



wwPDB NMR Structure Validation Summary Report ⓘ

Mar 15, 2026 – 03:35 PM UTC

PDB ID : 2V93 / pdb_00002v93
Title : EQUILLIBRIUM MIXTURE OF OPEN AND PARTIALLY-CLOSED SPECIES IN THE APO STATE OF MALTODEXTRIN-BINDING PROTEIN BY PARAMAGNETIC RELAXATION ENHANCEMENT NMR
Authors : Clore, G.M.; Tang, C.
Deposited on : 2007-08-21

This is a wwPDB NMR Structure 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/NMRValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

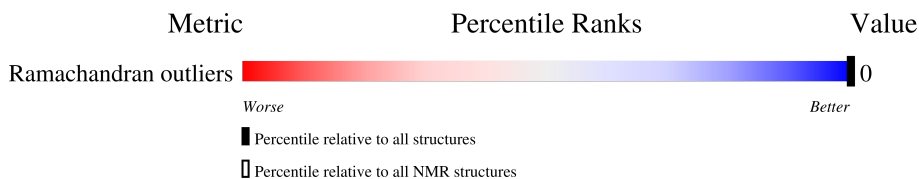
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR

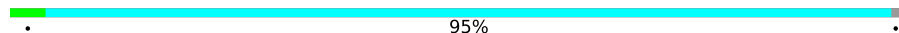
The overall completeness of chemical shifts assignment was not calculated.

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)	NMR archive (#Entries)
Ramachandran outliers	224038	12848

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	370	

2 Ensemble composition and analysis

This entry contains 50 models. The atoms present in the NMR models are not consistent. Some calculations may have failed as a result. All residues are included in the validation scores. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:81-A:87, A:103-A:105, A:266-A:268, A:311-A:313 (16)	0.00	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

NmrClust was unable to cluster the ensemble.

Error message: No clusters in NmrClust output

3 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 3792 atoms, of which 1003 are hydrogens and 0 are deuteriums.

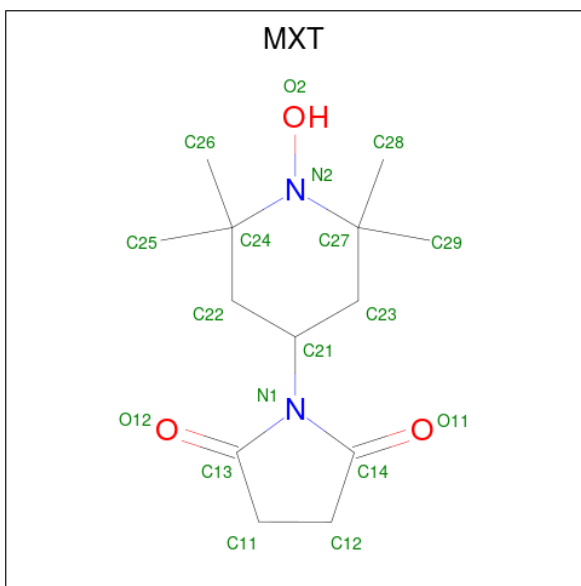
- Molecule 1 is a protein called MALTOSE-BINDING PERIPLASMIC PROTEIN.

Mol	Chain	Residues	Atoms					Trace	
			Total	C	H	N	O		S
1	A	366	2904	1169	547	583	581	24	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	CYS	ASP	engineered mutation	UNP P0AEY0
A	211	CYS	SER	engineered mutation	UNP P0AEY0

- Molecule 2 is 1-(1-HYDROXY-2,2,6,6-TETRAMETHYLPYRROLIDIN-4-YL)PYRROLIDIN E-2,5-DIONE (CCD ID: MXT) (formula: $C_{13}H_{22}N_2O_3$).



Mol	Chain	Residues	Atoms				
			Total	C	H	N	O
2	A	1	444	156	228	24	36
2	A	1	444	156	228	24	36

E309	L247	G187	K127
E310	P248	A188	T128
D314	T249	K189	W129
P315	F250	A190	E130
R316	K251	G191	E131
I317	G252	L192	I132
A318	Q253	T193	P133
A319	P254	F194	A134
T320	S255	L195	L135
M321	K256	V196	D136
E322	P257	D197	K137
M323	F258	L198	E138
A324	V259	I199	L139
Q325	G260	K200	K140
K326	V261	N201	A141
G327	L262	K202	K142
E328	S263	H203	G143
I329	A264	M204	K144
M330	G265	N205	S145
P331	A269	A206	A146
N332	S270	D207	L147
I333	P271	T208	M148
P334	N272	D209	F149
Q335	K273	Y210	N150
M336	E274	C211	L151
S337	L275	I212	Q152
F339	A276	A213	E153
W340	K277	E214	P154
Y341	E278	A215	Y155
A342	F279	A216	F156
V343	L280	F217	T157
R344	E281	N218	W158
T345	M282	K219	P159
A346	Y283	G220	L160
V347	L284	E221	I161
I348	L285	T222	A162
M349	T286	M224	A163
A350	D287	G165	D164
A351	E288	T225	G166
G353	G289	N227	Y167
R354	L290	G228	A168
Q355	E291	P229	F169
T356	V293	W230	K170
V357	M294	A231	Y171
D358	K295	W232	E172
E359	D296	S233	M173
A360	K297	N234	G174
L361	P298	I235	K175
K362	L299	D236	Y176
D363	G300	T237	D177
A364	A301	S238	I178
Q365	V302	K239	K179
T366	A303	V240	D180
R367	L304	M241	V181
I368	K305	Y242	G182
T369	S306	G243	V183
K370	Y307	V244	D184
	E308	T245	M185
		A246	A186

5 Refinement protocol and experimental data overview

The models were refined using the following method: *CONJOINED RIGID BODY/TORSION ANGLE SIMULATED ANNEALING DYNAMICS*.

Of the 100 calculated structures, 50 were deposited, based on the following criterion: *PRE AND VDW ENERGIES*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
NIH	refinement	
Xplor-NIH	structure solution	

No chemical shift data was provided.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MXT

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#Z>5	RMSZ	#Z>5
1	A	1.55±0.00	0±0/64 (0.0± 0.0%)	2.12±0.01	2±0/80 (2.5± 0.0%)
All	All	1.55	0/3200 (0.0%)	2.12	100/4000 (2.5%)

There are no bond-length outliers.

All unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
1	A	83	LYS	CA-C-N	5.08	127.08	120.28	1	50
1	A	83	LYS	C-N-CA	5.08	127.08	120.28	1	50

There are no chirality outliers.

There are no planarity outliers.

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes averaged over the ensemble.

Mol	Chain	Non-H	H(model)	H(added)	Clashes
1	A	-2113	-424	14	0±0
2	A	432	456	500	14±4
All	All	-84050	1600	25663	696

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

5 of 139 unique clashes are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Clash(Å)	Distance(Å)	Models	
				Worst	Total
2:A:402[A]:MXT:O11	2:A:402[A]:MXT:H231	0.83	1.73	29	11
2:A:402[B]:MXT:O11	2:A:402[B]:MXT:H231	0.83	1.73	46	12
2:A:401[F]:MXT:H231	2:A:401[F]:MXT:O11	0.83	1.73	24	12
2:A:401[D]:MXT:O11	2:A:401[D]:MXT:H231	0.83	1.73	10	14
2:A:401[A]:MXT:O11	2:A:401[A]:MXT:H231	0.82	1.75	24	6

6.3 Torsion angles [i](#)

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	16/370 (4%)	15±0 (94±0%)	1±0 (6±0%)	0±0 (0±0%)	100	100
All	All	800/18500 (4%)	750 (94%)	50 (6%)	0 (0%)	100	100

There are no Ramachandran outliers.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	0	-	-	-
All	All	0	-	-	-

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

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

Mol	Type	Chain	Res	Link	Bond lengths		
					Counts	RMSZ	#Z>2
2	MXT	A	401[D]	1	19,19,19	1.81±0.00	5±0 (26±0%)
2	MXT	A	401[C]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[E]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[V]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[Y]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[C]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[Y]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[W]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[X]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[A]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[Z]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[Z]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	402[V]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[U]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[F]	1	19,19,19	1.84±0.00	5±0 (26±0%)
2	MXT	A	401[U]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	401[B]	1	19,19,19	1.83±0.00	5±0 (26±0%)
2	MXT	A	402[B]	1	19,19,19	1.82±0.00	5±0 (26±0%)

Mol	Type	Chain	Res	Link	Counts	Bond lengths	
						RMSZ	#Z>2
2	MXT	A	402[A]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[X]	1	19,19,19	1.81±0.00	5±0 (26±0%)
2	MXT	A	401[E]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[F]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	401[W]	1	19,19,19	1.82±0.00	5±0 (26±0%)
2	MXT	A	402[D]	1	19,19,19	1.82±0.00	5±0 (26±0%)

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	MXT	A	401[D]	1	27,31,31	1.22±0.01	4±0 (13±1%)
2	MXT	A	401[C]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	402[E]	1	27,31,31	1.25±0.01	4±0 (14±1%)
2	MXT	A	401[V]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	402[Y]	1	27,31,31	1.25±0.01	4±0 (14±1%)
2	MXT	A	402[C]	1	27,31,31	1.24±0.01	4±0 (14±0%)
2	MXT	A	401[Y]	1	27,31,31	1.22±0.01	3±1 (10±2%)
2	MXT	A	402[W]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	402[X]	1	27,31,31	1.25±0.01	4±0 (13±1%)
2	MXT	A	401[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	402[Z]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	401[Z]	1	27,31,31	1.24±0.01	4±0 (14±1%)
2	MXT	A	402[V]	1	27,31,31	1.21±0.01	3±1 (11±2%)
2	MXT	A	402[U]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	401[F]	1	27,31,31	1.24±0.01	4±0 (13±1%)
2	MXT	A	401[U]	1	27,31,31	1.23±0.01	3±0 (11±1%)
2	MXT	A	401[B]	1	27,31,31	1.23±0.01	3±0 (12±1%)
2	MXT	A	402[B]	1	27,31,31	1.21±0.01	3±0 (11±1%)
2	MXT	A	402[A]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	401[X]	1	27,31,31	1.22±0.01	4±0 (13±1%)

Mol	Type	Chain	Res	Link	Counts	Bond angles	
						RMSZ	#Z>2
2	MXT	A	401[E]	1	27,31,31	1.22±0.01	3±1 (11±1%)
2	MXT	A	402[F]	1	27,31,31	1.21±0.01	3±1 (10±2%)
2	MXT	A	401[W]	1	27,31,31	1.23±0.01	3±0 (11±0%)
2	MXT	A	402[D]	1	27,31,31	1.25±0.01	4±0 (13±1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MXT	A	401[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[C]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[D]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[V]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[B]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[W]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[Z]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[F]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[A]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[Y]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[X]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[U]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	402[E]	1	-	0±0,4,39,39	0±0,2,2,2
2	MXT	A	401[C]	1	-	0±0,4,39,39	0±0,2,2,2

5 of 120 unique bond outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	401[A]	MXT	O2-N2	3.84	1.22	1.43	24	50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)	Models	
								Worst	Total
2	A	402[D]	MXT	O2-N2	3.84	1.22	1.43	49	50
2	A	401[U]	MXT	O2-N2	3.84	1.22	1.43	17	50
2	A	402[C]	MXT	O2-N2	3.84	1.22	1.43	21	50
2	A	402[U]	MXT	O2-N2	3.84	1.22	1.43	9	50

5 of 94 unique angle outliers are listed below. They are sorted according to the Z-score of the worst occurrence in the ensemble.

