



Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:34 AM JST

PDB ID : 8IYG
EMDB ID : EMD-35821
Title : Human neuronal gap junction channel connexin 36
Authors : Mao, W.X.; Chen, S.S.
Deposited on : 2023-04-04
Resolution : 2.69 Å(reported)

This is a Full wwPDB EM Validation 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 : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

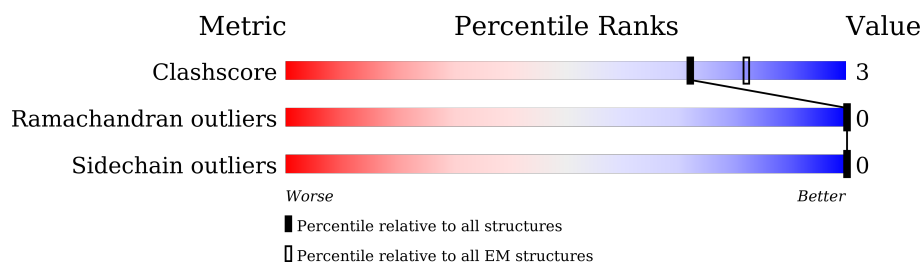
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.69 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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	321	53% 5% 42%
1	B	321	53% 5% 42%
1	C	321	53% 5% 42%
1	D	321	53% 5% 42%
1	E	321	52% 6% 42%
1	F	321	53% 5% 42%
1	G	321	53% 5% 42%
1	H	321	53% 5% 42%
1	I	321	53% 5% 42%

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Mol	Chain	Length	Quality of chain
1	J	321	 54%5%42%
1	K	321	 53%5%42%
1	L	321	 54%5%42%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 20532 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 Gap junction delta-2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	B	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	C	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	D	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	E	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	F	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	G	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	H	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	I	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	J	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	K	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		
1	L	187	Total	C	N	O	S	0	0
			1511	991	253	254	13		

- Molecule 2 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: C₃₁H₅₀O₄) (labeled as "Ligand of Interest" by depositor).



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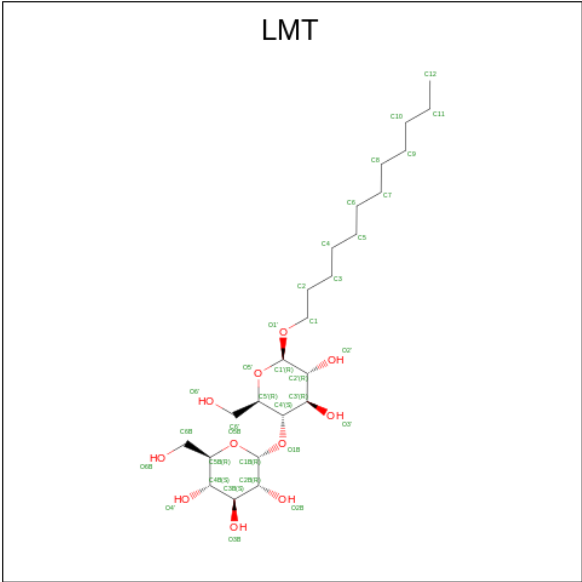
Mol	Chain	Residues	Atoms			AltConf
2	D	1	Total	C	O	0
			22	21	1	
2	D	1	Total	C	O	0
			26	24	2	
2	E	1	Total	C	O	0
			35	31	4	
2	E	1	Total	C	O	0
			26	24	2	
2	E	1	Total	C	O	0
			22	21	1	
2	E	1	Total	C	O	0
			26	24	2	
2	F	1	Total	C	O	0
			26	24	2	
2	F	1	Total	C	O	0
			35	31	4	
2	F	1	Total	C	O	0
			26	24	2	
2	F	1	Total	C	O	0
			22	21	1	
2	G	1	Total	C	O	0
			35	31	4	
2	G	1	Total	C	O	0
			26	24	2	
2	G	1	Total	C	O	0
			22	21	1	
2	G	1	Total	C	O	0
			26	24	2	
2	H	1	Total	C	O	0
			35	31	4	
2	H	1	Total	C	O	0
			26	24	2	
2	H	1	Total	C	O	0
			22	21	1	
2	H	1	Total	C	O	0
			26	24	2	
2	I	1	Total	C	O	0
			35	31	4	
2	I	1	Total	C	O	0
			26	24	2	
2	I	1	Total	C	O	0
			22	21	1	

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Mol	Chain	Residues	Atoms			AltConf
2	I	1	Total	C	O	0
			26	24	2	
2	J	1	Total	C	O	0
			35	31	4	
2	J	1	Total	C	O	0
			26	24	2	
2	J	1	Total	C	O	0
			22	21	1	
2	J	1	Total	C	O	0
			26	24	2	
2	K	1	Total	C	O	0
			35	31	4	
2	K	1	Total	C	O	0
			26	24	2	
2	K	1	Total	C	O	0
			22	21	1	
2	K	1	Total	C	O	0
			26	24	2	
2	L	1	Total	C	O	0
			26	24	2	
2	L	1	Total	C	O	0
			35	31	4	
2	L	1	Total	C	O	0
			26	24	2	
2	L	1	Total	C	O	0
			22	21	1	

- Molecule 3 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula: $C_{24}H_{46}O_{11}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total C O 35 24 11	0
3	A	1	Total C 10 10	0
3	A	1	Total C 10 10	0
3	A	1	Total C 9 9	0
3	A	1	Total C 7 7	0
3	A	1	Total C 8 8	0
3	A	1	Total C 12 12	0
3	B	1	Total C O 35 24 11	0
3	B	1	Total C 10 10	0
3	B	1	Total C 10 10	0
3	B	1	Total C 9 9	0
3	B	1	Total C 7 7	0
3	B	1	Total C 8 8	0
3	B	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
3	C	1	Total C O 35 24 11	0
3	C	1	Total C 10 10	0
3	C	1	Total C 10 10	0
3	C	1	Total C 9 9	0
3	C	1	Total C 7 7	0
3	C	1	Total C 8 8	0
3	C	1	Total C 12 12	0
3	D	1	Total C O 35 24 11	0
3	D	1	Total C 10 10	0
3	D	1	Total C 10 10	0
3	D	1	Total C 9 9	0
3	D	1	Total C 7 7	0
3	D	1	Total C 8 8	0
3	D	1	Total C 12 12	0
3	E	1	Total C O 35 24 11	0
3	E	1	Total C 10 10	0
3	E	1	Total C 10 10	0
3	E	1	Total C 9 9	0
3	E	1	Total C 7 7	0
3	E	1	Total C 8 8	0
3	E	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total C 12 12	0
3	F	1	Total C O 35 24 11	0
3	F	1	Total C 10 10	0
3	F	1	Total C 10 10	0
3	F	1	Total C 9 9	0
3	F	1	Total C 7 7	0
3	F	1	Total C 8 8	0
3	G	1	Total C O 35 24 11	0
3	G	1	Total C 10 10	0
3	G	1	Total C 10 10	0
3	G	1	Total C 9 9	0
3	G	1	Total C 7 7	0
3	G	1	Total C 8 8	0
3	G	1	Total C 12 12	0
3	H	1	Total C O 35 24 11	0
3	H	1	Total C 10 10	0
3	H	1	Total C 10 10	0
3	H	1	Total C 9 9	0
3	H	1	Total C 7 7	0
3	H	1	Total C 8 8	0
3	H	1	Total C 12 12	0

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Mol	Chain	Residues	Atoms	AltConf
3	I	1	Total C O 35 24 11	0
3	I	1	Total C 10 10	0
3	I	1	Total C 10 10	0
3	I	1	Total C 9 9	0
3	I	1	Total C 7 7	0
3	I	1	Total C 8 8	0
3	I	1	Total C 12 12	0
3	J	1	Total C O 35 24 11	0
3	J	1	Total C 10 10	0
3	J	1	Total C 10 10	0
3	J	1	Total C 9 9	0
3	J	1	Total C 7 7	0
3	J	1	Total C 8 8	0
3	J	1	Total C 12 12	0
3	K	1	Total C O 35 24 11	0
3	K	1	Total C 10 10	0
3	K	1	Total C 10 10	0
3	K	1	Total C 9 9	0
3	K	1	Total C 7 7	0
3	K	1	Total C 8 8	0
3	K	1	Total C 12 12	0

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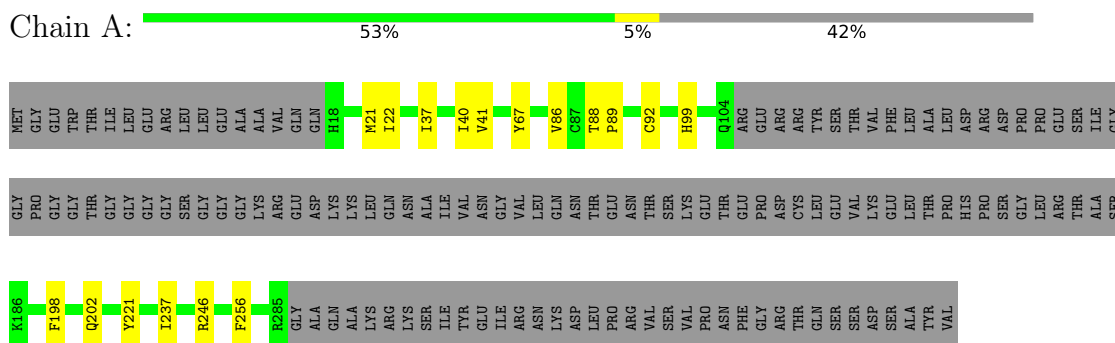
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Mol	Chain	Residues	Atoms	AltConf
3	L	1	Total C 12 12	0
3	L	1	Total C O 35 24 11	0
3	L	1	Total C 10 10	0
3	L	1	Total C 10 10	0
3	L	1	Total C 9 9	0
3	L	1	Total C 7 7	0
3	L	1	Total C 8 8	0

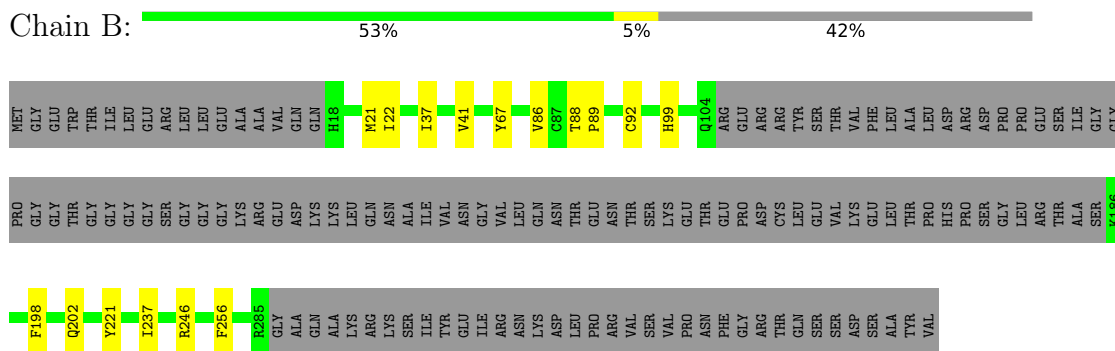
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

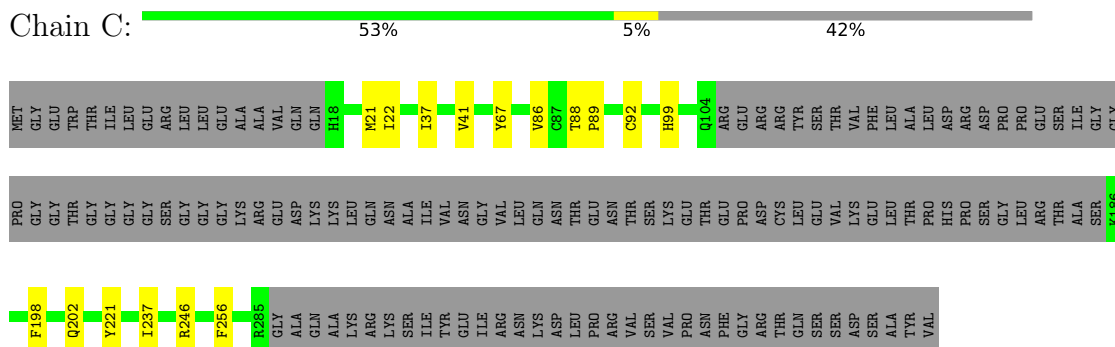
- Molecule 1: Gap junction delta-2 protein



- Molecule 1: Gap junction delta-2 protein

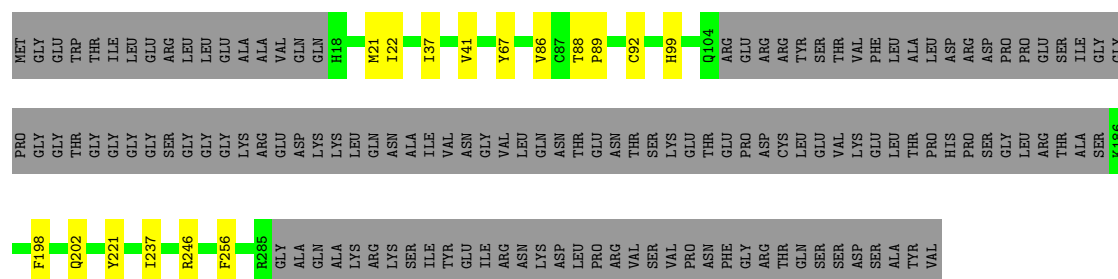


- Molecule 1: Gap junction delta-2 protein



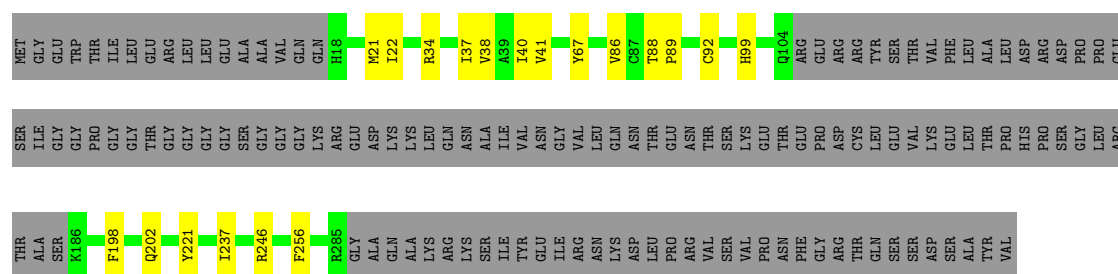
- Molecule 1: Gap junction delta-2 protein

Chain D:  53% 5% 42%



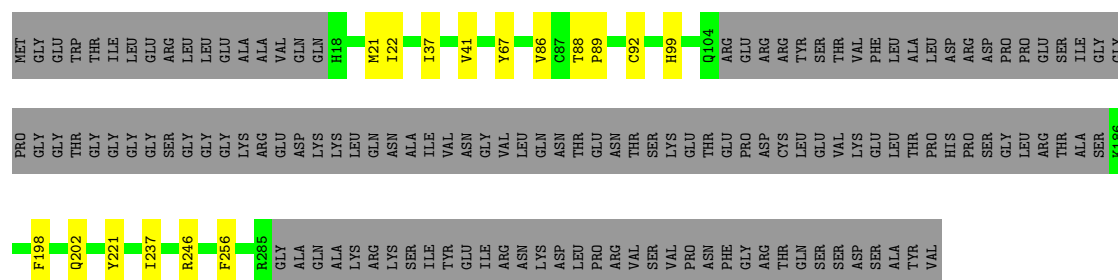
- Molecule 1: Gap junction delta-2 protein

Chain E:  52% 6% 42%



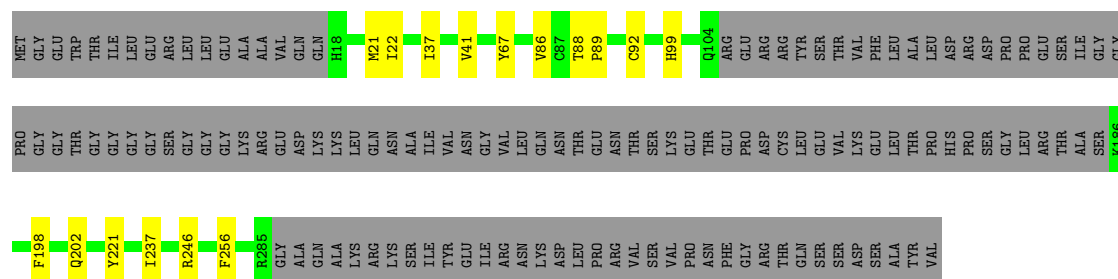
- Molecule 1: Gap junction delta-2 protein

Chain F:  53% 5% 42%



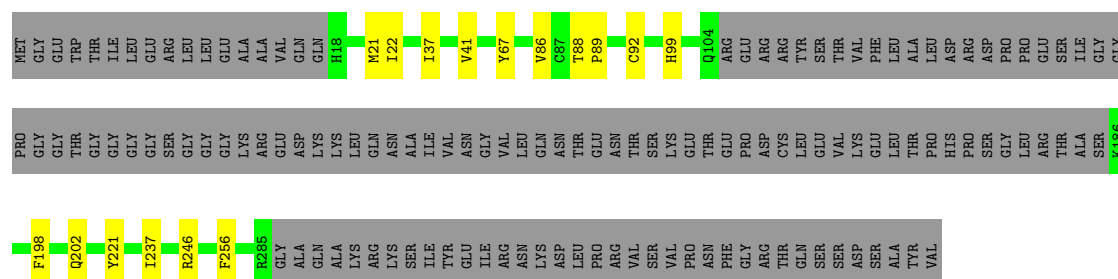
- Molecule 1: Gap junction delta-2 protein

Chain G:  53% 5% 42%



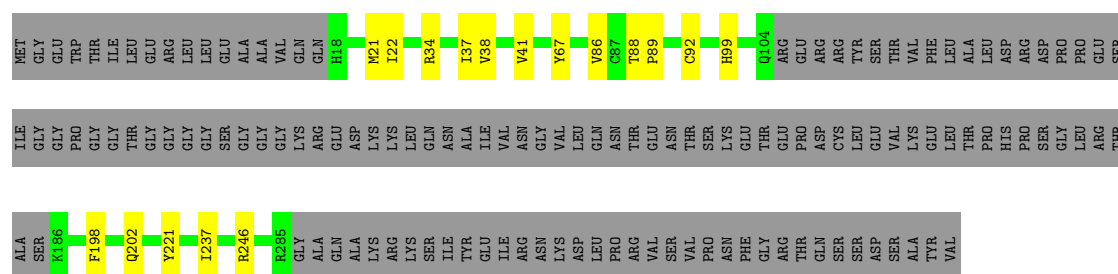
- Molecule 1: Gap junction delta-2 protein

Chain H:  53% 5% 42%



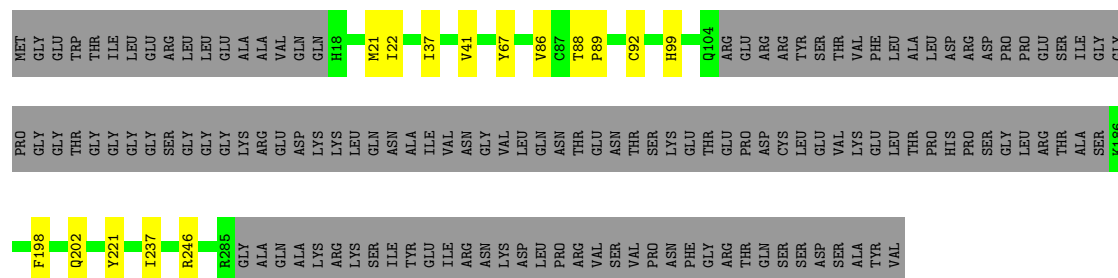
- Molecule 1: Gap junction delta-2 protein

Chain I:  53% 5% 42%



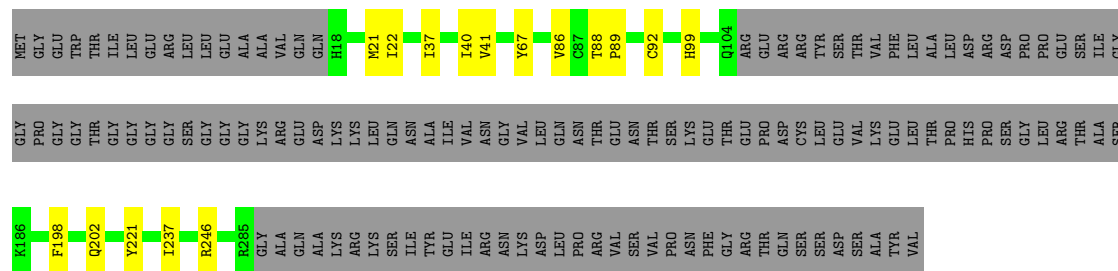
- Molecule 1: Gap junction delta-2 protein

Chain J:  54% 5% 42%



- Molecule 1: Gap junction delta-2 protein

Chain K:  53% 5% 42%



- Molecule 1: Gap junction delta-2 protein

Chain L:

54%

5%

42%

PRO	MET	GLY	GLY	TRP	THR	ILE	LEU	GLU	ARG	LEU	GLU	ALA	ALA	VAL	GLN	GLN	H18	M21	I22	I37	V41	Y67	V86	C87	T88	P89	C92	H99	Q104	ARG	GLU	ARG	ARG	ARG	TYR	SER	THR	THR	VAL	PHE	GLU	LEU	LEU	ALA	LEU	LEU	ASP	ARG	ASP	PRO	PRO	GLY	LEU	ARG	THR	ALA	ILE	GLY	GLY
		GLY	GLY	THR	GLY	GLY	GLY	SER	SER	GLY	GLY	LYS	ARG	GLU	ASP	LYS	LYS	LEU	GLN	ASN	ALA	ILE	VAL	ASN	GLY	VAL	LEU	GLN	ASN	THR	GLU	LYS	THR	GLU	PRO	ASP	CYS	LEU	GLU	VAL	LYS	GLU	THR	THR	PRO	HIS	PRO	SER	GLY	LEU	ARG	THR	ALA	SER					
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			
		F198	Q202	Y221	Y221	I237	R246	R285	GLY	ALA	GLN	ALA	LYS	ARG	LYS	LYS	LYS	LYS	SER	SER	ILE	TYR	GLU	ILE	ARG	ASN	LYS	ASP	LEU	PRO	ARG	THR	GLN	SER	SER	ASP	SER	ALA	TYR	VAL																			

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	117469	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 ($e^-/\text{\AA}^2$)	1.56	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	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: Y01, LMT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/1545	0.43	0/2093
1	B	0.24	0/1545	0.43	0/2093
1	C	0.24	0/1545	0.43	0/2093
1	D	0.24	0/1545	0.43	0/2093
1	E	0.24	0/1545	0.43	0/2093
1	F	0.24	0/1545	0.43	0/2093
1	G	0.24	0/1545	0.43	0/2093
1	H	0.24	0/1545	0.43	0/2093
1	I	0.24	0/1545	0.43	0/2093
1	J	0.24	0/1545	0.43	0/2093
1	K	0.24	0/1545	0.43	0/2093
1	L	0.24	0/1545	0.43	0/2093
All	All	0.24	0/18540	0.43	0/25116

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1511	0	1538	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1511	0	1538	13	0
1	C	1511	0	1538	13	0
1	D	1511	0	1538	13	0
1	E	1511	0	1538	15	0
1	F	1511	0	1538	13	0
1	G	1511	0	1538	13	0
1	H	1511	0	1538	13	0
1	I	1511	0	1538	13	0
1	J	1511	0	1538	12	0
1	K	1511	0	1538	13	0
1	L	1511	0	1538	12	0
2	A	109	0	141	3	0
2	B	109	0	141	3	0
2	C	109	0	141	2	0
2	D	109	0	141	2	0
2	E	109	0	141	2	0
2	F	109	0	141	2	0
2	G	109	0	141	2	0
2	H	109	0	141	2	0
2	I	109	0	141	2	0
2	J	109	0	141	2	0
2	K	109	0	141	3	0
2	L	109	0	141	3	0
3	A	91	0	136	2	0
3	B	91	0	136	2	0
3	C	91	0	136	2	0
3	D	91	0	136	2	0
3	E	91	0	136	2	0
3	F	91	0	136	2	0
3	G	91	0	136	2	0
3	H	91	0	136	2	0
3	I	91	0	137	1	0
3	J	91	0	136	1	0
3	K	91	0	136	1	0
3	L	91	0	136	1	0
All	All	20532	0	21781	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (137) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:92:CYS:SG	1:K:202:GLN:NE2	2.60	0.75
1:A:92:CYS:SG	1:A:202:GLN:NE2	2.60	0.75
1:I:92:CYS:SG	1:I:202:GLN:NE2	2.60	0.75
1:E:92:CYS:SG	1:E:202:GLN:NE2	2.60	0.75
1:D:92:CYS:SG	1:D:202:GLN:NE2	2.60	0.74
1:L:92:CYS:SG	1:L:202:GLN:NE2	2.60	0.74
1:H:92:CYS:SG	1:H:202:GLN:NE2	2.60	0.74
1:B:92:CYS:SG	1:B:202:GLN:NE2	2.60	0.74
1:F:92:CYS:SG	1:F:202:GLN:NE2	2.60	0.74
1:G:92:CYS:SG	1:G:202:GLN:NE2	2.60	0.73
1:J:92:CYS:SG	1:J:202:GLN:NE2	2.60	0.73
1:C:92:CYS:SG	1:C:202:GLN:NE2	2.60	0.73
1:K:37:ILE:O	1:K:41:VAL:HG22	2.14	0.48
1:A:22:ILE:HD11	2:B:409:Y01:HAT1	1.96	0.48
1:F:37:ILE:O	1:F:41:VAL:HG22	2.14	0.48
1:A:37:ILE:O	1:A:41:VAL:HG22	2.14	0.48
2:G:409:Y01:HAT1	1:L:22:ILE:HD11	1.96	0.47
1:J:22:ILE:HD11	2:K:409:Y01:HAT1	1.96	0.47
1:J:37:ILE:O	1:J:41:VAL:HG22	2.15	0.47
1:I:37:ILE:O	1:I:41:VAL:HG22	2.14	0.47
1:C:88:THR:OG1	1:C:89:PRO:HD3	2.14	0.47
1:H:88:THR:OG1	1:H:89:PRO:HD3	2.14	0.47
1:G:22:ILE:HD11	2:H:409:Y01:HAT1	1.97	0.47
1:D:88:THR:OG1	1:D:89:PRO:HD3	2.14	0.47
1:E:22:ILE:HD11	2:F:411:Y01:HAT1	1.97	0.47
1:G:88:THR:OG1	1:G:89:PRO:HD3	2.14	0.47
1:L:88:THR:OG1	1:L:89:PRO:HD3	2.14	0.47
1:A:88:THR:OG1	1:A:89:PRO:HD3	2.14	0.47
1:B:22:ILE:HD11	2:C:409:Y01:HAT1	1.97	0.47
1:B:88:THR:OG1	1:B:89:PRO:HD3	2.14	0.47
1:E:37:ILE:O	1:E:41:VAL:HG22	2.15	0.47
1:K:88:THR:OG1	1:K:89:PRO:HD3	2.14	0.47
1:I:22:ILE:HD11	2:J:409:Y01:HAT1	1.97	0.47
1:K:22:ILE:HD11	2:L:411:Y01:HAT1	1.97	0.47
1:L:37:ILE:O	1:L:41:VAL:HG22	2.14	0.47
1:B:37:ILE:O	1:B:41:VAL:HG22	2.15	0.47
1:H:37:ILE:O	1:H:41:VAL:HG22	2.14	0.47
1:D:37:ILE:O	1:D:41:VAL:HG22	2.14	0.47
1:F:88:THR:OG1	1:F:89:PRO:HD3	2.14	0.47
1:J:88:THR:OG1	1:J:89:PRO:HD3	2.14	0.47
1:C:37:ILE:O	1:C:41:VAL:HG22	2.14	0.46
1:I:88:THR:OG1	1:I:89:PRO:HD3	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:409:Y01:HAT1	1:F:22:ILE:HD11	1.98	0.46
1:D:22:ILE:HD11	2:E:409:Y01:HAT1	1.97	0.46
1:E:88:THR:OG1	1:E:89:PRO:HD3	2.14	0.46
1:G:37:ILE:O	1:G:41:VAL:HG22	2.14	0.46
1:C:22:ILE:HD11	2:D:409:Y01:HAT1	1.98	0.46
1:H:22:ILE:HD11	2:I:409:Y01:HAT1	1.97	0.46
1:C:198:PHE:CE1	2:C:409:Y01:HAT2	2.52	0.45
1:G:198:PHE:CE1	2:G:409:Y01:HAT2	2.52	0.45
1:K:221:TYR:O	3:K:403:LMT:O4'	2.32	0.45
1:B:198:PHE:CE1	2:B:409:Y01:HAT2	2.52	0.45
1:D:198:PHE:CE1	2:D:409:Y01:HAT2	2.52	0.45
1:K:198:PHE:CE1	2:K:409:Y01:HAT2	2.52	0.45
1:E:198:PHE:CE1	2:E:409:Y01:HAT2	2.52	0.45
1:H:198:PHE:CE1	2:H:409:Y01:HAT2	2.52	0.45
1:J:198:PHE:CE1	2:J:409:Y01:HAT2	2.52	0.45
1:A:198:PHE:CE1	2:A:409:Y01:HAT2	2.52	0.45
1:I:198:PHE:CE1	2:I:409:Y01:HAT2	2.52	0.45
1:L:198:PHE:CE1	2:L:411:Y01:HAT2	2.52	0.45
1:F:198:PHE:CE1	2:F:411:Y01:HAT2	2.52	0.45
1:L:221:TYR:O	3:L:405:LMT:O4'	2.32	0.45
1:A:221:TYR:O	3:A:403:LMT:O4'	2.33	0.45
1:C:221:TYR:O	3:C:403:LMT:O4'	2.32	0.44
1:G:221:TYR:O	3:G:403:LMT:O4'	2.33	0.44
1:B:221:TYR:O	3:B:403:LMT:O4'	2.32	0.44
1:I:246:ARG:HE	1:J:67:TYR:HE2	1.66	0.44
2:B:401:Y01:HAP1	2:B:401:Y01:HAO1	1.80	0.44
1:G:21:MET:HG2	1:H:99:HIS:CE1	2.53	0.44
2:A:401:Y01:HAP1	2:A:401:Y01:HAO1	1.80	0.44
1:J:21:MET:HG2	1:K:99:HIS:CE1	2.53	0.44
1:H:21:MET:HG2	1:I:99:HIS:CE1	2.53	0.43
1:G:99:HIS:CE1	1:L:21:MET:HG2	2.53	0.43
1:I:21:MET:HG2	1:J:99:HIS:CE1	2.53	0.43
1:E:246:ARG:HE	1:F:67:TYR:HE2	1.66	0.43
2:L:403:Y01:HAP1	2:L:403:Y01:HAO1	1.80	0.43
1:C:21:MET:HG2	1:D:99:HIS:CE1	2.53	0.43
1:F:221:TYR:O	3:F:405:LMT:O4'	2.32	0.43
1:J:221:TYR:O	3:J:403:LMT:O4'	2.33	0.43
1:D:21:MET:HG2	1:E:99:HIS:CE1	2.54	0.43
1:A:67:TYR:HE2	1:F:246:ARG:HE	1.67	0.43
2:K:401:Y01:HAP1	2:K:401:Y01:HAO1	1.80	0.43
1:A:99:HIS:CE1	1:F:21:MET:HG2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:MET:HG2	1:C:99:HIS:CE1	2.54	0.43
1:H:246:ARG:HE	1:I:67:TYR:HE2	1.67	0.43
1:K:246:ARG:HE	1:L:67:TYR:HE2	1.66	0.43
1:E:21:MET:HG2	1:F:99:HIS:CE1	2.54	0.43
1:D:86:VAL:O	1:D:89:PRO:HD2	2.19	0.43
1:G:67:TYR:HE2	1:L:246:ARG:HE	1.66	0.42
1:H:221:TYR:O	3:H:403:LMT:O4'	2.33	0.42
1:L:86:VAL:O	1:L:89:PRO:HD2	2.19	0.42
1:A:21:MET:HG2	1:B:99:HIS:CE1	2.53	0.42
1:A:86:VAL:O	1:A:89:PRO:HD2	2.19	0.42
1:D:246:ARG:HE	1:E:67:TYR:HE2	1.67	0.42
1:H:86:VAL:O	1:H:89:PRO:HD2	2.20	0.42
1:B:86:VAL:O	1:B:89:PRO:HD2	2.20	0.42
1:B:246:ARG:HE	1:C:67:TYR:HE2	1.66	0.42
1:K:21:MET:HG2	1:L:99:HIS:CE1	2.54	0.42
1:G:86:VAL:O	1:G:89:PRO:HD2	2.19	0.42
1:J:86:VAL:O	1:J:89:PRO:HD2	2.19	0.42
1:K:86:VAL:O	1:K:89:PRO:HD2	2.20	0.42
1:A:246:ARG:HE	1:B:67:TYR:HE2	1.67	0.42
1:C:246:ARG:HE	1:D:67:TYR:HE2	1.67	0.42
1:D:221:TYR:O	3:D:403:LMT:O4'	2.33	0.42
1:J:246:ARG:HE	1:K:67:TYR:HE2	1.68	0.42
1:C:86:VAL:O	1:C:89:PRO:HD2	2.20	0.42
1:F:86:VAL:O	1:F:89:PRO:HD2	2.20	0.42
1:G:246:ARG:HE	1:H:67:TYR:HE2	1.67	0.41
1:H:237:ILE:H	1:H:237:ILE:HD12	1.85	0.41
1:I:221:TYR:O	3:I:403:LMT:O4'	2.32	0.41
1:I:86:VAL:O	1:I:89:PRO:HD2	2.19	0.41
1:E:86:VAL:O	1:E:89:PRO:HD2	2.19	0.41
1:C:237:ILE:H	1:C:237:ILE:HD12	1.85	0.41
1:D:256:PHE:HE1	3:D:411:LMT:H122	1.85	0.41
1:D:237:ILE:H	1:D:237:ILE:HD12	1.86	0.41
1:E:221:TYR:O	3:E:403:LMT:O4'	2.33	0.41
1:E:237:ILE:HD12	1:E:237:ILE:H	1.86	0.41
1:I:237:ILE:HD12	1:I:237:ILE:H	1.86	0.41
1:C:256:PHE:HE1	3:C:411:LMT:H122	1.85	0.41
1:F:237:ILE:HD12	1:F:237:ILE:H	1.86	0.41
1:G:256:PHE:HE1	3:G:411:LMT:H122	1.85	0.41
1:G:237:ILE:H	1:G:237:ILE:HD12	1.86	0.41
1:J:237:ILE:HD12	1:J:237:ILE:H	1.85	0.41
1:H:256:PHE:HE1	3:H:411:LMT:H122	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ILE:HD13	1:A:40:ILE:HA	1.95	0.40
1:K:237:ILE:H	1:K:237:ILE:HD12	1.85	0.40
1:L:237:ILE:H	1:L:237:ILE:HD12	1.86	0.40
1:A:237:ILE:HD12	1:A:237:ILE:H	1.86	0.40
1:A:256:PHE:HE1	3:A:411:LMT:H122	1.85	0.40
1:B:237:ILE:H	1:B:237:ILE:HD12	1.86	0.40
1:E:40:ILE:HD13	1:E:40:ILE:HA	1.95	0.40
1:E:256:PHE:HE1	3:E:411:LMT:H122	1.85	0.40
1:B:256:PHE:HE1	3:B:411:LMT:H122	1.85	0.40
1:K:40:ILE:HD13	1:K:40:ILE:HA	1.95	0.40
1:E:34:ARG:O	1:E:38:VAL:HG12	2.22	0.40
1:F:256:PHE:HE1	3:F:402:LMT:H122	1.85	0.40
1:I:34:ARG:O	1:I:38:VAL:HG12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	B	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	C	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	D	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	E	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	F	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	G	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	H	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	I	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	J	183/321 (57%)	181 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
1	L	183/321 (57%)	181 (99%)	2 (1%)	0	100	100
All	All	2196/3852 (57%)	2172 (99%)	24 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	A	167/279 (60%)	167 (100%)	0	100	100
1	B	167/279 (60%)	167 (100%)	0	100	100
1	C	167/279 (60%)	167 (100%)	0	100	100
1	D	167/279 (60%)	167 (100%)	0	100	100
1	E	167/279 (60%)	167 (100%)	0	100	100
1	F	167/279 (60%)	167 (100%)	0	100	100
1	G	167/279 (60%)	167 (100%)	0	100	100
1	H	167/279 (60%)	167 (100%)	0	100	100
1	I	167/279 (60%)	167 (100%)	0	100	100
1	J	167/279 (60%)	167 (100%)	0	100	100
1	K	167/279 (60%)	167 (100%)	0	100	100
1	L	167/279 (60%)	167 (100%)	0	100	100
All	All	2004/3348 (60%)	2004 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

