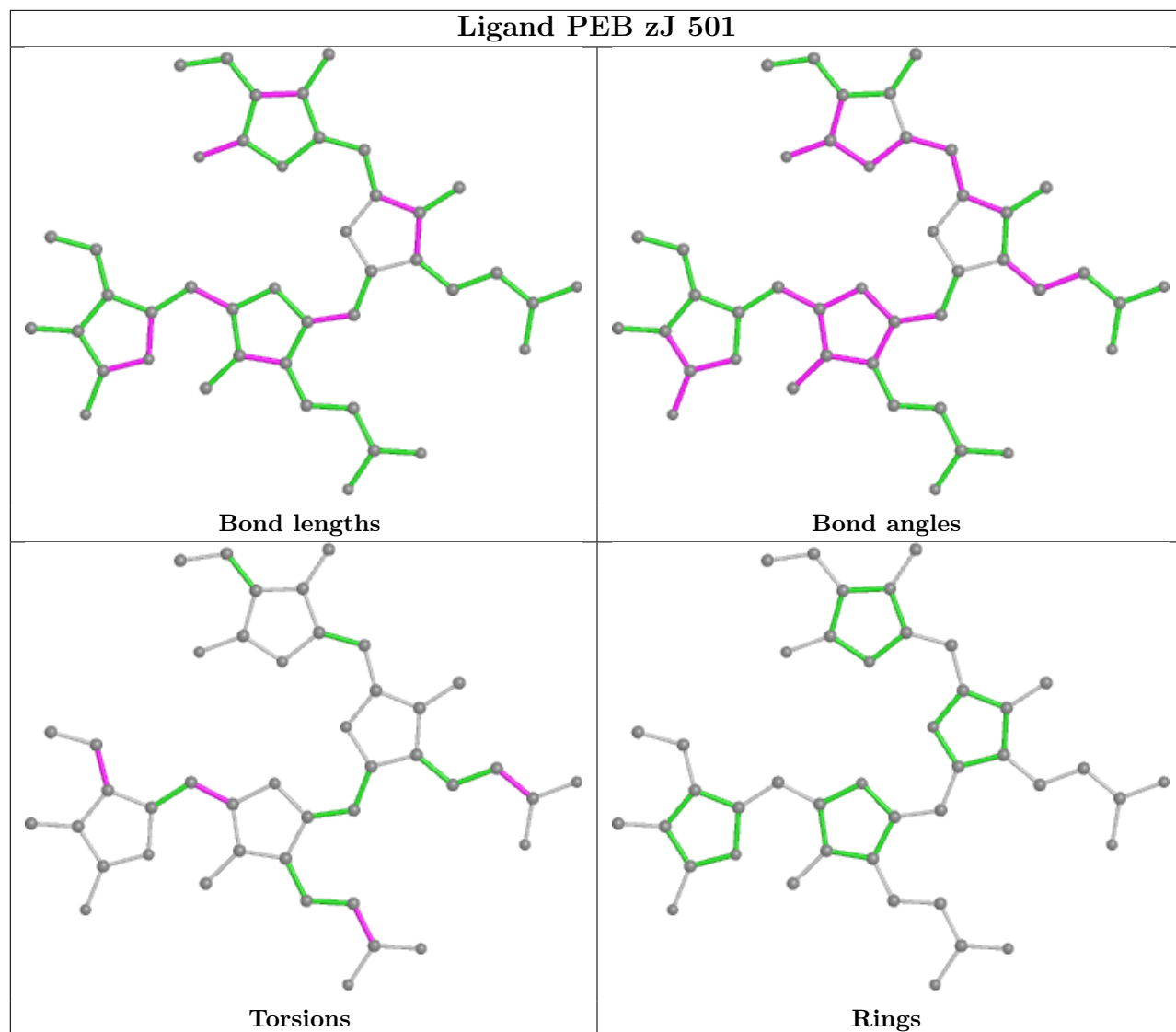


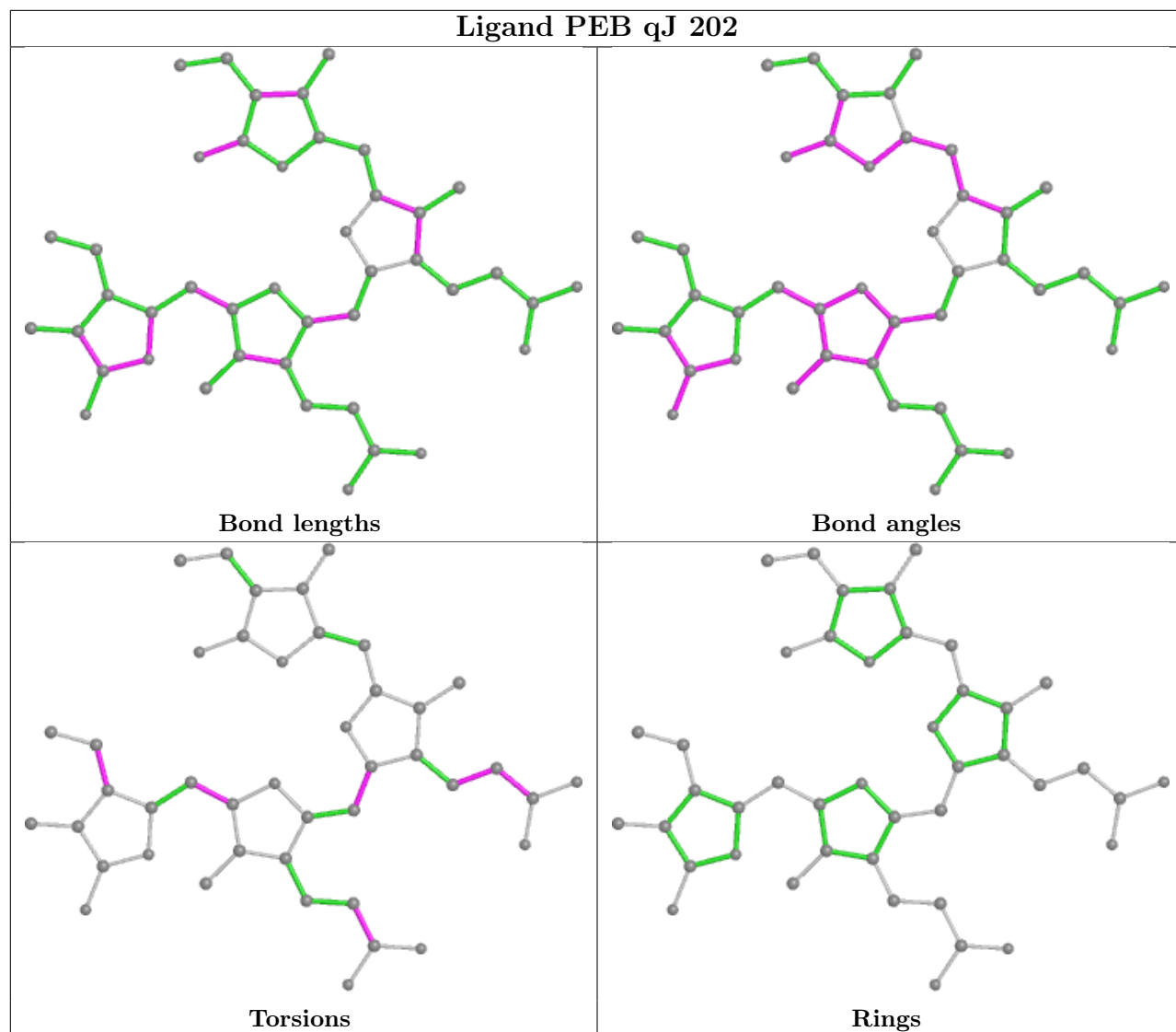


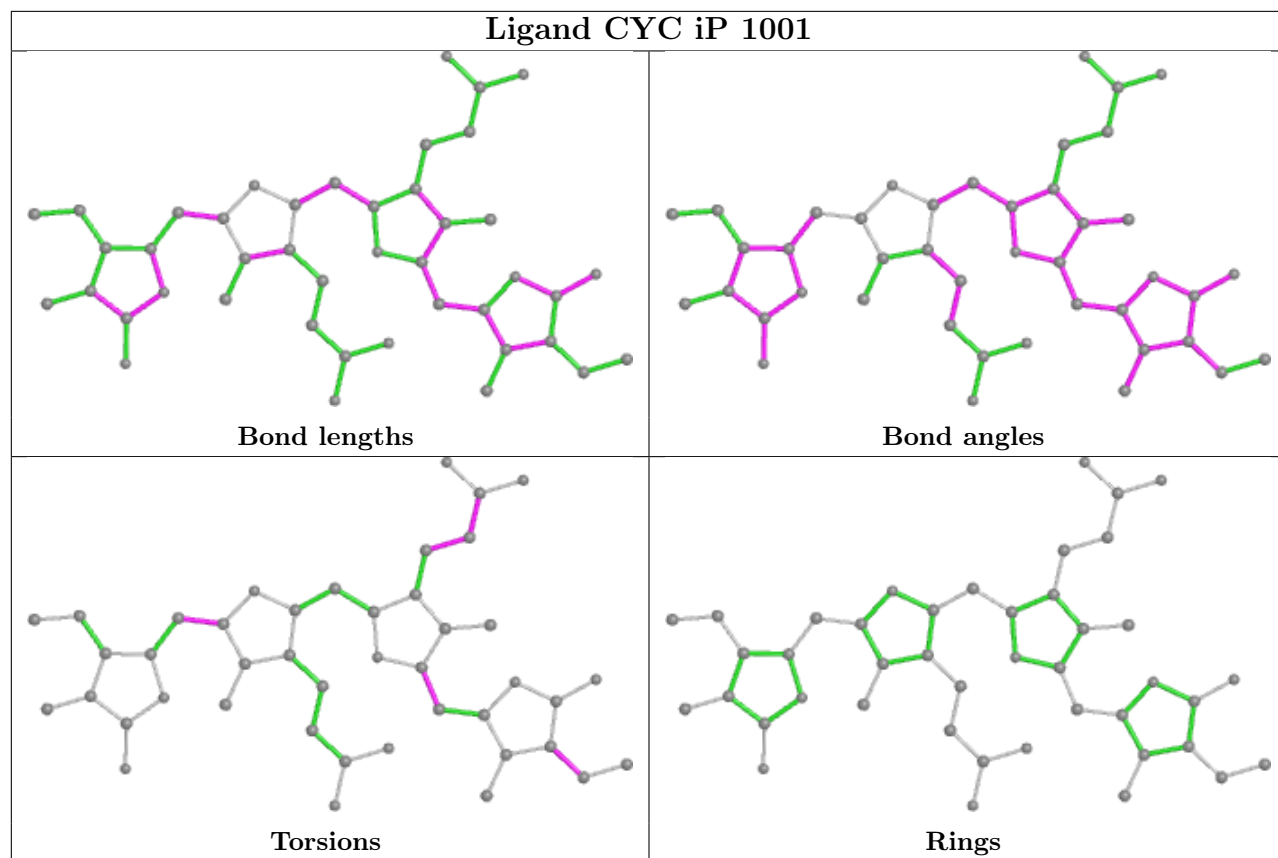


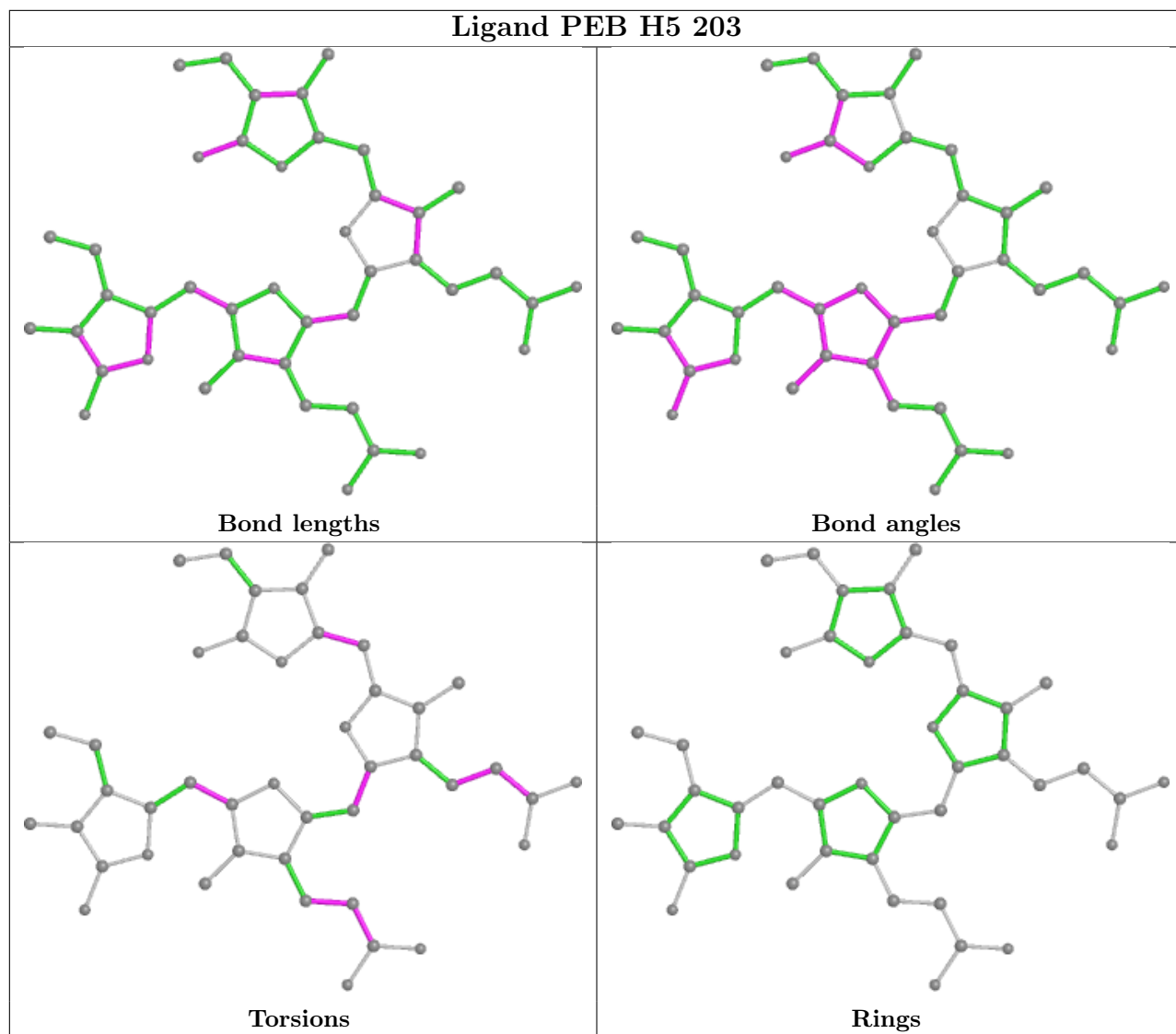


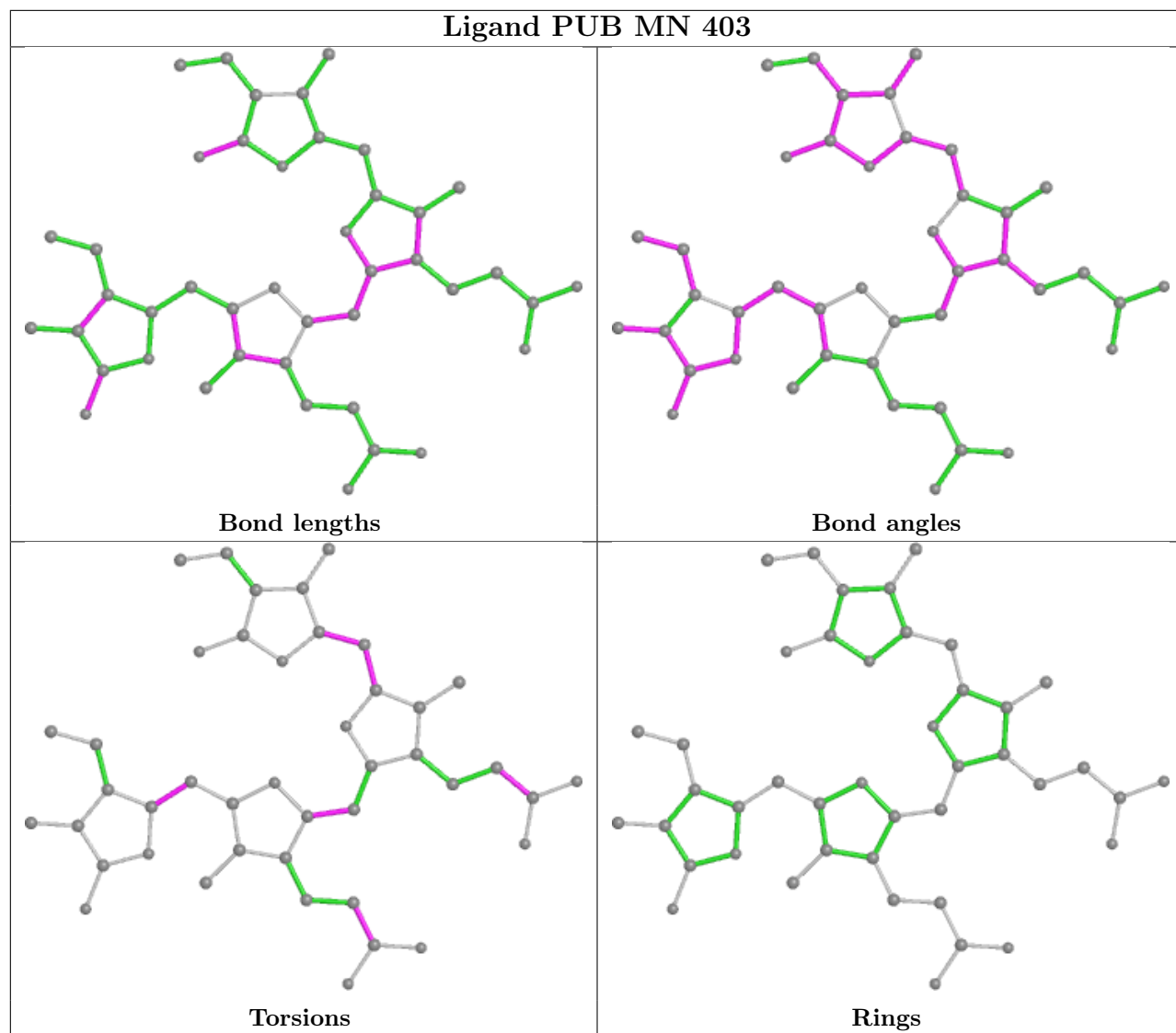


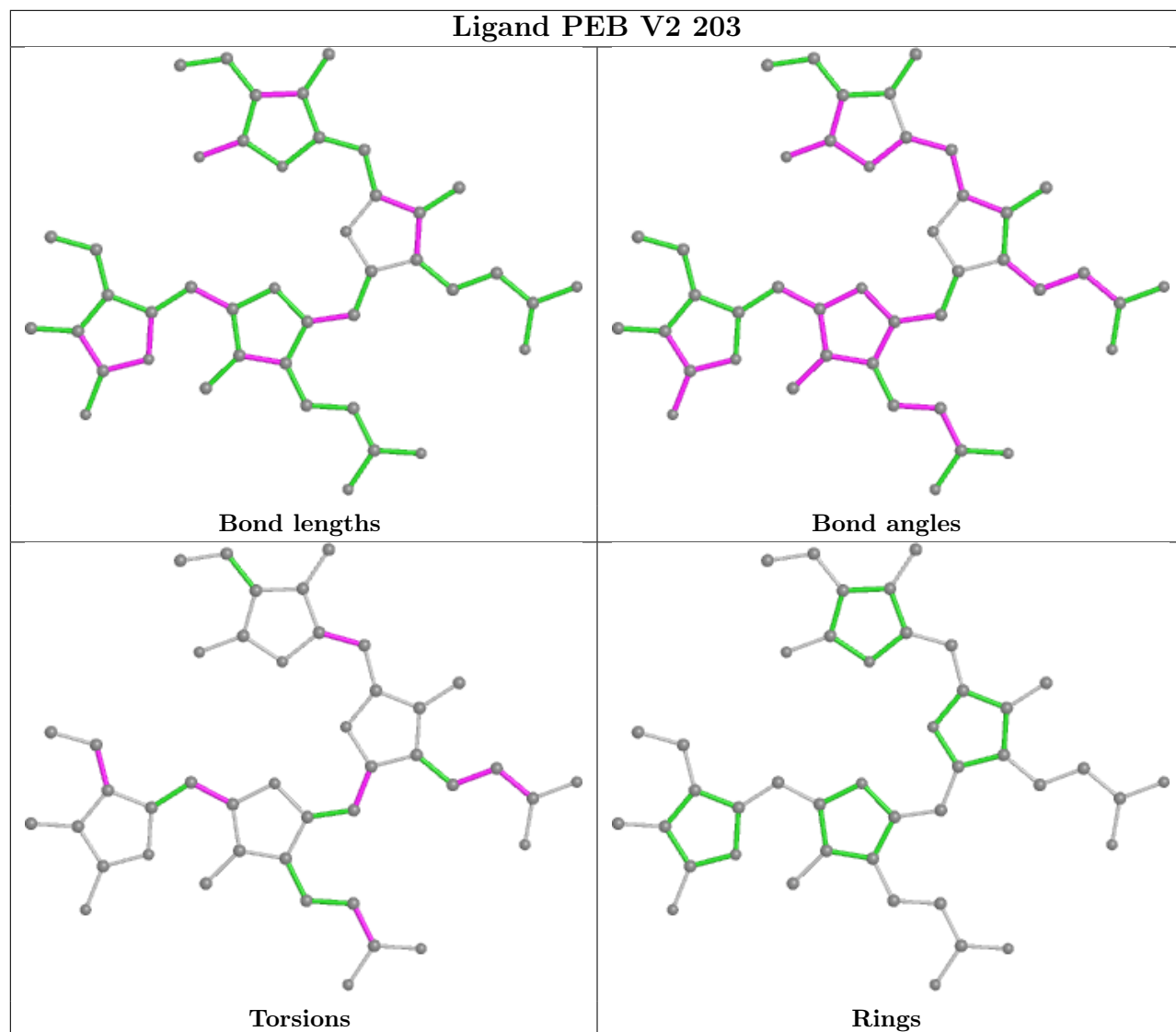


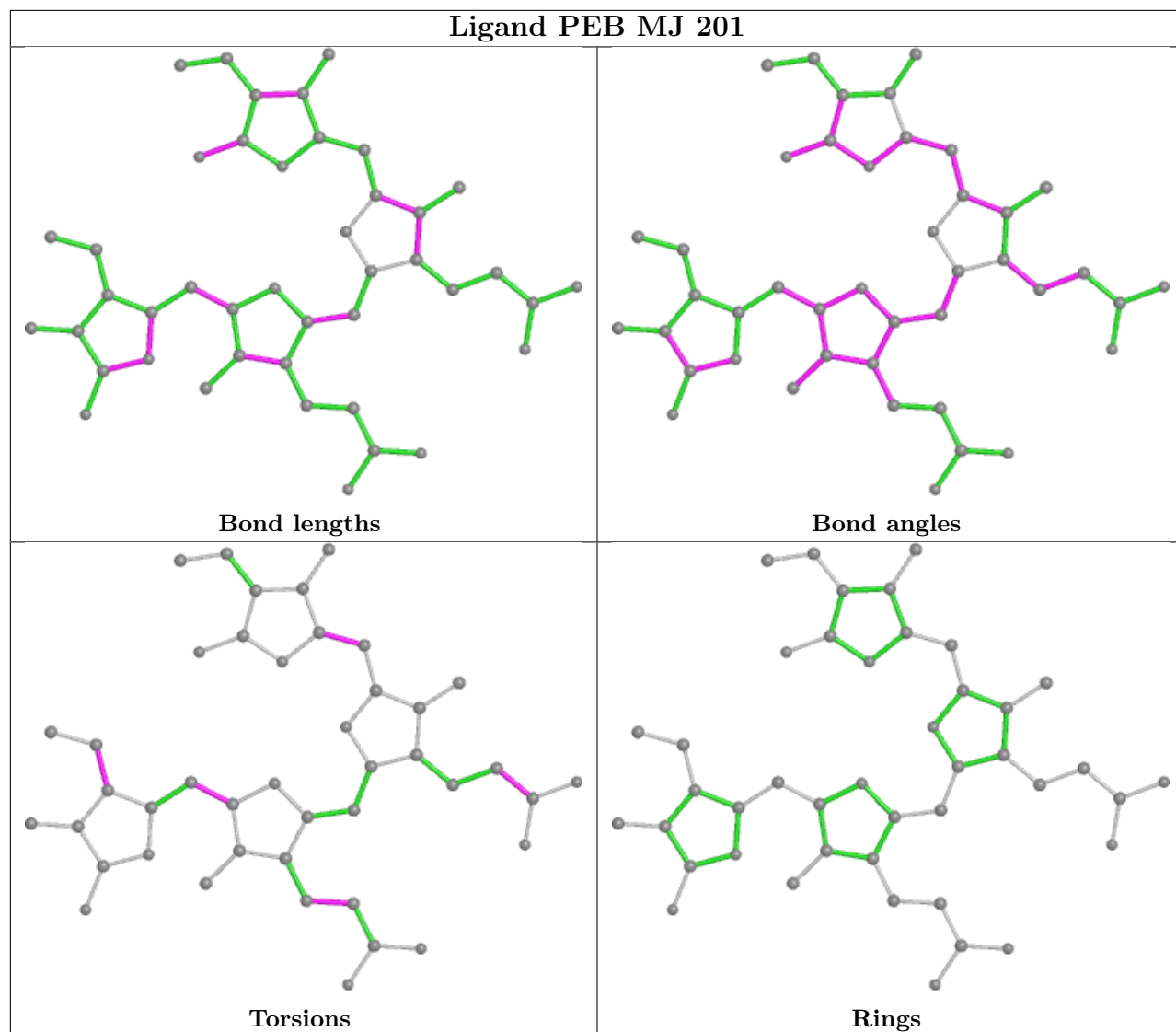


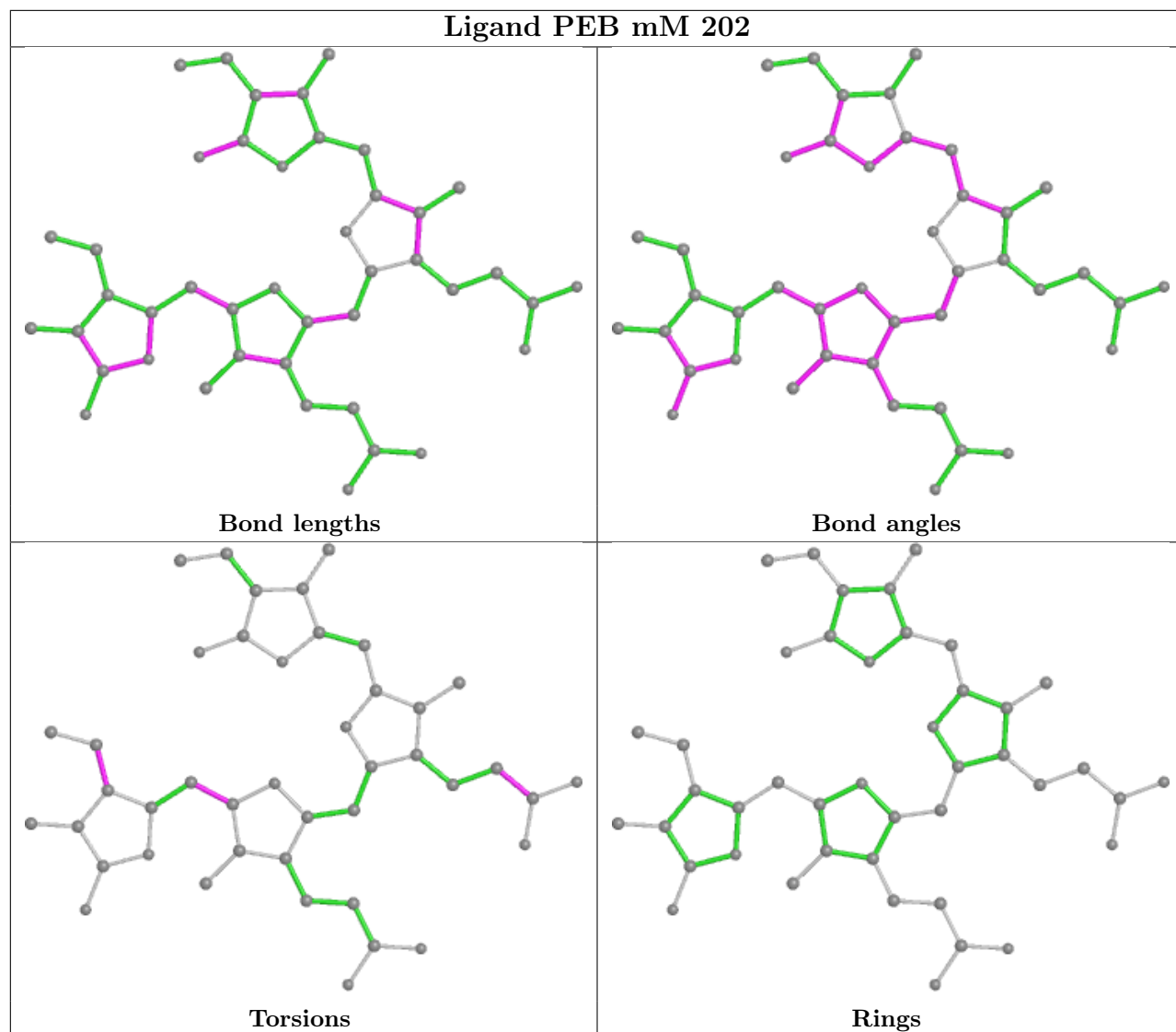


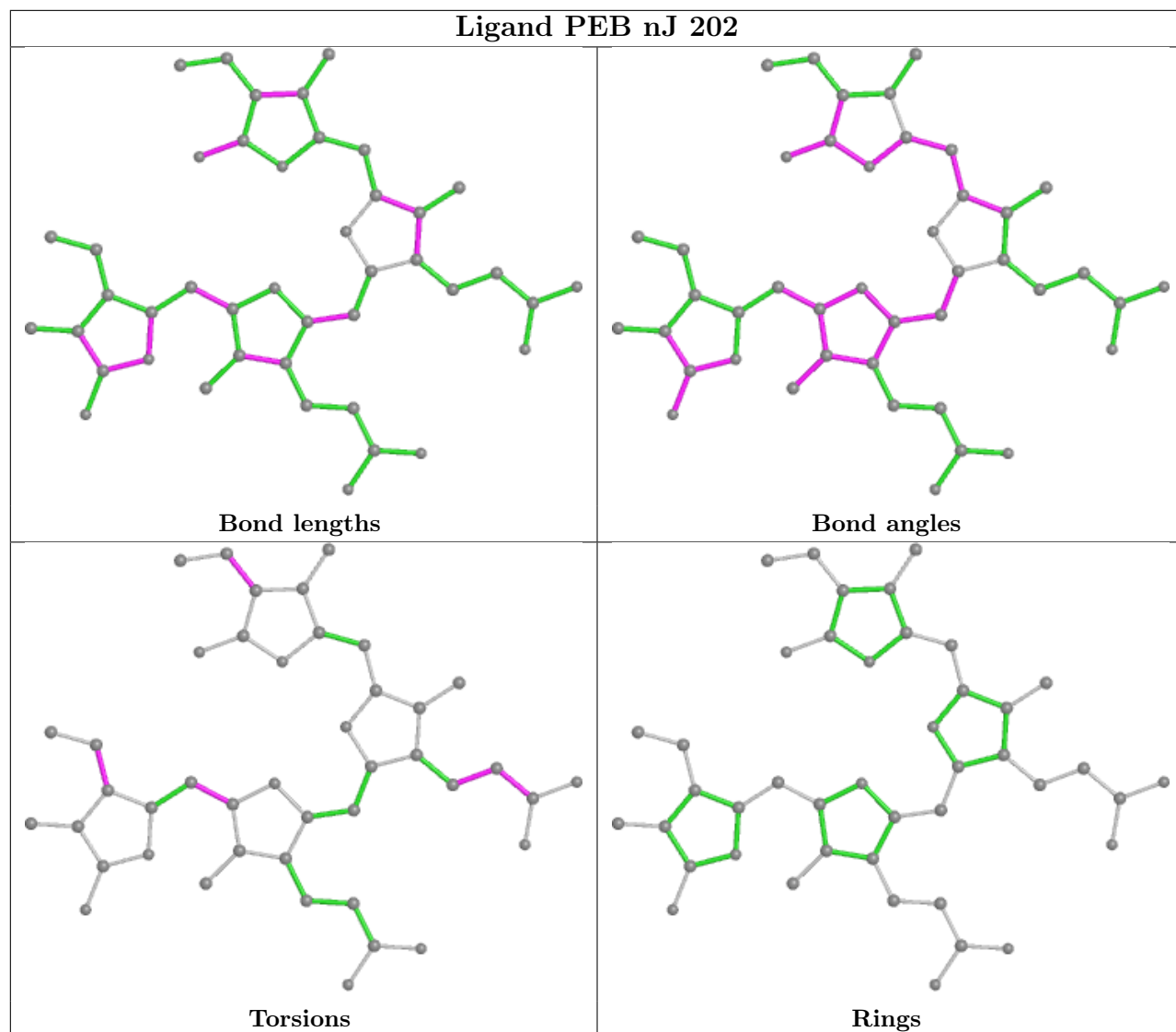


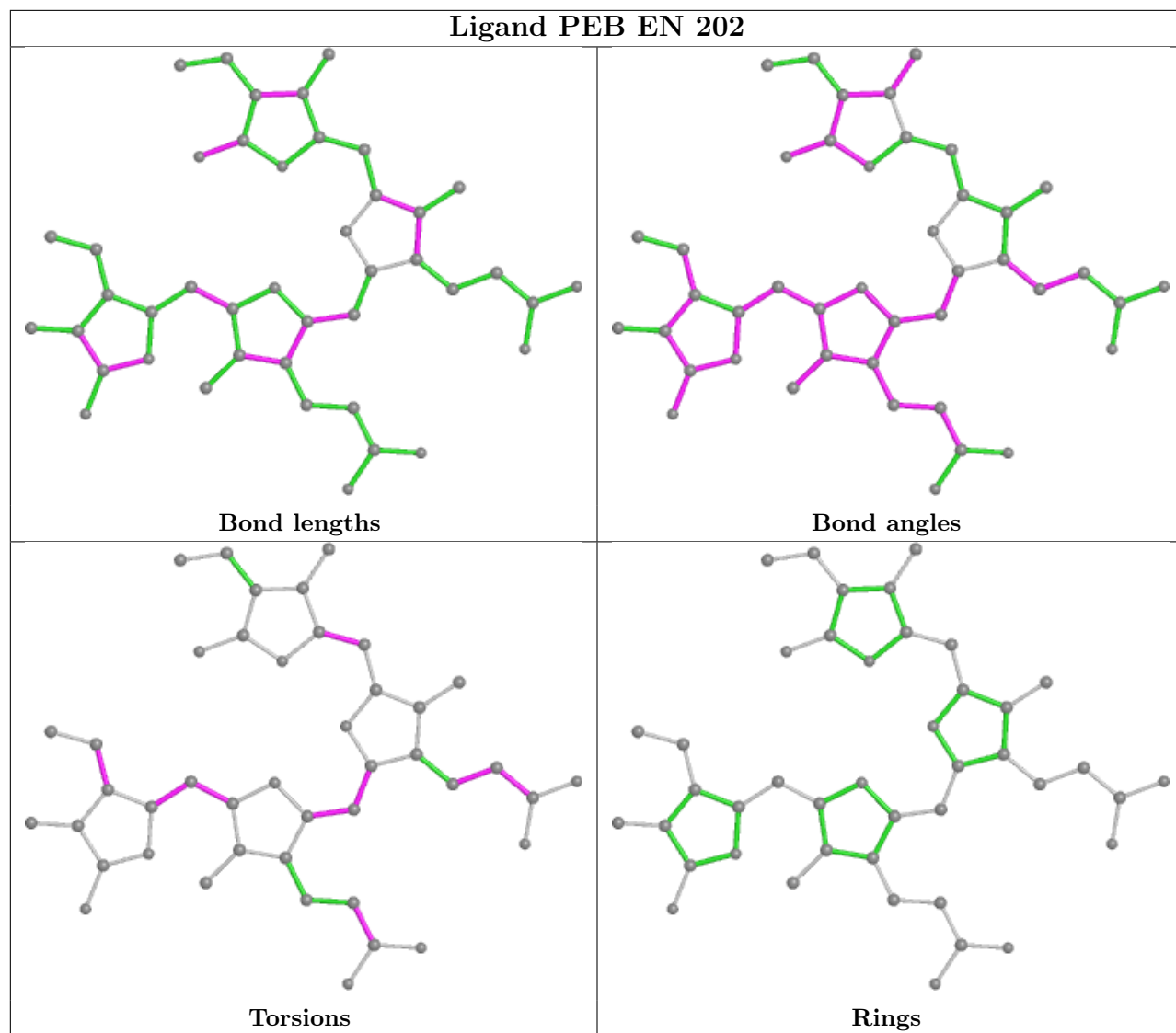


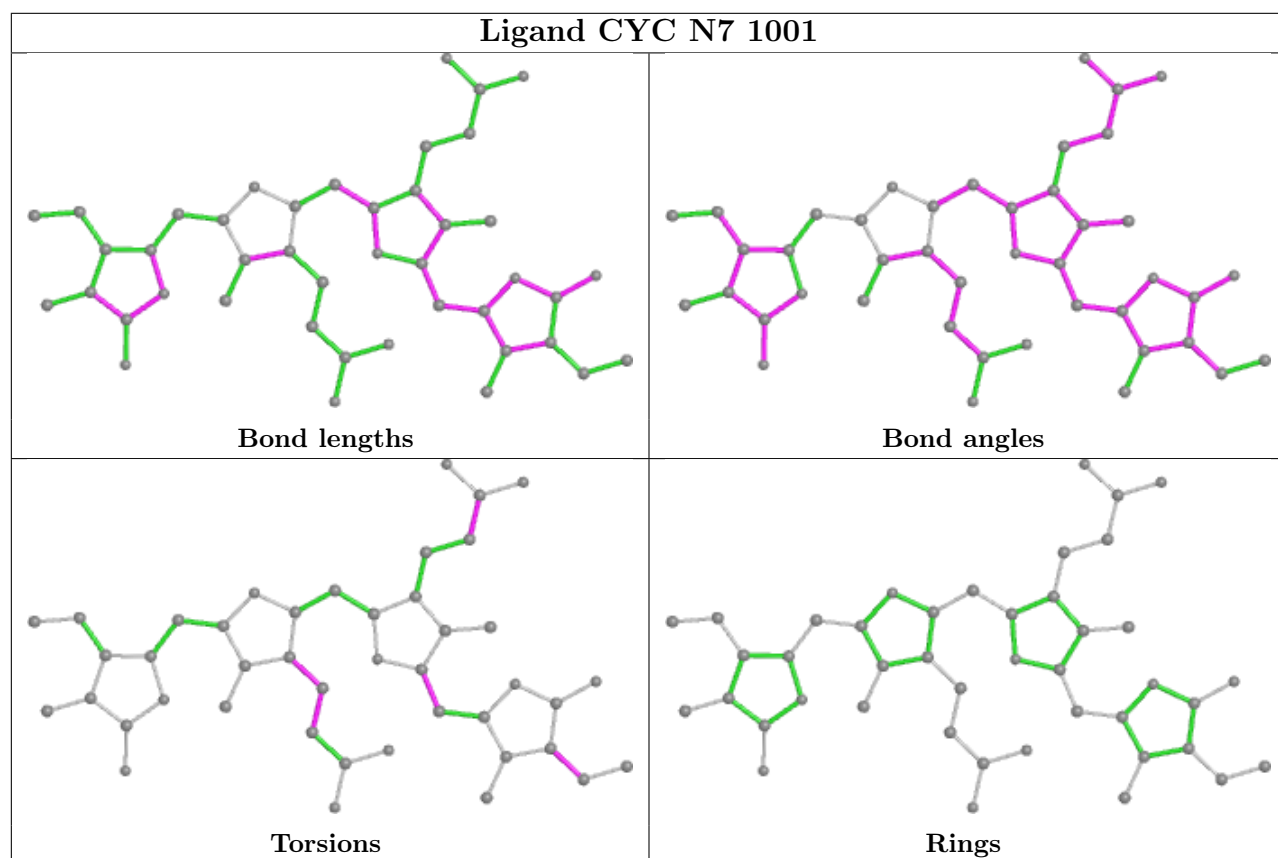
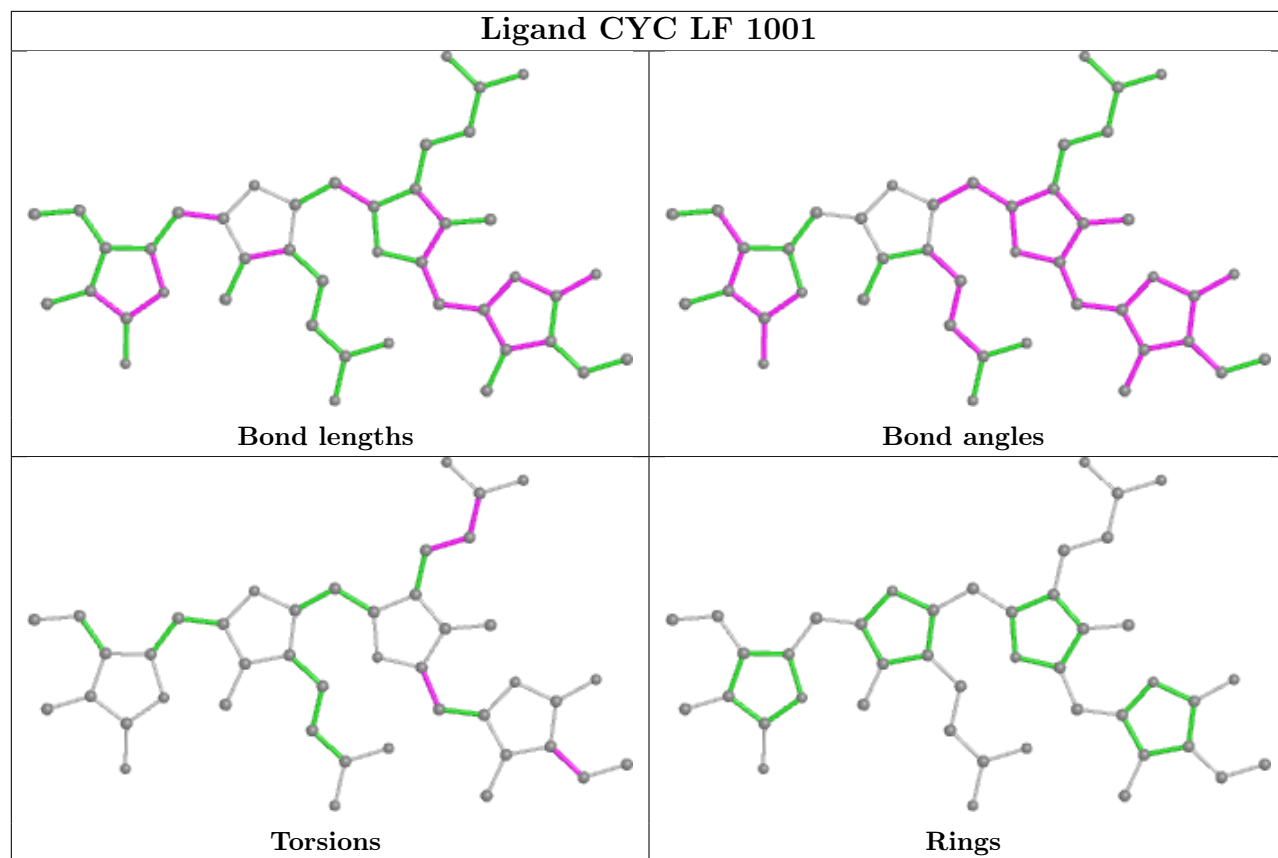


