



## wwPDB EM Validation Summary Report ⓘ

Nov 13, 2024 – 10:57 AM JST

PDB ID : 8Y1F  
EMDB ID : EMD-38834  
Title : The closed conformation of the HKU1-B S protein in the apo state  
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.  
Deposited on : 2024-01-24  
Resolution : 2.80 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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

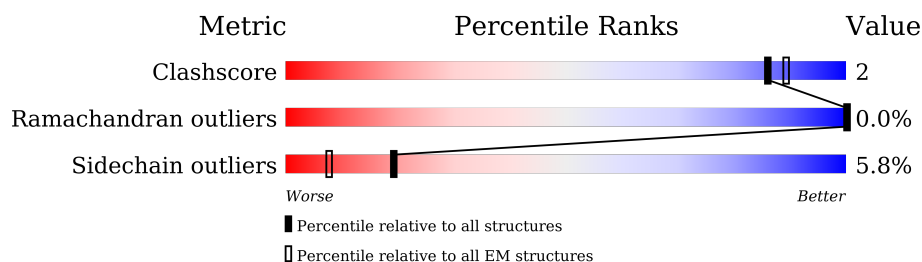
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.80 Å.

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












Metric	Whole archive (#Entries)	EM structures (#Entries)
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  $\geq 3$ , 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	1290	83% 10% • 6%
1	B	1290	84% 9% • 6%
1	C	1290	84% 9% • 6%
2	D	6	33% 67%
2	I	6	33% 67%
2	N	6	33% 67%
3	E	2	100%
3	F	2	50% 50%
3	G	2	100%

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	H	2	 100%
3	J	2	 100%
3	K	2	 50%50%
3	L	2	 100%
3	M	2	 100%
3	O	2	 100%
3	P	2	 50%50%
3	Q	2	 100%
3	R	2	 100%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29541 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.

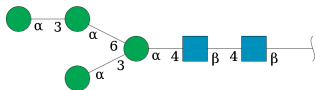
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		
1	B	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		
1	C	1208	Total	C	N	O	S	0	0
			9425	6003	1551	1814	57		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	752	GLY	ARG	conflict	UNP Q14EB0
A	753	SER	ARG	conflict	UNP Q14EB0
A	754	ALA	LYS	conflict	UNP Q14EB0
A	755	SER	ARG	conflict	UNP Q14EB0
A	1067	PRO	ASN	conflict	UNP Q14EB0
A	1068	PRO	LEU	conflict	UNP Q14EB0
B	752	GLY	ARG	conflict	UNP Q14EB0
B	753	SER	ARG	conflict	UNP Q14EB0
B	754	ALA	LYS	conflict	UNP Q14EB0
B	755	SER	ARG	conflict	UNP Q14EB0
B	1067	PRO	ASN	conflict	UNP Q14EB0
B	1068	PRO	LEU	conflict	UNP Q14EB0
C	752	GLY	ARG	conflict	UNP Q14EB0
C	753	SER	ARG	conflict	UNP Q14EB0
C	754	ALA	LYS	conflict	UNP Q14EB0
C	755	SER	ARG	conflict	UNP Q14EB0
C	1067	PRO	ASN	conflict	UNP Q14EB0
C	1068	PRO	LEU	conflict	UNP Q14EB0

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



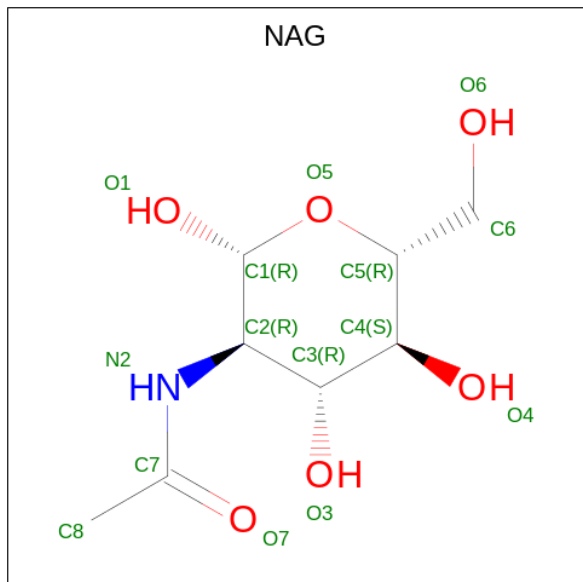
Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	6	Total	C	N	O	0	0
			72	40	2	30		
2	I	6	Total	C	N	O	0	0
			72	40	2	30		
2	N	6	Total	C	N	O	0	0
			72	40	2	30		

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	2	Total	C	N	O	0	0
			28	16	2	10		
3	F	2	Total	C	N	O	0	0
			28	16	2	10		
3	G	2	Total	C	N	O	0	0
			28	16	2	10		
3	H	2	Total	C	N	O	0	0
			28	16	2	10		
3	J	2	Total	C	N	O	0	0
			28	16	2	10		
3	K	2	Total	C	N	O	0	0
			28	16	2	10		
3	L	2	Total	C	N	O	0	0
			28	16	2	10		
3	M	2	Total	C	N	O	0	0
			28	16	2	10		
3	O	2	Total	C	N	O	0	0
			28	16	2	10		
3	P	2	Total	C	N	O	0	0
			28	16	2	10		
3	Q	2	Total	C	N	O	0	0
			28	16	2	10		
3	R	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0

*Continued on next page...*

*Continued from previous page...*

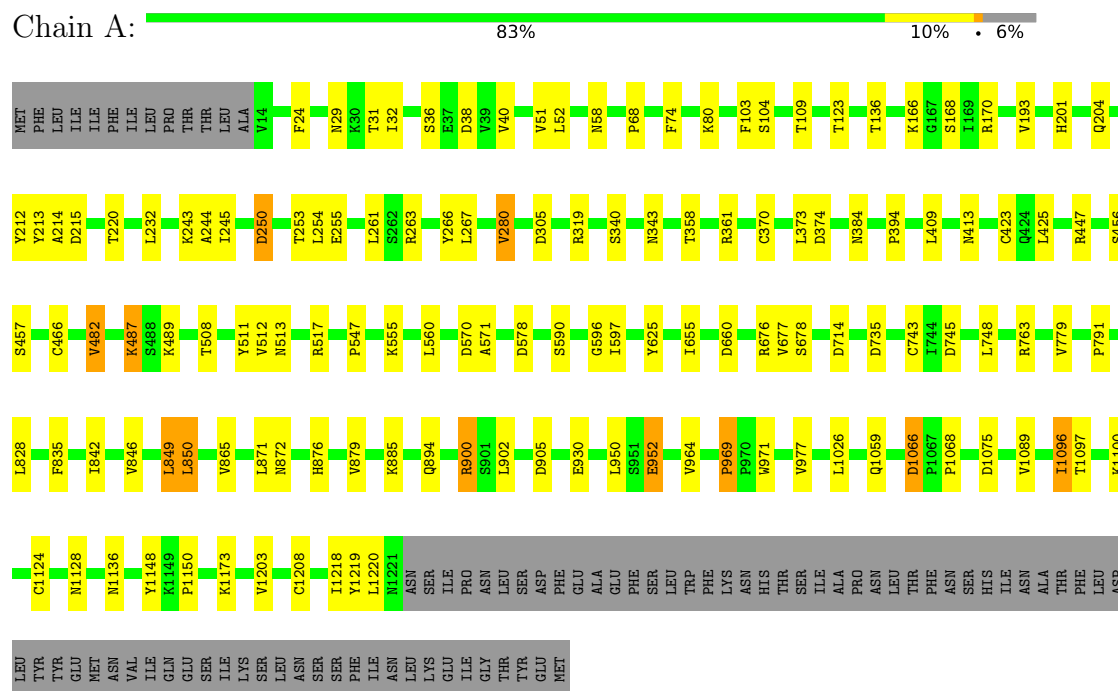
Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	



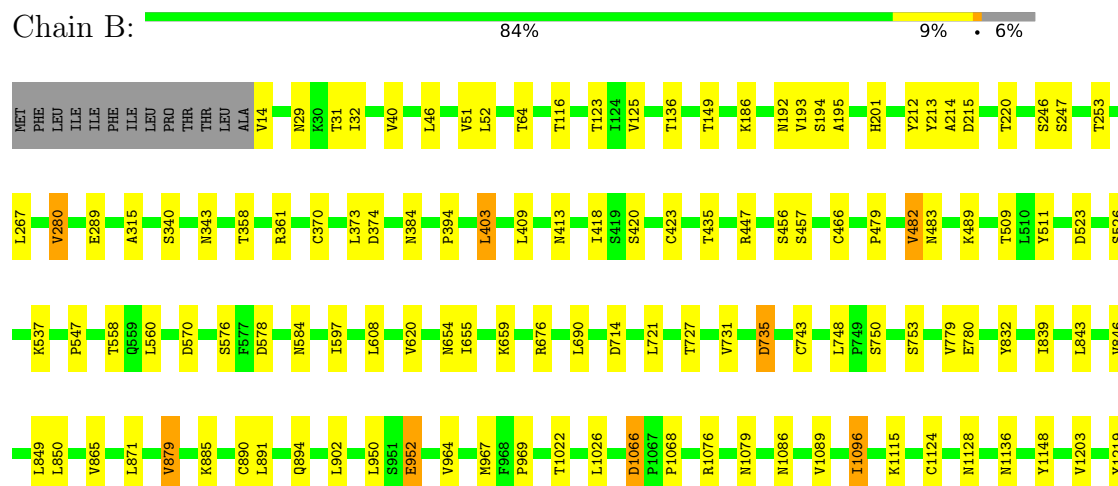
### 3 Residue-property plots

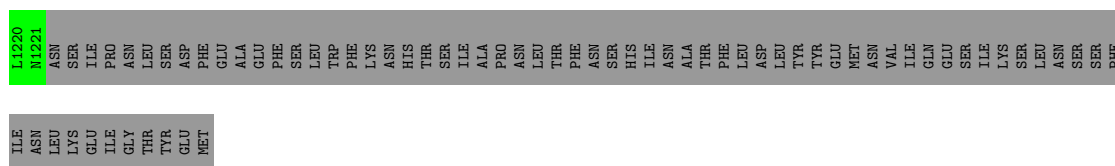
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



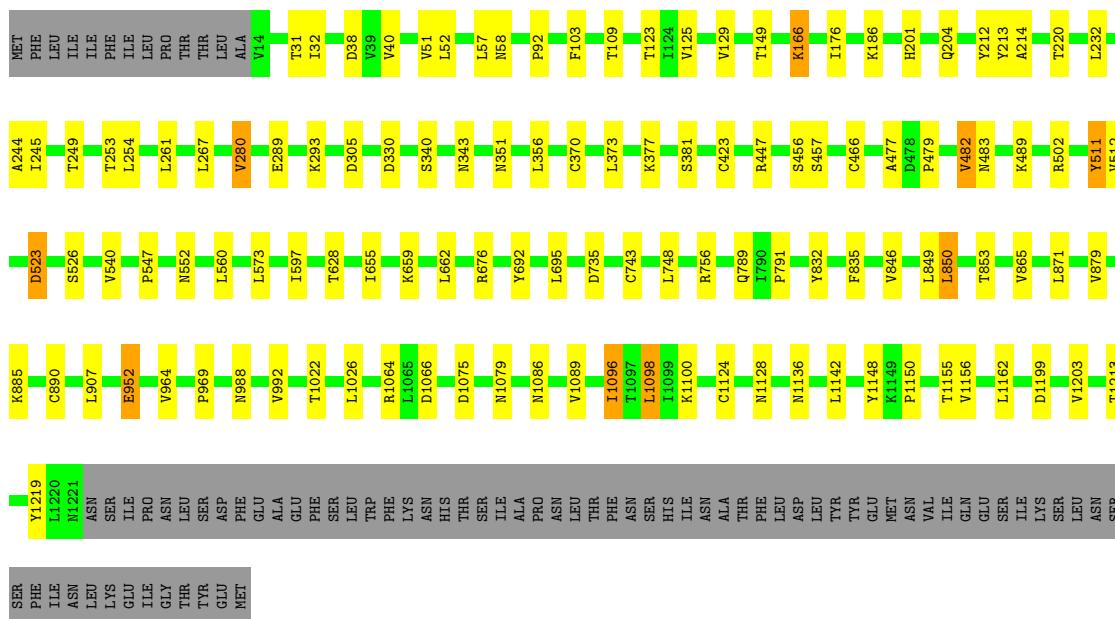
#### • Molecule 1: Spike glycoprotein





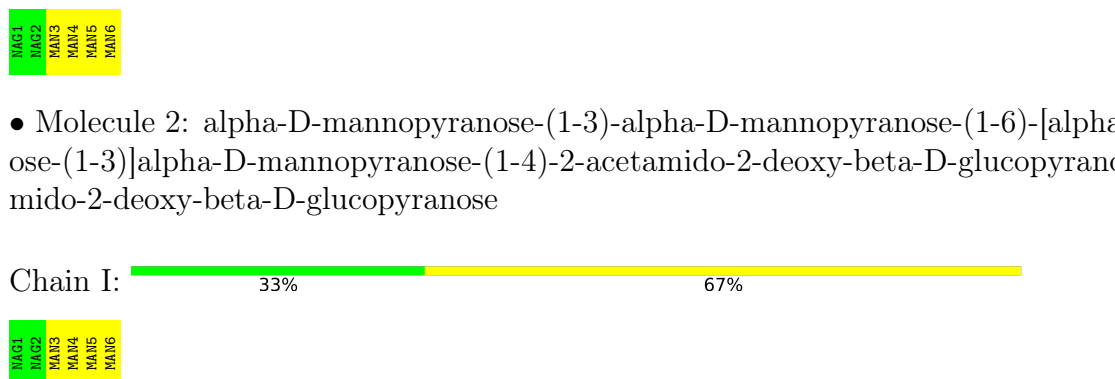
- Molecule 1: Spike glycoprotein

Chain C:



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:



- Molecule 2: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain N:  33% 67%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain R:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	104714	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor

## 5 Model quality

### 5.1 Standard geometry

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

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	0.29	0/9653	0.49	0/13146
1	B	0.29	0/9653	0.48	0/13146
1	C	0.29	0/9653	0.49	0/13146
All	All	0.29	0/28959	0.49	0/39438

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	969	PRO	Peptide
1	B	969	PRO	Peptide
1	C	92	PRO	Peptide
1	C	969	PRO	Peptide

## 5.2 Too-close contacts ⓘ

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	9425	0	9076	47	0
1	B	9425	0	9076	34	0
1	C	9425	0	9076	39	0
2	D	72	0	61	0	0
2	I	72	0	61	0	0
2	N	72	0	61	0	0
3	E	28	0	25	0	0
3	F	28	0	25	0	0
3	G	28	0	25	0	0
3	H	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
3	M	28	0	25	0	0
3	O	28	0	25	0	0
3	P	28	0	25	0	0
3	Q	28	0	25	0	0
3	R	28	0	25	0	0
4	A	238	0	221	0	0
4	B	238	0	221	0	0
4	C	238	0	221	0	0
All	All	29541	0	28374	116	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 2.

The worst 5 of 116 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:C:201:HIS:HB2	1:C:212:TYR:HB2	1.72	0.70
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.77	0.67
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.80	0.64
1:A:872:ASN:H	1:A:876:HIS:HD2	1.46	0.62
1:B:214:ALA:HB2	1:B:220:THR:HA	1.84	0.58

There are no symmetry-related clashes.

## 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	A	1206/1290 (94%)	1156 (96%)	49 (4%)	1 (0%)	48	77
1	B	1206/1290 (94%)	1147 (95%)	59 (5%)	0	100	100
1	C	1206/1290 (94%)	1146 (95%)	60 (5%)	0	100	100
All	All	3618/3870 (94%)	3449 (95%)	168 (5%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASP

### 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	1082/1159 (93%)	1021 (94%)	61 (6%)	17	47
1	B	1082/1159 (93%)	1014 (94%)	68 (6%)	15	42
1	C	1082/1159 (93%)	1023 (94%)	59 (6%)	18	47
All	All	3246/3477 (93%)	3058 (94%)	188 (6%)	19	45

5 of 188 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	B	894	GLN
1	C	245	ILE
1	B	964	VAL
1	C	32	ILE
1	C	351	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1059	GLN
1	C	1079	ASN
1	B	204	GLN
1	A	1180	GLN
1	C	1091	GLN

### 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 ⓘ

42 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	D	1	1,2	14,14,15	0.22	0	17,19,21	0.54	0
2	NAG	D	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	MAN	D	3	2	11,11,12	1.25	1 (9%)	15,15,17	1.83	3 (20%)
2	MAN	D	4	2	11,11,12	0.88	1 (9%)	15,15,17	1.36	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	MAN	D	5	2	11,11,12	0.75	0	15,15,17	1.12	2 (13%)
2	MAN	D	6	2	11,11,12	0.86	1 (9%)	15,15,17	1.38	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.28	0	17,19,21	0.51	0
3	NAG	E	2	3	14,14,15	0.33	0	17,19,21	0.48	0
3	NAG	F	1	3,1	14,14,15	0.24	0	17,19,21	0.45	0
3	NAG	F	2	3	14,14,15	0.32	0	17,19,21	0.64	1 (5%)
3	NAG	G	1	3,1	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	G	2	3	14,14,15	0.29	0	17,19,21	0.50	0
3	NAG	H	1	3,1	14,14,15	0.24	0	17,19,21	0.51	0
3	NAG	H	2	3	14,14,15	0.31	0	17,19,21	0.52	0
2	NAG	I	1	1,2	14,14,15	0.28	0	17,19,21	0.55	0
2	NAG	I	2	2	14,14,15	0.24	0	17,19,21	0.53	0
2	MAN	I	3	2	11,11,12	1.39	1 (9%)	15,15,17	1.79	3 (20%)
2	MAN	I	4	2	11,11,12	0.80	0	15,15,17	1.16	2 (13%)
2	MAN	I	5	2	11,11,12	0.78	0	15,15,17	1.09	2 (13%)
2	MAN	I	6	2	11,11,12	0.75	0	15,15,17	1.34	2 (13%)
3	NAG	J	1	3,1	14,14,15	0.33	0	17,19,21	0.51	0
3	NAG	J	2	3	14,14,15	0.40	0	17,19,21	0.46	0
3	NAG	K	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	K	2	3	14,14,15	0.34	0	17,19,21	0.57	1 (5%)
3	NAG	L	1	3,1	14,14,15	0.23	0	17,19,21	0.45	0
3	NAG	L	2	3	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	M	1	3,1	14,14,15	0.27	0	17,19,21	0.54	0
3	NAG	M	2	3	14,14,15	0.33	0	17,19,21	0.45	0
2	NAG	N	1	1,2	14,14,15	0.23	0	17,19,21	0.58	0
2	NAG	N	2	2	14,14,15	0.25	0	17,19,21	0.50	0
2	MAN	N	3	2	11,11,12	1.37	2 (18%)	15,15,17	1.76	3 (20%)
2	MAN	N	4	2	11,11,12	0.82	0	15,15,17	1.29	2 (13%)
2	MAN	N	5	2	11,11,12	0.85	0	15,15,17	0.98	2 (13%)
2	MAN	N	6	2	11,11,12	0.86	1 (9%)	15,15,17	1.31	2 (13%)
3	NAG	O	1	3,1	14,14,15	0.31	0	17,19,21	0.55	0
3	NAG	O	2	3	14,14,15	0.43	0	17,19,21	0.45	0
3	NAG	P	1	3,1	14,14,15	0.24	0	17,19,21	0.46	0
3	NAG	P	2	3	14,14,15	0.31	0	17,19,21	0.58	1 (5%)
3	NAG	Q	1	3,1	14,14,15	0.22	0	17,19,21	0.45	0
3	NAG	Q	2	3	14,14,15	0.28	0	17,19,21	0.54	0
3	NAG	R	1	3,1	14,14,15	0.25	0	17,19,21	0.57	0
3	NAG	R	2	3	14,14,15	0.32	0	17,19,21	0.53	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
2	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	0/2/19/22	0/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	0/2/19/22	0/1/1/1
2	MAN	D	6	2	-	2/2/19/22	0/1/1/1
3	NAG	E	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	0/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1
2	MAN	I	3	2	-	2/2/19/22	1/1/1/1
2	MAN	I	4	2	-	0/2/19/22	0/1/1/1
2	MAN	I	5	2	-	2/2/19/22	0/1/1/1
2	MAN	I	6	2	-	2/2/19/22	0/1/1/1
3	NAG	J	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	2/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	M	2	3	-	2/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	MAN	N	3	2	-	0/2/19/22	0/1/1/1
2	MAN	N	4	2	-	2/2/19/22	0/1/1/1
2	MAN	N	5	2	-	0/2/19/22	0/1/1/1
2	MAN	N	6	2	-	2/2/19/22	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	O	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	O	2	3	-	2/6/23/26	0/1/1/1
3	NAG	P	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	P	2	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	2/6/23/26	0/1/1/1
3	NAG	R	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	R	2	3	-	1/6/23/26	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	3	MAN	O5-C5	3.31	1.50	1.43
2	D	3	MAN	O5-C5	2.65	1.48	1.43
2	N	3	MAN	O5-C5	2.36	1.48	1.43
2	N	3	MAN	C1-C2	2.25	1.57	1.52
2	N	6	MAN	C1-C2	2.13	1.57	1.52

The worst 5 of 30 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	3	MAN	C1-O5-C5	5.44	119.56	112.19
2	N	3	MAN	C1-O5-C5	5.32	119.40	112.19
2	I	3	MAN	C1-O5-C5	5.06	119.04	112.19
2	D	6	MAN	C1-O5-C5	4.39	118.14	112.19
2	I	6	MAN	C1-O5-C5	4.28	118.00	112.19

There are no chirality outliers.

5 of 66 torsion outliers are listed below:

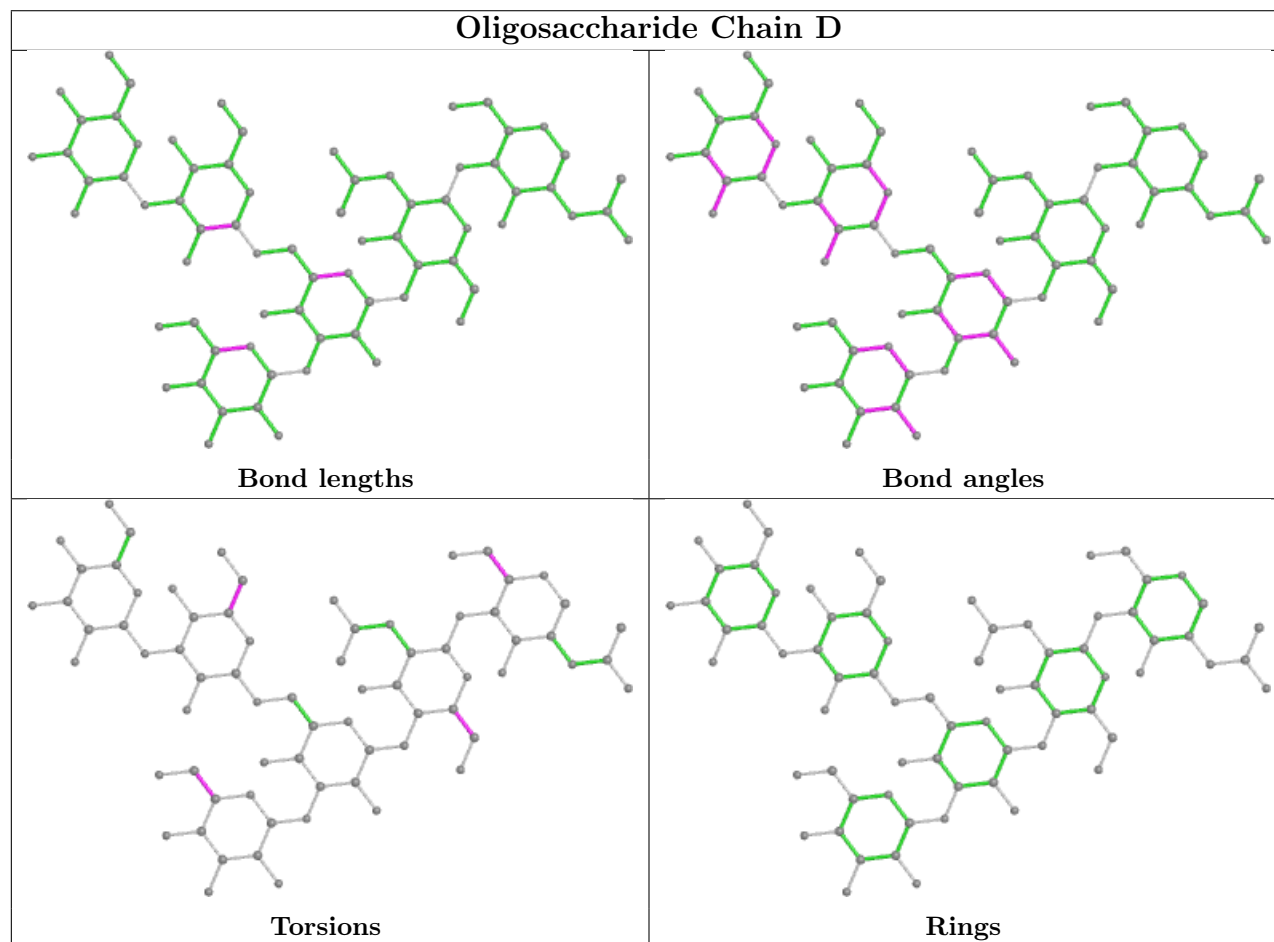
Mol	Chain	Res	Type	Atoms
2	N	1	NAG	O5-C5-C6-O6
2	N	4	MAN	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6

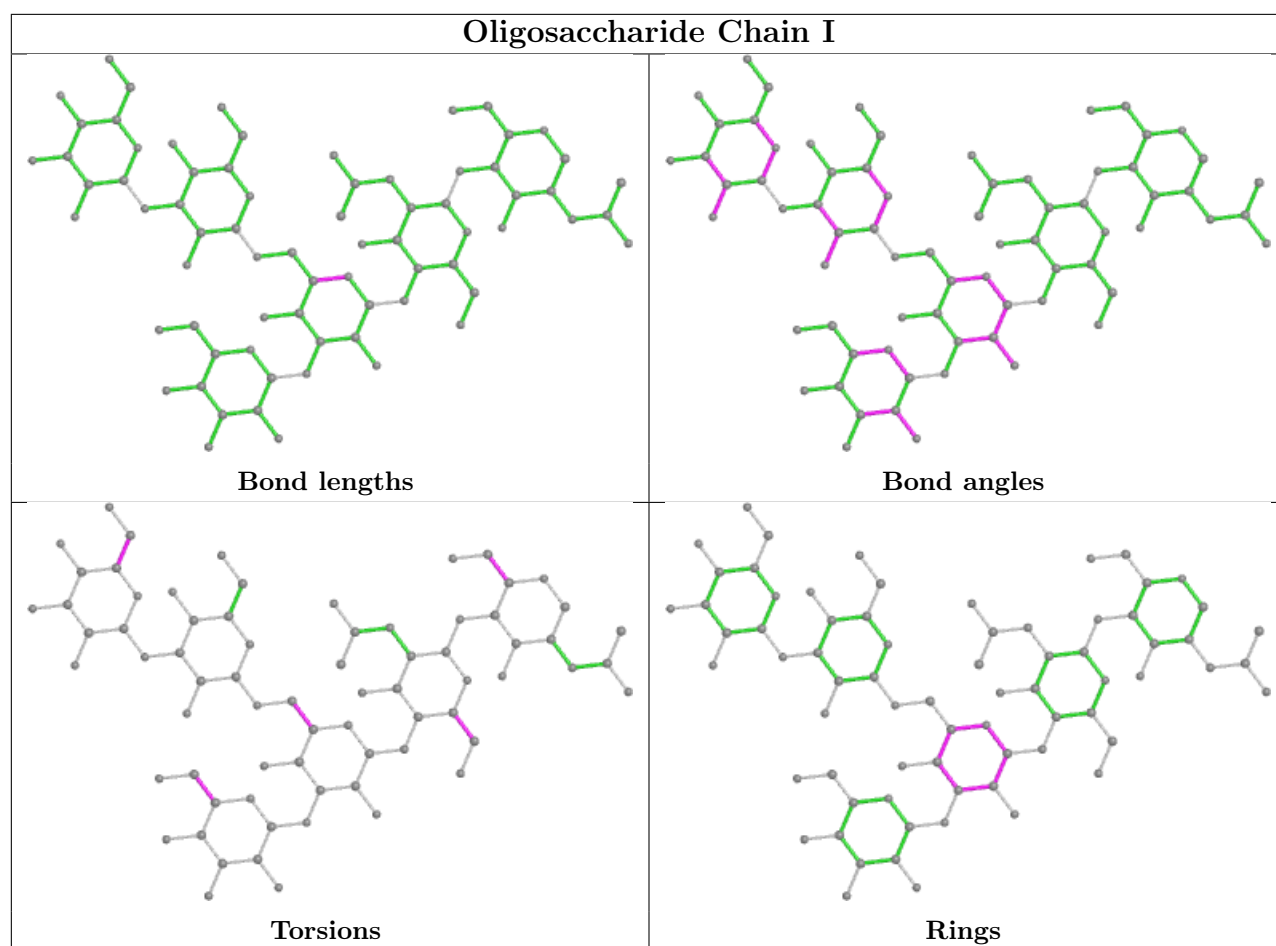
All (1) ring outliers are listed below:

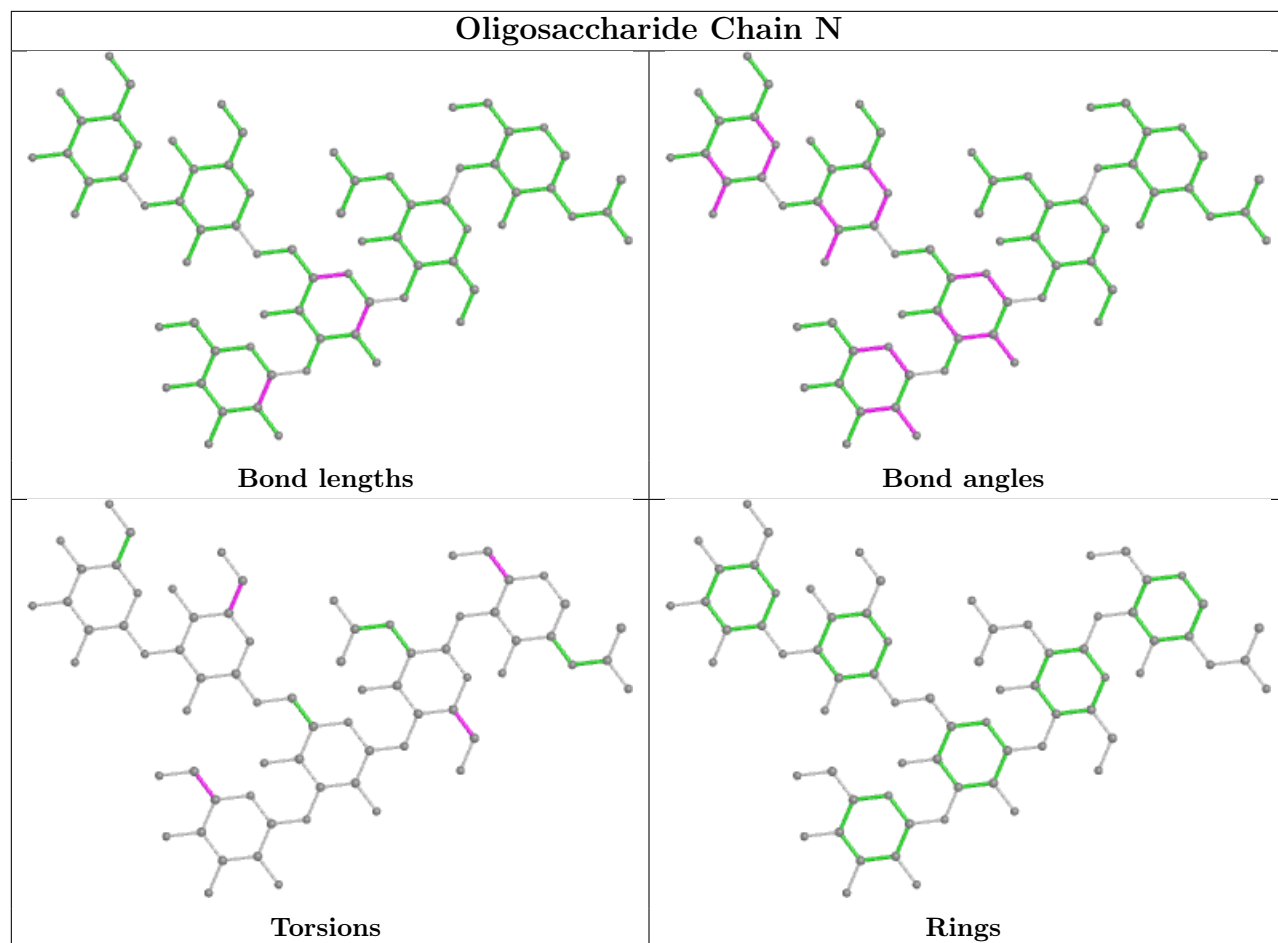
Mol	Chain	Res	Type	Atoms
2	I	3	MAN	C1-C2-C3-C4-C5-O5