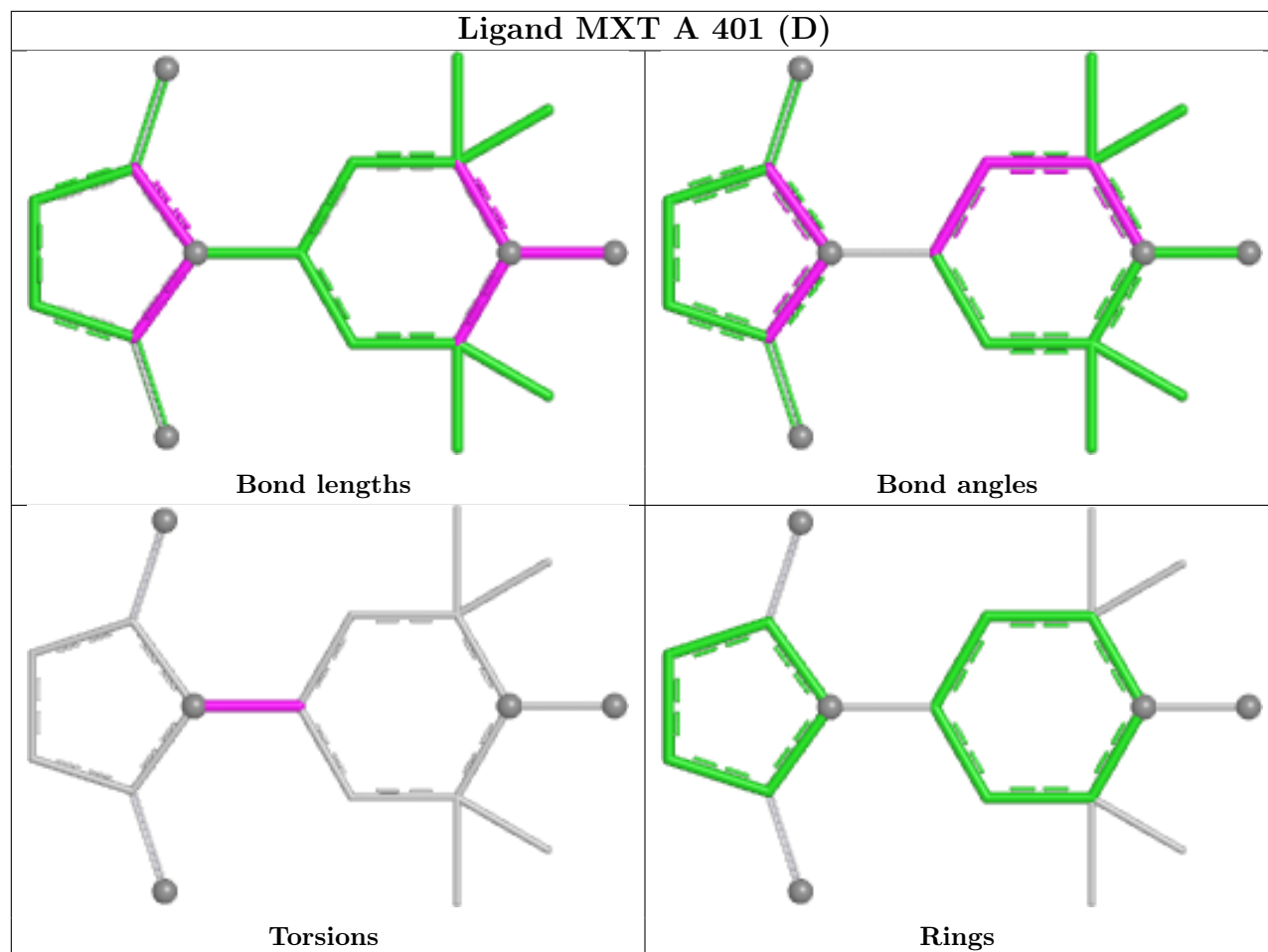
Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)	Models	
								Worst	Total
2	A	402[X]	MXT	C13-N1-C14	3.73	110.14	112.48	31	50
2	A	402[D]	MXT	C13-N1-C14	3.68	110.17	112.48	1	50
2	A	402[E]	MXT	C13-N1-C14	3.67	110.17	112.48	45	50
2	A	402[Y]	MXT	C13-N1-C14	3.66	110.18	112.48	38	50
2	A	401[F]	MXT	C13-N1-C14	3.63	110.20	112.48	33	50

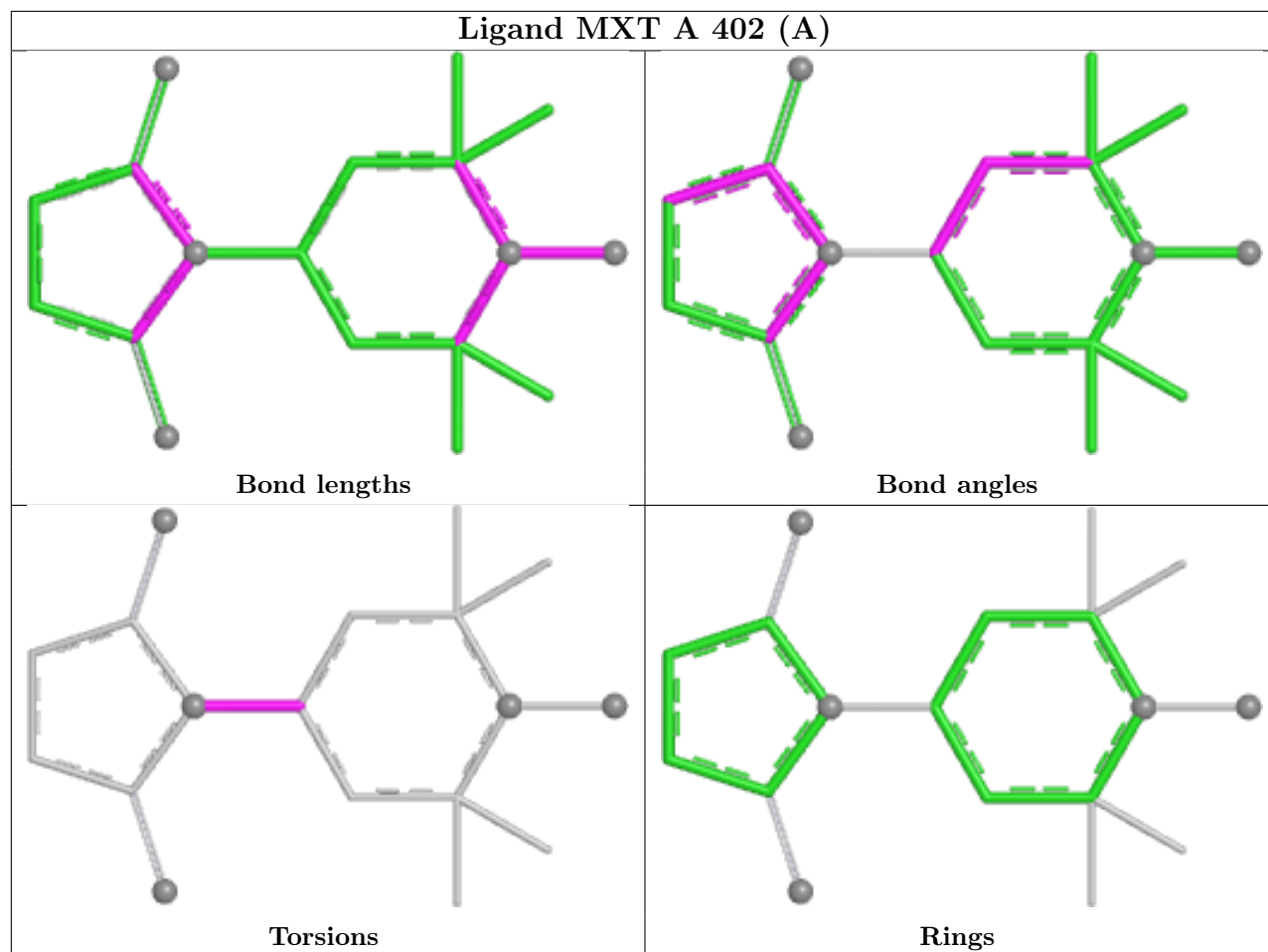
There are no chirality outliers.

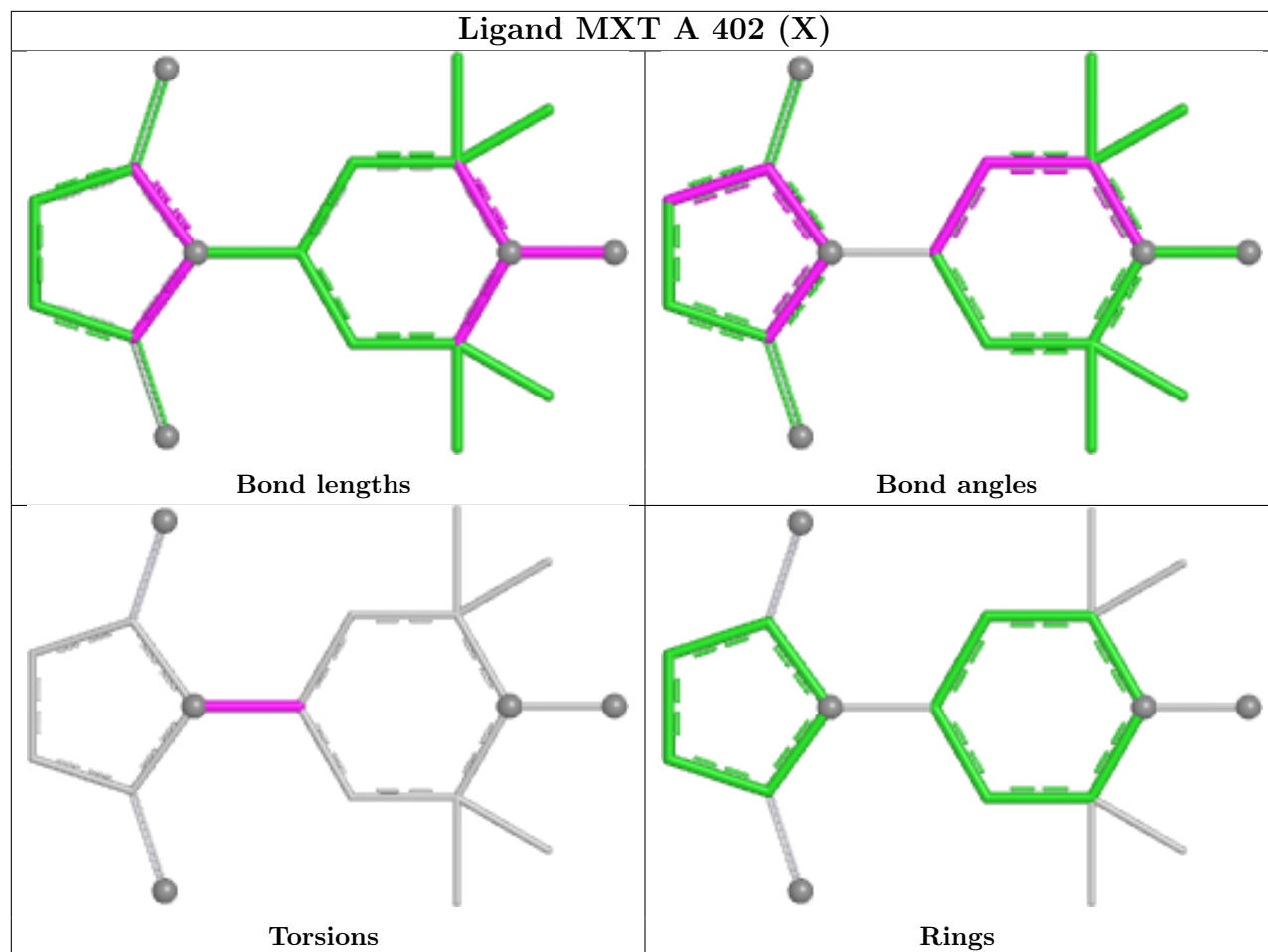
There are no torsion outliers.

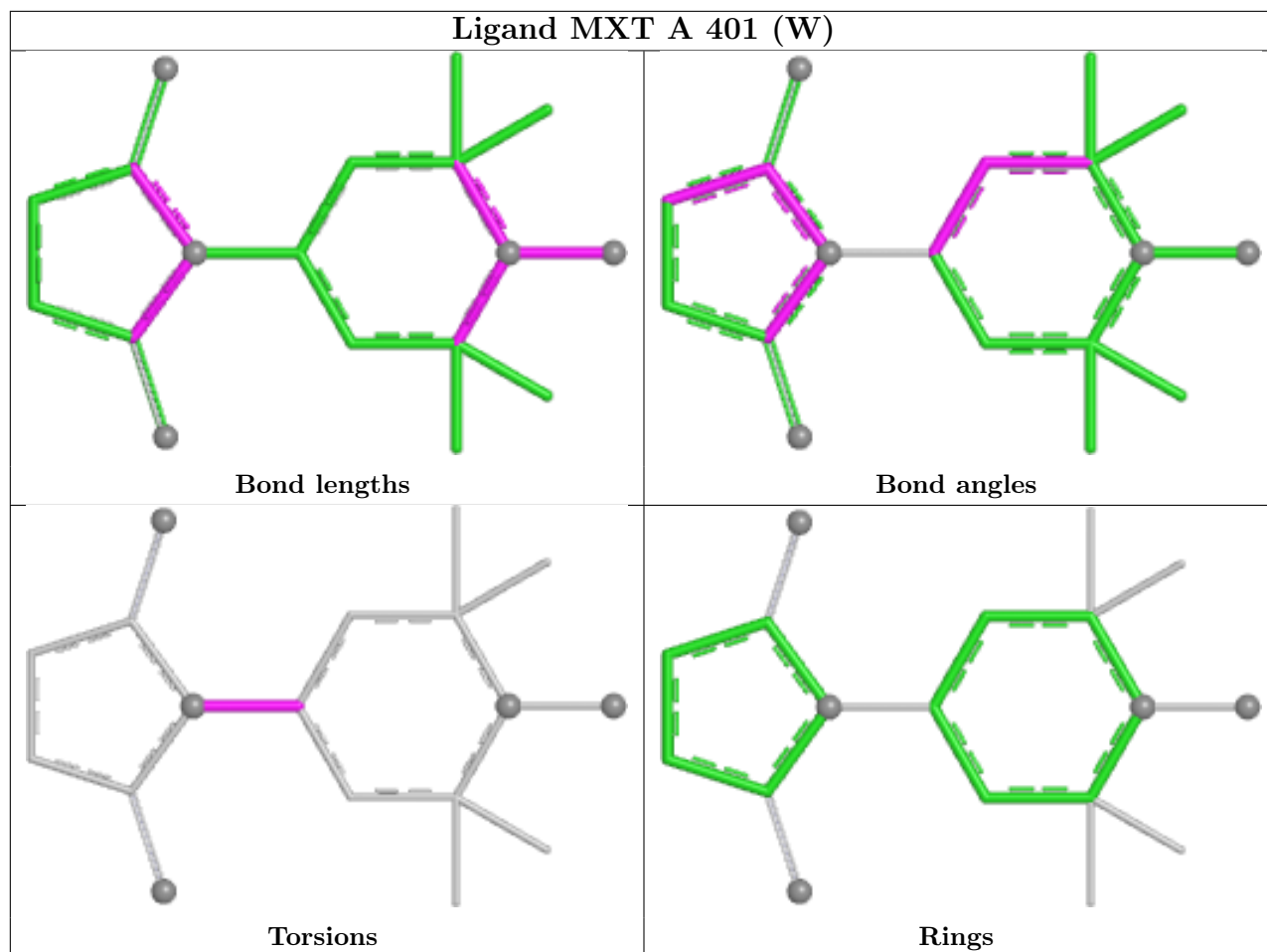
There are no ring outliers.