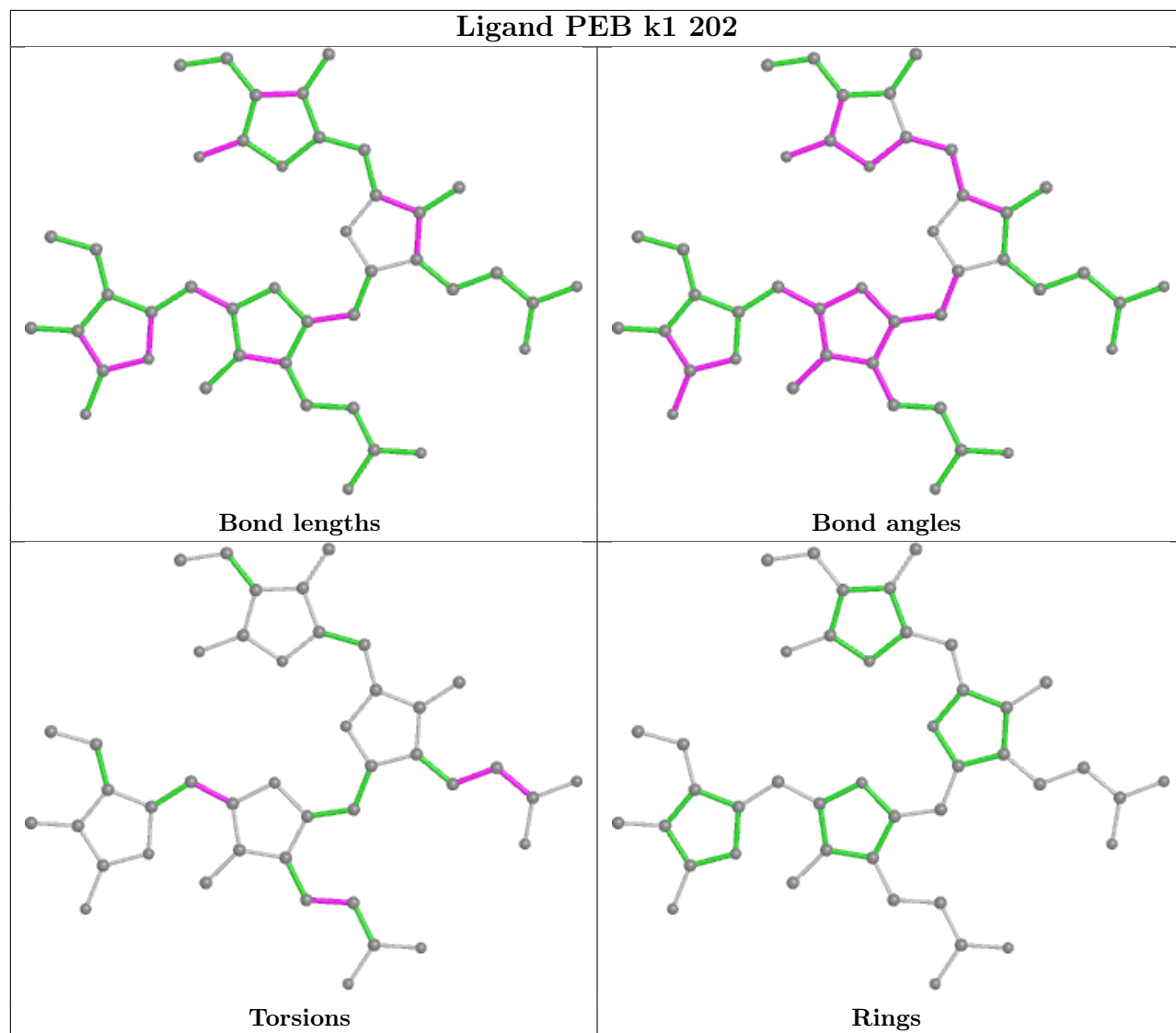


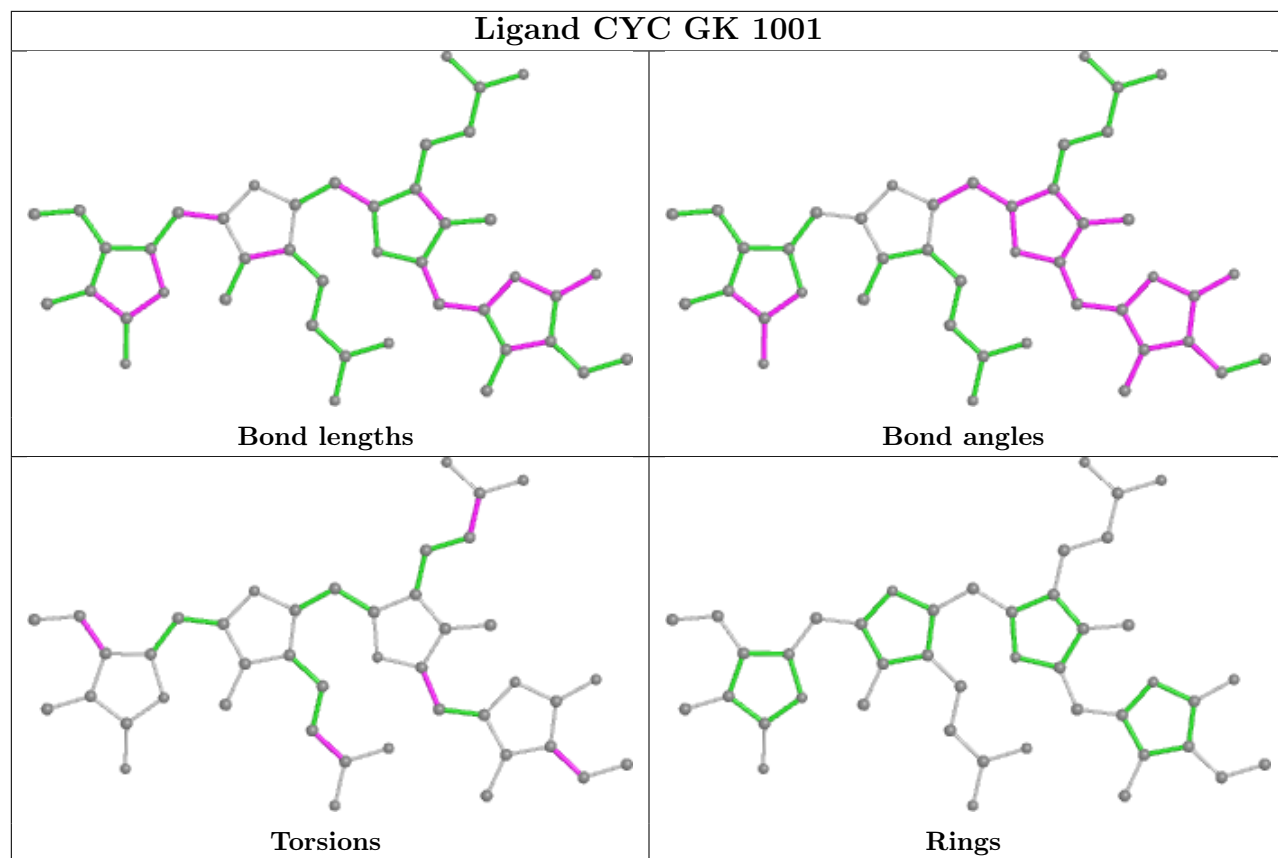


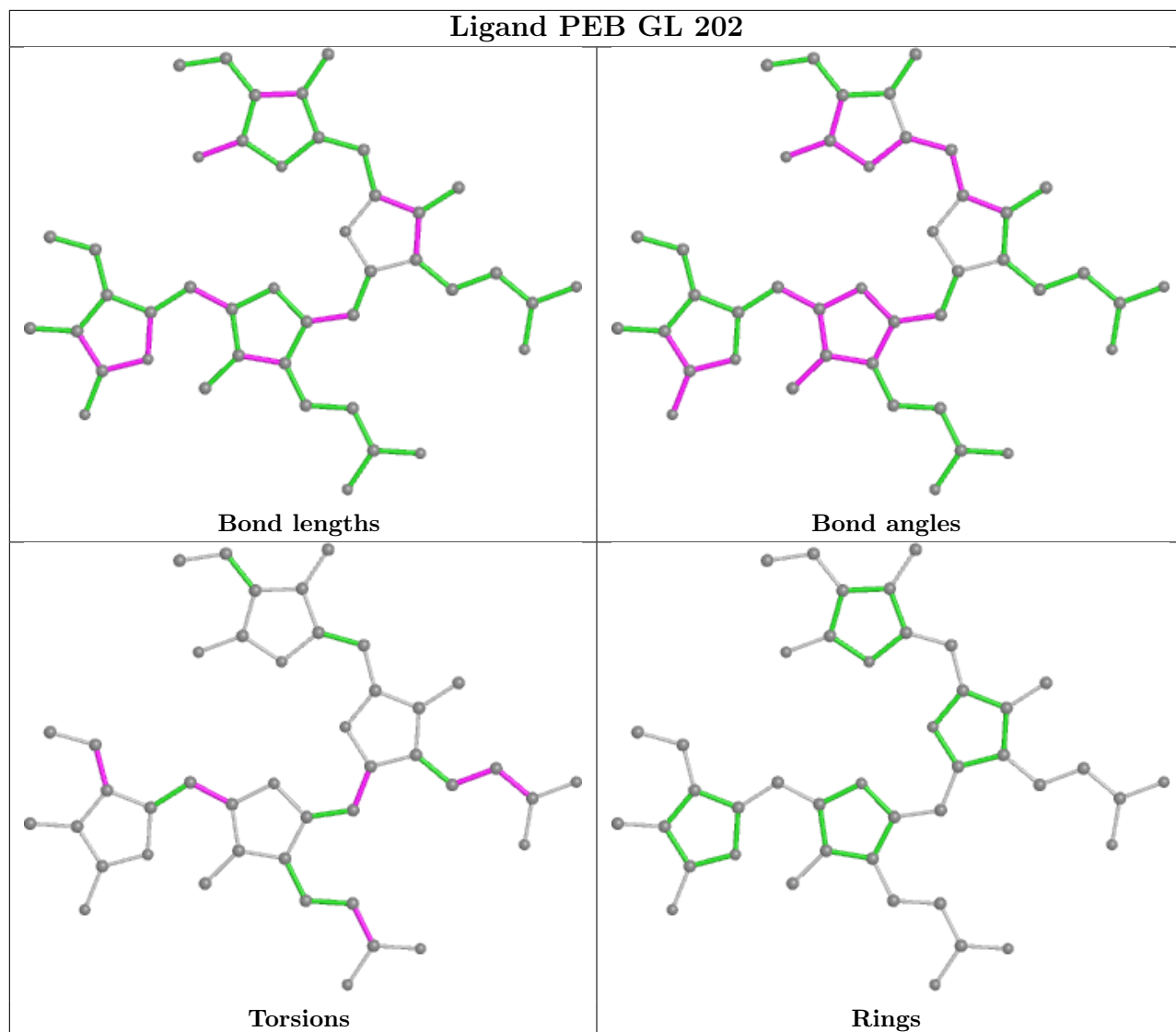


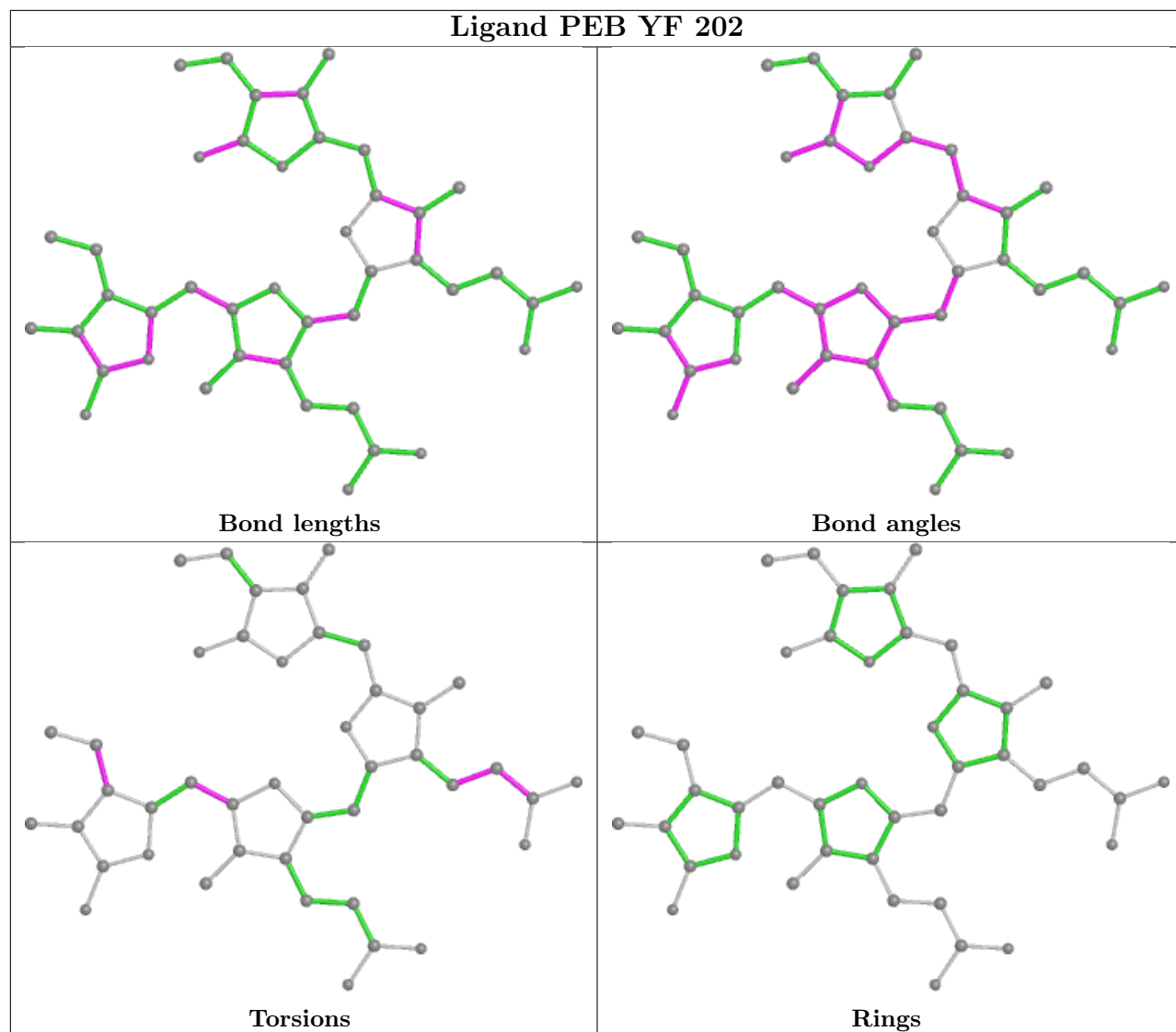


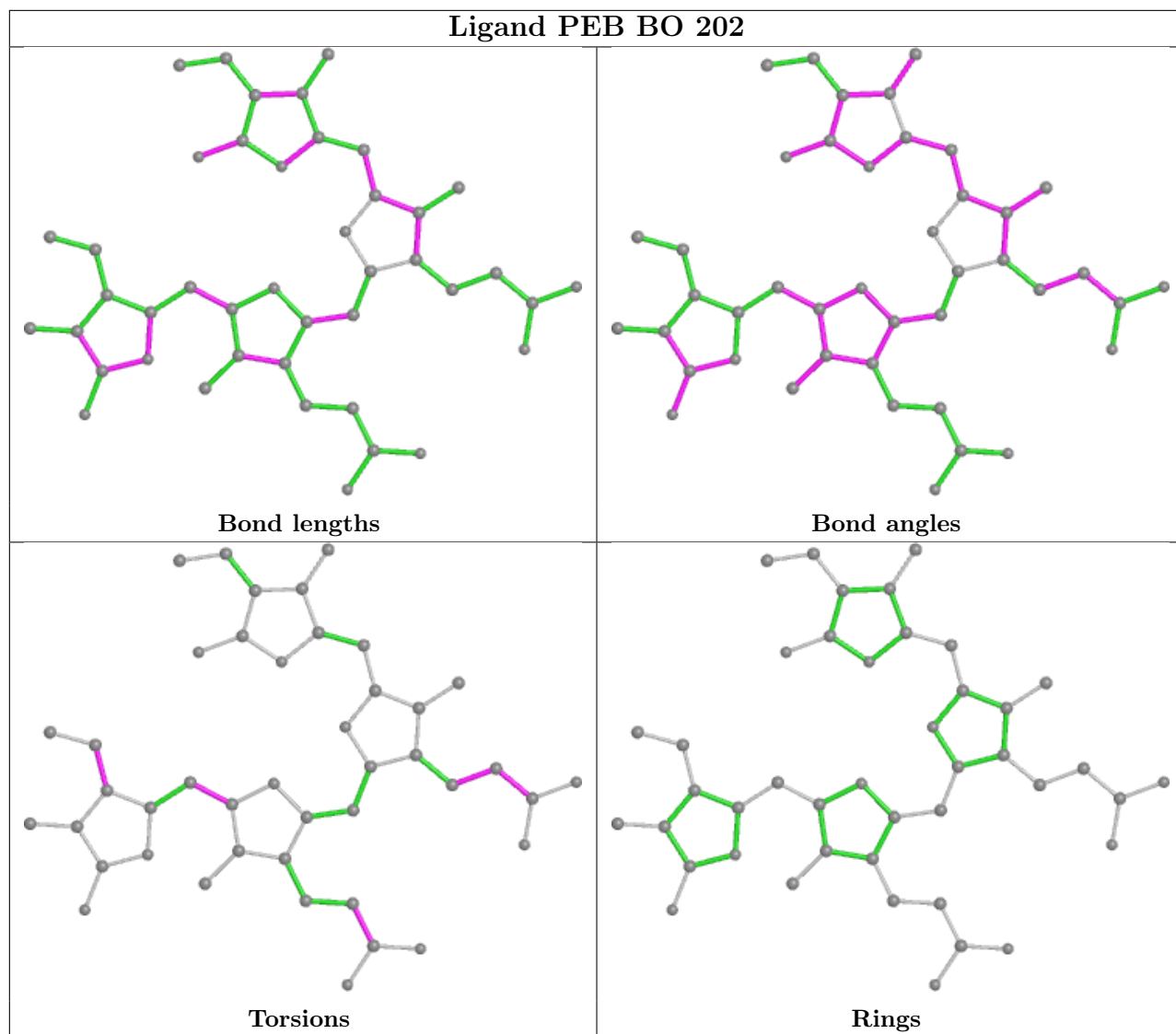


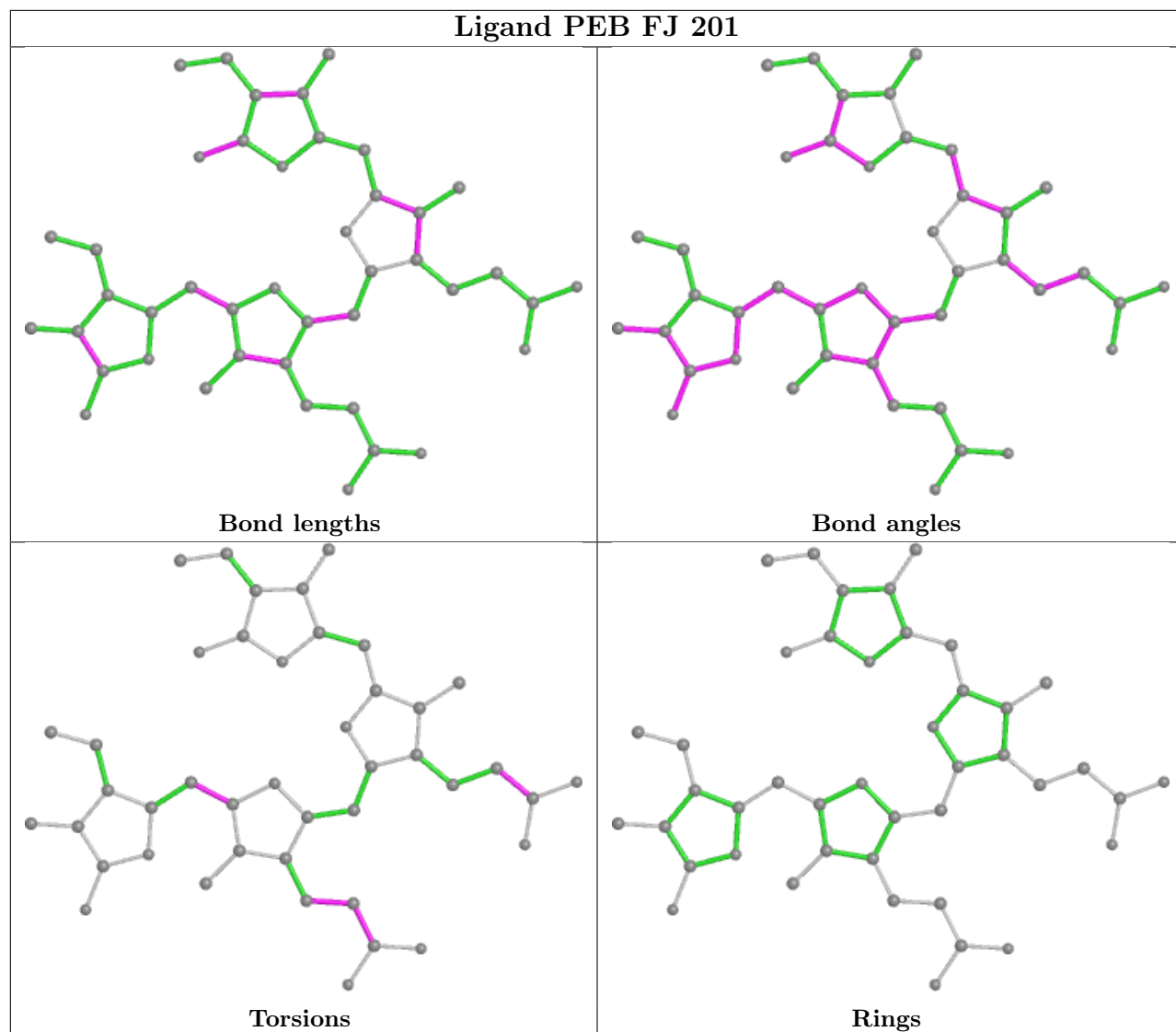


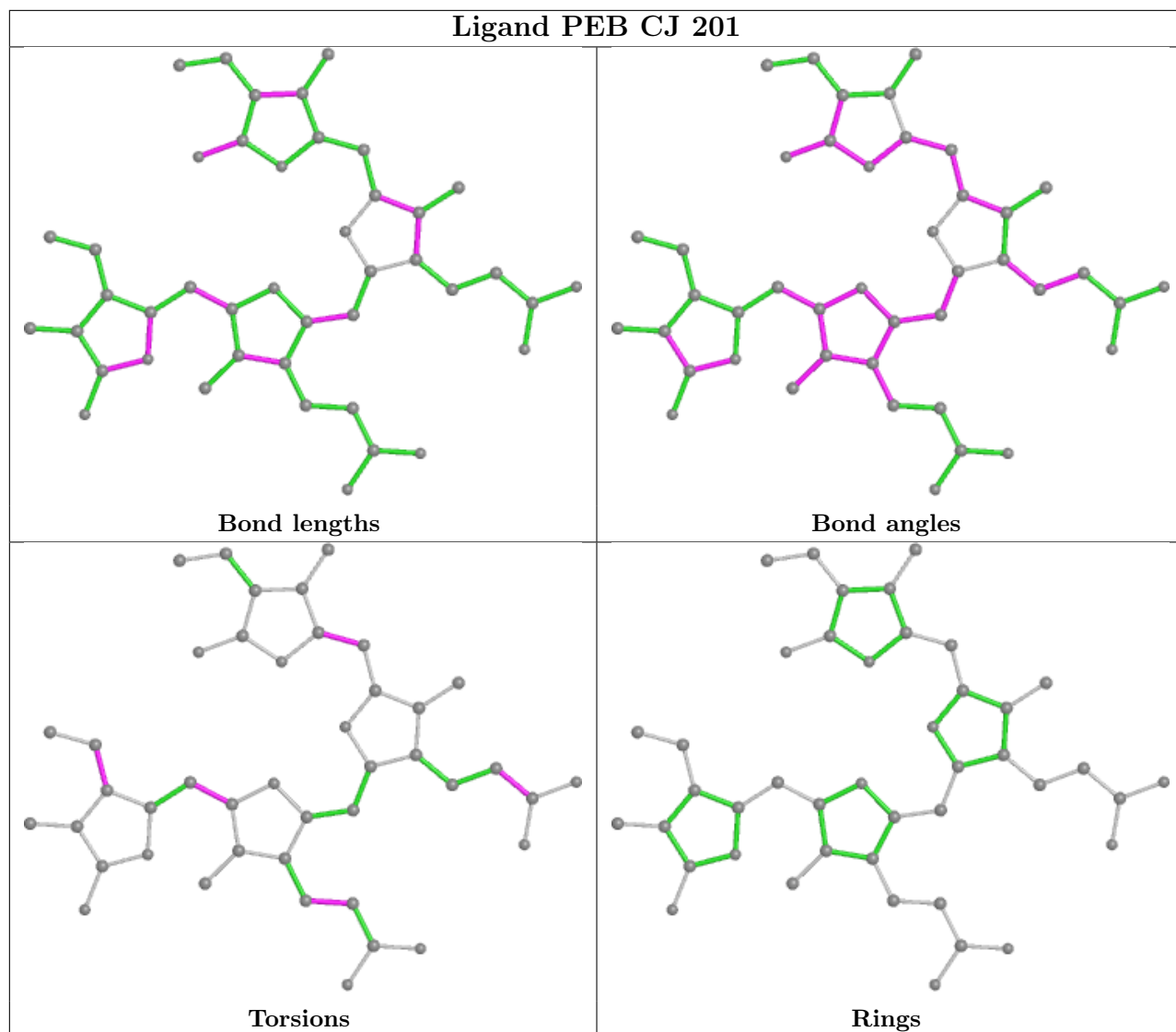


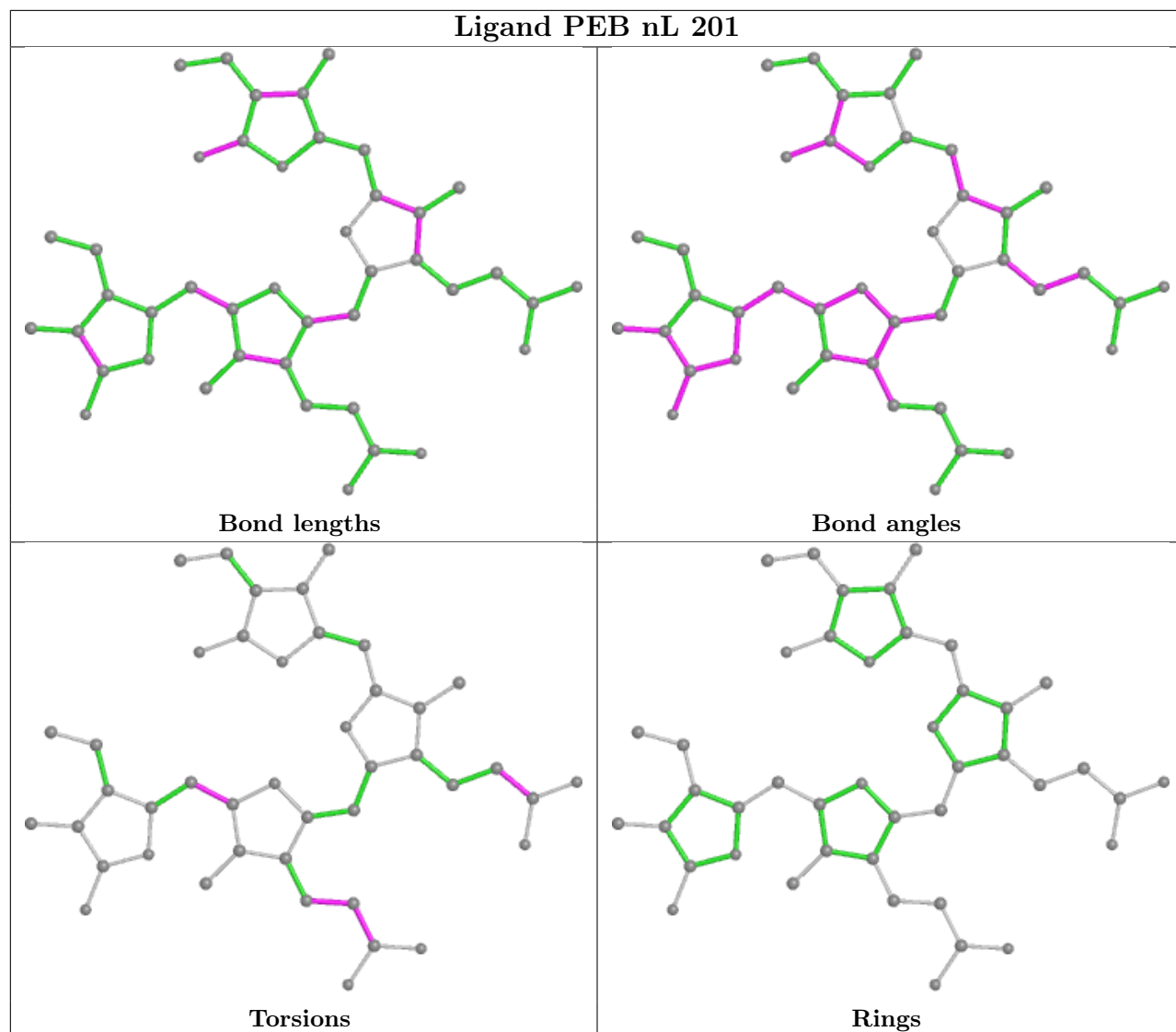


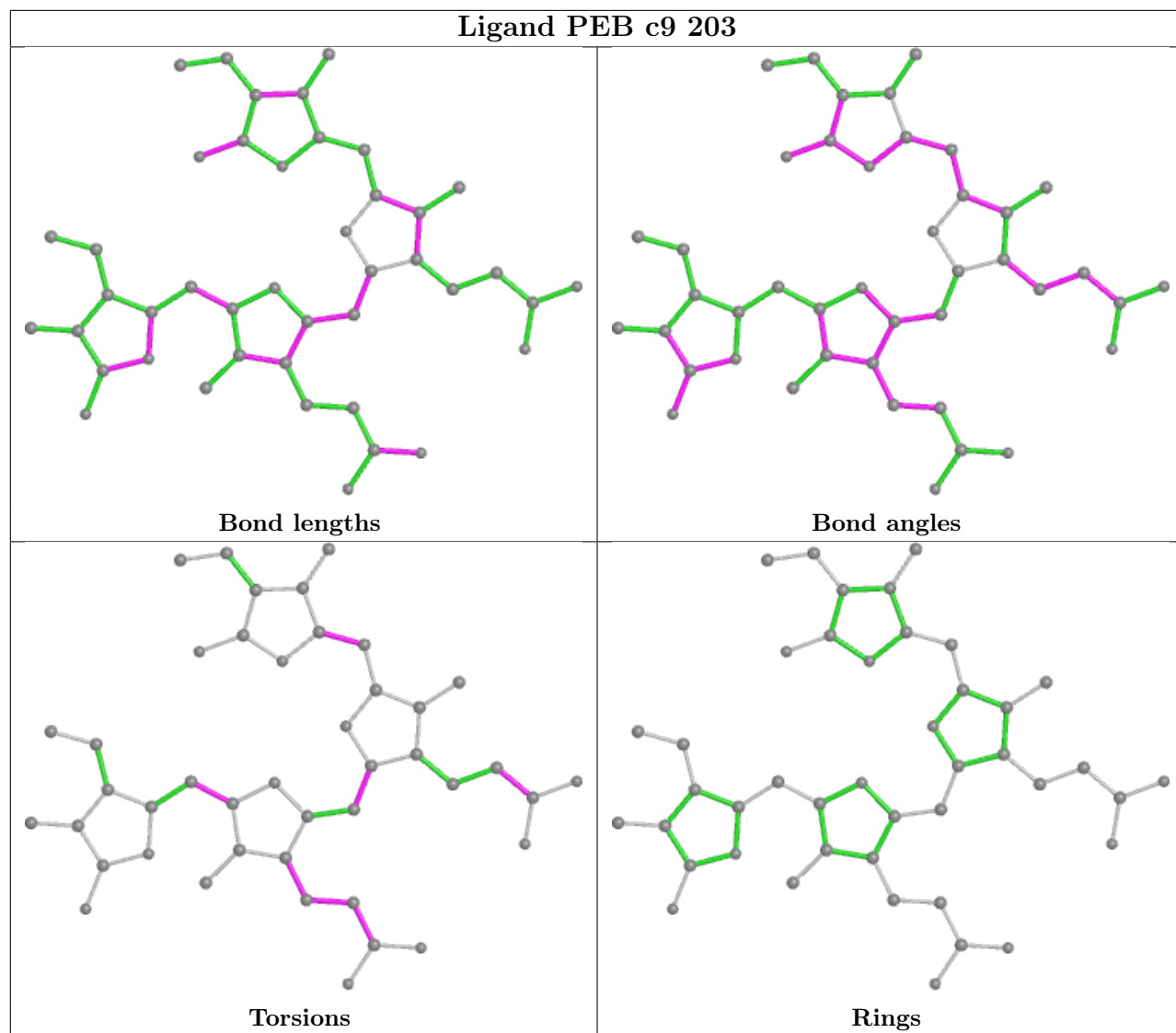


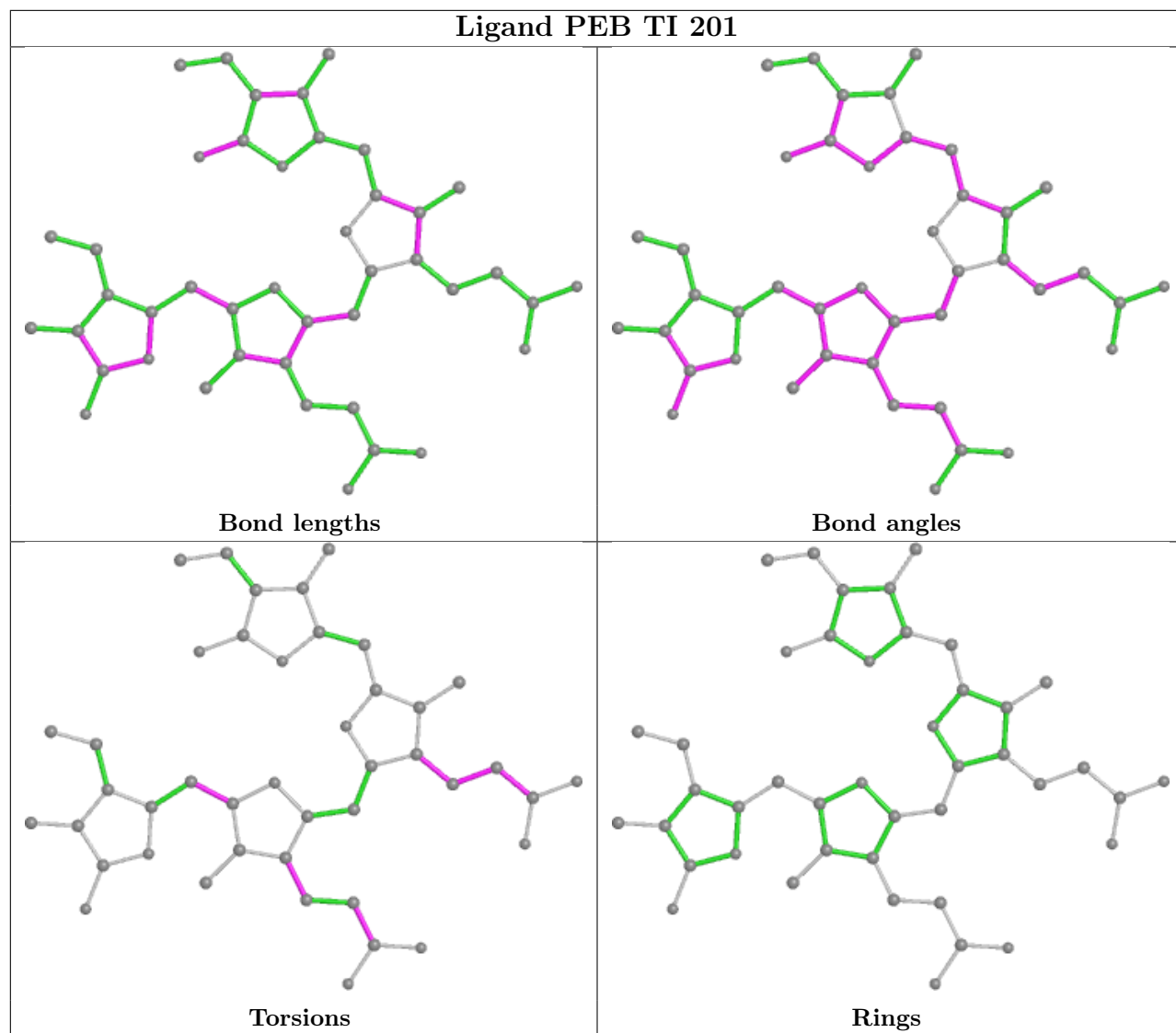


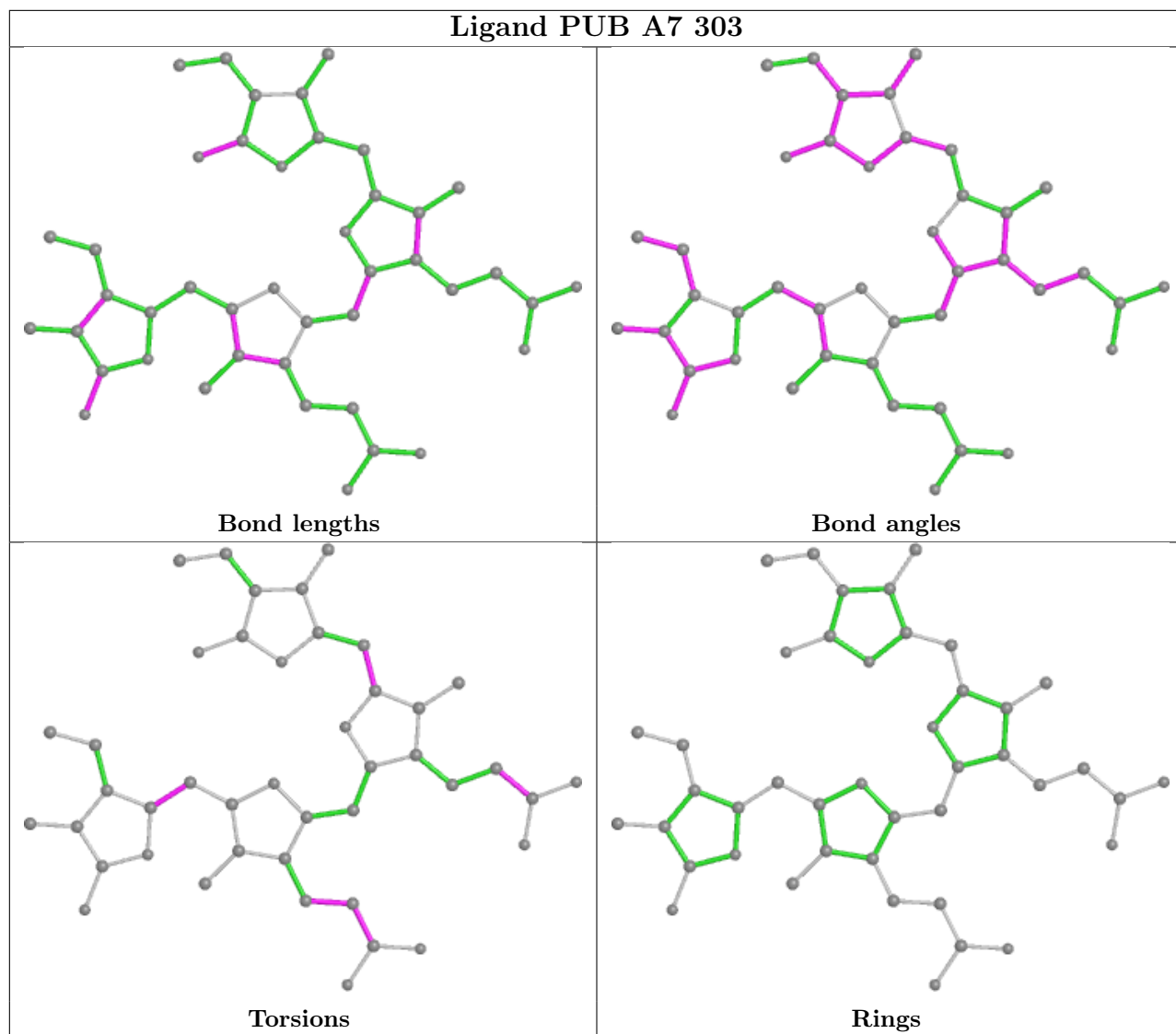


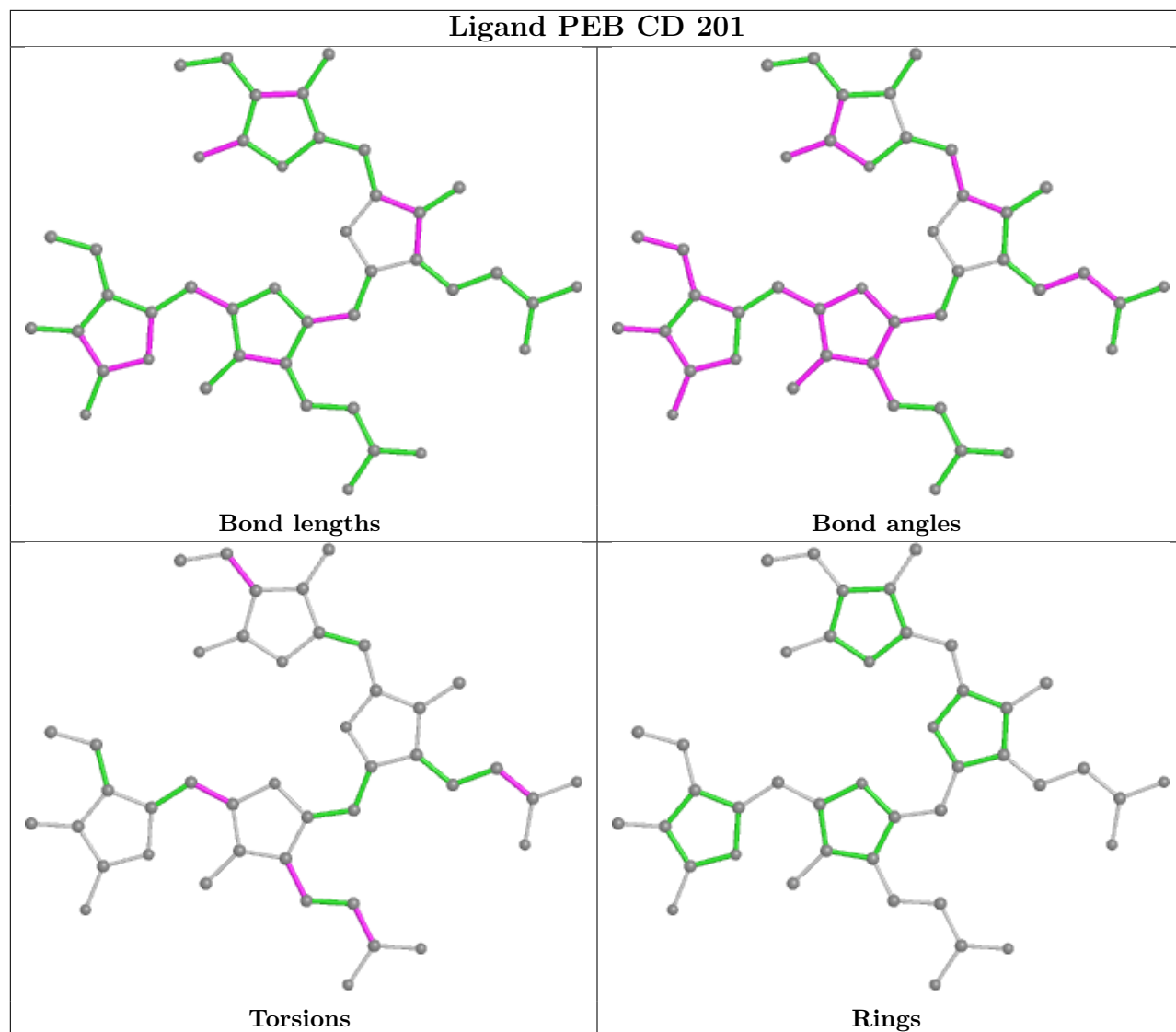


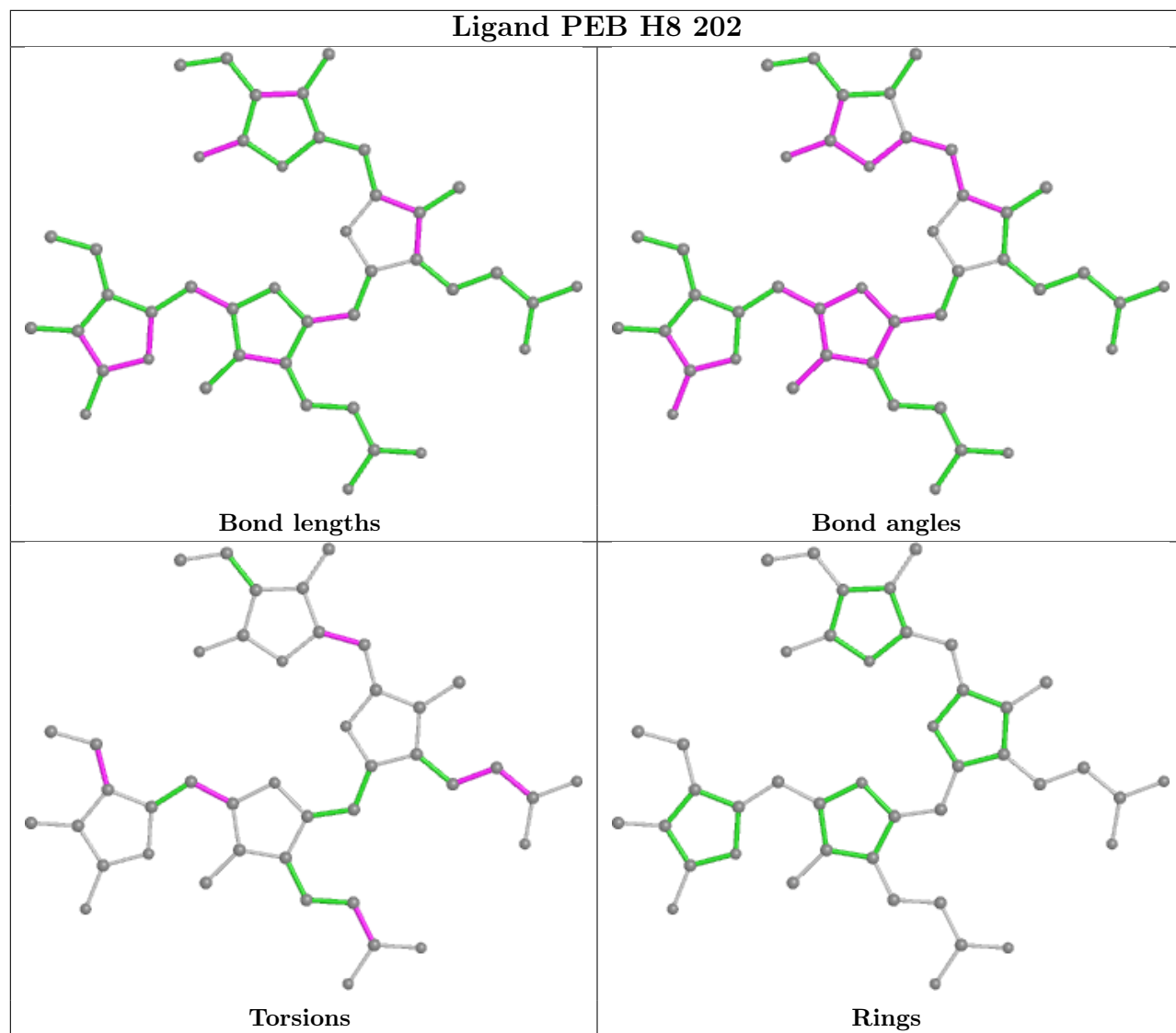


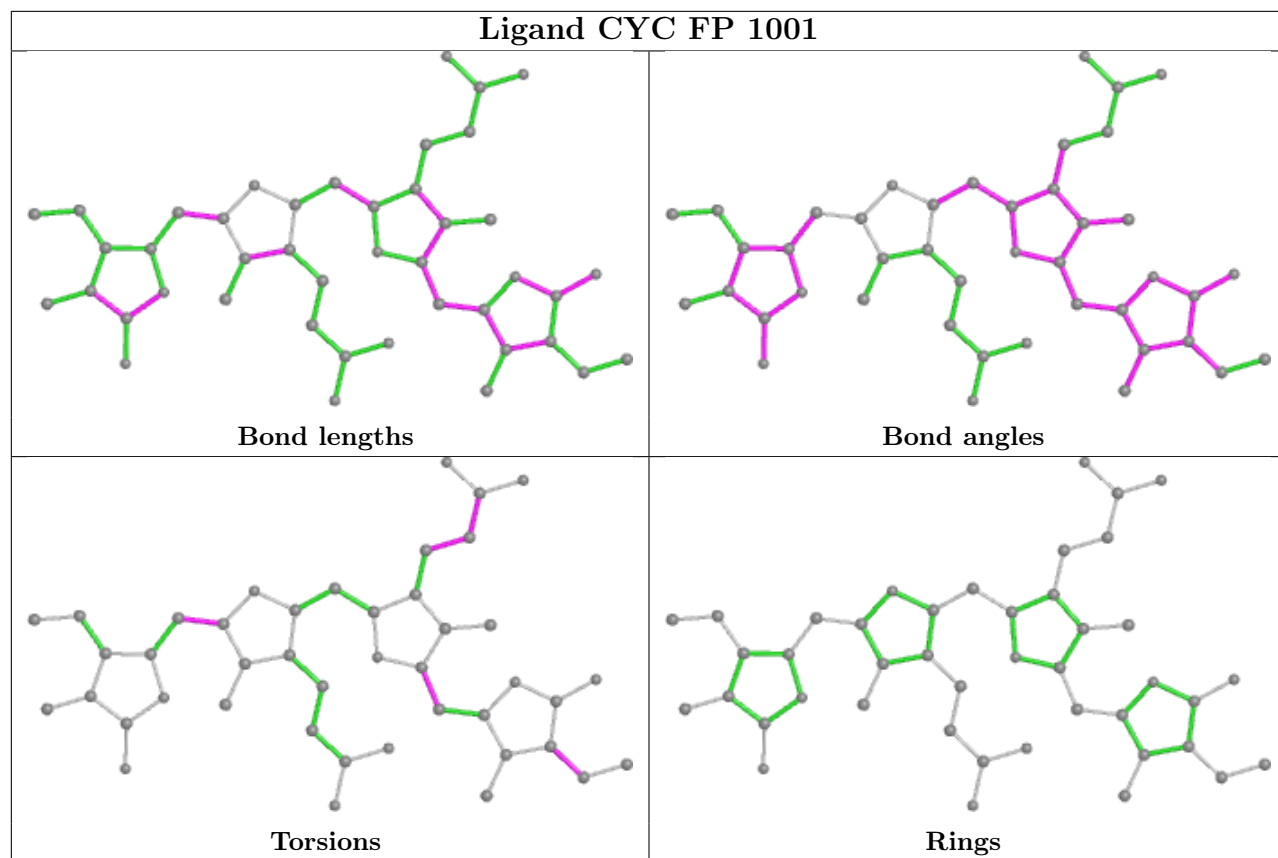


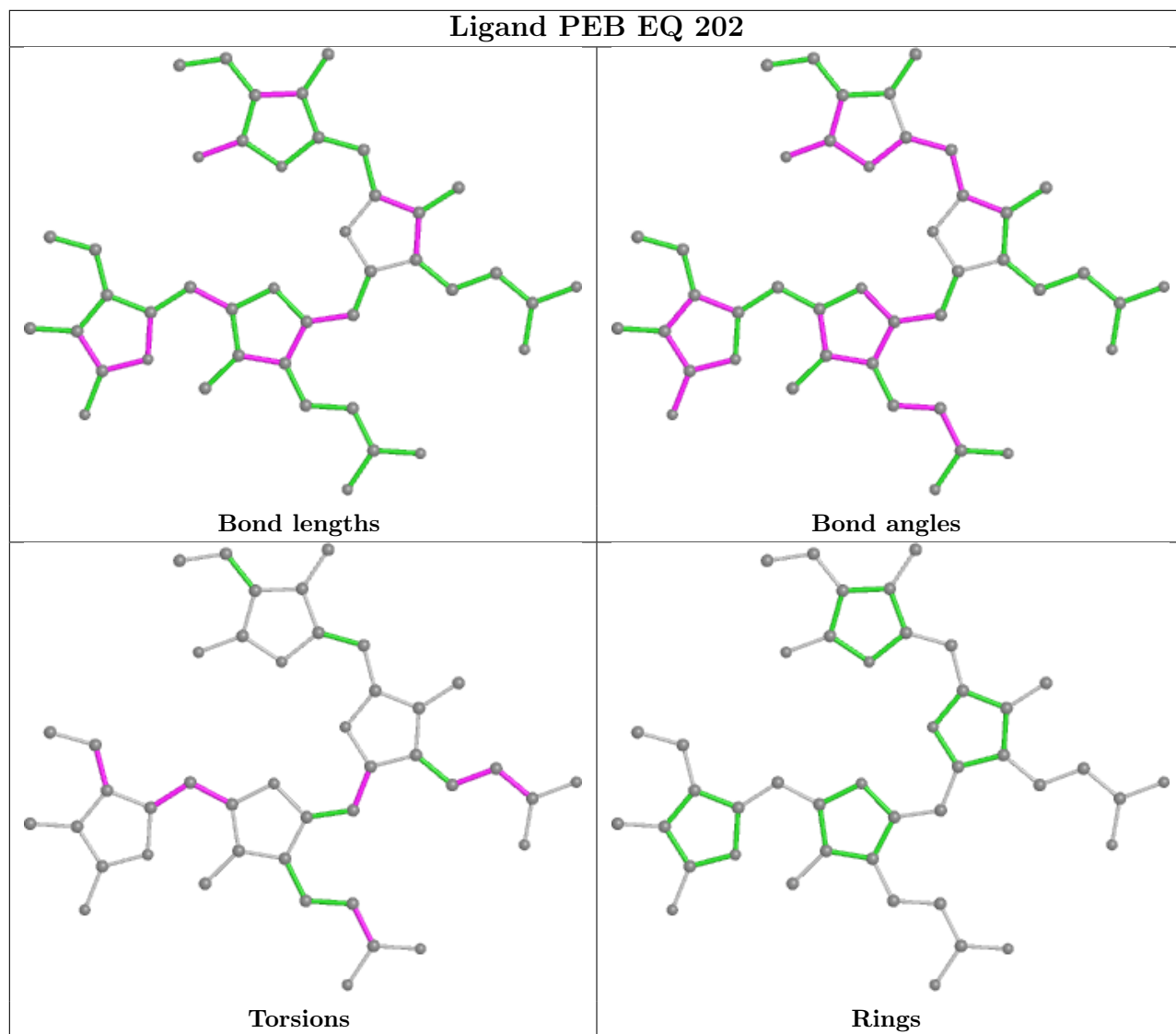


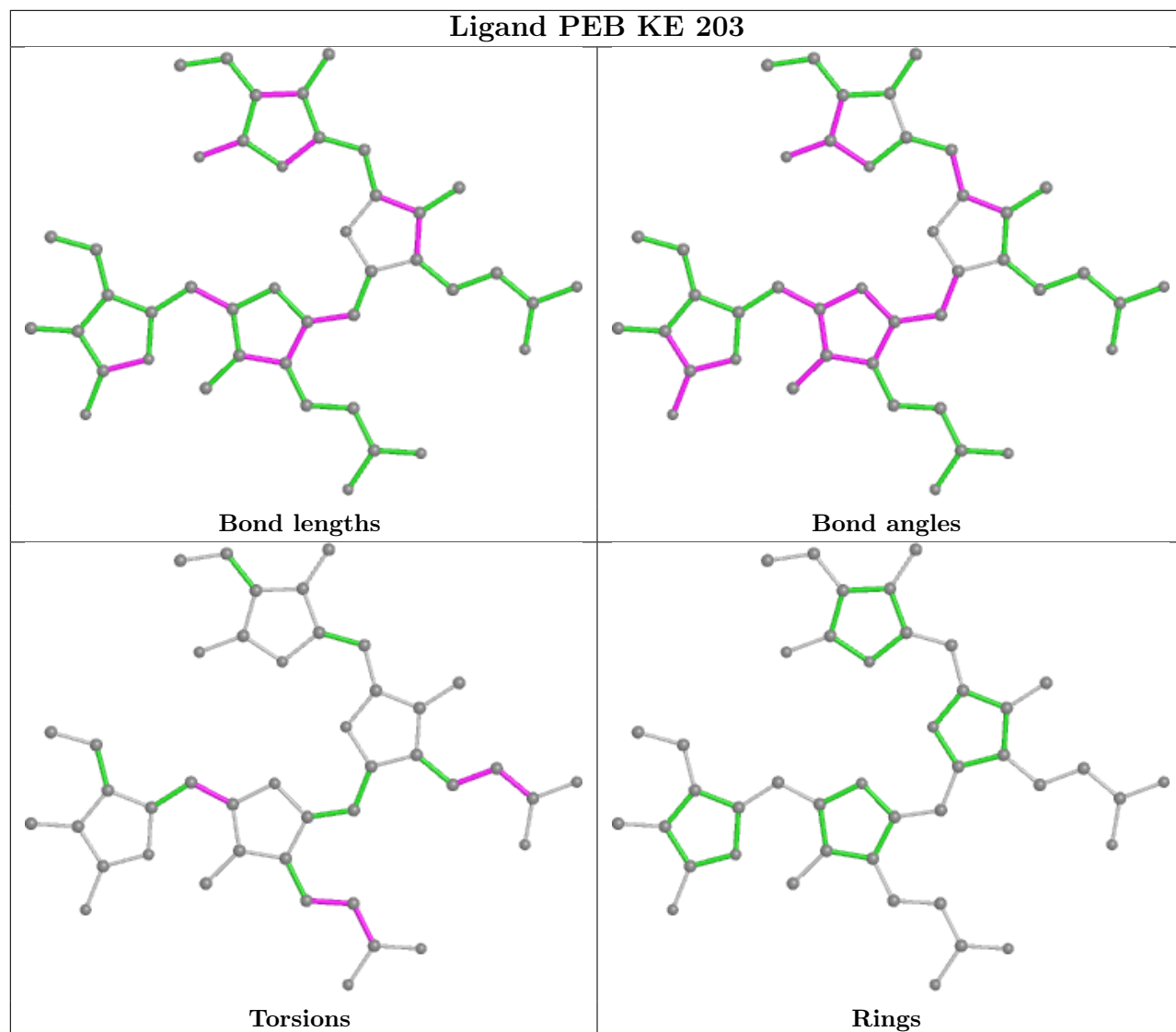


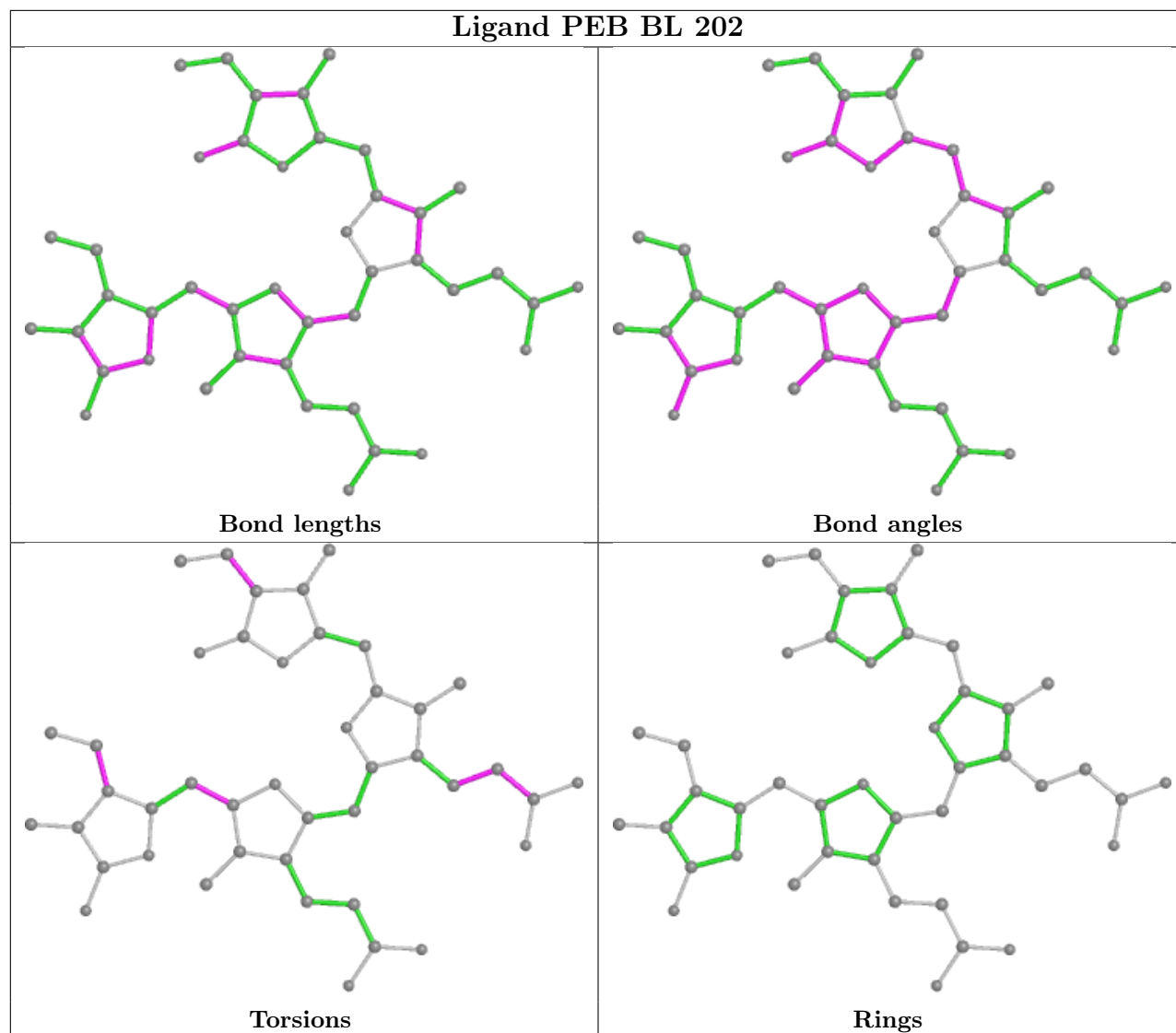


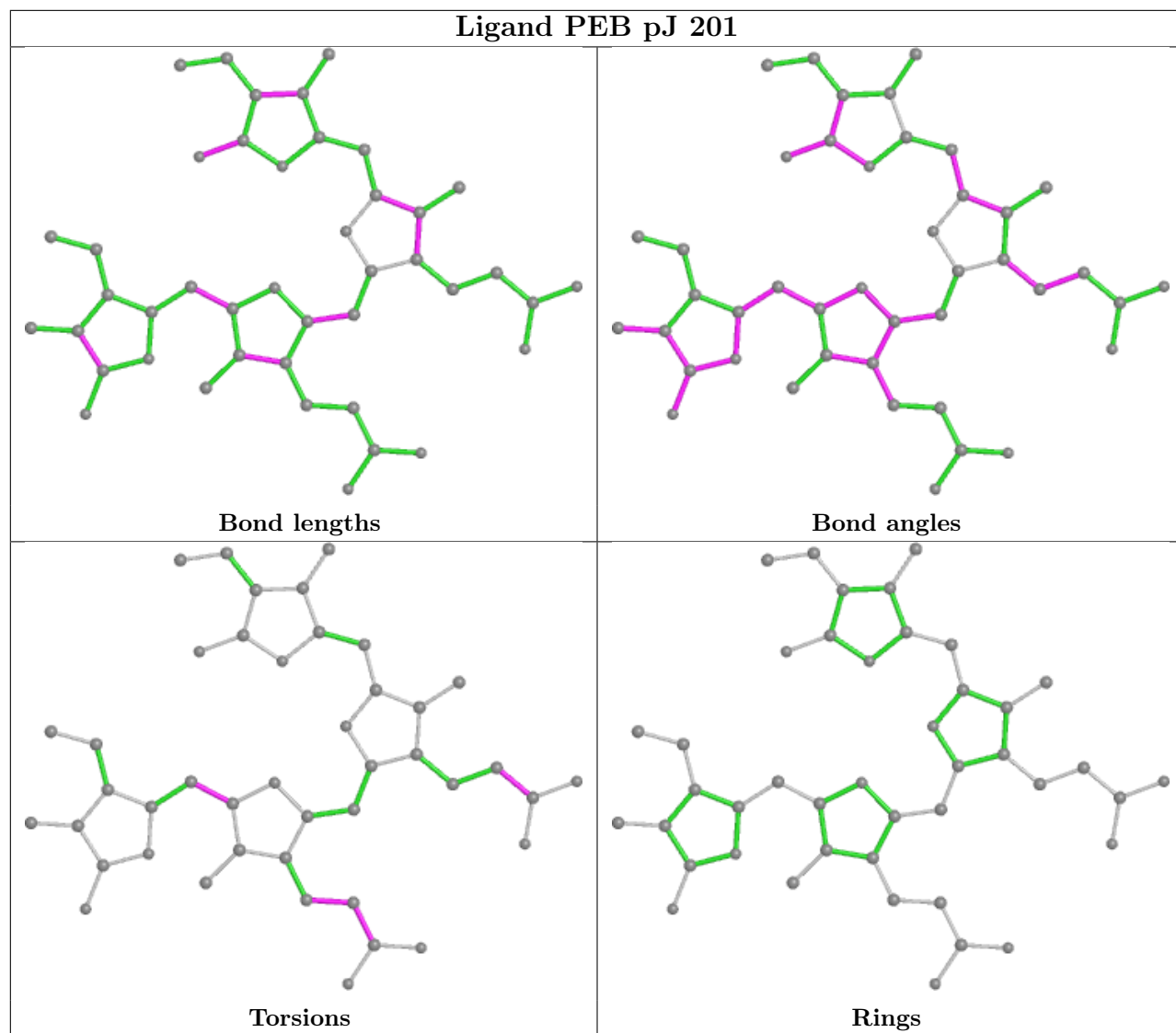


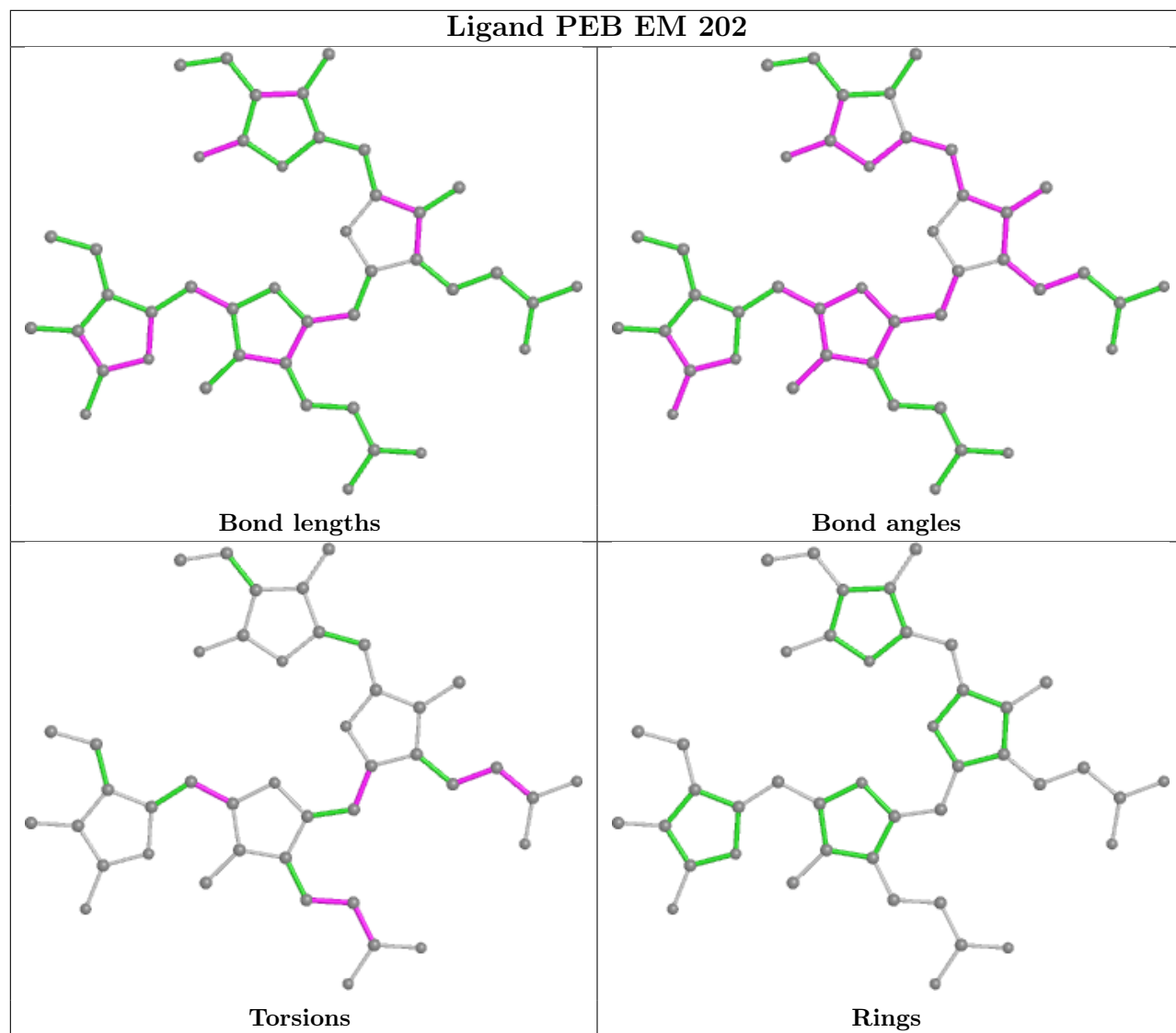


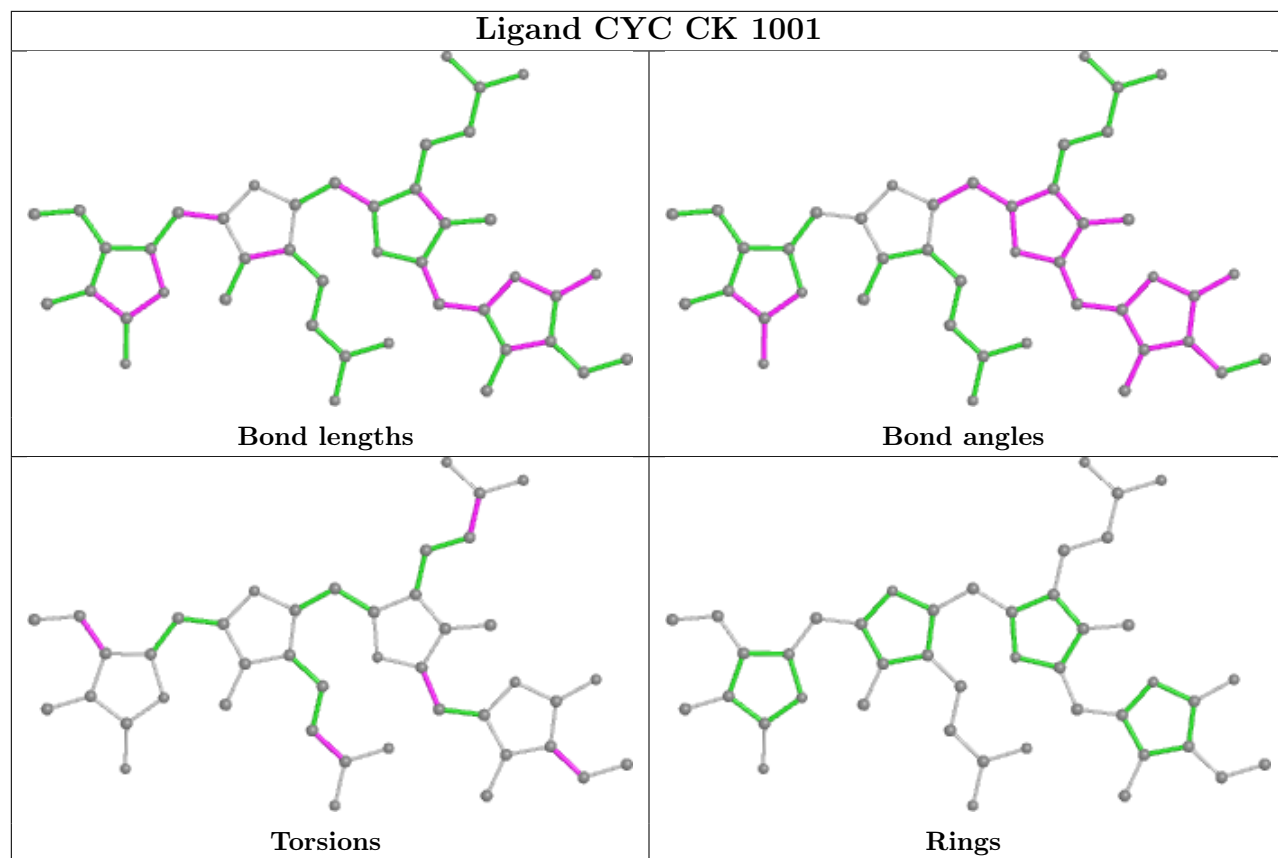


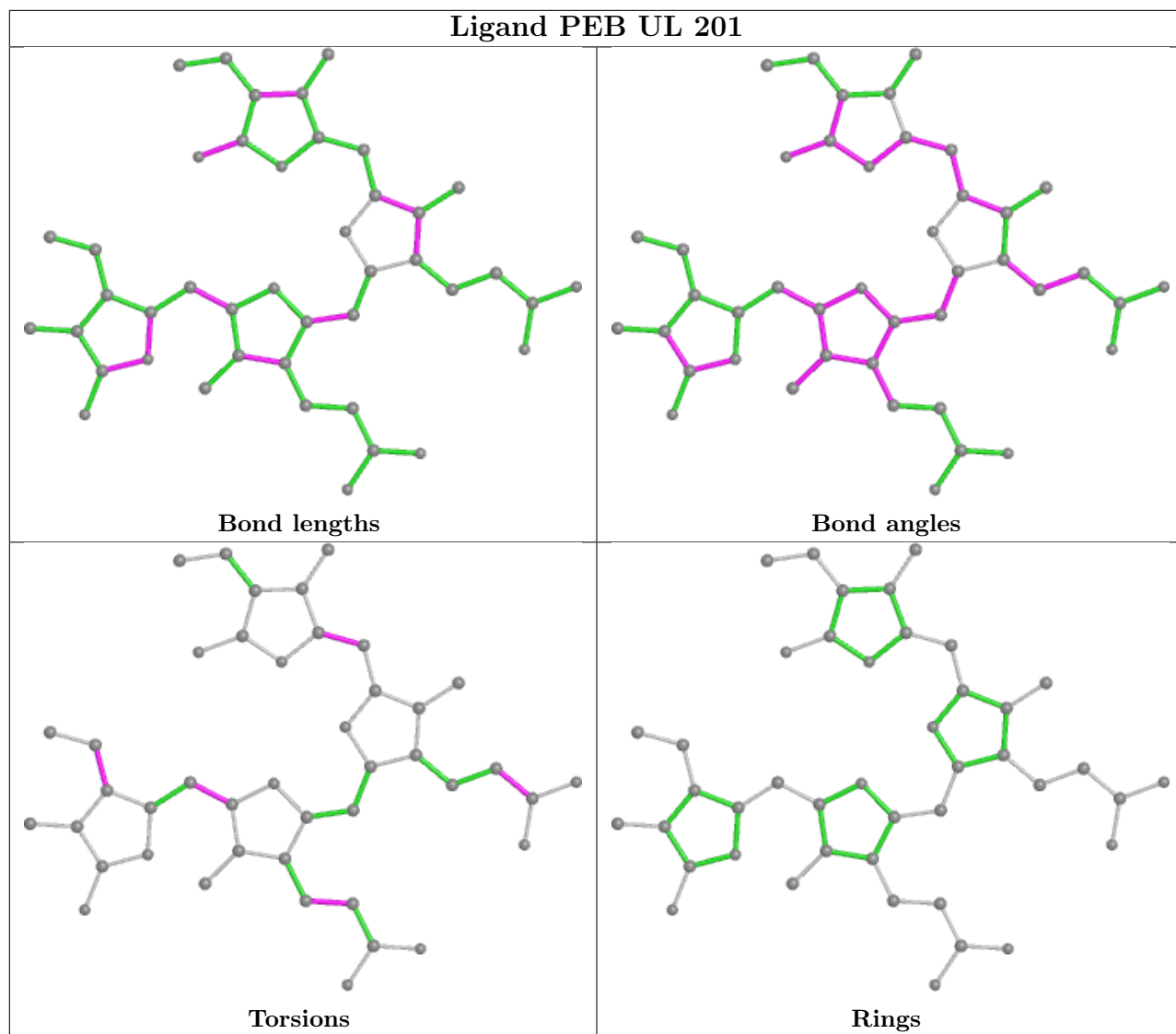


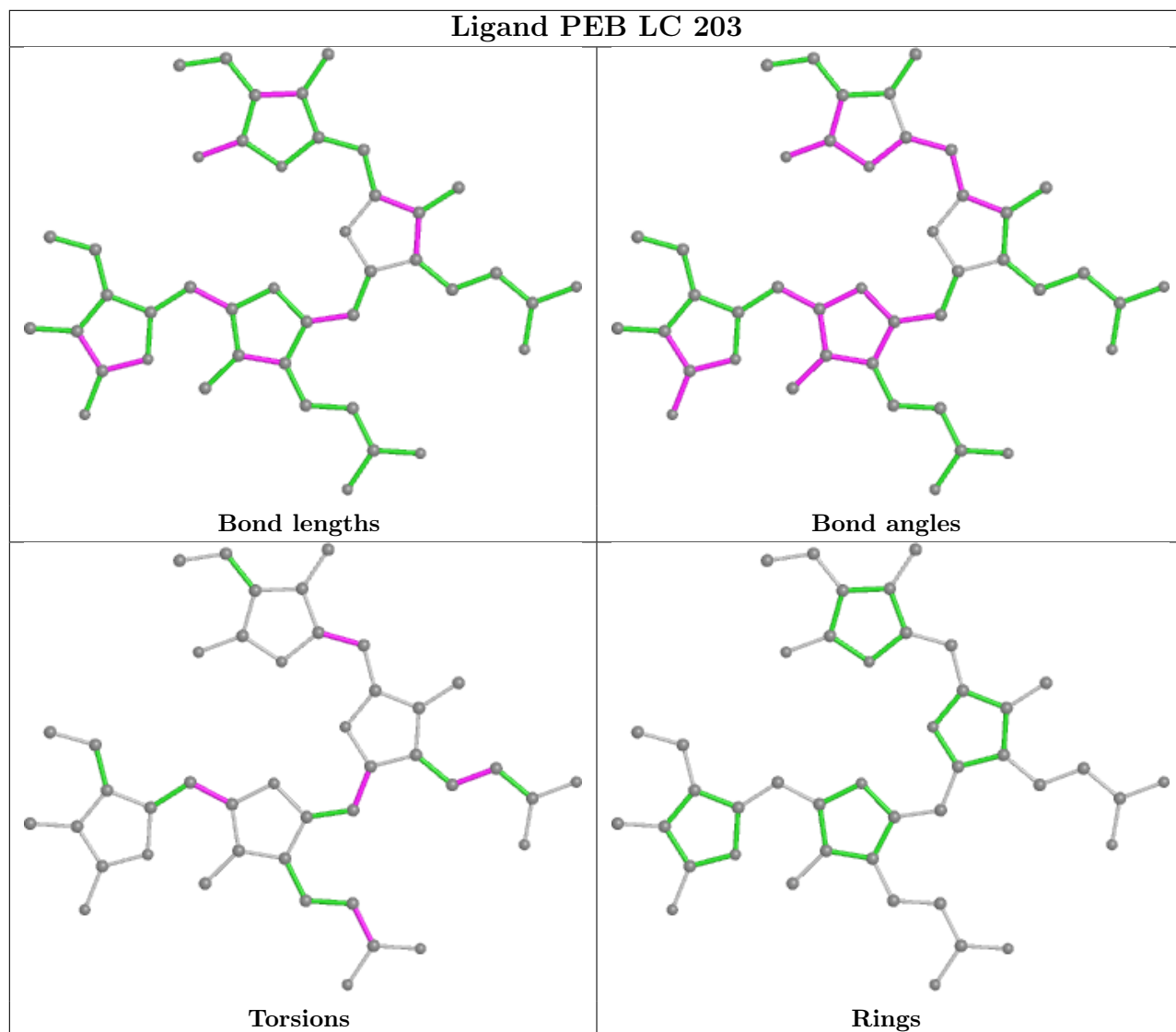


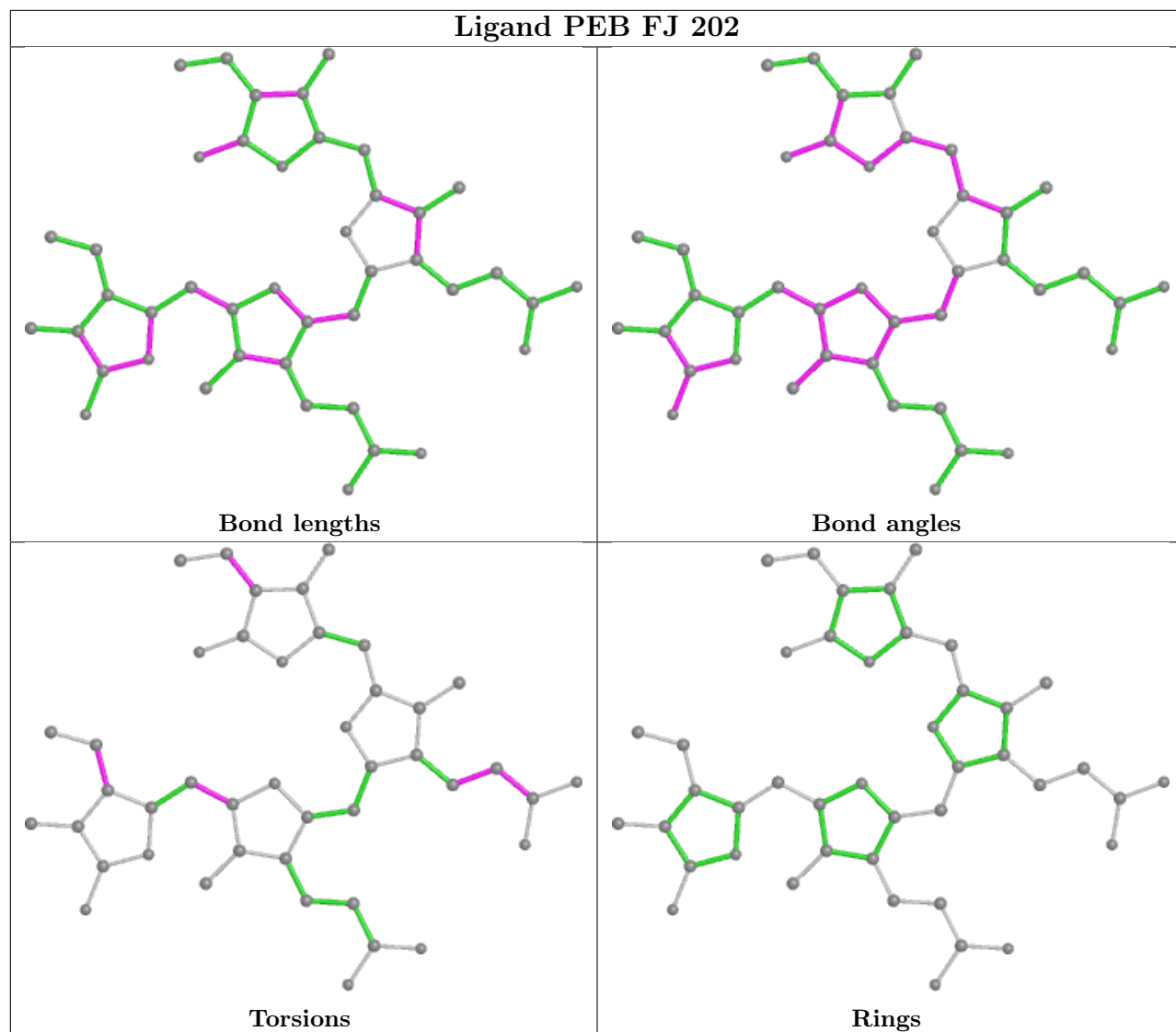


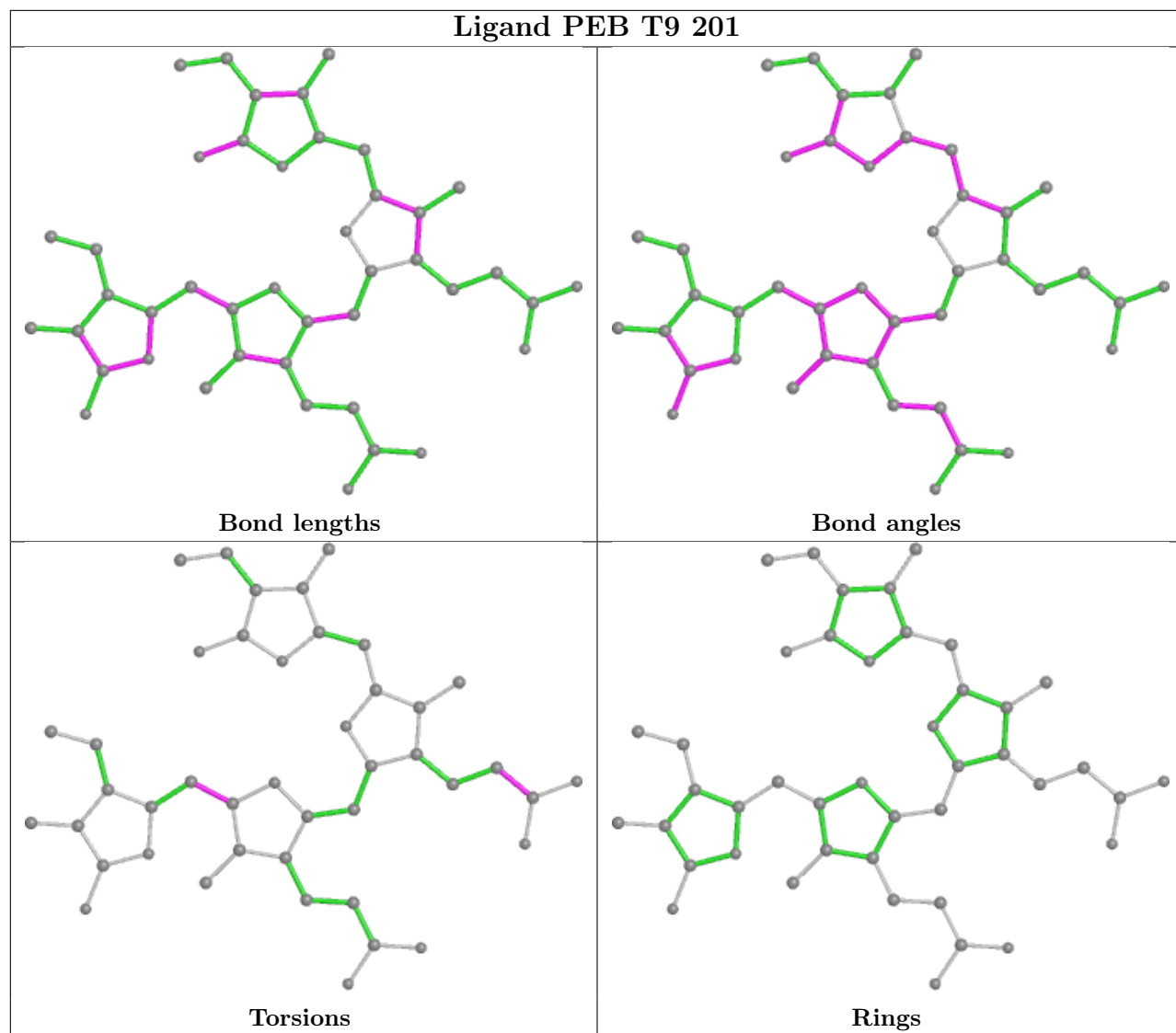


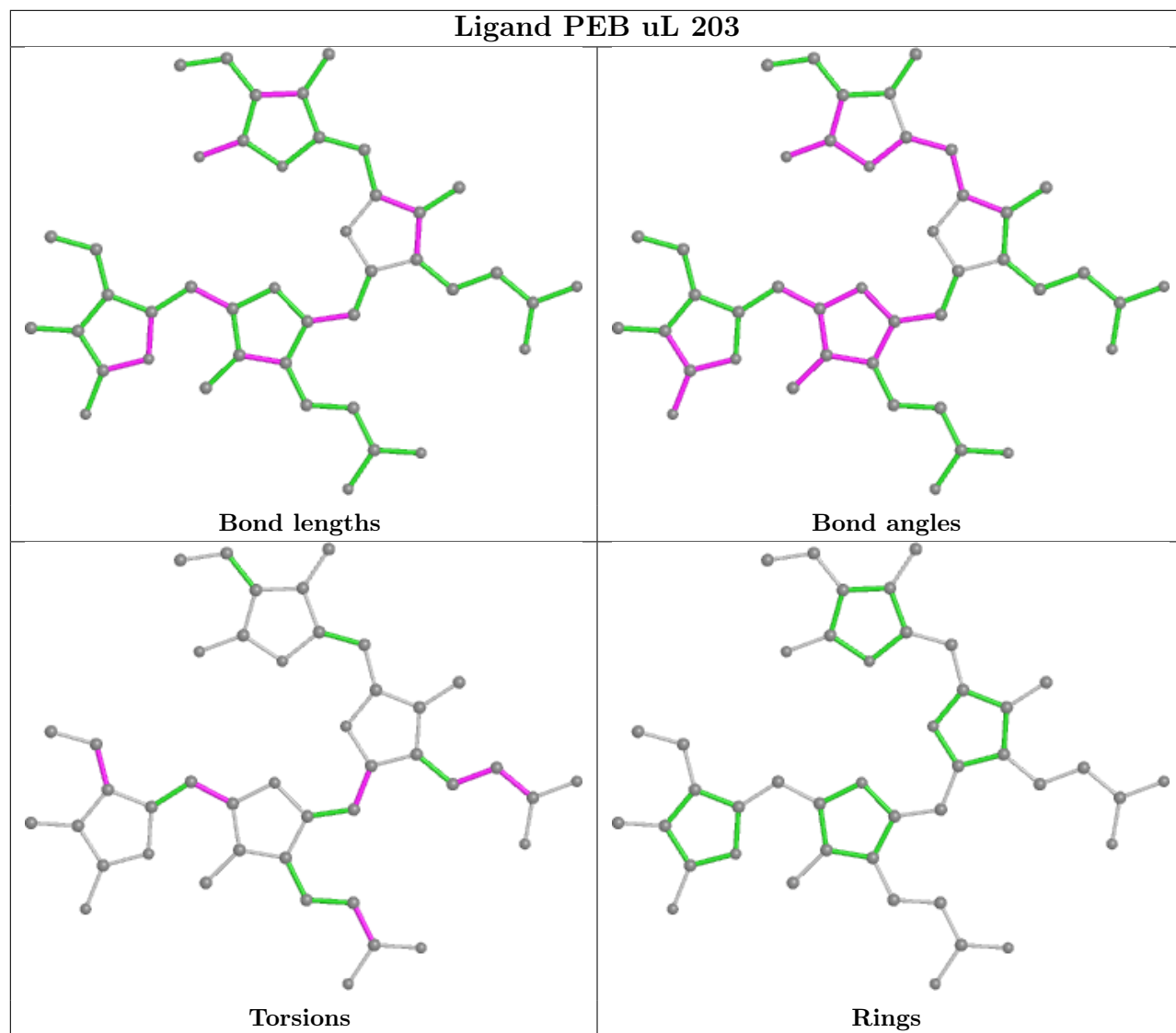


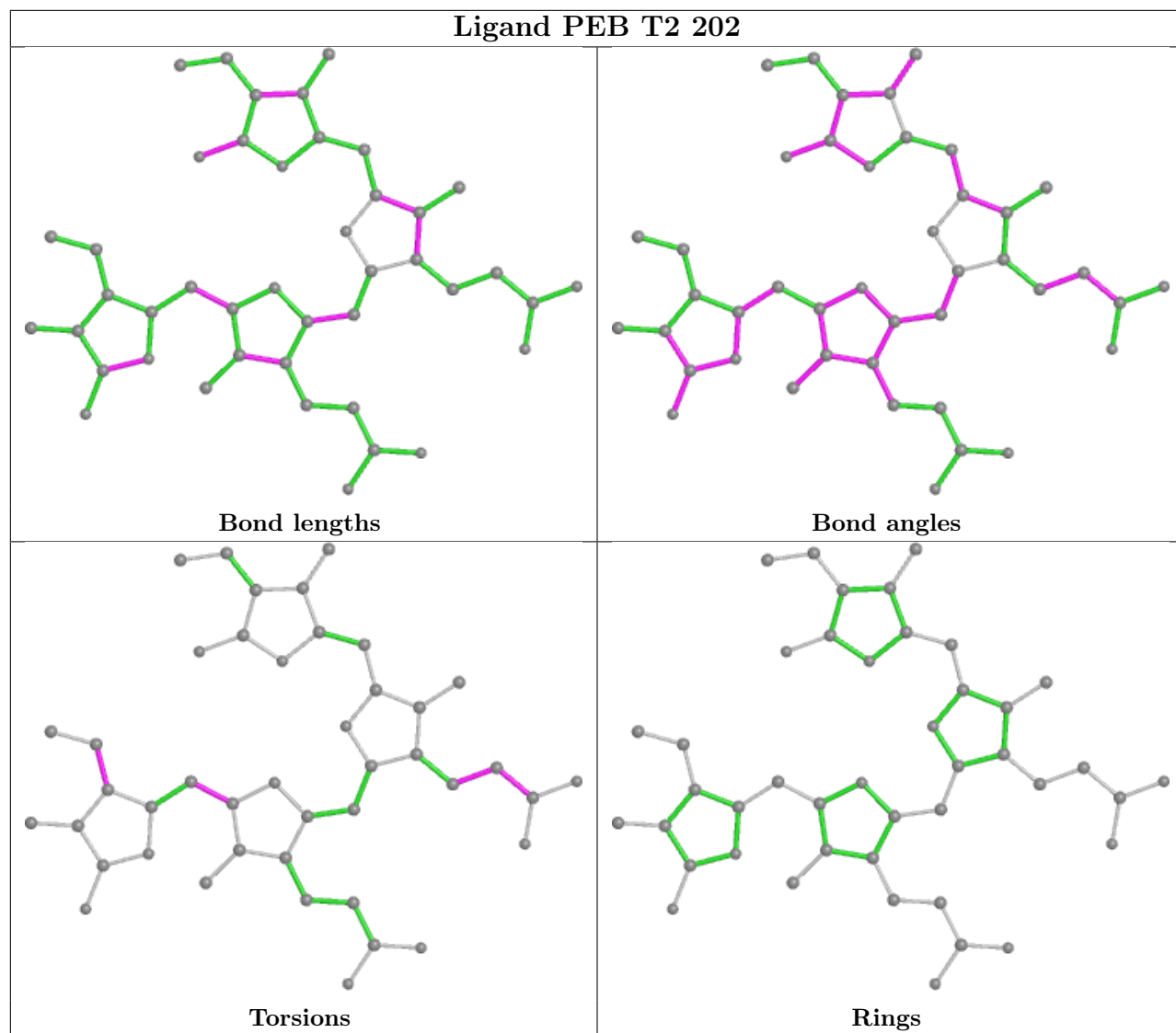


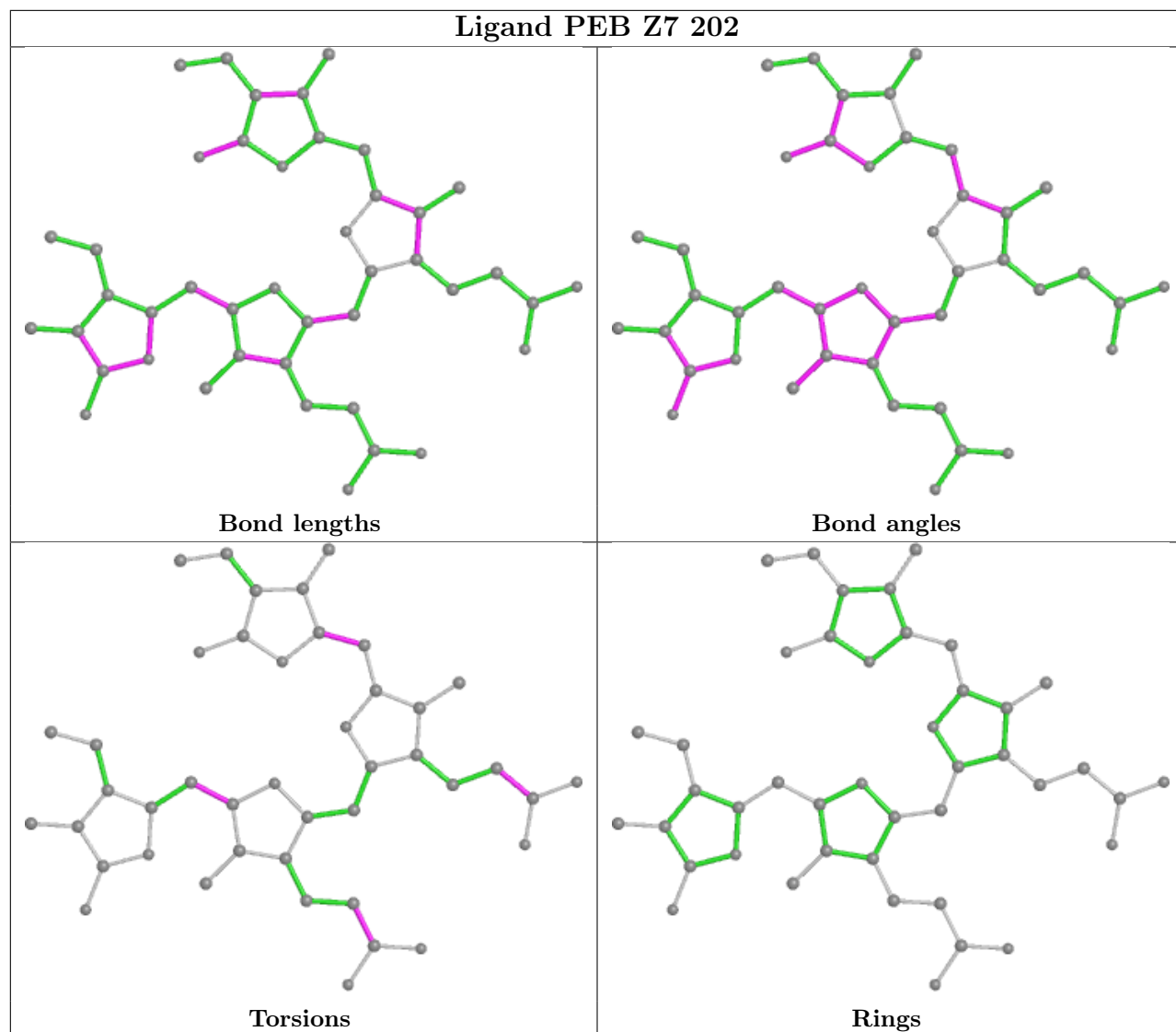


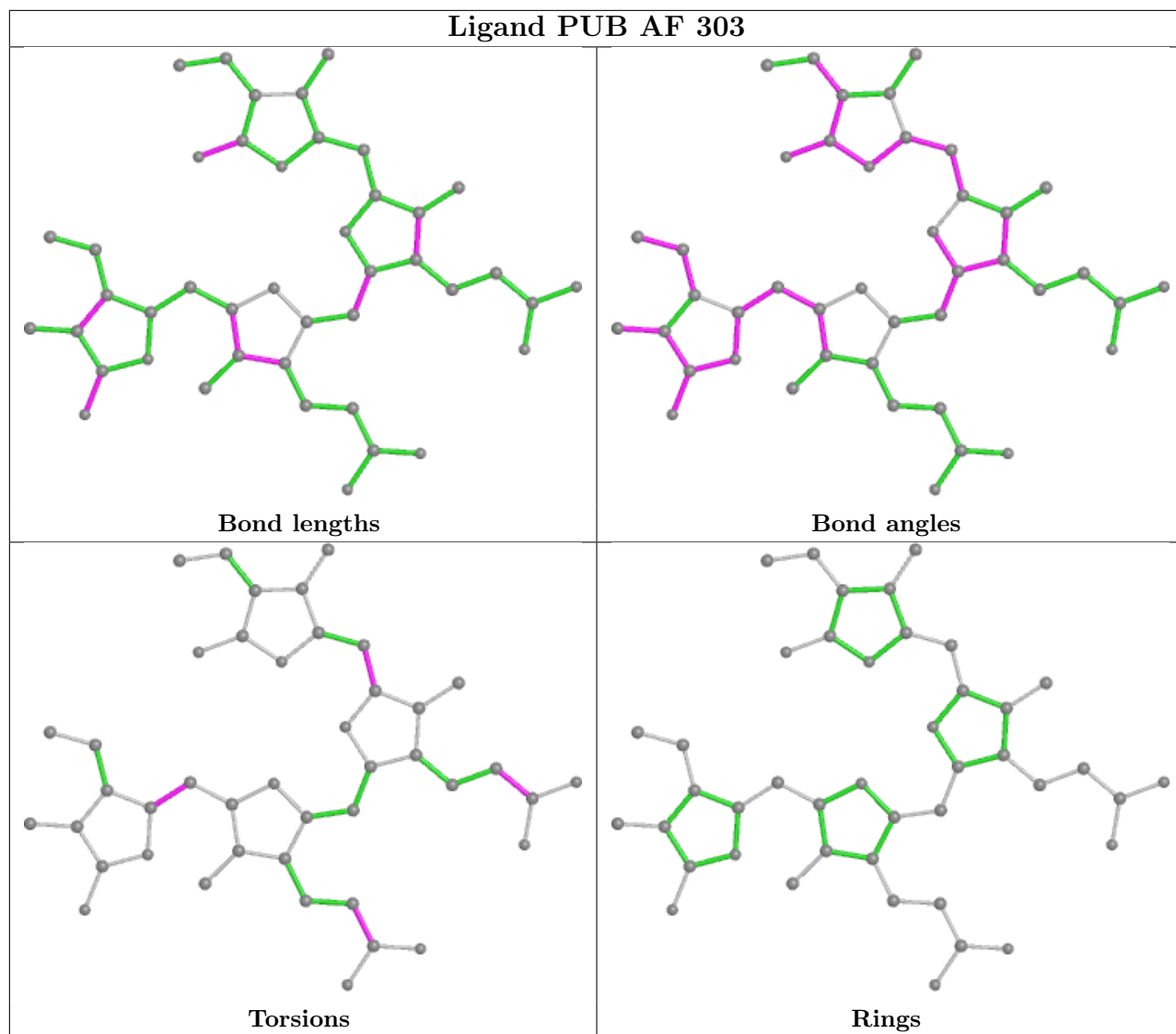


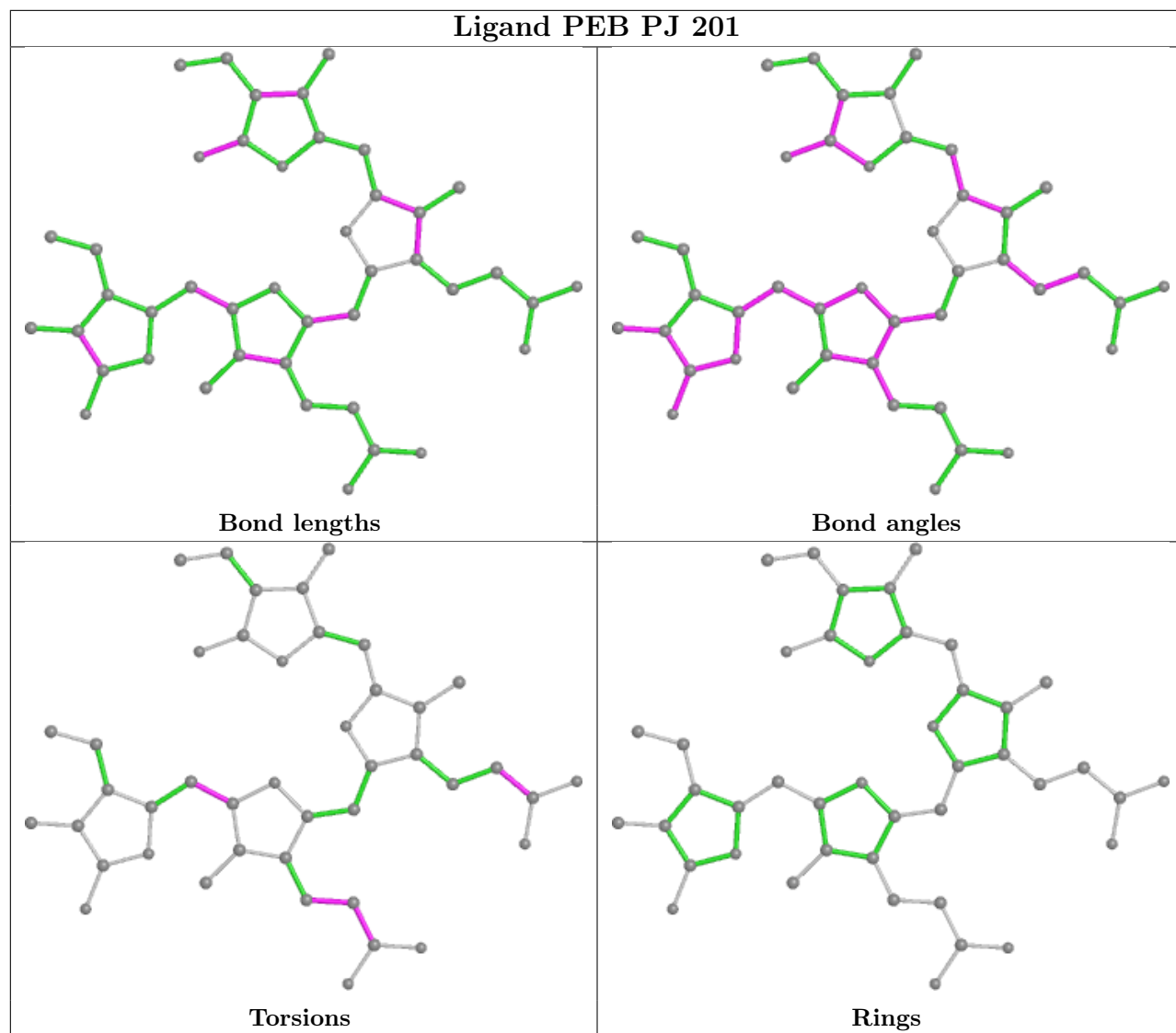


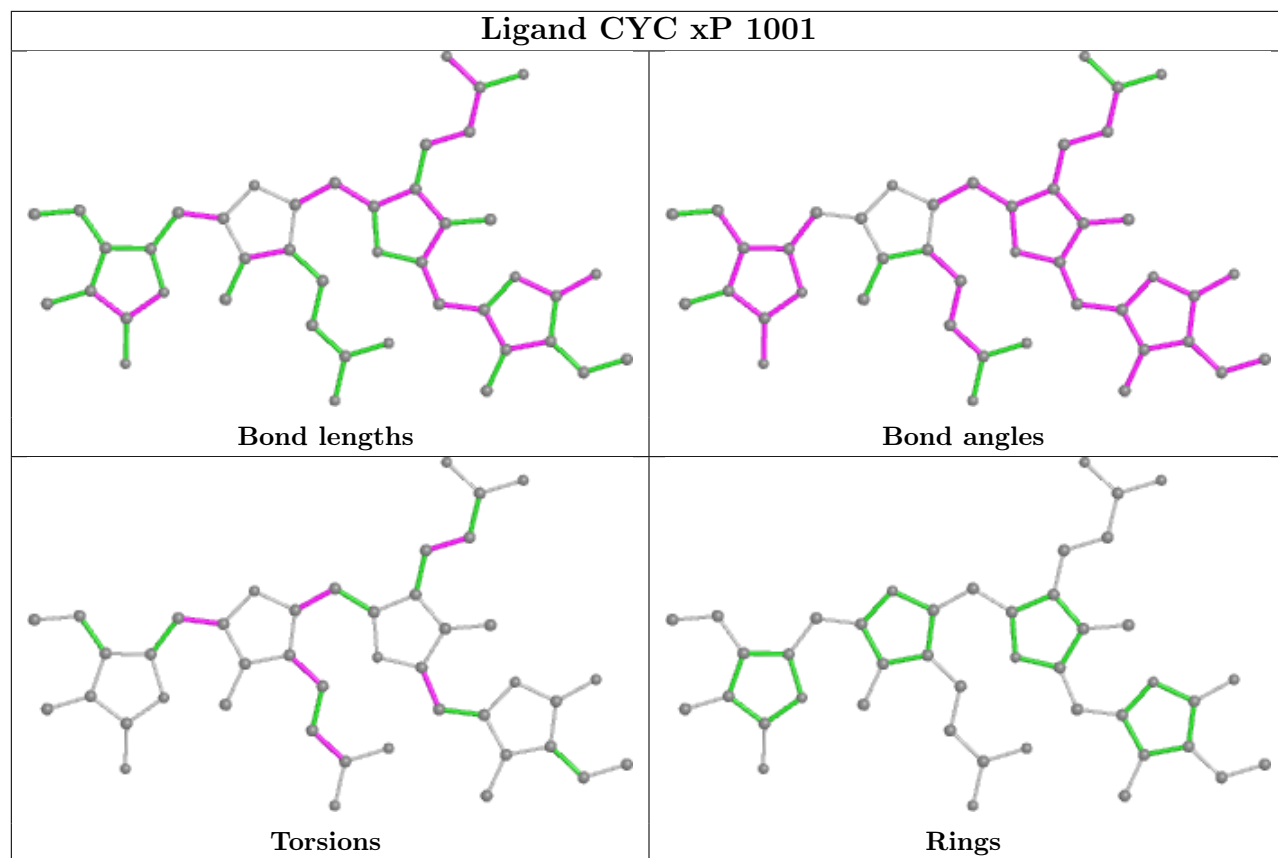


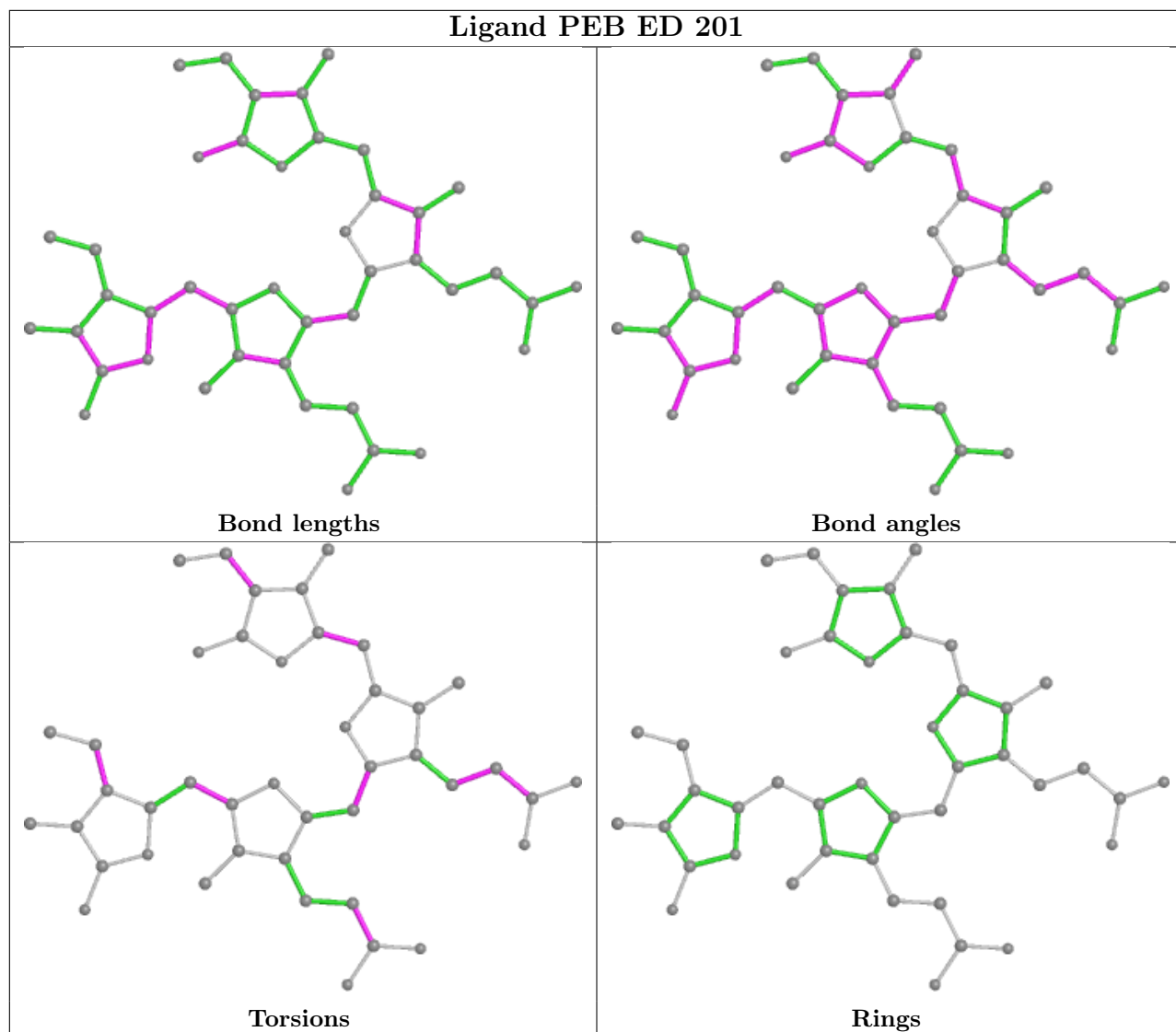


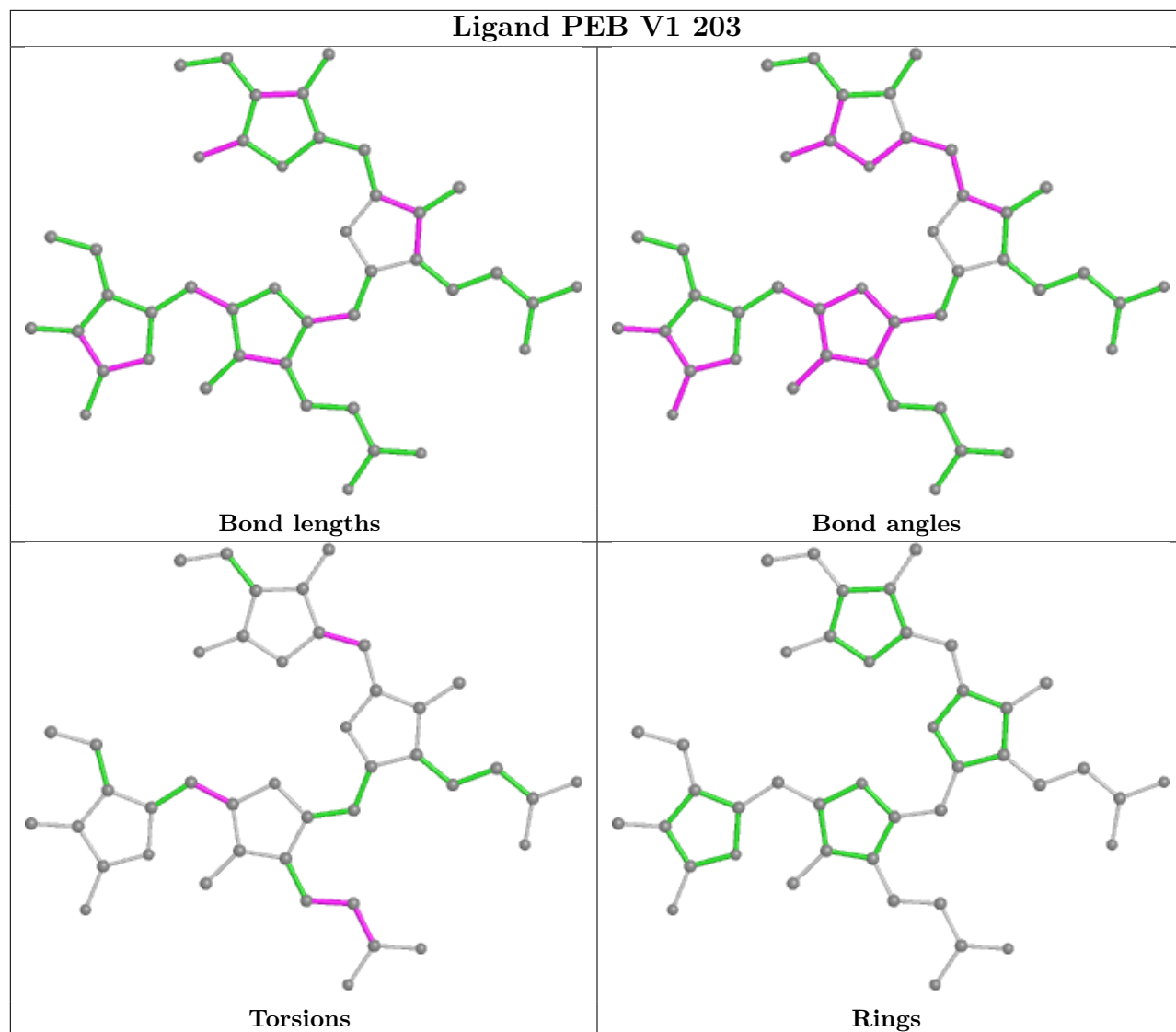


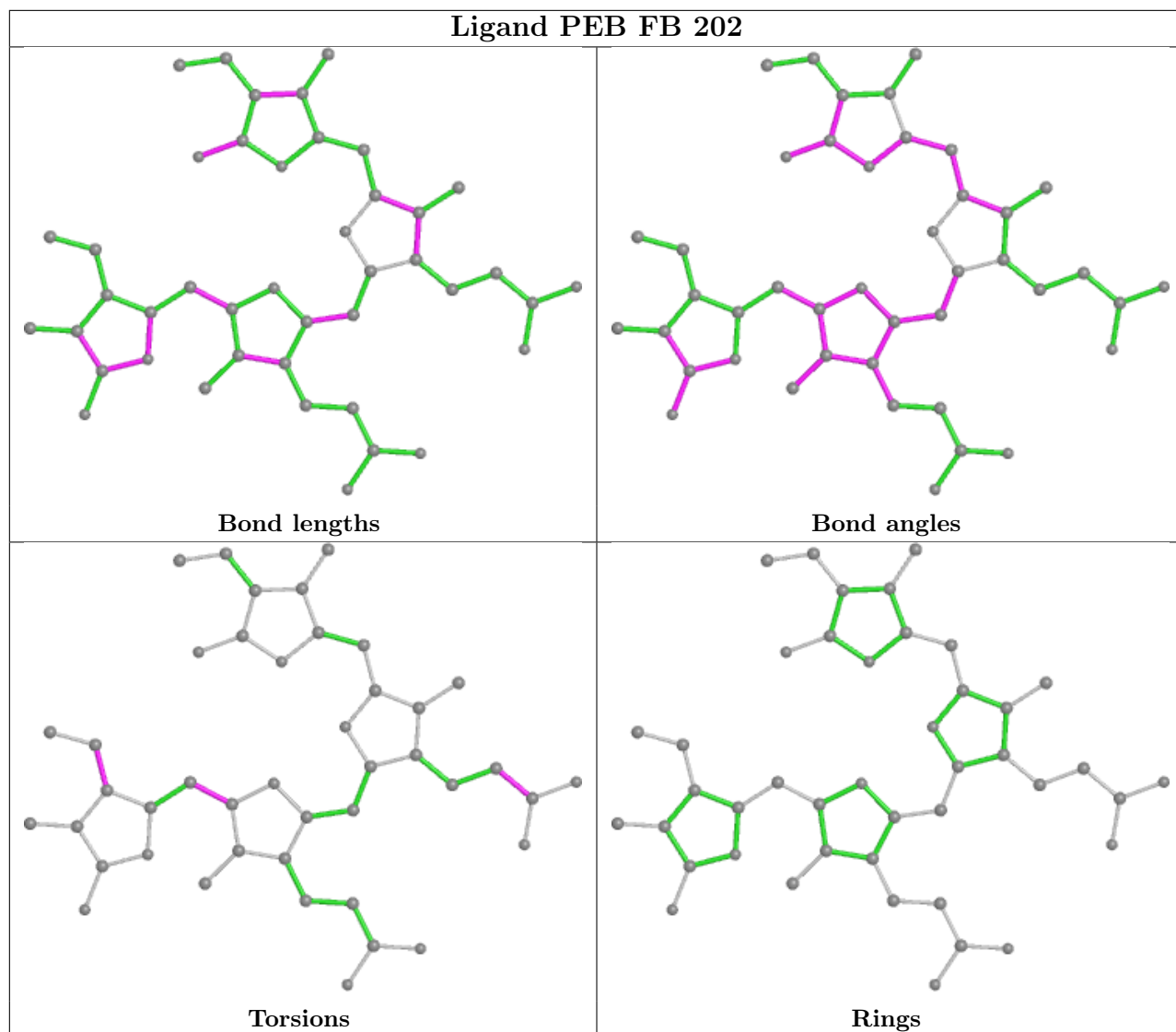


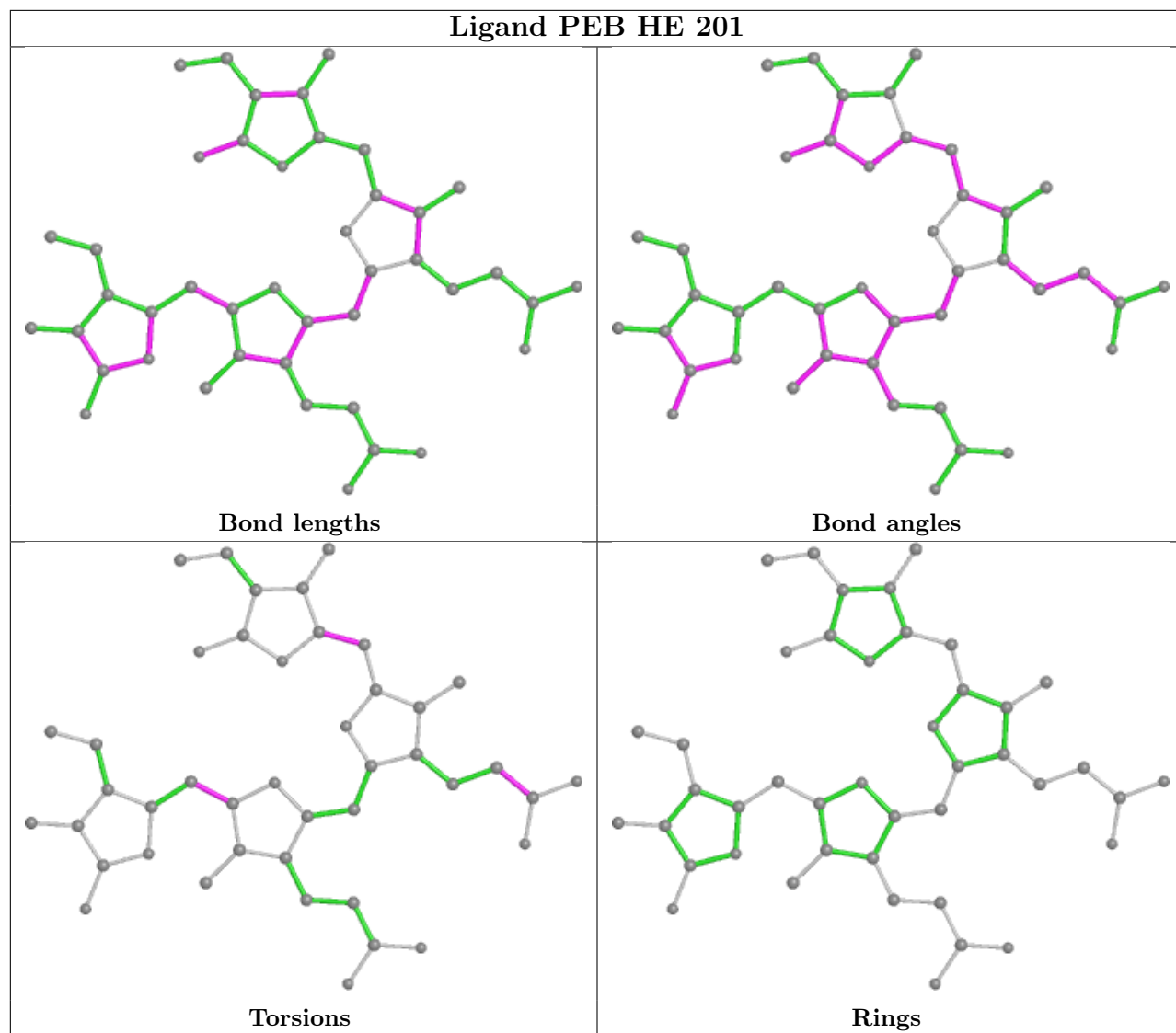


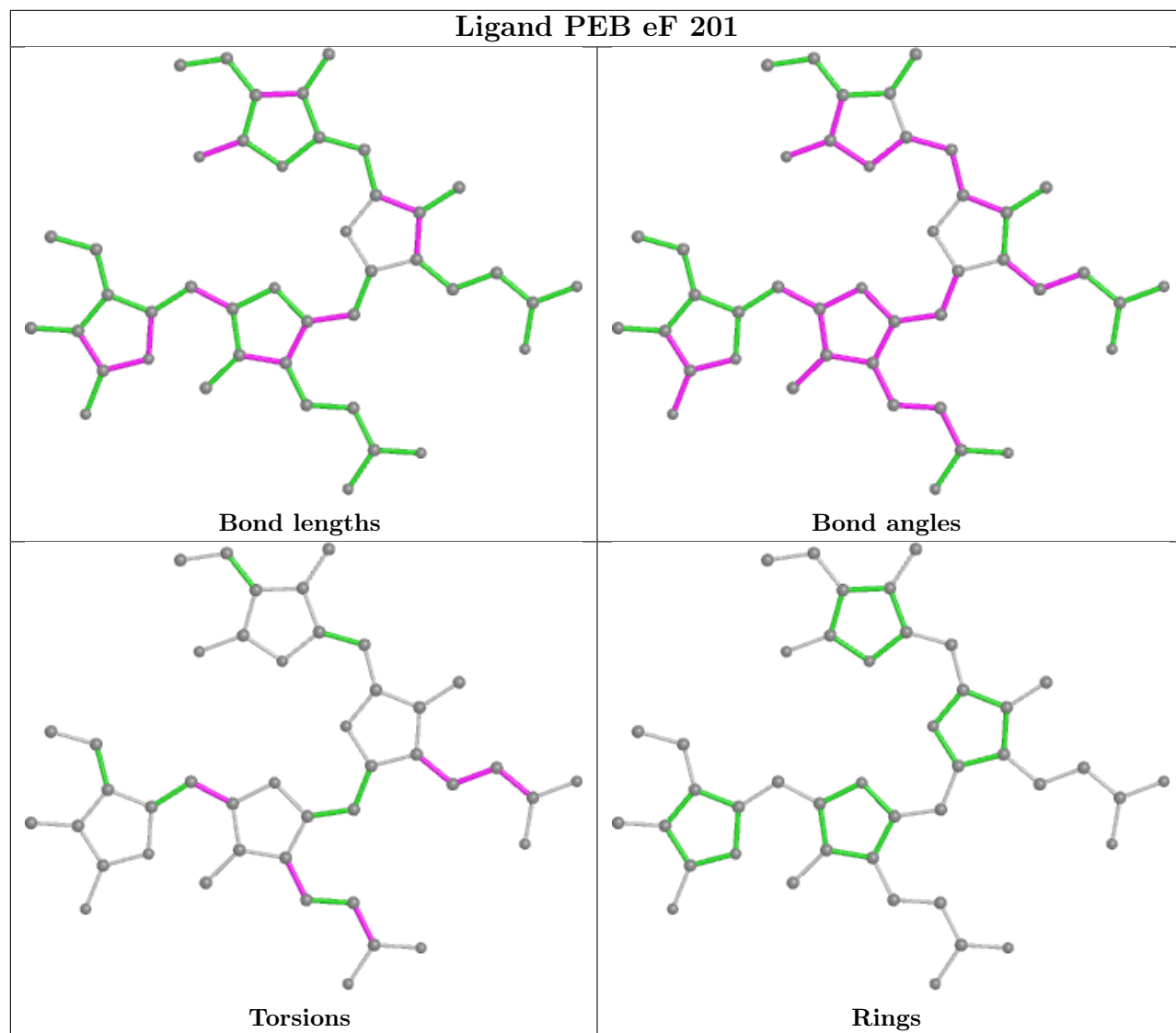


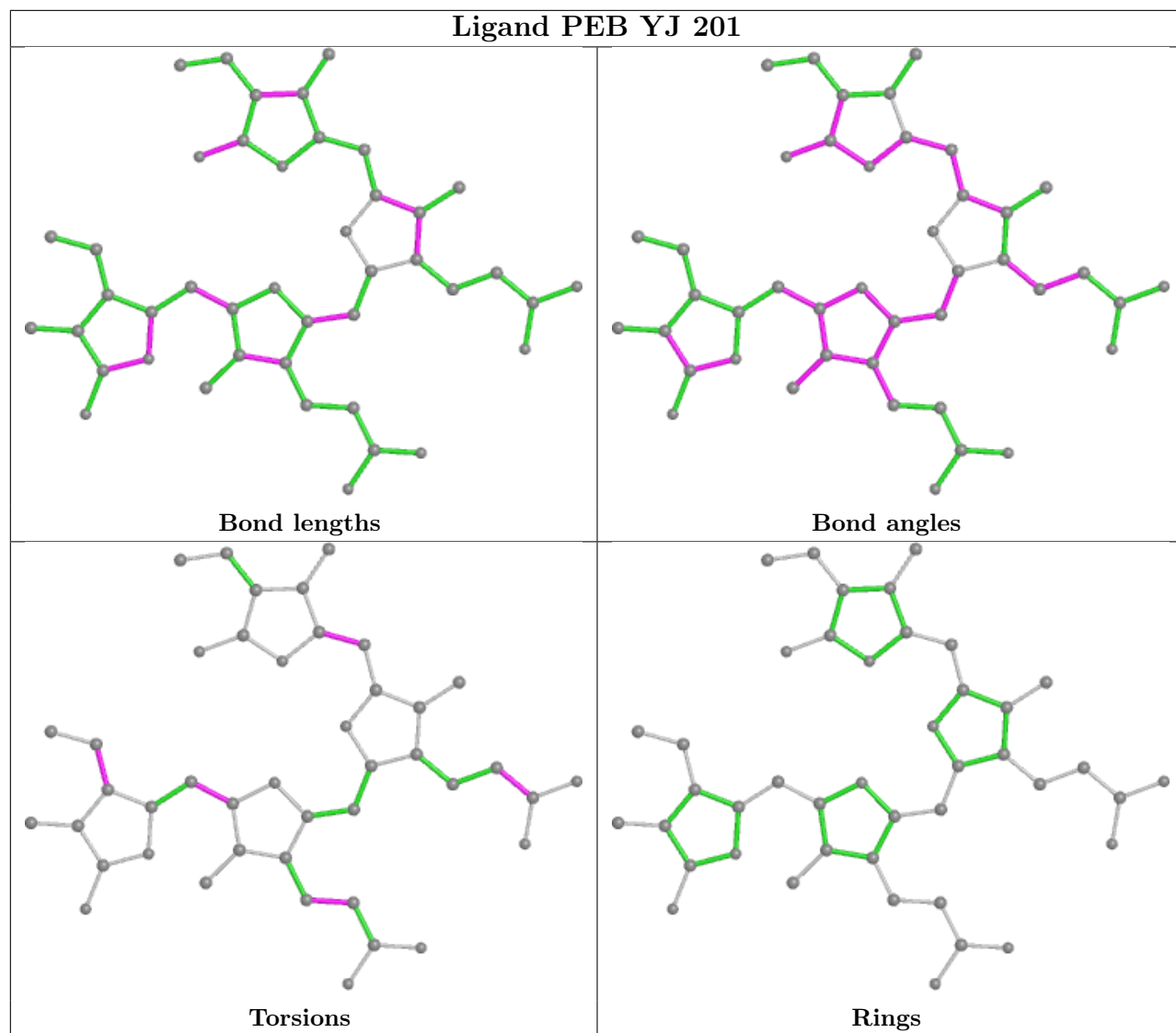


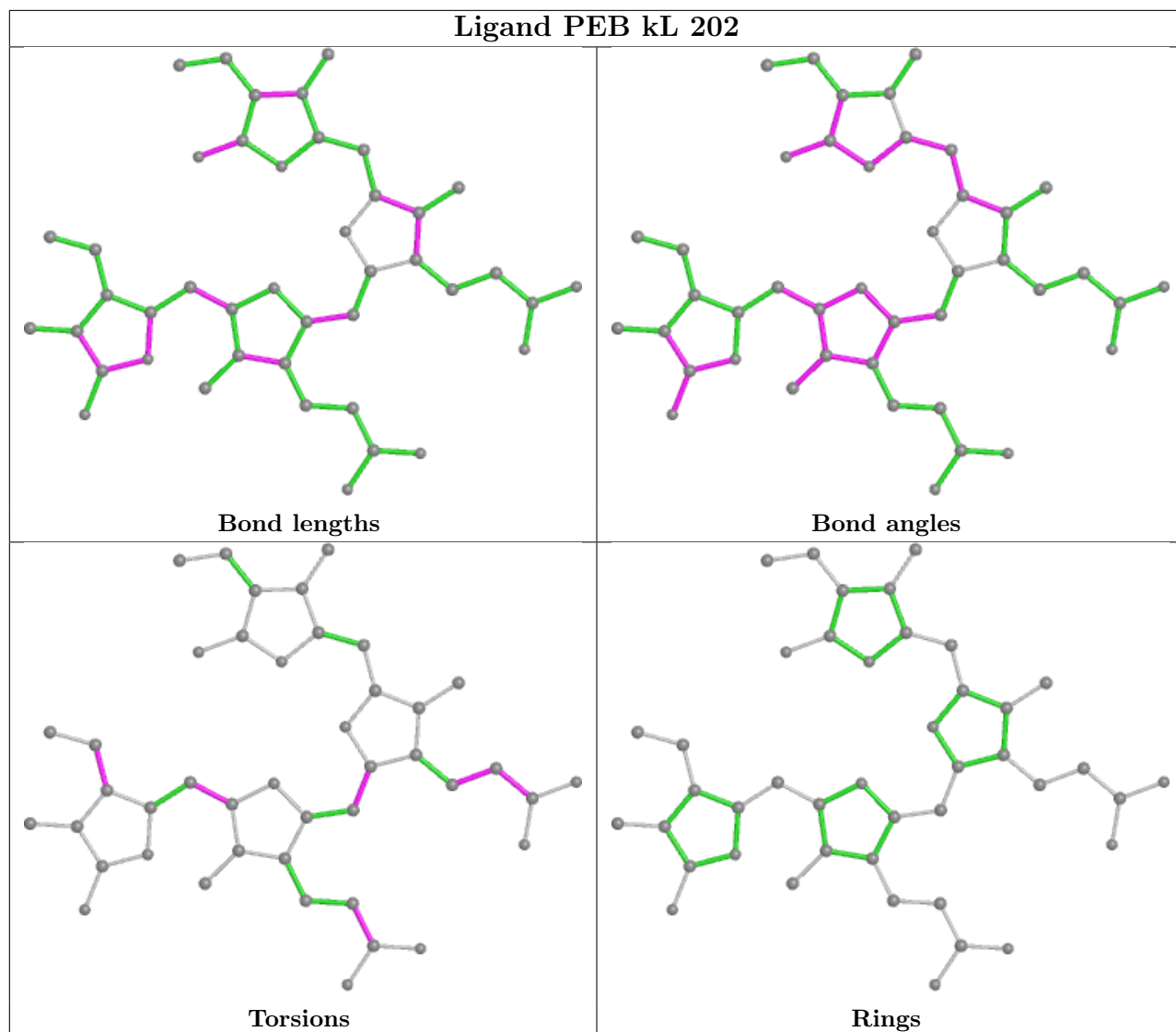


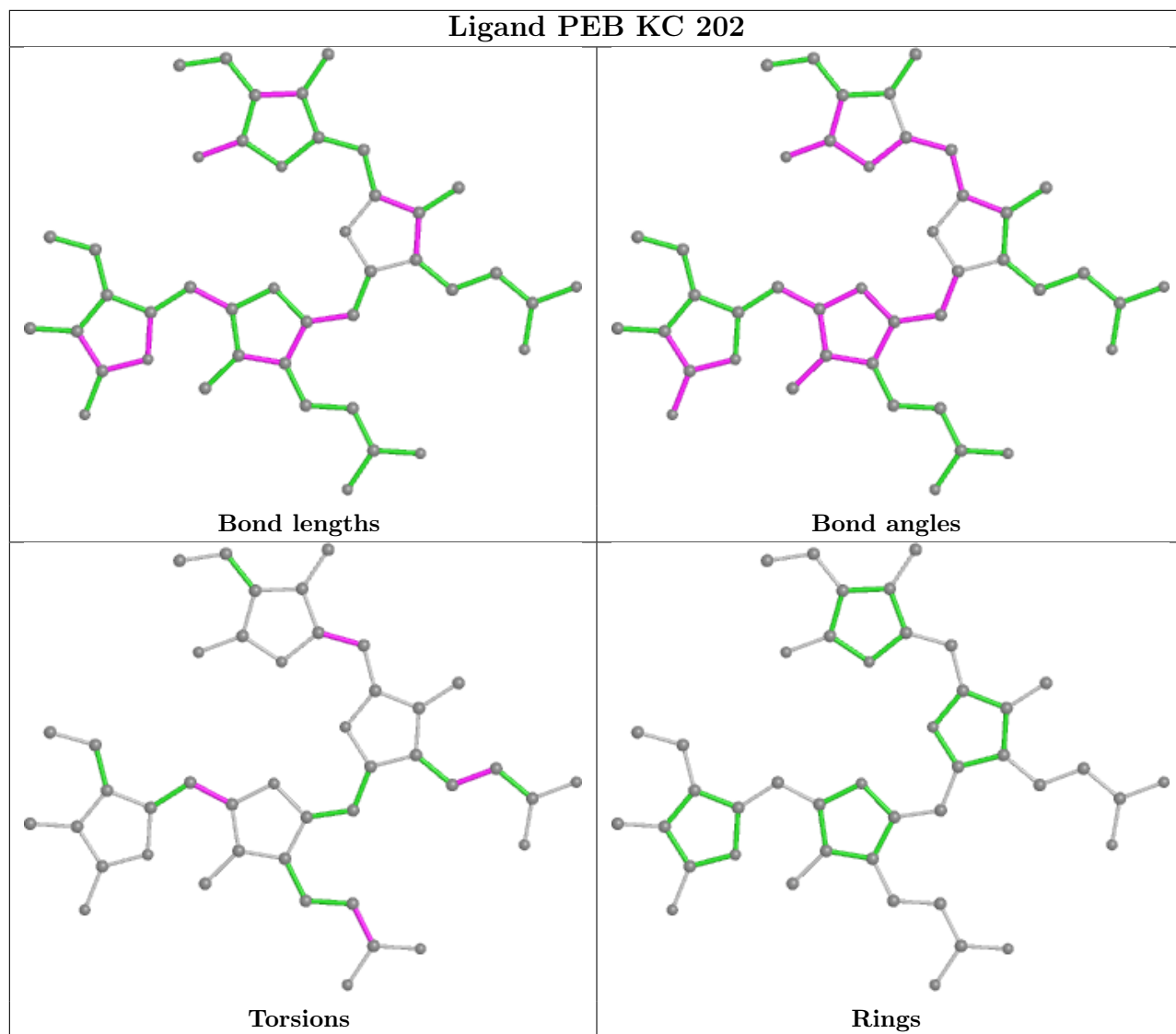


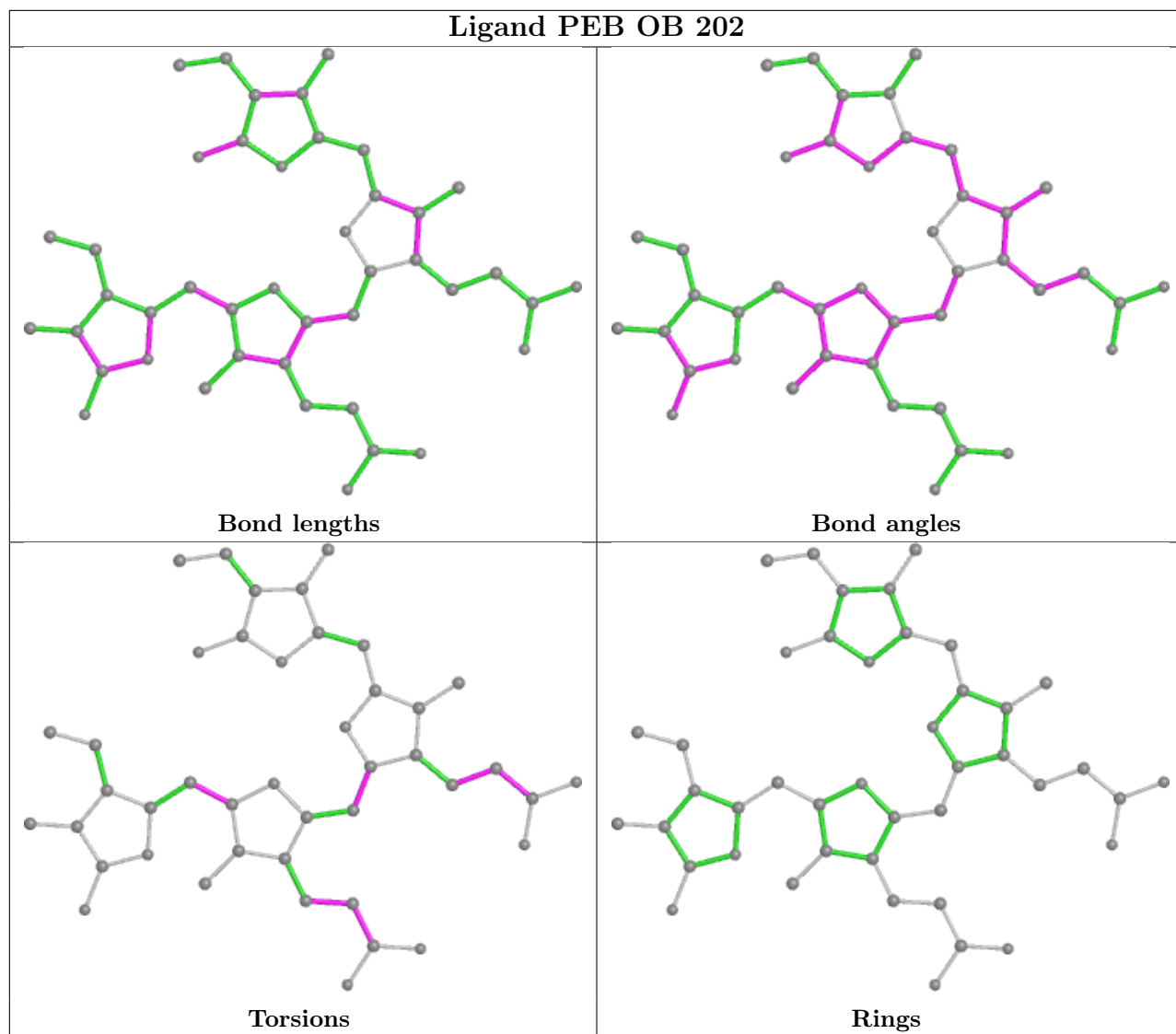


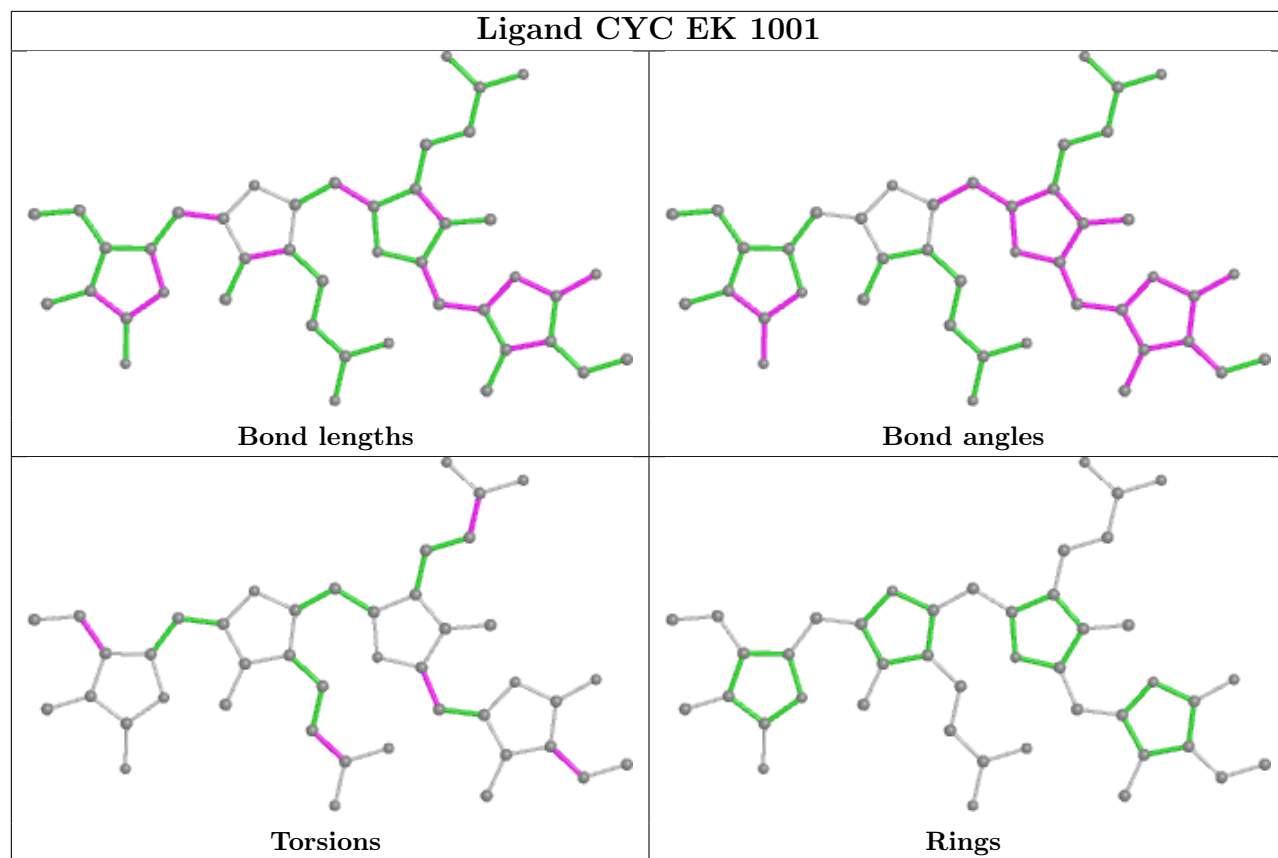


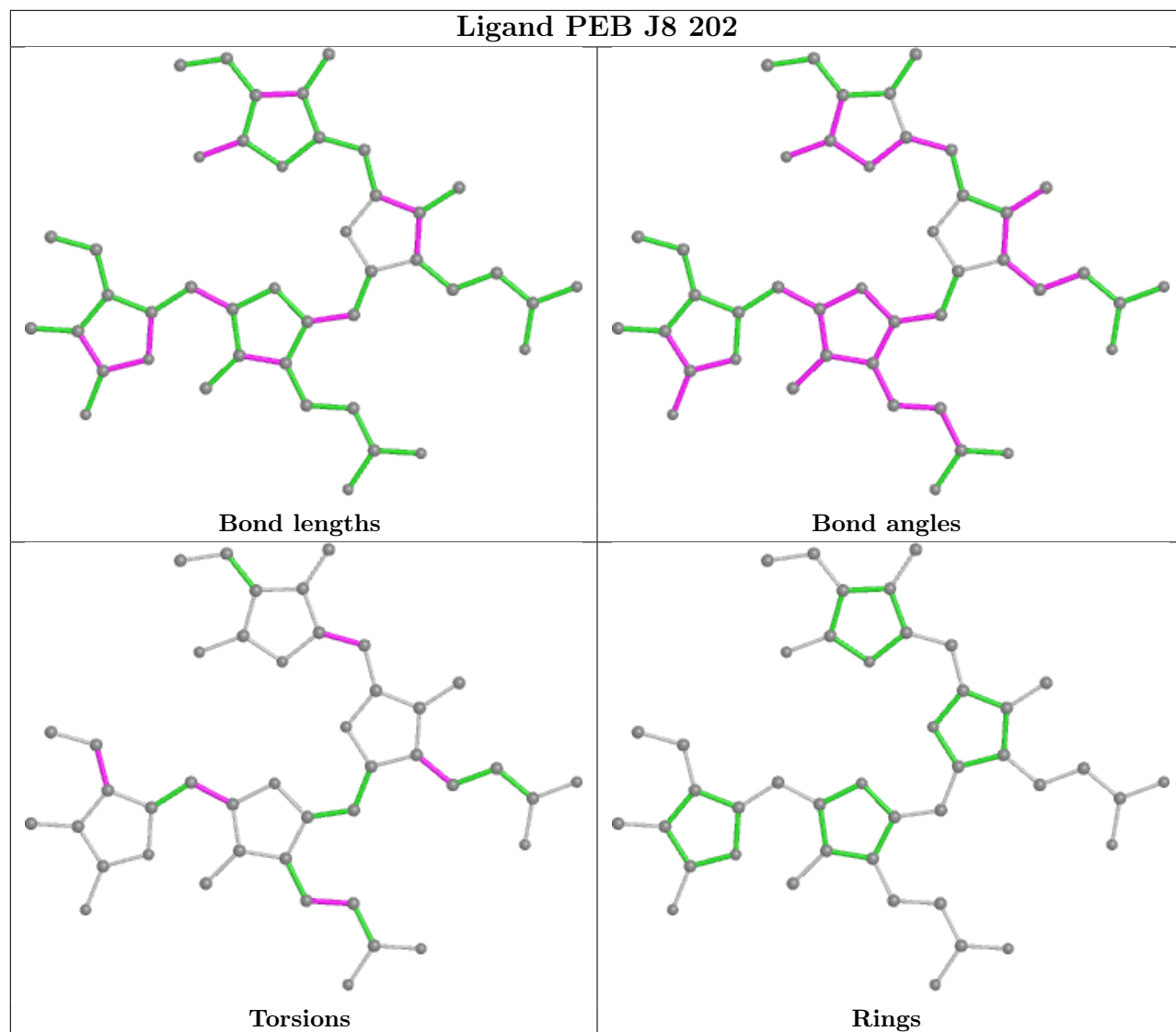


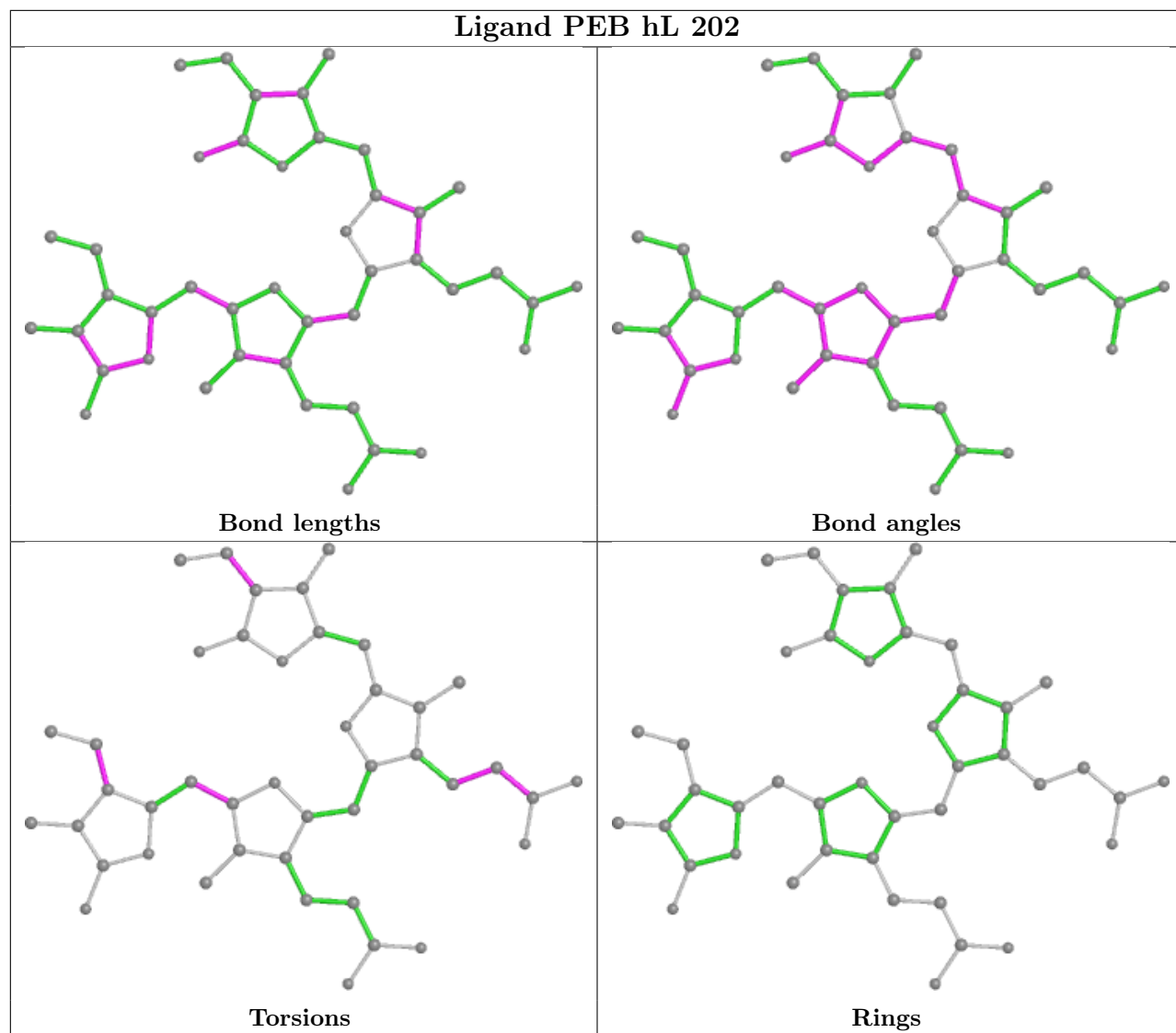


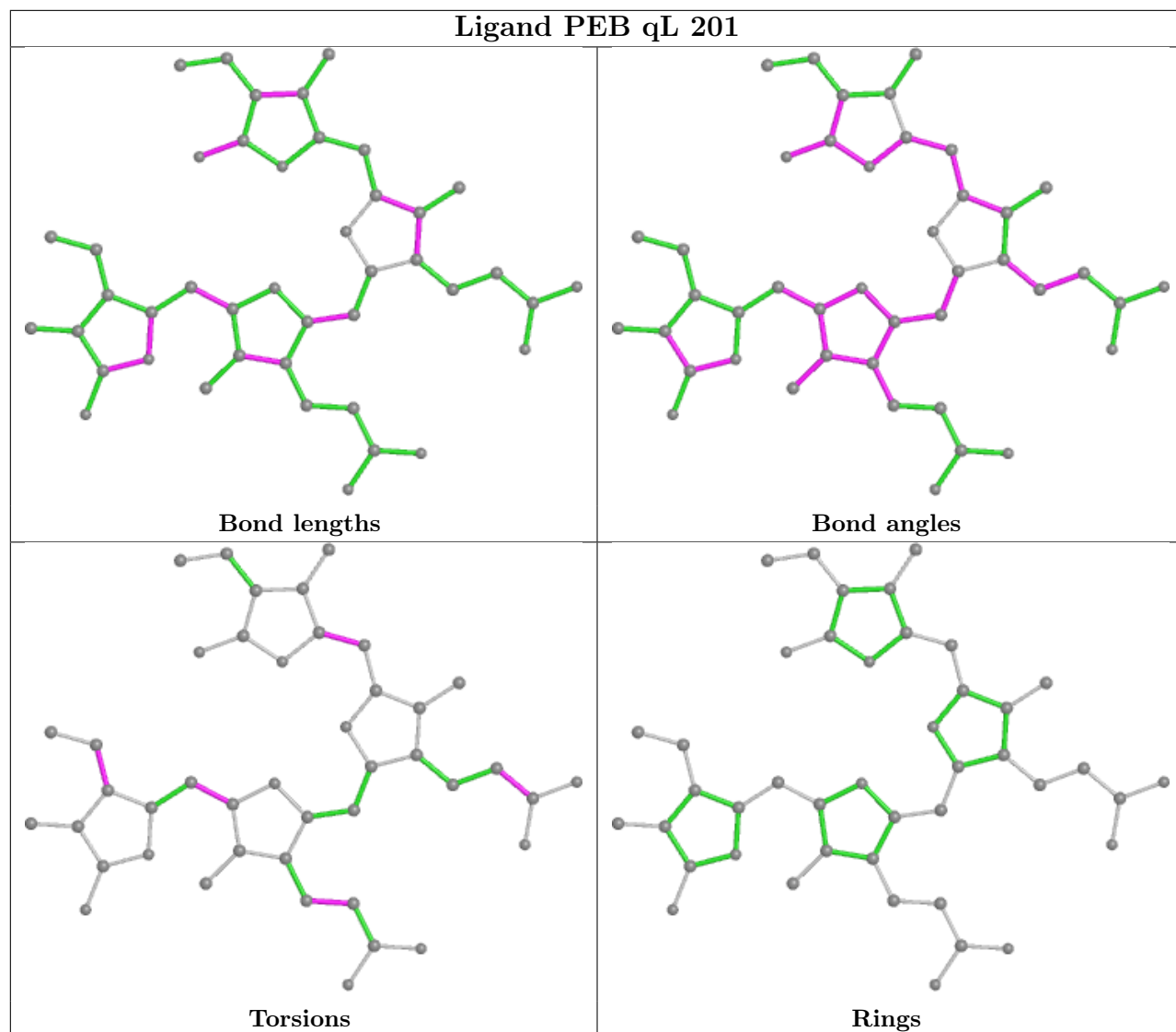


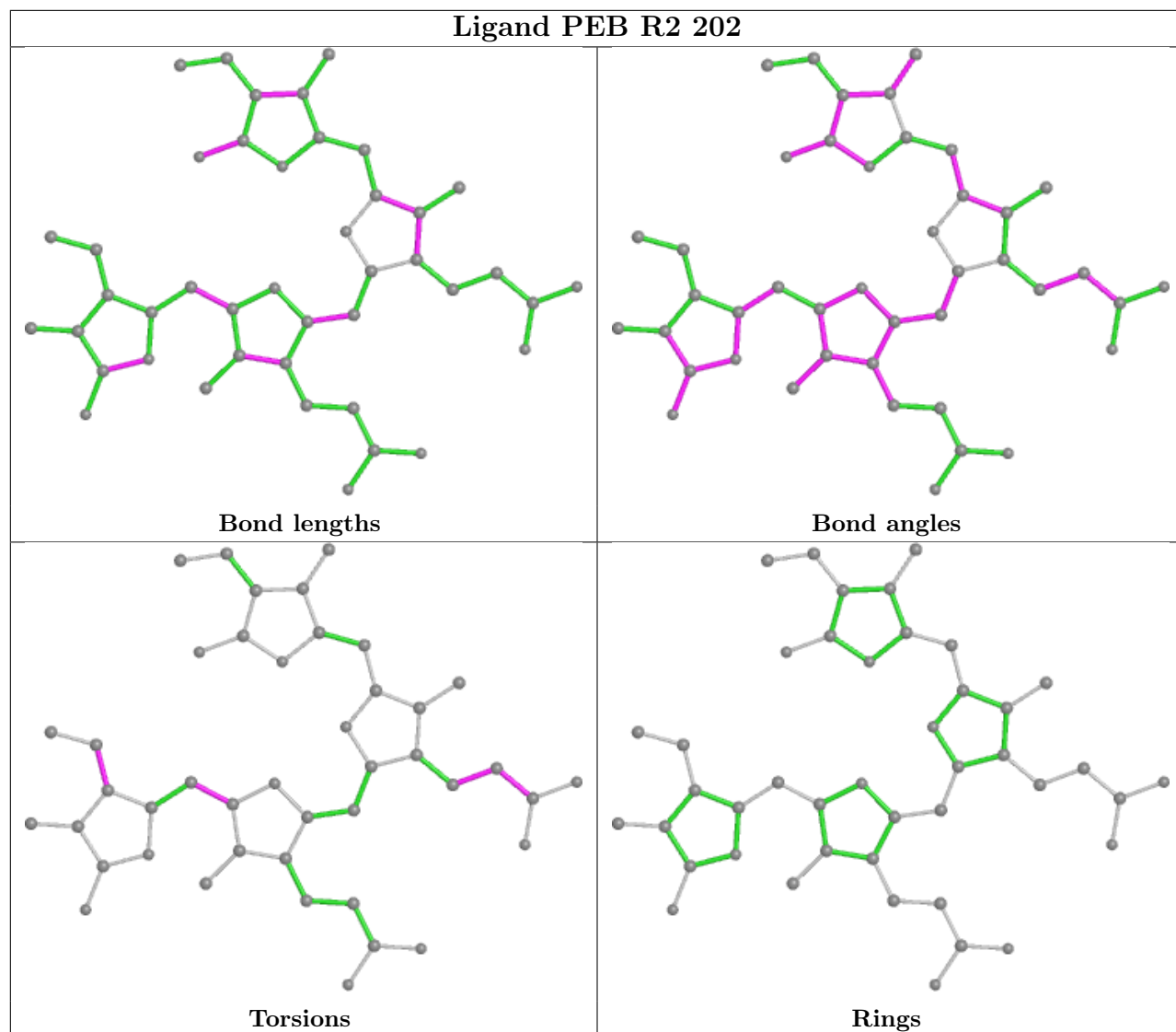


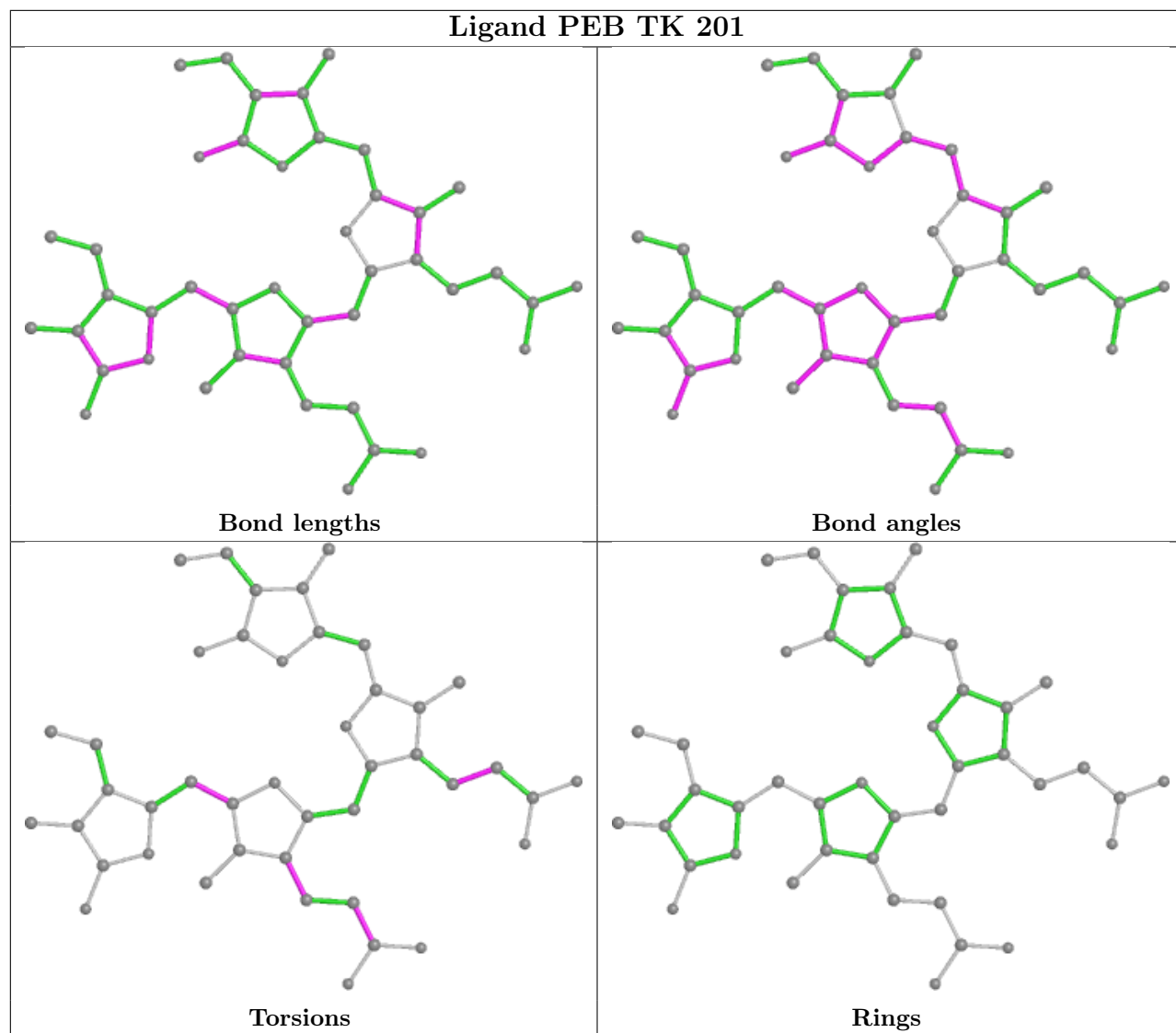


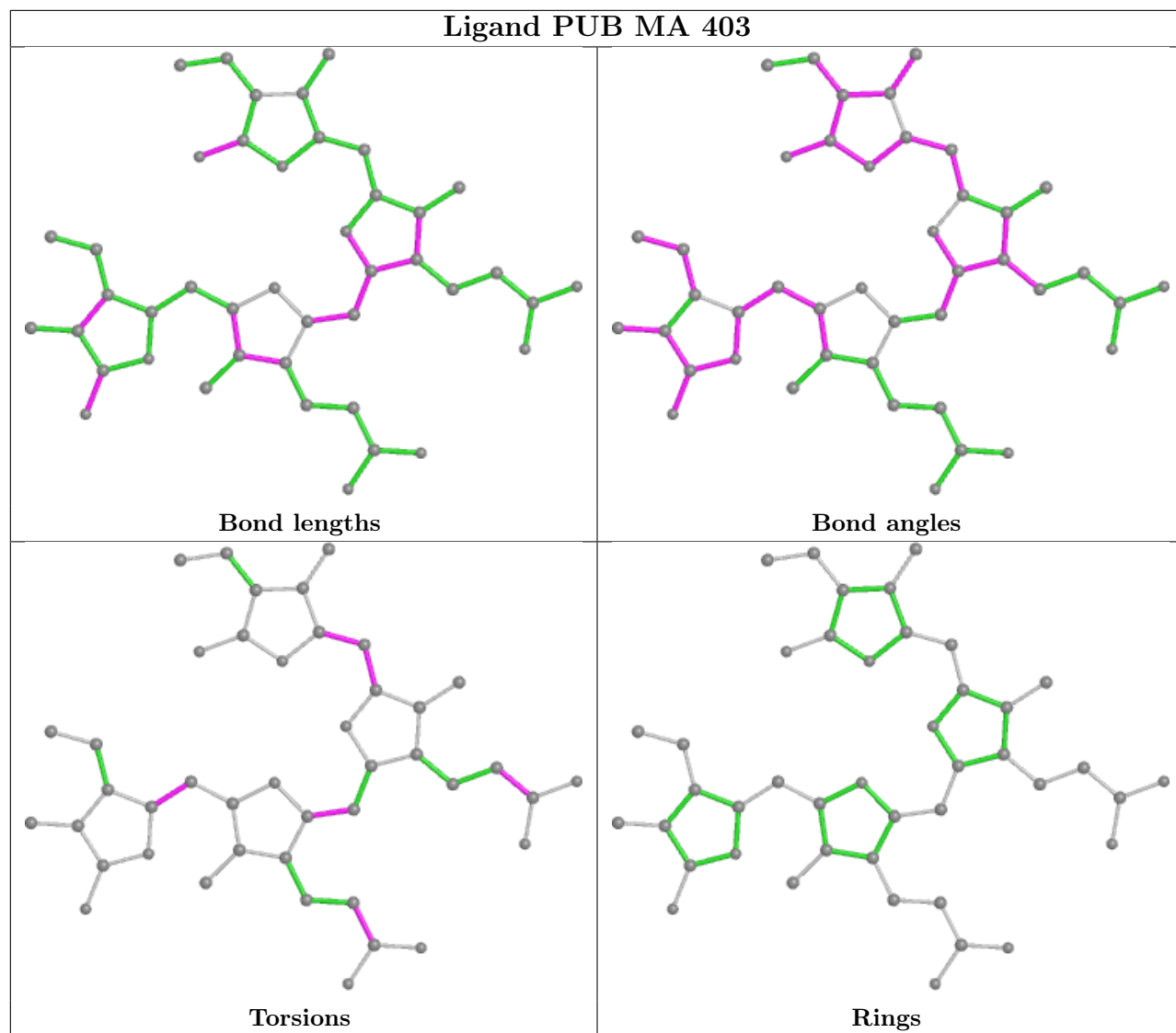


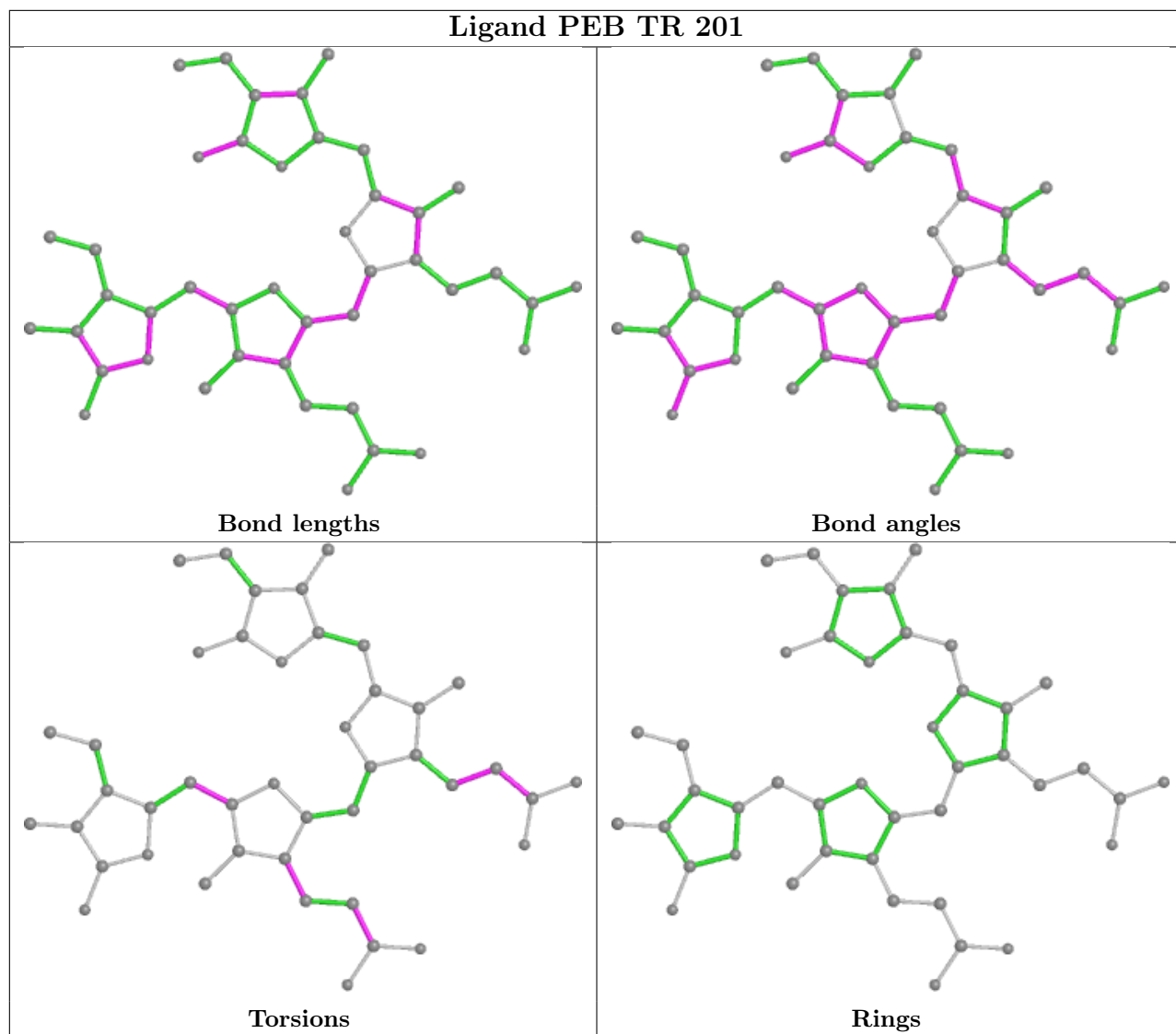


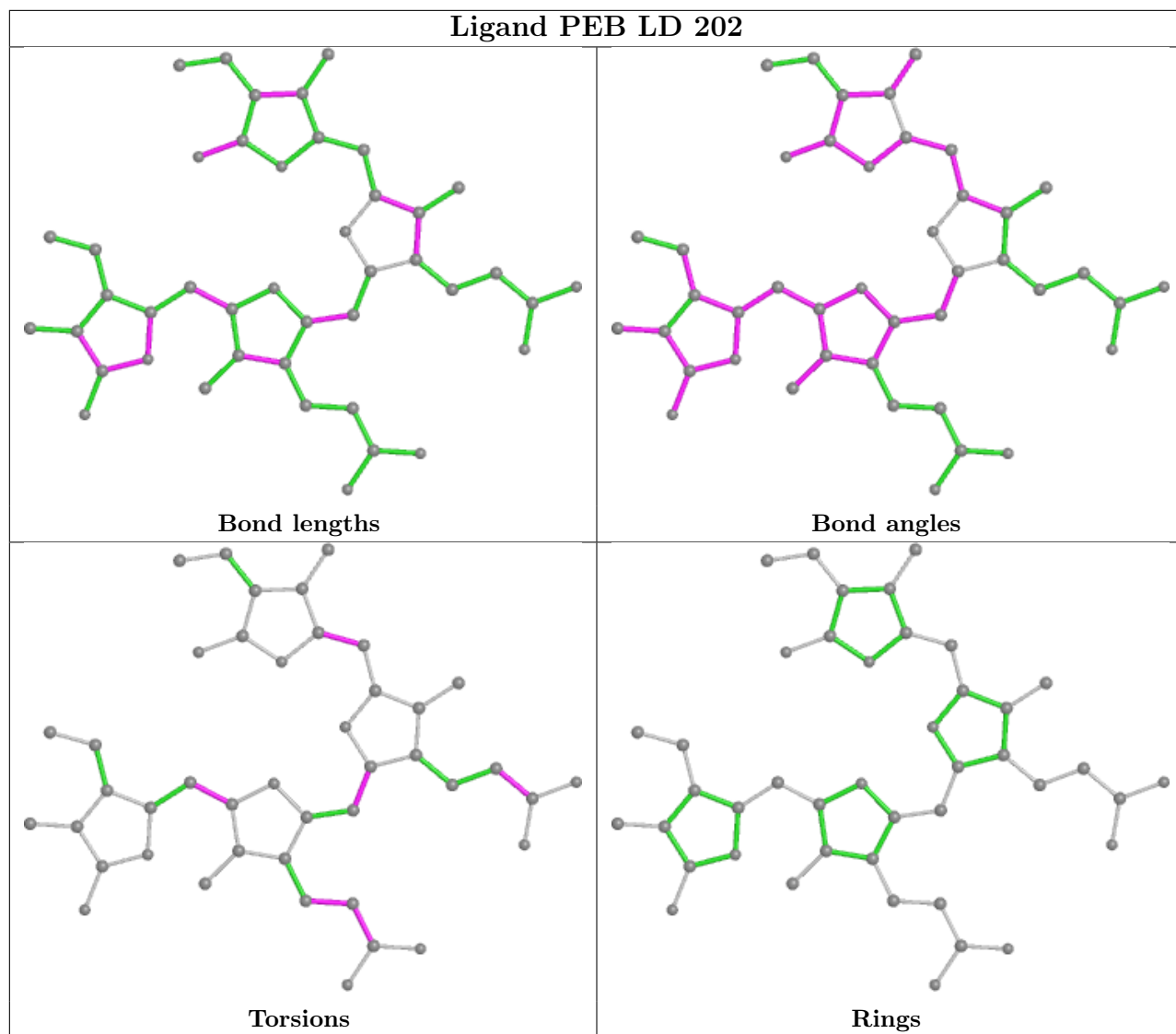


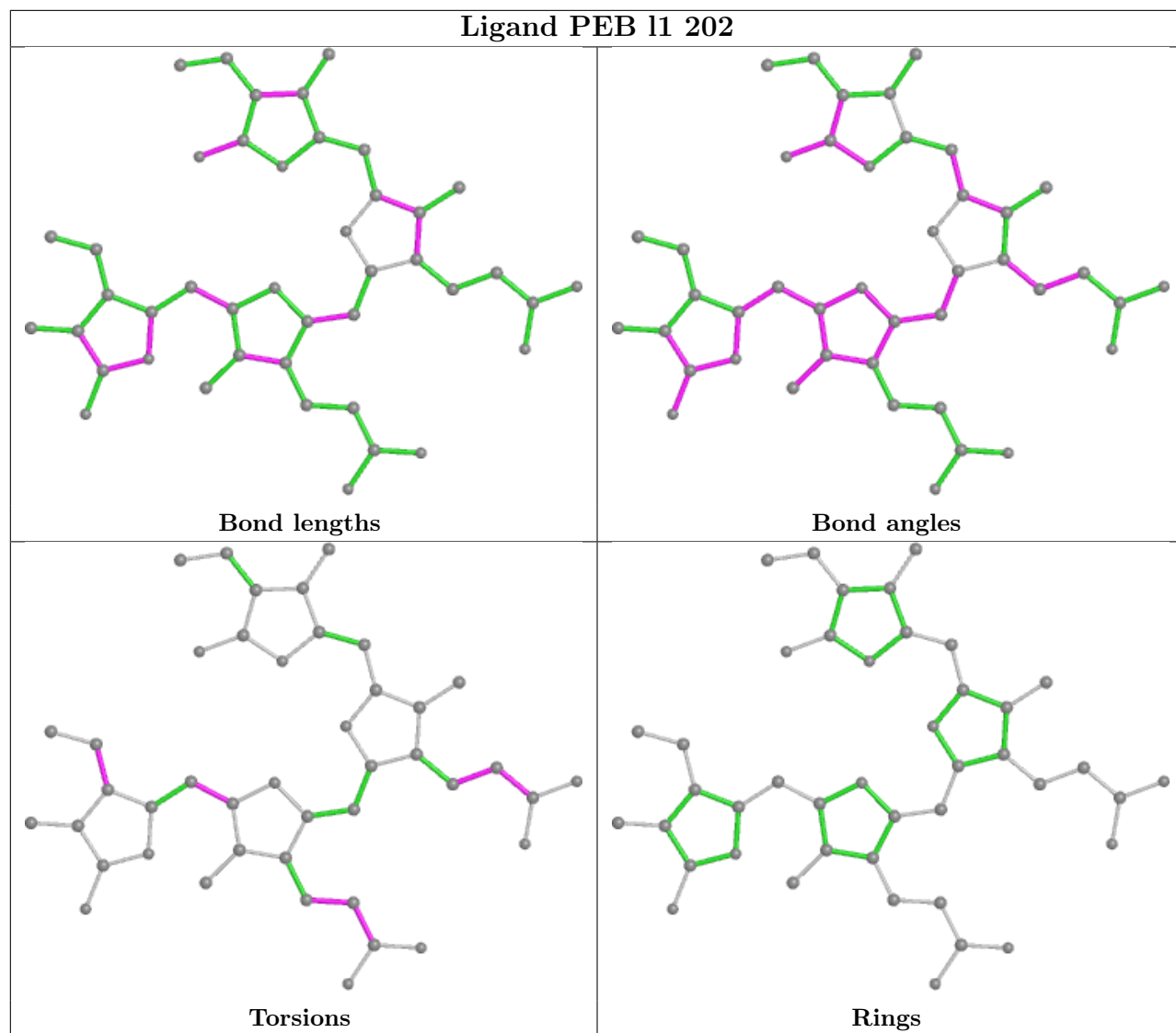


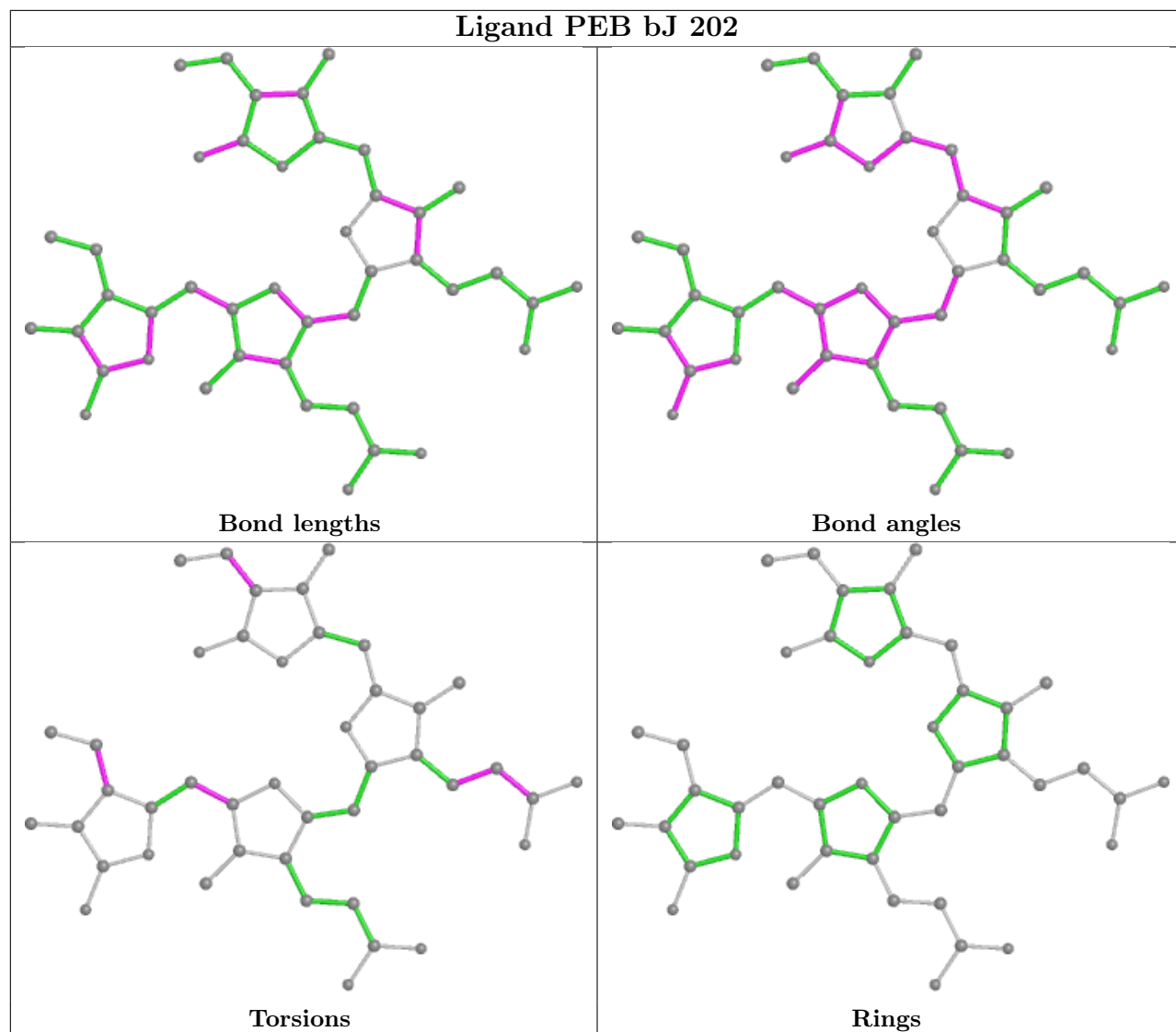


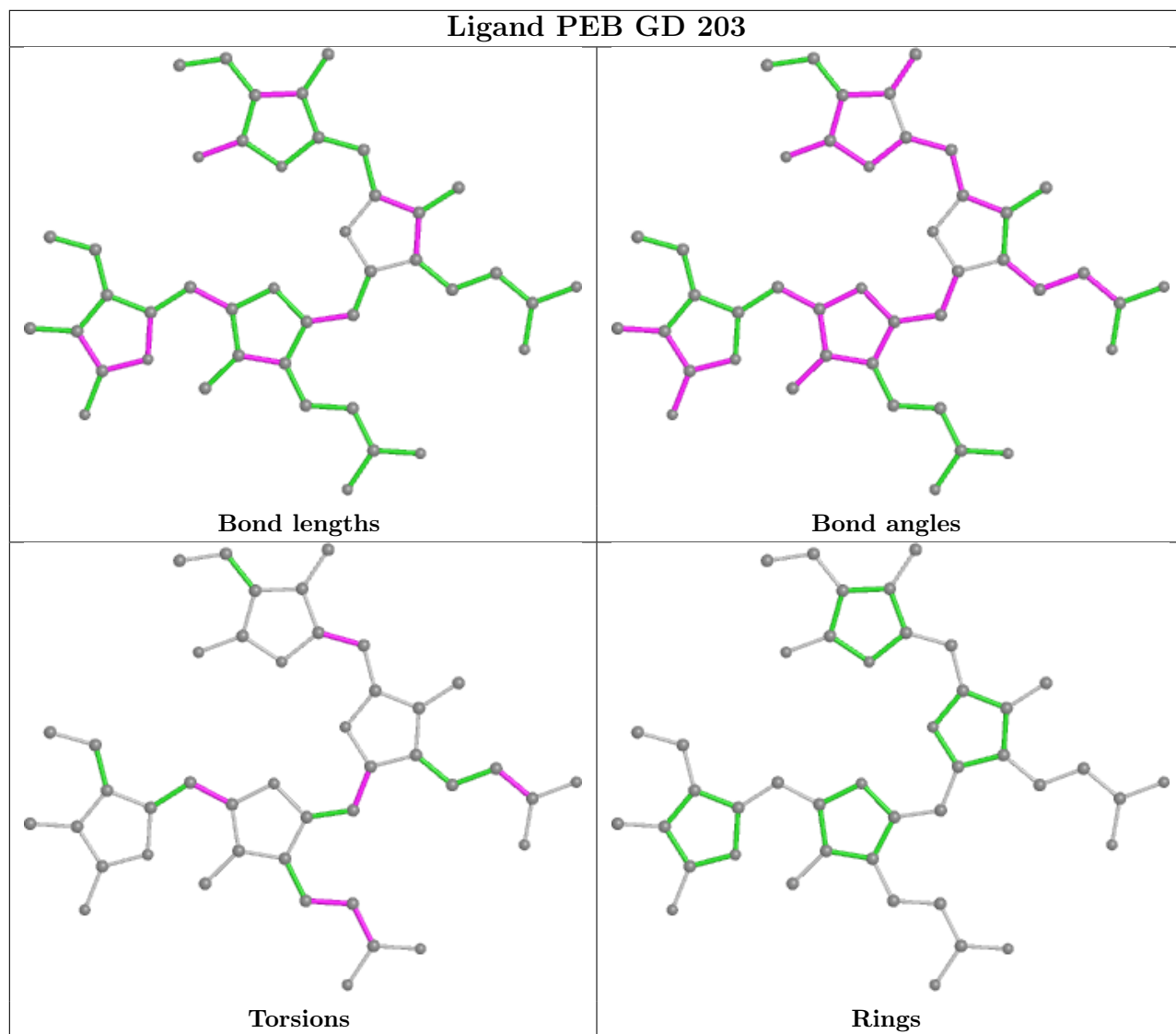


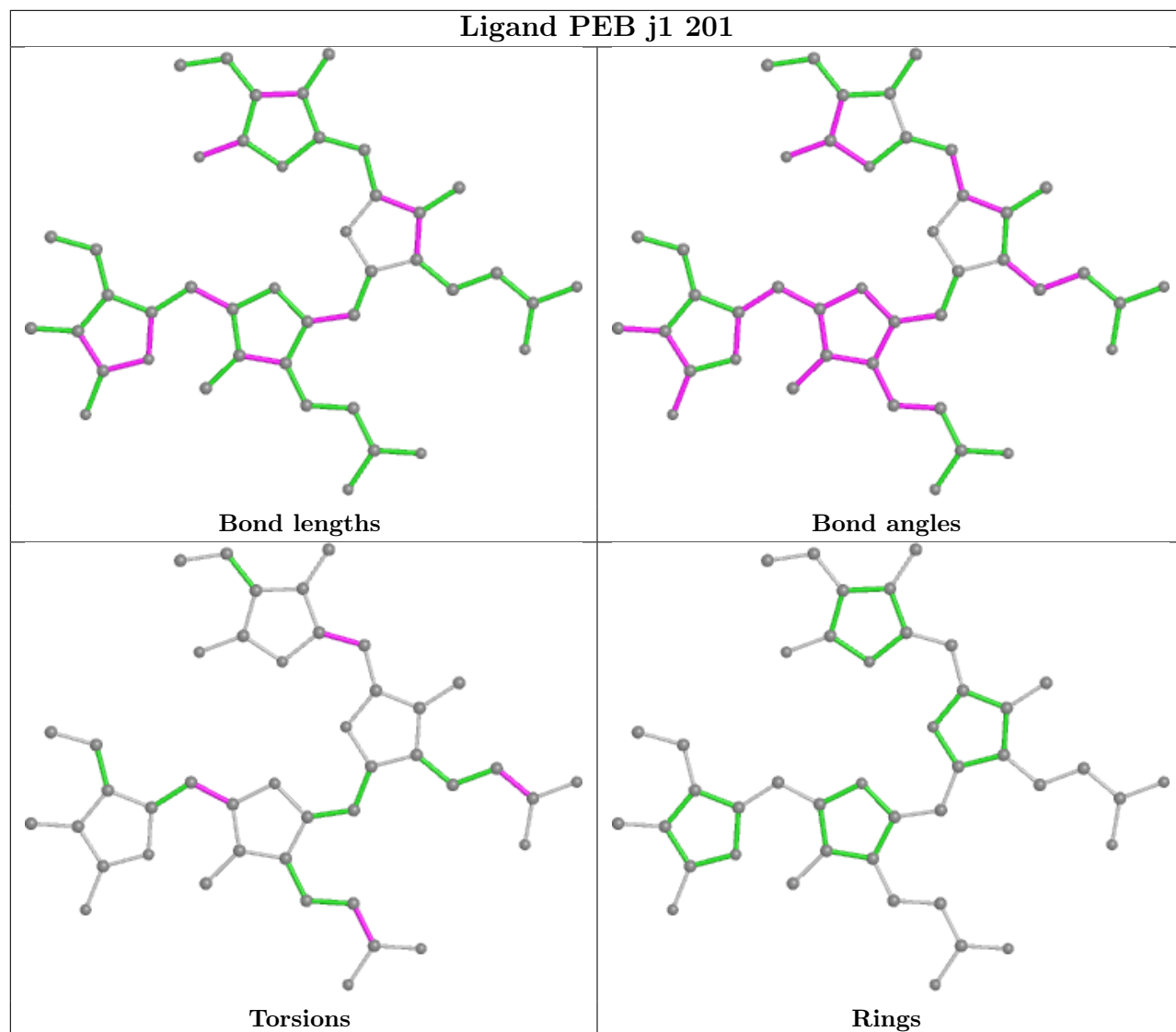


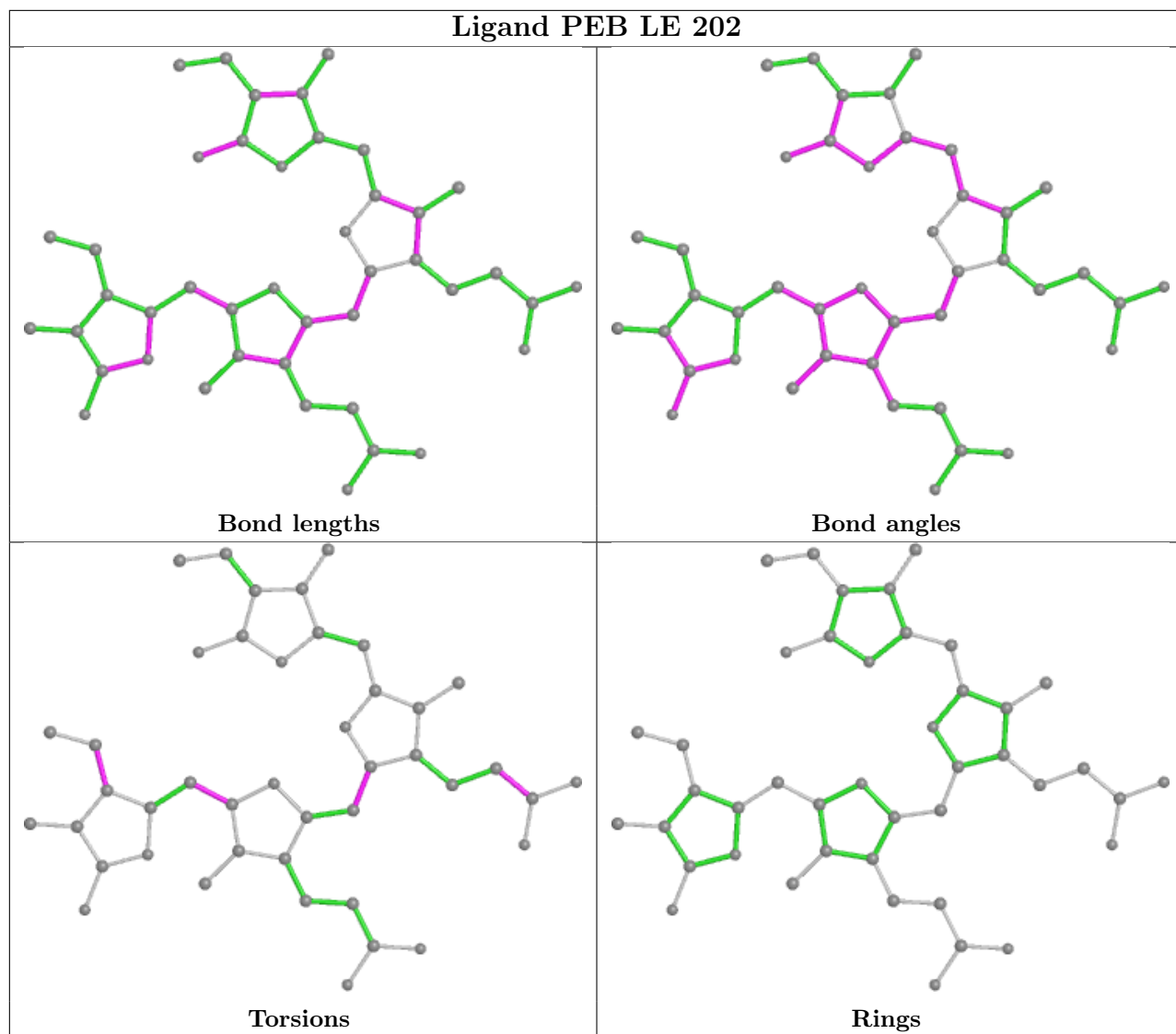


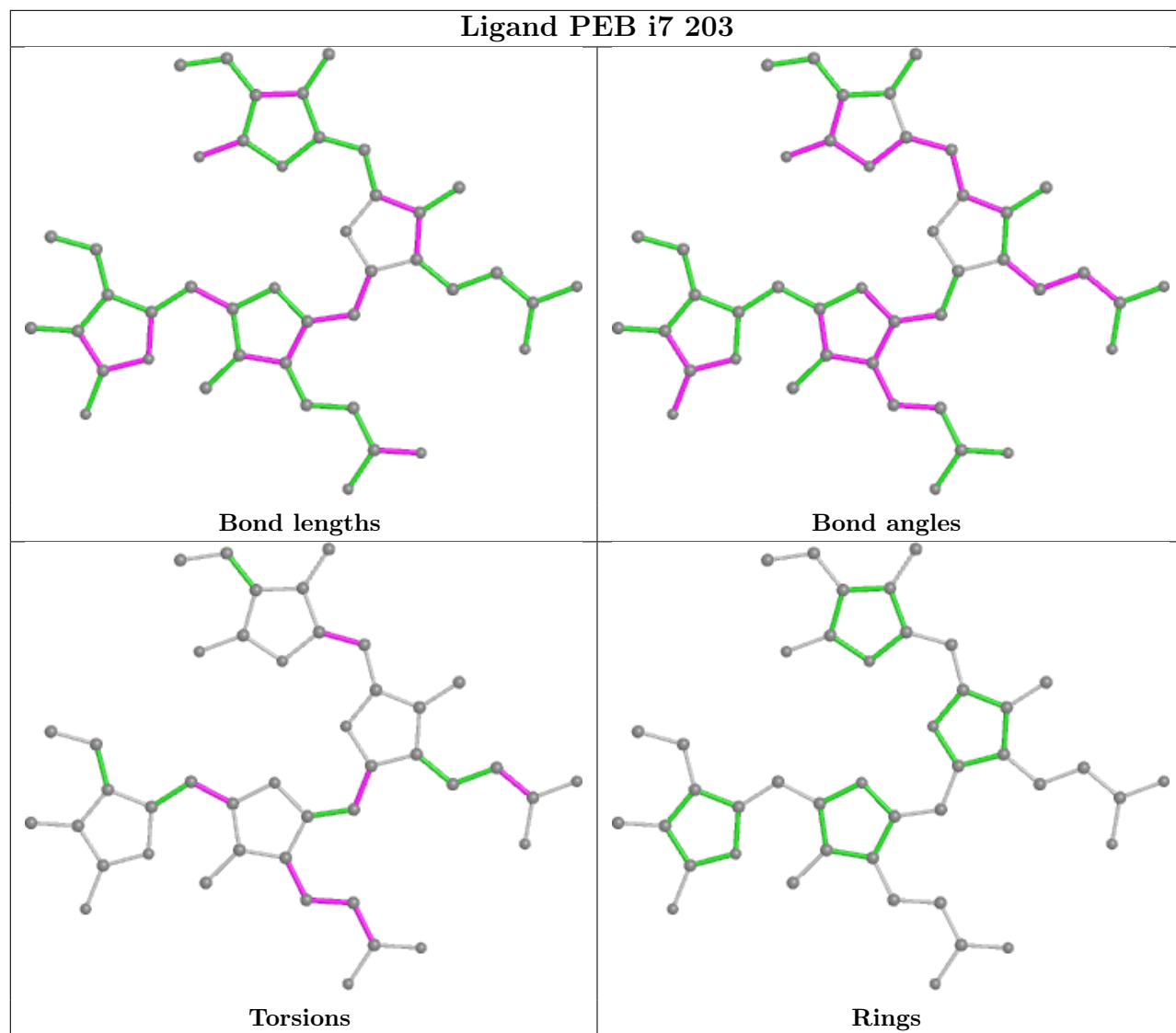


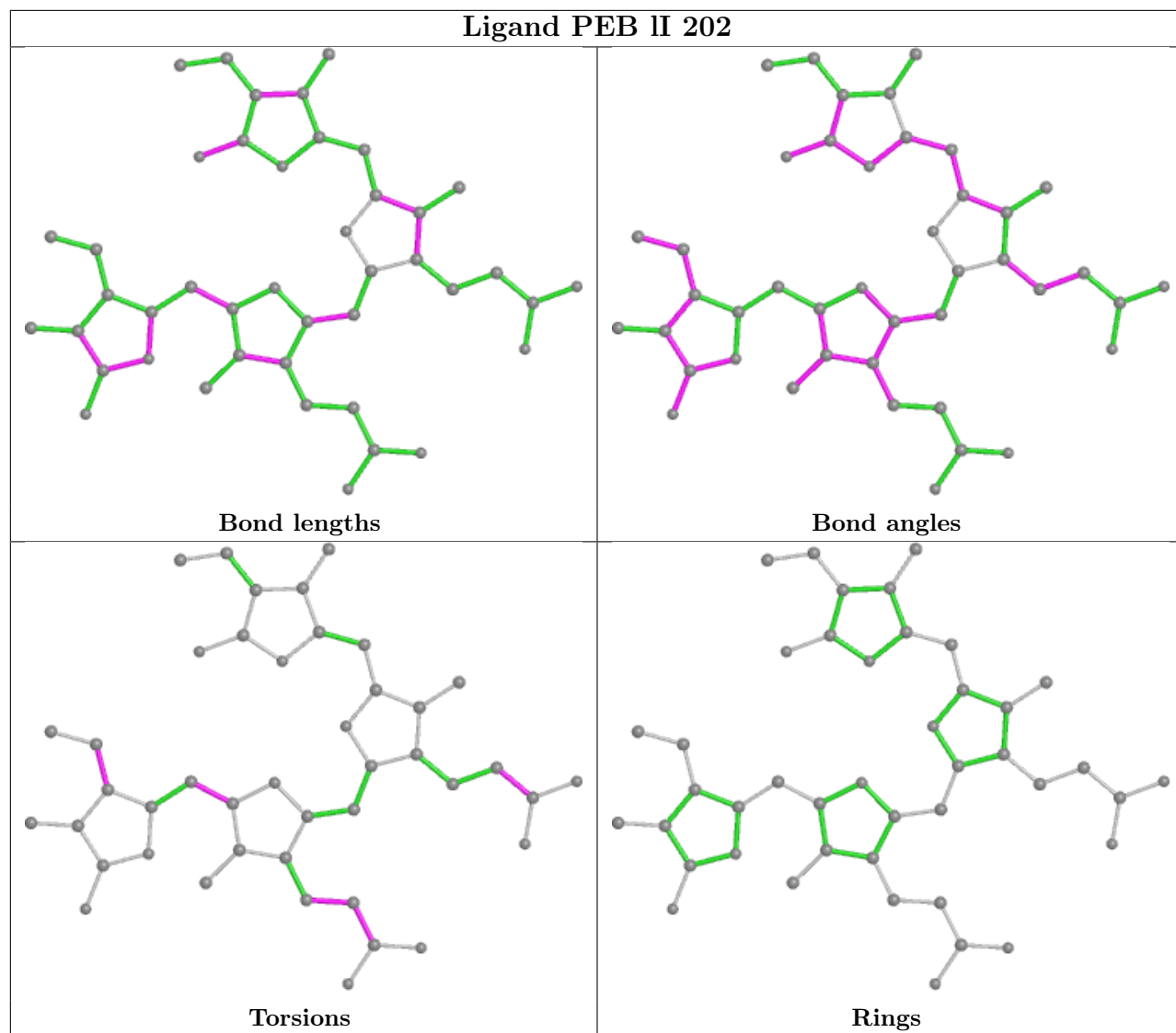


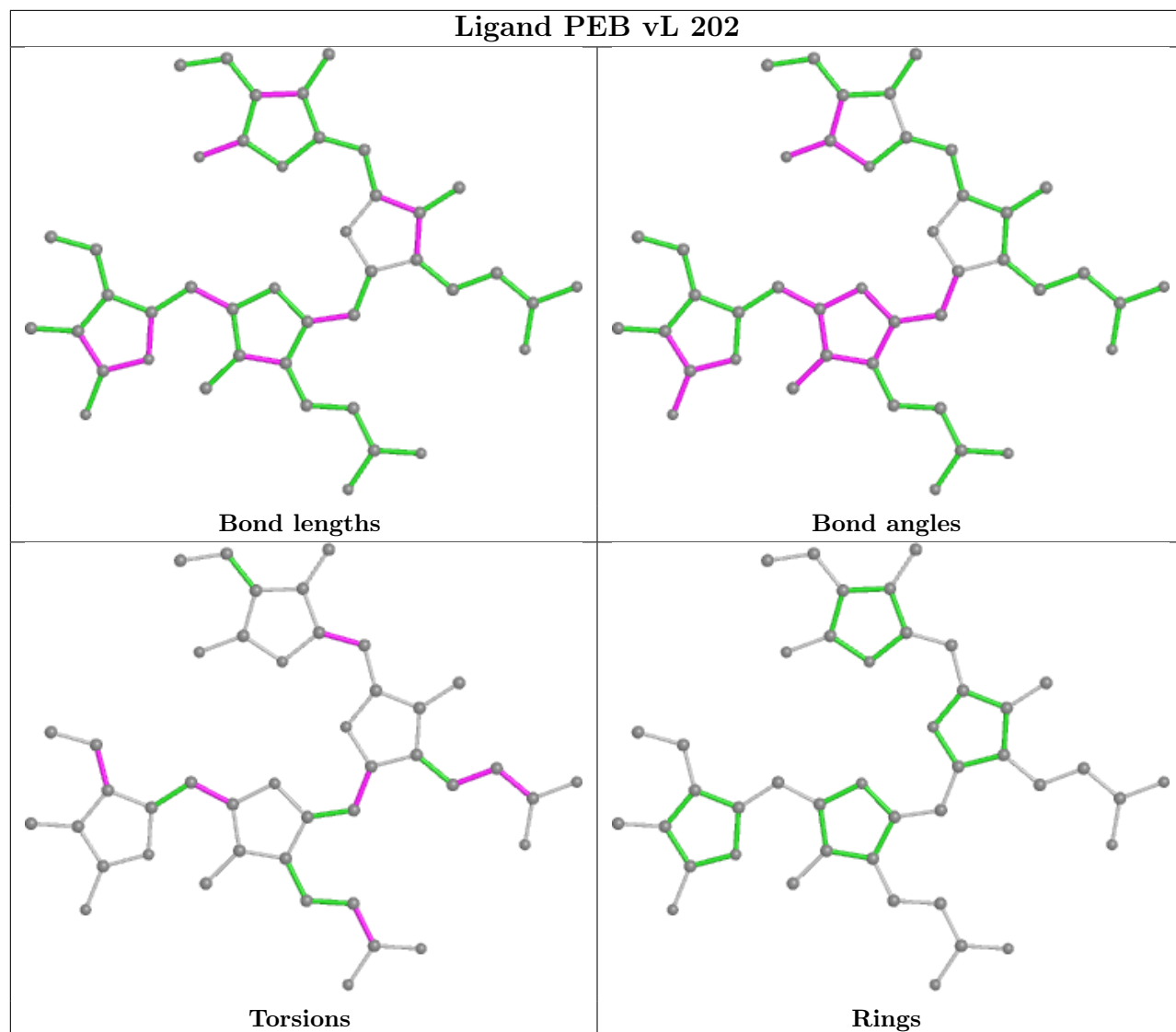


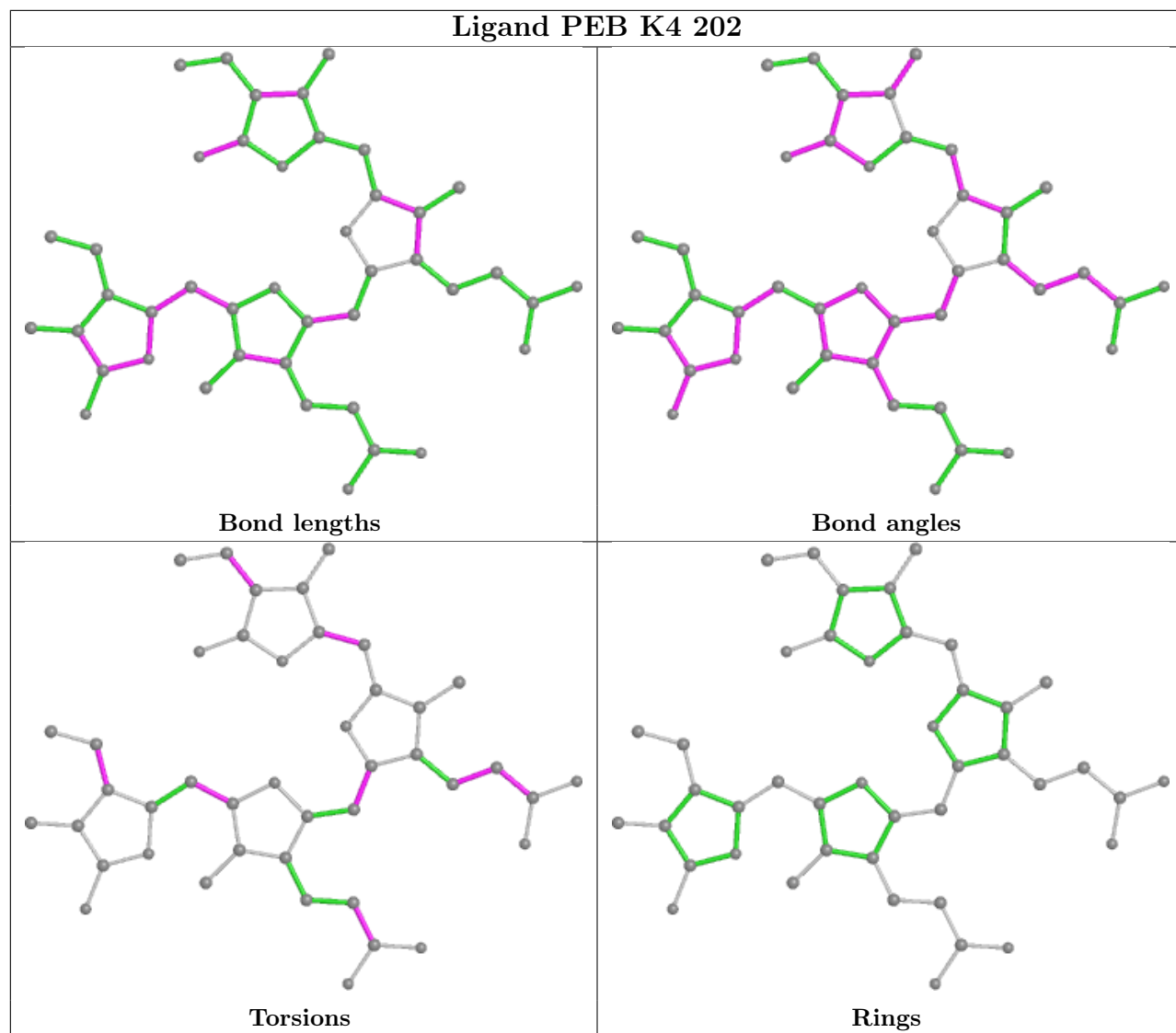


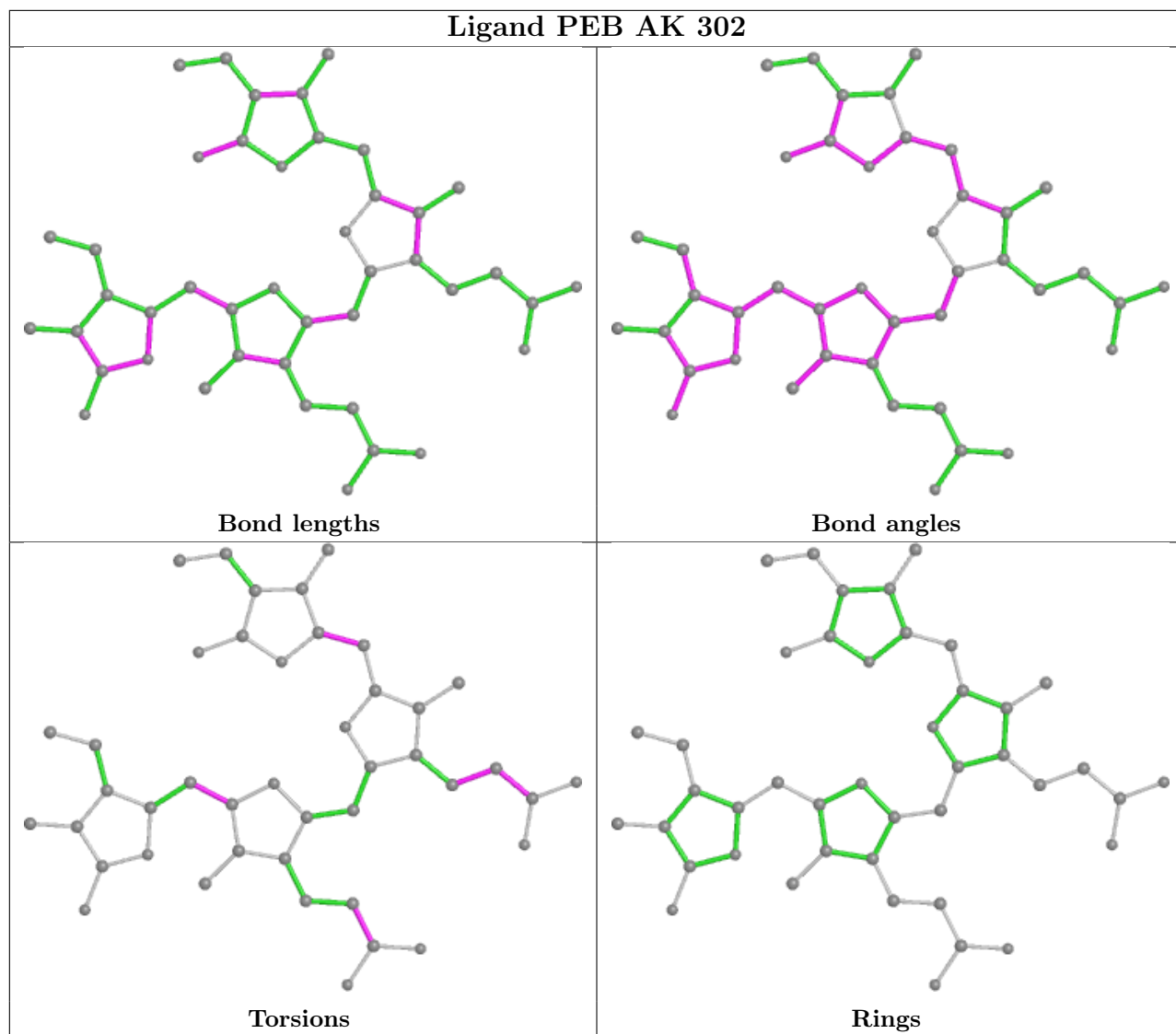


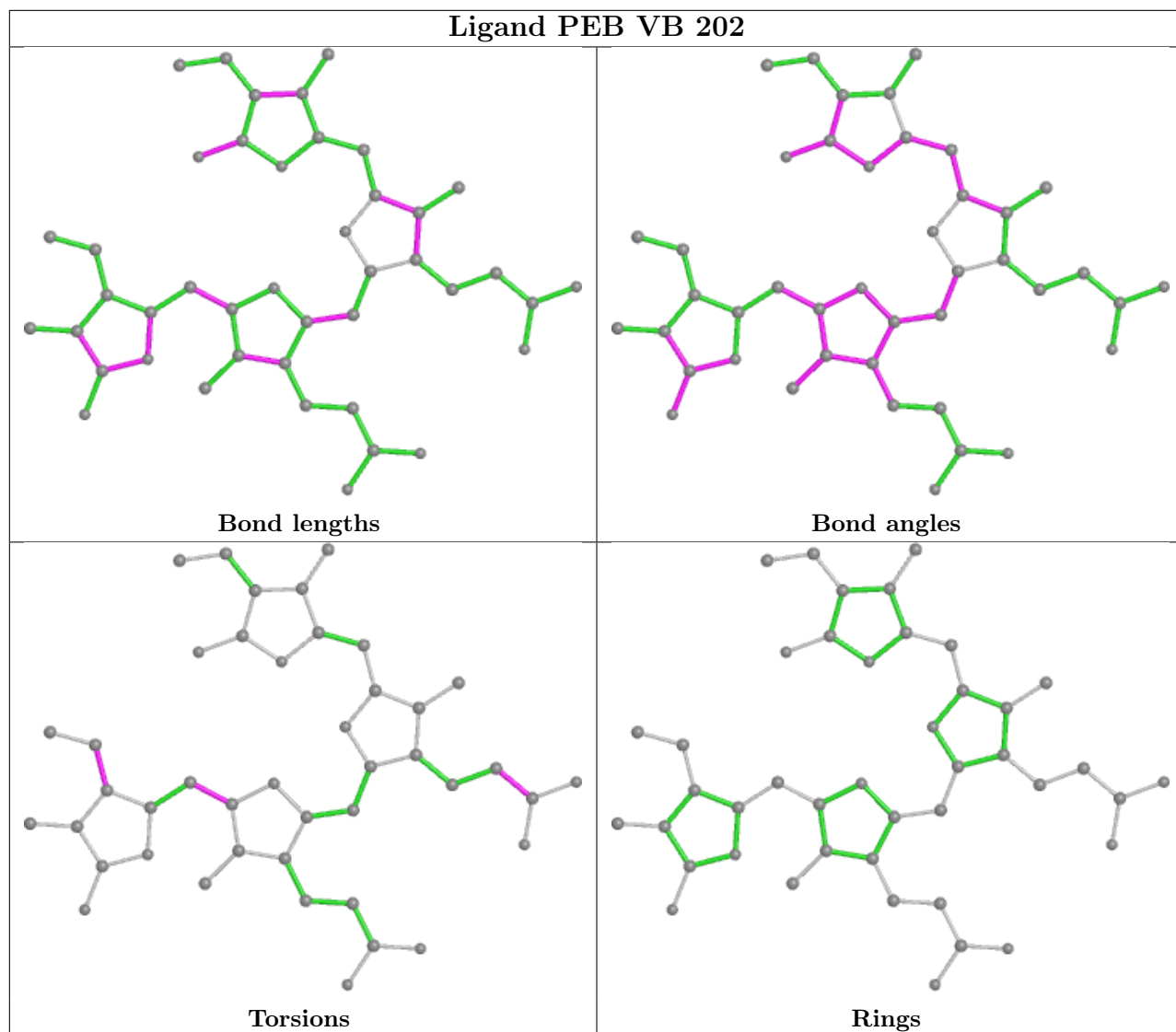


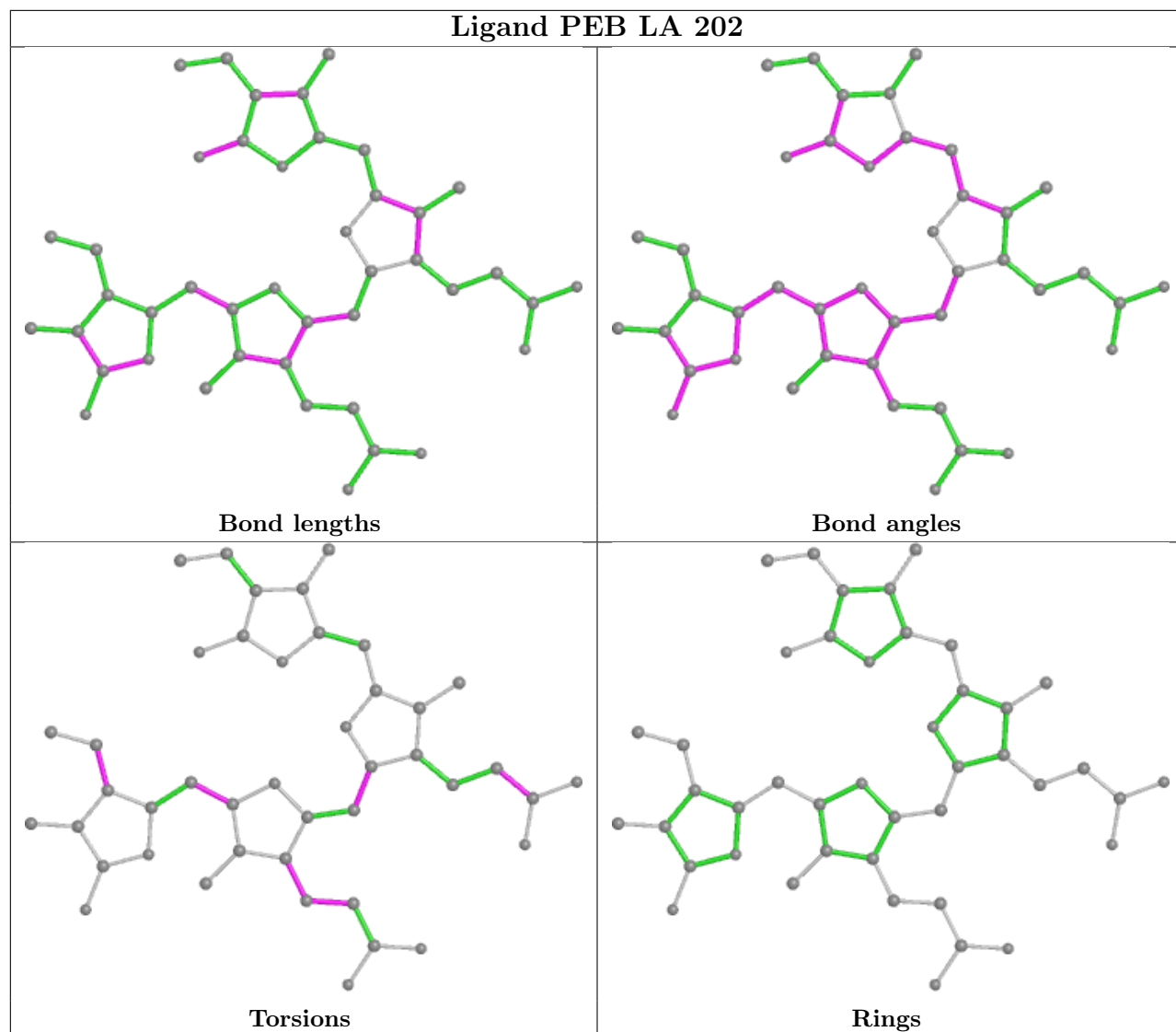


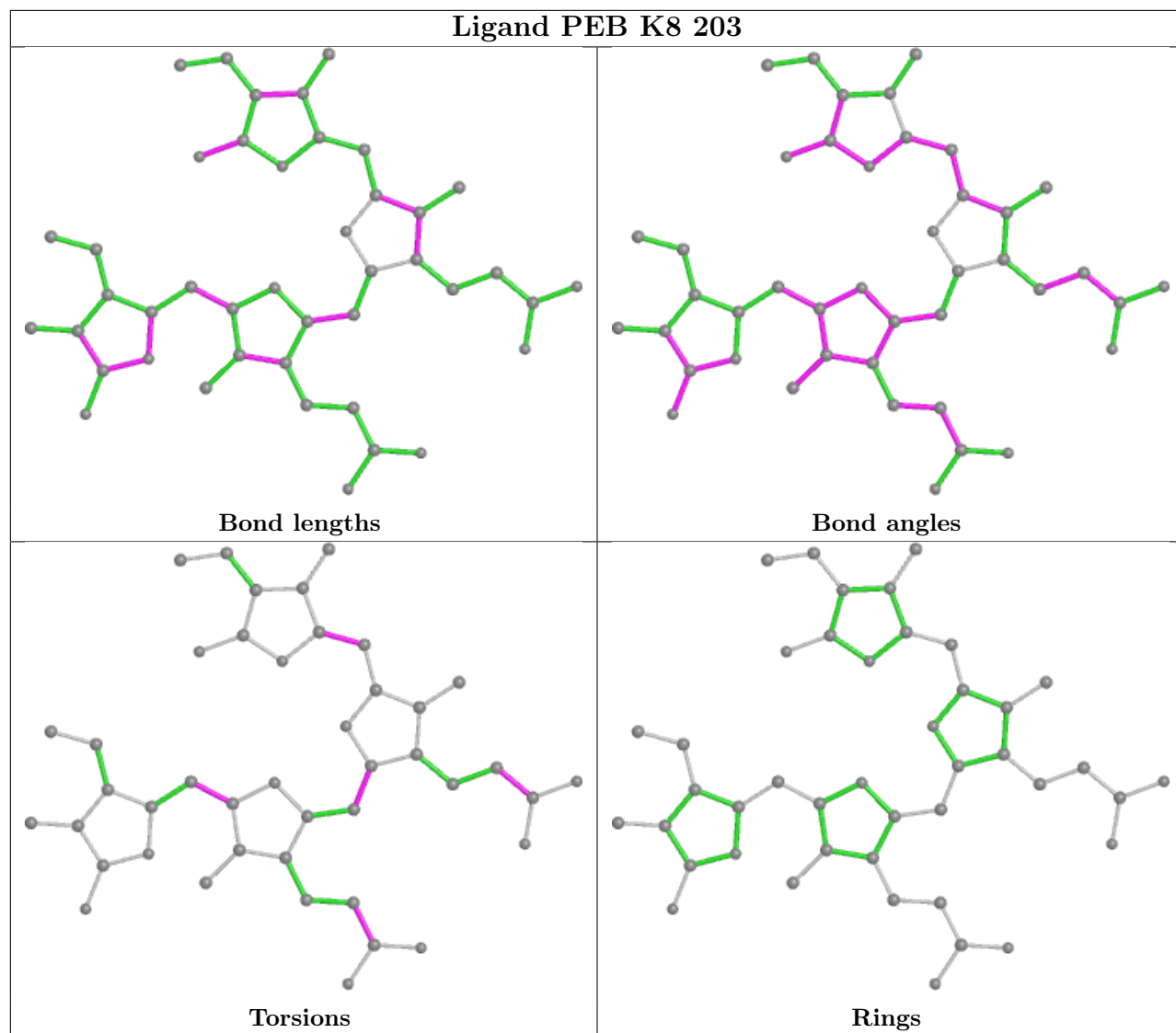


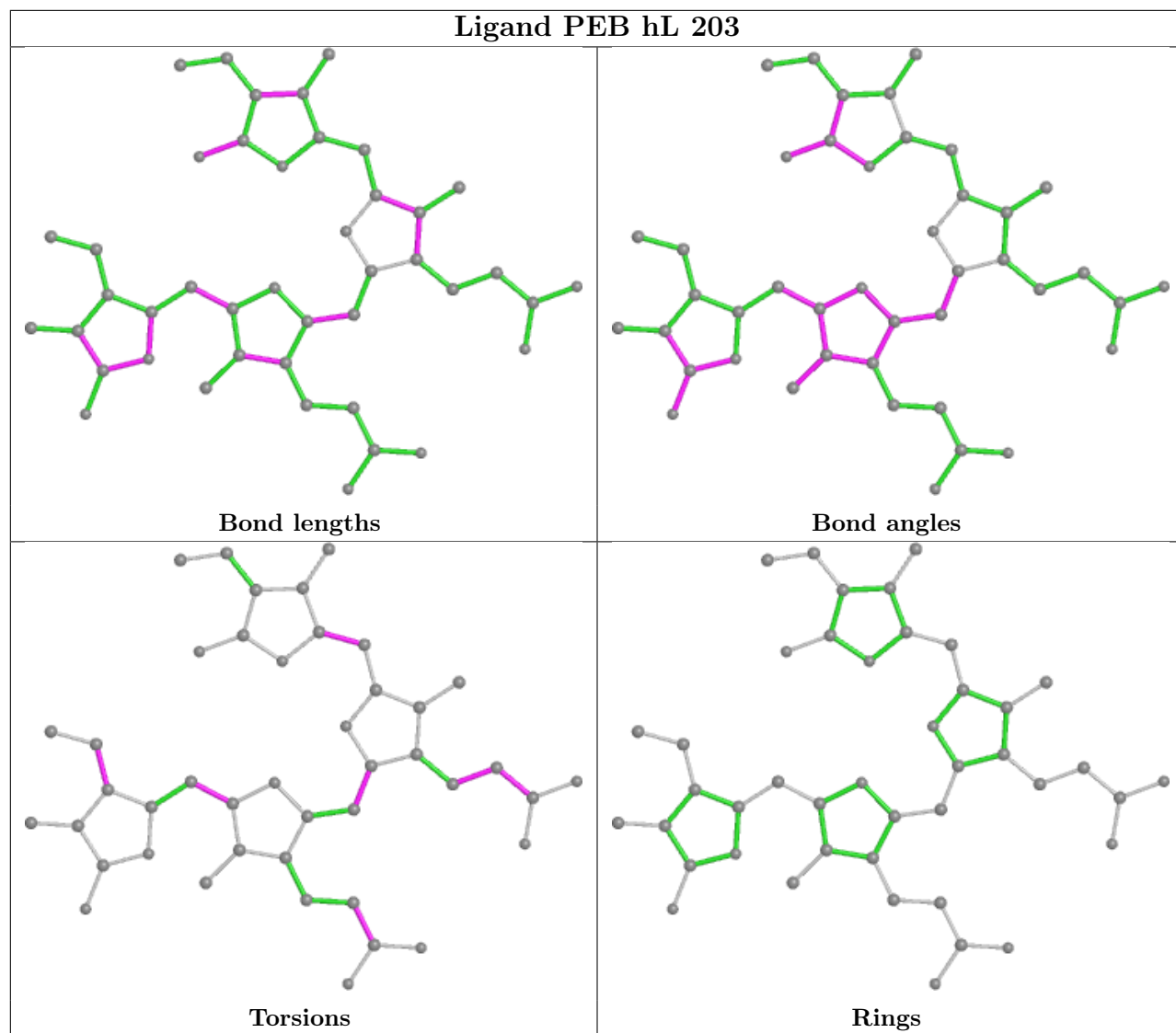


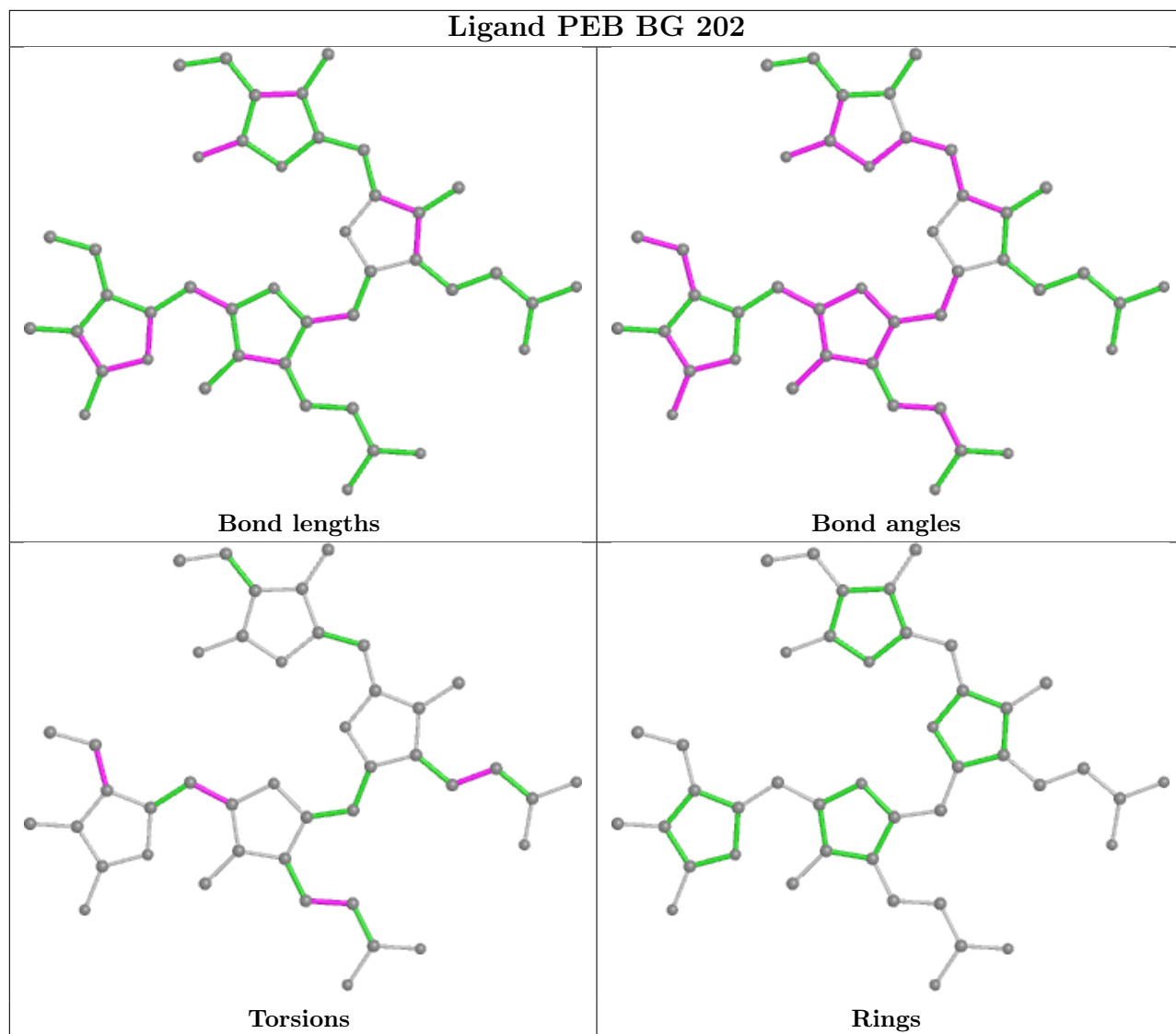


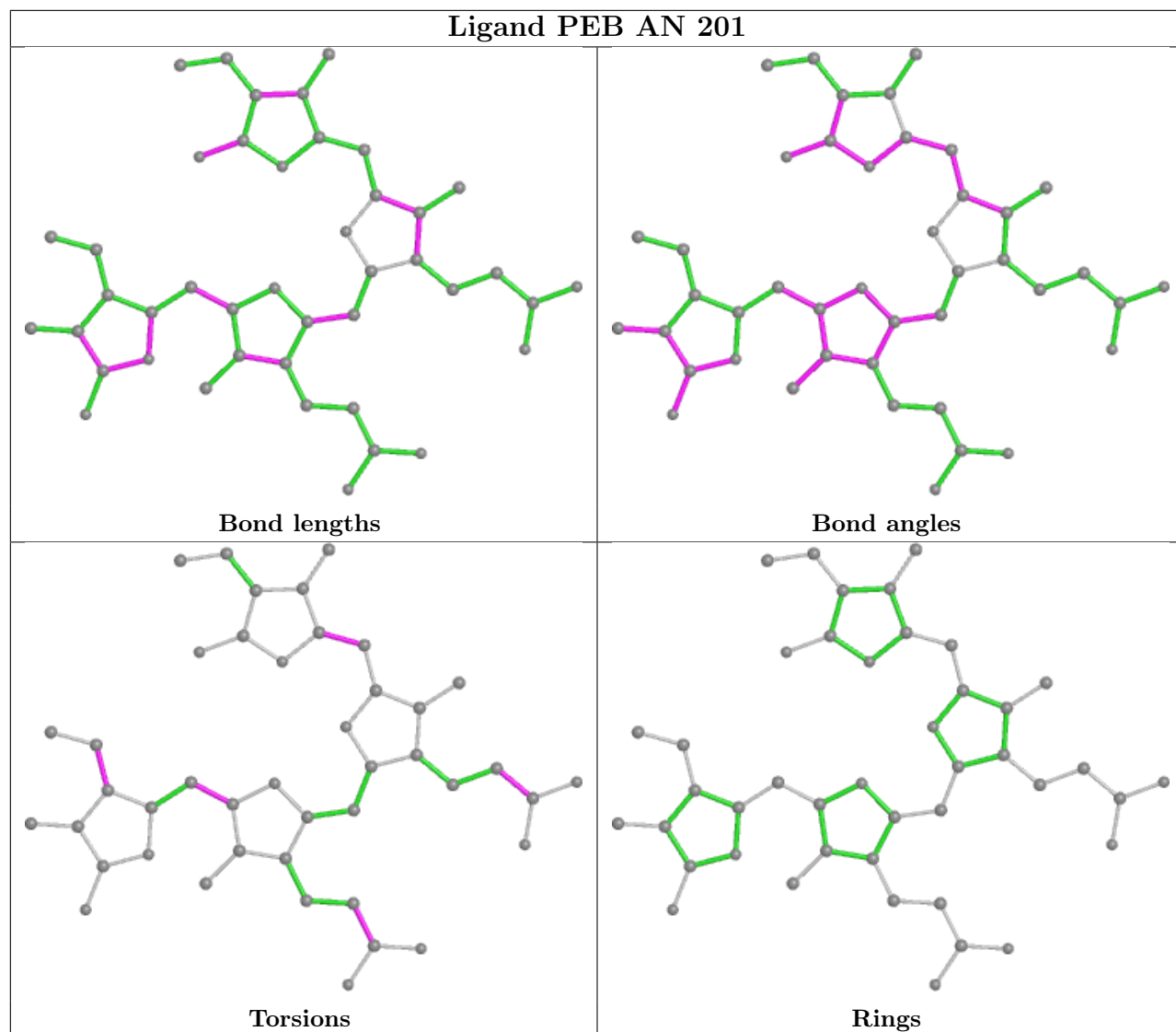


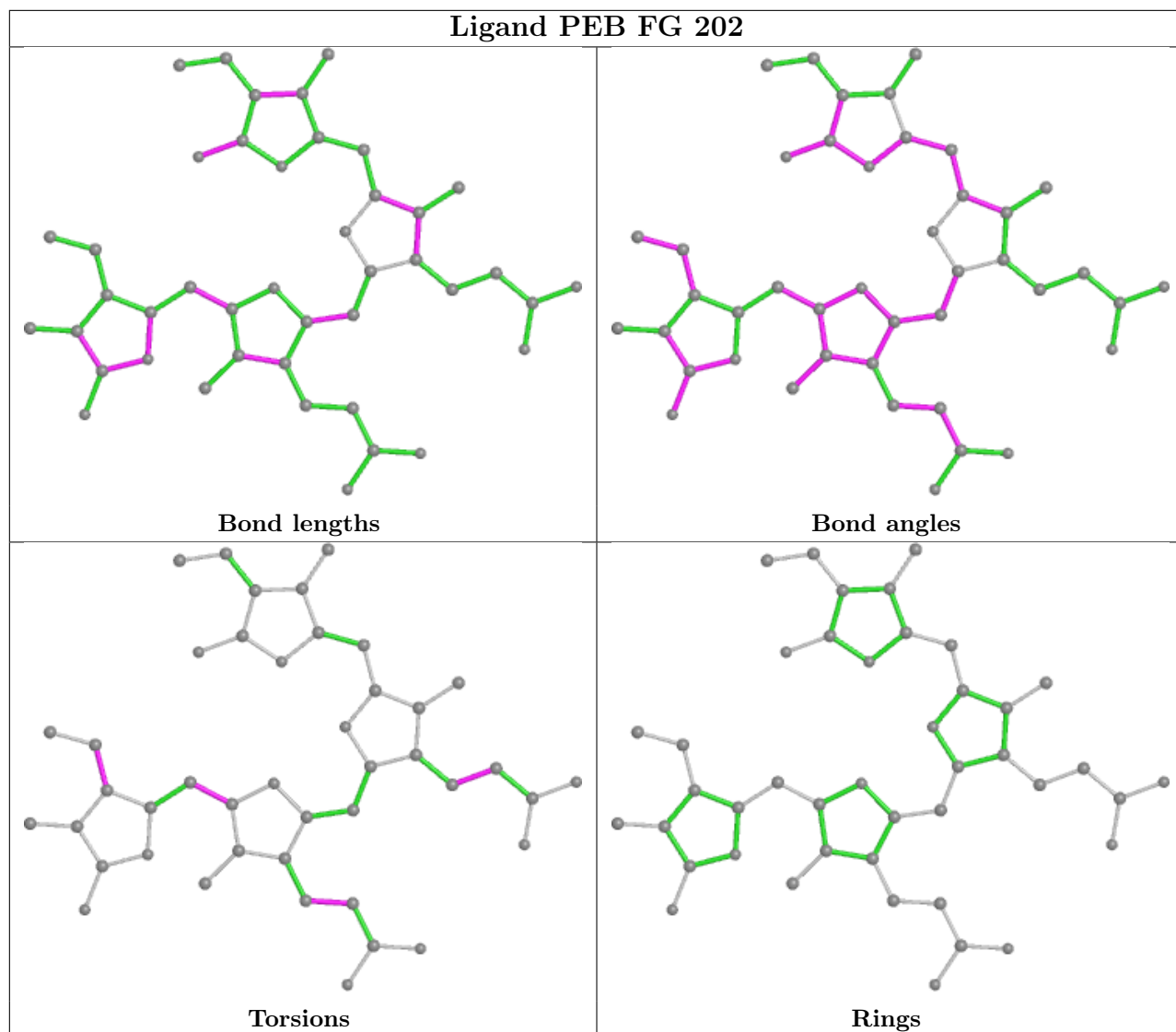


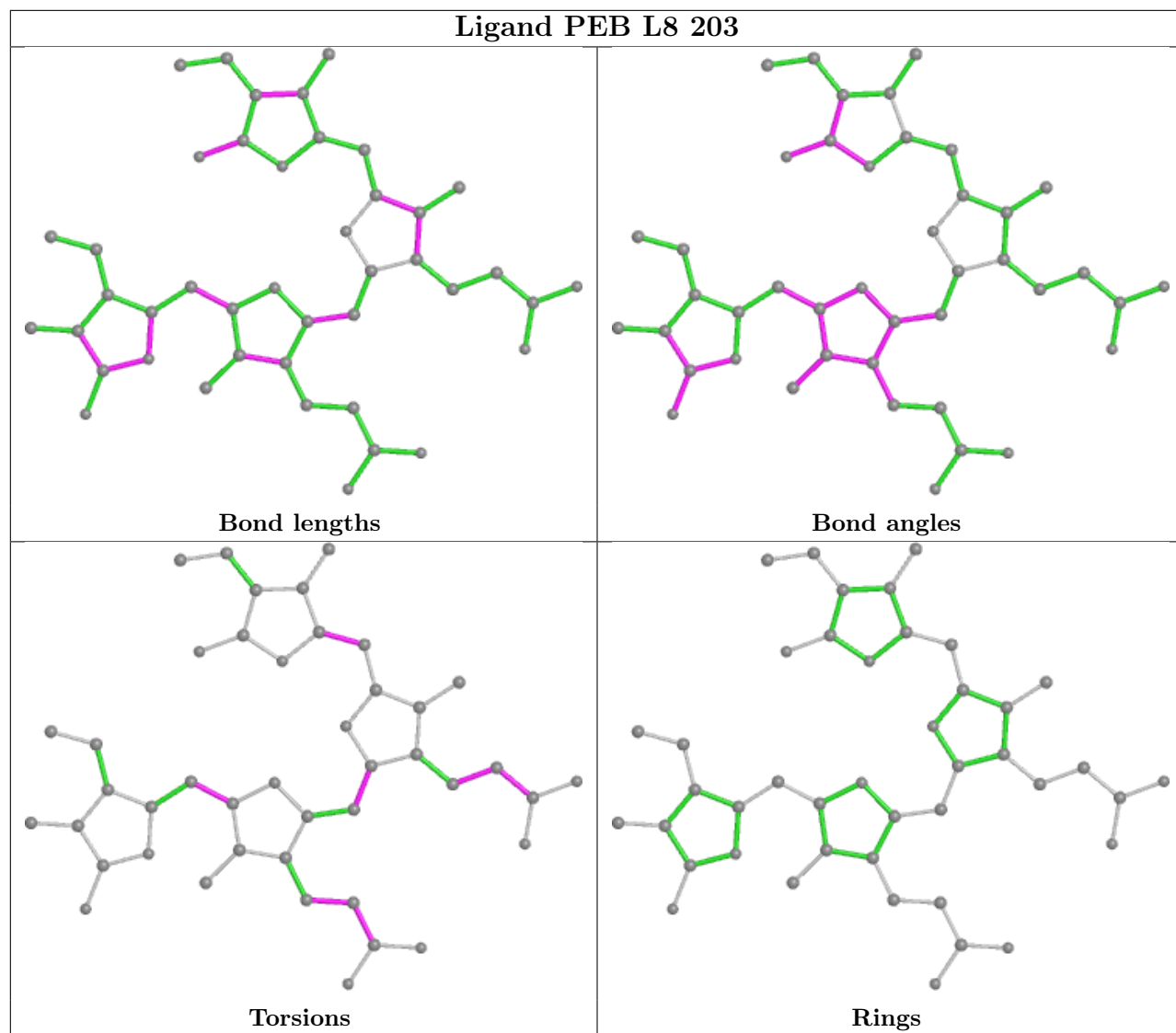


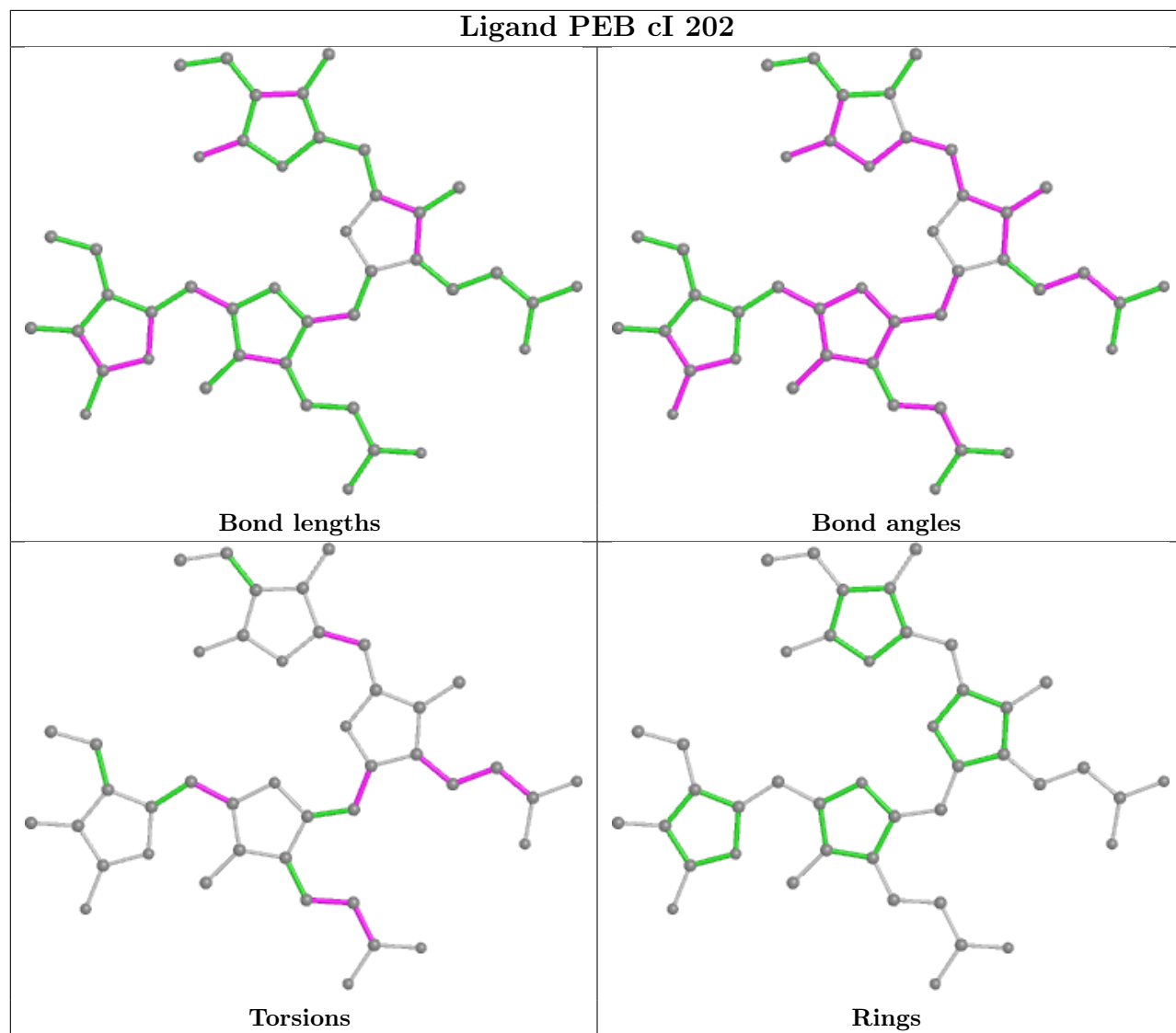


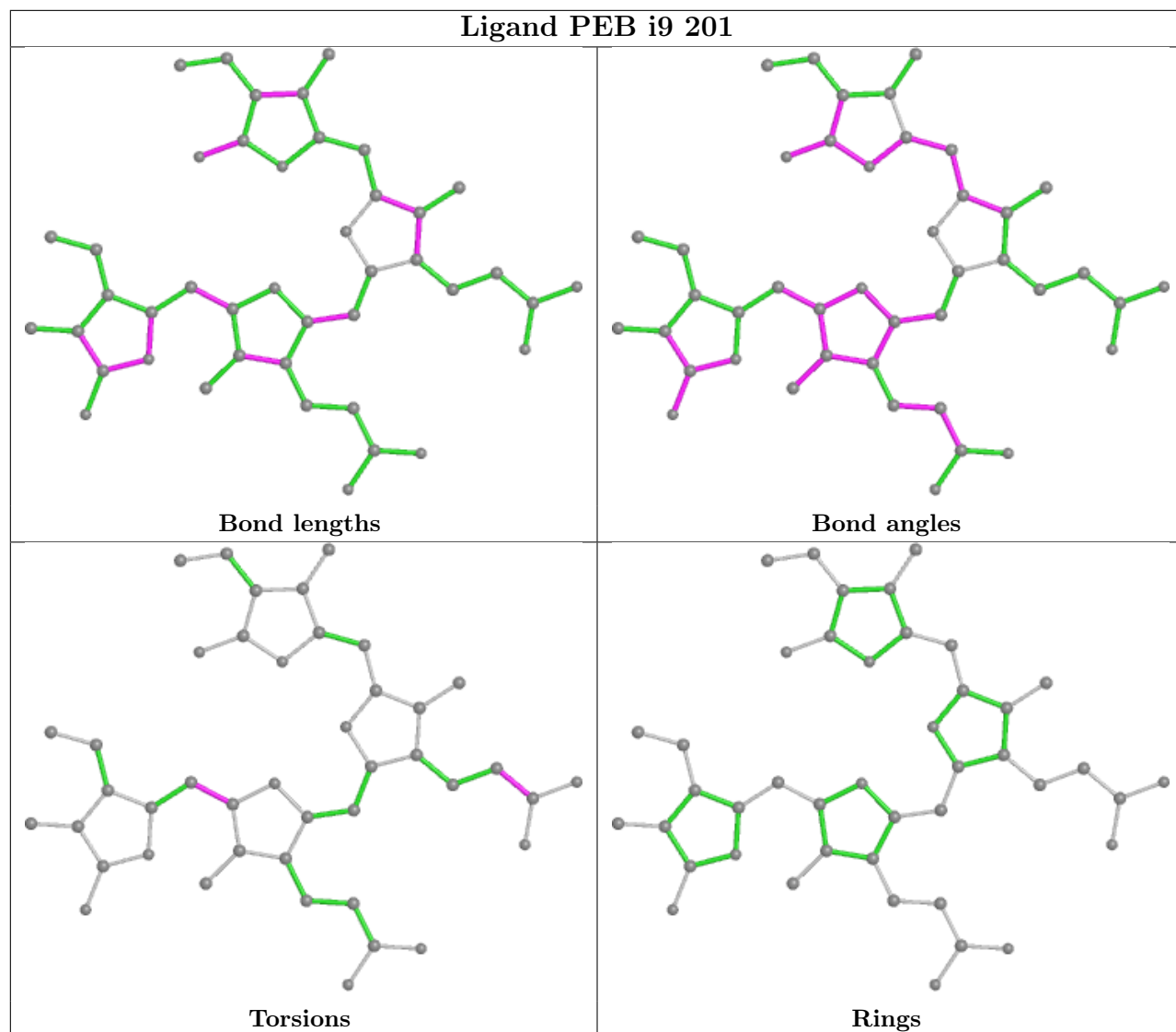


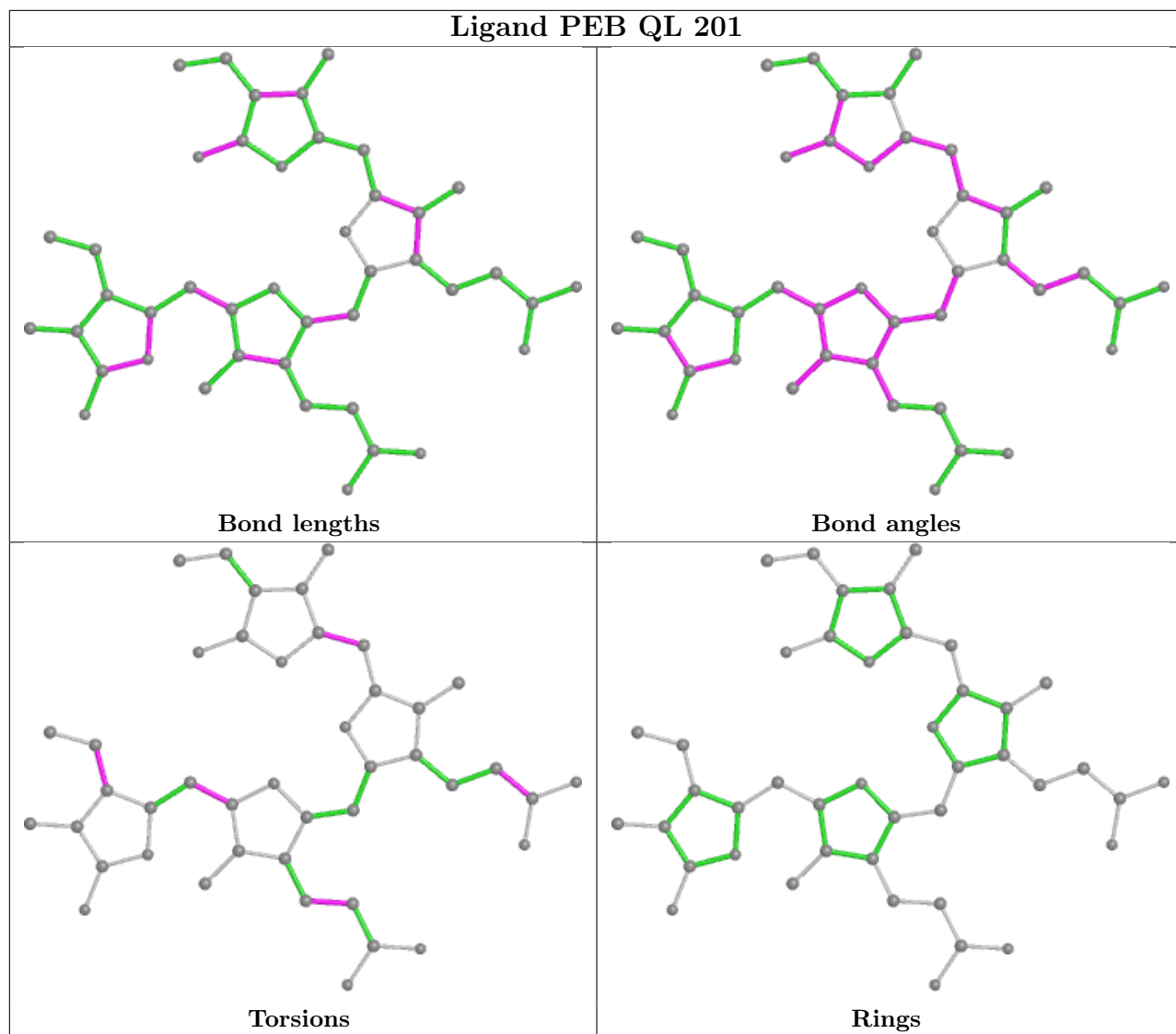


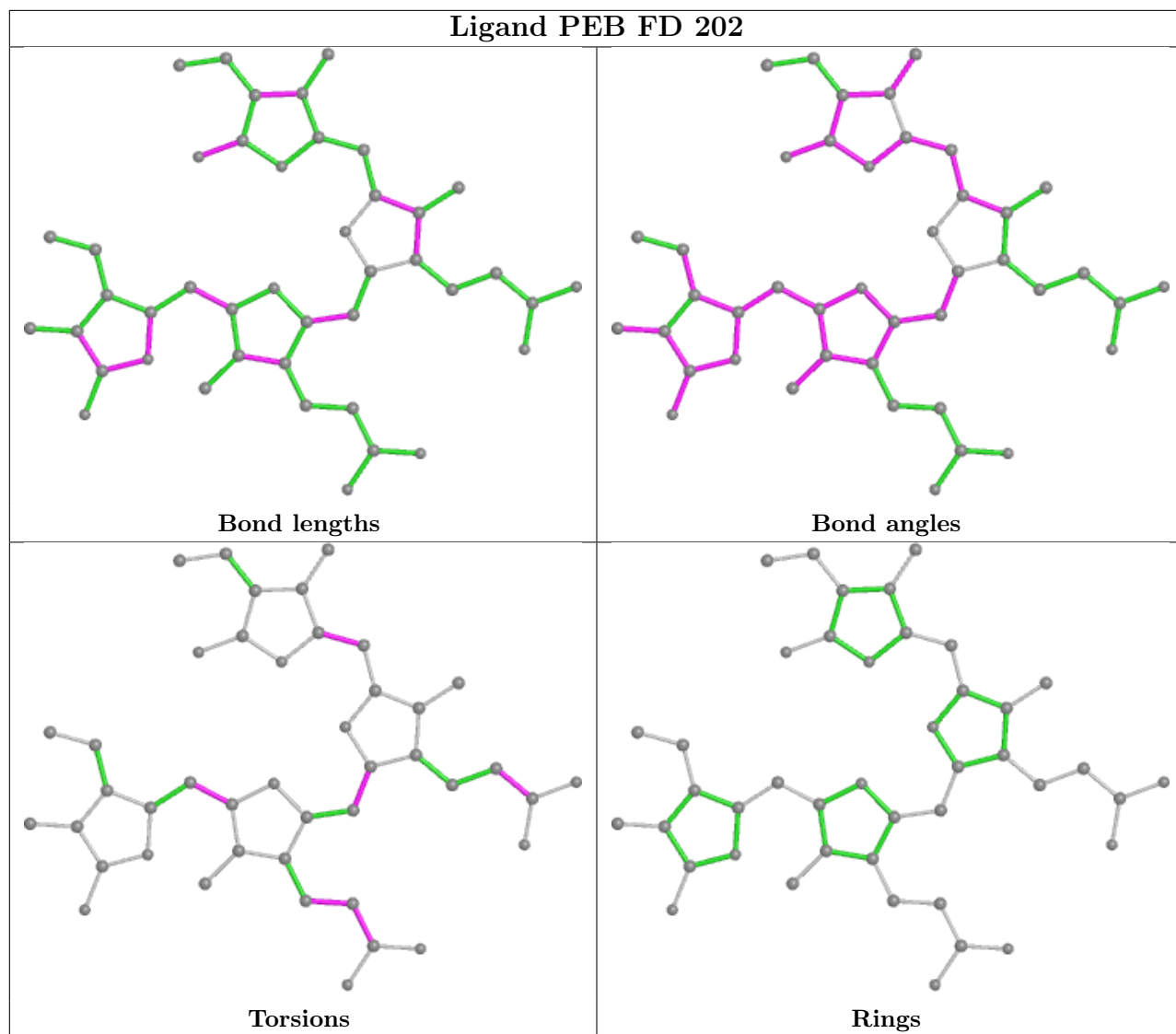


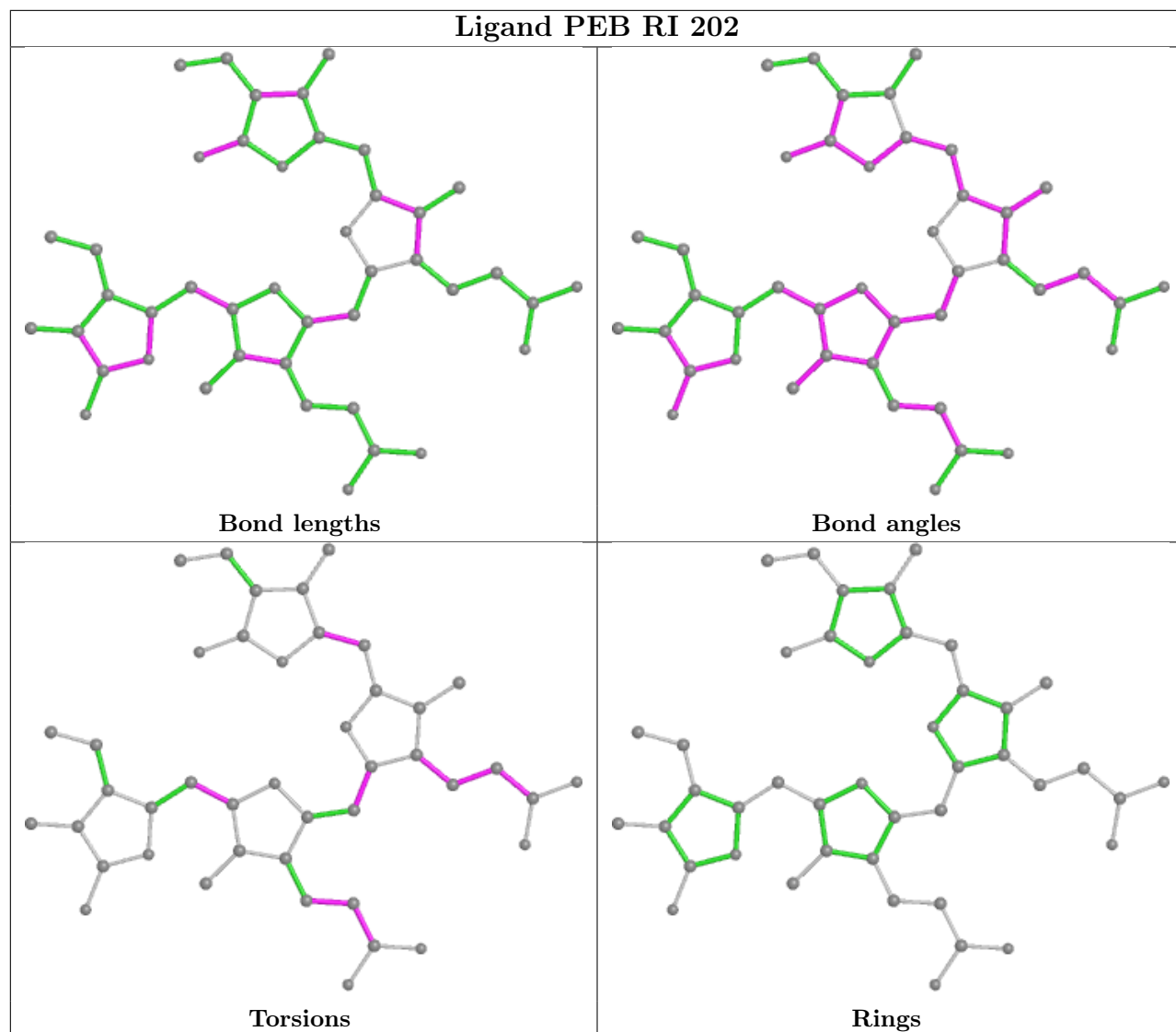


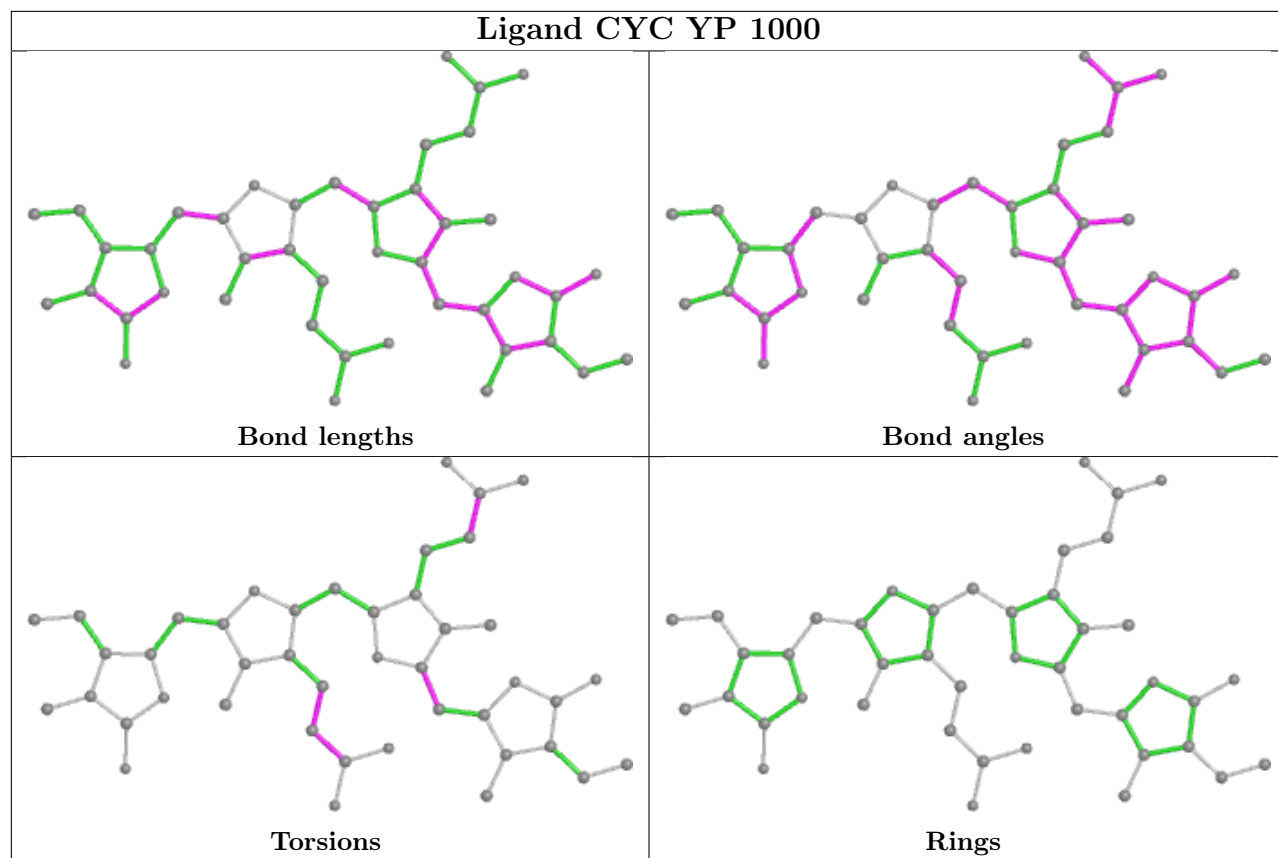


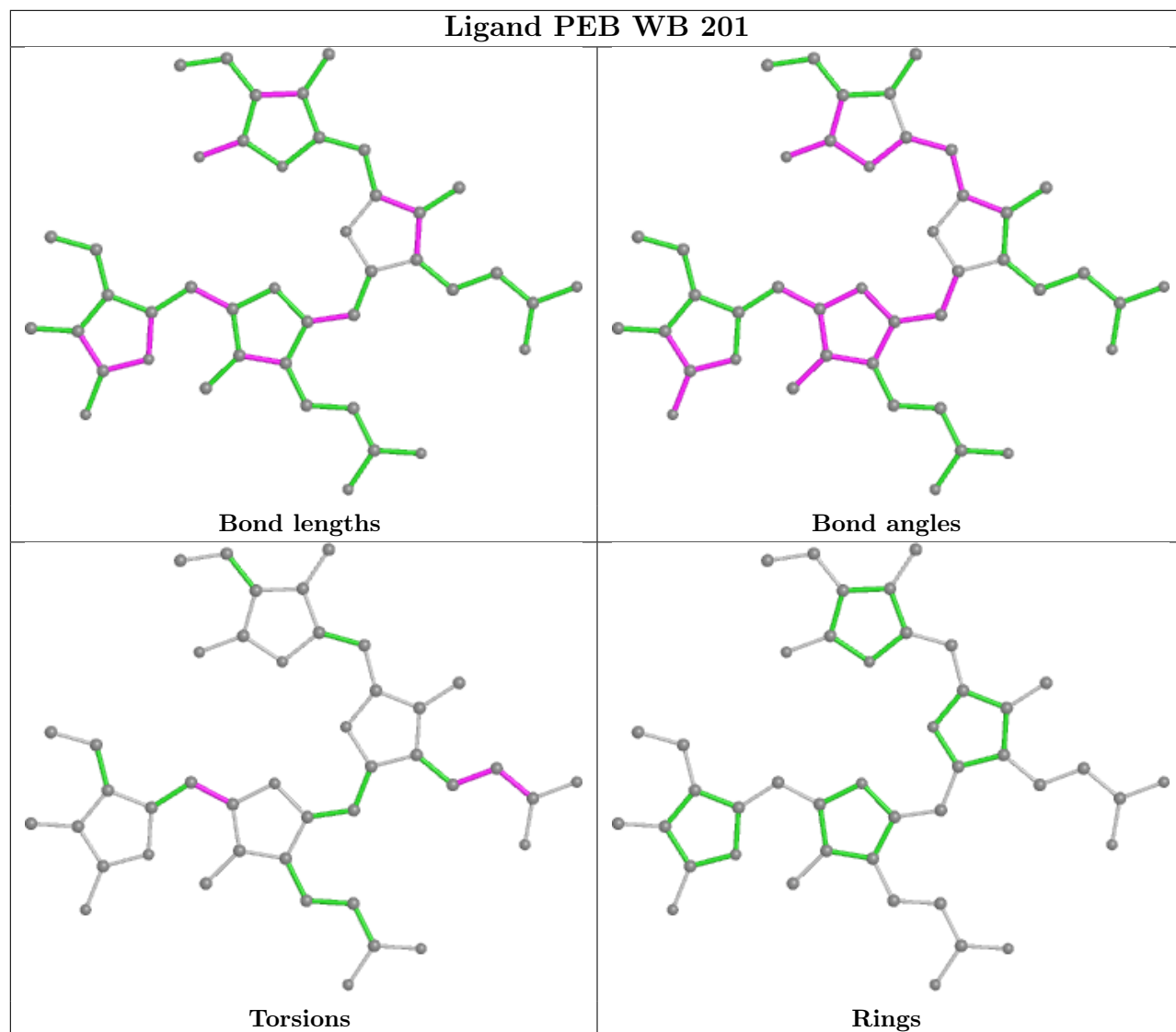


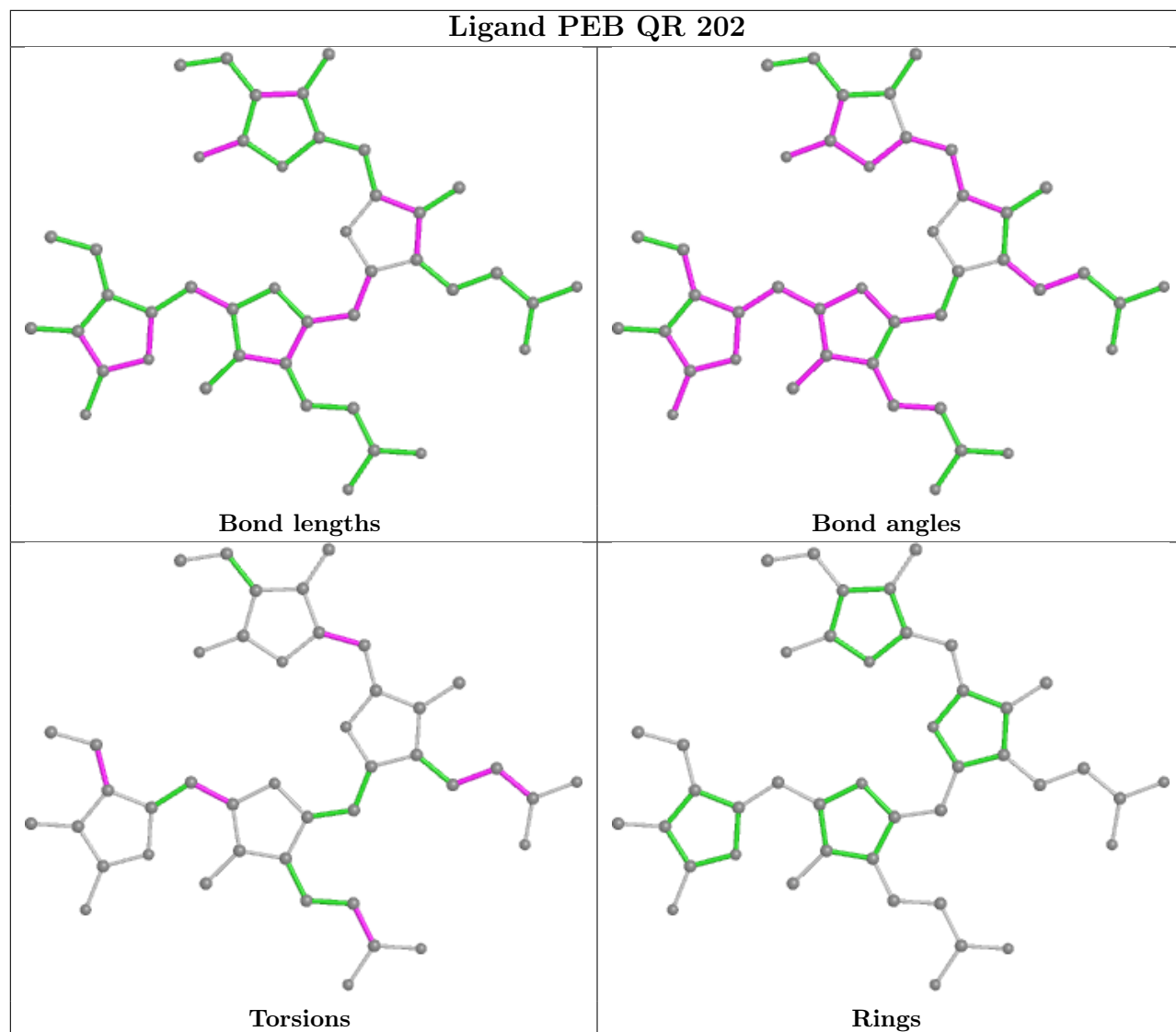


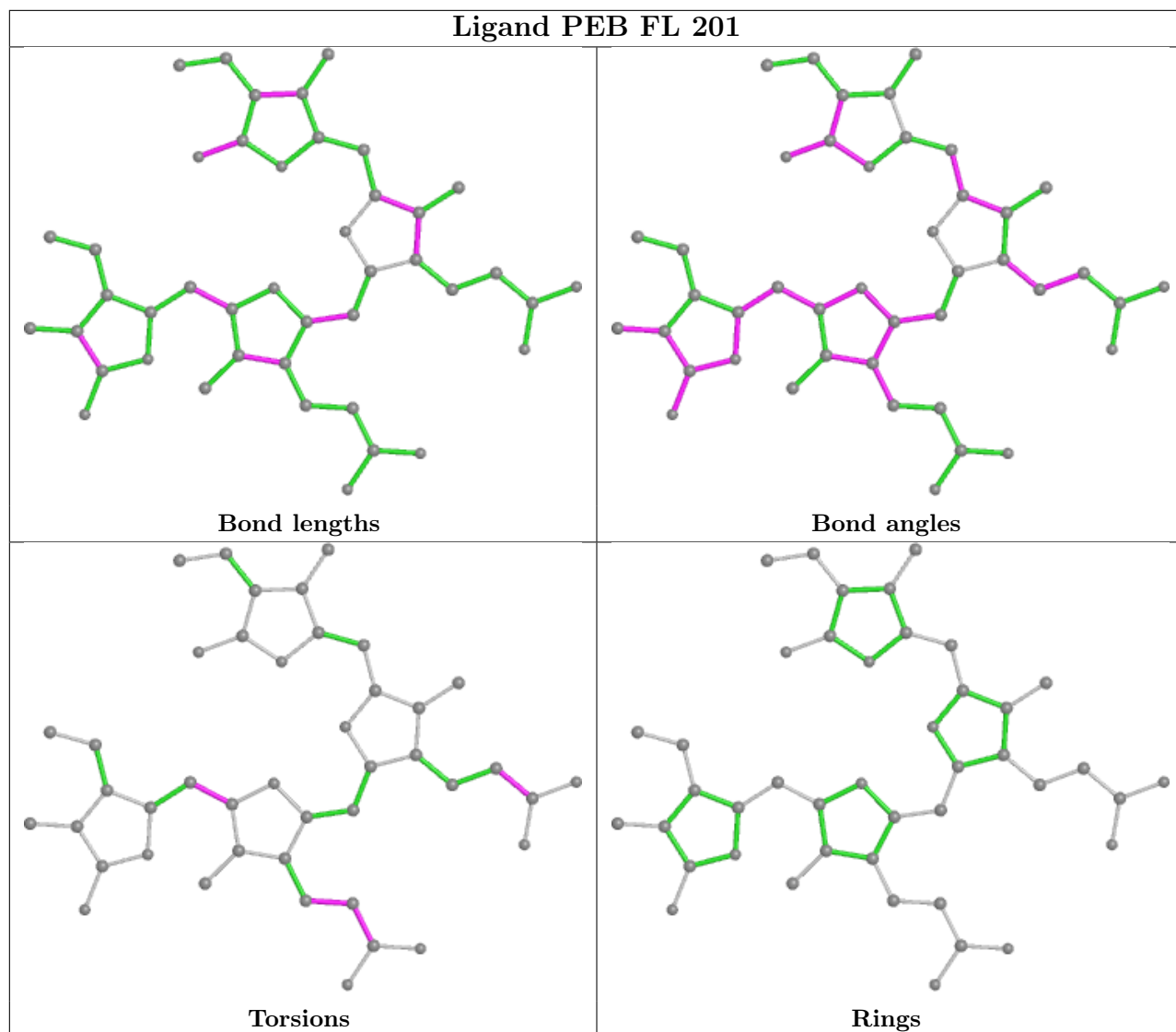


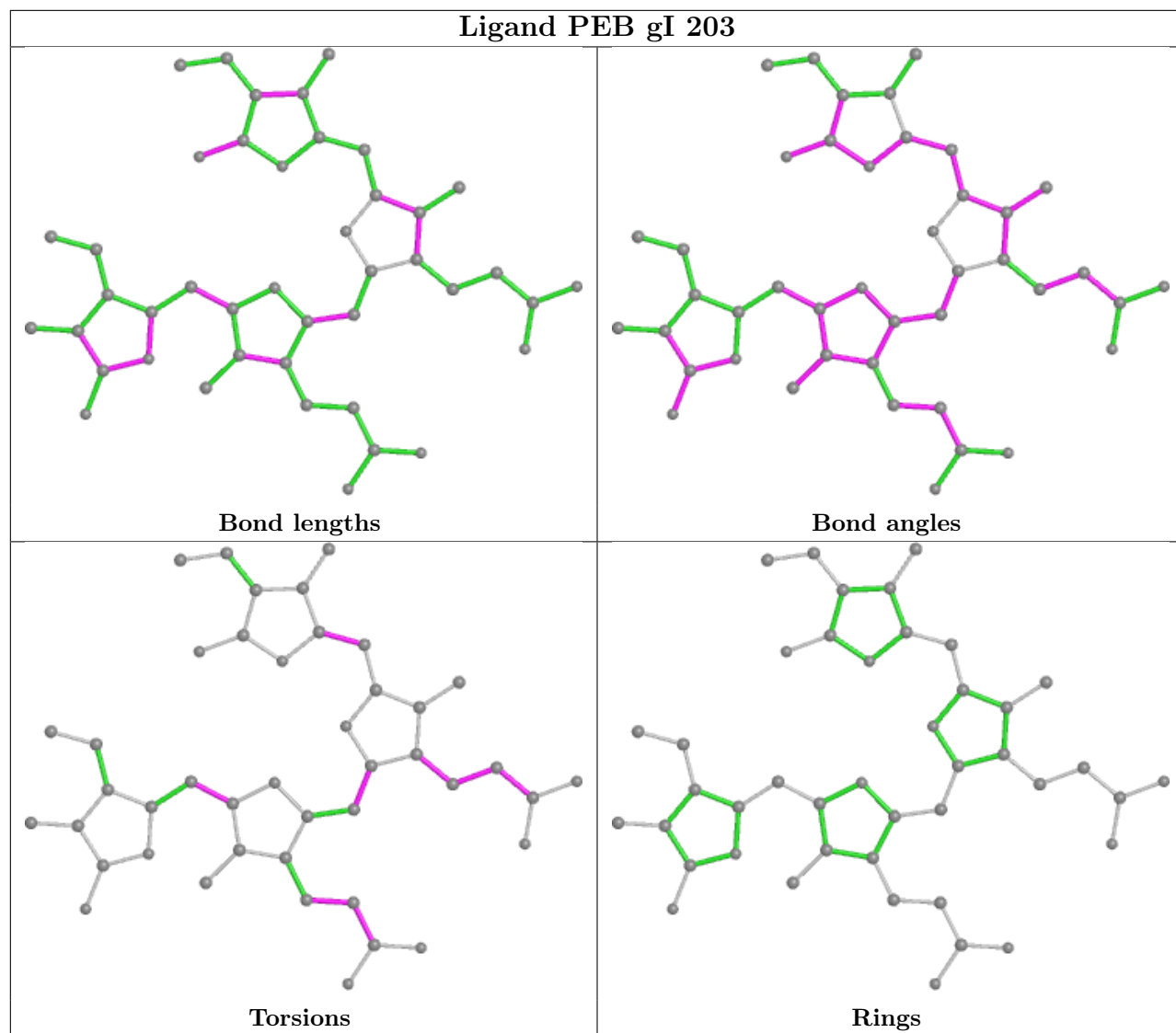


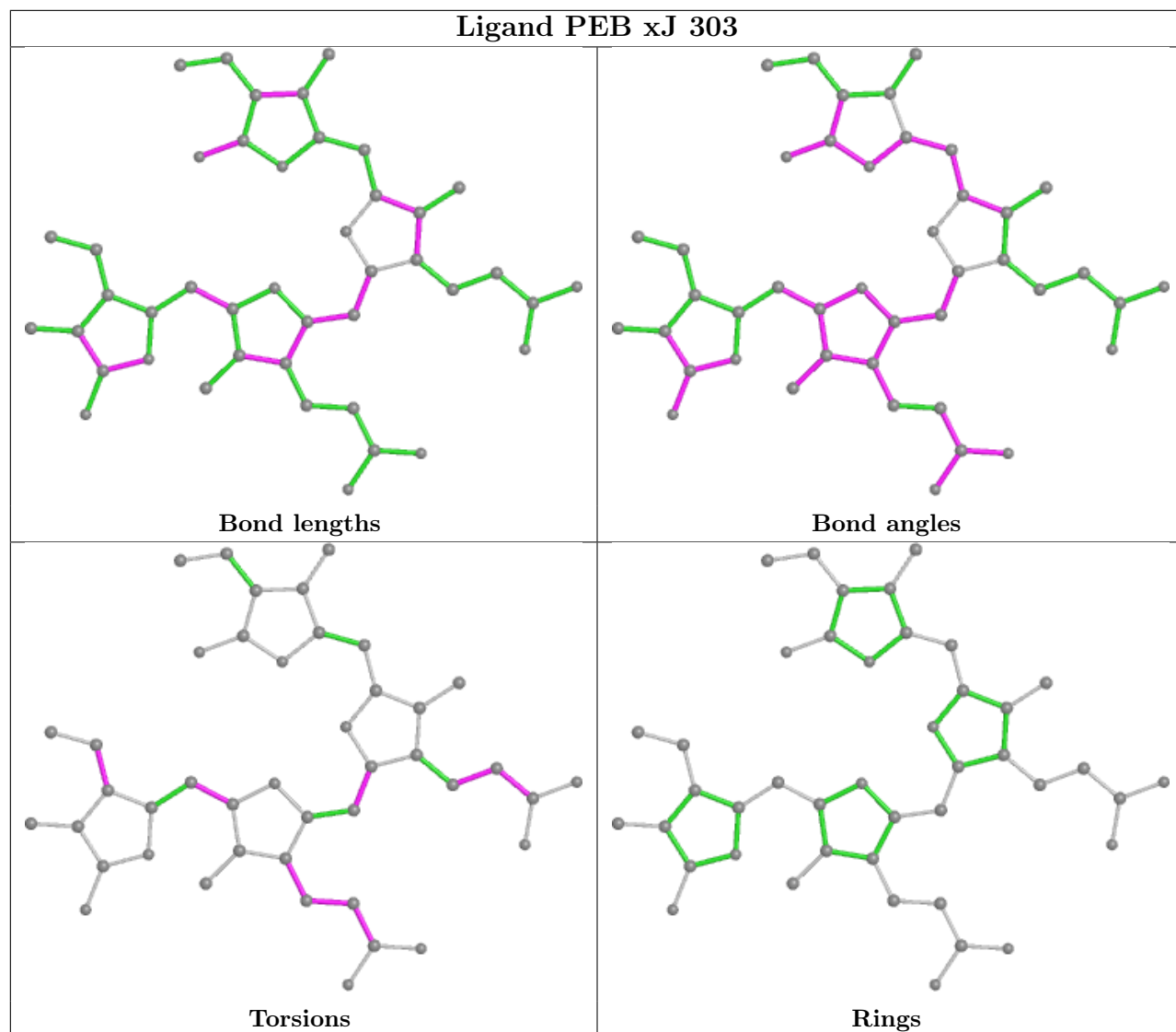


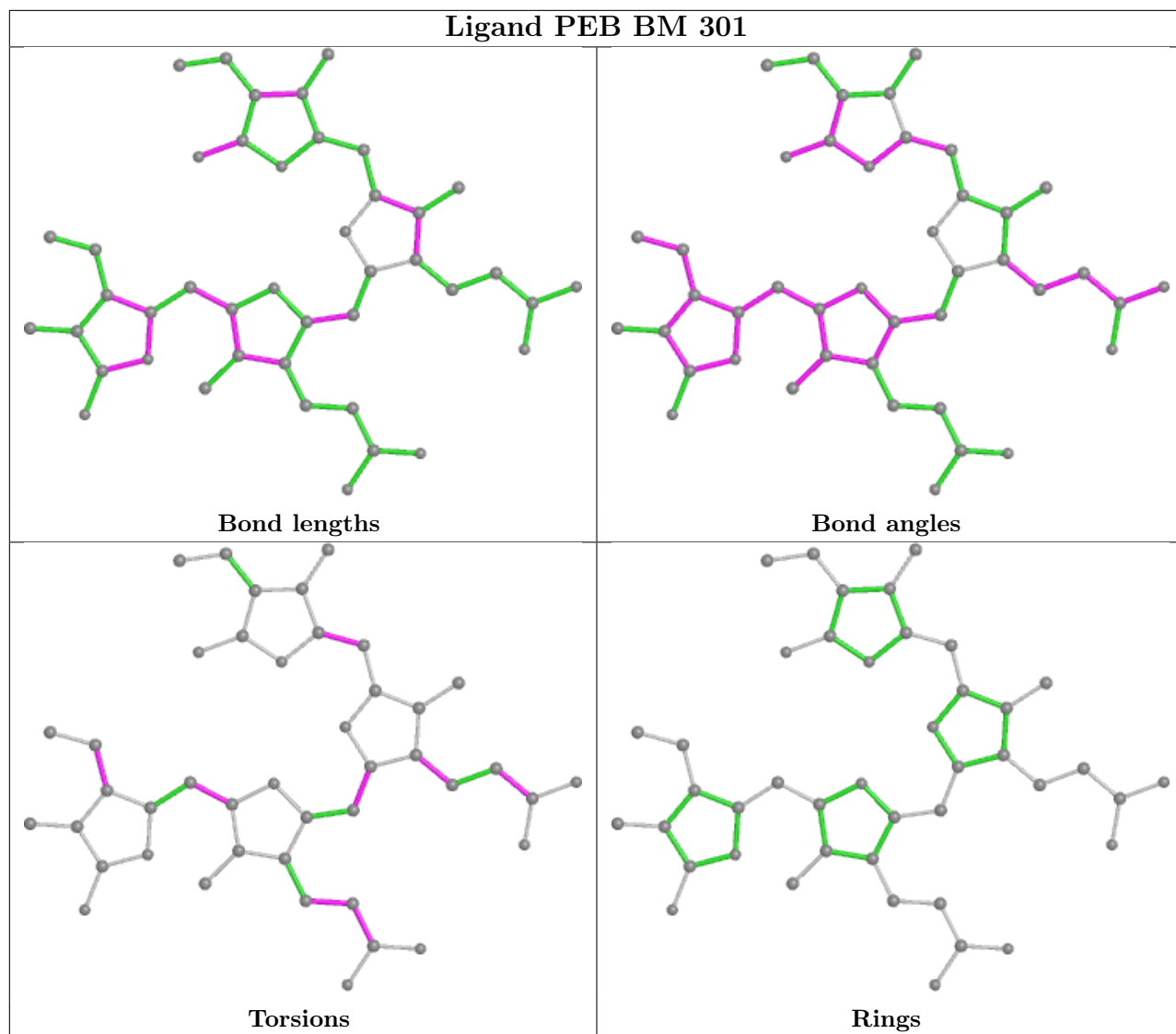


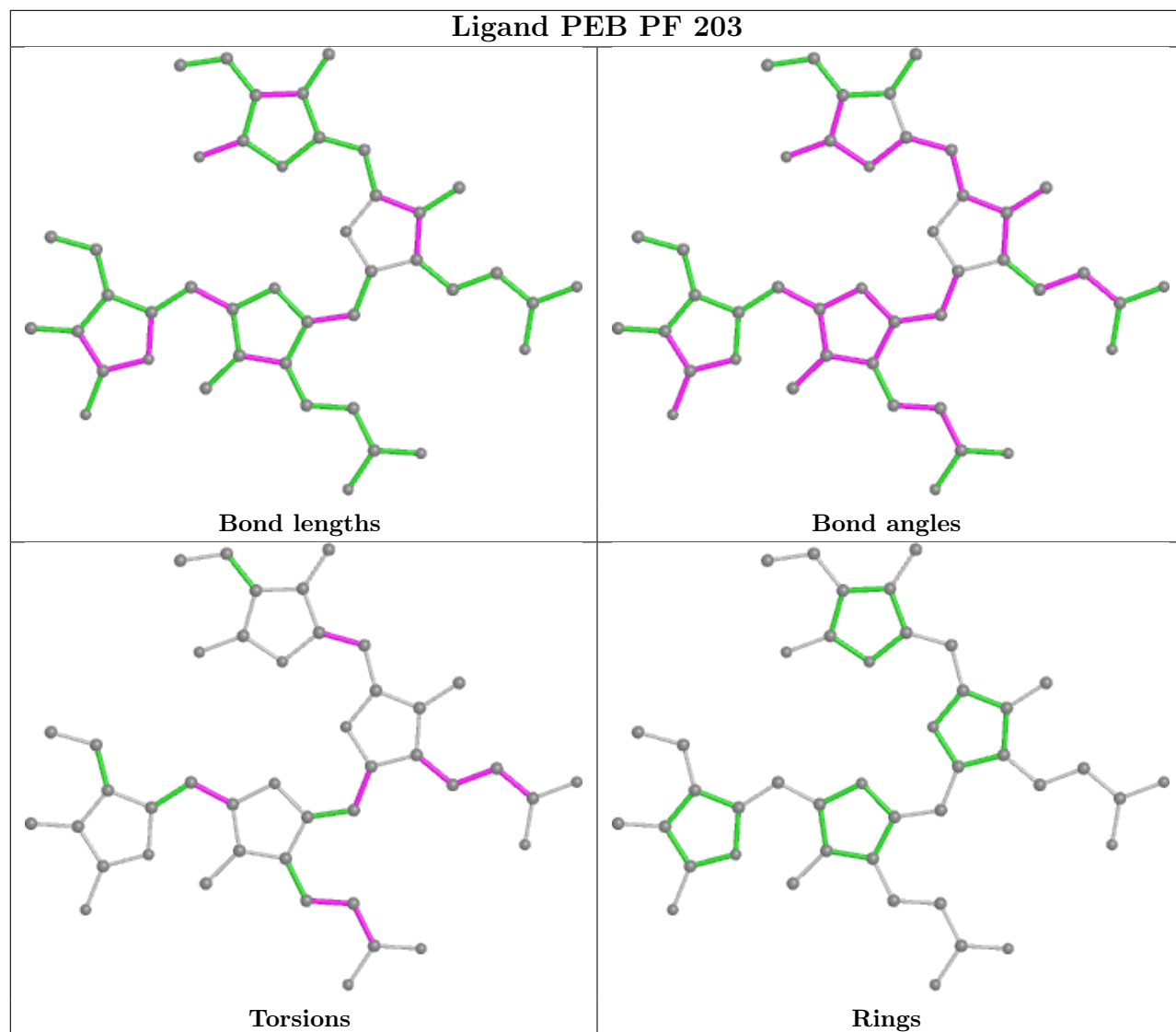


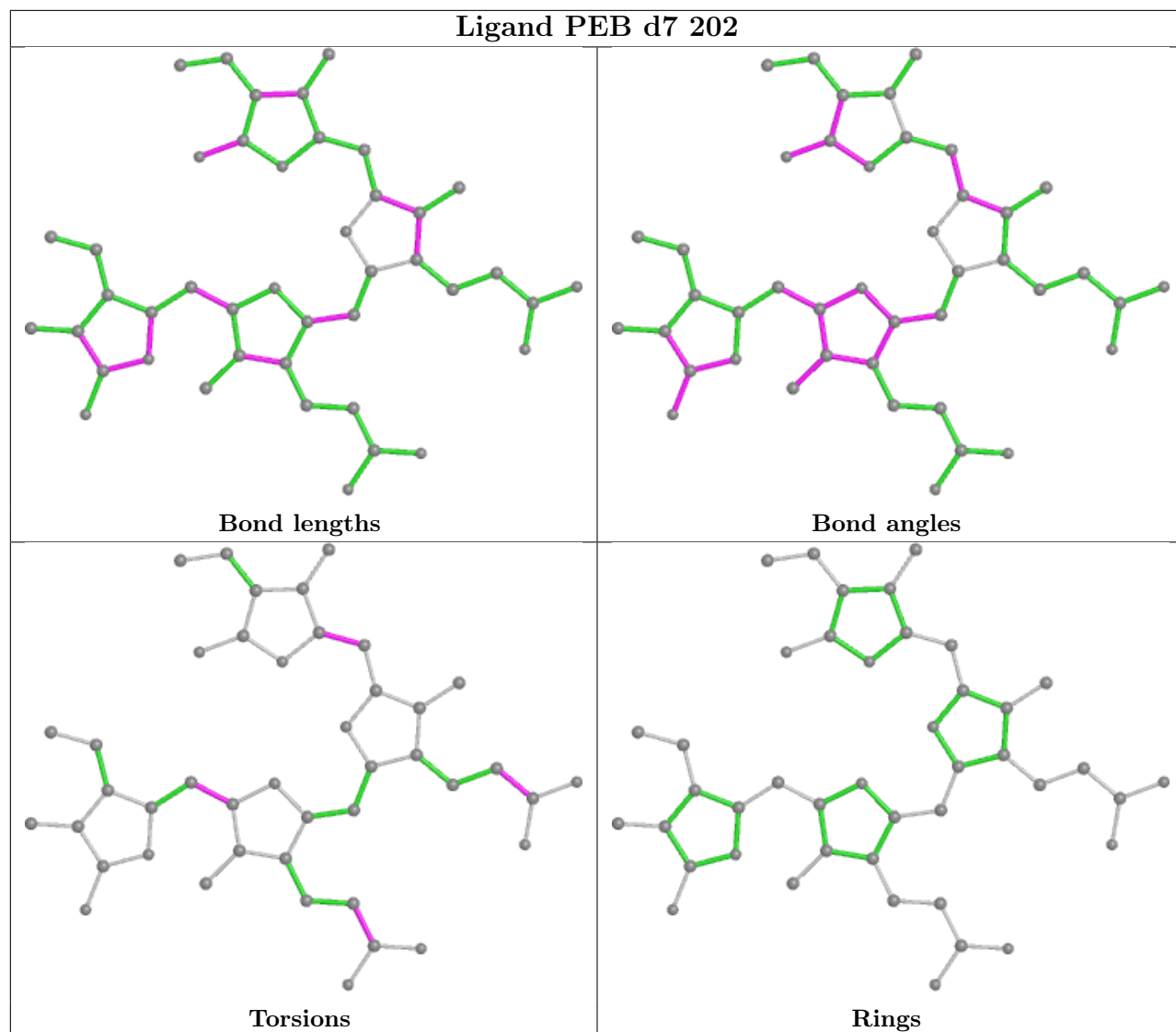


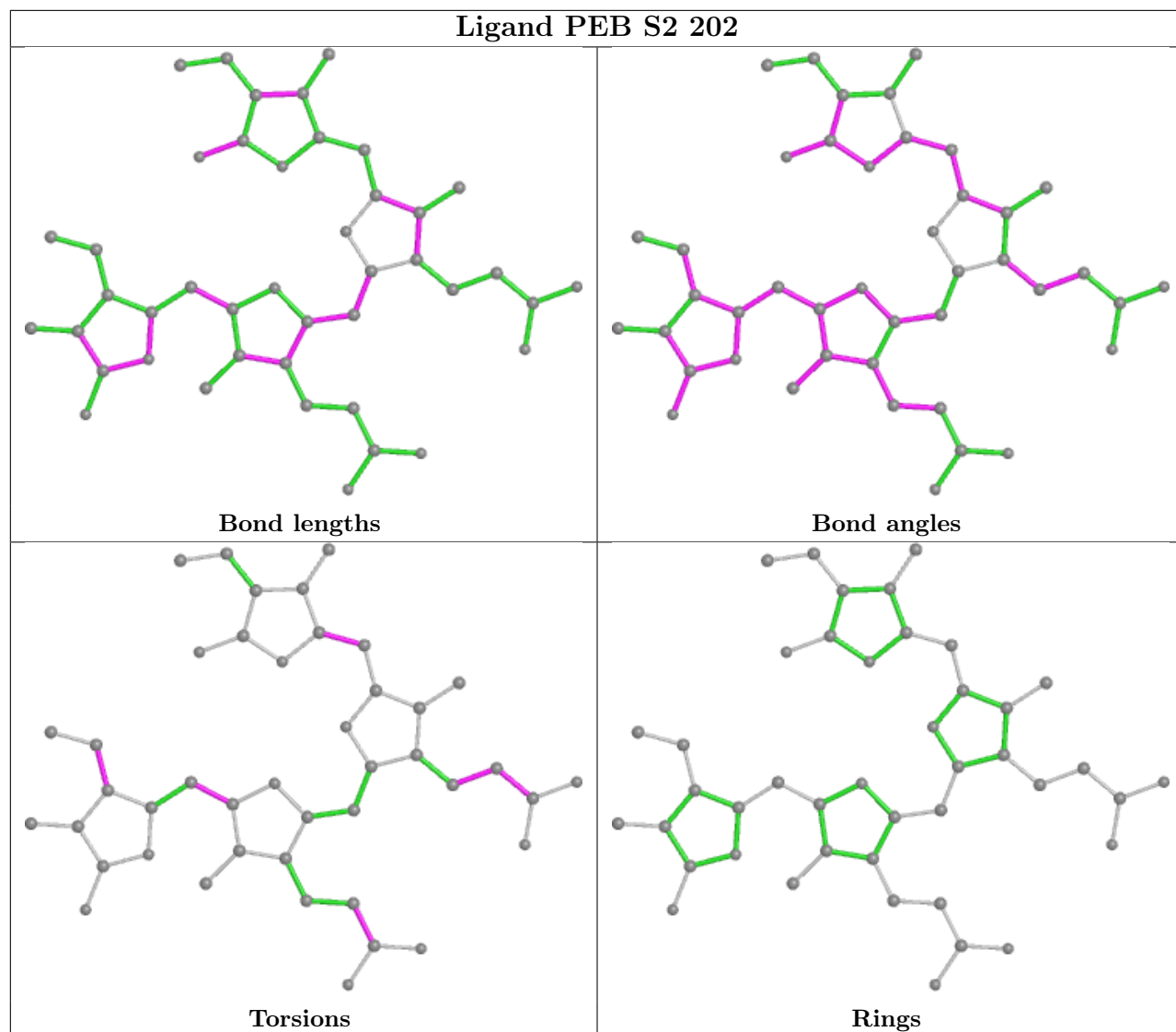


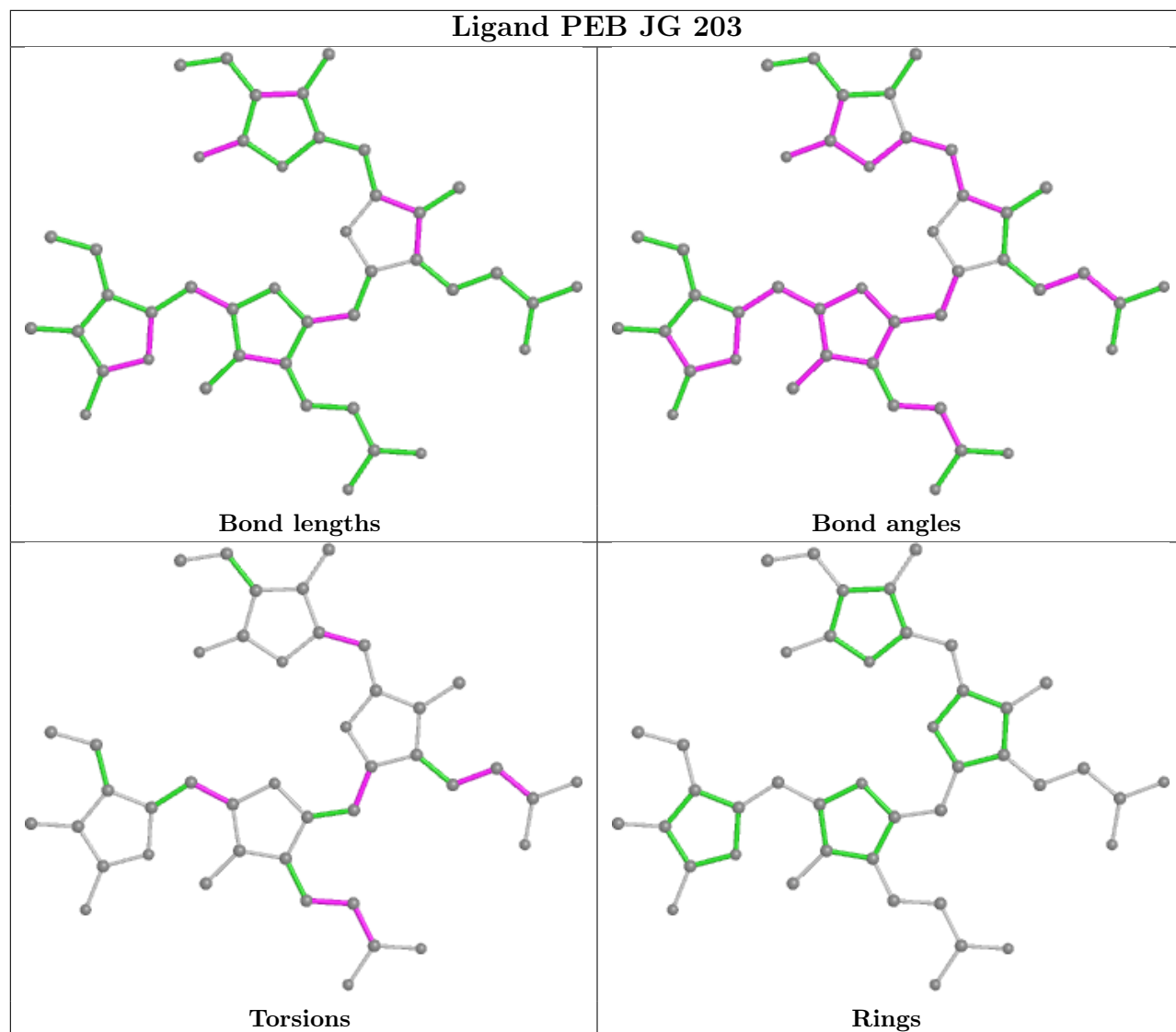


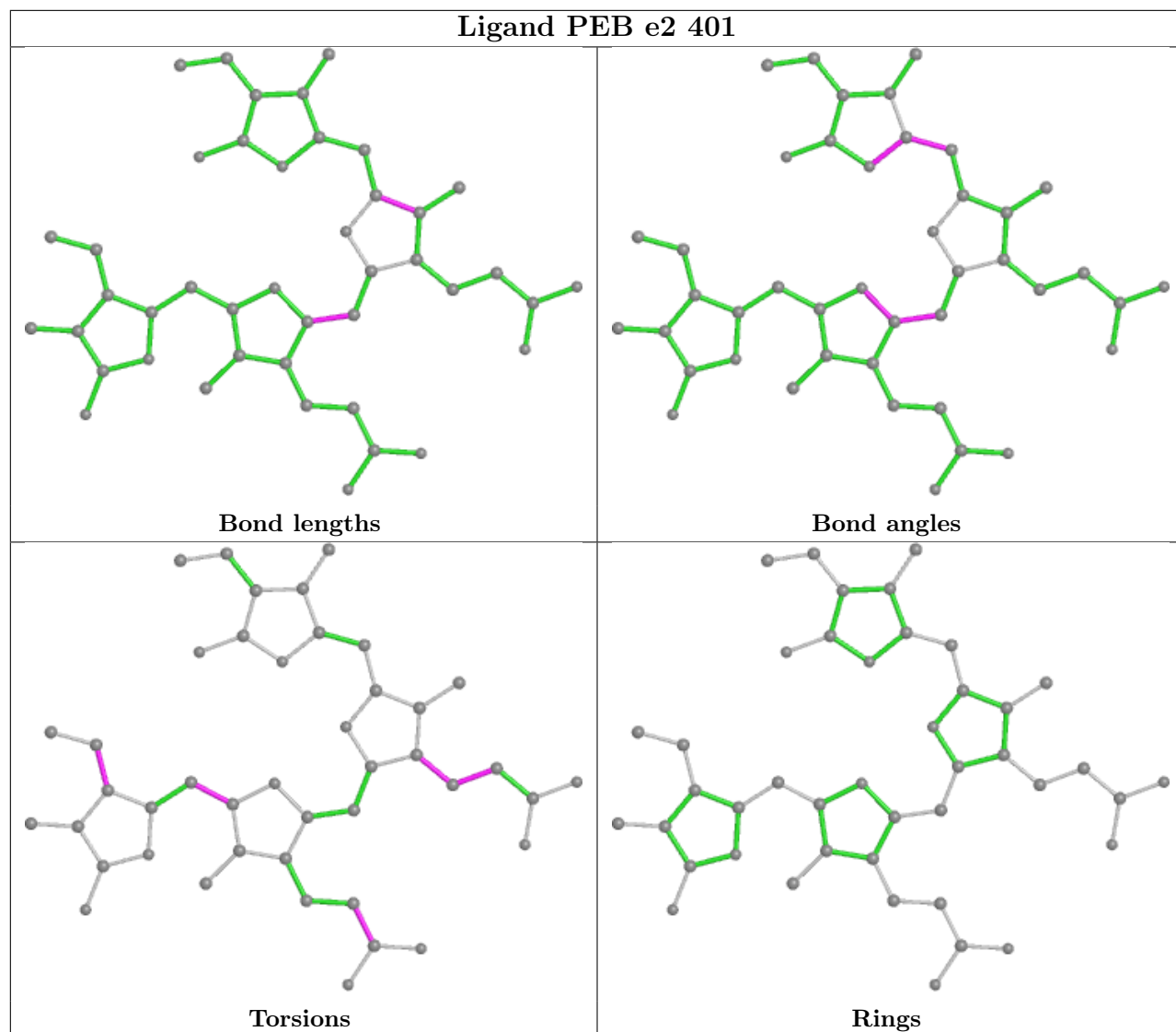


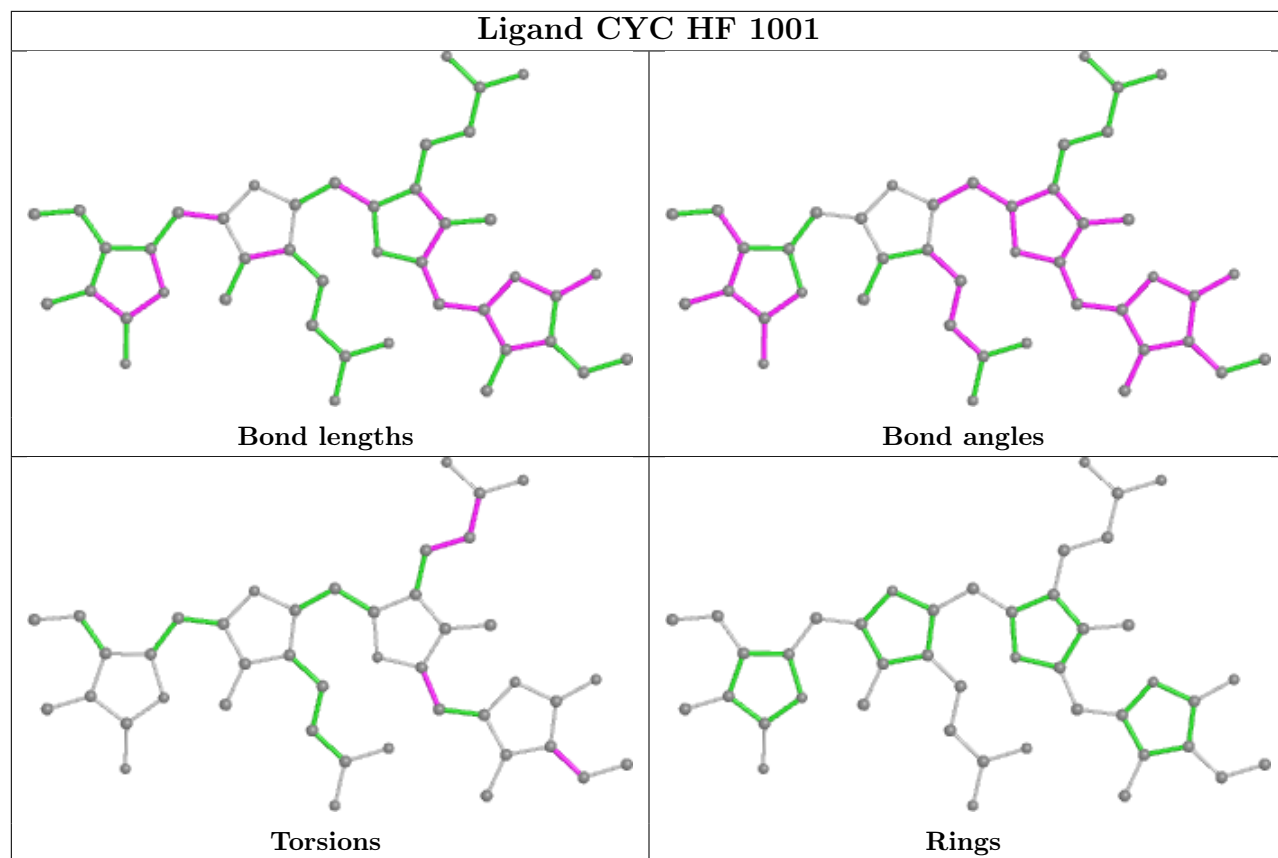


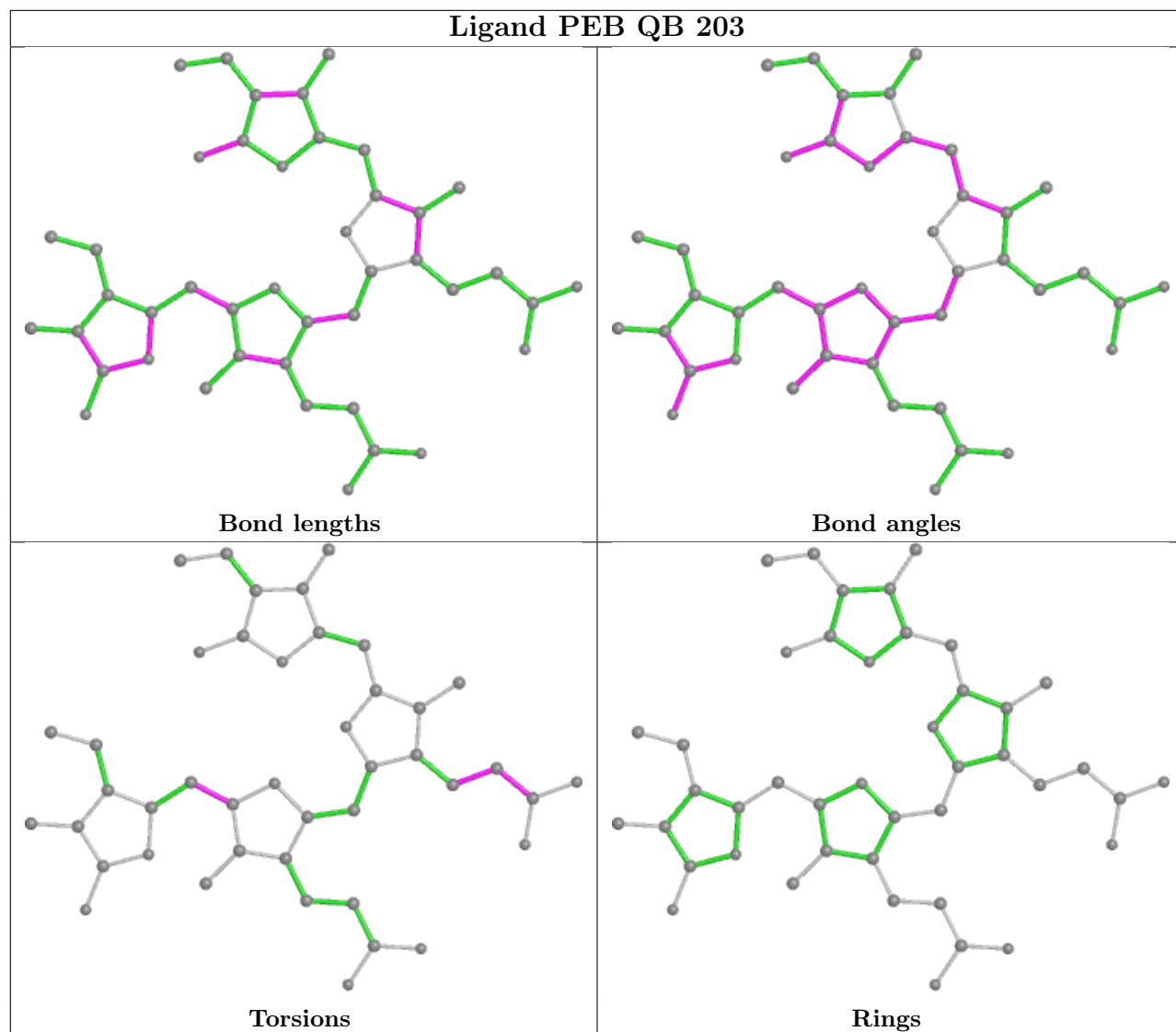


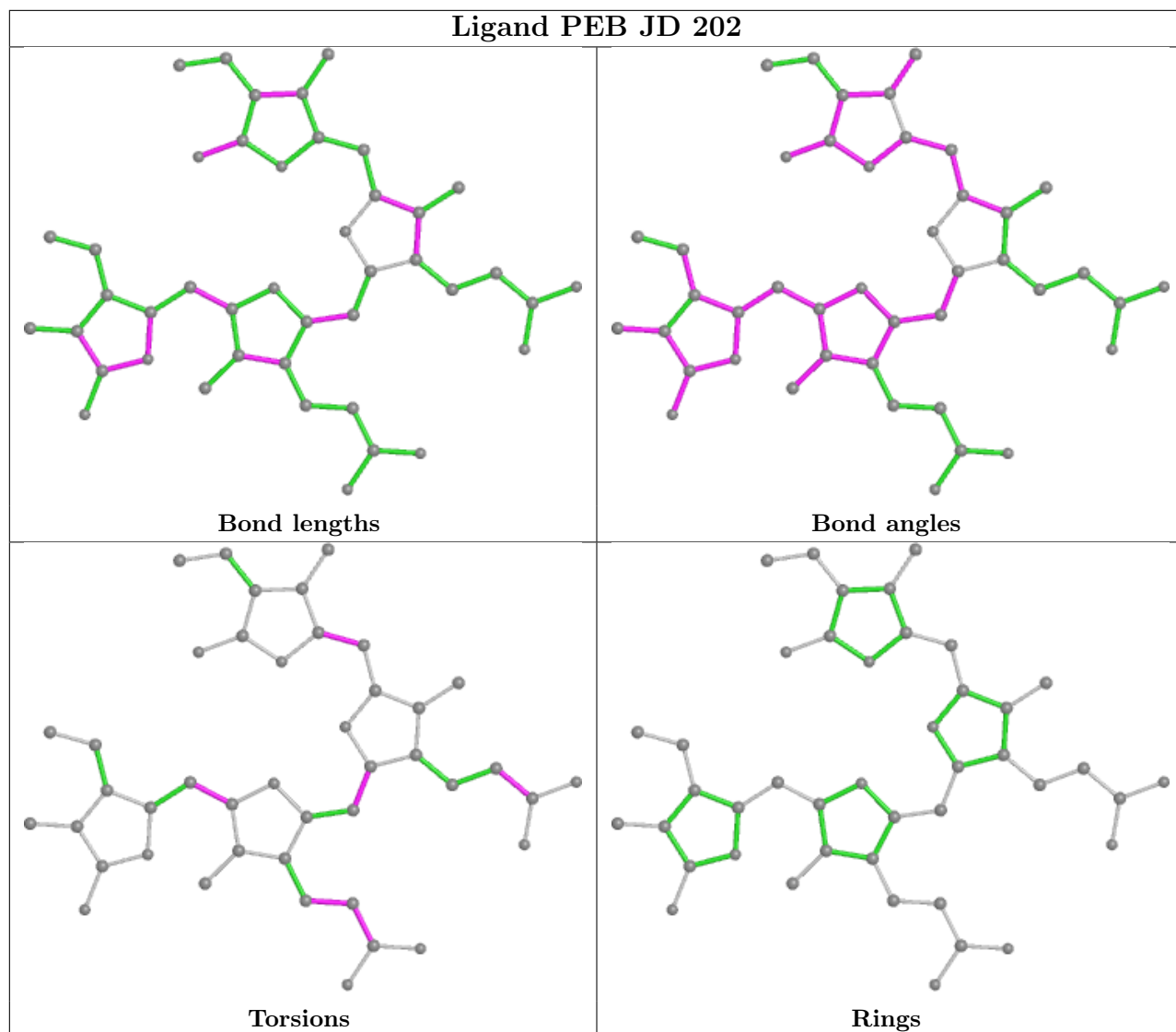


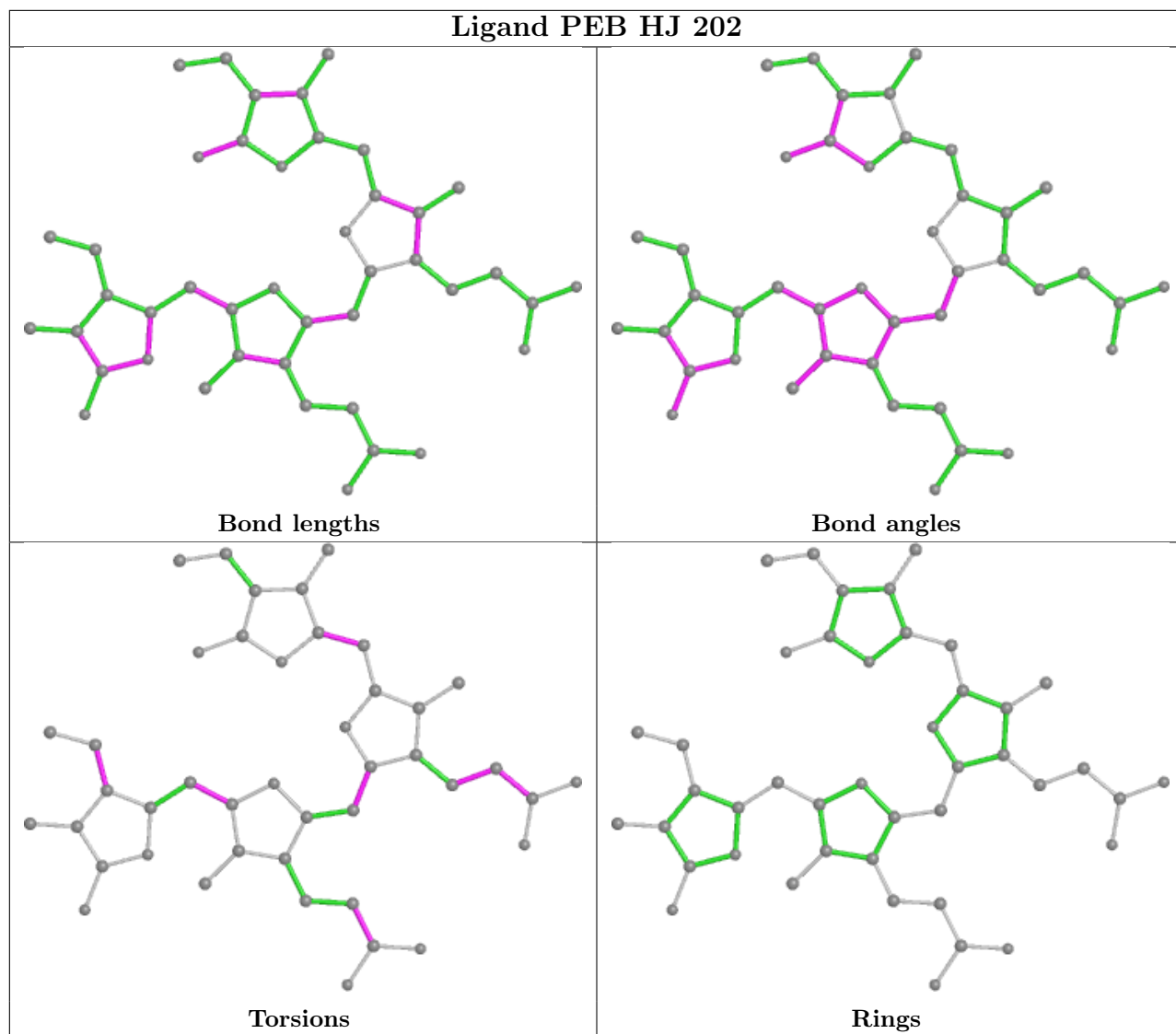


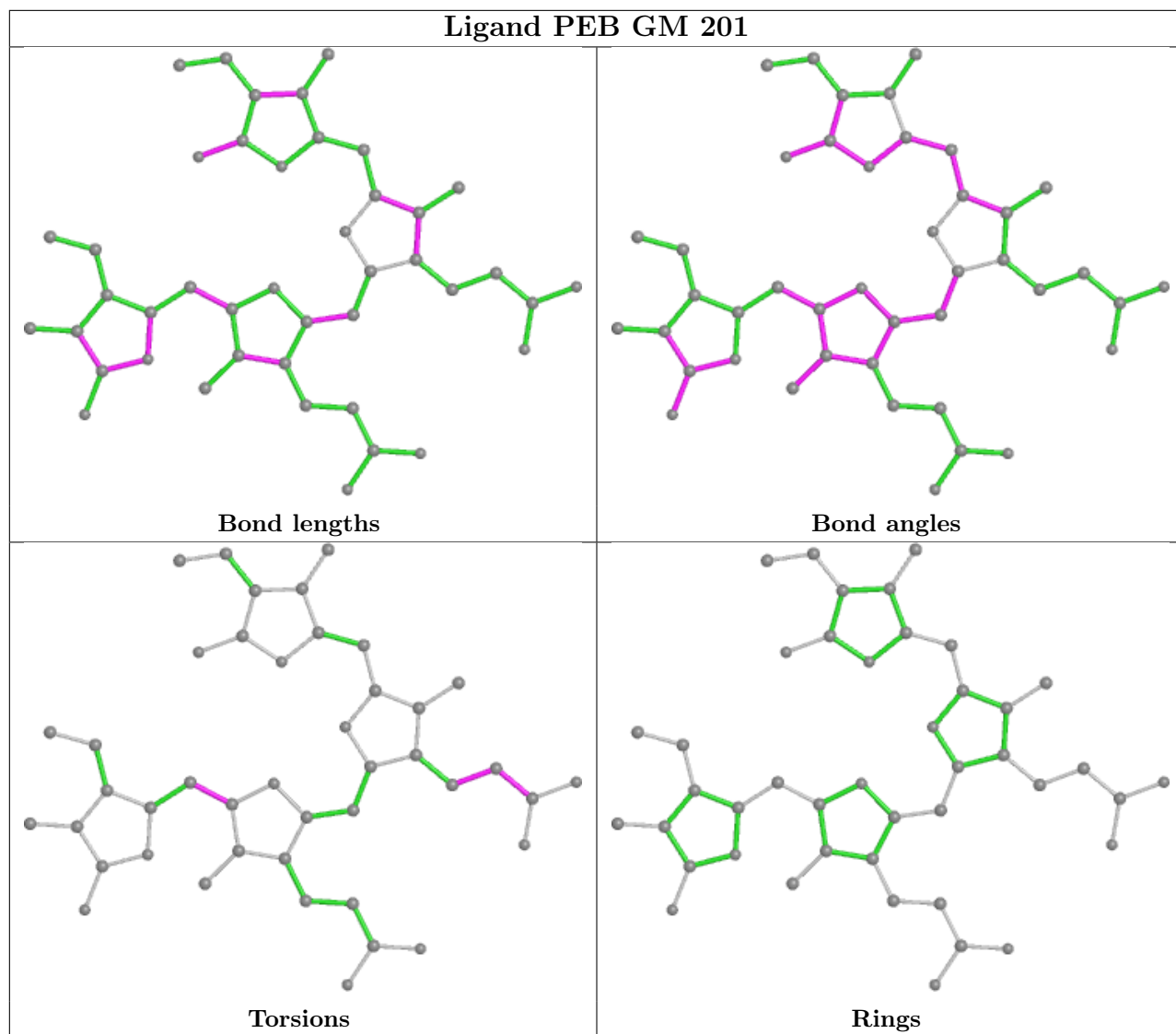


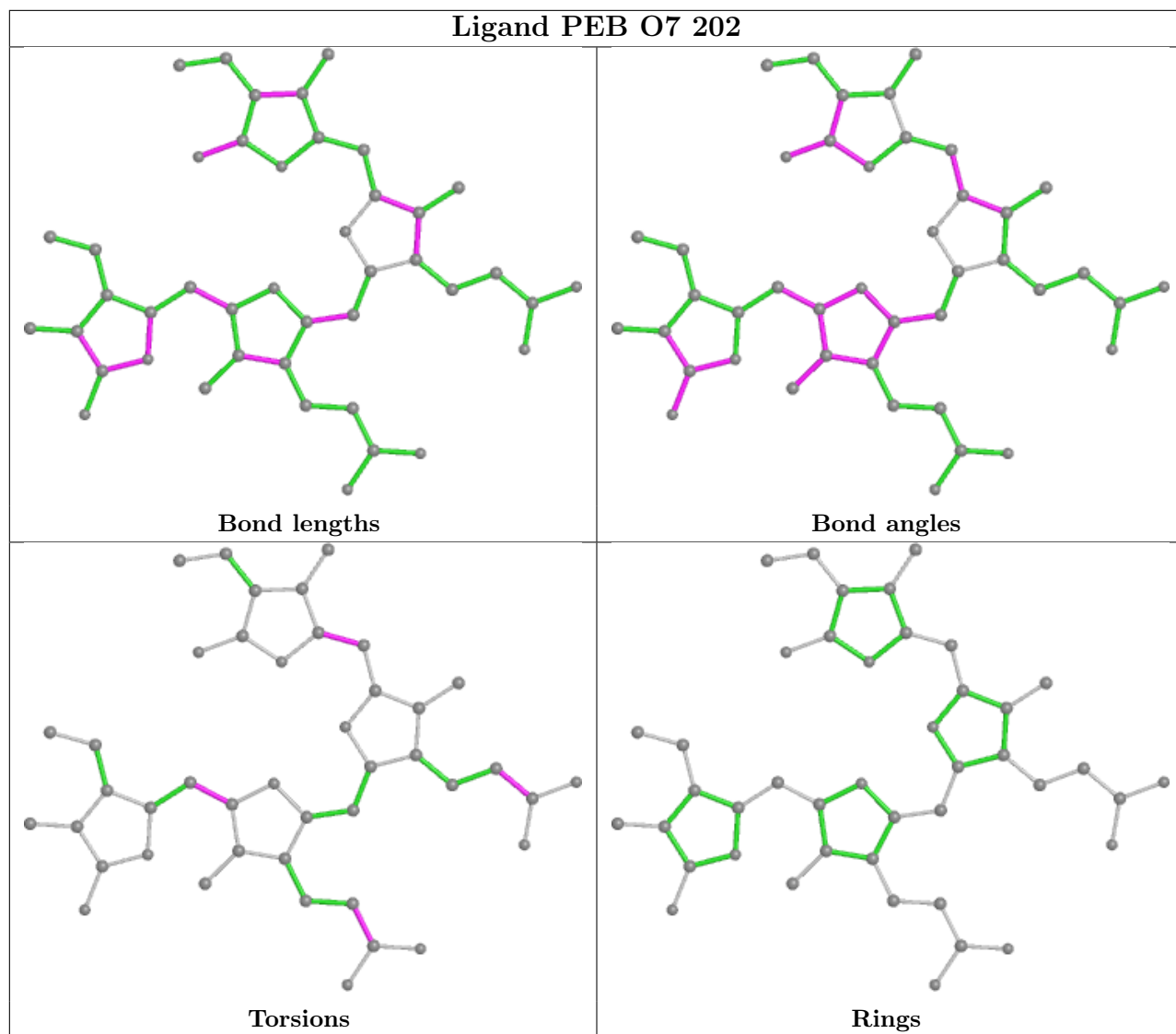


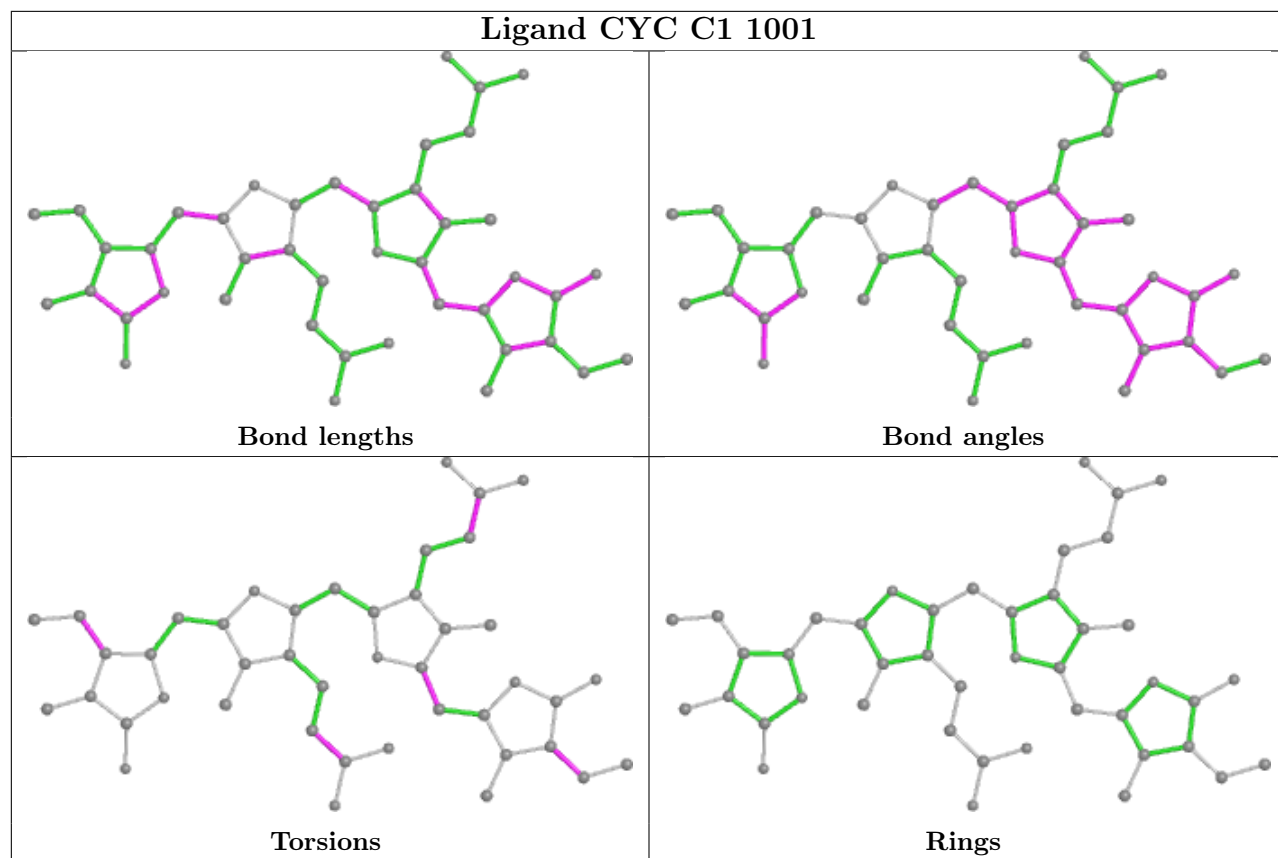


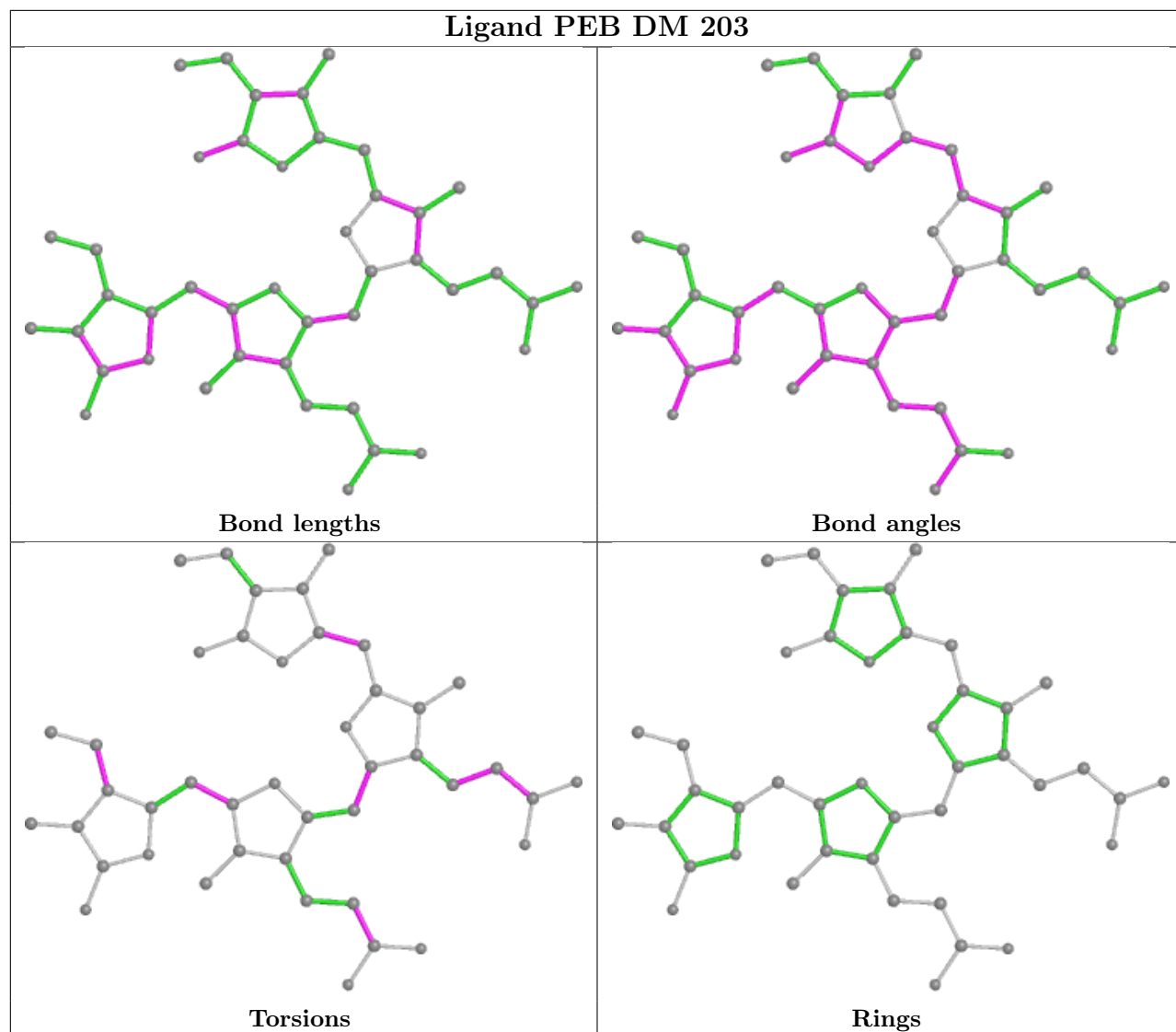


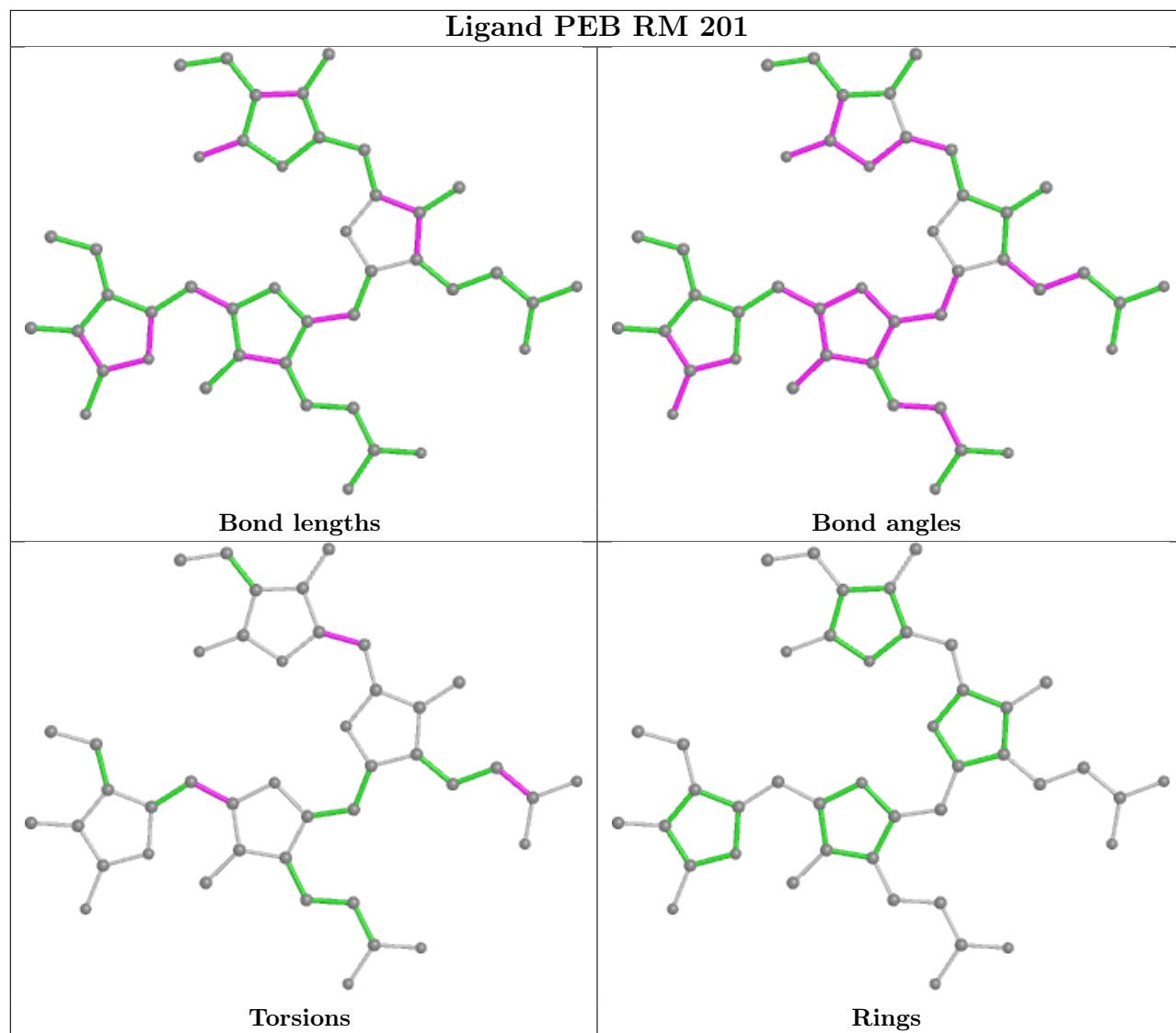


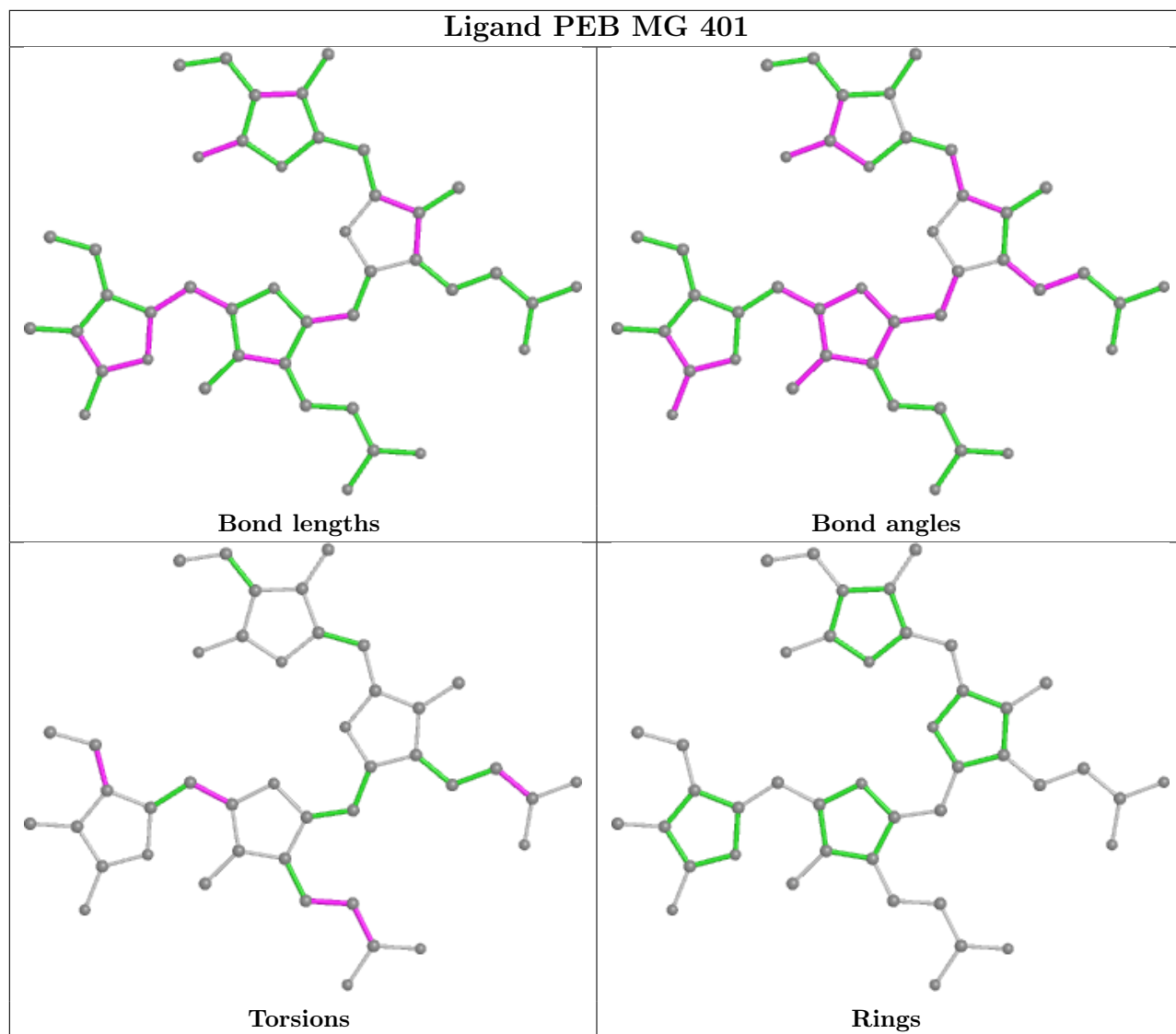


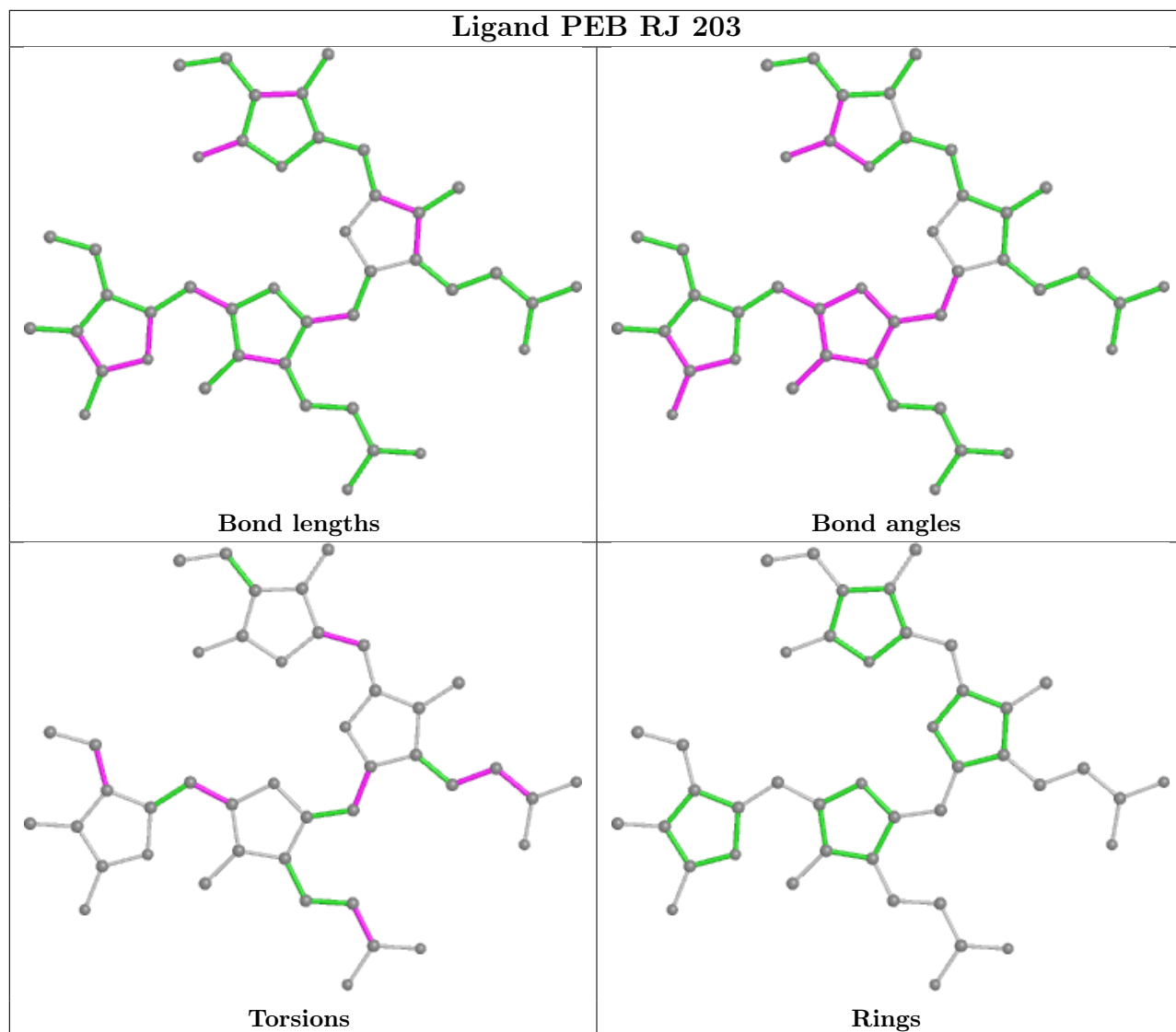


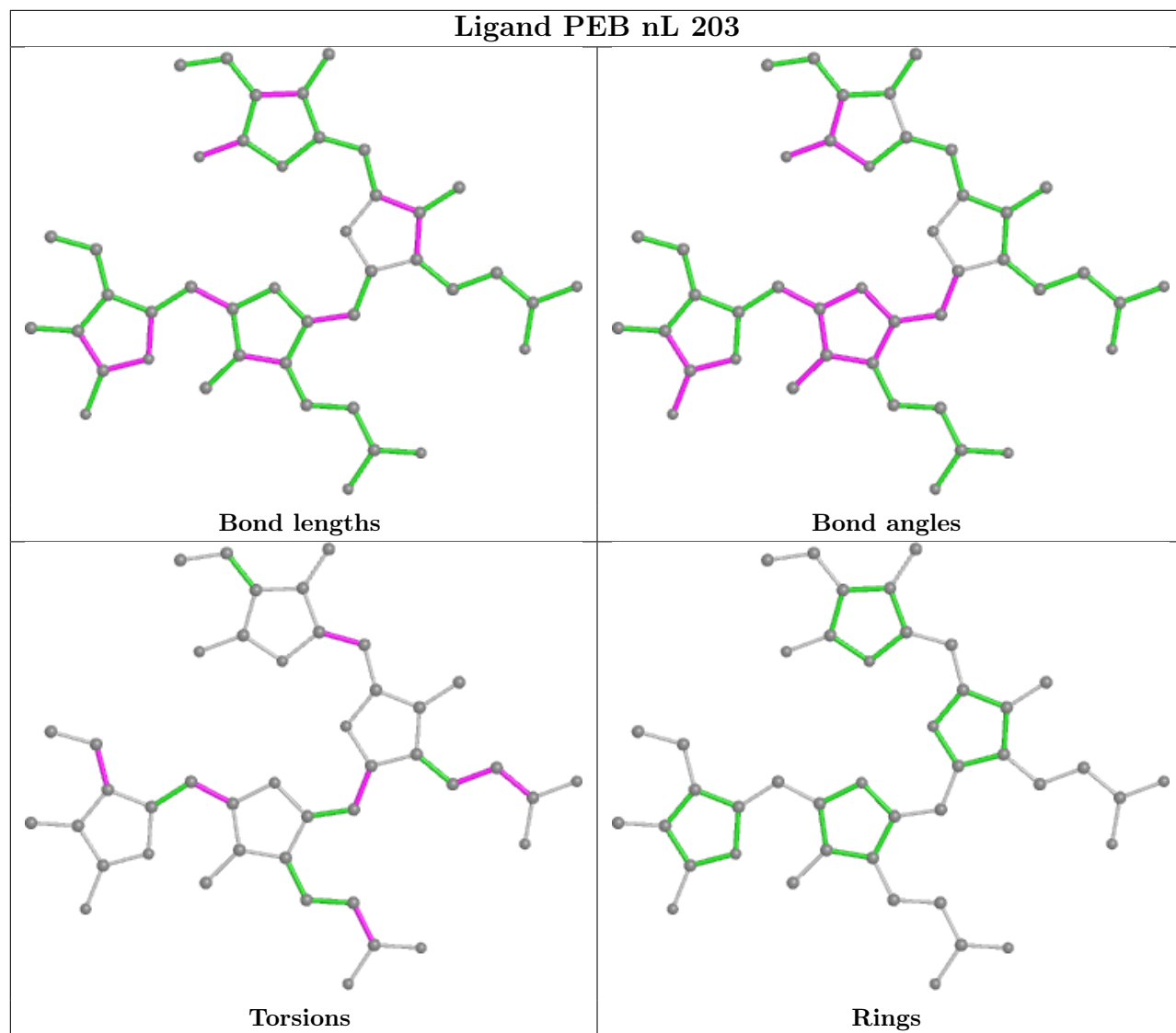


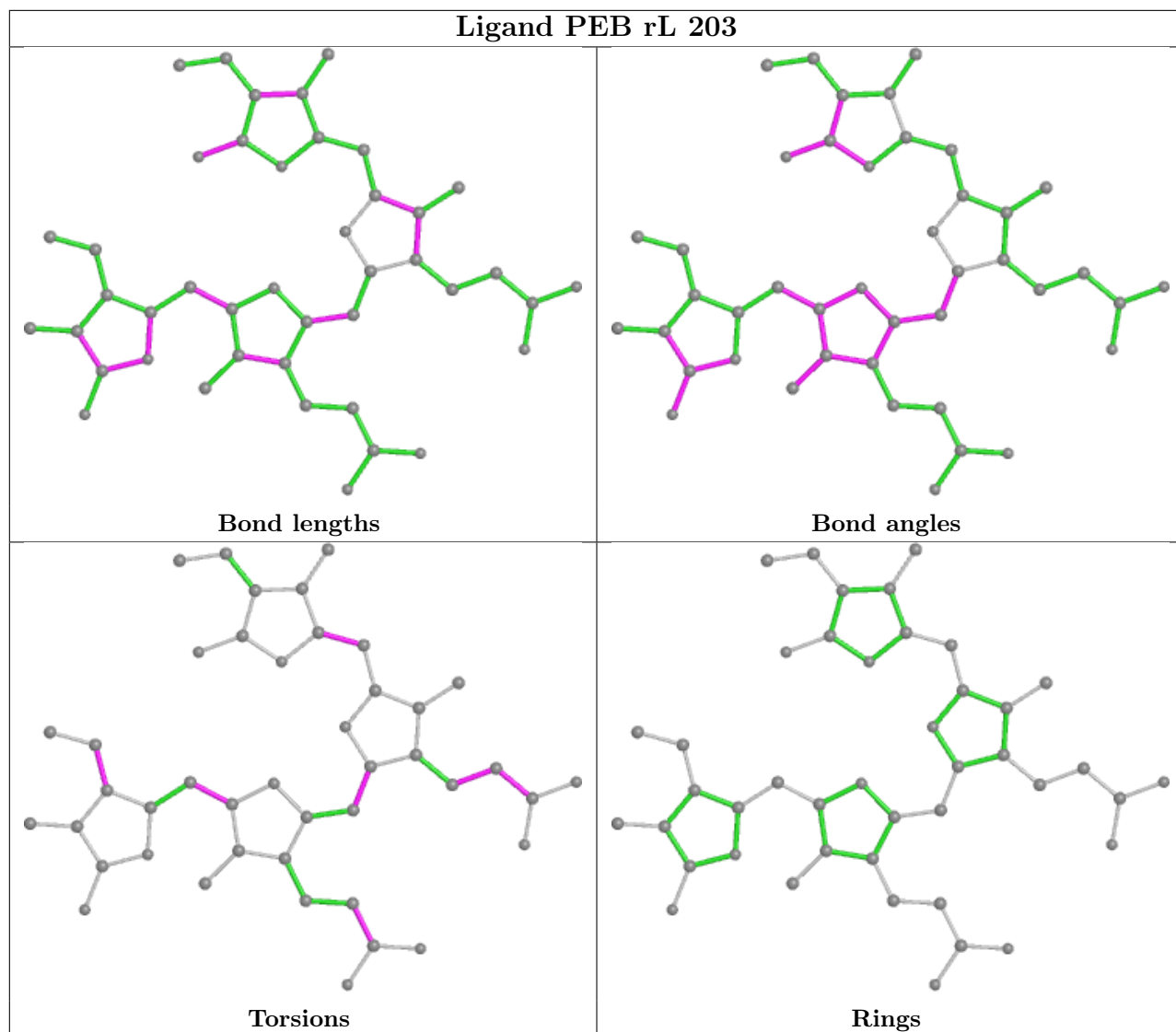


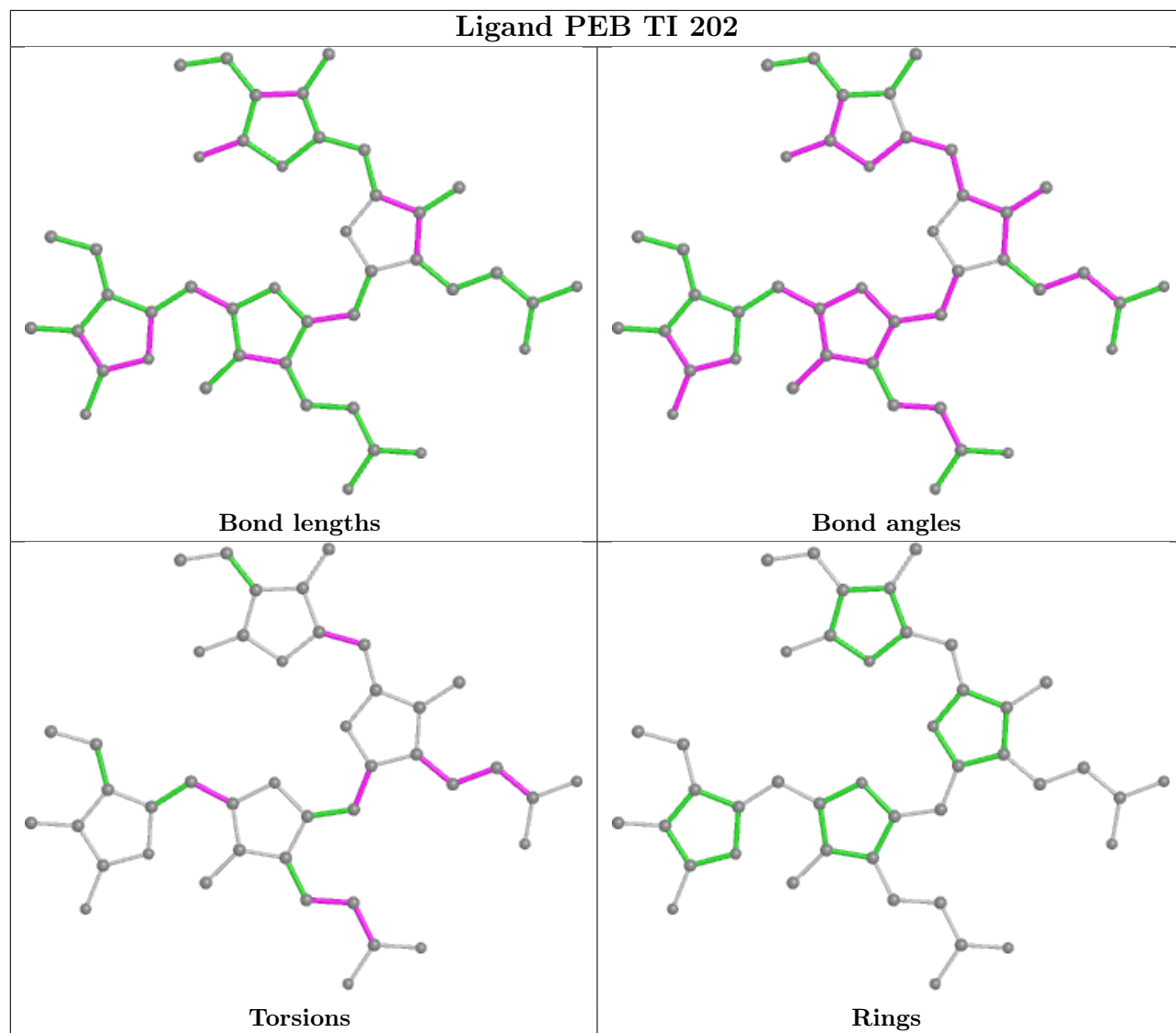


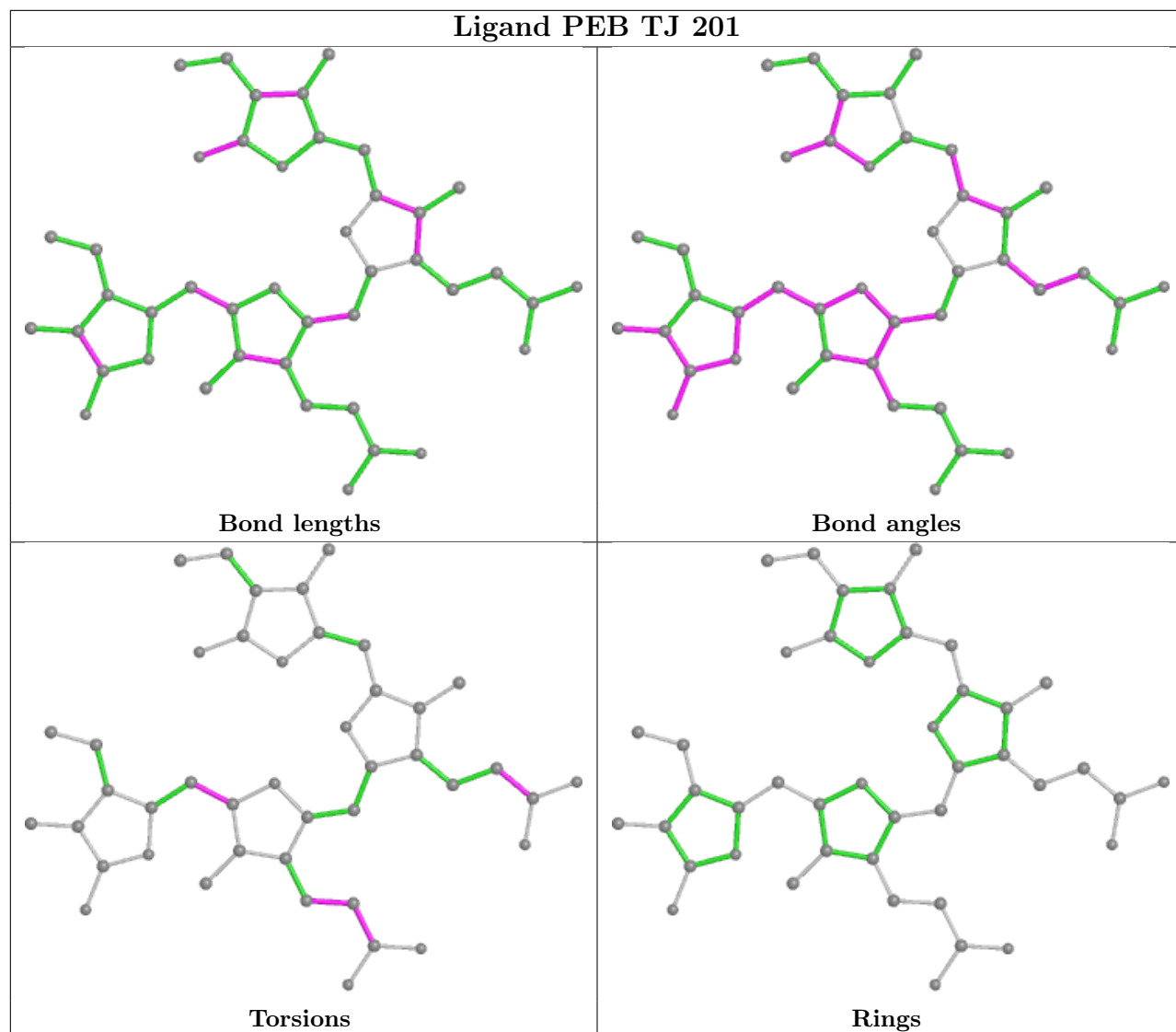


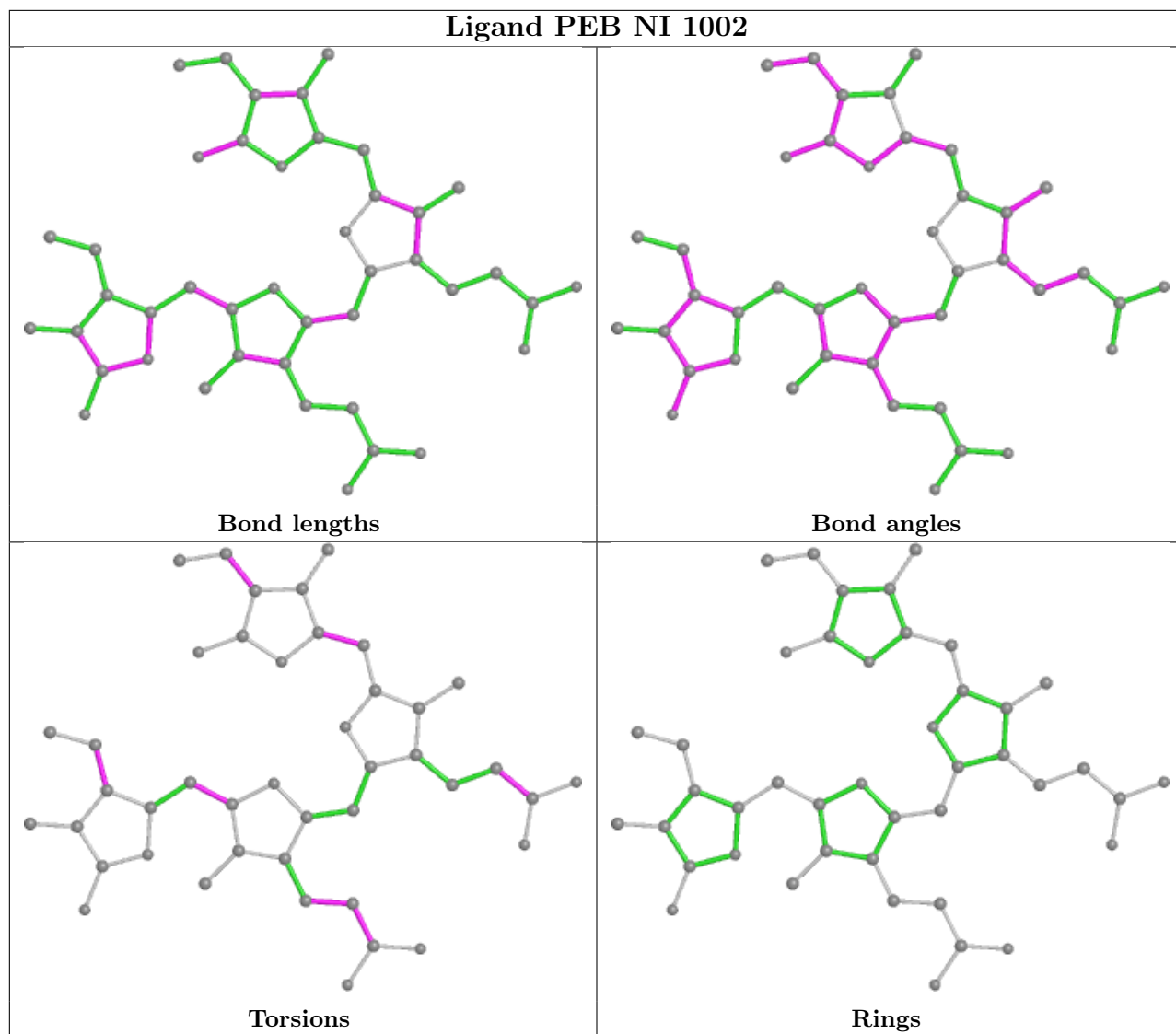


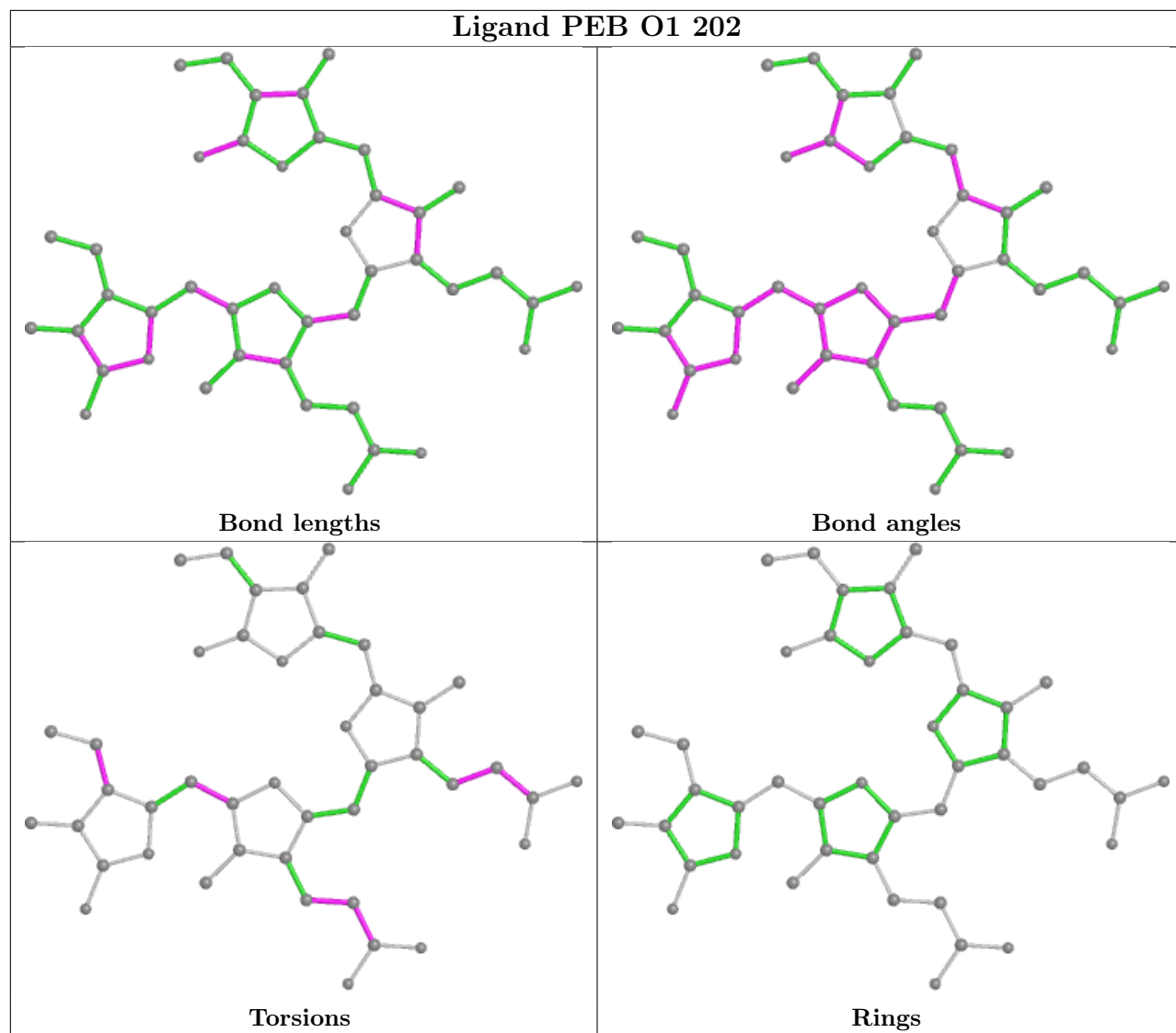


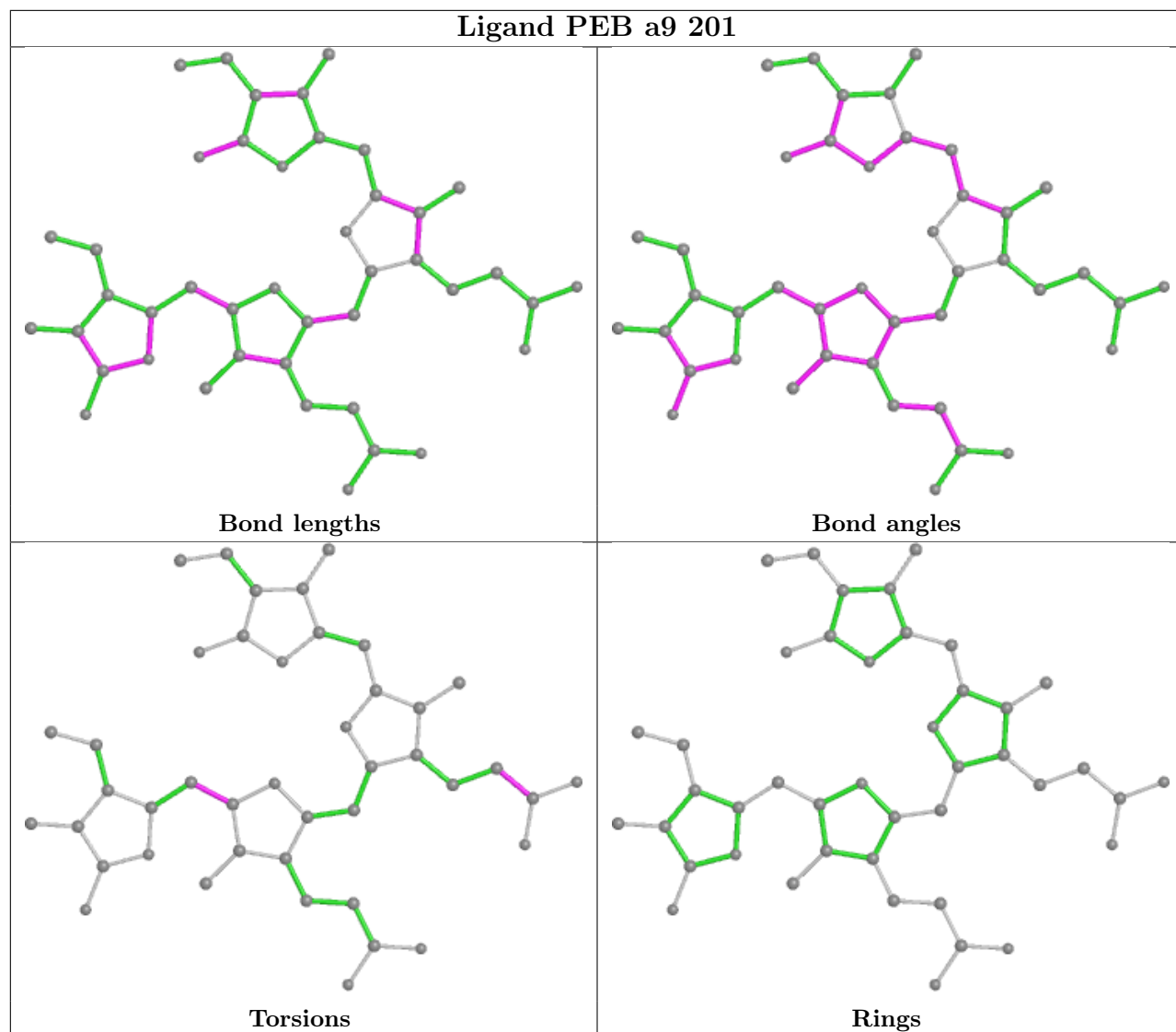


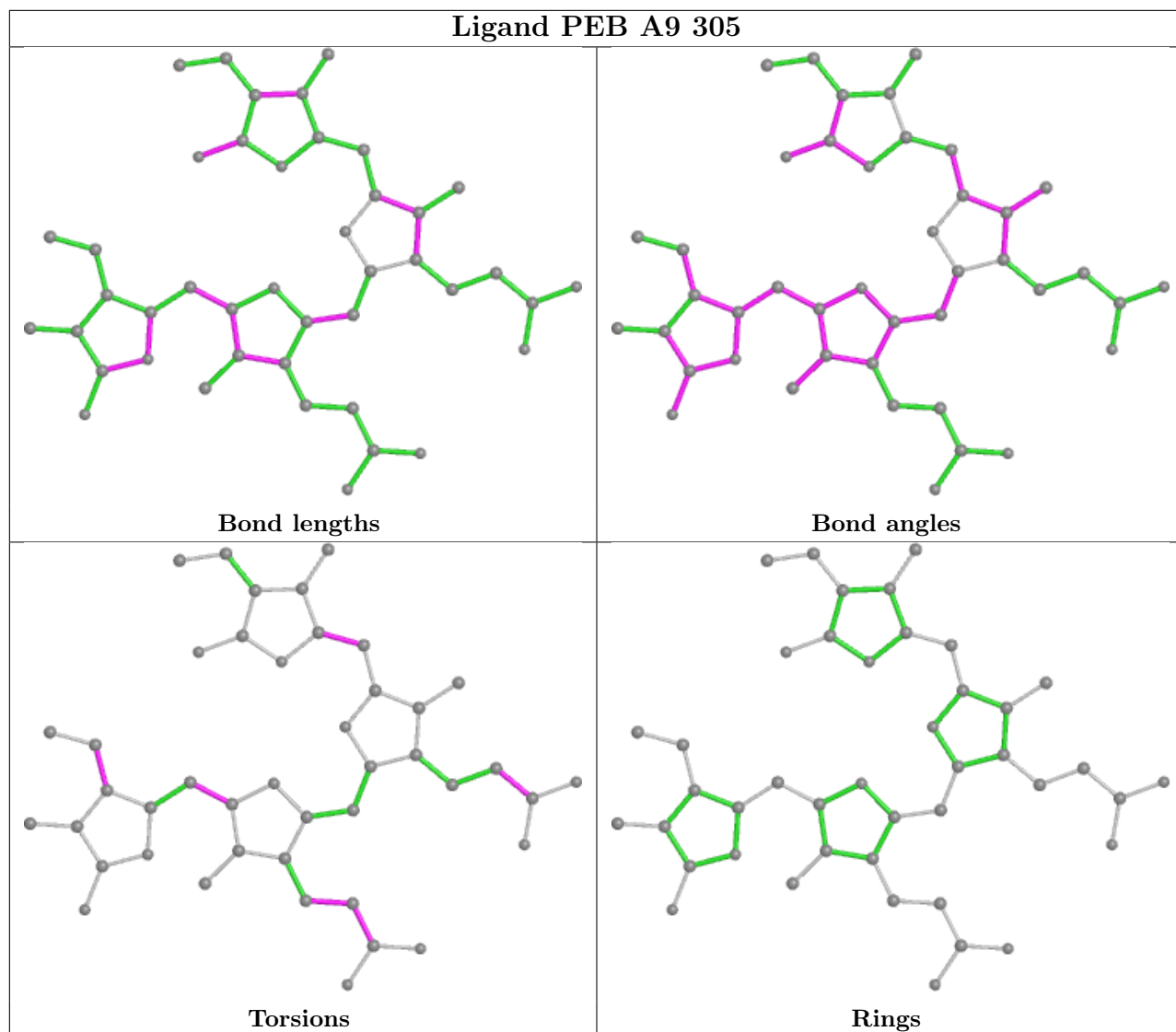


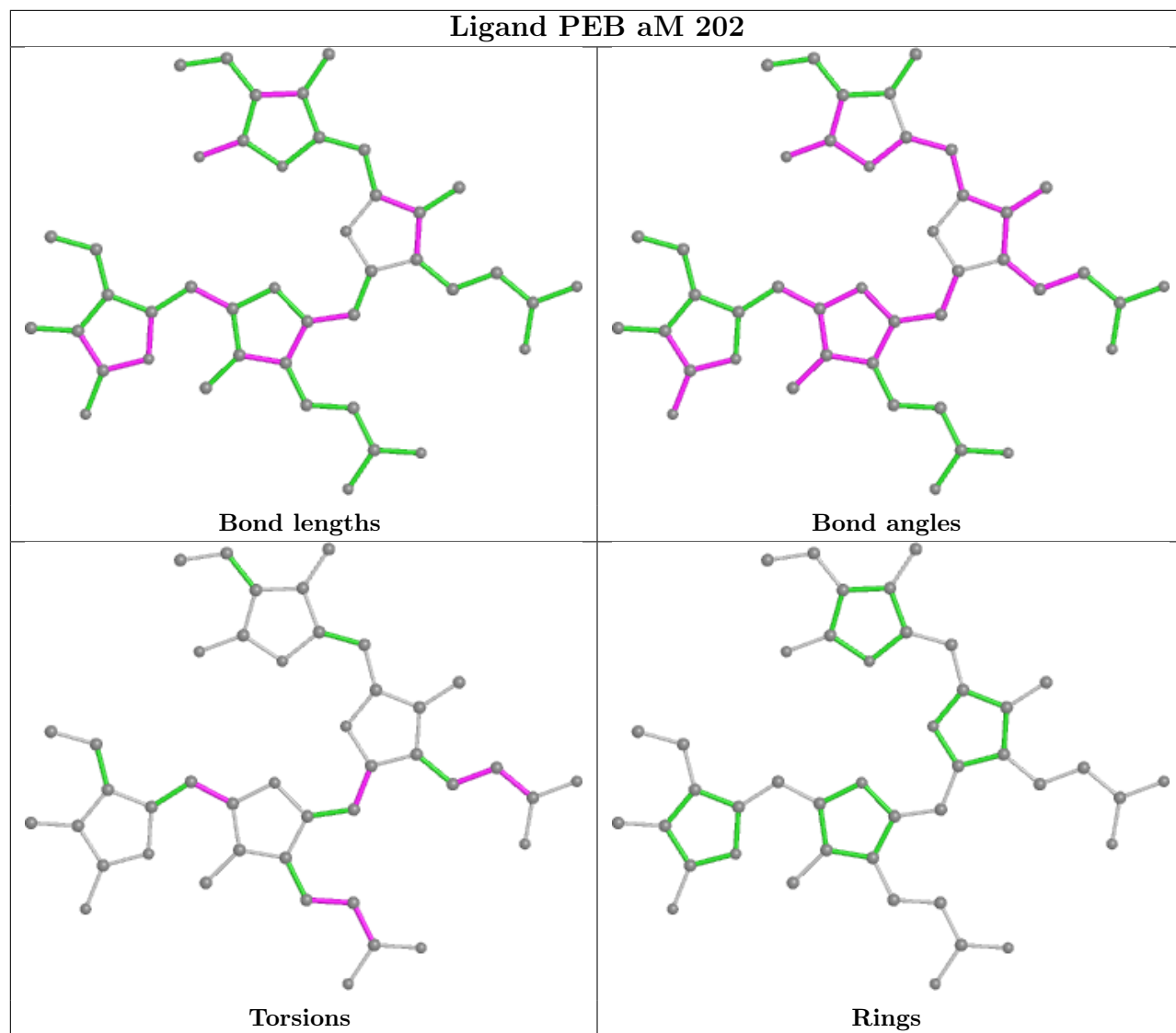


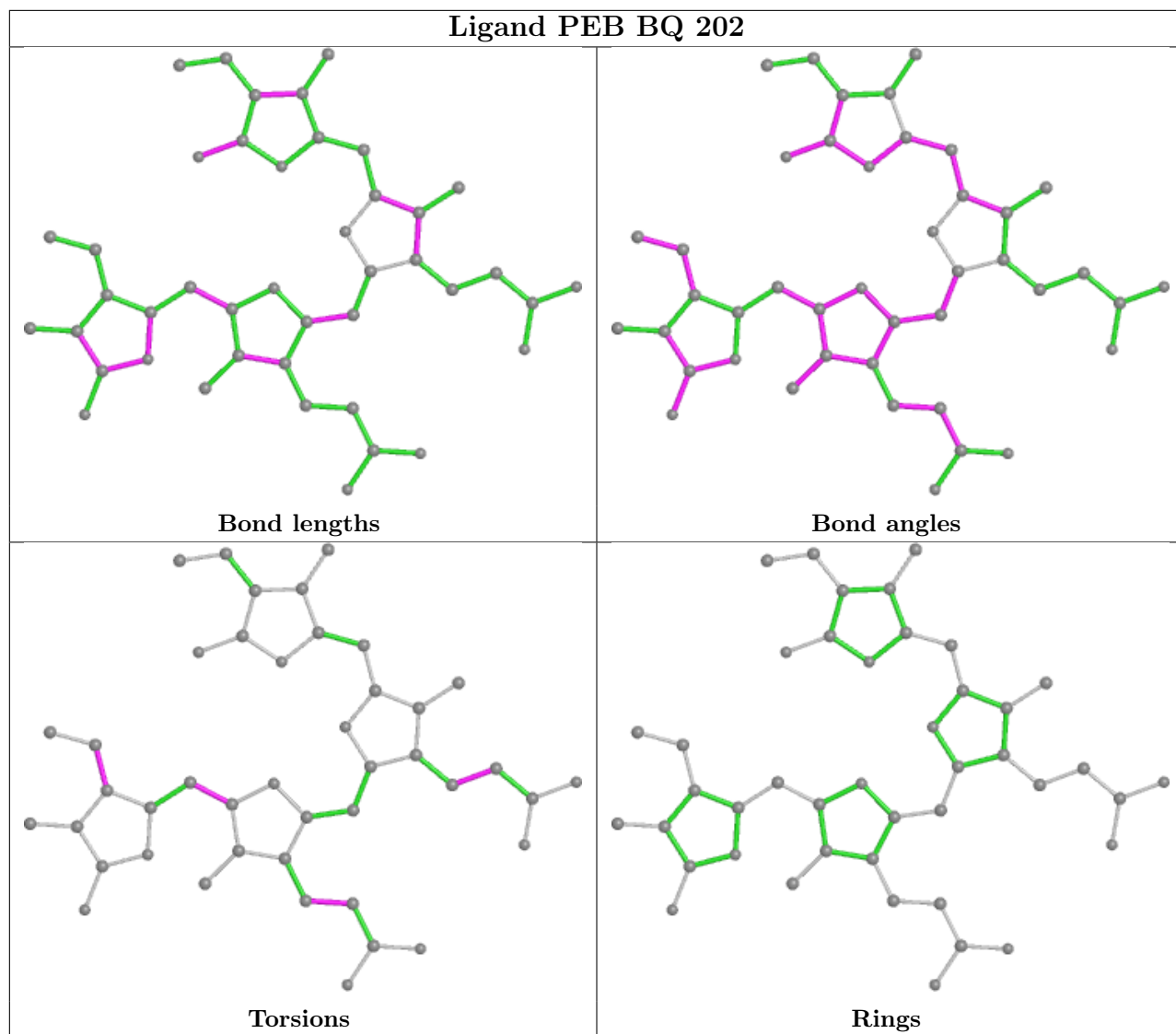


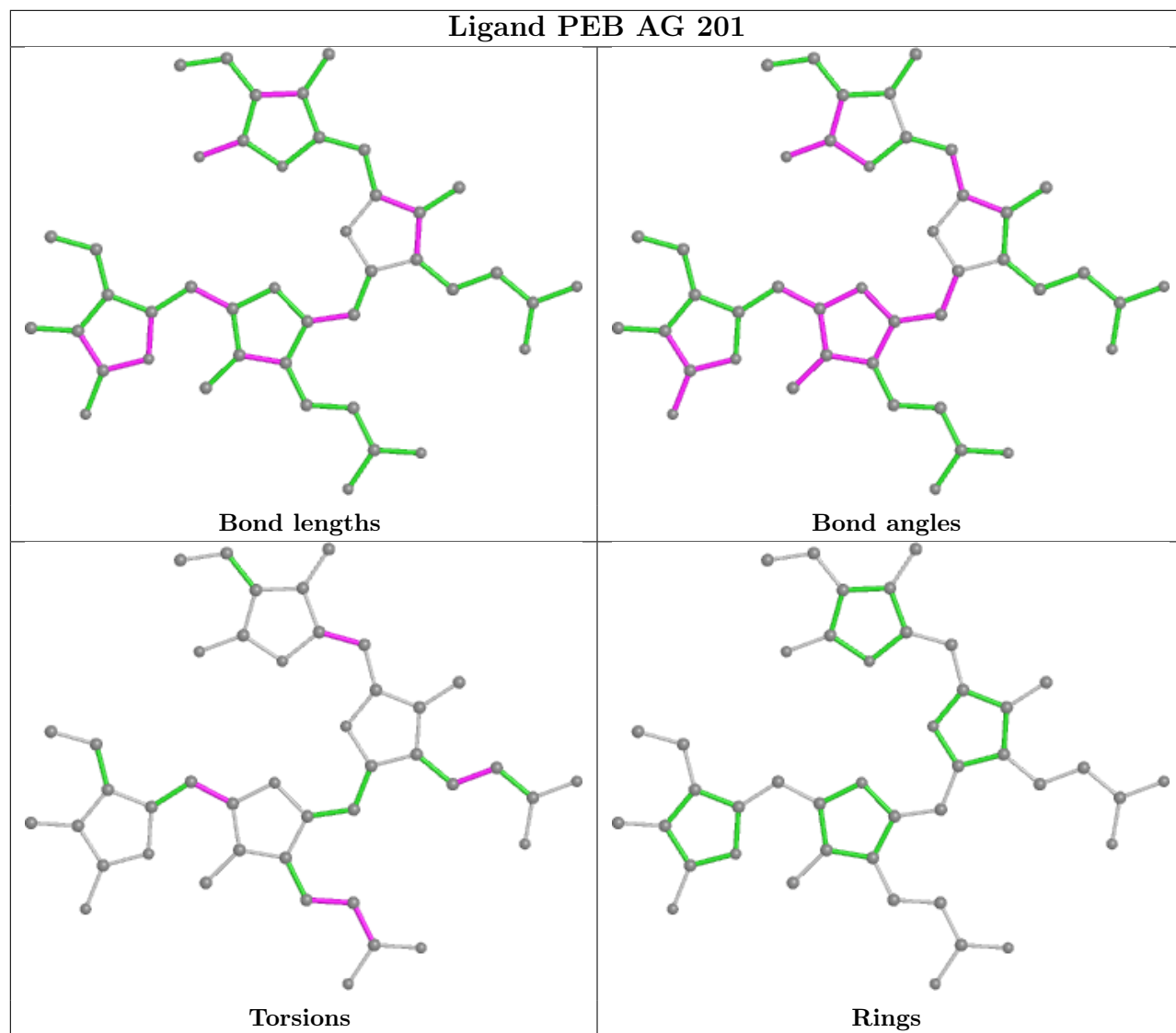


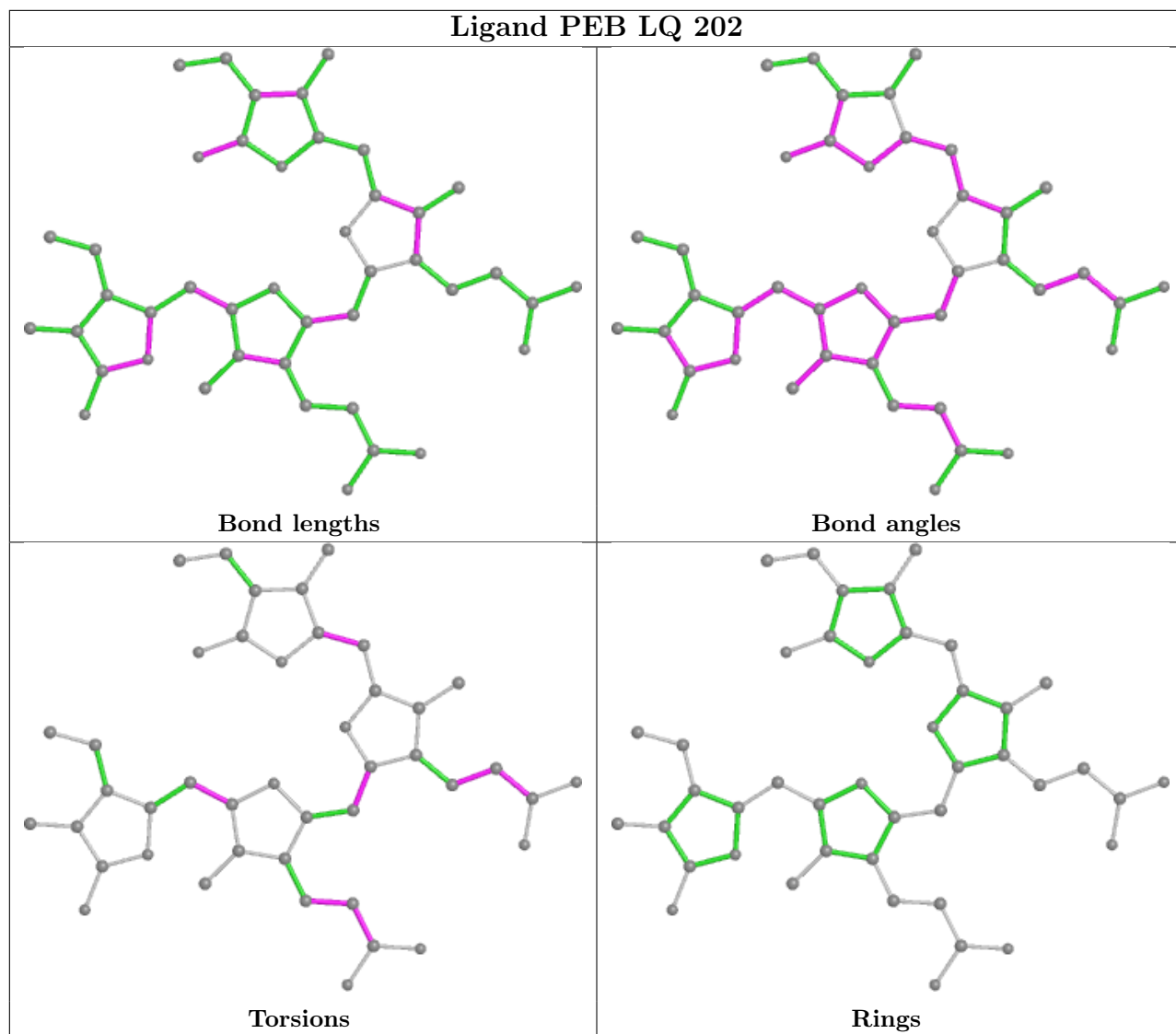


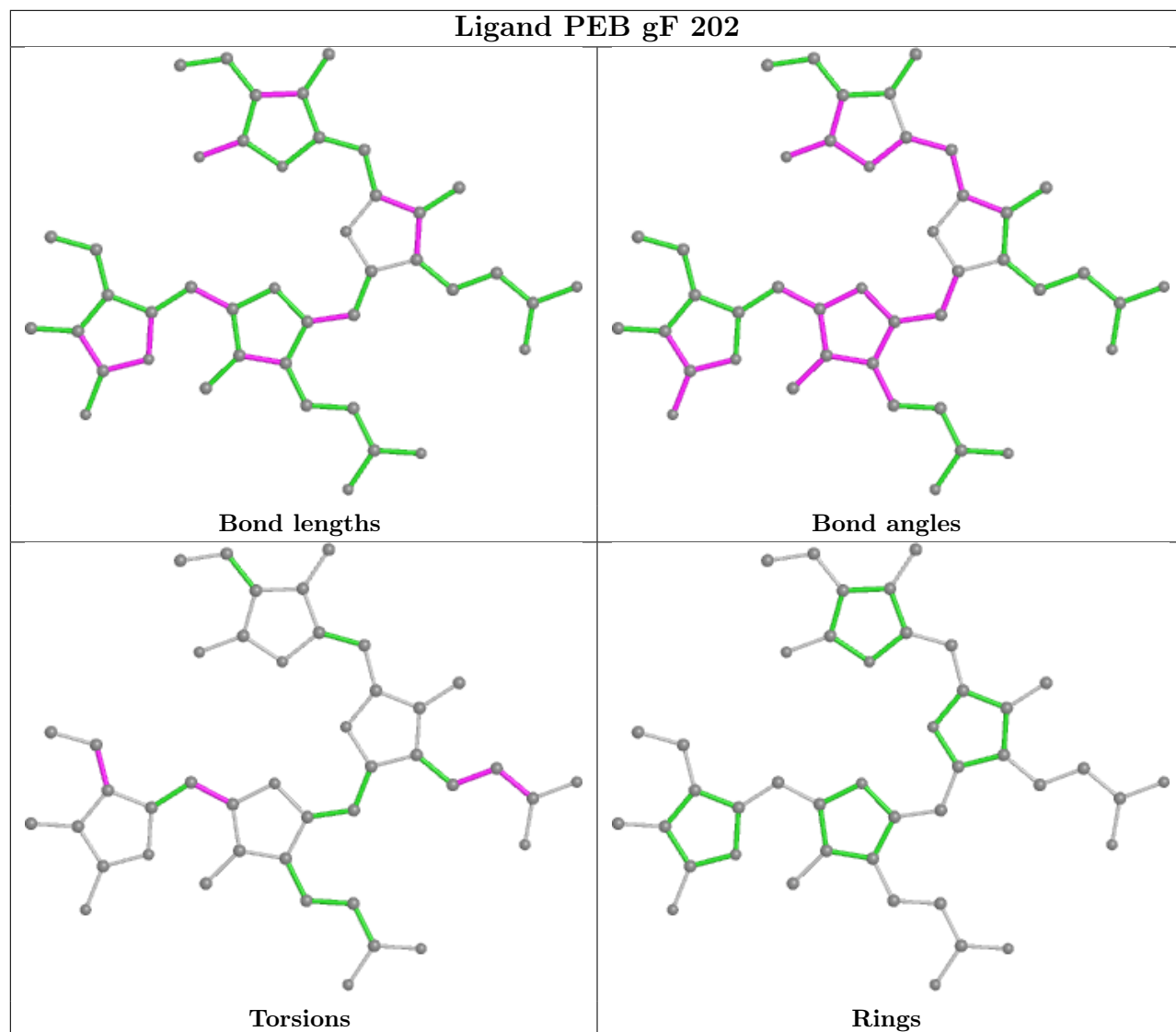


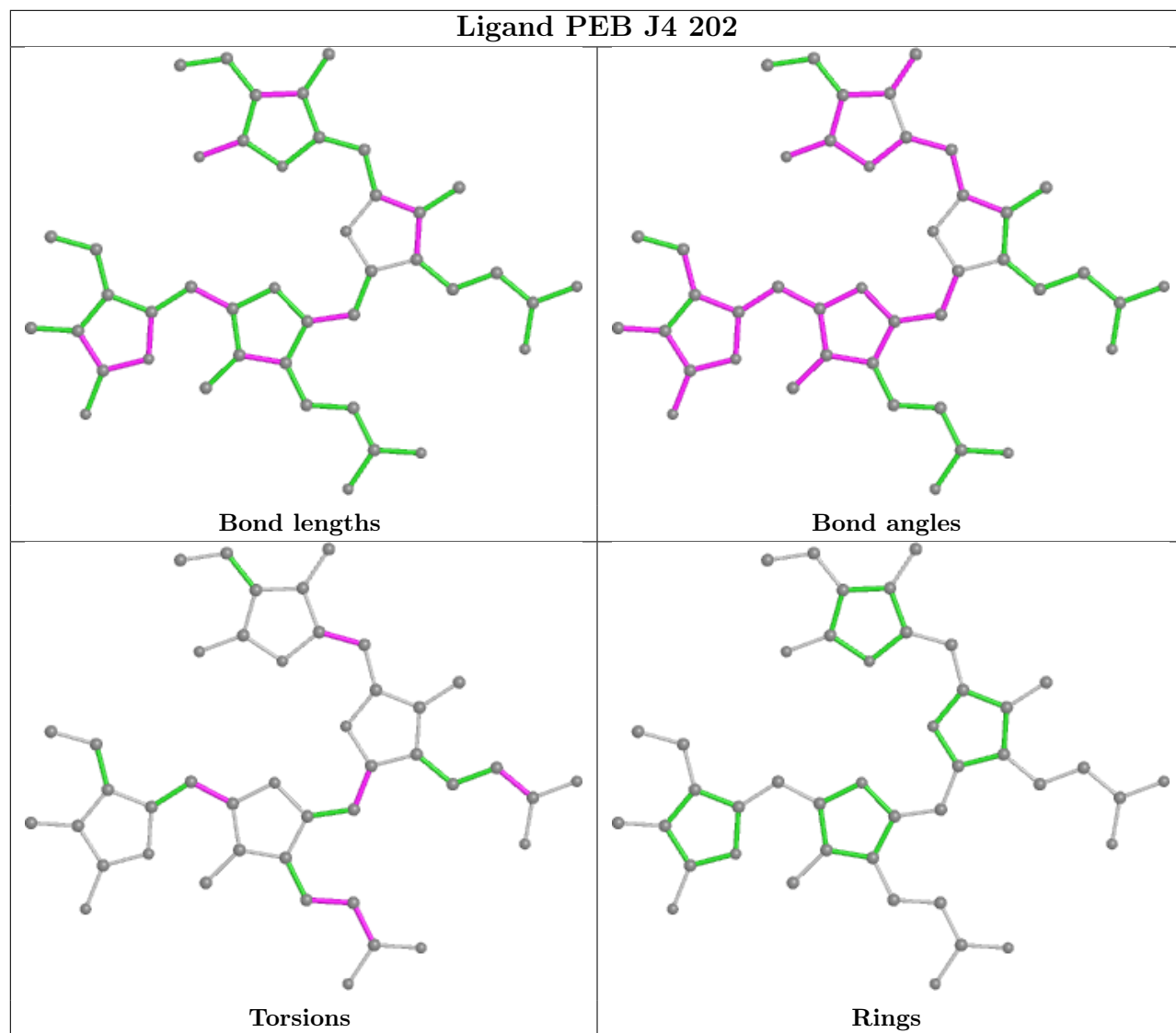


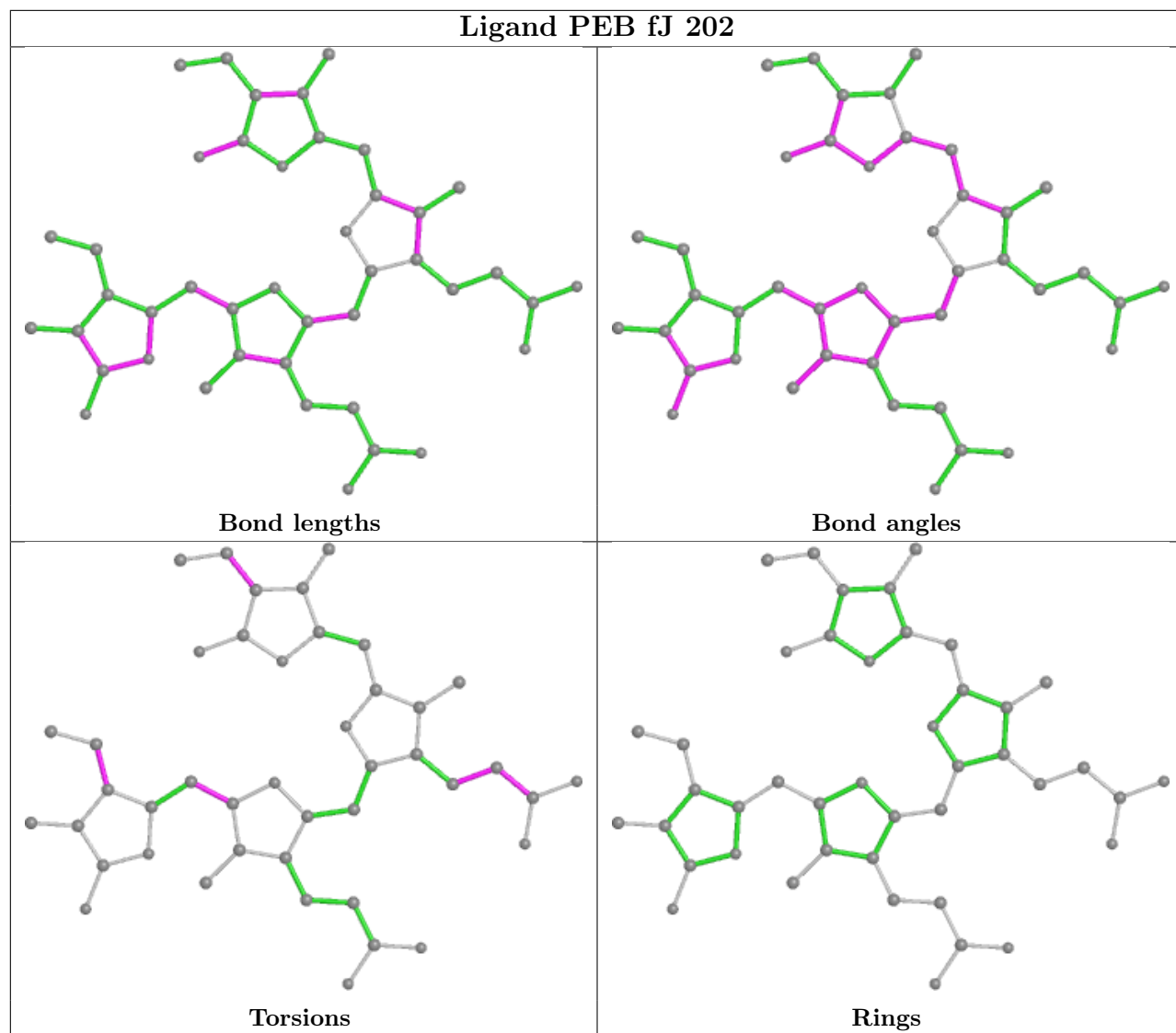


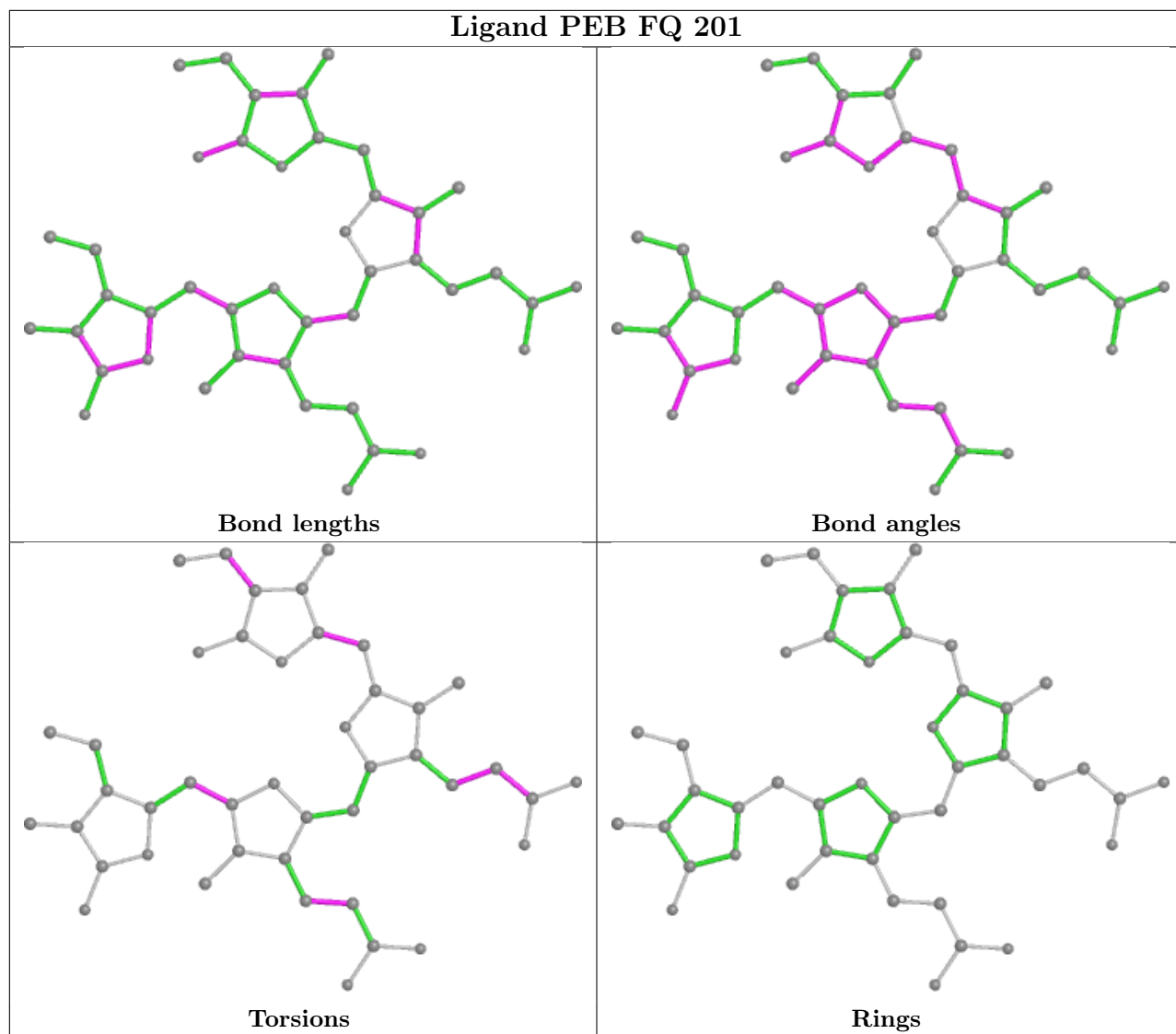


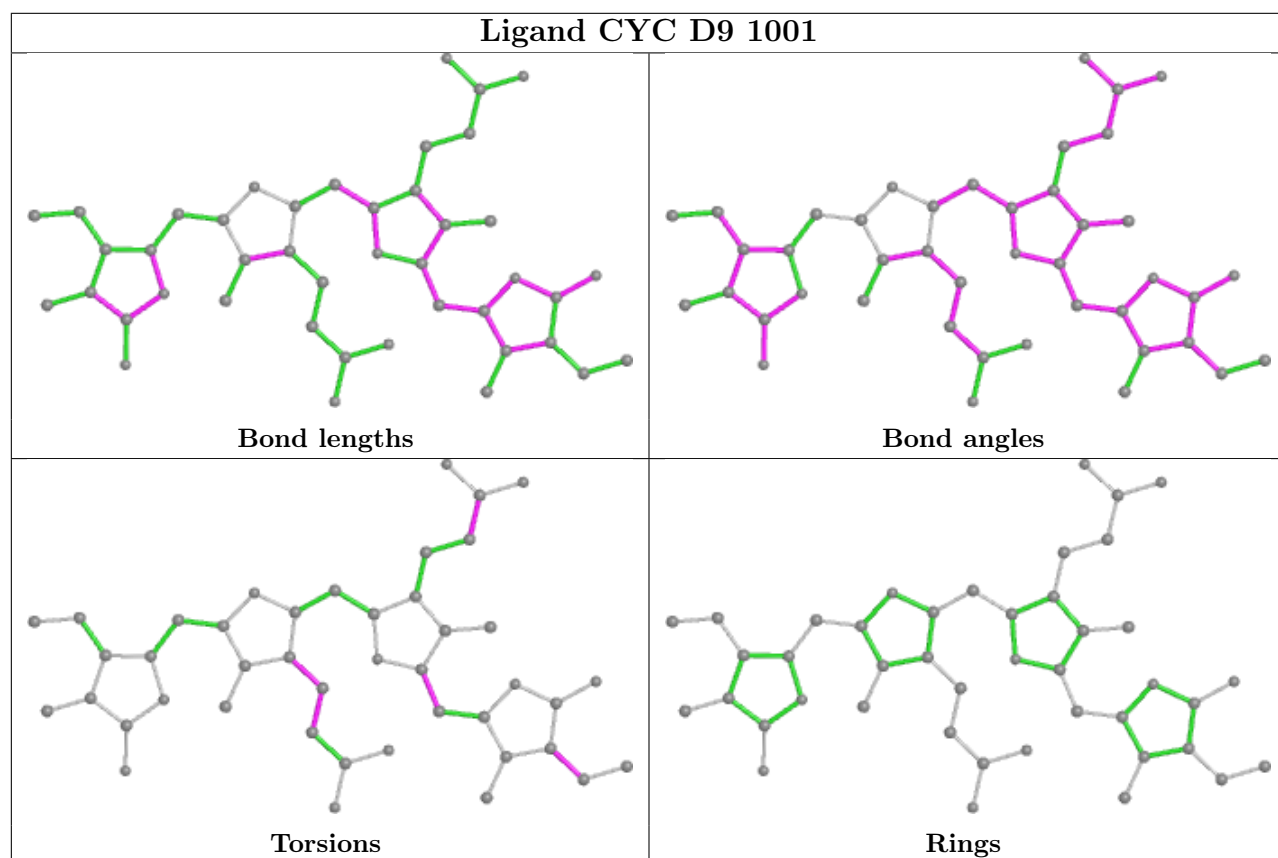
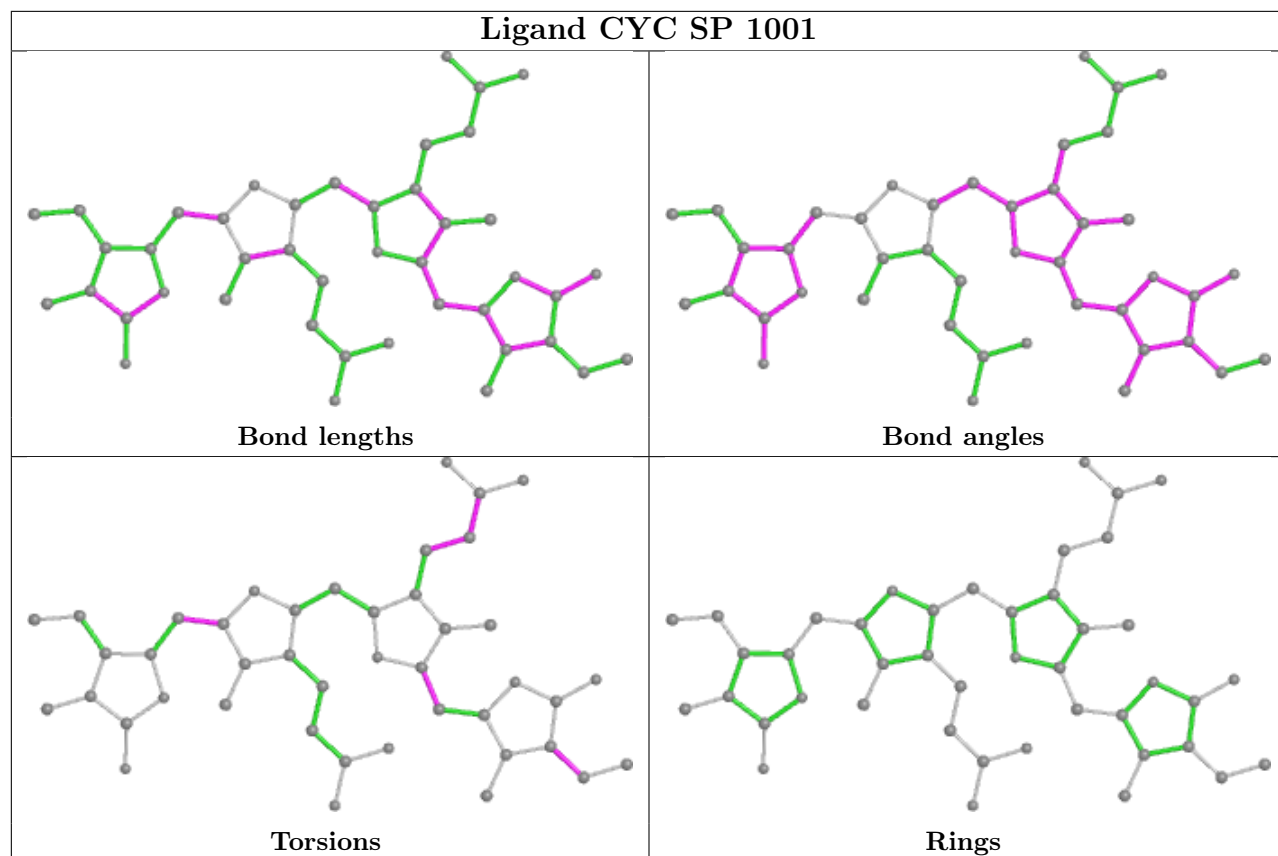


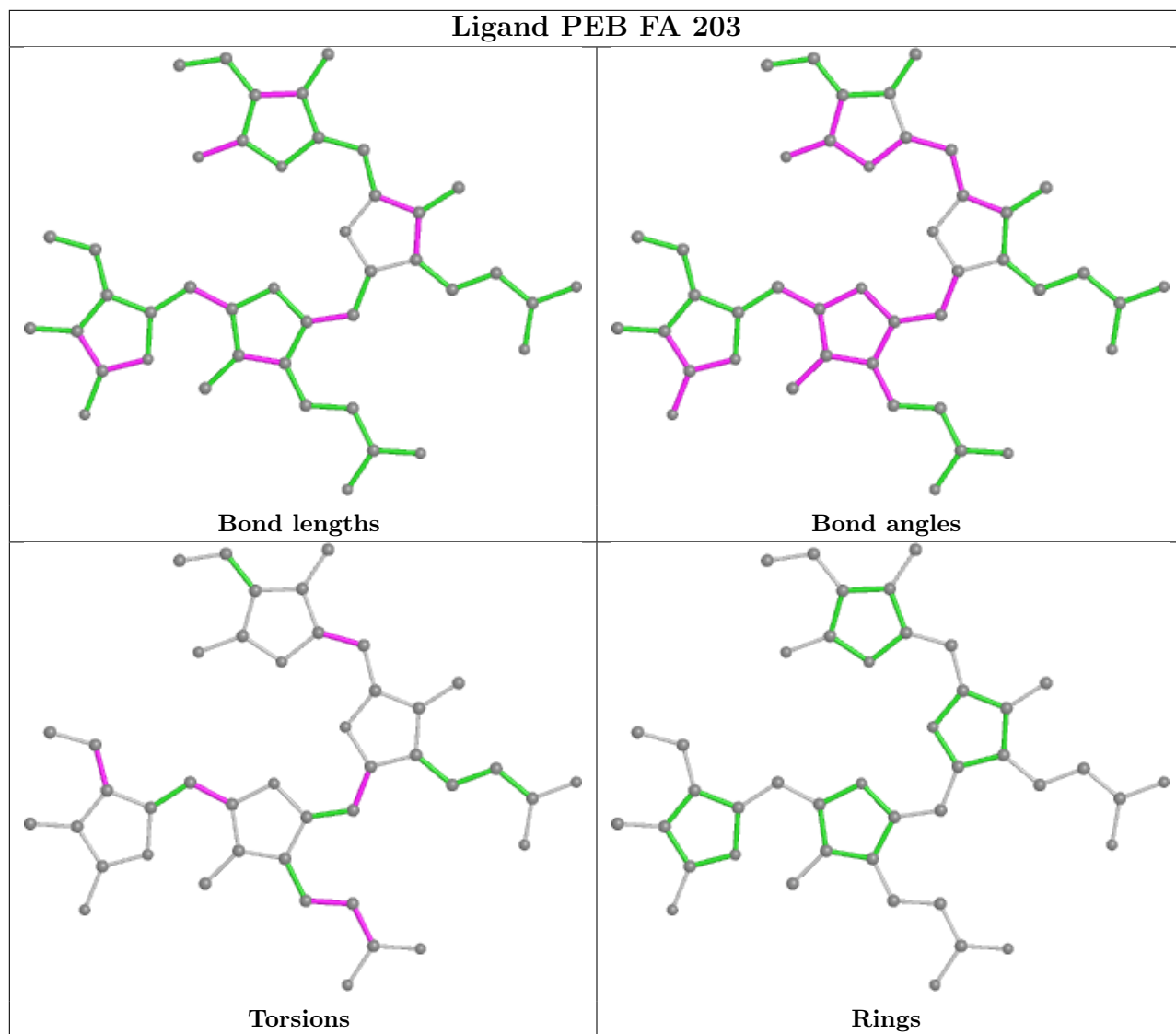


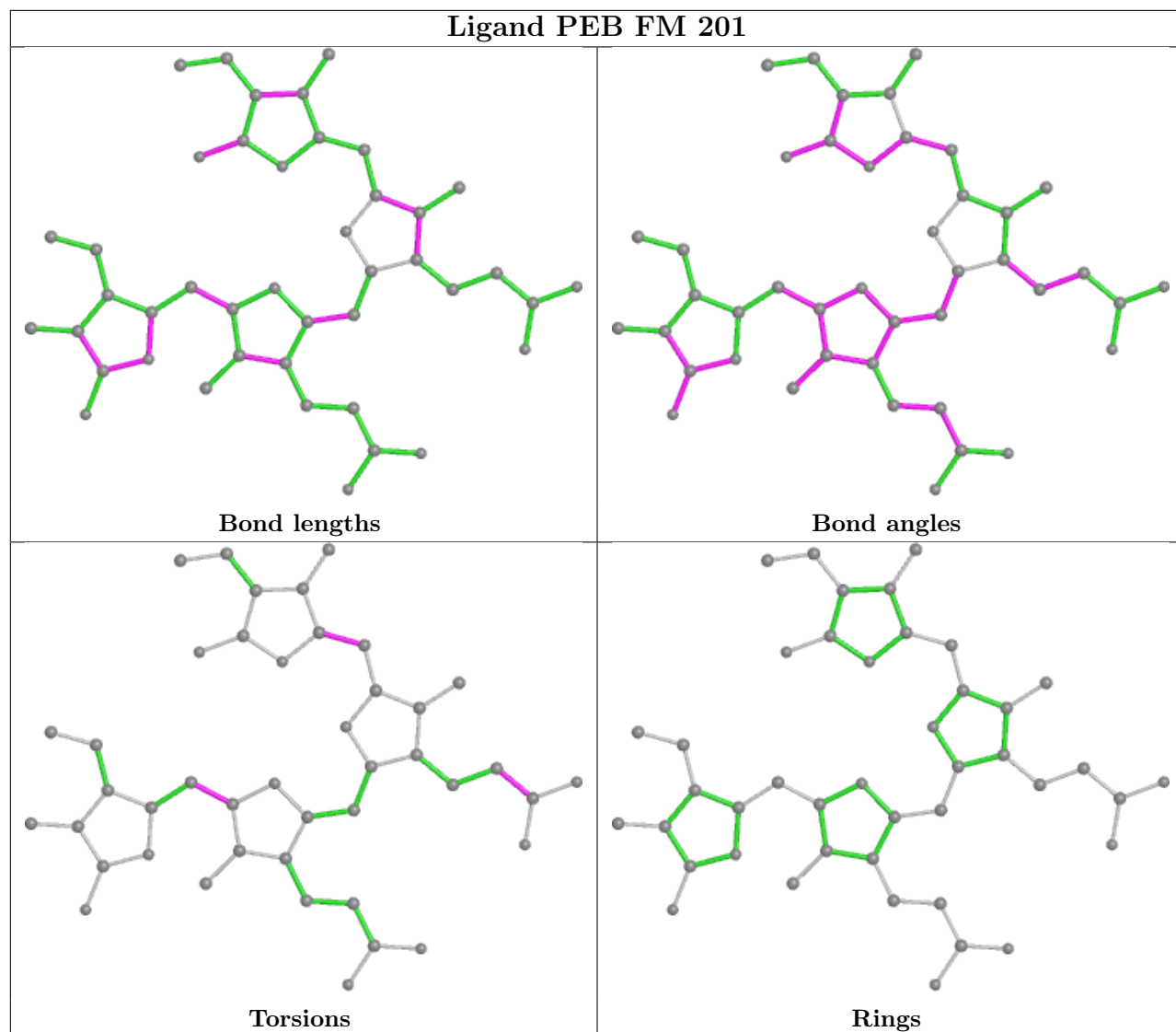


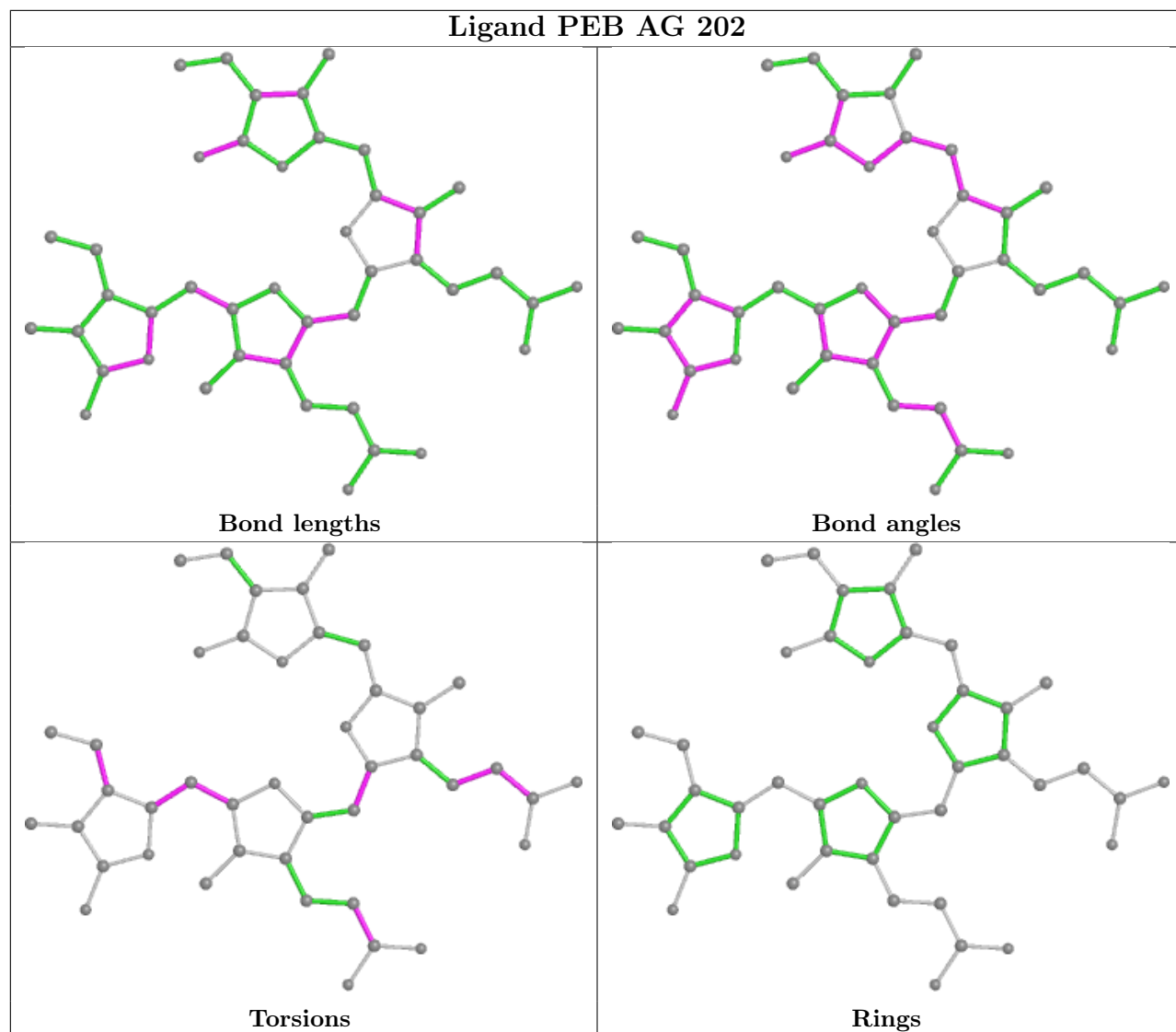


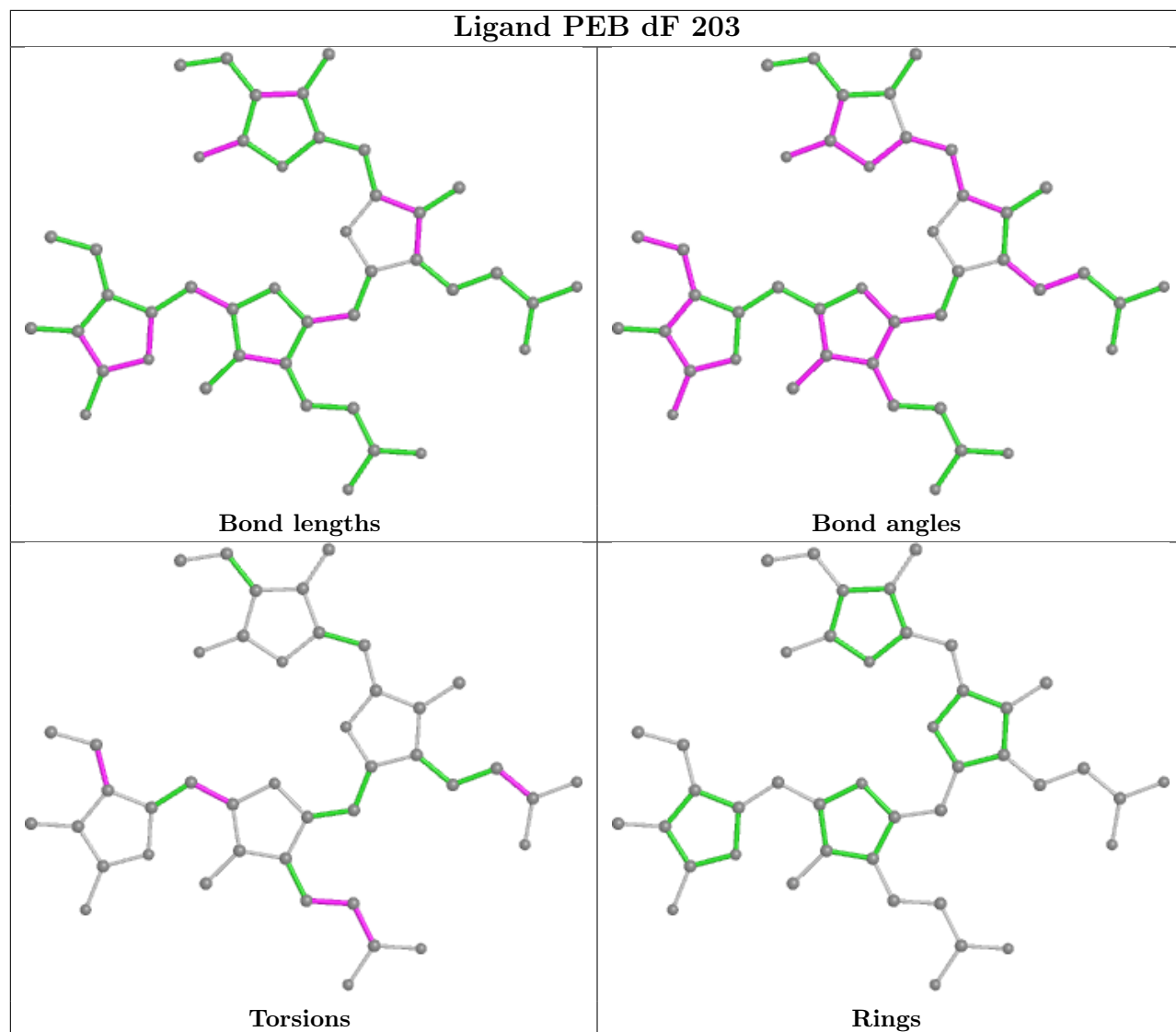


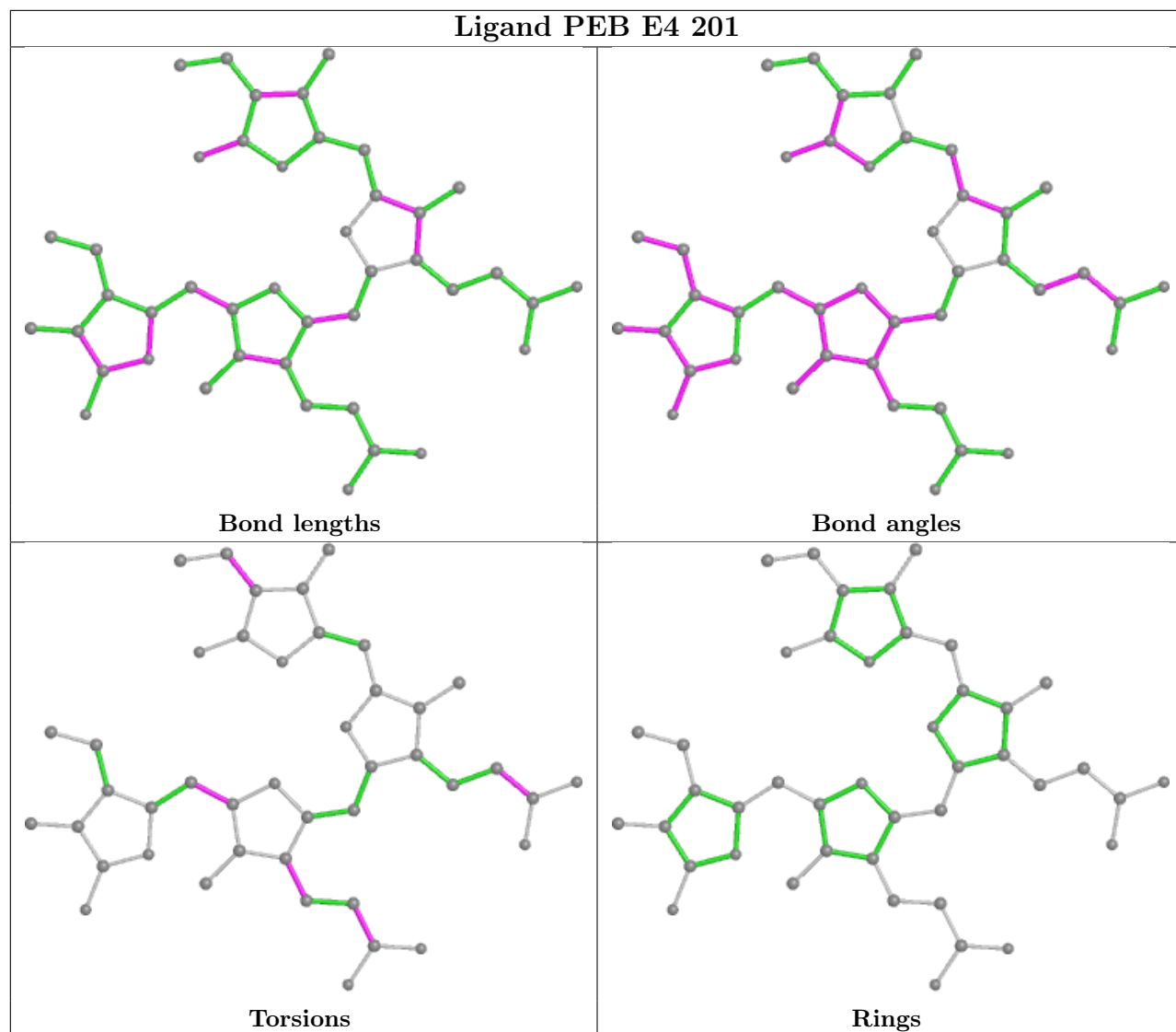


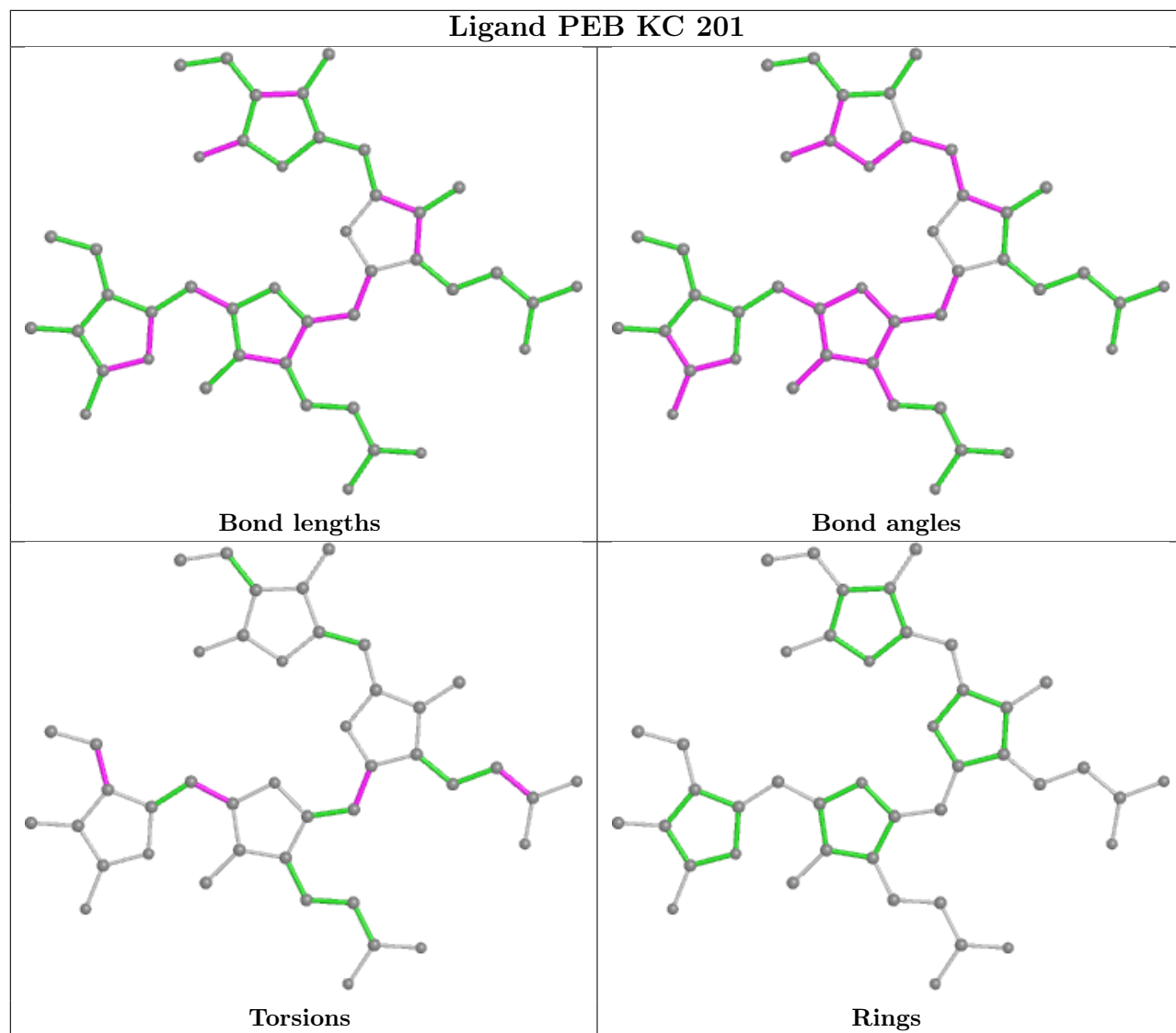


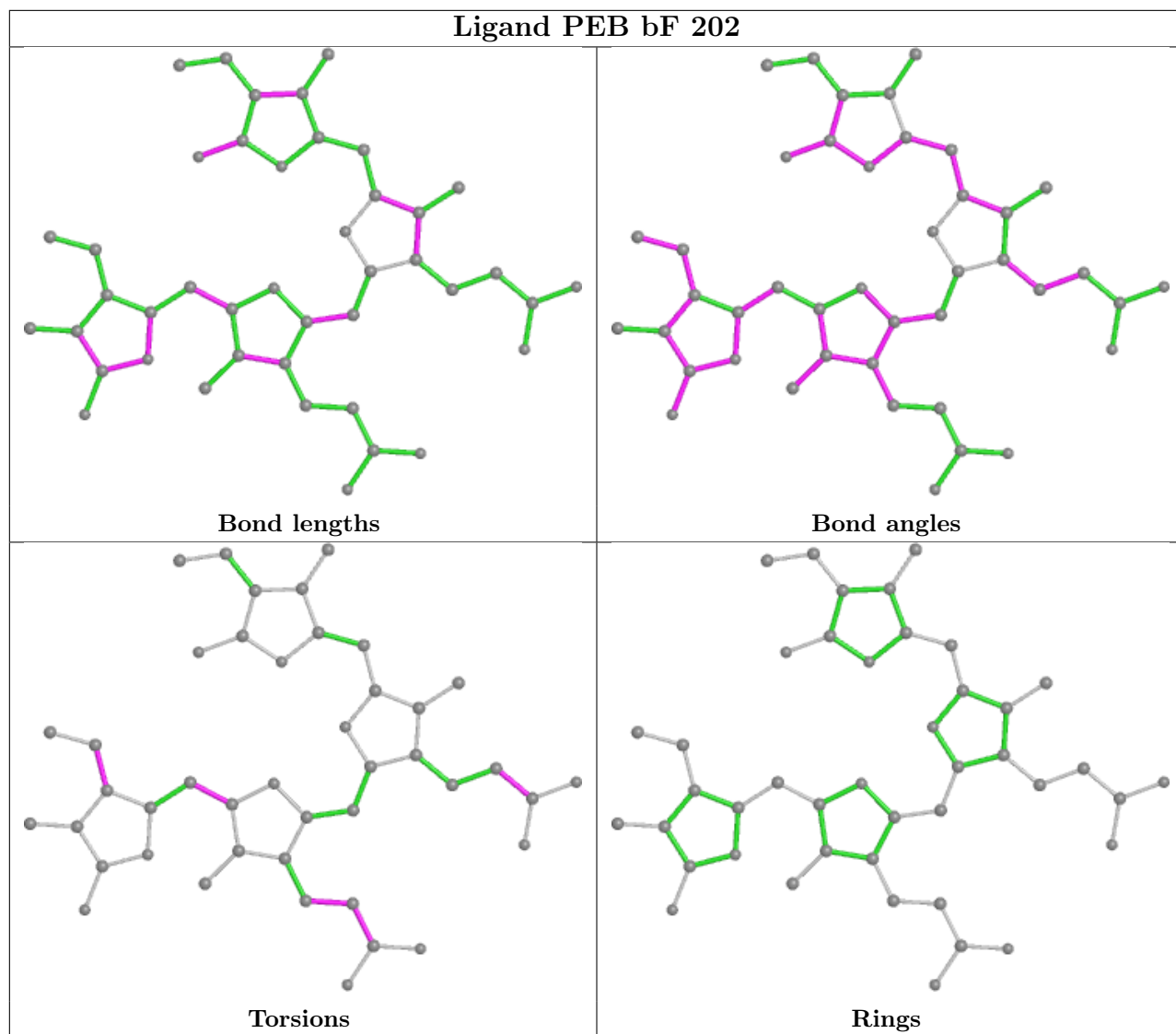


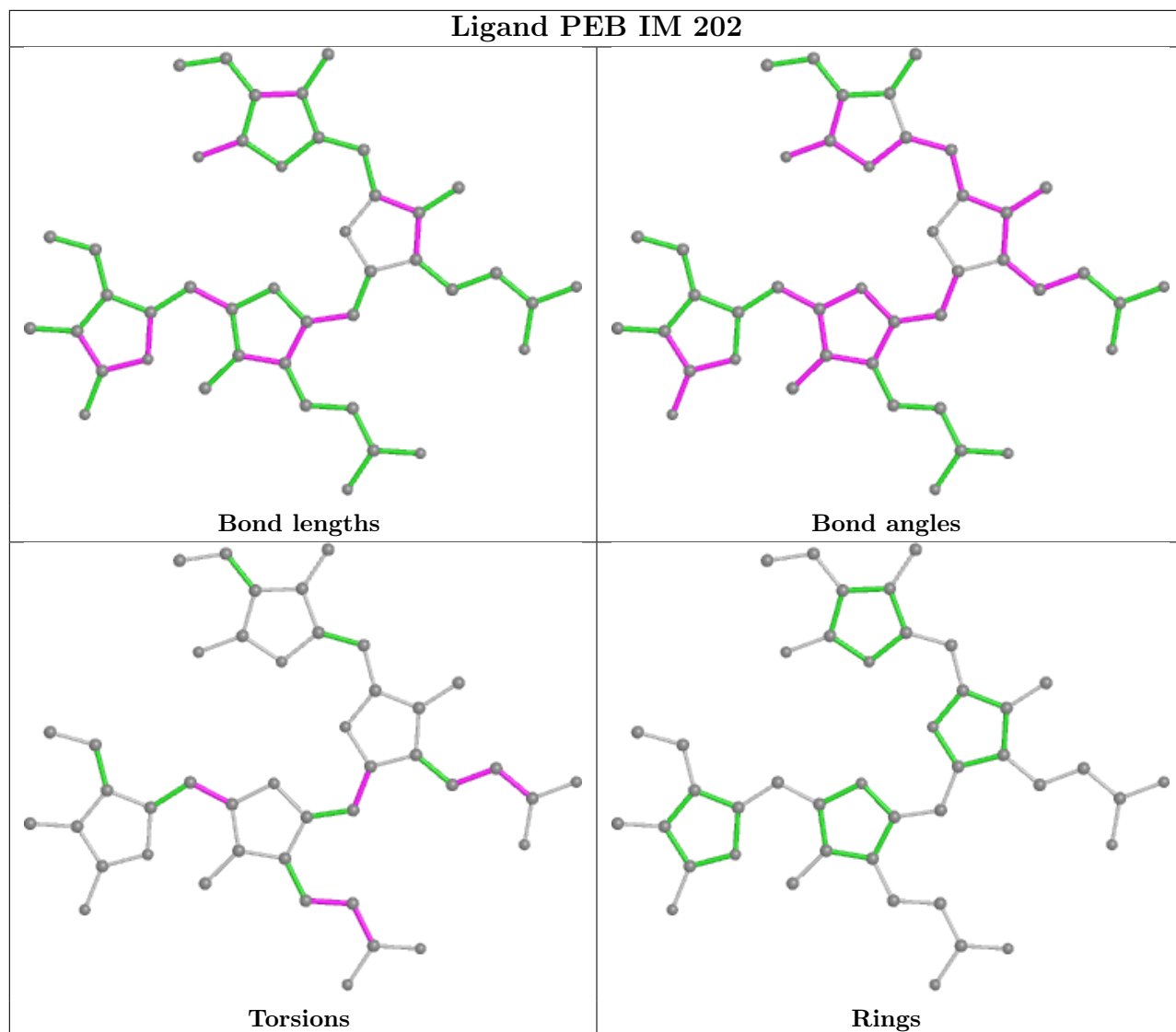


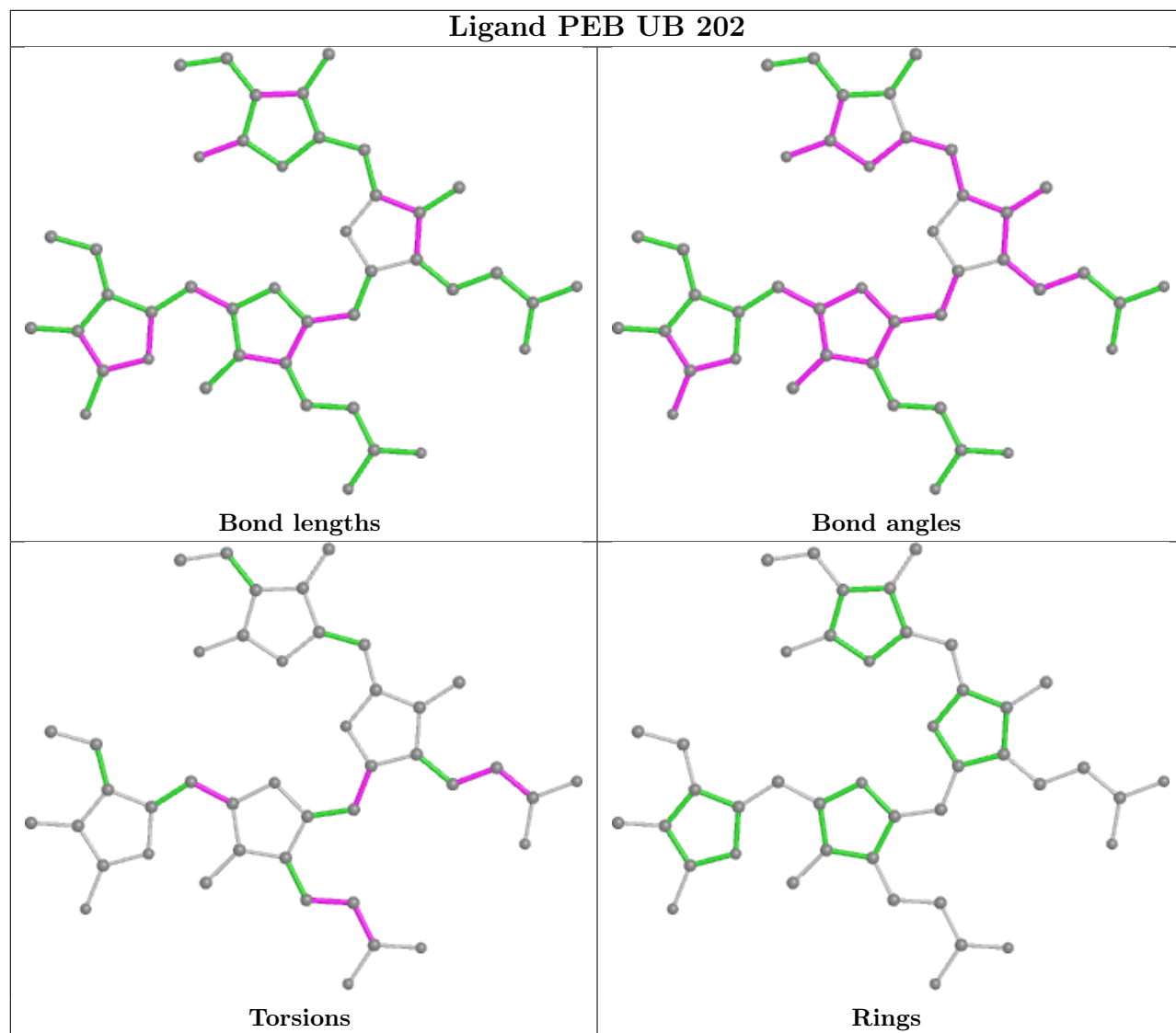


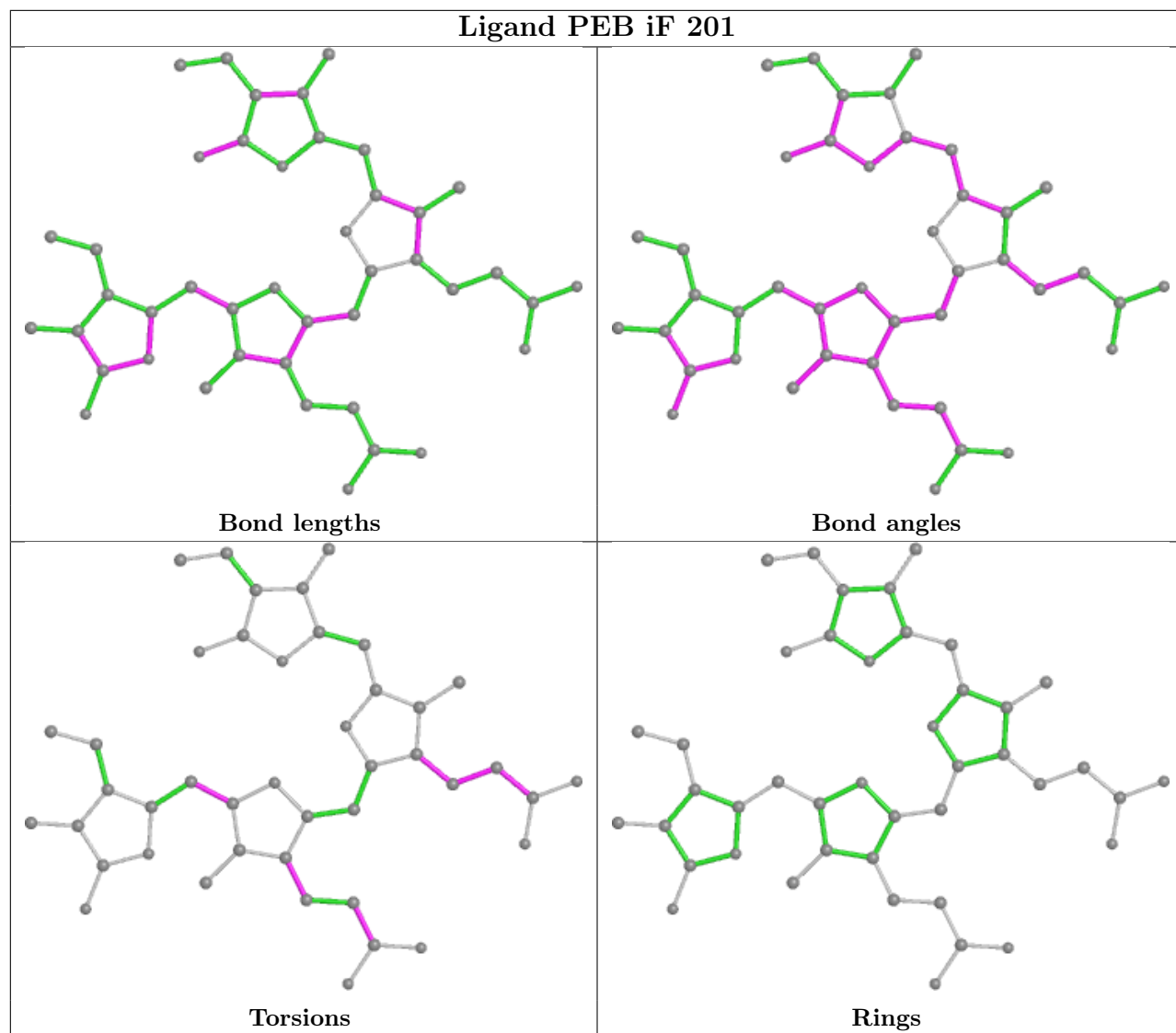


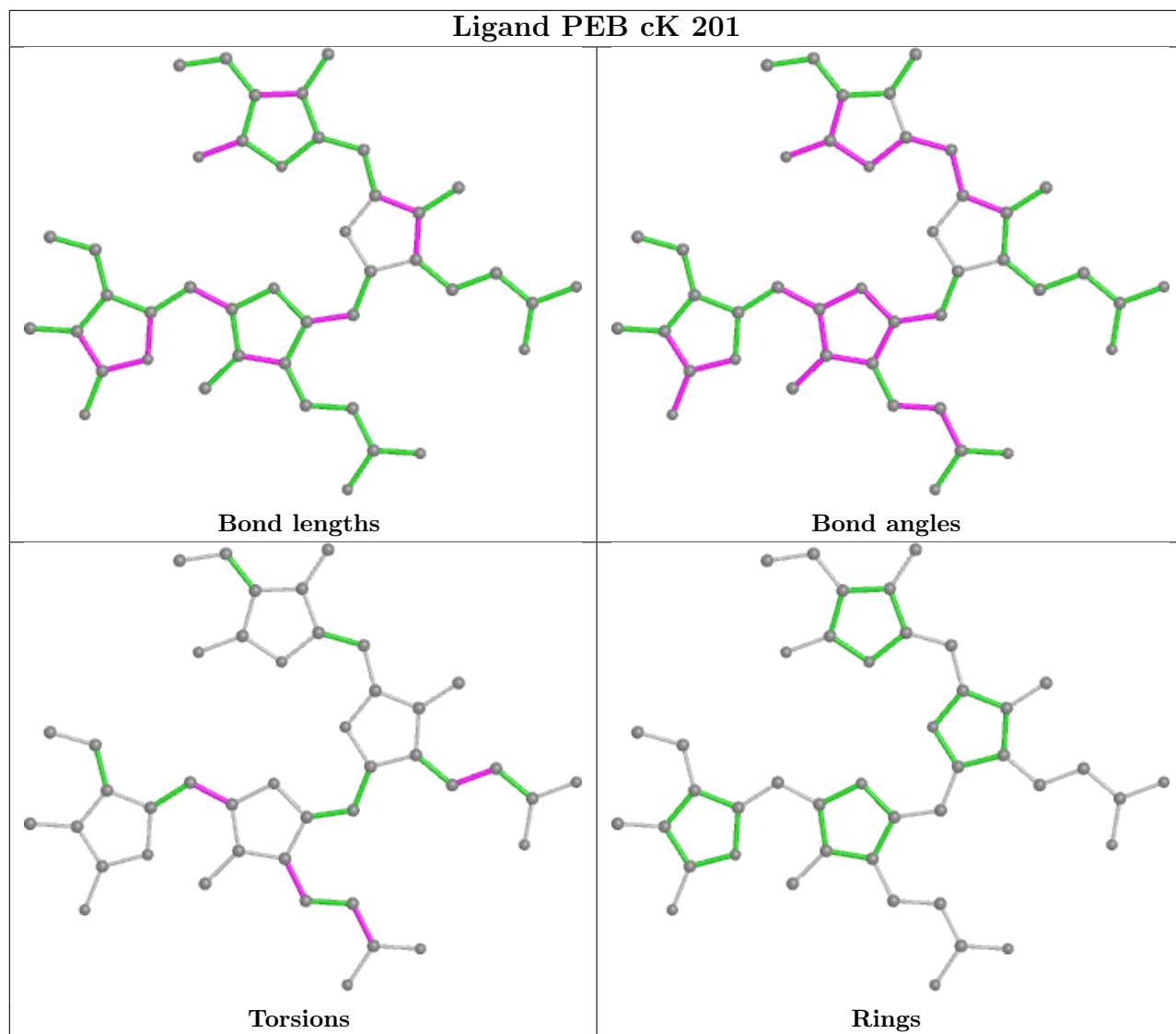


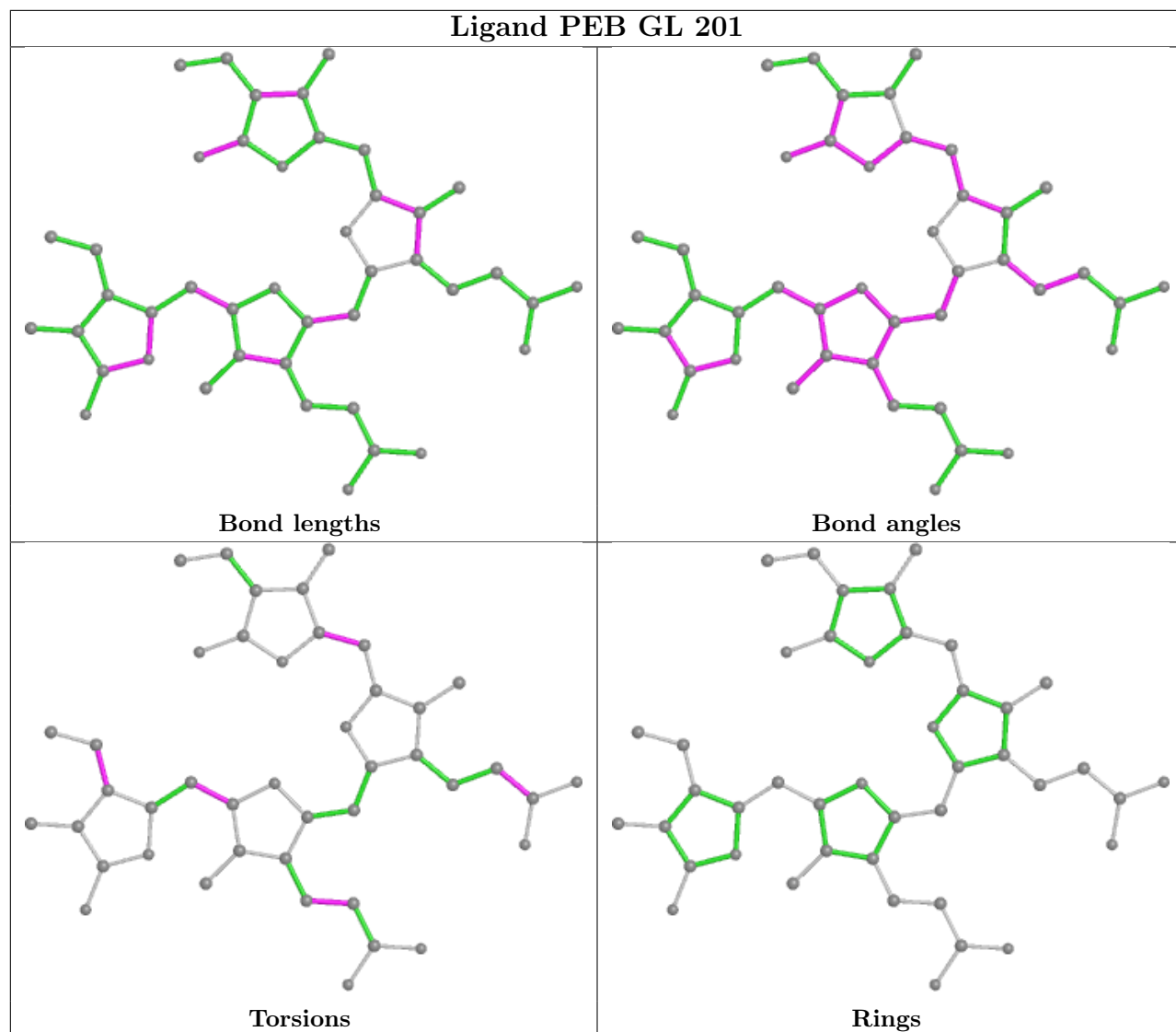


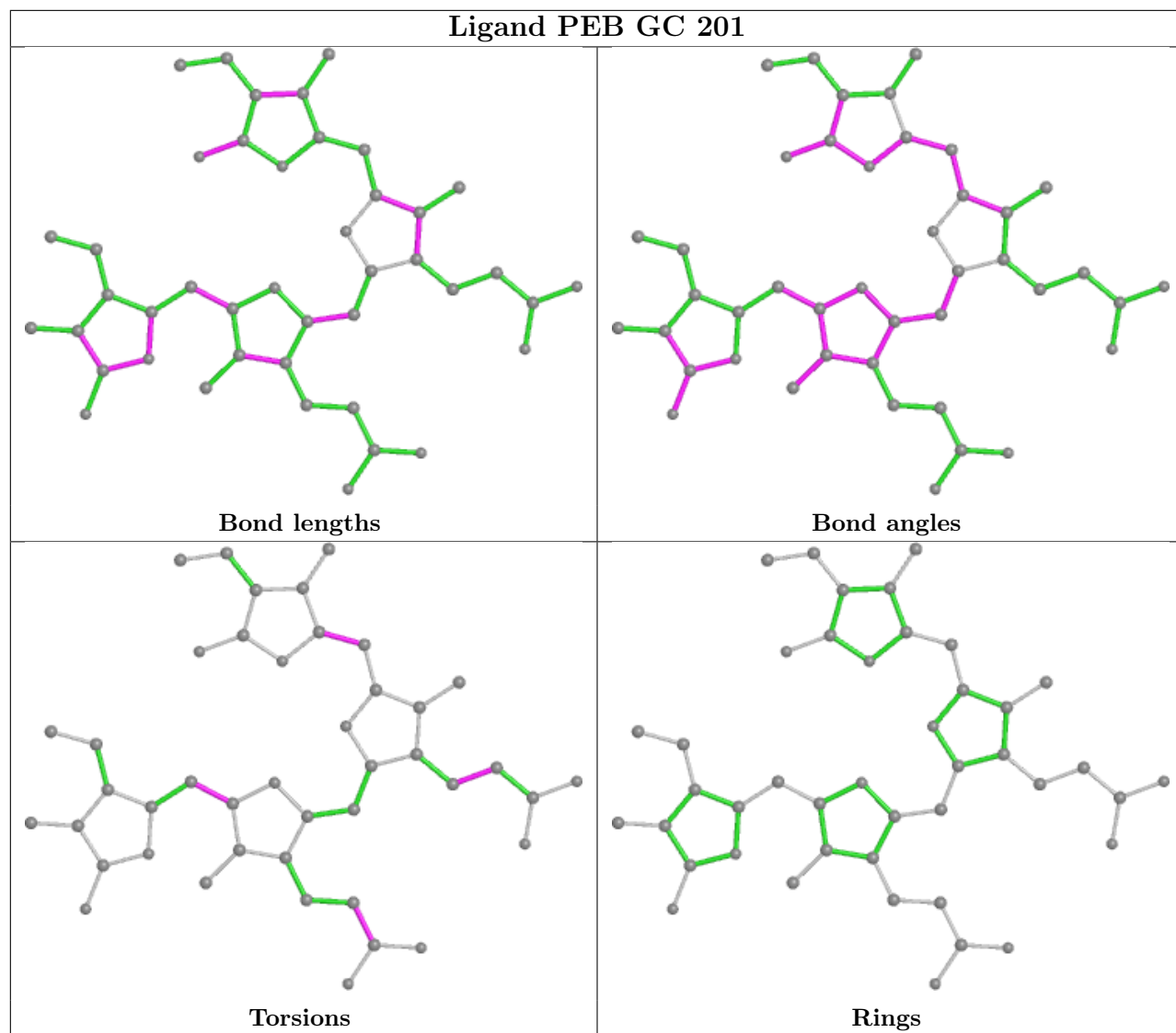


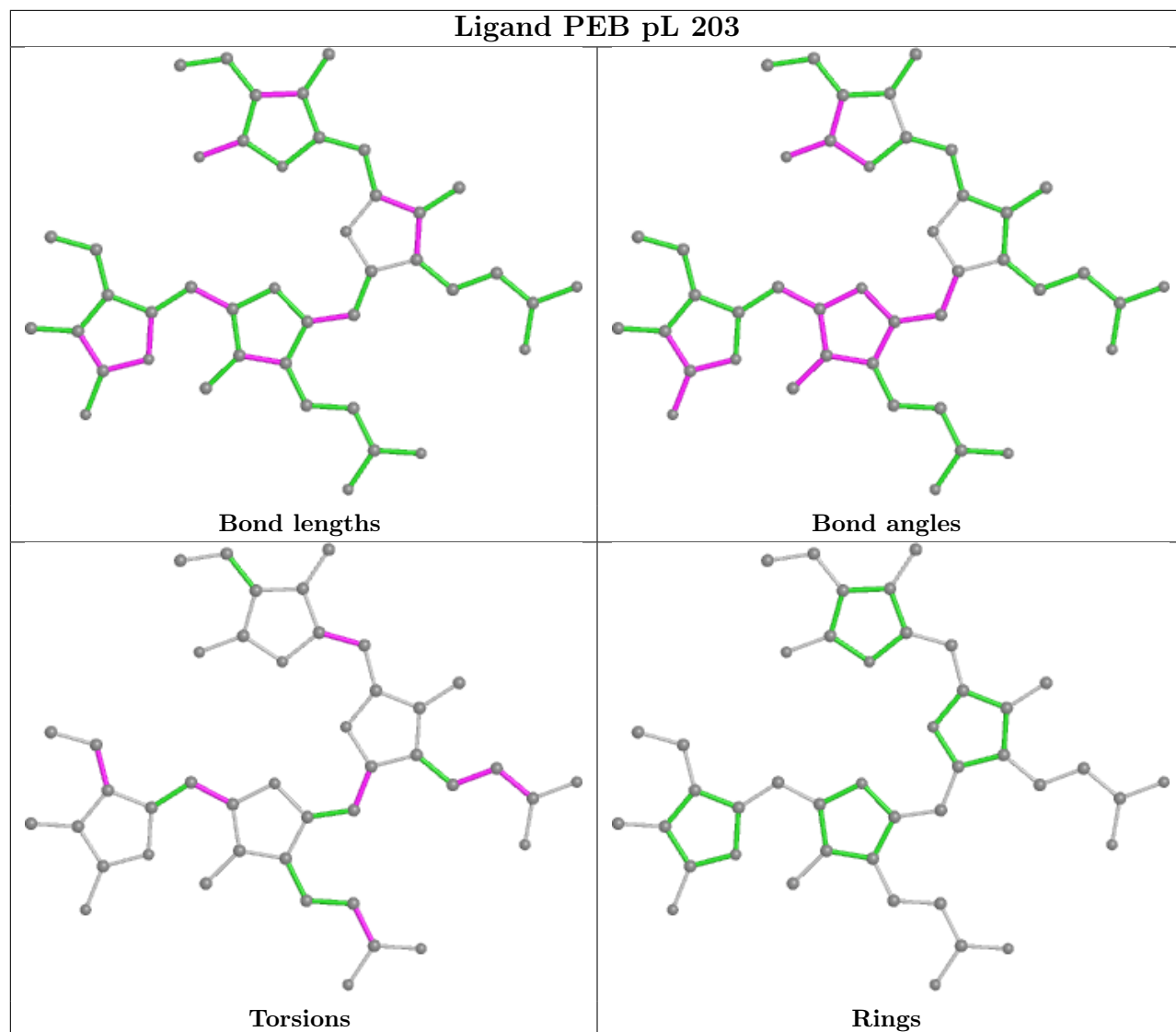


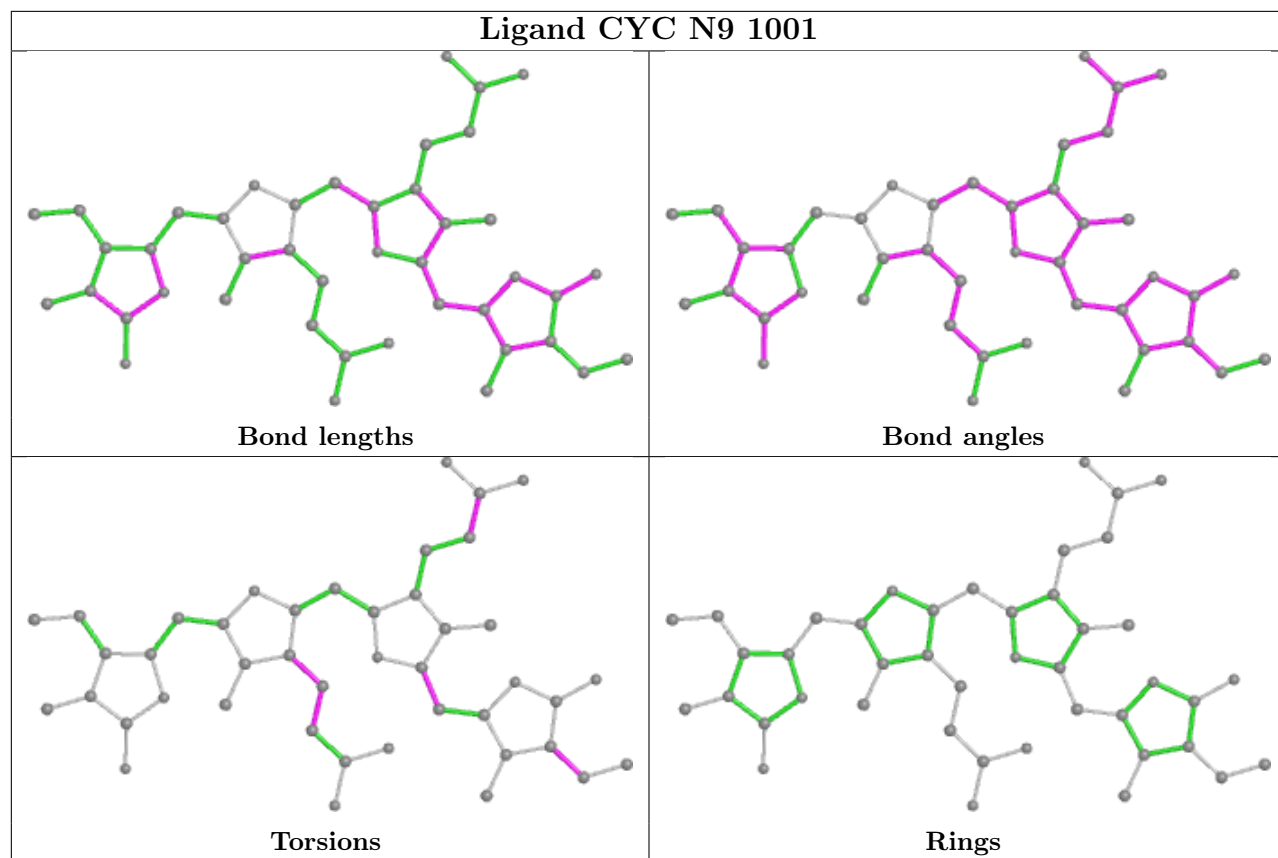


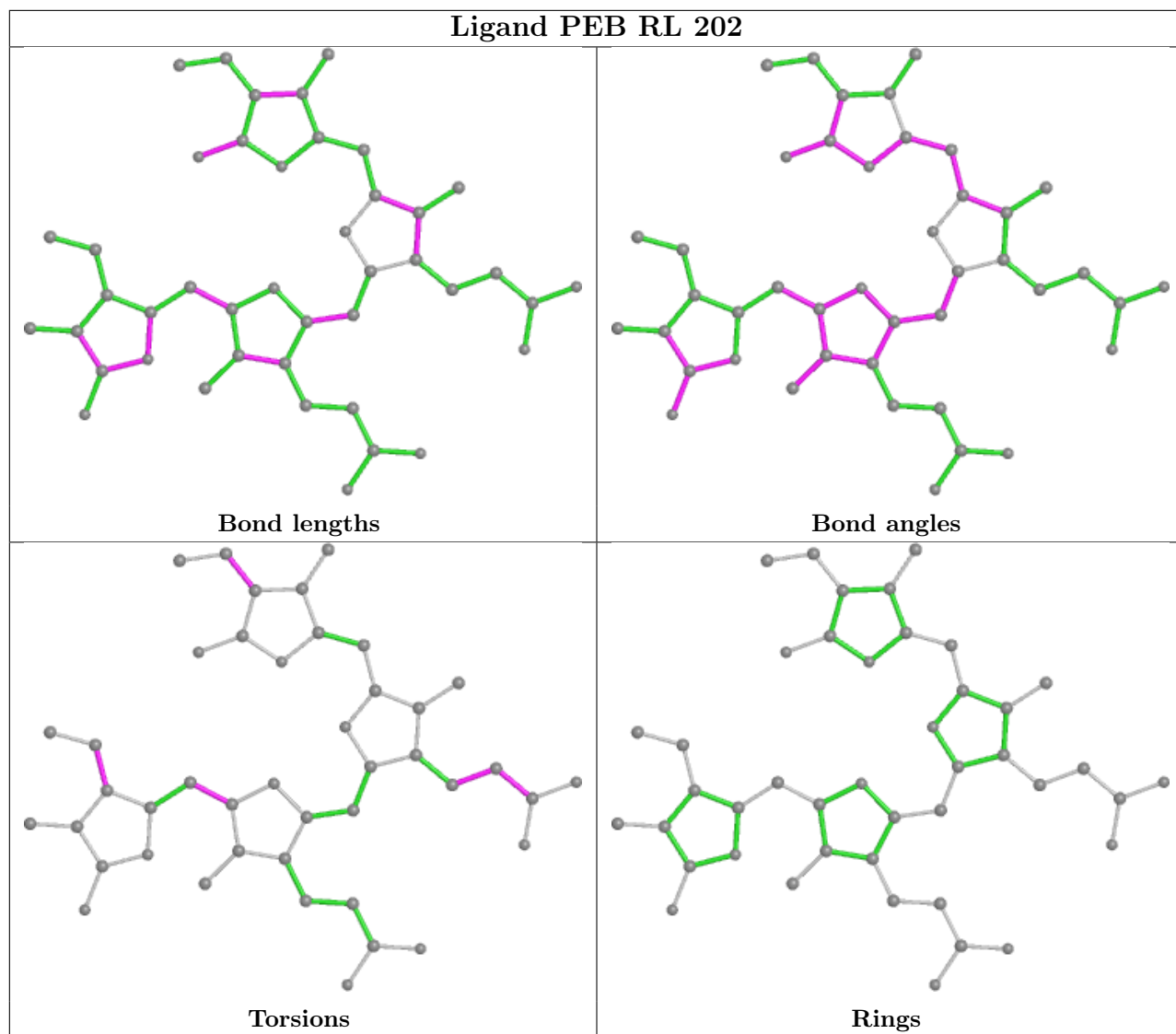


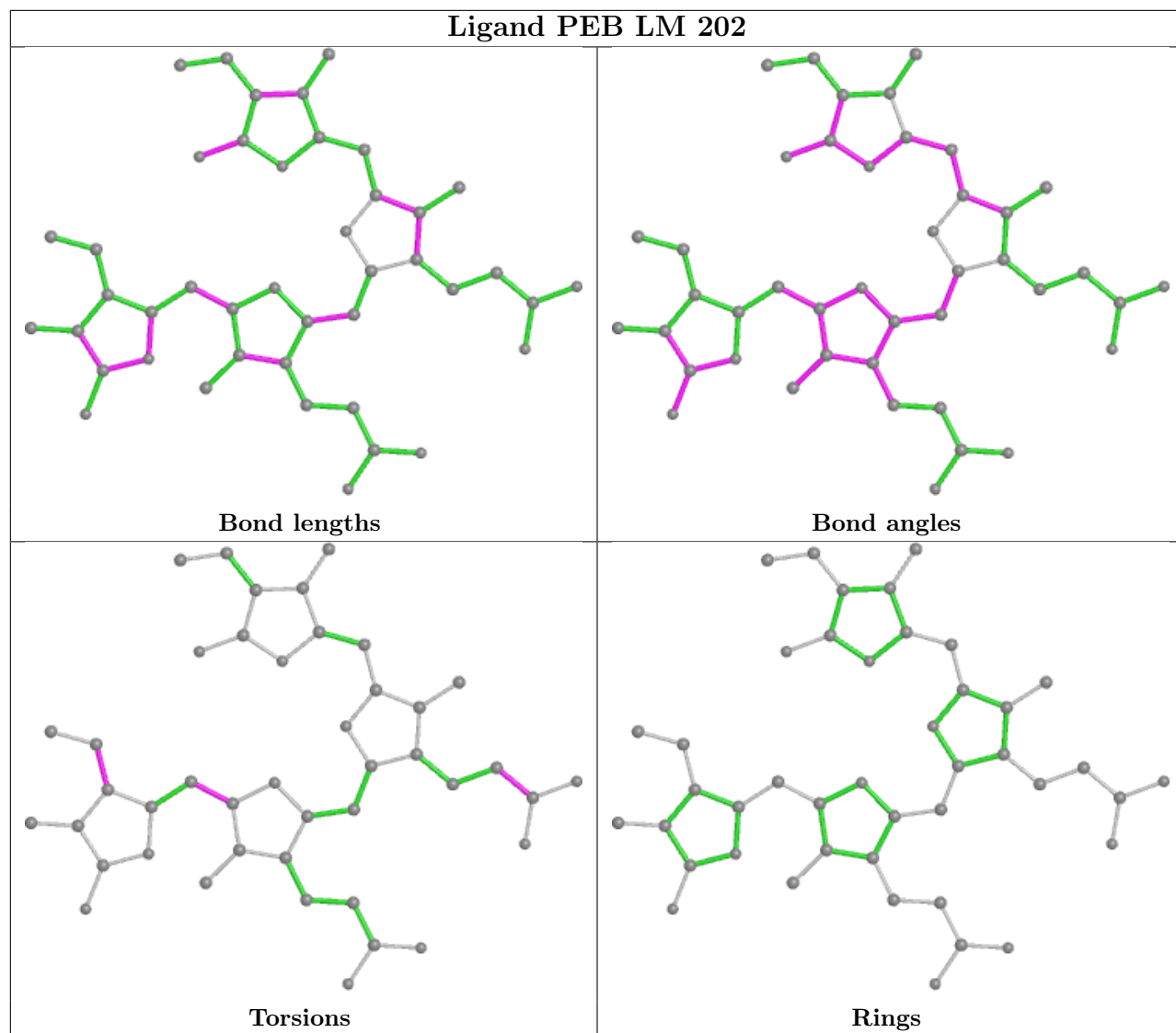


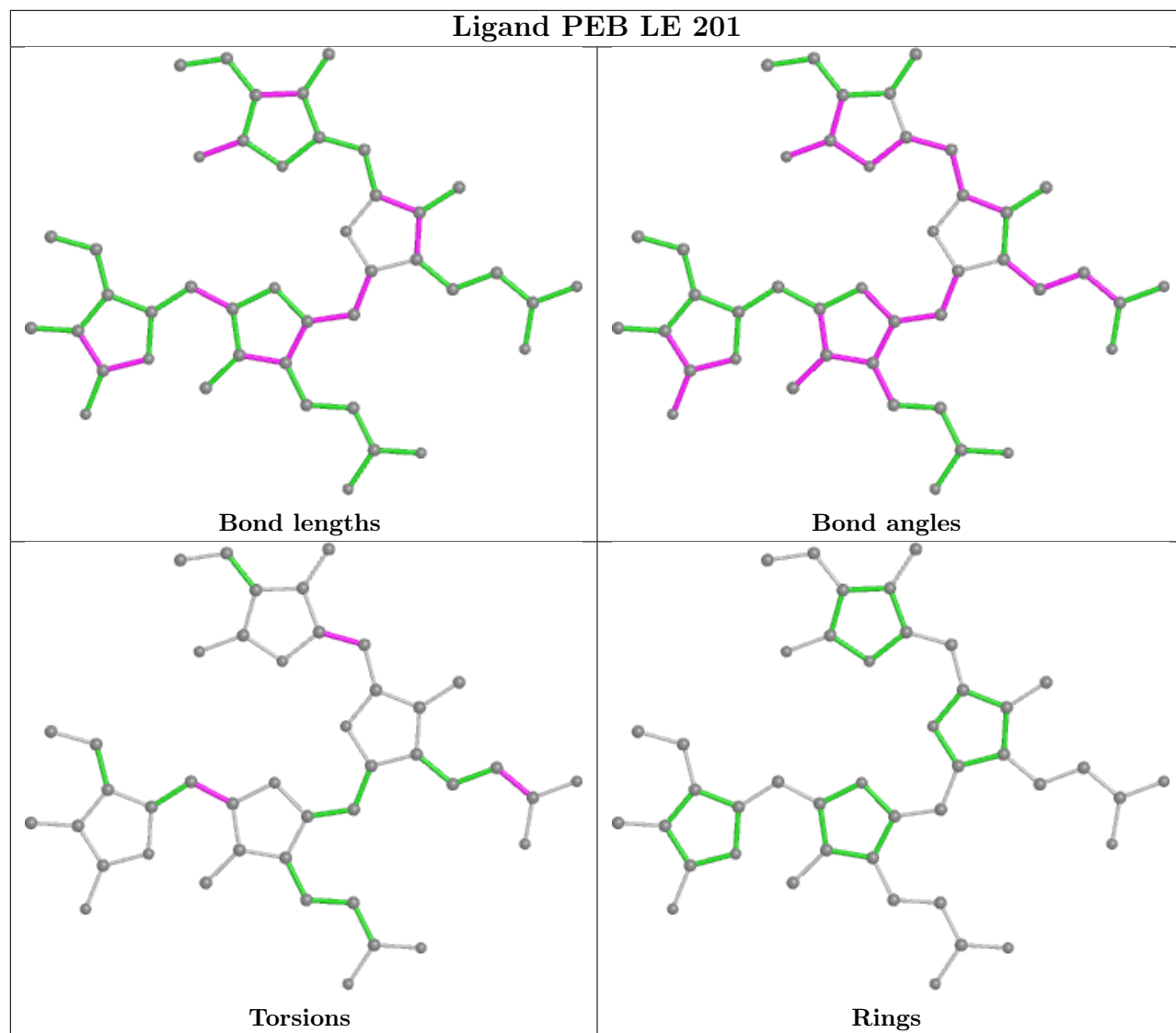


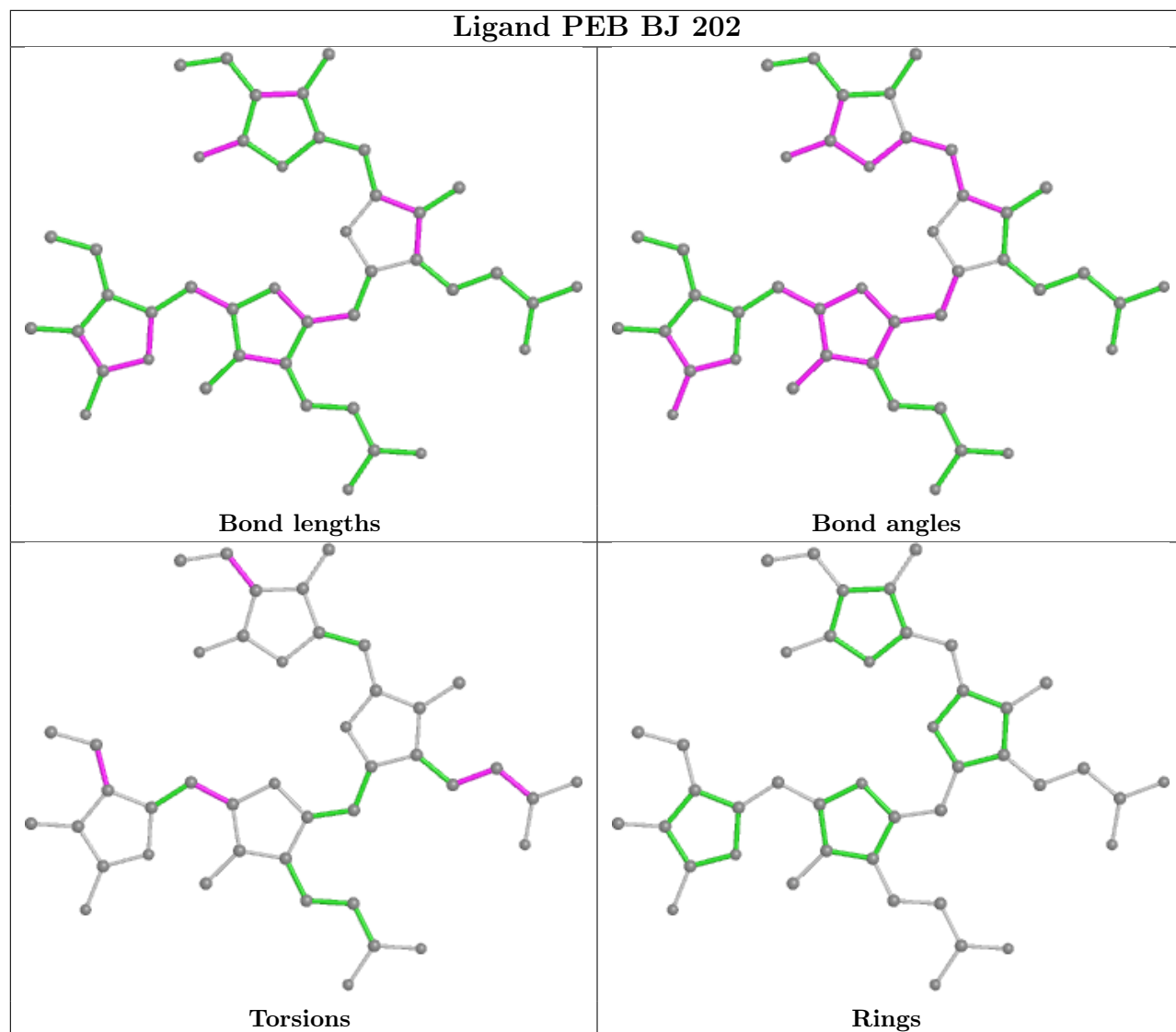


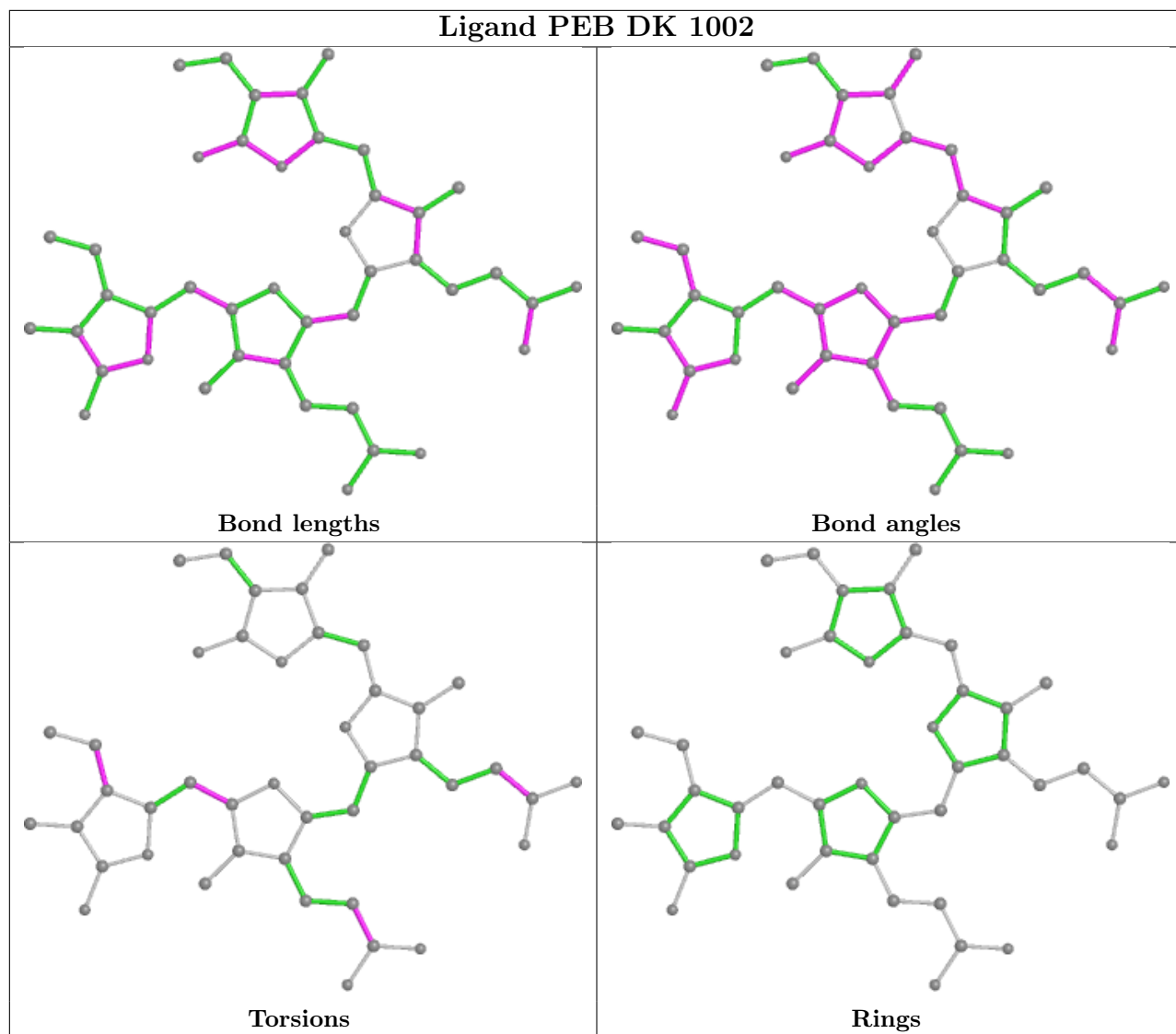


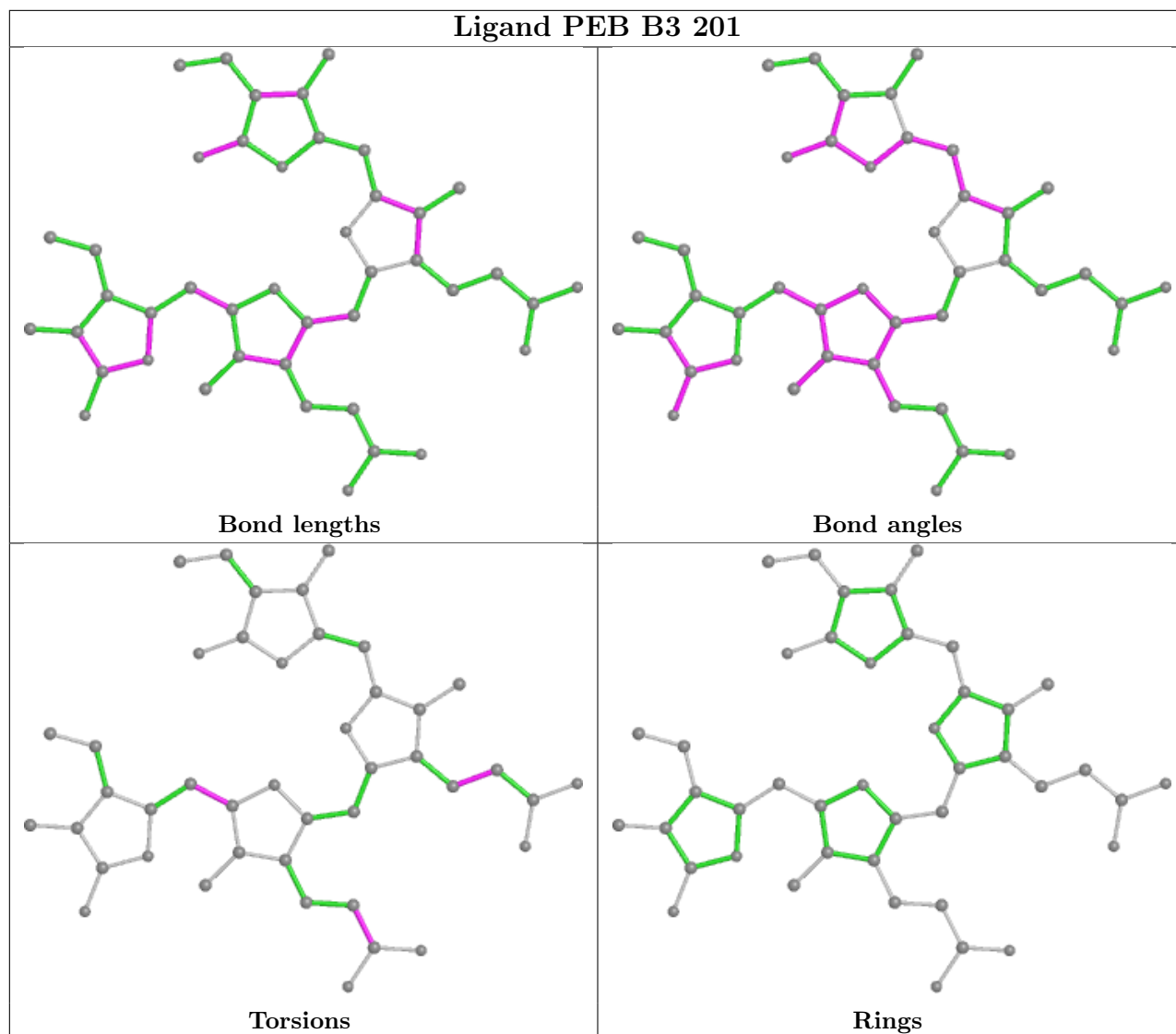


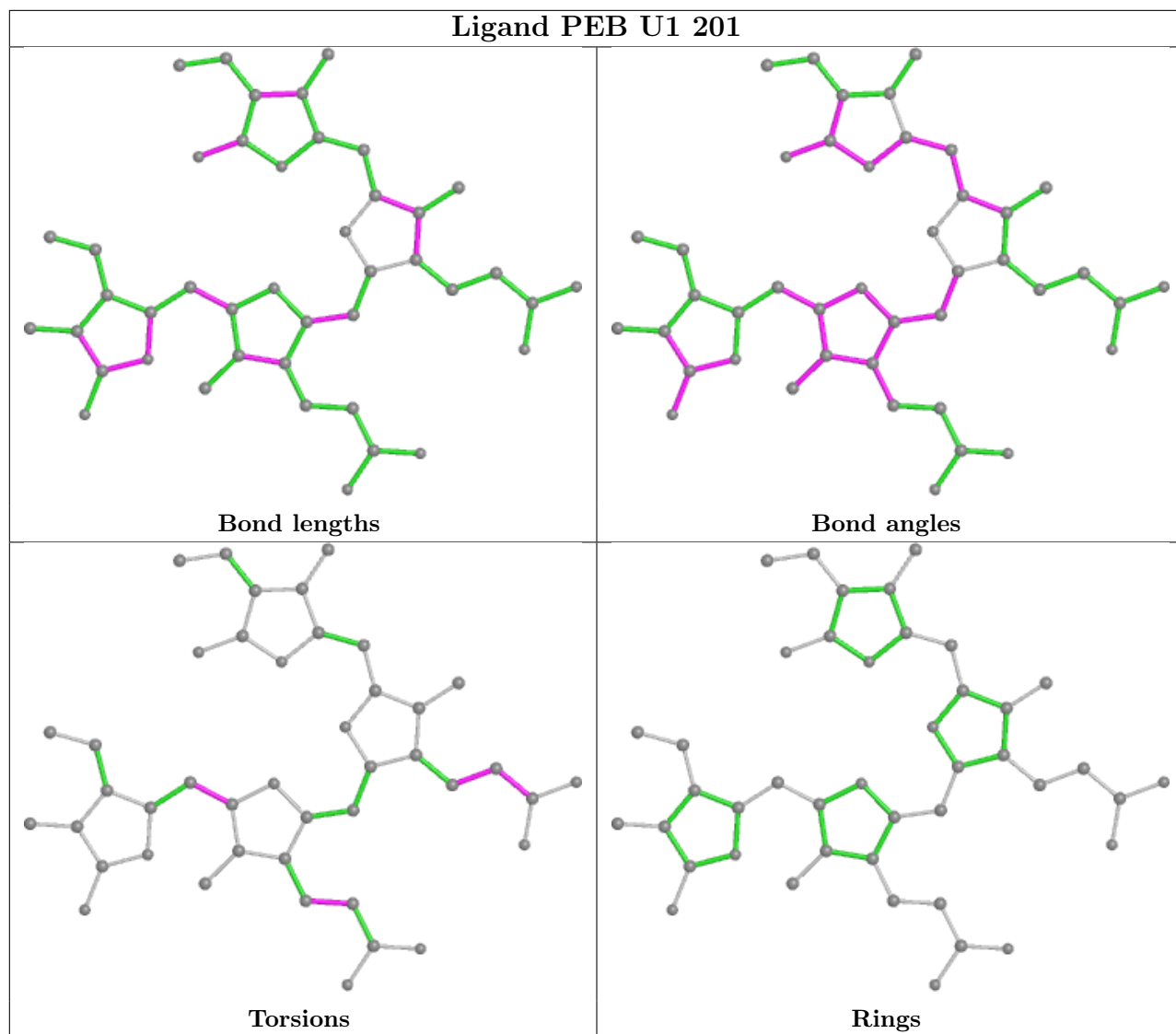


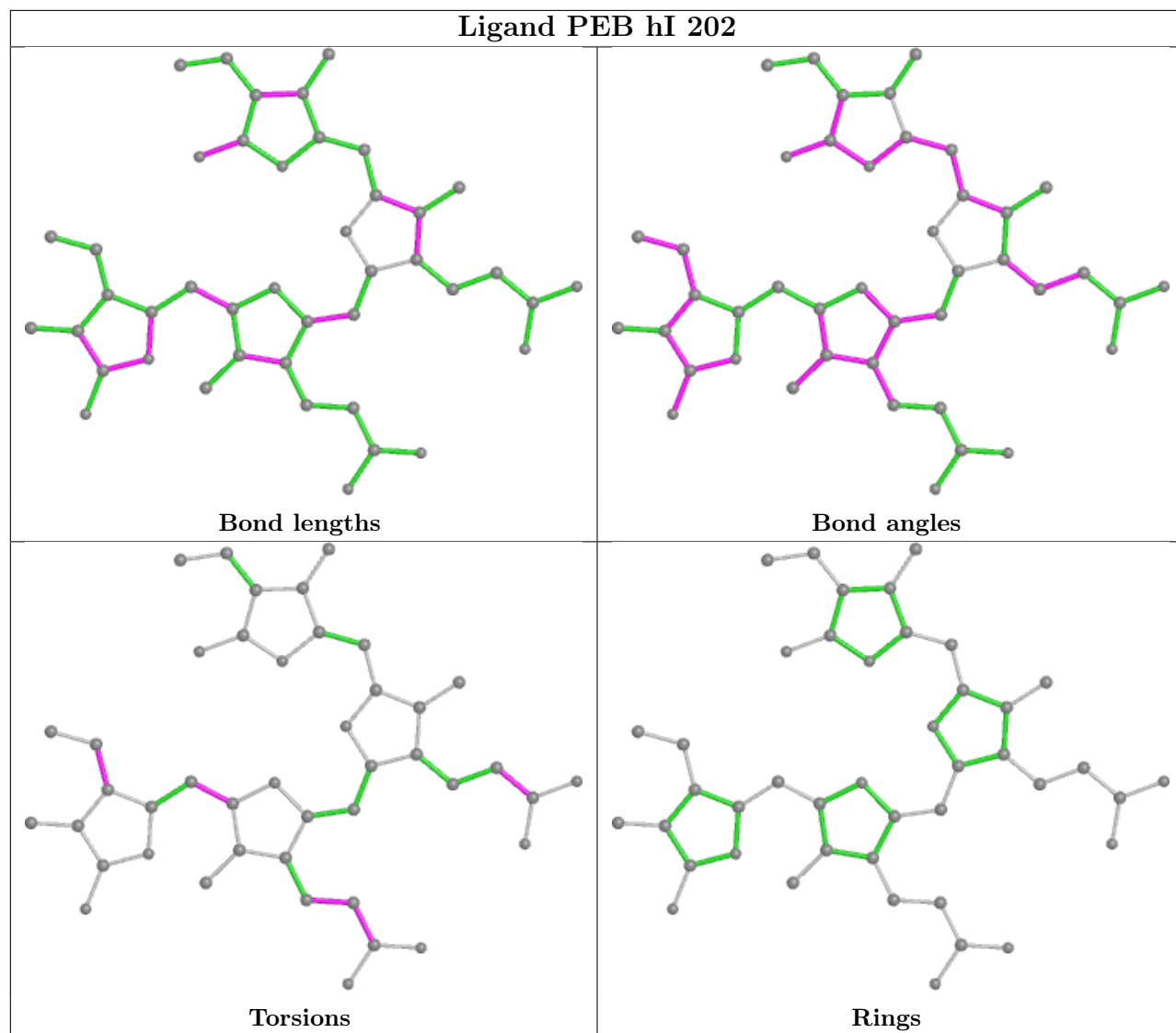


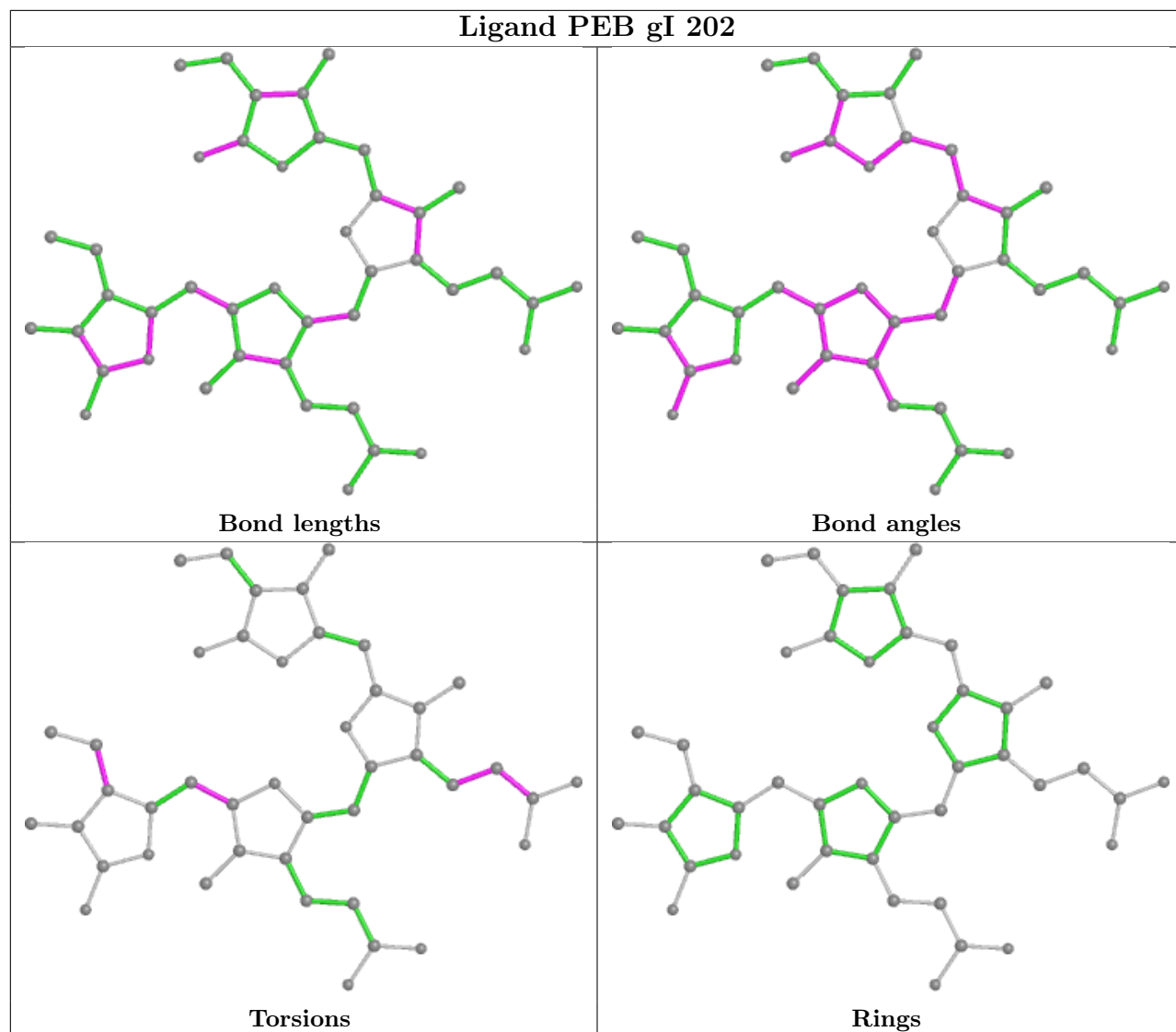


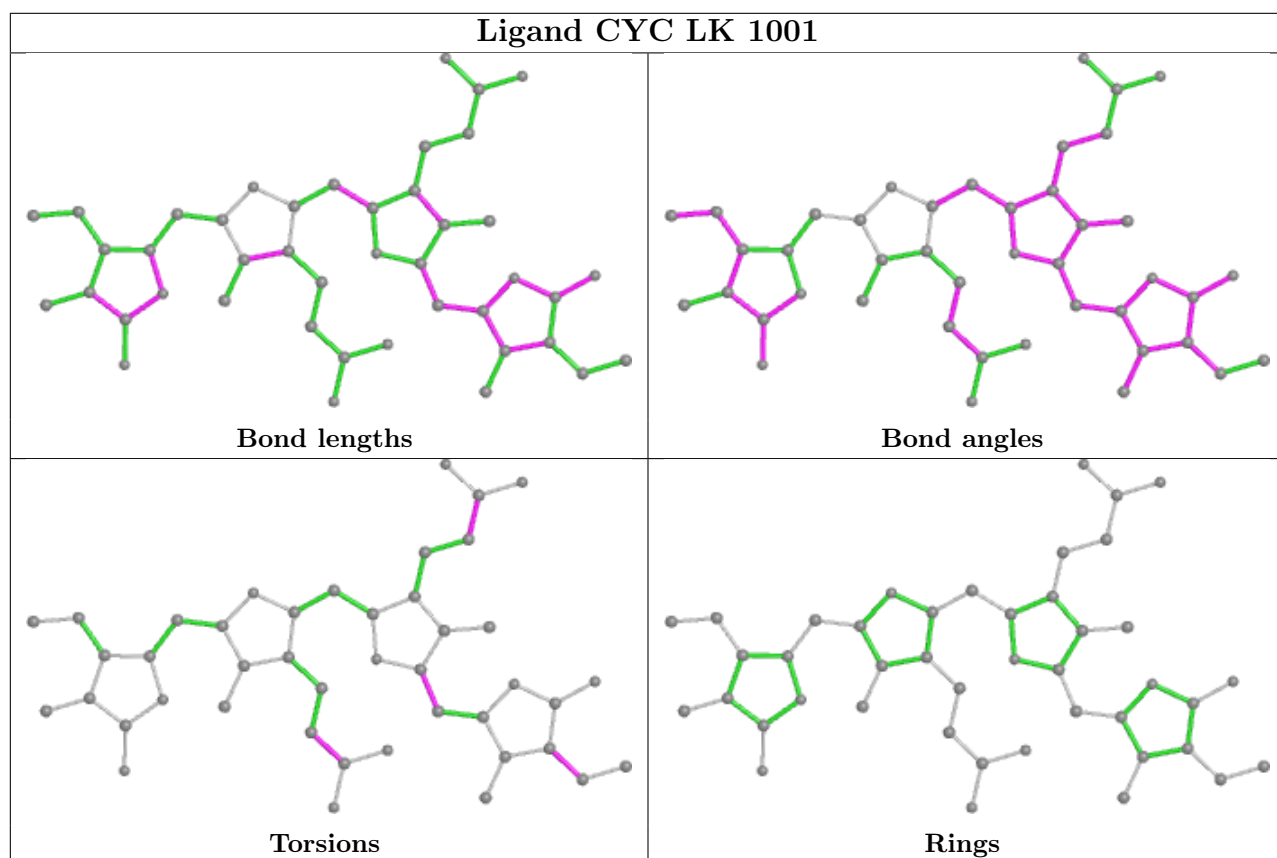
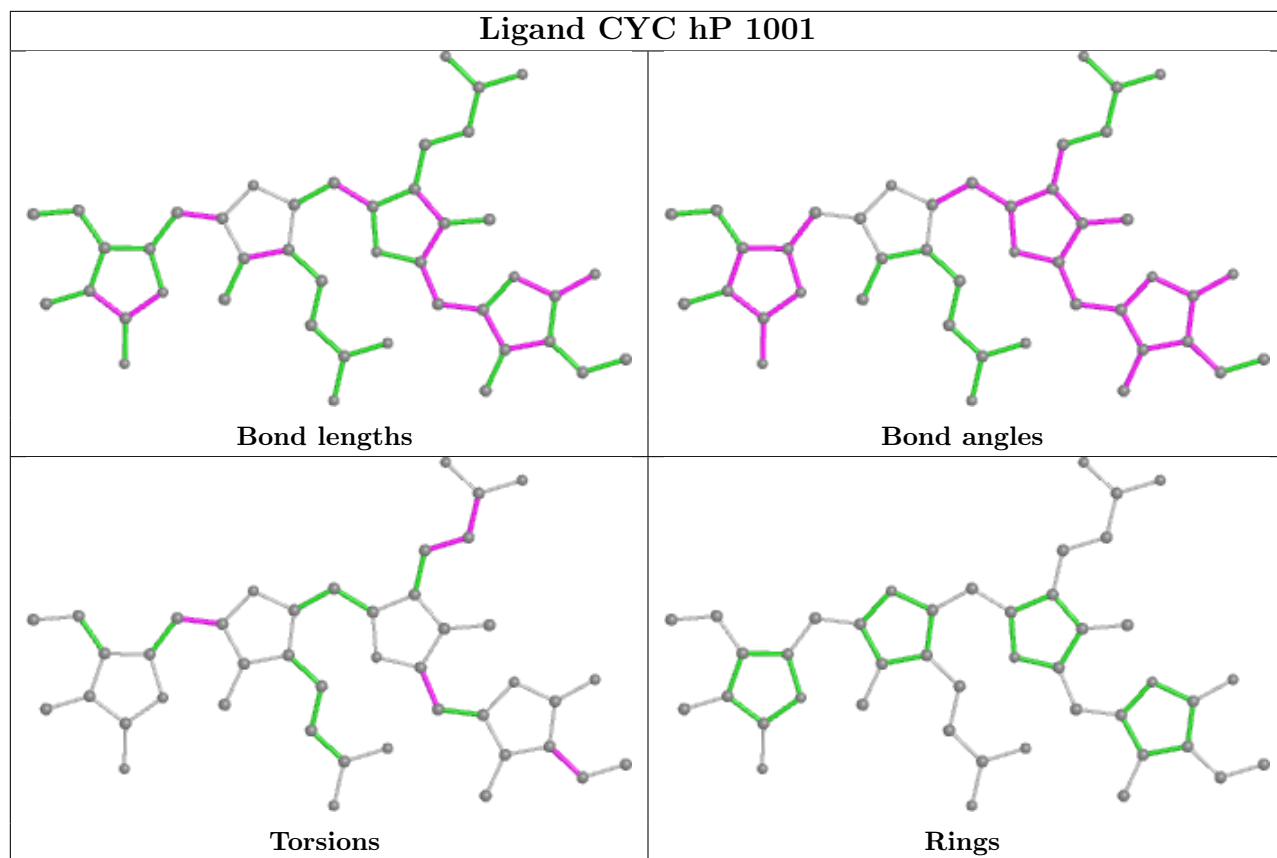