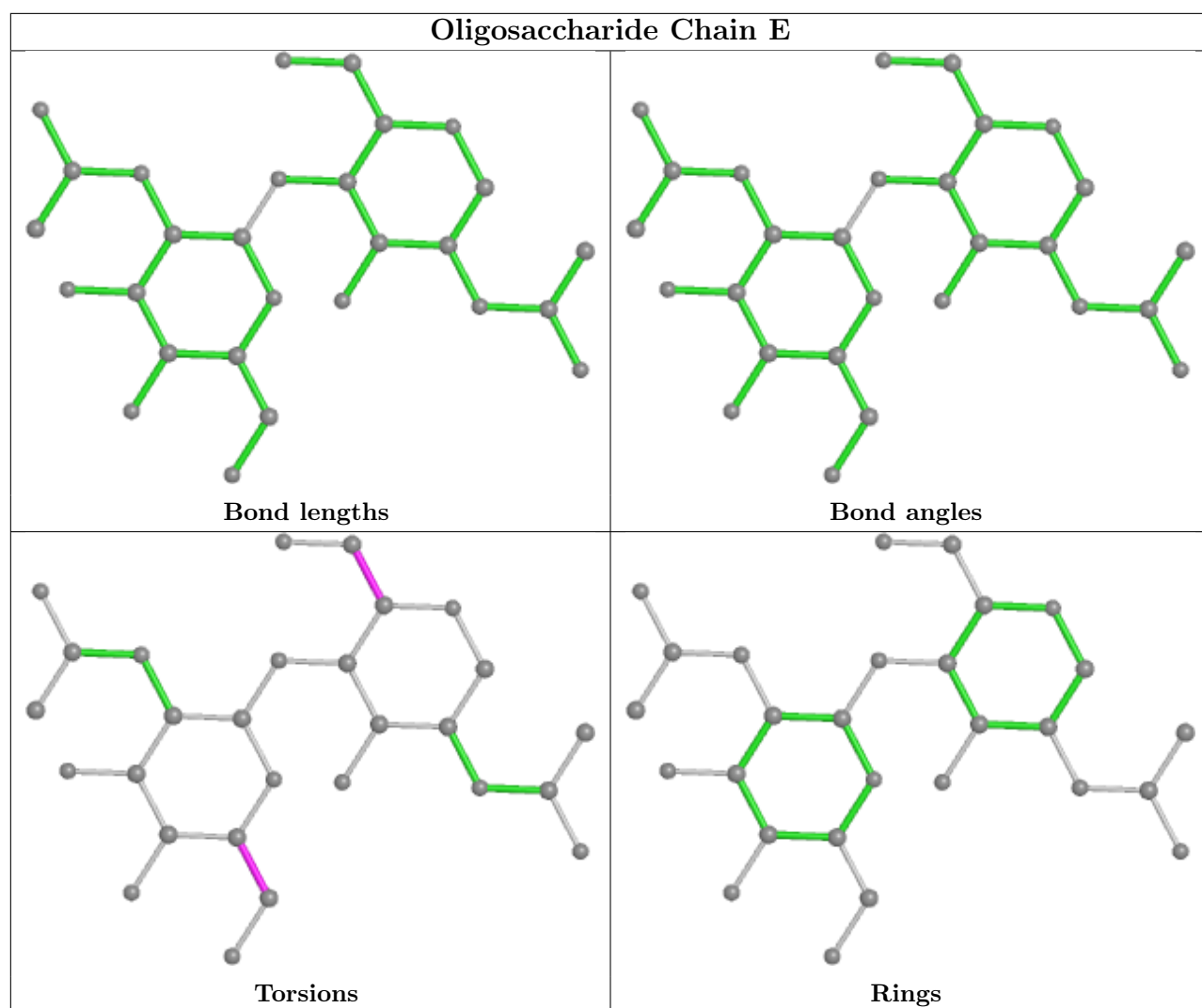
No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