132 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$
3	LMT	L	402	-	11,11,36	0.26	0	10,10,47	0.77	0
3	LMT	F	402	-	11,11,36	0.25	0	10,10,47	0.77	0
3	LMT	C	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	H	411	-	11,11,36	0.25	0	10,10,47	0.77	0
3	LMT	I	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	K	406	-	8,8,36	0.24	0	7,7,47	0.67	0
3	LMT	L	408	-	8,8,36	0.24	0	7,7,47	0.66	0
2	Y01	E	401	-	38,38,38	0.53	0	57,57,57	0.50	0
2	Y01	F	411	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
2	Y01	L	401	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	F	401	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	D	410	-	29,29,38	0.40	0	46,46,57	0.48	0
3	LMT	F	409	-	6,6,36	0.23	0	5,5,47	0.61	0
2	Y01	K	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
2	Y01	C	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
2	Y01	G	401	-	38,38,38	0.53	0	57,57,57	0.50	0
3	LMT	B	408	-	7,7,36	0.23	0	6,6,47	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	E	408	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	J	401	-	38,38,38	0.53	0	57,57,57	0.50	0
3	LMT	J	404	-	9,9,36	0.26	0	8,8,47	0.75	0
2	Y01	A	410	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	I	401	-	38,38,38	0.53	0	57,57,57	0.50	0
2	Y01	A	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	D	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	B	411	-	11,11,36	0.26	0	10,10,47	0.77	0
3	LMT	C	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	K	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	F	406	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	H	407	-	6,6,36	0.23	0	5,5,47	0.61	0
3	LMT	L	405	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	A	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	J	403	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	F	405	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
2	Y01	D	402	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	J	402	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	A	407	-	6,6,36	0.22	0	5,5,47	0.62	0
3	LMT	I	406	-	8,8,36	0.24	0	7,7,47	0.67	0
3	LMT	B	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	C	408	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	D	401	-	38,38,38	0.53	0	57,57,57	0.50	0
2	Y01	C	401	-	38,38,38	0.53	0	57,57,57	0.50	0
2	Y01	B	402	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	H	401	-	38,38,38	0.53	0	57,57,57	0.50	0
2	Y01	L	403	-	38,38,38	0.53	0	57,57,57	0.50	0
3	LMT	D	405	-	9,9,36	0.26	0	8,8,47	0.74	0
3	LMT	D	408	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	L	411	-	25,25,38	0.63	1 (4%)	38,40,57	0.68	1 (2%)
3	LMT	K	411	-	11,11,36	0.26	0	10,10,47	0.77	0
3	LMT	A	403	-	36,36,36	1.16	5 (13%)	47,47,47	1.00	2 (4%)
2	Y01	A	401	-	38,38,38	0.53	0	57,57,57	0.50	0
3	LMT	L	406	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	G	405	-	9,9,36	0.26	0	8,8,47	0.74	0
3	LMT	E	411	-	11,11,36	0.25	0	10,10,47	0.78	0
3	LMT	L	410	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	G	402	-	29,29,38	0.41	0	46,46,57	0.48	0
2	Y01	H	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	G	411	-	11,11,36	0.26	0	10,10,47	0.77	0
2	Y01	C	410	-	29,29,38	0.41	0	46,46,57	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	Y01	F	404	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	I	403	-	36,36,36	1.15	5 (13%)	47,47,47	1.00	2 (4%)
3	LMT	J	408	-	7,7,36	0.23	0	6,6,47	0.64	0
3	LMT	B	406	-	8,8,36	0.24	0	7,7,47	0.66	0
3	LMT	E	403	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	H	404	-	9,9,36	0.26	0	8,8,47	0.75	0
2	Y01	C	402	-	29,29,38	0.42	0	46,46,57	0.47	0
2	Y01	A	402	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	I	408	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	I	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	L	409	-	6,6,36	0.22	0	5,5,47	0.62	0
3	LMT	E	407	-	6,6,36	0.22	0	5,5,47	0.61	0
3	LMT	I	411	-	11,11,36	0.25	0	10,10,47	0.77	0
2	Y01	G	410	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	E	406	-	8,8,36	0.24	0	7,7,47	0.66	0
3	LMT	C	407	-	6,6,36	0.22	0	5,5,47	0.62	0
3	LMT	J	407	-	6,6,36	0.22	0	5,5,47	0.62	0
3	LMT	K	407	-	6,6,36	0.22	0	5,5,47	0.61	0
3	LMT	H	406	-	8,8,36	0.24	0	7,7,47	0.66	0
2	Y01	K	401	-	38,38,38	0.53	0	57,57,57	0.50	0
3	LMT	G	408	-	7,7,36	0.23	0	6,6,47	0.64	0
3	LMT	F	407	-	9,9,36	0.26	0	8,8,47	0.75	0
2	Y01	B	410	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	G	404	-	9,9,36	0.26	0	8,8,47	0.75	0
2	Y01	H	402	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	I	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	K	403	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	C	403	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	F	408	-	8,8,36	0.24	0	7,7,47	0.66	0
3	LMT	D	411	-	11,11,36	0.25	0	10,10,47	0.77	0
3	LMT	G	407	-	6,6,36	0.22	0	5,5,47	0.61	0
2	Y01	J	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
2	Y01	K	402	-	29,29,38	0.41	0	46,46,57	0.47	0
3	LMT	A	408	-	7,7,36	0.23	0	6,6,47	0.64	0
3	LMT	C	411	-	11,11,36	0.26	0	10,10,47	0.77	0
3	LMT	J	411	-	11,11,36	0.25	0	10,10,47	0.77	0
3	LMT	H	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	I	407	-	6,6,36	0.22	0	5,5,47	0.61	0
2	Y01	D	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	A	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	G	403	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	LMT	K	408	-	7,7,36	0.22	0	6,6,47	0.64	0
3	LMT	L	407	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	J	405	-	9,9,36	0.26	0	8,8,47	0.74	0
3	LMT	D	406	-	8,8,36	0.24	0	7,7,47	0.66	0
3	LMT	B	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	C	406	-	8,8,36	0.24	0	7,7,47	0.66	0
2	Y01	H	410	-	29,29,38	0.42	0	46,46,57	0.48	0
2	Y01	L	404	-	29,29,38	0.40	0	46,46,57	0.48	0
3	LMT	B	407	-	6,6,36	0.22	0	5,5,47	0.62	0
3	LMT	D	407	-	6,6,36	0.22	0	5,5,47	0.62	0
2	Y01	J	410	-	29,29,38	0.42	0	46,46,57	0.48	0
2	Y01	G	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	G	406	-	8,8,36	0.24	0	7,7,47	0.66	0
2	Y01	F	403	-	38,38,38	0.53	0	57,57,57	0.51	0
2	Y01	I	402	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	B	403	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	2 (4%)
2	Y01	E	410	-	29,29,38	0.42	0	46,46,57	0.48	0
3	LMT	J	406	-	8,8,36	0.24	0	7,7,47	0.66	0
3	LMT	D	403	-	36,36,36	1.16	5 (13%)	47,47,47	0.99	2 (4%)
3	LMT	H	403	-	36,36,36	1.15	5 (13%)	47,47,47	0.99	2 (4%)
2	Y01	E	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
3	LMT	K	405	-	9,9,36	0.26	0	8,8,47	0.75	0
2	Y01	B	401	-	38,38,38	0.54	0	57,57,57	0.50	0
2	Y01	E	402	-	29,29,38	0.42	0	46,46,57	0.48	0
3	LMT	A	406	-	8,8,36	0.25	0	7,7,47	0.66	0
3	LMT	E	405	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	E	404	-	9,9,36	0.26	0	8,8,47	0.75	0
3	LMT	F	410	-	7,7,36	0.23	0	6,6,47	0.64	0
2	Y01	B	409	-	25,25,38	0.63	1 (4%)	38,40,57	0.67	1 (2%)
2	Y01	I	410	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	A	411	-	11,11,36	0.25	0	10,10,47	0.77	0
2	Y01	K	410	-	29,29,38	0.41	0	46,46,57	0.48	0
3	LMT	H	408	-	7,7,36	0.23	0	6,6,47	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	L	402	-	-	0/9/9/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	F	402	-	-	0/9/9/61	-
3	LMT	C	405	-	-	0/7/7/61	-
3	LMT	H	411	-	-	0/9/9/61	-
3	LMT	I	404	-	-	0/7/7/61	-
3	LMT	K	406	-	-	0/6/6/61	-
3	LMT	L	408	-	-	0/6/6/61	-
2	Y01	E	401	-	-	8/19/77/77	0/4/4/4
2	Y01	F	411	-	-	1/2/60/77	0/4/4/4
2	Y01	L	401	-	-	4/8/66/77	0/4/4/4
2	Y01	F	401	-	-	4/8/66/77	0/4/4/4
2	Y01	D	410	-	-	4/8/66/77	0/4/4/4
3	LMT	F	409	-	-	0/4/4/61	-
2	Y01	K	409	-	-	1/2/60/77	0/4/4/4
2	Y01	C	409	-	-	1/2/60/77	0/4/4/4
2	Y01	G	401	-	-	7/19/77/77	0/4/4/4
3	LMT	B	408	-	-	0/5/5/61	-
3	LMT	E	408	-	-	0/5/5/61	-
2	Y01	J	401	-	-	7/19/77/77	0/4/4/4
3	LMT	J	404	-	-	0/7/7/61	-
2	Y01	A	410	-	-	4/8/66/77	0/4/4/4
2	Y01	I	401	-	-	8/19/77/77	0/4/4/4
2	Y01	A	409	-	-	1/2/60/77	0/4/4/4
3	LMT	D	404	-	-	0/7/7/61	-
3	LMT	B	411	-	-	0/9/9/61	-
3	LMT	C	404	-	-	0/7/7/61	-
3	LMT	K	404	-	-	0/7/7/61	-
3	LMT	F	406	-	-	0/7/7/61	-
3	LMT	H	407	-	-	0/4/4/61	-
3	LMT	L	405	-	-	6/21/61/61	0/2/2/2
3	LMT	A	404	-	-	0/7/7/61	-
3	LMT	J	403	-	-	6/21/61/61	0/2/2/2
3	LMT	F	405	-	-	6/21/61/61	0/2/2/2
2	Y01	D	402	-	-	4/8/66/77	0/4/4/4
2	Y01	J	402	-	-	4/8/66/77	0/4/4/4
3	LMT	A	407	-	-	0/4/4/61	-
3	LMT	I	406	-	-	0/6/6/61	-
3	LMT	B	405	-	-	0/7/7/61	-
3	LMT	C	408	-	-	0/5/5/61	-
2	Y01	D	401	-	-	7/19/77/77	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Y01	C	401	-	-	7/19/77/77	0/4/4/4
2	Y01	B	402	-	-	4/8/66/77	0/4/4/4
2	Y01	H	401	-	-	7/19/77/77	0/4/4/4
2	Y01	L	403	-	-	7/19/77/77	0/4/4/4
3	LMT	D	405	-	-	0/7/7/61	-
3	LMT	D	408	-	-	0/5/5/61	-
2	Y01	L	411	-	-	1/2/60/77	0/4/4/4
3	LMT	K	411	-	-	0/9/9/61	-
3	LMT	A	403	-	-	6/21/61/61	0/2/2/2
2	Y01	A	401	-	-	7/19/77/77	0/4/4/4
3	LMT	L	406	-	-	0/7/7/61	-
3	LMT	G	405	-	-	0/7/7/61	-
3	LMT	E	411	-	-	0/9/9/61	-
3	LMT	L	410	-	-	0/5/5/61	-
2	Y01	G	402	-	-	4/8/66/77	0/4/4/4
2	Y01	H	409	-	-	1/2/60/77	0/4/4/4
3	LMT	G	411	-	-	0/9/9/61	-
2	Y01	C	410	-	-	4/8/66/77	0/4/4/4
2	Y01	F	404	-	-	4/8/66/77	0/4/4/4
3	LMT	I	403	-	-	6/21/61/61	0/2/2/2
3	LMT	J	408	-	-	0/5/5/61	-
3	LMT	B	406	-	-	0/6/6/61	-
3	LMT	E	403	-	-	6/21/61/61	0/2/2/2
3	LMT	H	404	-	-	0/7/7/61	-
2	Y01	C	402	-	-	4/8/66/77	0/4/4/4
2	Y01	A	402	-	-	4/8/66/77	0/4/4/4
3	LMT	I	408	-	-	0/5/5/61	-
2	Y01	I	409	-	-	1/2/60/77	0/4/4/4
3	LMT	L	409	-	-	0/4/4/61	-
3	LMT	E	407	-	-	0/4/4/61	-
3	LMT	I	411	-	-	0/9/9/61	-
2	Y01	G	410	-	-	4/8/66/77	0/4/4/4
3	LMT	E	406	-	-	0/6/6/61	-
3	LMT	C	407	-	-	0/4/4/61	-
3	LMT	J	407	-	-	0/4/4/61	-
3	LMT	K	407	-	-	0/4/4/61	-
3	LMT	H	406	-	-	0/6/6/61	-
2	Y01	K	401	-	-	7/19/77/77	0/4/4/4
3	LMT	G	408	-	-	0/5/5/61	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	F	407	-	-	0/7/7/61	-
2	Y01	B	410	-	-	4/8/66/77	0/4/4/4
3	LMT	G	404	-	-	0/7/7/61	-
2	Y01	H	402	-	-	4/8/66/77	0/4/4/4
3	LMT	I	405	-	-	0/7/7/61	-
3	LMT	K	403	-	-	6/21/61/61	0/2/2/2
3	LMT	C	403	-	-	6/21/61/61	0/2/2/2
3	LMT	F	408	-	-	0/6/6/61	-
3	LMT	D	411	-	-	0/9/9/61	-
3	LMT	G	407	-	-	0/4/4/61	-
2	Y01	J	409	-	-	1/2/60/77	0/4/4/4
2	Y01	K	402	-	-	4/8/66/77	0/4/4/4
3	LMT	A	408	-	-	0/5/5/61	-
3	LMT	C	411	-	-	0/9/9/61	-
3	LMT	J	411	-	-	0/9/9/61	-
3	LMT	H	405	-	-	0/7/7/61	-
3	LMT	I	407	-	-	0/4/4/61	-
2	Y01	D	409	-	-	1/2/60/77	0/4/4/4
3	LMT	A	405	-	-	0/7/7/61	-
3	LMT	G	403	-	-	6/21/61/61	0/2/2/2
3	LMT	K	408	-	-	0/5/5/61	-
3	LMT	L	407	-	-	0/7/7/61	-
3	LMT	J	405	-	-	0/7/7/61	-
3	LMT	D	406	-	-	0/6/6/61	-
3	LMT	B	404	-	-	0/7/7/61	-
3	LMT	C	406	-	-	0/6/6/61	-
2	Y01	H	410	-	-	4/8/66/77	0/4/4/4
2	Y01	L	404	-	-	4/8/66/77	0/4/4/4
3	LMT	B	407	-	-	0/4/4/61	-
3	LMT	D	407	-	-	0/4/4/61	-
2	Y01	J	410	-	-	4/8/66/77	0/4/4/4
2	Y01	G	409	-	-	1/2/60/77	0/4/4/4
3	LMT	G	406	-	-	0/6/6/61	-
2	Y01	F	403	-	-	8/19/77/77	0/4/4/4
2	Y01	I	402	-	-	4/8/66/77	0/4/4/4
3	LMT	B	403	-	-	6/21/61/61	0/2/2/2
2	Y01	E	410	-	-	4/8/66/77	0/4/4/4
3	LMT	J	406	-	-	0/6/6/61	-
3	LMT	D	403	-	-	6/21/61/61	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	LMT	H	403	-	-	6/21/61/61	0/2/2/2
2	Y01	E	409	-	-	1/2/60/77	0/4/4/4
3	LMT	K	405	-	-	0/7/7/61	-
2	Y01	B	401	-	-	8/19/77/77	0/4/4/4
2	Y01	E	402	-	-	4/8/66/77	0/4/4/4
3	LMT	A	406	-	-	0/6/6/61	-
3	LMT	E	405	-	-	0/7/7/61	-
3	LMT	E	404	-	-	0/7/7/61	-
3	LMT	F	410	-	-	0/5/5/61	-
2	Y01	B	409	-	-	1/2/60/77	0/4/4/4
2	Y01	I	410	-	-	4/8/66/77	0/4/4/4
3	LMT	A	411	-	-	0/9/9/61	-
2	Y01	K	410	-	-	4/8/66/77	0/4/4/4
3	LMT	H	408	-	-	0/5/5/61	-

All (72) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	405	LMT	O3'-C3'	-2.67	1.36	1.43
3	A	403	LMT	O3'-C3'	-2.65	1.36	1.43
3	C	403	LMT	O3'-C3'	-2.64	1.36	1.43
3	J	403	LMT	O3'-C3'	-2.64	1.36	1.43
3	D	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	H	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	K	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	B	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	G	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	E	403	LMT	O3'-C3'	-2.62	1.36	1.43
3	L	405	LMT	O3'-C3'	-2.62	1.36	1.43
3	I	403	LMT	O3'-C3'	-2.57	1.36	1.43
2	C	409	Y01	OAW-CAY	-2.46	1.33	1.42
2	K	409	Y01	OAW-CAY	-2.45	1.33	1.42
2	I	409	Y01	OAW-CAY	-2.45	1.33	1.42
2	A	409	Y01	OAW-CAY	-2.45	1.33	1.42
2	D	409	Y01	OAW-CAY	-2.45	1.33	1.42
2	B	409	Y01	OAW-CAY	-2.44	1.33	1.42
2	J	409	Y01	OAW-CAY	-2.44	1.33	1.42
2	L	411	Y01	OAW-CAY	-2.44	1.33	1.42
2	F	411	Y01	OAW-CAY	-2.44	1.33	1.42
2	H	409	Y01	OAW-CAY	-2.44	1.33	1.42
2	E	409	Y01	OAW-CAY	-2.42	1.33	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	409	Y01	OAW-CAY	-2.42	1.33	1.42
3	D	403	LMT	O2B-C2B	-2.34	1.37	1.43
3	K	403	LMT	O2B-C2B	-2.33	1.37	1.43
3	J	403	LMT	O3B-C3B	-2.33	1.37	1.43
3	A	403	LMT	O2B-C2B	-2.32	1.37	1.43
3	J	403	LMT	O2B-C2B	-2.31	1.37	1.43
3	B	403	LMT	O3B-C3B	-2.31	1.37	1.43
3	B	403	LMT	O2B-C2B	-2.31	1.37	1.43
3	G	403	LMT	O3B-C3B	-2.31	1.37	1.43
3	K	403	LMT	O3B-C3B	-2.31	1.37	1.43
3	D	403	LMT	O2'-C2'	-2.30	1.37	1.43
3	A	403	LMT	O3B-C3B	-2.30	1.37	1.43
3	D	403	LMT	O3B-C3B	-2.30	1.37	1.43
3	H	403	LMT	O3B-C3B	-2.30	1.37	1.43
3	C	403	LMT	O2B-C2B	-2.30	1.37	1.43
3	F	405	LMT	O2B-C2B	-2.30	1.37	1.43
3	E	403	LMT	O3B-C3B	-2.30	1.37	1.43
3	G	403	LMT	O2B-C2B	-2.30	1.37	1.43
3	C	403	LMT	O3B-C3B	-2.30	1.37	1.43
3	F	405	LMT	O3B-C3B	-2.30	1.37	1.43
3	E	403	LMT	O2B-C2B	-2.30	1.37	1.43
3	I	403	LMT	O2B-C2B	-2.30	1.37	1.43
3	L	405	LMT	O2B-C2B	-2.29	1.37	1.43
3	H	403	LMT	O2B-C2B	-2.28	1.37	1.43
3	B	403	LMT	O2'-C2'	-2.28	1.37	1.43
3	L	405	LMT	O3B-C3B	-2.28	1.37	1.43
3	A	403	LMT	O2'-C2'	-2.27	1.37	1.43
3	J	403	LMT	O2'-C2'	-2.26	1.37	1.43
3	I	403	LMT	O3B-C3B	-2.26	1.37	1.43
3	L	405	LMT	O2'-C2'	-2.25	1.37	1.43
3	H	403	LMT	O2'-C2'	-2.25	1.37	1.43
3	E	403	LMT	O2'-C2'	-2.25	1.37	1.43
3	I	403	LMT	O2'-C2'	-2.25	1.37	1.43
3	C	403	LMT	O2'-C2'	-2.24	1.37	1.43
3	F	405	LMT	O2'-C2'	-2.24	1.37	1.43
3	G	403	LMT	O2'-C2'	-2.24	1.37	1.43
3	K	403	LMT	O2'-C2'	-2.21	1.37	1.43
3	I	403	LMT	O4'-C4B	-2.14	1.37	1.43
3	J	403	LMT	O4'-C4B	-2.12	1.38	1.43
3	D	403	LMT	O4'-C4B	-2.11	1.38	1.43
3	E	403	LMT	O4'-C4B	-2.09	1.38	1.43
3	L	405	LMT	O4'-C4B	-2.09	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	LMT	O4'-C4B	-2.09	1.38	1.43
3	G	403	LMT	O4'-C4B	-2.09	1.38	1.43
3	B	403	LMT	O4'-C4B	-2.08	1.38	1.43
3	A	403	LMT	O4'-C4B	-2.08	1.38	1.43
3	K	403	LMT	O4'-C4B	-2.08	1.38	1.43
3	H	403	LMT	O4'-C4B	-2.08	1.38	1.43
3	F	405	LMT	O4'-C4B	-2.07	1.38	1.43

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	403	LMT	C1'-O5'-C5'	-2.56	108.67	113.69
3	D	403	LMT	C1'-O5'-C5'	-2.55	108.69	113.69
3	A	403	LMT	C1'-O5'-C5'	-2.54	108.69	113.69
3	J	403	LMT	C1'-O5'-C5'	-2.54	108.70	113.69
3	C	403	LMT	C1'-O5'-C5'	-2.54	108.71	113.69
3	L	405	LMT	C1'-O5'-C5'	-2.53	108.72	113.69
3	G	403	LMT	C1'-O5'-C5'	-2.53	108.73	113.69
3	H	403	LMT	C1'-O5'-C5'	-2.53	108.73	113.69
3	B	403	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
3	F	405	LMT	C1'-O5'-C5'	-2.52	108.74	113.69
3	K	403	LMT	C1'-O5'-C5'	-2.51	108.76	113.69
3	E	403	LMT	C1'-O5'-C5'	-2.51	108.77	113.69
3	L	405	LMT	C3'-C4'-C5'	-2.42	105.37	110.93
3	G	403	LMT	C3'-C4'-C5'	-2.42	105.38	110.93
3	I	403	LMT	C3'-C4'-C5'	-2.42	105.38	110.93
3	D	403	LMT	C3'-C4'-C5'	-2.41	105.39	110.93
3	H	403	LMT	C3'-C4'-C5'	-2.41	105.39	110.93
3	E	403	LMT	C3'-C4'-C5'	-2.41	105.40	110.93
3	J	403	LMT	C3'-C4'-C5'	-2.41	105.40	110.93
3	A	403	LMT	C3'-C4'-C5'	-2.41	105.41	110.93
3	B	403	LMT	C3'-C4'-C5'	-2.40	105.42	110.93
3	C	403	LMT	C3'-C4'-C5'	-2.40	105.42	110.93
3	K	403	LMT	C3'-C4'-C5'	-2.40	105.44	110.93
3	F	405	LMT	C3'-C4'-C5'	-2.39	105.44	110.93
2	I	409	Y01	CAY-OAW-CBC	2.33	119.55	113.87
2	D	409	Y01	CAY-OAW-CBC	2.33	119.55	113.87
2	J	409	Y01	CAY-OAW-CBC	2.32	119.53	113.87
2	E	409	Y01	CAY-OAW-CBC	2.32	119.52	113.87
2	G	409	Y01	CAY-OAW-CBC	2.32	119.51	113.87
2	C	409	Y01	CAY-OAW-CBC	2.31	119.50	113.87
2	K	409	Y01	CAY-OAW-CBC	2.31	119.50	113.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	409	Y01	CAY-OAW-CBC	2.31	119.50	113.87
2	B	409	Y01	CAY-OAW-CBC	2.31	119.50	113.87
2	F	411	Y01	CAY-OAW-CBC	2.30	119.48	113.87
2	H	409	Y01	CAY-OAW-CBC	2.30	119.47	113.87
2	L	411	Y01	CAY-OAW-CBC	2.30	119.47	113.87

There are no chirality outliers.

All (268) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	LMT	C2'-C1'-O1'-C1
3	A	403	LMT	O5'-C1'-O1'-C1
3	B	403	LMT	C2'-C1'-O1'-C1
3	B	403	LMT	O5'-C1'-O1'-C1
3	C	403	LMT	C2'-C1'-O1'-C1
3	C	403	LMT	O5'-C1'-O1'-C1
3	D	403	LMT	C2'-C1'-O1'-C1
3	D	403	LMT	O5'-C1'-O1'-C1
3	E	403	LMT	C2'-C1'-O1'-C1
3	E	403	LMT	O5'-C1'-O1'-C1
3	F	405	LMT	C2'-C1'-O1'-C1
3	F	405	LMT	O5'-C1'-O1'-C1
3	G	403	LMT	C2'-C1'-O1'-C1
3	G	403	LMT	O5'-C1'-O1'-C1
3	H	403	LMT	C2'-C1'-O1'-C1
3	H	403	LMT	O5'-C1'-O1'-C1
3	I	403	LMT	C2'-C1'-O1'-C1
3	I	403	LMT	O5'-C1'-O1'-C1
3	J	403	LMT	C2'-C1'-O1'-C1
3	J	403	LMT	O5'-C1'-O1'-C1
3	K	403	LMT	C2'-C1'-O1'-C1
3	K	403	LMT	O5'-C1'-O1'-C1
3	L	405	LMT	C2'-C1'-O1'-C1
3	L	405	LMT	O5'-C1'-O1'-C1
3	A	403	LMT	O5'-C5'-C6'-O6'
3	B	403	LMT	O5'-C5'-C6'-O6'
3	C	403	LMT	O5'-C5'-C6'-O6'
3	D	403	LMT	O5'-C5'-C6'-O6'
3	E	403	LMT	O5'-C5'-C6'-O6'
3	F	405	LMT	O5'-C5'-C6'-O6'
3	G	403	LMT	O5'-C5'-C6'-O6'
3	H	403	LMT	O5'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
3	I	403	LMT	O5'-C5'-C6'-O6'
3	J	403	LMT	O5'-C5'-C6'-O6'
3	K	403	LMT	O5'-C5'-C6'-O6'
3	L	405	LMT	O5'-C5'-C6'-O6'
3	A	403	LMT	C4'-C5'-C6'-O6'
3	B	403	LMT	C4'-C5'-C6'-O6'
3	C	403	LMT	C4'-C5'-C6'-O6'
3	D	403	LMT	C4'-C5'-C6'-O6'
3	E	403	LMT	C4'-C5'-C6'-O6'
3	F	405	LMT	C4'-C5'-C6'-O6'
3	G	403	LMT	C4'-C5'-C6'-O6'
3	H	403	LMT	C4'-C5'-C6'-O6'
3	I	403	LMT	C4'-C5'-C6'-O6'
3	J	403	LMT	C4'-C5'-C6'-O6'
3	K	403	LMT	C4'-C5'-C6'-O6'
3	L	405	LMT	C4'-C5'-C6'-O6'
2	A	401	Y01	CAO-CBB-CBE-CBI
2	B	401	Y01	CAO-CBB-CBE-CBI
2	C	401	Y01	CAO-CBB-CBE-CBI
2	D	401	Y01	CAO-CBB-CBE-CBI
2	E	401	Y01	CAO-CBB-CBE-CBI
2	F	403	Y01	CAO-CBB-CBE-CBI
2	G	401	Y01	CAO-CBB-CBE-CBI
2	H	401	Y01	CAO-CBB-CBE-CBI
2	I	401	Y01	CAO-CBB-CBE-CBI
2	J	401	Y01	CAO-CBB-CBE-CBI
2	K	401	Y01	CAO-CBB-CBE-CBI
2	L	403	Y01	CAO-CBB-CBE-CBI
2	A	409	Y01	CAR-CBC-OAW-CAY
2	B	409	Y01	CAR-CBC-OAW-CAY
2	C	409	Y01	CAR-CBC-OAW-CAY
2	D	409	Y01	CAR-CBC-OAW-CAY
2	E	409	Y01	CAR-CBC-OAW-CAY
2	F	411	Y01	CAR-CBC-OAW-CAY
2	G	409	Y01	CAR-CBC-OAW-CAY
2	H	409	Y01	CAR-CBC-OAW-CAY
2	I	409	Y01	CAR-CBC-OAW-CAY
2	J	409	Y01	CAR-CBC-OAW-CAY
2	K	409	Y01	CAR-CBC-OAW-CAY
2	L	411	Y01	CAR-CBC-OAW-CAY
2	A	401	Y01	CAC-CBB-CBE-CAP
2	B	401	Y01	CAC-CBB-CBE-CAP

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Mol	Chain	Res	Type	Atoms
2	C	401	Y01	CAC-CBB-CBE-CAP
2	D	401	Y01	CAC-CBB-CBE-CAP
2	E	401	Y01	CAC-CBB-CBE-CAP
2	F	403	Y01	CAC-CBB-CBE-CAP
2	G	401	Y01	CAC-CBB-CBE-CAP
2	H	401	Y01	CAC-CBB-CBE-CAP
2	I	401	Y01	CAC-CBB-CBE-CAP
2	J	401	Y01	CAC-CBB-CBE-CAP
2	K	401	Y01	CAC-CBB-CBE-CAP
2	L	403	Y01	CAC-CBB-CBE-CAP
2	A	401	Y01	CAC-CBB-CBE-CBI
2	B	401	Y01	CAC-CBB-CBE-CBI
2	C	401	Y01	CAC-CBB-CBE-CBI
2	D	401	Y01	CAC-CBB-CBE-CBI
2	E	401	Y01	CAC-CBB-CBE-CBI
2	F	403	Y01	CAC-CBB-CBE-CBI
2	G	401	Y01	CAC-CBB-CBE-CBI
2	H	401	Y01	CAC-CBB-CBE-CBI
2	I	401	Y01	CAC-CBB-CBE-CBI
2	J	401	Y01	CAC-CBB-CBE-CBI
2	K	401	Y01	CAC-CBB-CBE-CBI
2	L	403	Y01	CAC-CBB-CBE-CBI
2	A	401	Y01	CAO-CBB-CBE-CAP
2	B	401	Y01	CAO-CBB-CBE-CAP
2	C	401	Y01	CAO-CBB-CBE-CAP
2	D	401	Y01	CAO-CBB-CBE-CAP
2	E	401	Y01	CAO-CBB-CBE-CAP
2	F	403	Y01	CAO-CBB-CBE-CAP
2	G	401	Y01	CAO-CBB-CBE-CAP
2	H	401	Y01	CAO-CBB-CBE-CAP
2	I	401	Y01	CAO-CBB-CBE-CAP
2	J	401	Y01	CAO-CBB-CBE-CAP
2	K	401	Y01	CAO-CBB-CBE-CAP
2	L	403	Y01	CAO-CBB-CBE-CAP
3	A	403	LMT	C2-C1-O1'-C1'
3	B	403	LMT	C2-C1-O1'-C1'
3	C	403	LMT	C2-C1-O1'-C1'
3	D	403	LMT	C2-C1-O1'-C1'
3	E	403	LMT	C2-C1-O1'-C1'
3	F	405	LMT	C2-C1-O1'-C1'
3	G	403	LMT	C2-C1-O1'-C1'
3	H	403	LMT	C2-C1-O1'-C1'