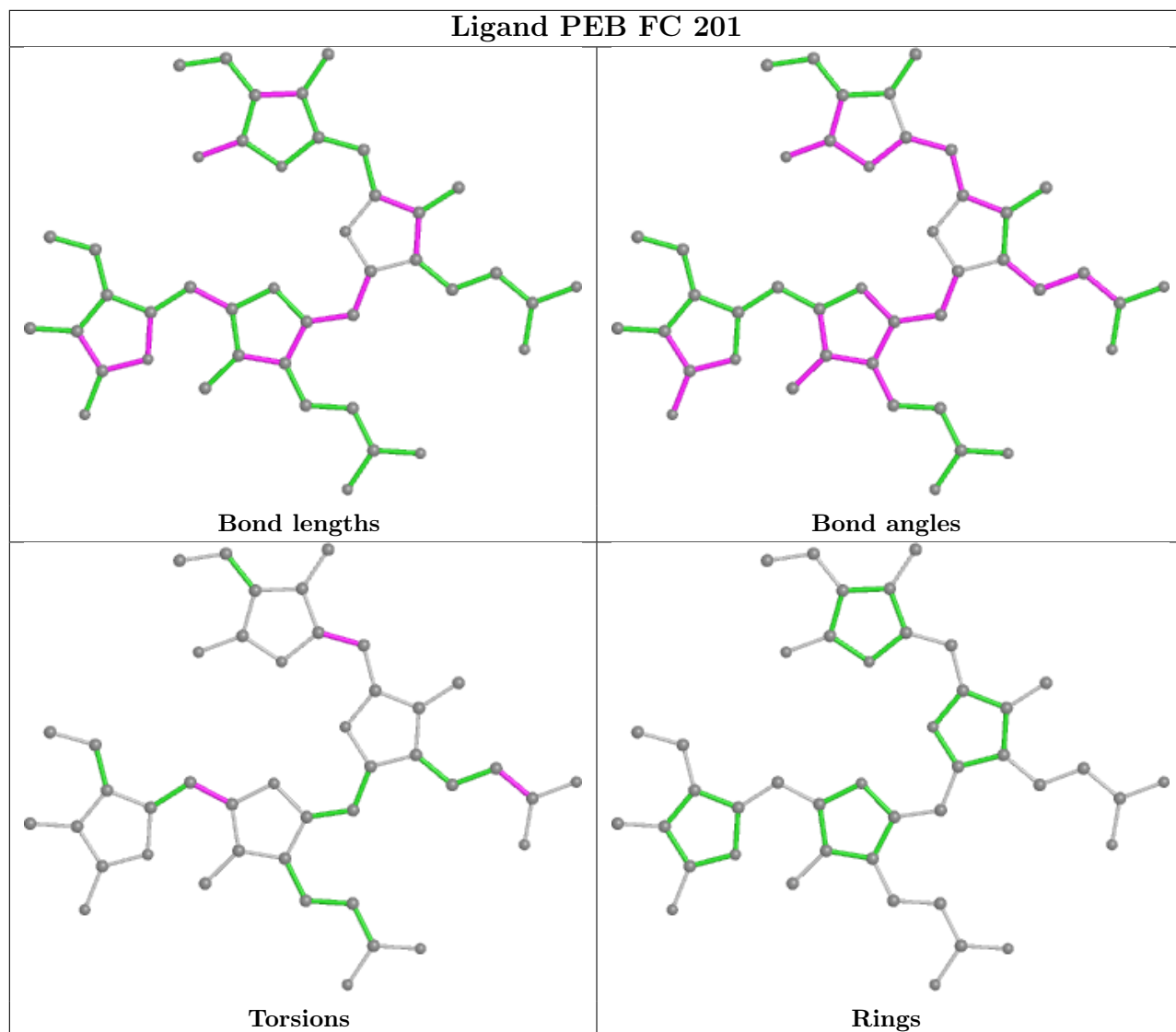


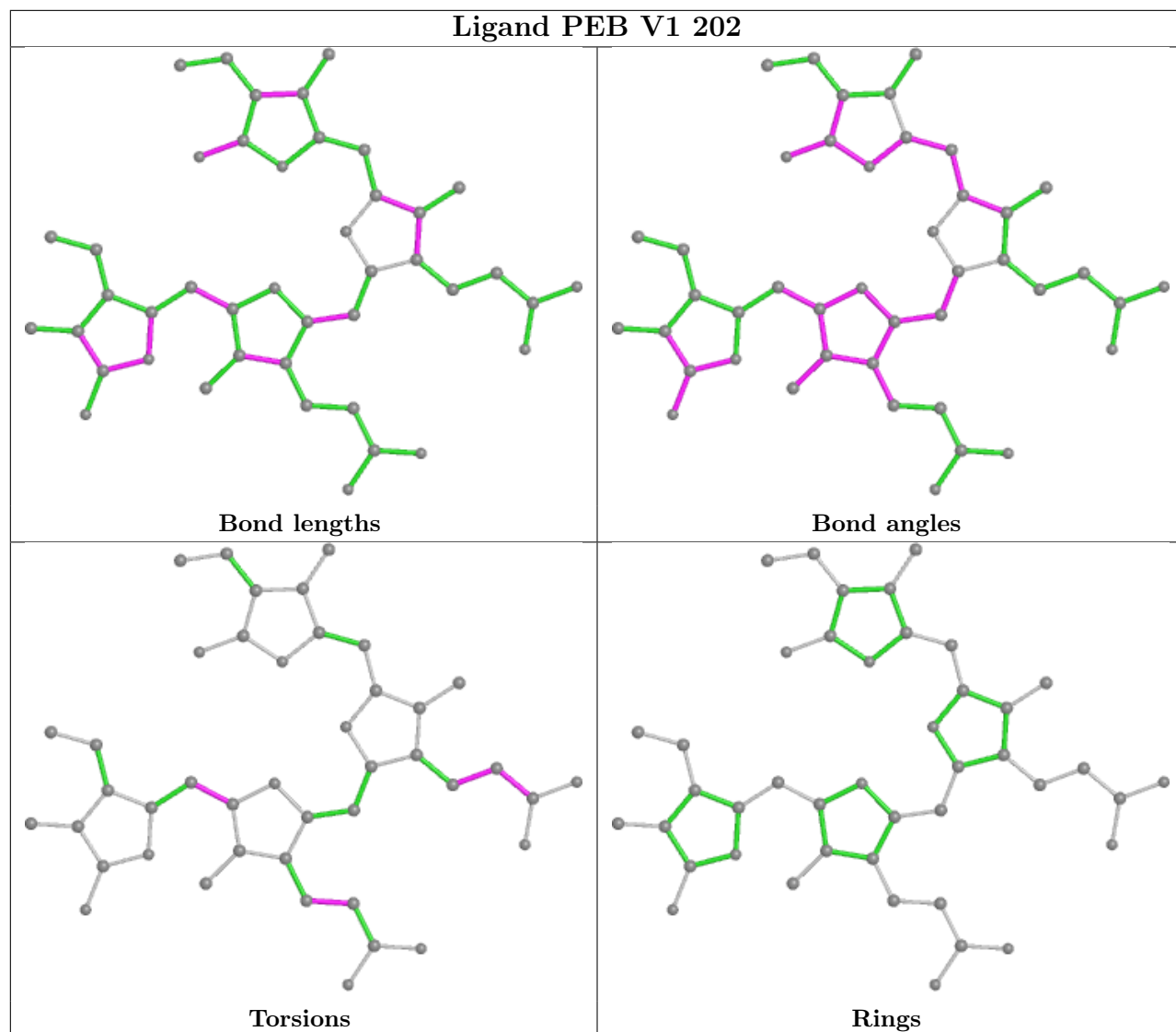


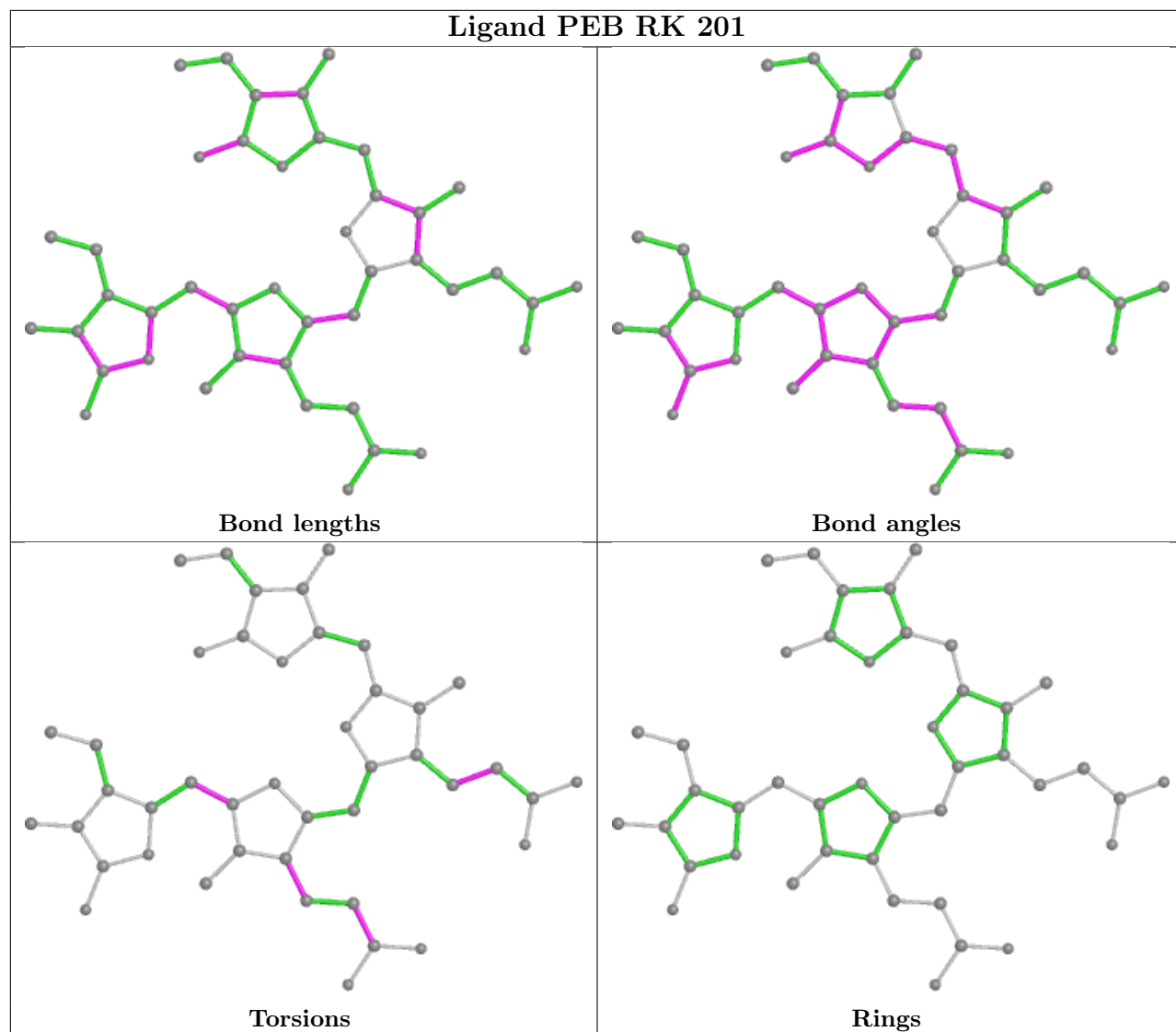


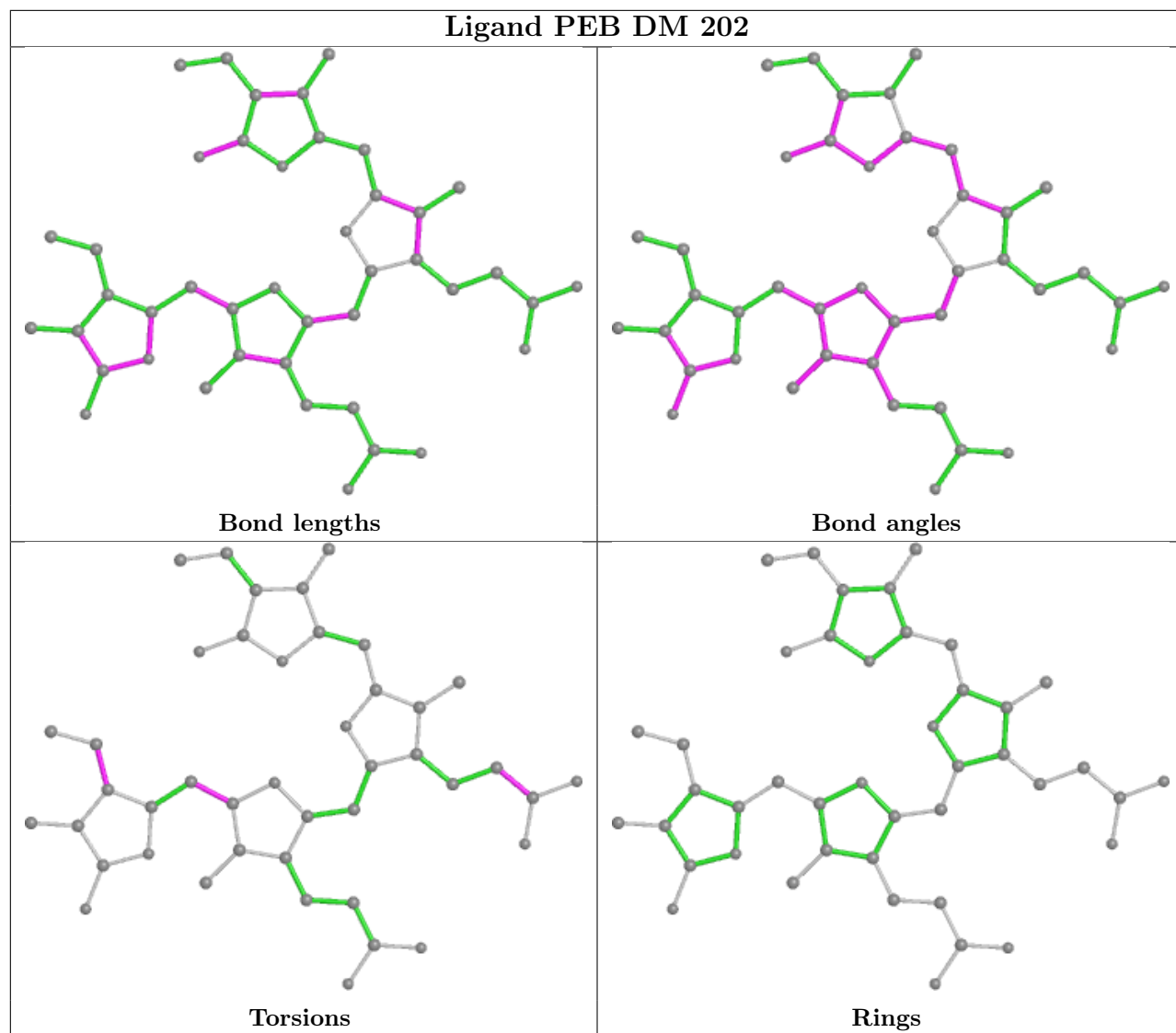


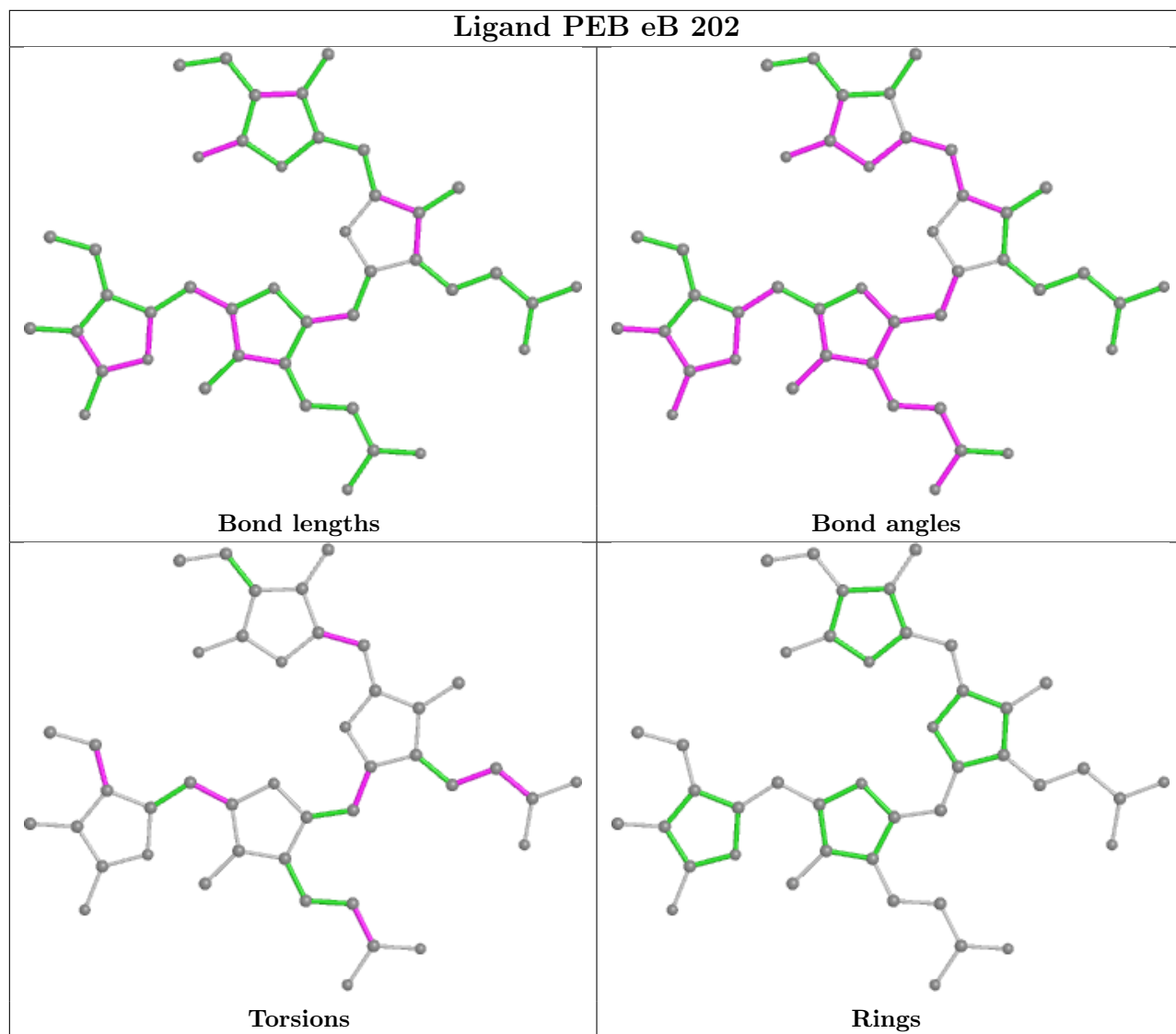


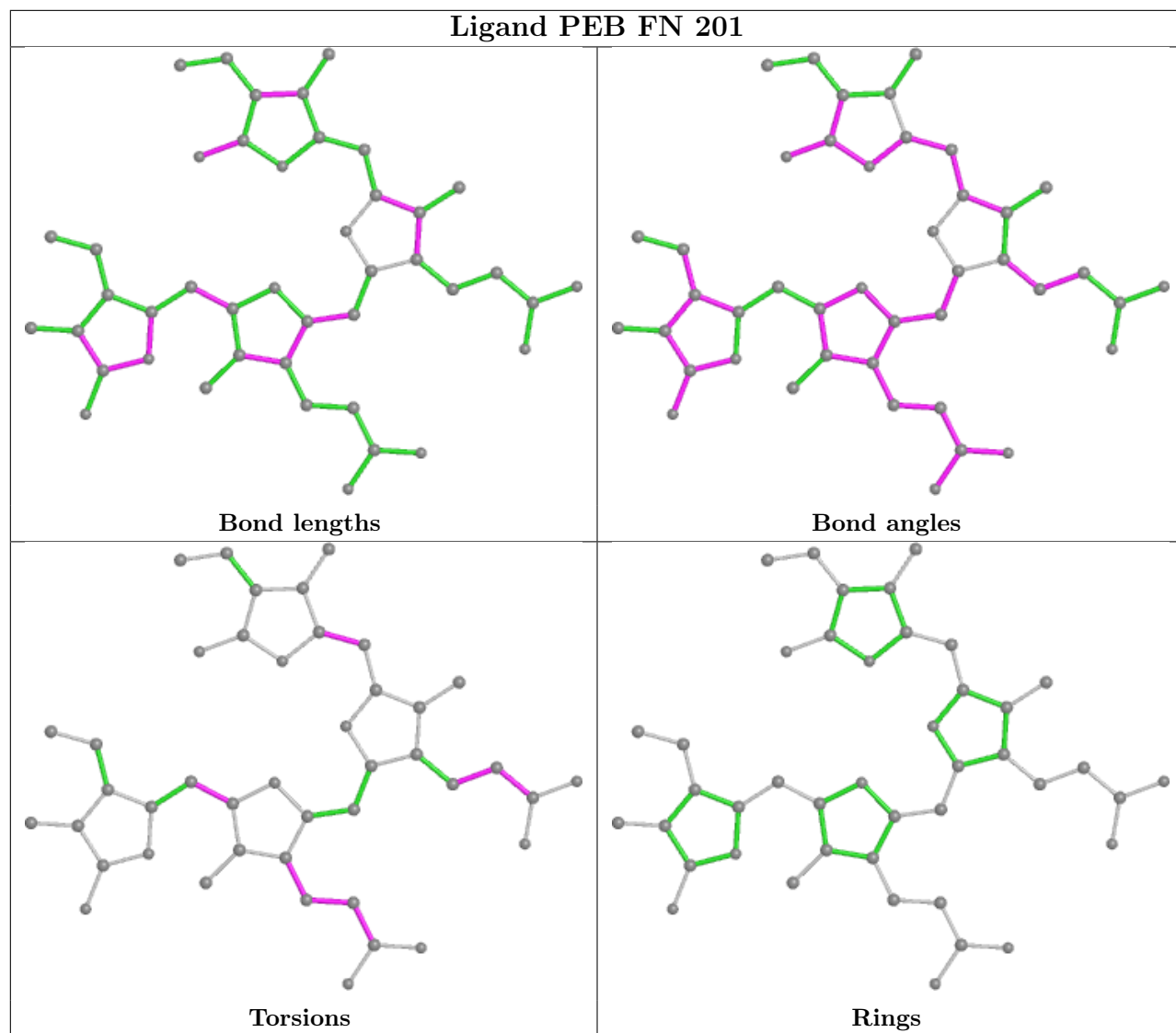


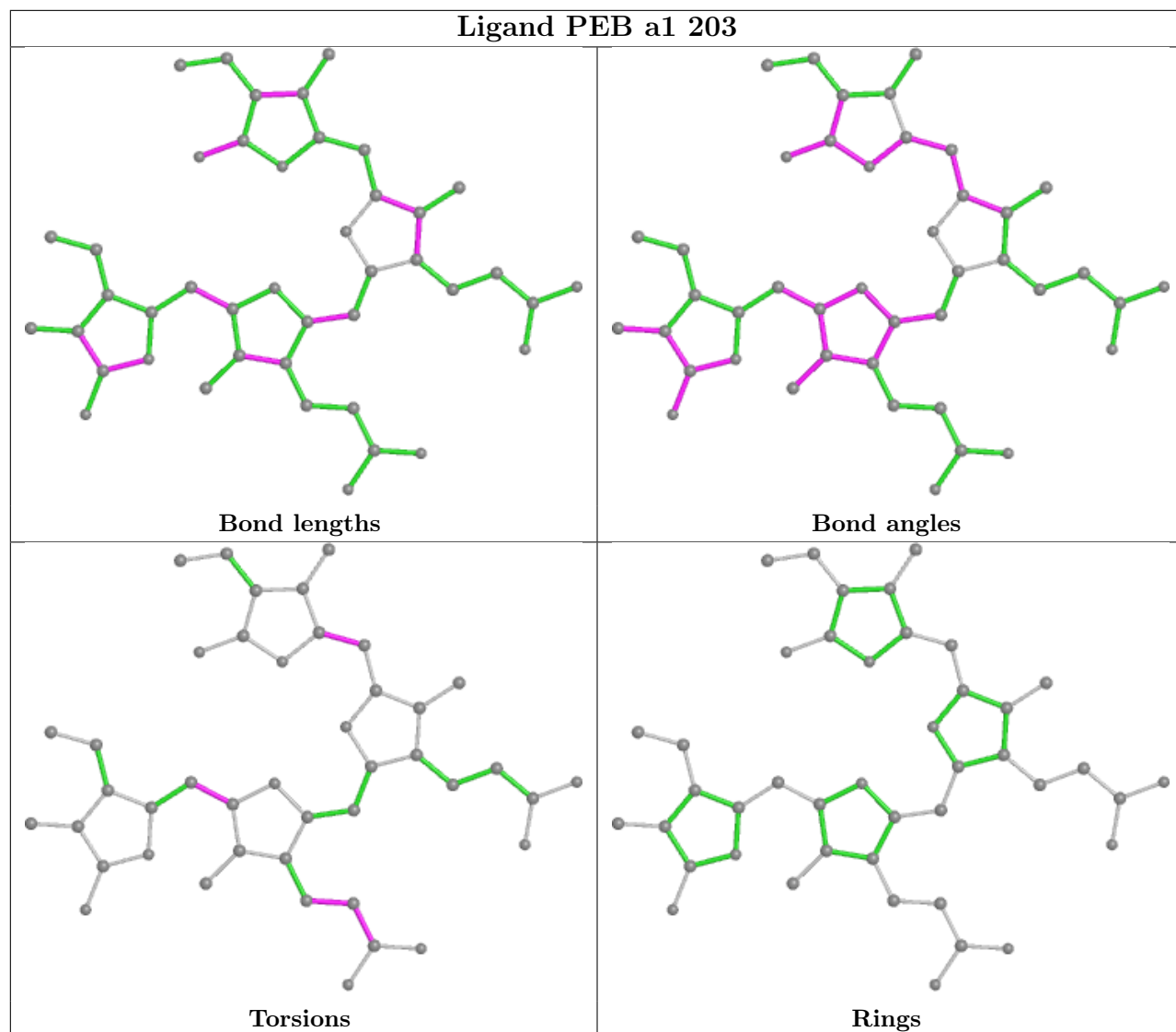


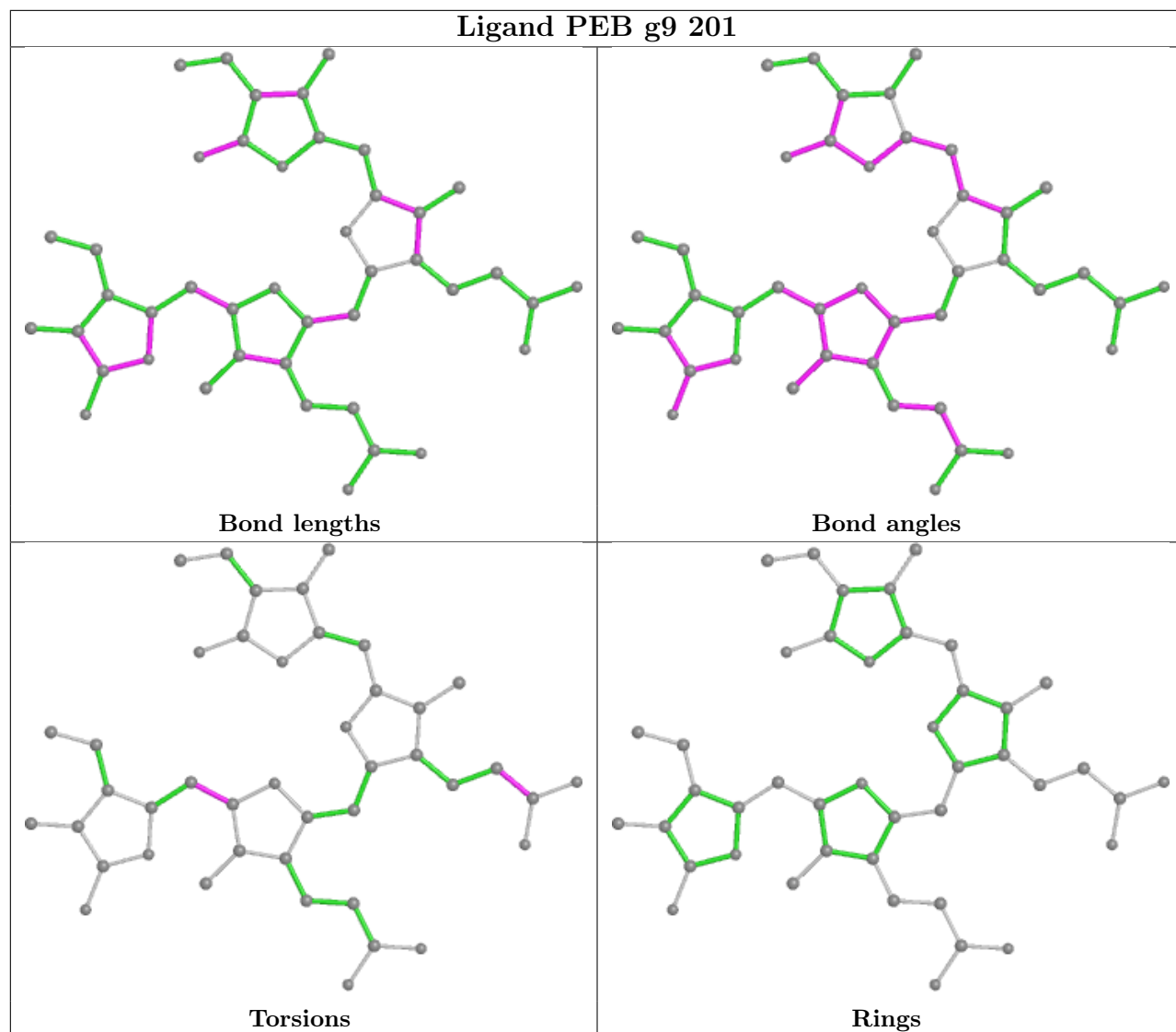


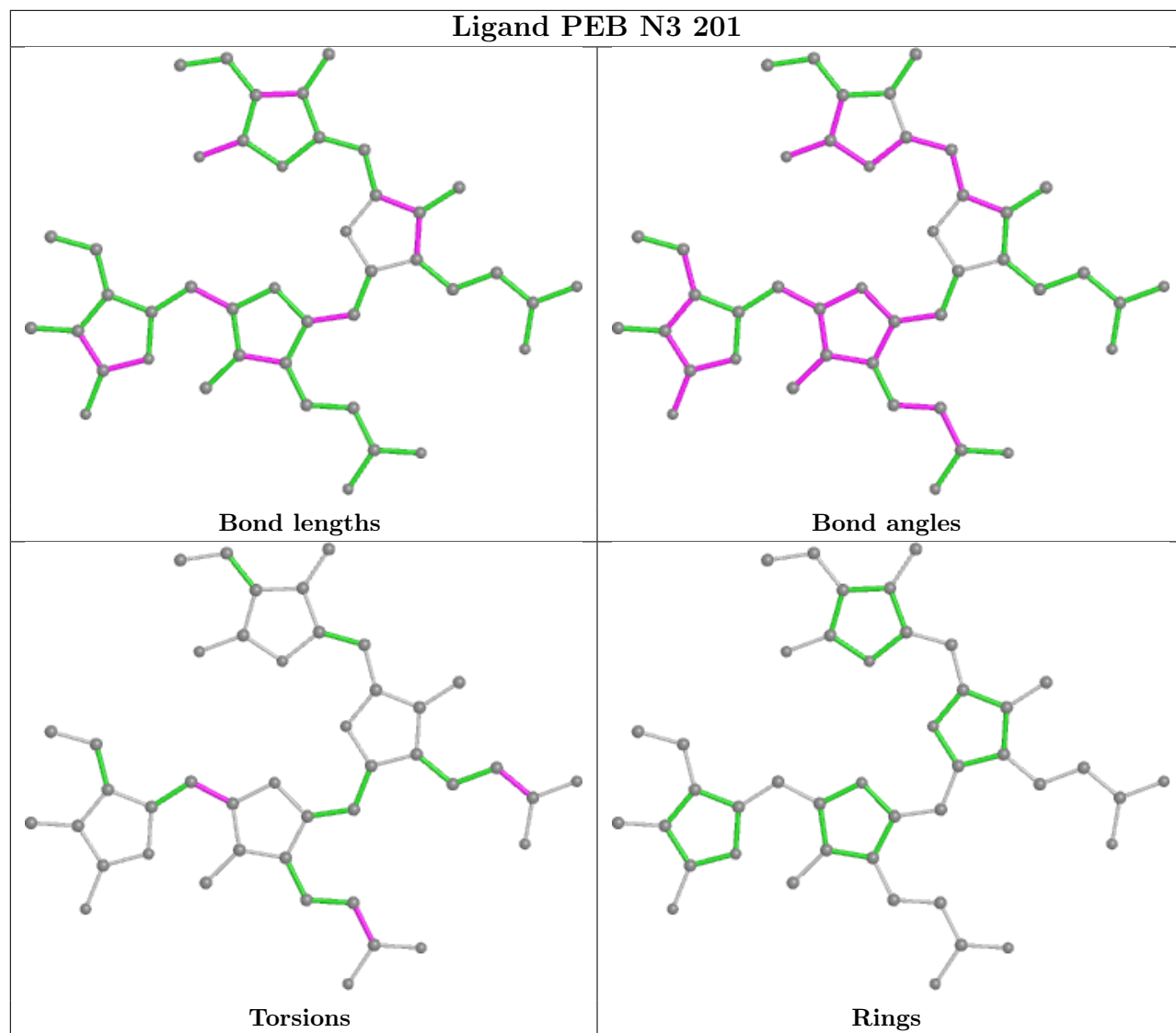


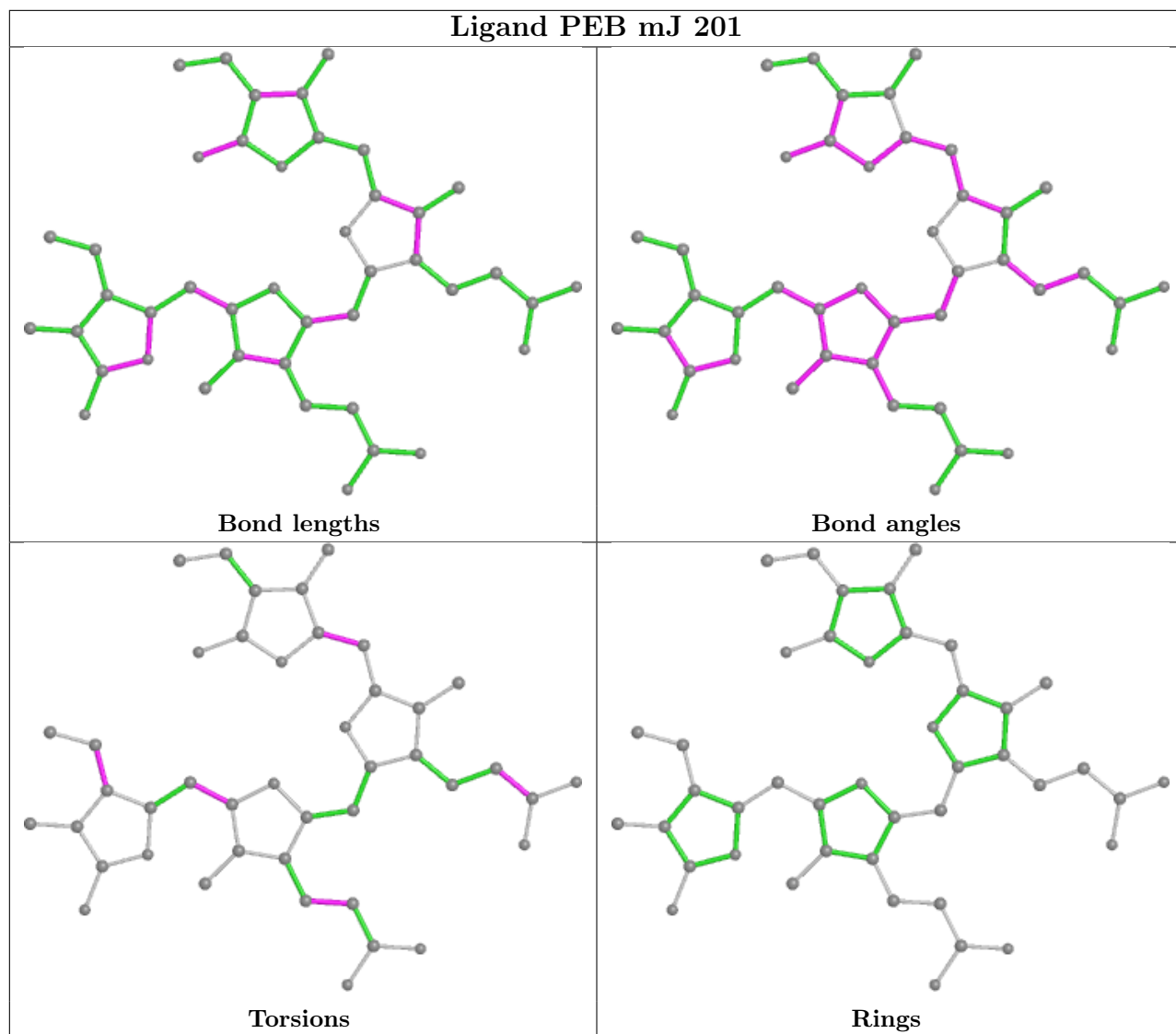


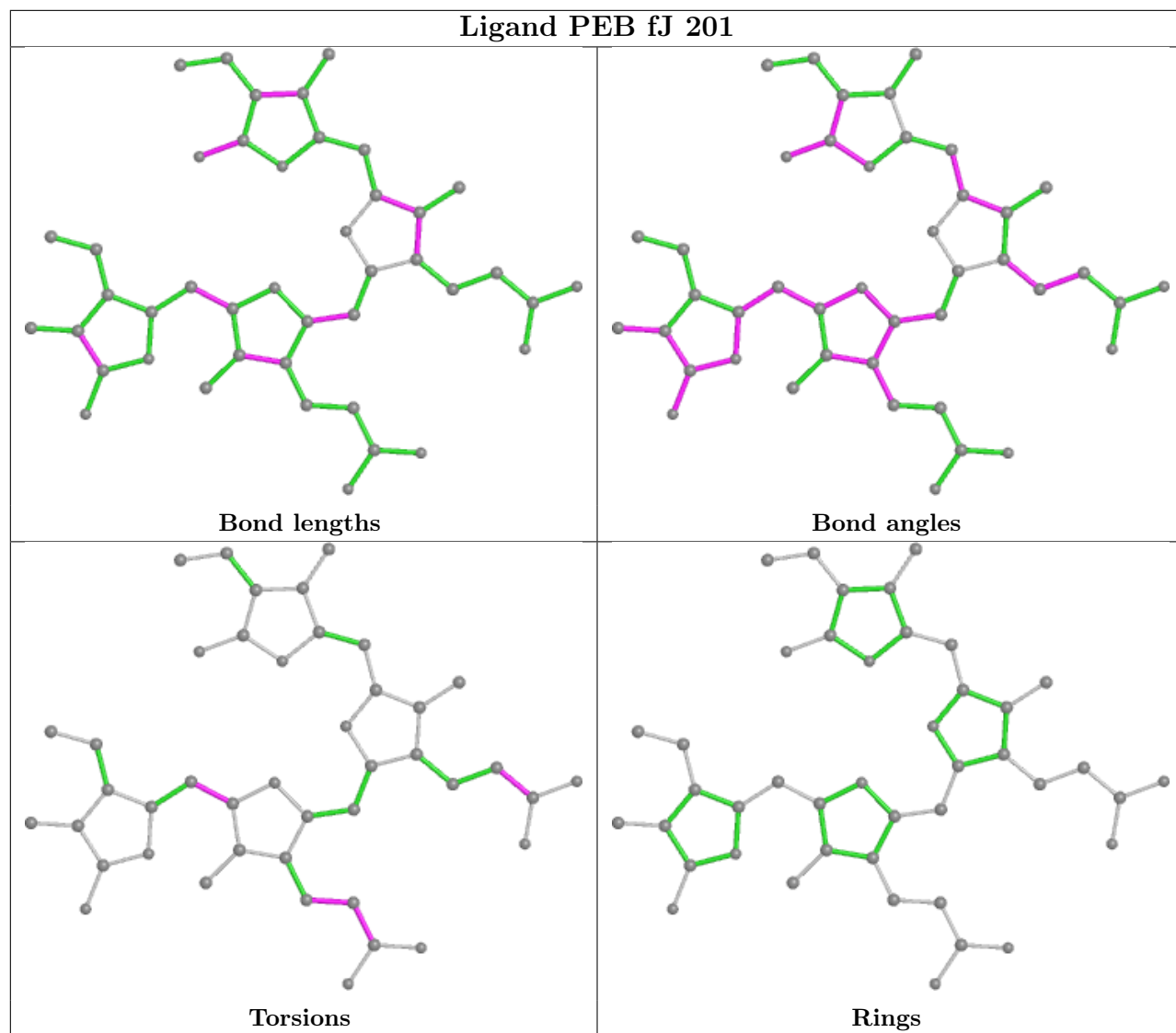


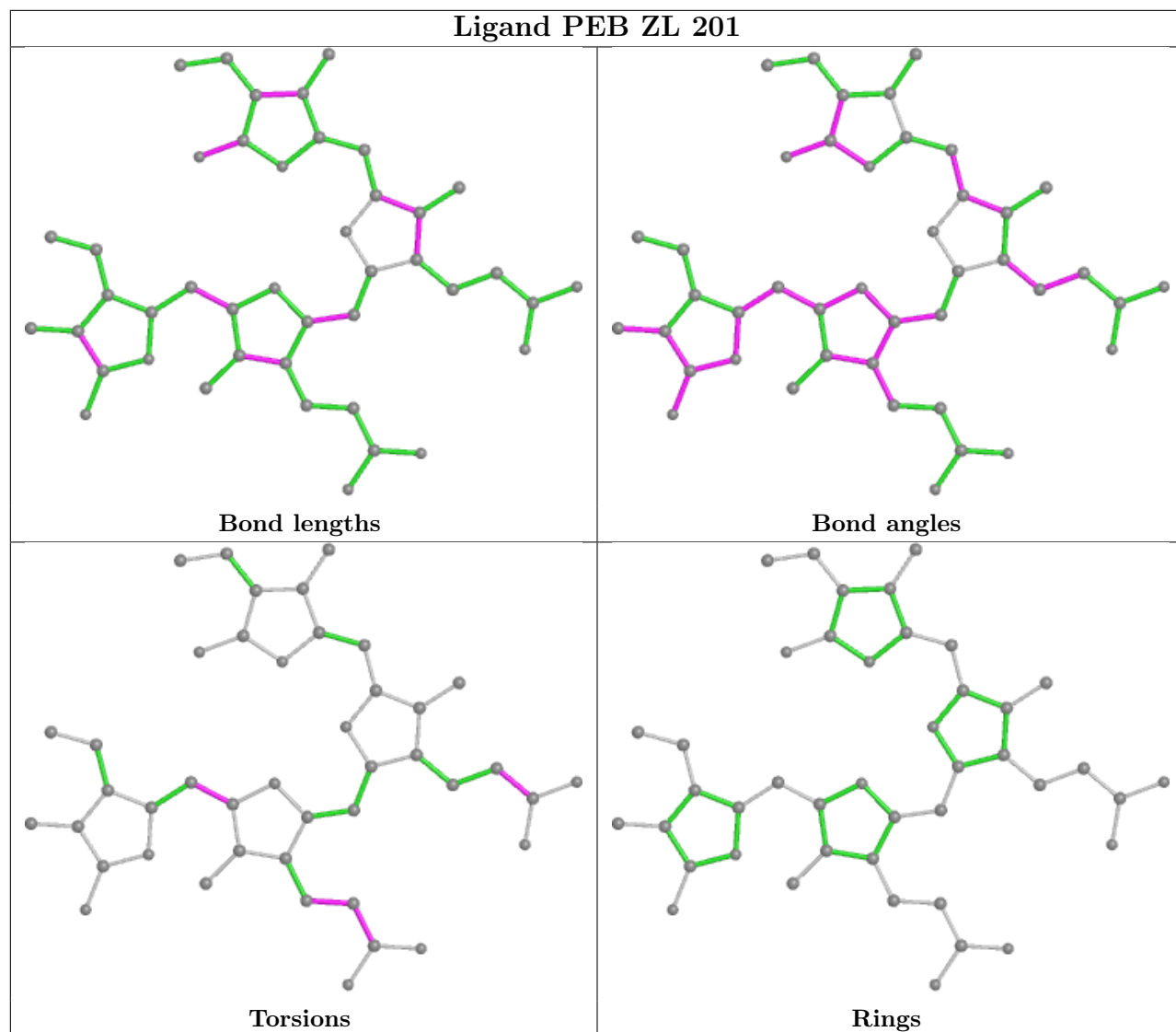


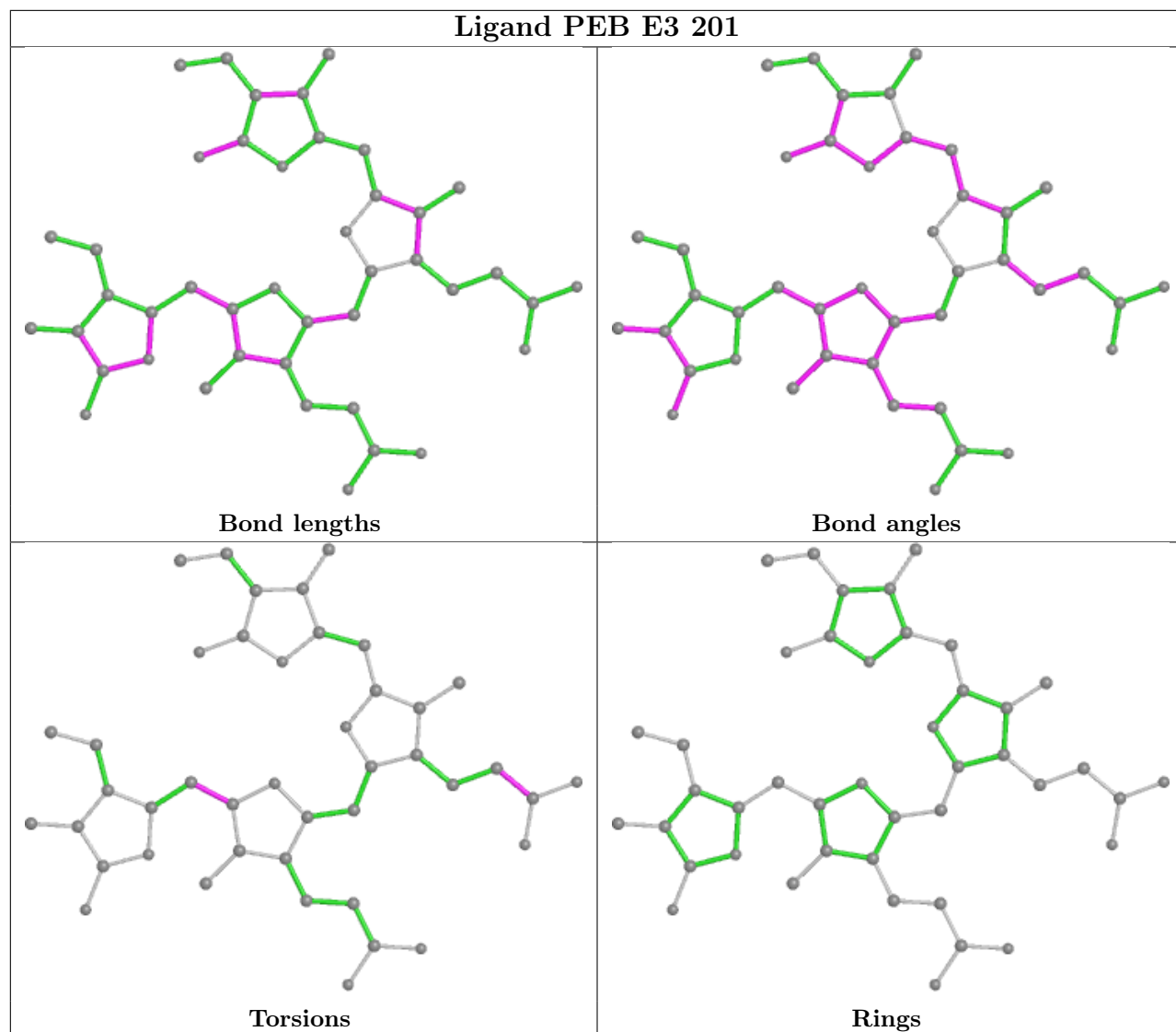


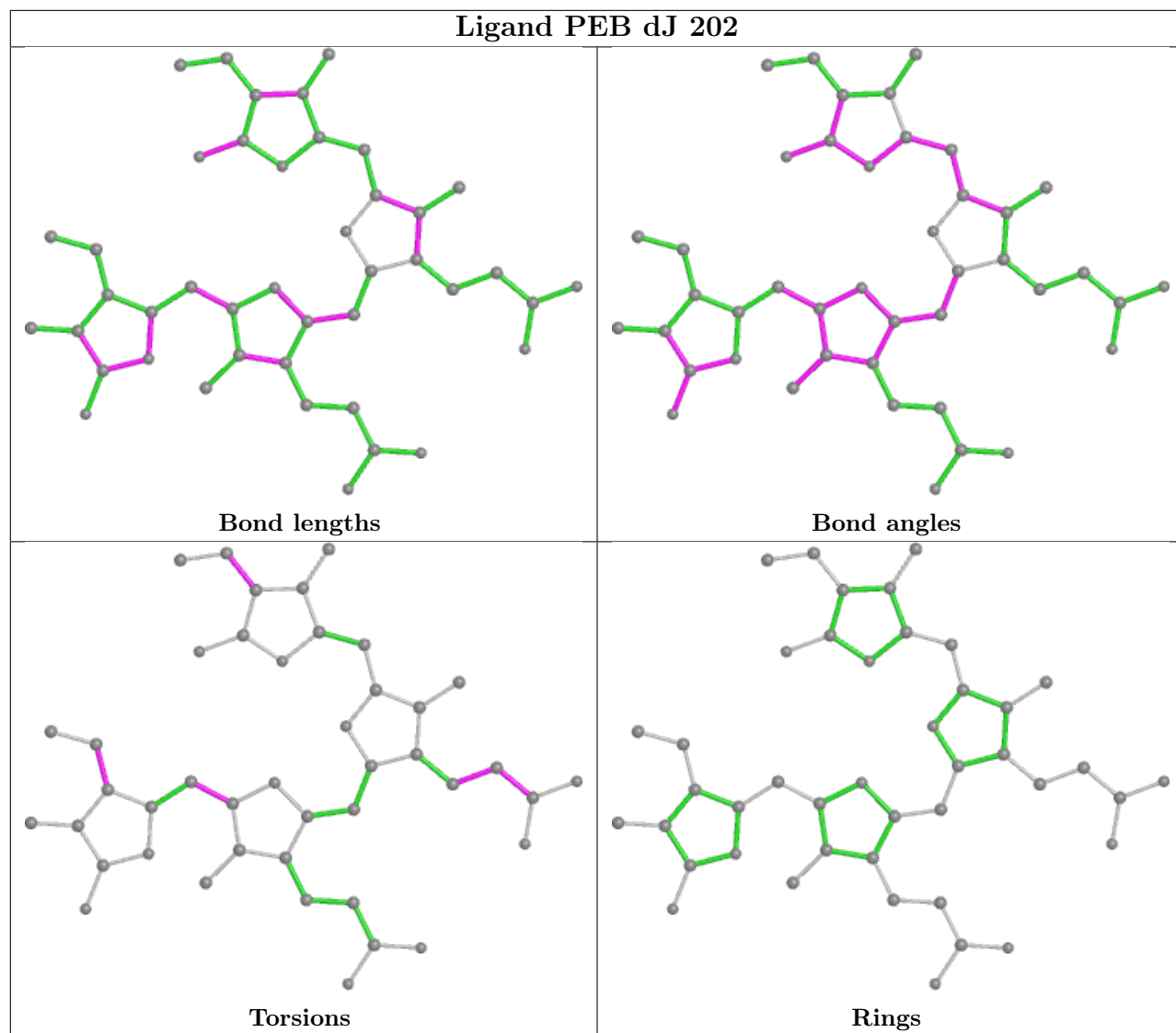


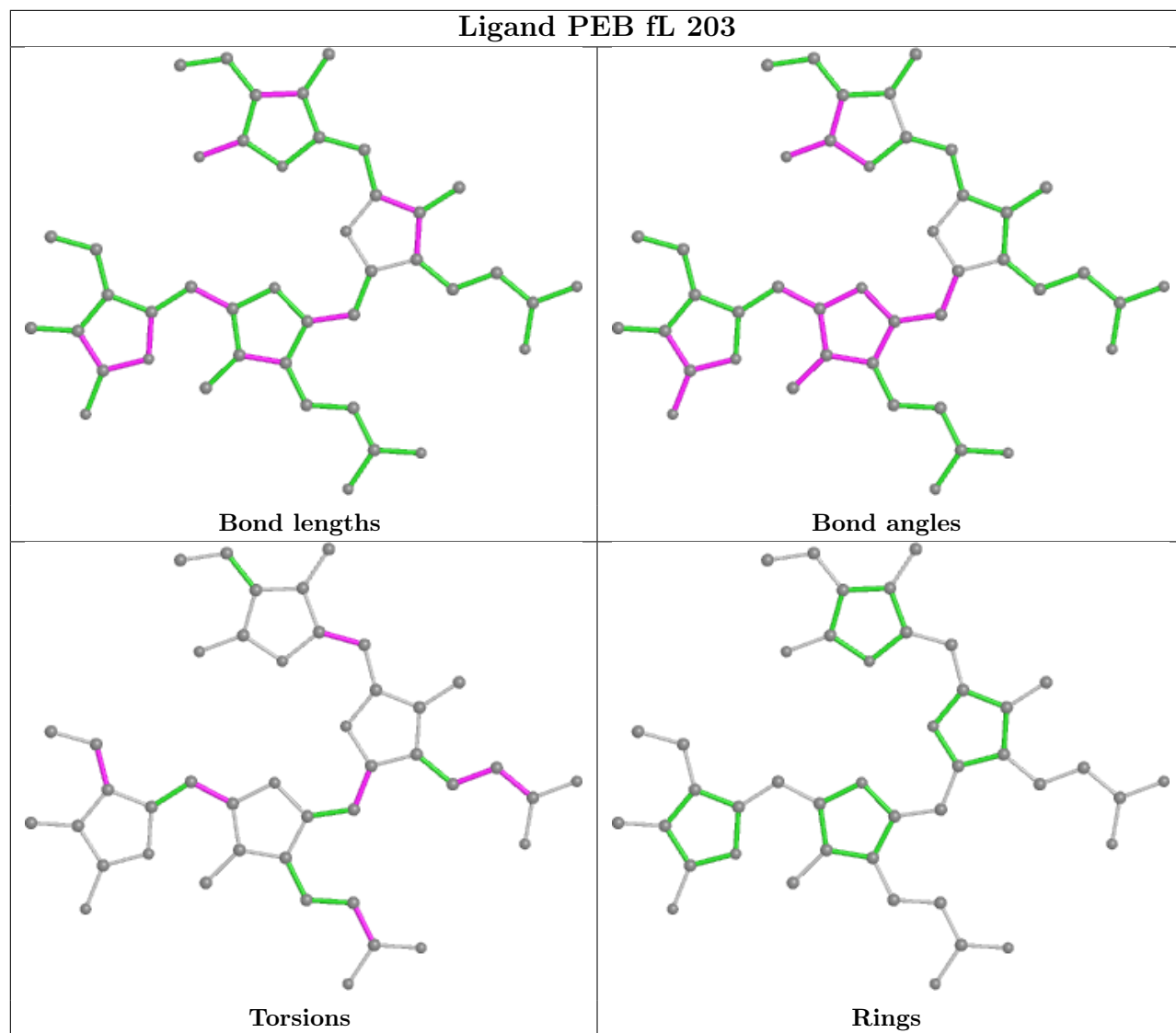


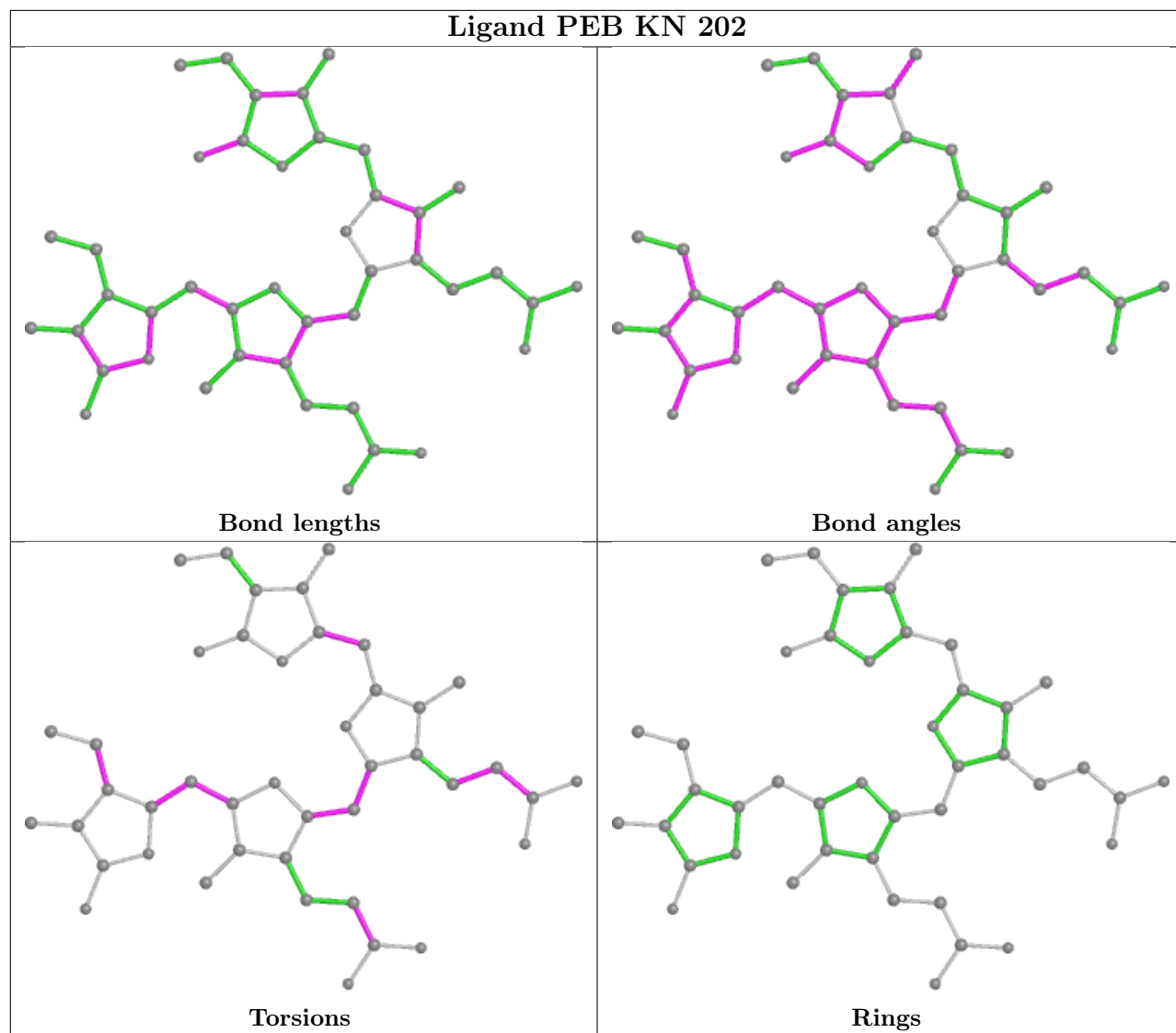


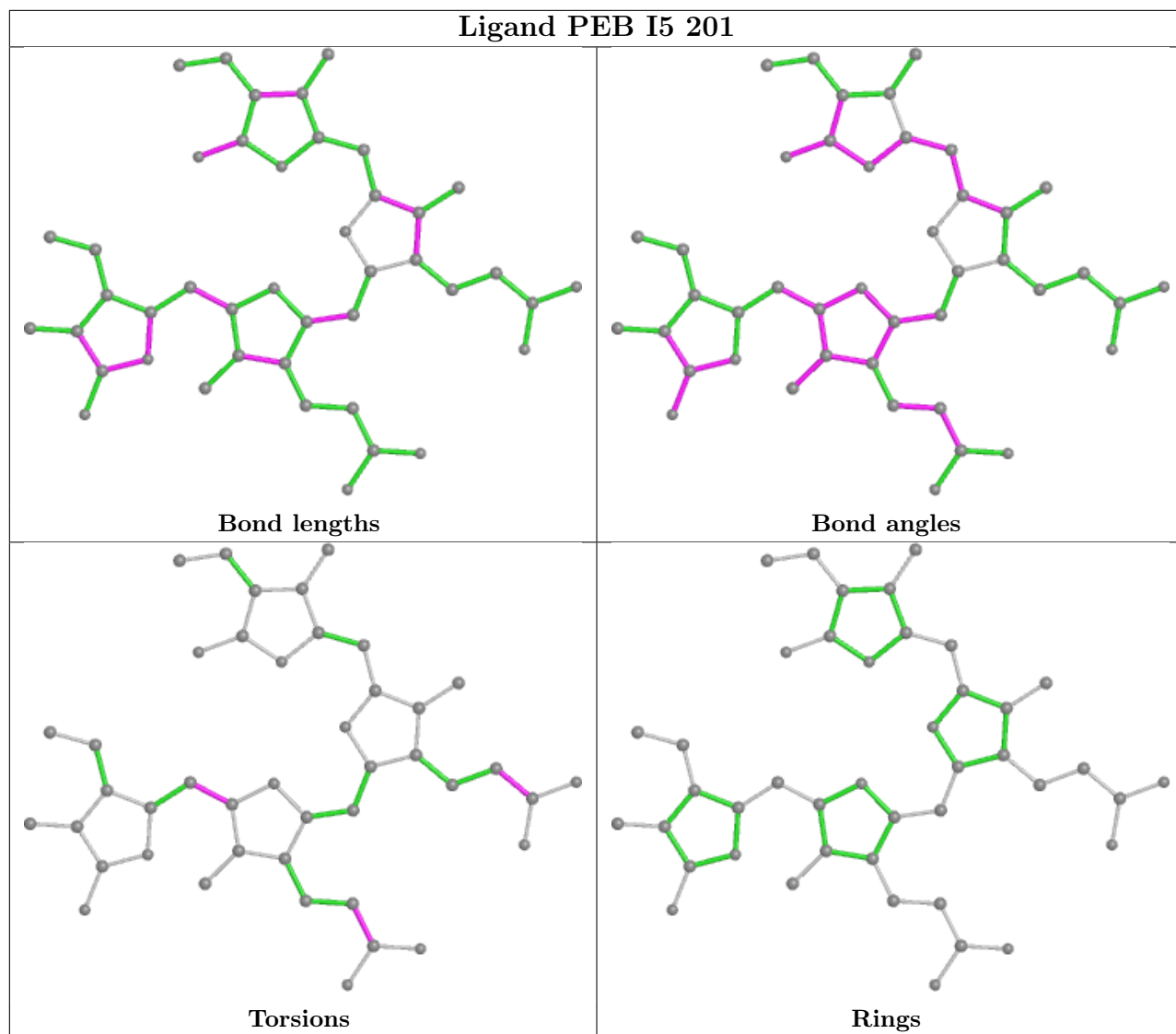


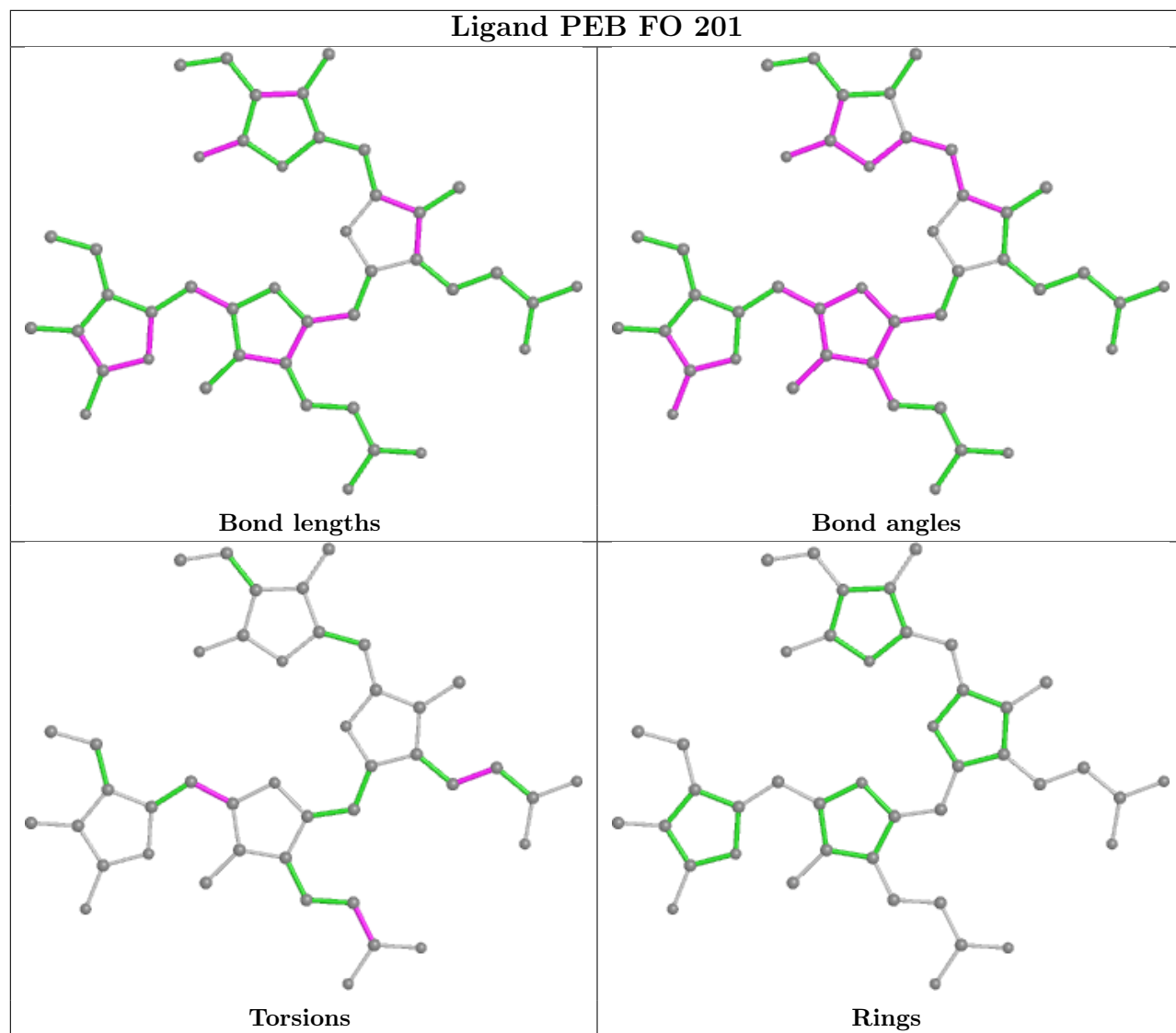


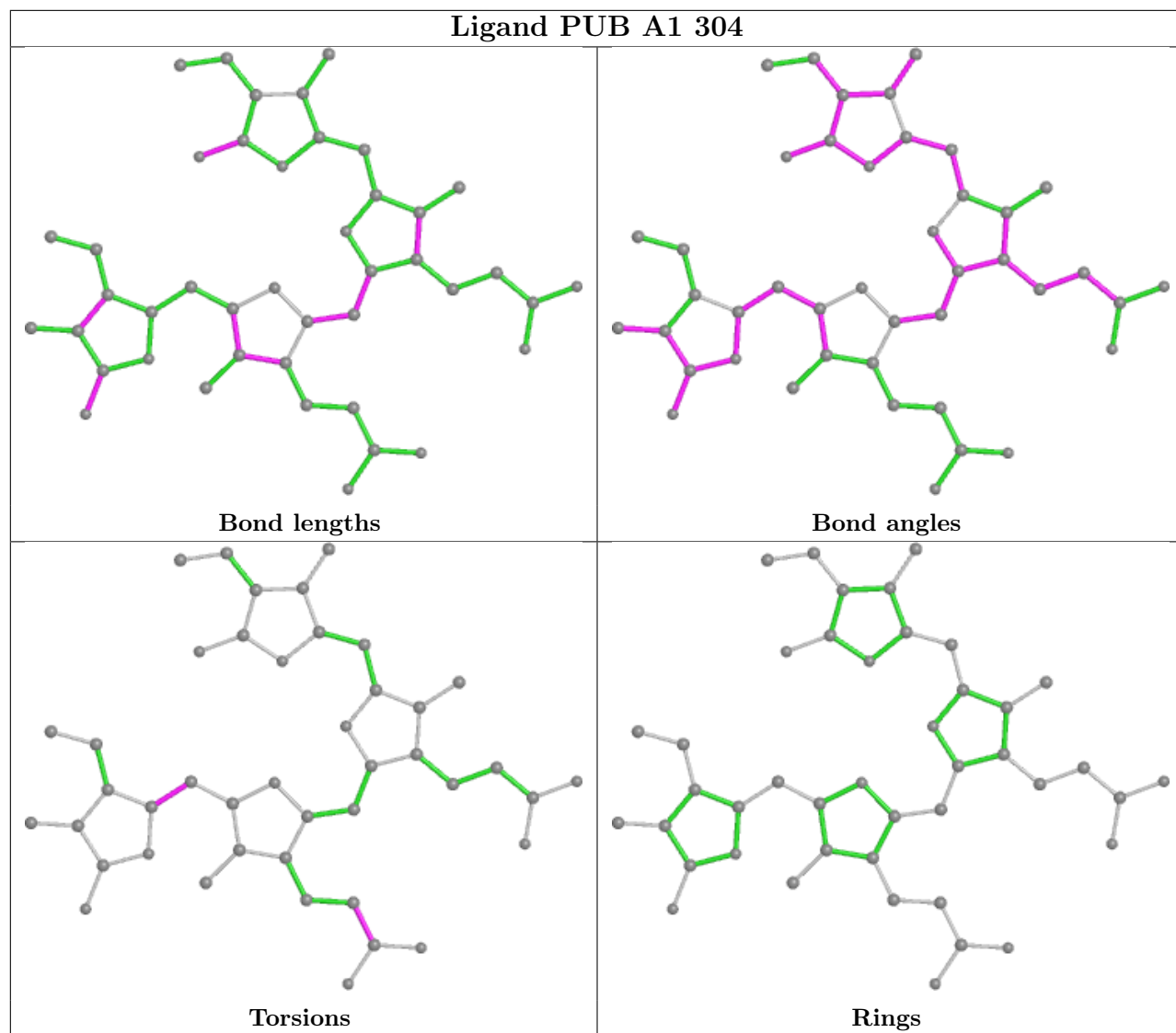


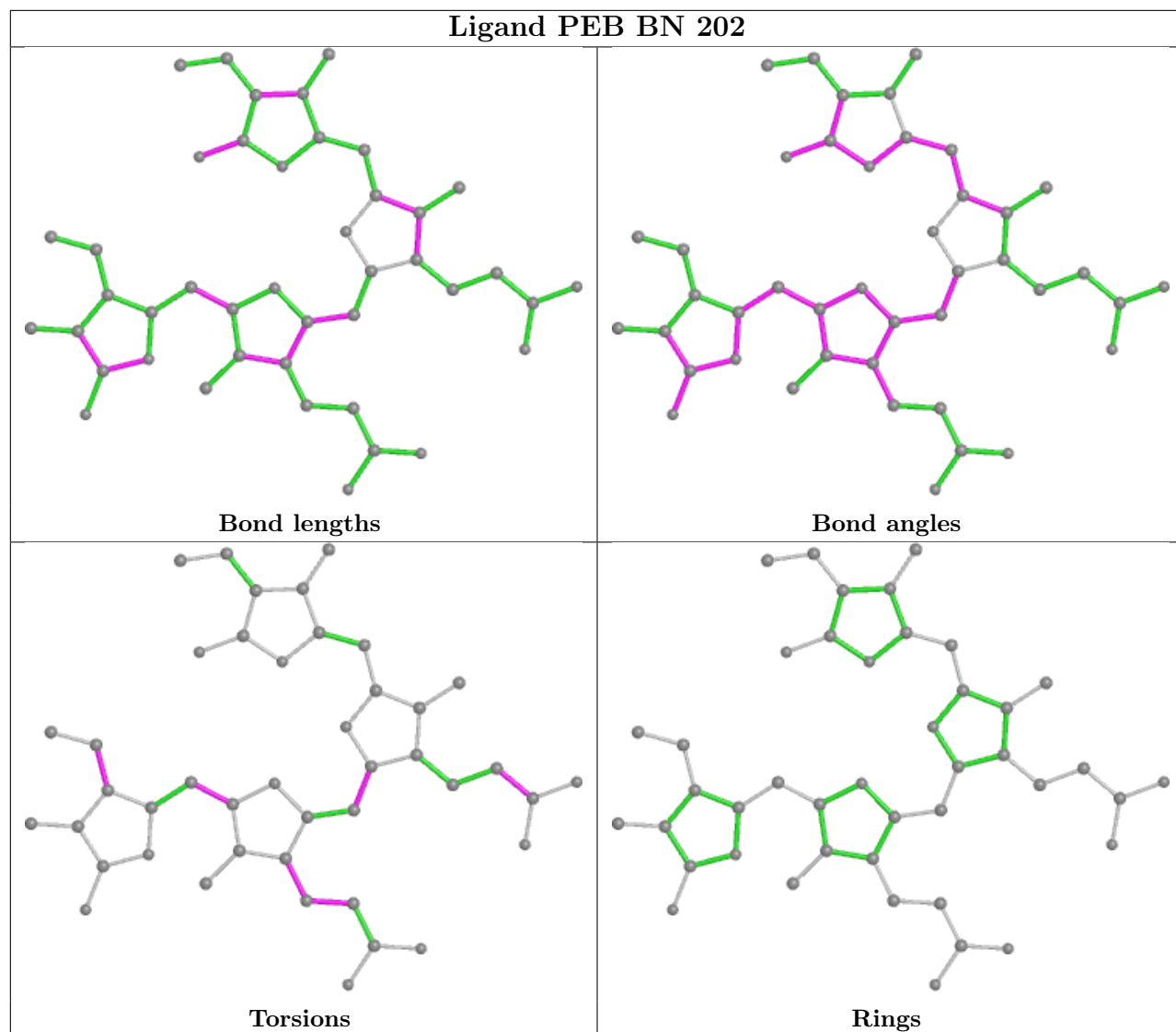


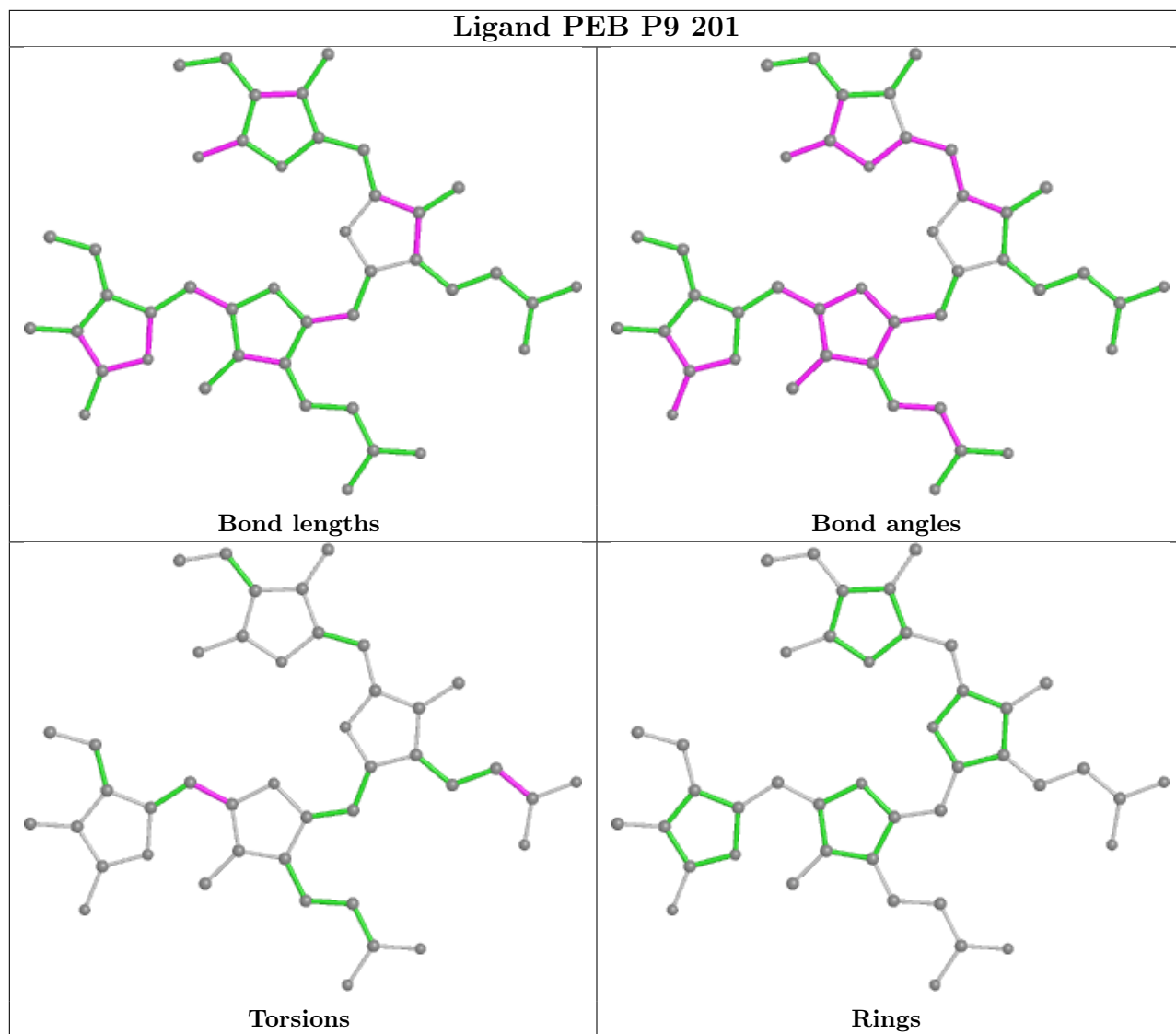


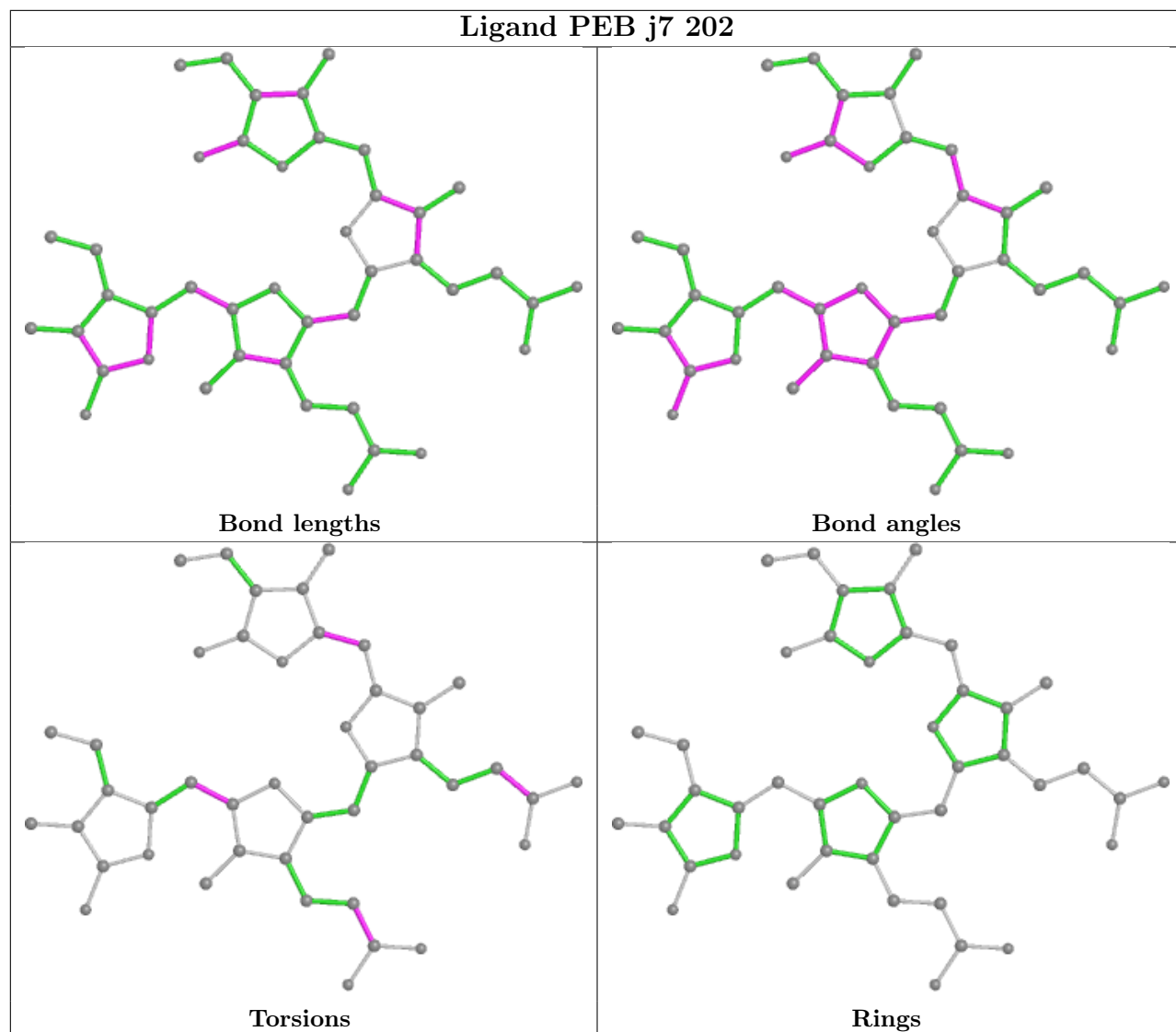


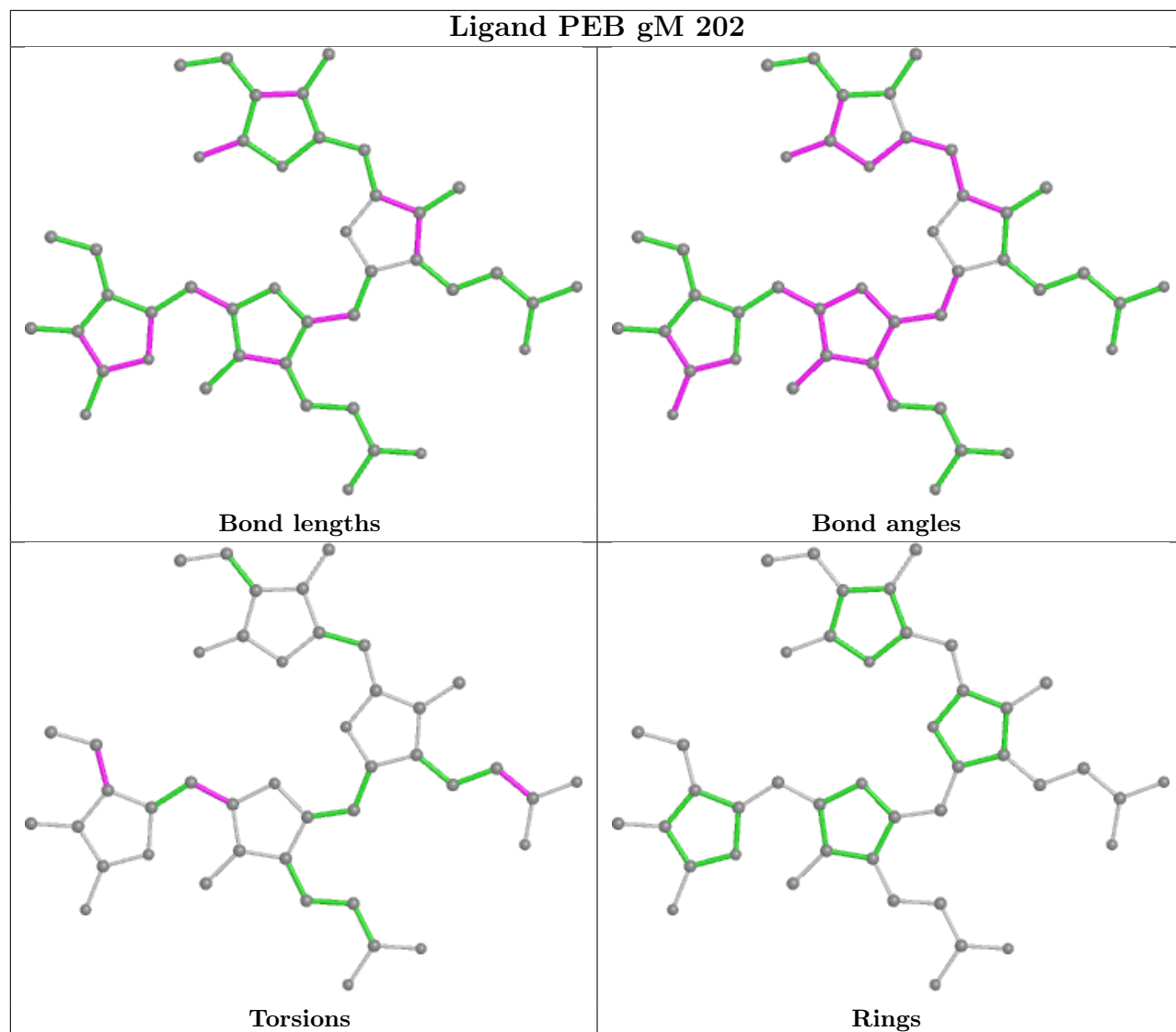


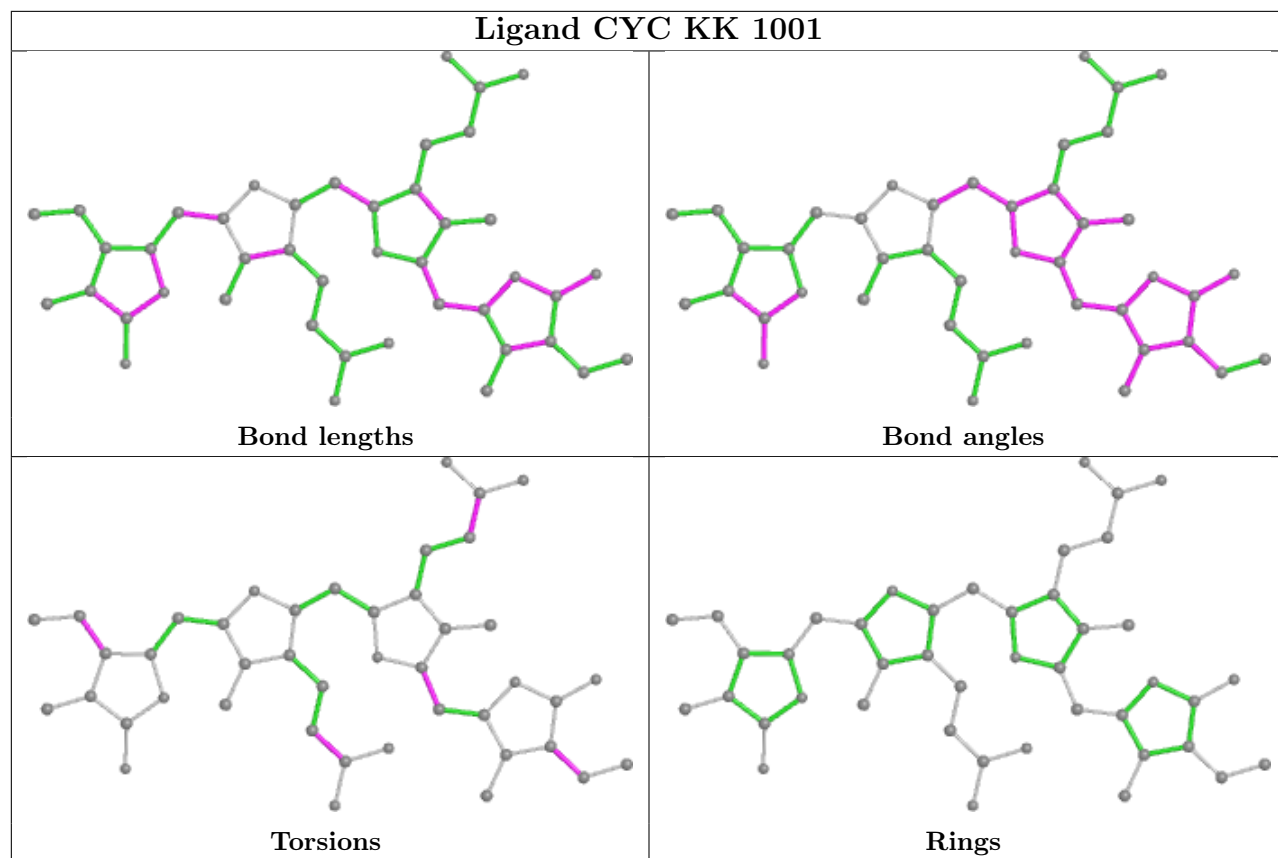


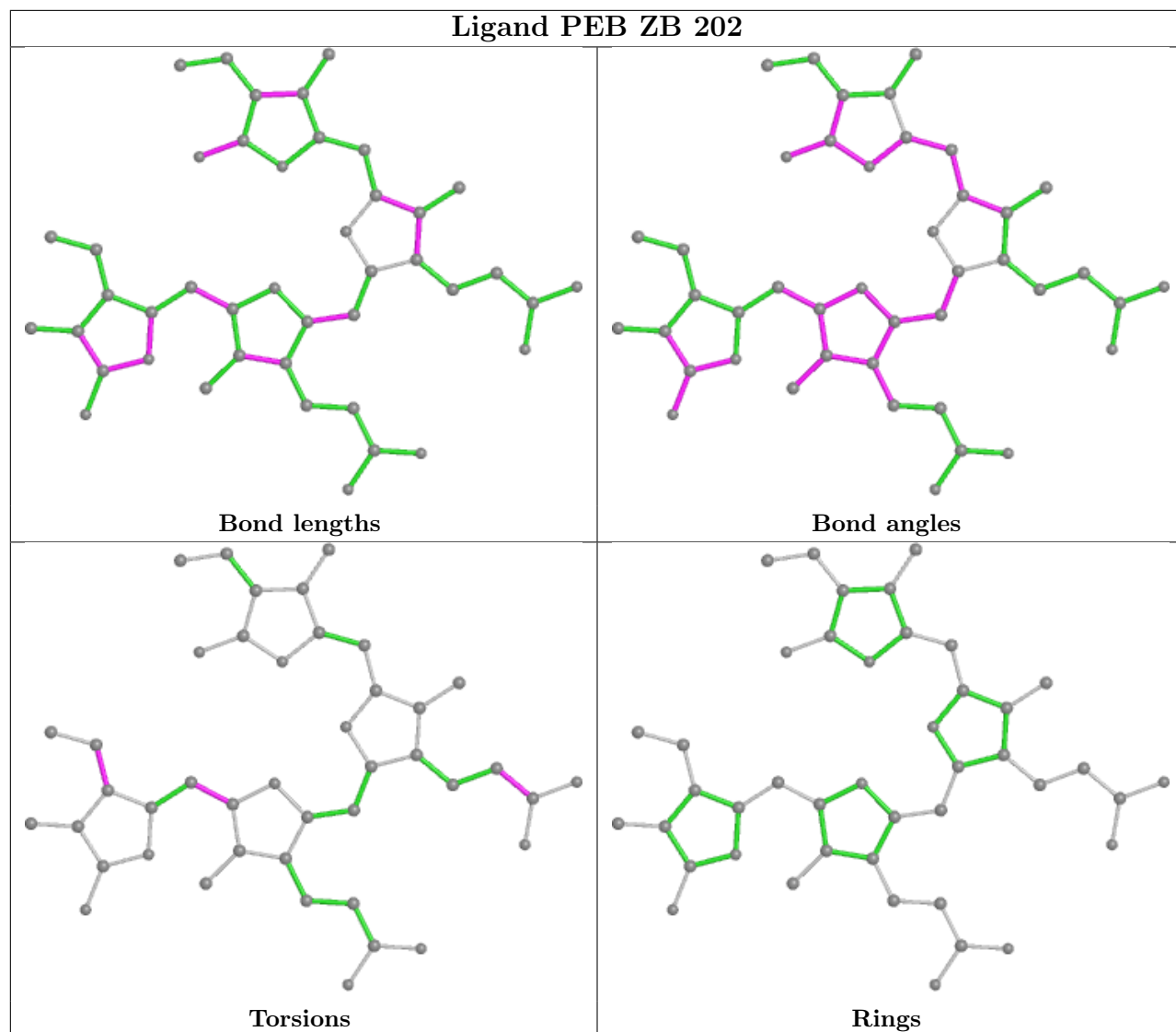


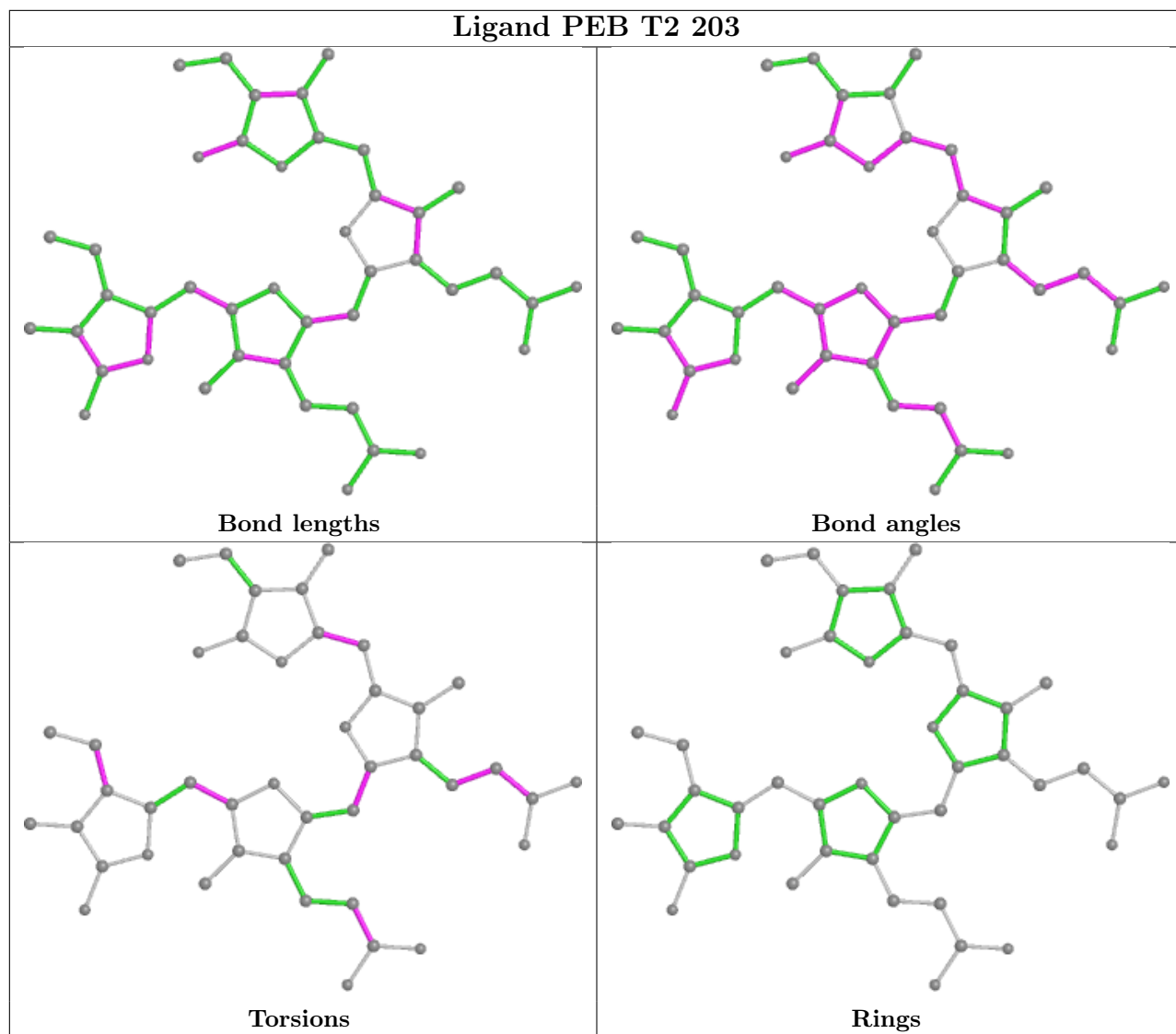


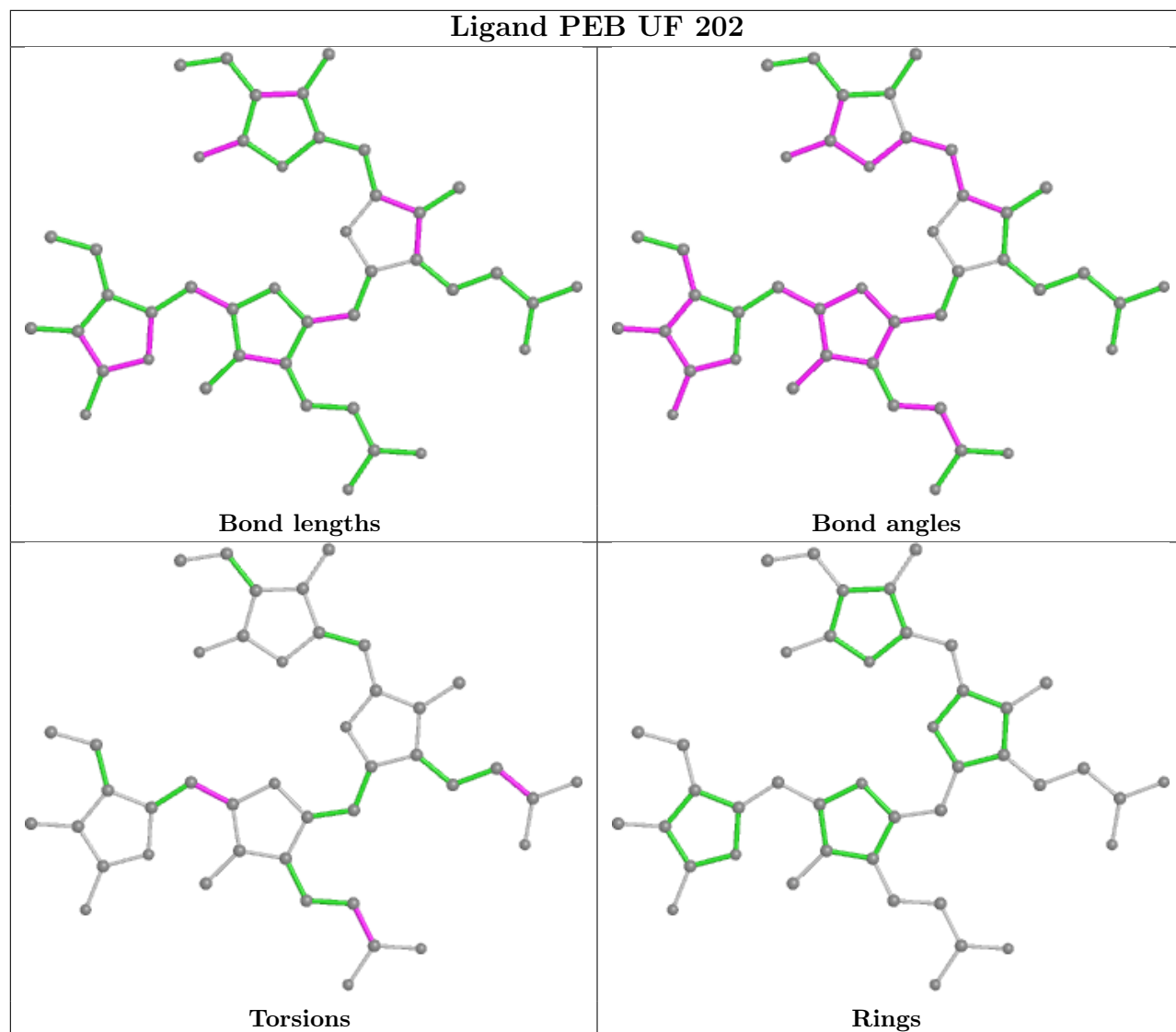


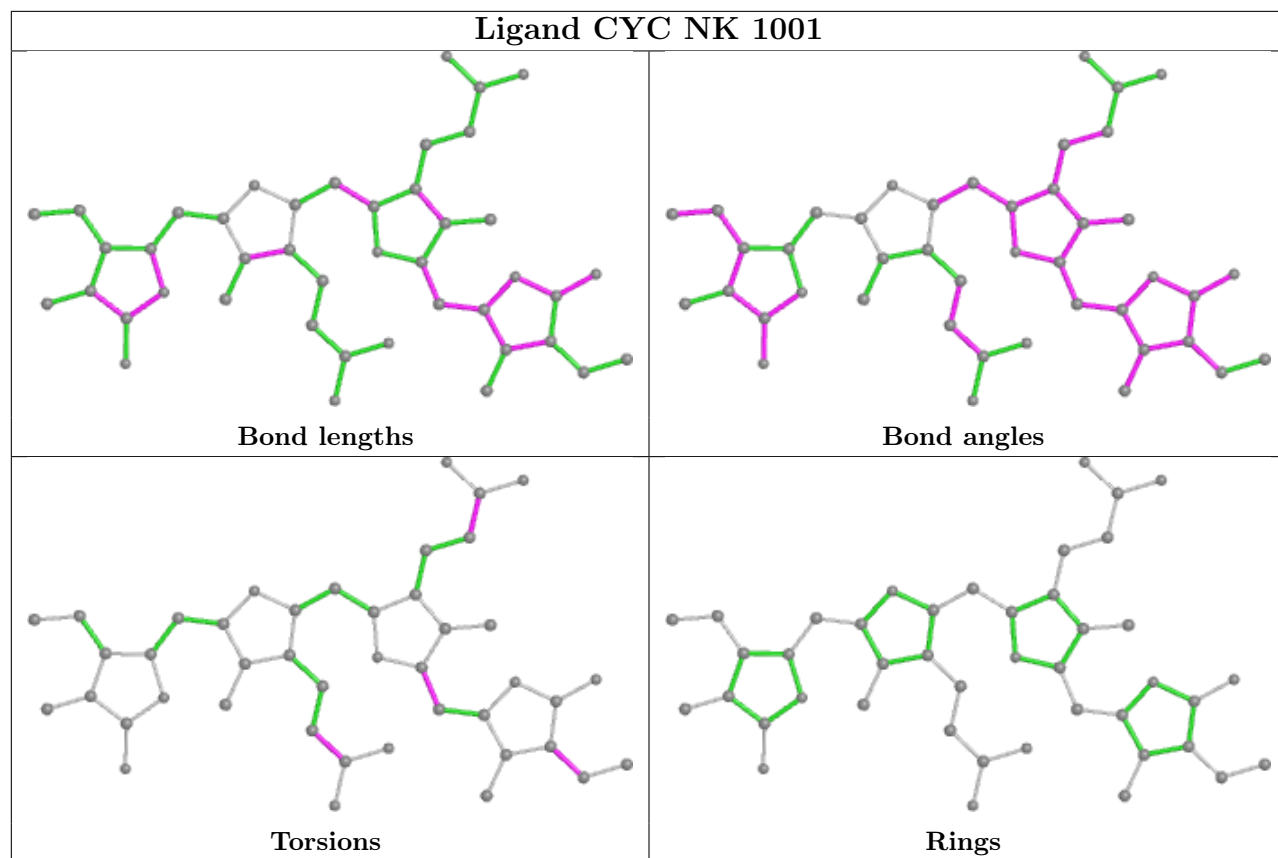


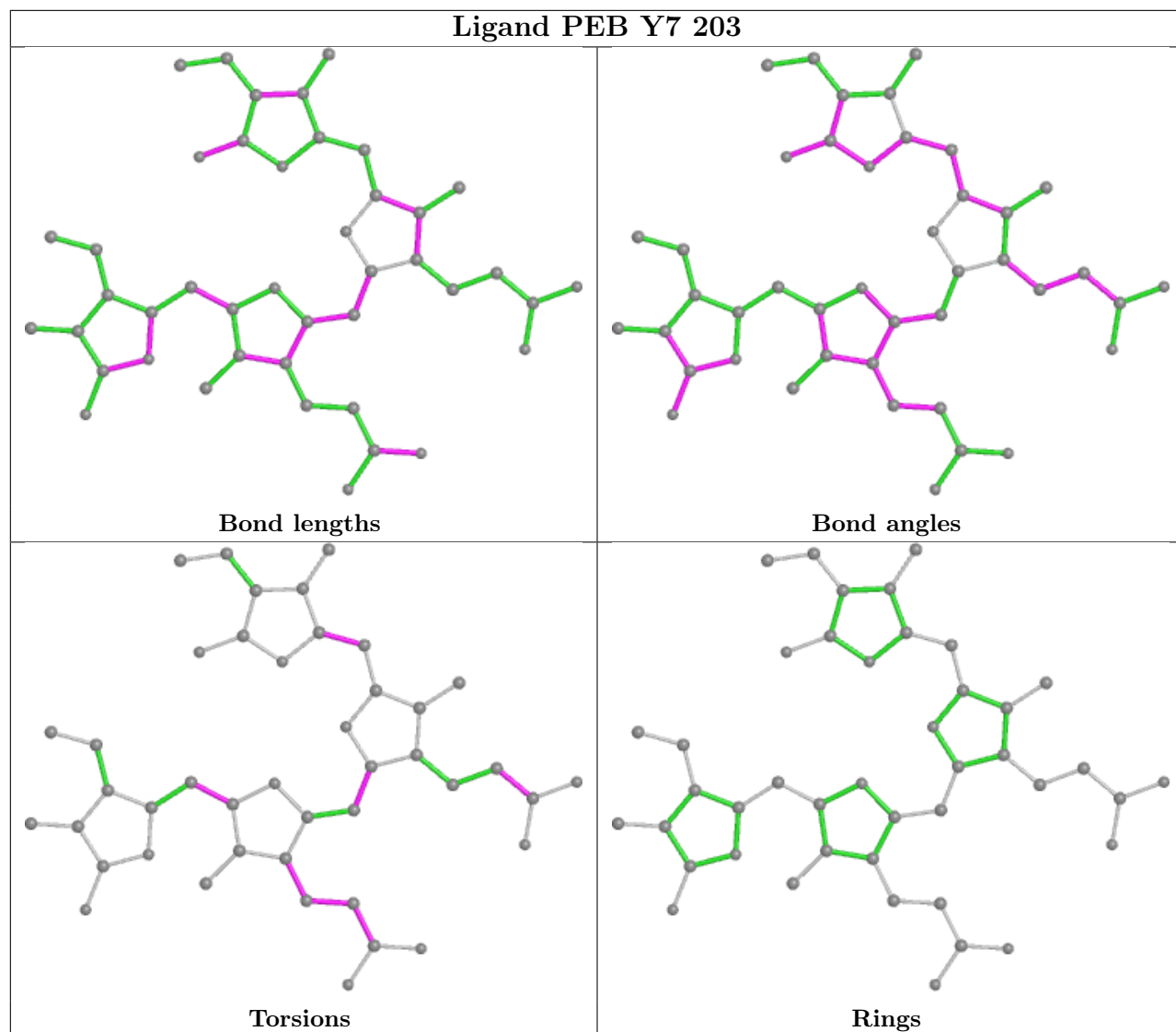


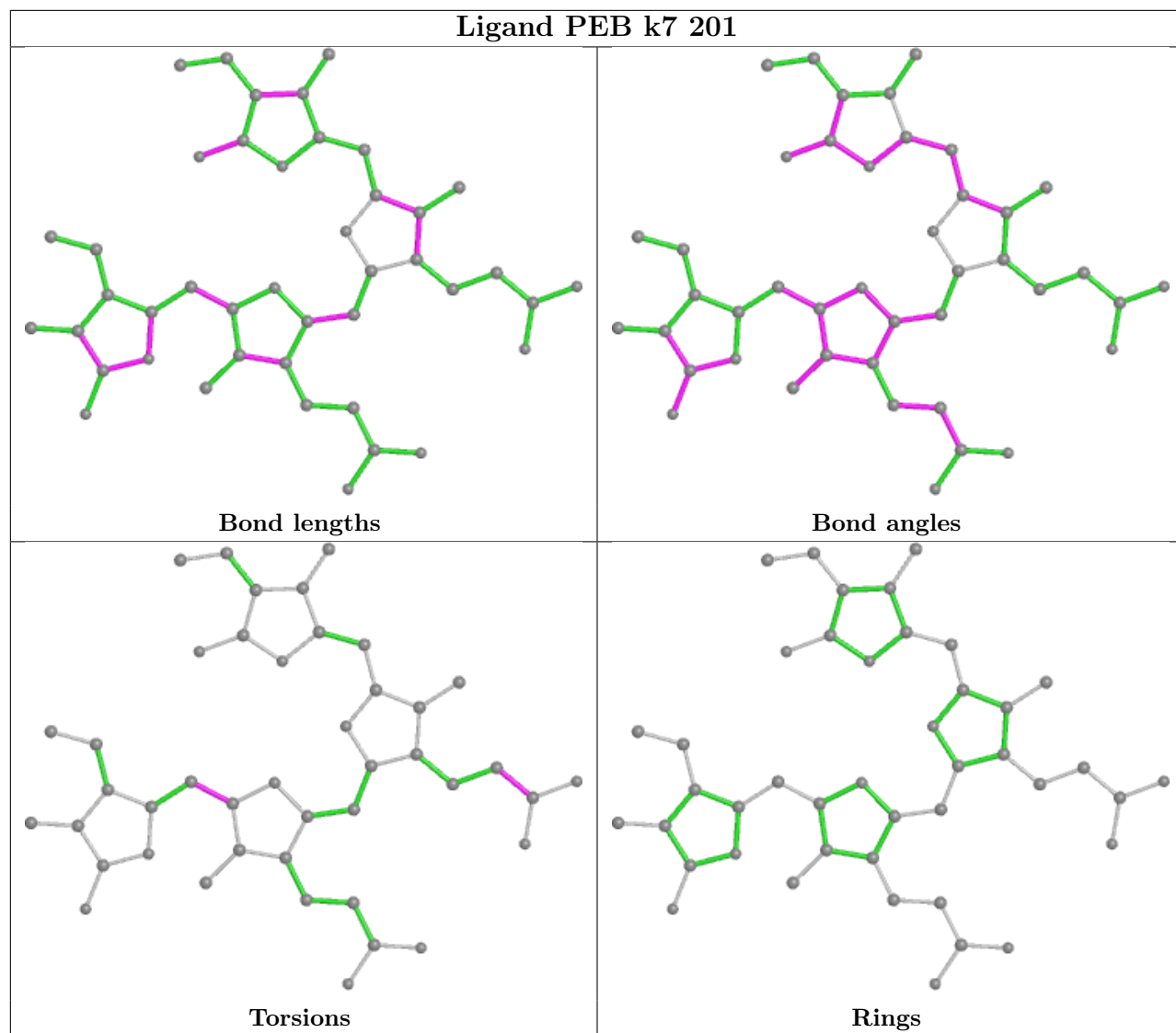


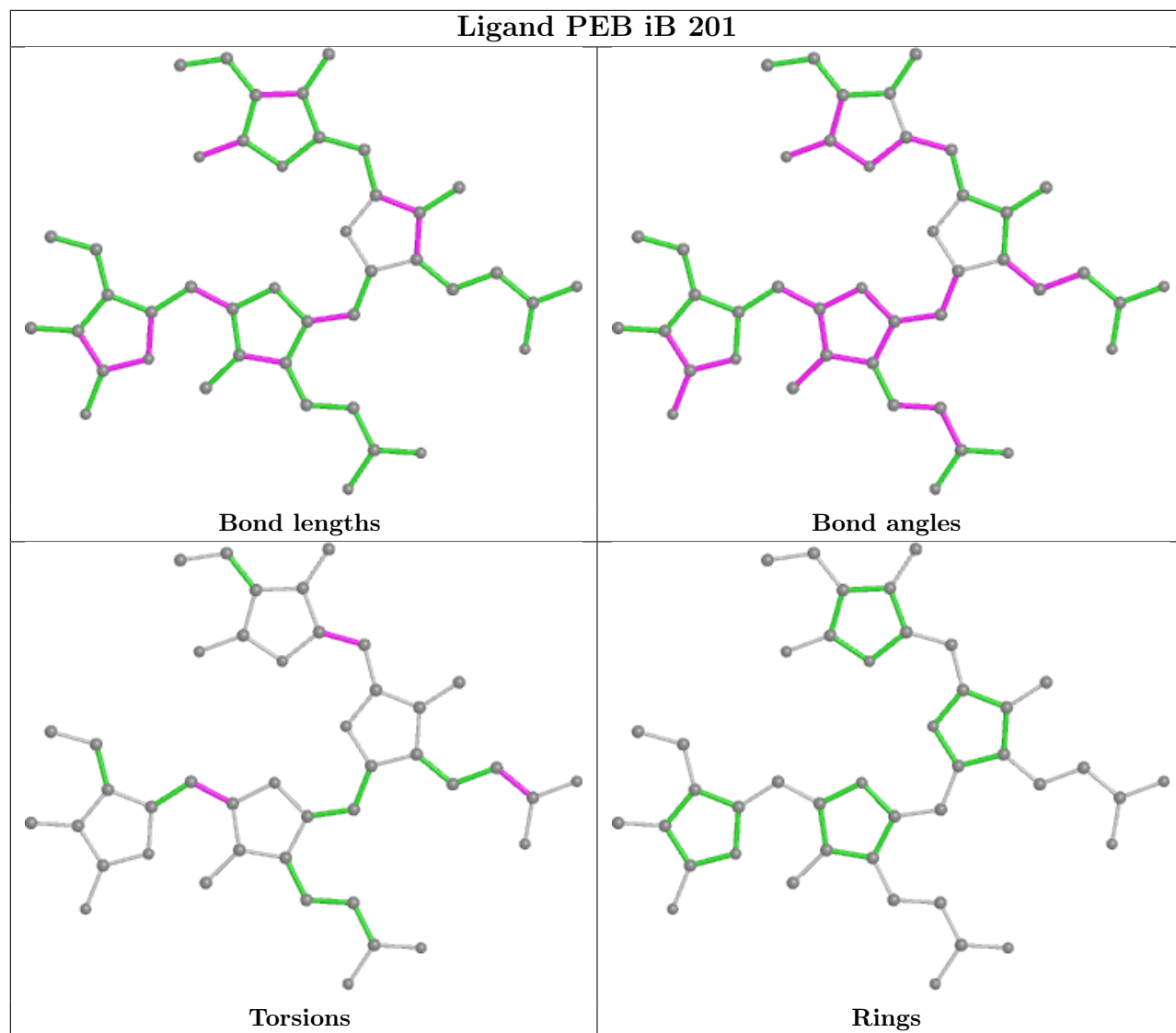


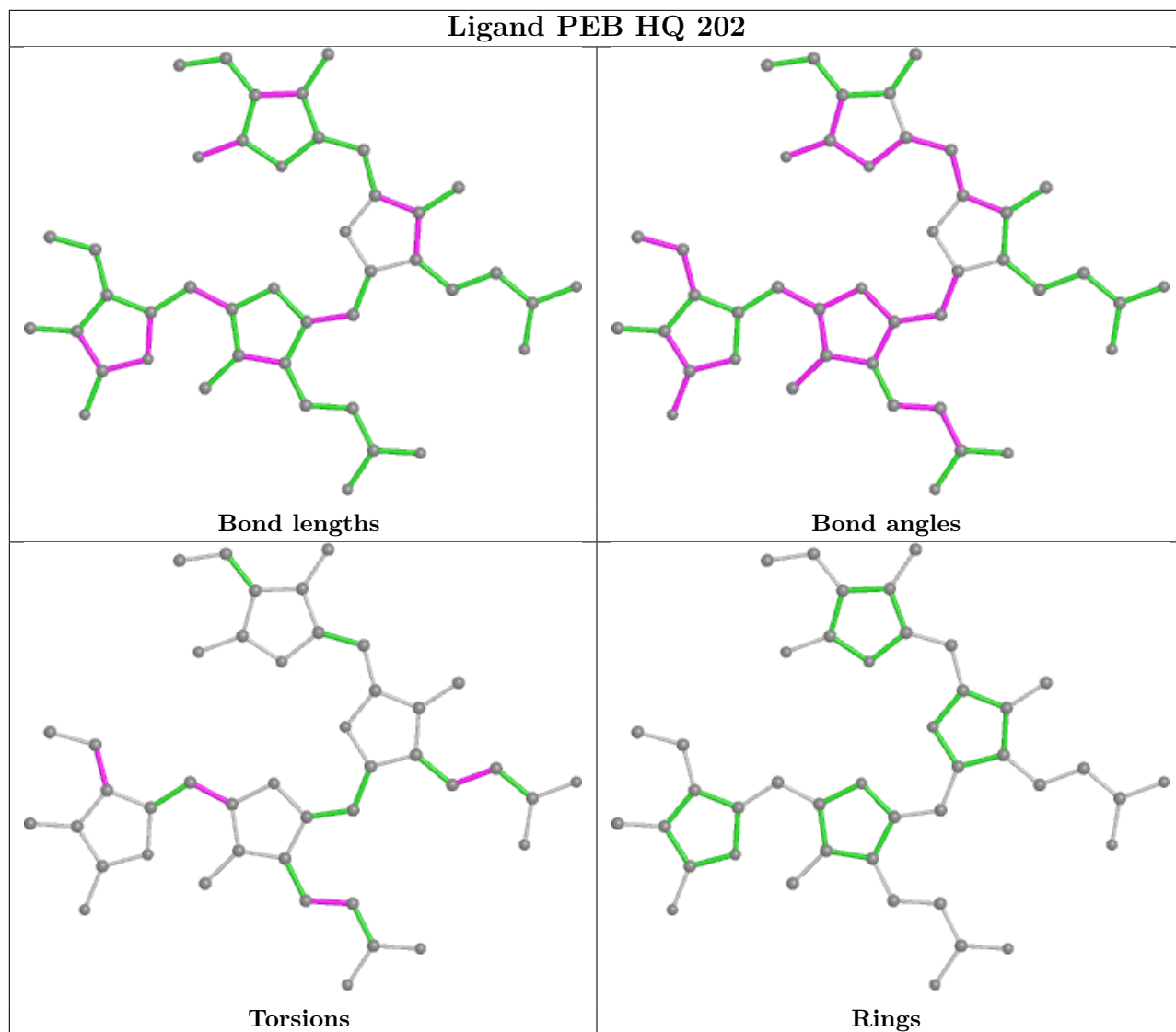


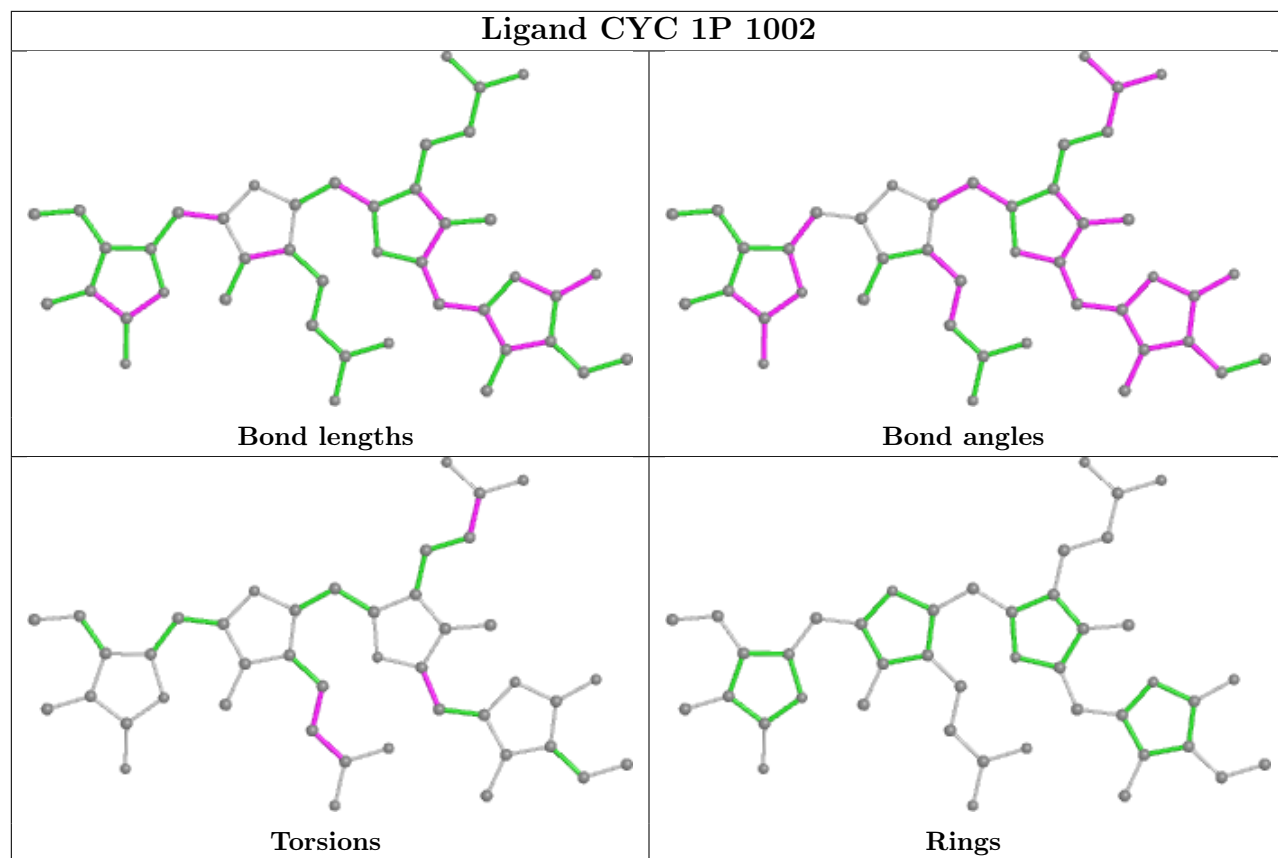


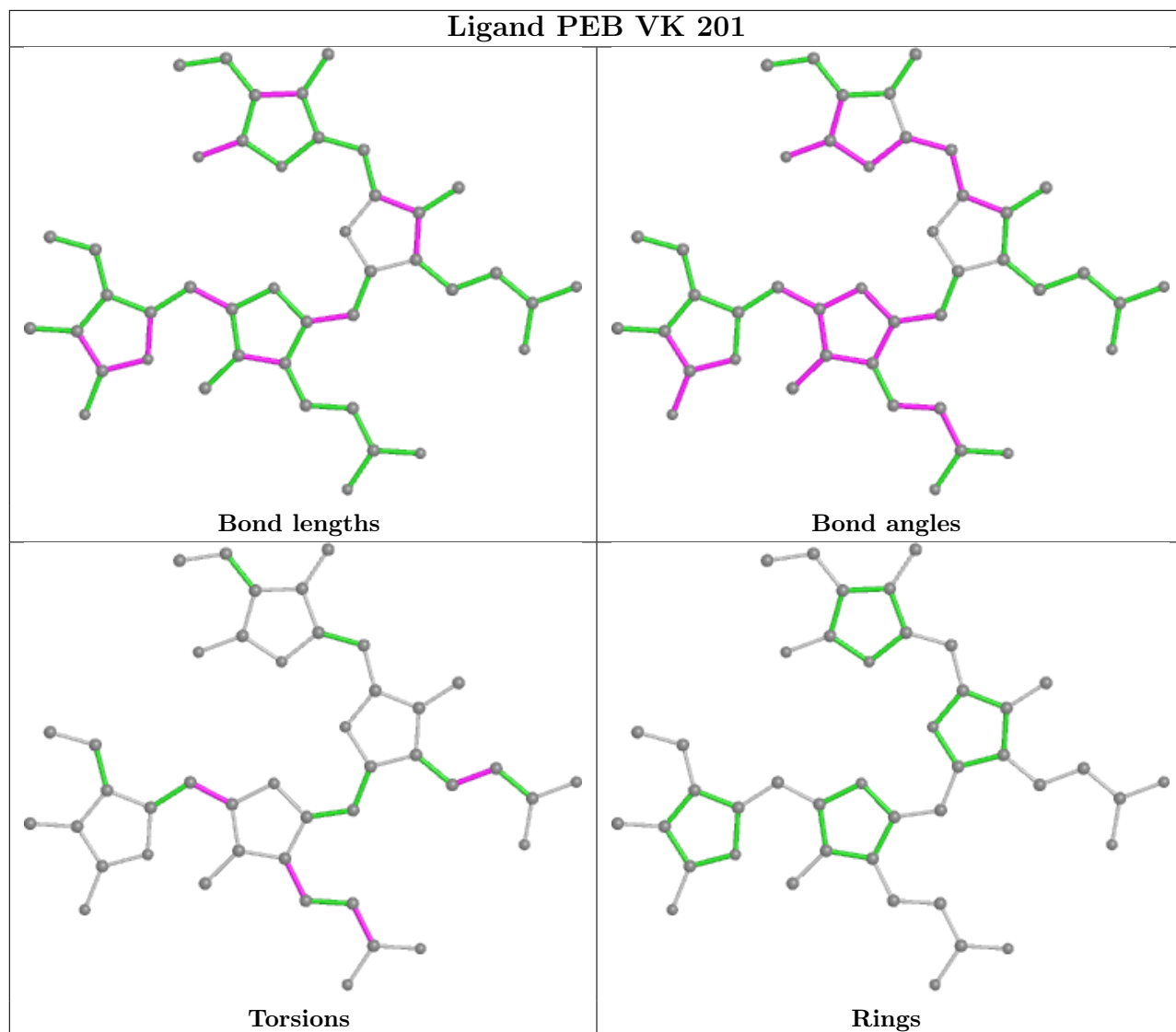


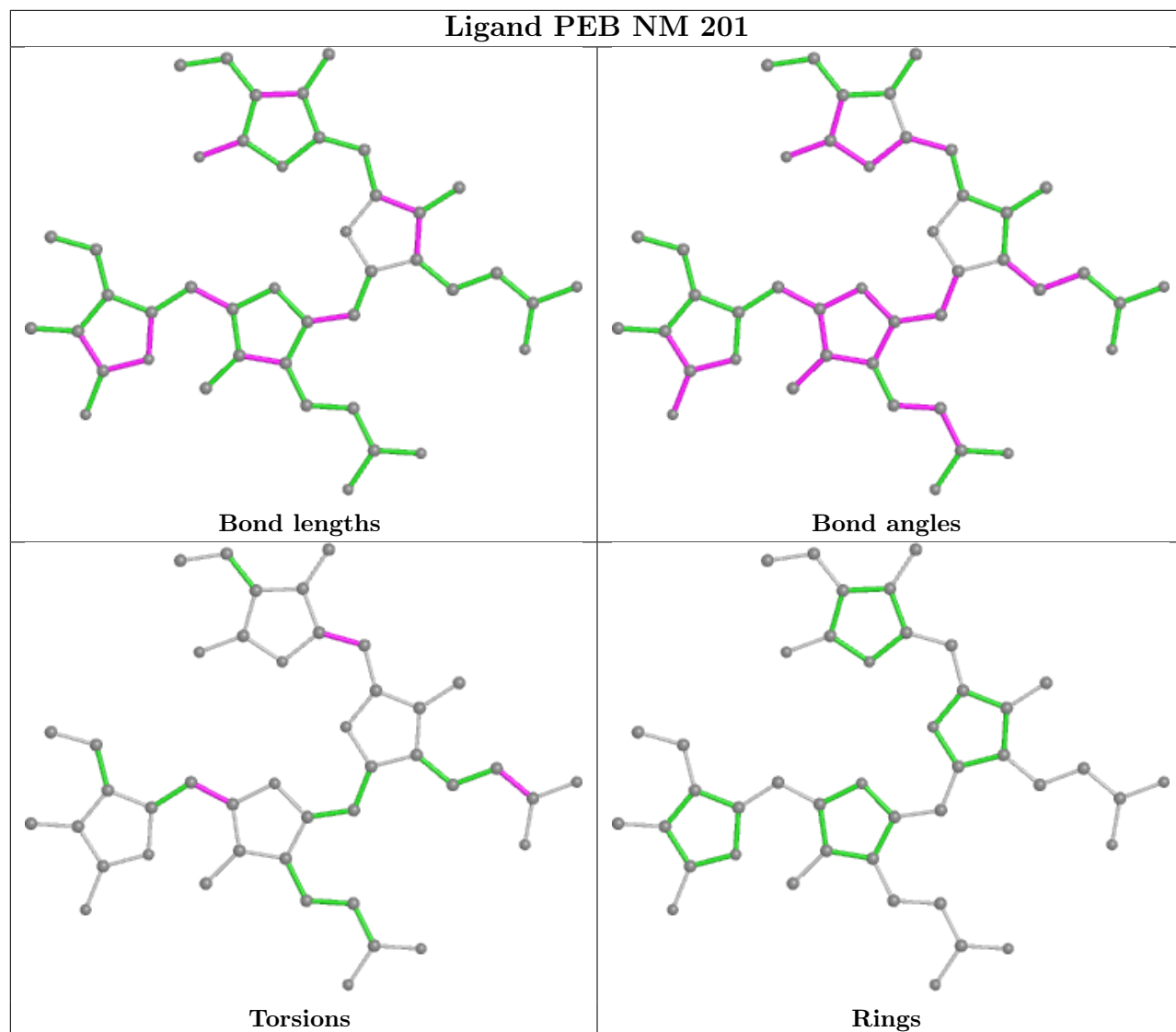


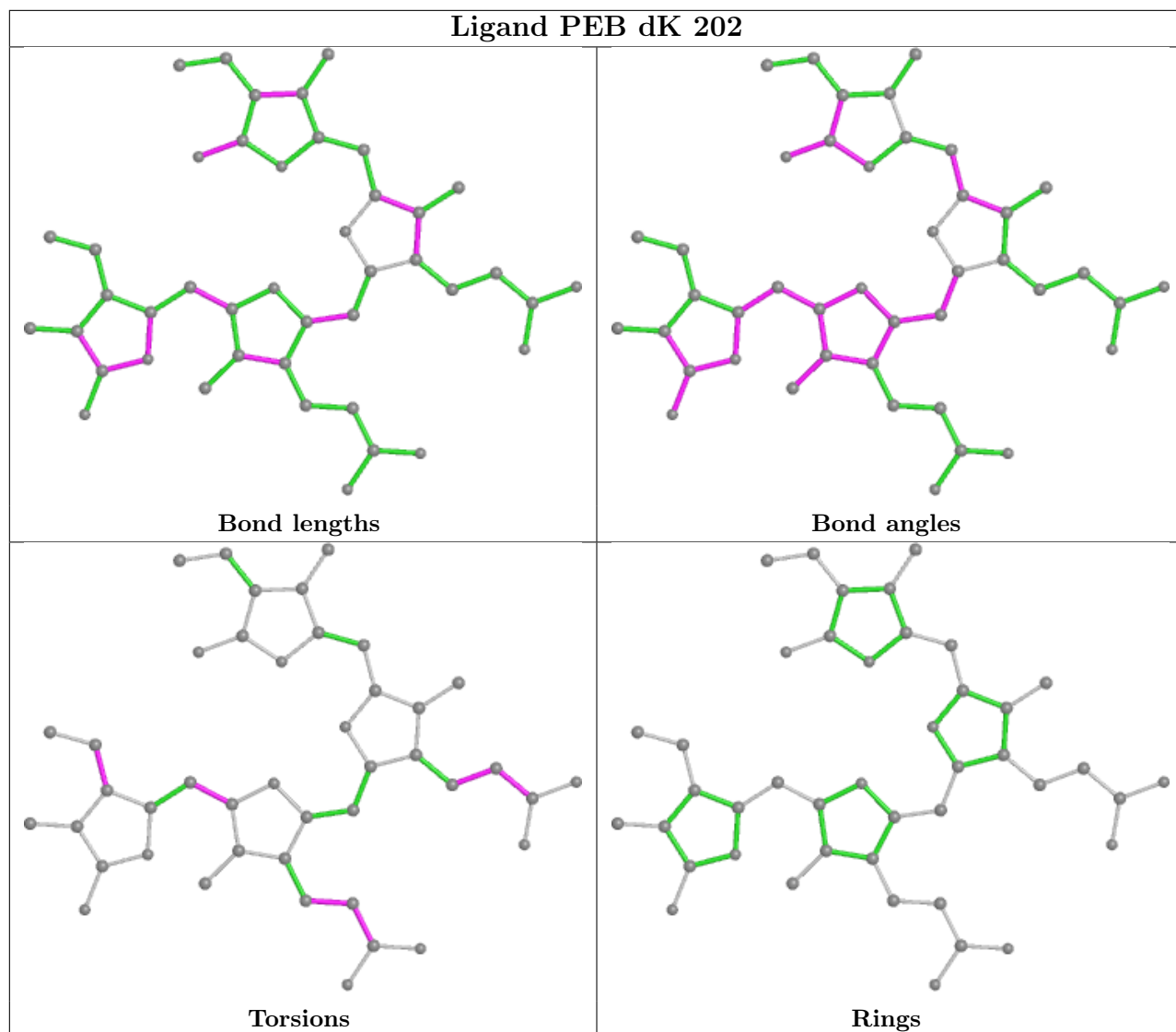


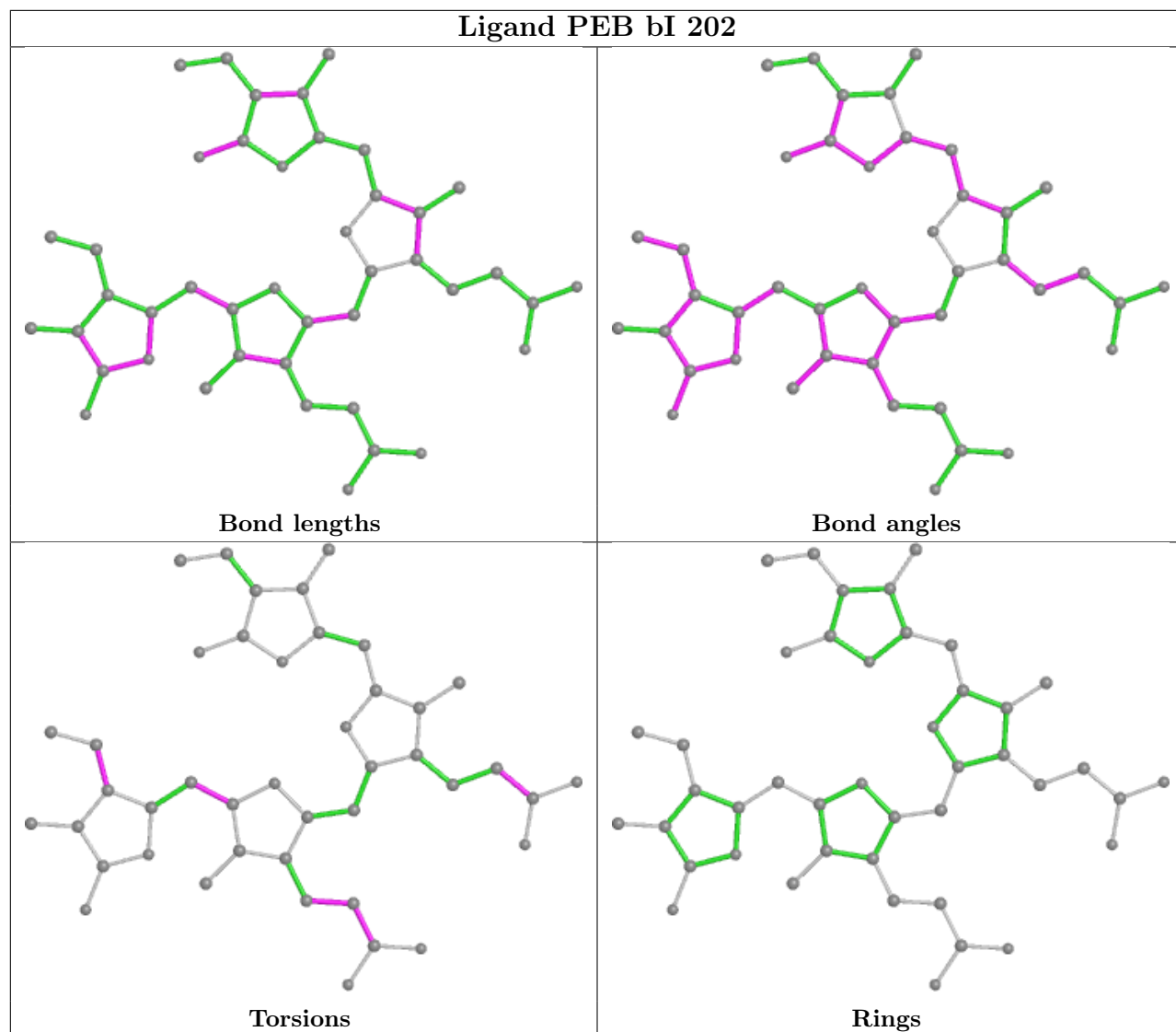


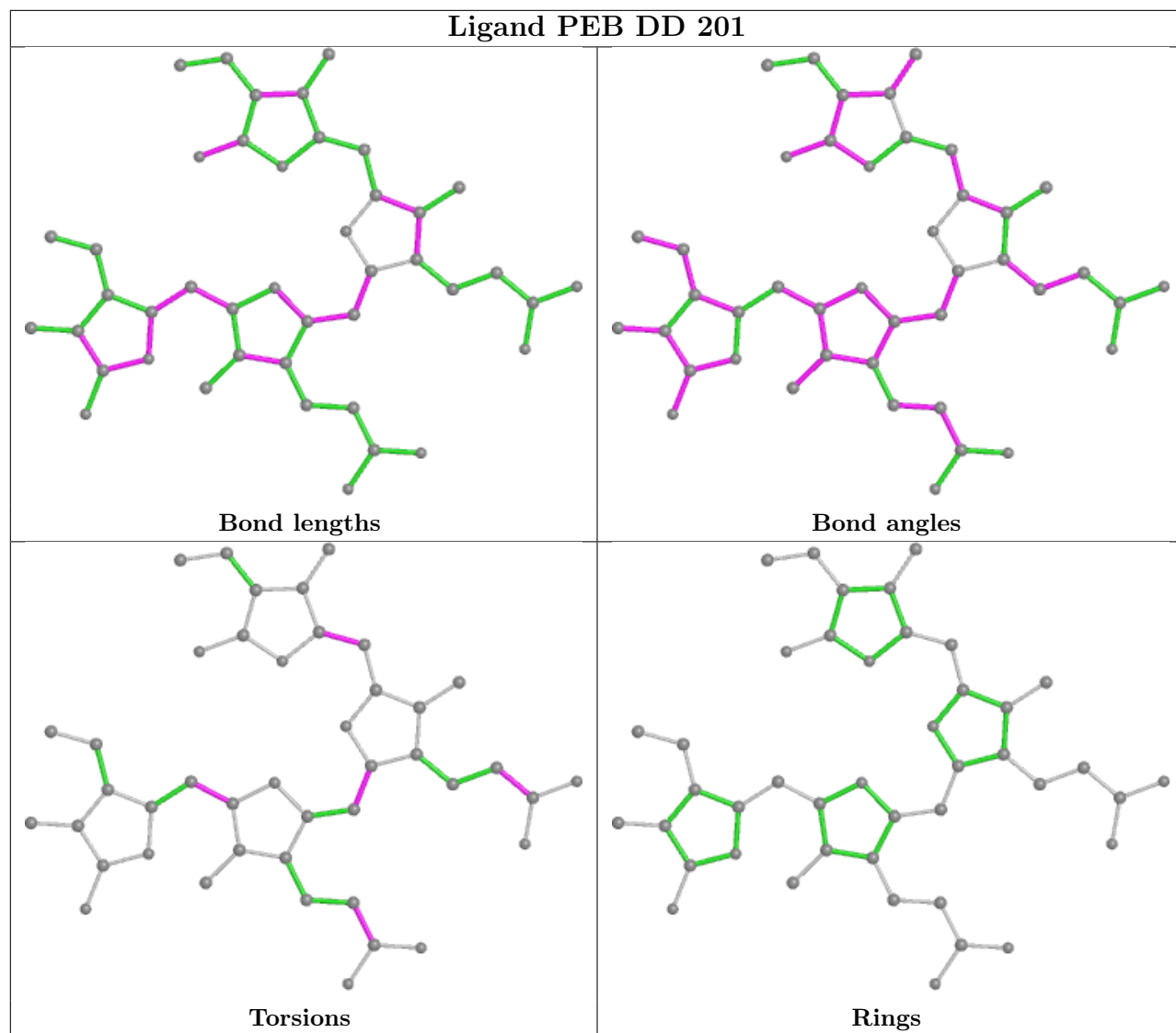


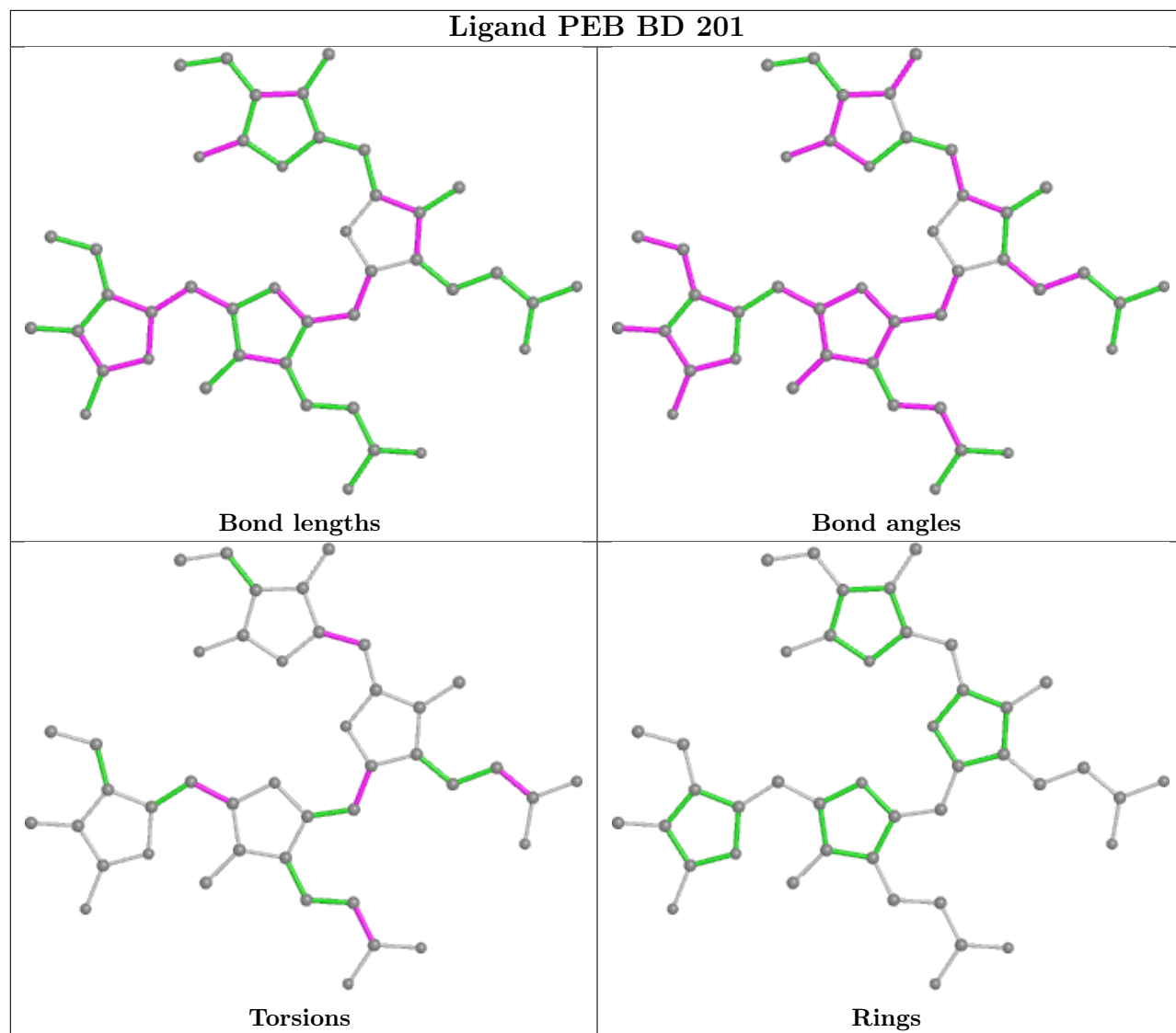


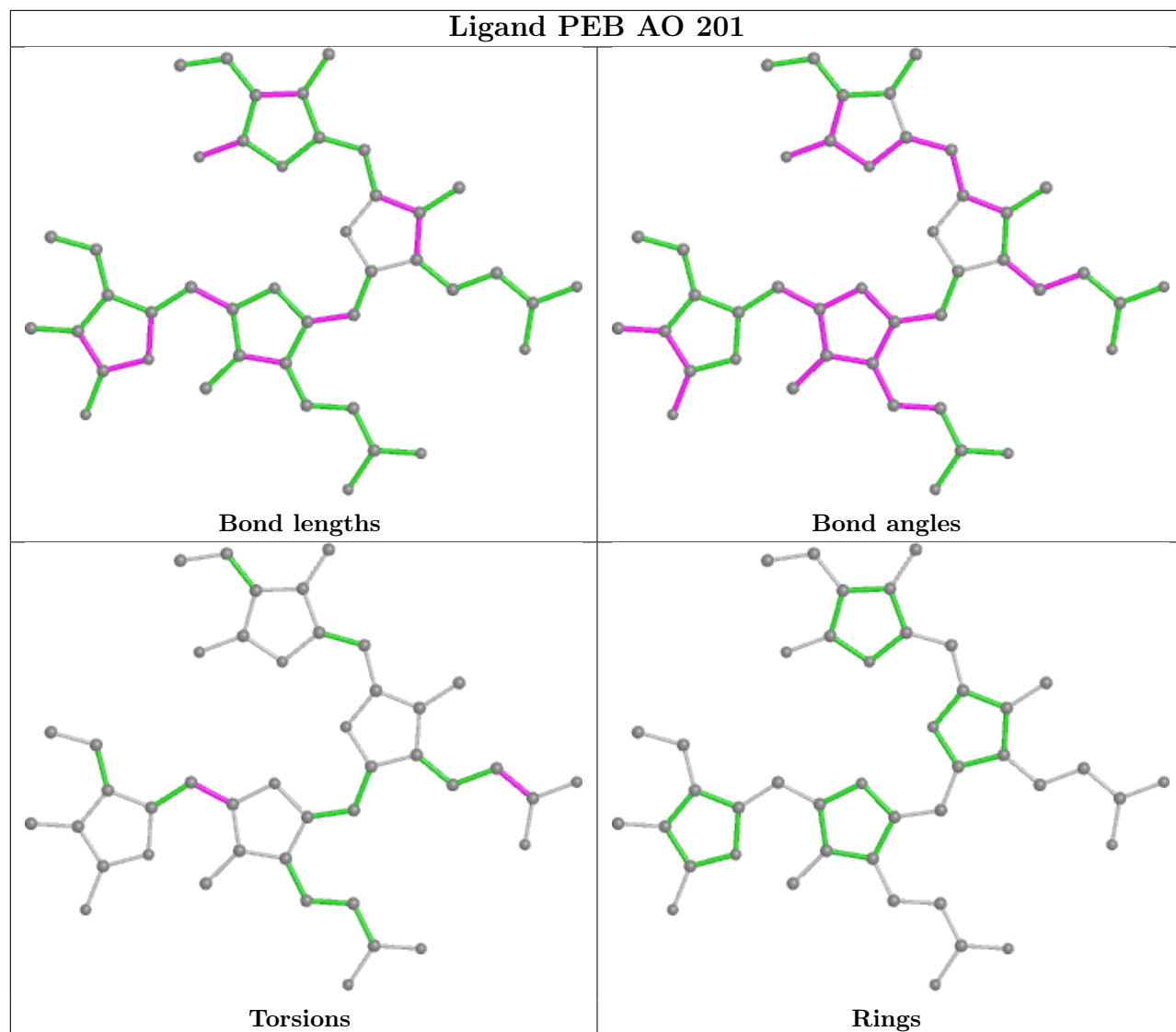


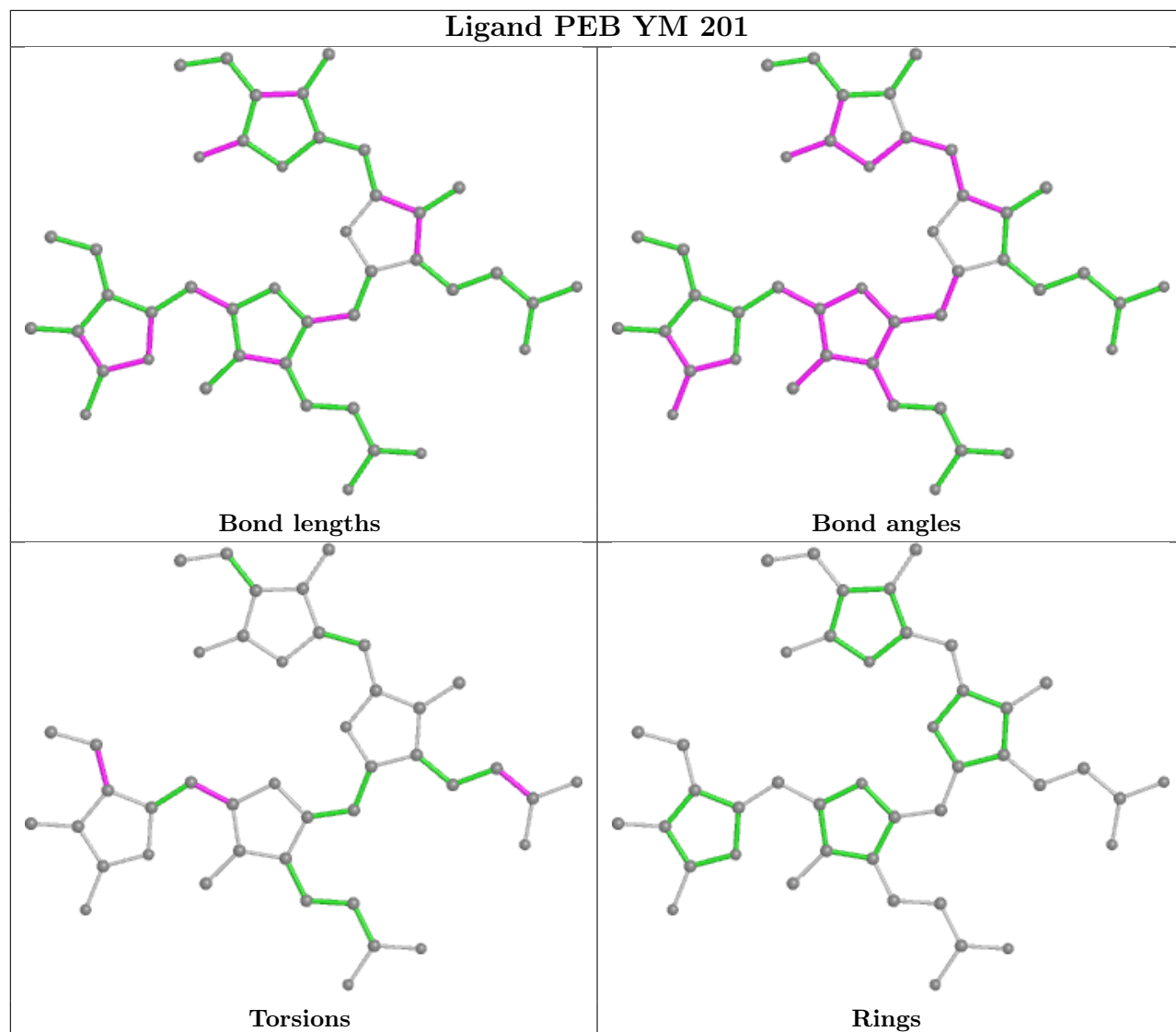


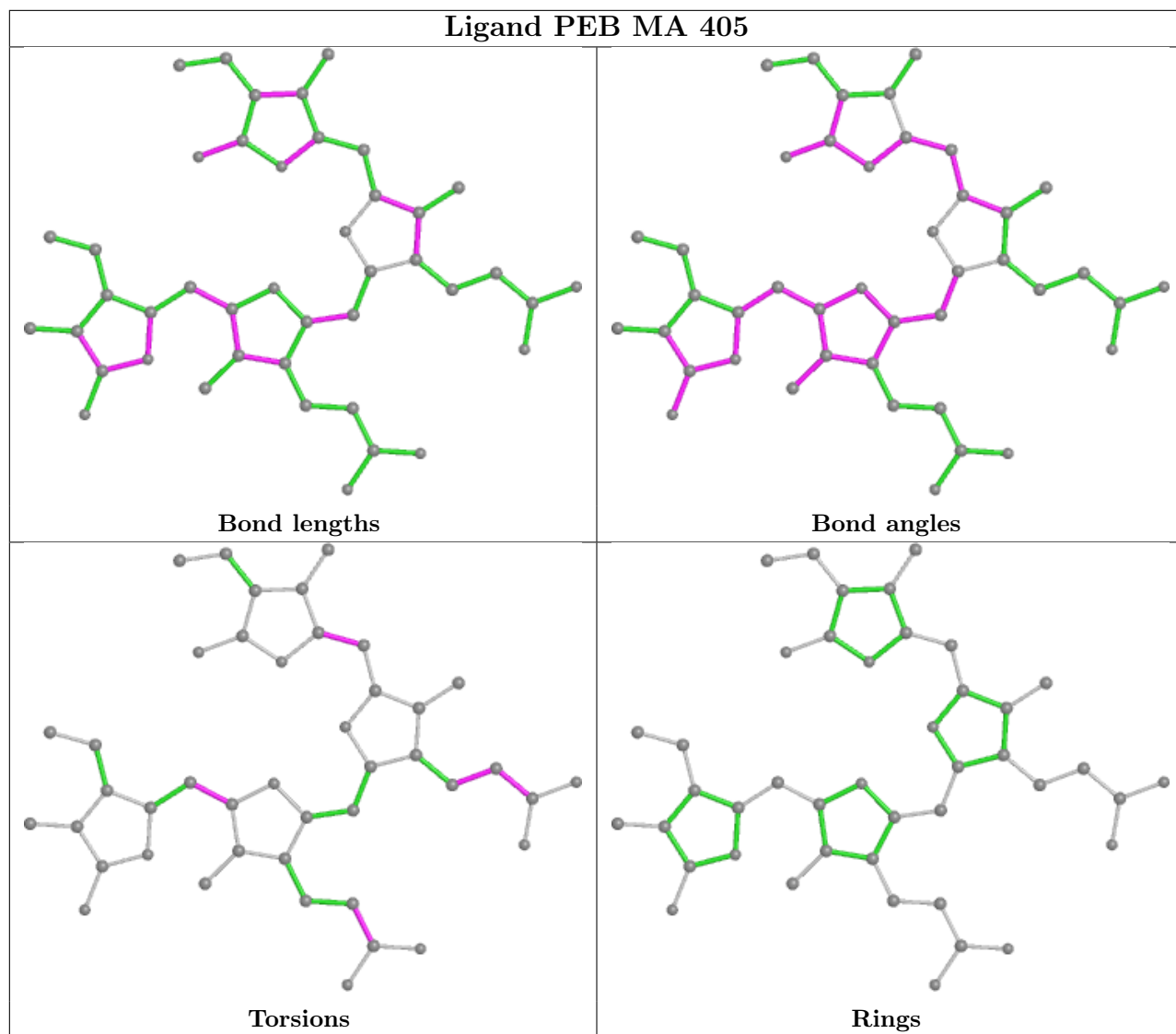


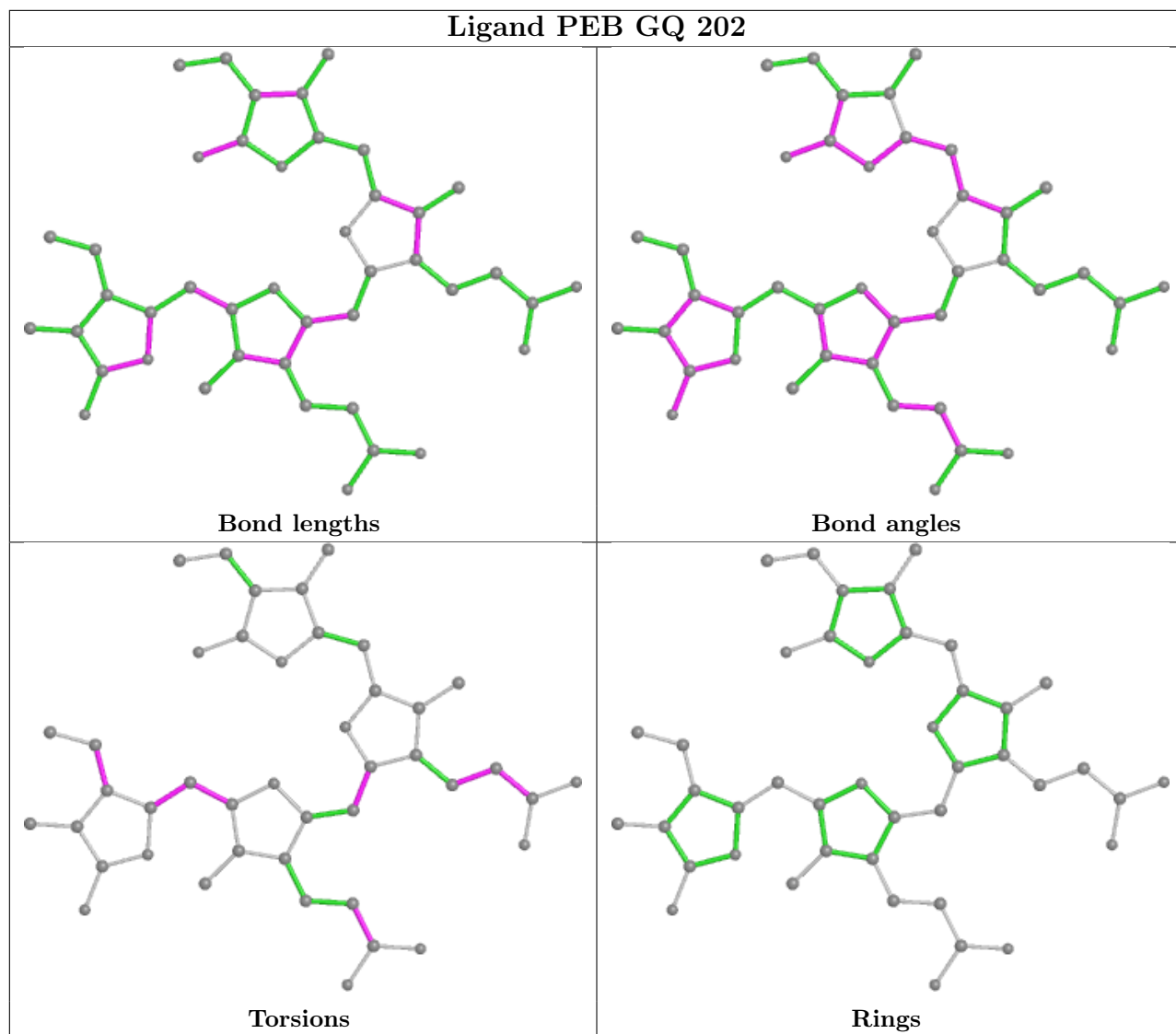


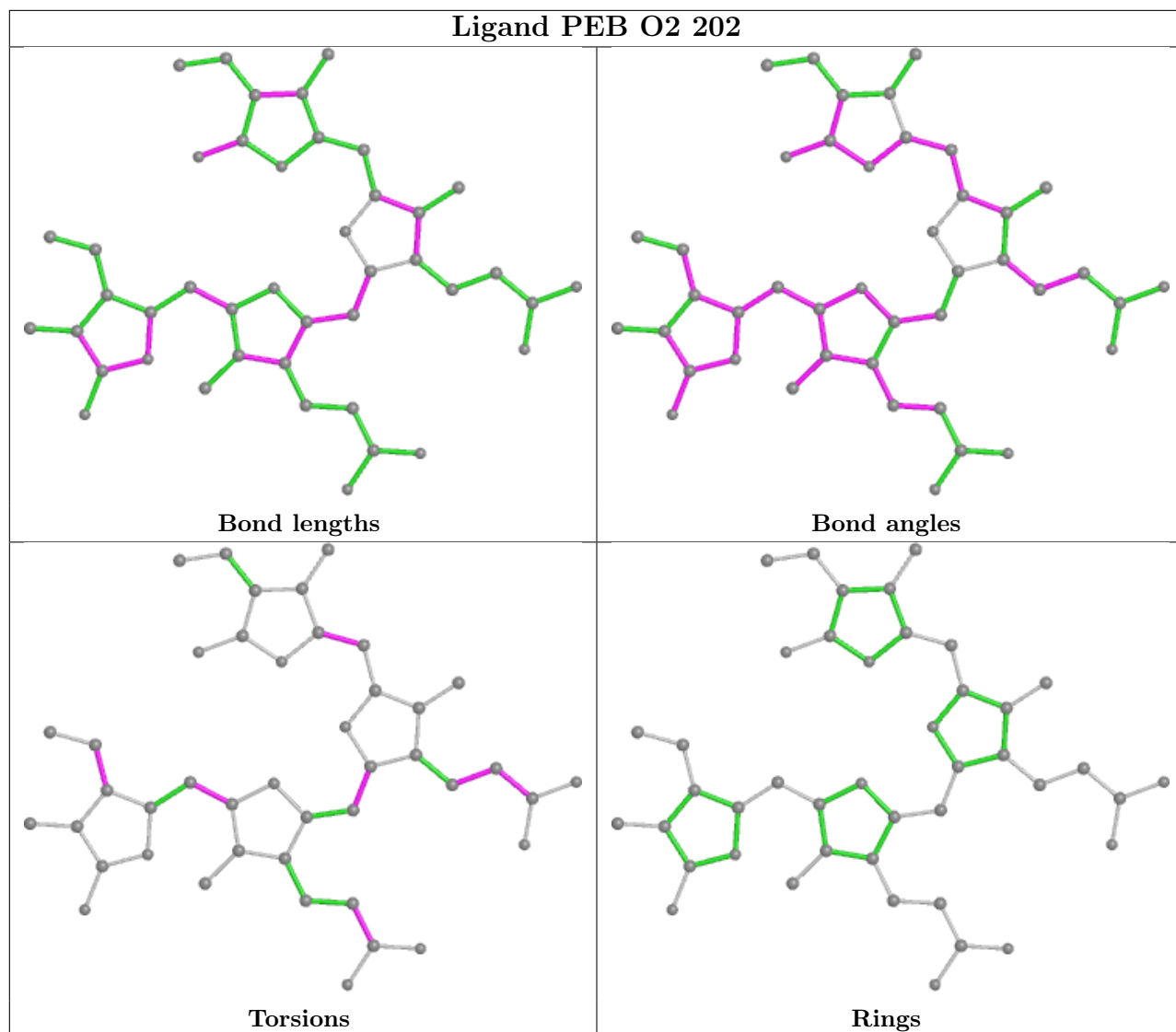


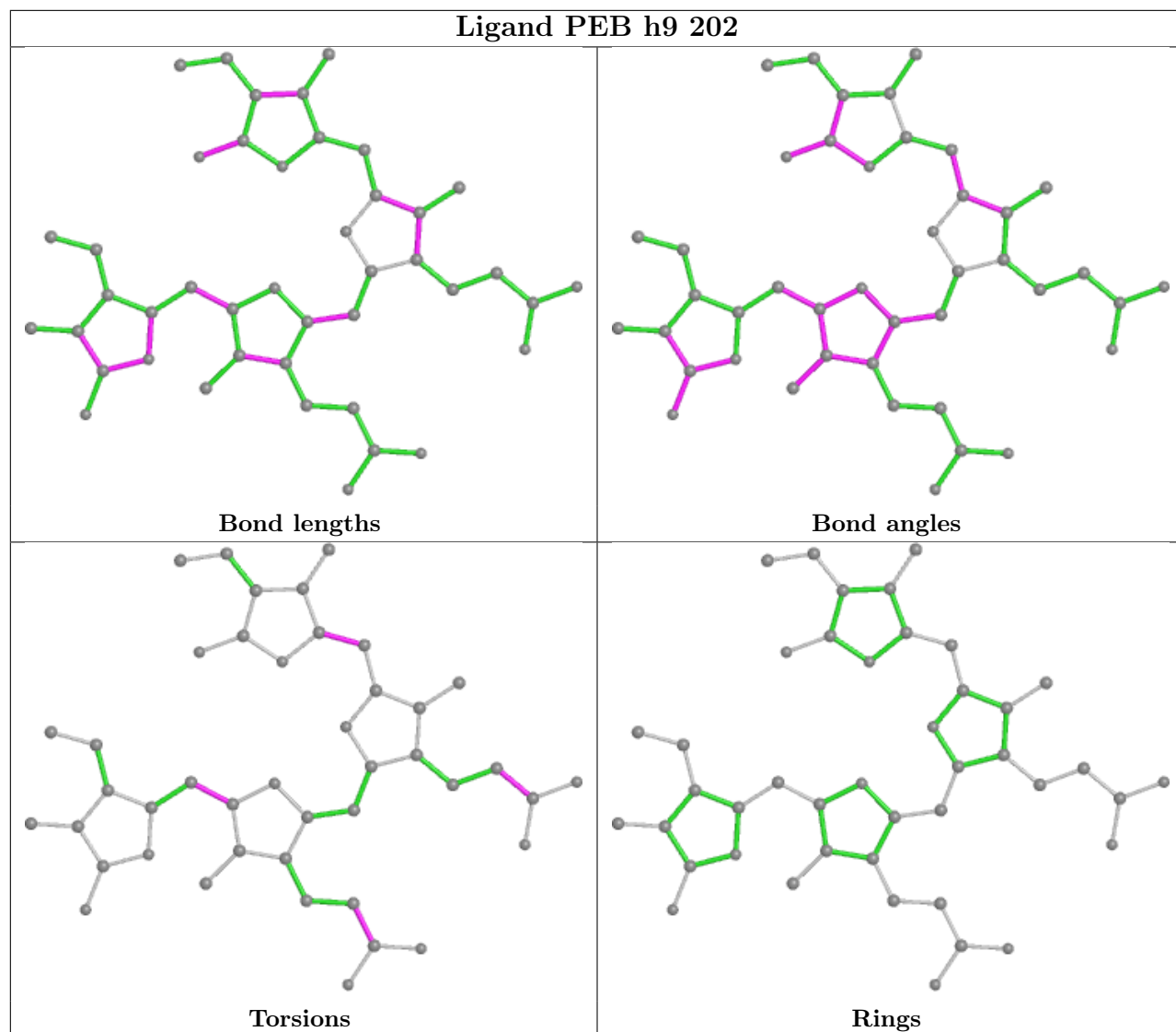


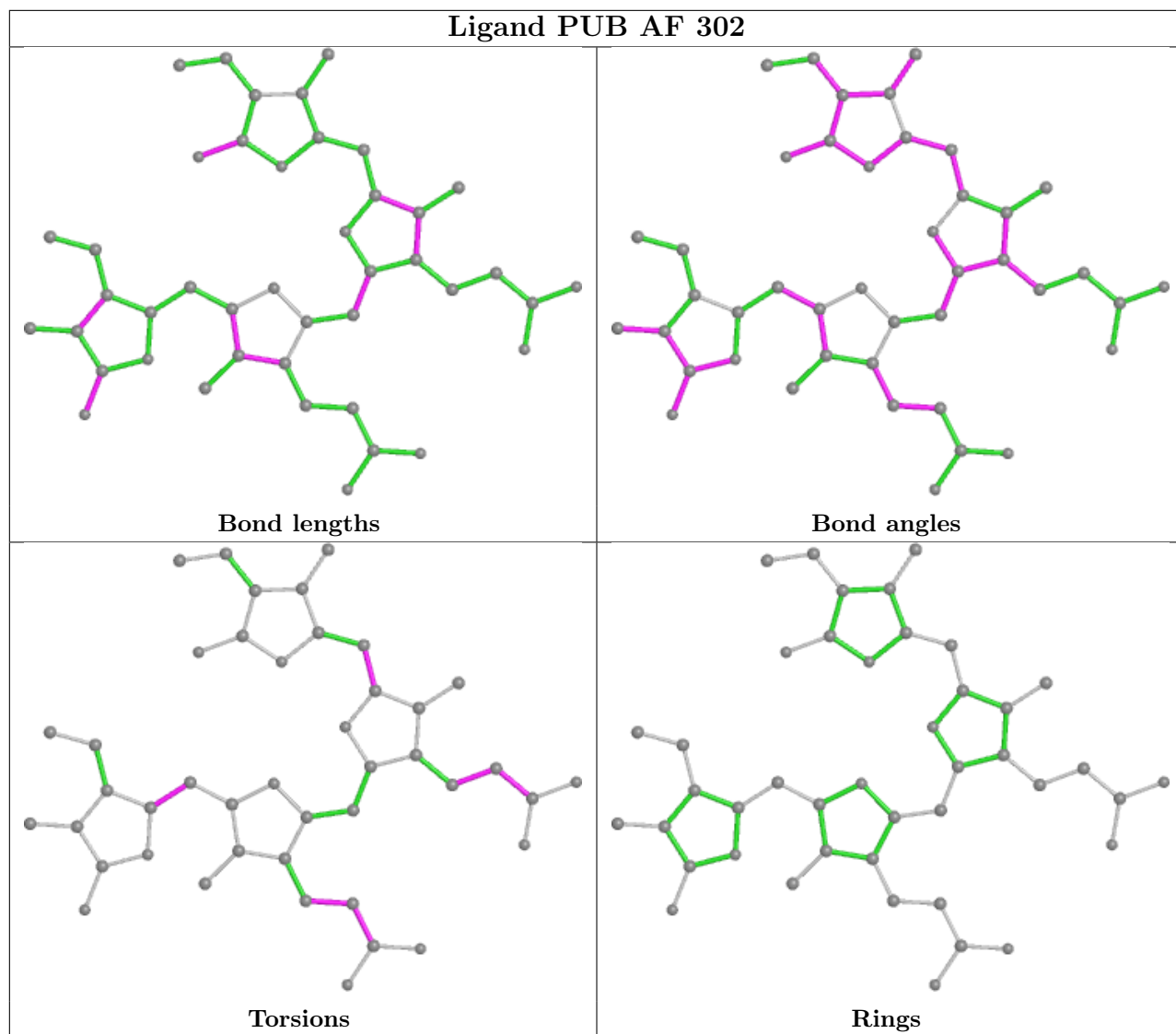


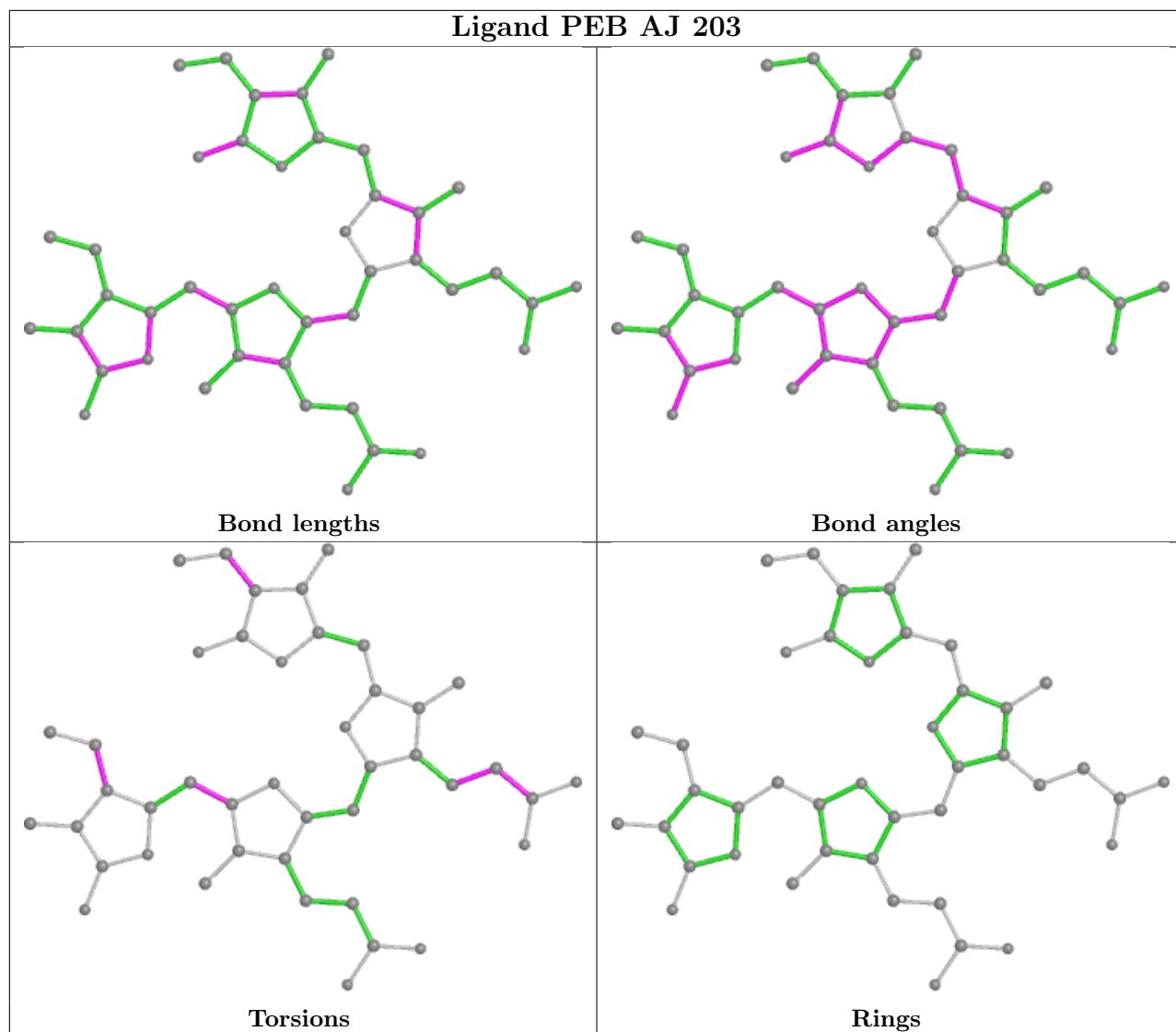


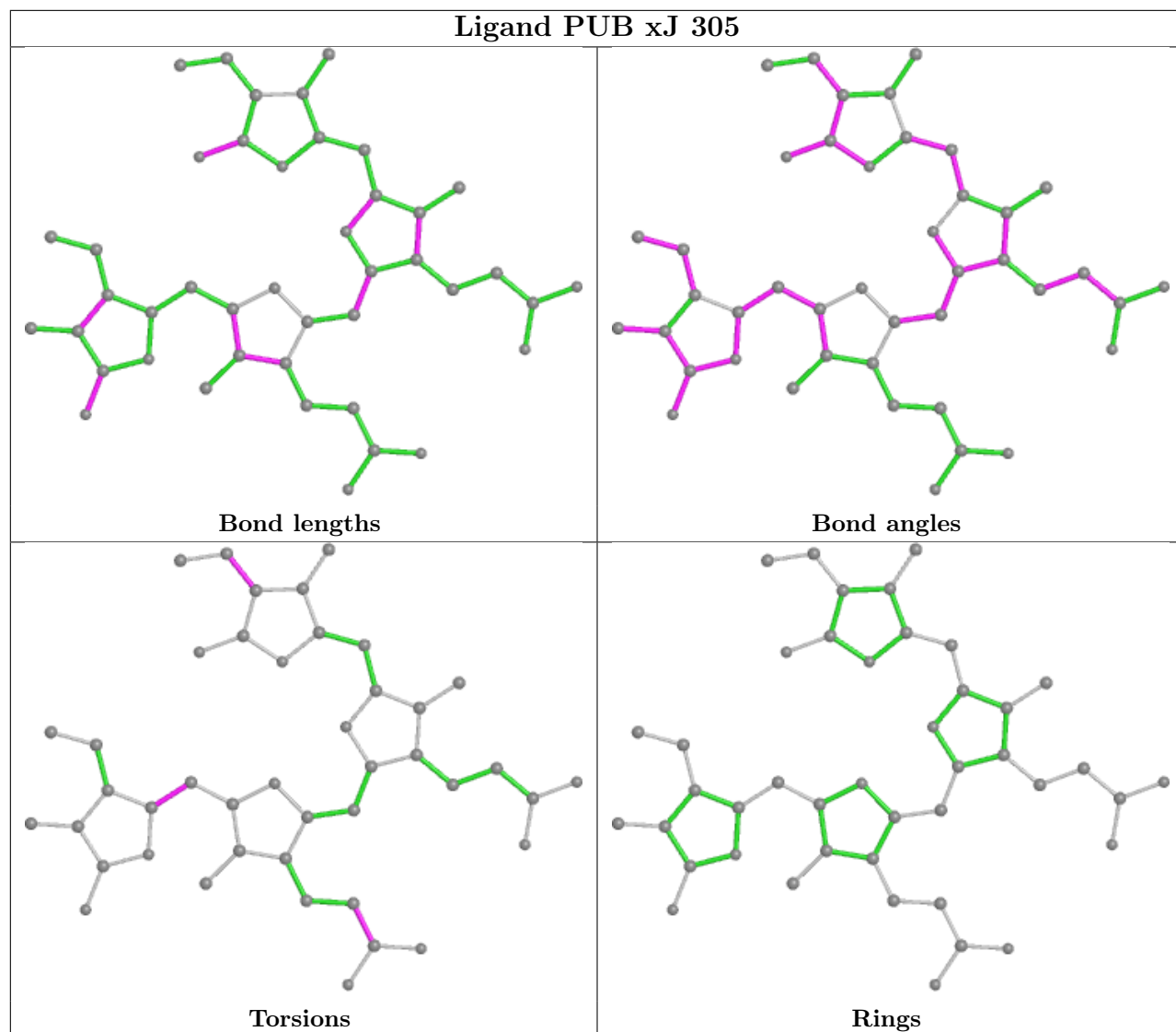


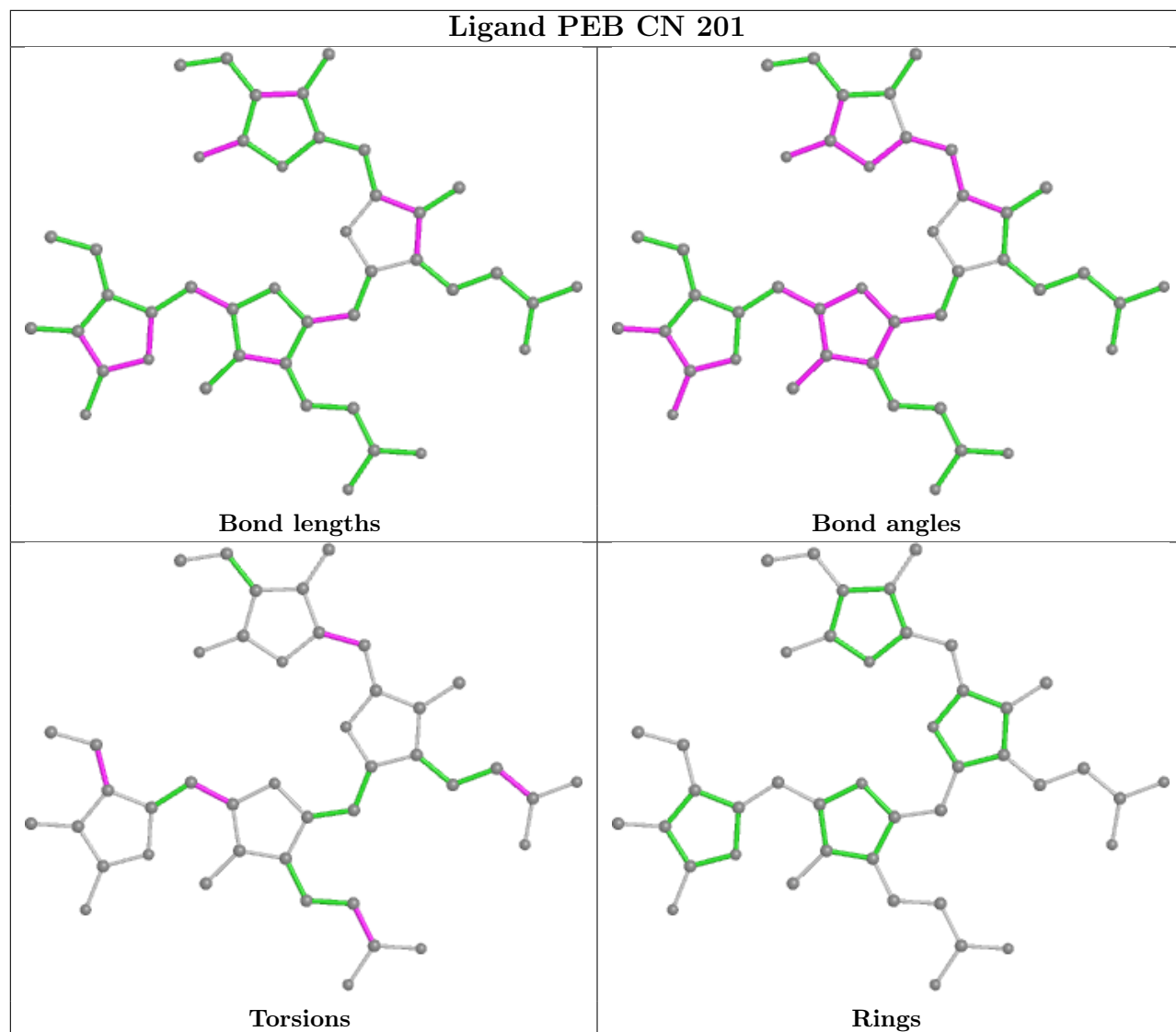


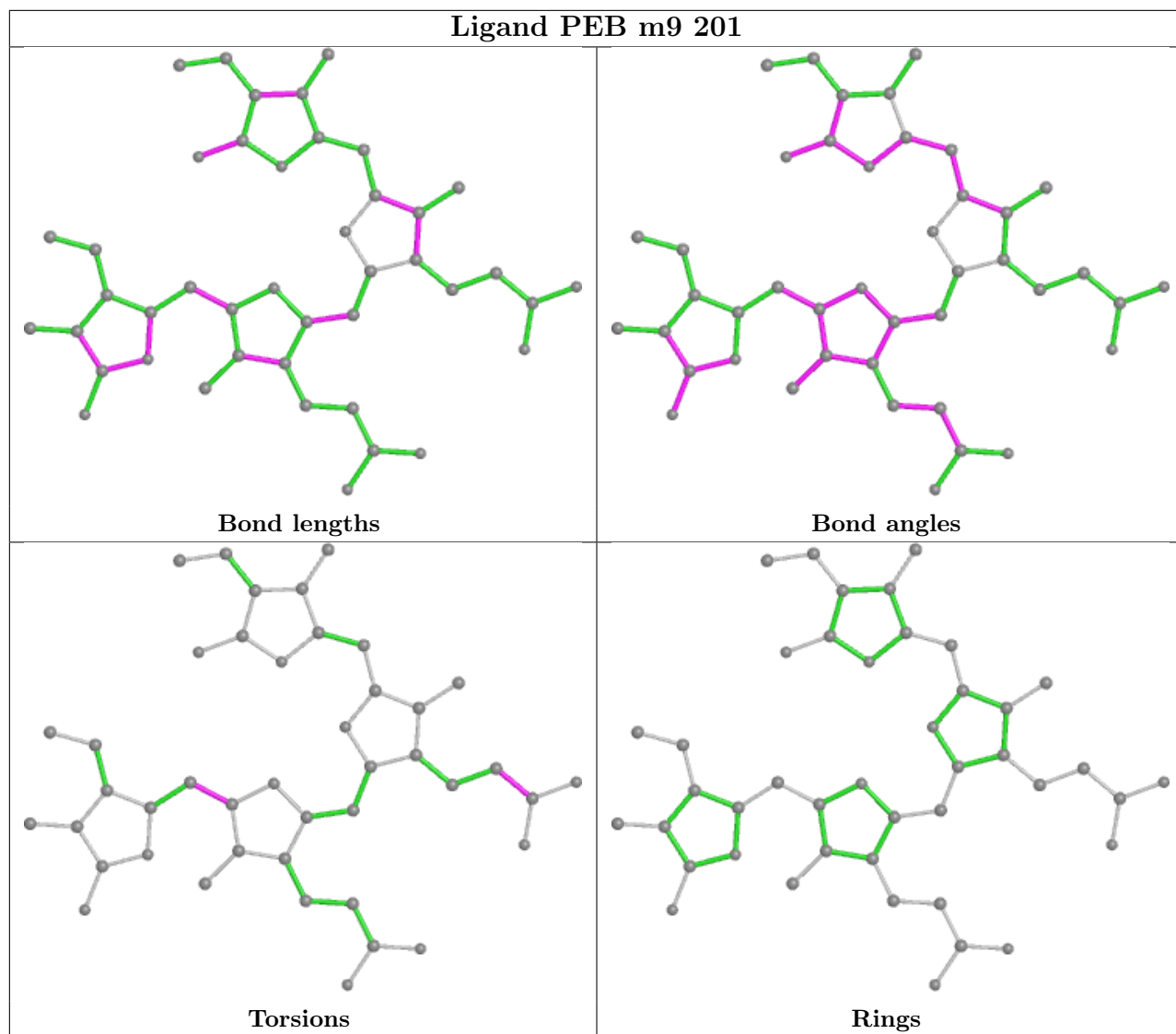


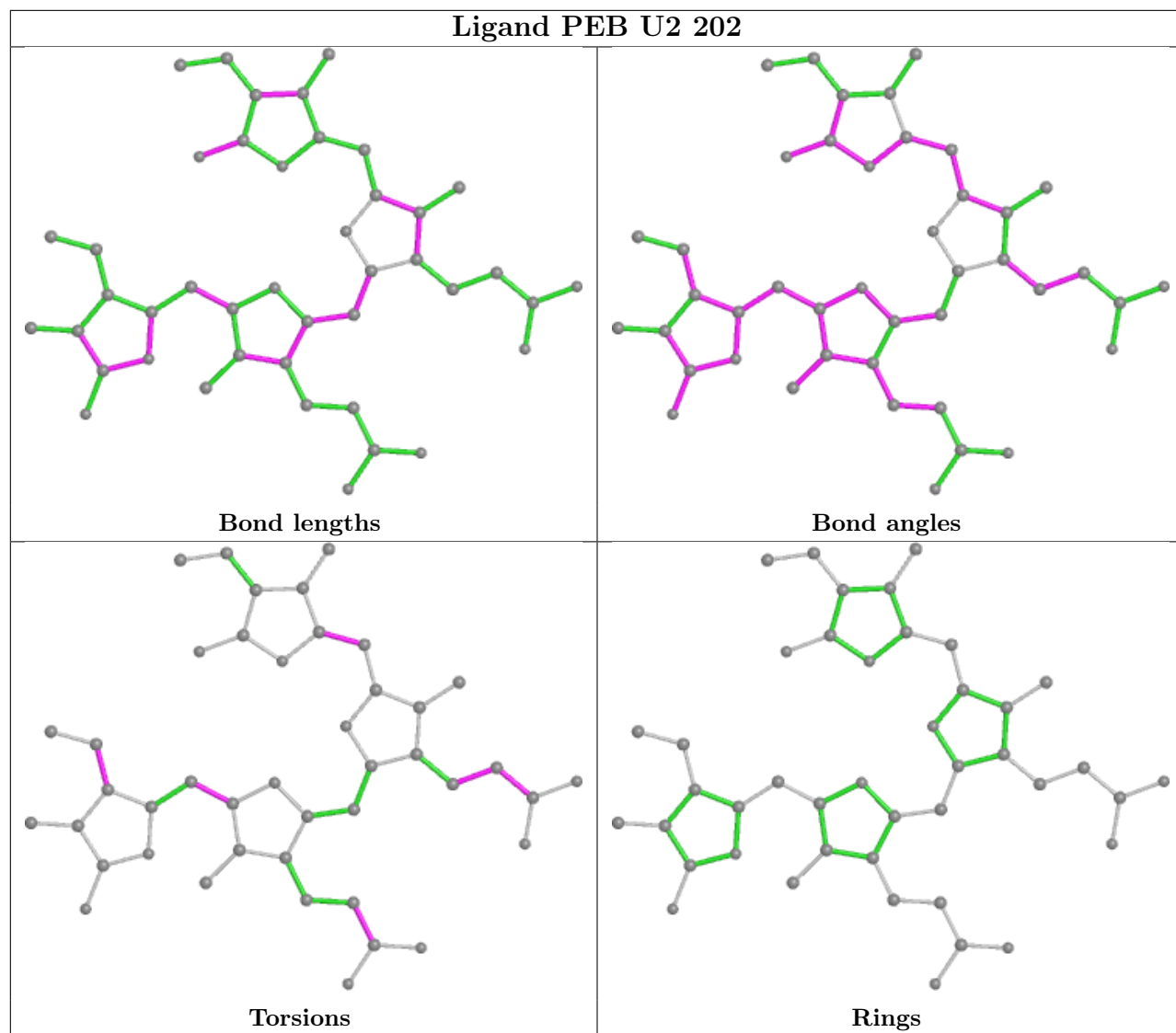


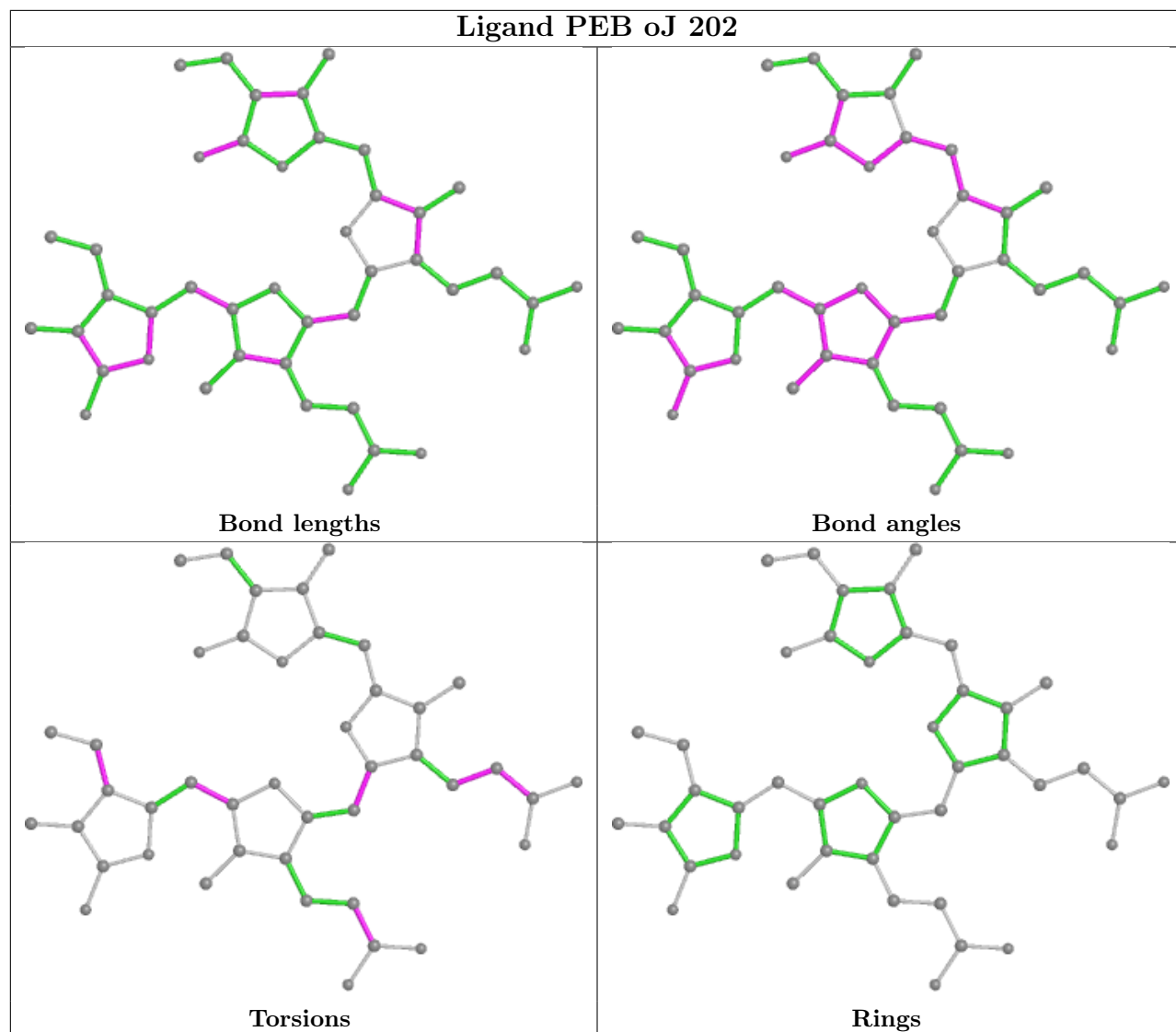


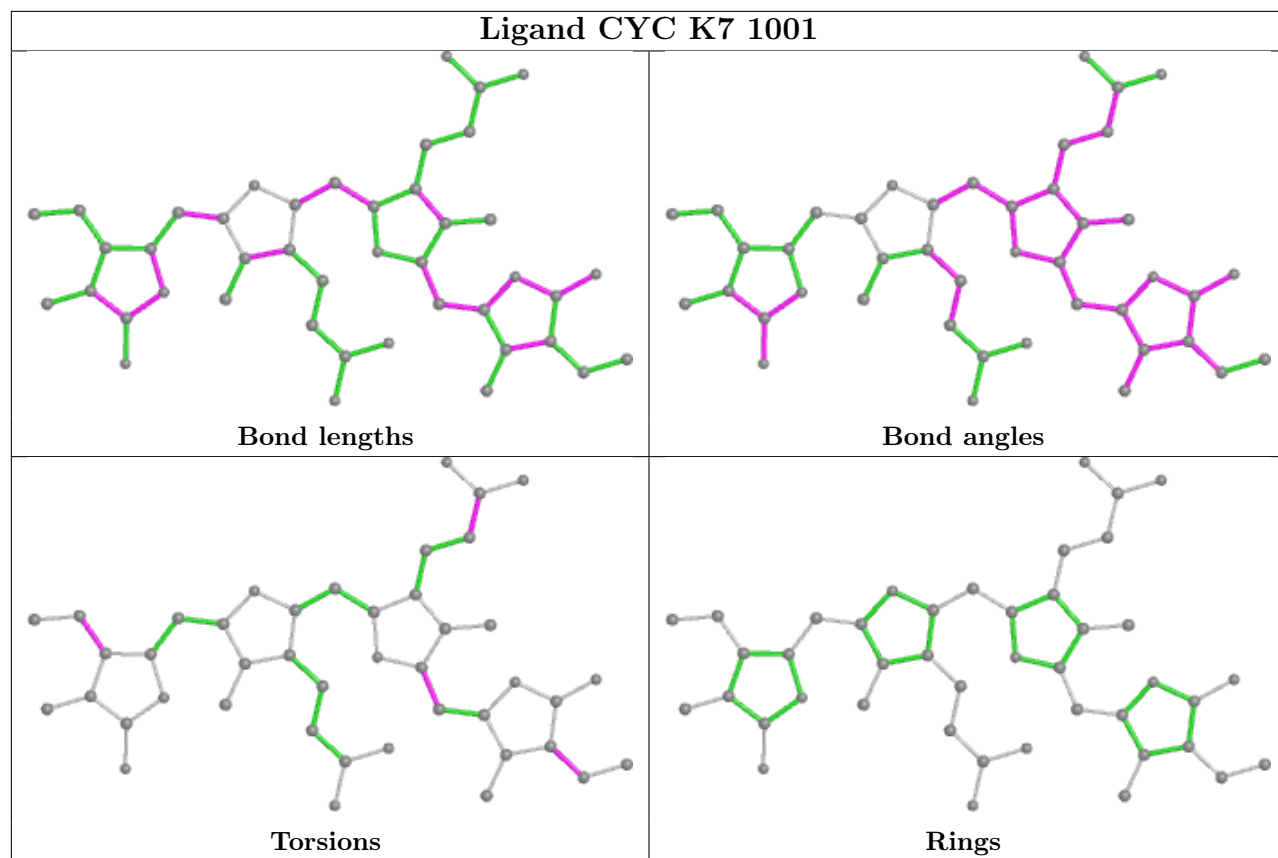


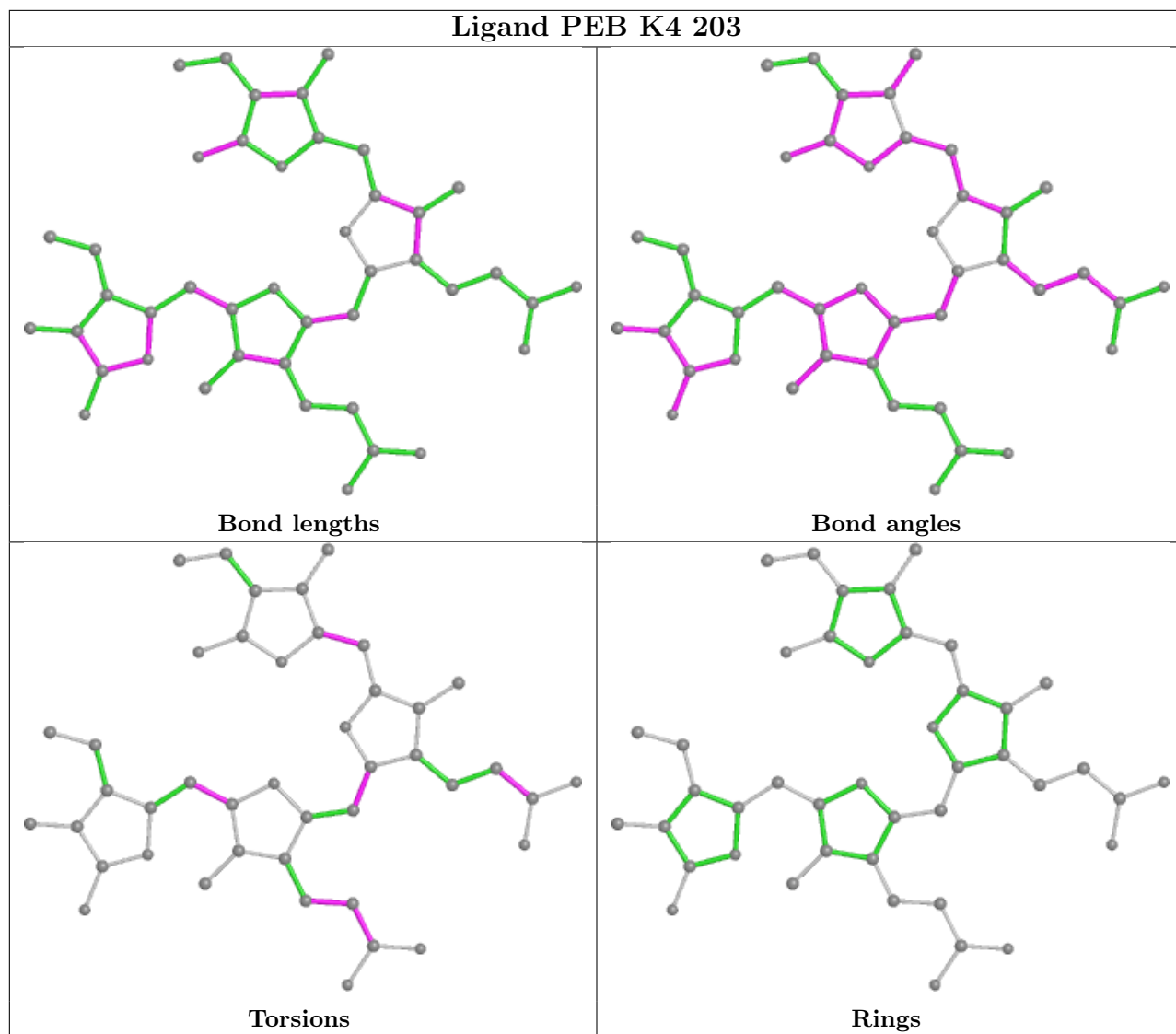


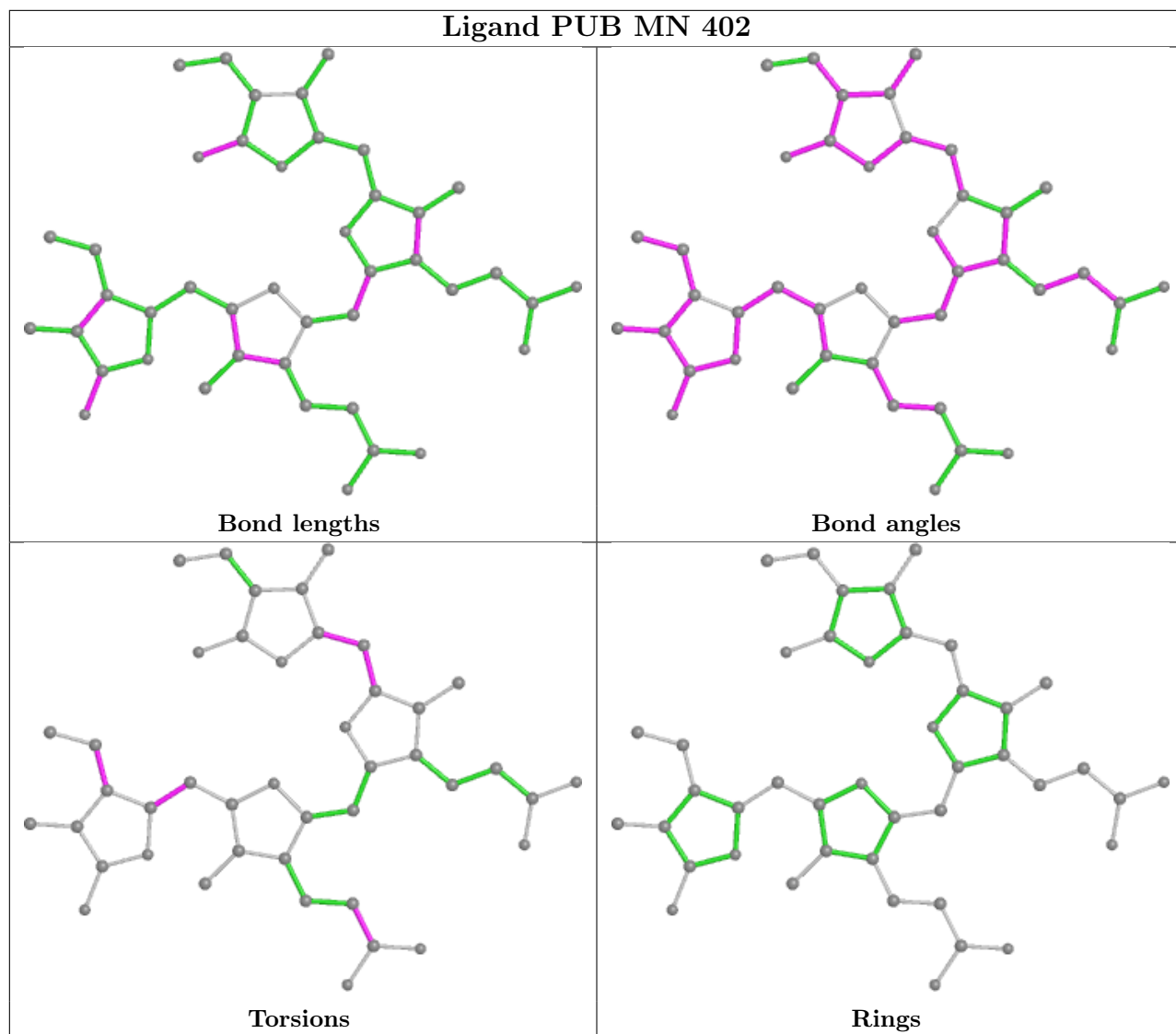


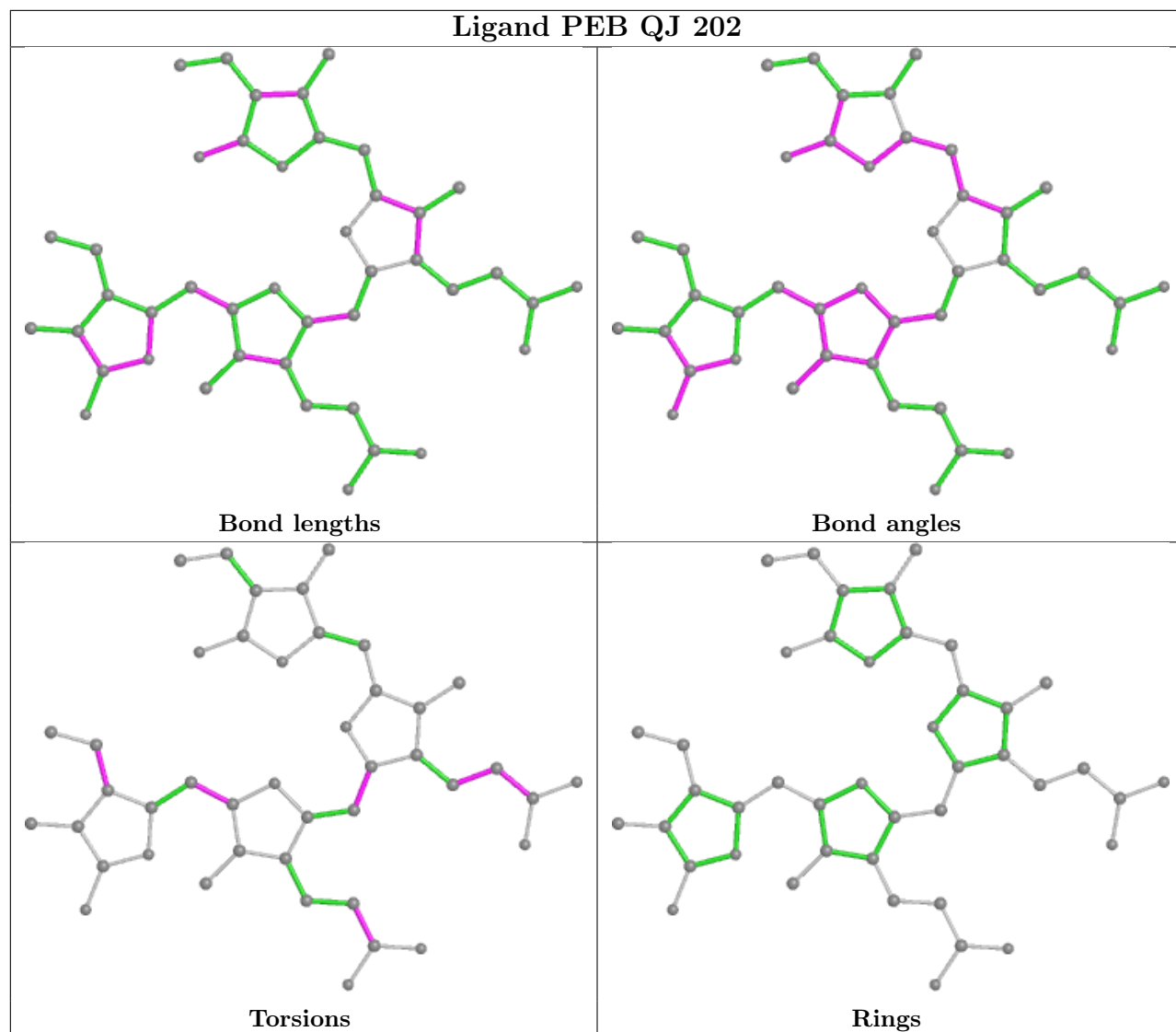


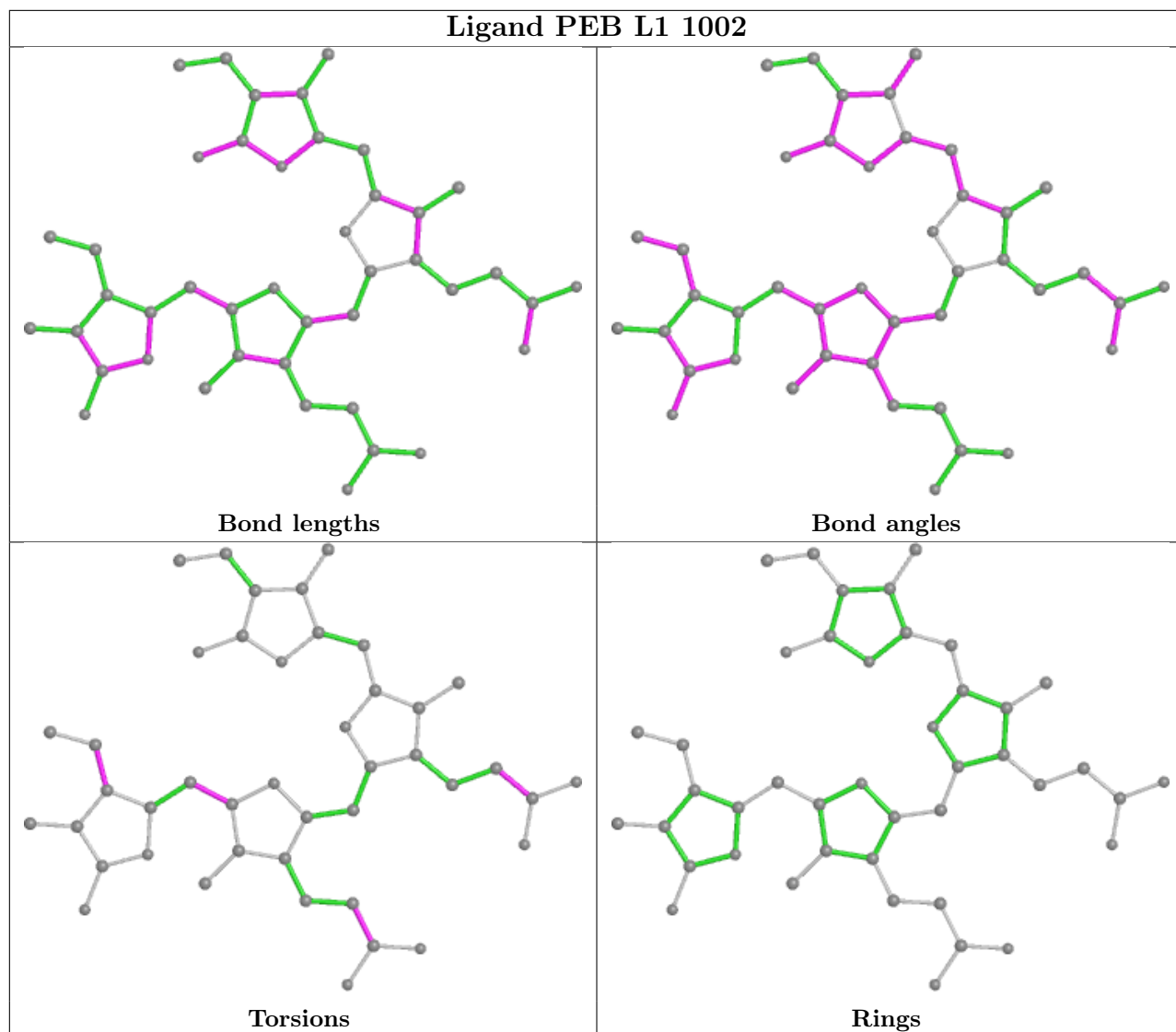


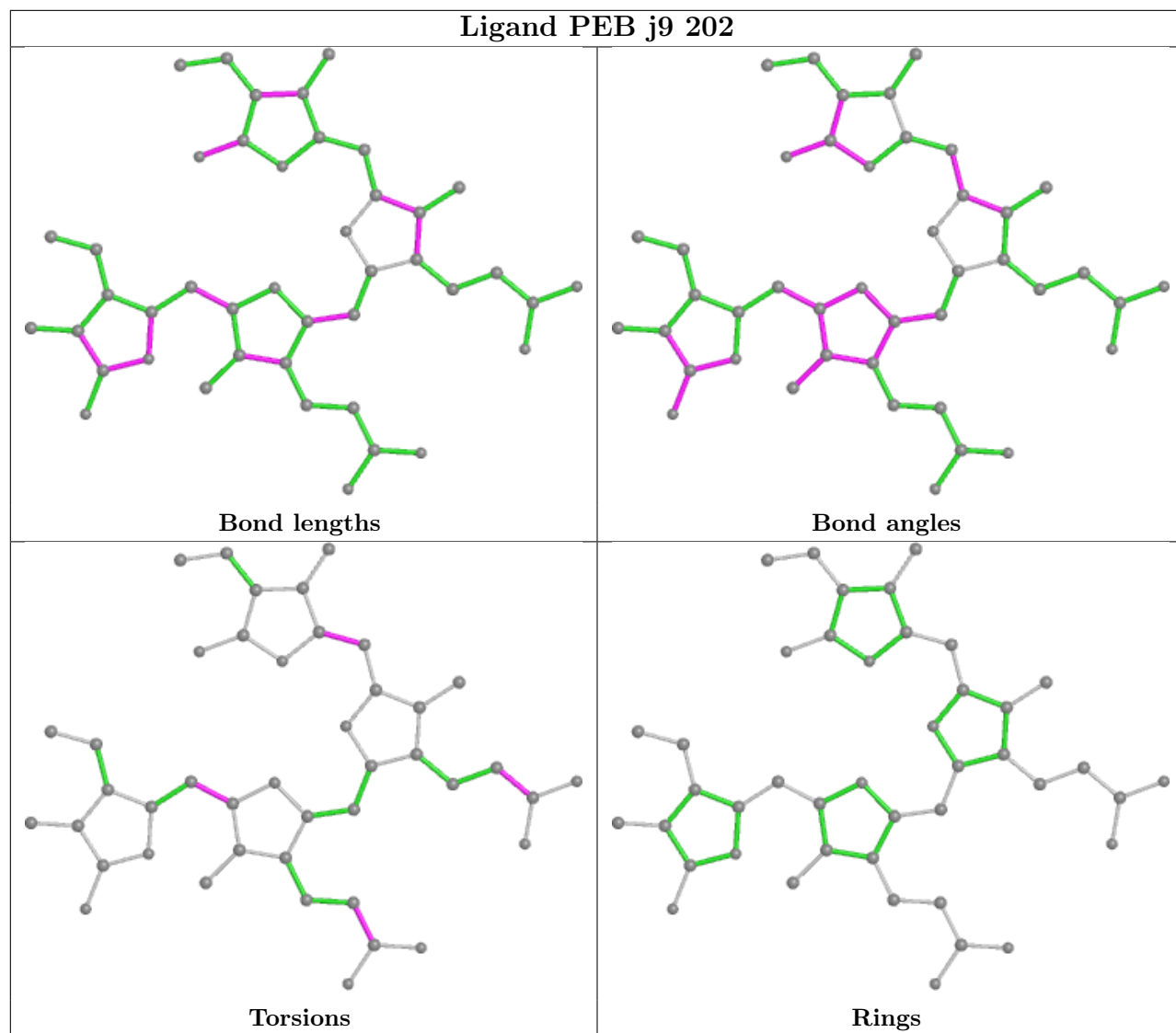


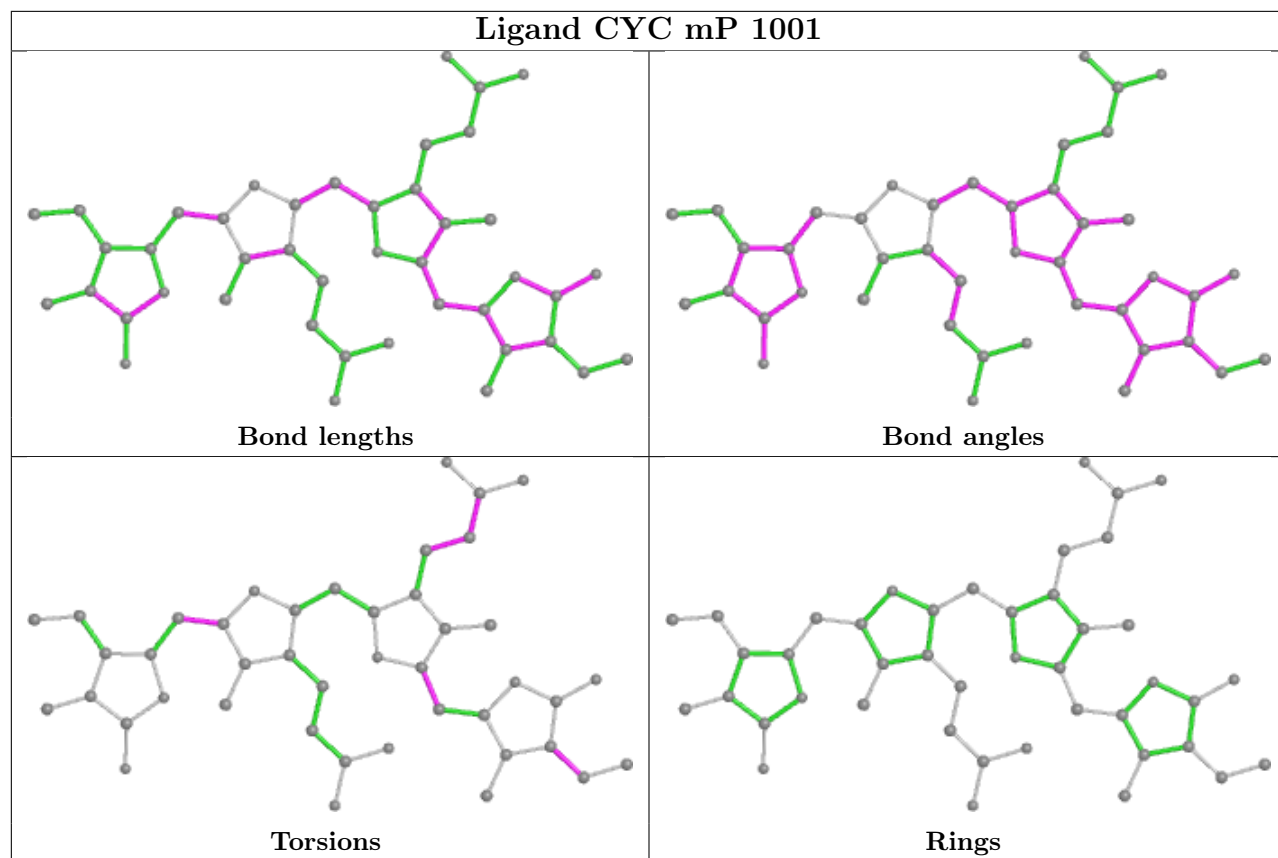


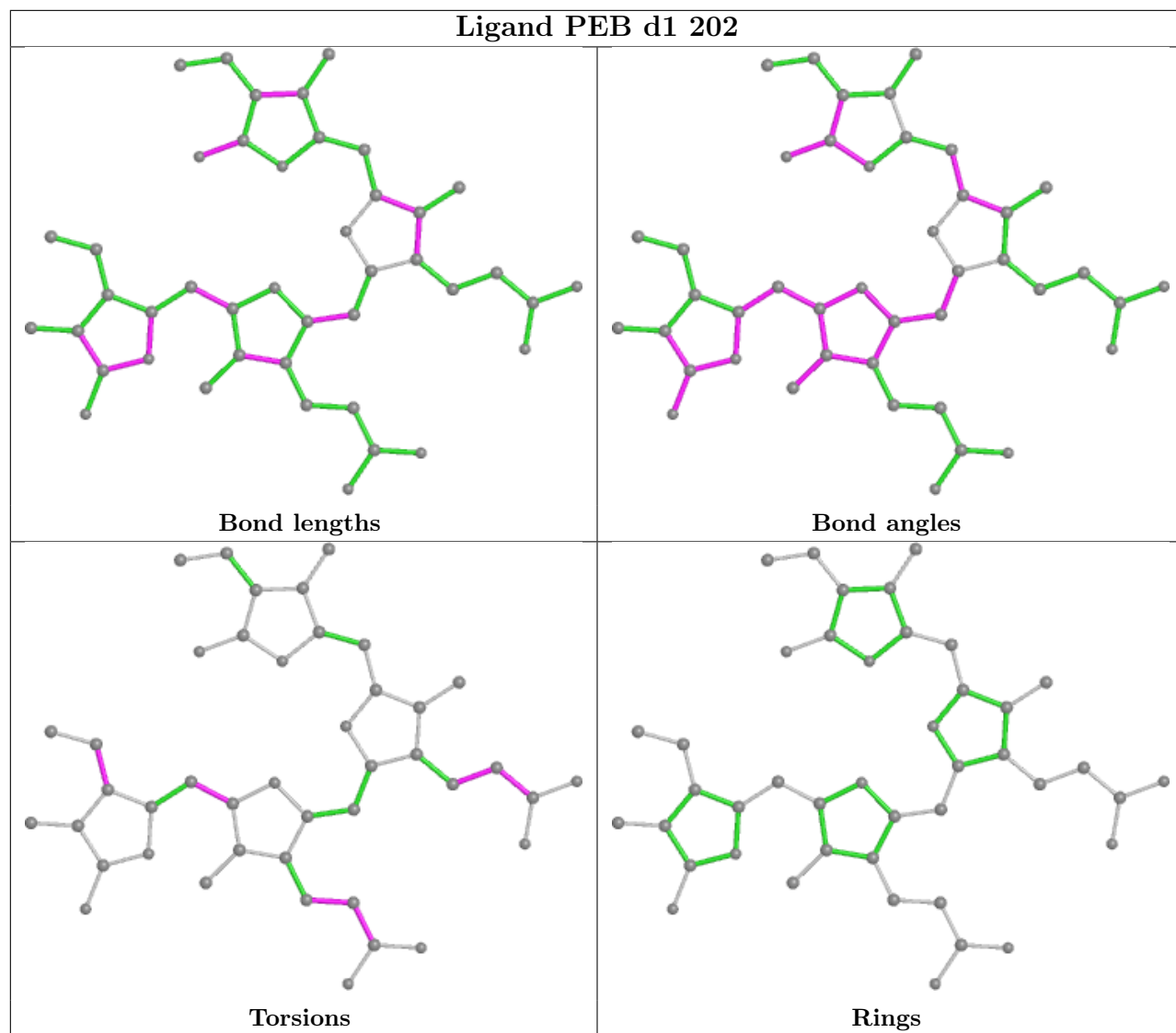


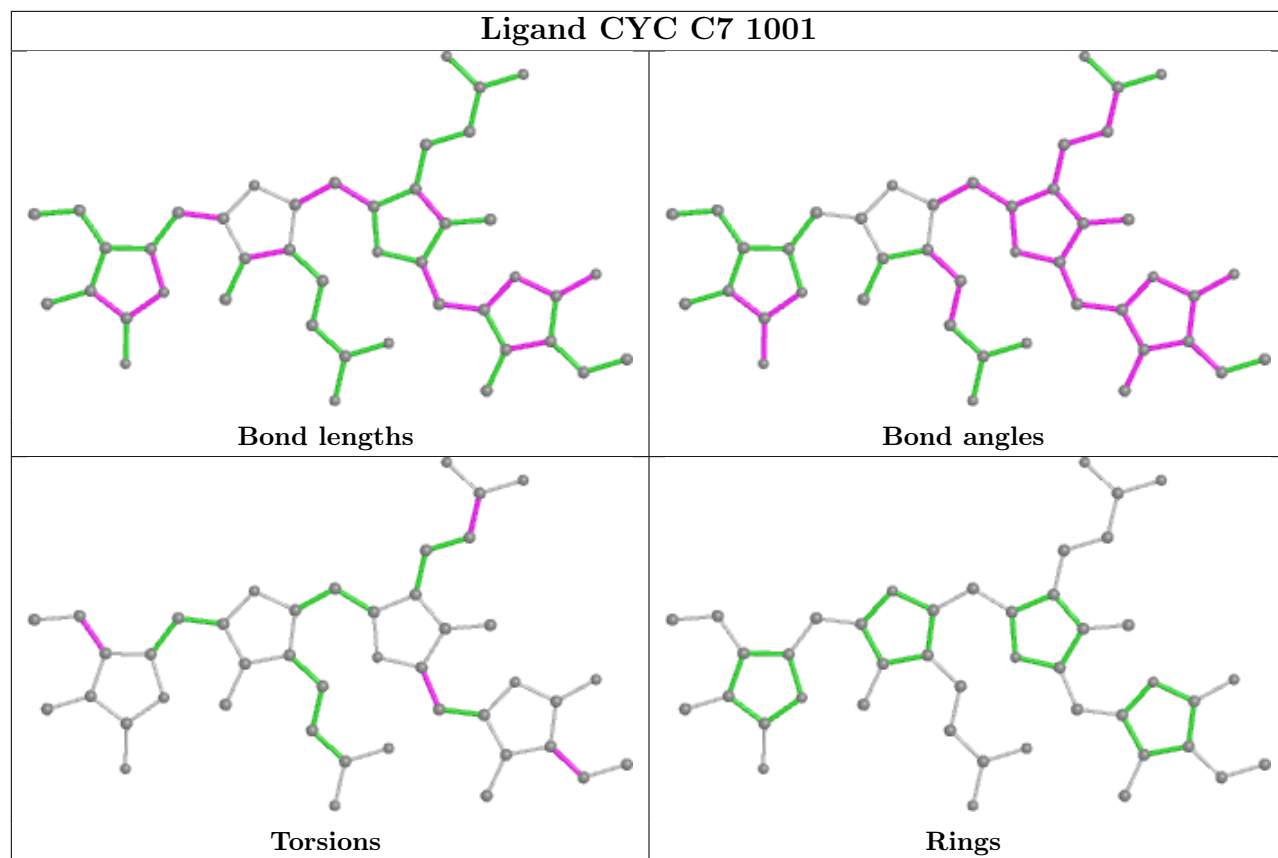


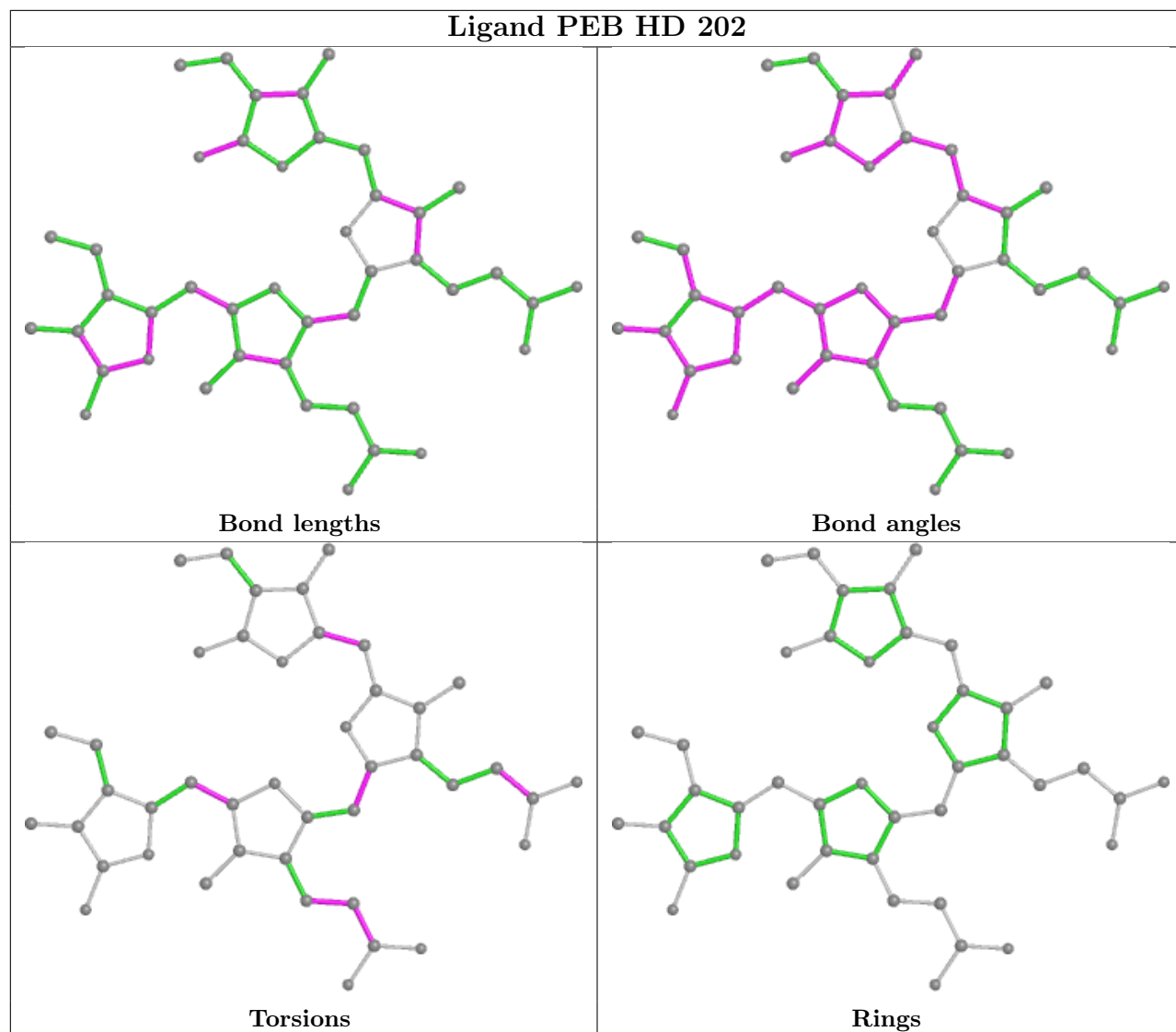


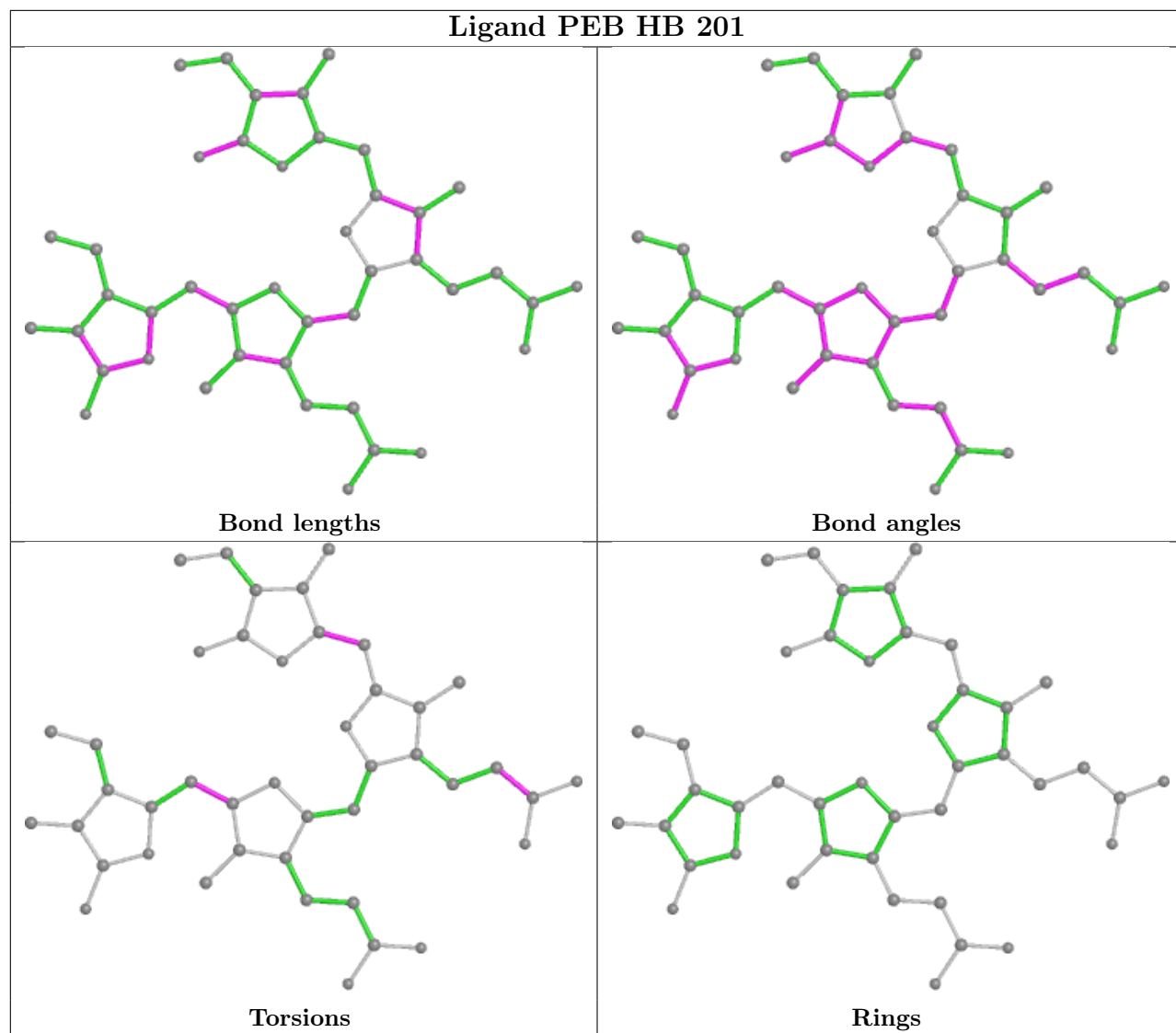


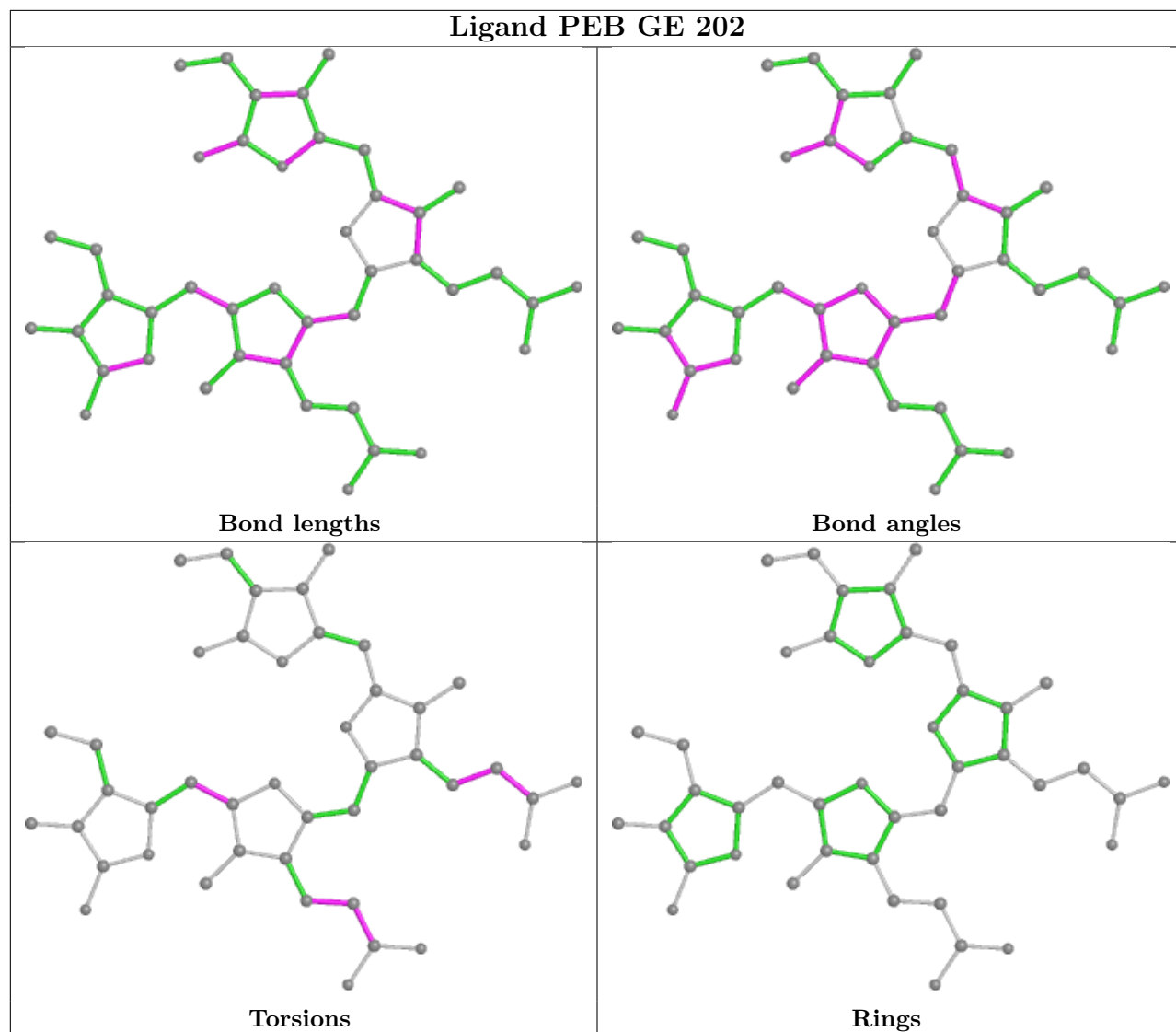


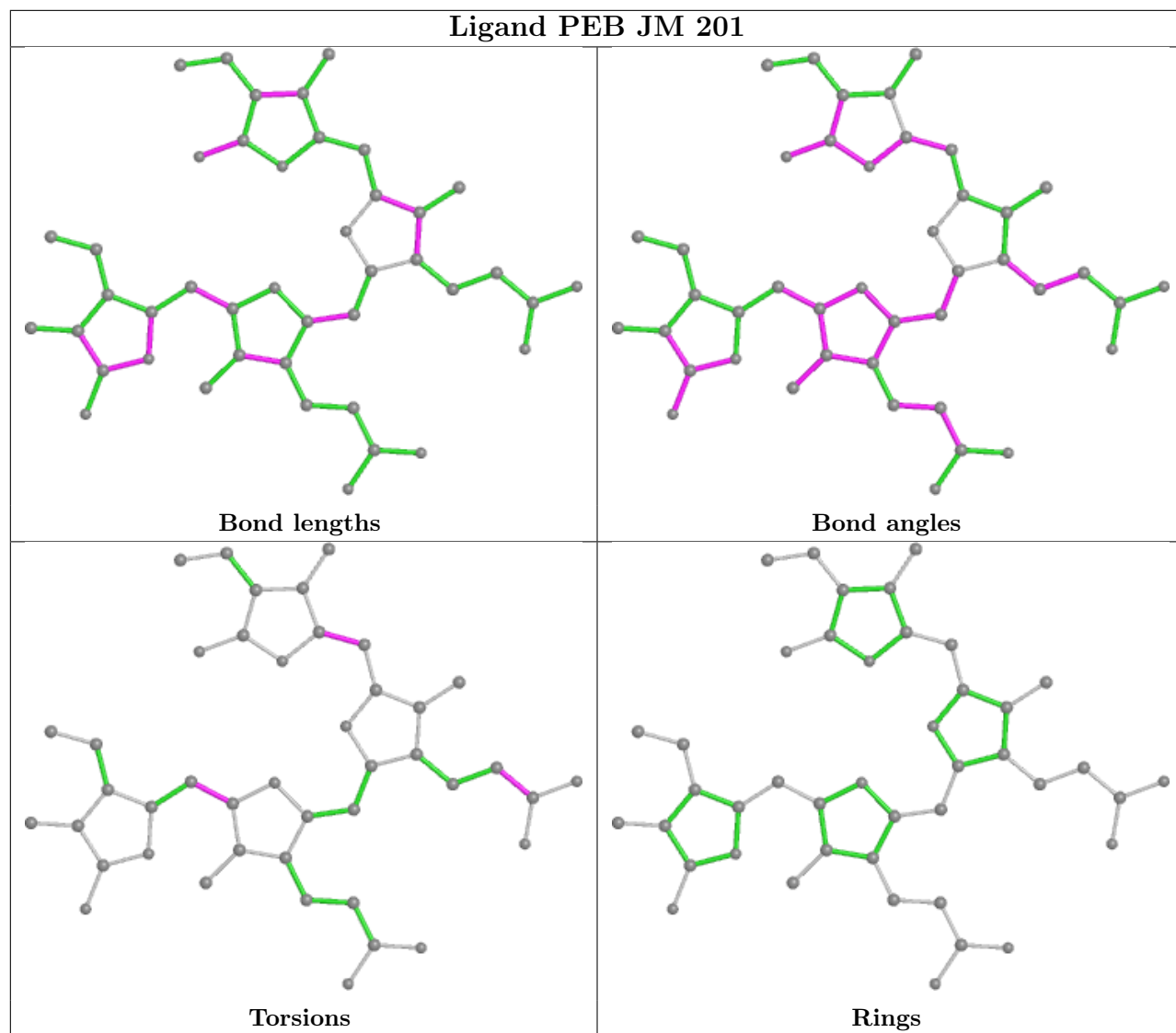


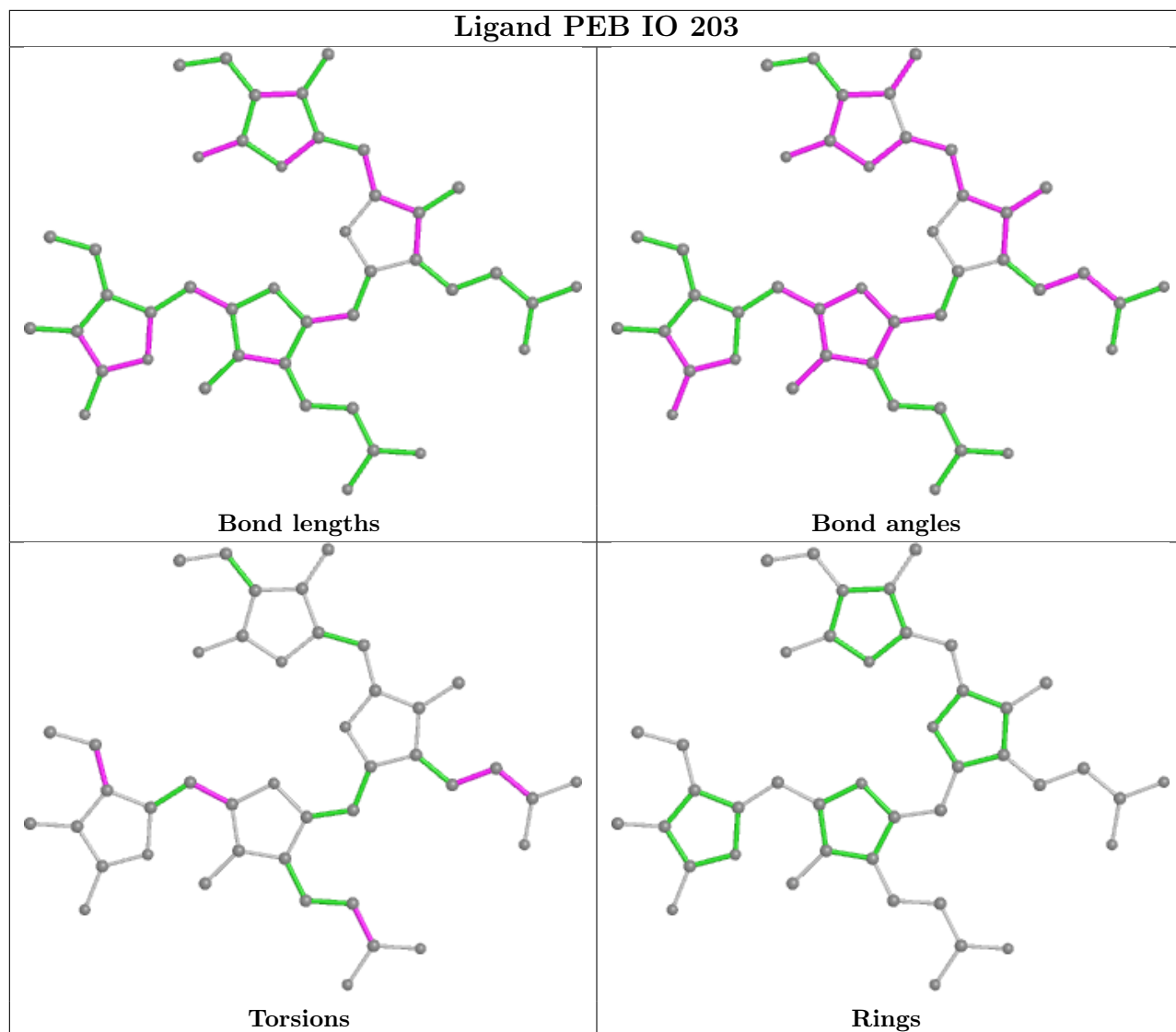


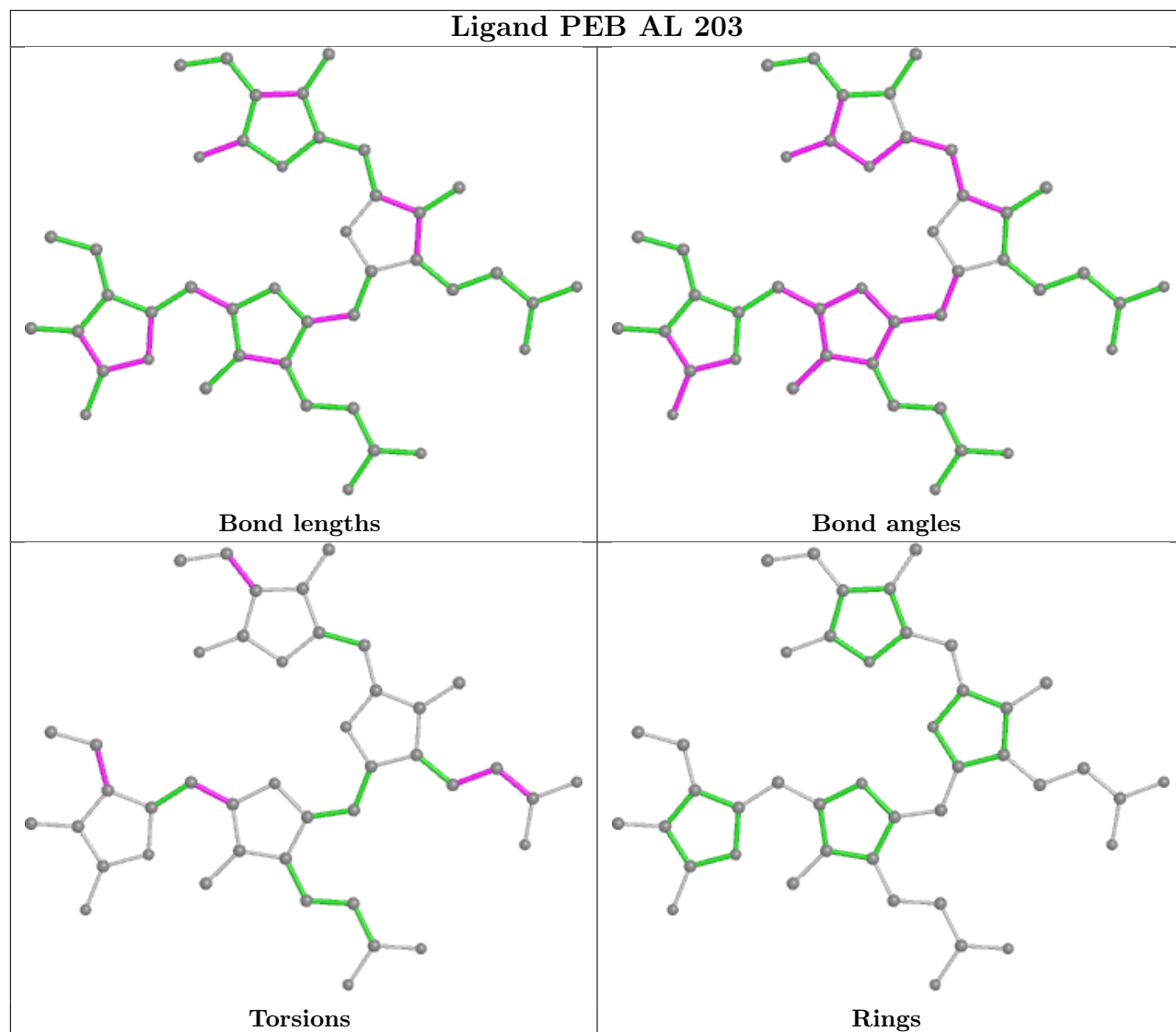


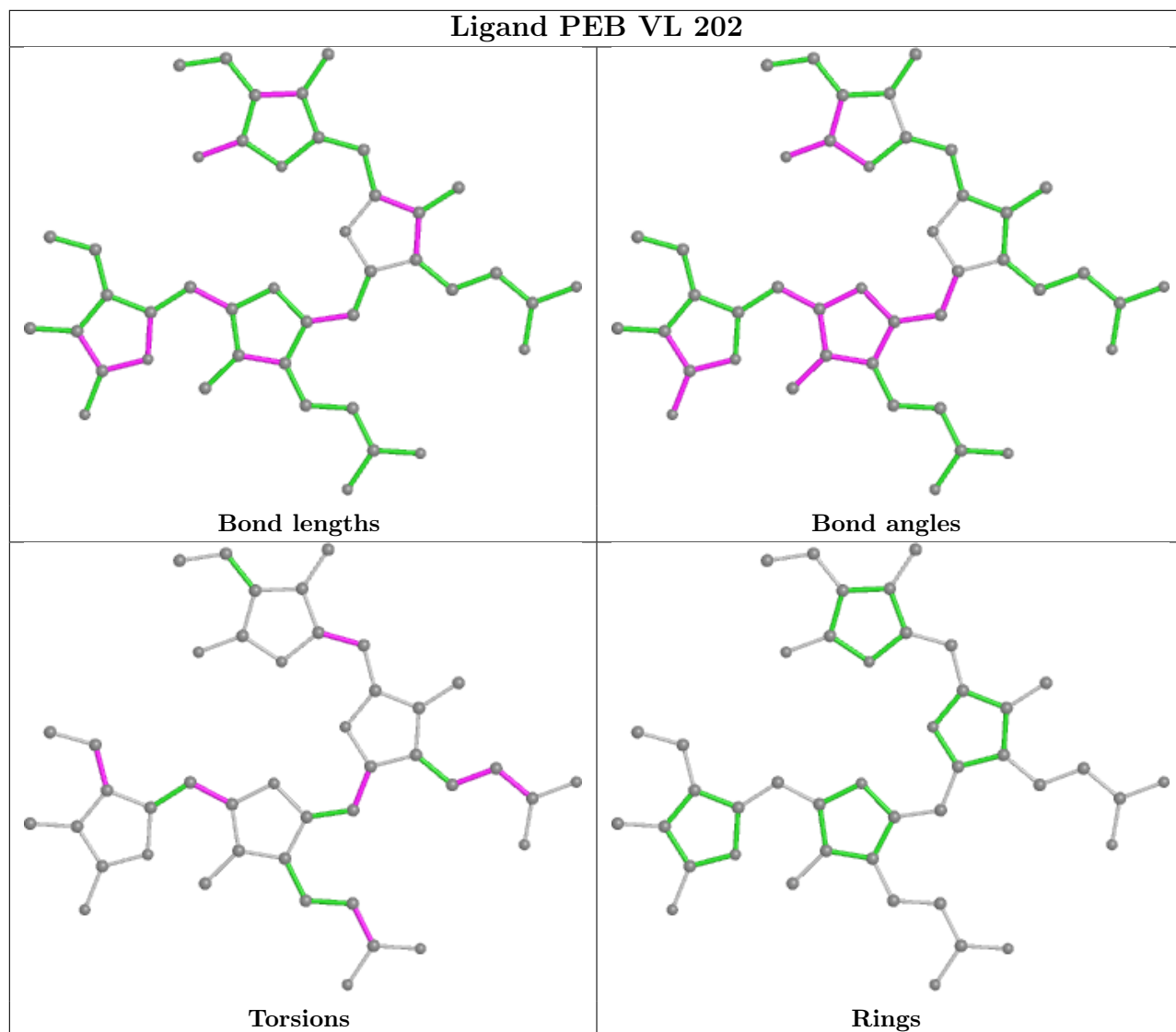


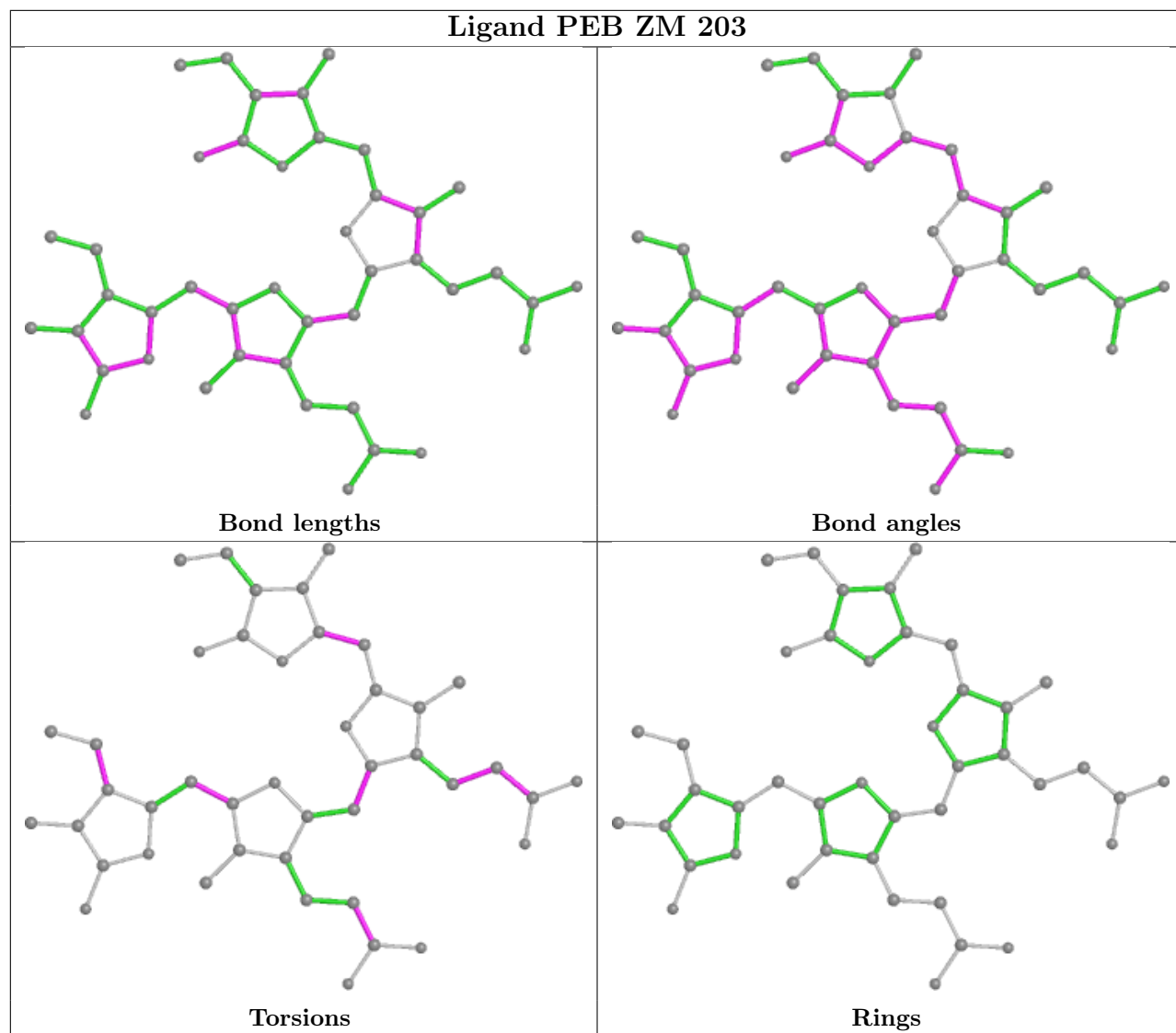


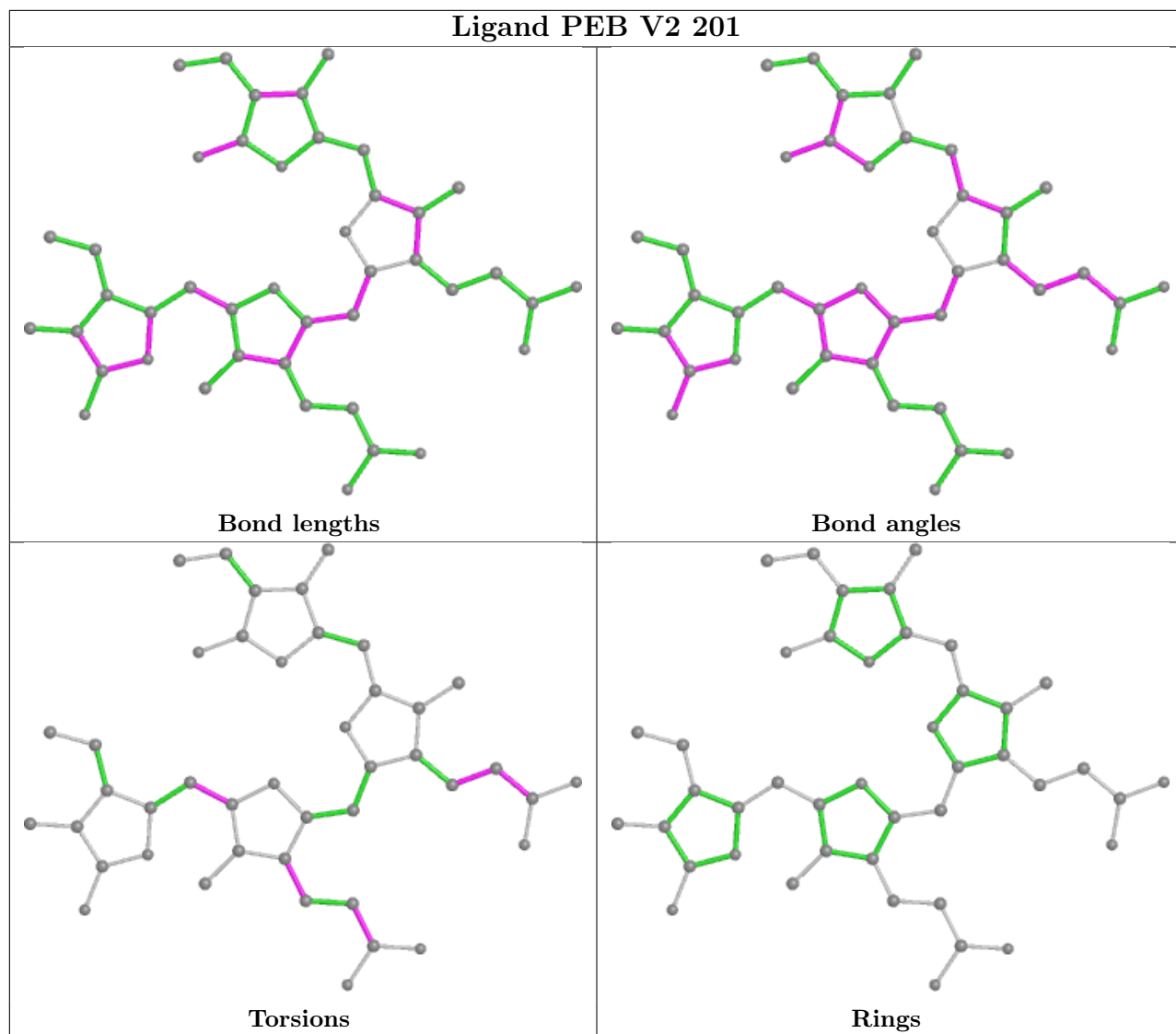


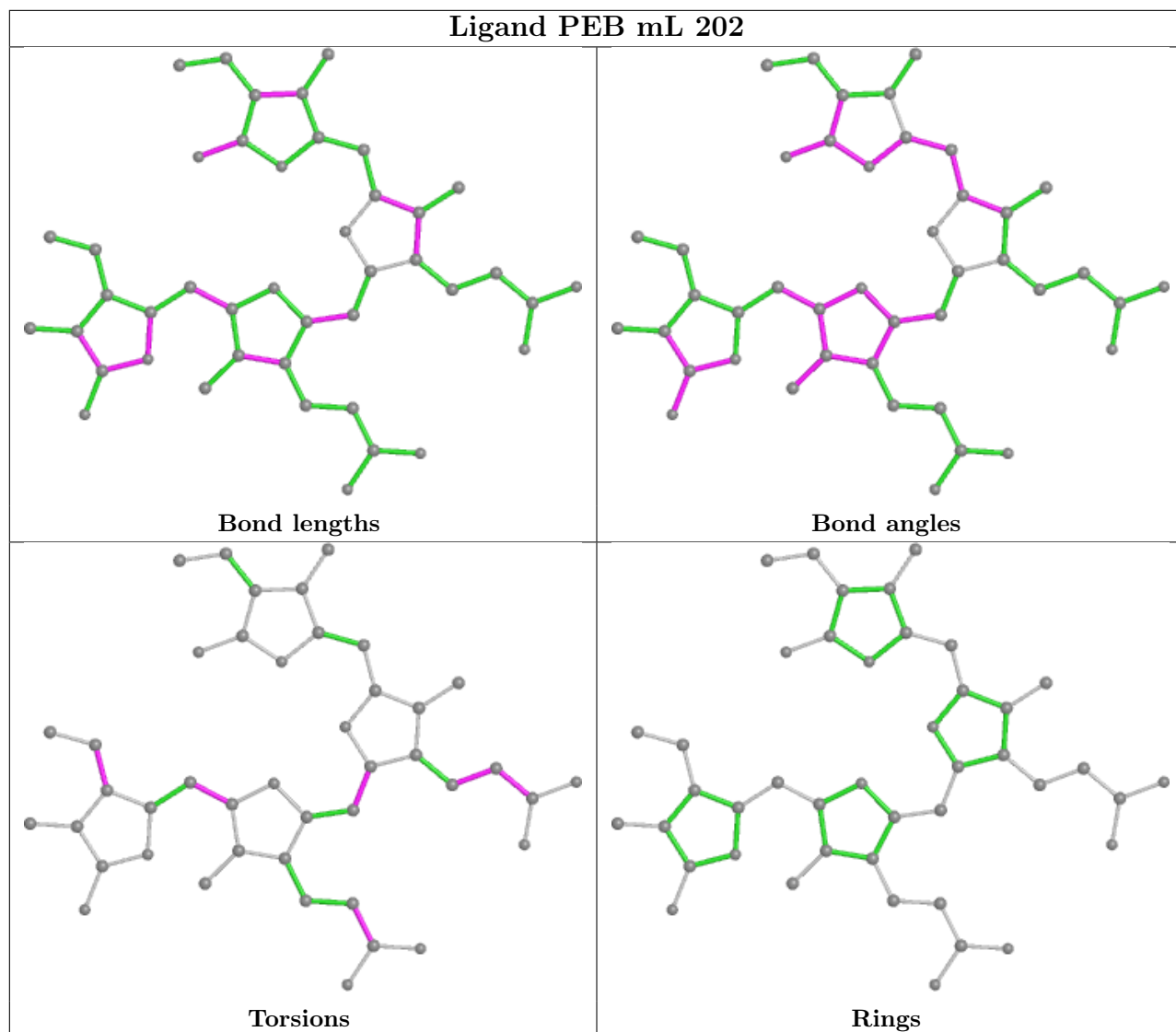


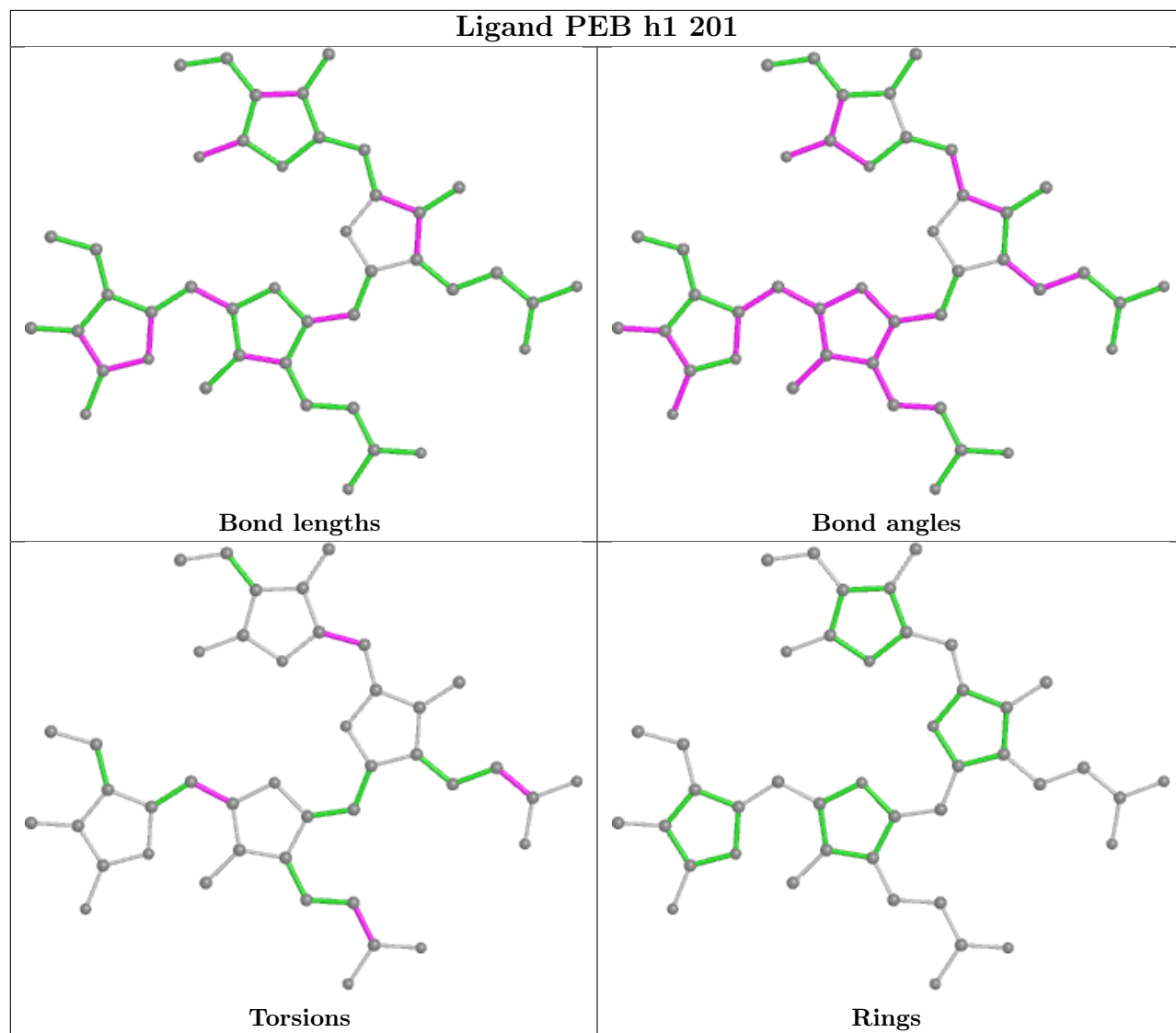


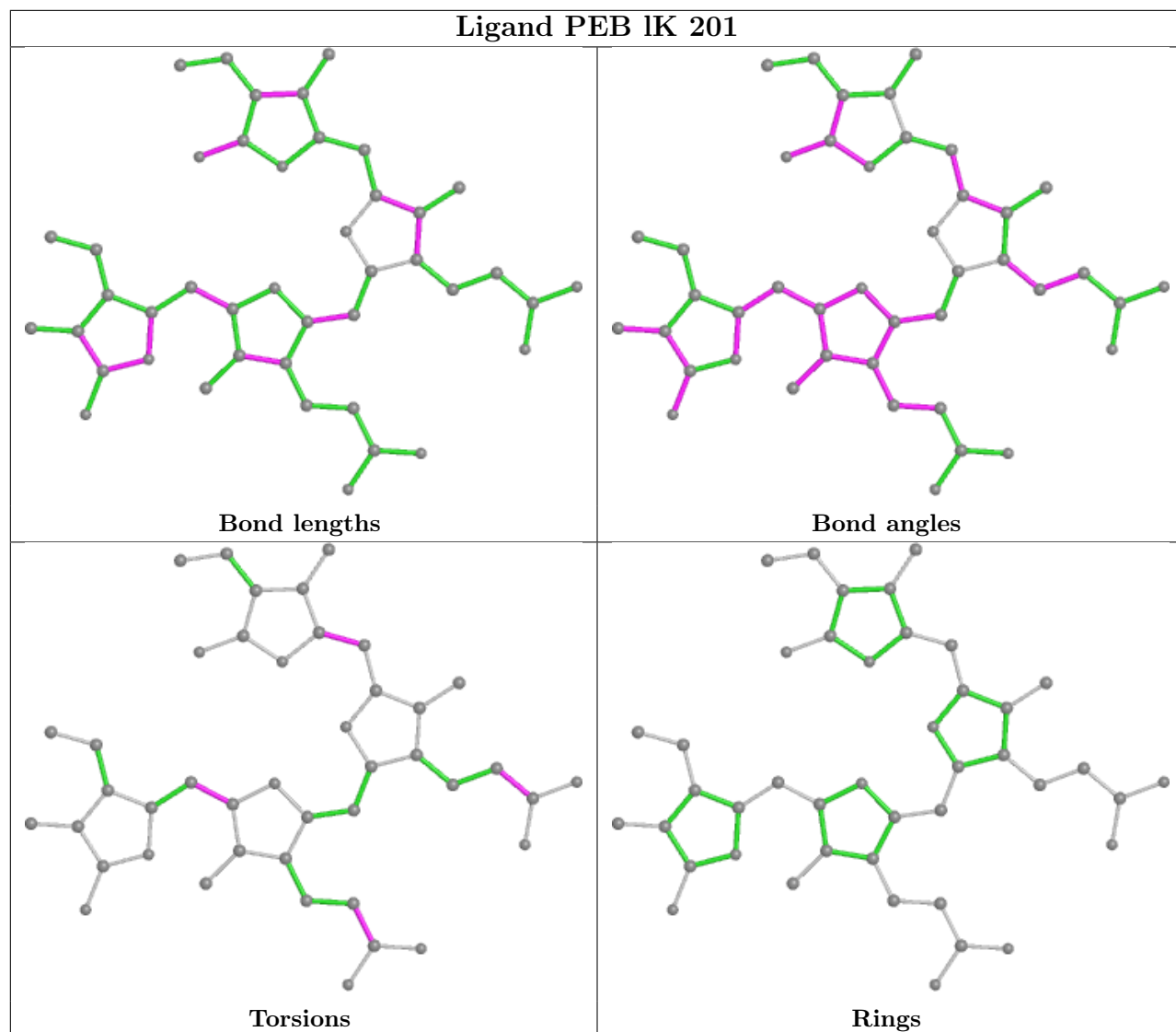


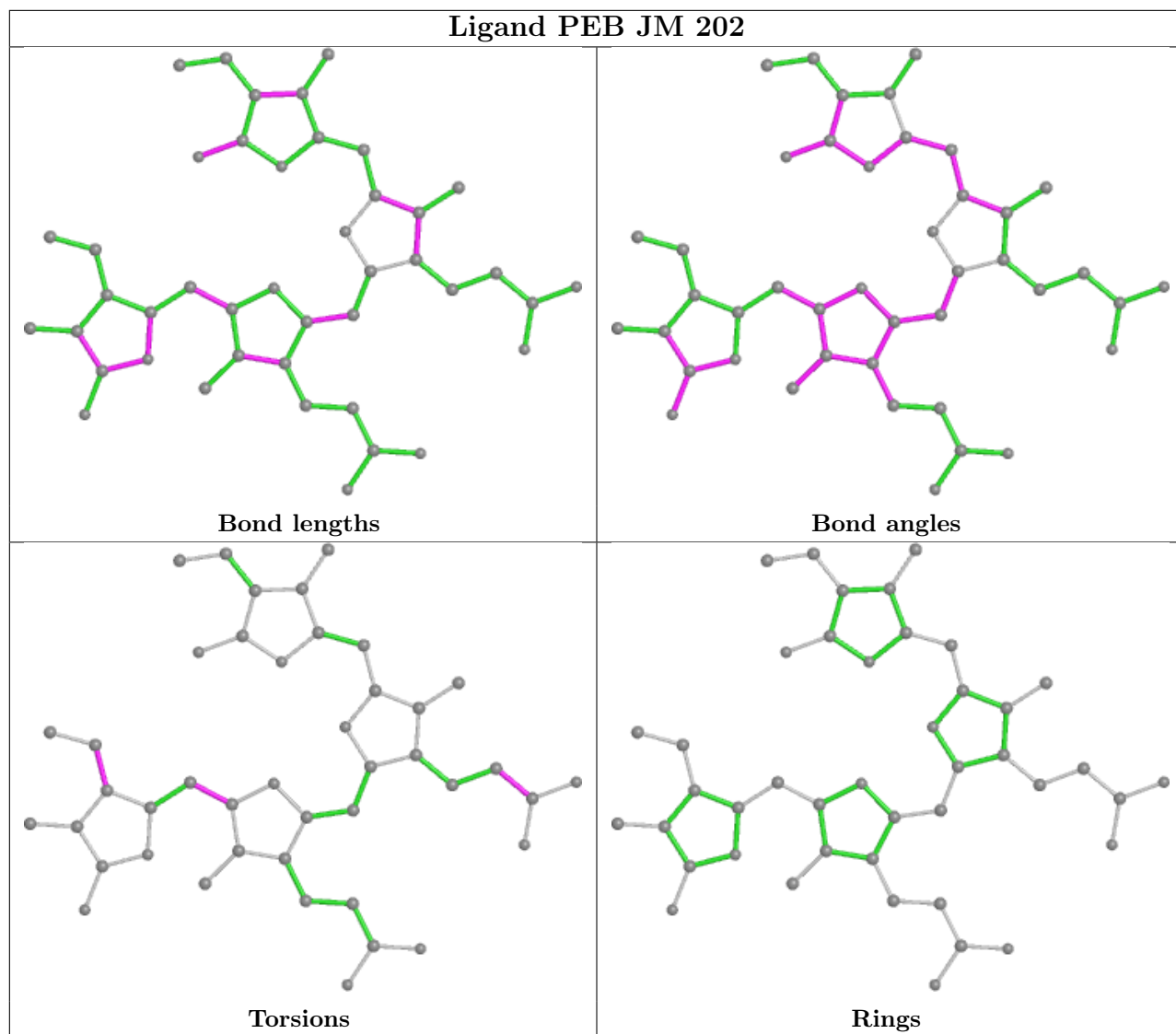


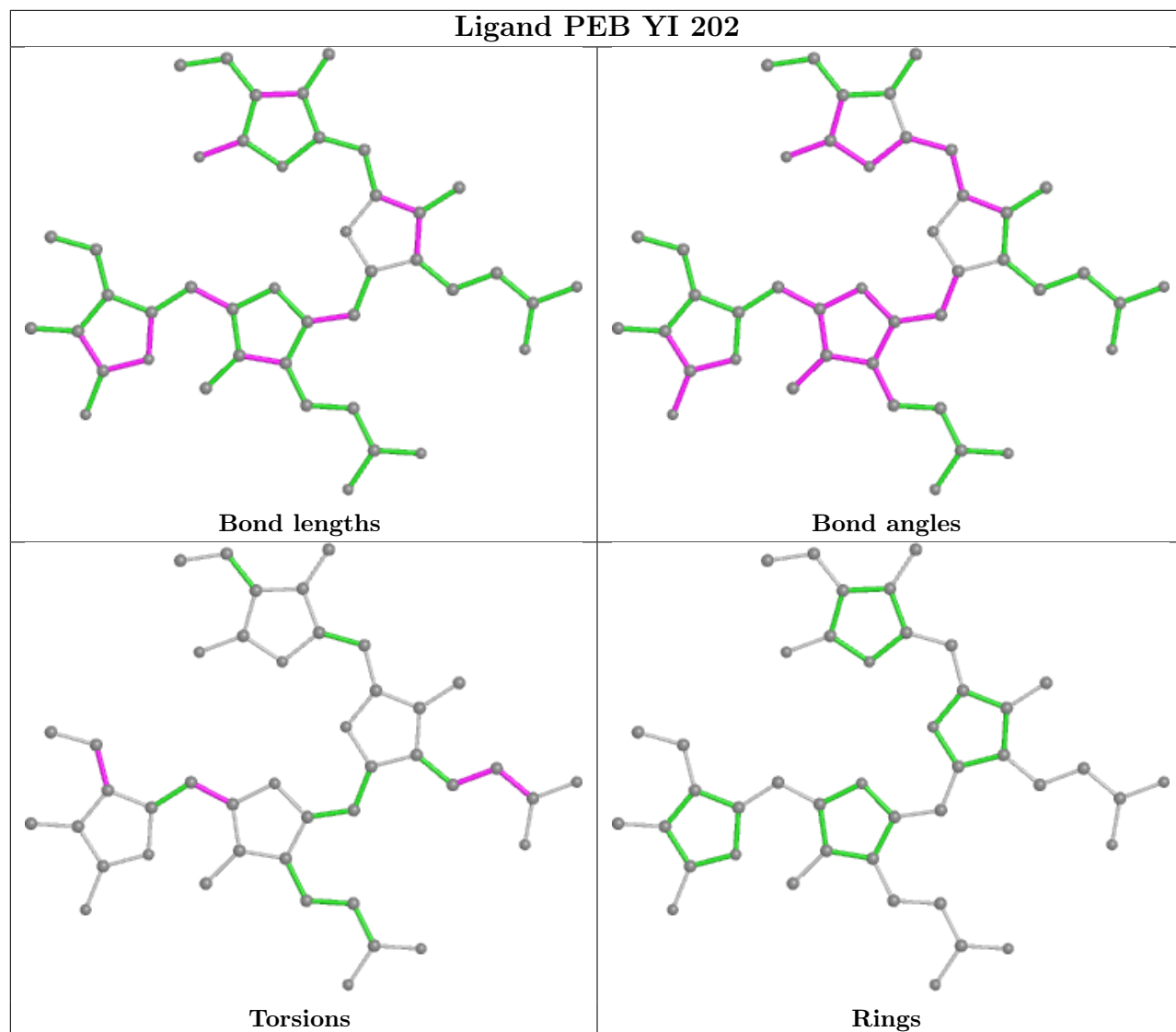


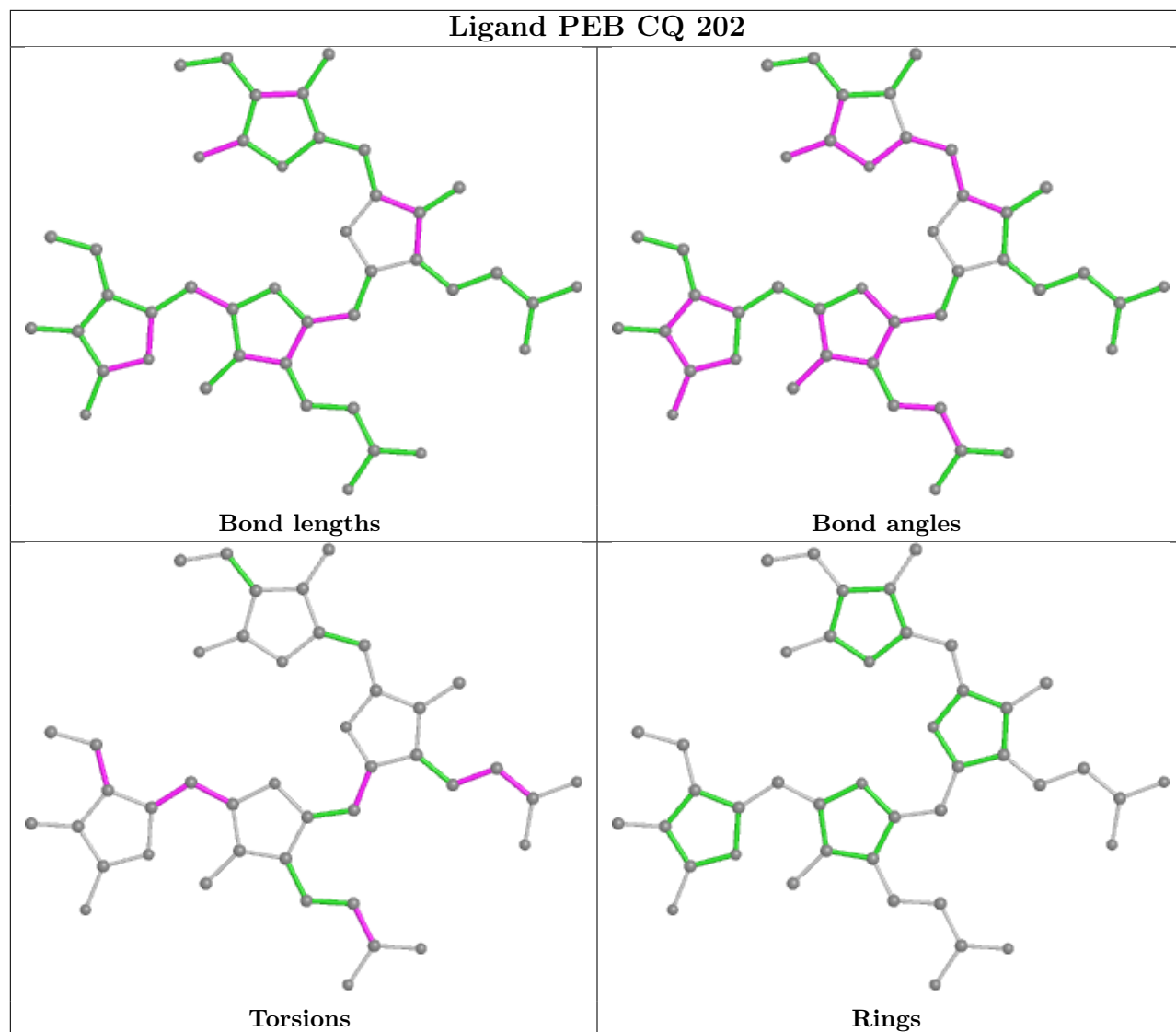


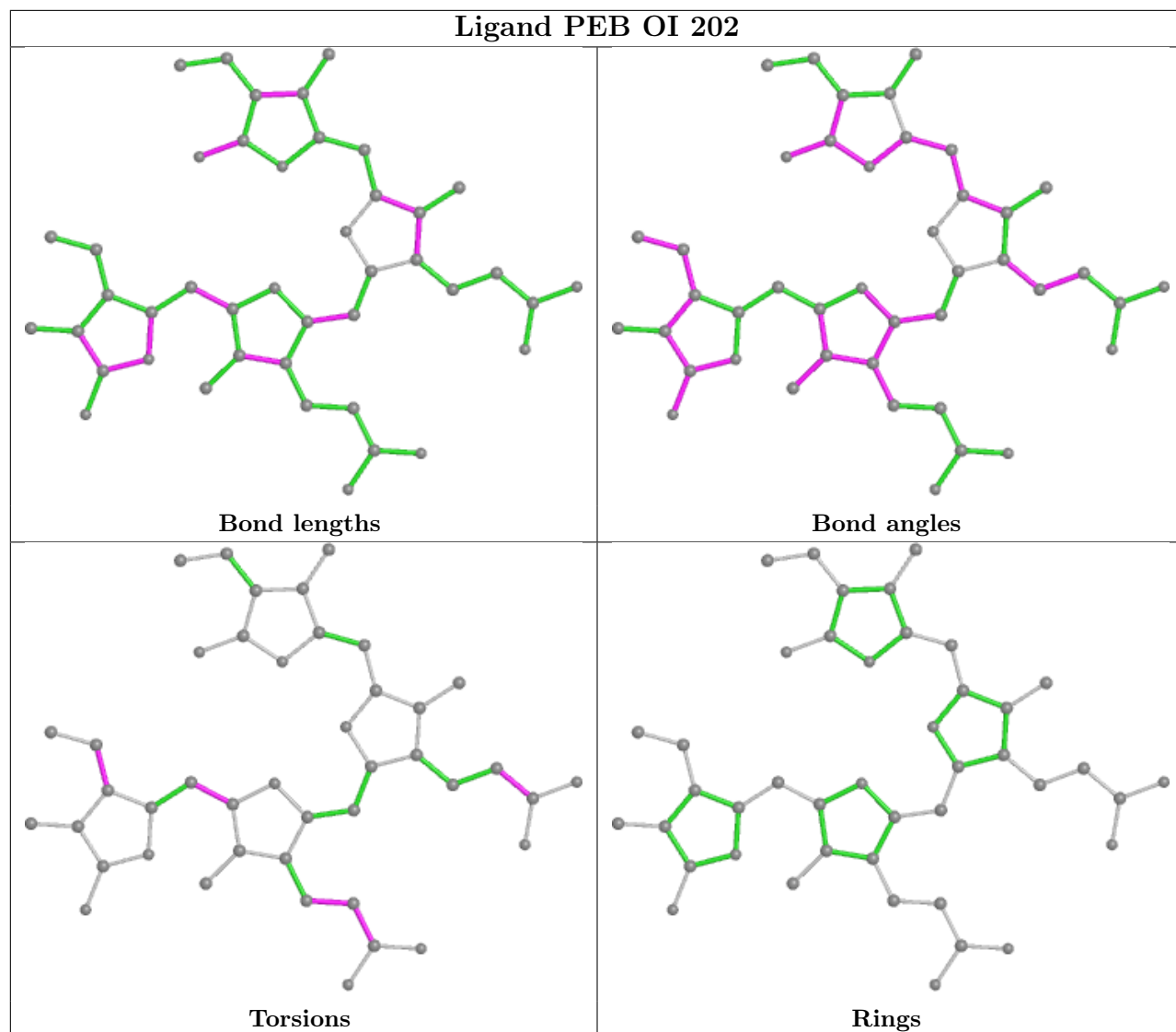


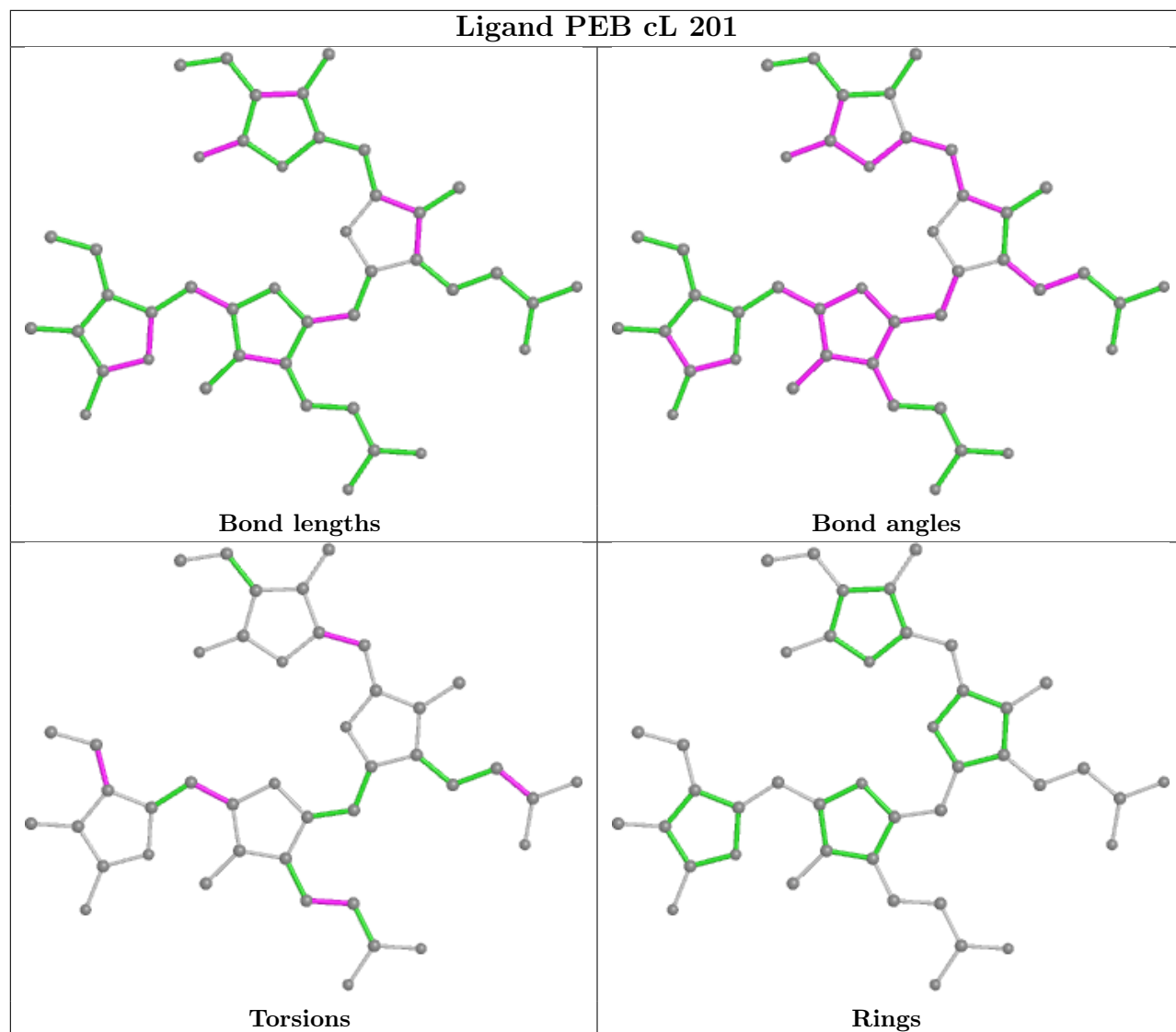


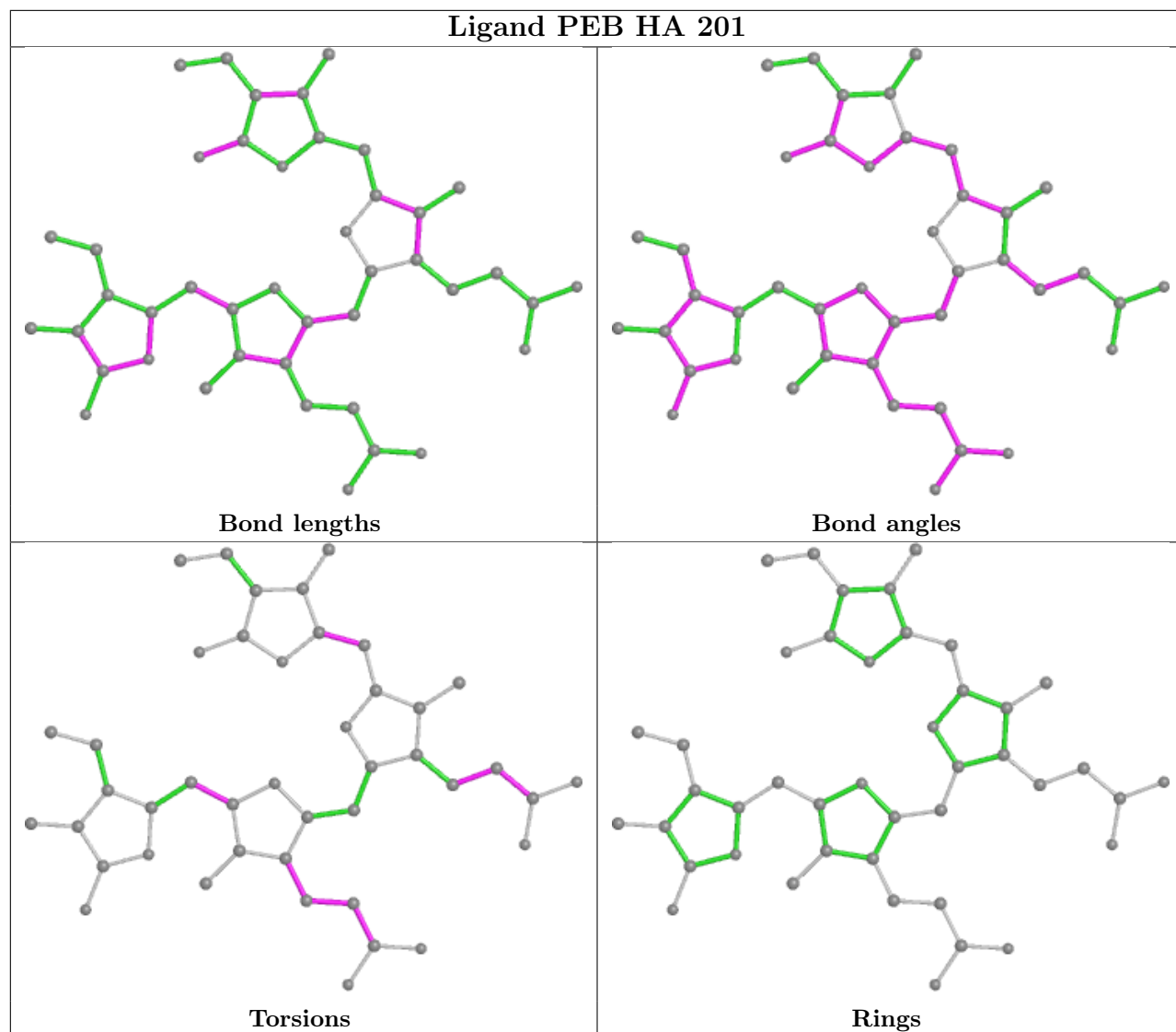


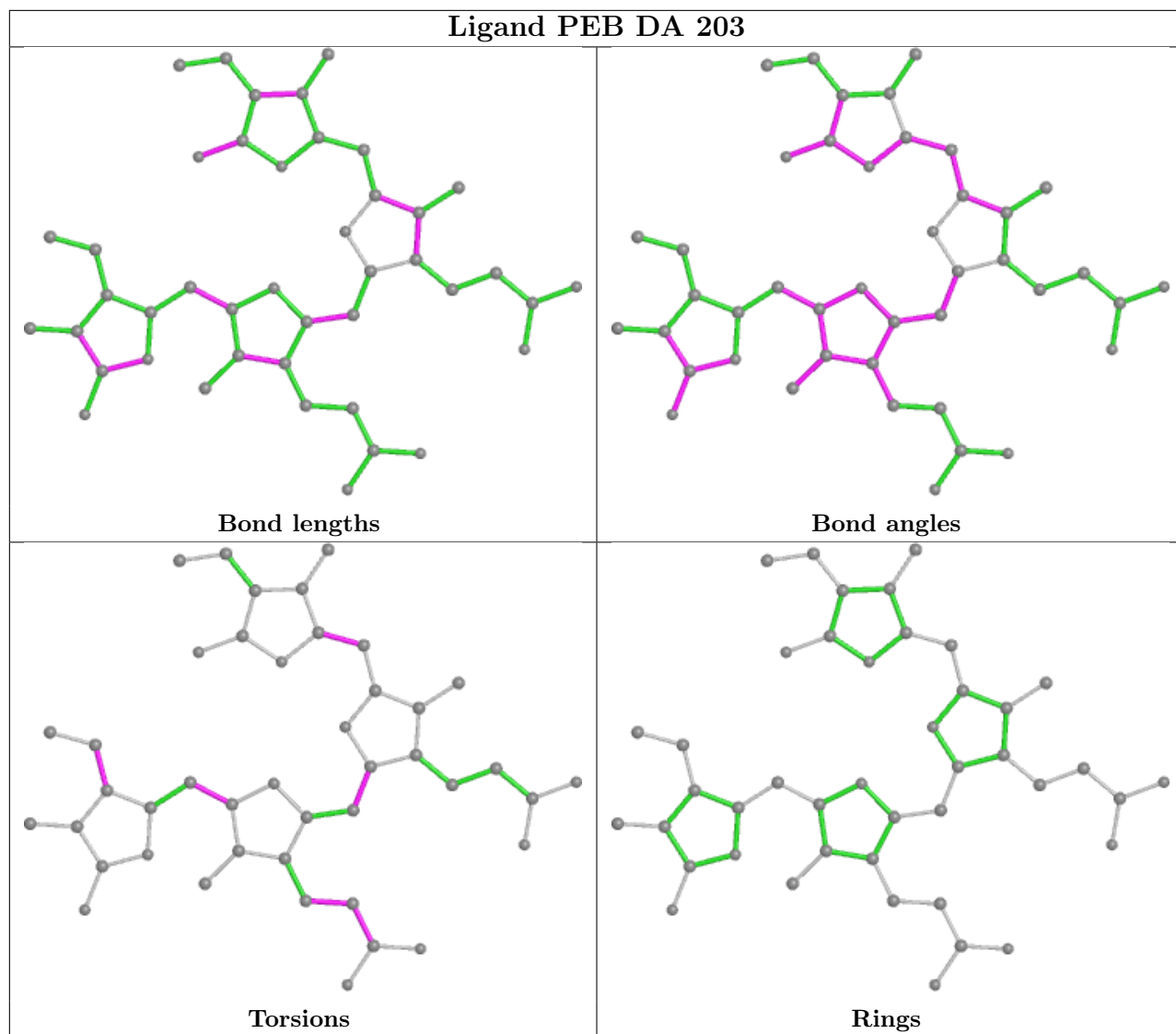


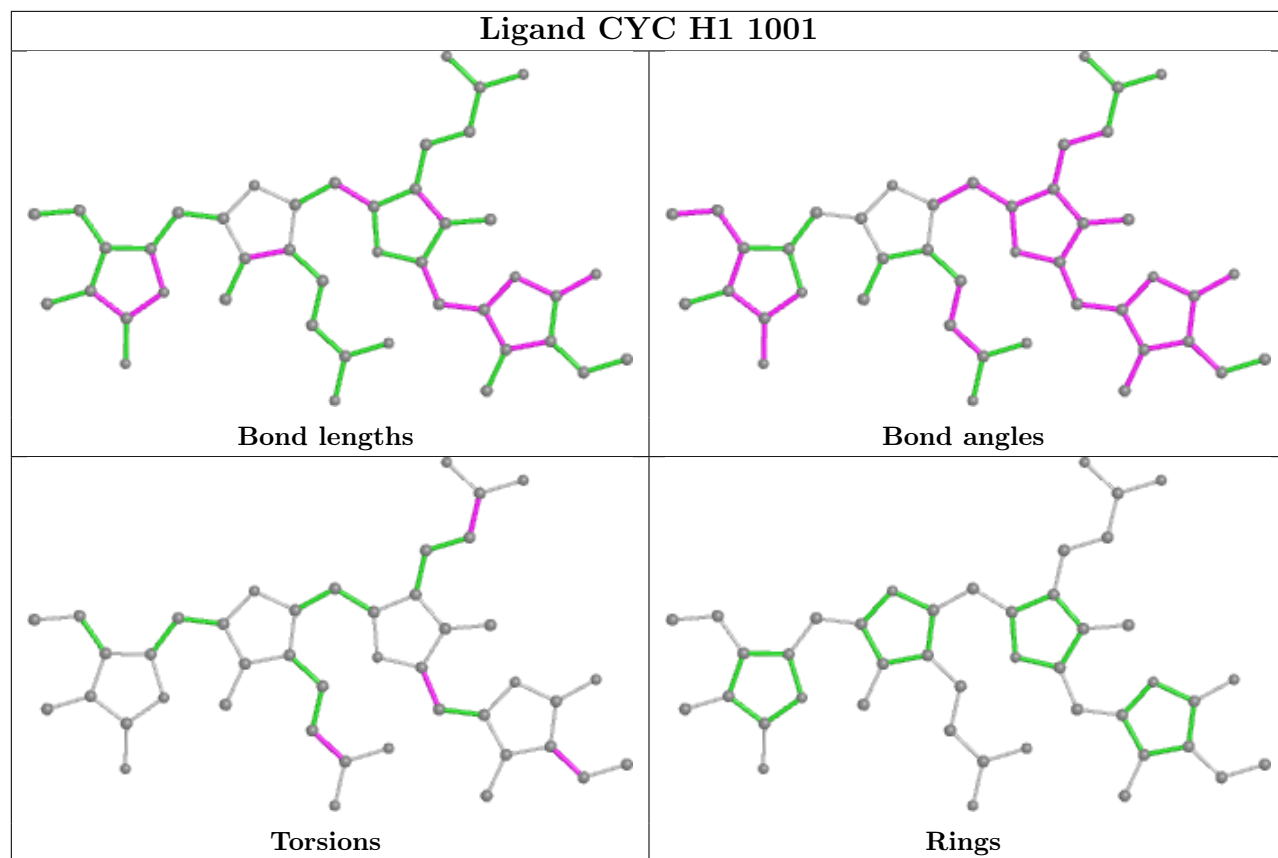


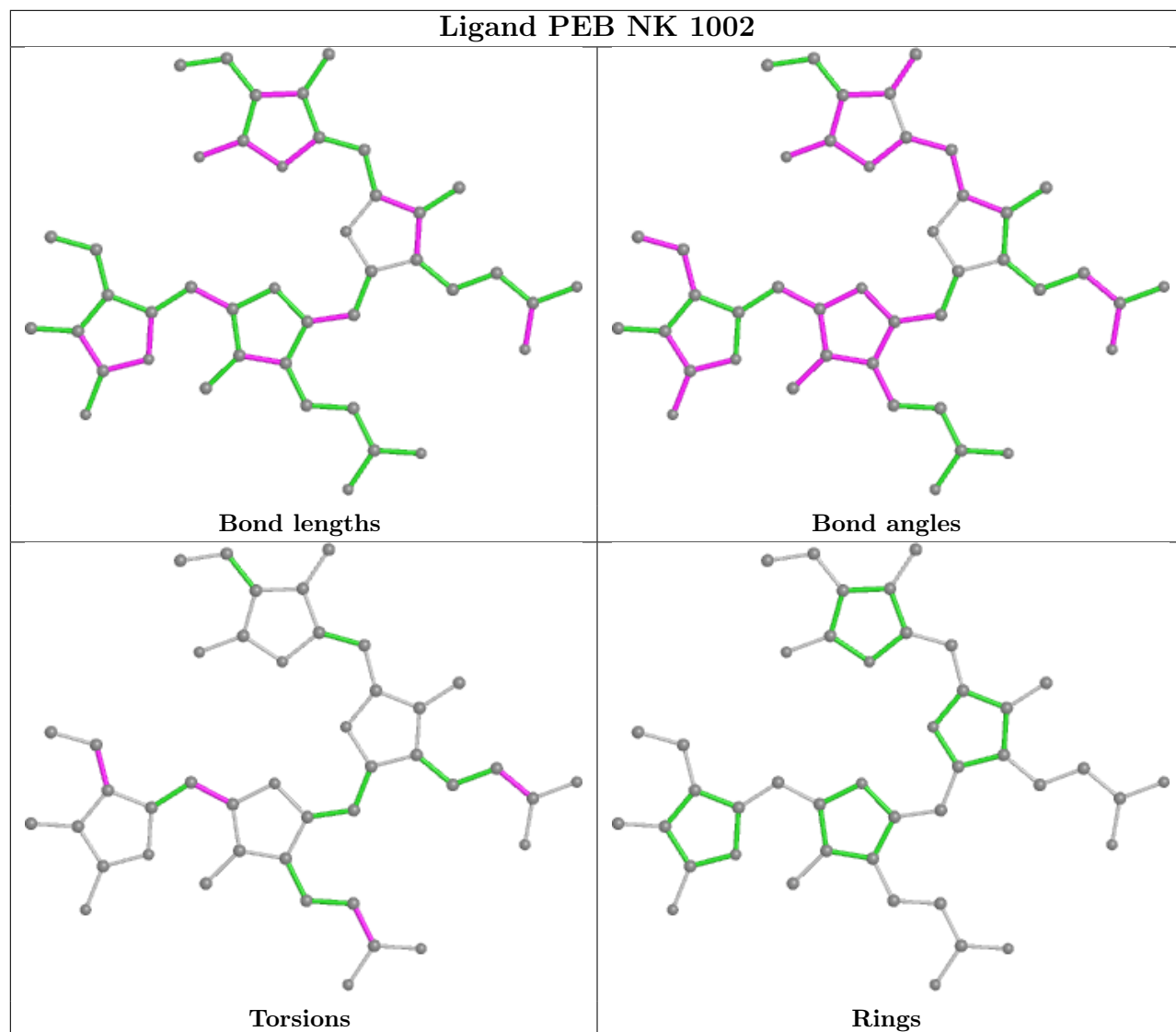


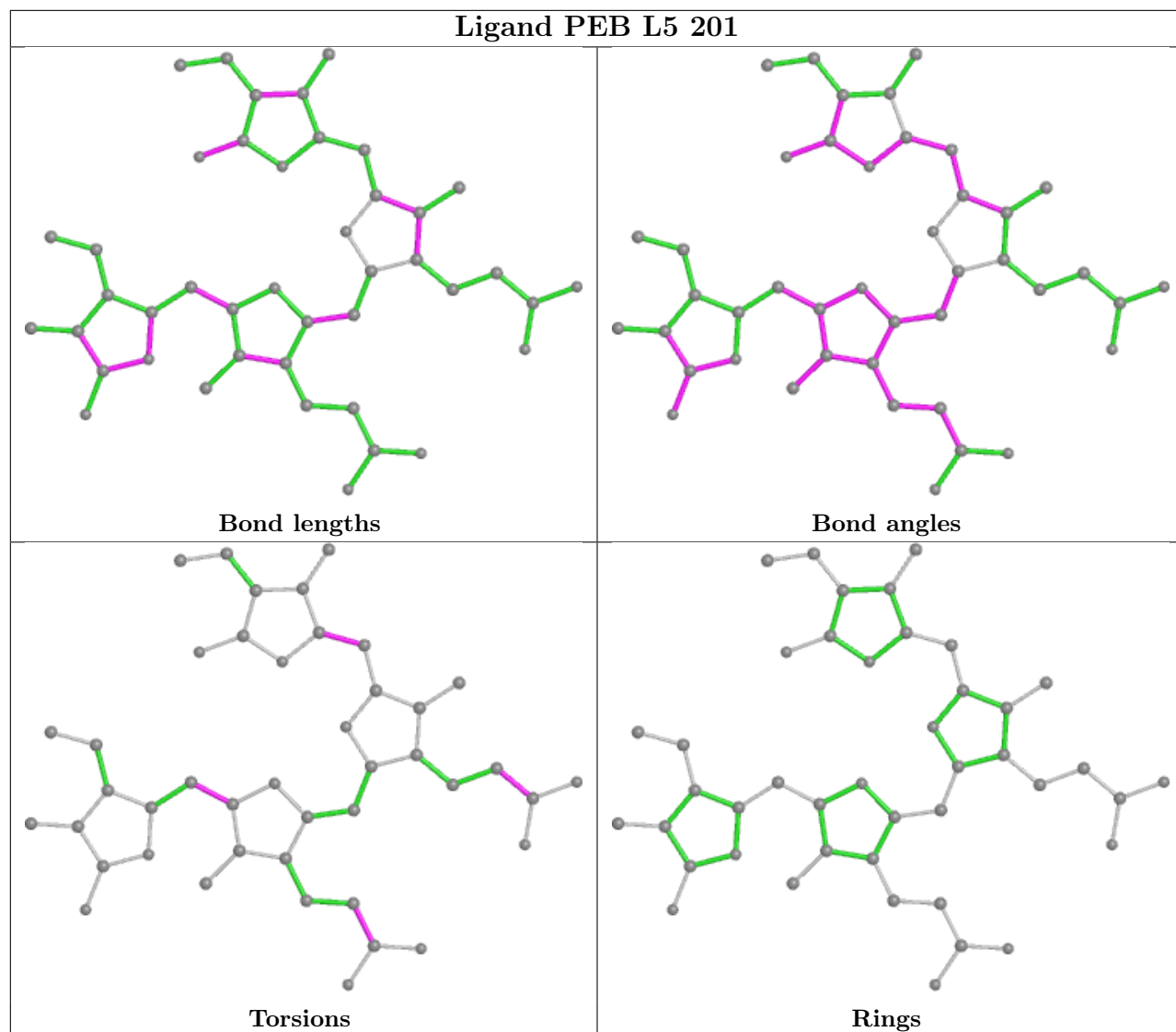


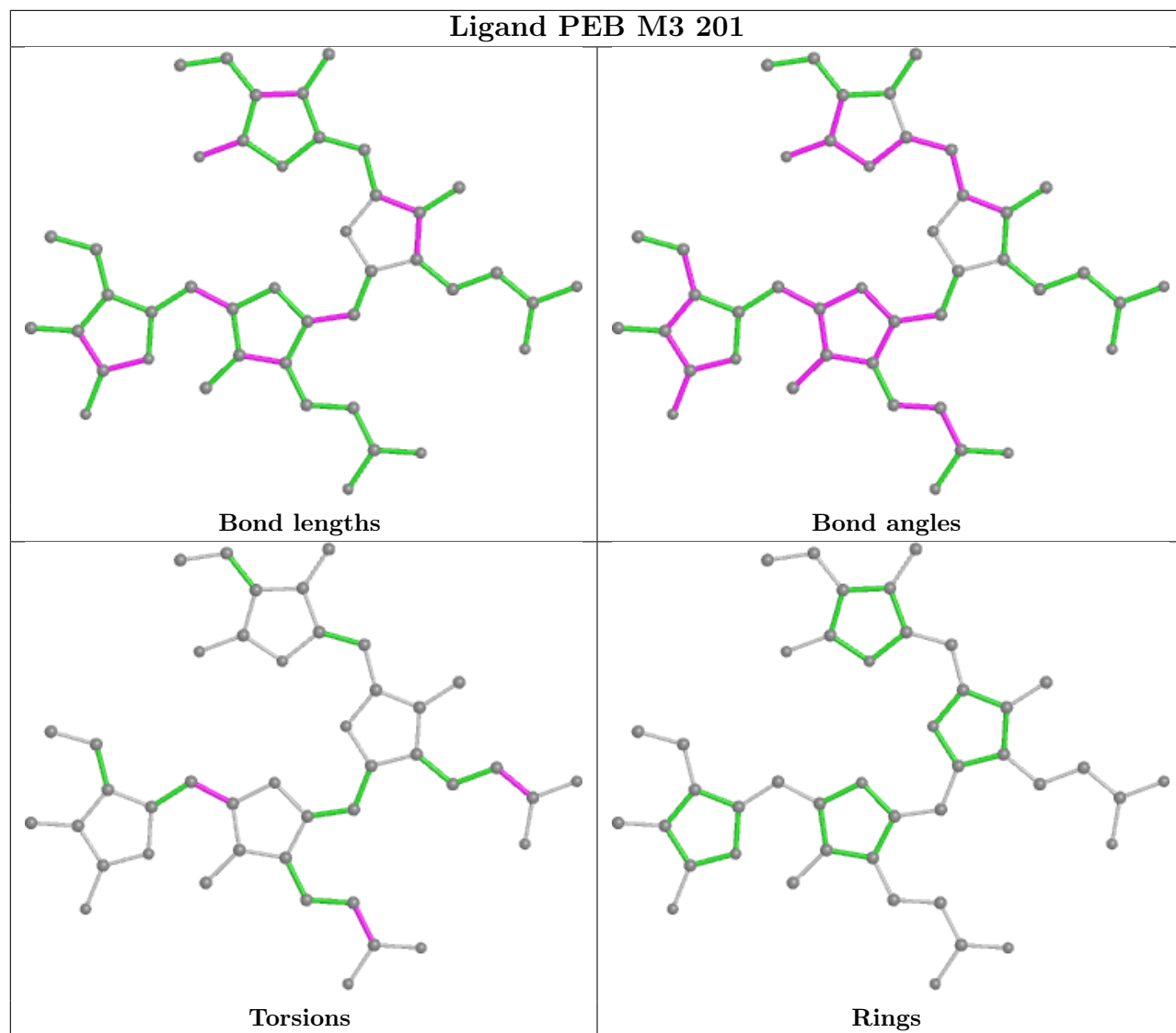


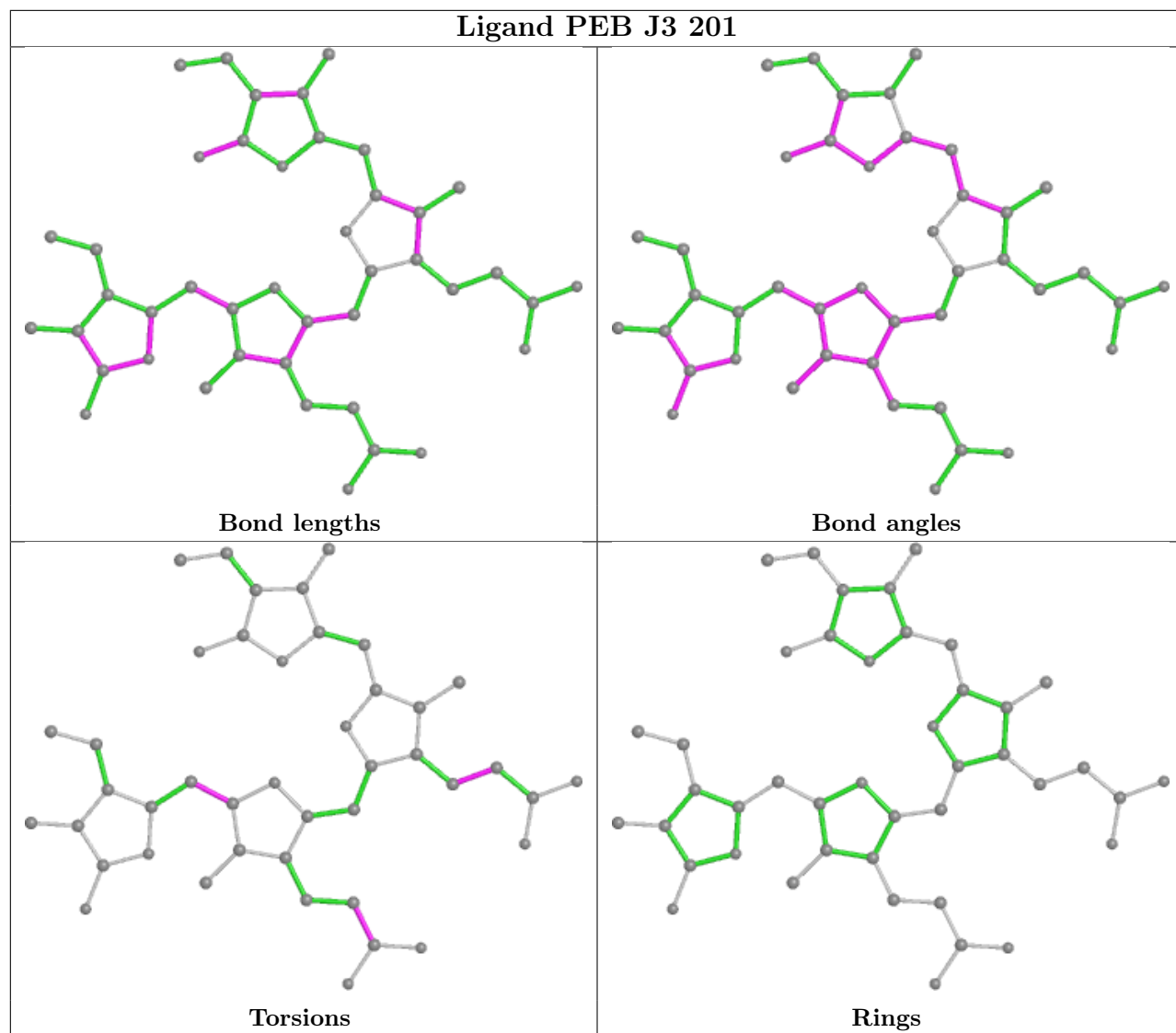


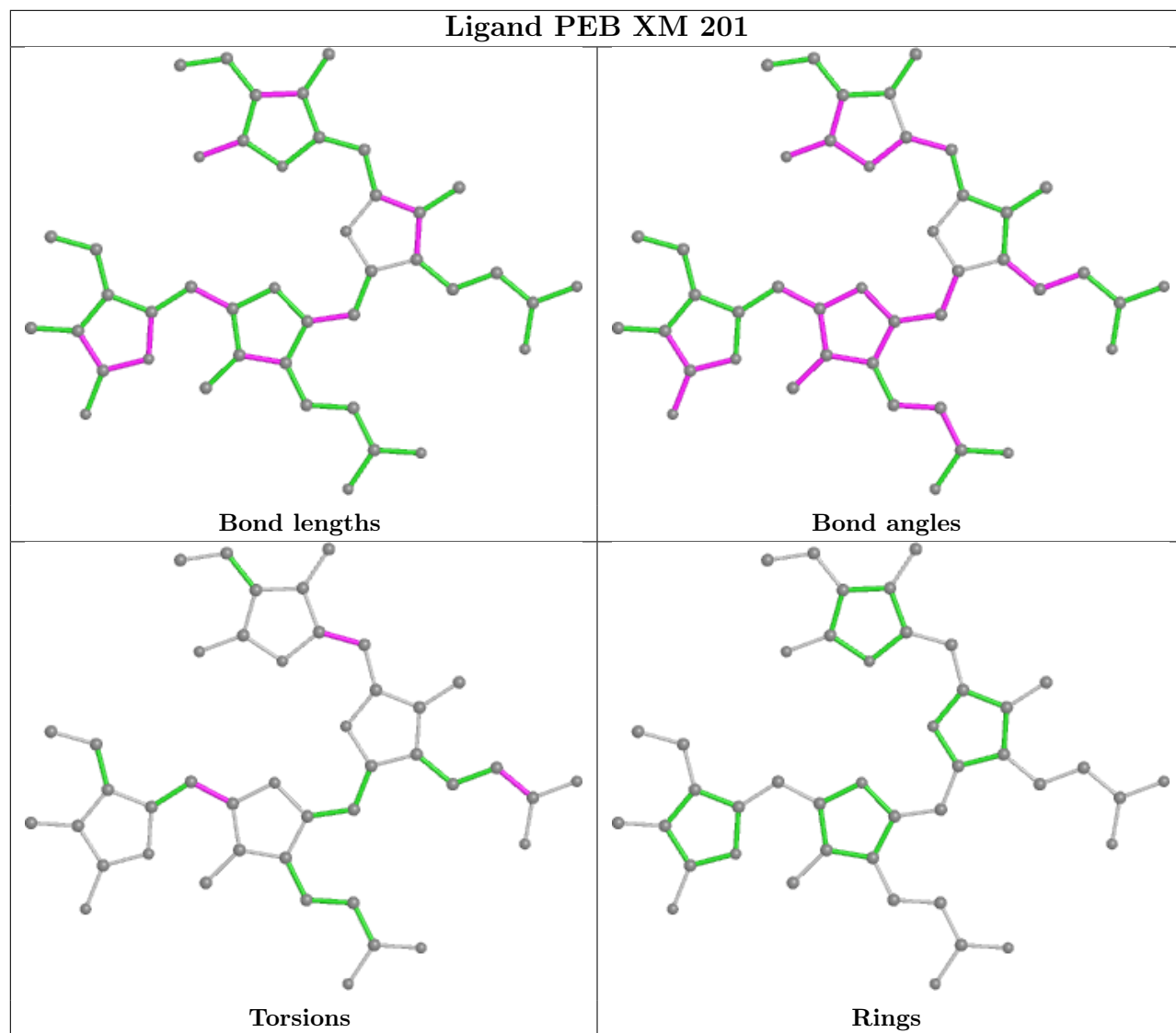


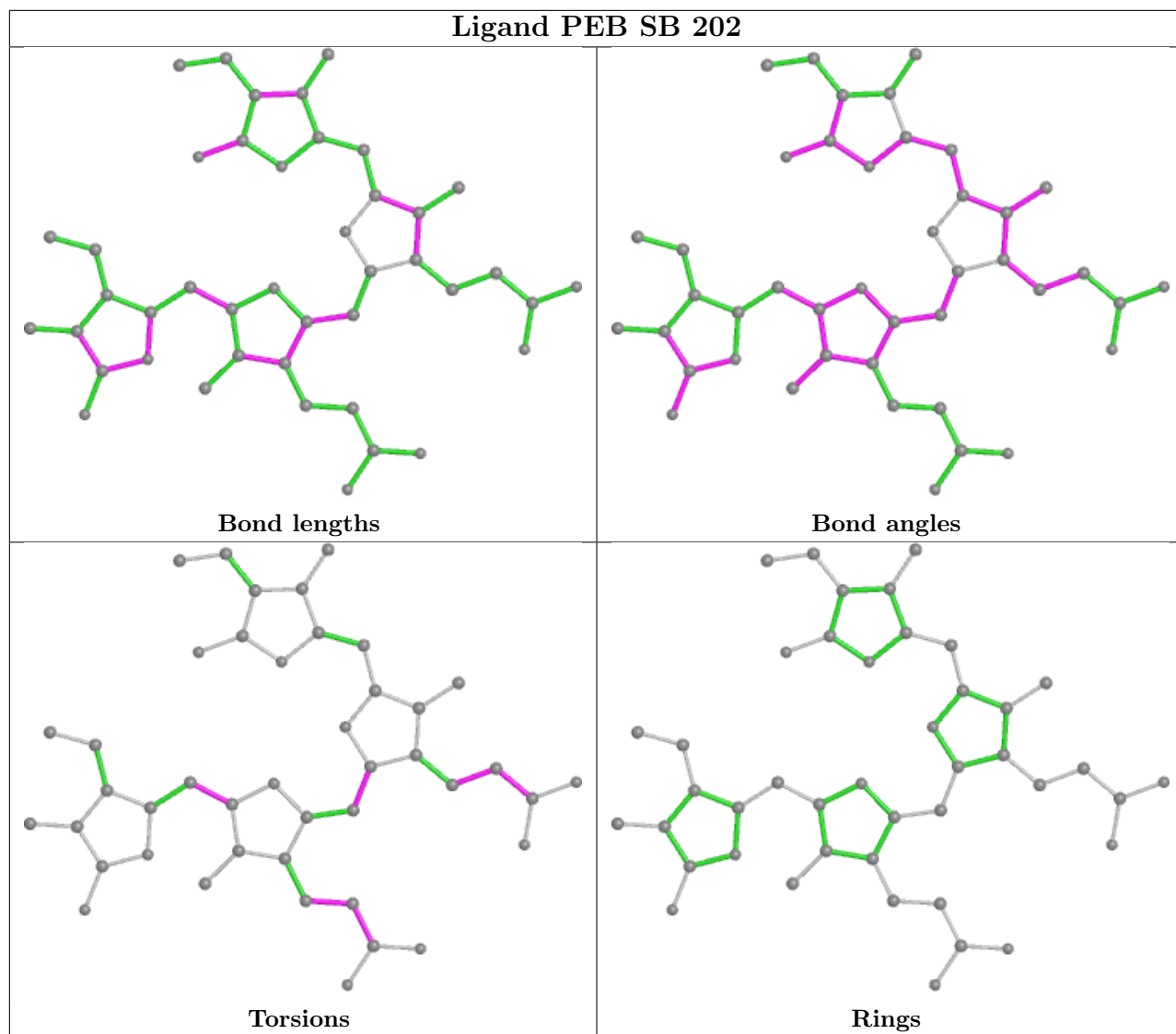


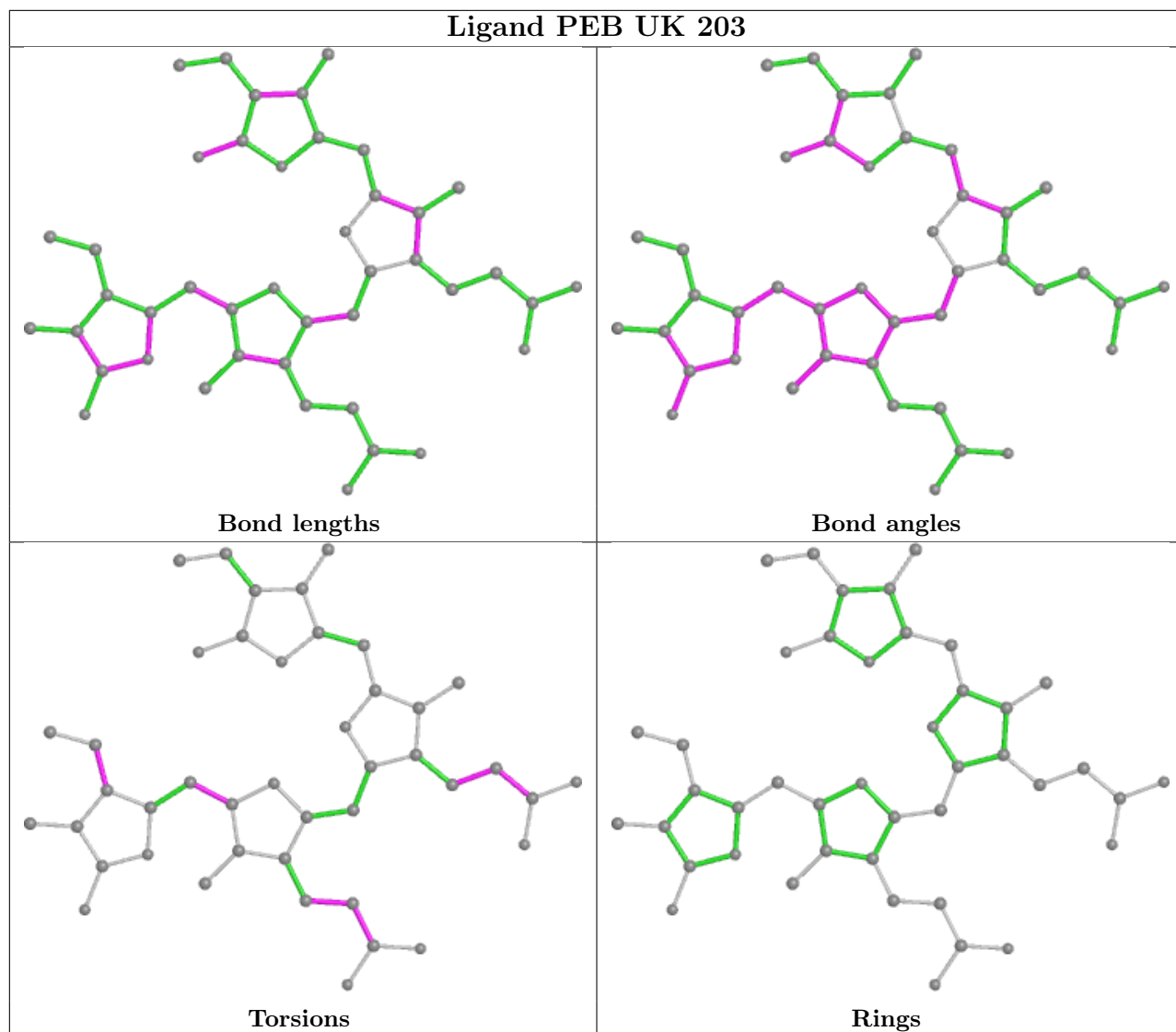


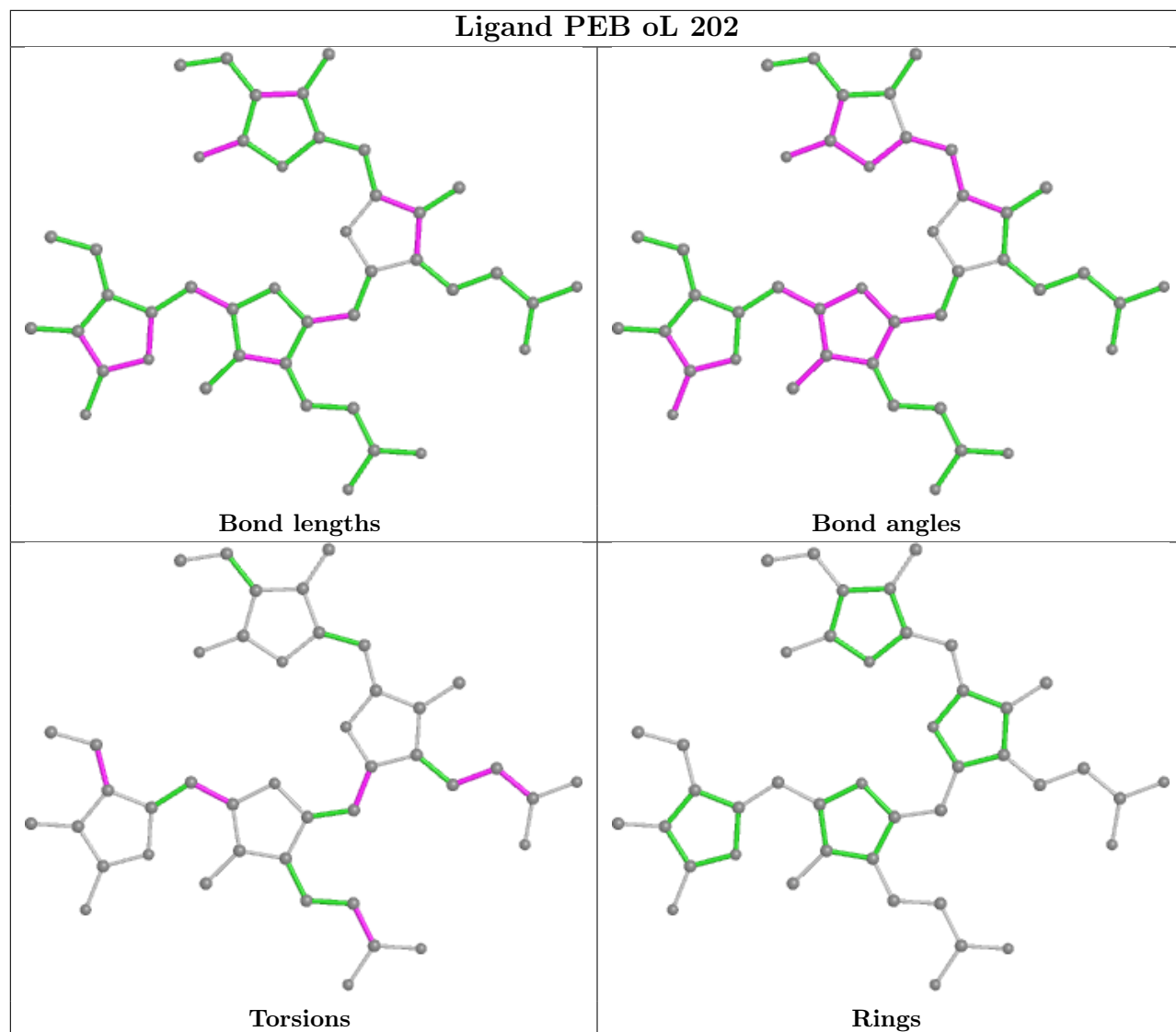


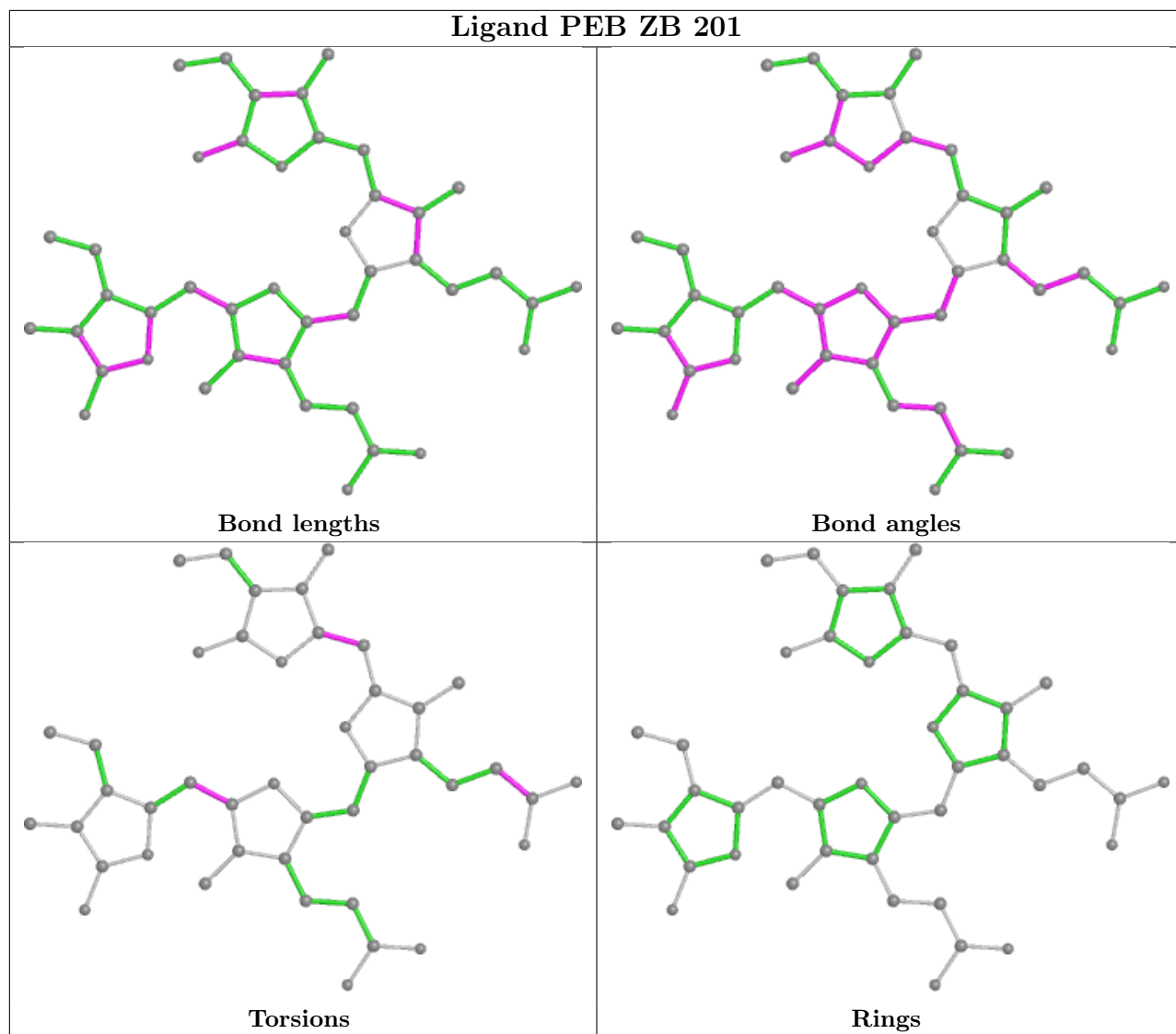


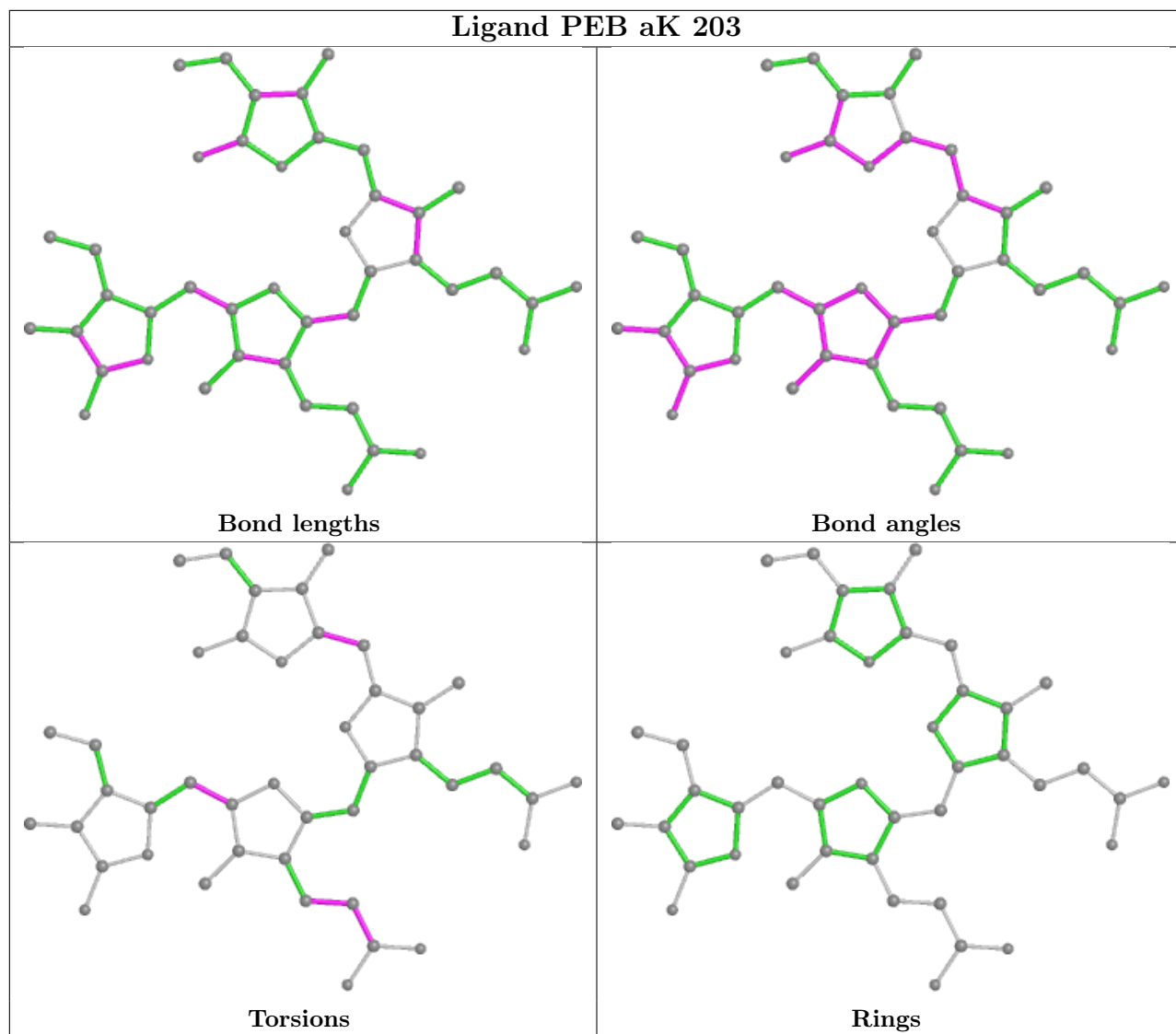


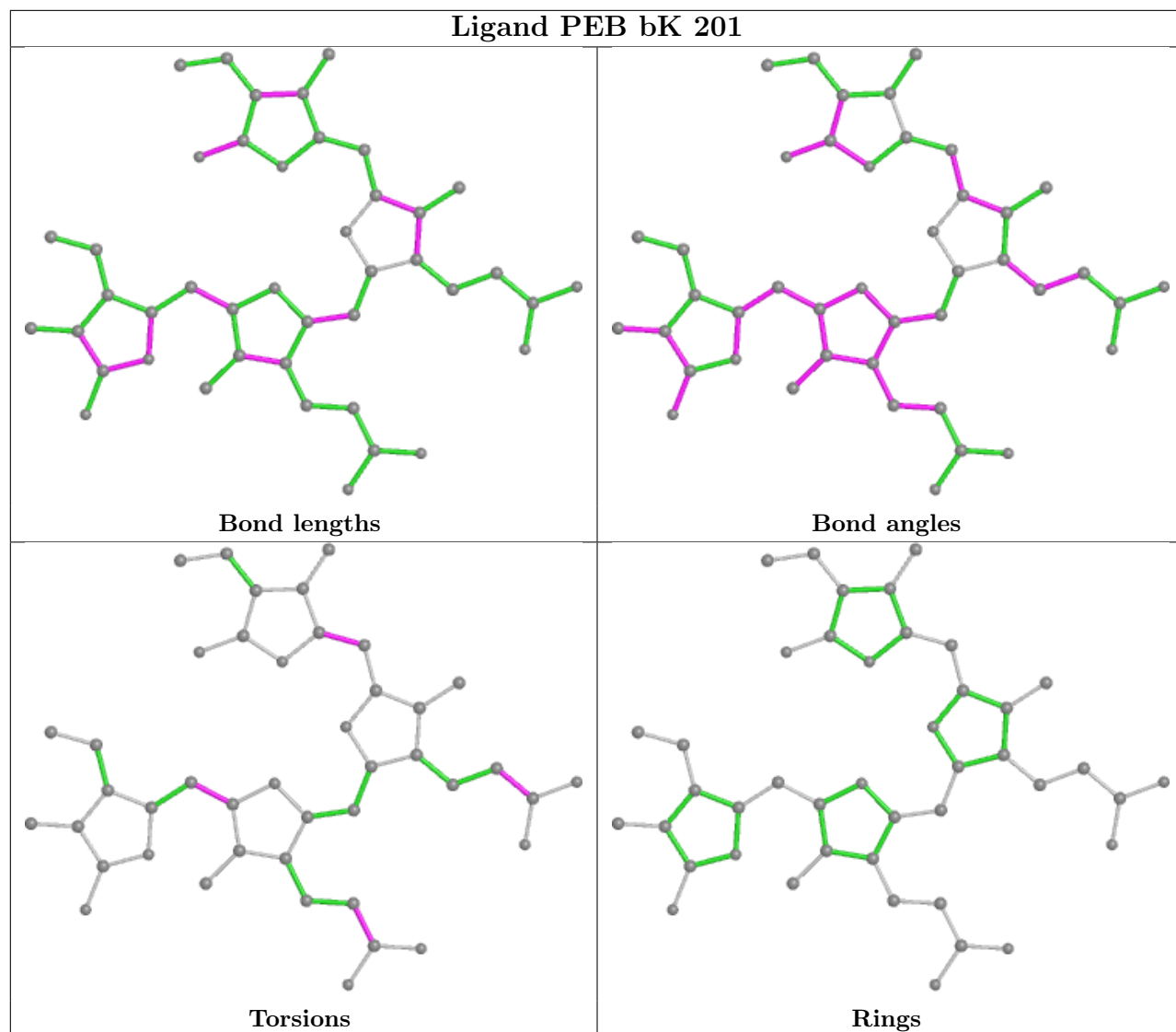


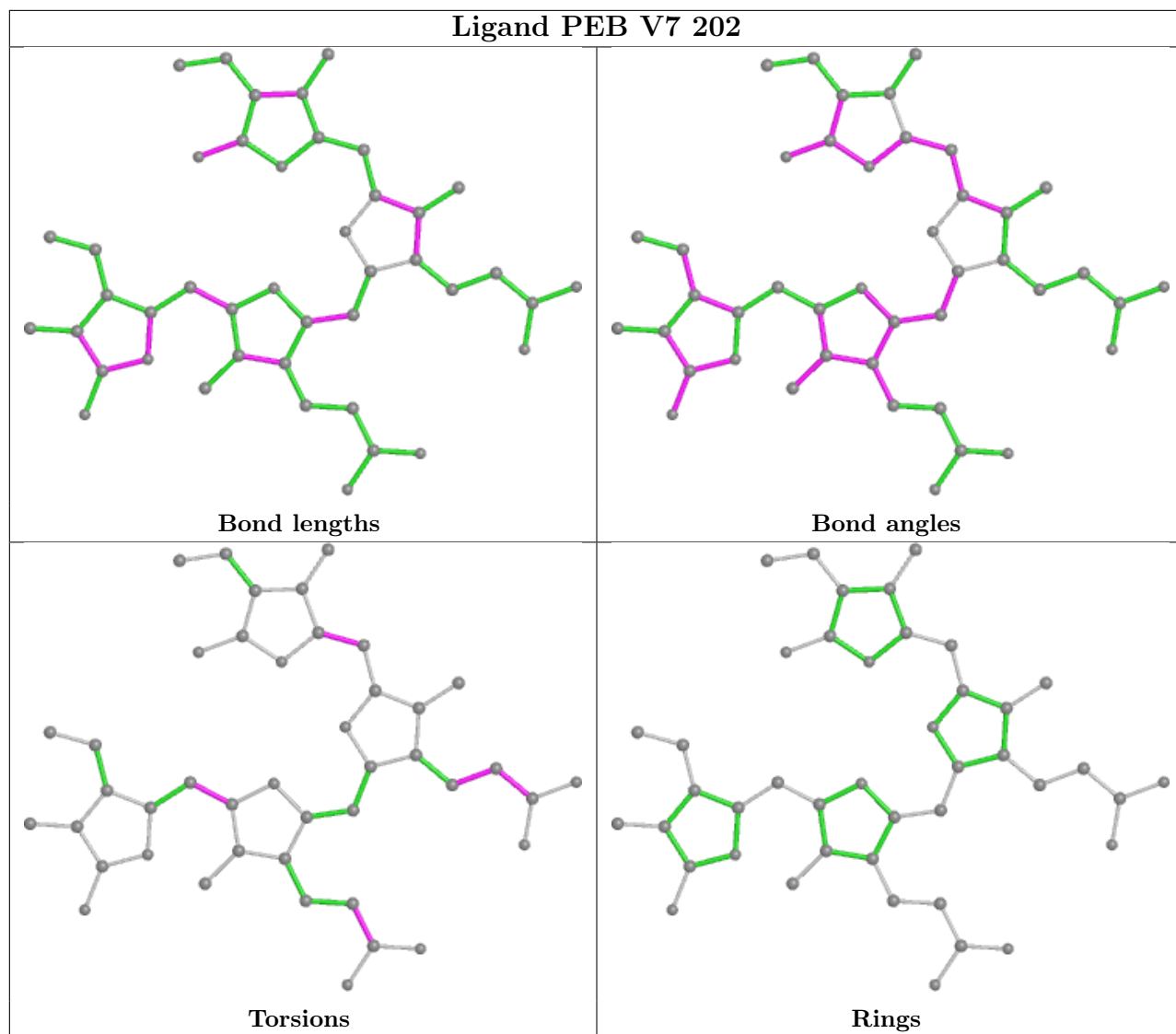


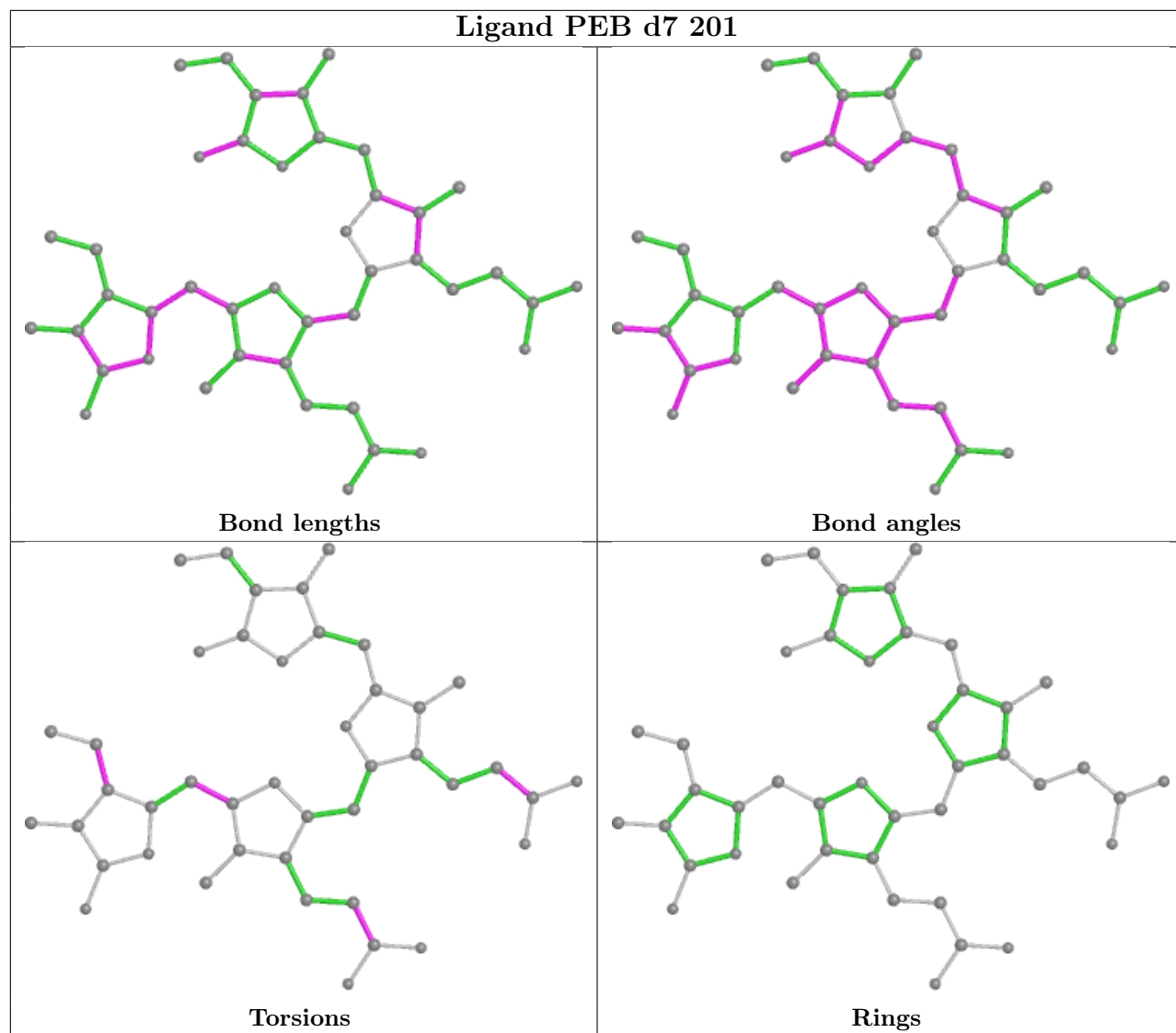


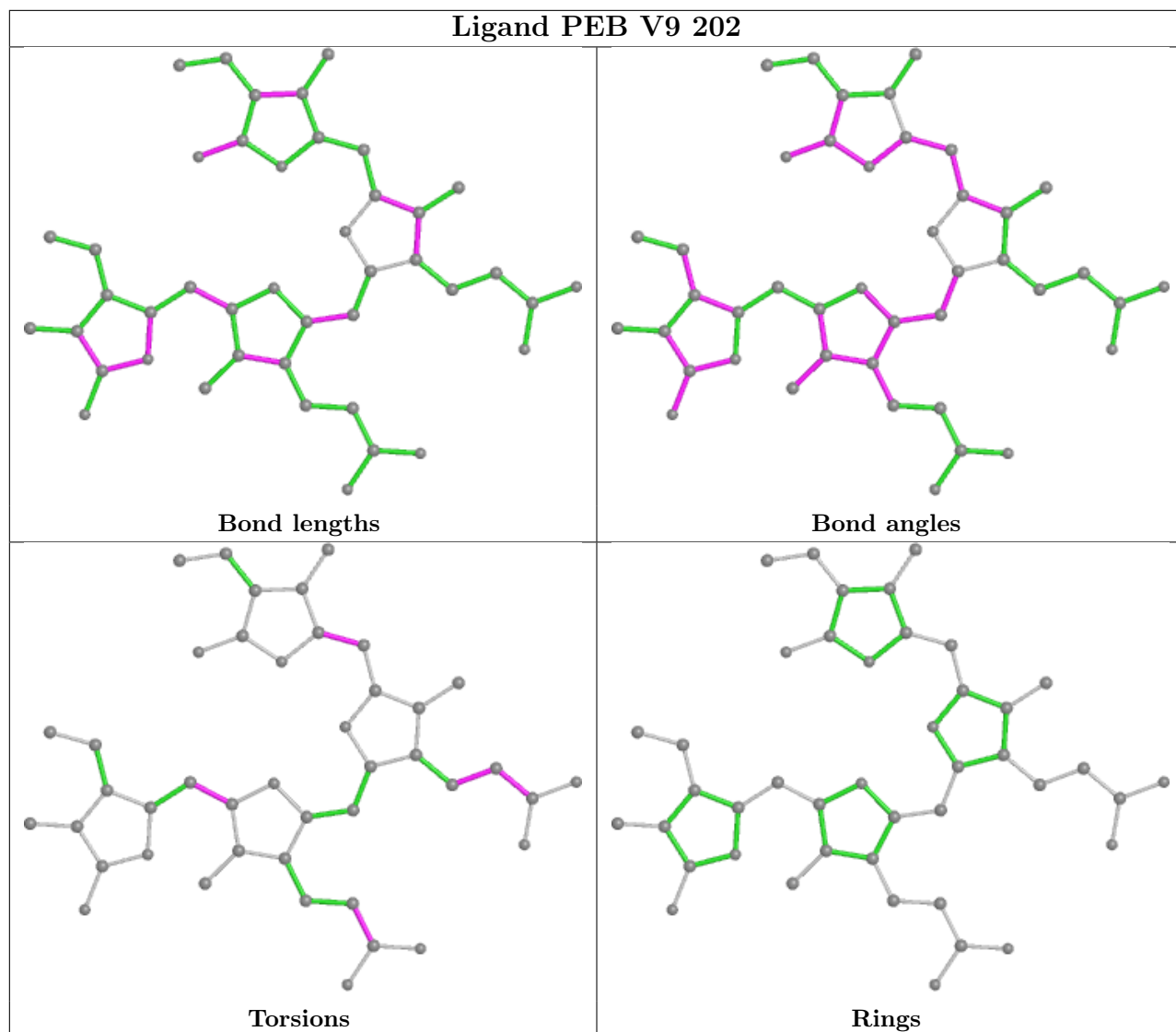


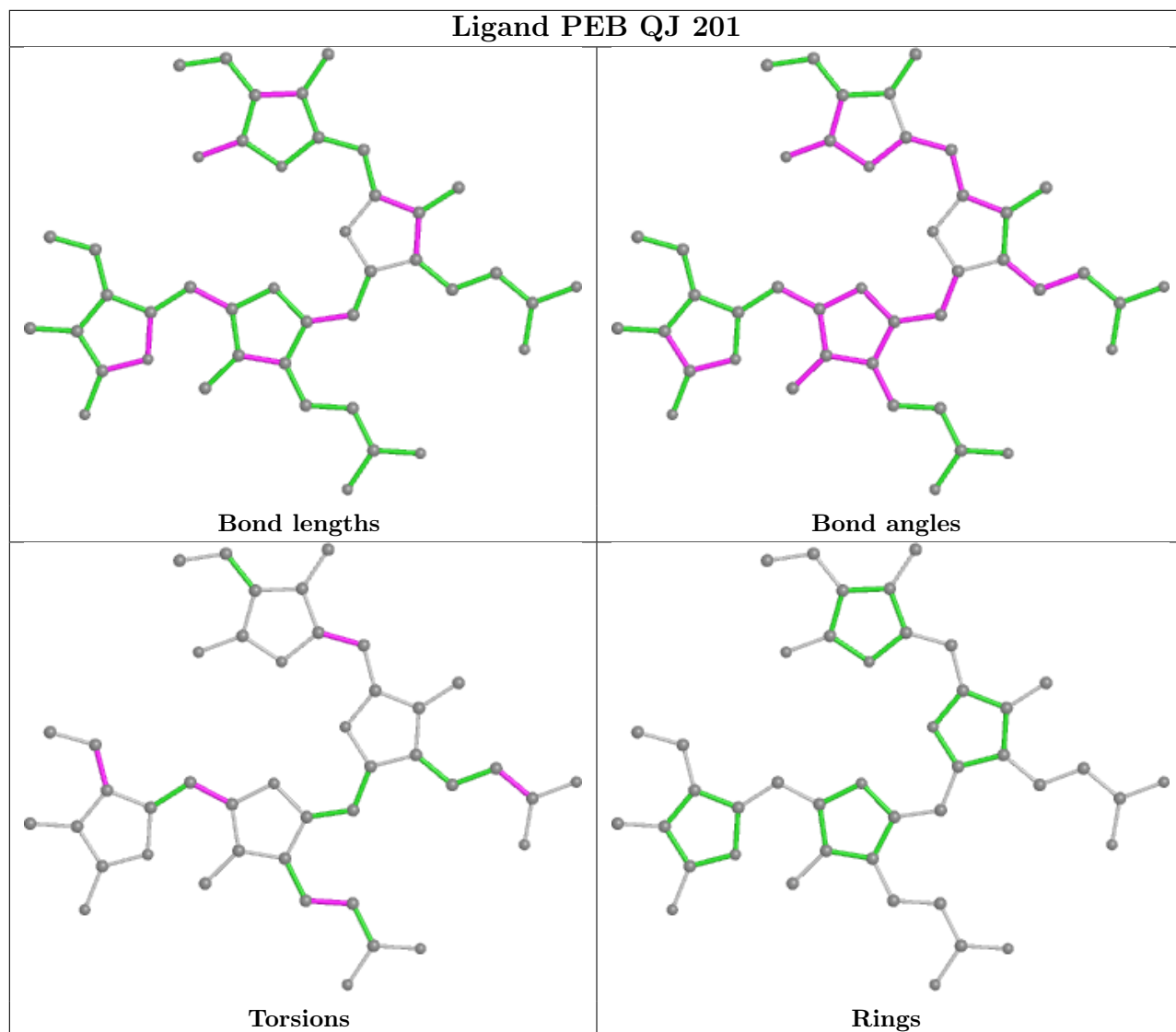


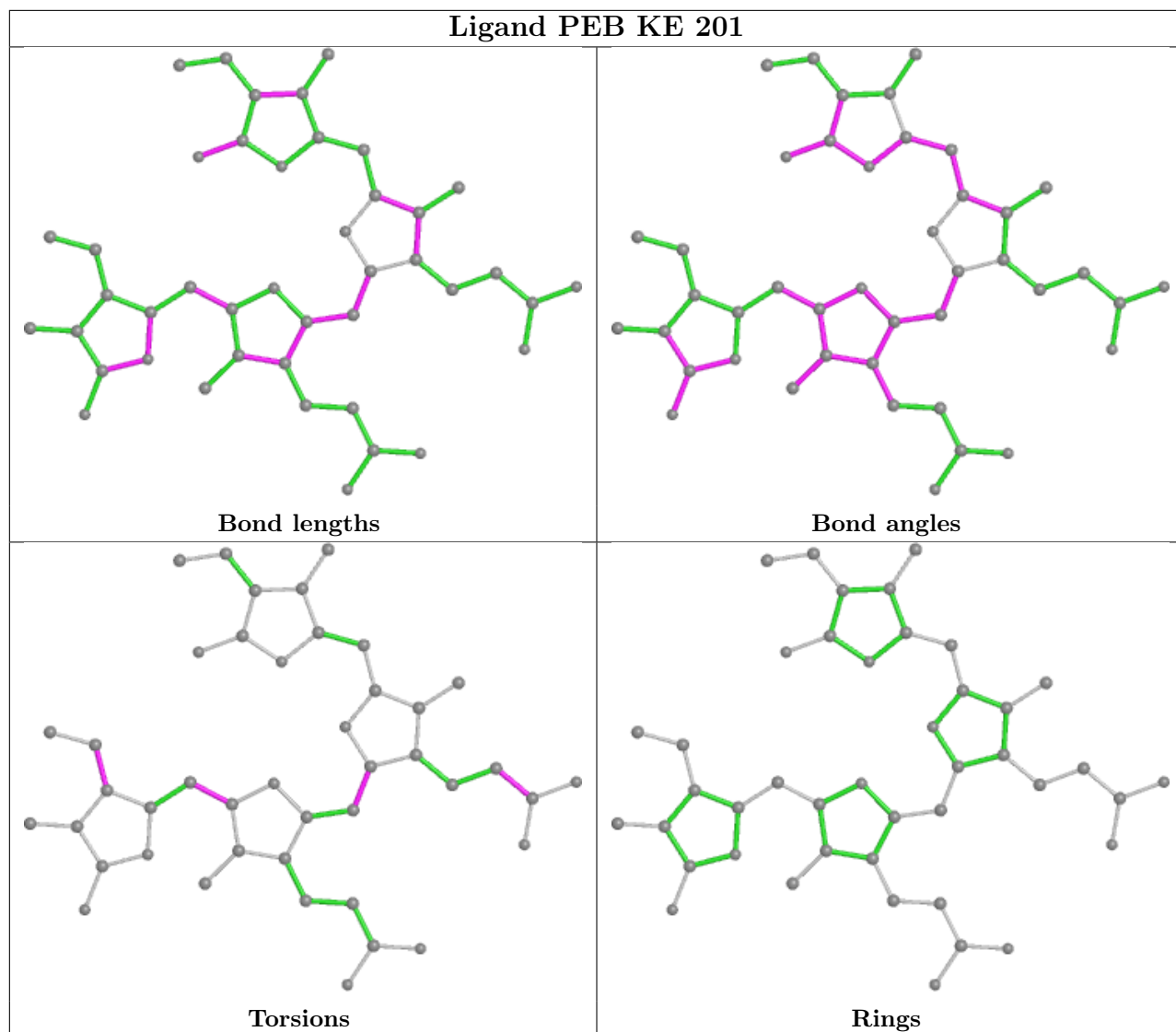


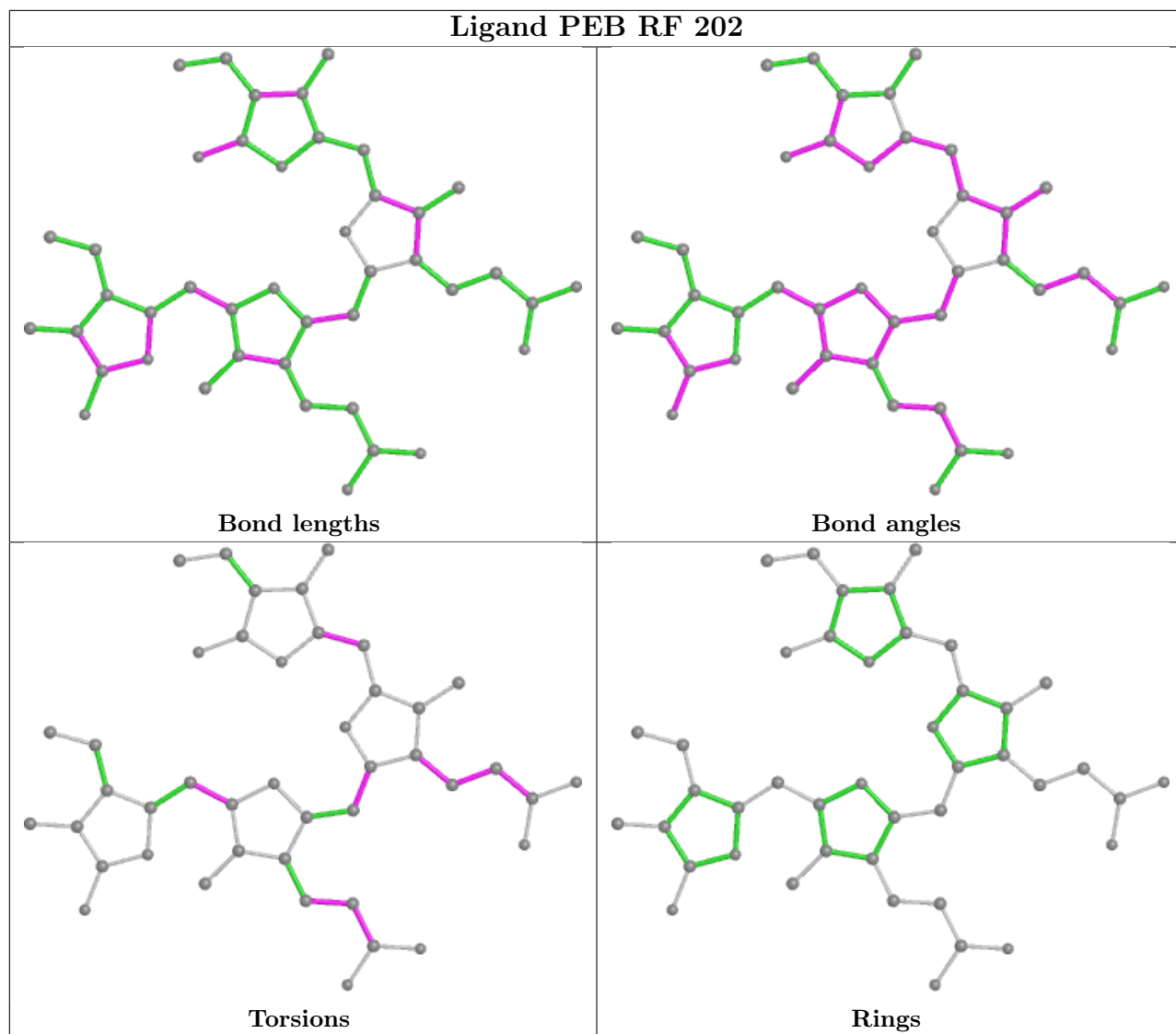


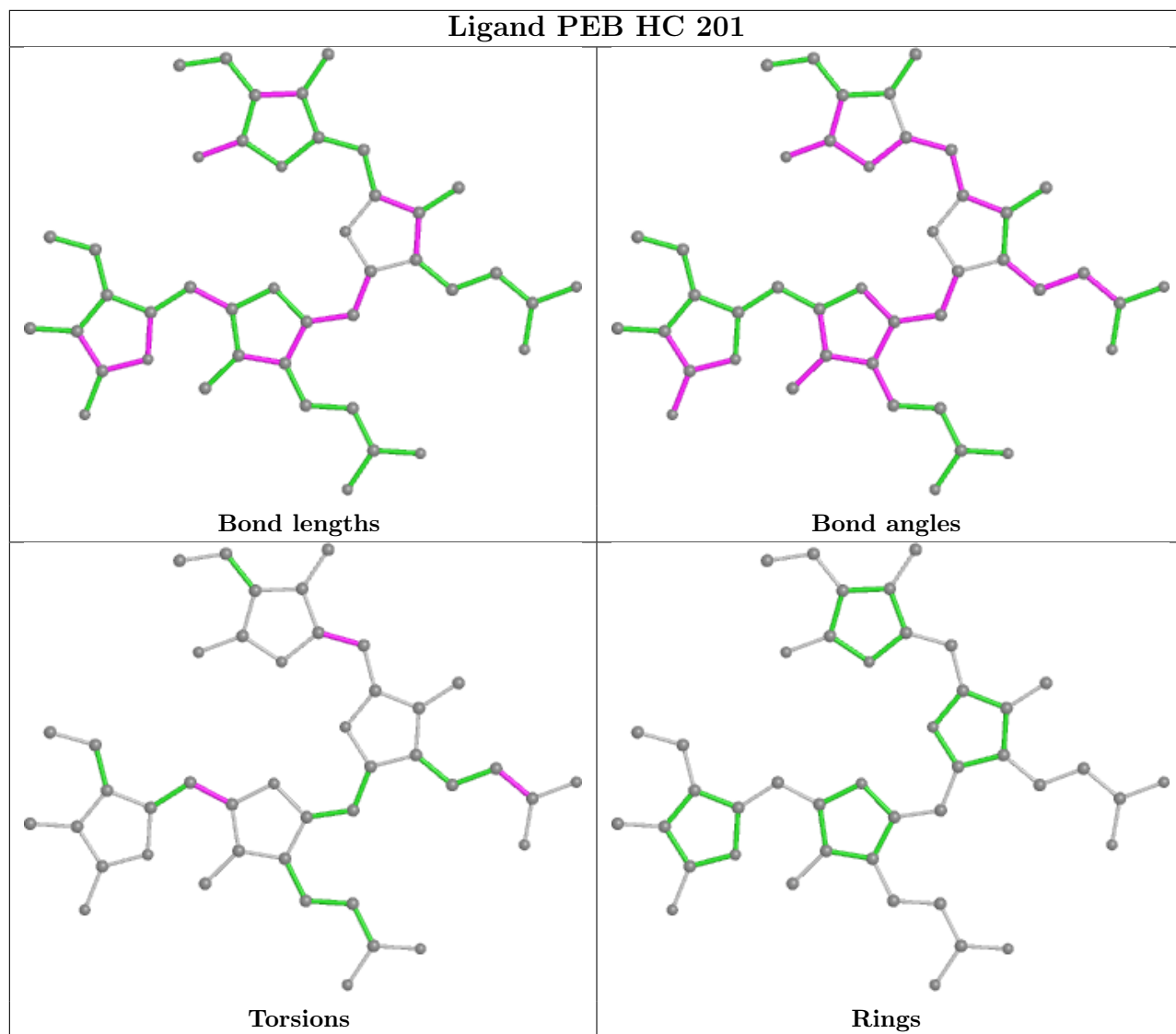


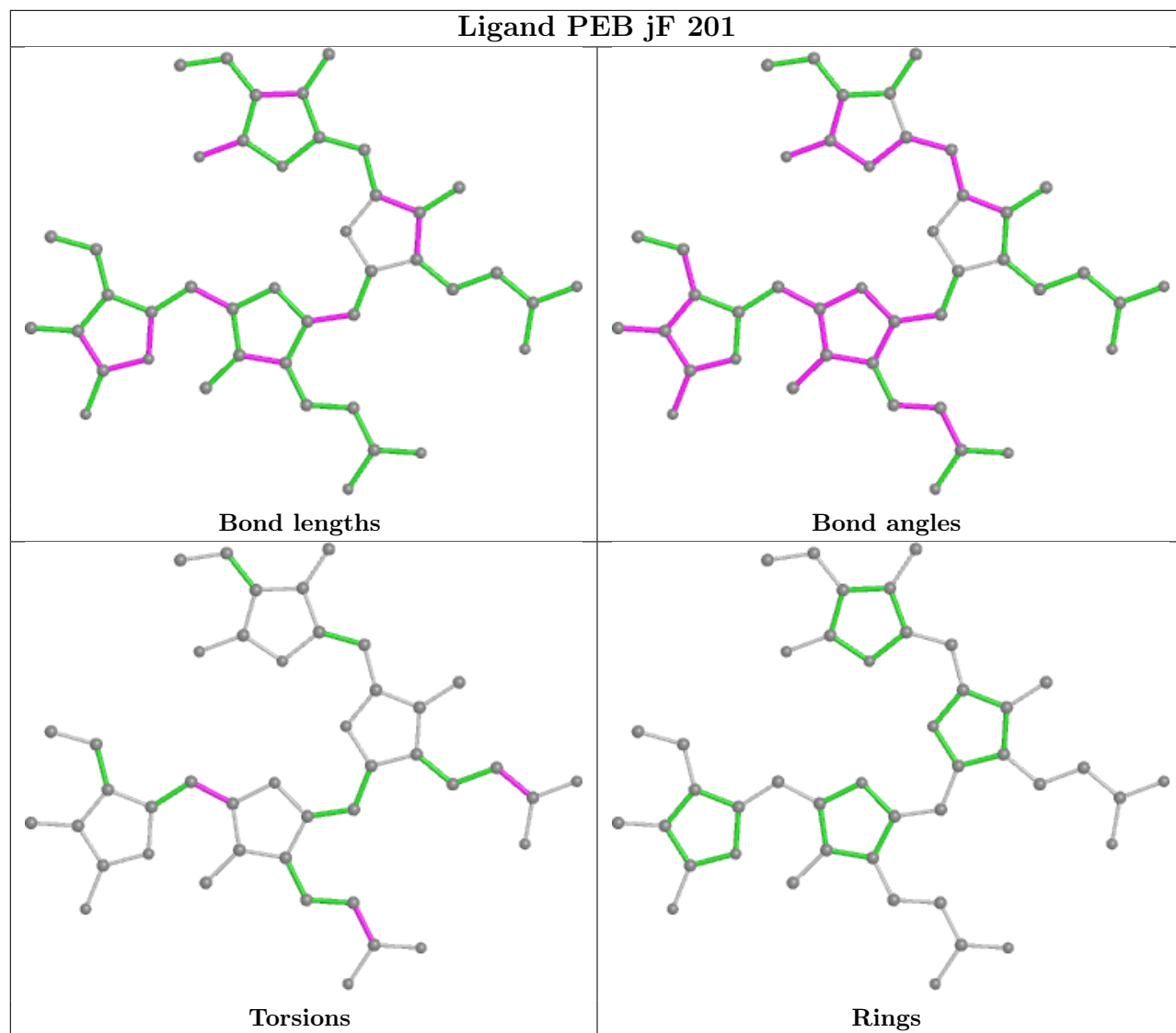