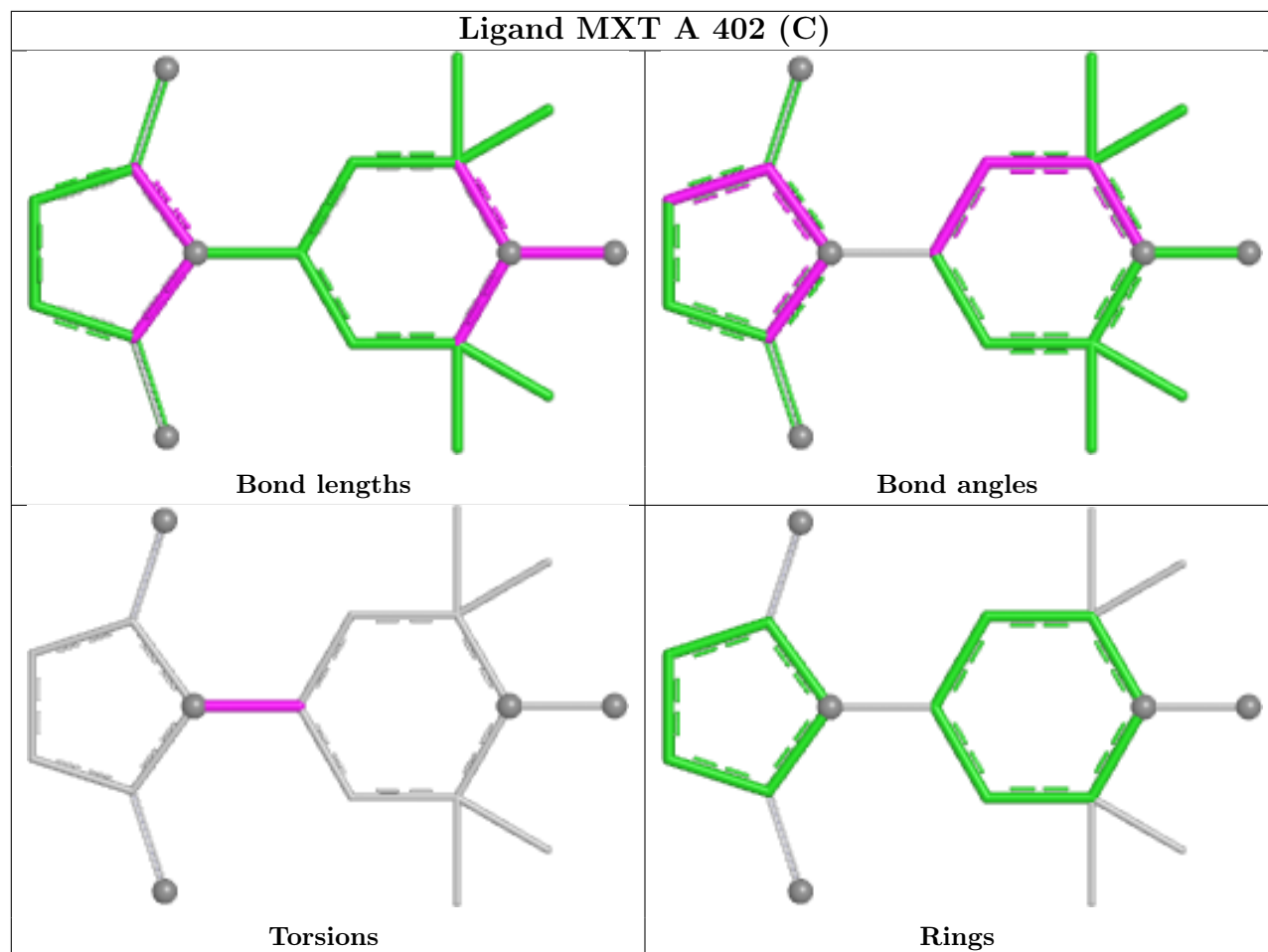
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