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Mol	Chain	Res	Type	Atoms
3	I	403	LMT	C2-C1-O1'-C1'
3	J	403	LMT	C2-C1-O1'-C1'
3	K	403	LMT	C2-C1-O1'-C1'
3	L	405	LMT	C2-C1-O1'-C1'
2	E	401	Y01	CAN-CAJ-CAO-CBB
2	I	401	Y01	CAN-CAJ-CAO-CBB
2	B	401	Y01	CAN-CAJ-CAO-CBB
2	L	403	Y01	CAN-CAJ-CAO-CBB
2	A	401	Y01	CAN-CAJ-CAO-CBB
2	C	401	Y01	CAN-CAJ-CAO-CBB
2	D	401	Y01	CAN-CAJ-CAO-CBB
2	F	403	Y01	CAN-CAJ-CAO-CBB
2	G	401	Y01	CAN-CAJ-CAO-CBB
2	H	401	Y01	CAN-CAJ-CAO-CBB
2	J	401	Y01	CAN-CAJ-CAO-CBB
2	K	401	Y01	CAN-CAJ-CAO-CBB
2	A	402	Y01	CAC-CBB-CBE-CAP
2	A	410	Y01	CAC-CBB-CBE-CAP
2	B	402	Y01	CAC-CBB-CBE-CAP
2	B	410	Y01	CAC-CBB-CBE-CAP
2	C	402	Y01	CAC-CBB-CBE-CAP
2	C	410	Y01	CAC-CBB-CBE-CAP
2	D	402	Y01	CAC-CBB-CBE-CAP
2	D	410	Y01	CAC-CBB-CBE-CAP
2	E	402	Y01	CAC-CBB-CBE-CAP
2	E	410	Y01	CAC-CBB-CBE-CAP
2	F	401	Y01	CAC-CBB-CBE-CAP
2	F	404	Y01	CAC-CBB-CBE-CAP
2	G	402	Y01	CAC-CBB-CBE-CAP
2	G	410	Y01	CAC-CBB-CBE-CAP
2	H	402	Y01	CAC-CBB-CBE-CAP
2	H	410	Y01	CAC-CBB-CBE-CAP
2	I	402	Y01	CAC-CBB-CBE-CAP
2	I	410	Y01	CAC-CBB-CBE-CAP
2	J	402	Y01	CAC-CBB-CBE-CAP
2	J	410	Y01	CAC-CBB-CBE-CAP
2	K	402	Y01	CAC-CBB-CBE-CAP
2	K	410	Y01	CAC-CBB-CBE-CAP
2	L	401	Y01	CAC-CBB-CBE-CAP
2	L	404	Y01	CAC-CBB-CBE-CAP
3	E	403	LMT	O5B-C5B-C6B-O6B
3	L	405	LMT	O5B-C5B-C6B-O6B

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Mol	Chain	Res	Type	Atoms
3	I	403	LMT	O5B-C5B-C6B-O6B
3	A	403	LMT	O5B-C5B-C6B-O6B
3	B	403	LMT	O5B-C5B-C6B-O6B
3	G	403	LMT	O5B-C5B-C6B-O6B
3	J	403	LMT	O5B-C5B-C6B-O6B
3	D	403	LMT	O5B-C5B-C6B-O6B
3	H	403	LMT	O5B-C5B-C6B-O6B
3	K	403	LMT	O5B-C5B-C6B-O6B
2	B	401	Y01	CAM-CAL-CAX-OAH
2	E	401	Y01	CAM-CAL-CAX-OAH
2	F	403	Y01	CAM-CAL-CAX-OAH
2	G	401	Y01	CAM-CAL-CAX-OAH
2	H	401	Y01	CAM-CAL-CAX-OAH
2	I	401	Y01	CAM-CAL-CAX-OAH
2	J	401	Y01	CAM-CAL-CAX-OAH
3	C	403	LMT	O5B-C5B-C6B-O6B
3	F	405	LMT	O5B-C5B-C6B-O6B
2	A	401	Y01	CAM-CAL-CAX-OAH
2	C	401	Y01	CAM-CAL-CAX-OAH
2	D	401	Y01	CAM-CAL-CAX-OAH
2	K	401	Y01	CAM-CAL-CAX-OAH
2	L	403	Y01	CAM-CAL-CAX-OAH
2	E	401	Y01	CAM-CAL-CAX-OAF
2	I	401	Y01	CAM-CAL-CAX-OAF
2	A	401	Y01	CAM-CAL-CAX-OAF
2	B	401	Y01	CAM-CAL-CAX-OAF
2	C	401	Y01	CAM-CAL-CAX-OAF
2	D	401	Y01	CAM-CAL-CAX-OAF
2	F	403	Y01	CAM-CAL-CAX-OAF
2	G	401	Y01	CAM-CAL-CAX-OAF
2	H	401	Y01	CAM-CAL-CAX-OAF
2	J	401	Y01	CAM-CAL-CAX-OAF
2	K	401	Y01	CAM-CAL-CAX-OAF
2	L	403	Y01	CAM-CAL-CAX-OAF
2	A	402	Y01	CAO-CBB-CBE-CBI
2	B	402	Y01	CAO-CBB-CBE-CBI
2	D	402	Y01	CAO-CBB-CBE-CBI
2	E	402	Y01	CAO-CBB-CBE-CBI
2	F	404	Y01	CAO-CBB-CBE-CBI
2	G	402	Y01	CAO-CBB-CBE-CBI
2	H	402	Y01	CAO-CBB-CBE-CBI
2	I	402	Y01	CAO-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
2	J	402	Y01	CAO-CBB-CBE-CBI
2	K	402	Y01	CAO-CBB-CBE-CBI
2	L	404	Y01	CAO-CBB-CBE-CBI
2	A	402	Y01	CAO-CBB-CBE-CAP
2	A	410	Y01	CAO-CBB-CBE-CAP
2	B	402	Y01	CAO-CBB-CBE-CAP
2	B	410	Y01	CAO-CBB-CBE-CAP
2	C	402	Y01	CAO-CBB-CBE-CAP
2	C	410	Y01	CAO-CBB-CBE-CAP
2	D	402	Y01	CAO-CBB-CBE-CAP
2	D	410	Y01	CAO-CBB-CBE-CAP
2	E	402	Y01	CAO-CBB-CBE-CAP
2	E	410	Y01	CAO-CBB-CBE-CAP
2	F	401	Y01	CAO-CBB-CBE-CAP
2	F	404	Y01	CAO-CBB-CBE-CAP
2	G	402	Y01	CAO-CBB-CBE-CAP
2	G	410	Y01	CAO-CBB-CBE-CAP
2	H	402	Y01	CAO-CBB-CBE-CAP
2	H	410	Y01	CAO-CBB-CBE-CAP
2	I	402	Y01	CAO-CBB-CBE-CAP
2	I	410	Y01	CAO-CBB-CBE-CAP
2	J	402	Y01	CAO-CBB-CBE-CAP
2	J	410	Y01	CAO-CBB-CBE-CAP
2	K	402	Y01	CAO-CBB-CBE-CAP
2	K	410	Y01	CAO-CBB-CBE-CAP
2	L	401	Y01	CAO-CBB-CBE-CAP
2	L	404	Y01	CAO-CBB-CBE-CAP
2	F	403	Y01	CAJ-CAO-CBB-CBE
2	A	402	Y01	CAC-CBB-CBE-CBI
2	A	410	Y01	CAO-CBB-CBE-CBI
2	A	410	Y01	CAC-CBB-CBE-CBI
2	B	402	Y01	CAC-CBB-CBE-CBI
2	B	410	Y01	CAO-CBB-CBE-CBI
2	B	410	Y01	CAC-CBB-CBE-CBI
2	C	402	Y01	CAO-CBB-CBE-CBI
2	C	402	Y01	CAC-CBB-CBE-CBI
2	C	410	Y01	CAO-CBB-CBE-CBI
2	C	410	Y01	CAC-CBB-CBE-CBI
2	D	402	Y01	CAC-CBB-CBE-CBI
2	D	410	Y01	CAO-CBB-CBE-CBI
2	D	410	Y01	CAC-CBB-CBE-CBI
2	E	402	Y01	CAC-CBB-CBE-CBI

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Mol	Chain	Res	Type	Atoms
2	E	410	Y01	CAO-CBB-CBE-CBI
2	E	410	Y01	CAC-CBB-CBE-CBI
2	F	401	Y01	CAO-CBB-CBE-CBI
2	F	401	Y01	CAC-CBB-CBE-CBI
2	F	404	Y01	CAC-CBB-CBE-CBI
2	G	402	Y01	CAC-CBB-CBE-CBI
2	G	410	Y01	CAO-CBB-CBE-CBI
2	G	410	Y01	CAC-CBB-CBE-CBI
2	H	402	Y01	CAC-CBB-CBE-CBI
2	H	410	Y01	CAO-CBB-CBE-CBI
2	H	410	Y01	CAC-CBB-CBE-CBI
2	I	402	Y01	CAC-CBB-CBE-CBI
2	I	410	Y01	CAO-CBB-CBE-CBI
2	I	410	Y01	CAC-CBB-CBE-CBI
2	J	402	Y01	CAC-CBB-CBE-CBI
2	J	410	Y01	CAO-CBB-CBE-CBI
2	J	410	Y01	CAC-CBB-CBE-CBI
2	K	402	Y01	CAC-CBB-CBE-CBI
2	K	410	Y01	CAO-CBB-CBE-CBI
2	K	410	Y01	CAC-CBB-CBE-CBI
2	L	401	Y01	CAO-CBB-CBE-CBI
2	L	401	Y01	CAC-CBB-CBE-CBI
2	L	404	Y01	CAC-CBB-CBE-CBI
2	B	401	Y01	CAJ-CAO-CBB-CBE
2	E	401	Y01	CAJ-CAO-CBB-CBE
2	I	401	Y01	CAJ-CAO-CBB-CBE

There are no ring outliers.

36 monomers are involved in 48 short contacts:

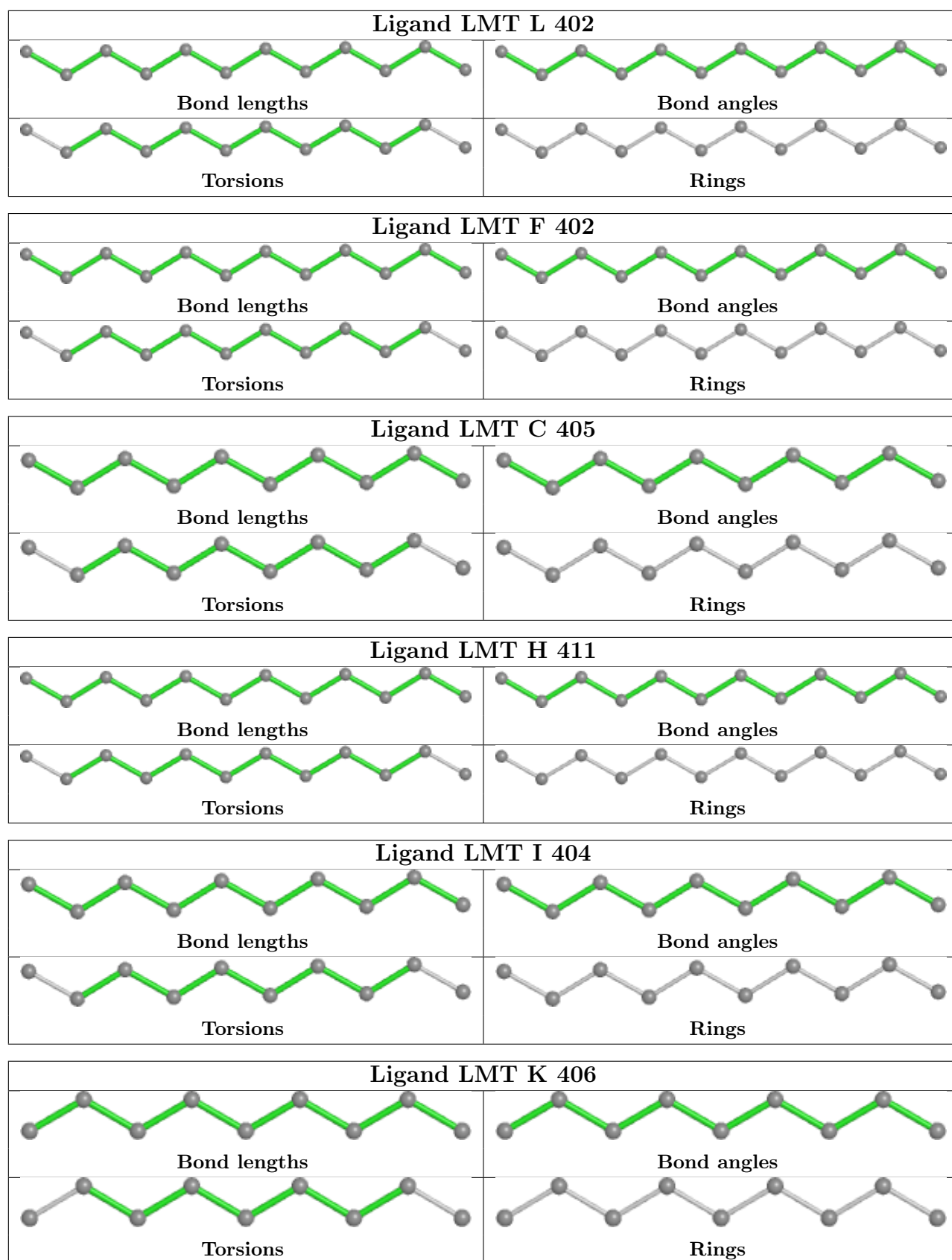
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	402	LMT	1	0
3	H	411	LMT	1	0
2	F	411	Y01	2	0
2	K	409	Y01	2	0
2	C	409	Y01	2	0
2	A	409	Y01	2	0
3	B	411	LMT	1	0
3	L	405	LMT	1	0
3	J	403	LMT	1	0
3	F	405	LMT	1	0
2	L	403	Y01	1	0

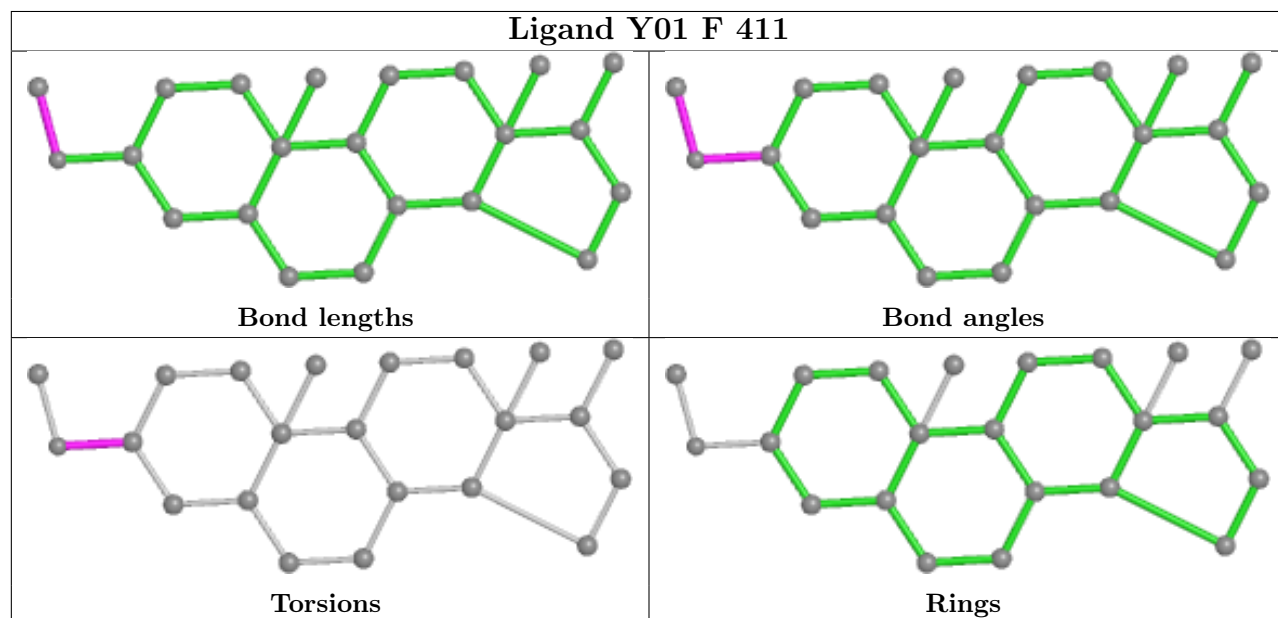
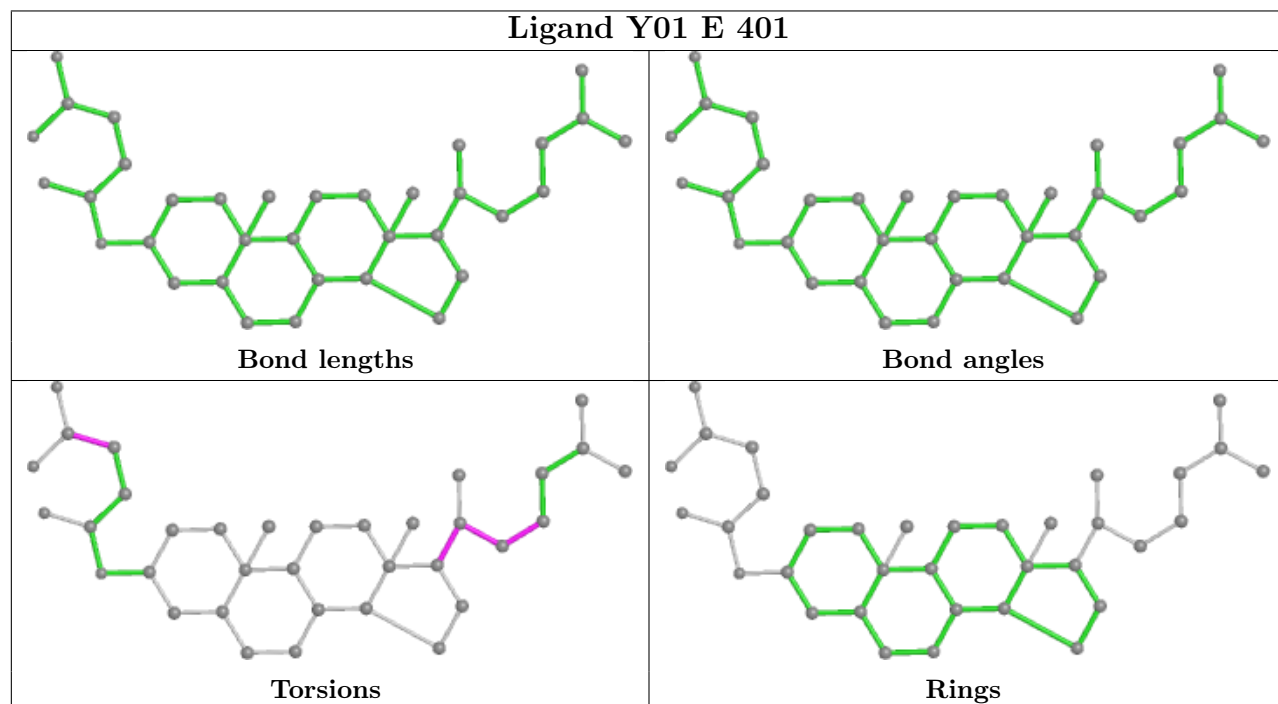
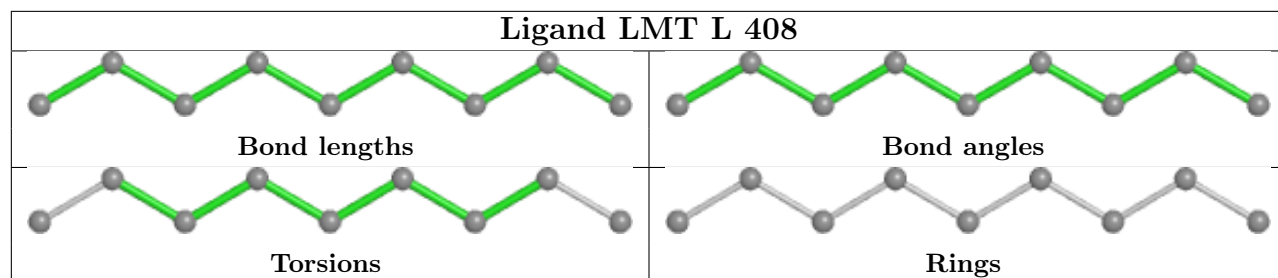
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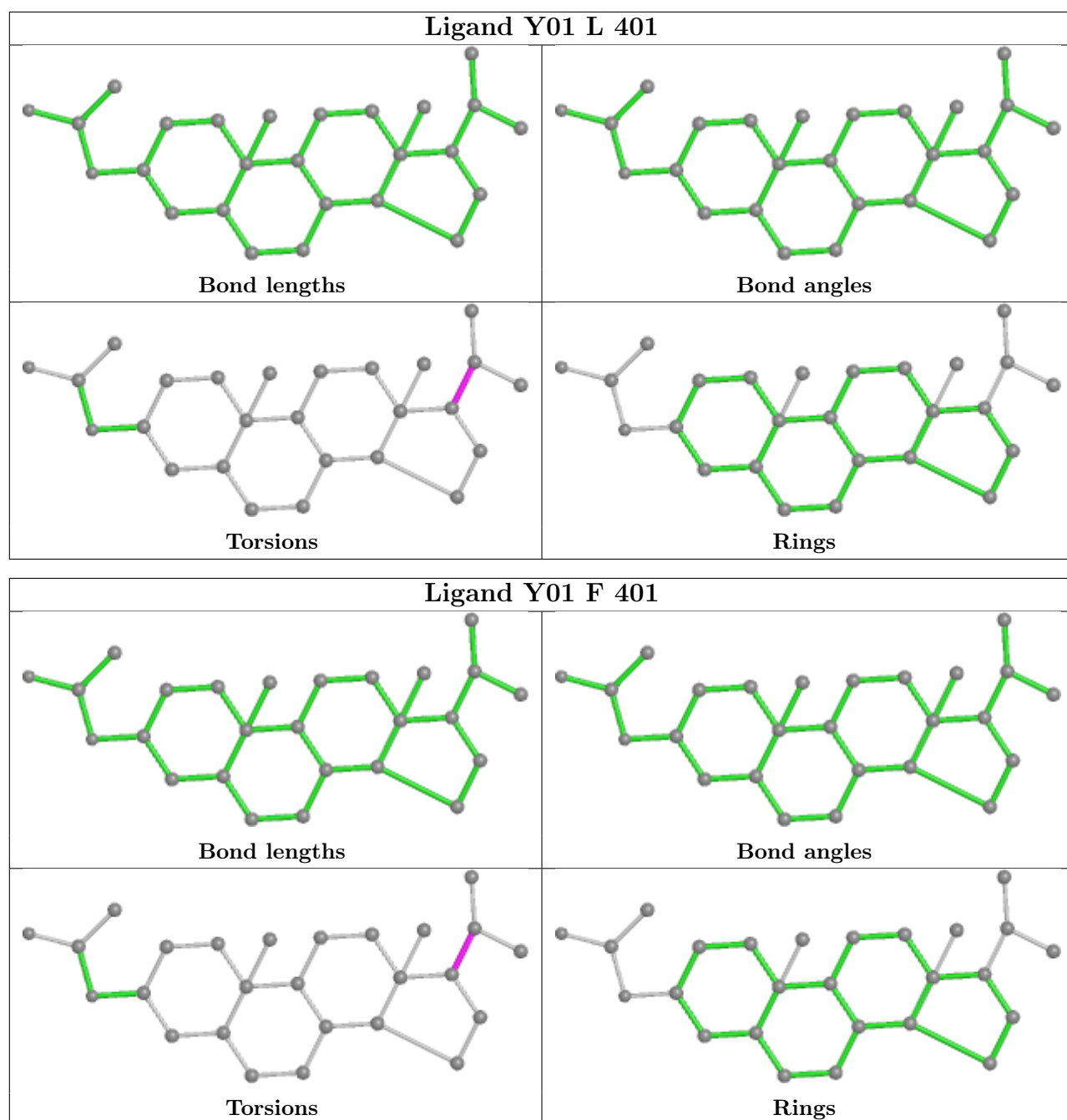
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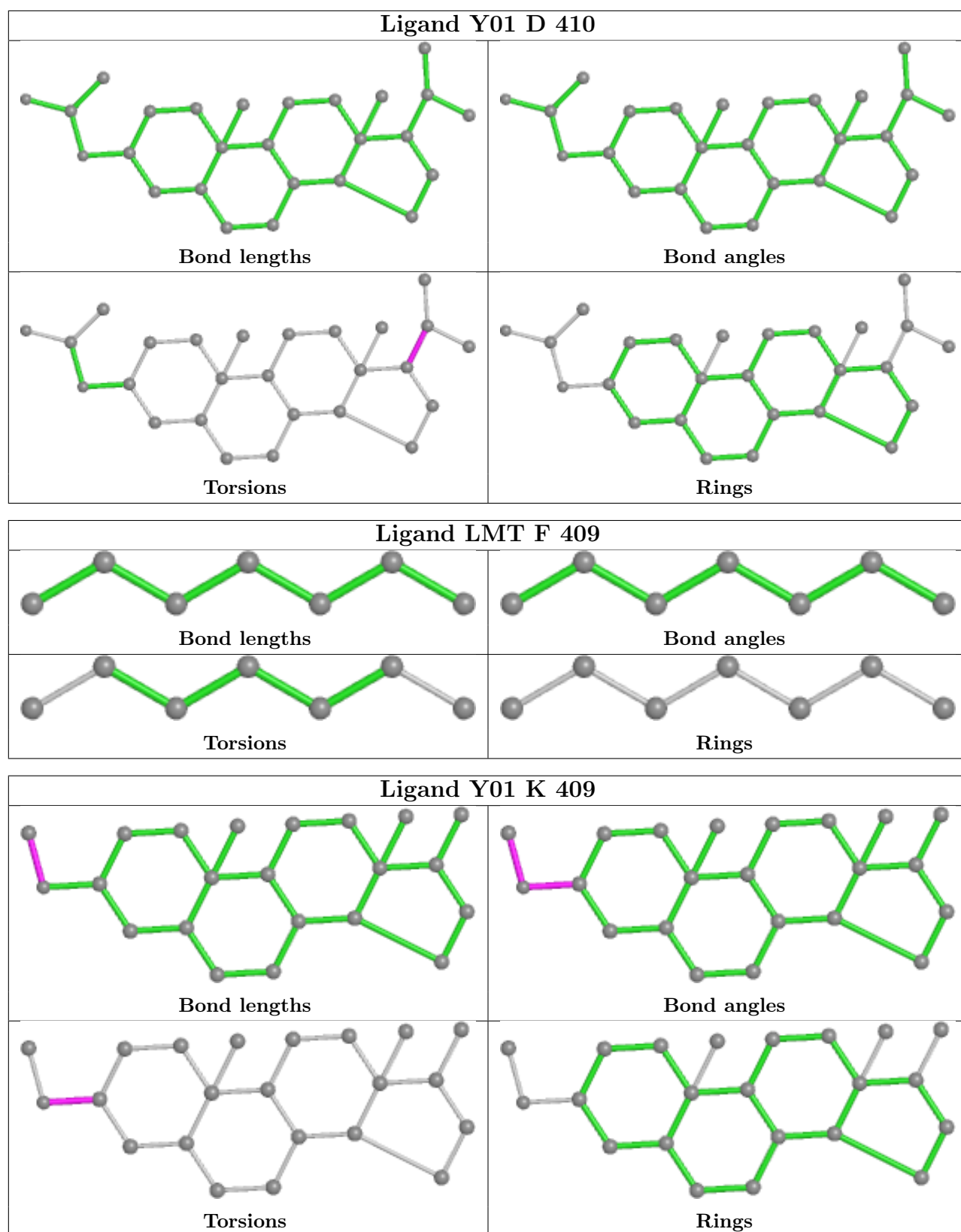
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	411	Y01	2	0
3	A	403	LMT	1	0
2	A	401	Y01	1	0
3	E	411	LMT	1	0
2	H	409	Y01	2	0
3	G	411	LMT	1	0
3	I	403	LMT	1	0
3	E	403	LMT	1	0
2	I	409	Y01	2	0
2	K	401	Y01	1	0
3	K	403	LMT	1	0
3	C	403	LMT	1	0
3	D	411	LMT	1	0
2	J	409	Y01	2	0
3	C	411	LMT	1	0
2	D	409	Y01	2	0
3	G	403	LMT	1	0
2	G	409	Y01	2	0
3	B	403	LMT	1	0
3	D	403	LMT	1	0
3	H	403	LMT	1	0
2	E	409	Y01	2	0
2	B	401	Y01	1	0
2	B	409	Y01	2	0
3	A	411	LMT	1	0

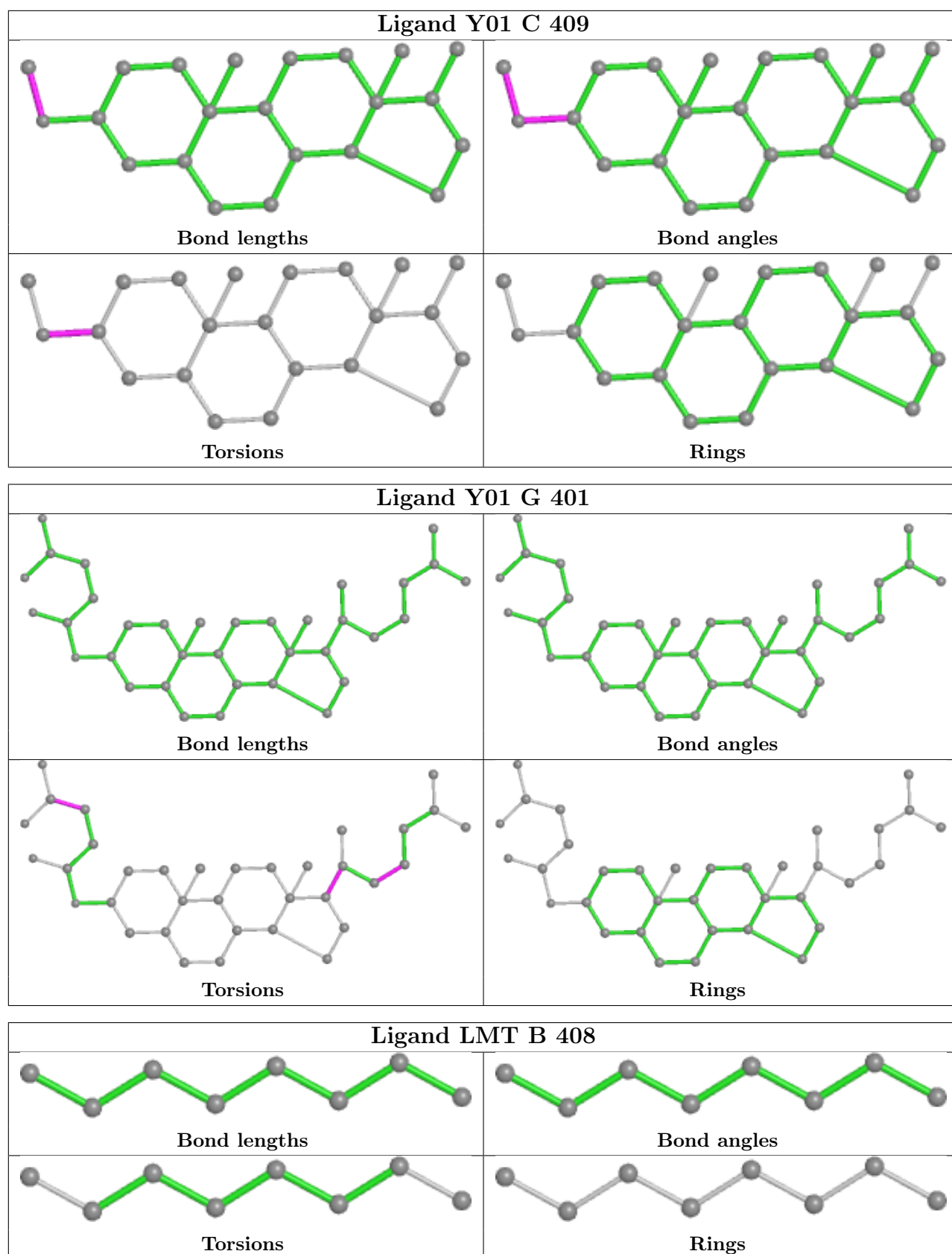
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