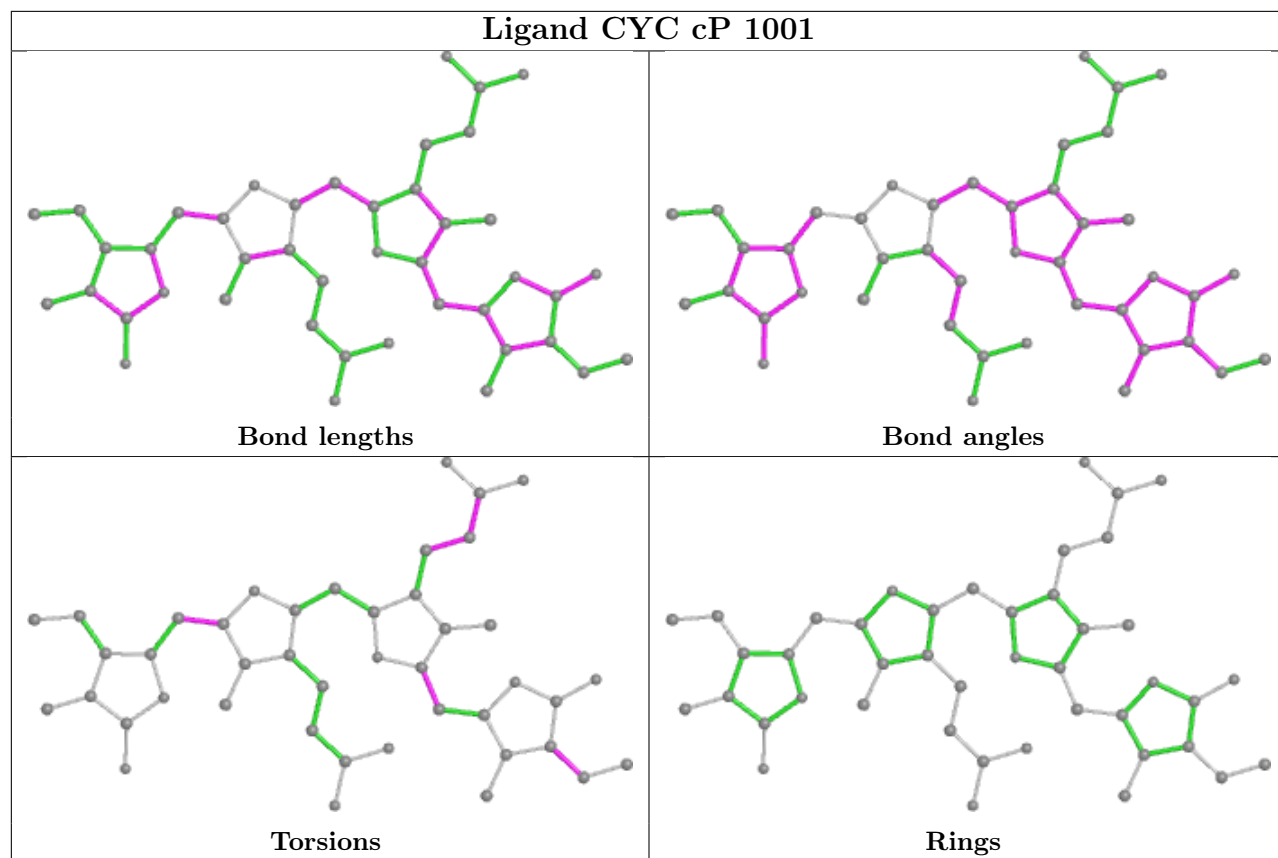


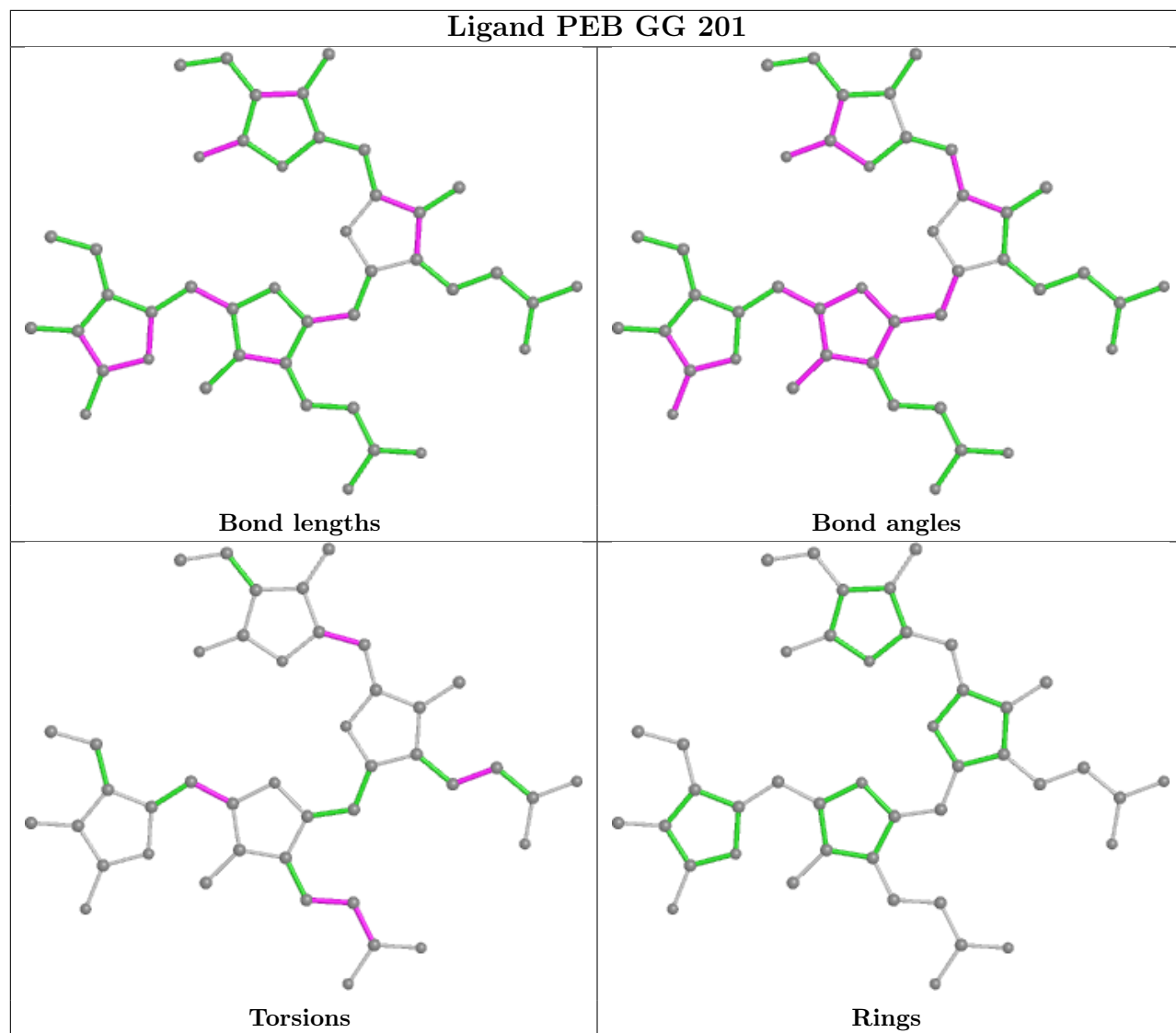


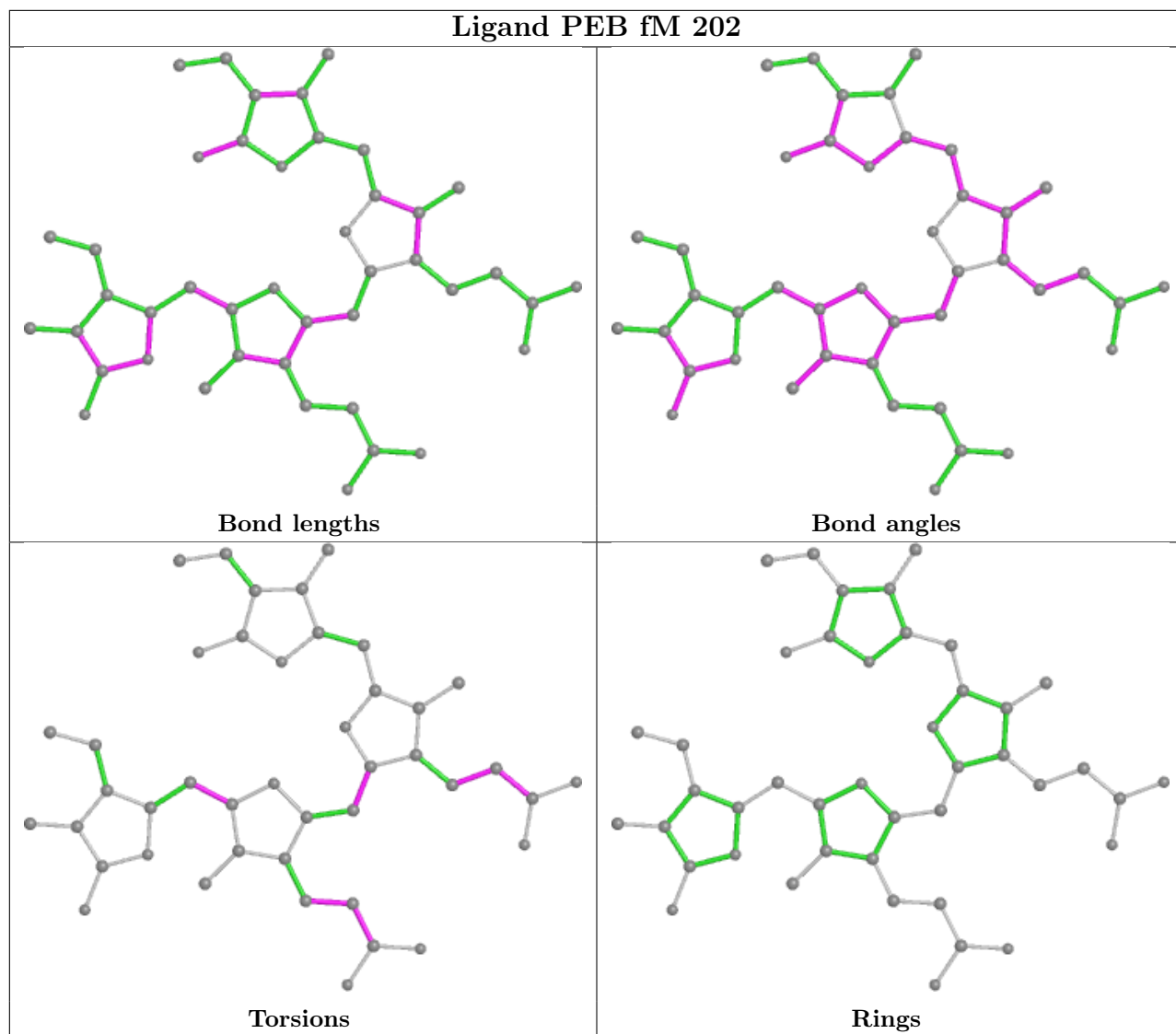


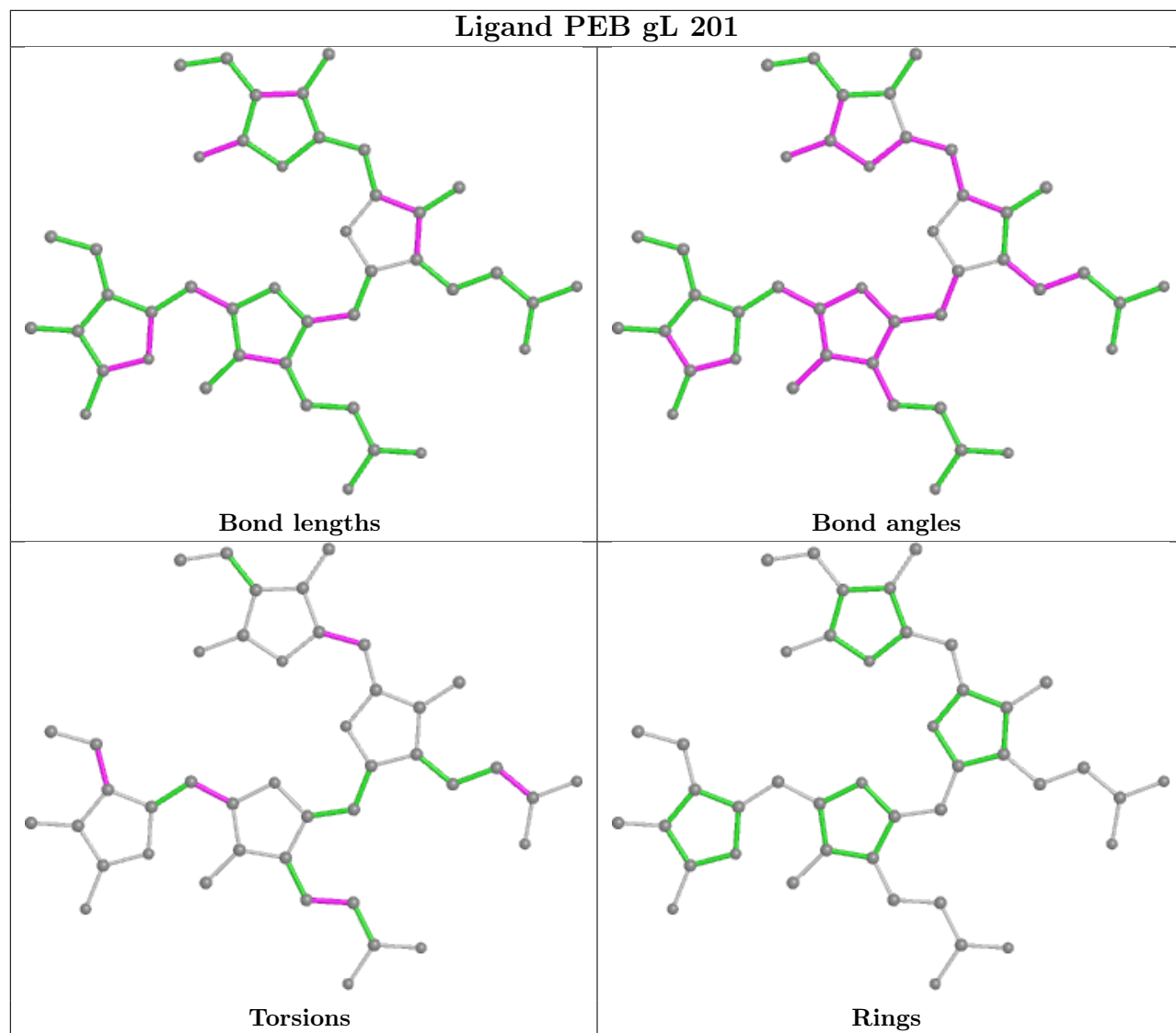


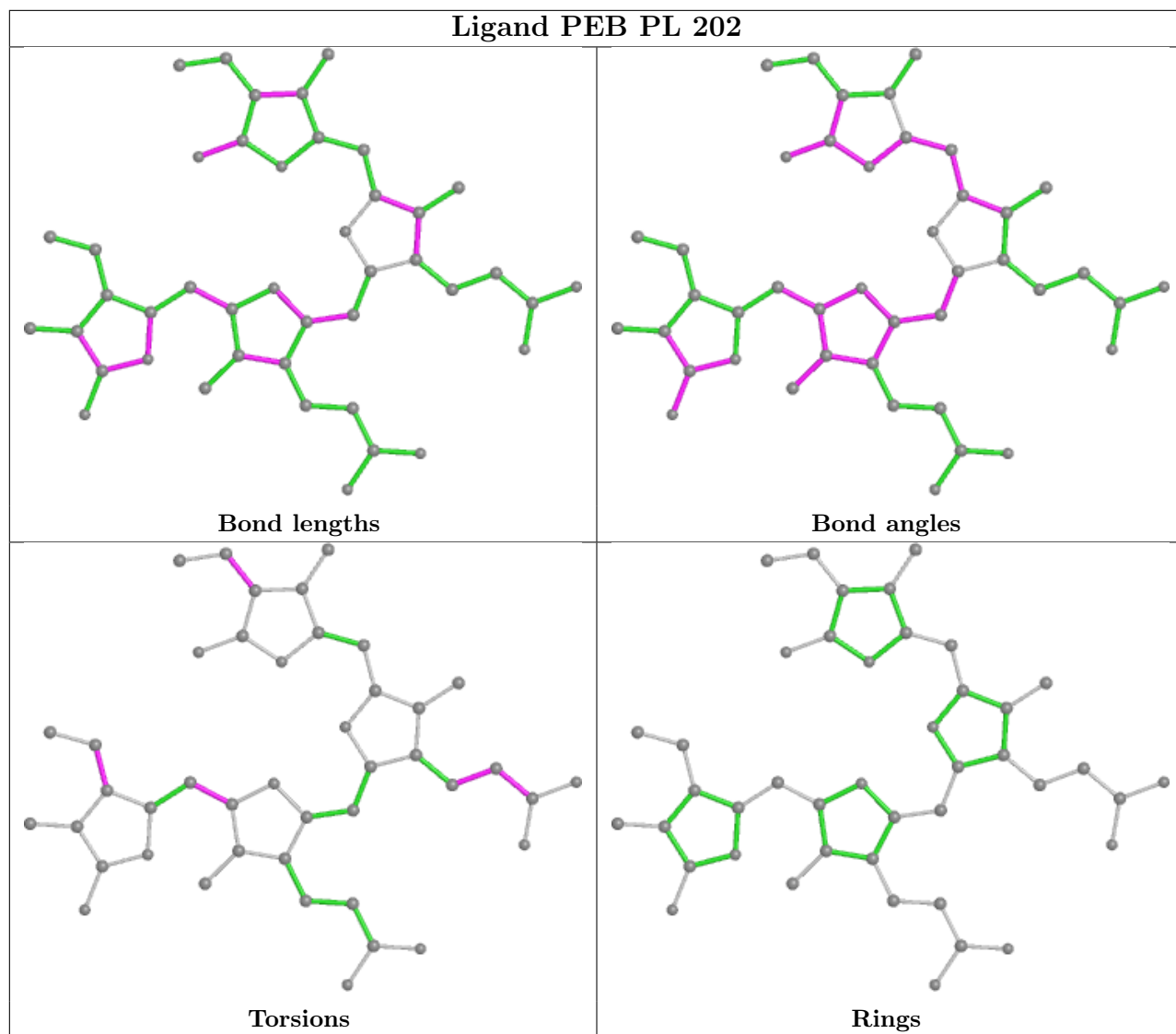


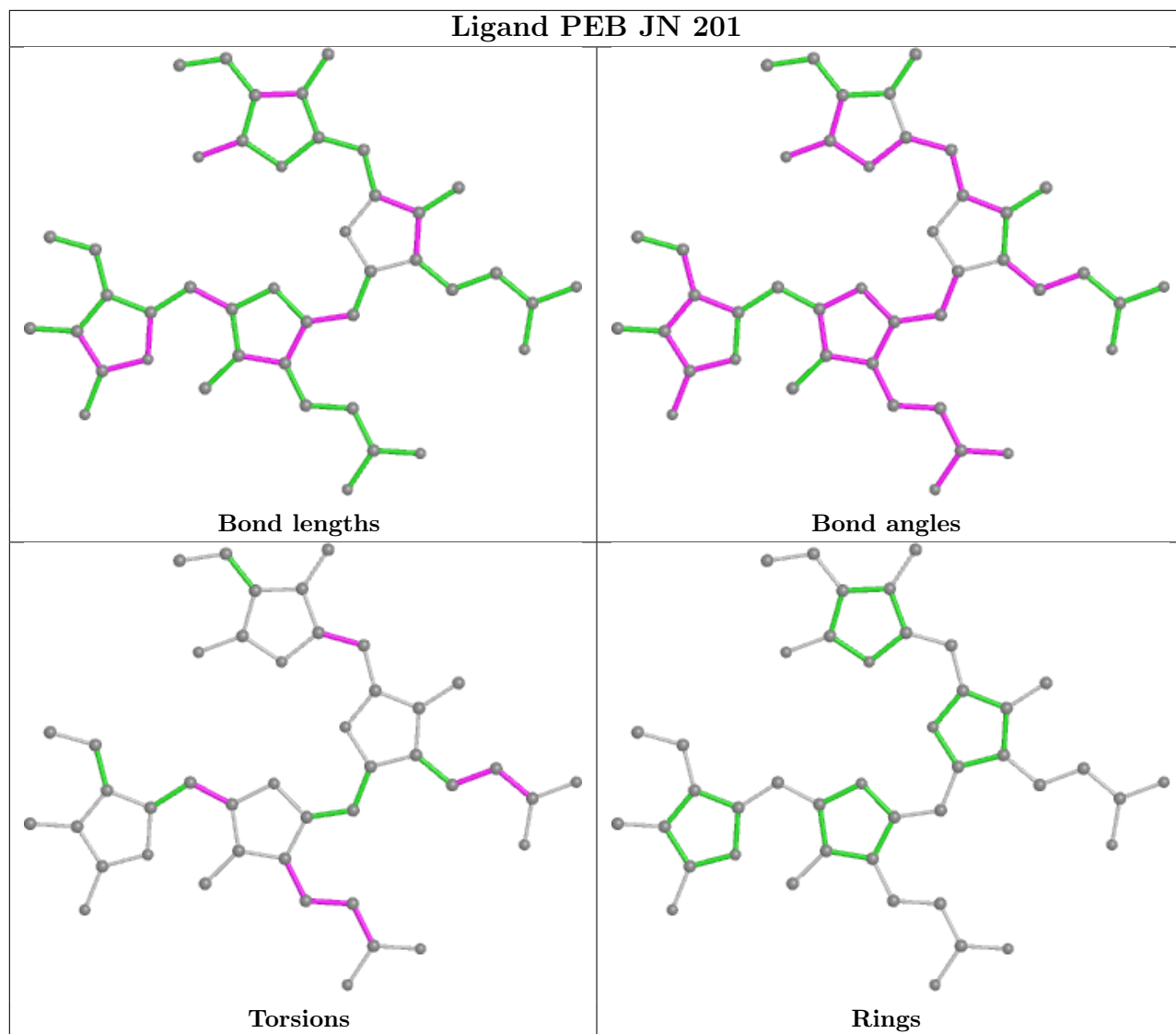


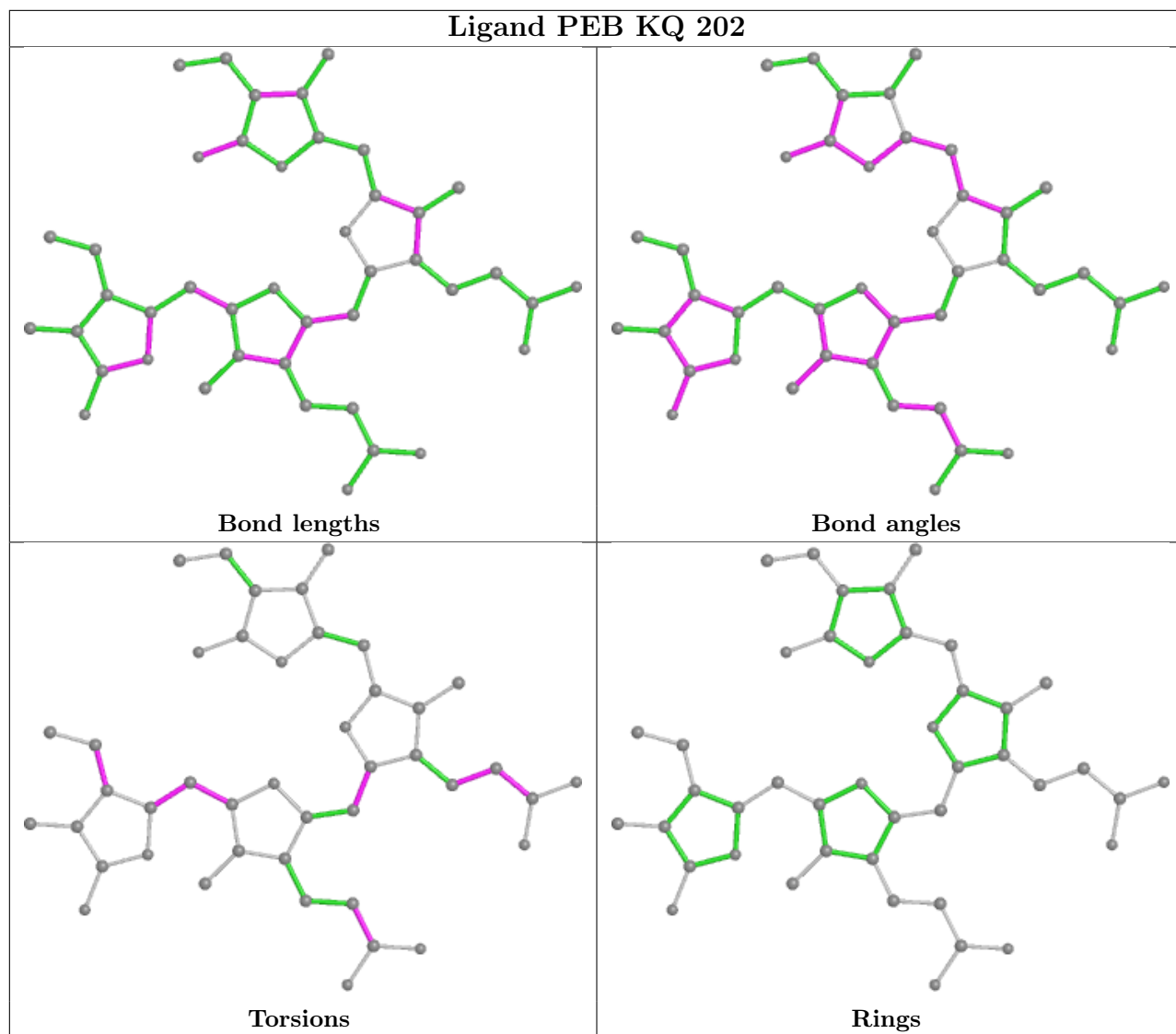


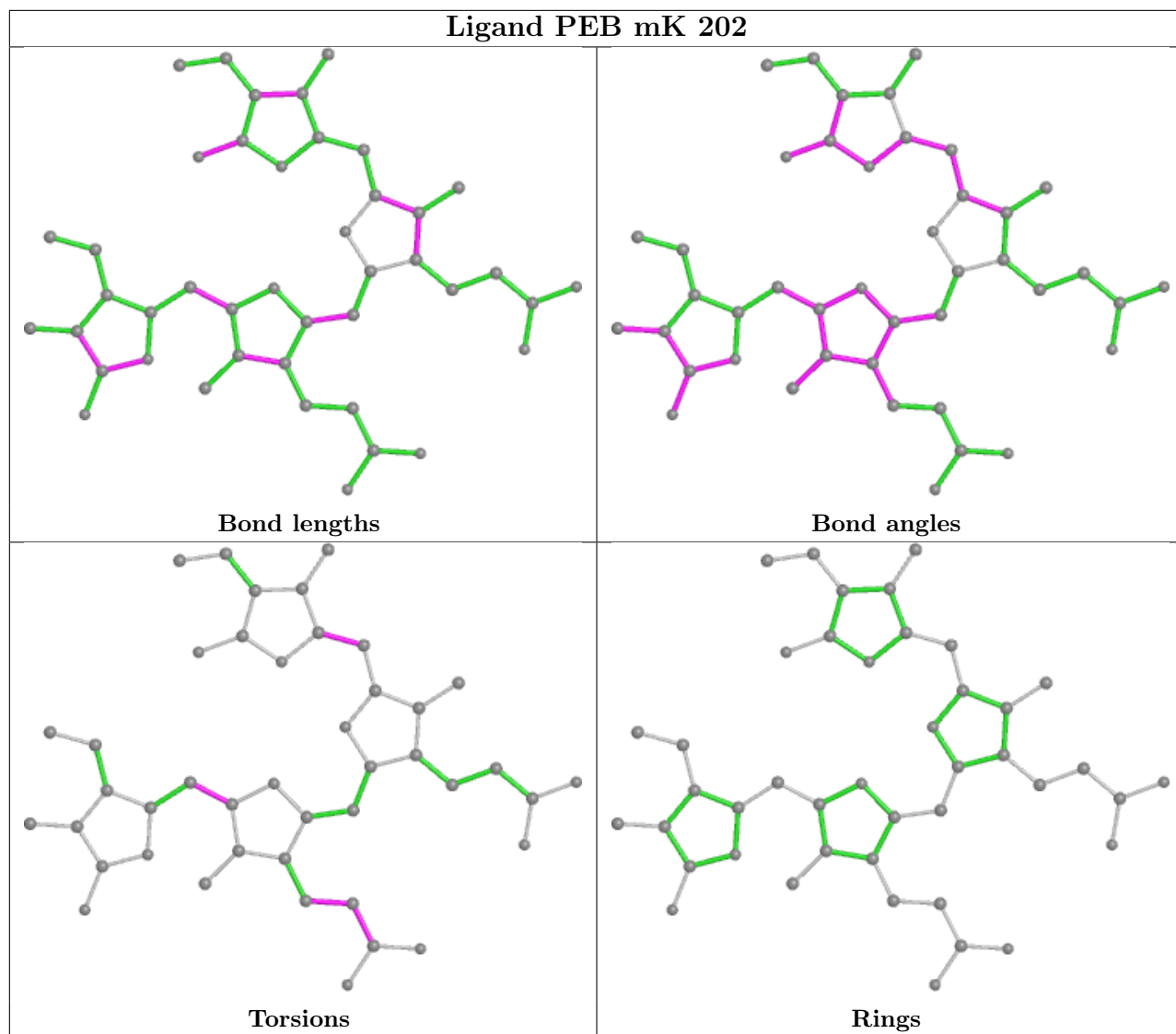


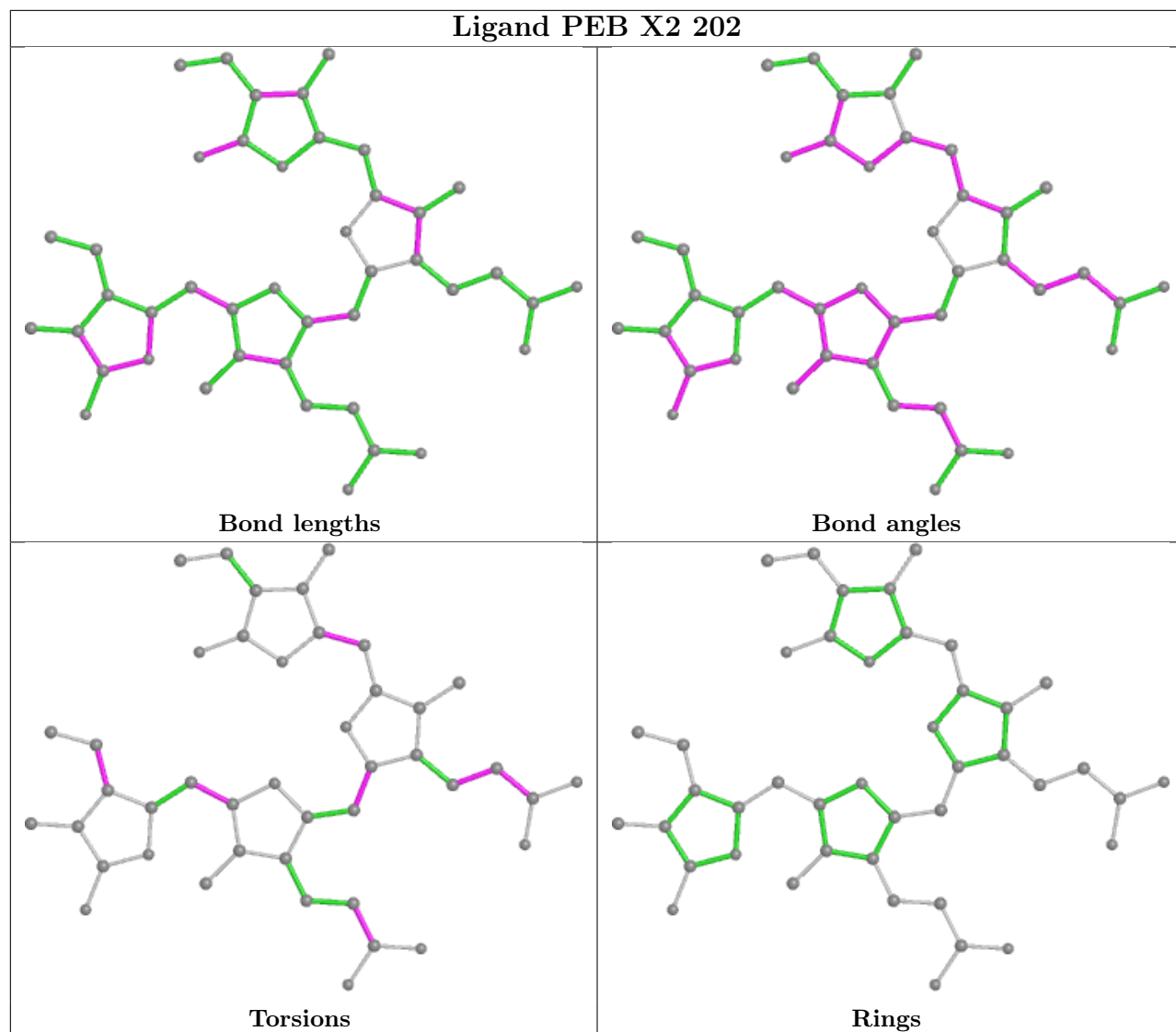


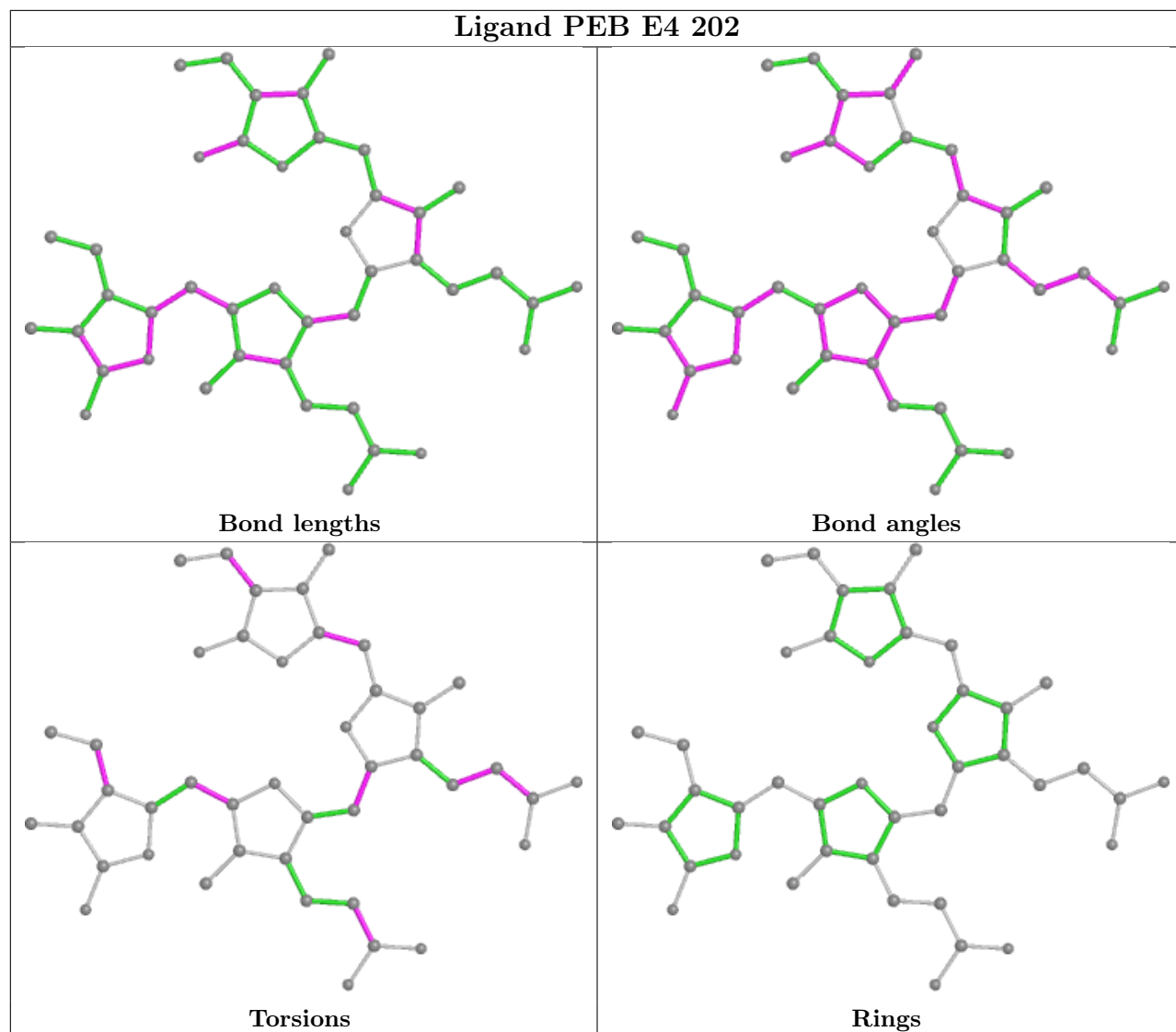


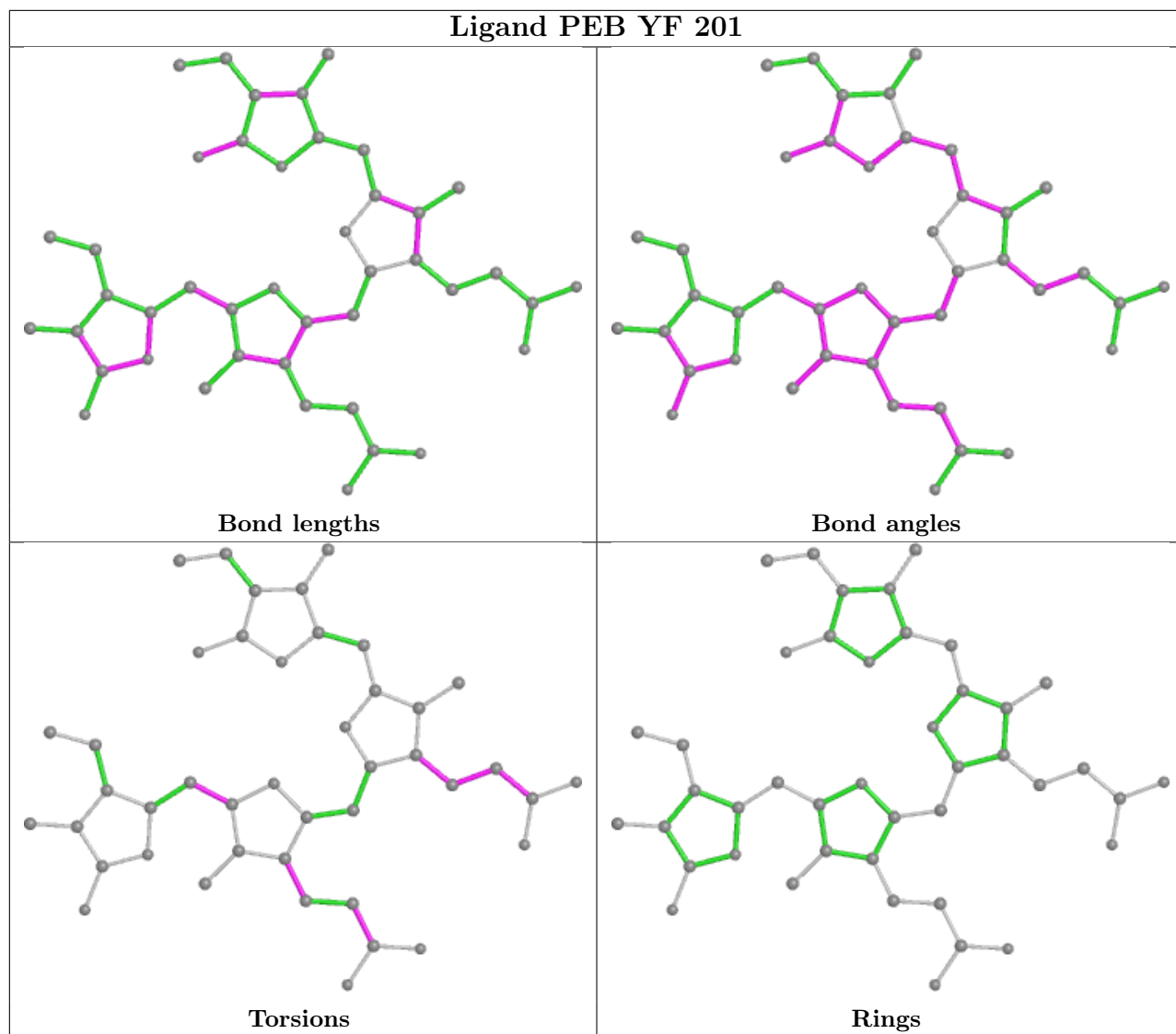


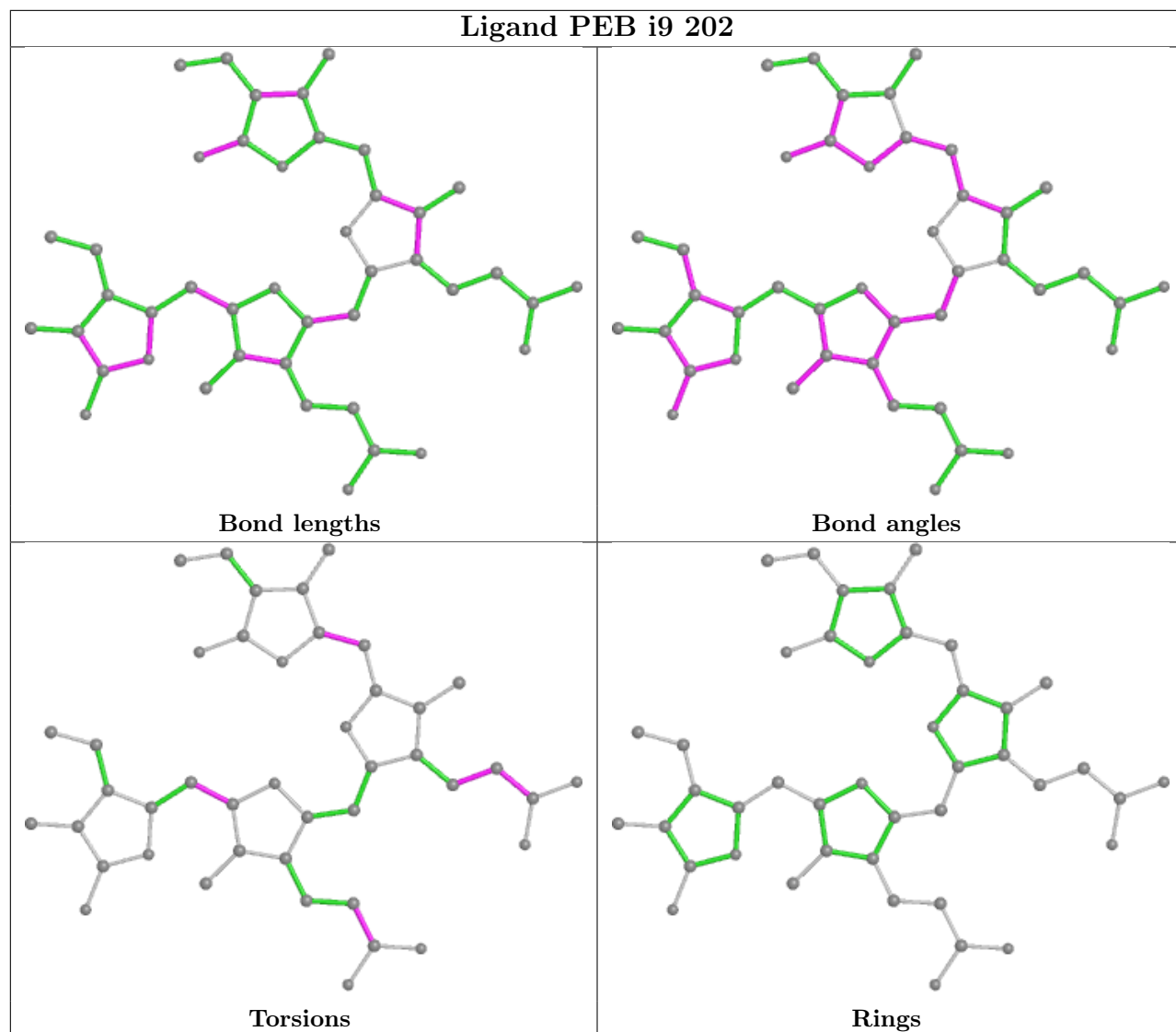


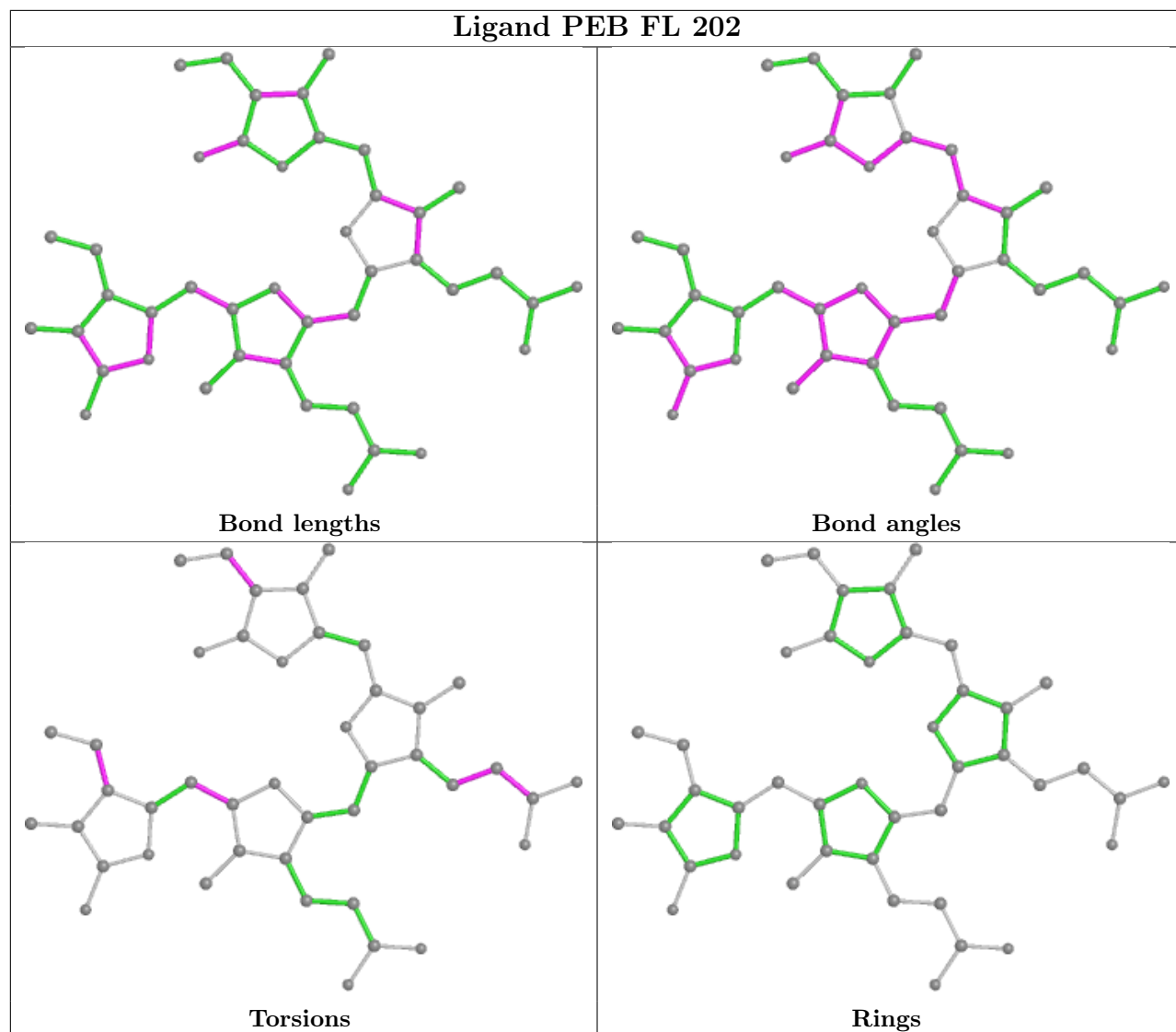


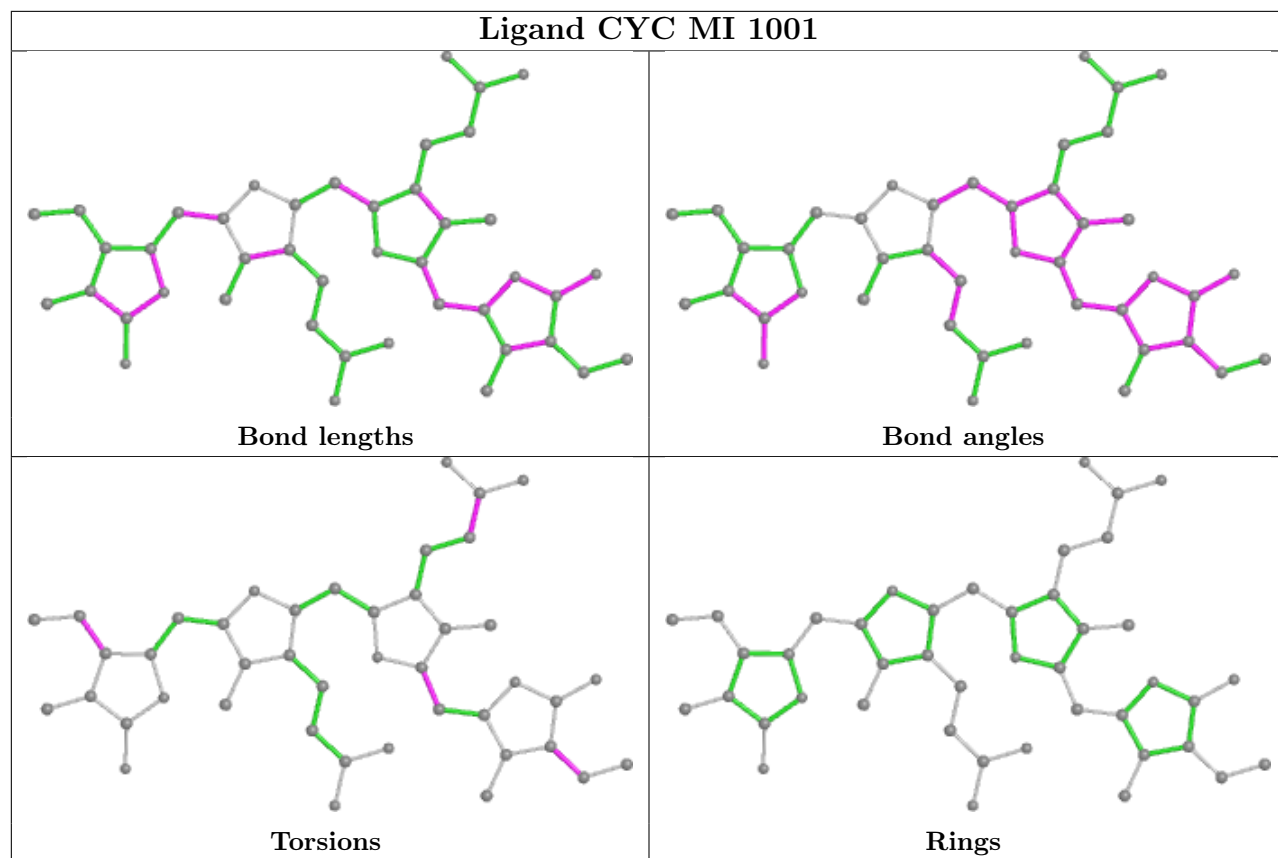


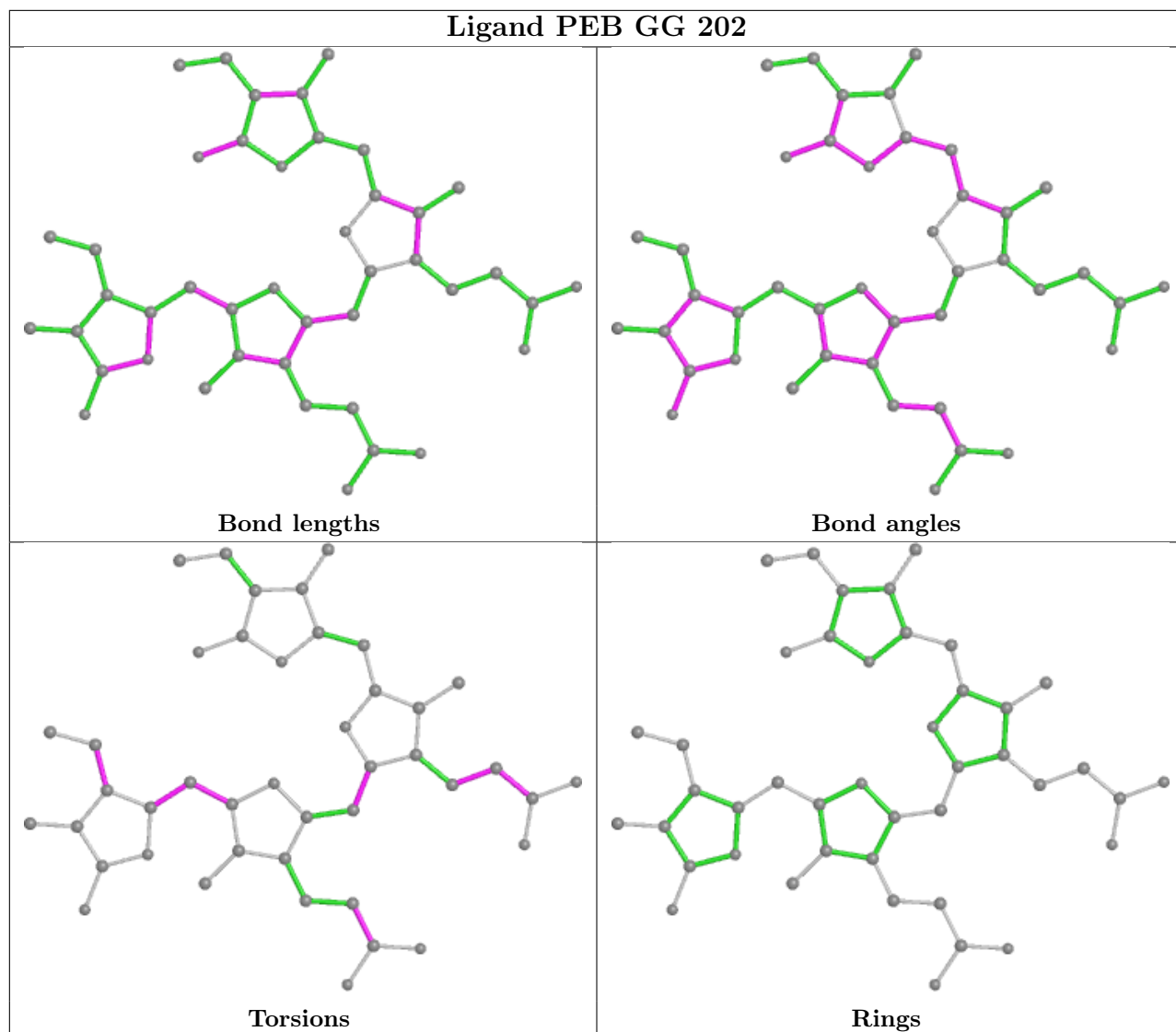


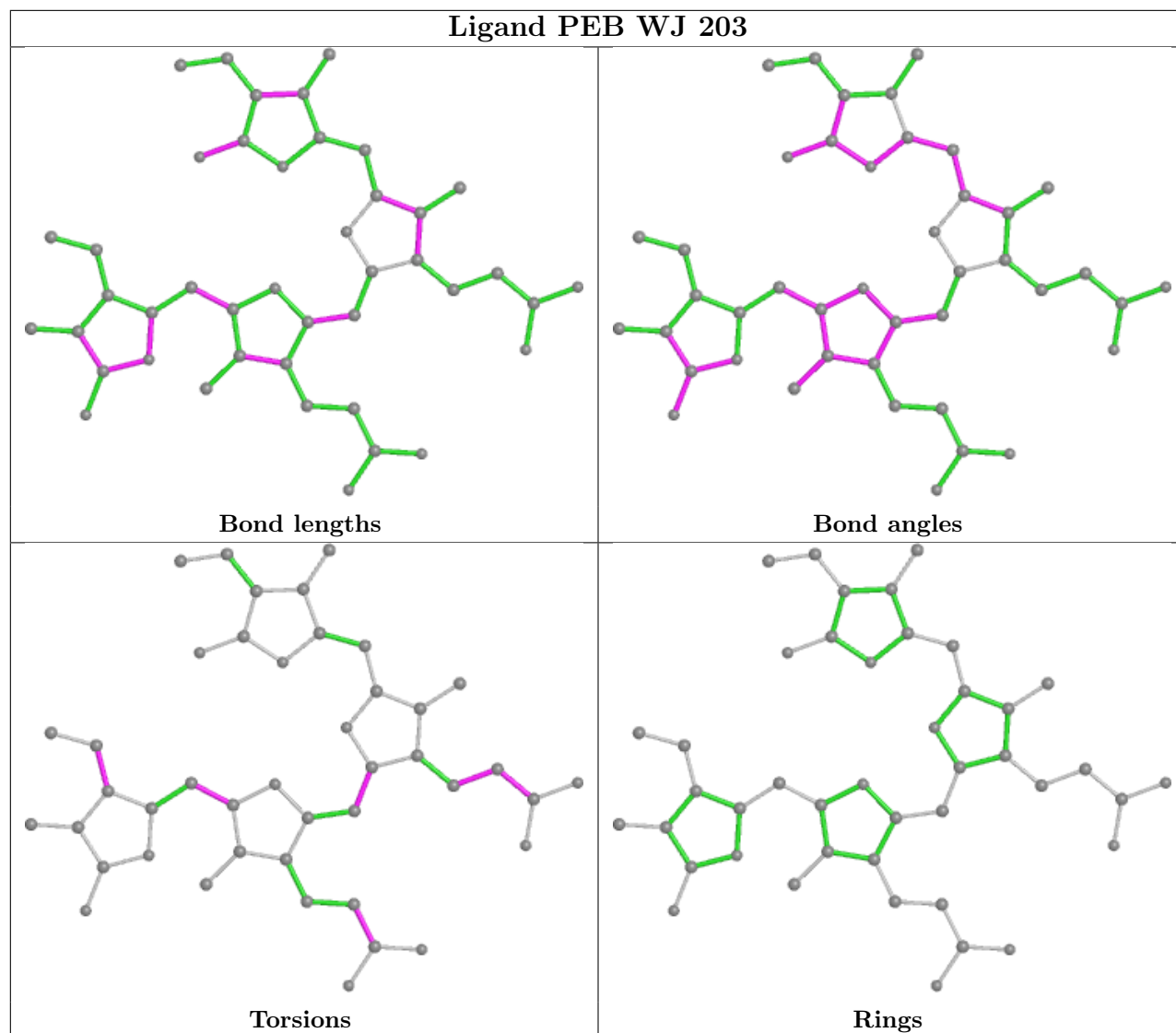


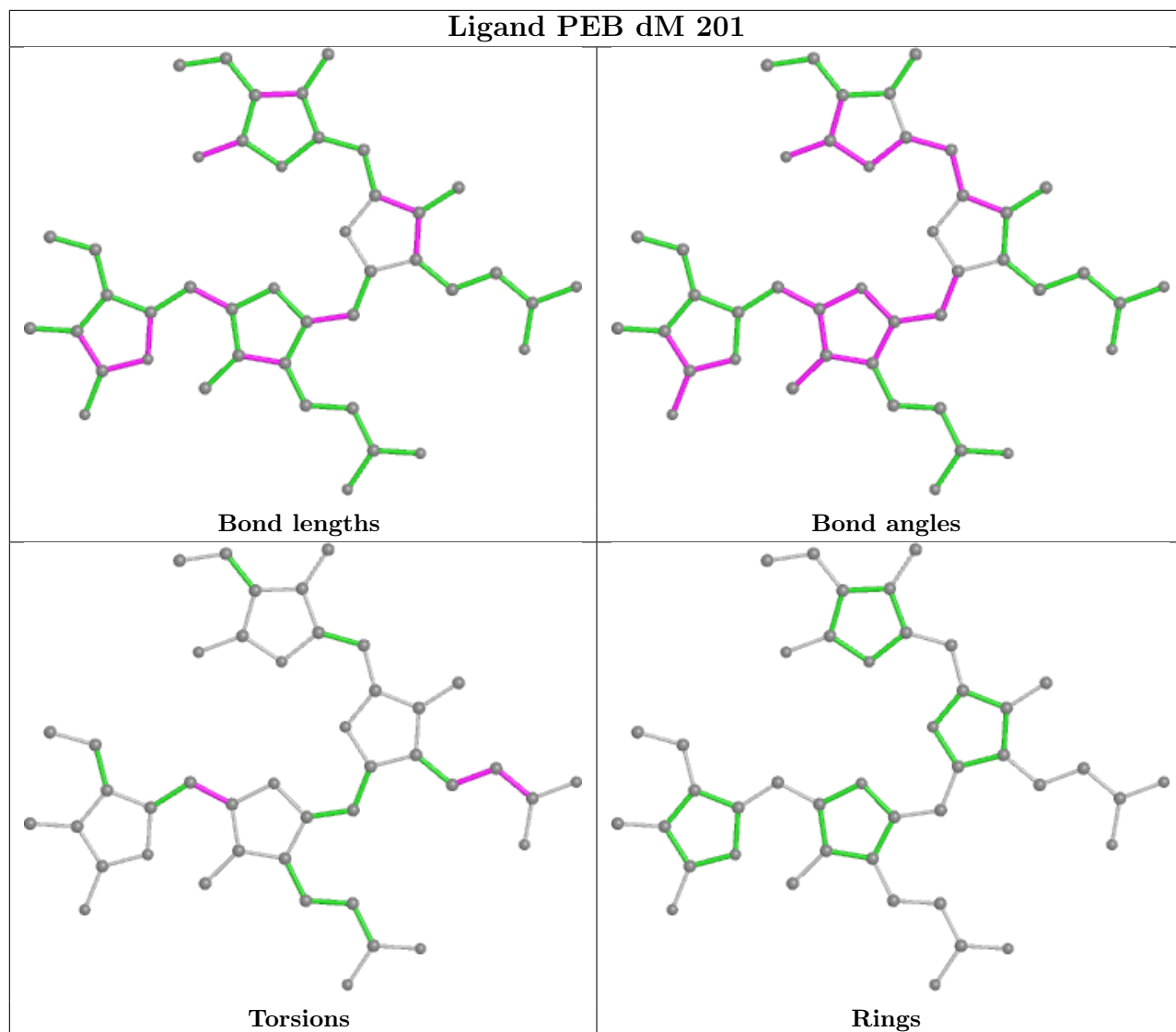


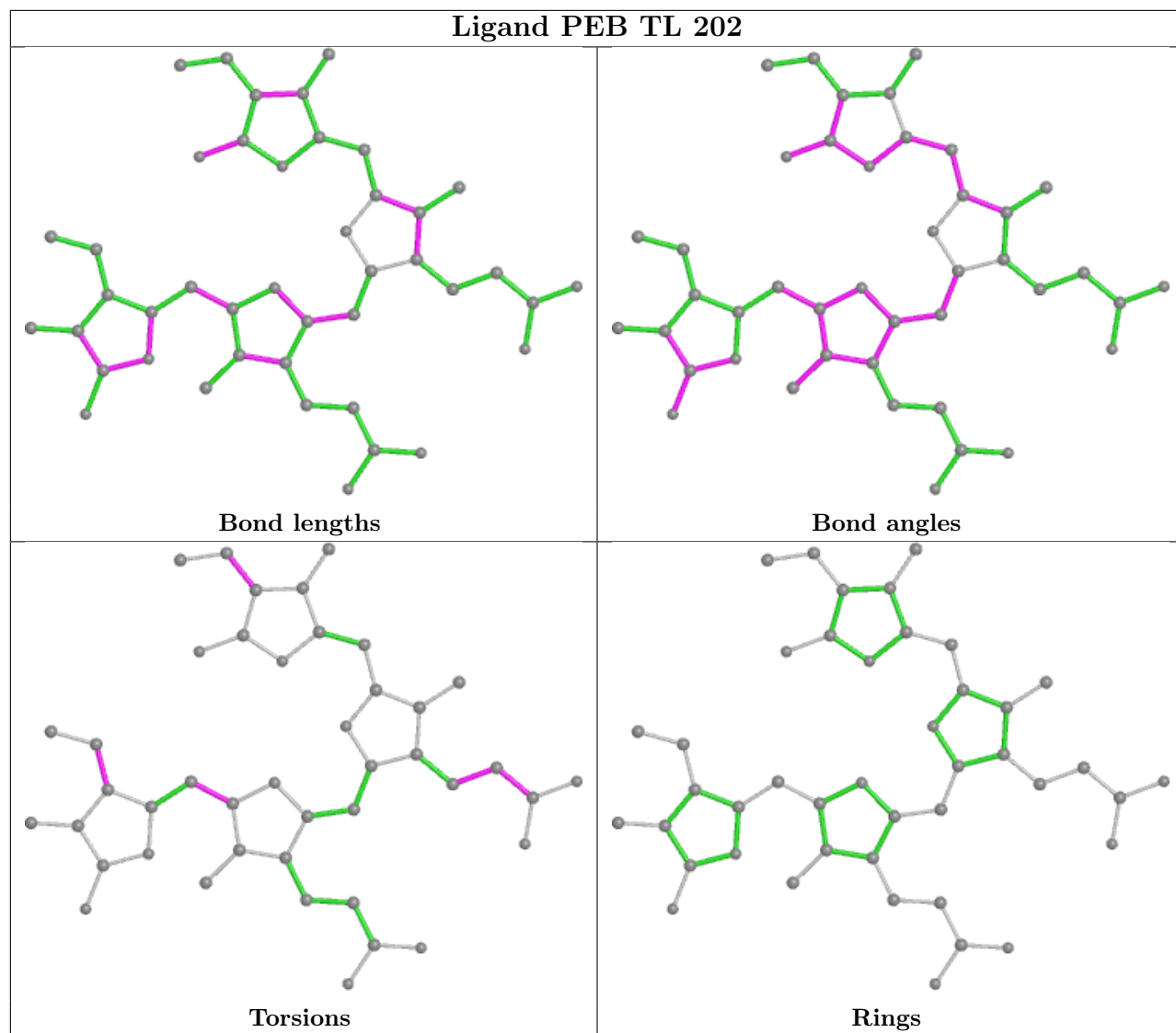


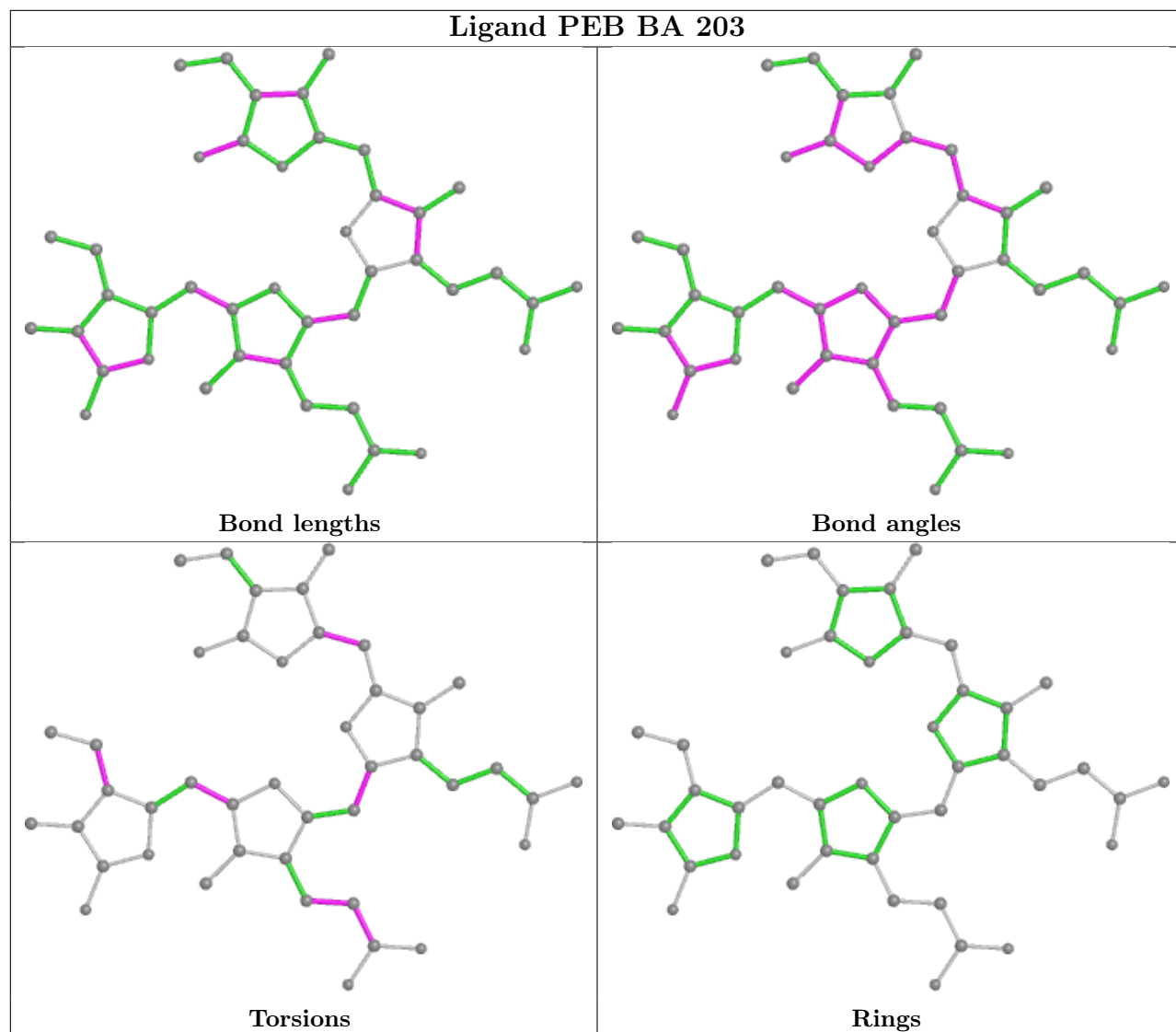


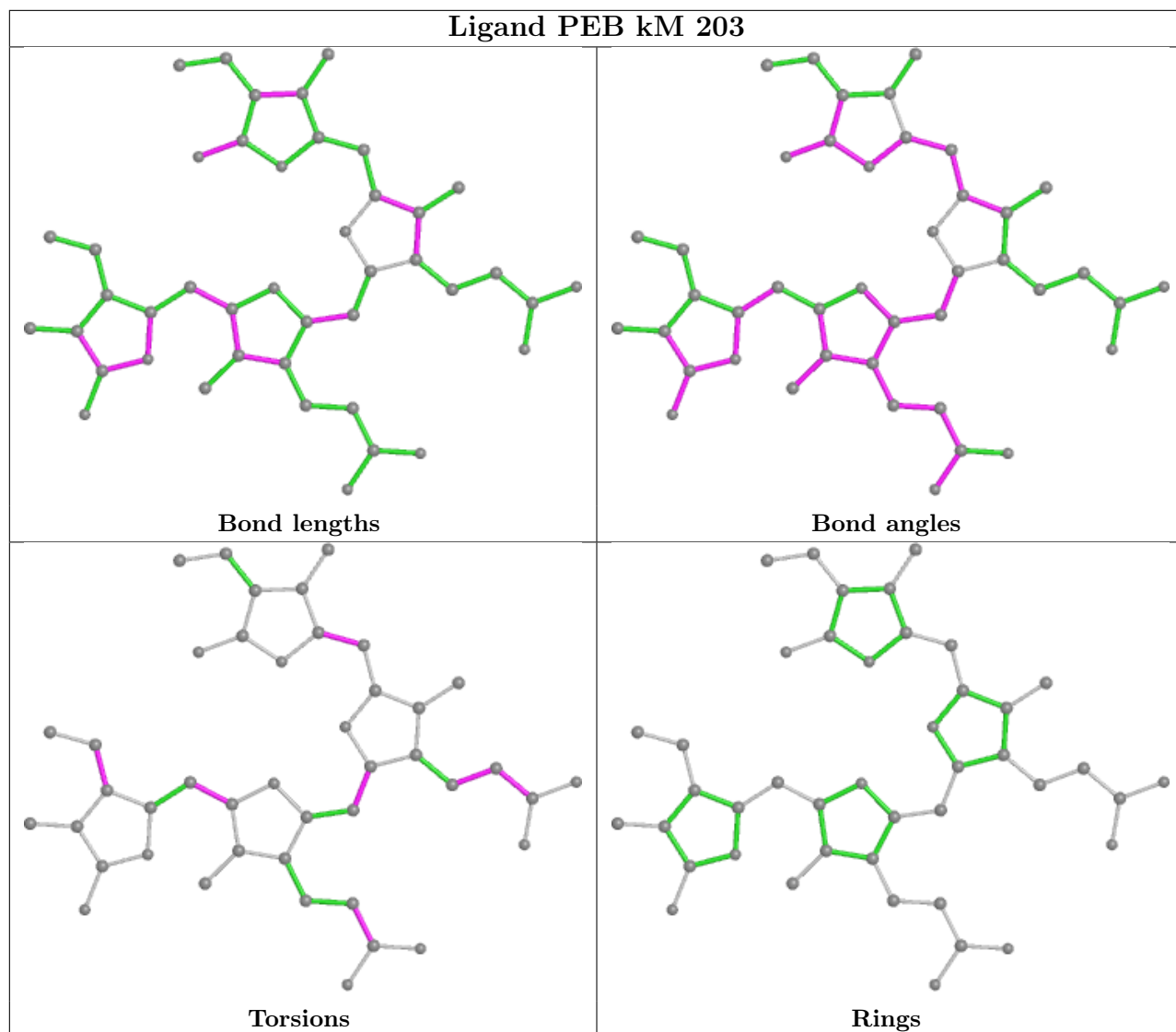


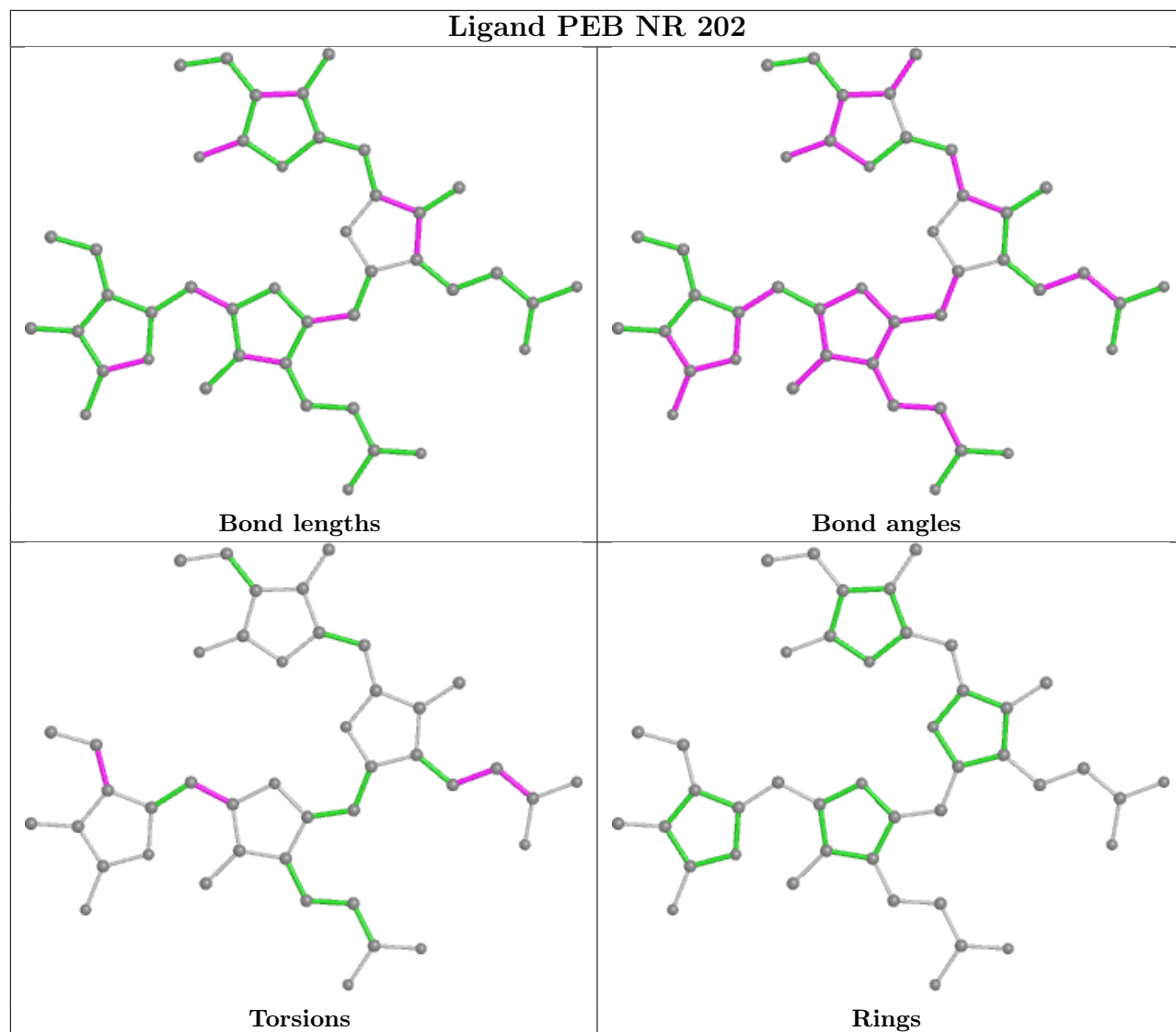


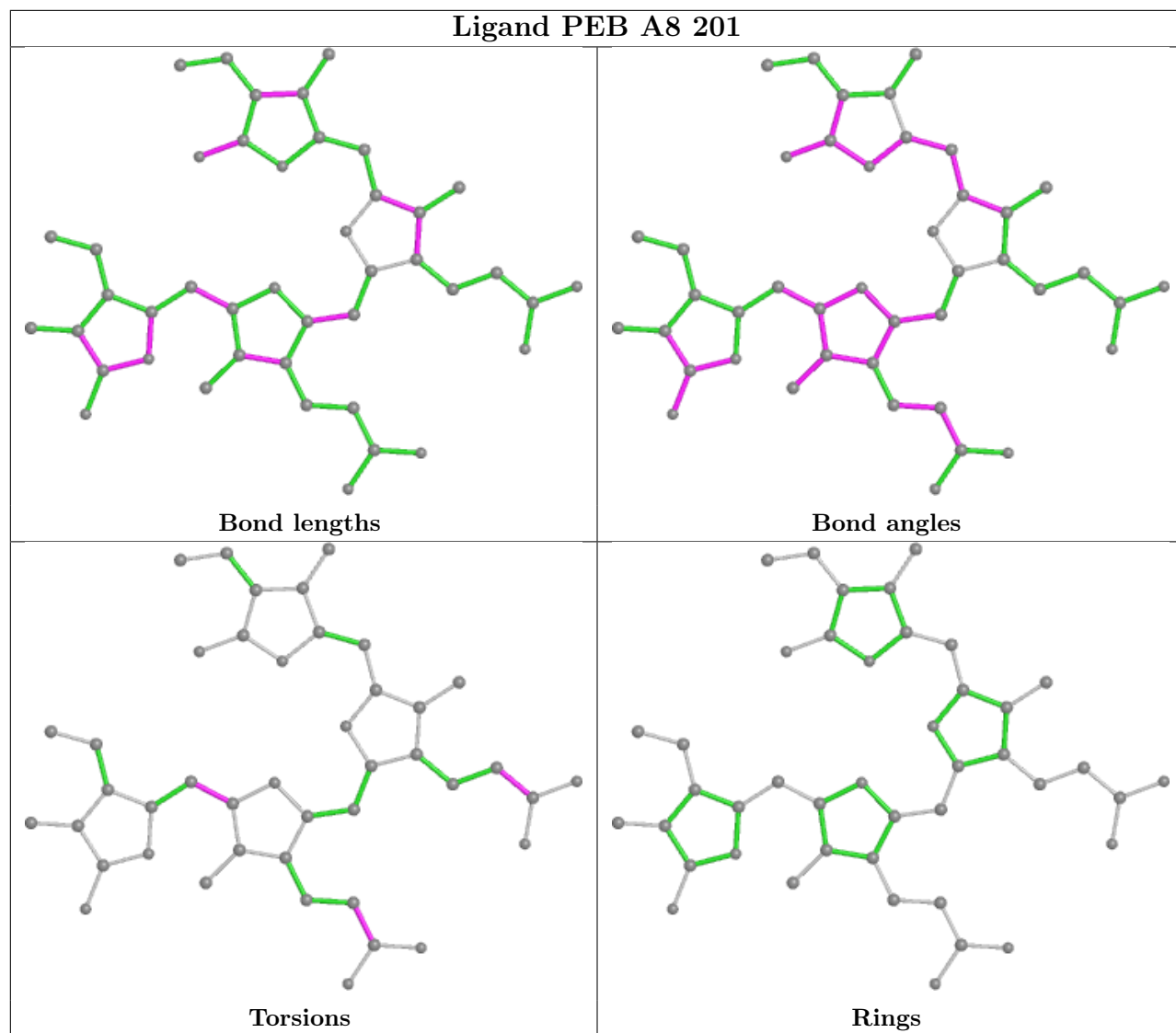


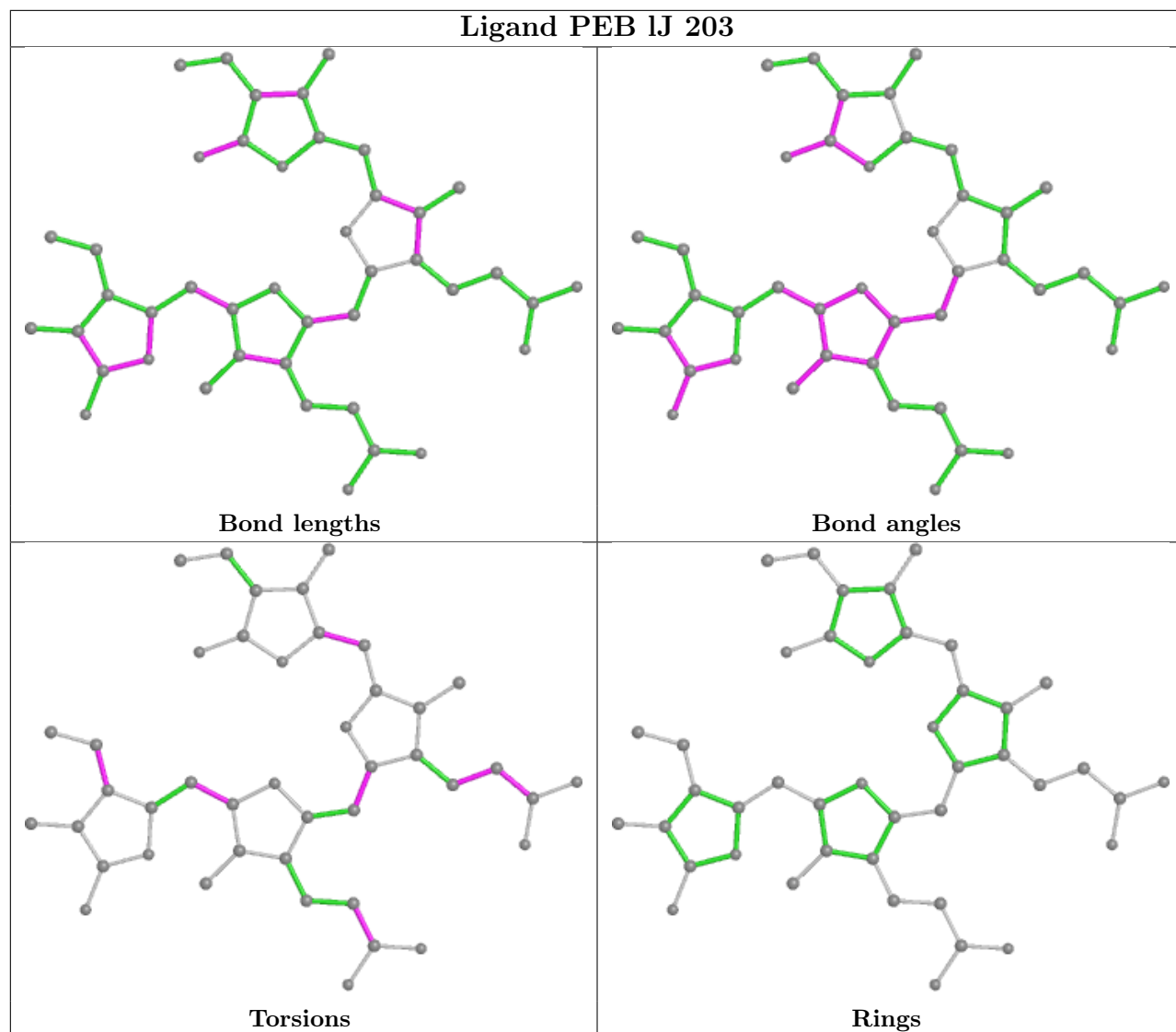


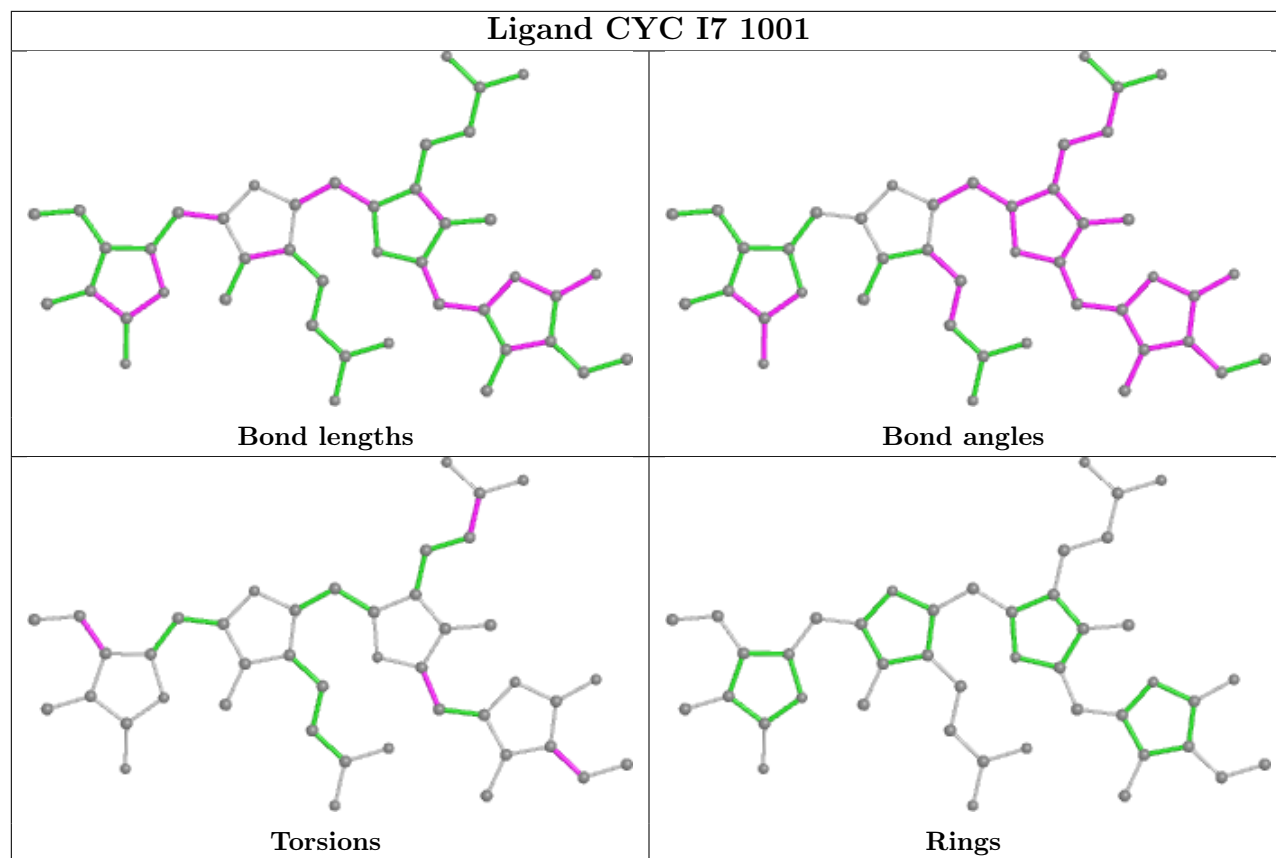


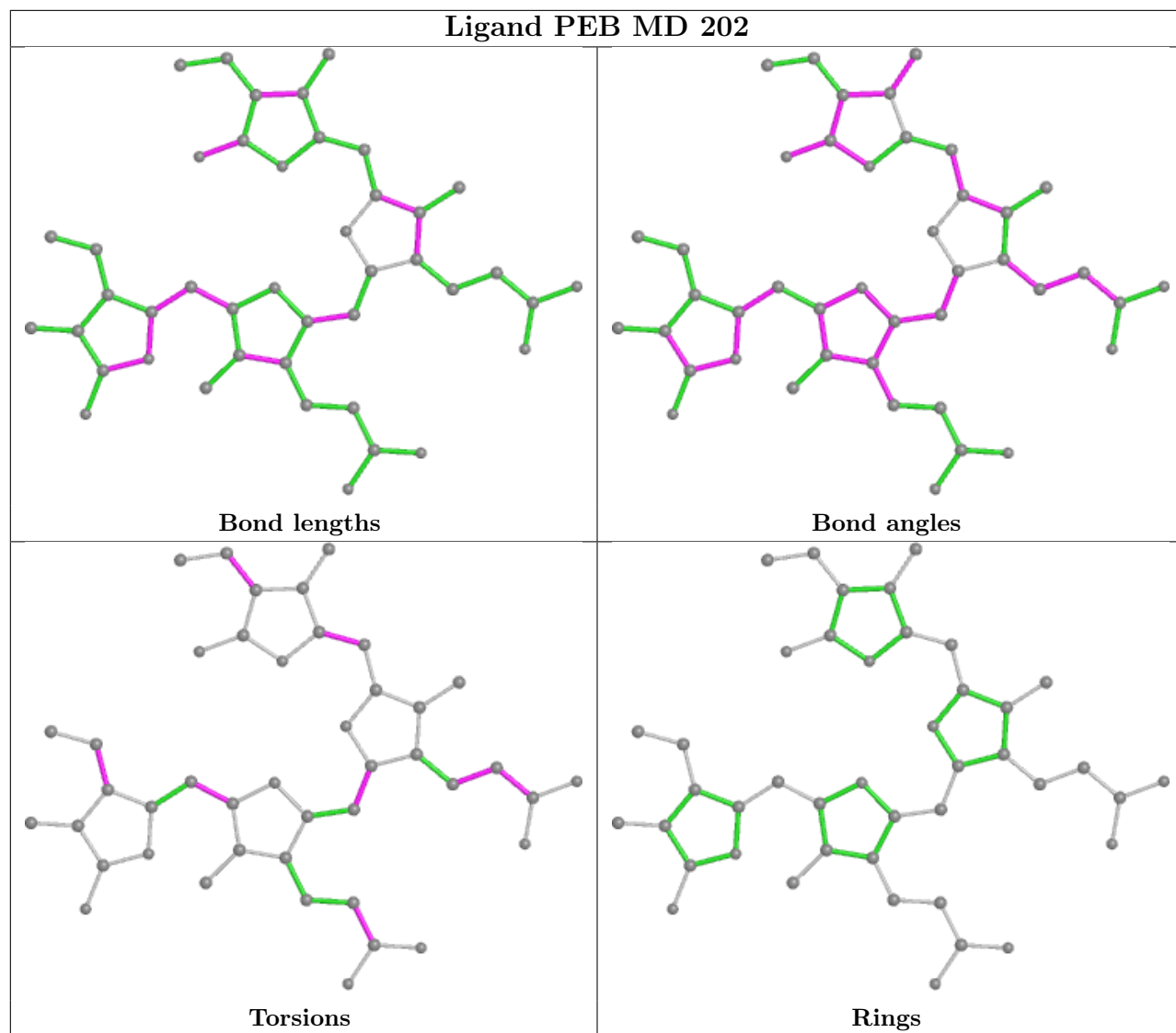


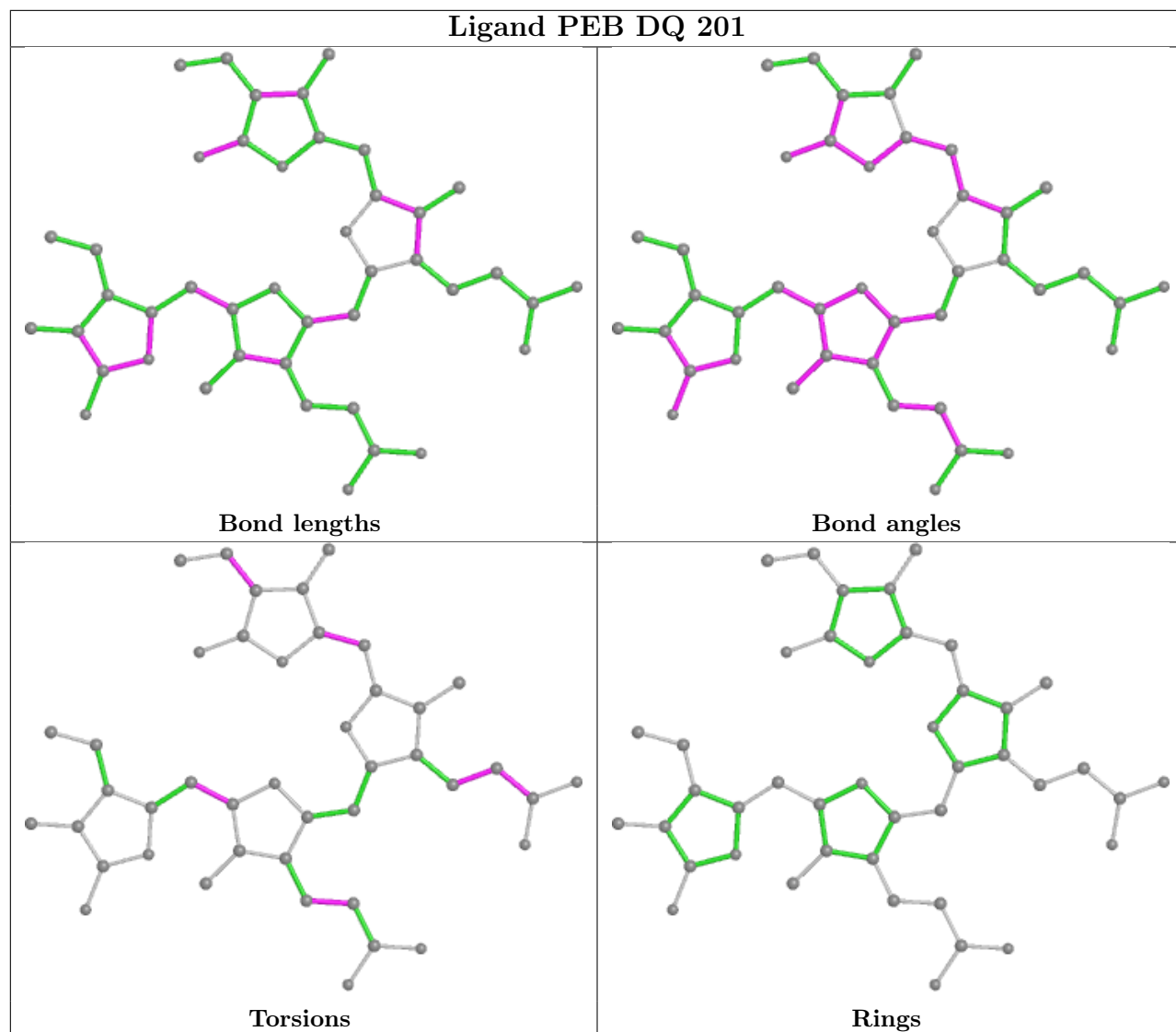


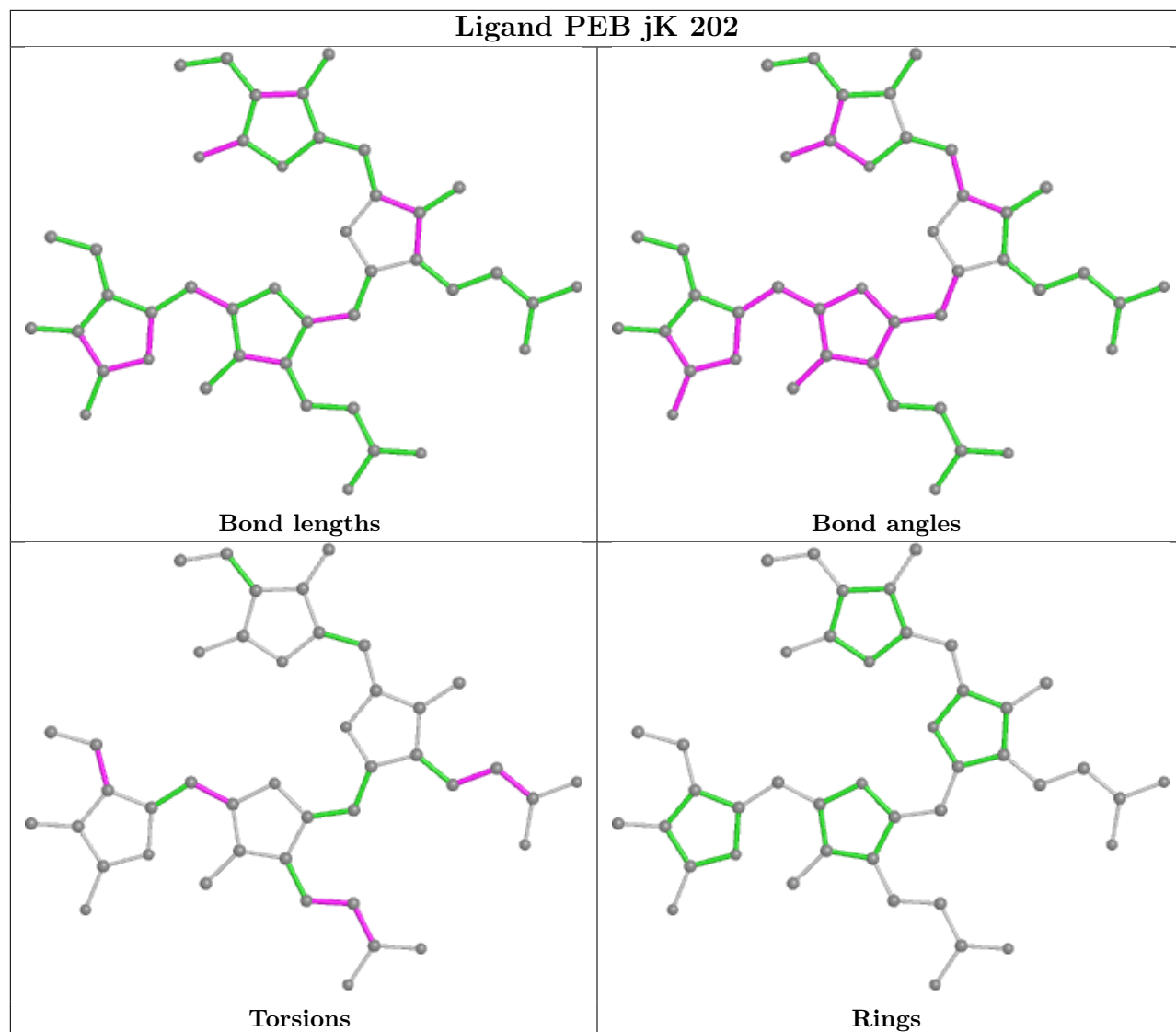


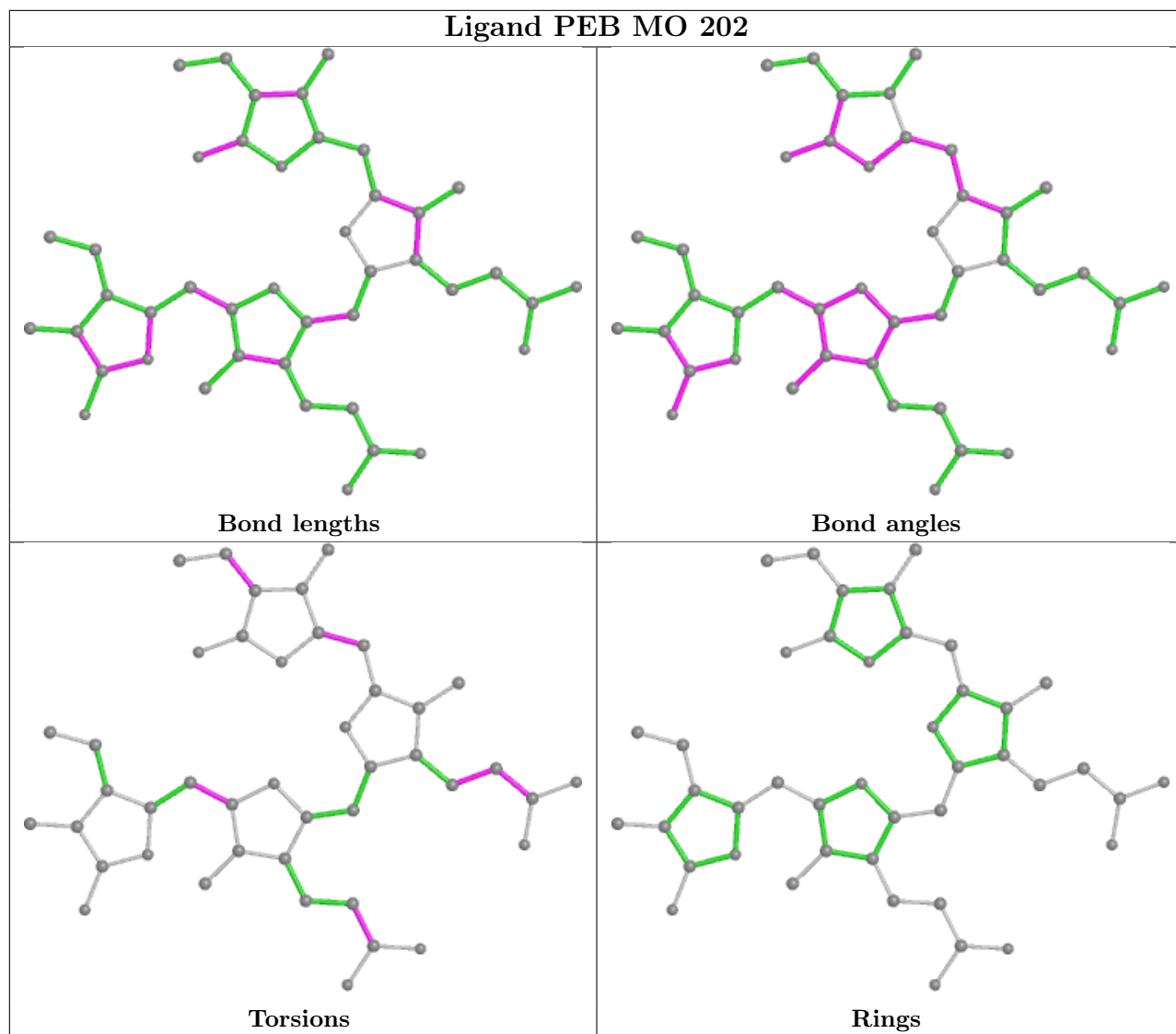


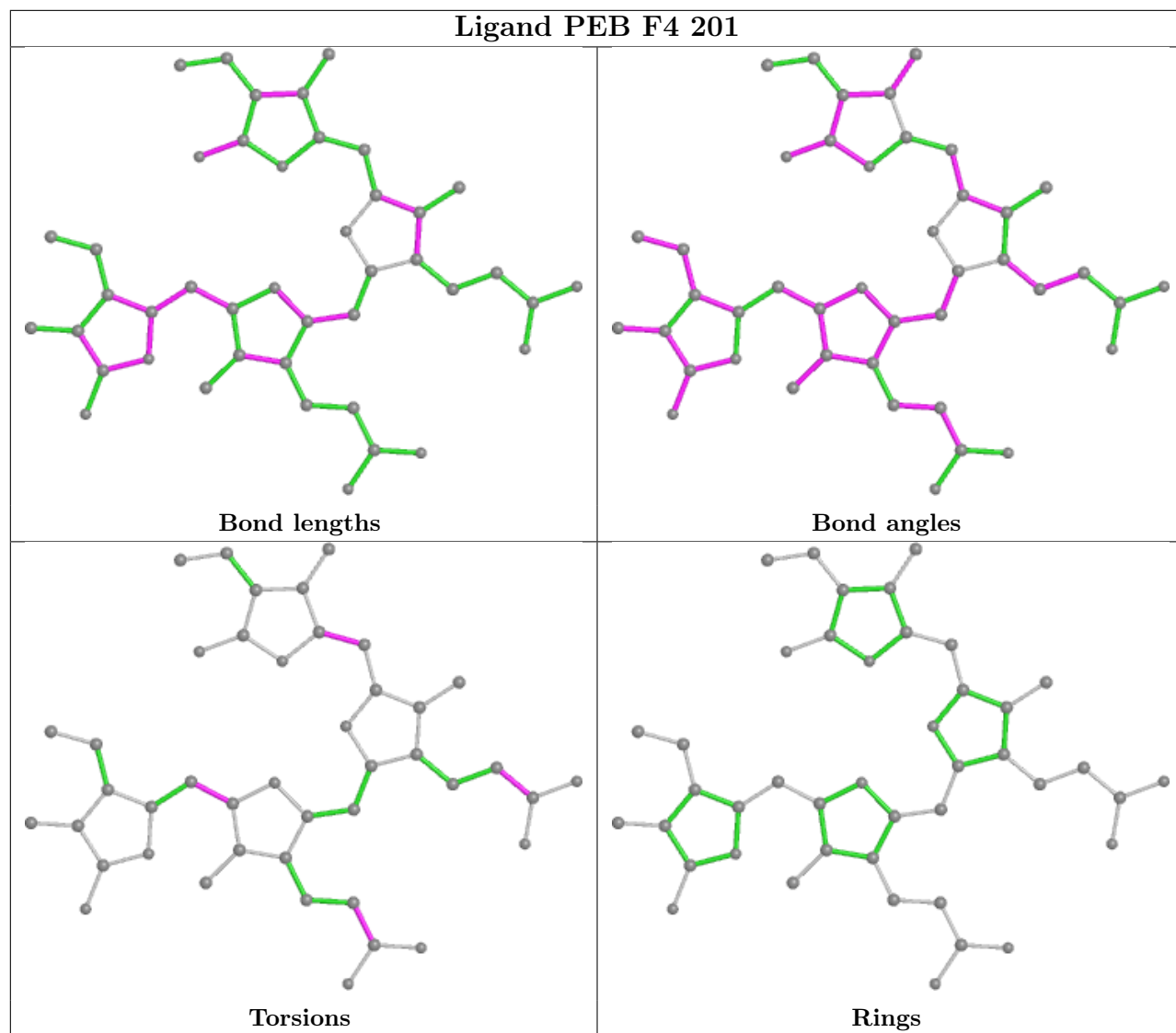


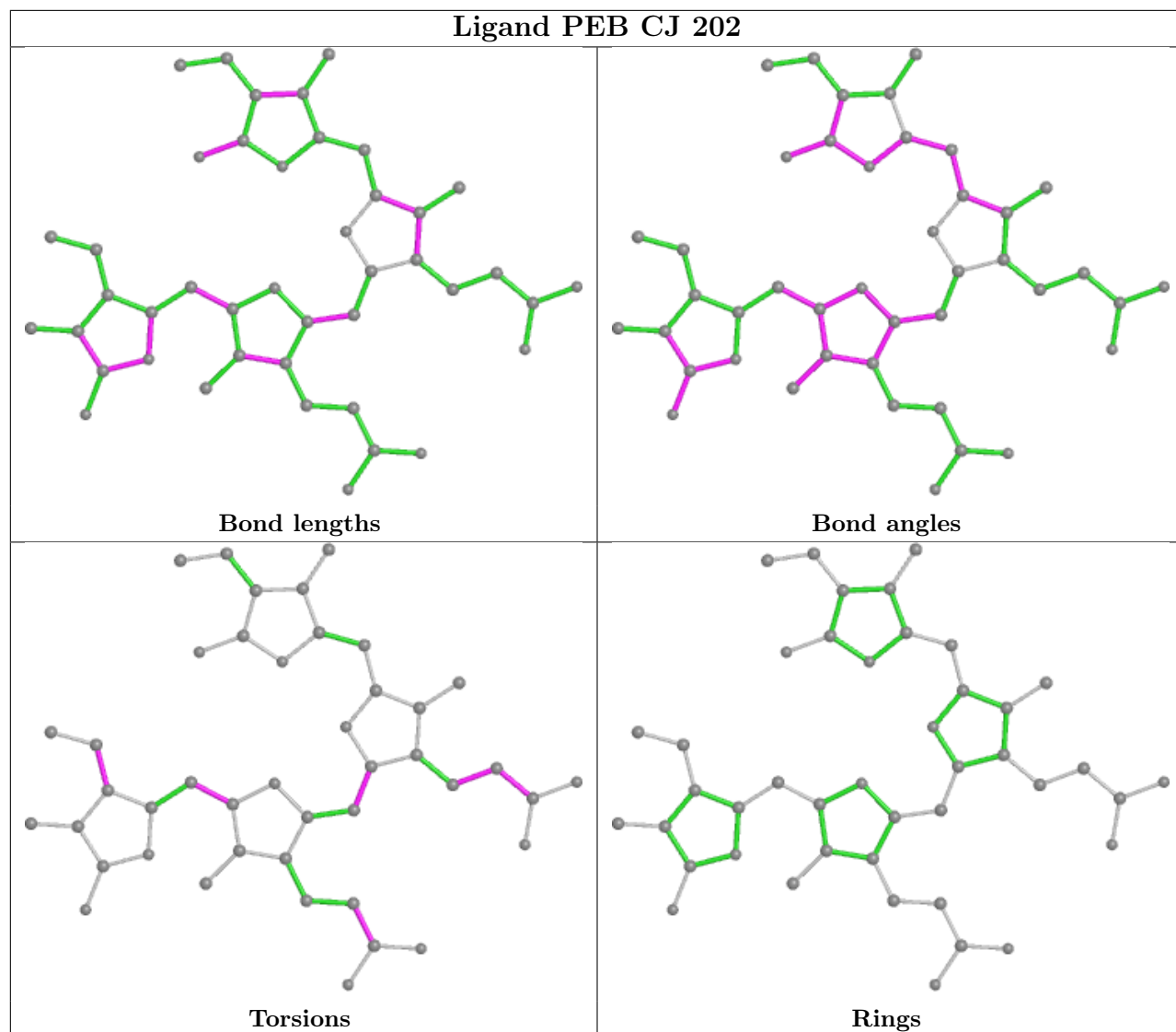


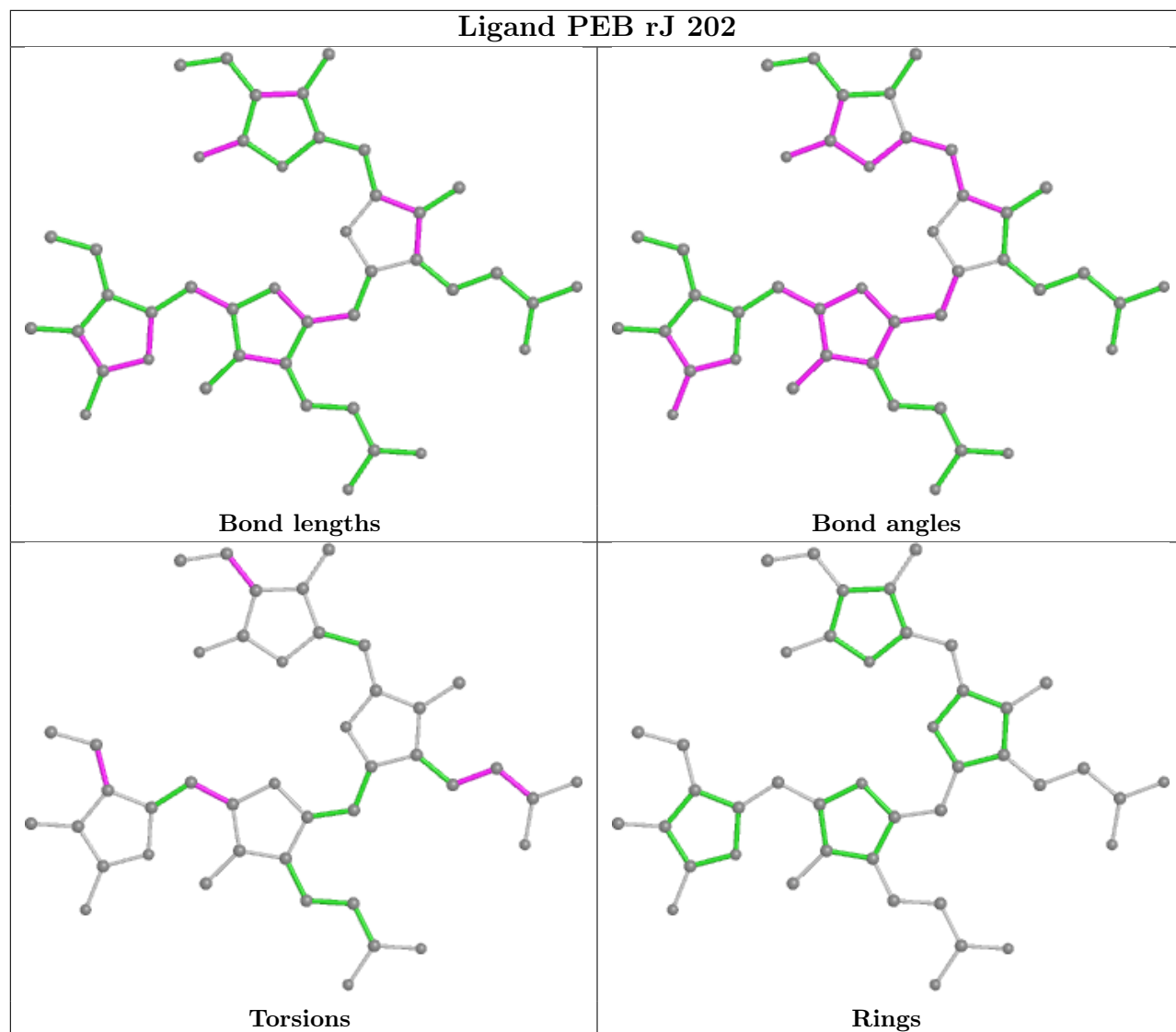


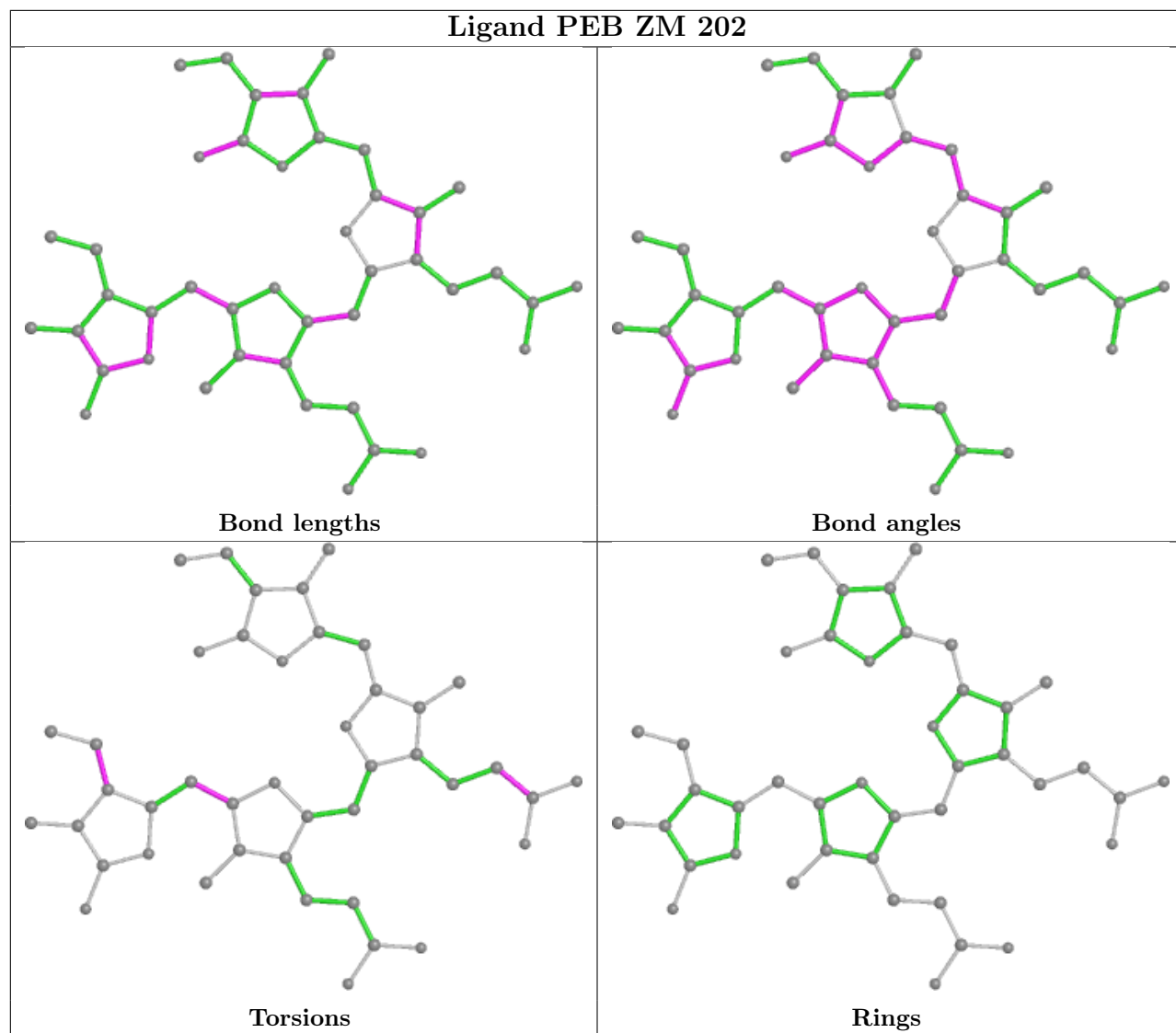


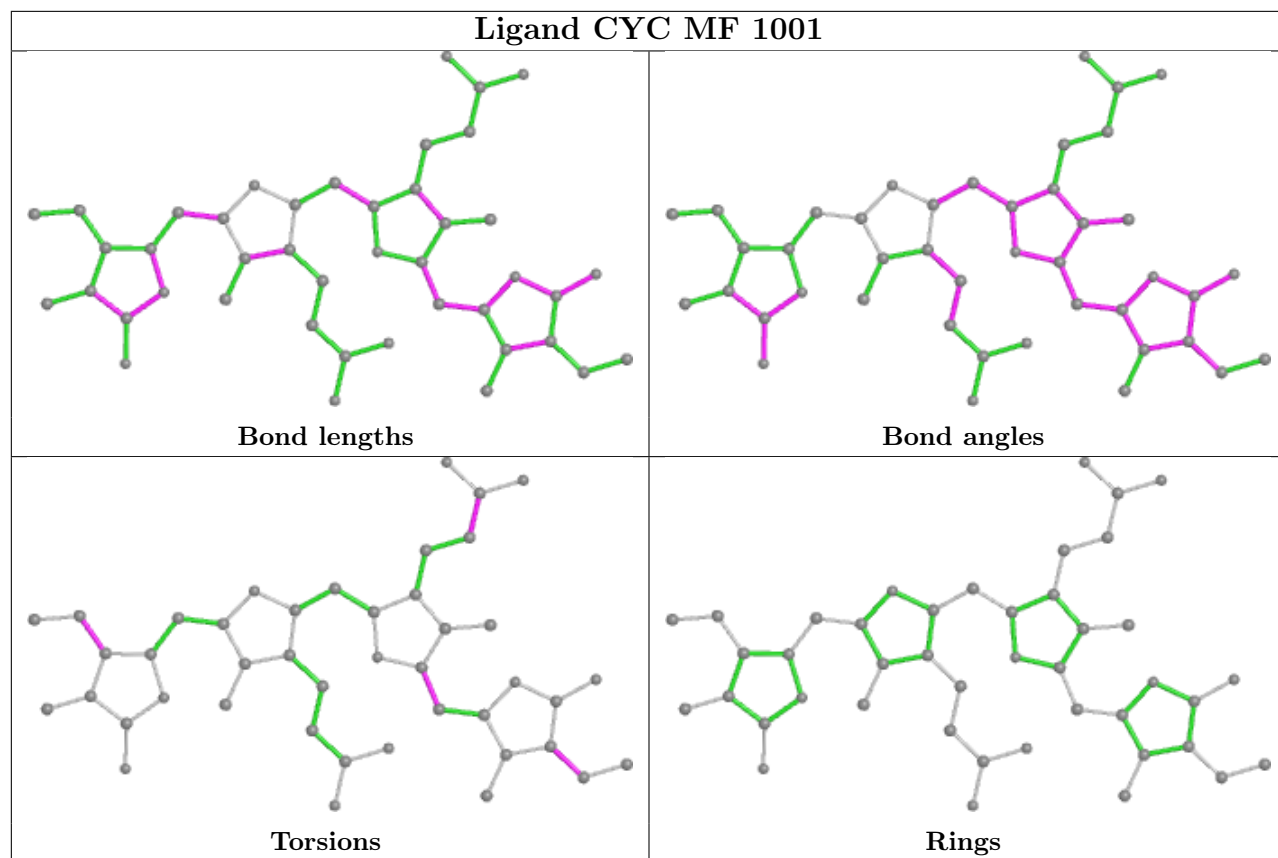


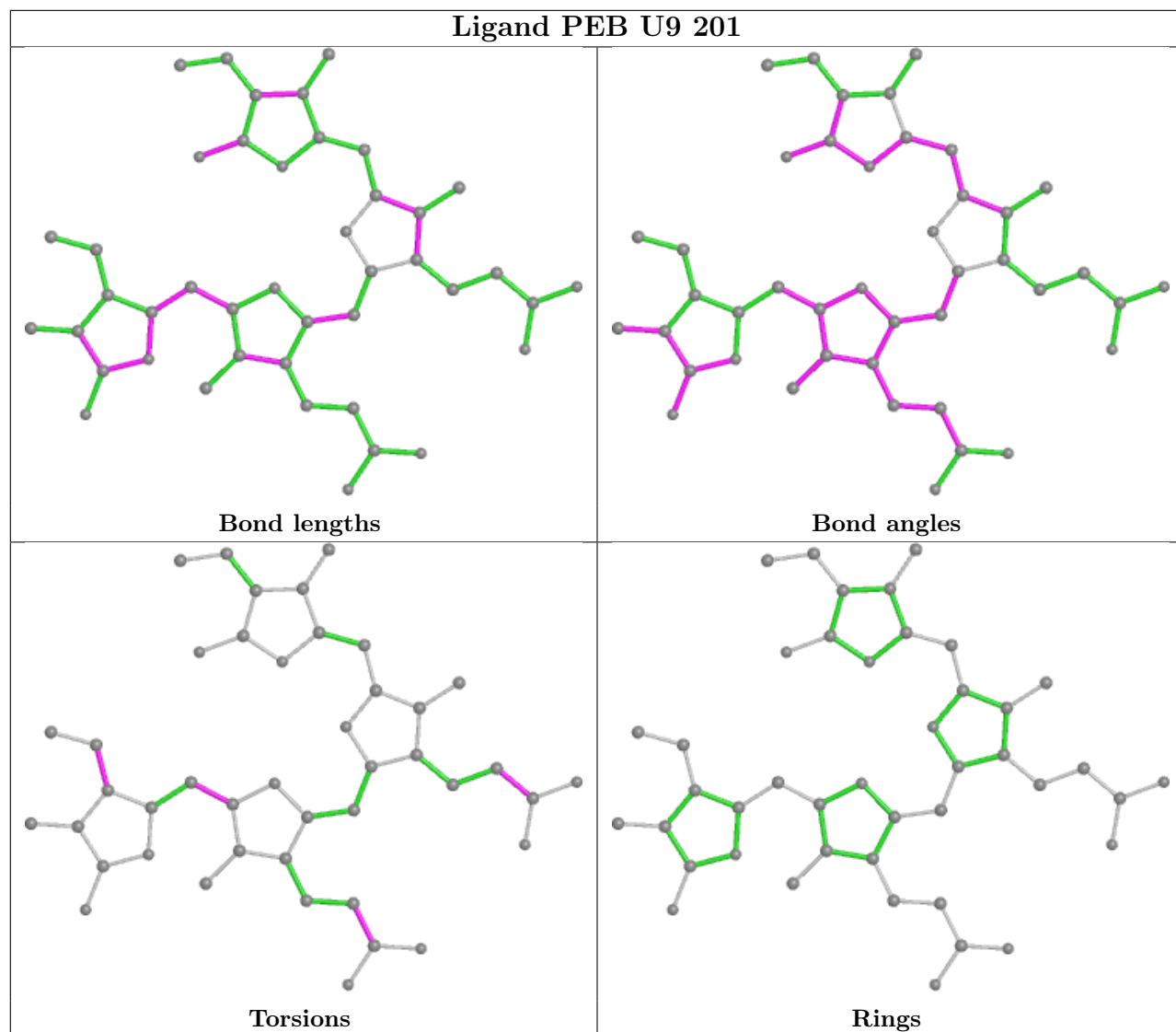


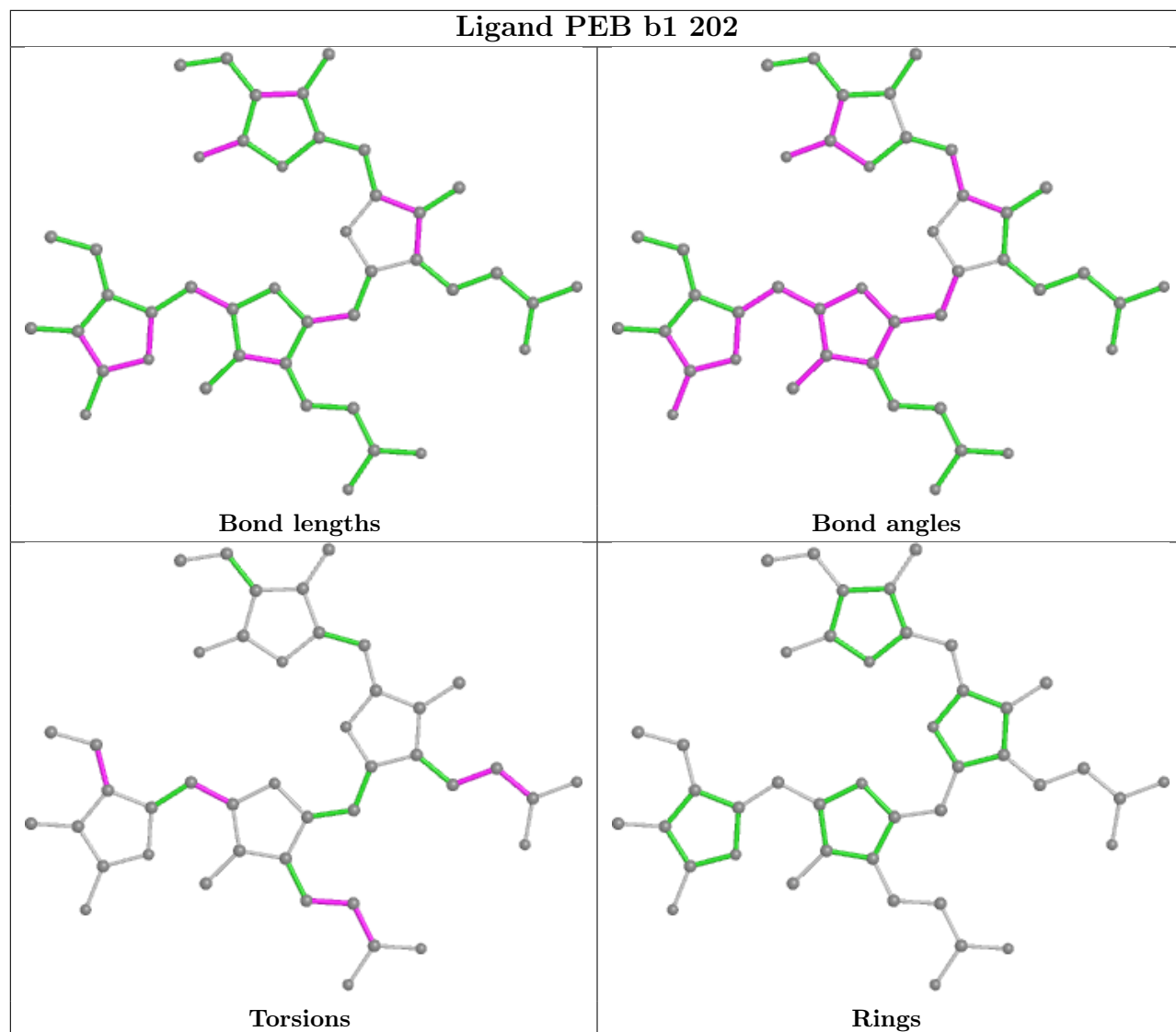


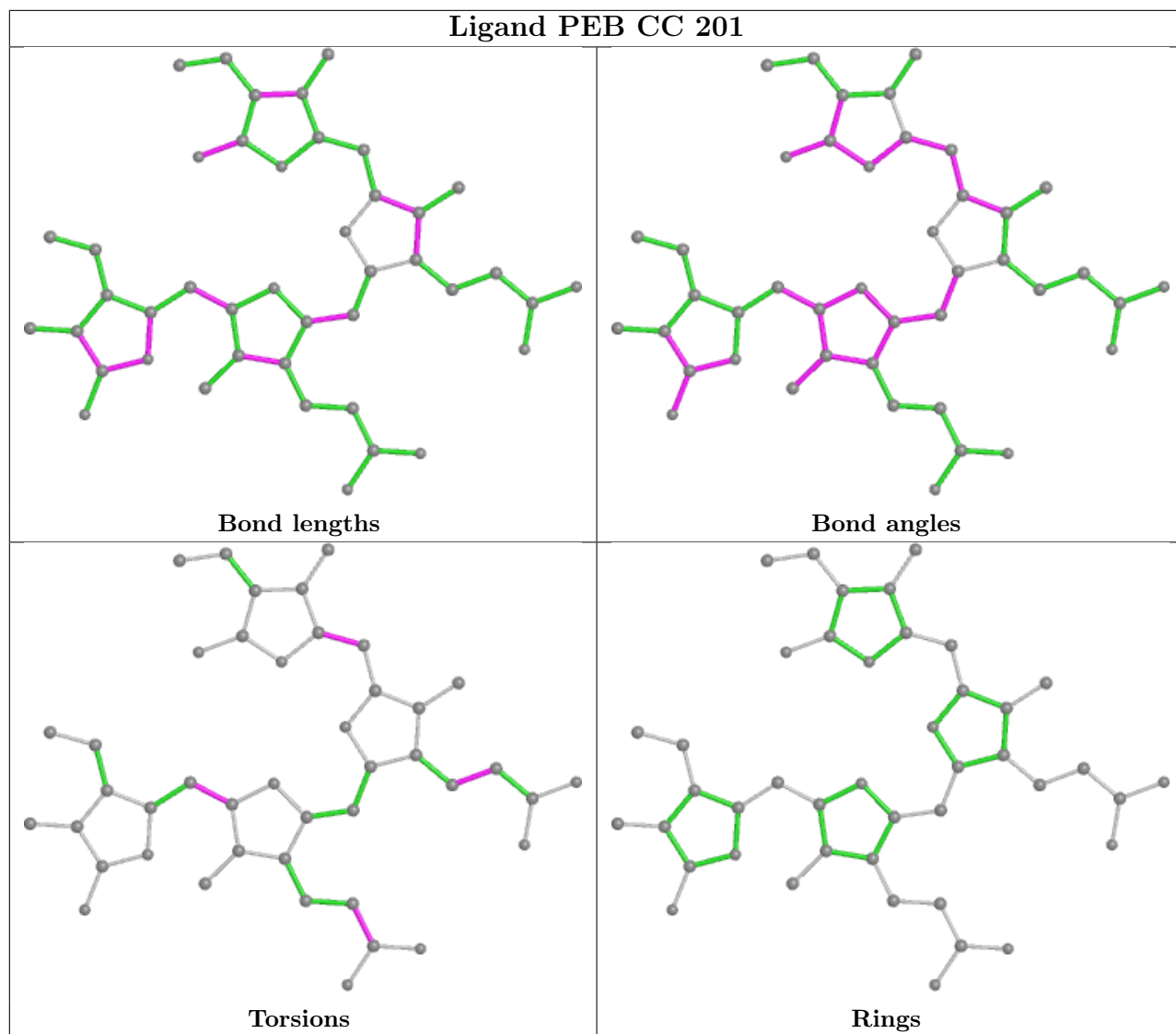


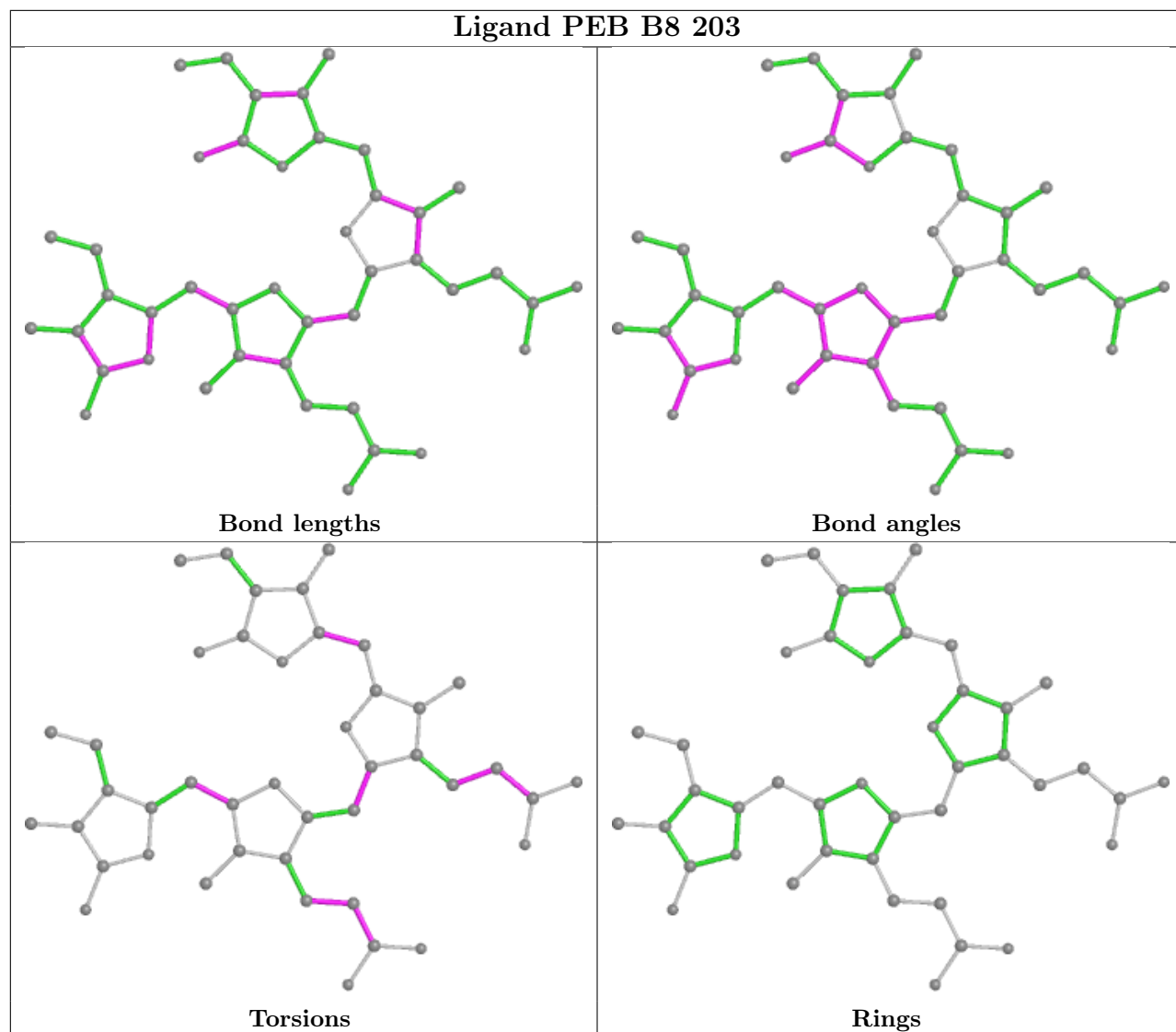


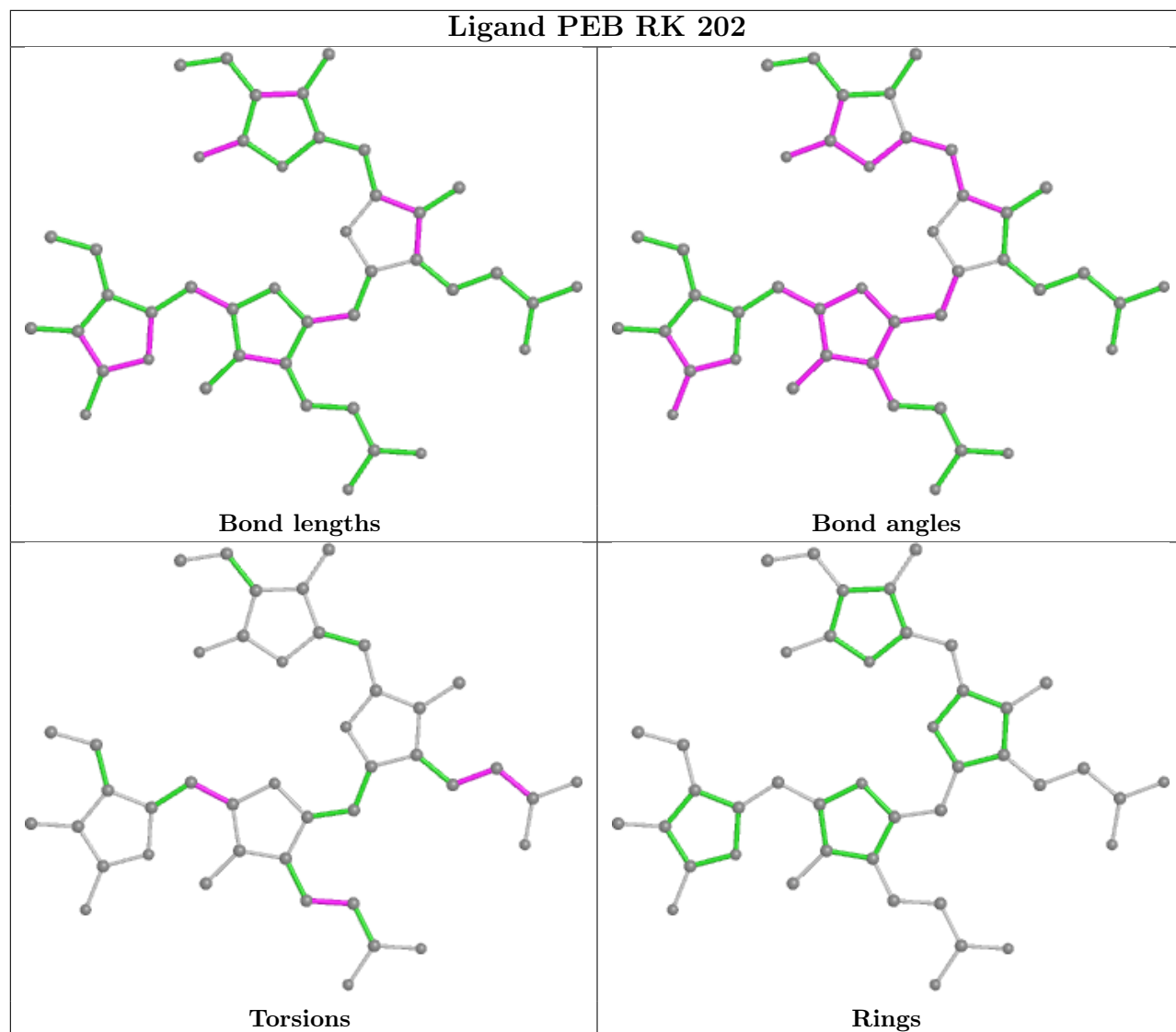


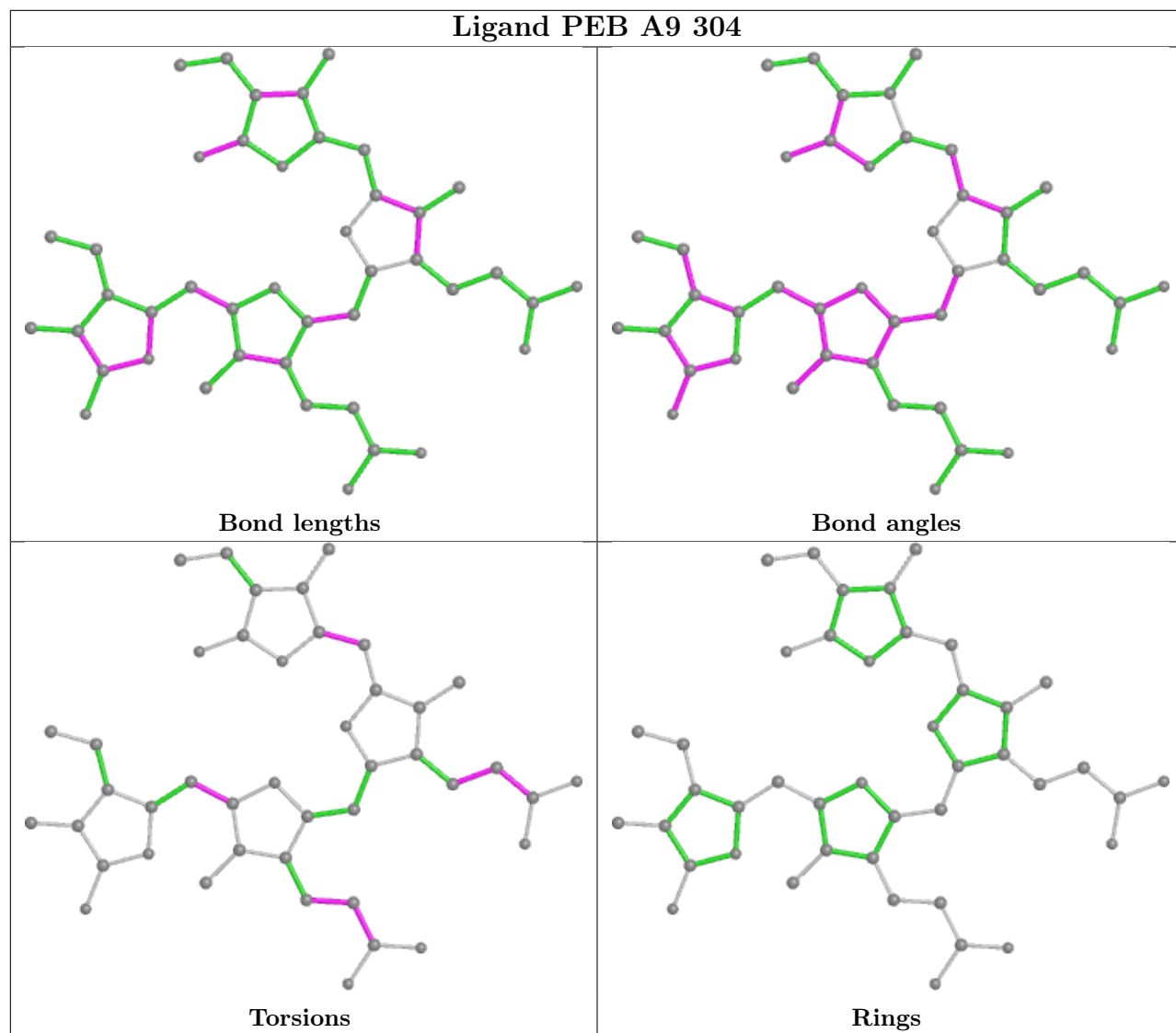


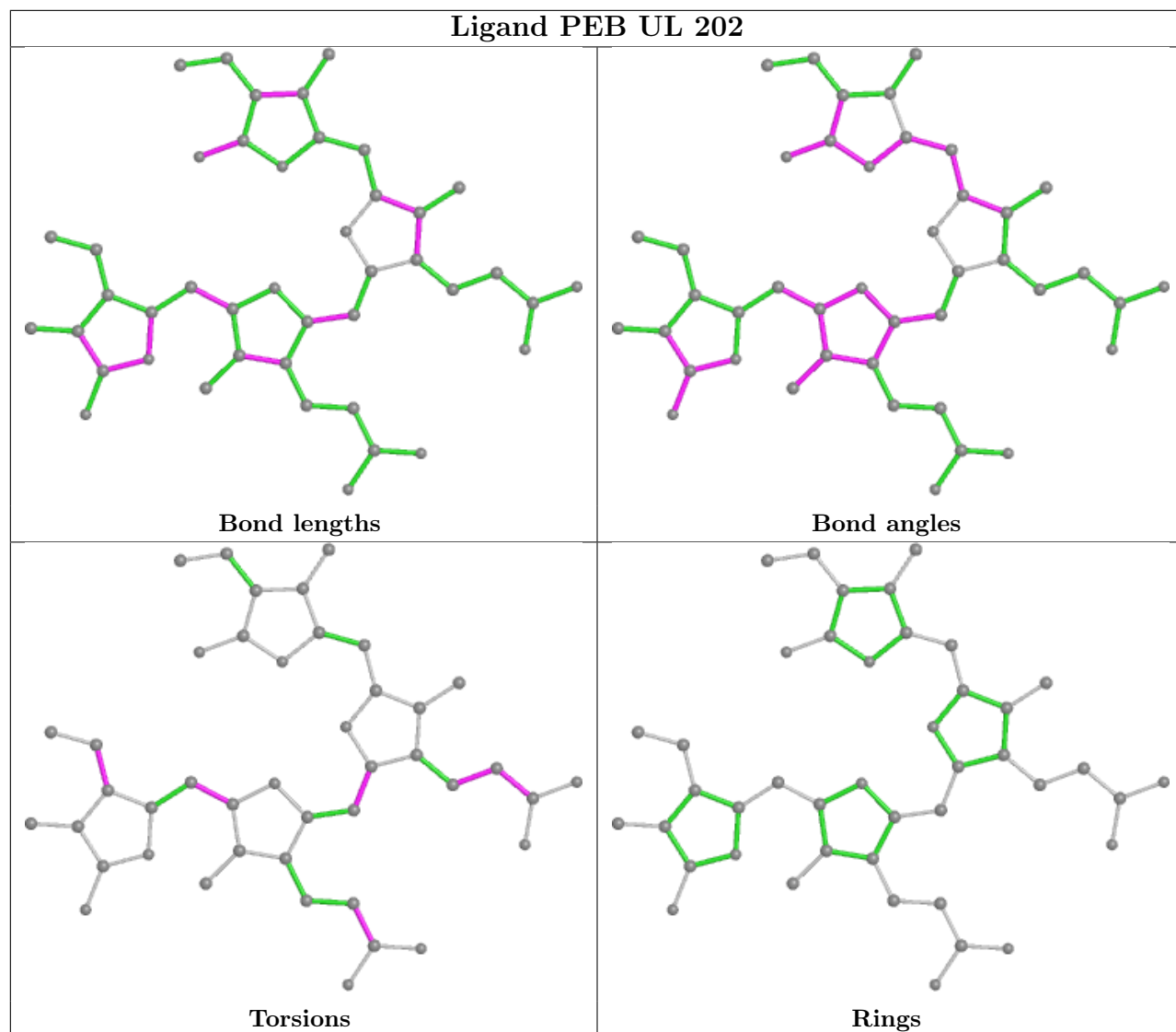


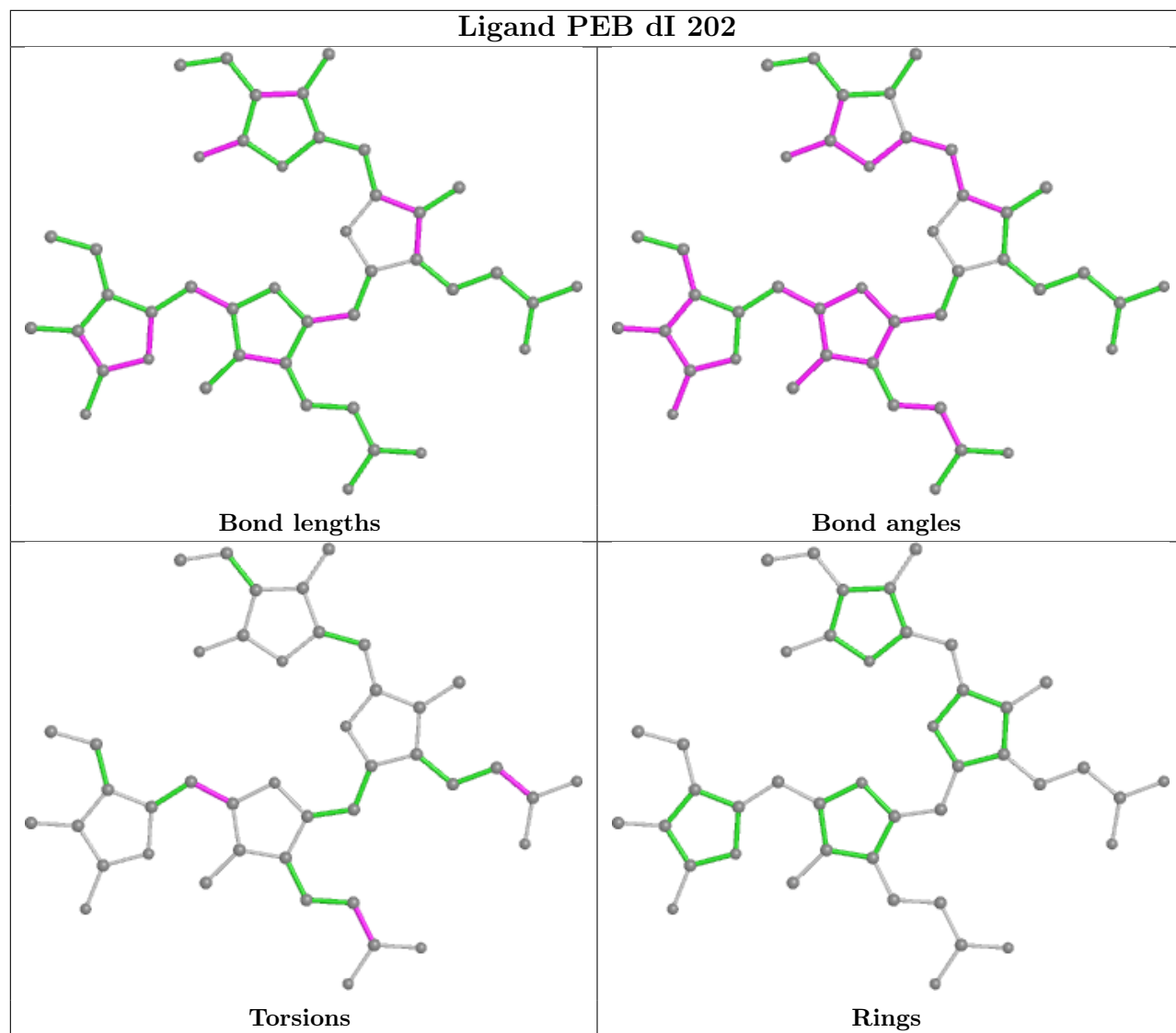


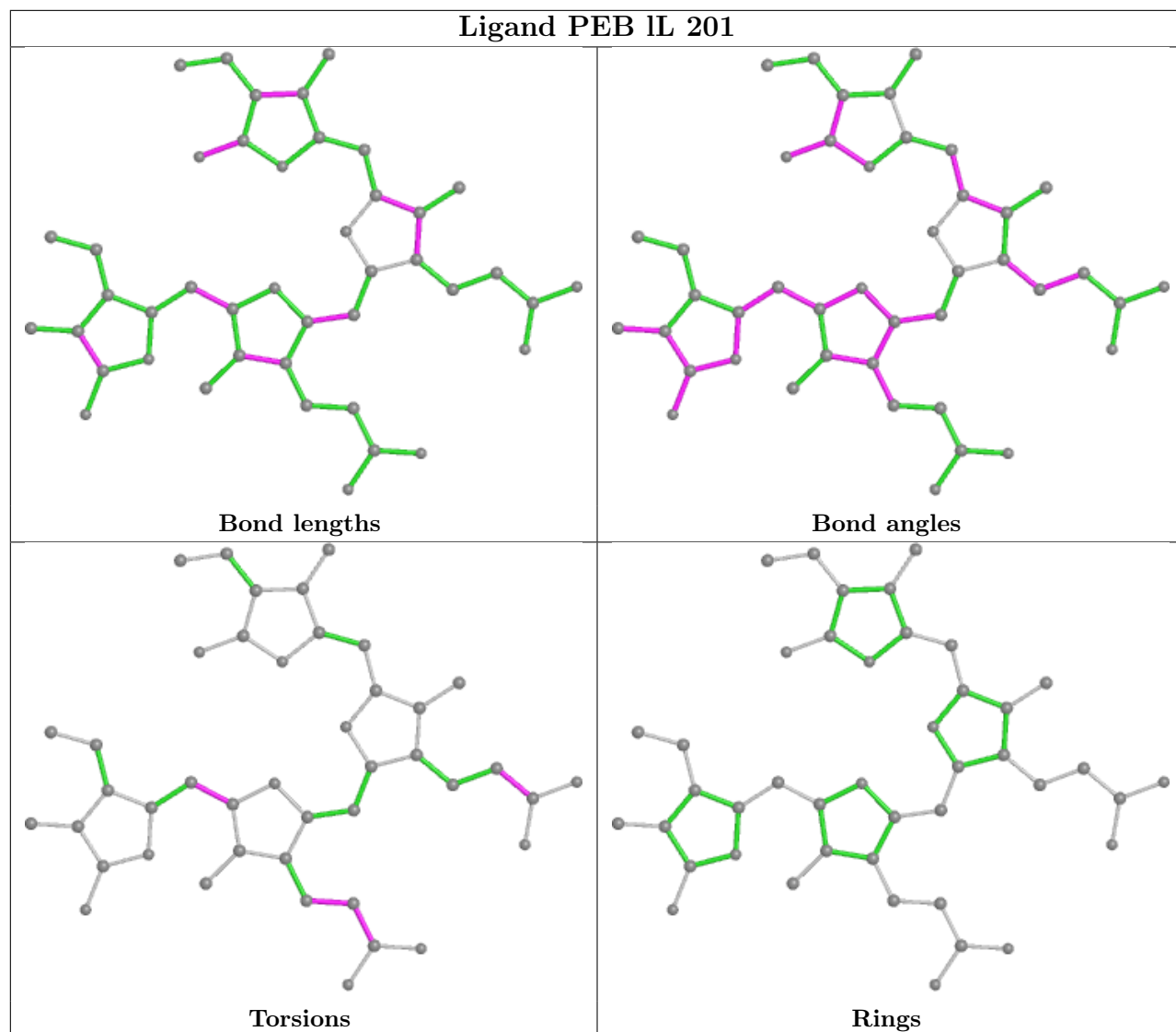


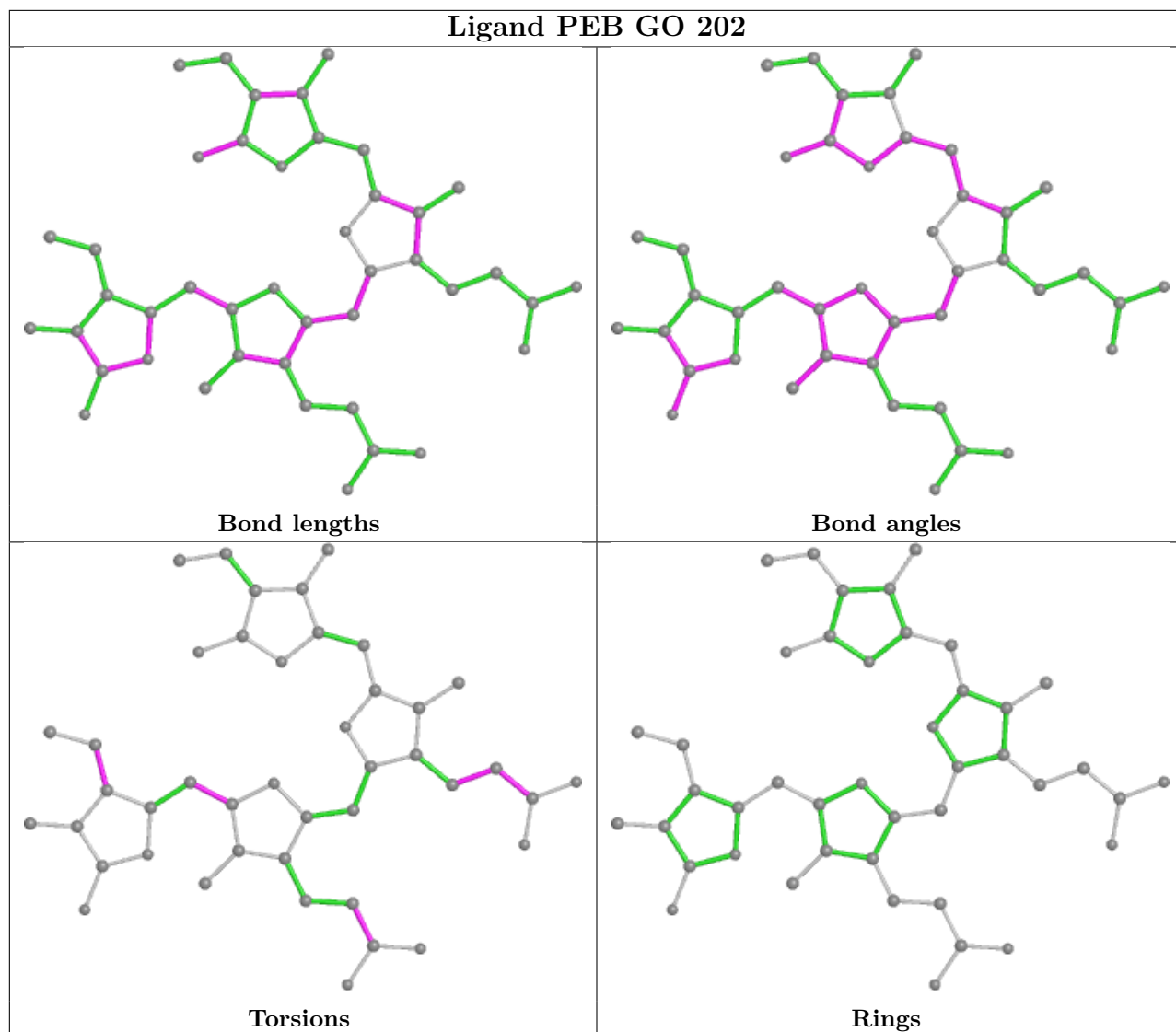


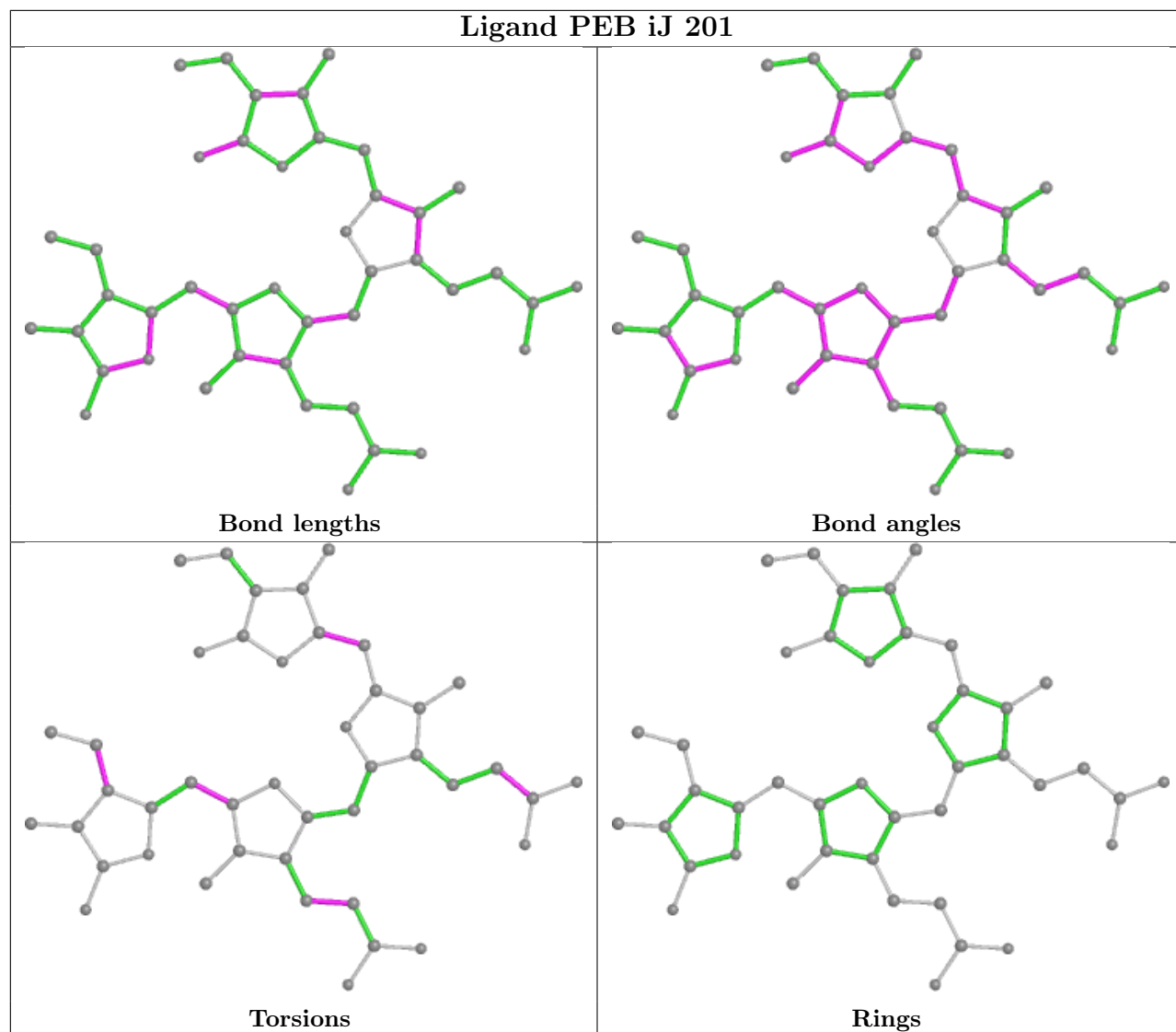


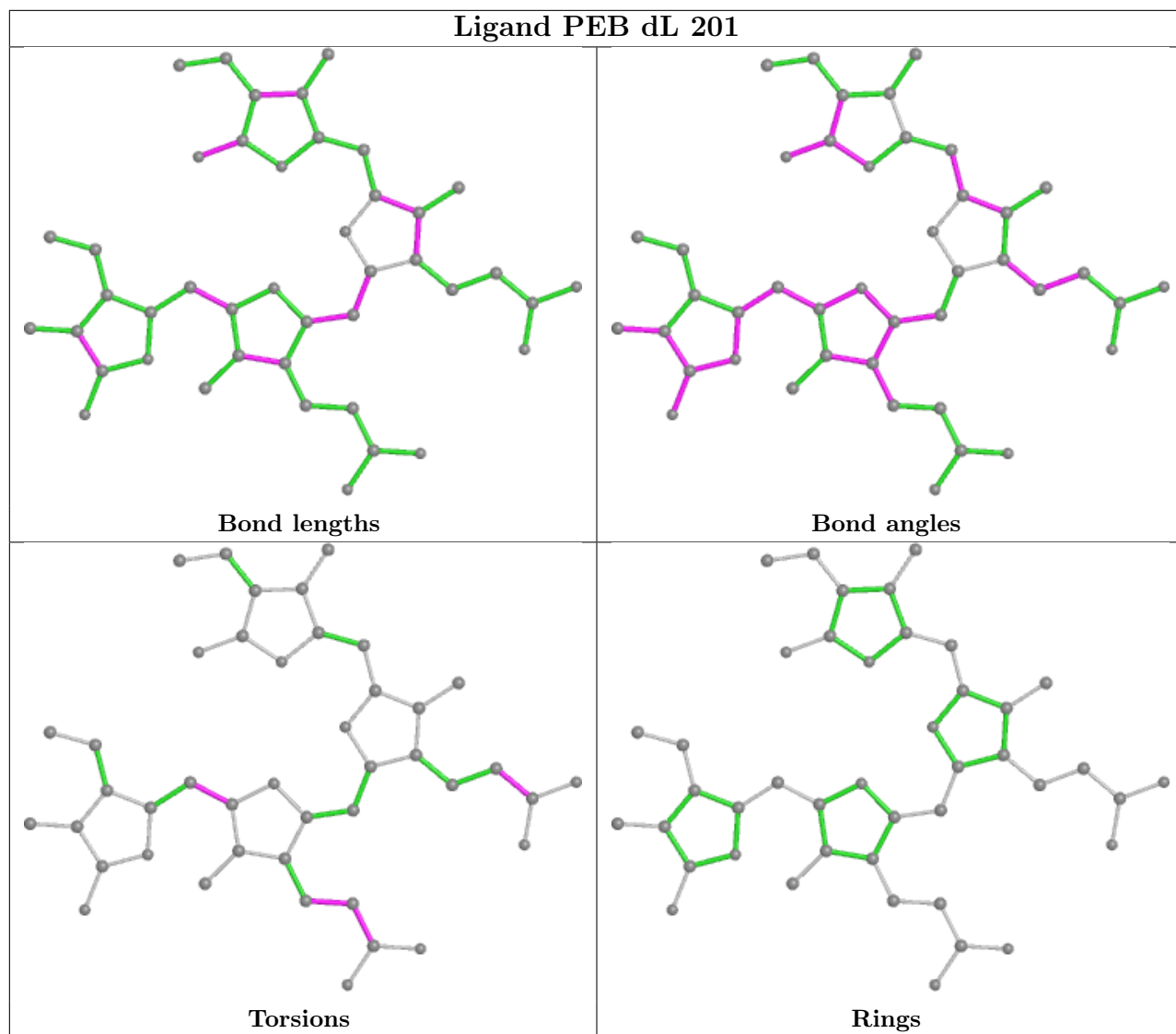


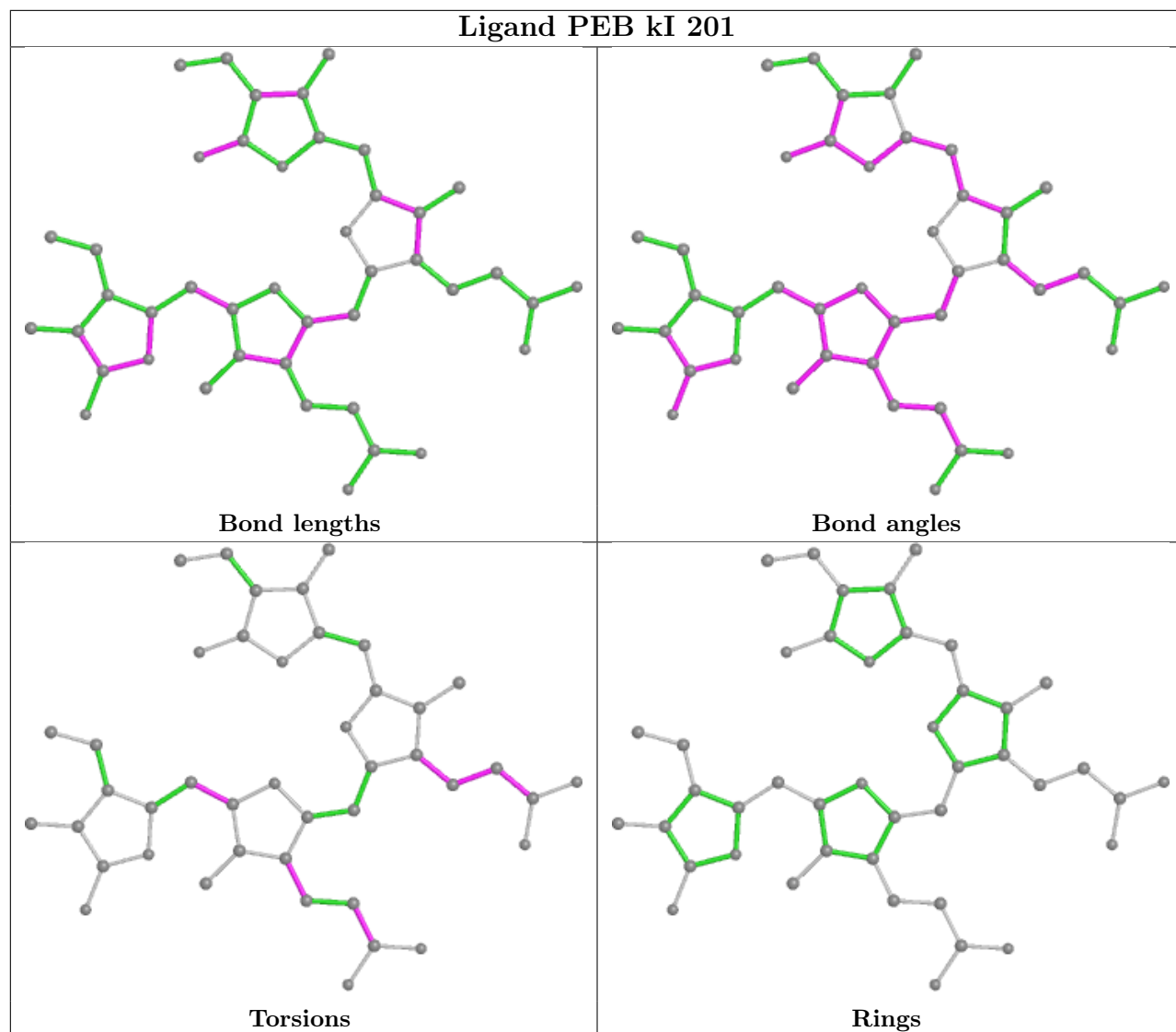


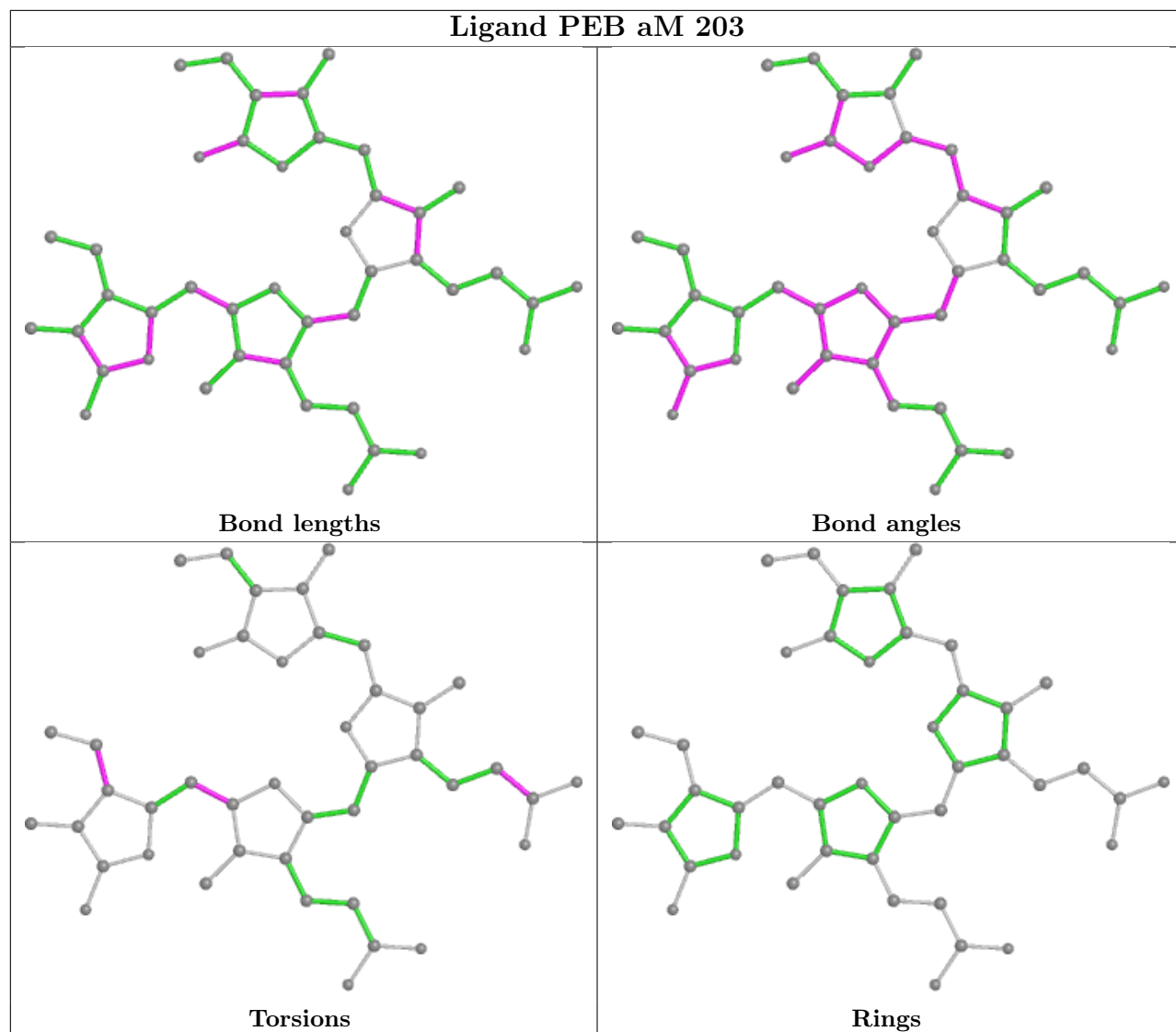


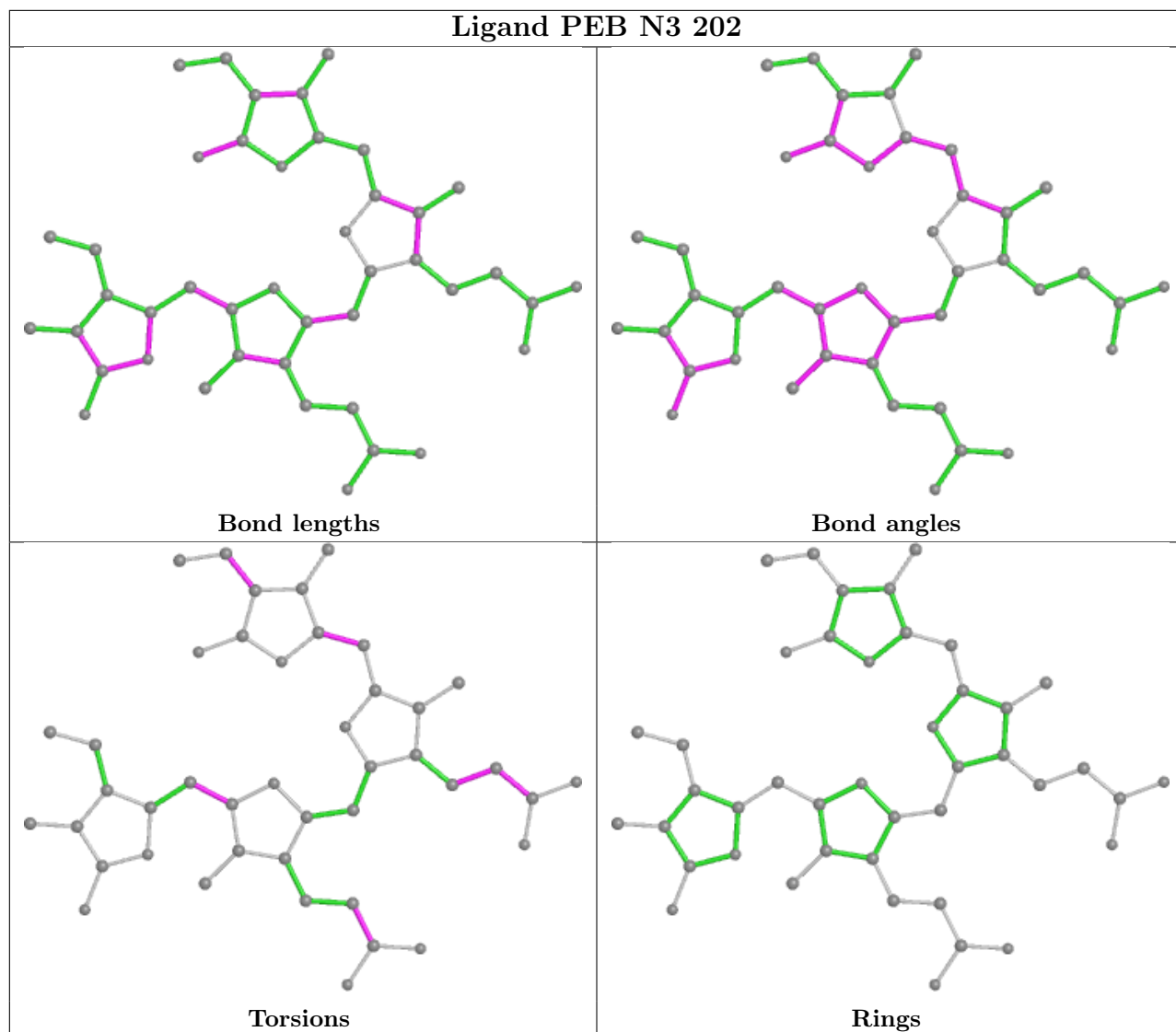


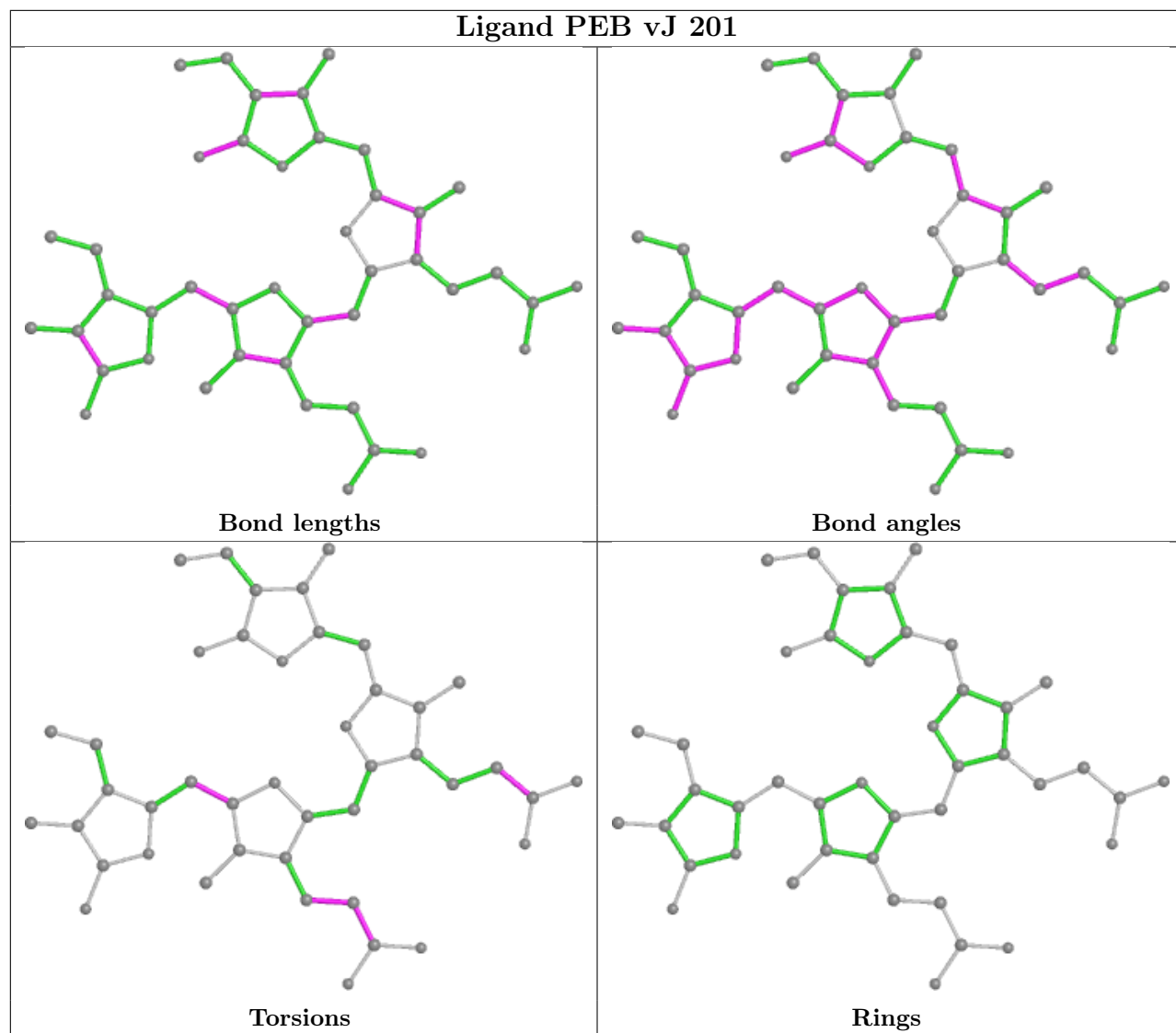


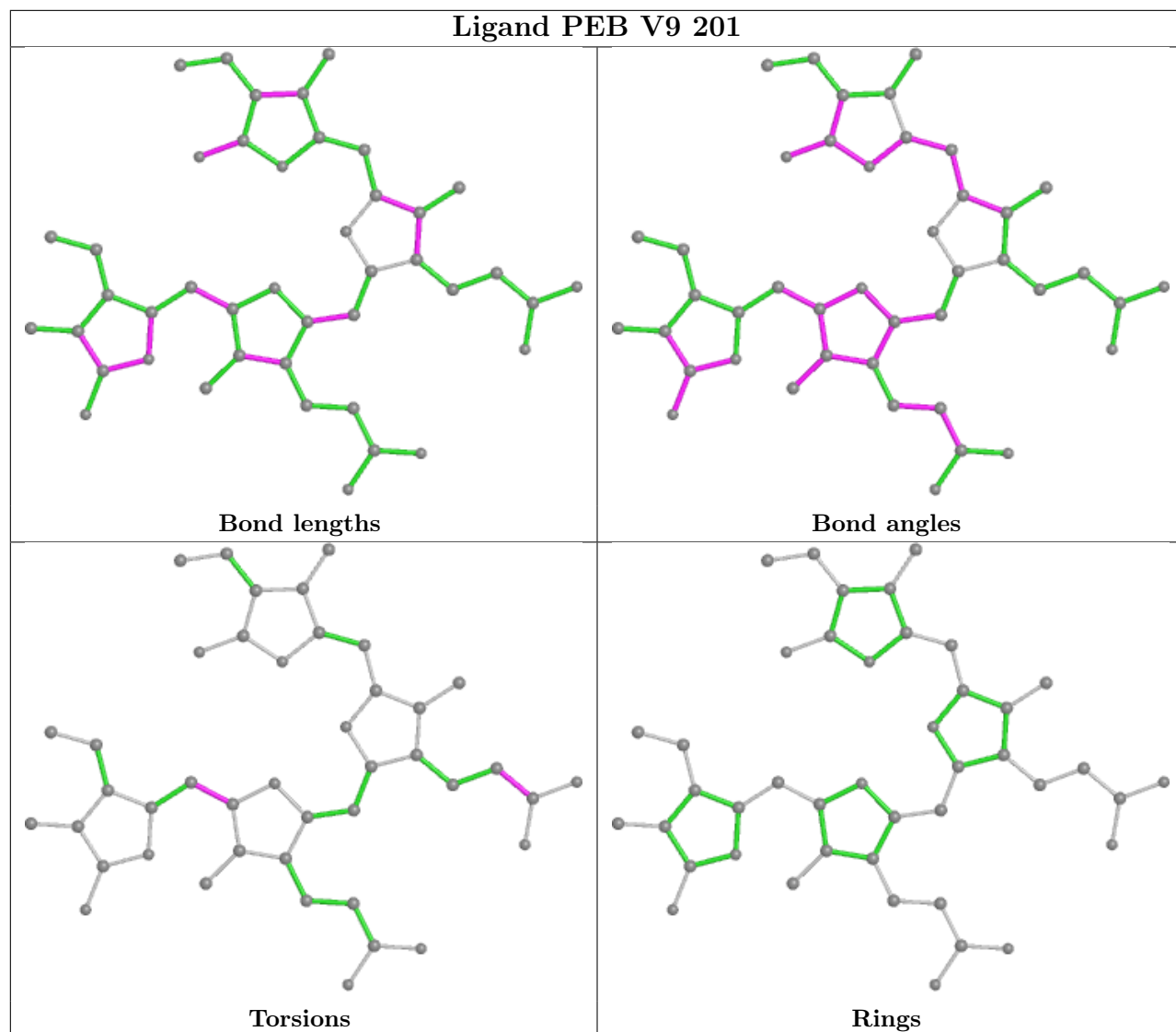


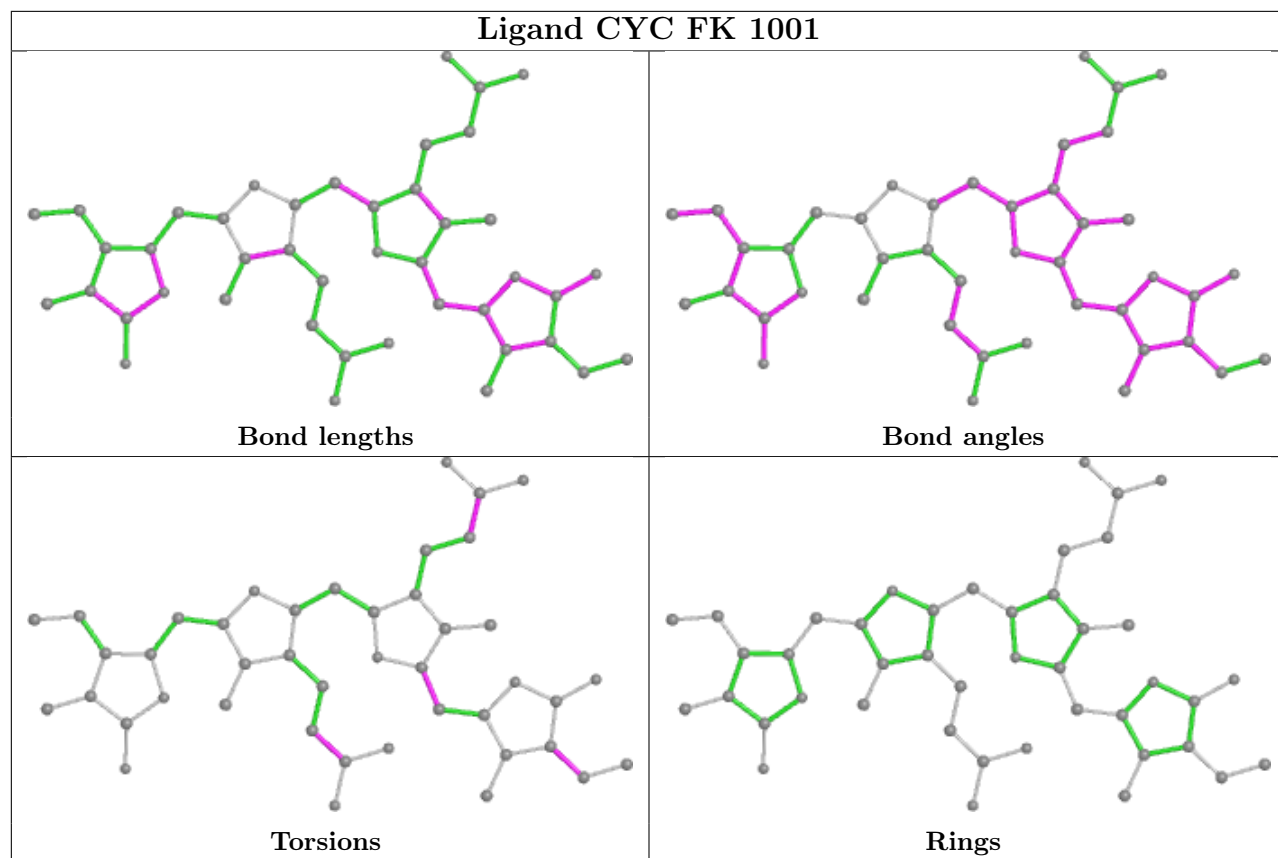


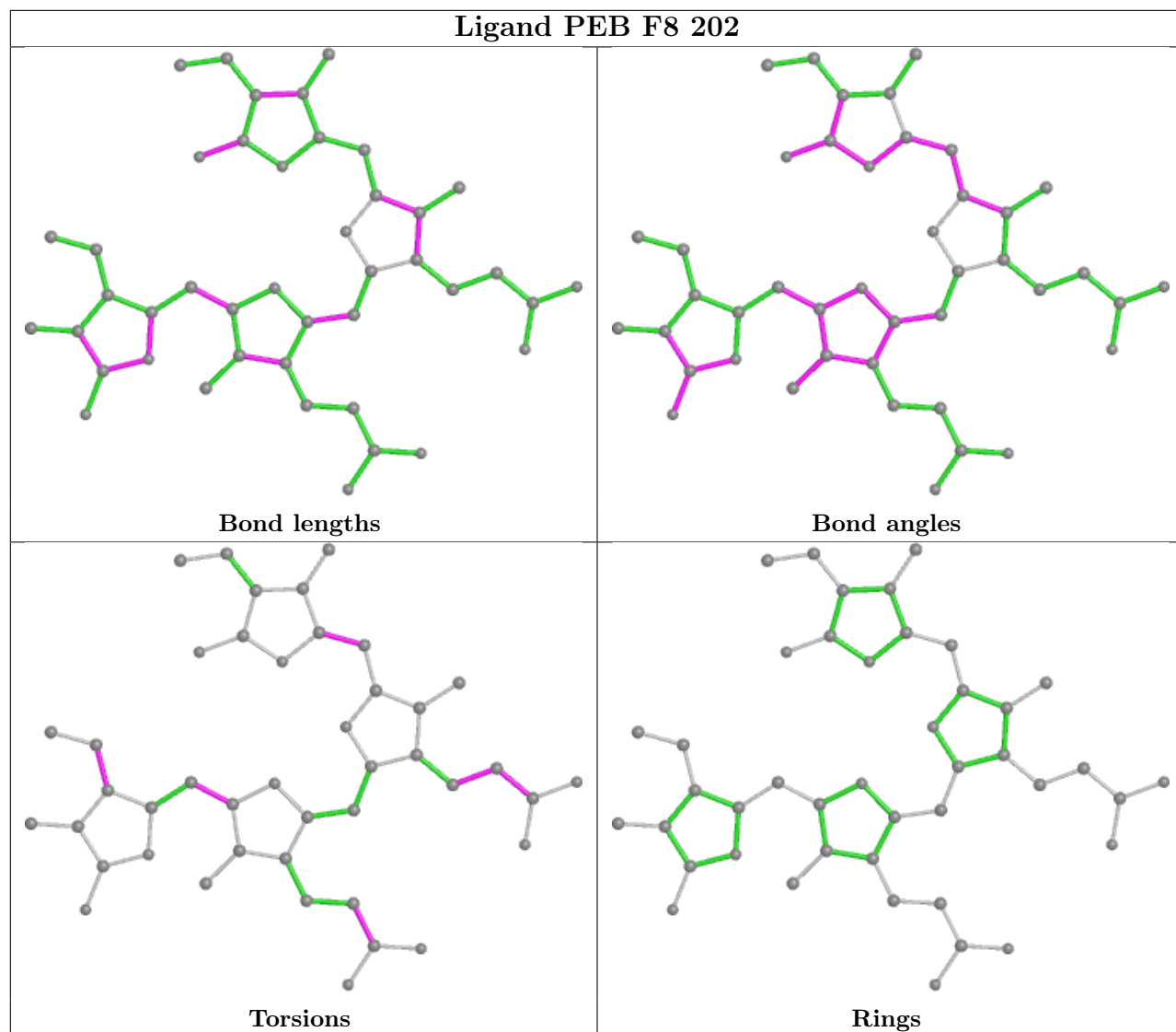


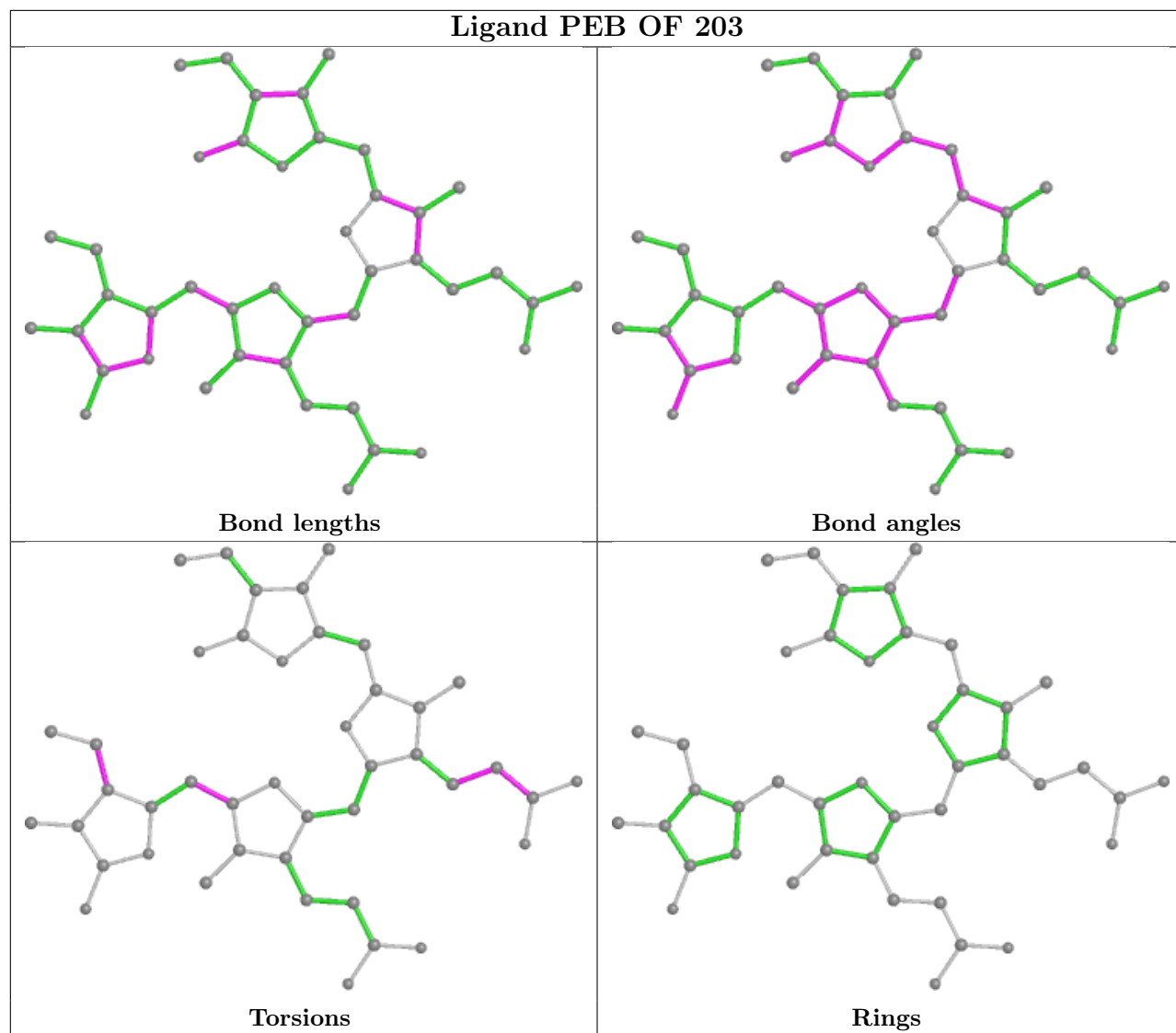


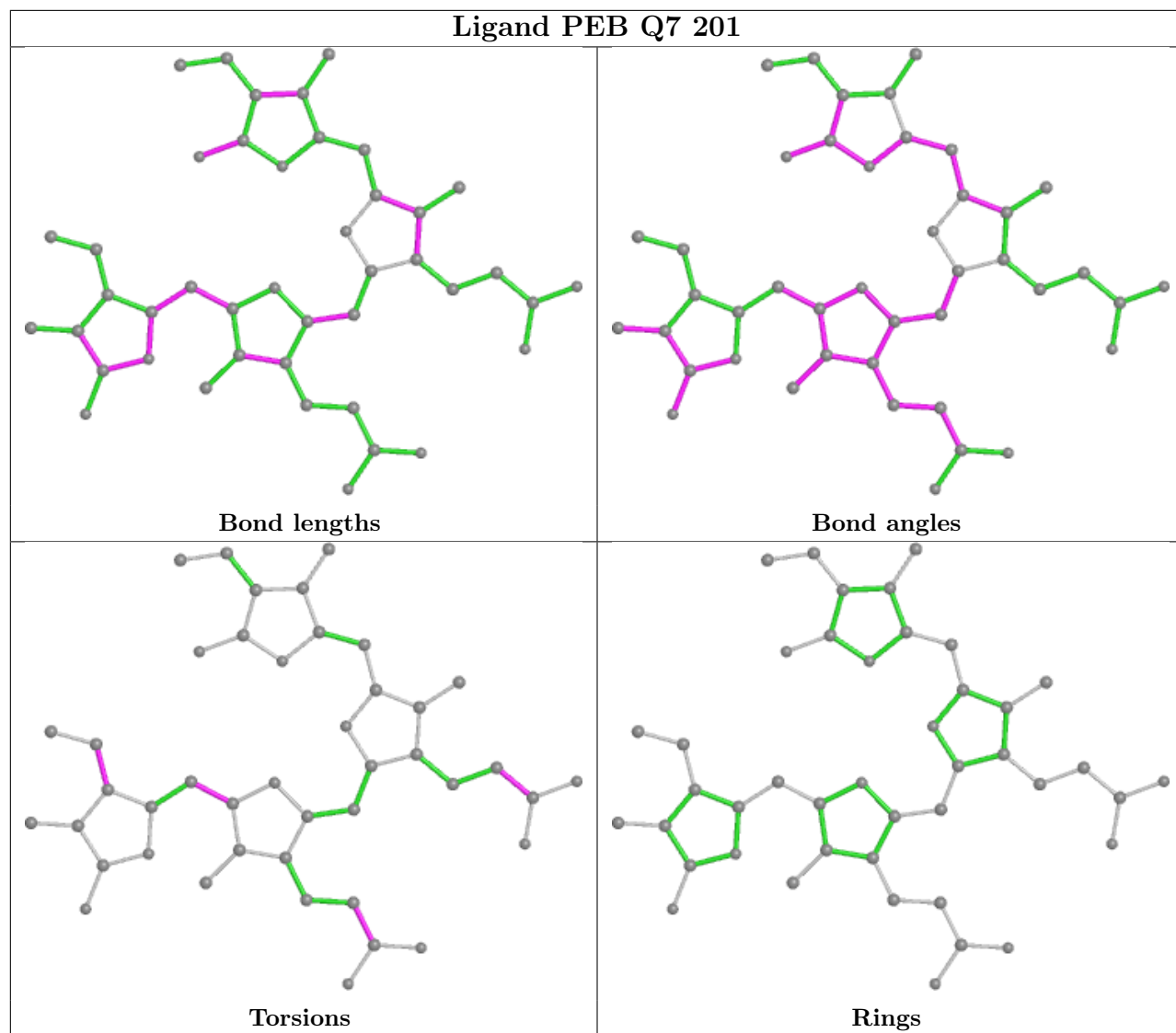


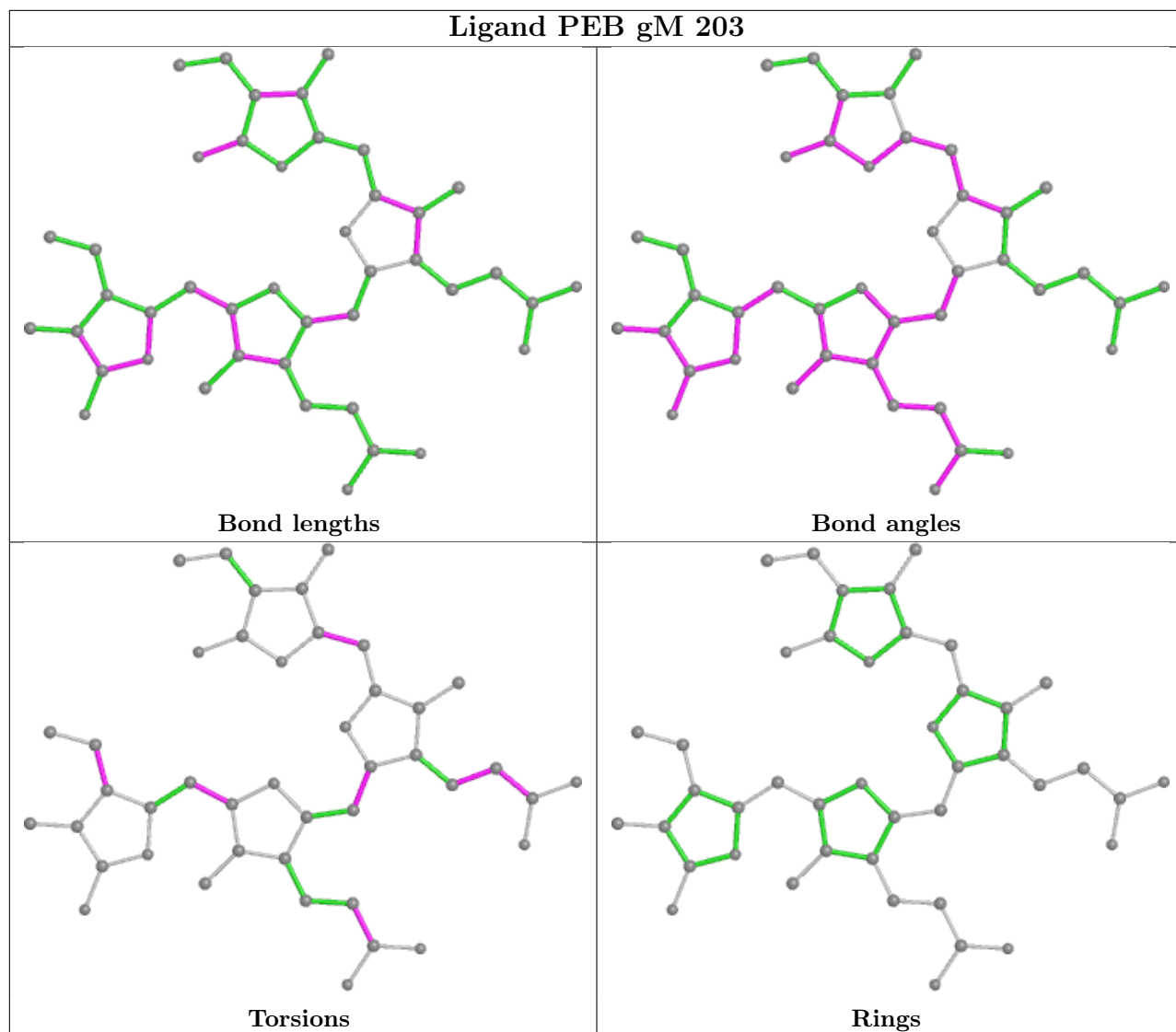


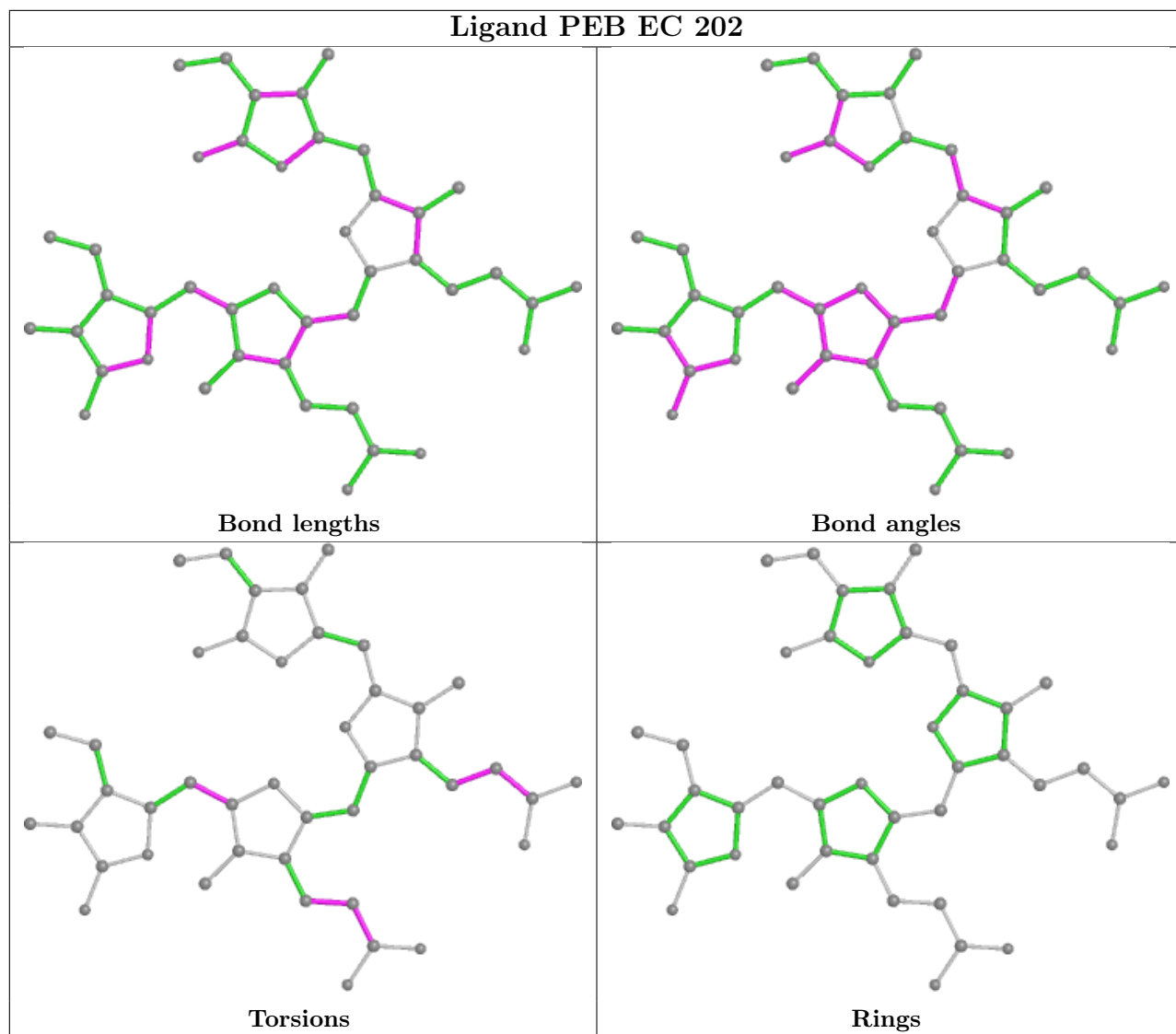


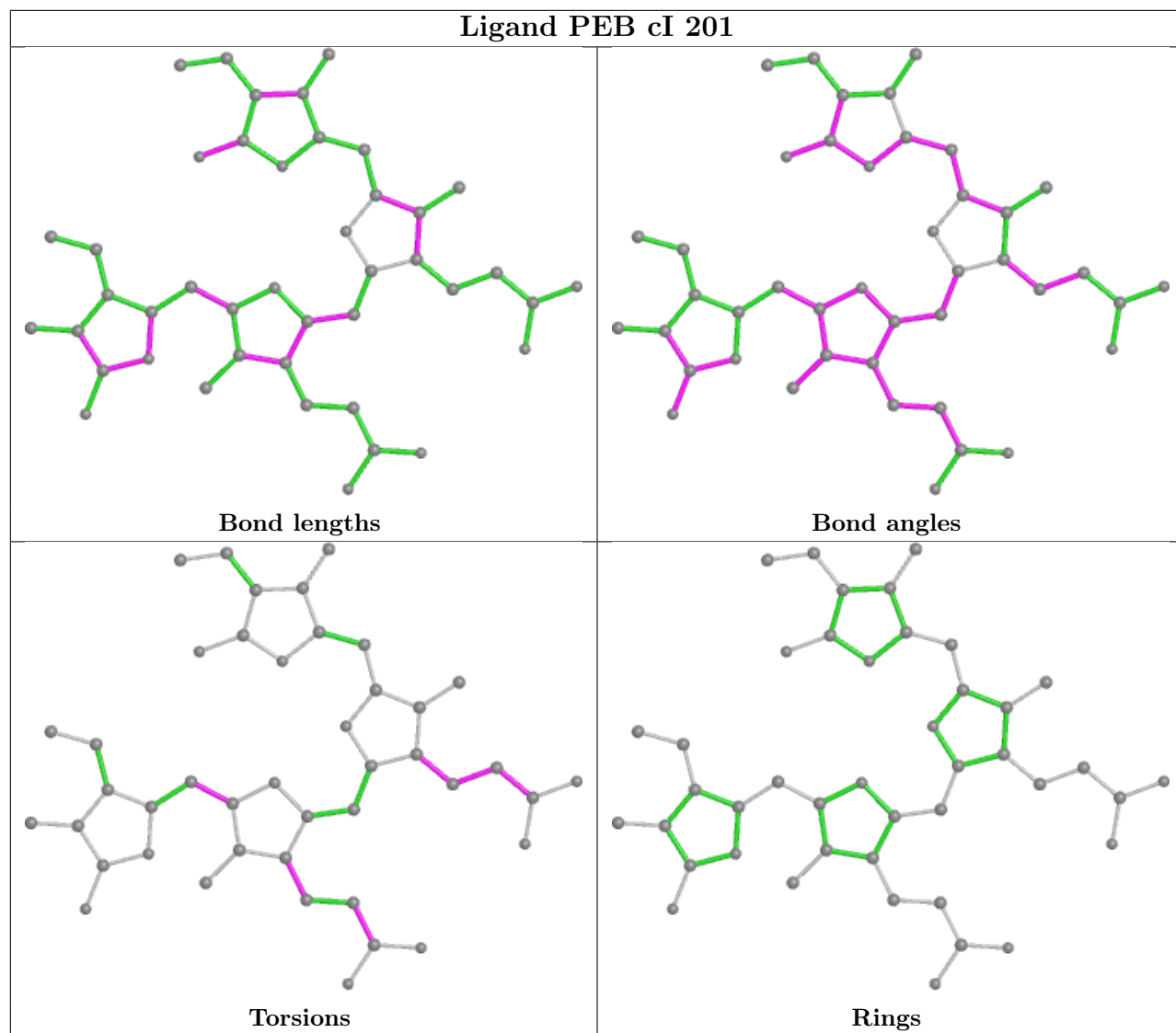


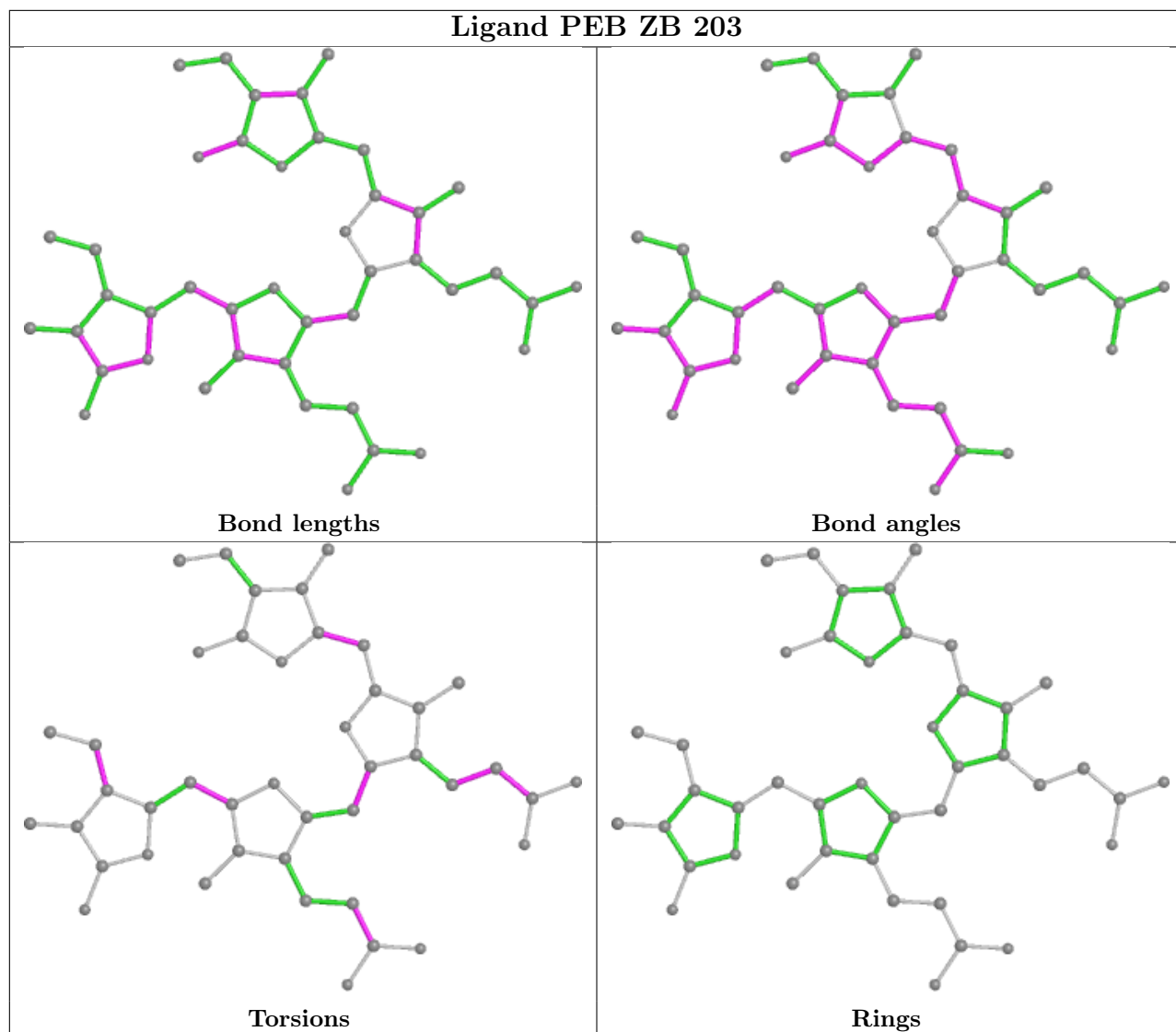


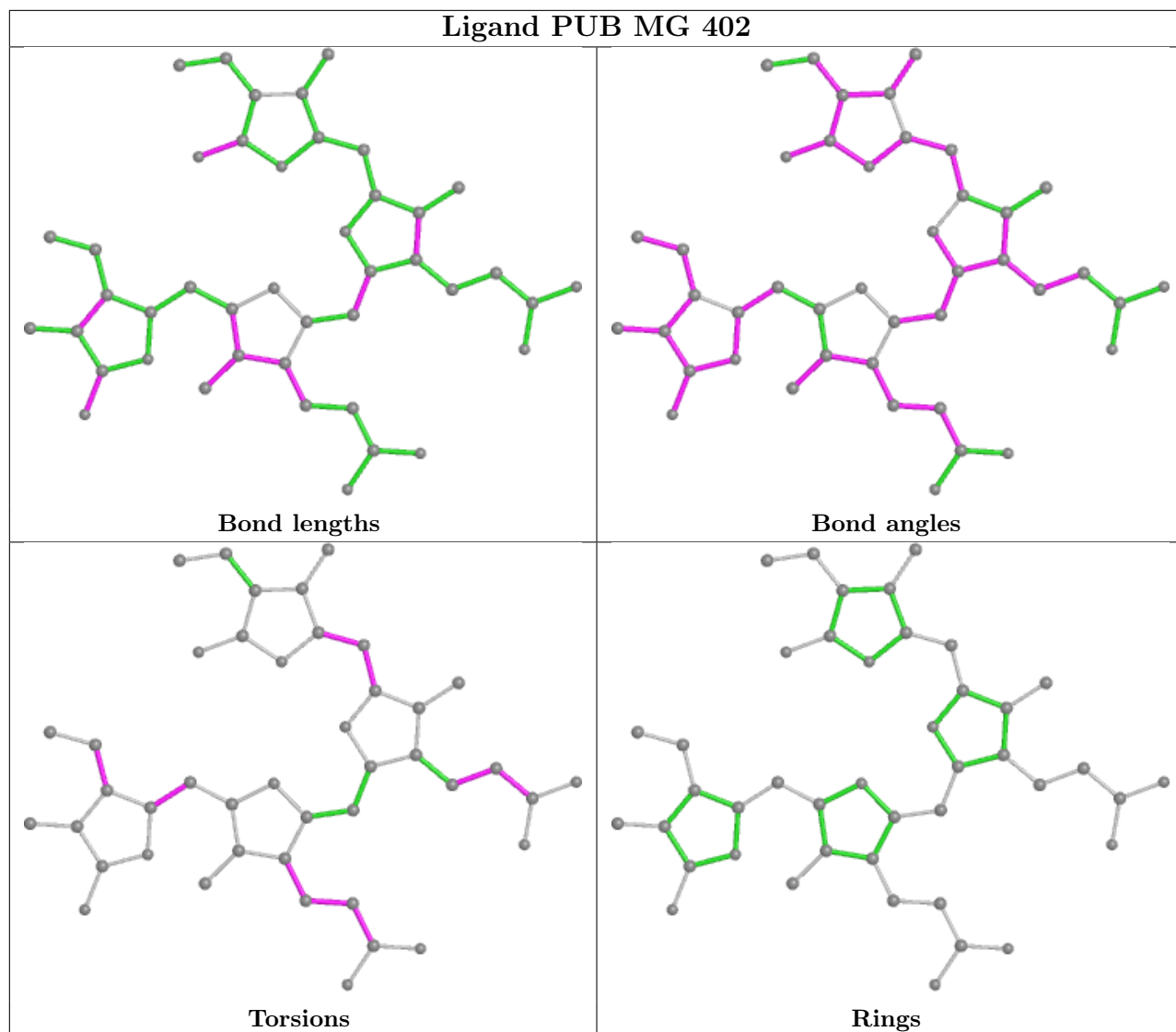


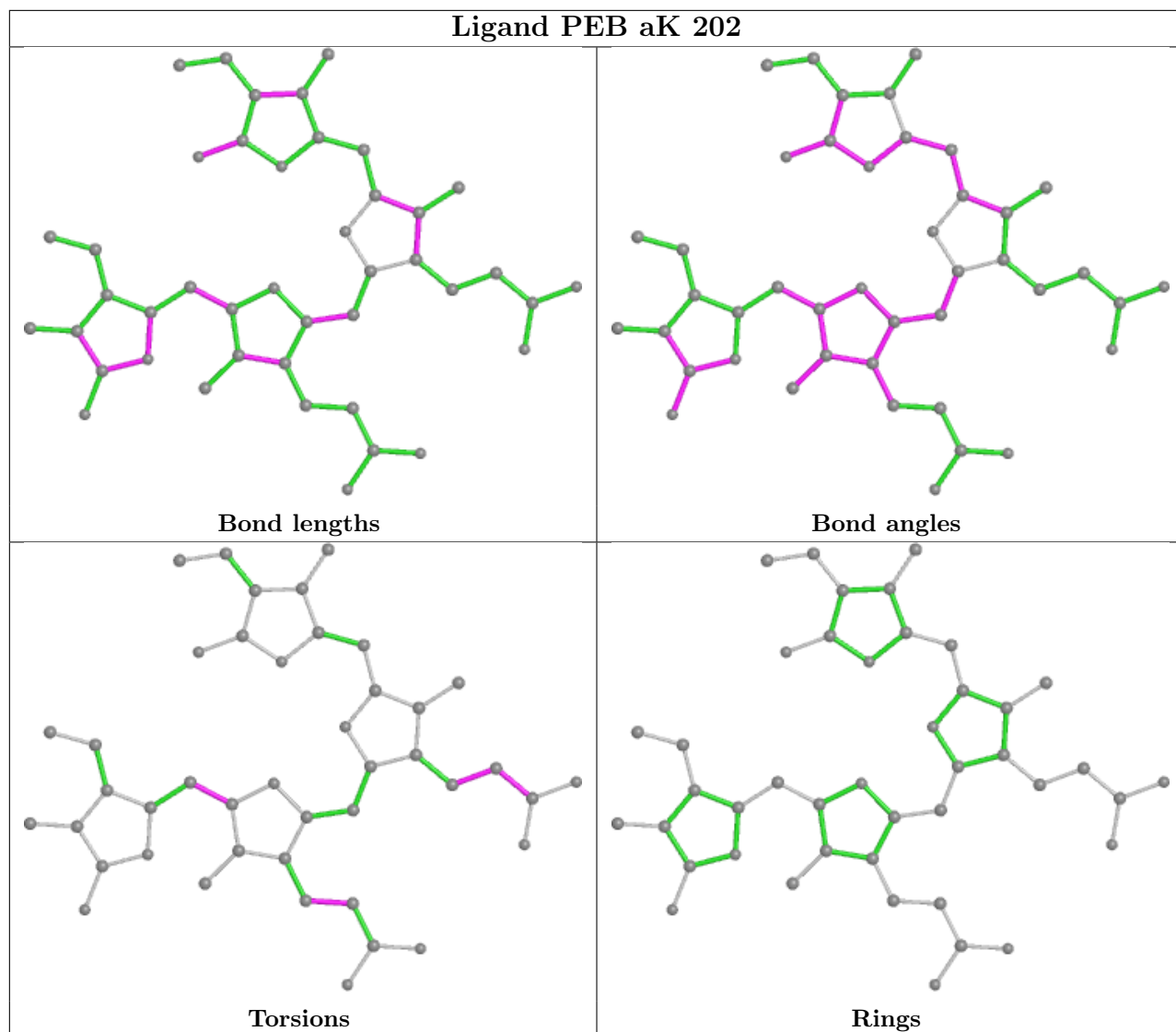


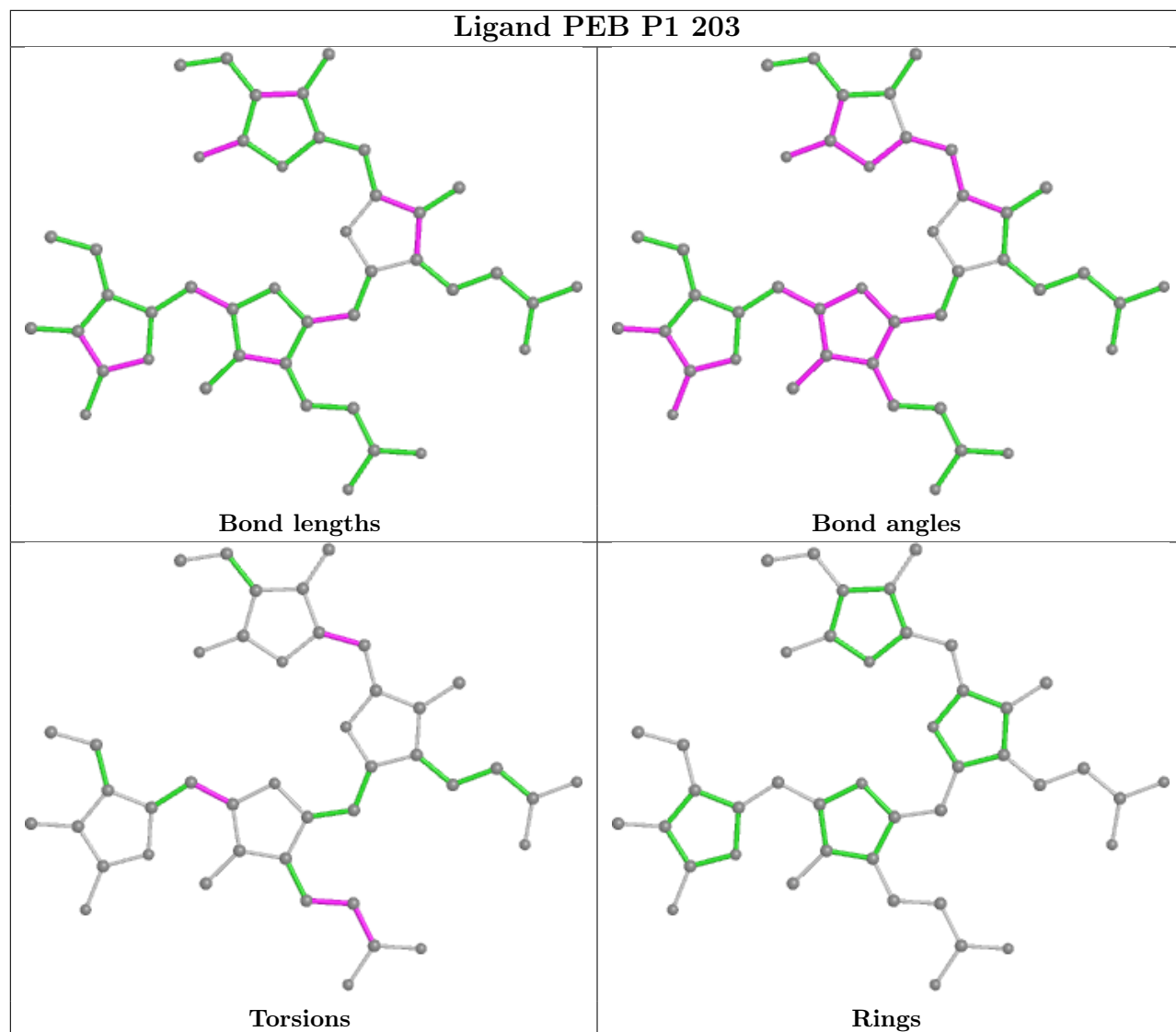


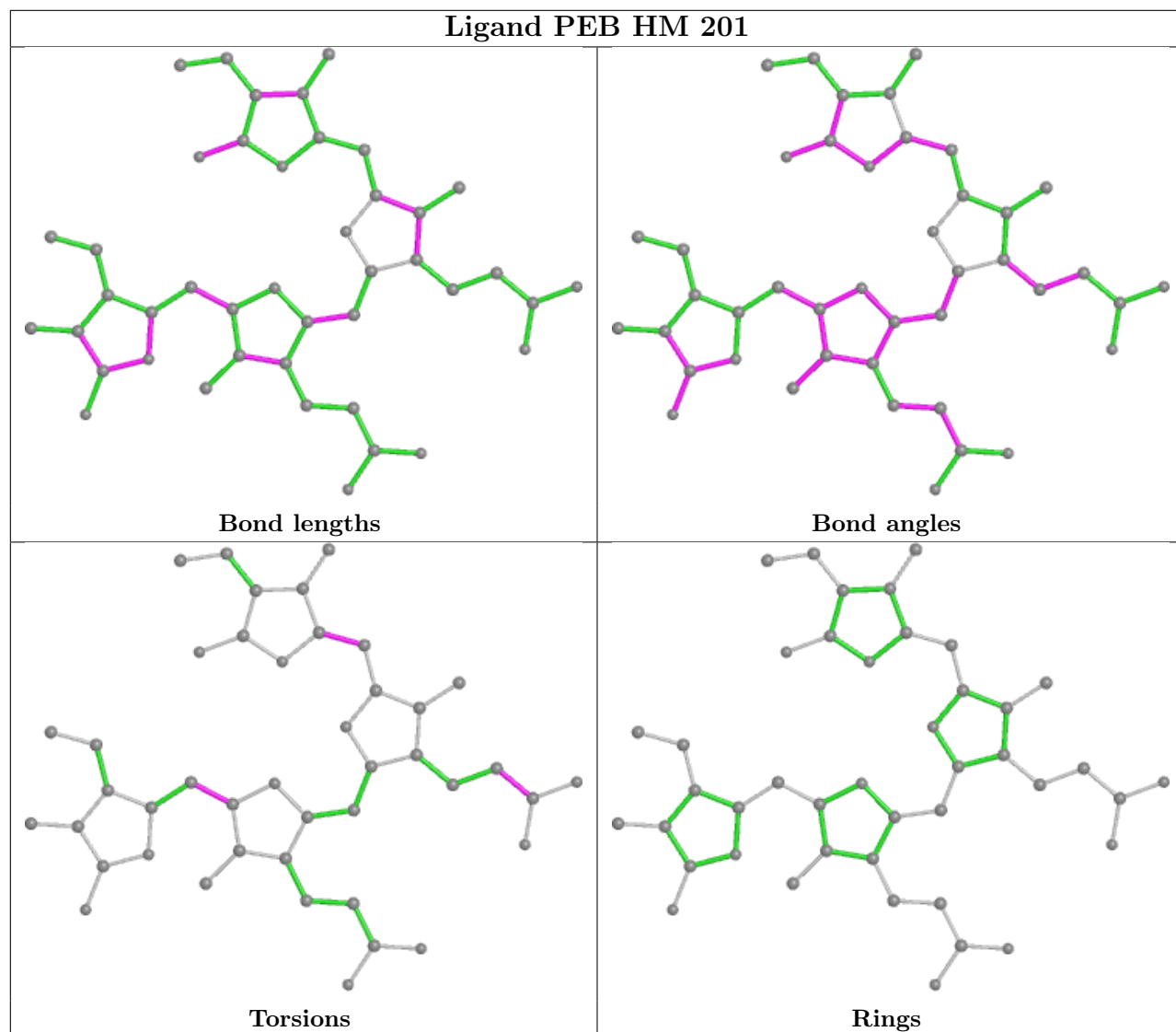


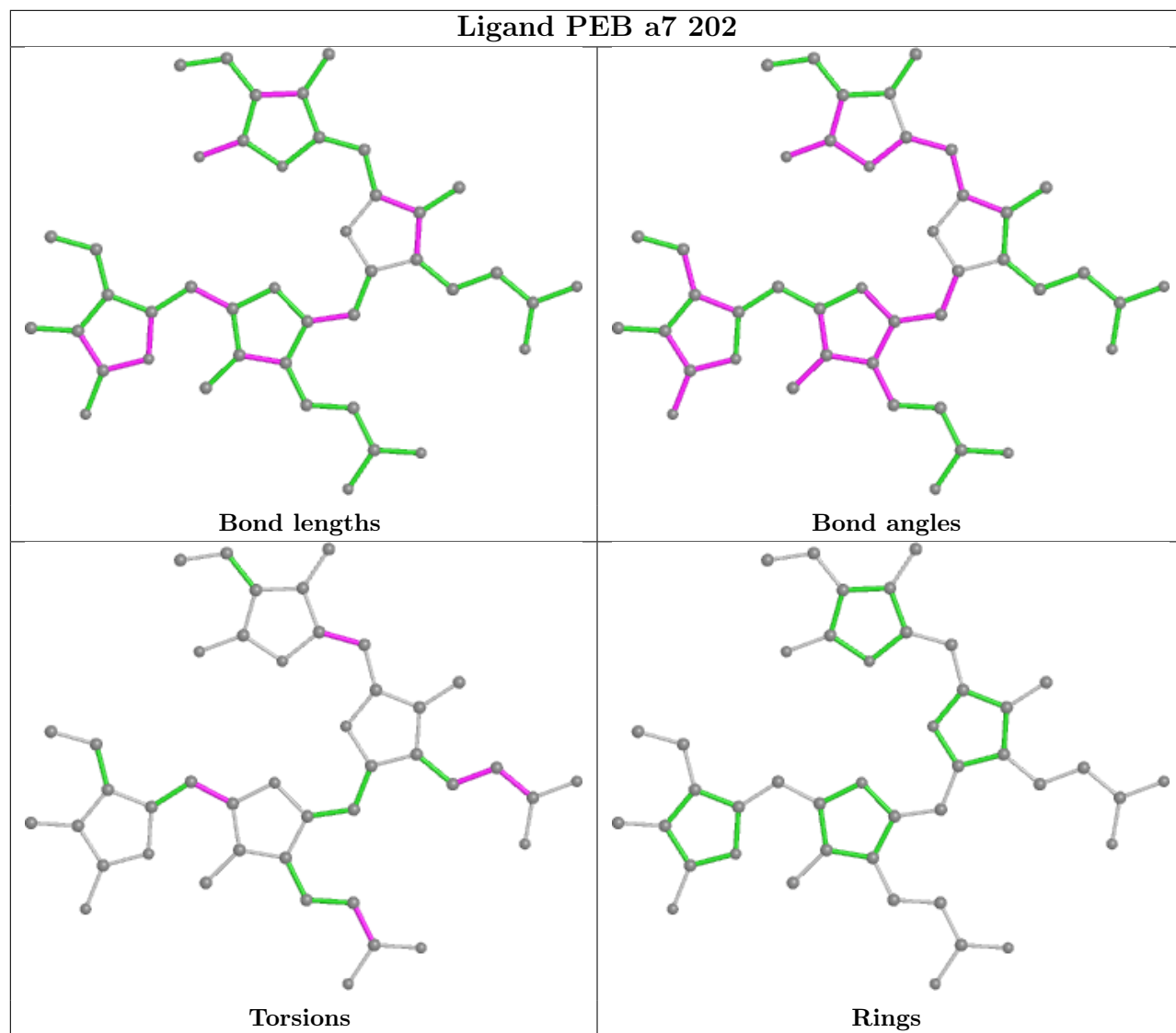


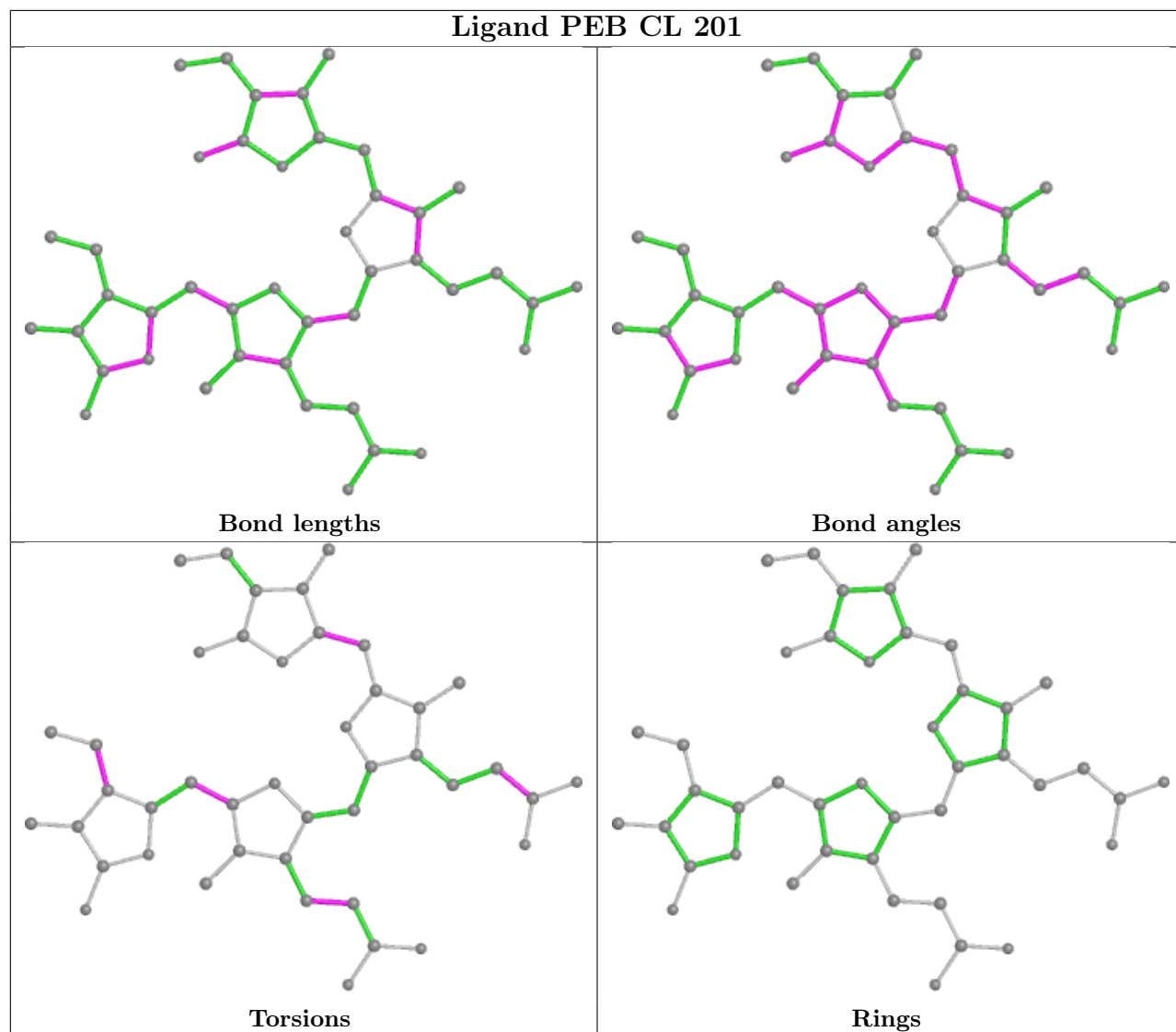


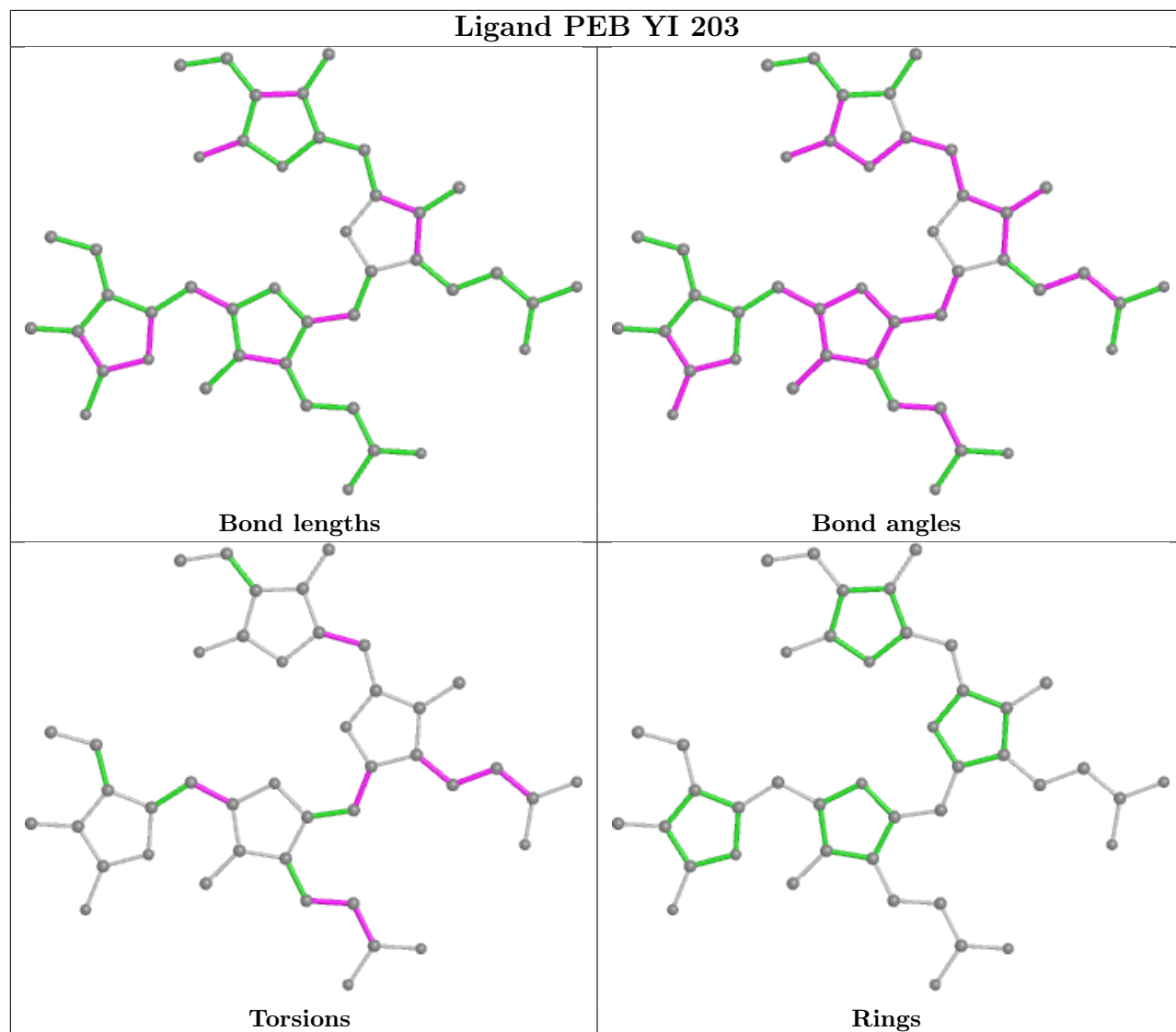


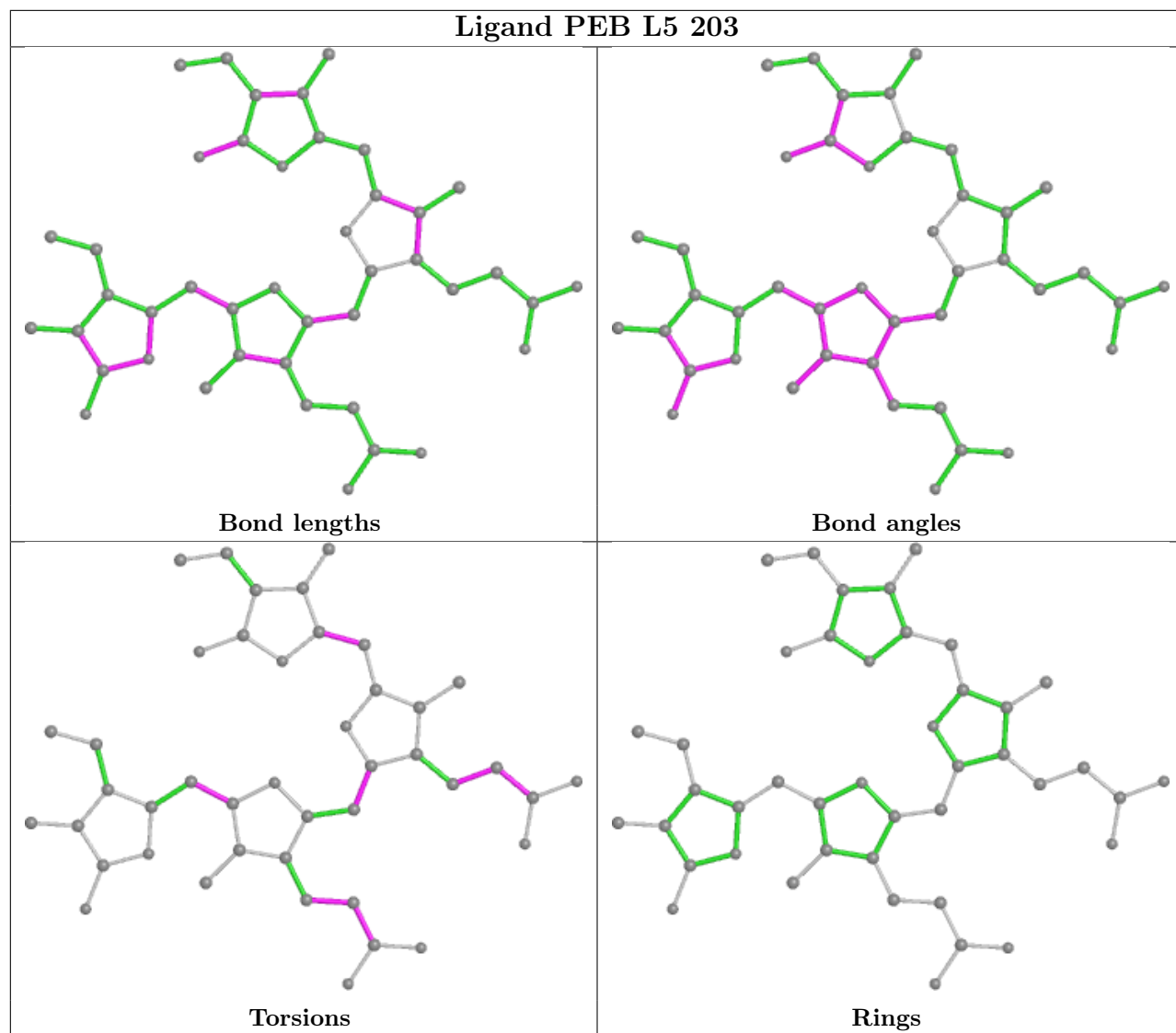


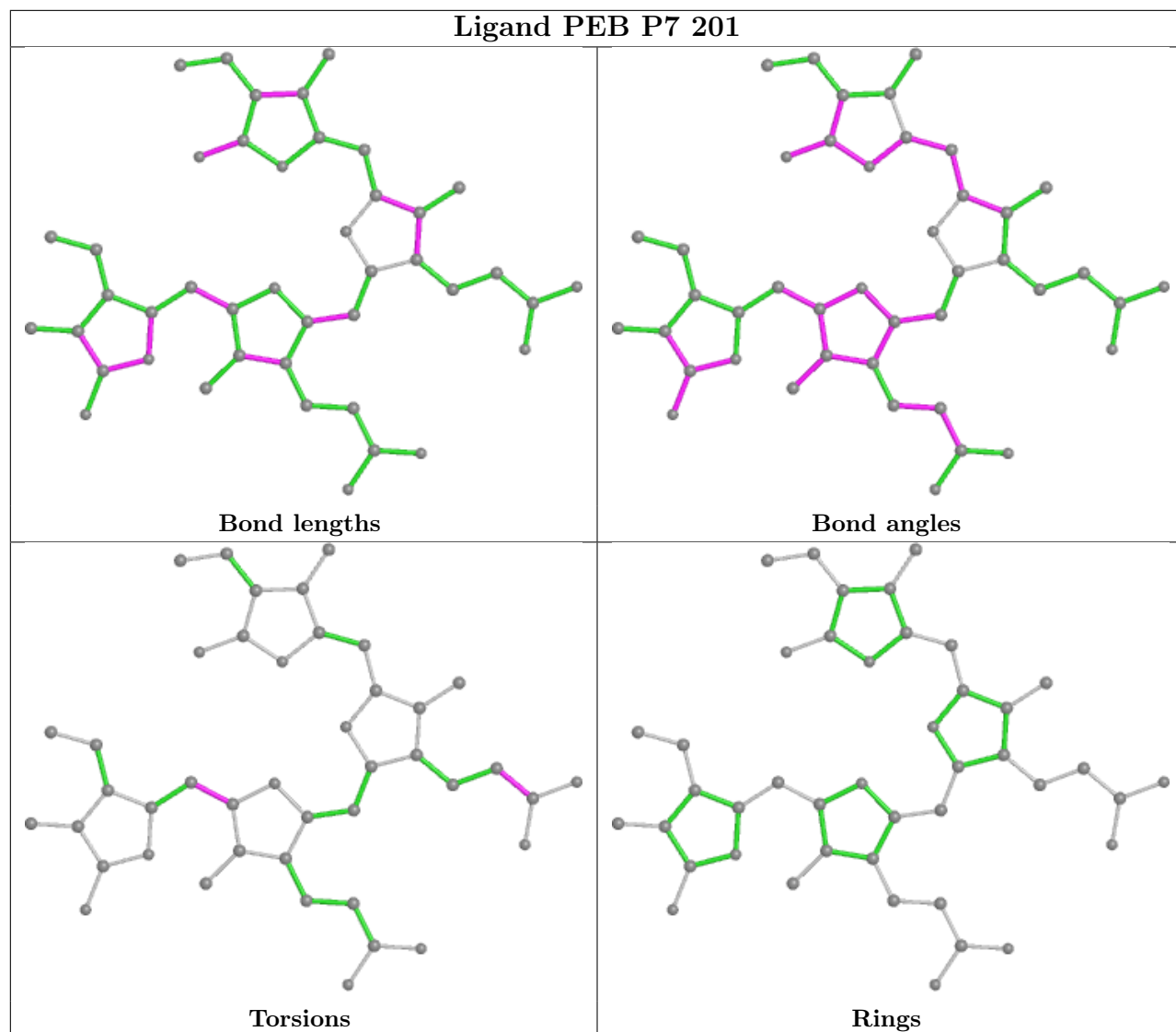


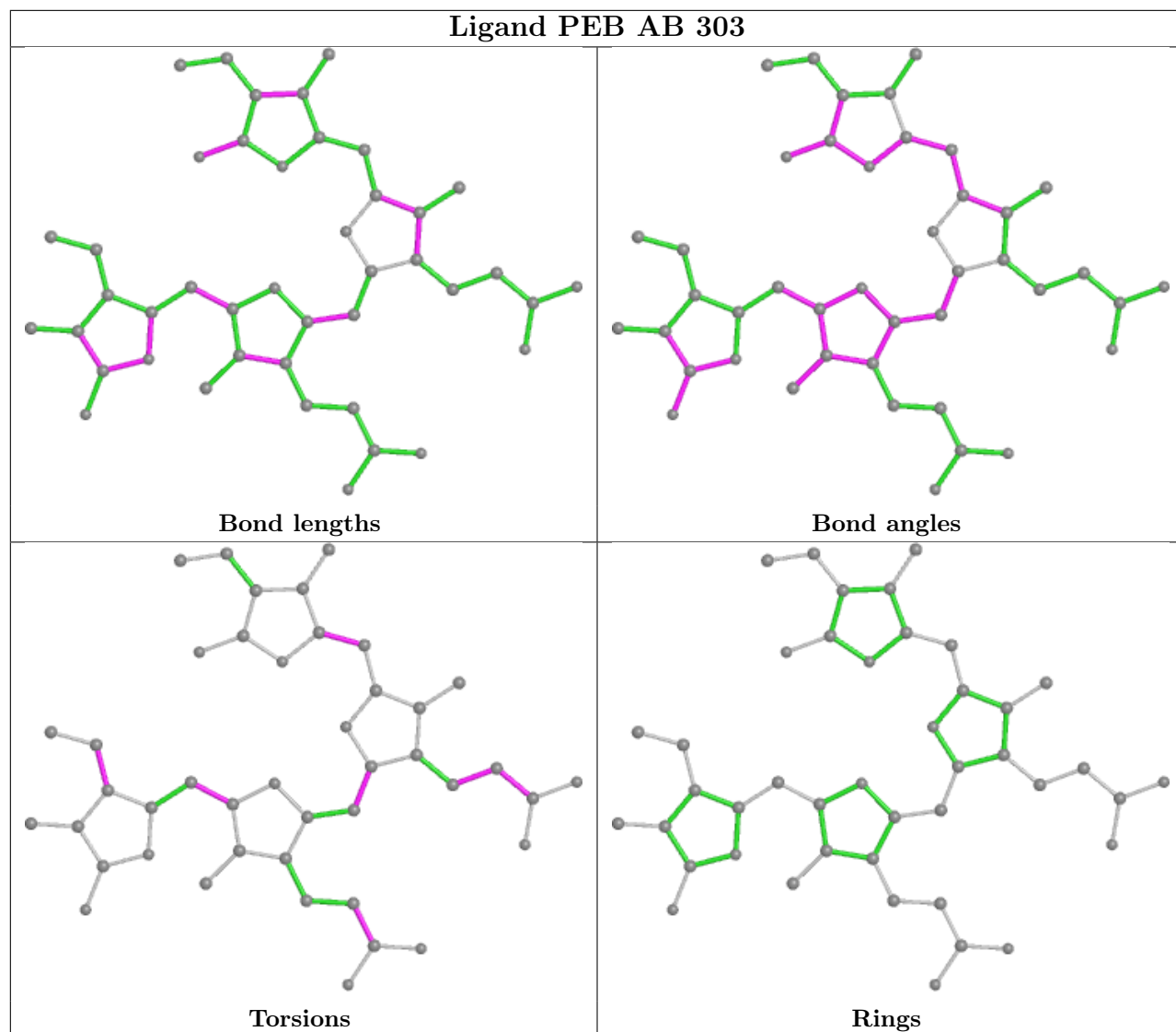


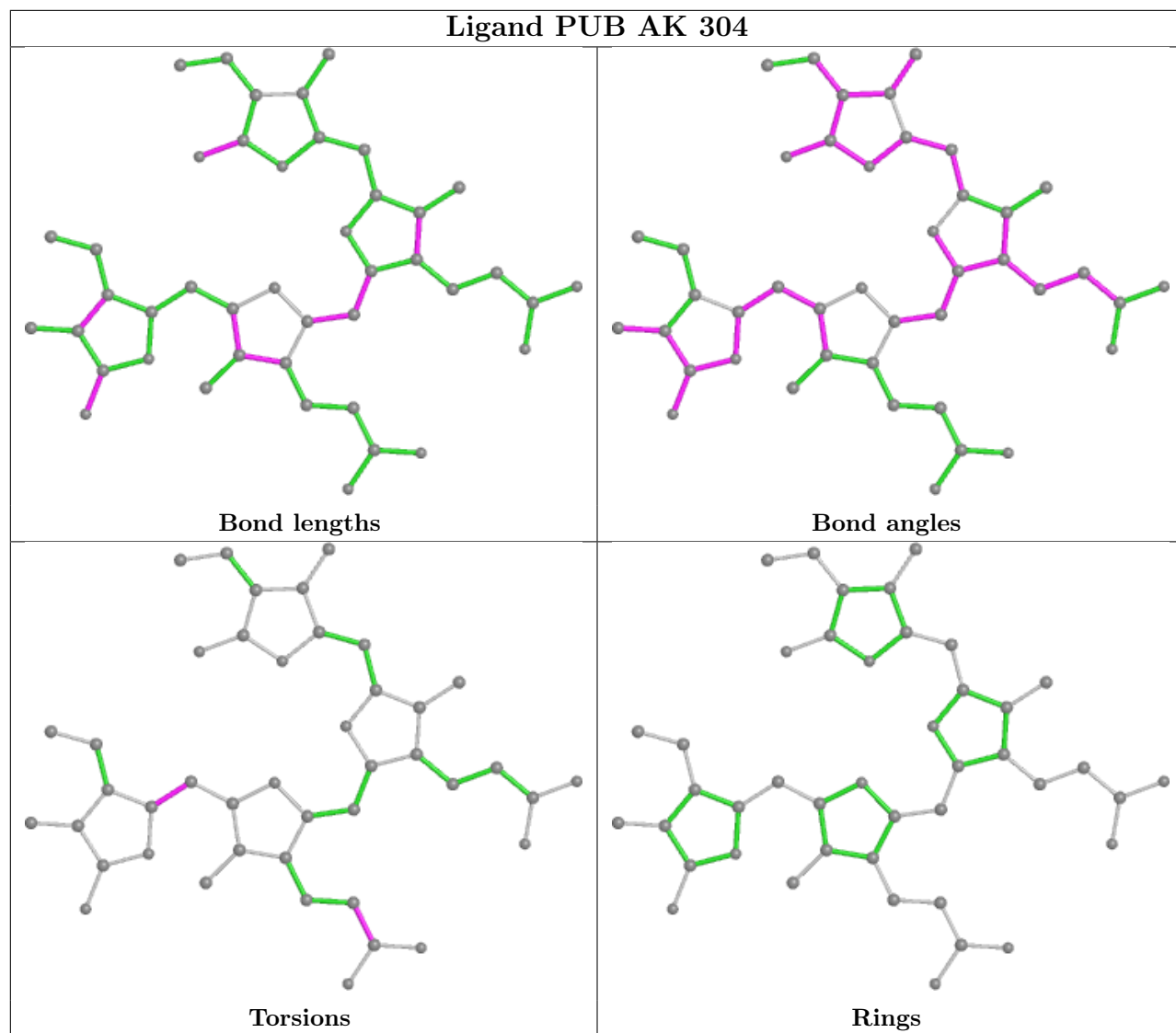


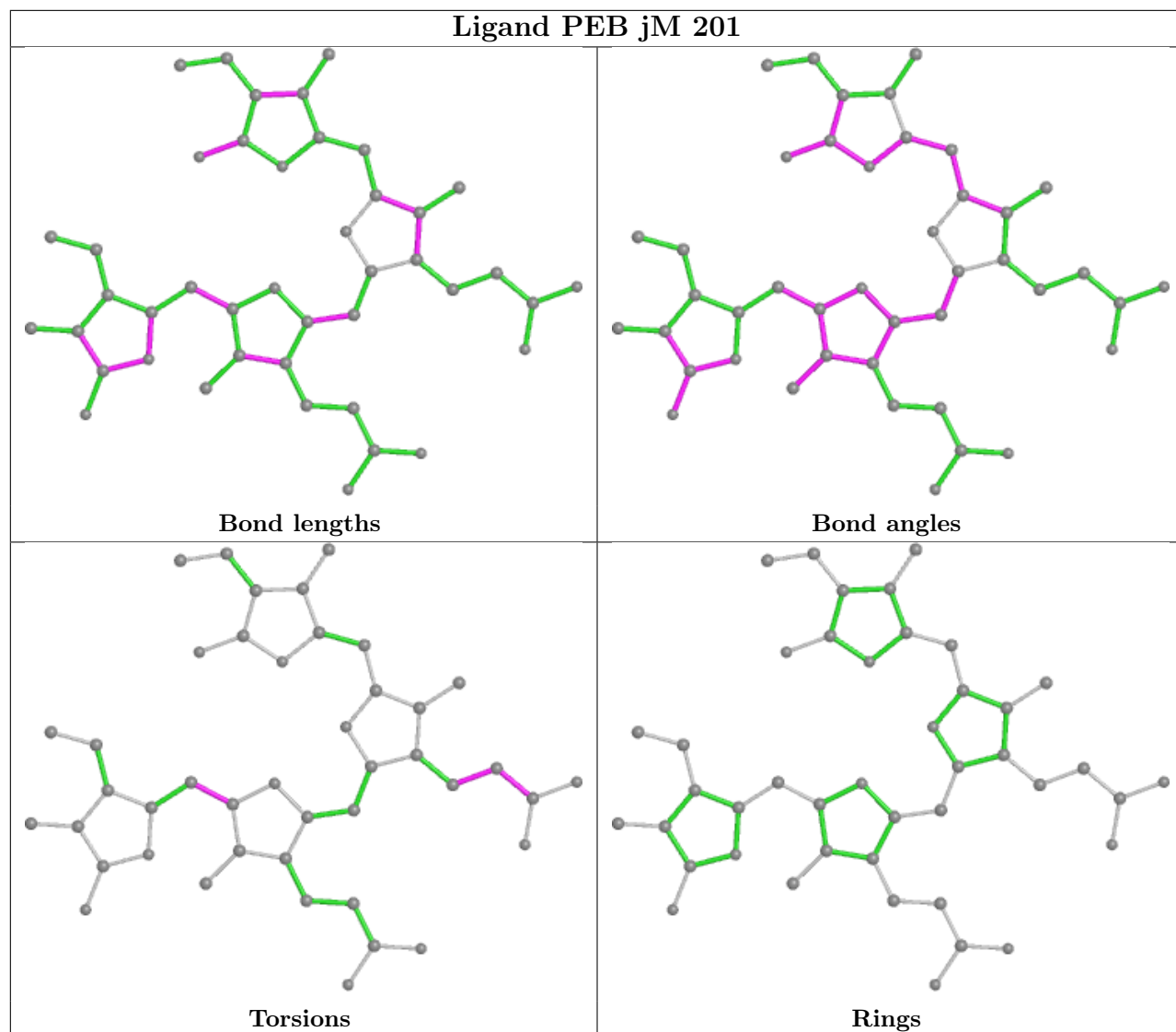


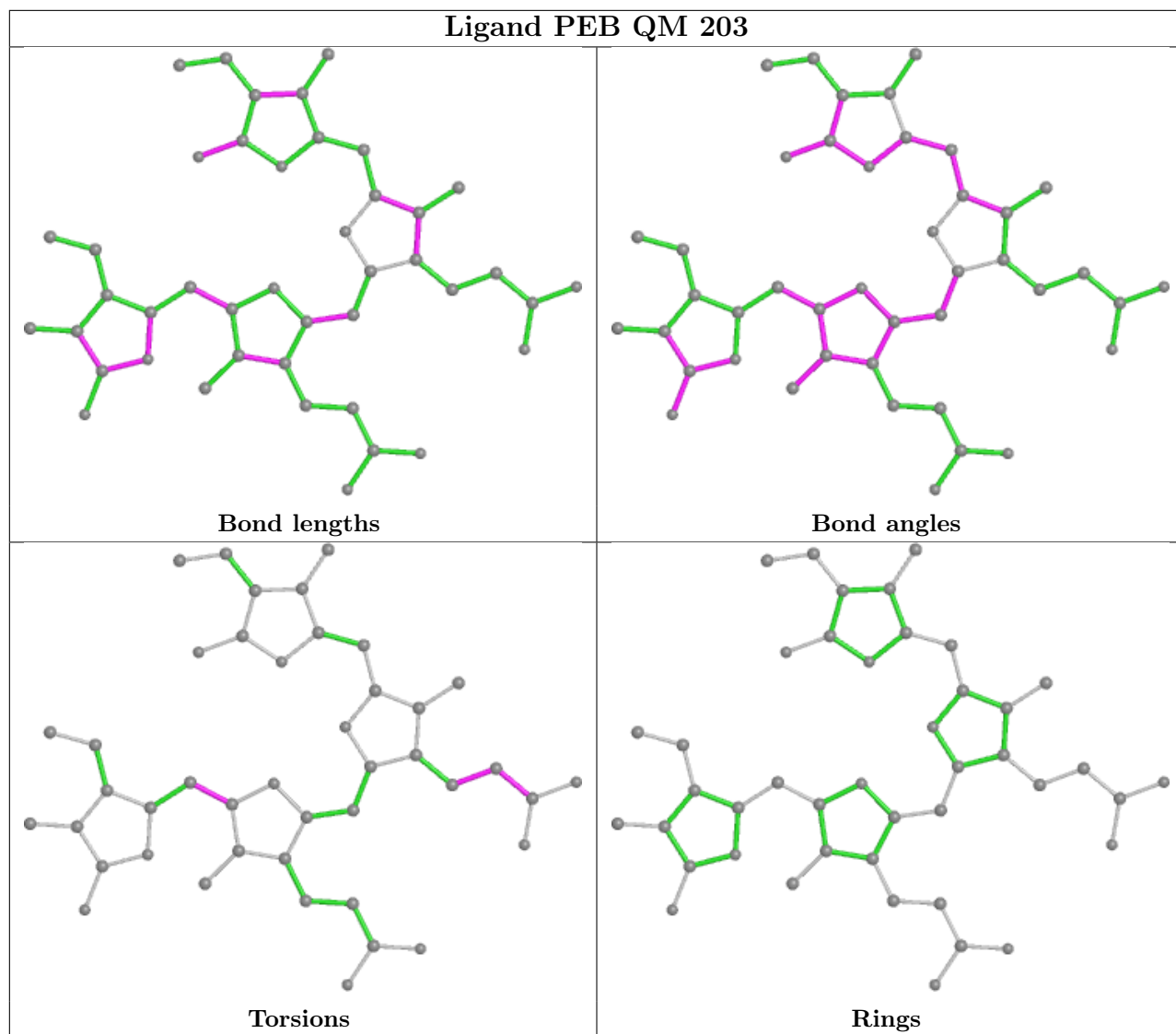


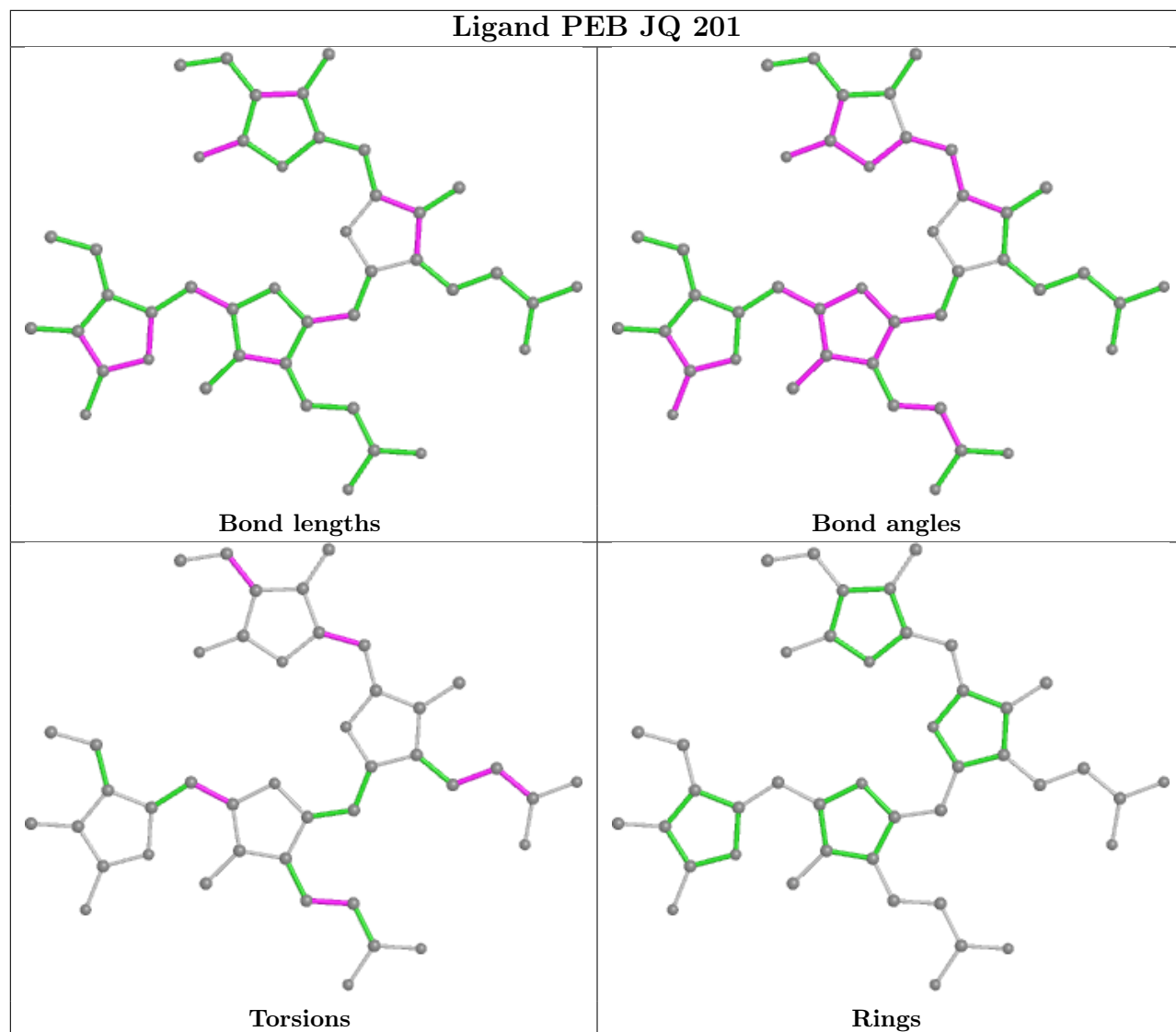


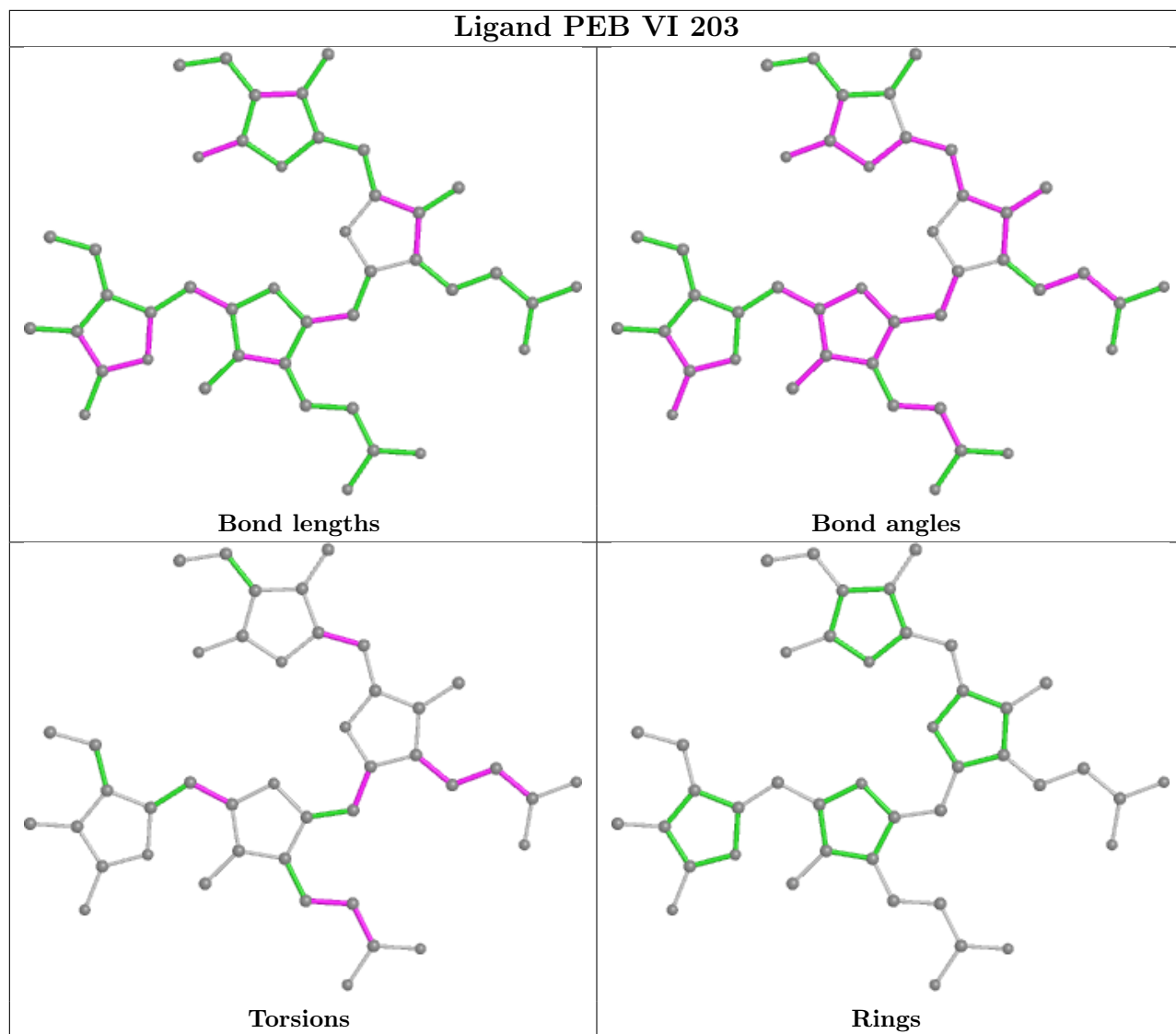


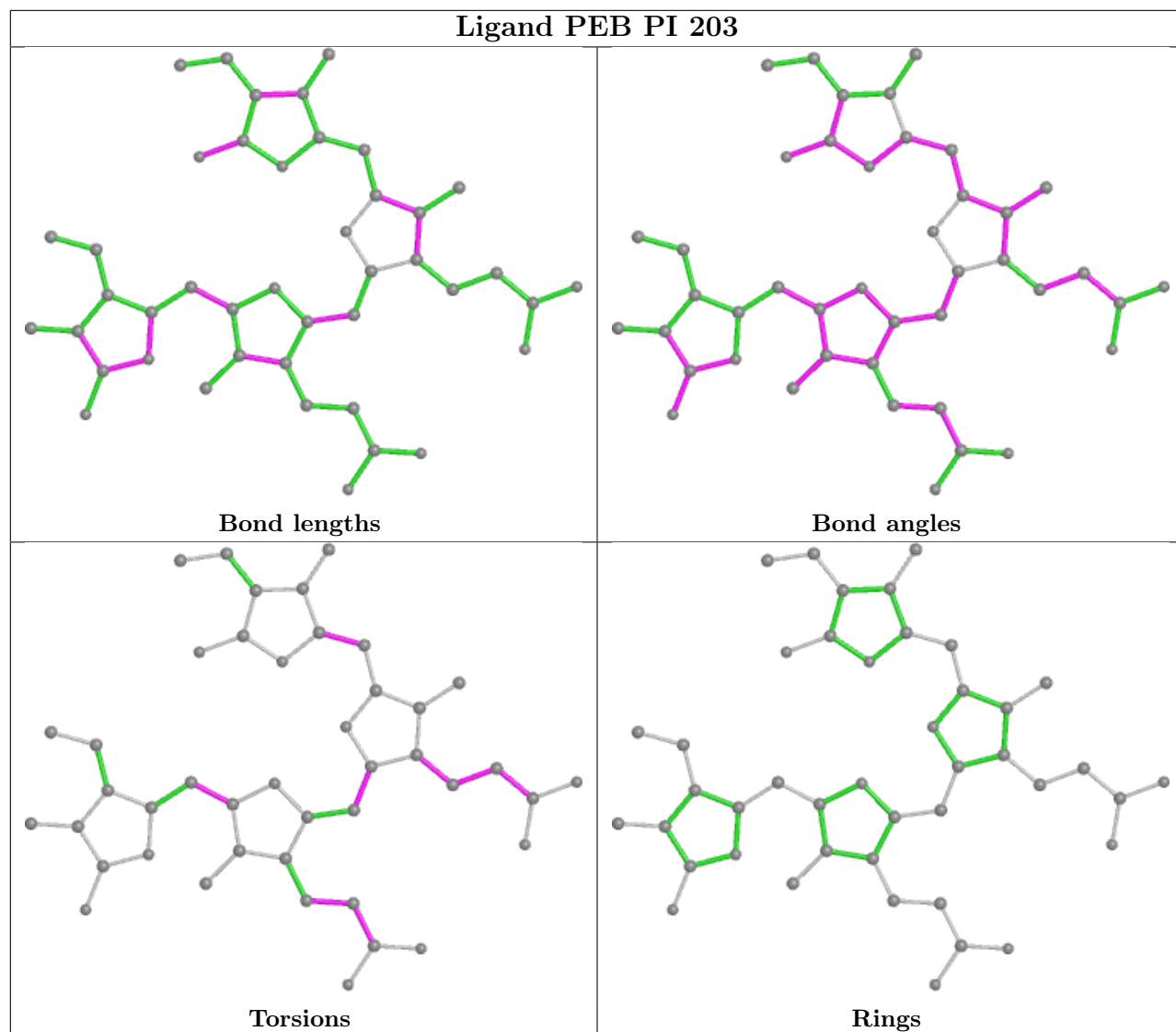


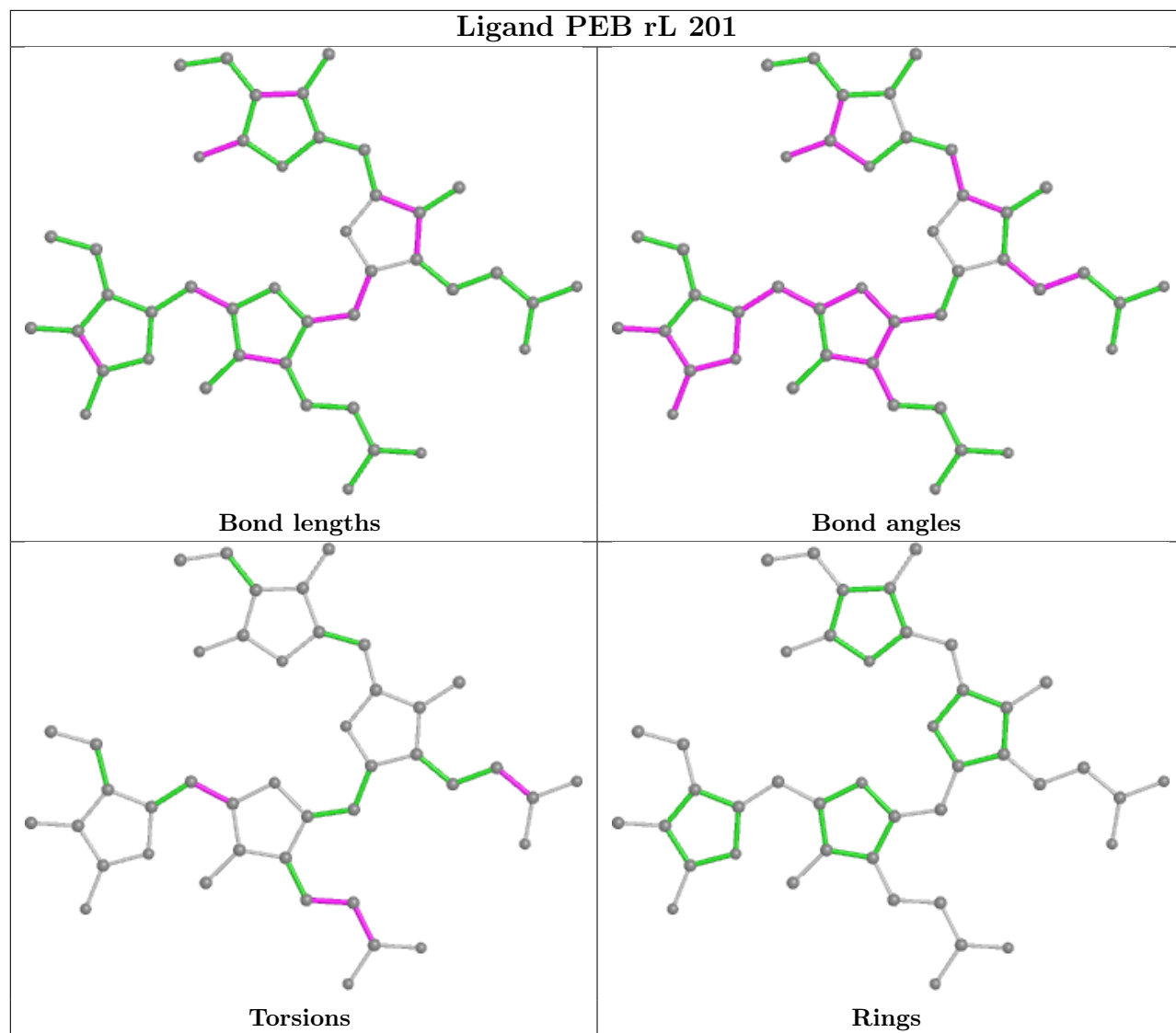


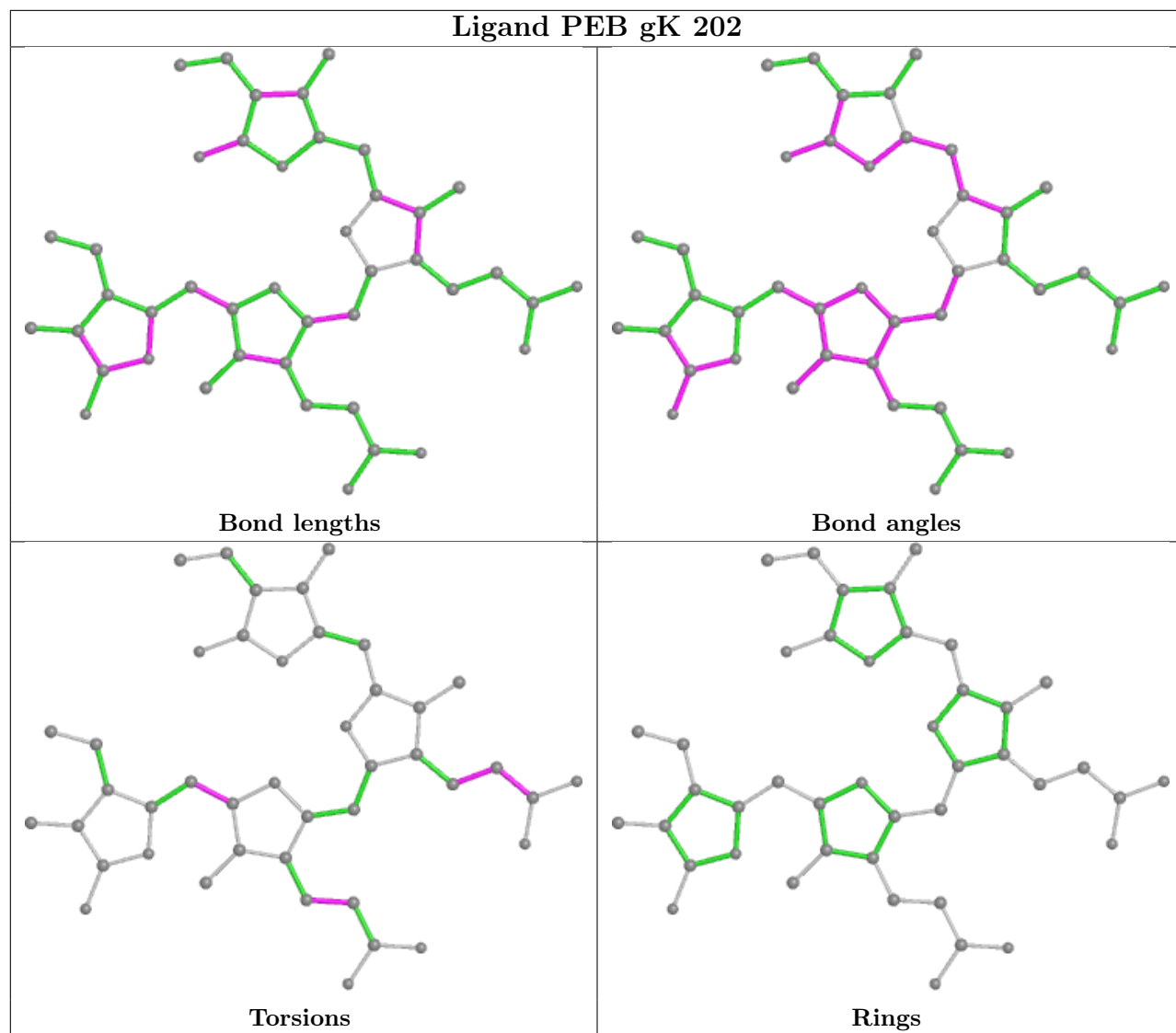


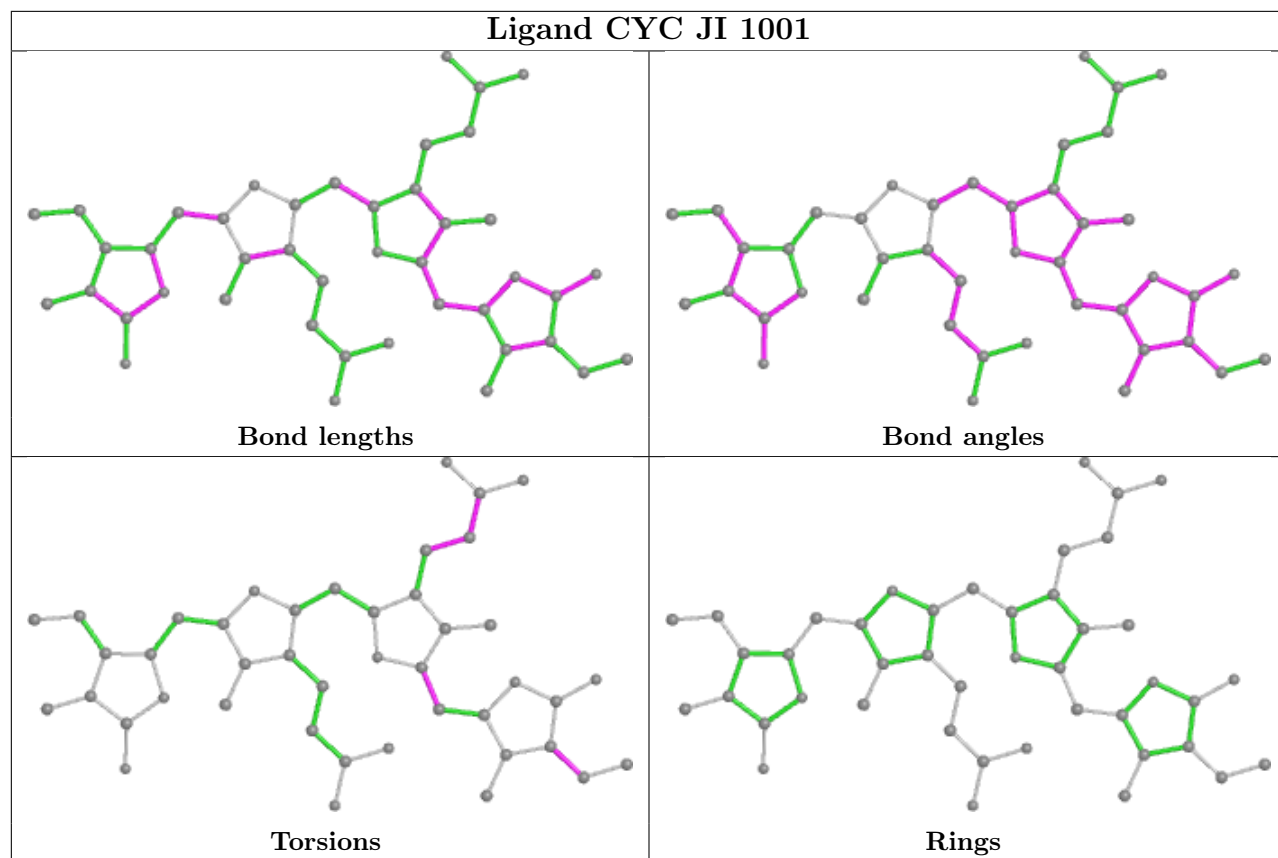


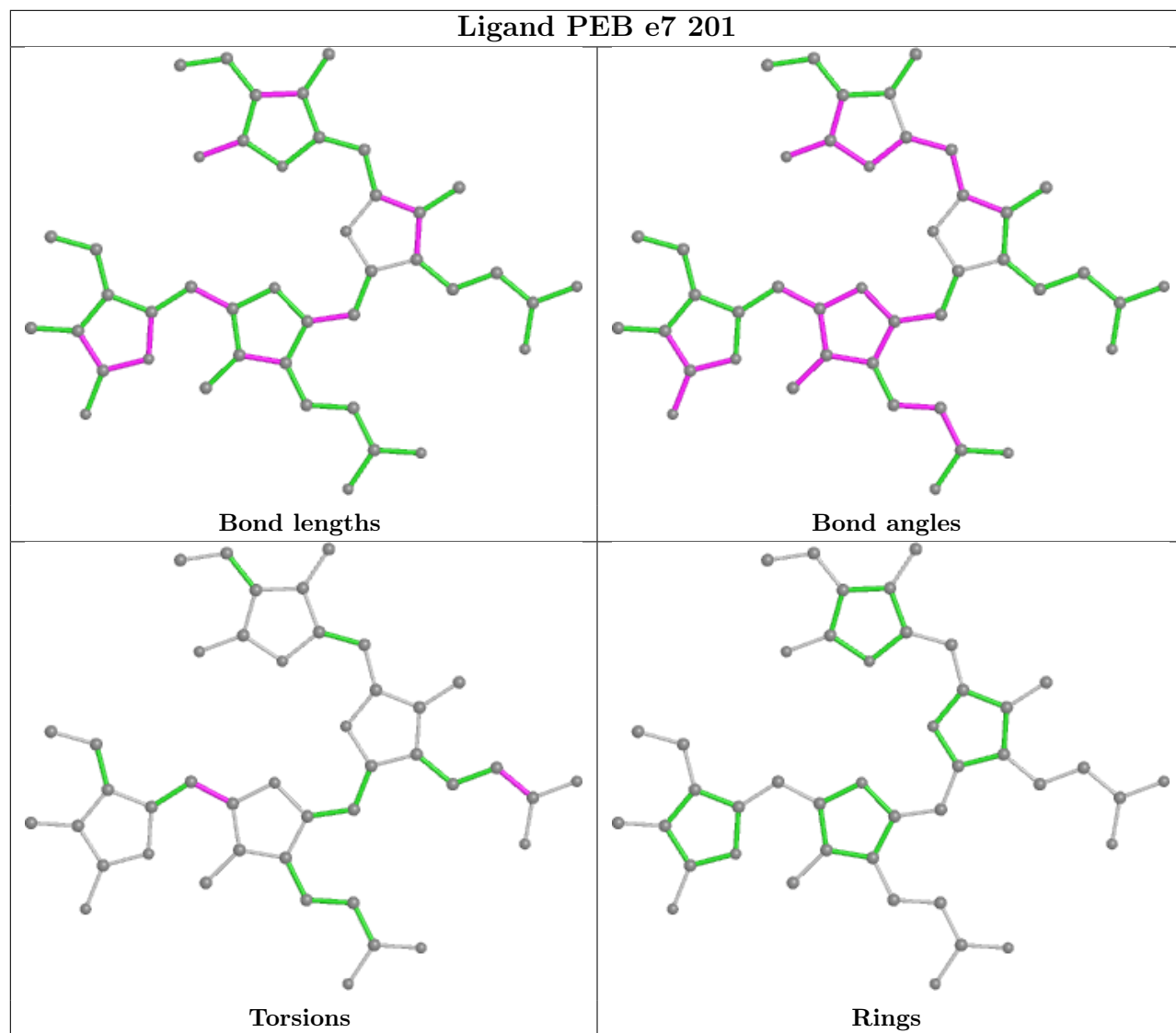


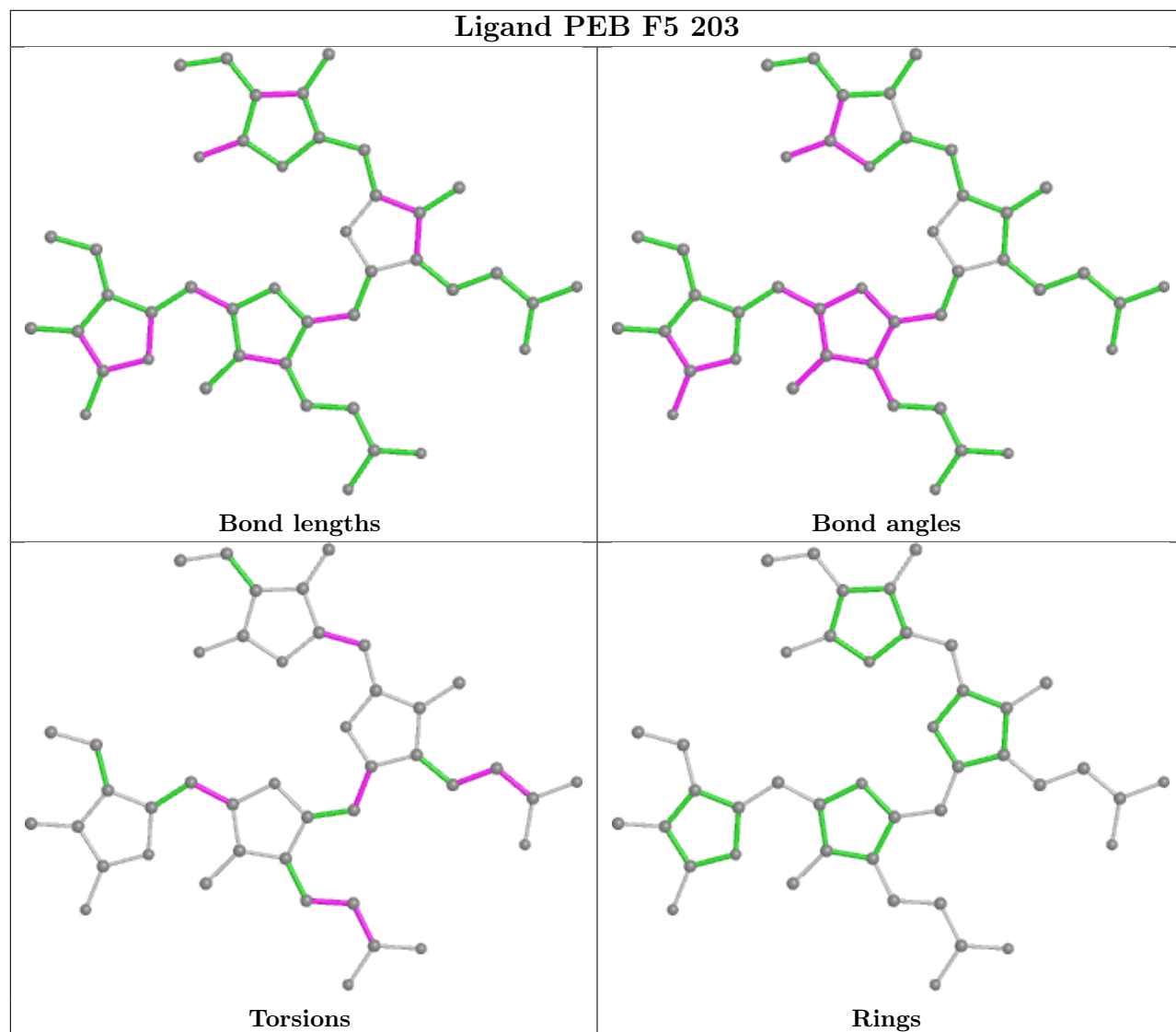


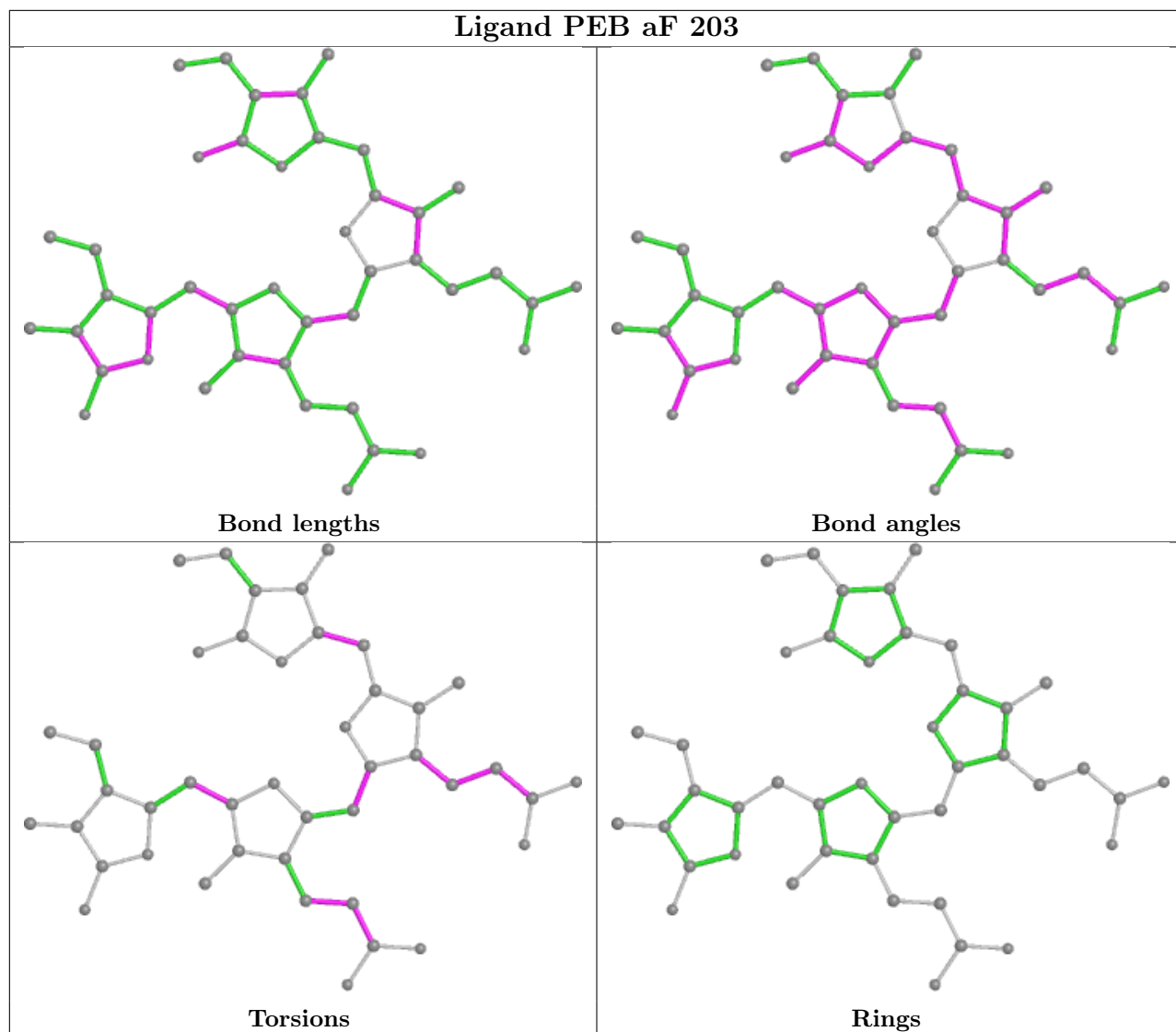


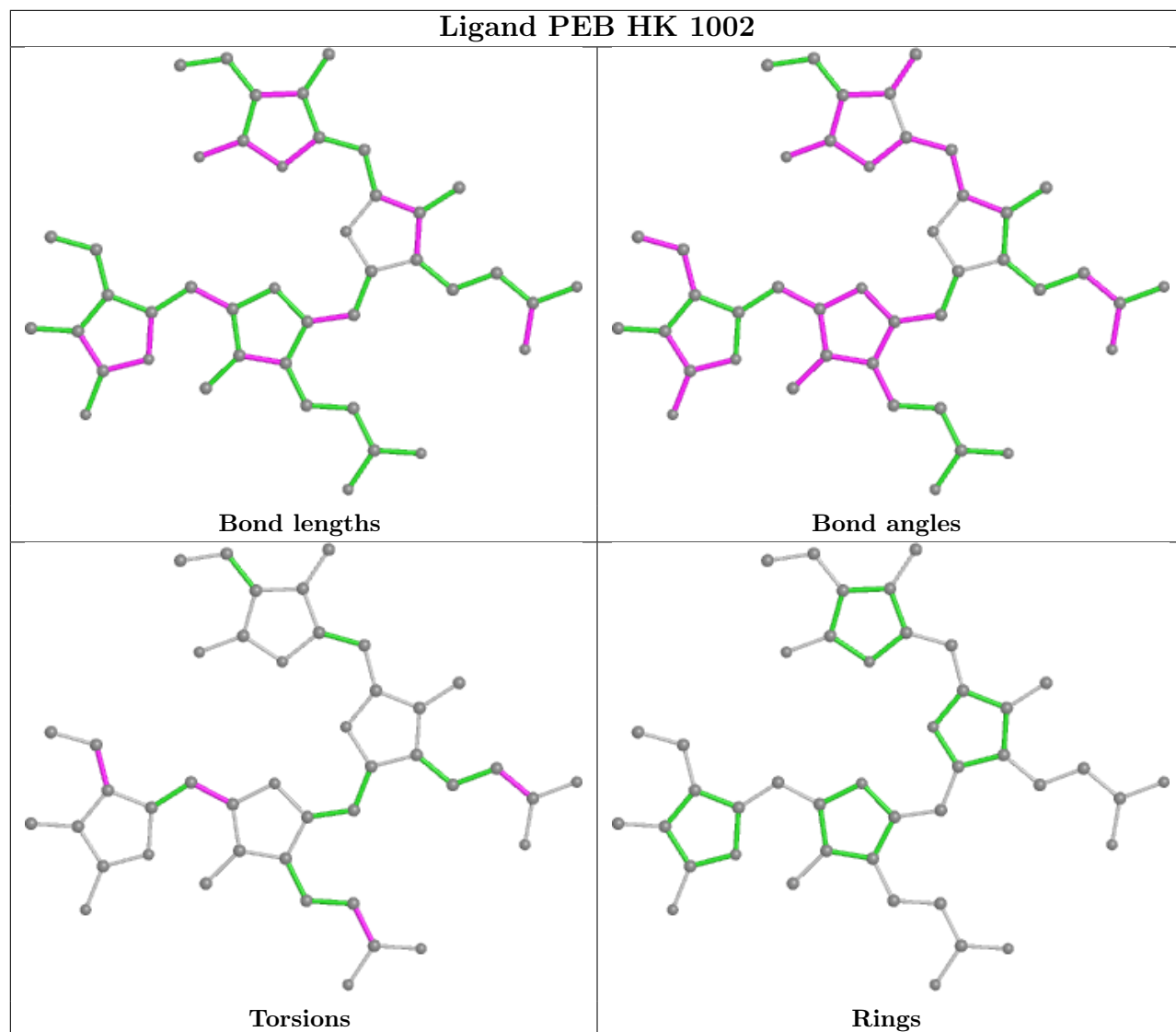


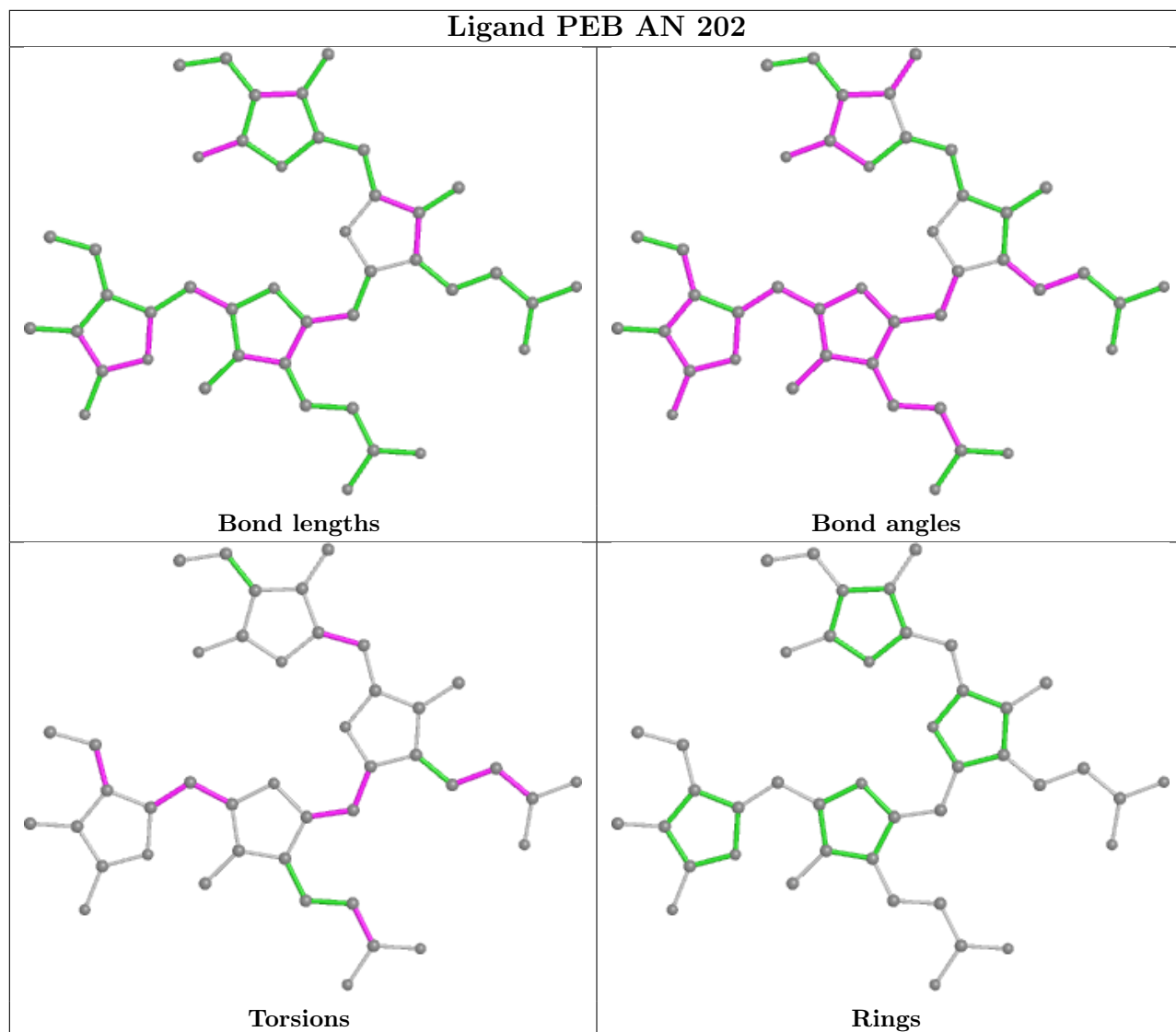


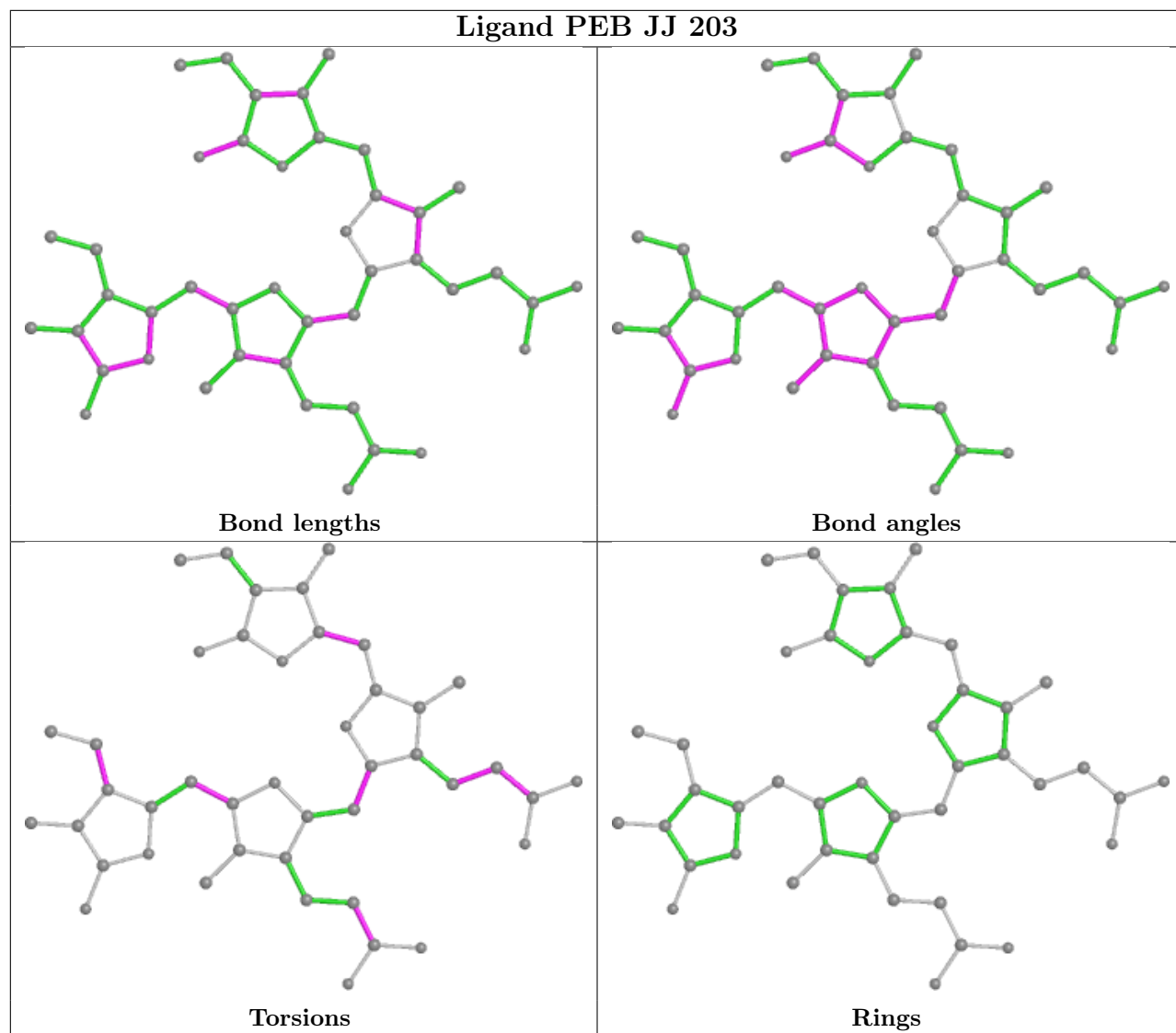


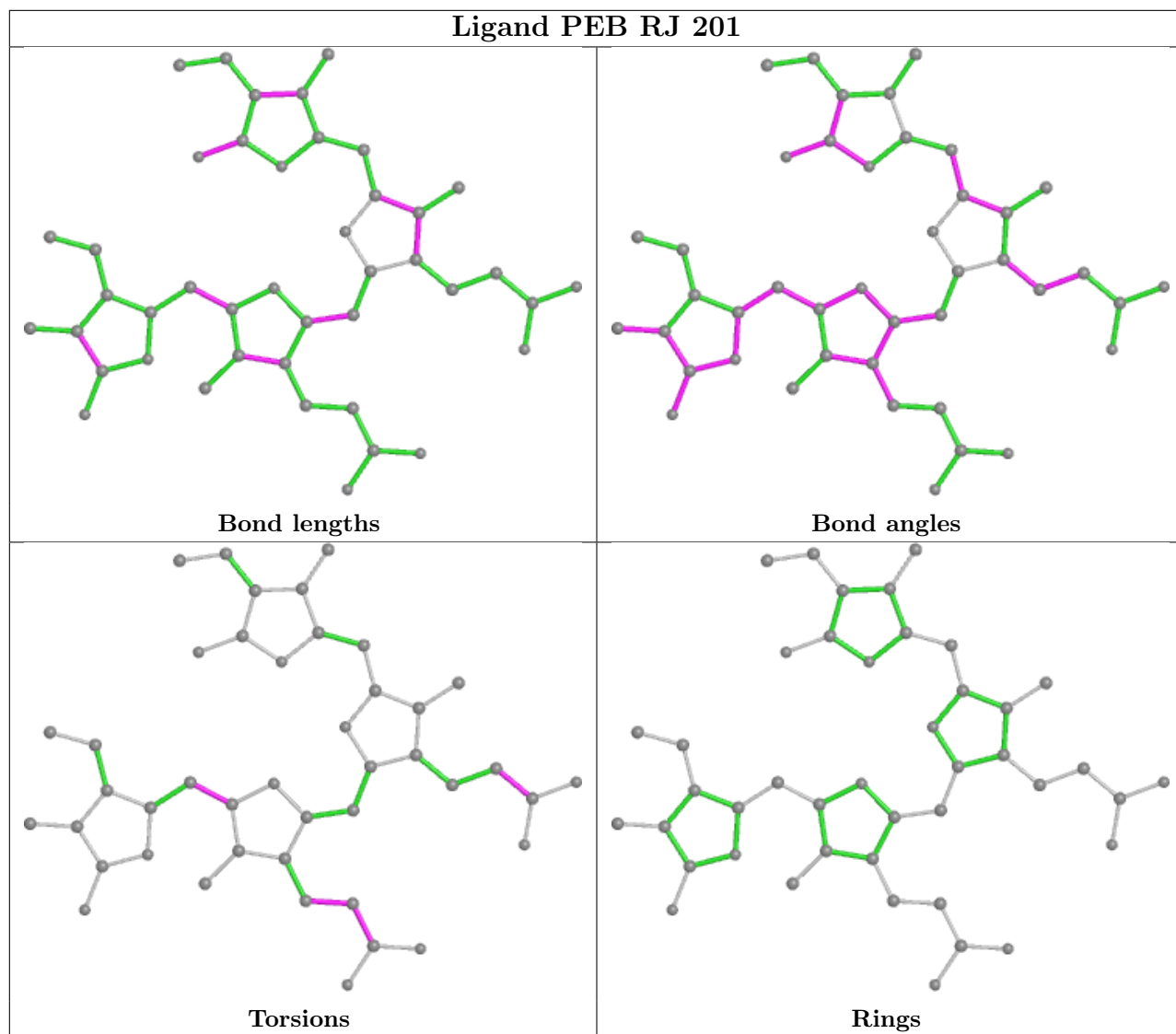


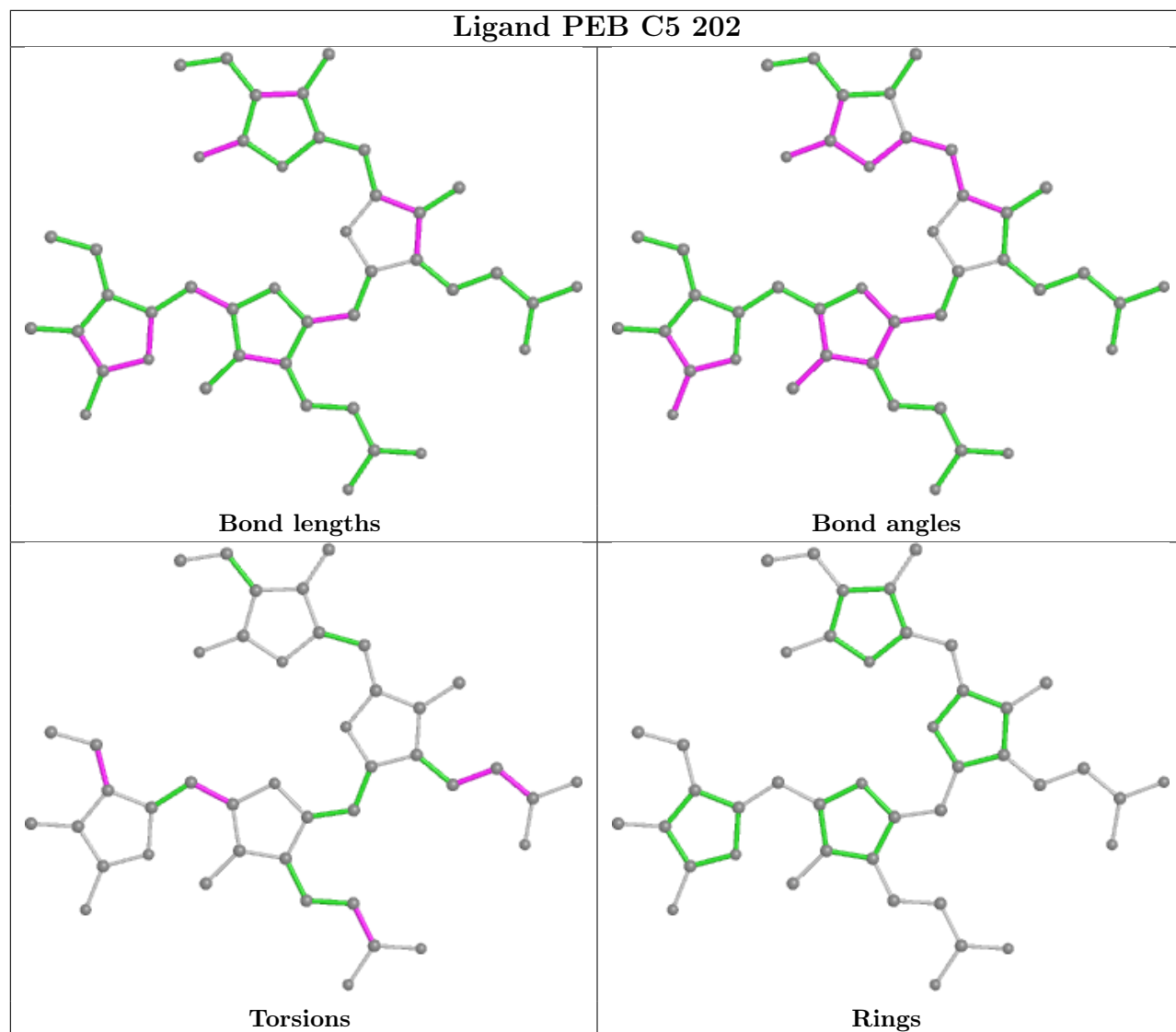


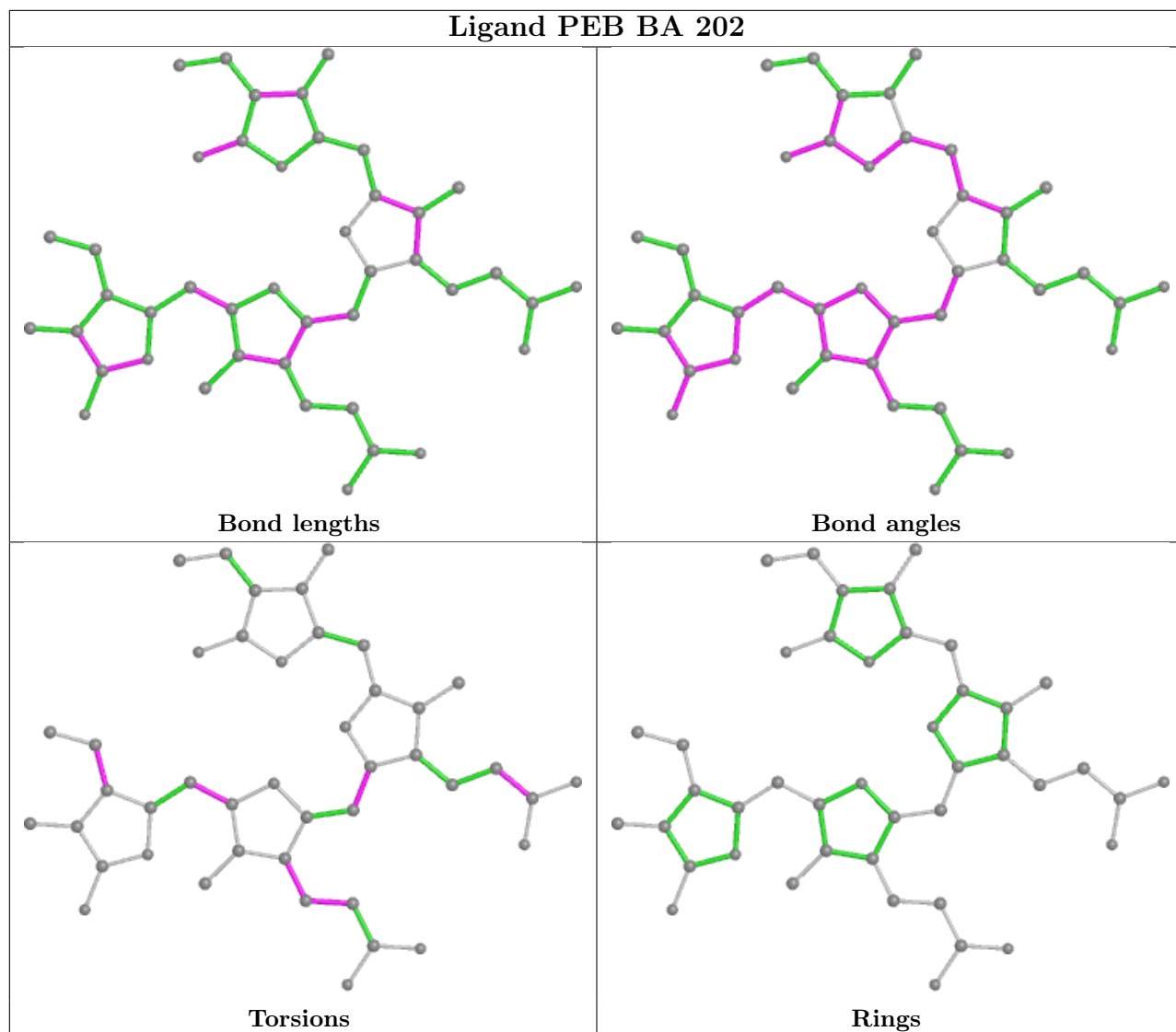


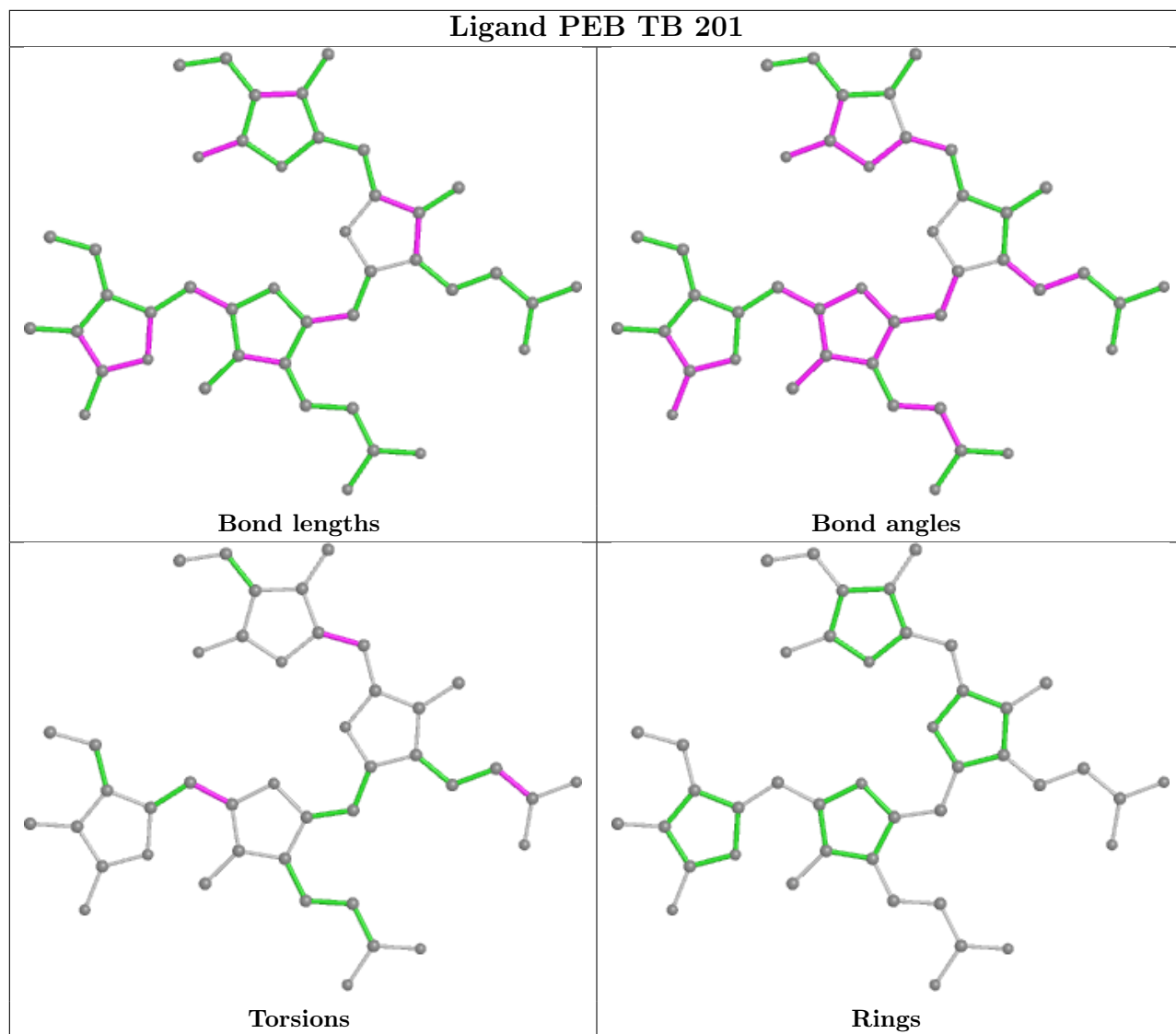


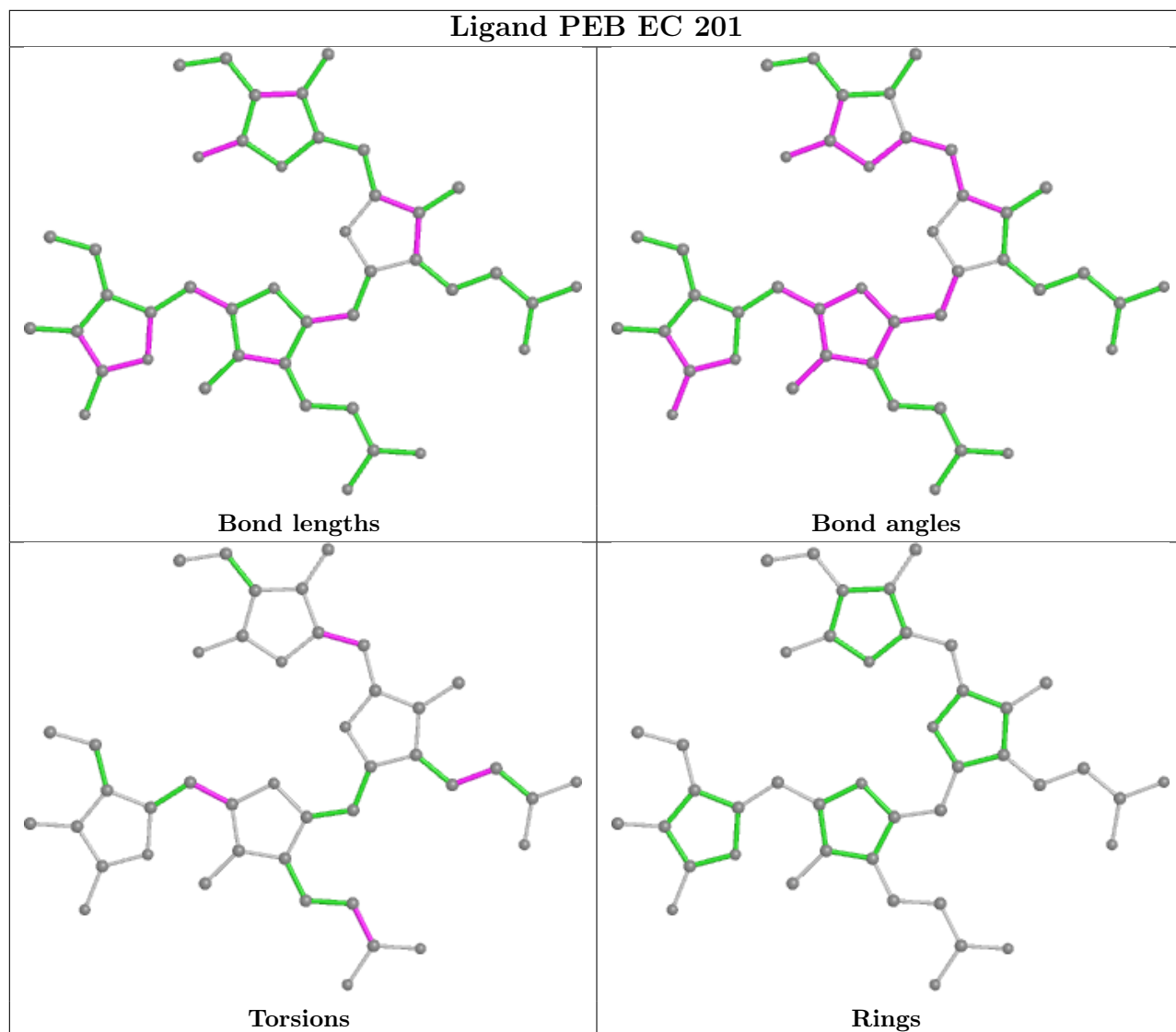


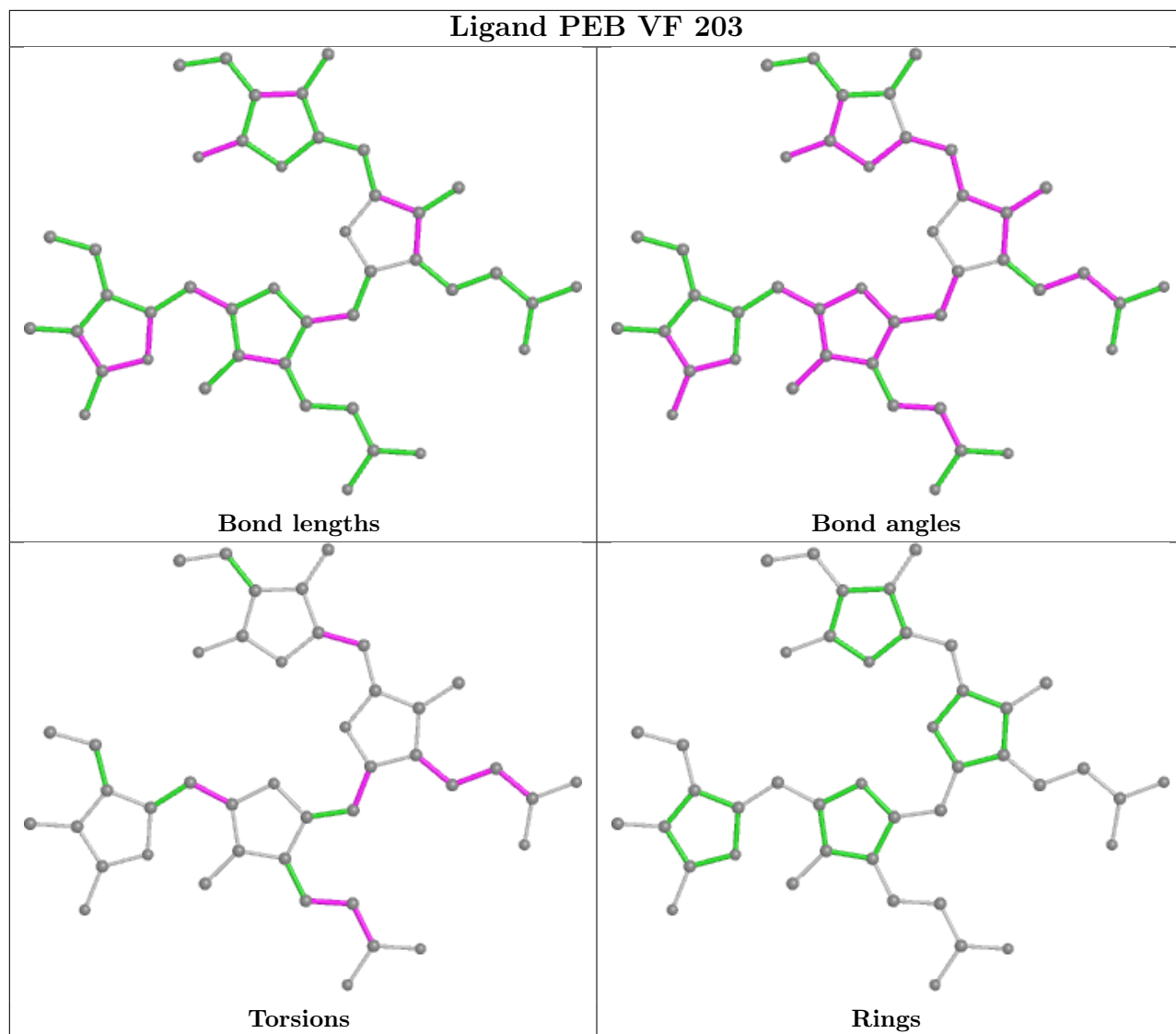


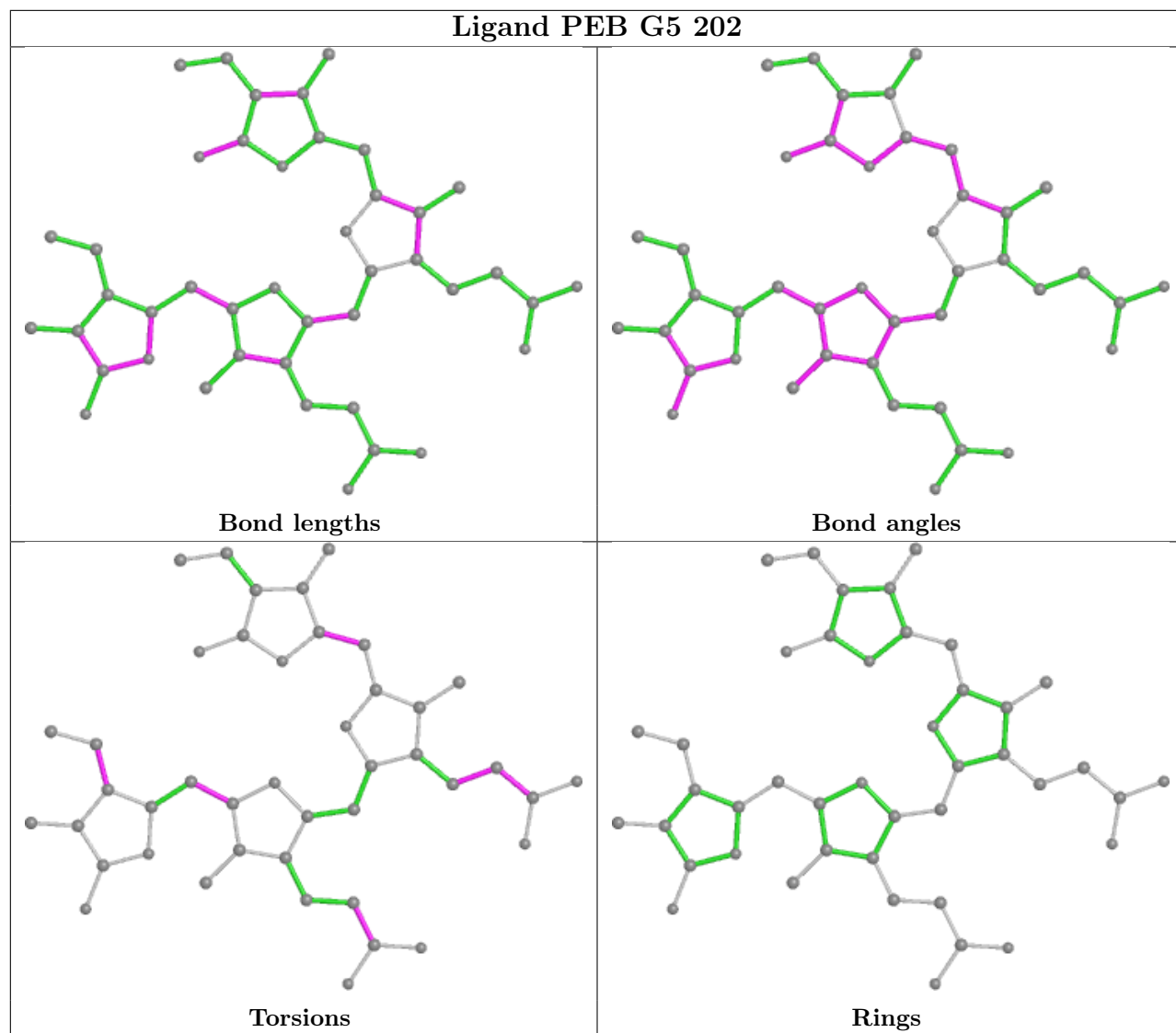


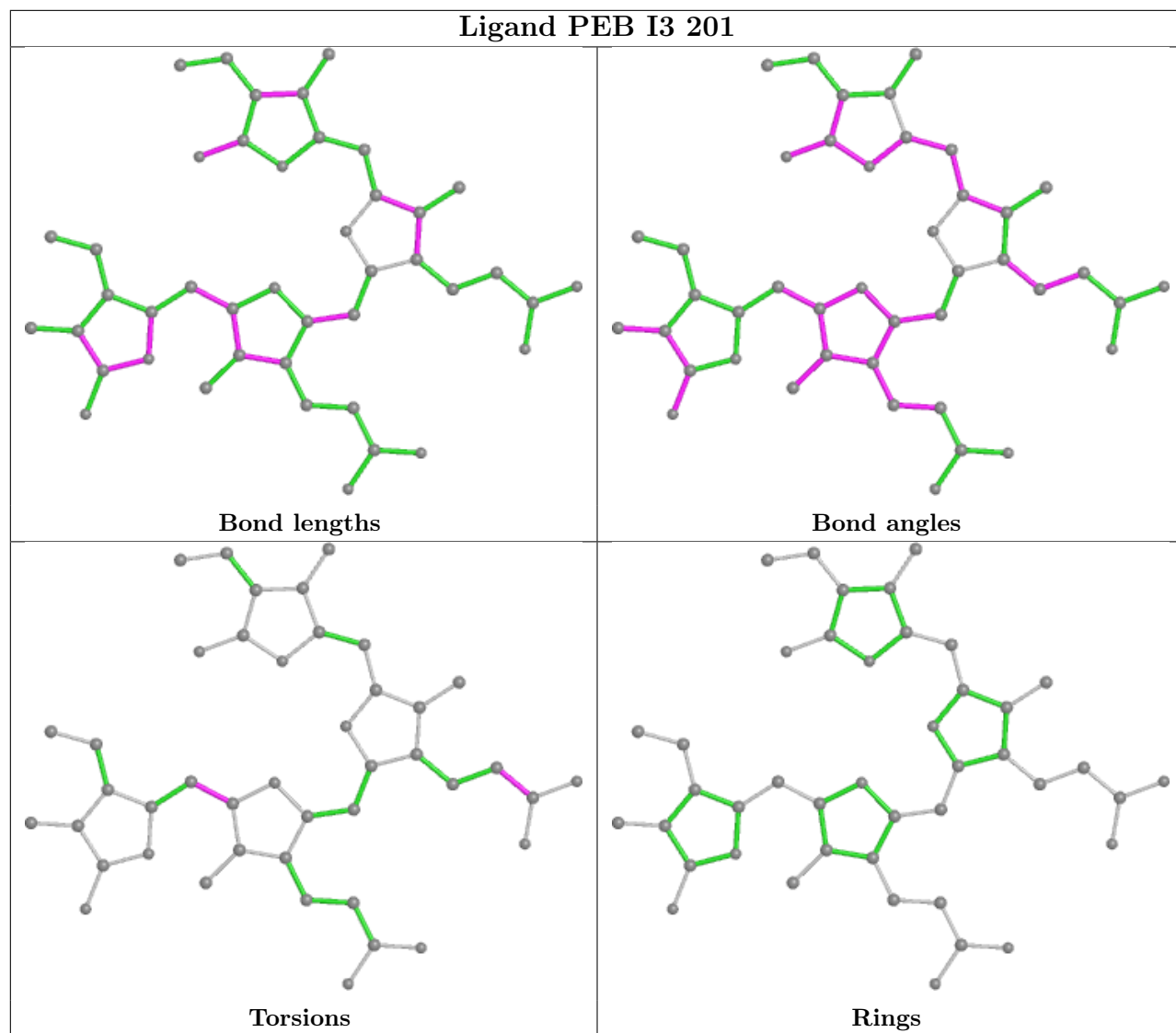


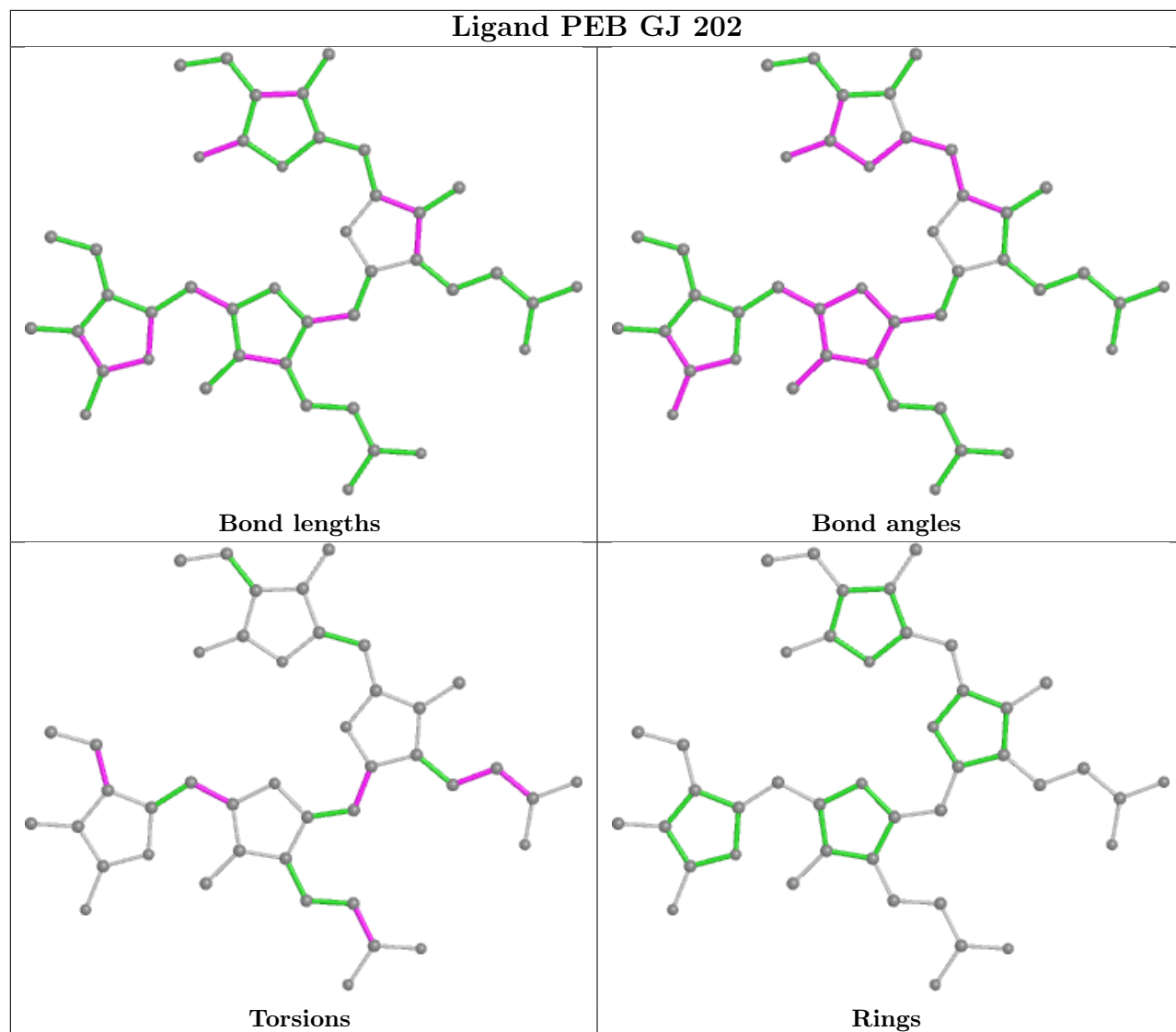


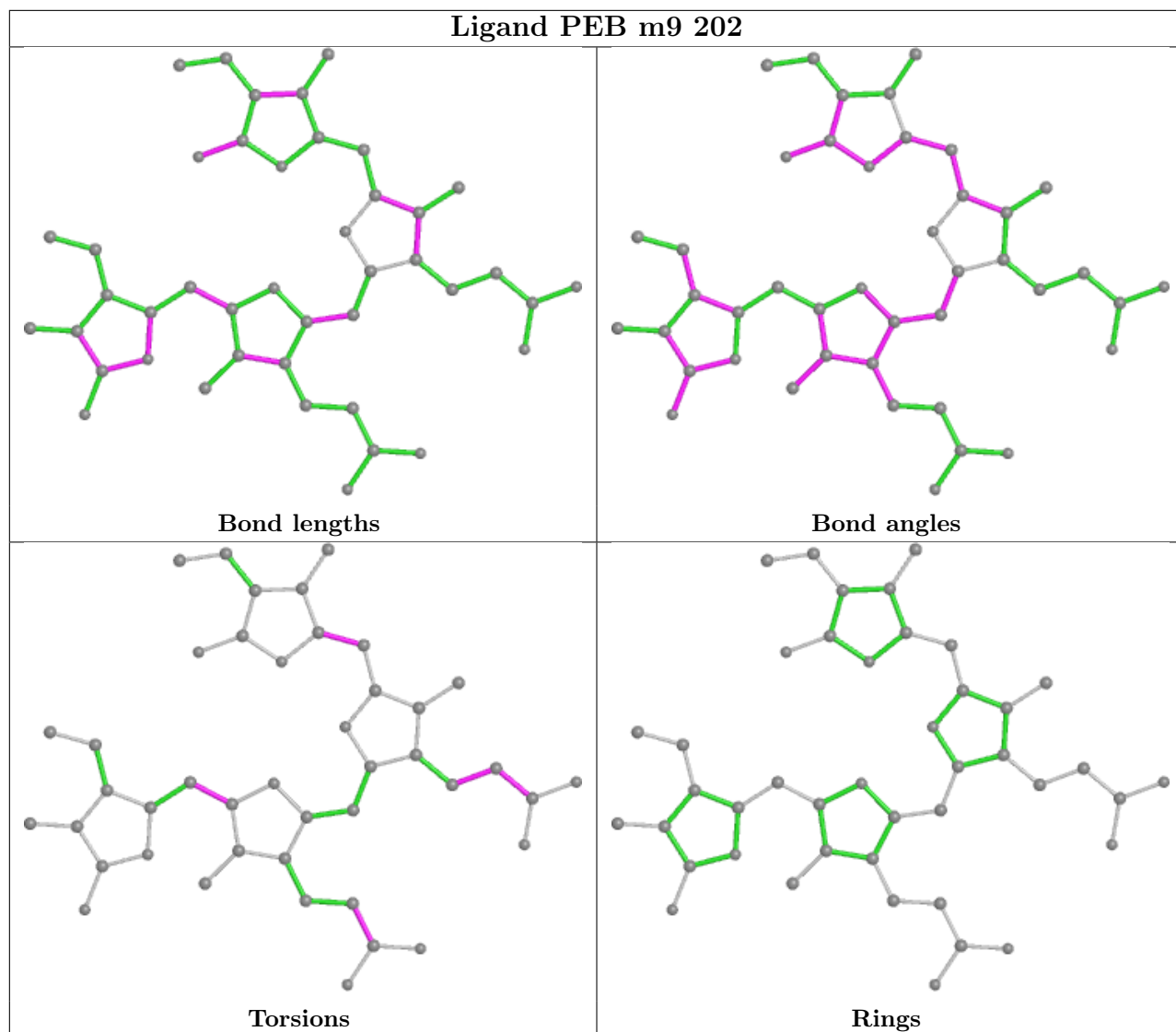


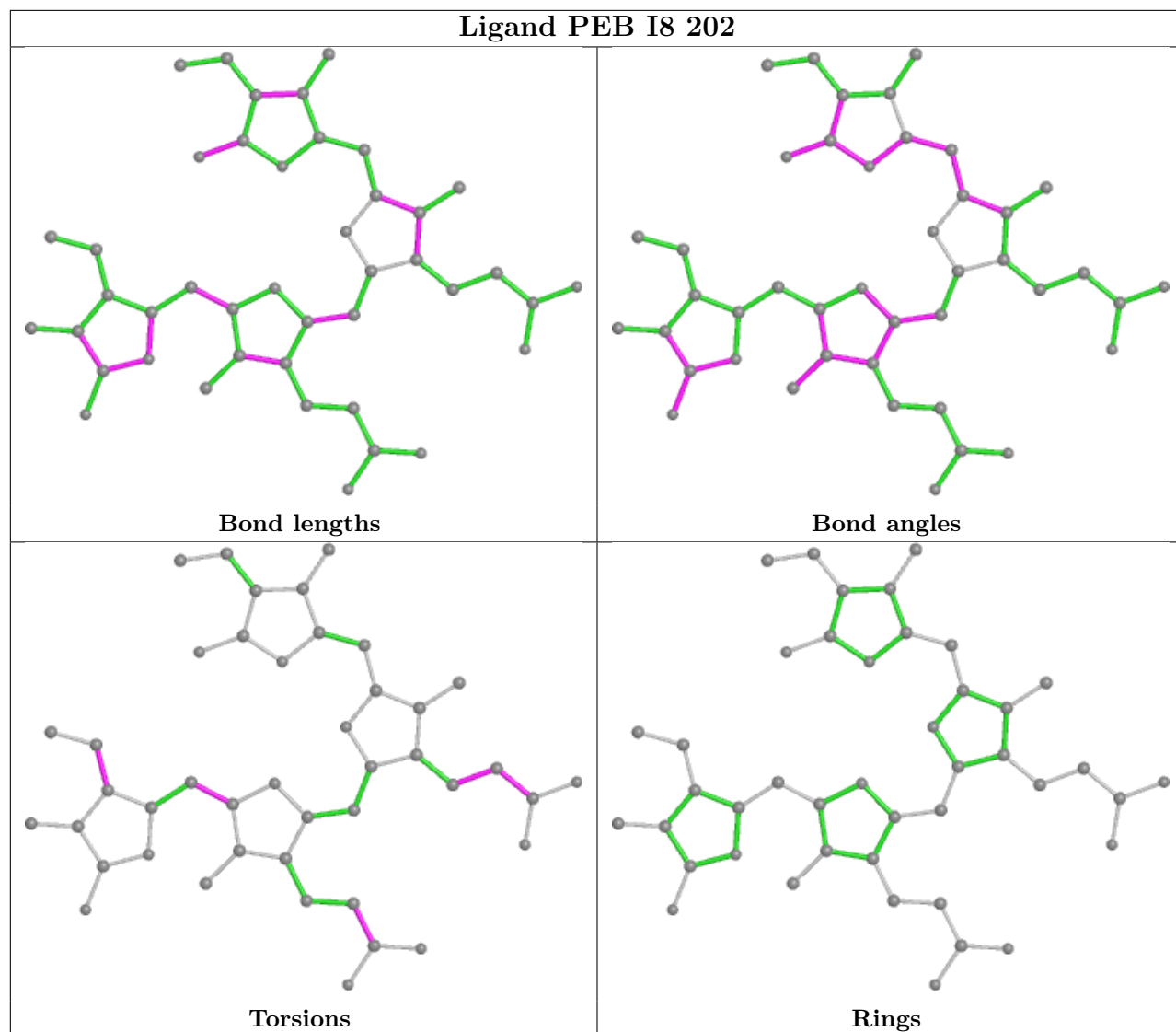


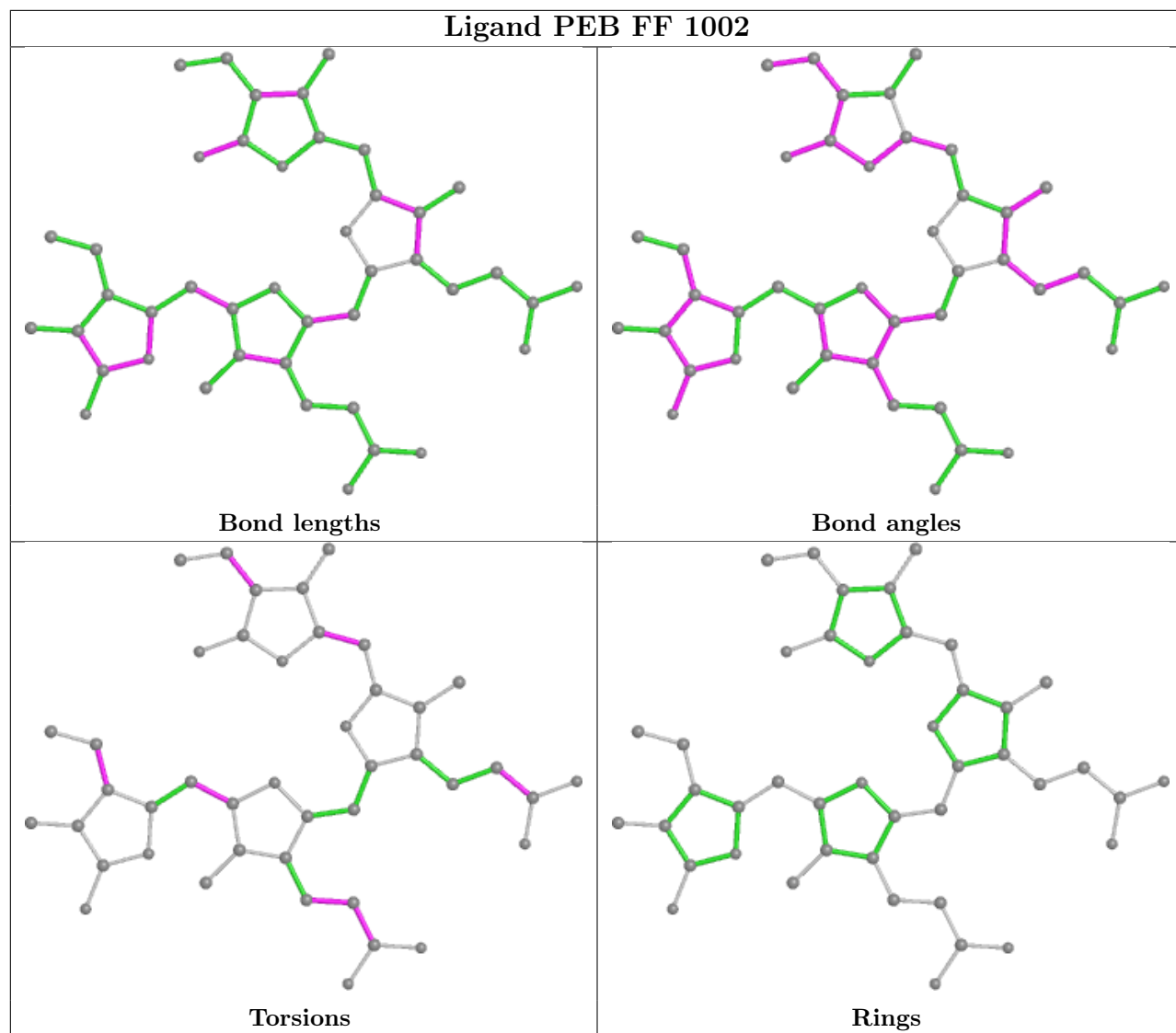


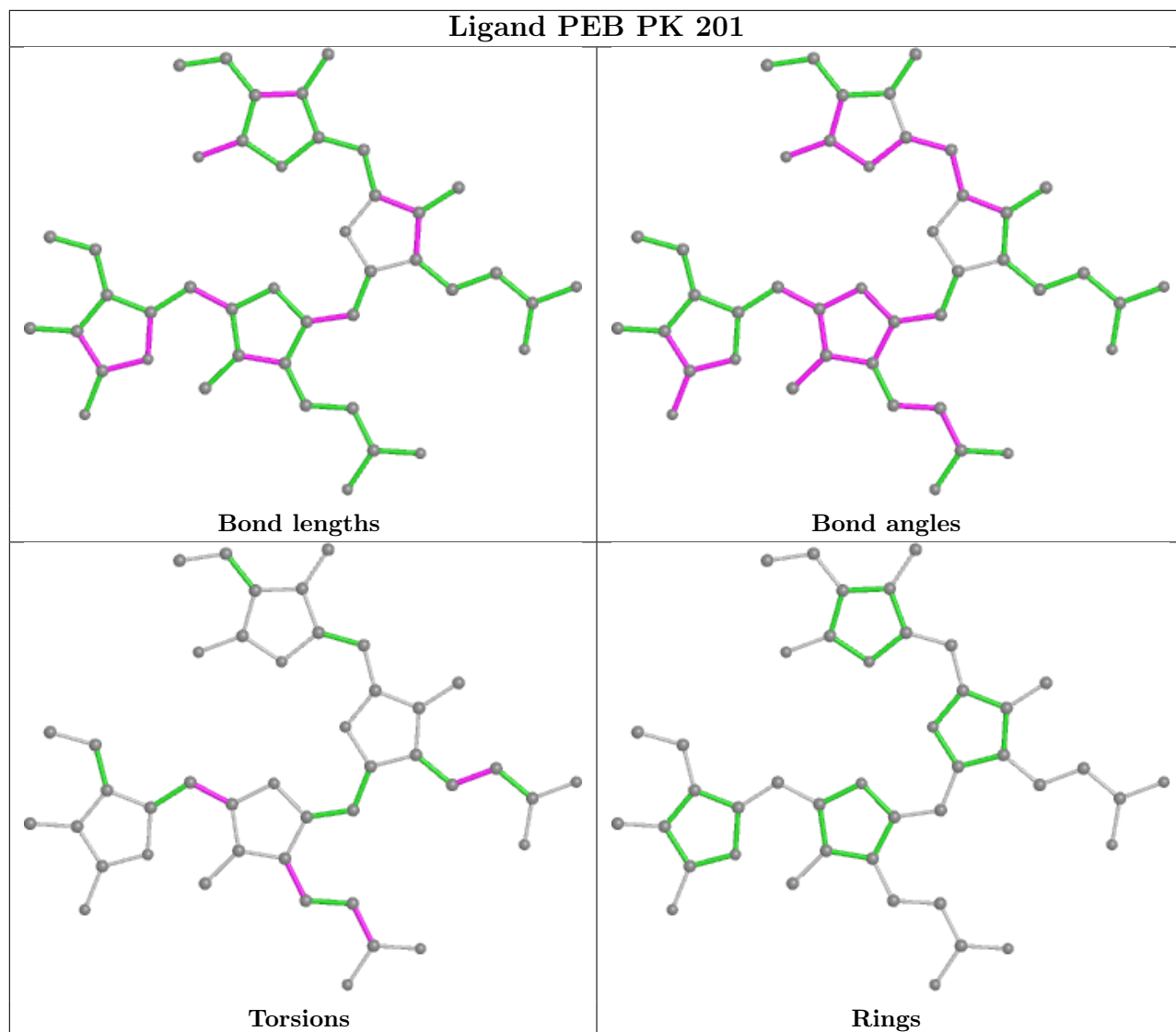


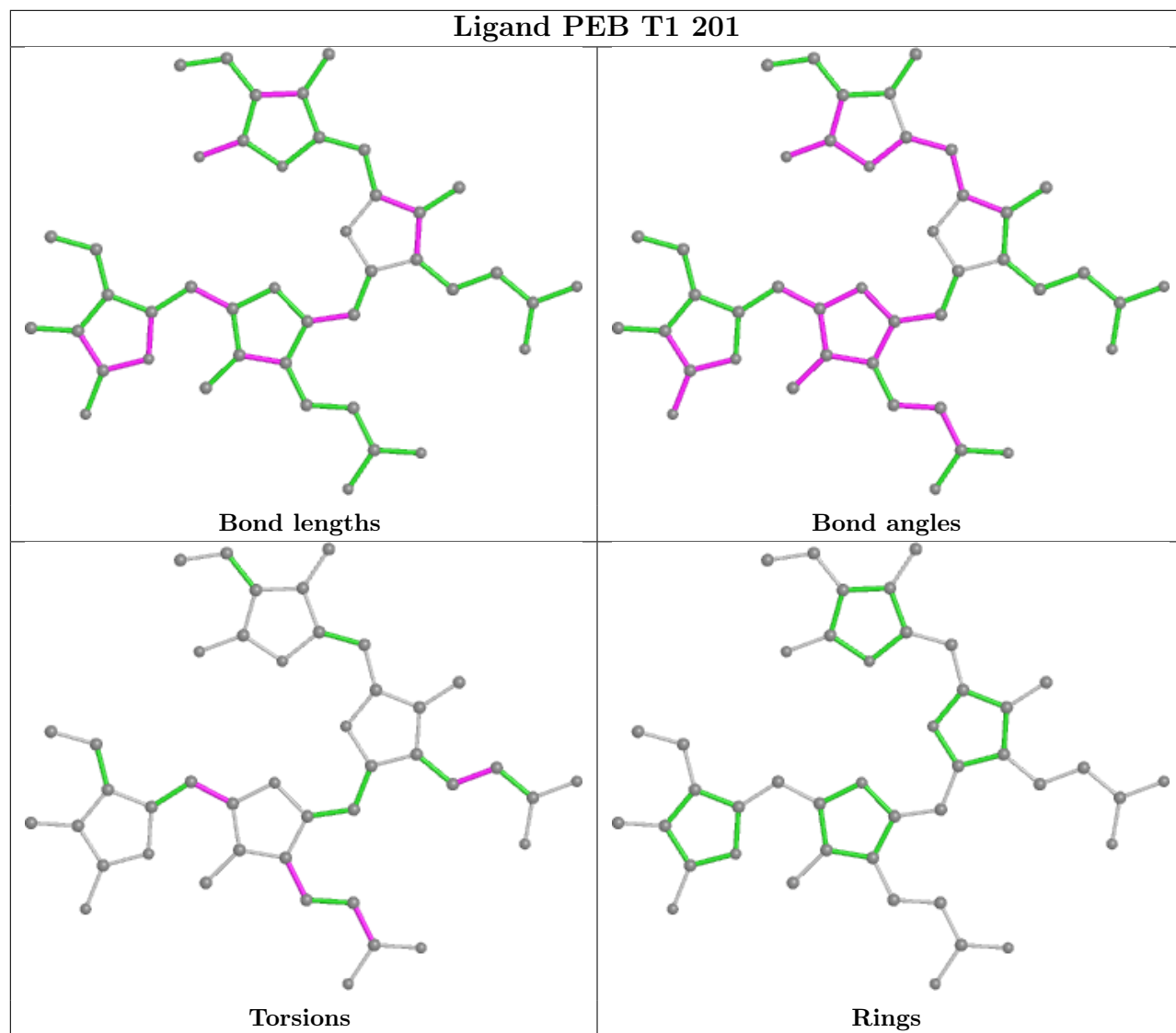


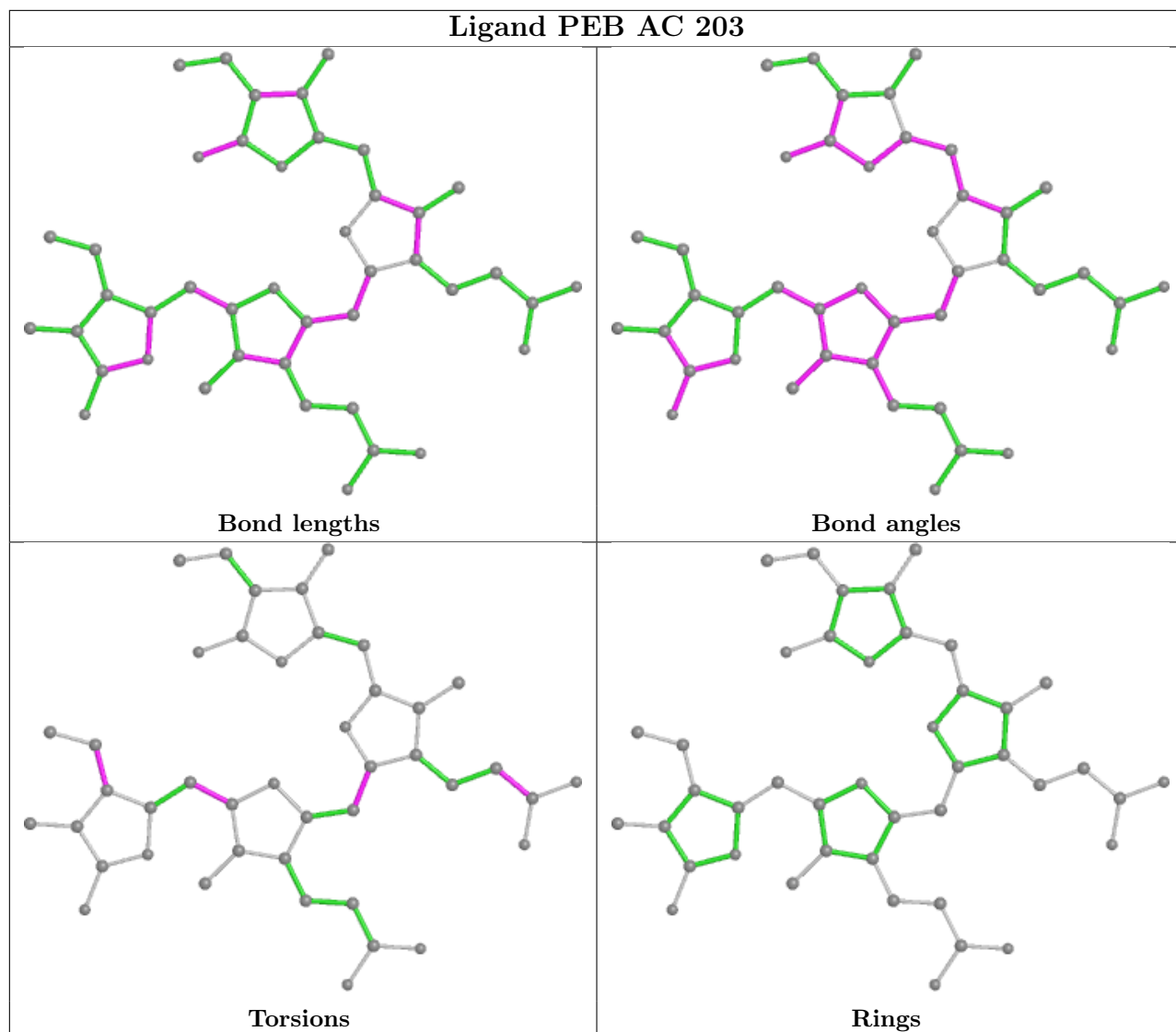


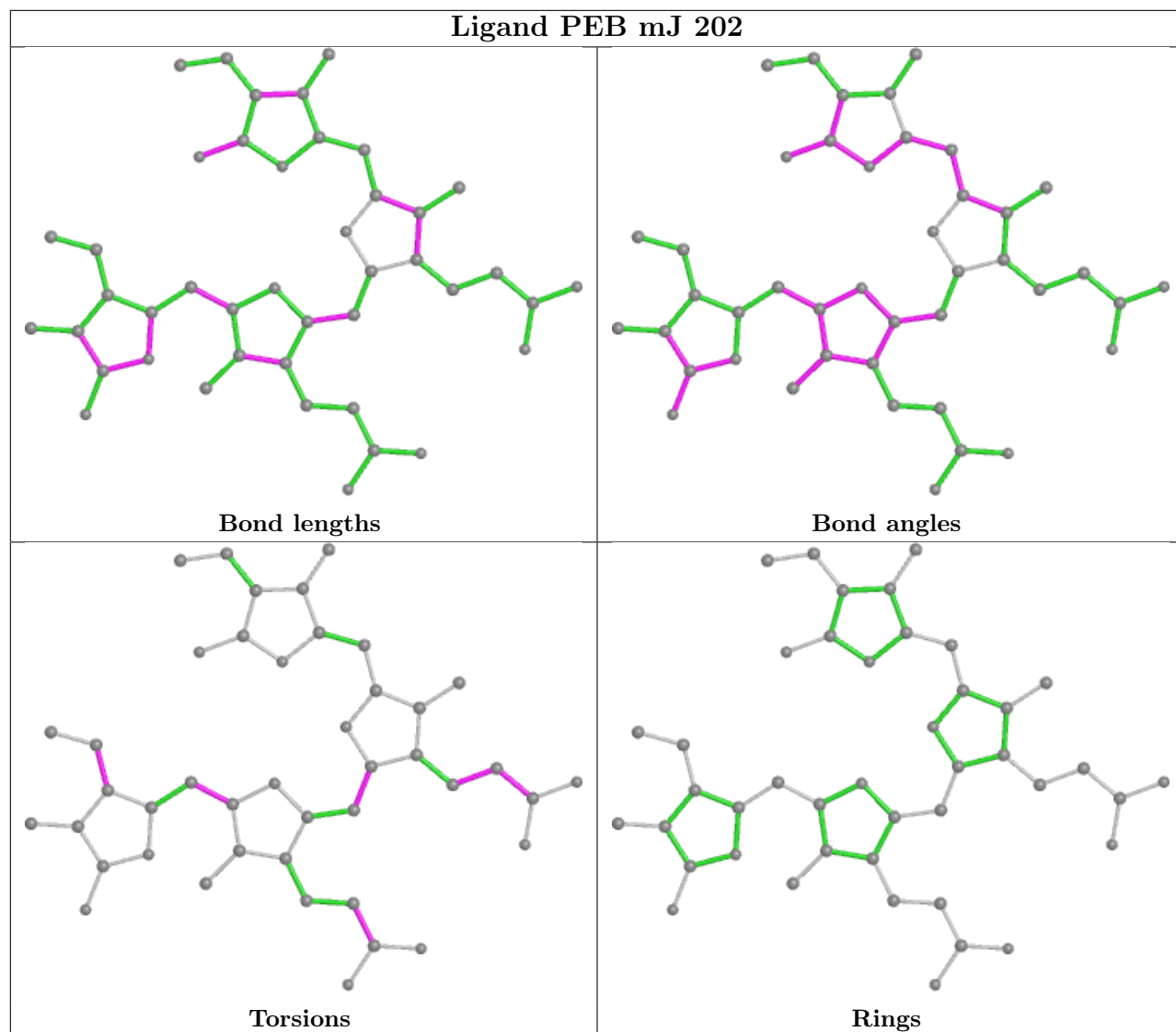


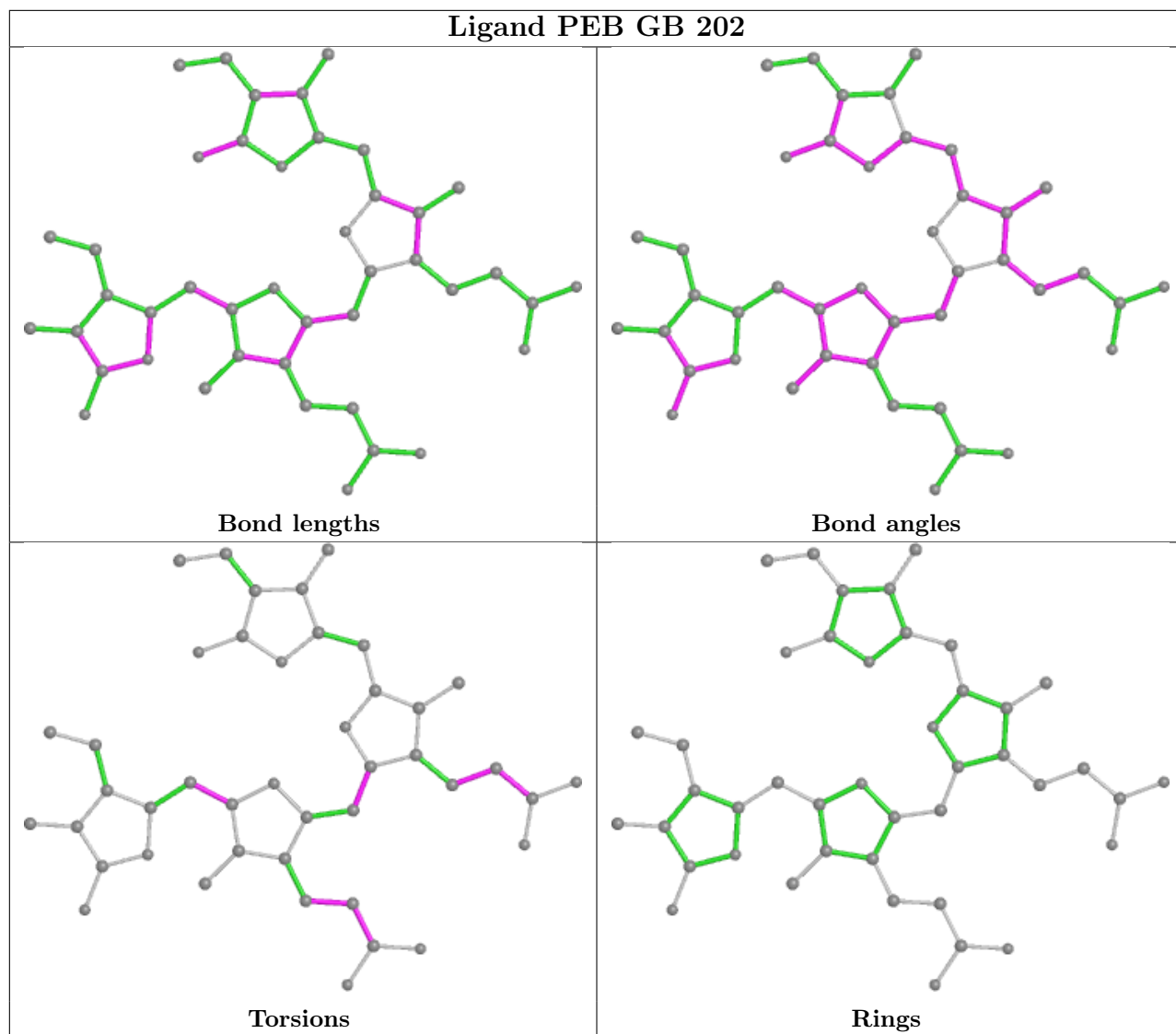


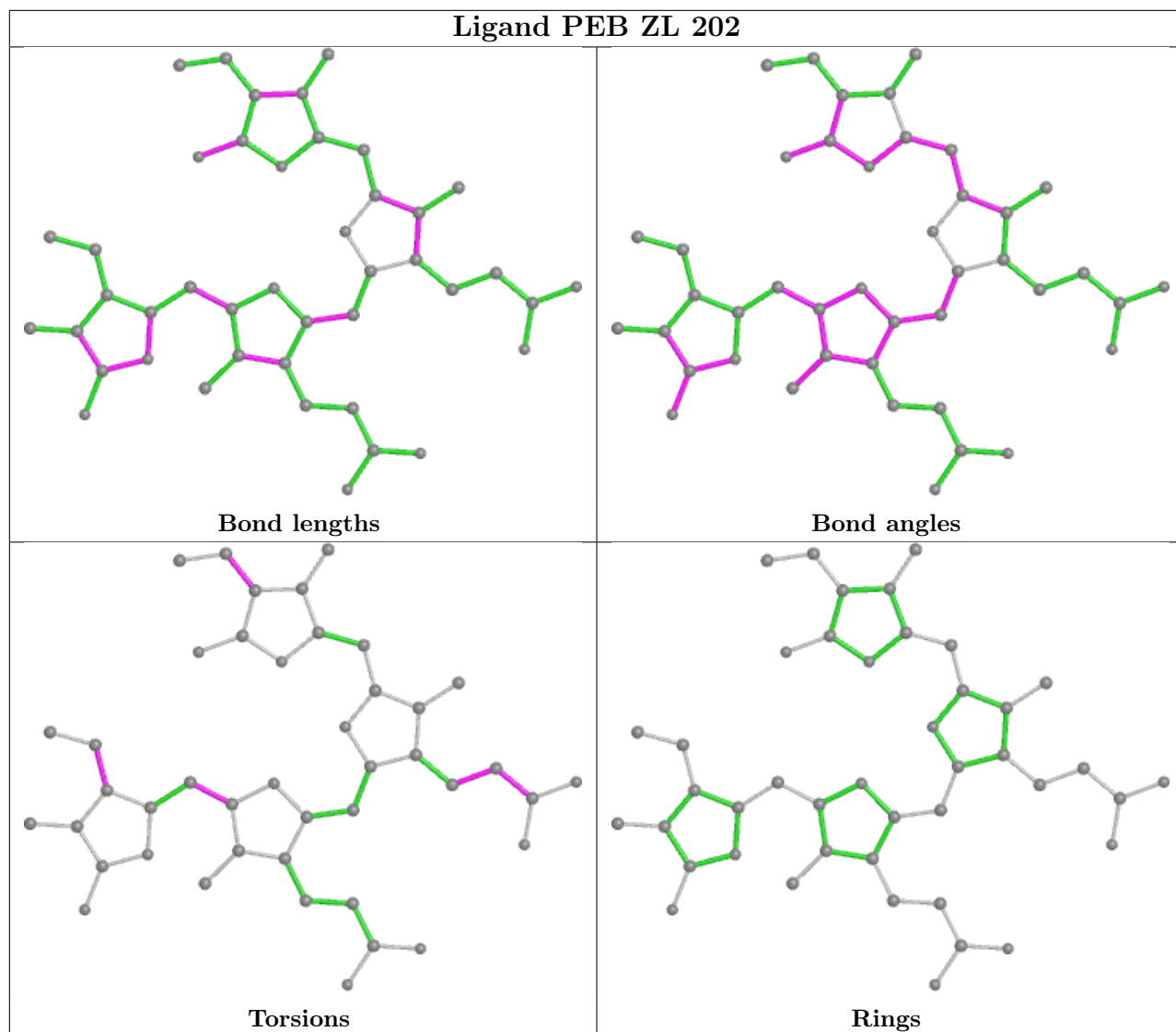