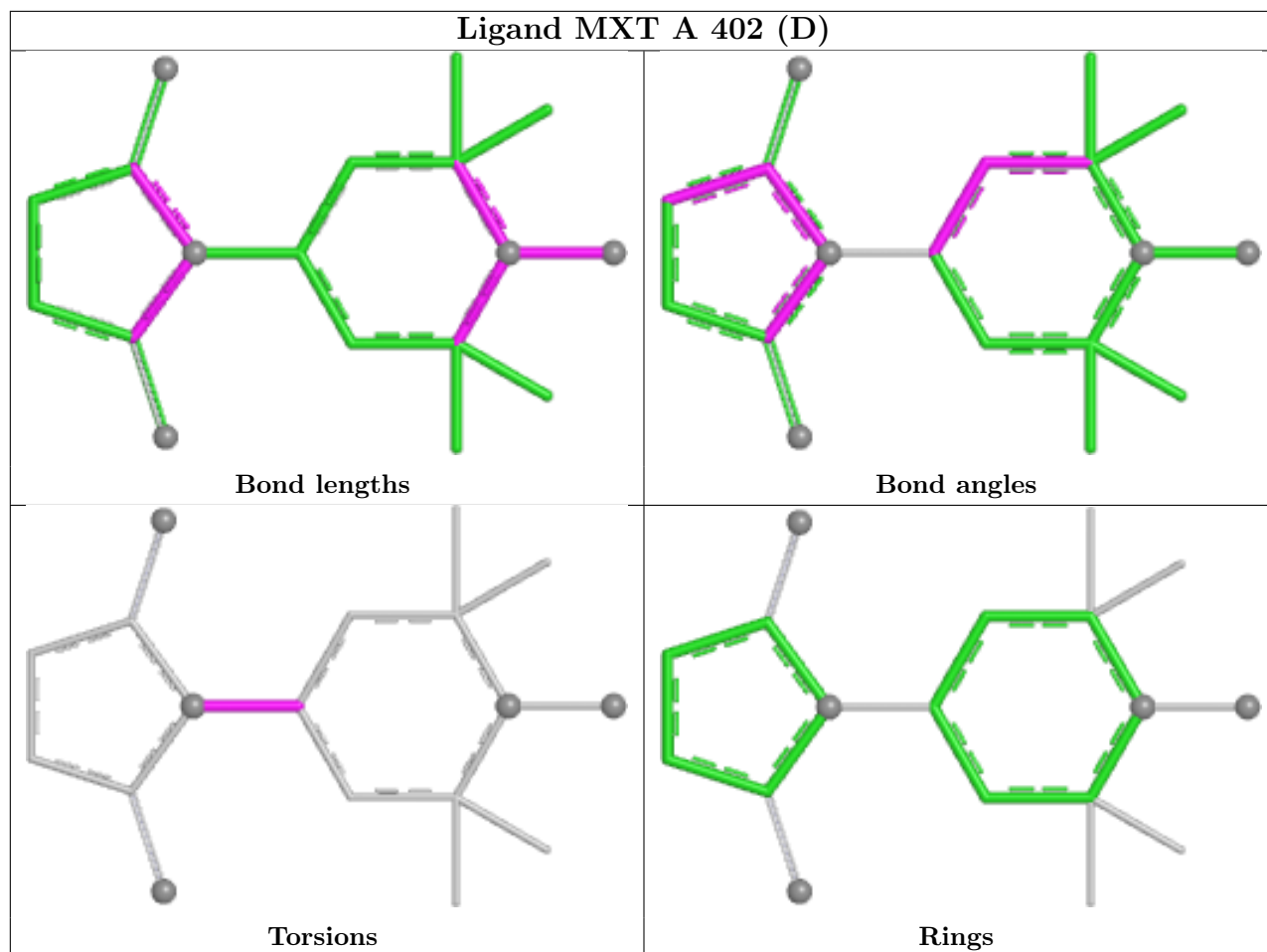


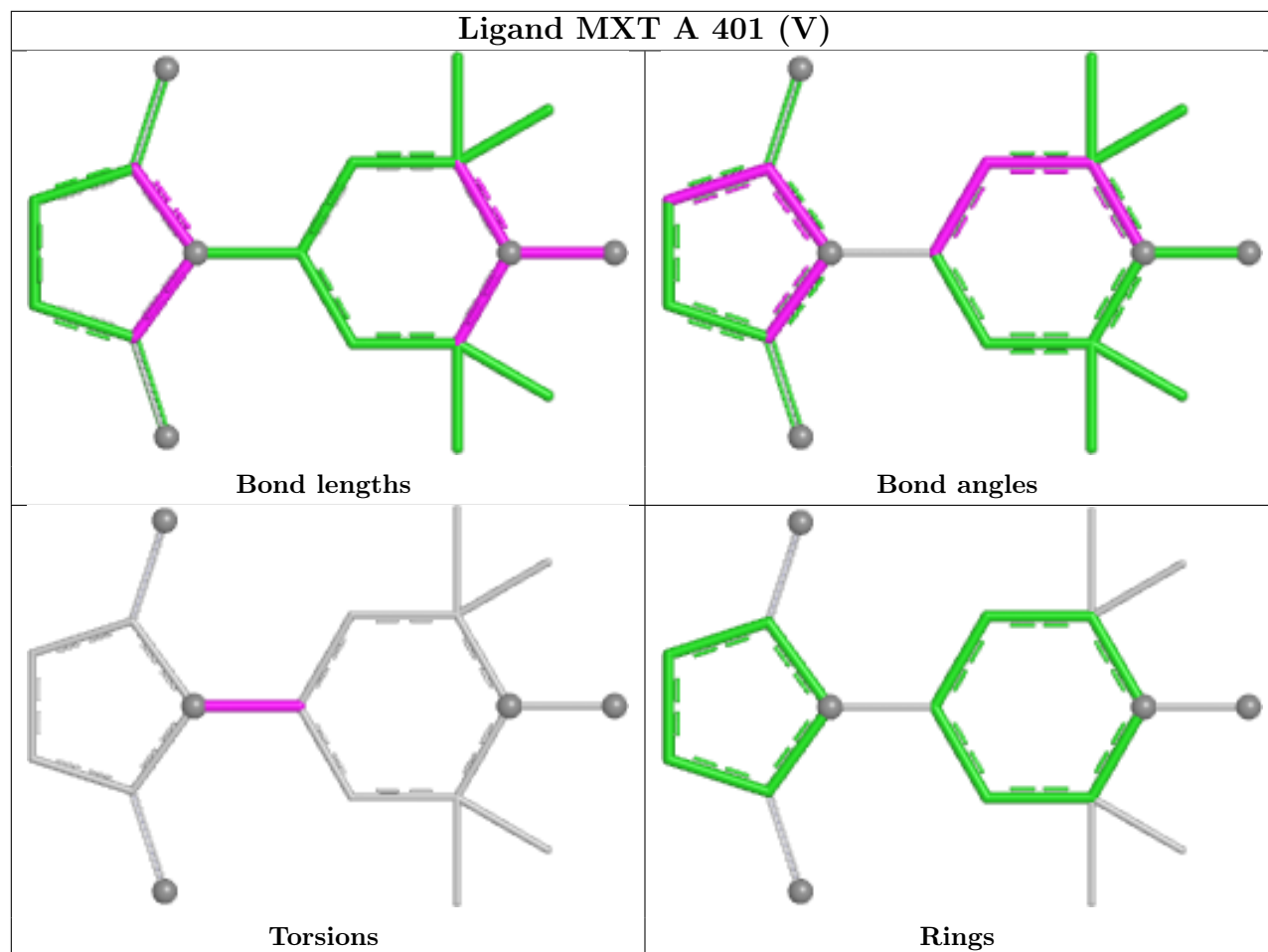


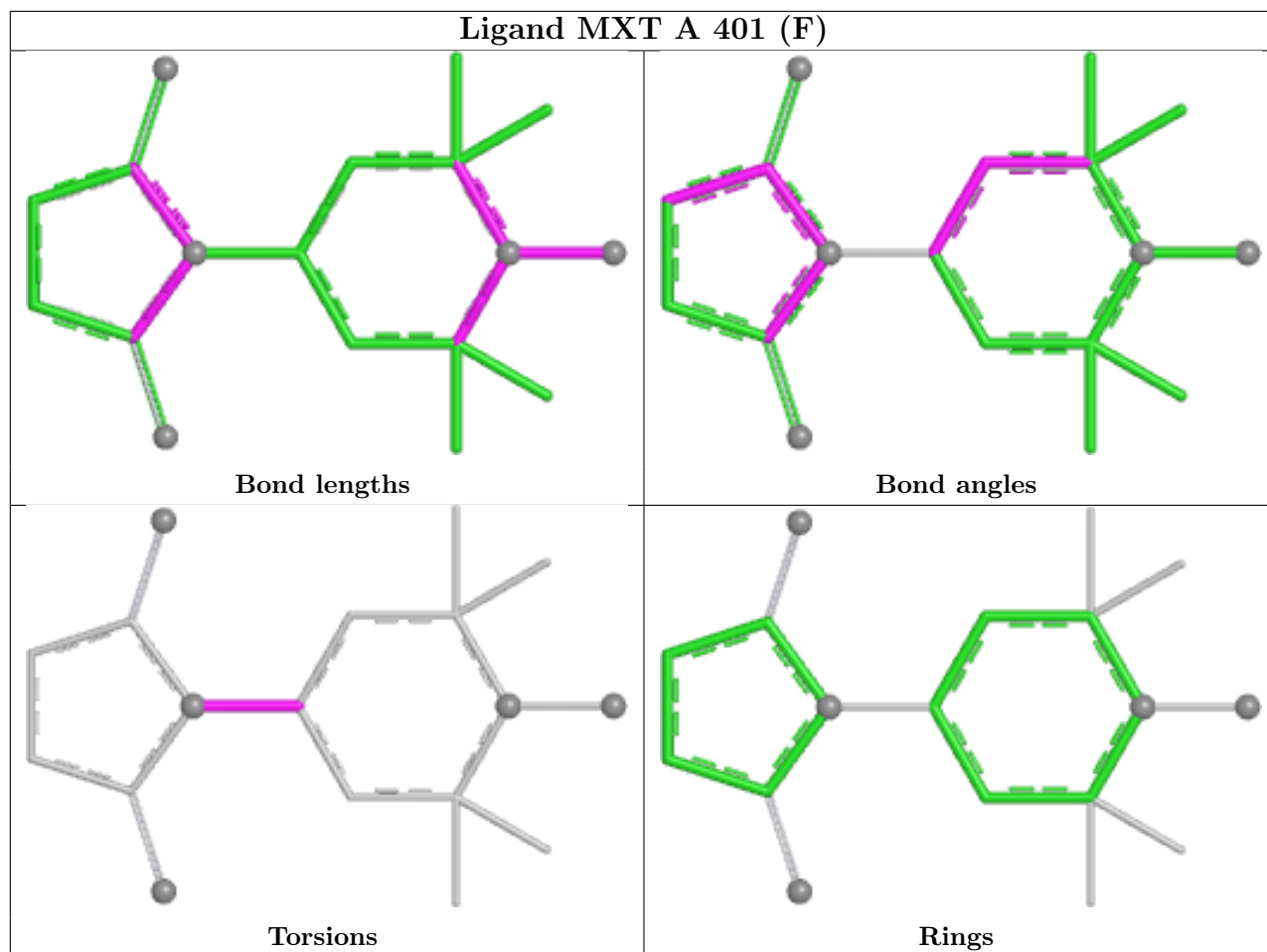


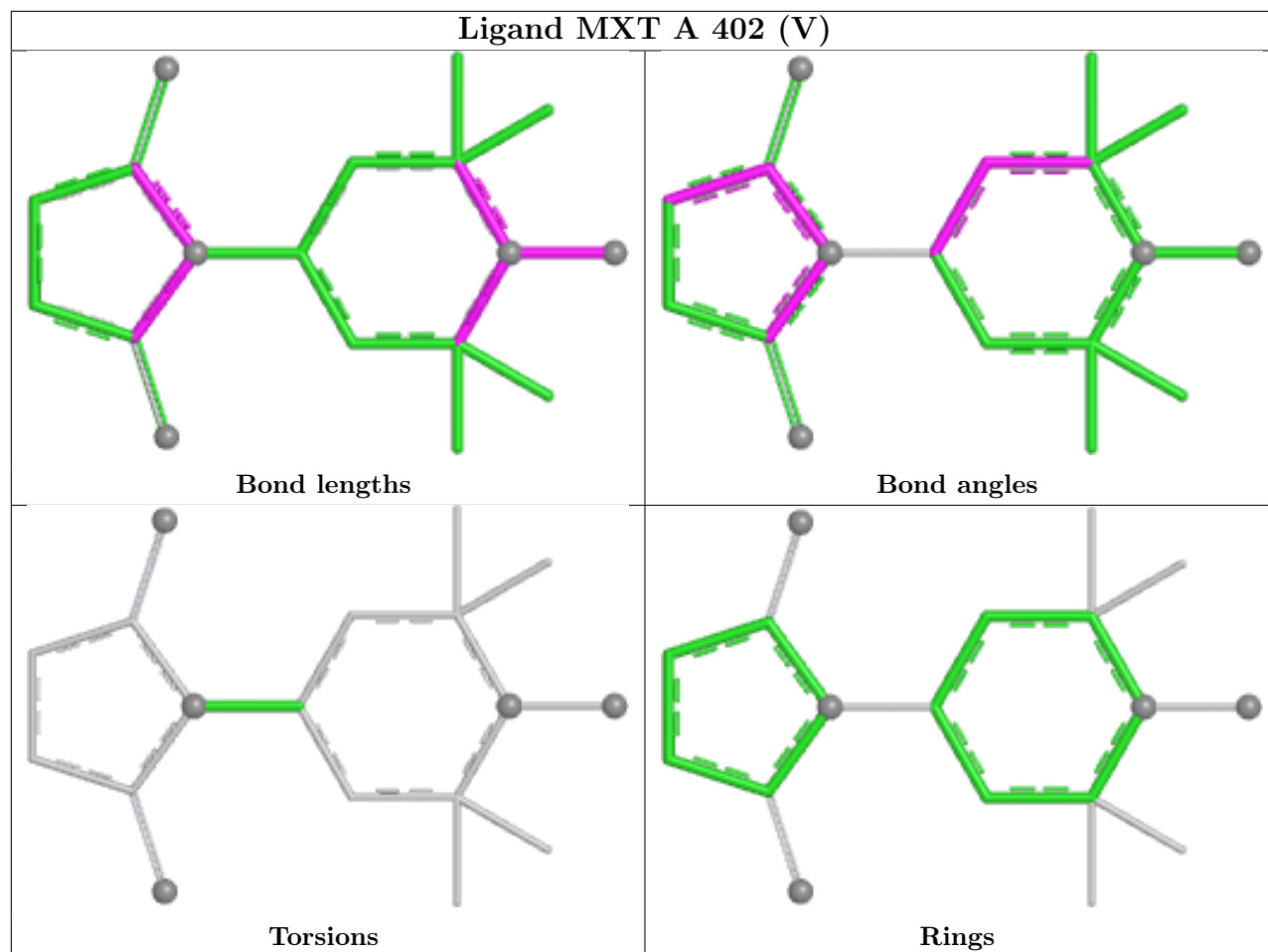


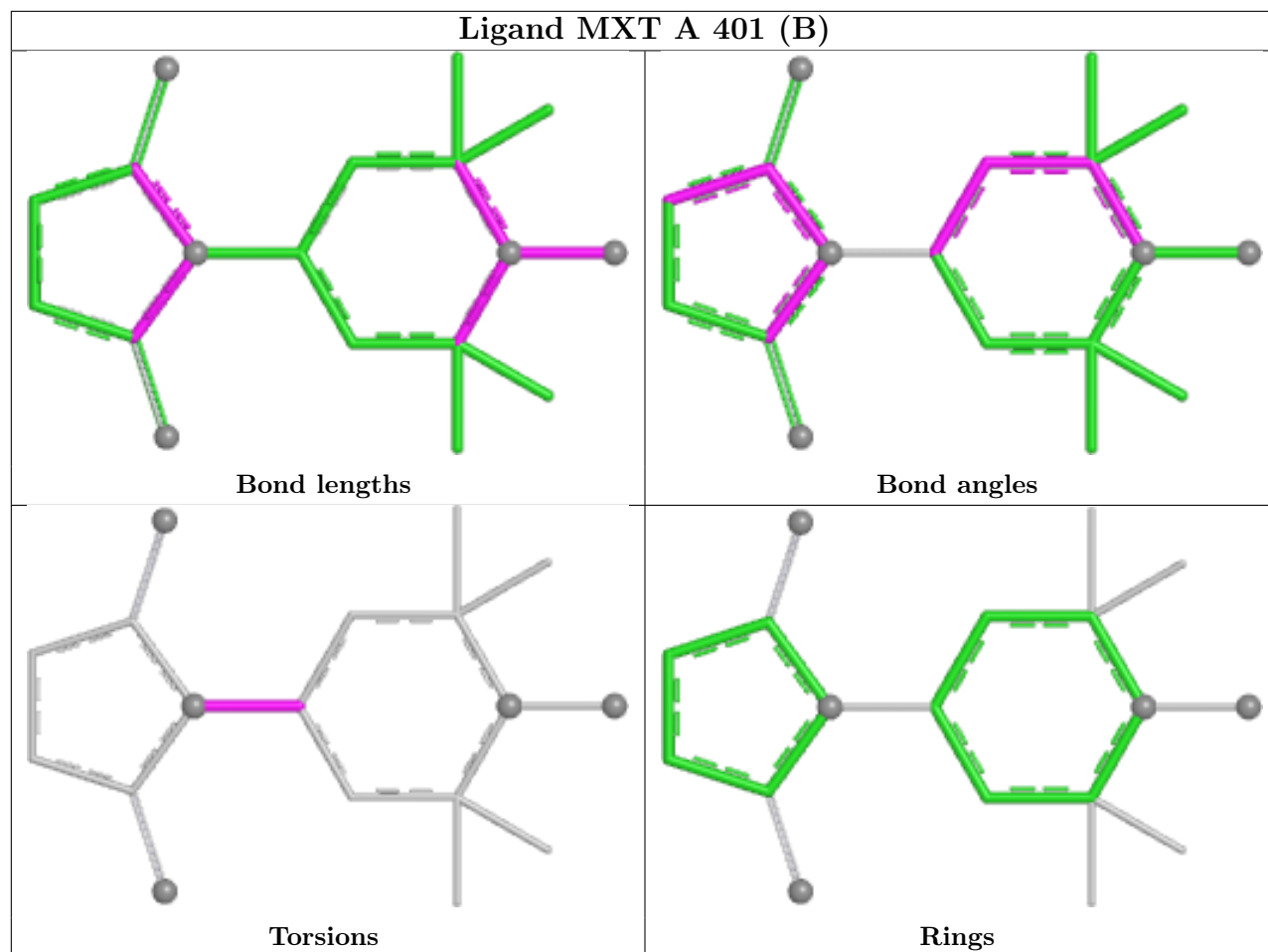