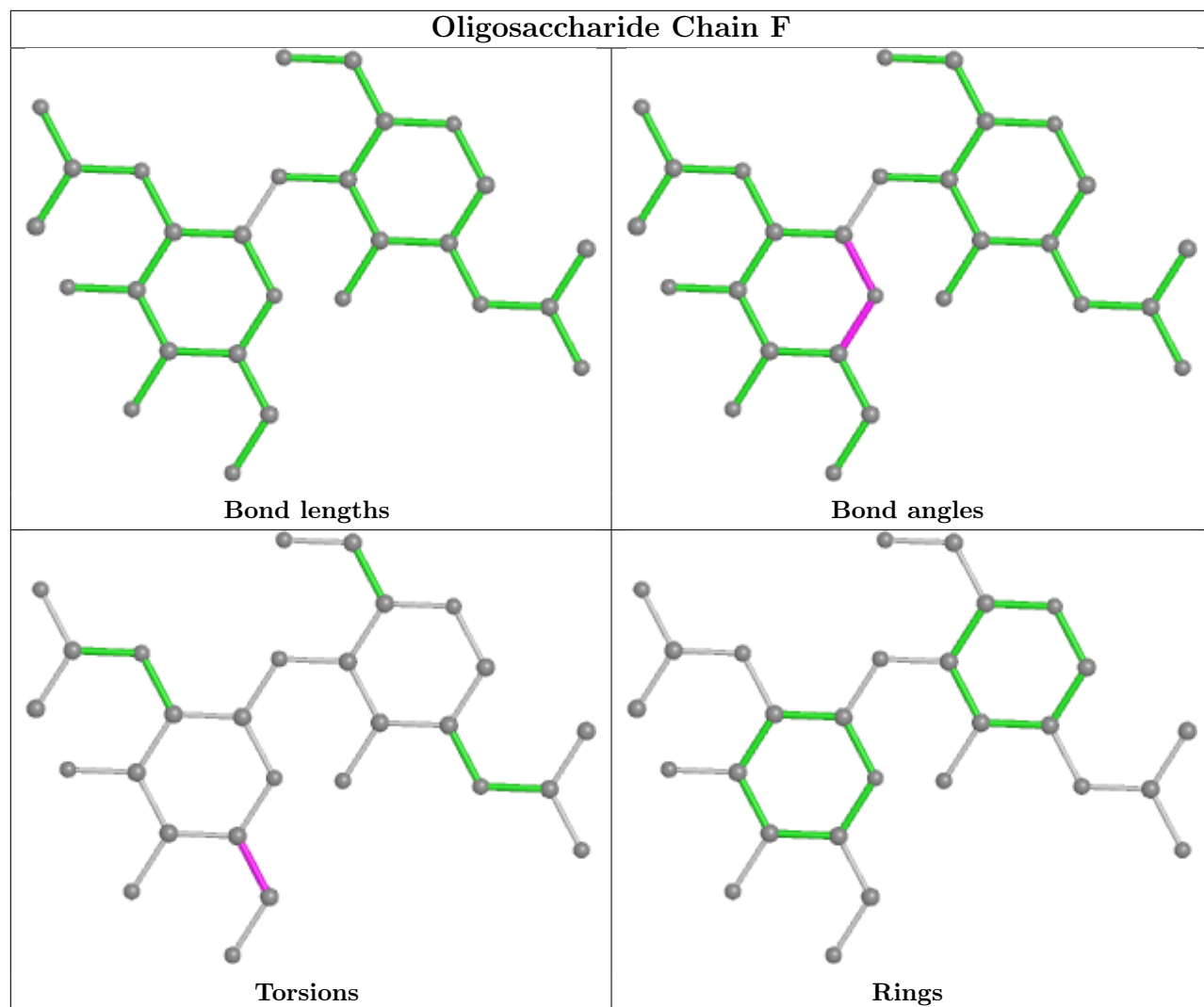


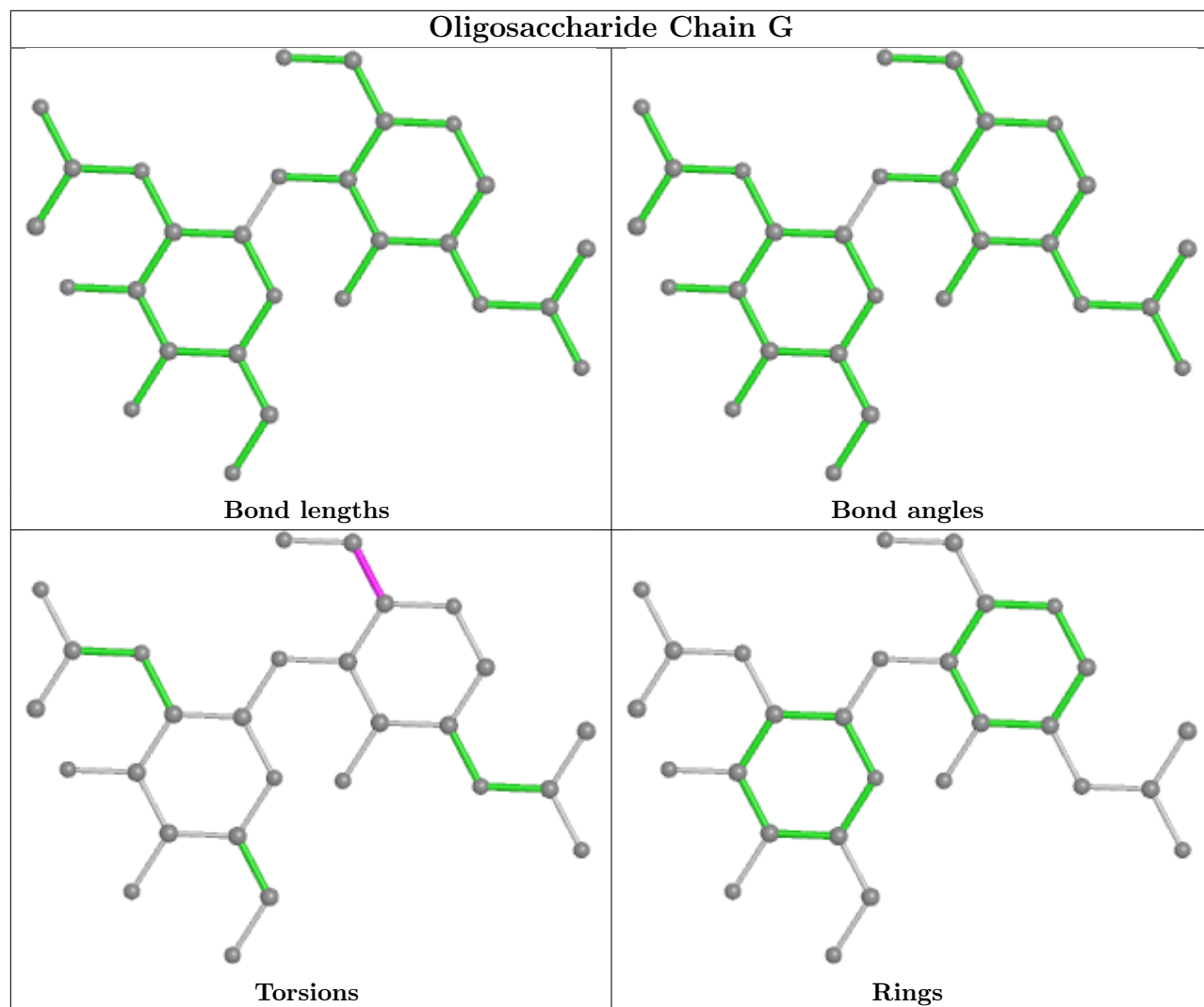


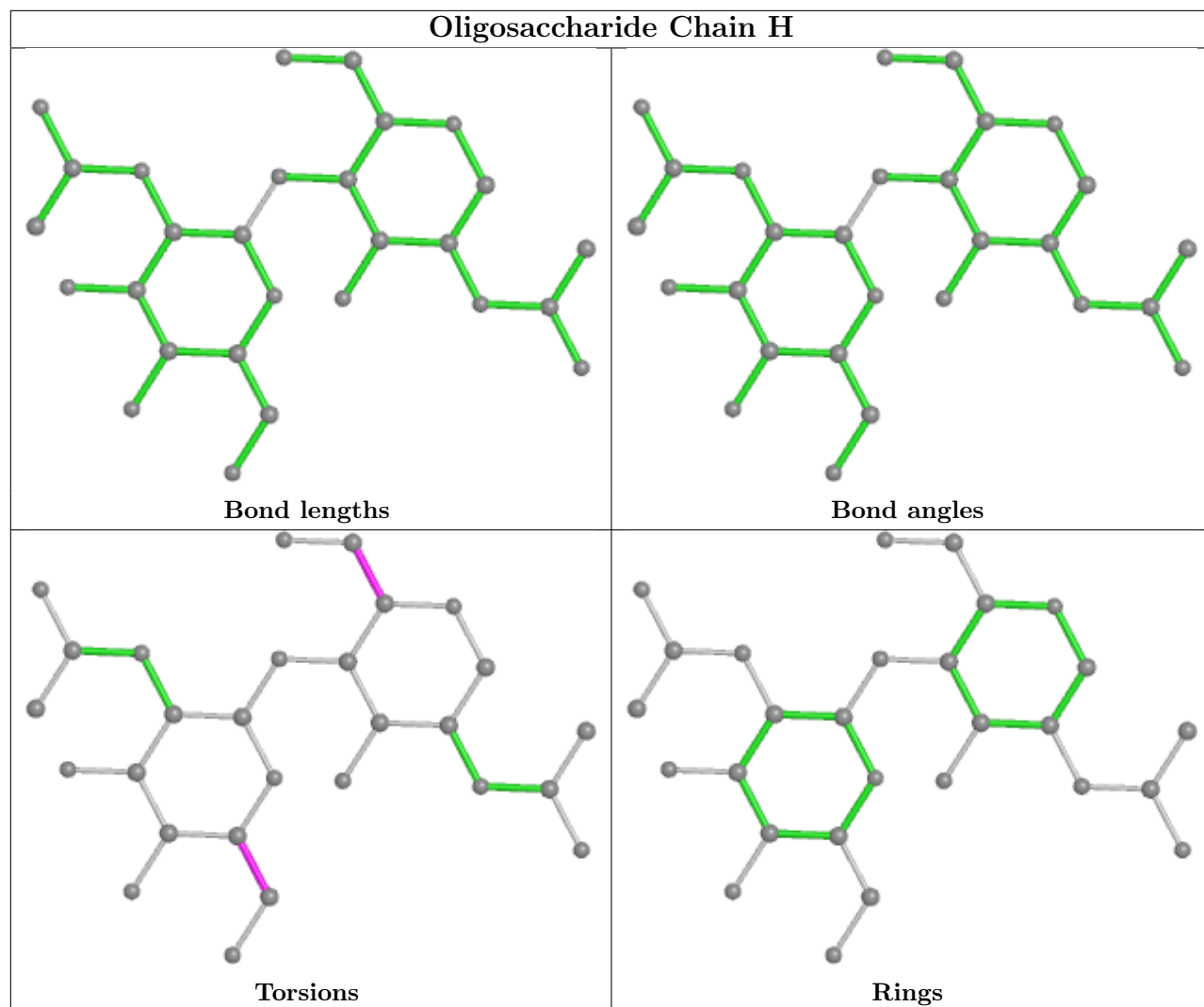


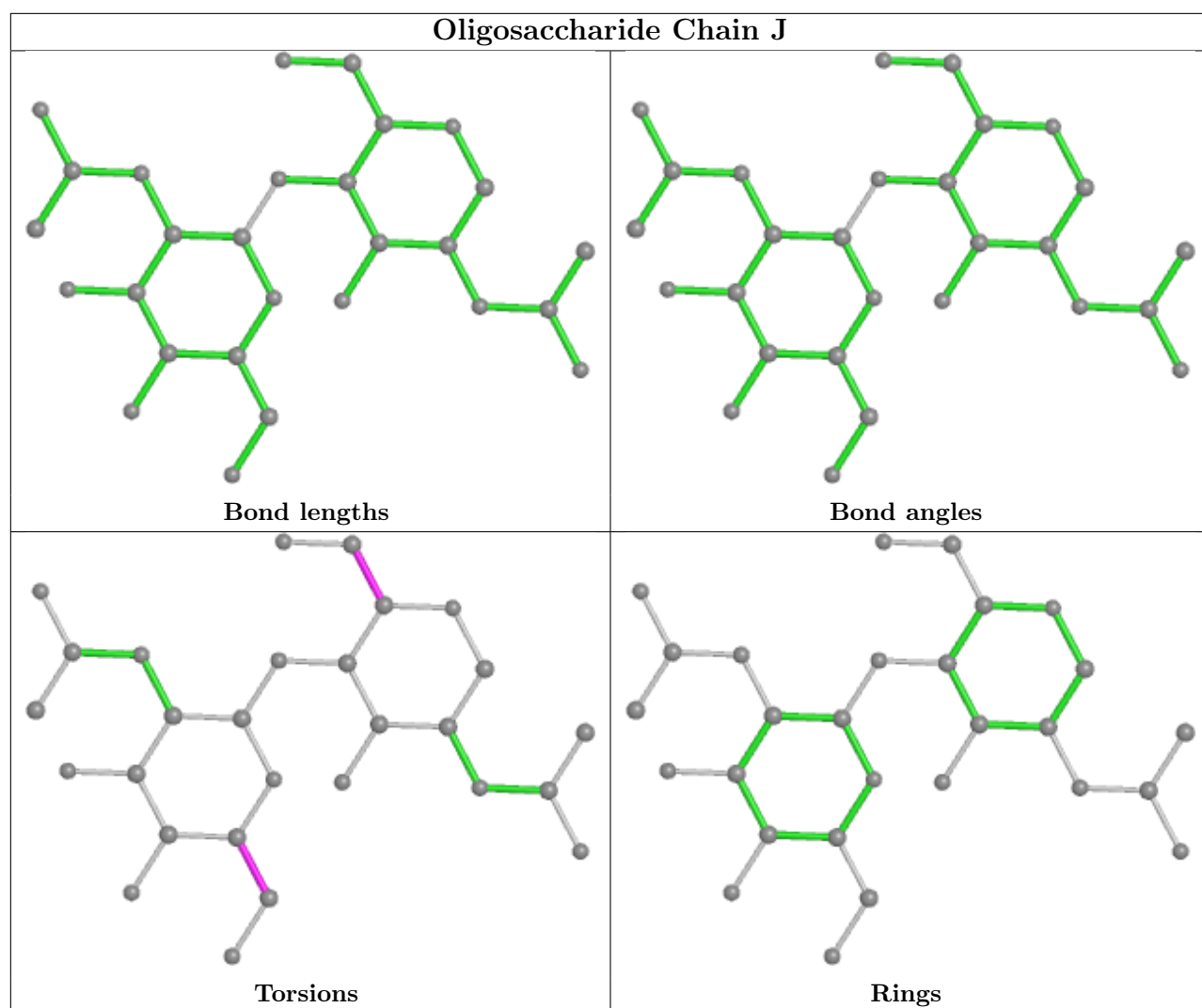


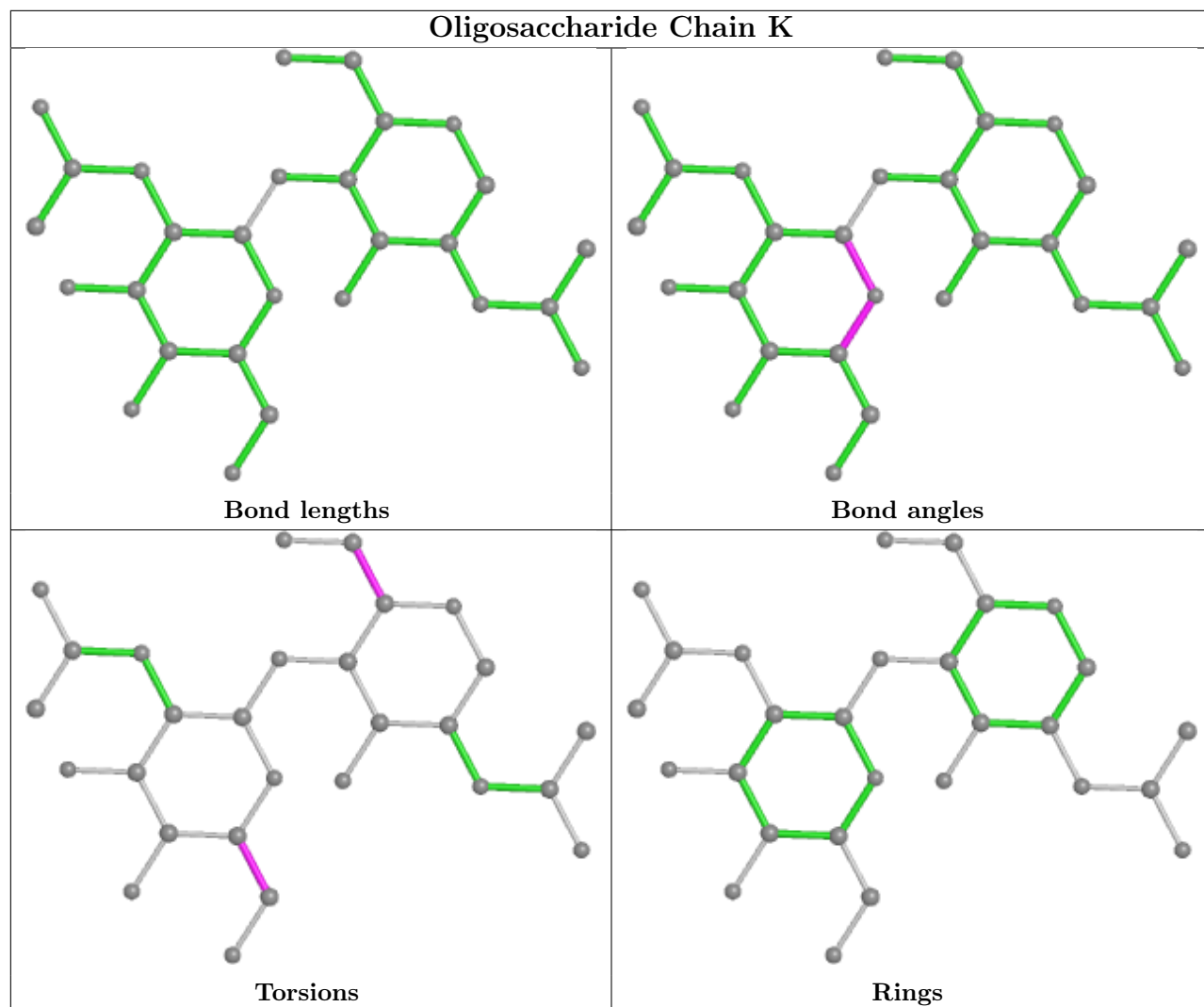


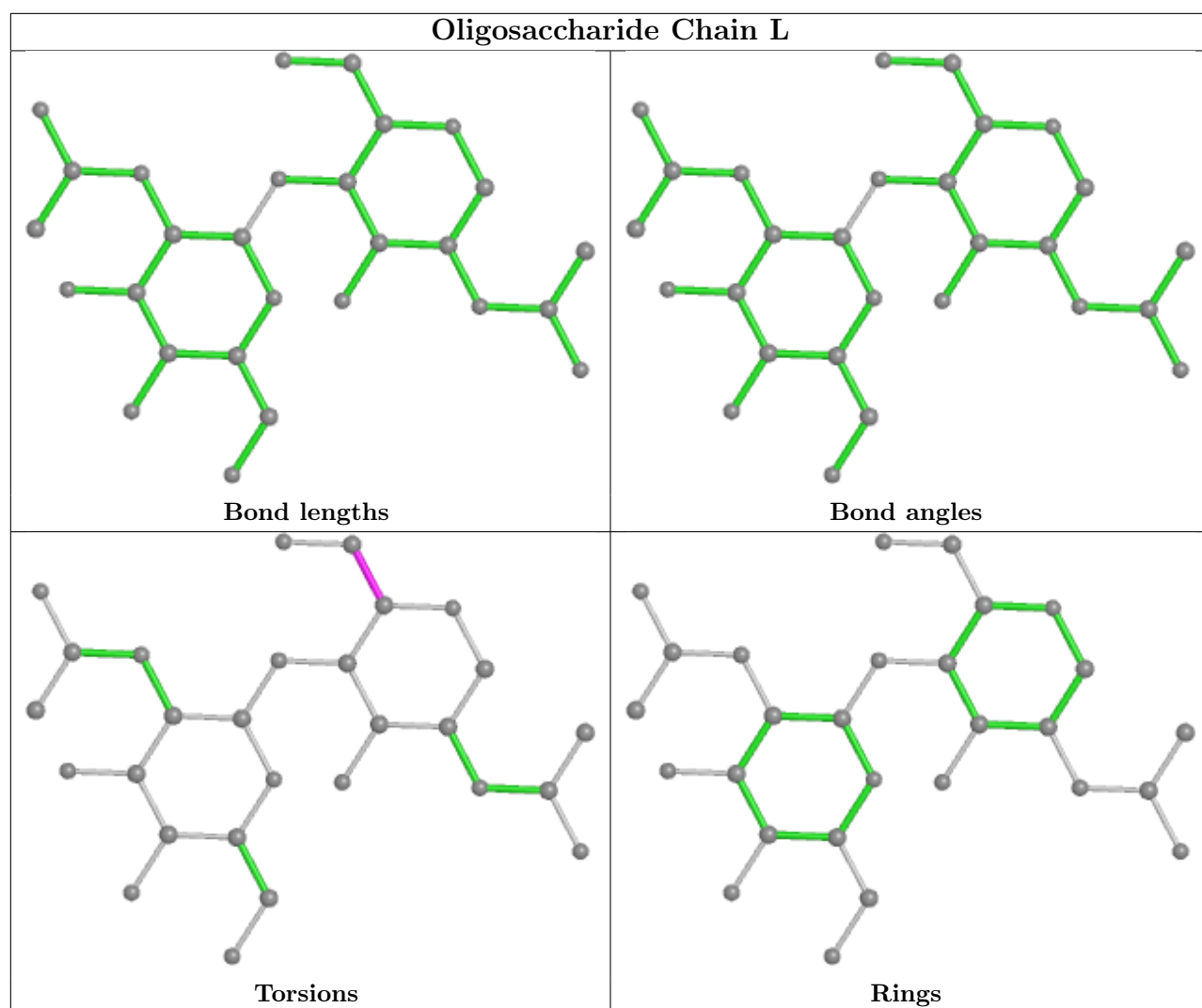


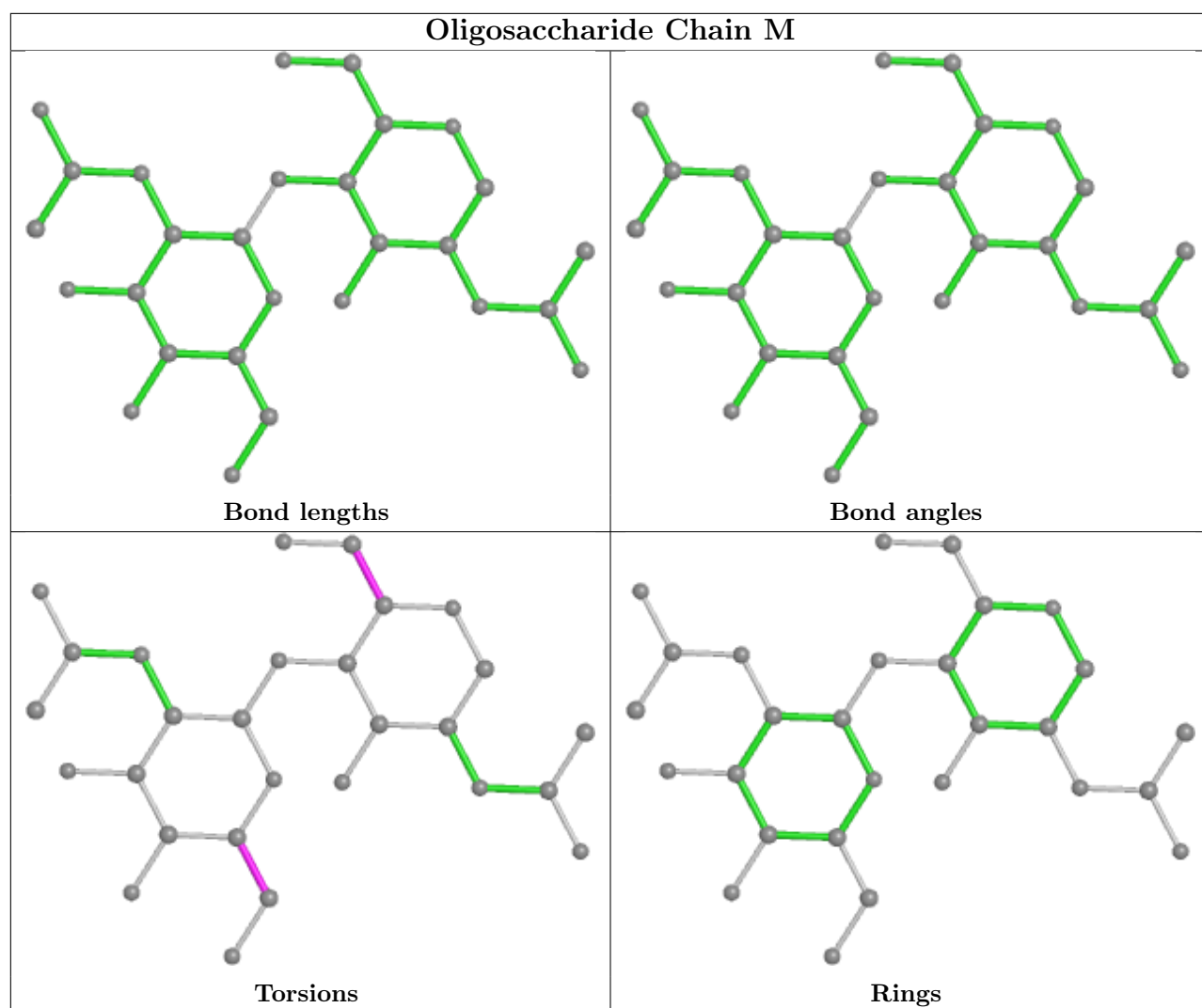


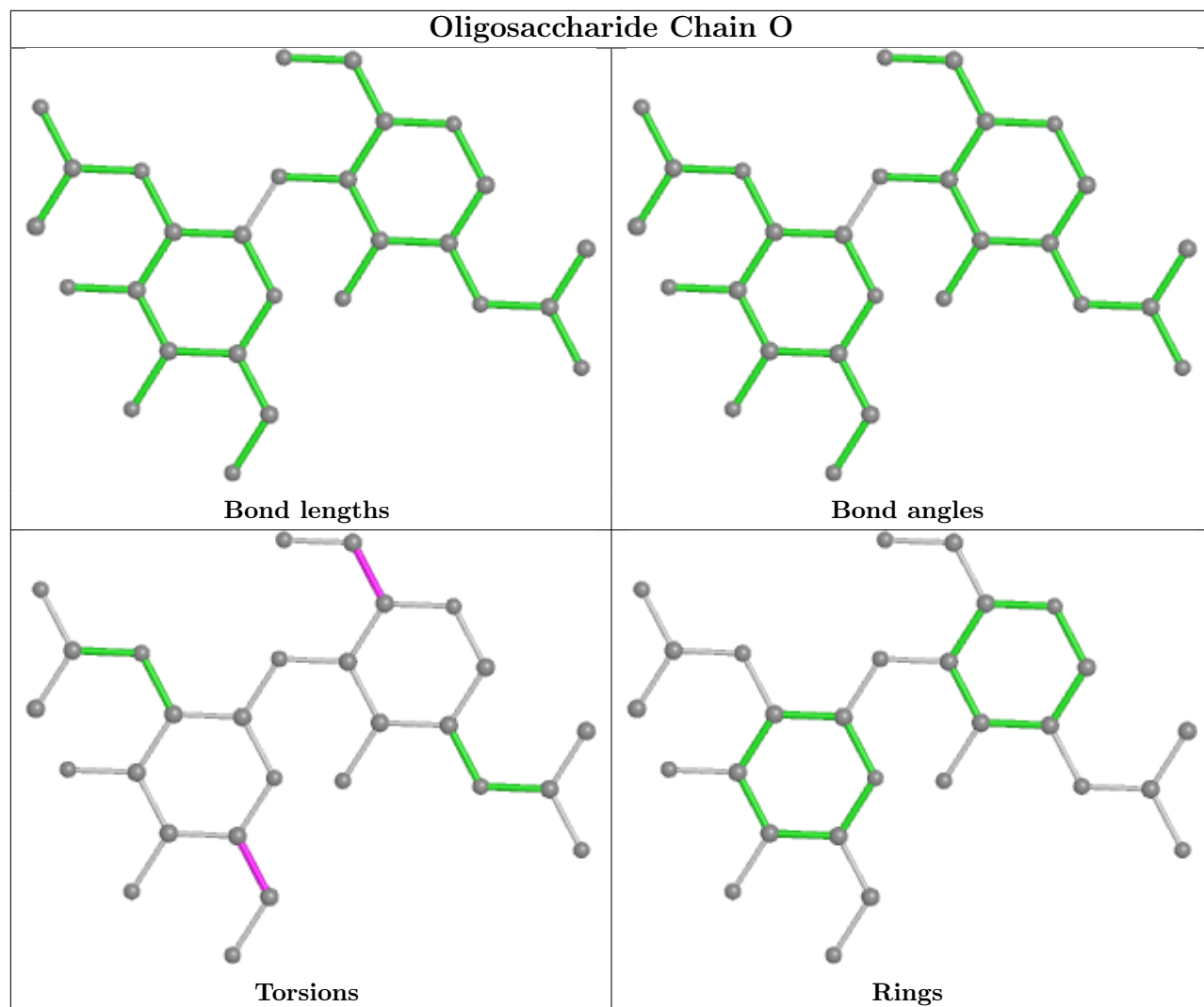




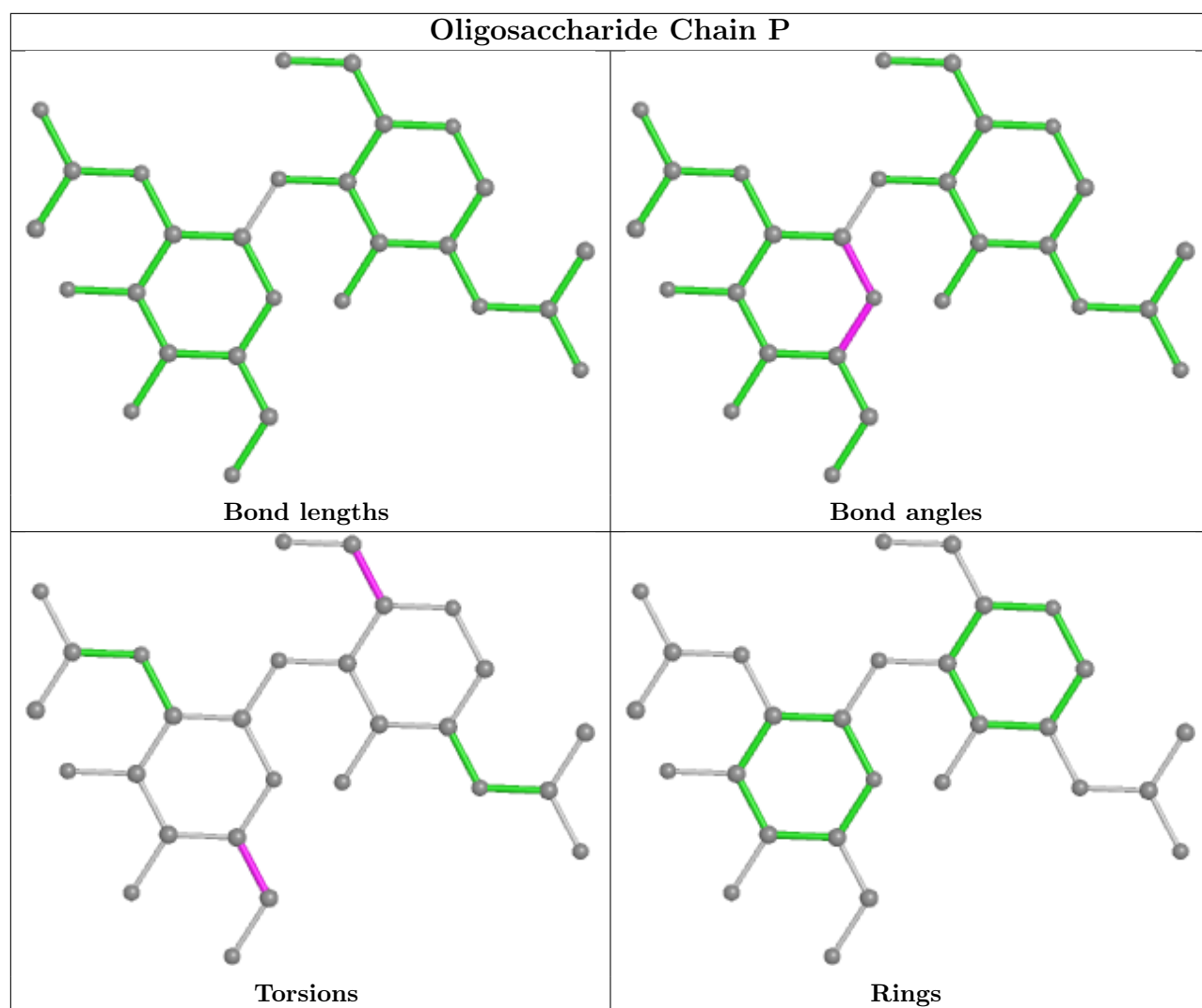


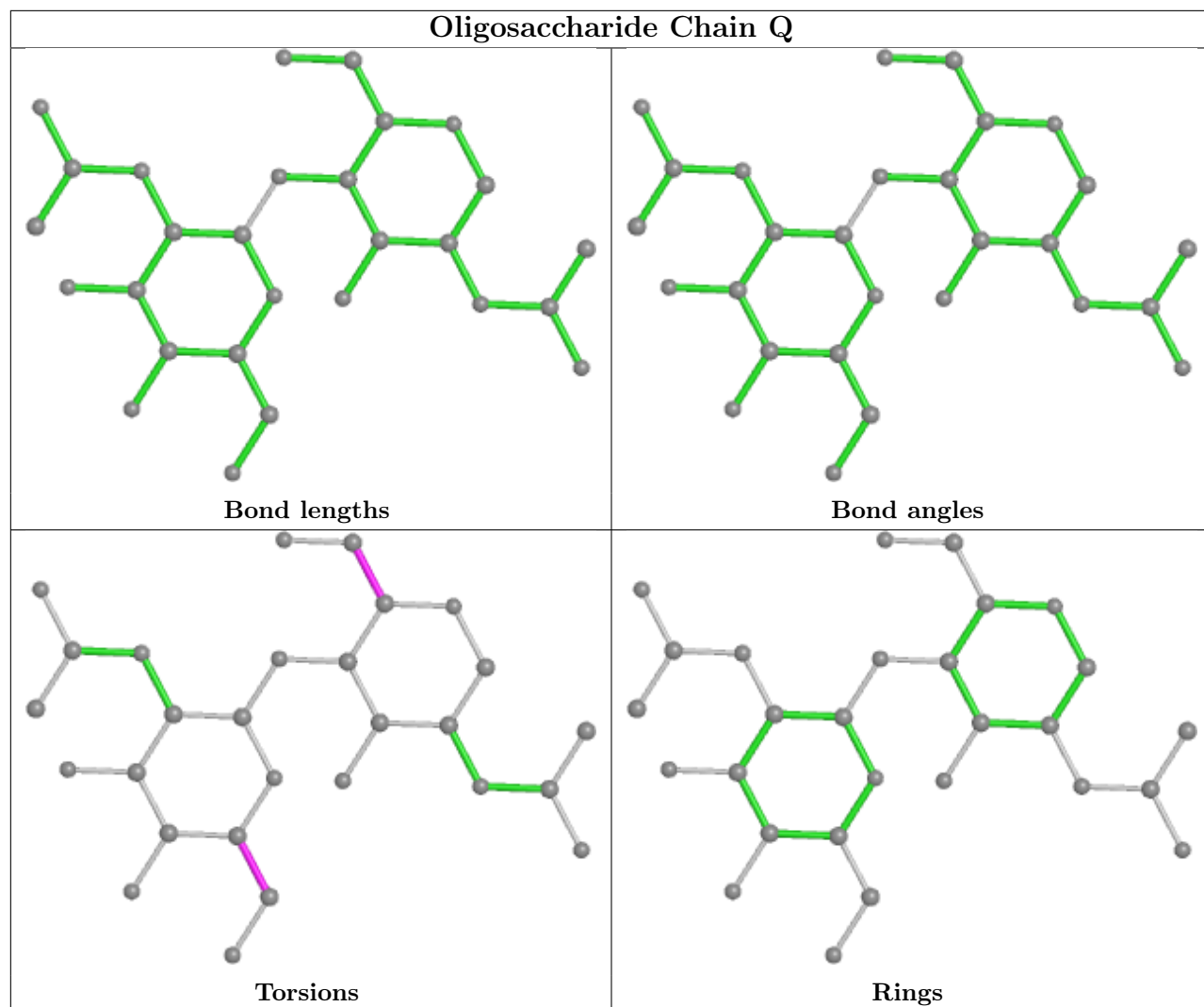


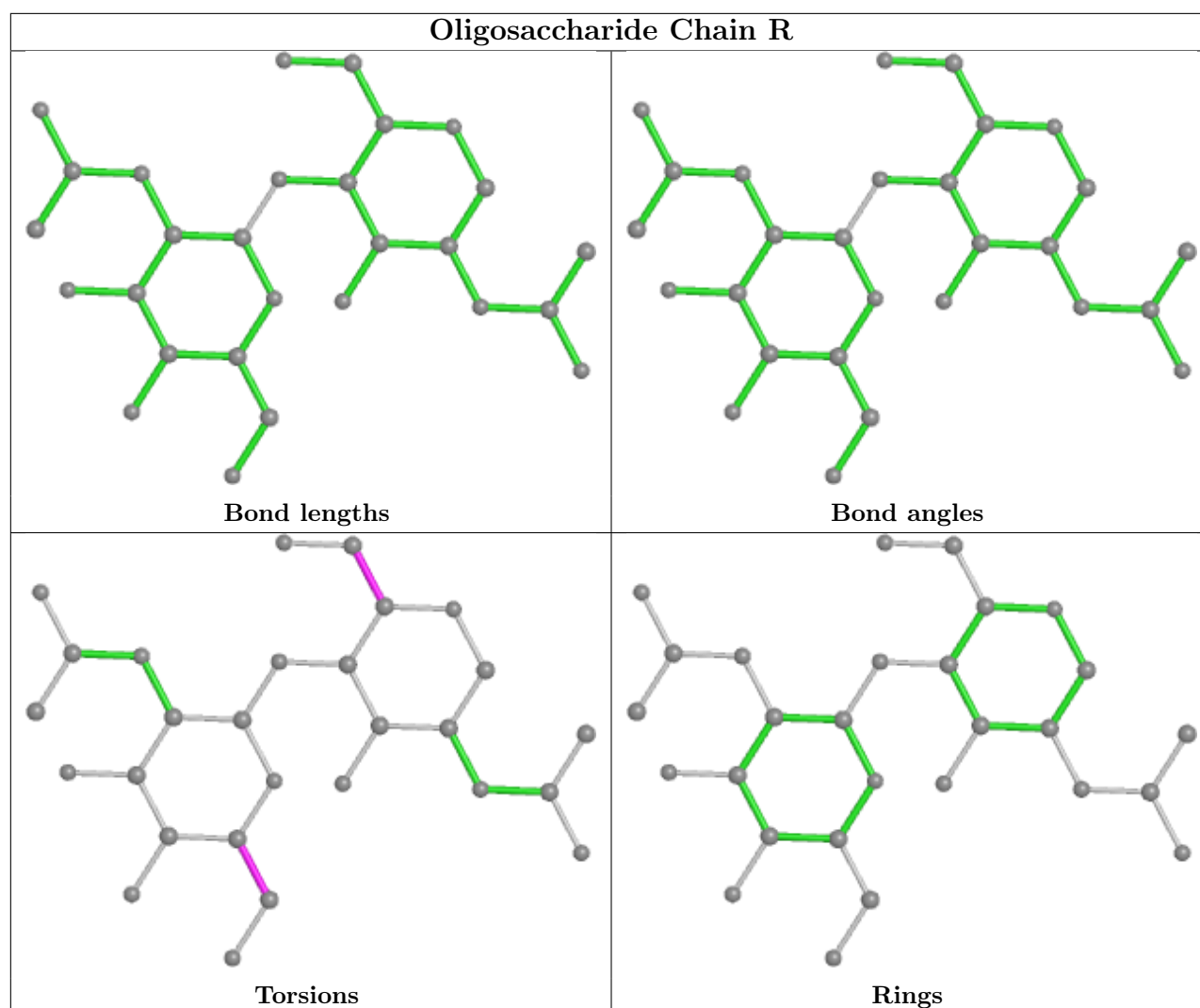












## 5.6 Ligand geometry [i](#)

51 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	$\# Z  > 2$
4	NAG	C	2016	1	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	B	2013	1	14,14,15	0.27	0	17,19,21	0.49	0
4	NAG	B	2012	1	14,14,15	0.35	0	17,19,21	0.59	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	2016	1	14,14,15	0.41	0	17,19,21	0.54	0
4	NAG	C	2003	1	14,14,15	0.42	0	17,19,21	0.39	0
4	NAG	C	2006	1	14,14,15	0.37	0	17,19,21	0.47	0
4	NAG	A	2009	1	14,14,15	0.35	0	17,19,21	0.59	1 (5%)
4	NAG	A	2012	1	14,14,15	0.30	0	17,19,21	0.61	1 (5%)
4	NAG	A	2010	1	14,14,15	0.35	0	17,19,21	0.41	0
4	NAG	B	2009	1	14,14,15	0.30	0	17,19,21	0.58	0
4	NAG	A	2002	1	14,14,15	0.48	0	17,19,21	0.49	0
4	NAG	C	2014	1	14,14,15	0.46	0	17,19,21	0.50	0
4	NAG	C	2009	1	14,14,15	0.33	0	17,19,21	0.59	1 (5%)
4	NAG	C	2010	1	14,14,15	0.33	0	17,19,21	0.37	0
4	NAG	C	2011	1	14,14,15	0.36	0	17,19,21	0.55	0
4	NAG	B	2002	1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	A	2013	1	14,14,15	0.40	0	17,19,21	0.43	0
4	NAG	B	2010	1	14,14,15	0.34	0	17,19,21	0.39	0
4	NAG	A	2016	1	14,14,15	0.38	0	17,19,21	0.60	1 (5%)
4	NAG	A	2007	1	14,14,15	0.36	0	17,19,21	0.51	0
4	NAG	C	2008	1	14,14,15	0.48	0	17,19,21	0.60	1 (5%)
4	NAG	A	2005	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	B	2006	1	14,14,15	0.33	0	17,19,21	0.47	0
4	NAG	A	2015	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	A	2017	1	14,14,15	0.41	0	17,19,21	0.51	0
4	NAG	C	2005	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	2007	1	14,14,15	0.41	0	17,19,21	0.58	1 (5%)
4	NAG	C	2004	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	C	2017	1	14,14,15	0.32	0	17,19,21	0.51	0
4	NAG	C	2012	1	14,14,15	0.34	0	17,19,21	0.57	0
4	NAG	B	2005	1	14,14,15	0.40	0	17,19,21	0.52	0
4	NAG	B	2015	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	2003	1	14,14,15	0.47	0	17,19,21	0.39	0
4	NAG	B	2017	1	14,14,15	0.37	0	17,19,21	0.52	0
4	NAG	A	2014	1	14,14,15	0.33	0	17,19,21	0.43	0
4	NAG	B	2014	1	14,14,15	0.45	0	17,19,21	0.48	0
4	NAG	C	2007	1	14,14,15	0.41	0	17,19,21	0.45	0
4	NAG	C	2013	1	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	2001	1	14,14,15	0.51	0	17,19,21	0.52	0
4	NAG	A	2008	1	14,14,15	0.37	0	17,19,21	0.57	0
4	NAG	A	2003	1	14,14,15	0.44	0	17,19,21	0.40	0
4	NAG	A	2001	1	14,14,15	0.41	0	17,19,21	0.49	0
4	NAG	A	2011	1	14,14,15	0.32	0	17,19,21	0.56	0
4	NAG	B	2011	1	14,14,15	0.43	0	17,19,21	0.65	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	2001	1	14,14,15	0.41	0	17,19,21	0.50	0
4	NAG	C	2015	1	14,14,15	0.32	0	17,19,21	0.53	0
4	NAG	C	2002	1	14,14,15	0.50	0	17,19,21	0.53	0
4	NAG	A	2006	1	14,14,15	0.36	0	17,19,21	0.47	0
4	NAG	A	2004	1	14,14,15	0.38	0	17,19,21	0.54	0
4	NAG	B	2008	1	14,14,15	0.42	0	17,19,21	0.58	0
4	NAG	B	2004	1	14,14,15	0.34	0	17,19,21	0.49	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
4	NAG	C	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2011	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2016	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	2/6/23/26	0/1/1/1

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2001	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2011	NAG	C1-O5-C5	2.28	115.28	112.19
4	C	2008	NAG	C1-O5-C5	2.11	115.06	112.19
4	A	2012	NAG	C1-O5-C5	2.08	115.01	112.19
4	A	2009	NAG	C1-O5-C5	2.07	115.00	112.19
4	B	2012	NAG	C1-O5-C5	2.07	115.00	112.19

There are no chirality outliers.

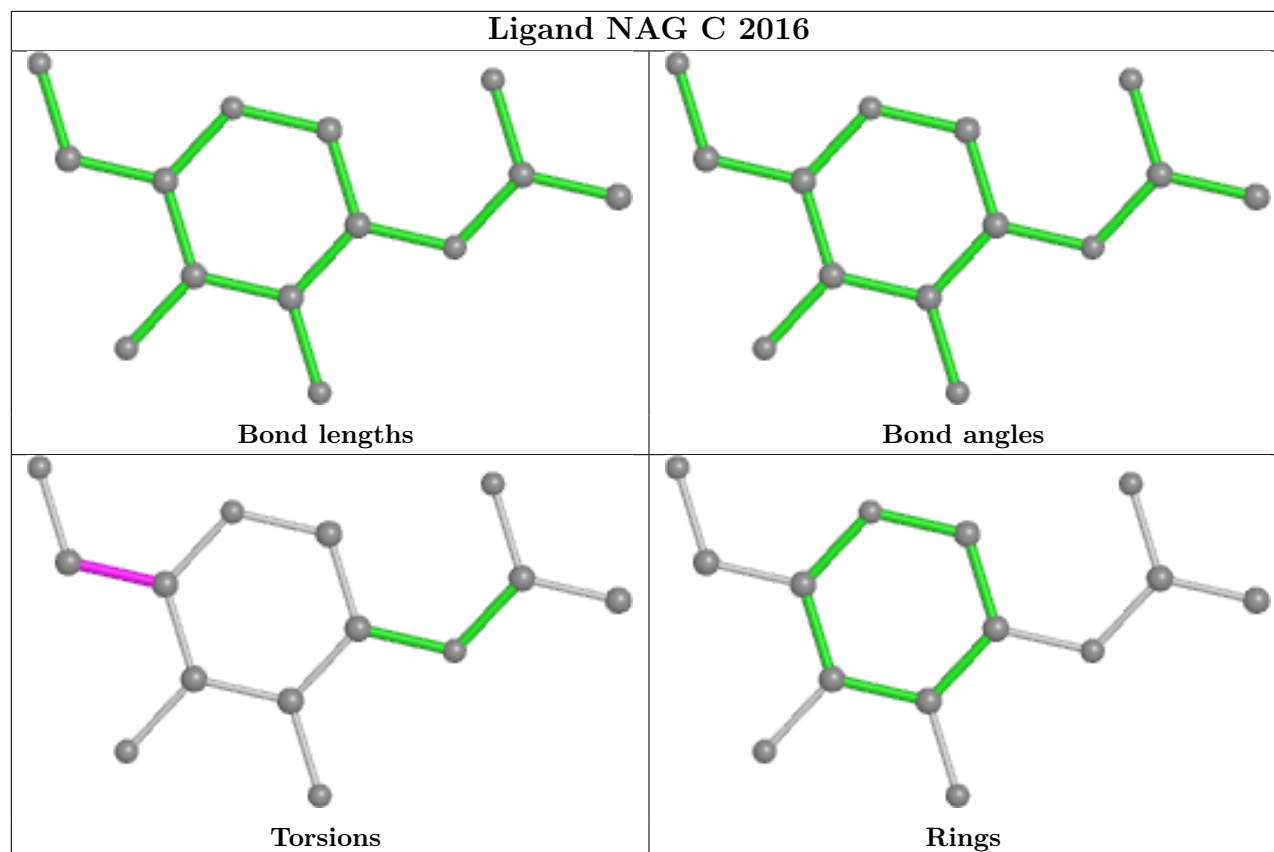
5 of 74 torsion outliers are listed below:

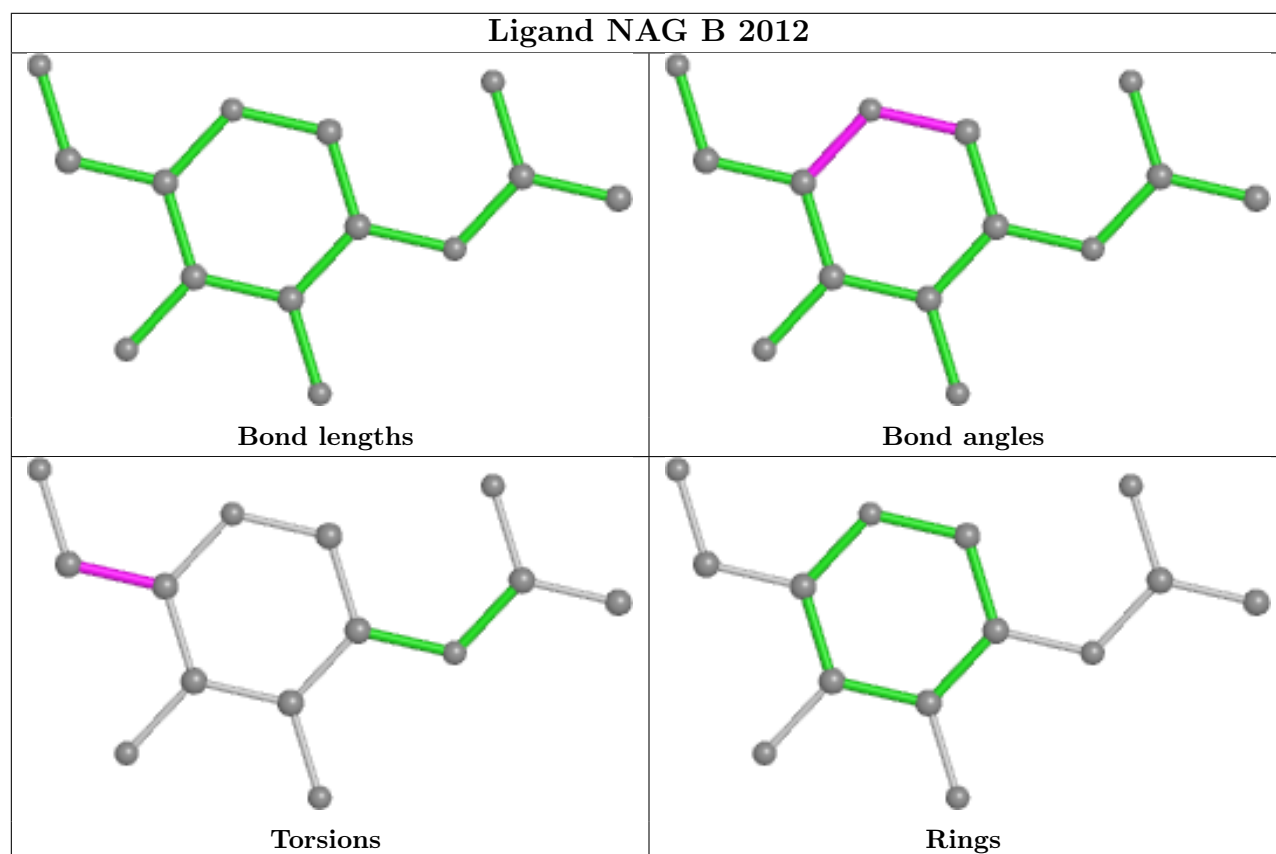
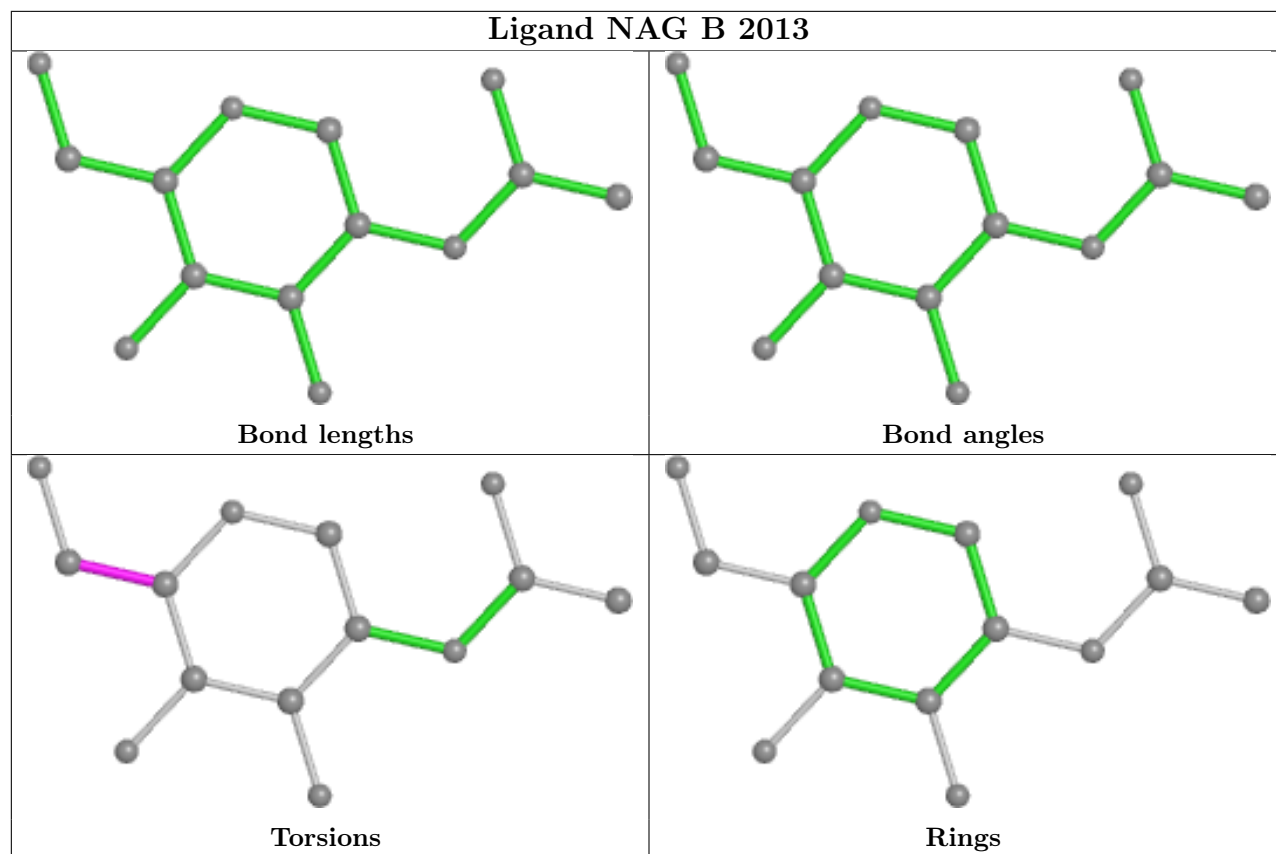
Mol	Chain	Res	Type	Atoms
4	A	2012	NAG	O5-C5-C6-O6
4	A	2015	NAG	O5-C5-C6-O6
4	C	2014	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6

There are no ring outliers.

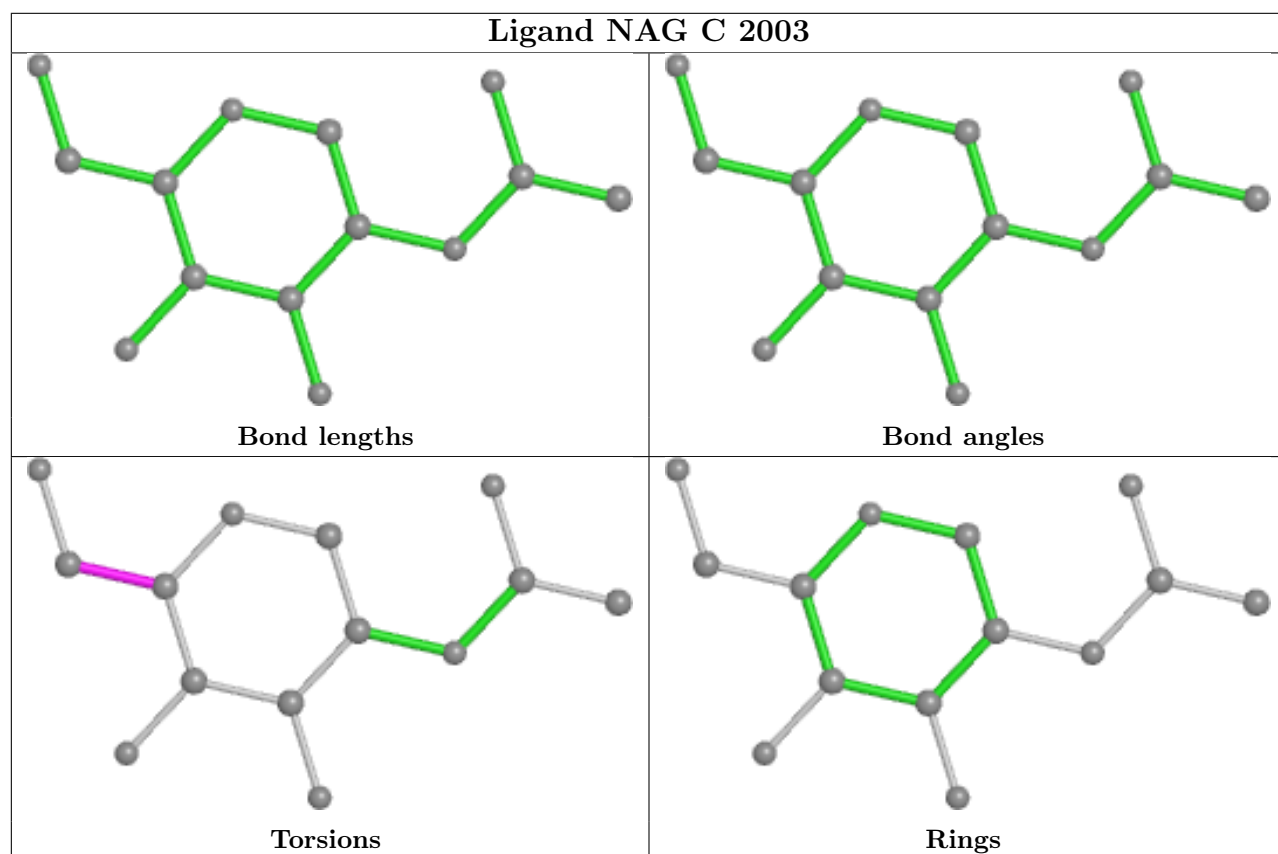
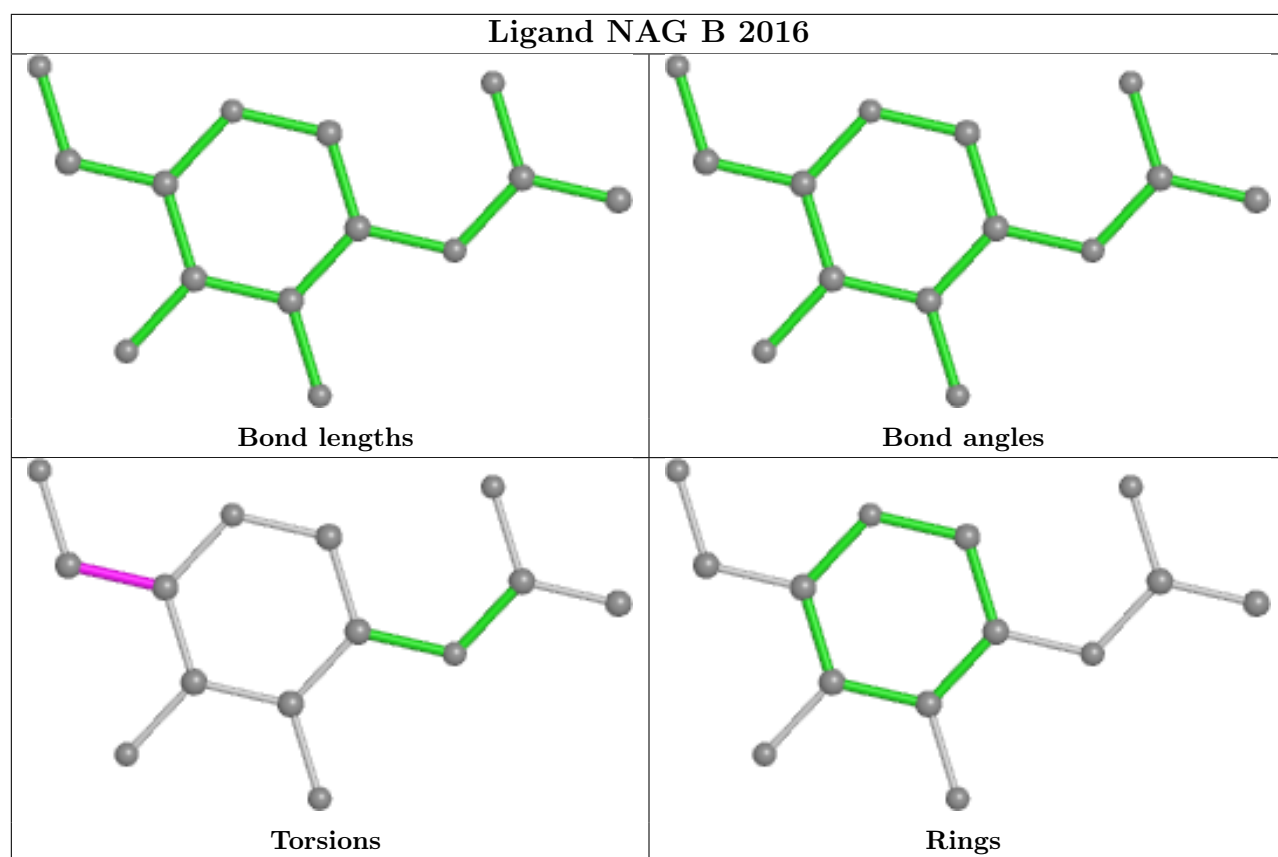
No monomer is involved in short contacts.