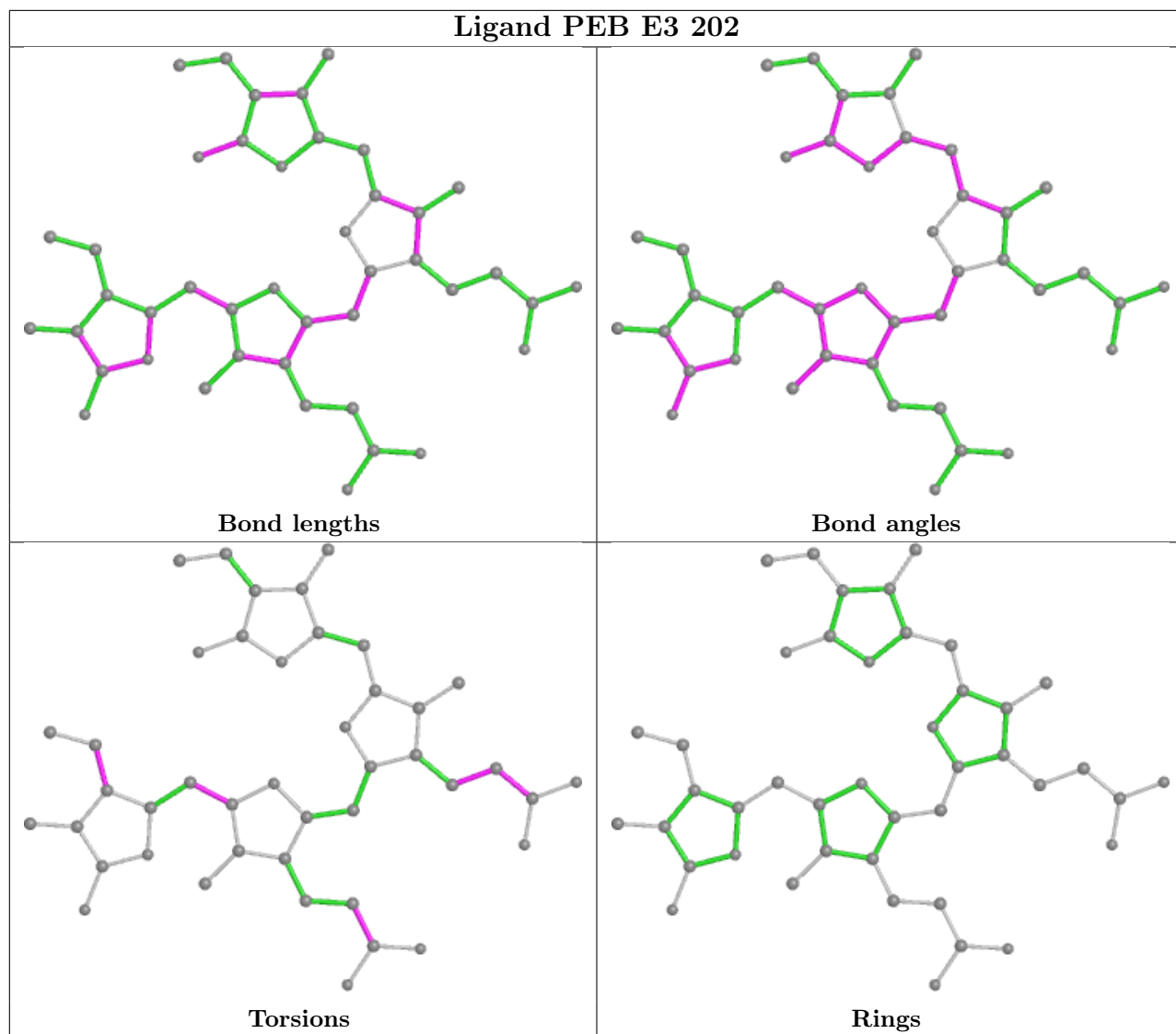


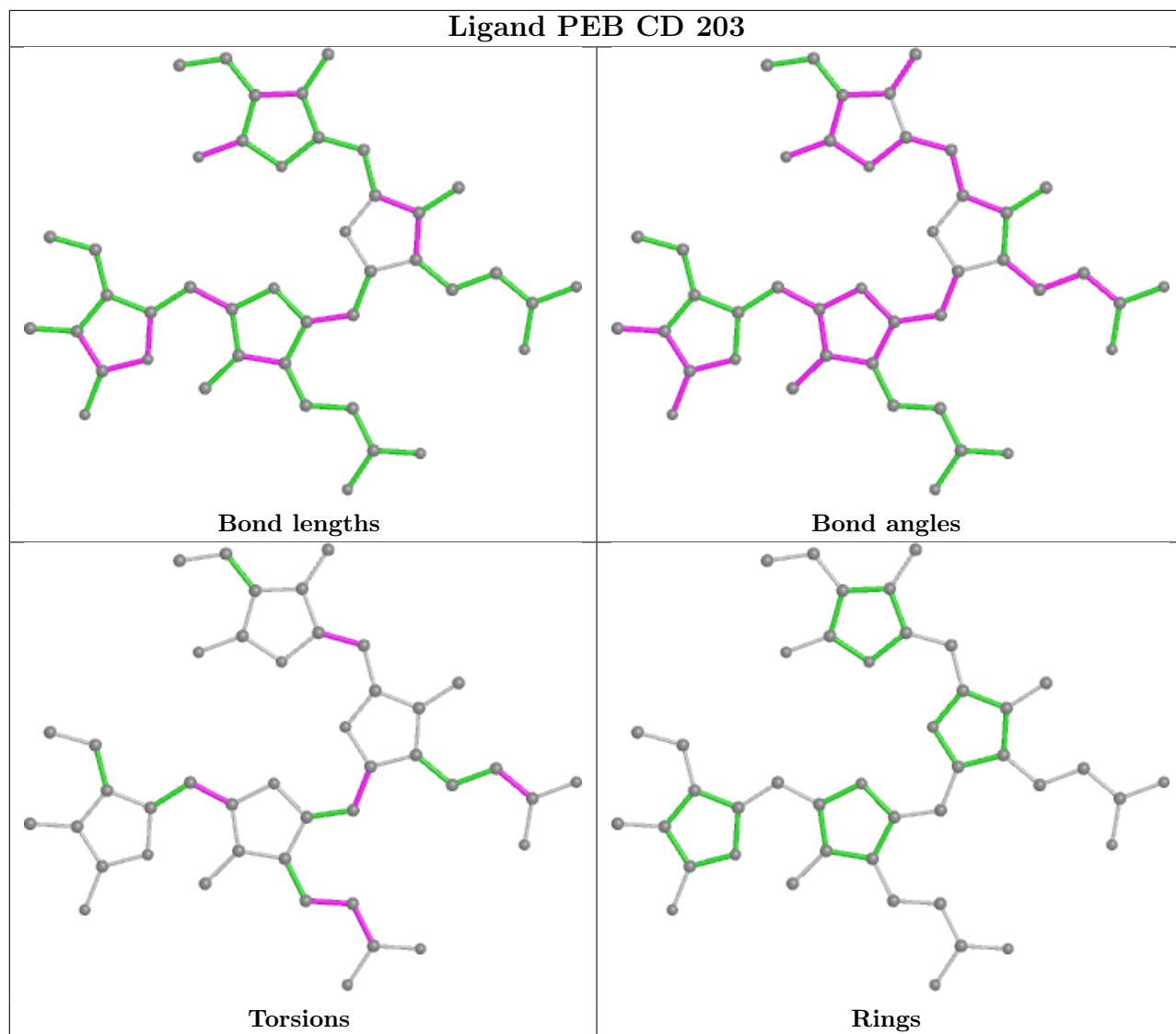


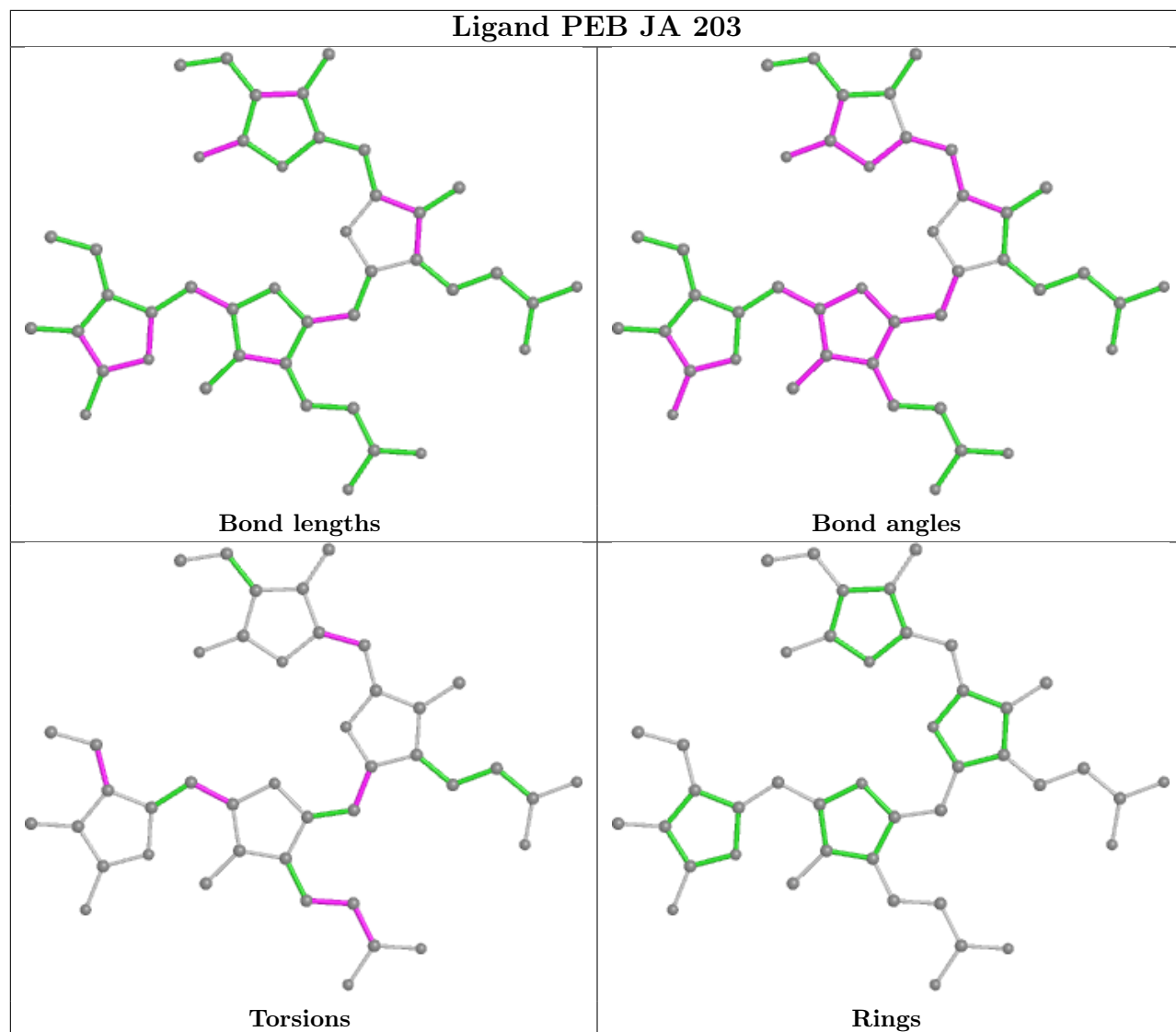


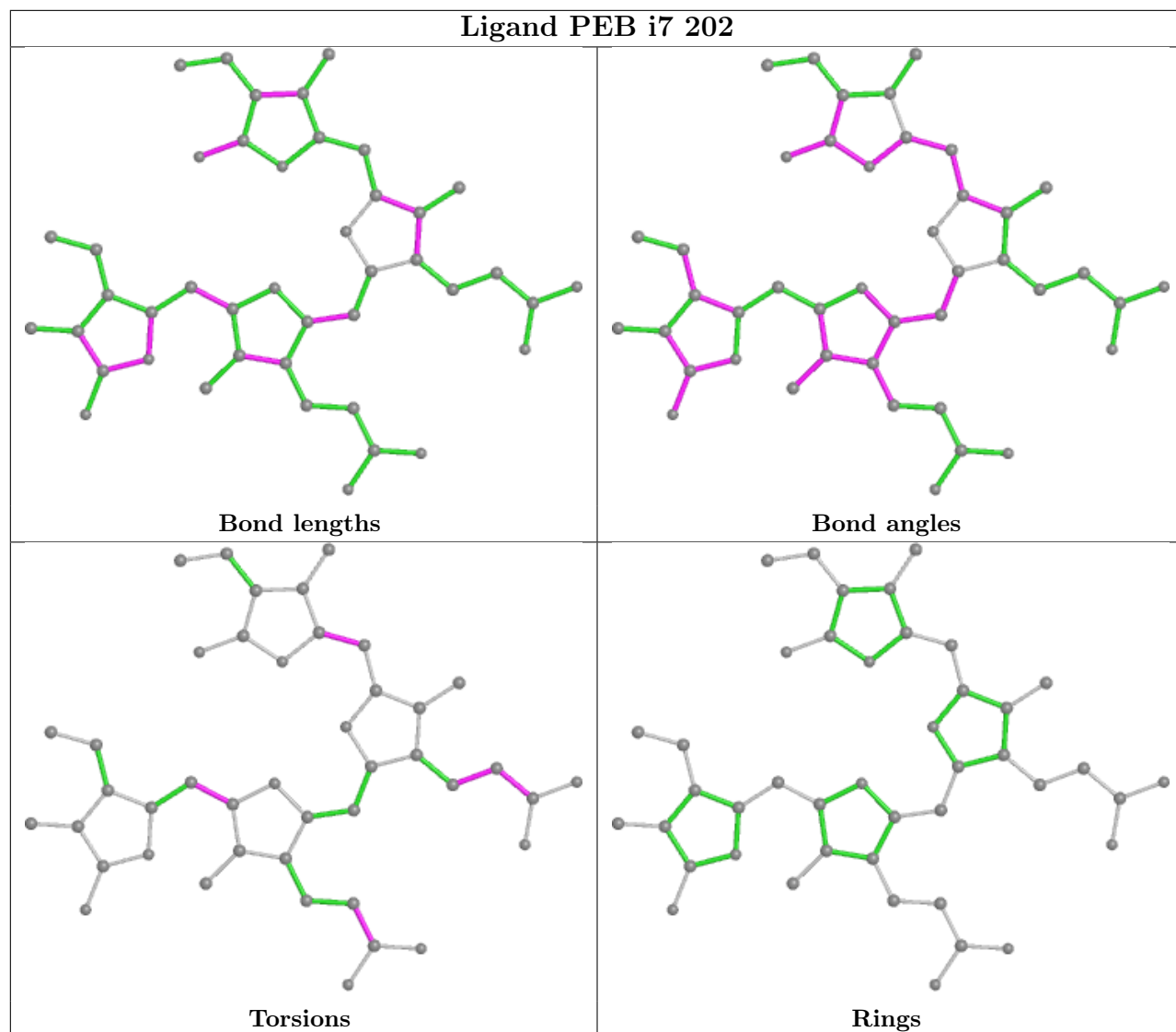


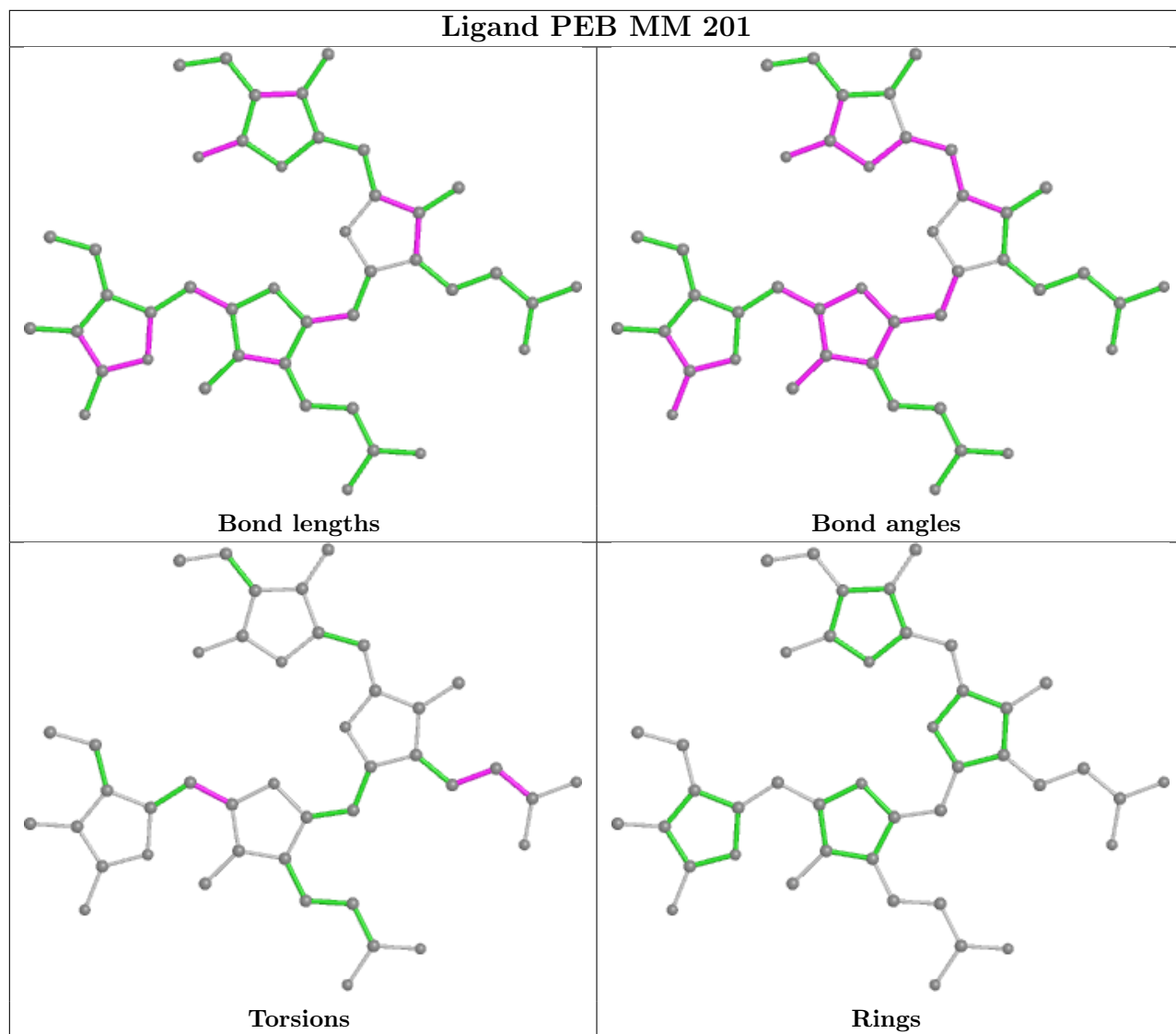


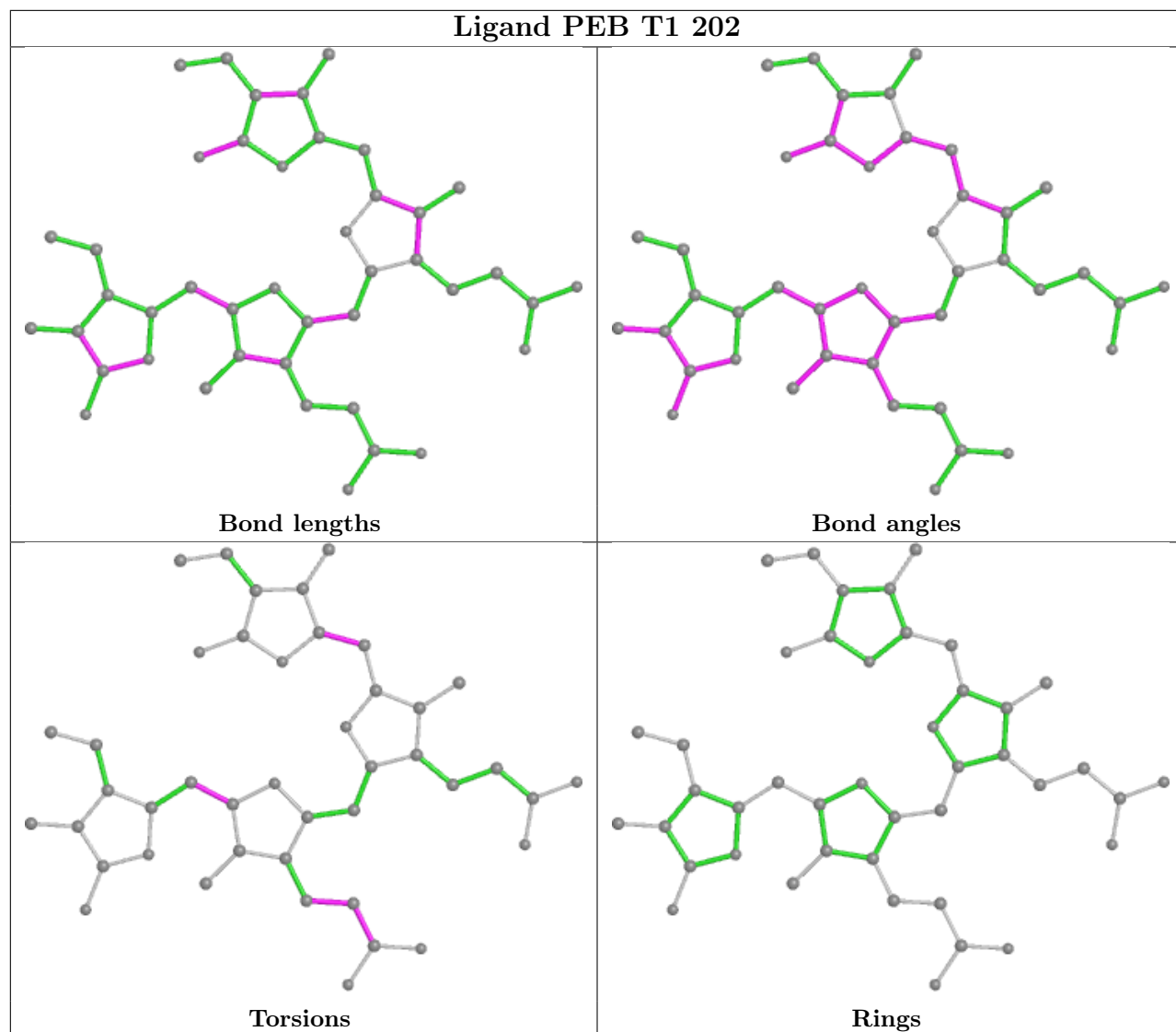


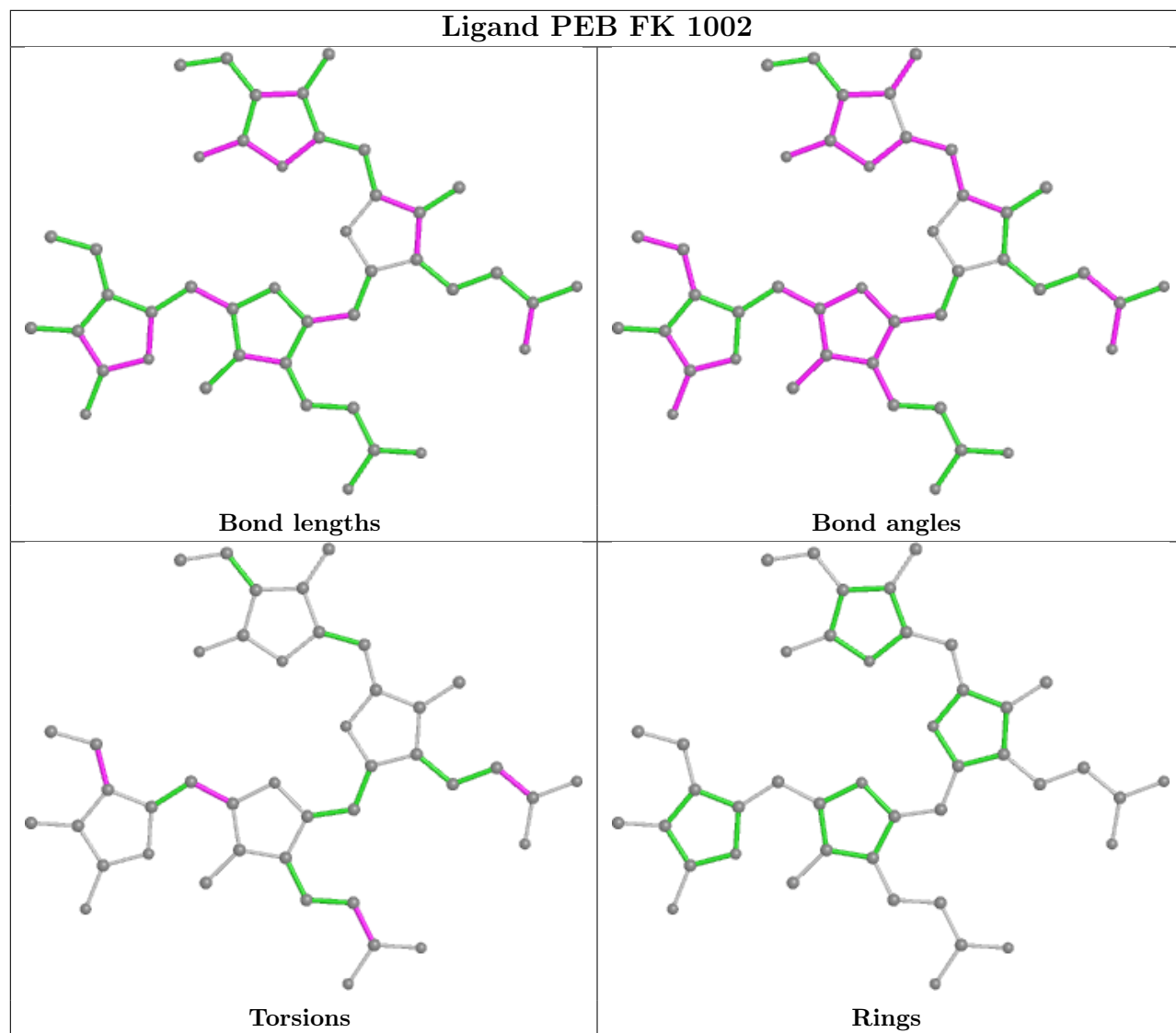


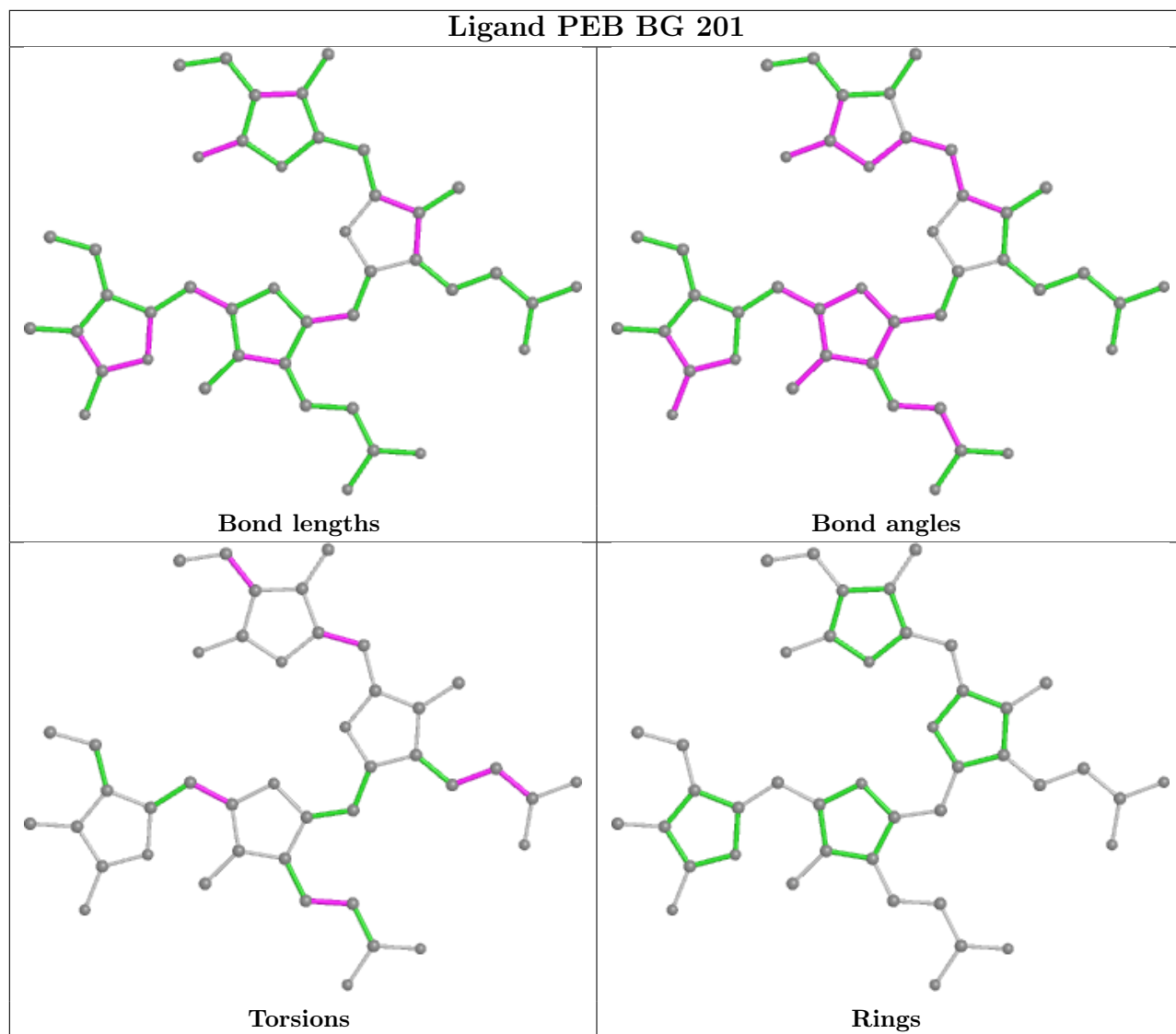


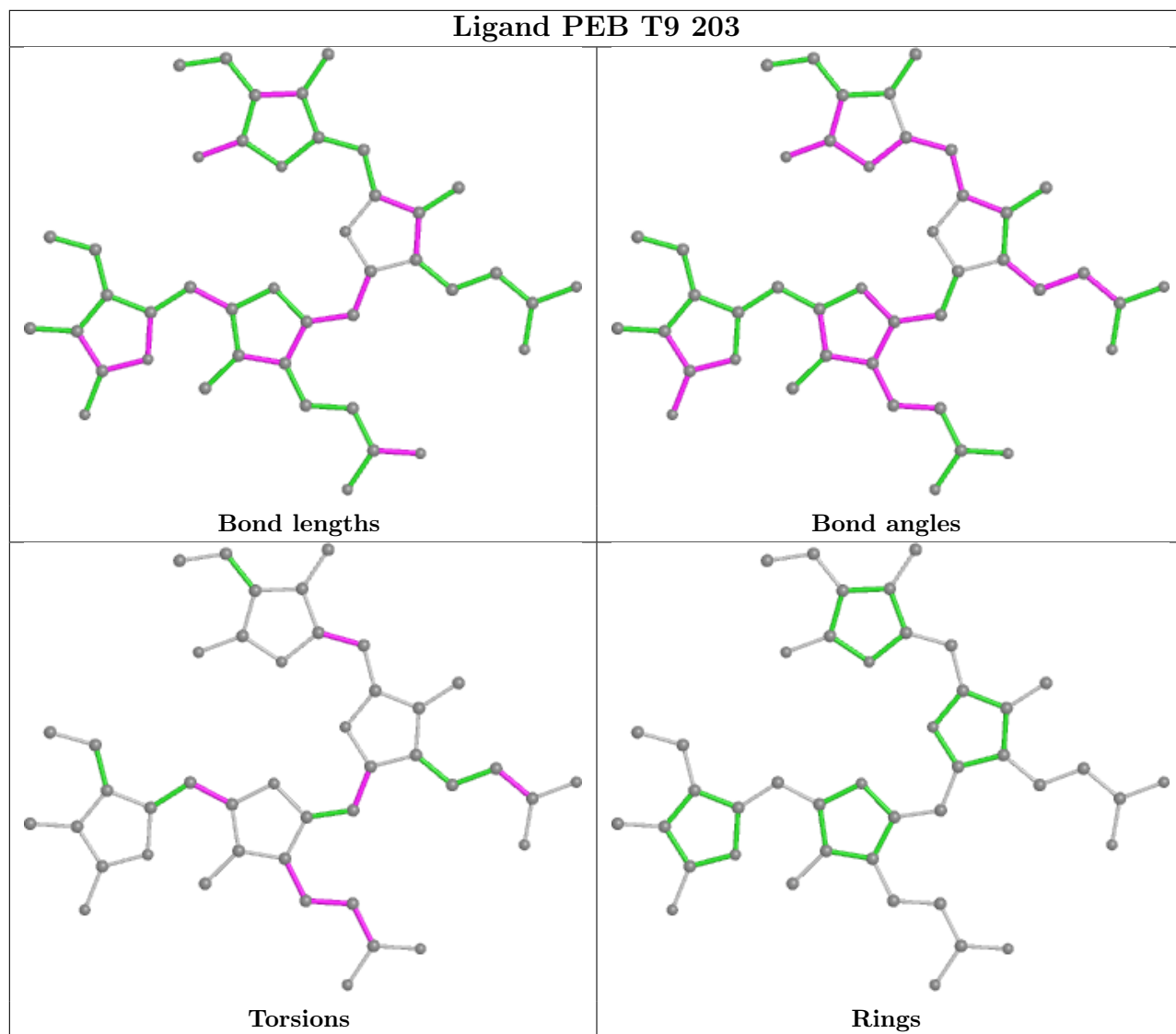


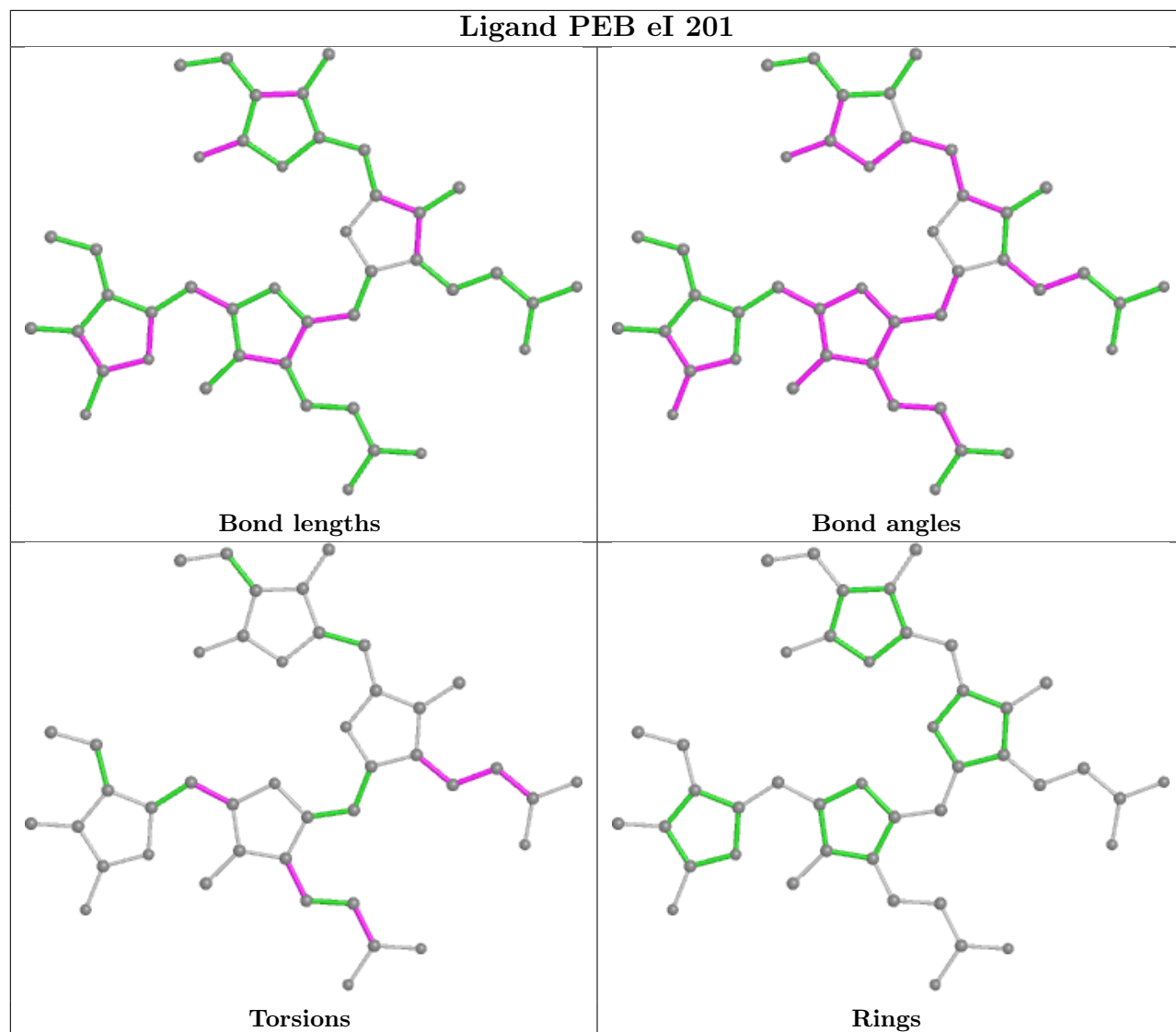


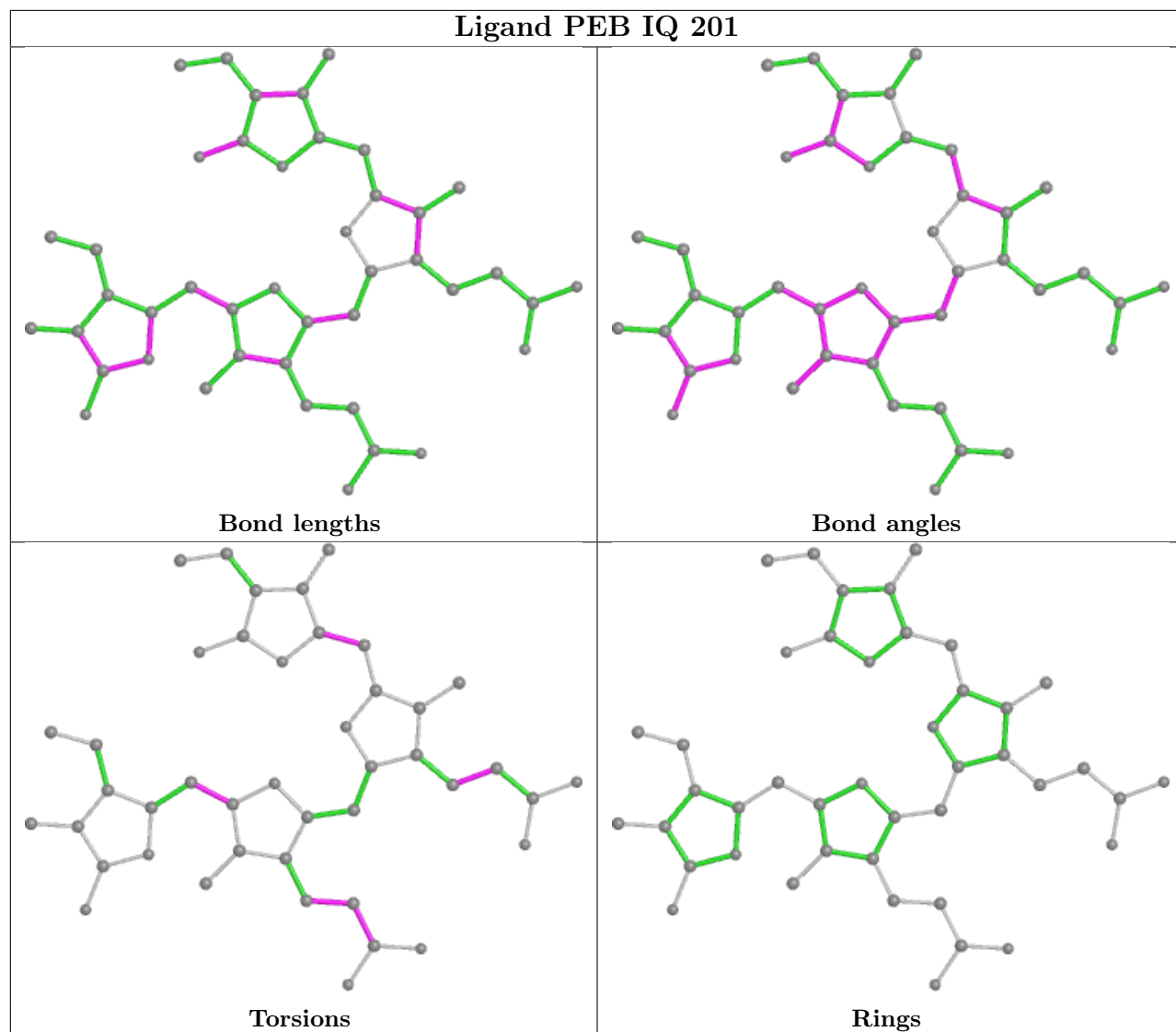


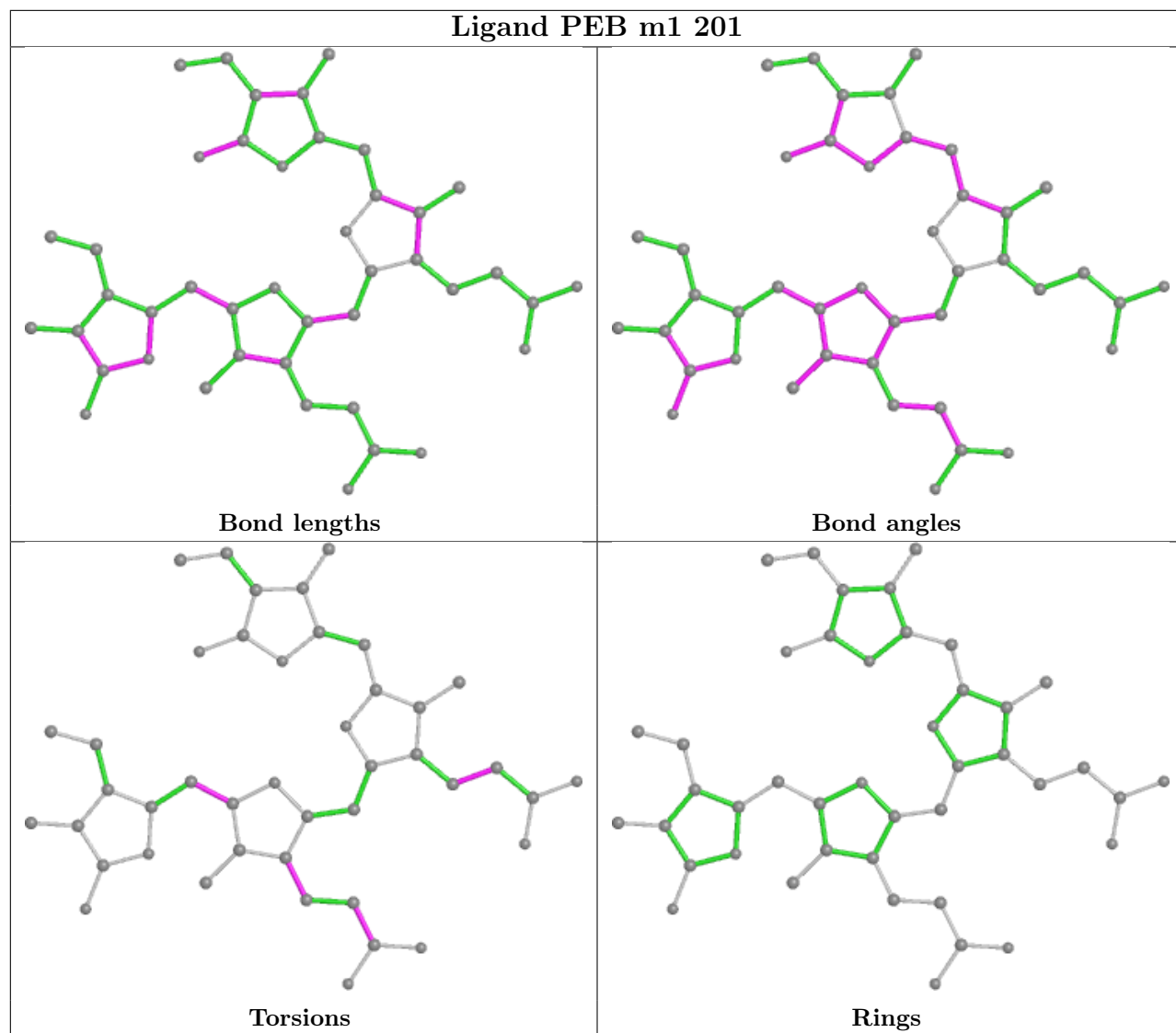


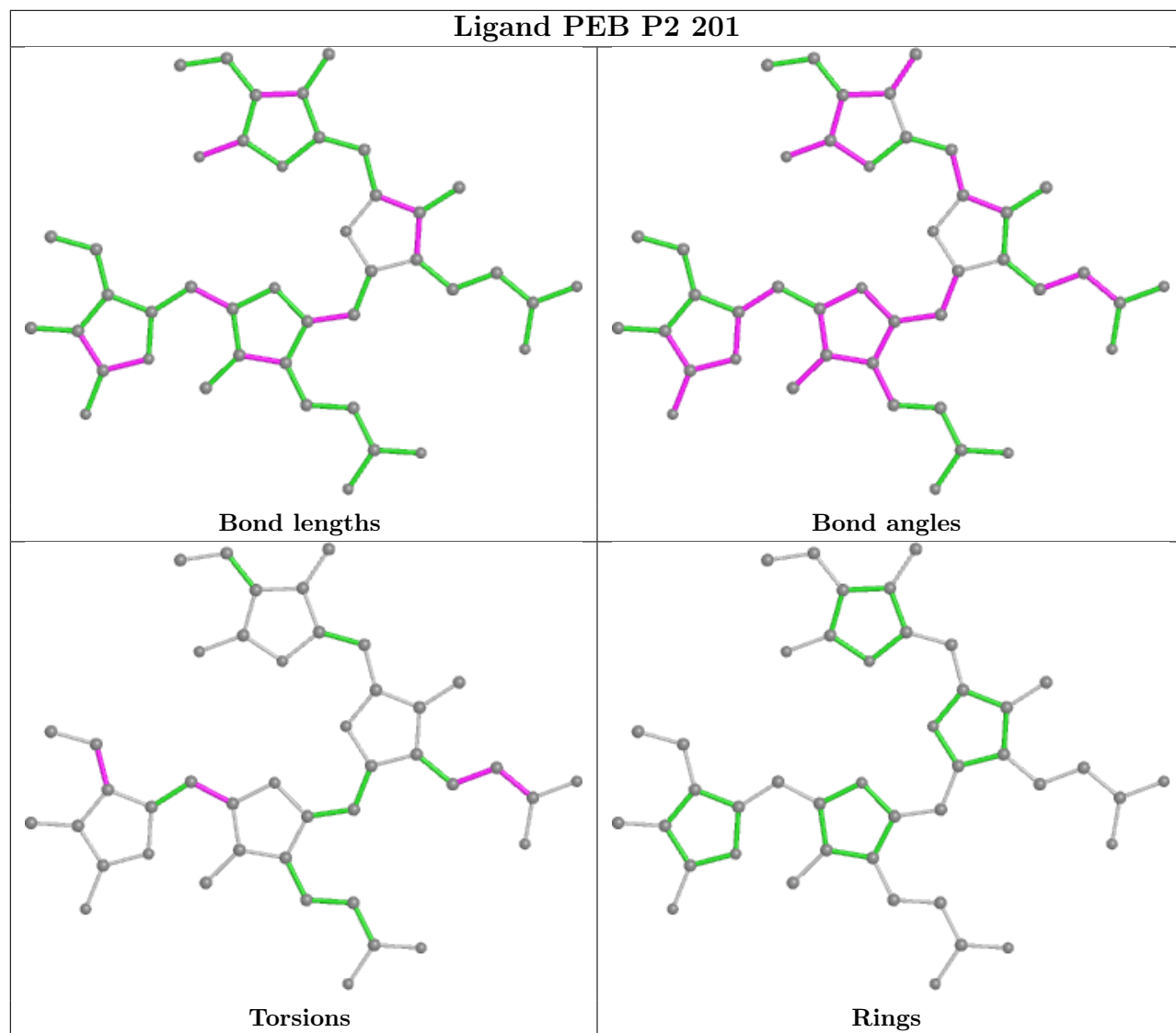


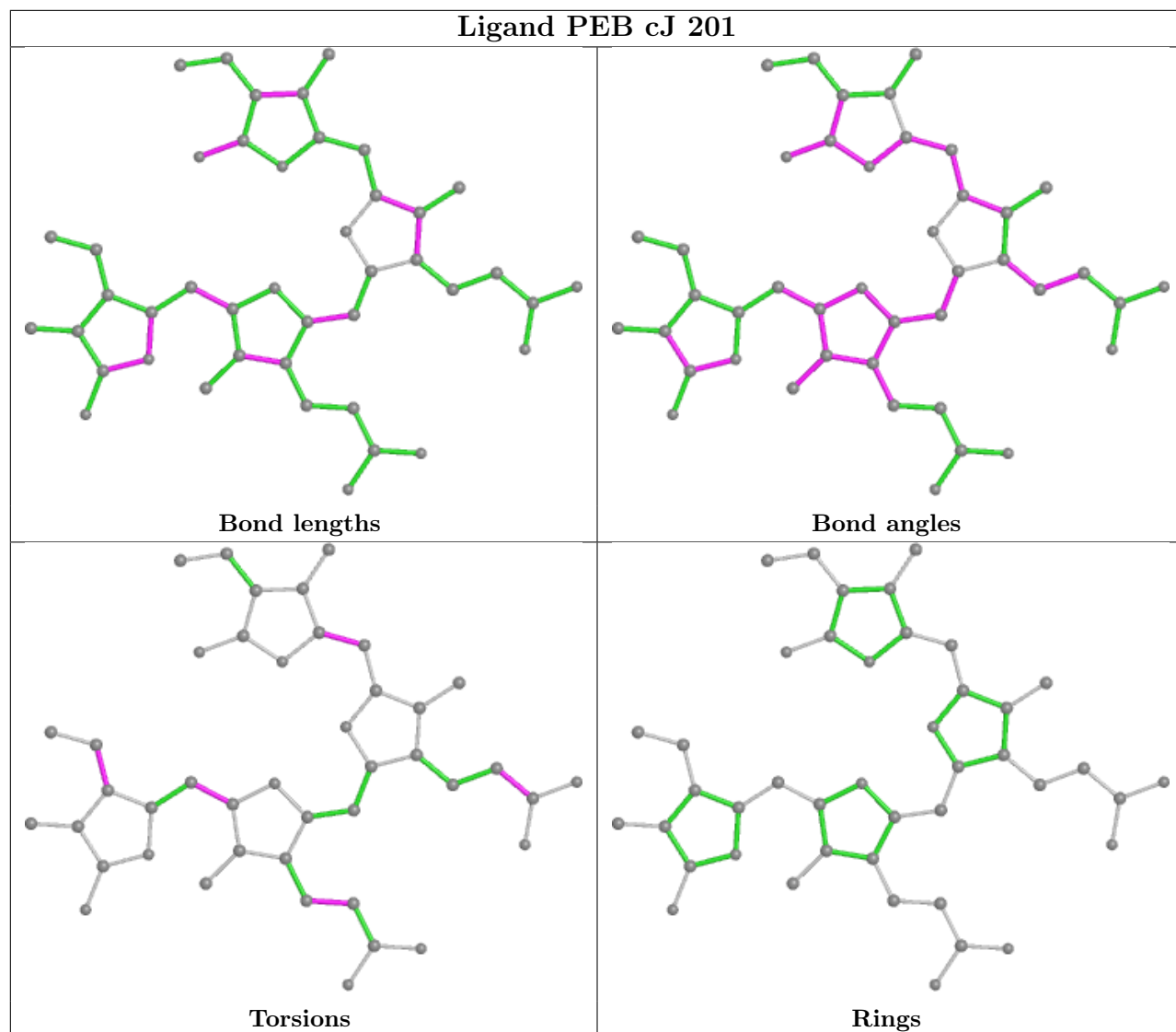


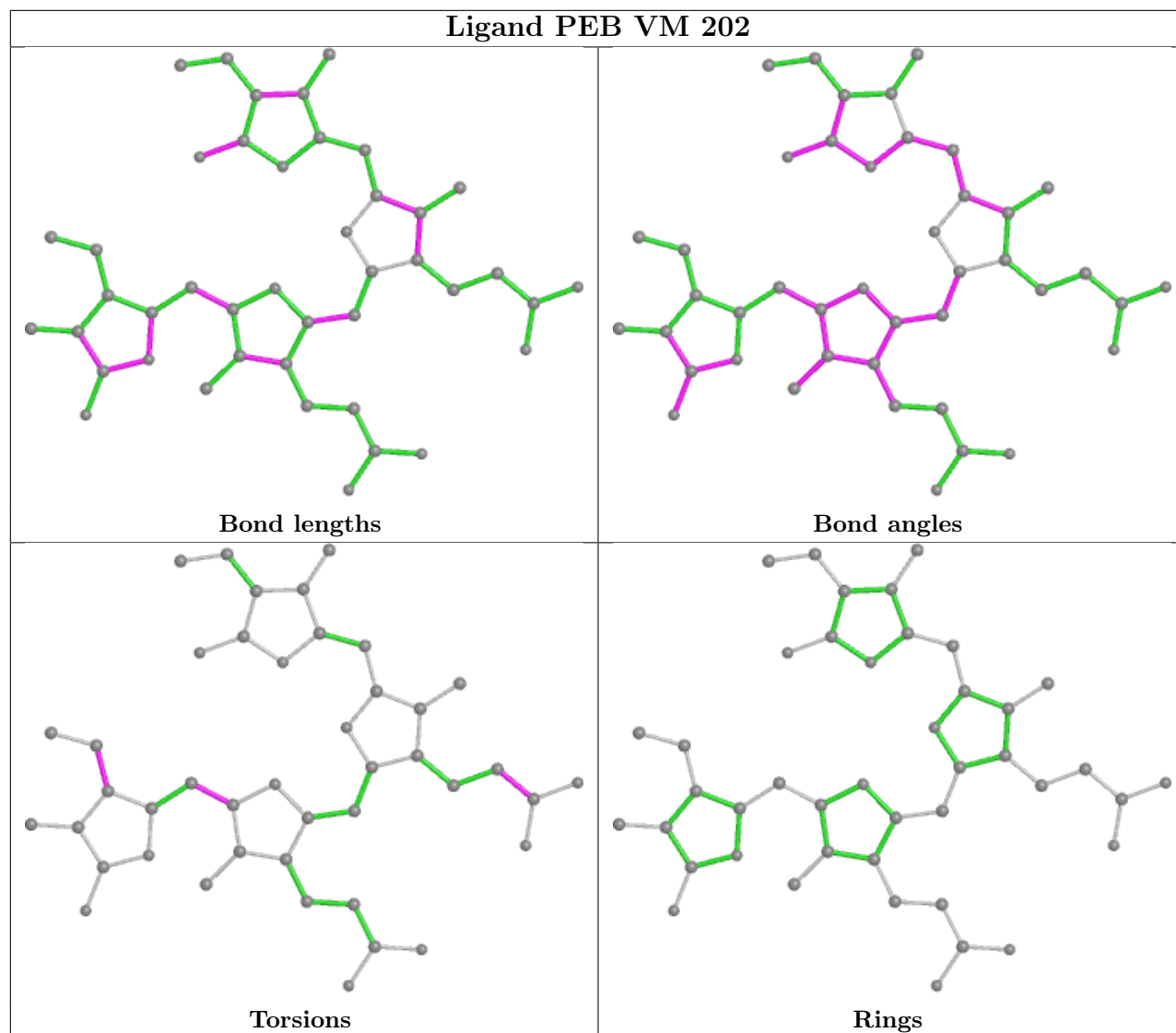


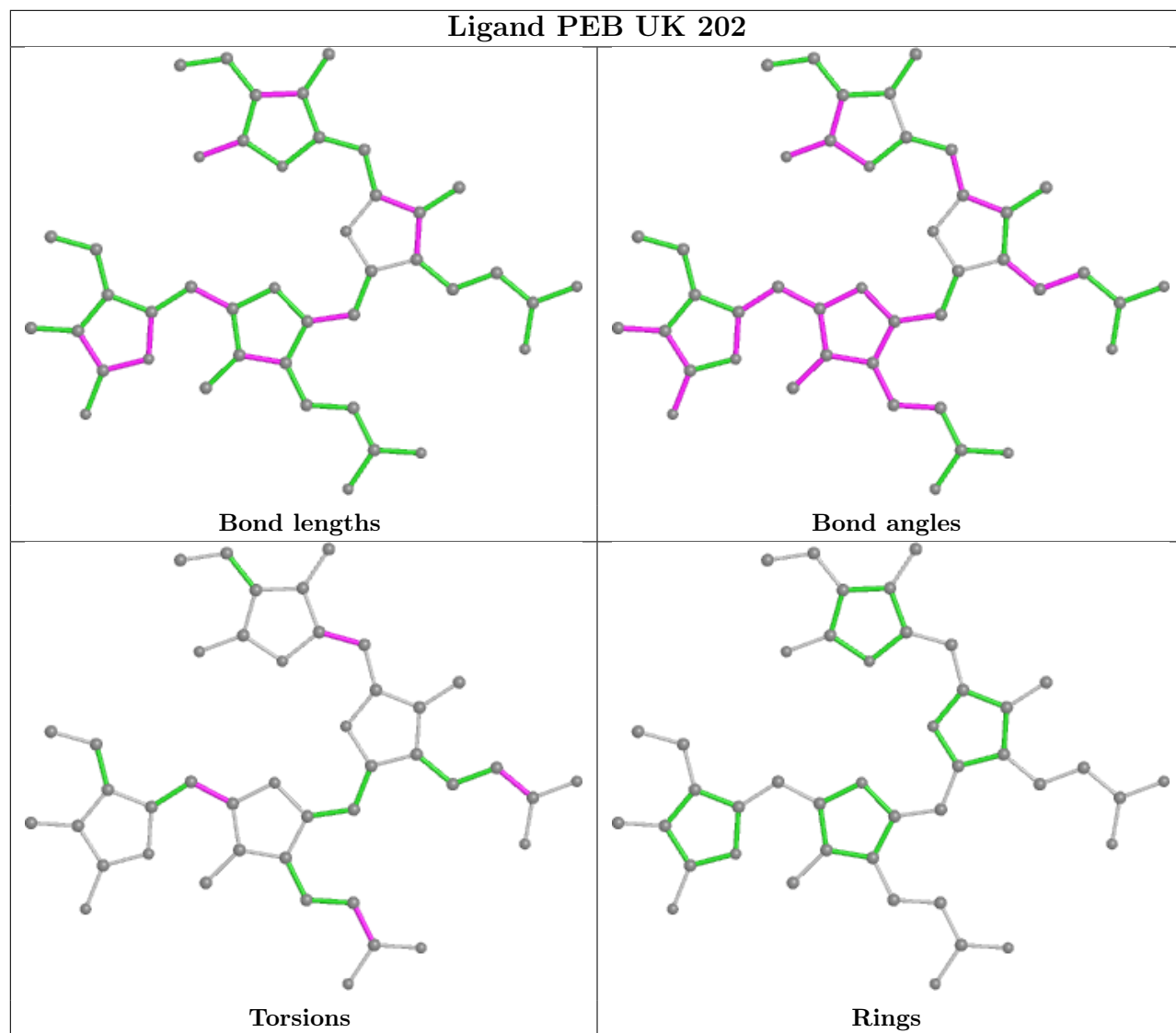


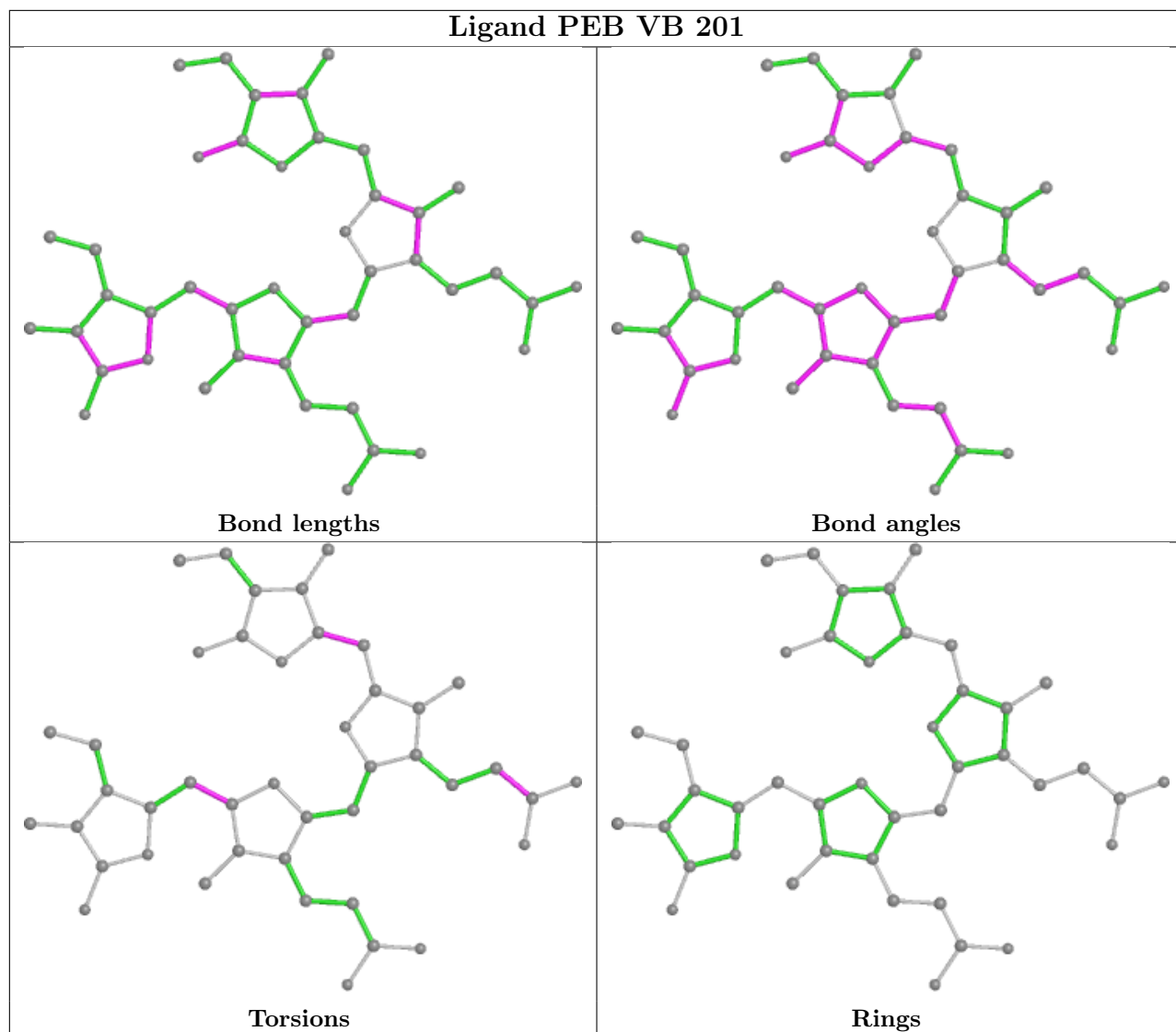


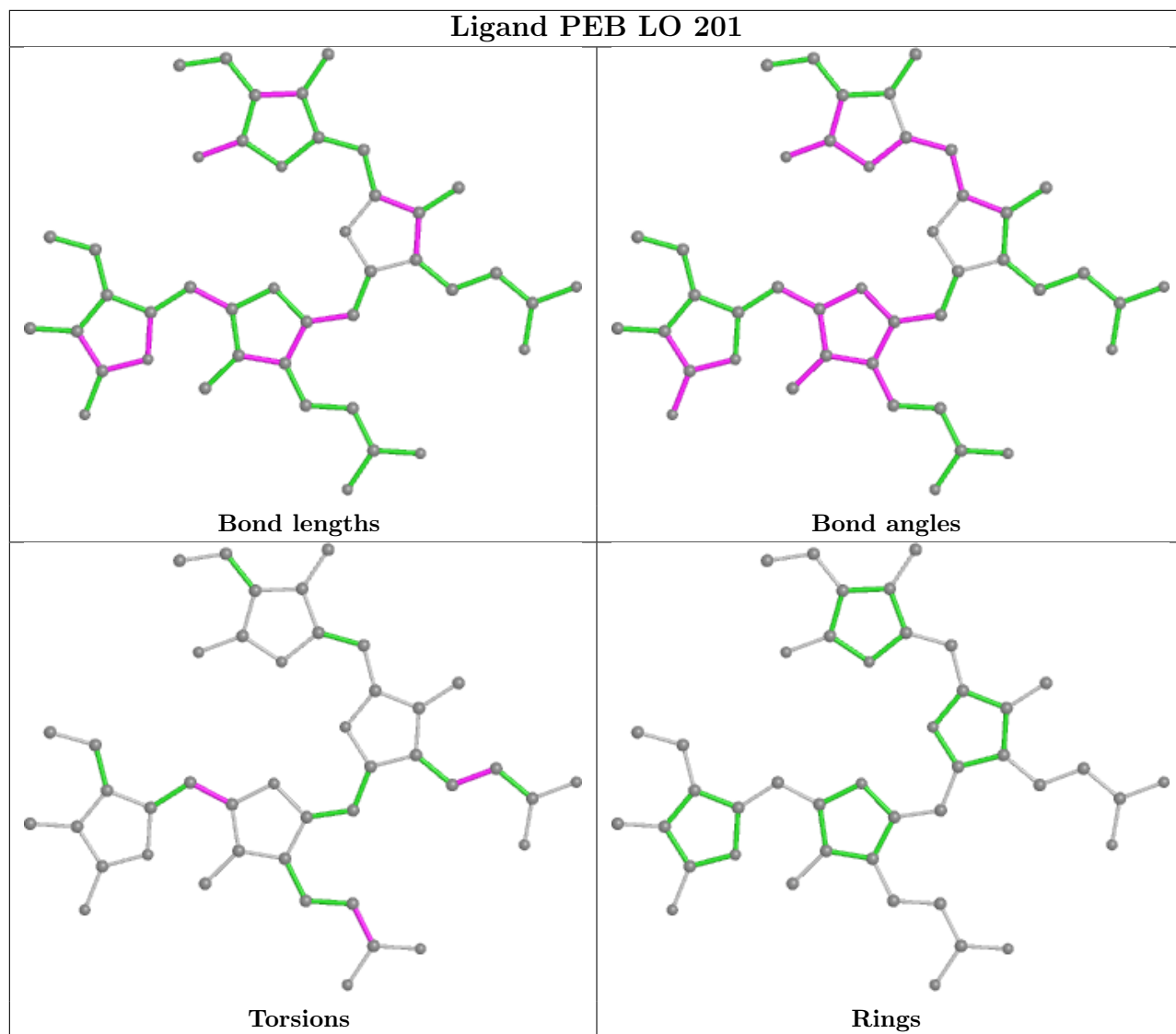


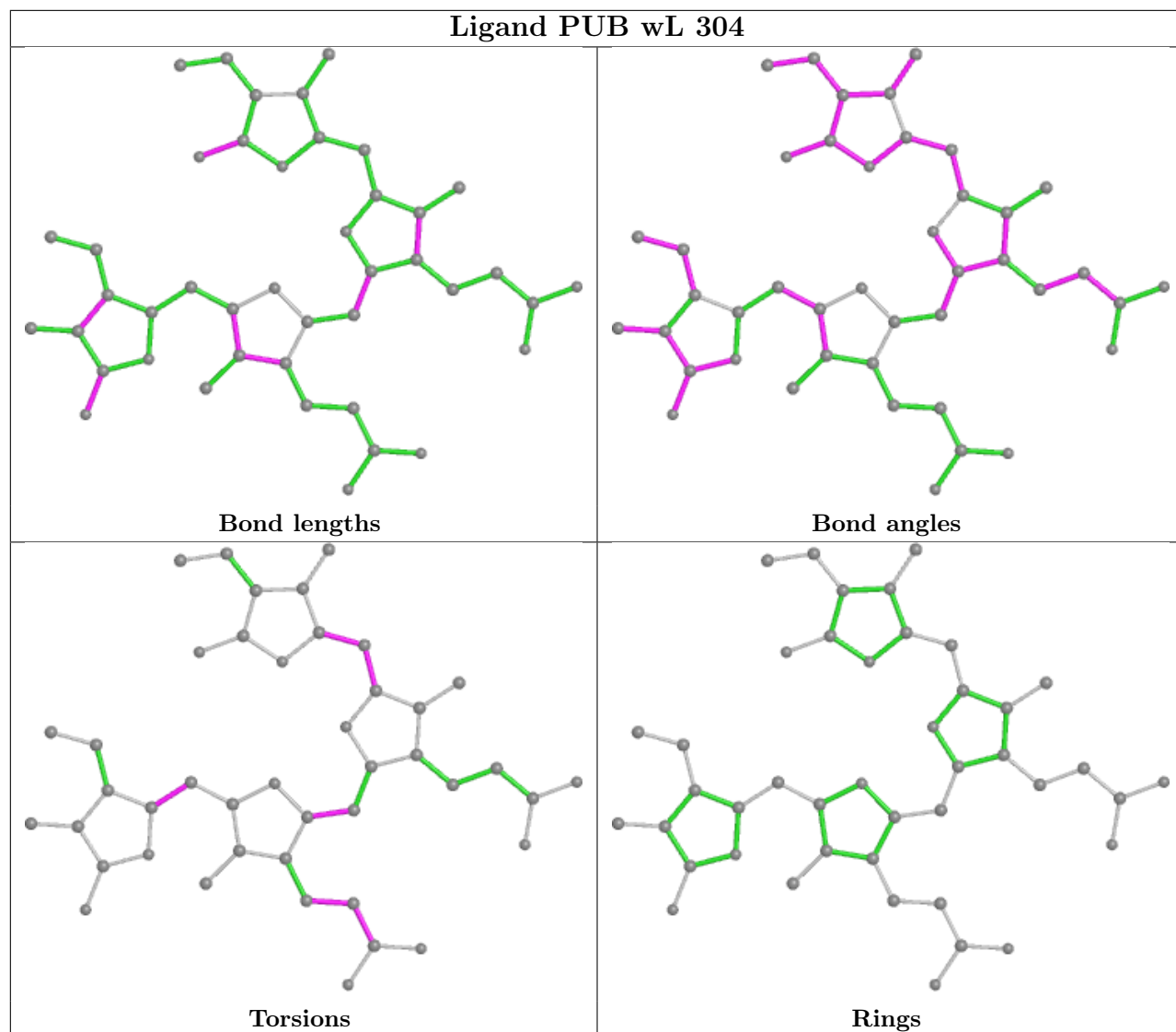


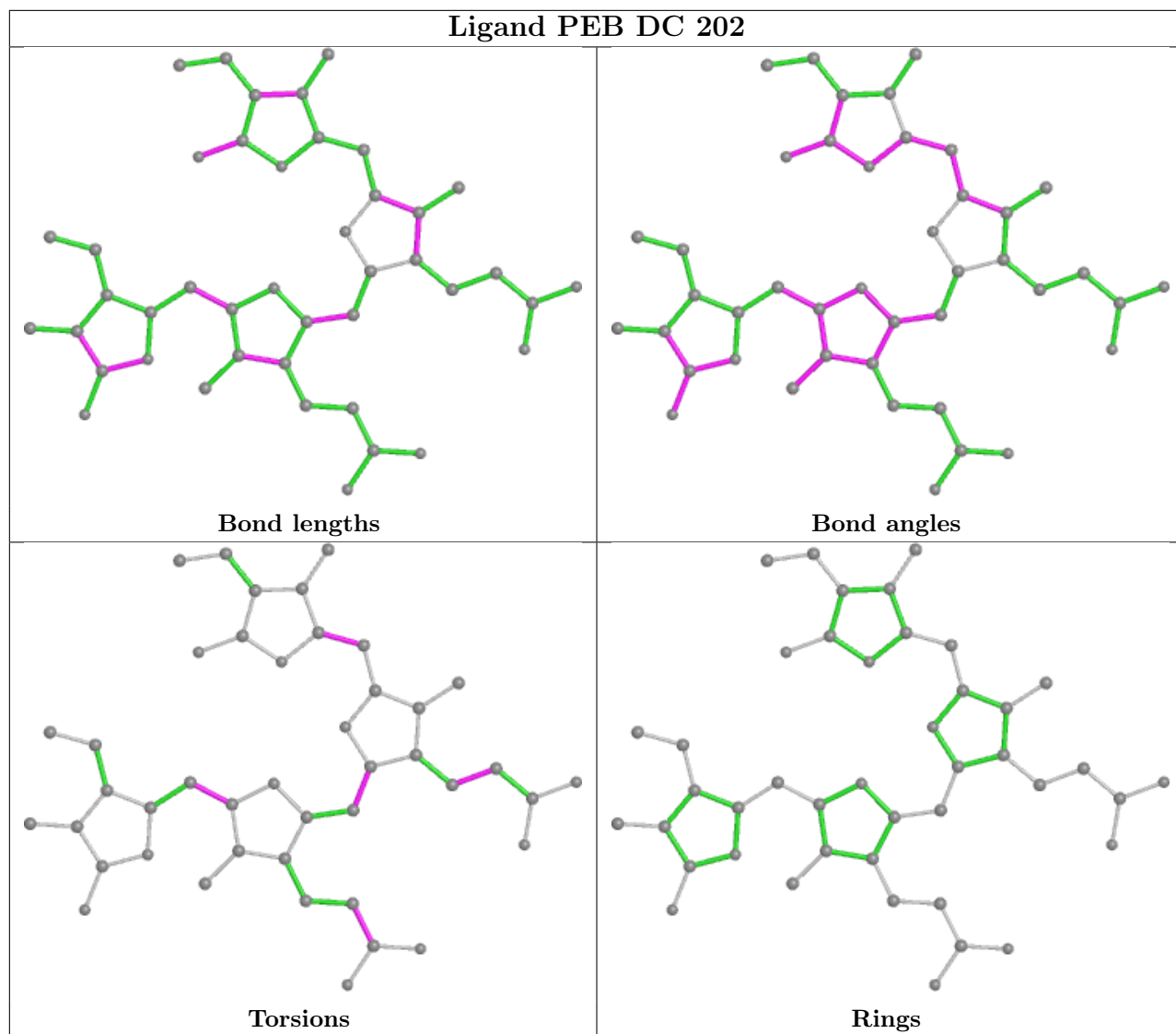


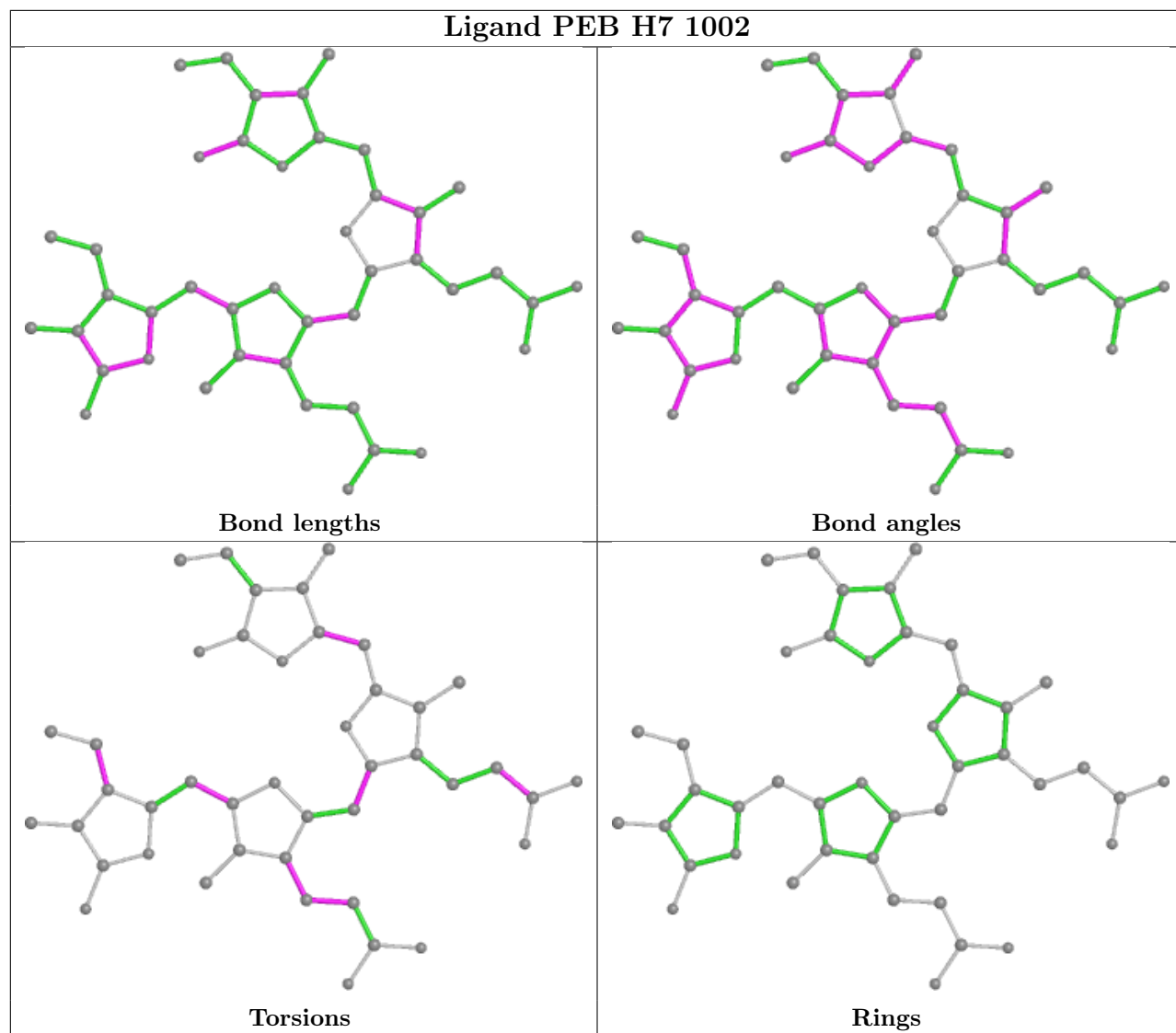


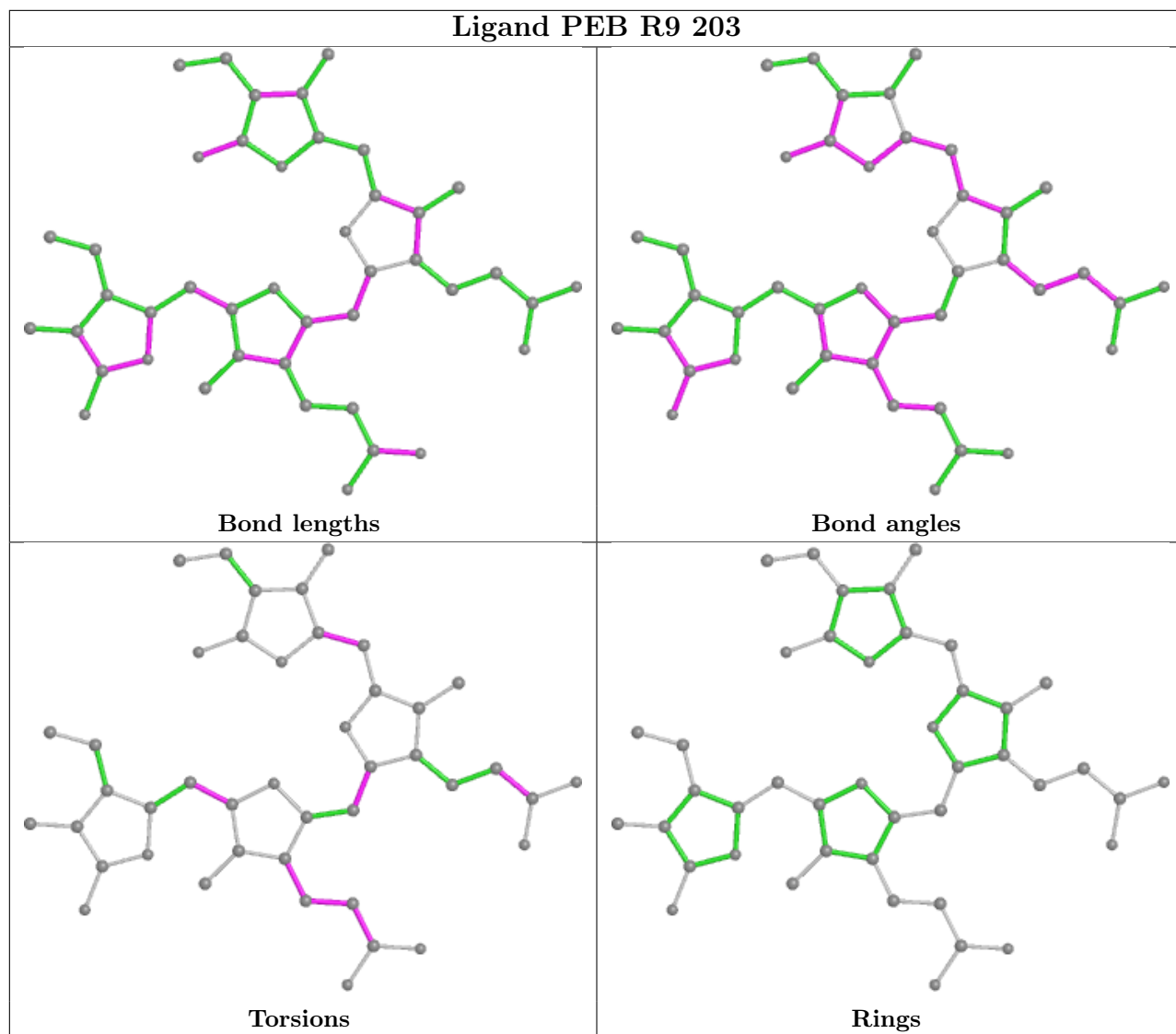


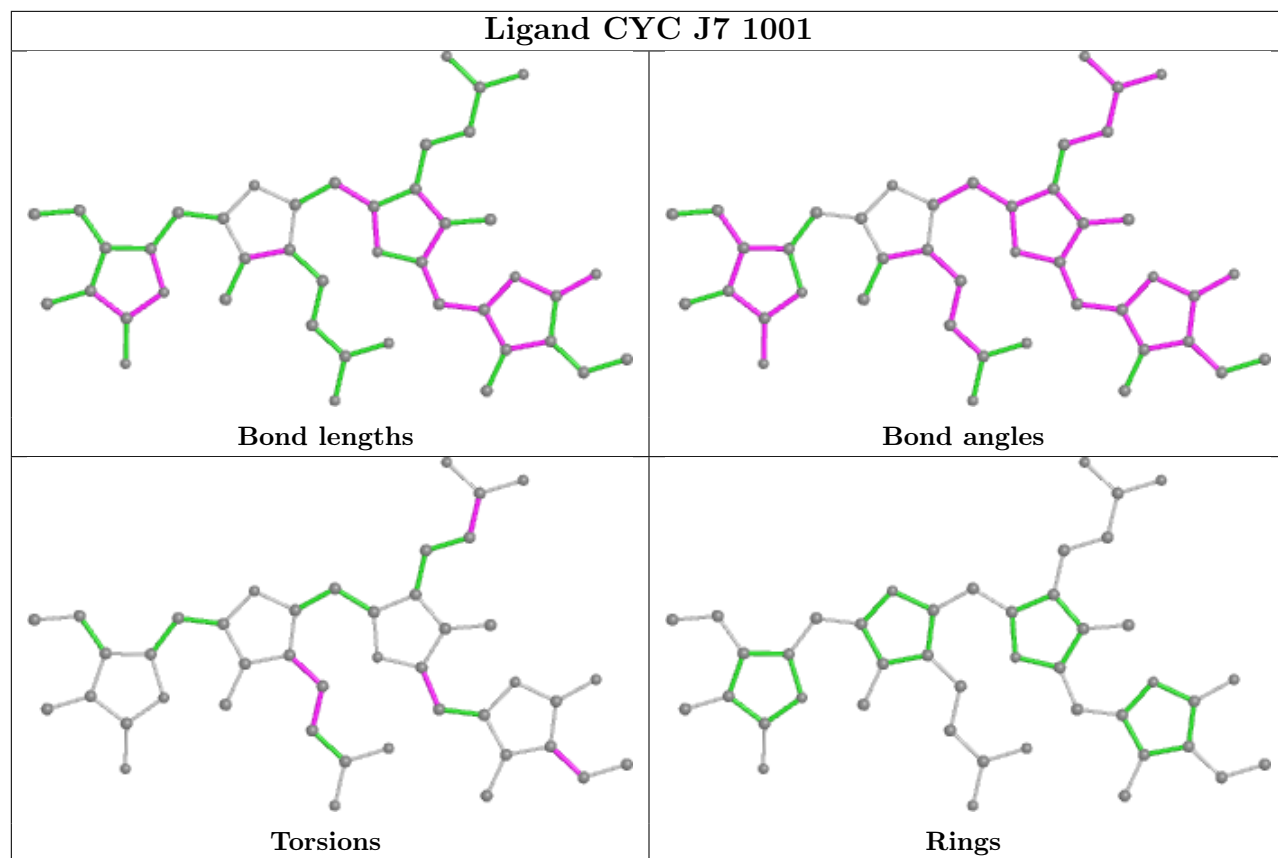


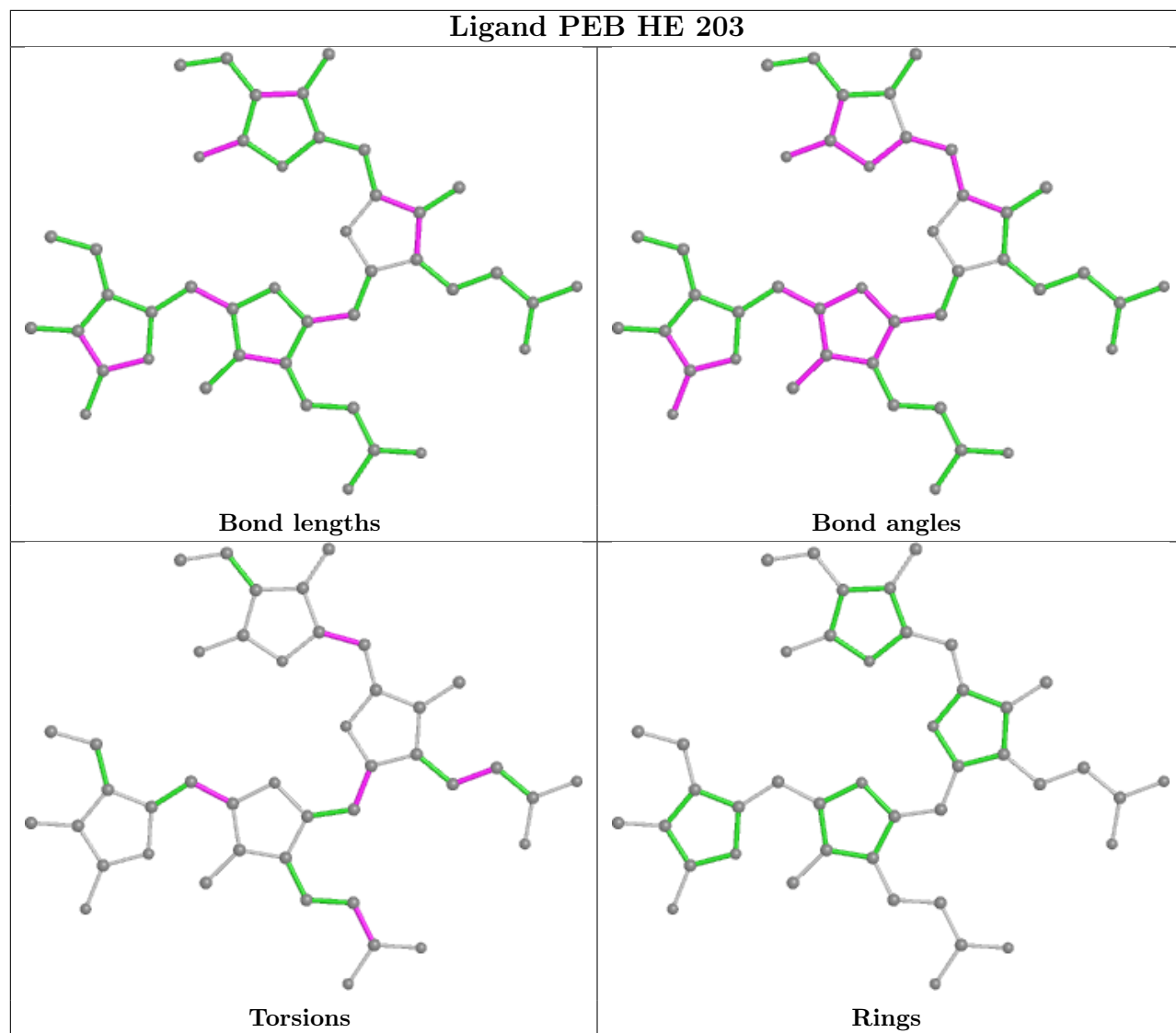


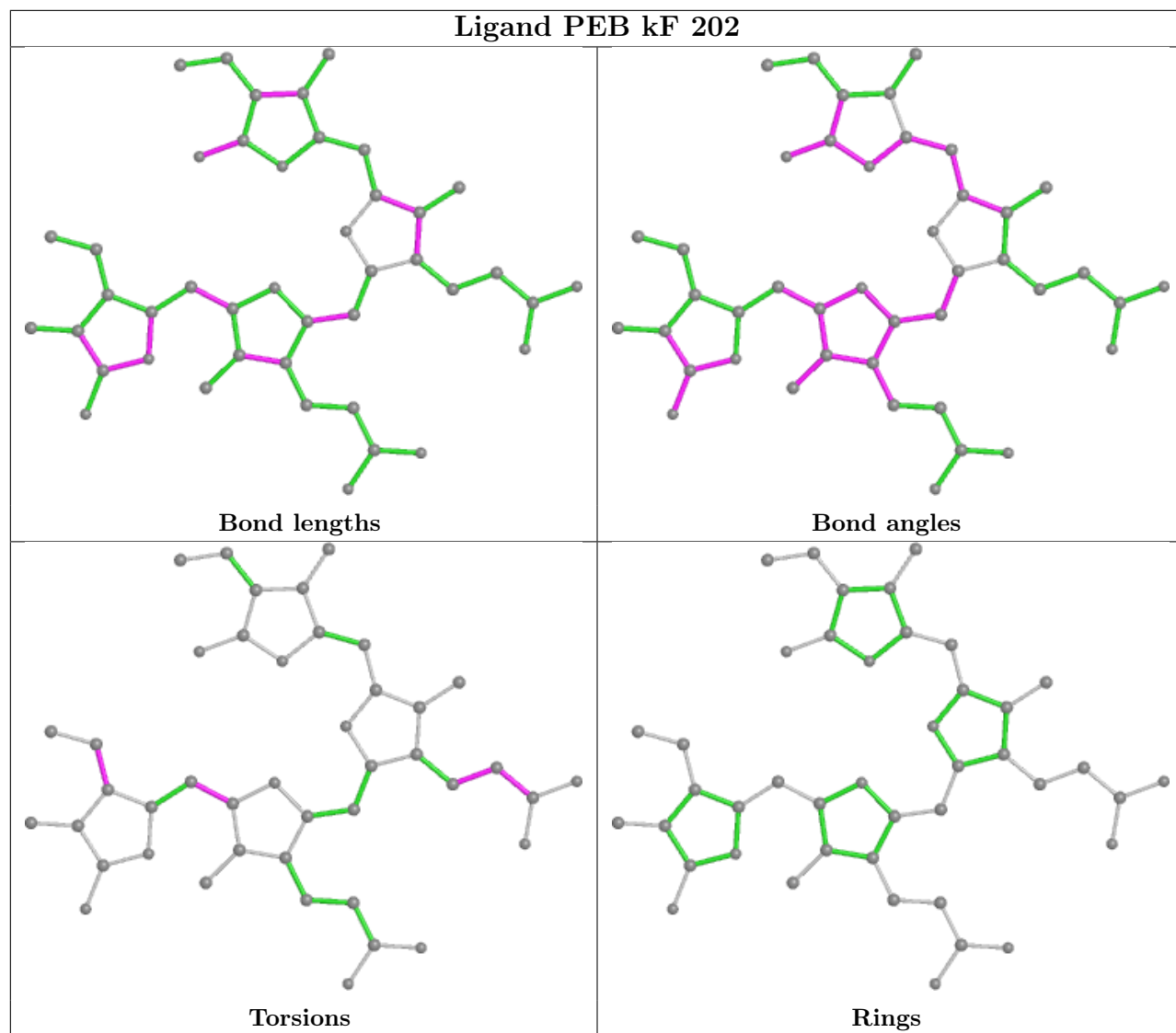


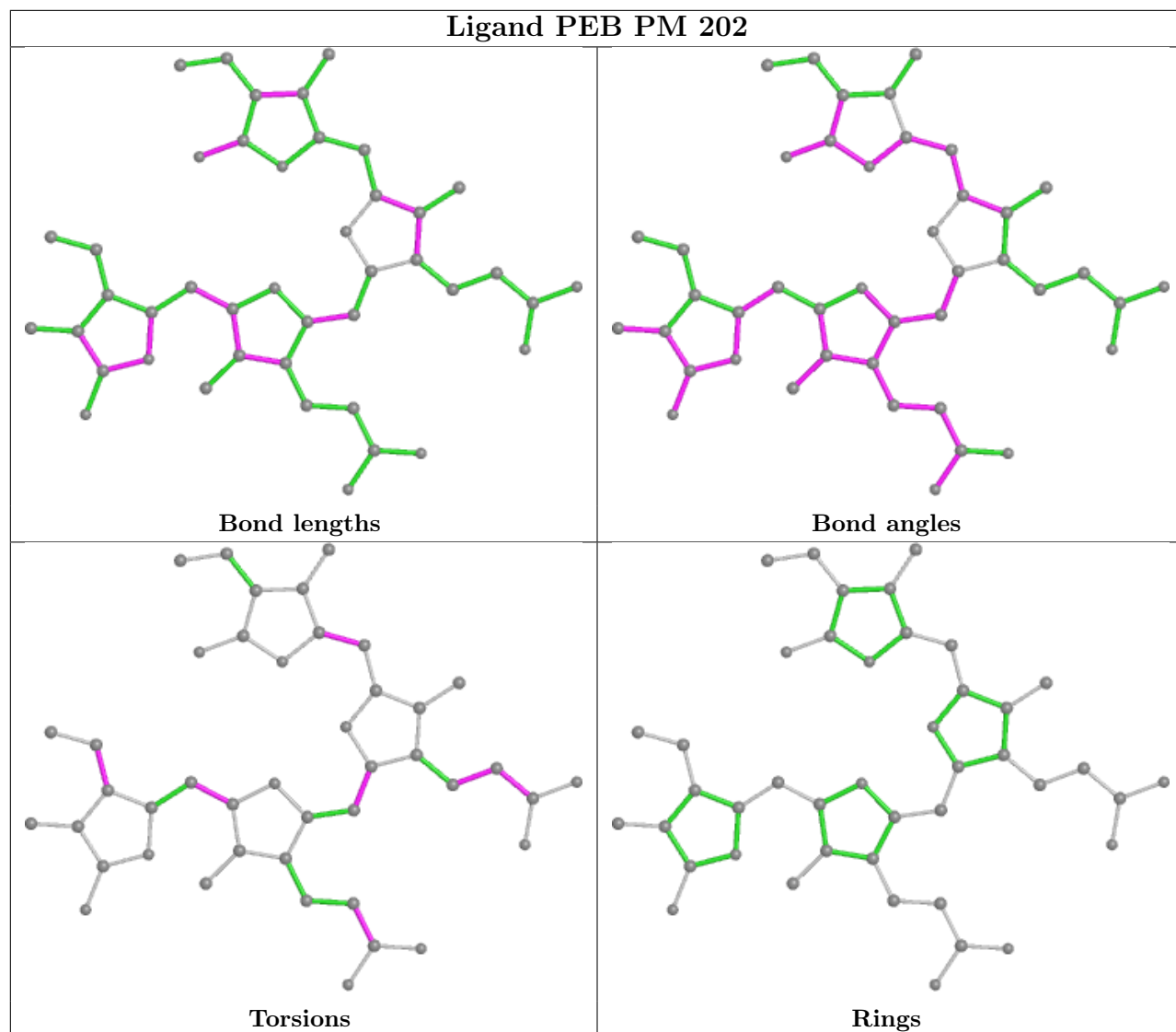


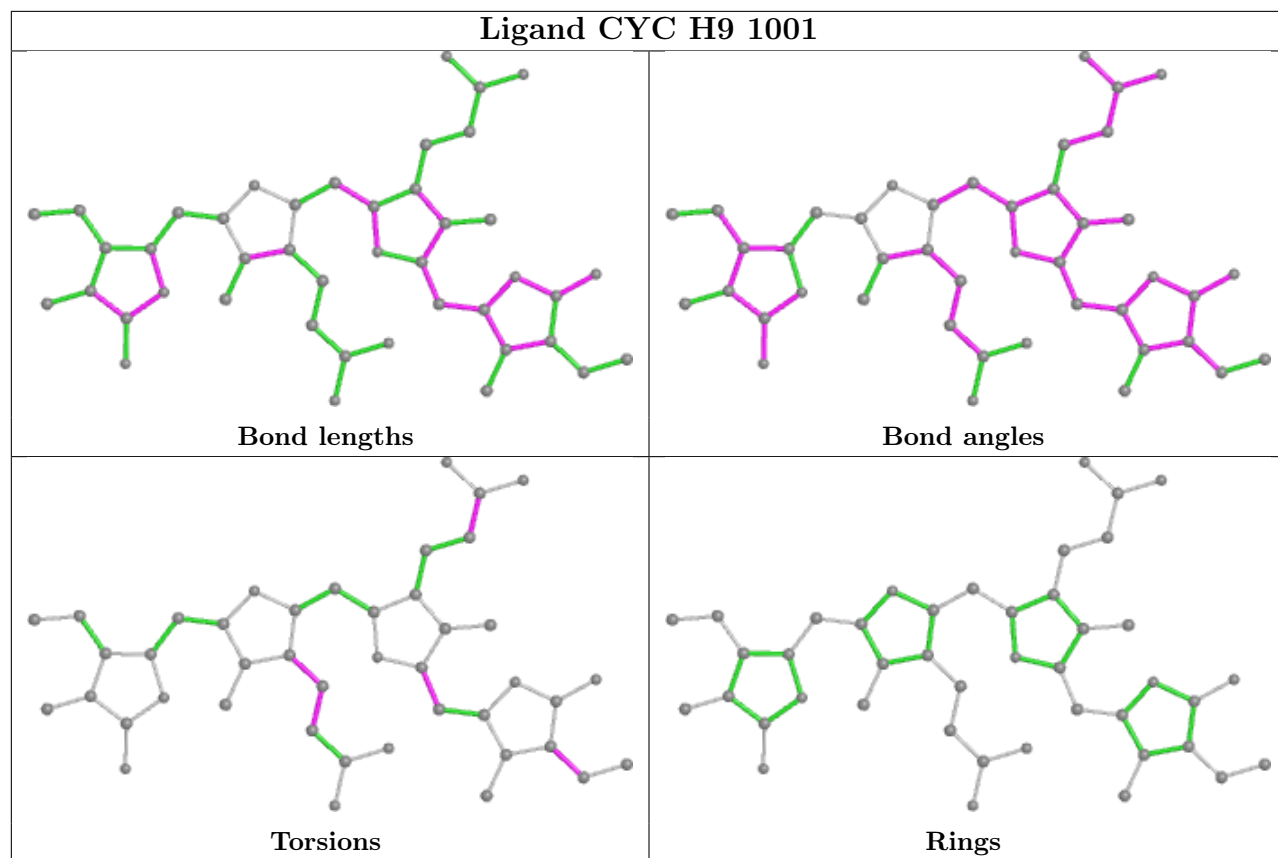


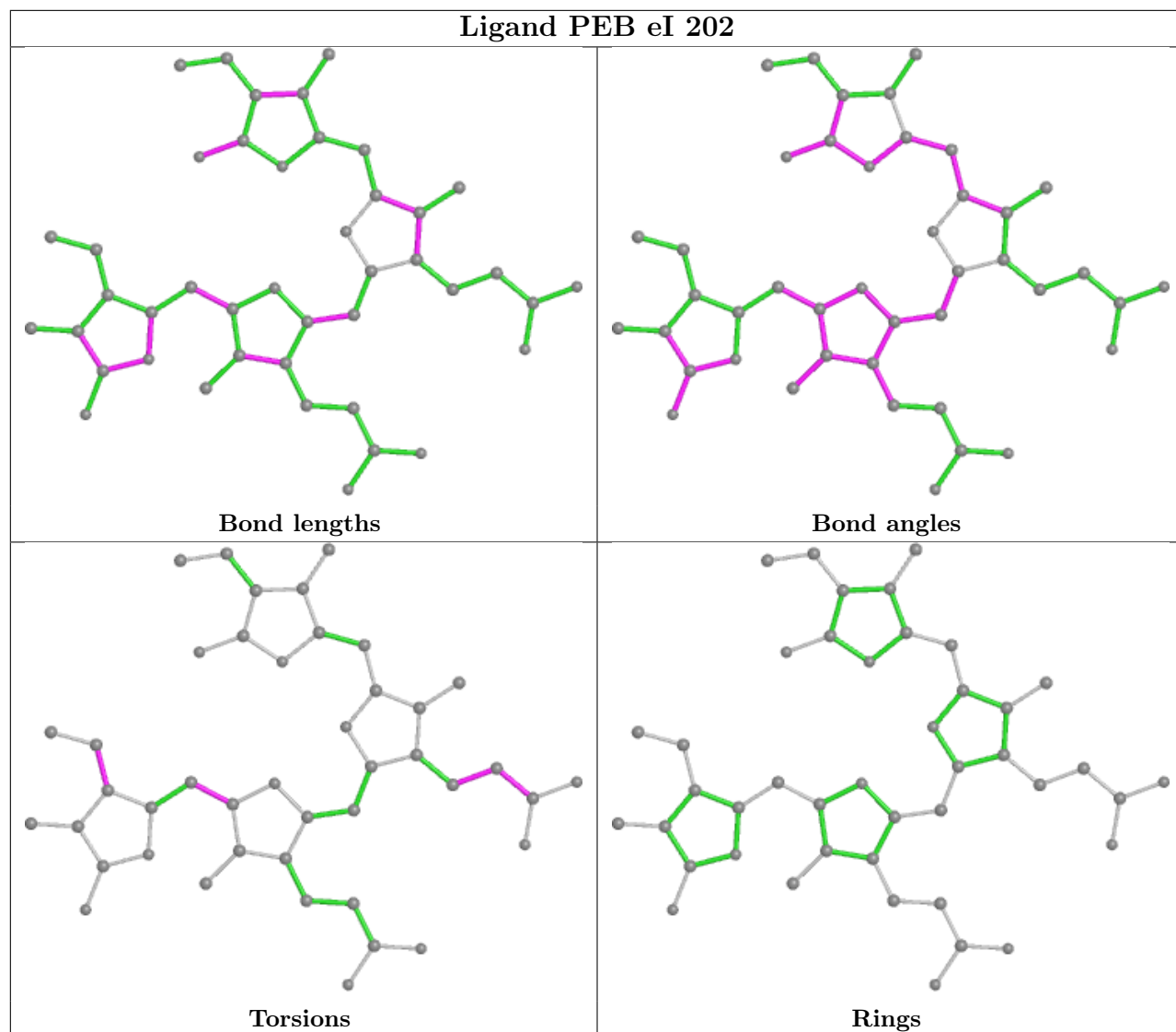


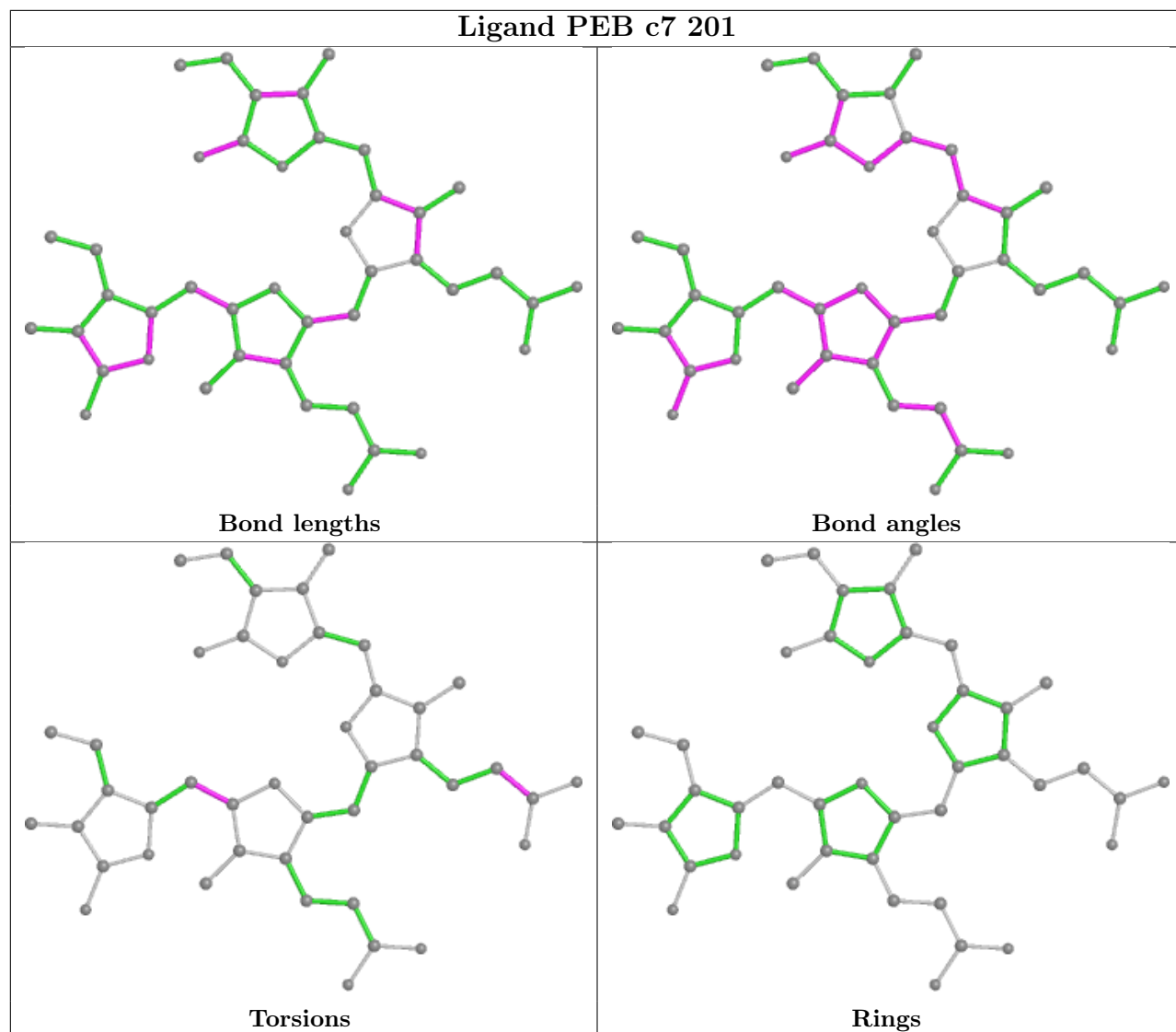


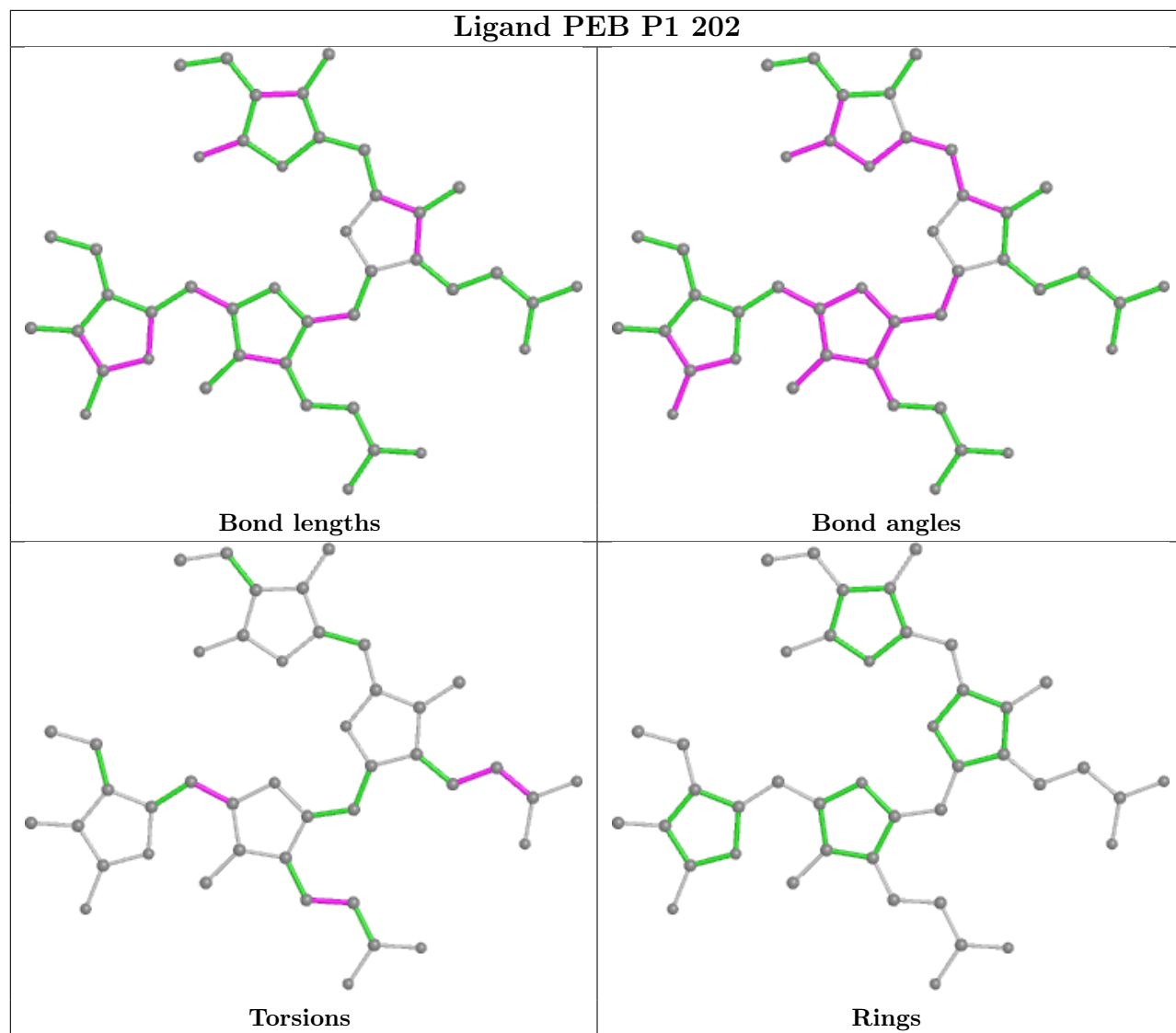


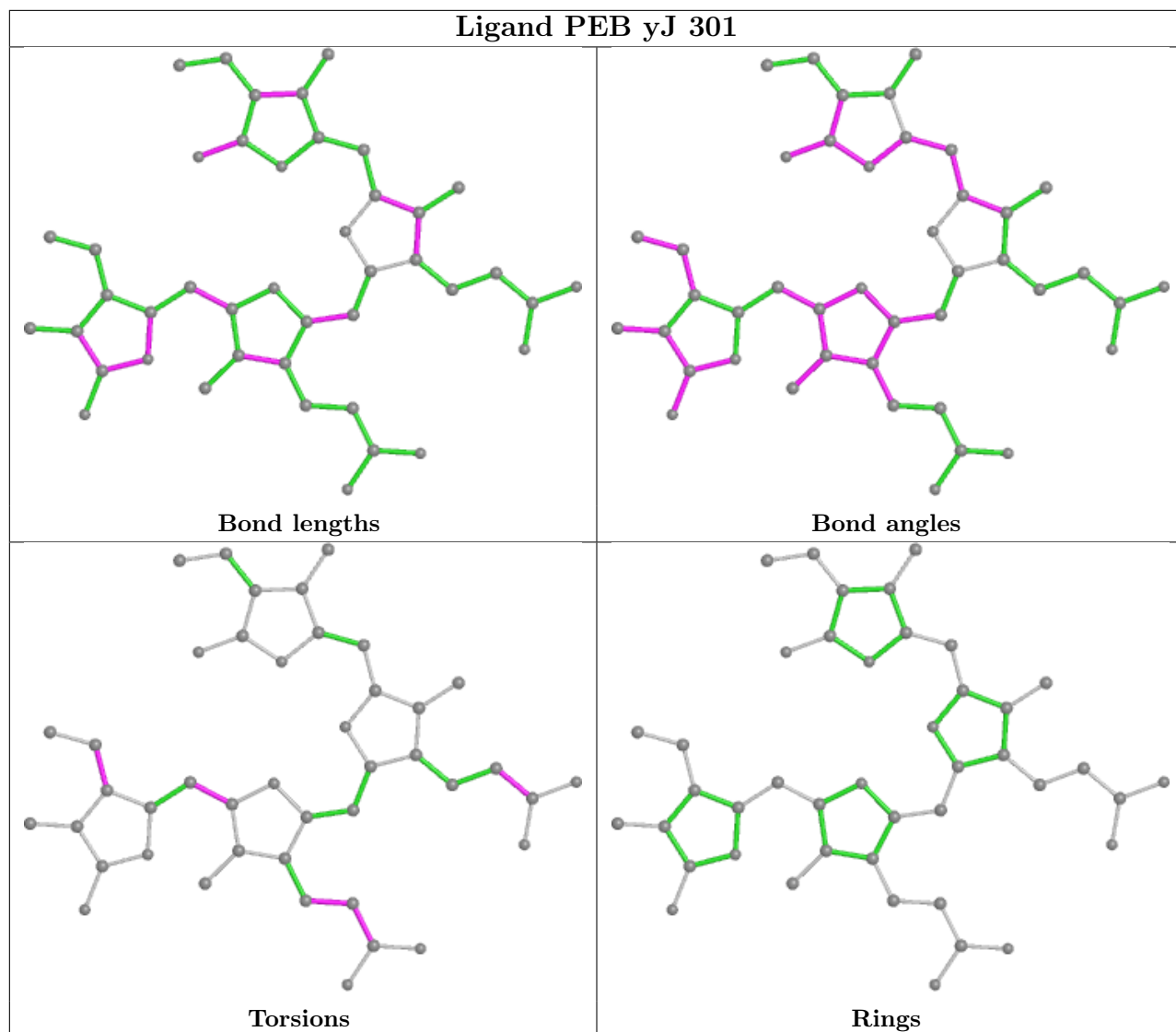


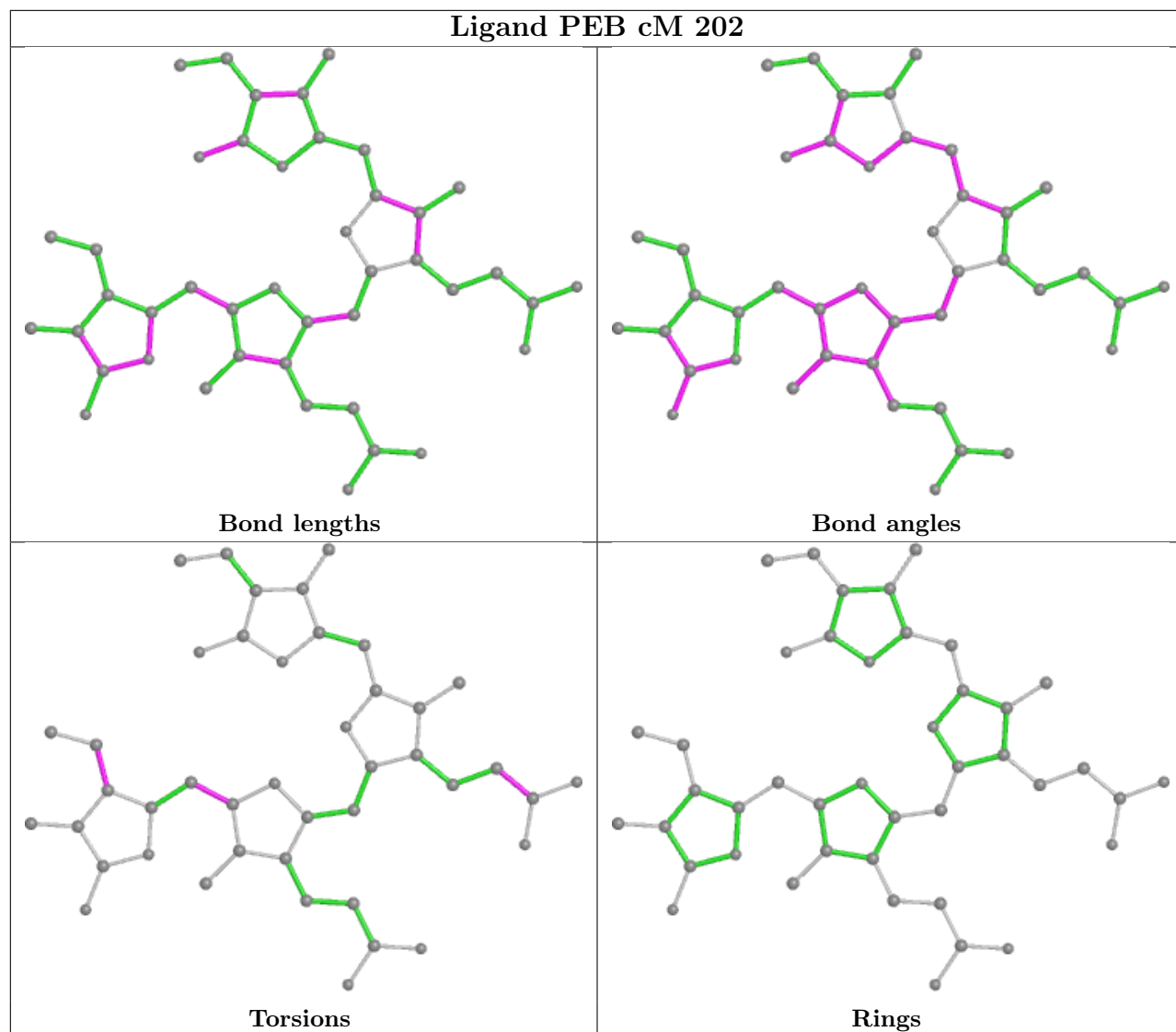


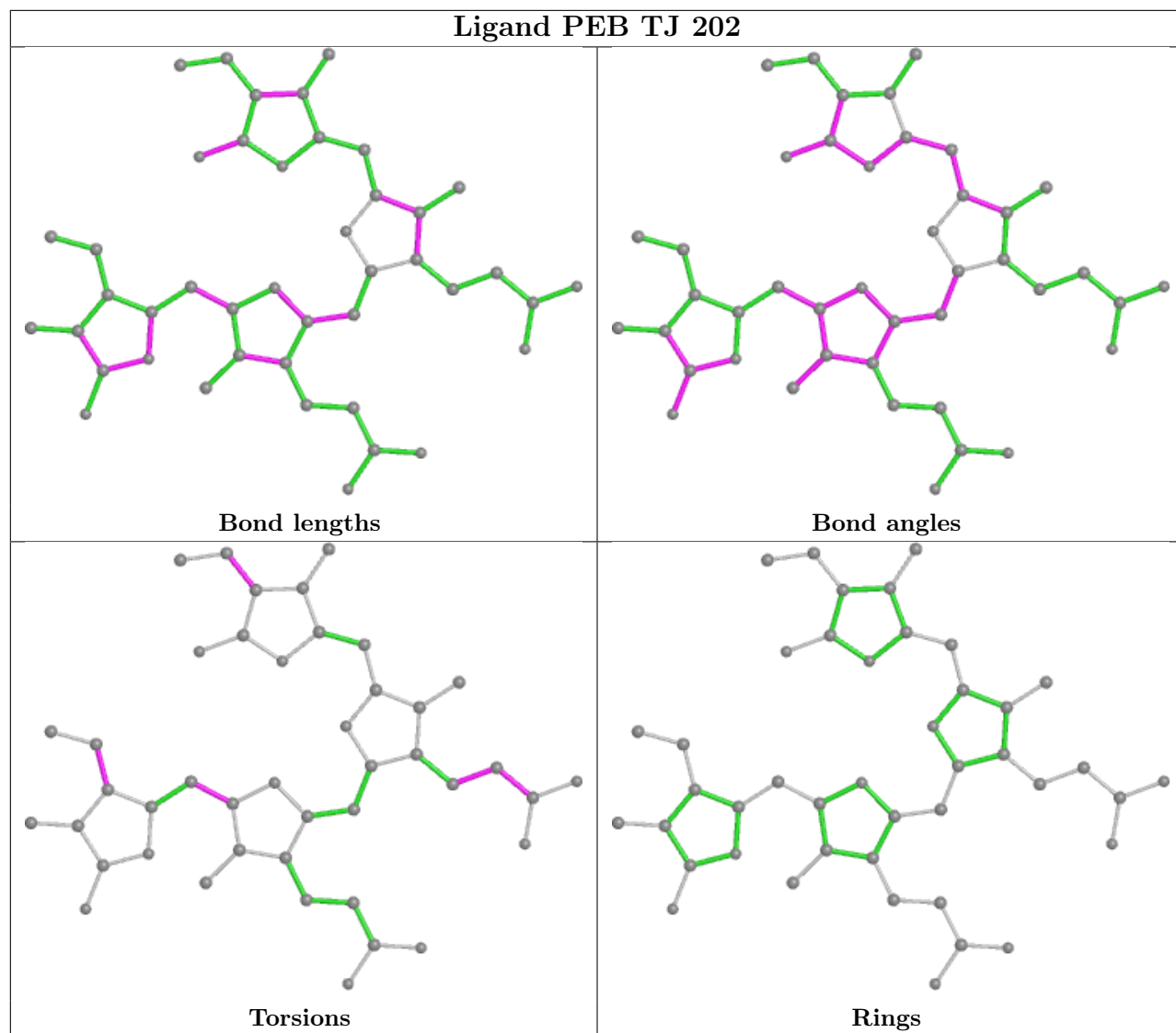


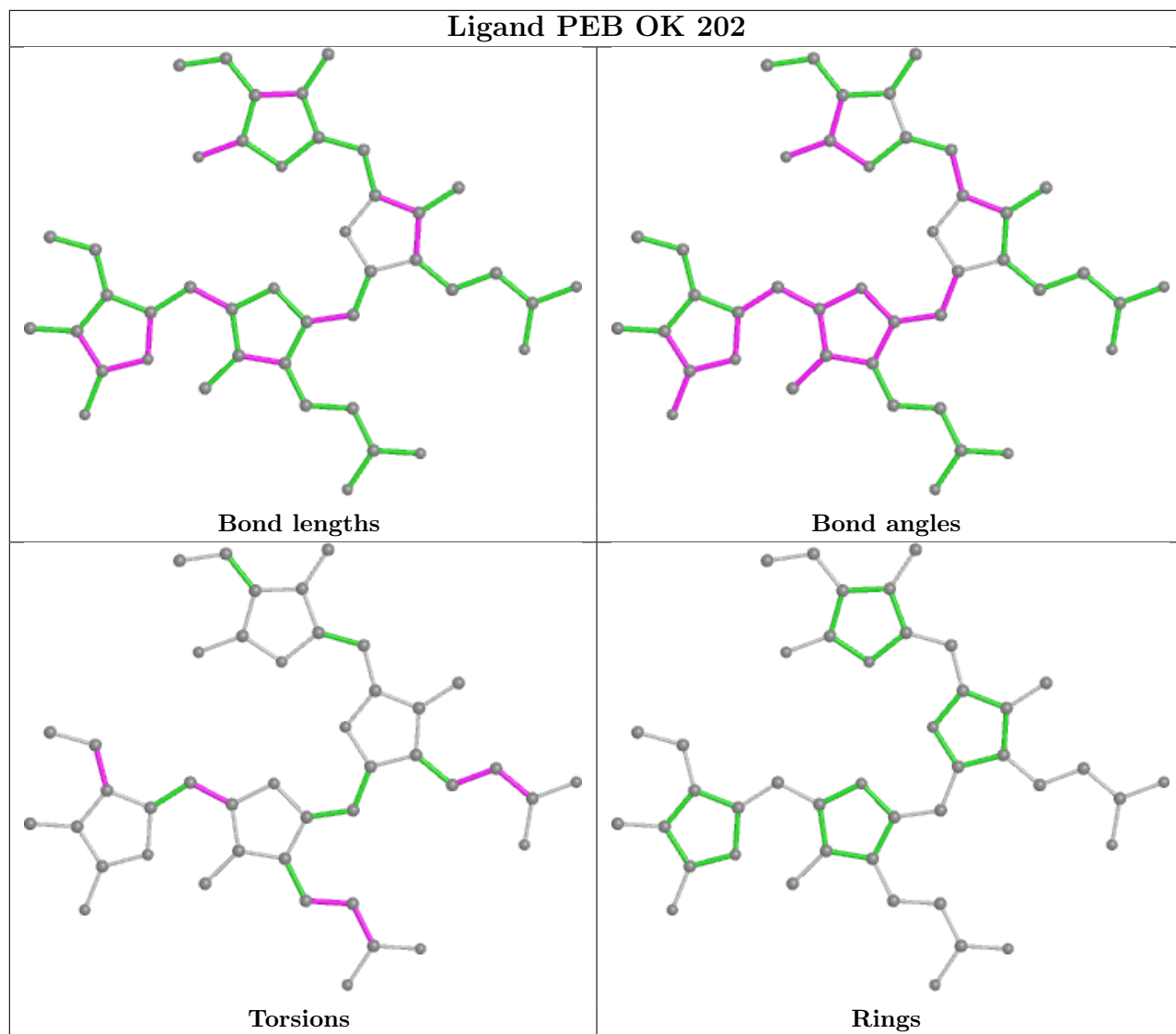


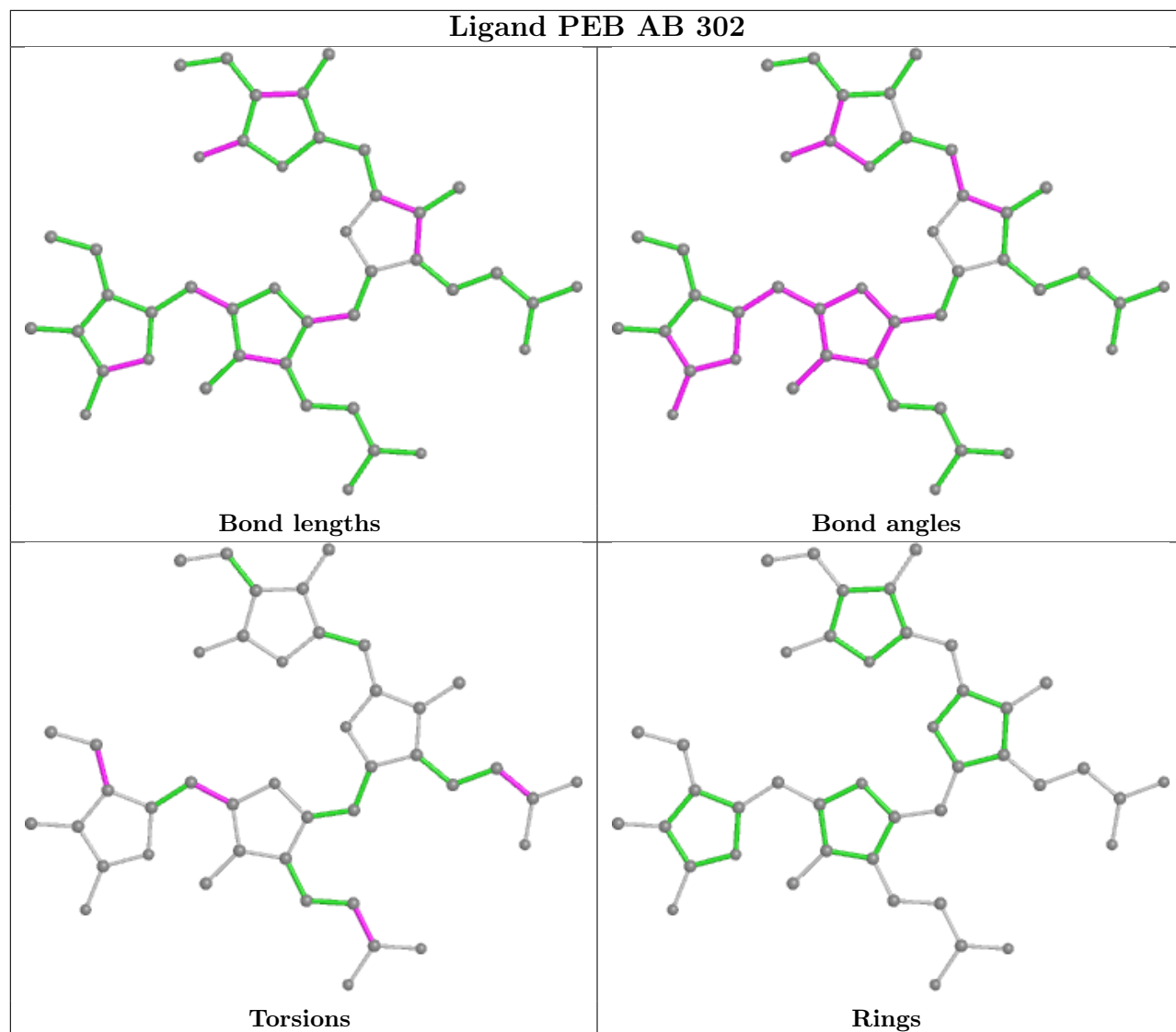


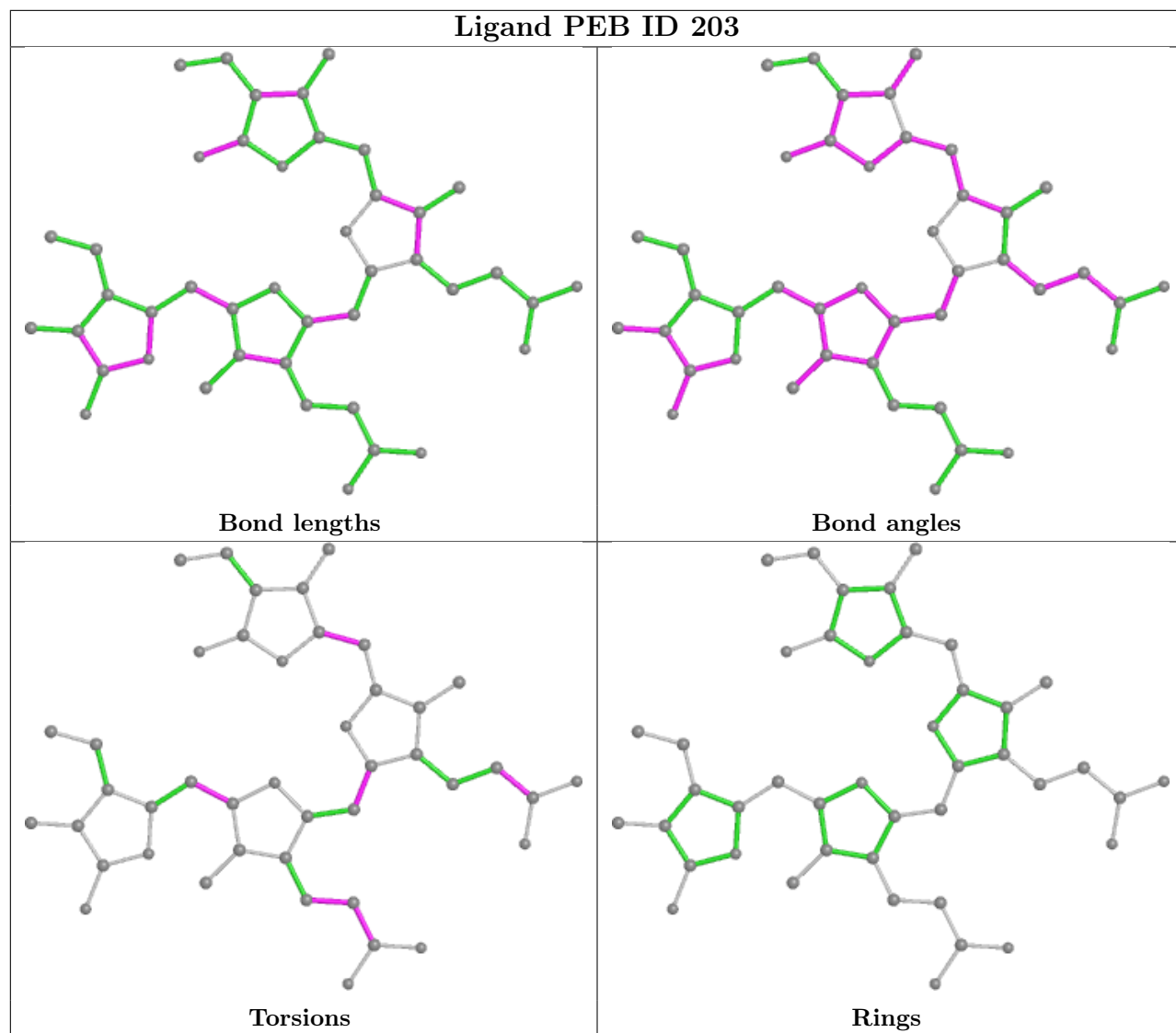


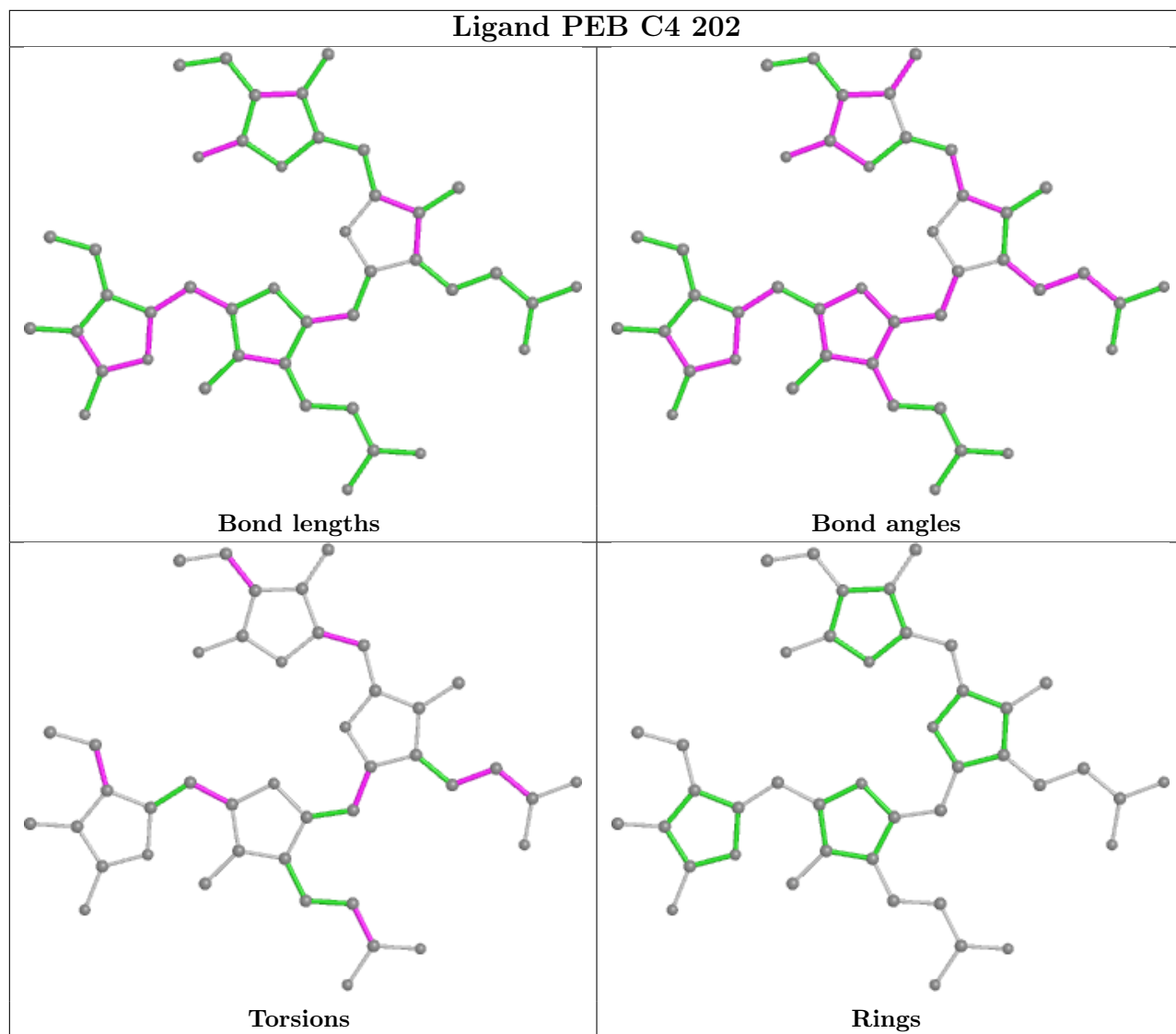


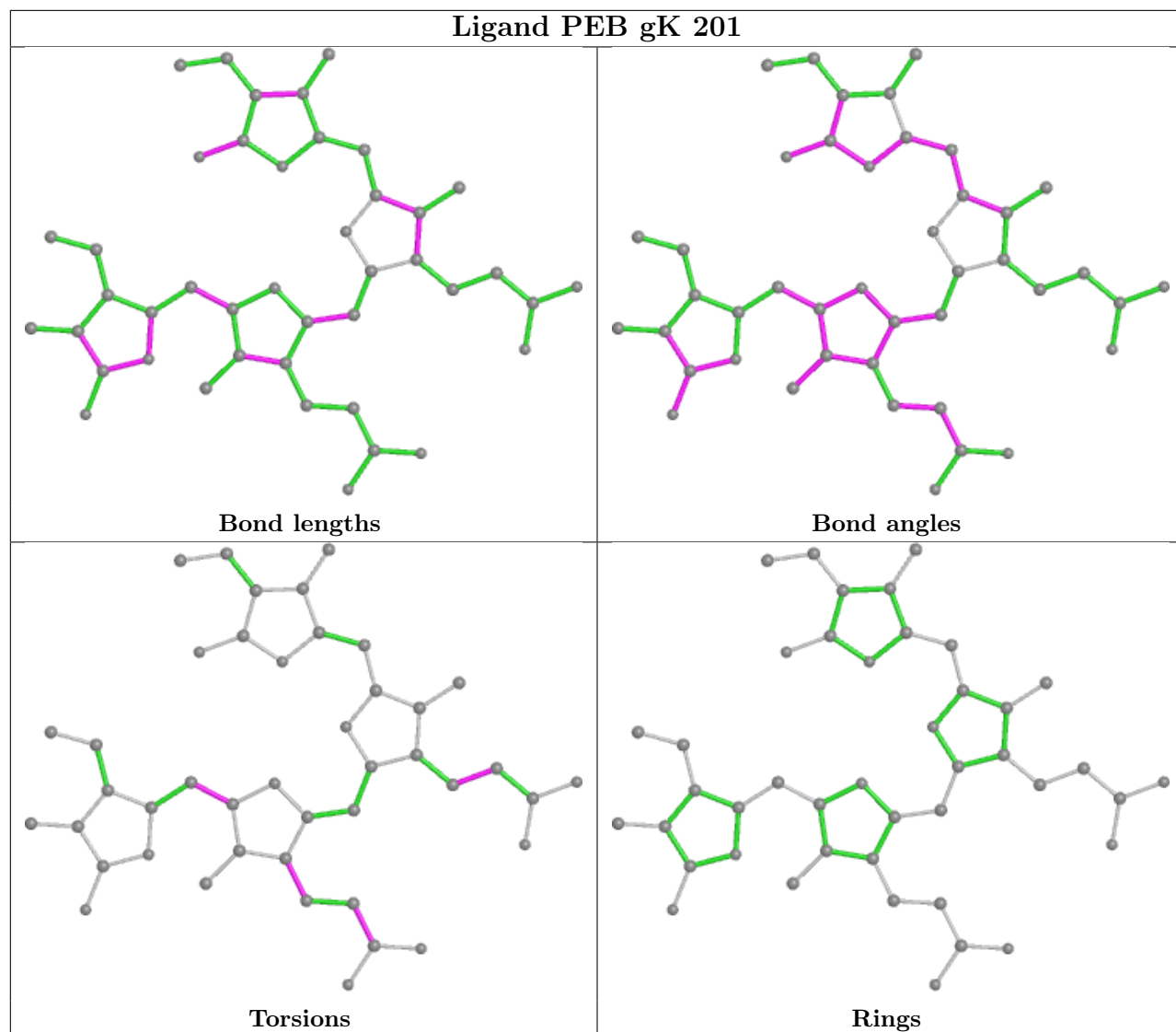


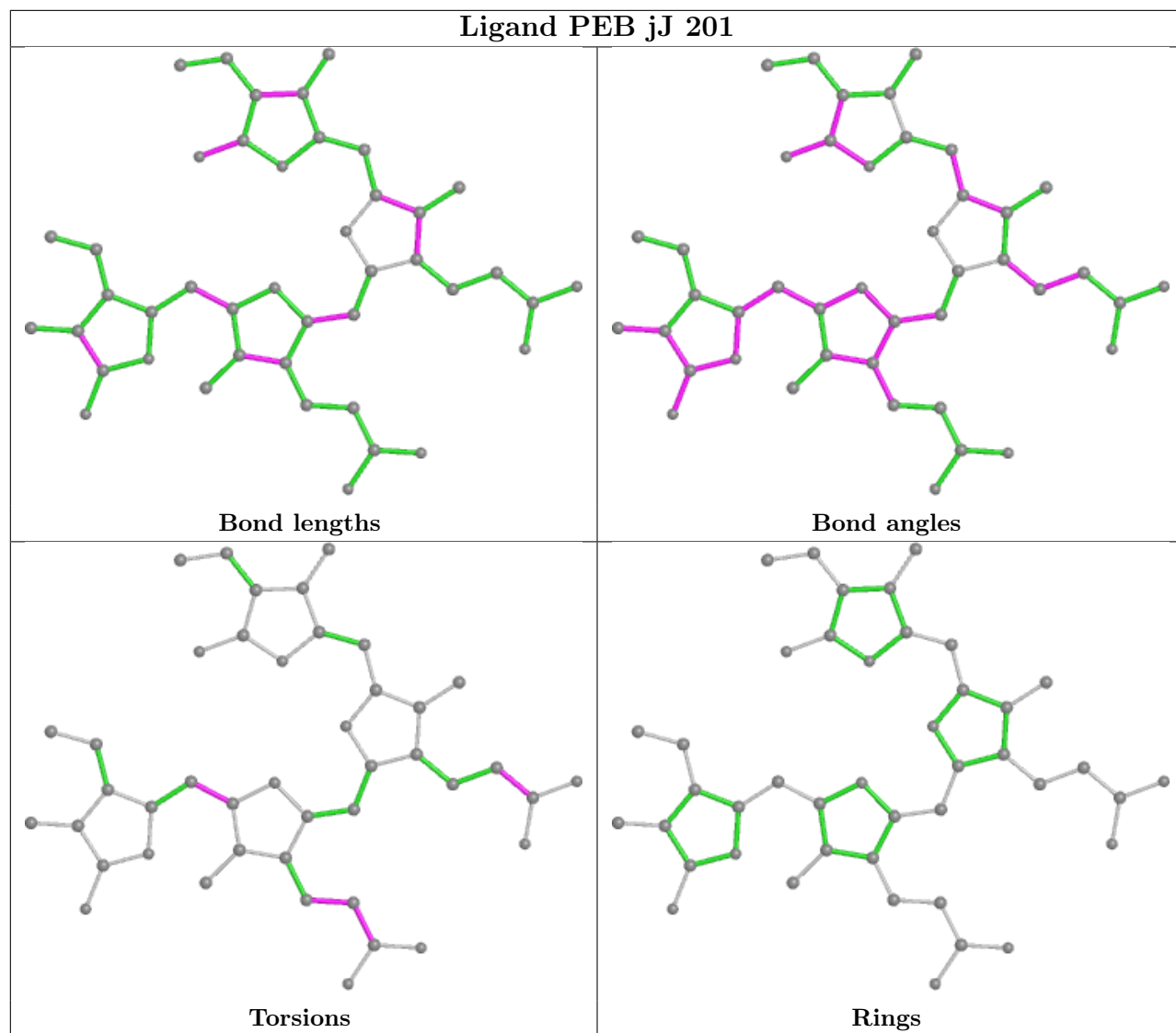


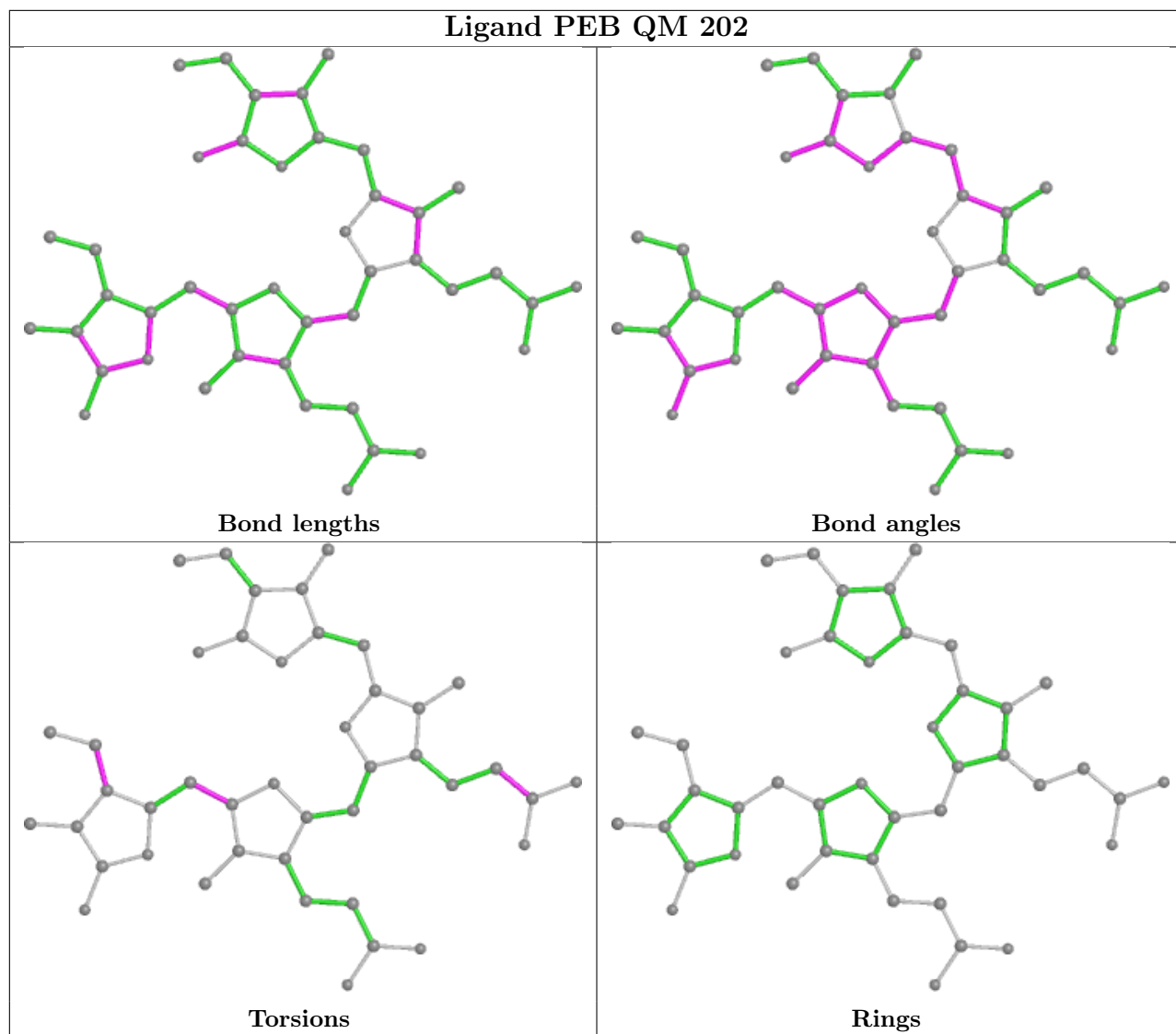


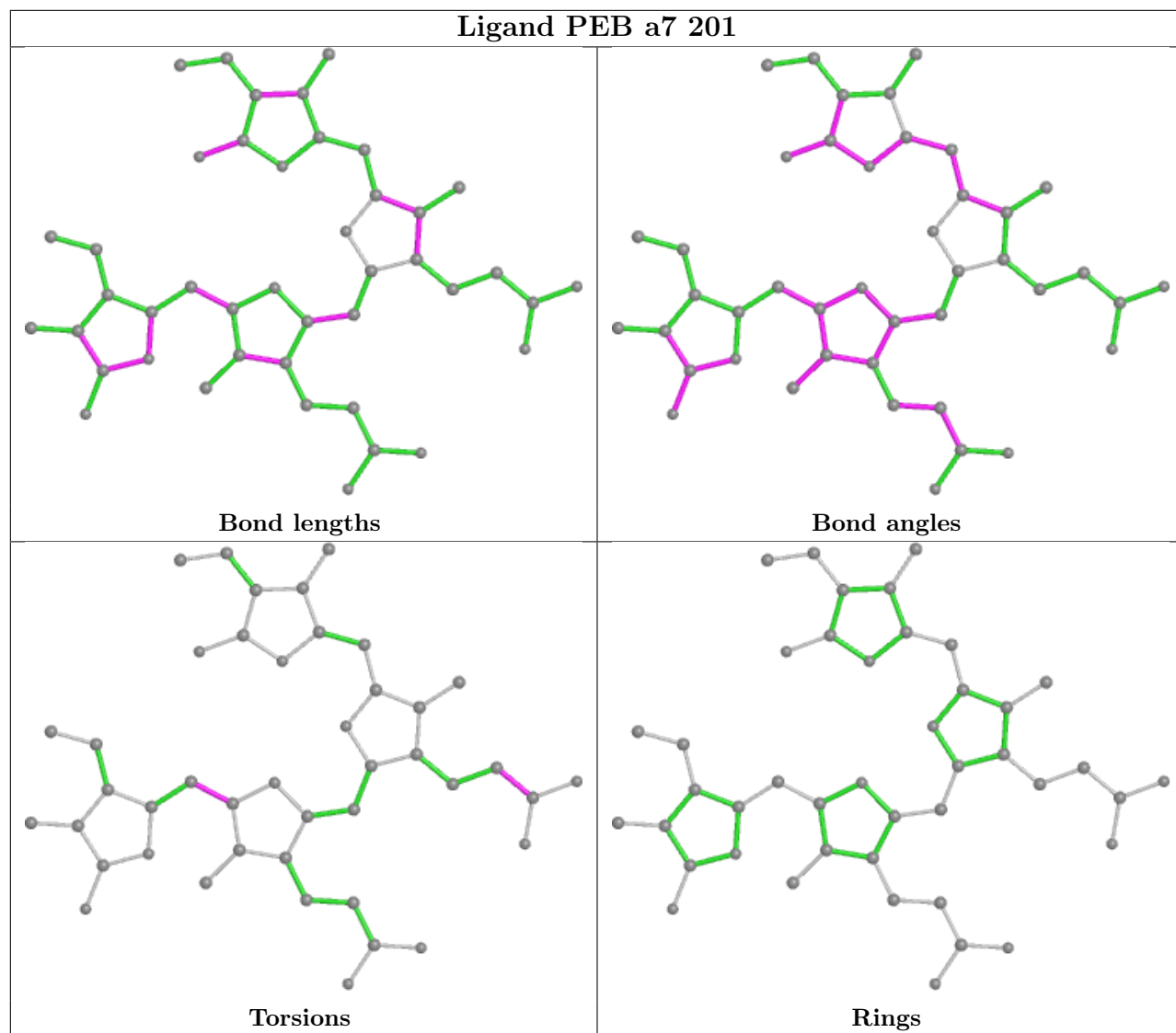


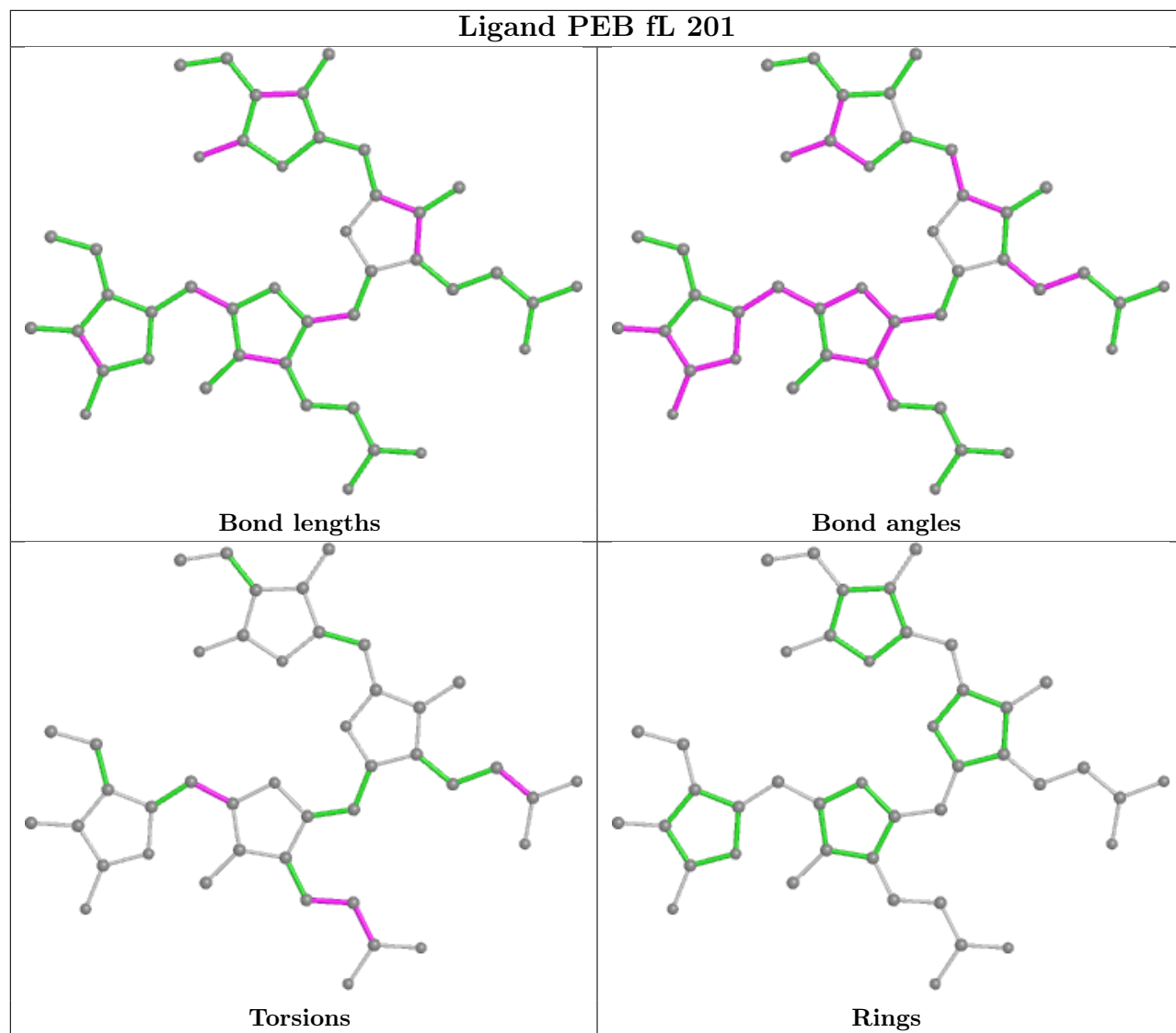


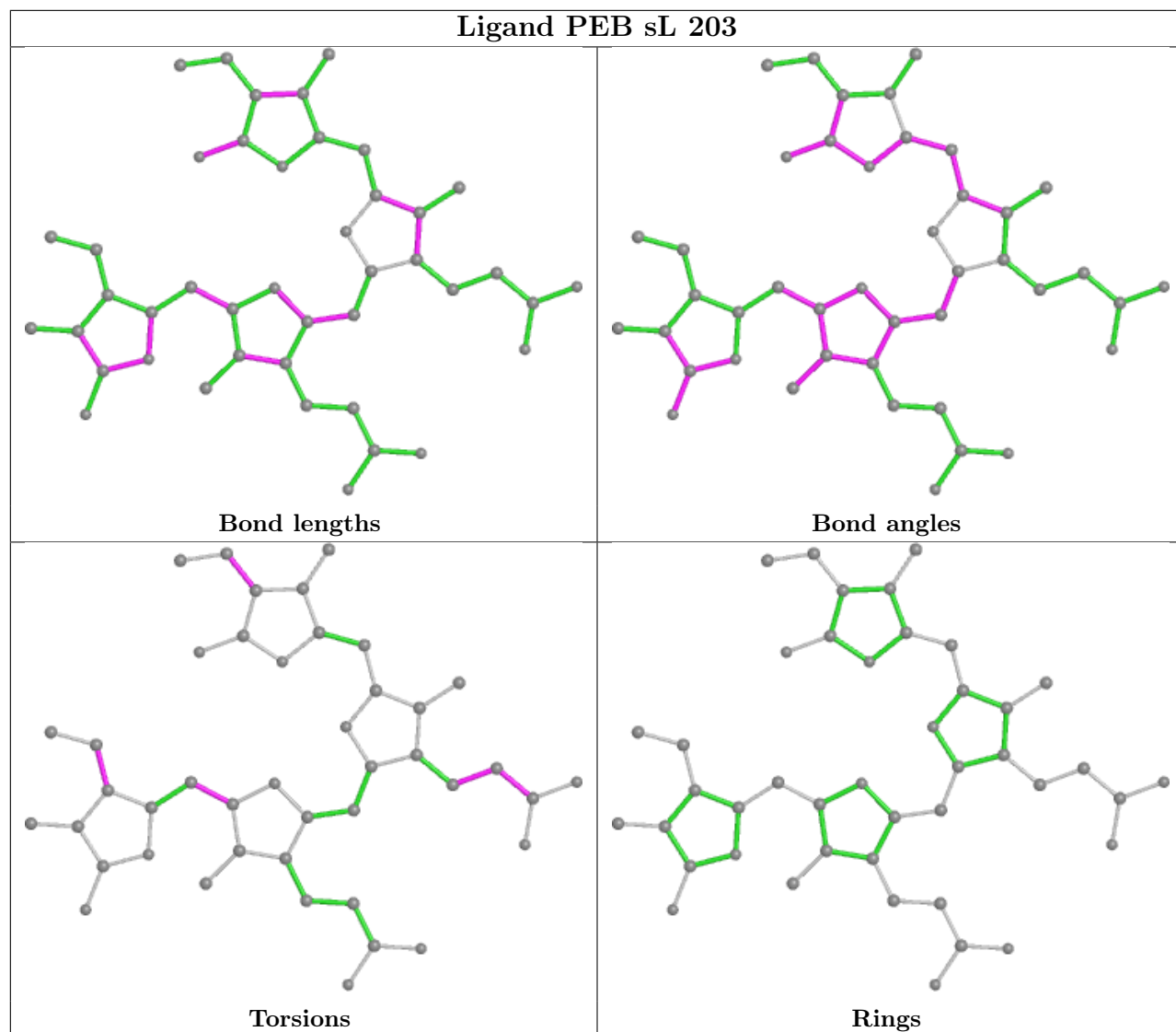


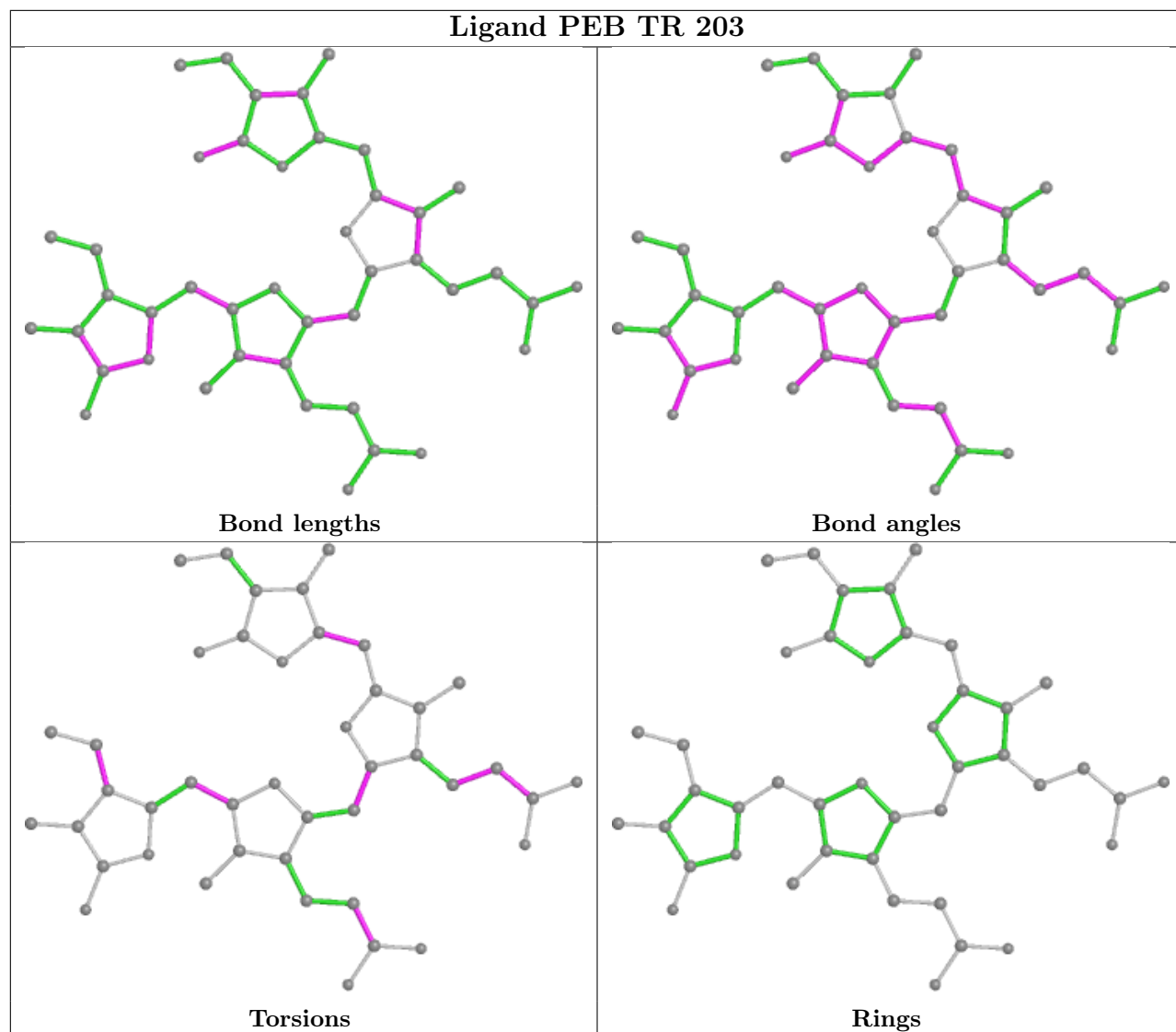


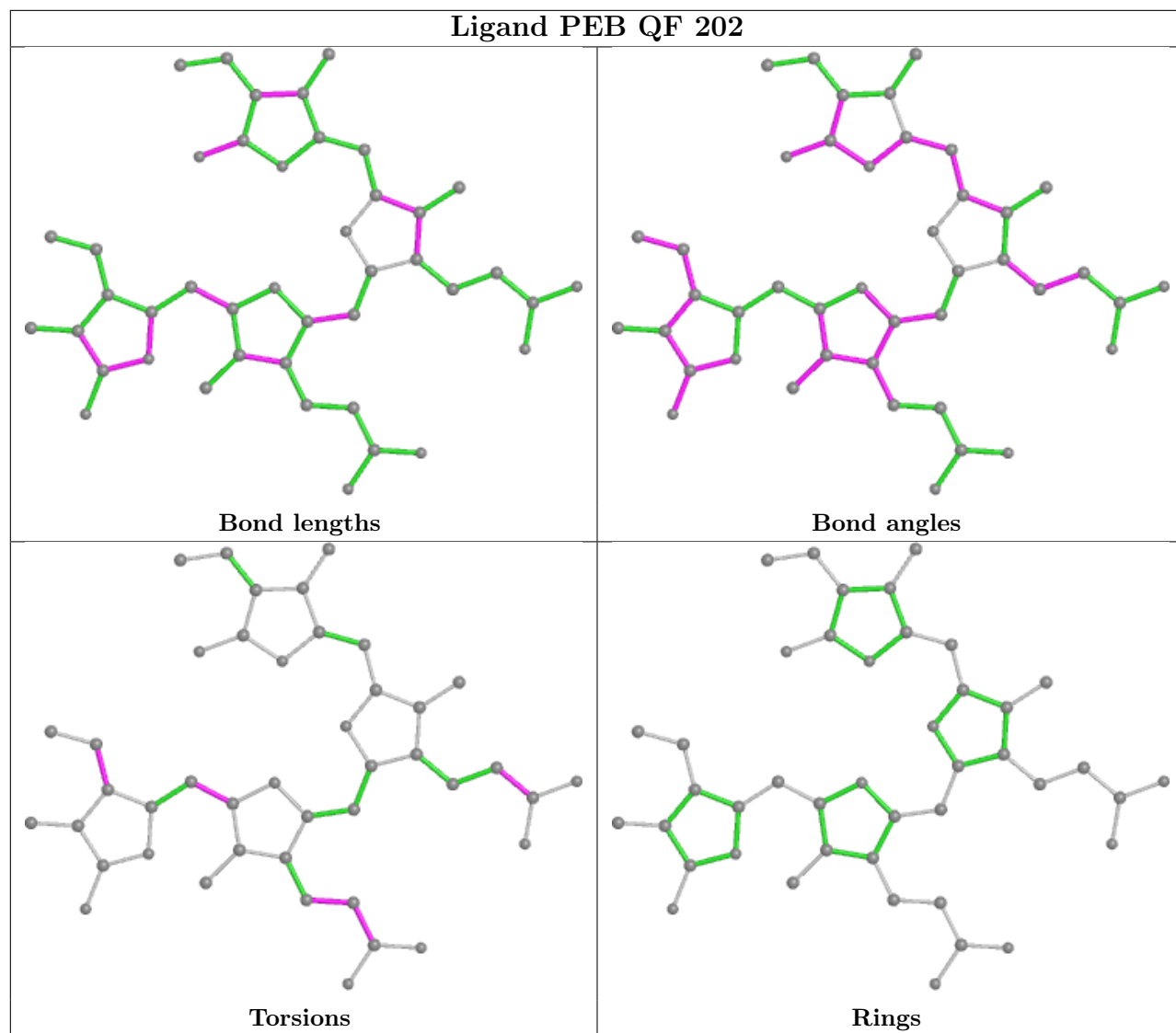


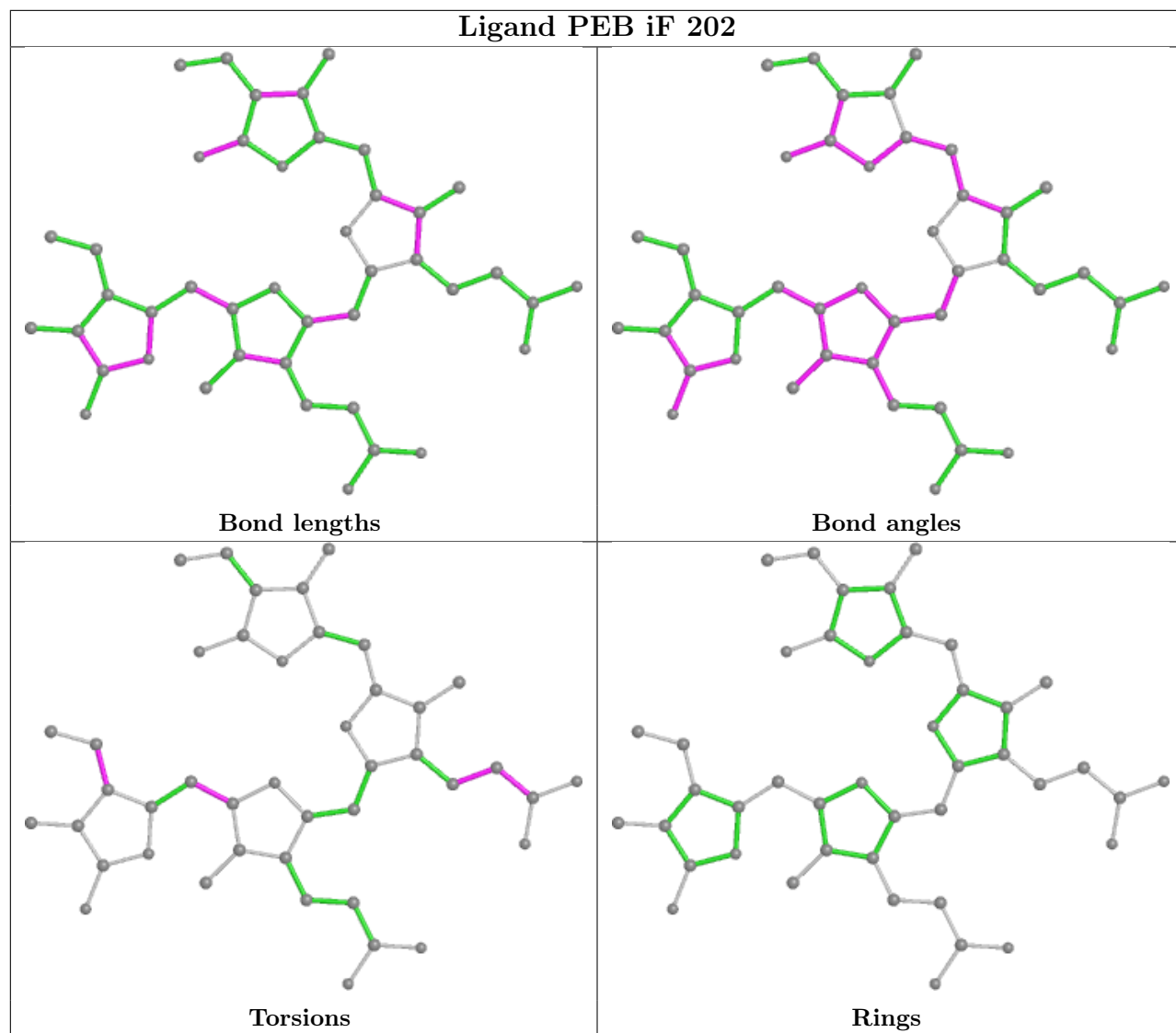


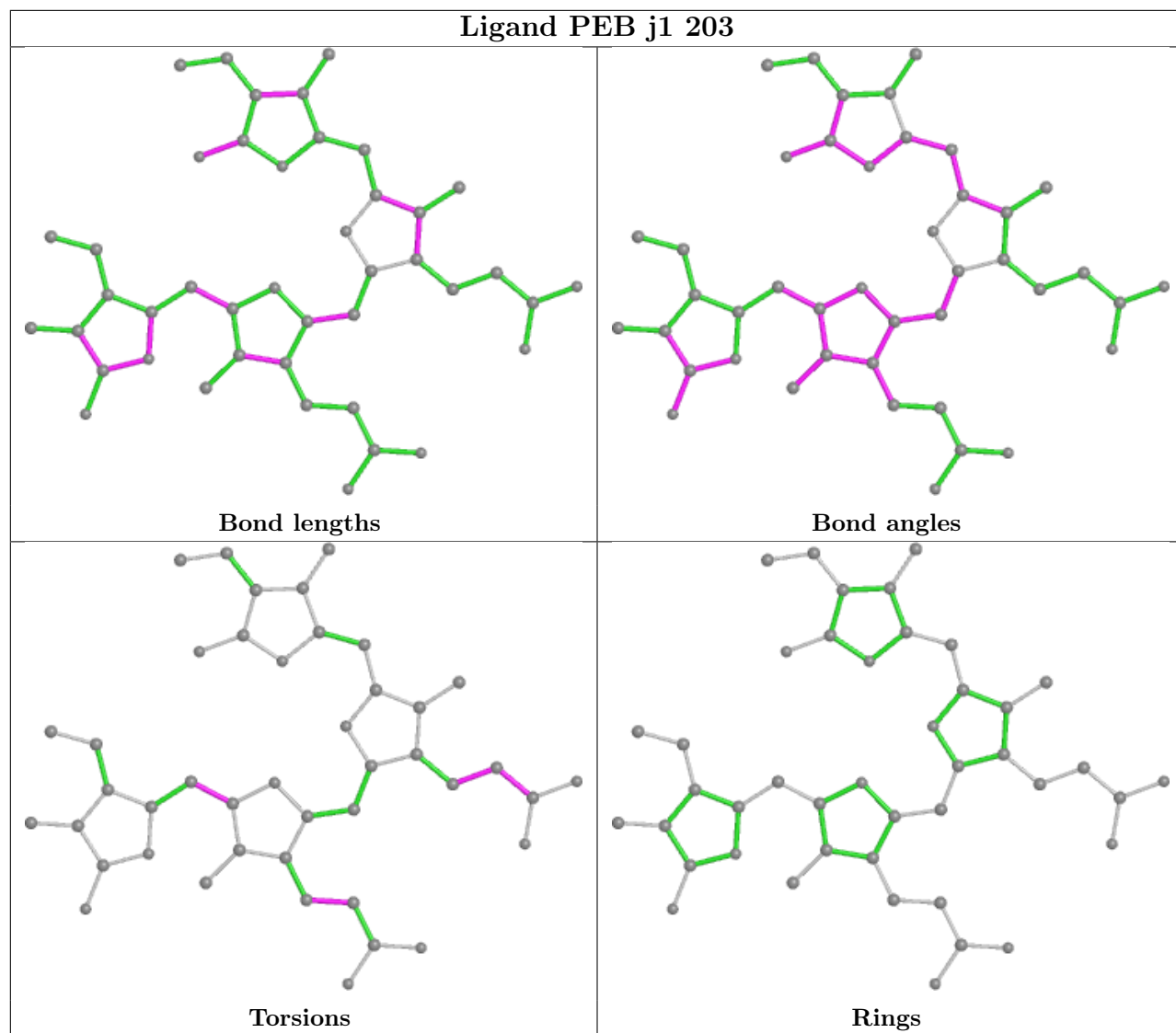


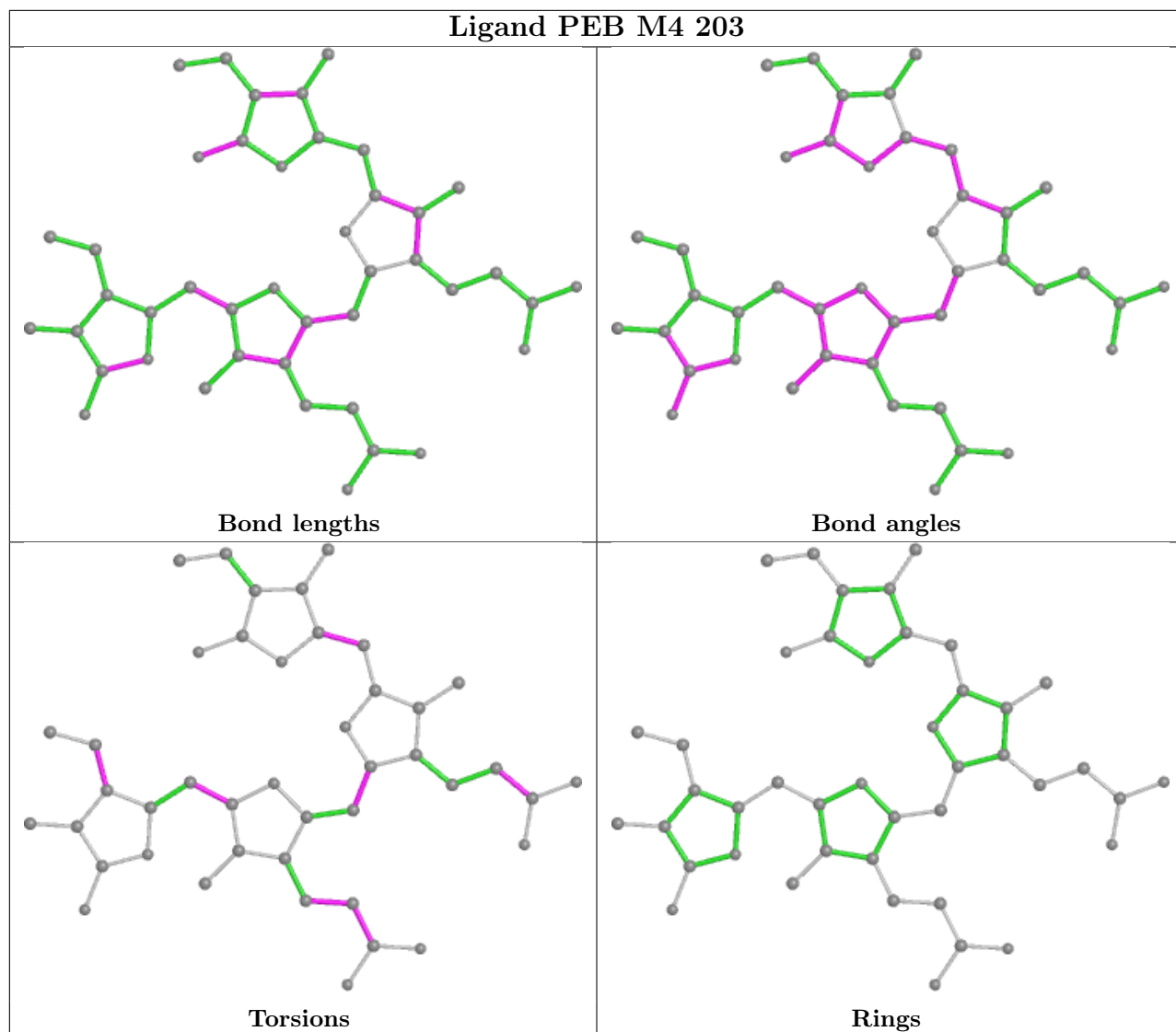


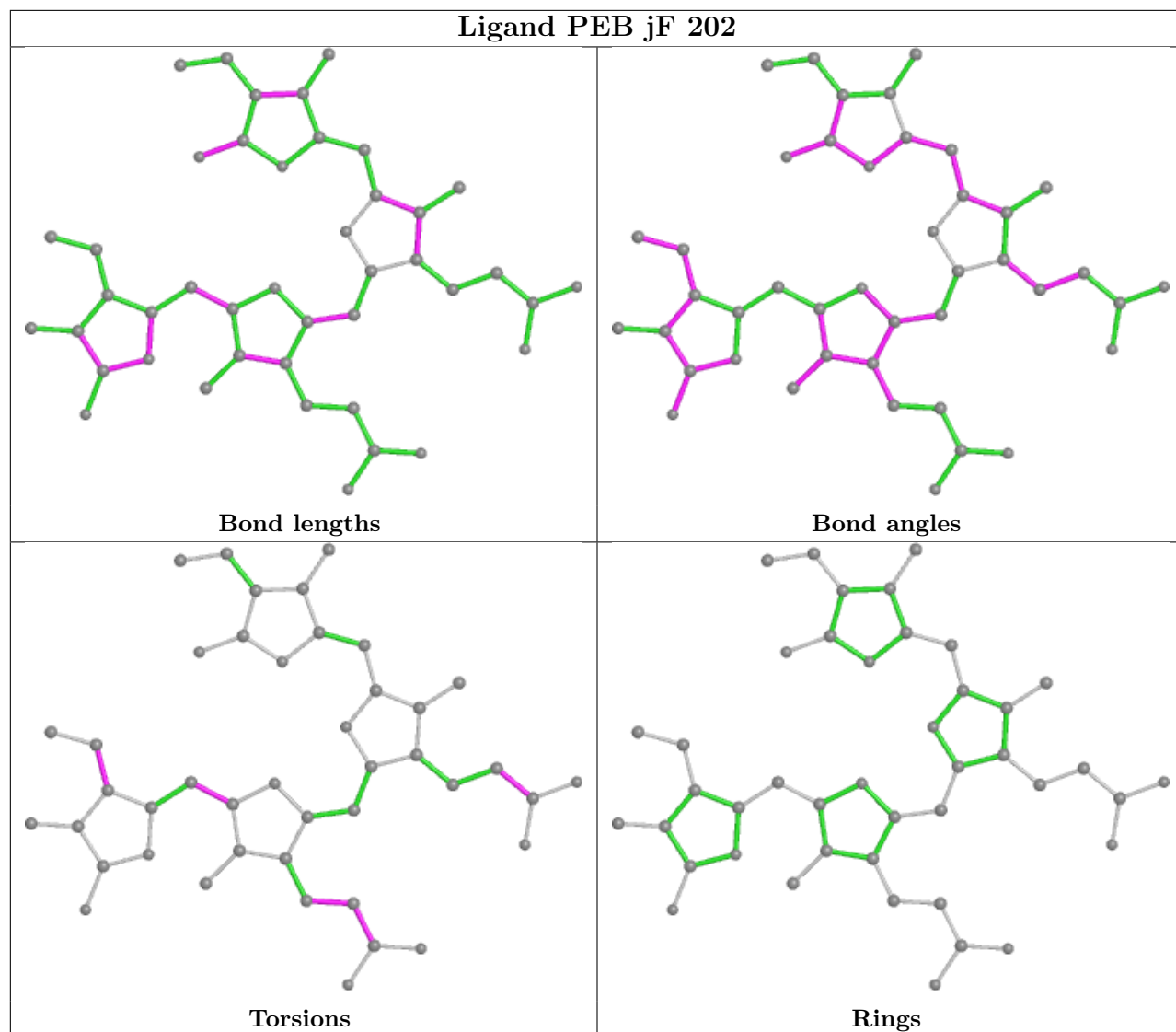


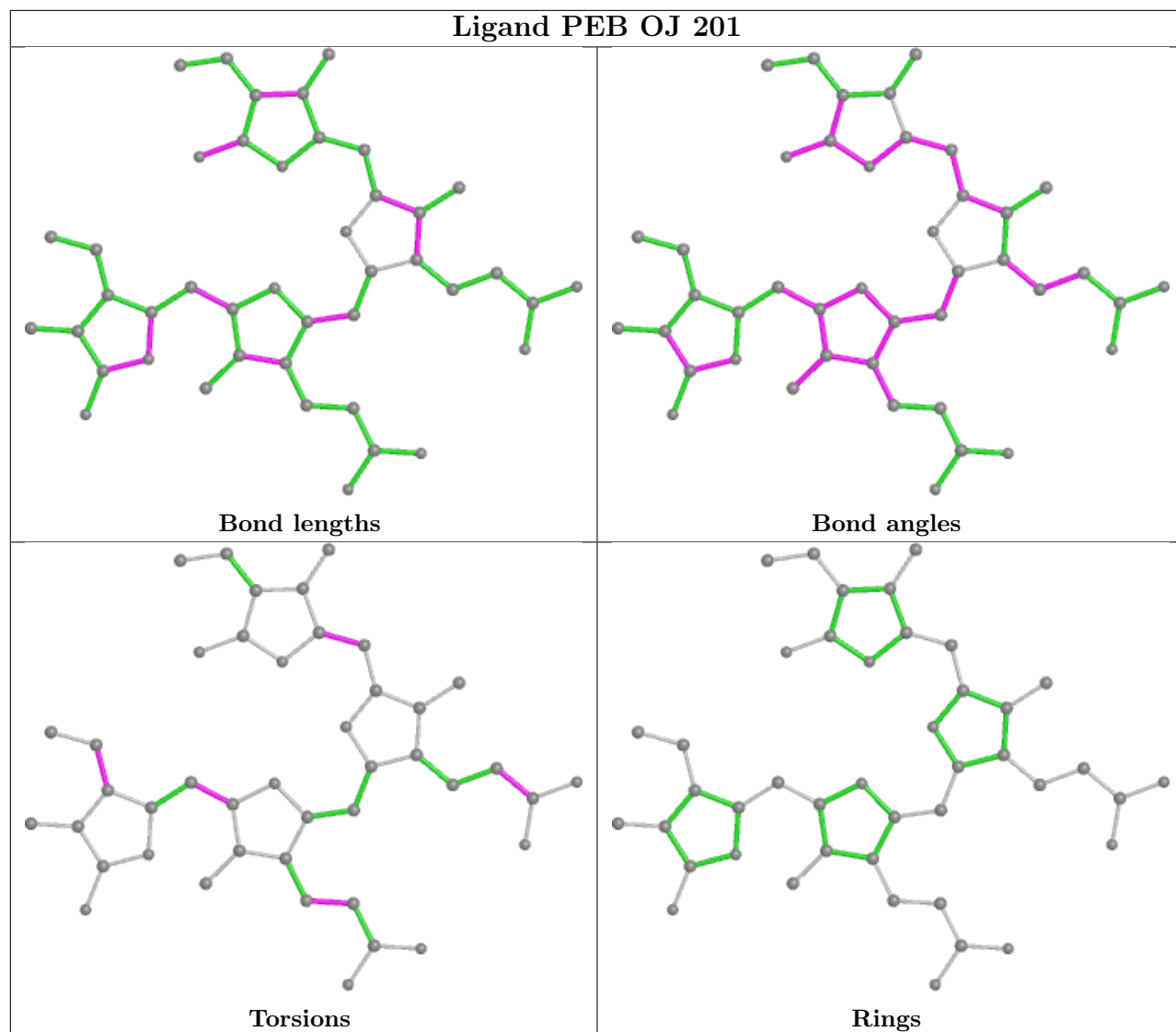


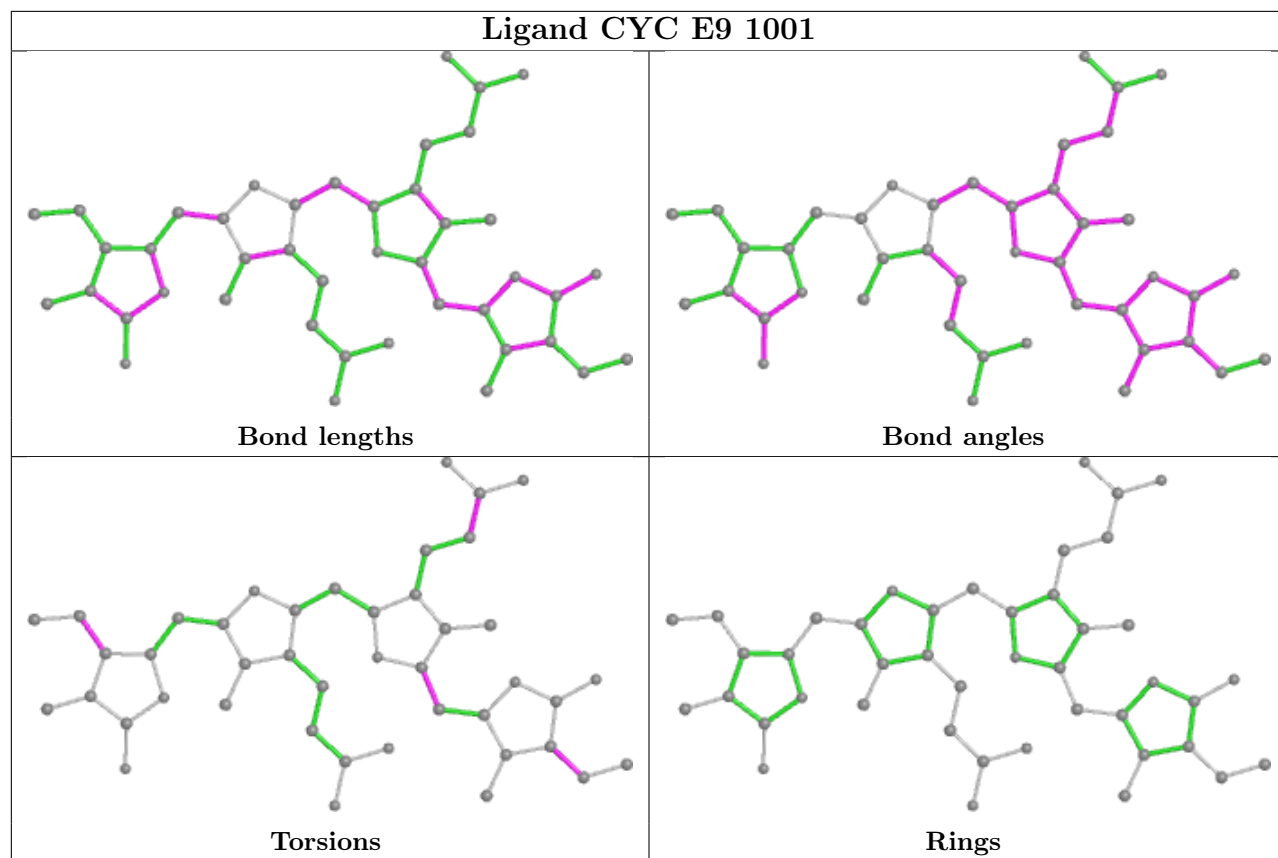


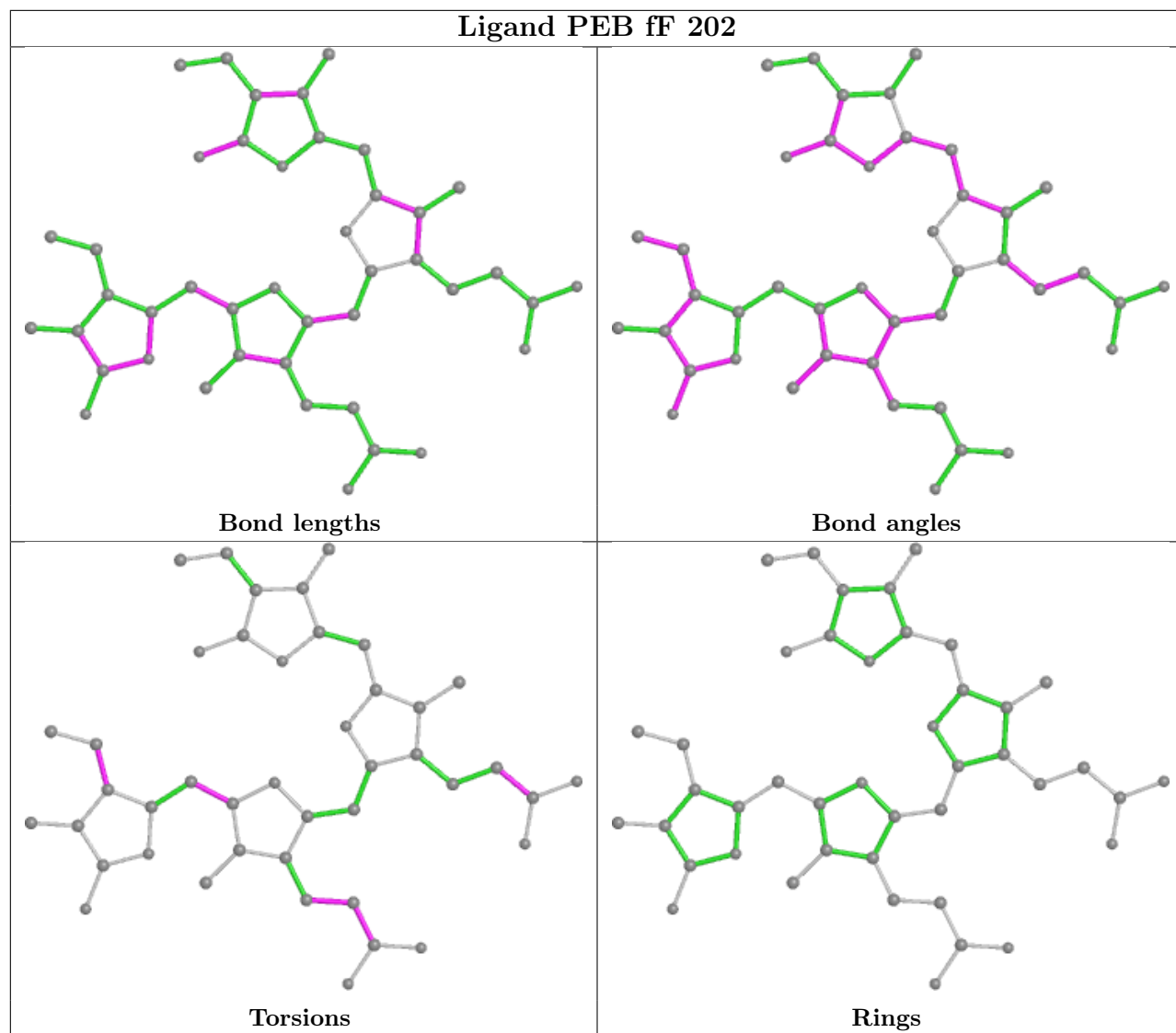


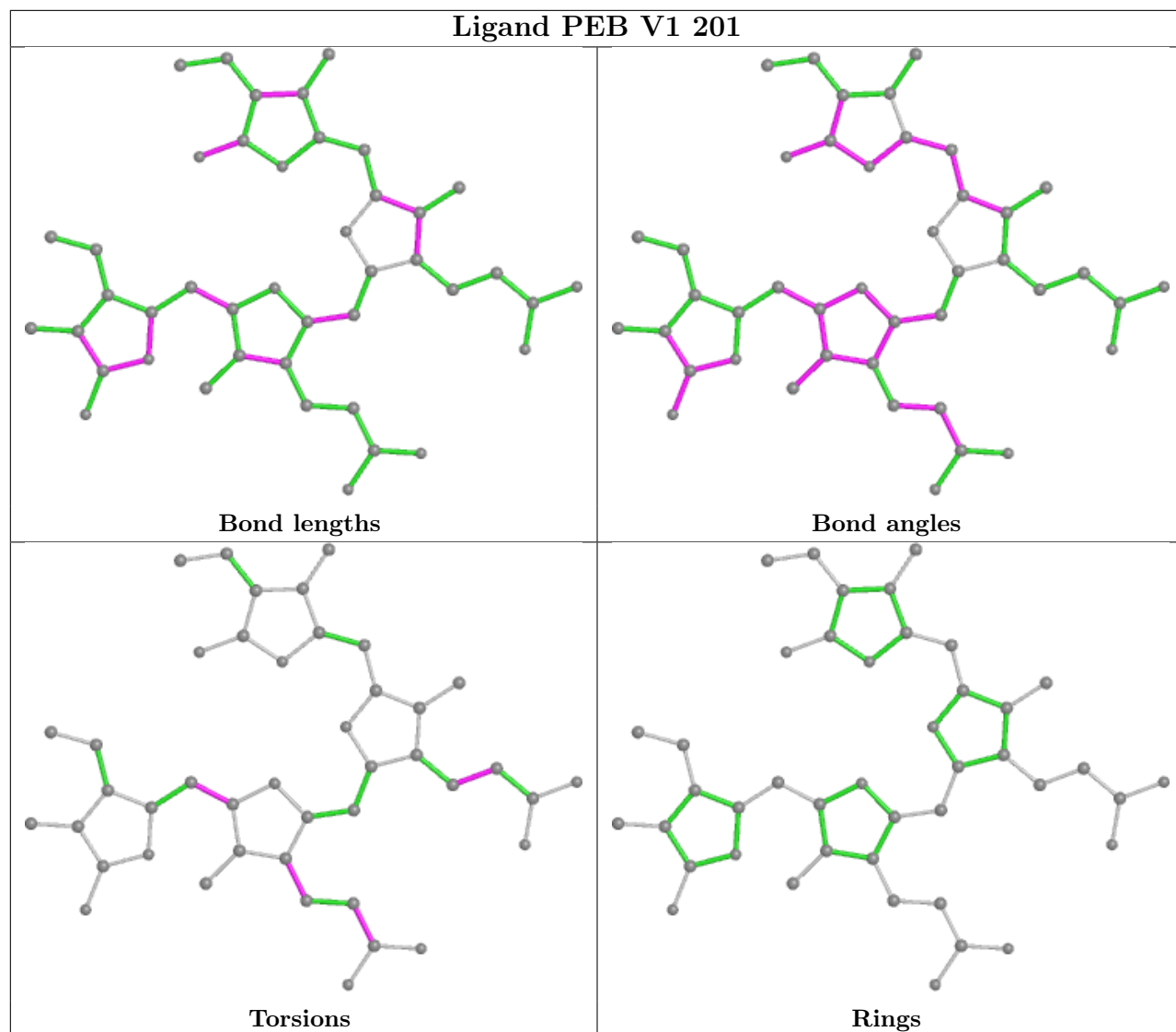


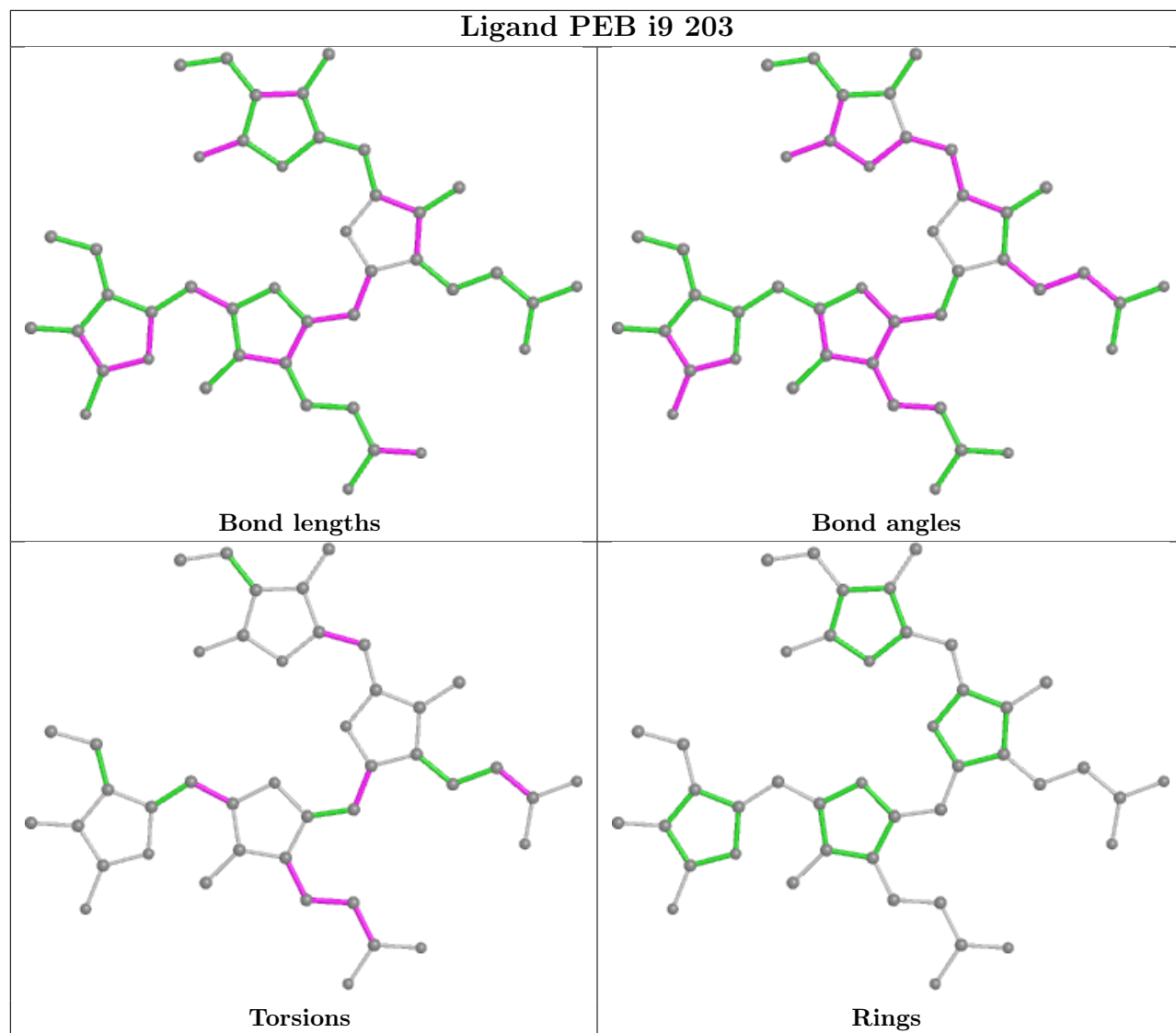


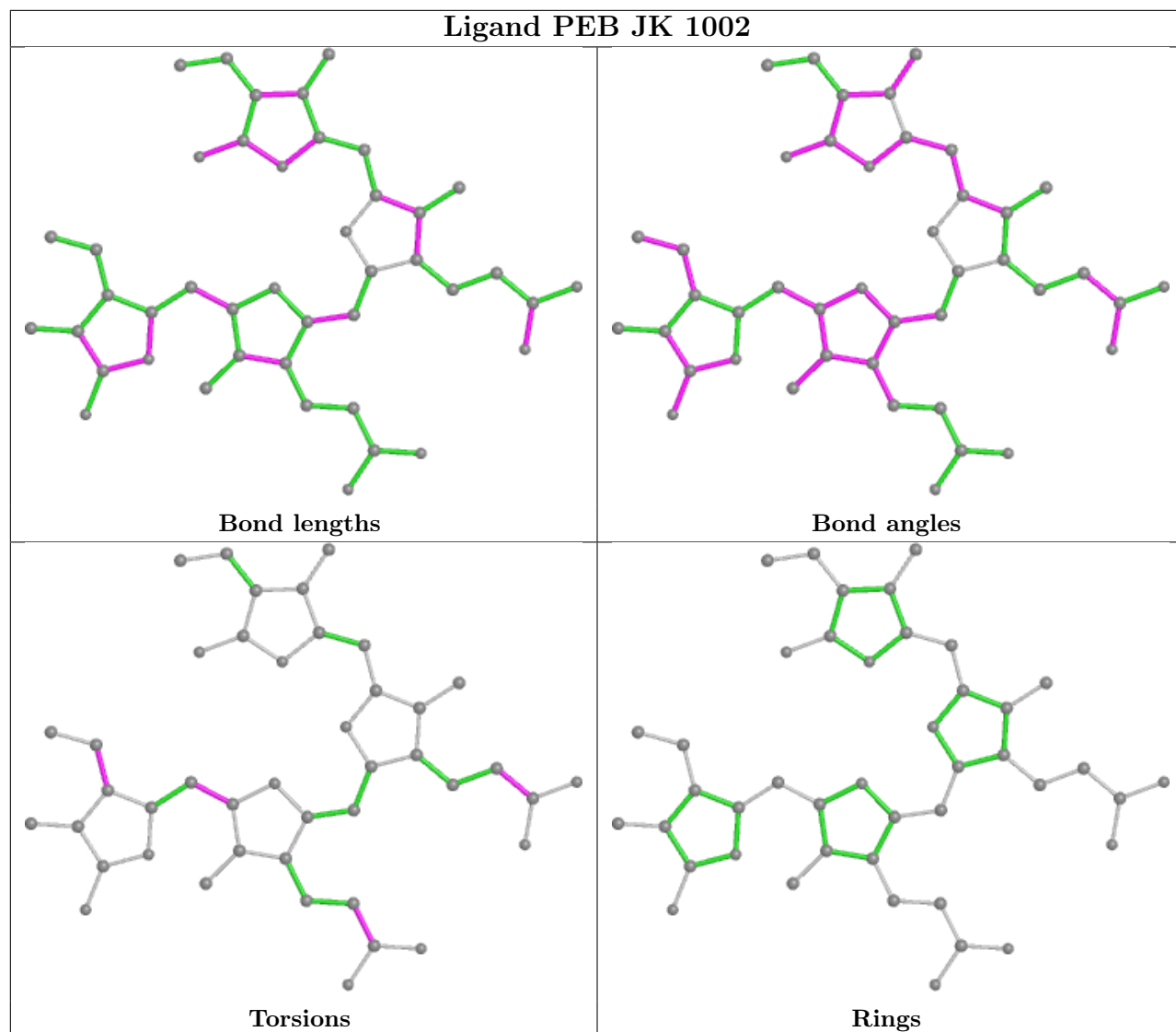


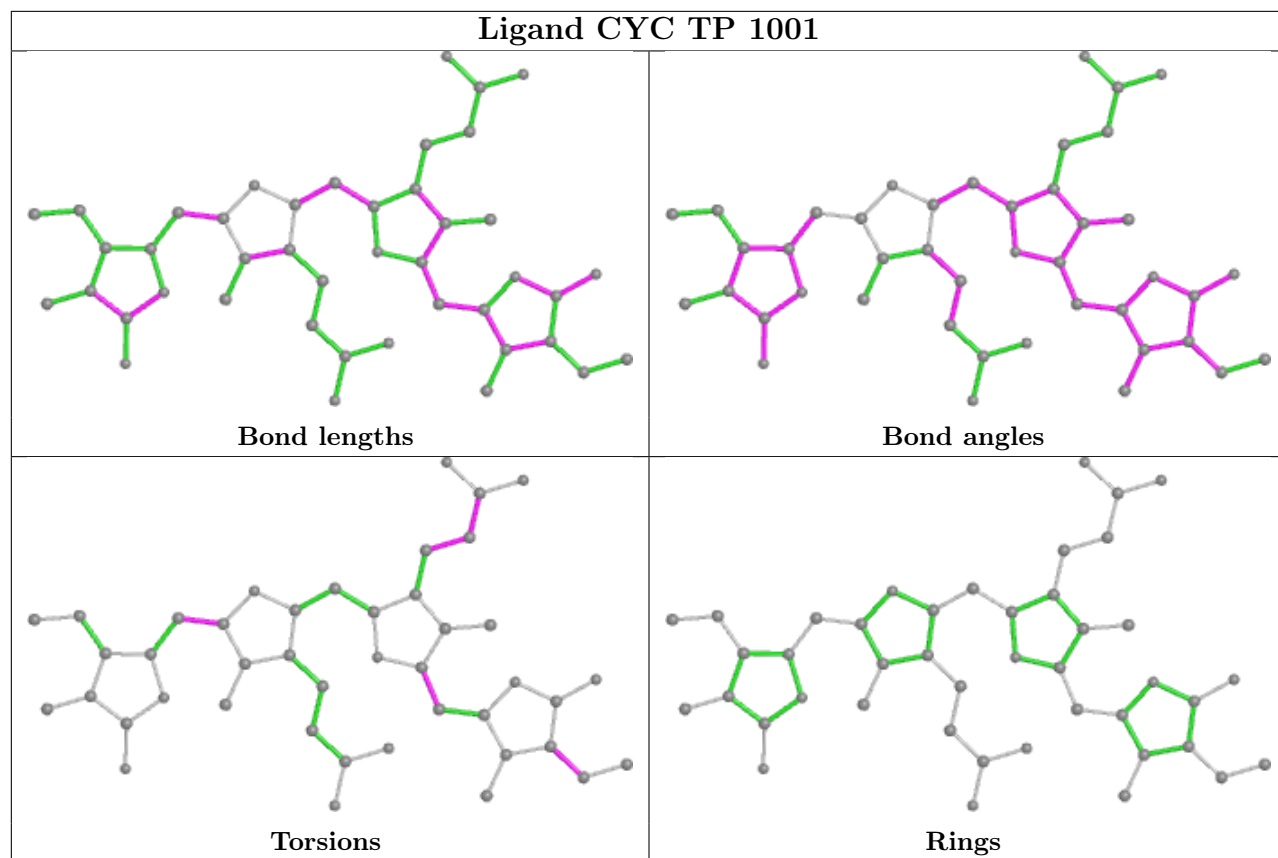


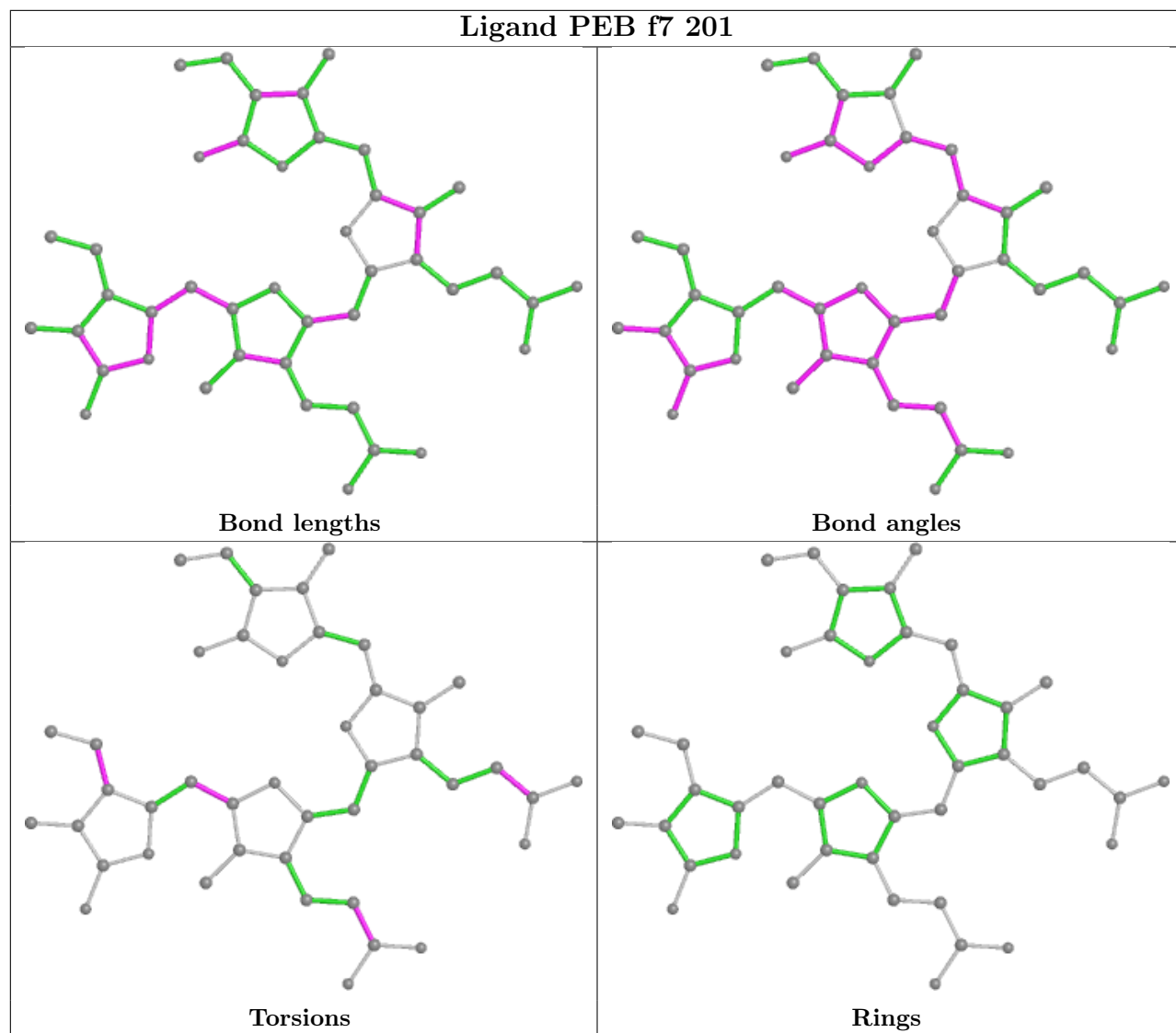


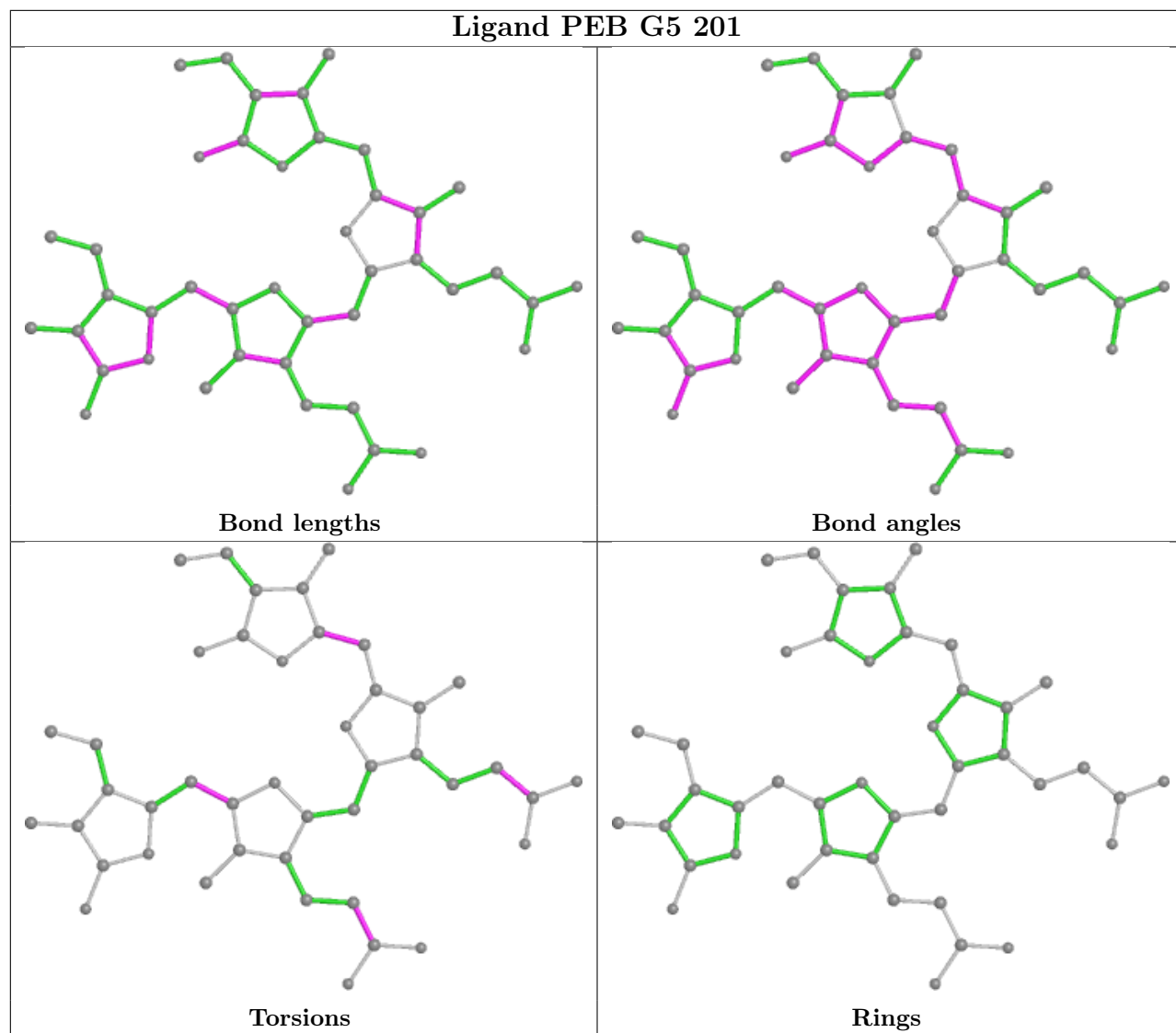


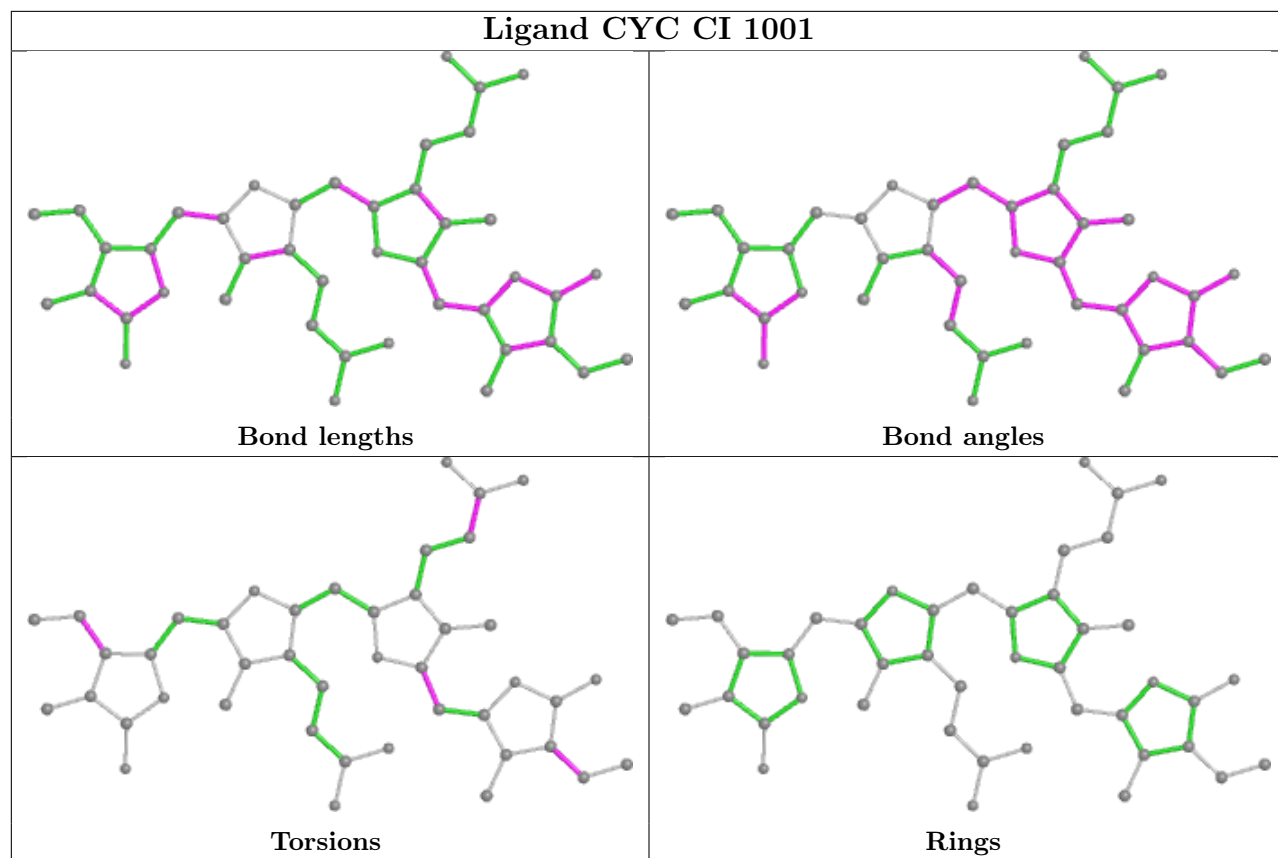


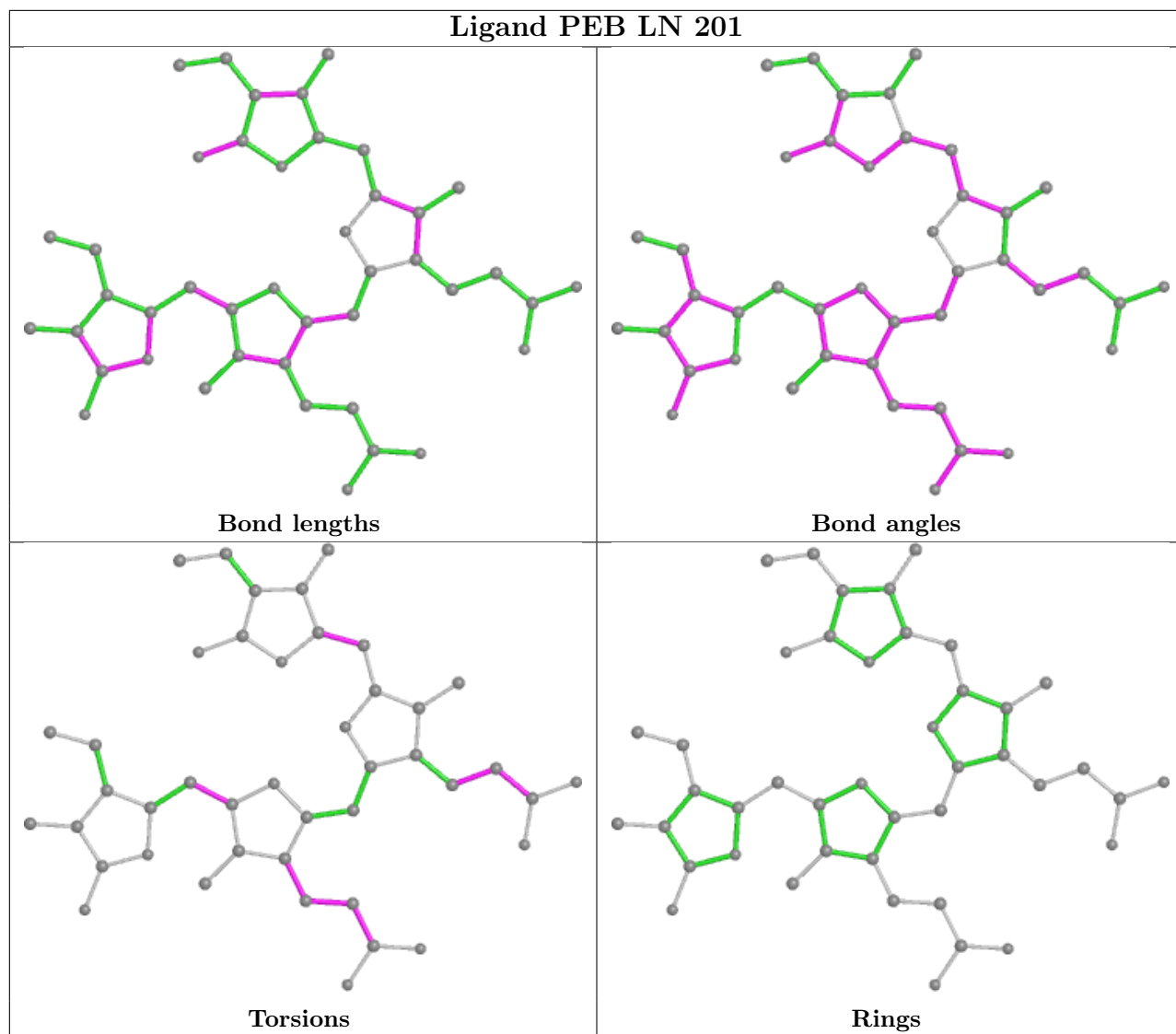


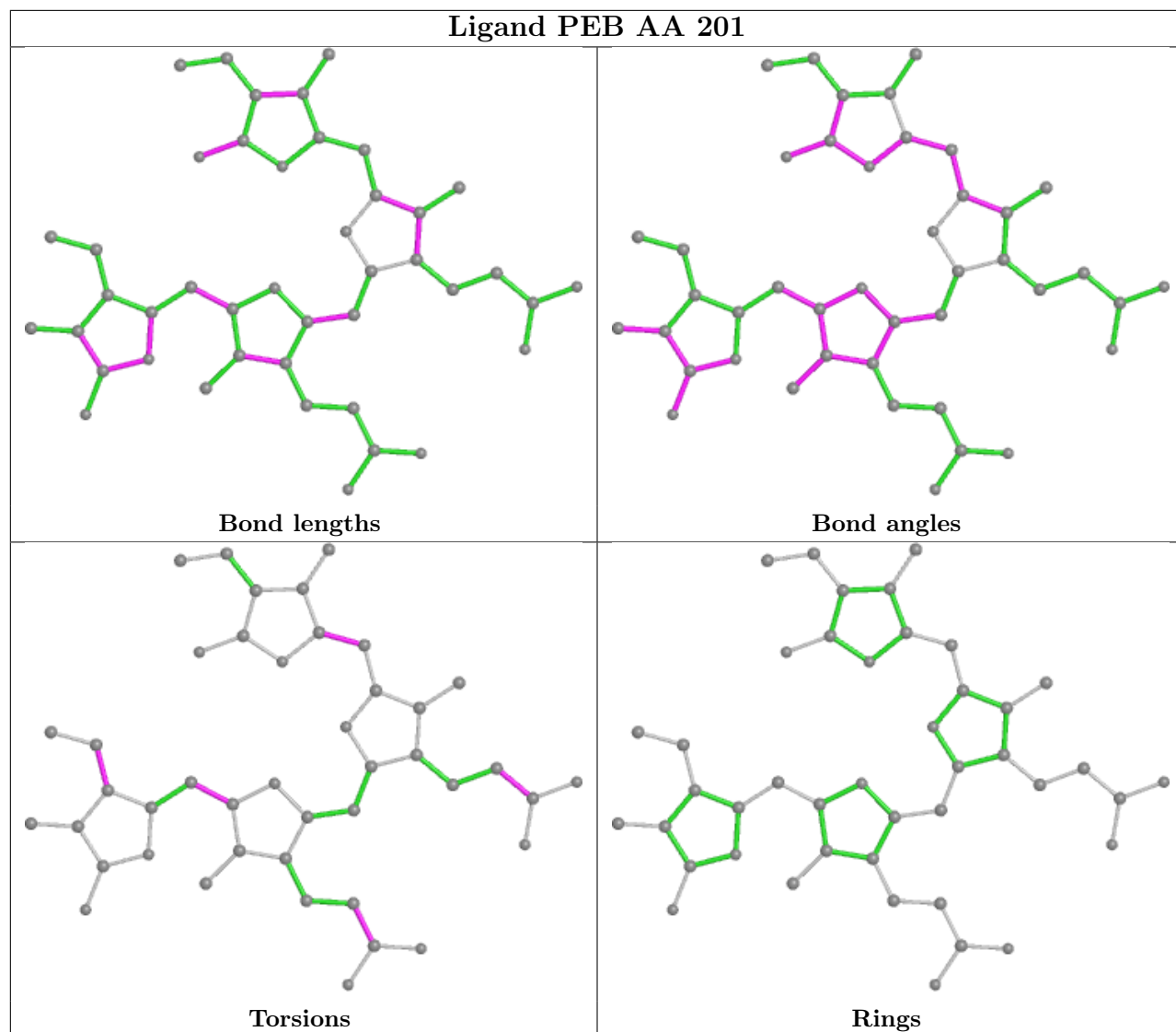


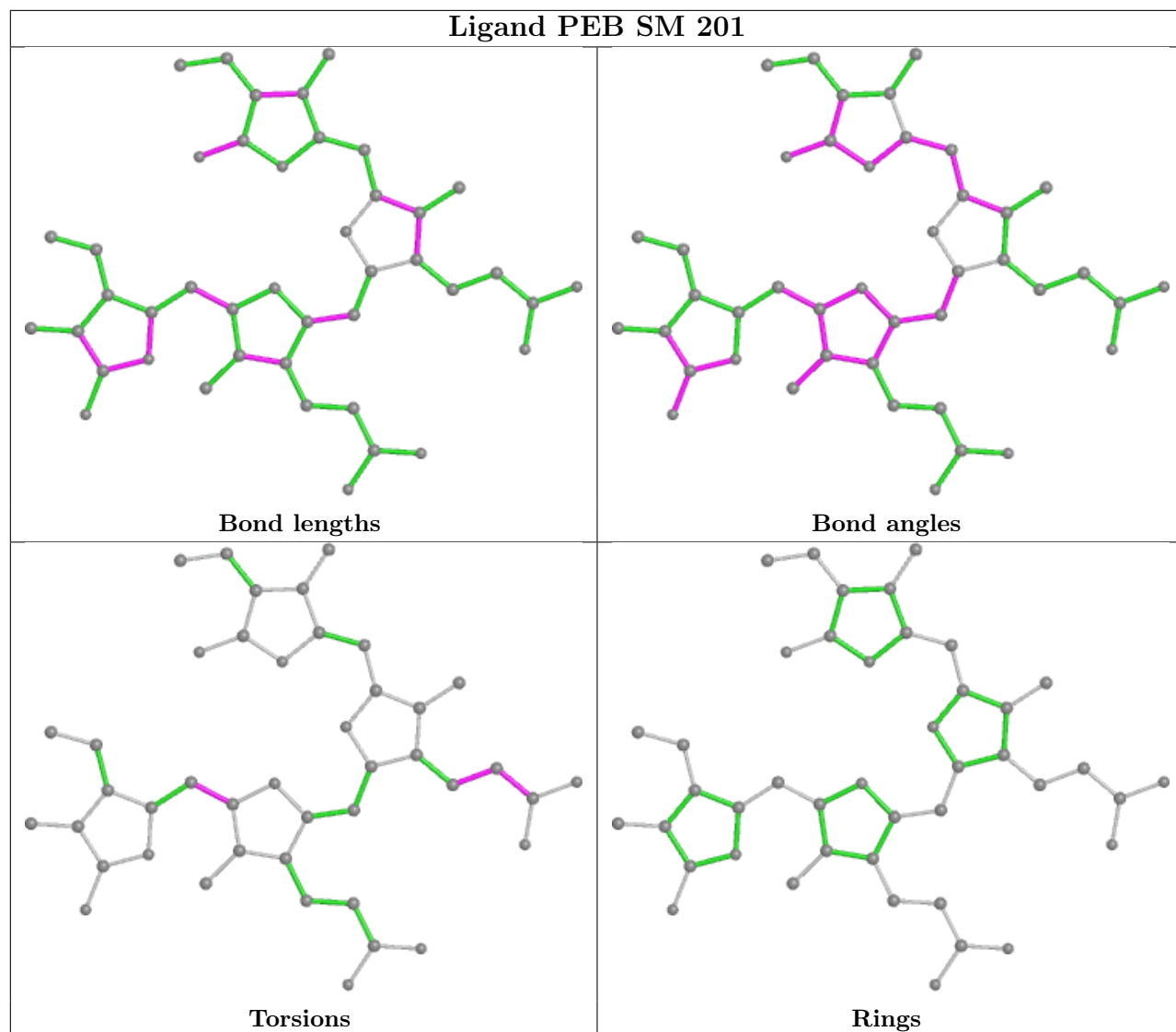


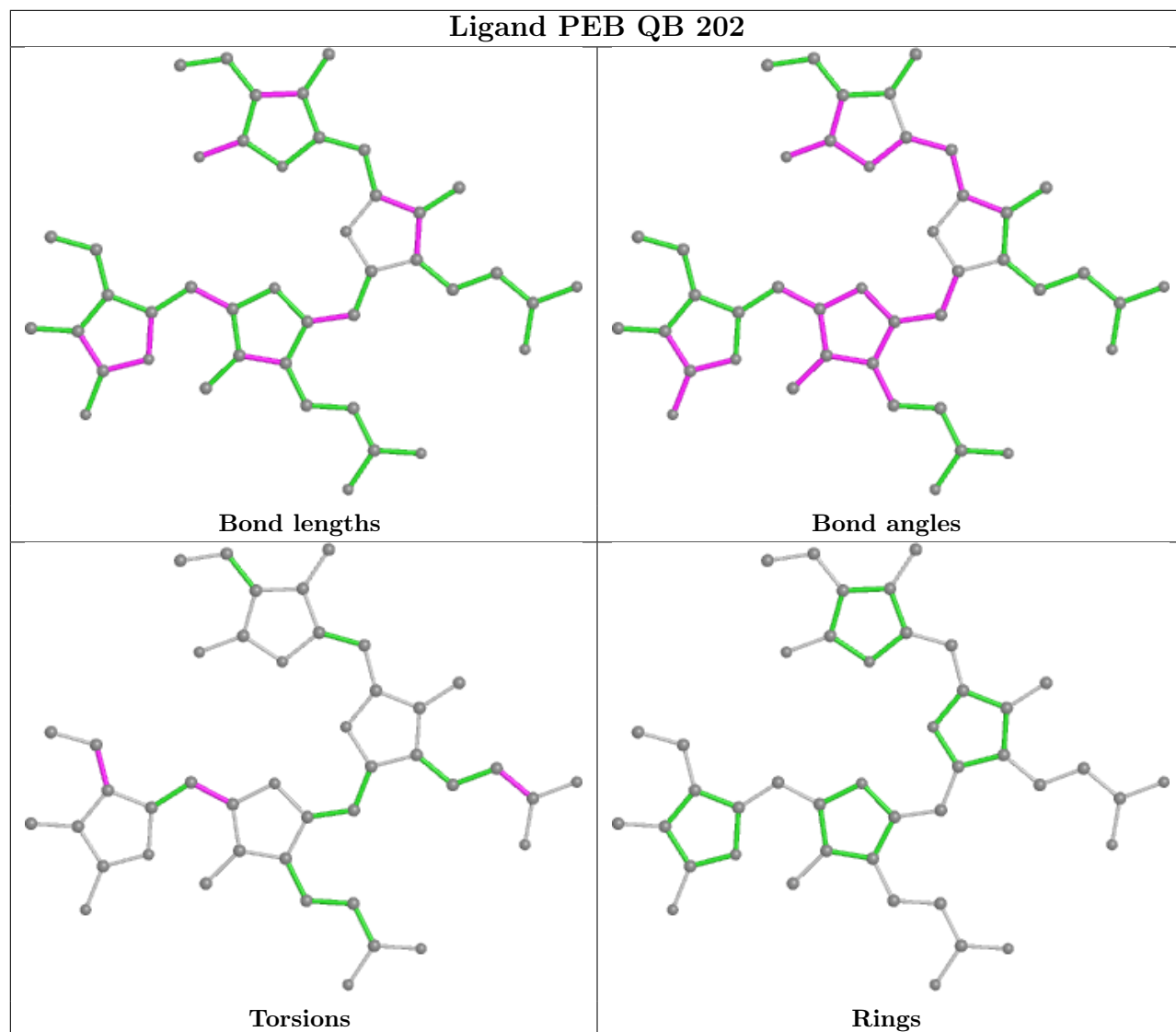


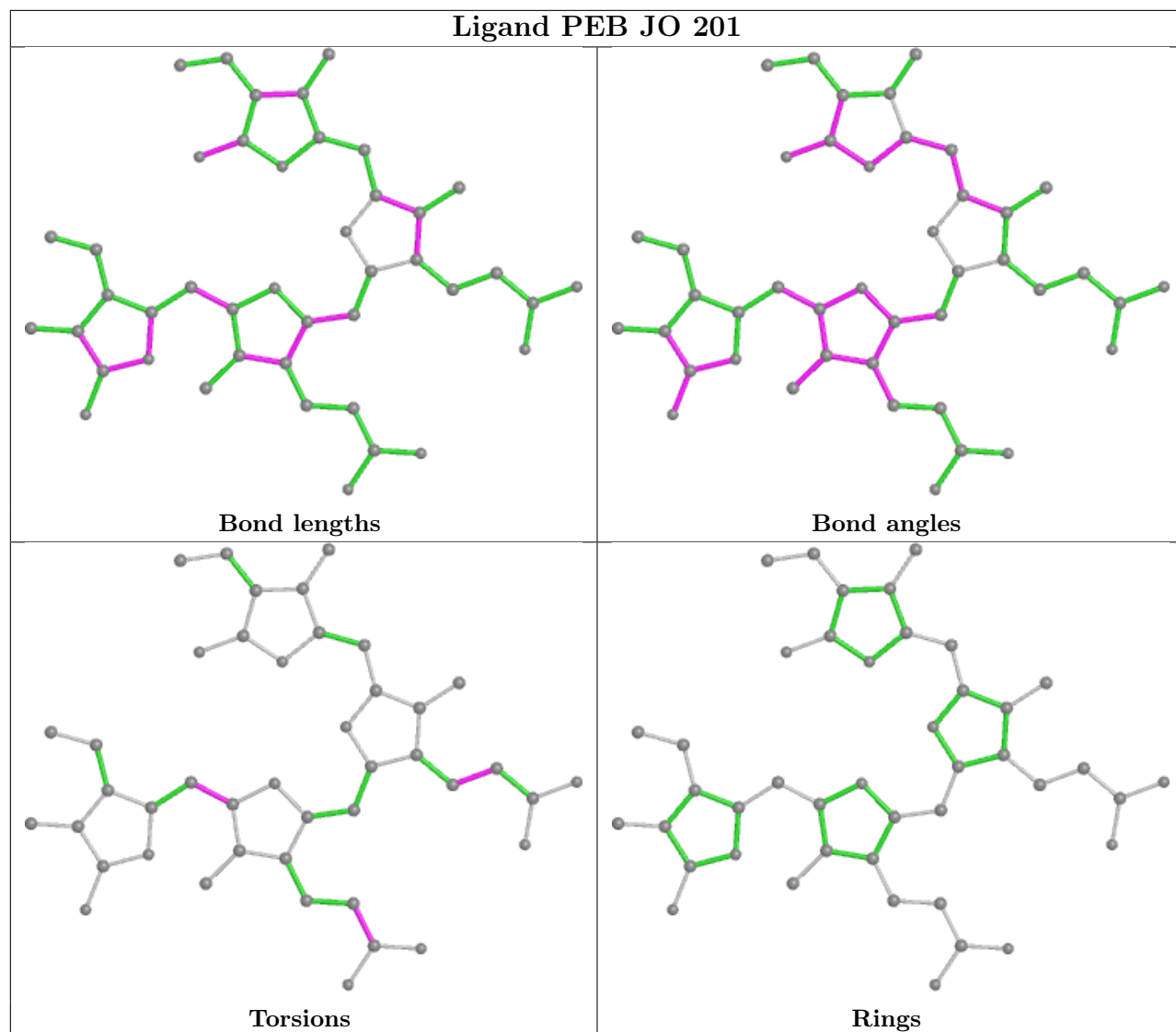


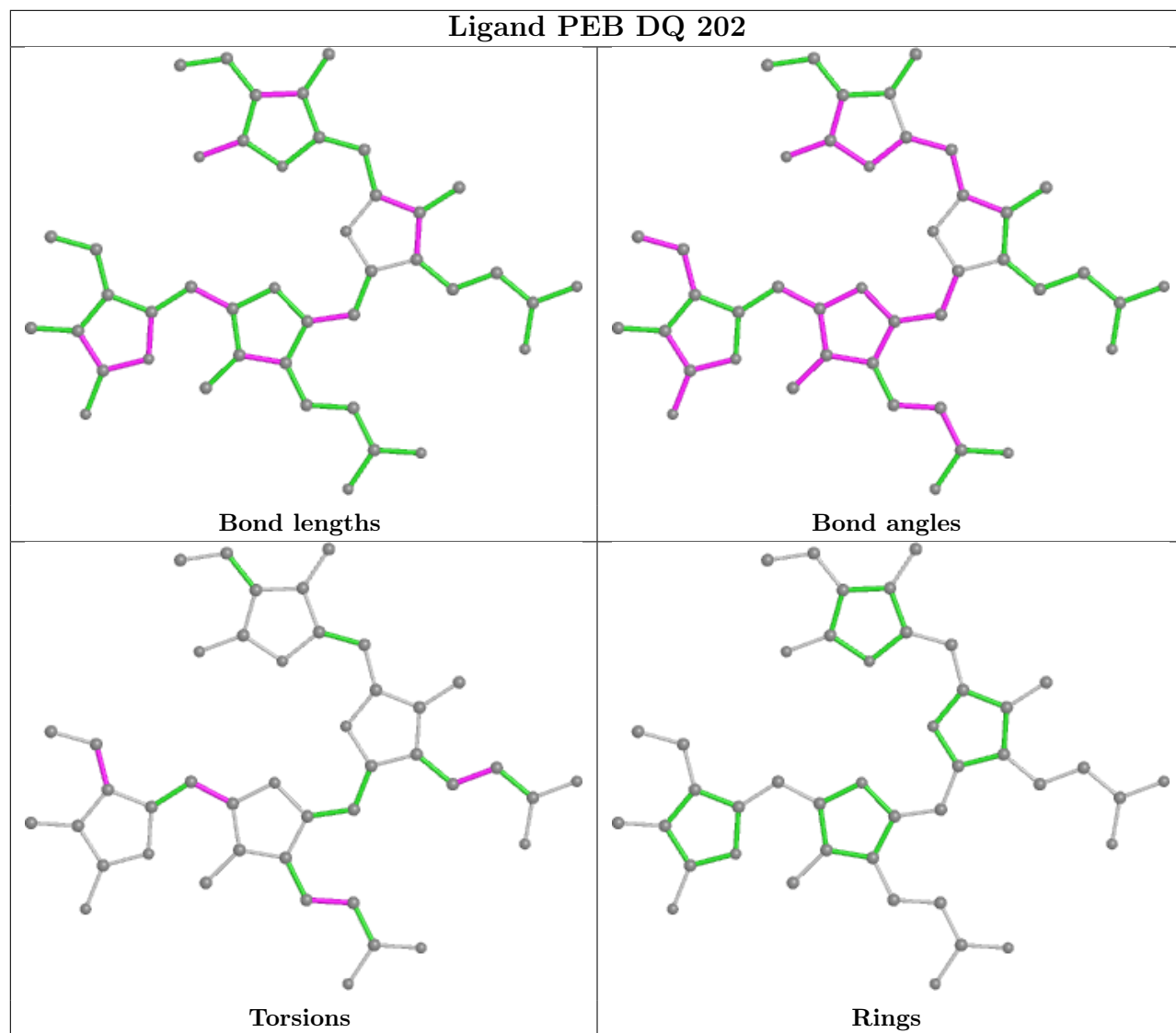


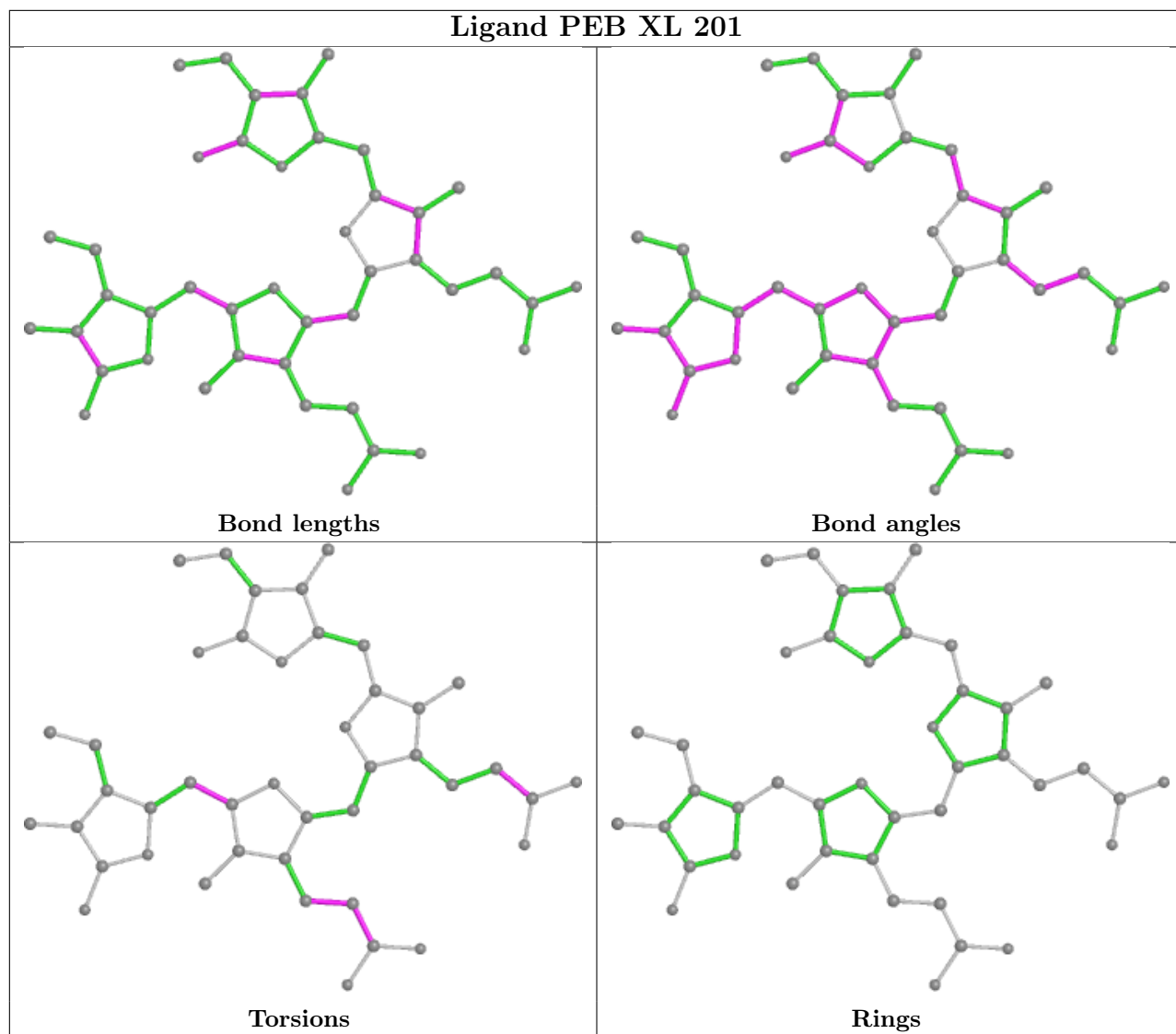


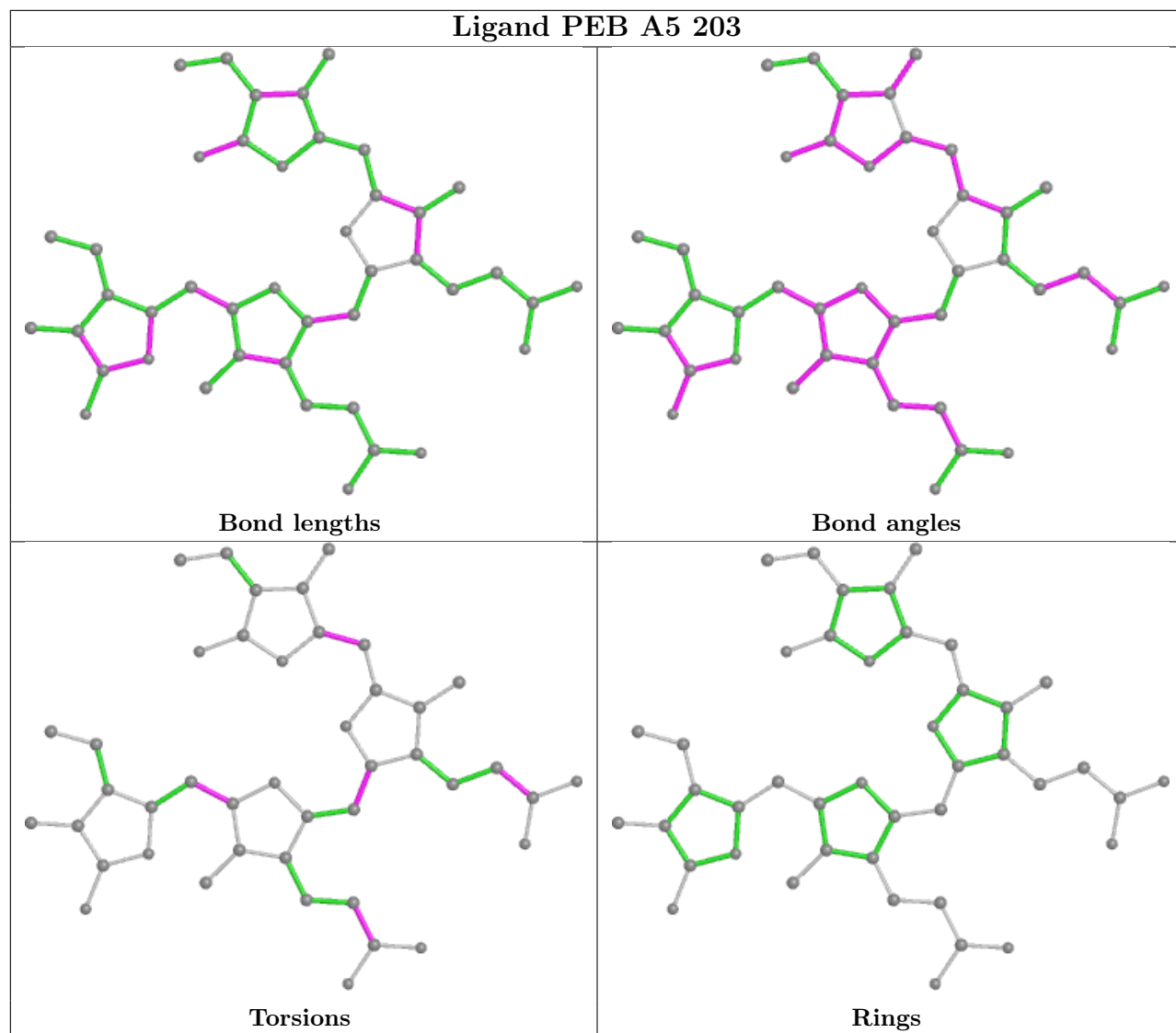


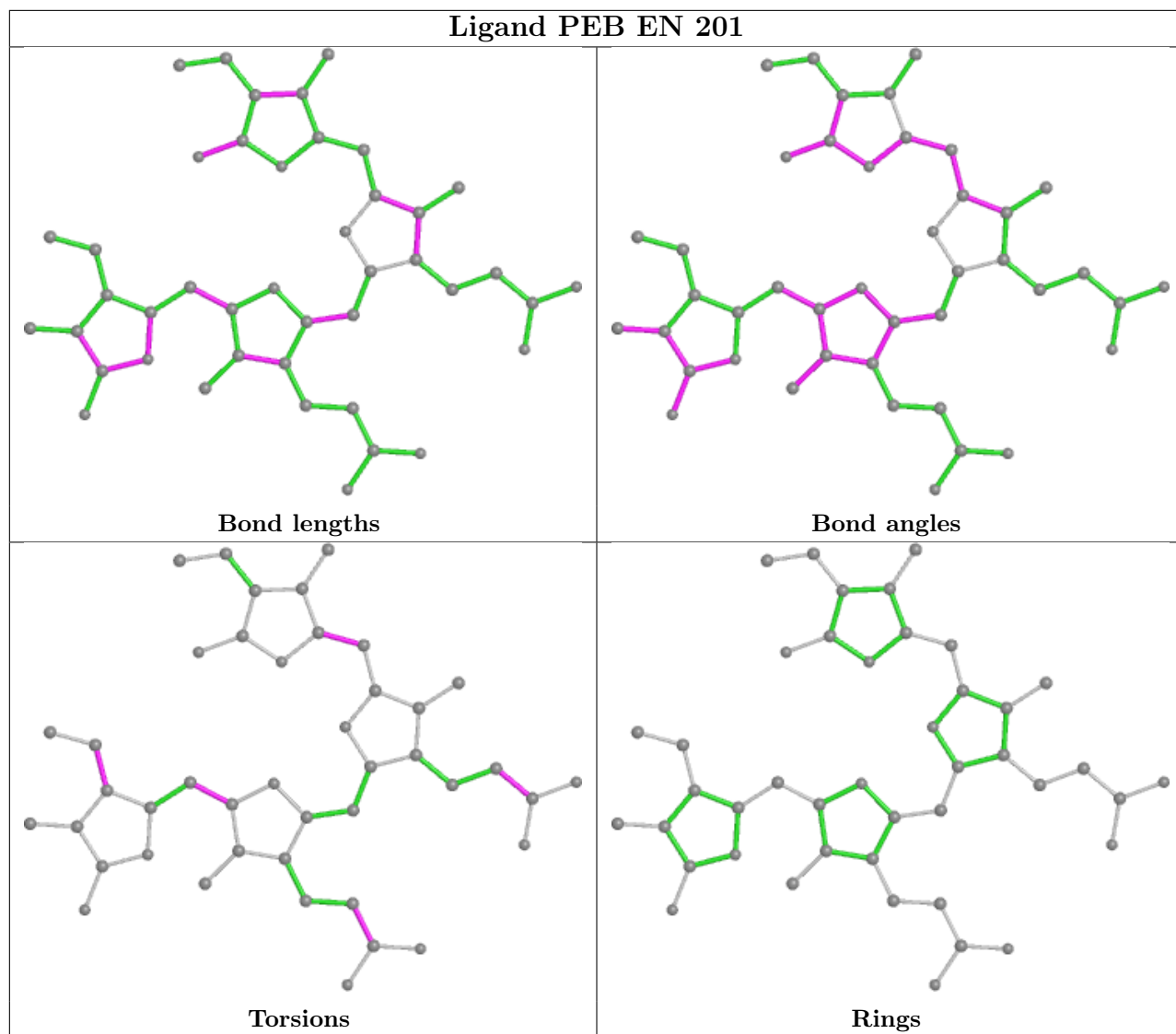


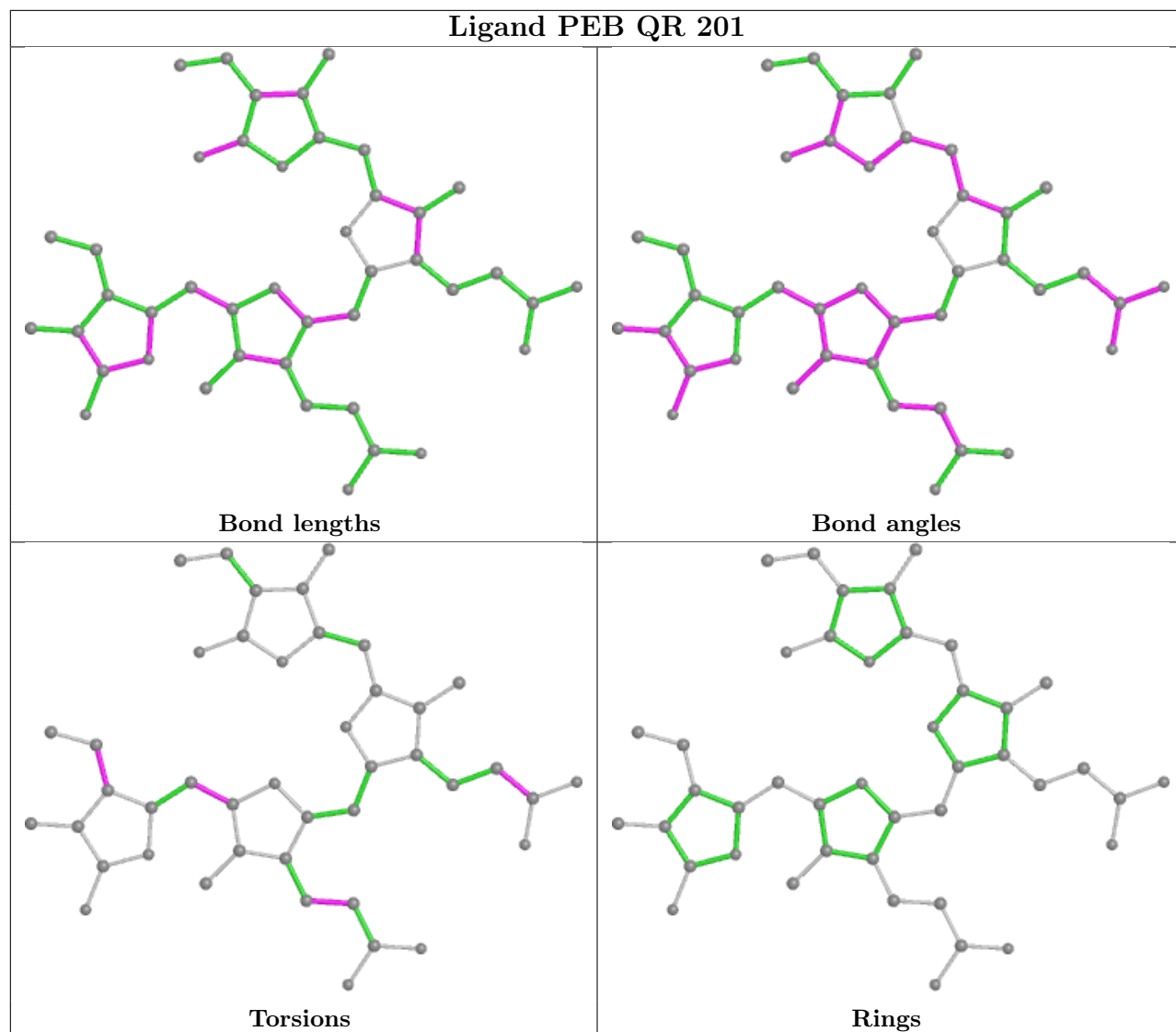


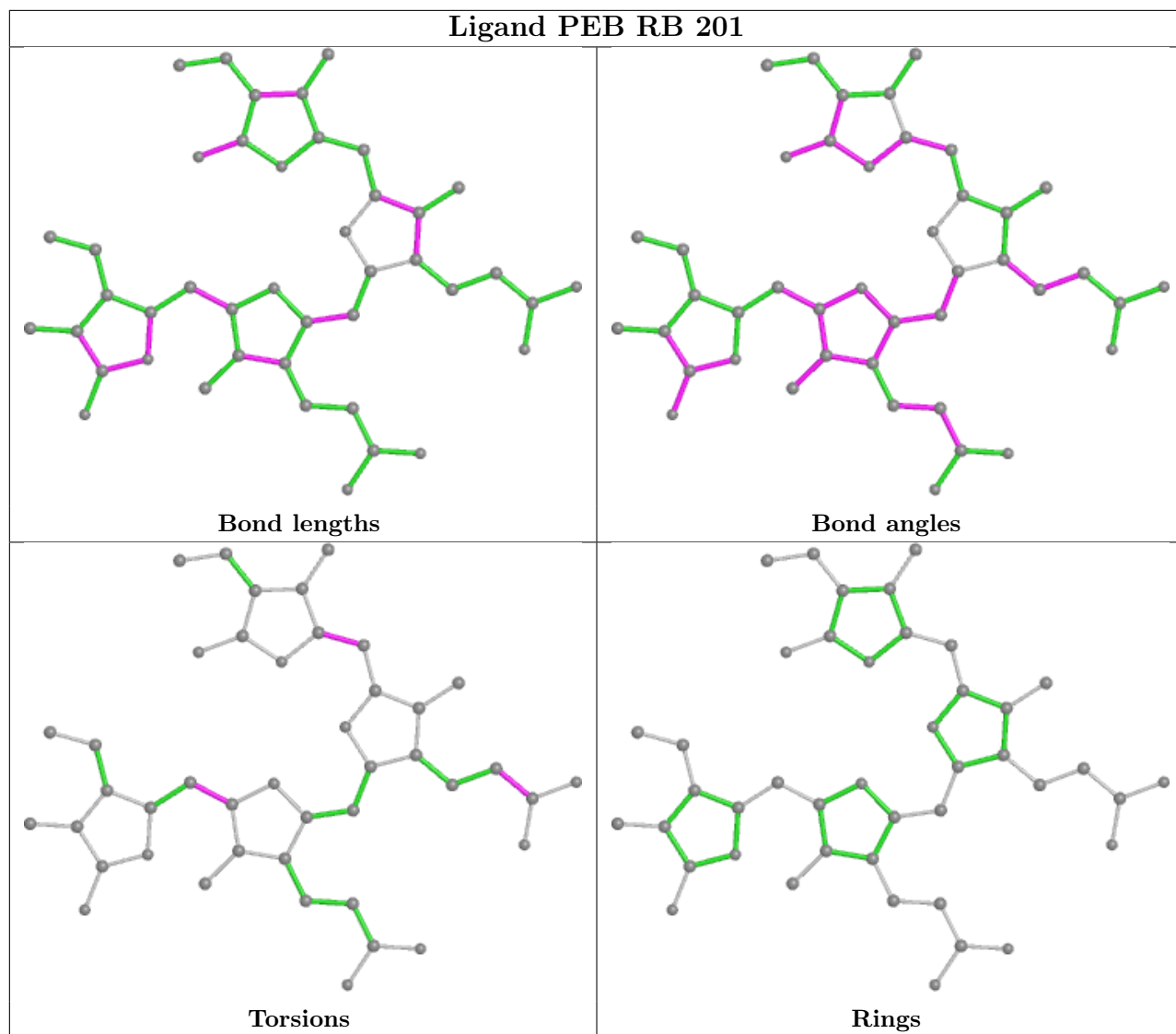


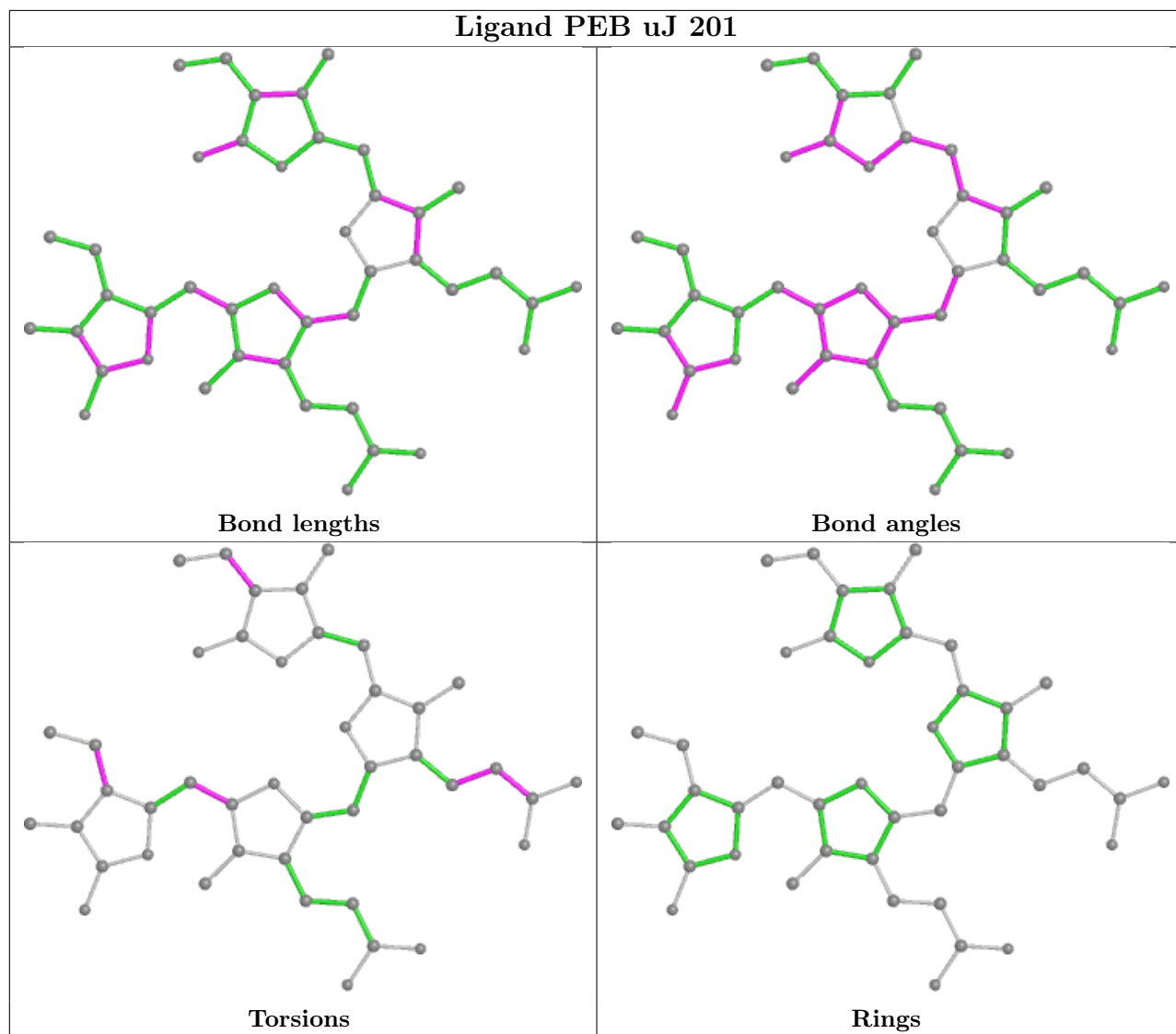


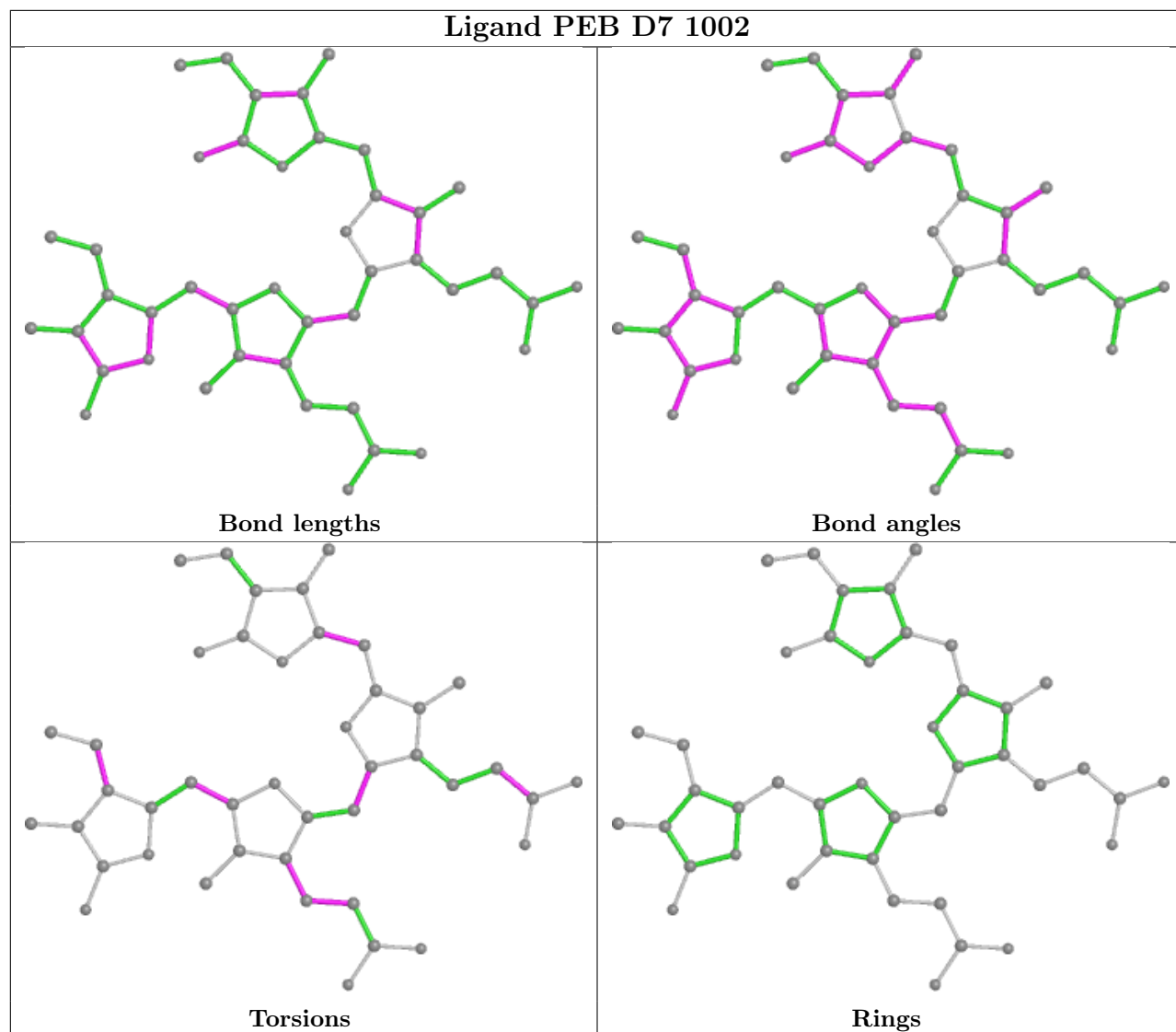


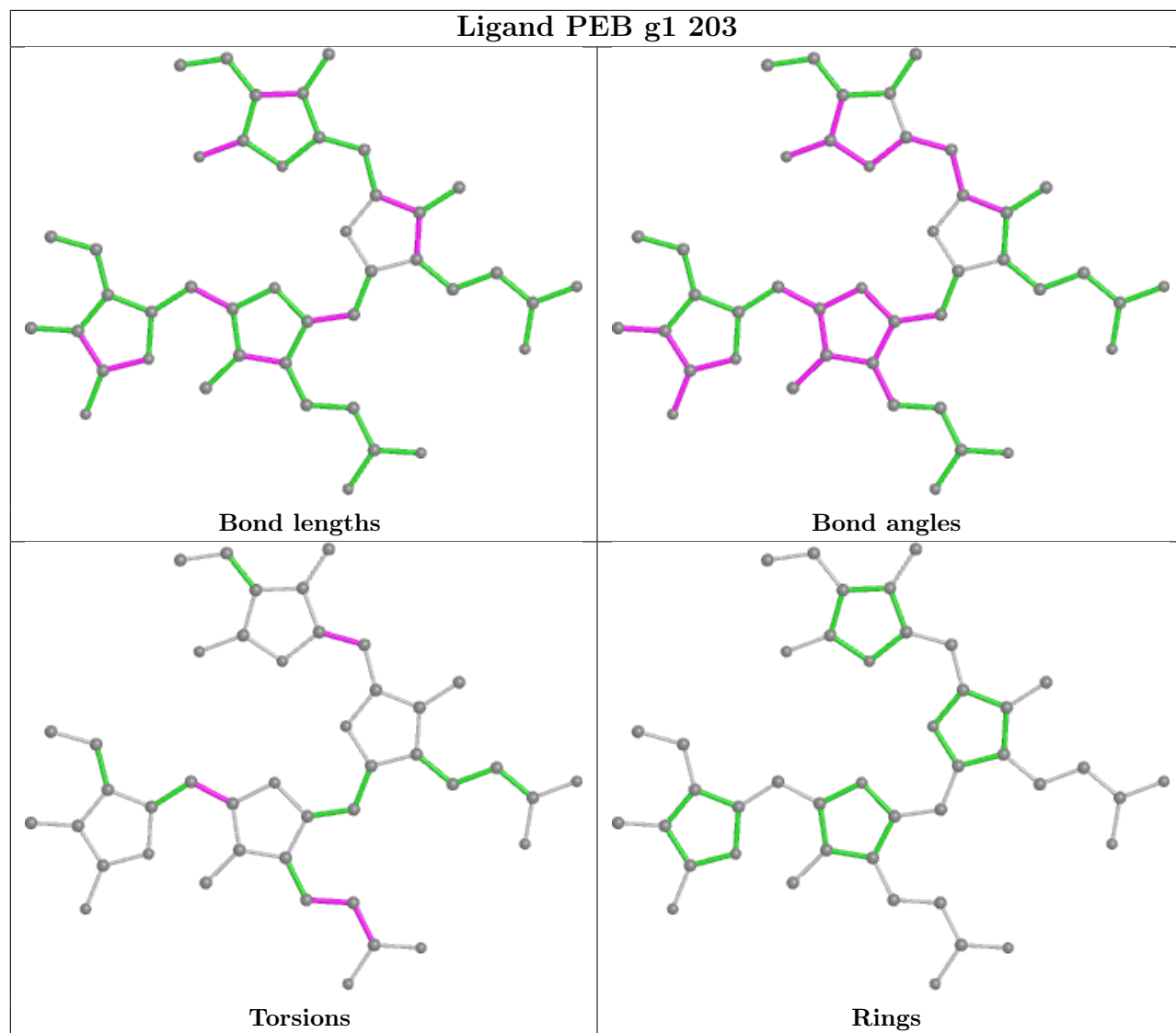


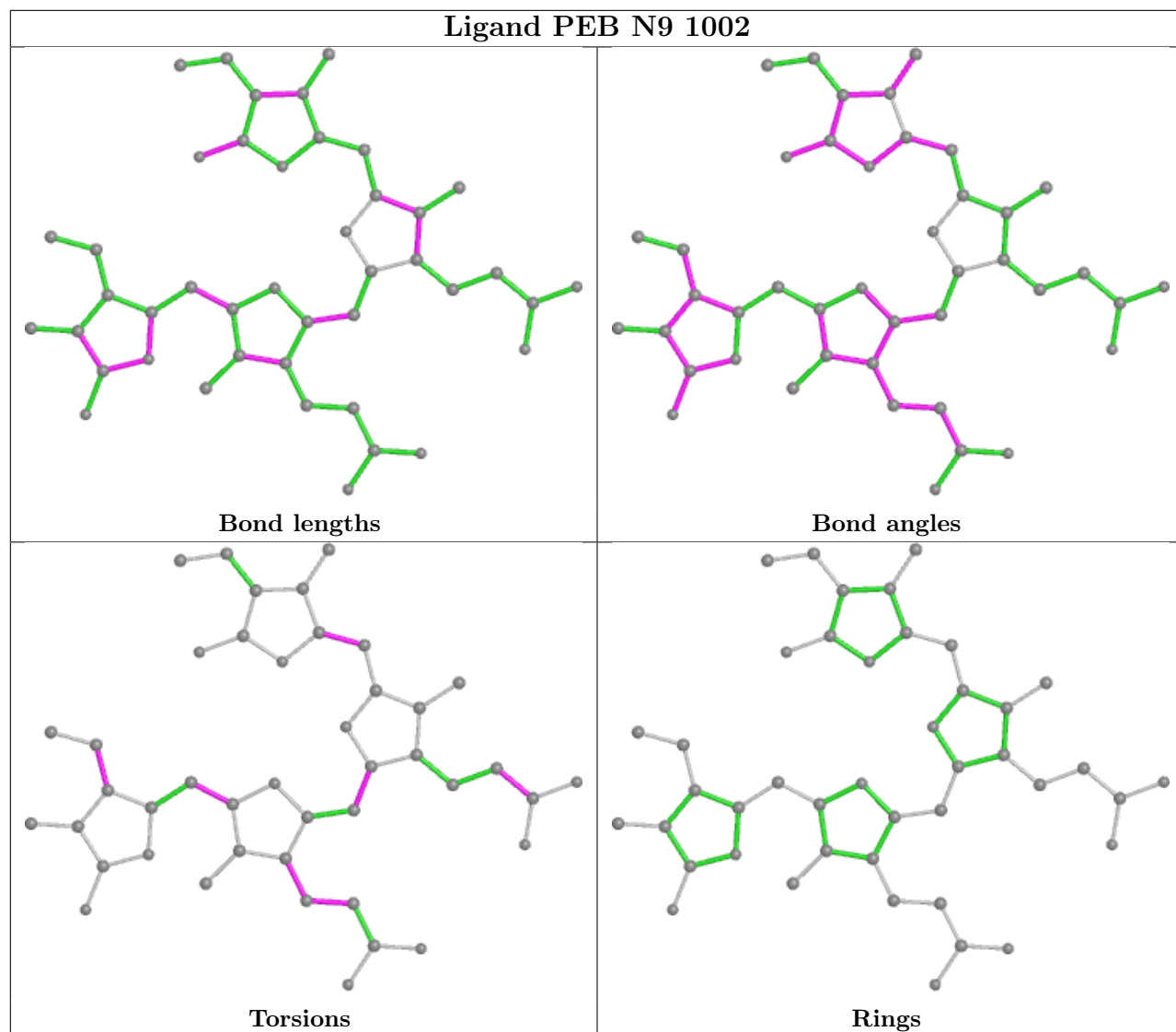


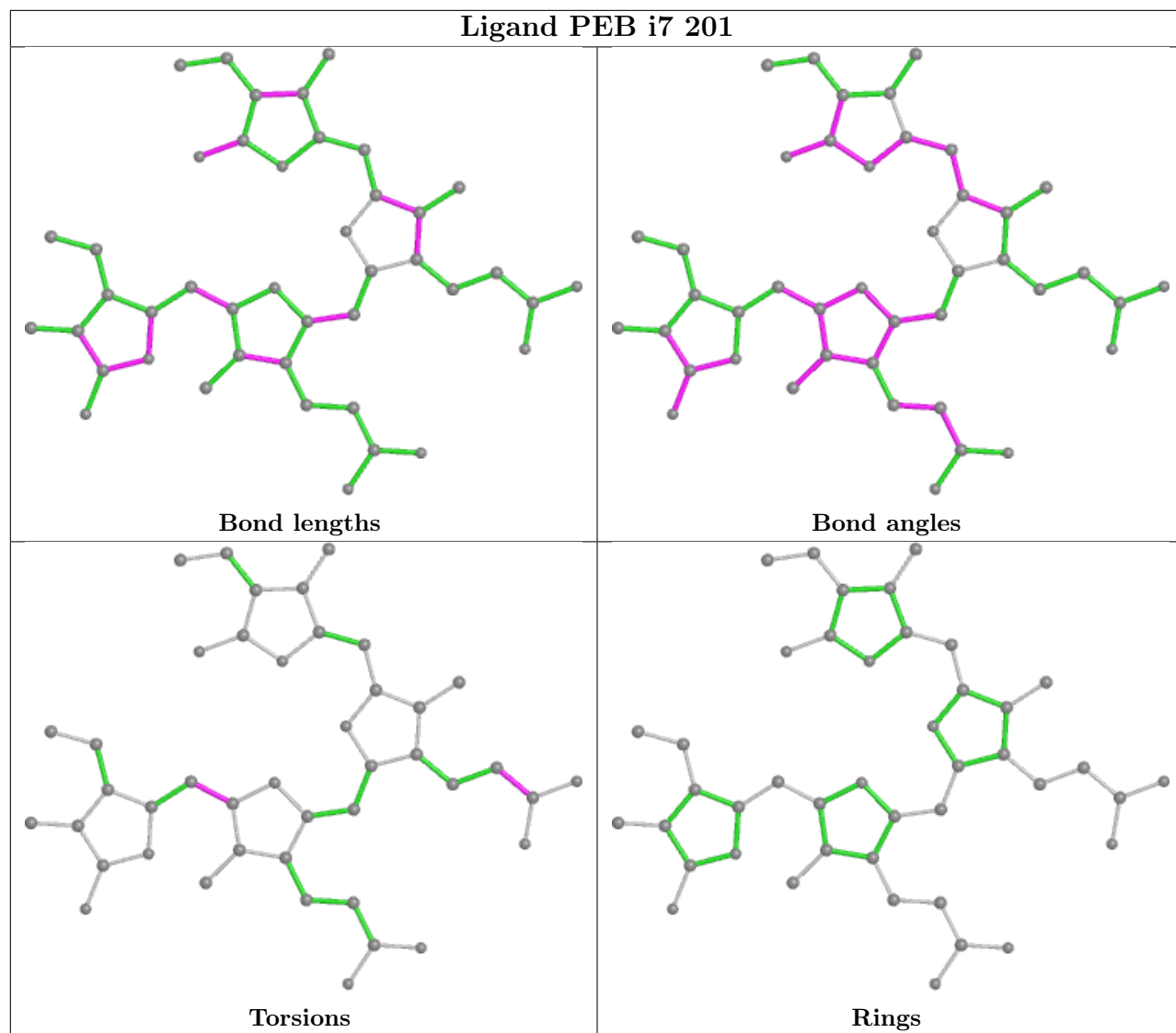


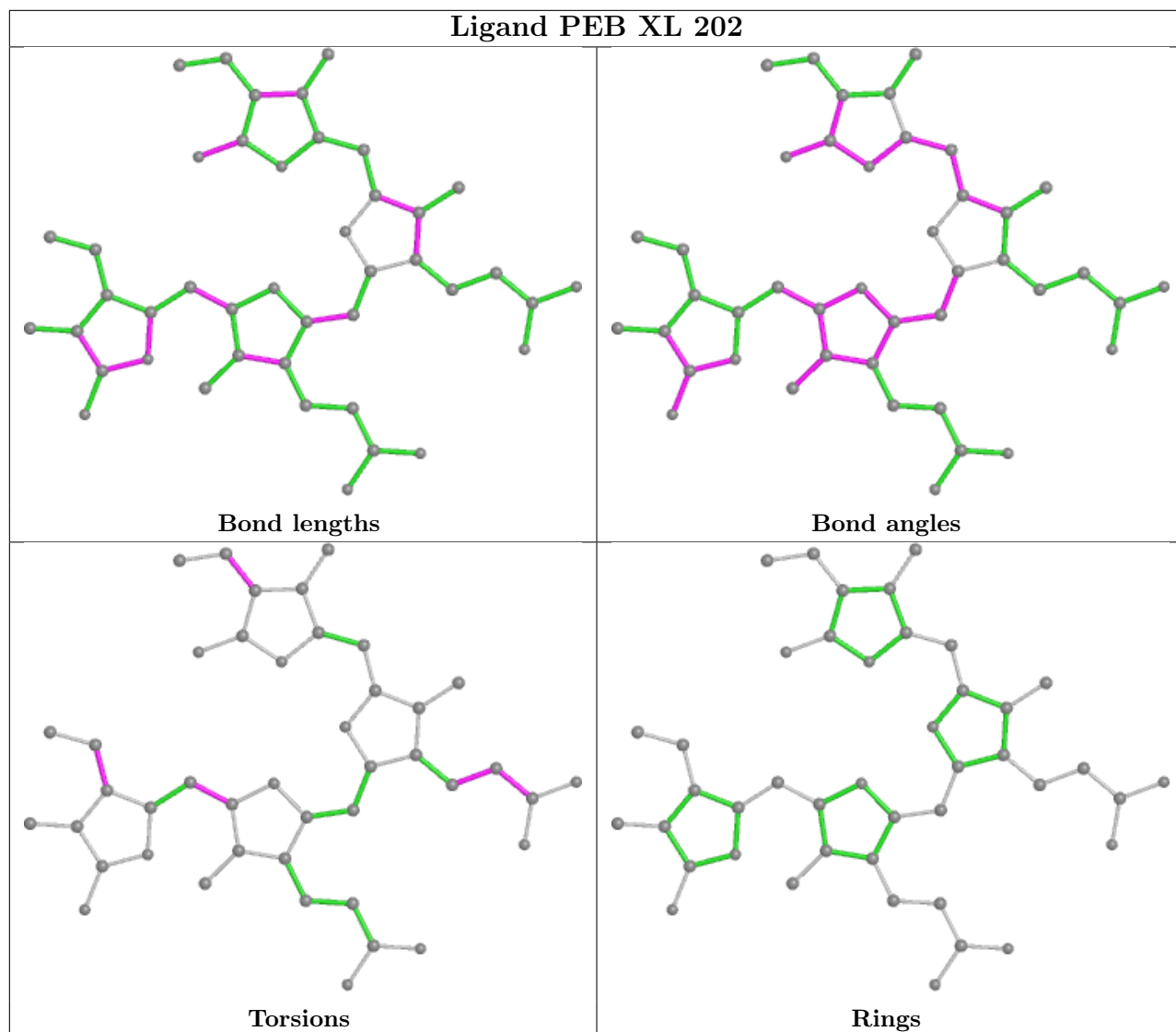


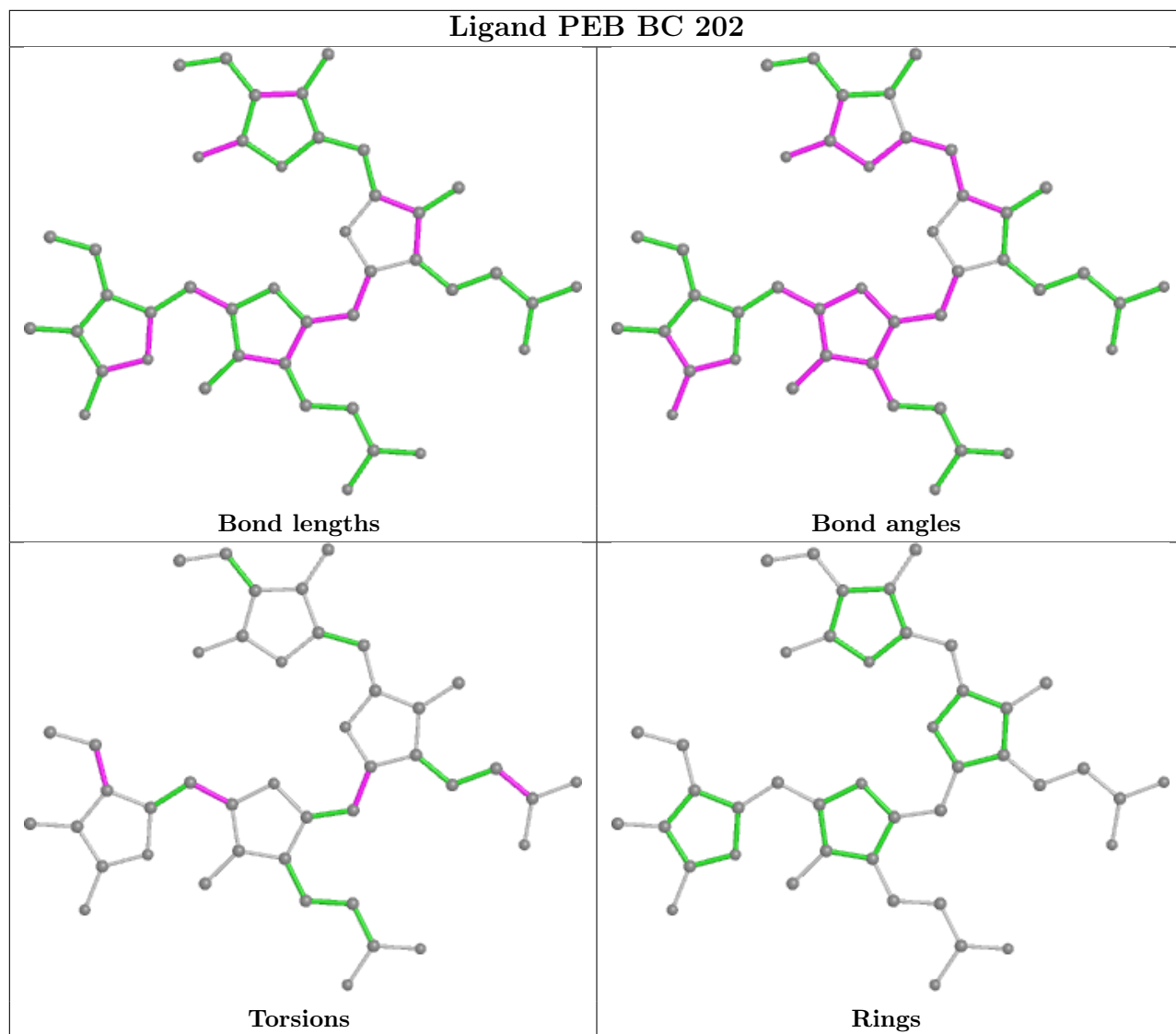


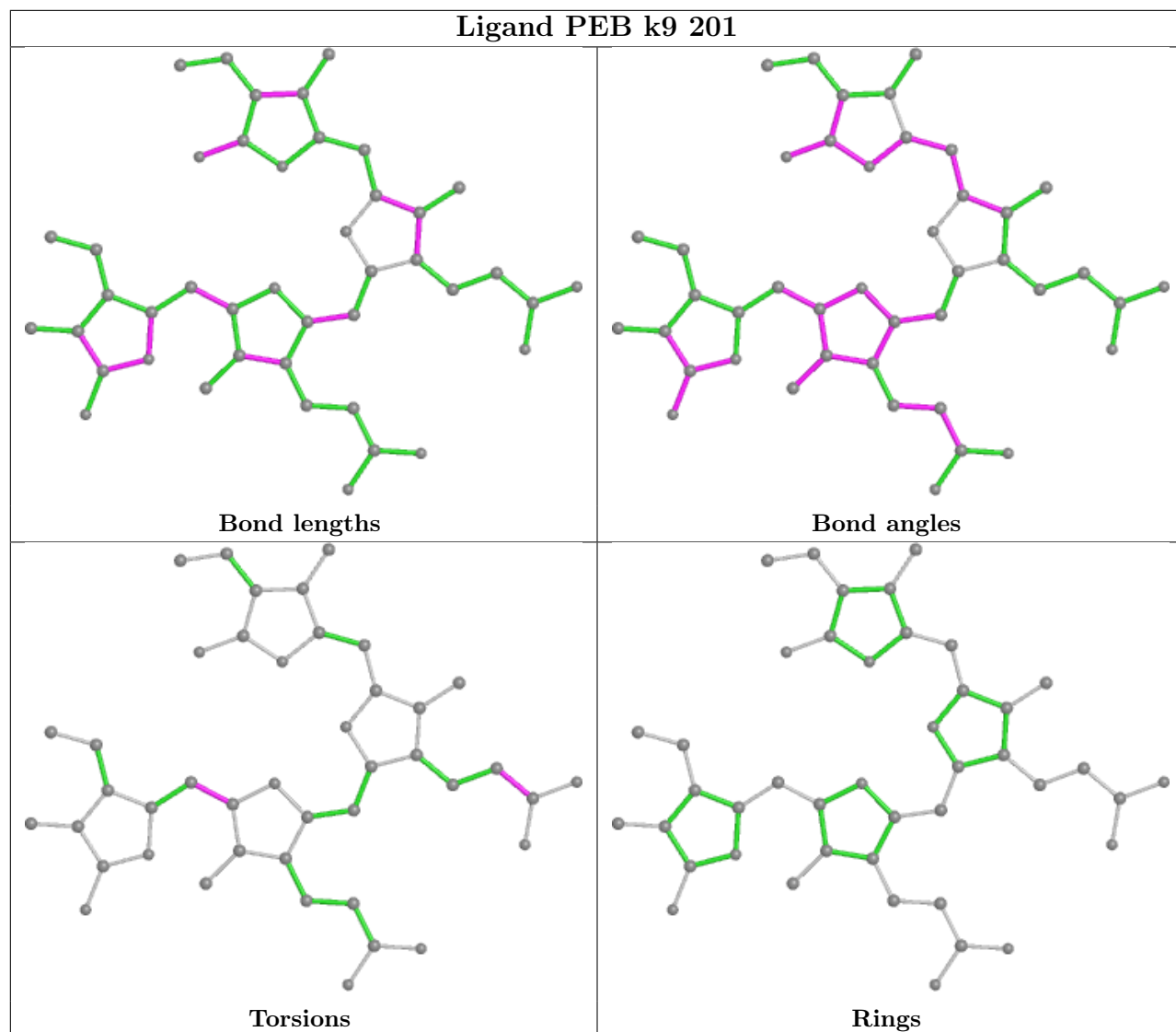


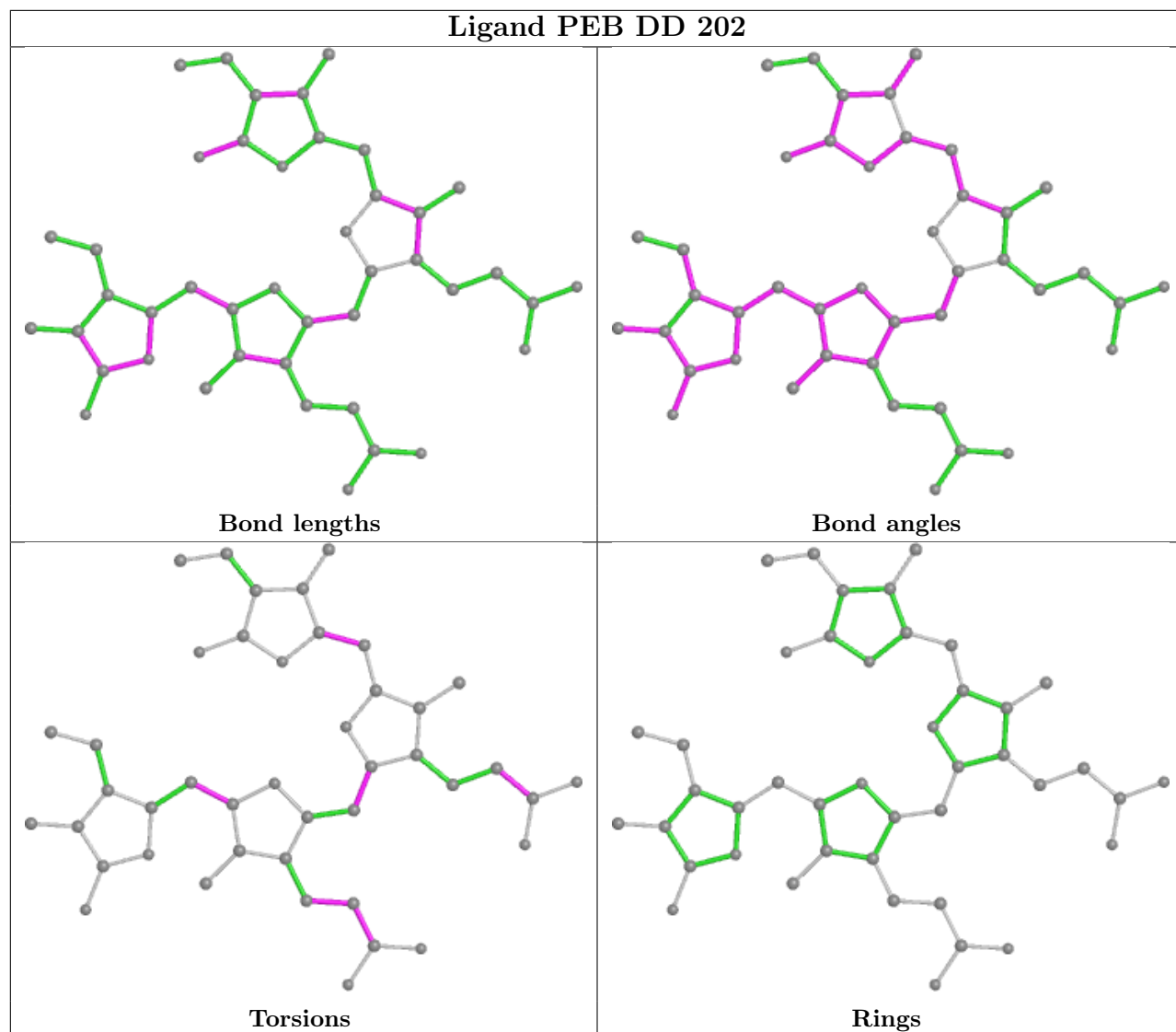


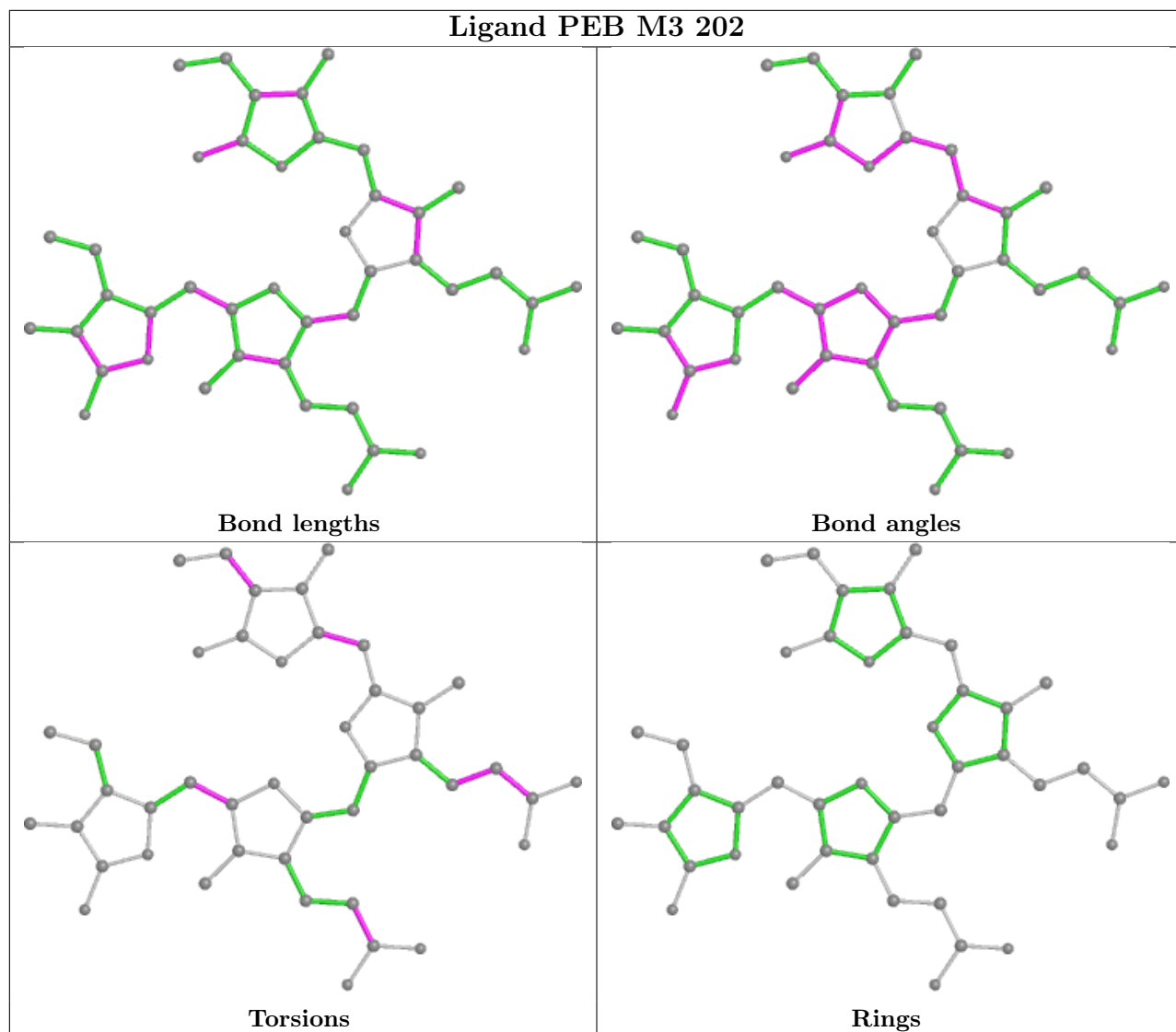


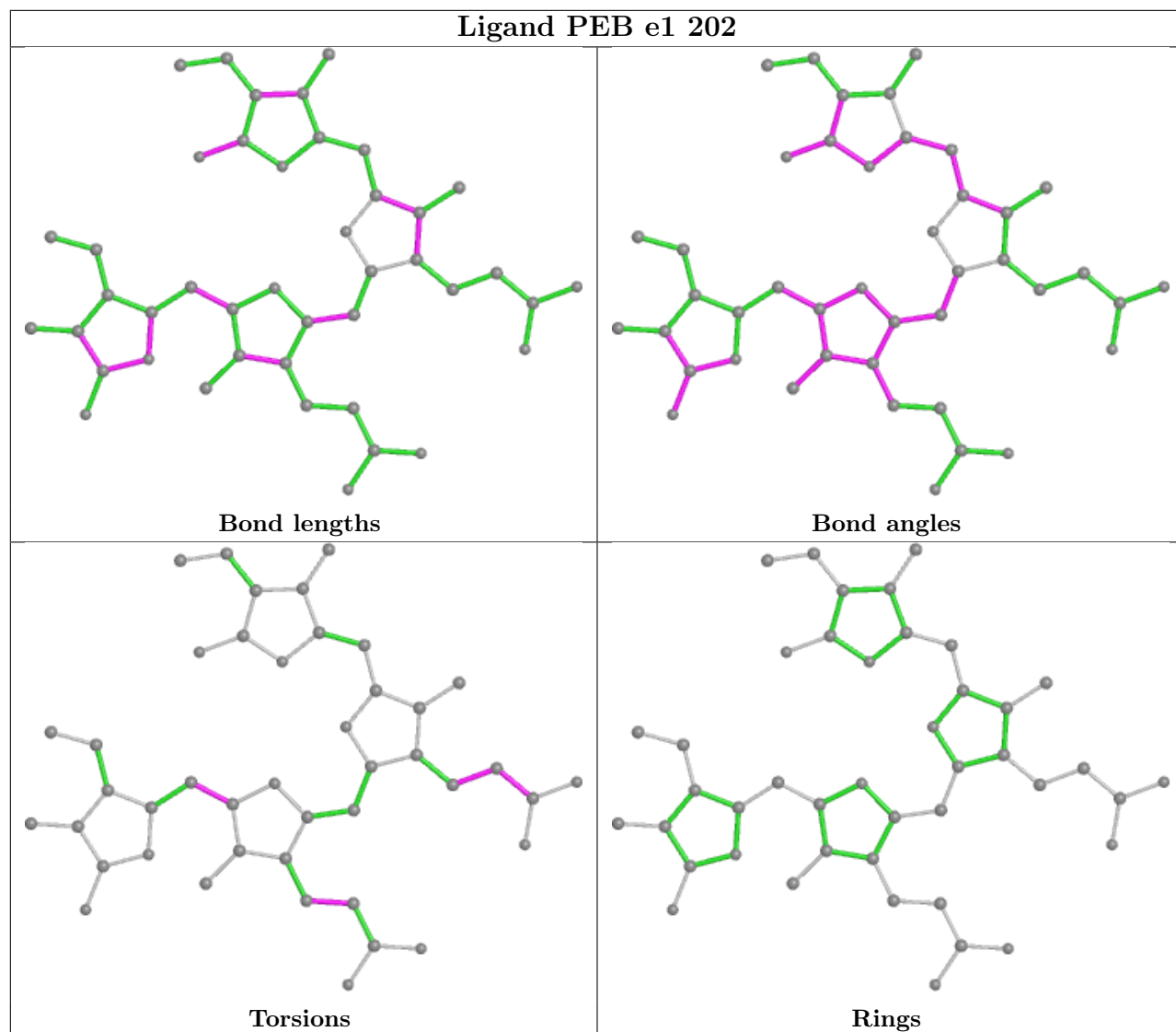


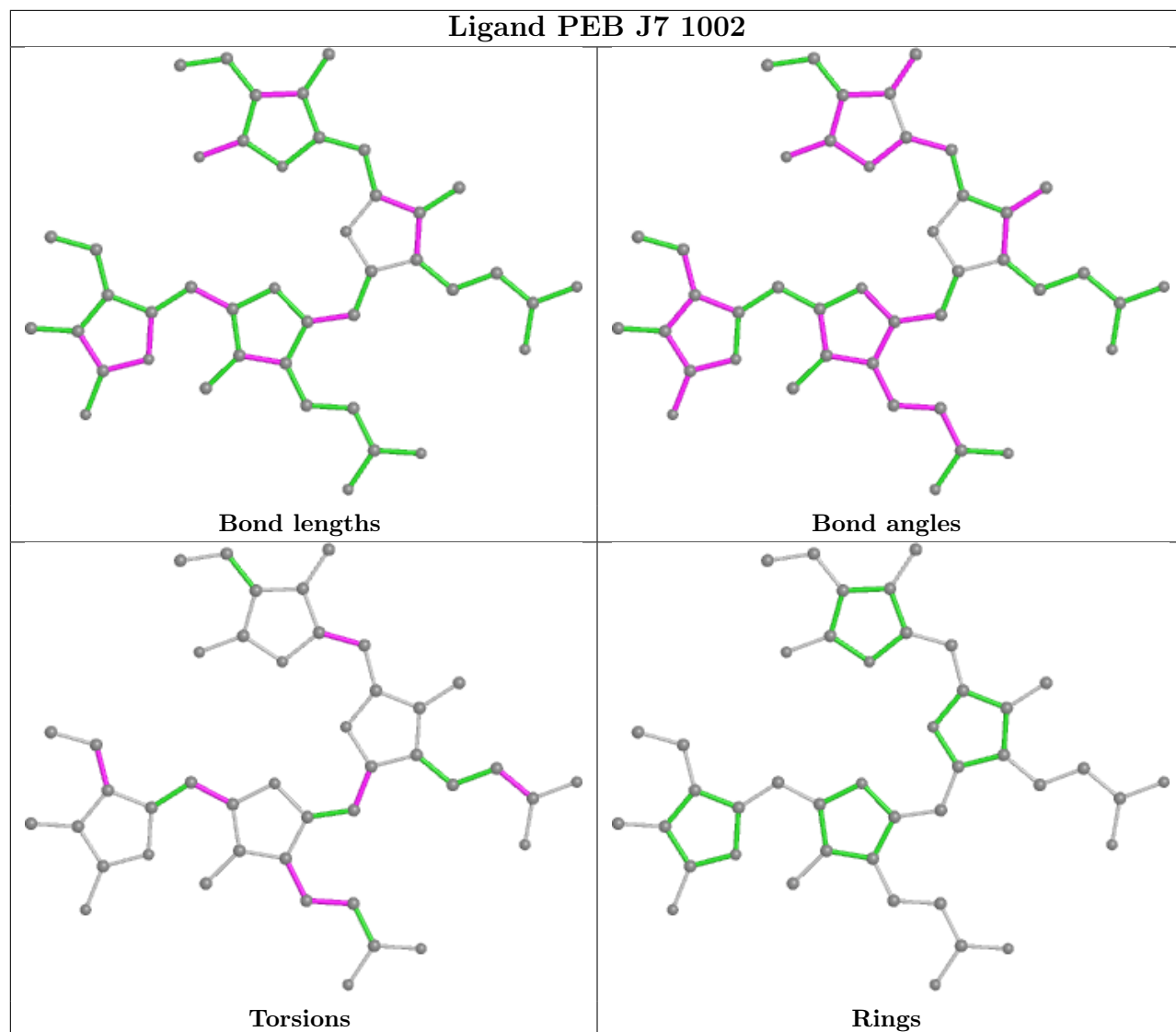


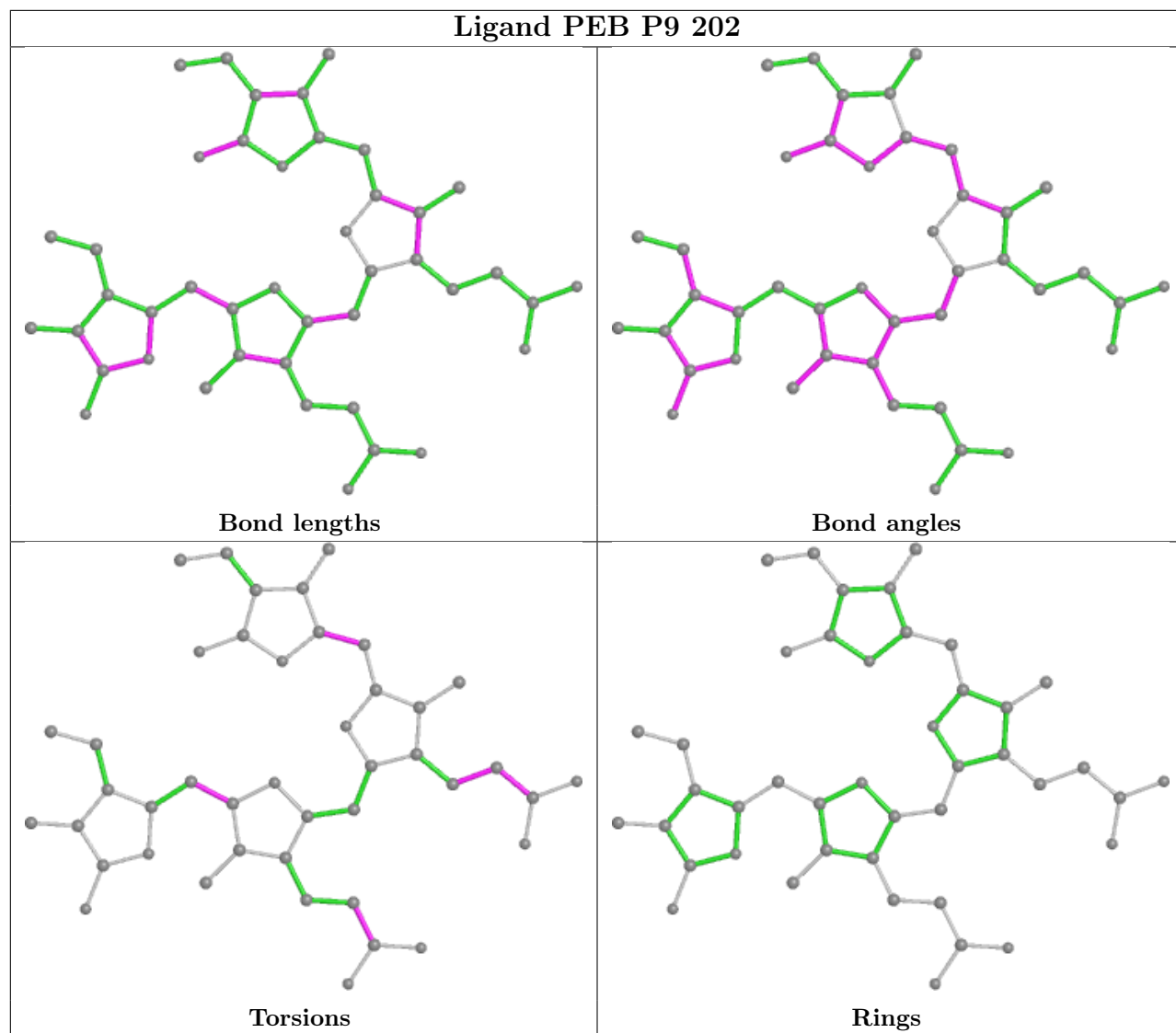


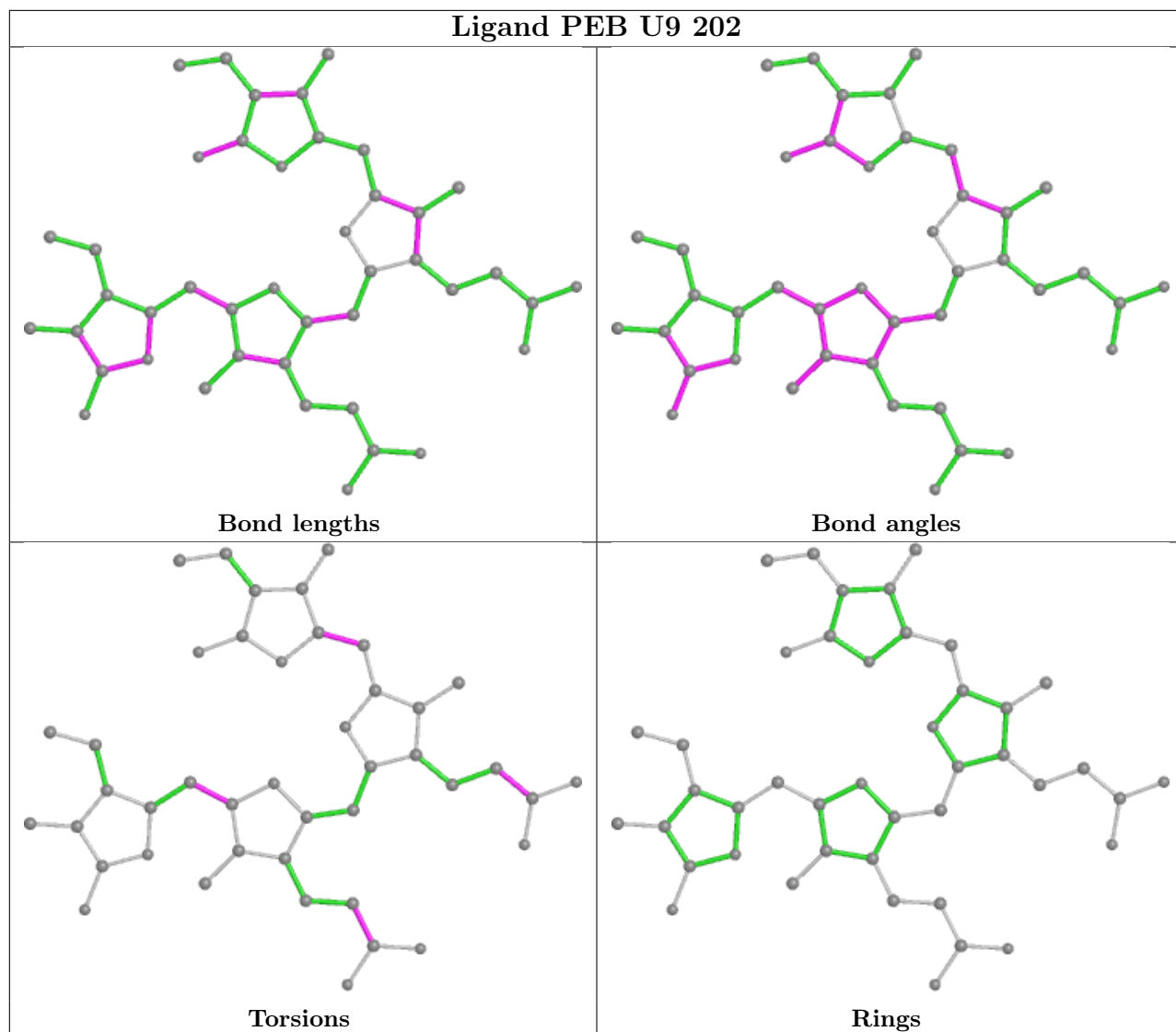


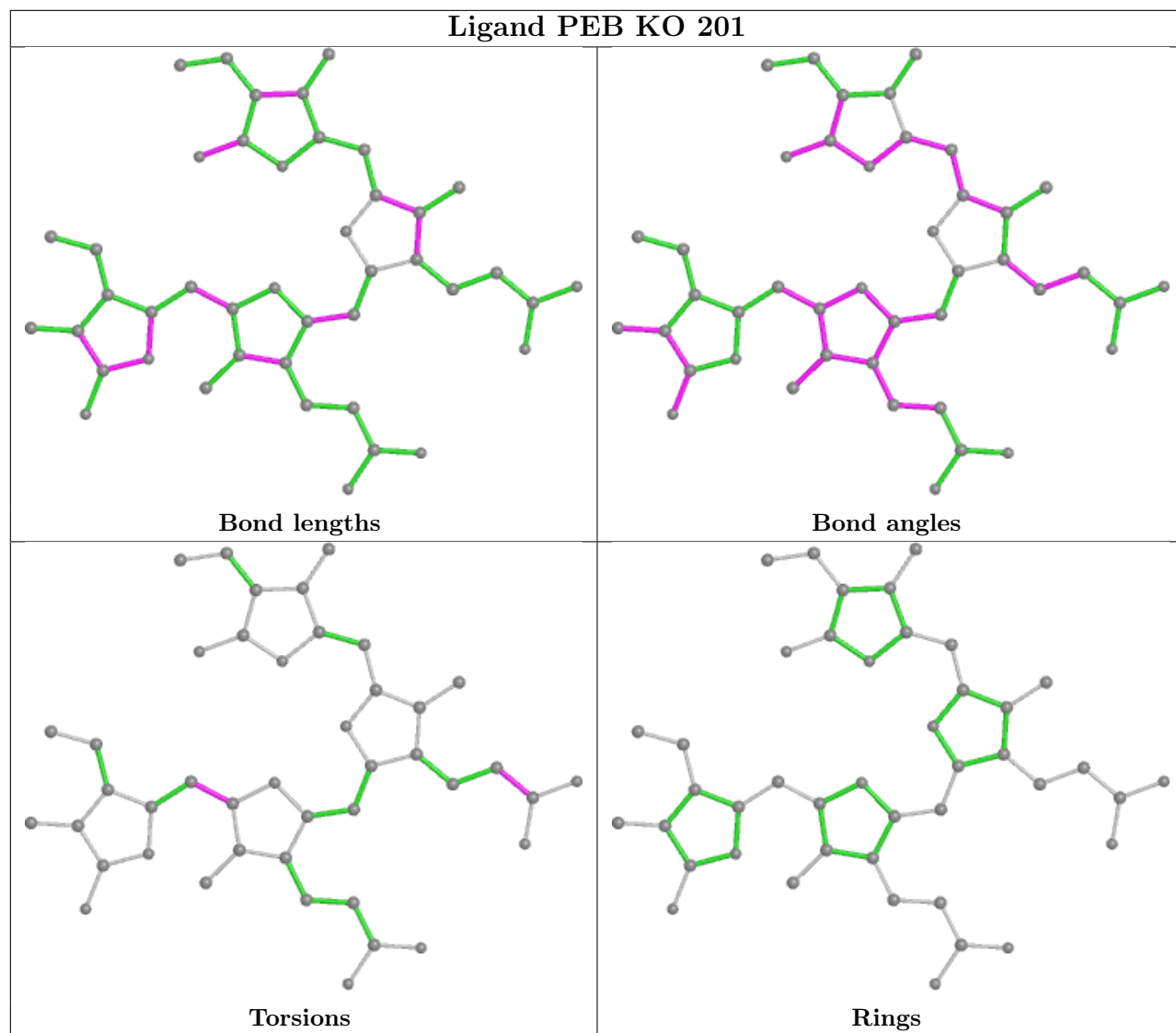


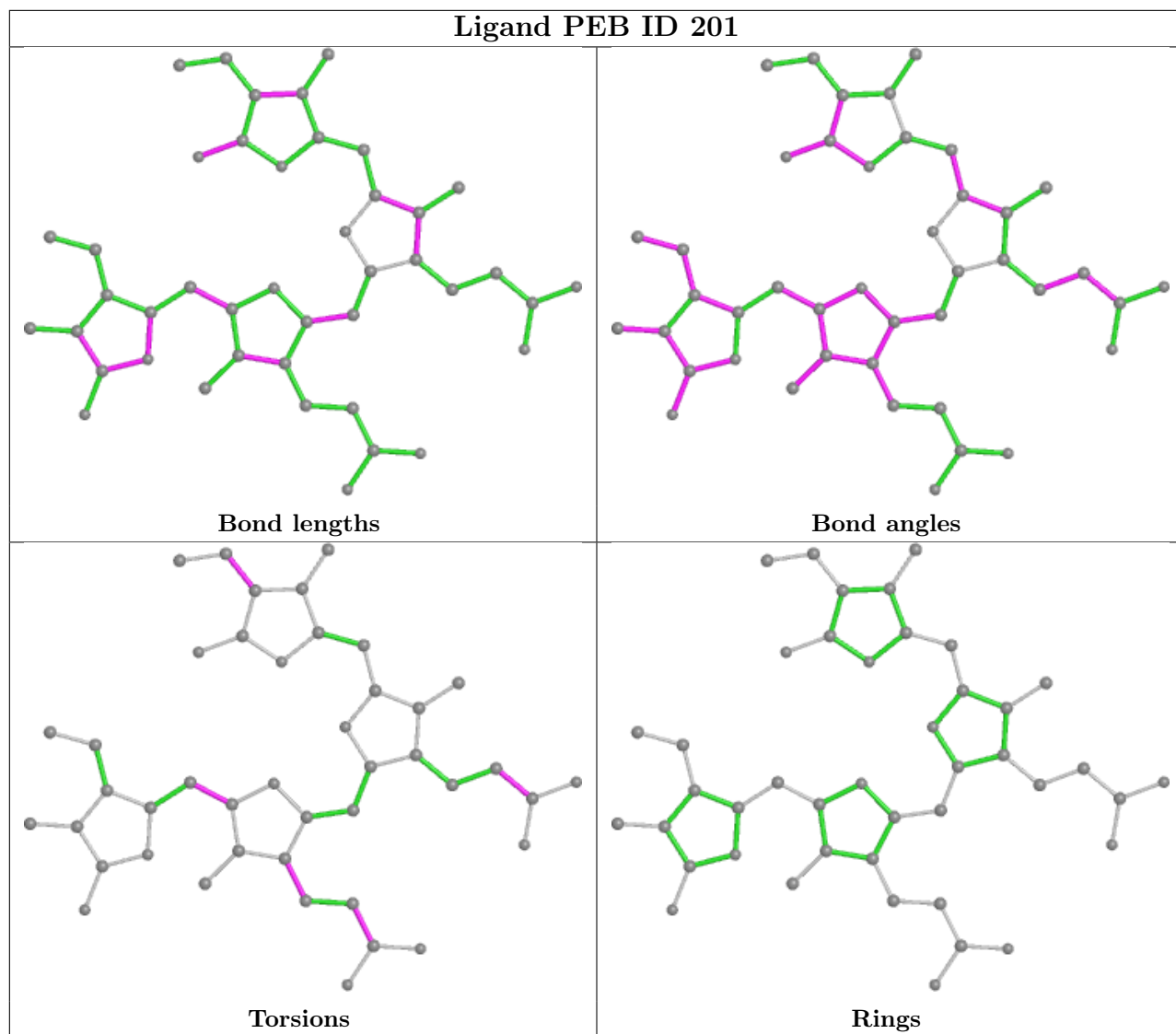


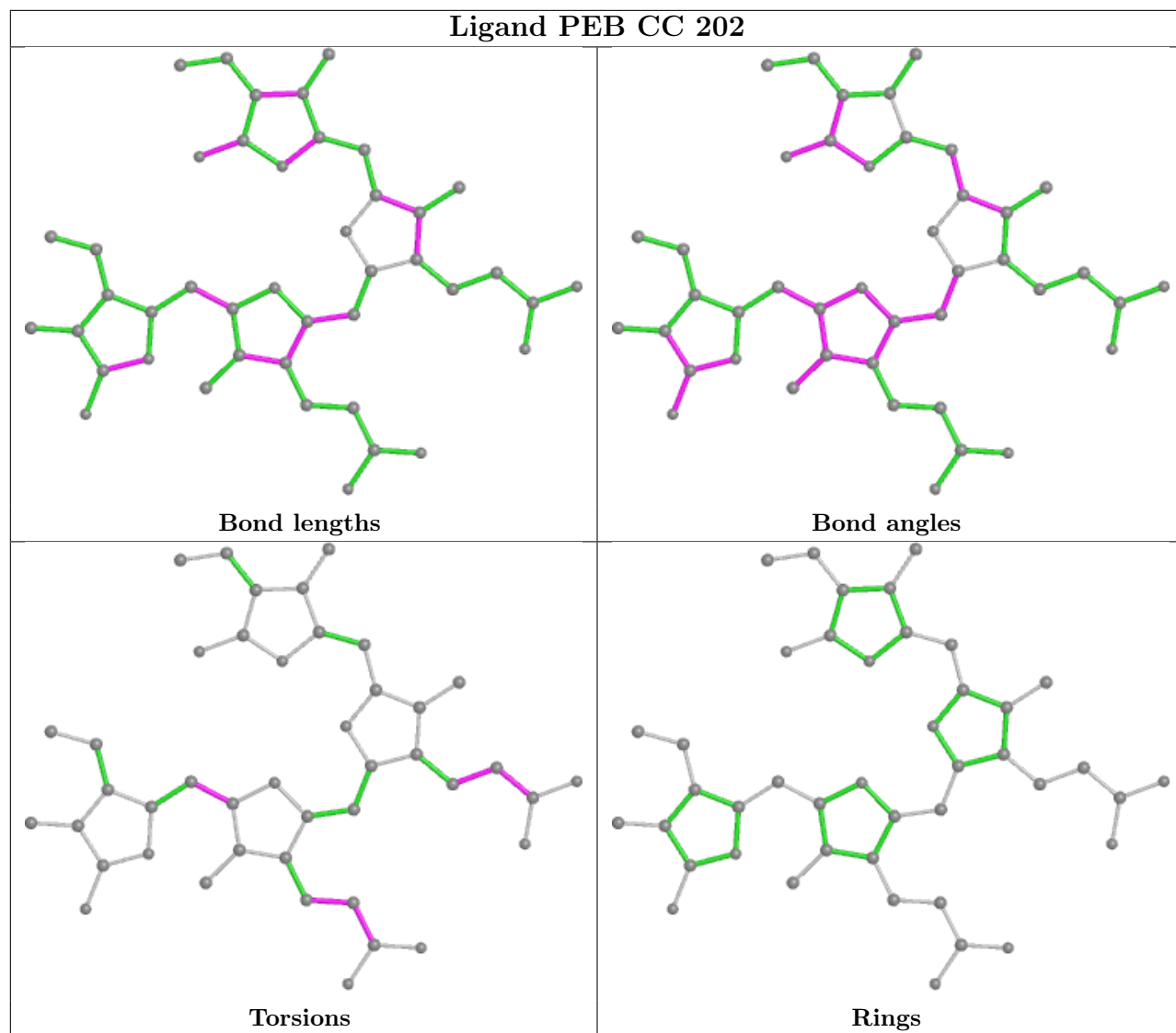


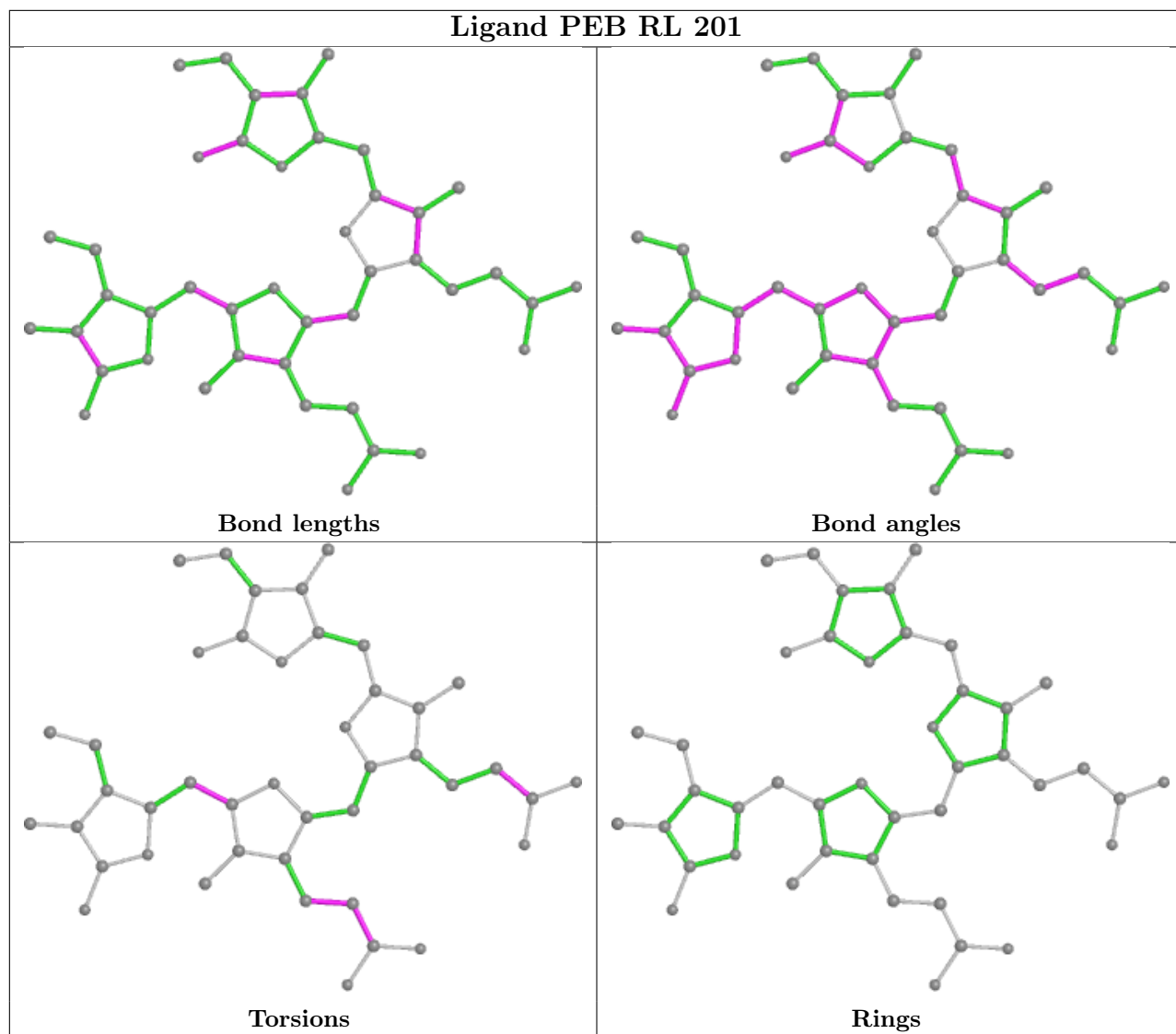


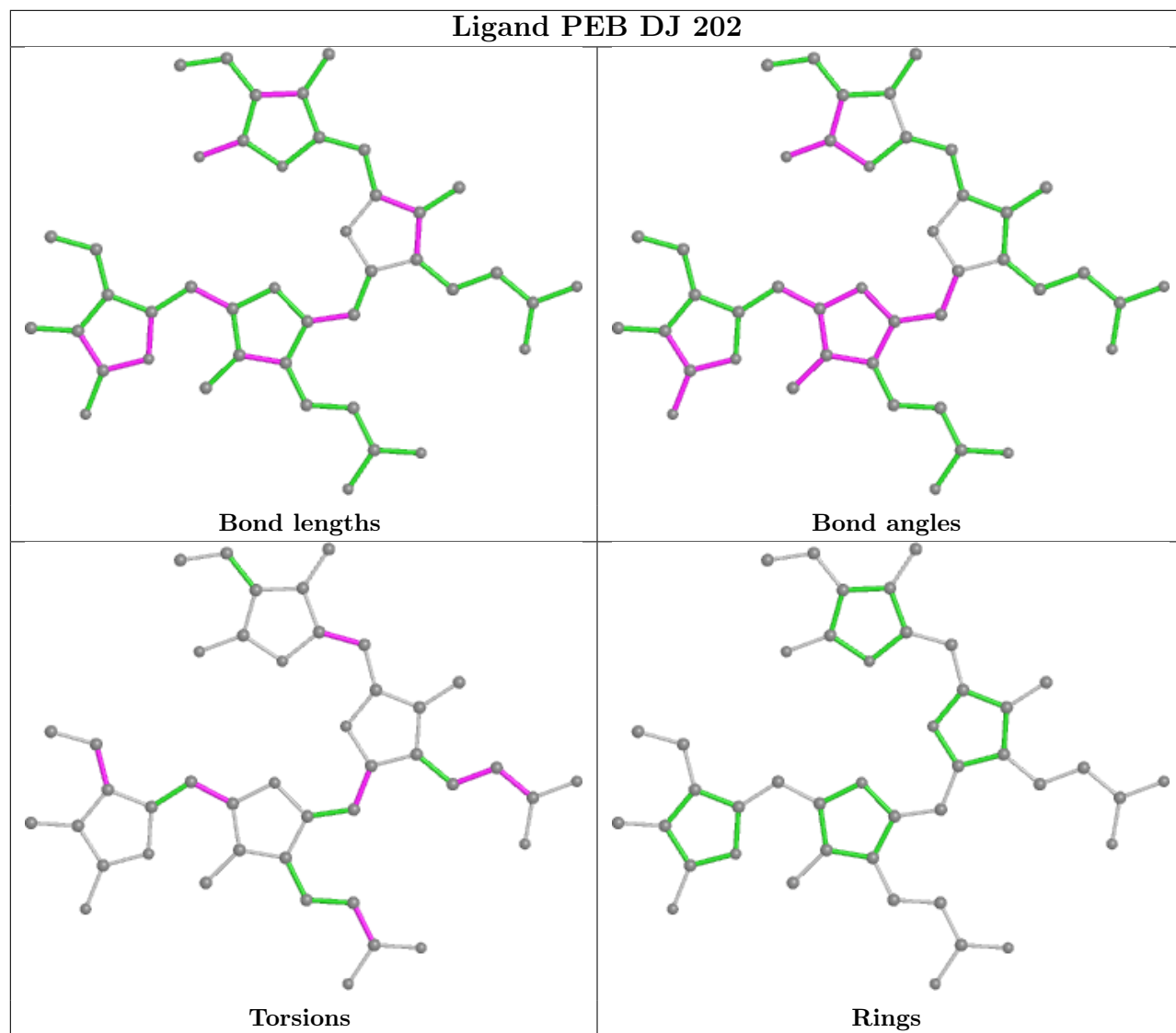


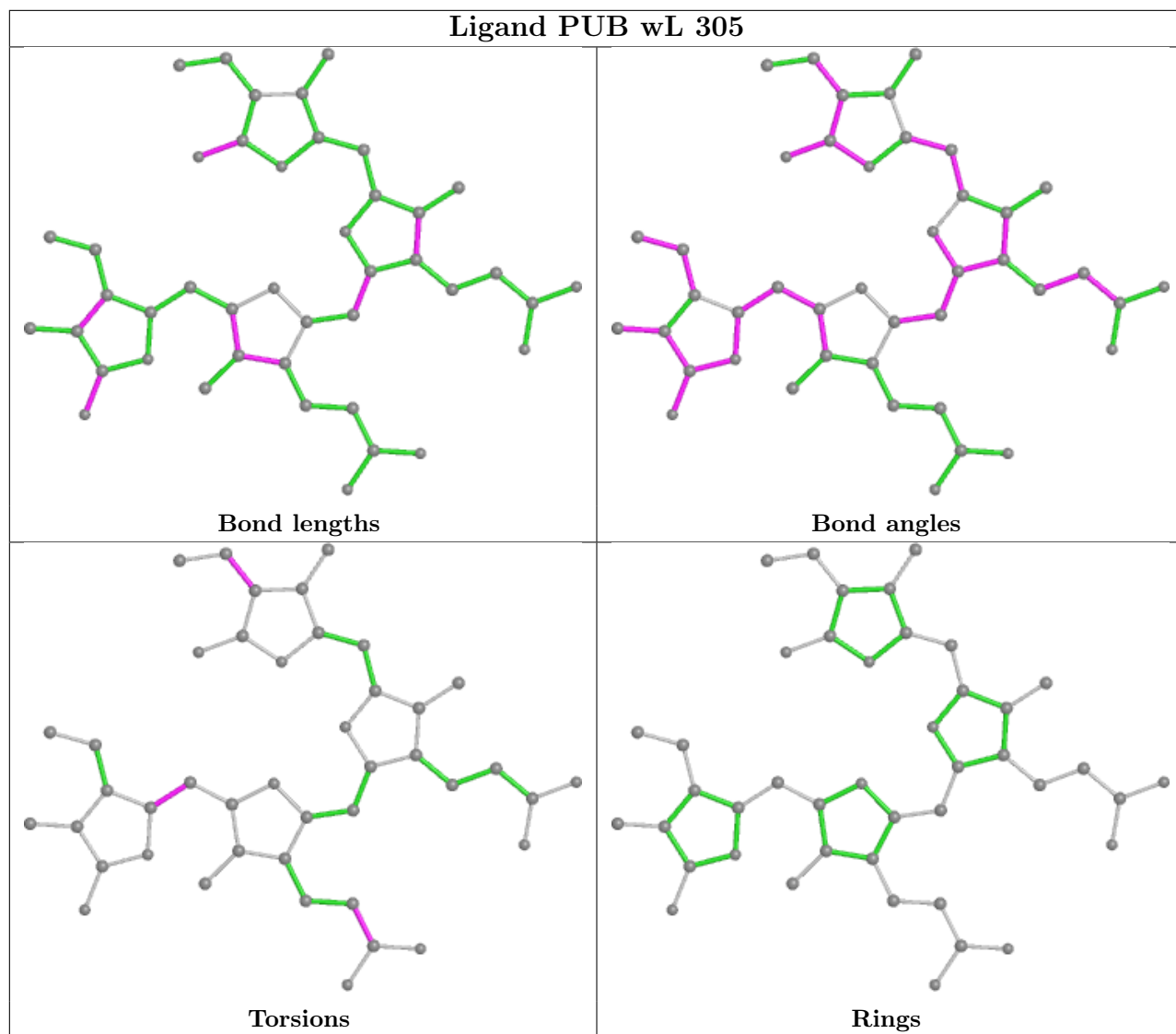


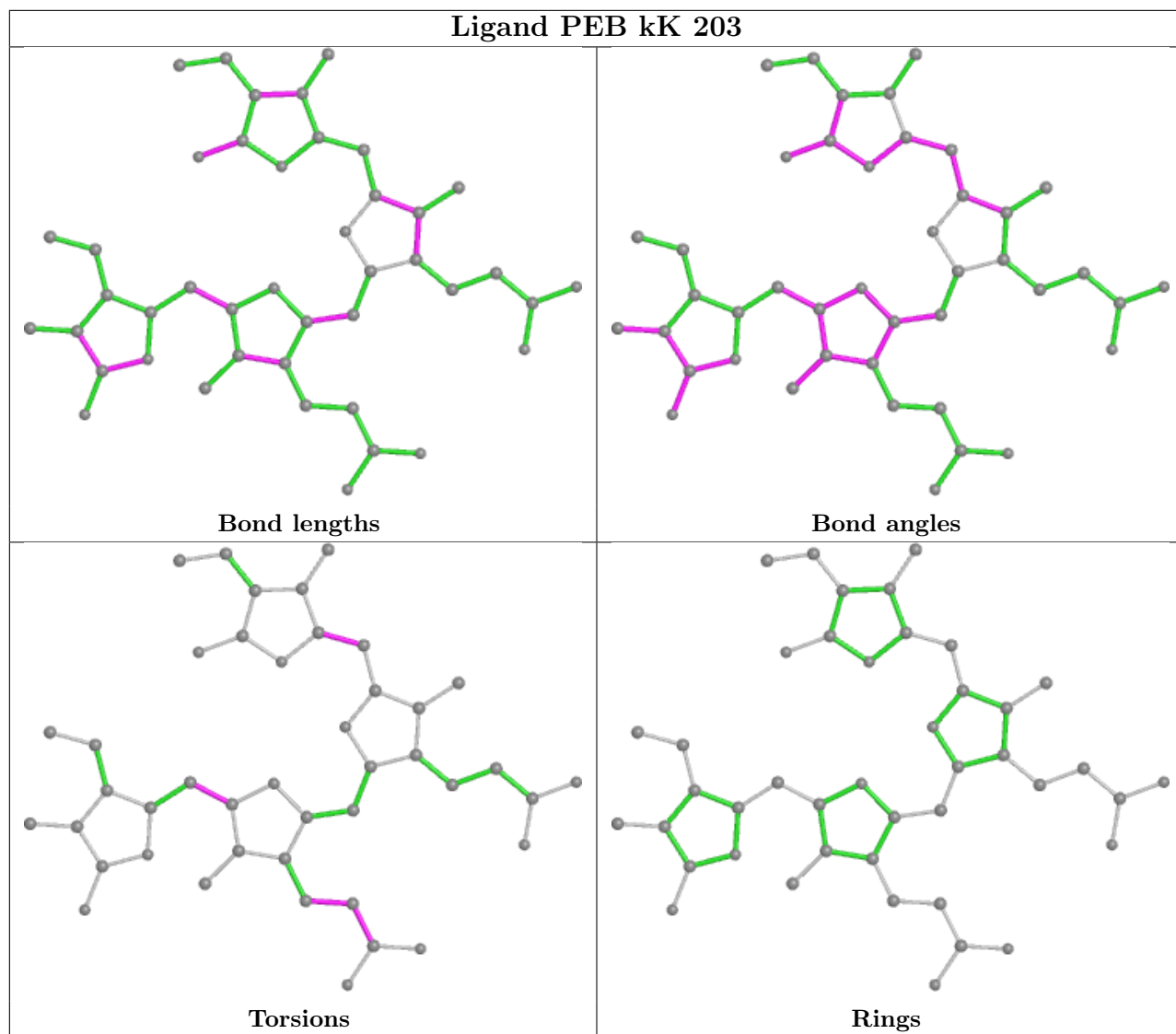


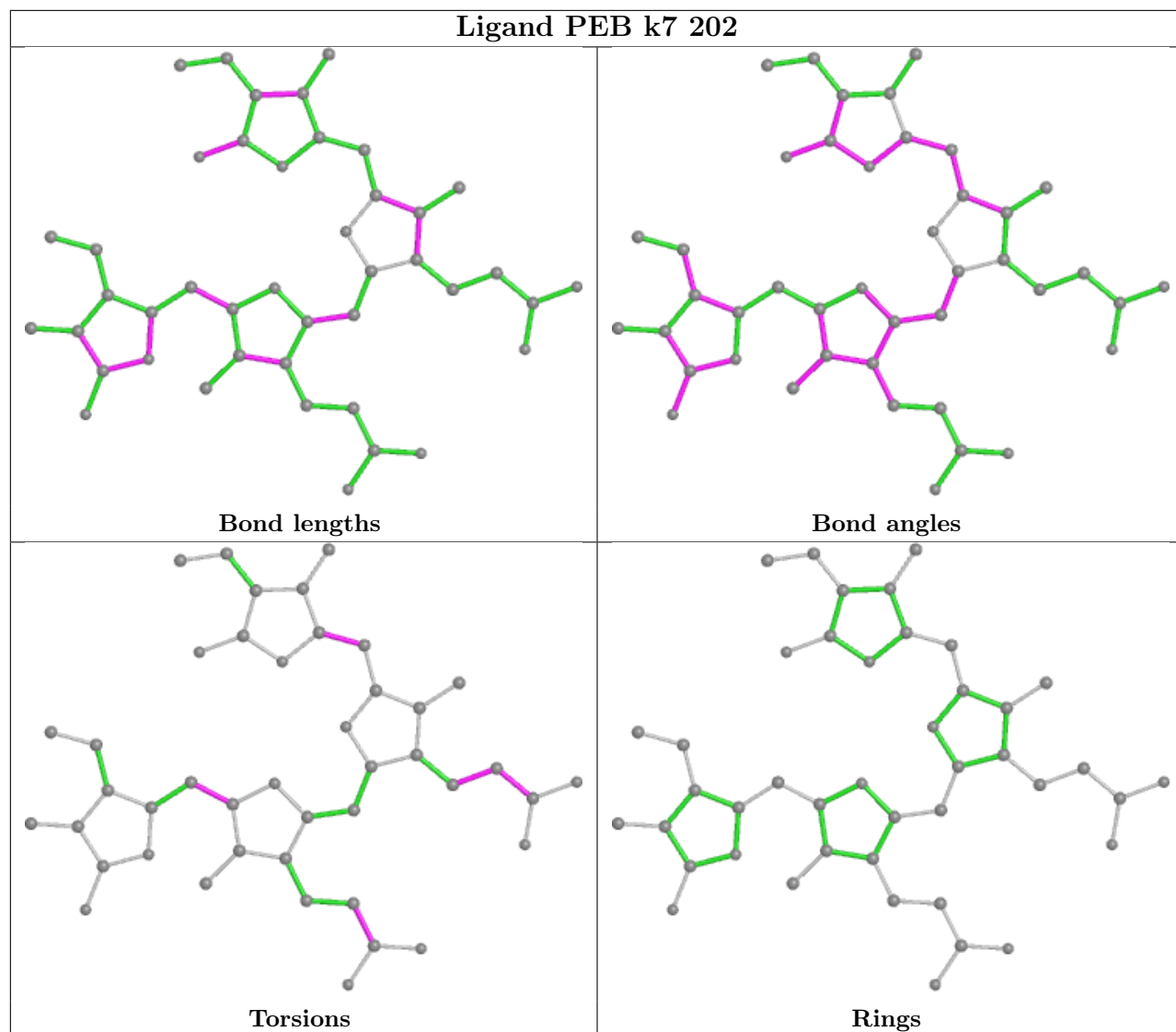


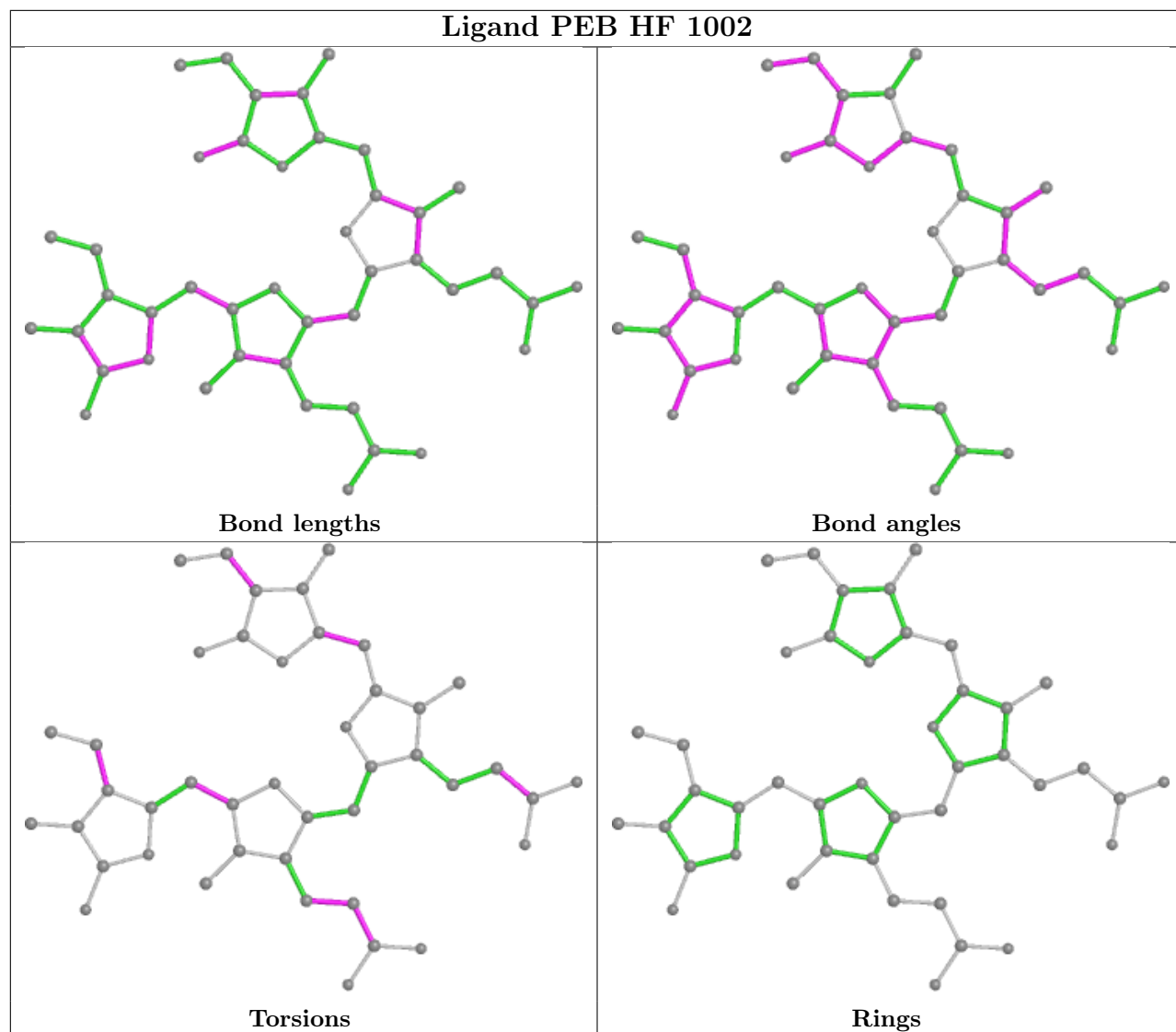


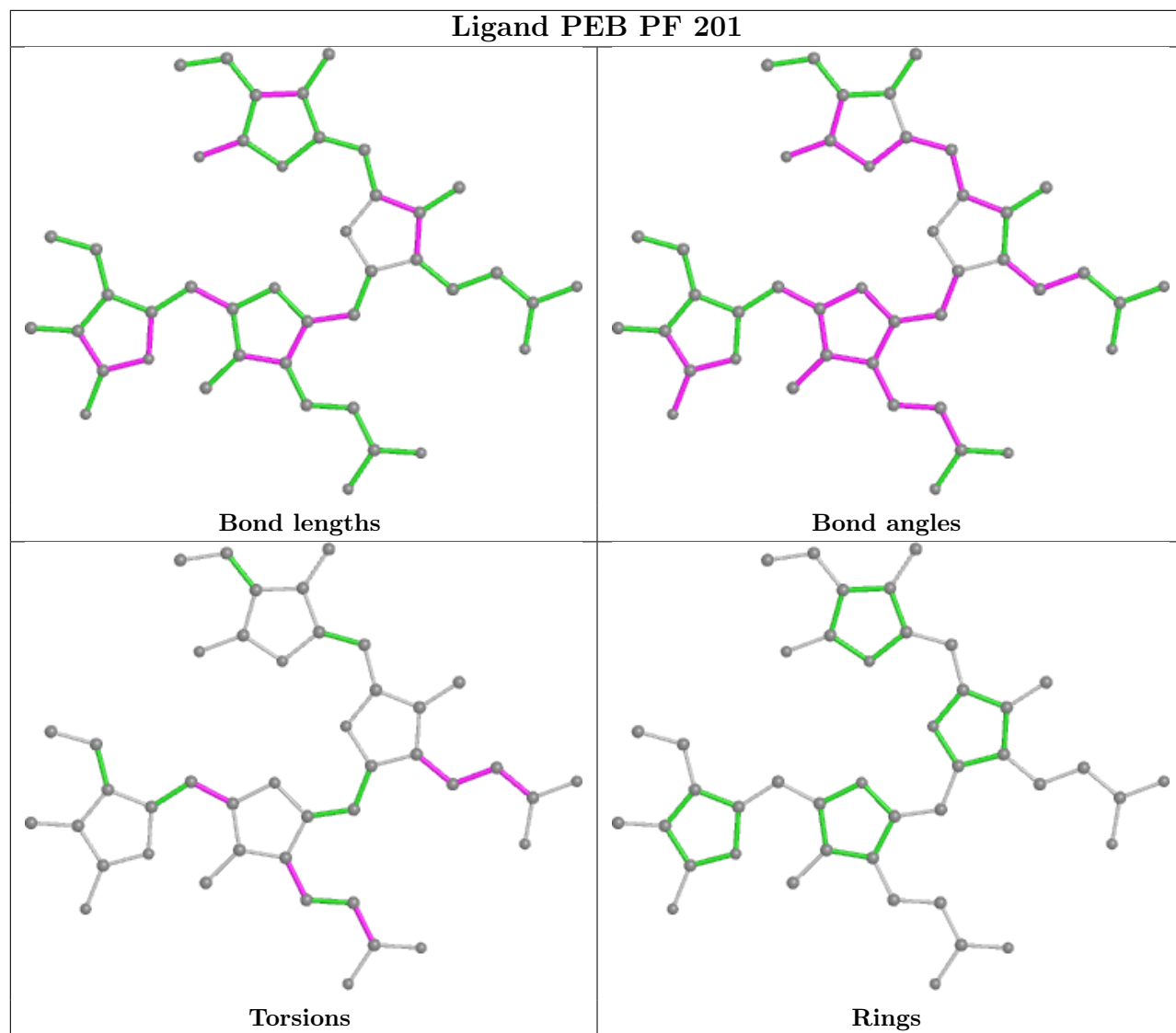


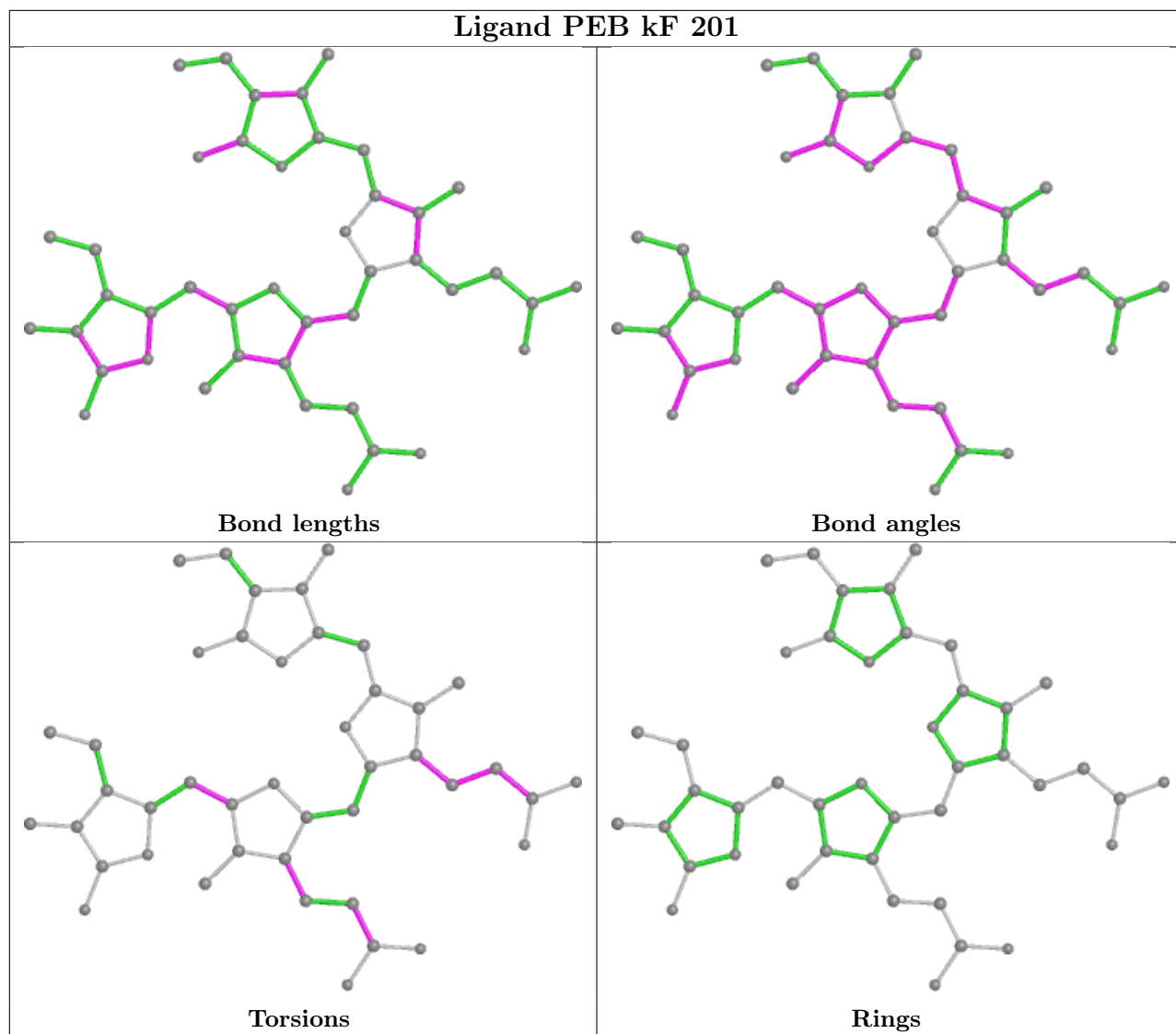


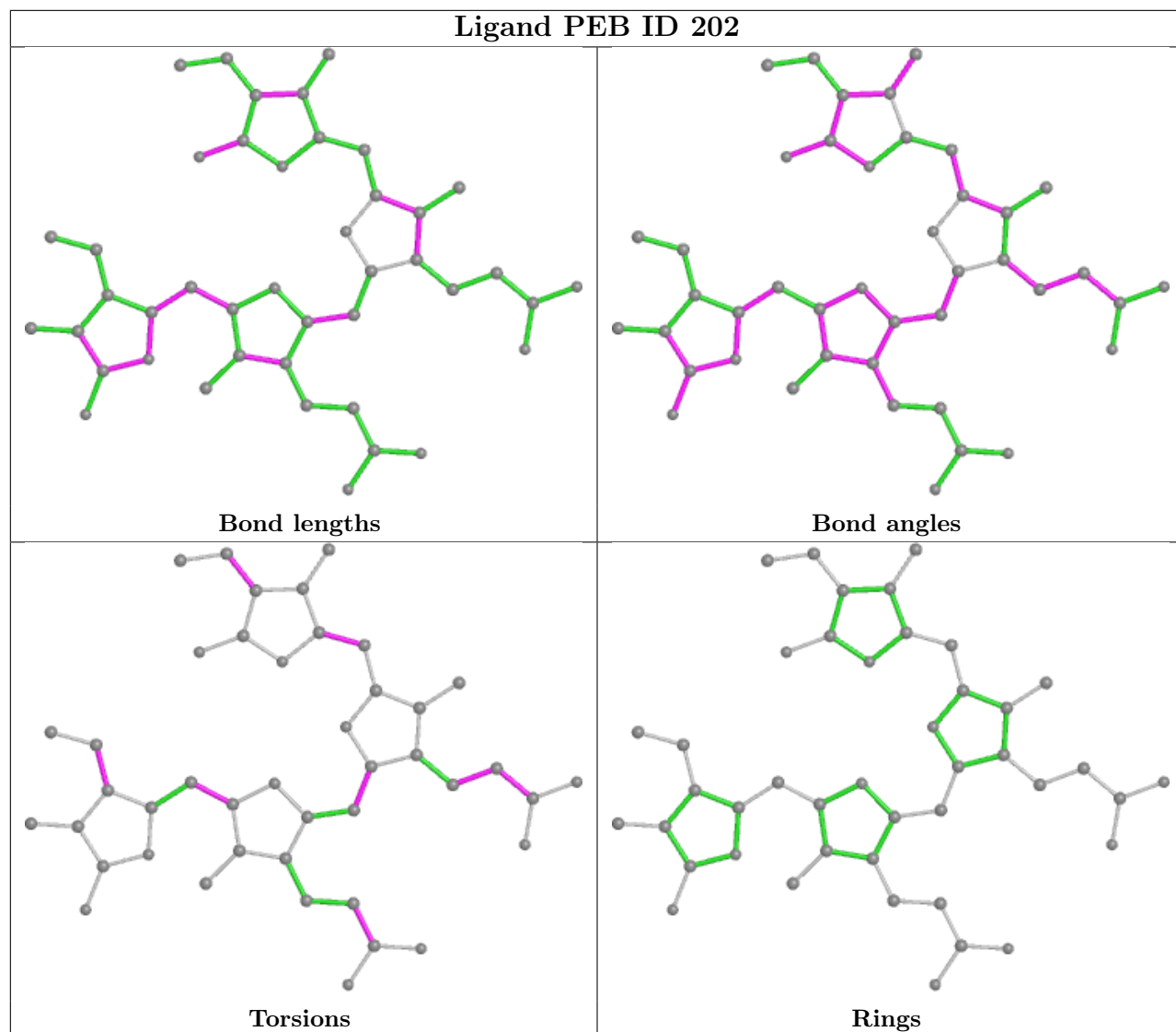


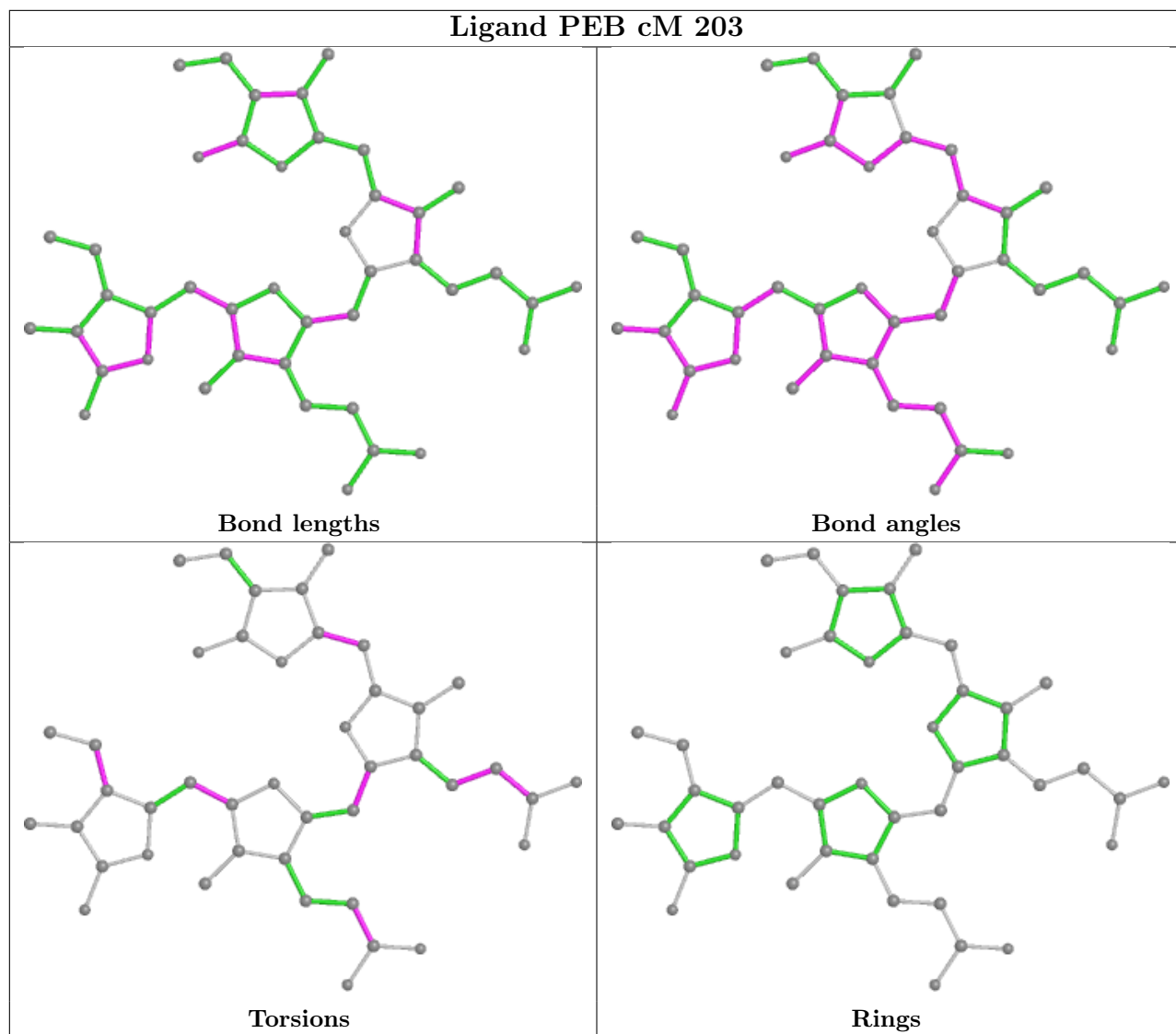


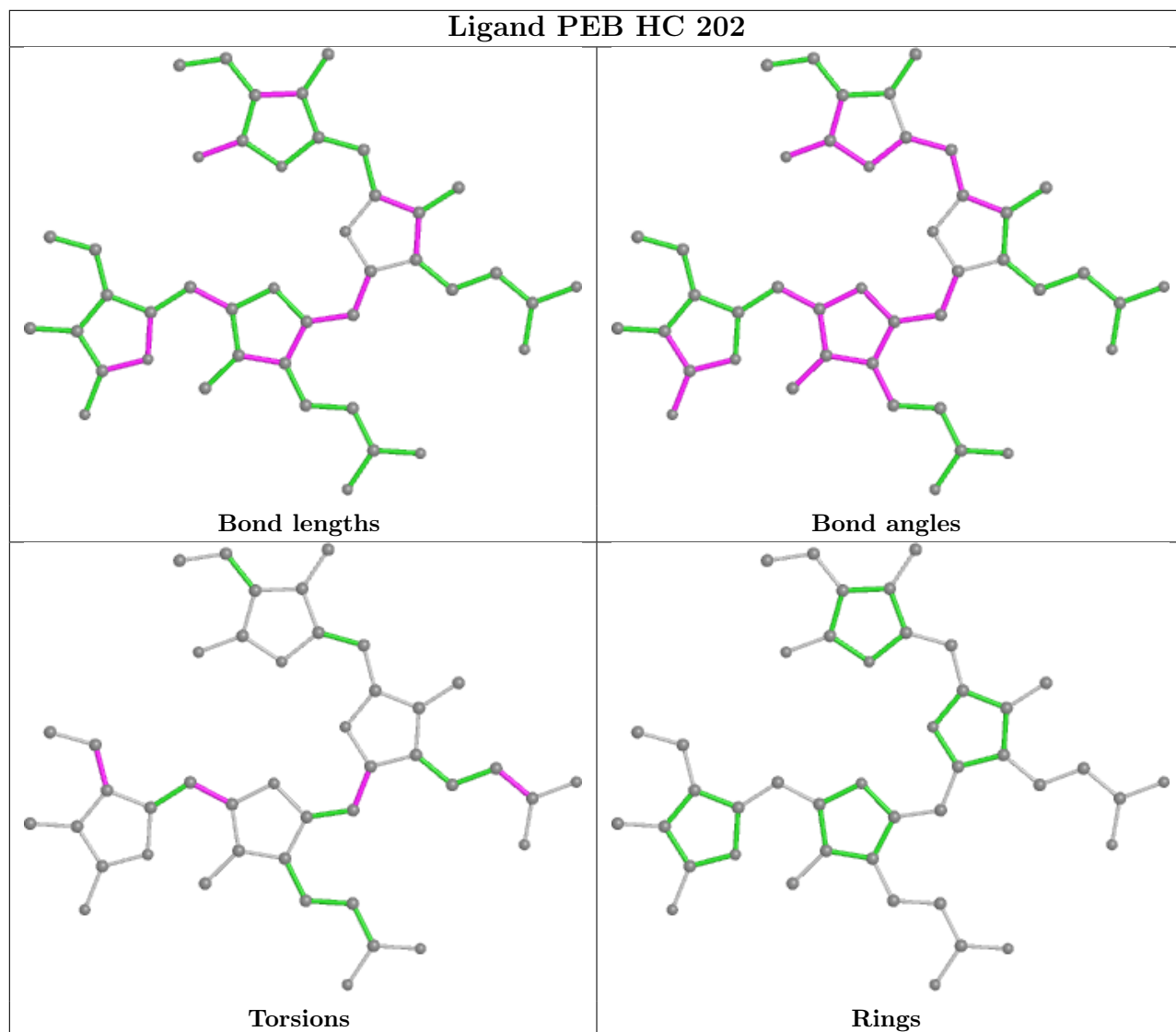


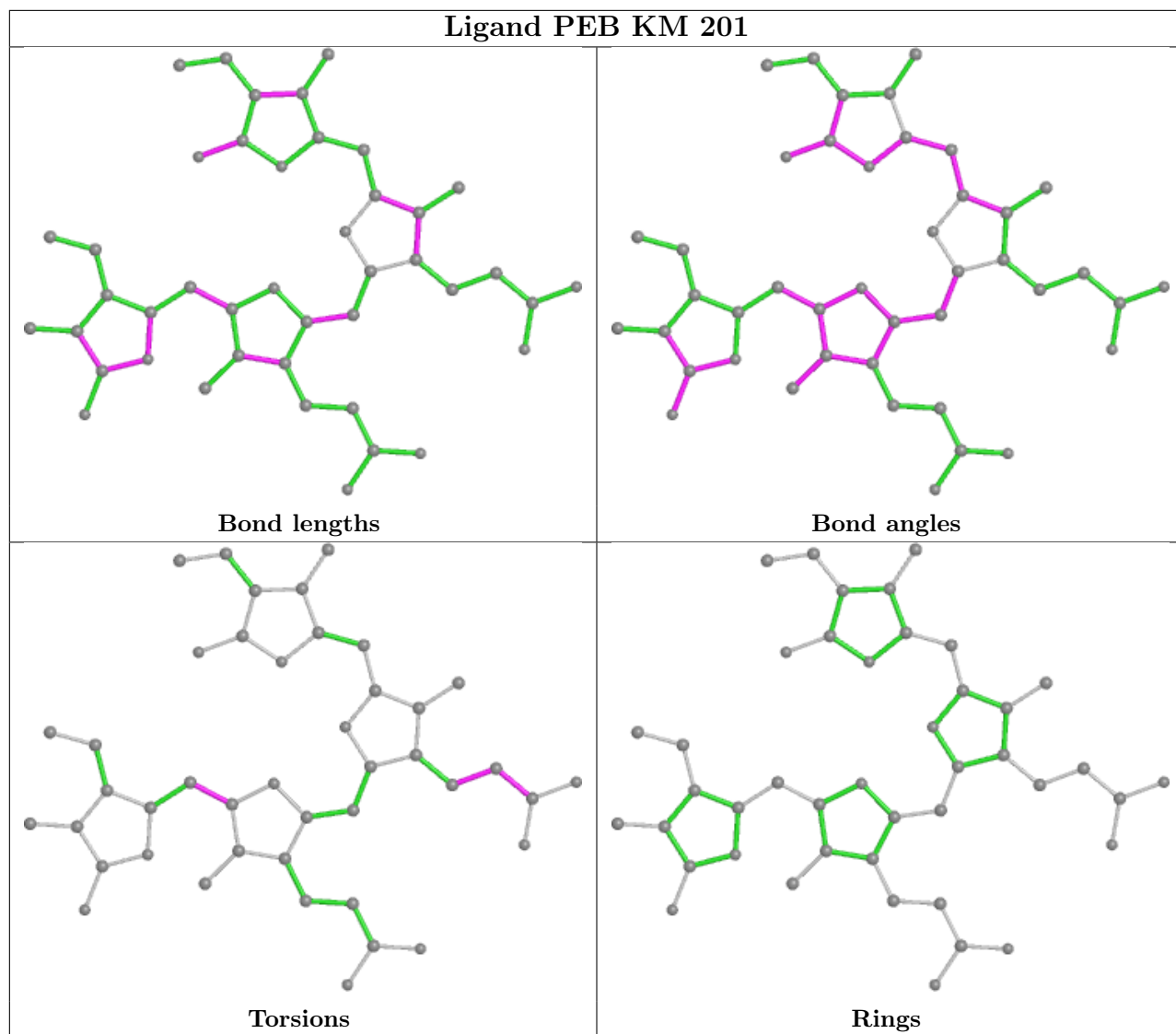


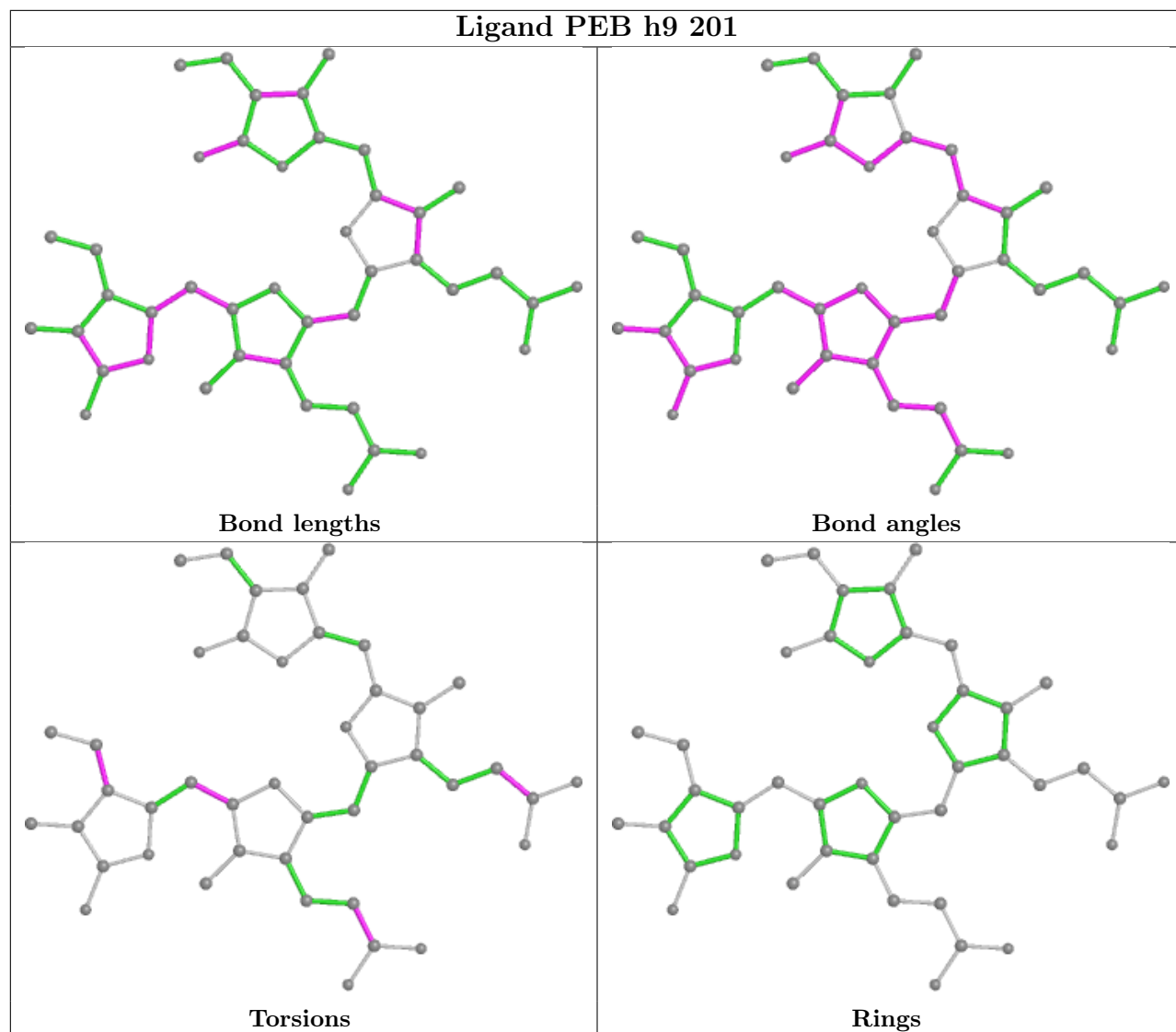