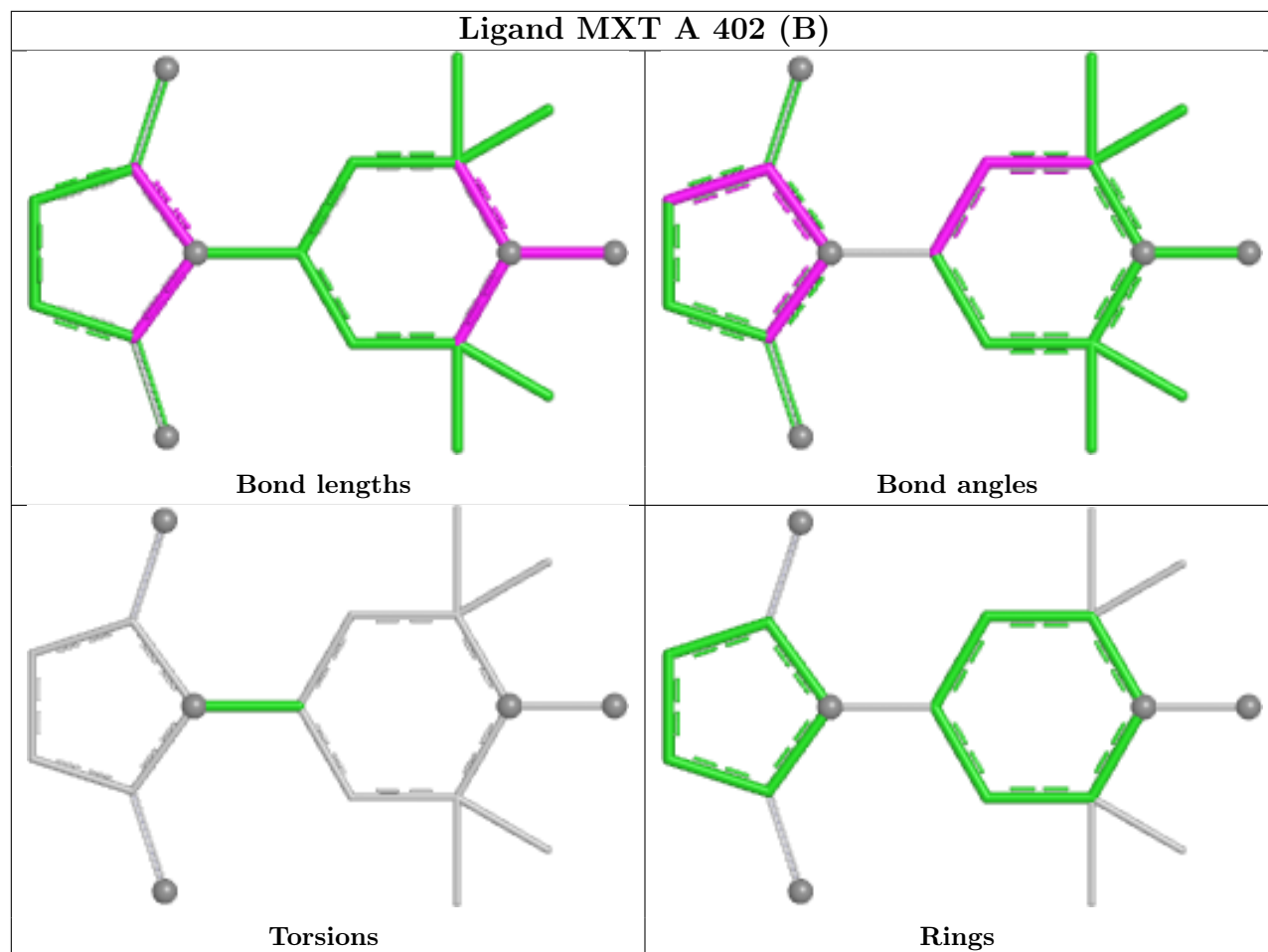


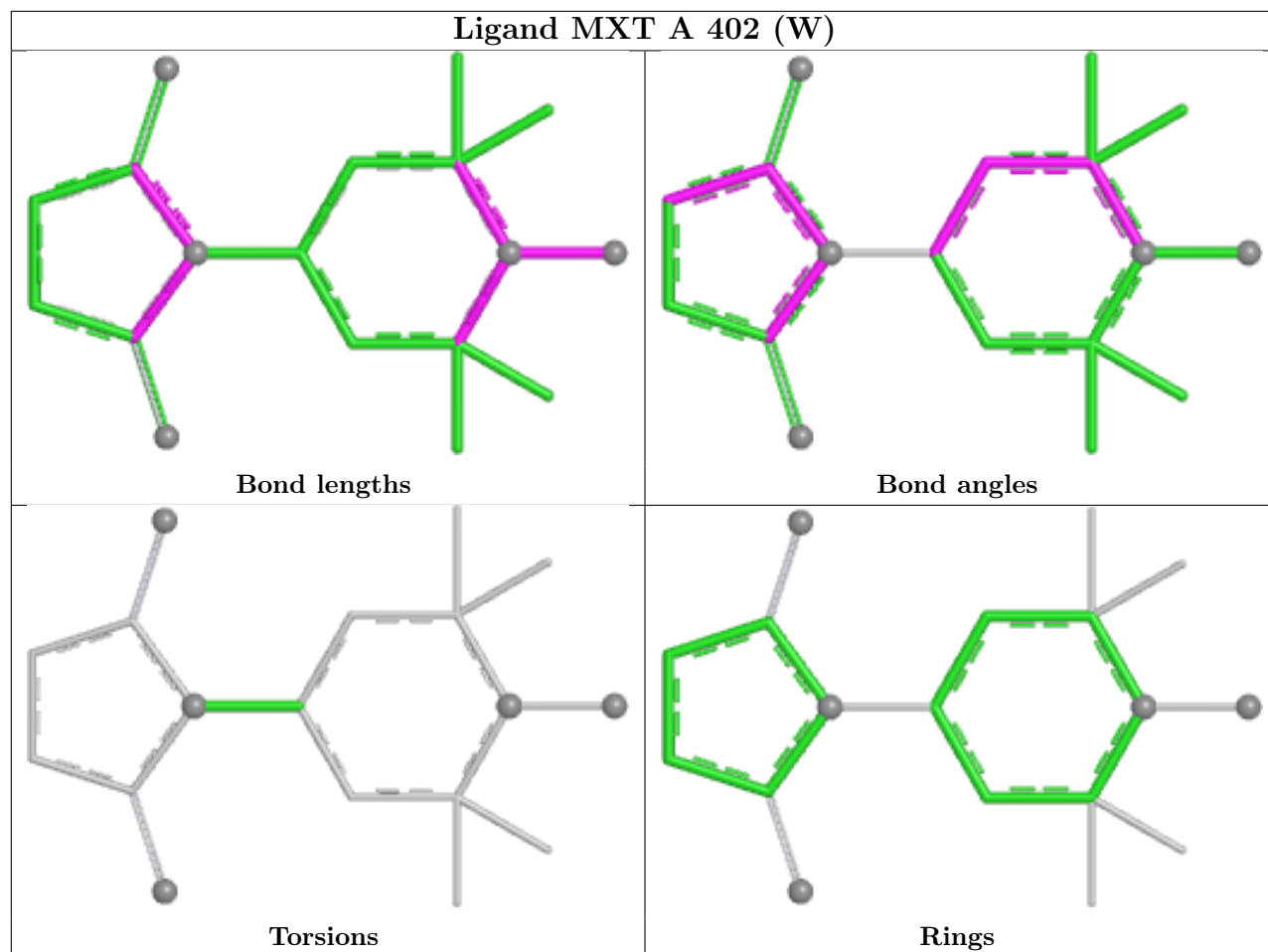


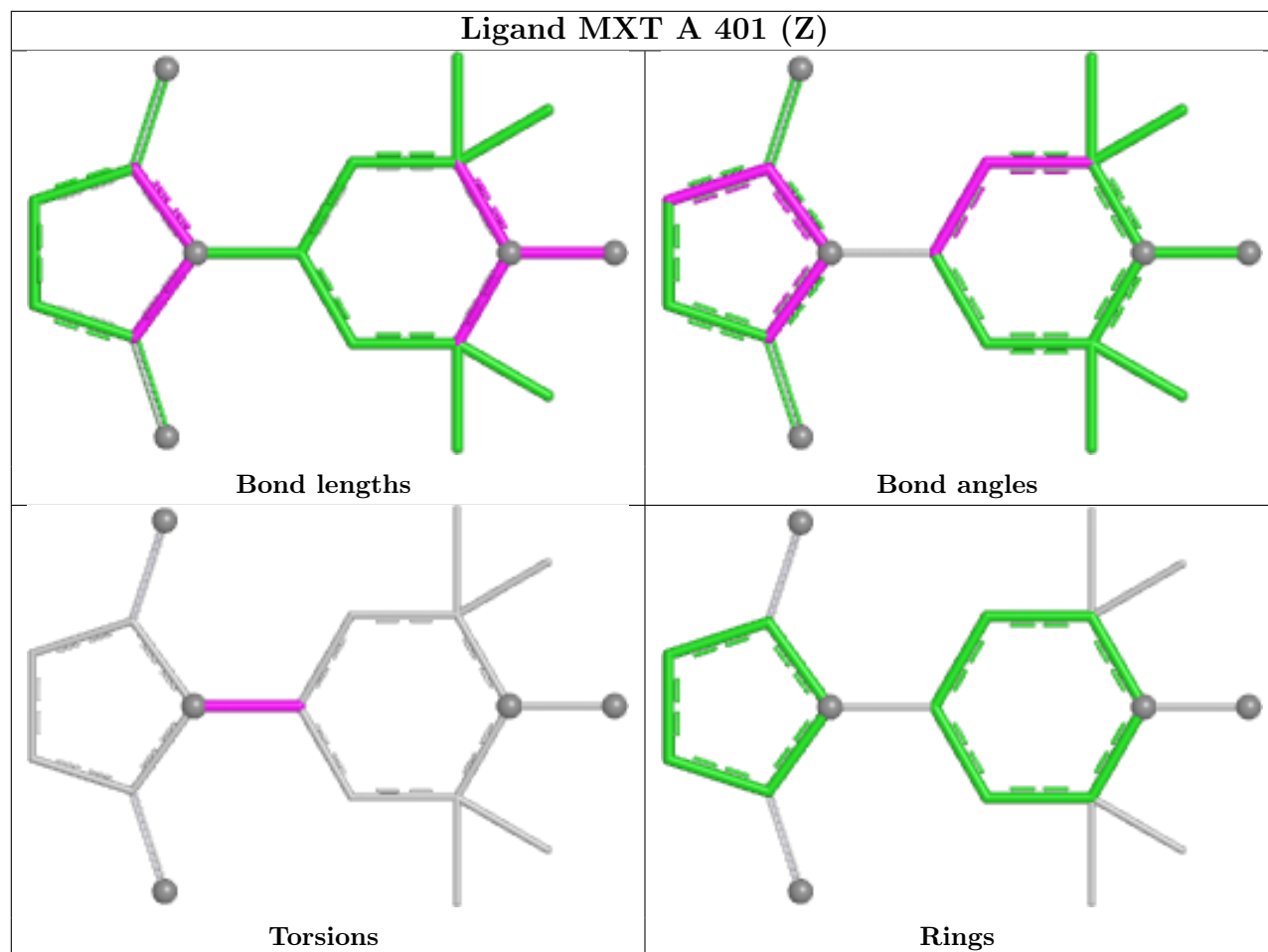


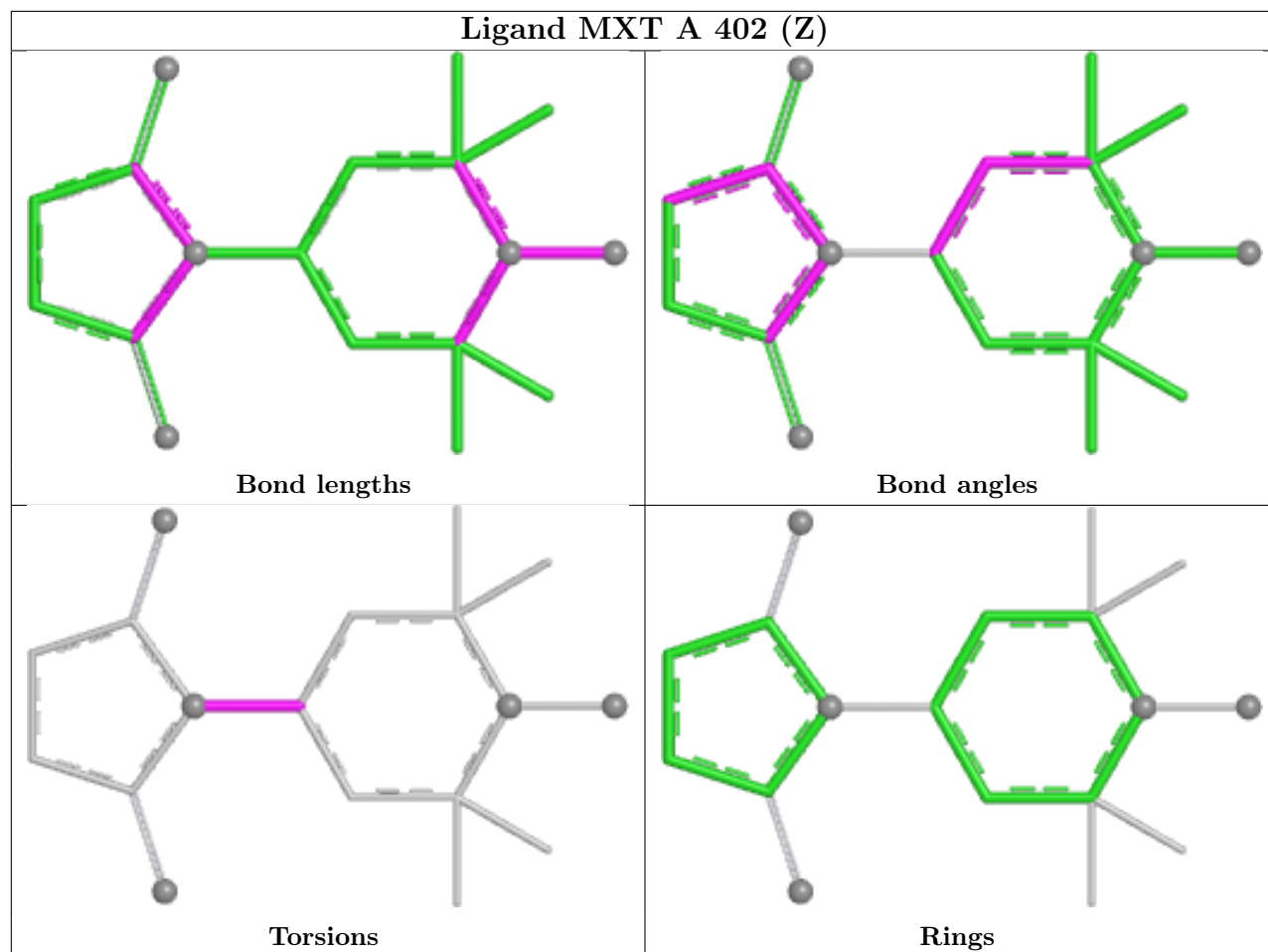