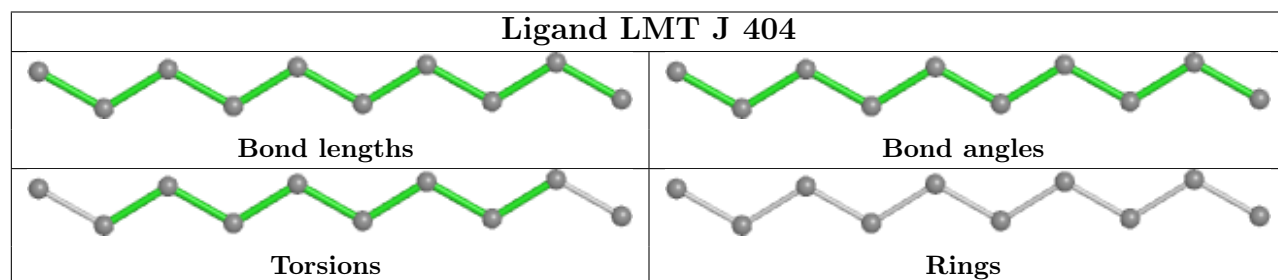
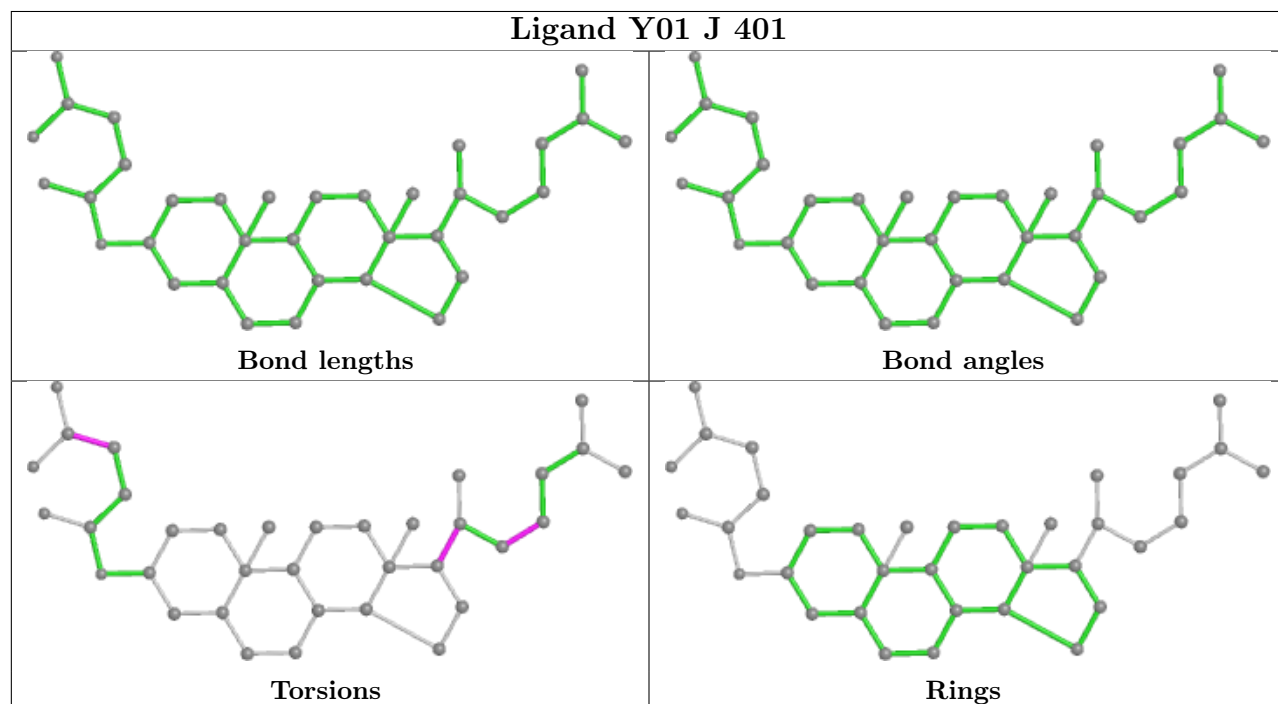
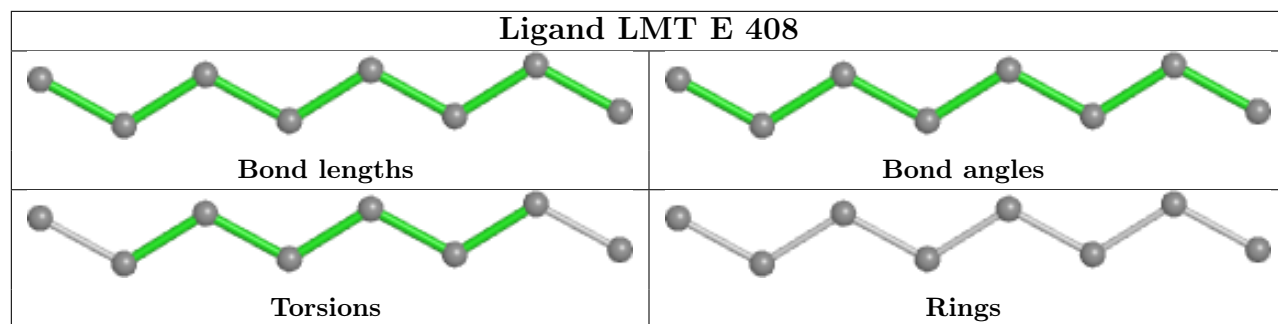


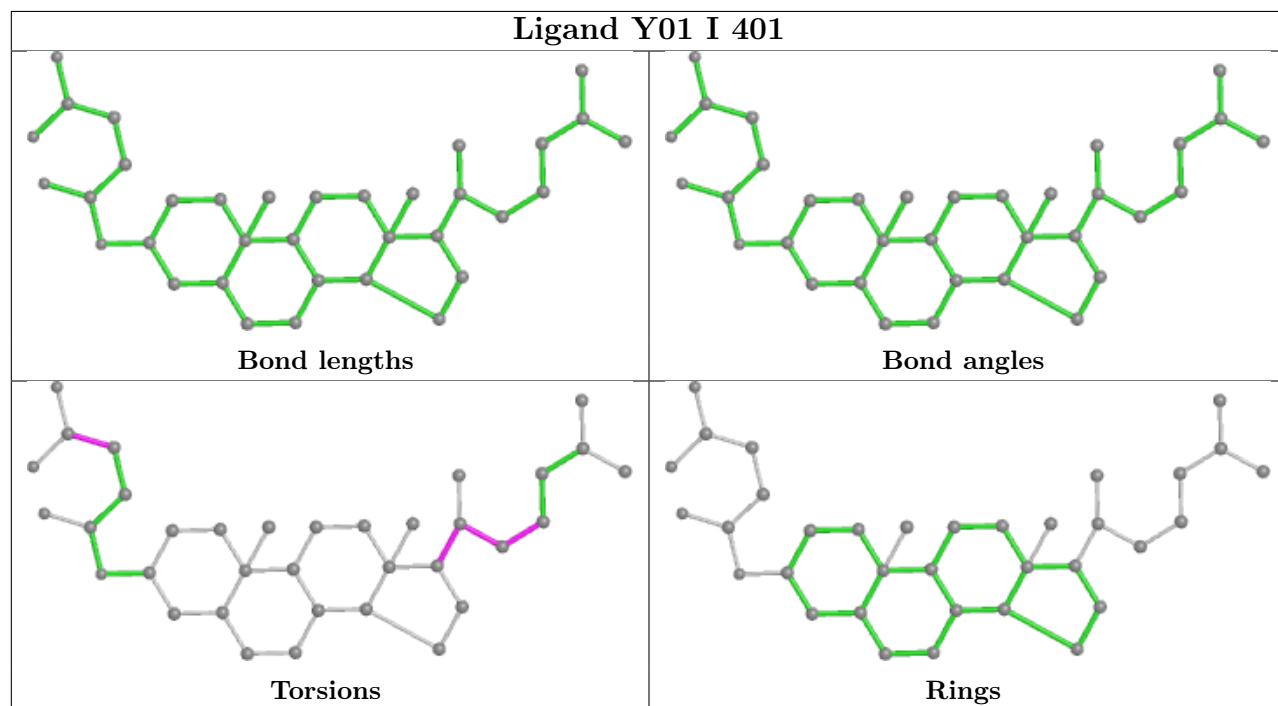
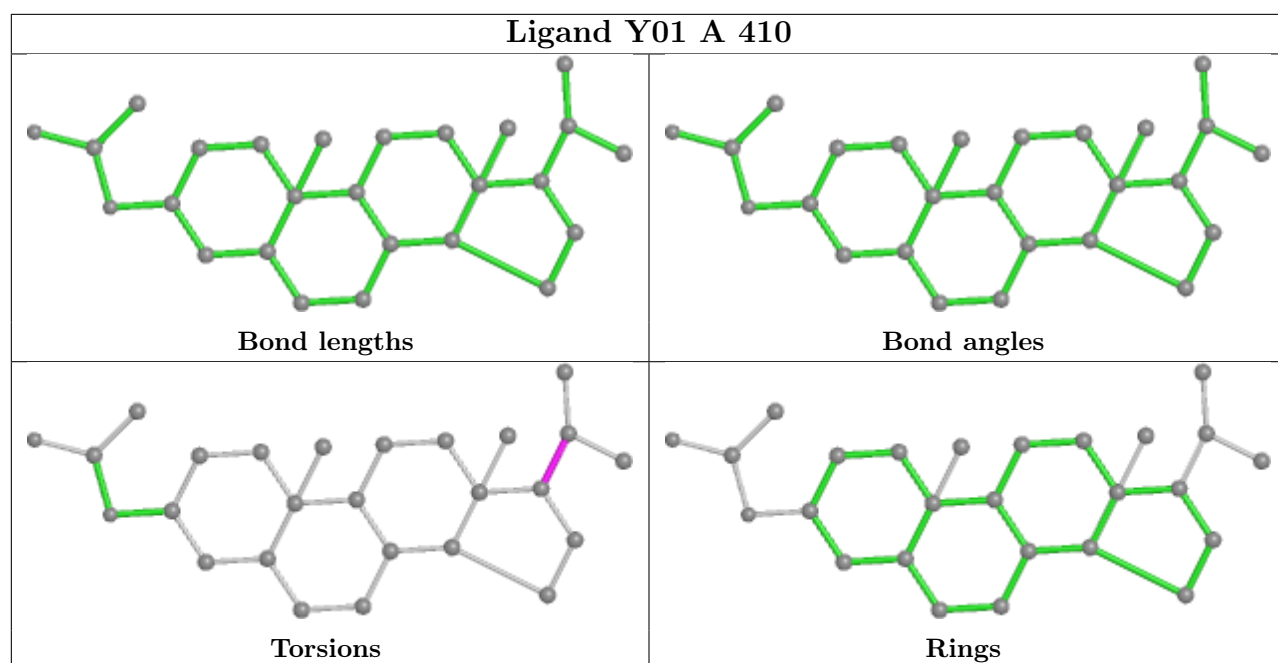


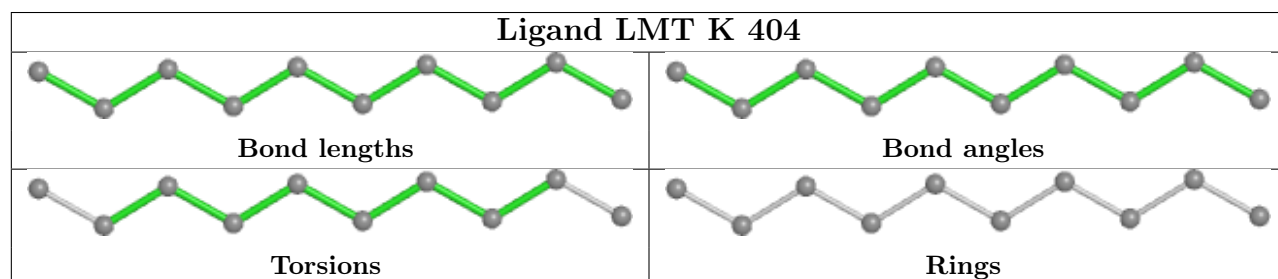
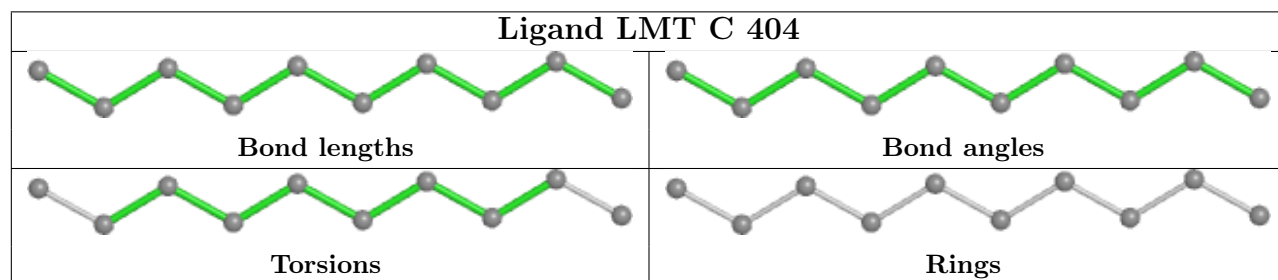
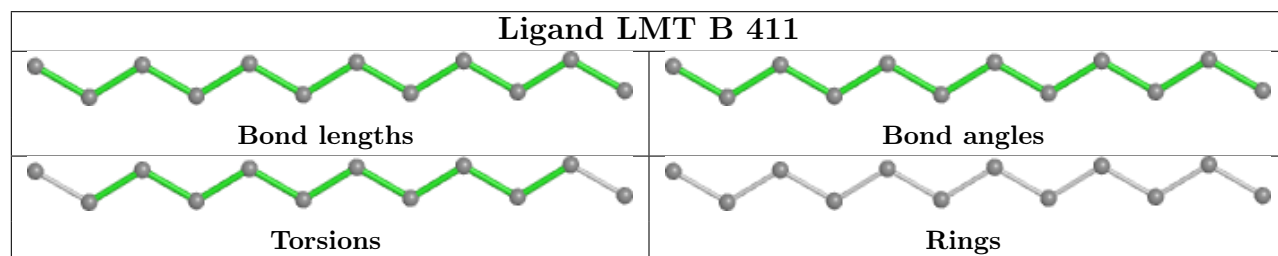
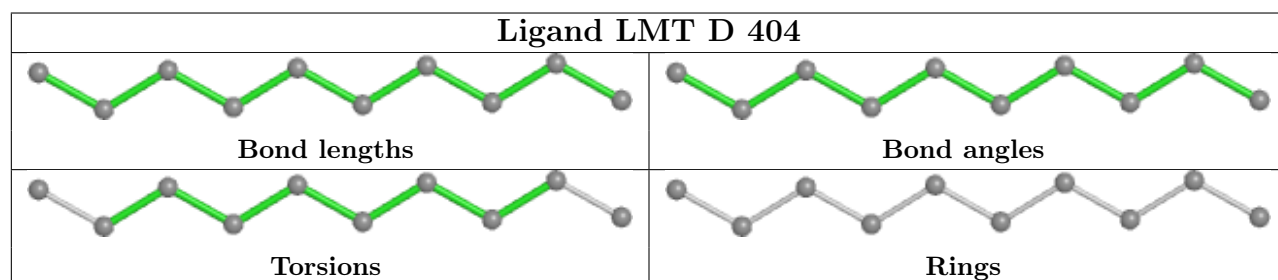
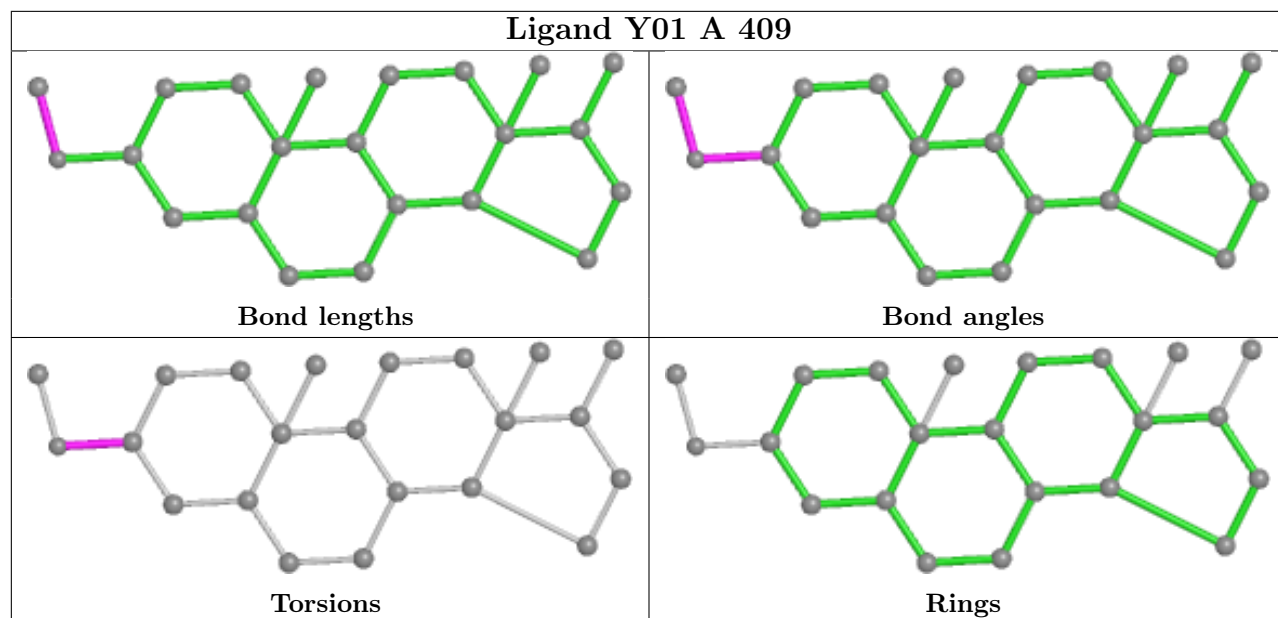


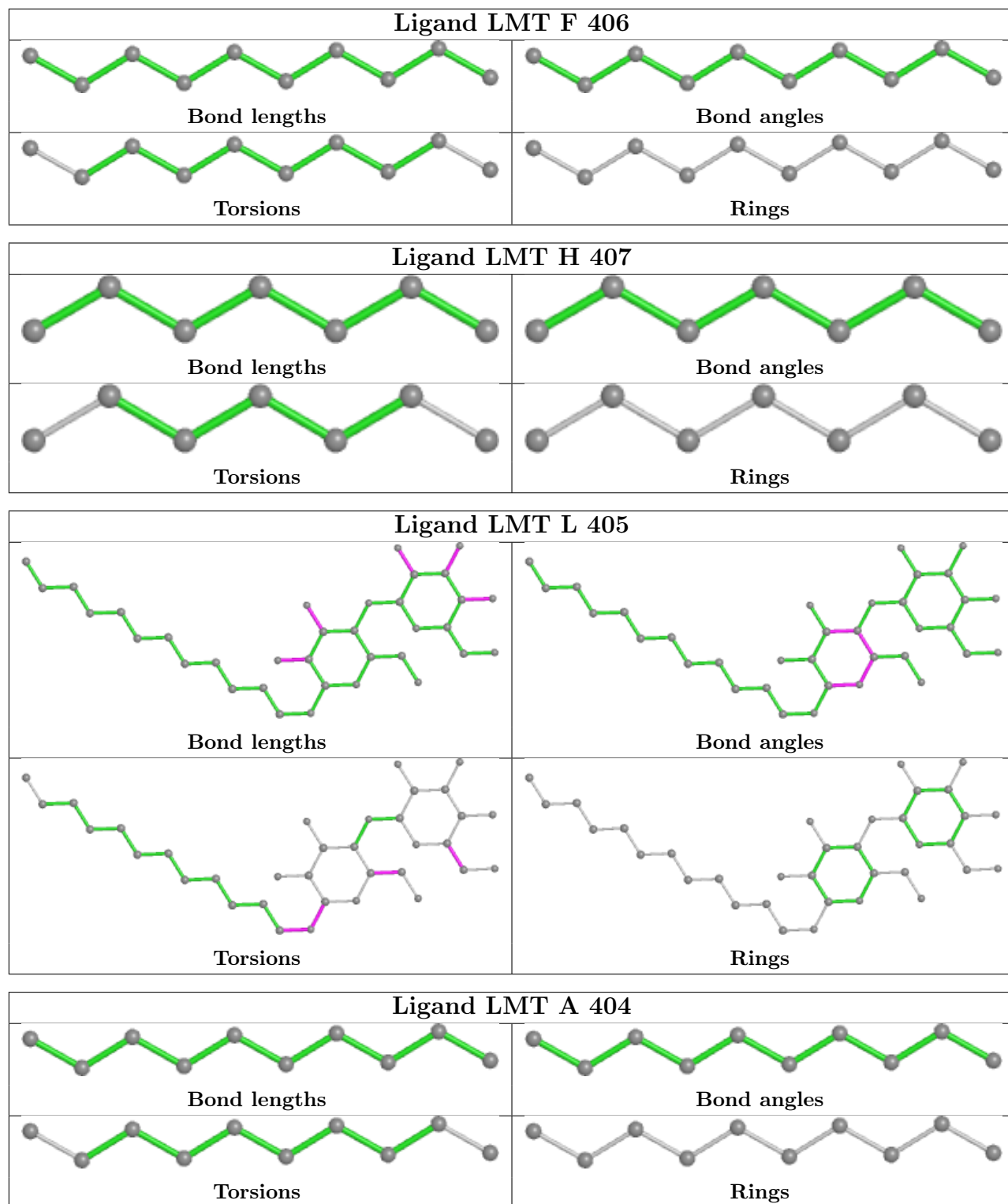


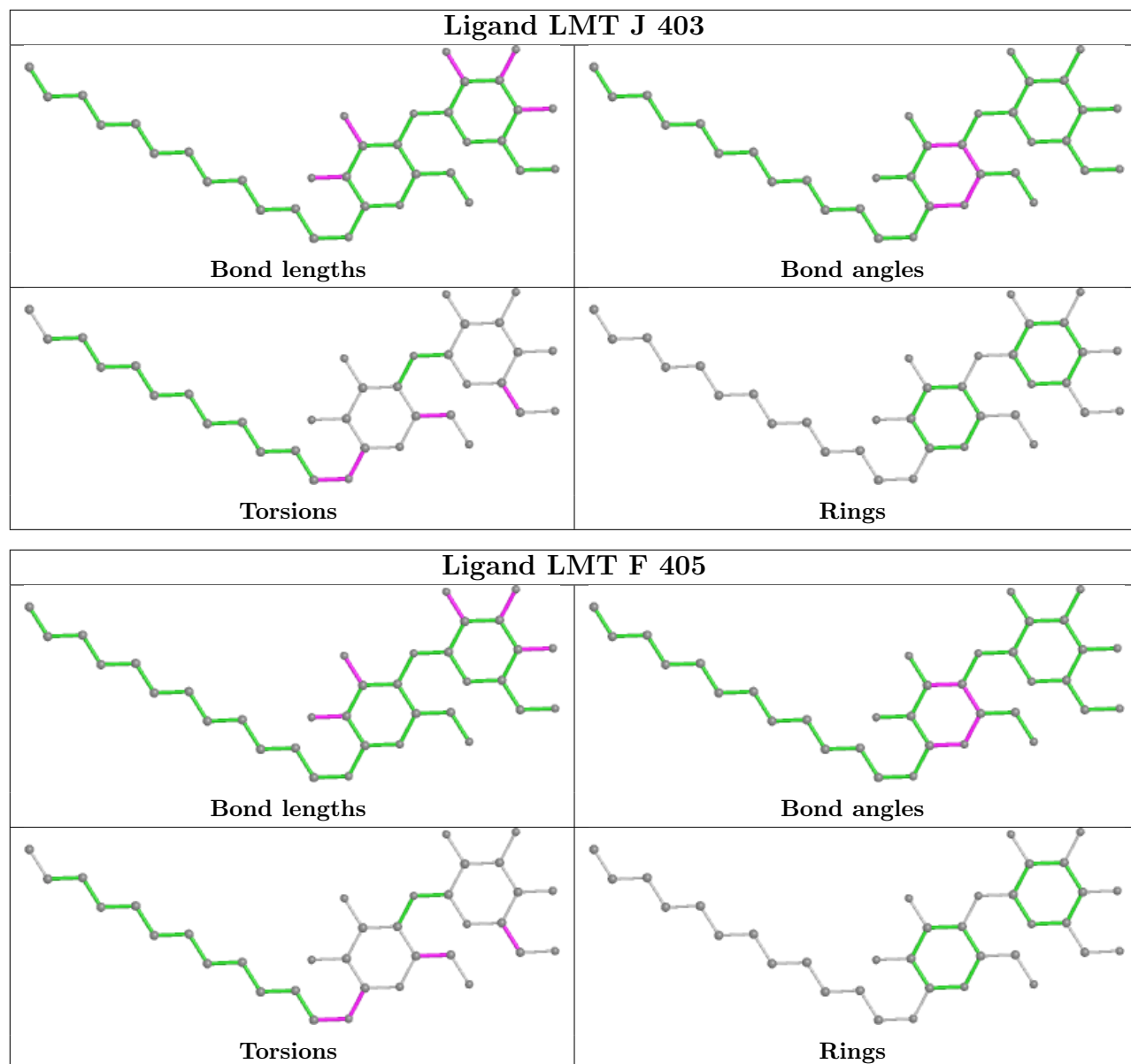


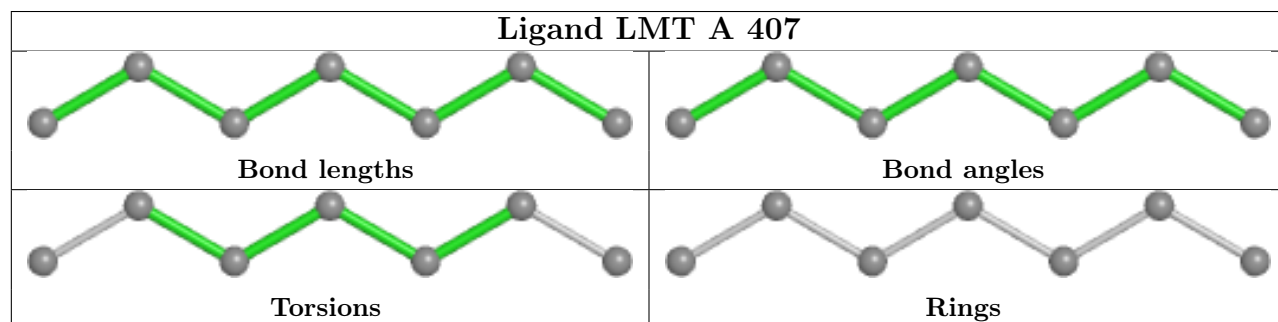
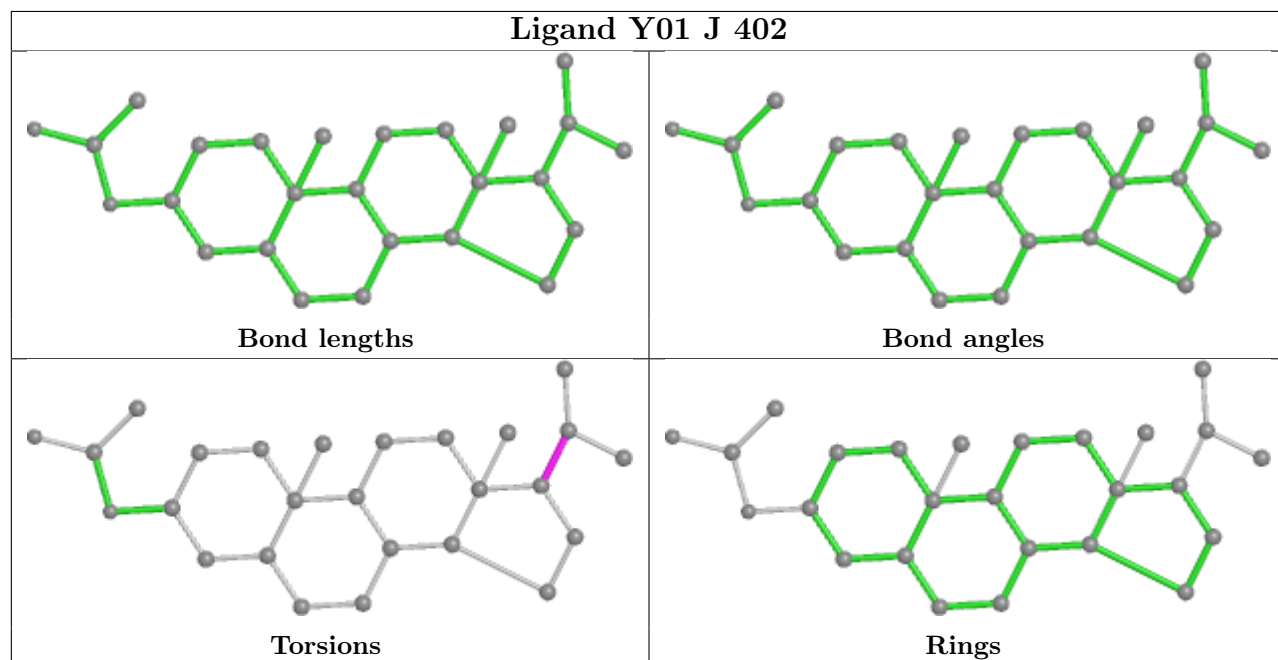
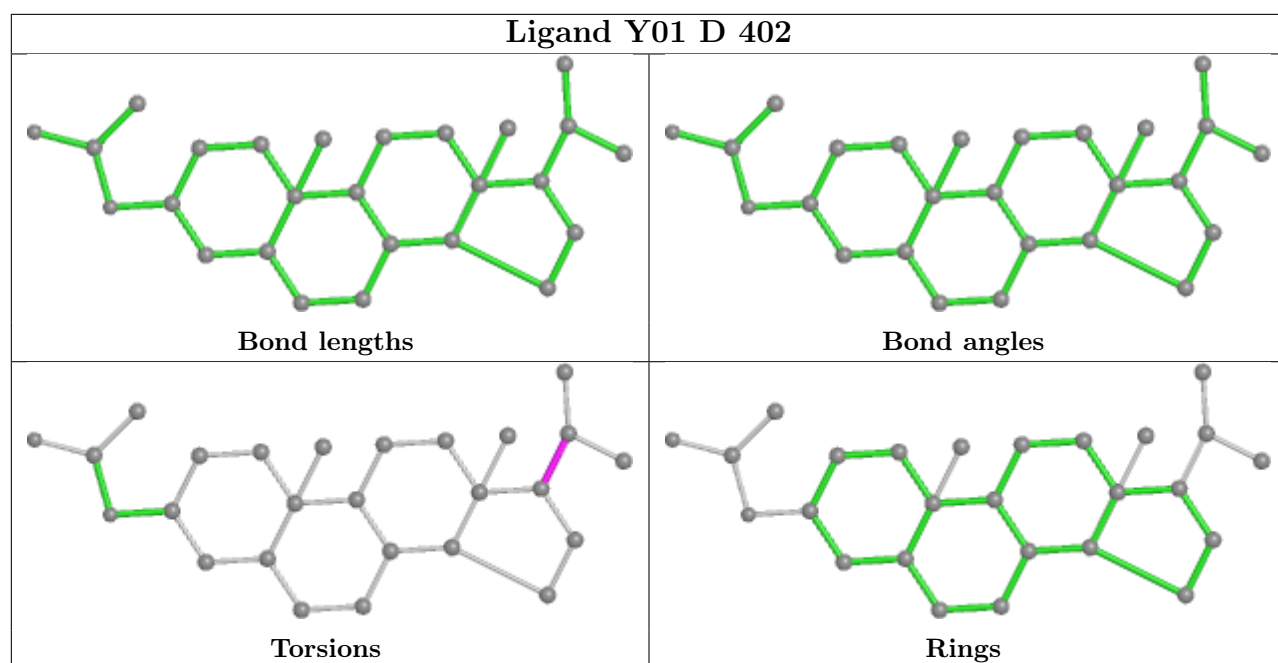