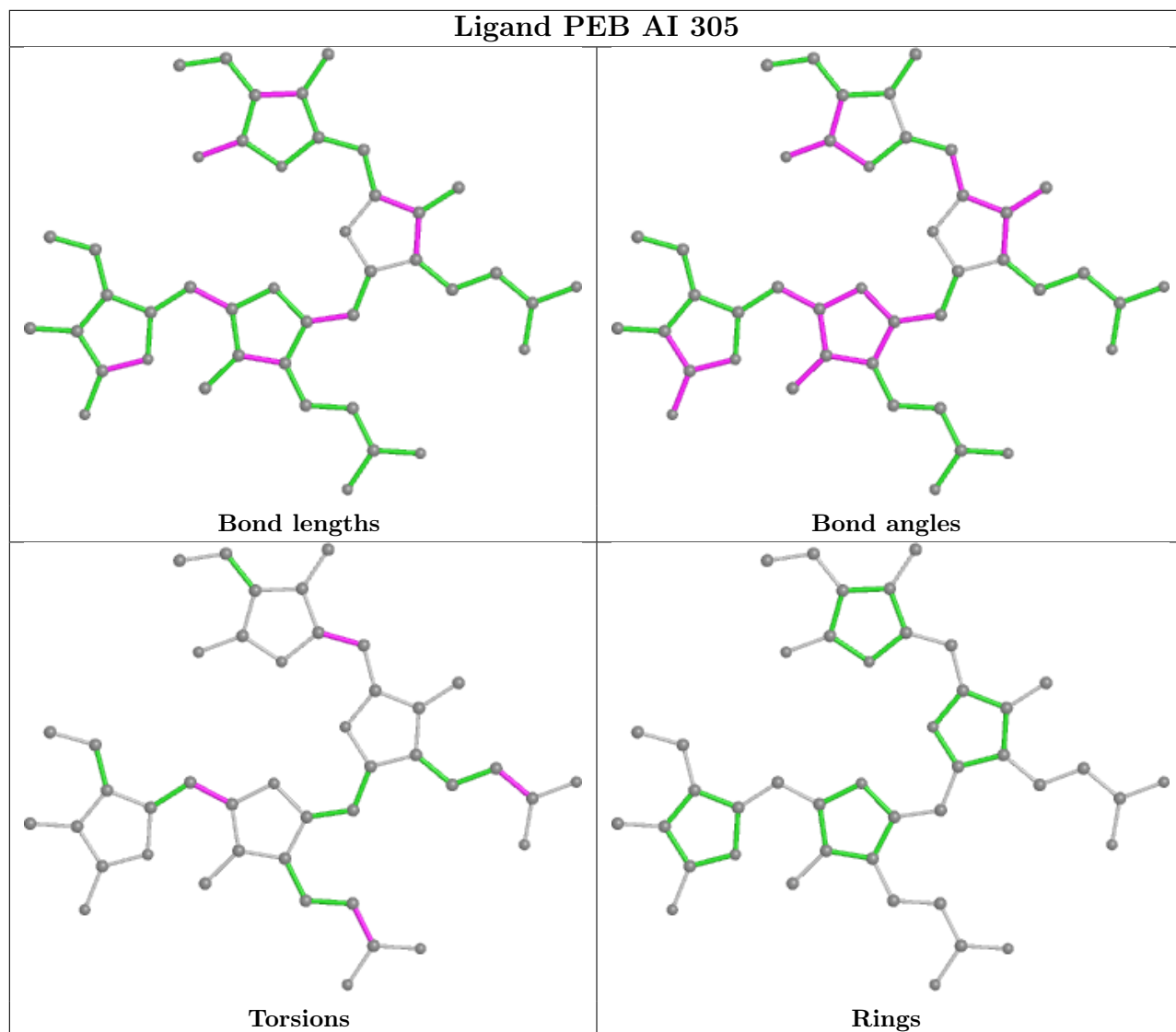


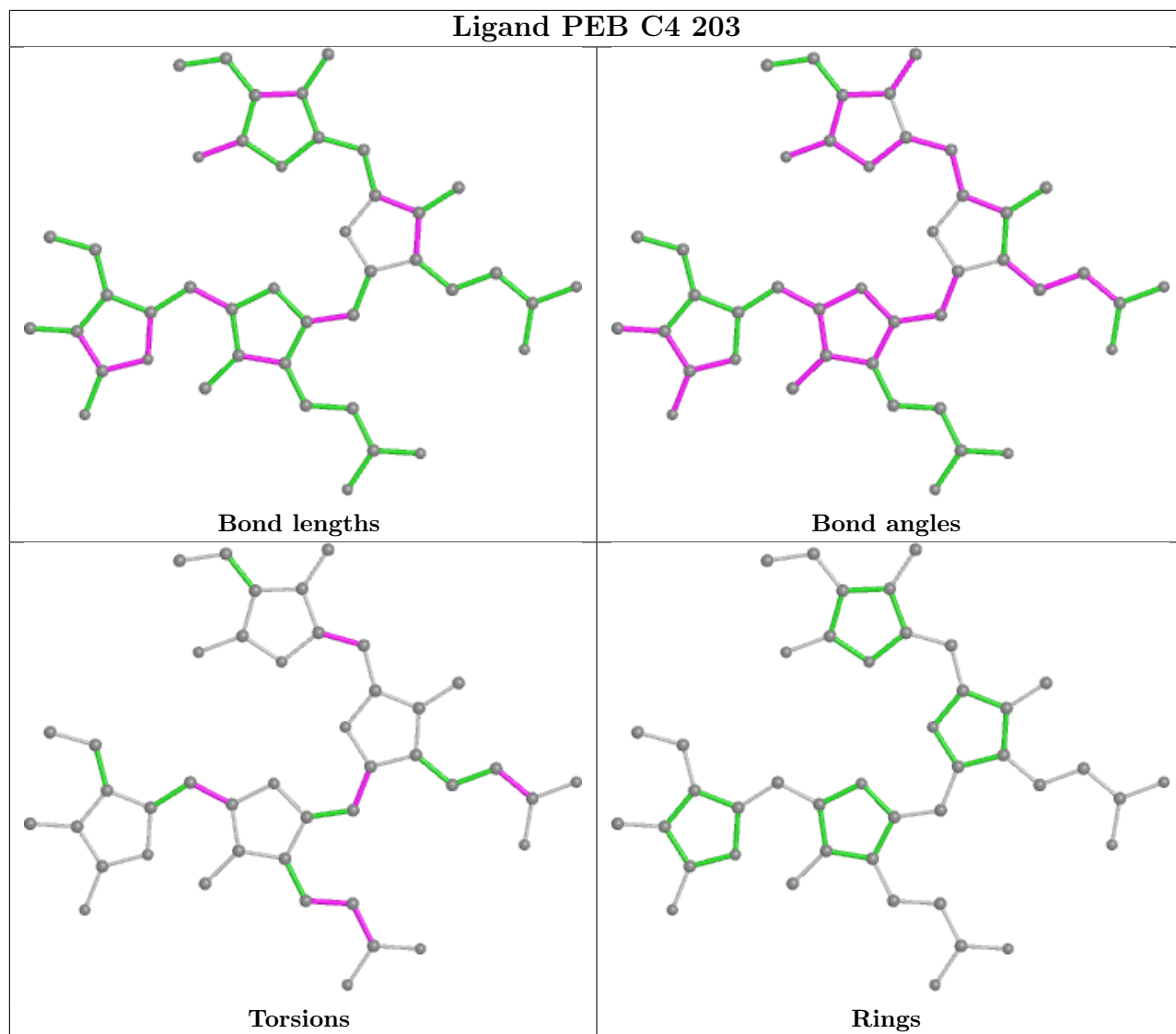


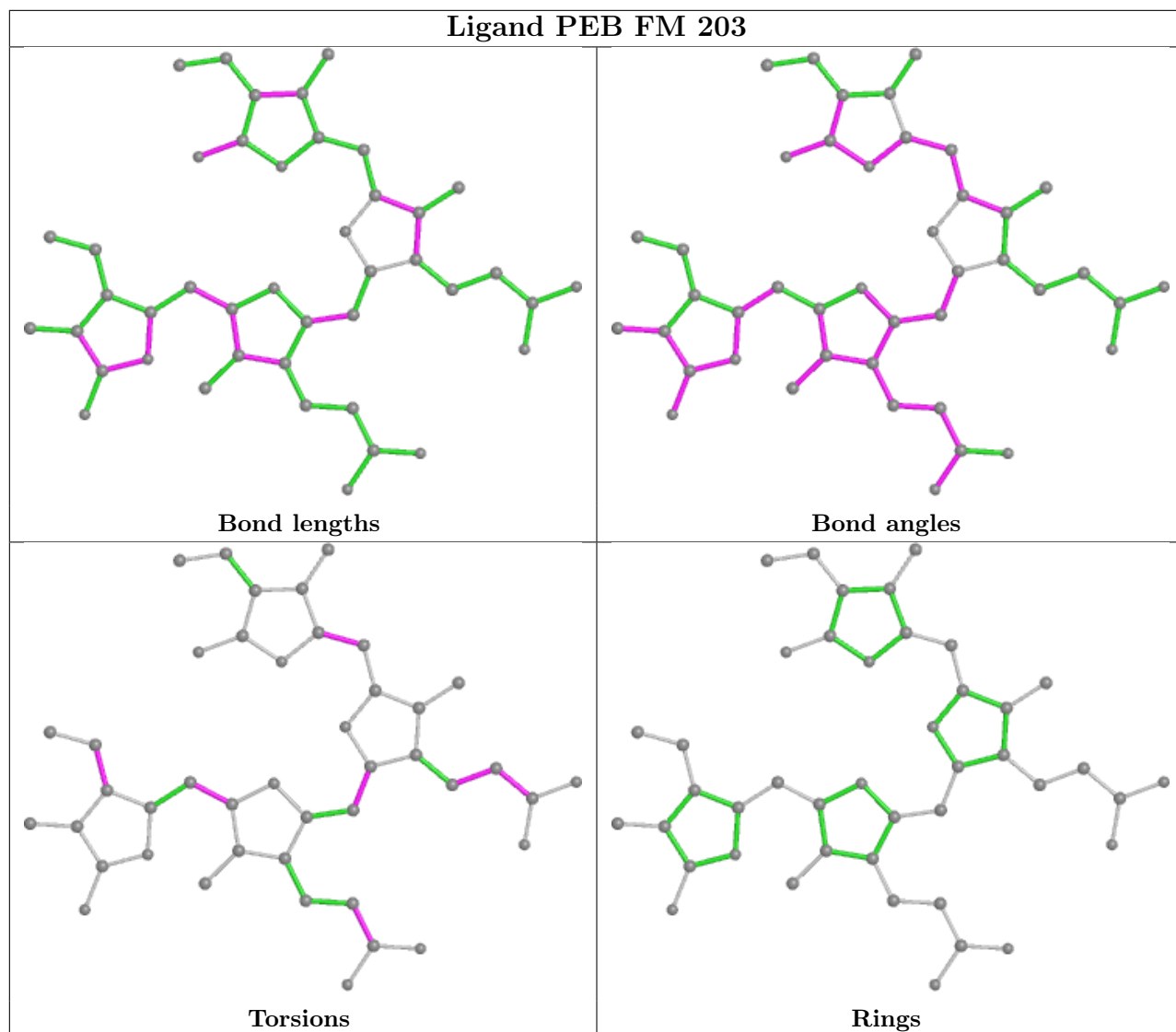


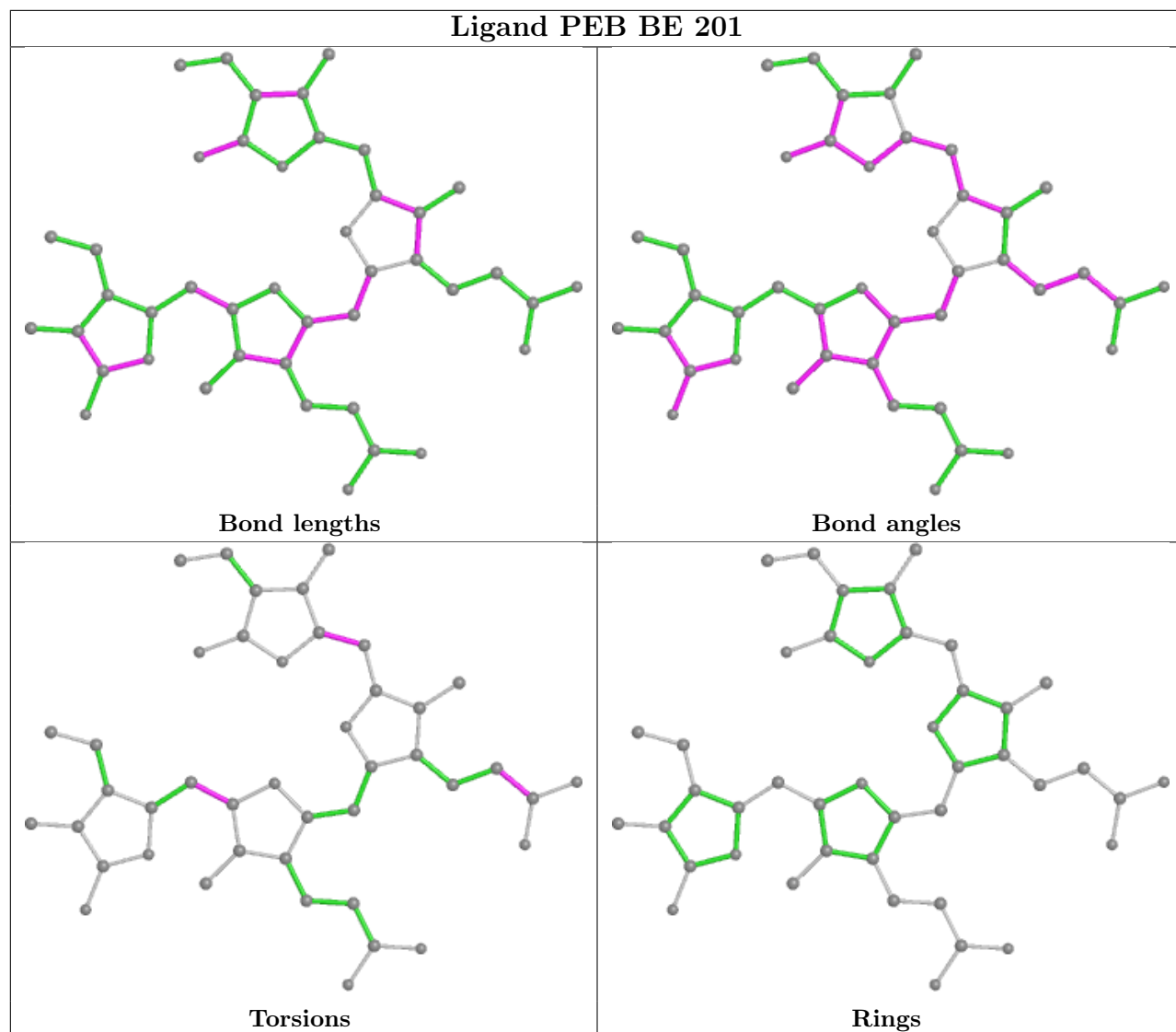


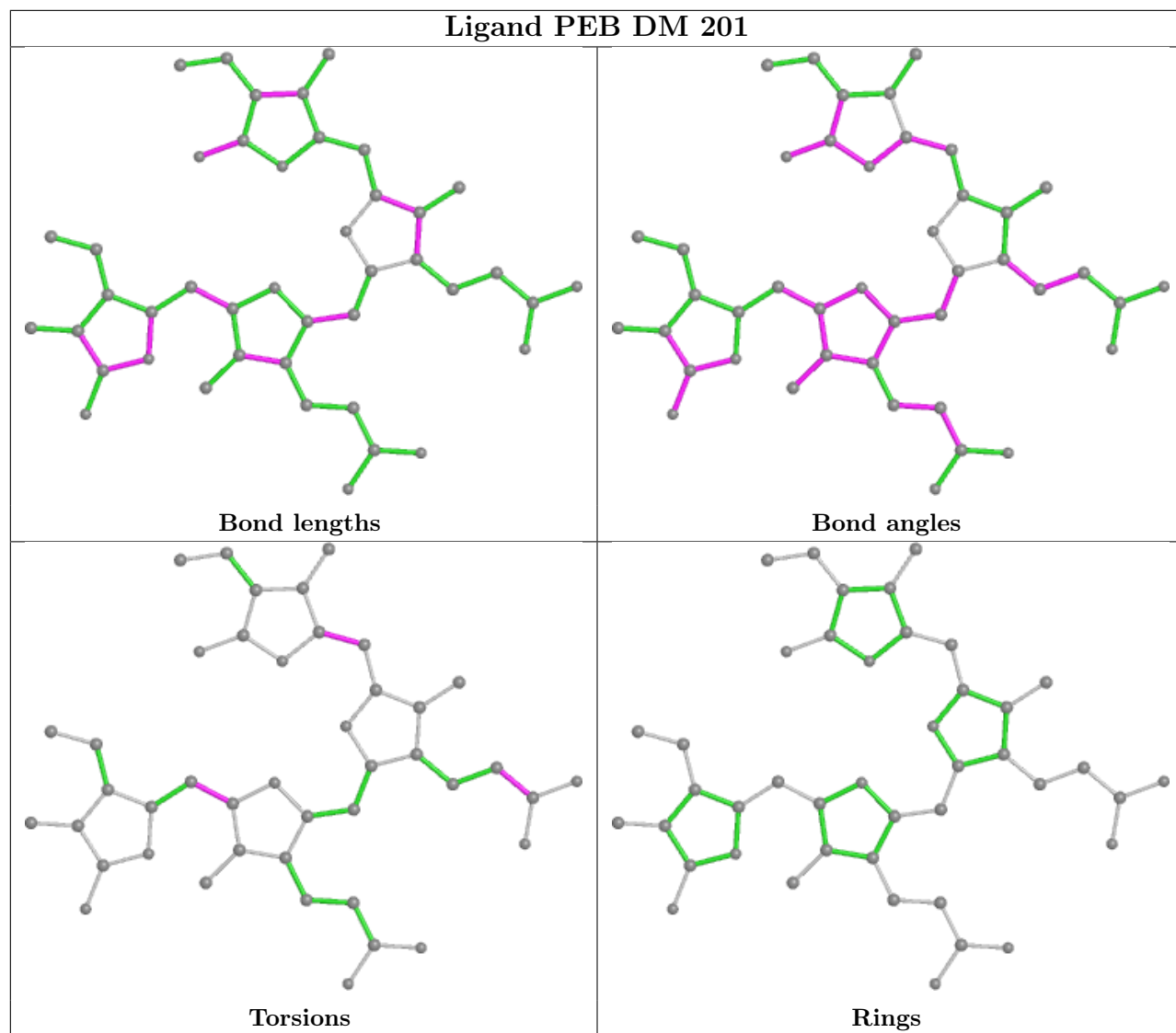


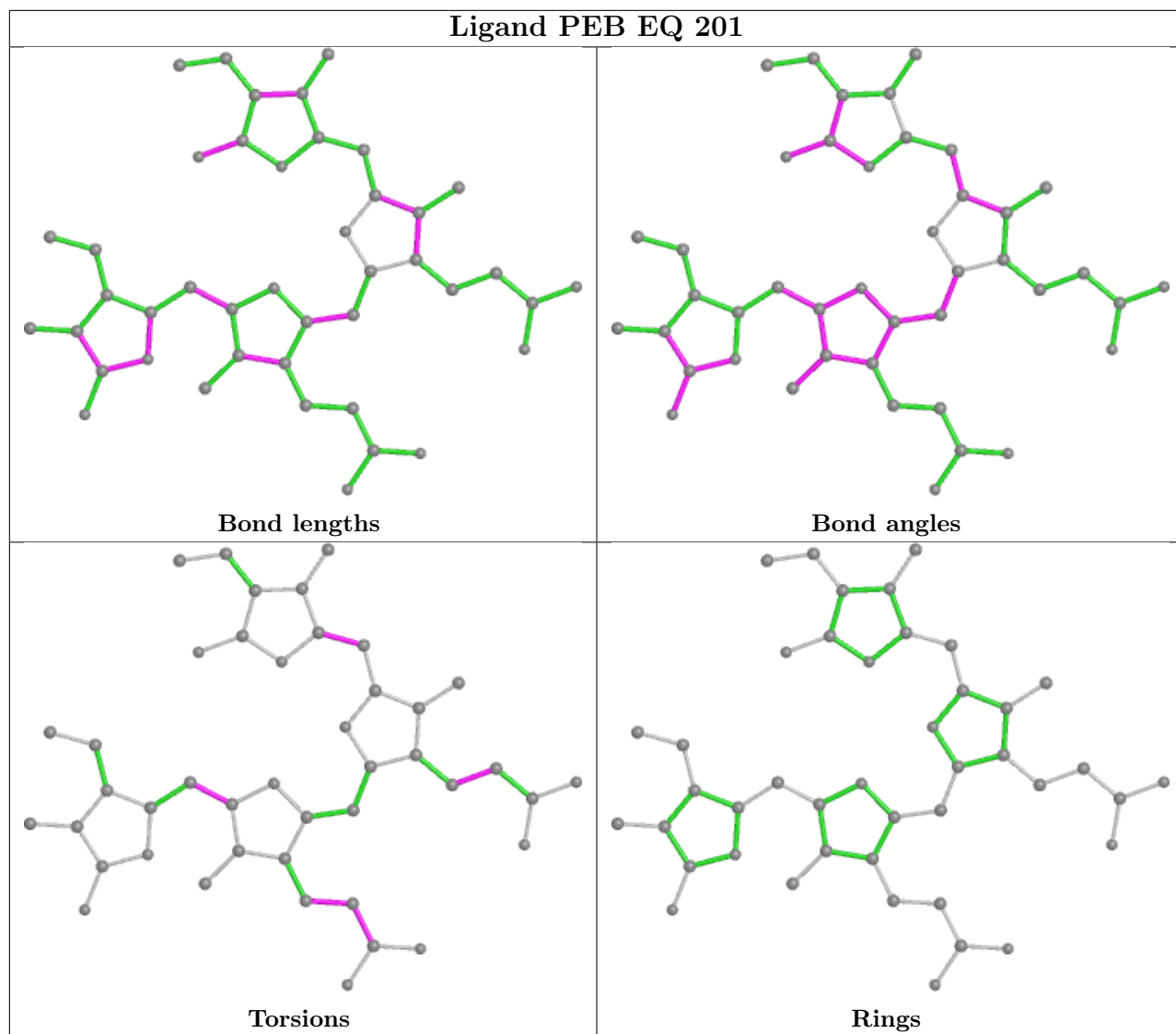


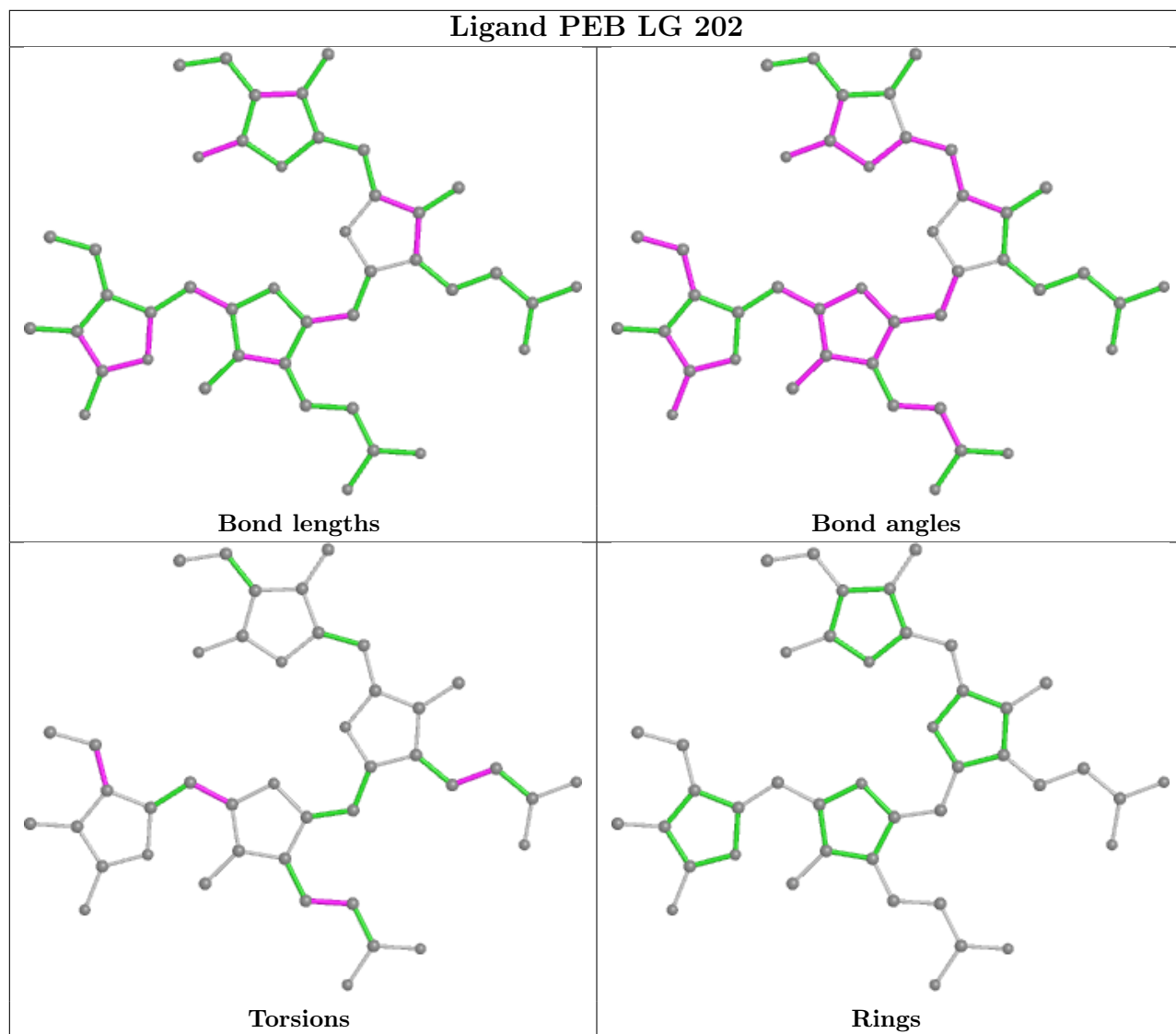


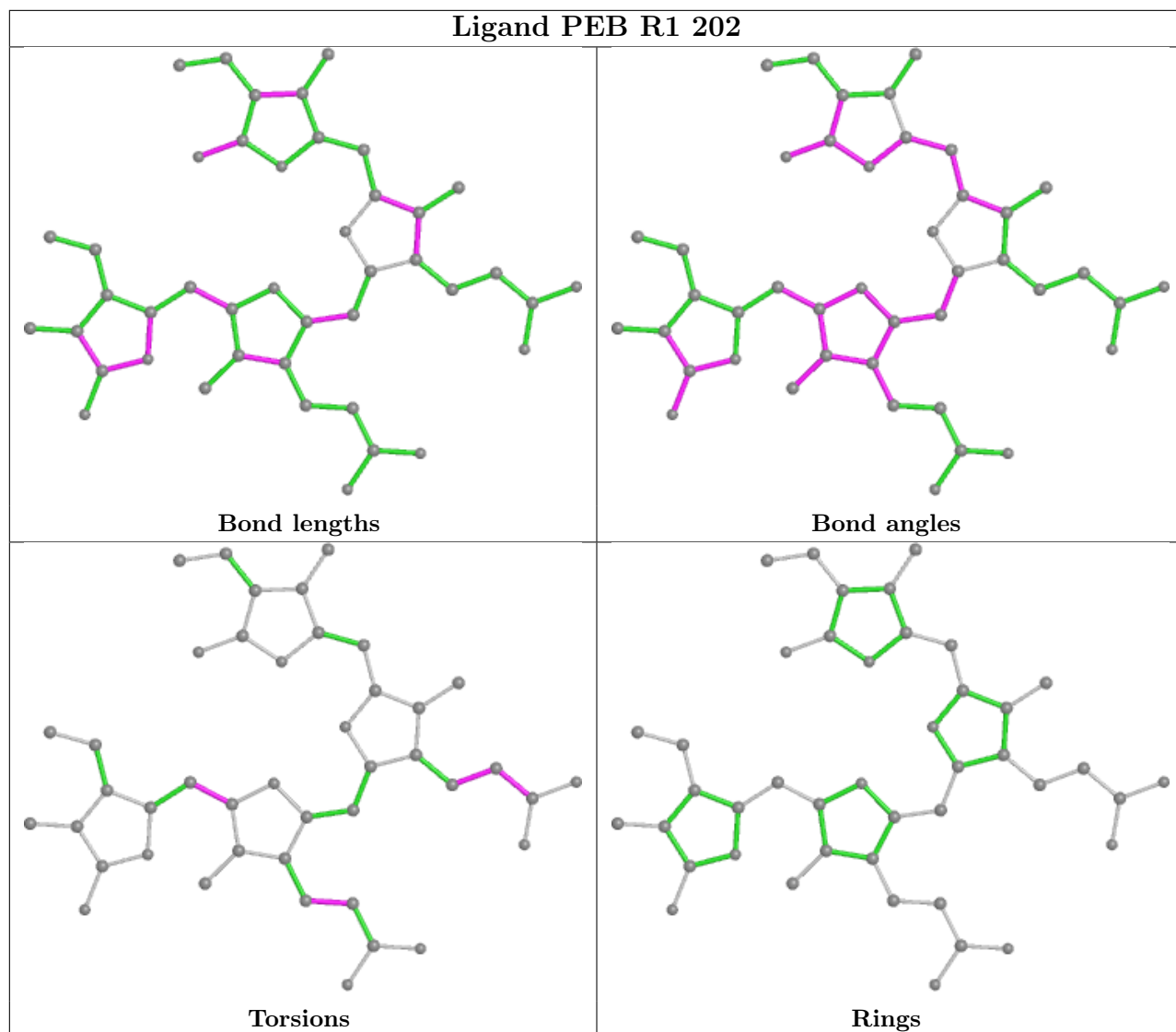


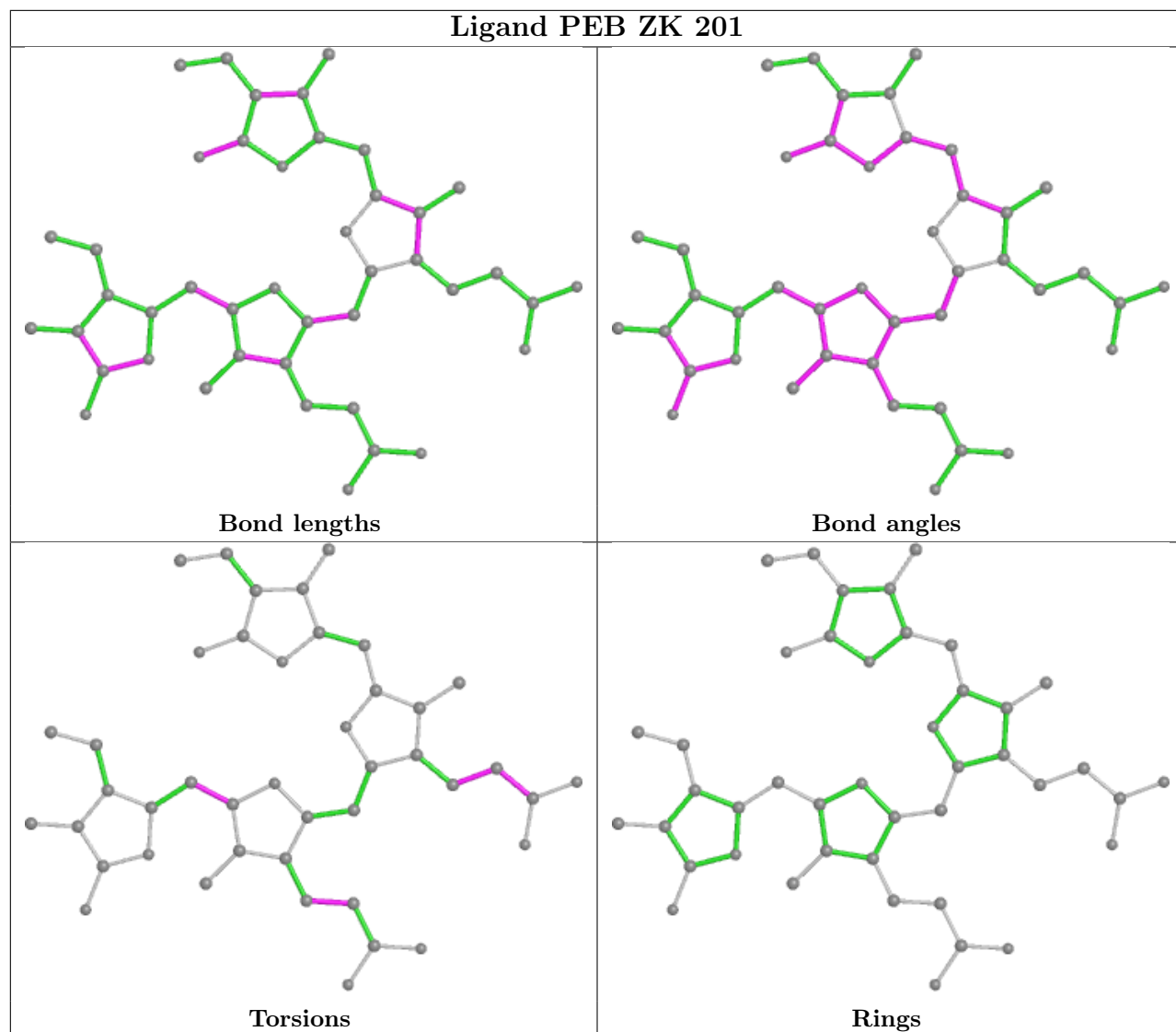


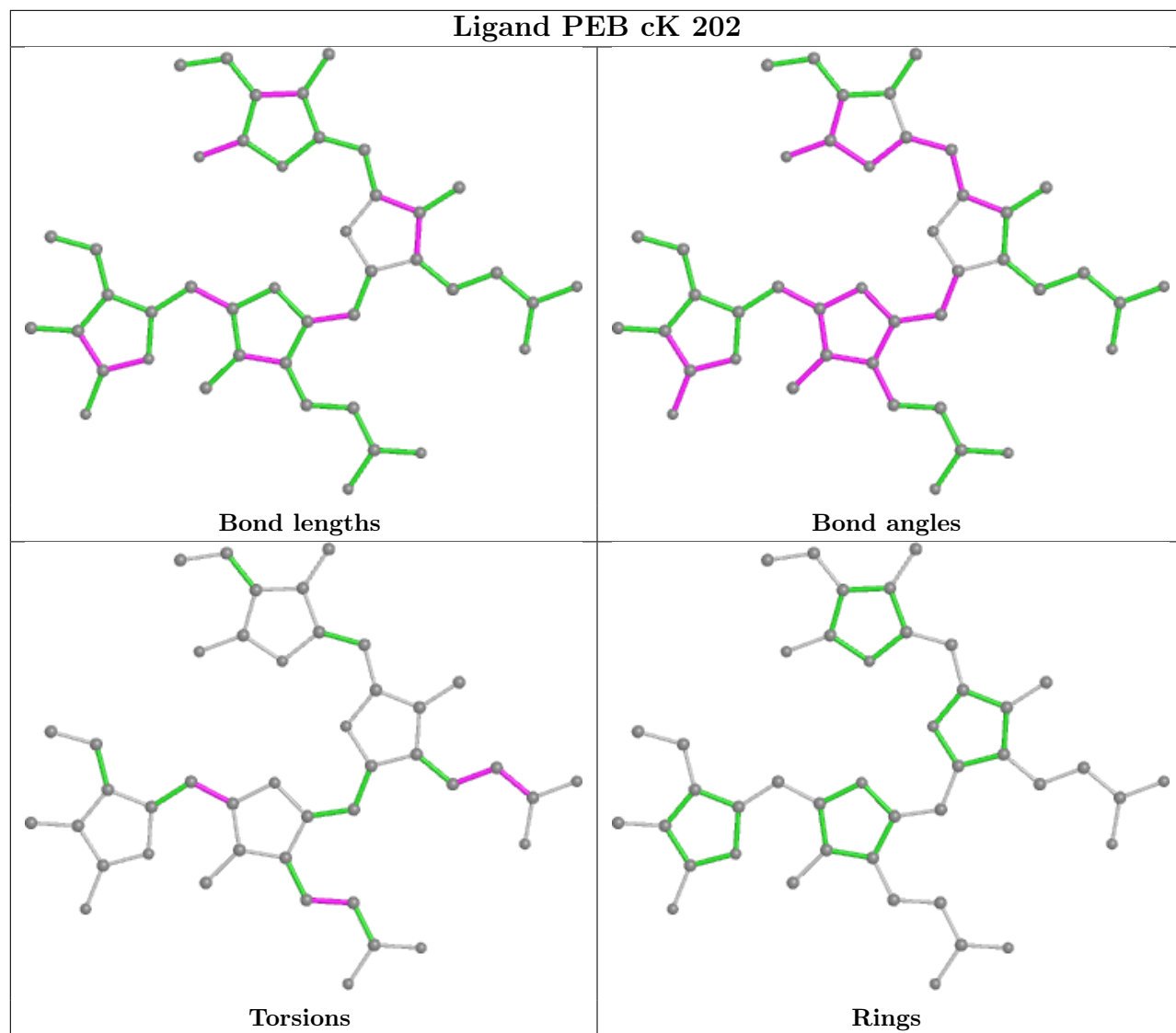


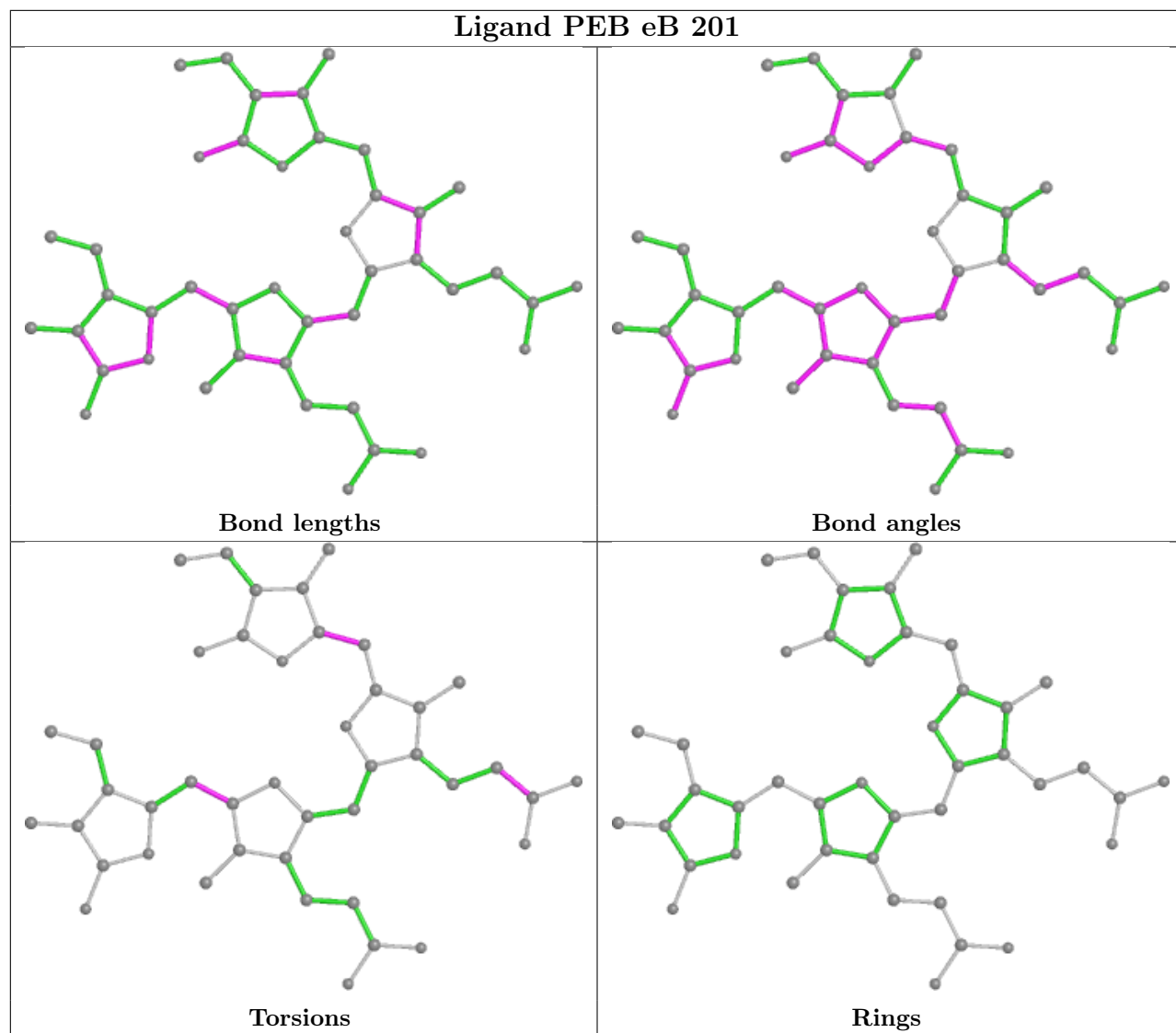


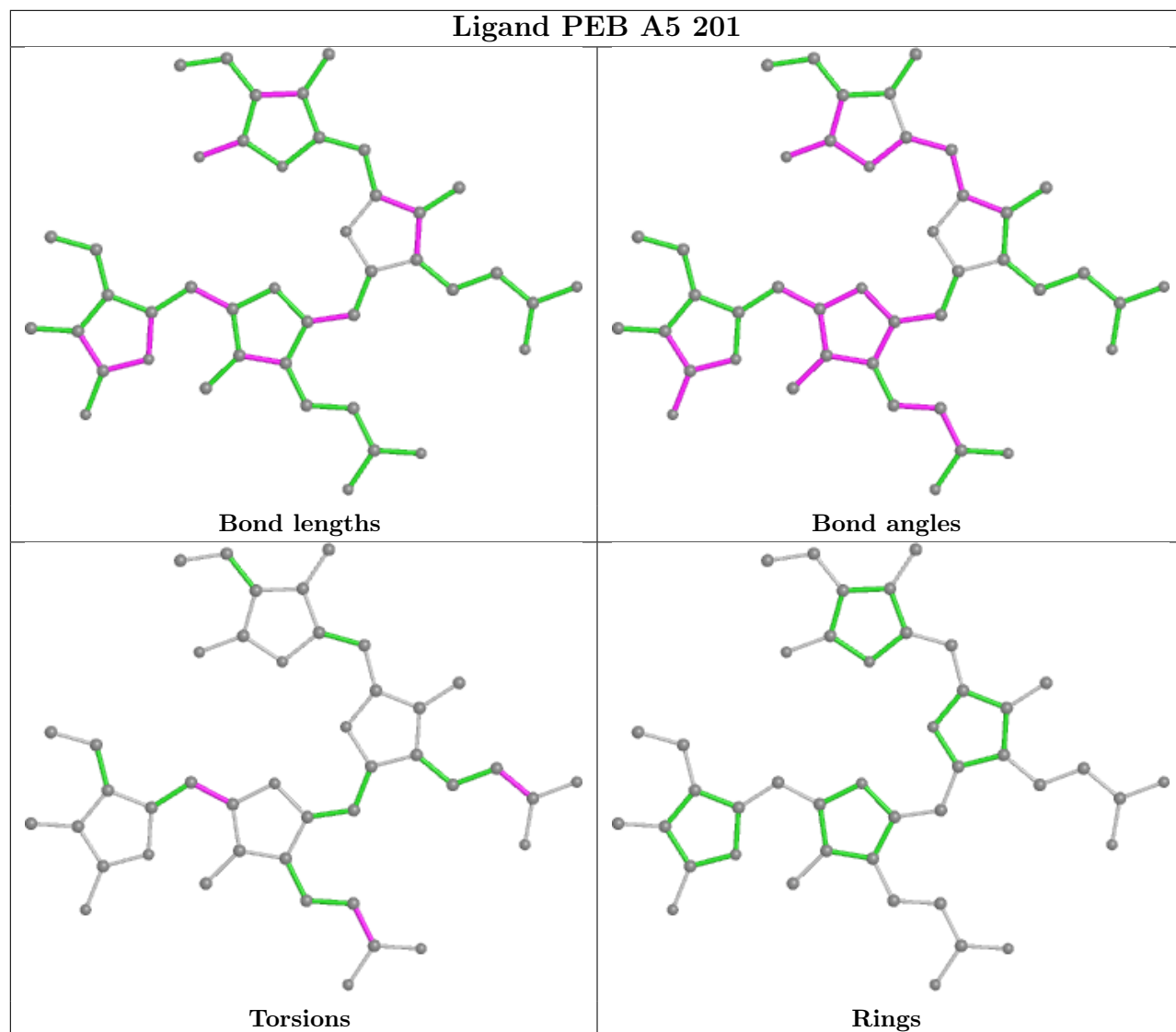


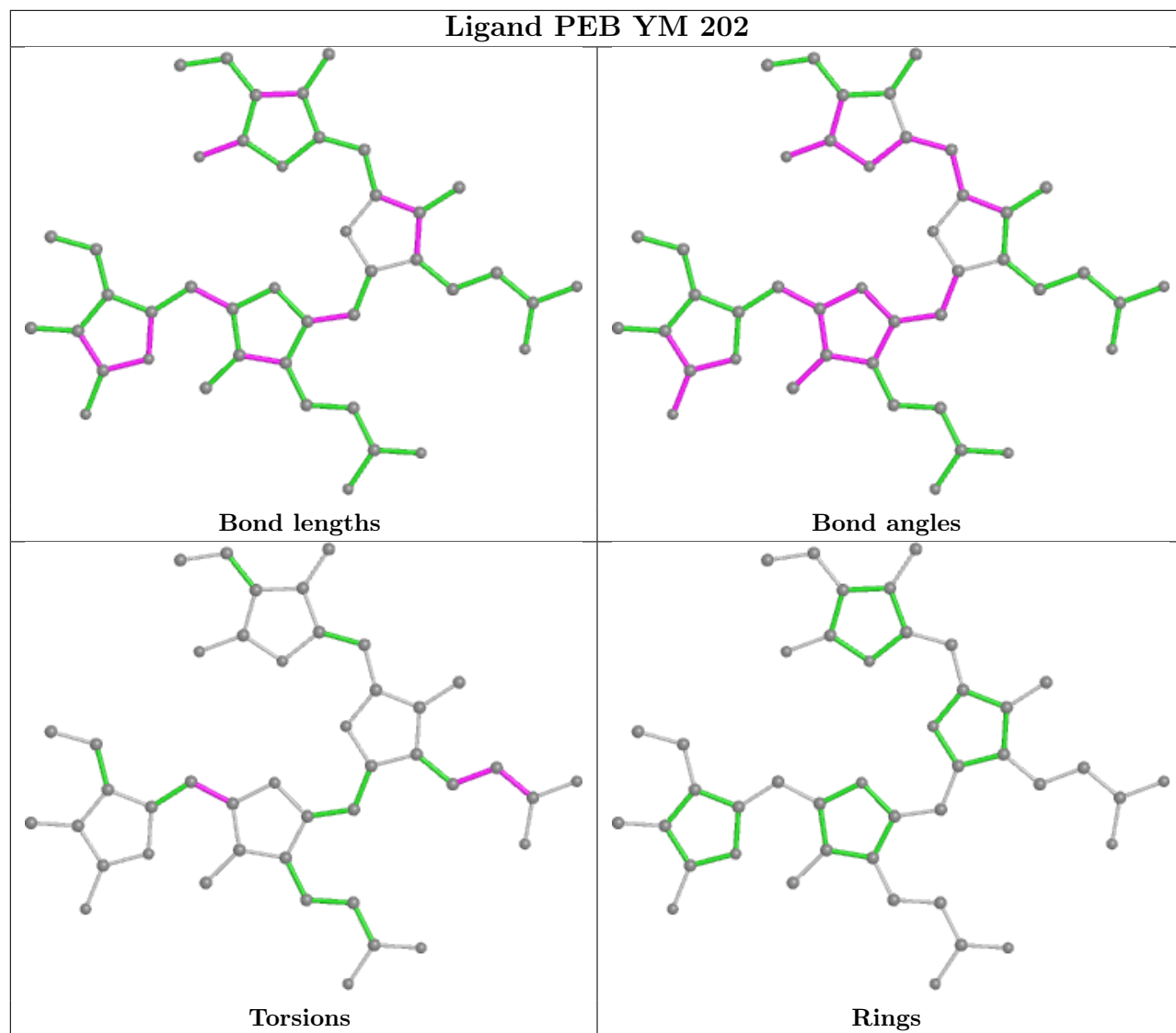


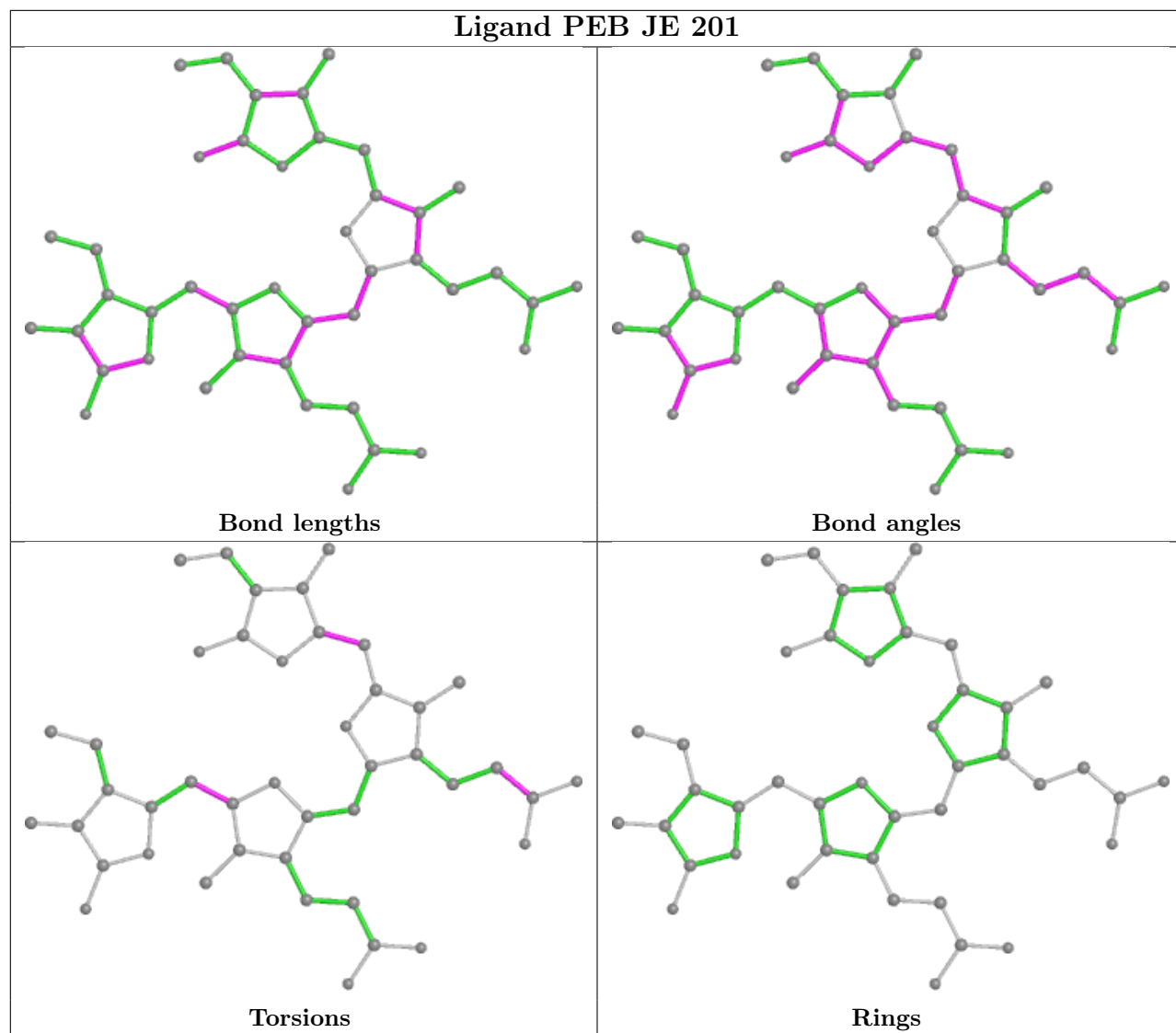


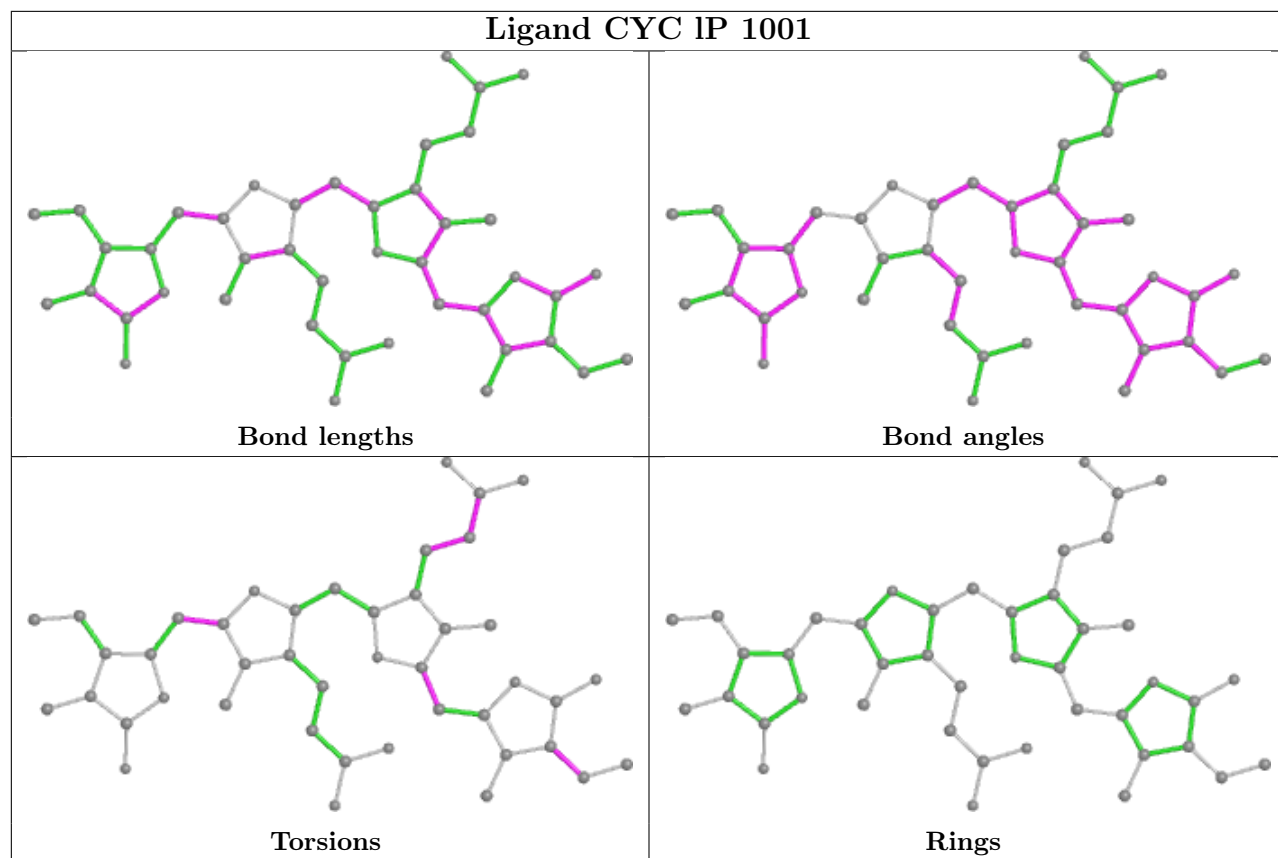


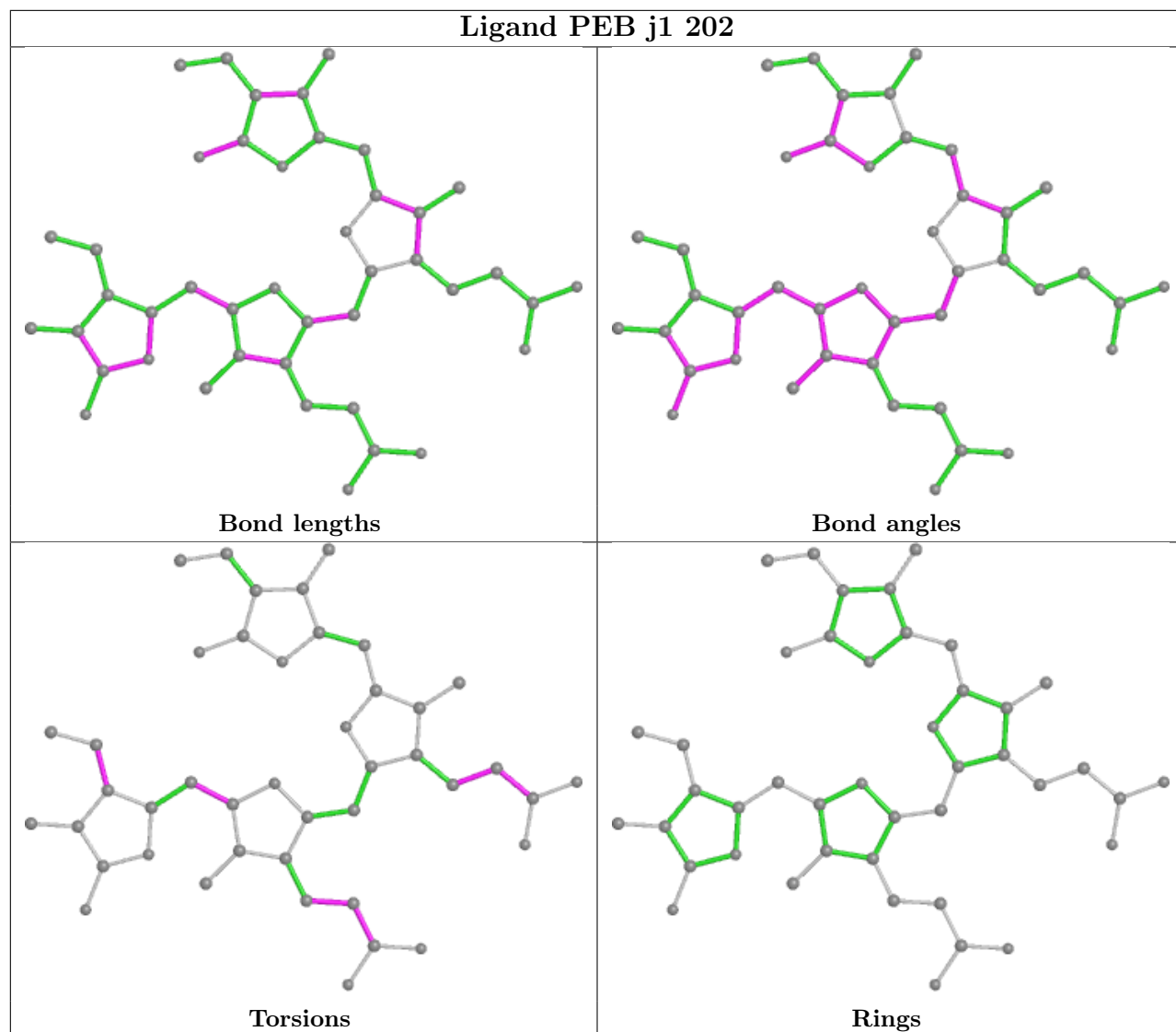


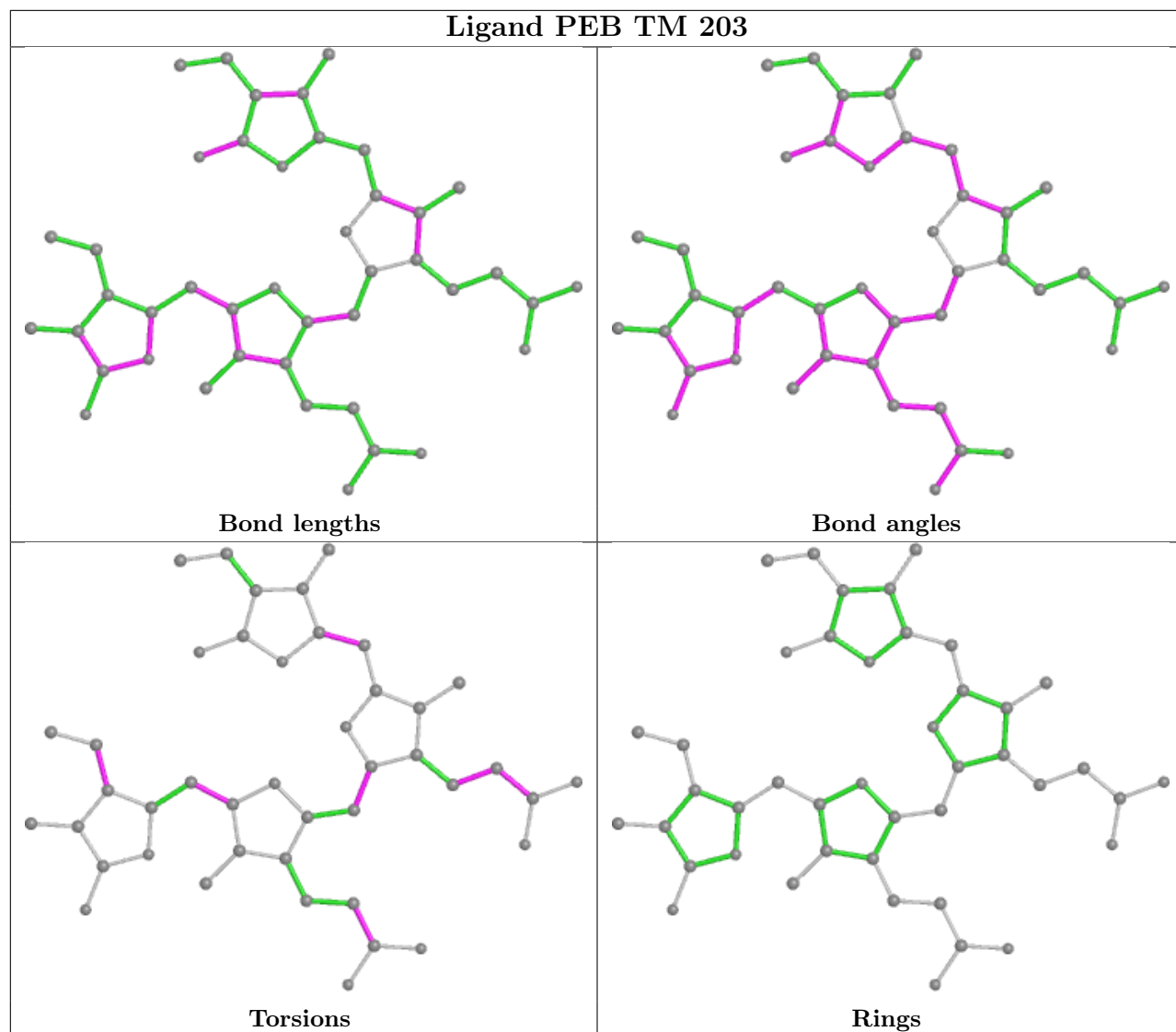


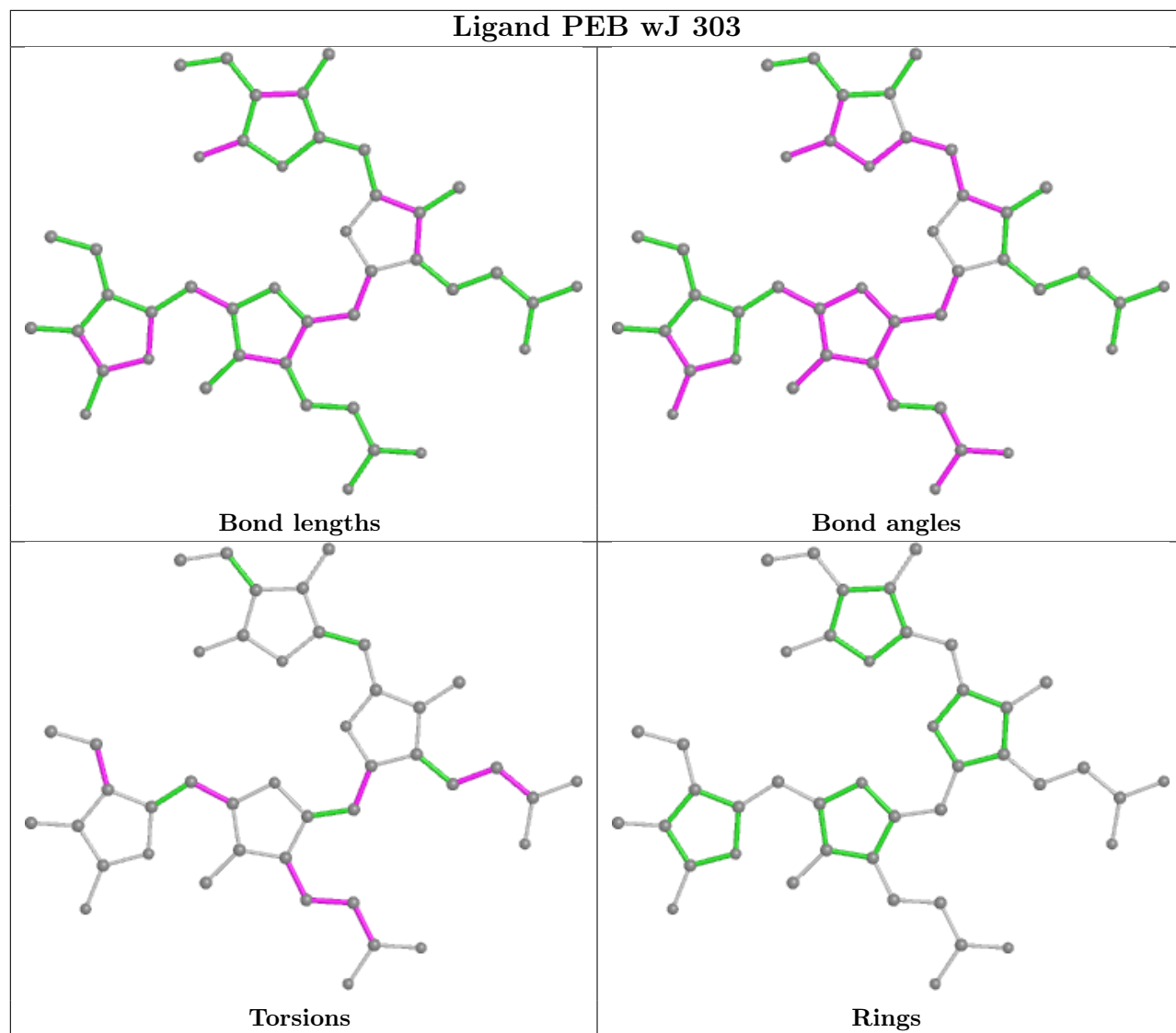


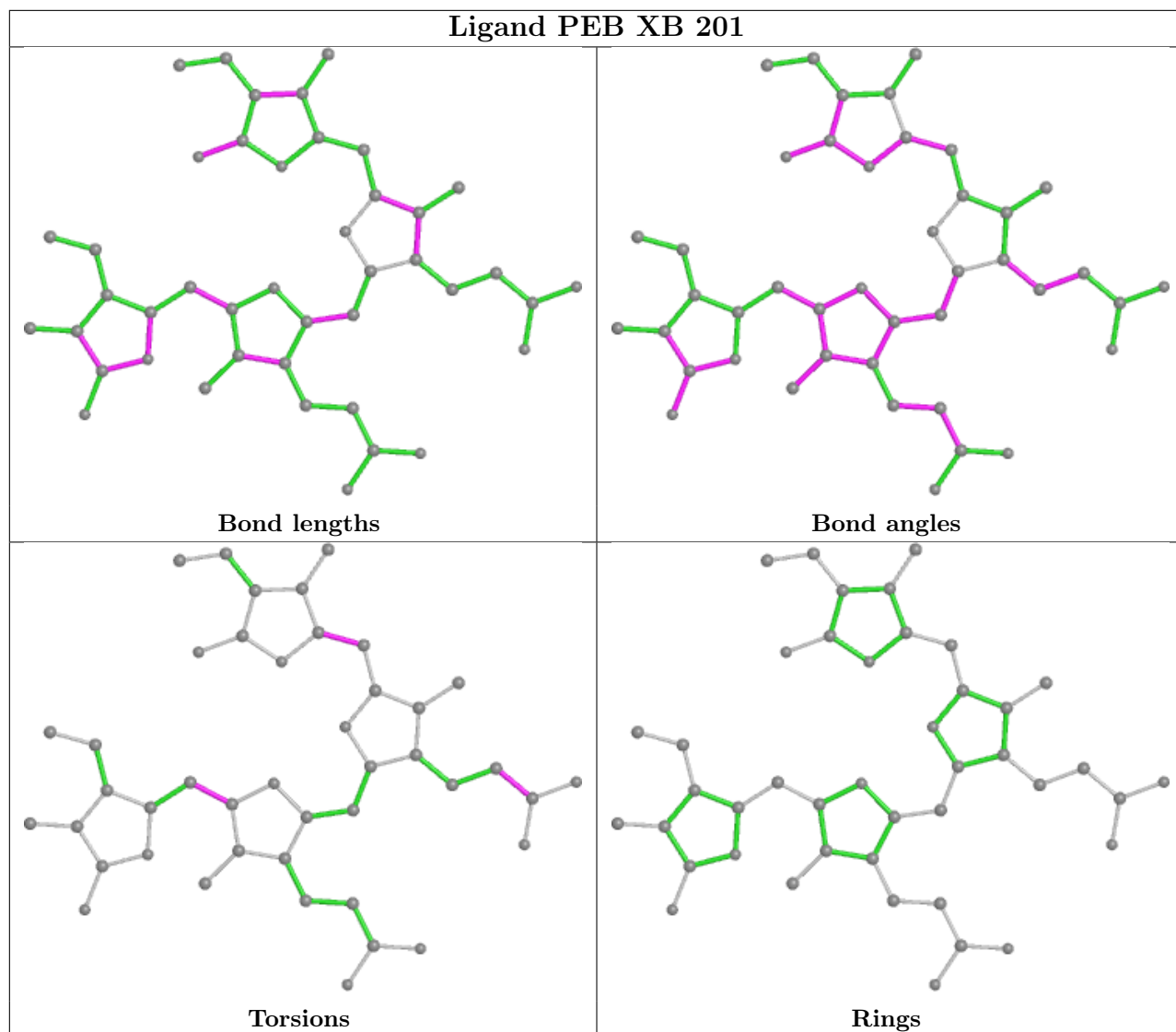


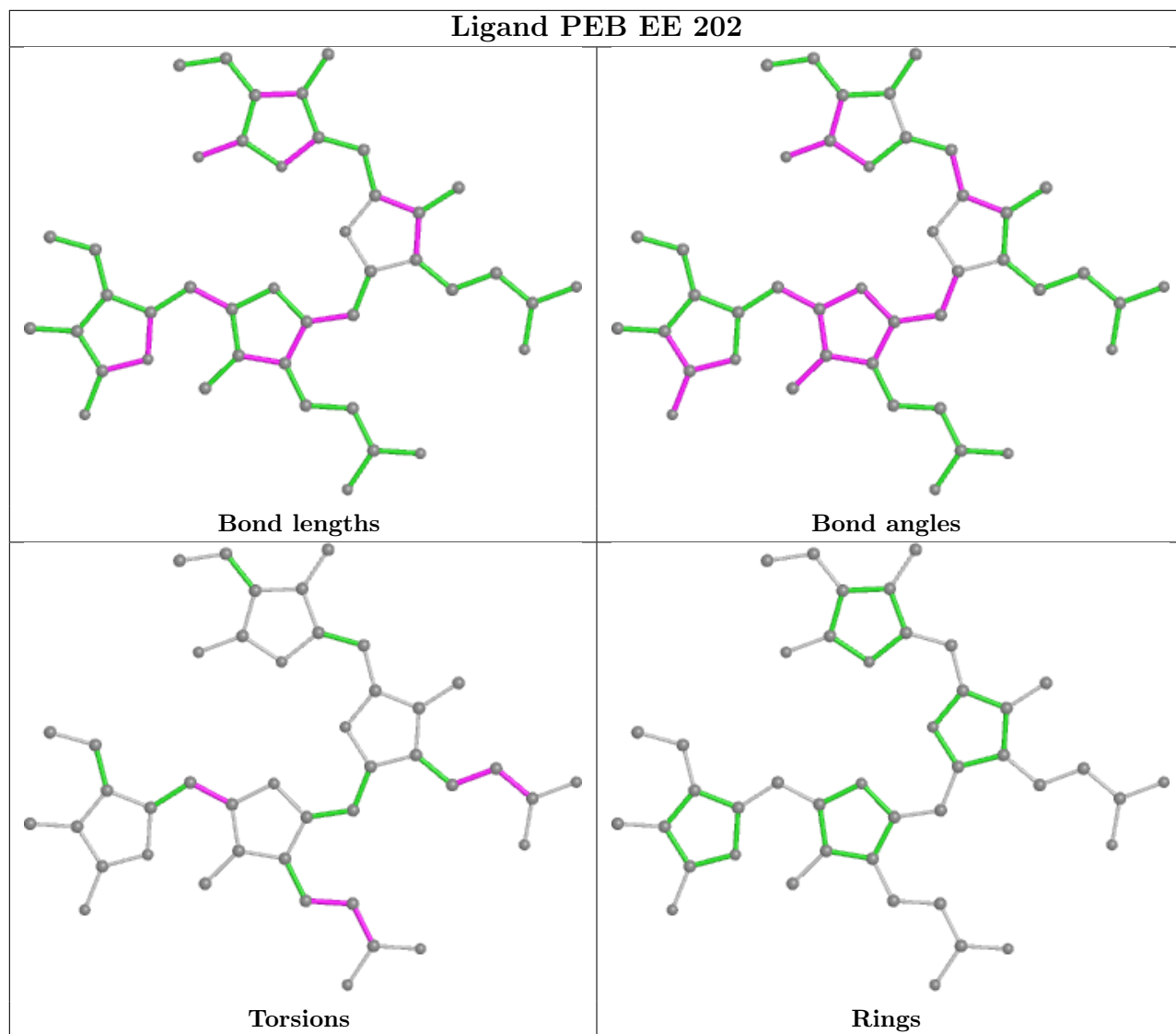


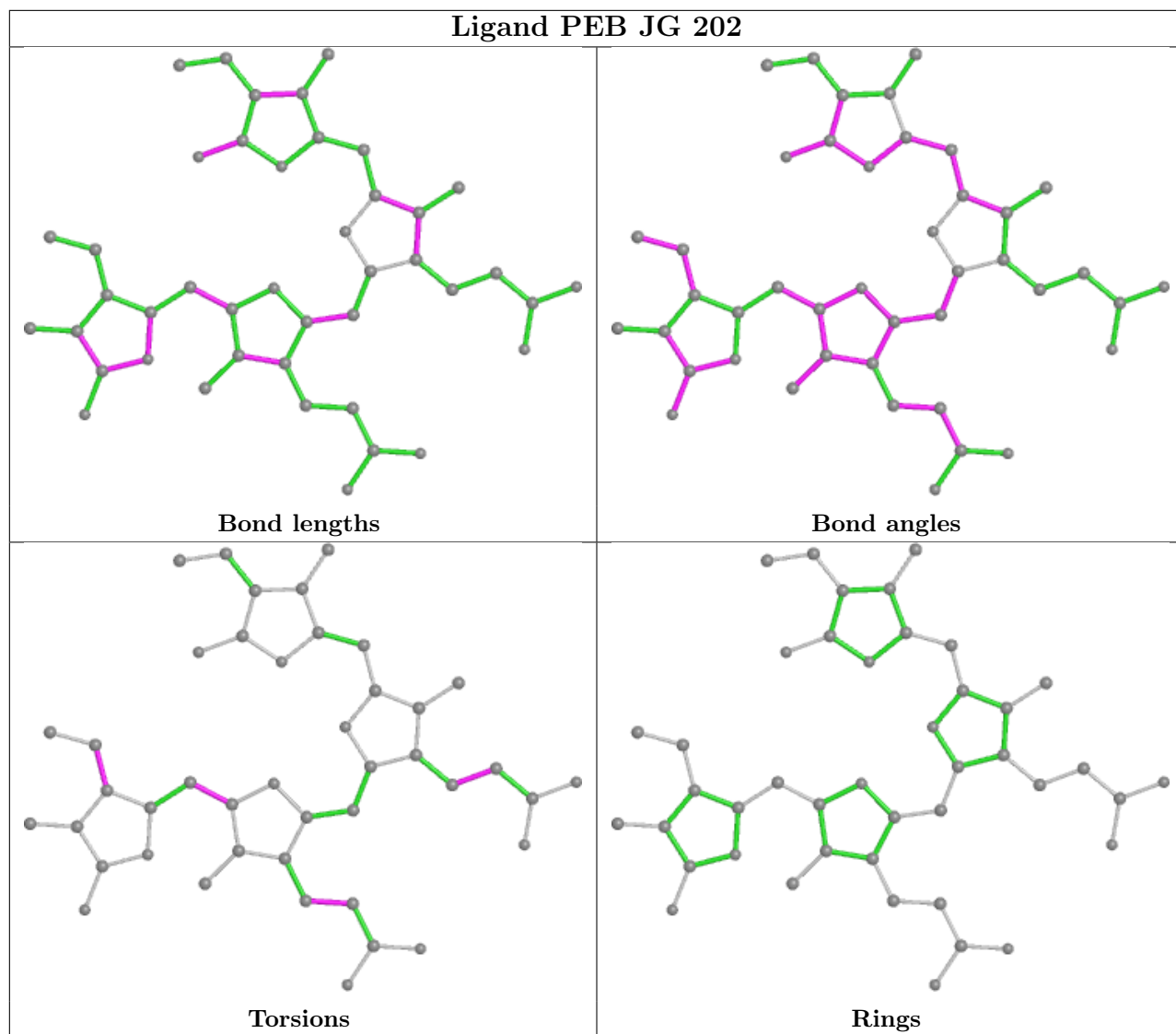


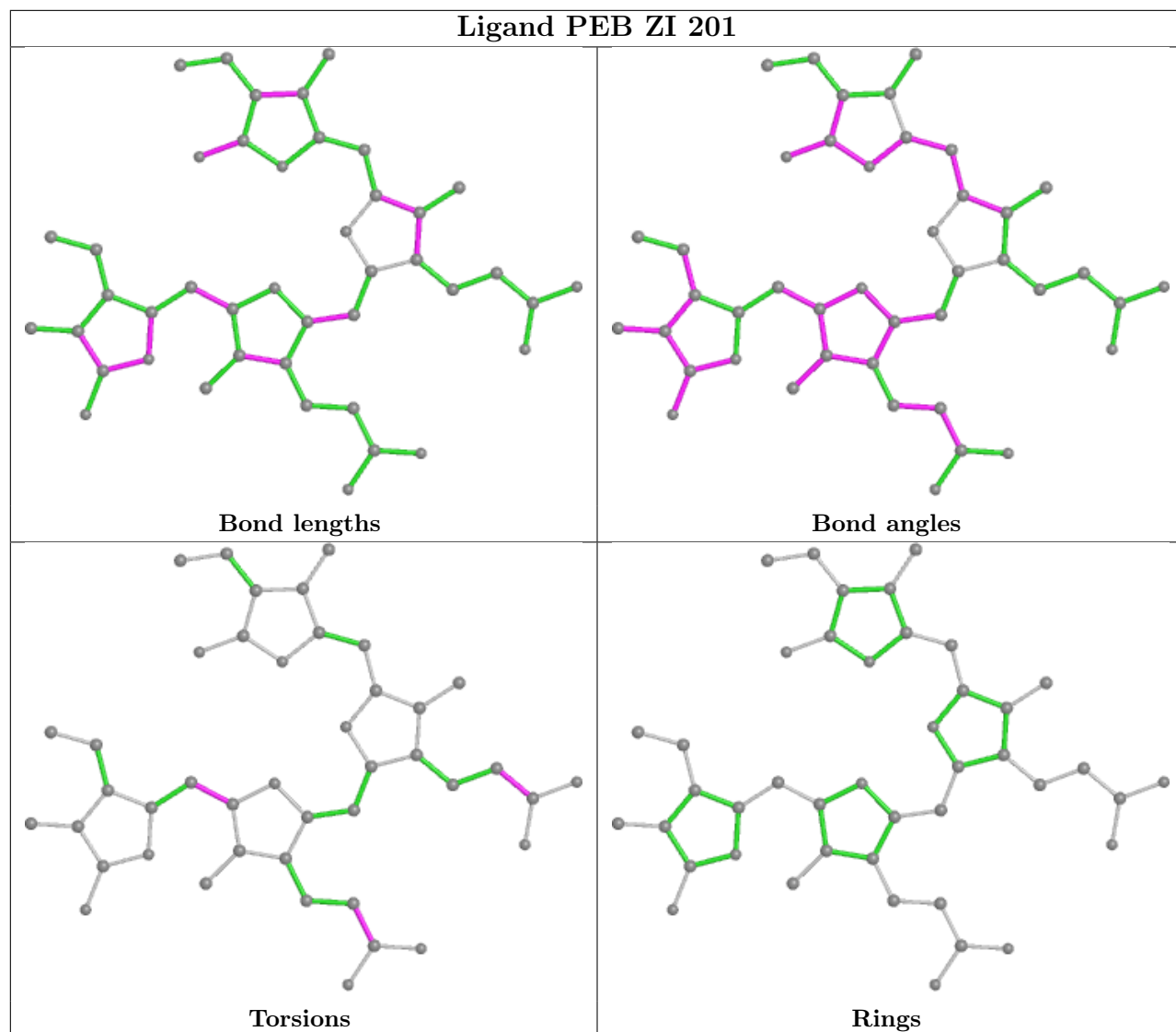


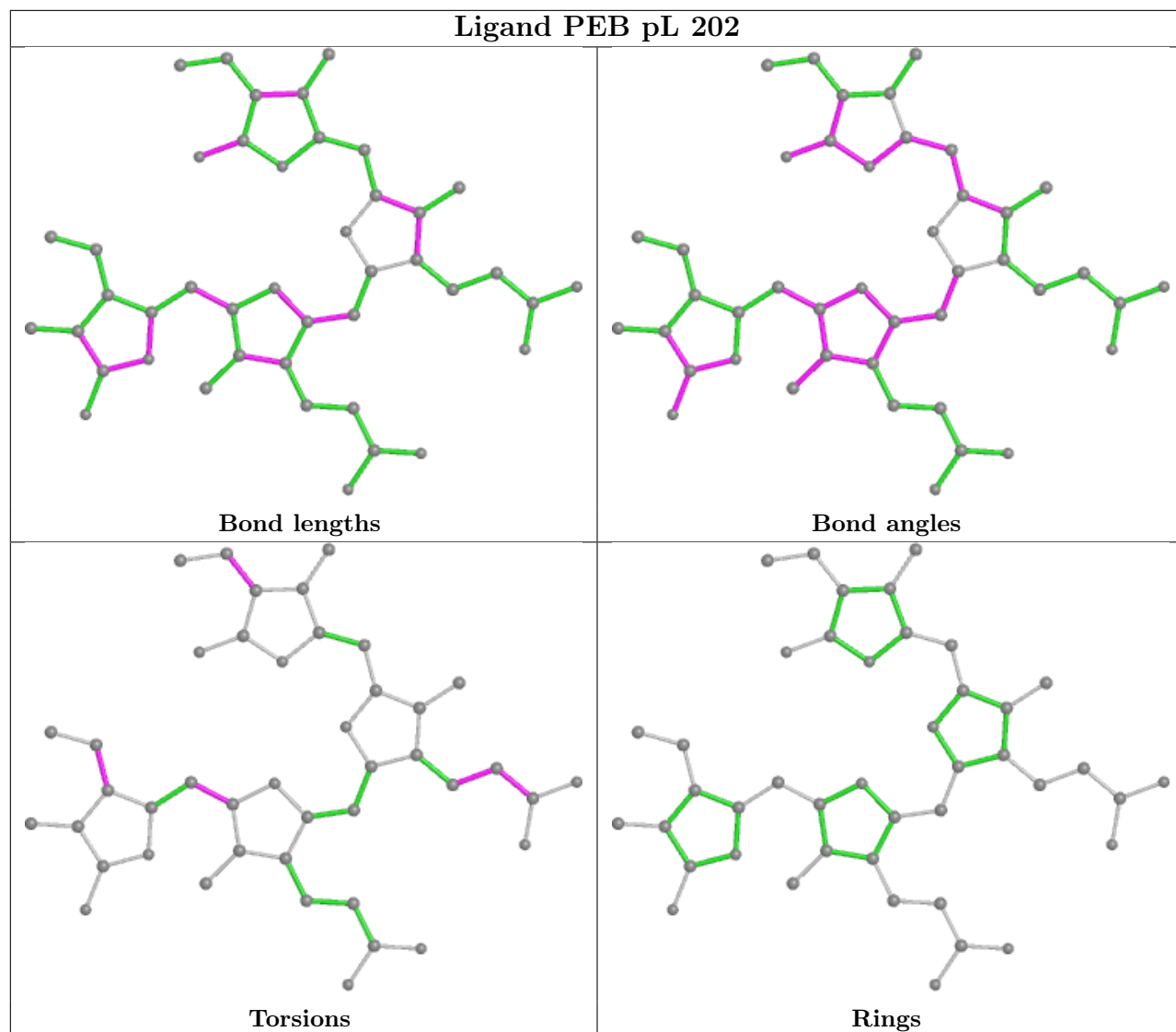


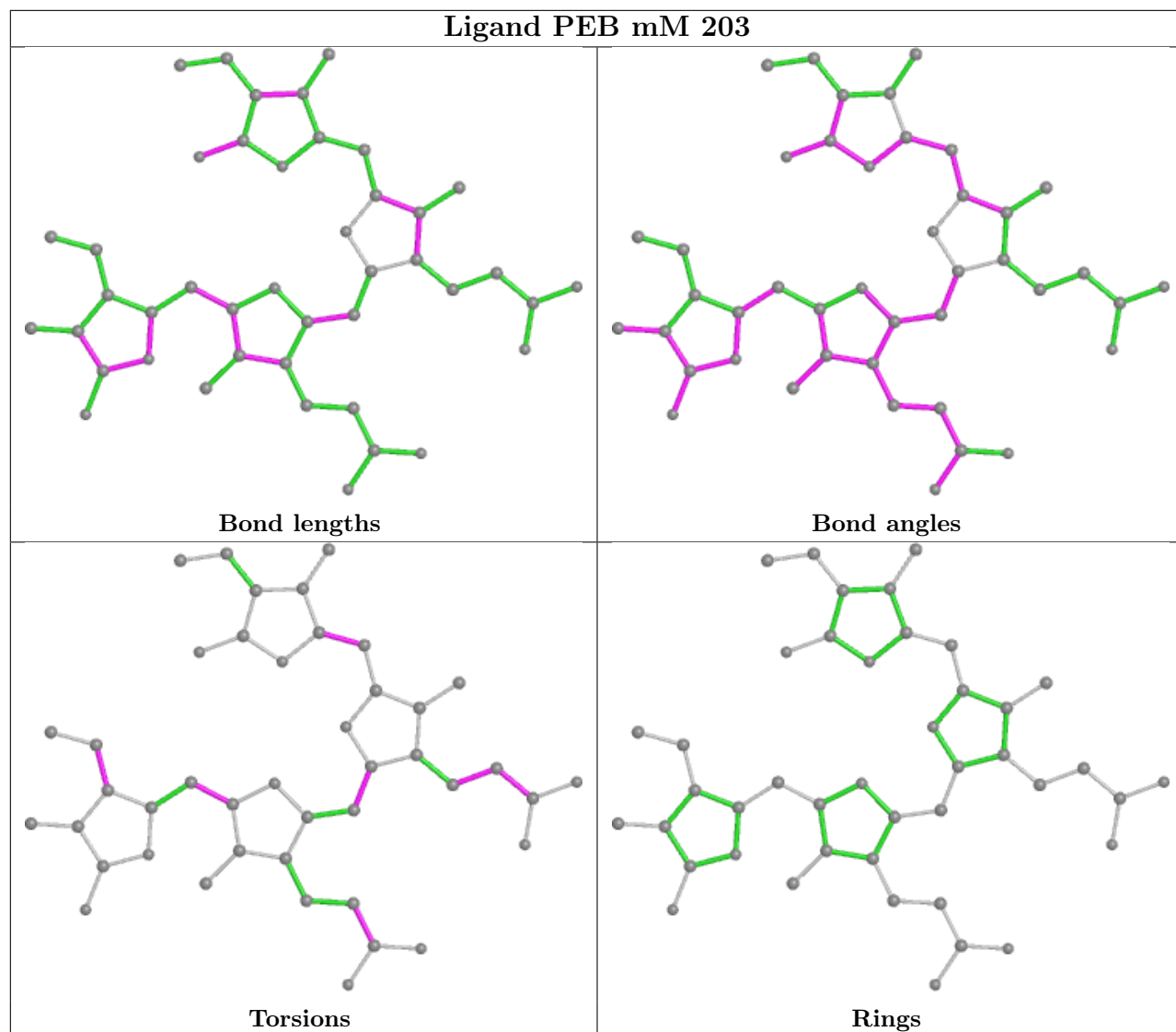


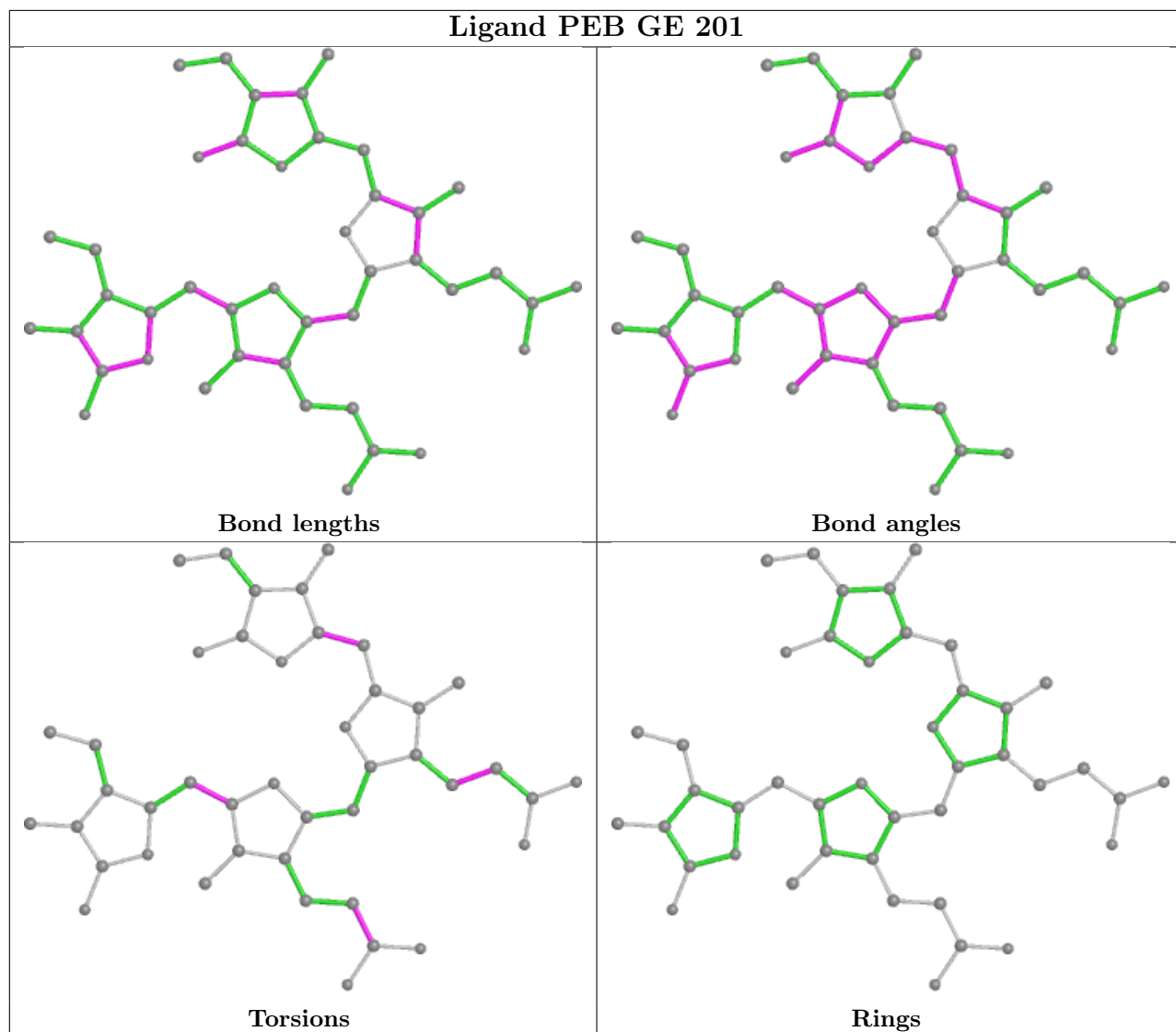


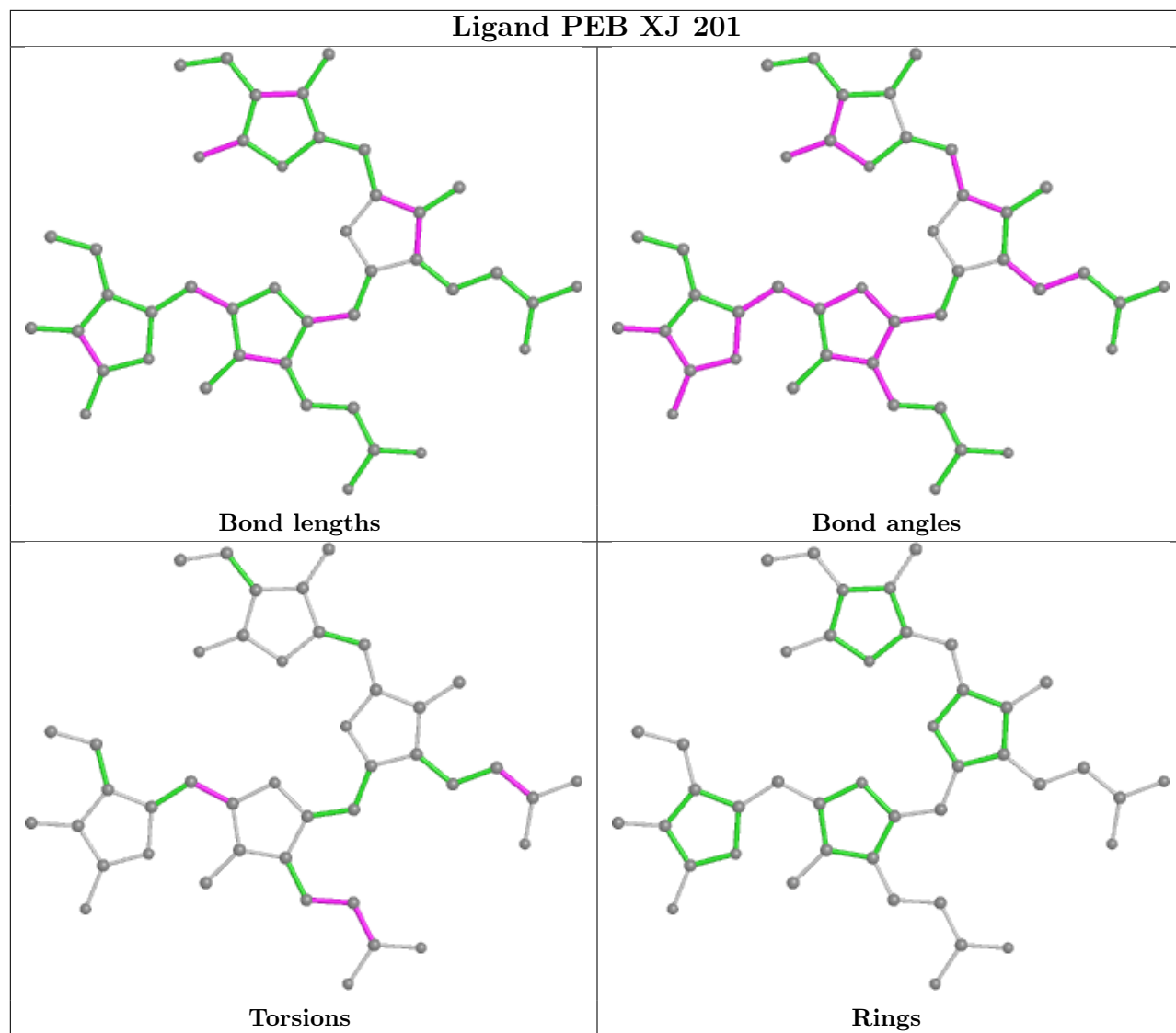


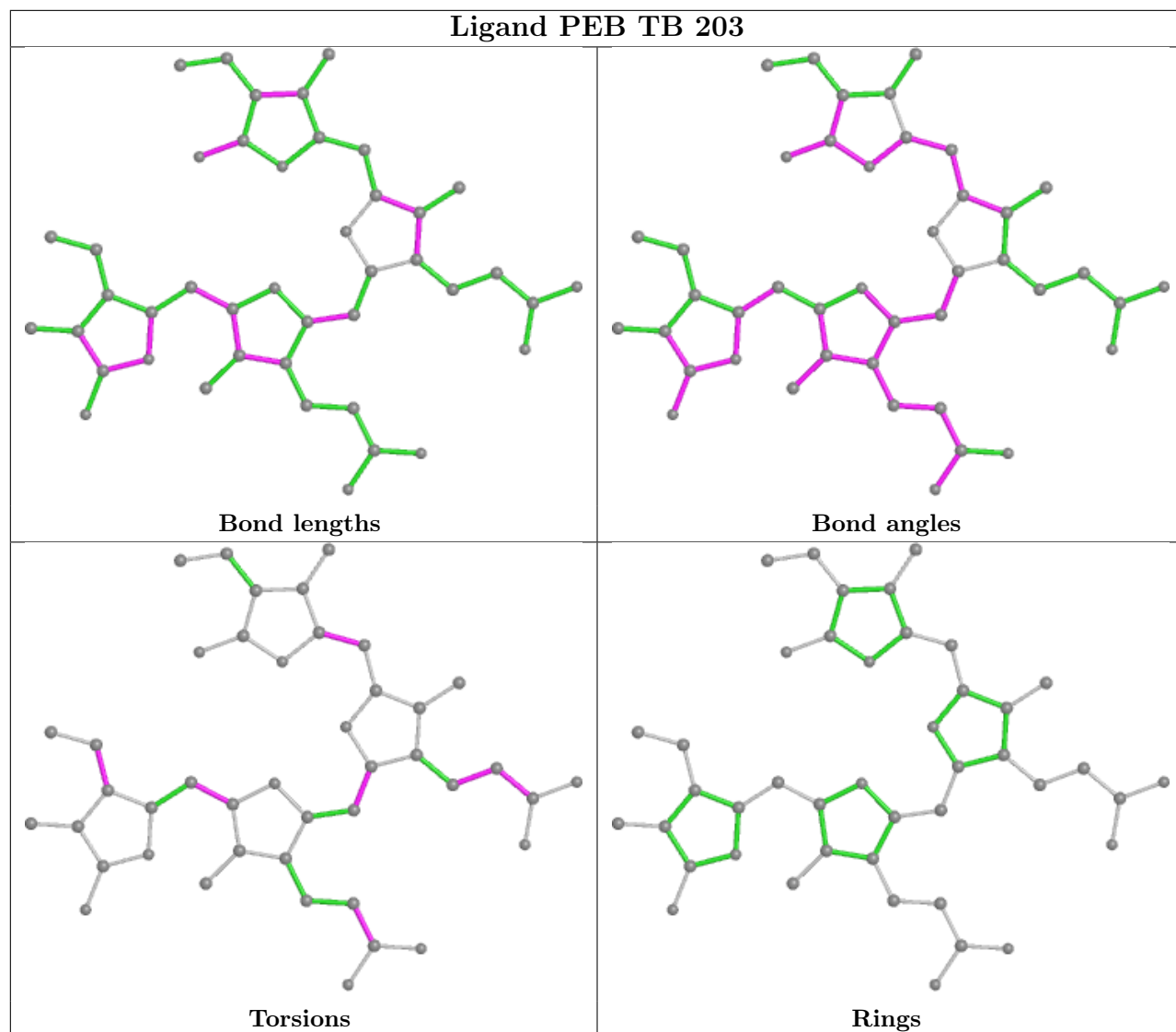


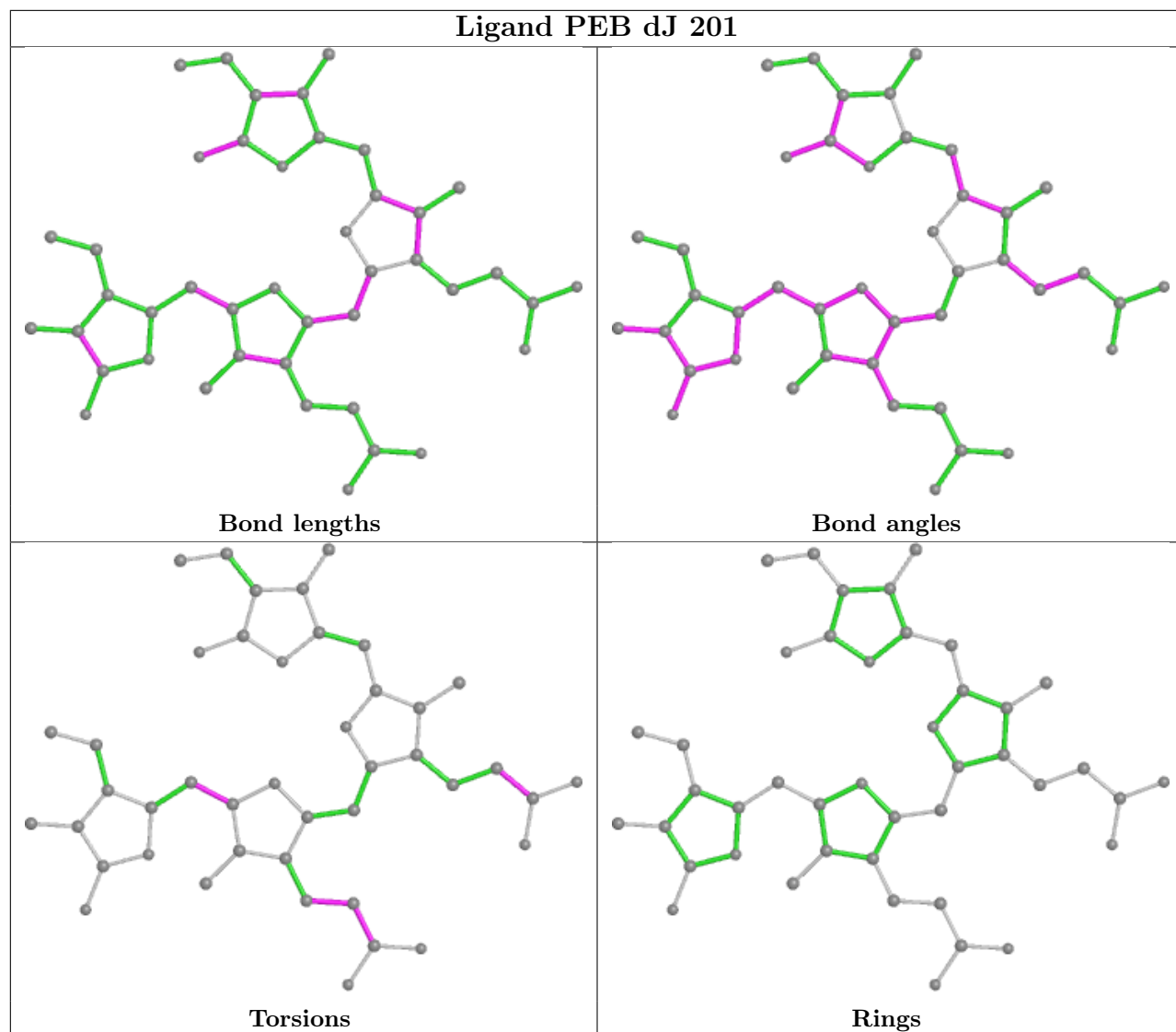


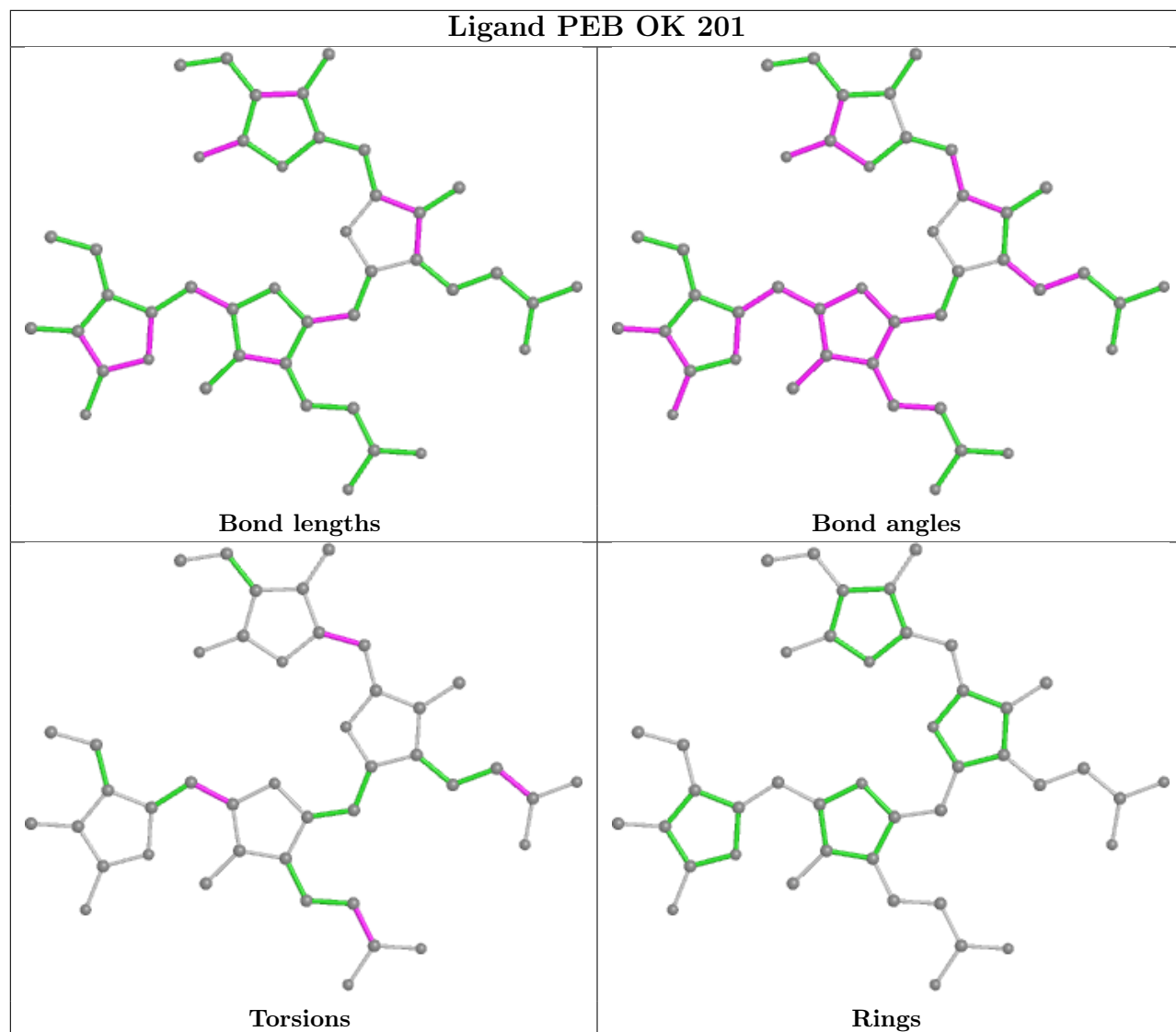


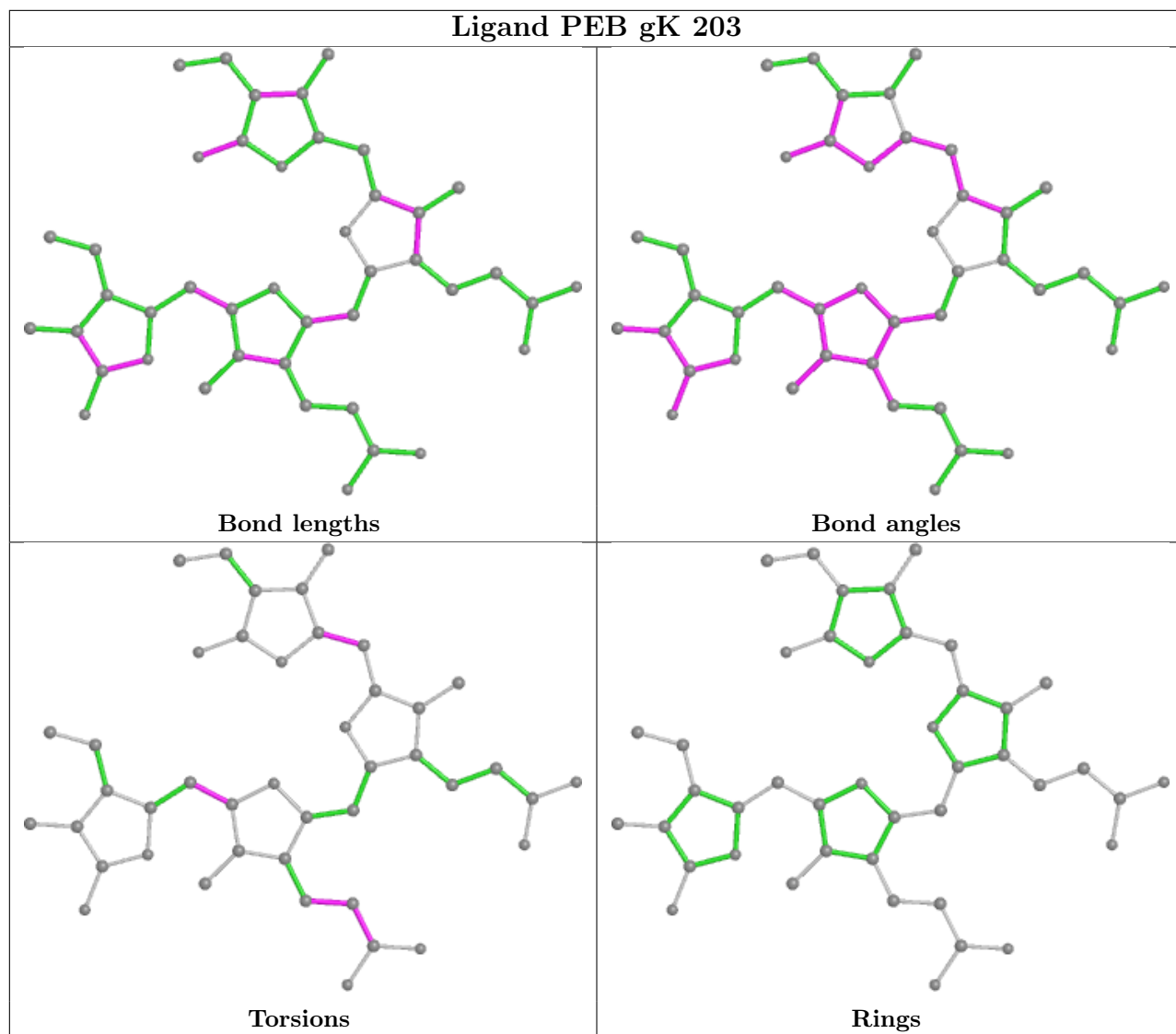


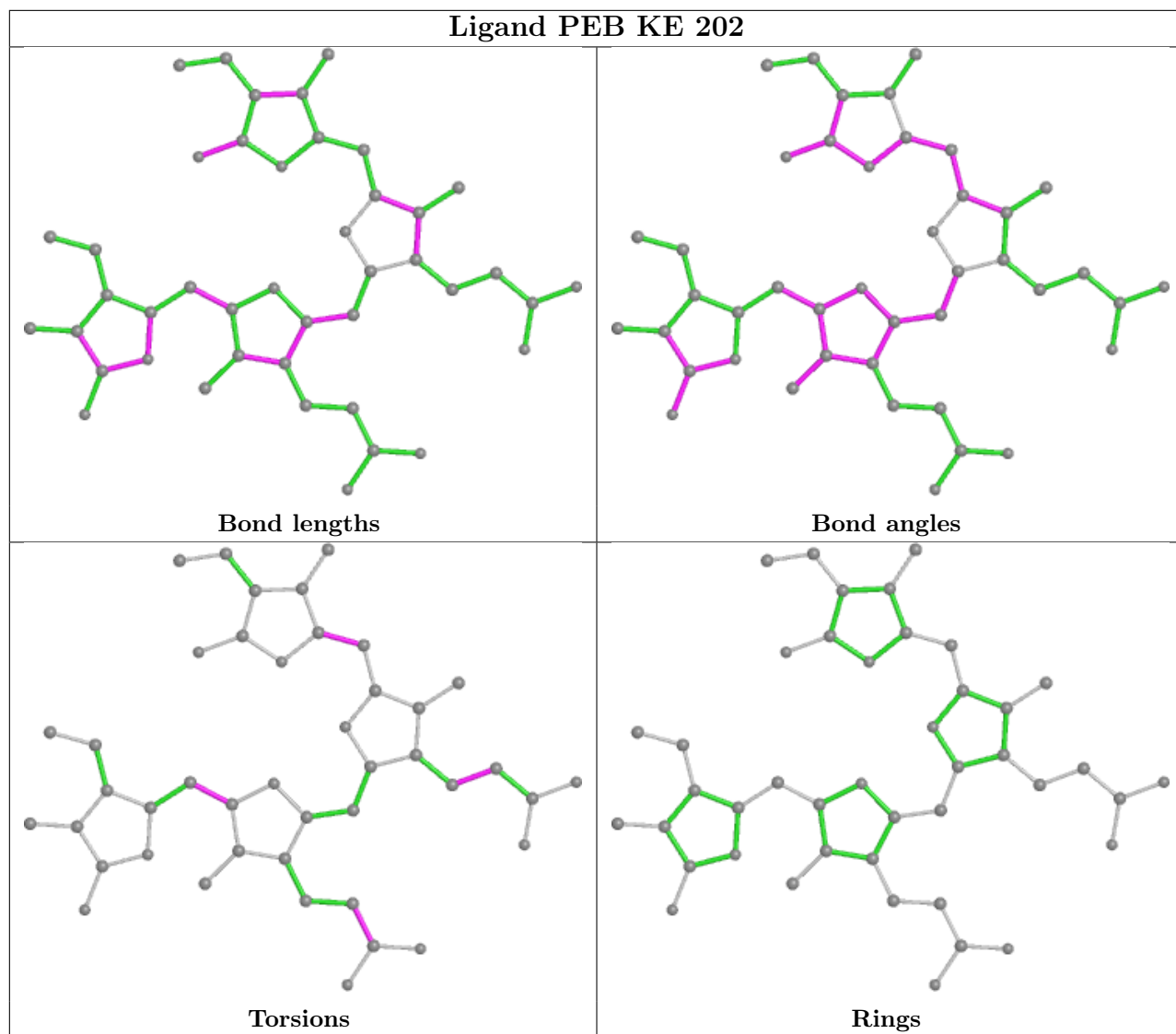


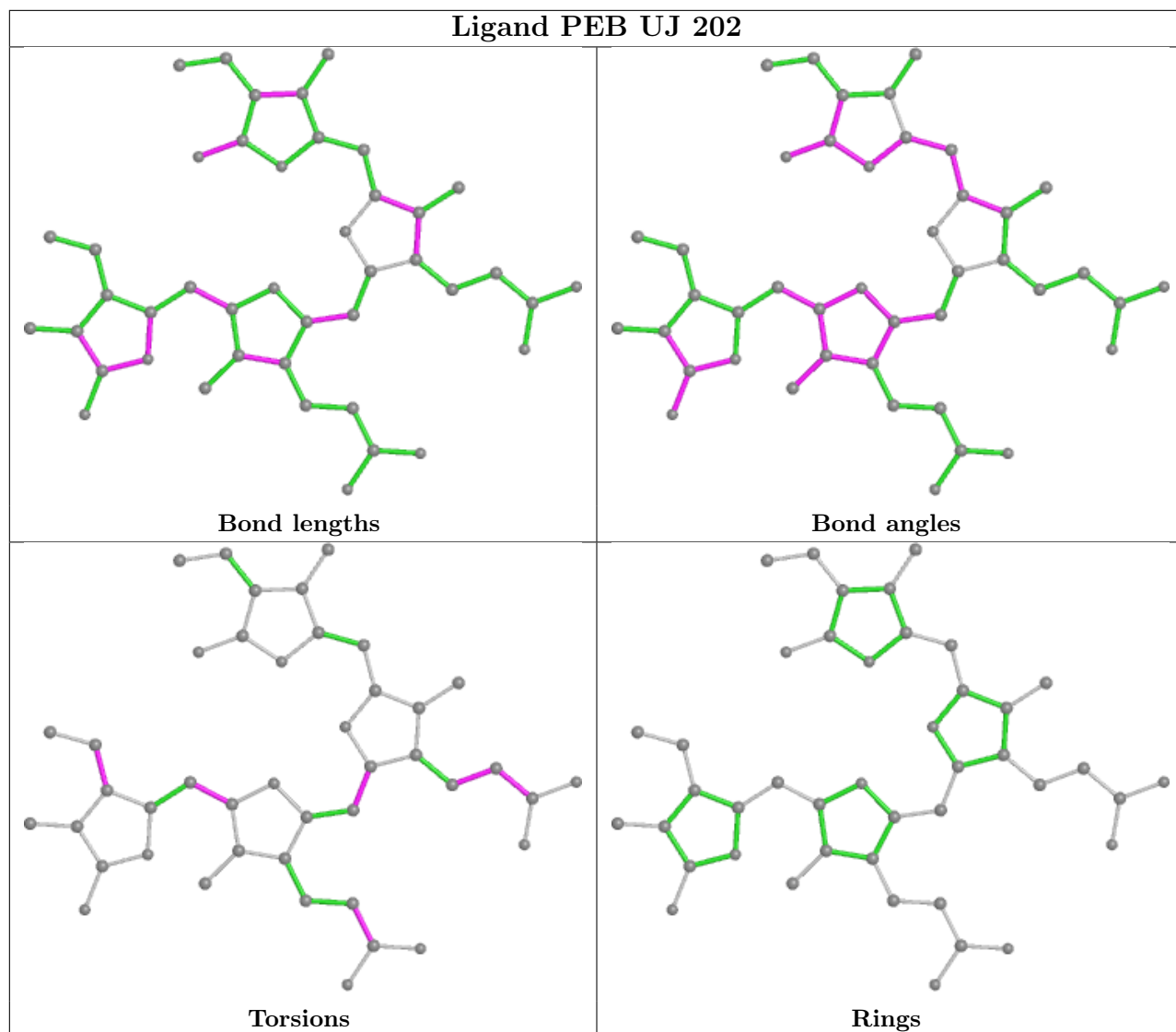


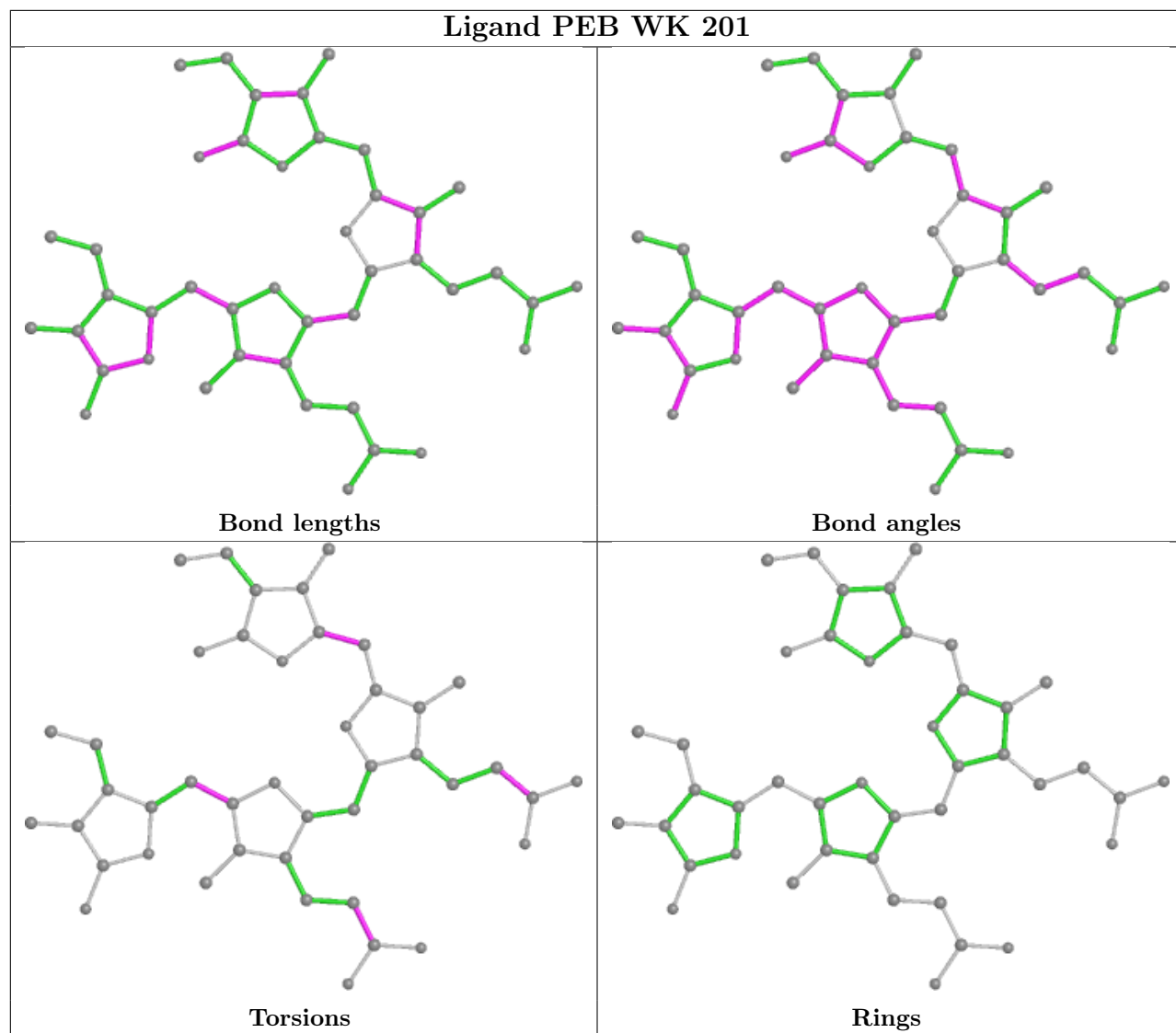


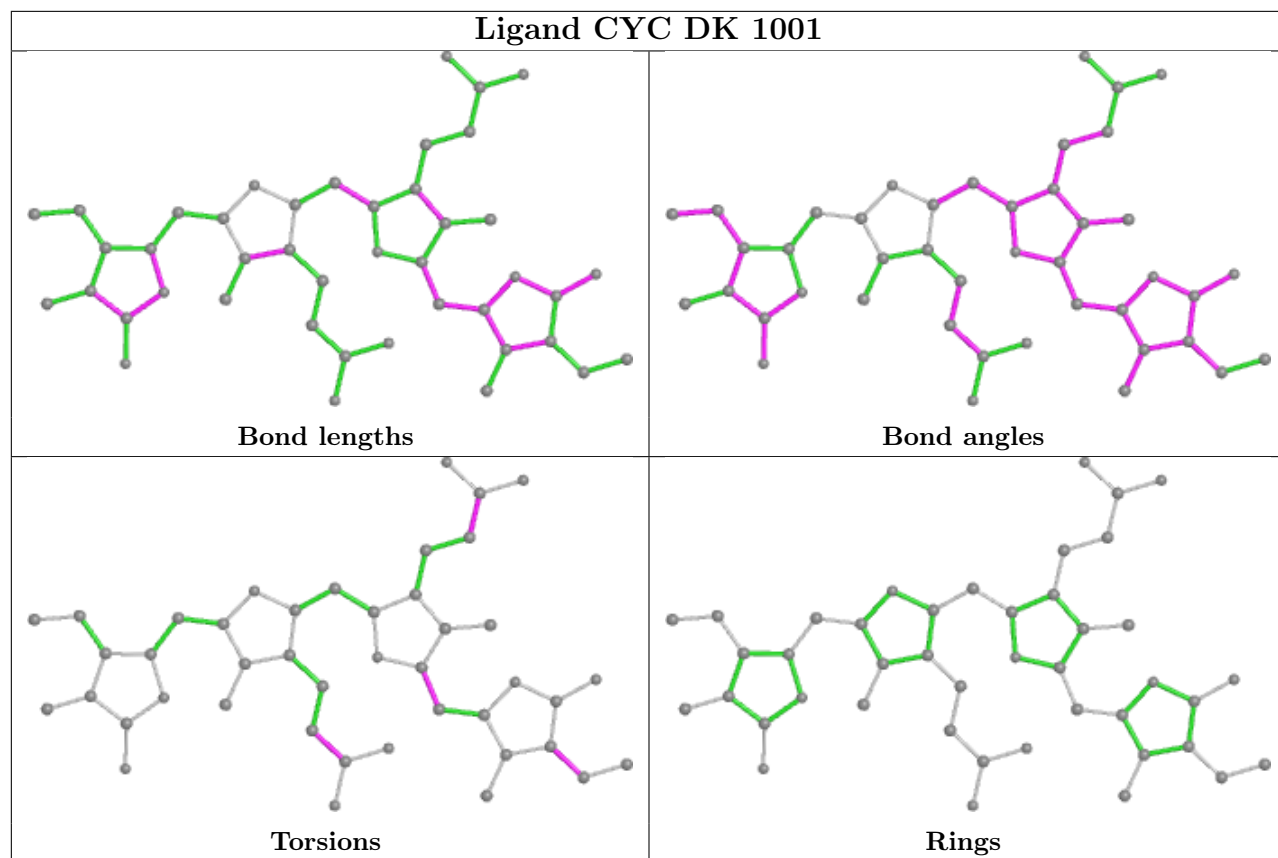


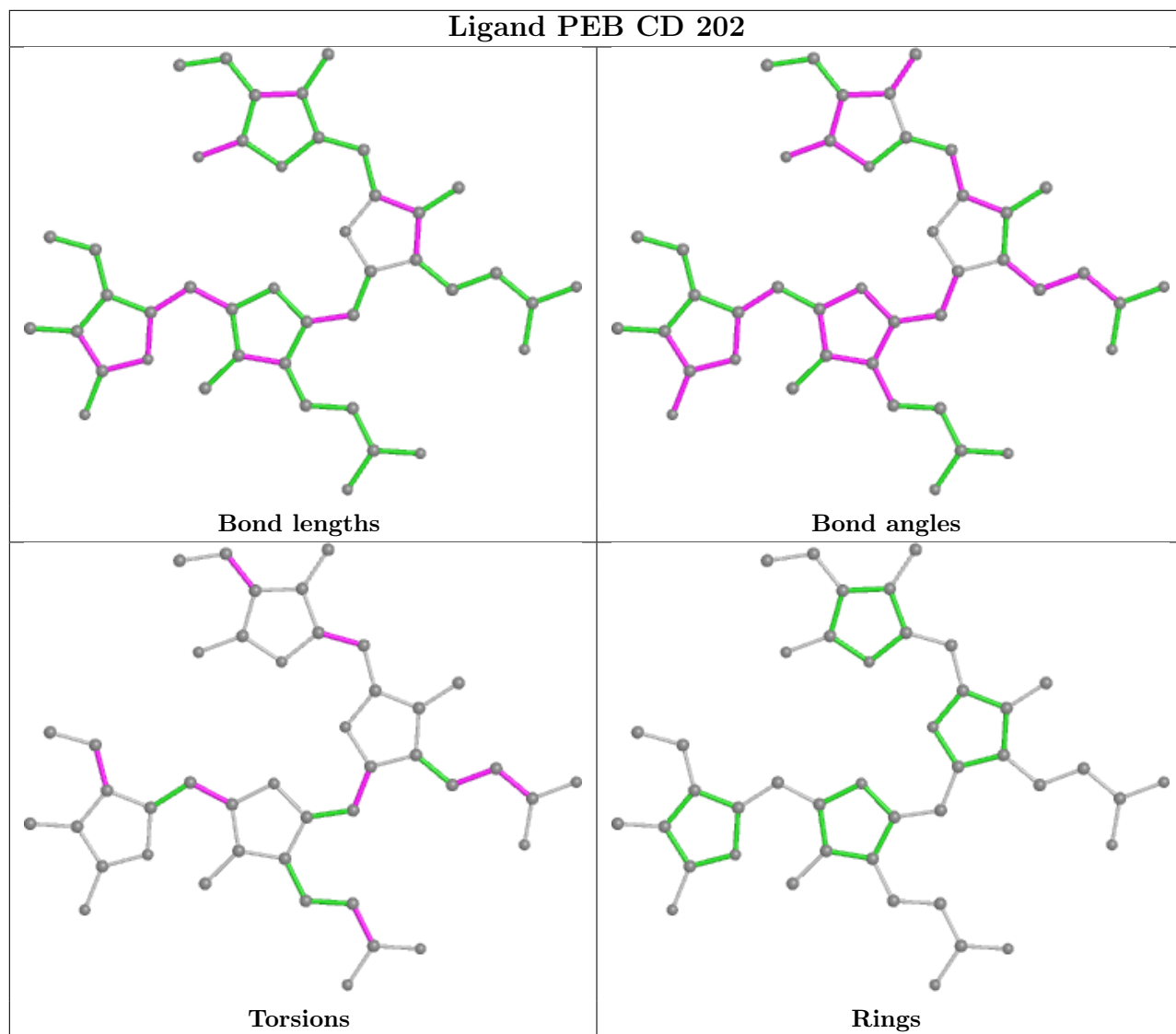


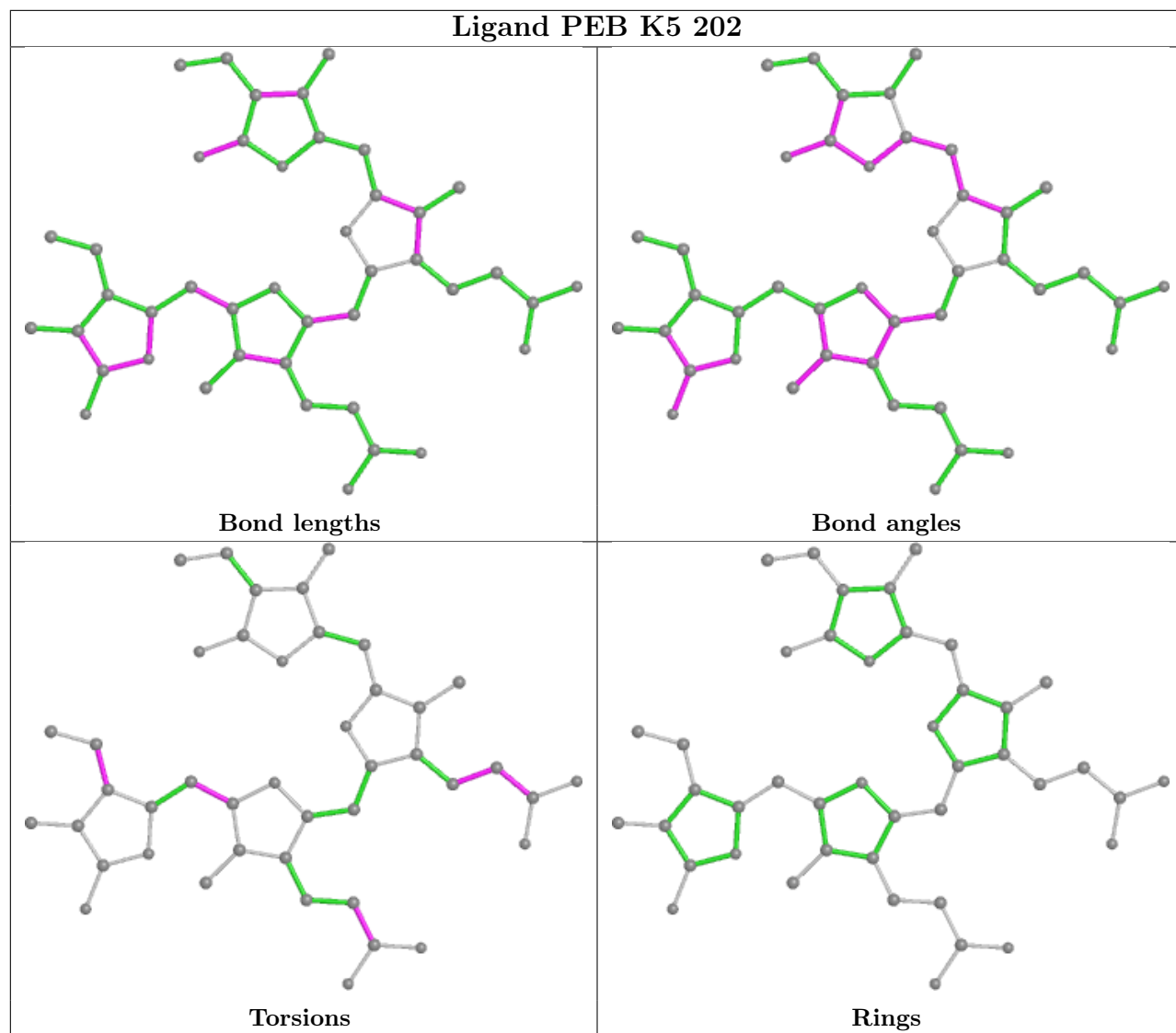


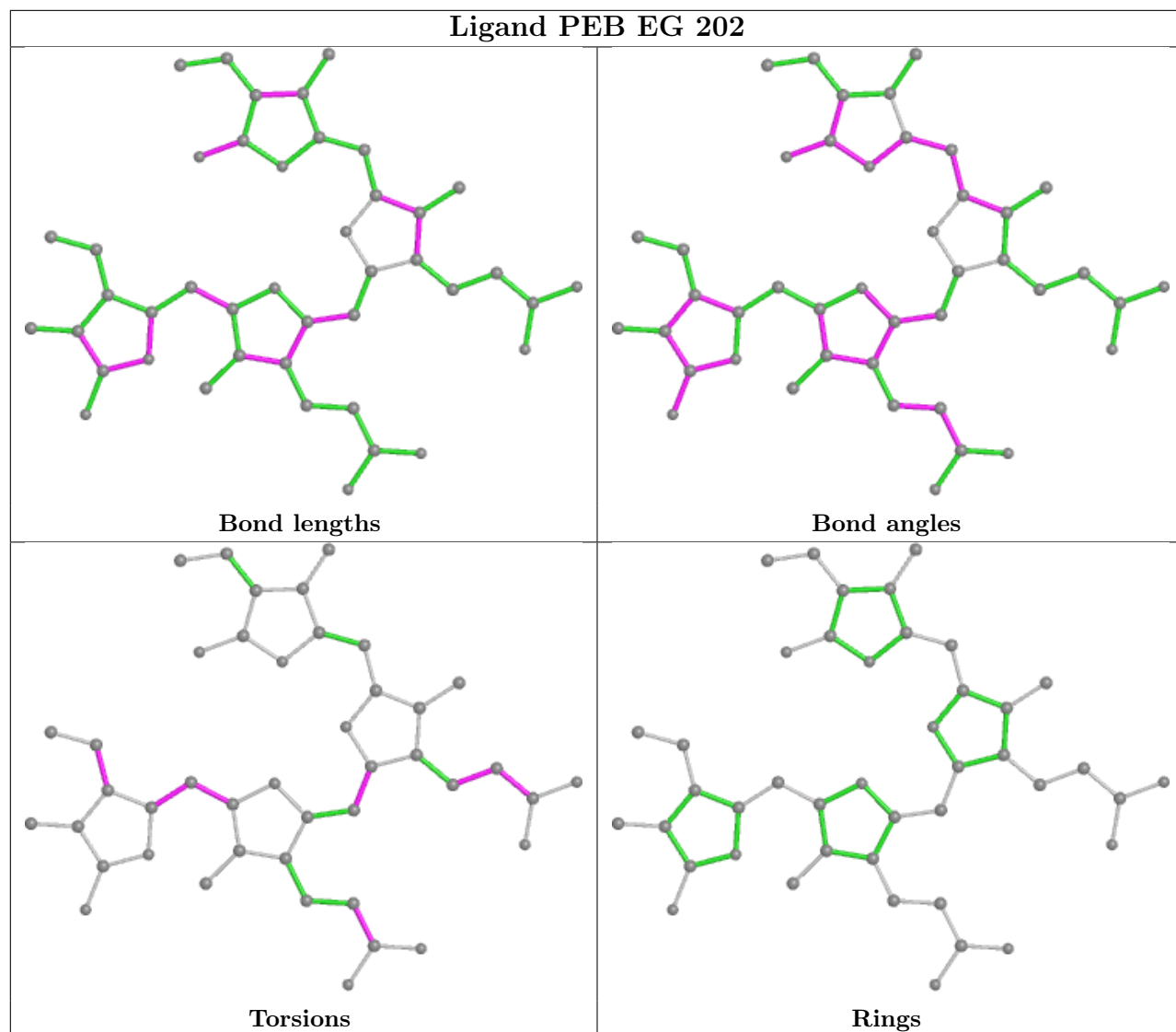


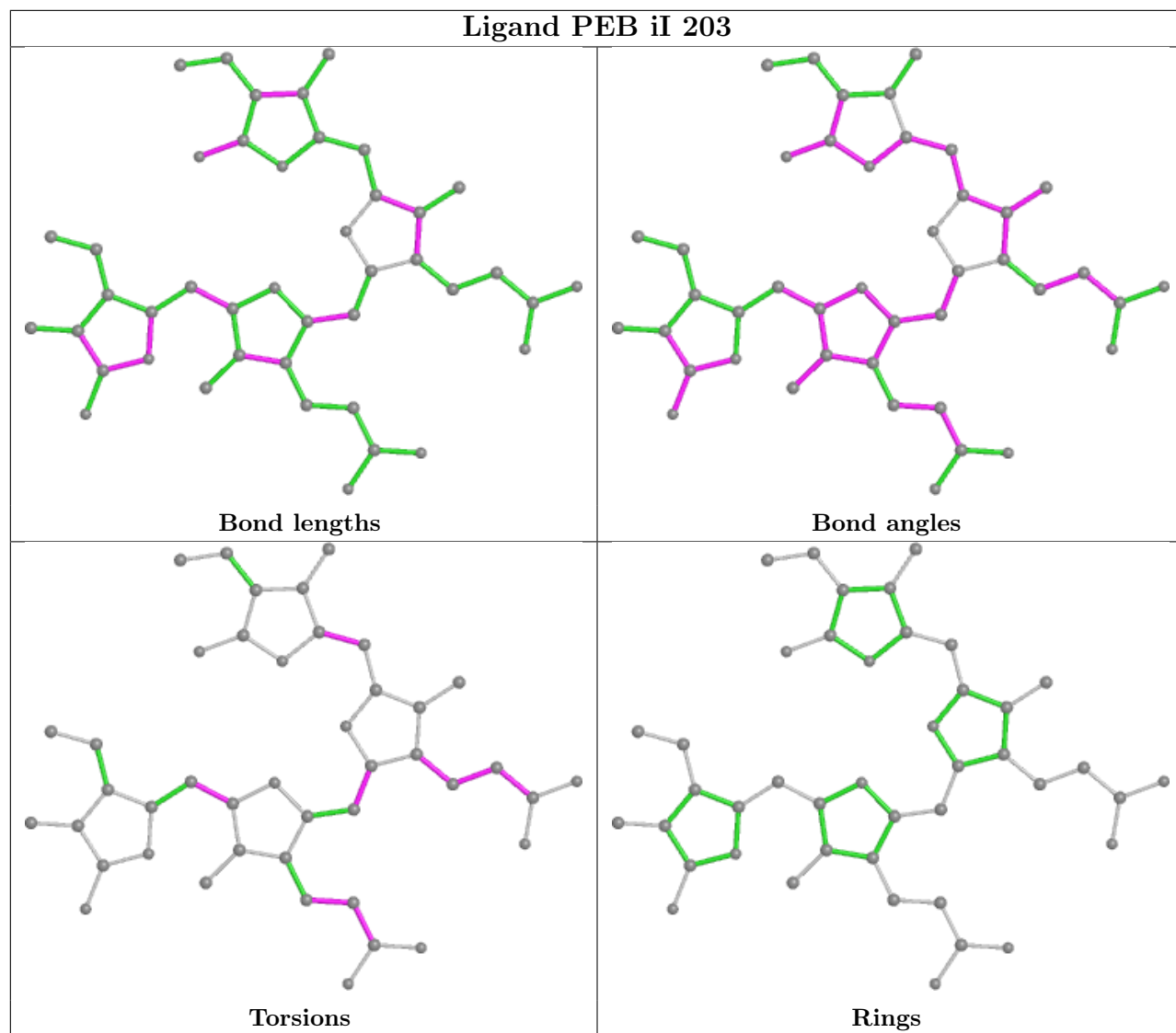


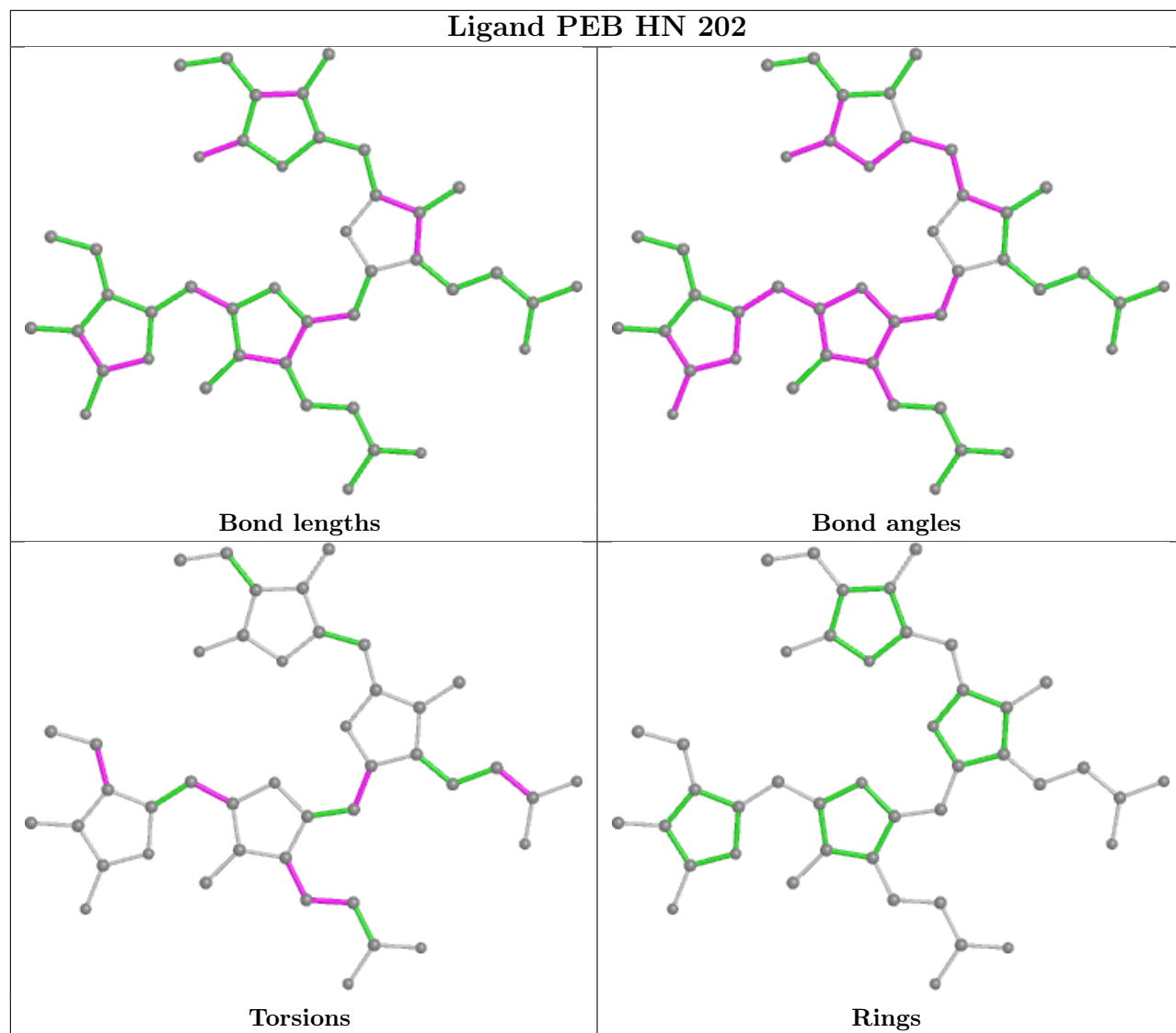


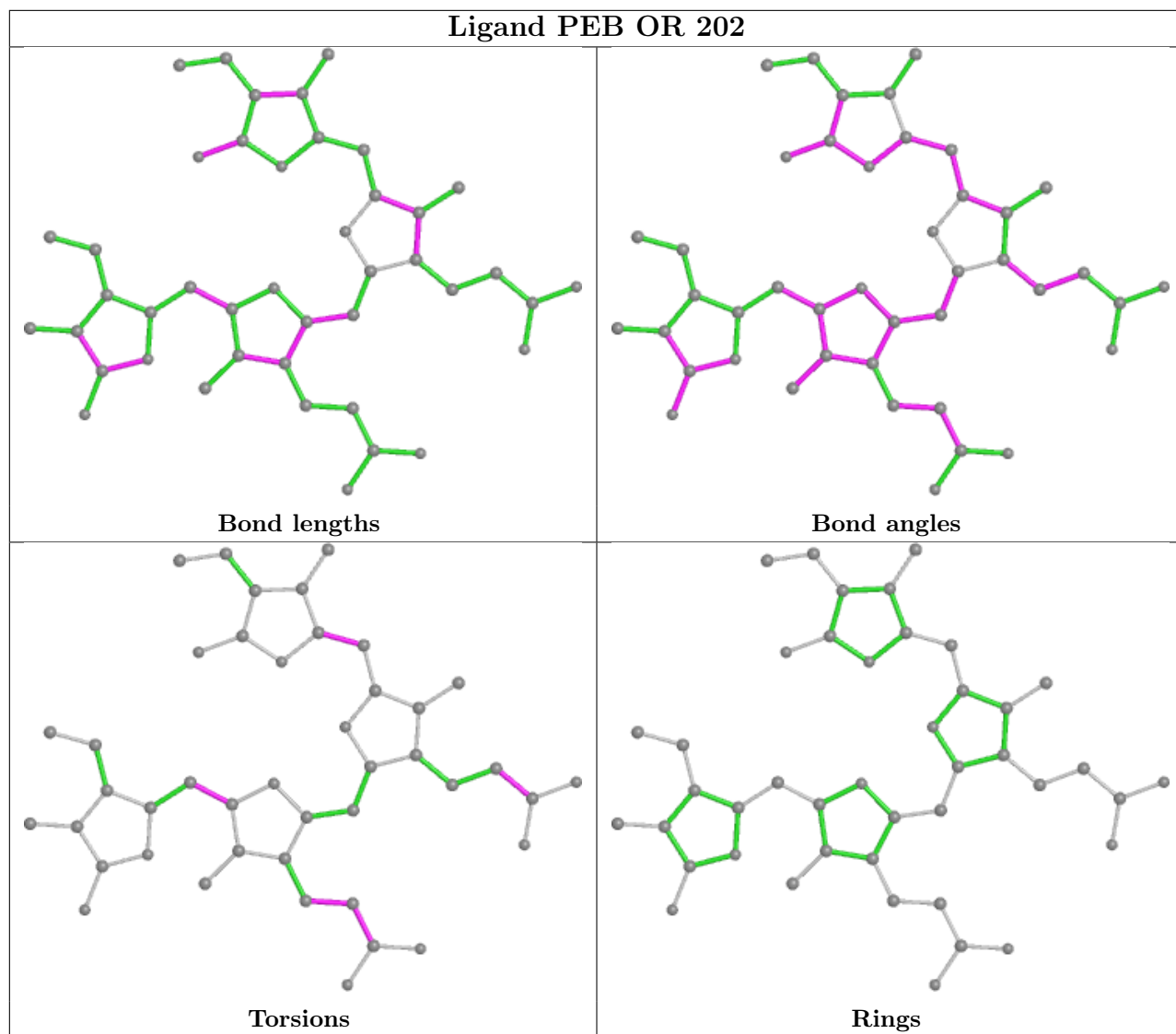


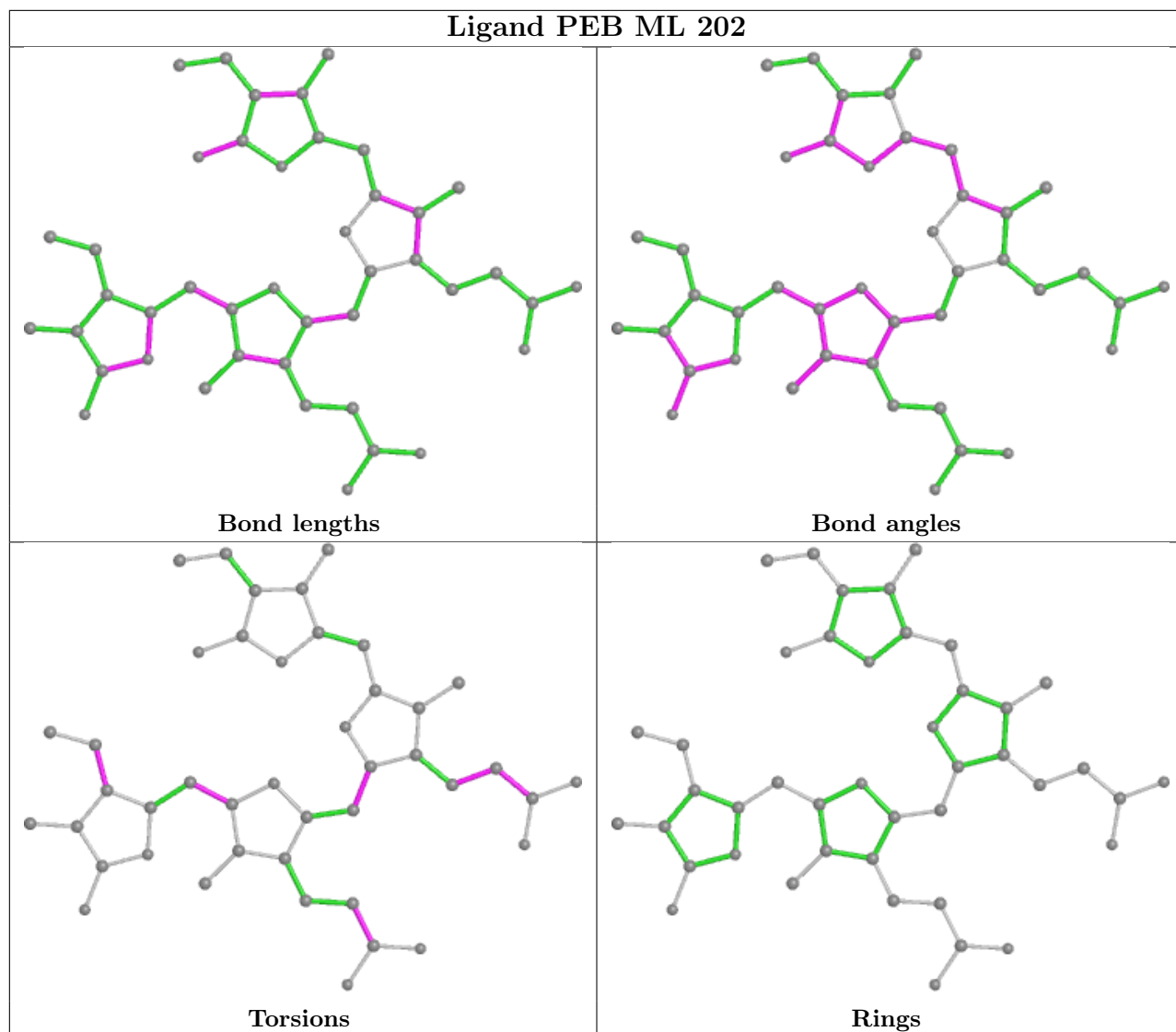


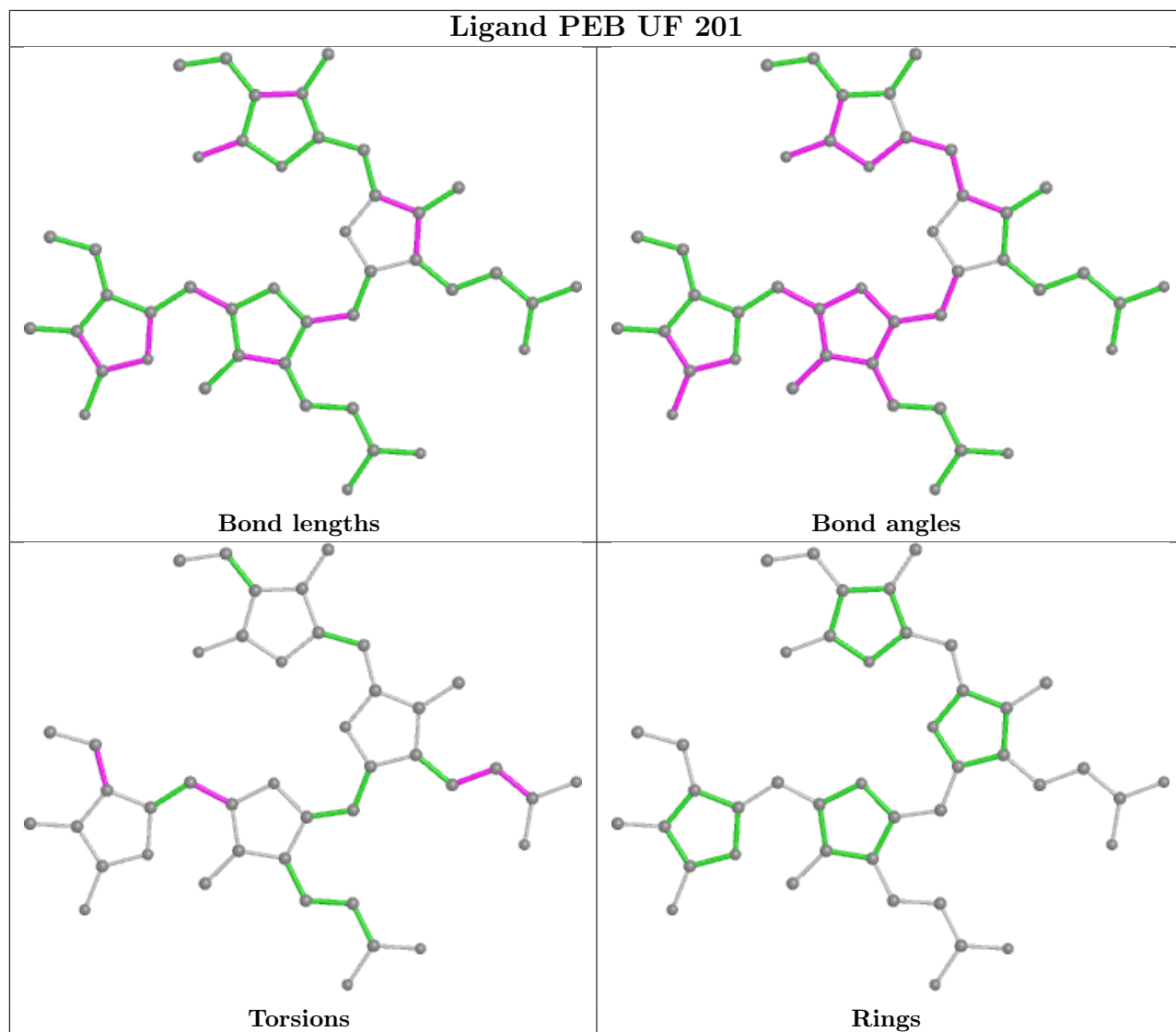


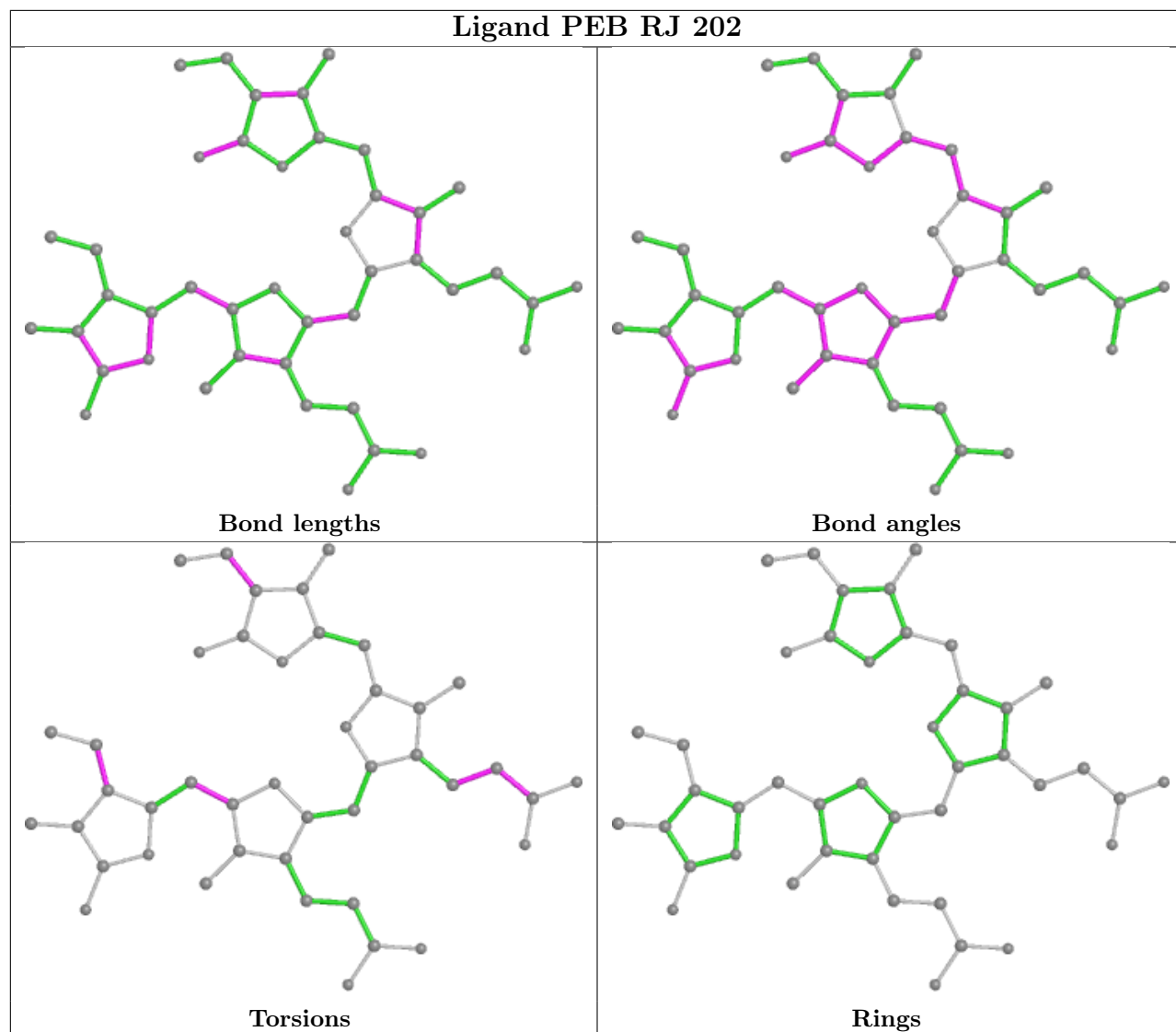


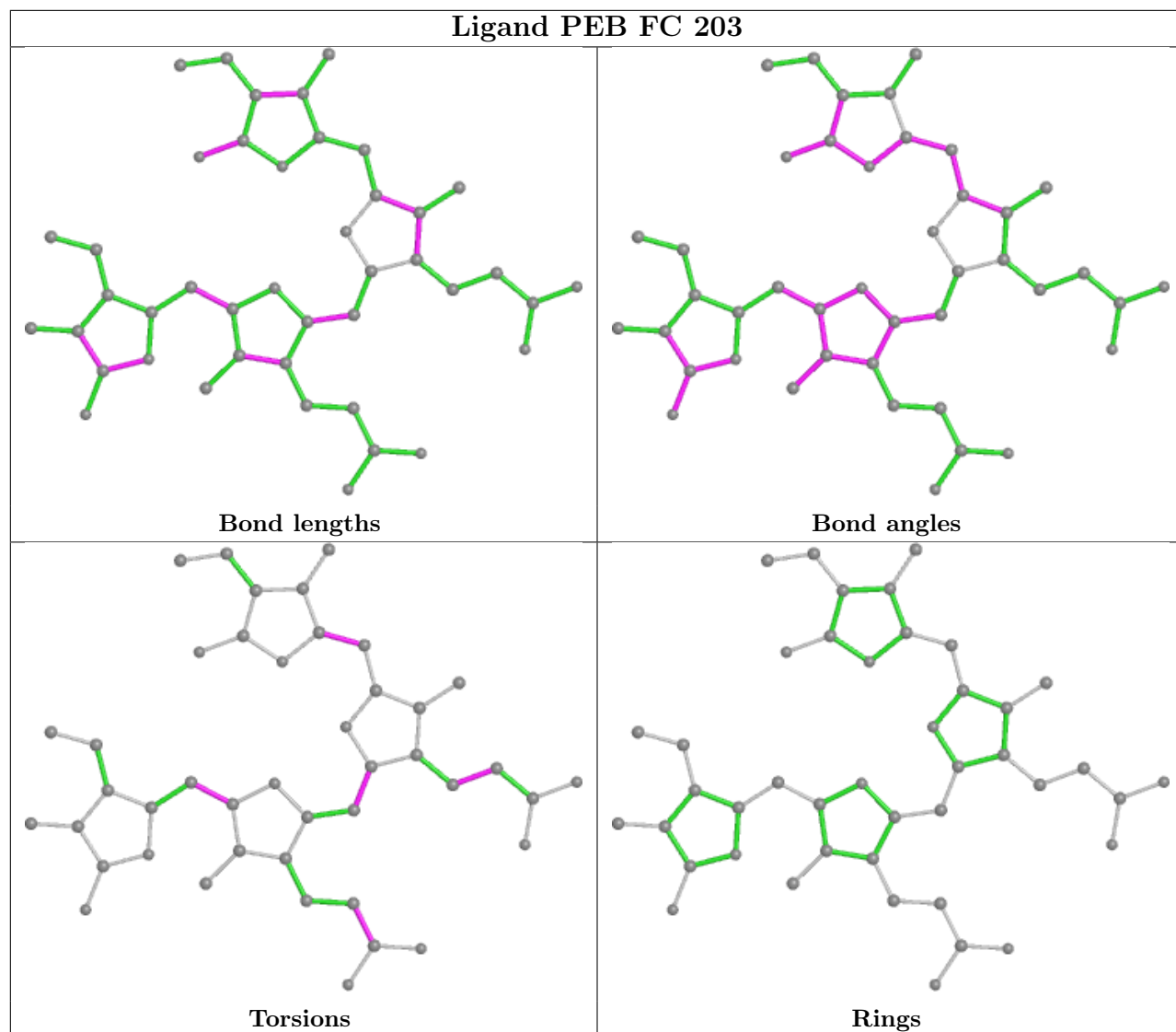


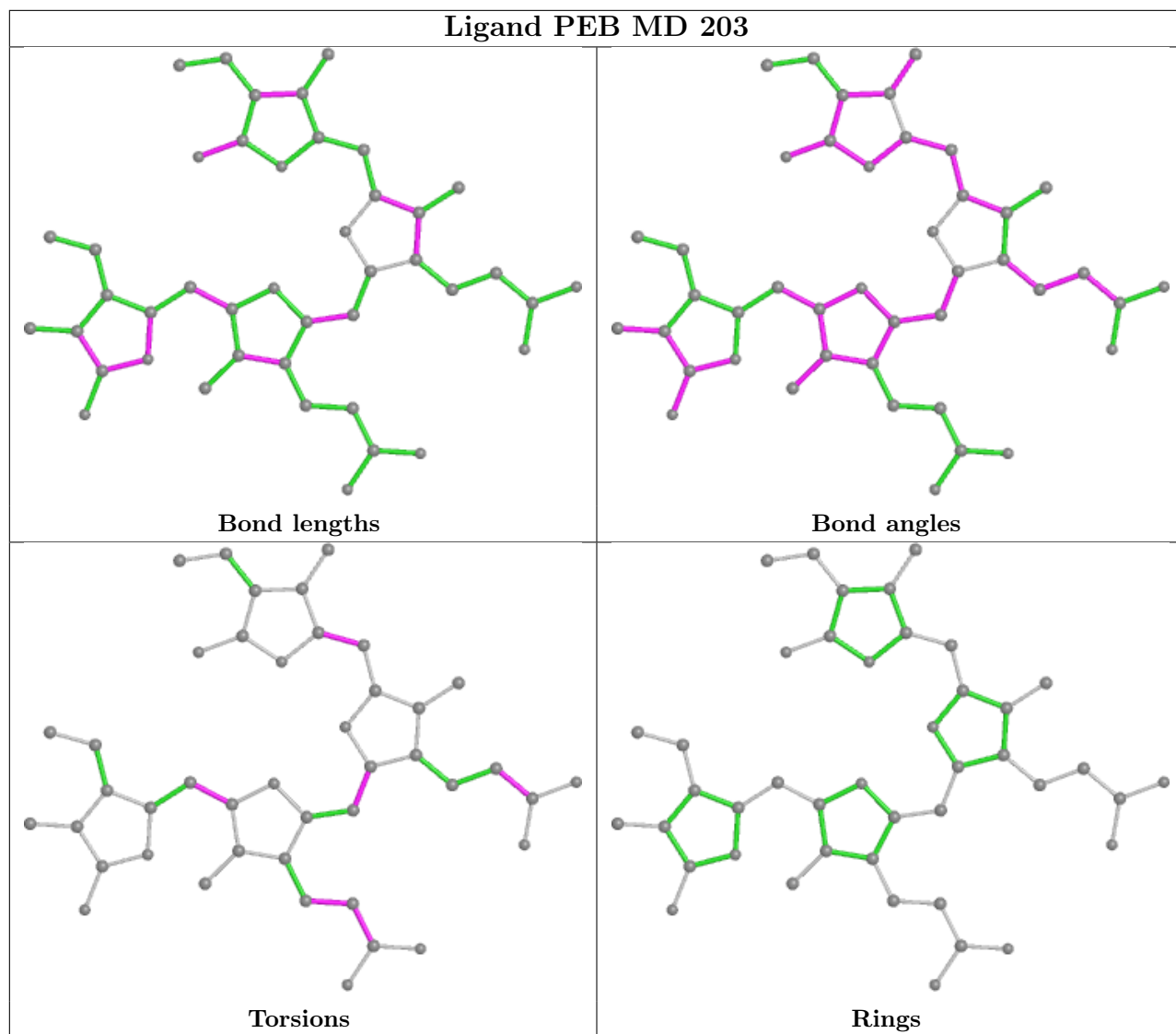


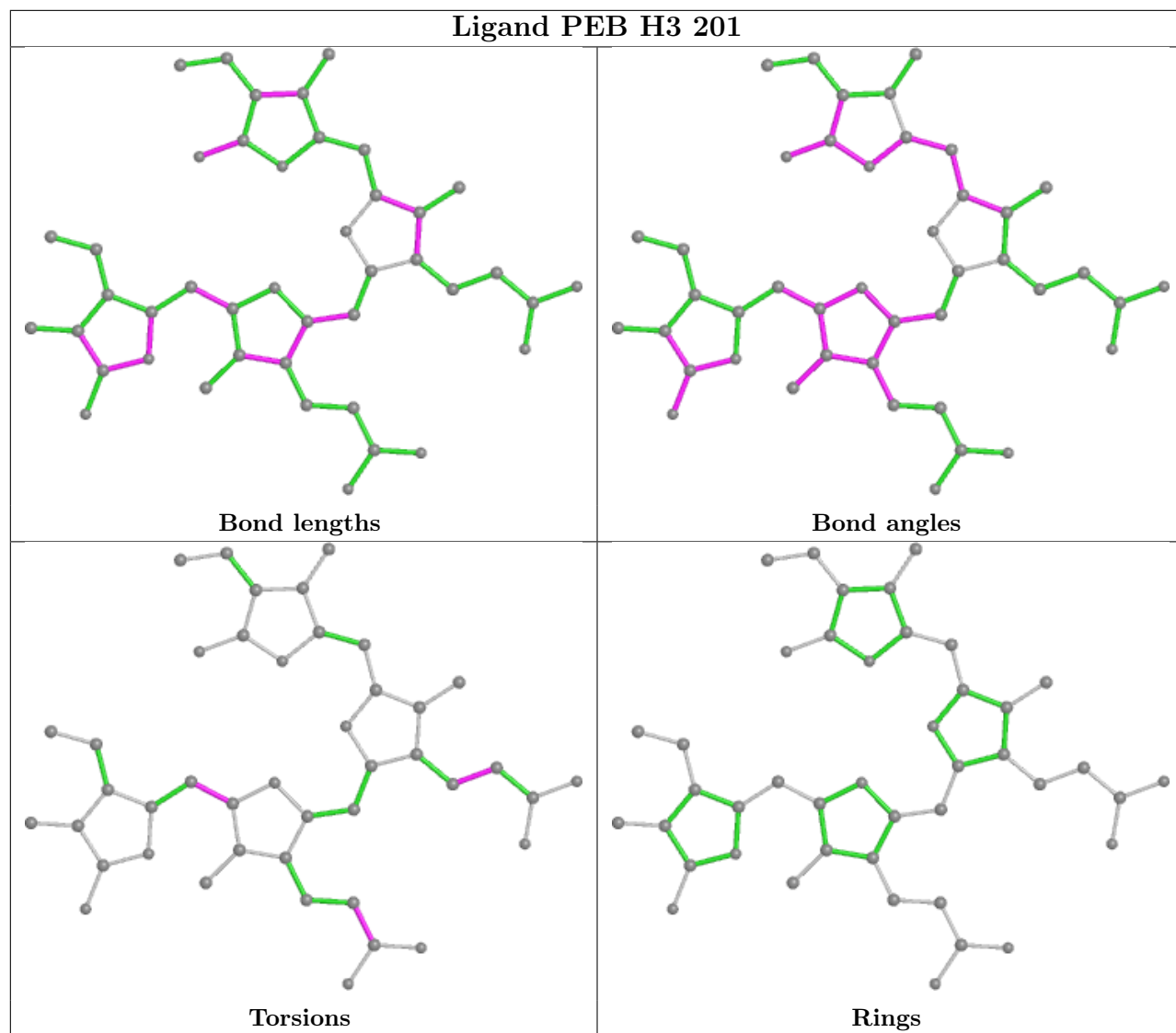


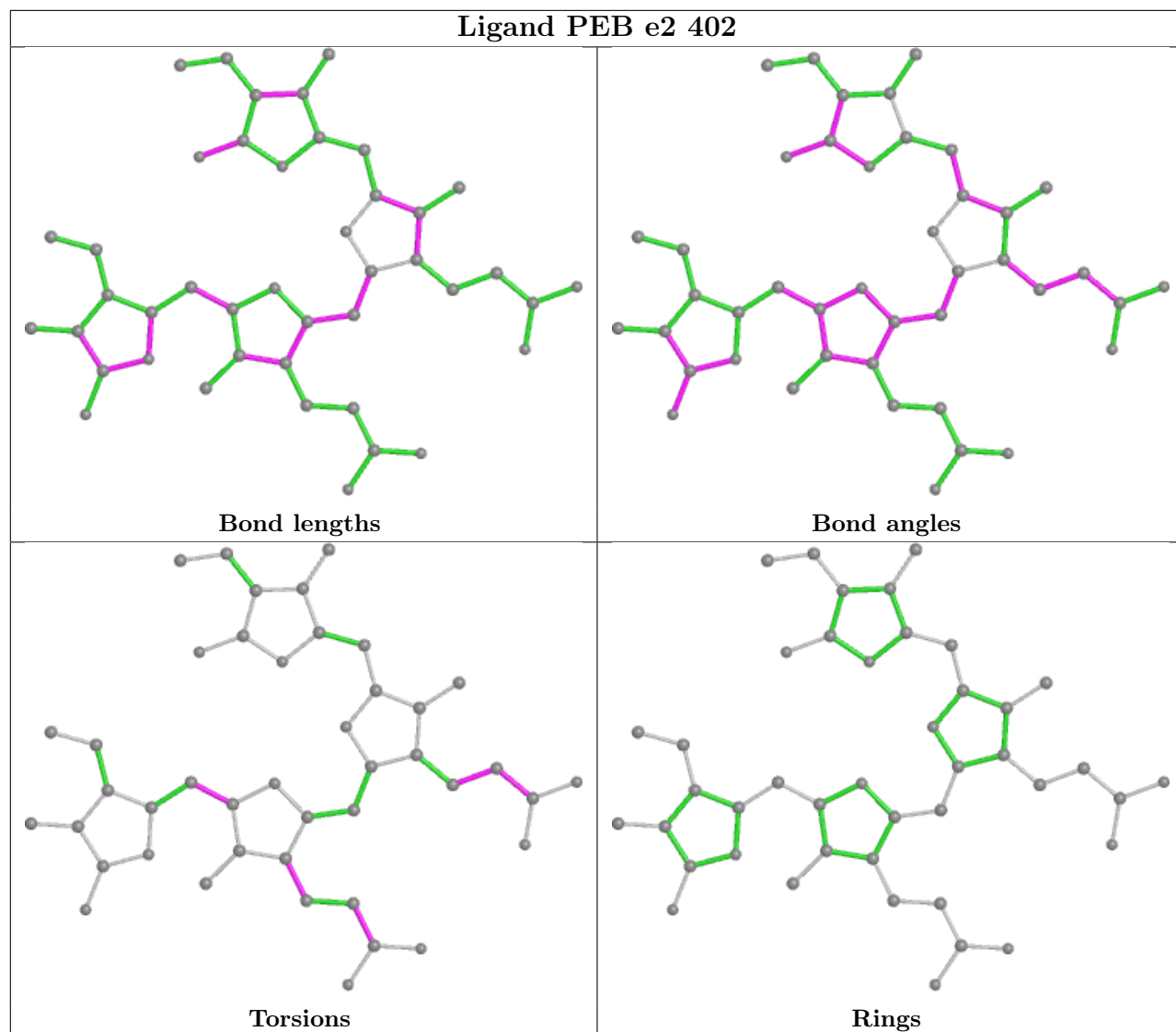


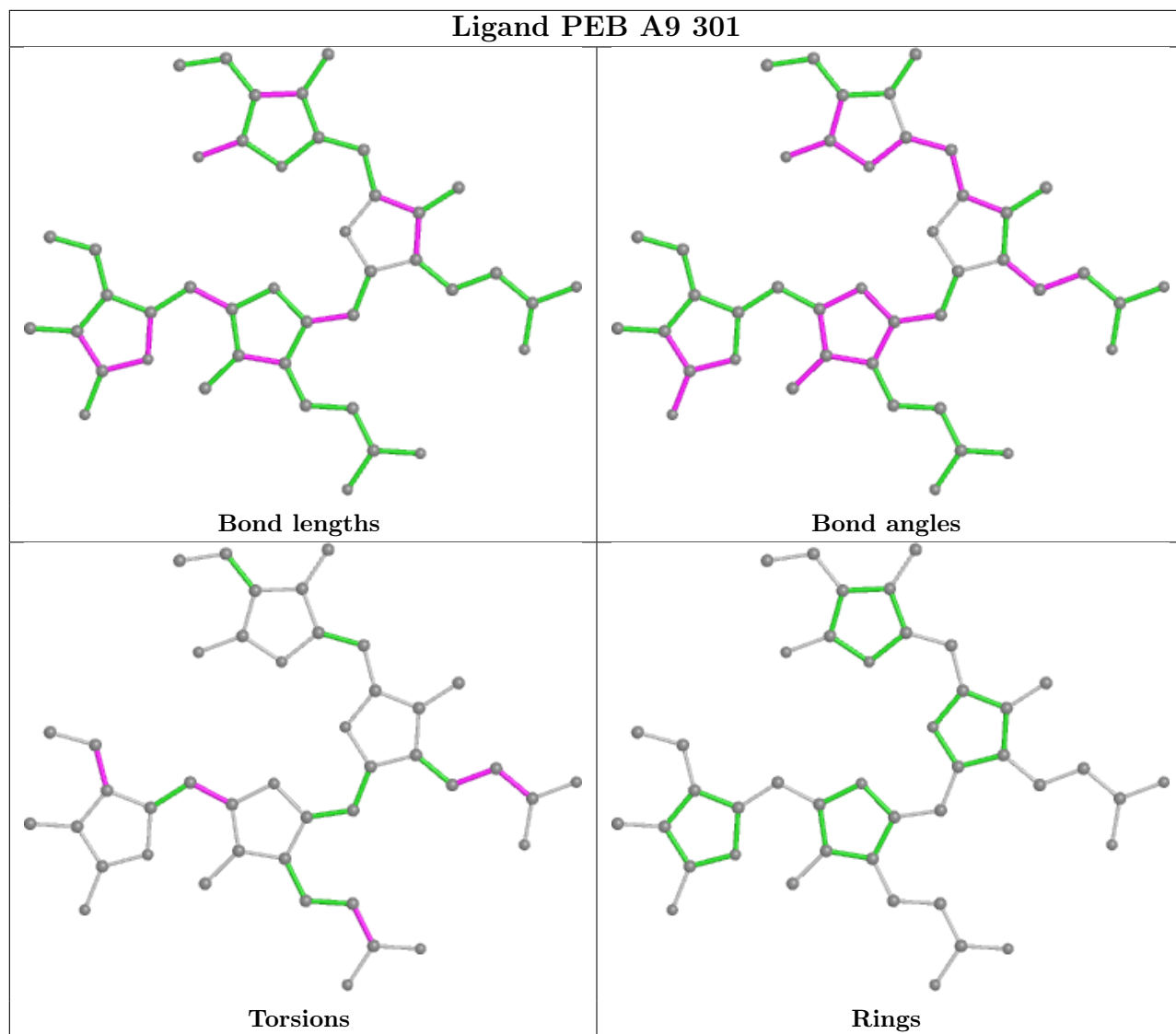


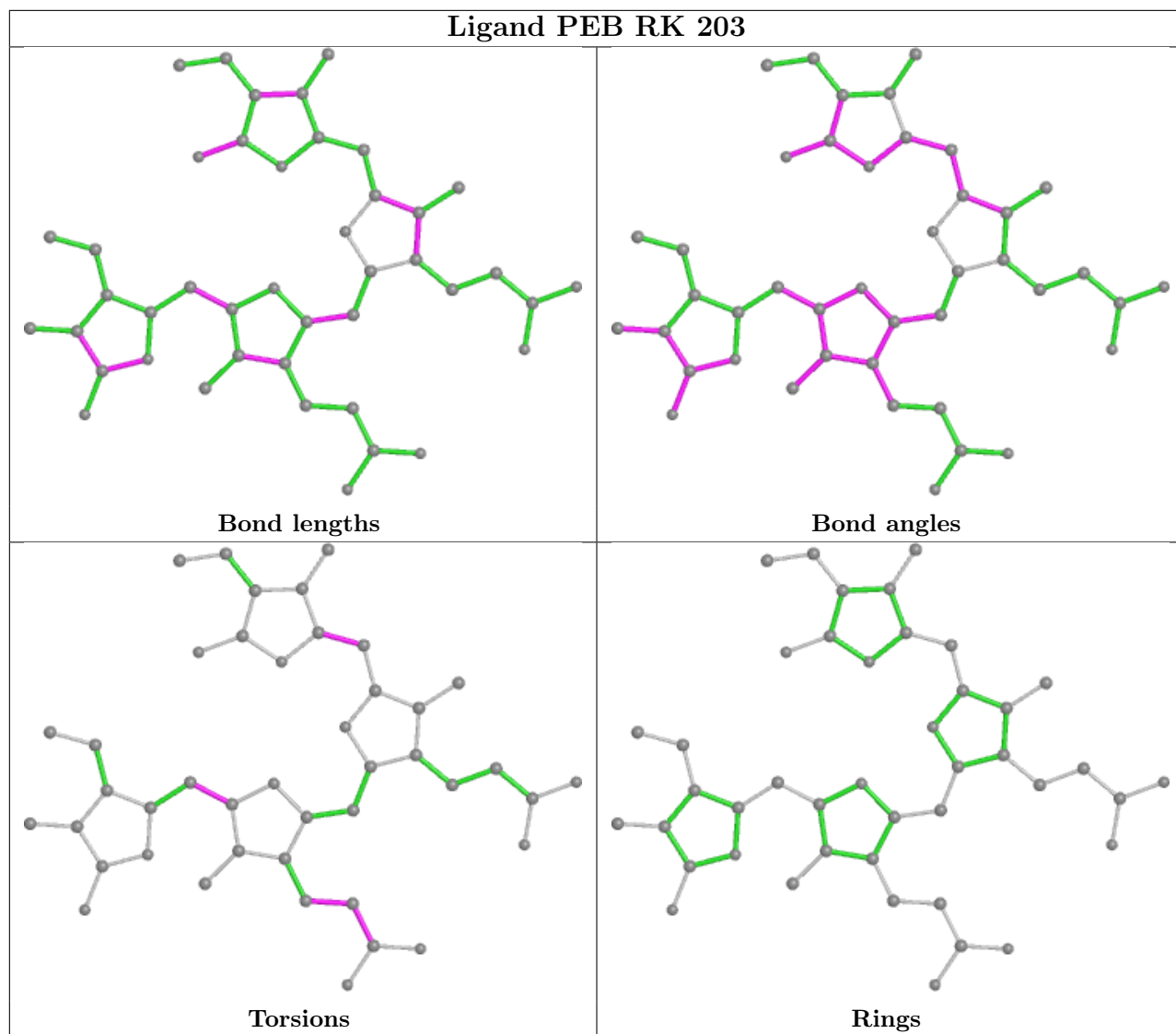


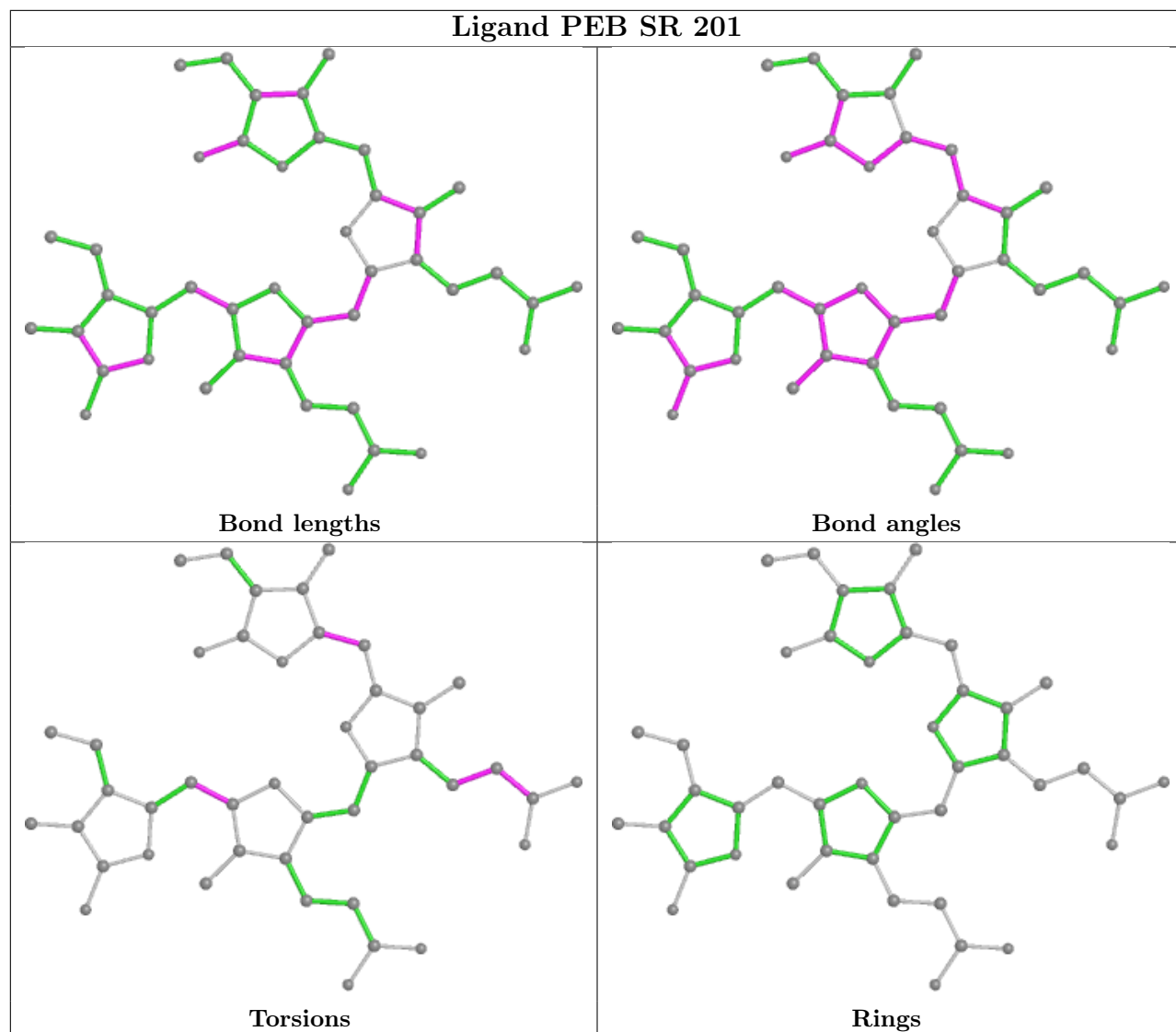


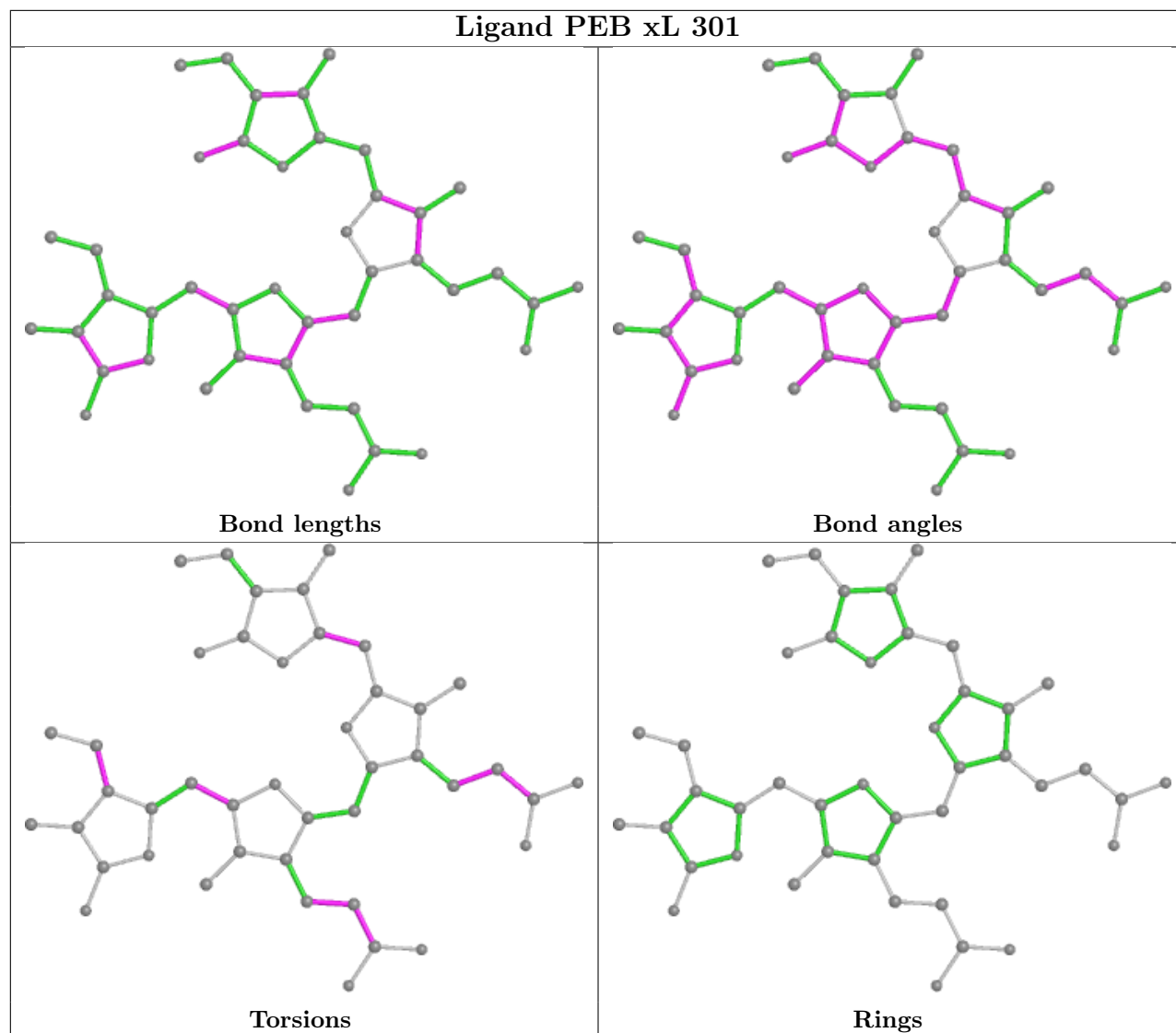


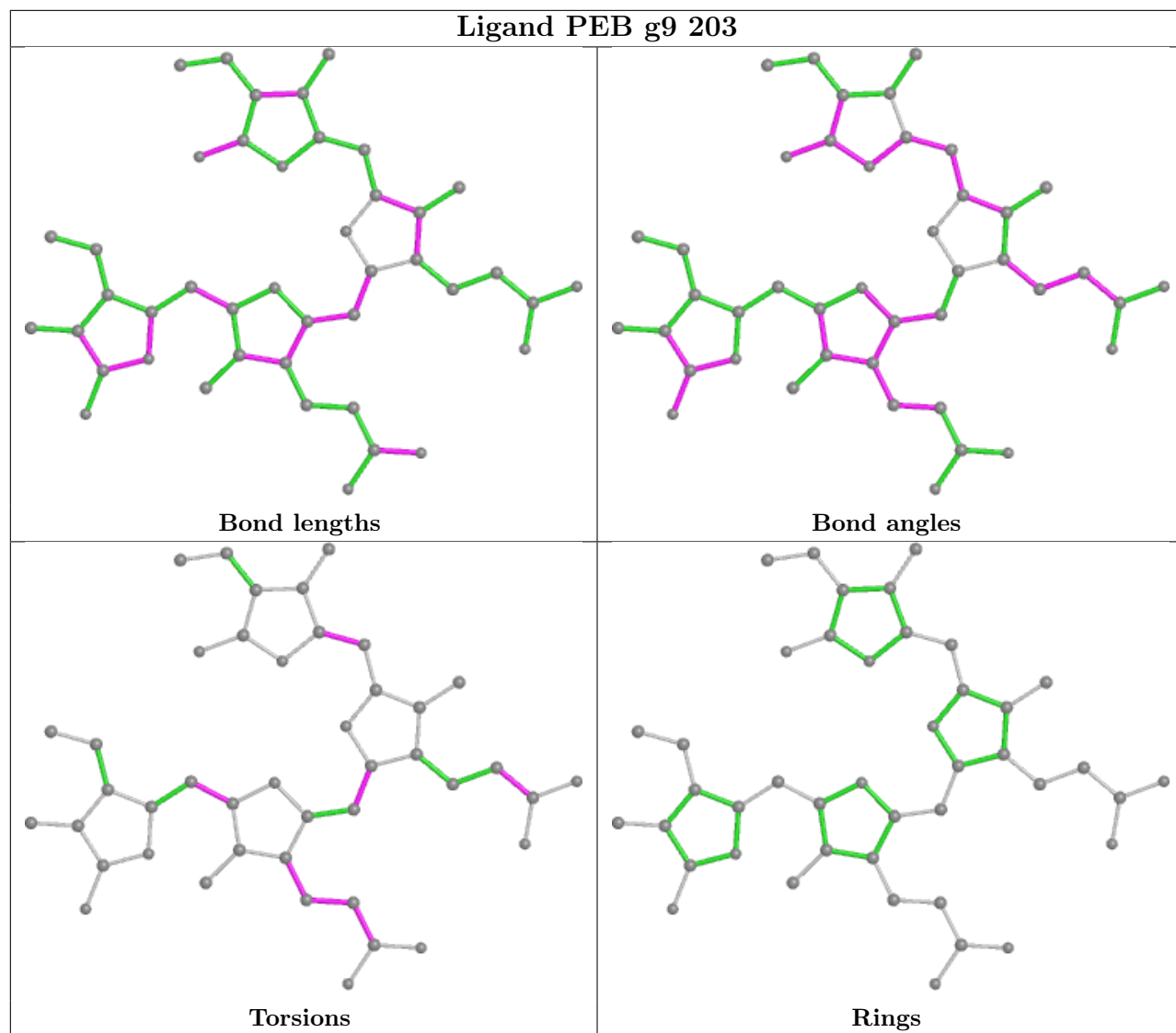


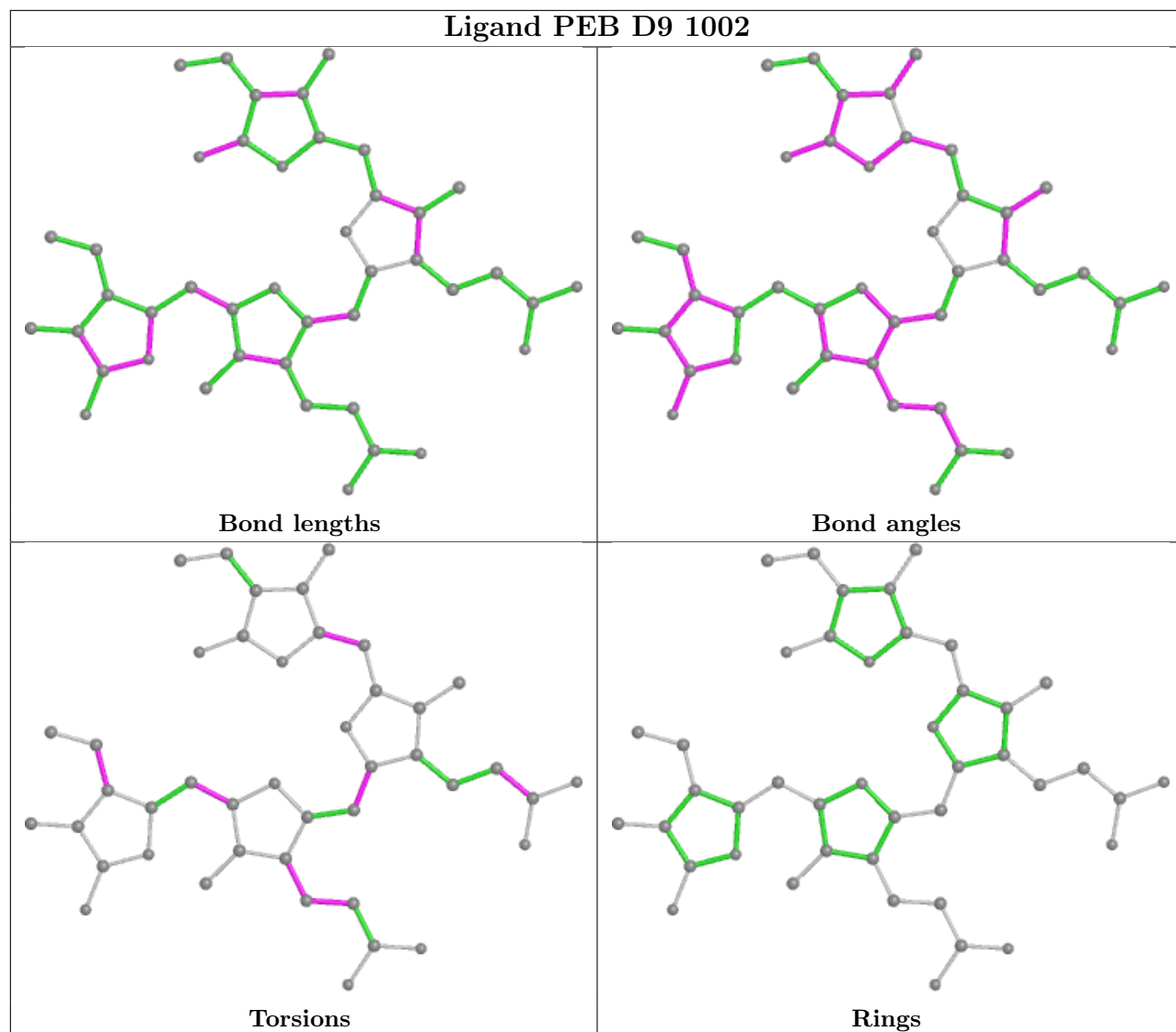


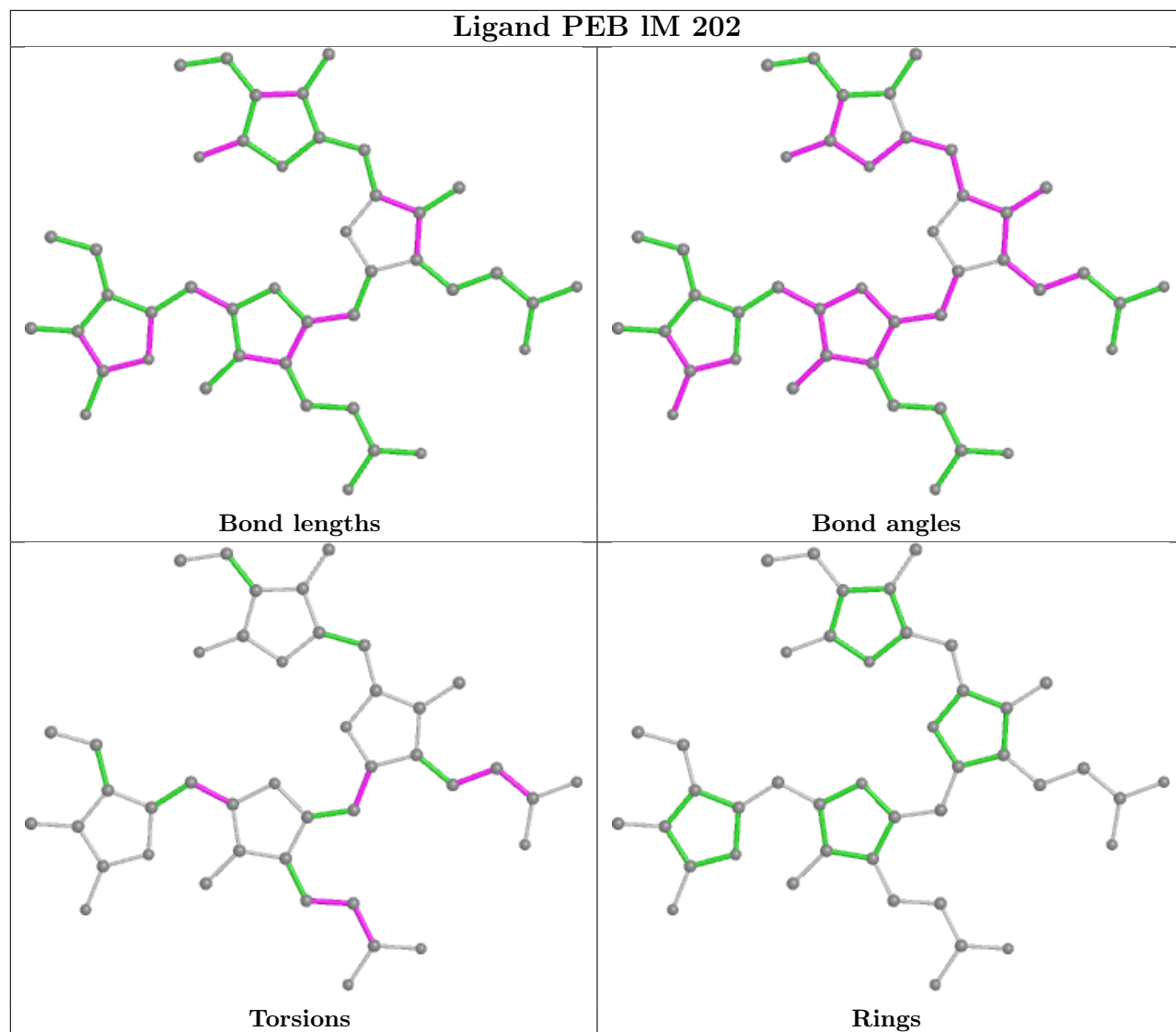


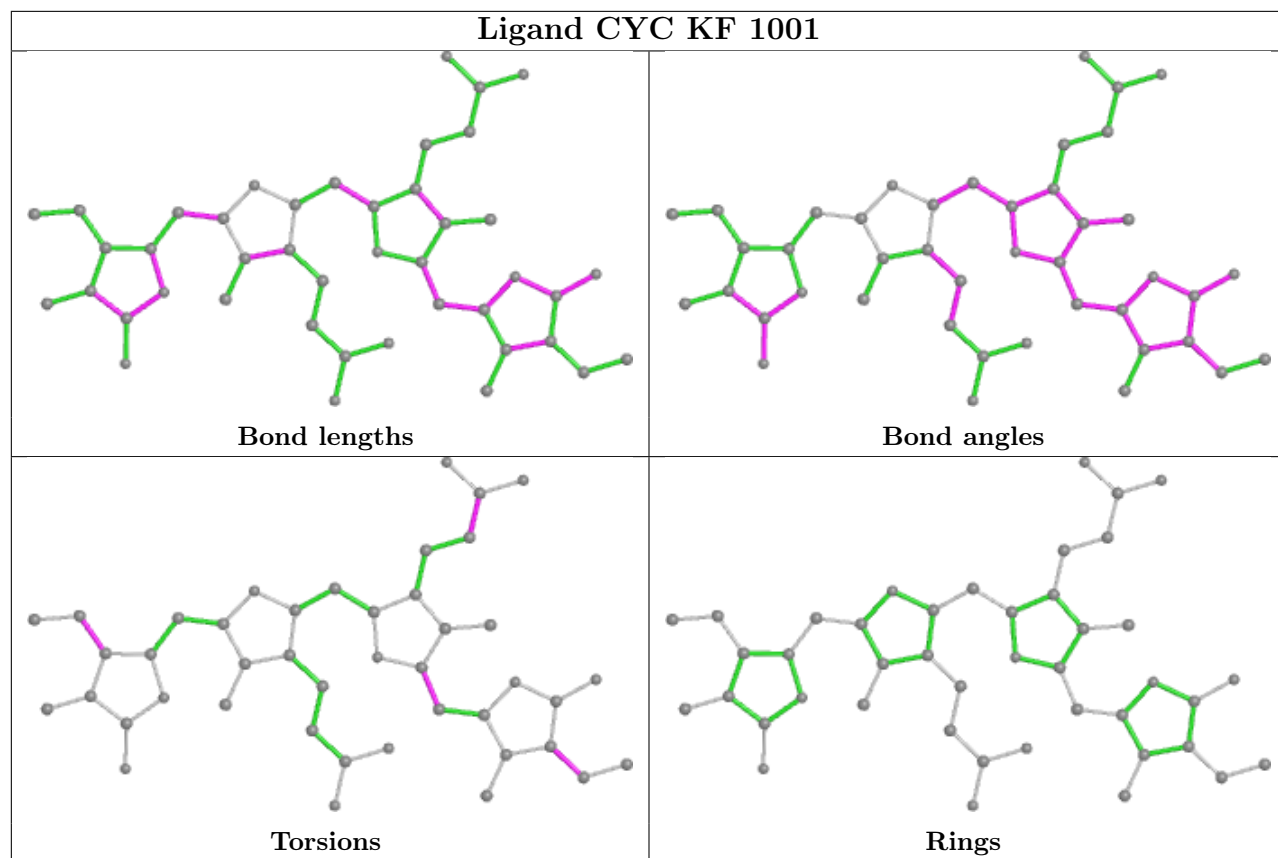


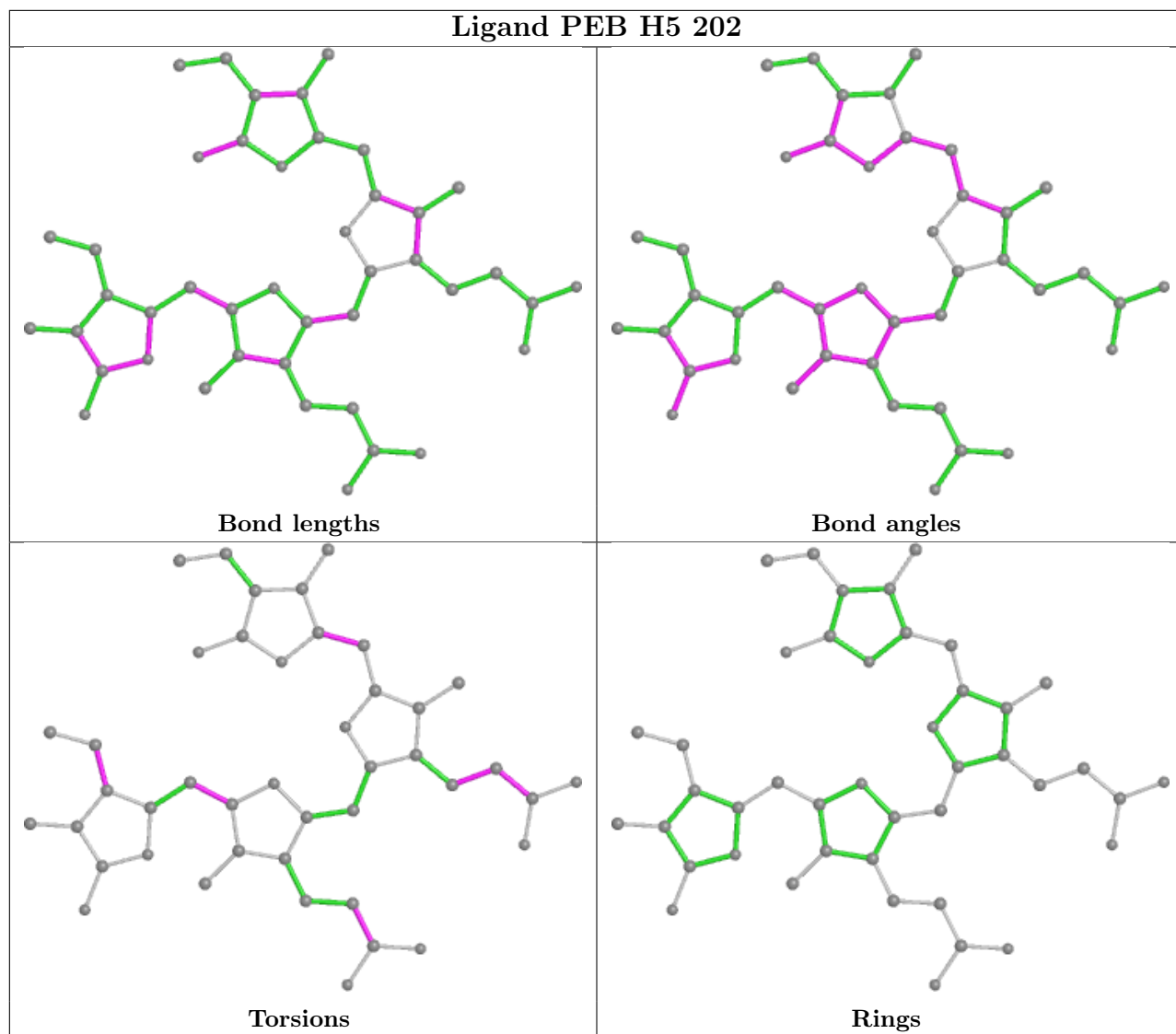


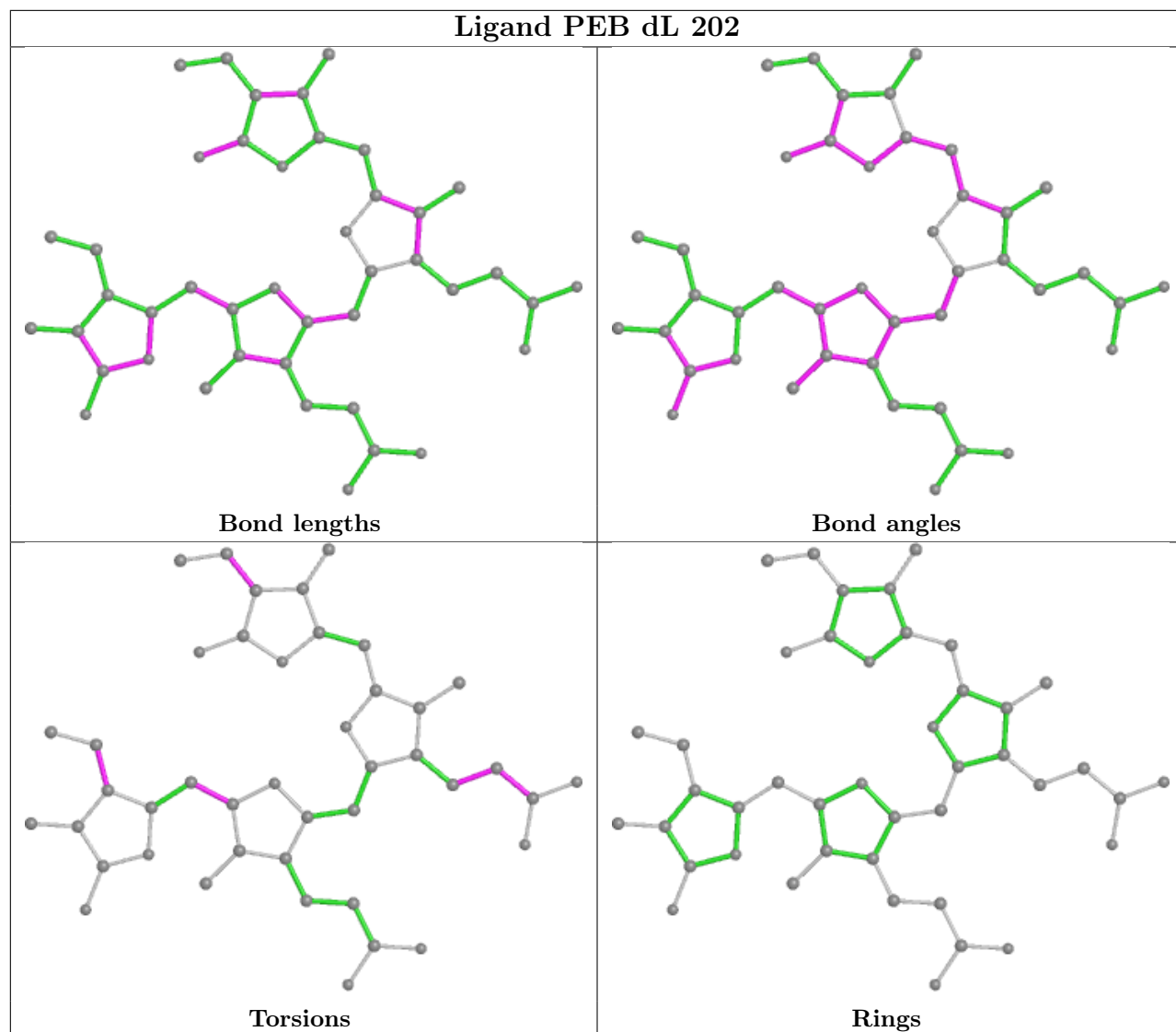


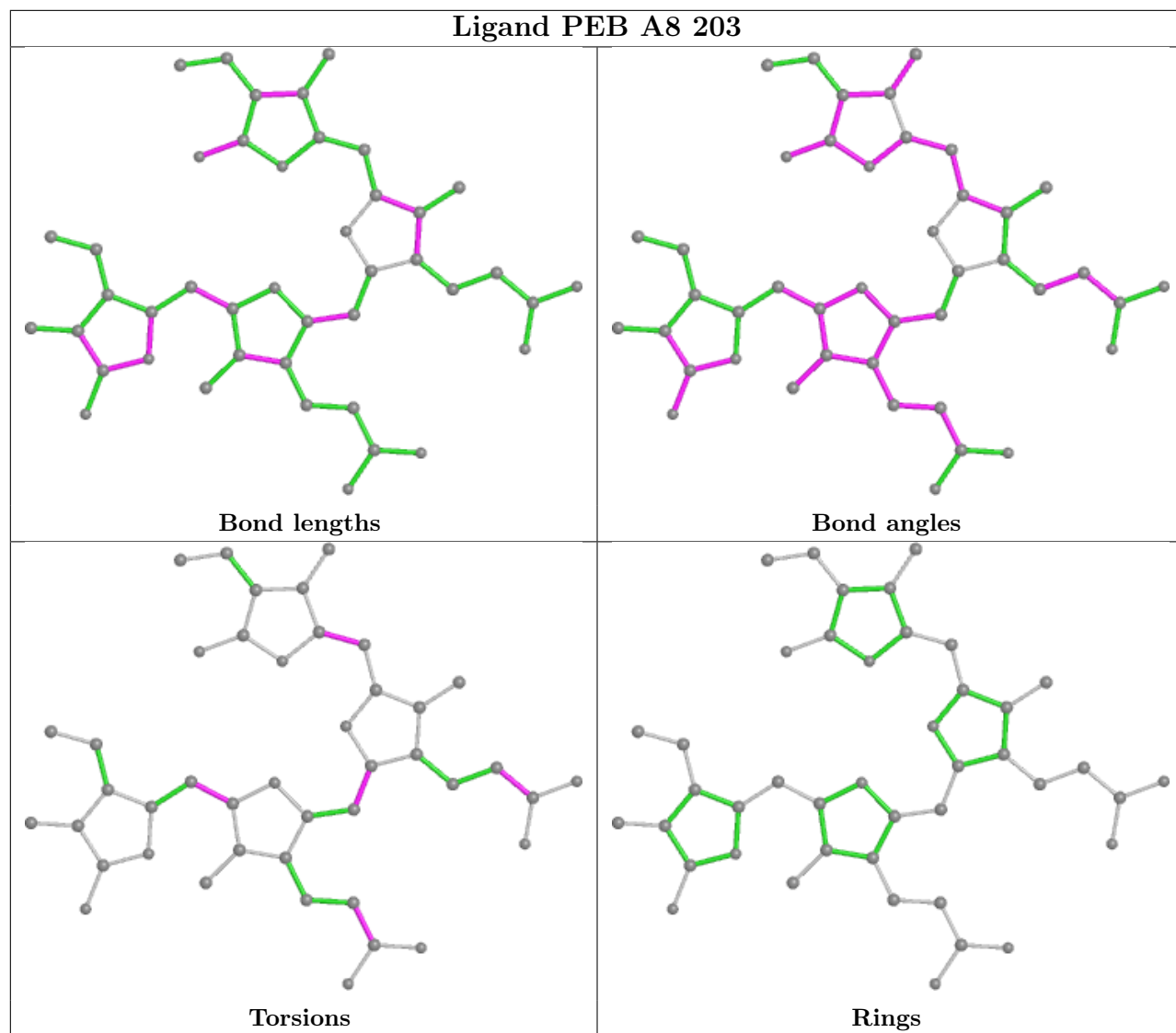


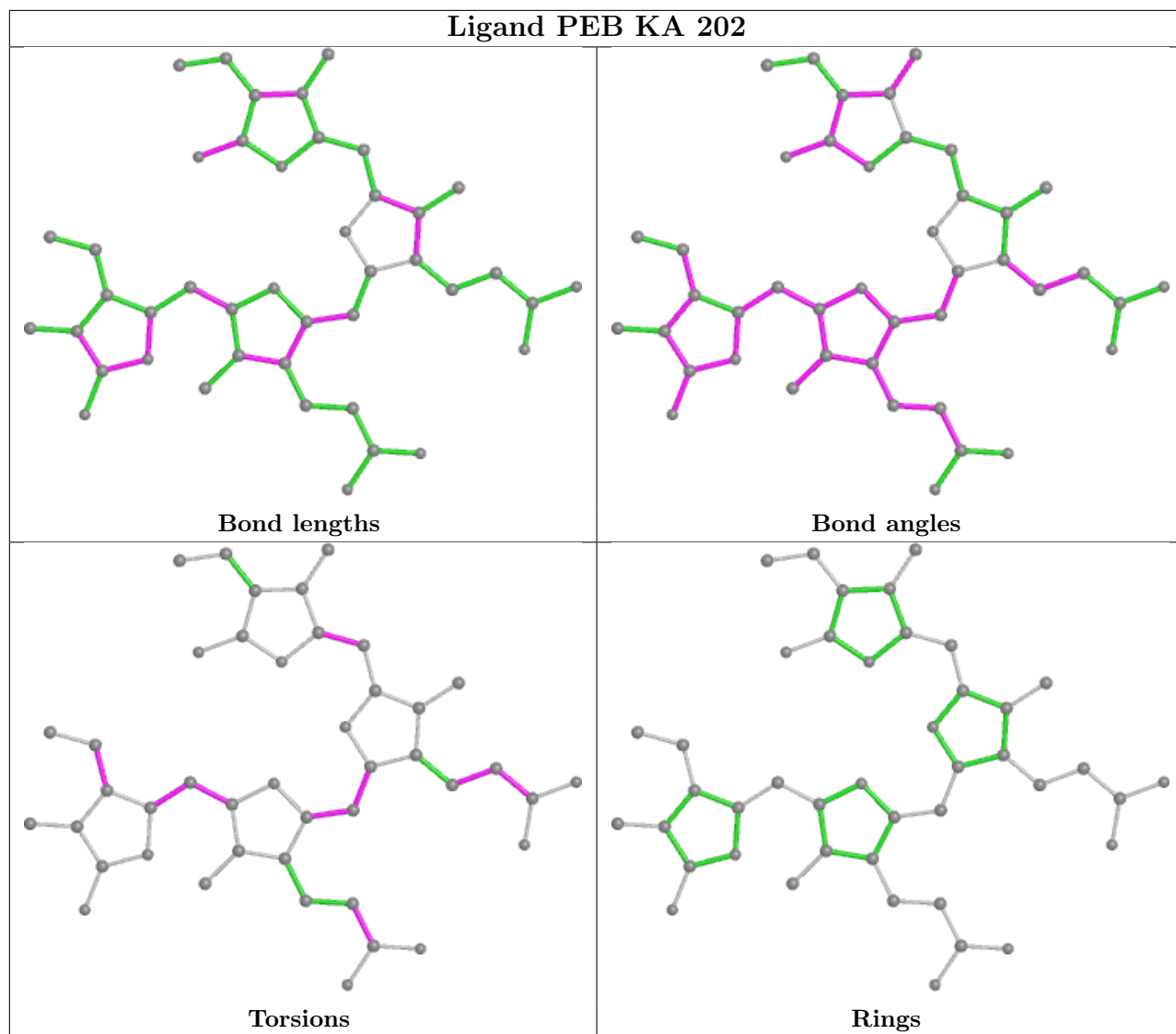


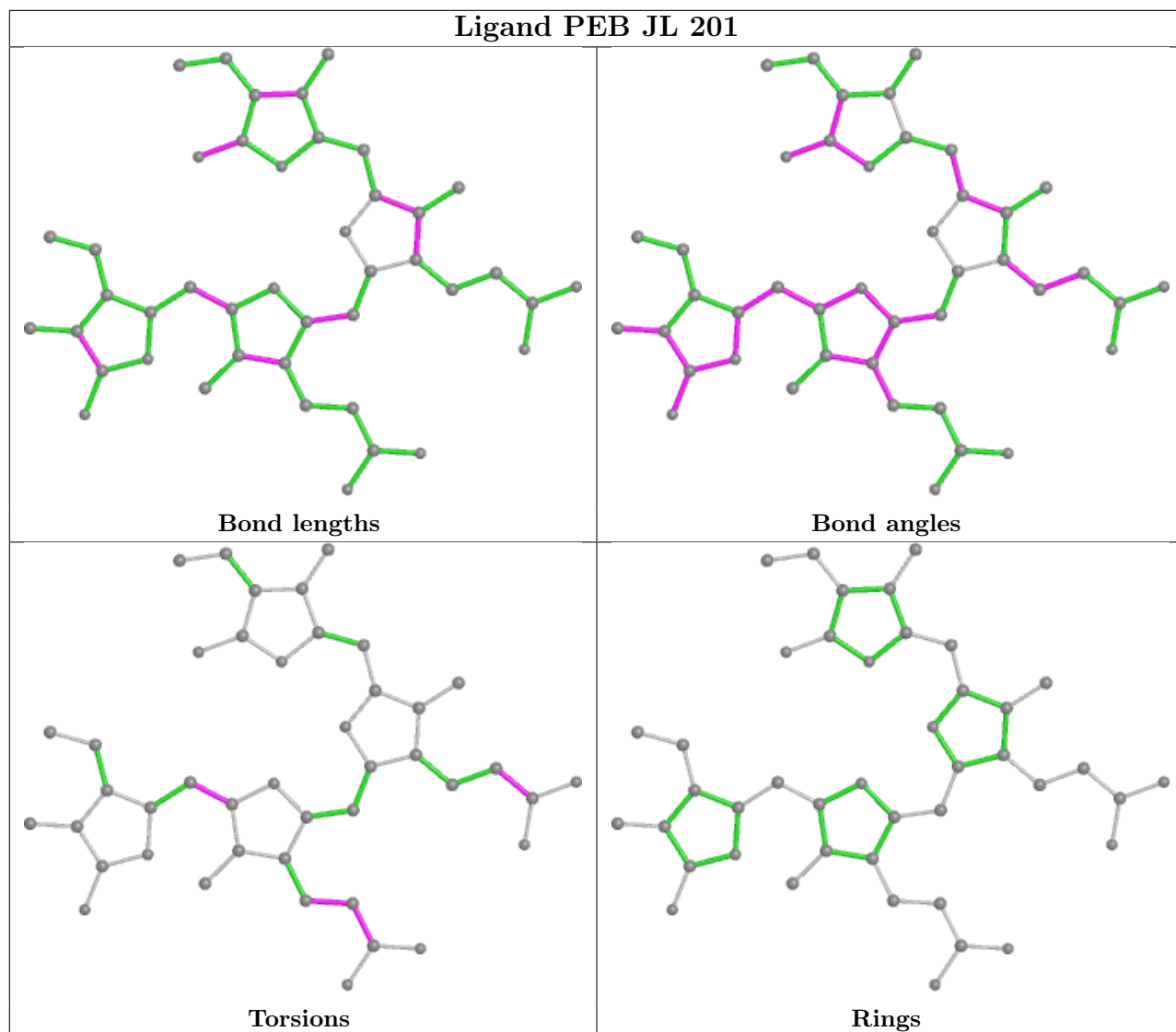


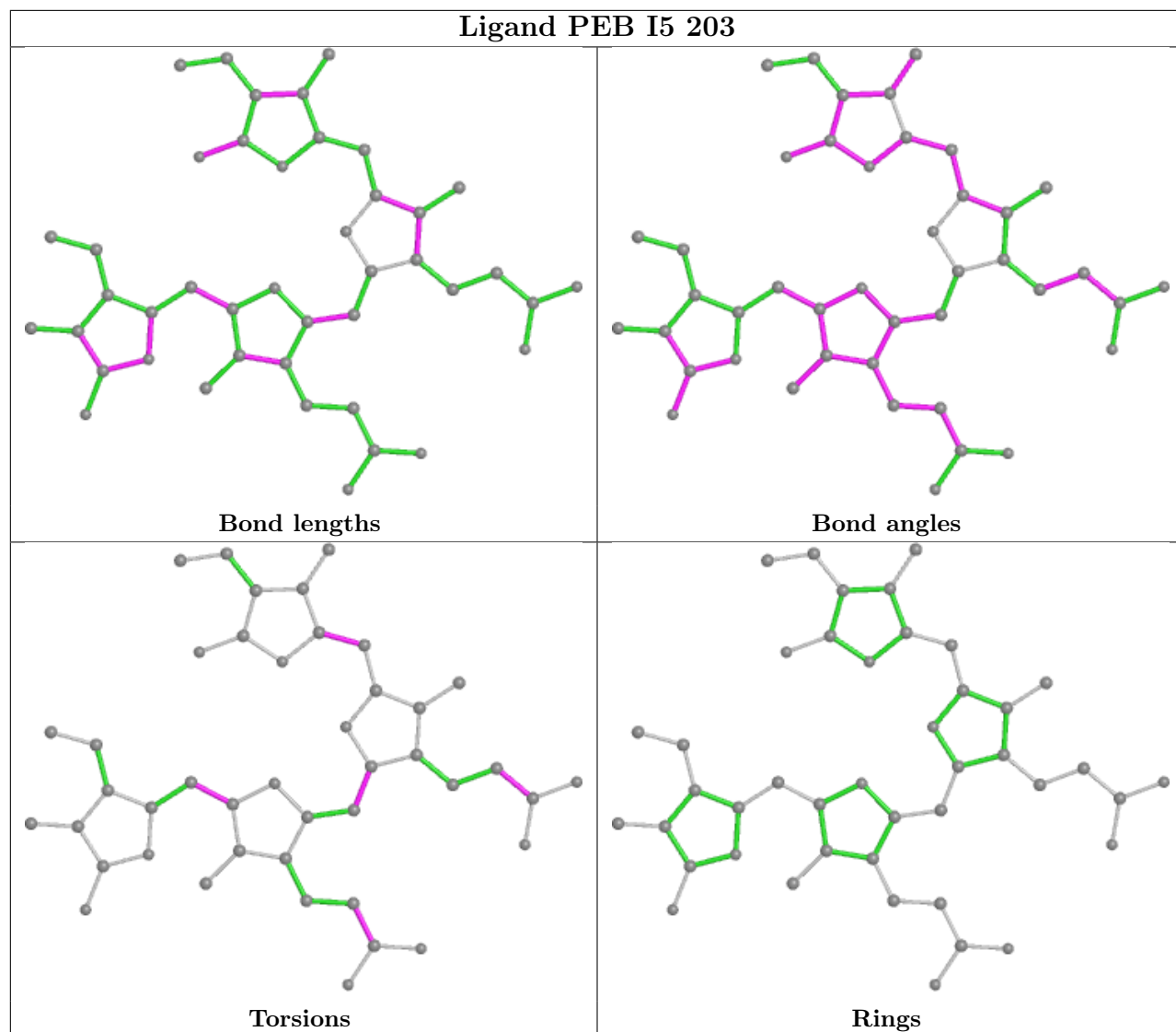


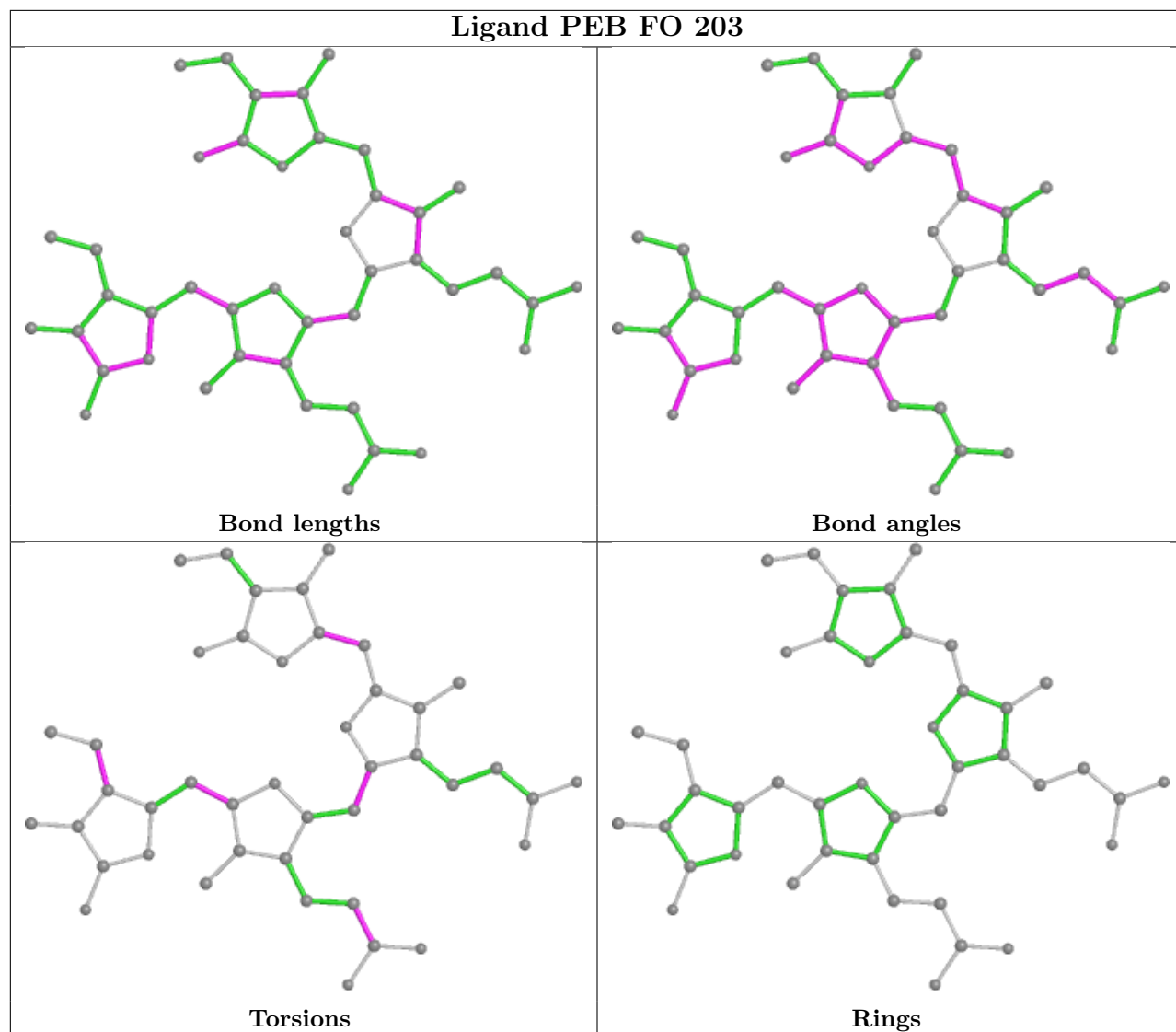


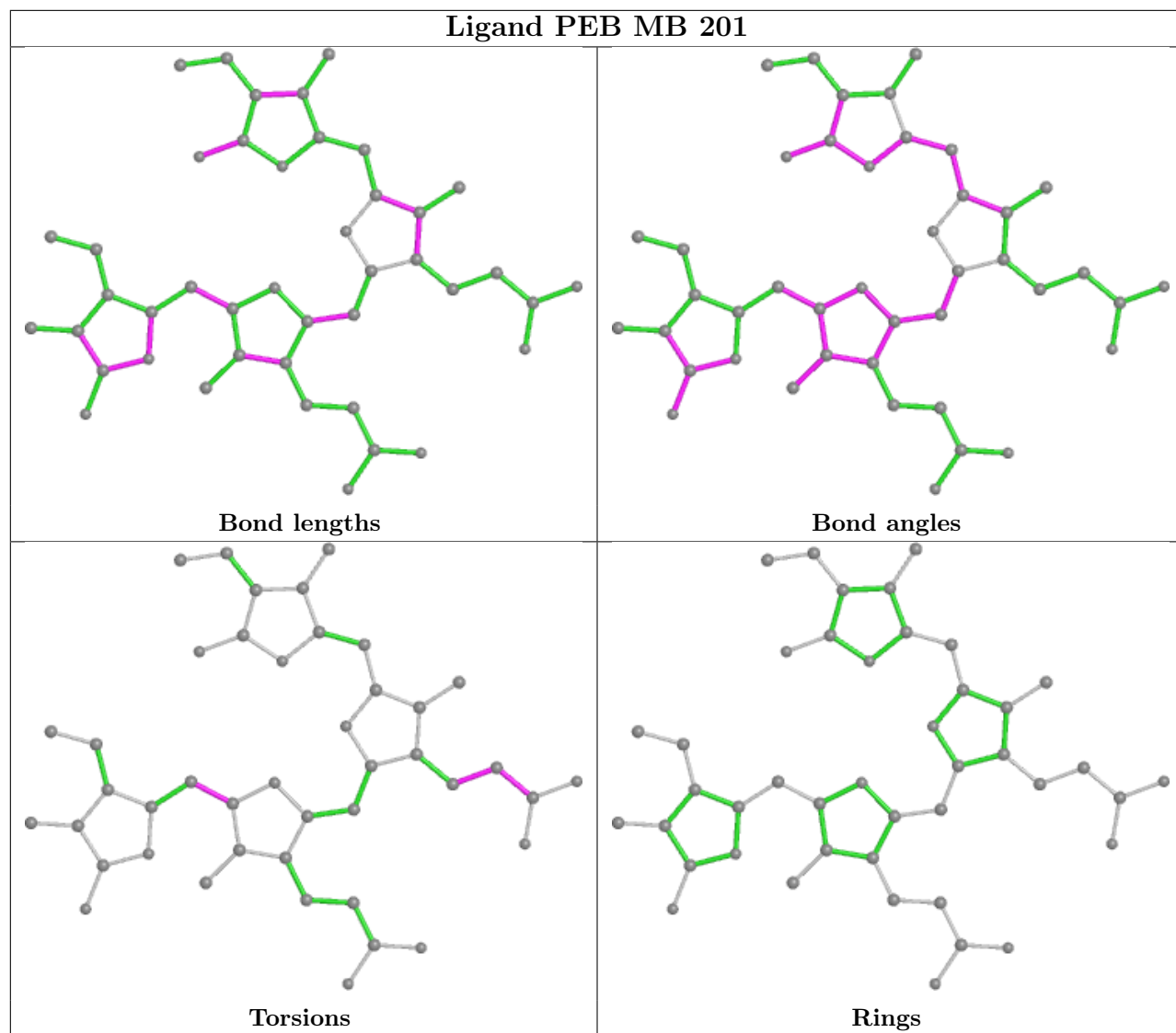


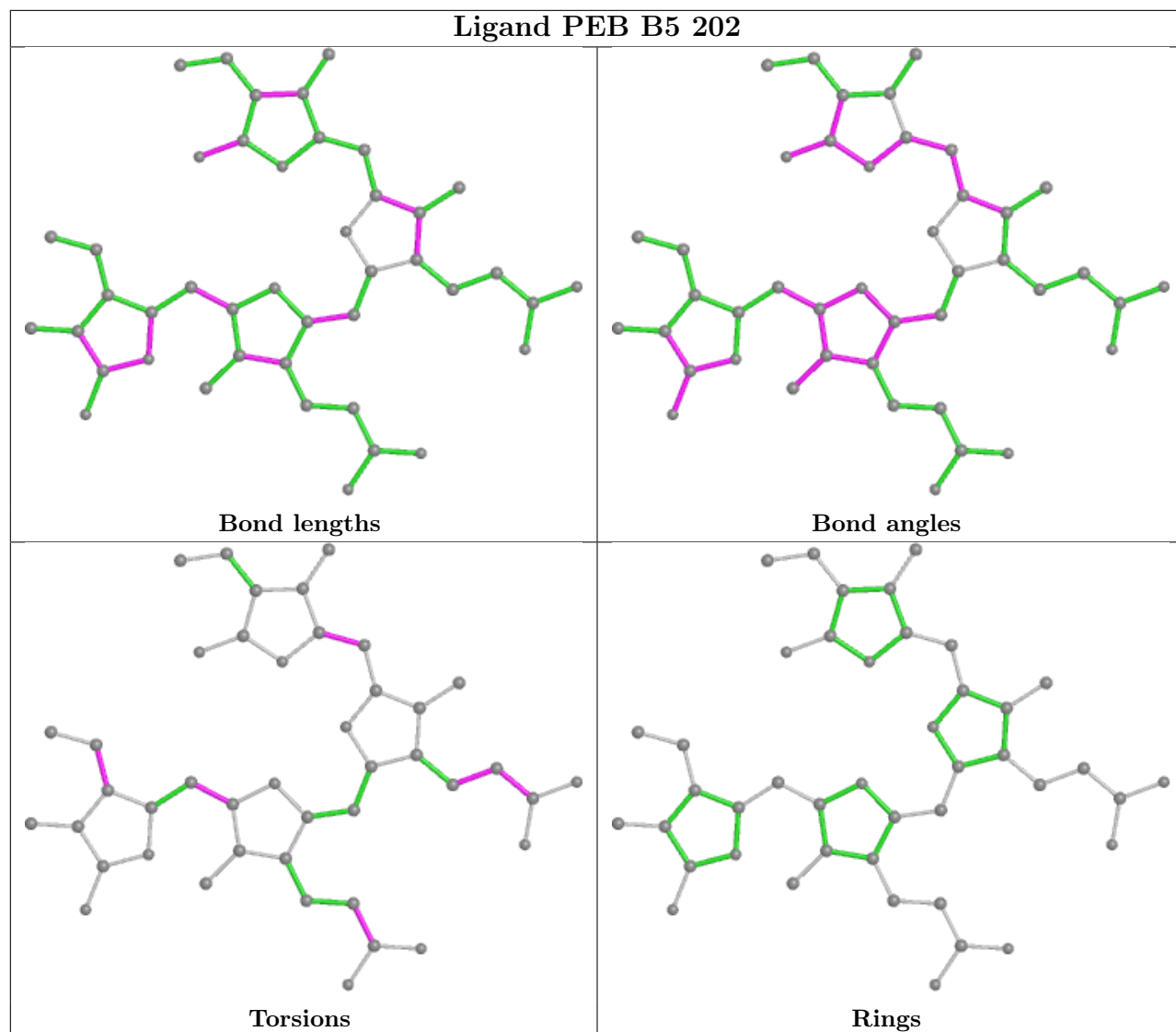


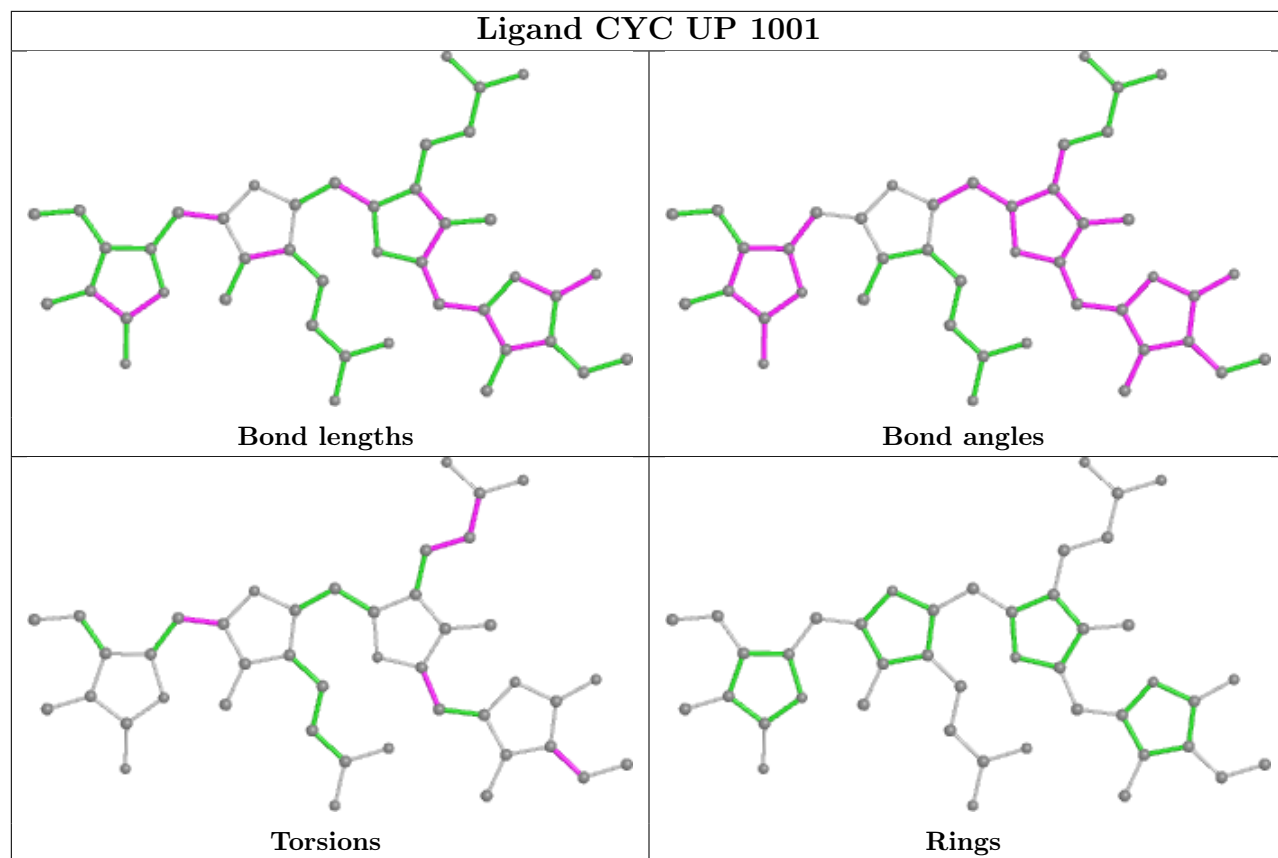


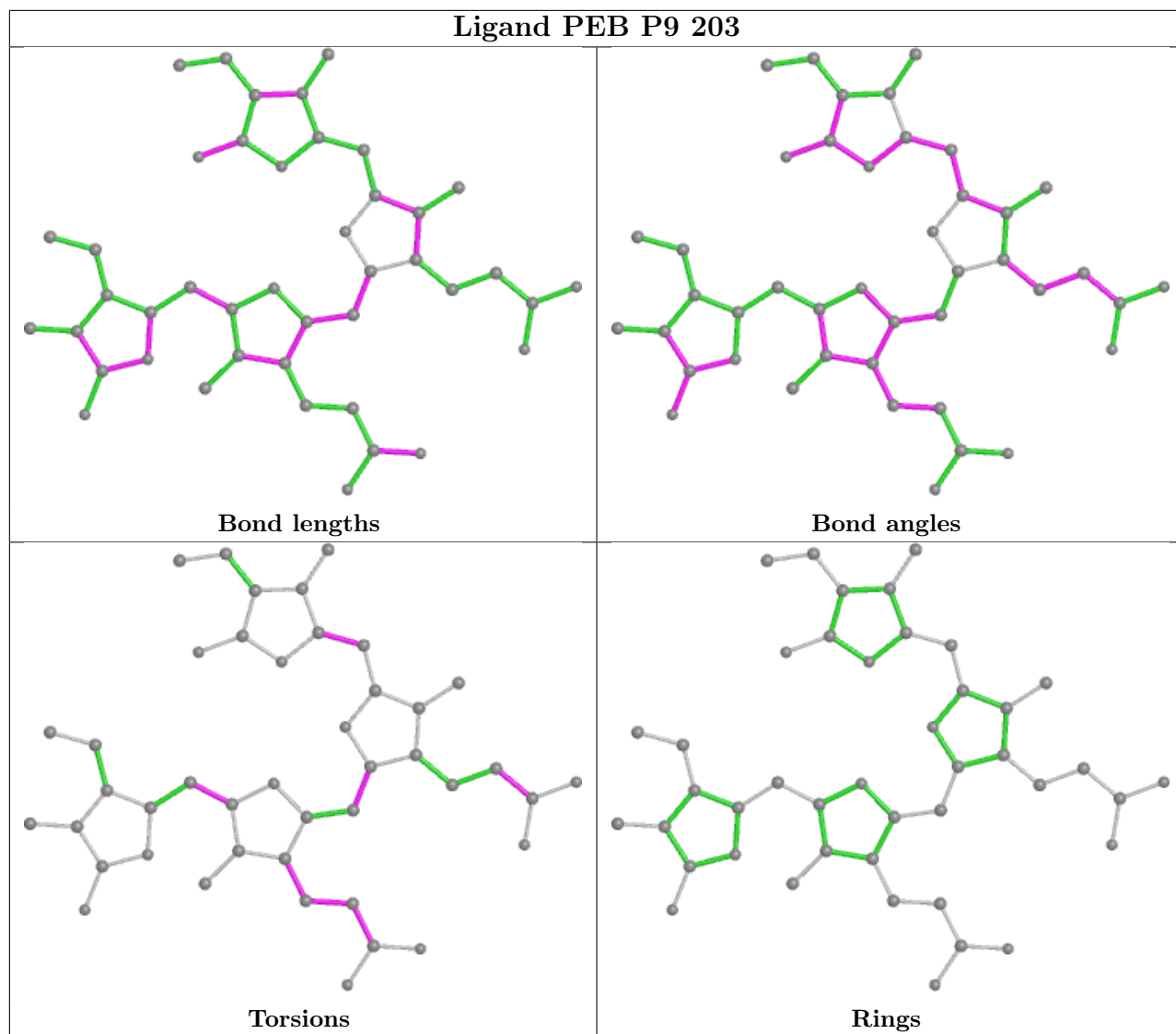


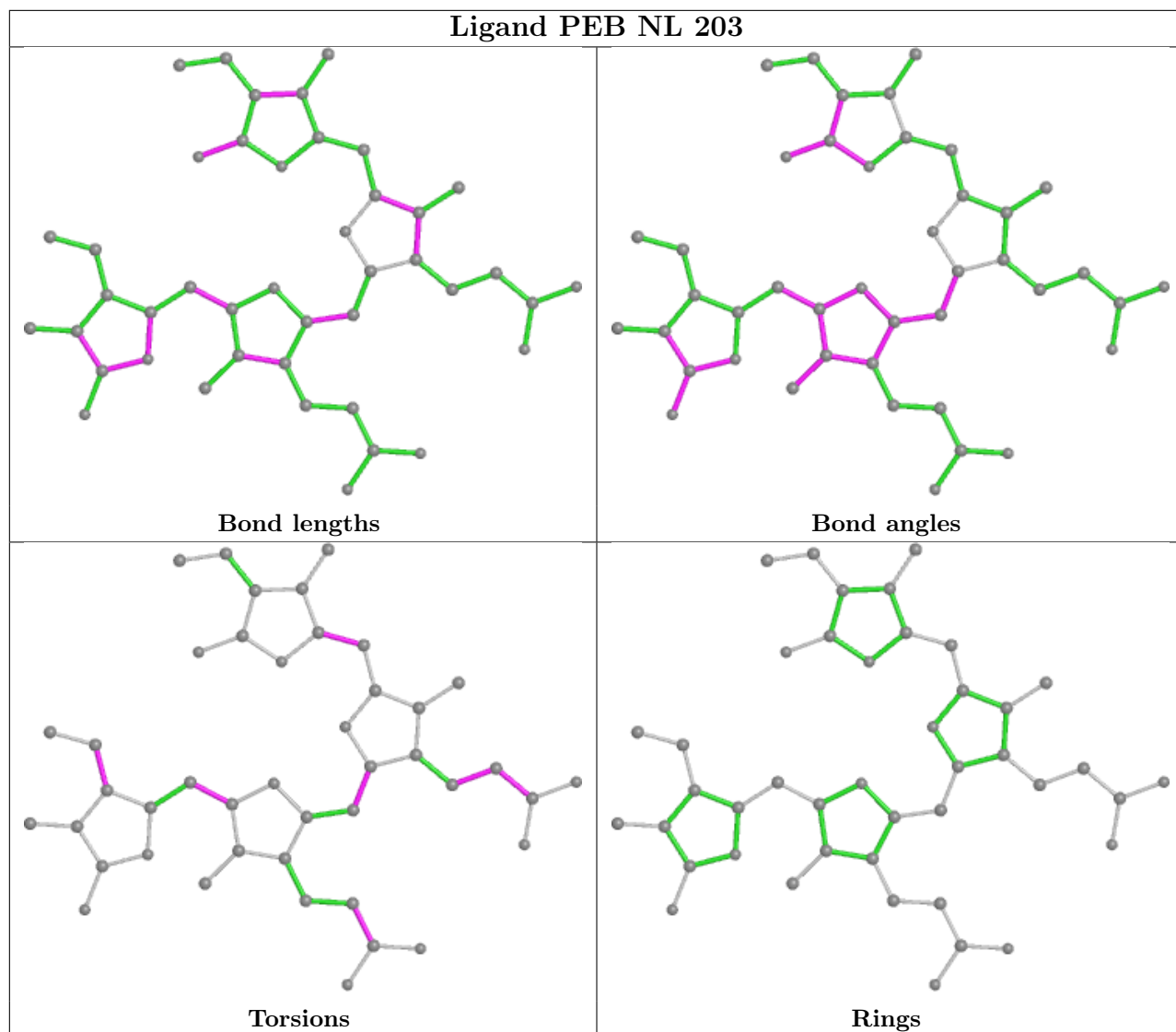


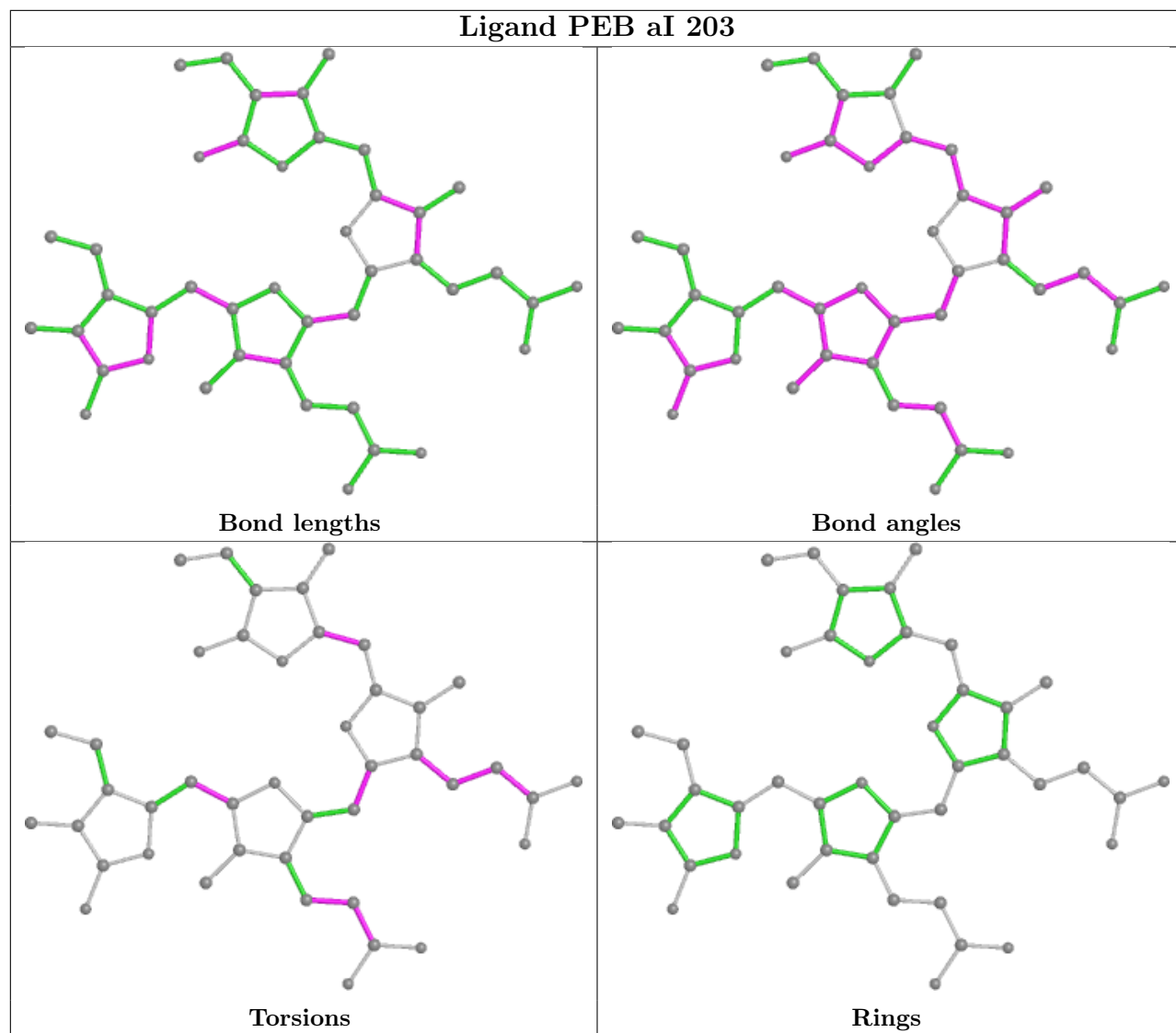


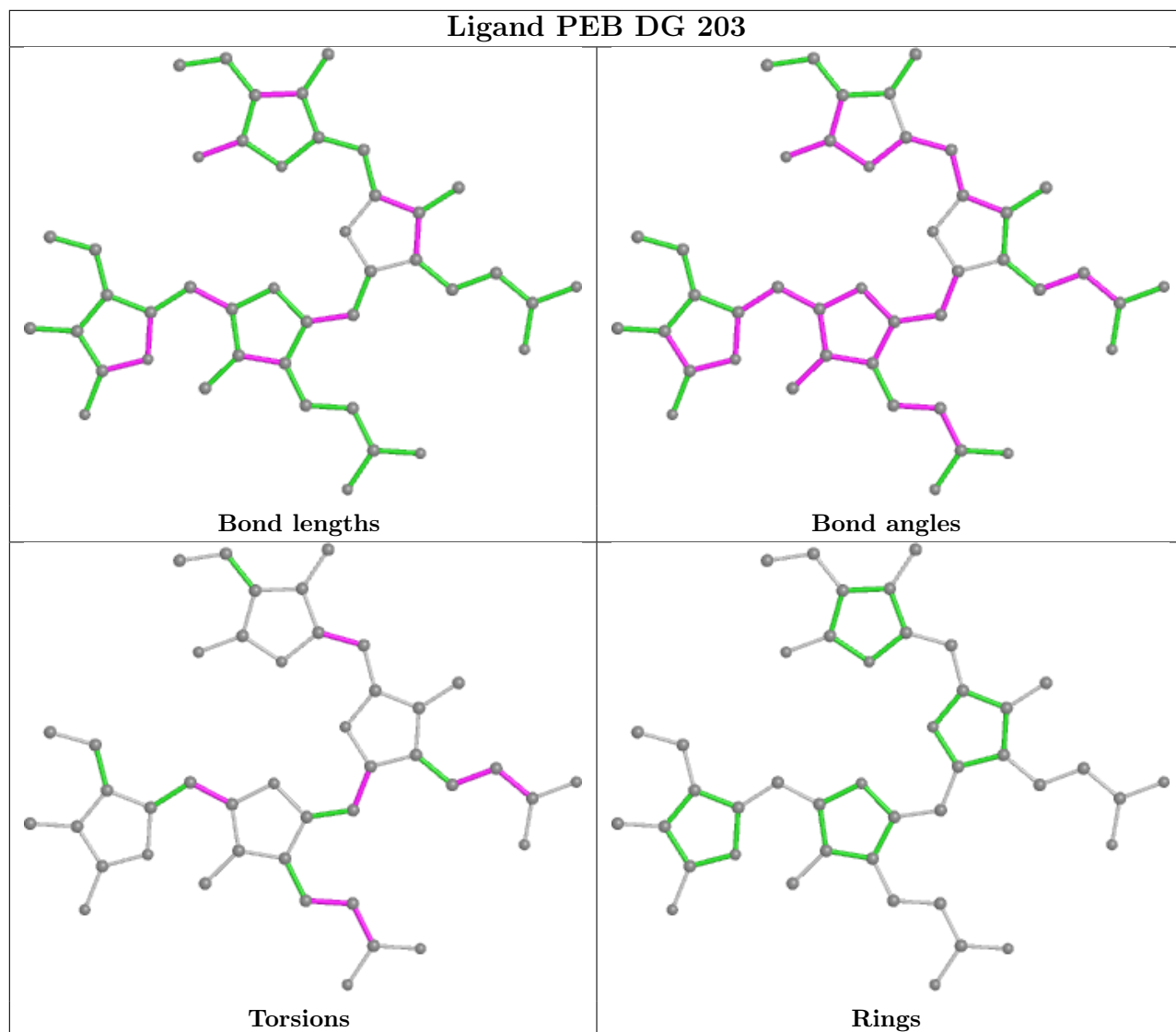


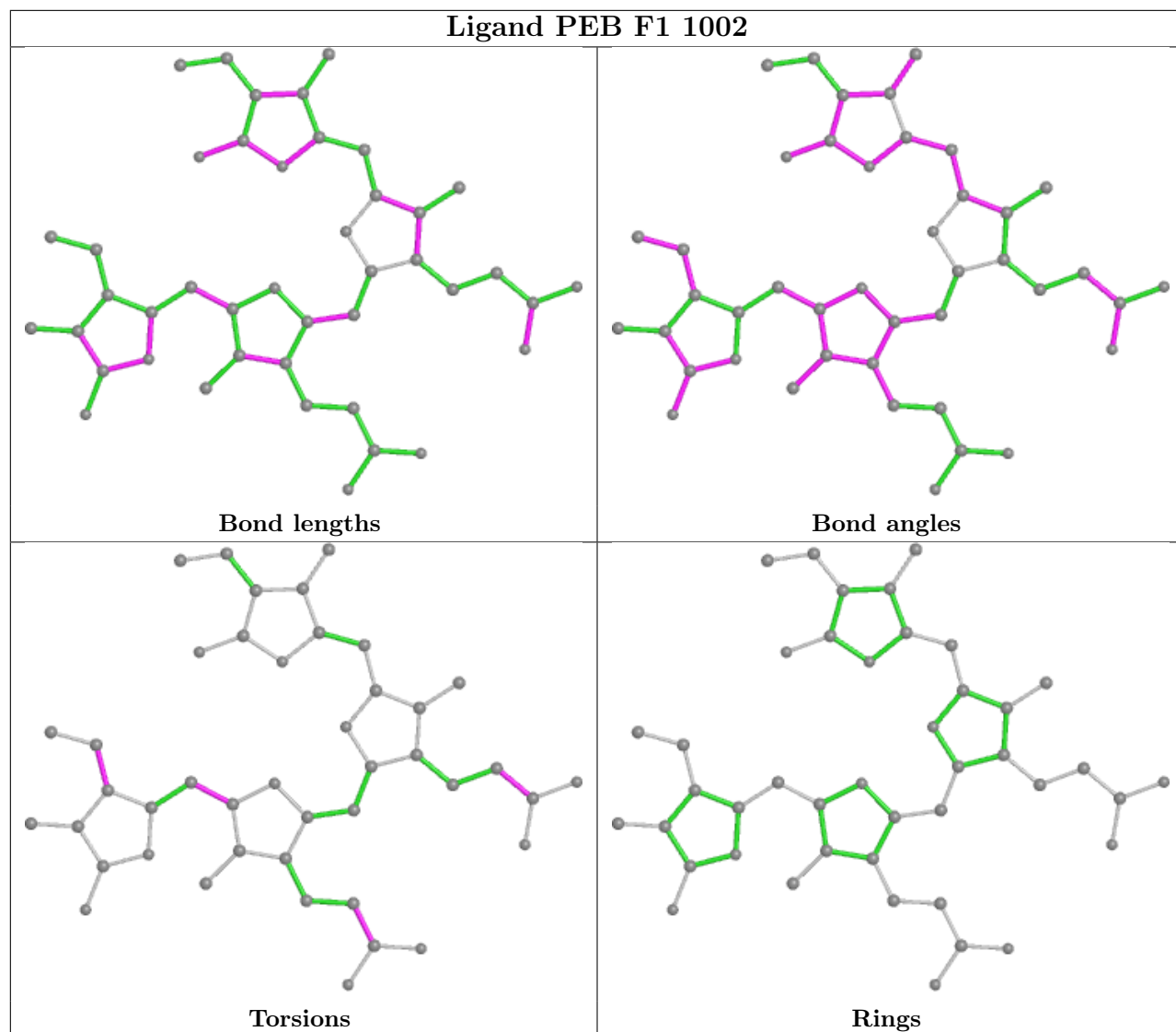


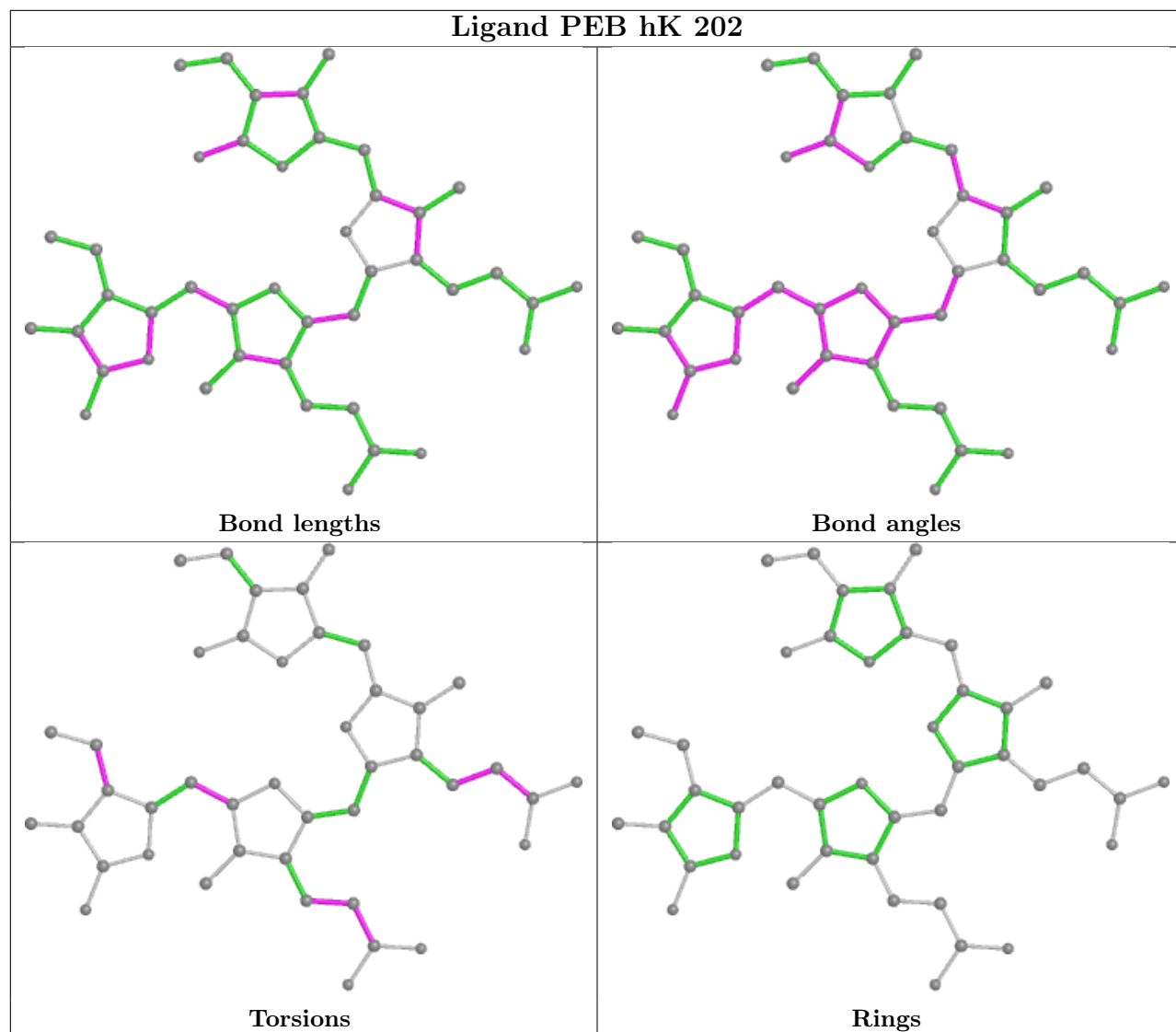


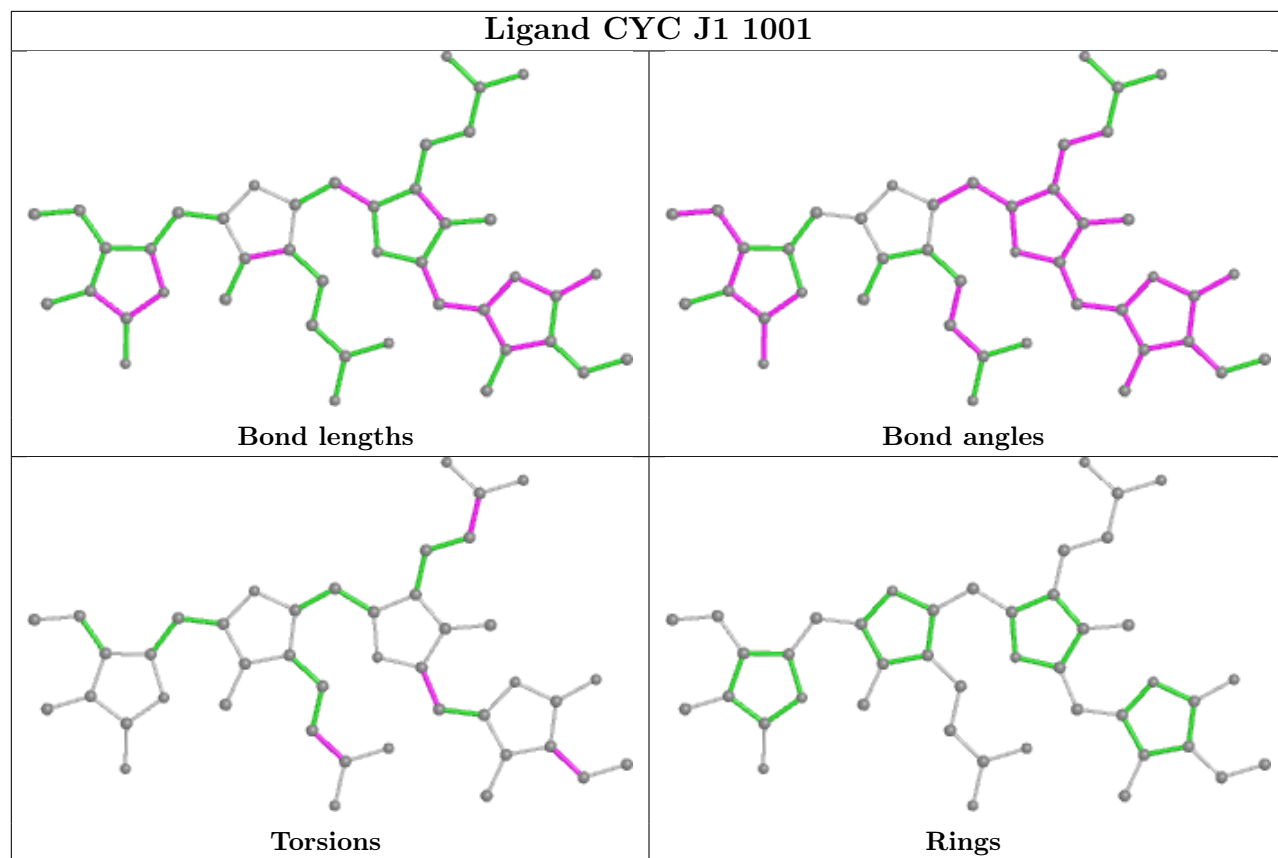


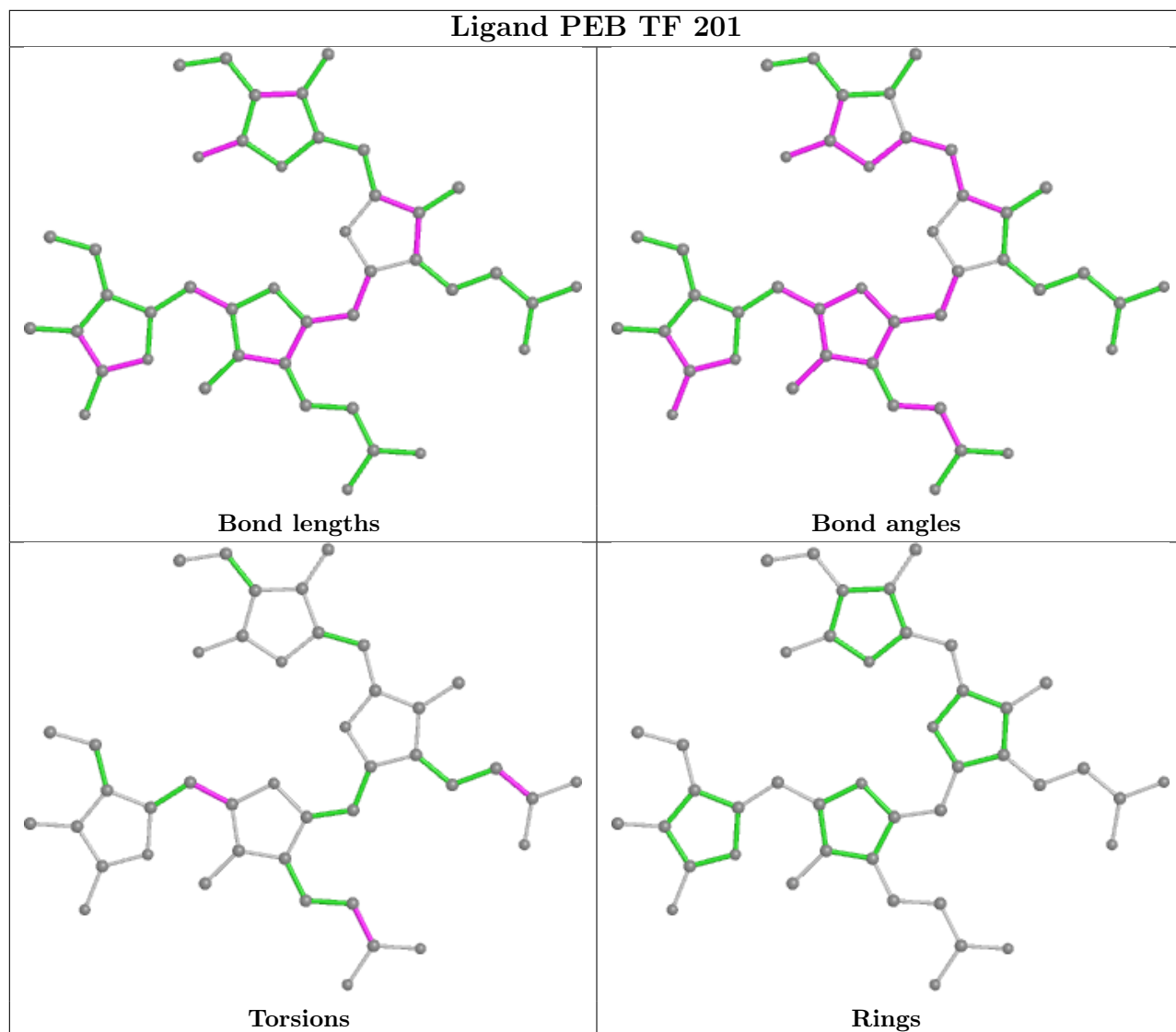


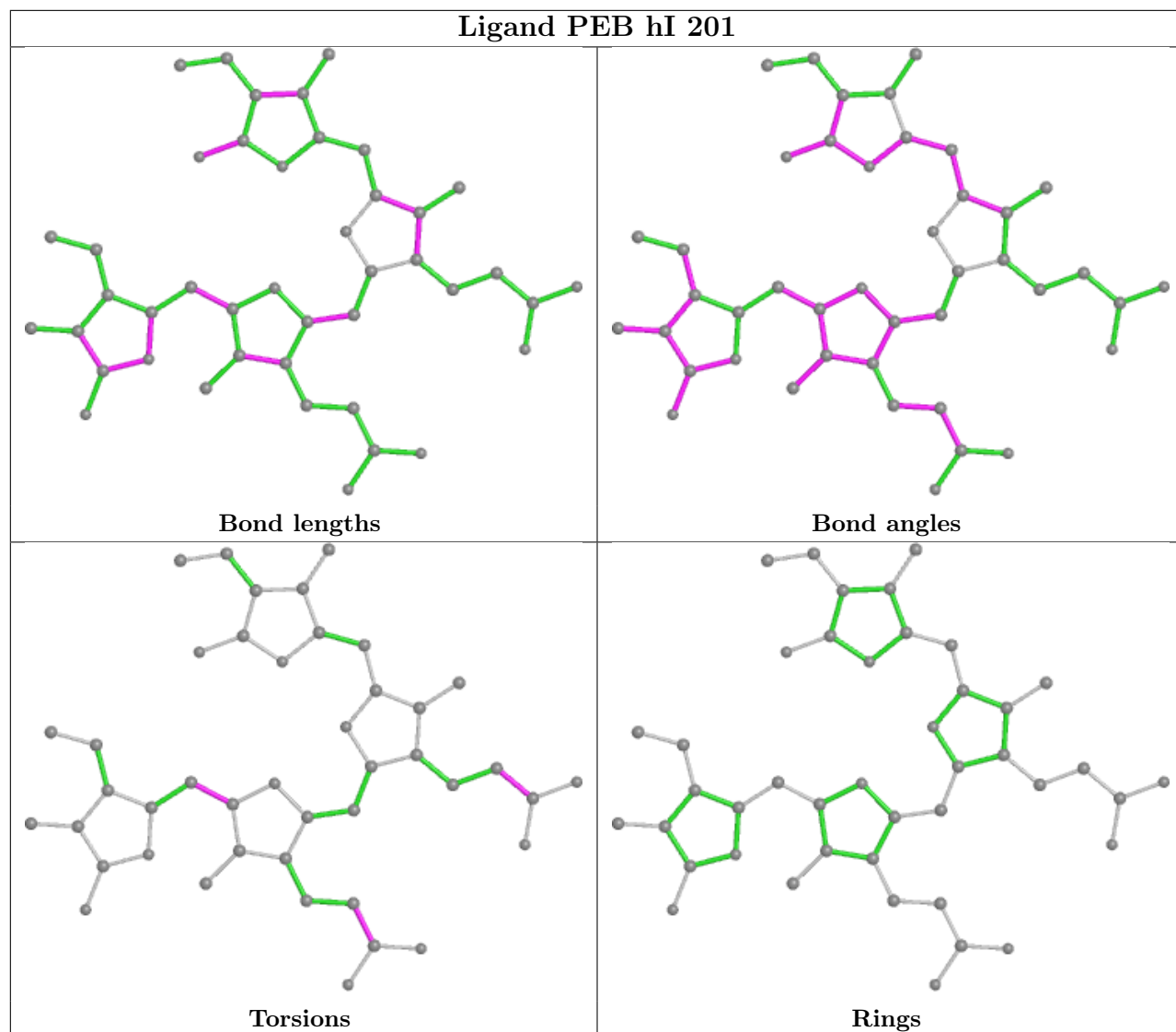


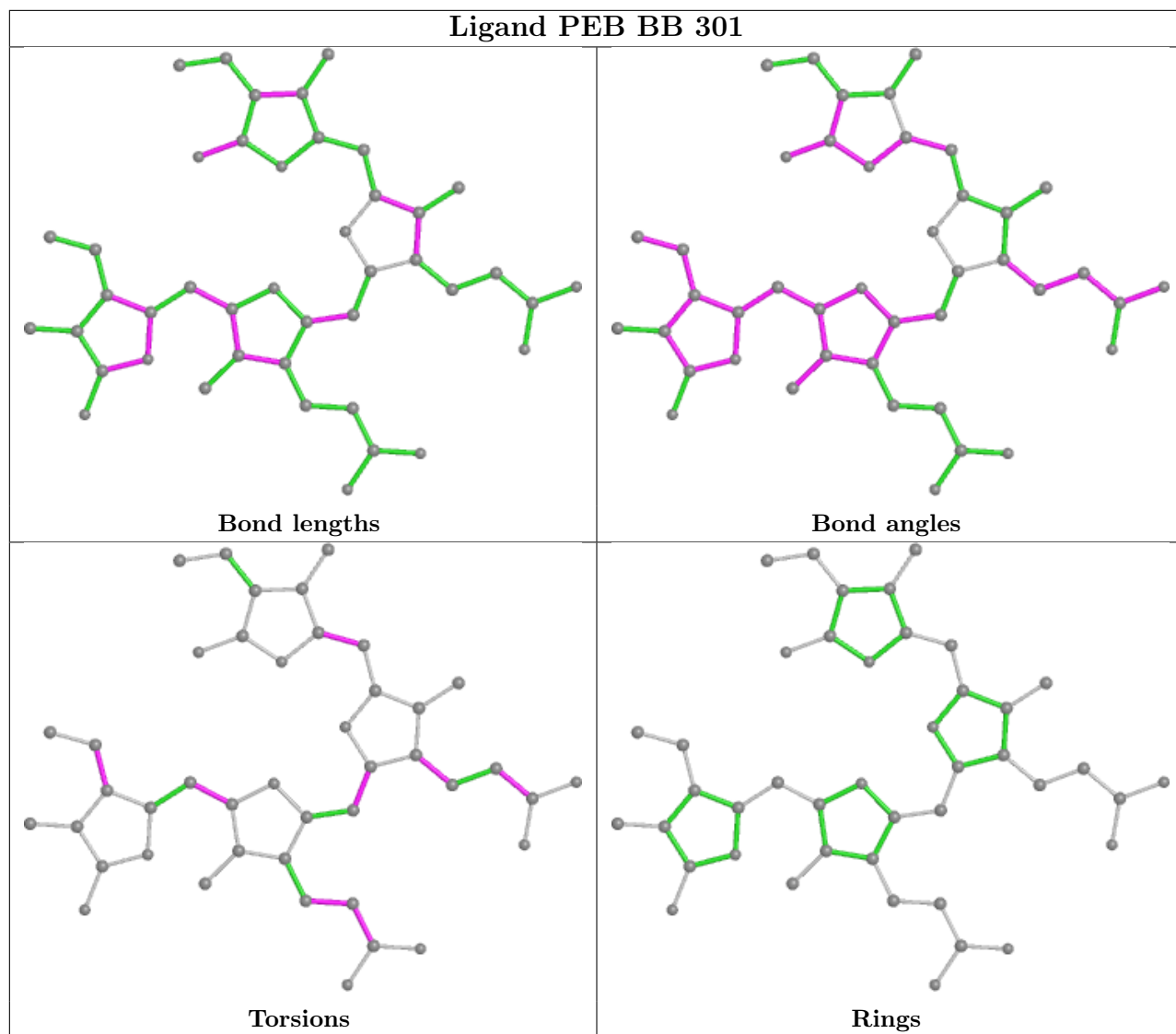


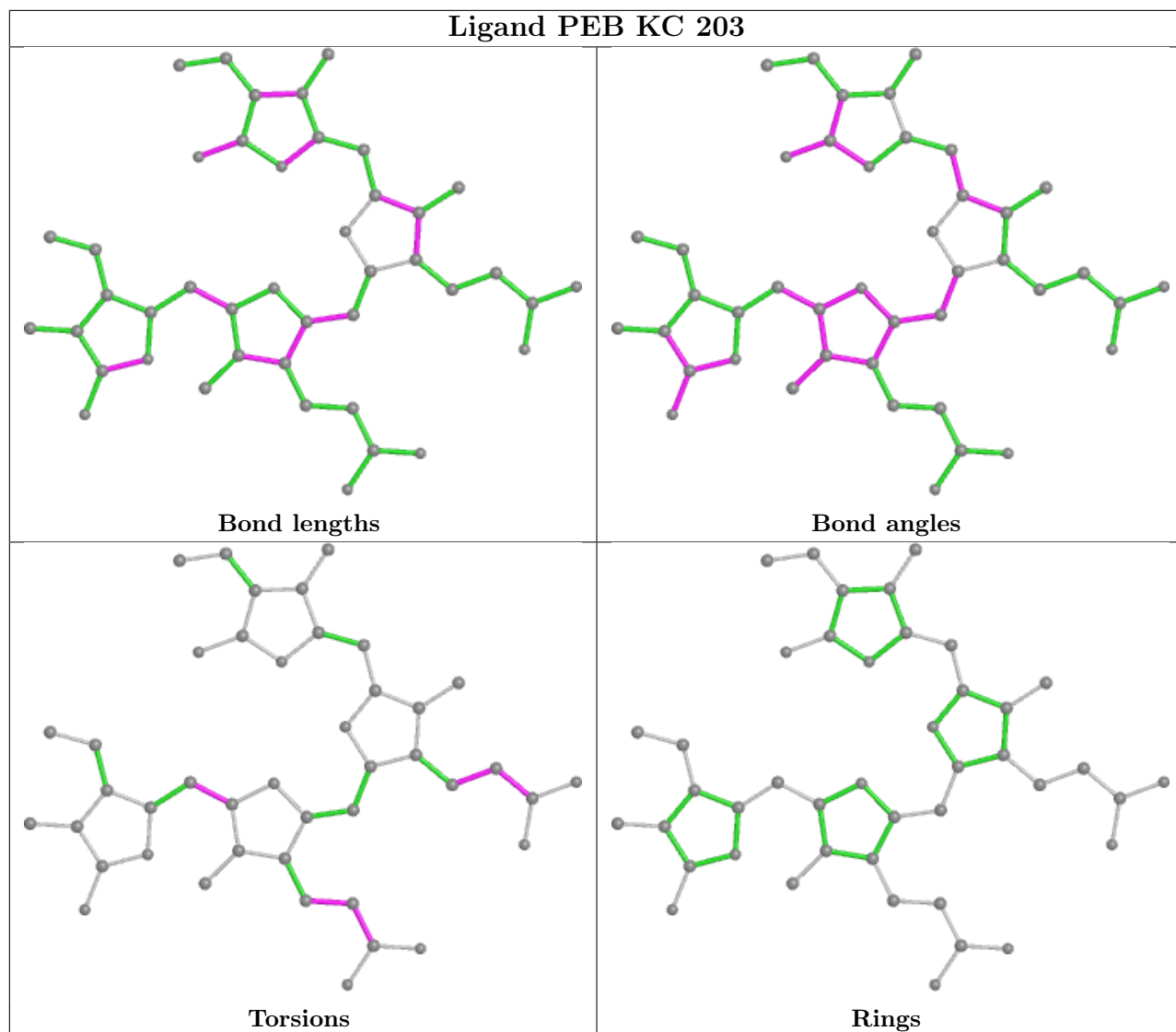


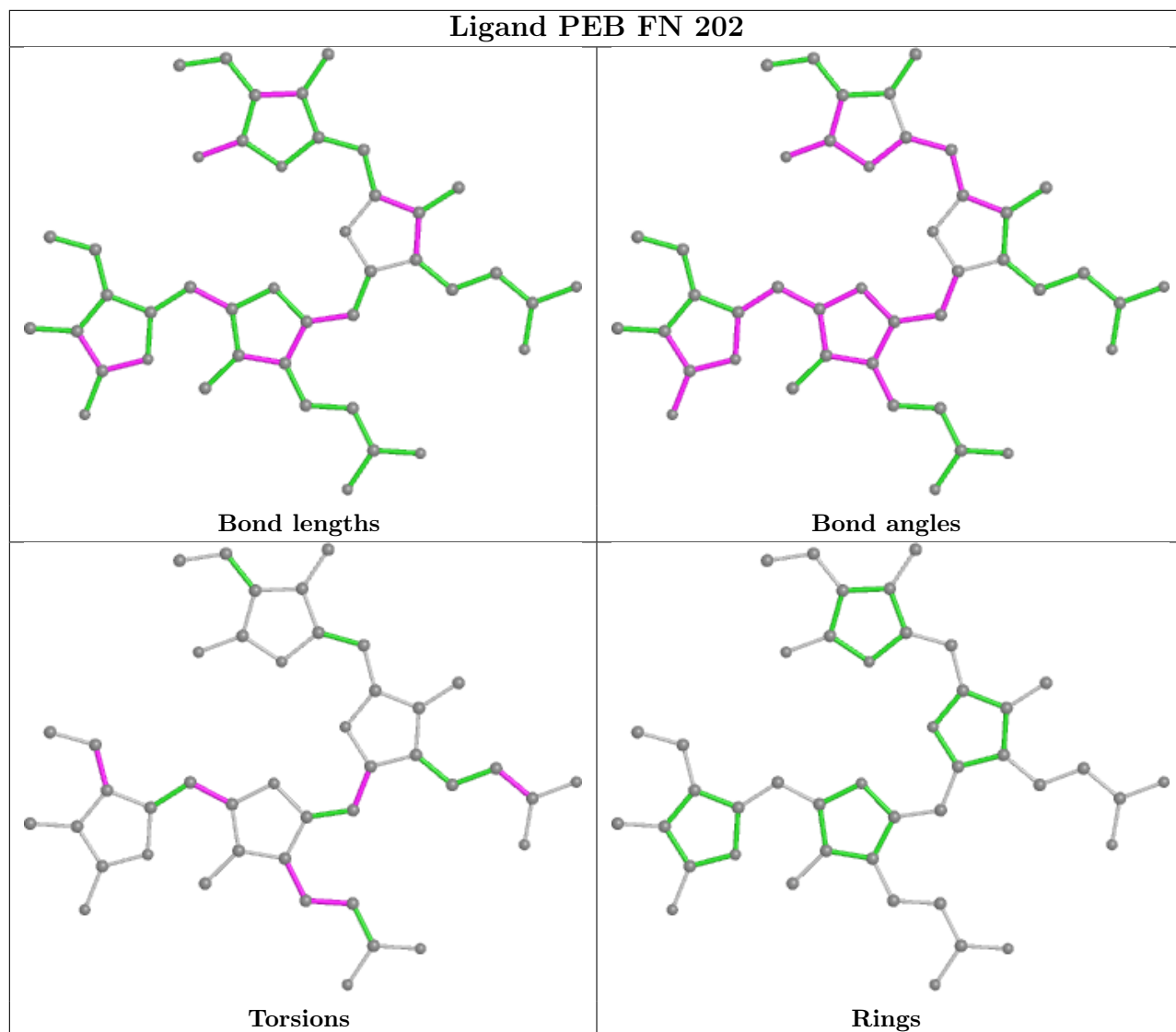


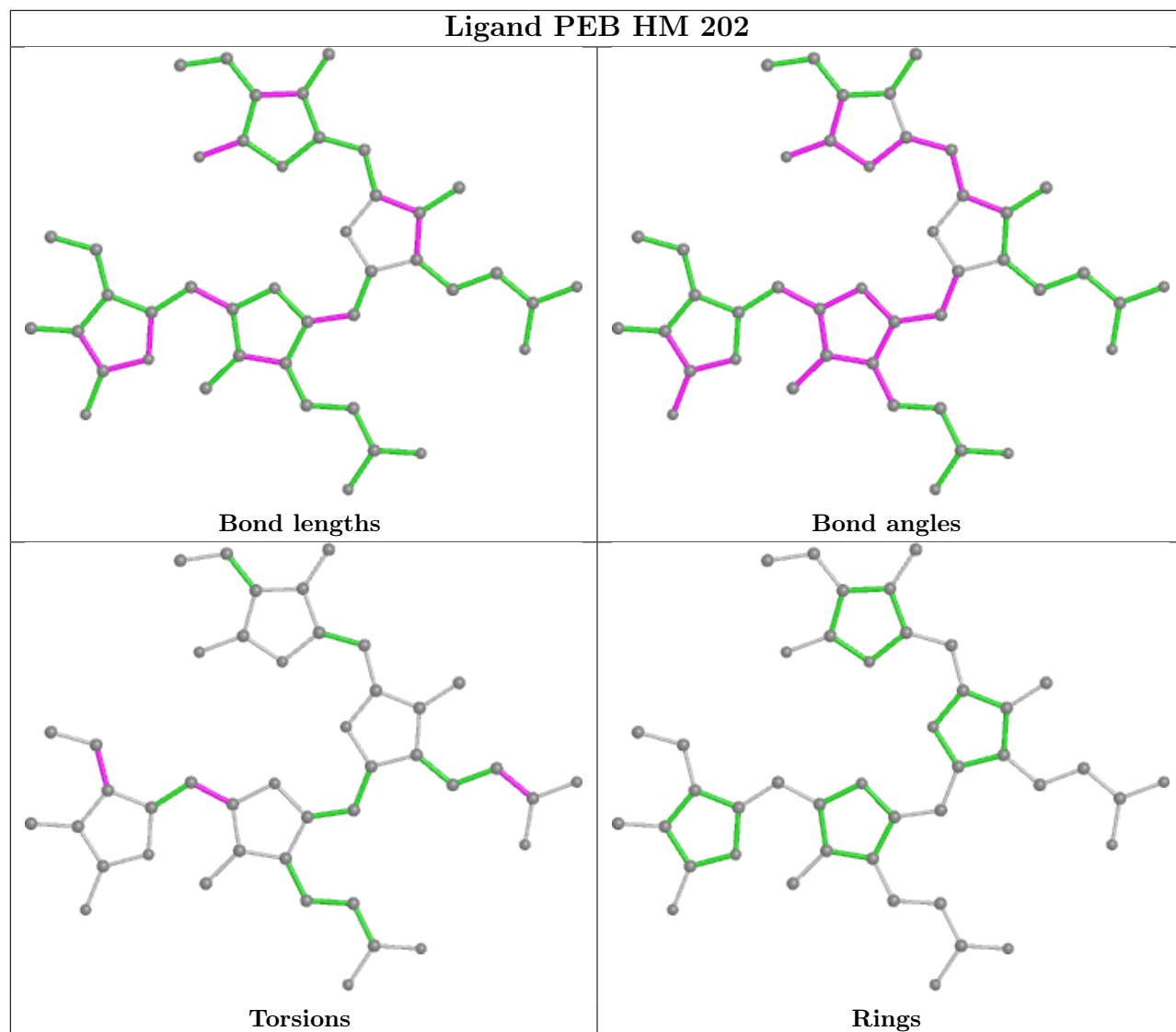


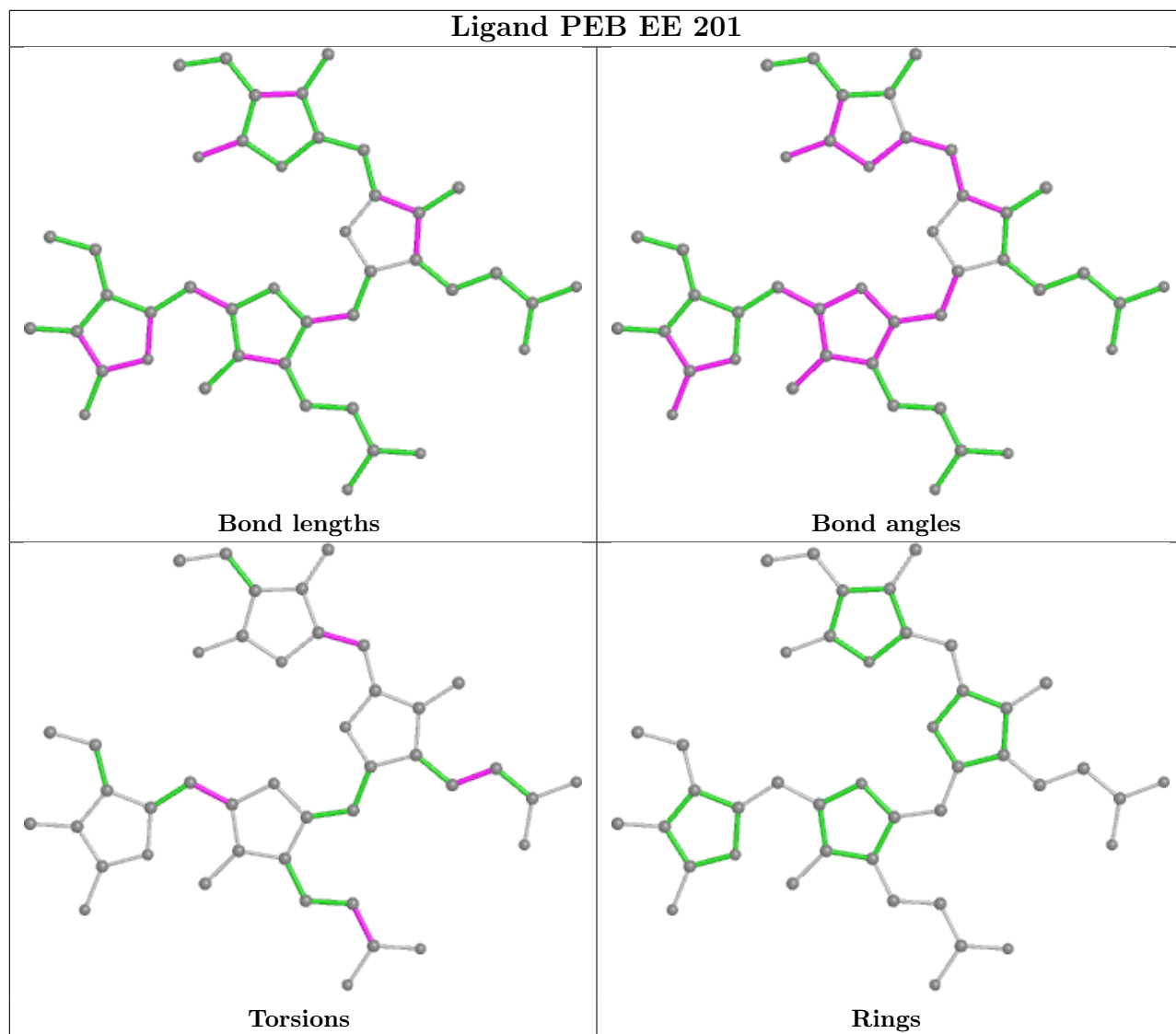


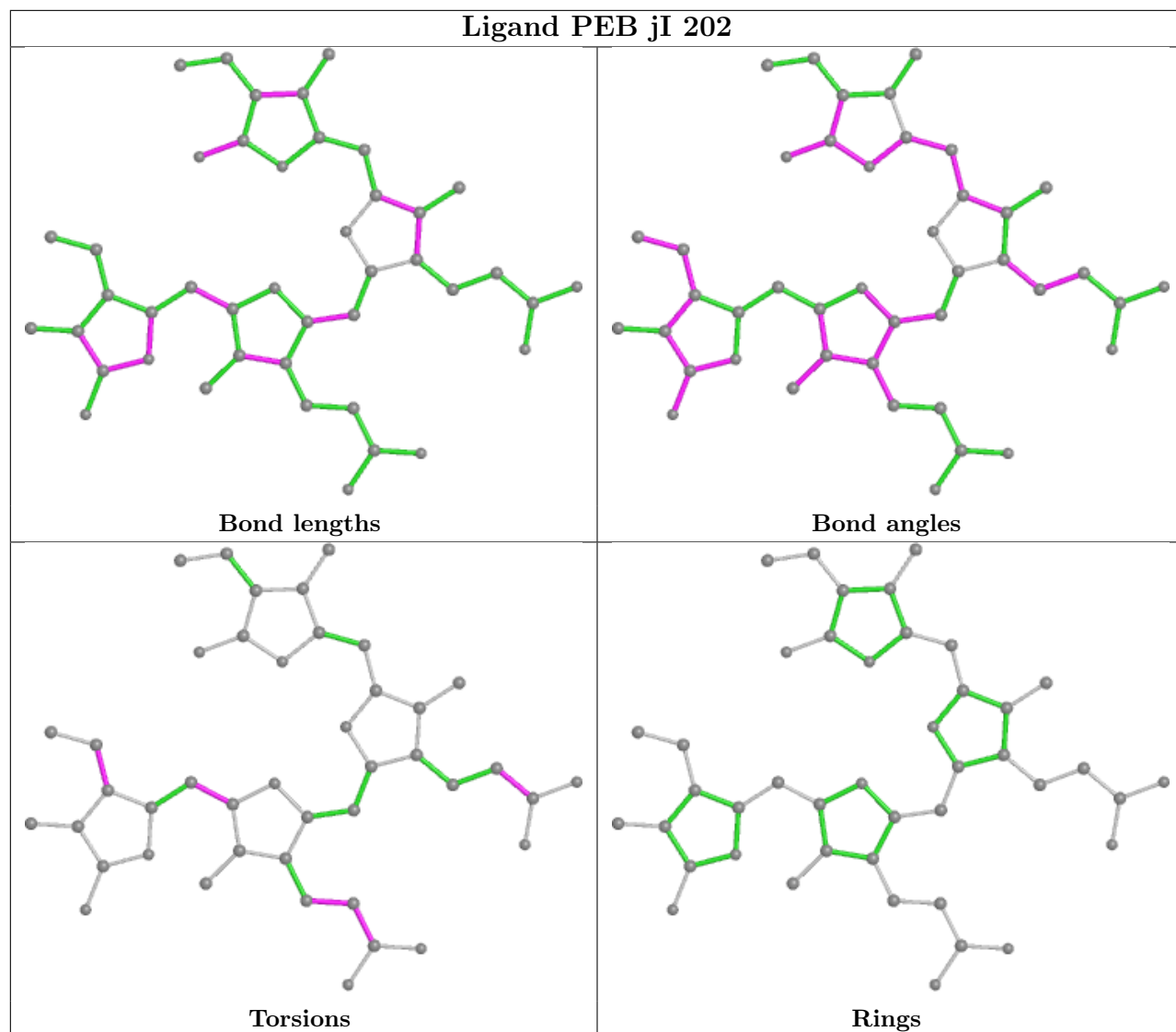


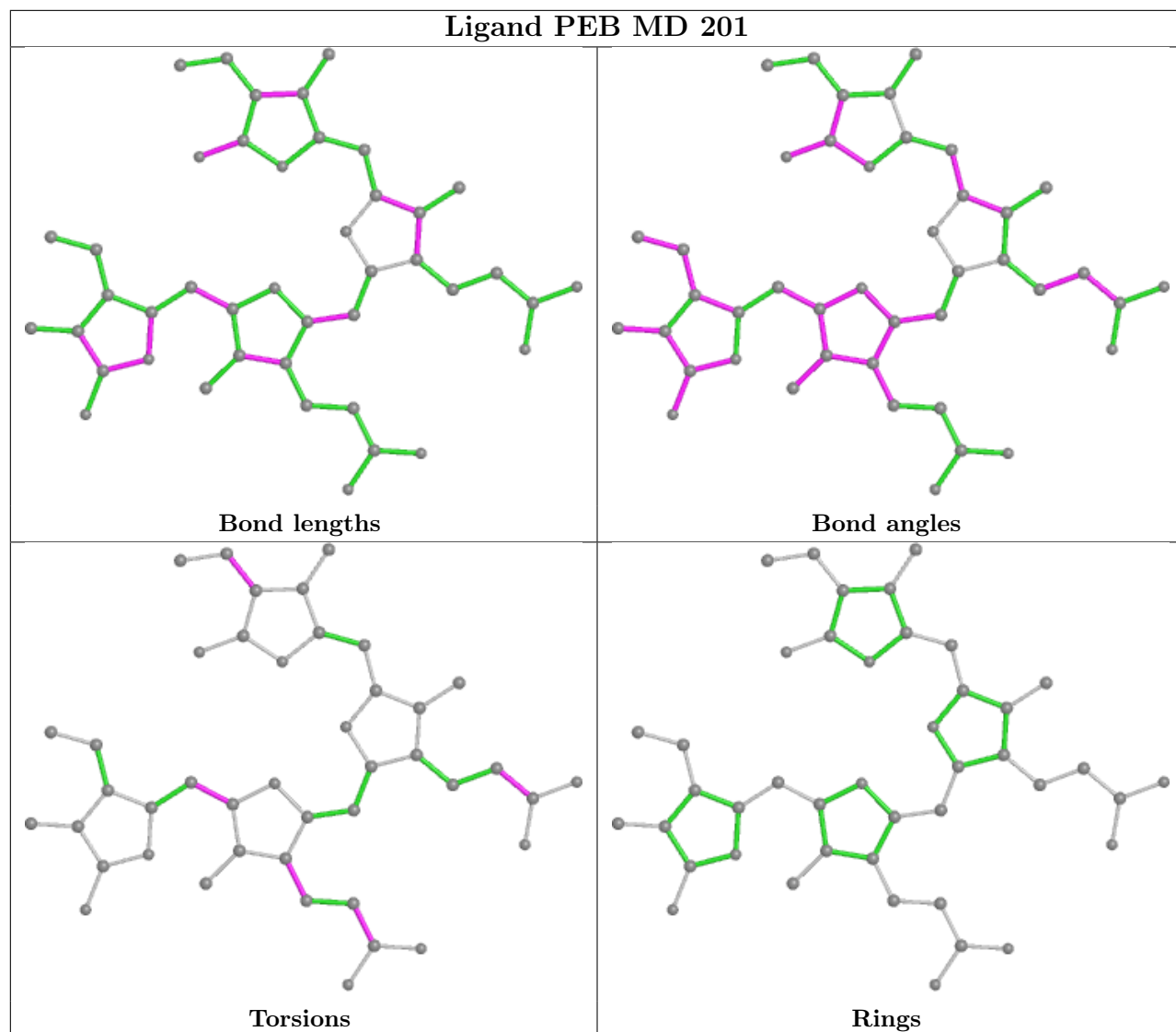


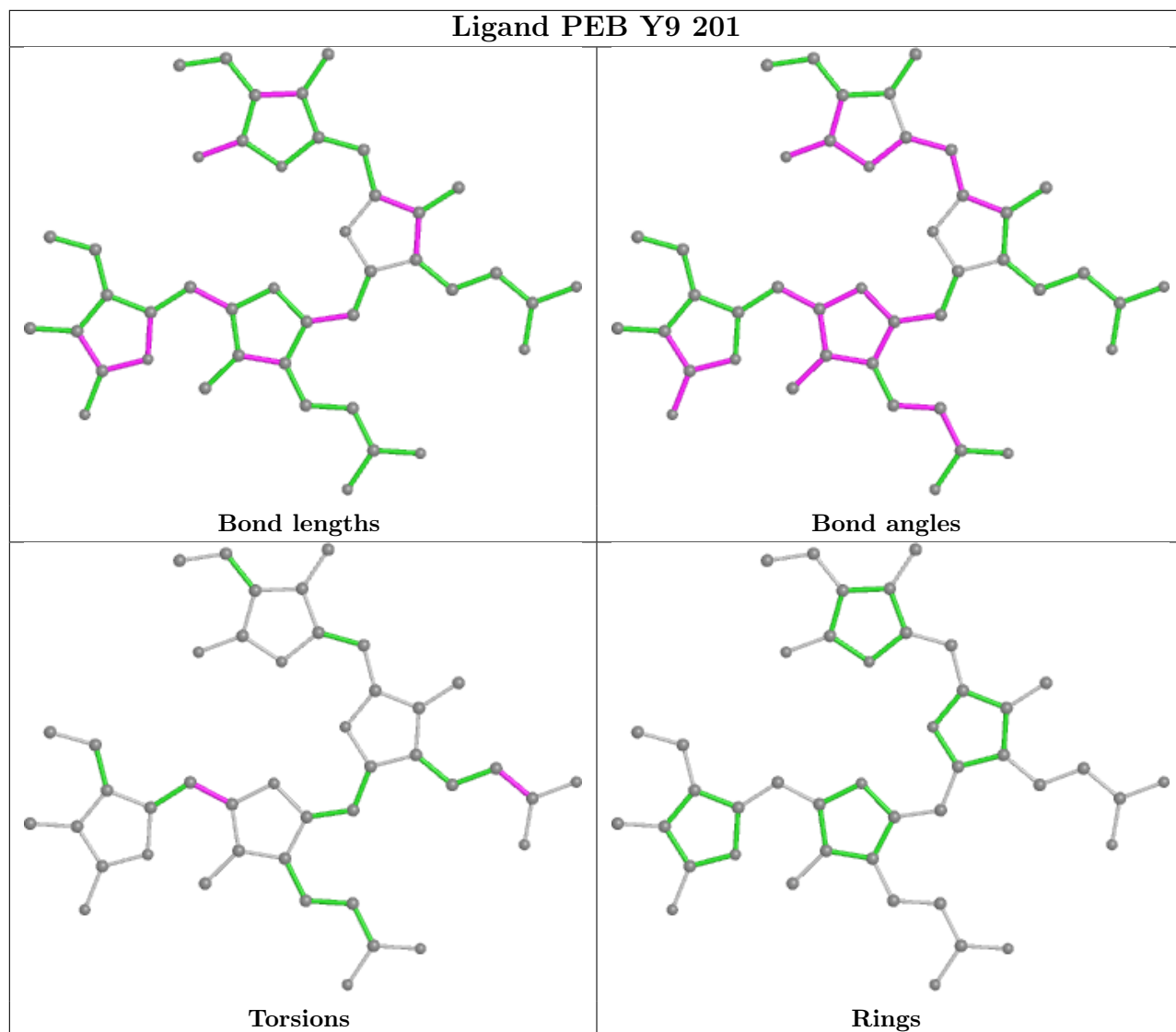


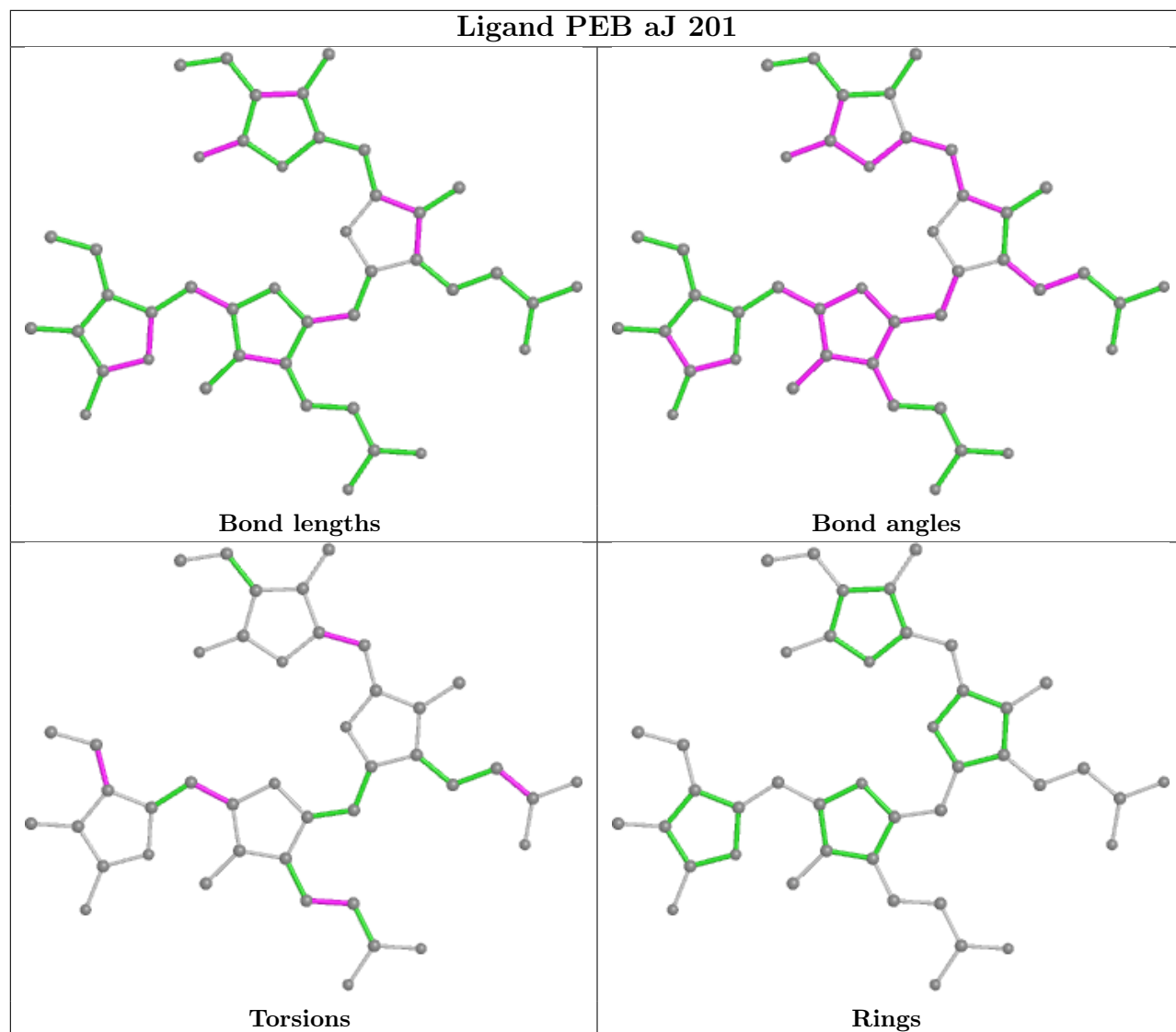


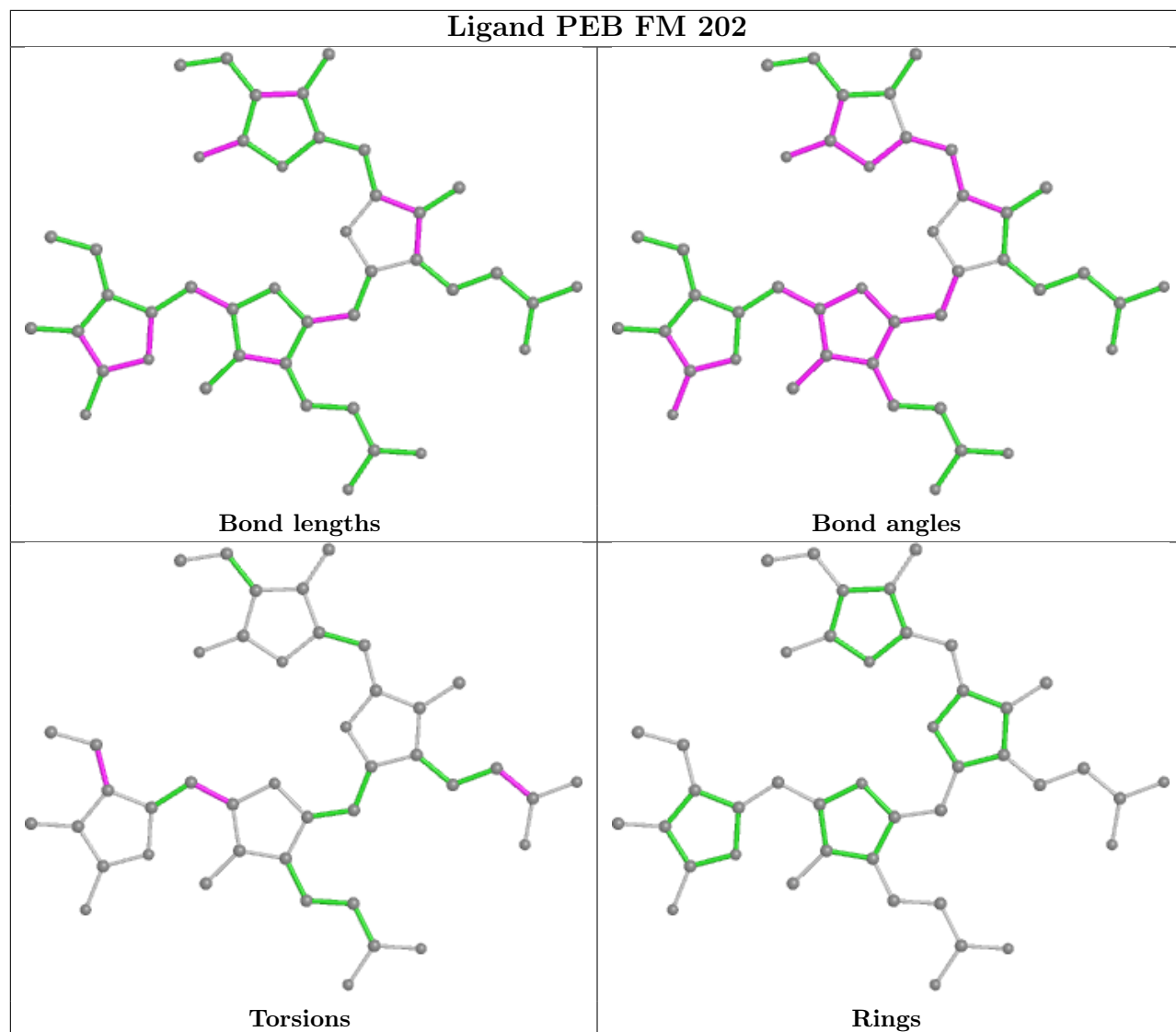


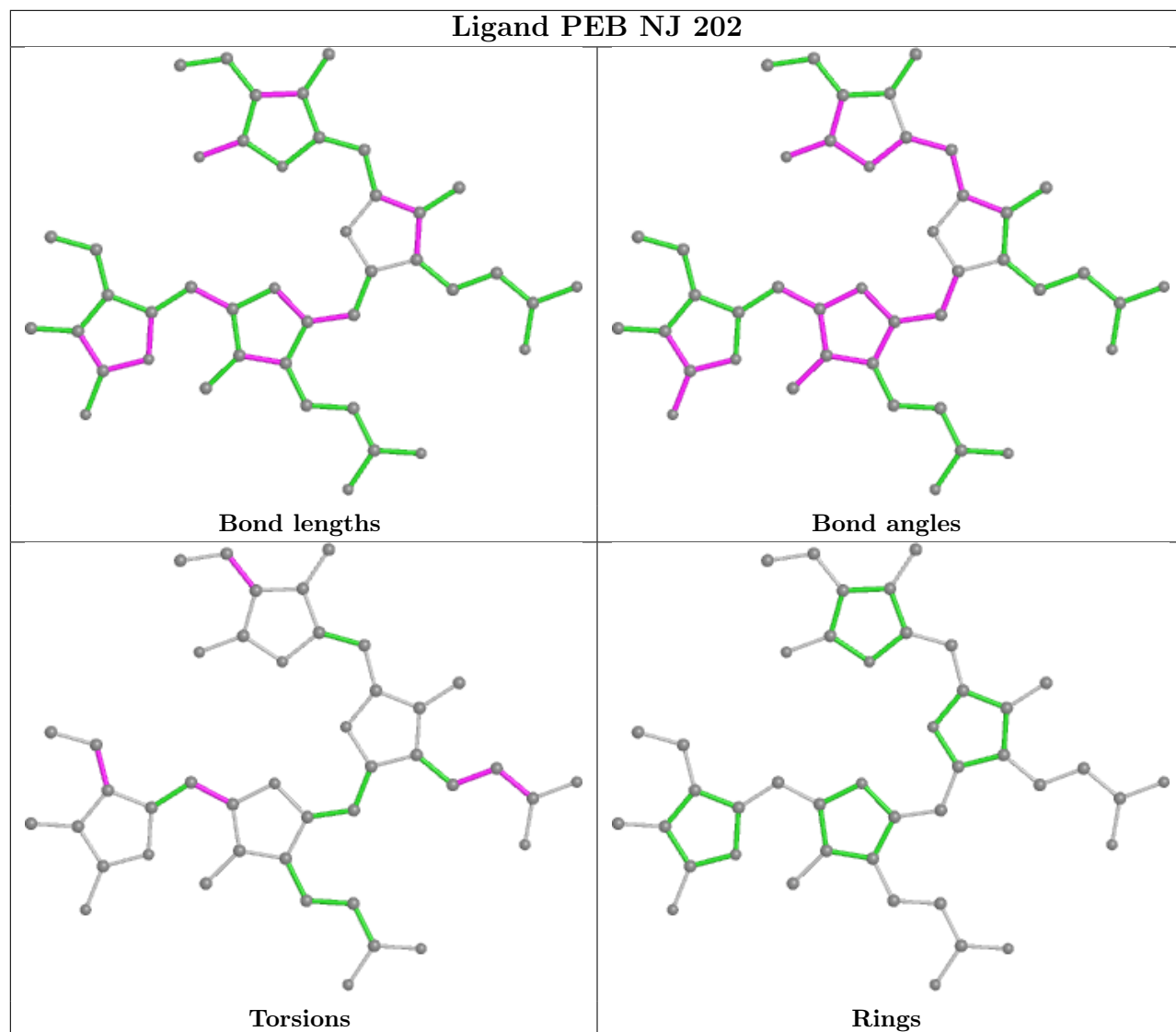


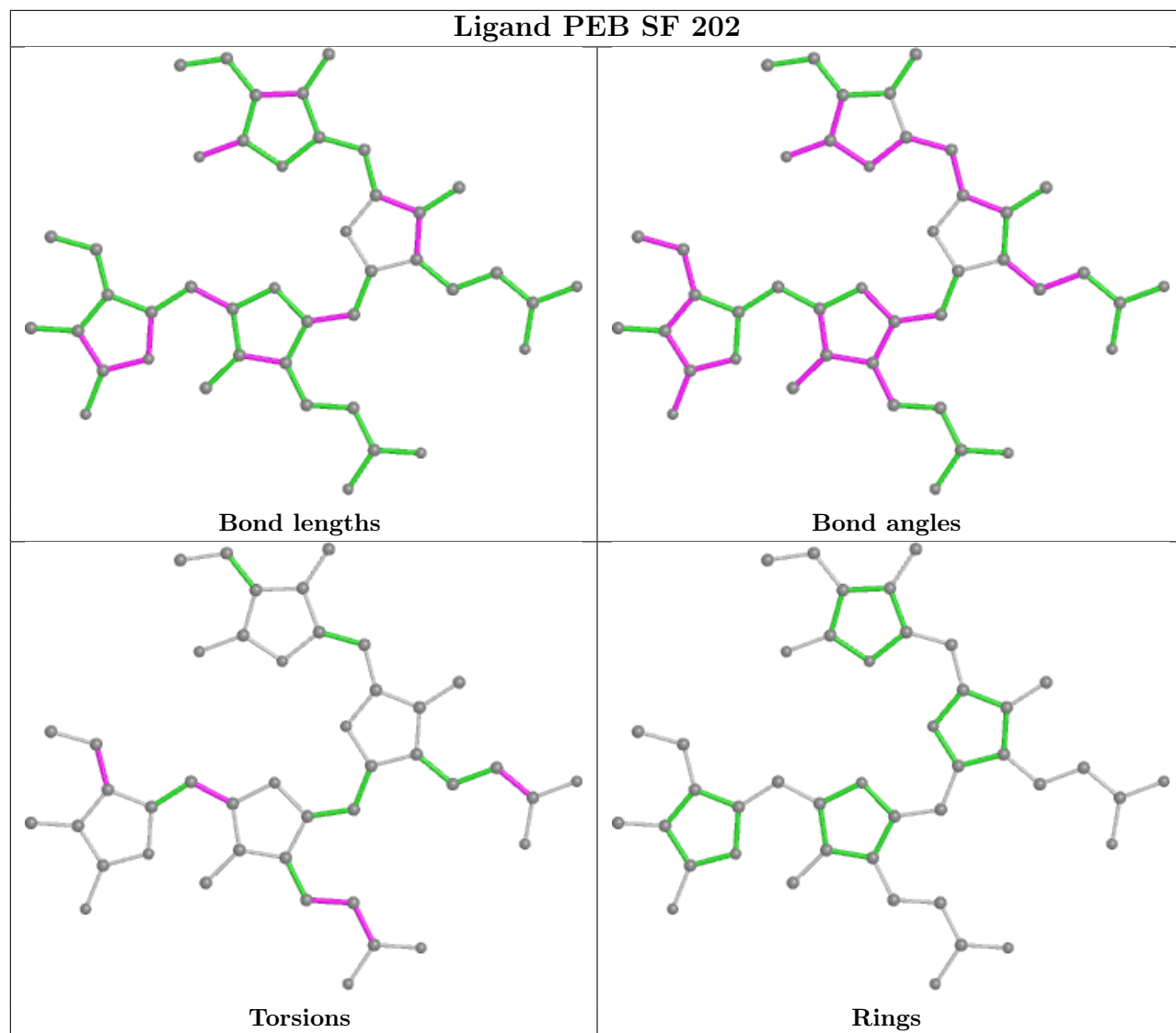


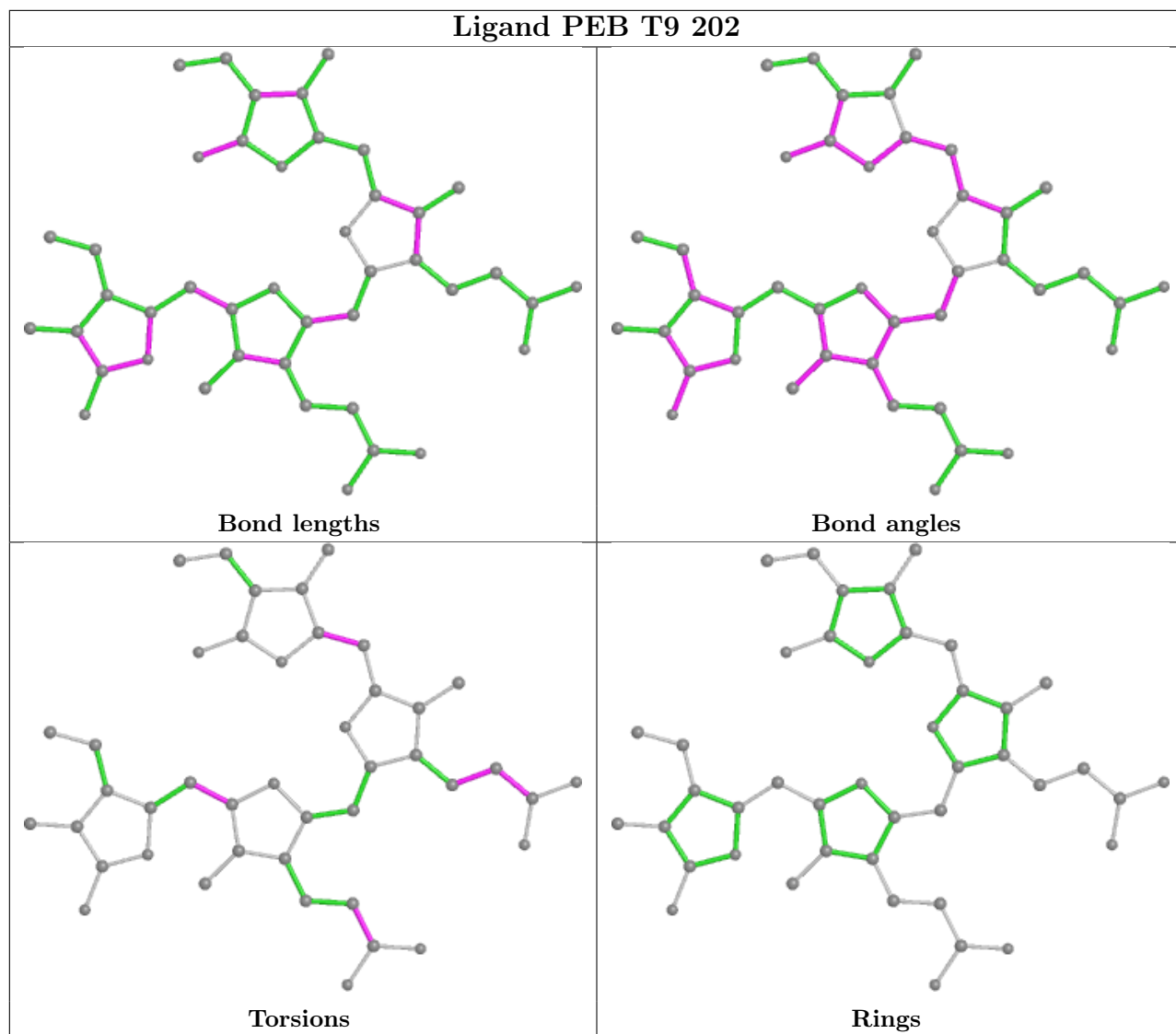


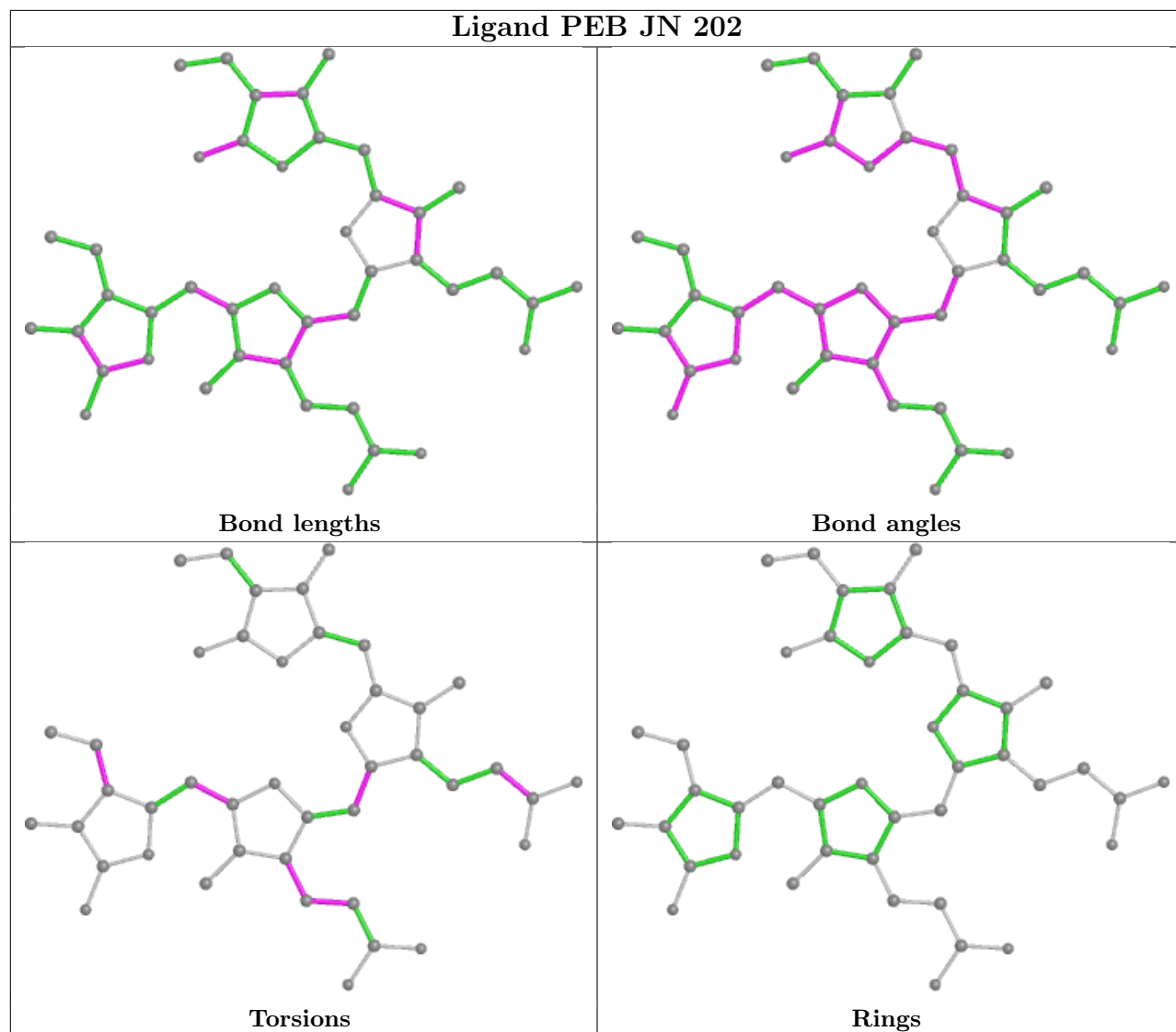


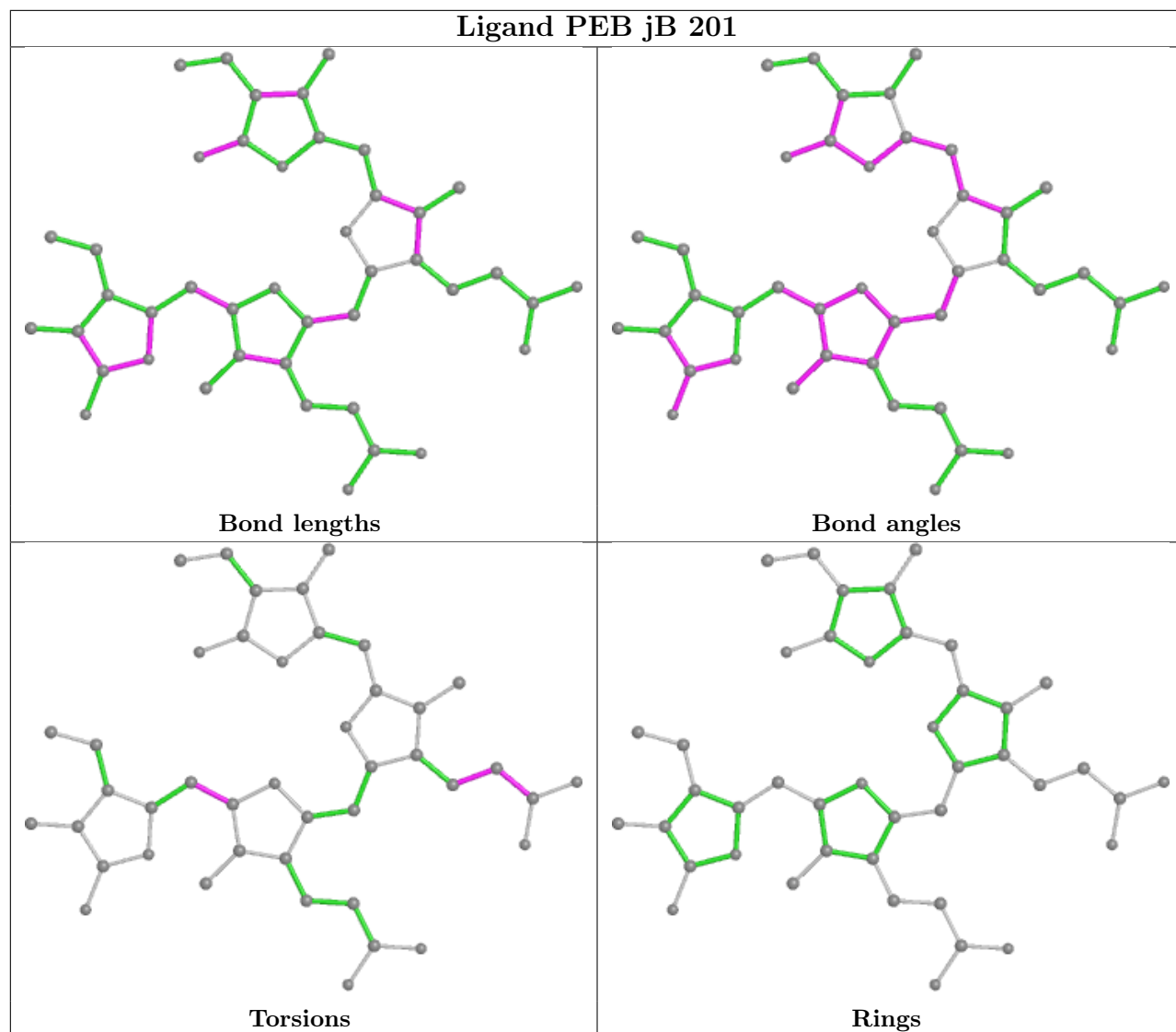


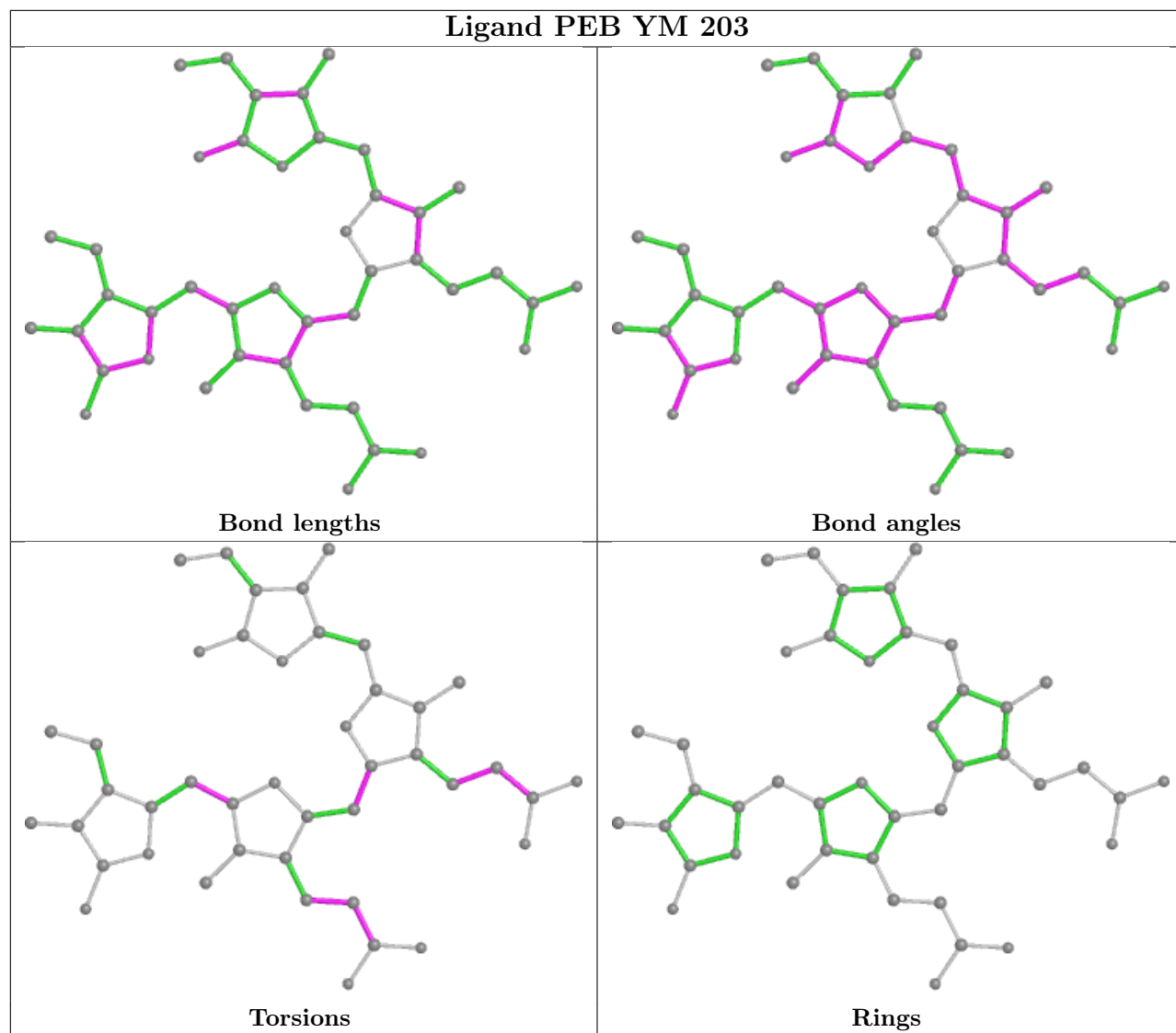


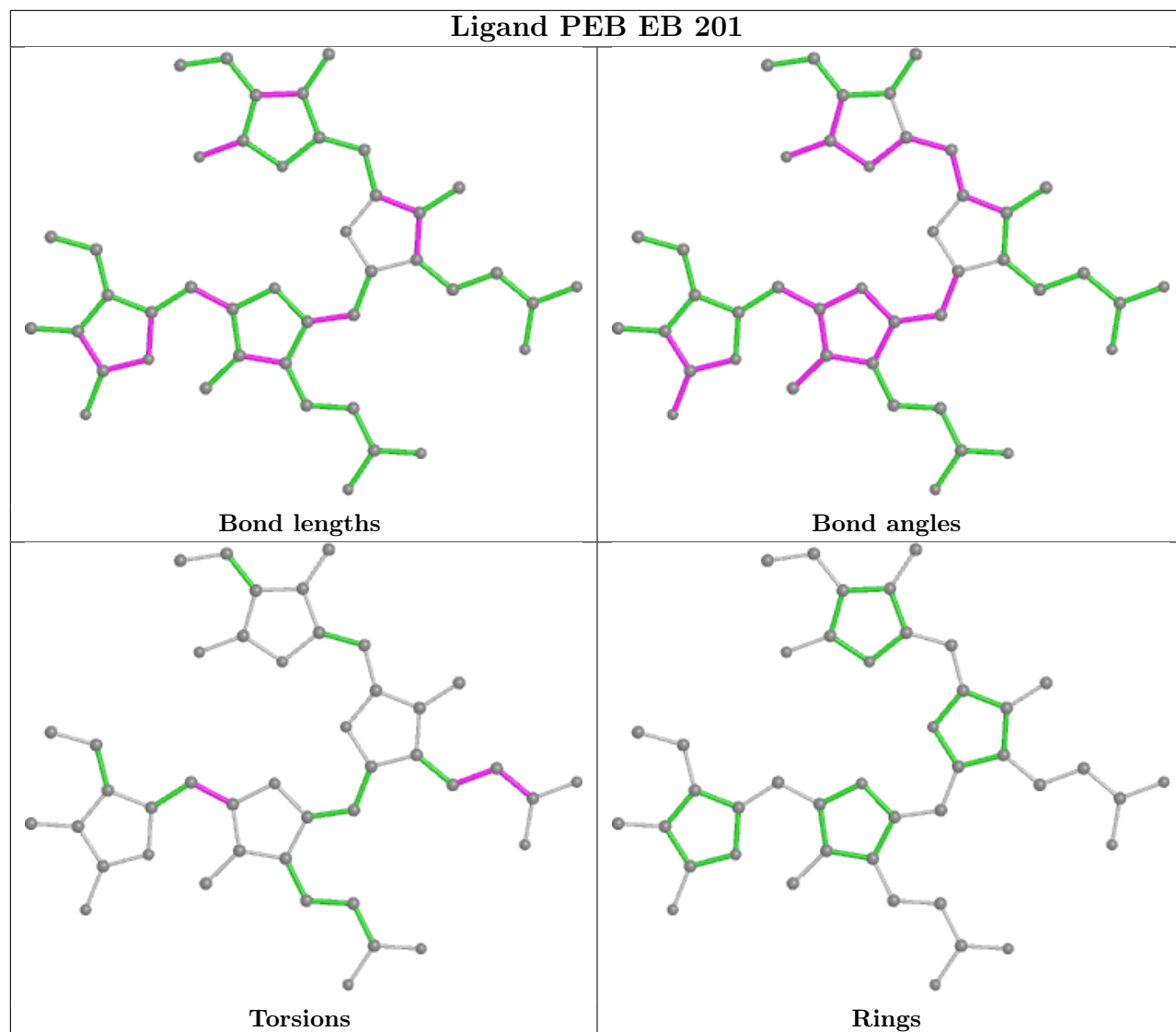


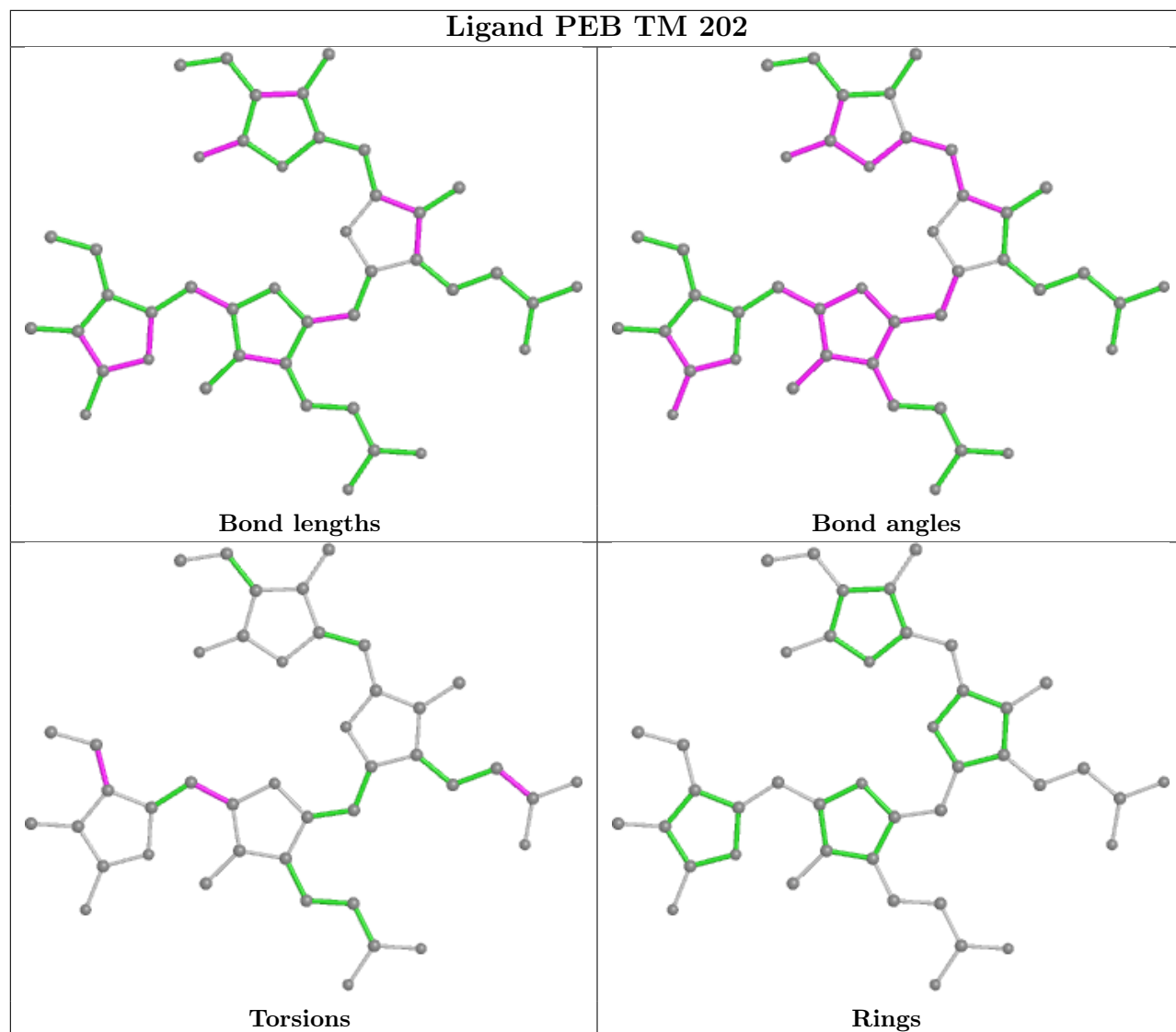


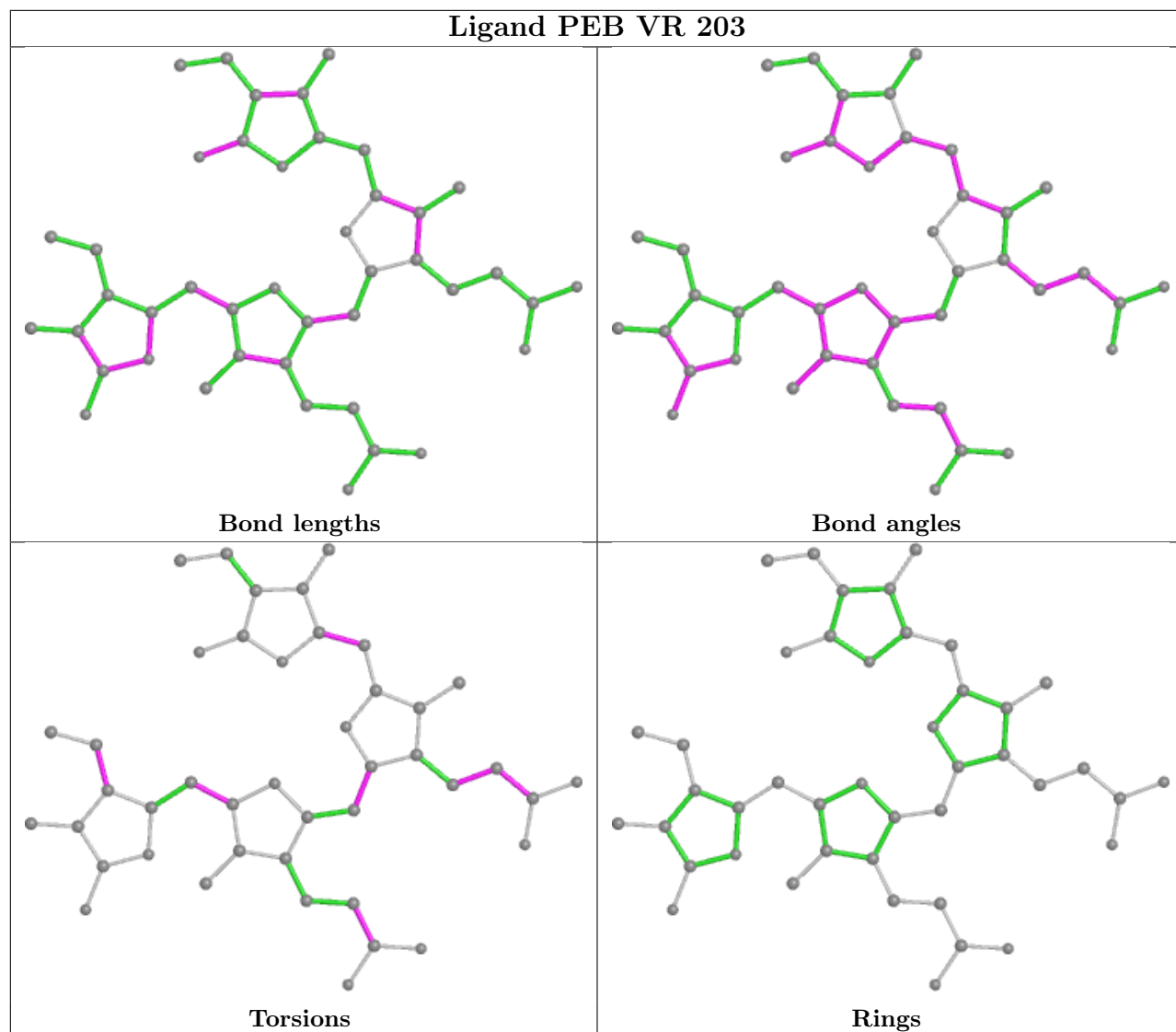


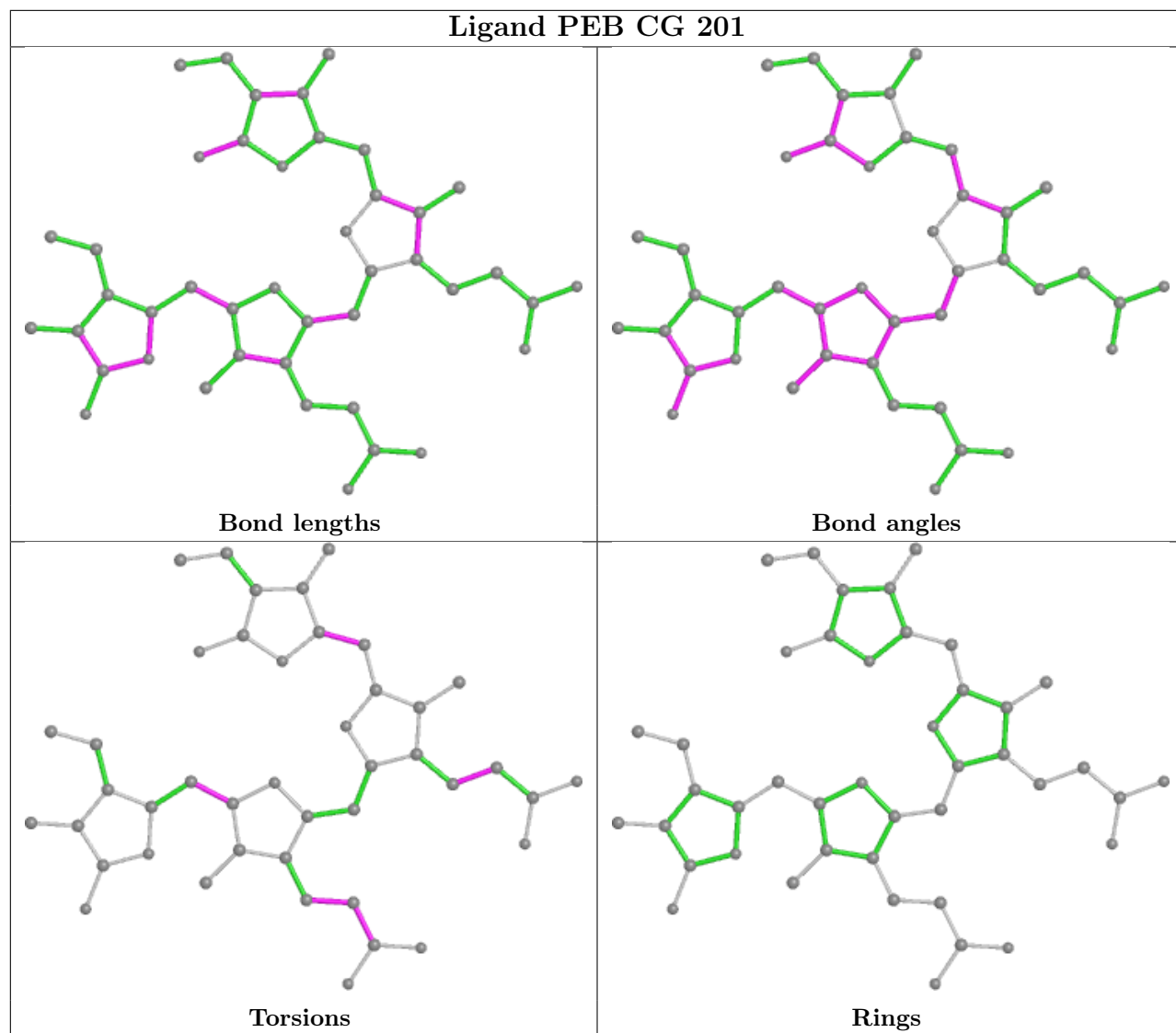


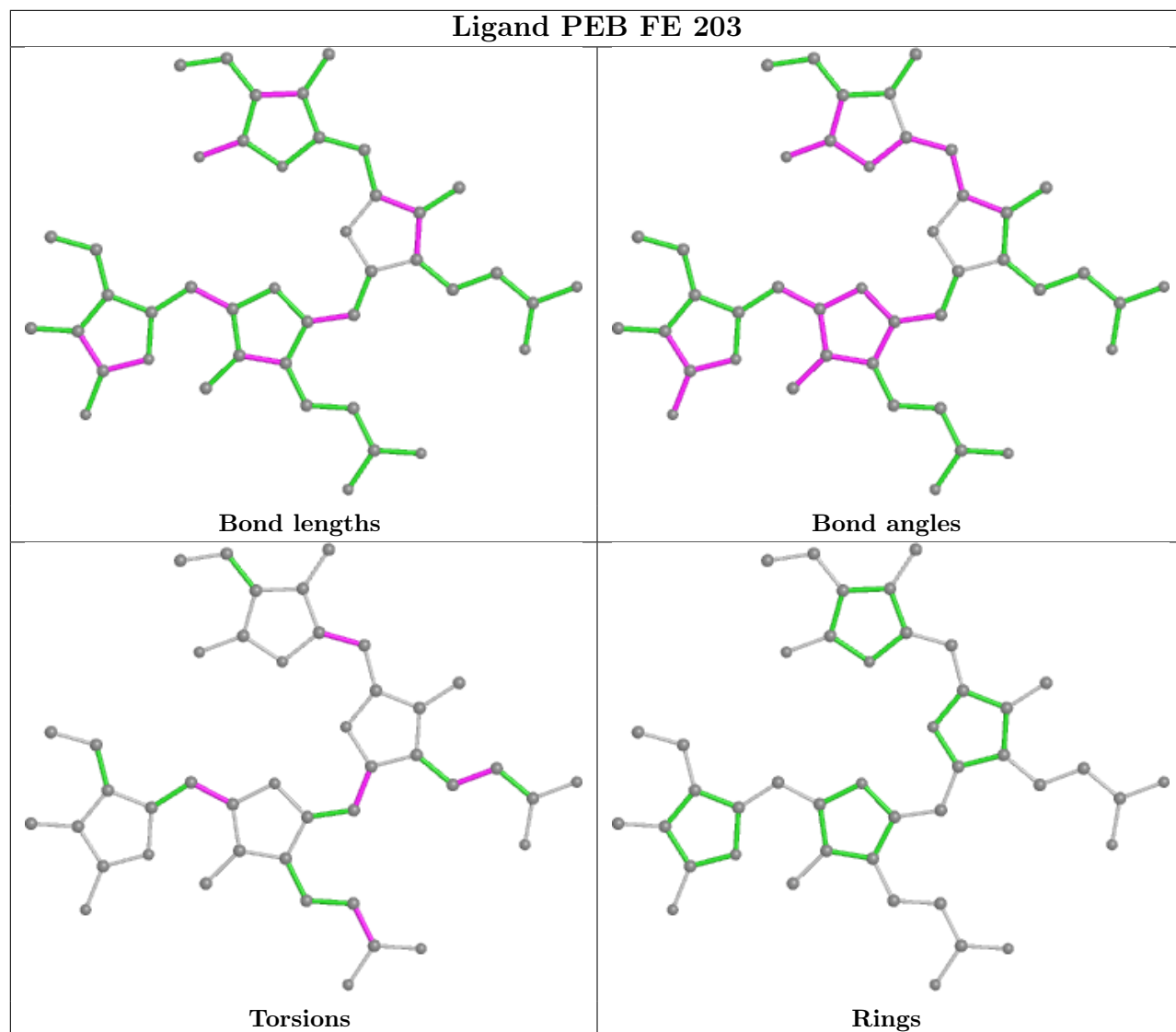


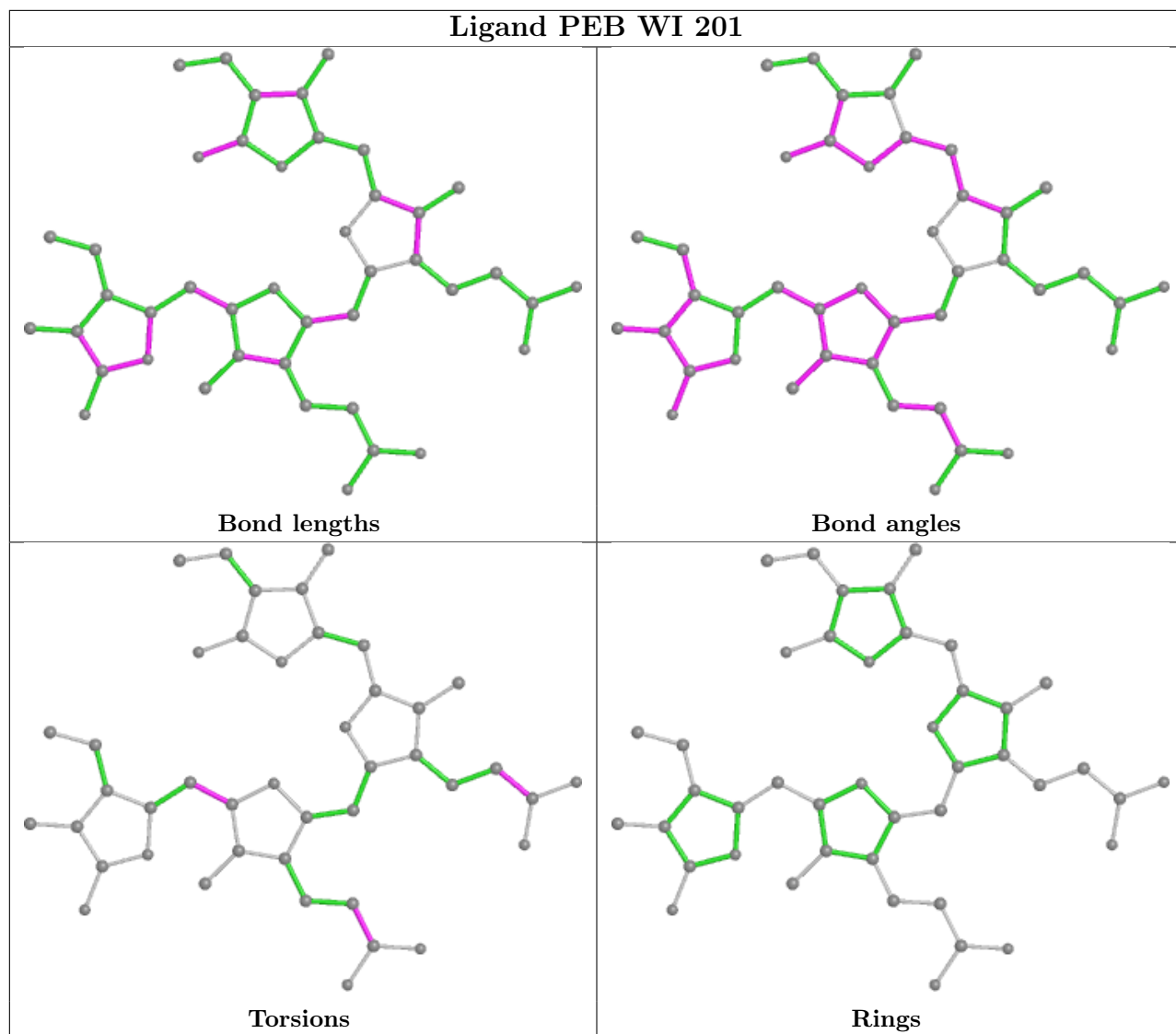


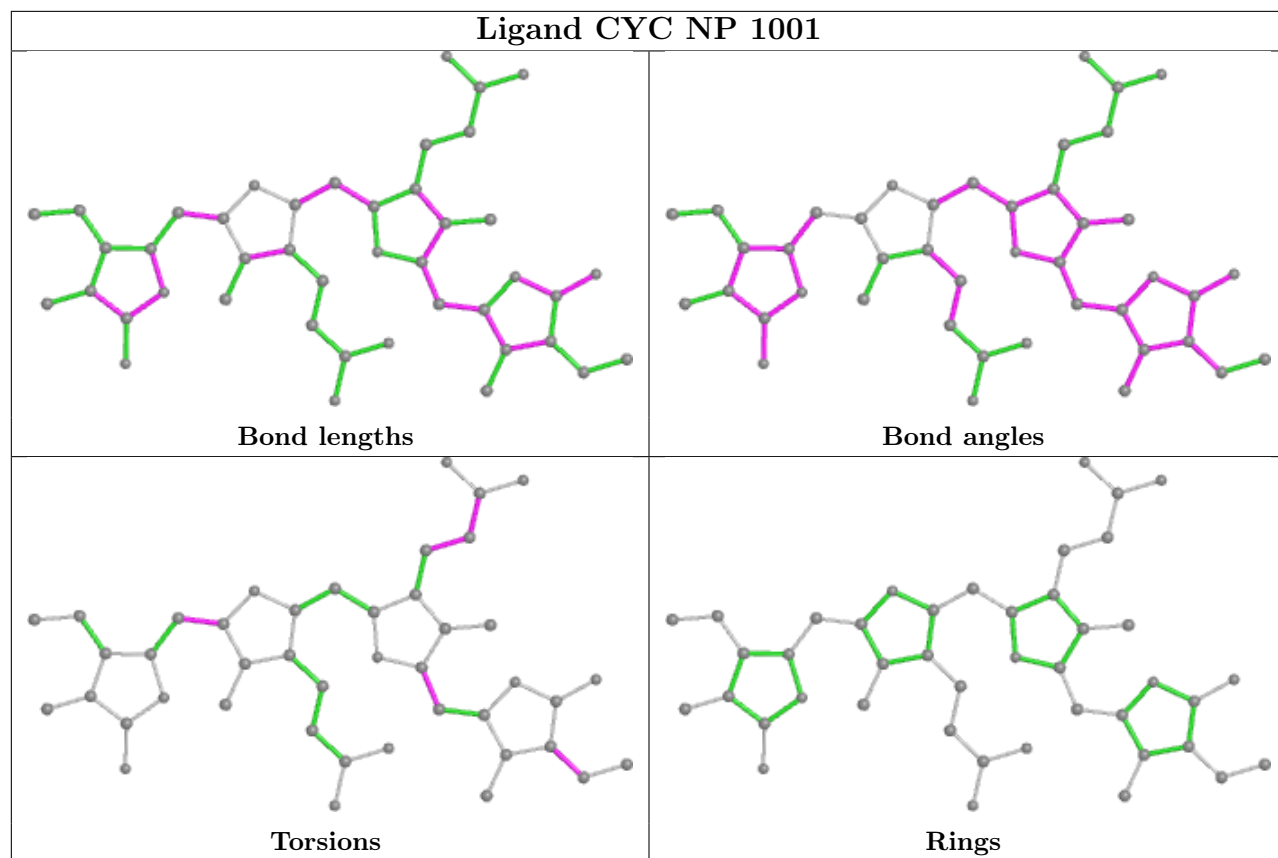


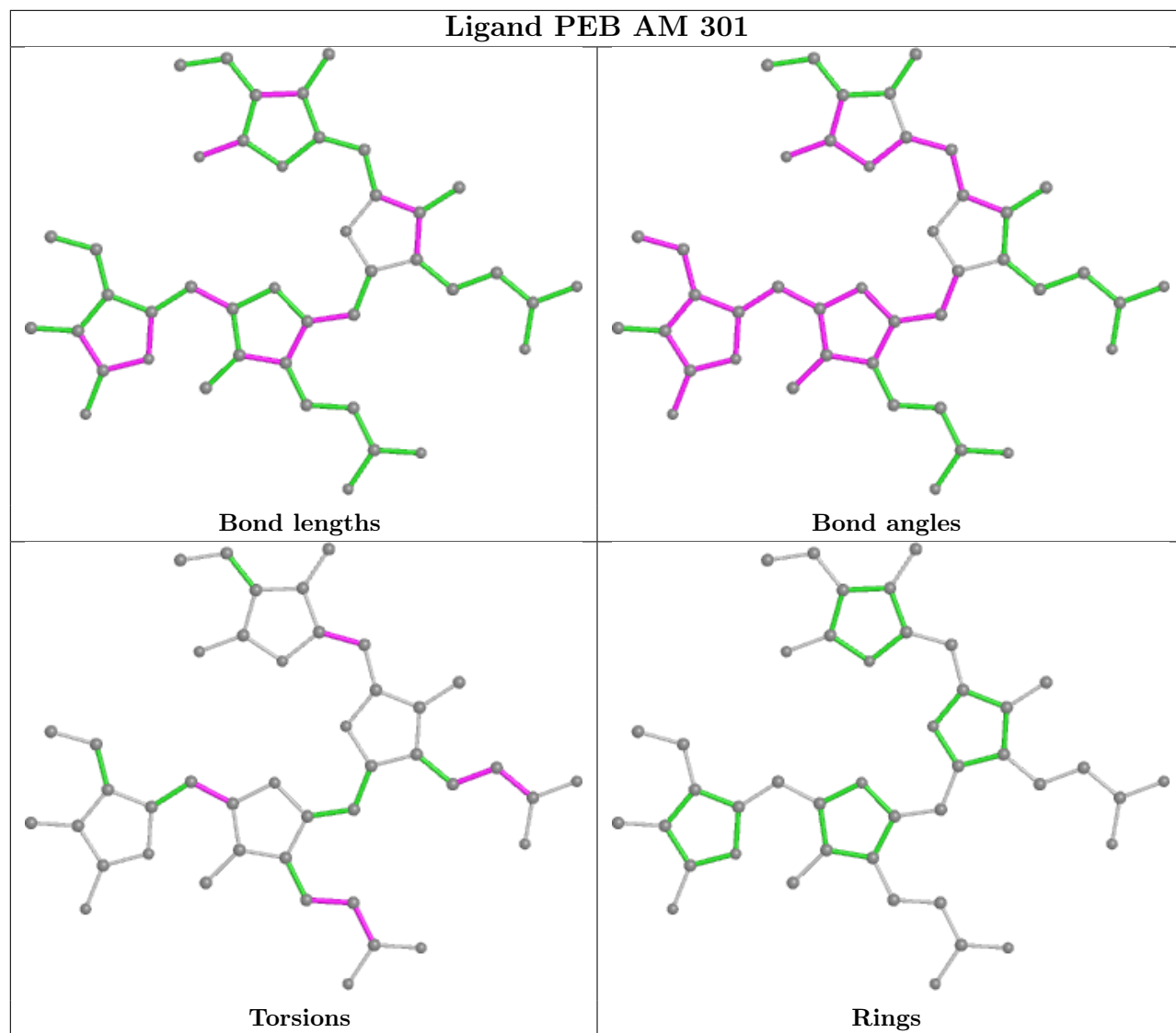


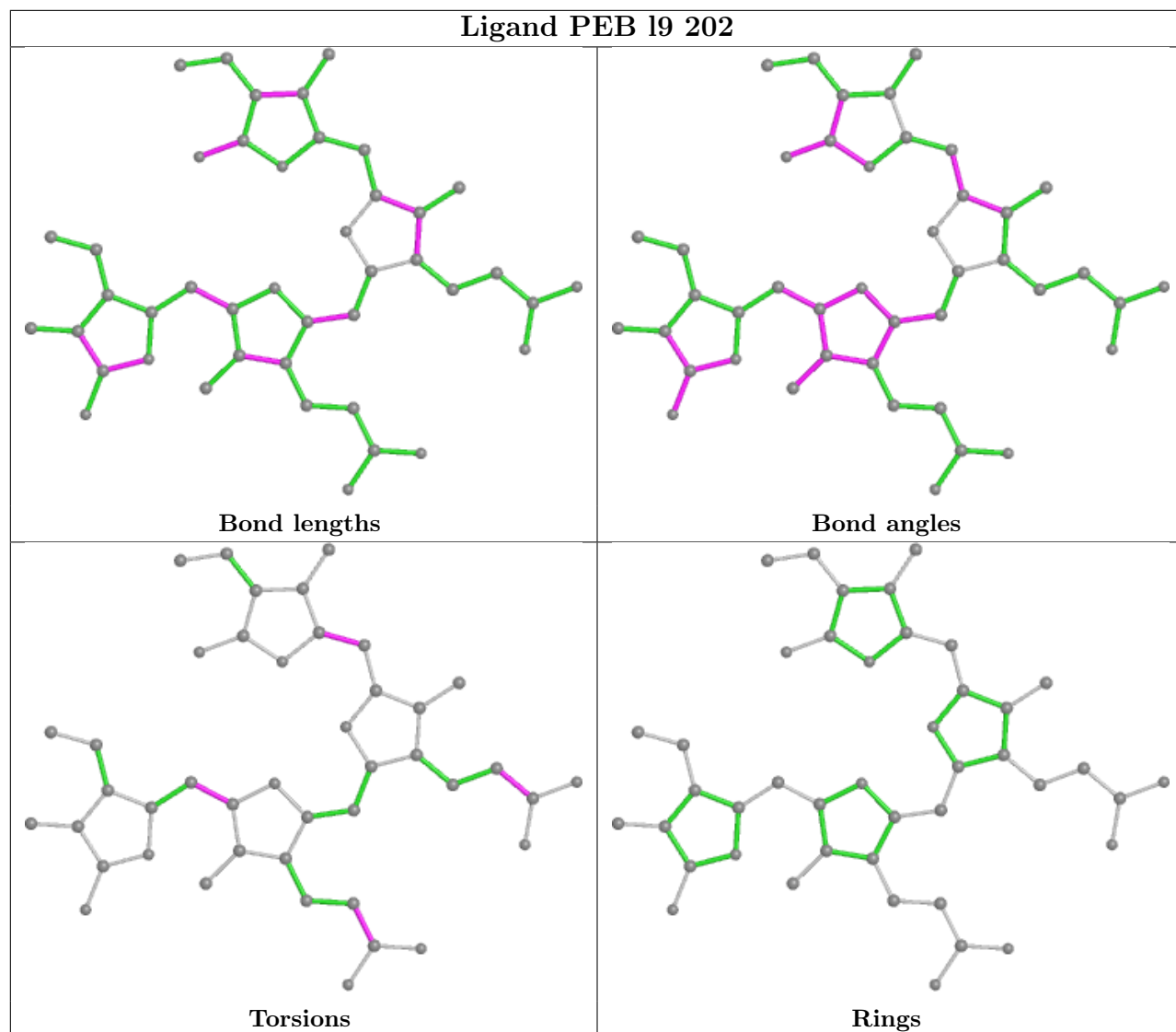


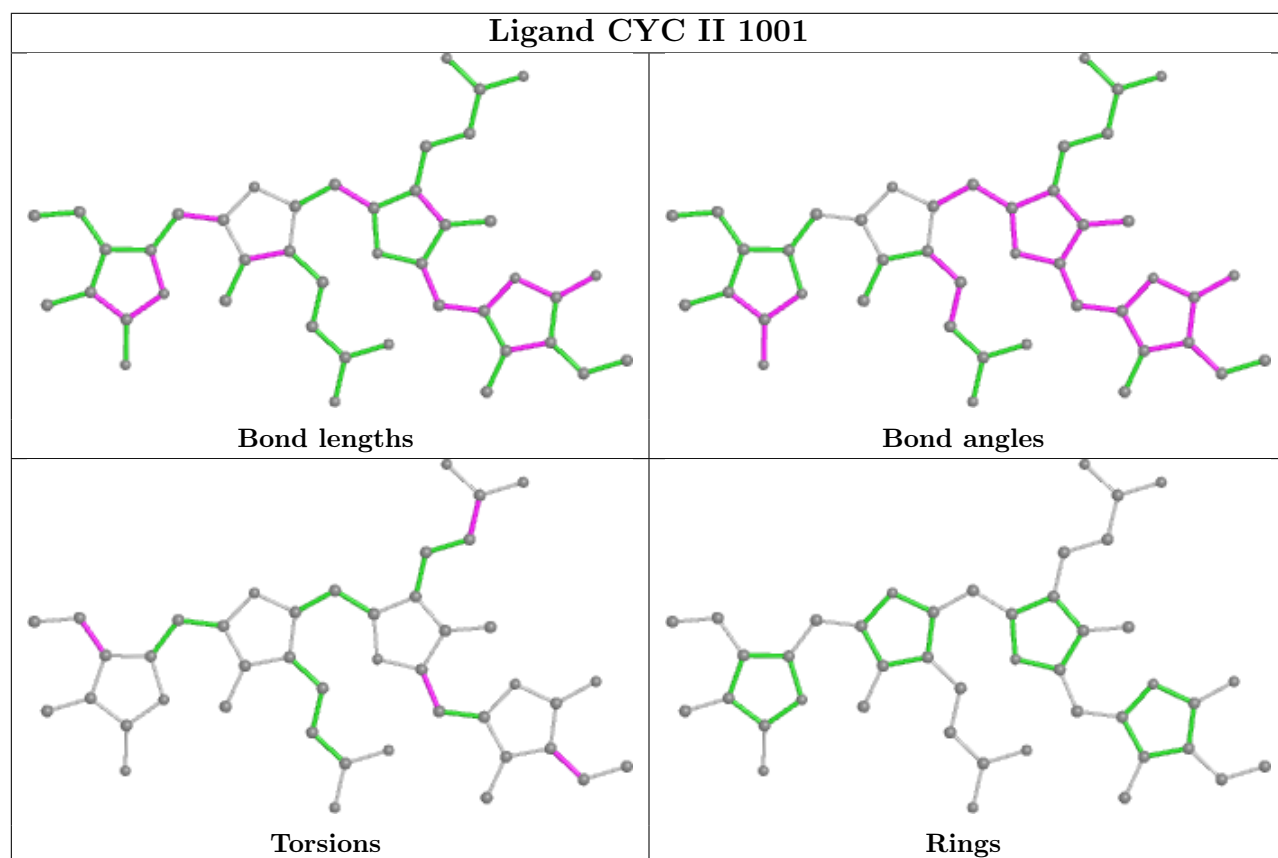
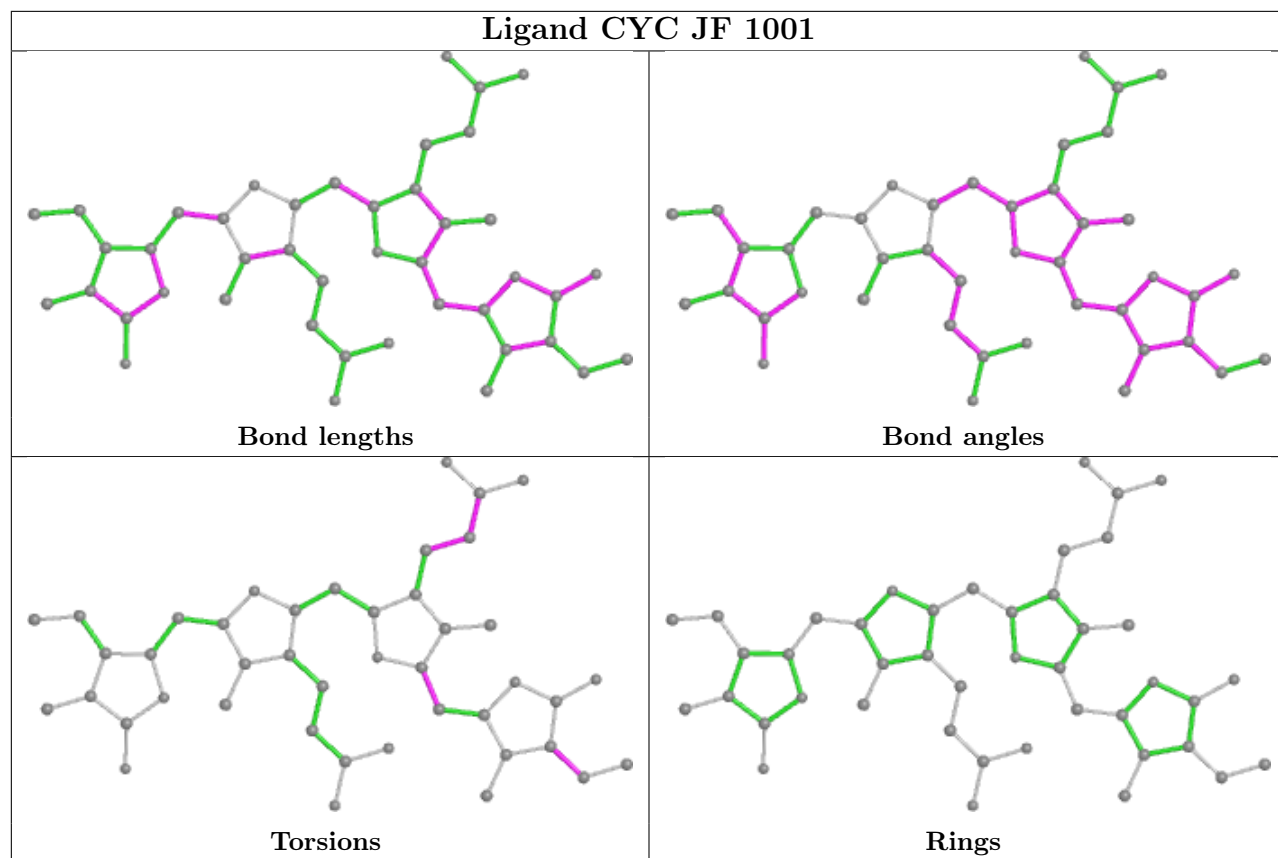


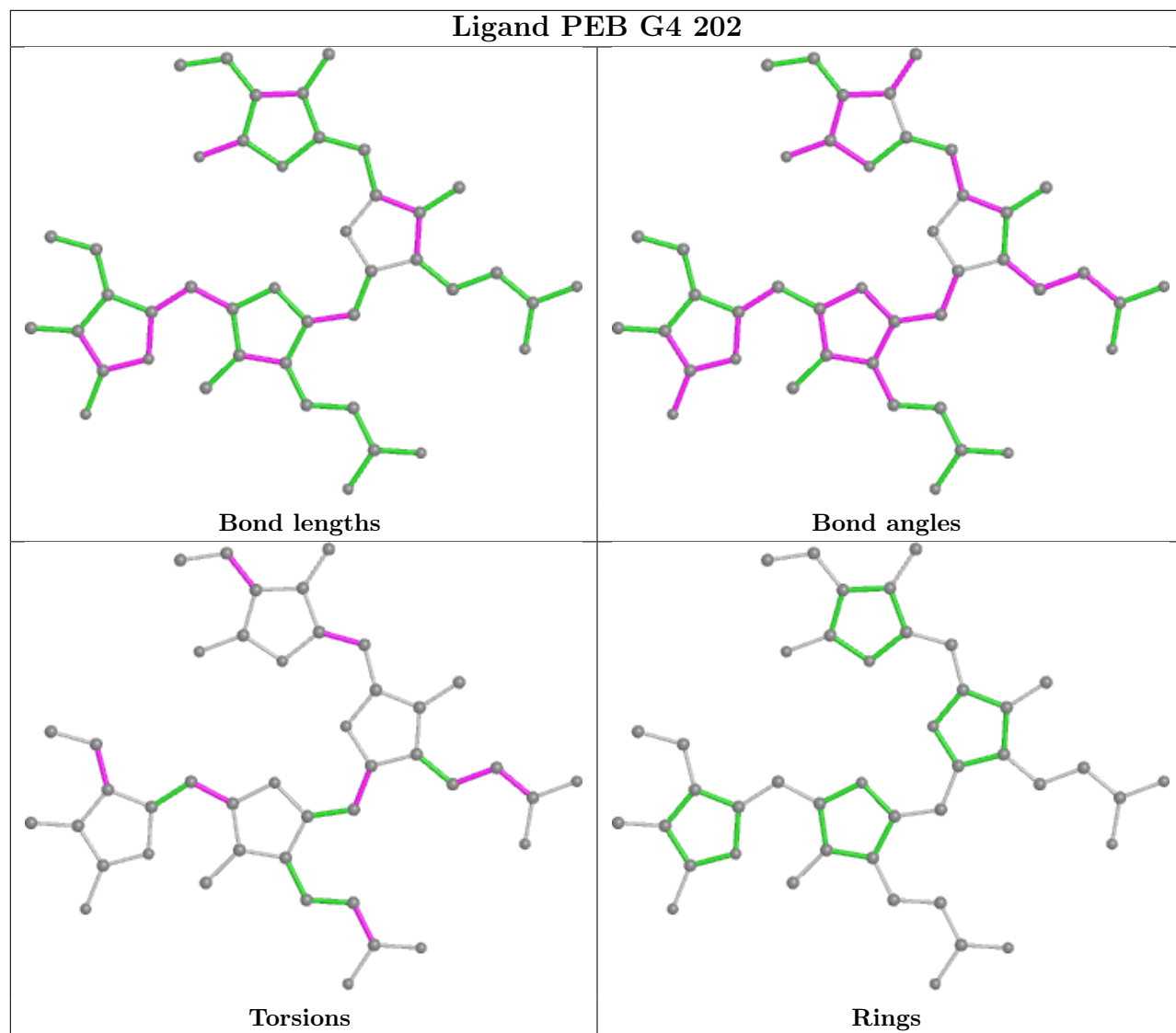


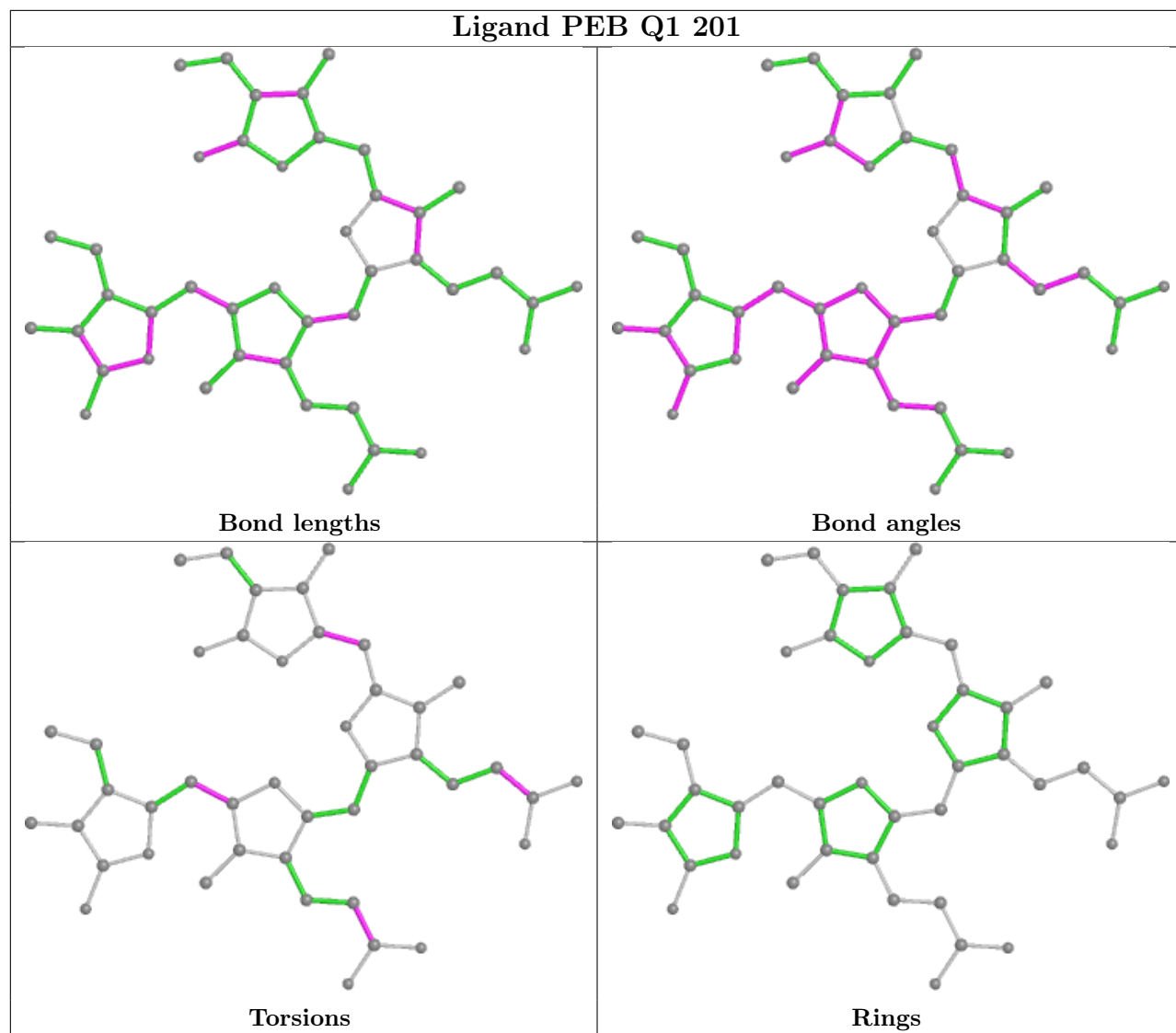


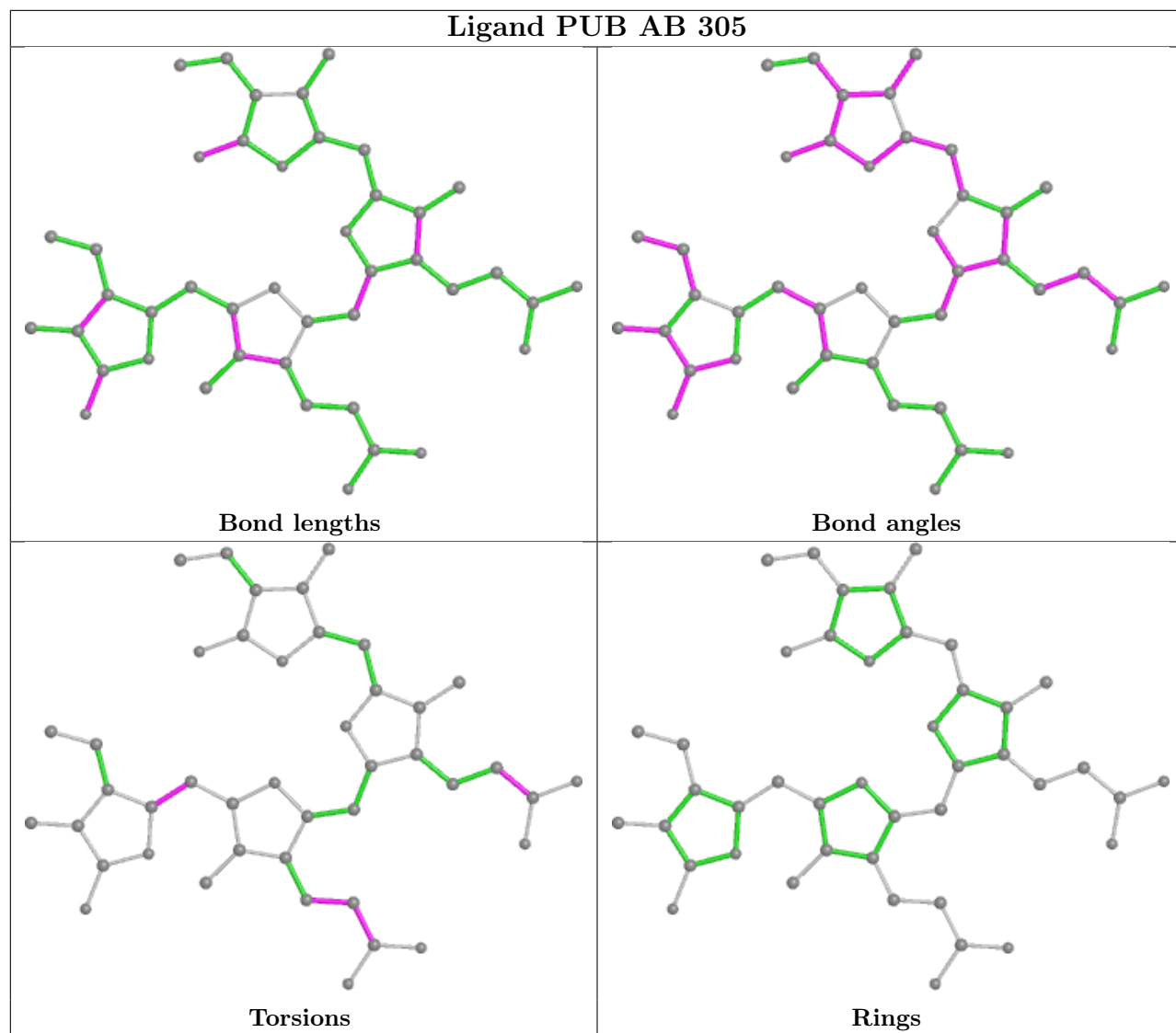


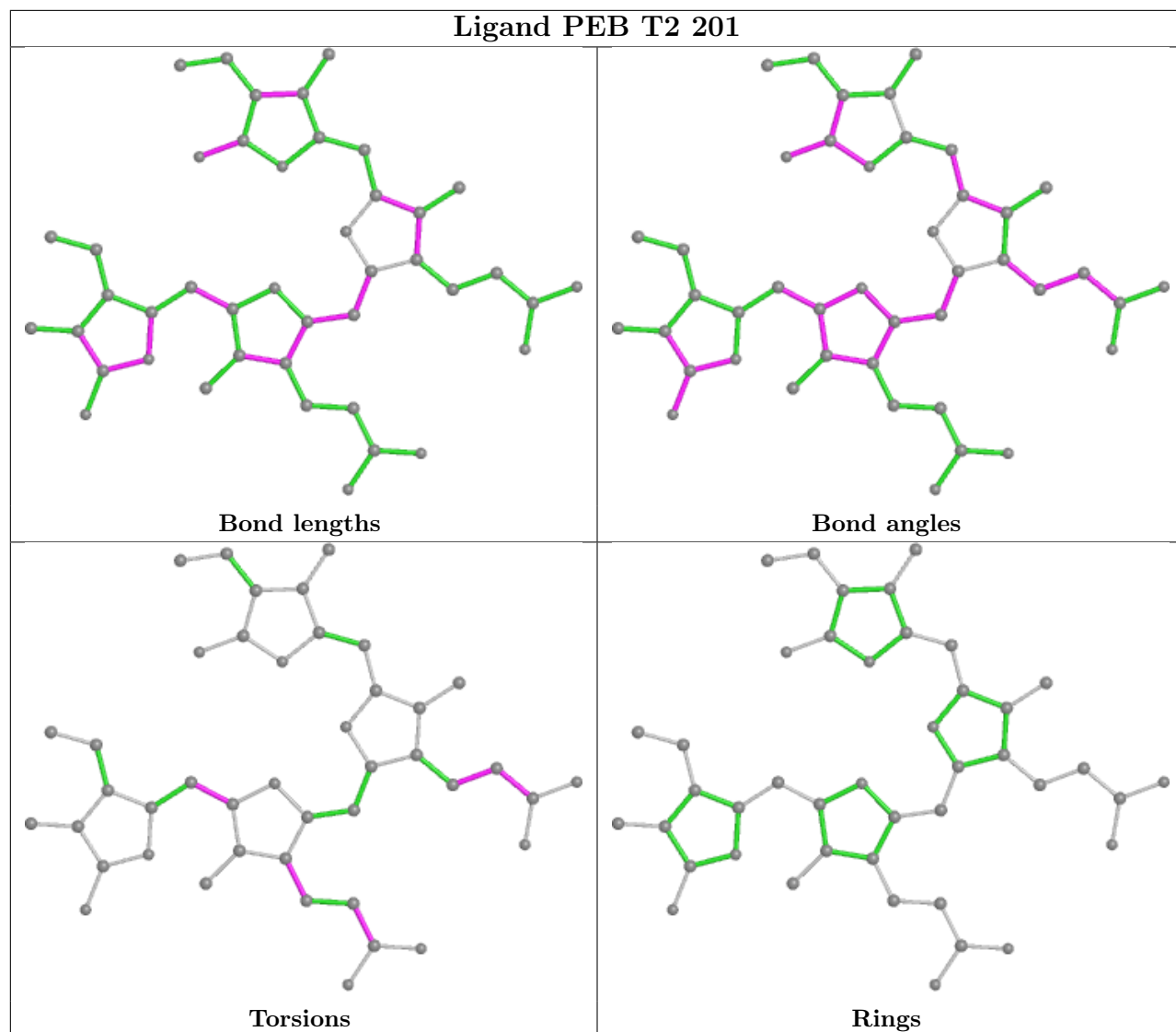


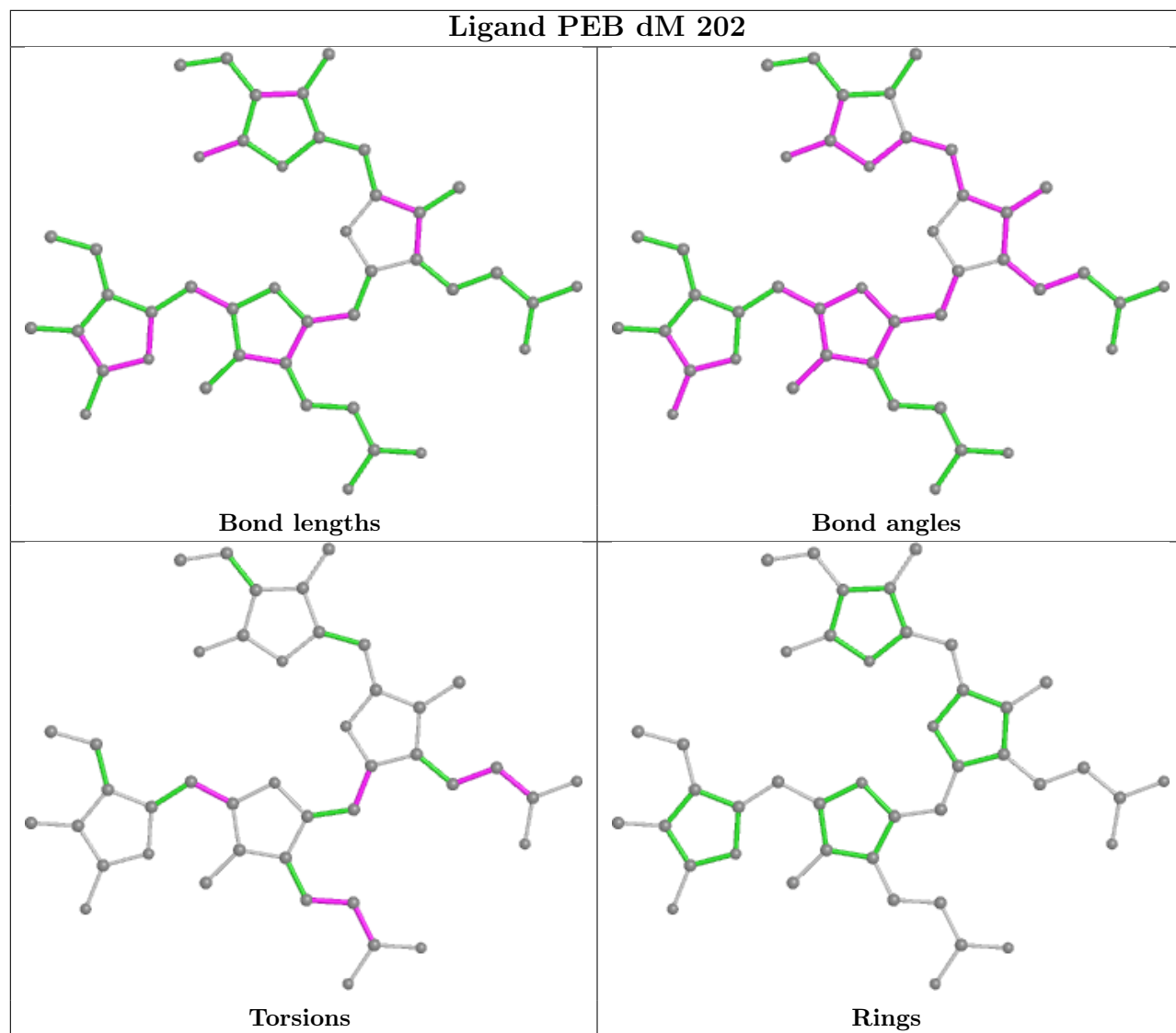


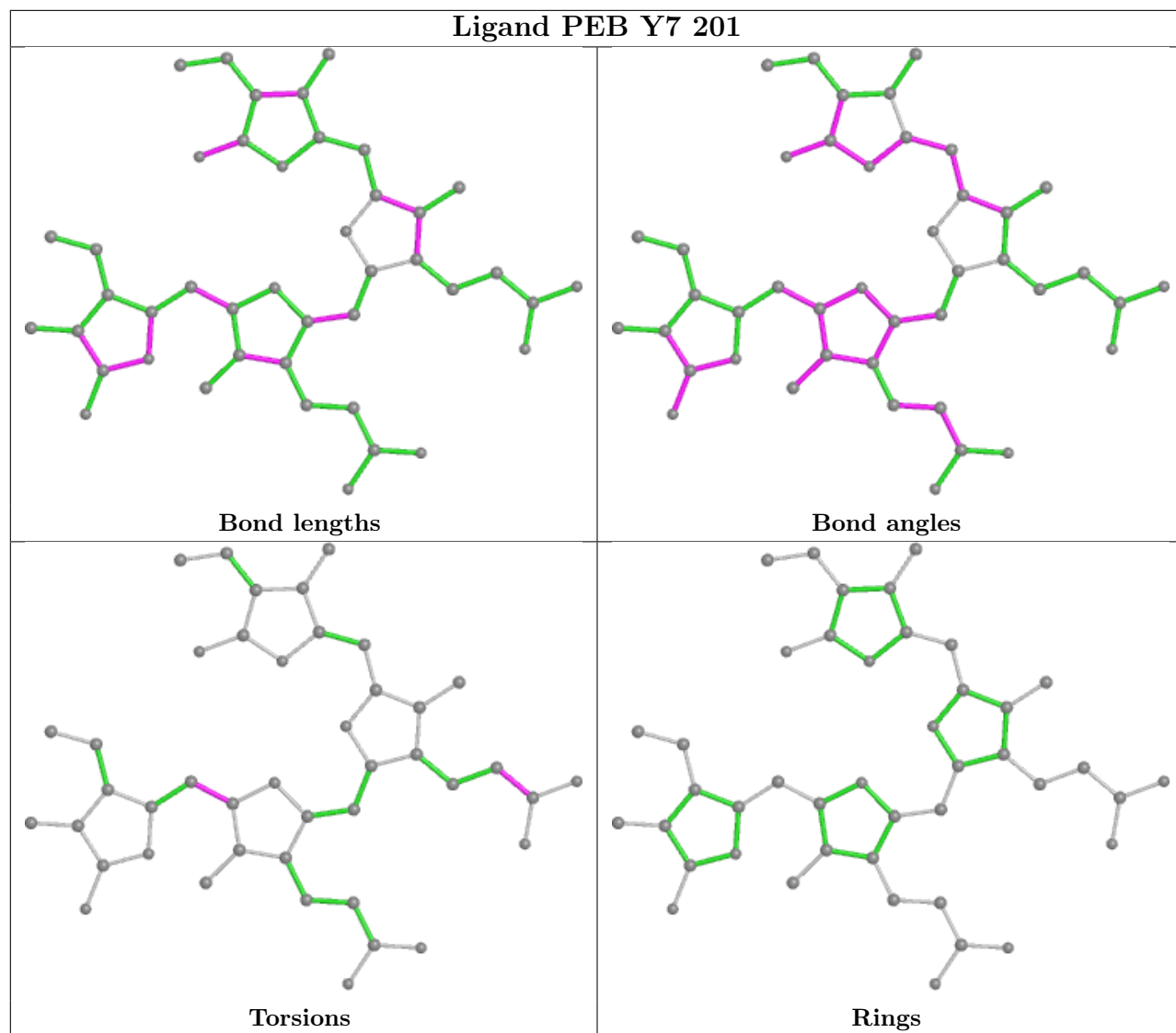


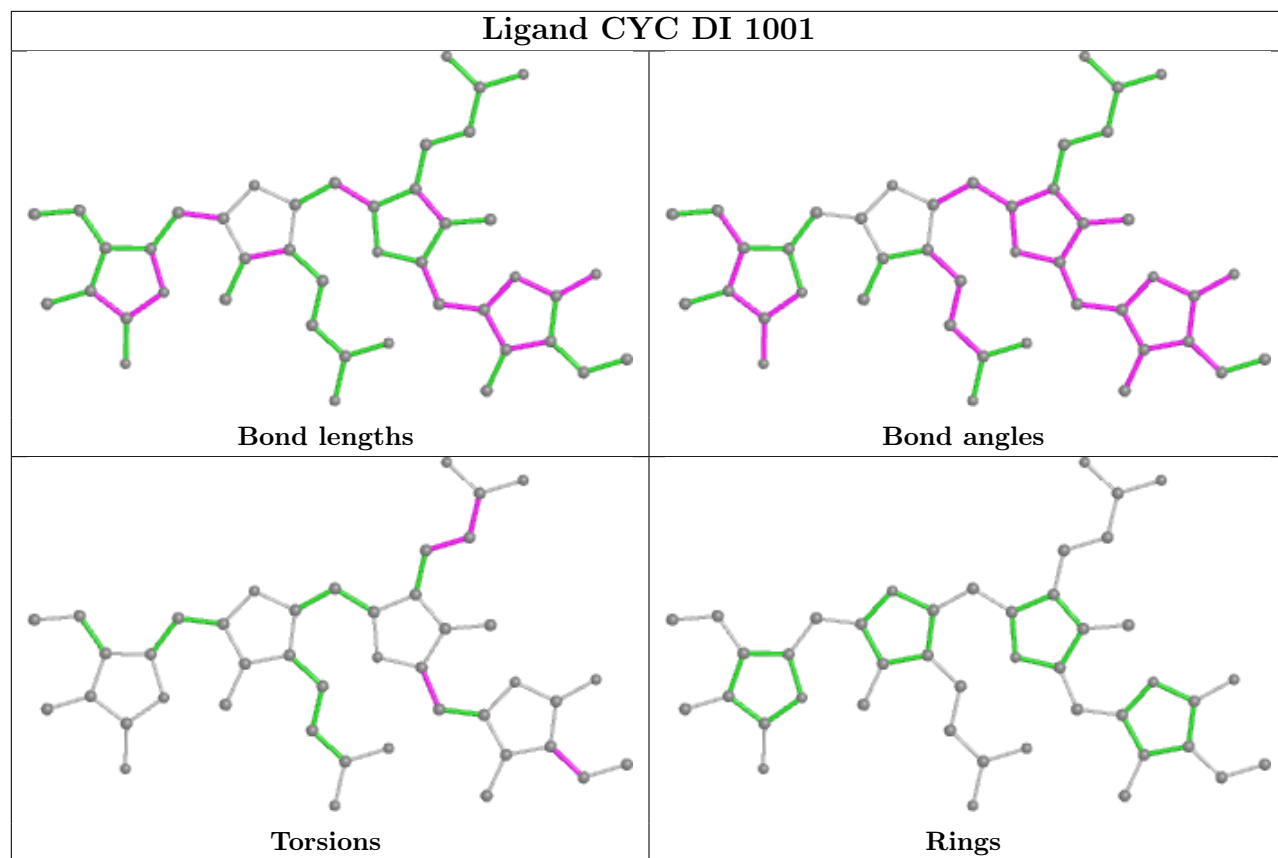


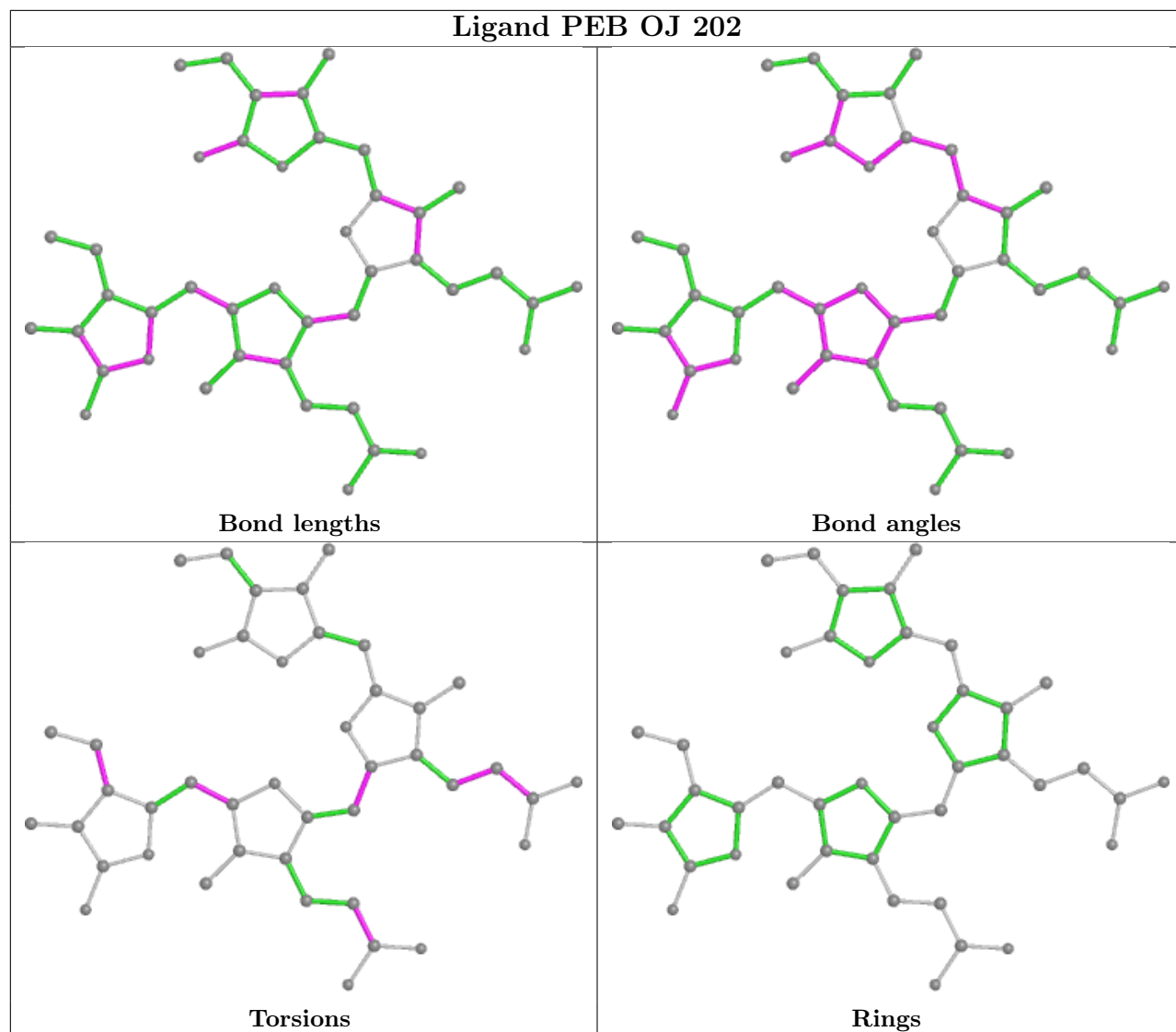


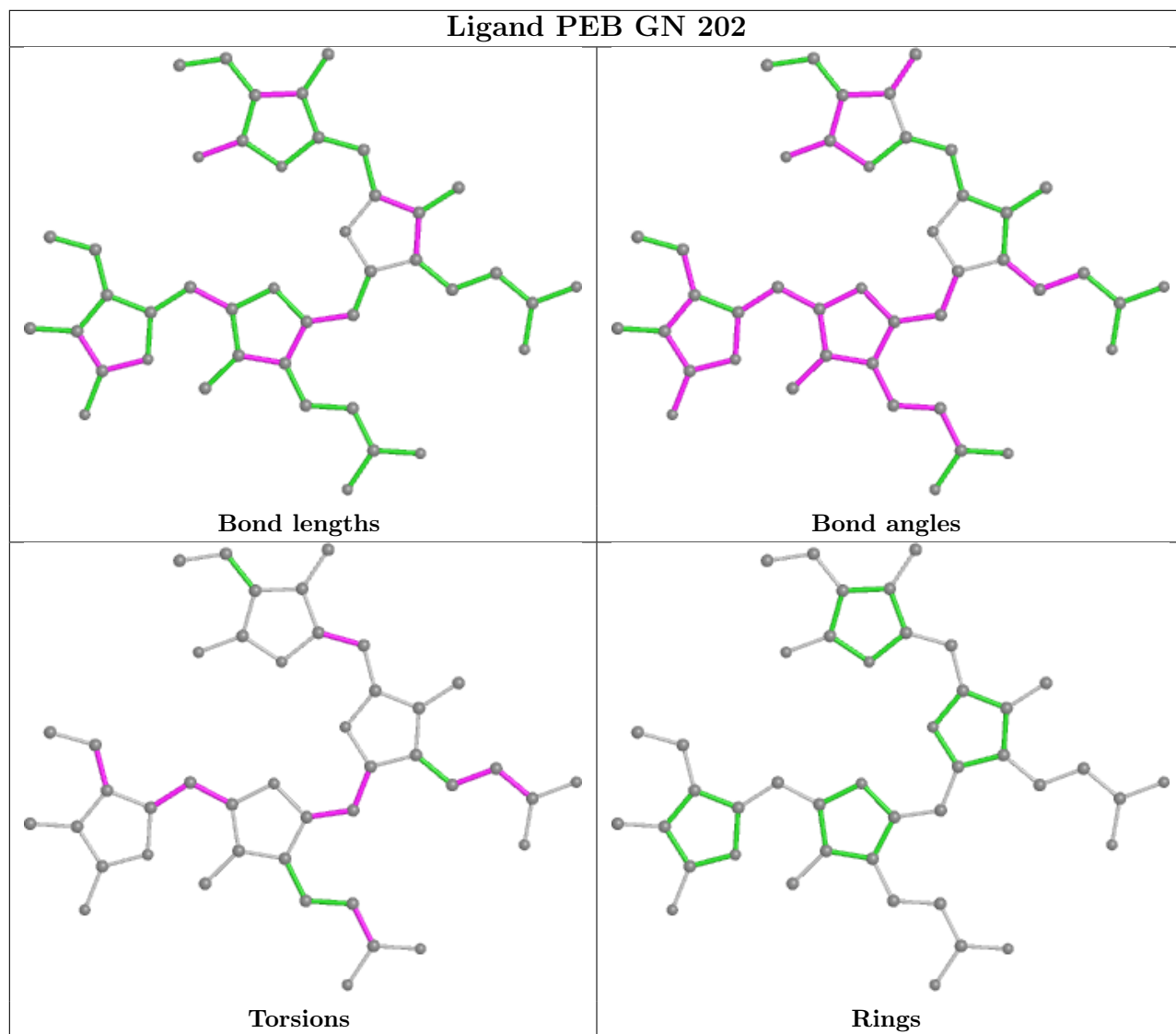


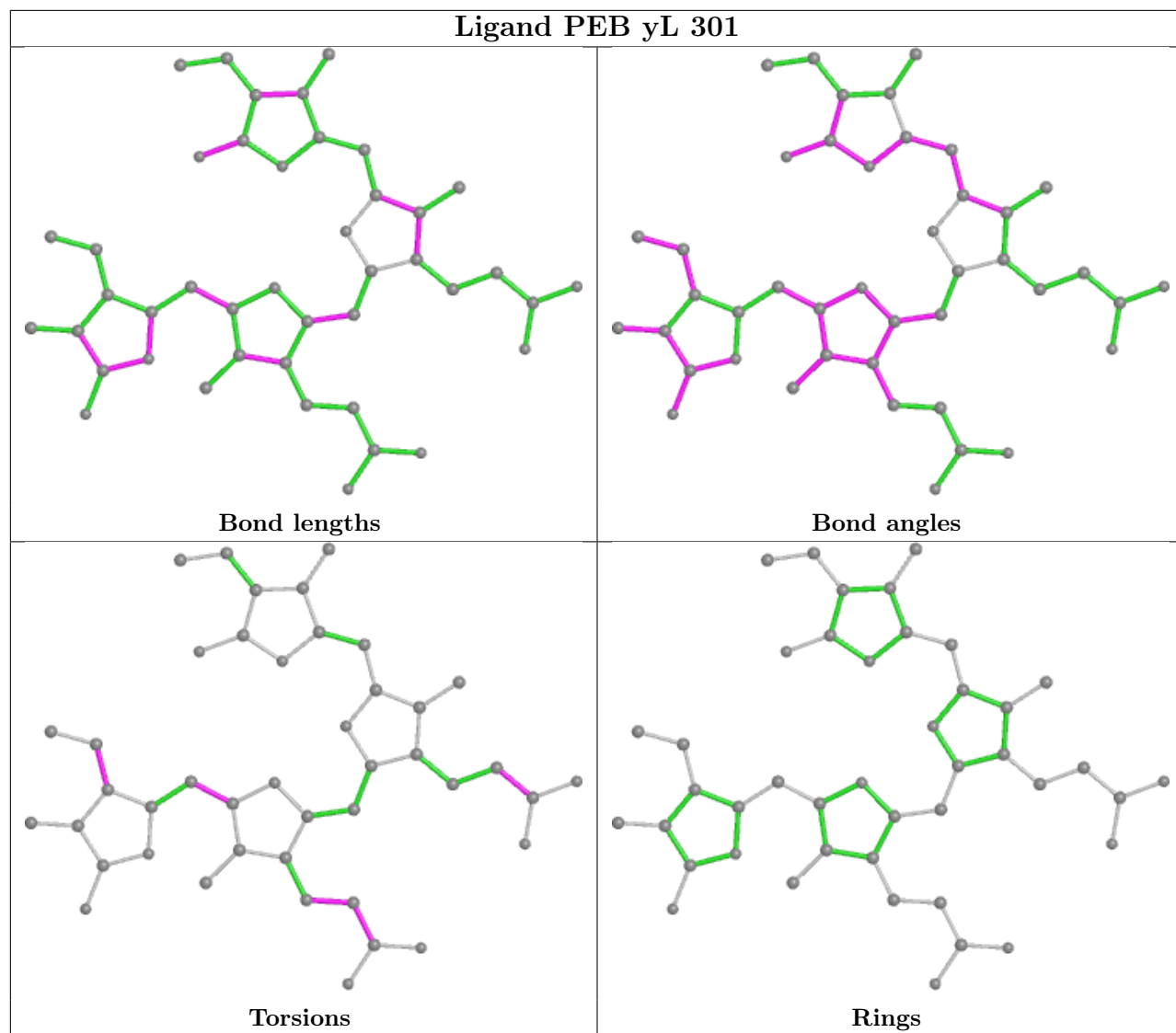


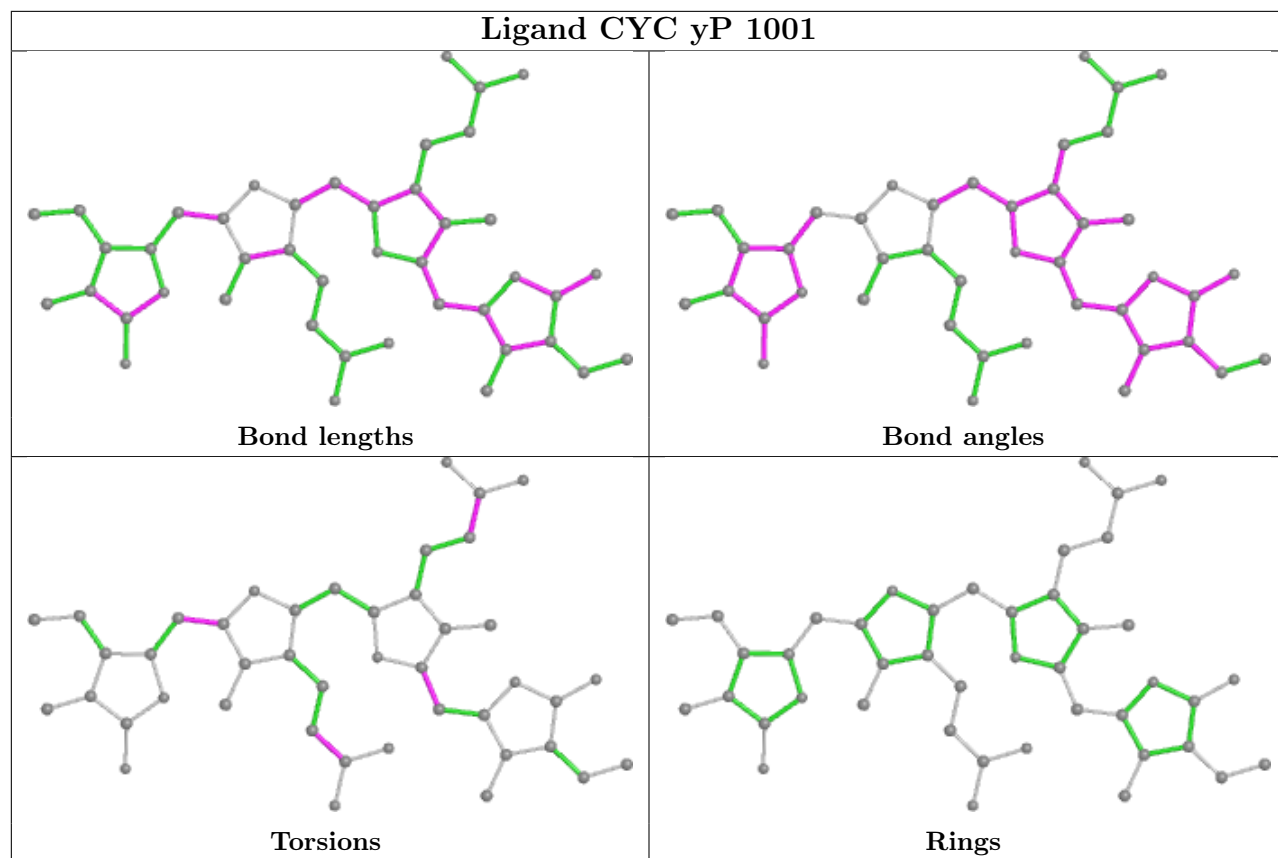


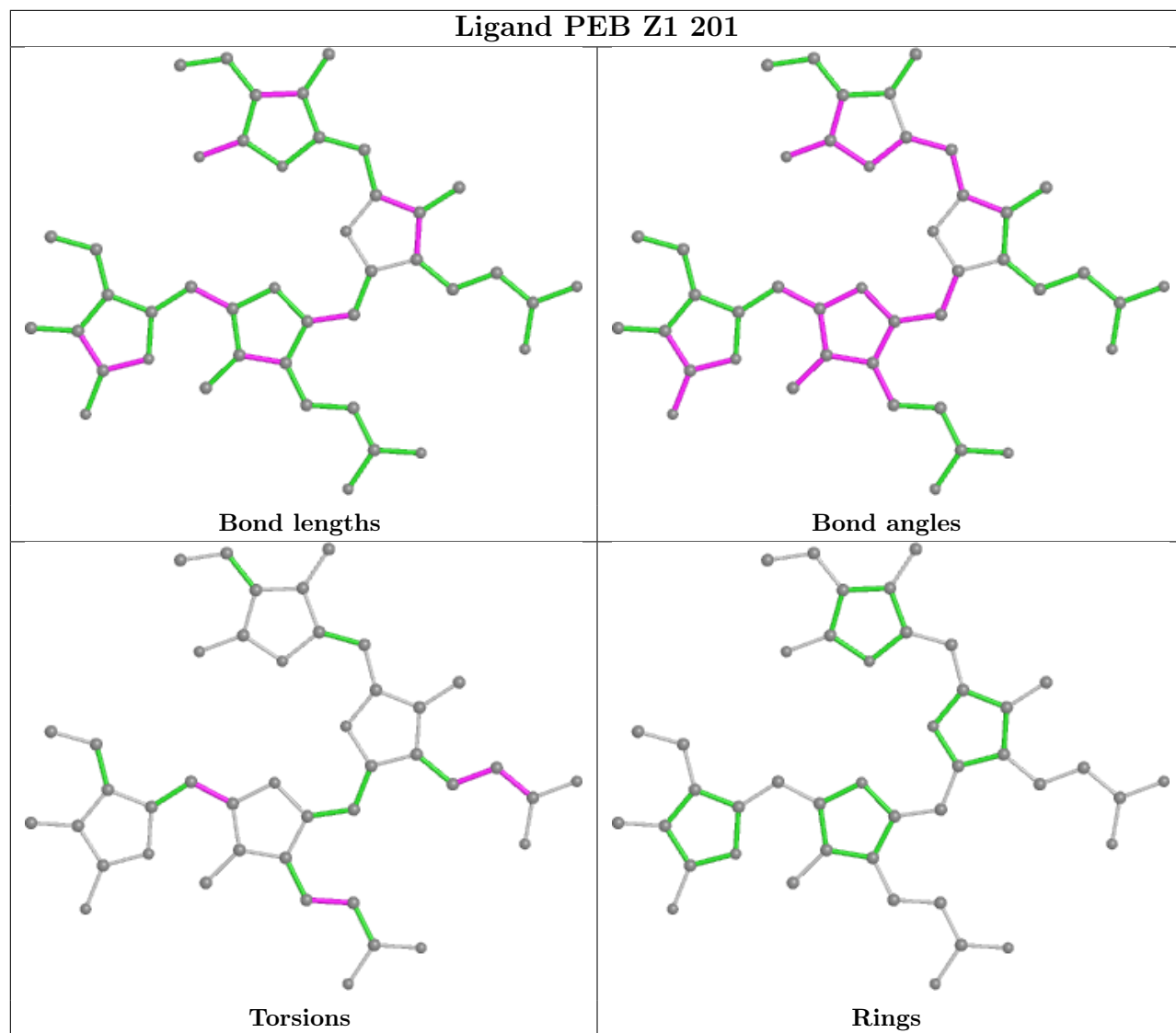


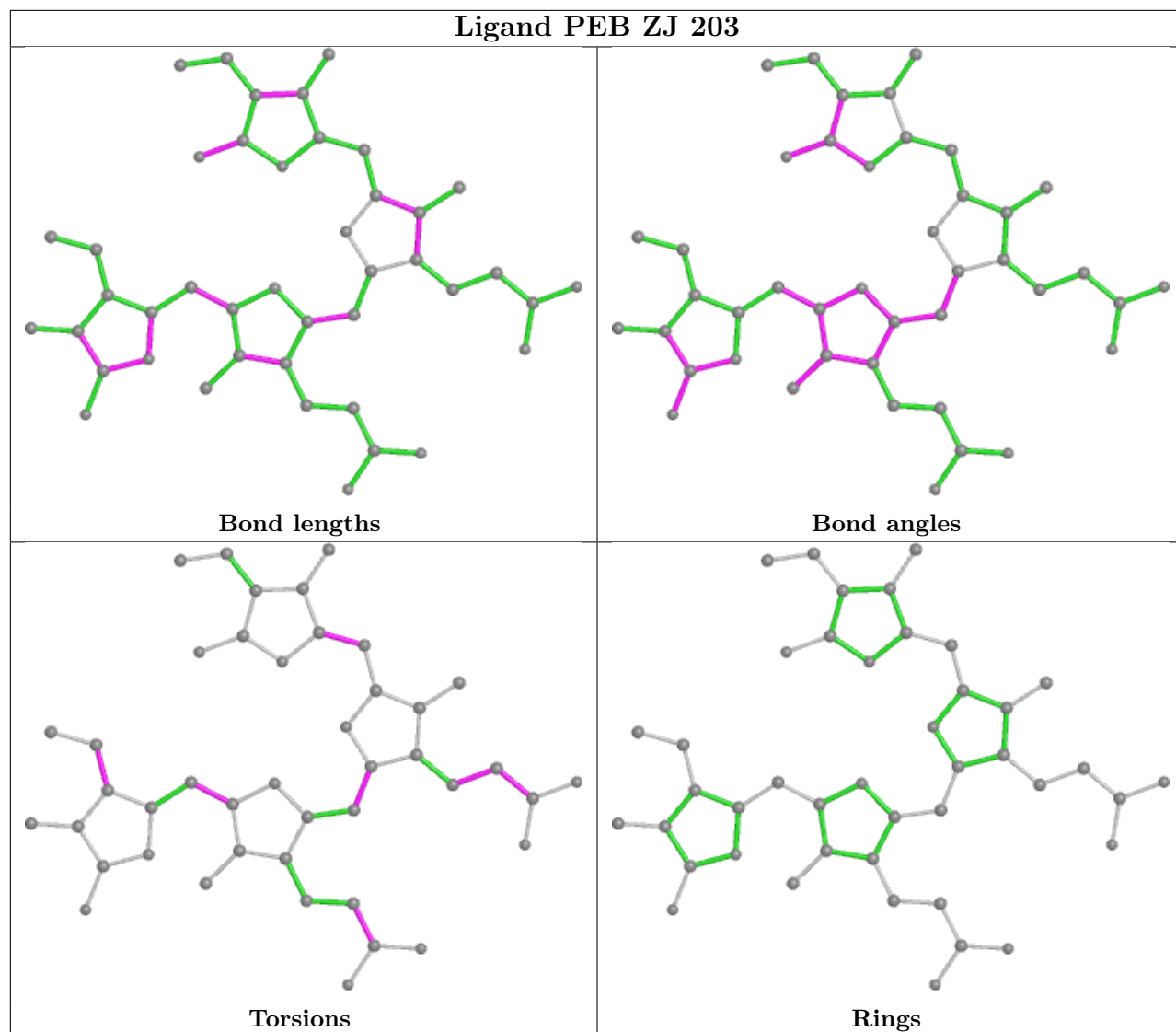


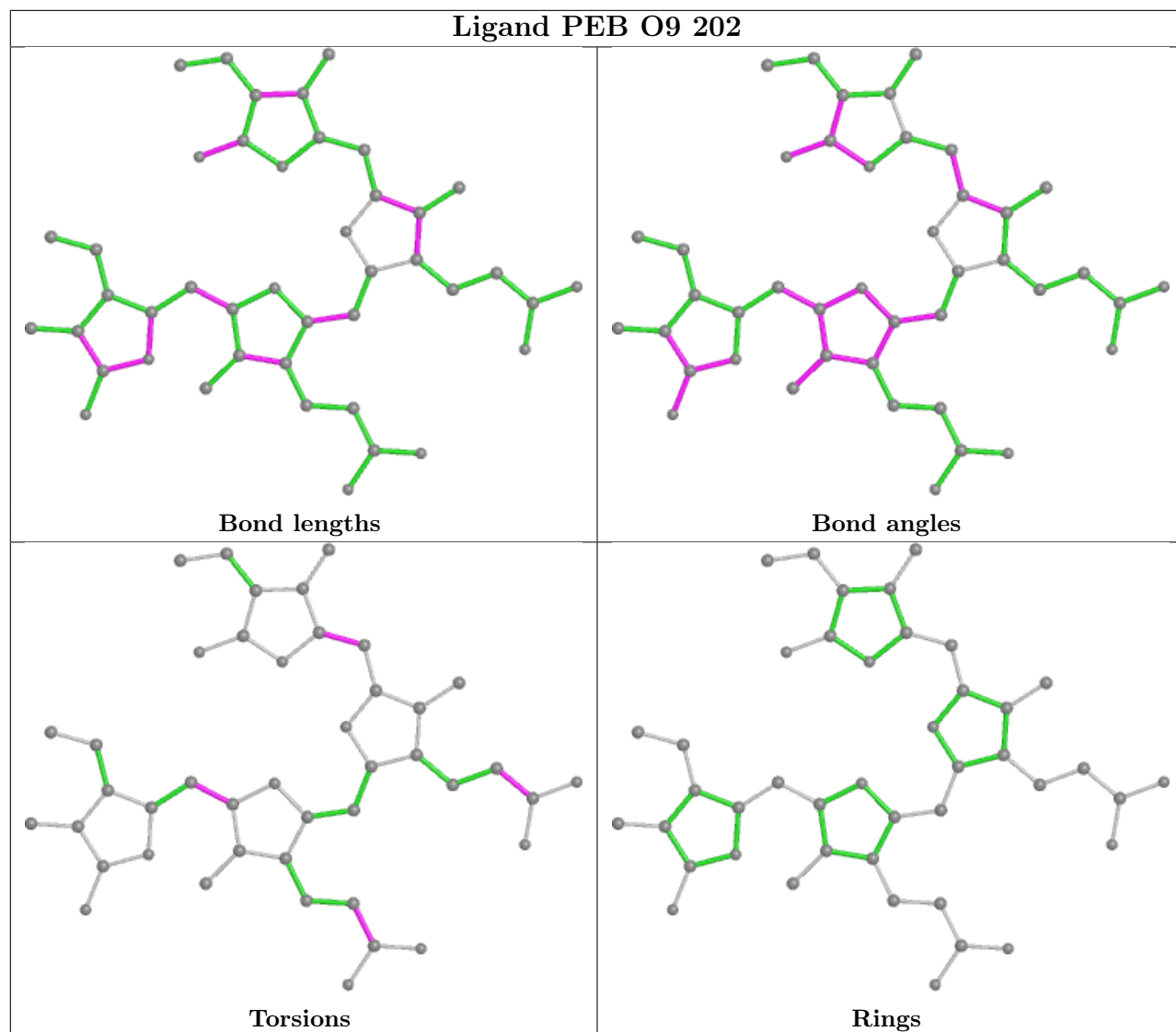


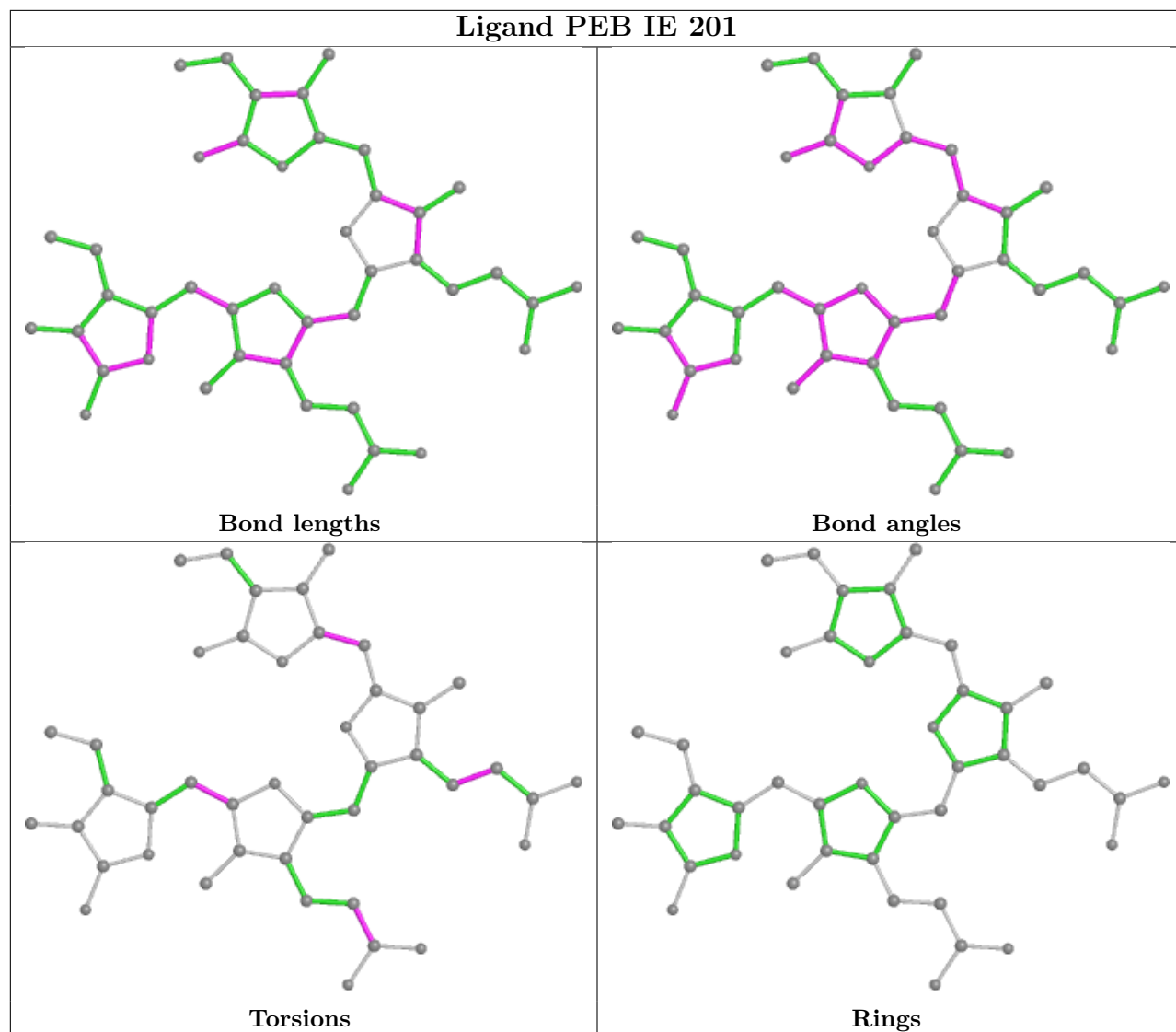


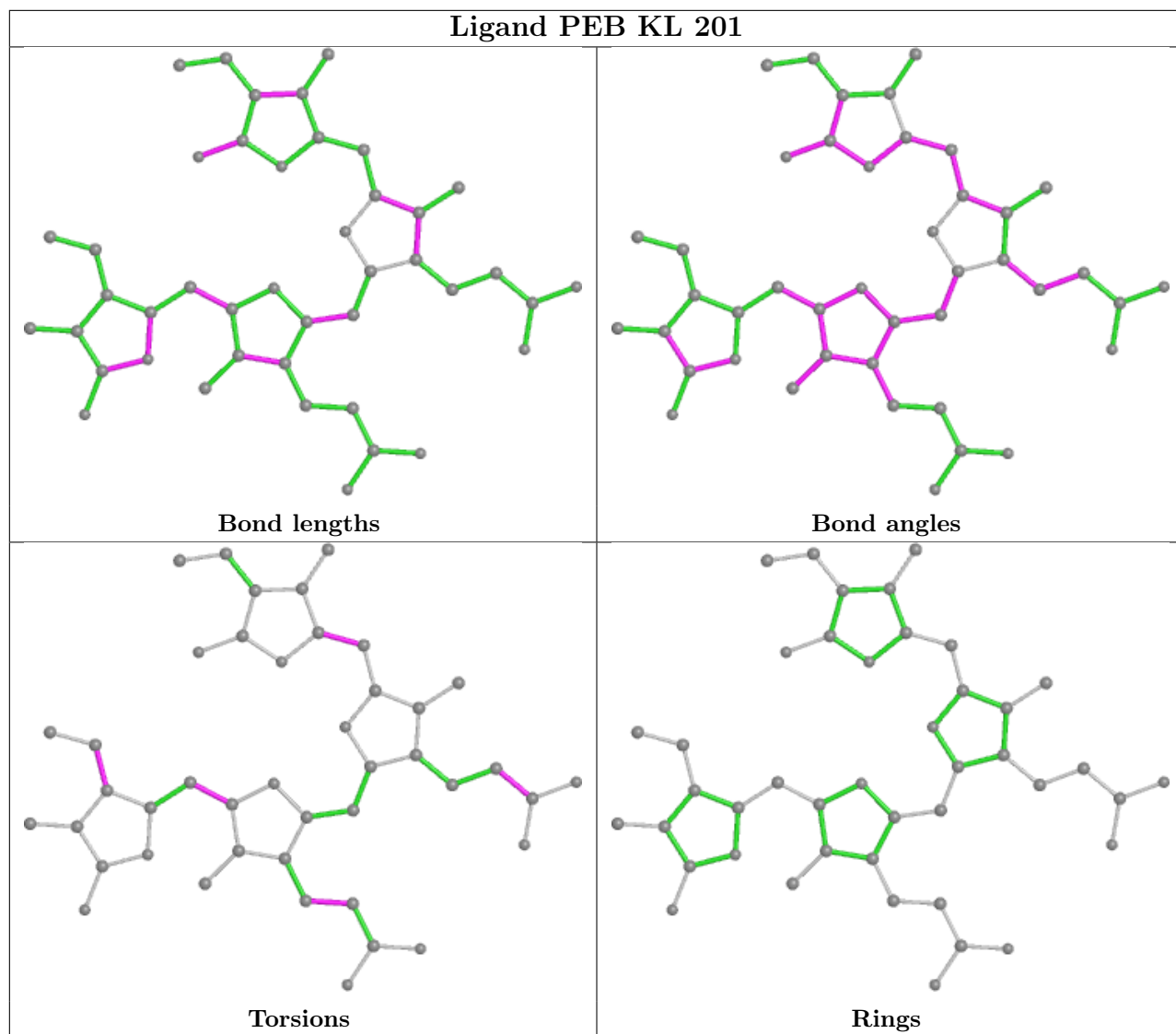


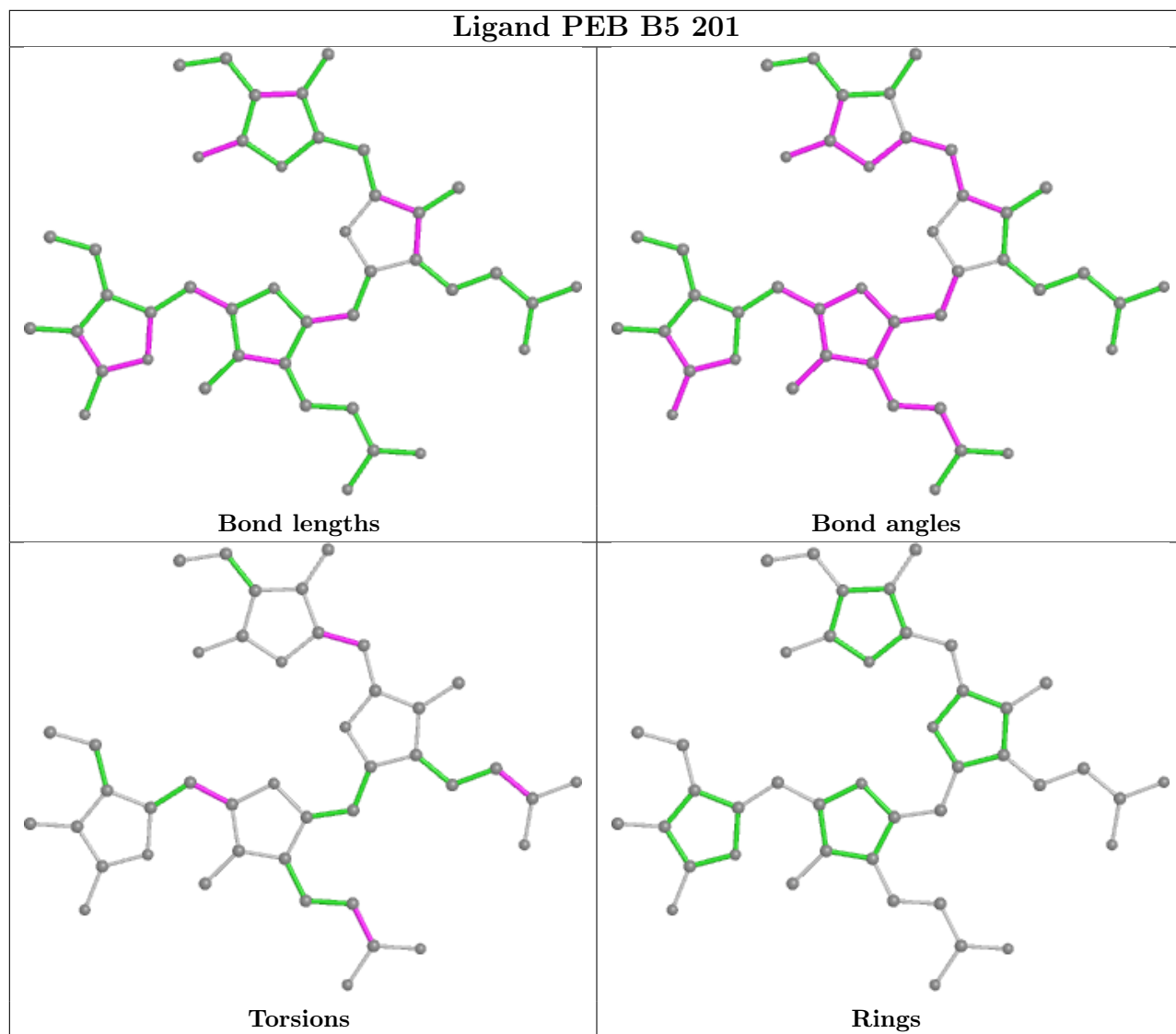


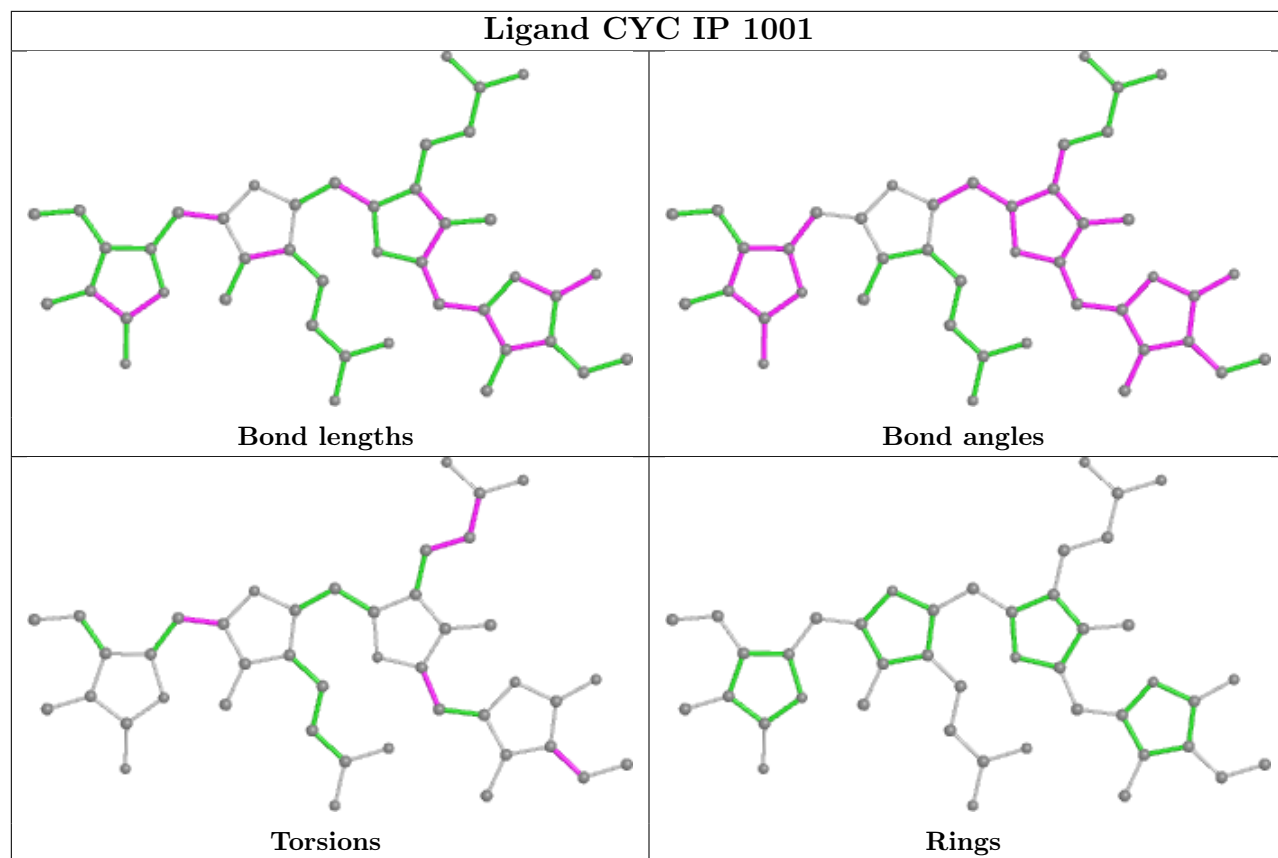


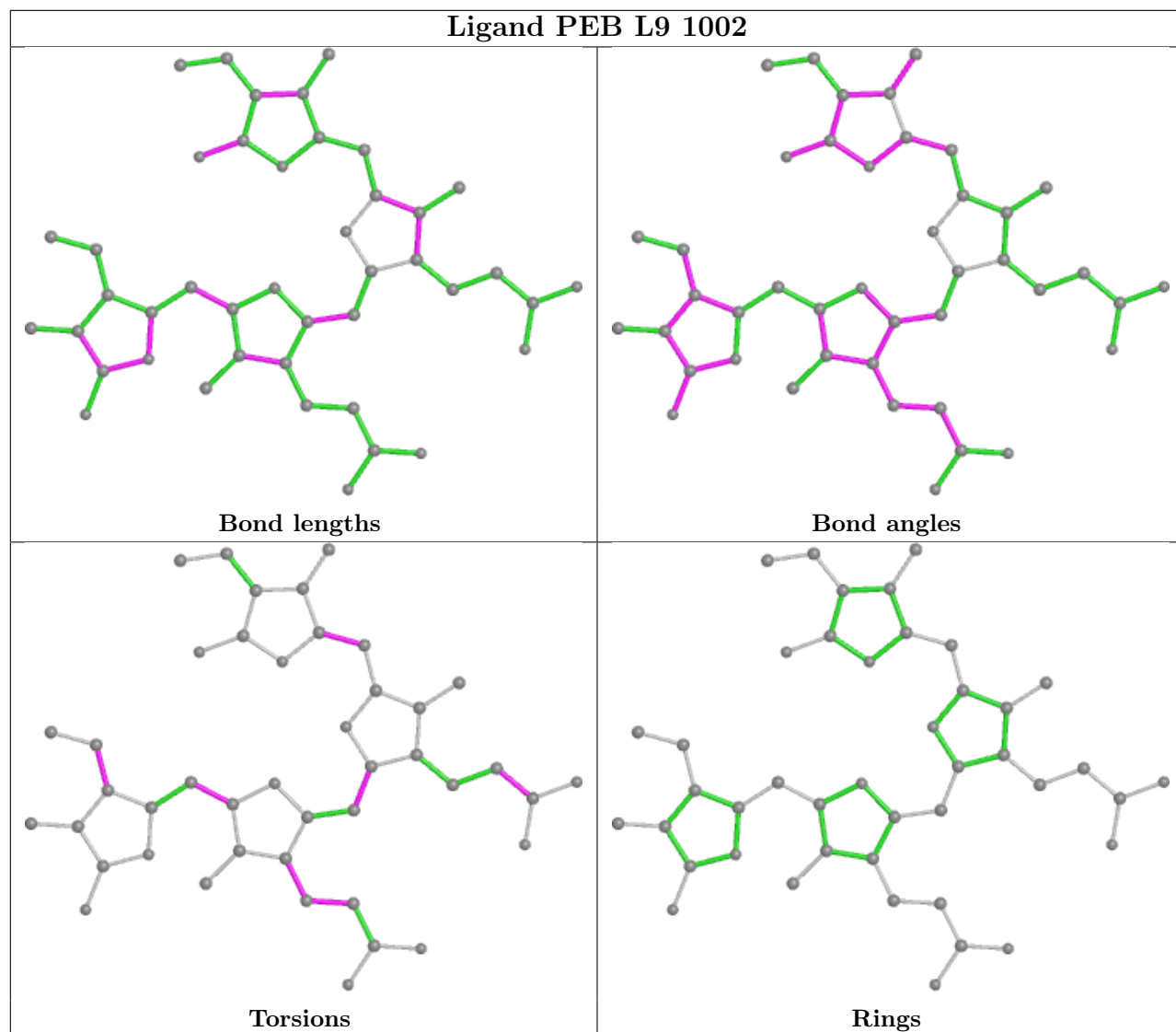


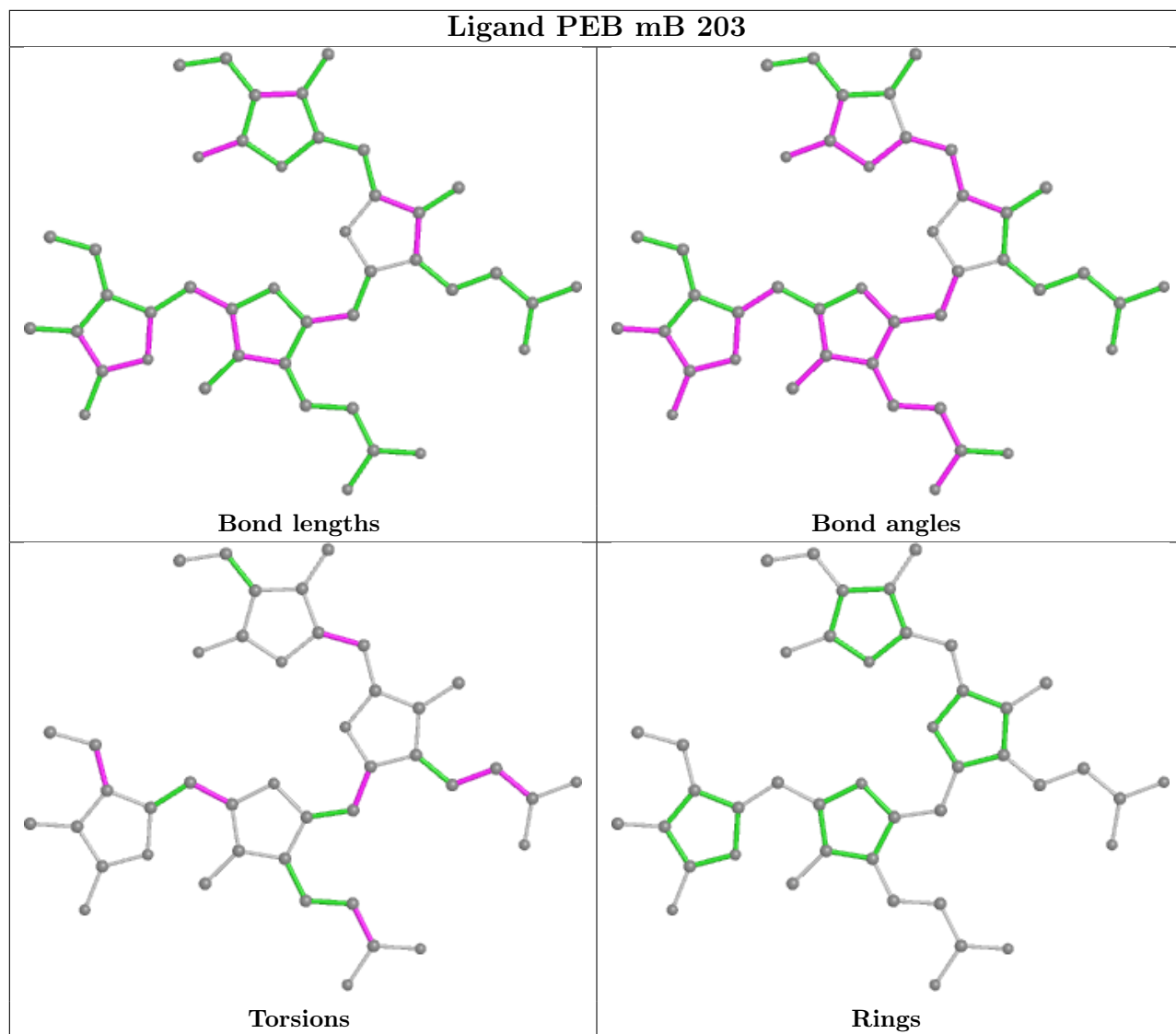


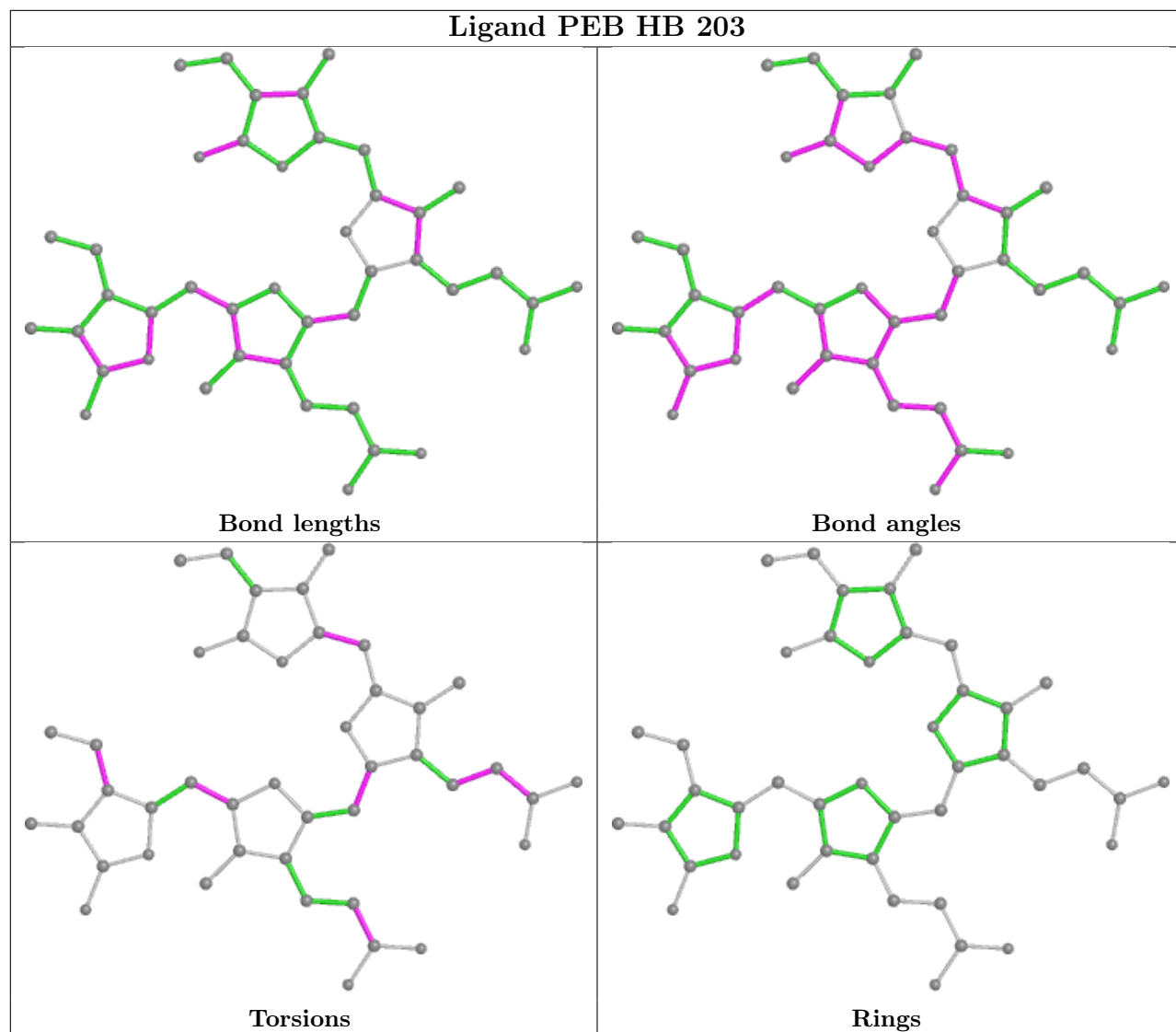


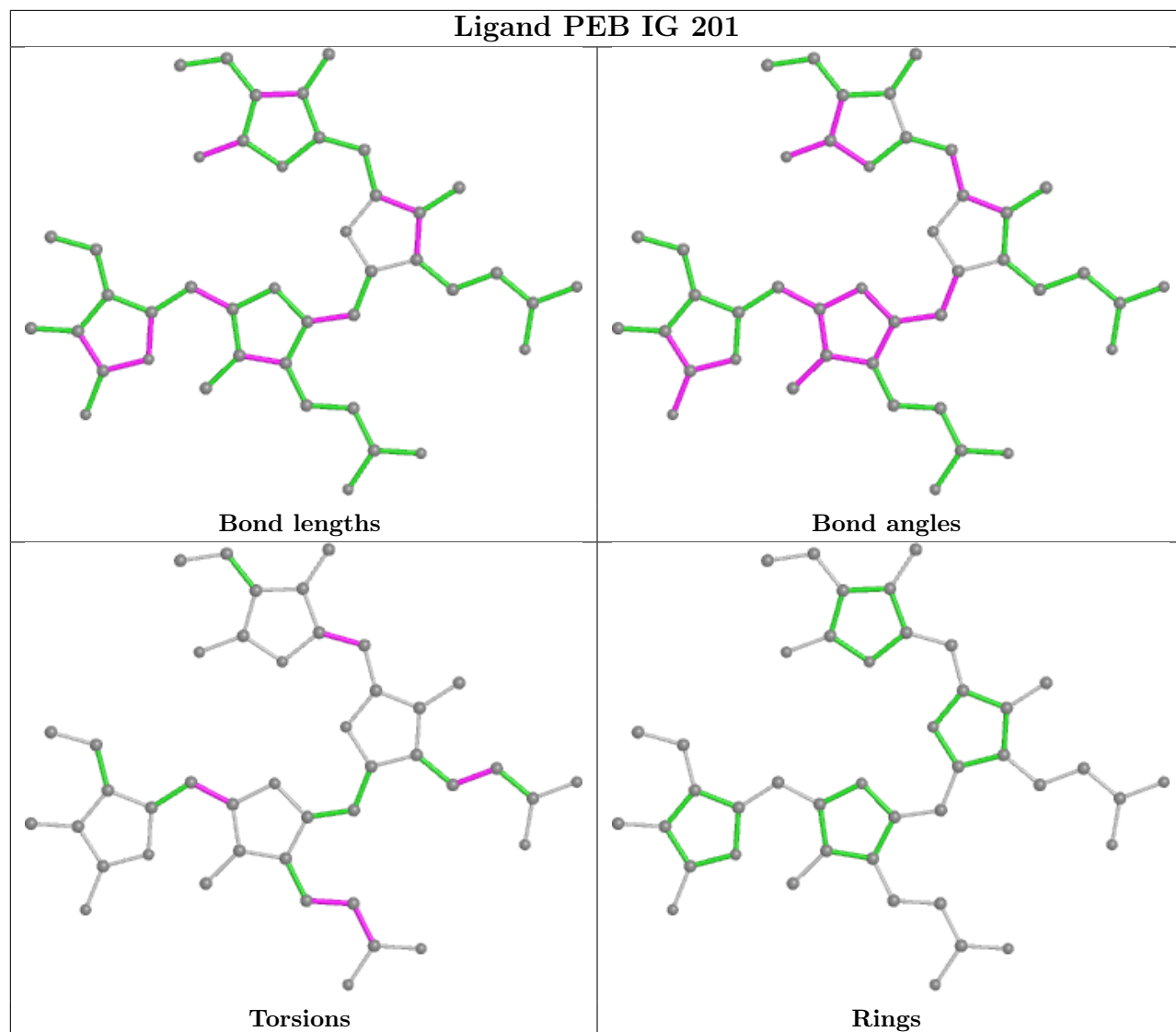


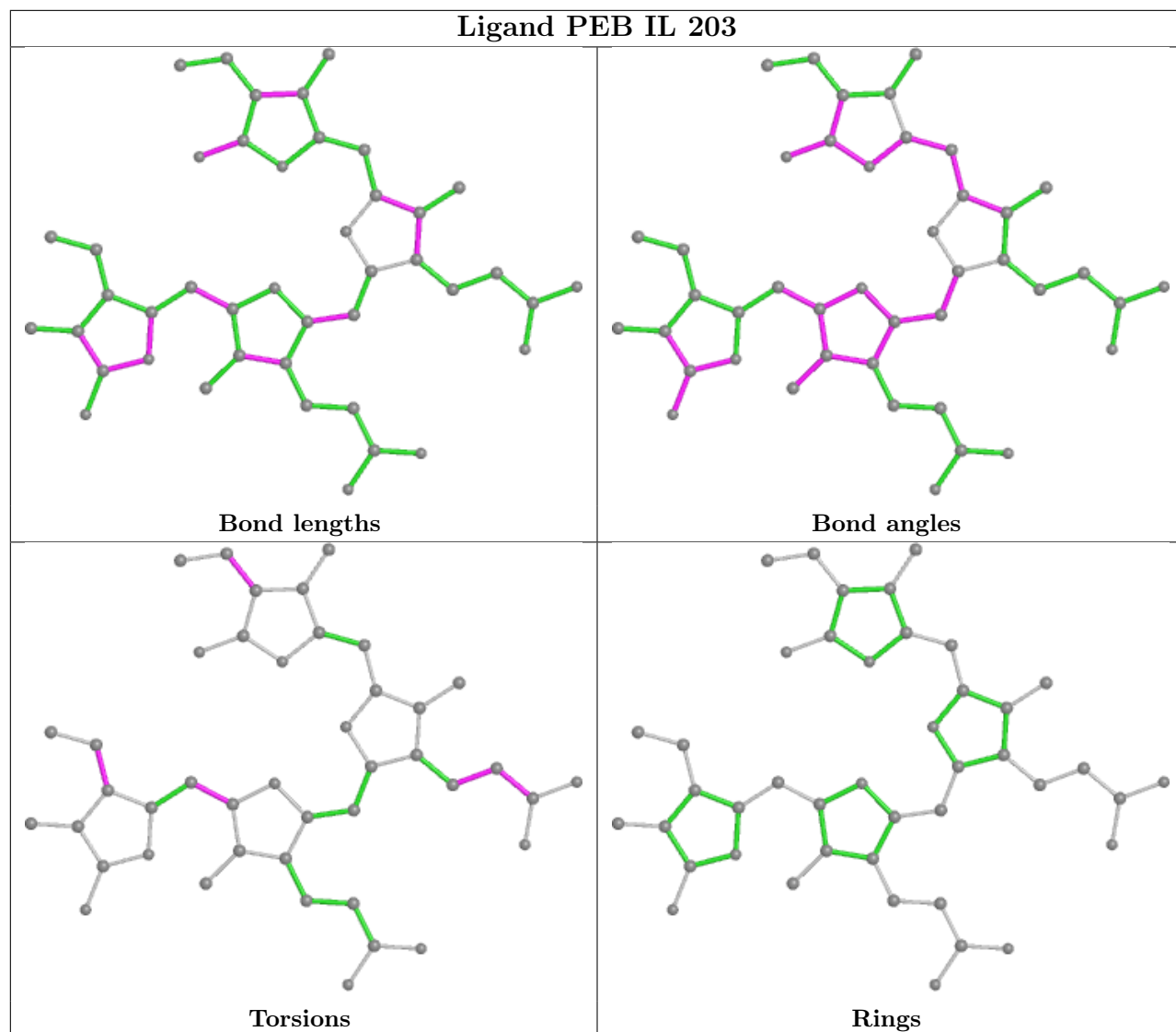


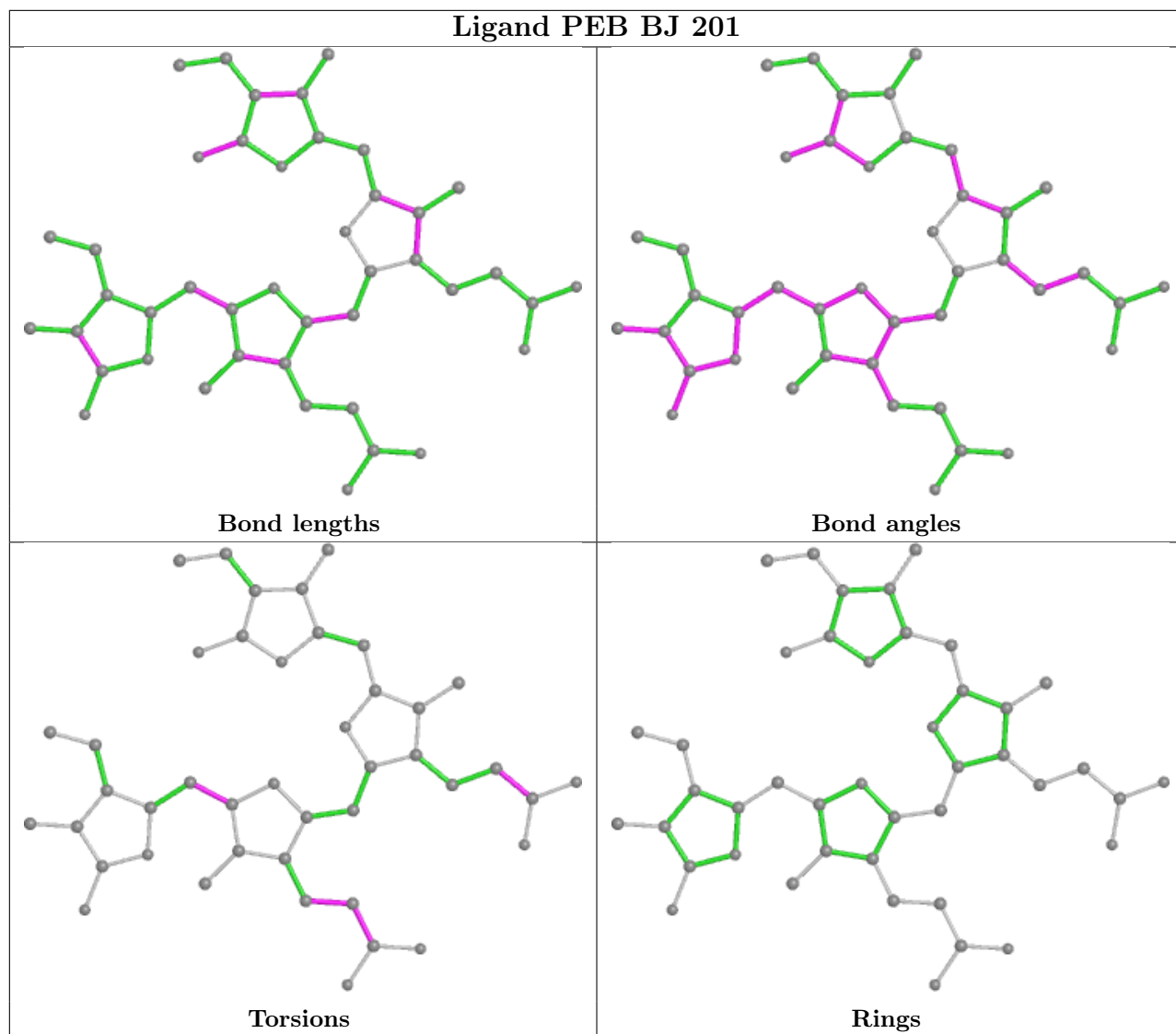


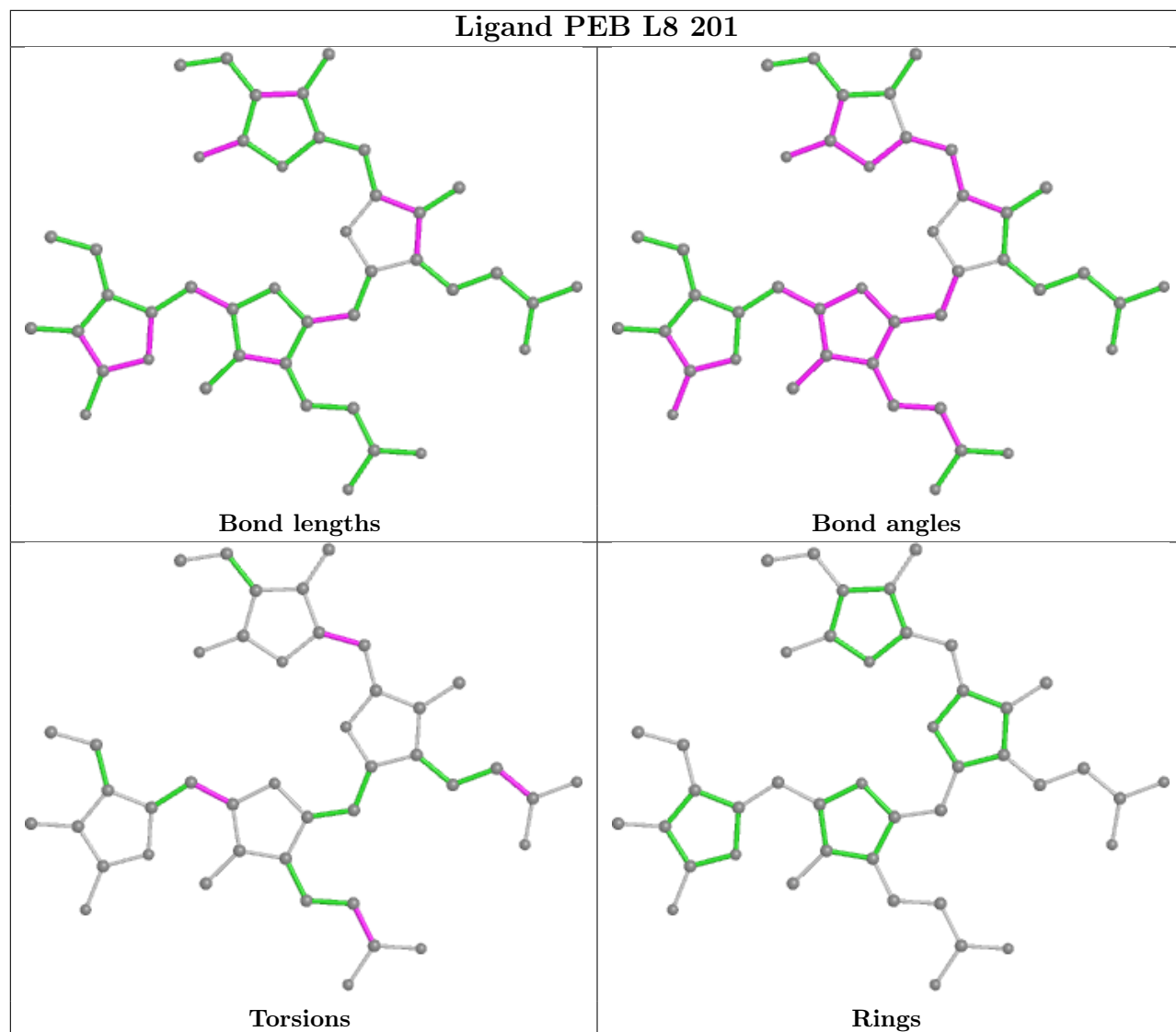


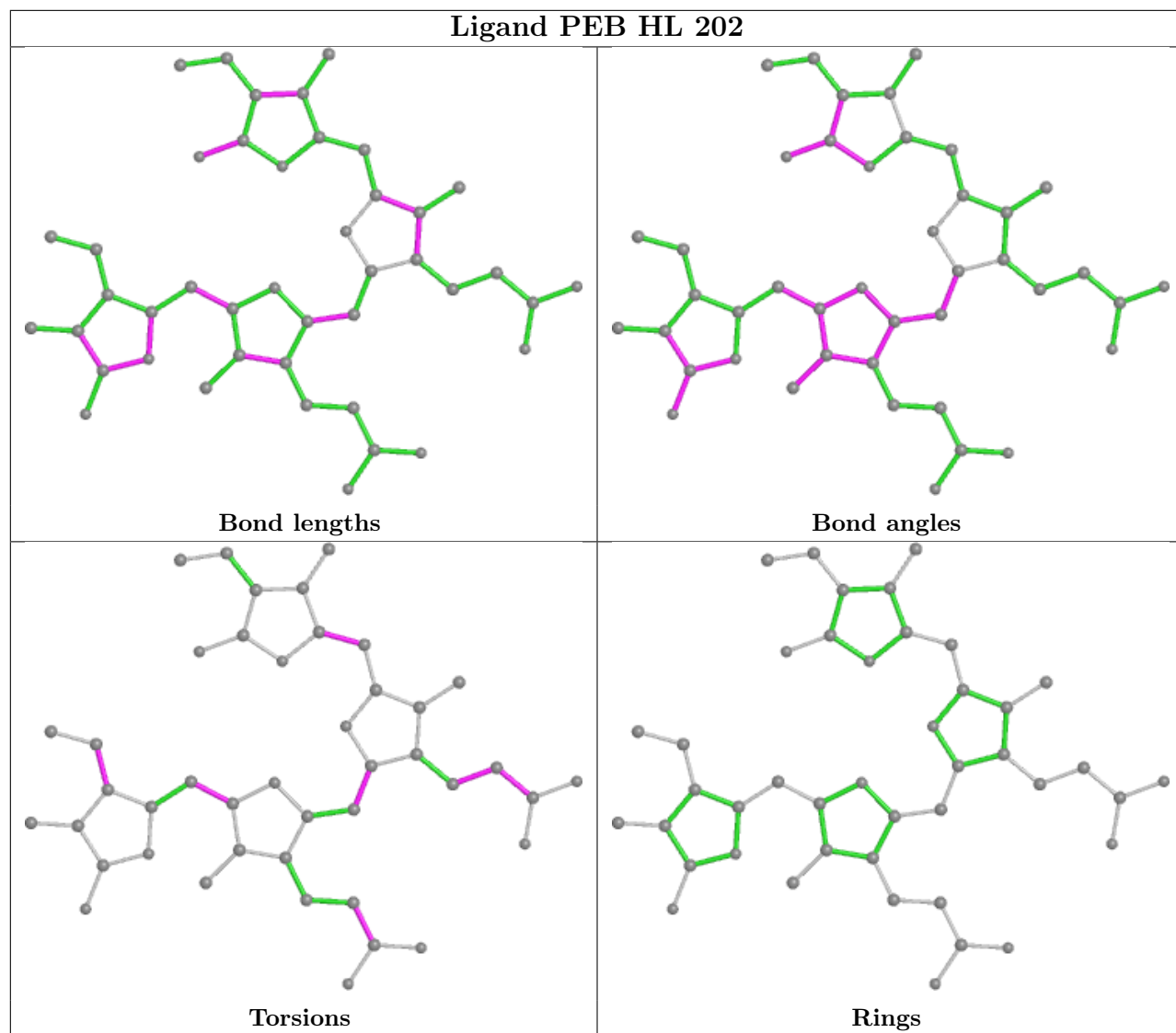


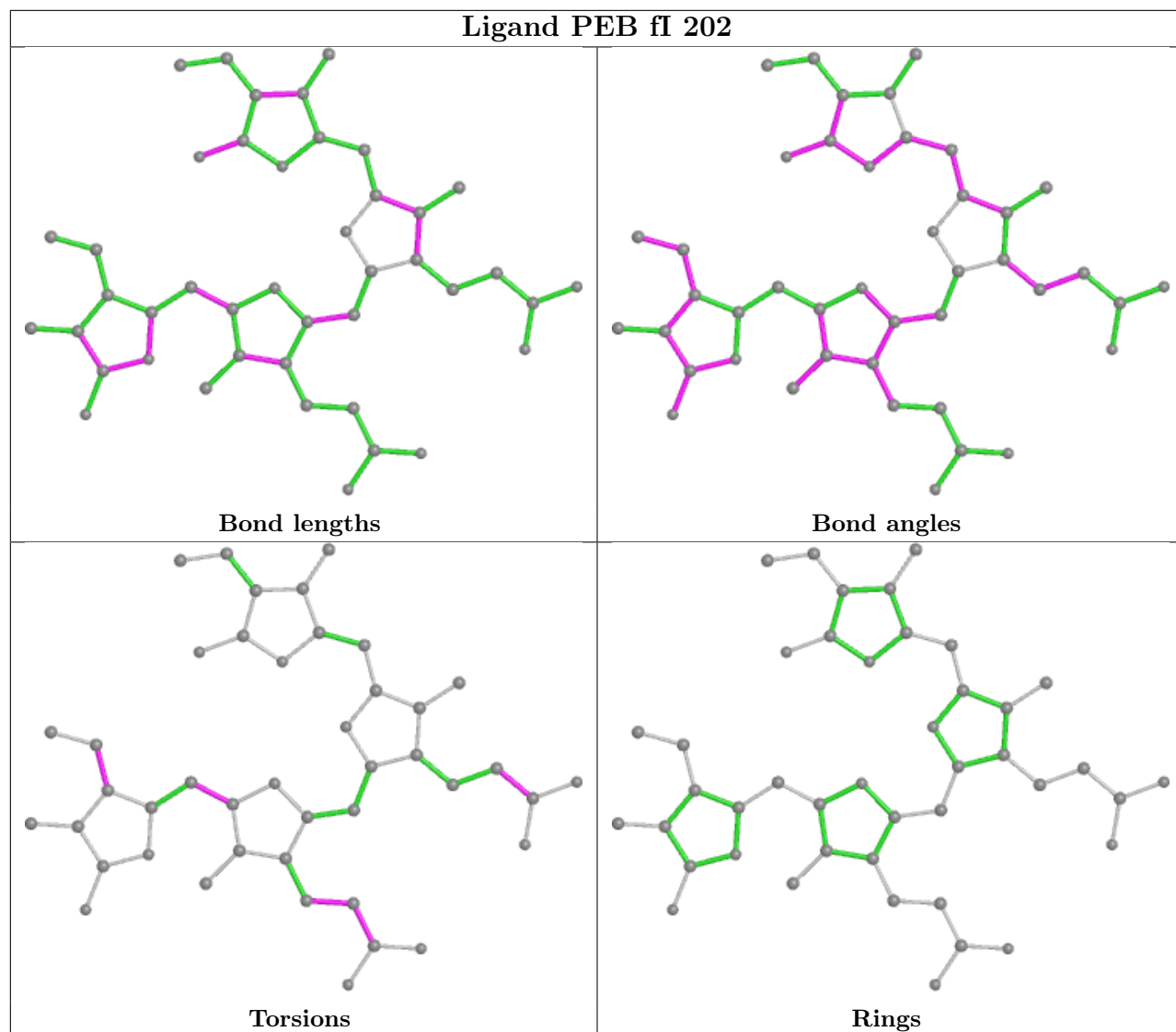


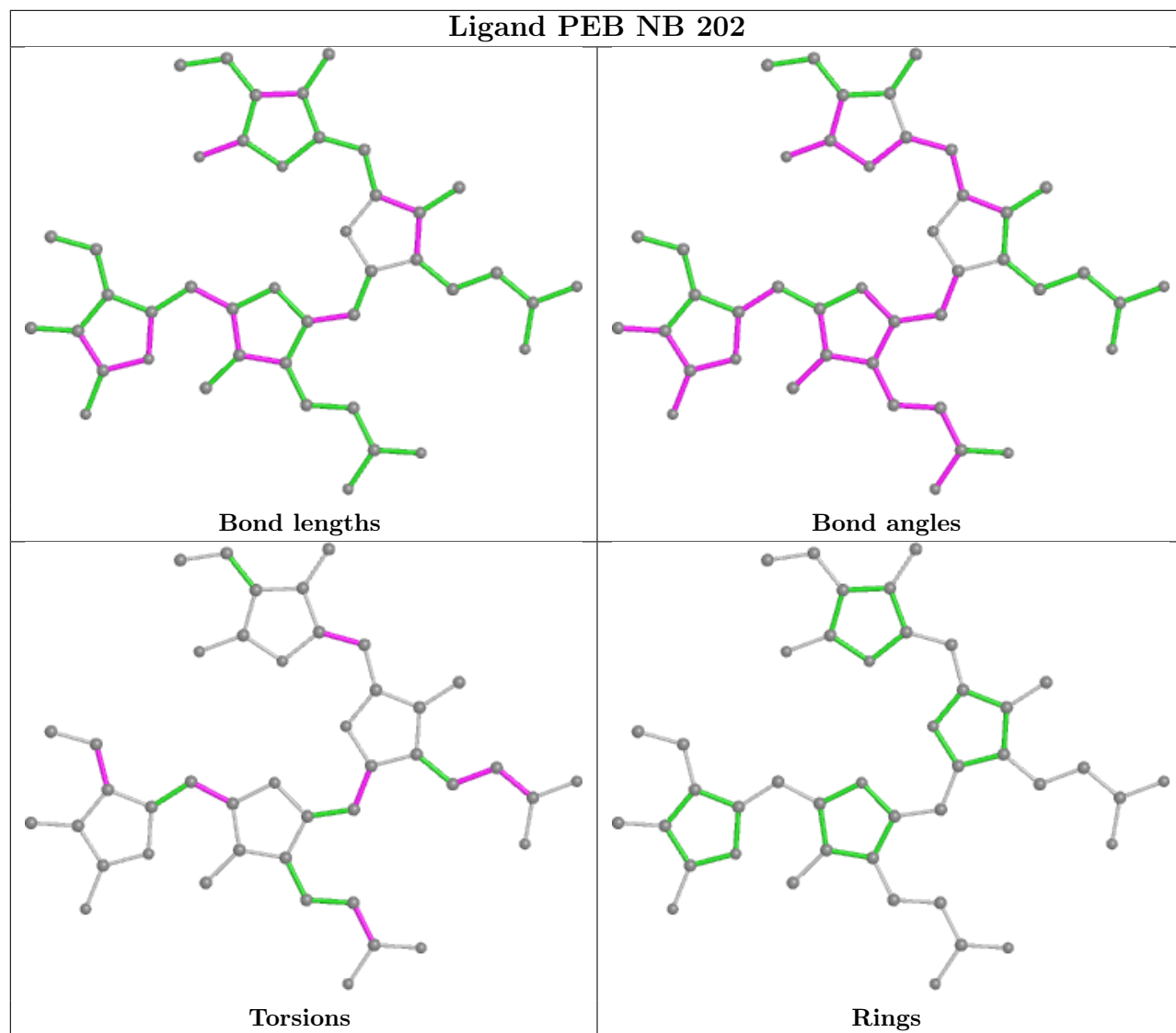


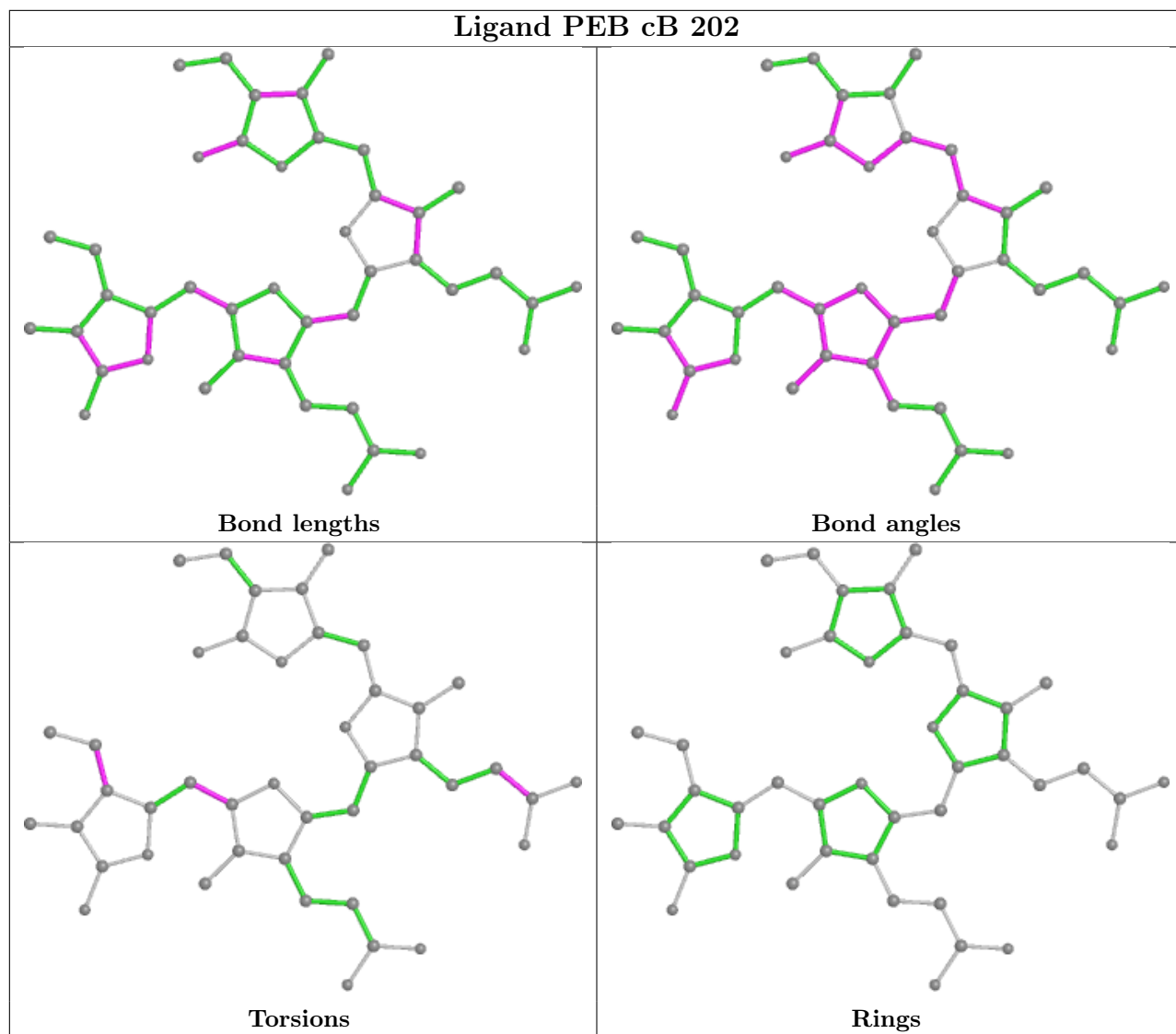


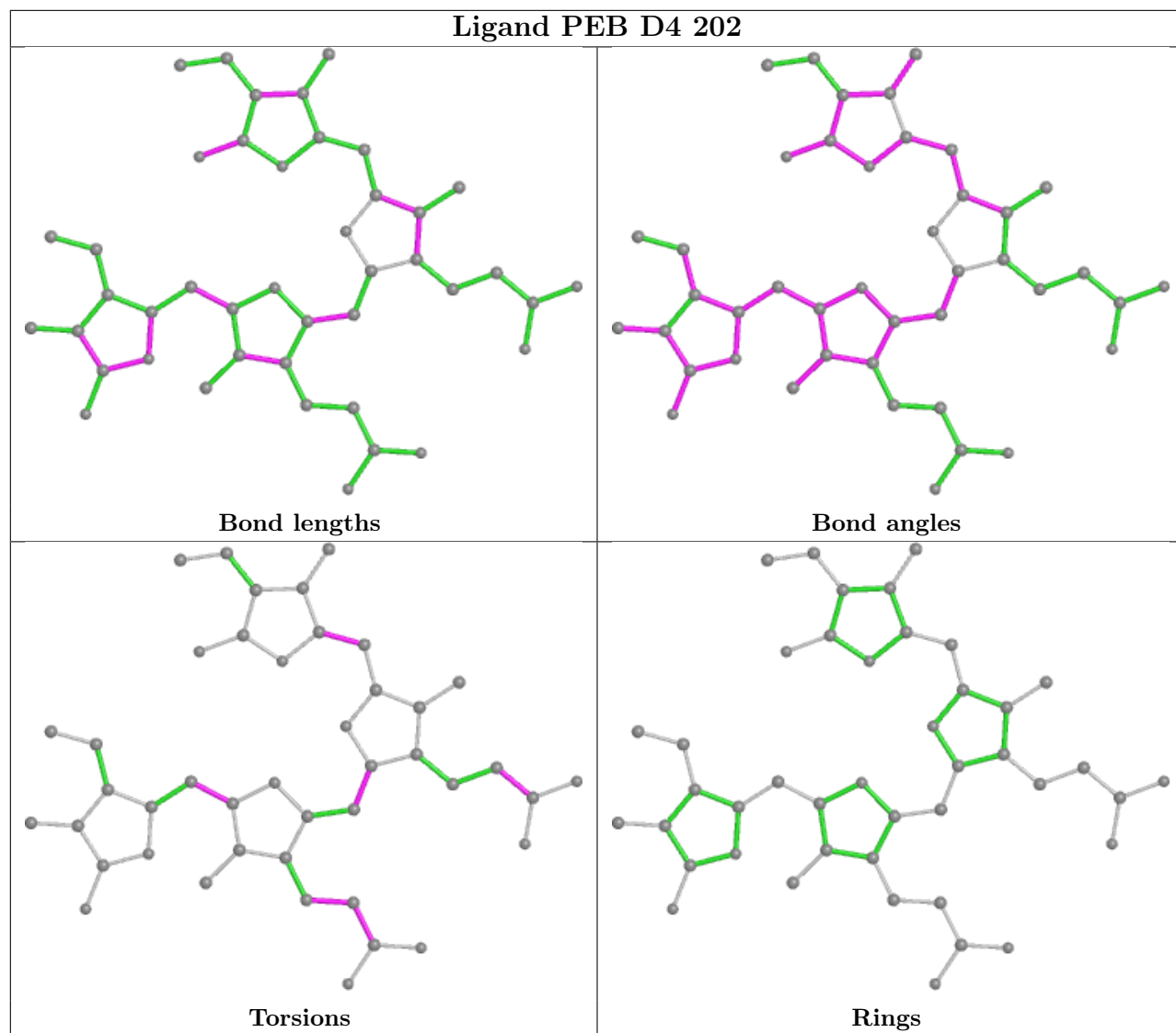


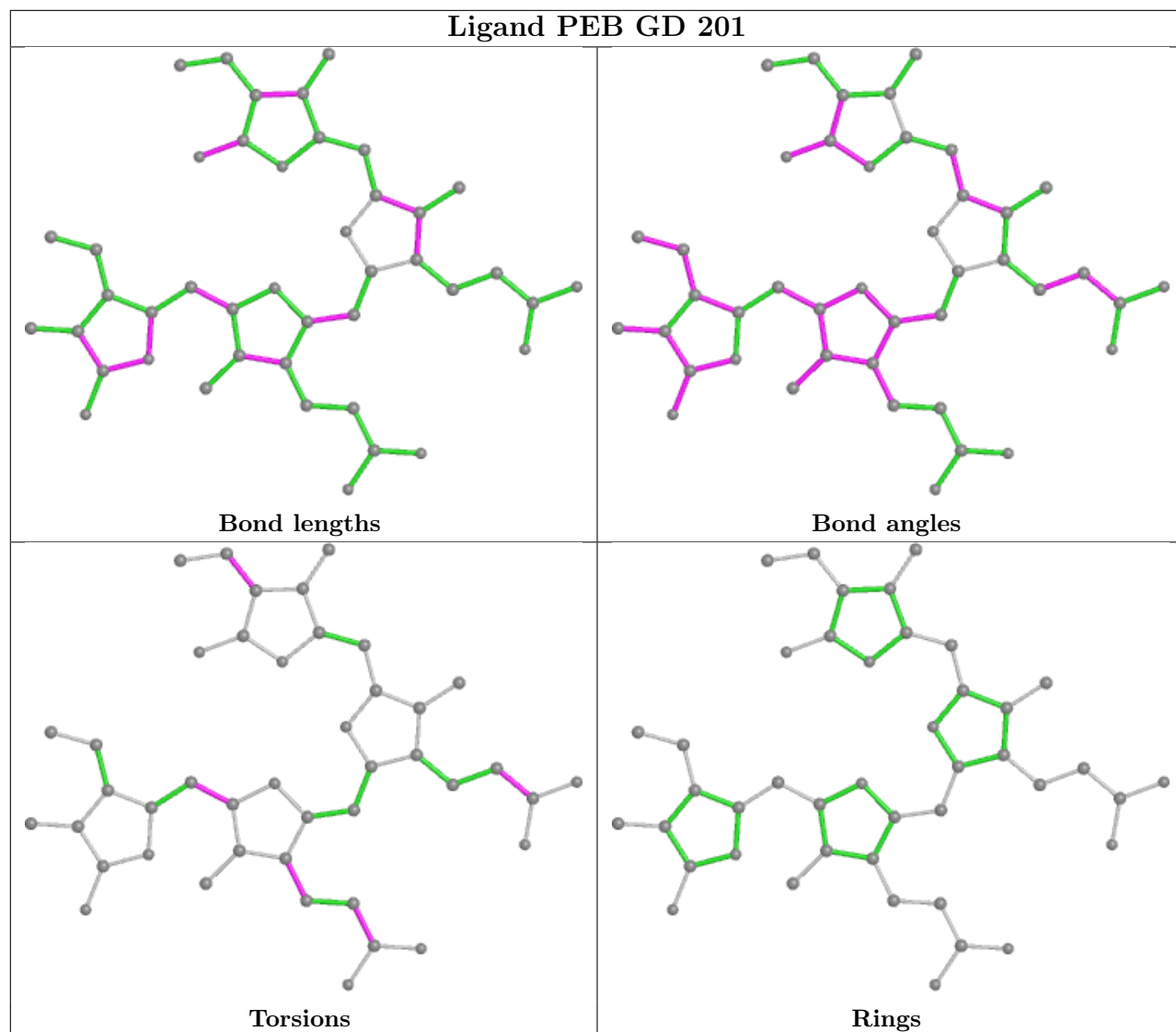


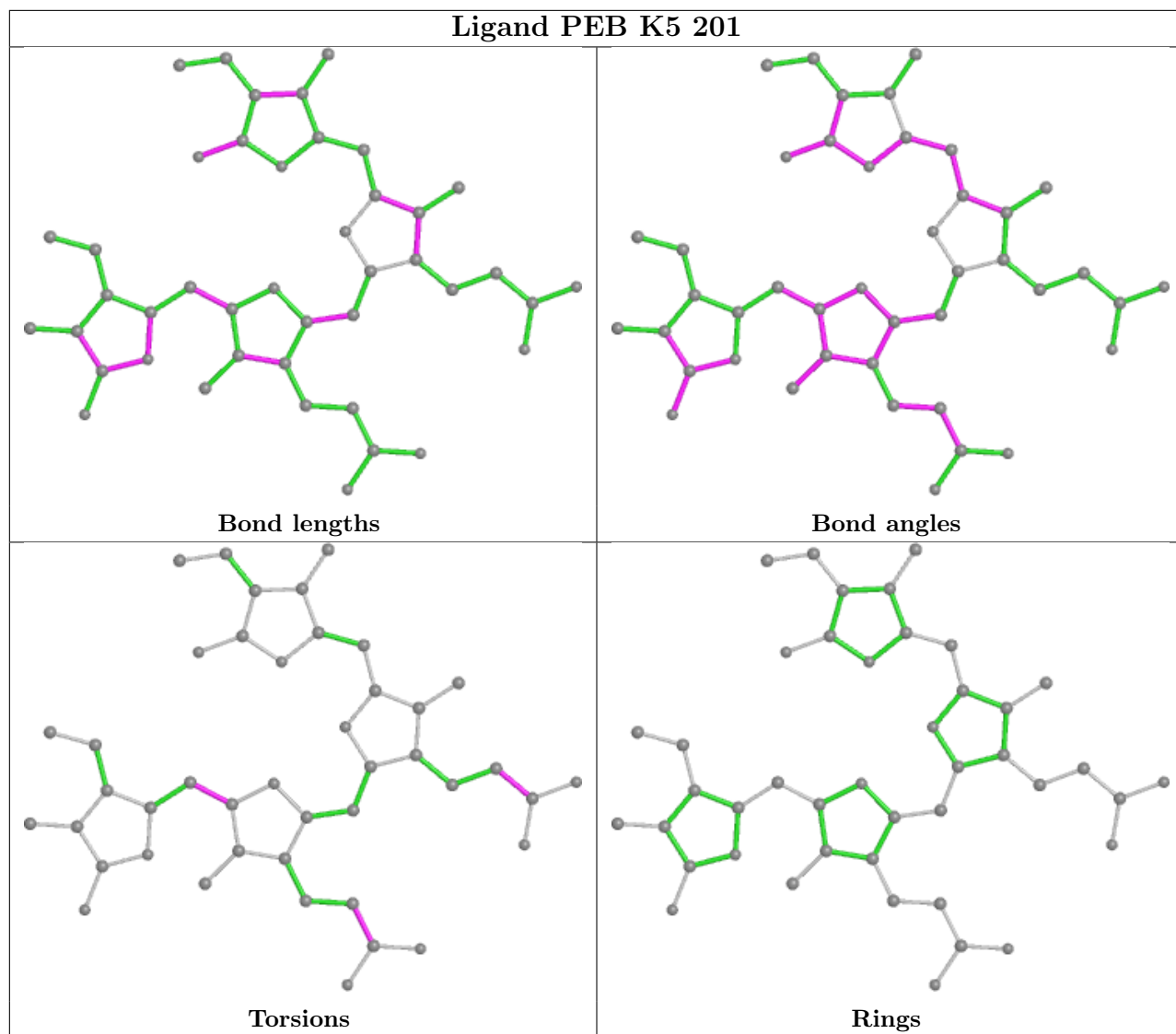


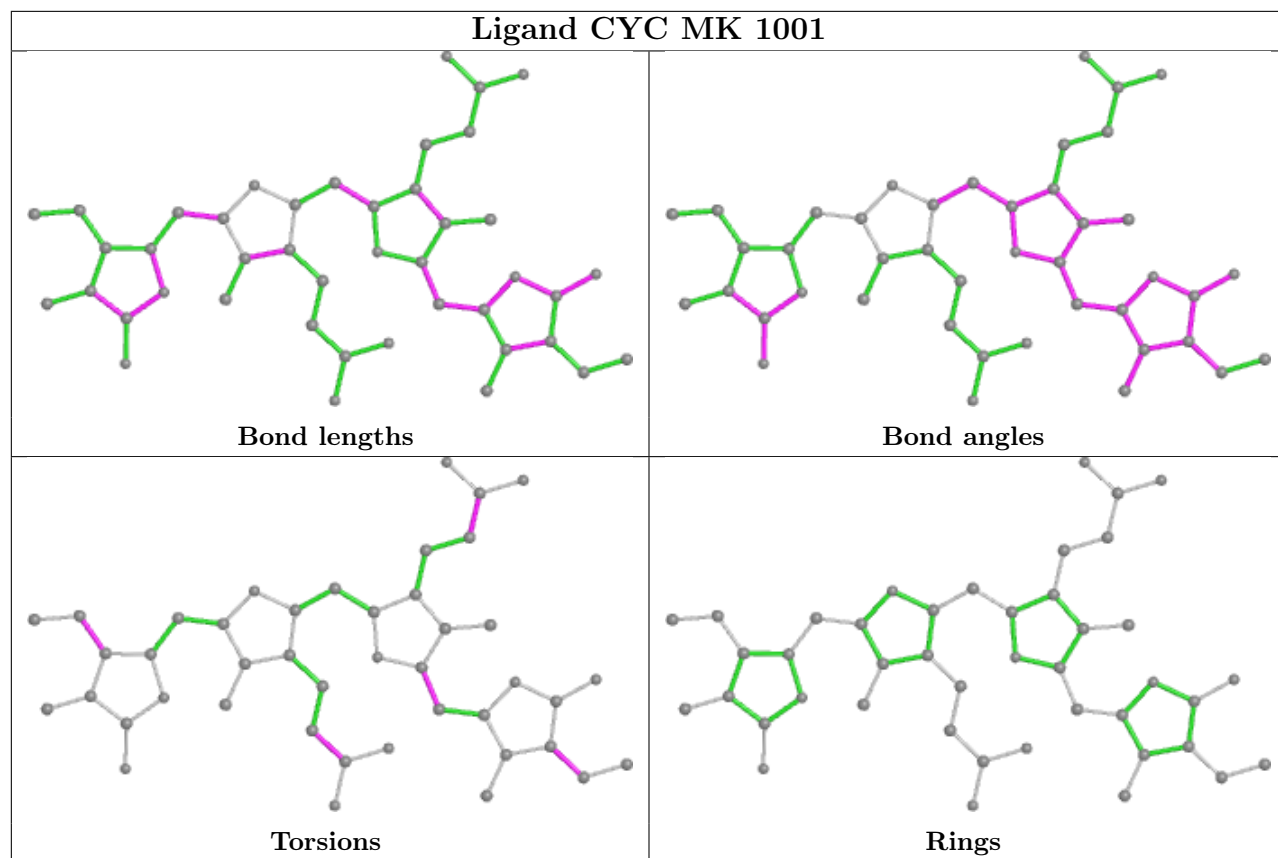


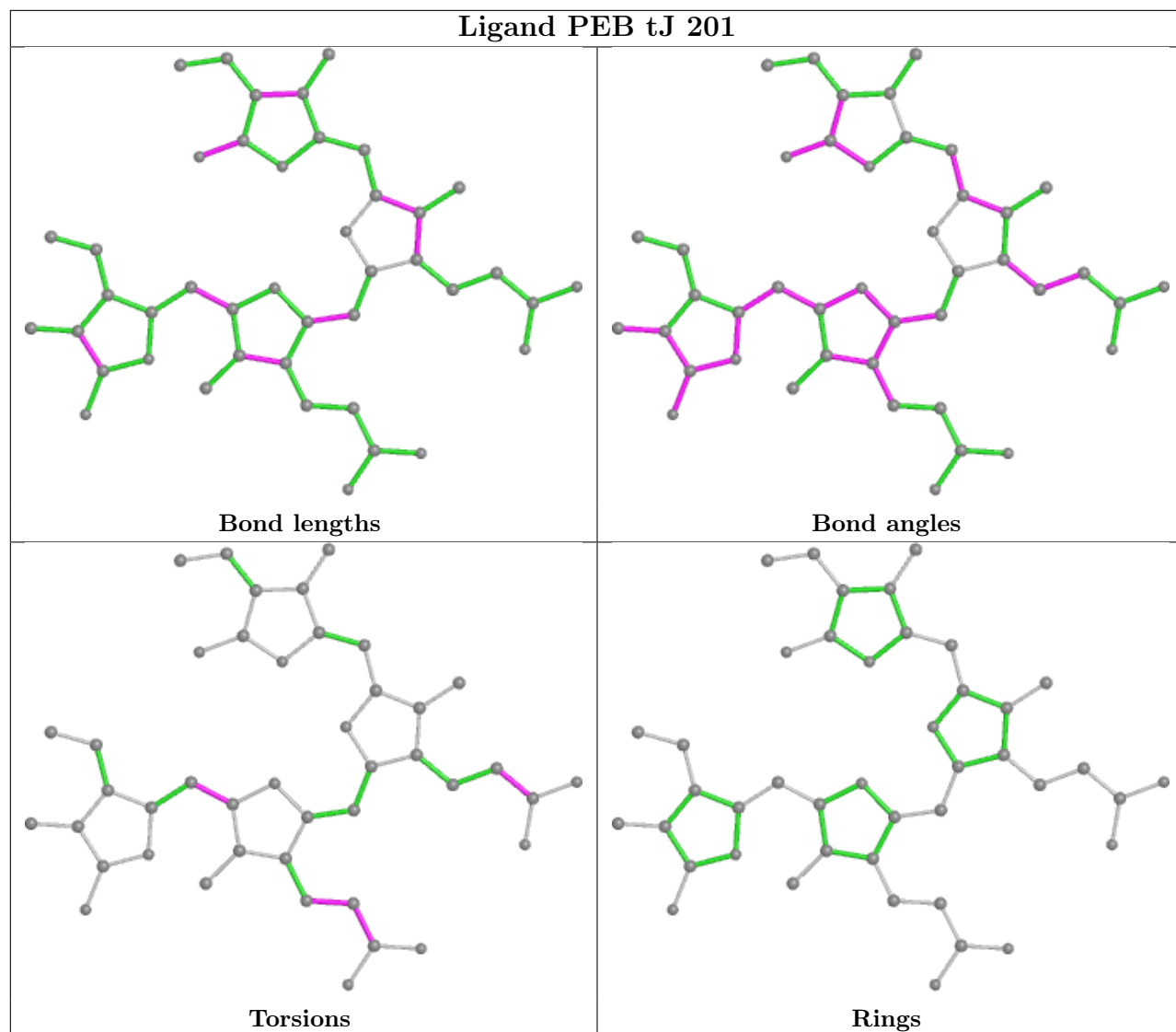


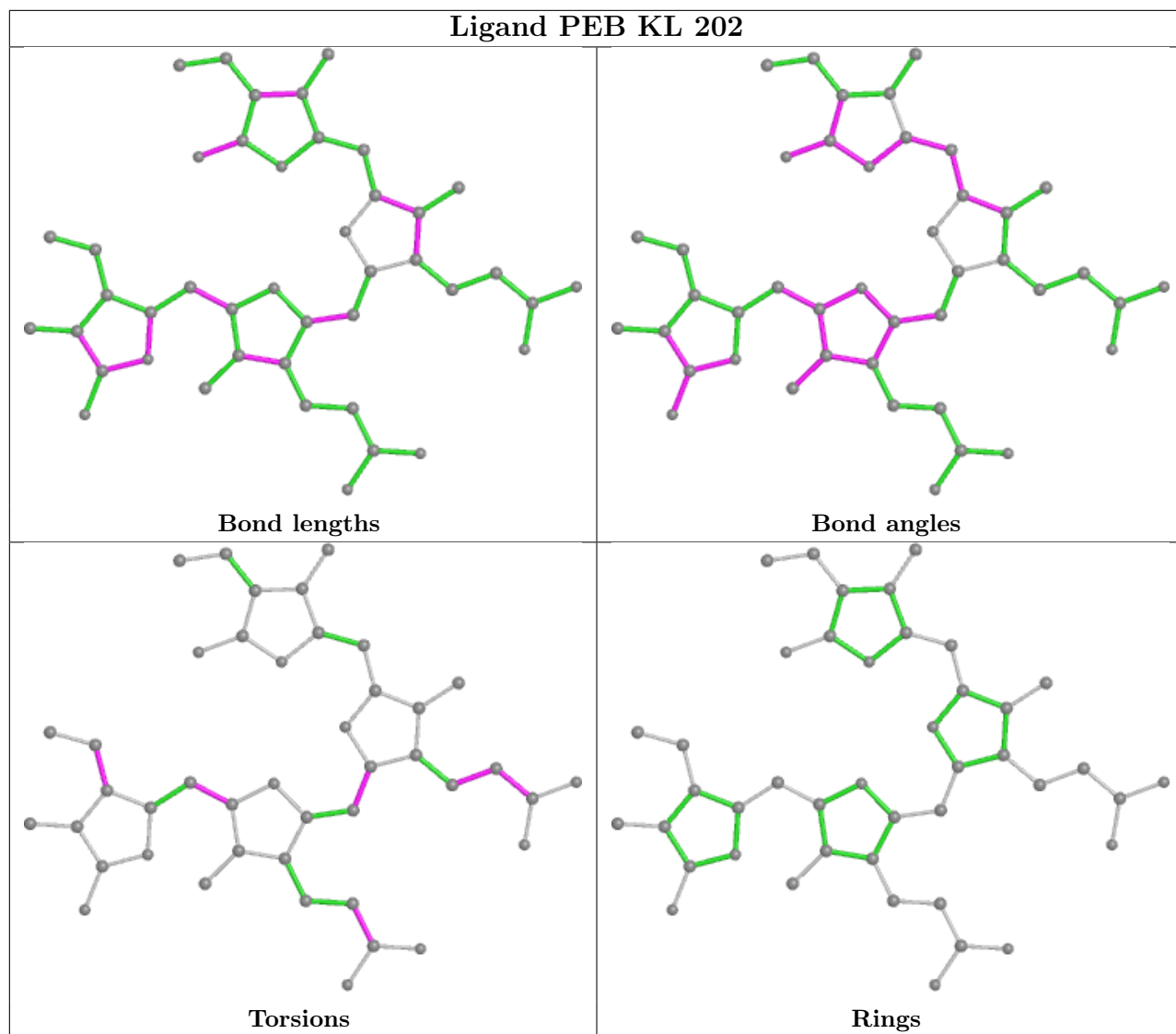


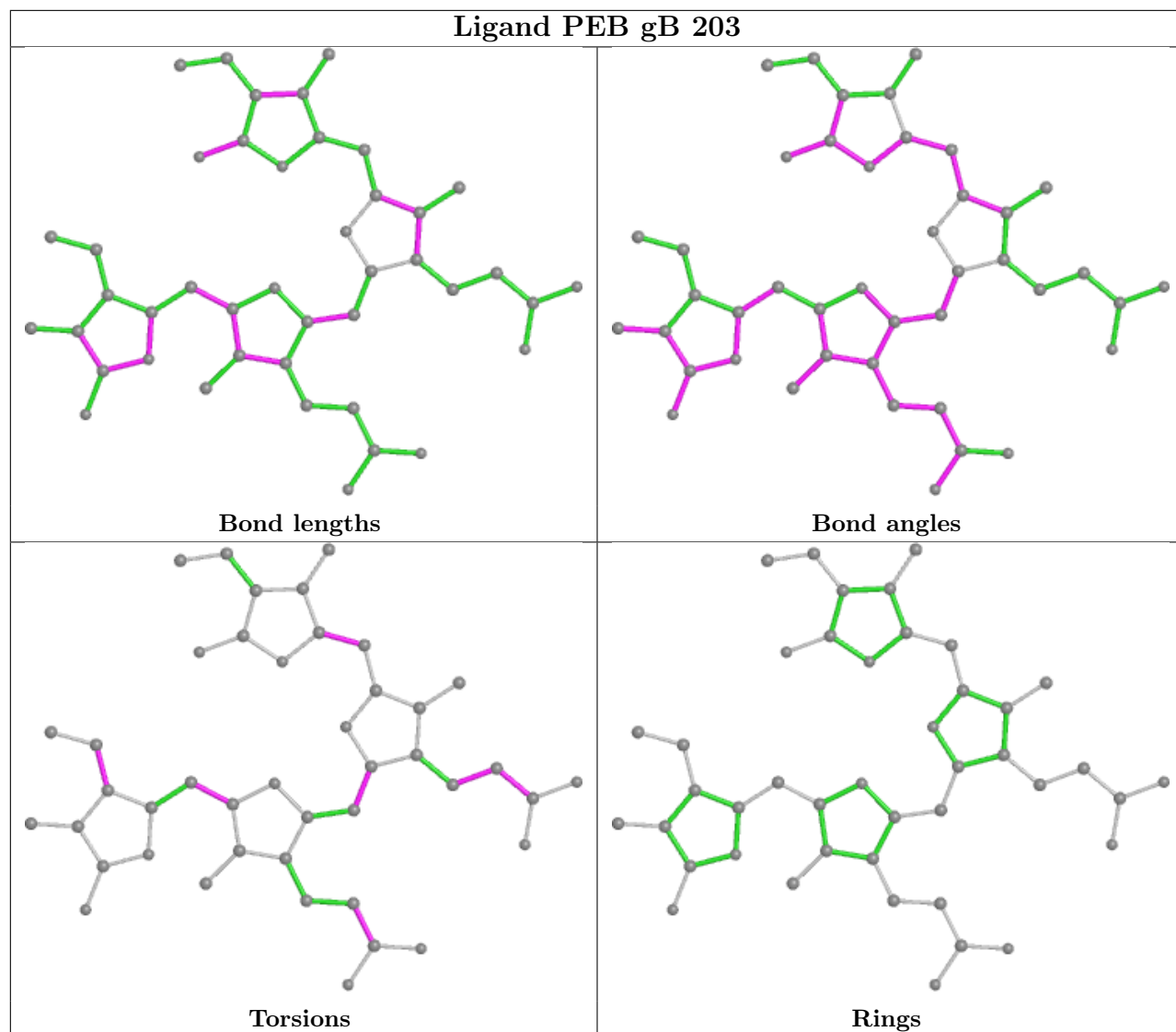


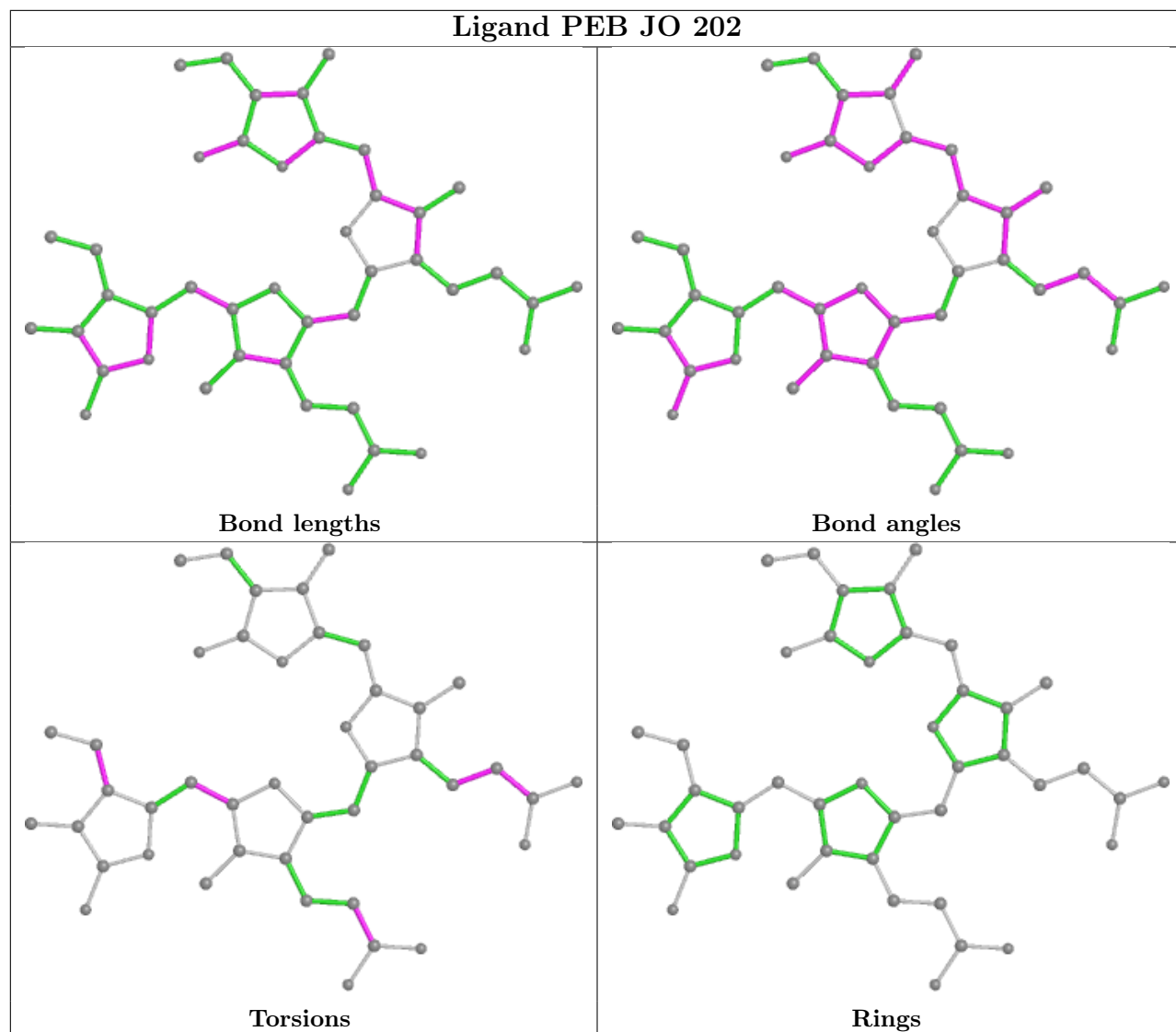


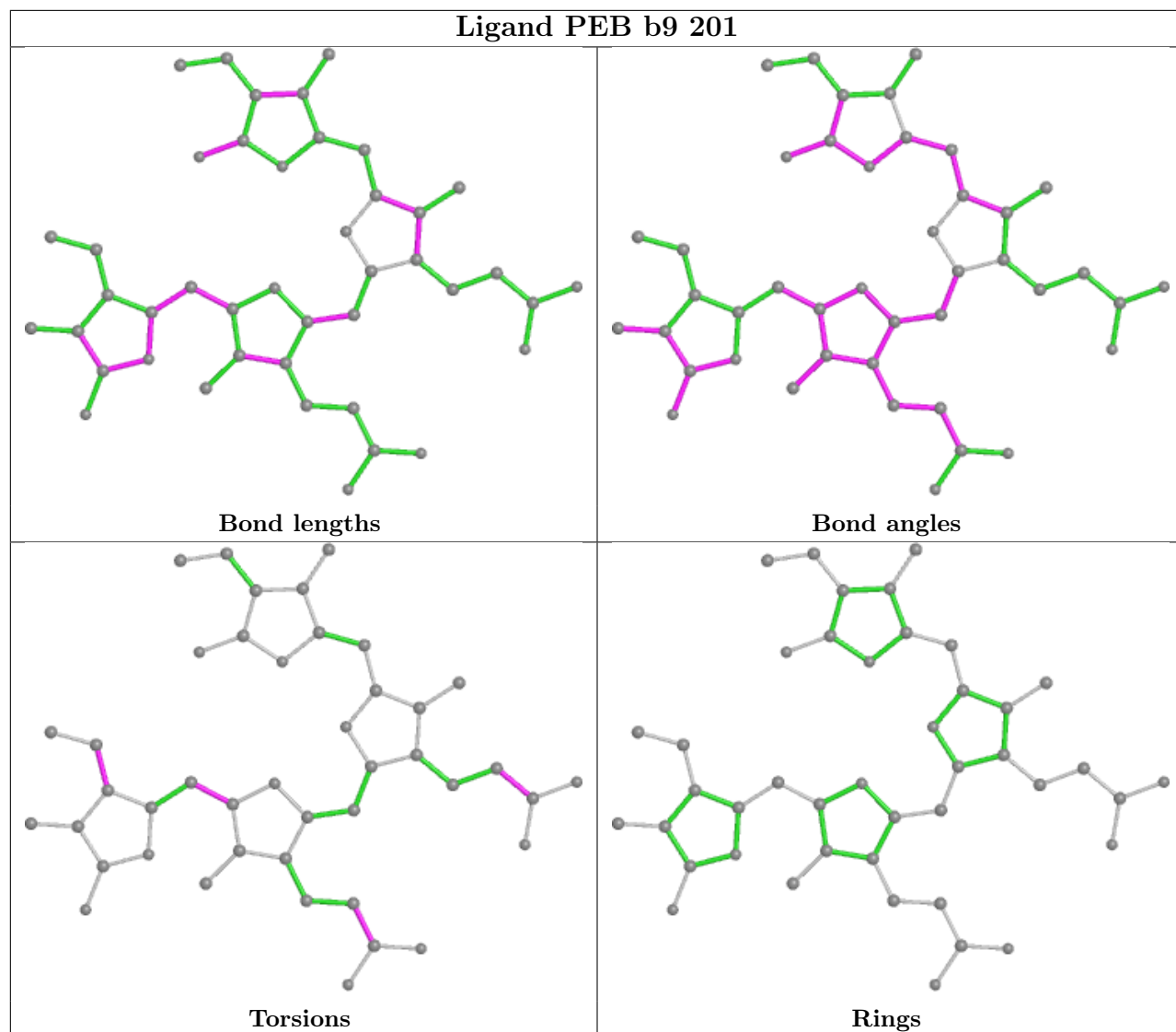


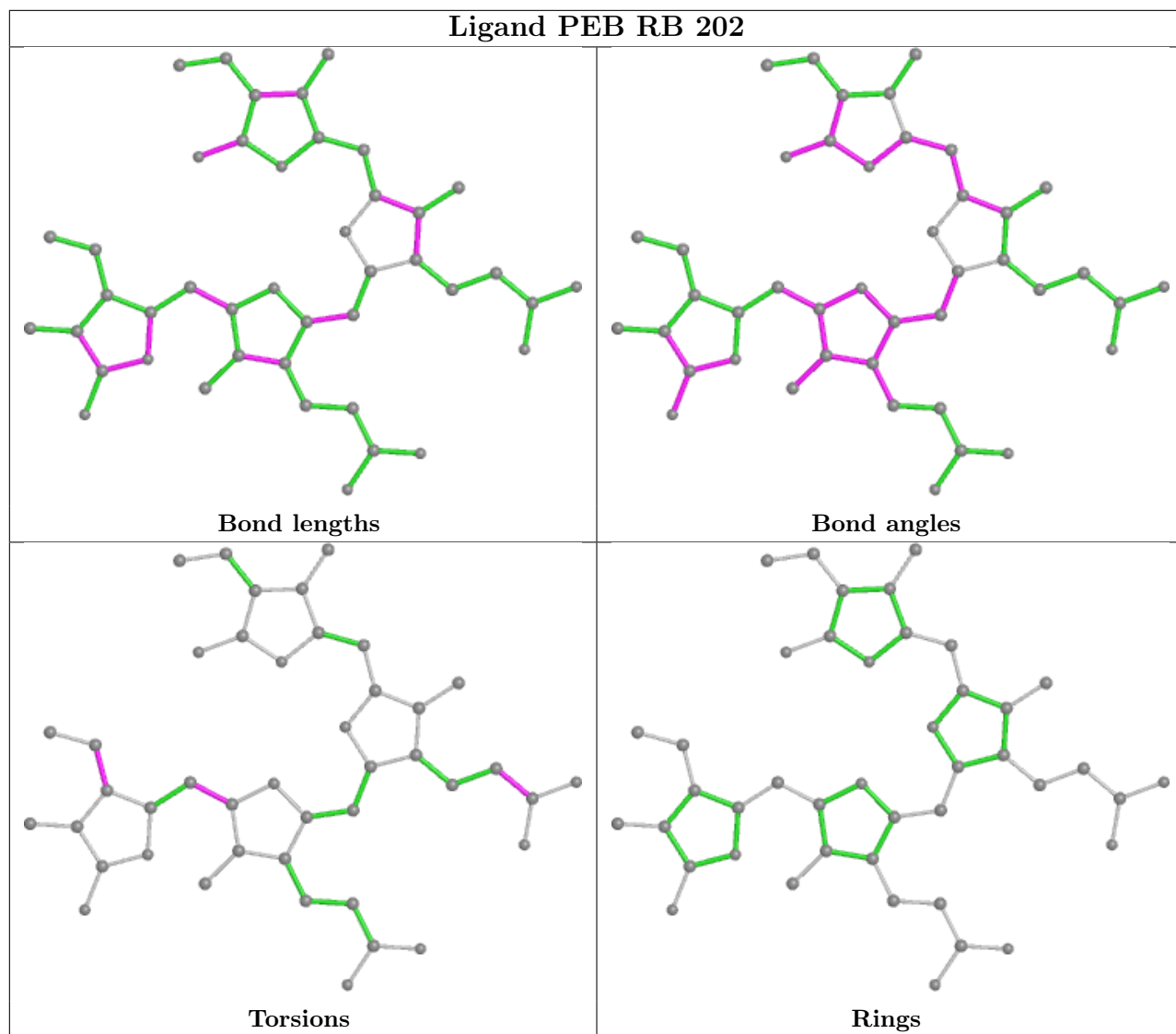


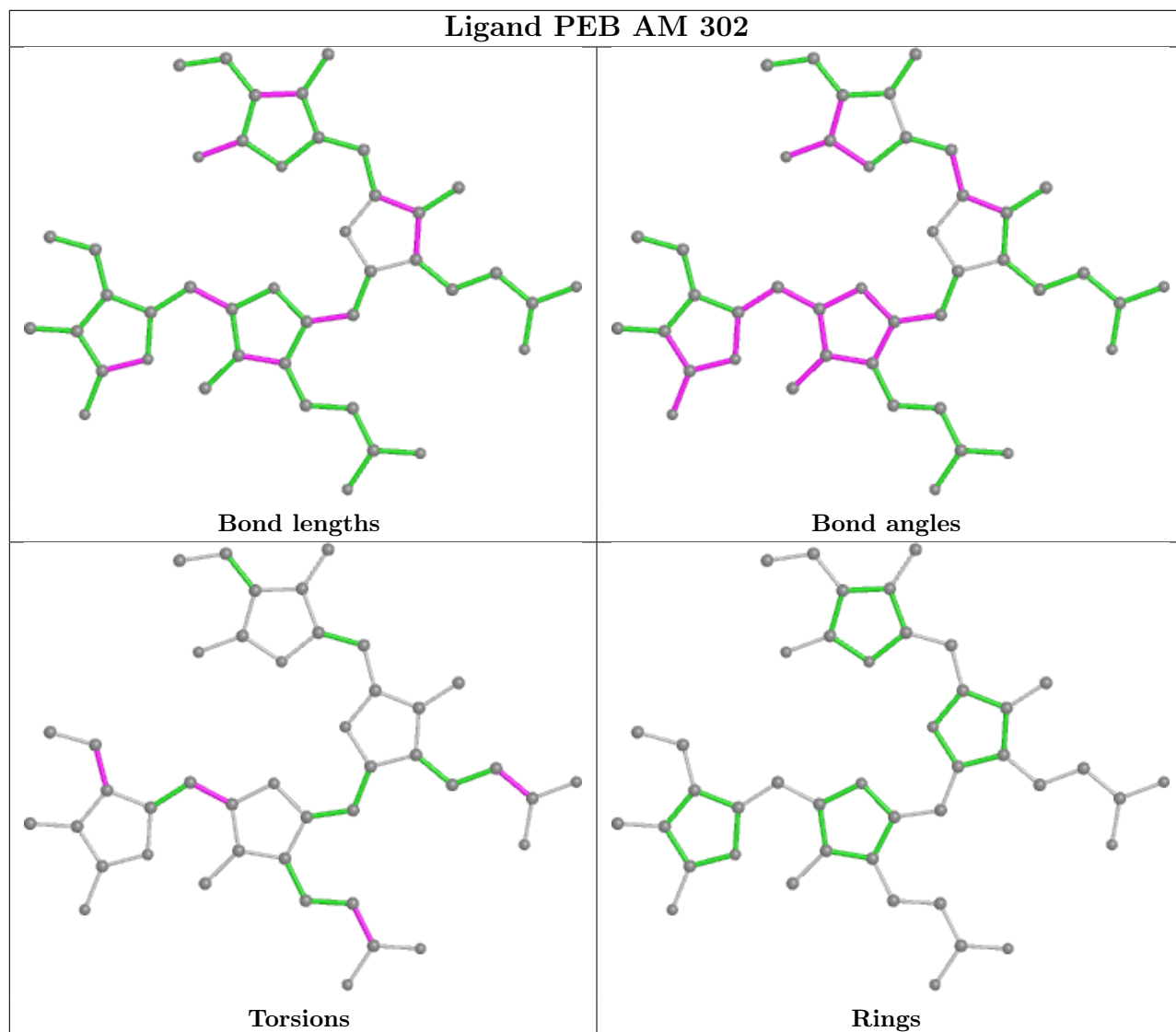


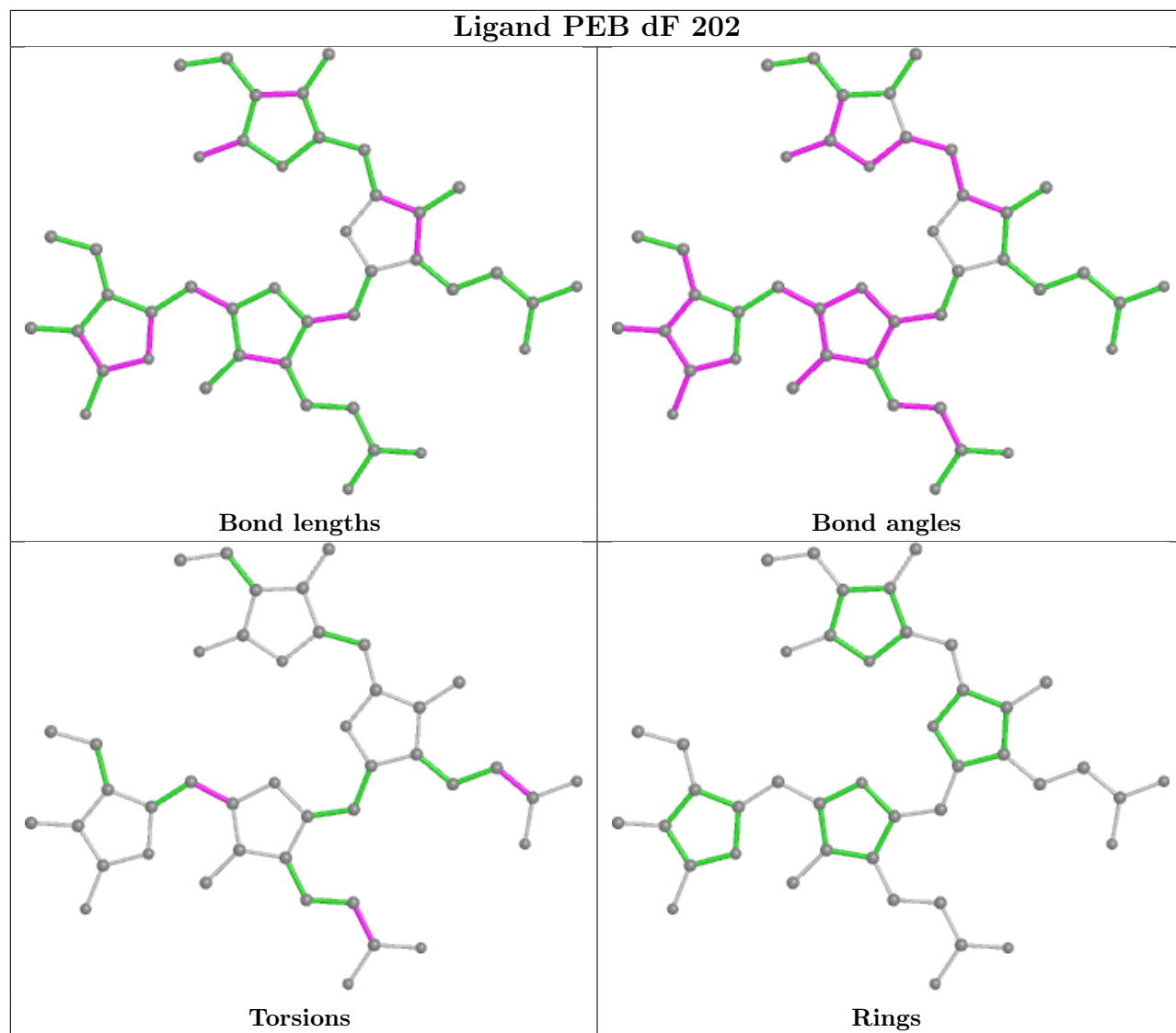


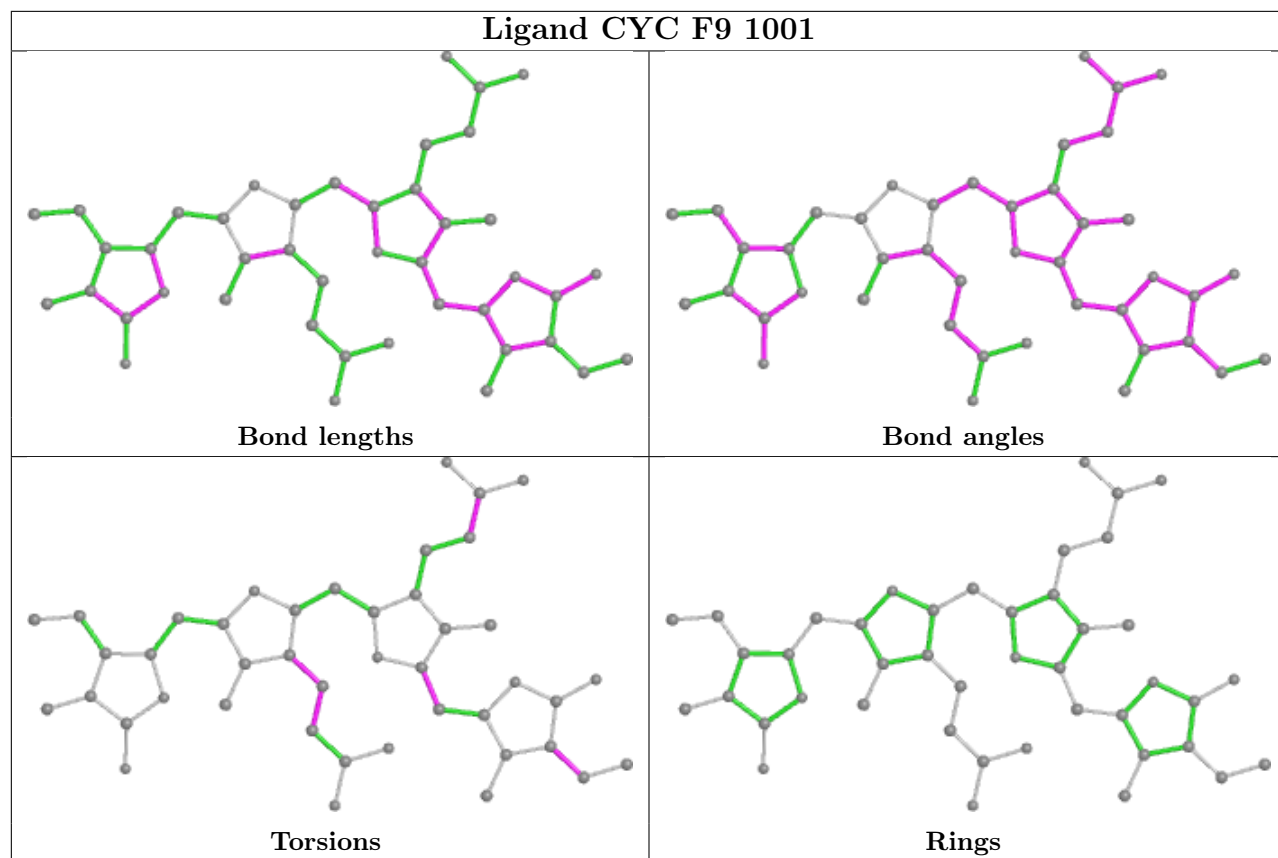


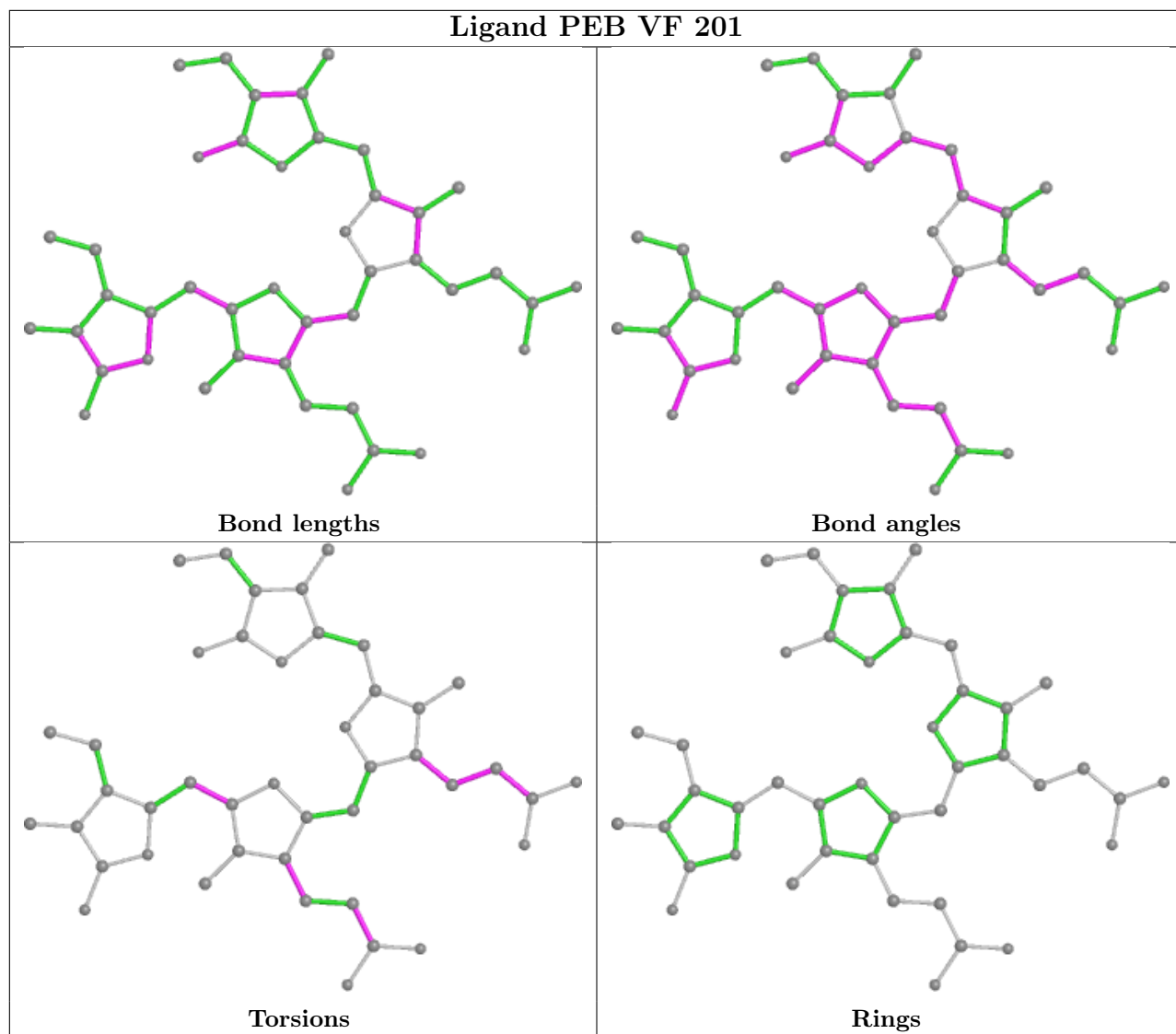


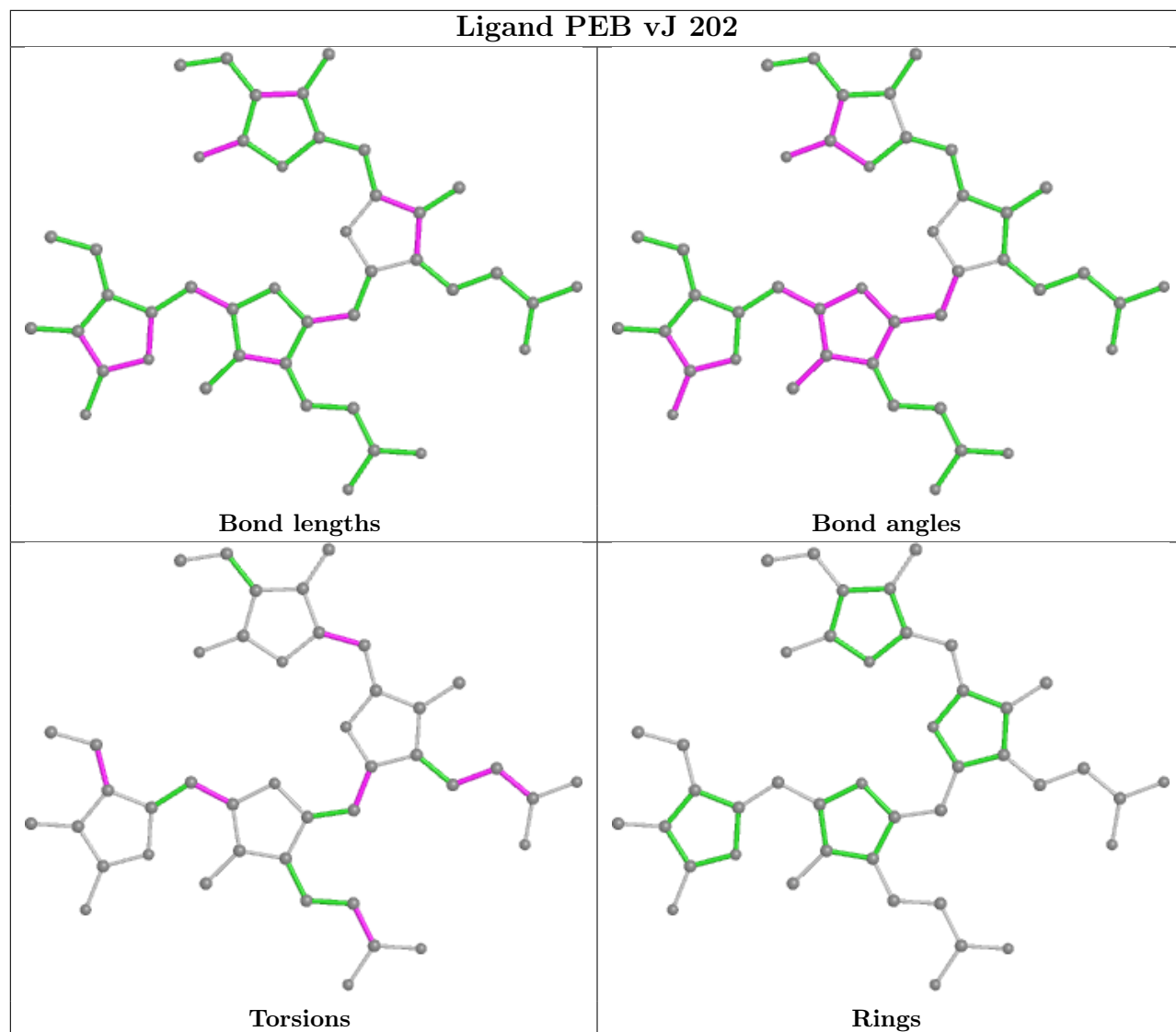


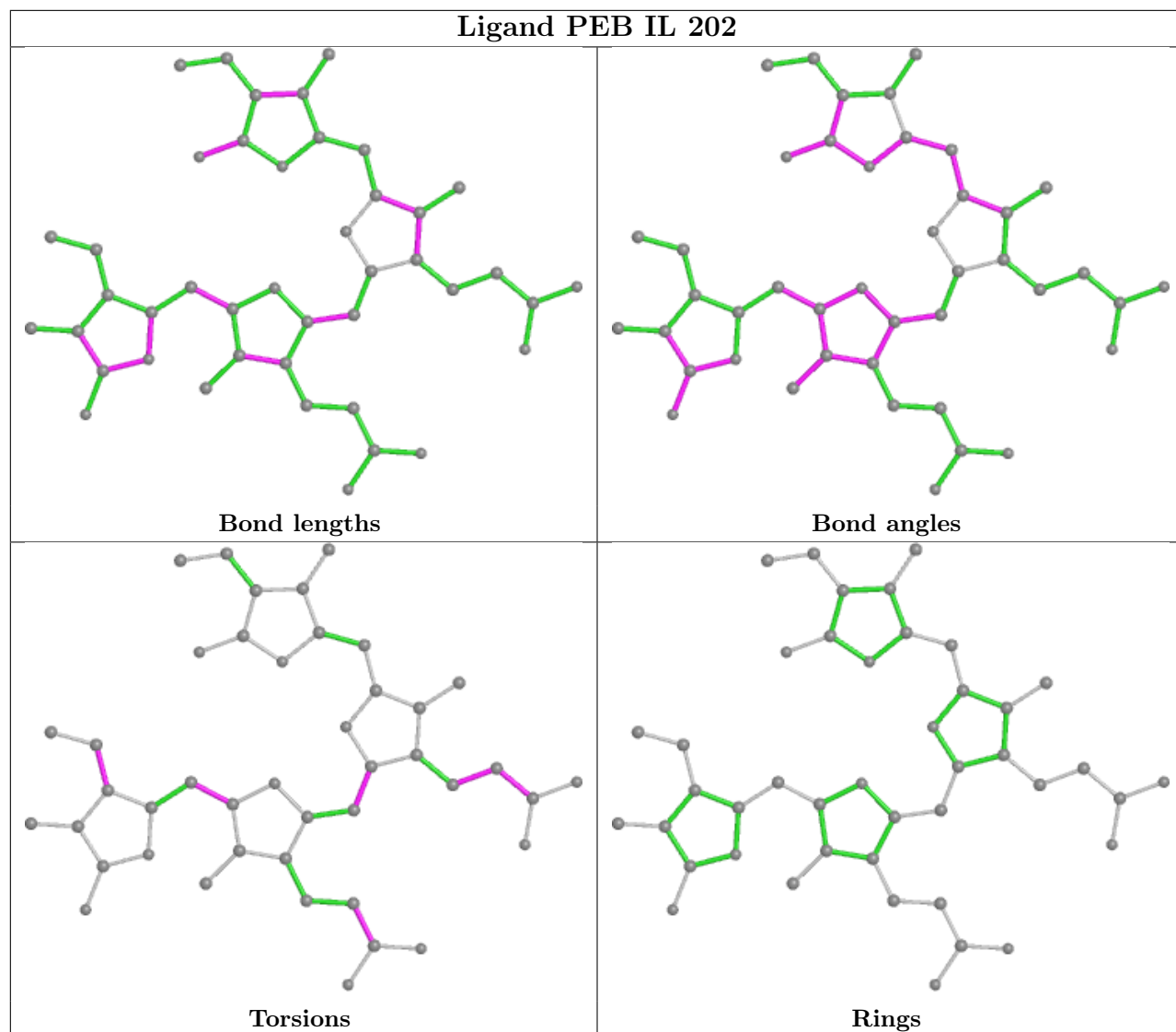


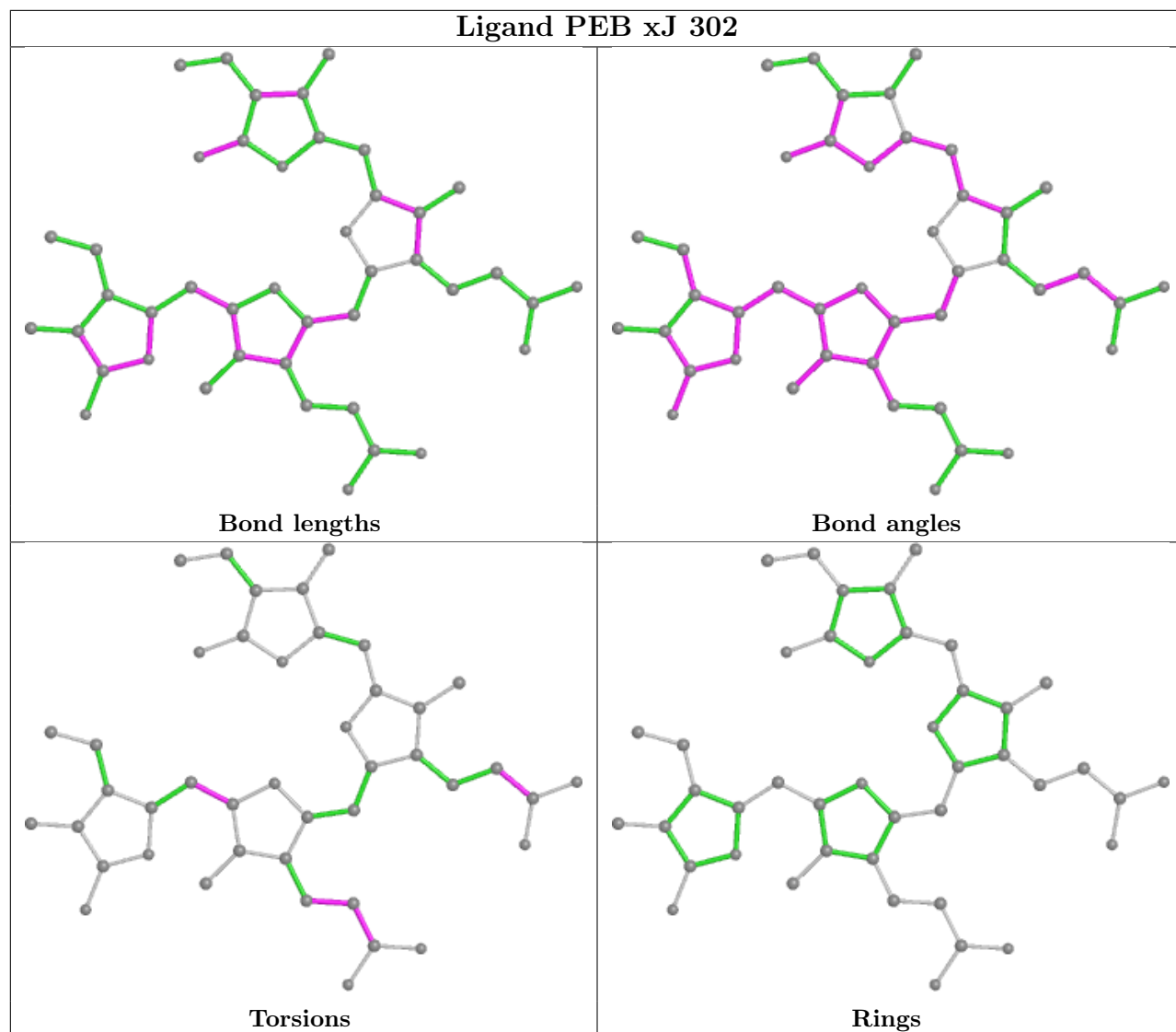


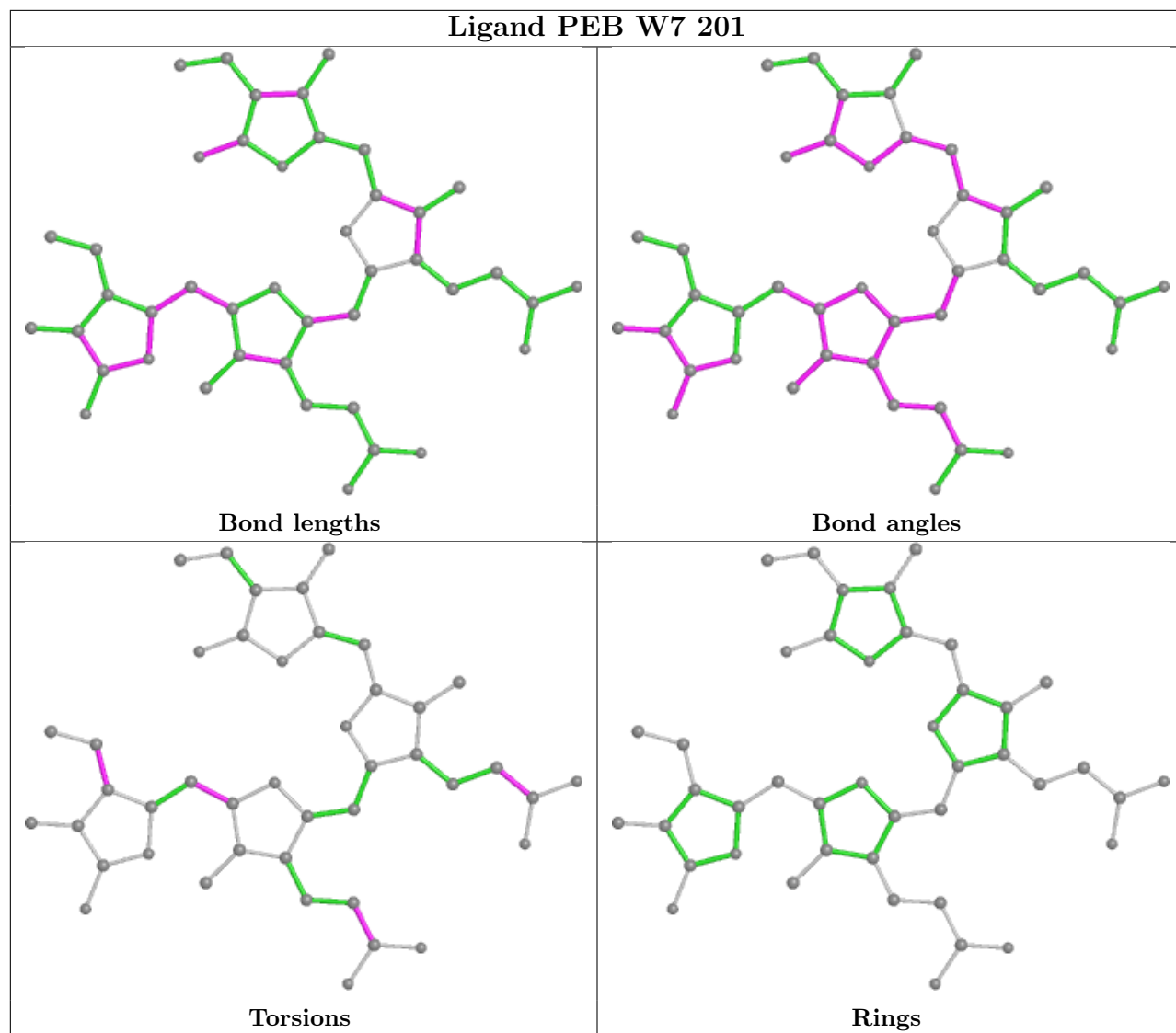


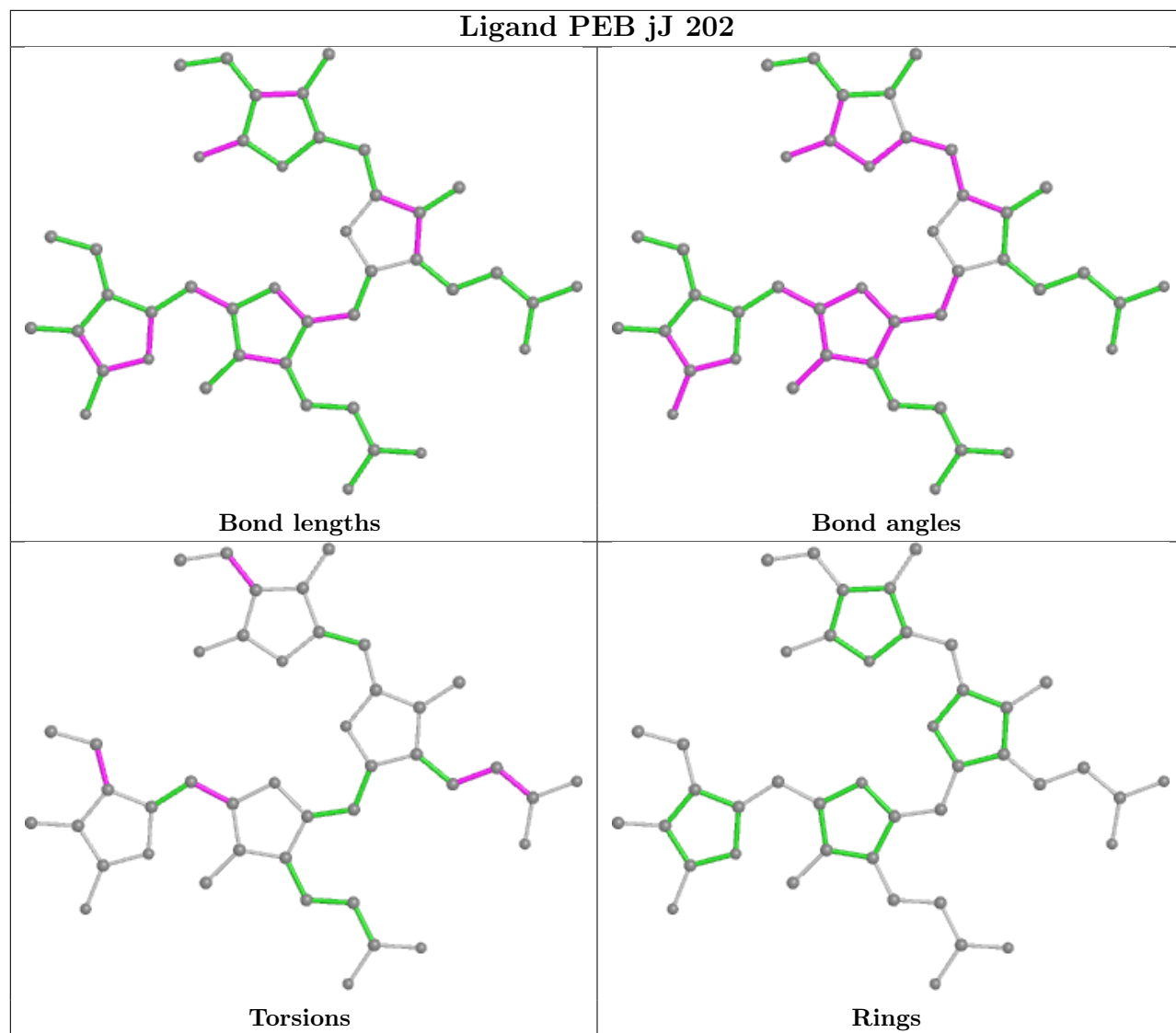


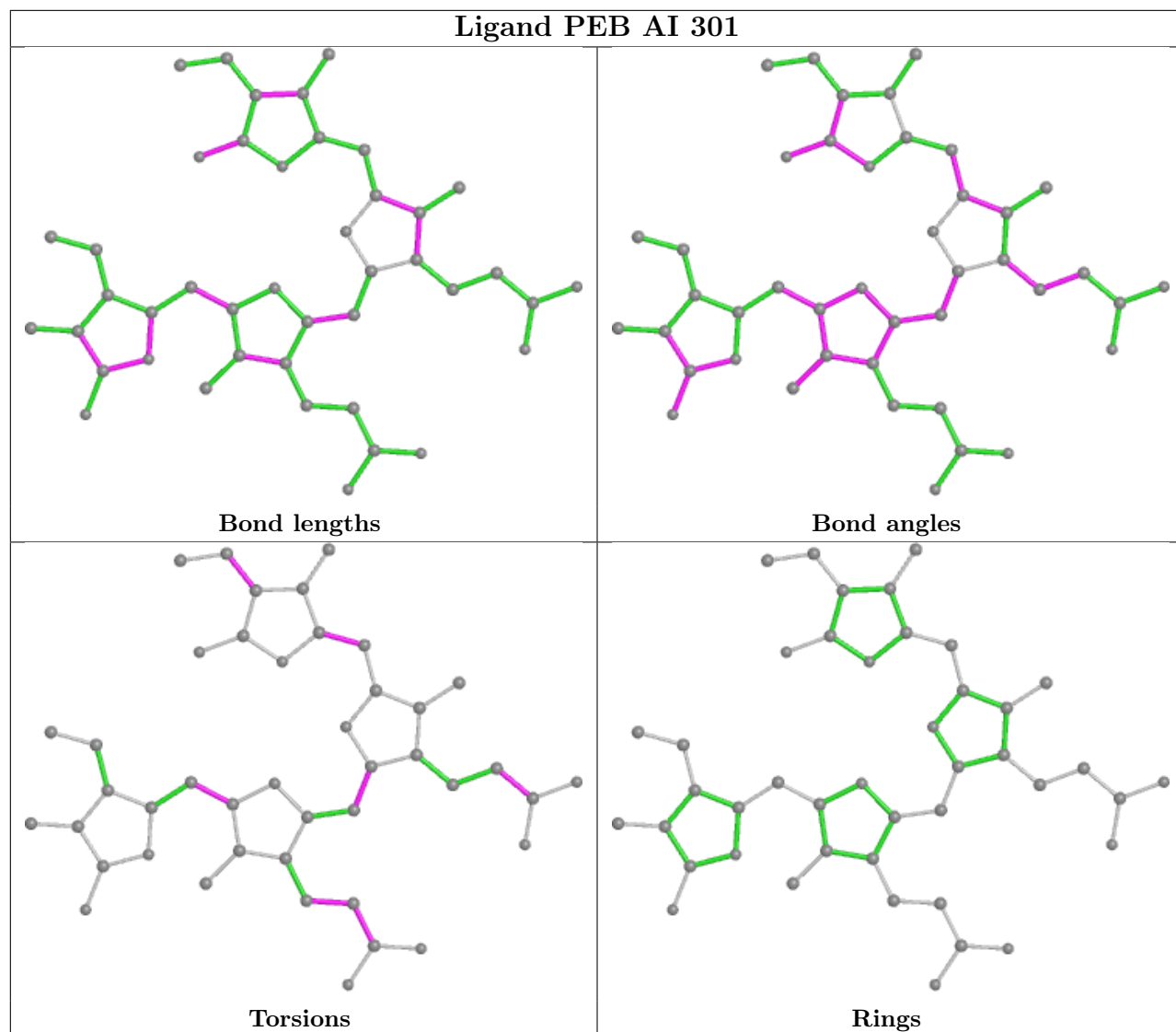


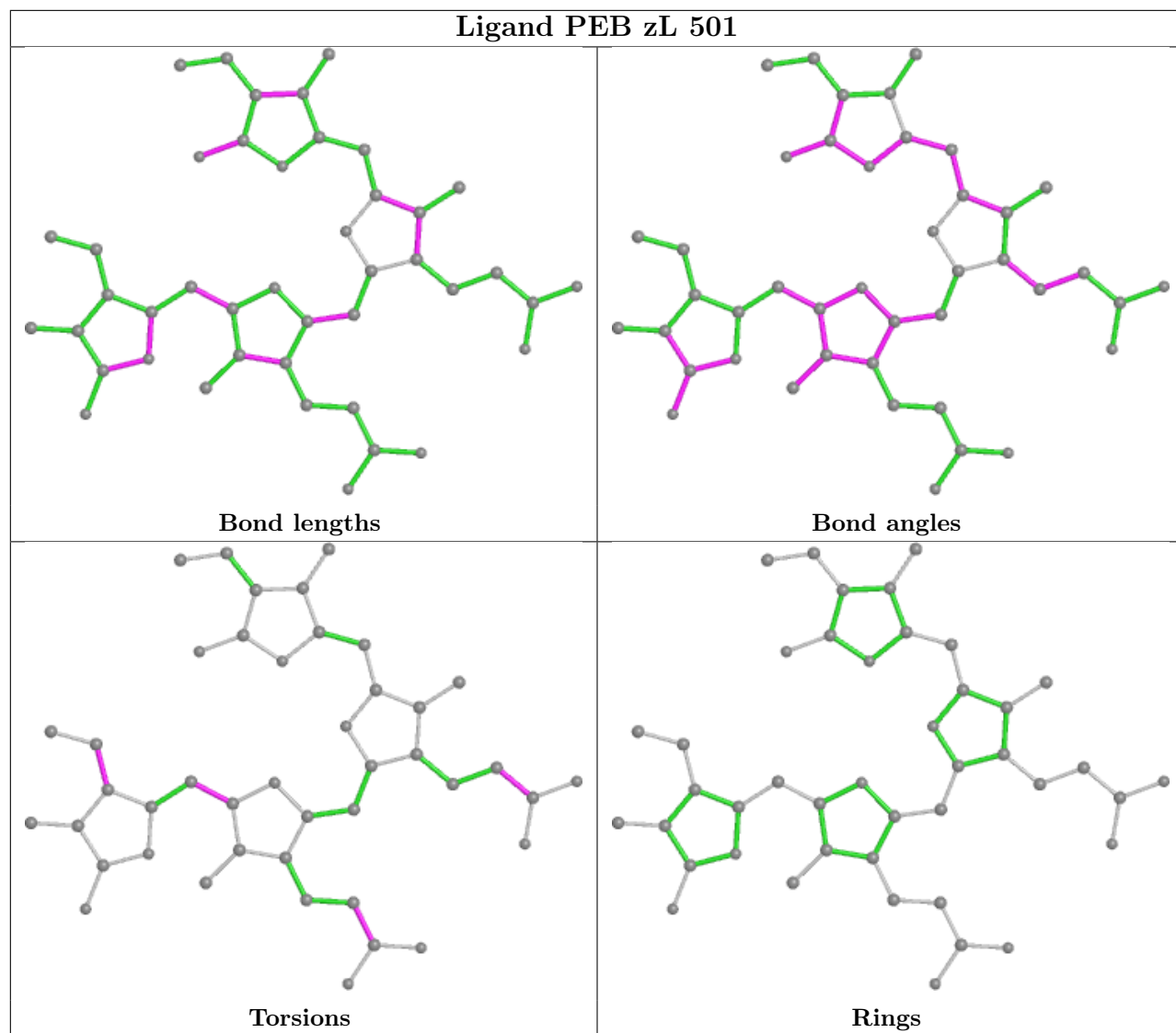


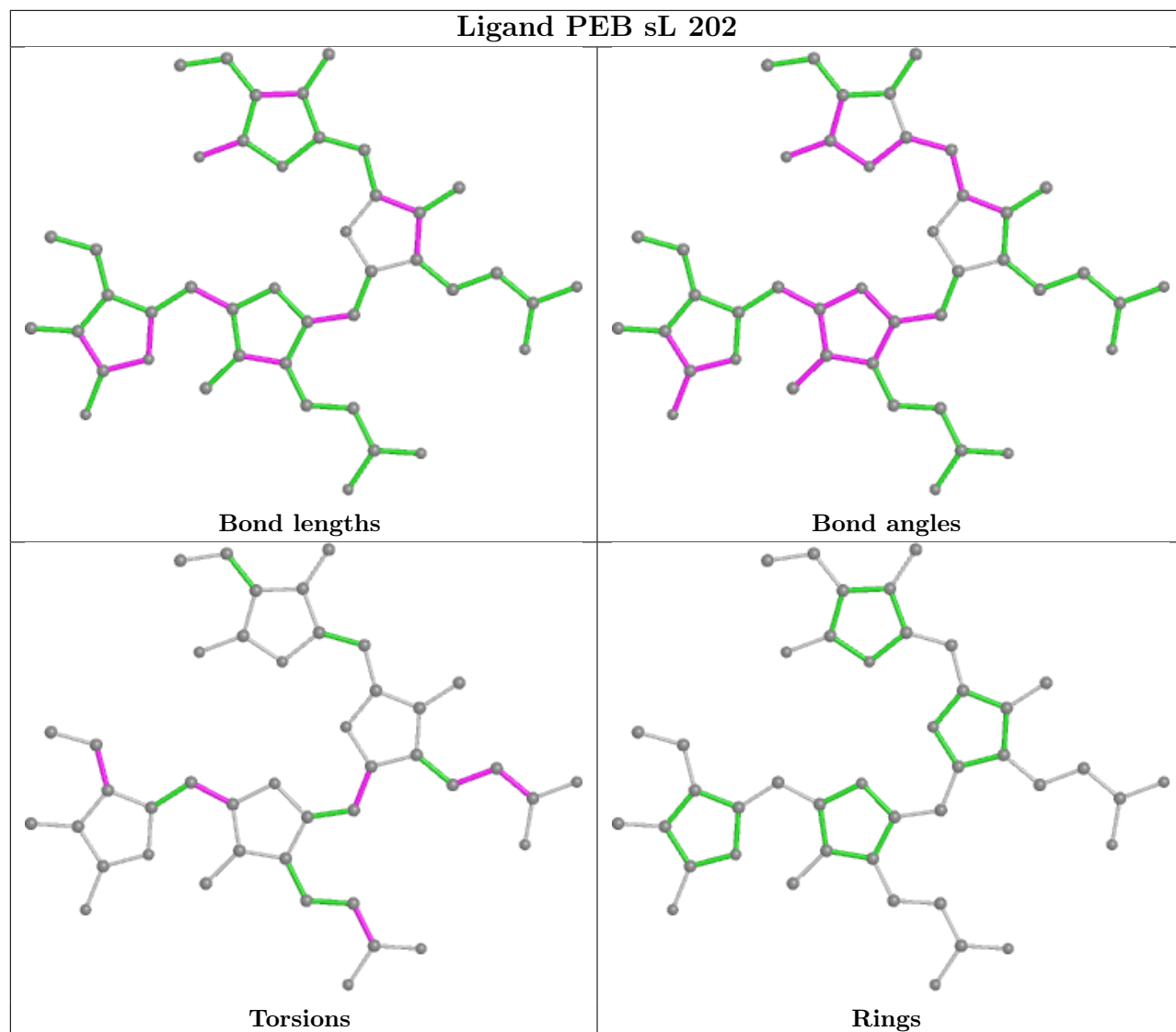


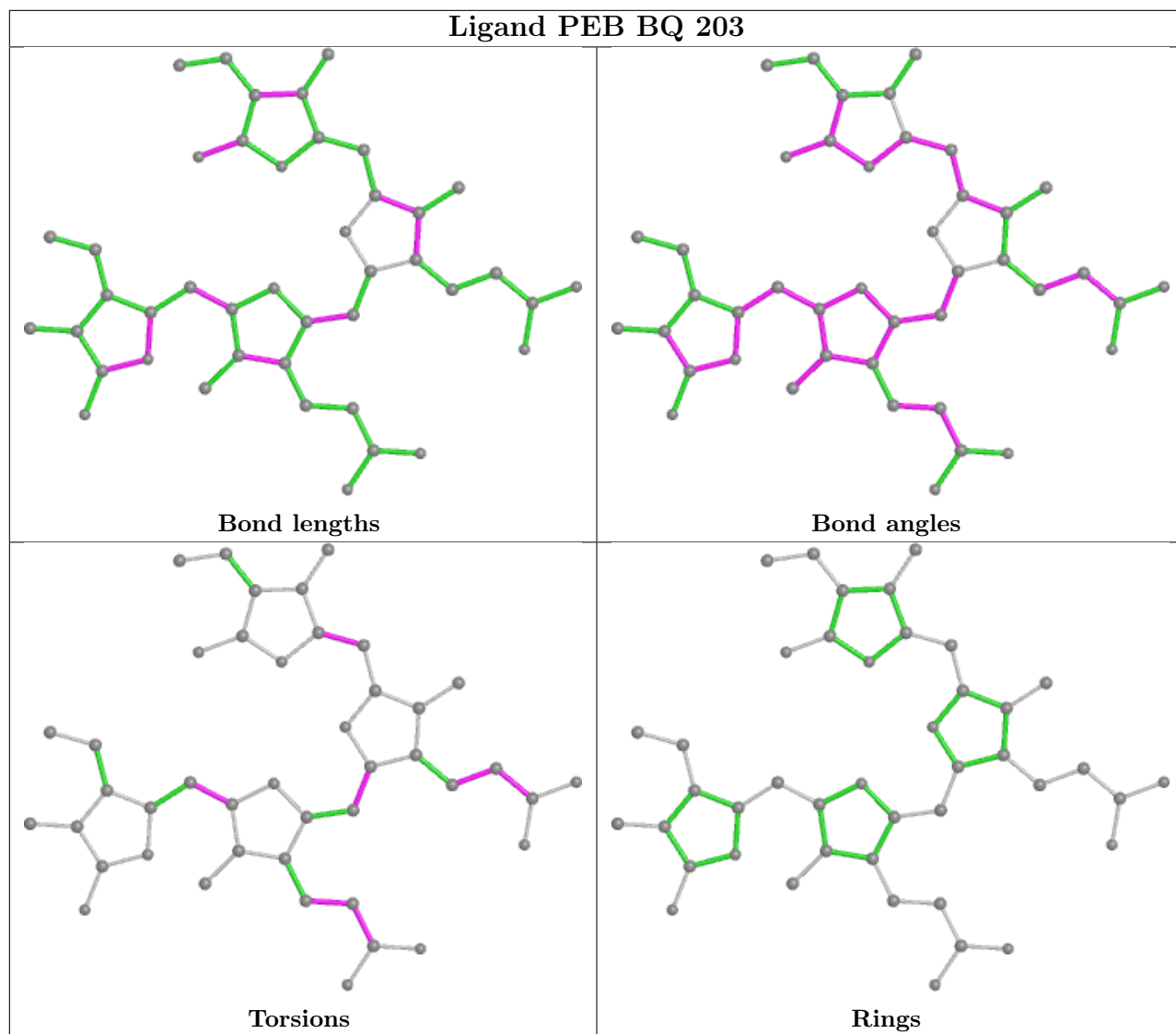


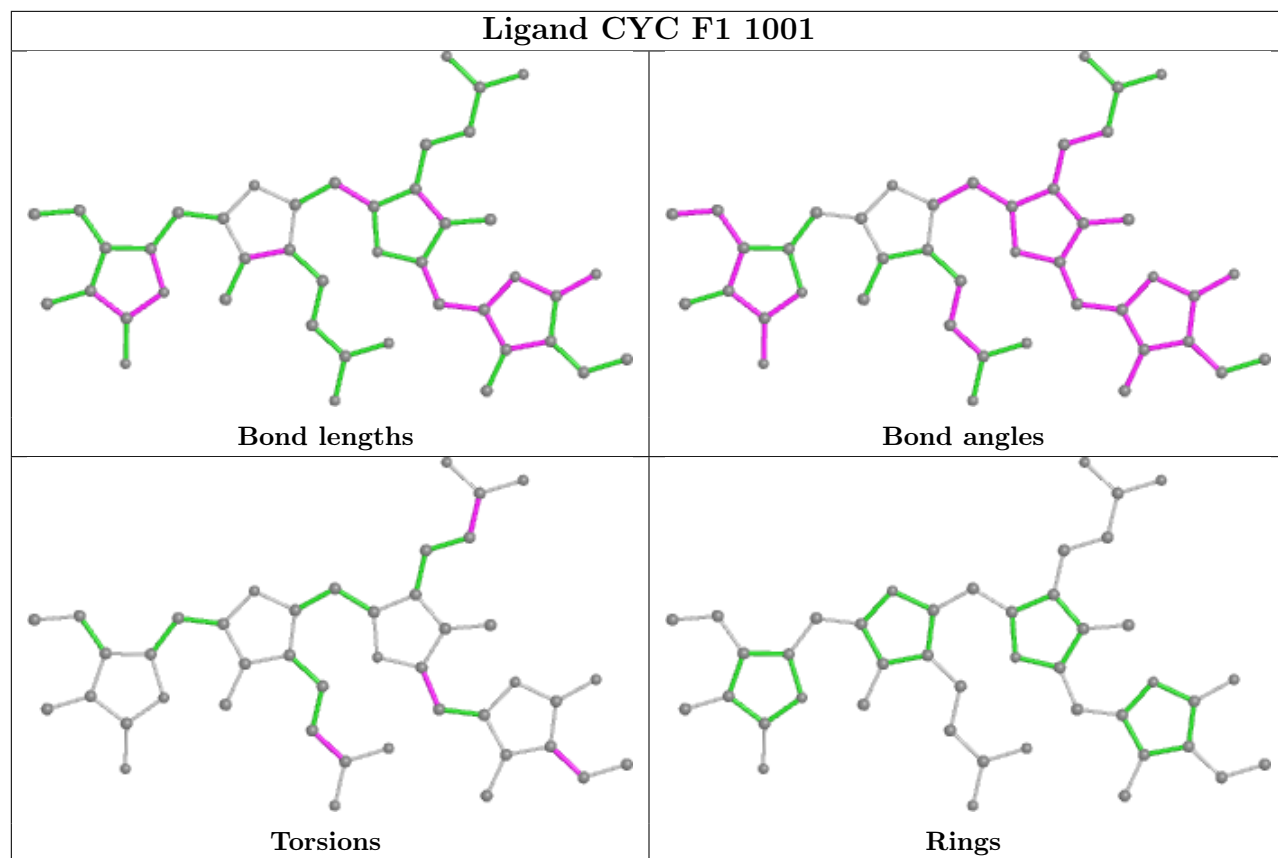


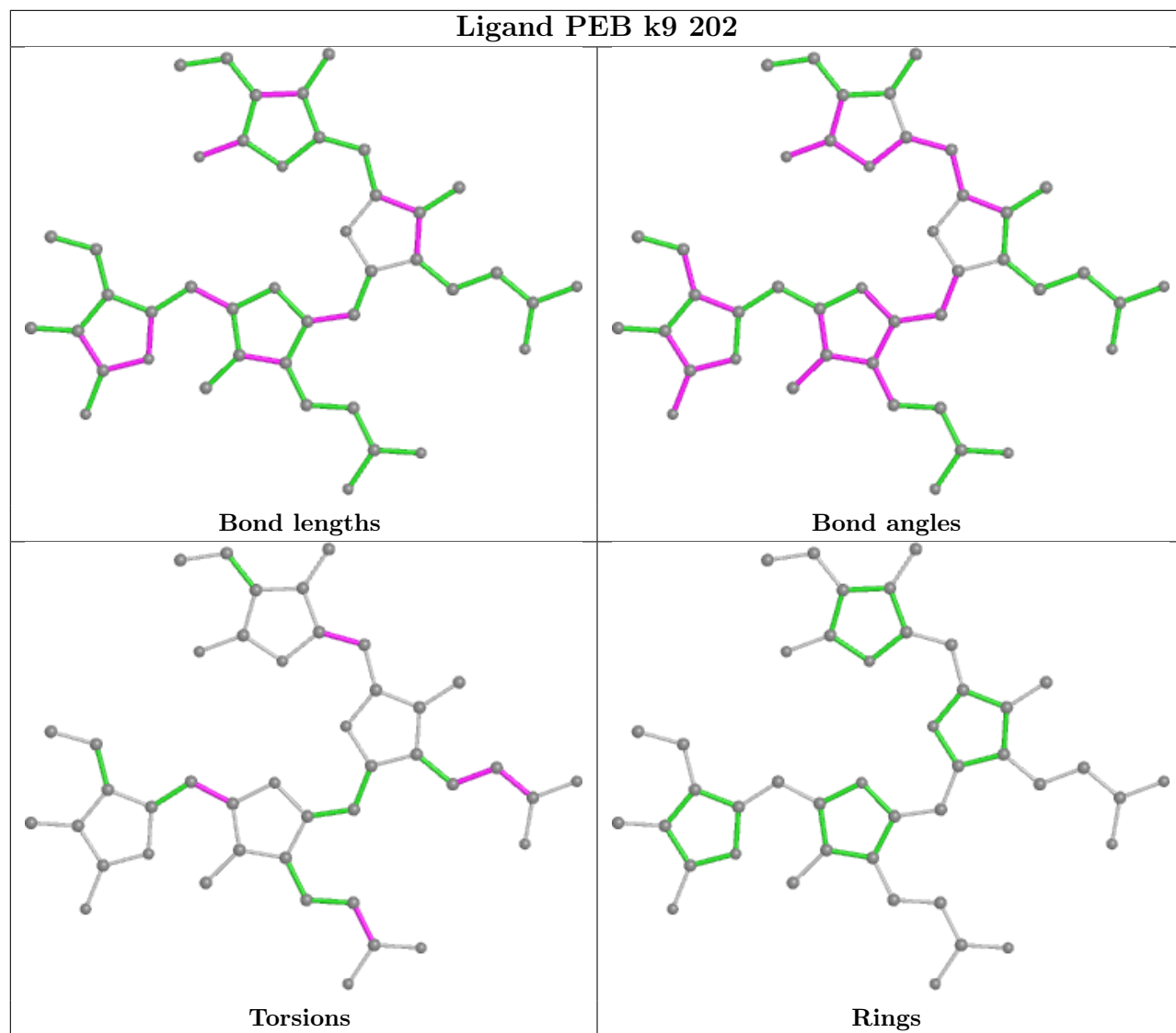


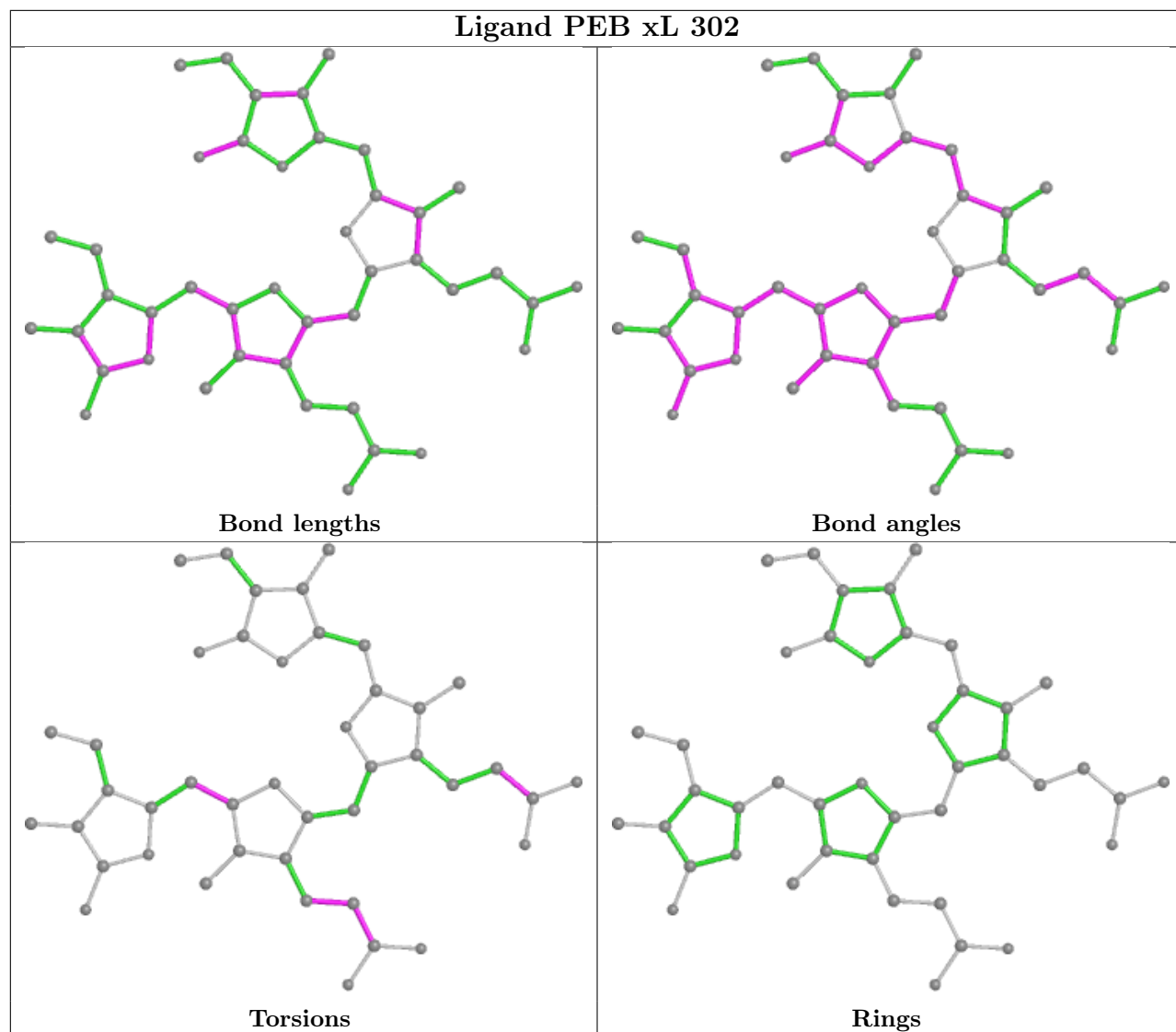


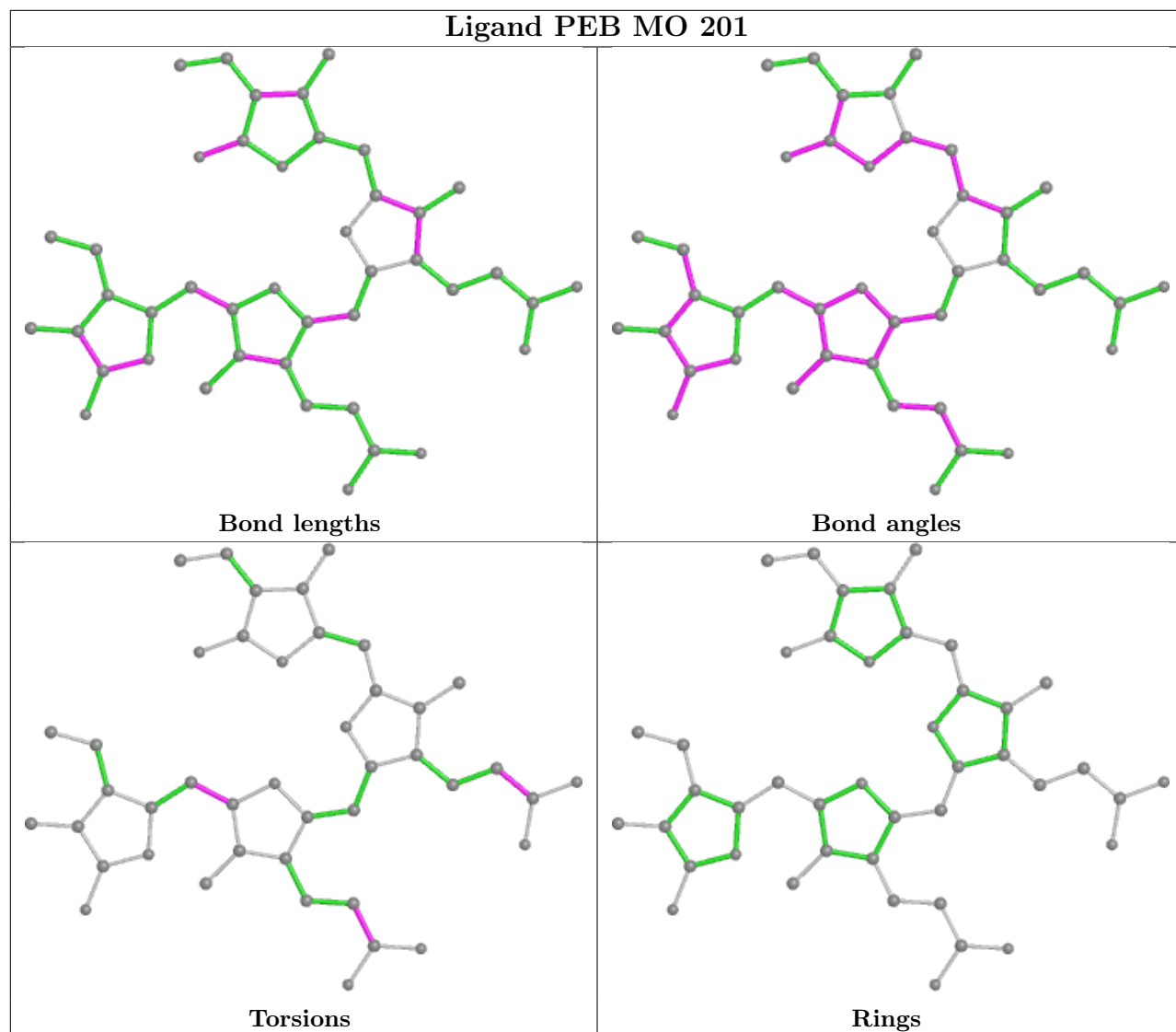


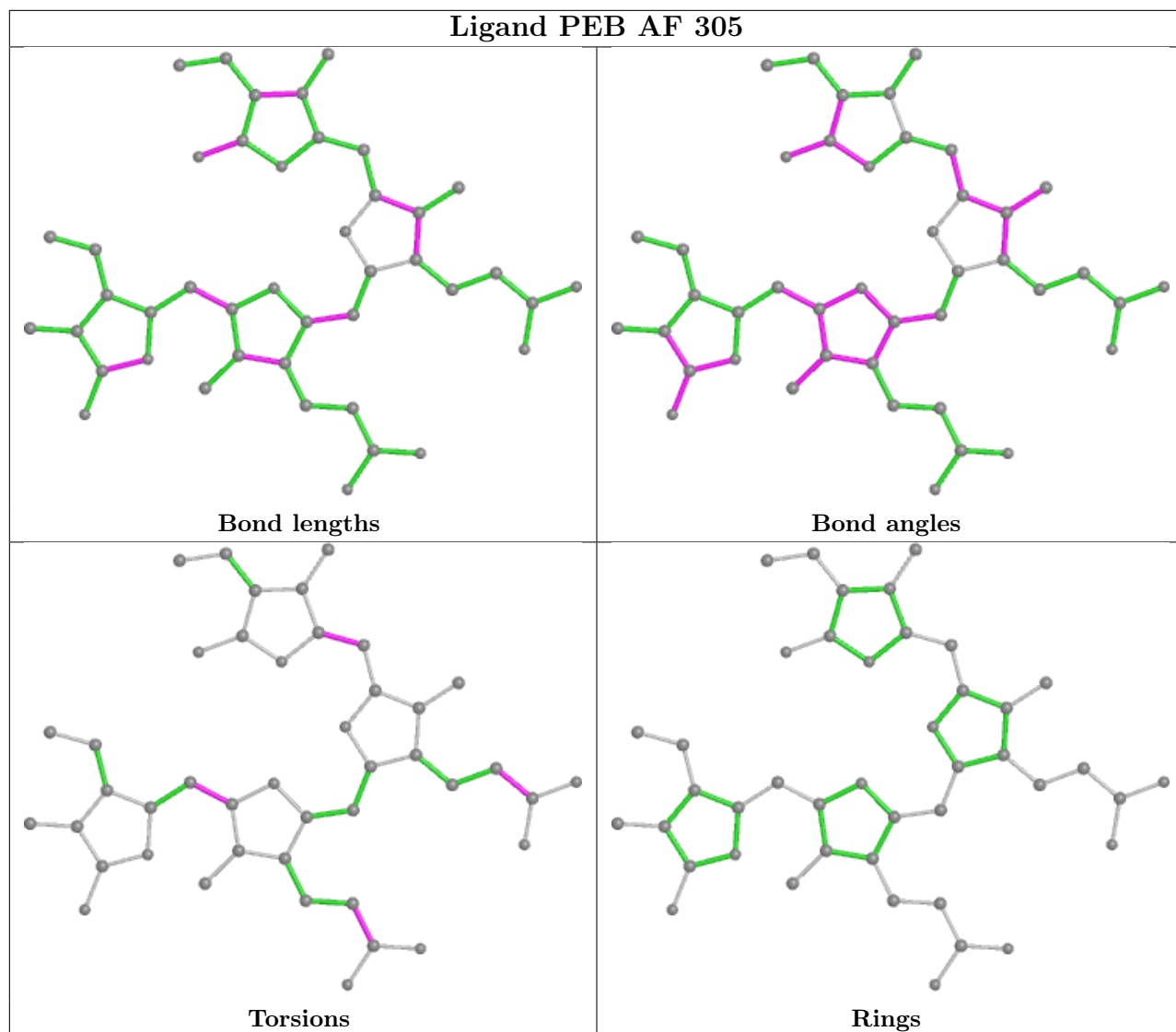


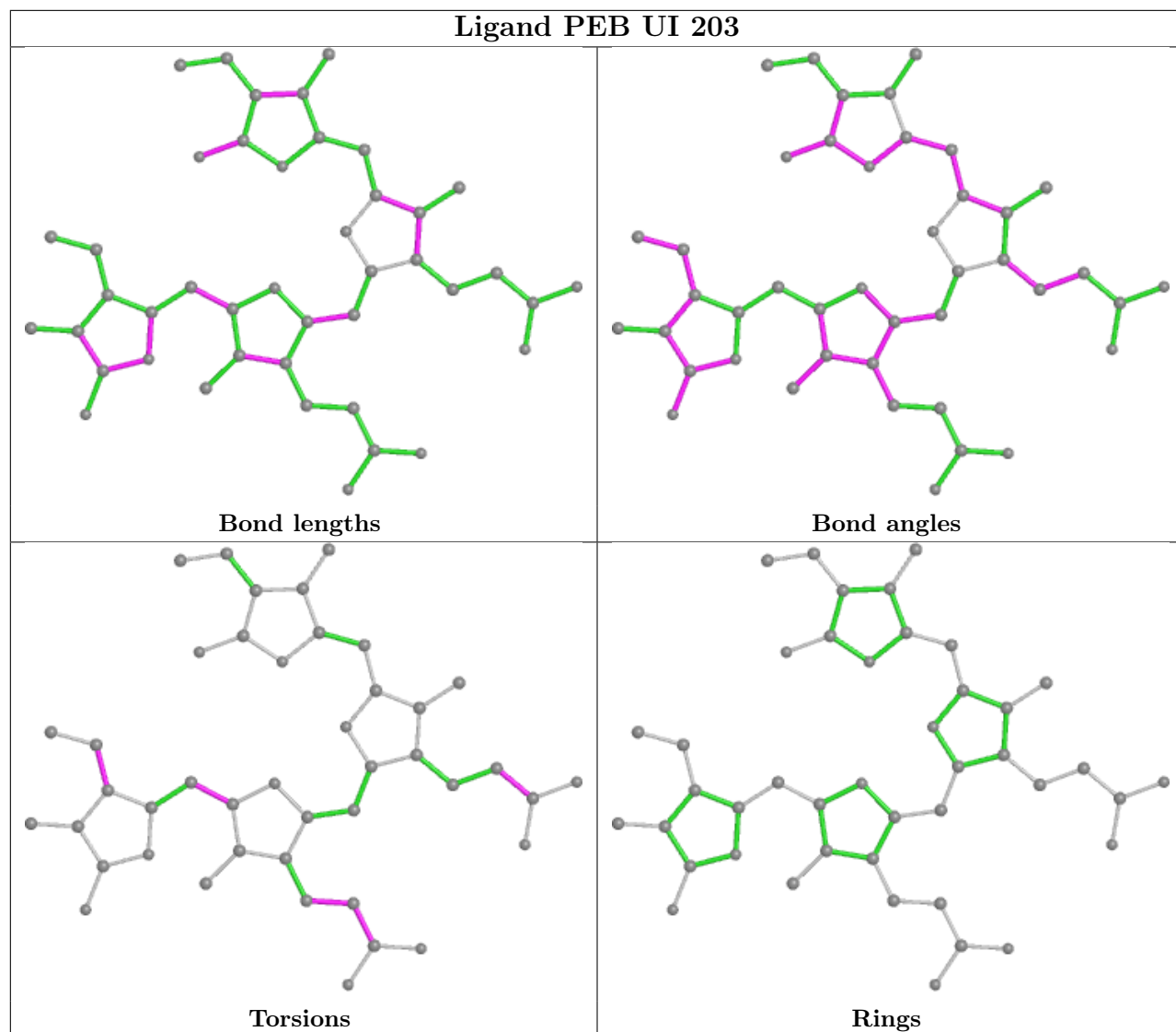


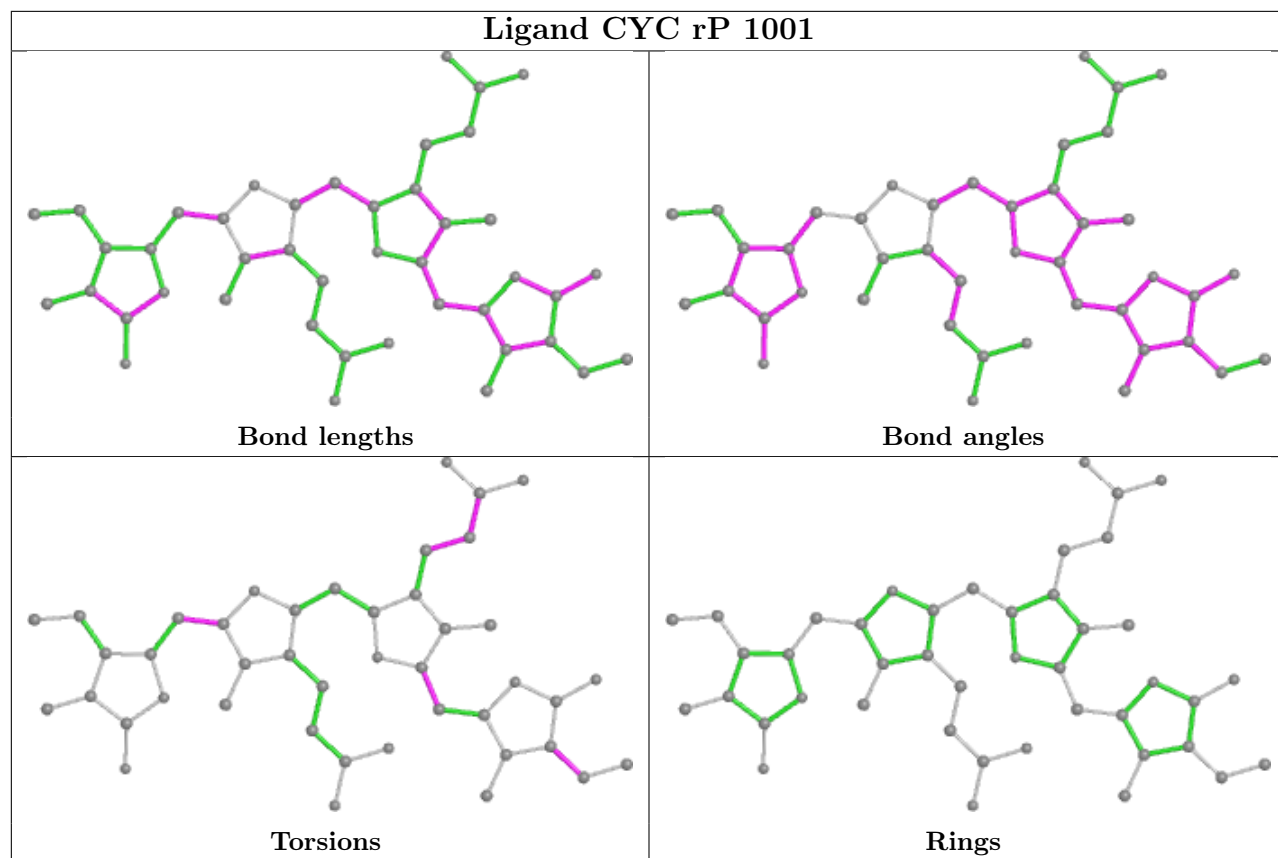


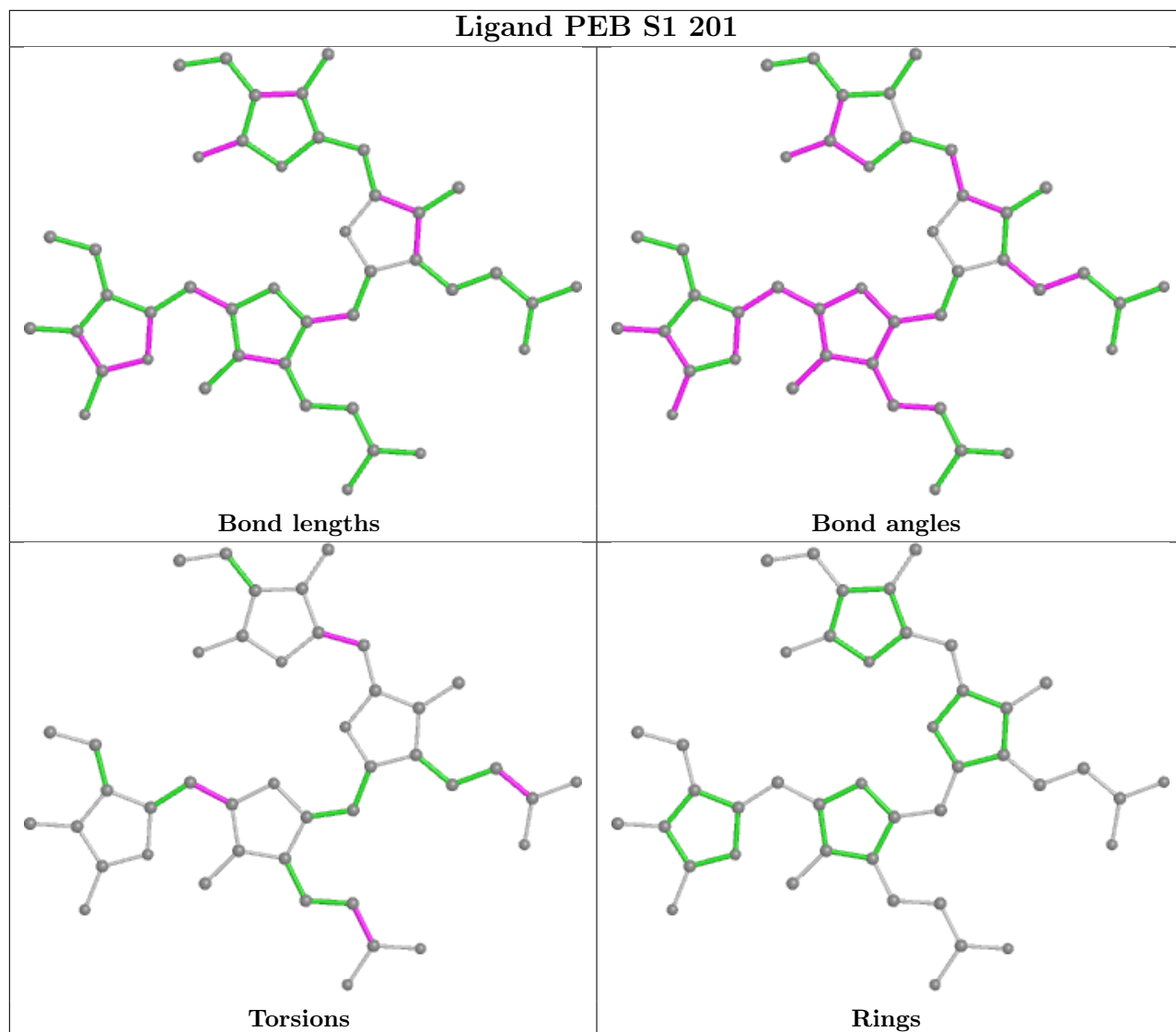


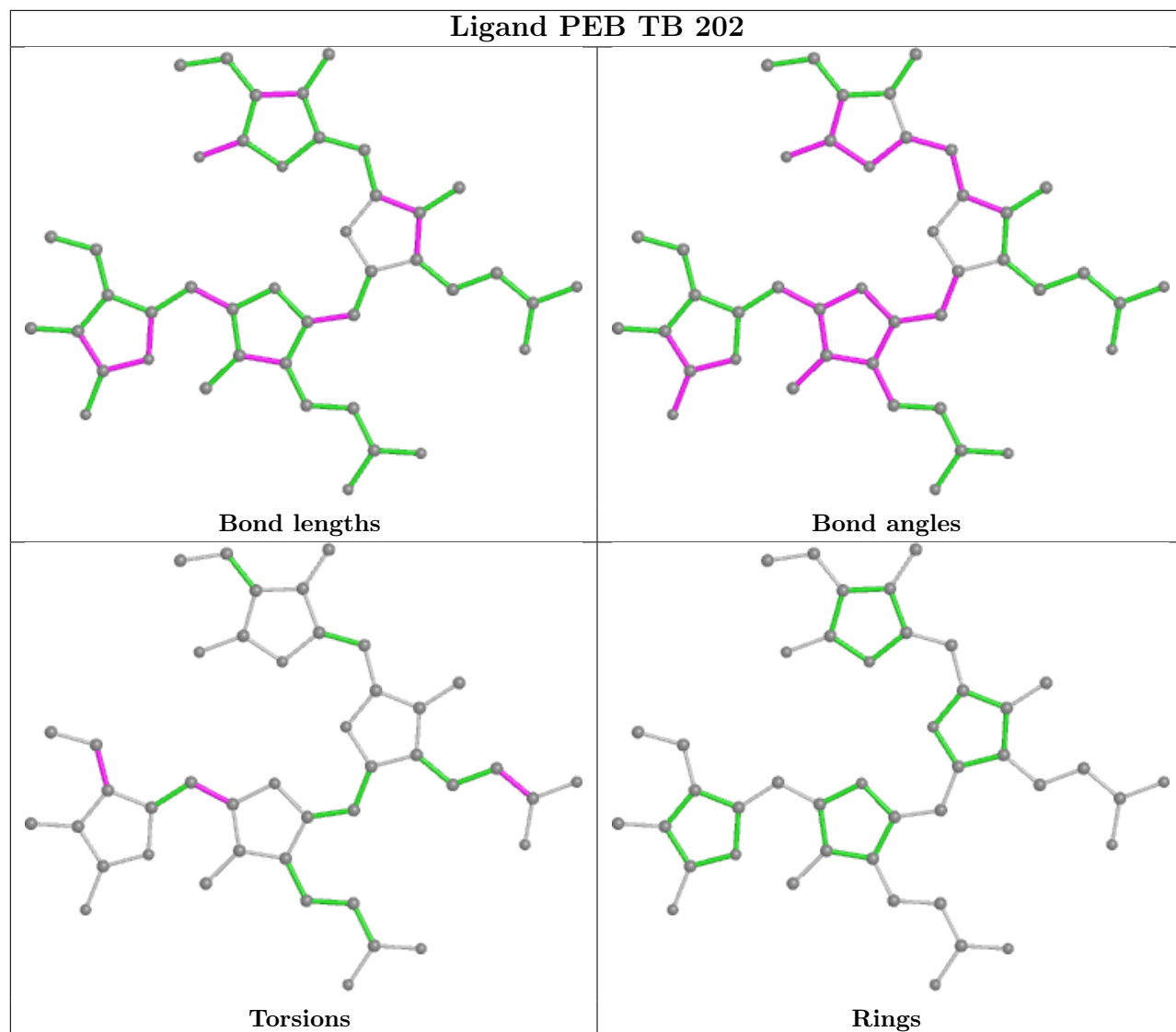


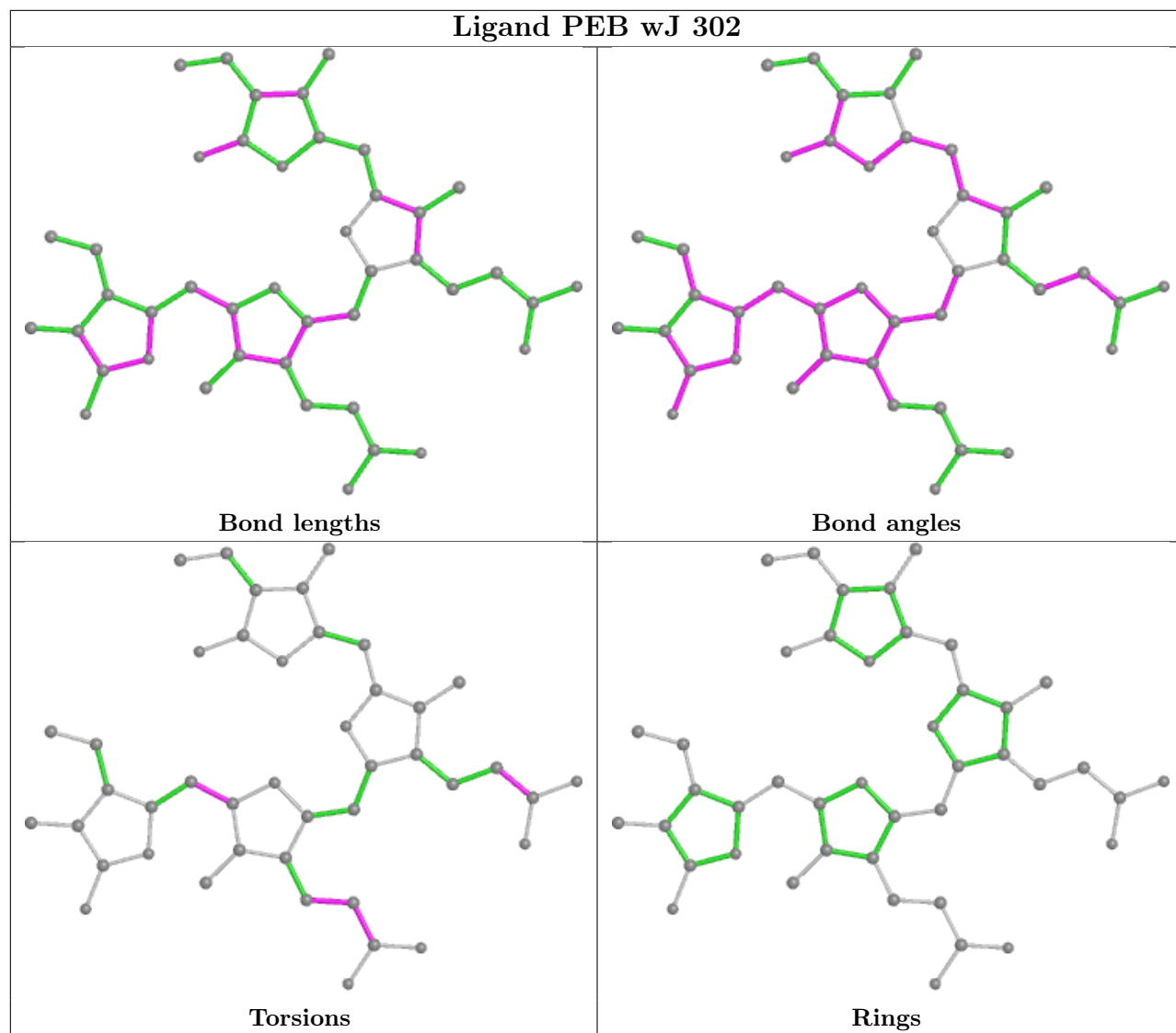


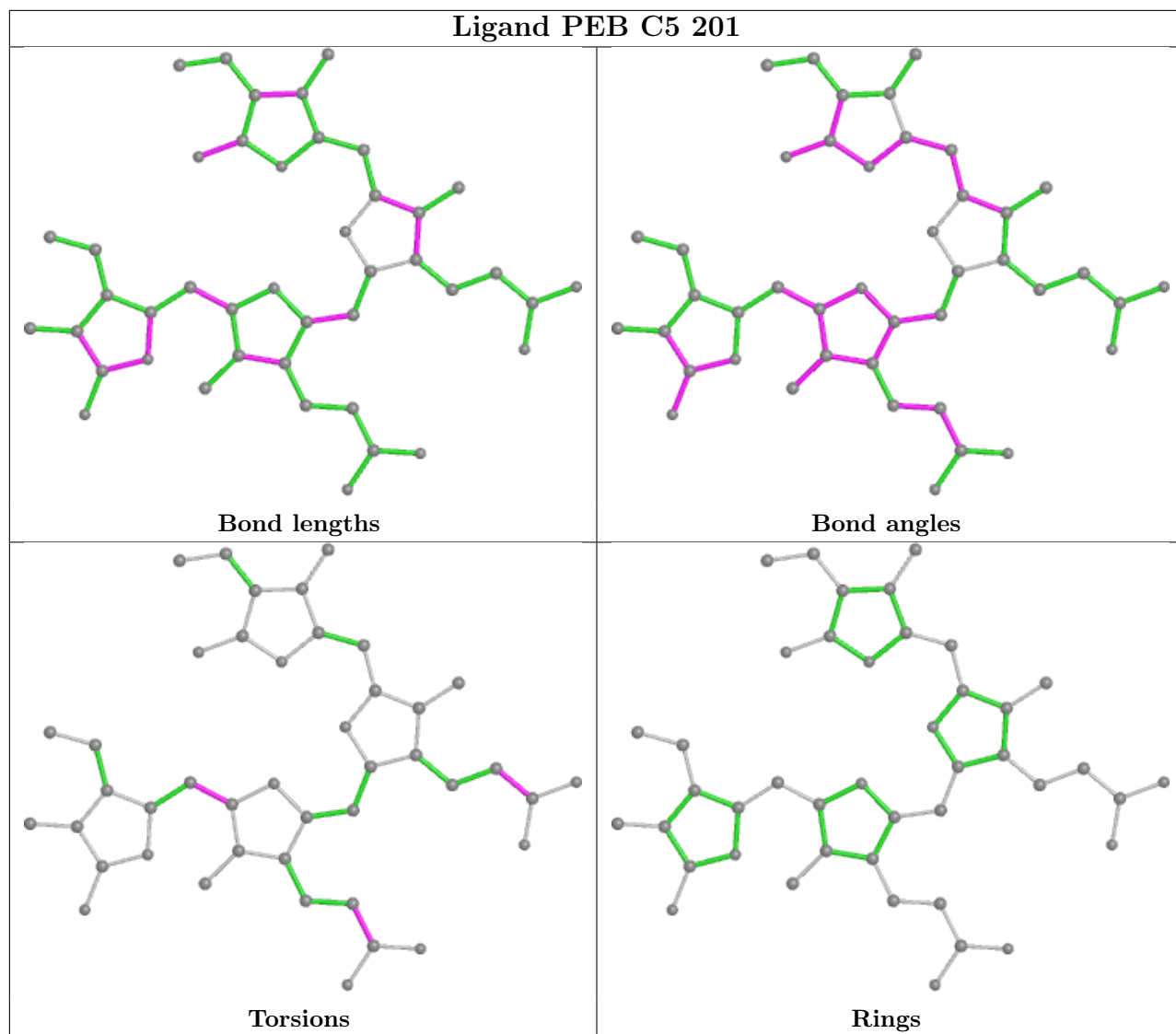


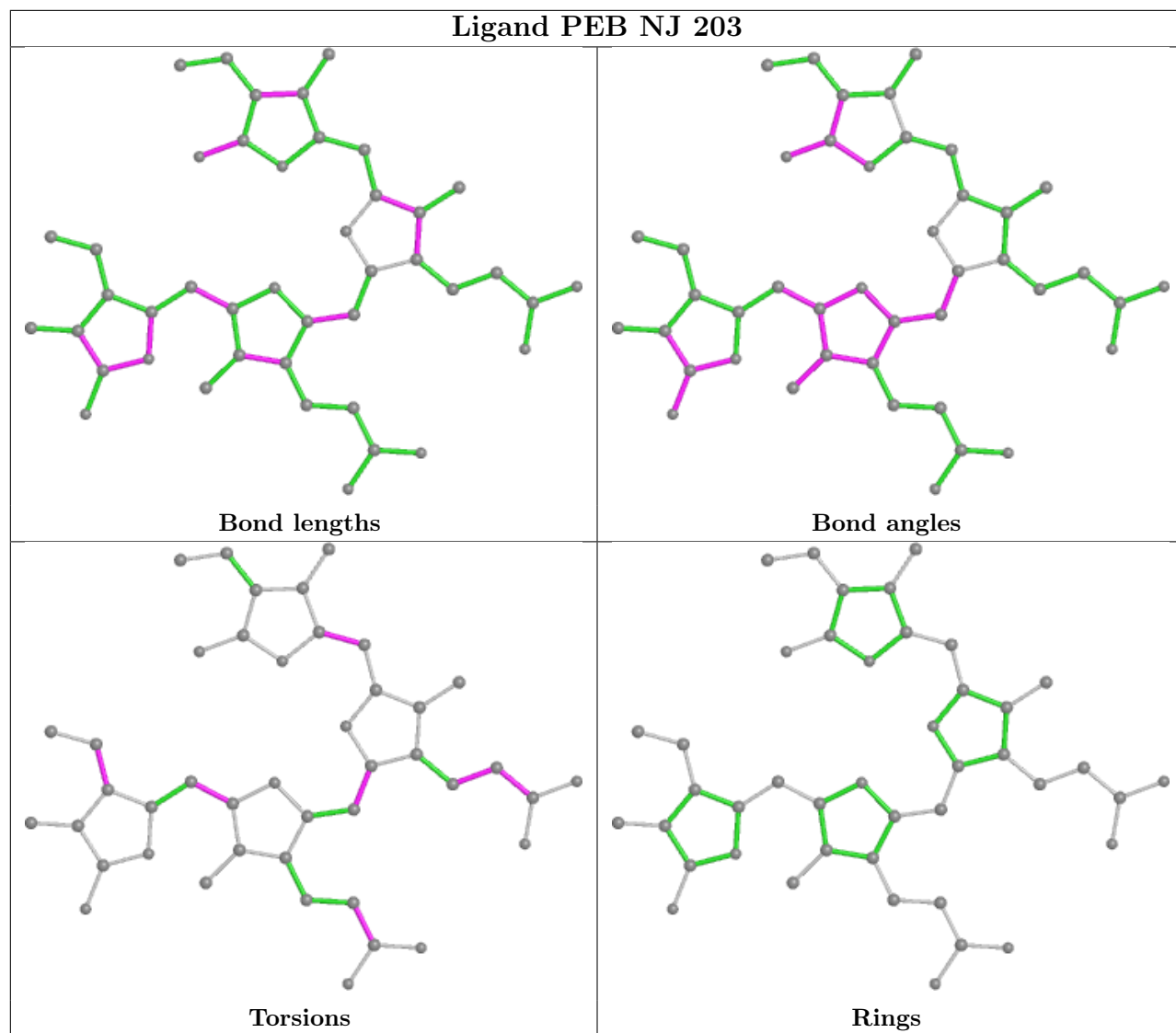


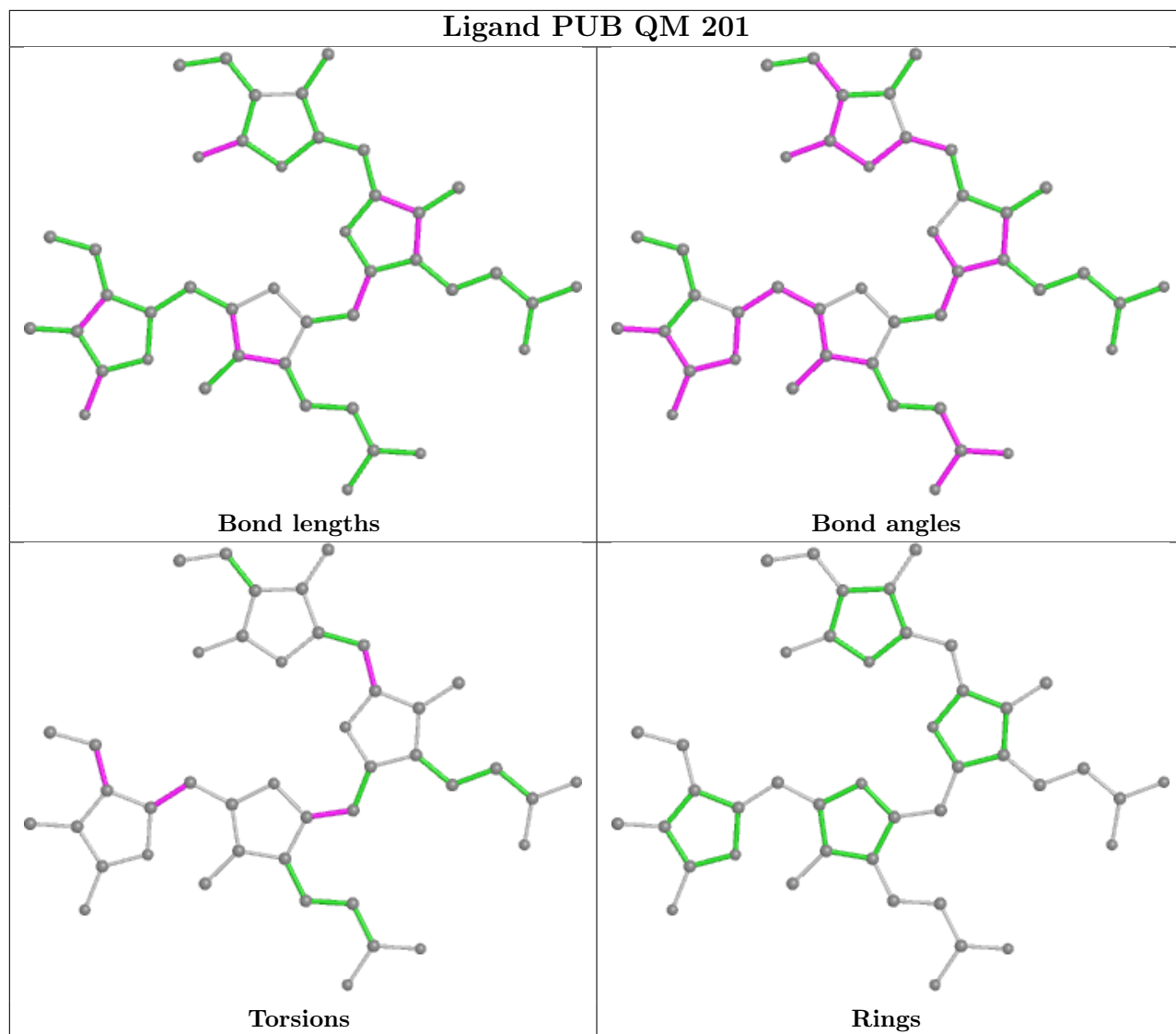


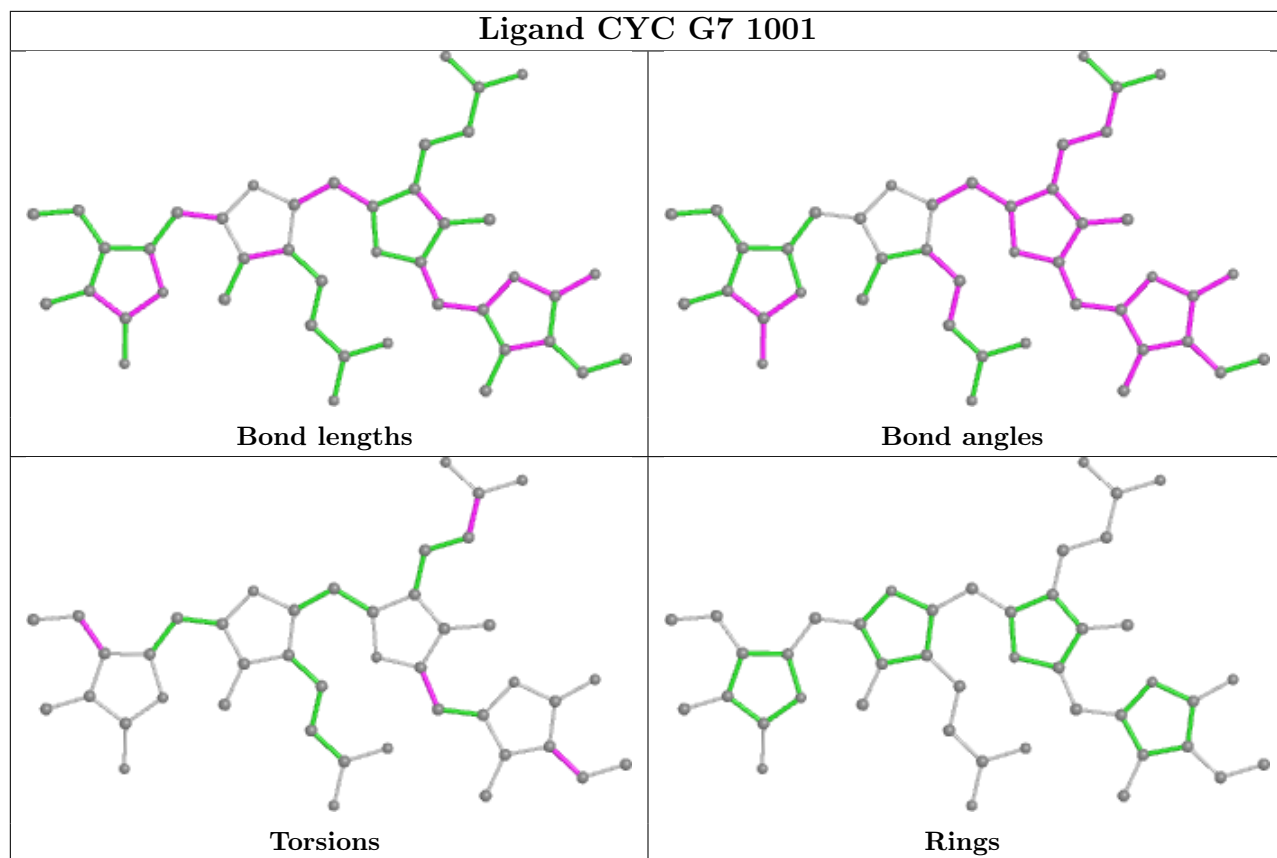


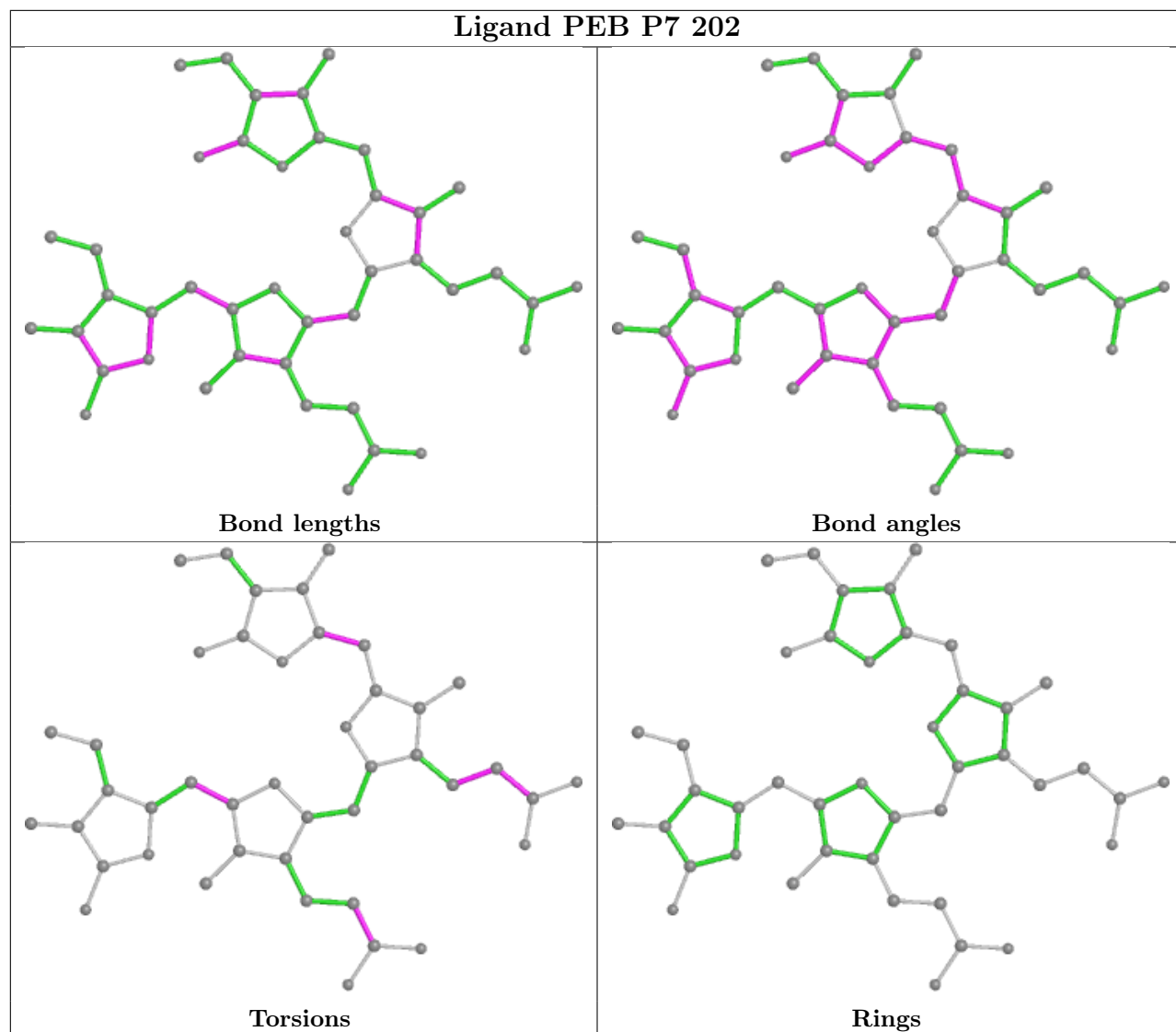


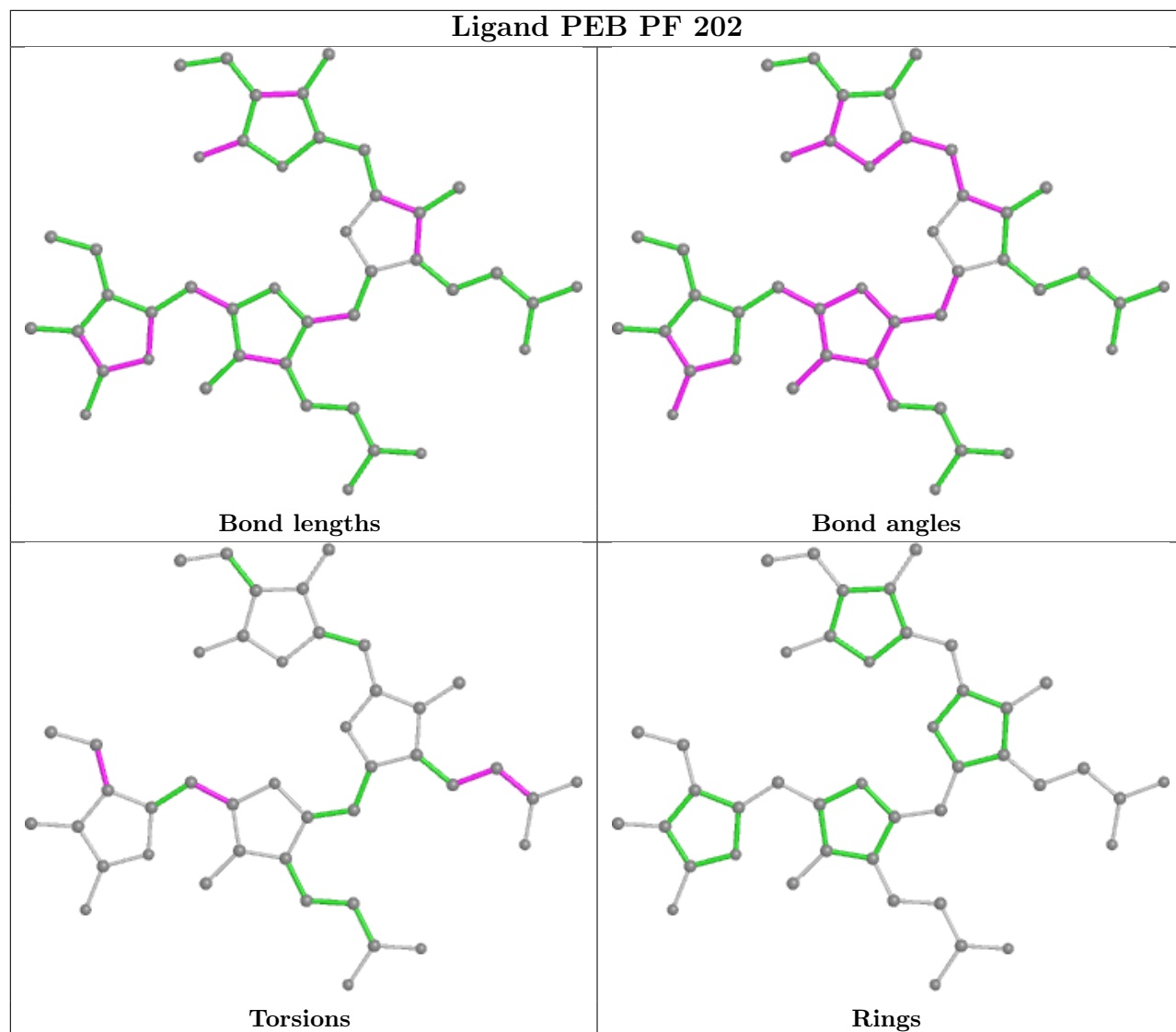


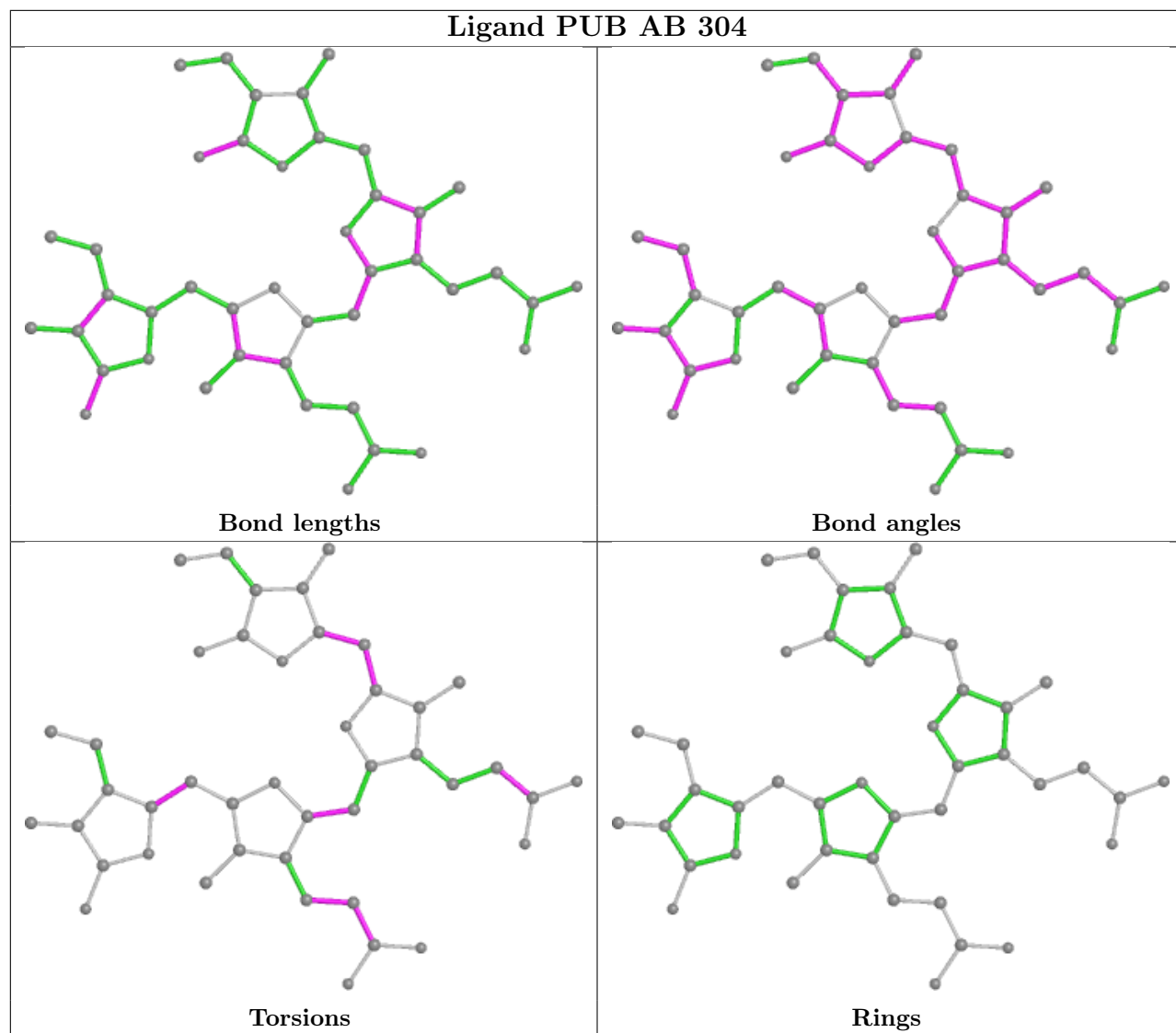


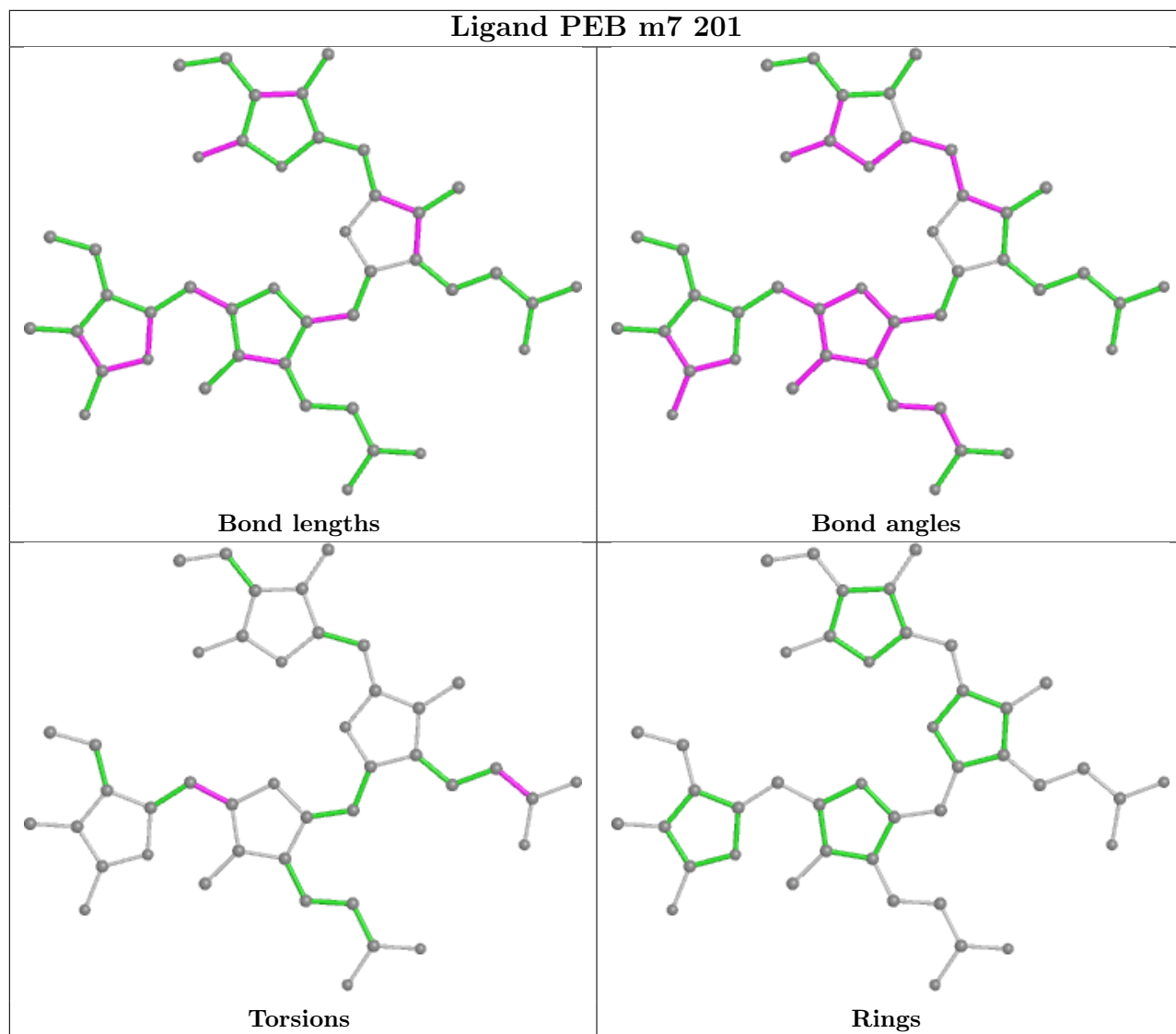


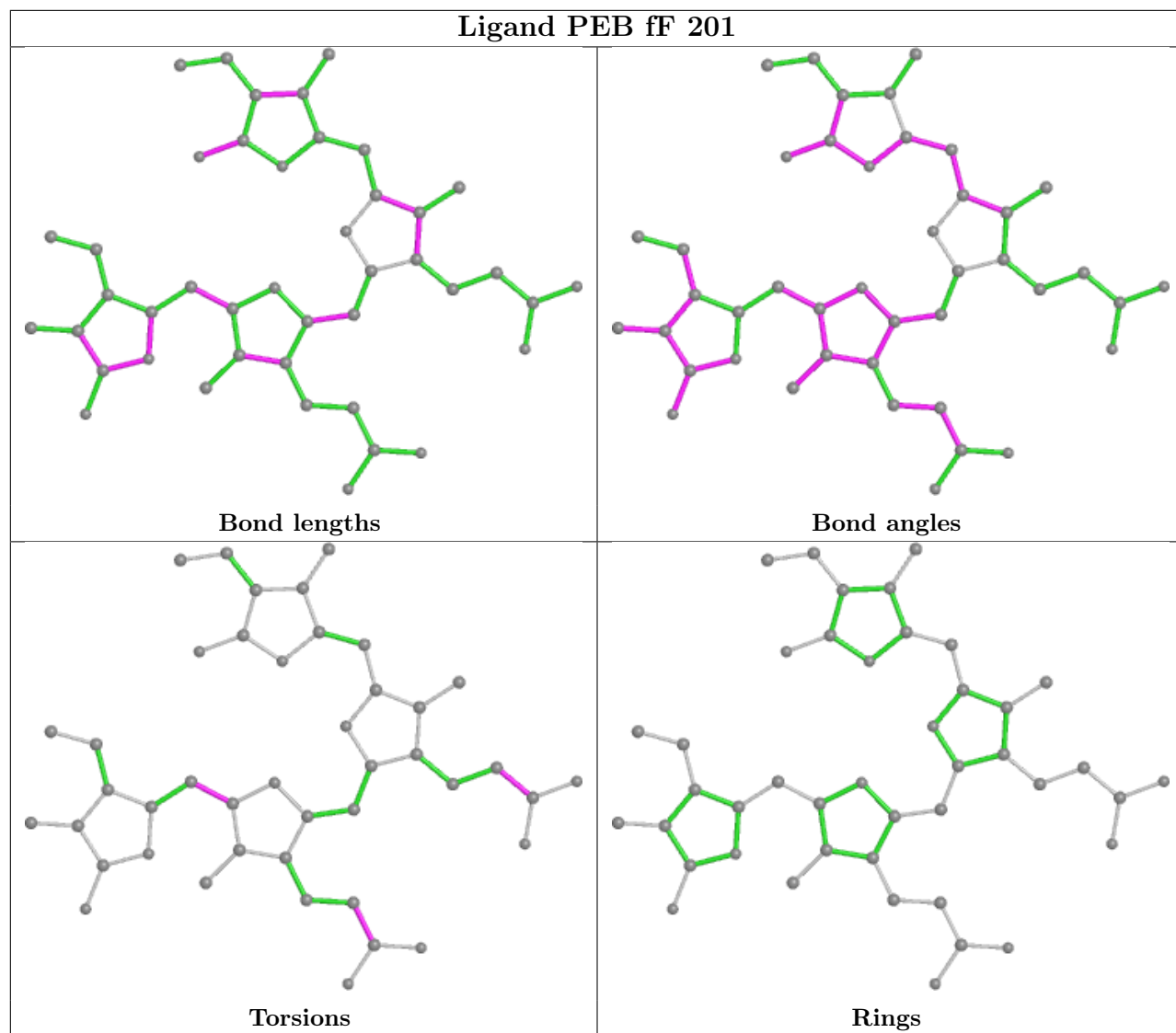


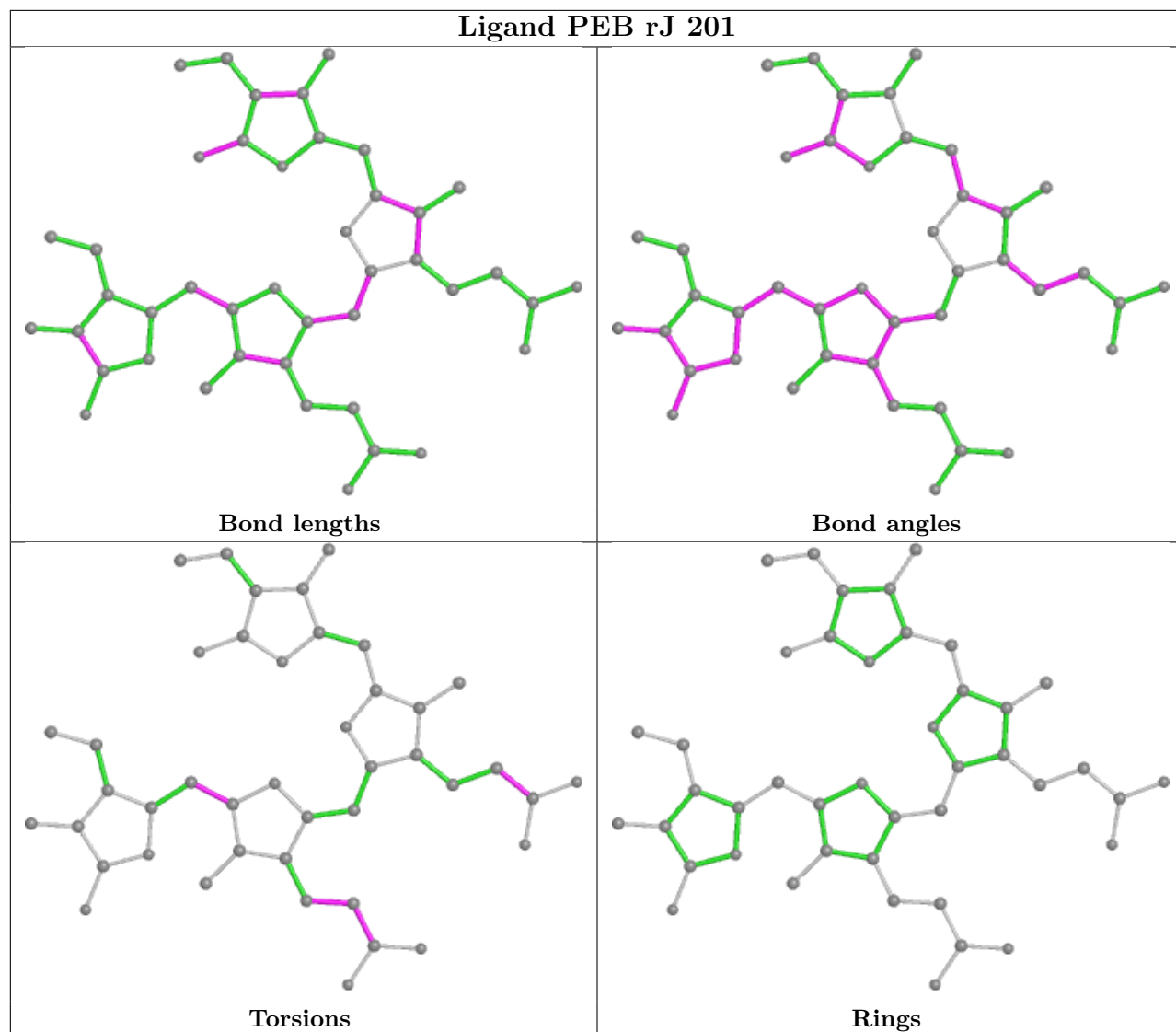


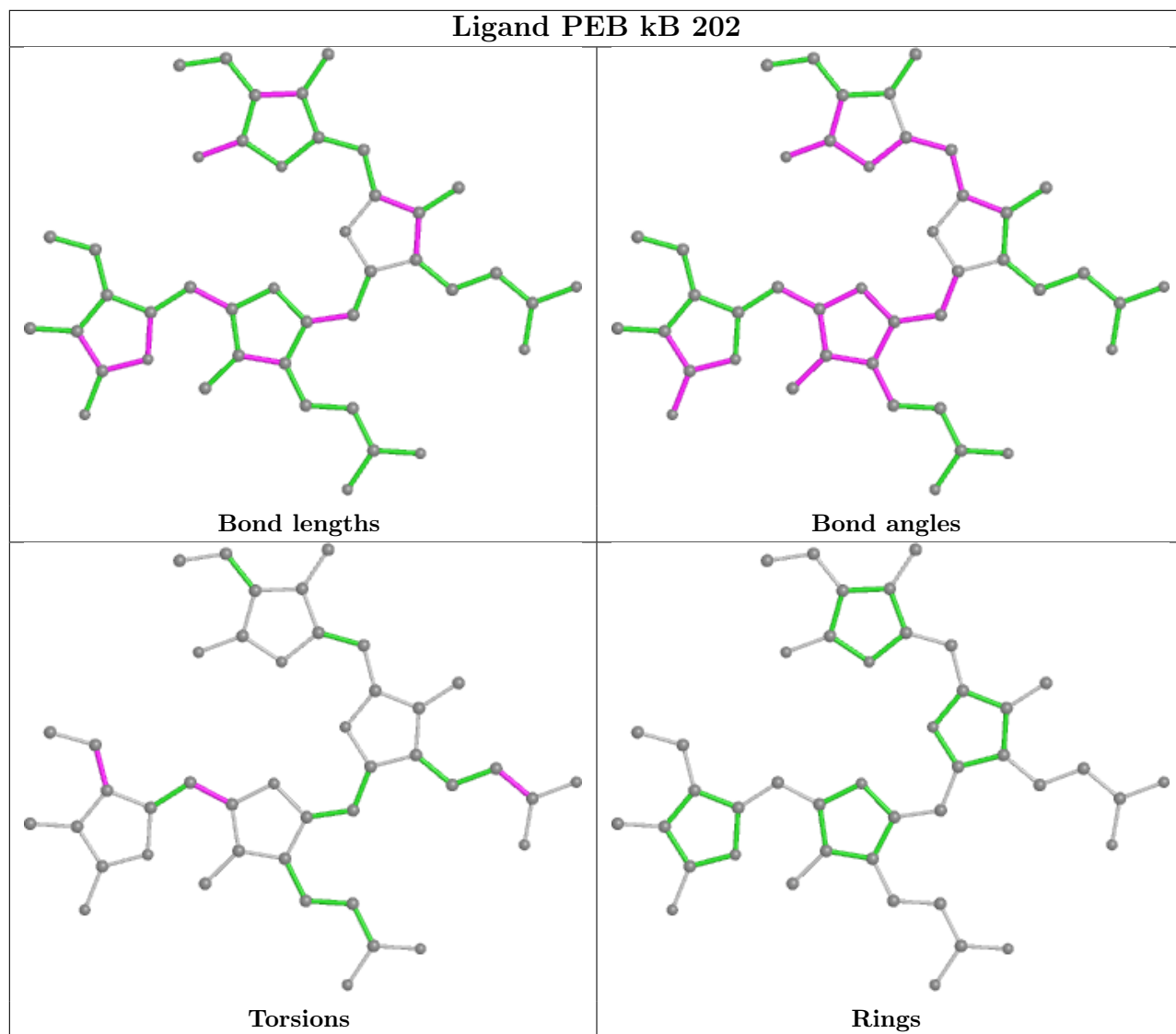


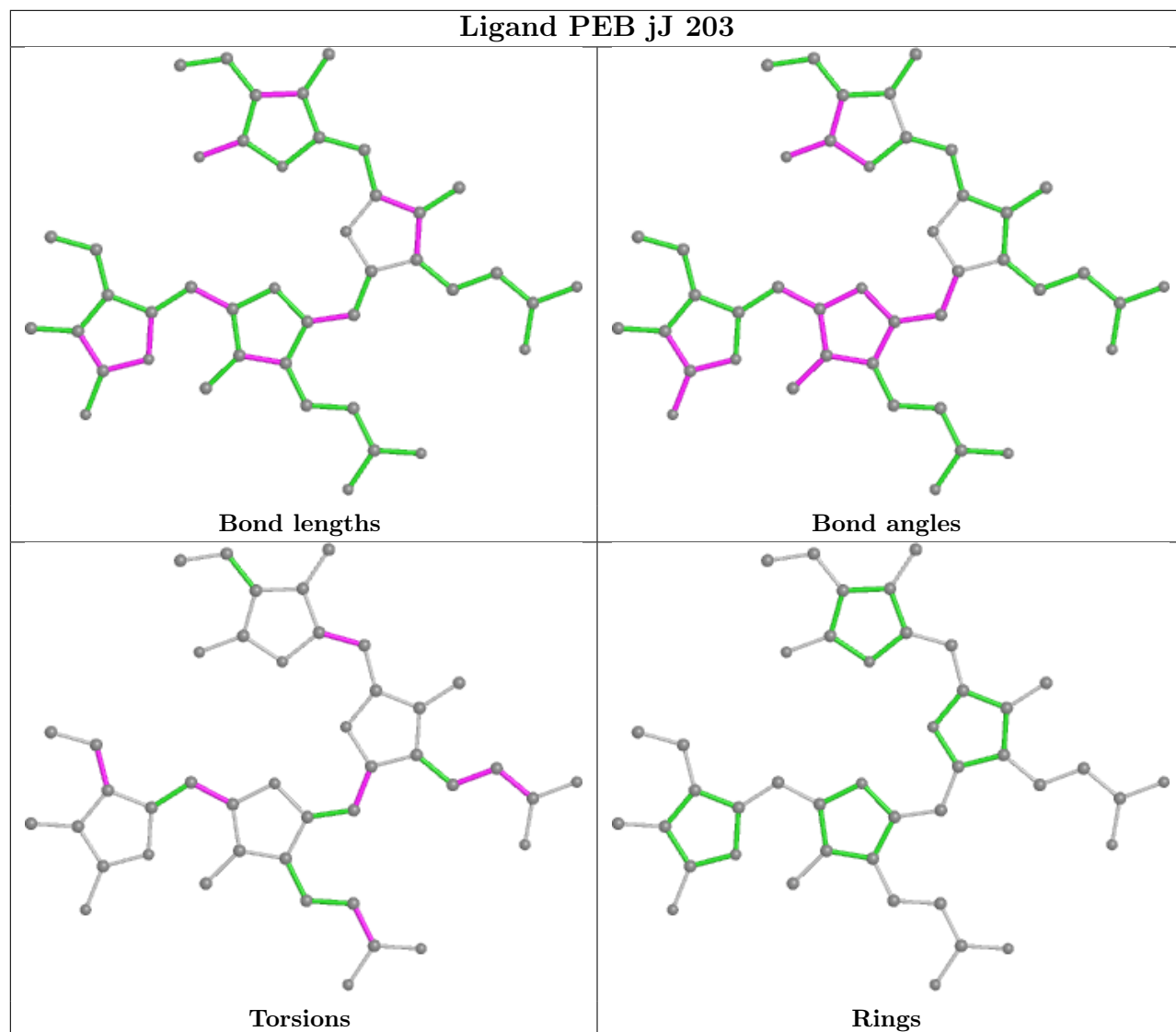


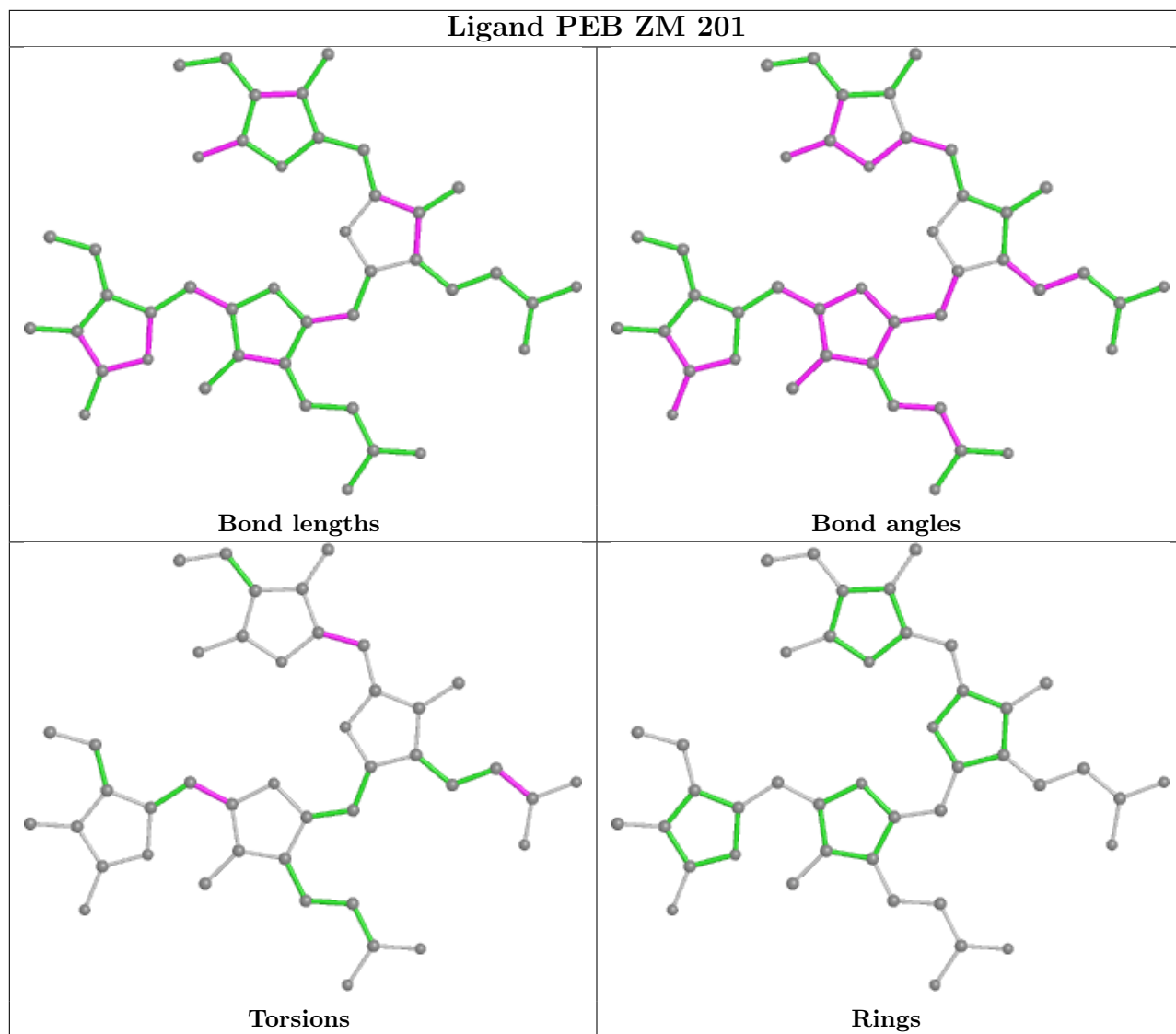


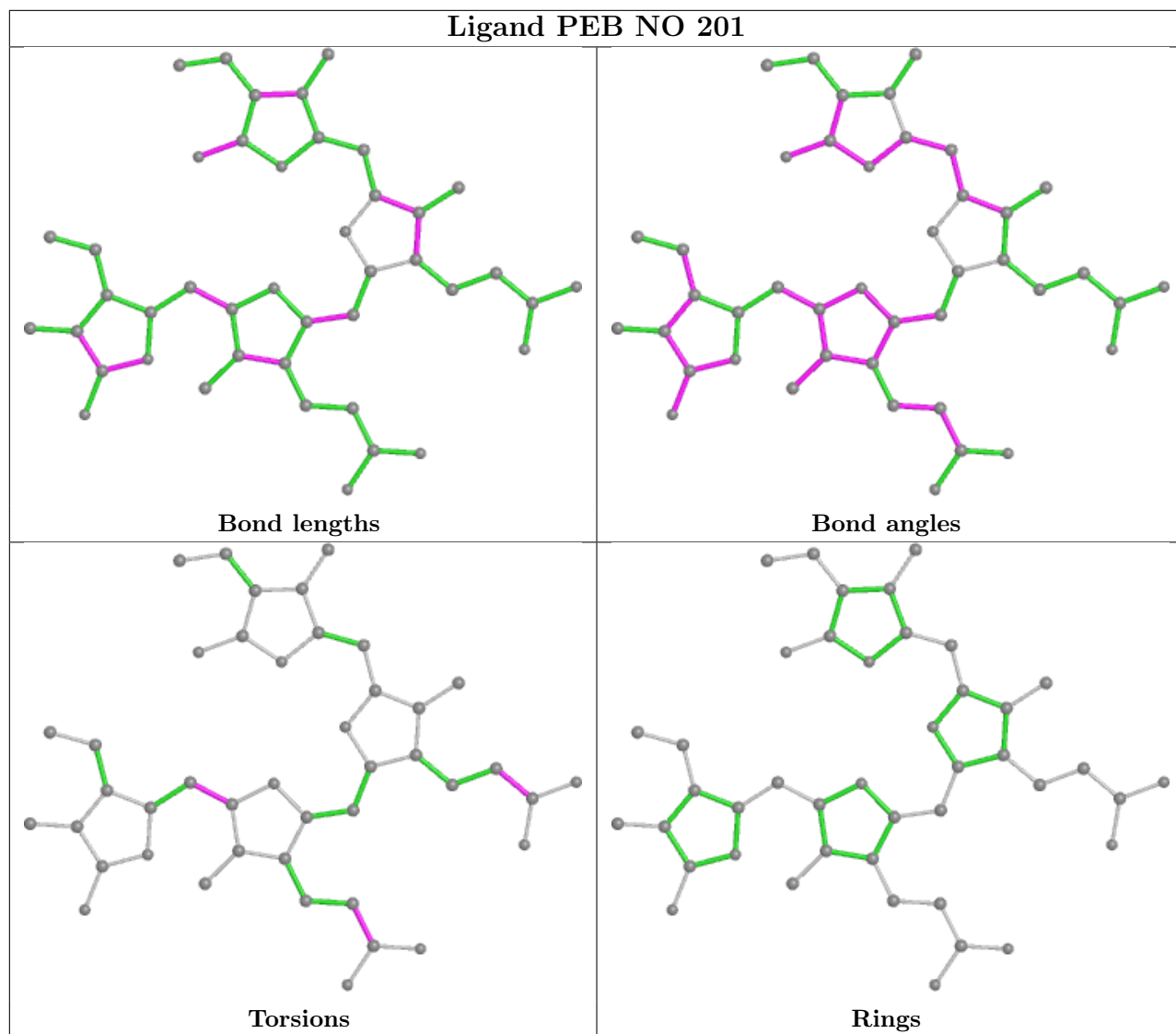




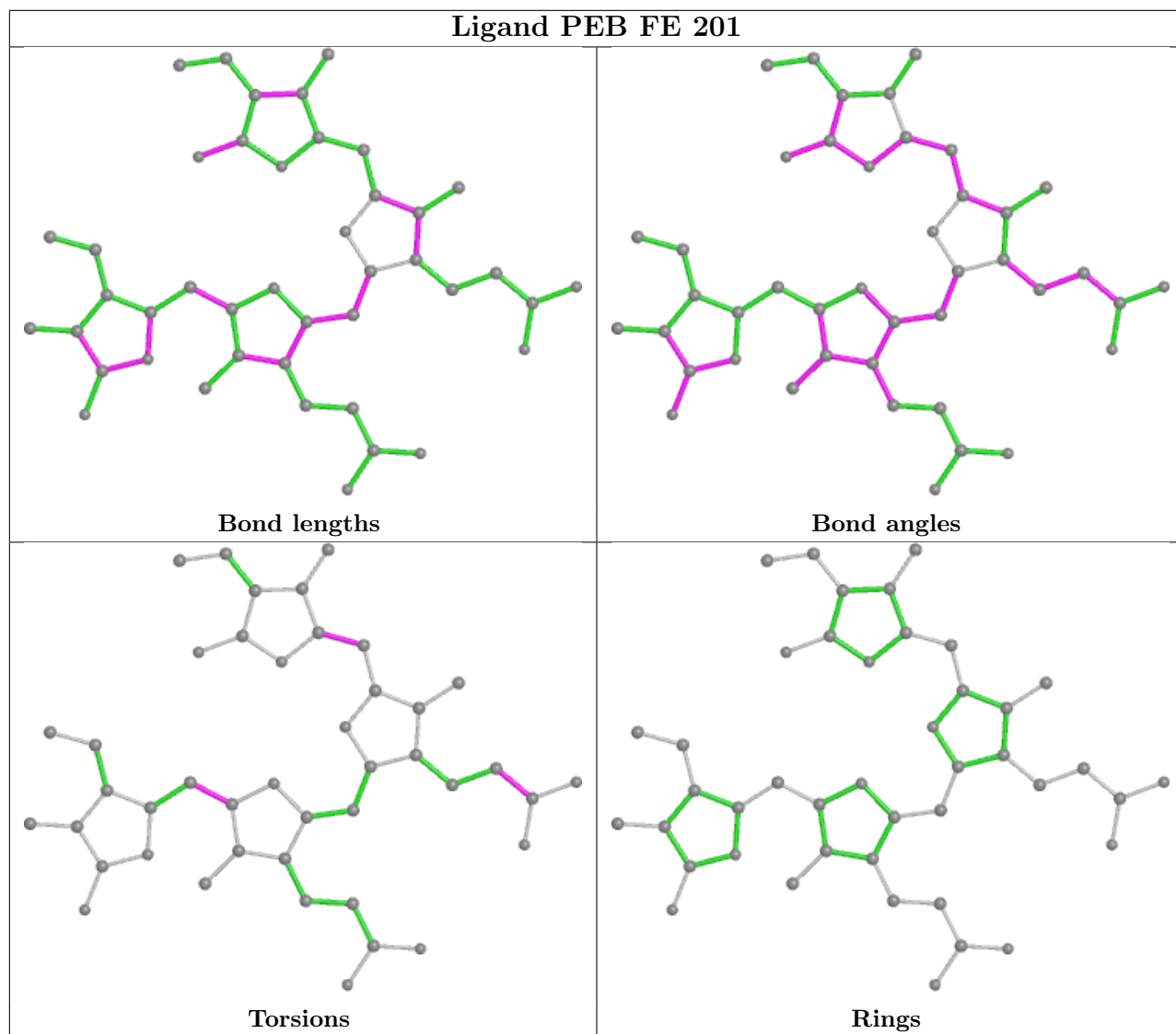


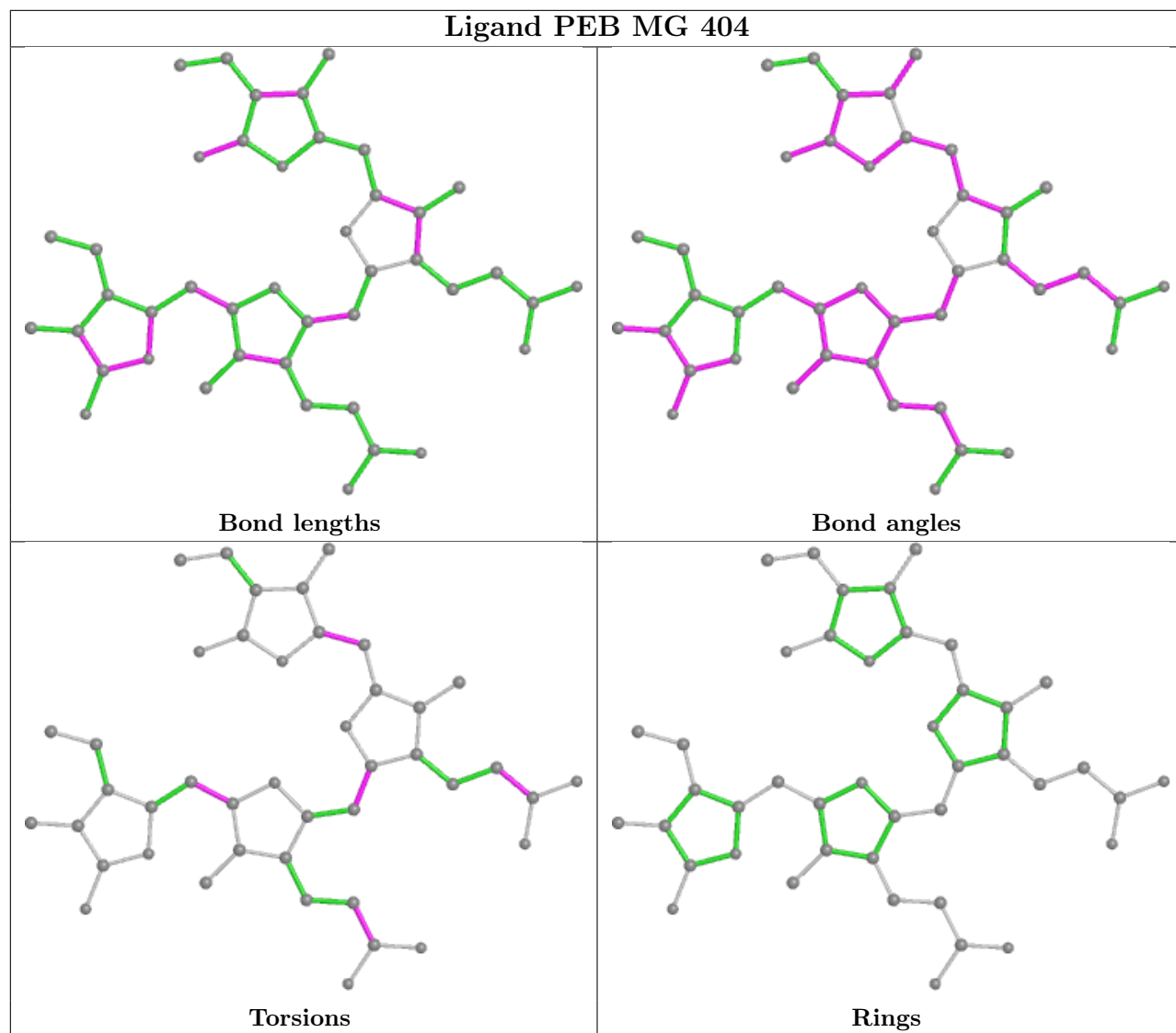


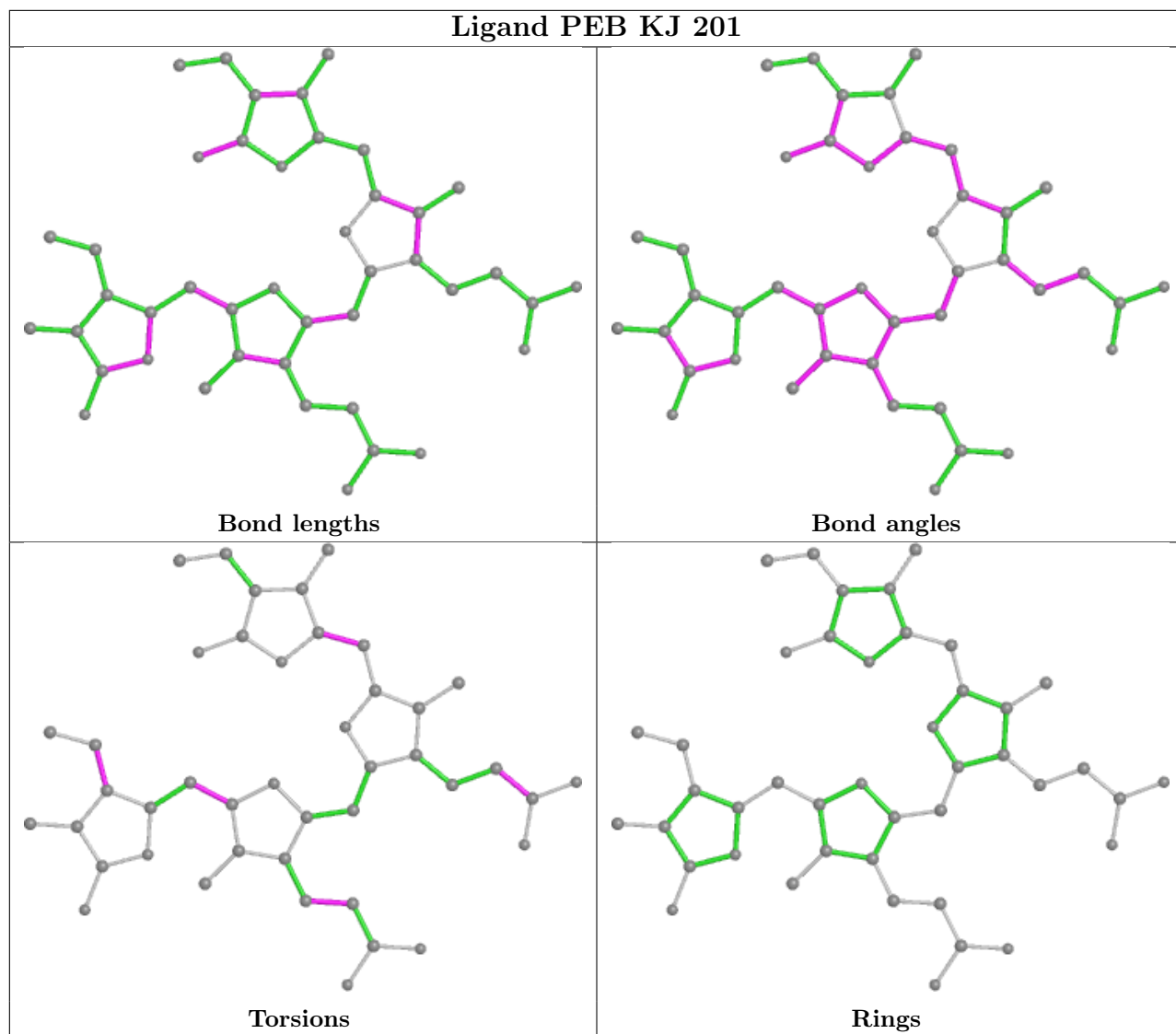


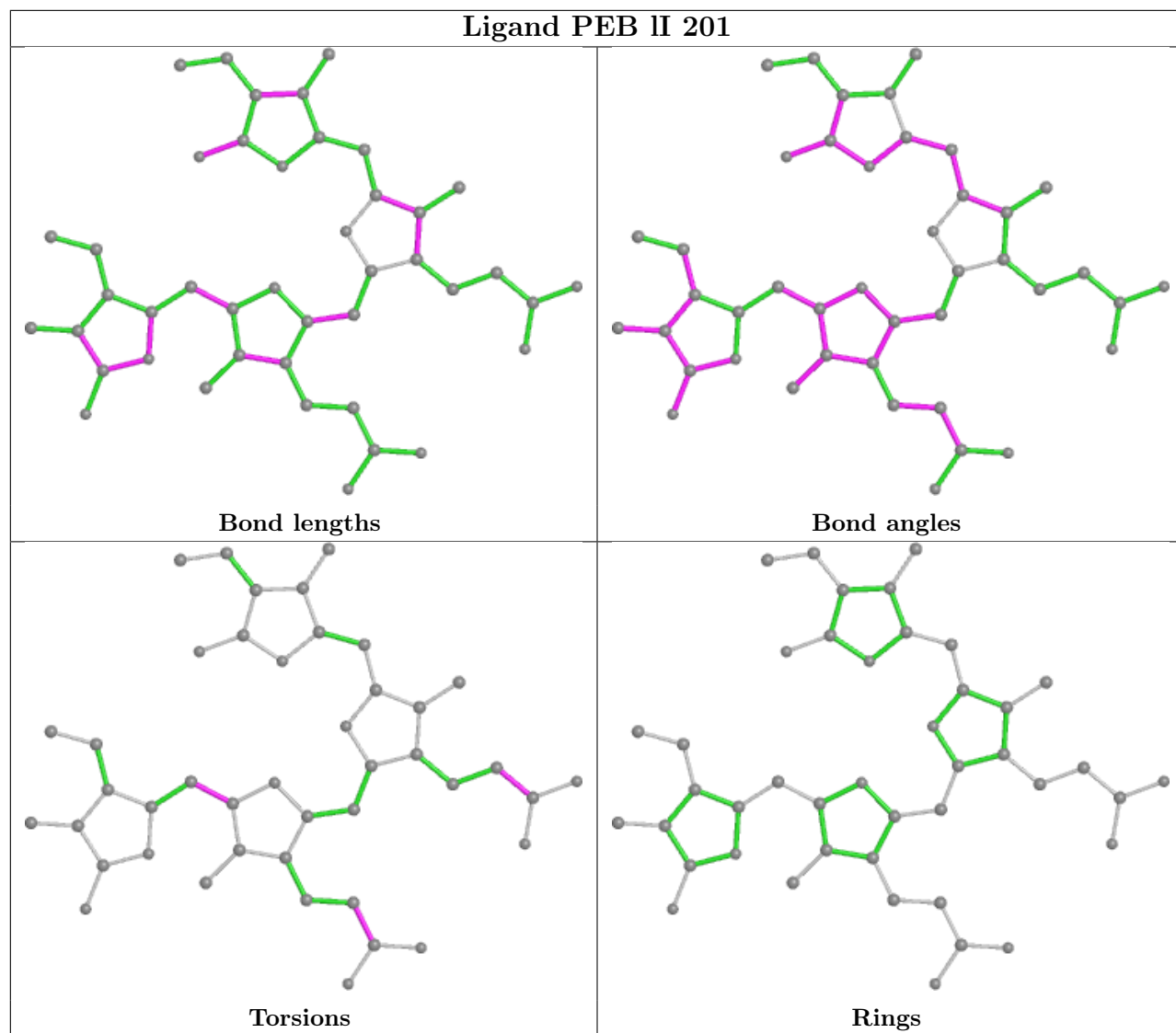


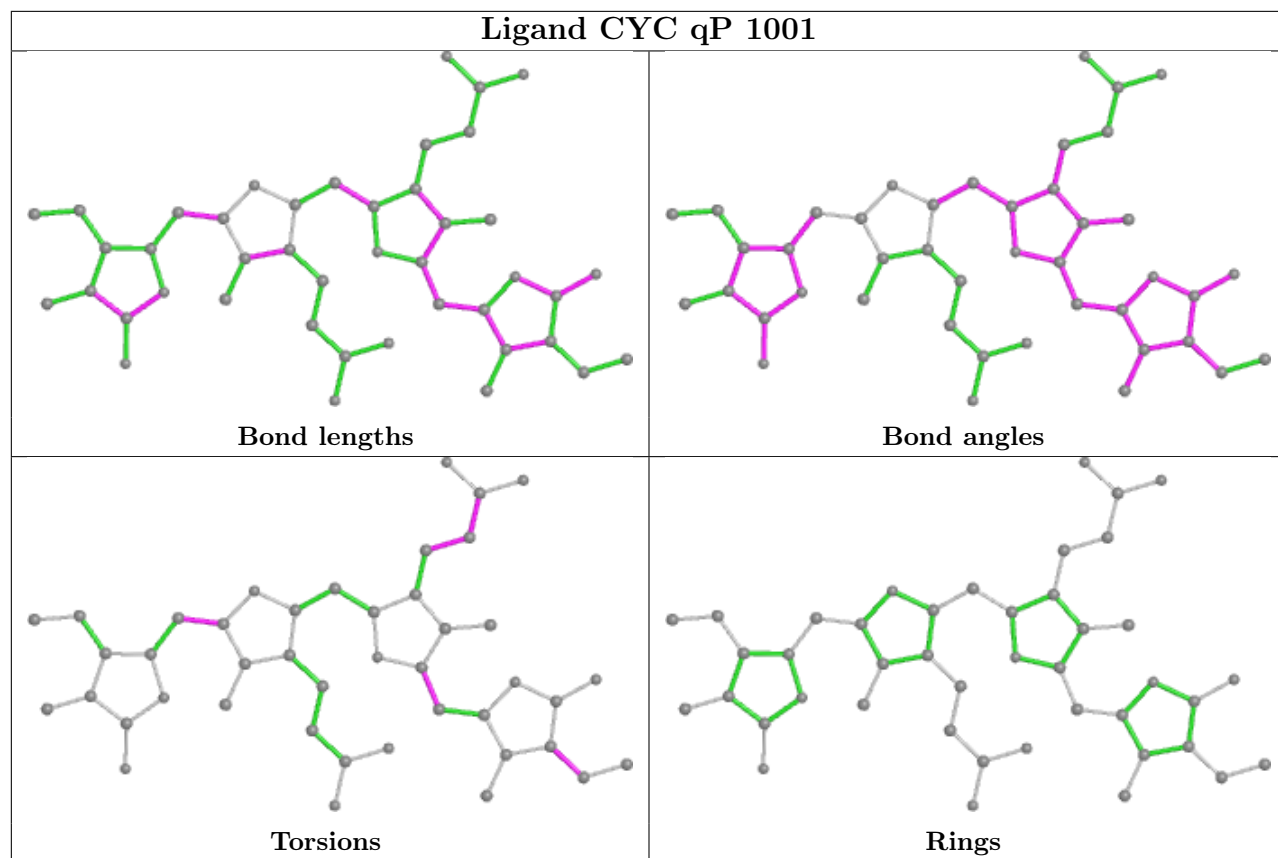


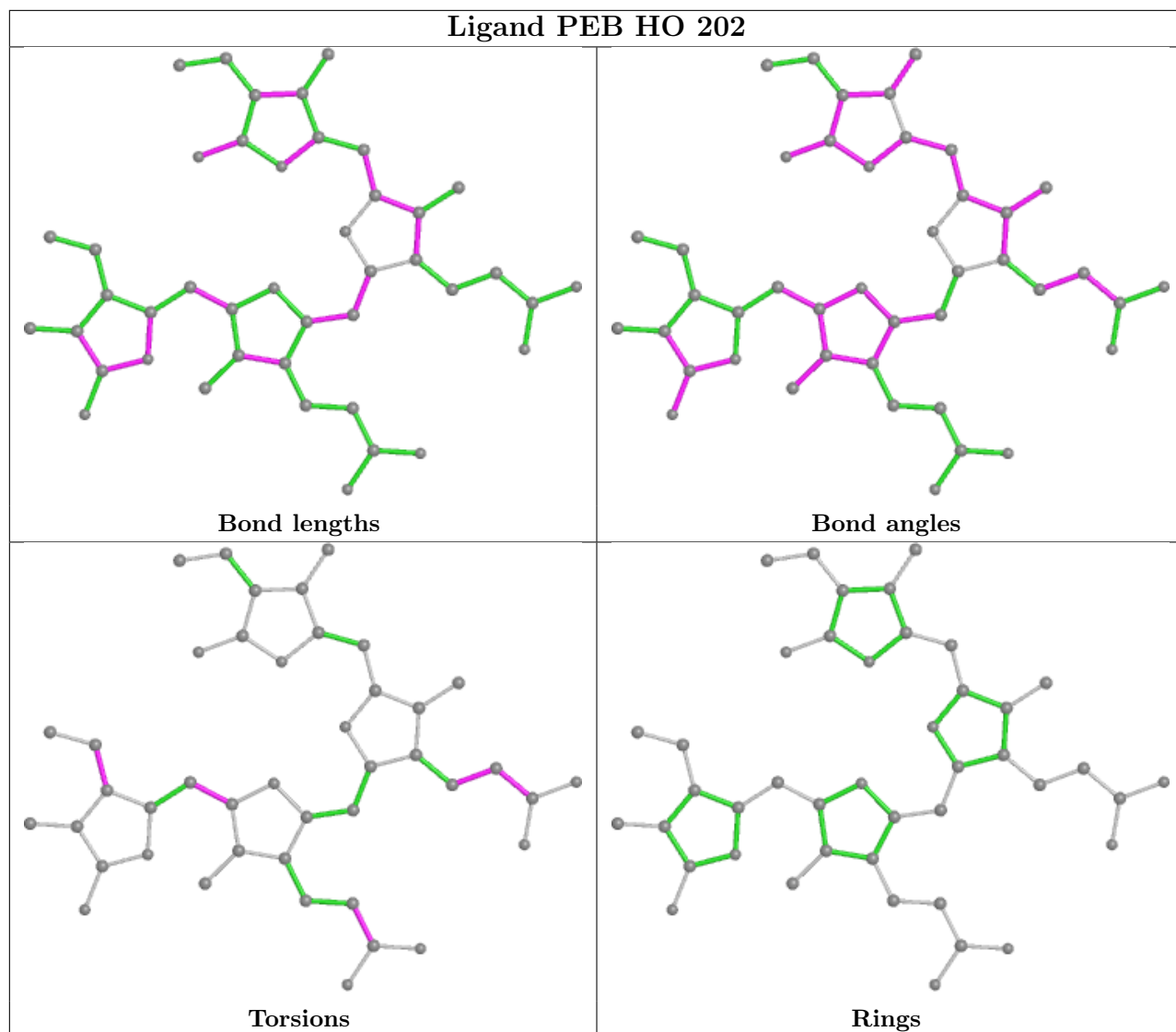


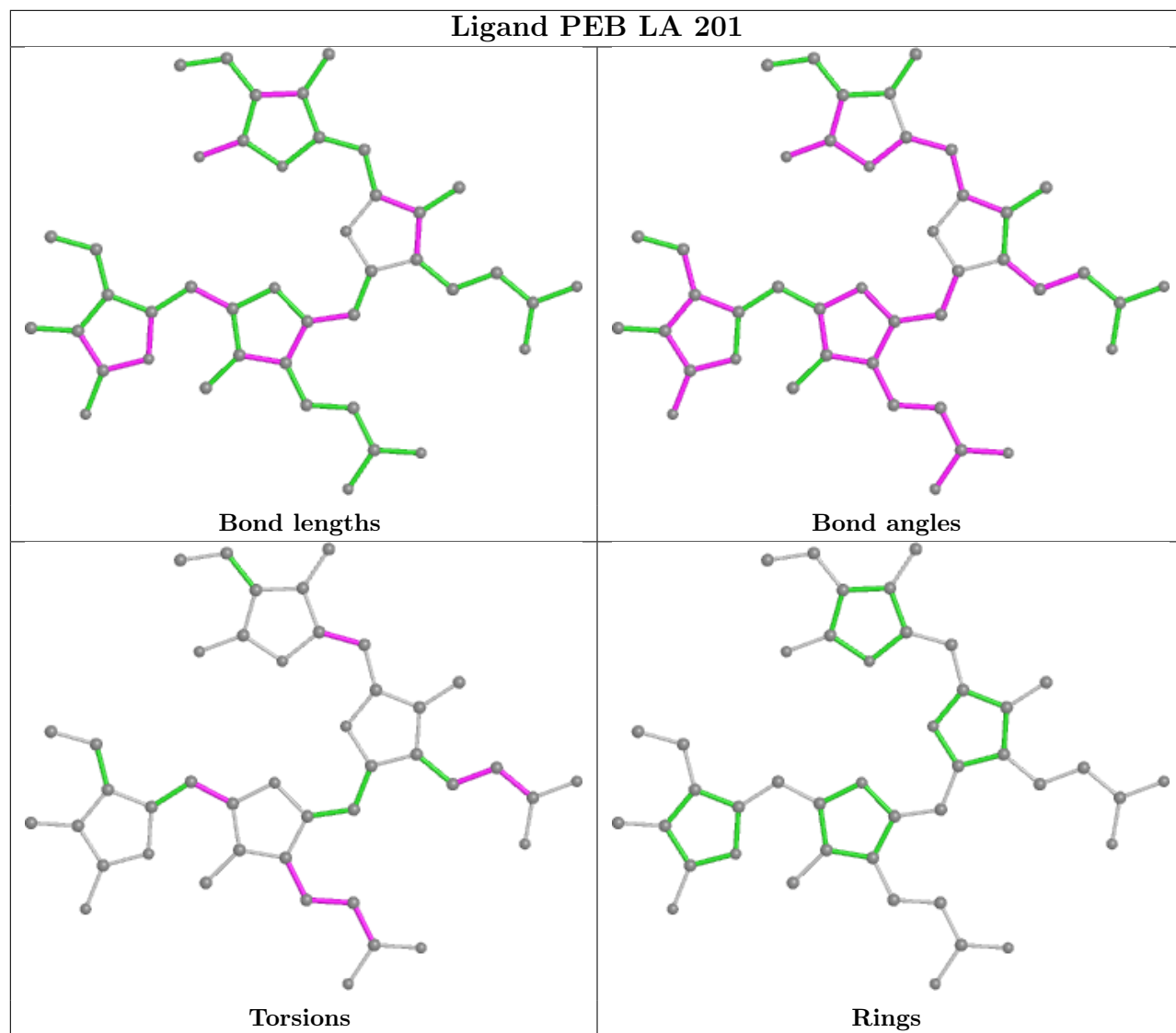


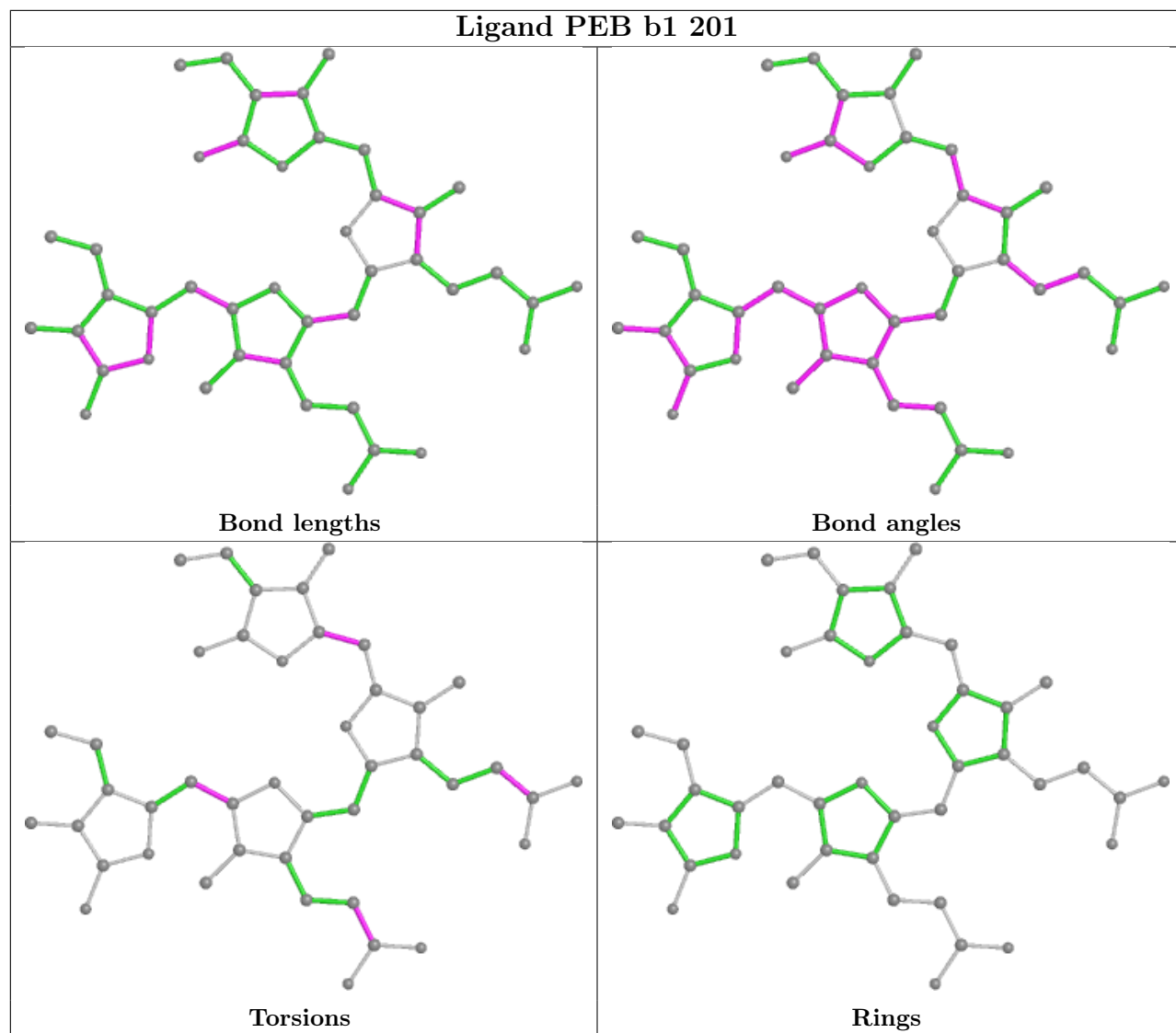


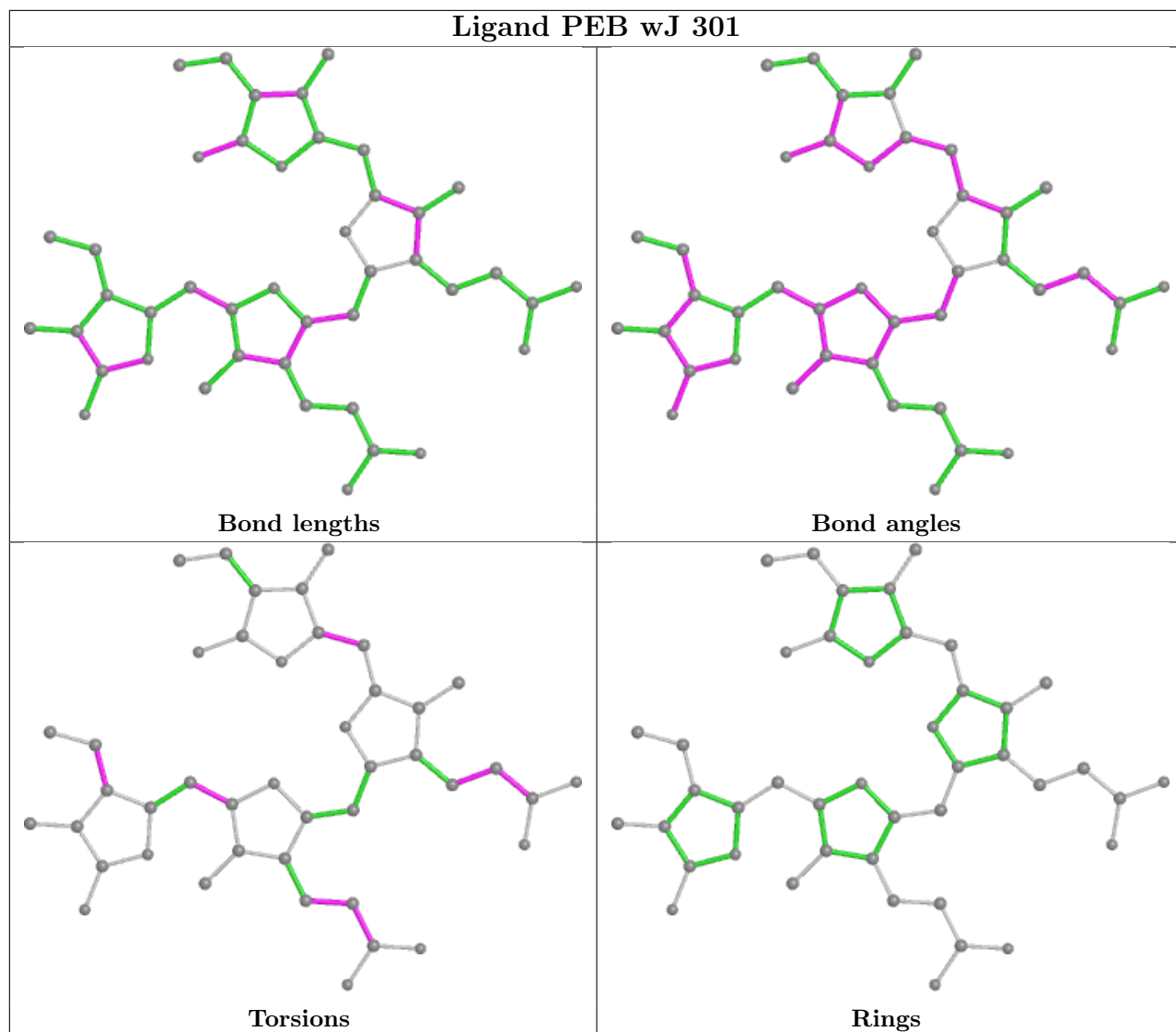


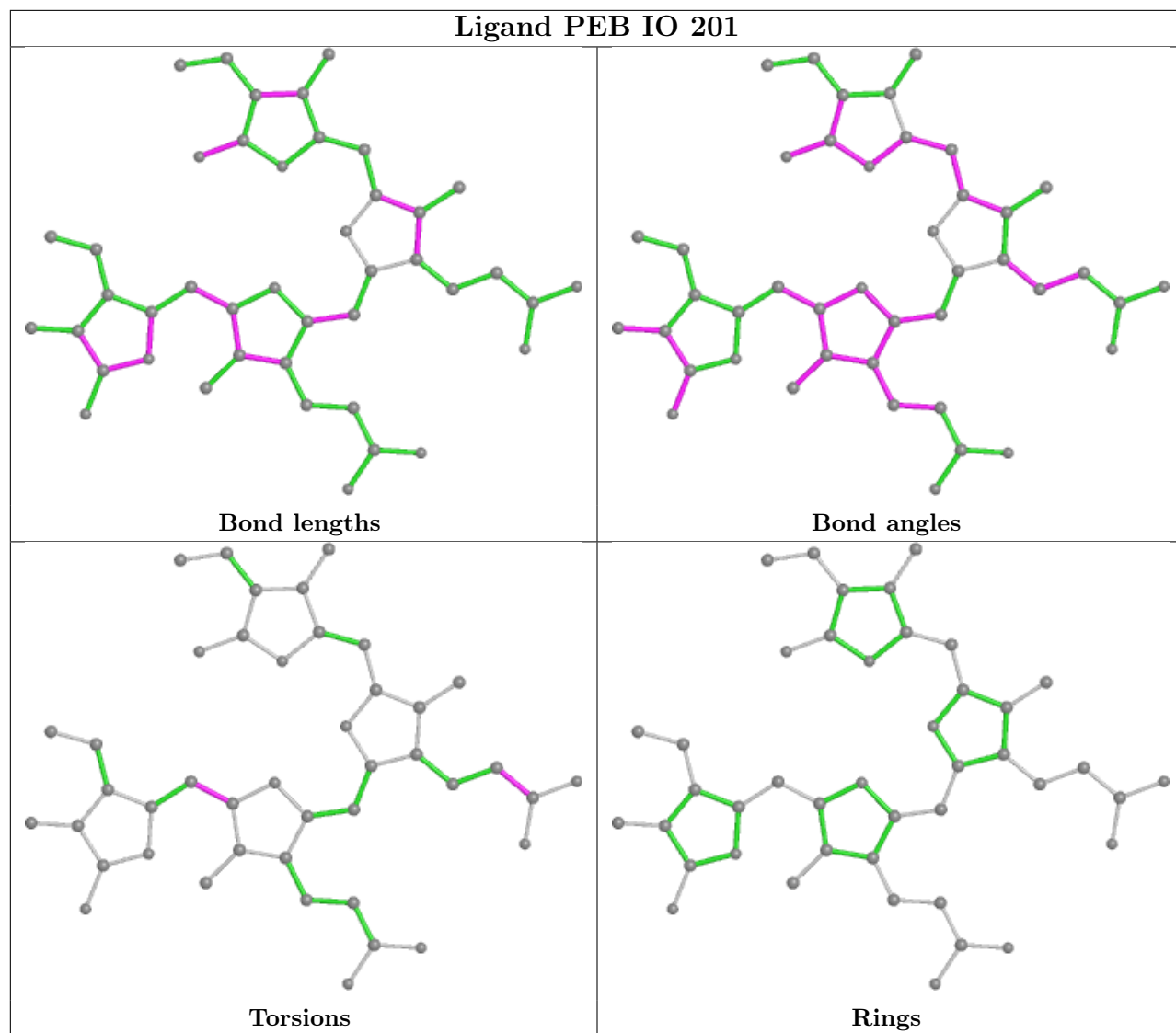


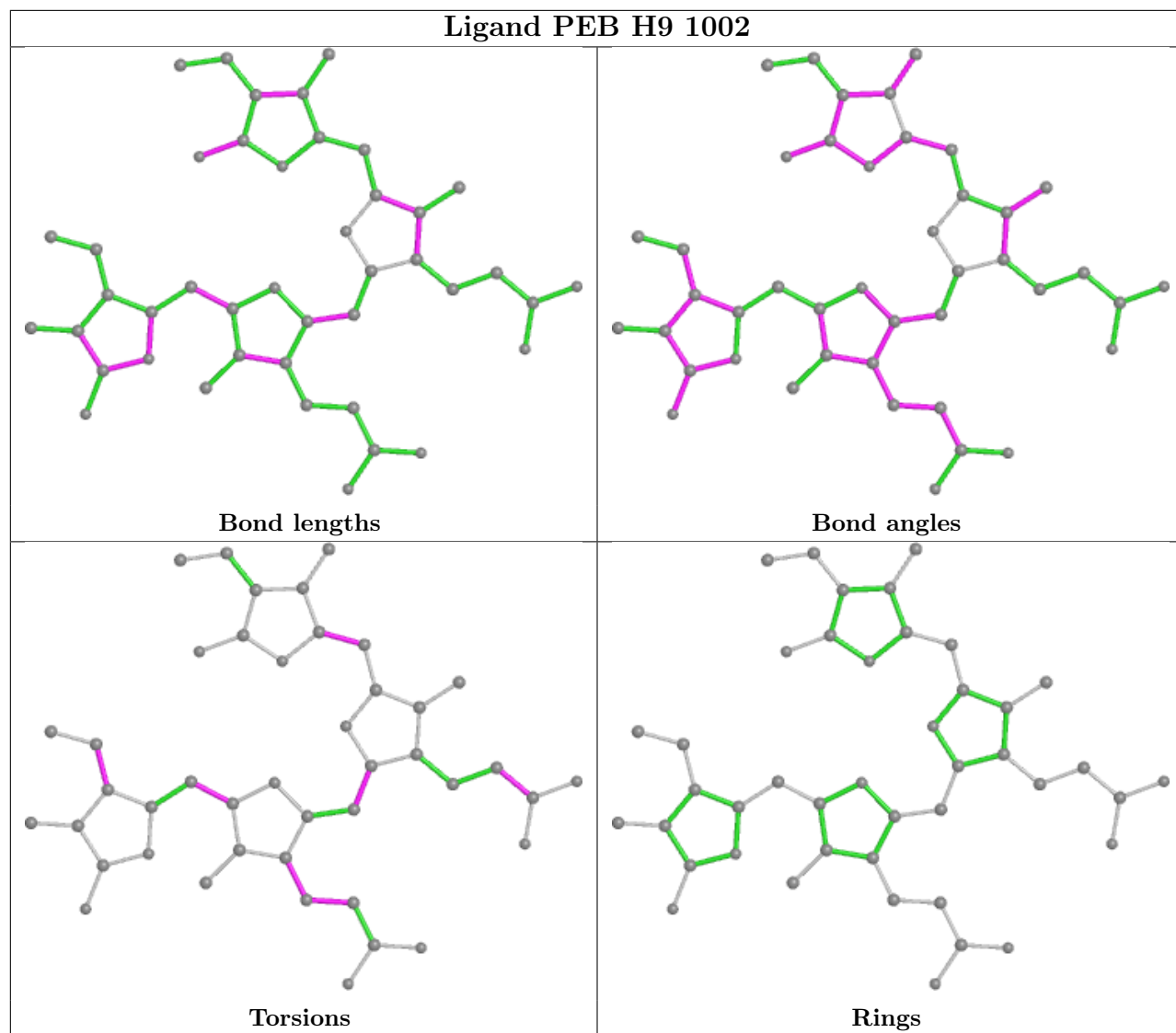


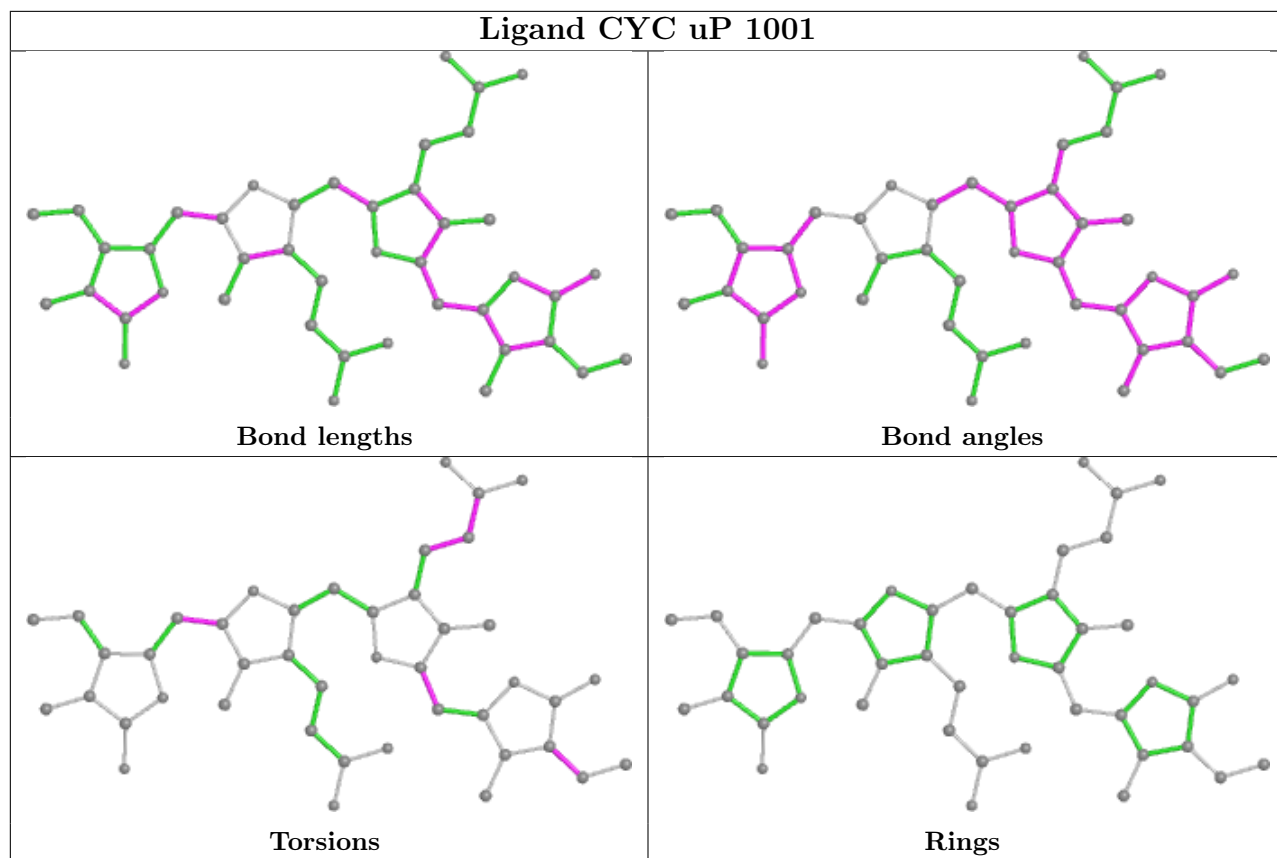


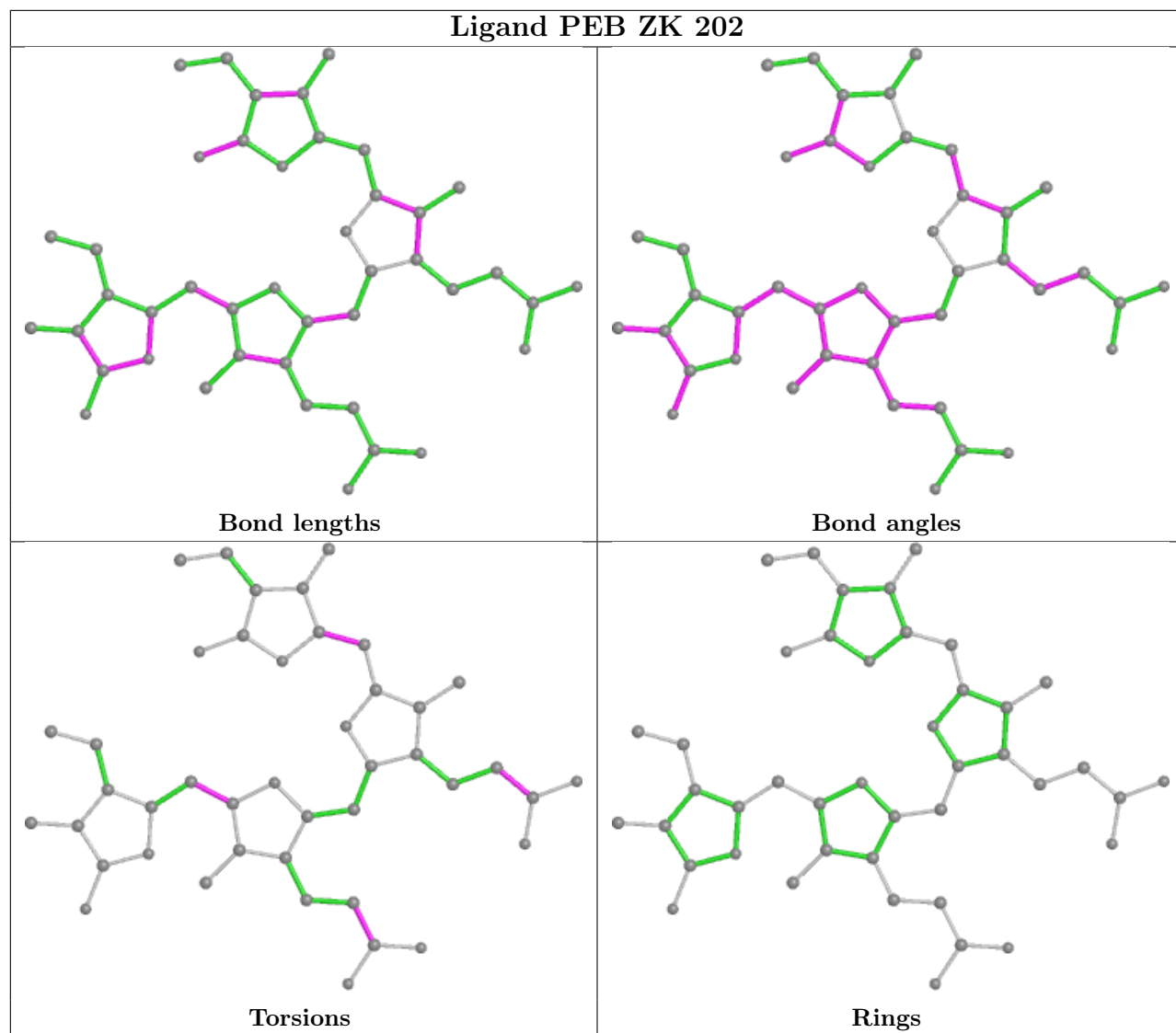


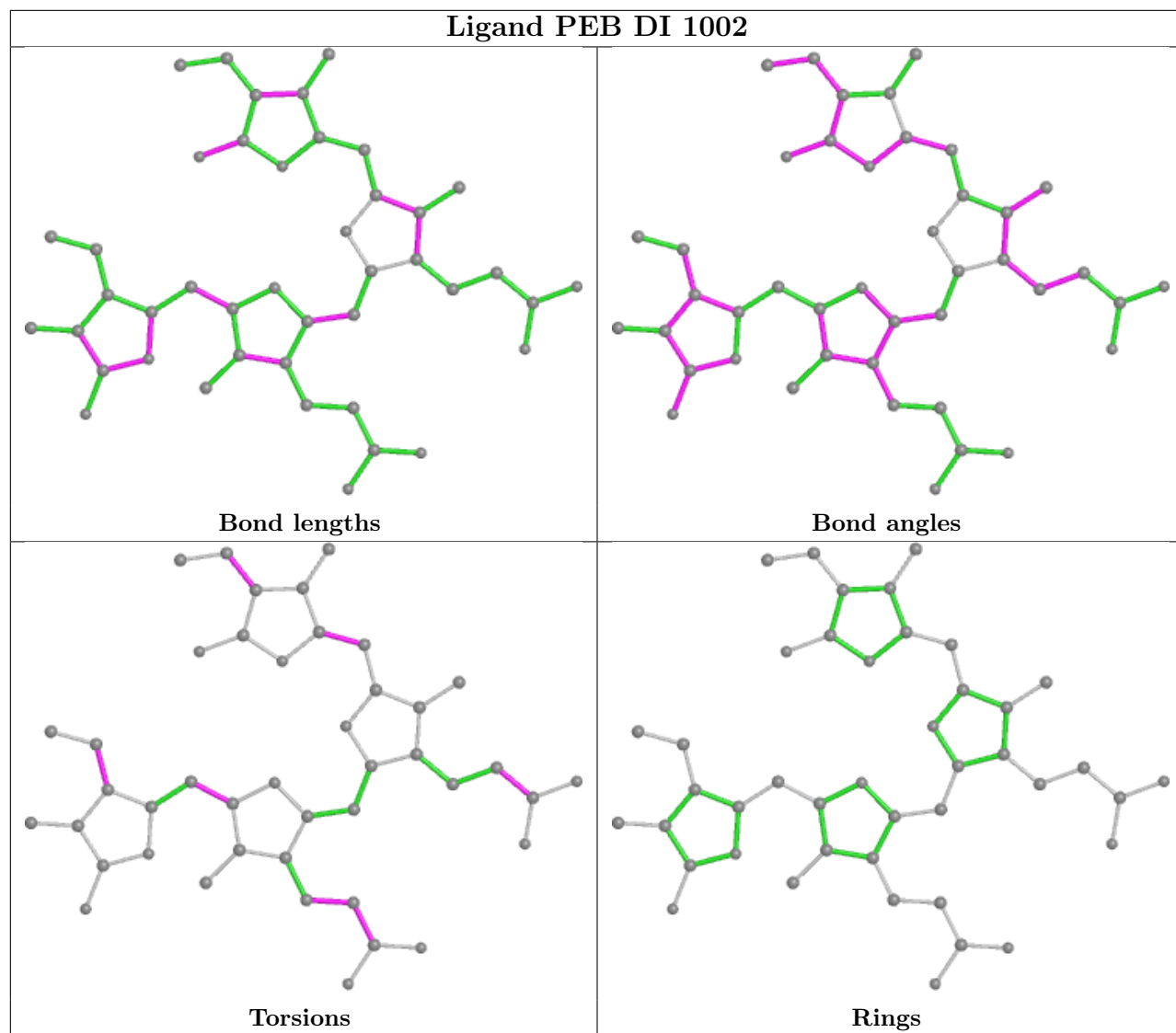


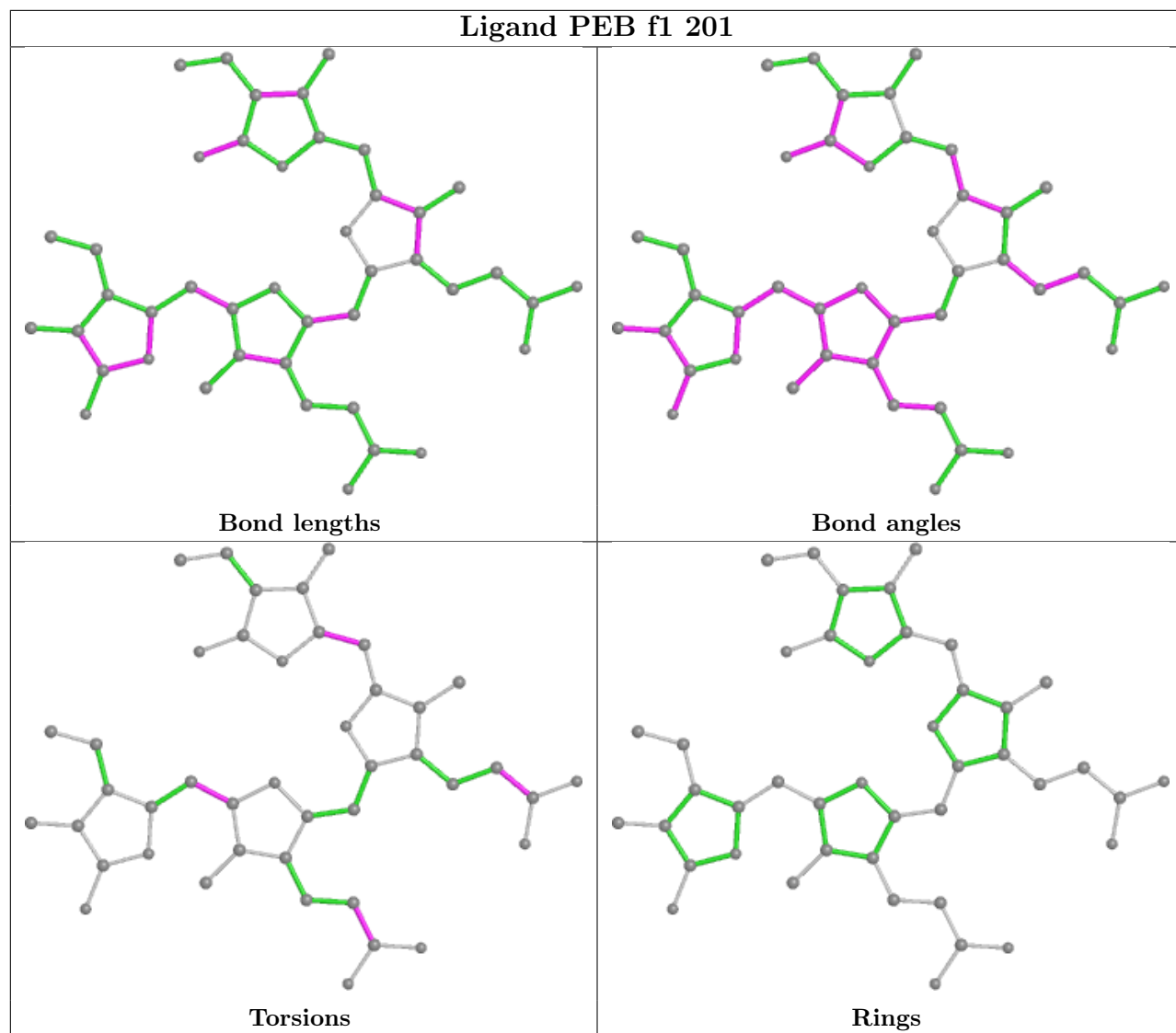


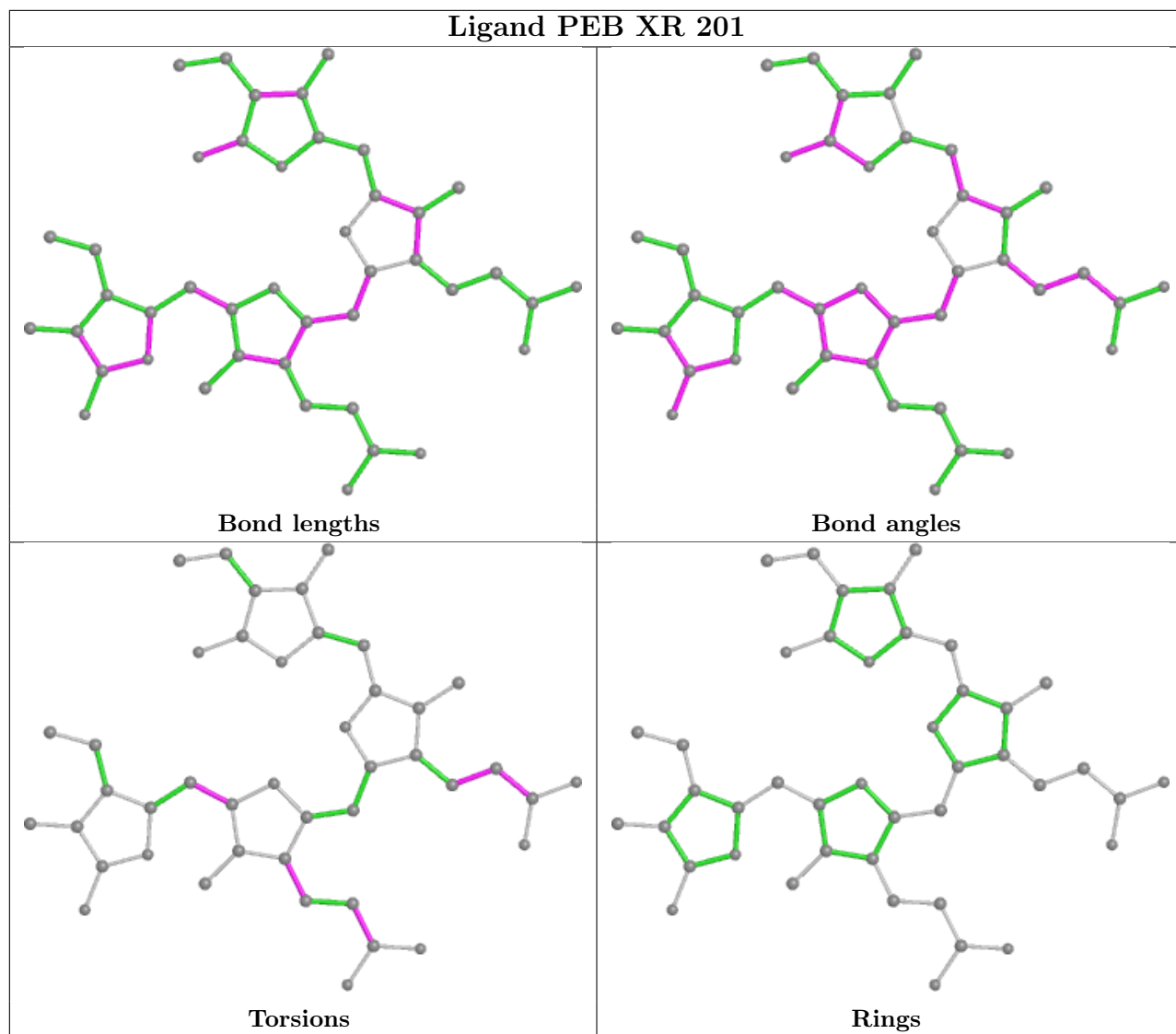


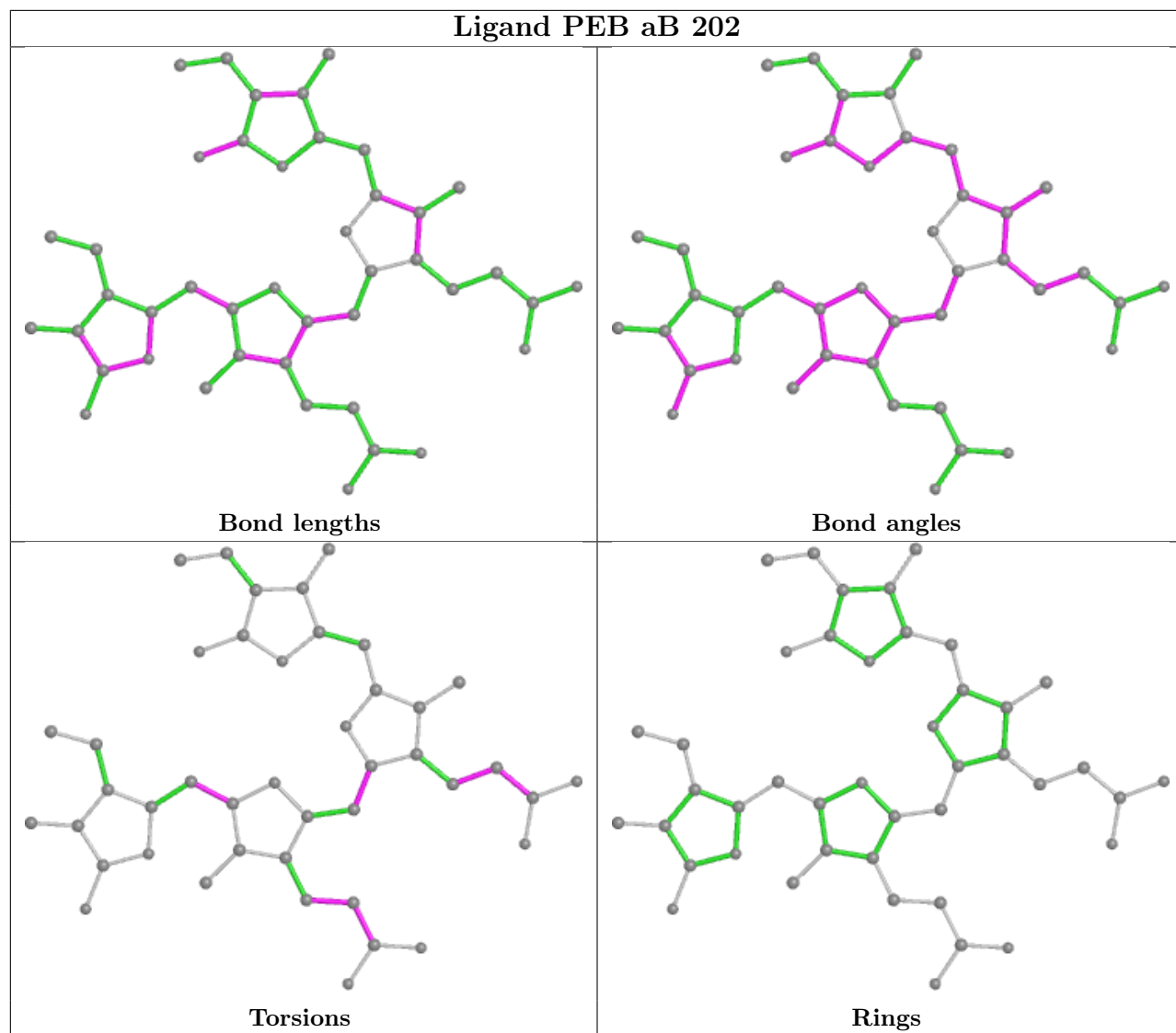


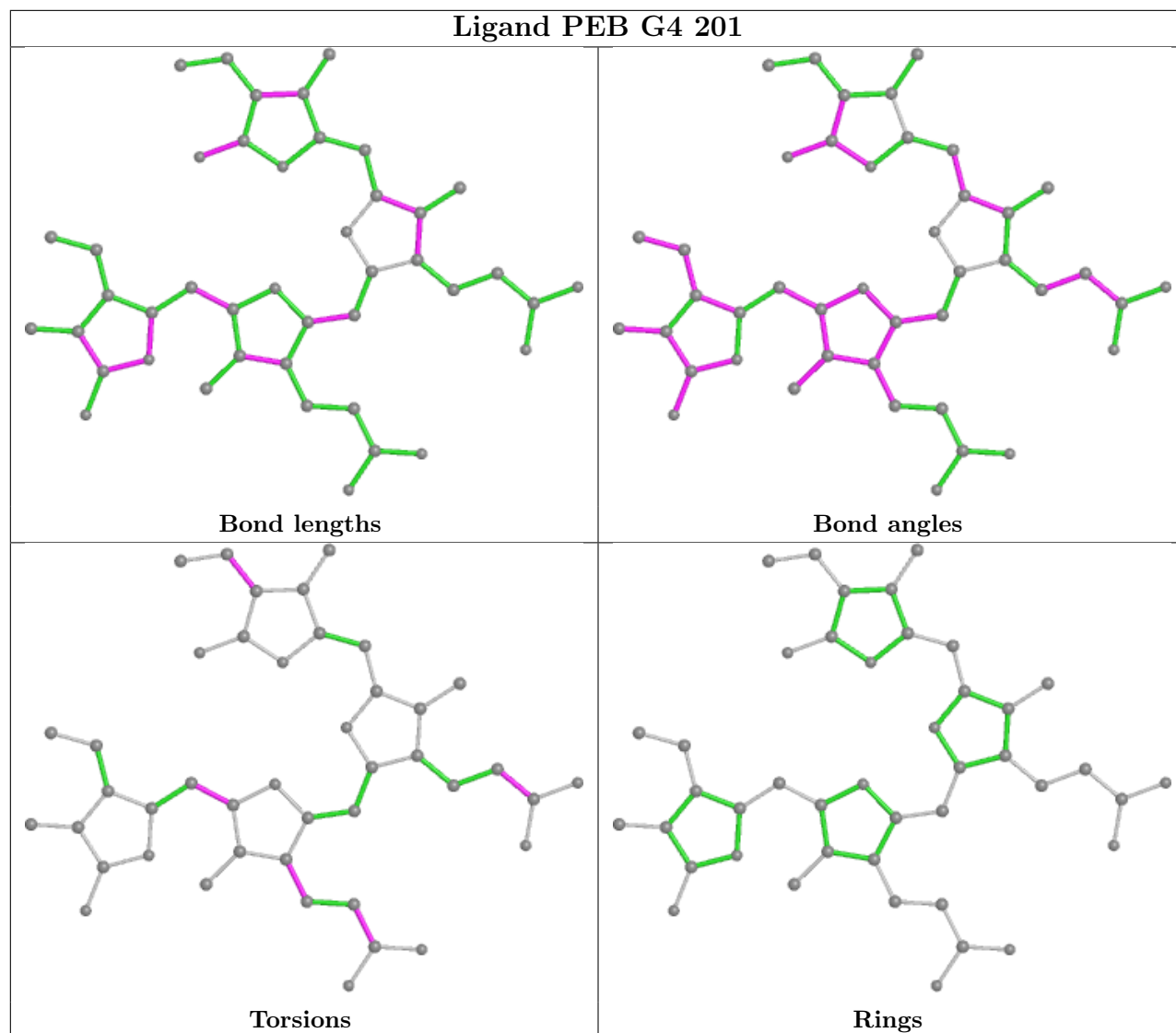


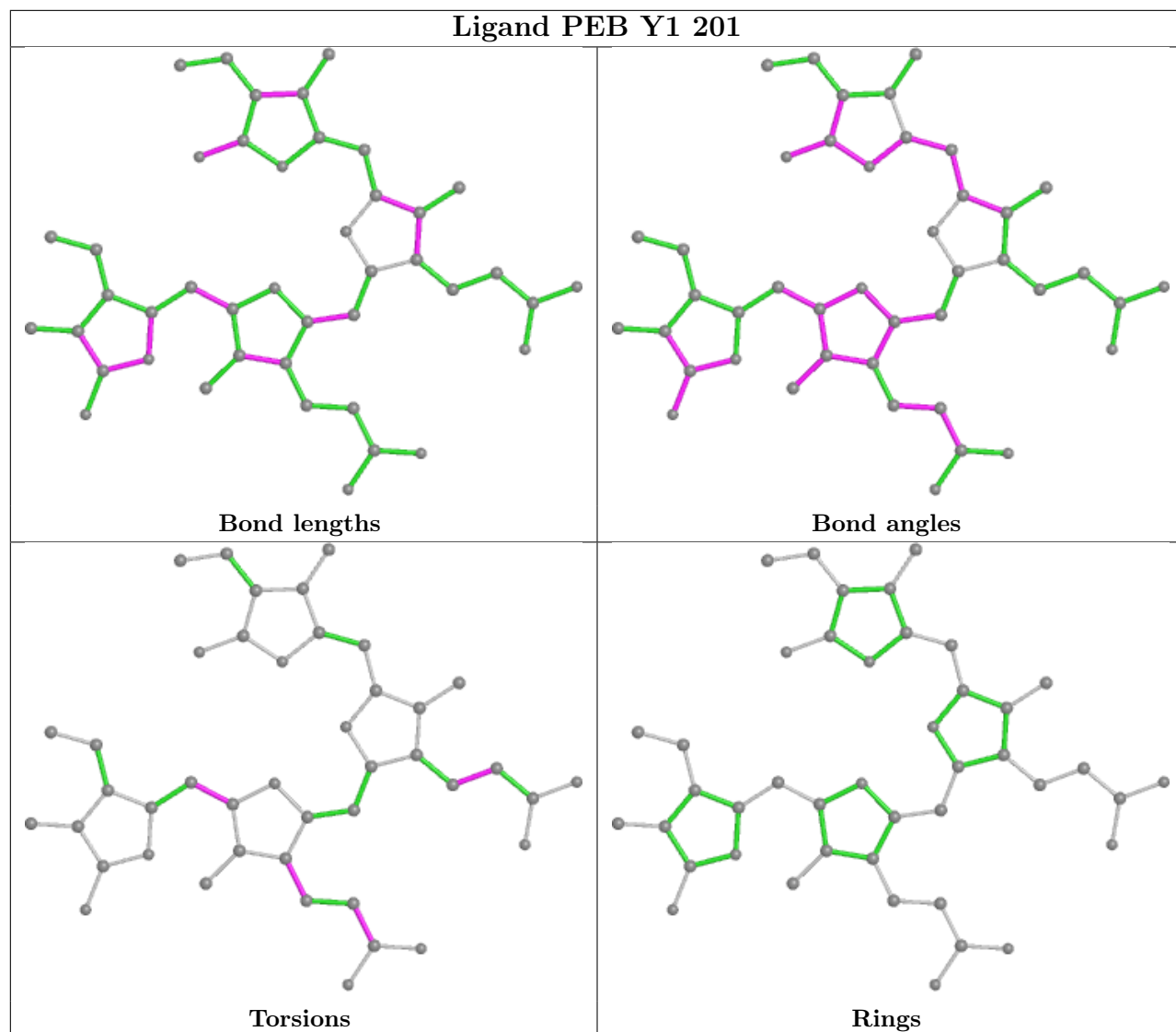


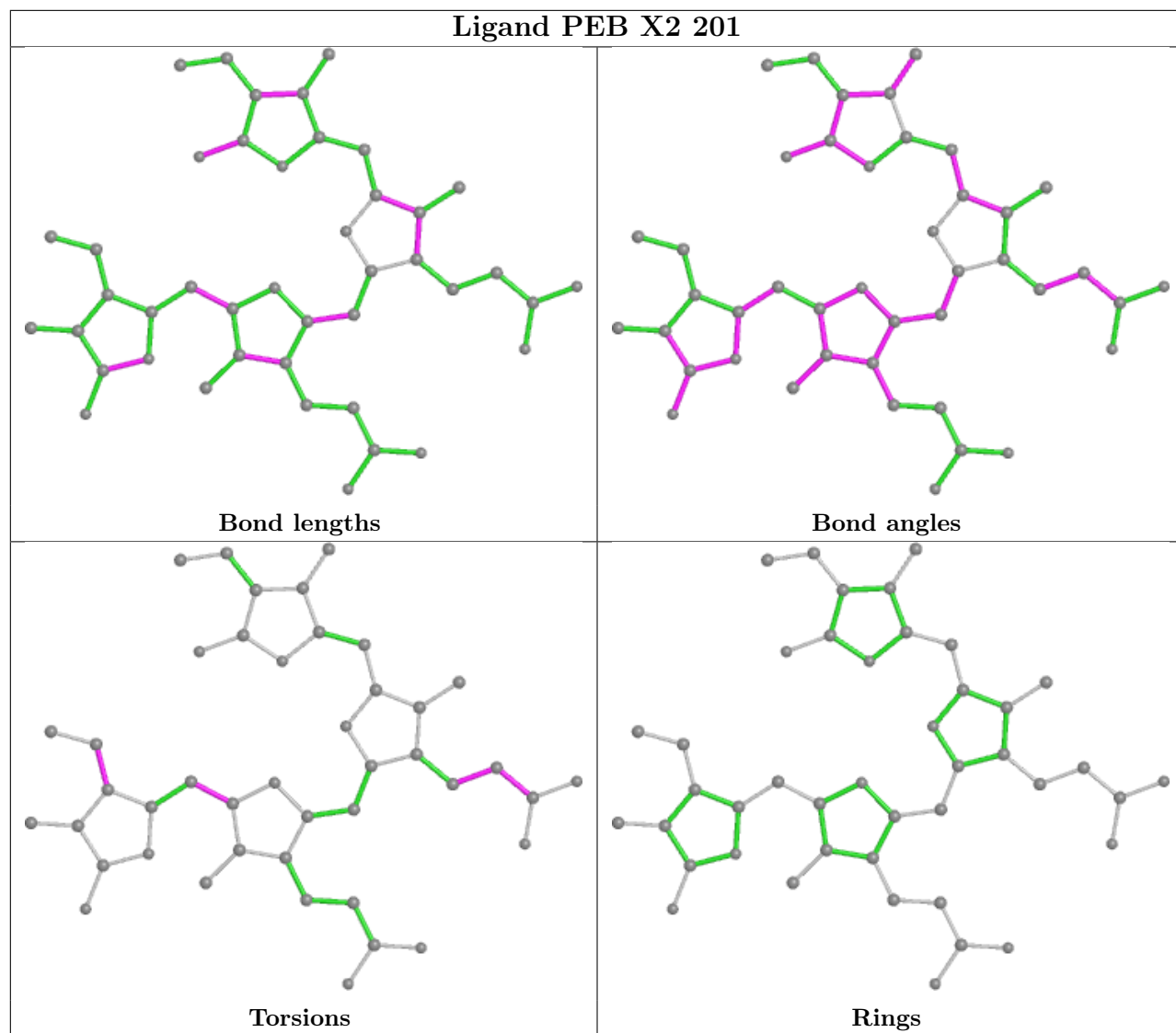


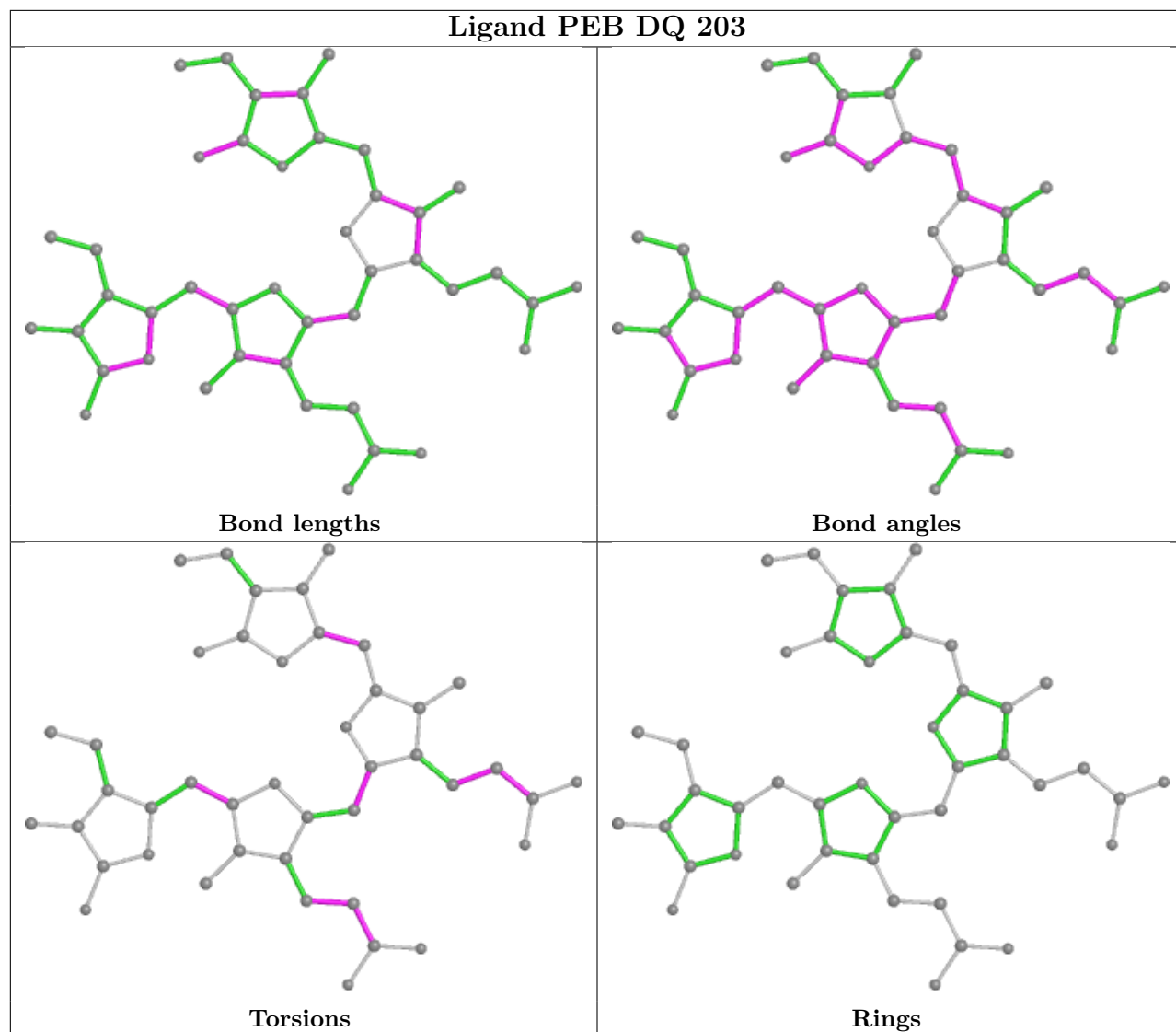


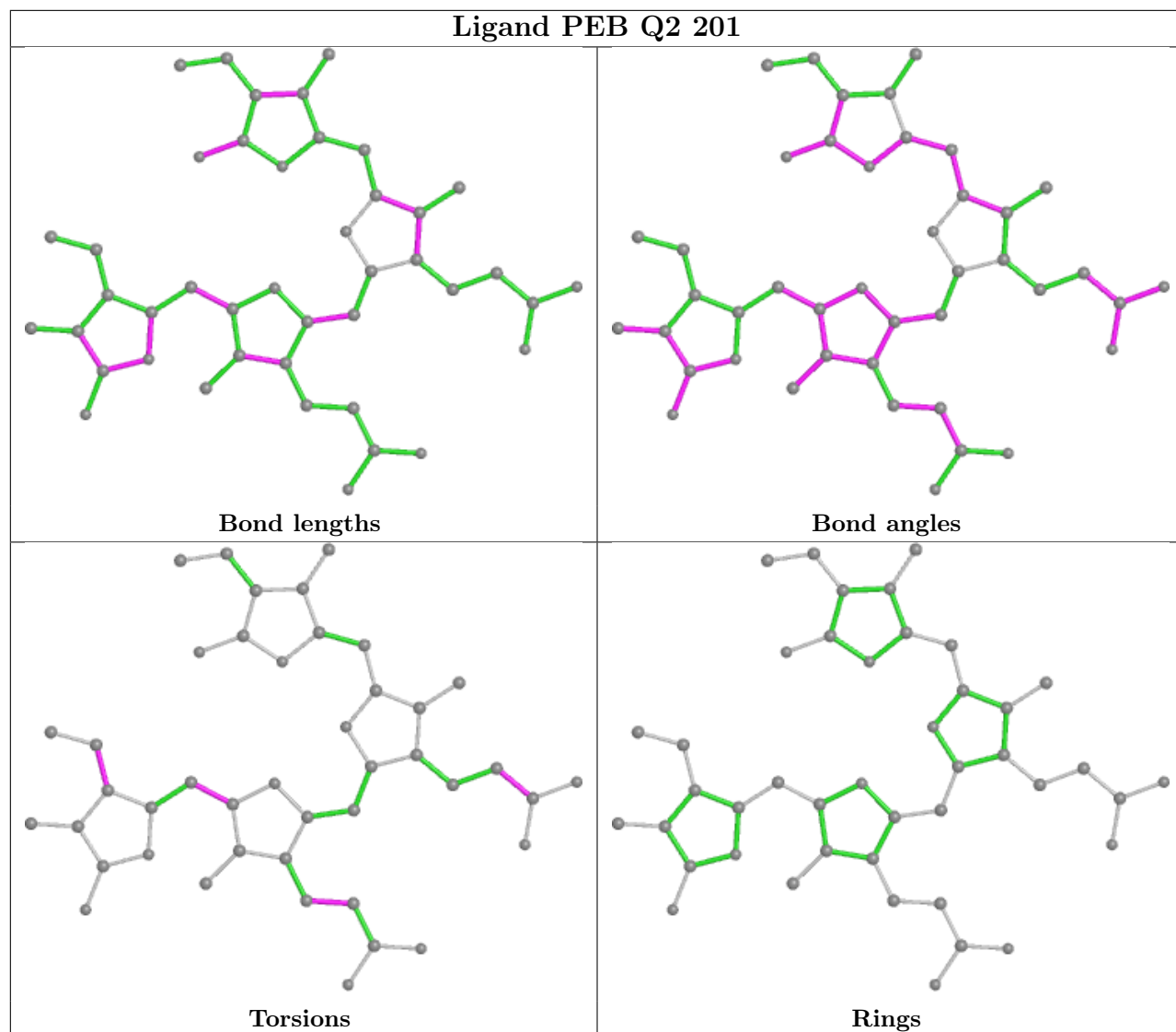


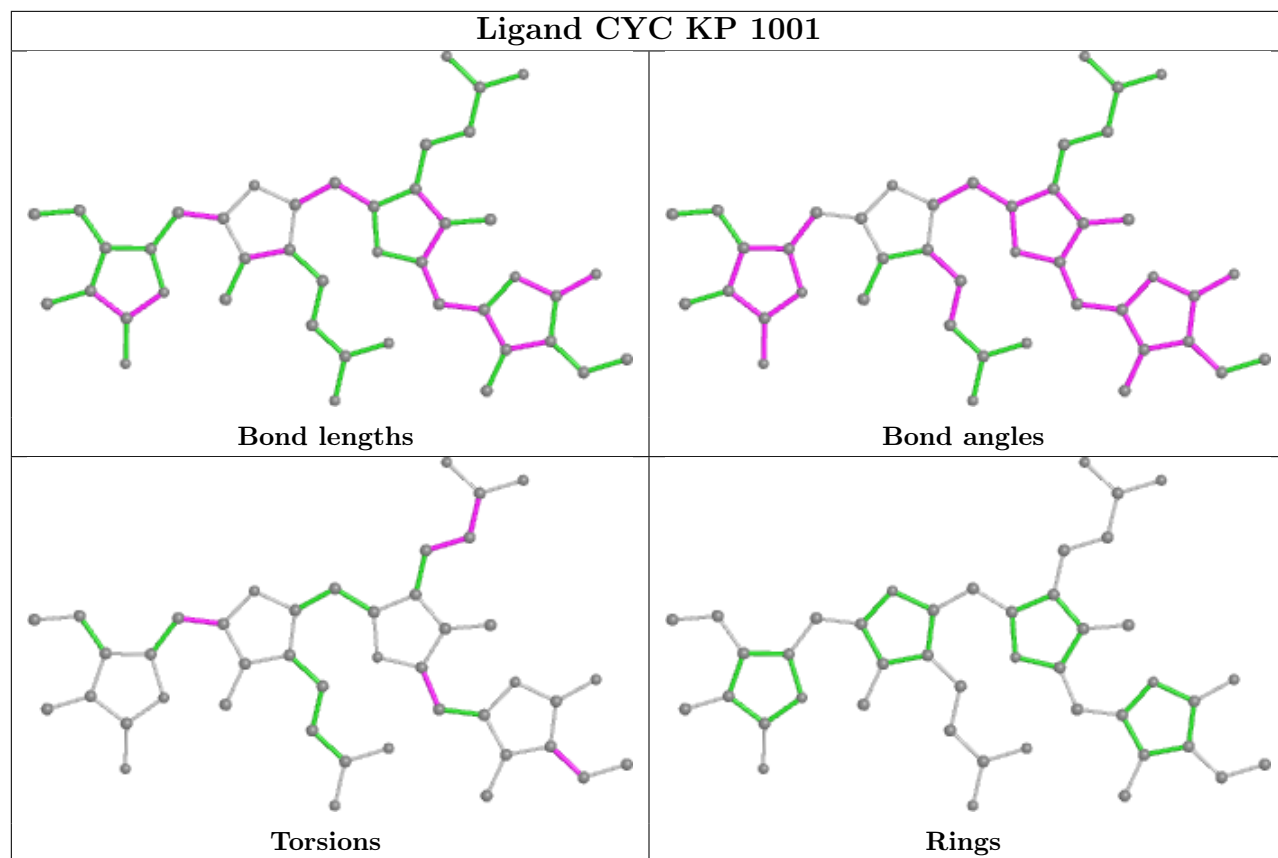


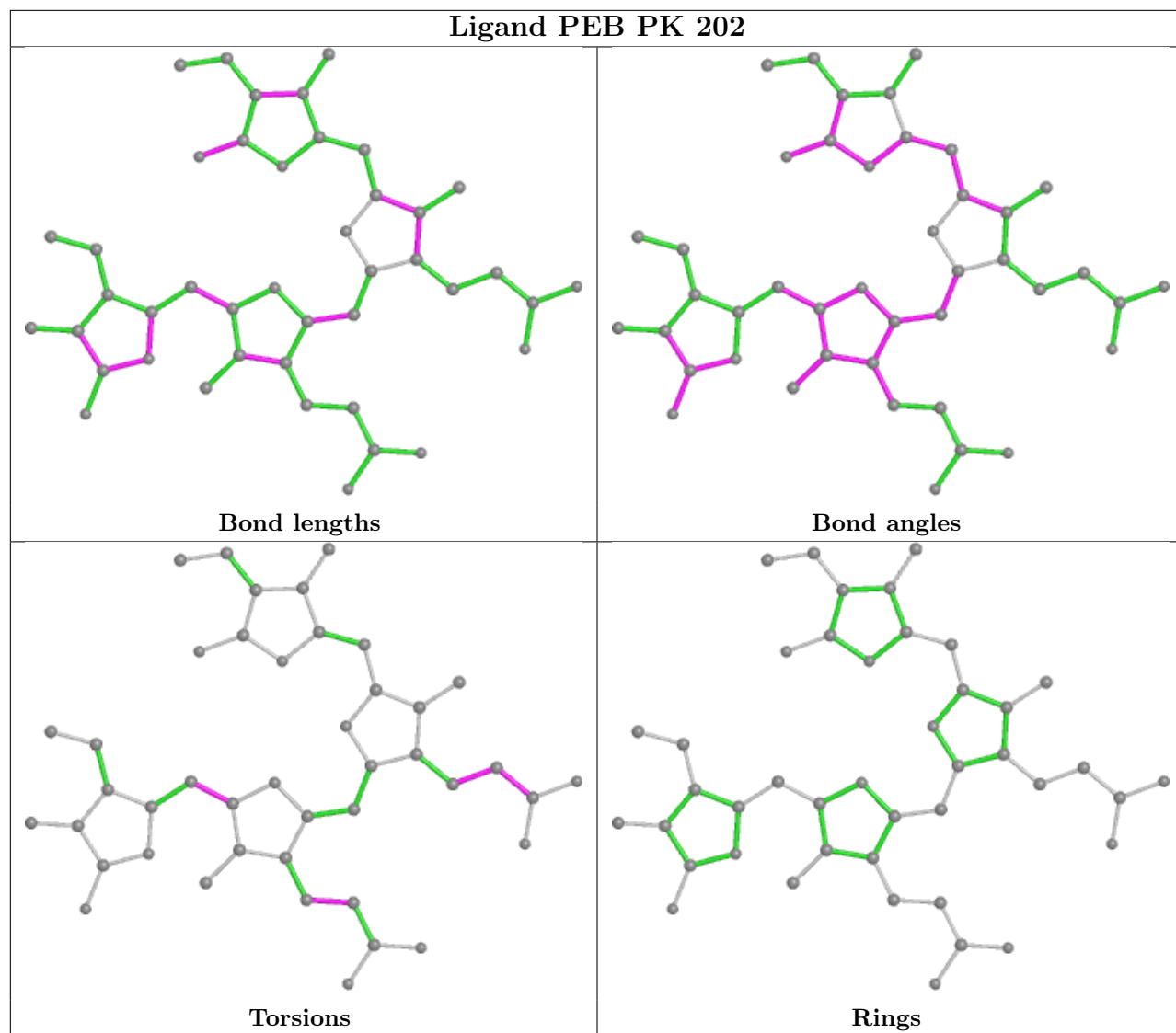


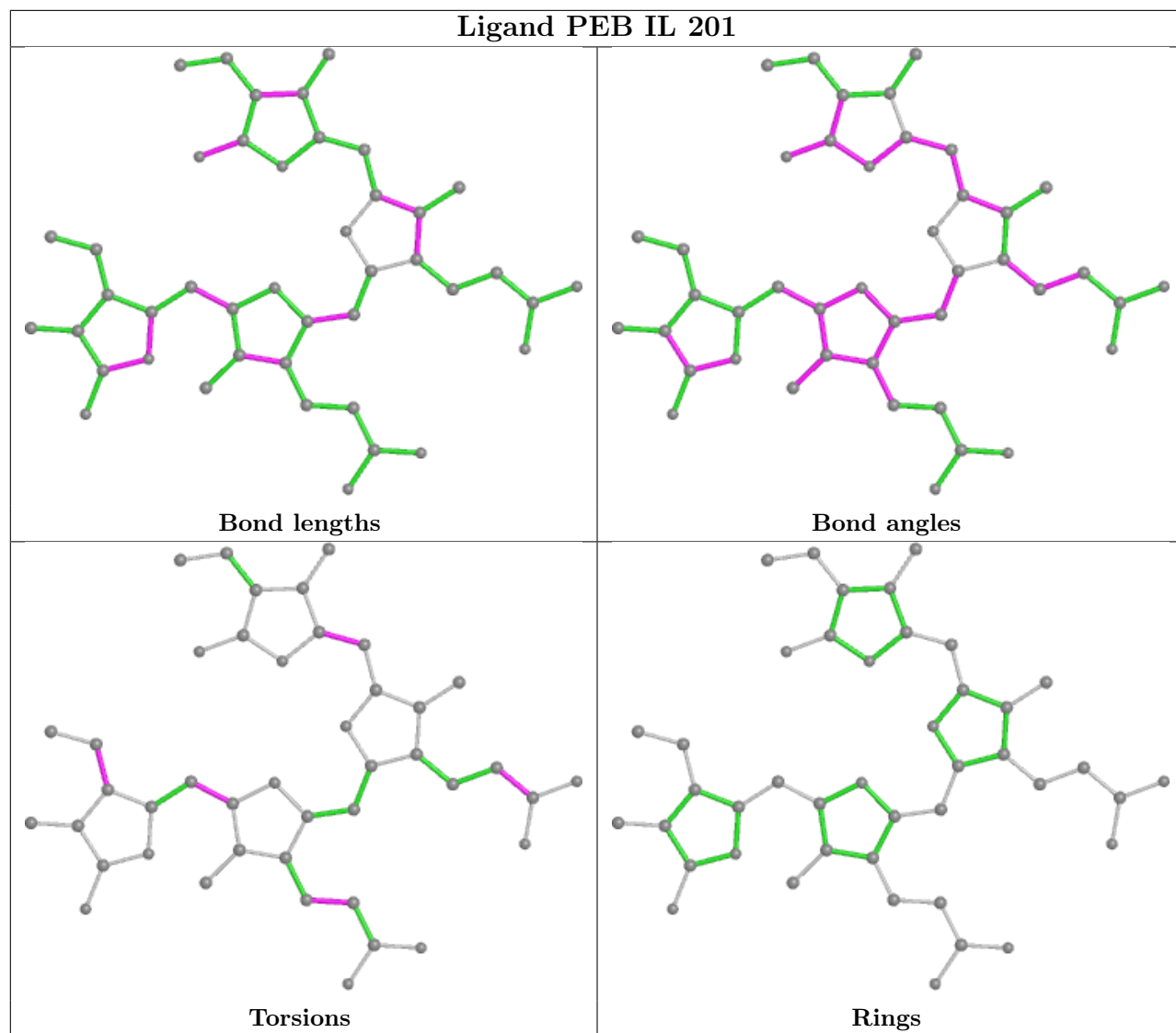


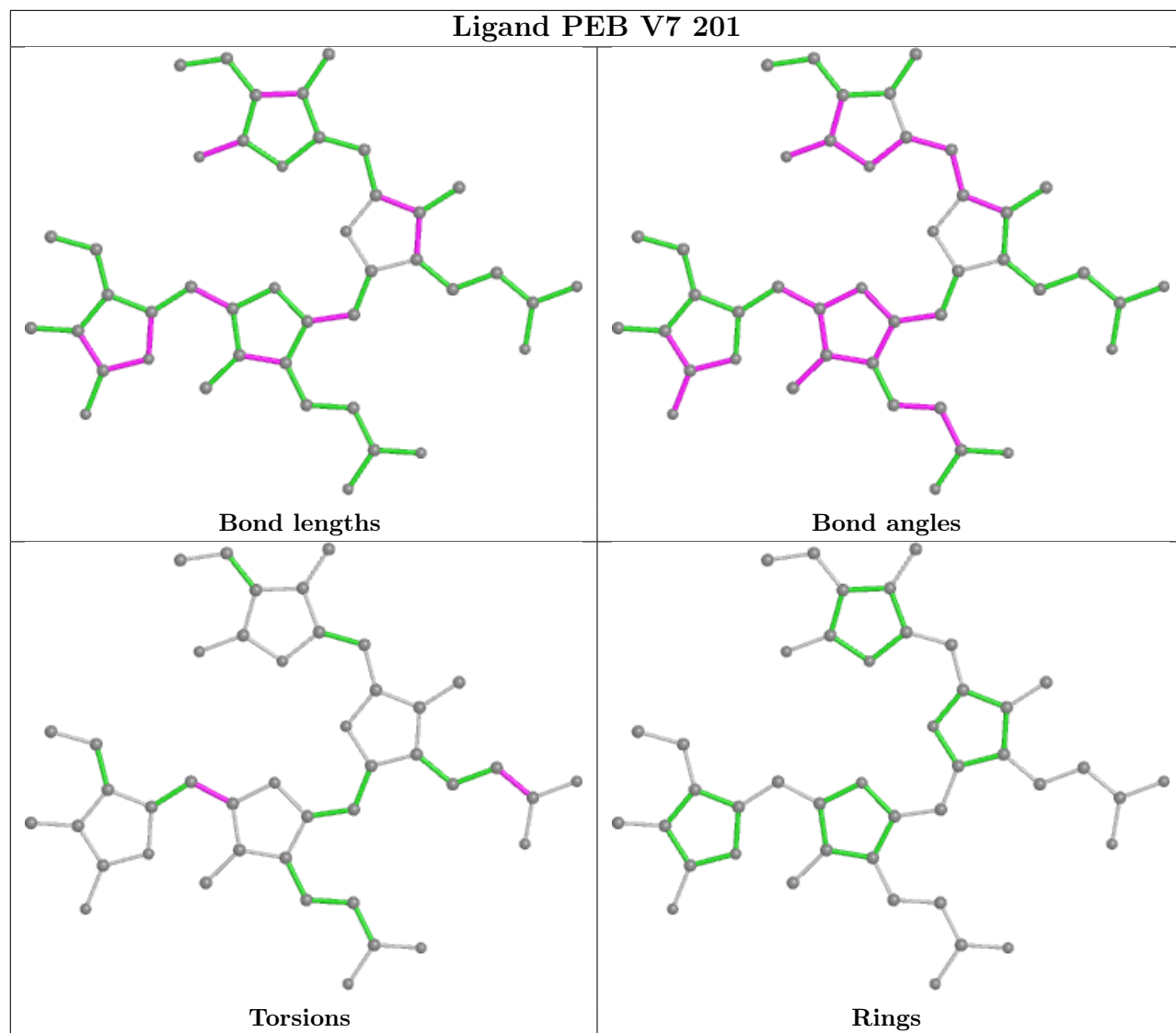


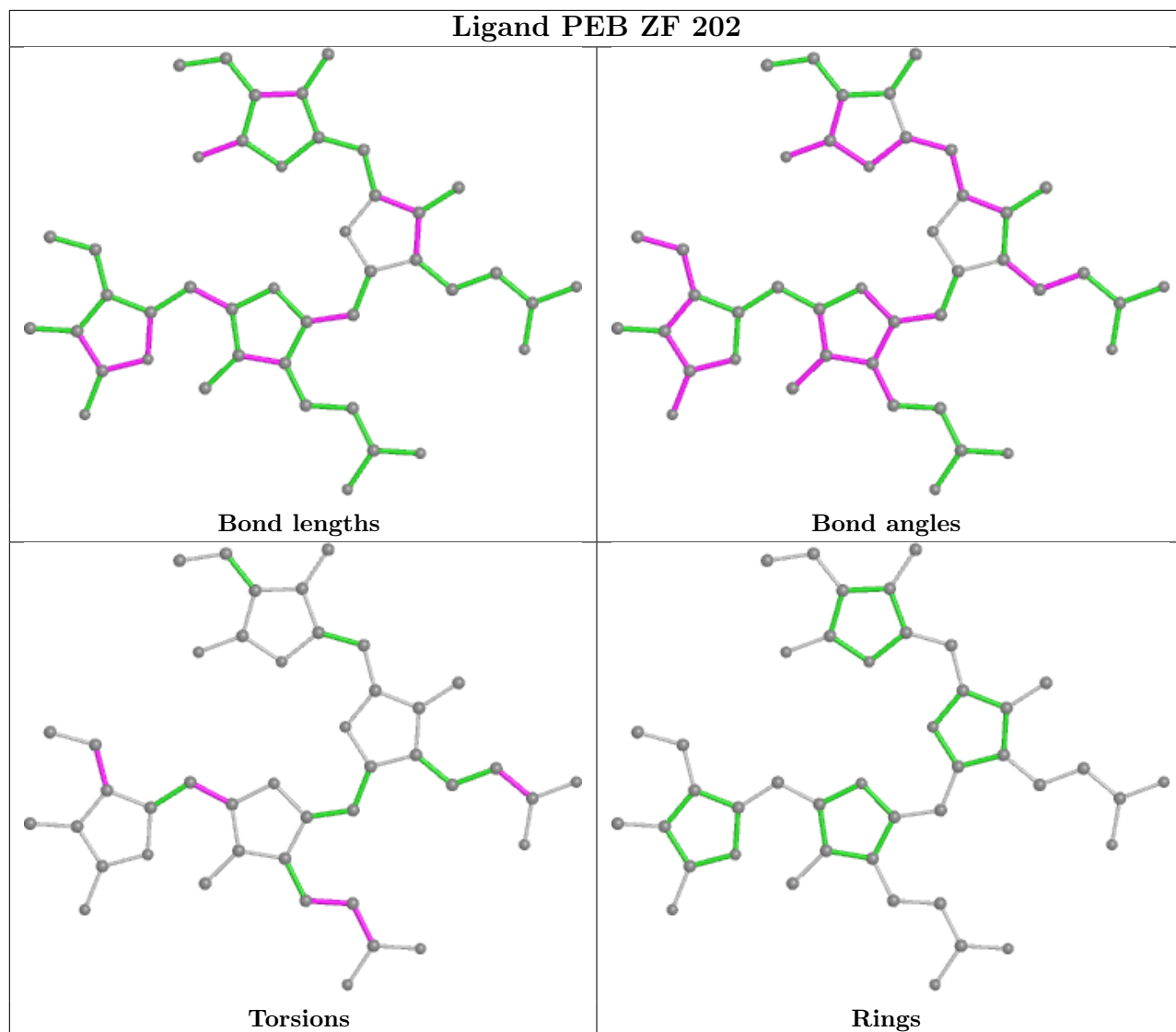


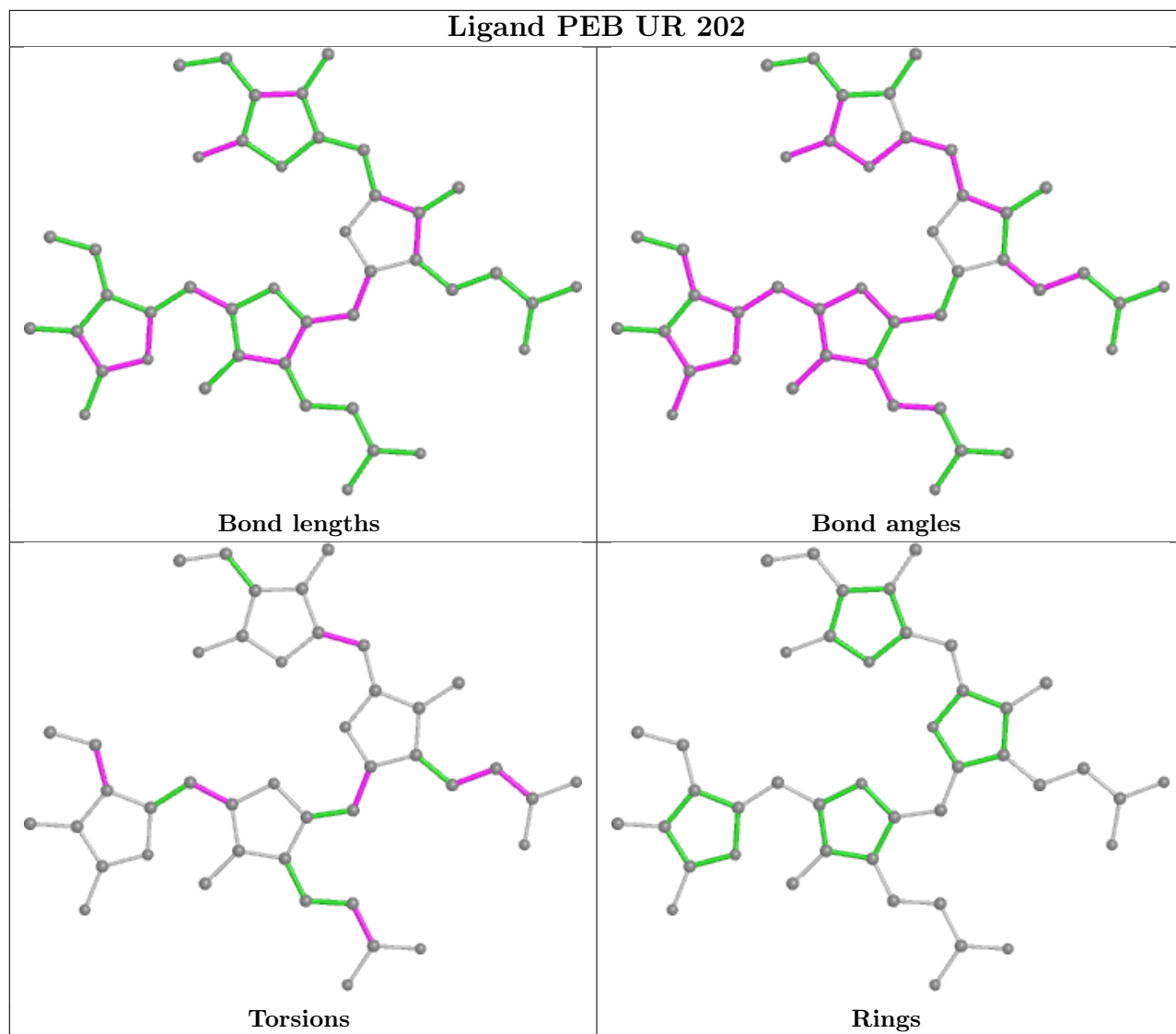


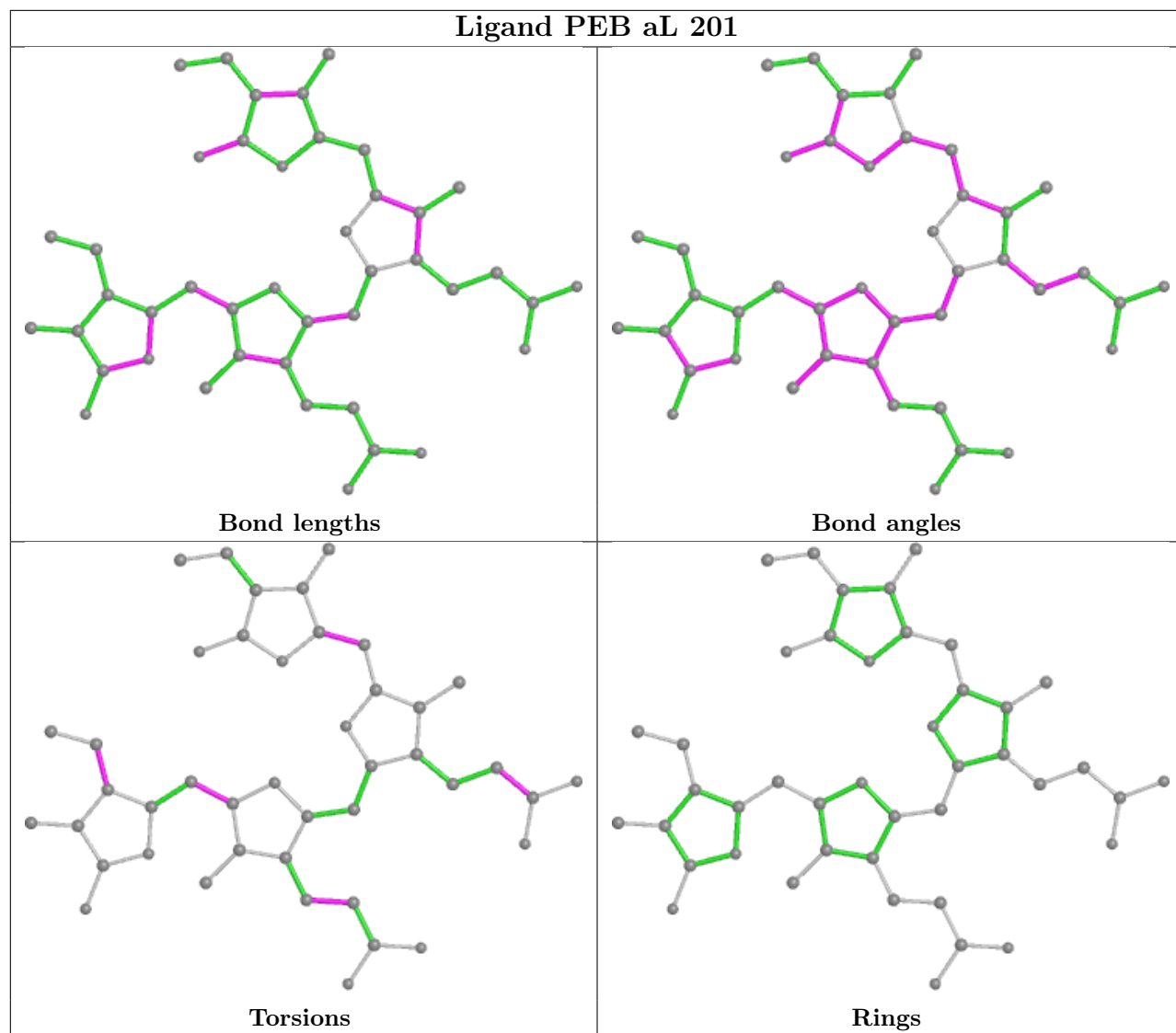


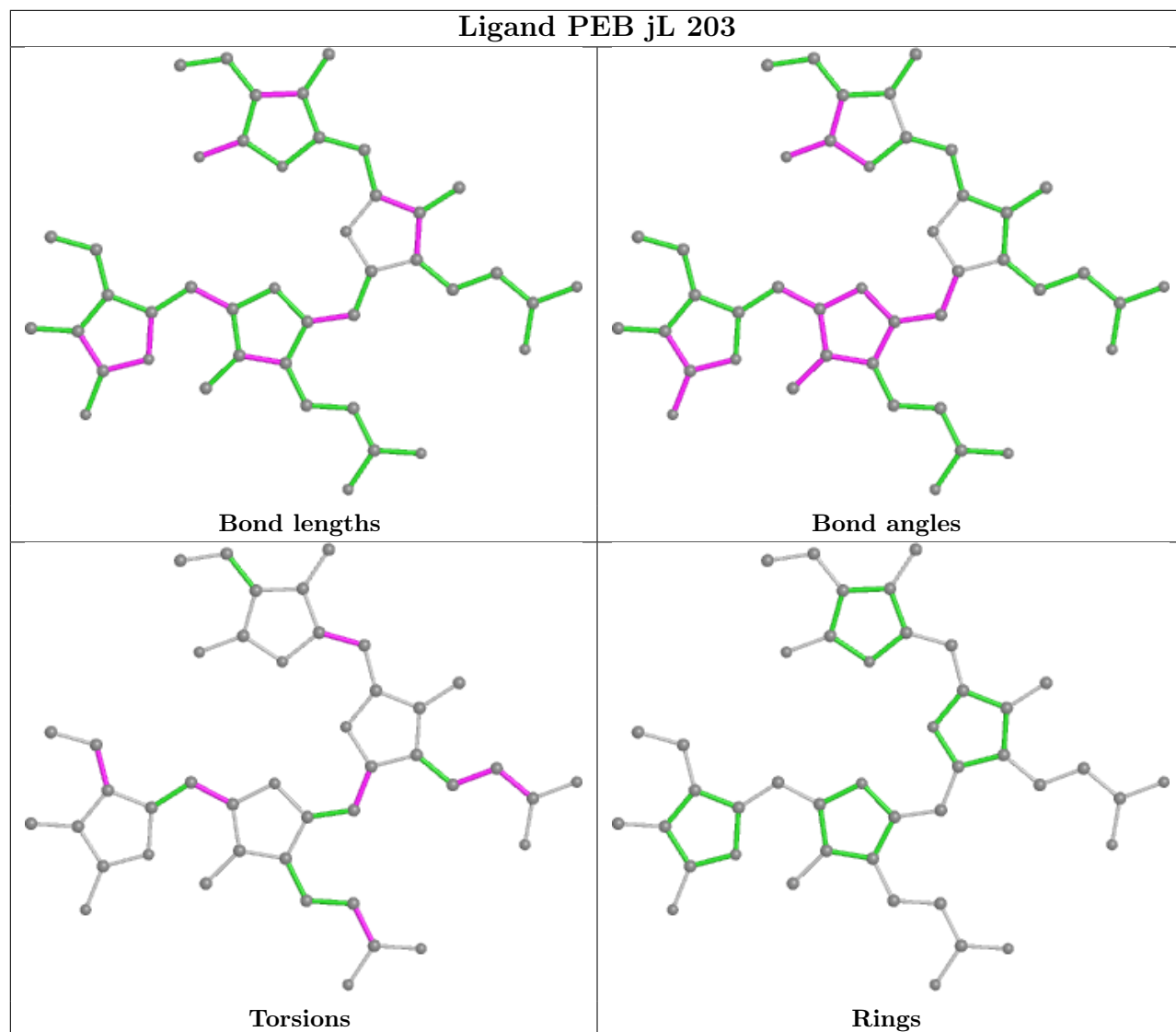


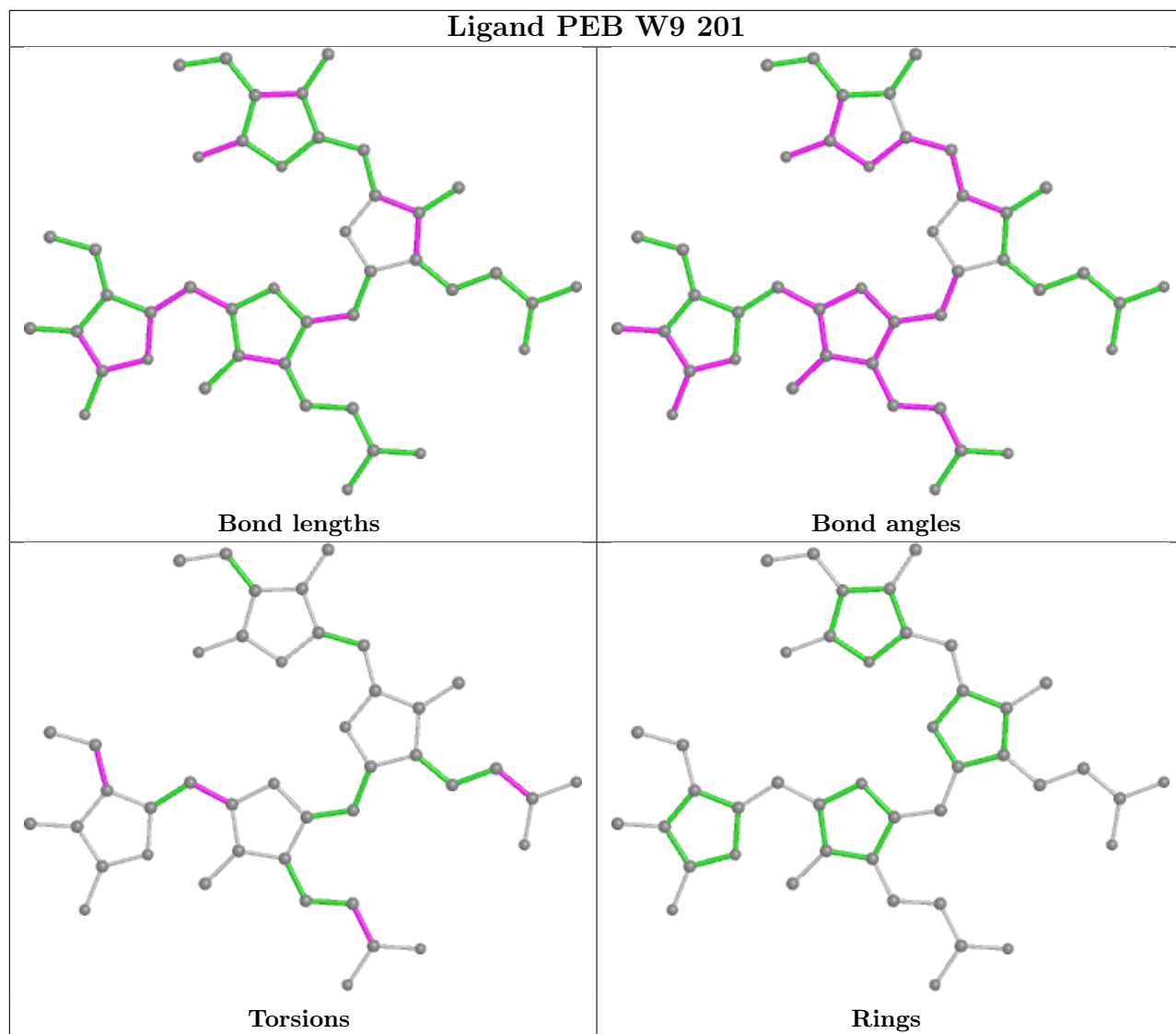


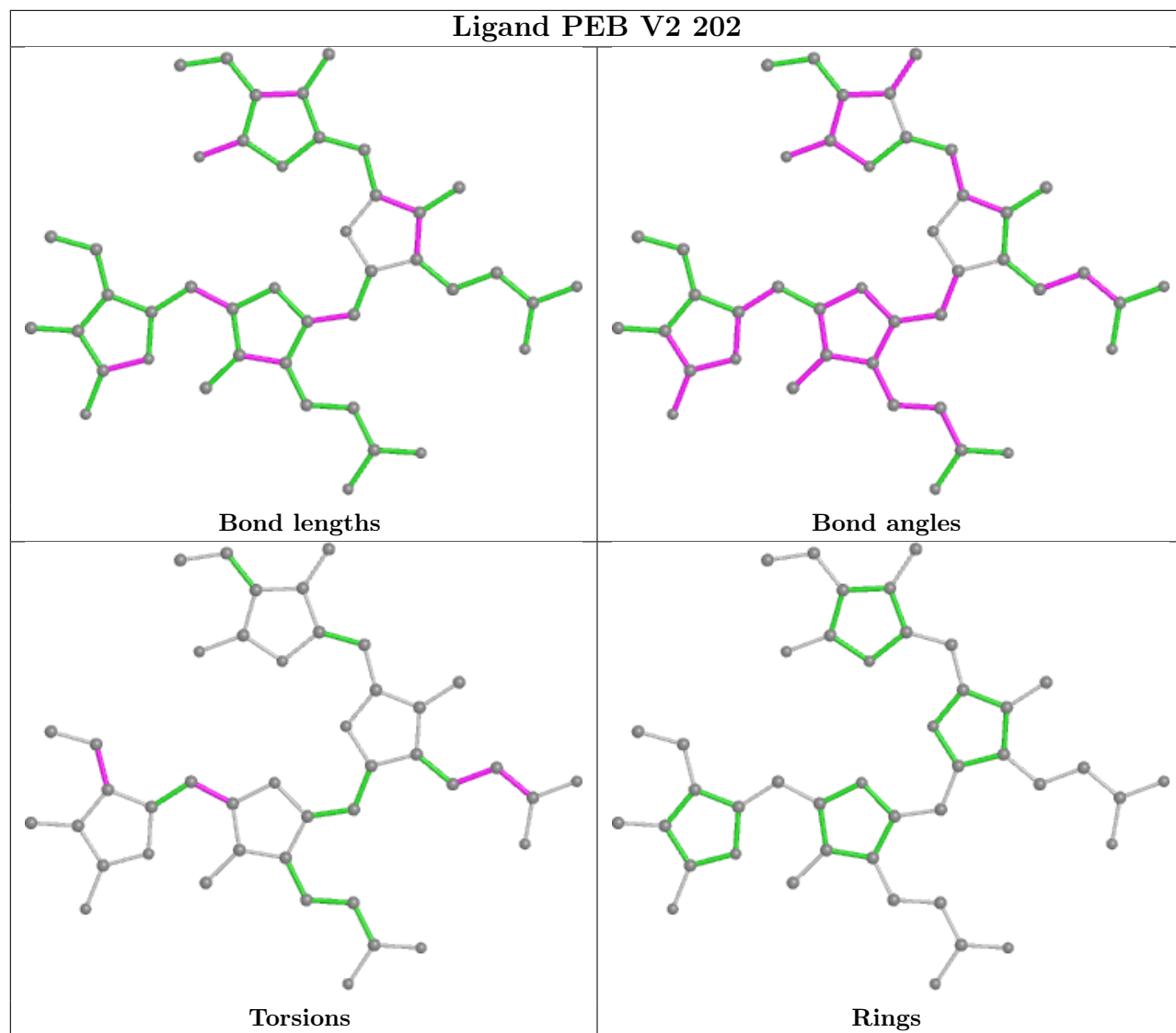


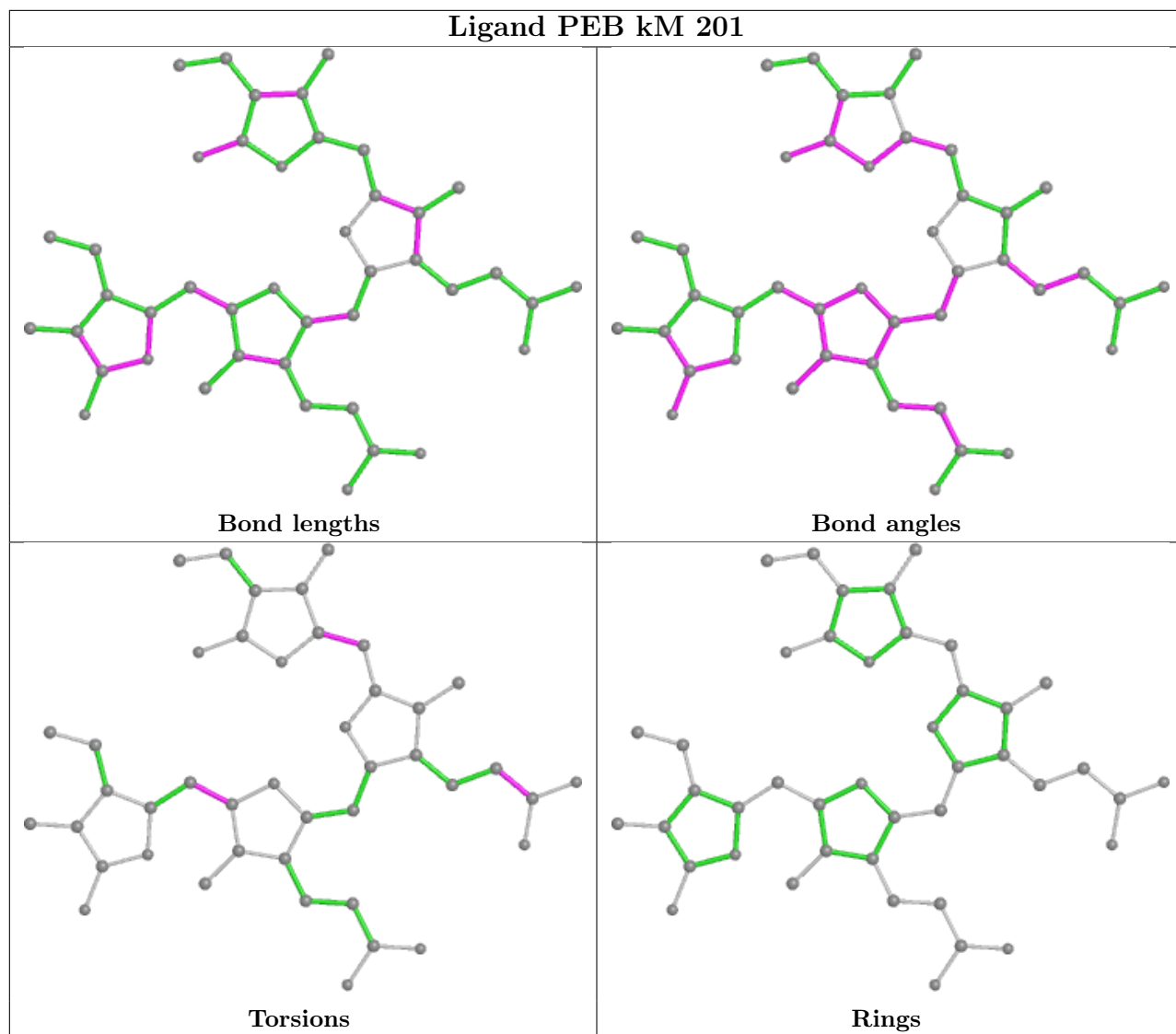


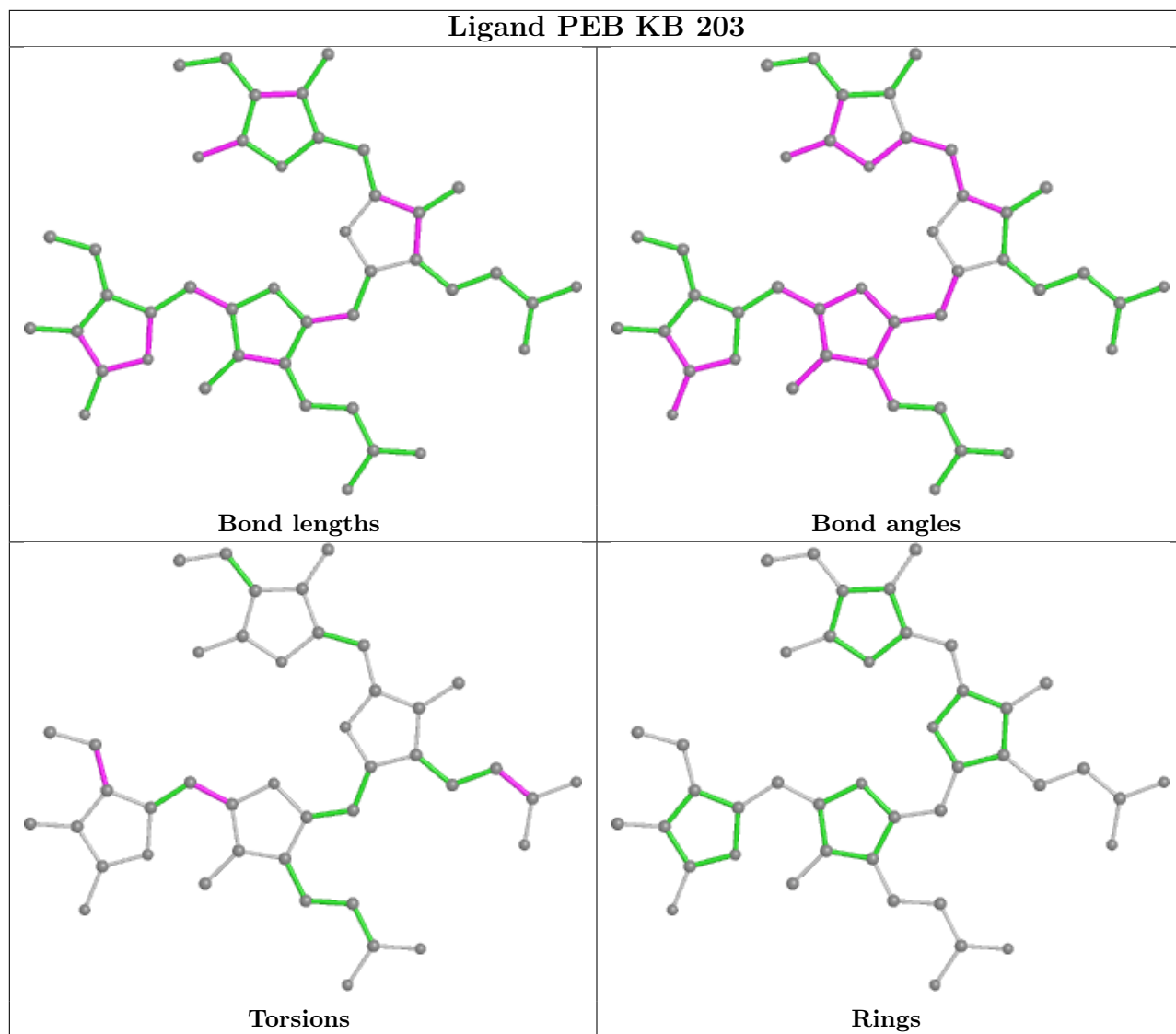


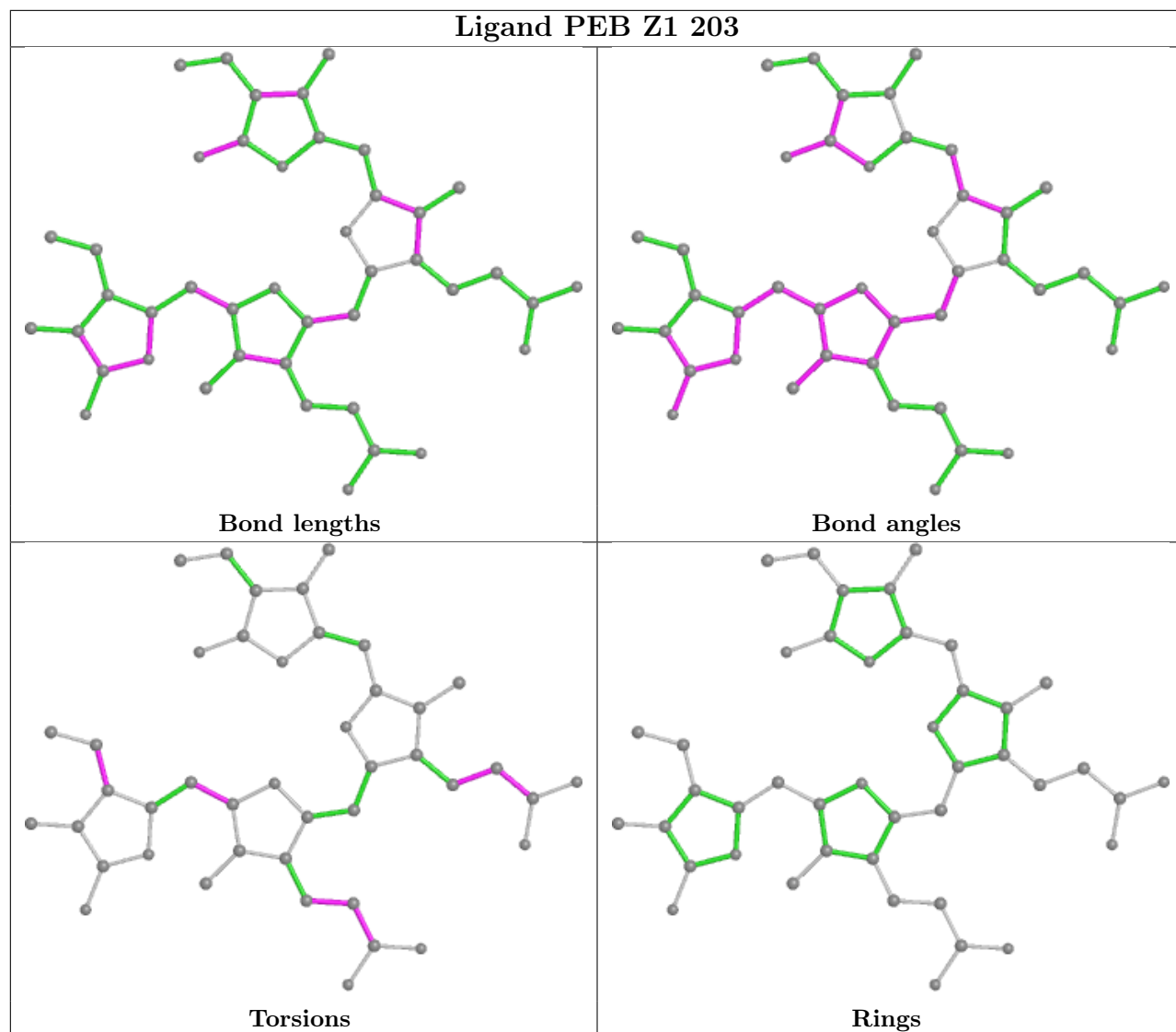


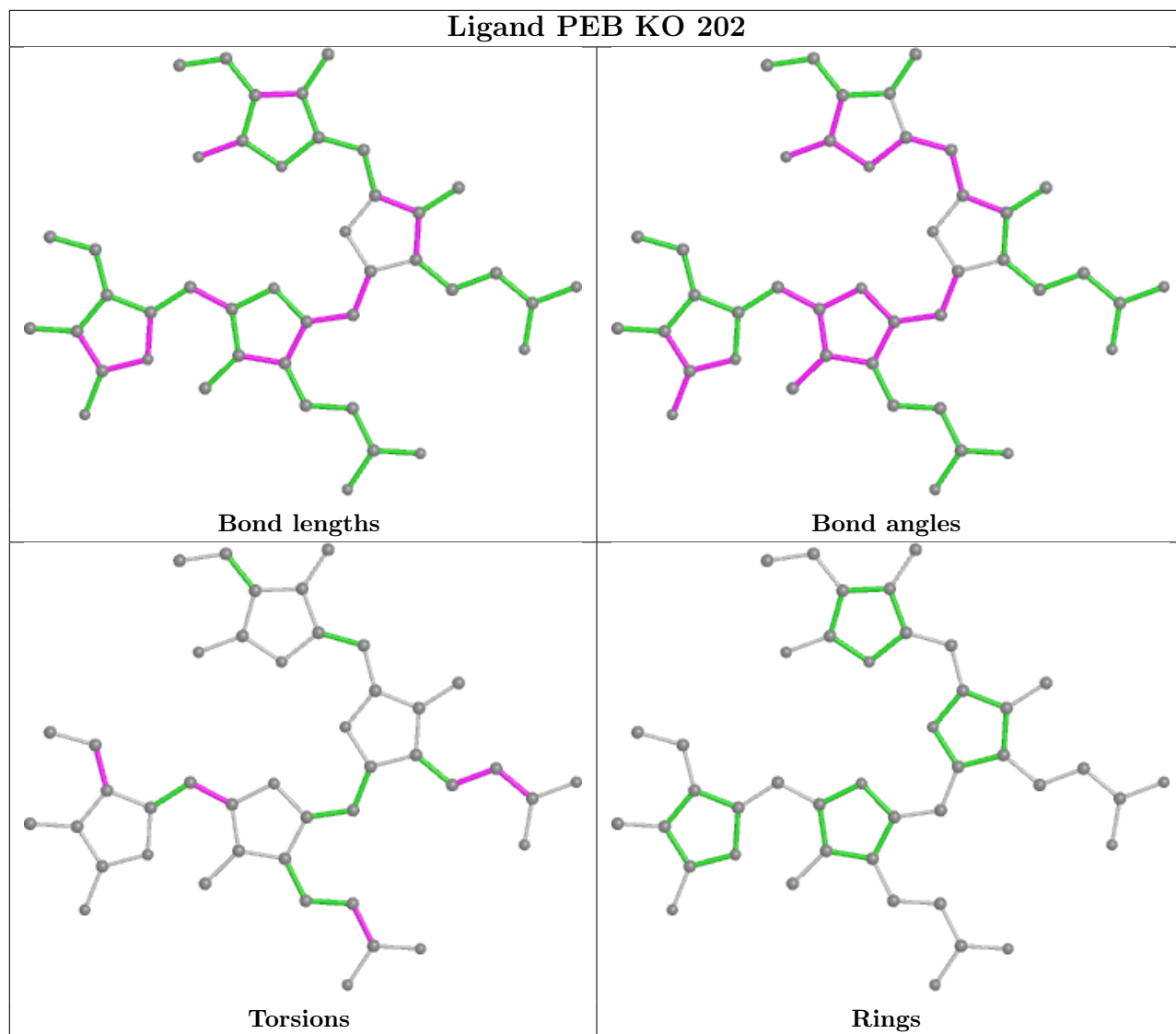


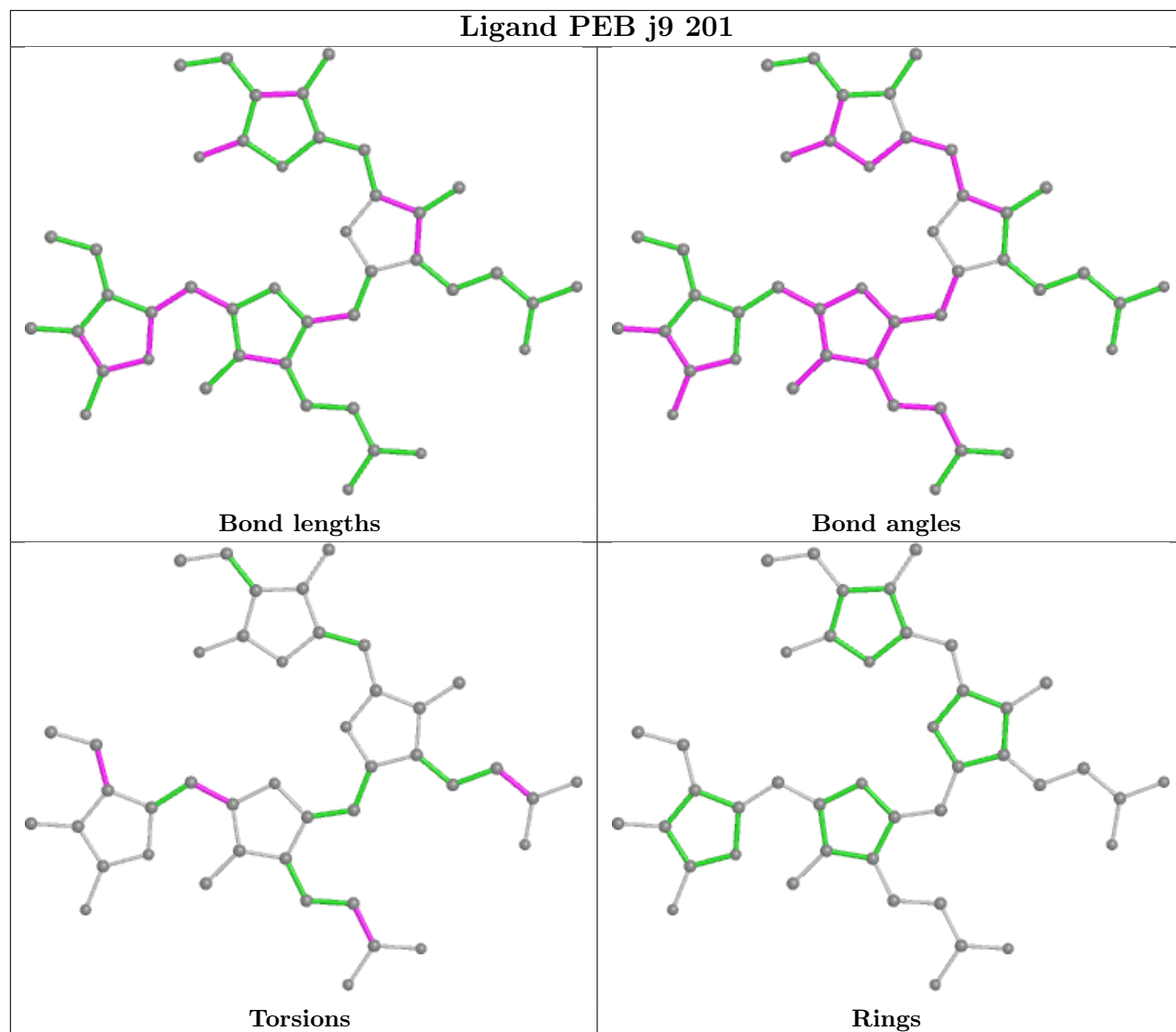


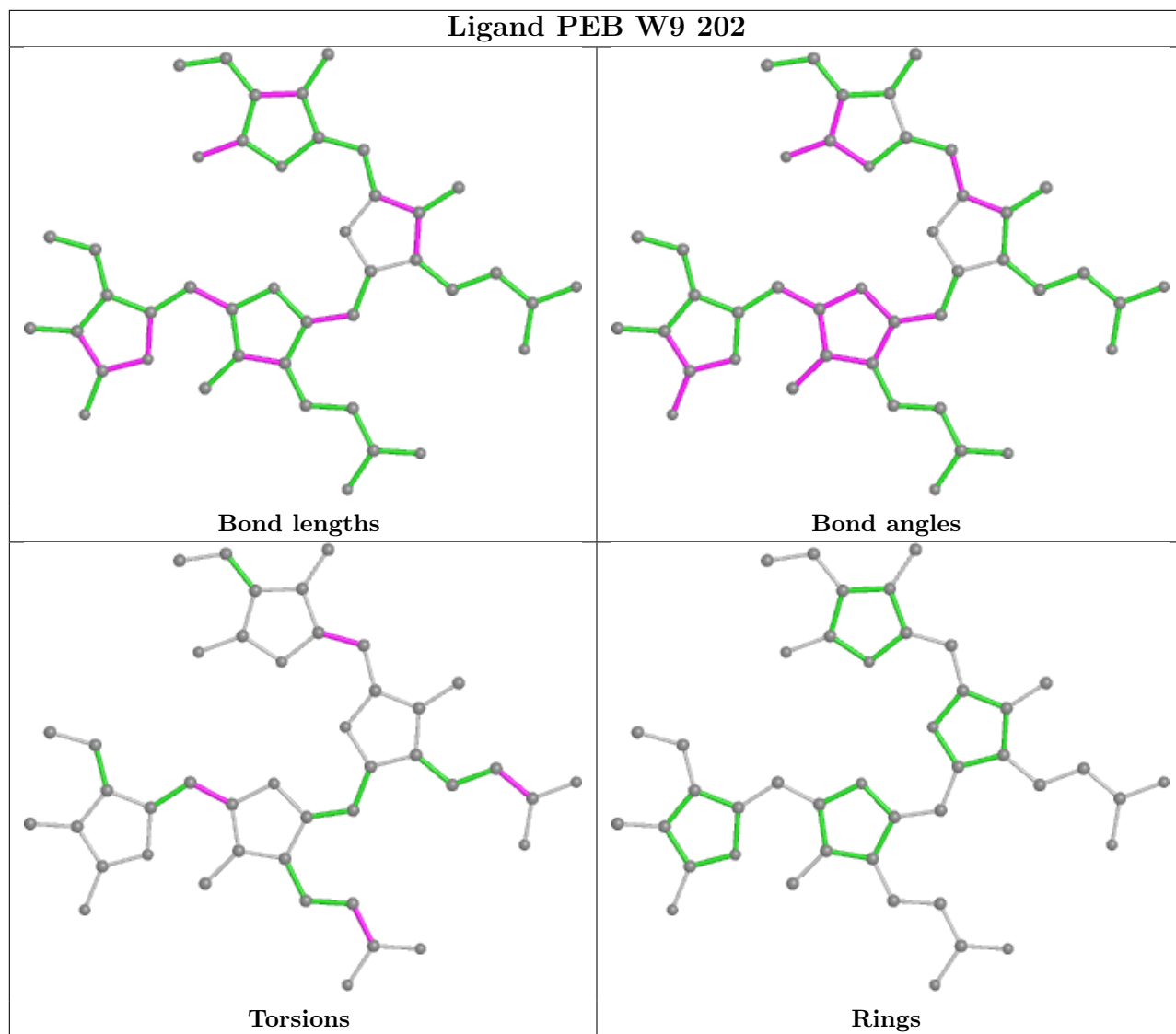


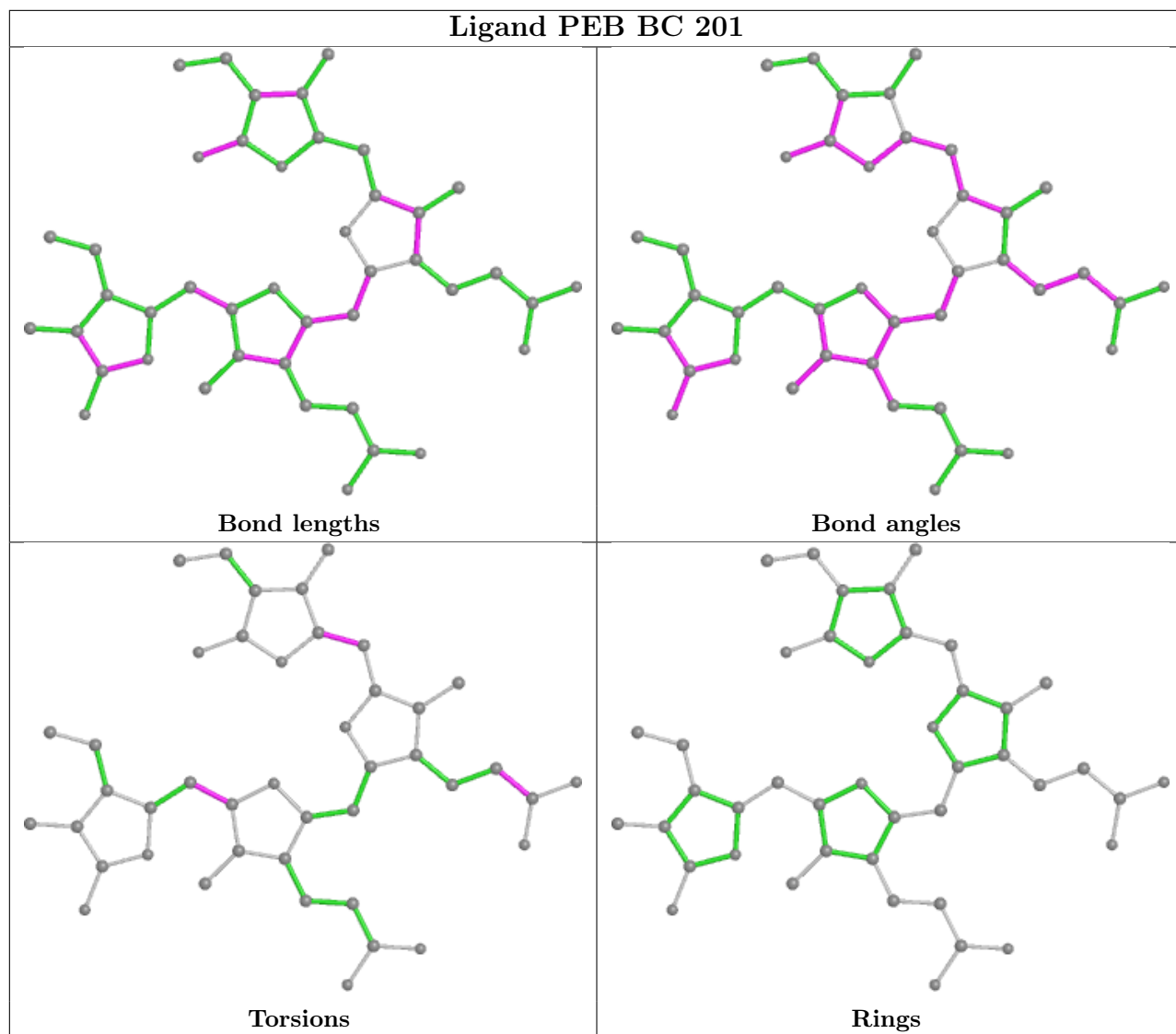


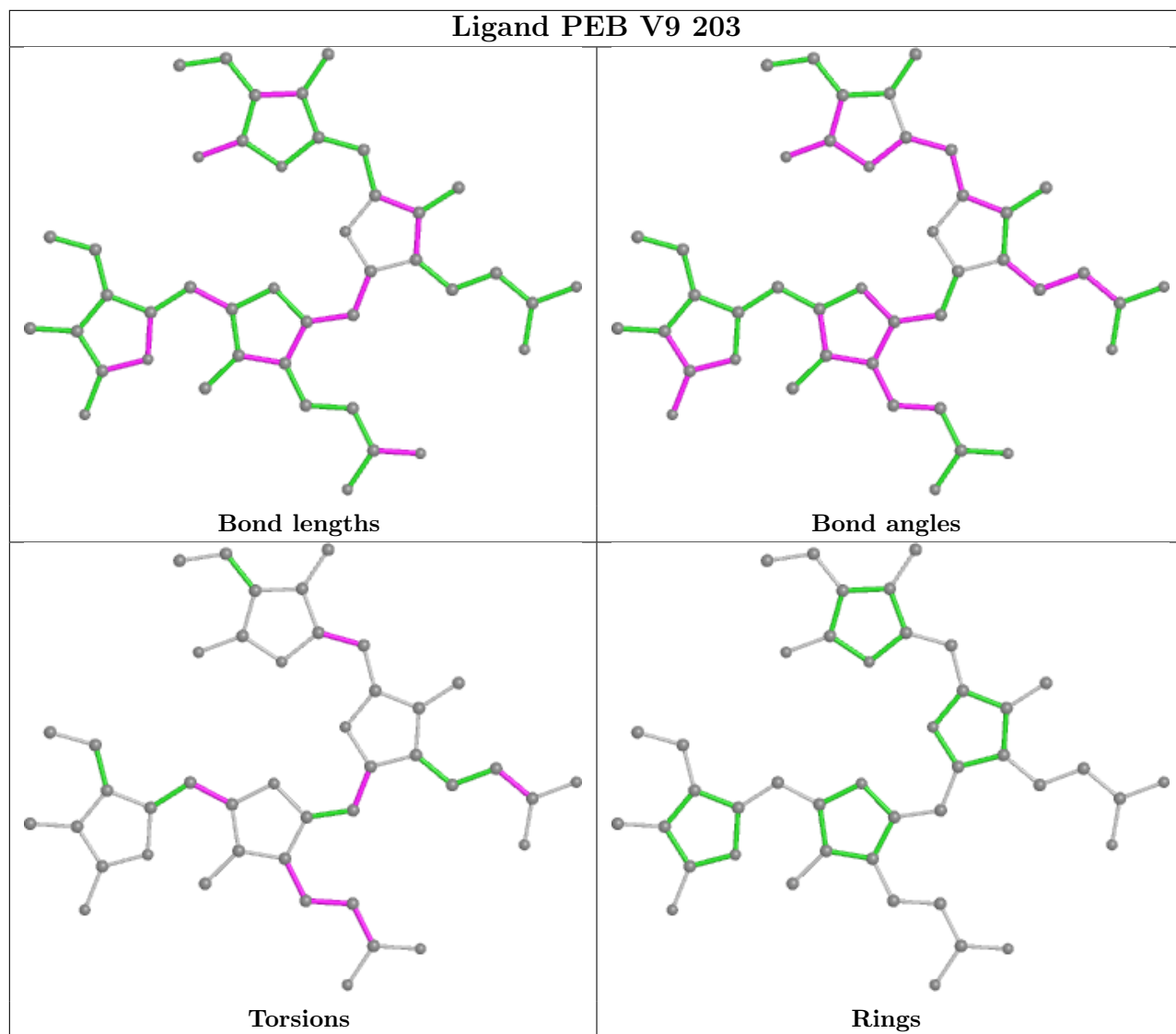


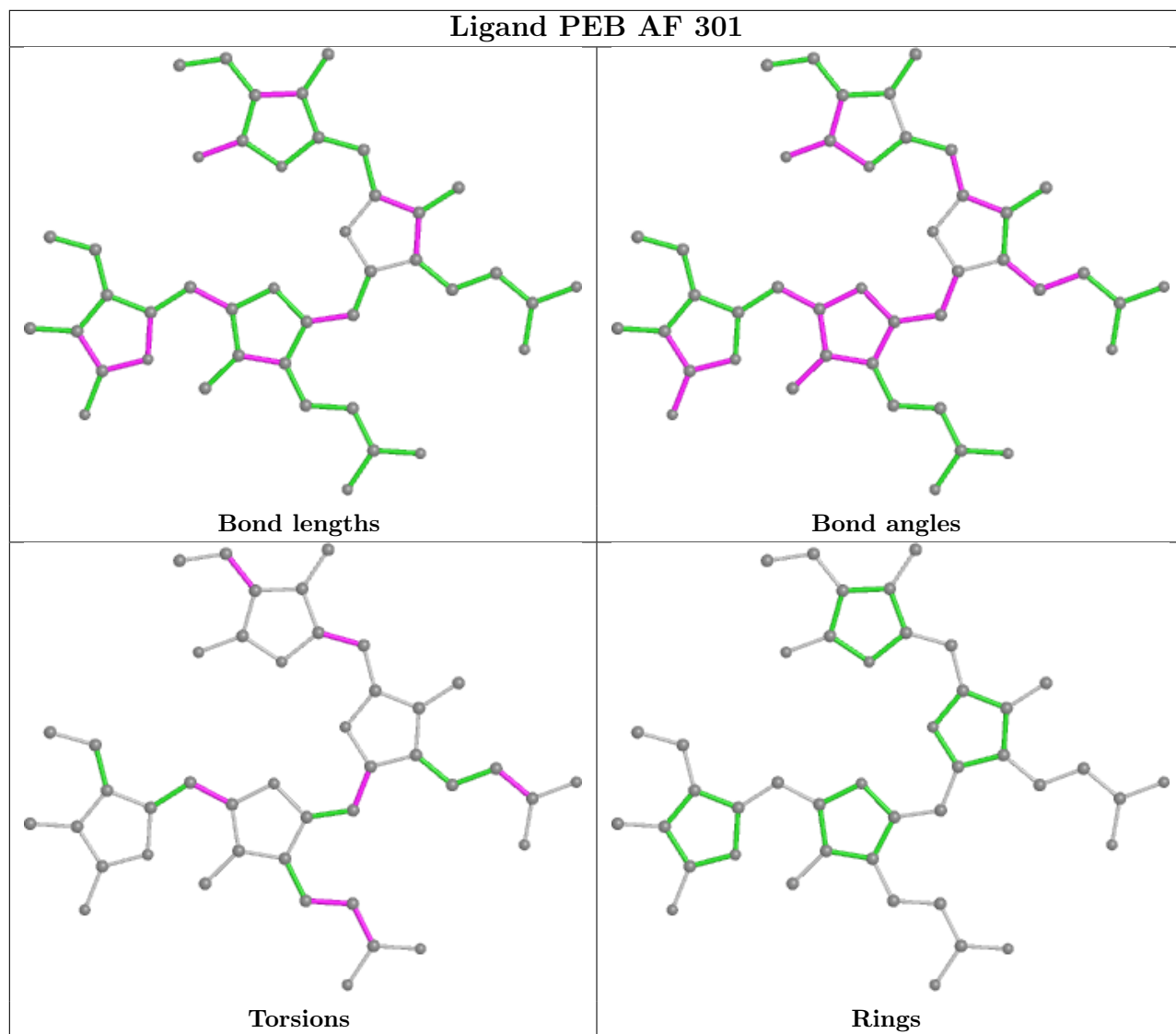


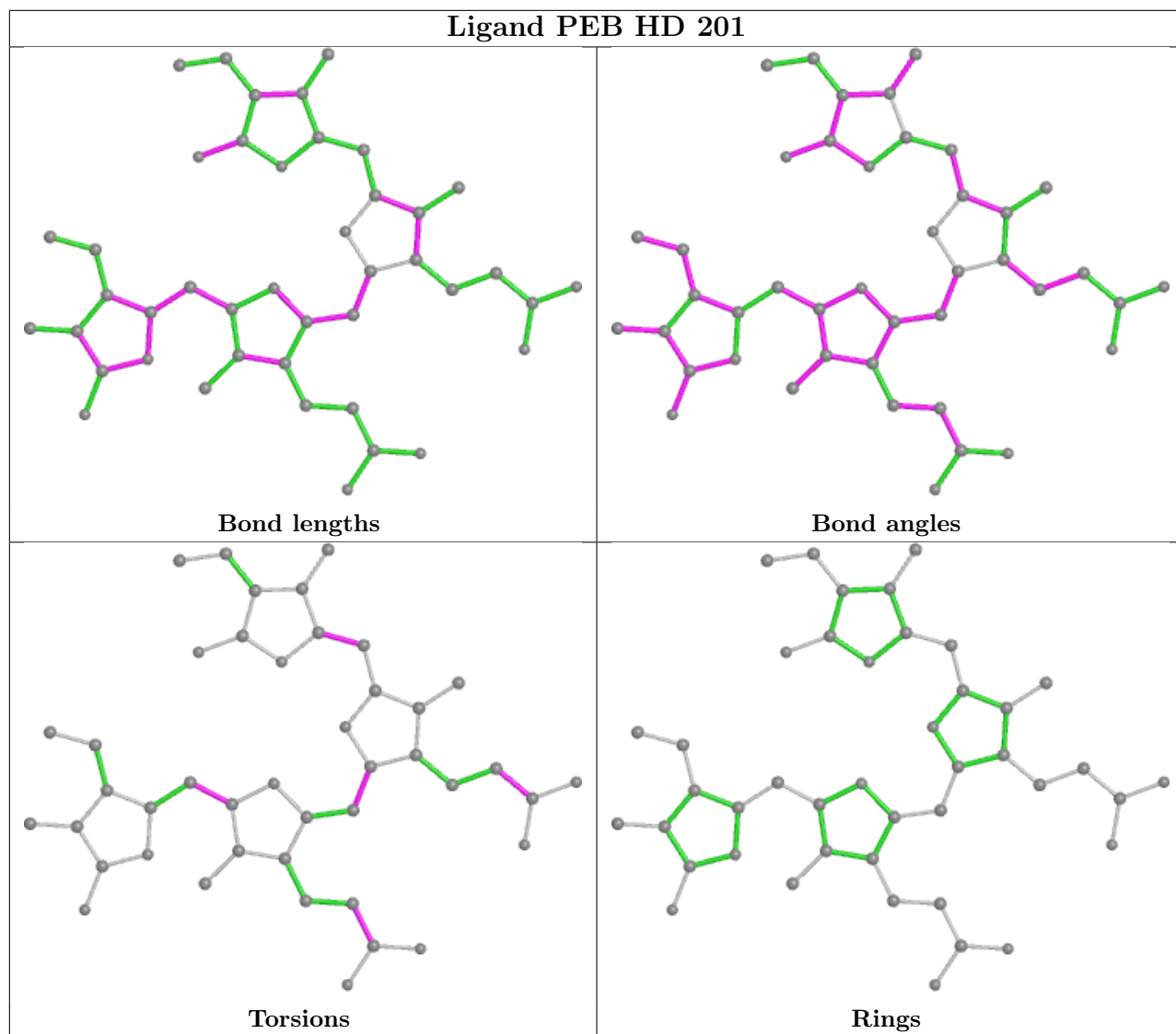


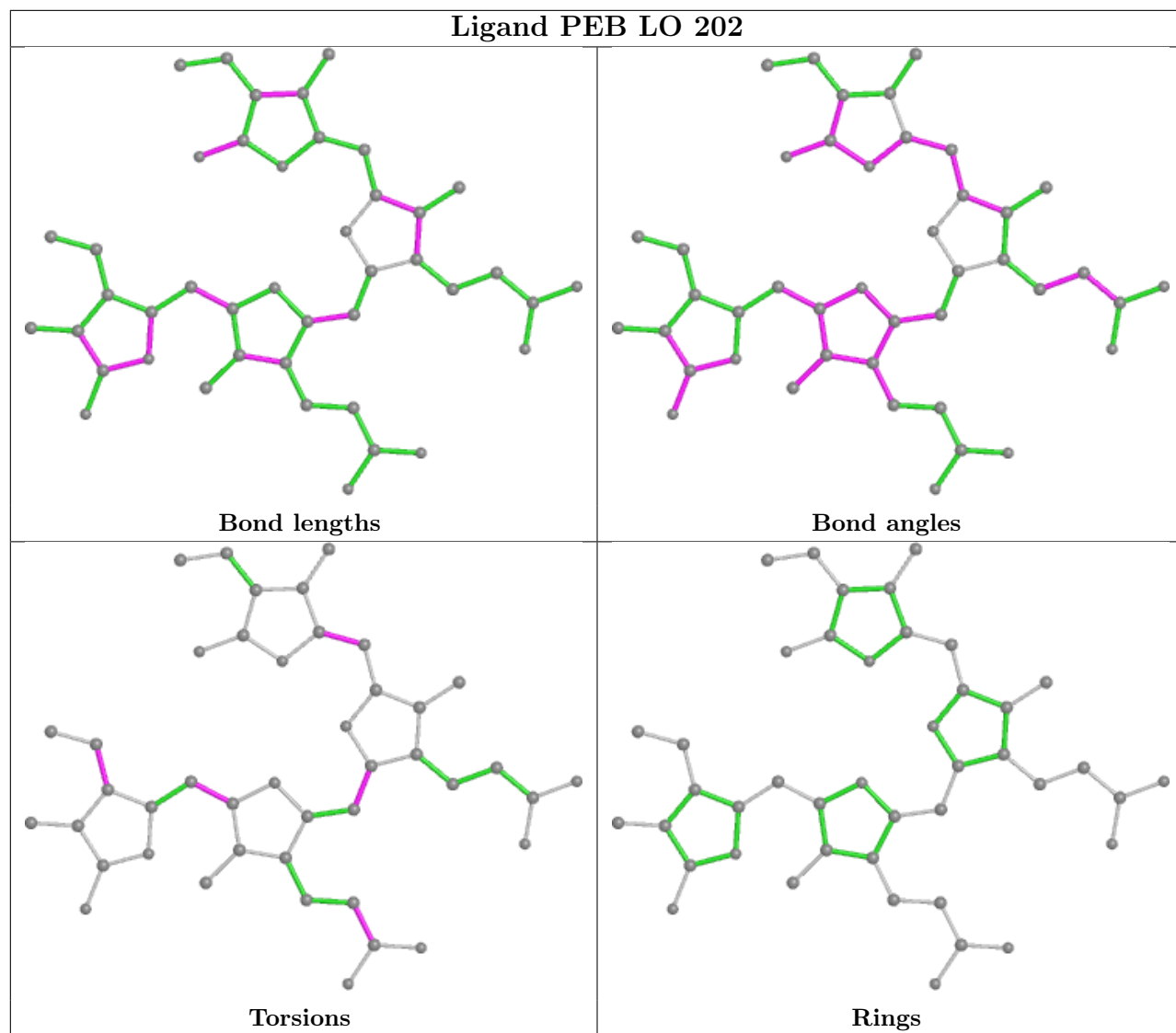


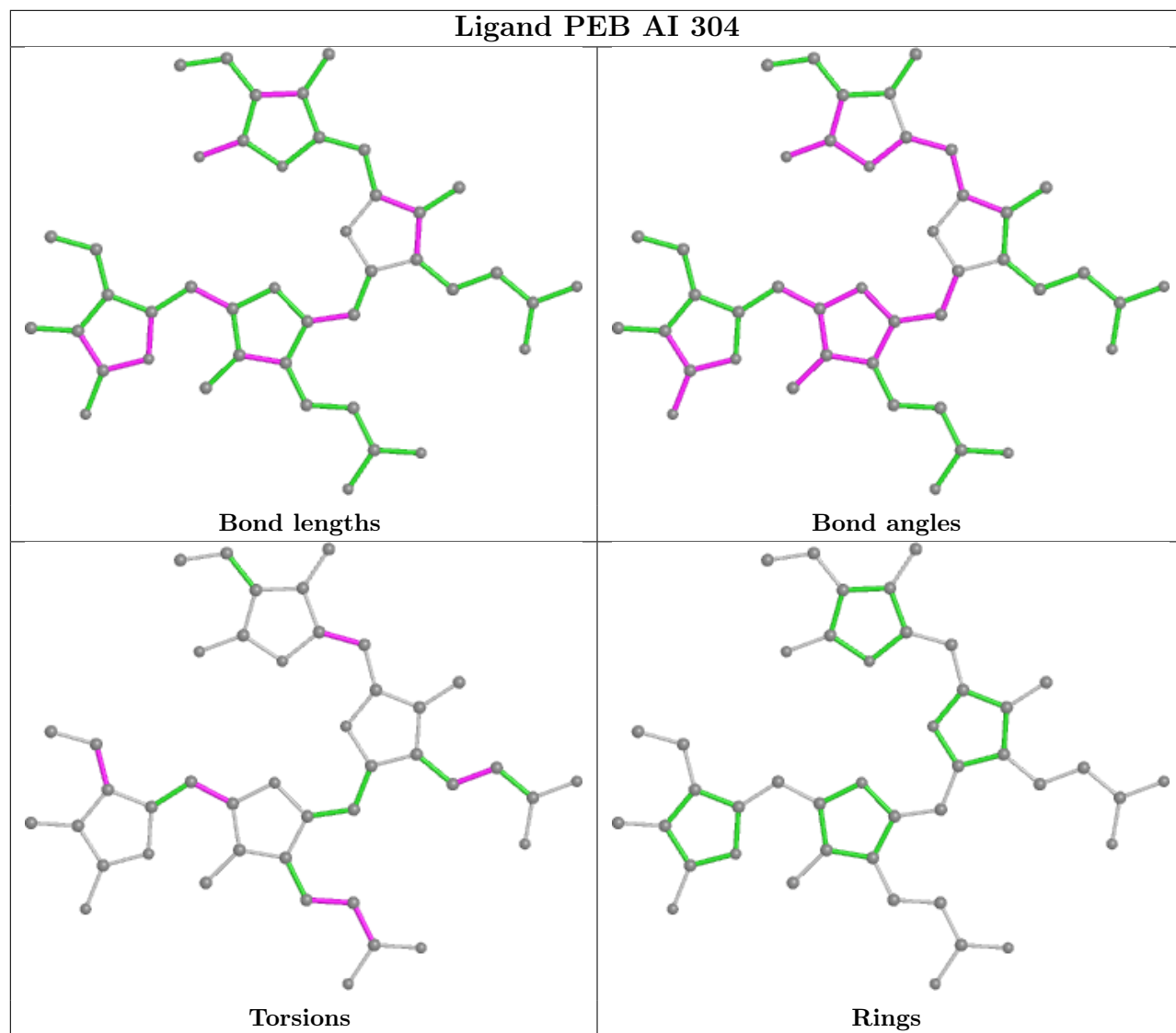


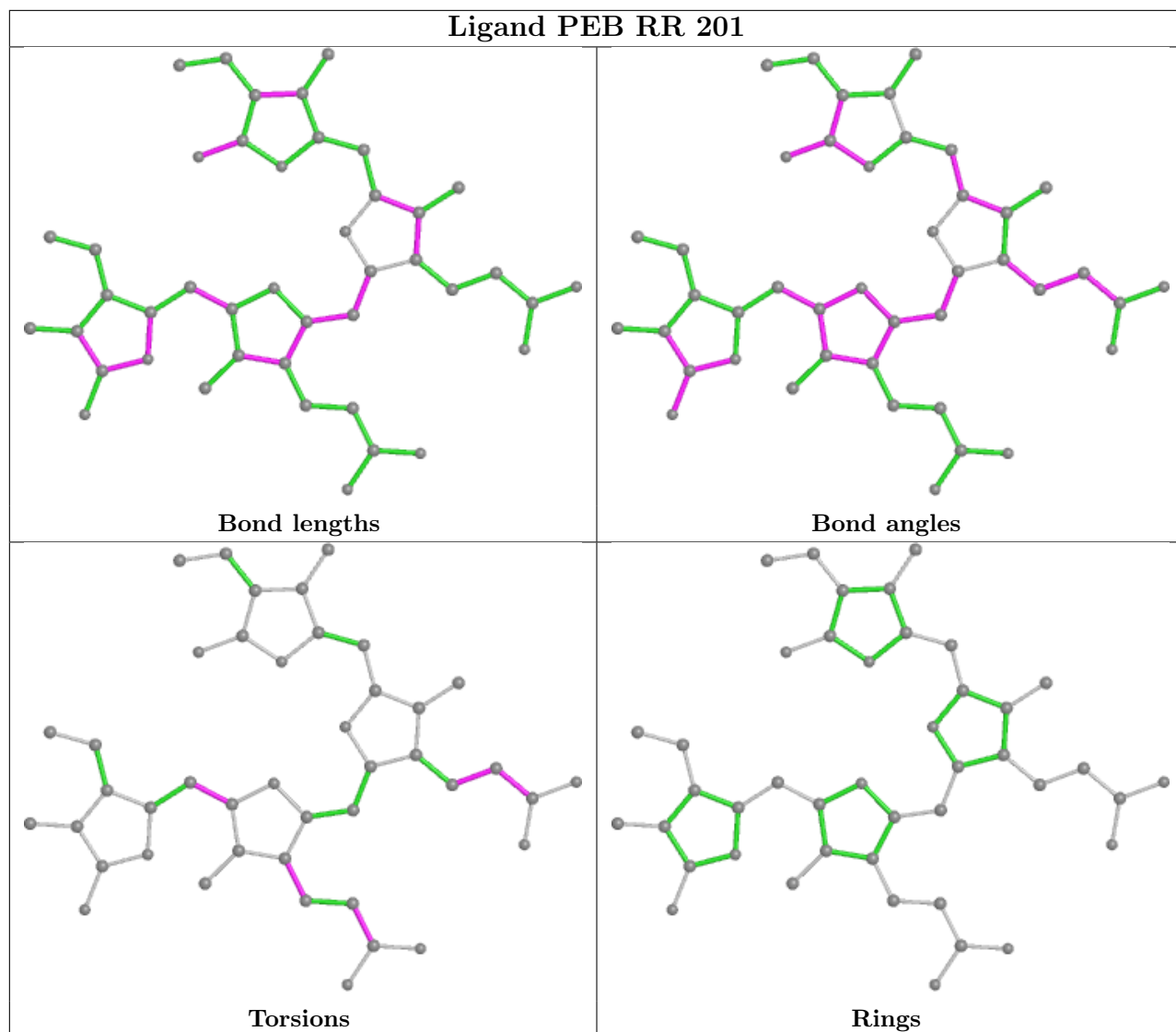


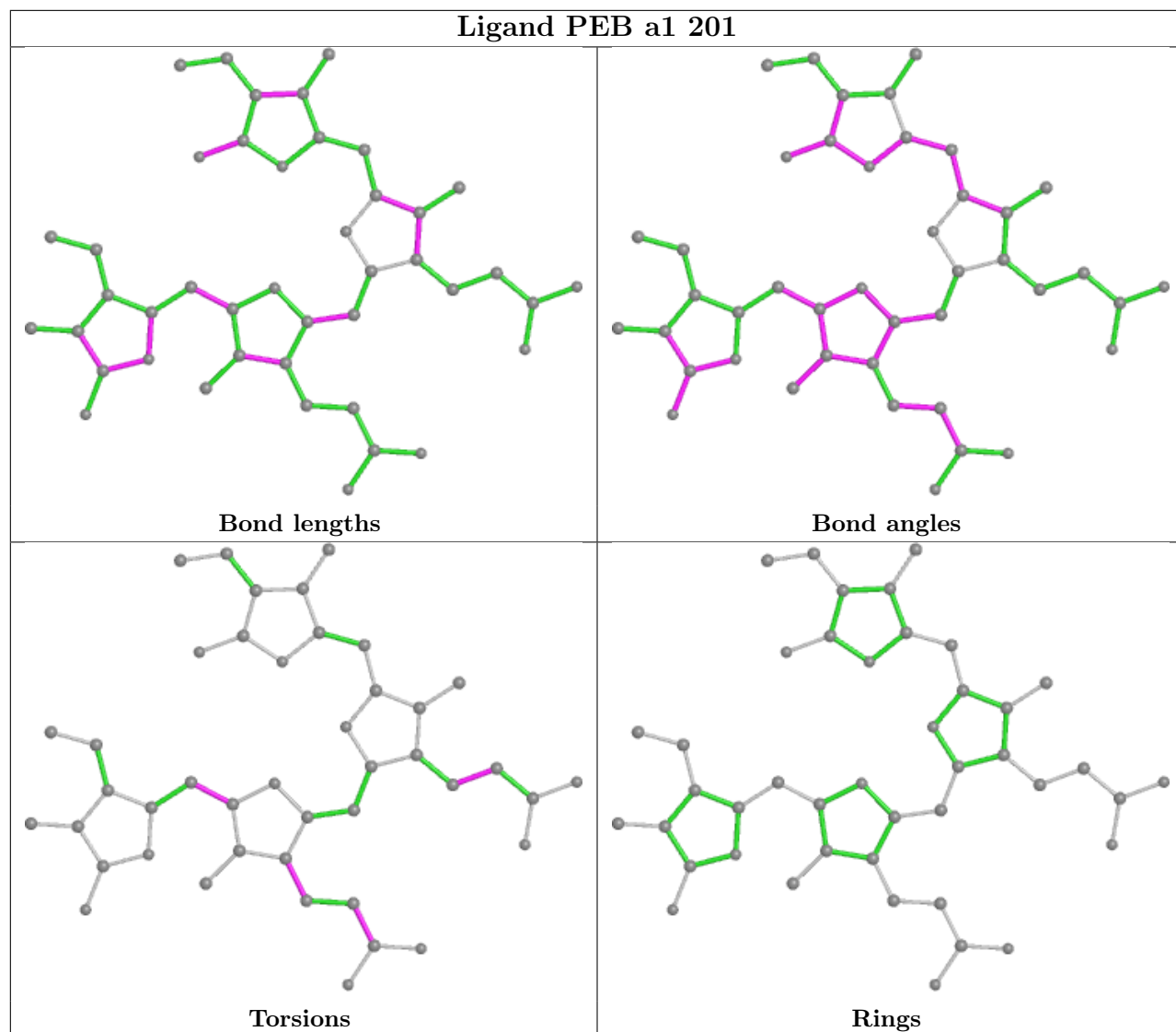


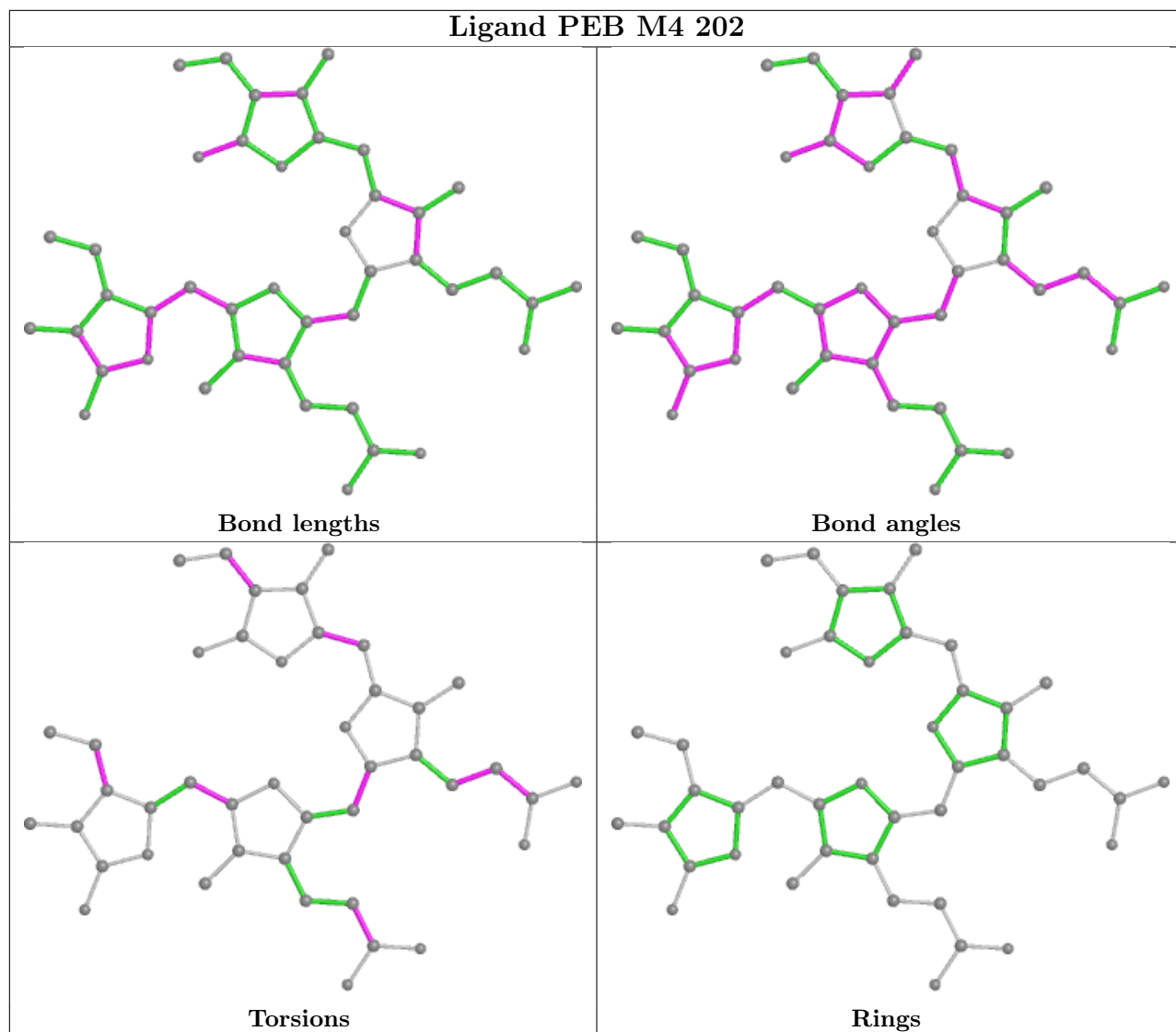


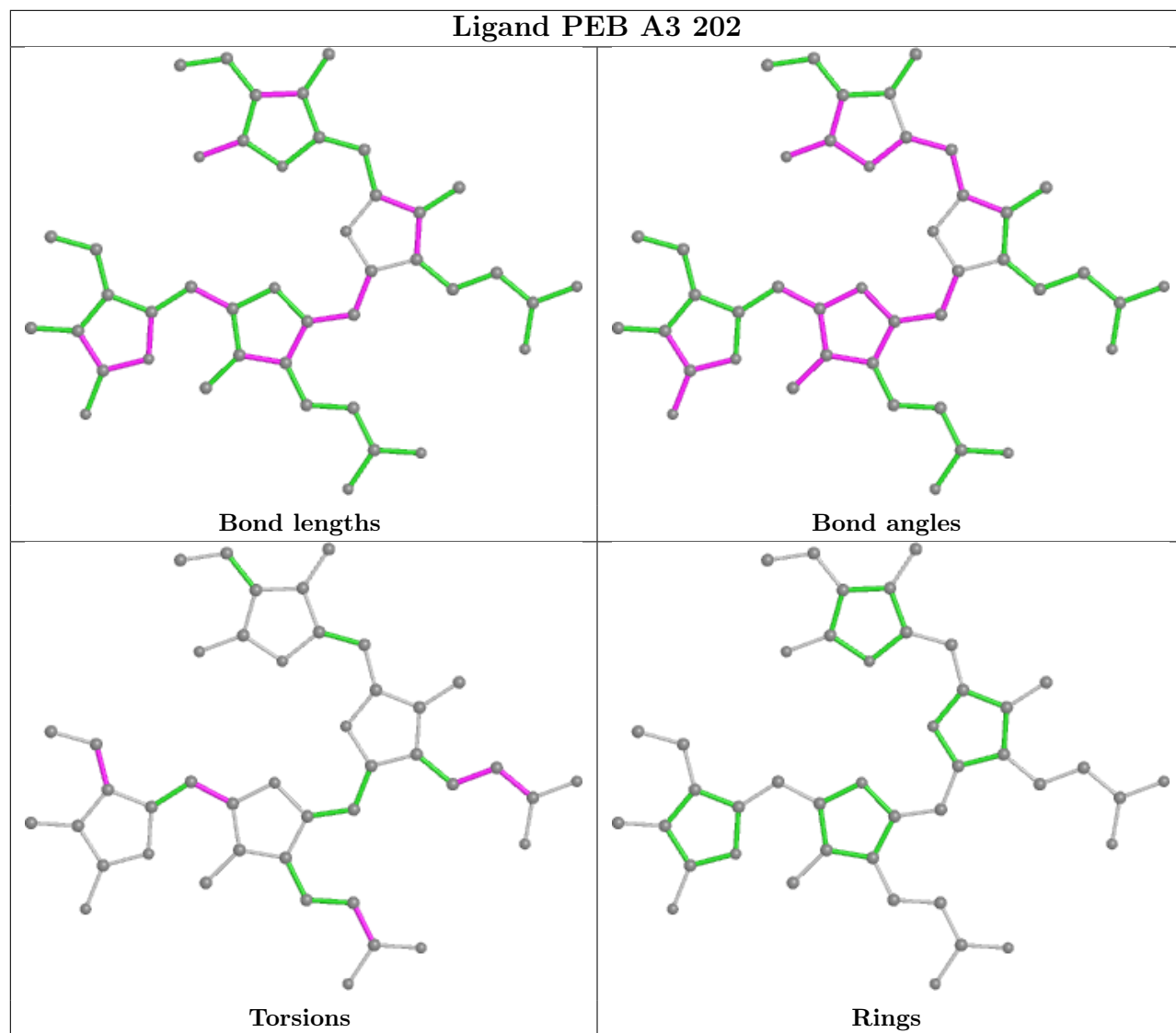


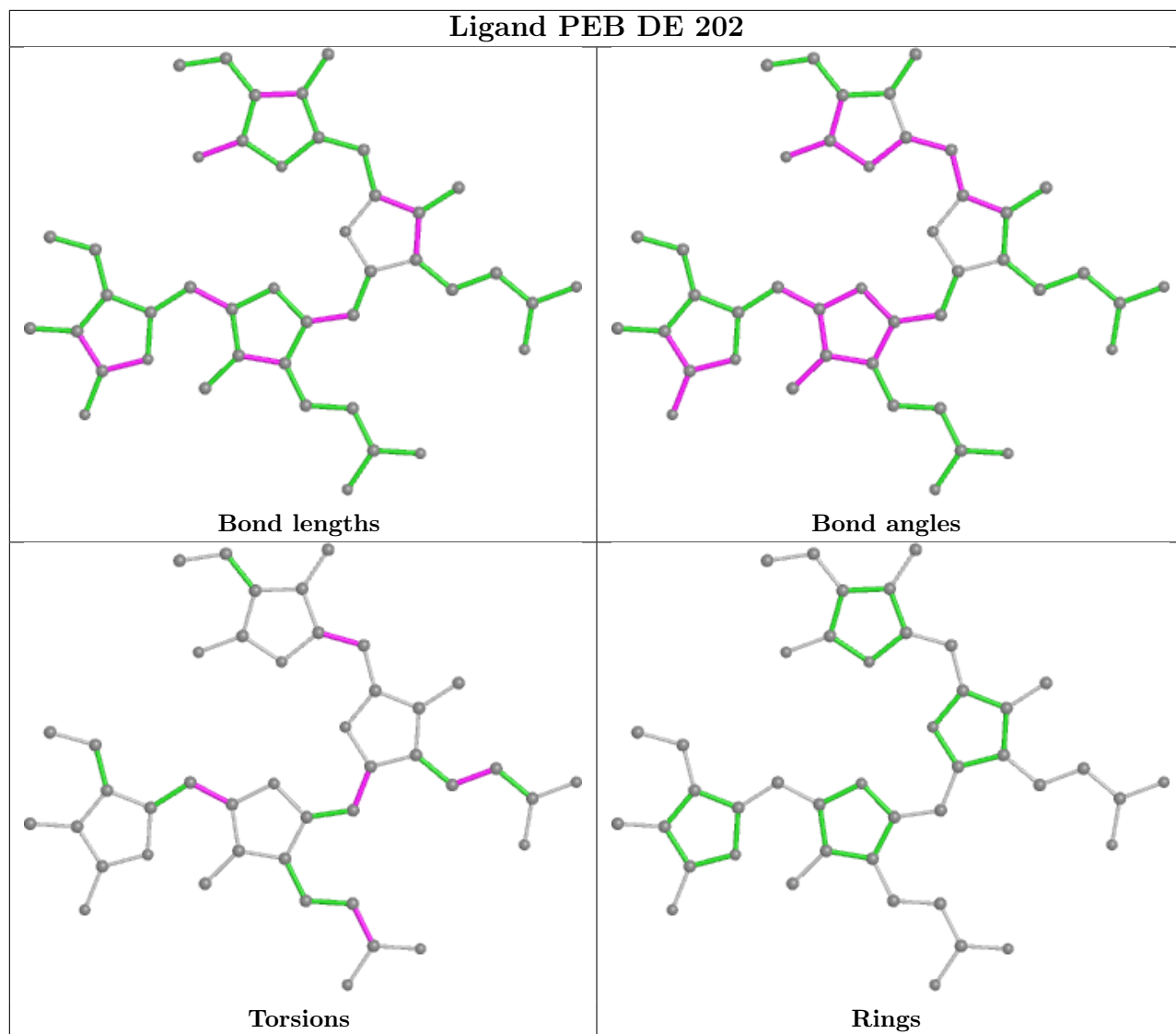


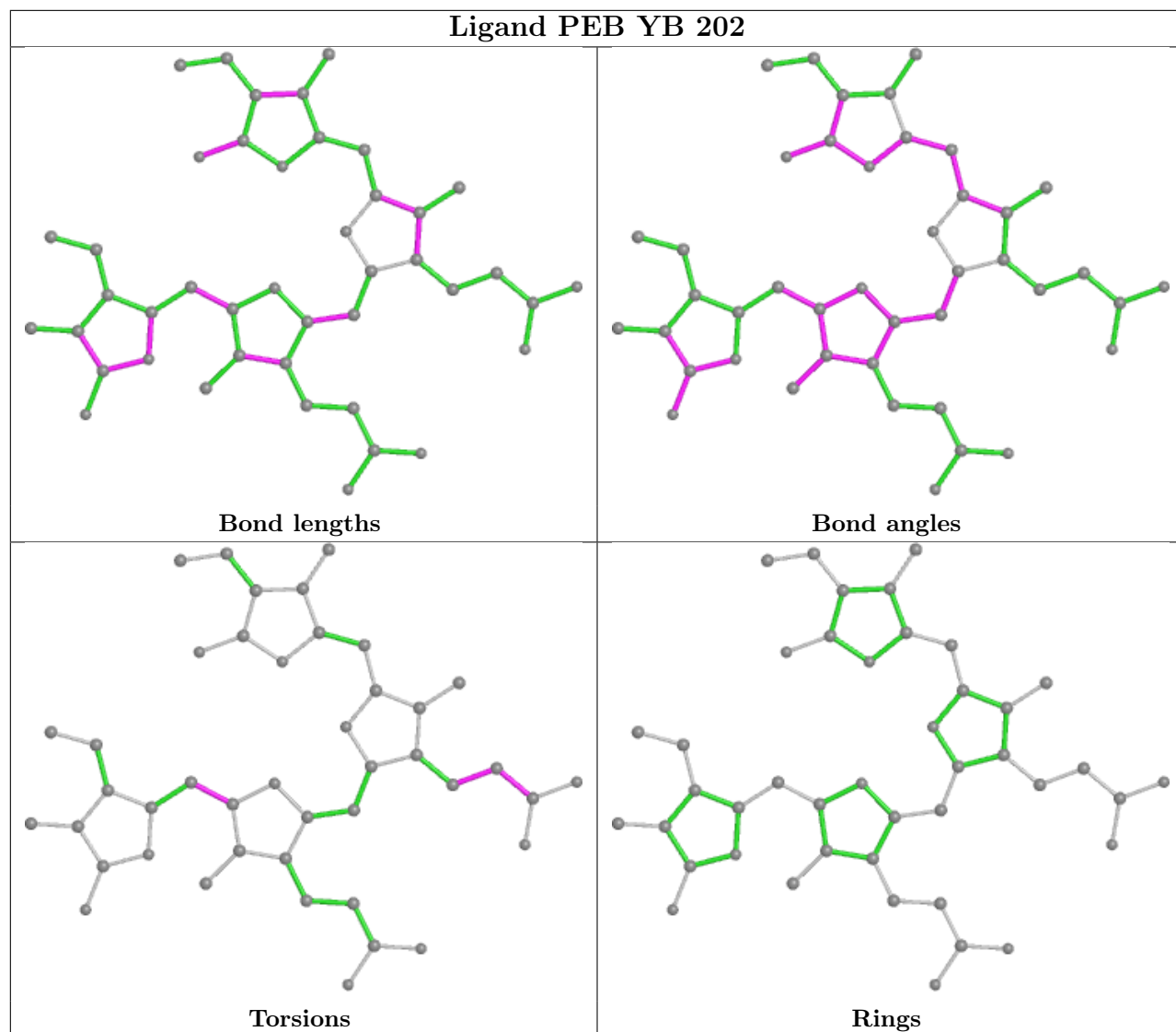


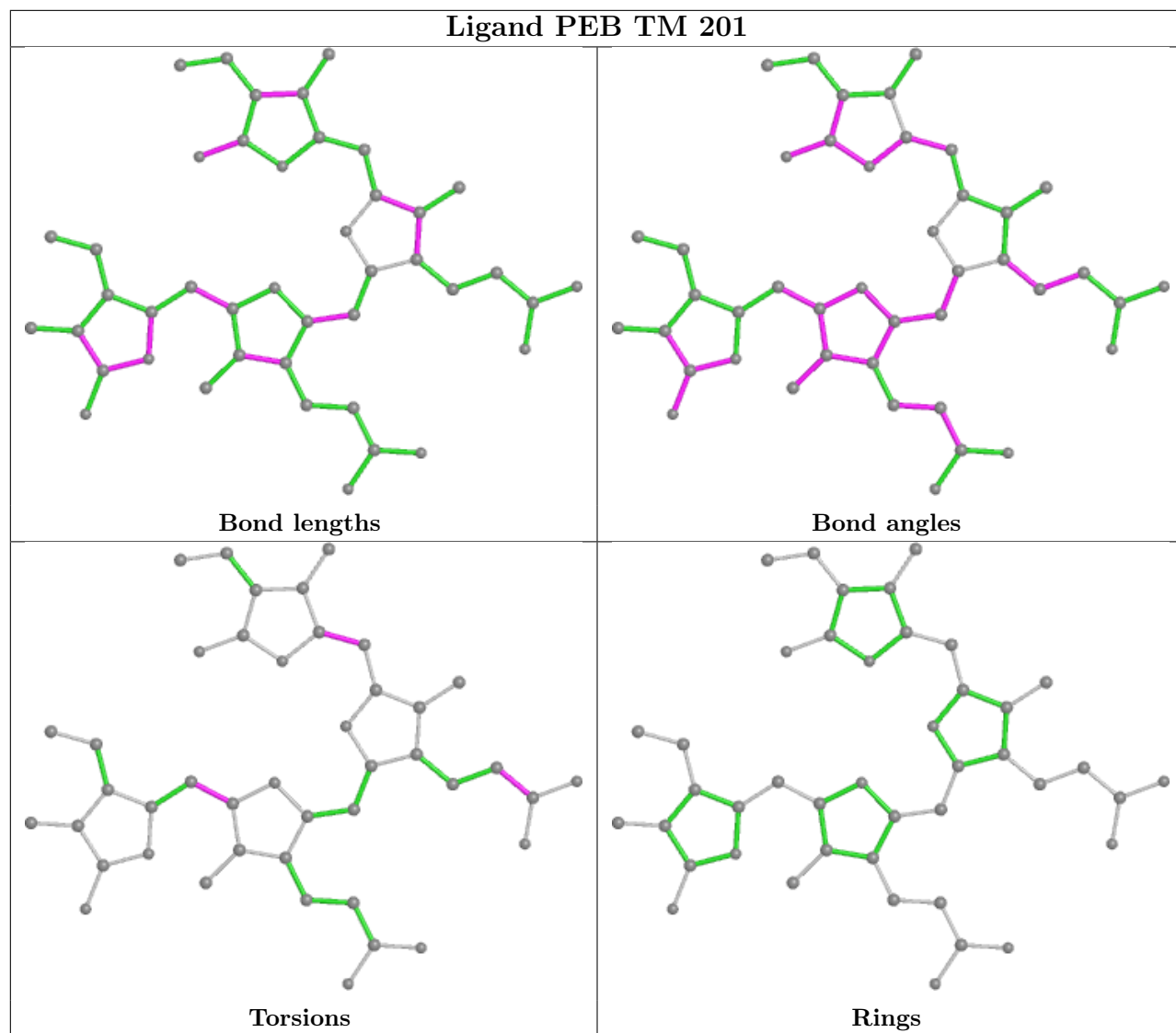


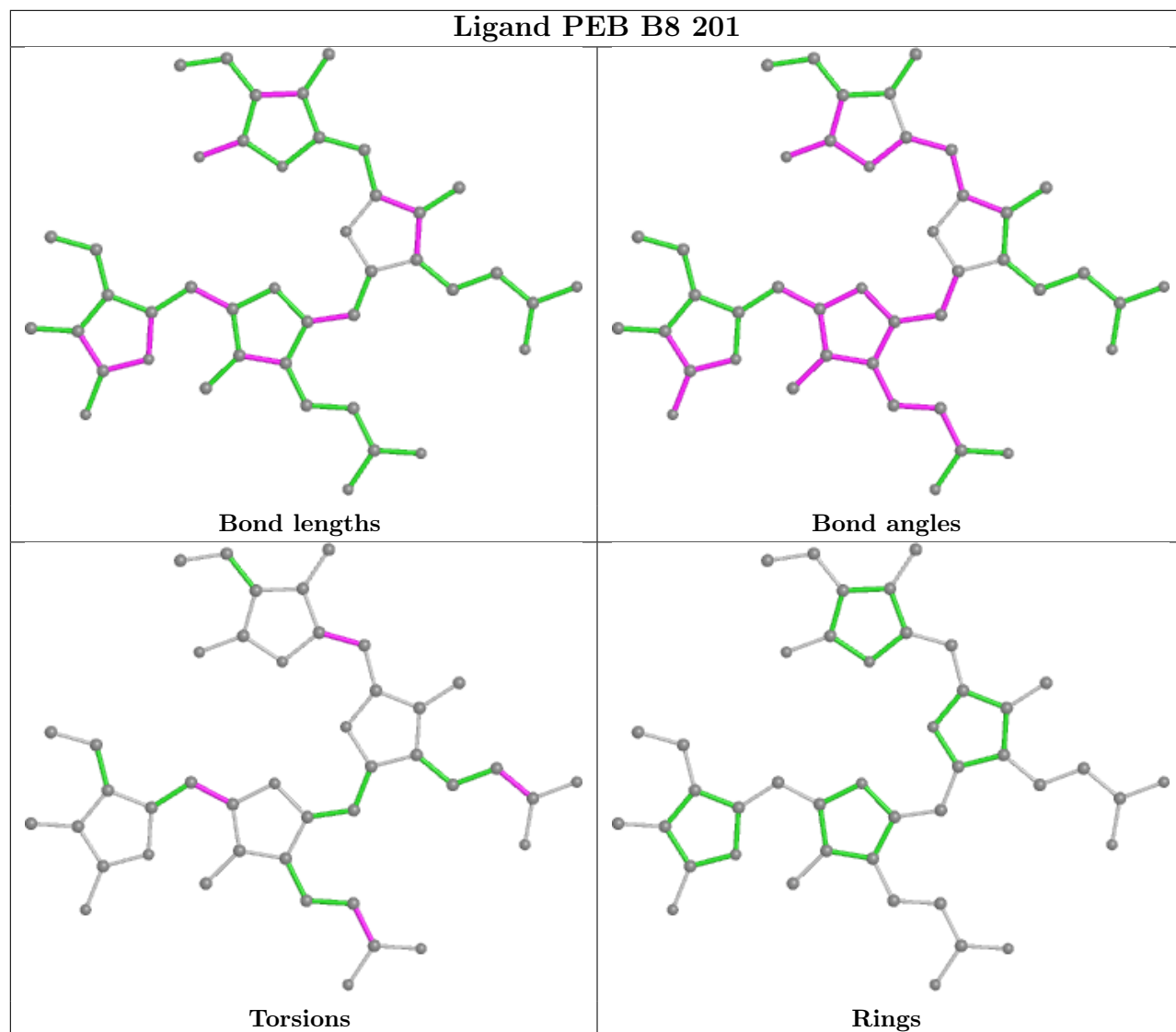


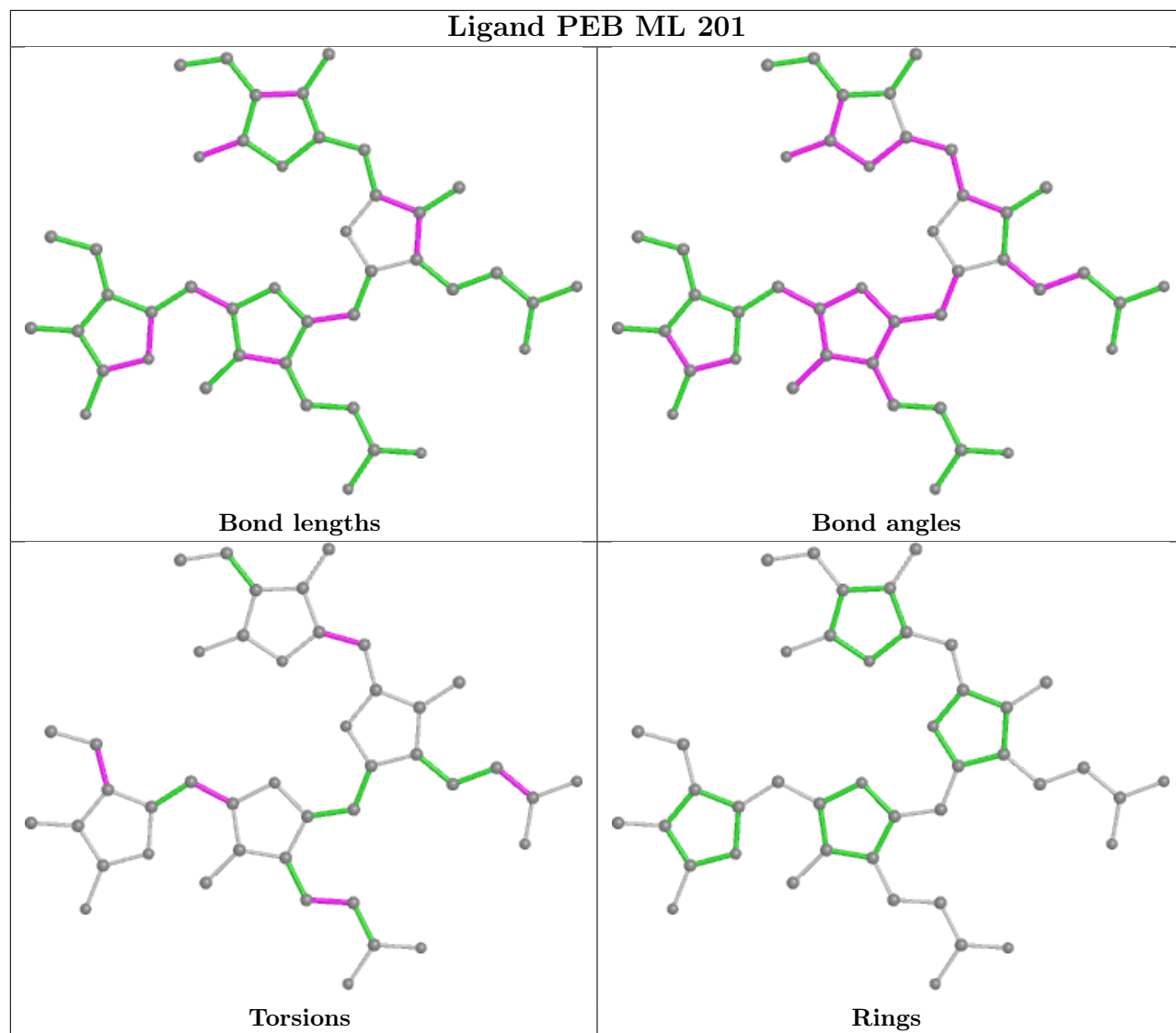


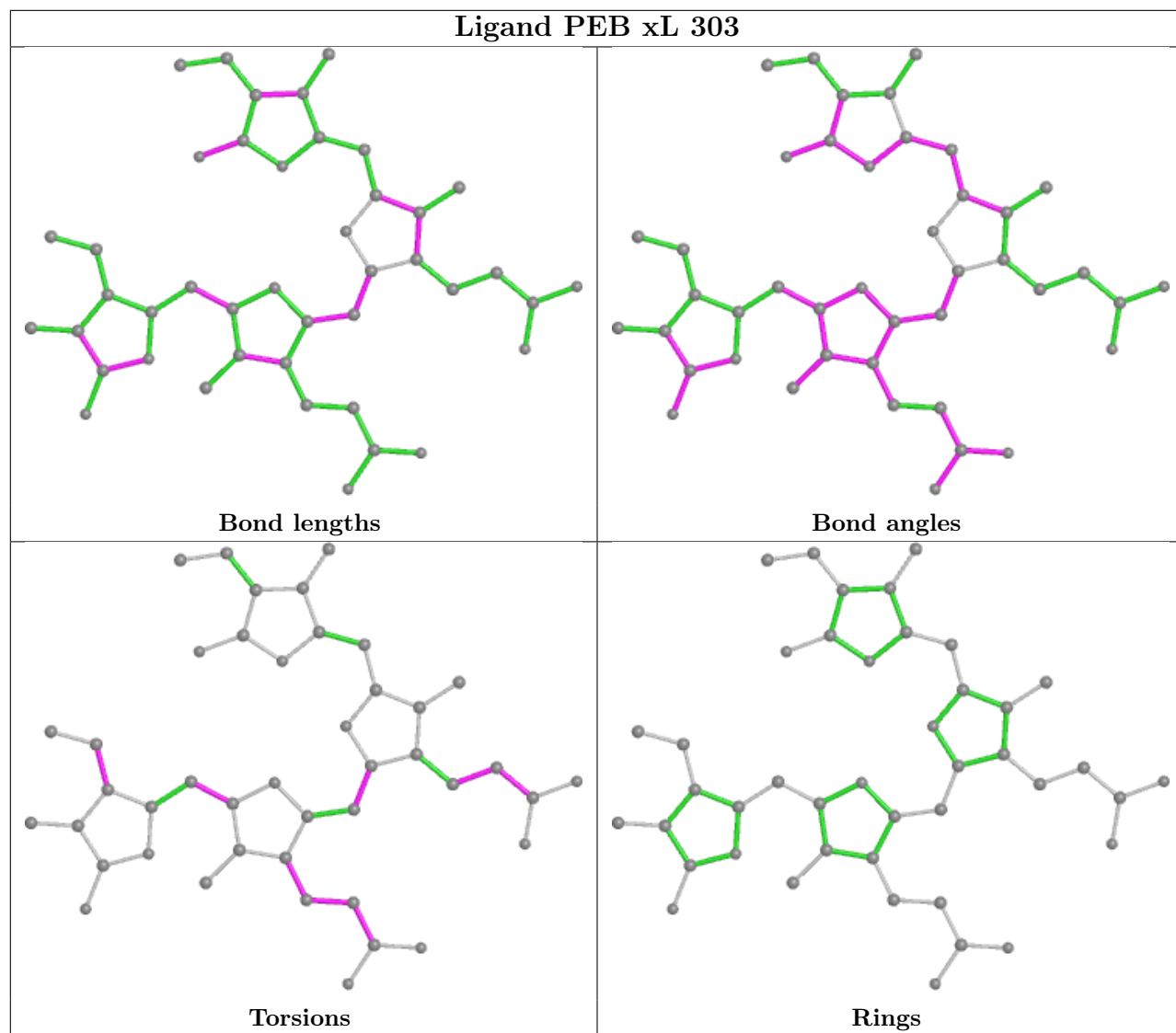


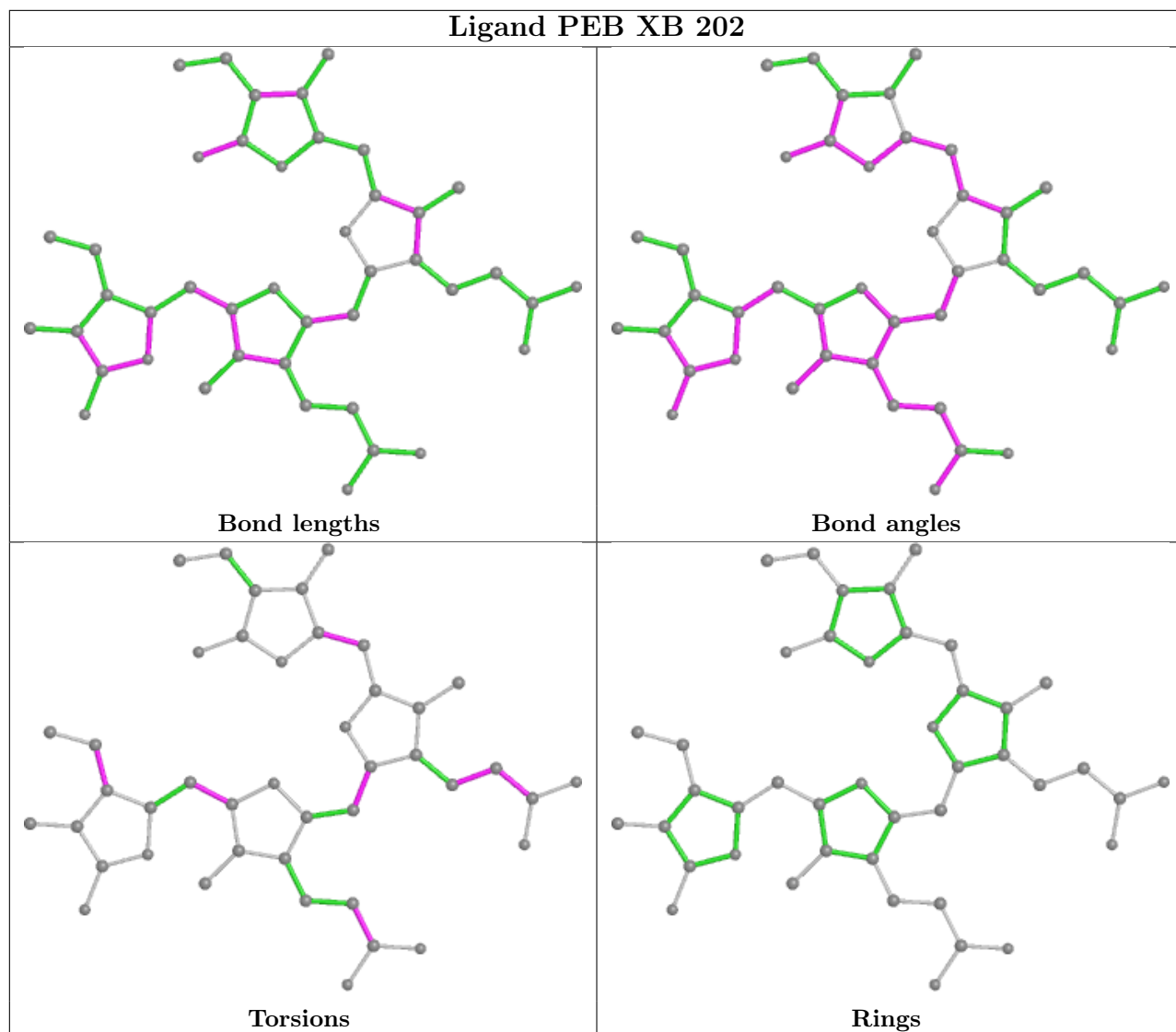


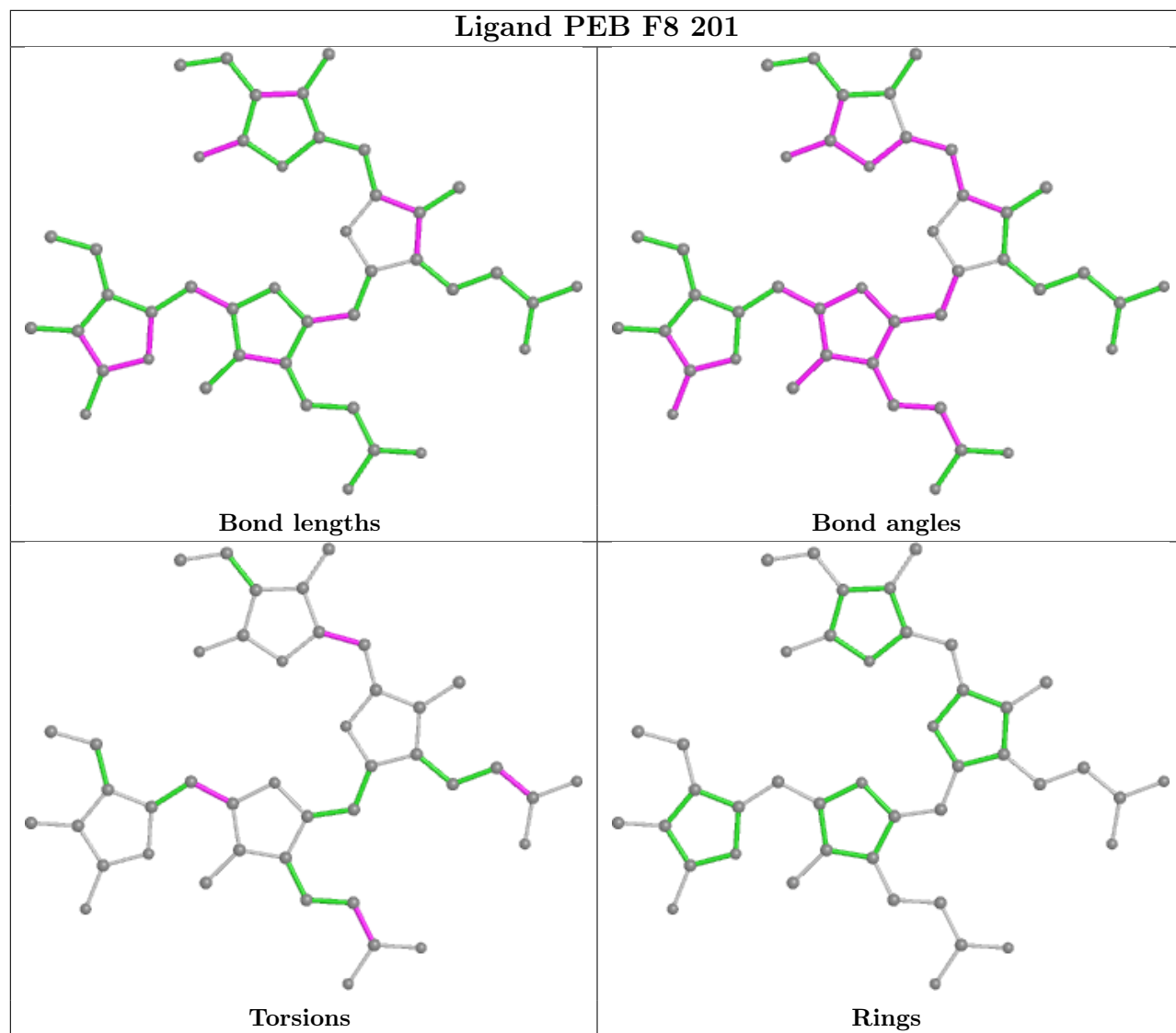


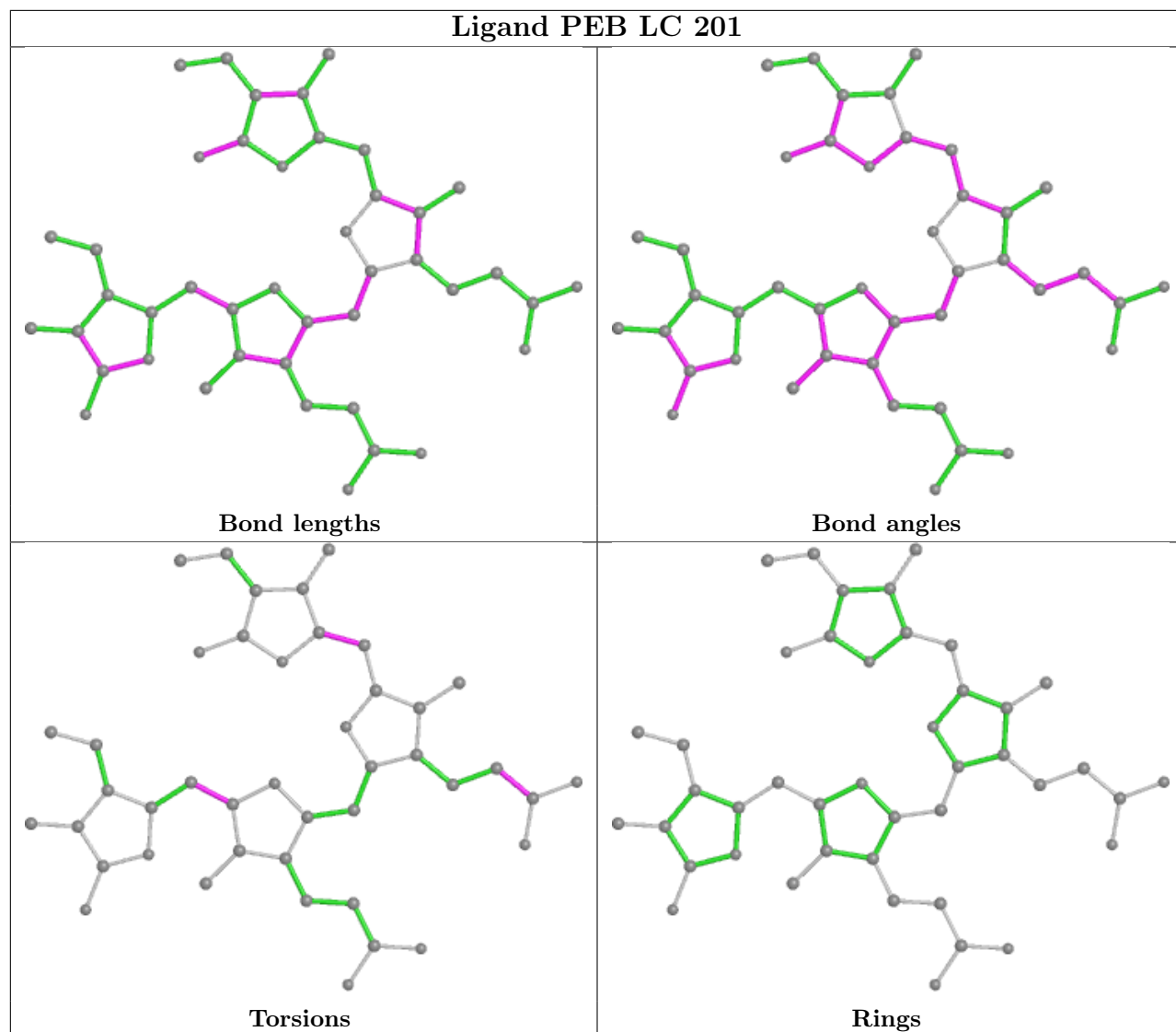


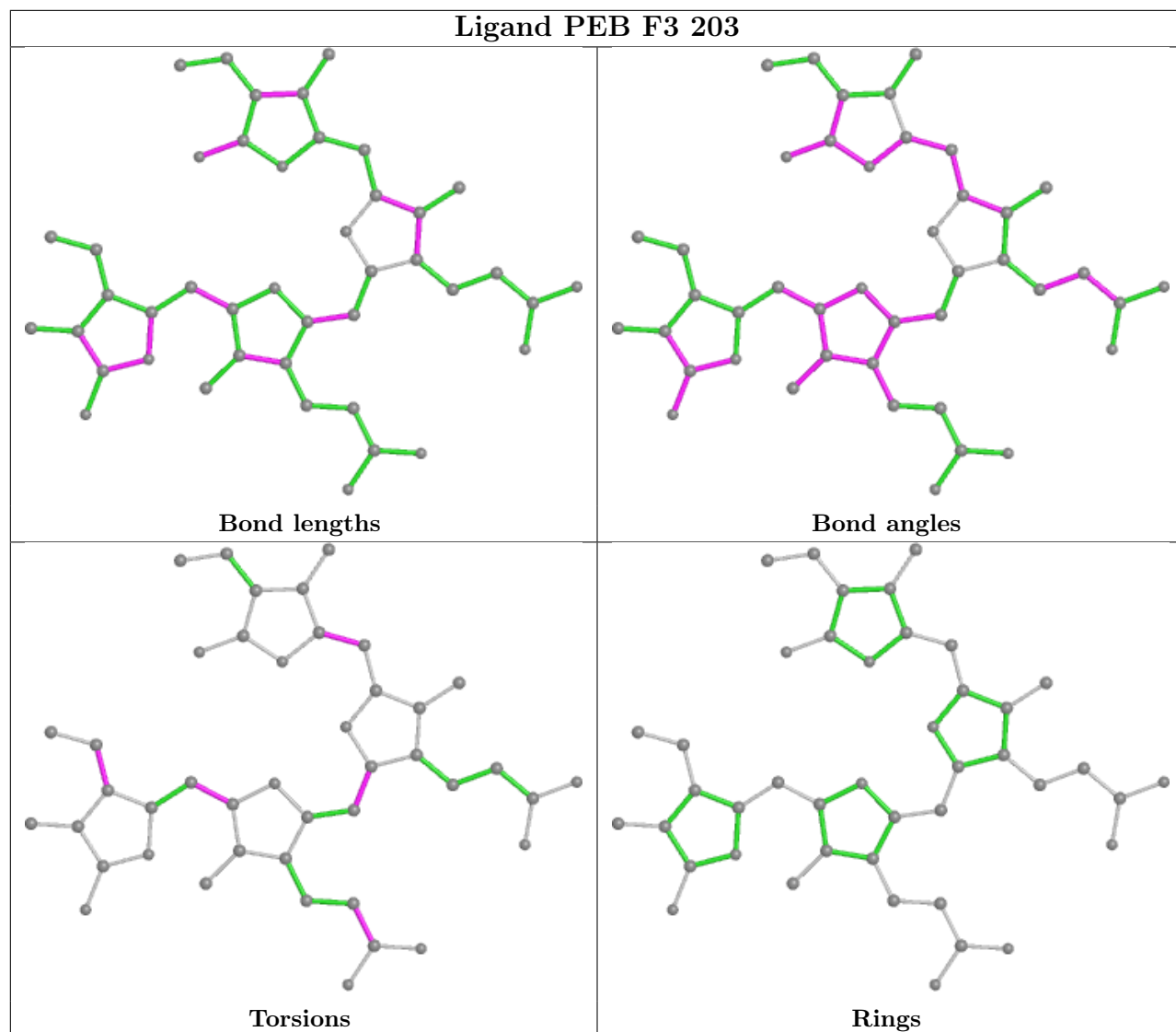


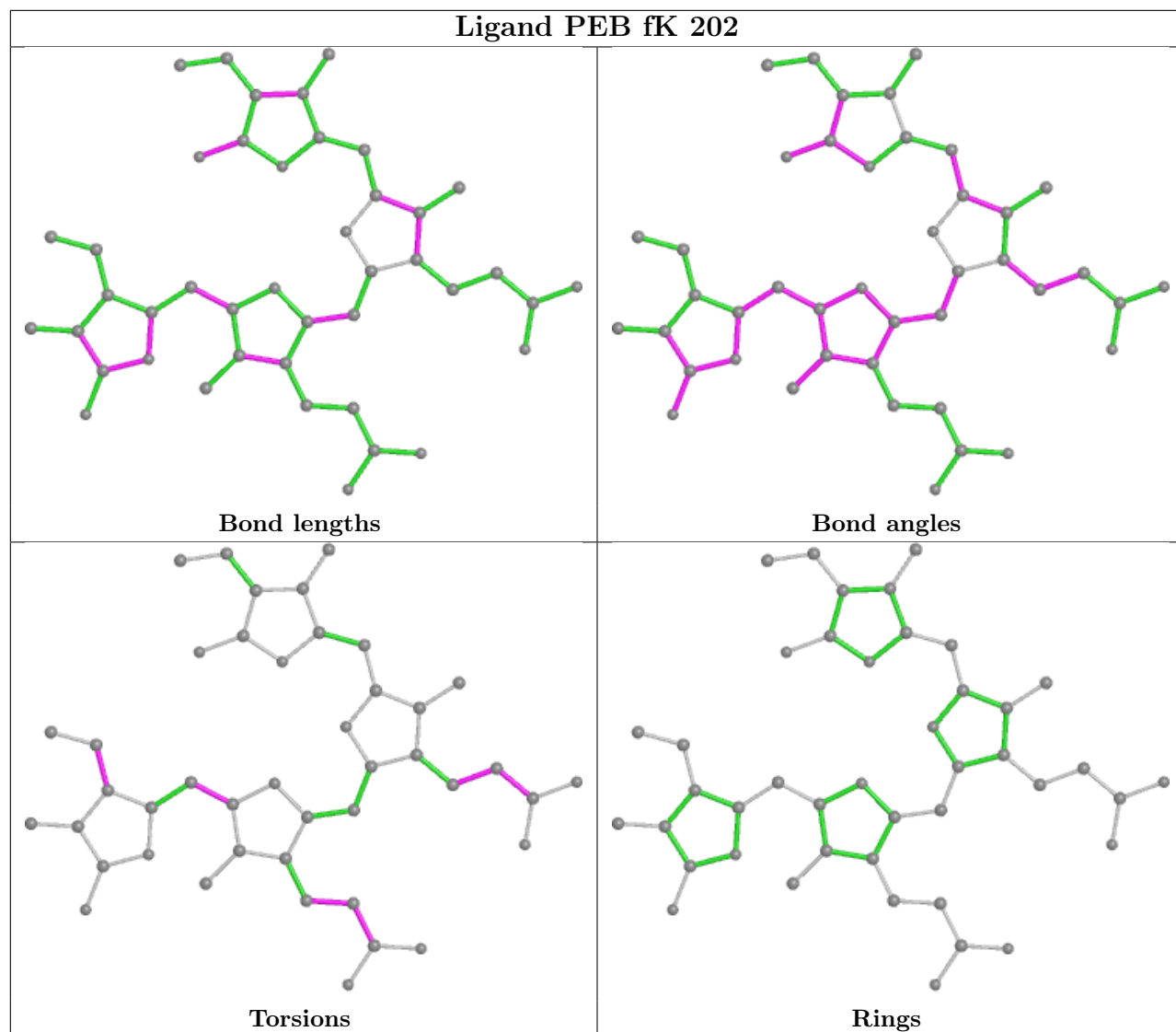


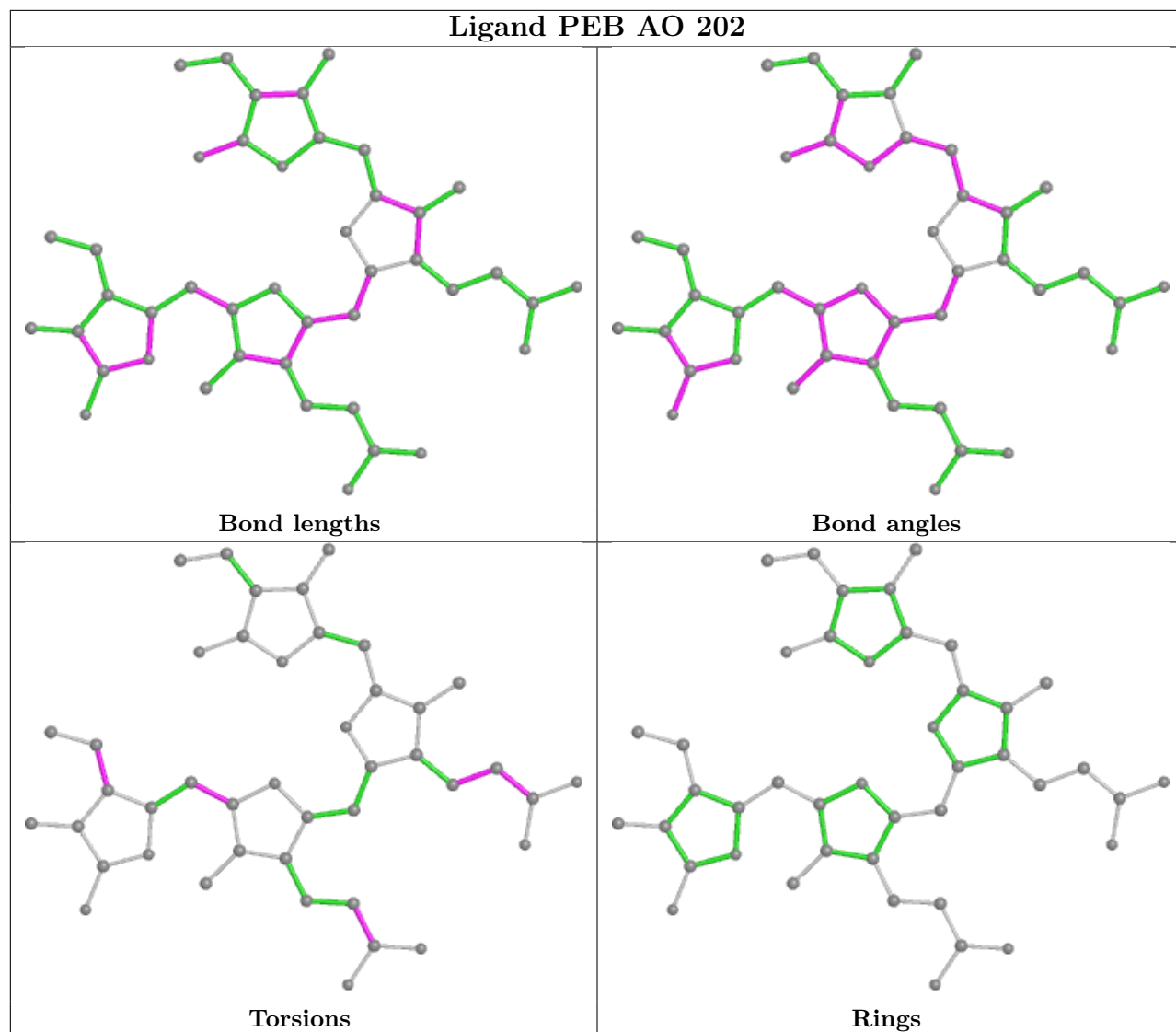


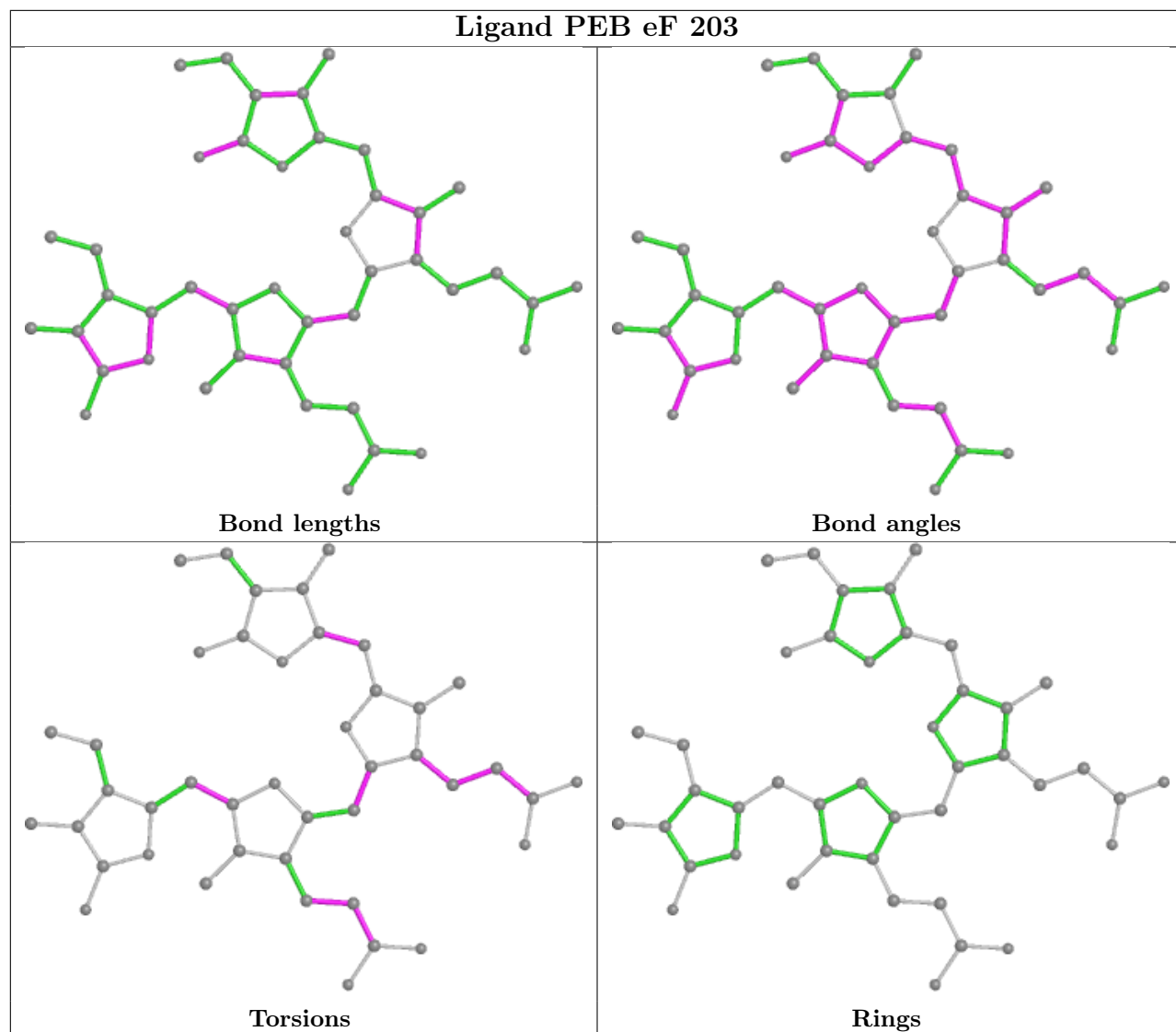


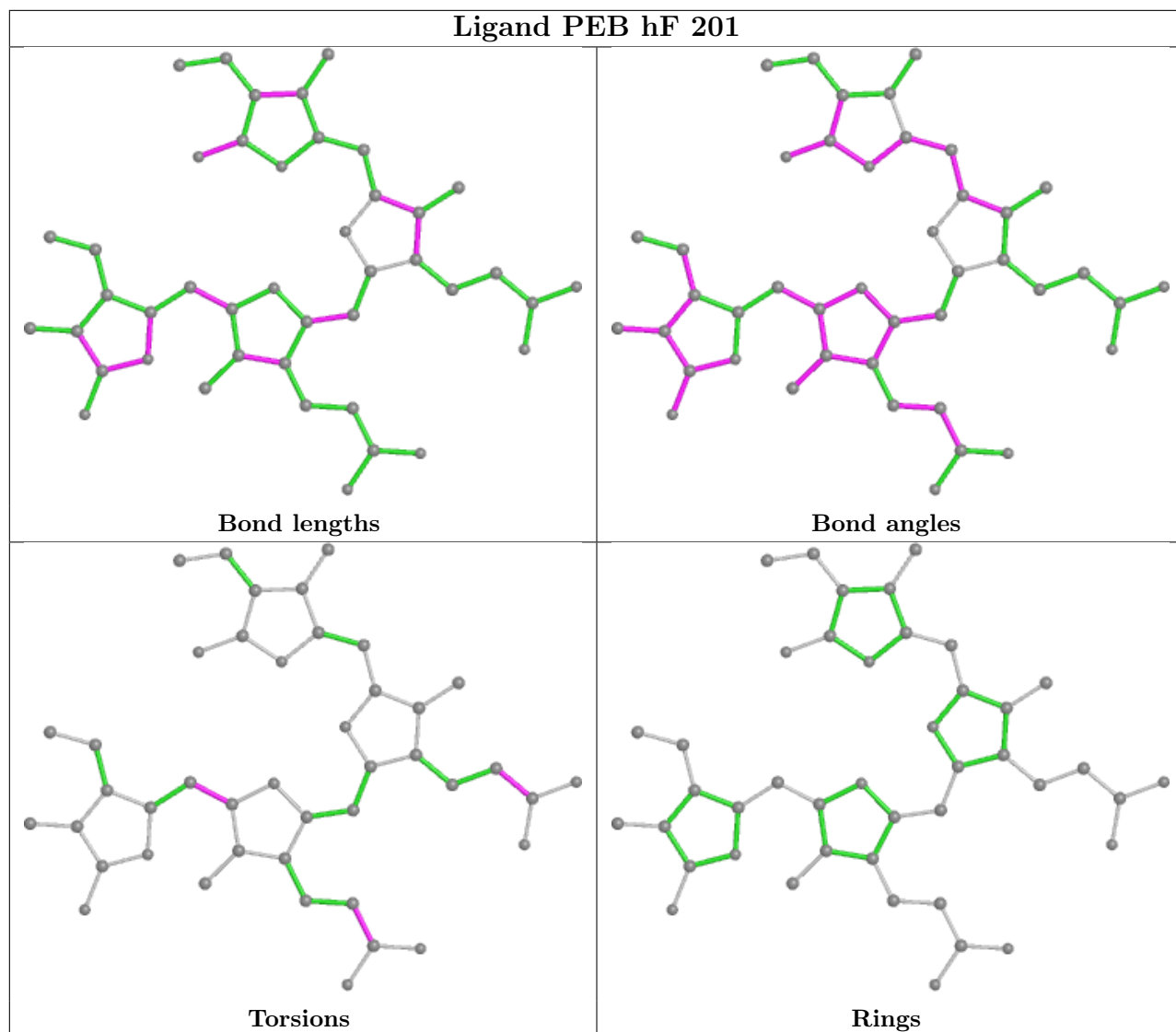


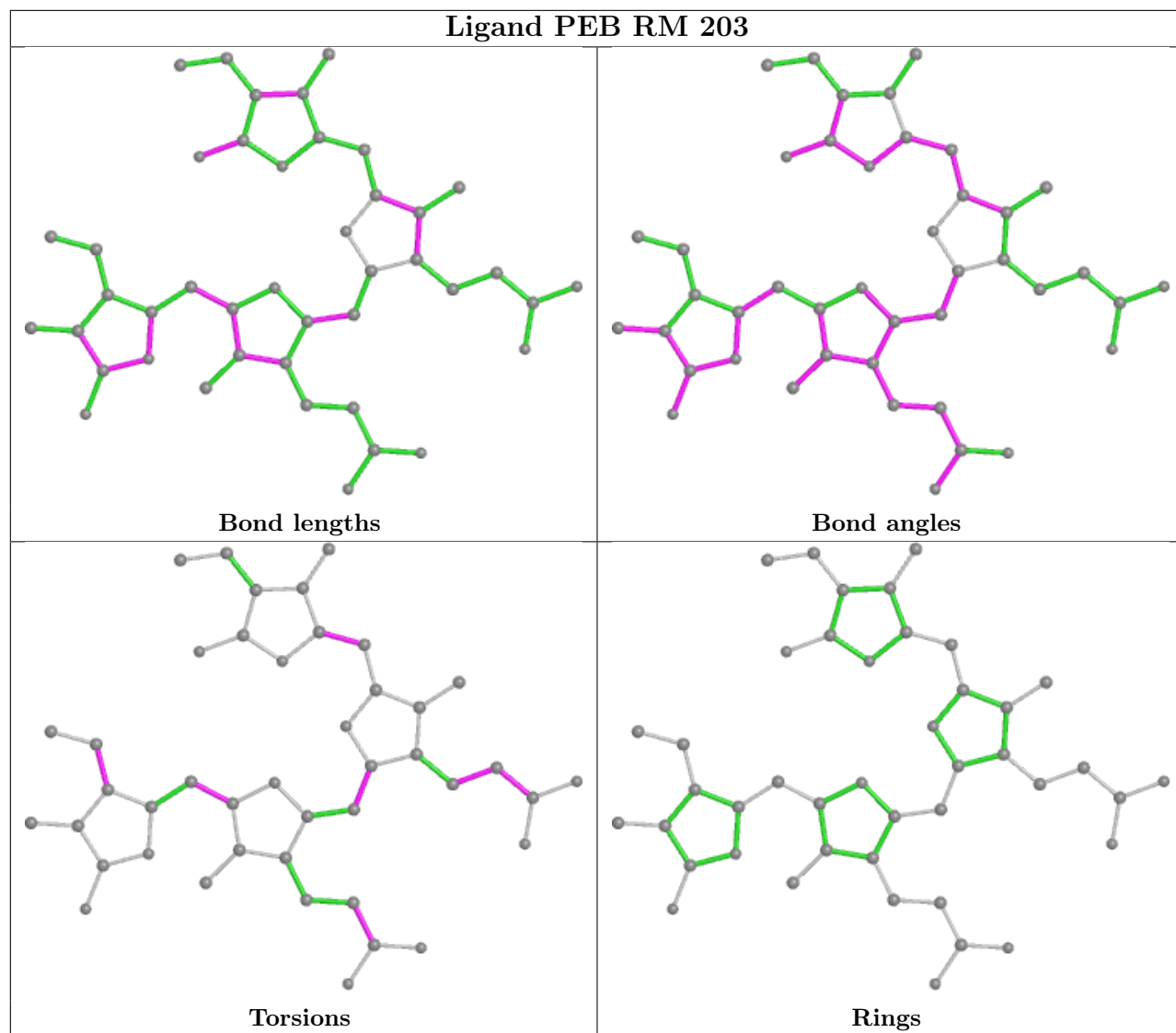


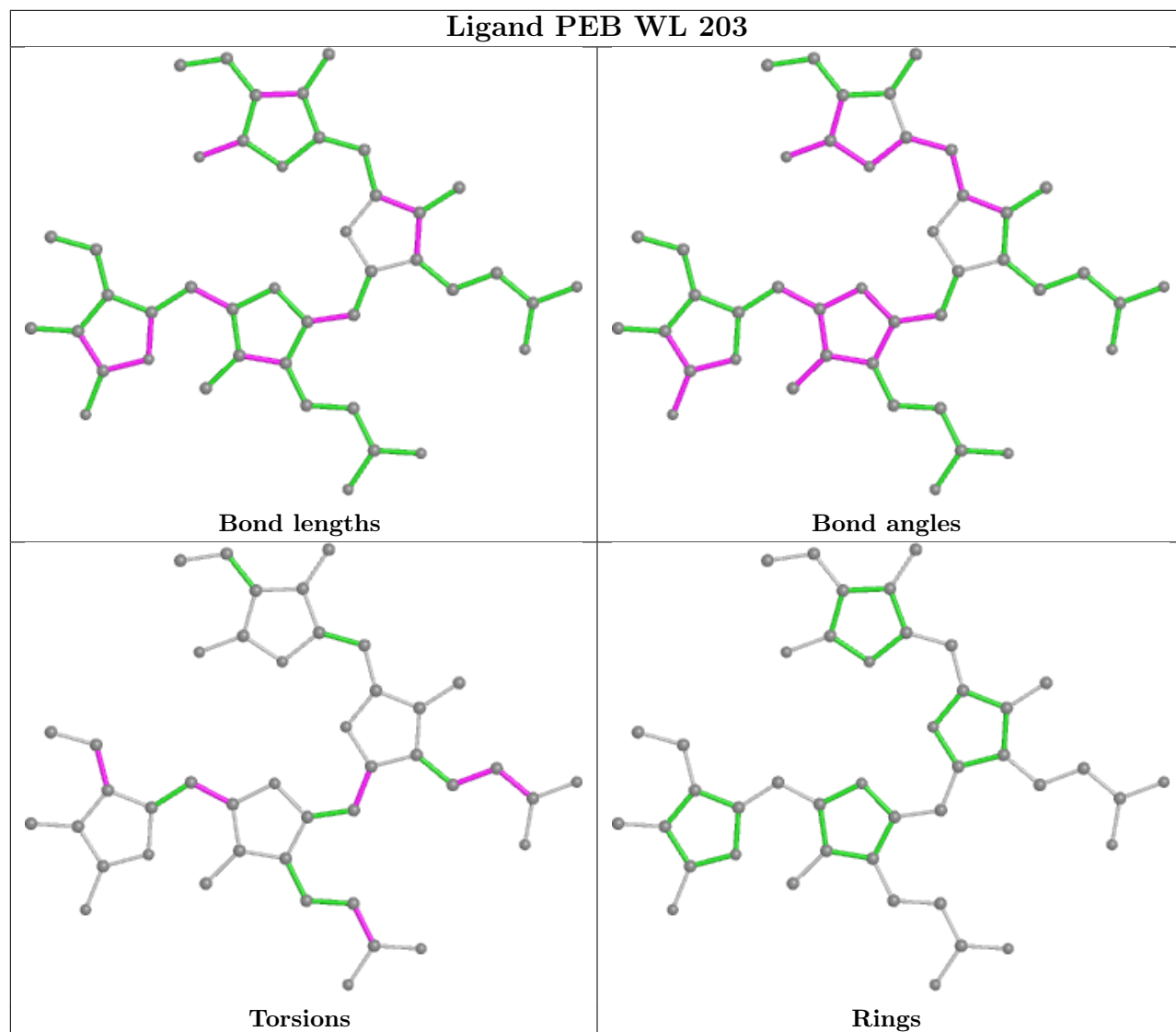


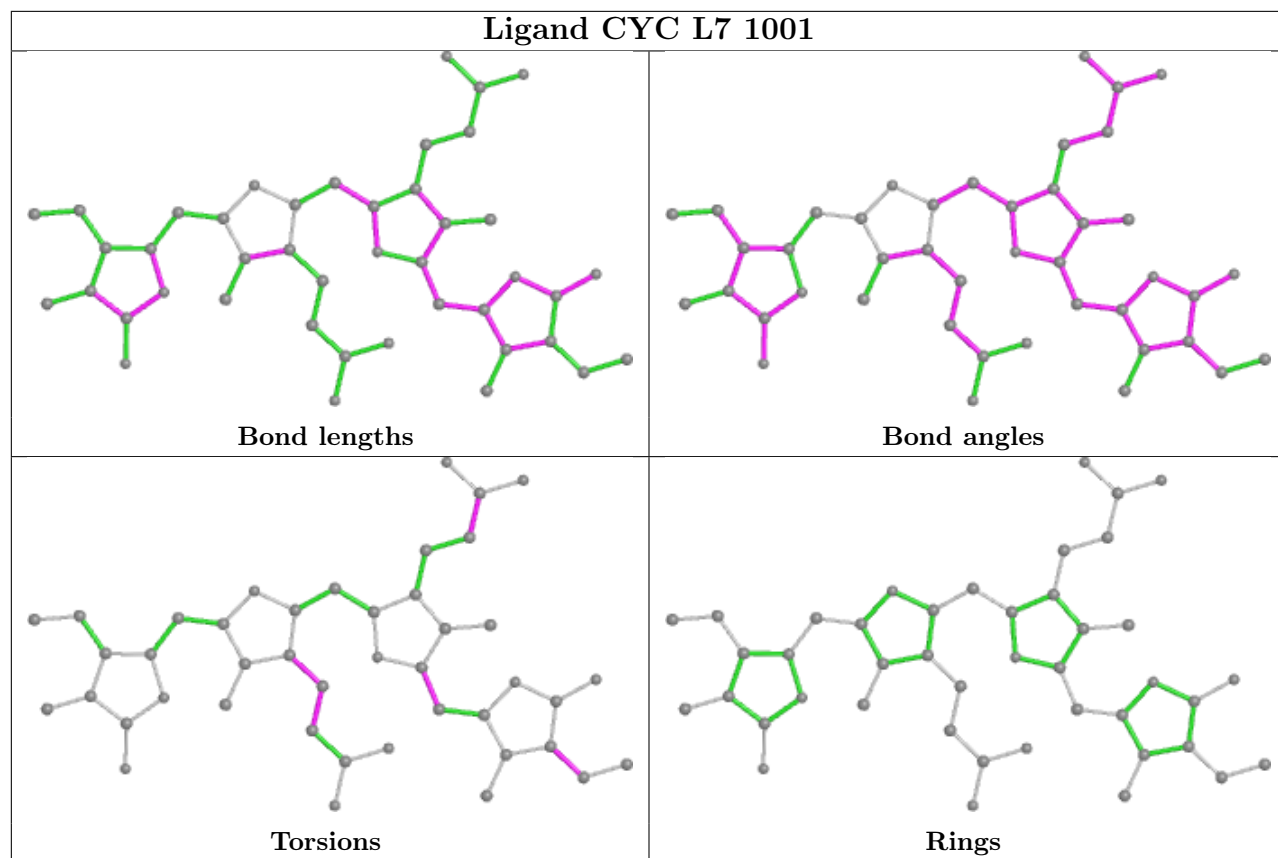


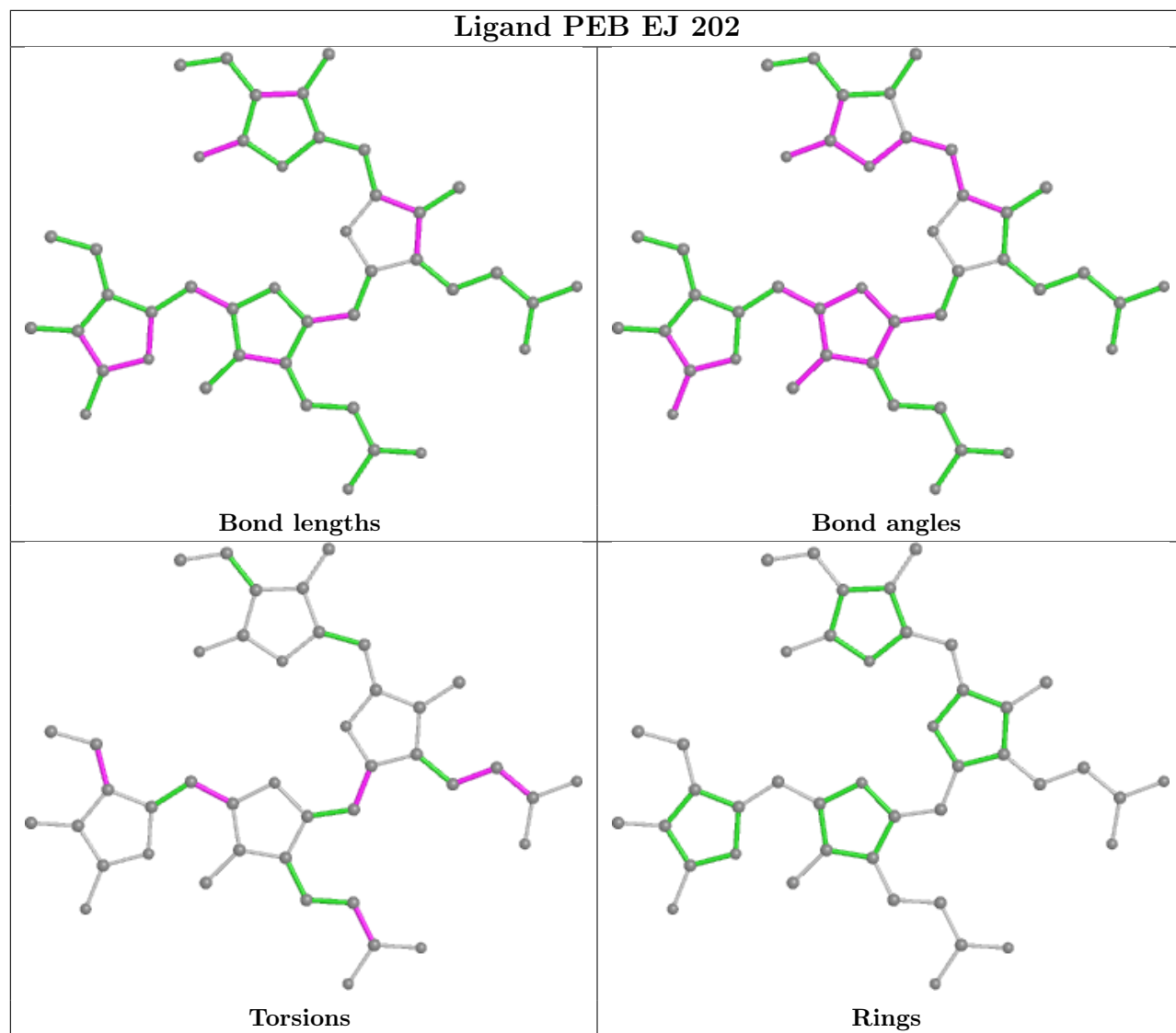


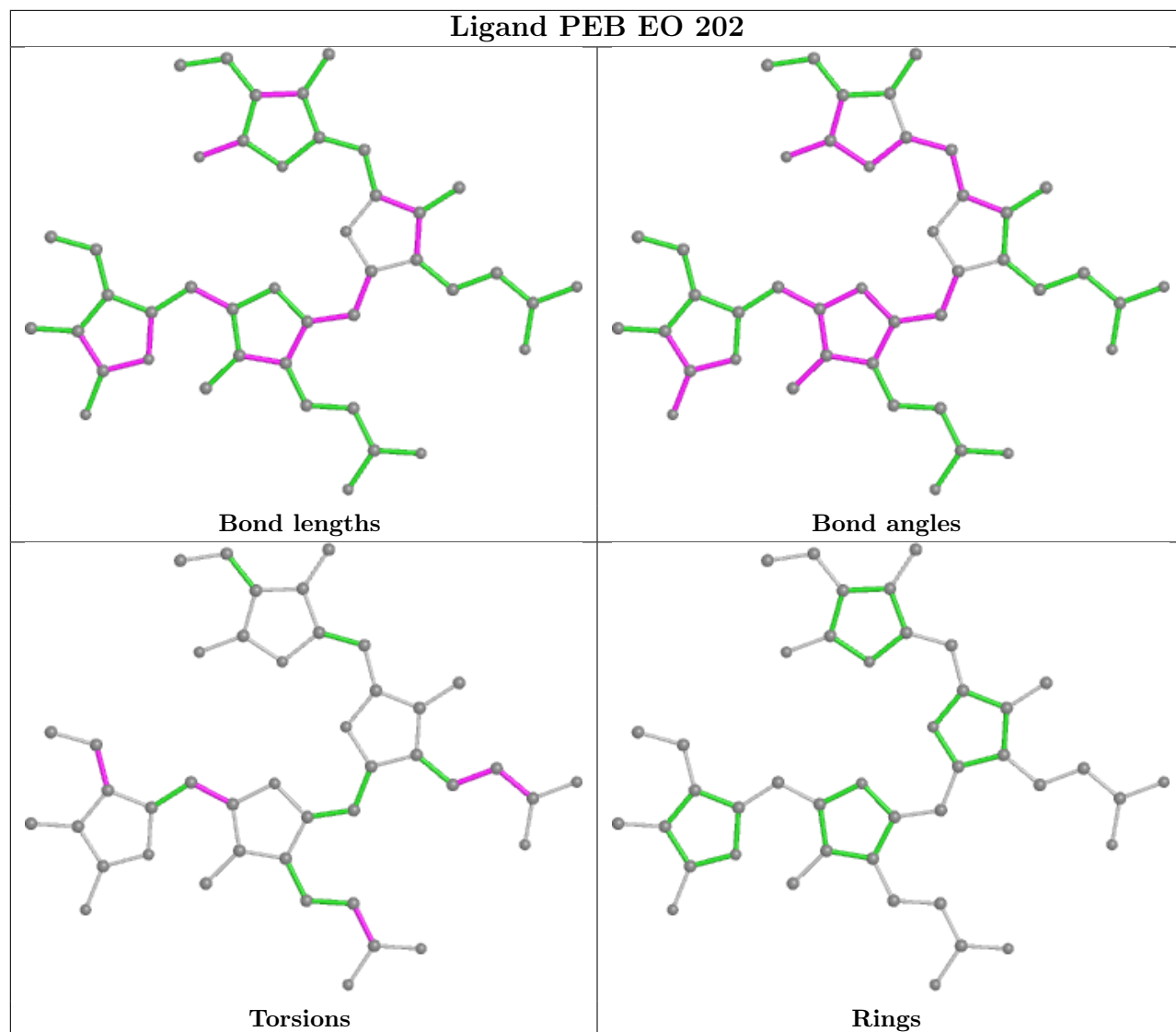


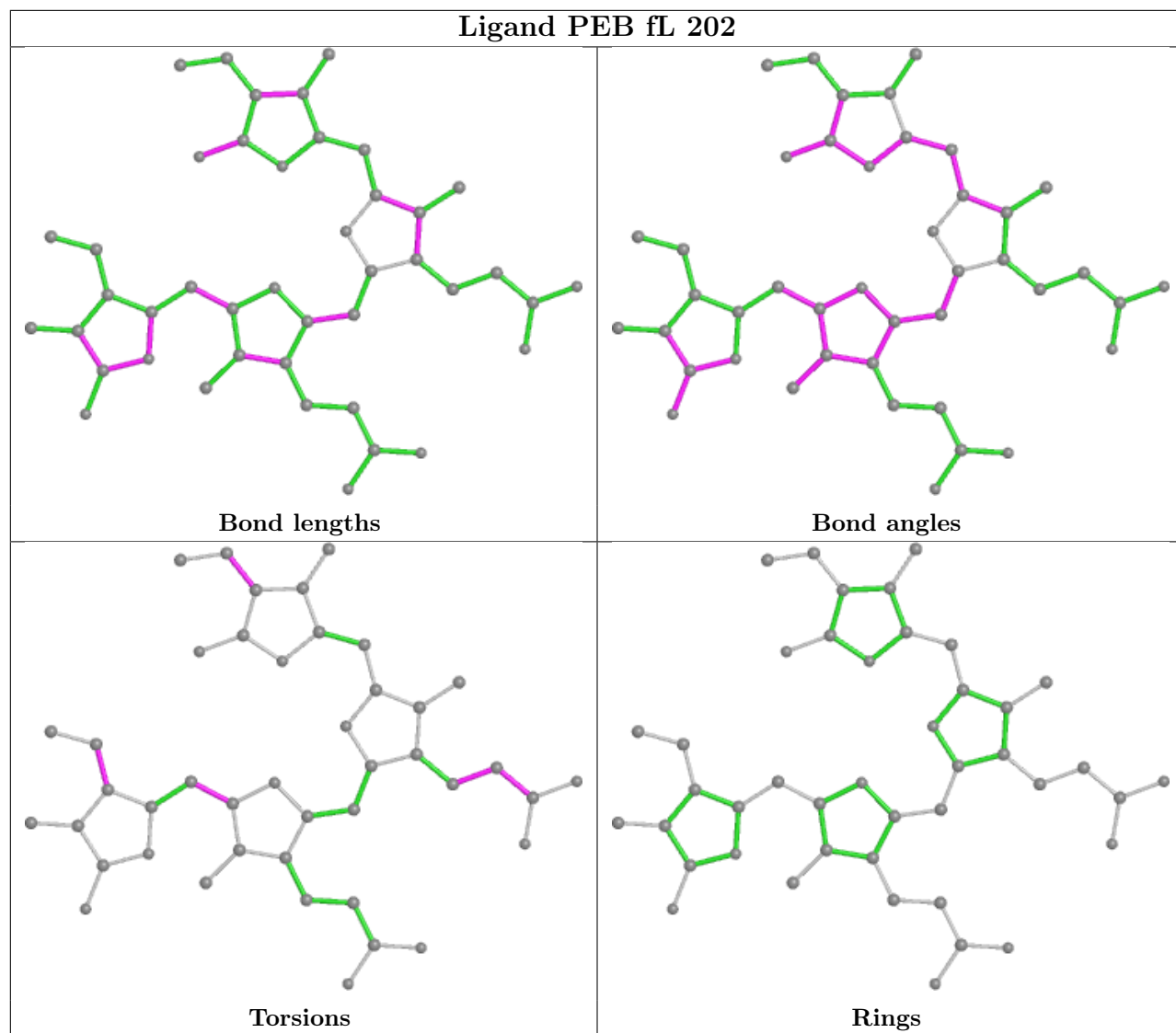


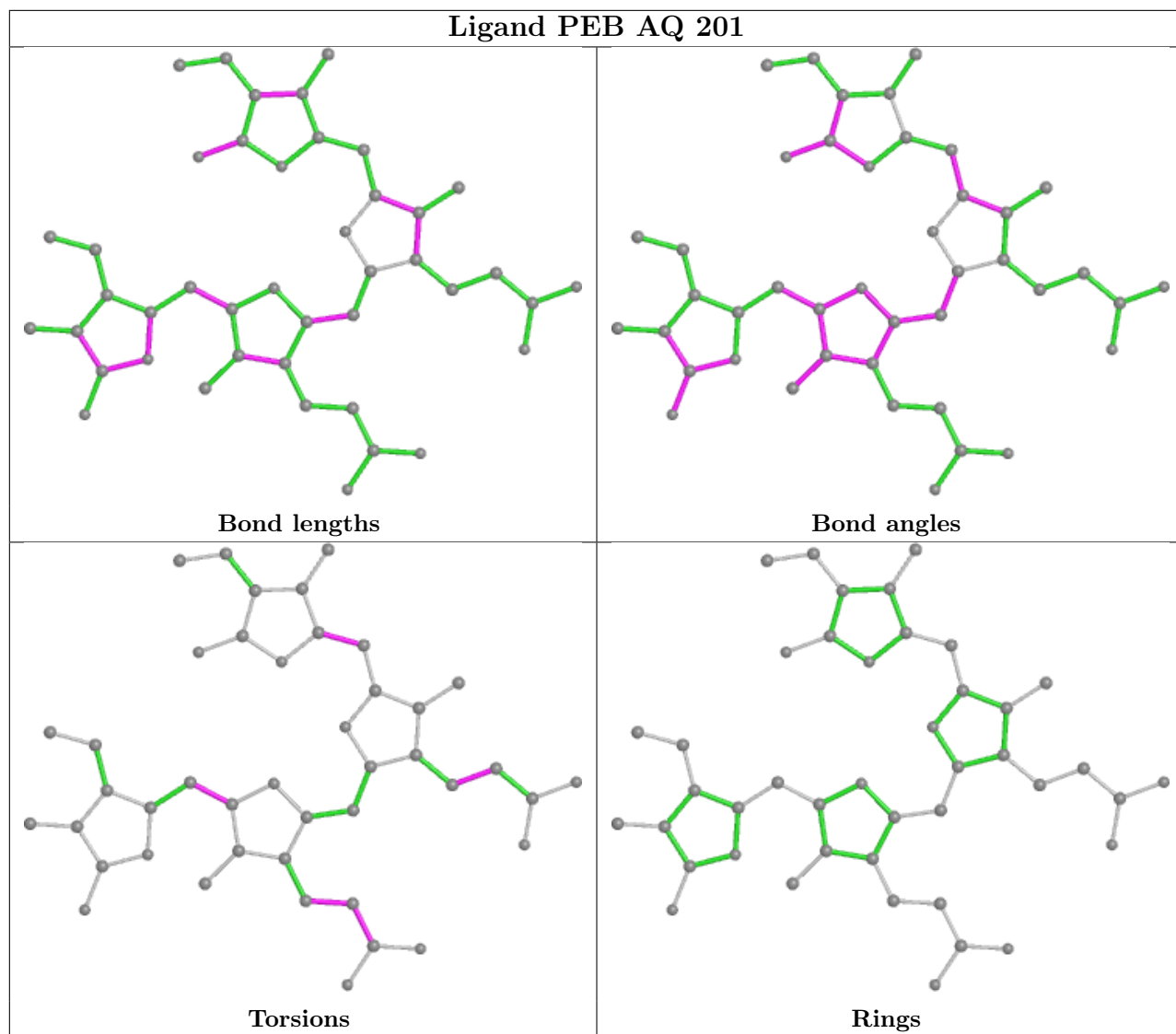


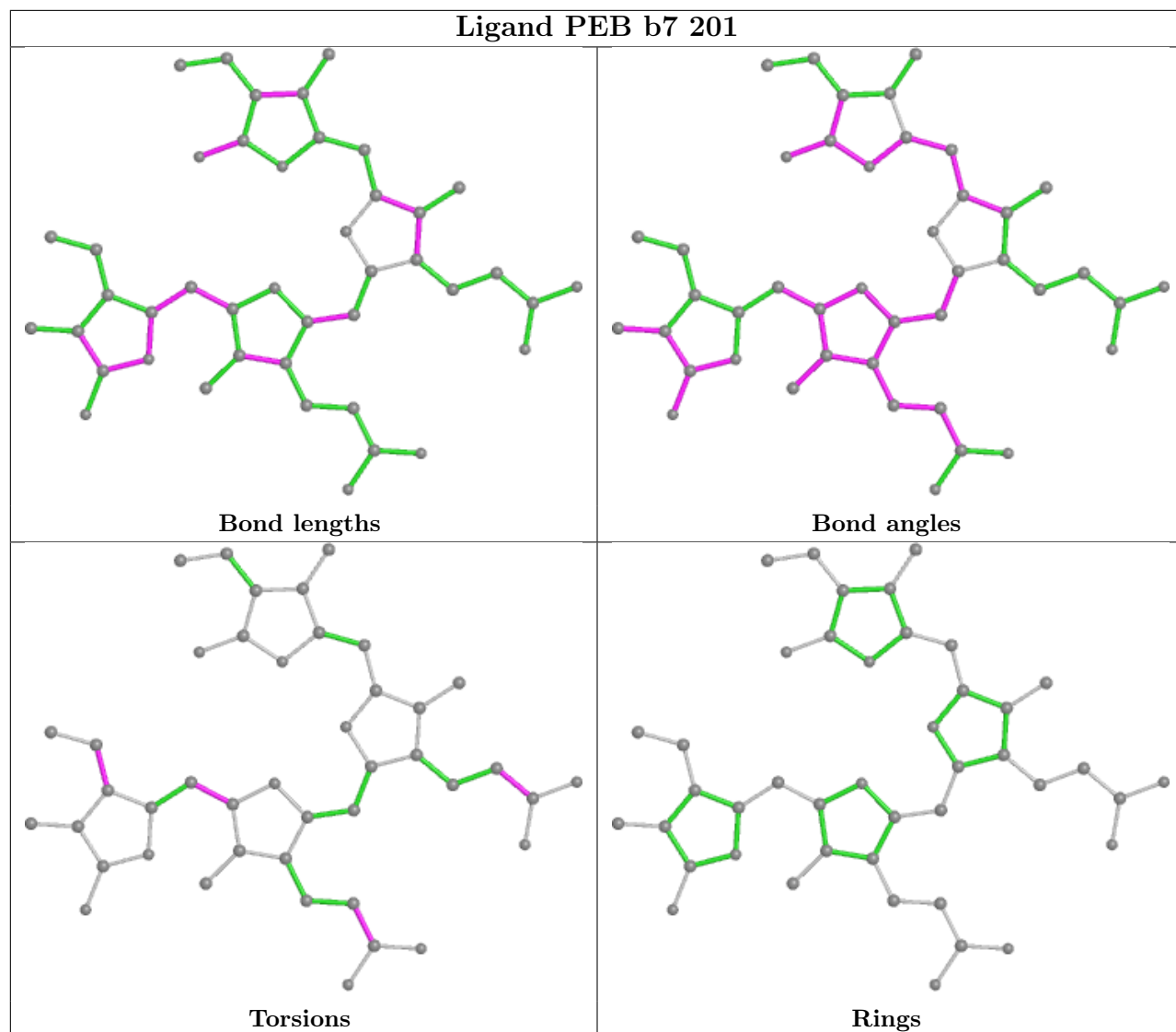


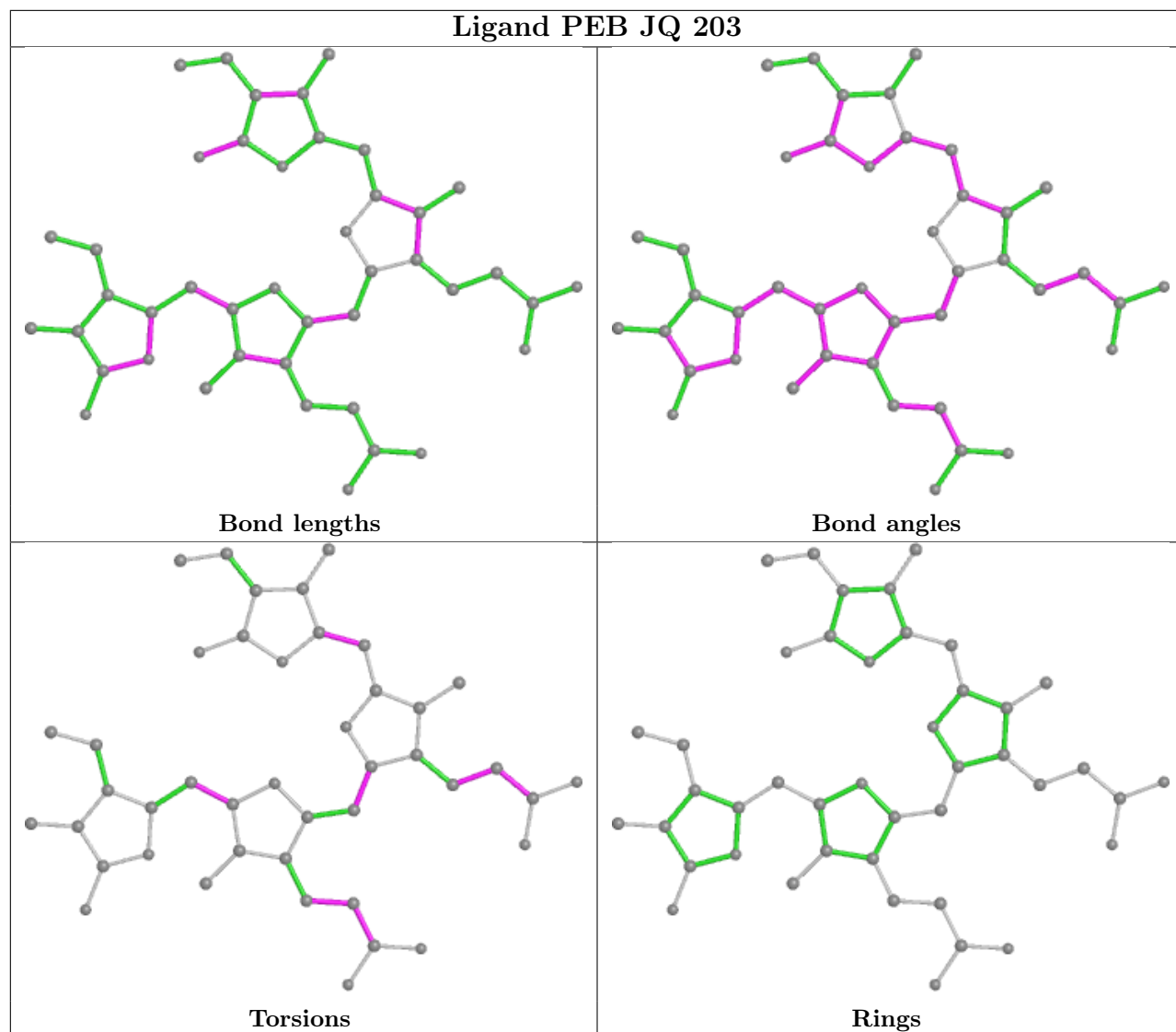


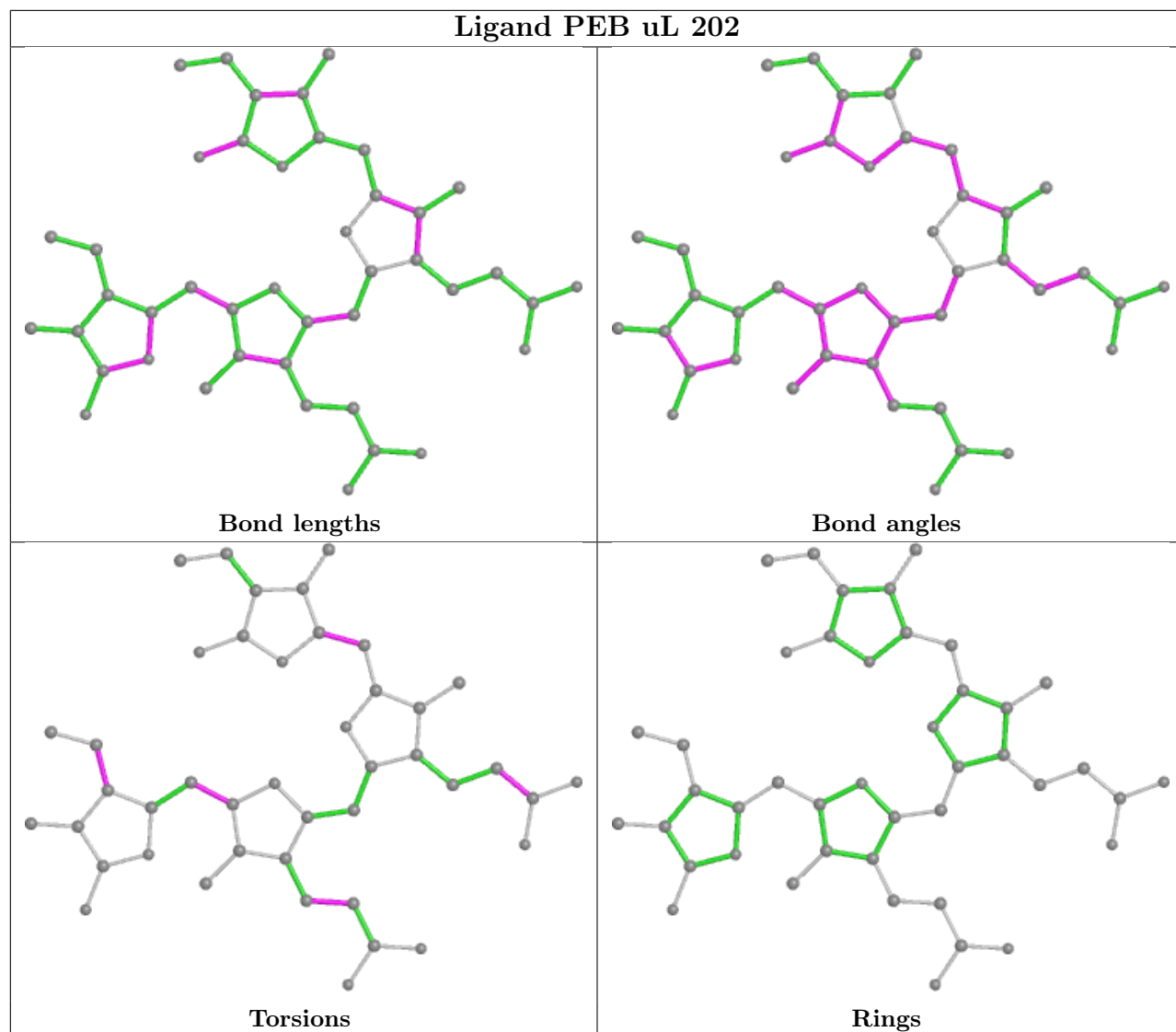


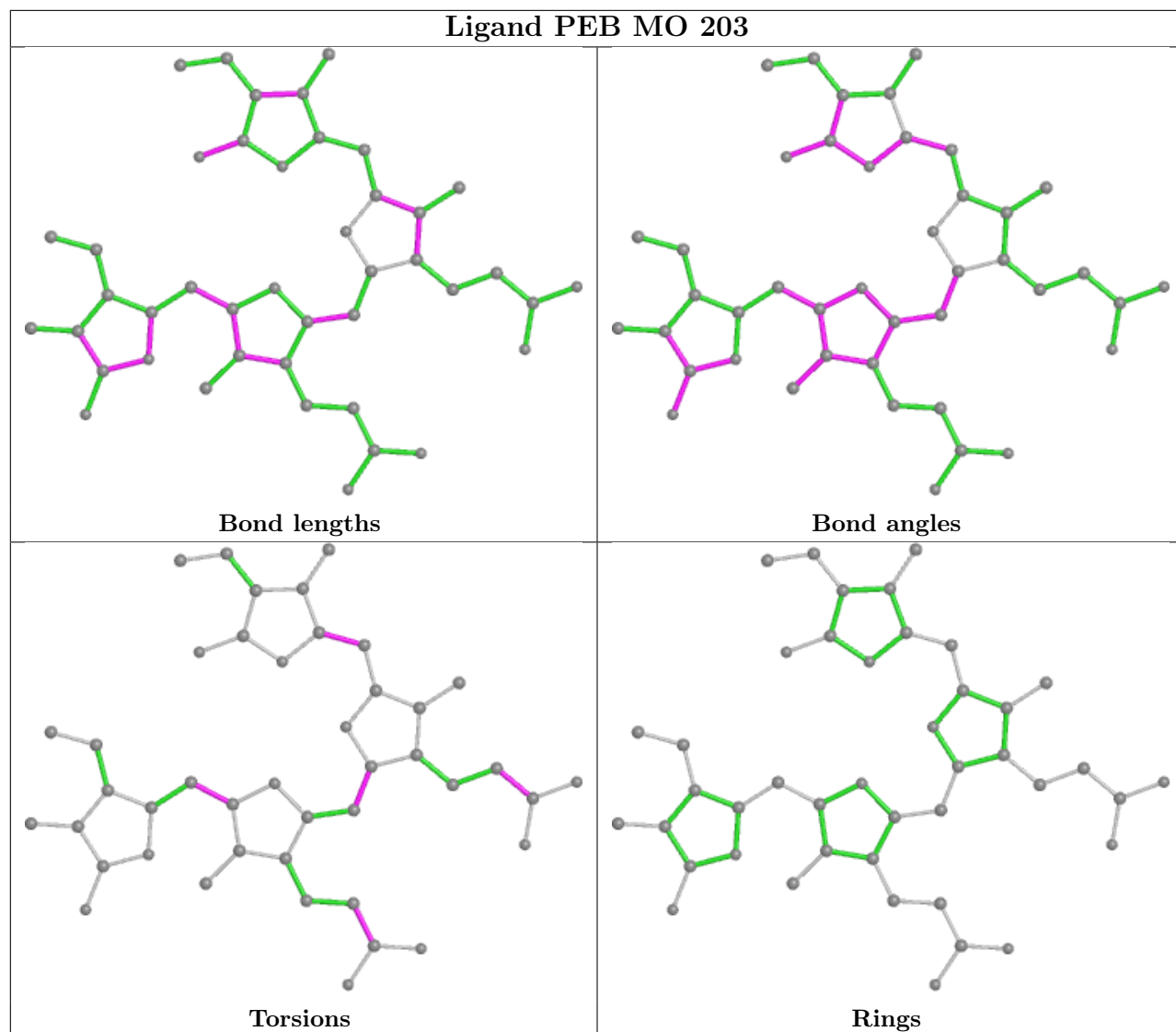


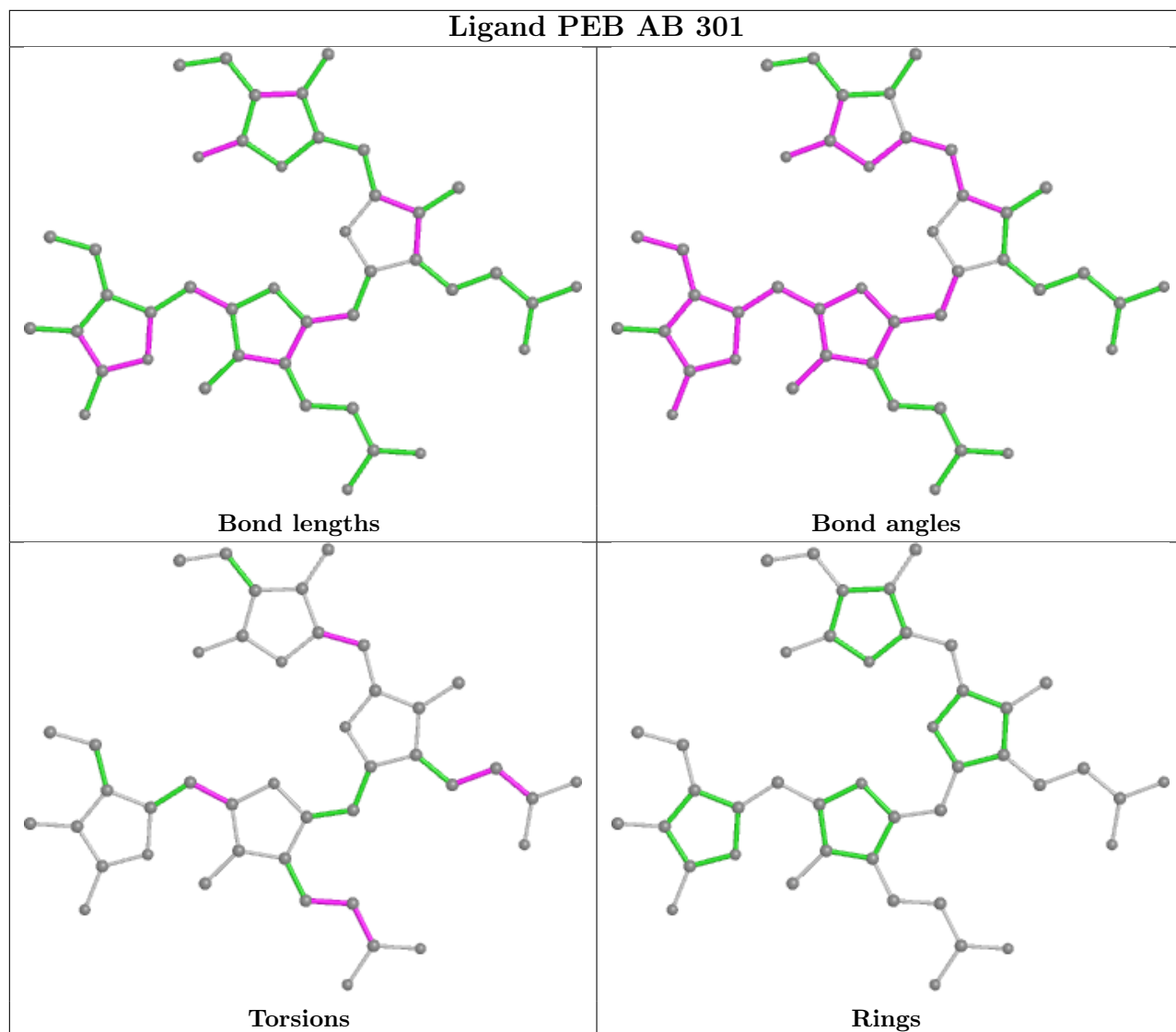


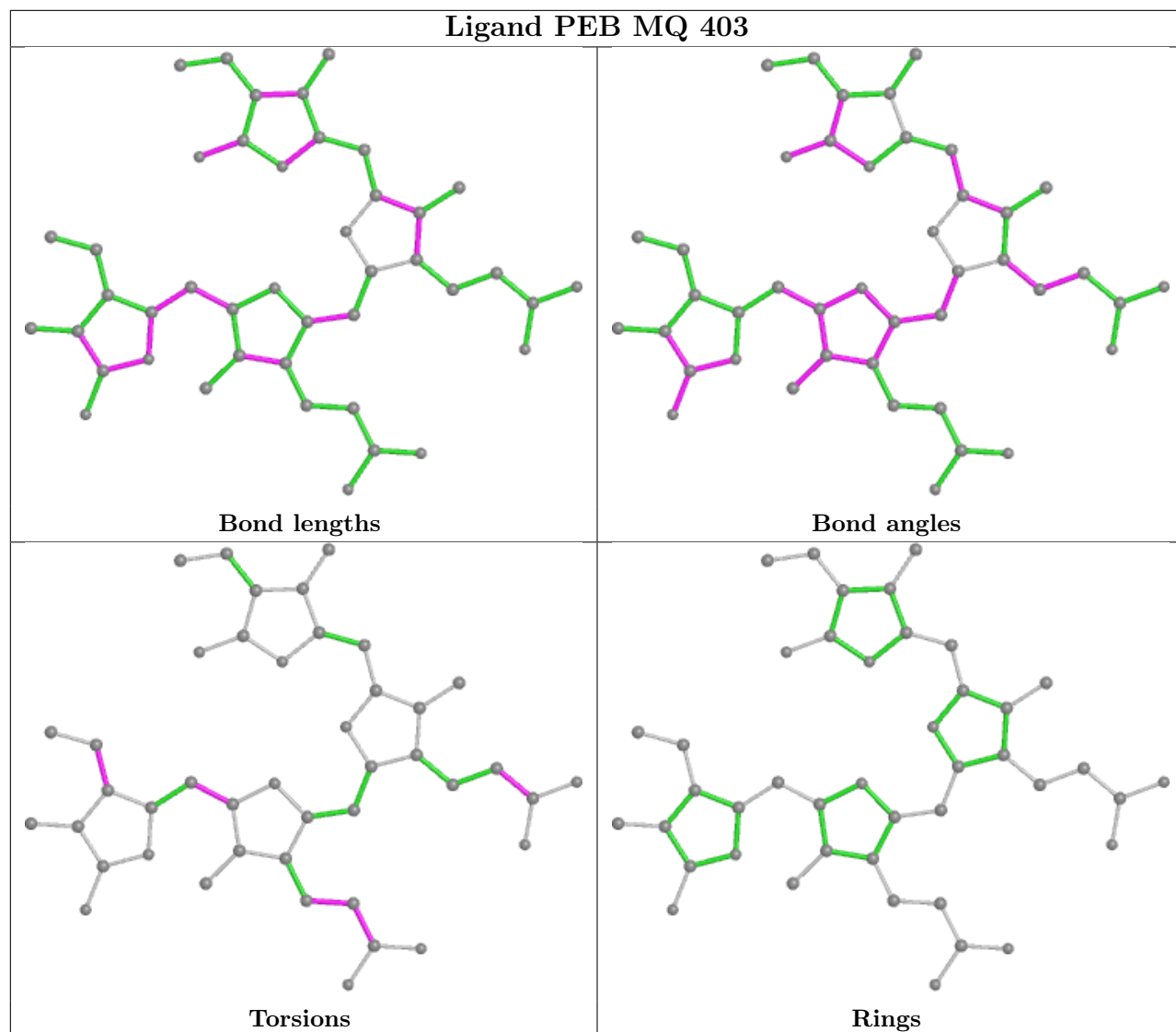


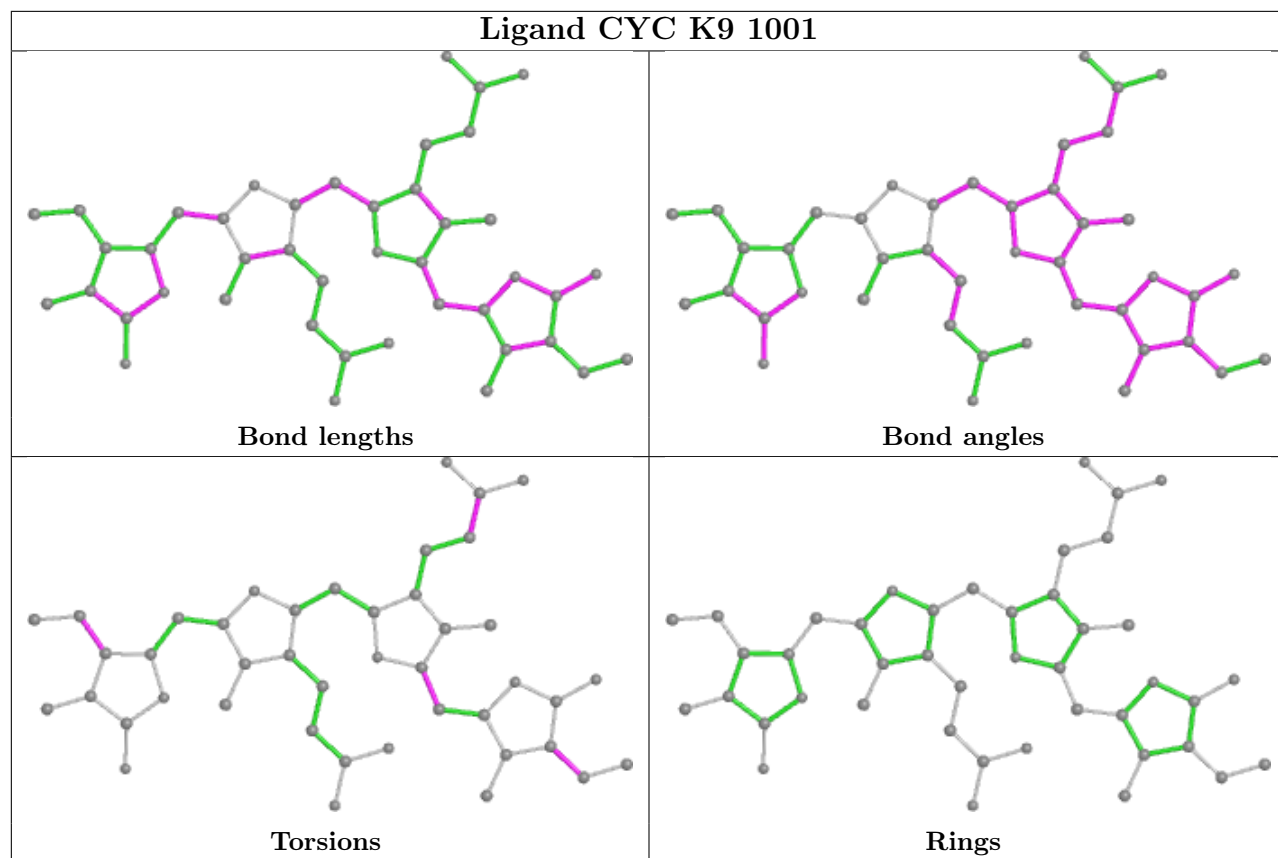


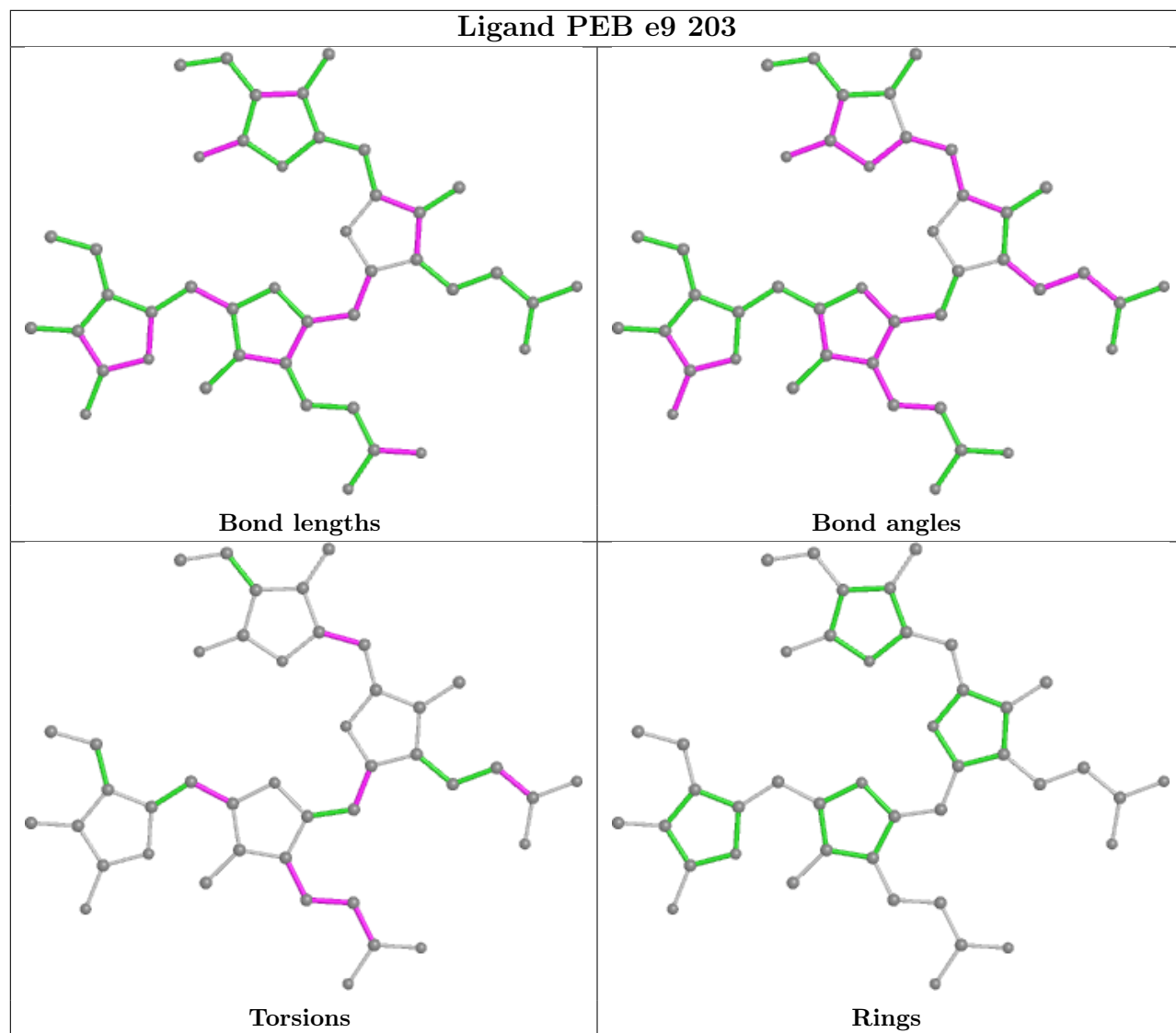


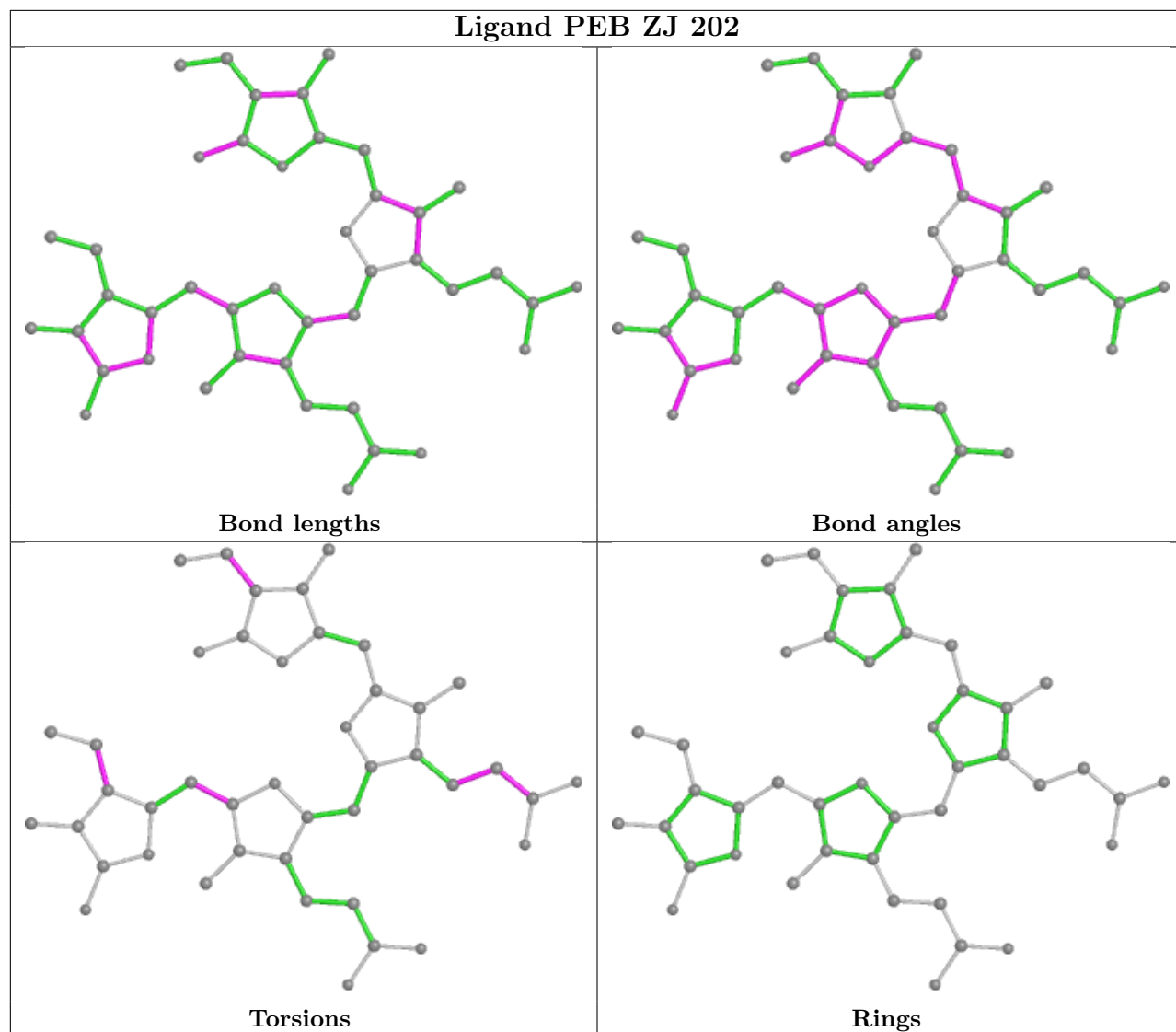


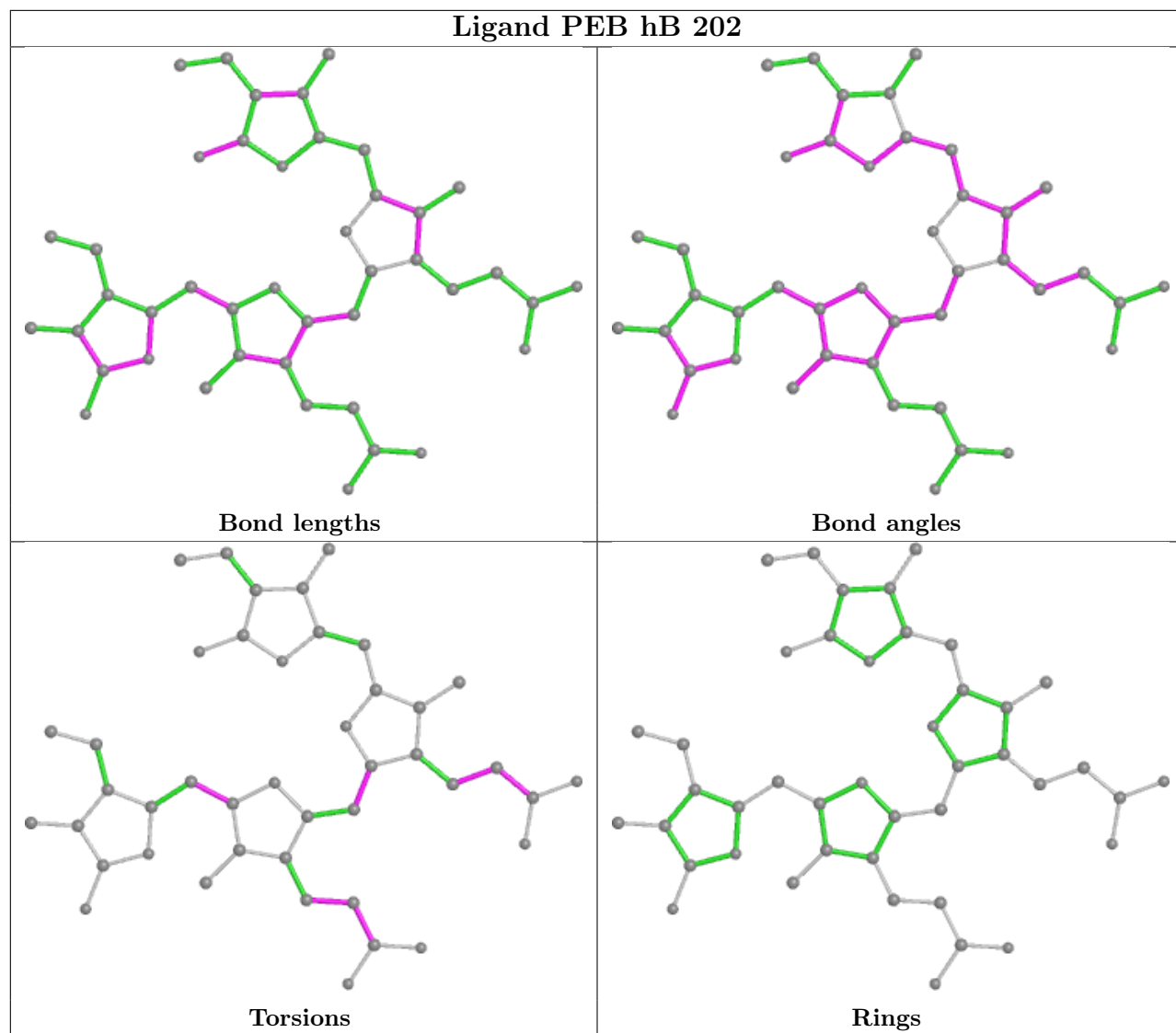


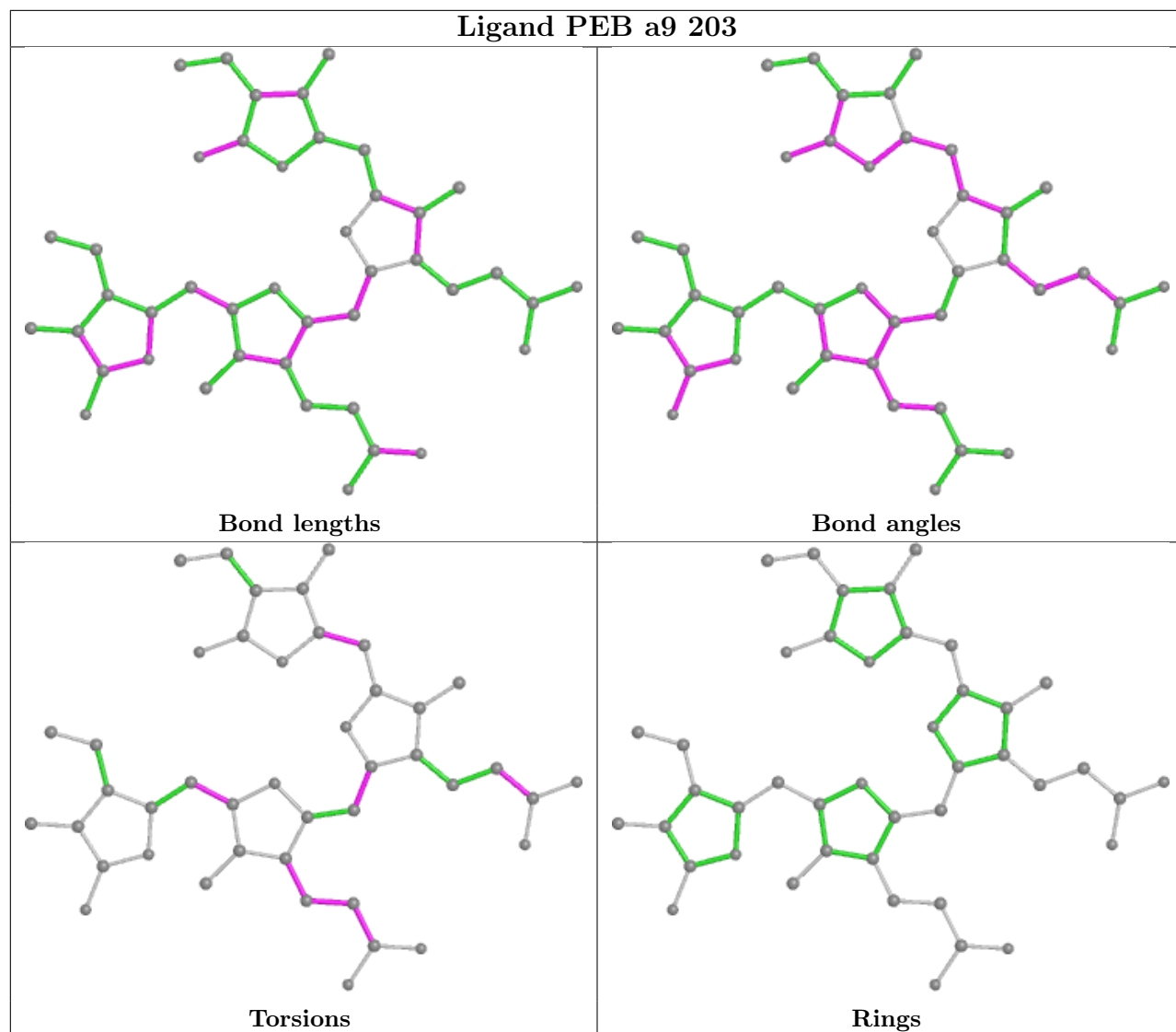


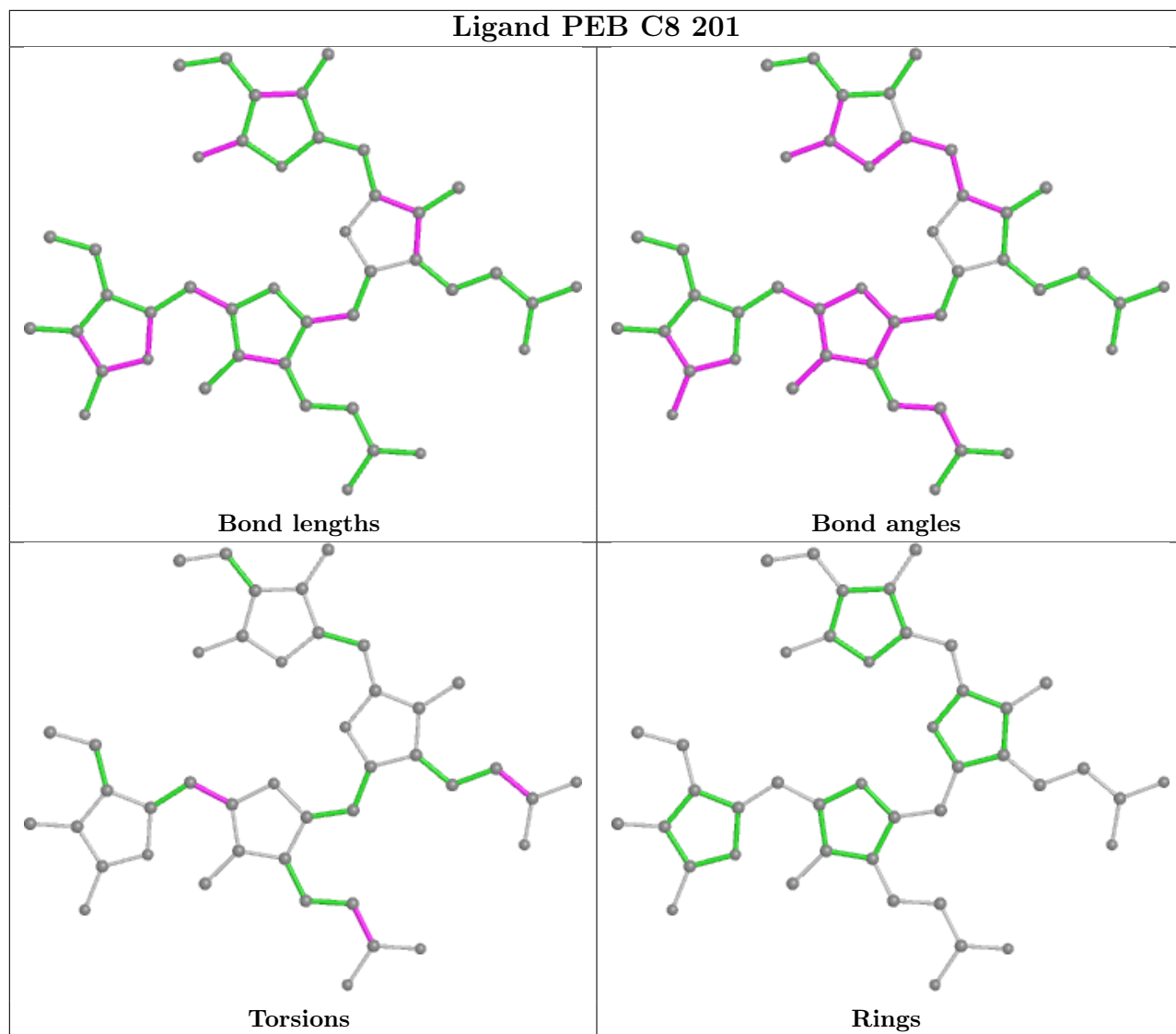


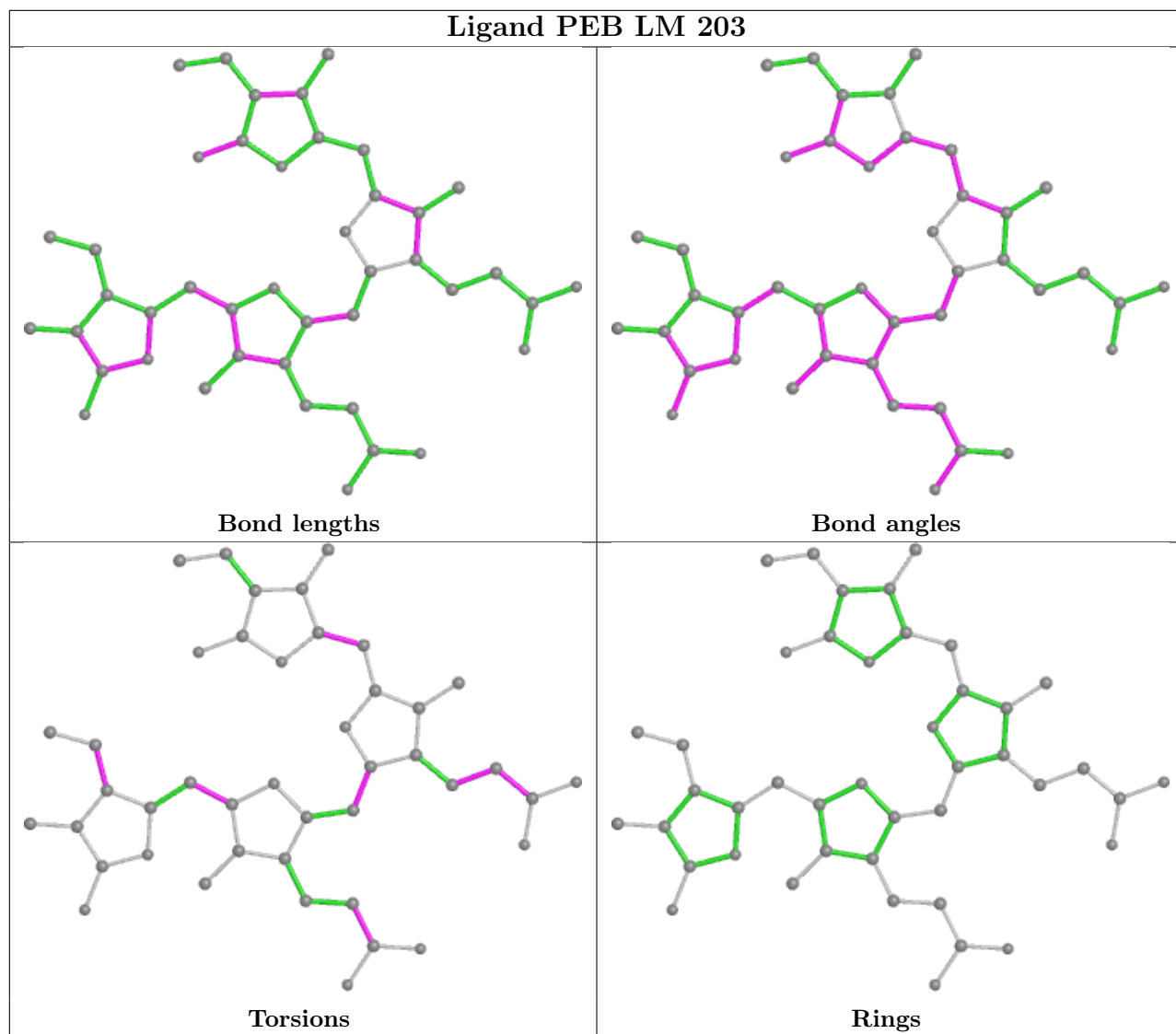


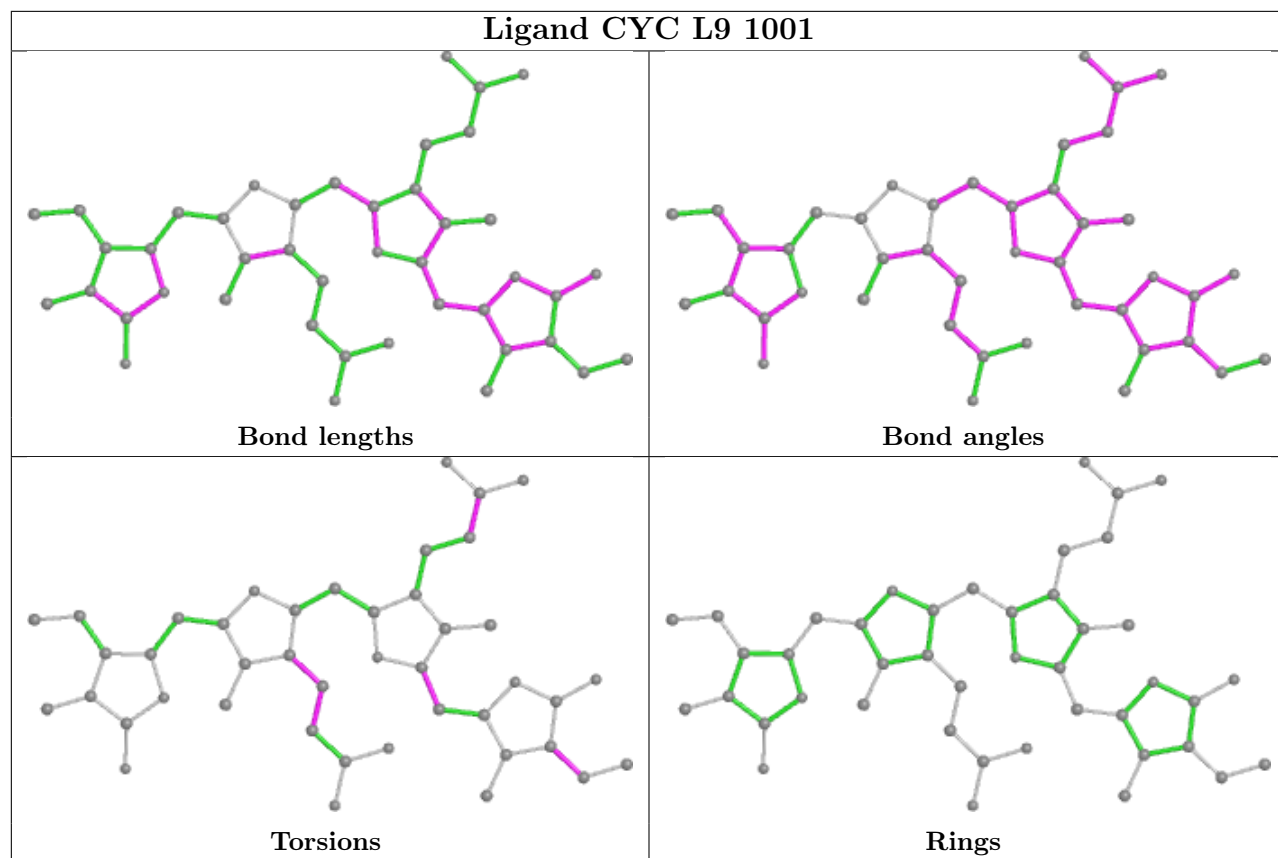


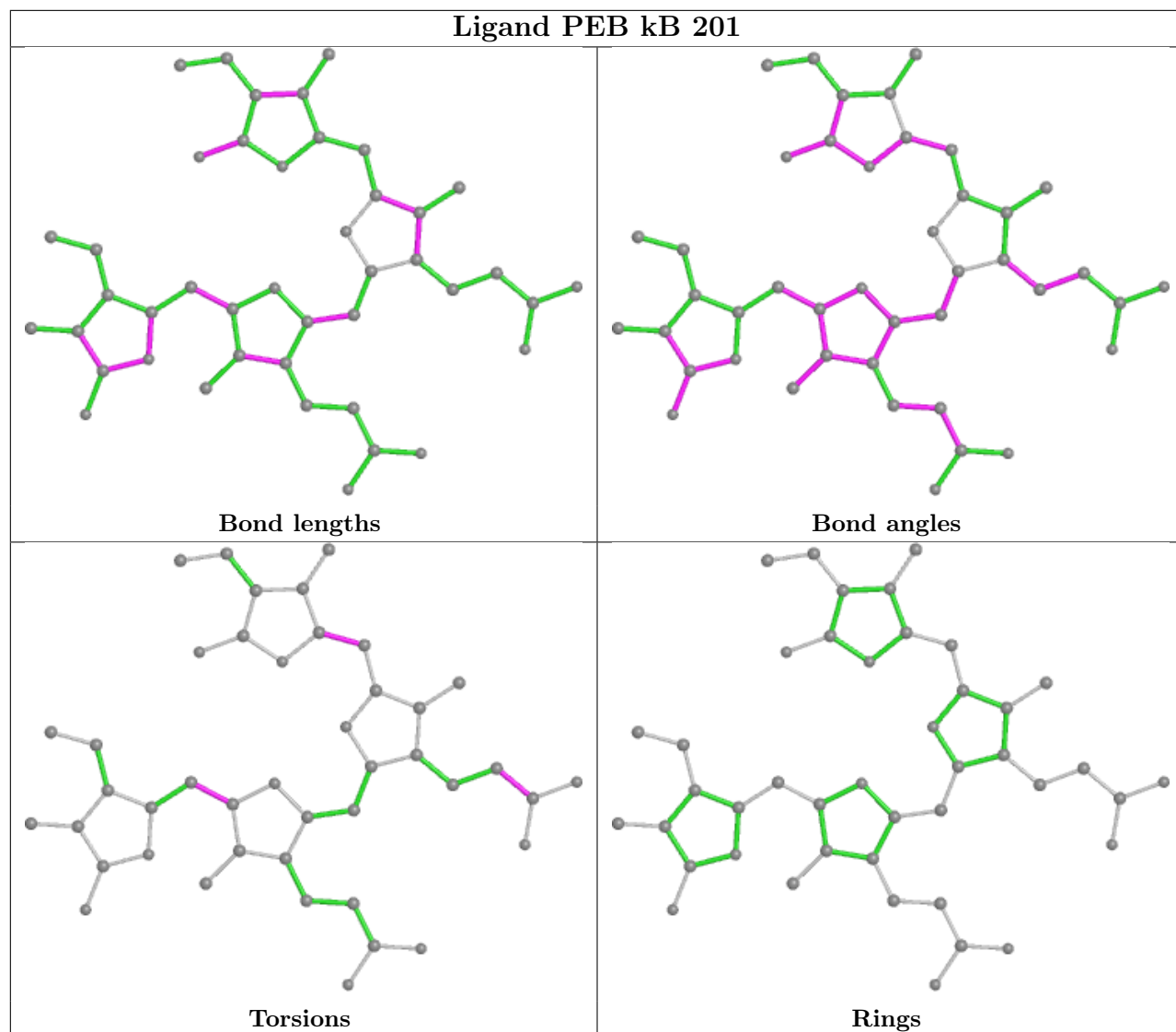


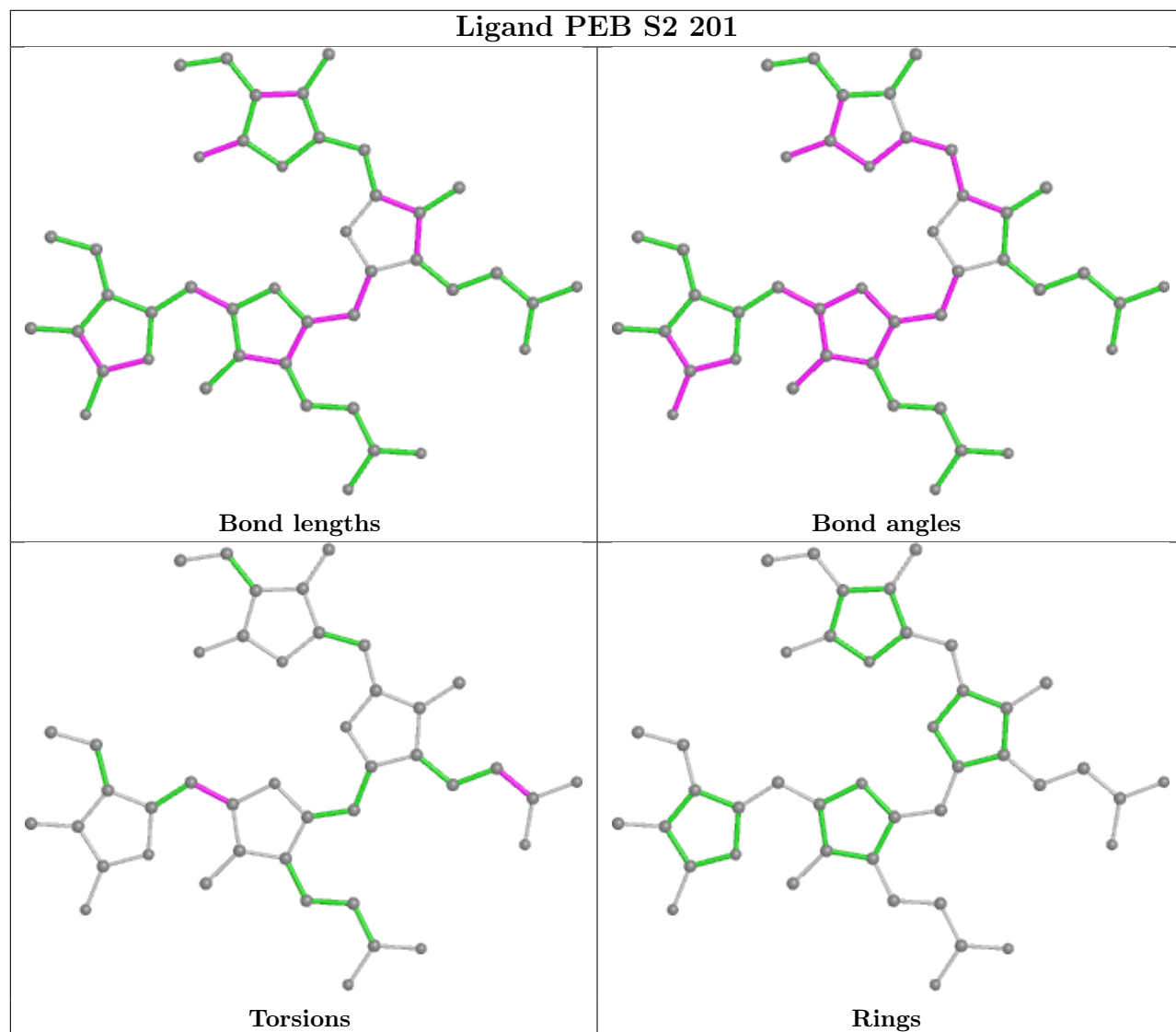


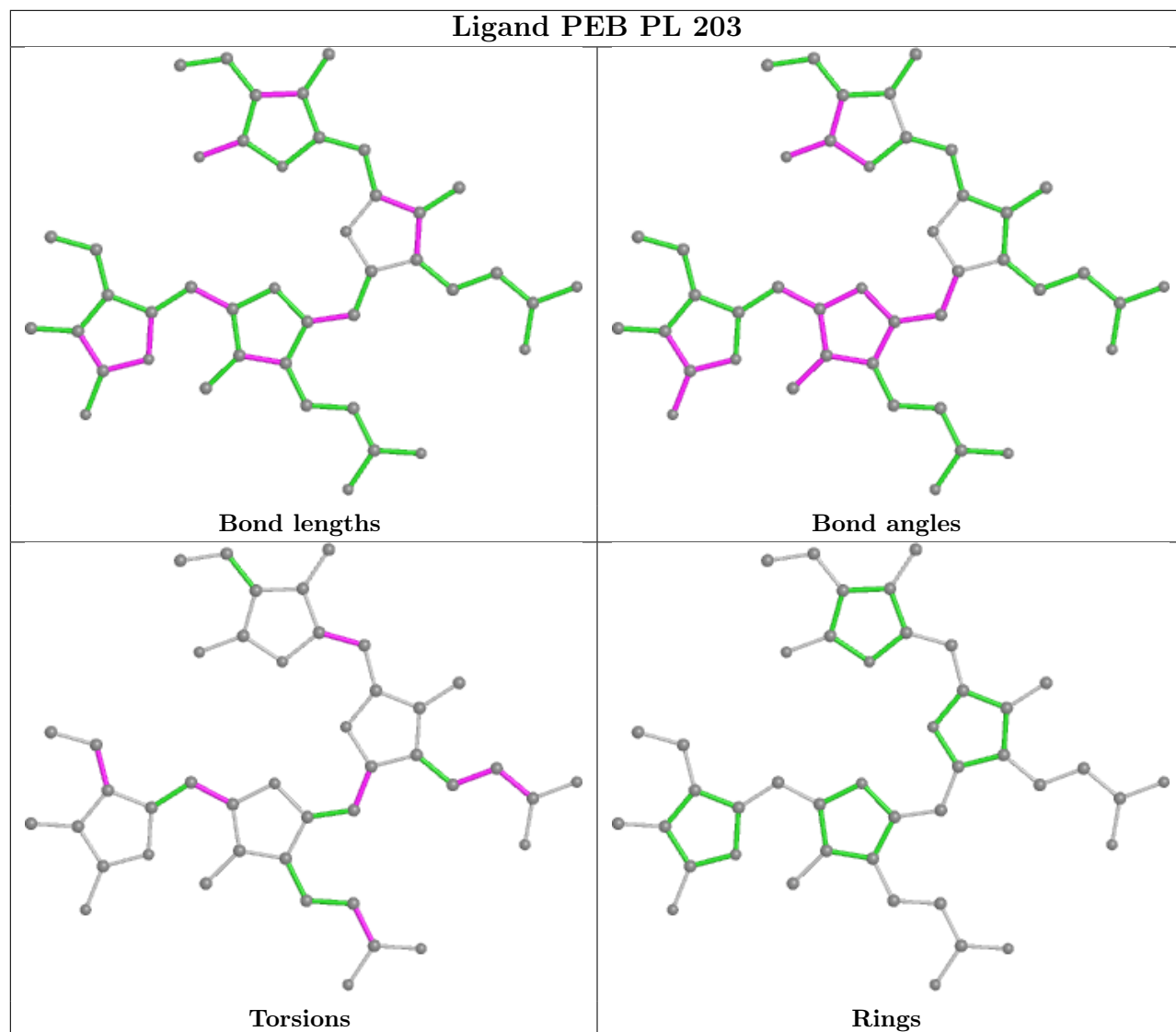


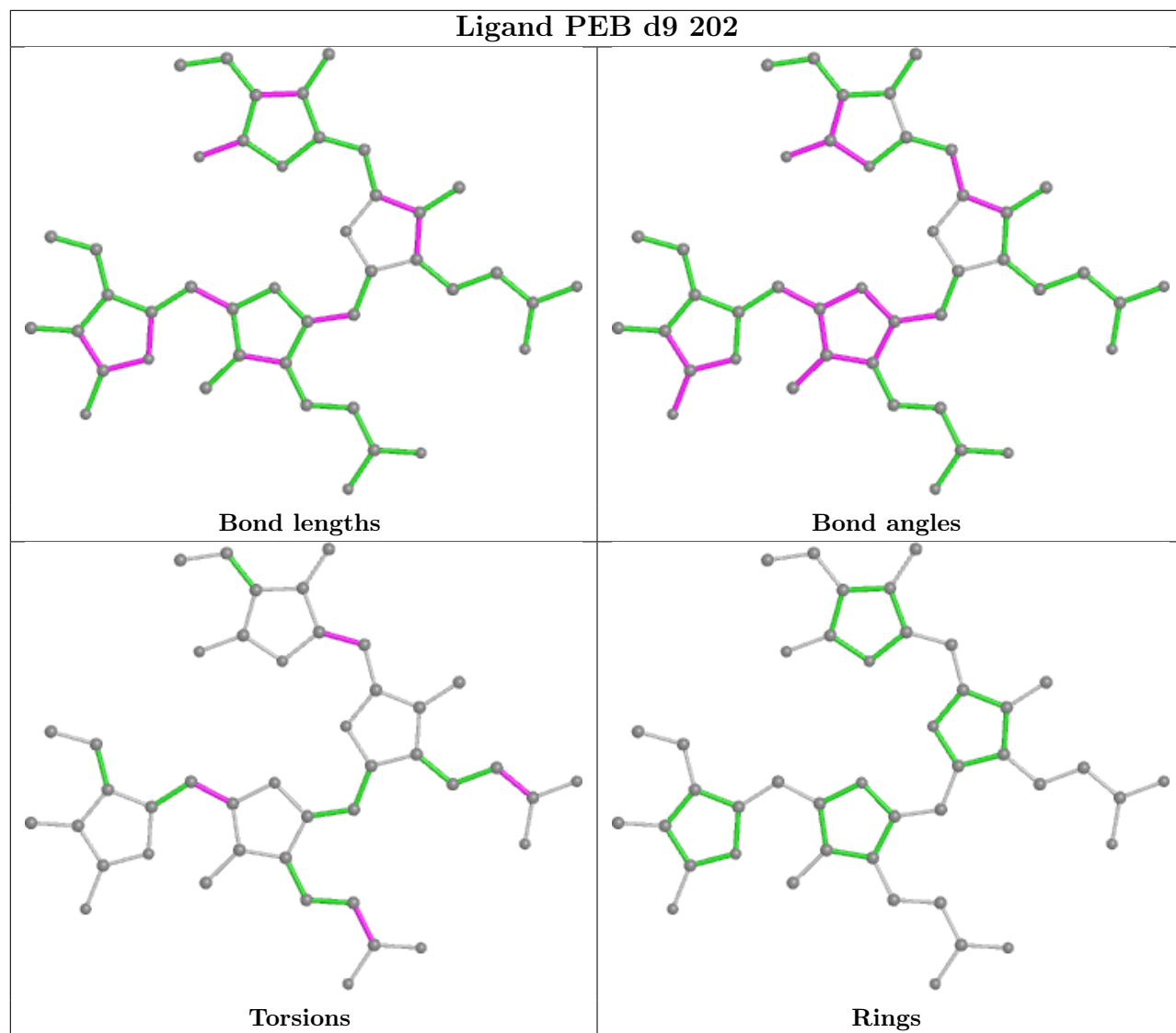


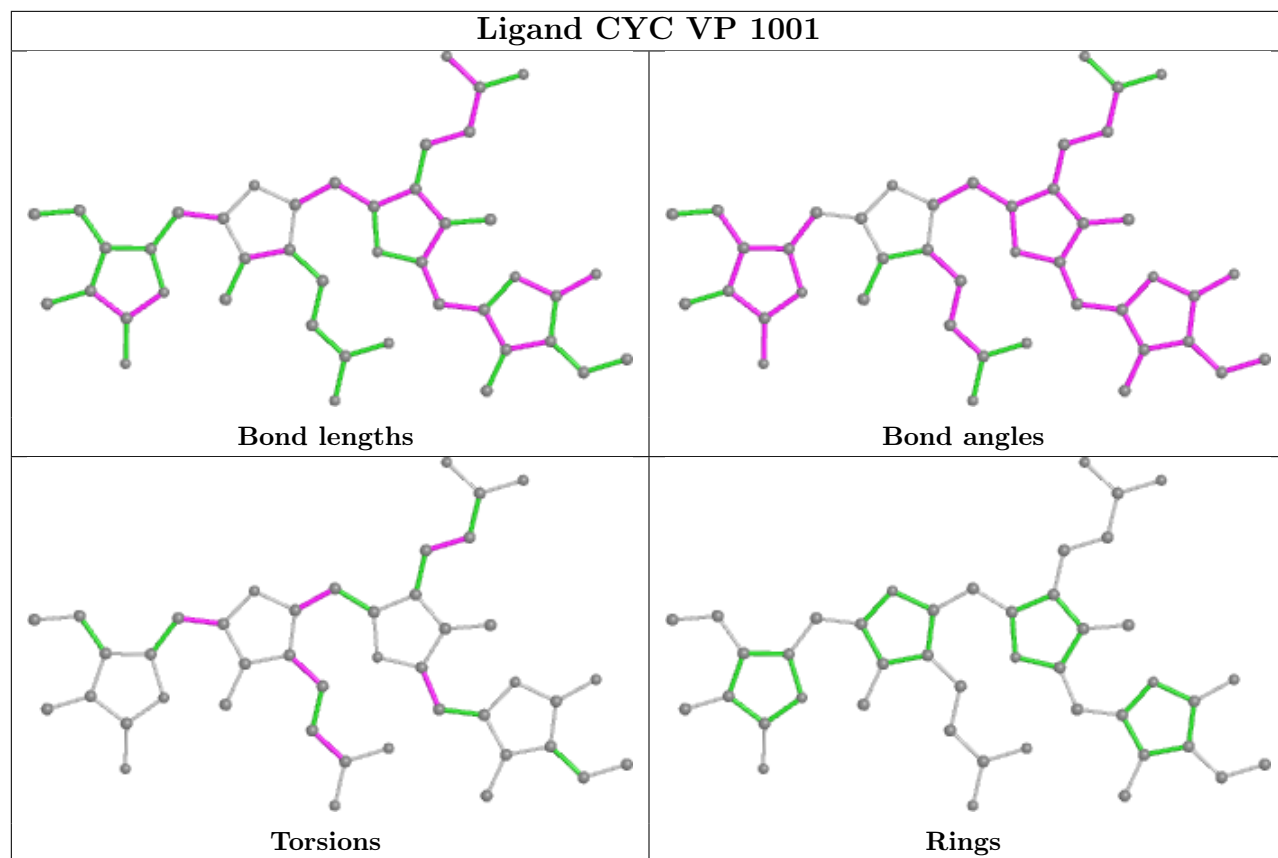


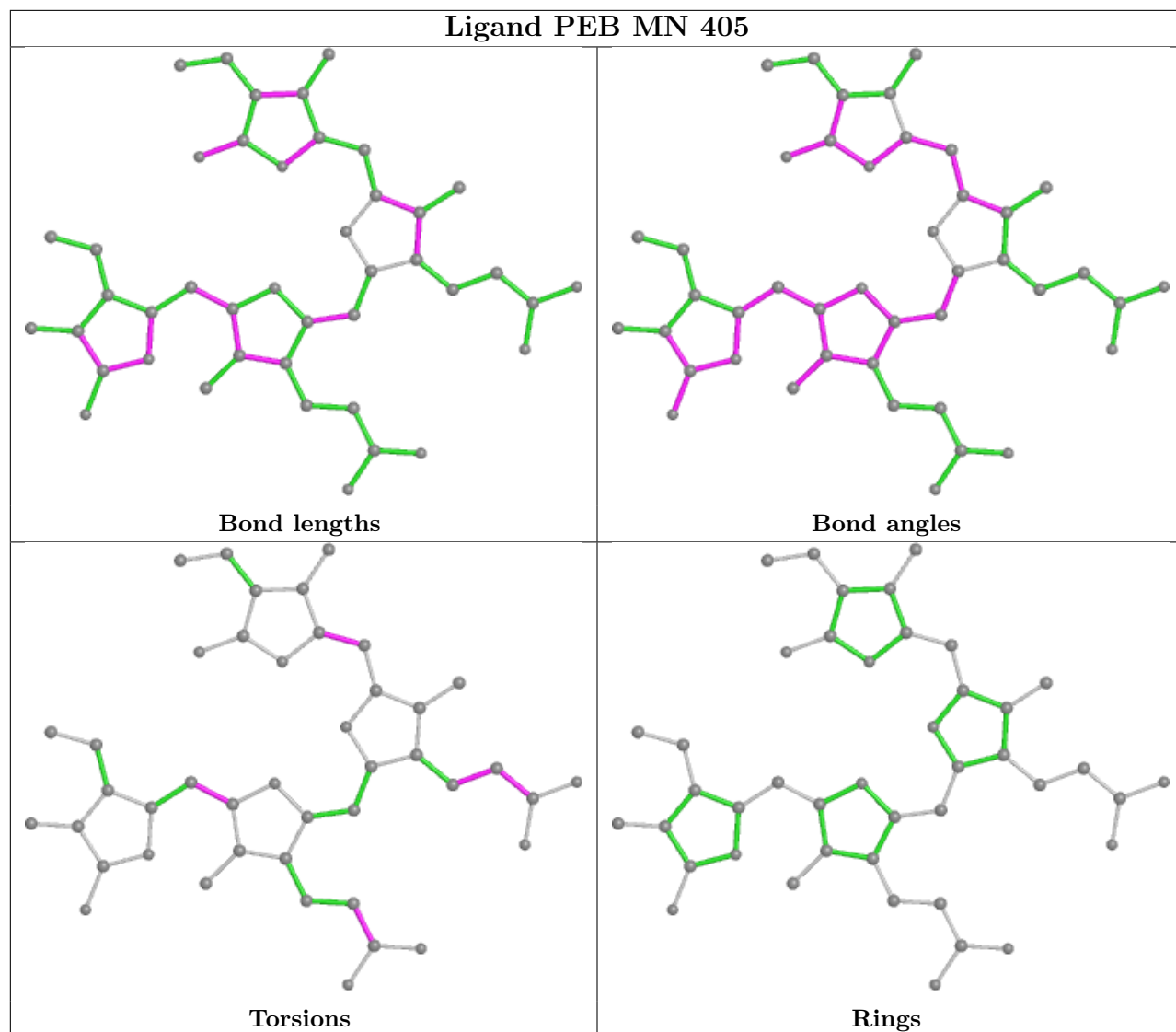


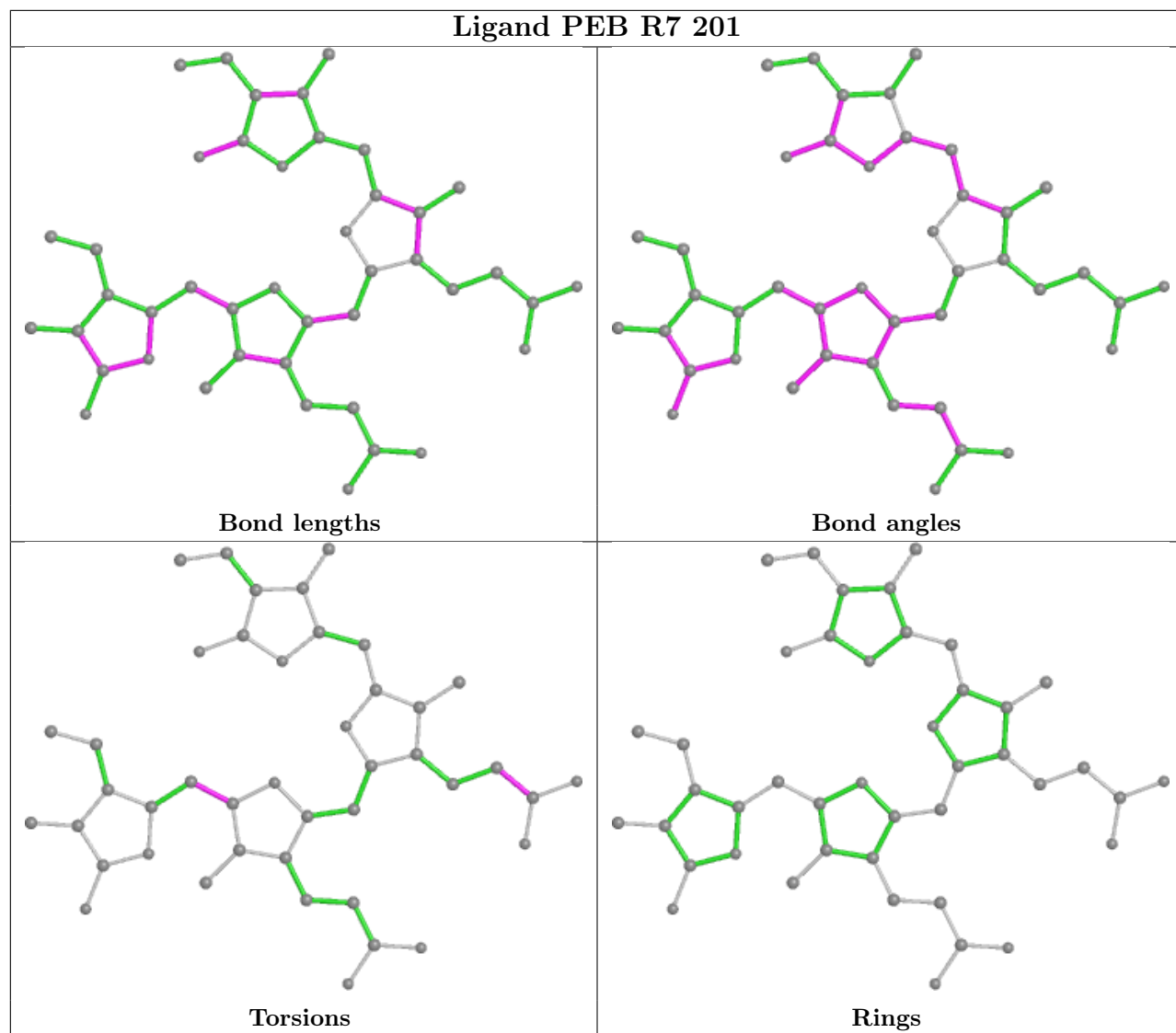


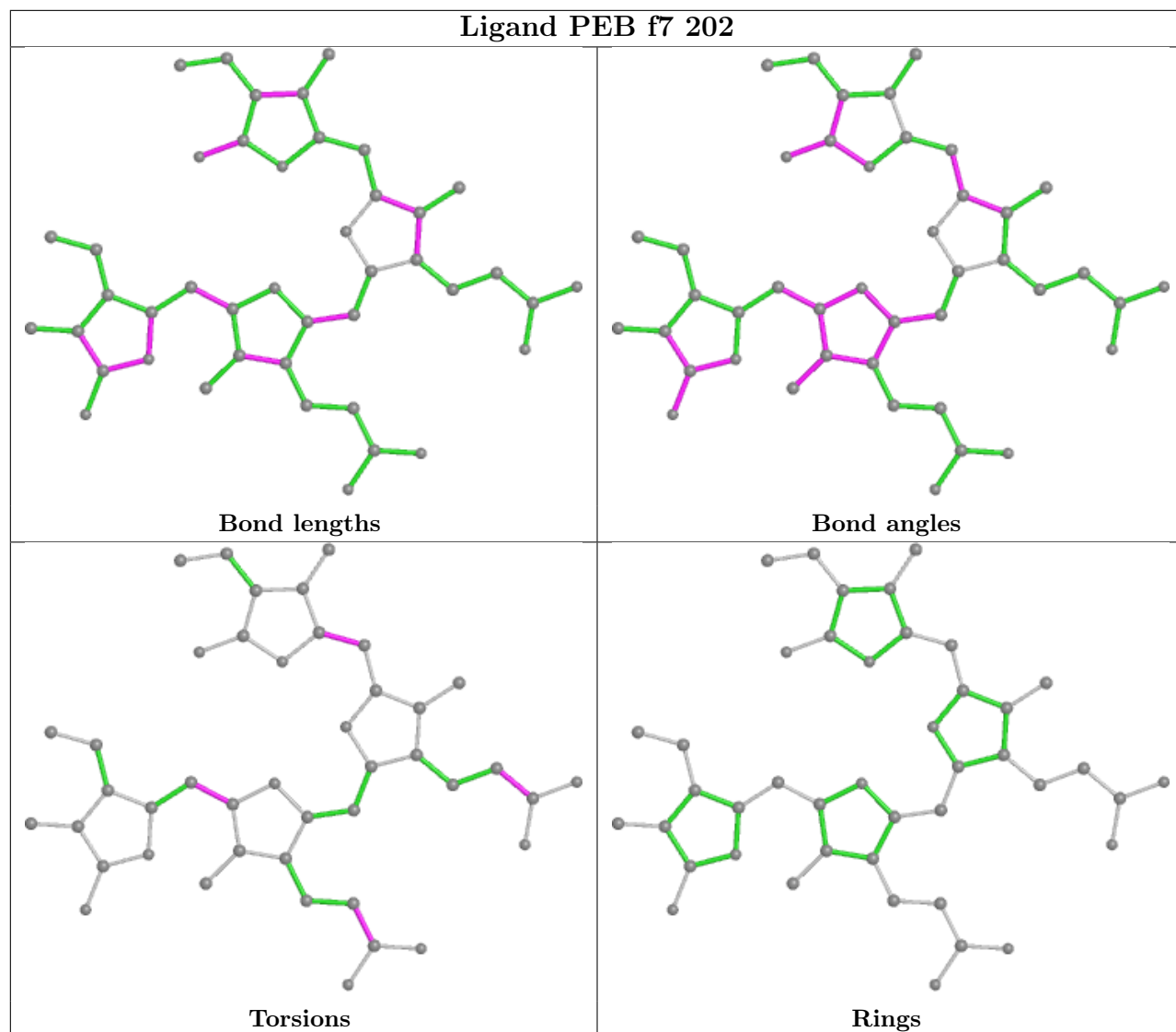


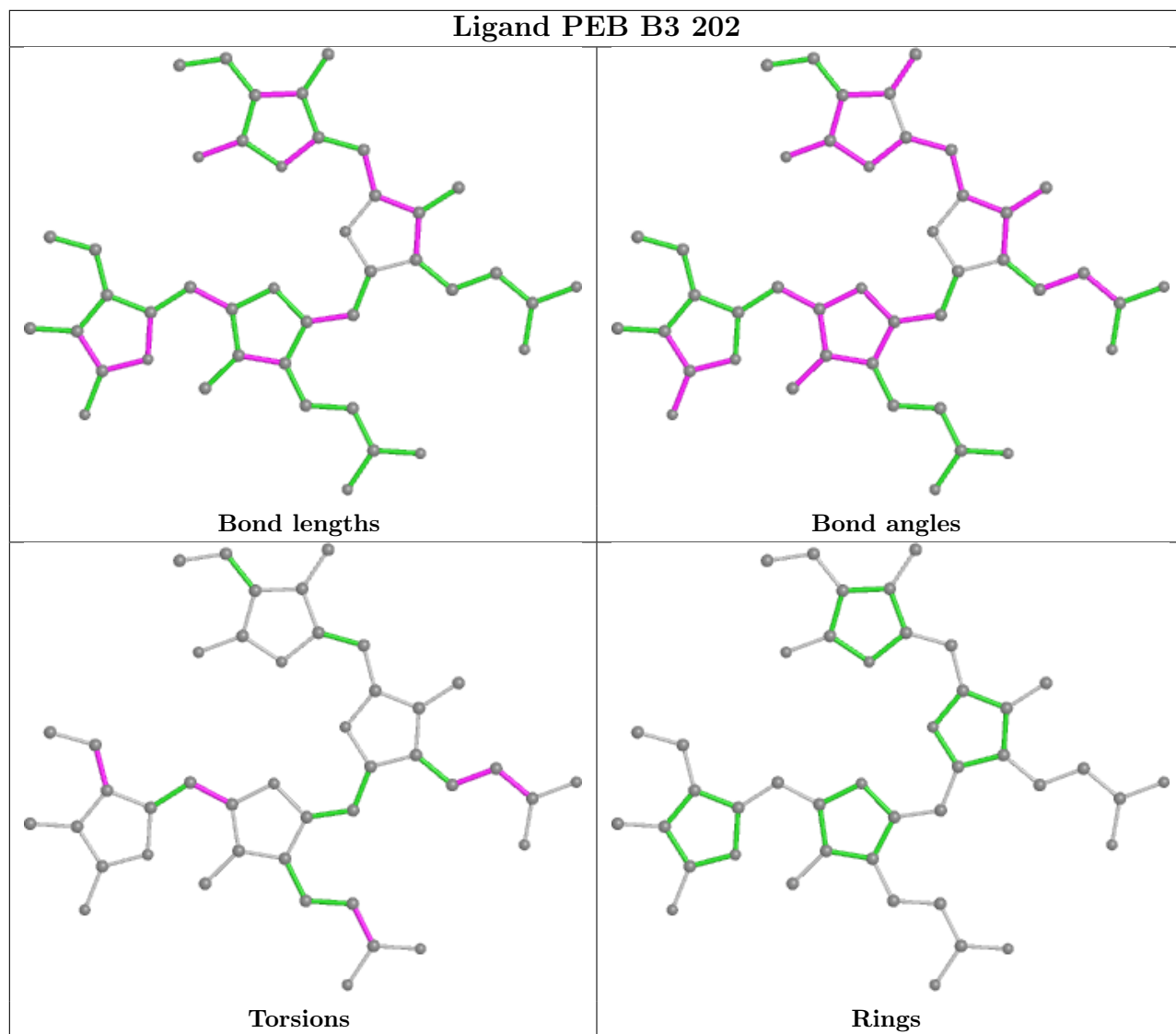


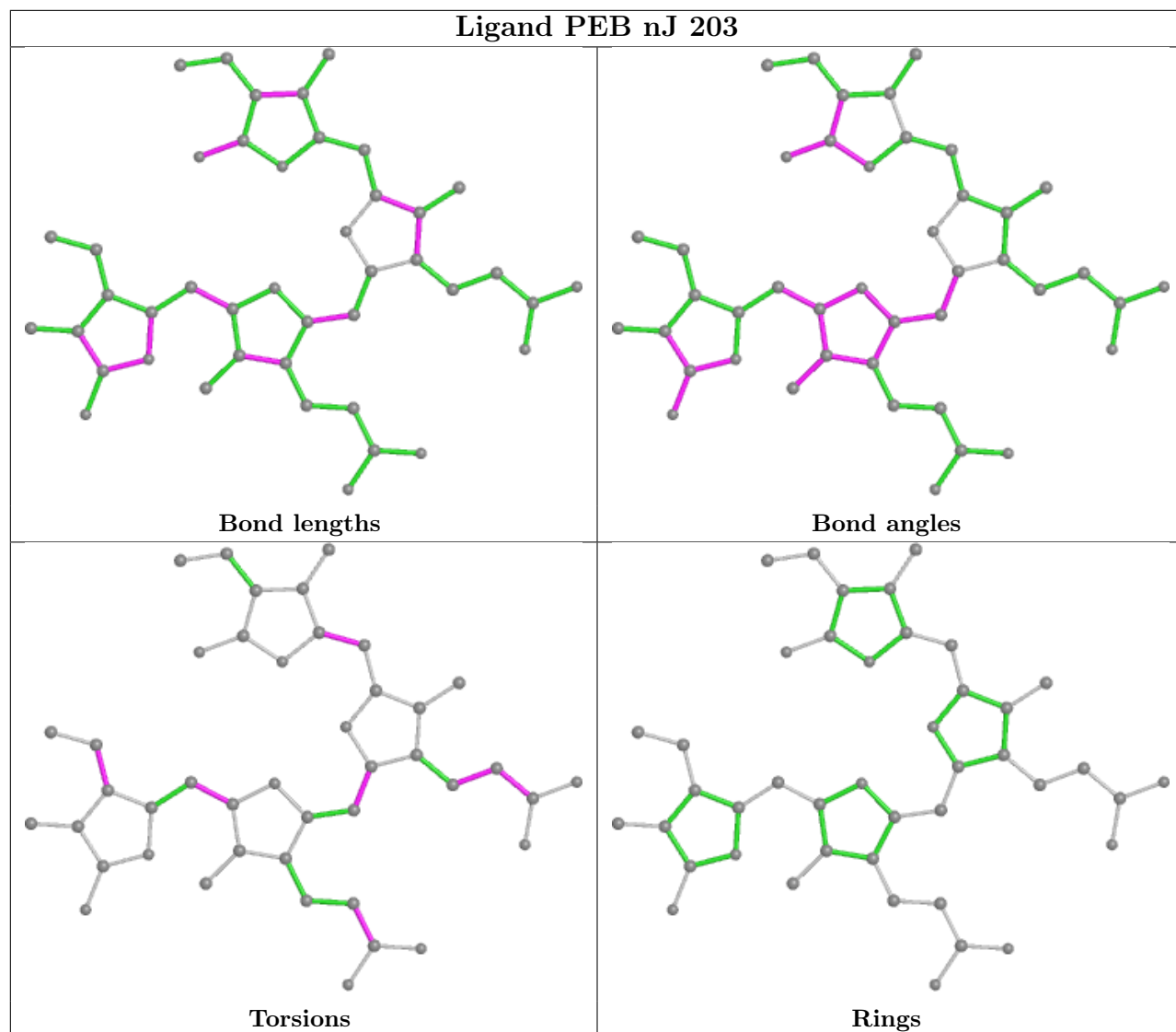


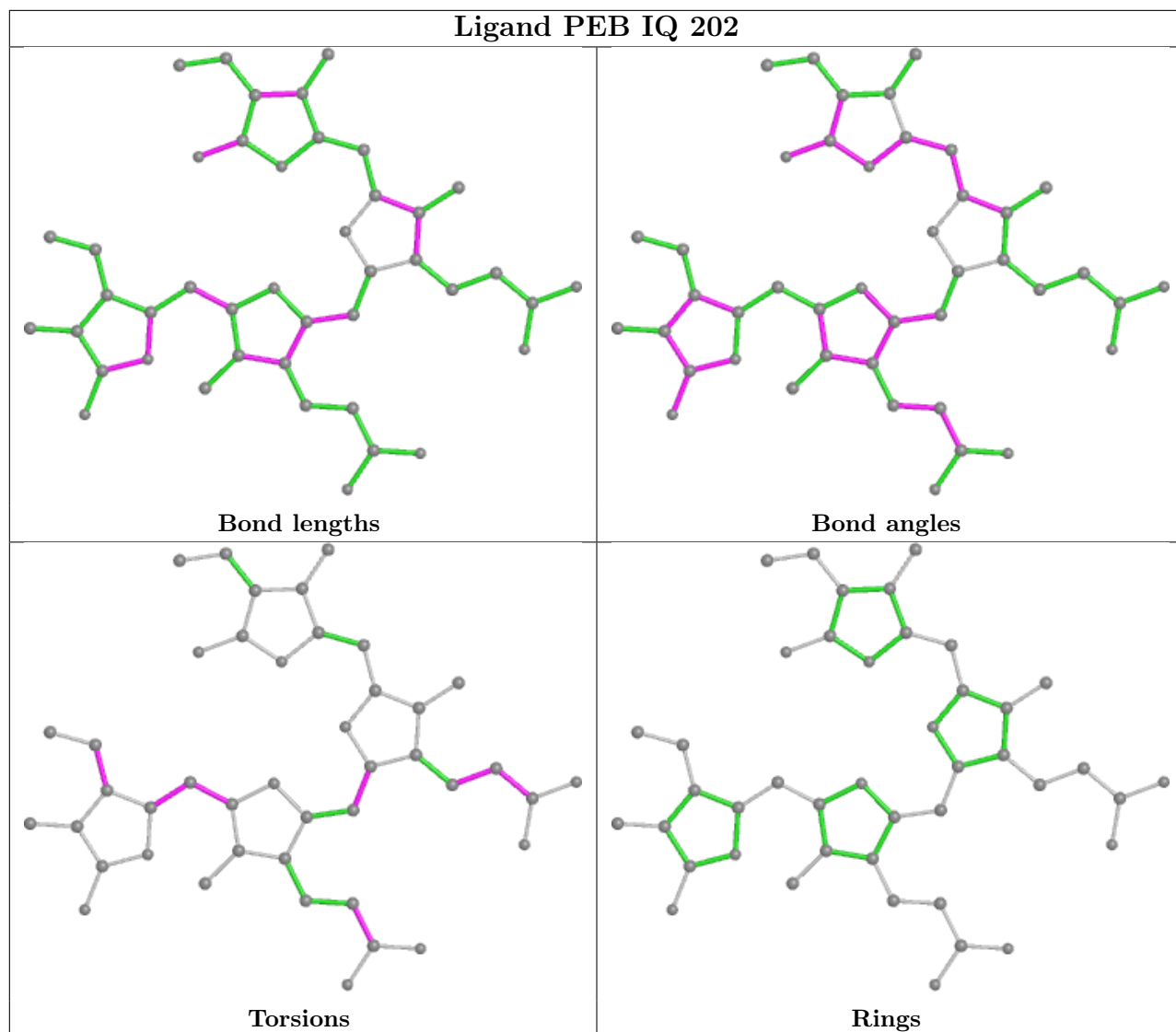


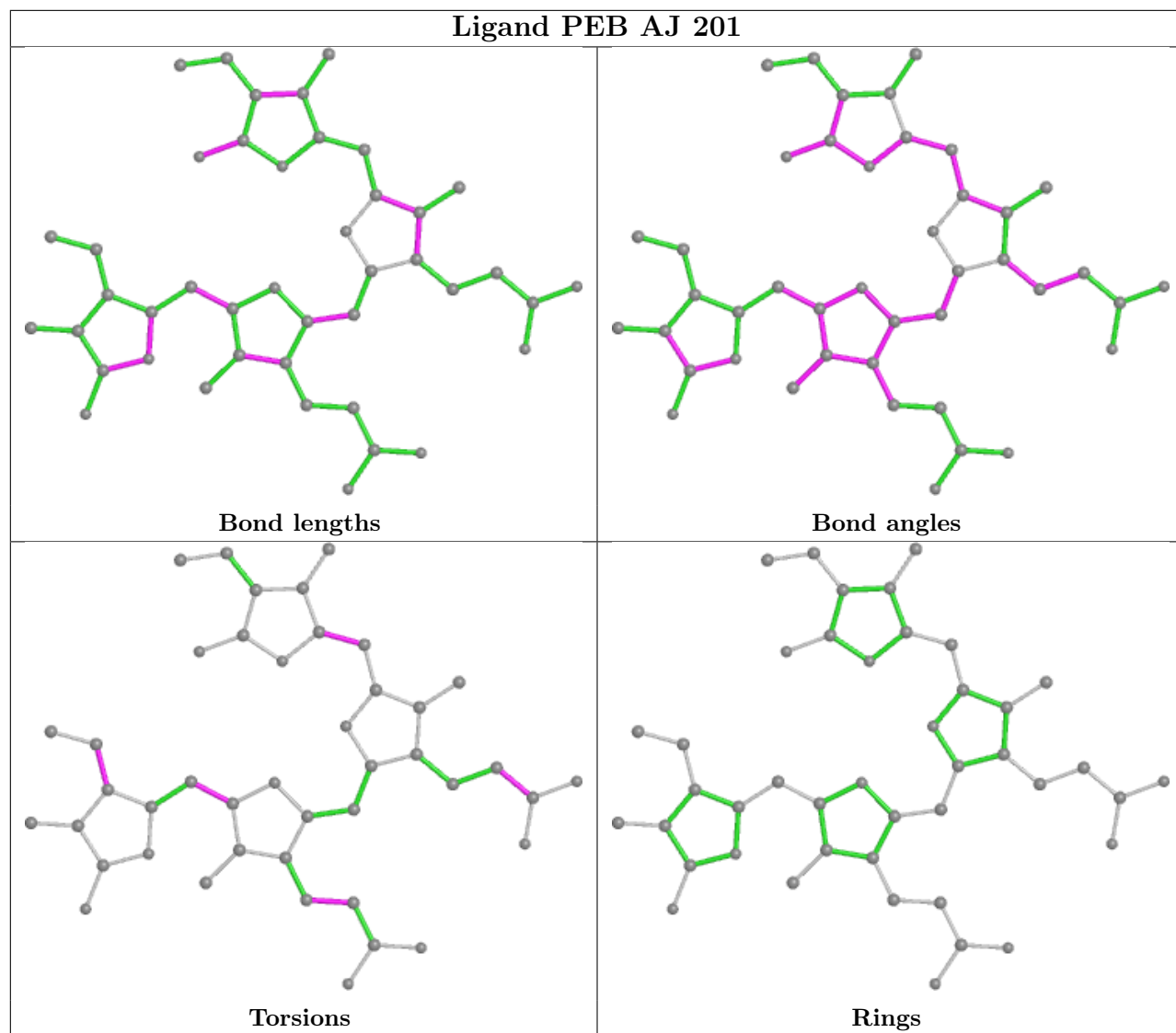


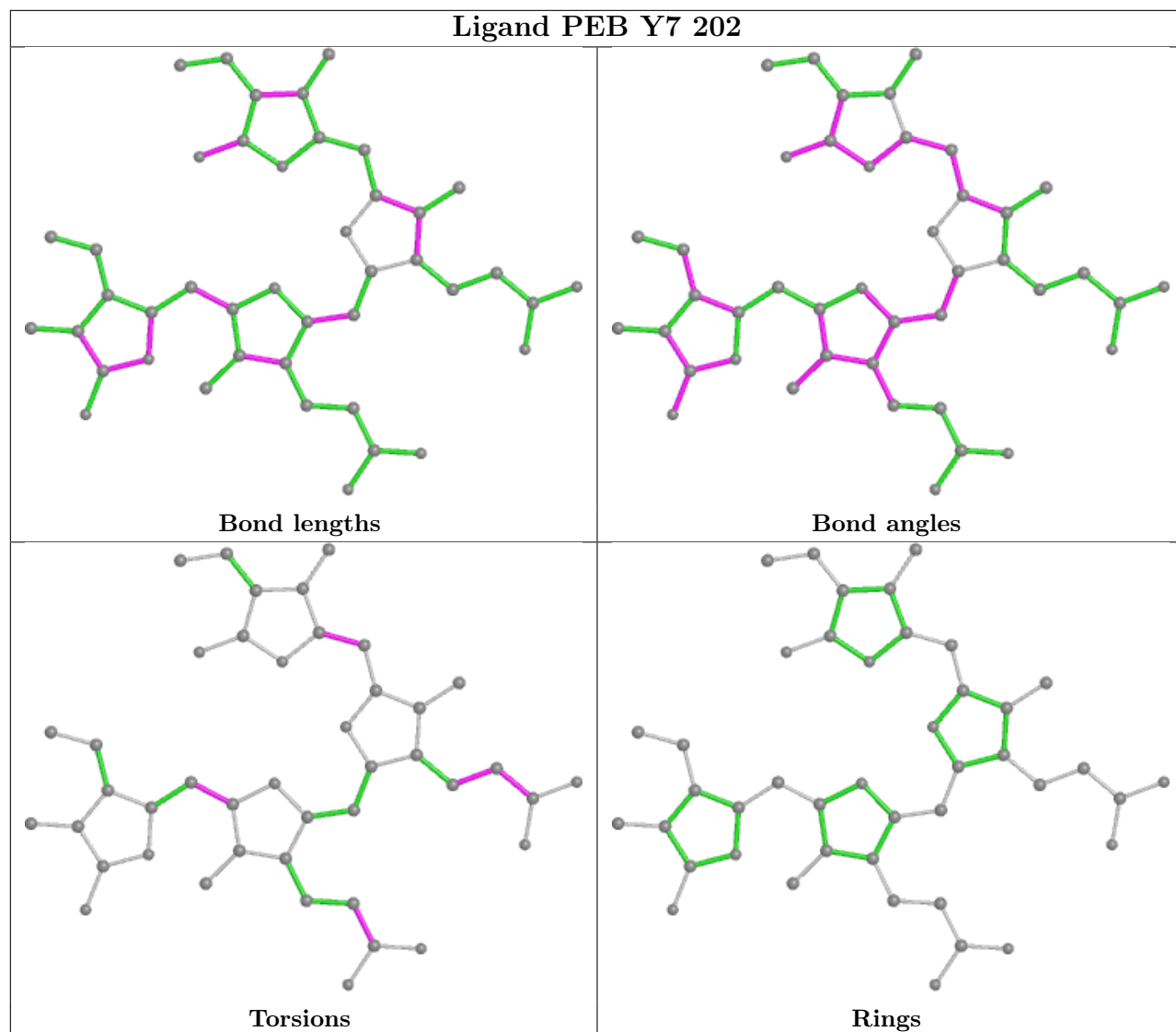


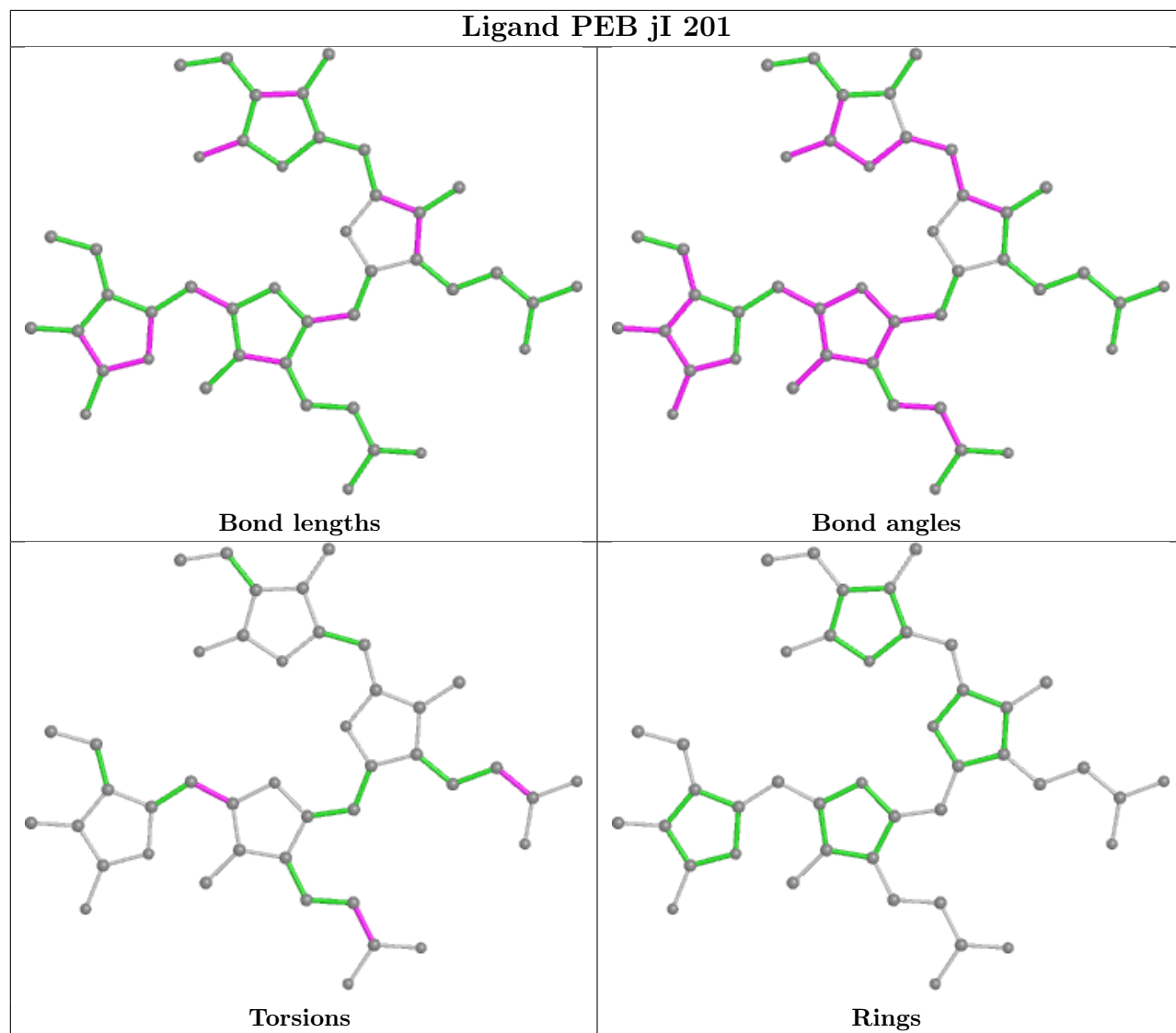


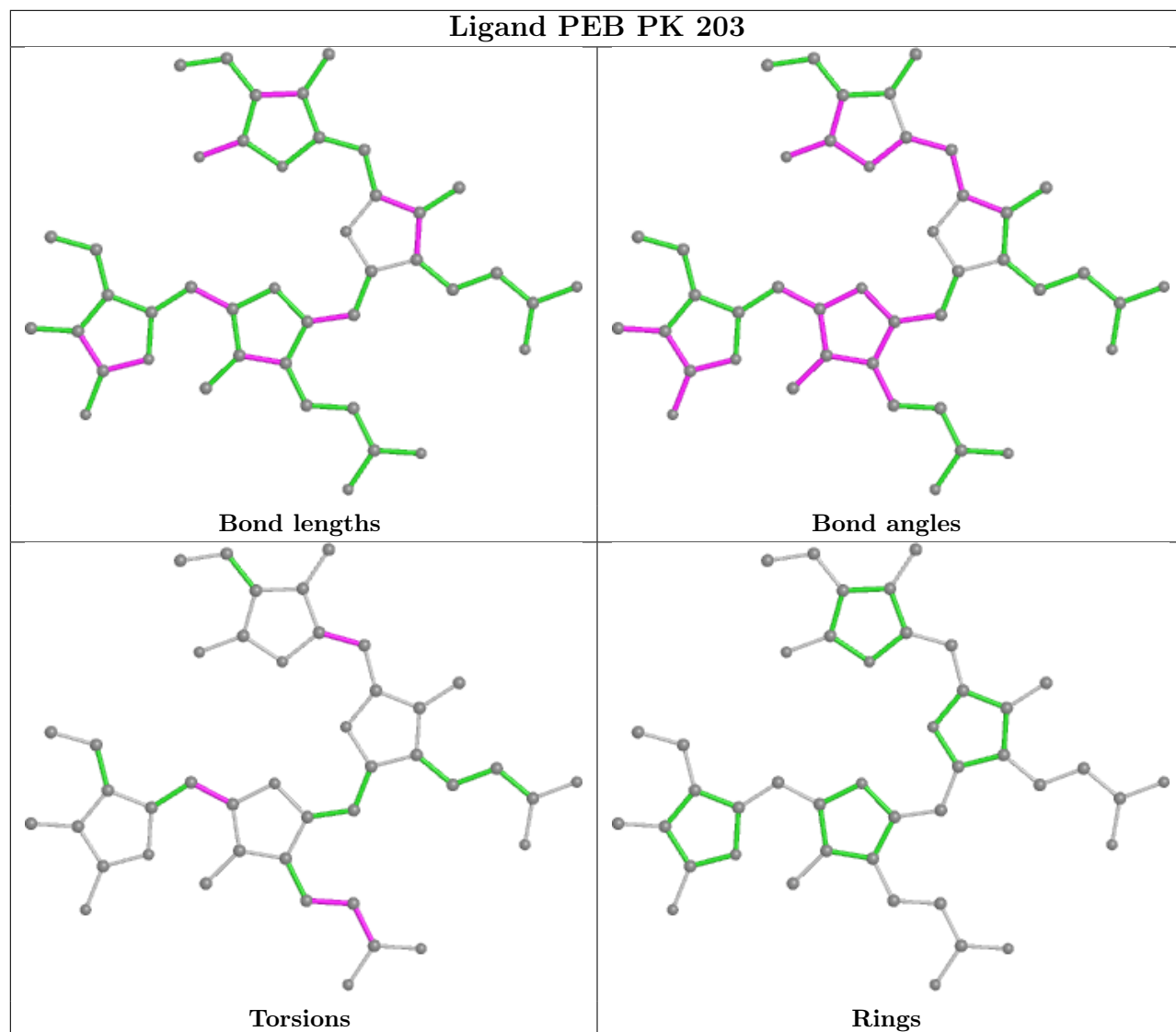


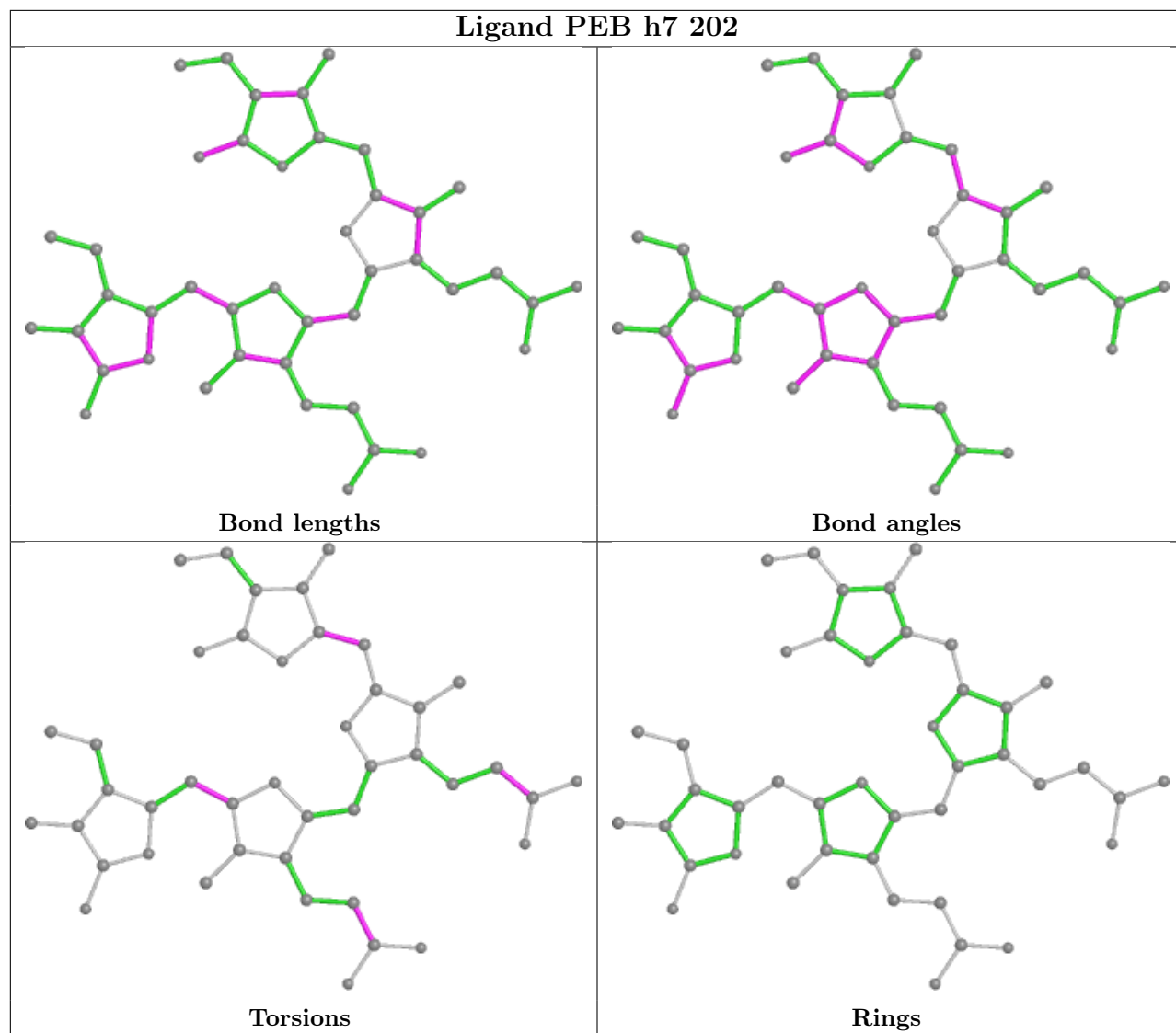


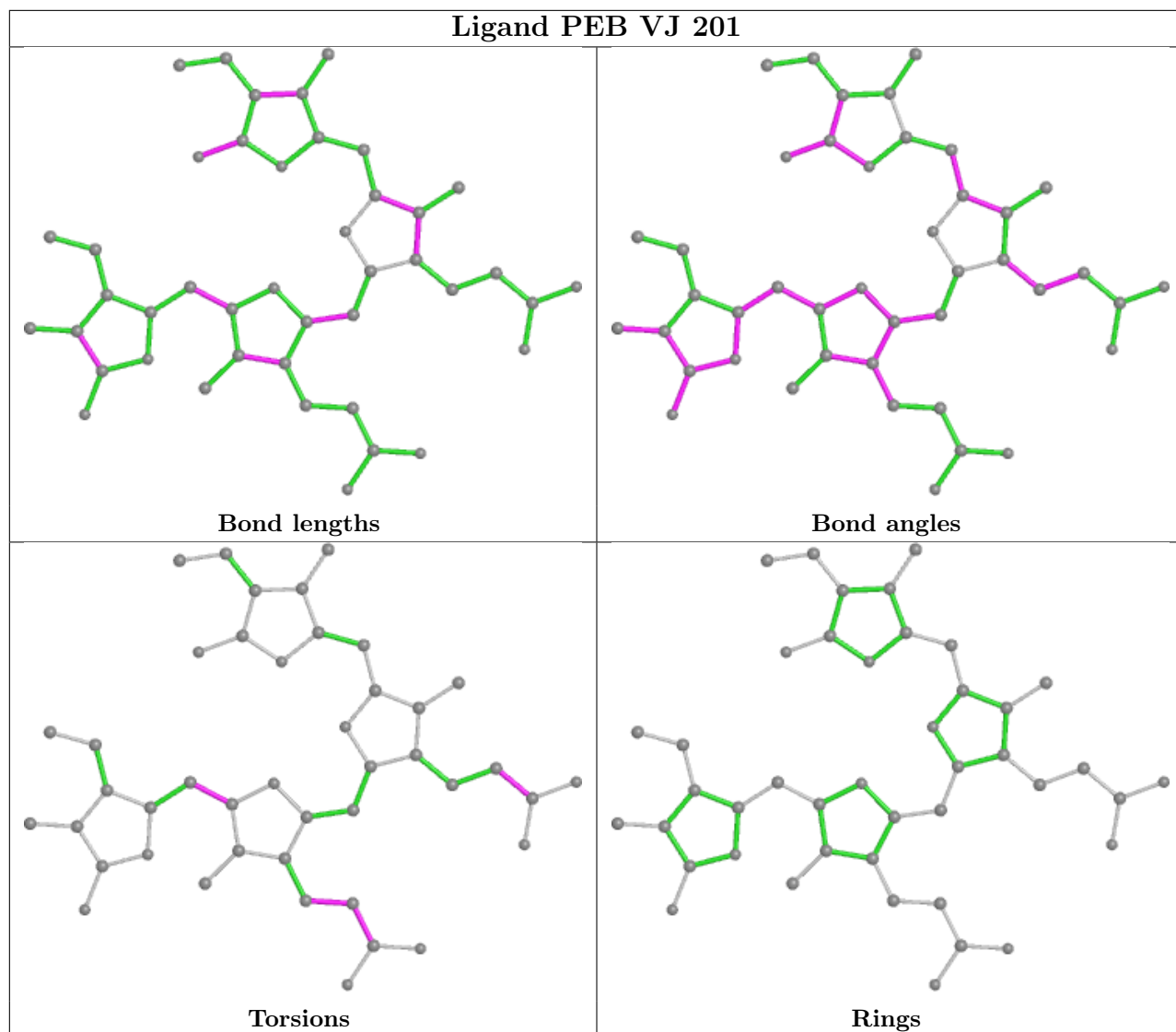


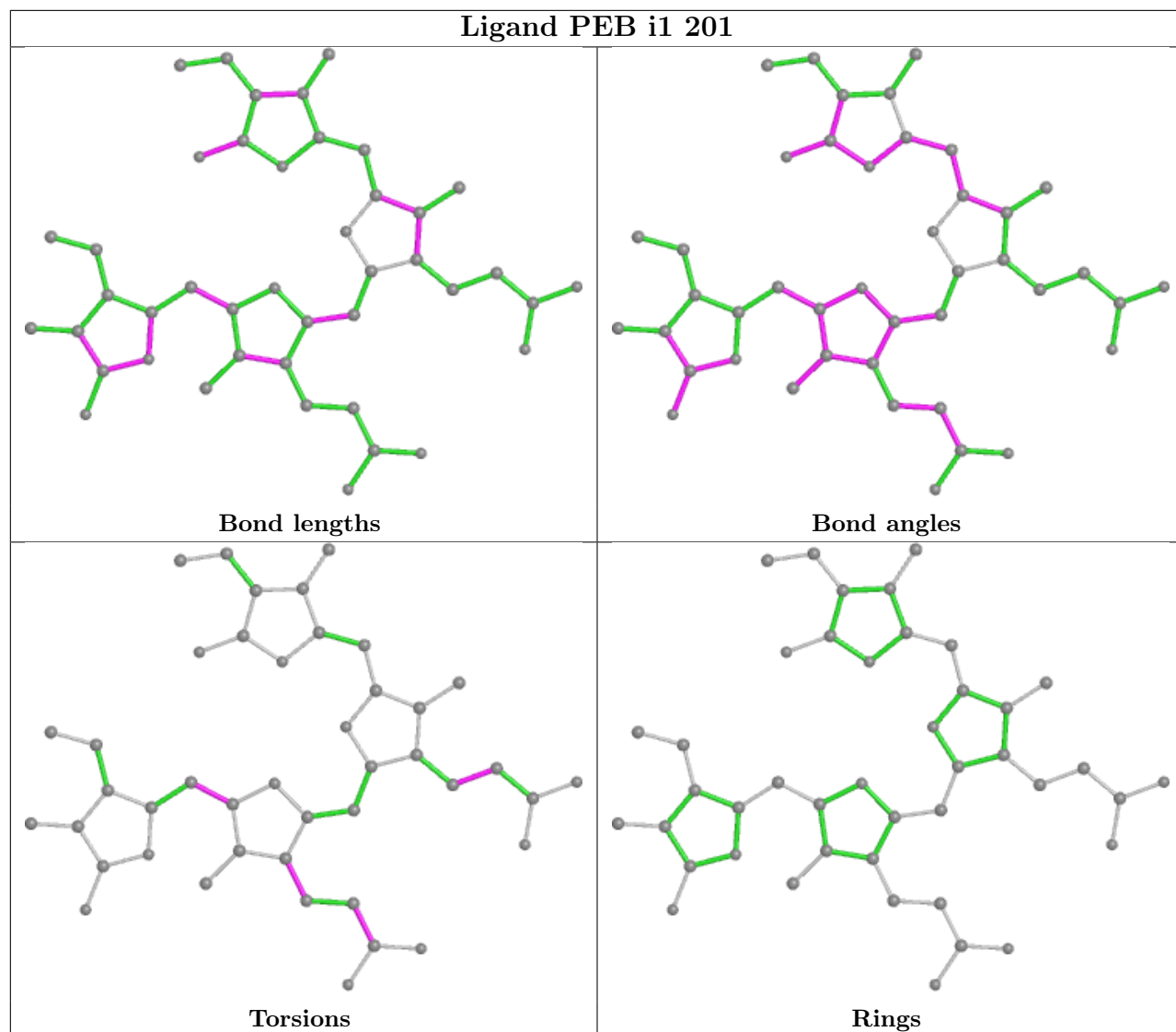


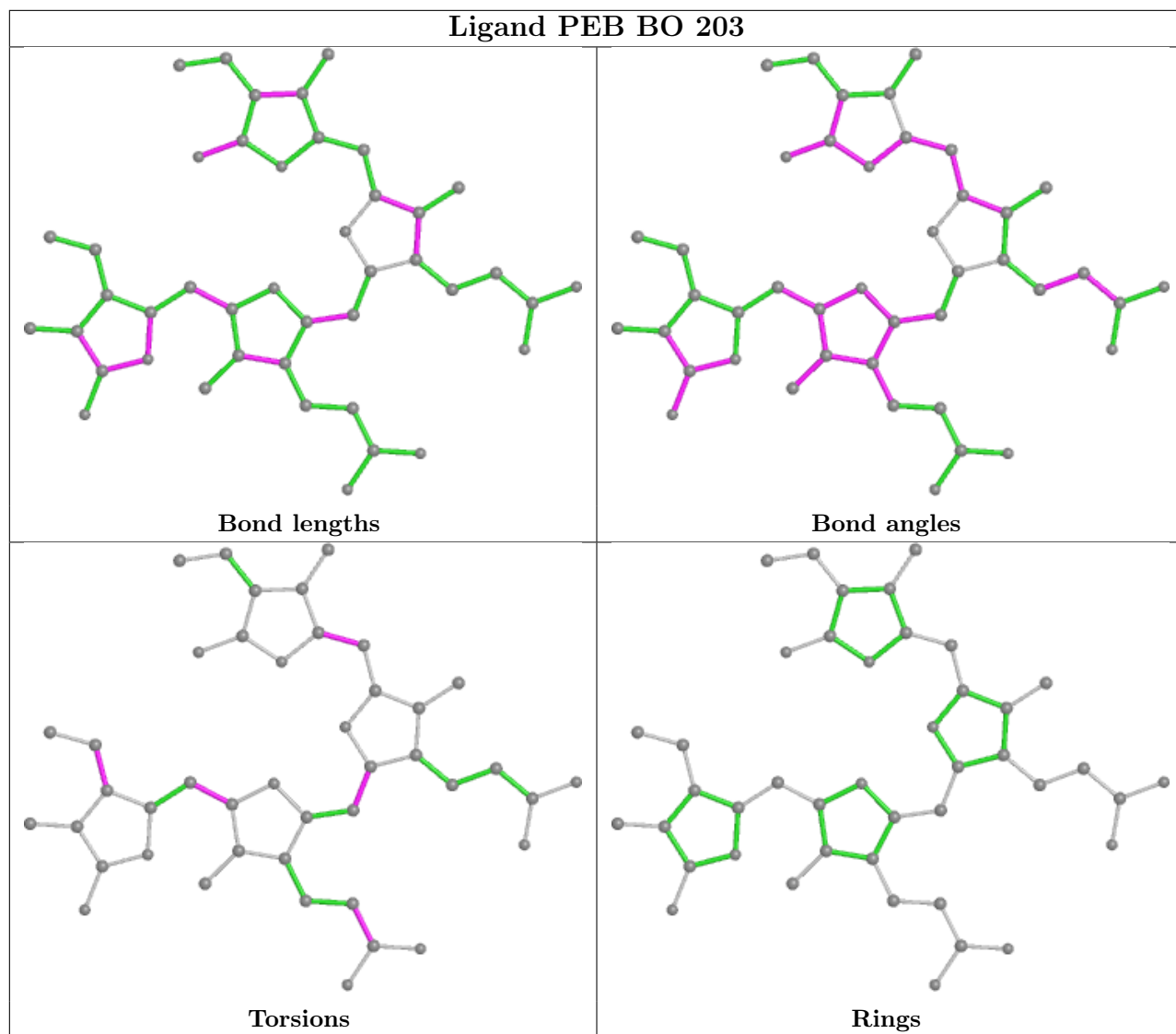


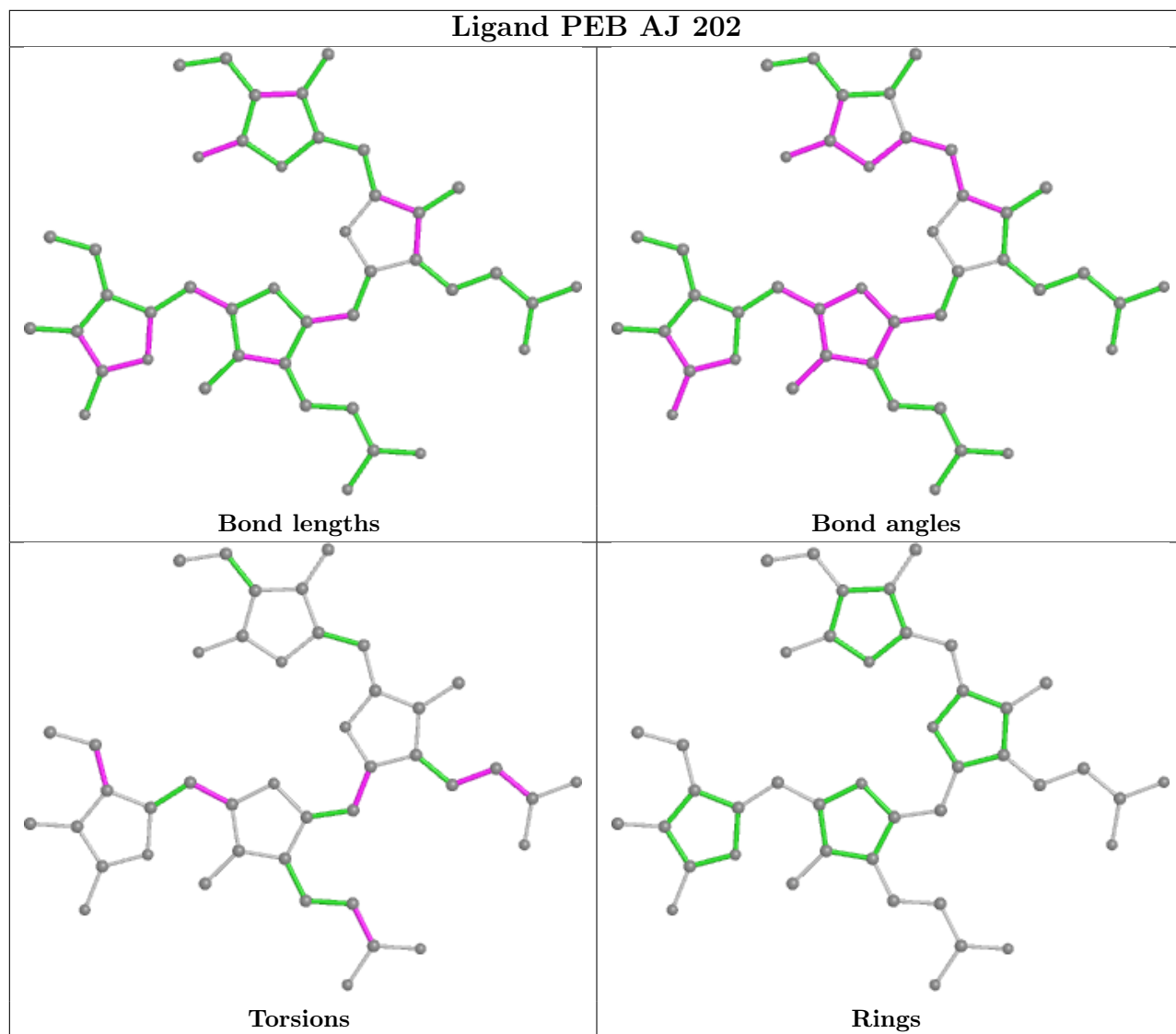


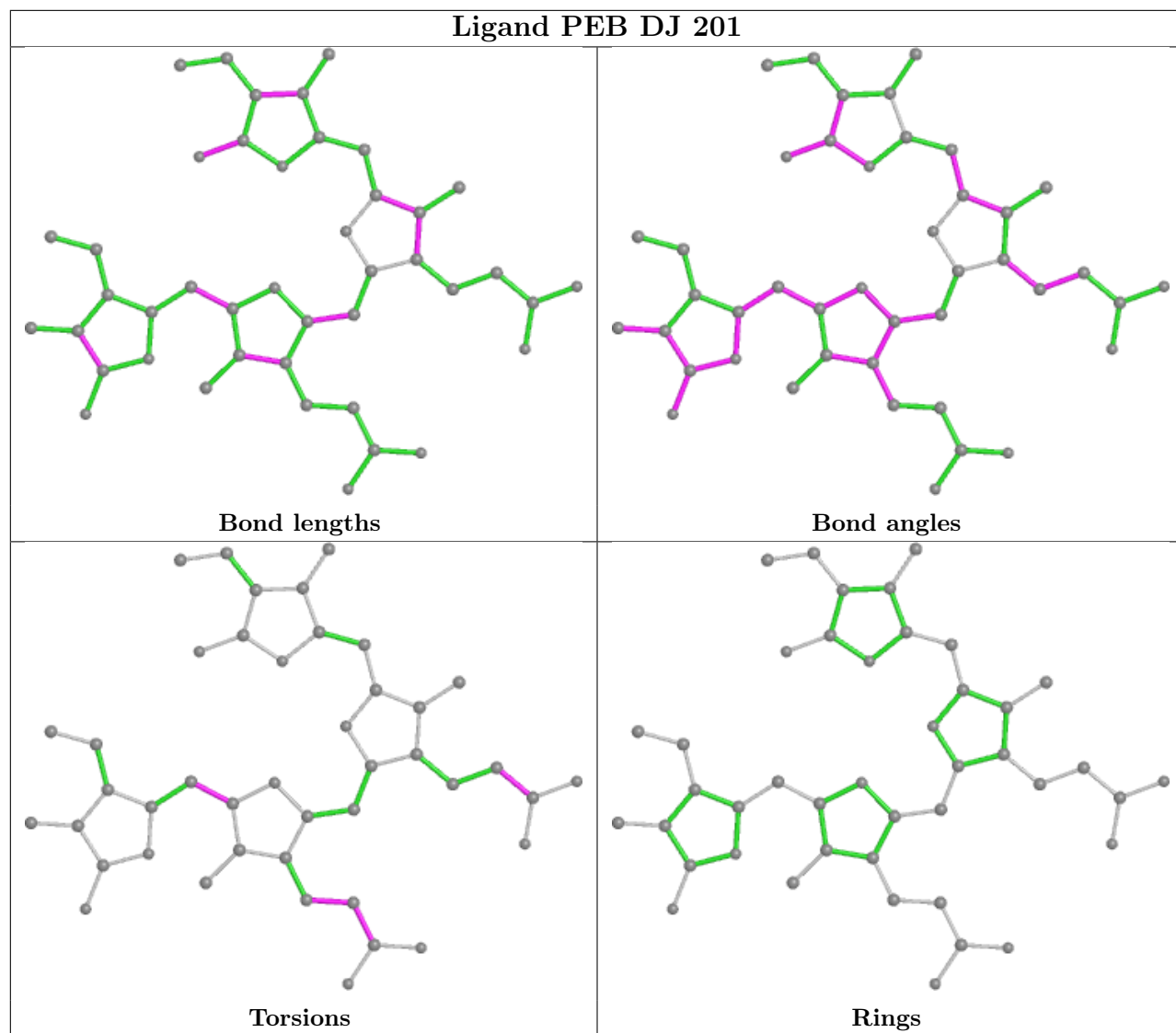


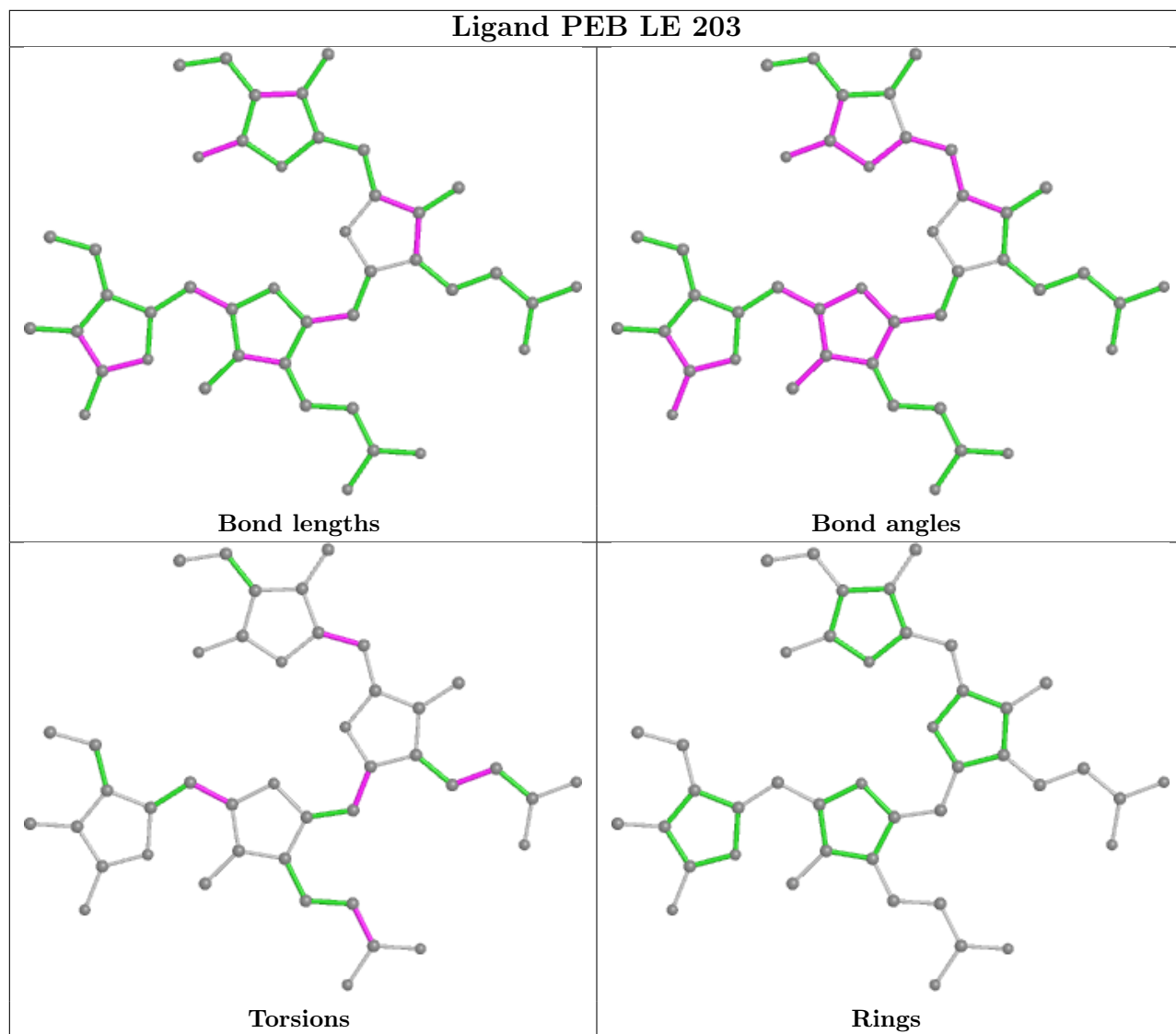


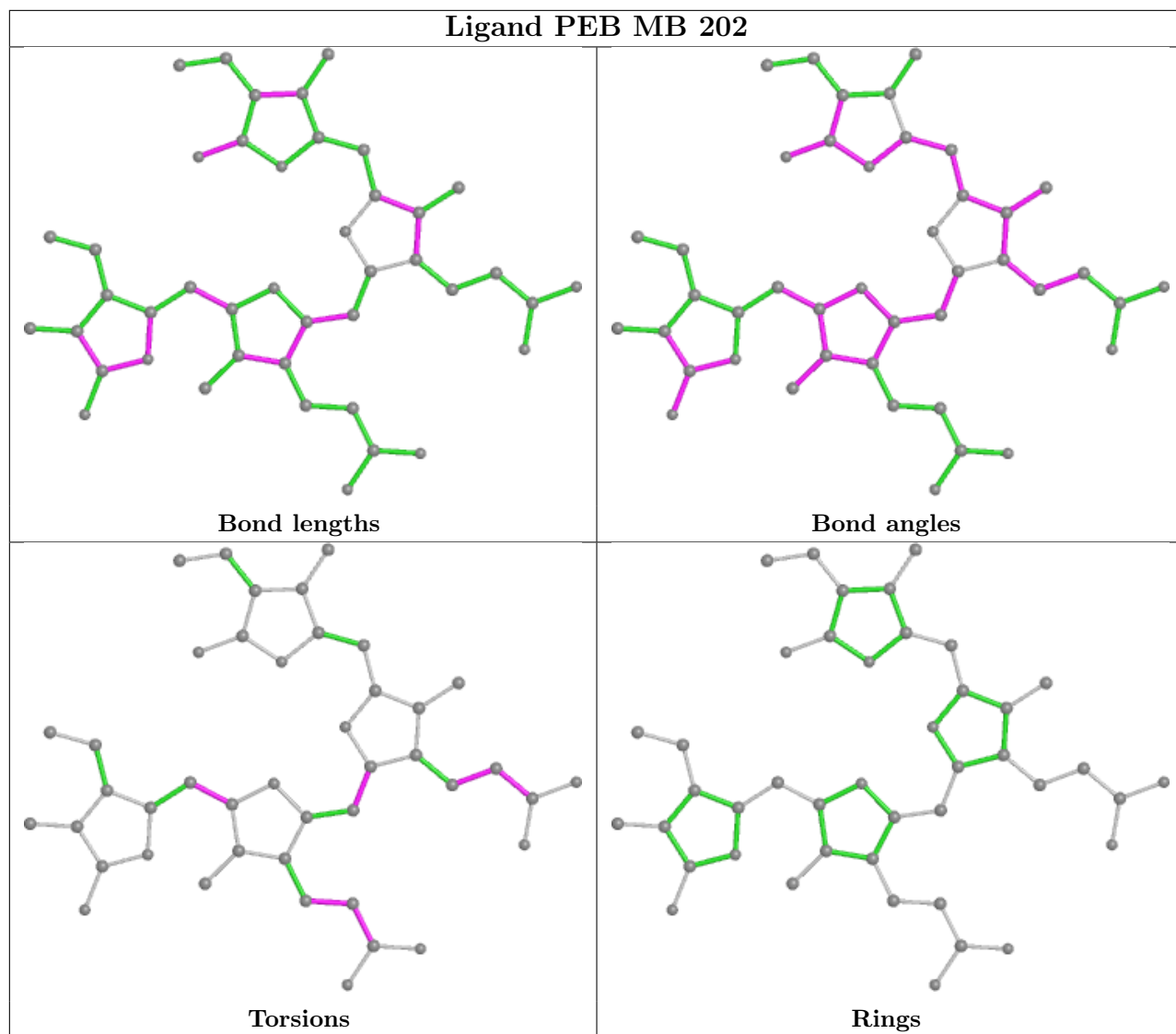


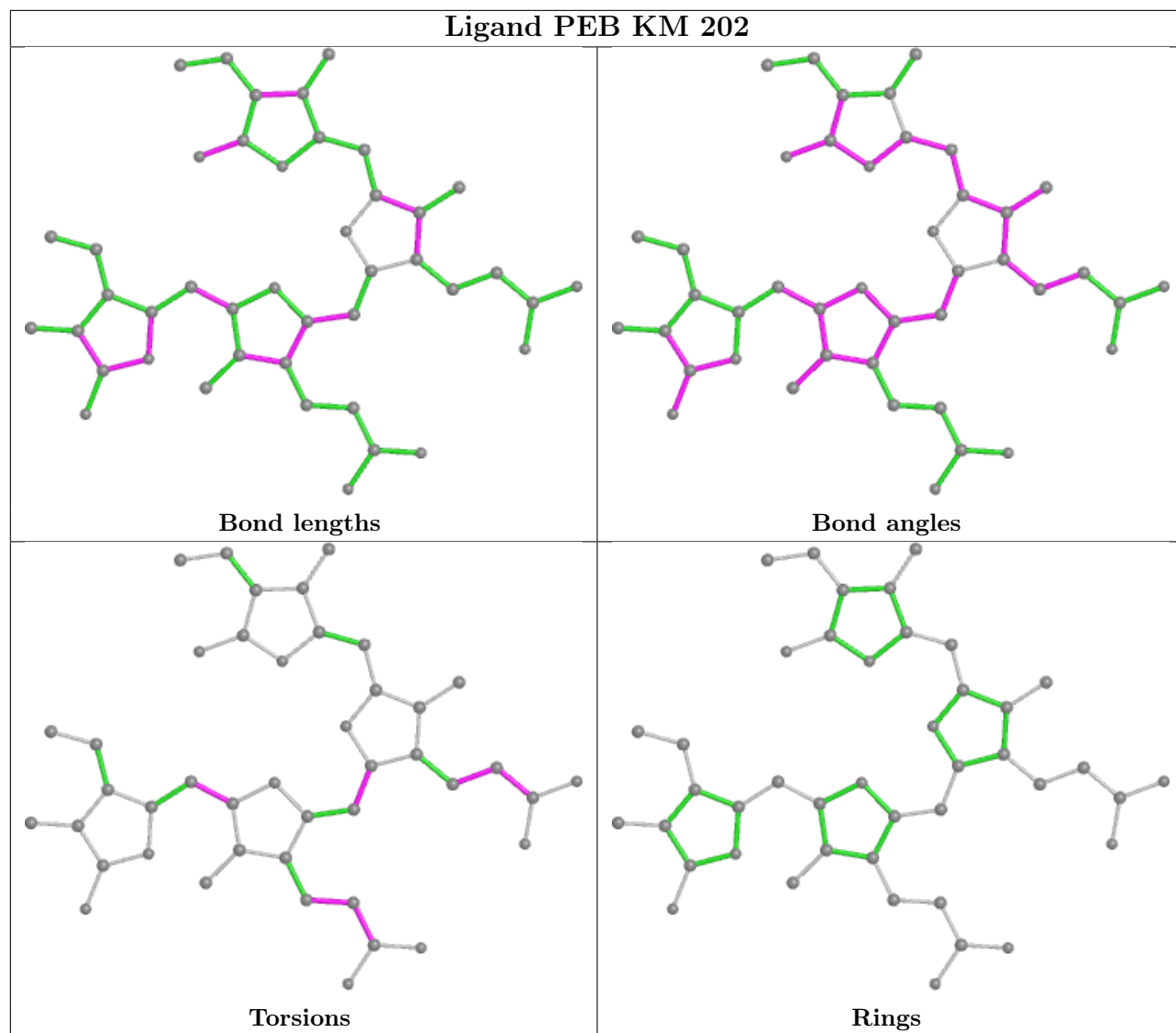


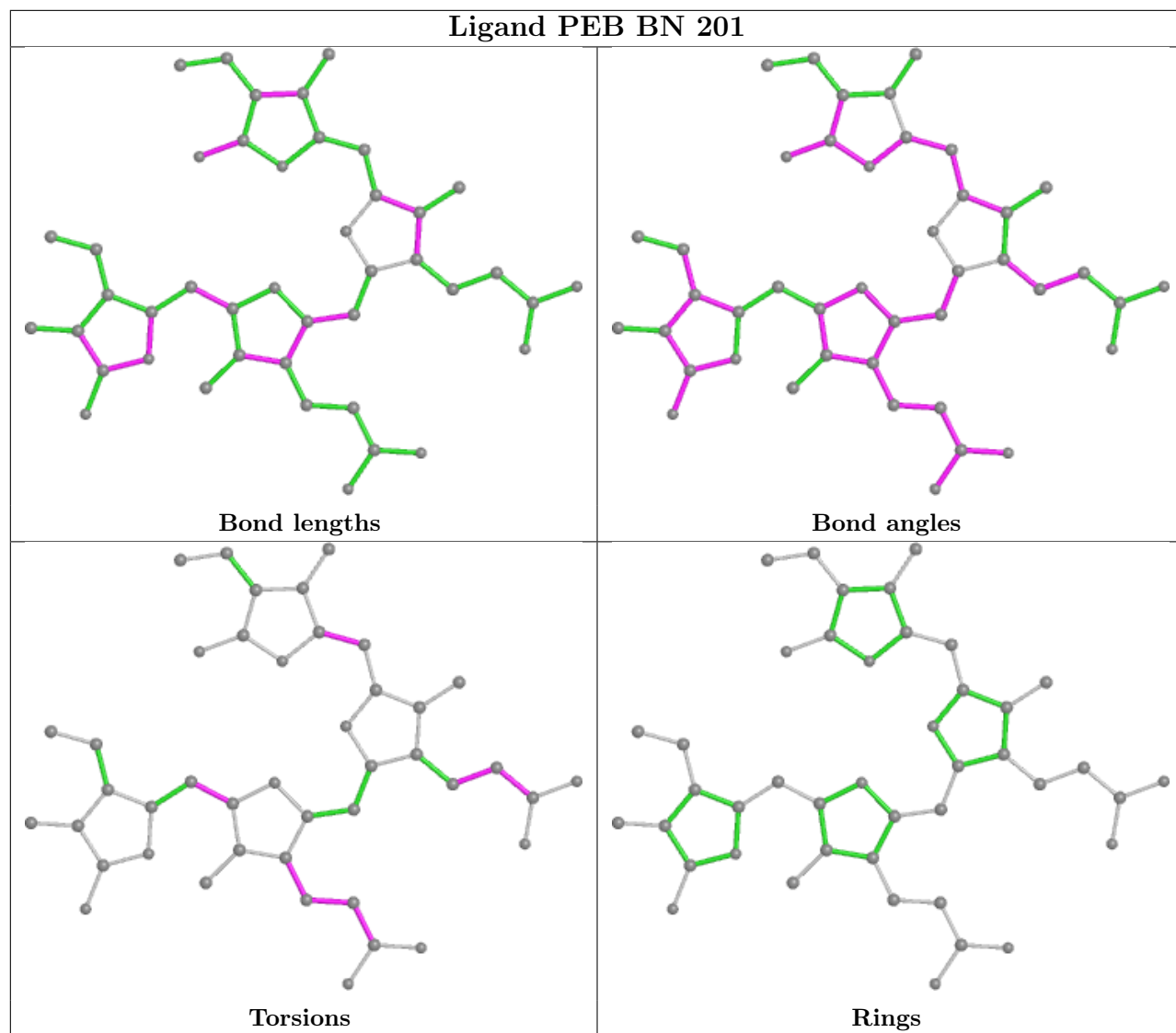


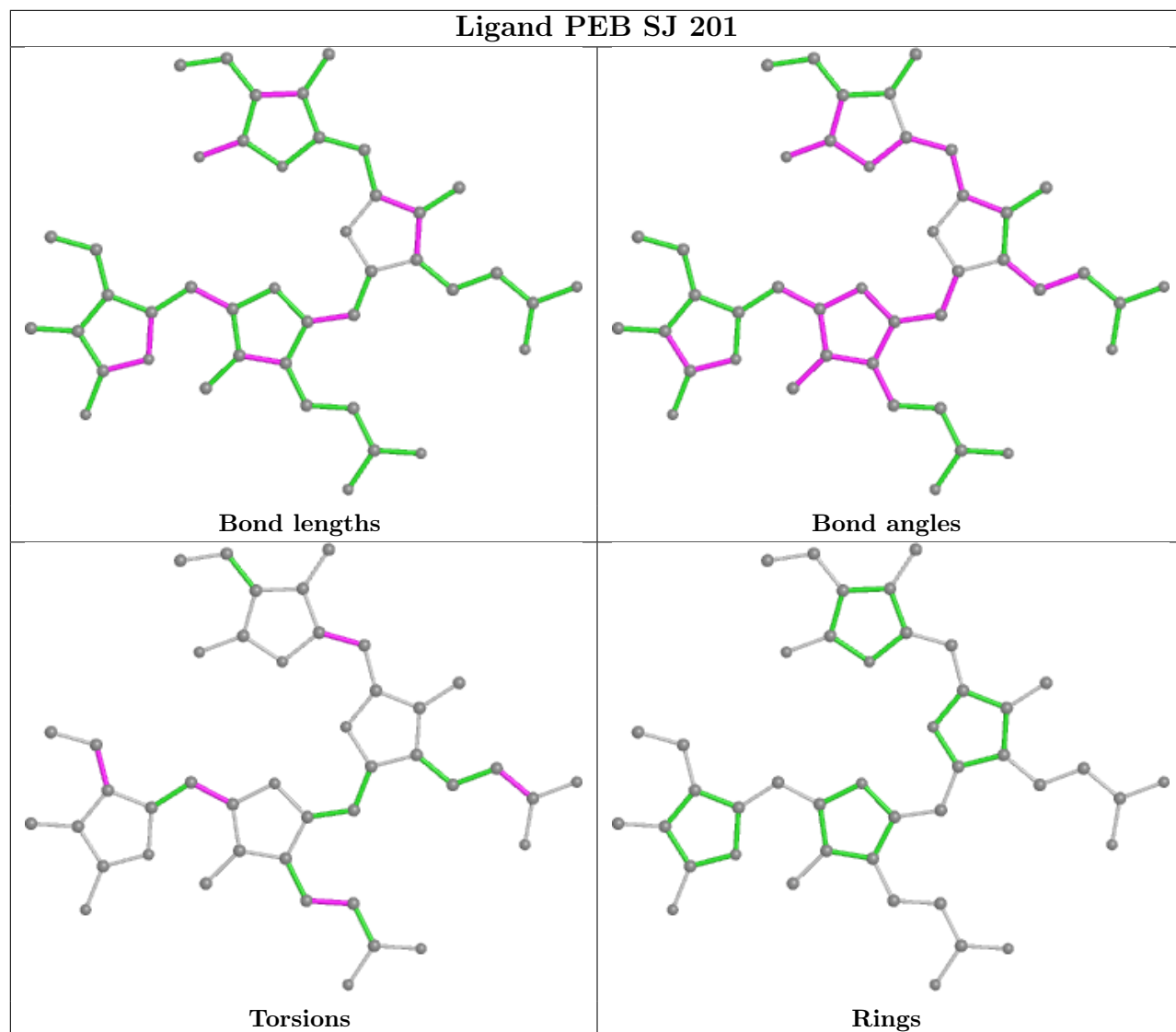


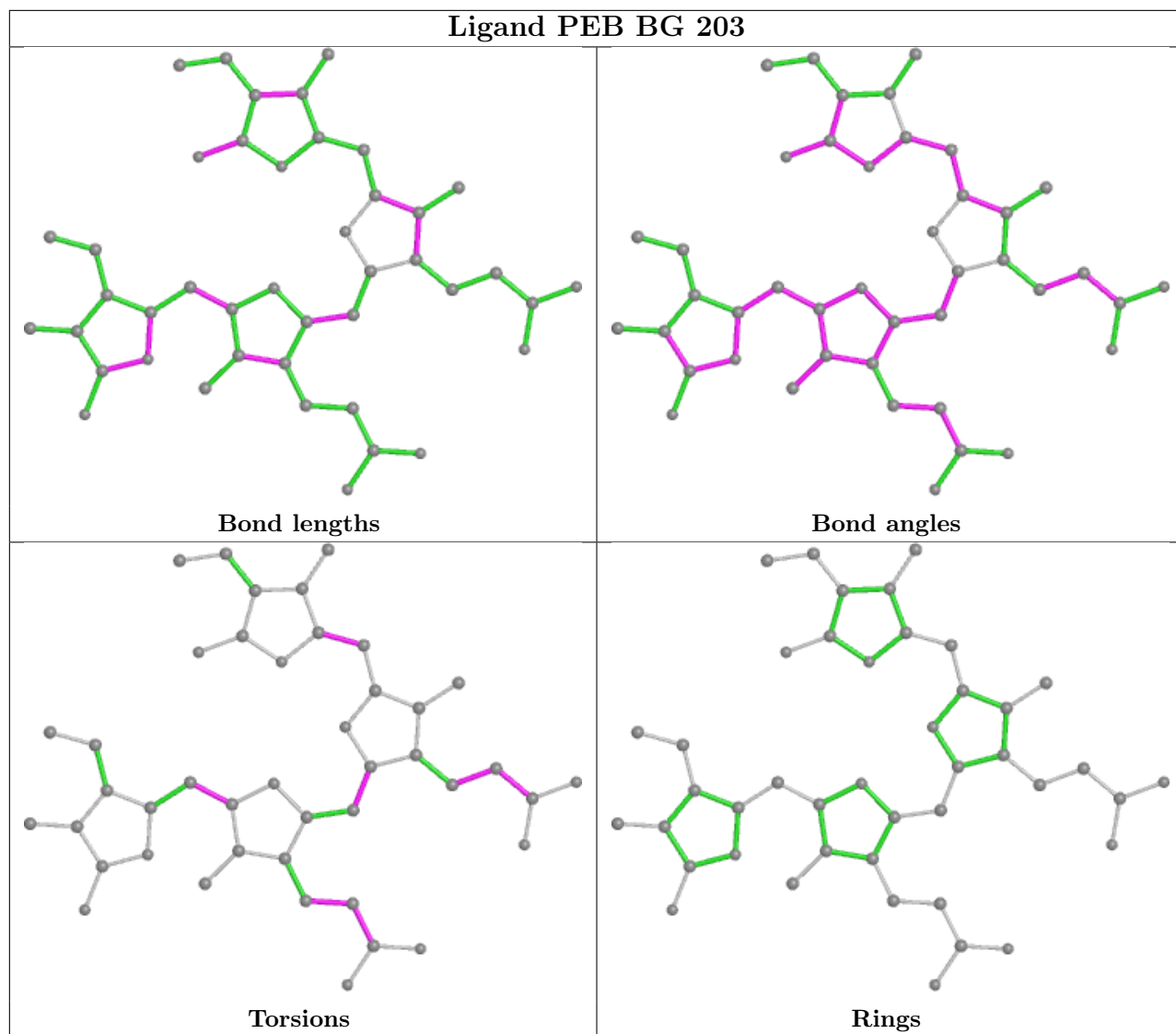


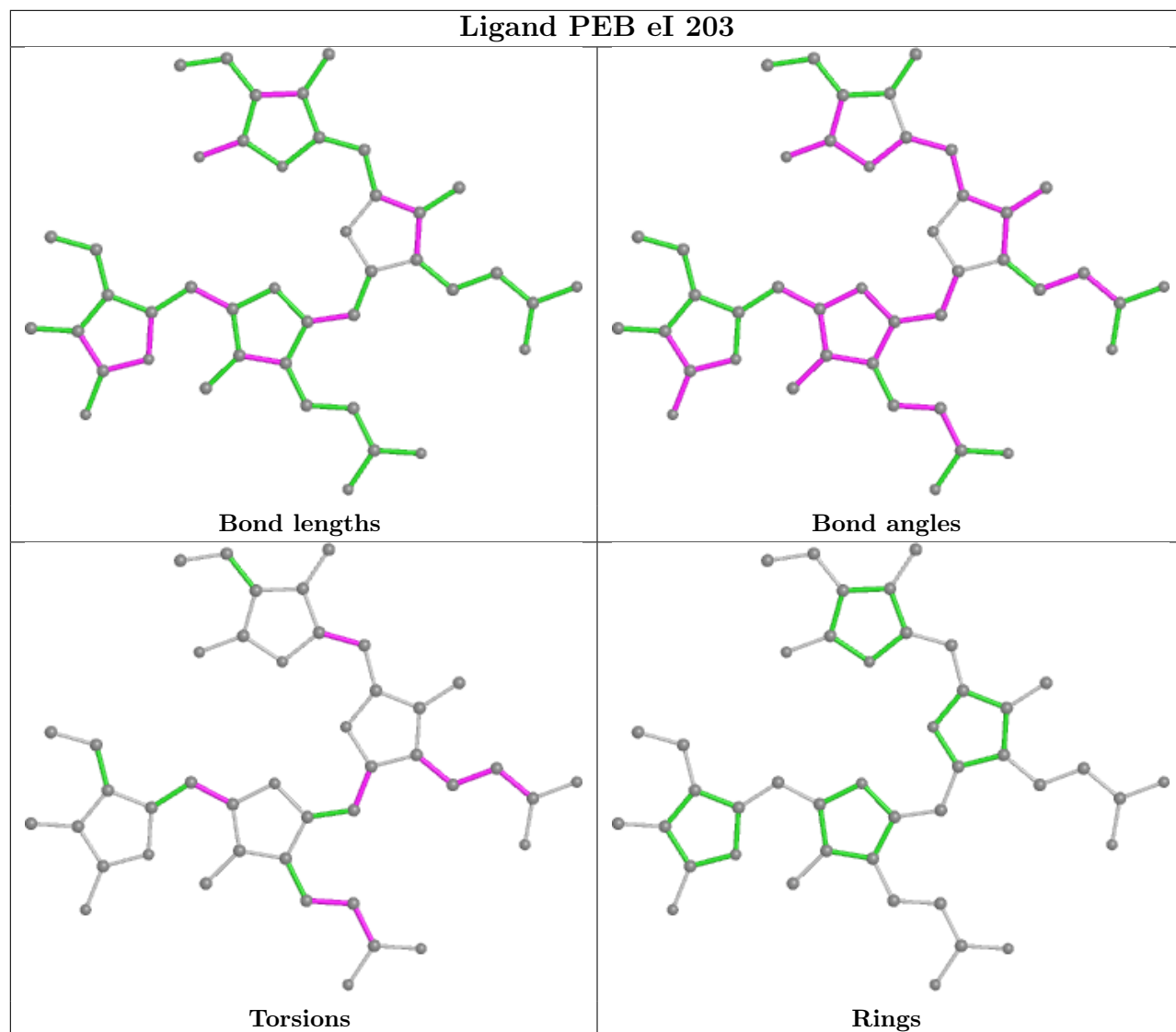


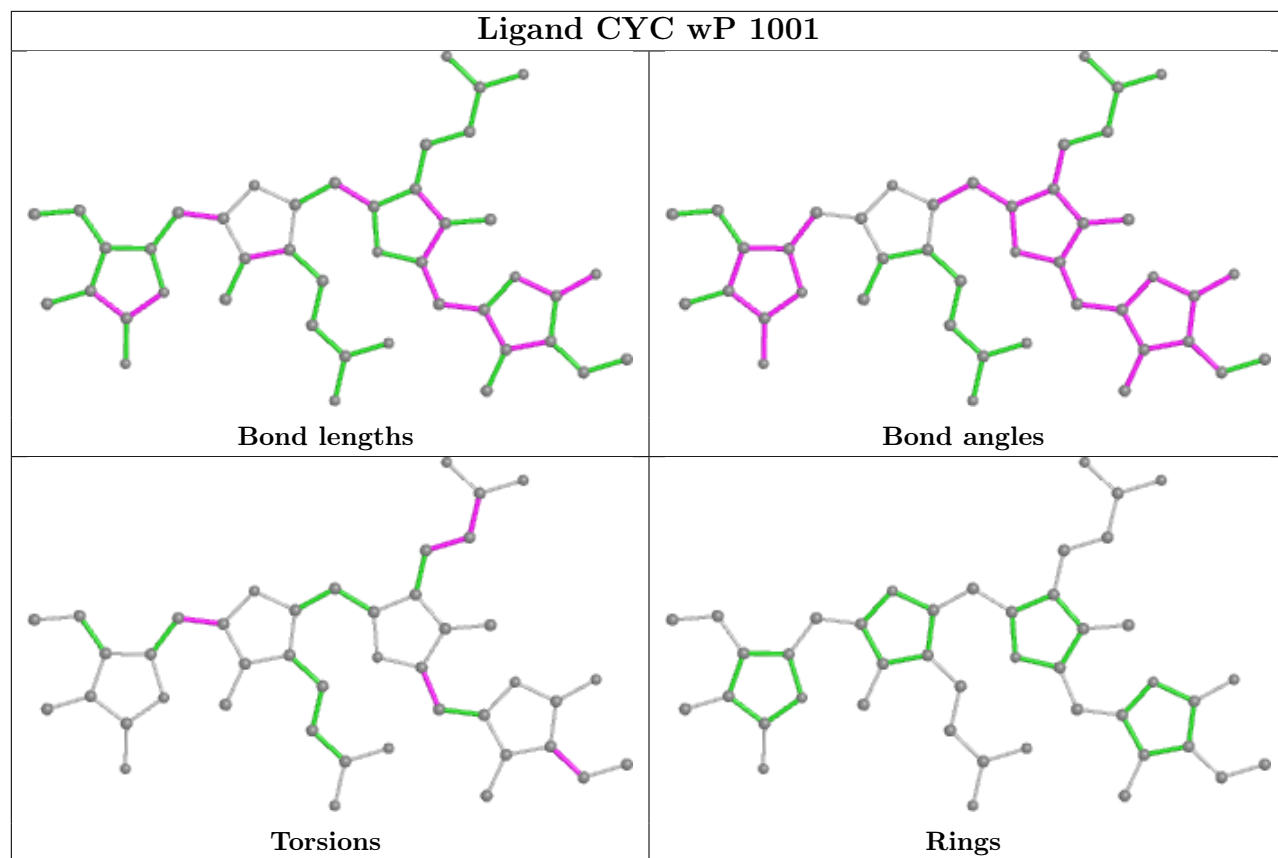


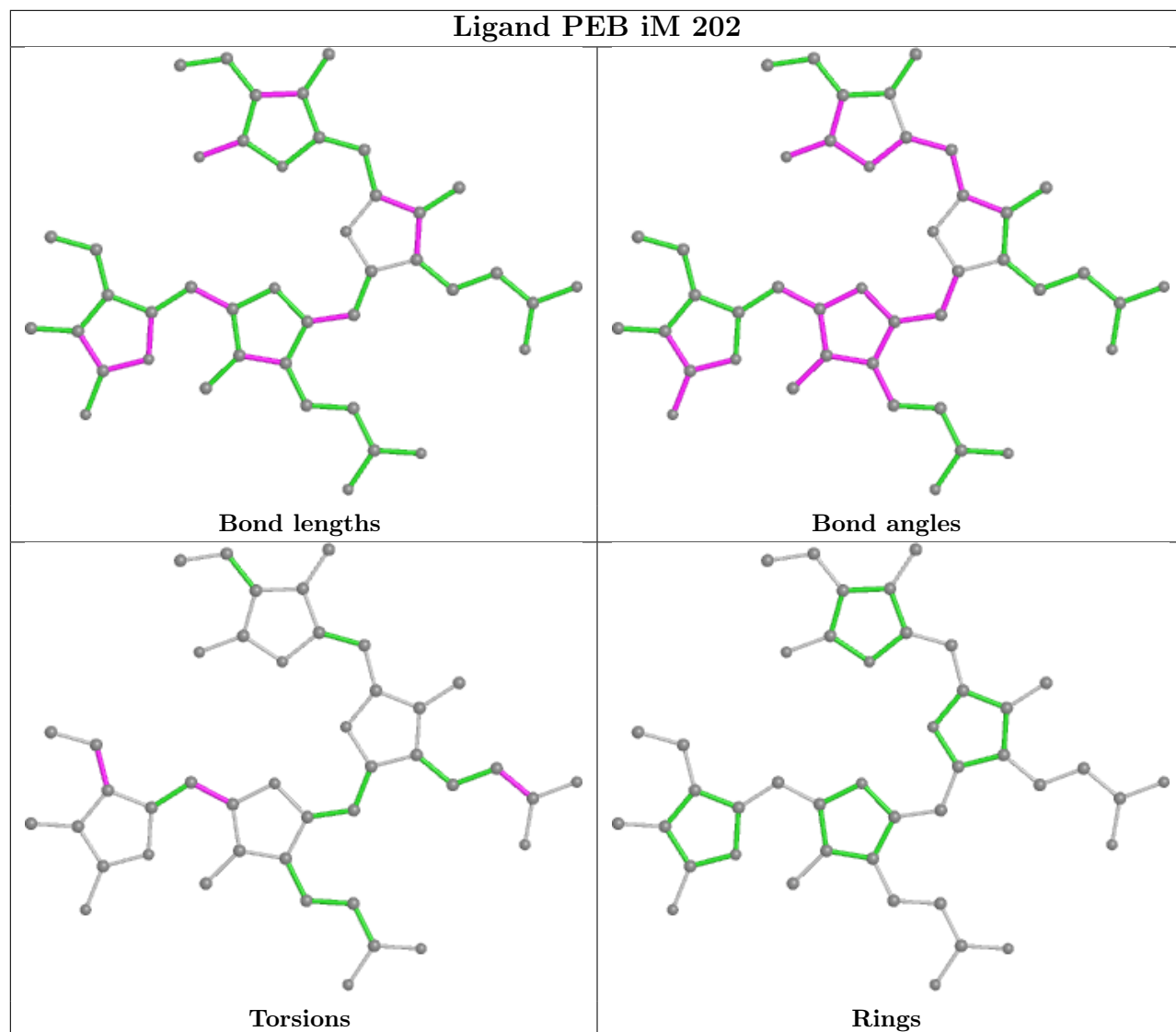


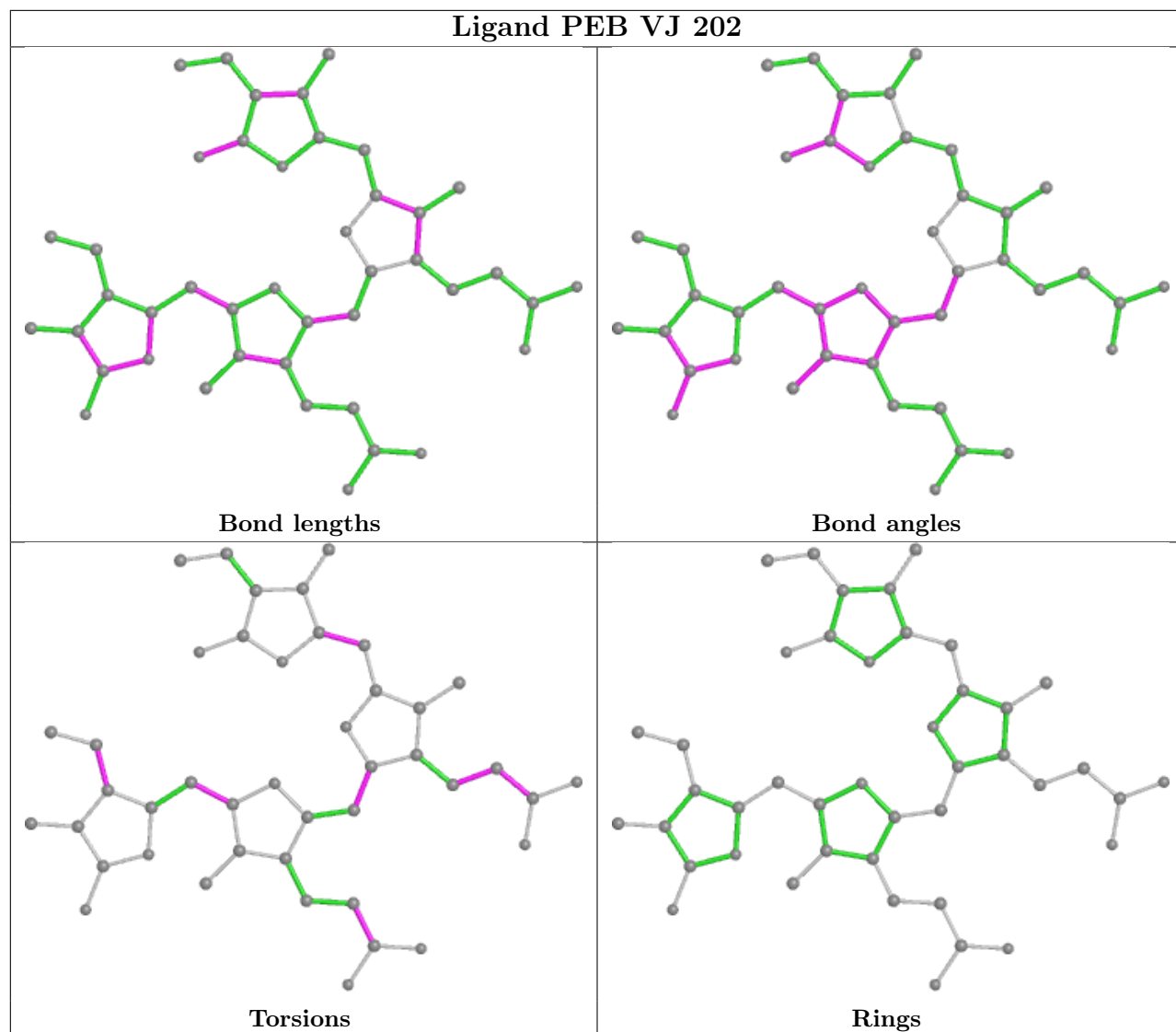


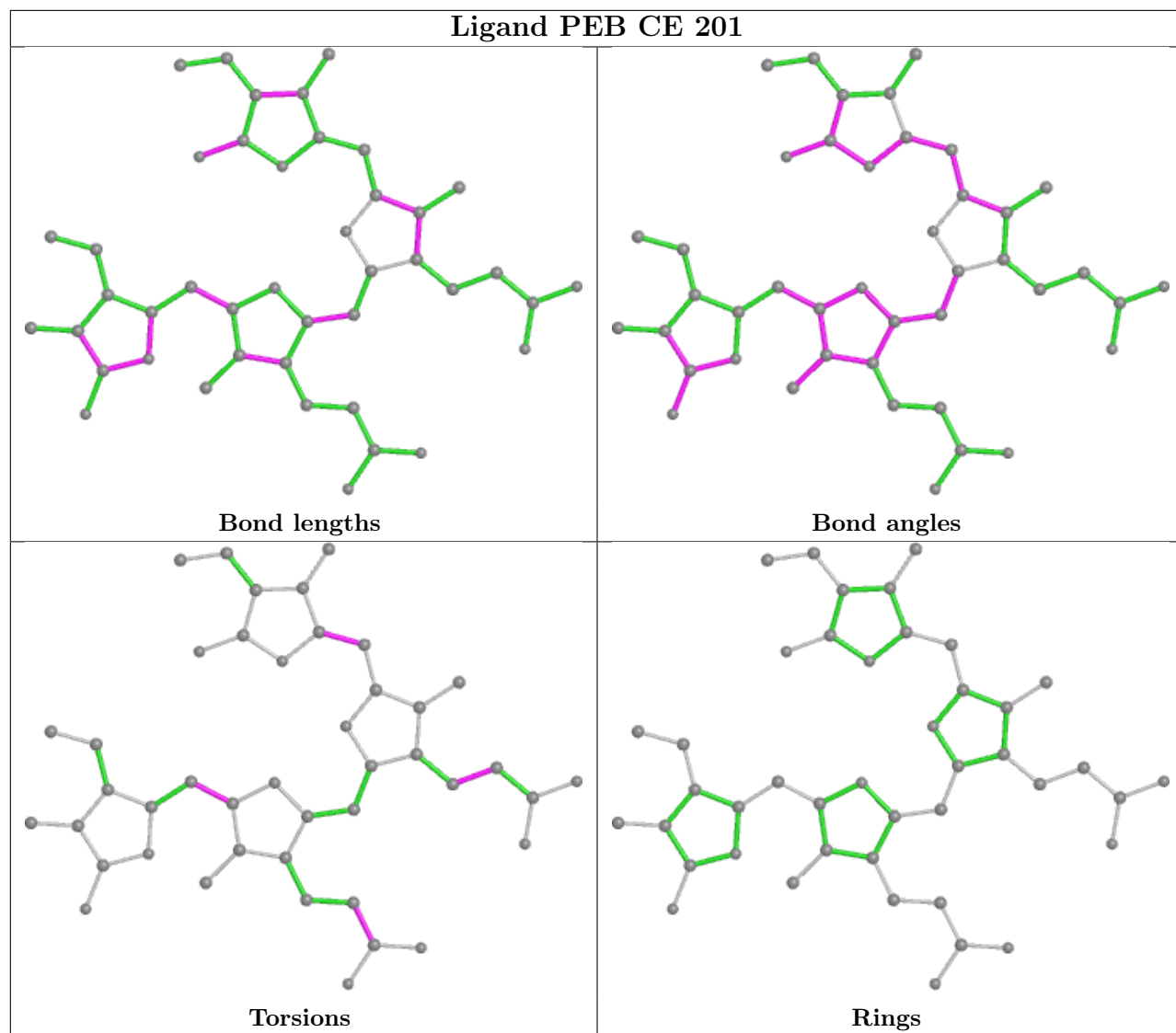


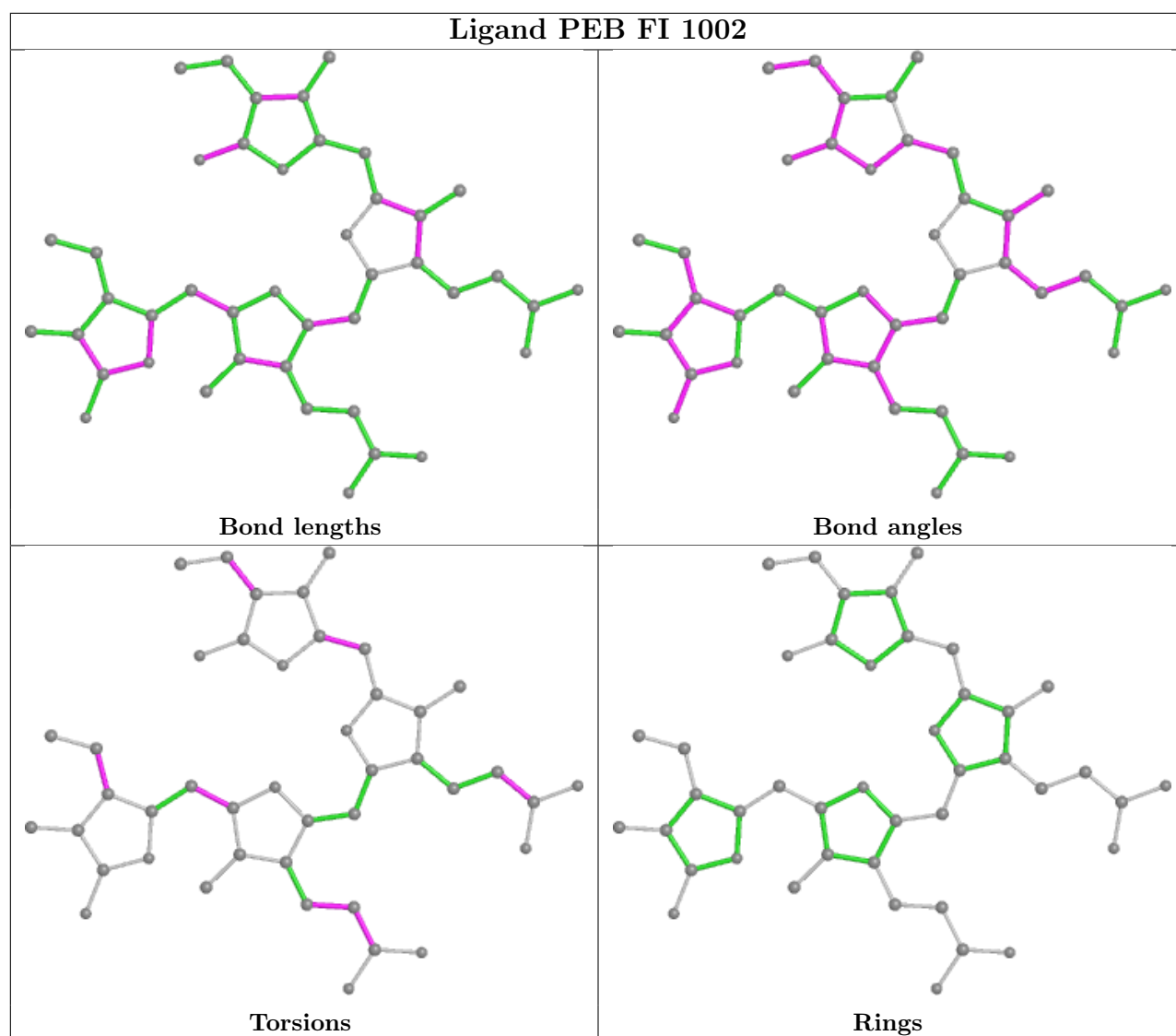












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

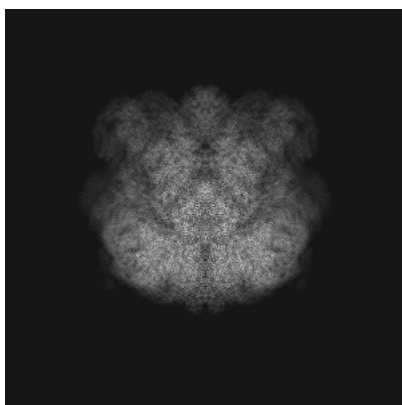
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31393. These allow visual inspection of the internal detail of the map and identification of artifacts.

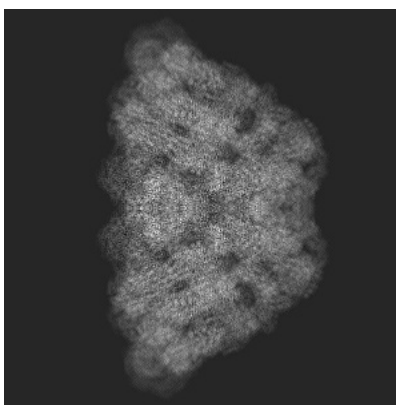
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

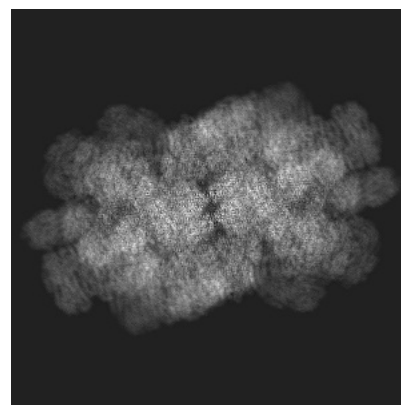
6.1.1 Primary map



X



Y



Z

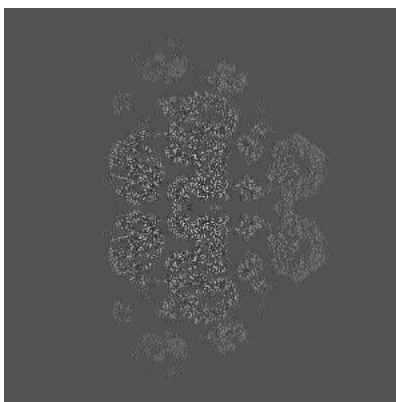
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

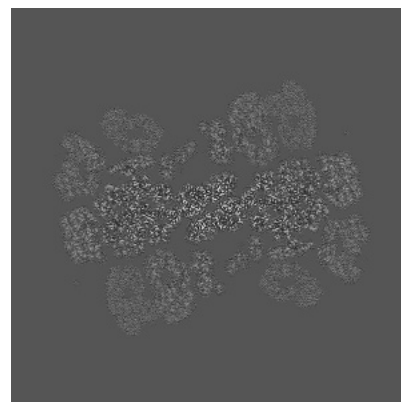
6.2.1 Primary map



X Index: 290



Y Index: 290

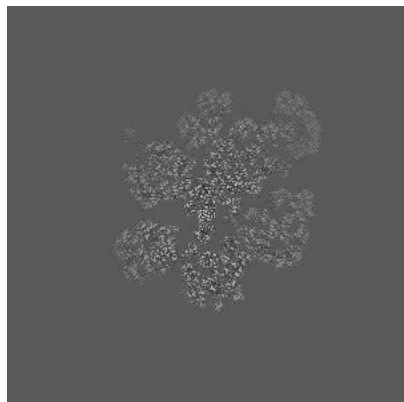


Z Index: 290

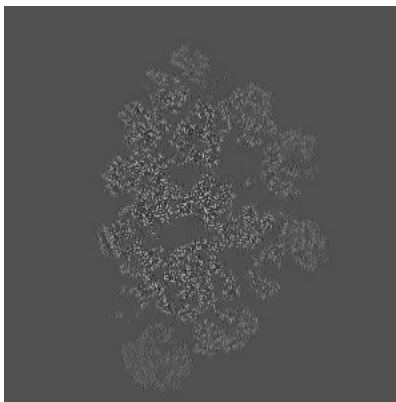
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

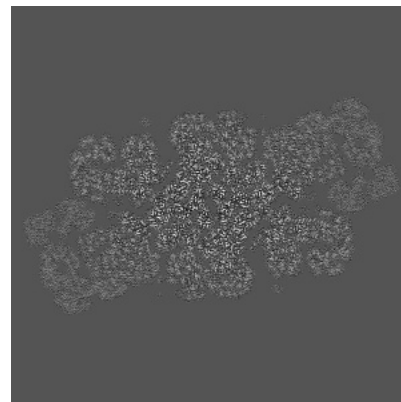
6.3.1 Primary map



X Index: 322



Y Index: 271

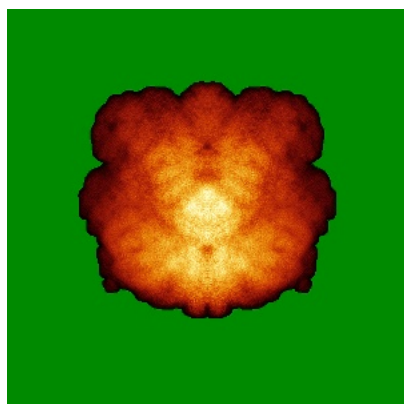


Z Index: 217

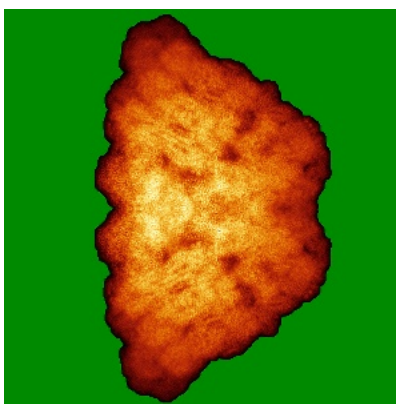
The images above show the largest variance slices of the map in three orthogonal directions.

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

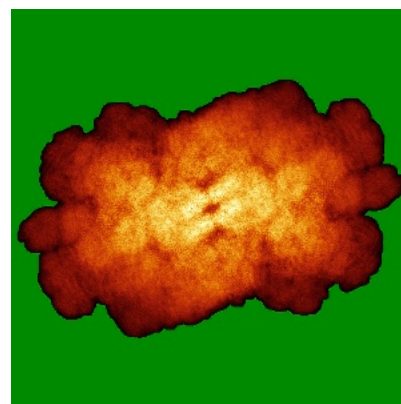
6.4.1 Primary map



X



Y

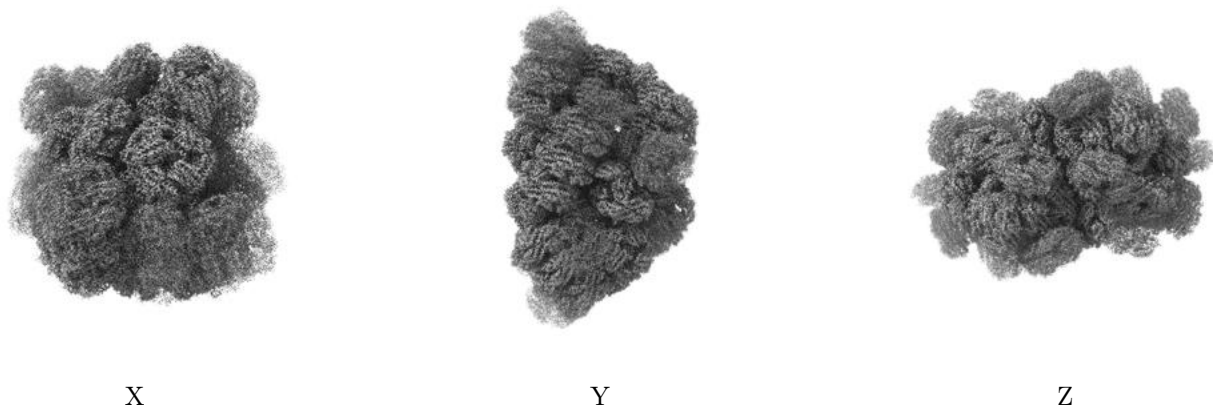


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

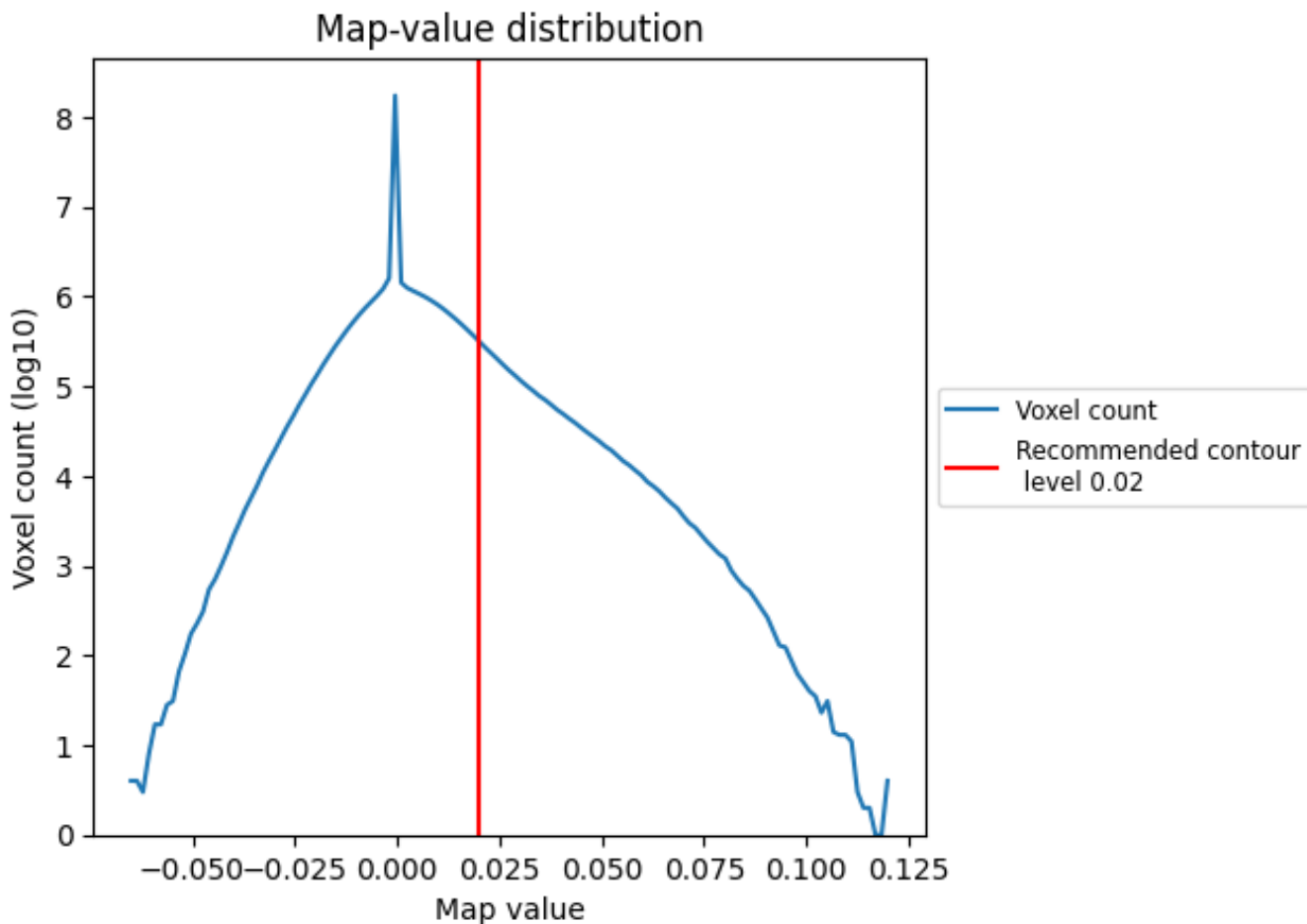
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

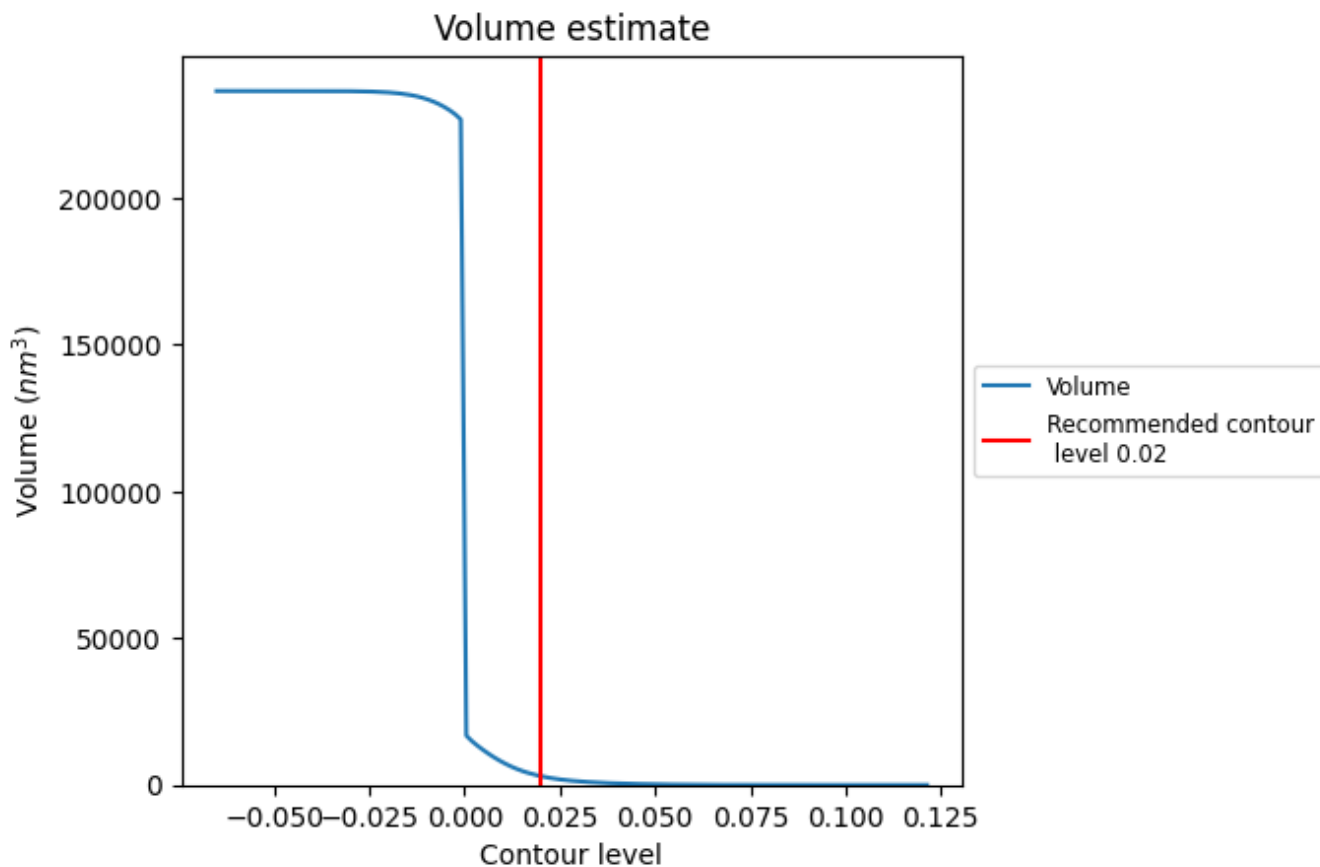
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

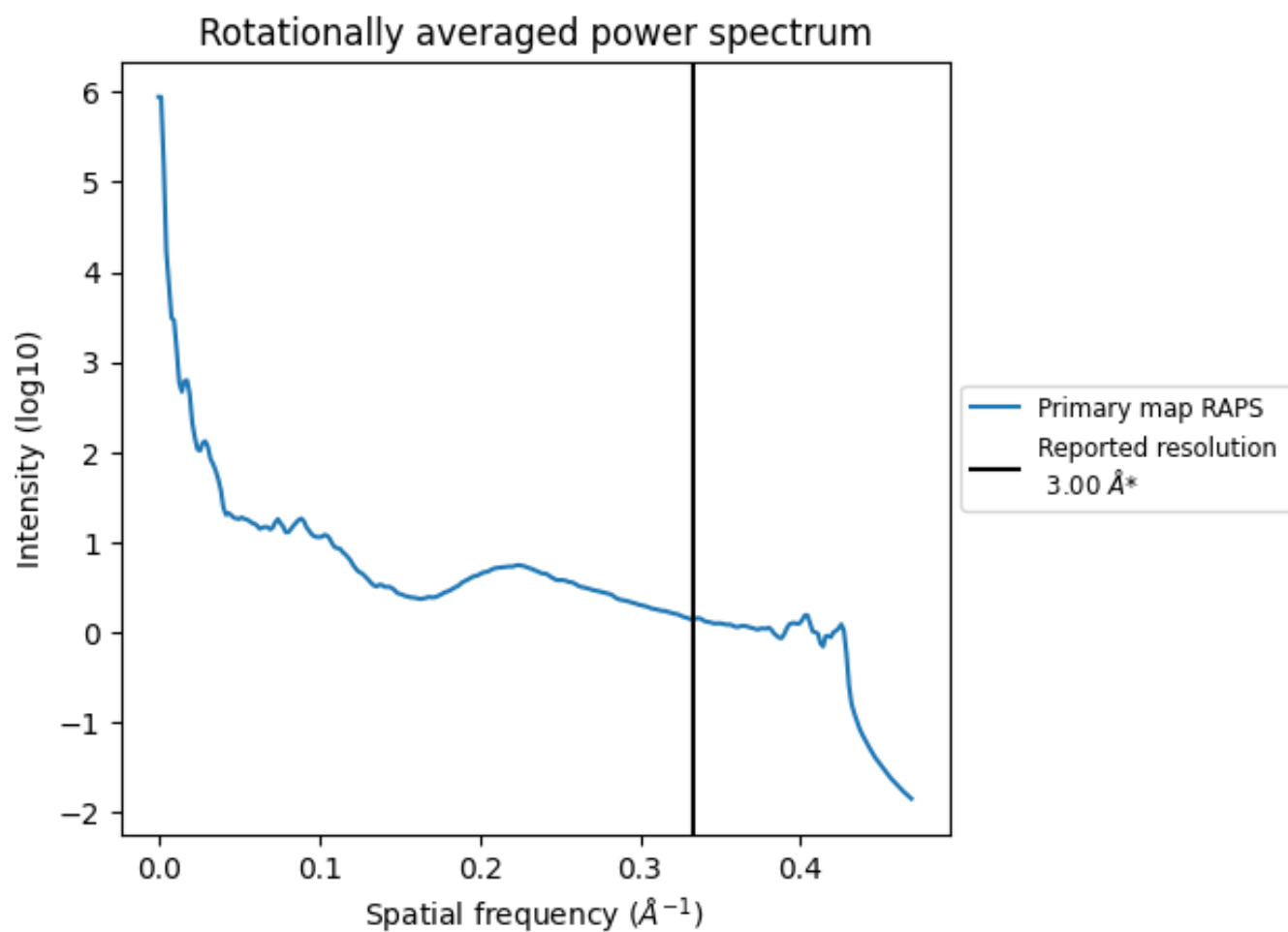
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 3006 nm^3 ; this corresponds to an approximate mass of 2716 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 0.333 \AA^{-1}

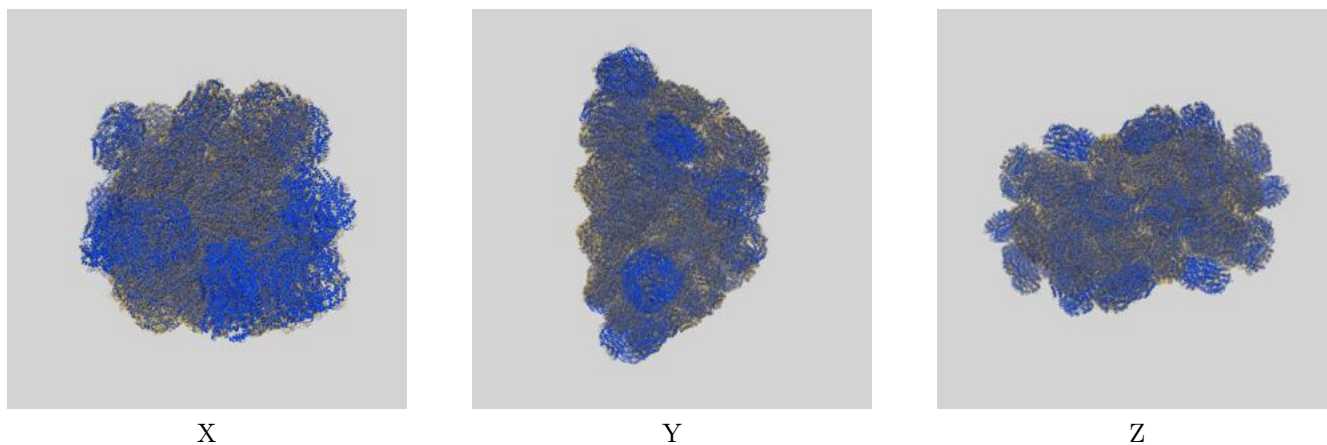
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

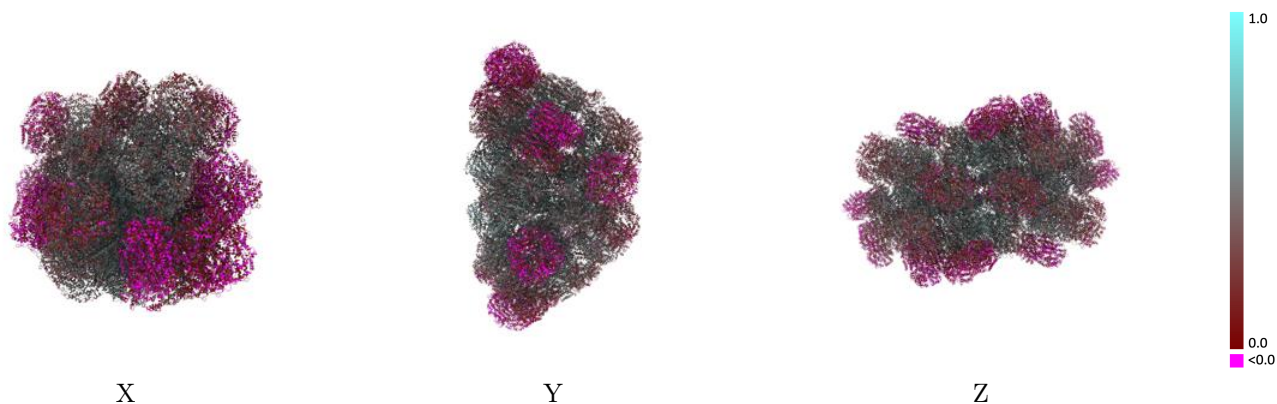
This section contains information regarding the fit between EMDB map EMD-31393 and PDB model 7EZX. Per-residue inclusion information can be found in section 3 on page 136.

9.1 Map-model overlay [i](#)



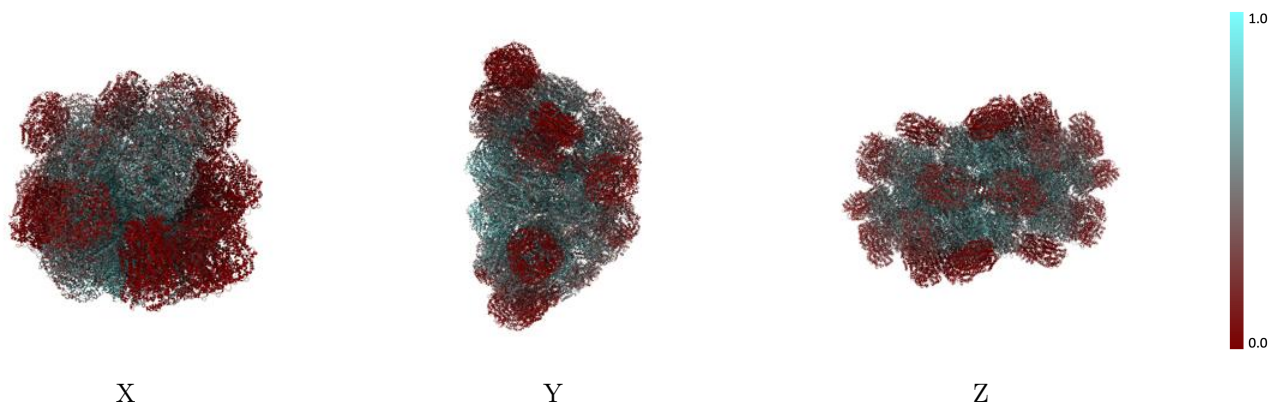
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



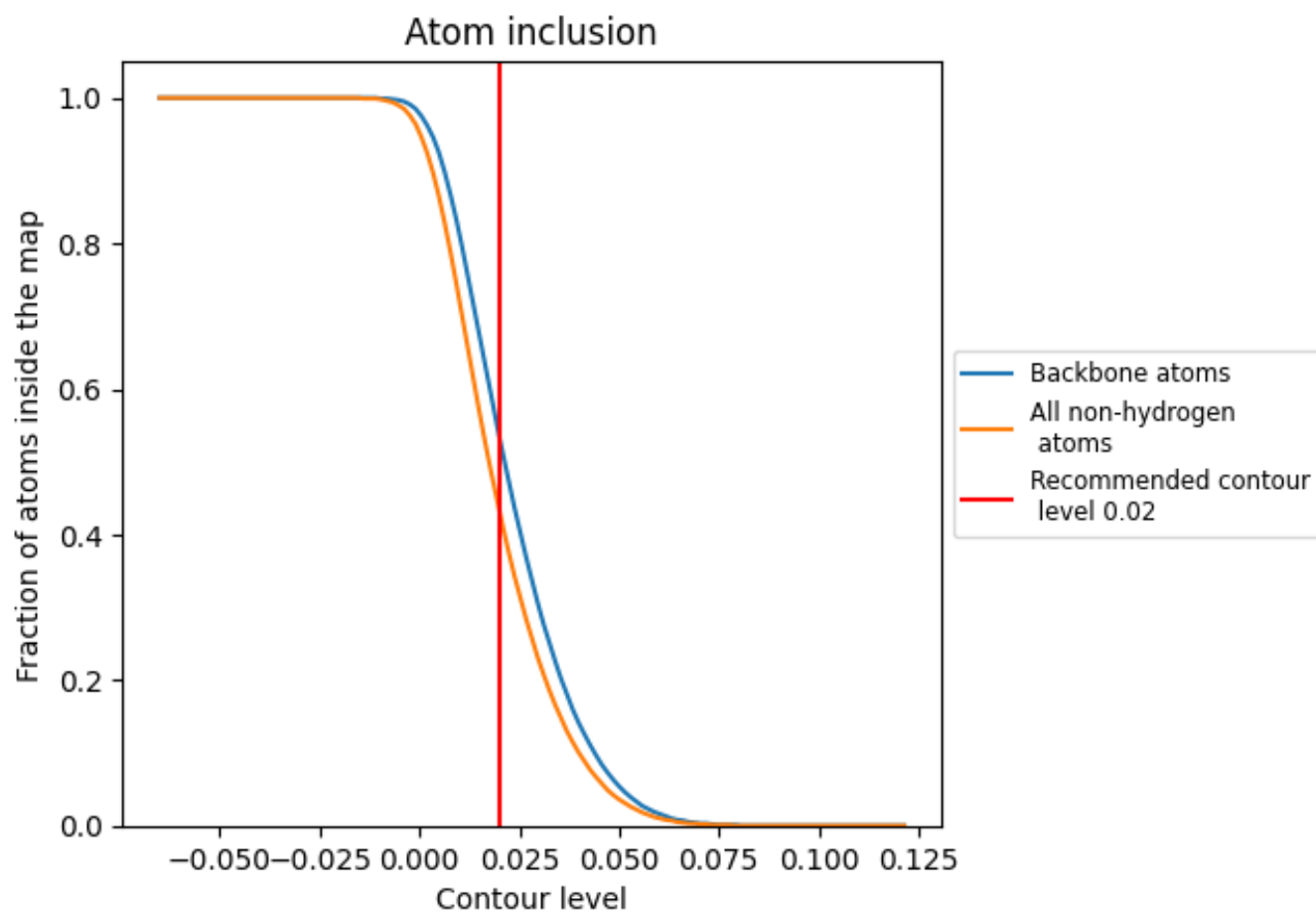
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 53% of all backbone atoms, 43% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4330	 0.3580
1P	 0.8010	 0.5930
2P	 0.7070	 0.5460
3P	 0.7460	 0.5620
4P	 0.7640	 0.5730
A1	 0.0690	 0.1470
A3	 0.6740	 0.4950
A5	 0.0320	 0.1800
A7	 0.5670	 0.4590
A8	 0.0310	 0.1830
A9	 0.5670	 0.4600
AA	 0.0120	 0.0270
AB	 0.1980	 0.2990
AC	 0.0370	 0.0570
AE	 0.0380	 0.0560
AF	 0.3850	 0.3680
AG	 0.0110	 0.0240
AI	 0.3830	 0.3670
AJ	 0.5360	 0.4260
AK	 0.0650	 0.1500
AL	 0.5290	 0.4200
AM	 0.1990	 0.3000
AN	 0.0140	 0.0330
AO	 0.6770	 0.5020
AP	 0.6920	 0.4990
AQ	 0.0110	 0.0200
B1	 0.5950	 0.4650
B3	 0.5890	 0.4590
B4	 0.2360	 0.2570
B5	 0.1220	 0.2730
B7	 0.8120	 0.5680
B8	 0.1150	 0.2790
B9	 0.8150	 0.5740
BA	 0.0090	 0.0390
BB	 0.5720	 0.4690























































































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Chain	Atom inclusion	Q-score
BC	0.0370	0.0800
BD	0.2360	0.2570
BE	0.0360	0.0820
BF	0.7370	0.5270
BG	0.0170	0.0910
BI	0.7400	0.5250
BJ	0.4870	0.3810
BK	0.5950	0.4580
BL	0.5000	0.3980
BM	0.5710	0.4710
BN	0.0110	0.0380
BO	0.5960	0.4640
BP	0.7410	0.5240
BQ	0.0180	0.0940
C1	0.3030	0.3140
C3	0.4610	0.3940
C4	0.2490	0.2710
C5	0.0140	0.1360
C7	0.8450	0.5720
C8	0.0130	0.1380
C9	0.8360	0.5750
CA	0.0110	0.0180
CB	0.6470	0.4950
CC	0.0740	0.1300
CD	0.2490	0.2710
CE	0.0710	0.1320
CF	0.7330	0.5380
CG	0.0090	0.0270
CI	0.7320	0.5450
CJ	0.5250	0.4110
CK	0.2960	0.3100
CL	0.5260	0.4170
CM	0.6520	0.4970
CN	0.0120	0.0210
CO	0.4640	0.3980
CP	0.6520	0.4590
CQ	0.0080	0.0260
D1	0.2580	0.2830
D3	0.6430	0.4900
D4	0.3670	0.3420
D5	0.0510	0.2170
D7	0.8090	0.5680

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Chain	Atom inclusion	Q-score
D8	 0.0510	 0.2130
D9	 0.8080	 0.5700
DA	 0.0080	 0.0270
DB	 0.5260	 0.4300
DC	 0.0900	 0.1420
DD	 0.3690	 0.3420
DE	 0.0900	 0.1420
DF	 0.6830	 0.4980
DG	 0.0080	 0.0470
DI	 0.6840	 0.4990
DJ	 0.5610	 0.4460
DK	 0.2680	 0.2850
DL	 0.5560	 0.4380
DM	 0.5230	 0.4300
DN	 0.0090	 0.0270
DO	 0.6380	 0.4830
DP	 0.7400	 0.4920
DQ	 0.0090	 0.0520
E1	 0.7280	 0.5280
E3	 0.4340	 0.3640
E4	 0.3390	 0.3150
E5	 0.4760	 0.4280
E7	 0.8070	 0.5670
E8	 0.4740	 0.4280
E9	 0.8080	 0.5750
EA	 0.0140	 0.0450
EB	 0.4860	 0.4170
EC	 0.0350	 0.0760
ED	 0.3400	 0.3130
EE	 0.0350	 0.0770
EF	 0.7620	 0.5600
EG	 0.0100	 0.0330
EI	 0.7600	 0.5550
EJ	 0.6040	 0.4530
EK	 0.7280	 0.5300
EL	 0.6060	 0.4490
EM	 0.4910	 0.4190
EN	 0.0150	 0.0470
EO	 0.4400	 0.3700
EP	 0.7350	 0.4910
EQ	 0.0100	 0.0390
F1	 0.4890	 0.4170

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Chain	Atom inclusion	Q-score
F3	0.5210	0.4120
F4	0.3200	0.3160
F5	0.4860	0.4310
F7	0.7390	0.5280
F8	0.4880	0.4300
F9	0.7530	0.5440
FA	0.0350	0.1250
FB	0.6430	0.4680
FC	0.0480	0.0870
FD	0.3280	0.3150
FE	0.0470	0.0870
FF	0.6780	0.5180
FG	0.0170	0.0700
FI	0.6830	0.5170
FJ	0.6890	0.4780
FK	0.4920	0.4190
FL	0.6980	0.4920
FM	0.6420	0.4670
FN	0.0360	0.1320
FO	0.5190	0.4110
FP	0.8010	0.5580
FQ	0.0180	0.0730
G1	0.4050	0.3670
G3	0.4570	0.3870
G4	0.1900	0.2260
G5	0.3210	0.3360
G7	0.8450	0.6000
G8	0.3240	0.3340
G9	0.8540	0.5990
GA	0.0410	0.0870
GB	0.4570	0.3940
GC	0.1010	0.1560
GD	0.1950	0.2310
GE	0.0960	0.1540
GF	0.8180	0.5740
GG	0.0140	0.0220
GI	0.8220	0.5790
GJ	0.7510	0.5180
GK	0.3940	0.3590
GL	0.7590	0.5230
GM	0.4610	0.3990
GN	0.0380	0.0860





















































































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Chain	Atom inclusion	Q-score
GO	0.4520	0.3890
GP	0.7790	0.5360
GQ	0.0140	0.0230
H1	0.5400	0.4200
H3	0.4370	0.3720
H4	0.2490	0.2680
H5	0.5370	0.4570
H7	0.7700	0.5520
H8	0.5400	0.4540
H9	0.7710	0.5570
HA	0.0210	0.0580
HB	0.5500	0.4460
HC	0.0910	0.1360
HD	0.2550	0.2790
HE	0.0910	0.1330
HF	0.7580	0.5570
HG	0.0110	0.0380
HI	0.7600	0.5610
HJ	0.6820	0.4860
HK	0.5520	0.4370
HL	0.6880	0.4940
HM	0.5450	0.4500
HN	0.0180	0.0590
HO	0.4350	0.3800
HP	0.7350	0.5180
HQ	0.0110	0.0440
I1	0.7370	0.5350
I3	0.6030	0.4670
I4	0.4630	0.3880
I5	0.6430	0.4640
I7	0.8320	0.5850
I8	0.6400	0.4570
I9	0.8330	0.5890
IA	0.0110	0.0340
IB	0.6130	0.4680
IC	0.0700	0.1410
ID	0.4680	0.3850
IE	0.0660	0.1420
IF	0.8100	0.5670
IG	0.0110	0.0750
II	0.8090	0.5690
IJ	0.7300	0.5200





















































































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Chain	Atom inclusion	Q-score
IK	 0.7400	 0.5360
IL	 0.7270	 0.5170
IM	 0.6050	 0.4660
IN	 0.0090	 0.0280
IO	 0.5970	 0.4660
IP	 0.8340	 0.5860
IQ	 0.0100	 0.0740
J1	 0.5130	 0.4220
J3	 0.7390	 0.5350
J4	 0.1720	 0.2200
J5	 0.7120	 0.5230
J7	 0.8120	 0.5570
J8	 0.7120	 0.5190
J9	 0.8130	 0.5550
JA	 0.0100	 0.0350
JB	 0.5410	 0.4470
JC	 0.0300	 0.0890
JD	 0.1680	 0.2200
JE	 0.0330	 0.0860
JF	 0.8120	 0.5690
JG	 0.0220	 0.1200
JI	 0.8160	 0.5760
JJ	 0.6600	 0.4940
JK	 0.5150	 0.4250
JL	 0.6670	 0.5010
JM	 0.5460	 0.4480
JN	 0.0070	 0.0340
JO	 0.7400	 0.5340
JP	 0.7870	 0.5560
JQ	 0.0190	 0.1200
K1	 0.4830	 0.4140
K3	 0.7540	 0.5360
K4	 0.1600	 0.1990
K5	 0.4850	 0.4120
K7	 0.8280	 0.5730
K8	 0.4840	 0.4120
K9	 0.8430	 0.5880
KA	 0.0090	 0.0150
KB	 0.6980	 0.5190
KC	 0.0460	 0.0820
KD	 0.1590	 0.1980
KE	 0.0460	 0.0860

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Chain	Atom inclusion	Q-score
KF	 0.7660	 0.5560
KG	 0.0120	 0.0830
KI	 0.7710	 0.5610
KJ	 0.6170	 0.4410
KK	 0.4860	 0.4180
KL	 0.6310	 0.4570
KM	 0.6910	 0.5180
KN	 0.0080	 0.0170
KO	 0.7510	 0.5370
KP	 0.7150	 0.5100
KQ	 0.0120	 0.0770
L1	 0.6910	 0.5110
L3	 0.6210	 0.4850
L4	 0.2050	 0.2400
L5	 0.5460	 0.4460
L7	 0.7820	 0.5510
L8	 0.5410	 0.4390
L9	 0.7910	 0.5560
LA	 0.0140	 0.0190
LB	 0.6820	 0.5030
LC	 0.1230	 0.1900
LD	 0.2010	 0.2410
LE	 0.1200	 0.1880
LF	 0.7400	 0.5340
LG	 0.0170	 0.0710
LI	 0.7390	 0.5330
LJ	 0.7400	 0.5150
LK	 0.6900	 0.5120
LL	 0.7450	 0.5140
LM	 0.6970	 0.5080
LN	 0.0140	 0.0190
LO	 0.6190	 0.4910
LP	 0.7510	 0.5010
LQ	 0.0180	 0.0860
M1	 0.3130	 0.2940
M2	 0.3810	 0.3270
M3	 0.5320	 0.4050
M4	 0.2360	 0.2480
M7	 0.8390	 0.5740
M9	 0.8500	 0.5950
MA	 0.0260	 0.0750
MB	 0.7400	 0.5360

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Chain	Atom inclusion	Q-score
MC	0.1530	0.1960
MD	0.2260	0.2390
ME	0.1500	0.1870
MF	0.8160	0.5810
MG	0.0180	0.0900
MI	0.8190	0.5850
MJ	0.4290	0.3720
MK	0.3170	0.2930
ML	0.4370	0.3740
MM	0.7440	0.5370
MN	0.0210	0.0740
MO	0.5390	0.4110
MP	0.7520	0.5250
MQ	0.0260	0.1110
MR	0.3870	0.3380
N1	0.3610	0.3230
N2	0.4860	0.4000
N3	0.3620	0.3330
N7	0.8170	0.5670
N9	0.8130	0.5640
NB	0.7480	0.5330
NF	0.7290	0.5290
NI	0.7370	0.5300
NJ	0.4510	0.3900
NK	0.3670	0.3260
NL	0.4500	0.3960
NM	0.7480	0.5320
NO	0.3670	0.3240
NP	0.8090	0.5670
NR	0.4820	0.3990
O1	0.2300	0.2790
O2	0.6140	0.4530
O3	0.5460	0.4280
O7	0.6760	0.4980
O9	0.6760	0.5020
OB	0.5080	0.4260
OF	0.6330	0.4950
OI	0.6360	0.5010
OJ	0.5190	0.4260
OK	0.2300	0.2800
OL	0.5210	0.4310
OM	0.5070	0.4310





















































































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Chain	Atom inclusion	Q-score
OO	0.5500	0.4330
OP	0.7090	0.5010
OR	0.6190	0.4560
P1	0.4100	0.3910
P2	0.5380	0.4350
P7	0.7000	0.5120
P9	0.7020	0.5180
PB	0.4120	0.3740
PF	0.6300	0.4840
PI	0.6340	0.4900
PJ	0.5330	0.4390
PK	0.4060	0.3920
PL	0.5390	0.4460
PM	0.4120	0.3750
PP	0.7930	0.5300
PR	0.5360	0.4310
Q1	0.2790	0.3130
Q2	0.5570	0.4310
Q7	0.7450	0.5290
Q9	0.7440	0.5330
QB	0.4150	0.3640
QF	0.5370	0.4400
QI	0.5390	0.4430
QJ	0.4970	0.4280
QK	0.2800	0.3070
QL	0.5020	0.4300
QM	0.4150	0.3610
QP	0.8290	0.5660
QR	0.5610	0.4340
R1	0.1950	0.2420
R2	0.5240	0.4300
R7	0.7790	0.5470
R9	0.7760	0.5520
RB	0.5560	0.4460
RF	0.6080	0.4830
RI	0.6140	0.4870
RJ	0.5490	0.4430
RK	0.1920	0.2430
RL	0.5580	0.4480
RM	0.5550	0.4440
RP	0.7910	0.5260
RR	0.5190	0.4330





















































































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Chain	Atom inclusion	Q-score
S1	 0.2420	 0.2700
S2	 0.5960	 0.4650
S7	 0.7330	 0.5410
S9	 0.7350	 0.5450
SB	 0.3820	 0.3610
SF	 0.5650	 0.4500
SI	 0.5650	 0.4520
SJ	 0.6200	 0.4480
SK	 0.2460	 0.2760
SL	 0.6240	 0.4620
SM	 0.3860	 0.3610
SP	 0.8210	 0.5620
SR	 0.5920	 0.4630
T1	 0.2390	 0.2820
T2	 0.6910	 0.5140
T7	 0.6950	 0.5250
T9	 0.7020	 0.5340
TB	 0.5170	 0.4350
TF	 0.6630	 0.4980
TI	 0.6550	 0.4980
TJ	 0.6380	 0.4900
TK	 0.2380	 0.2820
TL	 0.6470	 0.4950
TM	 0.5150	 0.4390
TP	 0.7840	 0.5270
TR	 0.6840	 0.5140
U1	 0.1460	 0.2190
U2	 0.4560	 0.3930
U7	 0.7240	 0.5170
U9	 0.7250	 0.5230
UB	 0.5720	 0.4560
UF	 0.5510	 0.4490
UI	 0.5530	 0.4430
UJ	 0.6140	 0.4740
UK	 0.1500	 0.2220
UL	 0.6160	 0.4750
UM	 0.5770	 0.4680
UP	 0.8590	 0.5930
UR	 0.4600	 0.3970
V1	 0.1840	 0.2560
V2	 0.3530	 0.3210
V7	 0.7910	 0.5610

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Chain	Atom inclusion	Q-score
V9	 0.7950	 0.5610
VB	 0.4570	 0.4060
VF	 0.5290	 0.4350
VI	 0.5270	 0.4410
VJ	 0.4980	 0.4090
VK	 0.1900	 0.2590
VL	 0.5140	 0.4130
VM	 0.4550	 0.4060
VP	 0.7470	 0.5580
VR	 0.3520	 0.3250
W1	 0.1290	 0.1740
W2	 0.4220	 0.3610
W7	 0.7080	 0.5190
W9	 0.7140	 0.5270
WB	 0.6780	 0.5150
WF	 0.6380	 0.4890
WI	 0.6370	 0.4900
WJ	 0.5380	 0.4220
WK	 0.1300	 0.1760
WL	 0.5470	 0.4280
WM	 0.6810	 0.5150
WP	 0.7840	 0.5900
WR	 0.4190	 0.3600
X1	 0.3370	 0.3640
X2	 0.5510	 0.4570
X7	 0.7790	 0.5530
X9	 0.7830	 0.5600
XB	 0.6110	 0.4790
XF	 0.6800	 0.5230
XI	 0.6840	 0.5270
XJ	 0.6500	 0.4860
XK	 0.3400	 0.3620
XL	 0.6480	 0.4880
XM	 0.6190	 0.4840
XP	 0.8550	 0.6050
XR	 0.5550	 0.4600
Y1	 0.1950	 0.2540
Y7	 0.6750	 0.5020
Y9	 0.6850	 0.5120
YB	 0.6400	 0.4960
YF	 0.7040	 0.5280
YI	 0.7140	 0.5330

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Chain	Atom inclusion	Q-score
YJ	0.0960	0.1130
YK	0.1880	0.2550
YL	0.0950	0.1180
YM	0.6420	0.5030
YP	0.8020	0.5920
Z1	0.1210	0.1860
Z7	0.6970	0.5010
Z9	0.7040	0.5110
ZB	0.6920	0.5120
ZF	0.6520	0.4990
ZI	0.6510	0.4970
ZJ	0.1110	0.1350
ZK	0.1200	0.1850
ZL	0.1170	0.1330
ZM	0.6960	0.5210
ZP	0.7060	0.5470
a1	0.1050	0.1590
a7	0.7220	0.5080
a9	0.7300	0.5160
aB	0.1990	0.3080
aF	0.5610	0.4540
aI	0.5630	0.4590
aJ	0.1930	0.2190
aK	0.1040	0.1610
aL	0.1930	0.2200
aM	0.1980	0.3130
aP	0.7500	0.5660
b1	0.0540	0.0950
b7	0.4930	0.3940
b9	0.5000	0.3990
bB	0.6780	0.4980
bF	0.4800	0.4160
bI	0.4770	0.4160
bJ	0.2130	0.2240
bK	0.0580	0.0960
bL	0.2180	0.2330
bM	0.6720	0.4940
bP	0.7620	0.5710
c1	0.0800	0.1740
c7	0.4460	0.3870
c9	0.4560	0.3890
cB	0.1140	0.2190

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Chain	Atom inclusion	Q-score
cF	█ 0.4320	█ 0.4060
cI	█ 0.4340	█ 0.4080
cJ	█ 0.1850	█ 0.2160
cK	█ 0.0820	█ 0.1770
cL	█ 0.1810	█ 0.2220
cM	█ 0.1120	█ 0.2220
cP	█ 0.6940	█ 0.4970
d1	█ 0.0600	█ 0.1020
d4	█ 0.3220	█ 0.2860
d7	█ 0.5490	█ 0.4500
d9	█ 0.5460	█ 0.4520
dB	█ 0.1750	█ 0.2800
dD	█ 0.3520	█ 0.3250
dF	█ 0.3350	█ 0.3150
dI	█ 0.3390	█ 0.3170
dJ	█ 0.1360	█ 0.1860
dK	█ 0.0580	█ 0.1030
dL	█ 0.1350	█ 0.1850
dM	█ 0.1740	█ 0.2810
dP	█ 0.7500	█ 0.4920
e1	█ 0.0460	█ 0.0860
e2	█ 0.4980	█ 0.3770
e7	█ 0.6080	█ 0.4870
e9	█ 0.6100	█ 0.4870
eB	█ 0.3450	█ 0.3970
eF	█ 0.3620	█ 0.3580
eI	█ 0.3650	█ 0.3600
eJ	█ 0.1620	█ 0.1830
eK	█ 0.0460	█ 0.0880
eL	█ 0.1630	█ 0.1840
eM	█ 0.3470	█ 0.4040
eP	█ 0.6500	█ 0.4610
eR	█ 0.4730	█ 0.3480
f1	█ 0.0670	█ 0.1320
f7	█ 0.4800	█ 0.3960
f9	█ 0.4730	█ 0.3930
fB	█ 0.0900	█ 0.1660
fF	█ 0.2990	█ 0.3030
fI	█ 0.3020	█ 0.3040
fJ	█ 0.2530	█ 0.2880
fK	█ 0.0710	█ 0.1370
fL	█ 0.2580	█ 0.2890

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Chain	Atom inclusion	Q-score
fM	0.0870	0.1680
fP	0.7990	0.5580
g1	0.0660	0.1250
g7	0.4290	0.3880
g9	0.4310	0.3890
gB	0.0810	0.1520
gF	0.3770	0.3550
gI	0.3800	0.3540
gJ	0.1560	0.2020
gK	0.0630	0.1300
gL	0.1590	0.2010
gM	0.0750	0.1520
gP	0.7480	0.4980
h1	0.0380	0.0730
h7	0.5170	0.4340
h9	0.5190	0.4340
hB	0.1290	0.2340
hF	0.2280	0.2660
hI	0.2240	0.2640
hJ	0.1170	0.1620
hK	0.0350	0.0760
hL	0.1200	0.1580
hM	0.1310	0.2330
hP	0.7330	0.5150
i1	0.0470	0.1020
i7	0.6070	0.4830
i9	0.6000	0.4860
iB	0.2080	0.3100
iF	0.2440	0.2850
iI	0.2380	0.2850
iJ	0.2110	0.2480
iK	0.0480	0.1050
iL	0.2050	0.2490
iM	0.2070	0.3130
iP	0.7810	0.5350
j1	0.0410	0.0830
j7	0.4570	0.3850
j9	0.4500	0.3880
jB	0.1050	0.2080
jF	0.3400	0.3340
jI	0.3360	0.3320
jJ	0.2770	0.3000









































































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Chain	Atom inclusion	Q-score
jK	0.0450	0.0830
jL	0.2730	0.2990
jM	0.1050	0.2100
jP	0.7270	0.5150
k1	0.0310	0.1040
k6	0.7730	0.6030
k7	0.4560	0.3930
k9	0.4650	0.3960
kB	0.1410	0.2320
kF	0.4940	0.4310
kH	0.7760	0.6060
kI	0.4900	0.4330
kJ	0.0080	0.0370
kK	0.0330	0.1060
kL	0.0100	0.0400
kM	0.1390	0.2300
kP	0.8360	0.5830
l1	0.0250	0.0520
l7	0.5400	0.4290
l9	0.5560	0.4330
lB	0.2980	0.3490
lF	0.3900	0.3730
lI	0.3940	0.3760
lJ	0.0100	0.0320
lK	0.0250	0.0460
lL	0.0110	0.0310
lM	0.2950	0.3600
lP	0.7950	0.5530
m1	0.0320	0.0470
m7	0.5780	0.4660
m9	0.5710	0.4700
mB	0.2240	0.3160
mF	0.2740	0.2810
mI	0.2700	0.2860
mJ	0.0100	0.0360
mK	0.0320	0.0460
mL	0.0120	0.0350
mM	0.2240	0.3170
mP	0.7190	0.5090
nJ	0.0110	0.0220
nL	0.0110	0.0230
nP	0.7520	0.5010

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Chain	Atom inclusion	Q-score
oJ	 0.0150	 0.0220
oL	 0.0150	 0.0220
oP	 0.7500	 0.5240
pJ	 0.0160	 0.0280
pL	 0.0140	 0.0250
pP	 0.8230	 0.5750
qJ	 0.0140	 0.0500
qL	 0.0120	 0.0470
qP	 0.7130	 0.5040
rJ	 0.0160	 0.0620
rL	 0.0150	 0.0630
rP	 0.7860	 0.5290
sJ	 0.0150	 0.0450
sL	 0.0130	 0.0460
sP	 0.8290	 0.5650
tJ	 0.0130	 0.0390
tL	 0.0130	 0.0360
tP	 0.7830	 0.5350
uJ	 0.0120	 0.0080
uL	 0.0080	 0.0100
uP	 0.8200	 0.5630
vJ	 0.0180	 0.0660
vL	 0.0160	 0.0630
vP	 0.7870	 0.5260
wJ	 0.2660	 0.2830
wL	 0.2670	 0.2880
wP	 0.8620	 0.5950
xJ	 0.0110	 0.0530
xL	 0.0120	 0.0400
xP	 0.7400	 0.5590
yJ	 0.6260	 0.5070
yL	 0.6230	 0.5050
yP	 0.7810	 0.5880
zJ	 0.7150	 0.5140
zL	 0.7130	 0.5130
zP	 0.8450	 0.6020