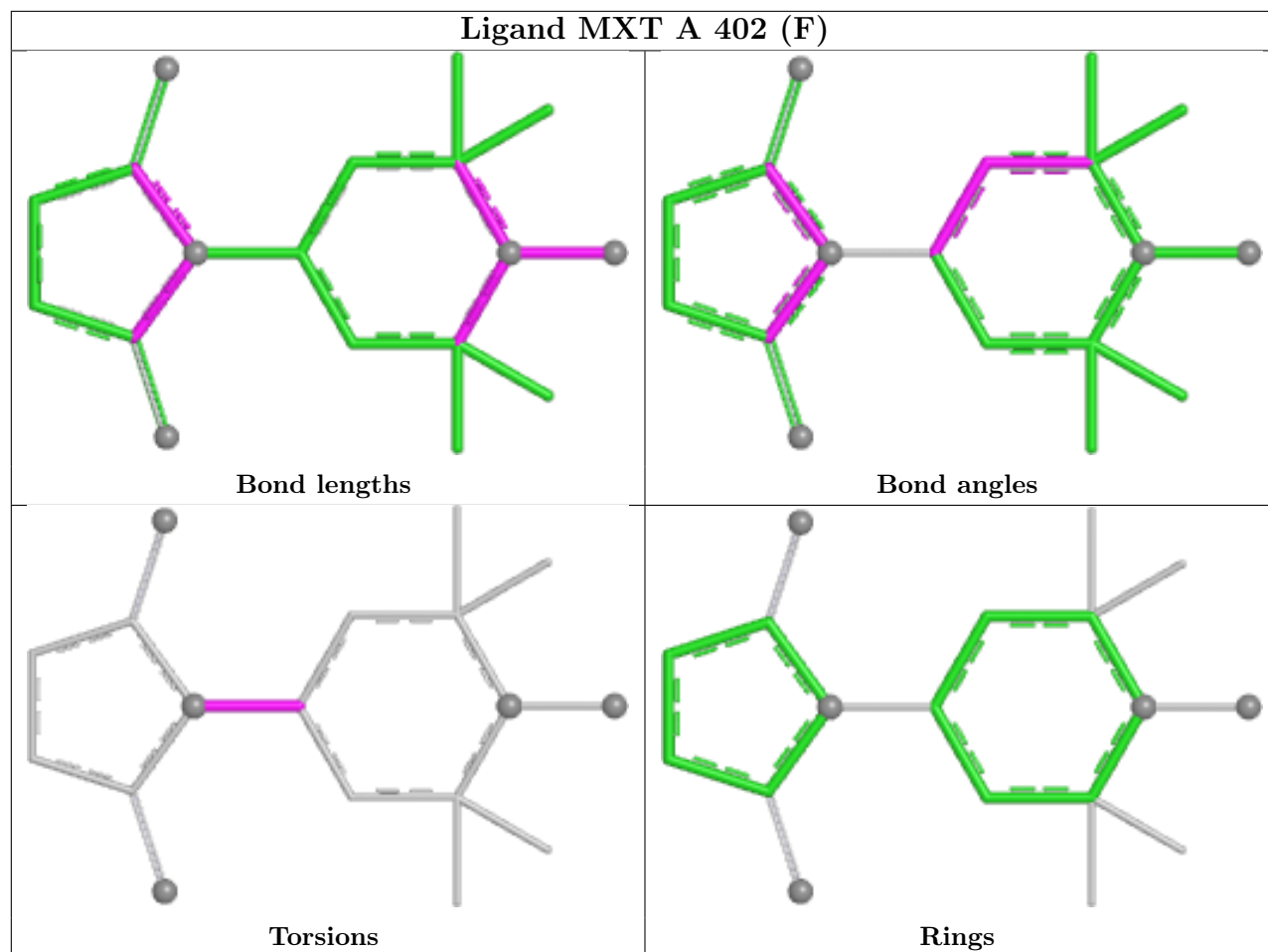


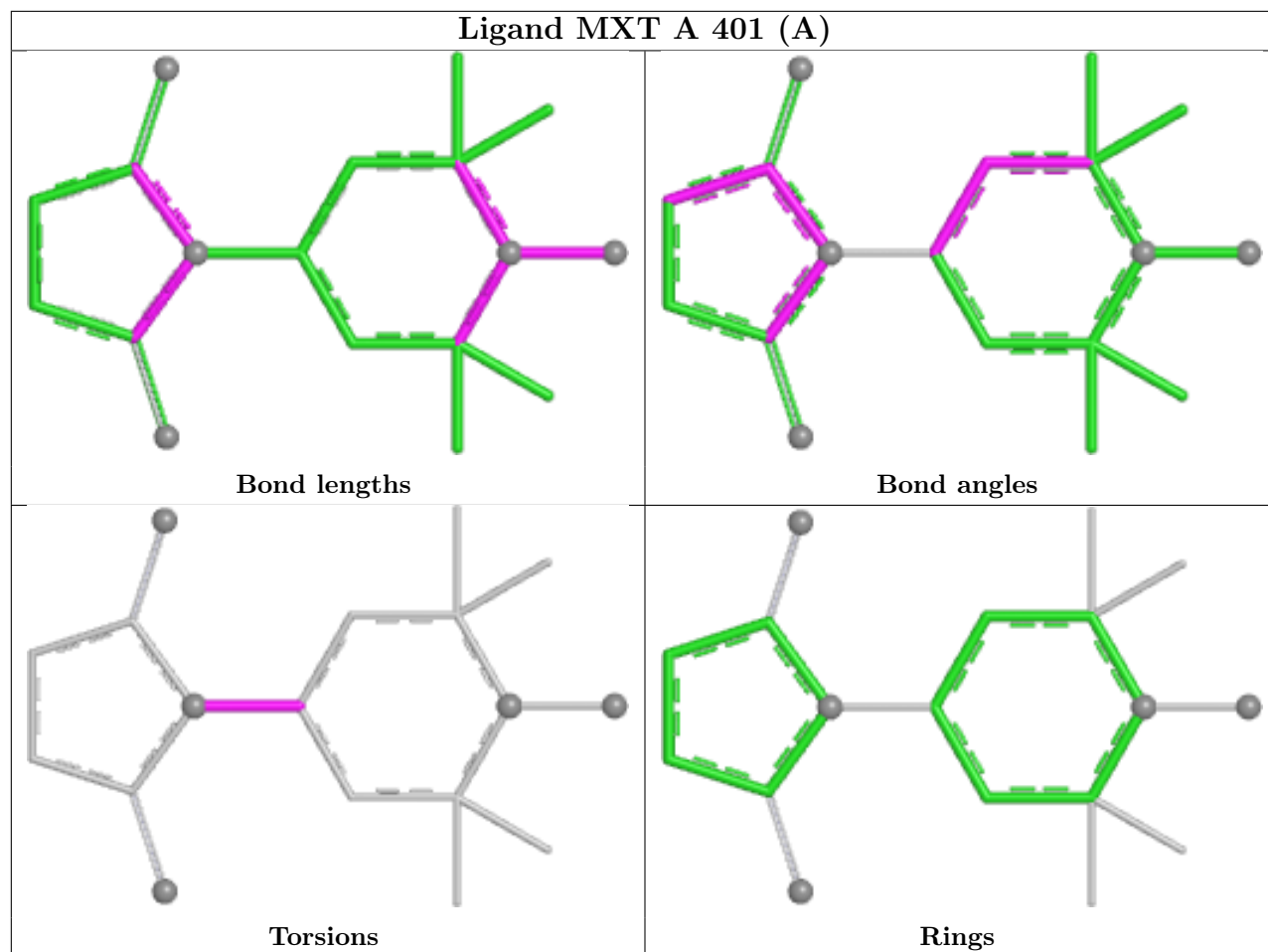


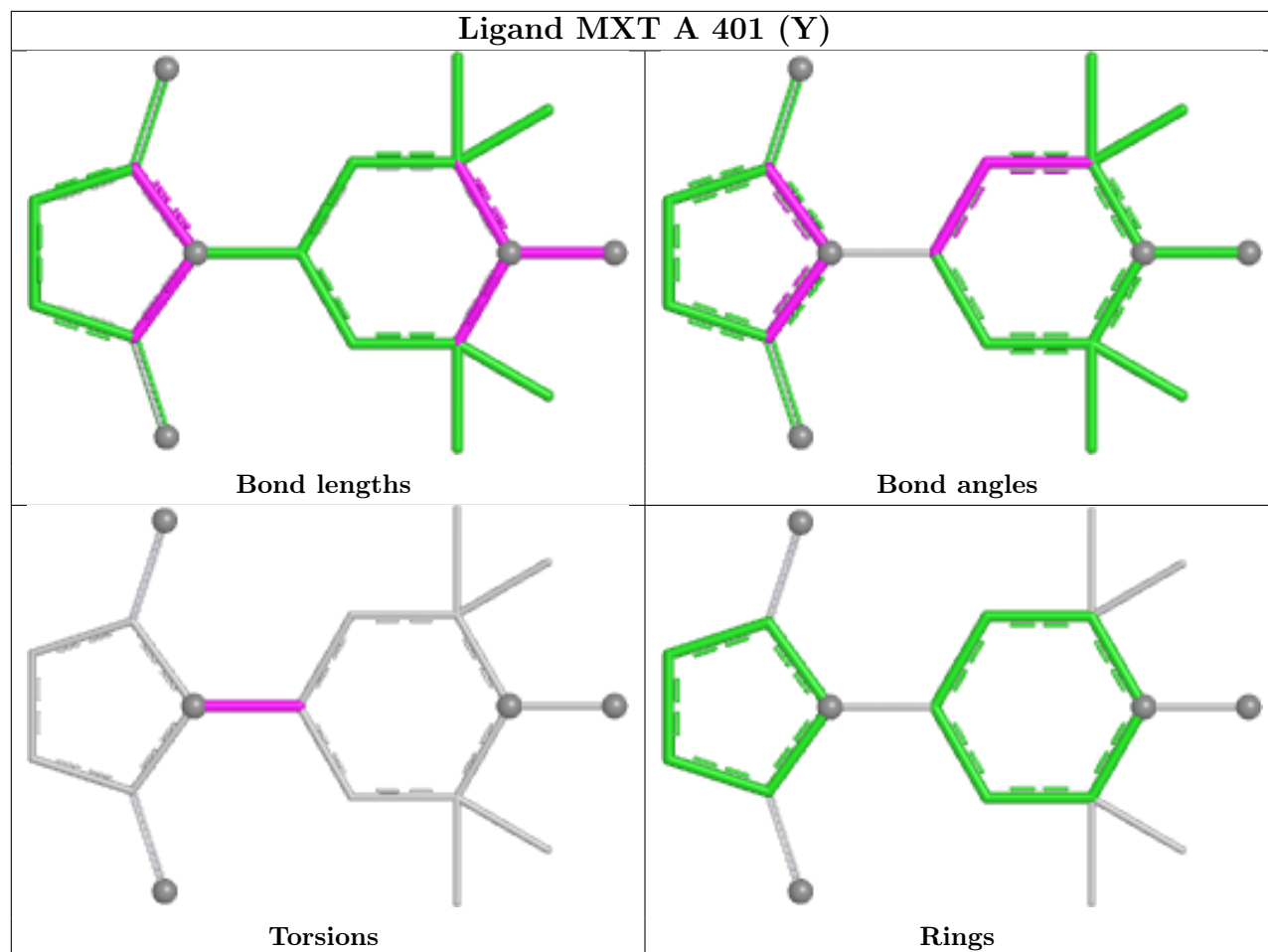


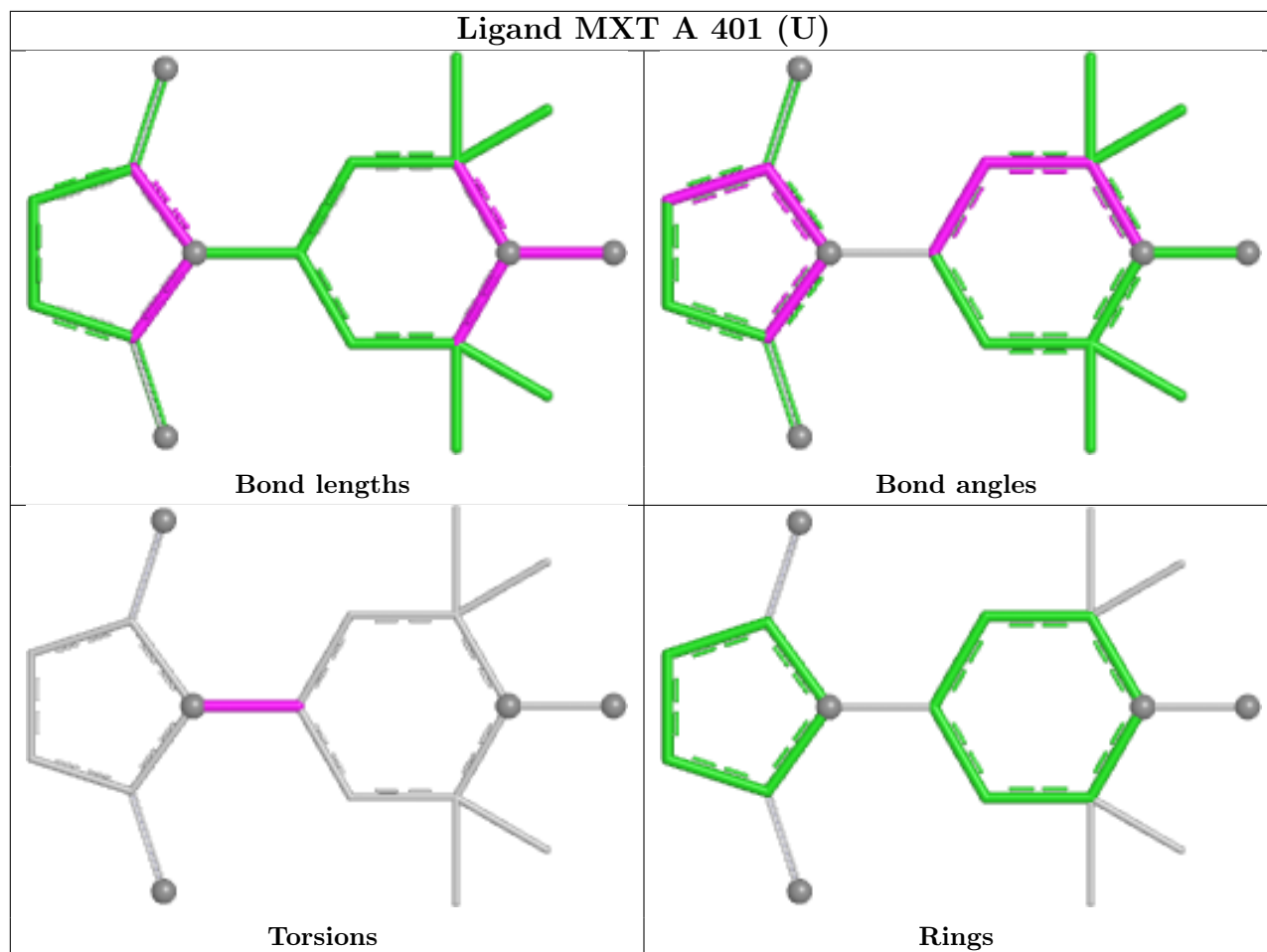


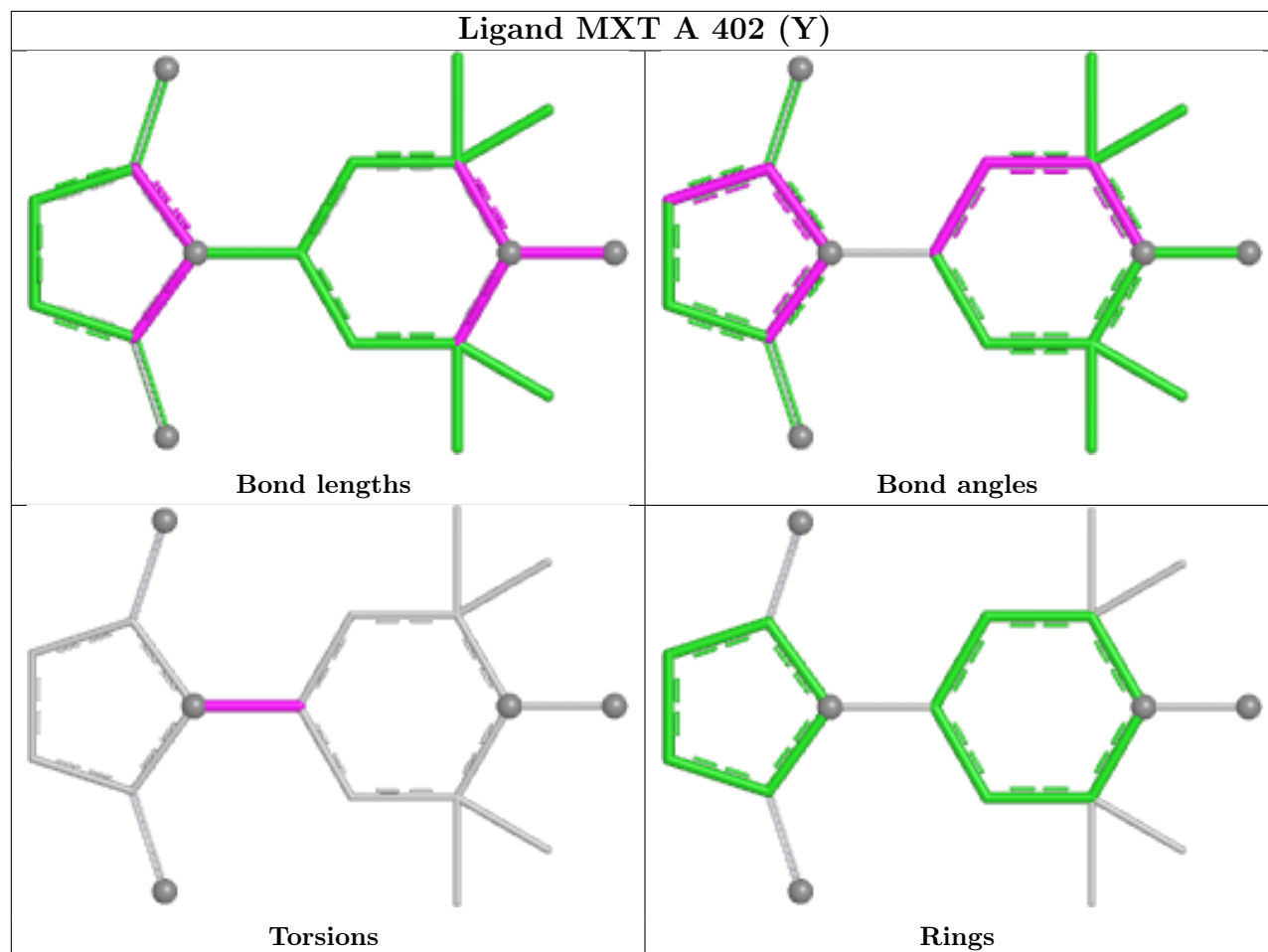