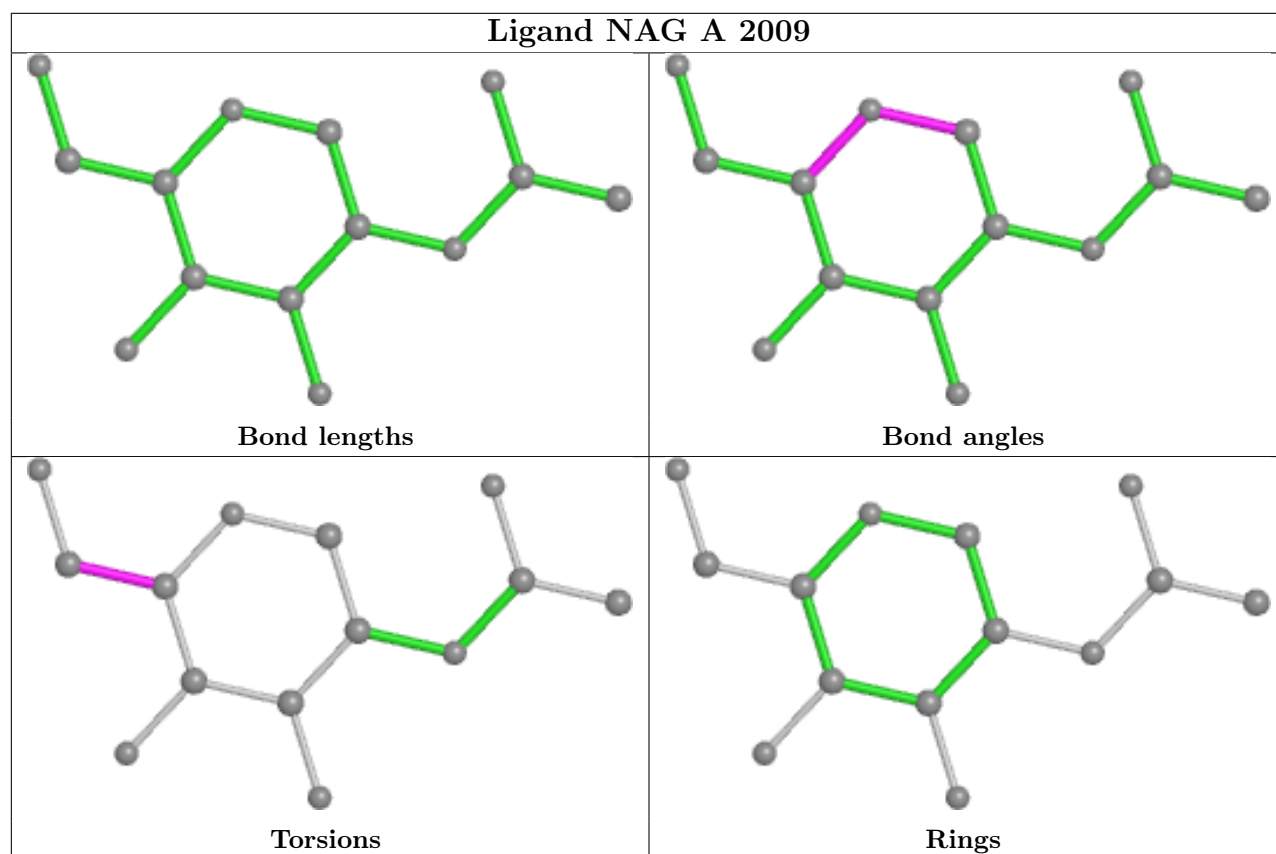
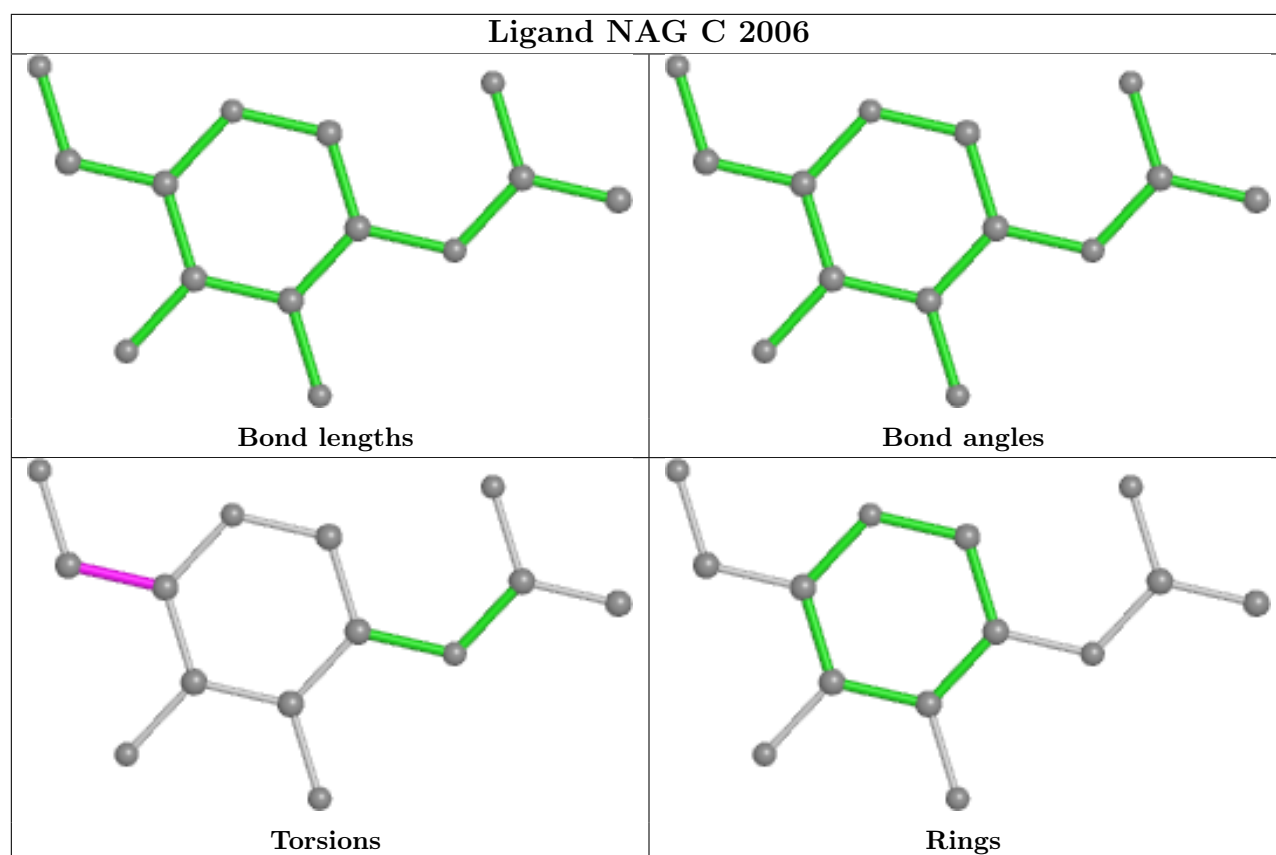
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

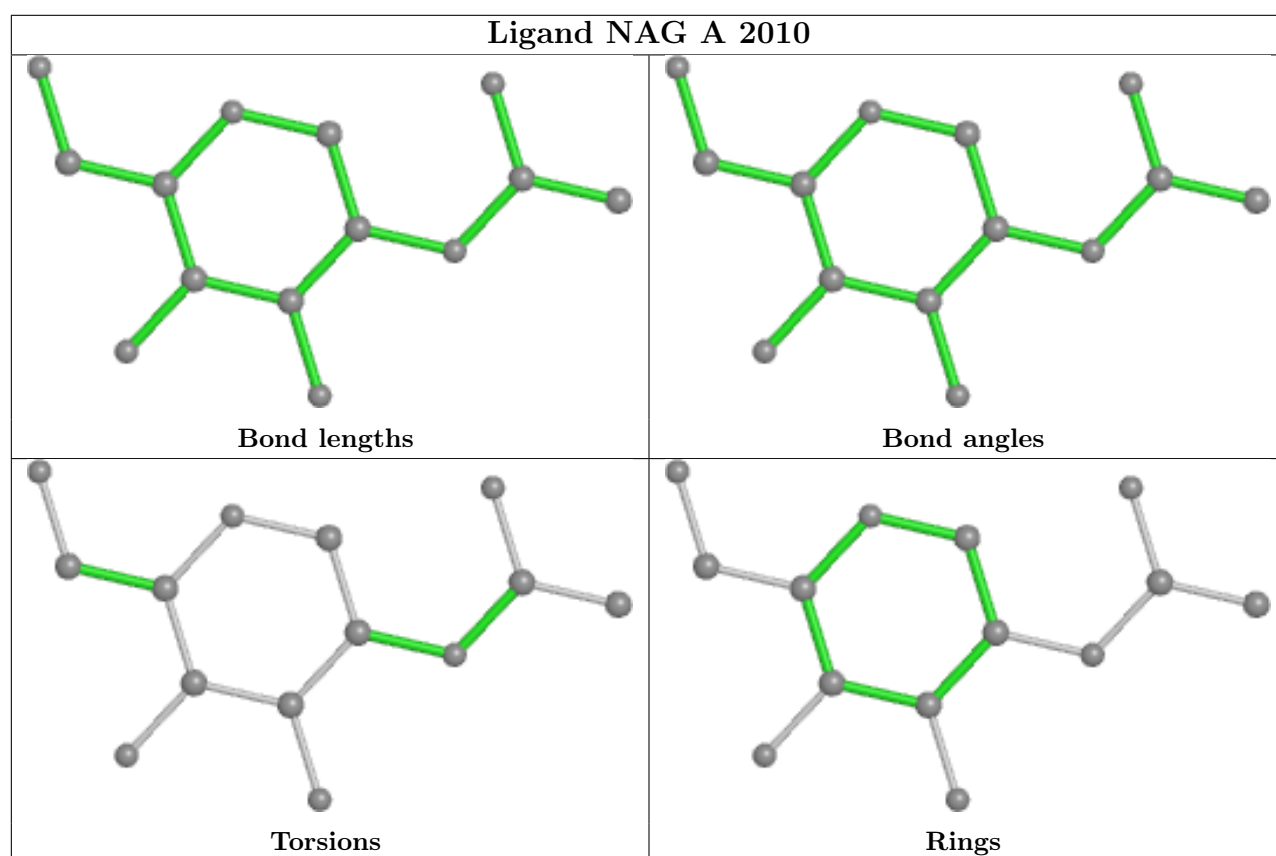
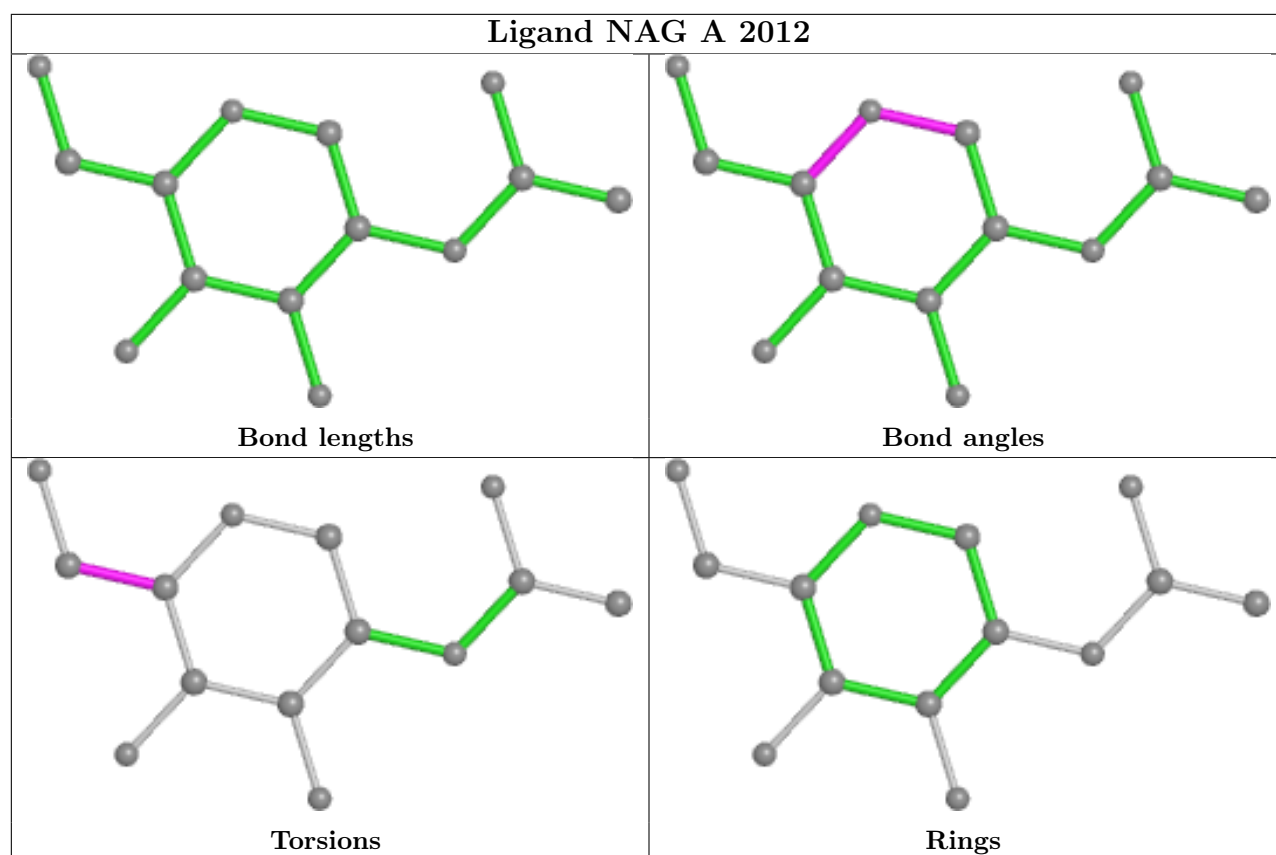


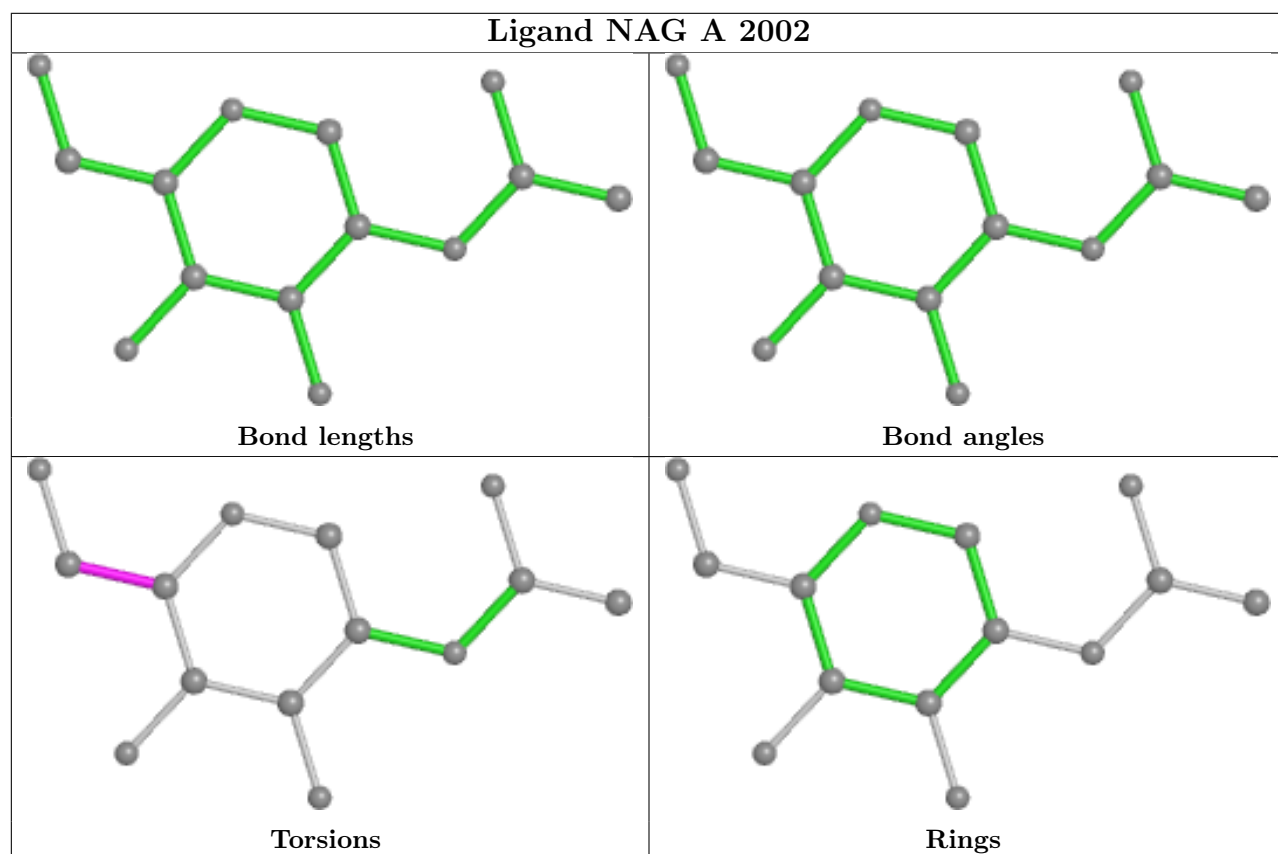
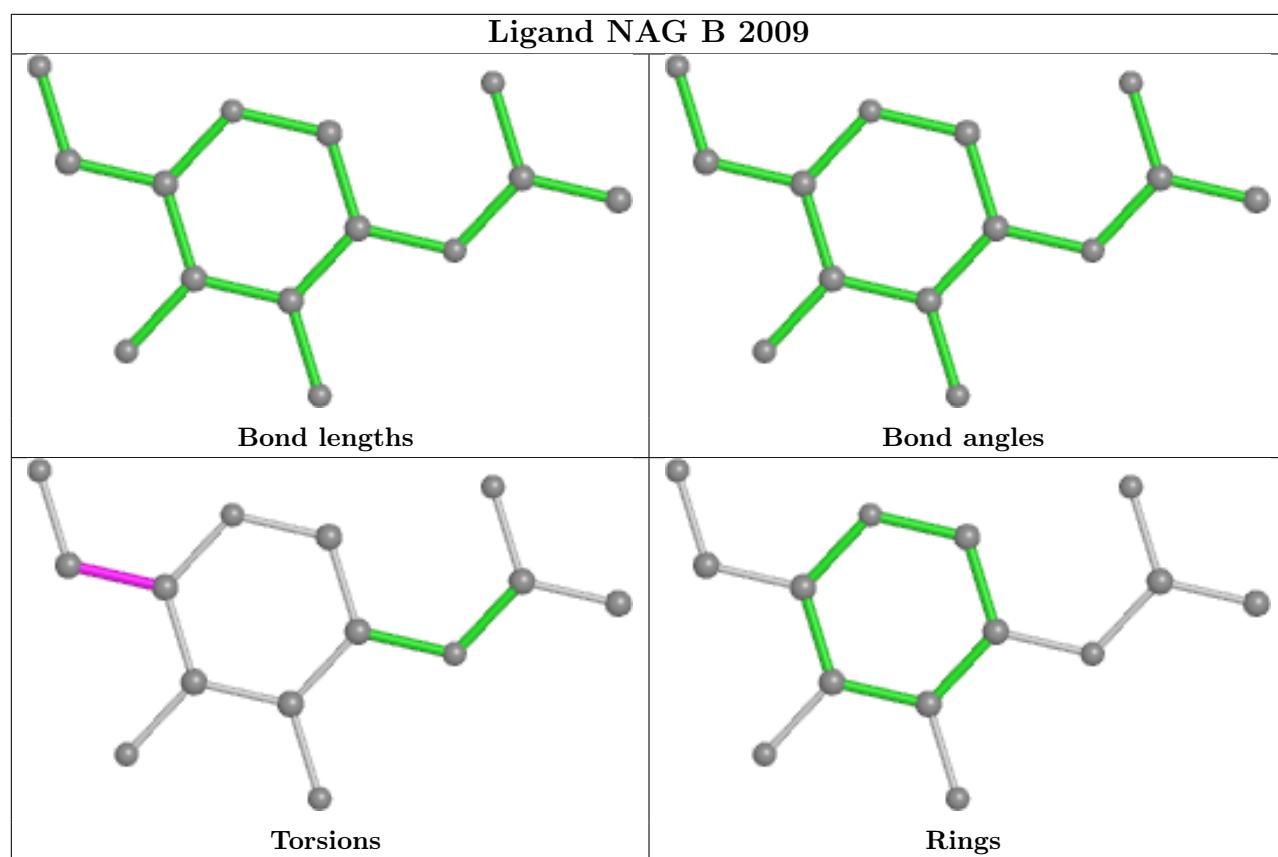


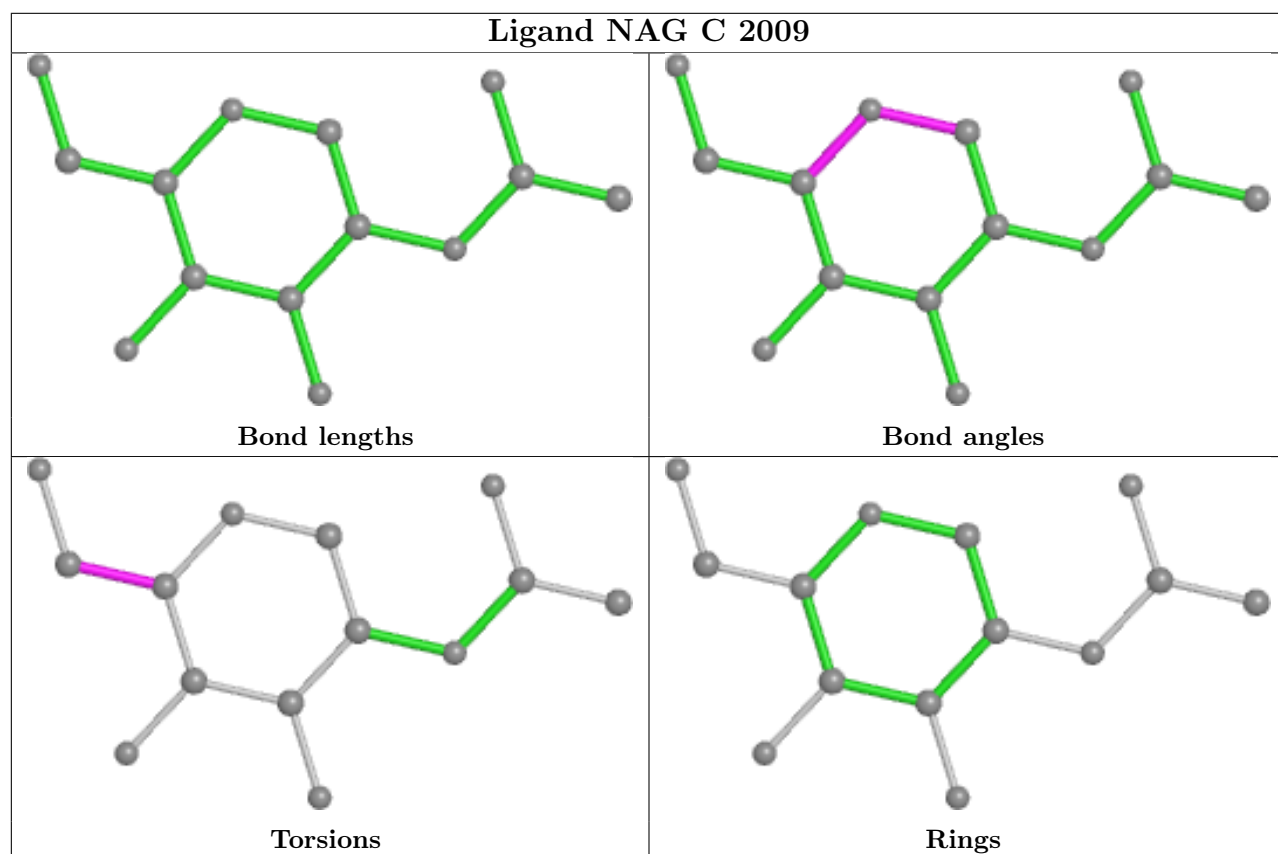
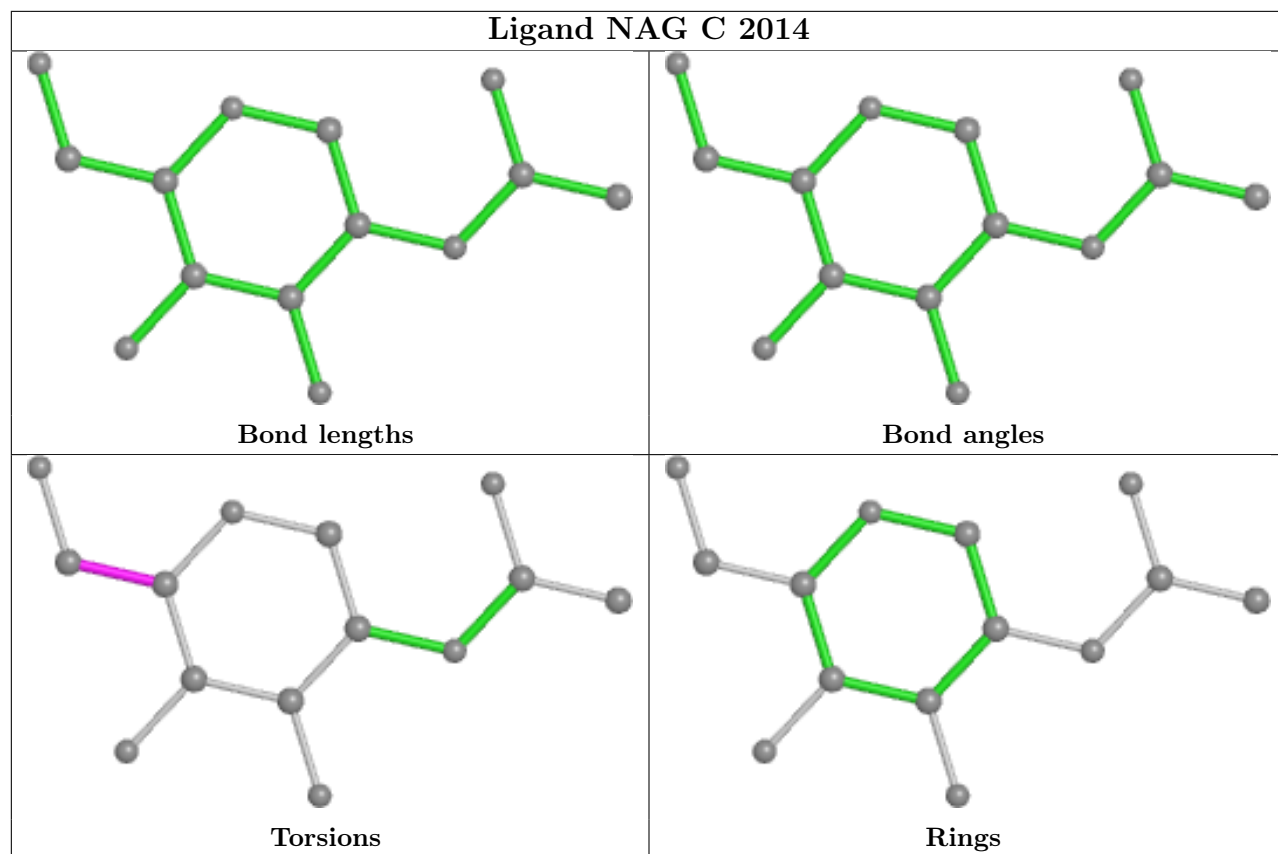


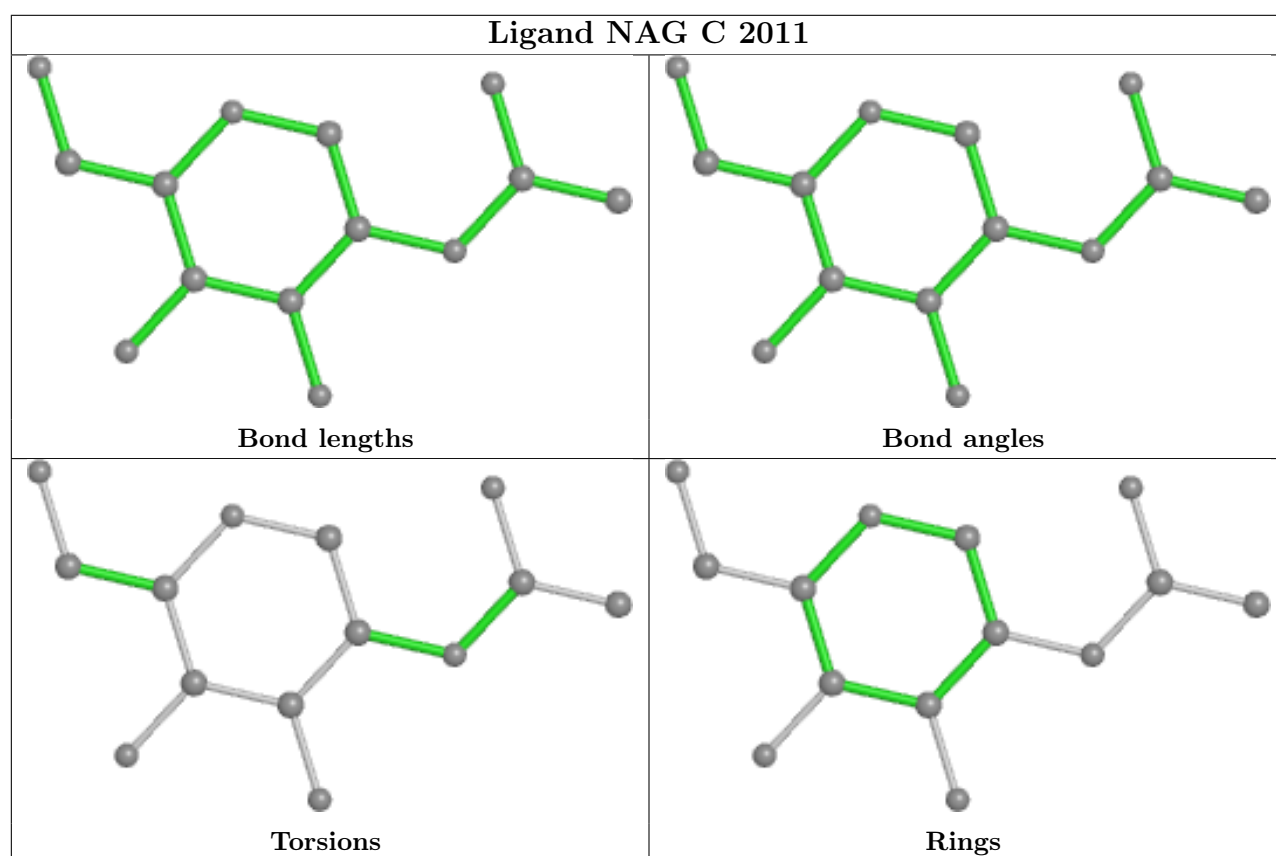
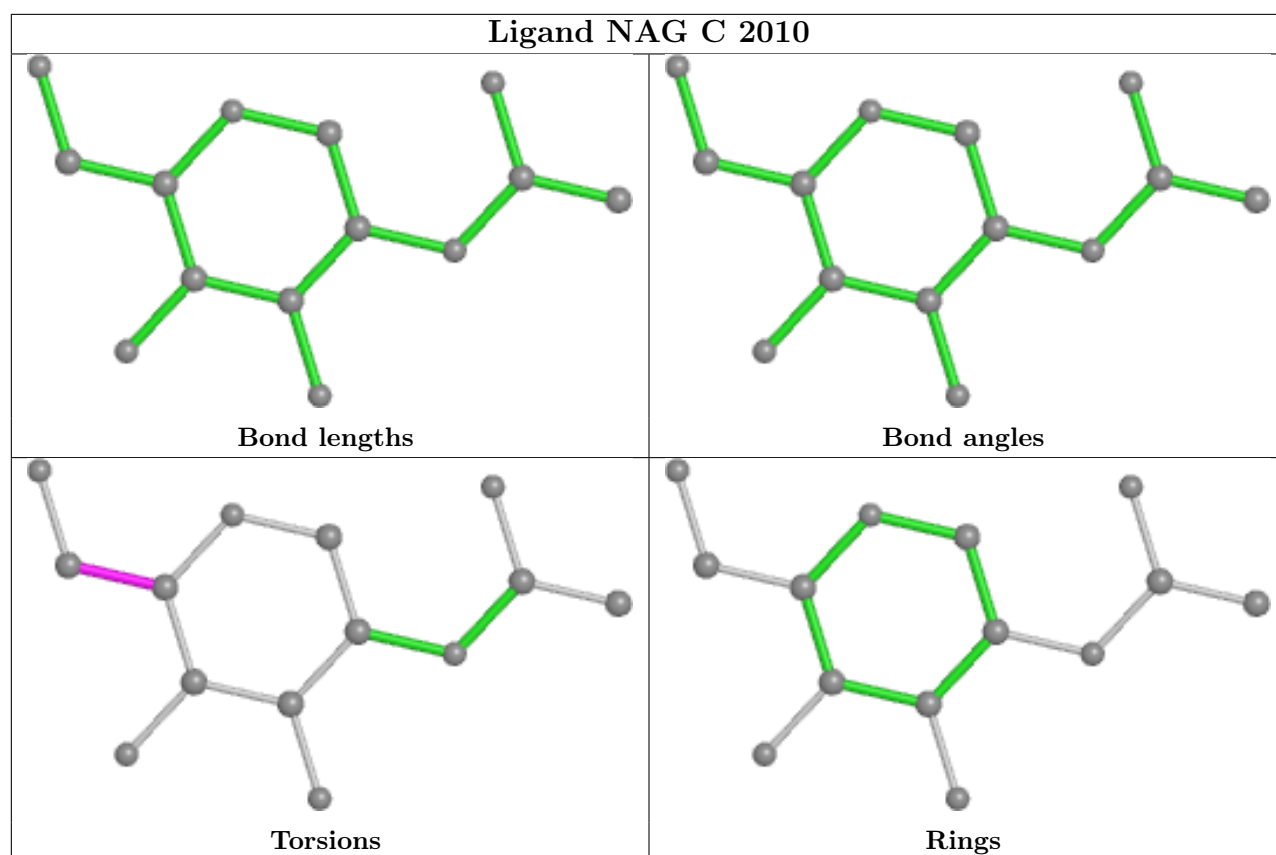


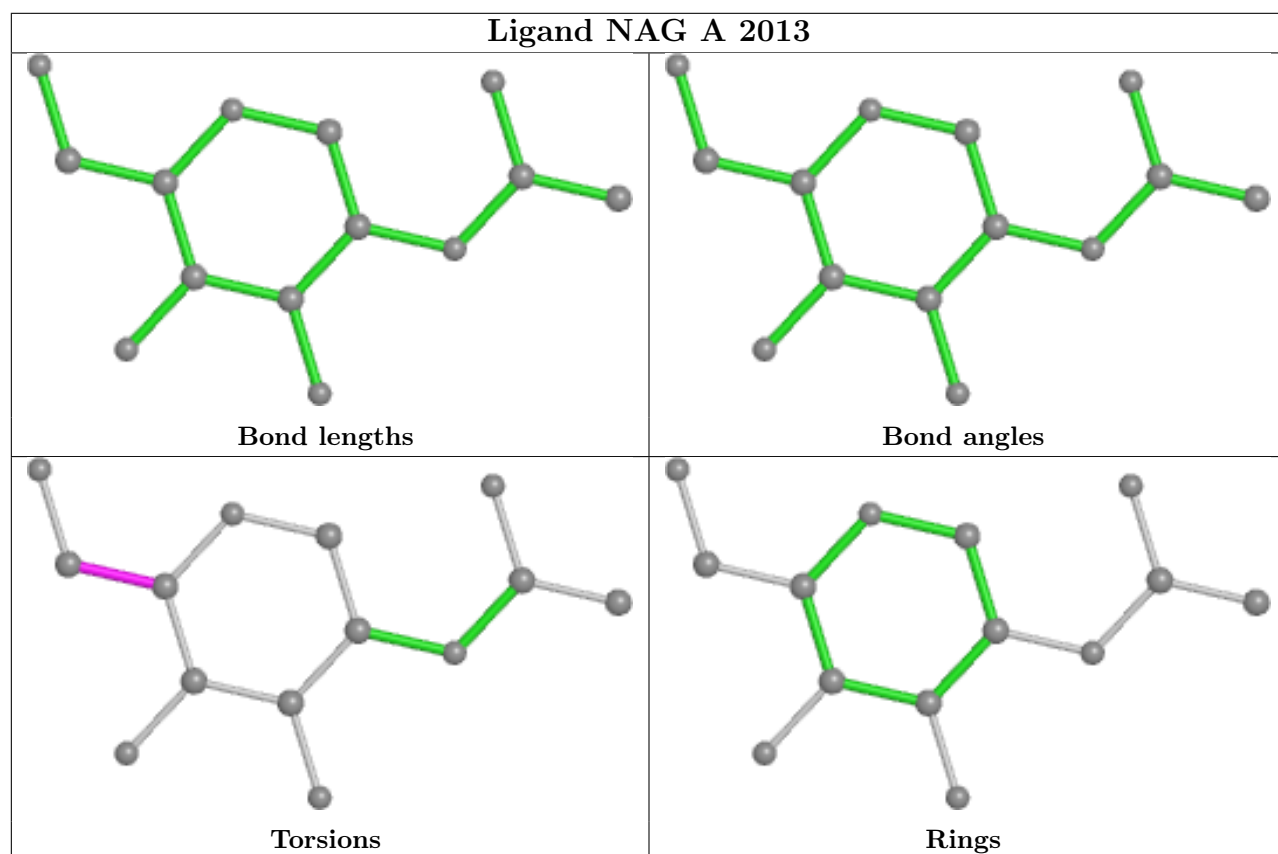
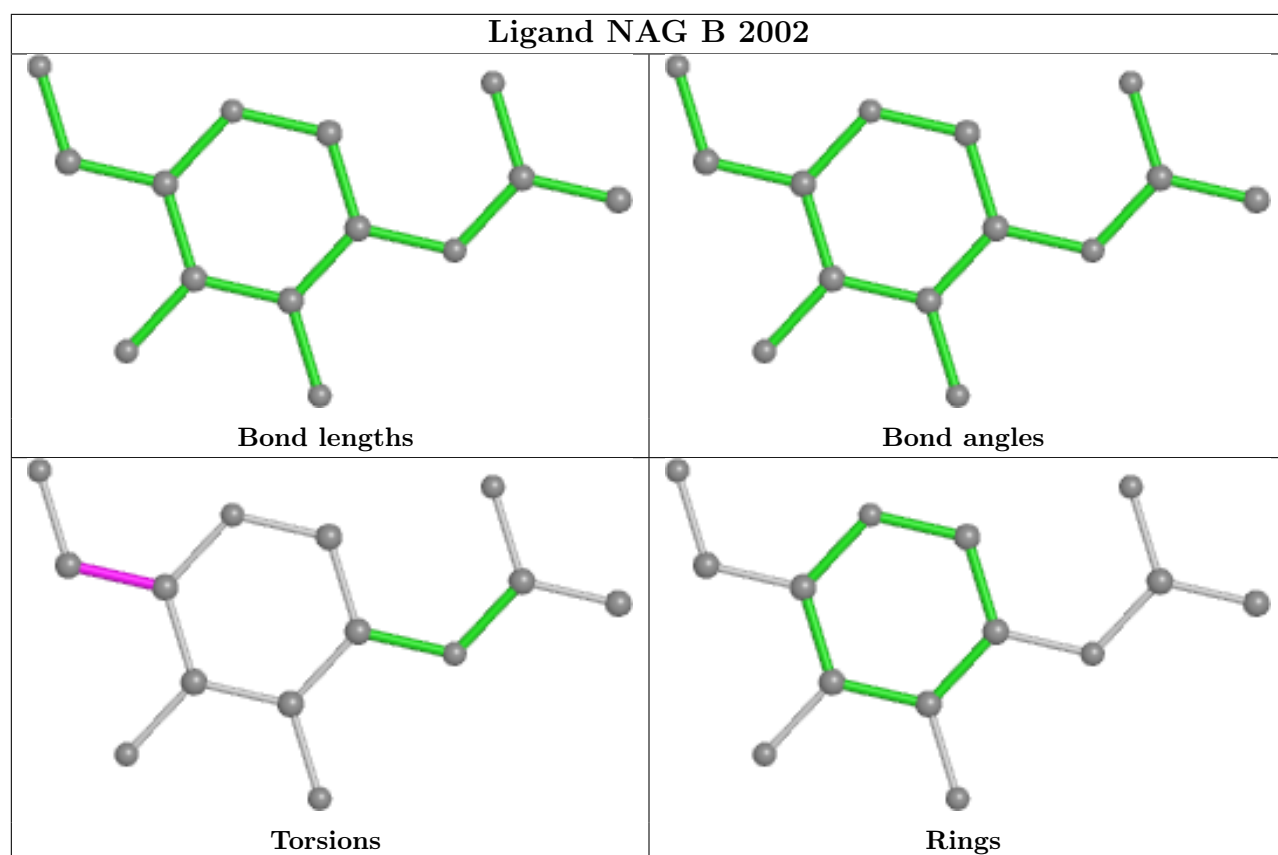


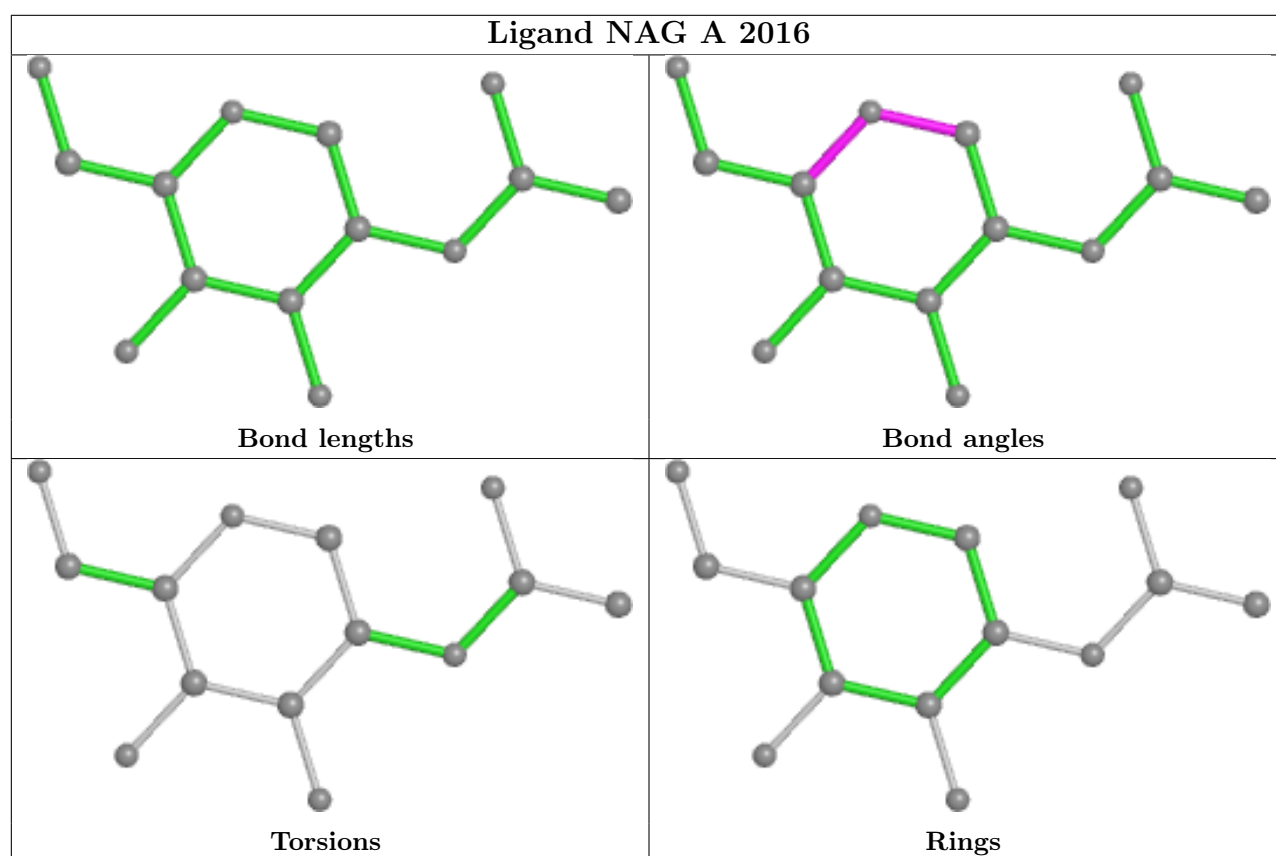
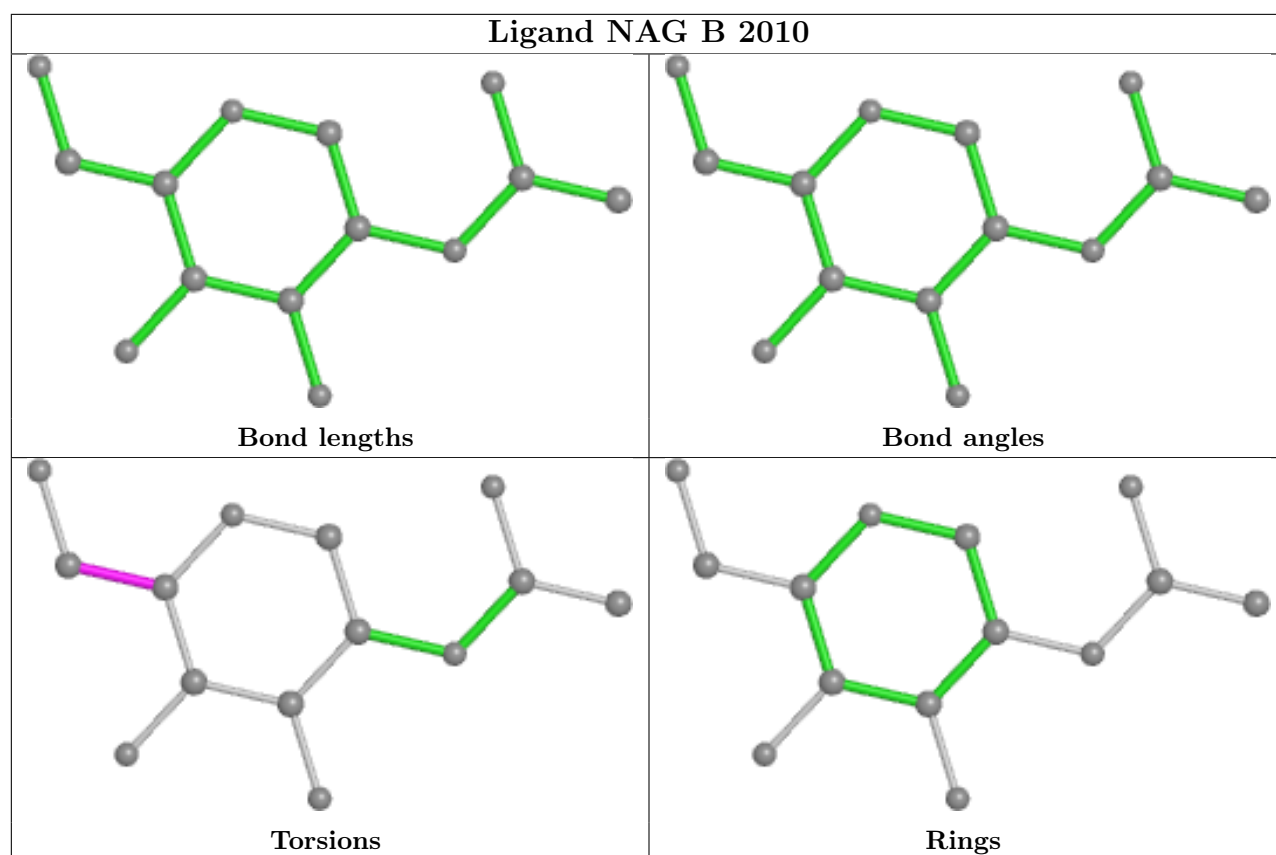




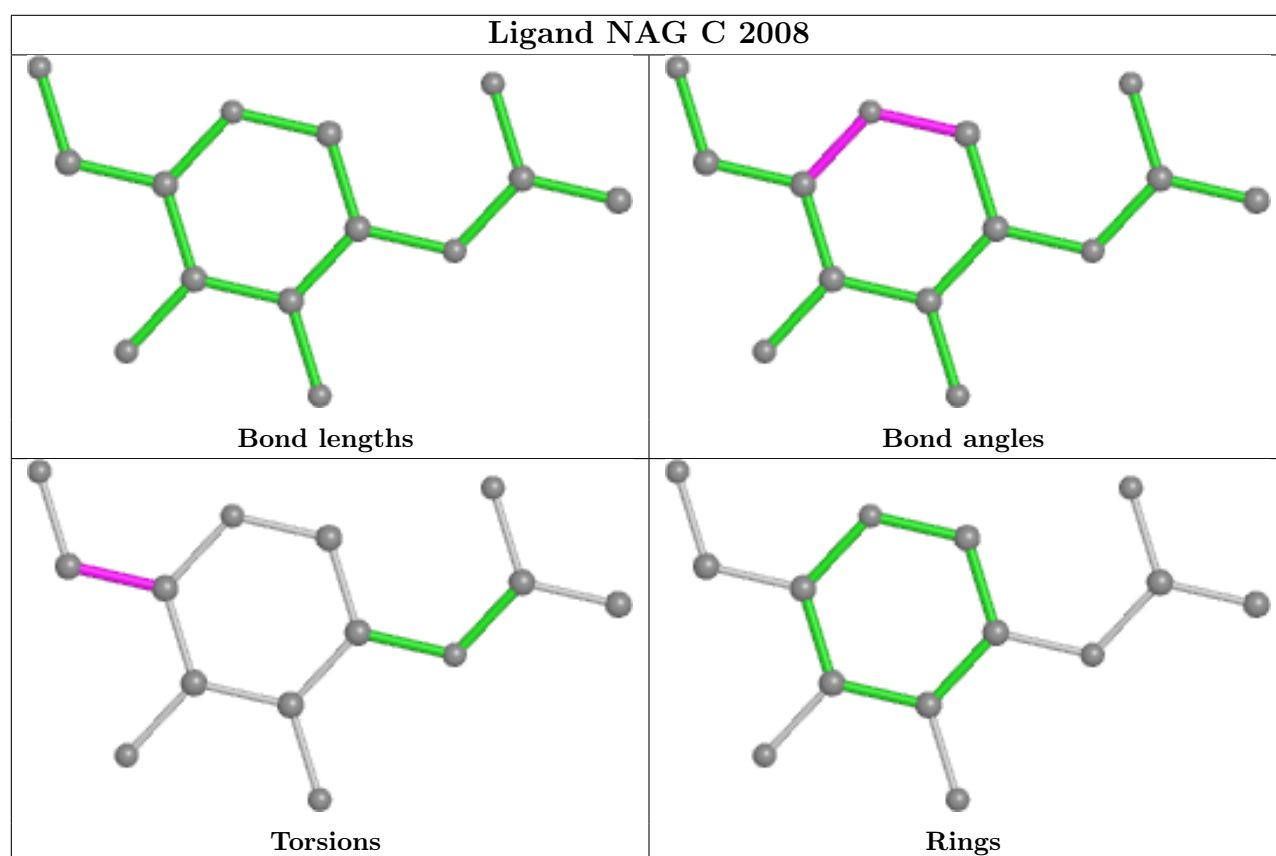
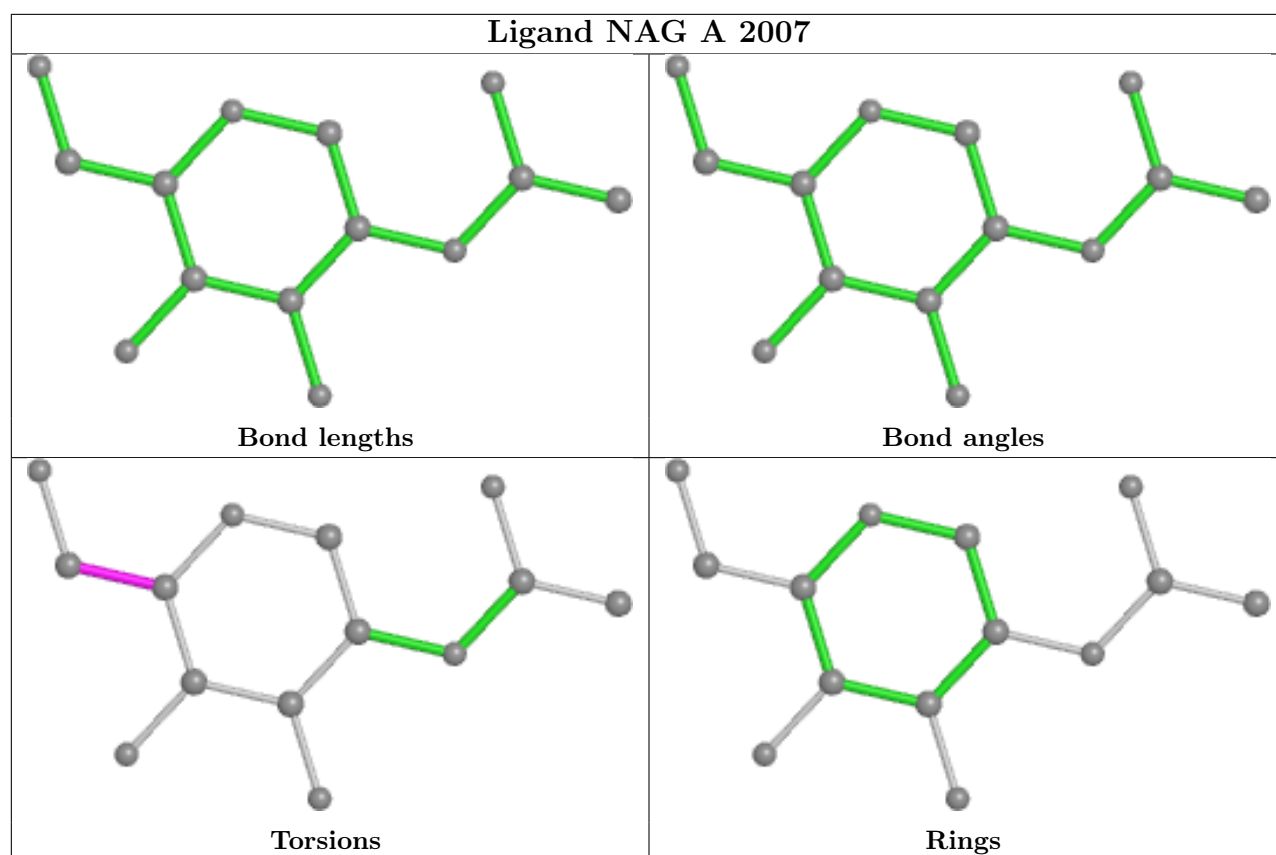


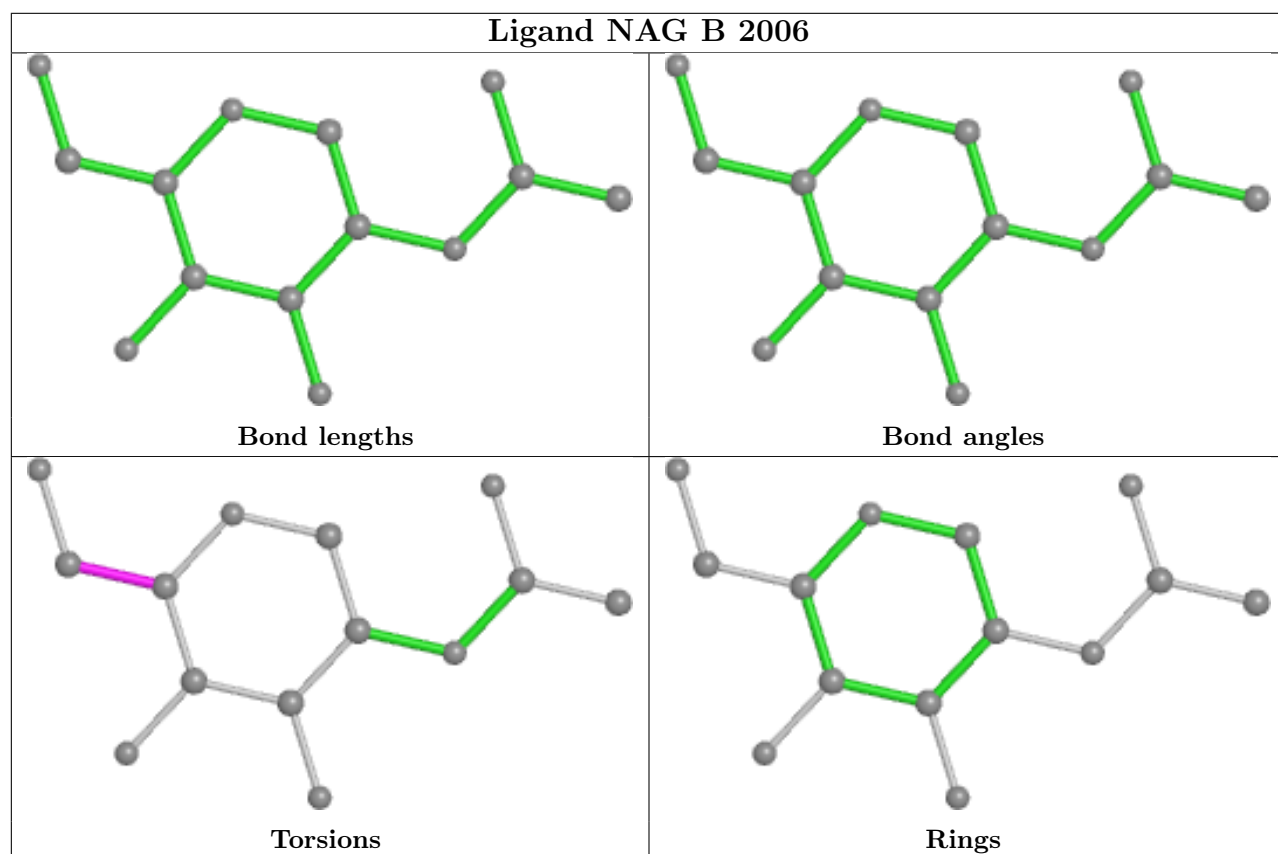
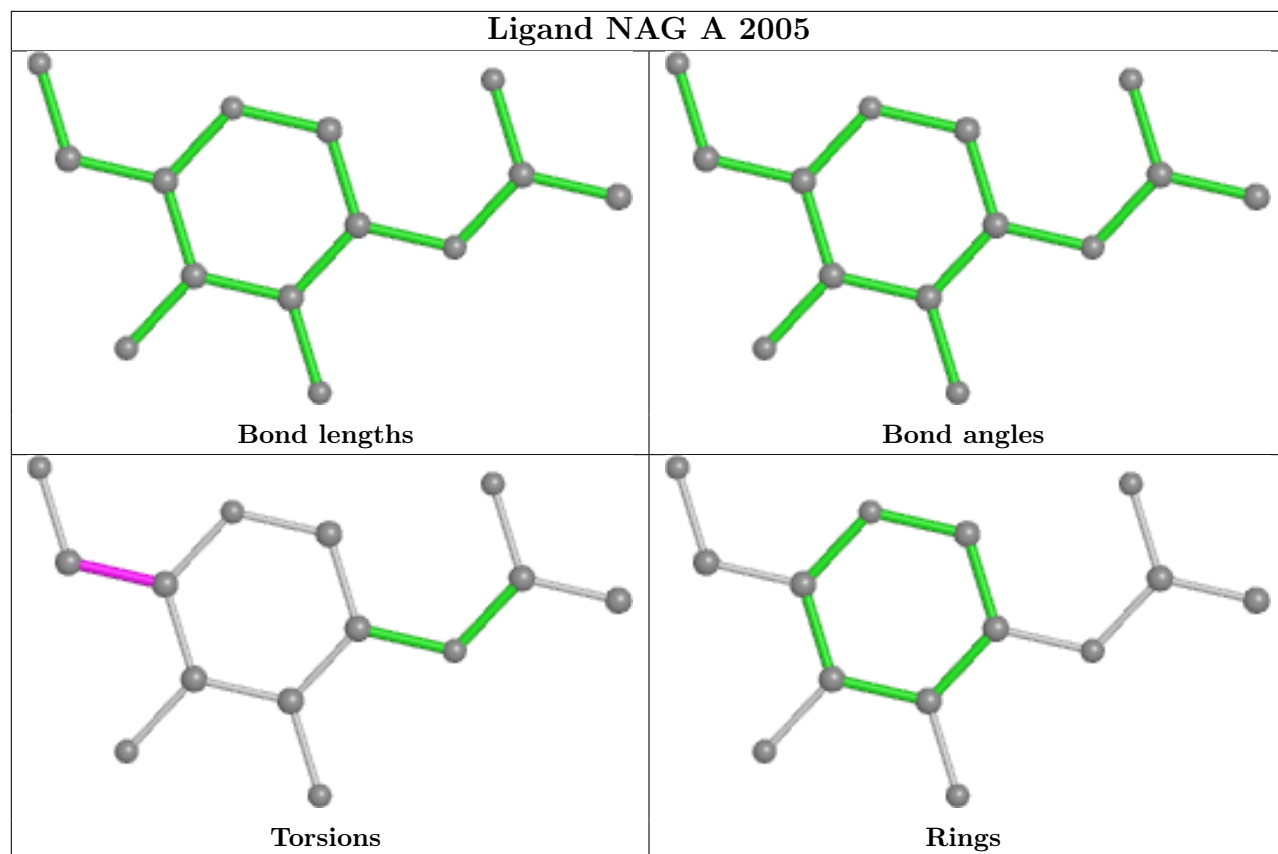


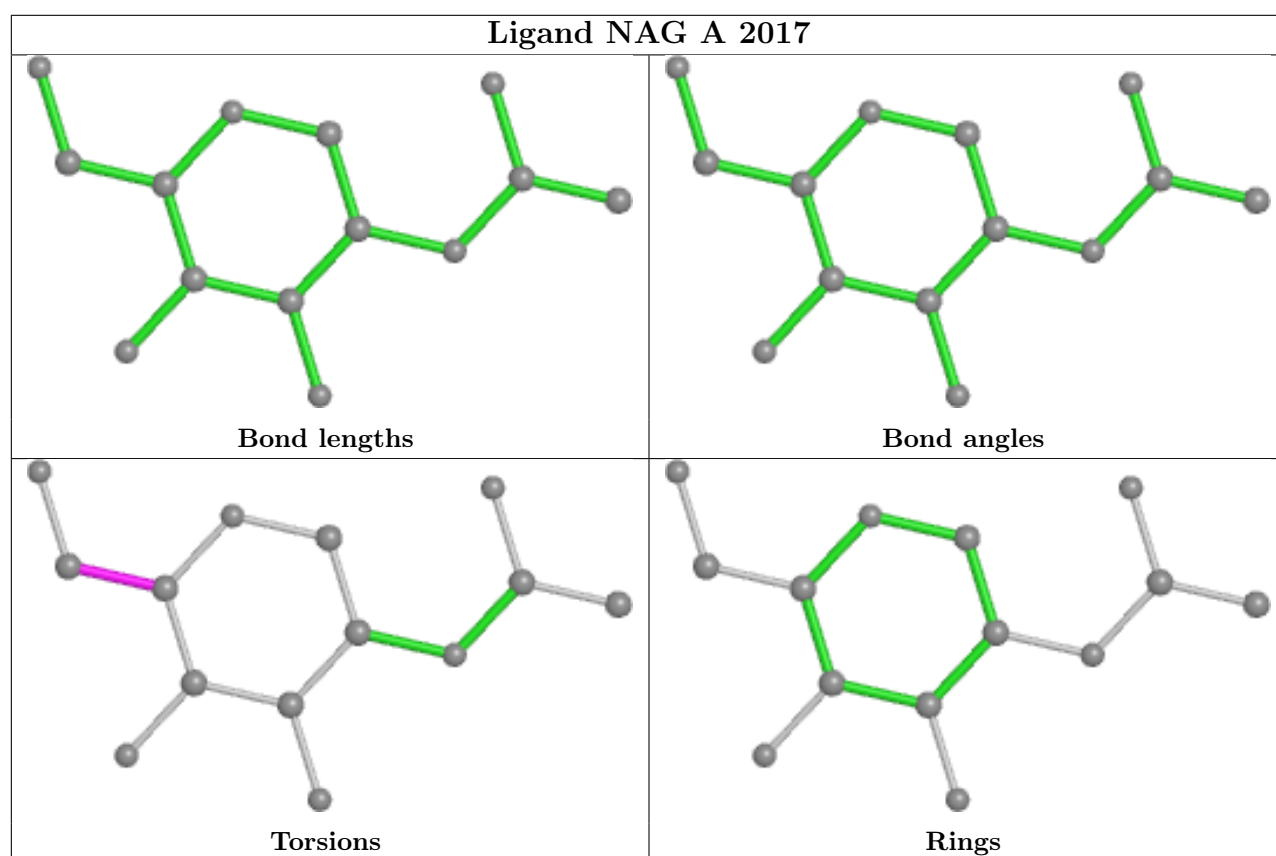
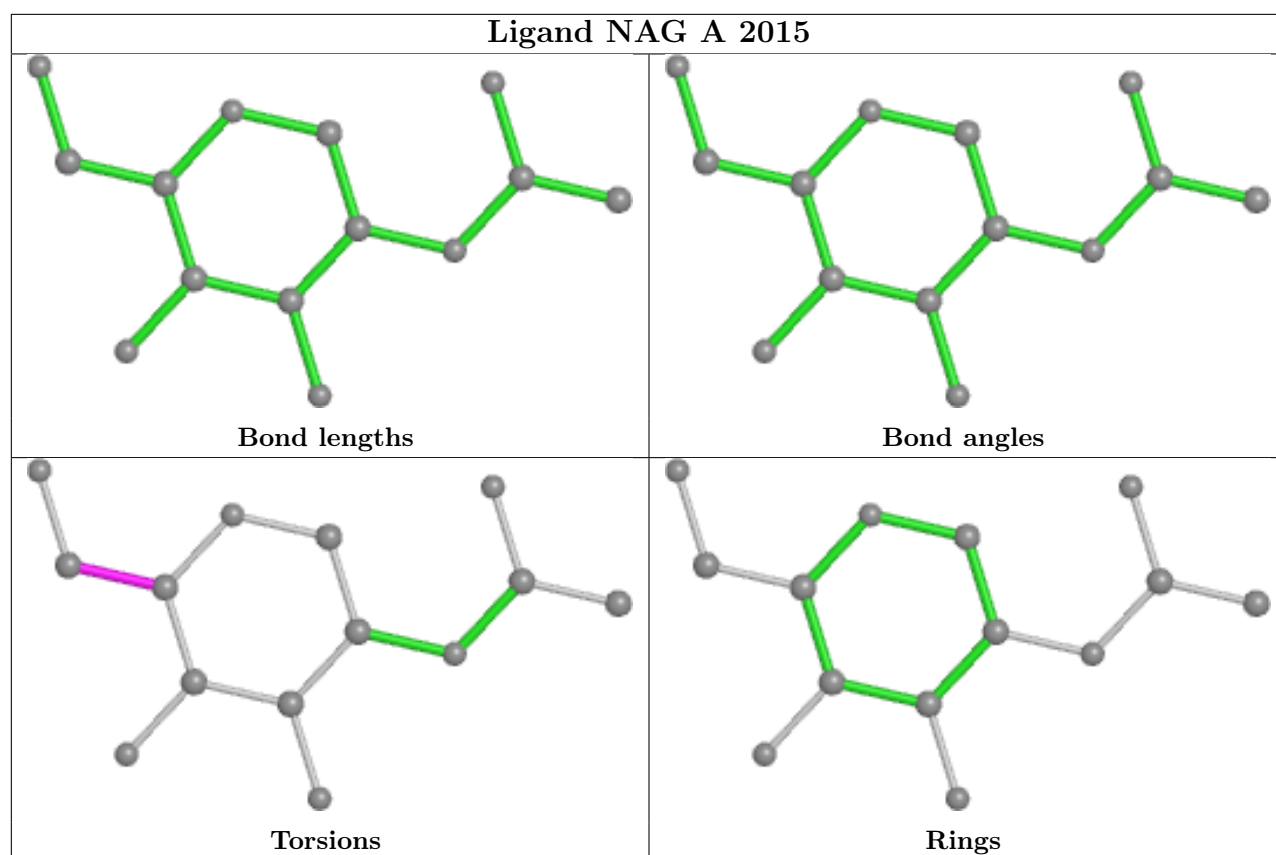


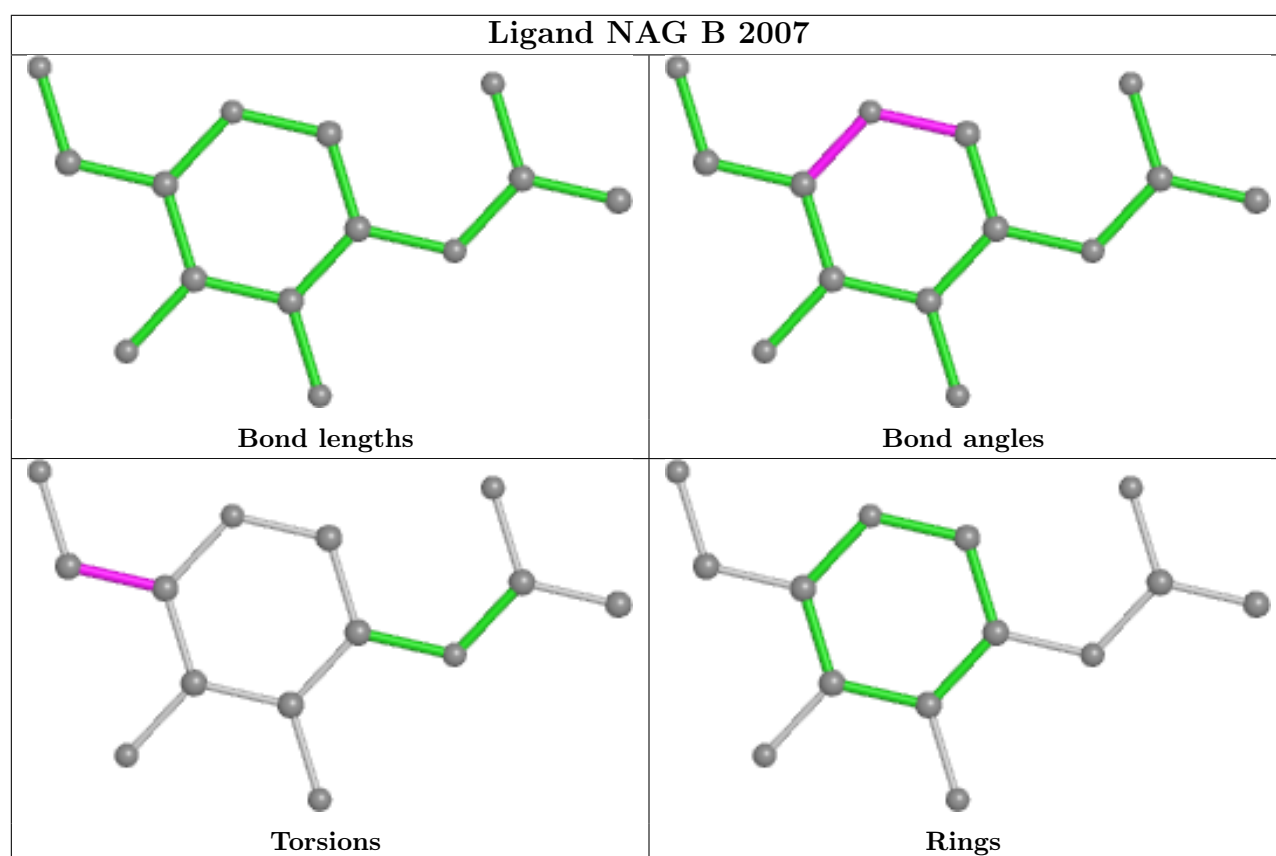
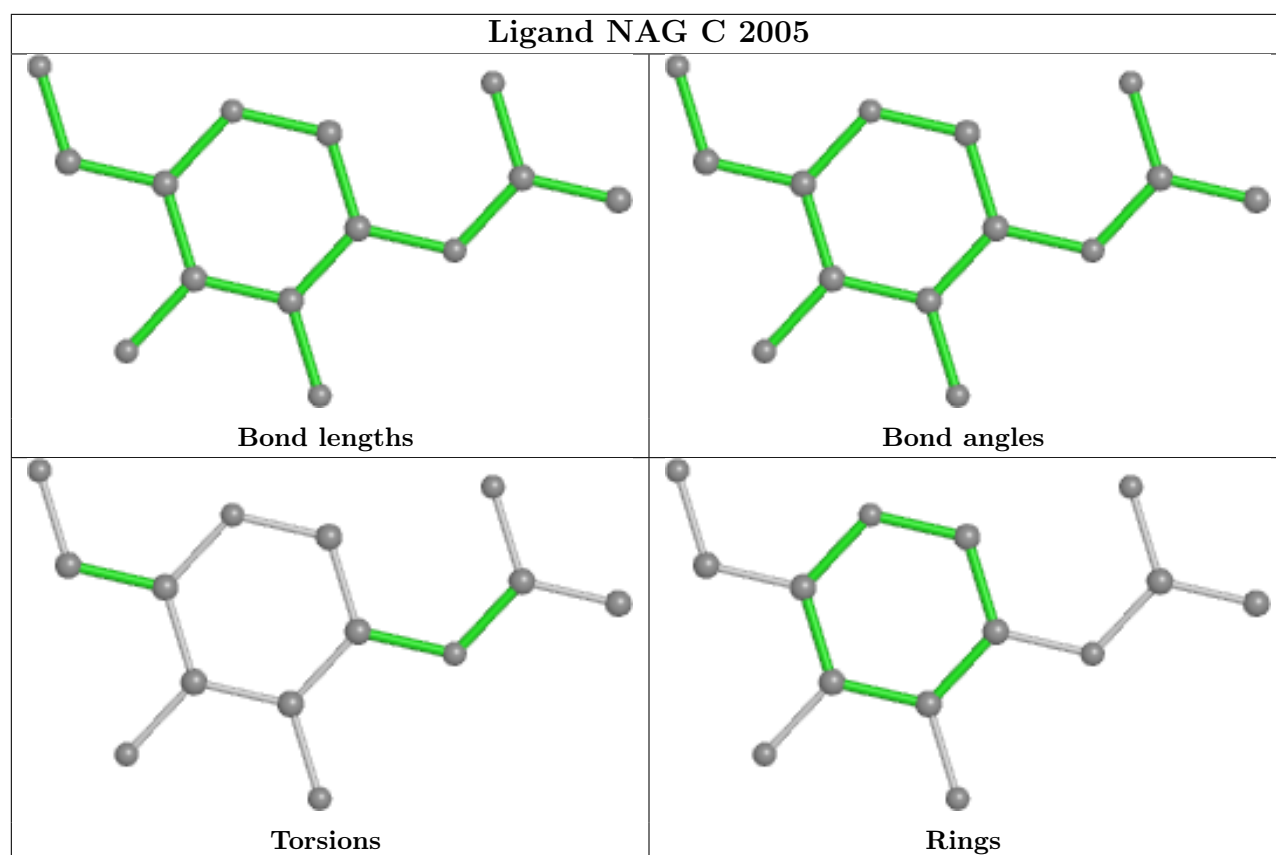


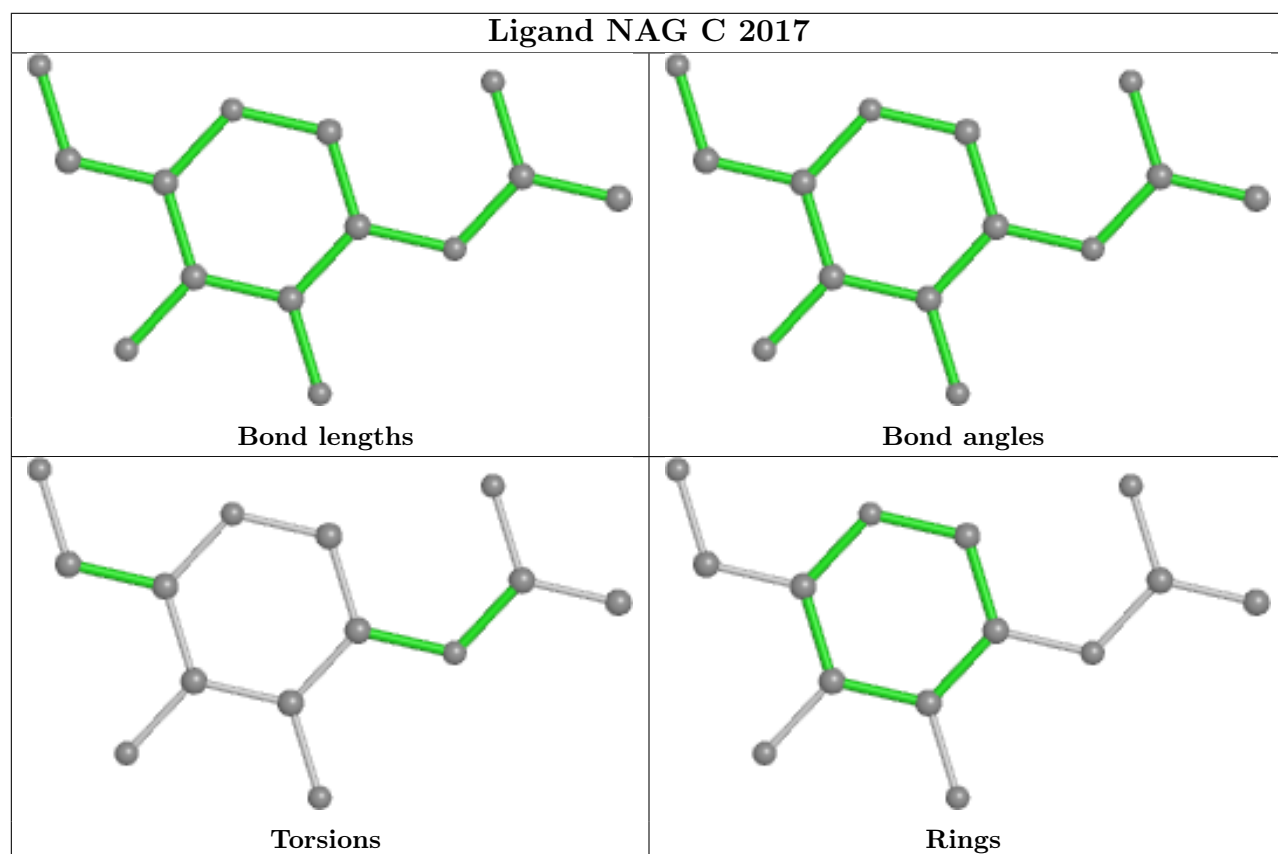
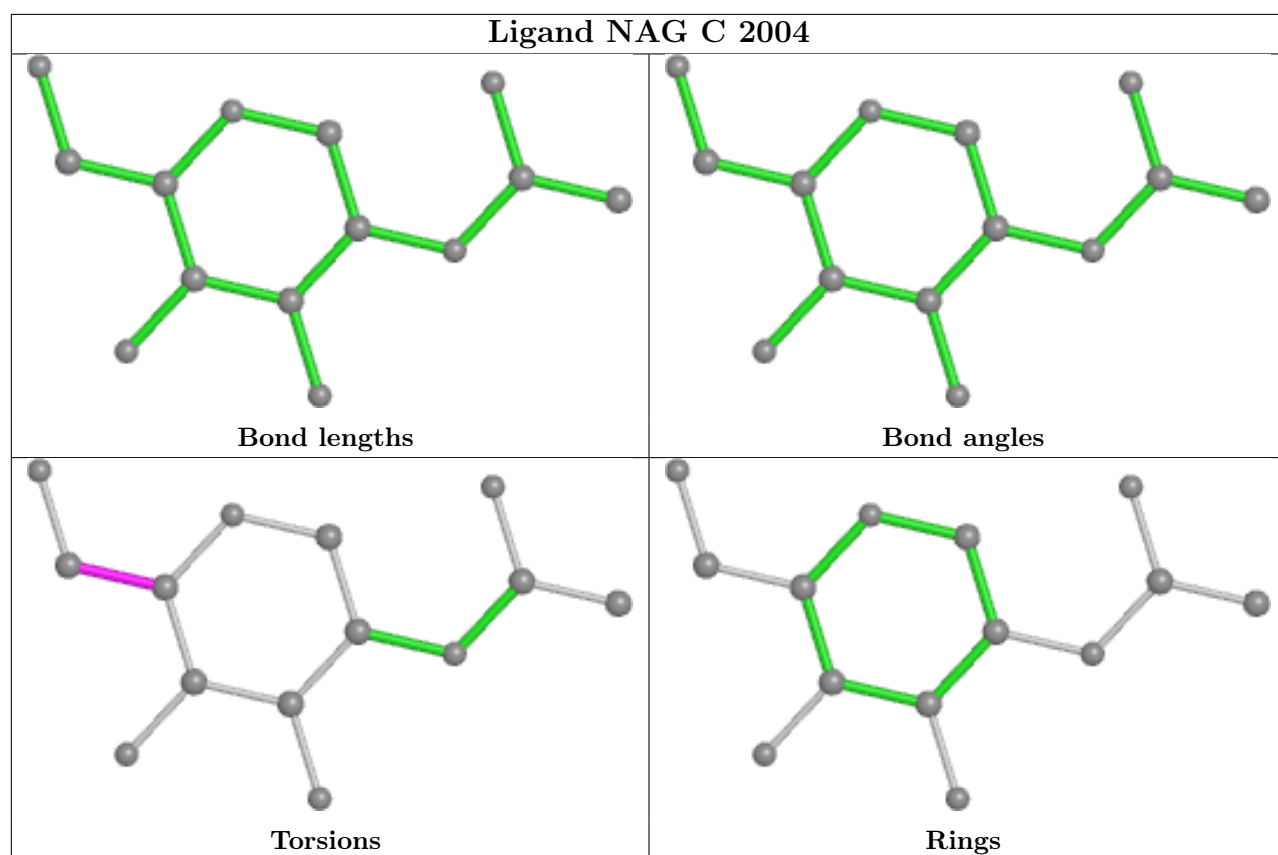


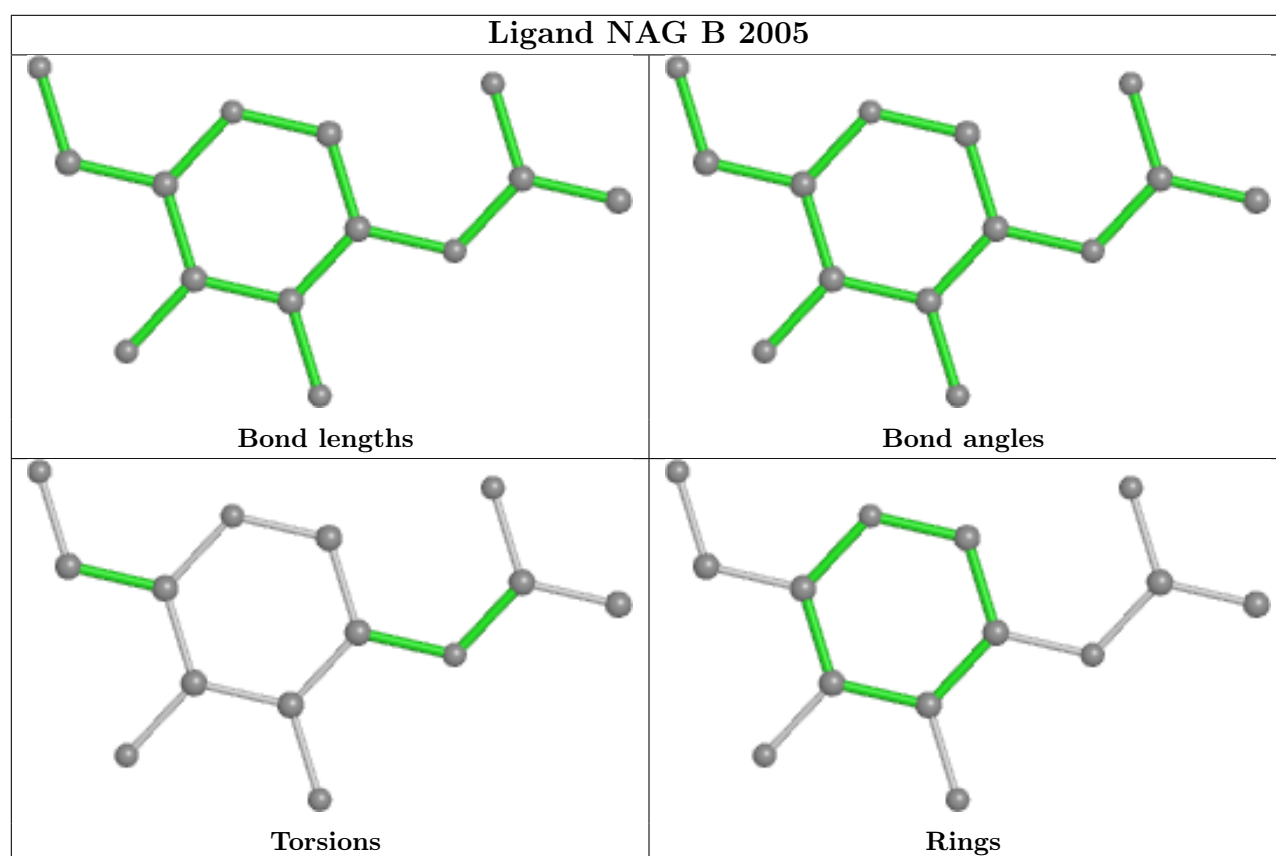
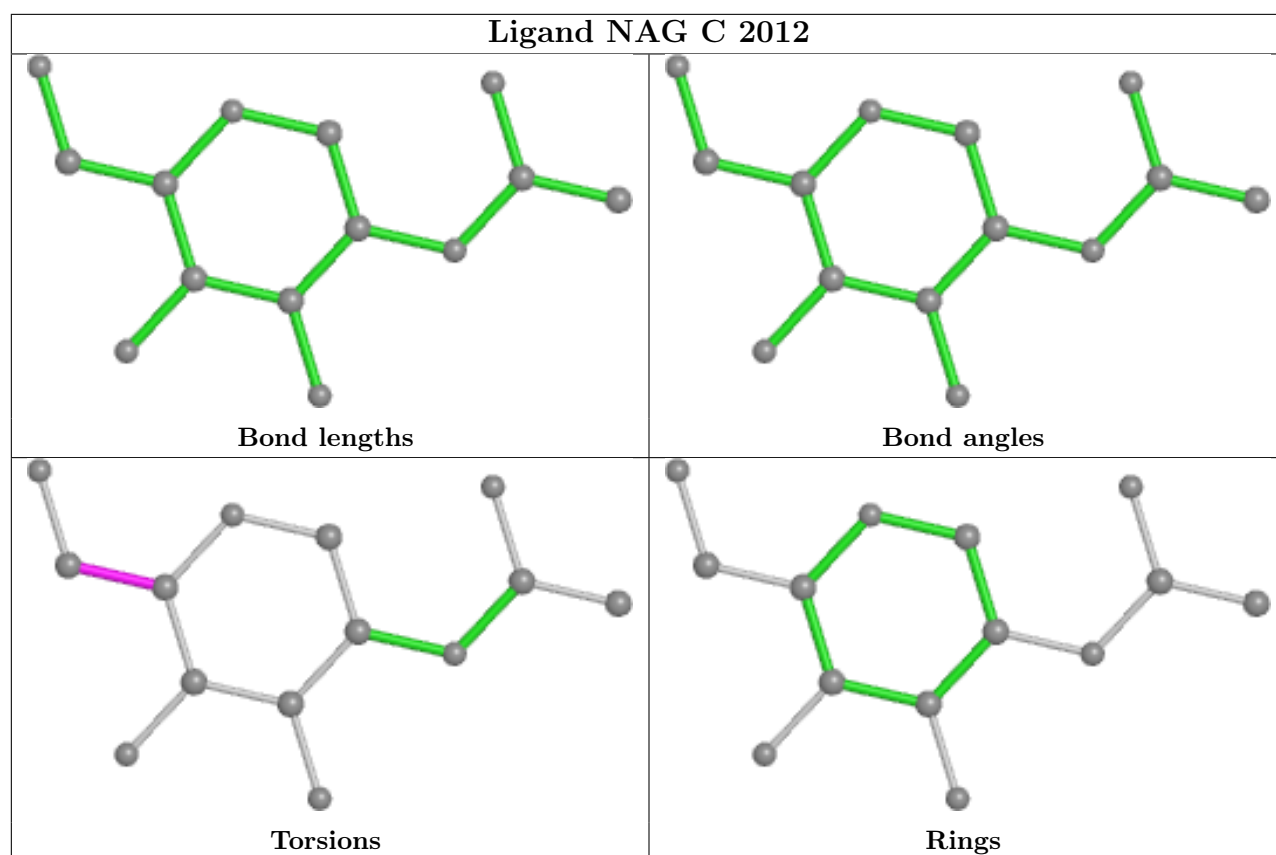


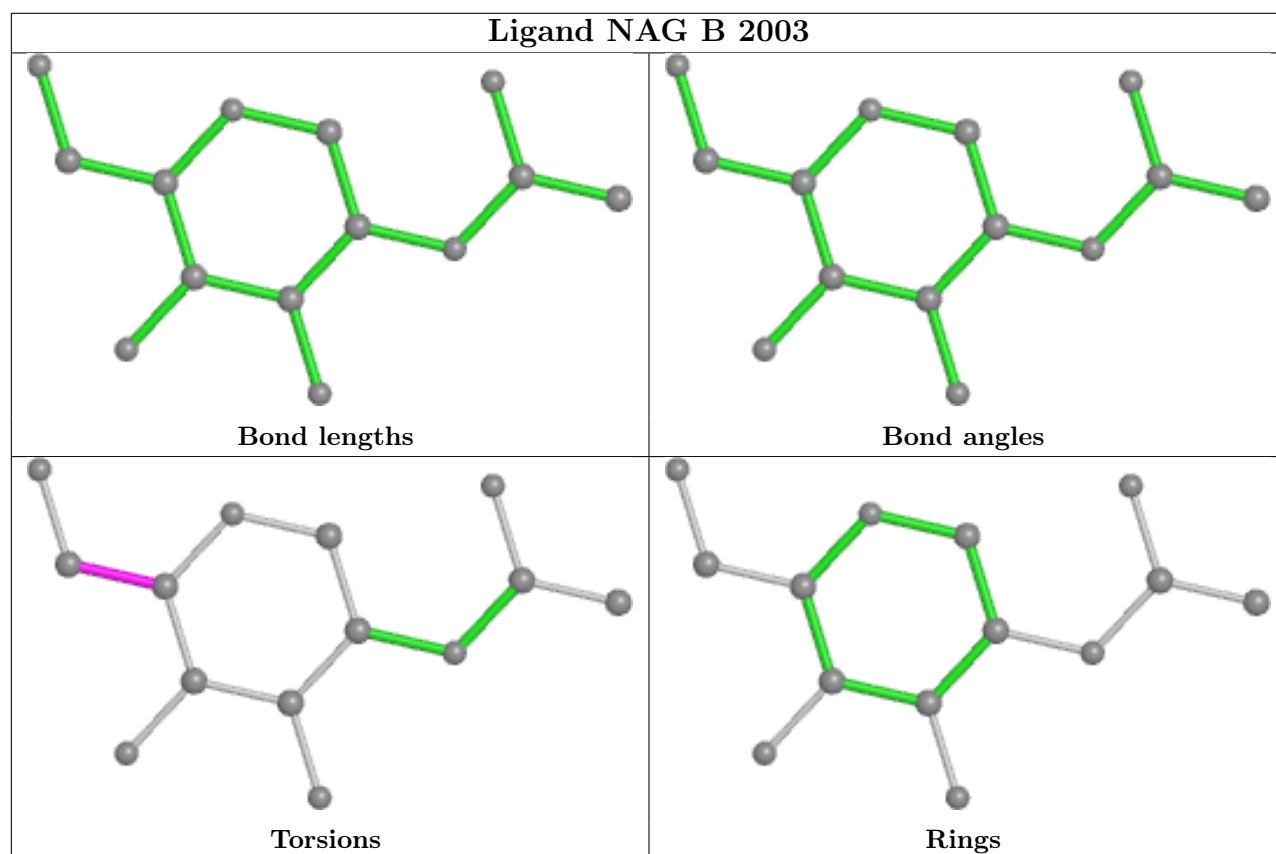
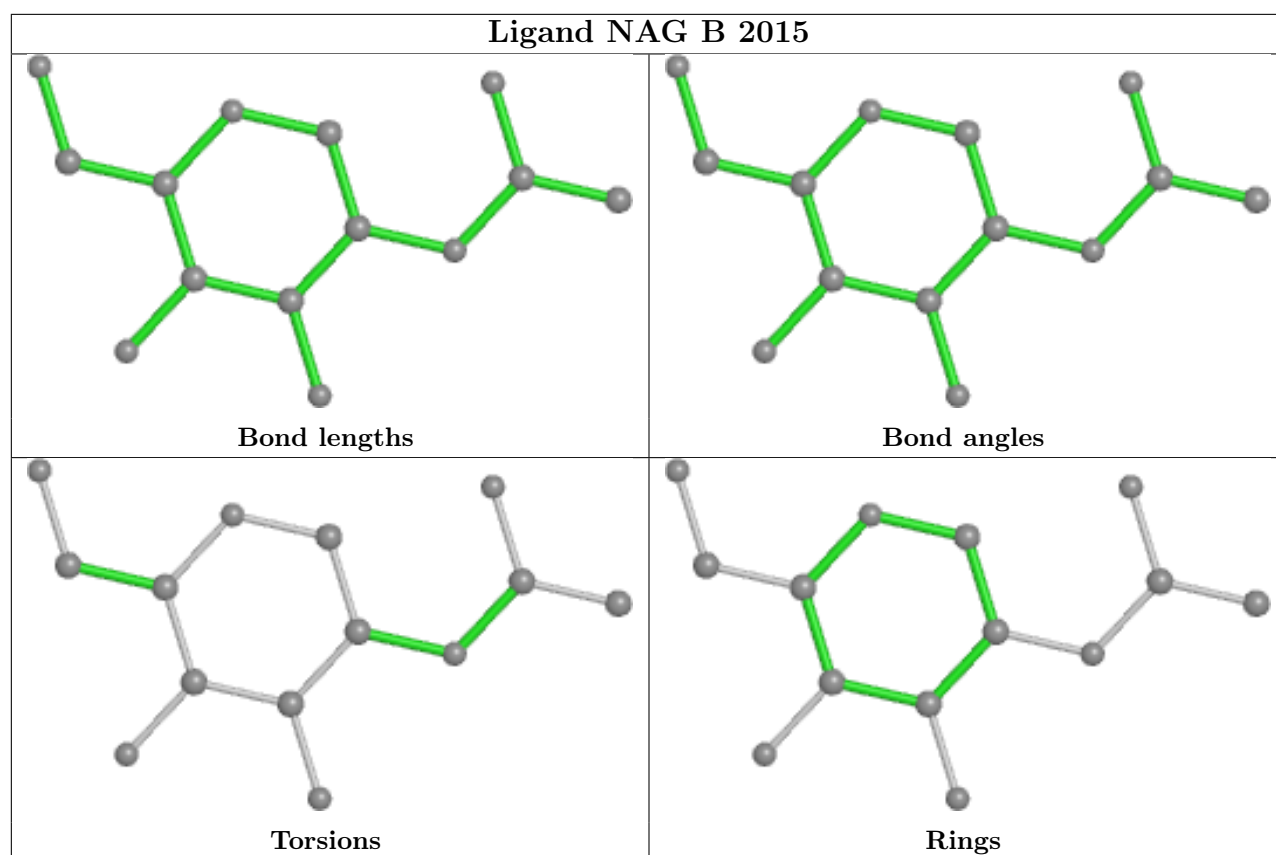


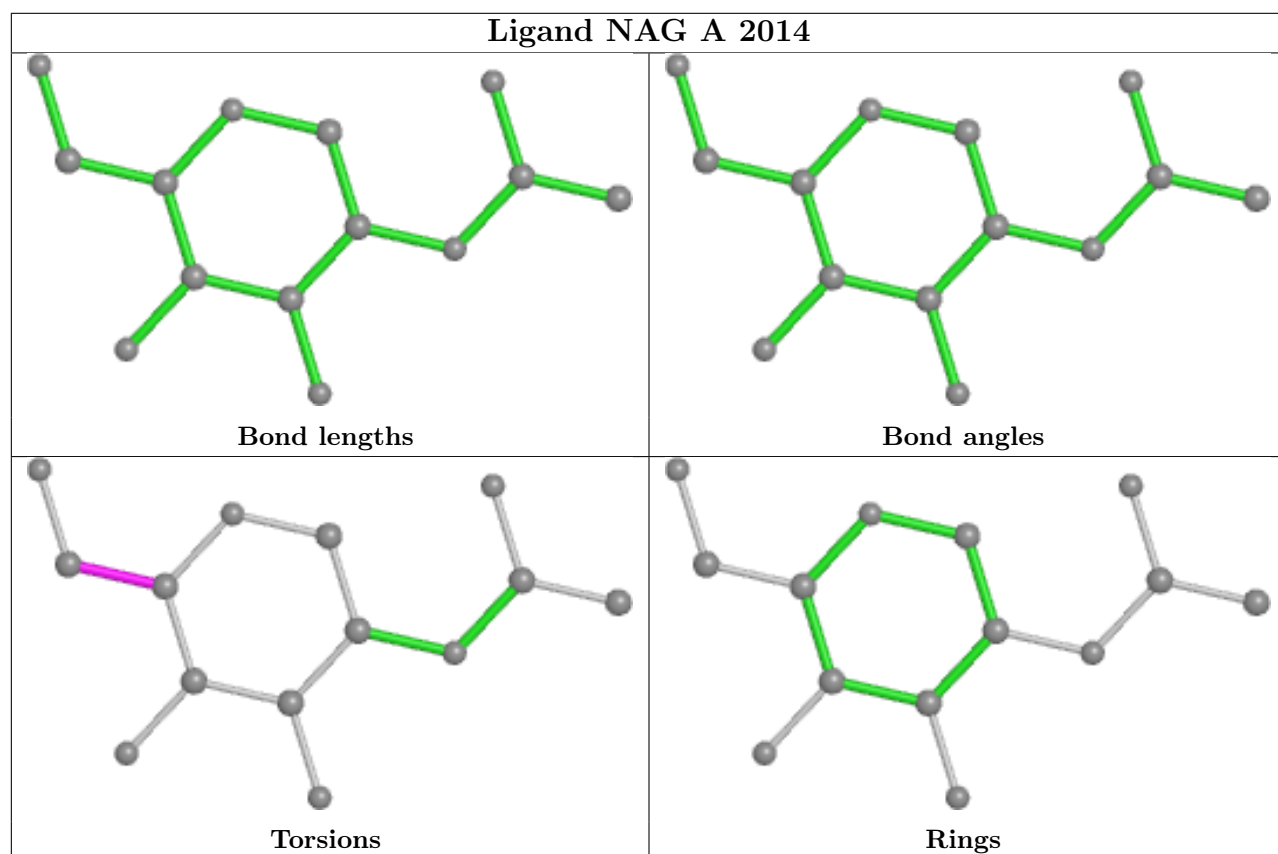
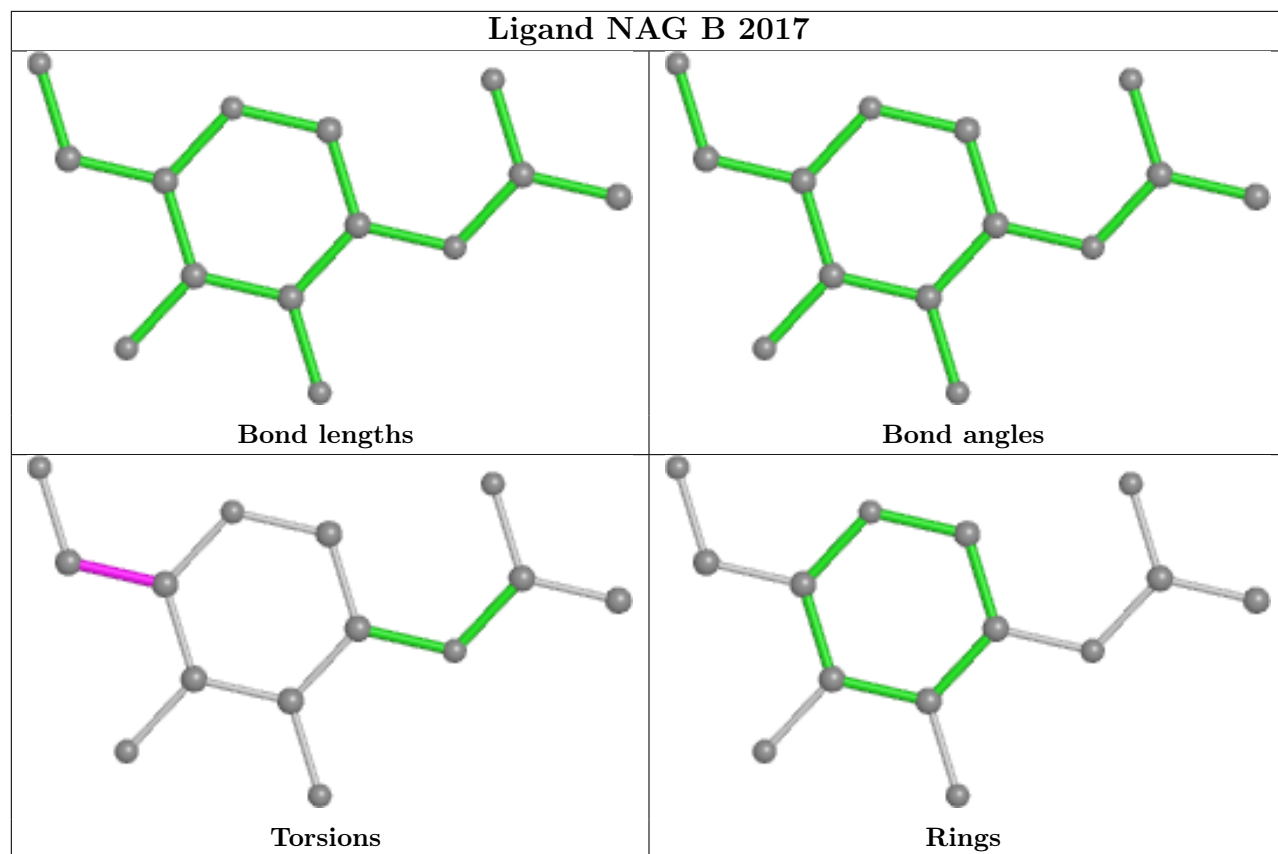




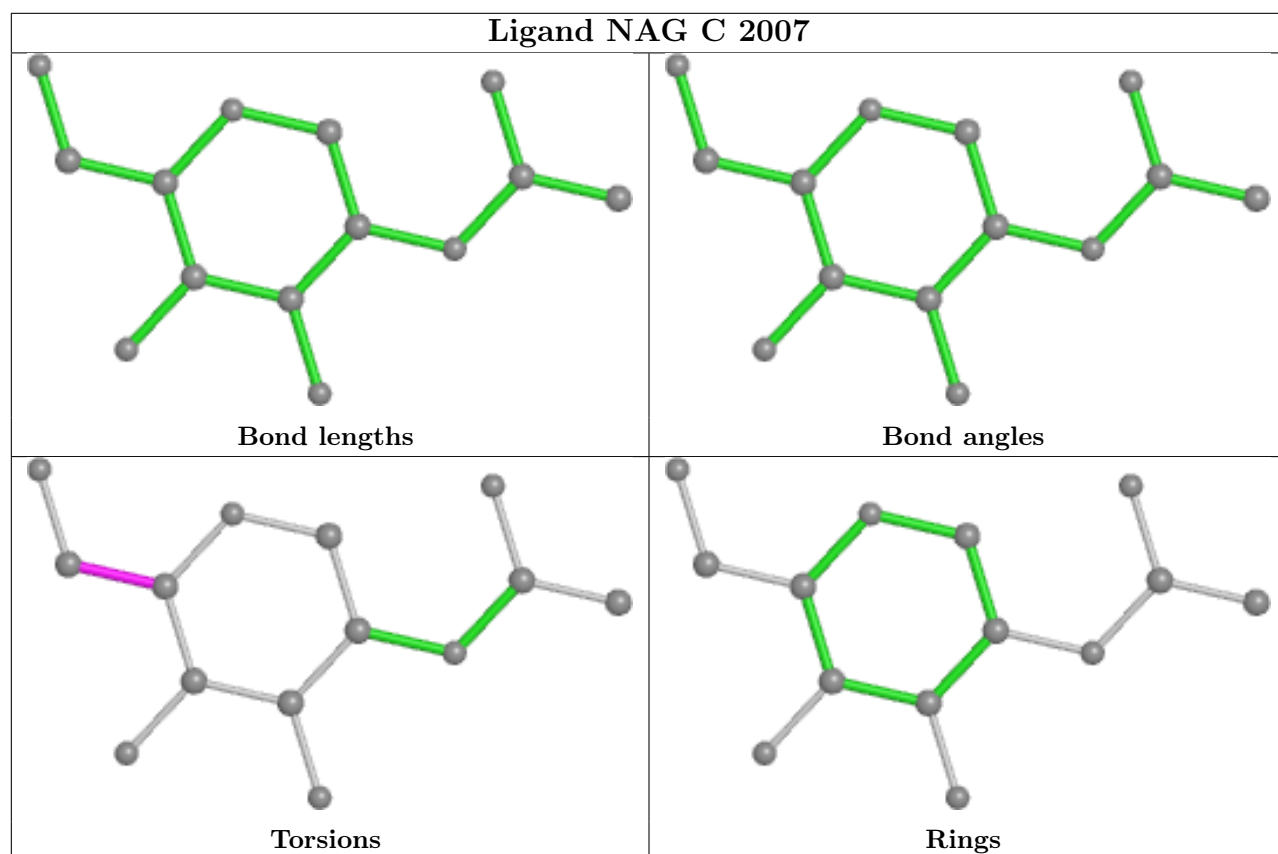
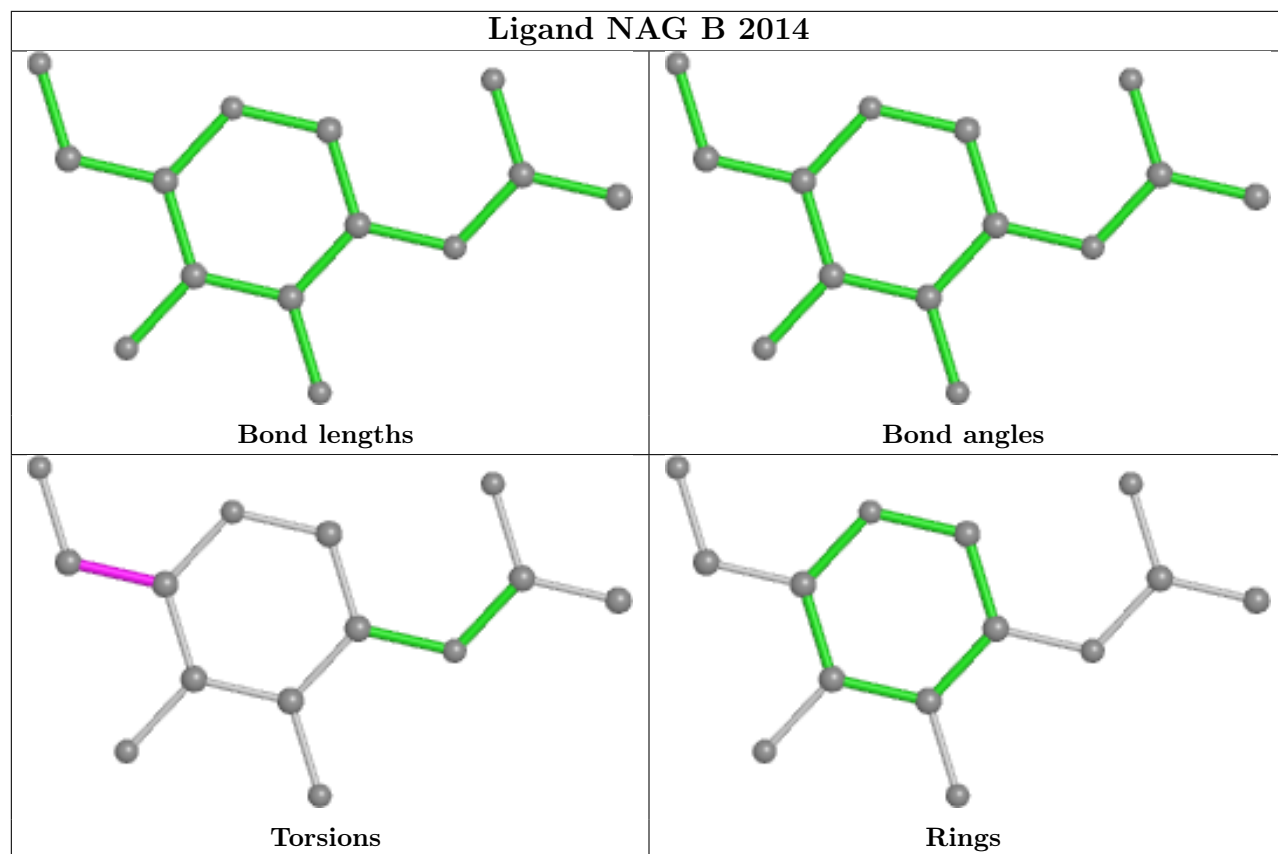


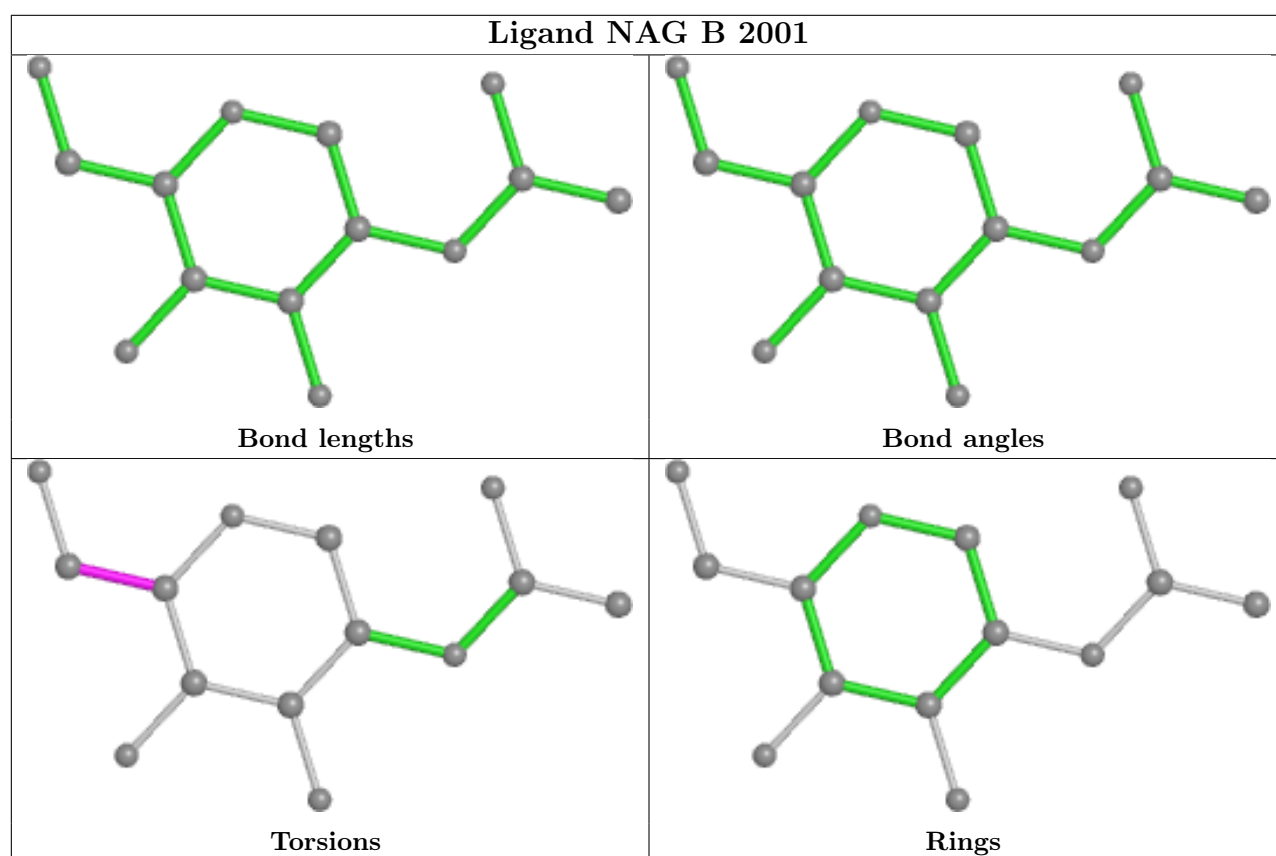
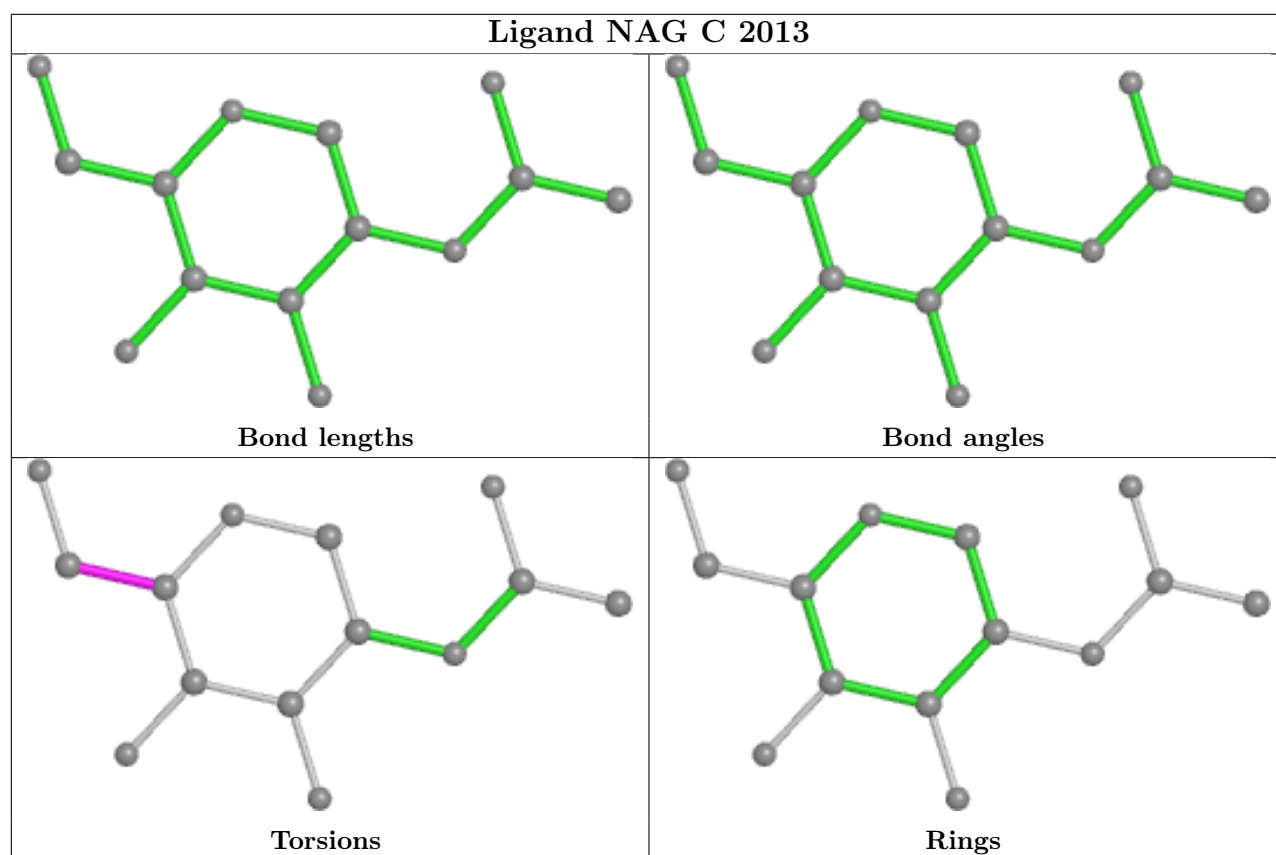


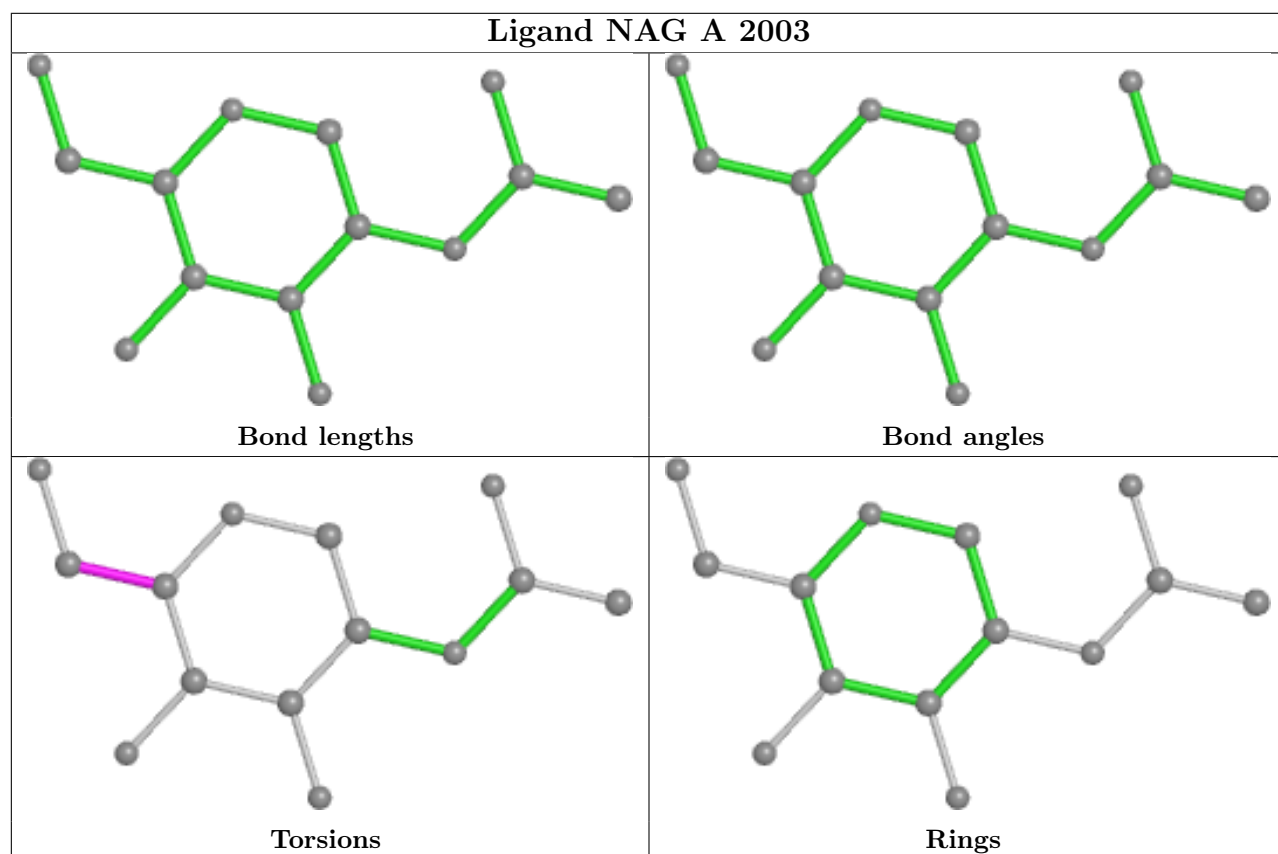
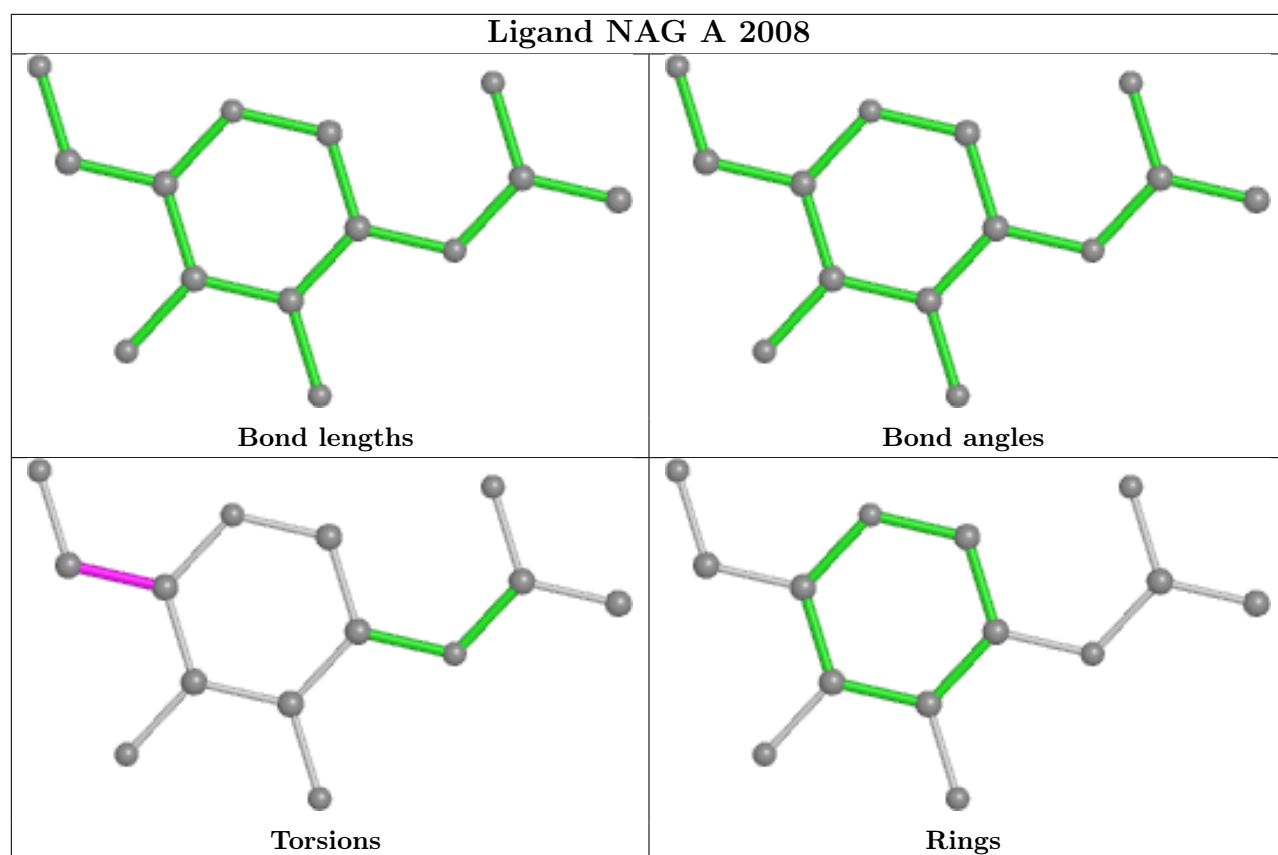


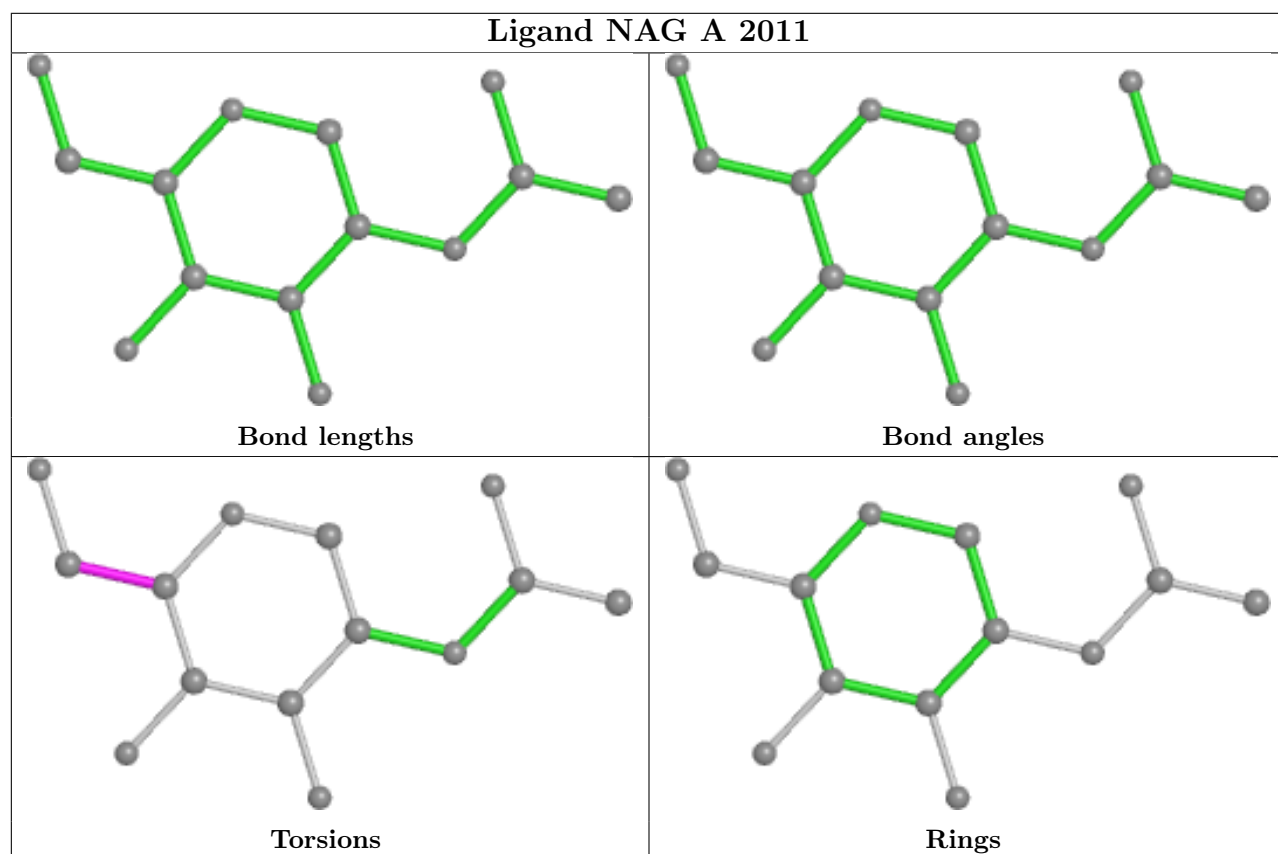
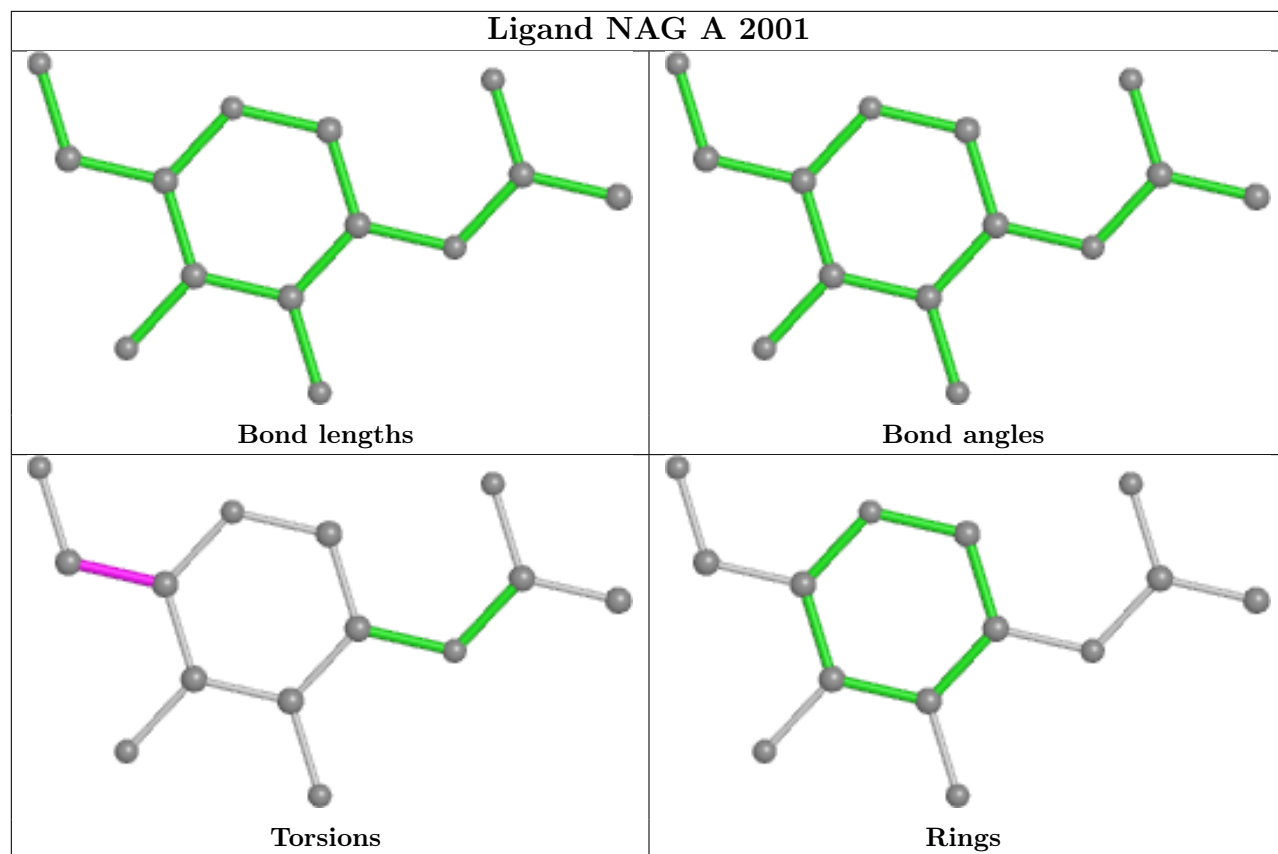


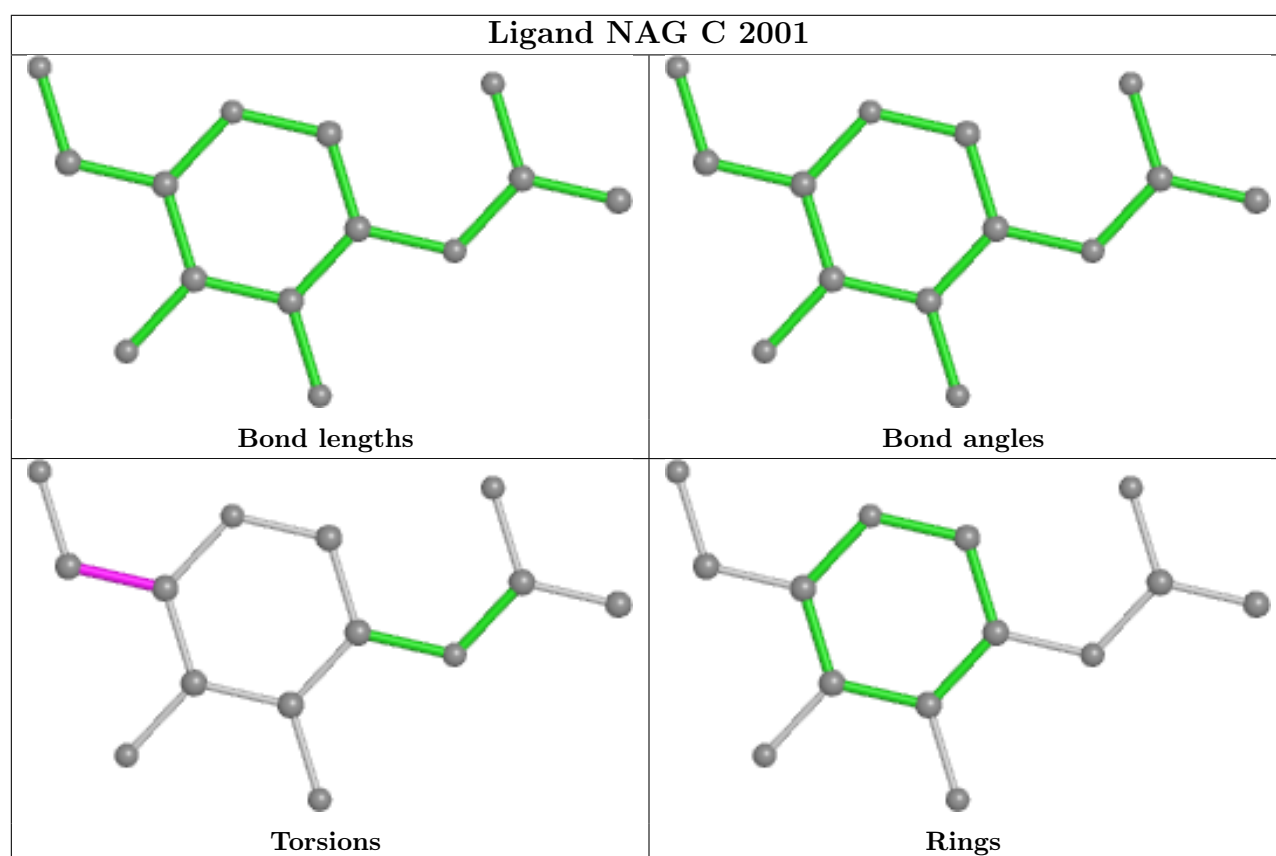
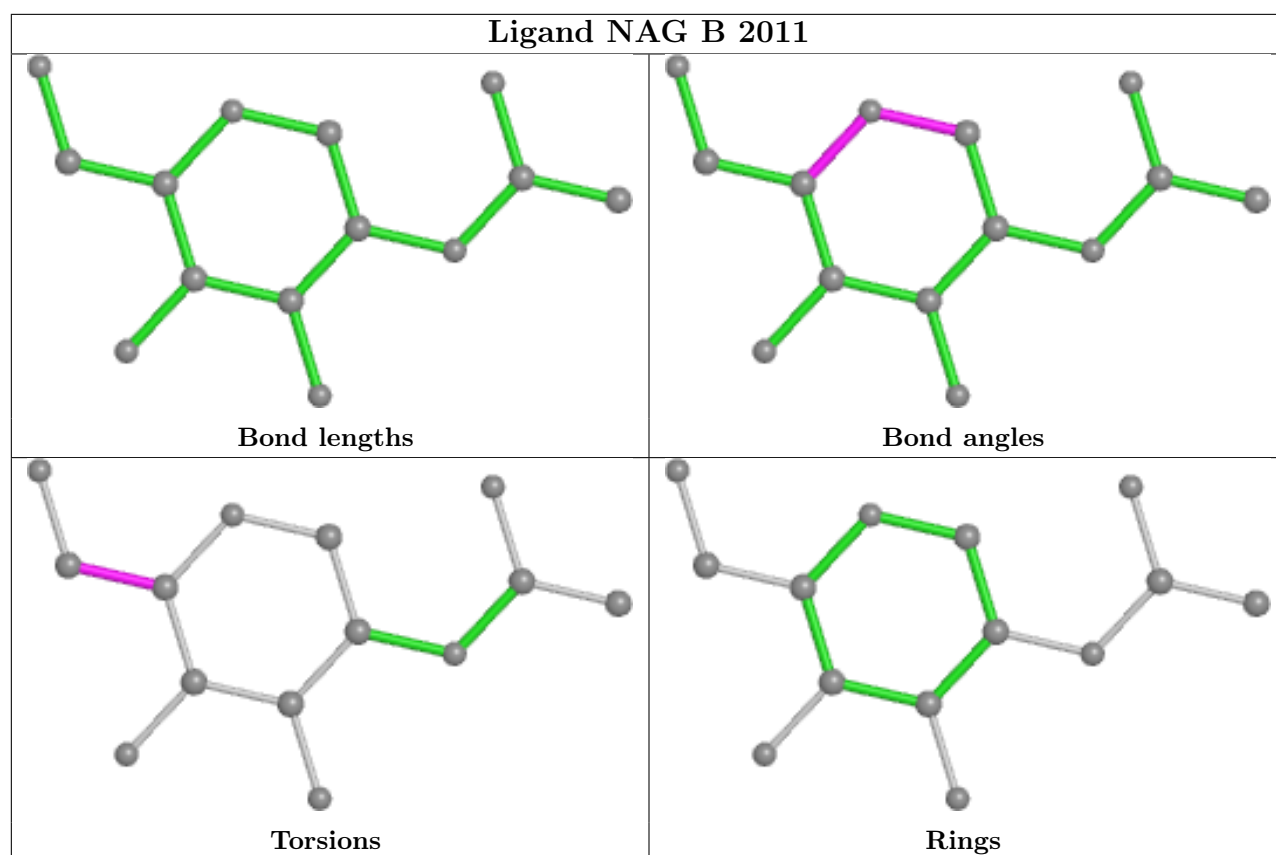


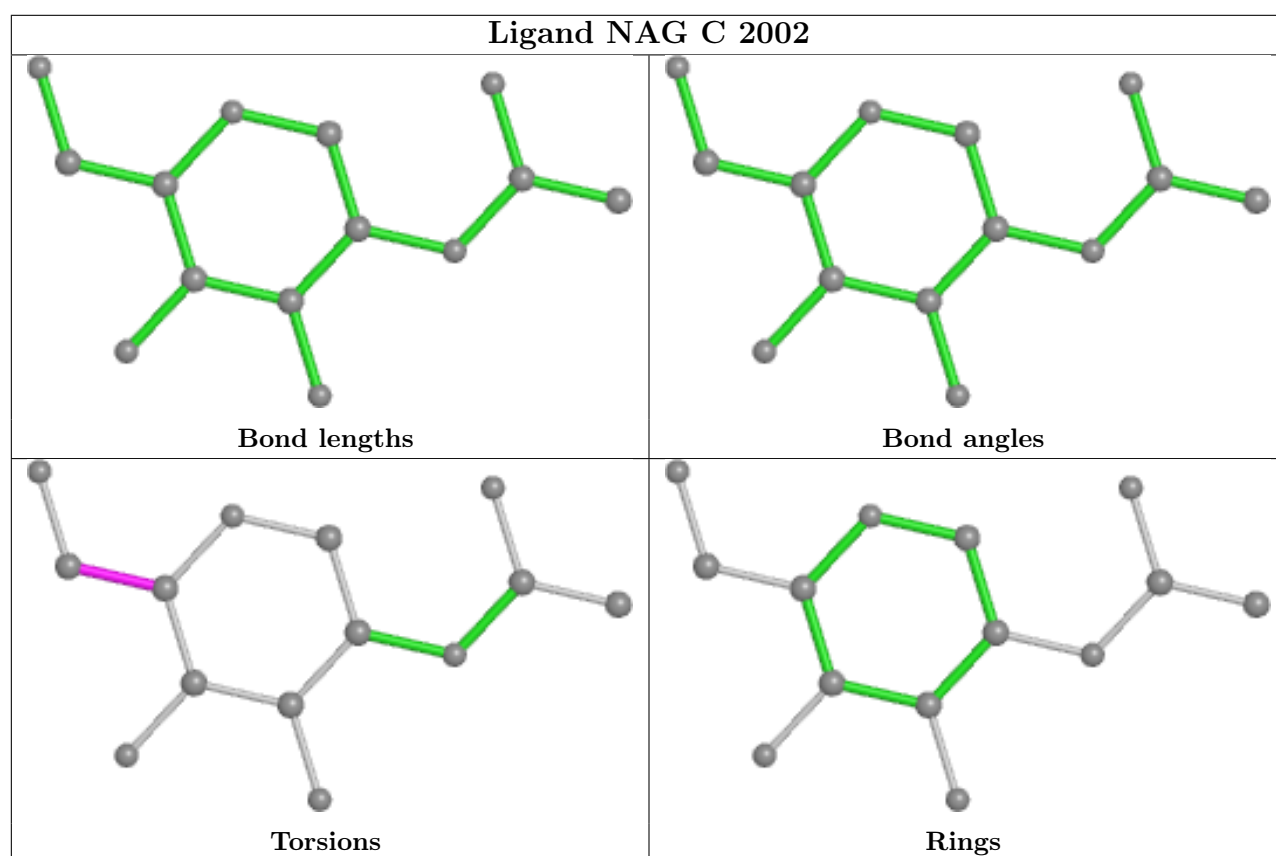
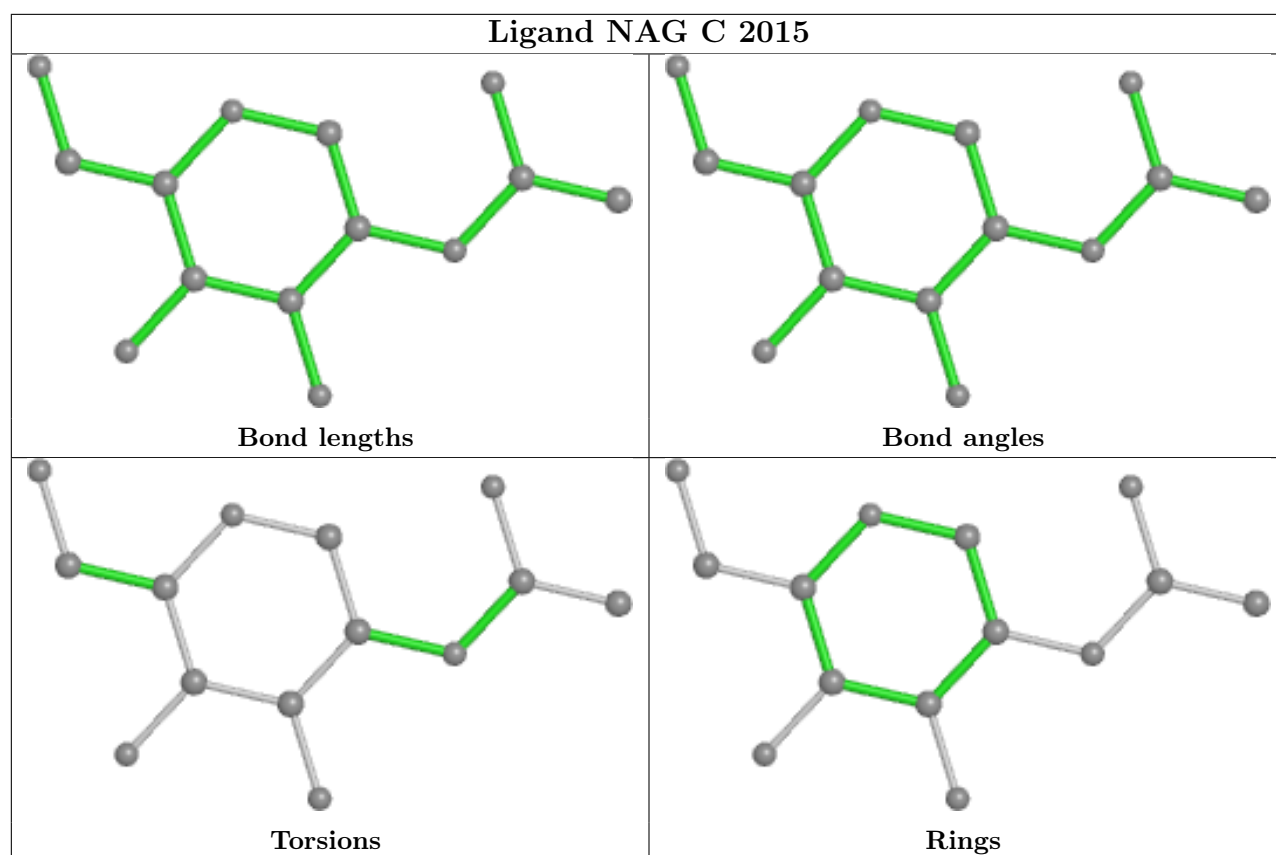


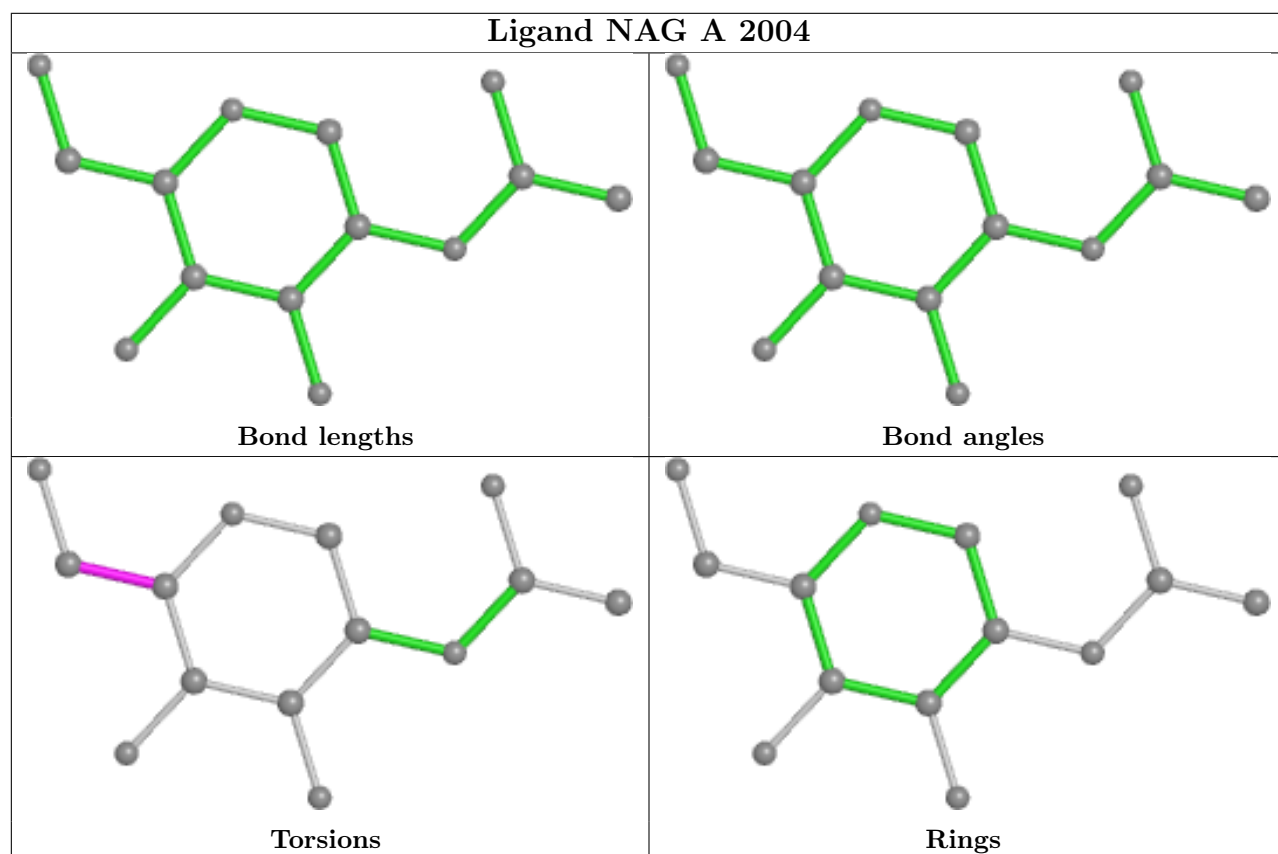
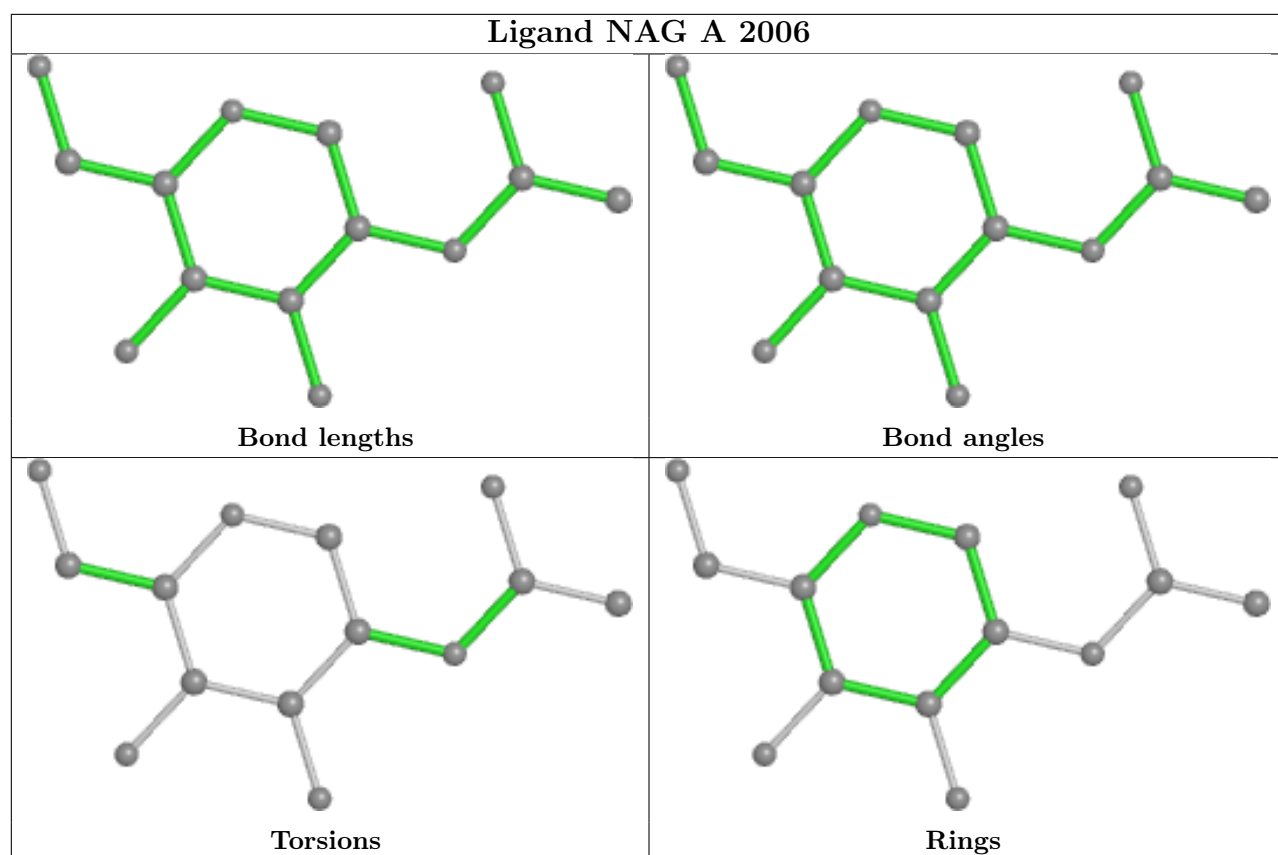


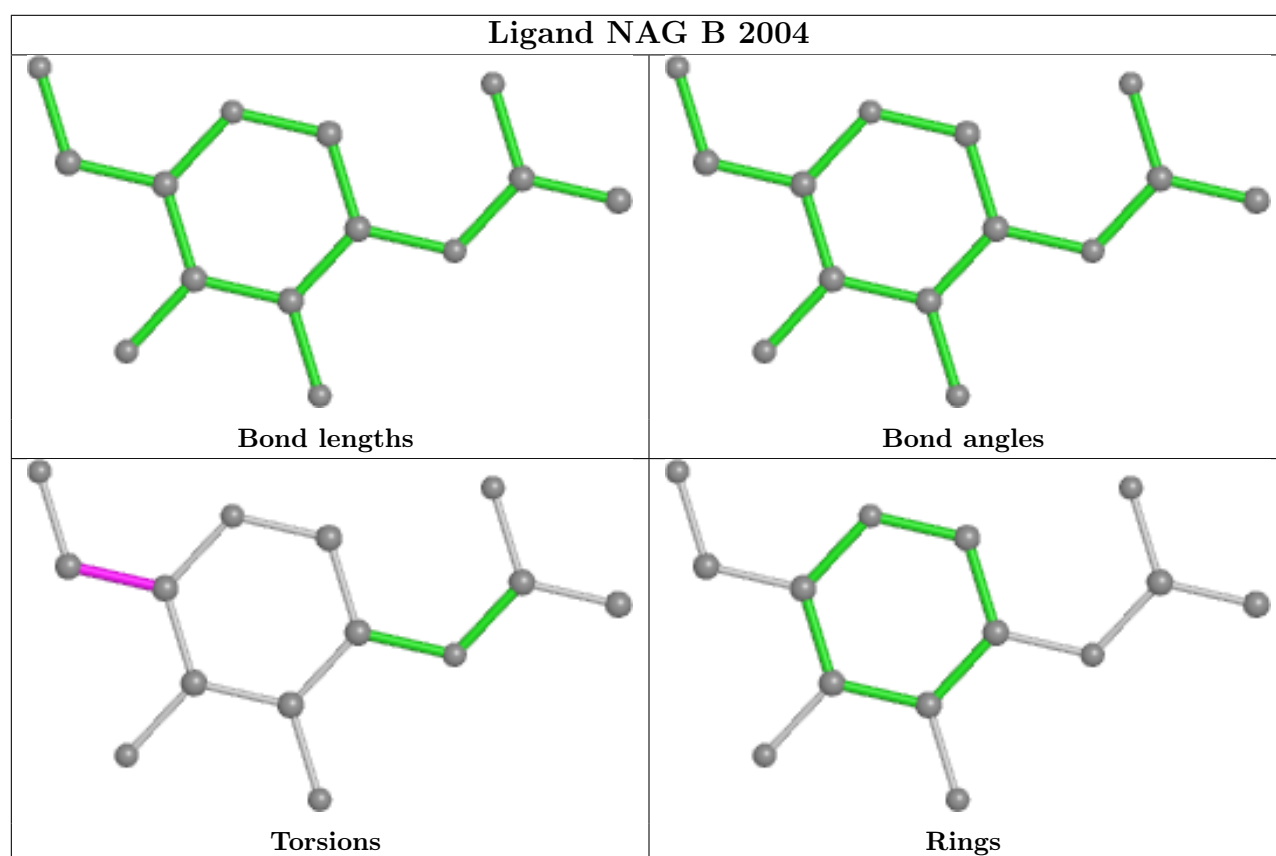
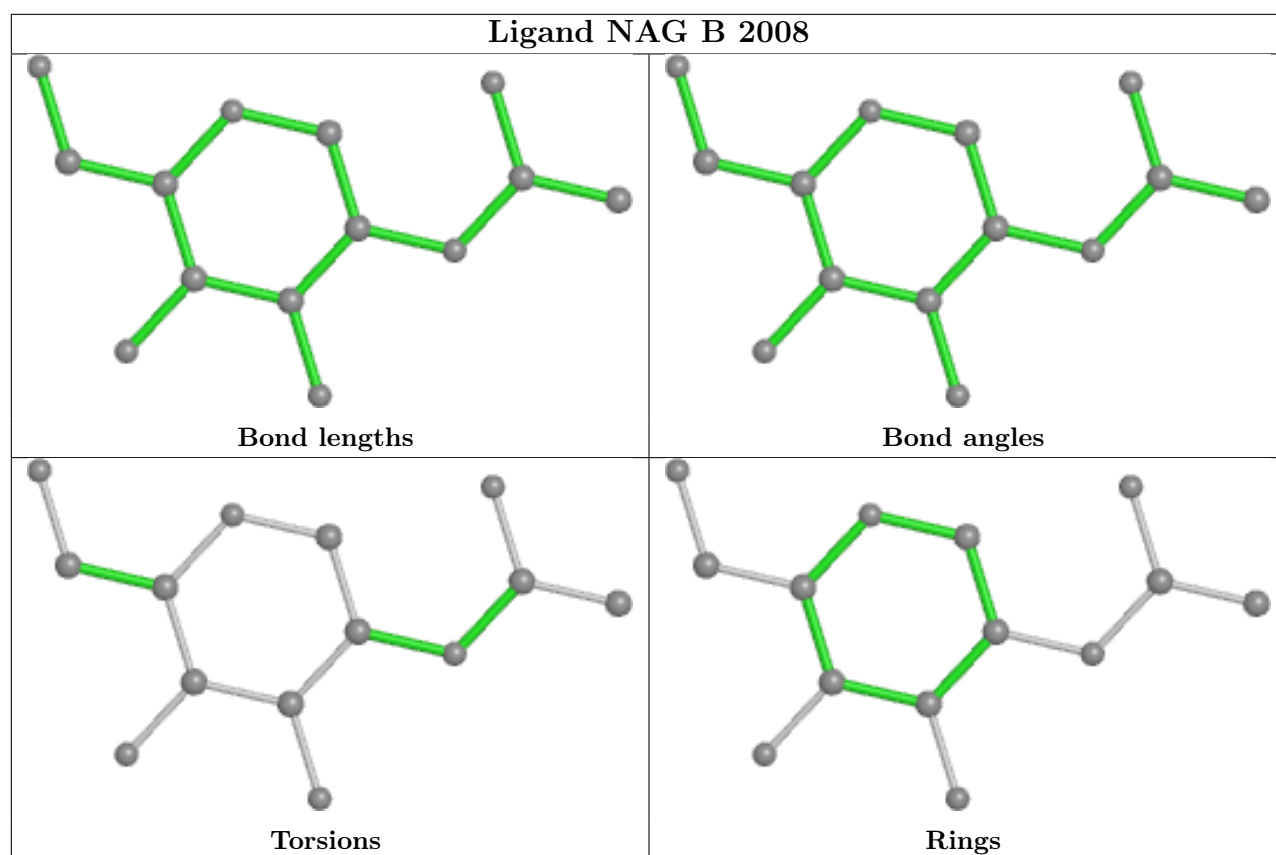














## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.