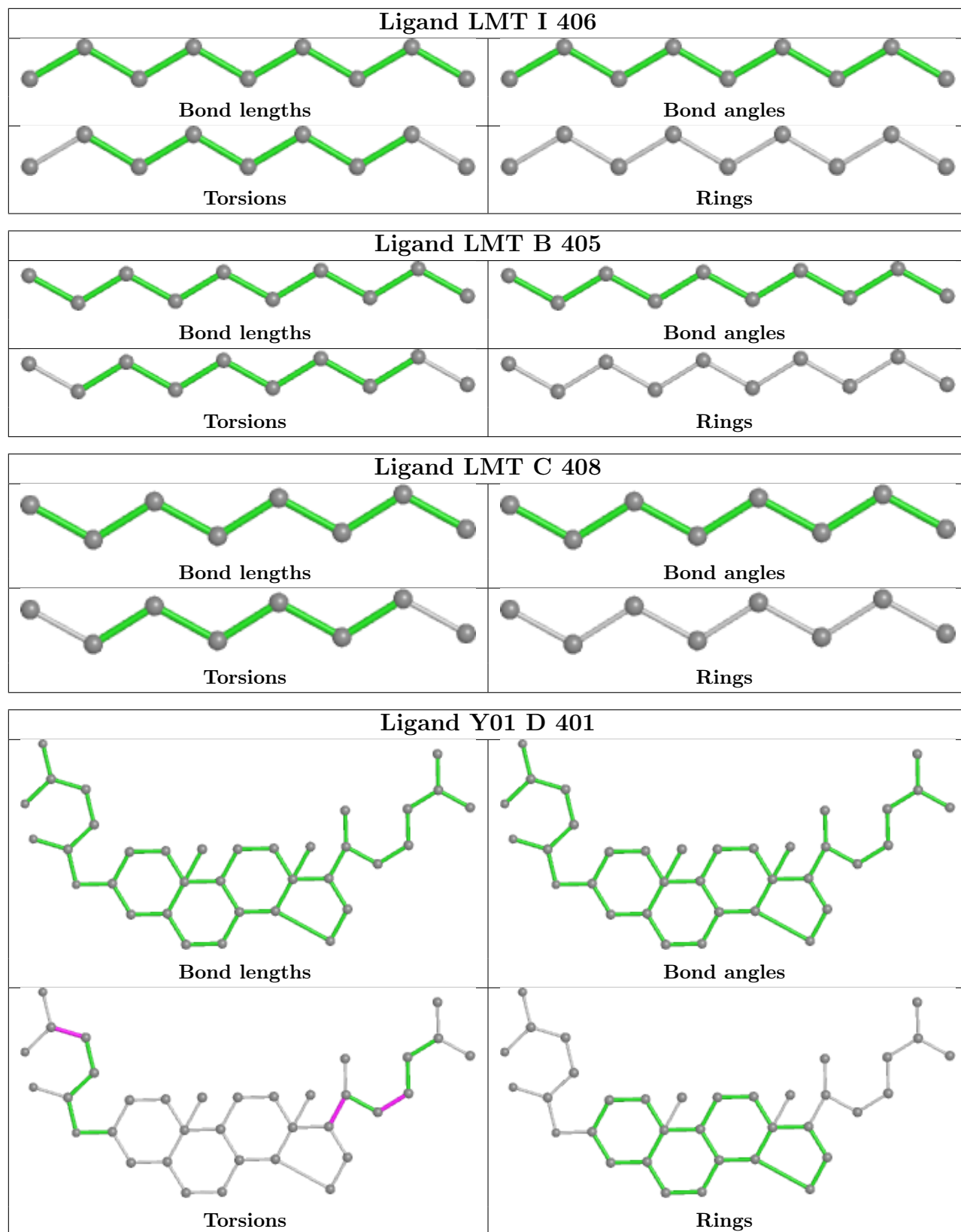




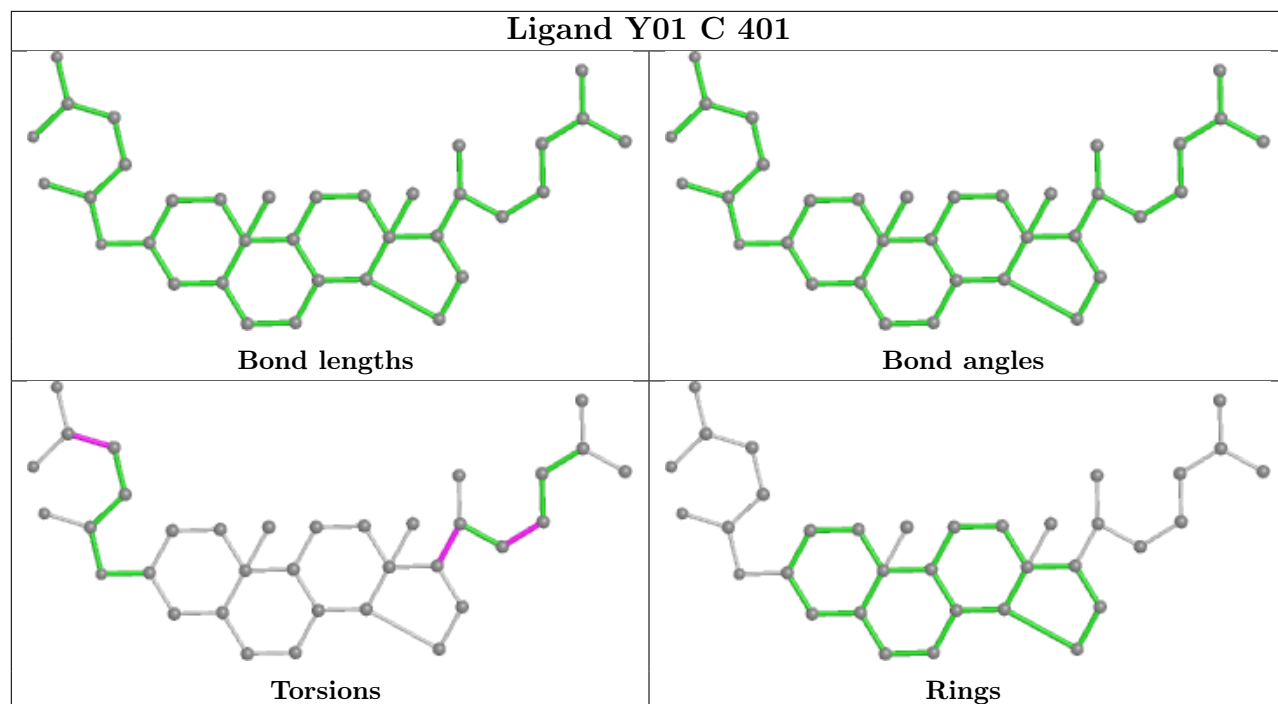




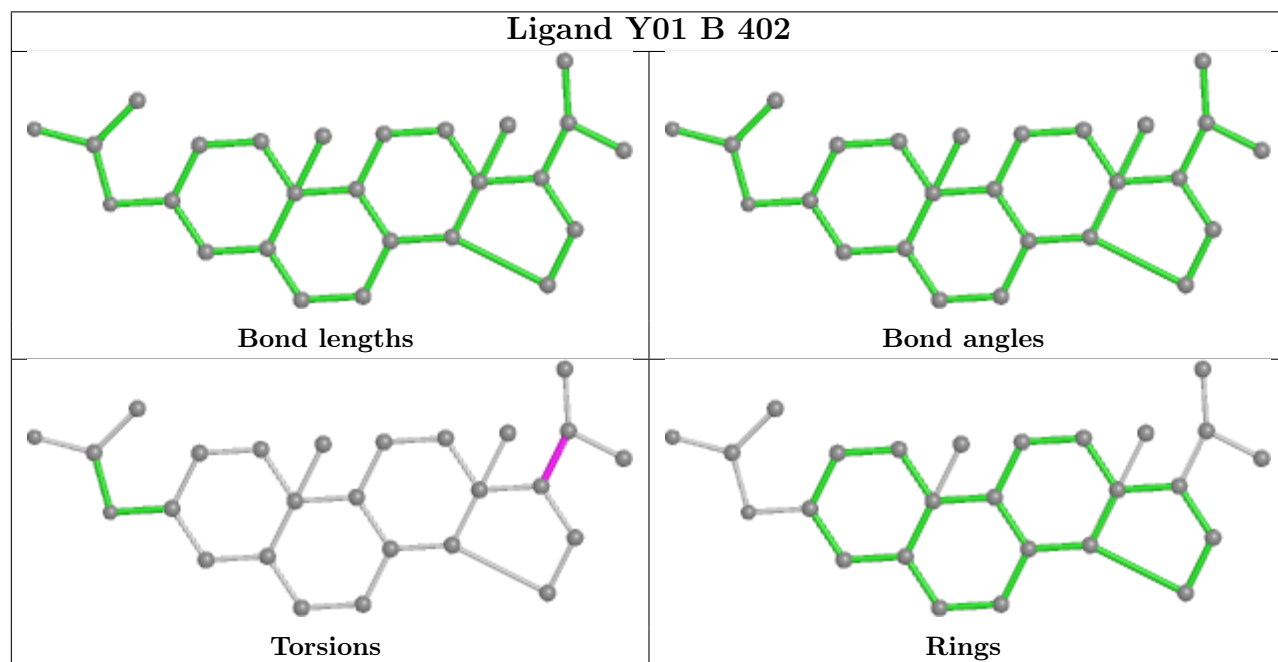


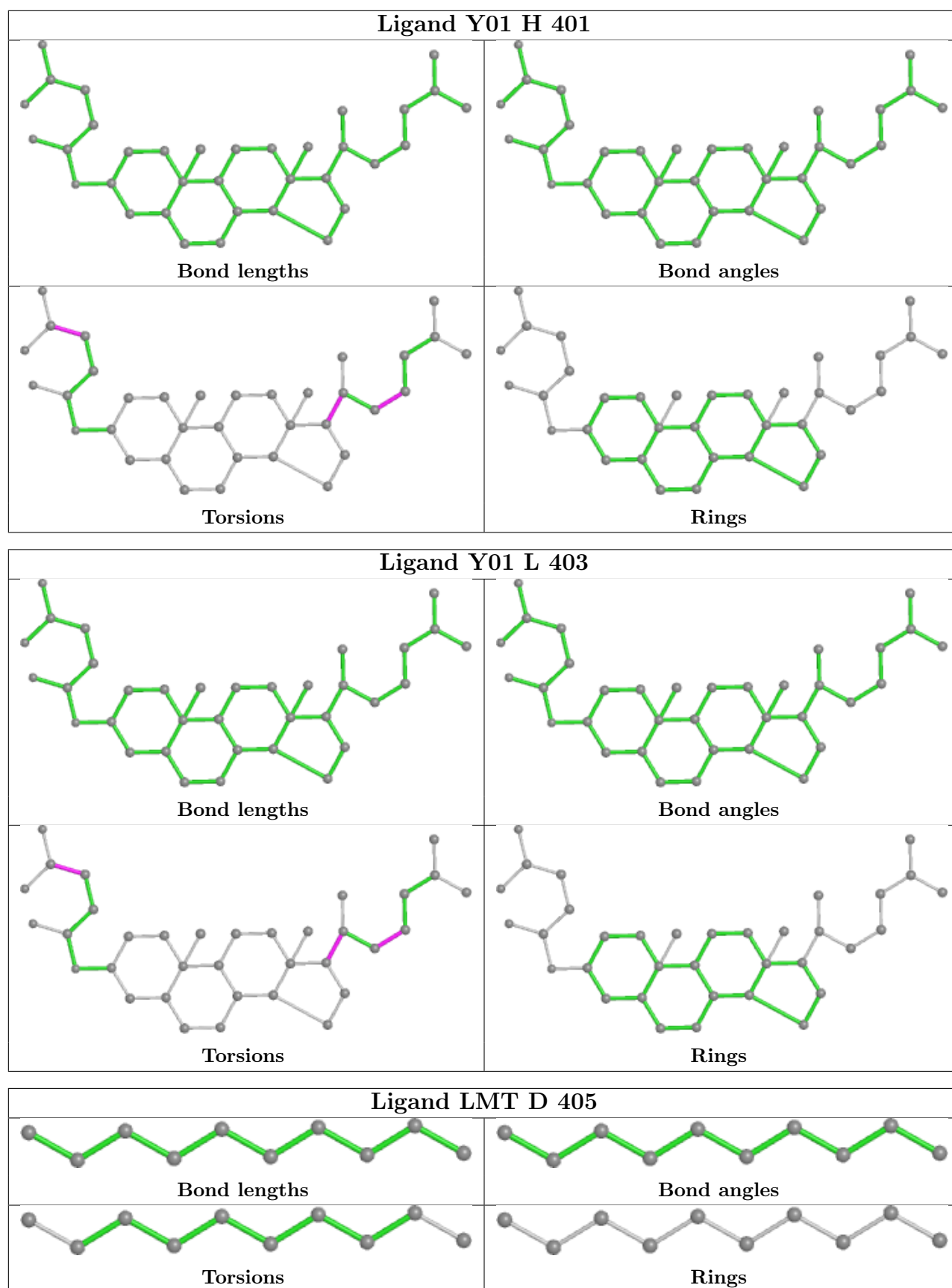


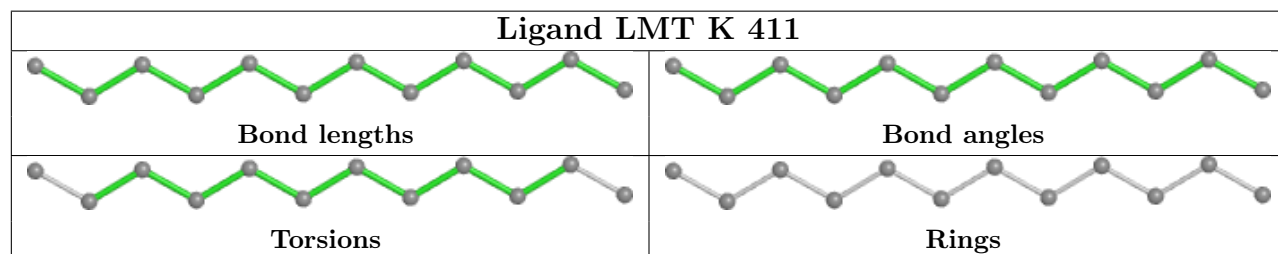
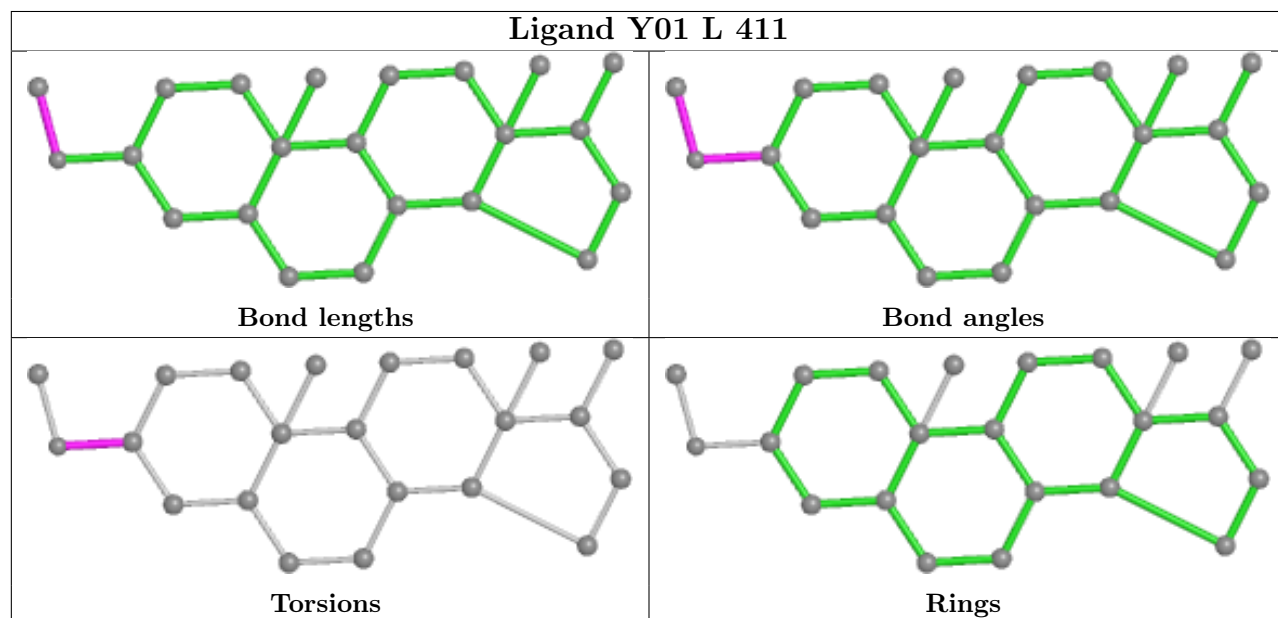
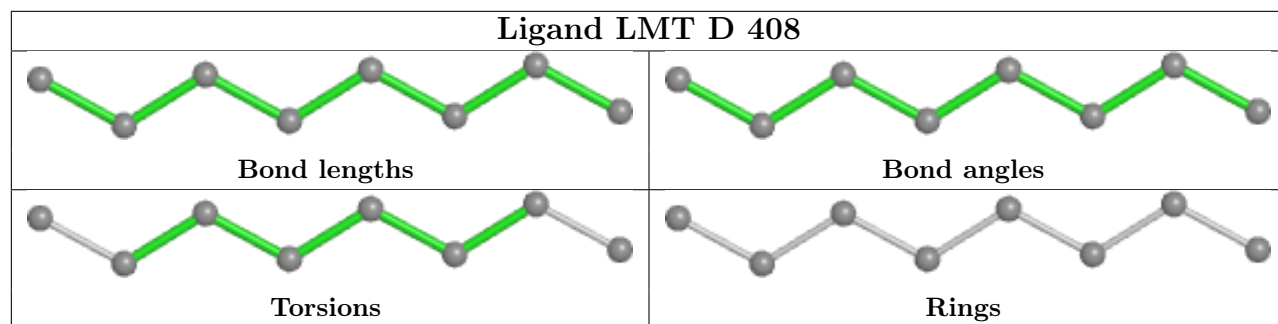
Ligand Y01 C 401

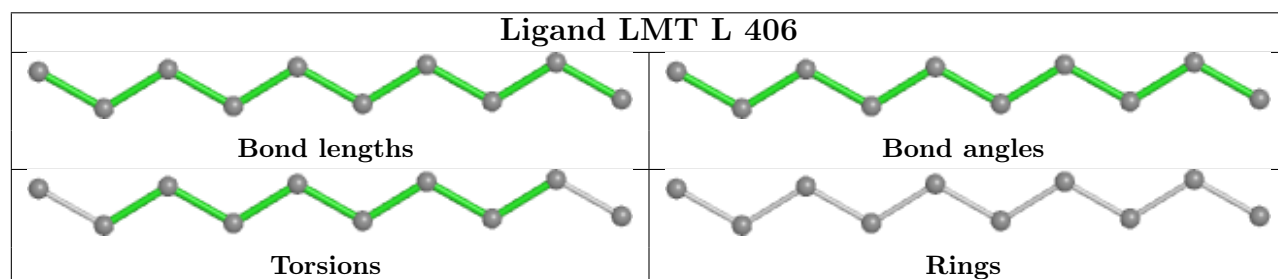
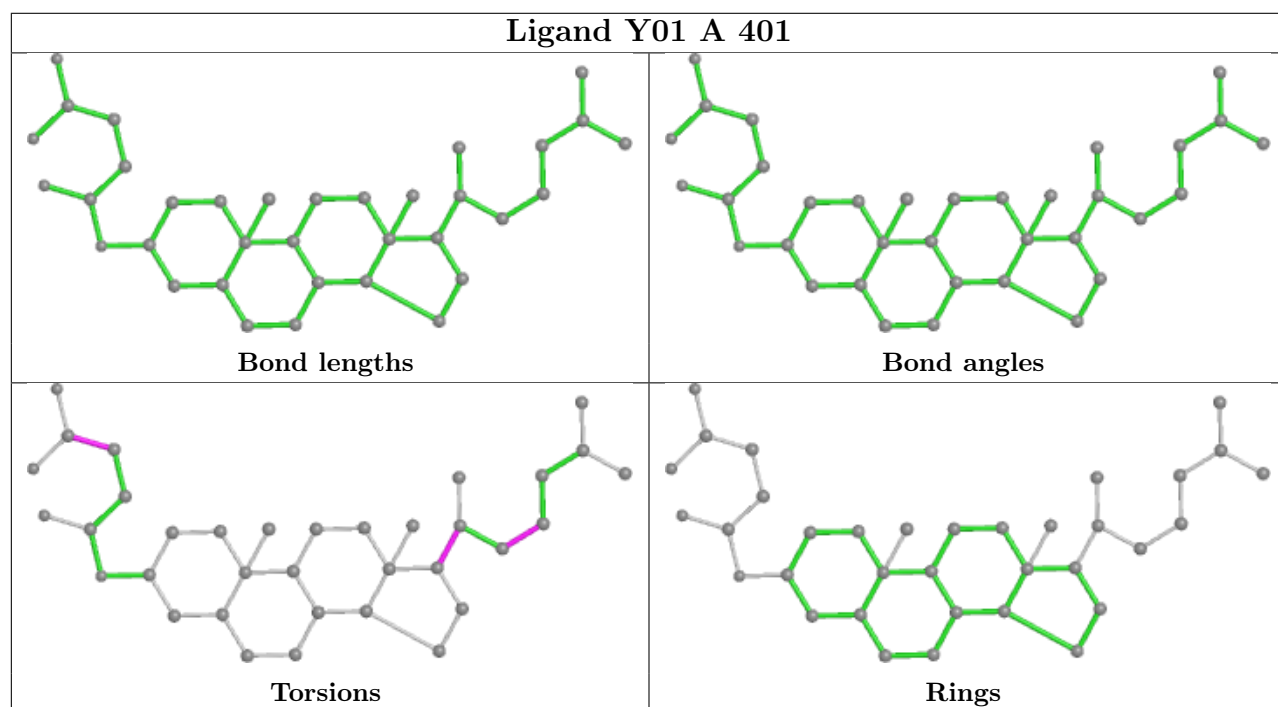
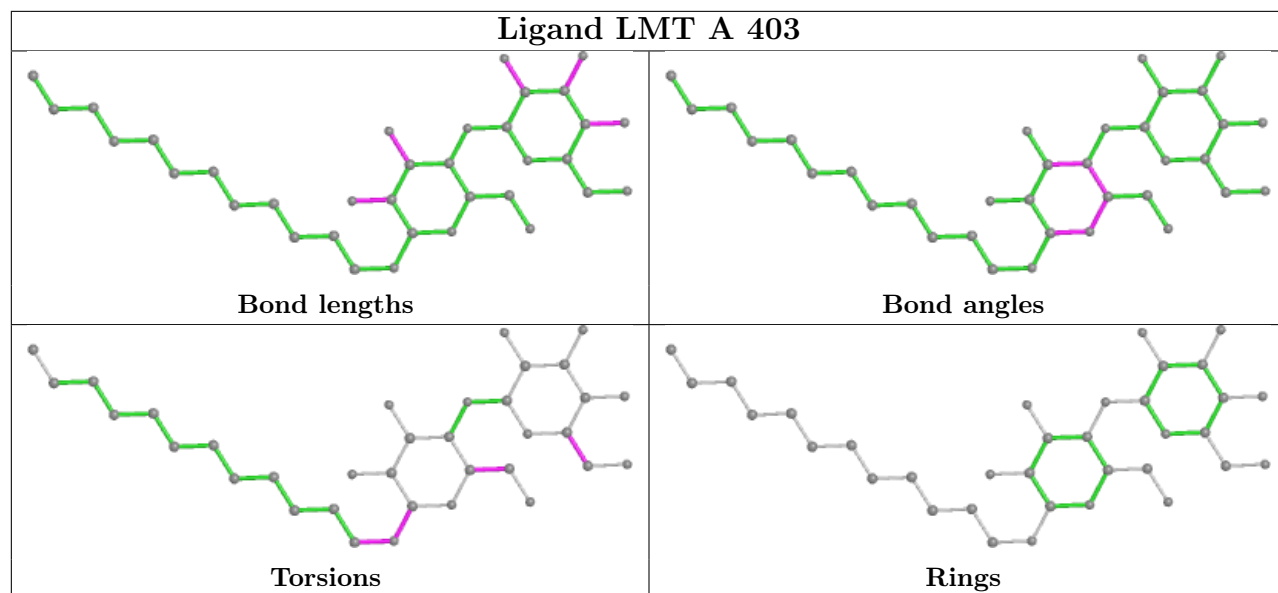


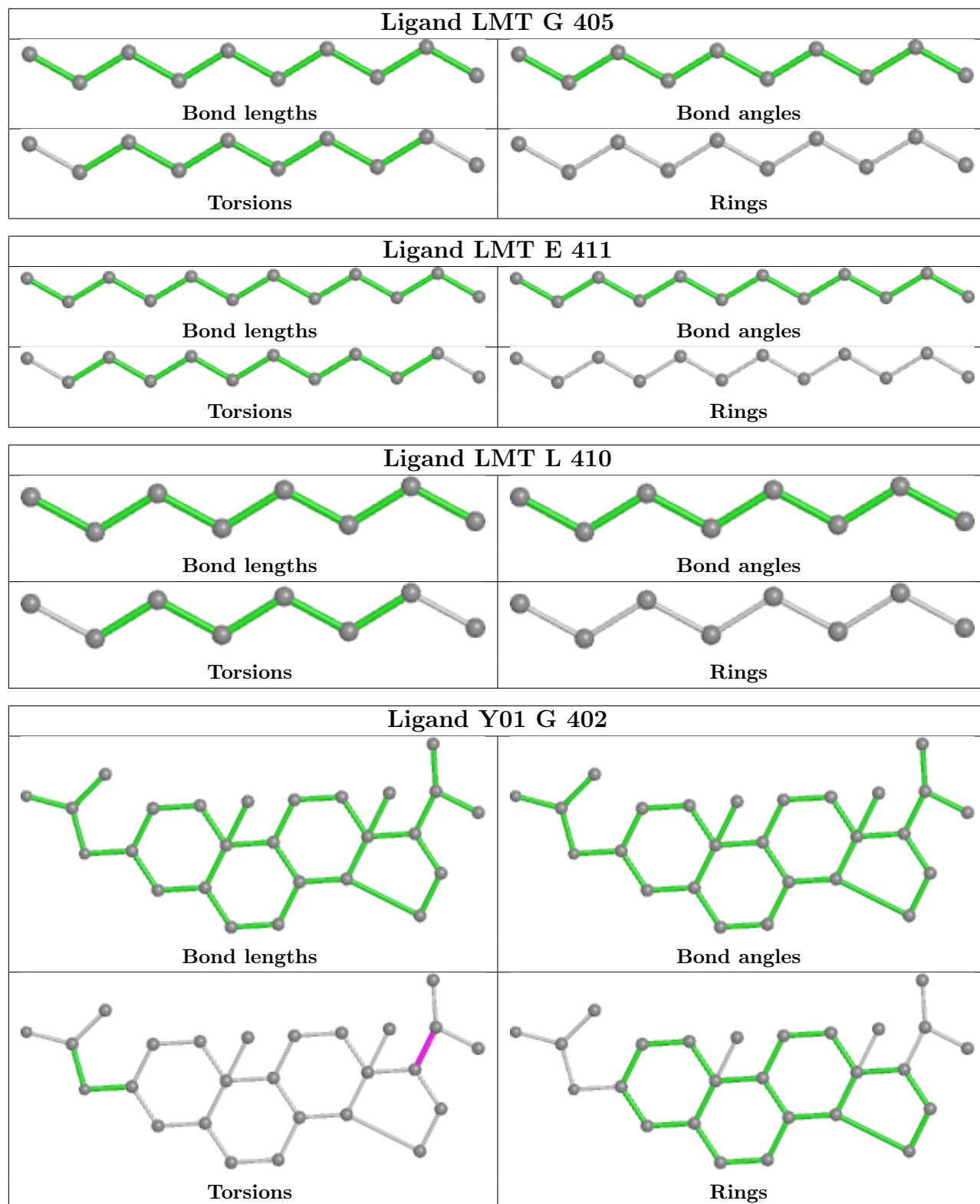
Ligand Y01 B 402

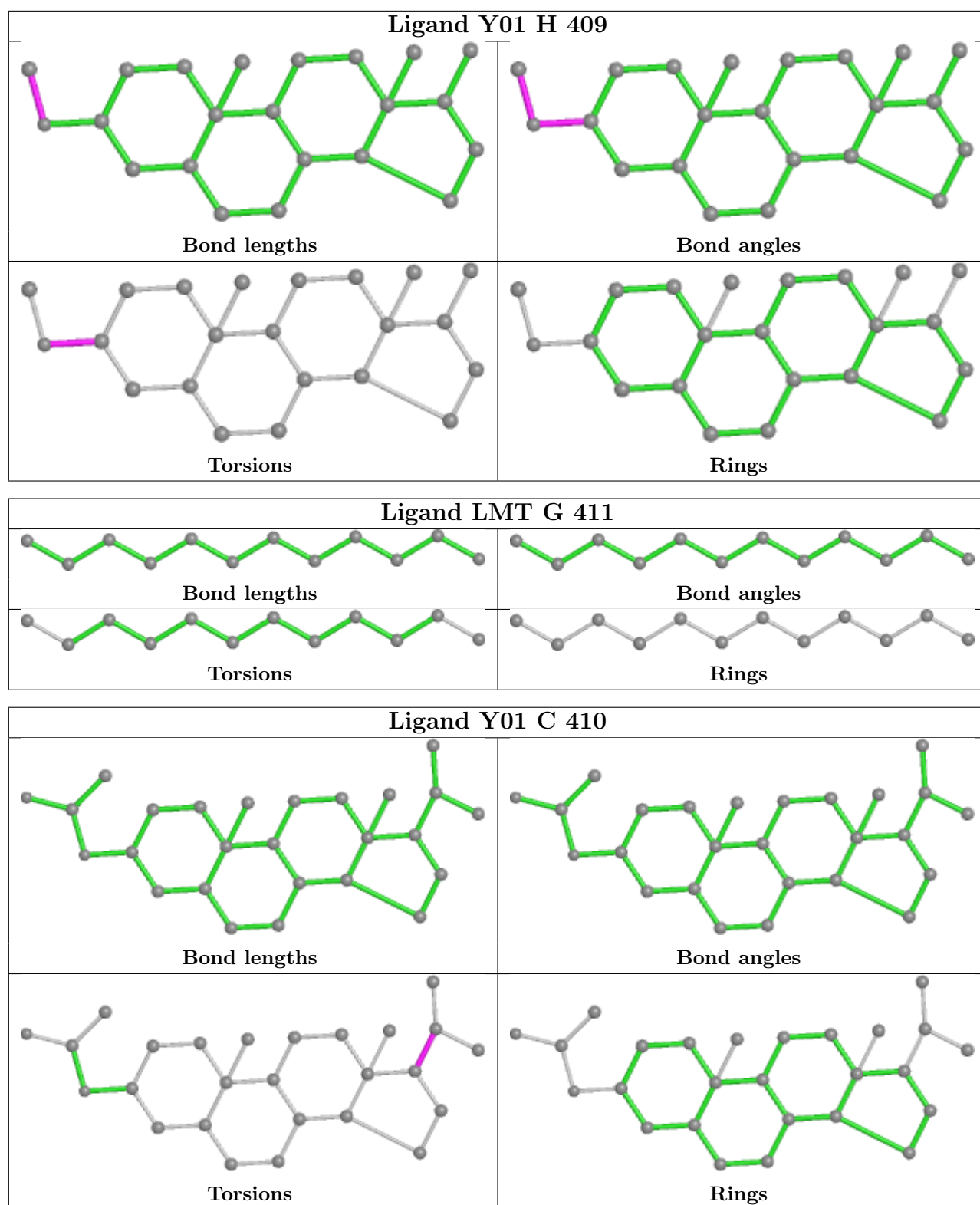


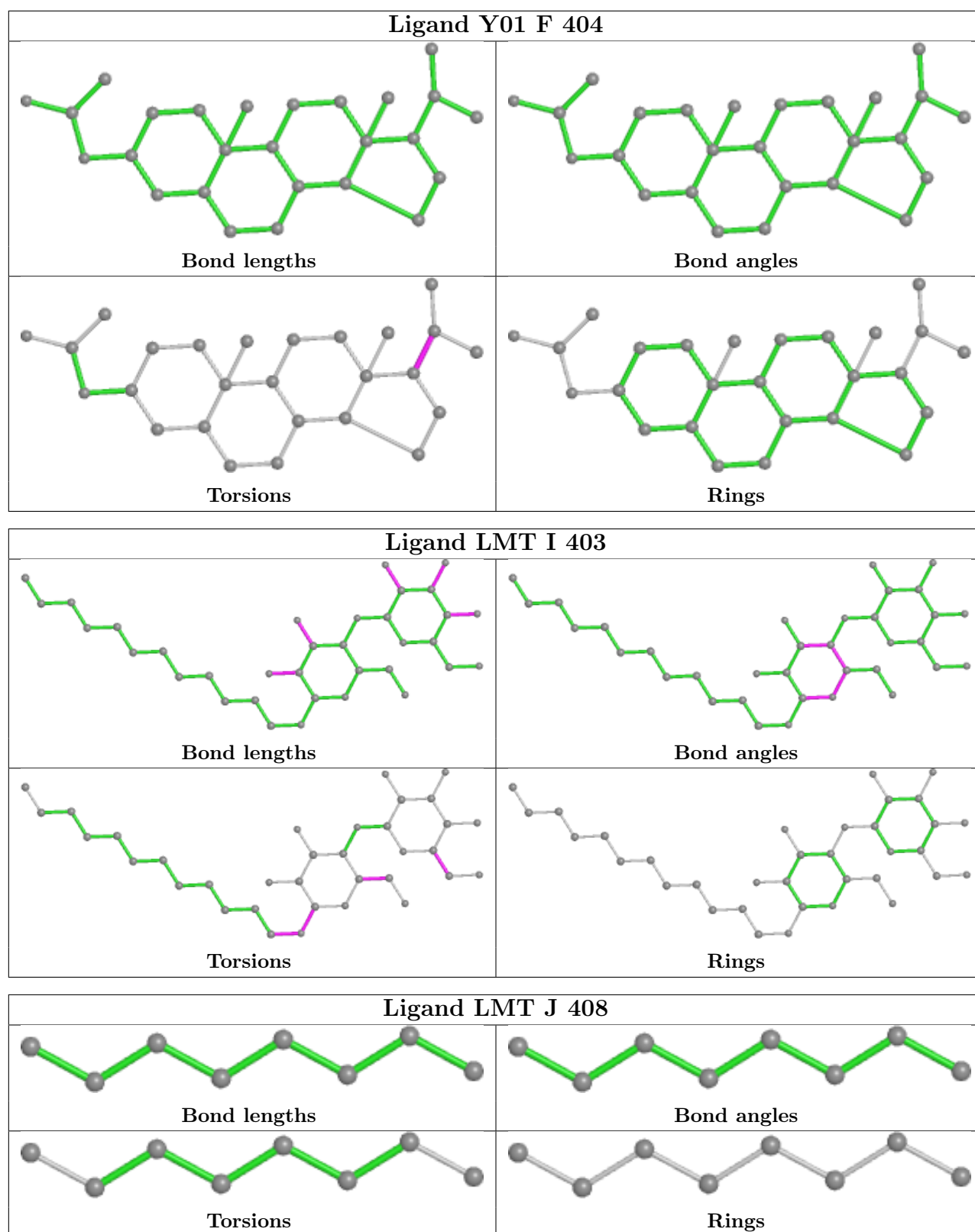


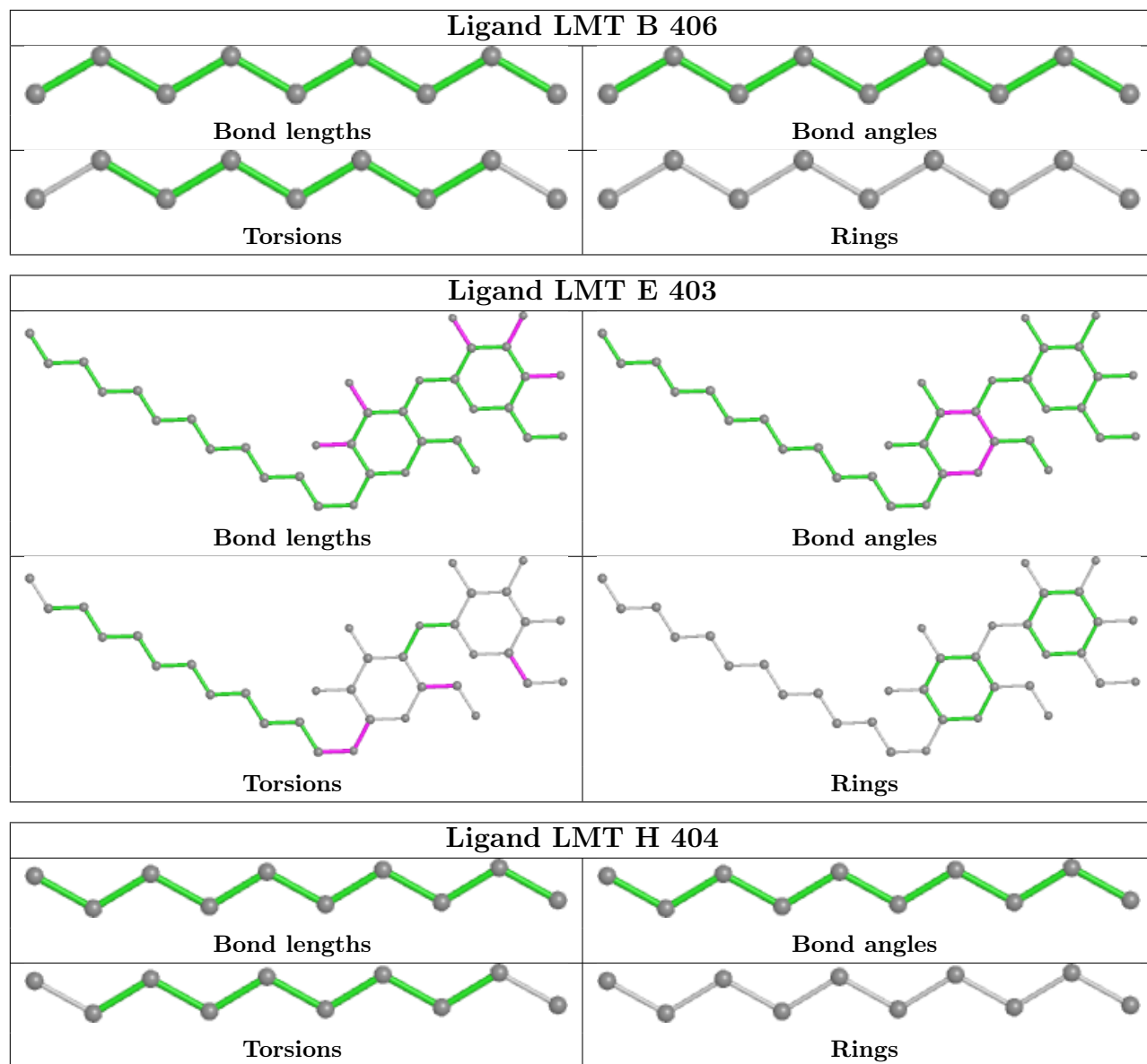


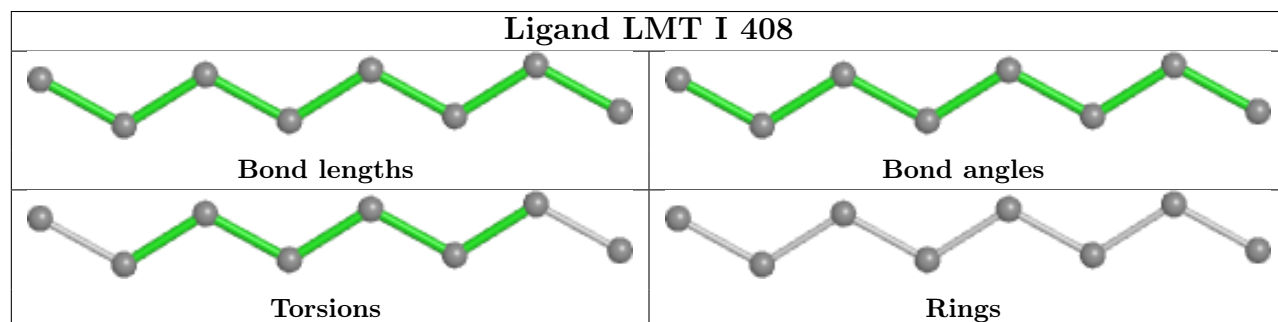
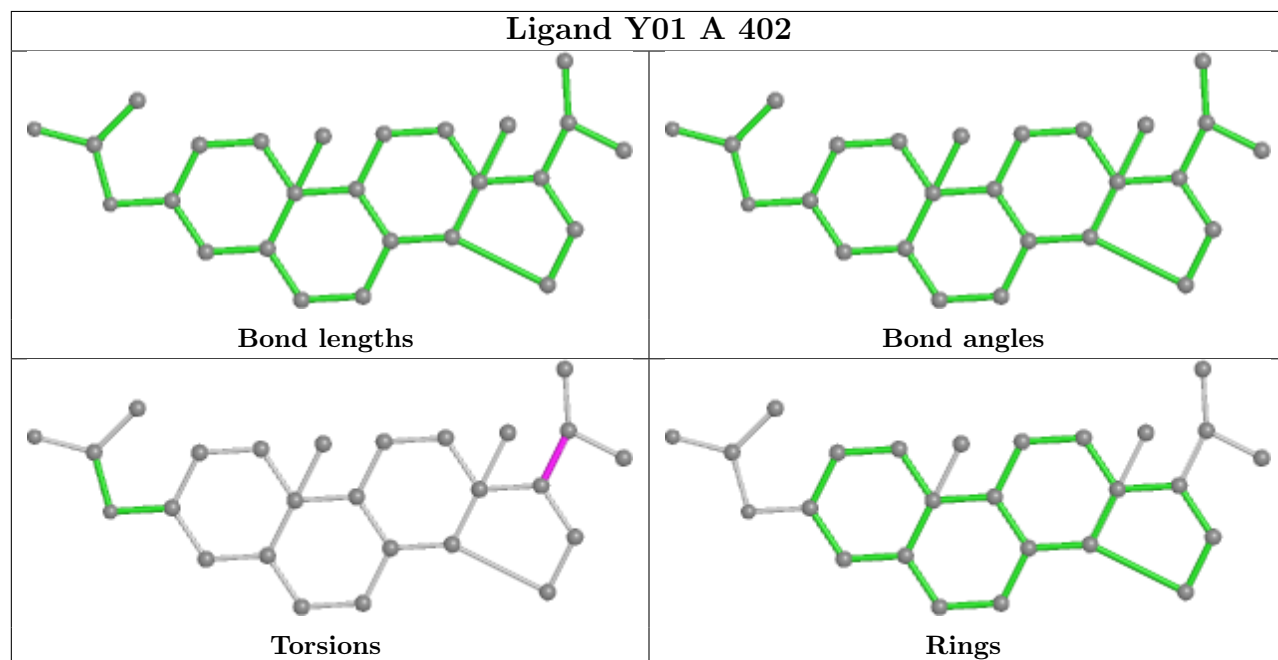
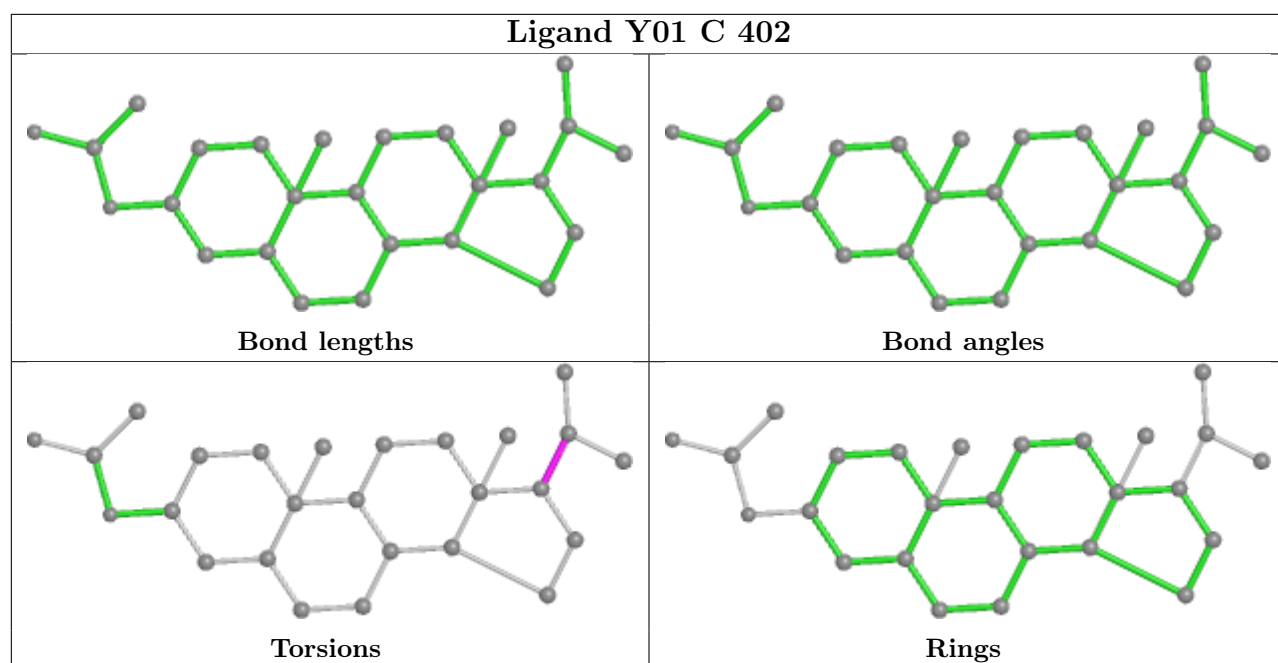


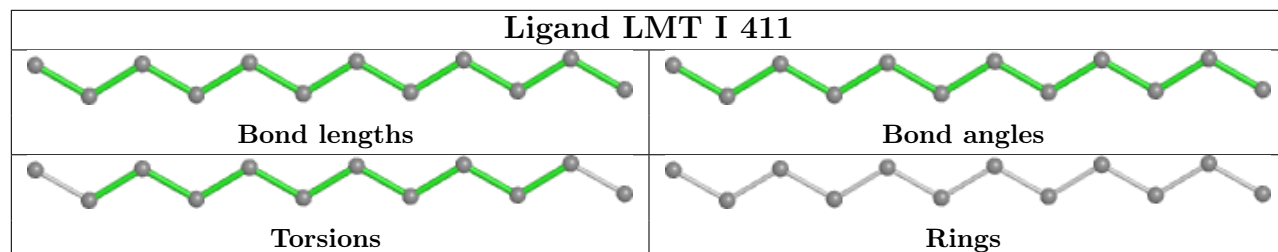
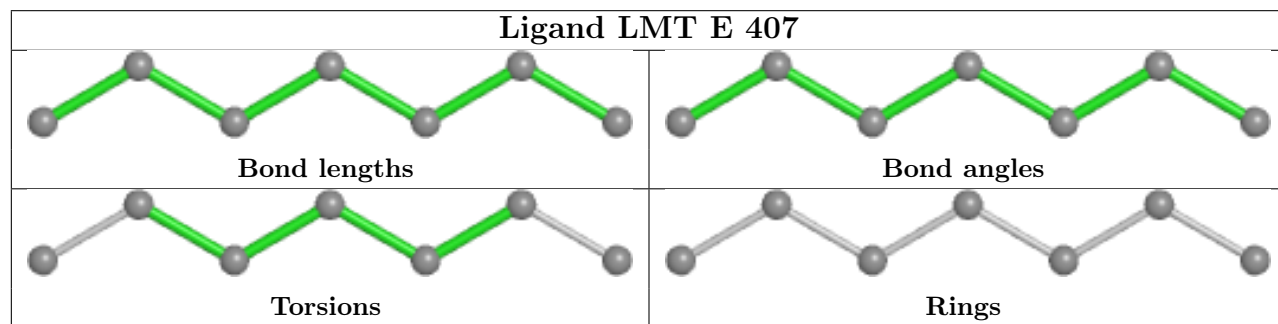
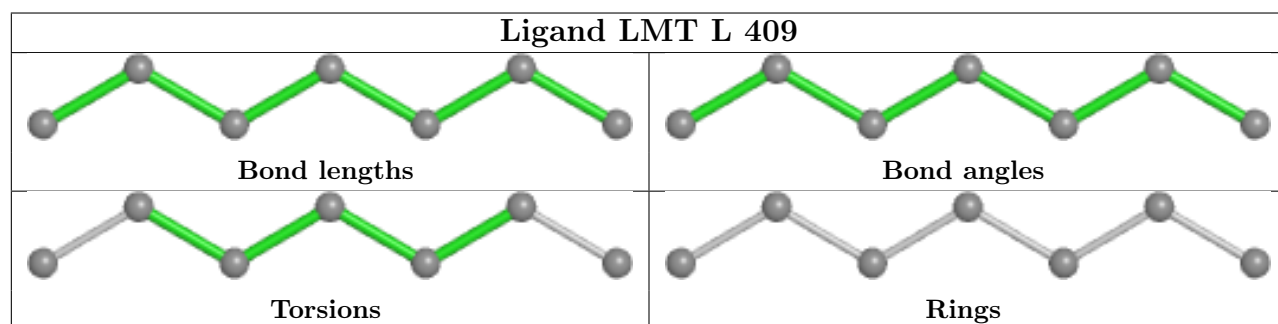
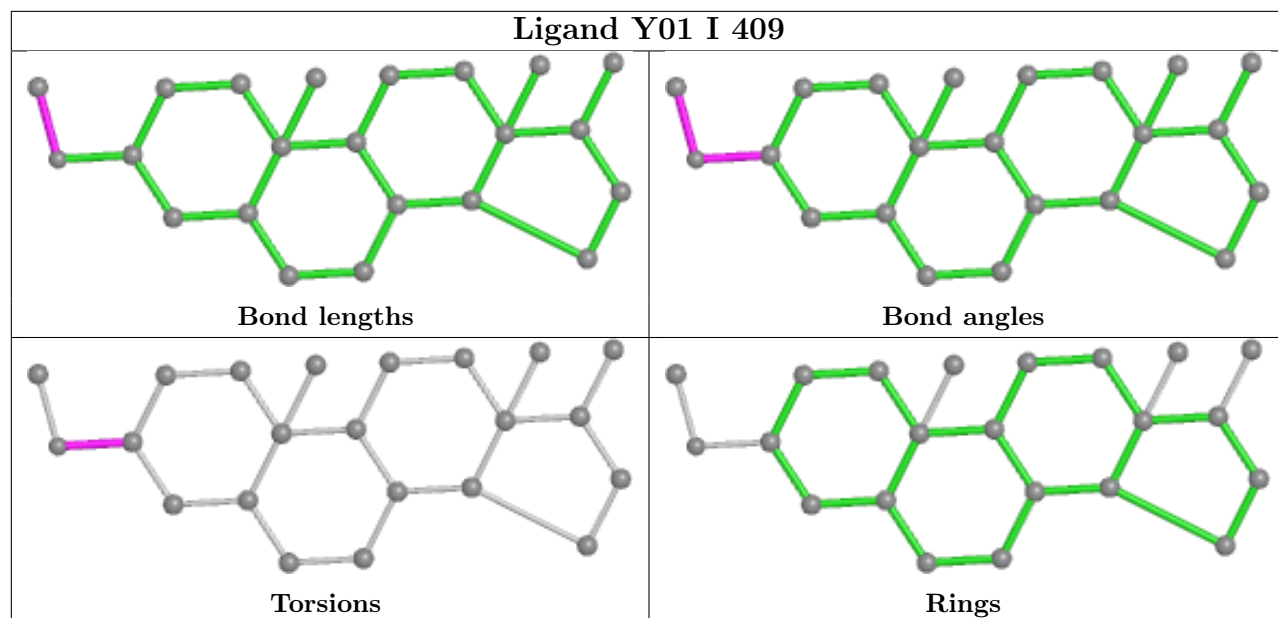


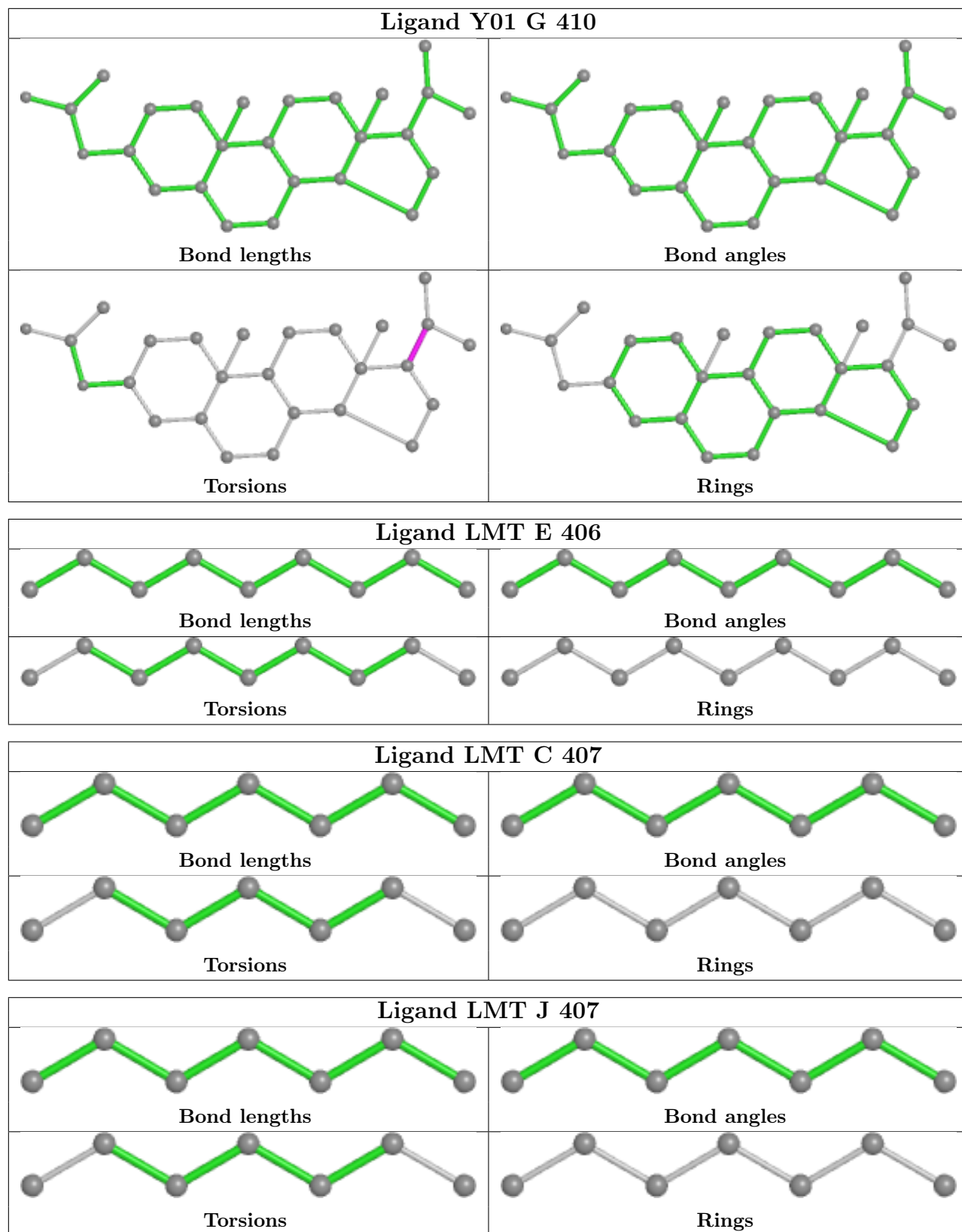


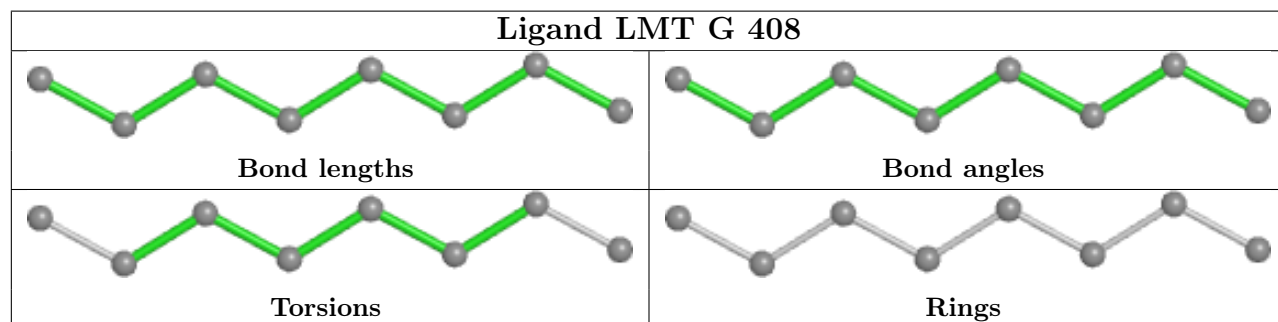
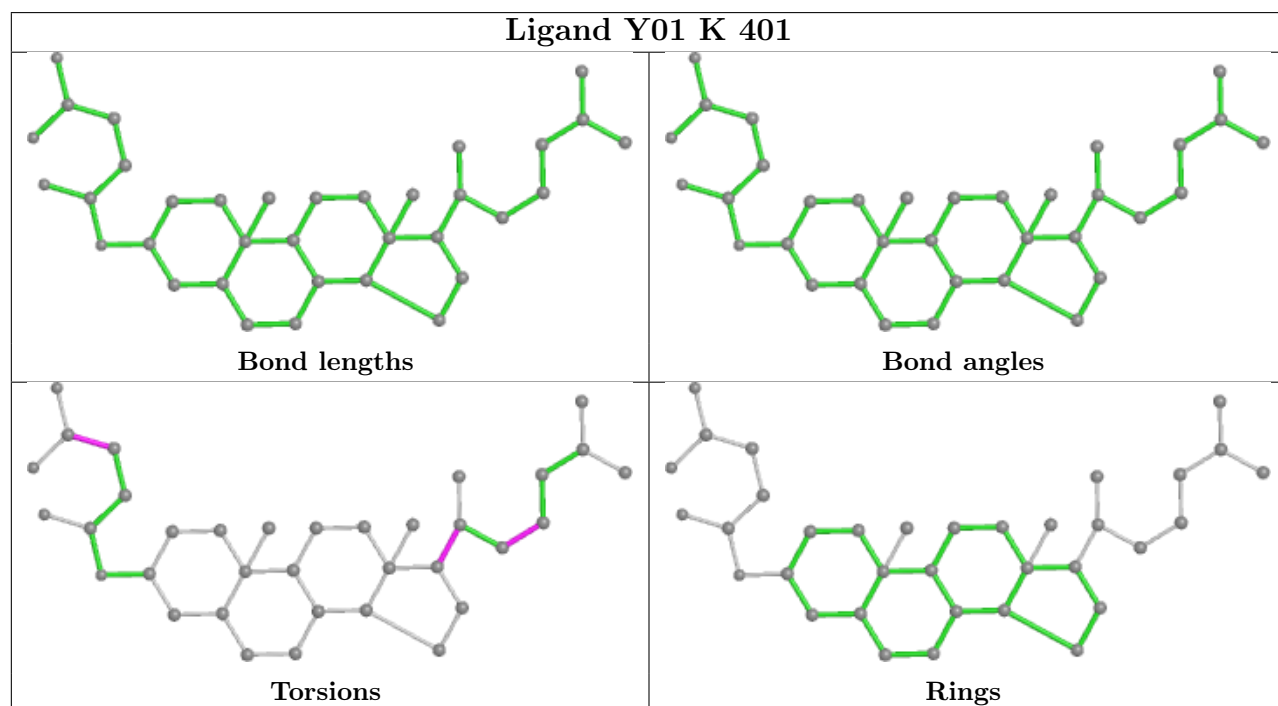
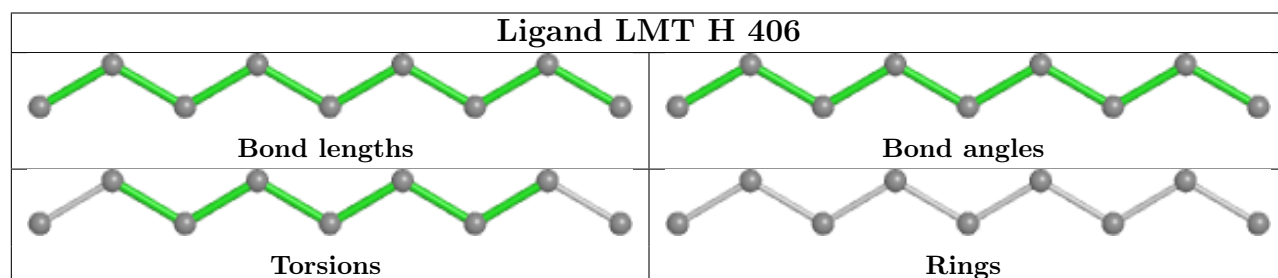
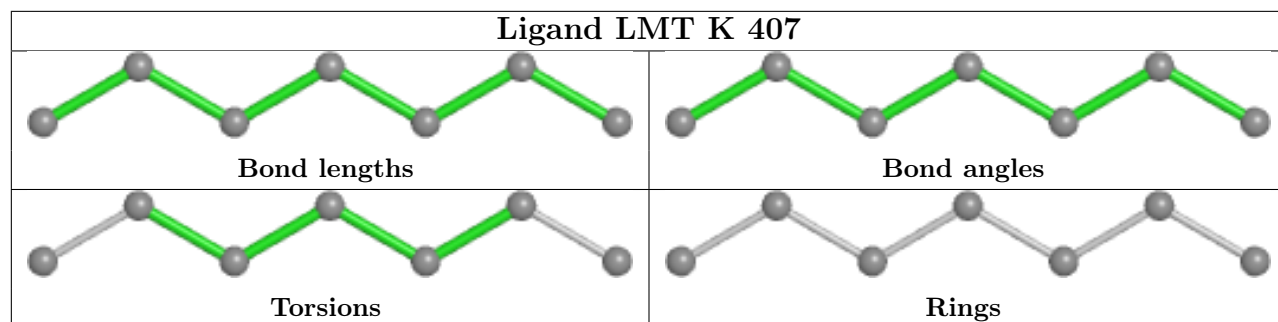


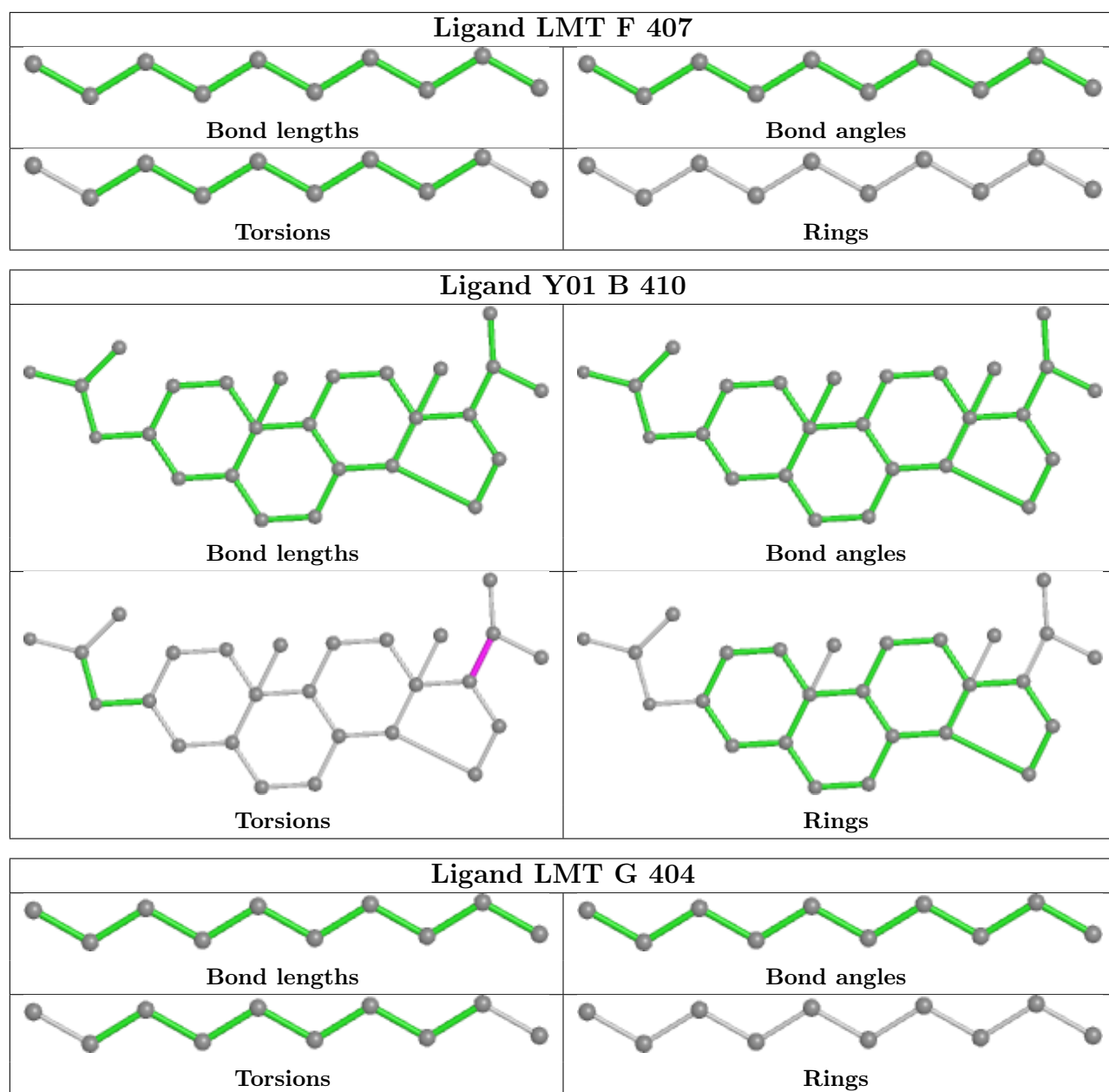


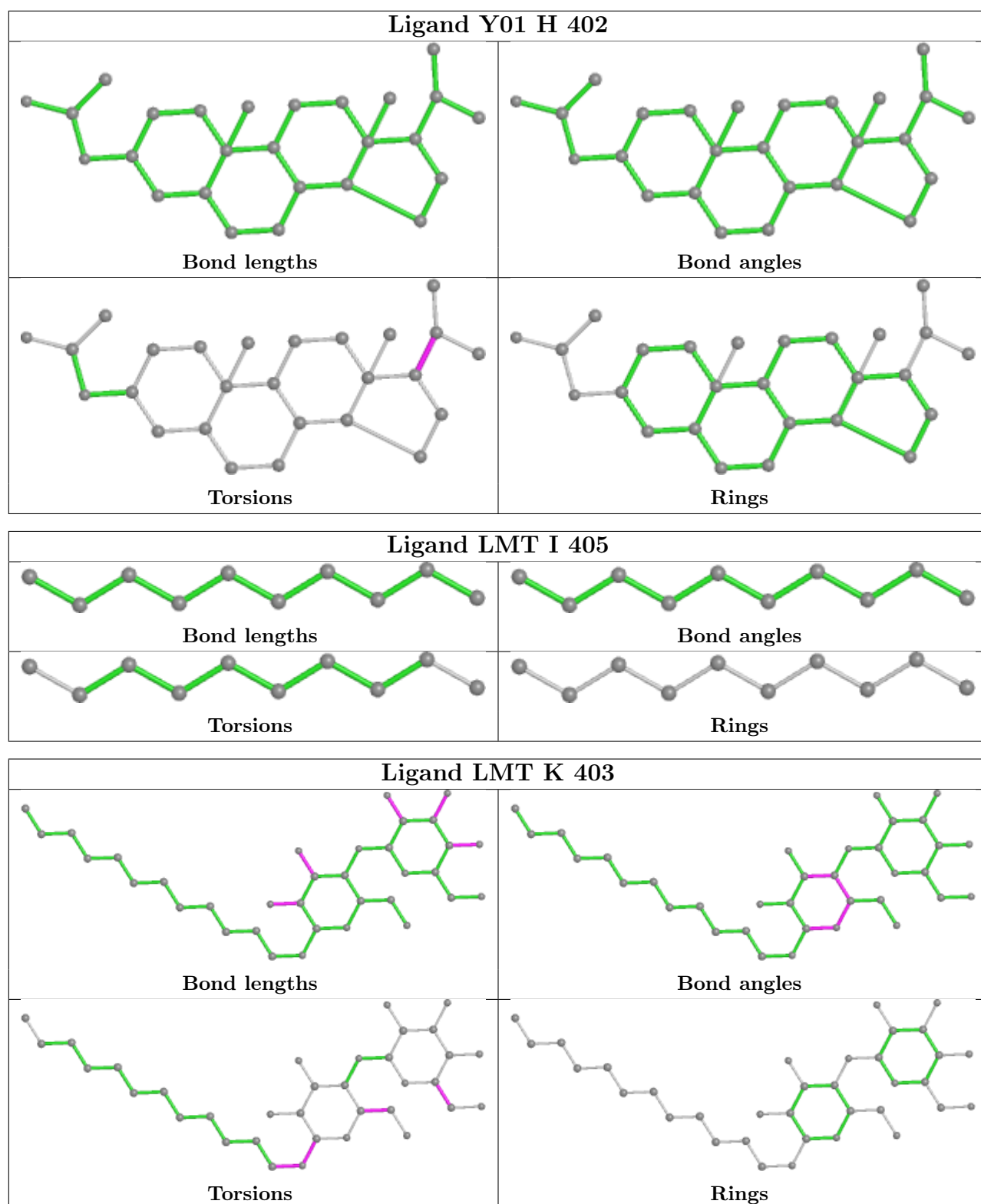


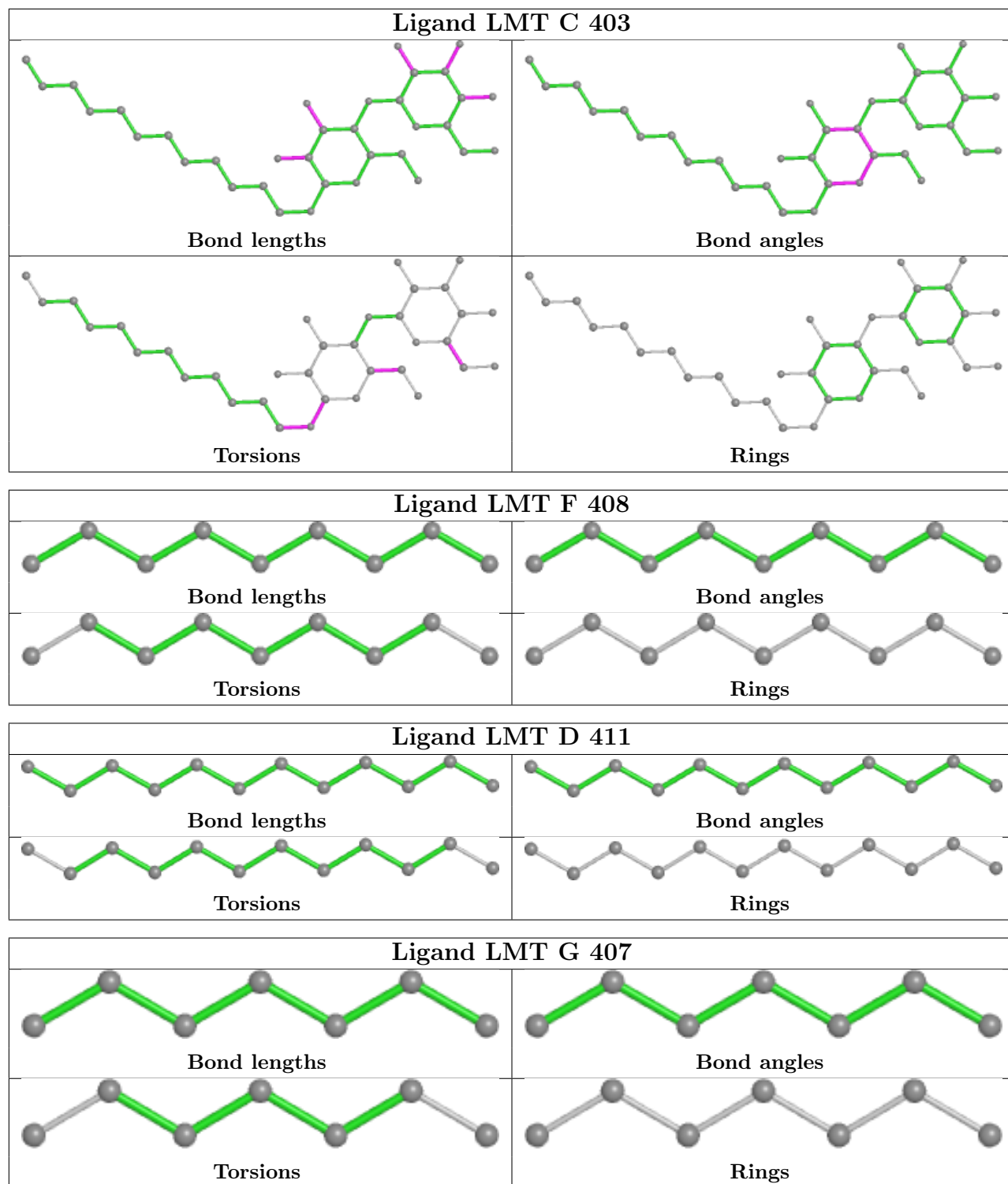


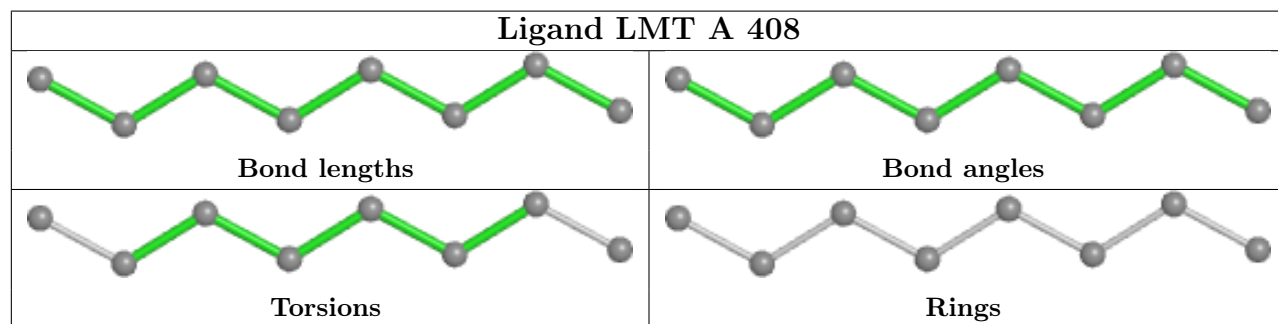
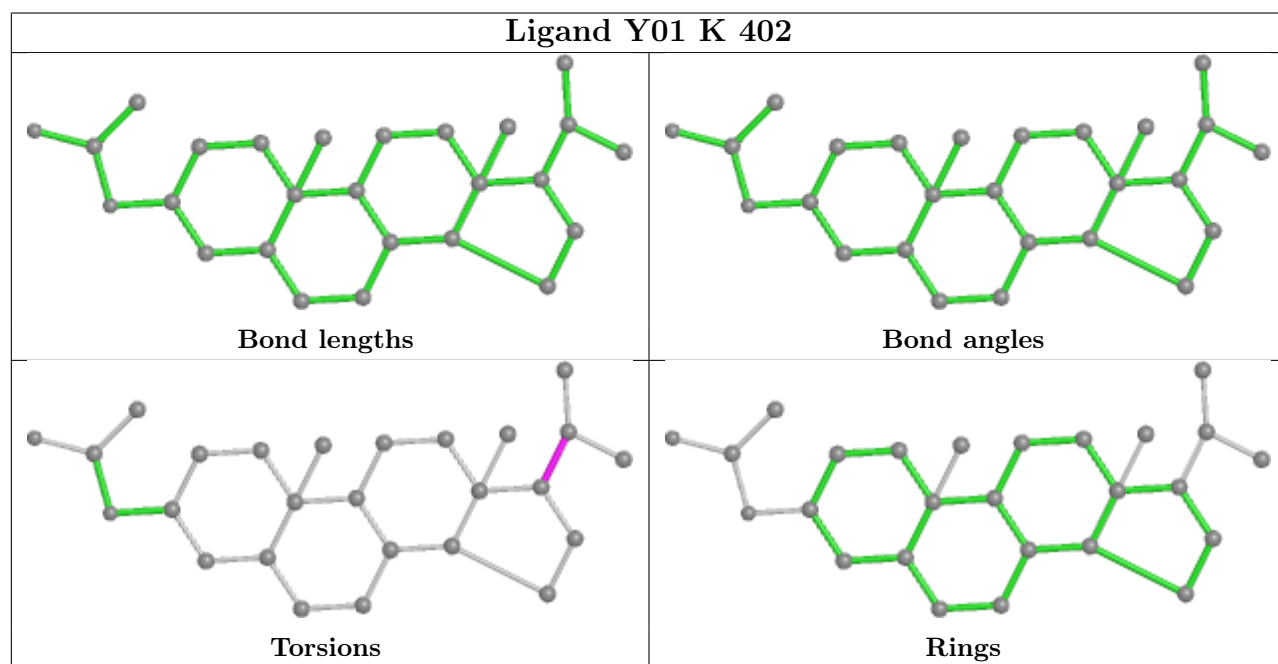
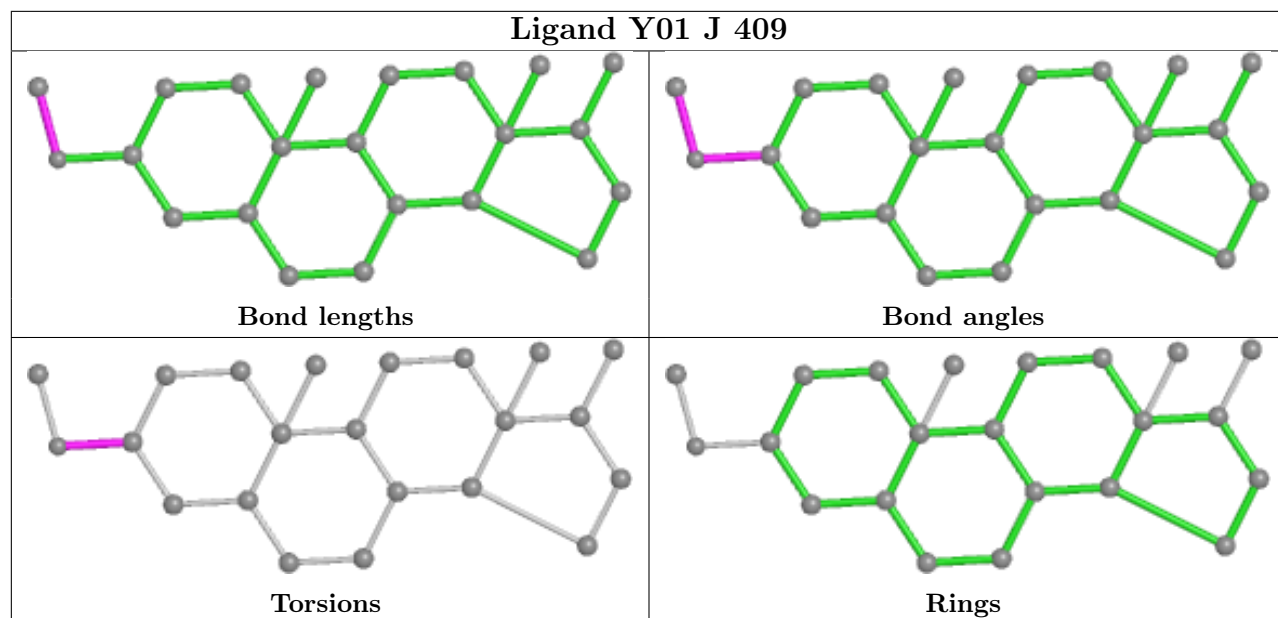


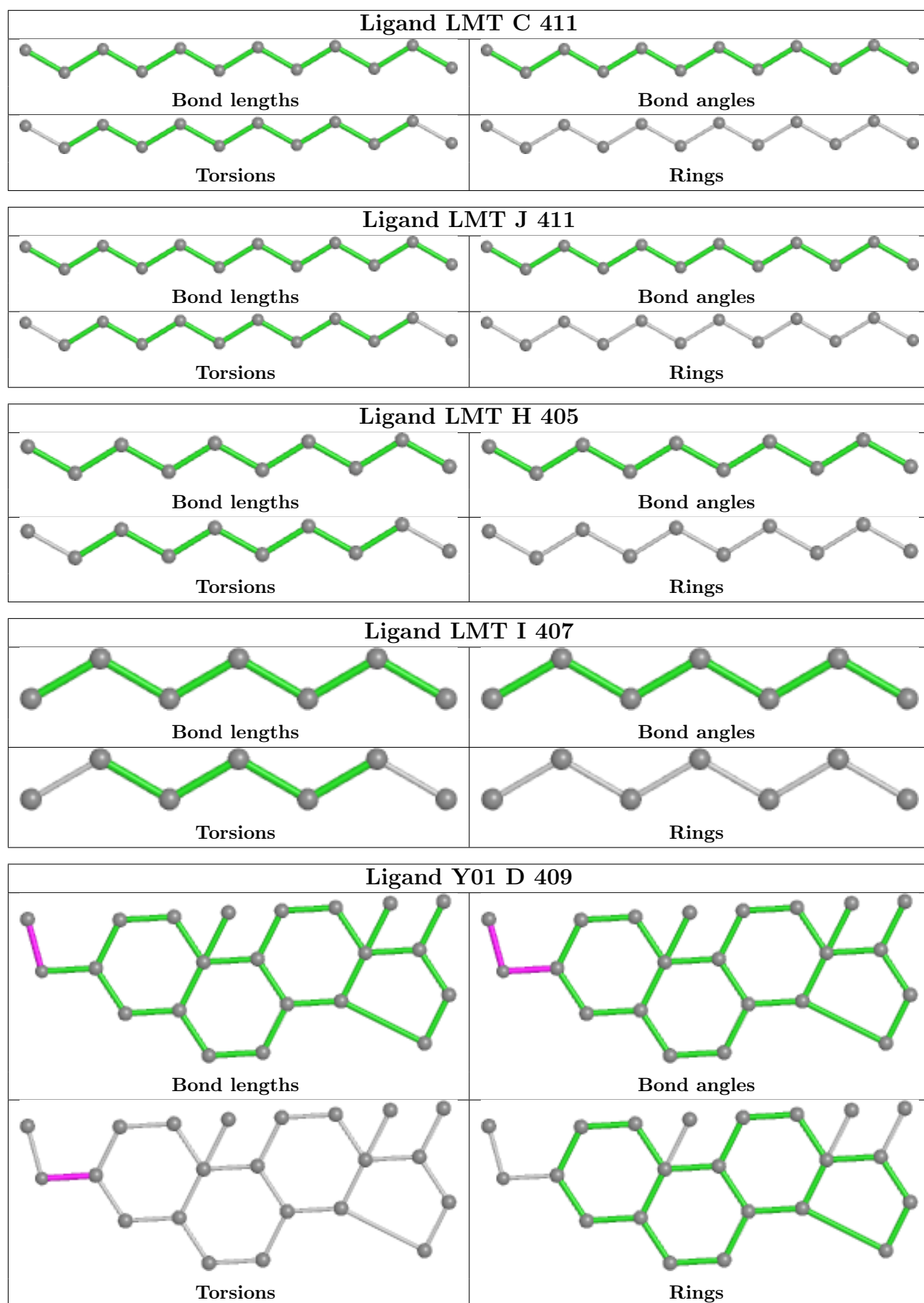


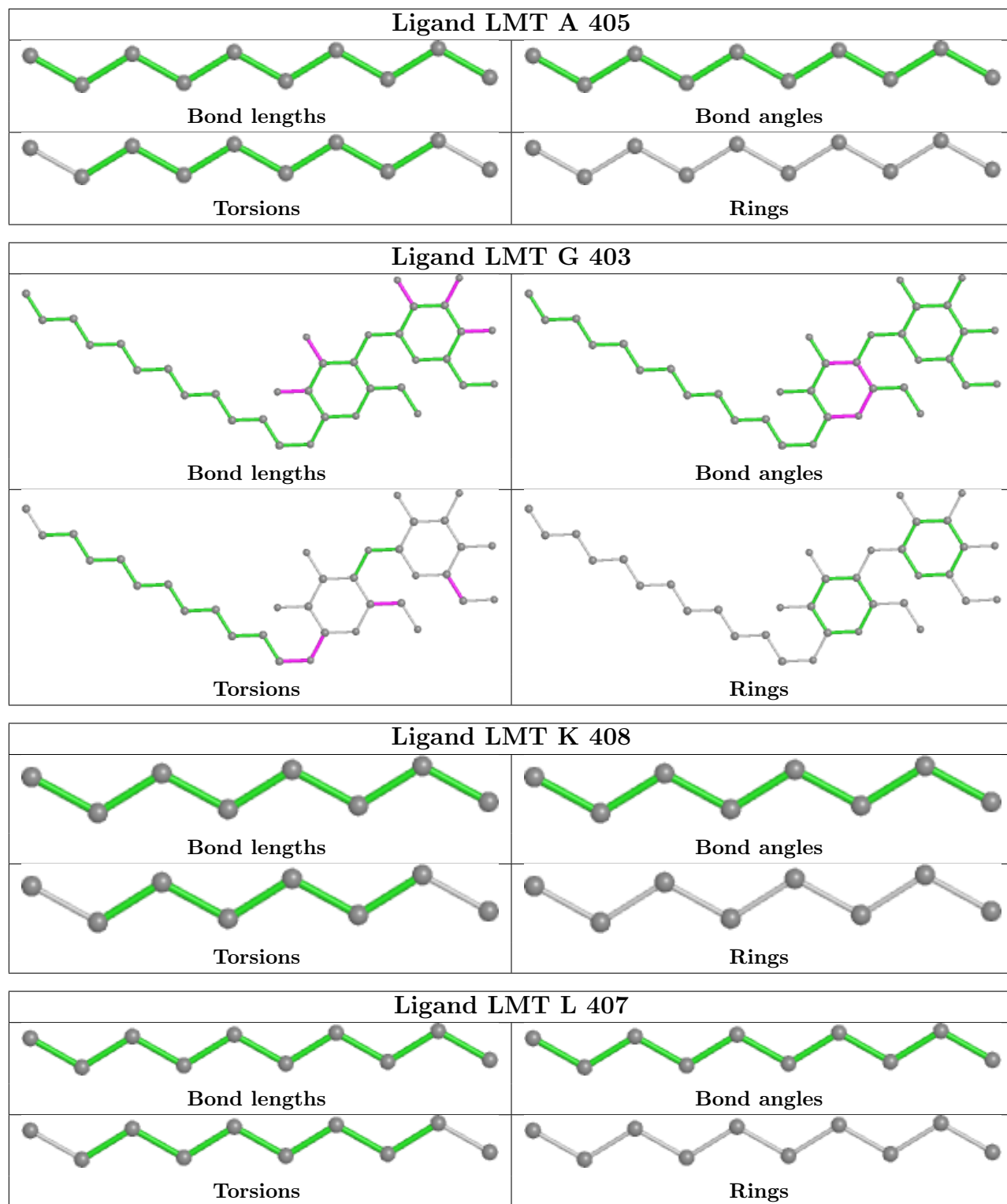


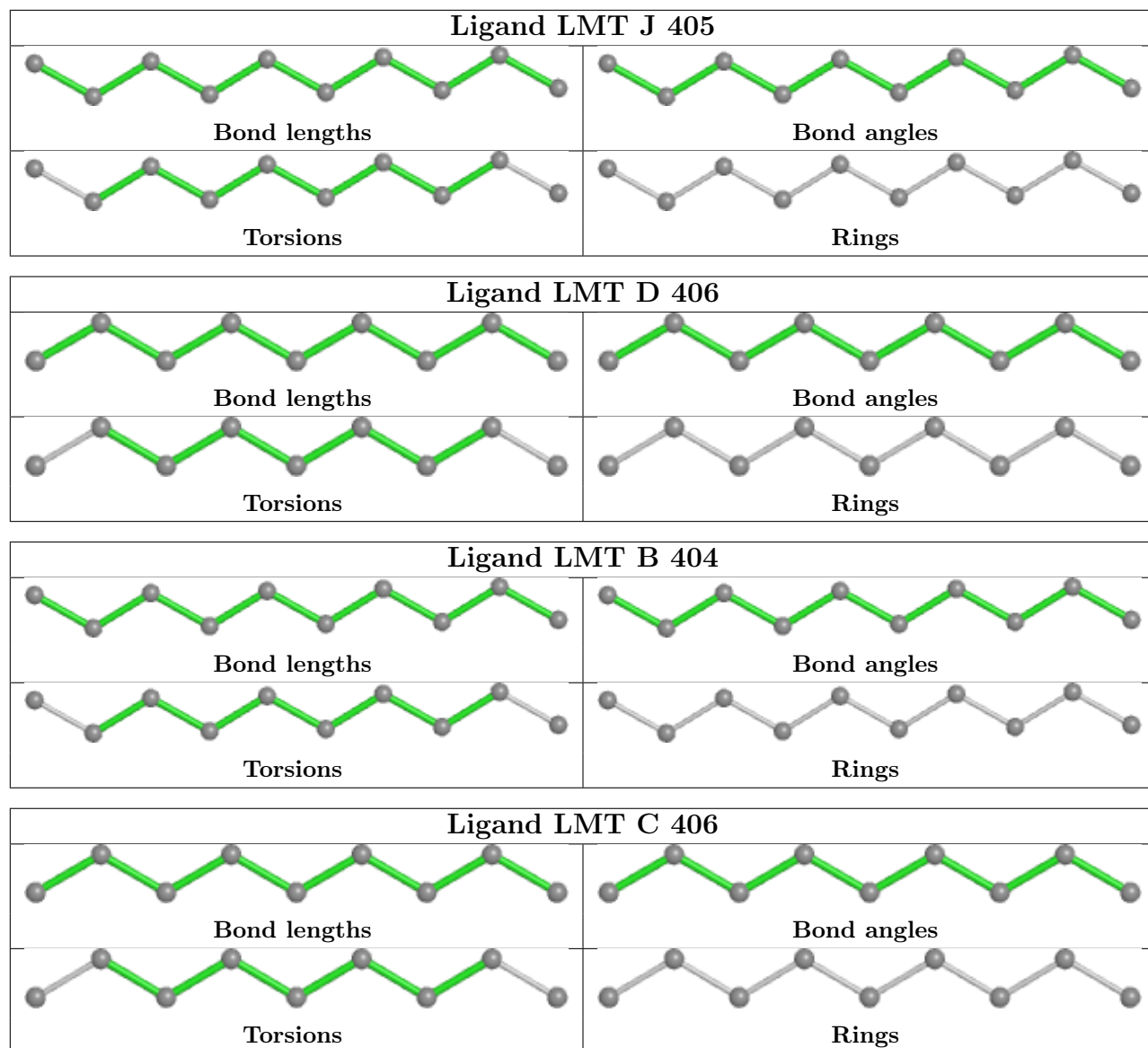


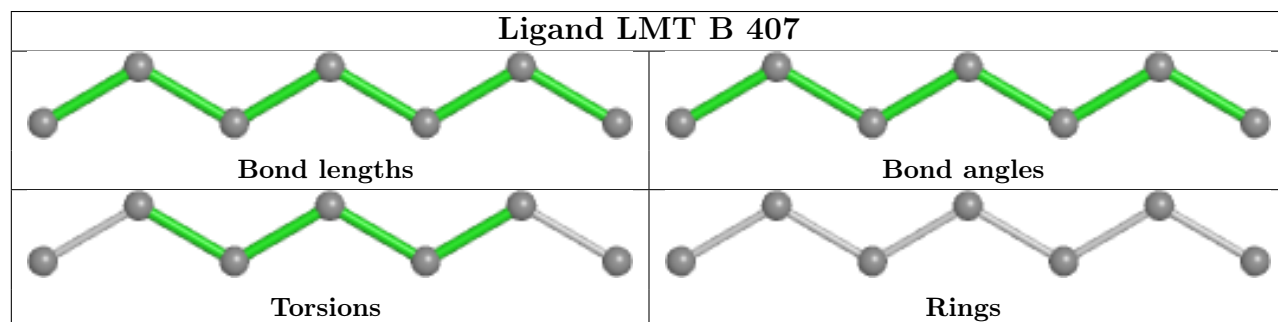
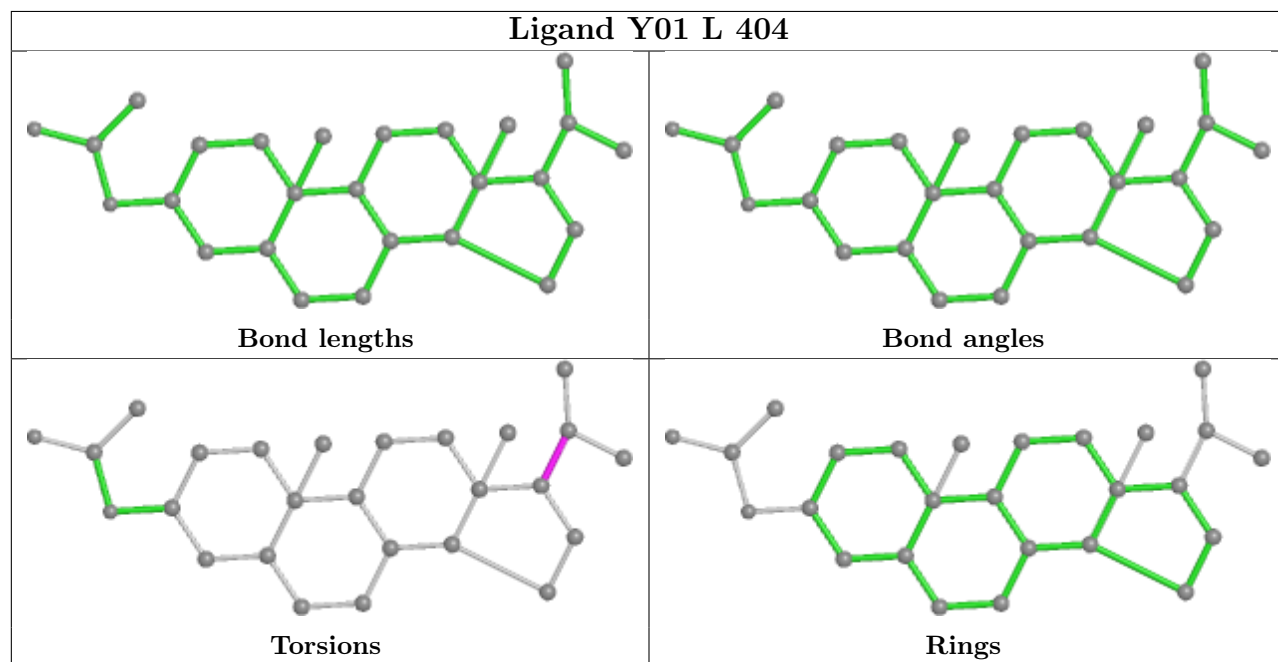
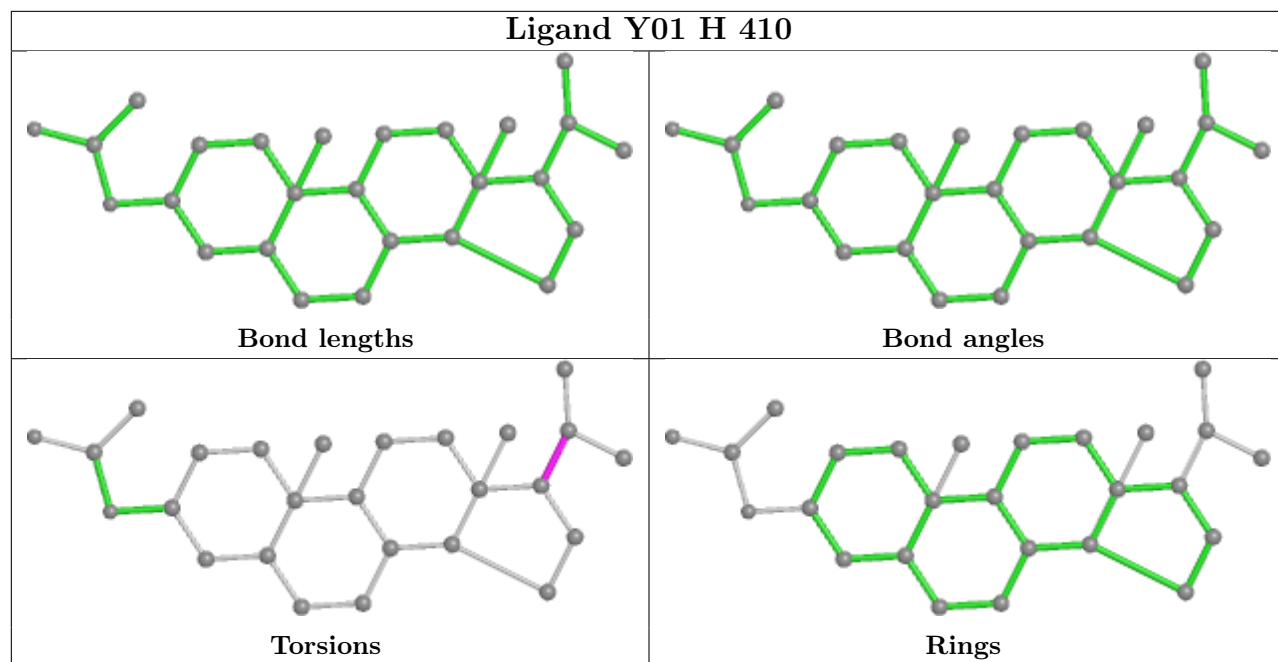


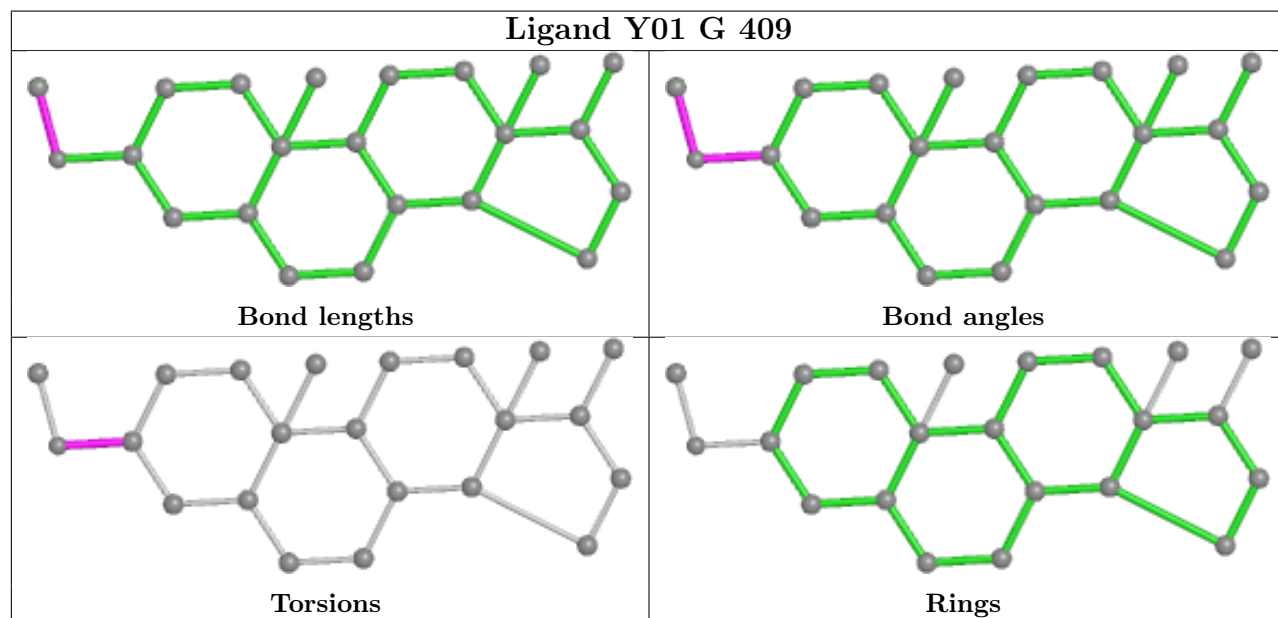
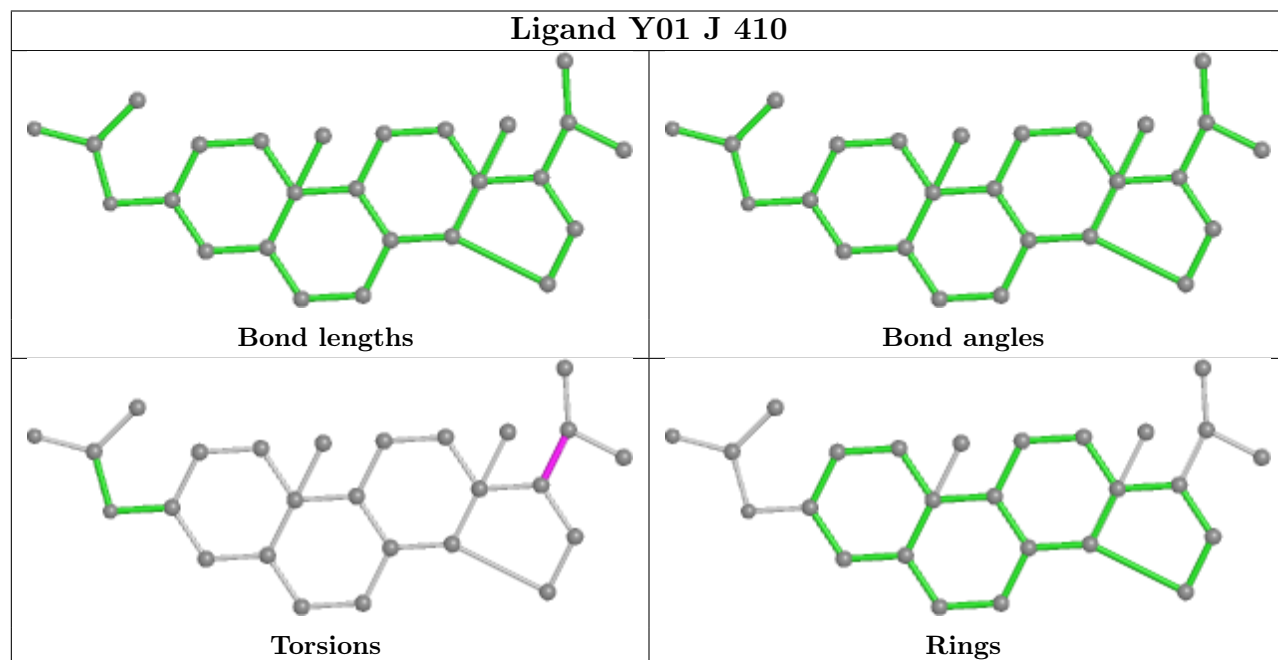
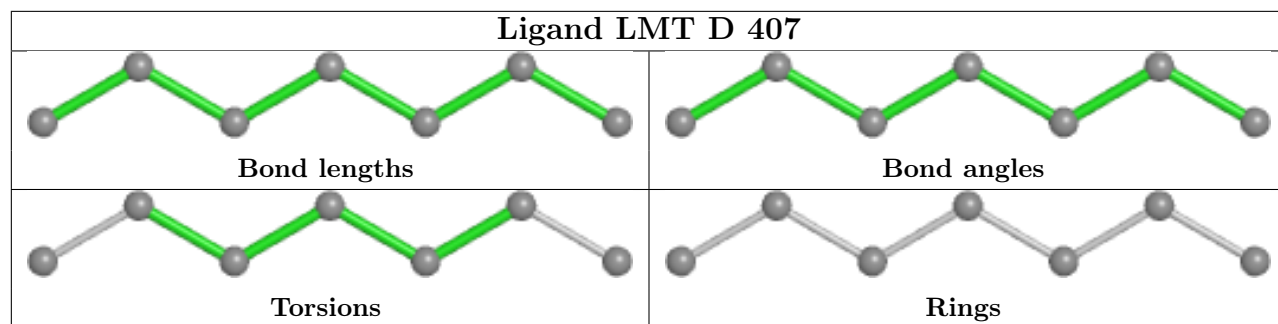


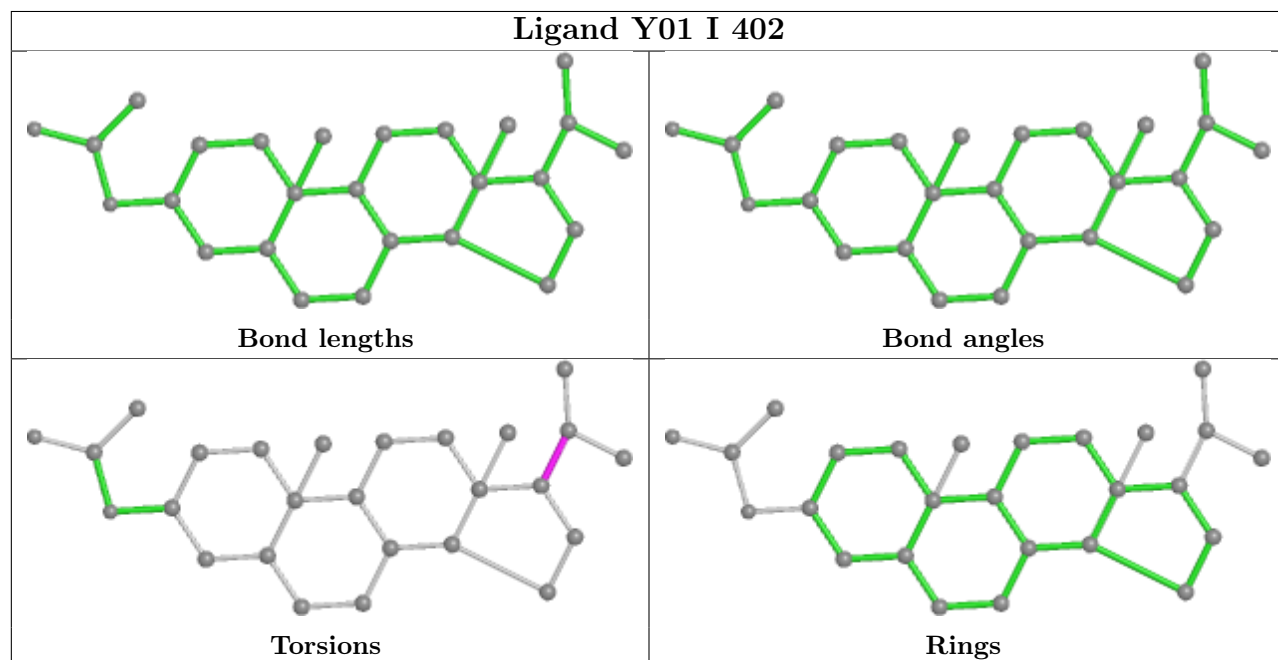
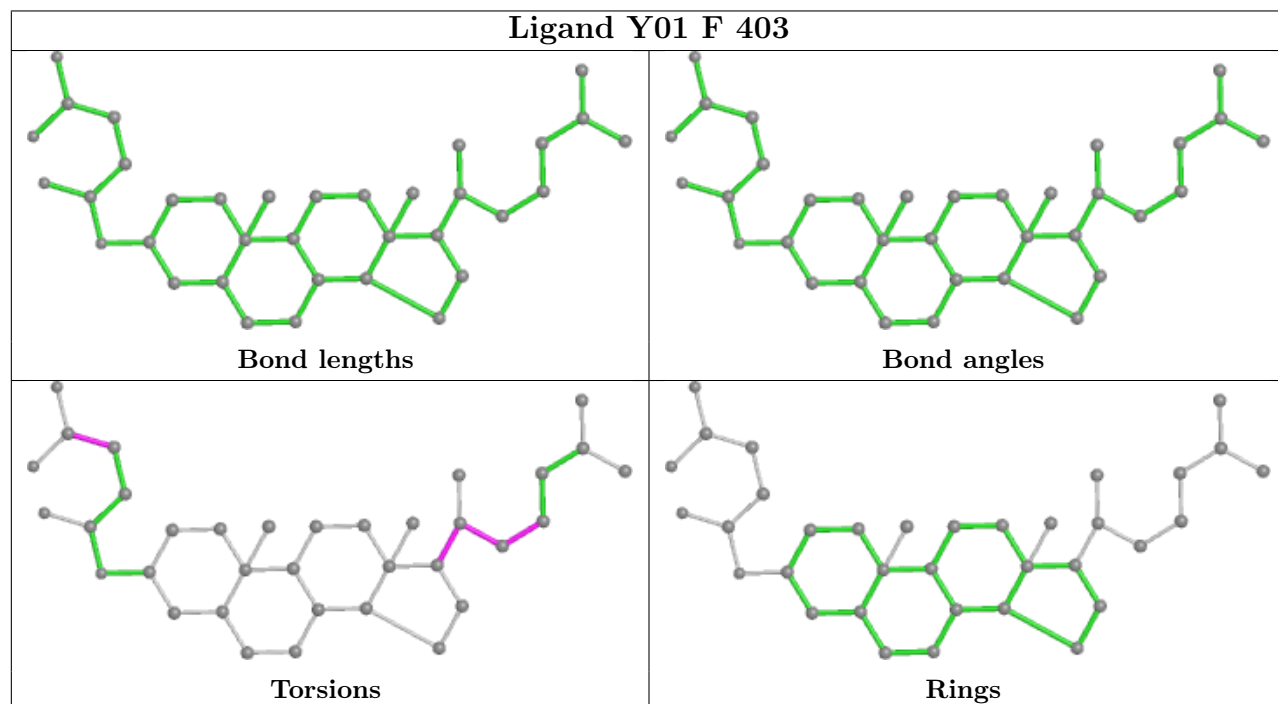
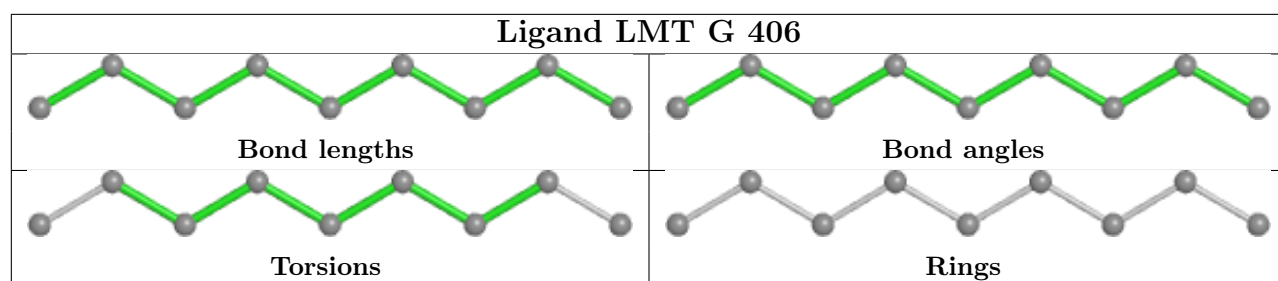


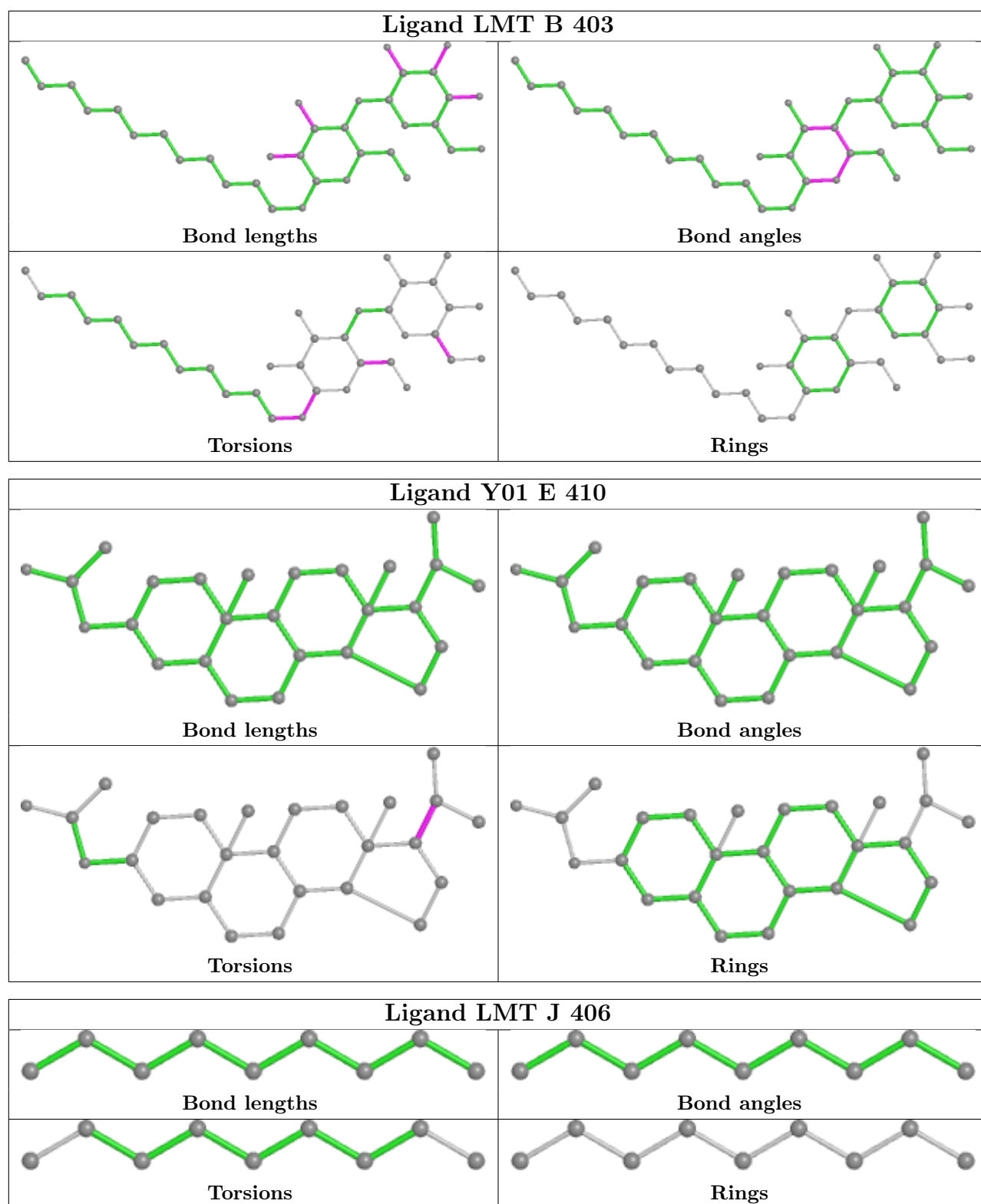


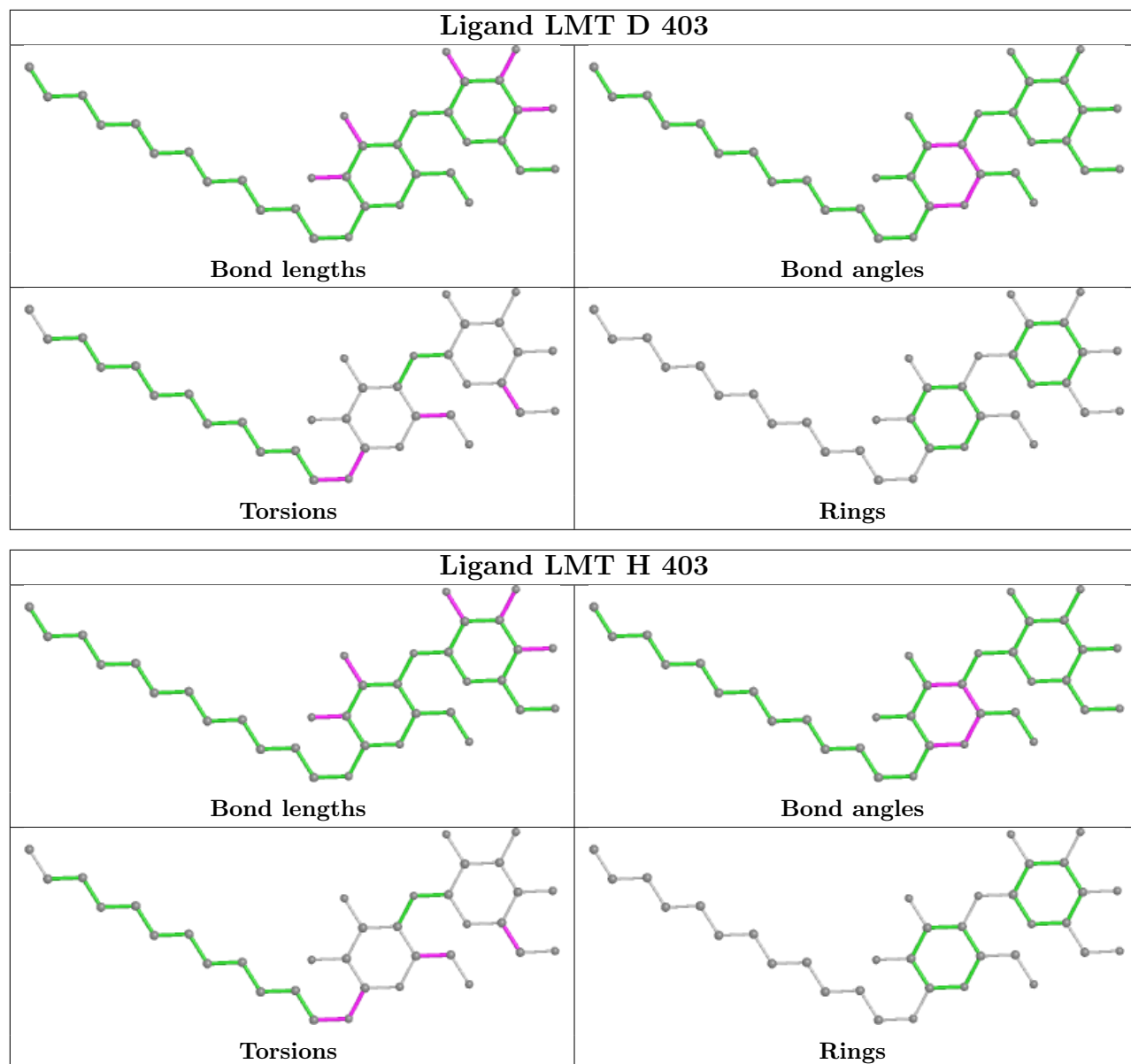


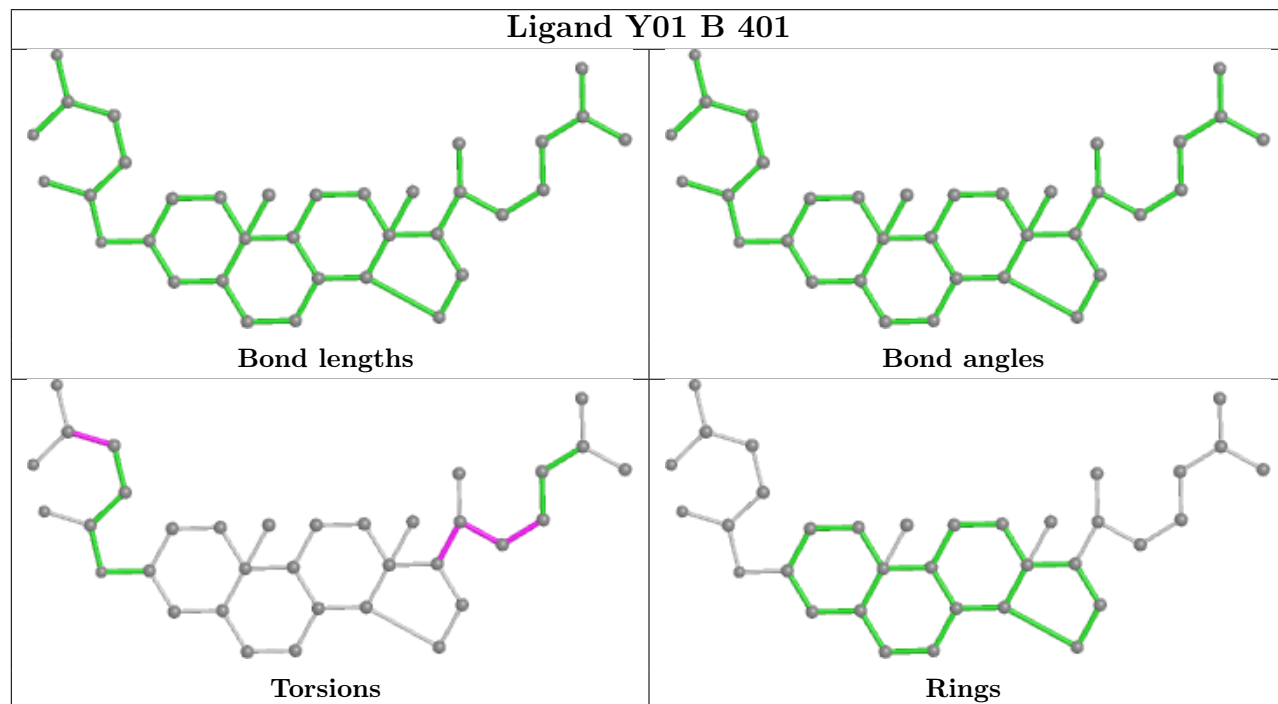
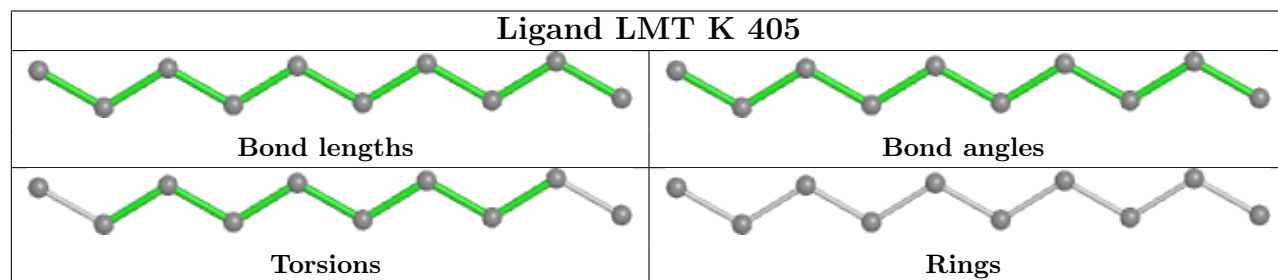
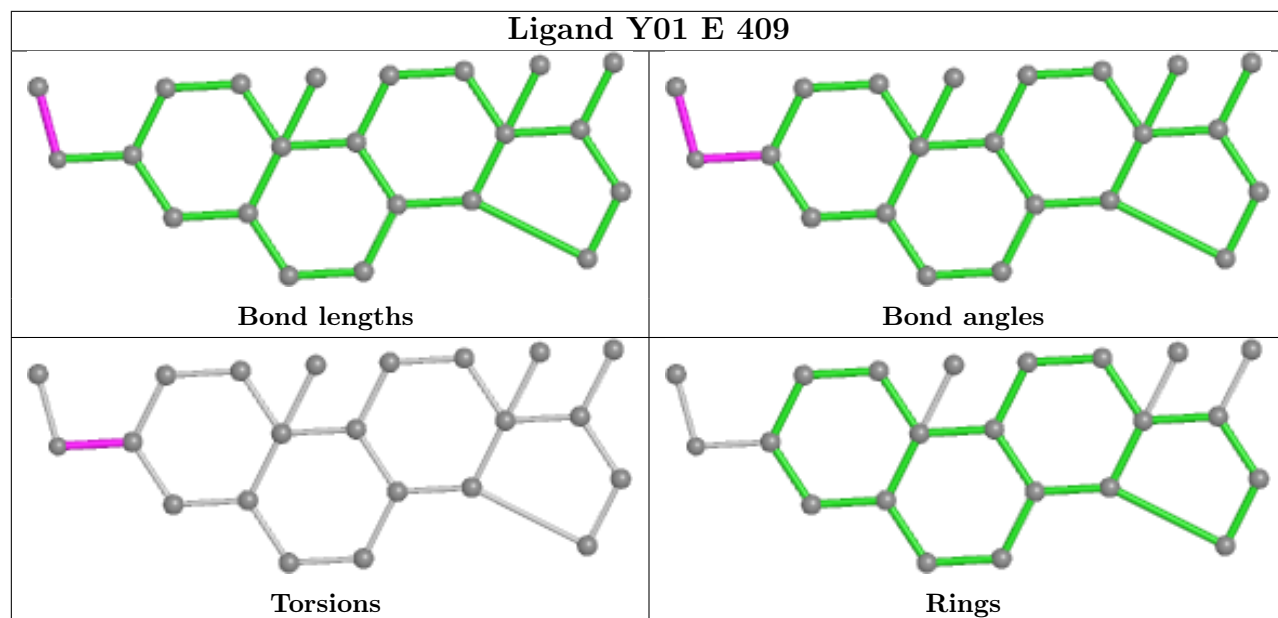


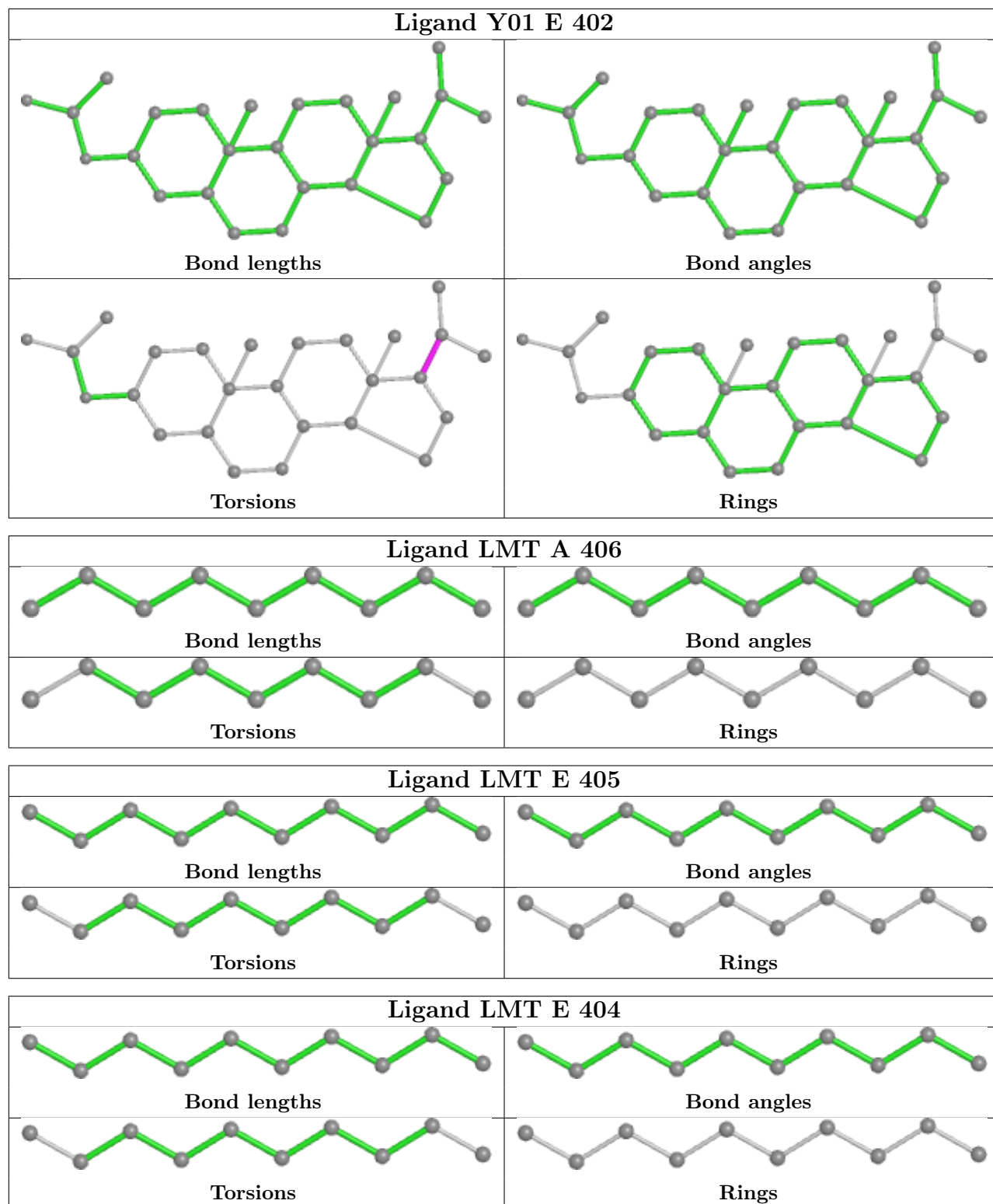


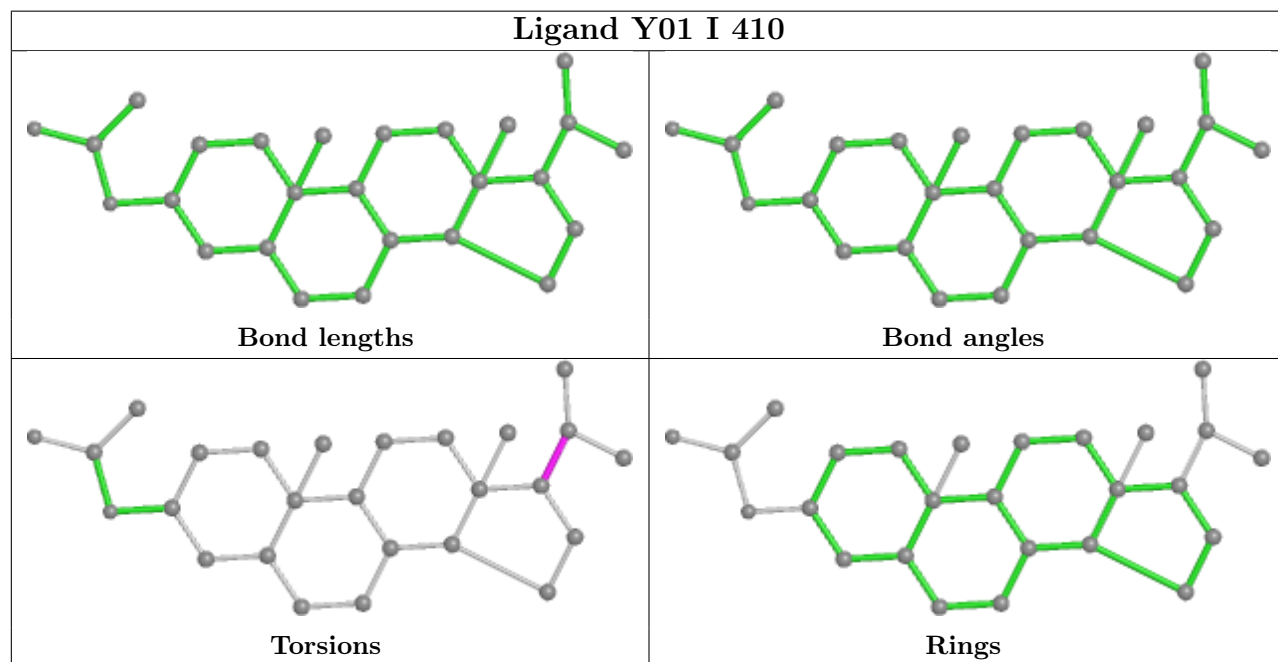
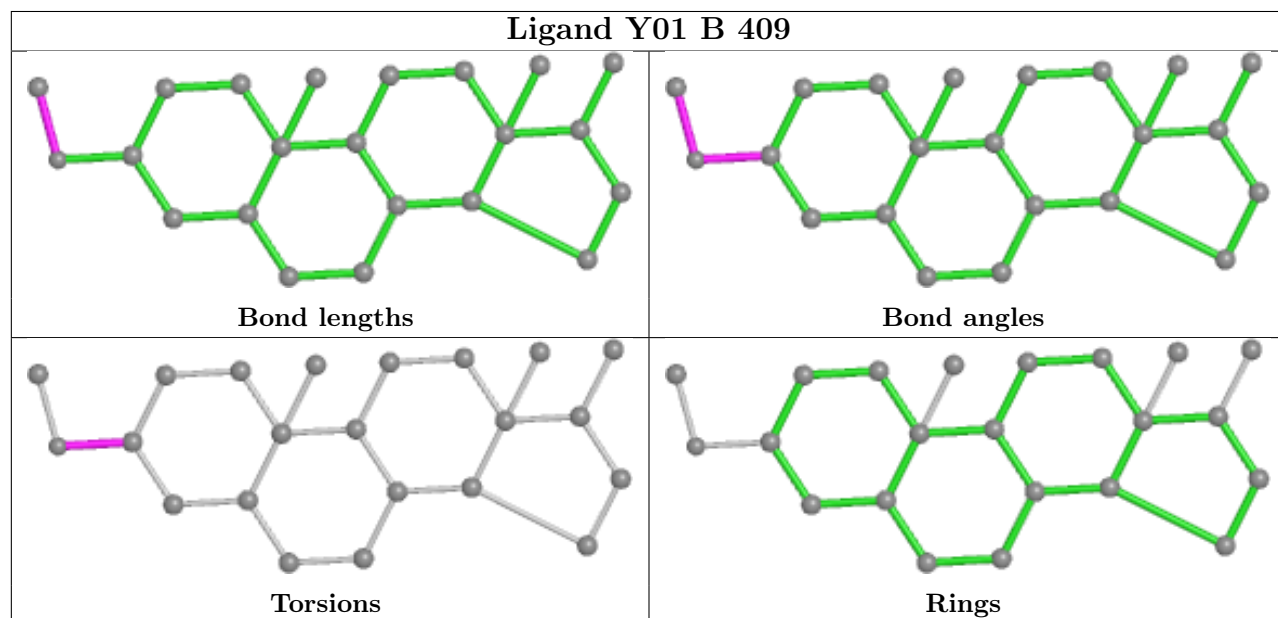
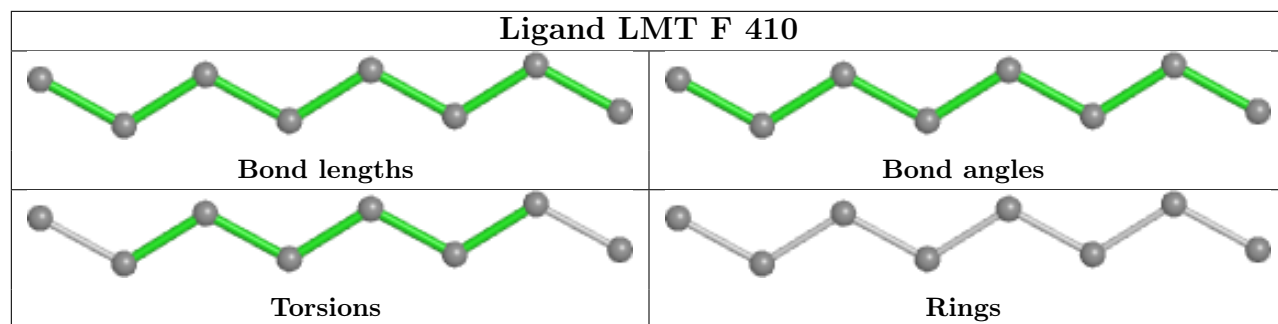


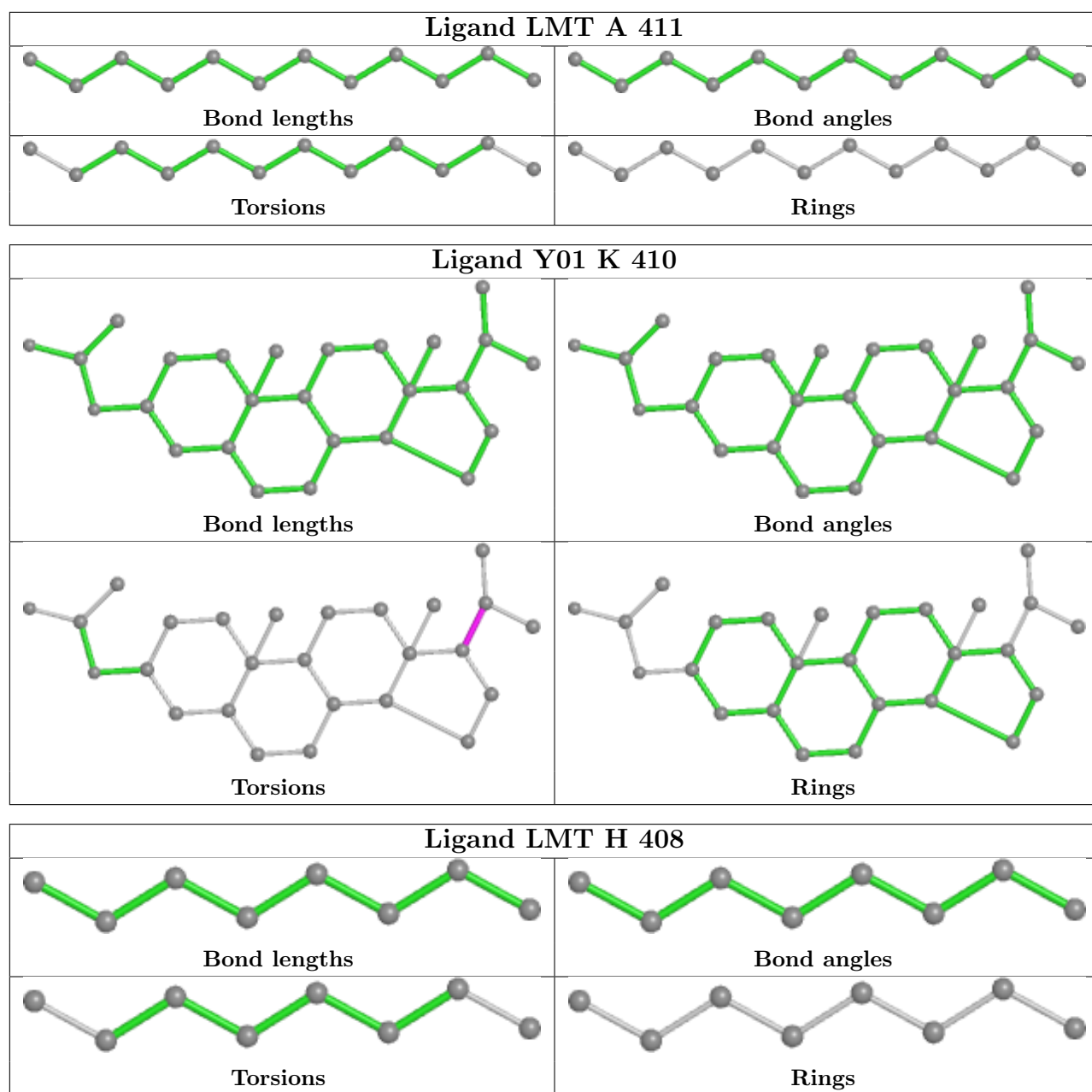












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.