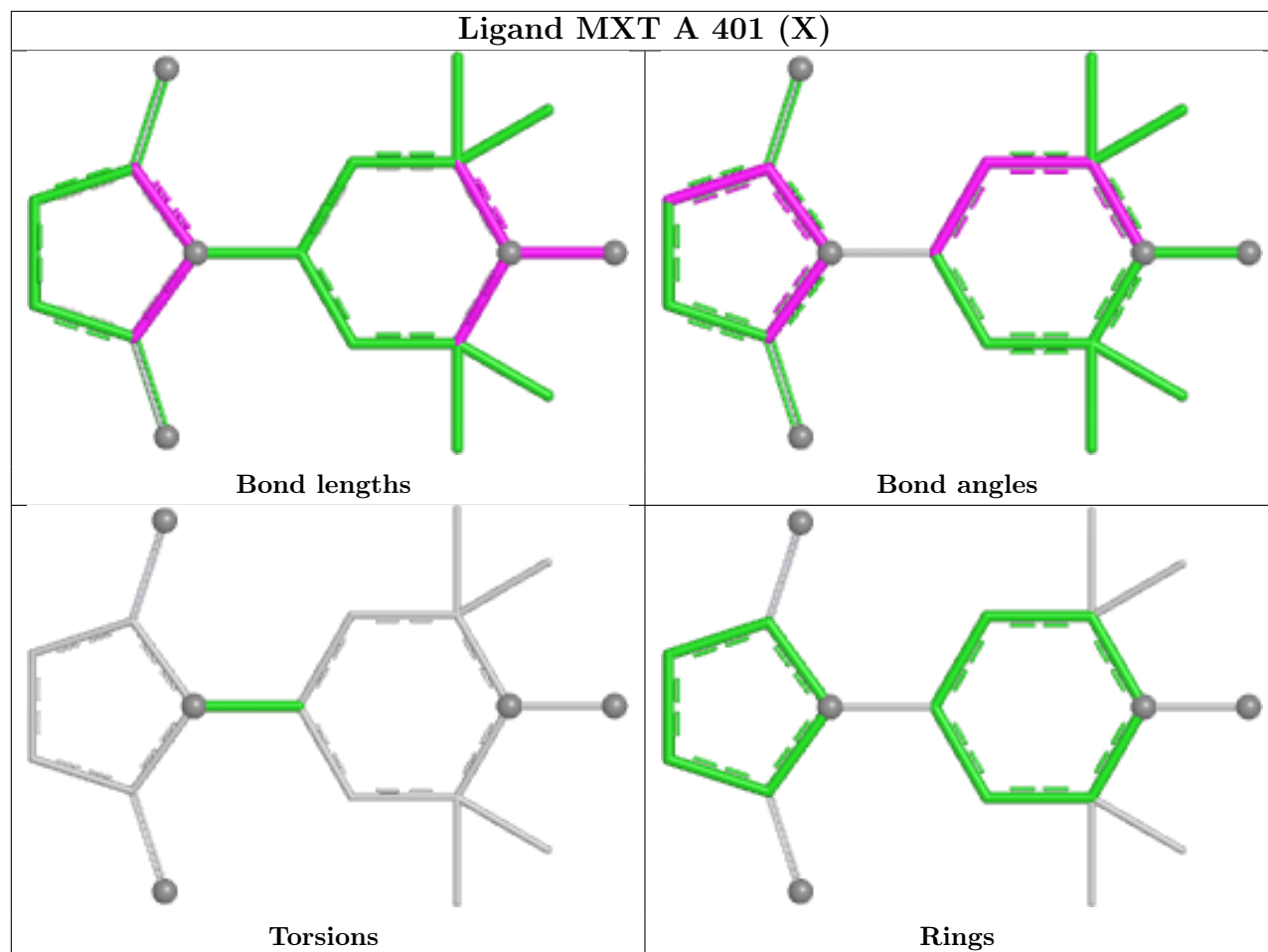


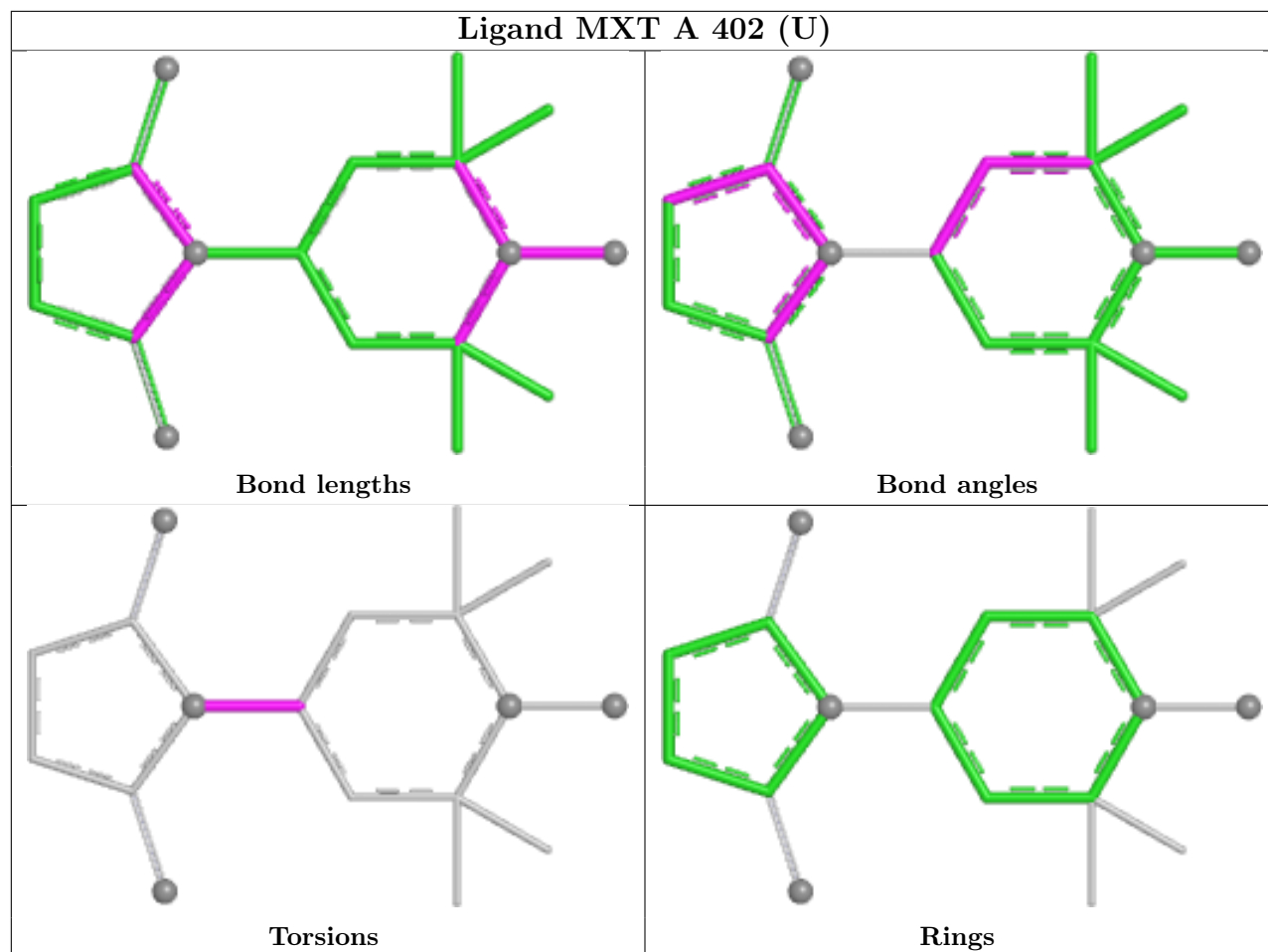


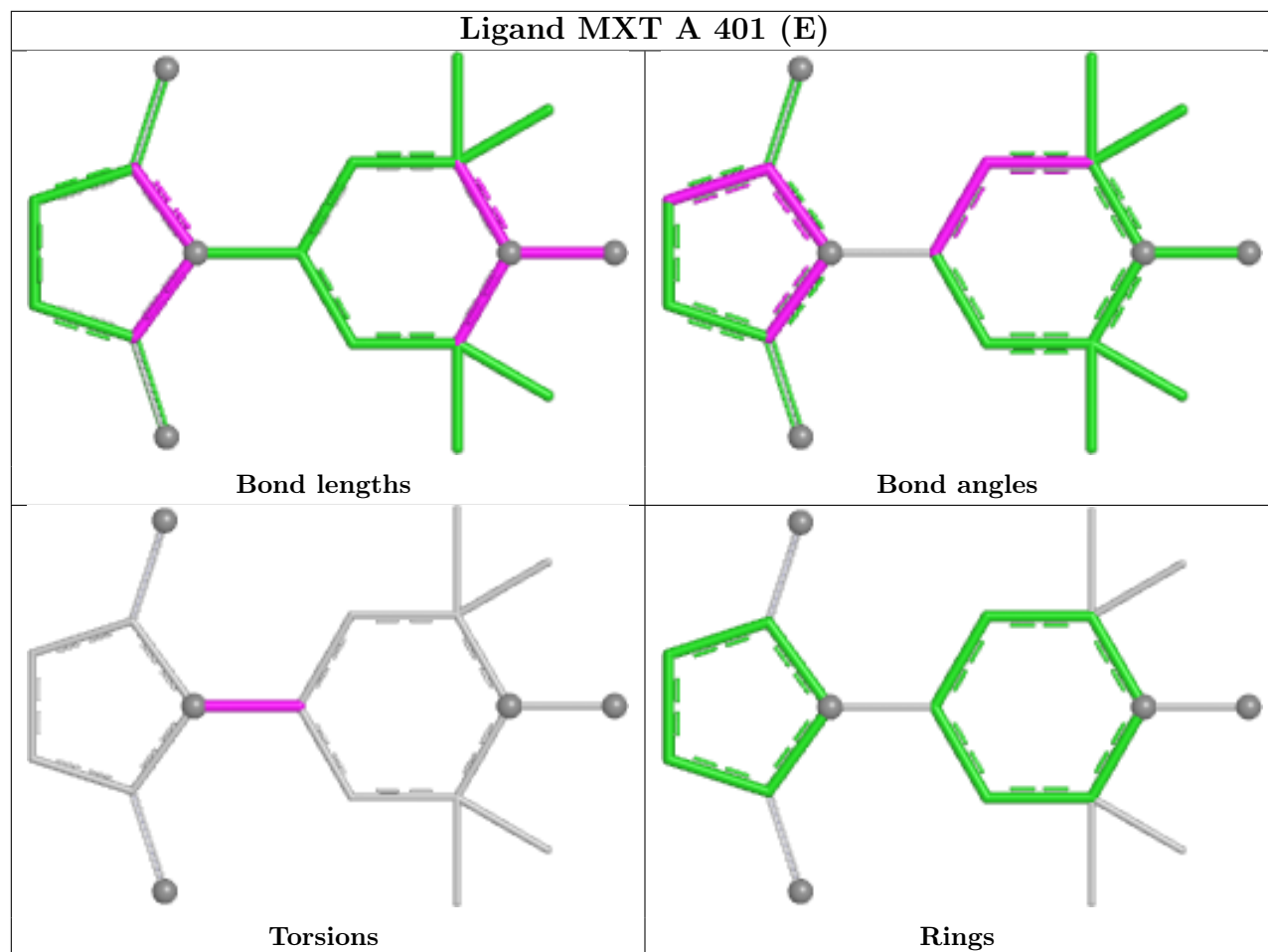


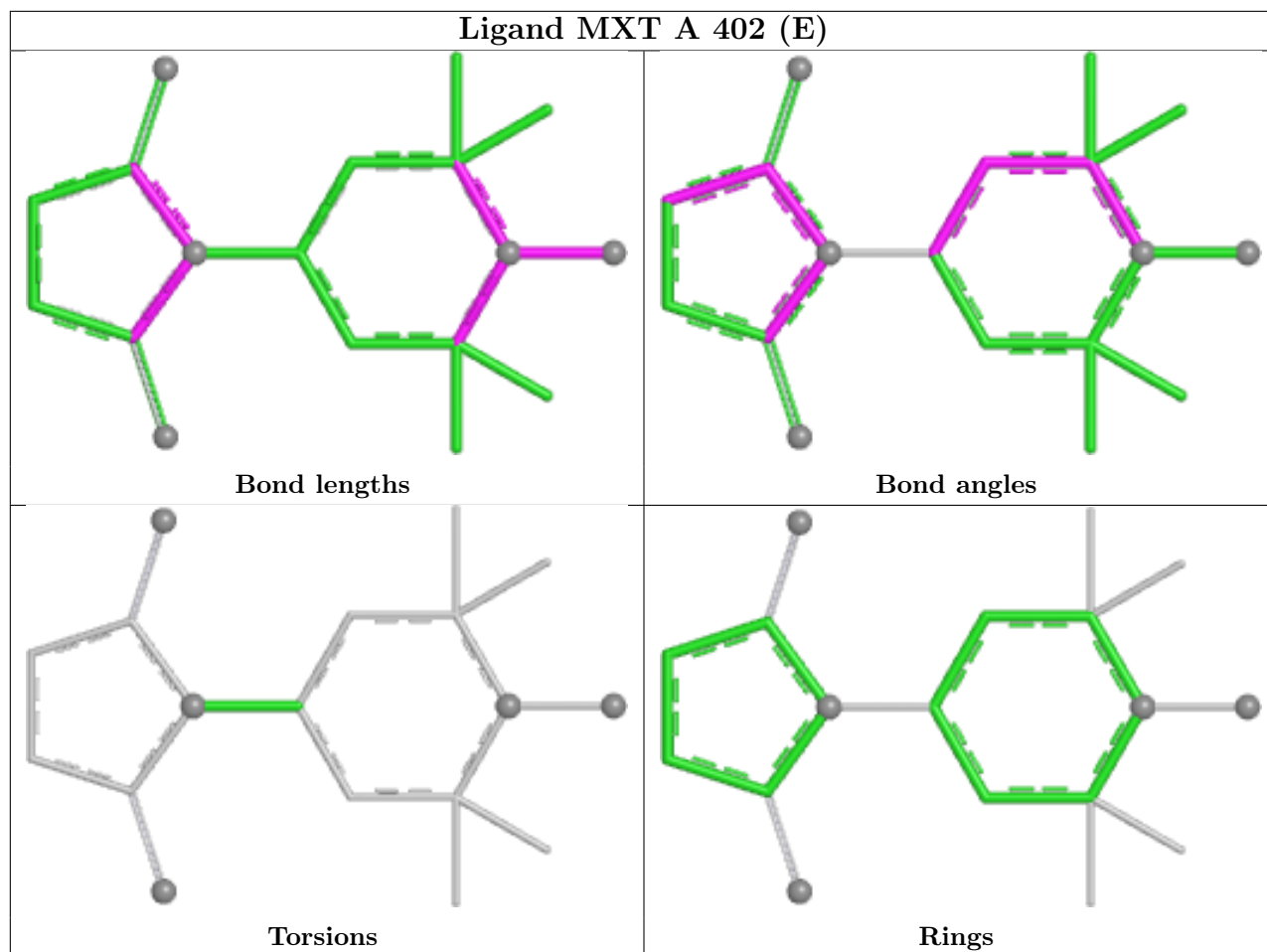


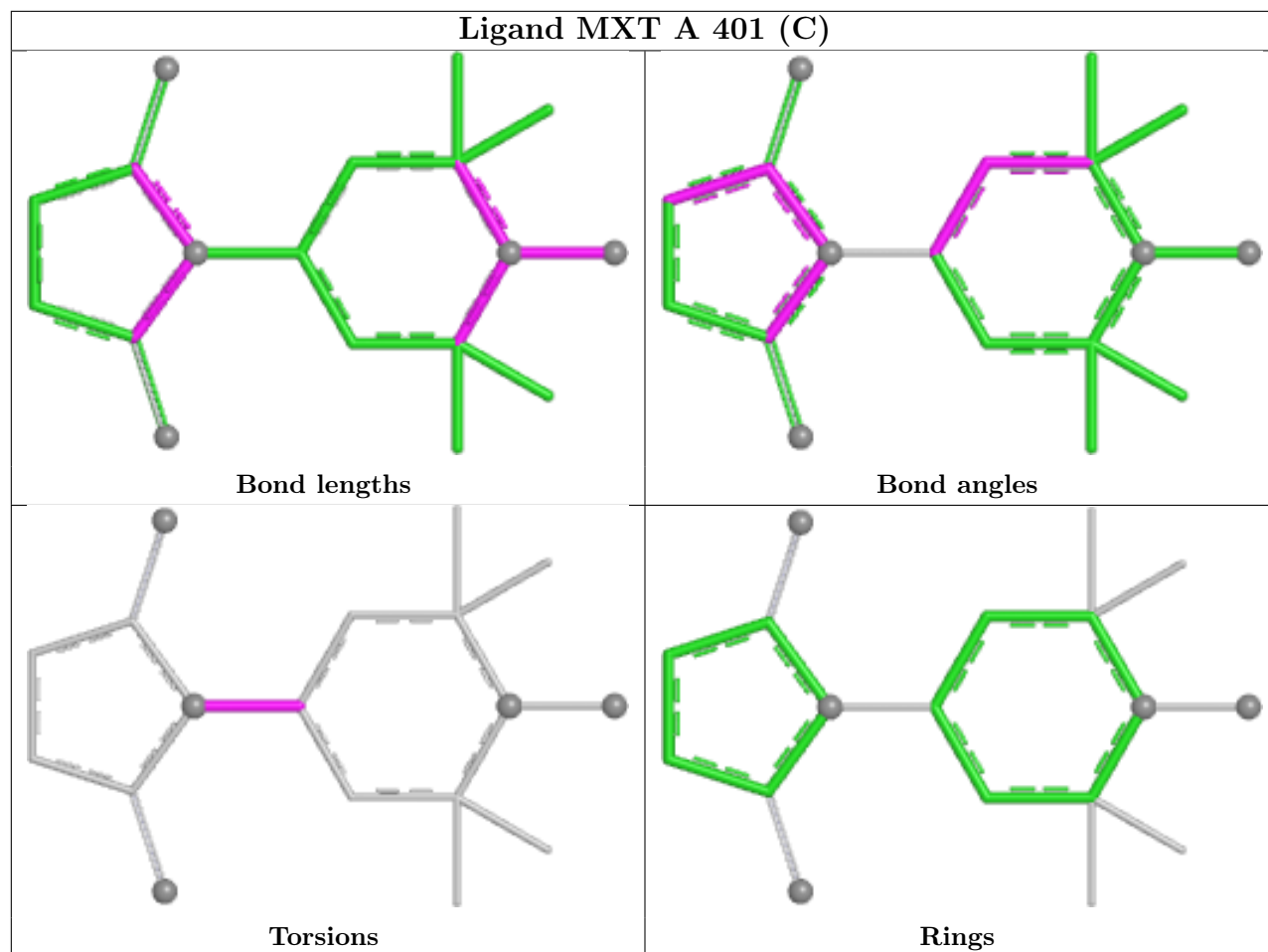












6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

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

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided