



Full wwPDB EM Validation Report ⓘ

Oct 16, 2024 – 01:00 AM JST

PDB ID : 8Y1G
EMDB ID : EMD-38835
Title : The 1up 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 : 2.99 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

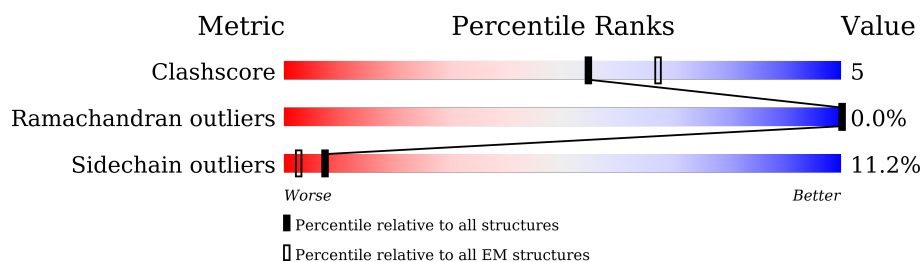
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.99 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	1290	73% 18% • 6%
1	B	1290	74% 18% • 6%
1	C	1290	75% 17% • 6%
2	D	6	33% 67%
2	I	6	33% 67%
2	N	6	33% 67%
3	E	2	100%
3	F	2	100%
3	G	2	50% 50%

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

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.

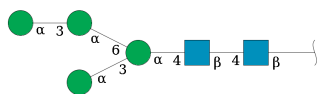
- Molecule 1 is a protein called Spike glycoprotein.

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	

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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	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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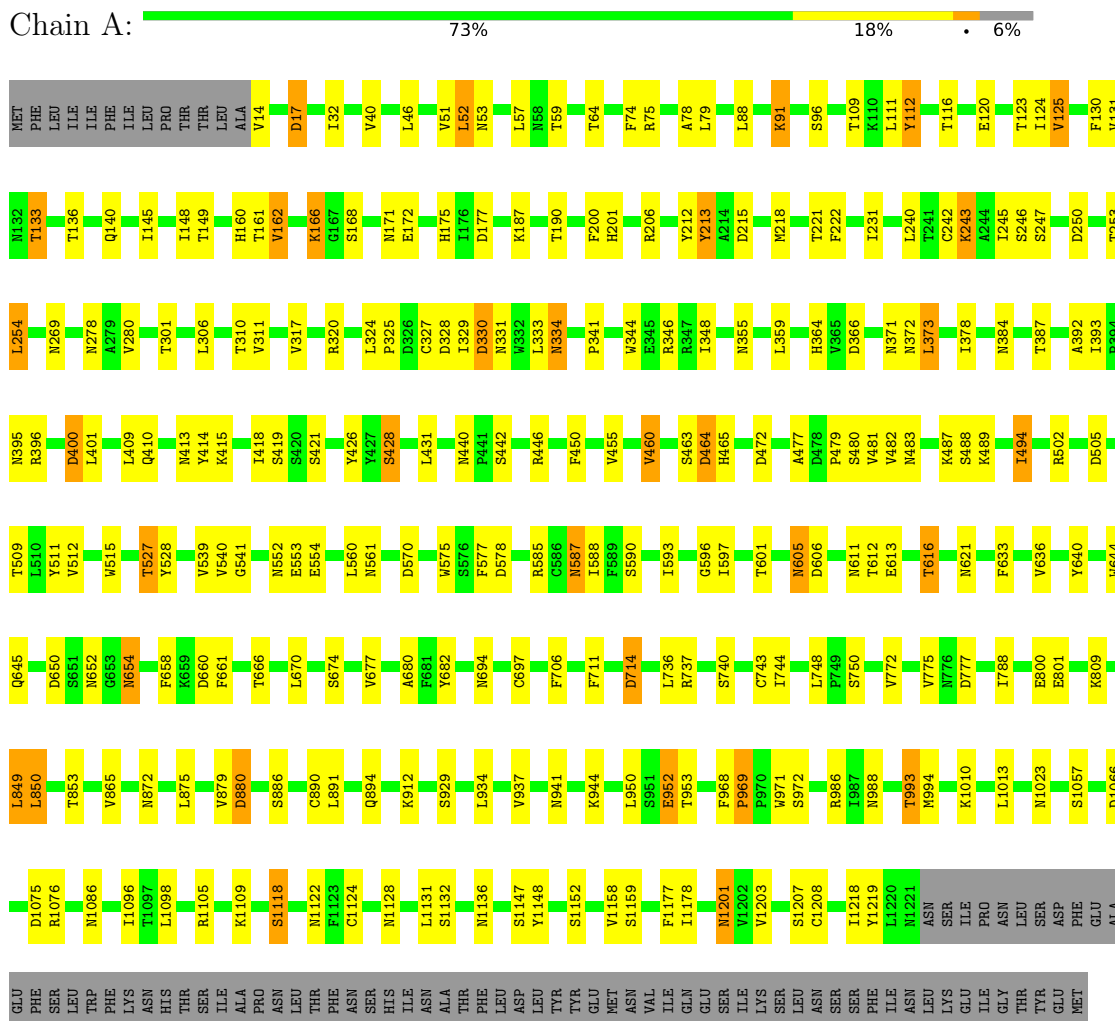
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Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C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

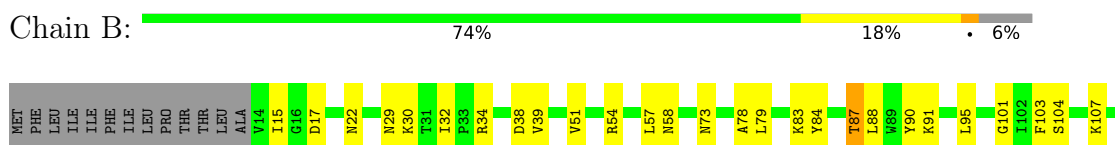
3 Residue-property plots

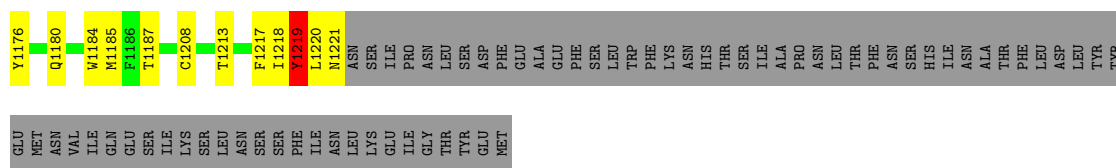
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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 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: 33% 67%



- 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 I: 33% 67%



- 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: 100%



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

Chain G:  50% 50%

WAG1
WAG2

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

Chain H:  100%

WAG1
WAG2

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

Chain J:  100%

WAG1
WAG2

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

Chain K:  100%

WAG1
WAG2

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

Chain L:  100%

WAG1
WAG2

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

Chain M:  100%

WAG1
WAG2

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

Chain O:  50% 50%

WAG1
WAG2

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

Chain P:  100%

MAG1
MAG2

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

Chain Q:  100%

MAG1
MAG2

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

Chain R:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	148802	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: NAG, MAN

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	0.47	0/9653	0.56	0/13146
1	B	0.44	0/9653	0.56	0/13146
1	C	0.48	0/9653	0.56	0/13146
All	All	0.47	0/28959	0.56	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	4
1	B	0	2
1	C	0	3
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1218	ILE	Peptide
1	A	929	SER	Peptide
1	A	968	PHE	Peptide
1	A	969	PRO	Peptide
1	B	968	PHE	Peptide
1	B	969	PRO	Peptide
1	C	1219	TYR	Peptide

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

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	9425	0	9076	104	0
1	B	9425	0	9076	102	0
1	C	9425	0	9076	92	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	1	0
All	All	29541	0	28374	285	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 5.

All (285) 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:B:651:SER:HG	1:C:59:THR:HG1	1.38	0.72
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.75	0.68
1:A:560:LEU:H	1:A:560:LEU:HD23	1.59	0.67
1:A:392:ALA:HA	1:A:588:ILE:HA	1.79	0.65
1:C:214:ALA:HB2	1:C:220:THR:HA	1.80	0.63
1:A:463:SER:HA	1:A:575:TRP:HA	1.80	0.62
1:A:1128:ASN:HB3	1:A:1148:TYR:HB3	1.82	0.62
1:C:332:TRP:O	1:C:390:LYS:NZ	2.33	0.61
1:B:249:THR:OG1	1:B:250:ASP:N	2.33	0.61
1:A:611:ASN:HB2	1:A:613:GLU:HG2	1.82	0.61
1:C:262:SER:OG	1:C:264:ARG:NH1	2.35	0.59
1:B:563:SER:OG	1:B:564:SER:N	2.34	0.59
1:C:952:GLU:HG3	1:C:1136:ASN:HD21	1.67	0.59
1:B:1132:SER:OG	1:B:1145:HIS:ND1	2.36	0.58
1:C:688:PRO:O	1:C:722:ASN:ND2	2.36	0.58
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.85	0.58
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.85	0.58
1:B:79:LEU:HB2	1:B:239:PRO:HB3	1.84	0.58
1:A:242:CYS:SG	1:A:243:LYS:N	2.77	0.58
1:A:387:THR:HB	1:A:593:ILE:HB	1.86	0.58
1:C:479:PRO:O	1:C:483:ASN:ND2	2.37	0.57
1:A:1122:ASN:O	1:B:1111:ASN:ND2	2.36	0.57
1:C:938:GLN:NE2	1:C:1041:ASN:OD1	2.37	0.57
1:B:470:ASN:N	1:B:470:ASN:OD1	2.37	0.57
1:B:400:ASP:OD1	1:B:400:ASP:N	2.34	0.57
1:C:394:PRO:HB3	1:C:578:ASP:HB3	1.87	0.56
1:C:1108:GLU:OE2	1:C:1120:ARG:NH2	2.32	0.56
1:B:482:VAL:O	1:B:489:LYS:NZ	2.37	0.56
1:C:745:ASP:OD2	1:C:763:ARG:NH2	2.38	0.56
1:A:160:HIS:NE2	1:A:171:ASN:O	2.37	0.56
1:A:246:SER:OG	1:A:247:SER:N	2.38	0.56
1:A:400:ASP:OD1	1:A:400:ASP:N	2.36	0.56
1:A:464:ASP:N	1:A:464:ASP:OD1	2.37	0.56
1:C:301:THR:HG23	1:C:682:TYR:HA	1.86	0.56
1:B:354:PHE:O	1:B:605:ASN:ND2	2.38	0.56
1:B:456:SER:OG	1:B:457:SER:N	2.39	0.56
1:C:1126:ASN:ND2	1:C:1127:GLY:O	2.39	0.56
1:A:301:THR:HG23	1:A:682:TYR:HA	1.87	0.56
1:B:150:ALA:HB3	1:B:185:PHE:HB3	1.88	0.56
1:B:900:ARG:NH1	1:B:905:ASP:OD1	2.38	0.56
1:B:425:LEU:HB3	1:B:590:SER:HB3	1.86	0.56
1:C:951:SER:OG	1:C:952:GLU:N	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:HD22	1:A:596:GLY:HA3	1.70	0.55
1:A:348:ILE:HG12	1:A:387:THR:HG23	1.87	0.55
1:C:139:VAL:HG22	1:C:148:ILE:HG12	1.89	0.55
1:B:872:ASN:OD1	1:B:894:GLN:NE2	2.39	0.55
1:C:395:ASN:ND2	1:C:579:SER:O	2.39	0.55
1:C:431:LEU:O	1:C:458:TYR:OH	2.24	0.55
1:B:996:VAL:O	1:B:1000:ASN:ND2	2.39	0.55
1:A:487:LYS:NZ	1:A:488:SER:OG	2.40	0.55
1:A:221:THR:OG1	1:A:222:PHE:N	2.40	0.55
1:C:456:SER:OG	1:C:457:SER:N	2.40	0.54
1:C:496:PRO:O	1:C:499:THR:OG1	2.24	0.54
1:A:400:ASP:O	1:A:410:GLN:NE2	2.39	0.54
1:C:863:GLN:O	1:C:1115:LYS:NZ	2.34	0.54
1:B:160:HIS:NE2	1:B:171:ASN:O	2.36	0.54
1:B:994:MET:HA	1:B:997:LEU:HD12	1.89	0.54
1:B:15:ILE:HD11	1:B:90:TYR:HB3	1.88	0.54
1:A:409:LEU:O	1:A:414:TYR:N	2.39	0.54
1:A:395:ASN:N	1:A:578:ASP:OD2	2.41	0.54
1:A:396:ARG:NH1	1:A:578:ASP:OD1	2.42	0.53
1:B:118:TYR:HA	1:B:143:ASN:HD21	1.72	0.53
1:B:262:SER:OG	1:B:264:ARG:NH1	2.42	0.53
1:A:777:ASP:O	1:B:870:ASN:ND2	2.41	0.53
1:C:215:ASP:OD1	1:C:215:ASP:N	2.41	0.53
1:A:112:TYR:O	1:A:166:LYS:NZ	2.42	0.53
1:B:319:ARG:NH1	1:B:612:THR:O	2.38	0.53
1:A:341:PRO:HD3	1:A:460:VAL:HG12	1.91	0.53
1:A:372:ASN:ND2	1:A:419:SER:O	2.43	0.52
1:A:409:LEU:HA	1:A:413:ASN:HB2	1.91	0.52
1:B:886:SER:O	1:B:901:SER:OG	2.27	0.52
1:A:344:TRP:HZ3	1:A:346:ARG:HB2	1.74	0.52
1:C:409:LEU:HA	1:C:413:ASN:HD22	1.73	0.52
1:C:604:SER:OG	1:C:606:ASP:OD2	2.28	0.52
1:C:828:LEU:HD11	1:C:1071:GLN:HG2	1.90	0.52
1:C:735:ASP:N	1:C:735:ASP:OD1	2.37	0.52
1:C:1154:LYS:NZ	1:C:1155:THR:O	2.42	0.52
1:B:1066:ASP:OD1	1:B:1066:ASP:N	2.38	0.52
1:B:246:SER:OG	1:B:247:SER:N	2.42	0.52
1:B:995:ASP:N	1:B:995:ASP:OD1	2.40	0.52
1:C:625:TYR:OH	1:C:660:ASP:OD1	2.27	0.52
1:B:214:ALA:HB2	1:B:220:THR:HA	1.90	0.52
1:A:393:ILE:HD12	1:A:587:ASN:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ASP:N	1:A:17:ASP:OD1	2.43	0.52
1:B:400:ASP:O	1:B:410:GLN:NE2	2.42	0.51
1:C:1180:GLN:HB3	1:C:1185:MET:HG3	1.91	0.51
1:A:162:VAL:HB	1:A:172:GLU:HB2	1.91	0.51
1:B:401:LEU:HA	1:B:410:GLN:HE21	1.76	0.51
1:B:146:LEU:HB3	1:B:189:PHE:HB2	1.93	0.51
1:B:789:GLN:NE2	1:B:1155:THR:OG1	2.39	0.51
1:A:324:LEU:HD23	1:A:325:PRO:HD2	1.92	0.51
1:A:396:ARG:NH2	1:A:577:PHE:O	2.41	0.51
1:B:358:THR:HA	1:B:361:ARG:HG2	1.92	0.51
1:A:480:SER:O	1:A:483:ASN:ND2	2.42	0.51
1:A:1147:SER:OG	1:A:1148:TYR:N	2.43	0.51
1:B:142:HIS:HB2	1:B:145:ILE:HB	1.92	0.51
1:B:739:GLY:HA2	1:C:949:ILE:HA	1.92	0.51
1:C:617:GLY:O	4:C:2011:NAG:O3	2.28	0.51
1:C:97:ASP:OD1	1:C:97:ASP:N	2.41	0.51
1:C:124:ILE:HG13	1:C:237:VAL:HG22	1.93	0.51
1:A:200:PHE:HD1	1:A:213:TYR:HB2	1.75	0.50
1:A:680:ALA:HB1	1:A:736:LEU:HD13	1.94	0.50
1:A:1207:SER:OG	1:B:998:ASN:ND2	2.42	0.50
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.93	0.50
1:A:1159:SER:N	1:A:1177:PHE:O	2.40	0.50
1:C:879:VAL:HG21	1:C:967:MET:HB3	1.93	0.50
1:A:440:ASN:HD21	1:A:442:SER:HB3	1.77	0.50
1:C:125:VAL:HG23	1:C:138:VAL:HG22	1.93	0.50
1:C:1130:ILE:HG22	1:C:1131:LEU:HG	1.94	0.50
1:C:986:ARG:HH11	1:C:1117:GLN:HG2	1.77	0.49
1:A:373:LEU:HG	1:A:421:SER:HB3	1.93	0.49
1:B:1196:PRO:O	1:B:1201:ASN:ND2	2.46	0.49
1:A:937:VAL:O	1:A:941:ASN:ND2	2.44	0.49
1:B:382:CYS:HA	1:B:603:CYS:HA	1.94	0.49
1:A:743:CYS:SG	1:A:744:ILE:N	2.86	0.49
1:B:1158:VAL:HG12	1:B:1178:ILE:HG22	1.93	0.49
1:B:446:ARG:NH2	1:C:133:THR:O	2.46	0.49
1:A:986:ARG:NH2	1:A:1118:SER:O	2.45	0.49
1:B:119:SER:OG	1:B:193:VAL:O	2.29	0.49
1:A:392:ALA:HB3	1:A:460:VAL:HG11	1.95	0.48
1:A:560:LEU:H	1:A:560:LEU:CD2	2.26	0.48
1:B:735:ASP:OD1	1:B:735:ASP:N	2.44	0.48
1:C:509:THR:HG1	1:C:515:TRP:HE1	1.60	0.48
1:B:130:PHE:HB3	1:B:155:MET:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:VAL:HG13	1:B:433:ASN:HB3	1.94	0.48
1:B:795:THR:OG1	1:B:796:ILE:N	2.46	0.48
1:C:340:SER:OG	1:C:461:VAL:O	2.31	0.48
1:C:590:SER:OG	1:C:591:ASN:N	2.47	0.48
1:B:1163:CYS:N	1:B:1213:THR:O	2.46	0.48
1:C:334:ASN:HA	1:C:429:LEU:HD11	1.95	0.47
1:C:448:TYR:OH	1:C:473:PHE:O	2.29	0.47
1:C:503:HIS:NE2	1:C:505:ASP:OD1	2.47	0.47
1:A:334:ASN:OD1	1:A:334:ASN:N	2.46	0.47
1:B:369:SER:OG	1:B:370:CYS:N	2.46	0.47
1:A:650:ASP:OD1	1:A:650:ASP:N	2.48	0.47
1:A:46:LEU:HD12	1:A:218:MET:HG2	1.97	0.47
1:C:75:ARG:NH2	1:C:96:SER:OG	2.48	0.47
1:B:269:ASN:ND2	1:B:277:THR:OG1	2.44	0.47
1:B:791:PRO:HB3	1:B:1150:PRO:HB3	1.97	0.47
1:C:552:ASN:HB2	1:C:573:LEU:HD11	1.97	0.47
1:A:1158:VAL:HG12	1:A:1178:ILE:HG22	1.95	0.47
1:B:83:LYS:HE3	1:B:84:TYR:CZ	2.50	0.47
1:A:775:VAL:O	1:B:869:SER:OG	2.27	0.46
1:B:1187:THR:OG1	1:B:1188:GLY:N	2.47	0.46
1:B:335:ASN:OD1	1:B:336:VAL:N	2.44	0.46
1:B:837:ASP:OD1	1:B:837:ASP:N	2.49	0.46
1:A:801:GLU:OE2	1:A:1109:LYS:NZ	2.49	0.46
1:C:246:SER:OG	1:C:247:SER:N	2.48	0.46
1:A:482:VAL:O	1:A:489:LYS:NZ	2.48	0.46
1:B:215:ASP:OD1	1:B:215:ASP:N	2.49	0.46
1:B:926:THR:O	1:B:926:THR:OG1	2.34	0.46
1:A:125:VAL:HG22	1:A:130:PHE:HE2	1.79	0.46
1:A:269:ASN:ND2	1:A:278:ASN:OD1	2.47	0.46
1:A:654:ASN:OD1	1:A:654:ASN:N	2.46	0.46
1:B:692:TYR:HB3	1:B:695:LEU:HD12	1.98	0.46
1:B:1207:SER:O	1:C:998:ASN:ND2	2.48	0.46
1:B:165:SER:OG	1:B:166:LYS:N	2.46	0.46
1:B:478:ASP:HB3	1:B:481:VAL:HG23	1.98	0.46
1:A:502:ARG:NH1	1:A:553:GLU:O	2.49	0.46
1:A:636:VAL:O	1:A:666:THR:OG1	2.33	0.46
1:B:15:ILE:HD12	1:B:95:LEU:HD13	1.98	0.46
1:B:1184:TRP:HB2	1:B:1218:ILE:HD11	1.97	0.46
1:A:240:LEU:HB3	1:A:254:LEU:HD11	1.97	0.45
1:C:196:ASP:OD1	1:C:196:ASP:N	2.49	0.45
1:A:872:ASN:HD22	1:A:875:LEU:HD23	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HA	1:B:413:ASN:HD22	1.81	0.45
1:C:162:VAL:HG22	1:C:241:THR:HB	1.98	0.45
1:A:560:LEU:HG	1:A:561:ASN:N	2.31	0.45
1:A:373:LEU:HD13	1:A:378:ILE:HG12	1.99	0.45
1:A:477:ALA:HA	1:A:502:ARG:HB3	1.99	0.45
1:B:1086:ASN:O	1:B:1090:SER:OG	2.34	0.45
1:A:131:VAL:HG23	1:A:133:THR:H	1.81	0.45
1:A:415:LYS:HD3	1:A:541:GLY:HA2	1.98	0.45
1:A:463:SER:OG	1:A:465:HIS:O	2.35	0.45
1:A:969:PRO:HA	1:A:971:TRP:CE2	2.51	0.45
1:B:162:VAL:HB	1:B:172:GLU:HB2	1.98	0.45
1:A:78:ALA:HB1	1:A:254:LEU:HB3	1.98	0.45
1:A:944:LYS:NZ	1:C:694:ASN:OD1	2.48	0.45
1:C:330:ASP:HA	1:C:333:LEU:HB2	1.99	0.45
1:B:405:SER:OG	1:B:406:SER:N	2.49	0.44
1:C:693:ARG:HH12	1:C:717:LEU:HD22	1.82	0.44
1:C:1085:LEU:HD23	1:C:1085:LEU:HA	1.83	0.44
1:C:756:ARG:HD3	1:C:756:ARG:HA	1.72	0.44
1:C:1158:VAL:HB	1:C:1176:TYR:HB3	1.99	0.44
1:B:935:LEU:O	1:B:939:SER:OG	2.22	0.44
1:A:1201:ASN:OD1	1:A:1201:ASN:N	2.48	0.44
1:A:809:LYS:HG2	1:A:850:LEU:HD23	1.99	0.44
1:B:103:PHE:HB2	1:B:261:LEU:HD21	2.00	0.44
1:B:1100:LYS:HE3	1:B:1100:LYS:HB3	1.80	0.44
1:A:215:ASP:N	1:A:215:ASP:OD1	2.51	0.44
1:A:872:ASN:ND2	1:A:894:GLN:OE1	2.45	0.44
1:B:1098:LEU:HD13	1:C:1097:THR:HG23	1.99	0.44
1:C:1219:TYR:H	1:C:1220:LEU:HD22	1.82	0.44
1:A:53:ASN:OD1	1:A:53:ASN:N	2.50	0.44
1:A:880:ASP:OD1	1:A:880:ASP:N	2.50	0.44
1:B:1013:LEU:O	1:B:1017:ASN:ND2	2.35	0.44
1:A:355:ASN:HA	1:A:605:ASN:HB3	2.00	0.44
1:A:645:GLN:NE2	1:B:54:ARG:O	2.51	0.44
1:C:105:LYS:HB3	1:C:257:TRP:HB2	1.99	0.44
1:C:496:PRO:HD2	1:C:499:THR:HG21	1.99	0.44
1:B:552:ASN:HB2	1:B:573:LEU:HD21	1.98	0.43
1:C:876:HIS:HB3	1:C:968:PHE:CZ	2.53	0.43
1:B:132:ASN:OD1	1:B:132:ASN:N	2.50	0.43
1:A:527:THR:OG1	1:A:528:TYR:N	2.50	0.43
1:B:216:VAL:HG13	1:B:218:MET:HG2	2.00	0.43
1:C:1066:ASP:HB3	1:C:1068:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1076:ARG:NH2	1:B:1075:ASP:OD2	2.52	0.43
1:C:358:THR:HA	1:C:361:ARG:HG2	2.01	0.43
1:A:512:VAL:HG11	1:A:515:TRP:HB3	2.00	0.43
1:B:88:LEU:HD12	1:B:91:LYS:HZ1	1.83	0.43
1:B:1206:ASN:OD1	1:B:1206:ASN:N	2.52	0.43
1:A:91:LYS:HD3	1:A:91:LYS:HA	1.68	0.43
1:B:130:PHE:HD2	1:B:155:MET:HG3	1.84	0.43
1:A:333:LEU:HD12	1:A:359:LEU:HD11	2.00	0.43
1:B:853:THR:HG21	1:B:1100:LYS:HG2	2.00	0.43
1:A:328:ASP:HB2	1:A:331:ASN:HB2	1.99	0.43
1:A:366:ASP:OD1	1:A:428:SER:OG	2.32	0.43
1:B:1164:LEU:HD21	1:B:1170:ILE:HD11	2.00	0.43
1:A:123:THR:HG21	1:A:140:GLN:HG3	2.01	0.42
1:C:392:ALA:HB3	1:C:460:VAL:HG11	2.01	0.42
1:A:440:ASN:O	1:A:446:ARG:NE	2.51	0.42
1:C:791:PRO:HB3	1:C:1150:PRO:HB3	2.01	0.42
1:A:401:LEU:O	1:A:426:TYR:OH	2.36	0.42
1:B:1075:ASP:O	1:B:1079:ASN:ND2	2.37	0.42
1:C:17:ASP:N	1:C:17:ASP:OD1	2.52	0.42
1:C:34:ARG:HE	1:C:34:ARG:HB3	1.61	0.42
1:A:52:LEU:H	1:A:52:LEU:HG	1.47	0.42
1:B:397:ARG:NE	1:B:400:ASP:OD2	2.45	0.42
1:A:552:ASN:HD21	1:A:554:GLU:HB2	1.84	0.42
1:A:993:THR:OG1	1:A:994:MET:N	2.52	0.42
1:B:104:SER:HB2	1:B:200:PHE:HB2	2.02	0.42
1:B:264:ARG:HD3	1:B:266:TYR:HE1	1.84	0.42
1:B:487:LYS:HB2	1:B:515:TRP:HB2	2.00	0.42
1:A:694:ASN:ND2	1:B:923:ASN:OD1	2.37	0.42
1:B:835:PHE:HD2	1:B:1082:LEU:HD22	1.84	0.42
1:C:103:PHE:HB2	1:C:261:LEU:HD21	2.01	0.42
1:C:636:VAL:O	1:C:666:THR:OG1	2.34	0.42
1:C:689:ALA:HA	1:C:722:ASN:HB3	2.01	0.42
1:A:330:ASP:N	1:A:330:ASP:OD1	2.52	0.42
1:B:88:LEU:HA	1:B:91:LYS:HZ3	1.84	0.42
1:A:32:ILE:HD13	1:A:88:LEU:HD13	2.02	0.42
1:A:616:THR:HA	1:A:633:PHE:HB2	2.02	0.42
1:B:506:LEU:H	1:B:506:LEU:HG	1.69	0.42
1:C:485:CYS:SG	1:C:516:CYS:N	2.93	0.42
1:B:462:TYR:CZ	1:B:576:SER:HB2	2.54	0.41
1:B:879:VAL:HG21	1:B:967:MET:HB3	2.01	0.41
1:A:740:SER:O	1:A:740:SER:OG	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:912:LYS:HE2	1:A:912:LYS:HB3	1.87	0.41
1:B:140:GLN:HE21	1:B:142:HIS:HE1	1.67	0.41
1:C:389:ASP:OD2	1:C:414:TYR:OH	2.31	0.41
1:B:969:PRO:HA	1:B:971:TRP:CE2	2.55	0.41
1:C:447:ARG:HH12	1:C:496:PRO:HG2	1.85	0.41
1:A:145:ILE:HG12	1:A:190:THR:HG22	2.03	0.41
1:C:1062:LEU:HD23	1:C:1062:LEU:HA	1.91	0.41
1:A:428:SER:HB2	1:A:585:ARG:HD2	2.02	0.41
1:C:319:ARG:HH21	1:C:611:ASN:HB3	1.85	0.41
1:C:508:THR:HG23	1:C:513:ASN:HA	2.03	0.41
1:C:561:ASN:HD22	1:C:562:HIS:H	1.67	0.41
1:C:1184:TRP:HB2	1:C:1218:ILE:HD11	2.03	0.41
1:B:823:ALA:HA	1:B:826:HIS:HB2	2.02	0.41
1:A:697:CYS:N	1:A:714:ASP:OD2	2.44	0.41
1:B:101:GLY:HA3	1:B:261:LEU:HD12	2.03	0.41
1:C:267:LEU:HB3	1:C:280:VAL:HG12	2.01	0.41
1:A:472:ASP:OD1	1:A:472:ASP:N	2.54	0.41
1:C:185:PHE:HB2	1:C:226:LEU:HD13	2.03	0.41
1:C:264:ARG:HH11	1:C:264:ARG:HD2	1.77	0.41
1:C:570:ASP:OD1	1:C:570:ASP:N	2.41	0.41
1:C:659:LYS:HB2	1:C:666:THR:HG22	2.03	0.41
1:C:1023:ASN:HB3	1:C:1026:LEU:HB2	2.01	0.41
1:C:1091:GLN:HE21	1:C:1091:GLN:HB2	1.50	0.41
1:C:632:ILE:N	1:C:670:LEU:O	2.54	0.41
1:C:1015:ILE:HD13	1:C:1015:ILE:HA	1.92	0.41
1:B:87:THR:O	1:B:91:LYS:NZ	2.51	0.40
1:B:269:ASN:HB2	1:B:297:PHE:CE1	2.57	0.40
1:A:952:GLU:HG3	1:A:1136:ASN:HD21	1.86	0.40
1:B:78:ALA:HB1	1:B:254:LEU:HD12	2.03	0.40
1:C:1100:LYS:HE2	1:C:1100:LYS:HB3	1.94	0.40
1:A:479:PRO:HG3	1:A:494:ILE:HA	2.02	0.40
1:A:849:LEU:O	1:A:853:THR:HG23	2.22	0.40
1:B:405:SER:OG	1:B:406:SER:O	2.36	0.40
1:B:1114:VAL:HG11	1:B:1134:VAL:HG12	2.03	0.40
1:C:566:SER:OG	1:C:567:CYS:N	2.54	0.40
1:A:570:ASP:OD1	1:A:570:ASP:N	2.50	0.40
1:C:329:ILE:HB	1:C:359:LEU:HD11	2.03	0.40
1:C:346:ARG:HE	1:C:346:ARG:HB2	1.67	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	1206/1290 (94%)	1105 (92%)	101 (8%)	0	100	100
1	B	1206/1290 (94%)	1100 (91%)	106 (9%)	0	100	100
1	C	1206/1290 (94%)	1123 (93%)	82 (7%)	1 (0%)	48	81
All	All	3618/3870 (94%)	3328 (92%)	289 (8%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	970	PRO

5.3.2 Protein sidechains

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%)	952 (88%)	130 (12%)	4	18
1	B	1082/1159 (93%)	963 (89%)	119 (11%)	5	22
1	C	1082/1159 (93%)	969 (90%)	113 (10%)	5	23
All	All	3246/3477 (93%)	2884 (89%)	362 (11%)	7	21

All (362) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	17	ASP

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Mol	Chain	Res	Type
1	A	40	VAL
1	A	51	VAL
1	A	52	LEU
1	A	57	LEU
1	A	59	THR
1	A	64	THR
1	A	74	PHE
1	A	75	ARG
1	A	79	LEU
1	A	91	LYS
1	A	96	SER
1	A	109	THR
1	A	111	LEU
1	A	112	TYR
1	A	116	THR
1	A	120	GLU
1	A	124	ILE
1	A	125	VAL
1	A	133	THR
1	A	136	THR
1	A	148	ILE
1	A	149	THR
1	A	161	THR
1	A	162	VAL
1	A	166	LYS
1	A	168	SER
1	A	175	HIS
1	A	177	ASP
1	A	187	LYS
1	A	206	ARG
1	A	213	TYR
1	A	231	ILE
1	A	243	LYS
1	A	245	ILE
1	A	250	ASP
1	A	253	THR
1	A	254	LEU
1	A	280	VAL
1	A	306	LEU
1	A	310	THR
1	A	311	VAL
1	A	317	VAL

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Mol	Chain	Res	Type
1	A	320	ARG
1	A	327	CYS
1	A	329	ILE
1	A	330	ASP
1	A	334	ASN
1	A	364	HIS
1	A	371	ASN
1	A	373	LEU
1	A	400	ASP
1	A	418	ILE
1	A	428	SER
1	A	431	LEU
1	A	450	PHE
1	A	455	VAL
1	A	460	VAL
1	A	464	ASP
1	A	481	VAL
1	A	494	ILE
1	A	505	ASP
1	A	509	THR
1	A	511	TYR
1	A	527	THR
1	A	539	VAL
1	A	540	VAL
1	A	587	ASN
1	A	590	SER
1	A	597	ILE
1	A	601	THR
1	A	605	ASN
1	A	606	ASP
1	A	612	THR
1	A	616	THR
1	A	621	ASN
1	A	640	TYR
1	A	644	TRP
1	A	652	ASN
1	A	654	ASN
1	A	658	PHE
1	A	660	ASP
1	A	661	PHE
1	A	670	LEU
1	A	674	SER

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Mol	Chain	Res	Type
1	A	677	VAL
1	A	706	PHE
1	A	711	PHE
1	A	714	ASP
1	A	737	ARG
1	A	748	LEU
1	A	750	SER
1	A	772	VAL
1	A	788	ILE
1	A	800	GLU
1	A	849	LEU
1	A	850	LEU
1	A	865	VAL
1	A	879	VAL
1	A	880	ASP
1	A	886	SER
1	A	890	CYS
1	A	891	LEU
1	A	934	LEU
1	A	950	LEU
1	A	952	GLU
1	A	953	THR
1	A	972	SER
1	A	988	ASN
1	A	993	THR
1	A	1010	LYS
1	A	1013	LEU
1	A	1023	ASN
1	A	1057	SER
1	A	1066	ASP
1	A	1075	ASP
1	A	1086	ASN
1	A	1096	ILE
1	A	1098	LEU
1	A	1105	ARG
1	A	1118	SER
1	A	1124	CYS
1	A	1131	LEU
1	A	1132	SER
1	A	1152	SER
1	A	1201	ASN
1	A	1203	VAL

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Mol	Chain	Res	Type
1	A	1208	CYS
1	A	1219	TYR
1	B	17	ASP
1	B	22	ASN
1	B	29	ASN
1	B	30	LYS
1	B	32	ILE
1	B	34	ARG
1	B	38	ASP
1	B	39	VAL
1	B	51	VAL
1	B	57	LEU
1	B	58	ASN
1	B	73	ASN
1	B	87	THR
1	B	107	LYS
1	B	116	THR
1	B	125	VAL
1	B	132	ASN
1	B	133	THR
1	B	136	THR
1	B	143	ASN
1	B	154	THR
1	B	175	HIS
1	B	184	LEU
1	B	190	THR
1	B	213	TYR
1	B	241	THR
1	B	249	THR
1	B	254	LEU
1	B	259	THR
1	B	307	SER
1	B	310	THR
1	B	311	VAL
1	B	346	ARG
1	B	350	SER
1	B	351	ASN
1	B	369	SER
1	B	373	LEU
1	B	374	ASP
1	B	375	LYS
1	B	378	ILE

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Mol	Chain	Res	Type
1	B	381	SER
1	B	400	ASP
1	B	412	SER
1	B	418	ILE
1	B	447	ARG
1	B	470	ASN
1	B	481	VAL
1	B	482	VAL
1	B	506	LEU
1	B	507	ASP
1	B	511	TYR
1	B	527	THR
1	B	531	ASN
1	B	540	VAL
1	B	560	LEU
1	B	563	SER
1	B	573	LEU
1	B	583	ASN
1	B	601	THR
1	B	606	ASP
1	B	624	LEU
1	B	636	VAL
1	B	644	TRP
1	B	655	ILE
1	B	668	THR
1	B	670	LEU
1	B	676	ARG
1	B	677	VAL
1	B	683	GLN
1	B	690	LEU
1	B	711	PHE
1	B	731	VAL
1	B	735	ASP
1	B	743	CYS
1	B	763	ARG
1	B	766	THR
1	B	781	THR
1	B	788	ILE
1	B	828	LEU
1	B	837	ASP
1	B	838	ASN
1	B	849	LEU

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Mol	Chain	Res	Type
1	B	850	LEU
1	B	865	VAL
1	B	879	VAL
1	B	881	ASN
1	B	886	SER
1	B	895	CYS
1	B	915	ASP
1	B	930	GLU
1	B	931	ILE
1	B	950	LEU
1	B	964	VAL
1	B	977	VAL
1	B	986	ARG
1	B	995	ASP
1	B	1000	ASN
1	B	1012	LEU
1	B	1023	ASN
1	B	1028	LYS
1	B	1058	LEU
1	B	1066	ASP
1	B	1086	ASN
1	B	1089	VAL
1	B	1090	SER
1	B	1091	GLN
1	B	1096	ILE
1	B	1098	LEU
1	B	1108	GLU
1	B	1117	GLN
1	B	1135	GLN
1	B	1142	LEU
1	B	1147	SER
1	B	1159	SER
1	B	1180	GLN
1	B	1190	SER
1	B	1195	GLU
1	B	1203	VAL
1	B	1213	THR
1	C	14	VAL
1	C	21	THR
1	C	28	TYR
1	C	29	ASN
1	C	31	THR

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Mol	Chain	Res	Type
1	C	32	ILE
1	C	40	VAL
1	C	52	LEU
1	C	97	ASP
1	C	99	ASN
1	C	123	THR
1	C	128	SER
1	C	129	VAL
1	C	136	THR
1	C	161	THR
1	C	178	SER
1	C	182	LEU
1	C	187	LYS
1	C	190	THR
1	C	193	VAL
1	C	196	ASP
1	C	204	GLN
1	C	213	TYR
1	C	221	THR
1	C	241	THR
1	C	243	LYS
1	C	250	ASP
1	C	253	THR
1	C	258	VAL
1	C	277	THR
1	C	289	GLU
1	C	305	ASP
1	C	330	ASP
1	C	337	SER
1	C	350	SER
1	C	351	ASN
1	C	356	LEU
1	C	358	THR
1	C	359	LEU
1	C	373	LEU
1	C	375	LYS
1	C	376	SER
1	C	384	ASN
1	C	399	ASP
1	C	418	ILE
1	C	456	SER
1	C	457	SER

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Mol	Chain	Res	Type
1	C	460	VAL
1	C	472	ASP
1	C	481	VAL
1	C	484	SER
1	C	509	THR
1	C	560	LEU
1	C	561	ASN
1	C	590	SER
1	C	597	ILE
1	C	608	LEU
1	C	612	THR
1	C	615	SER
1	C	636	VAL
1	C	644	TRP
1	C	646	ASN
1	C	651	SER
1	C	659	LYS
1	C	676	ARG
1	C	717	LEU
1	C	731	VAL
1	C	743	CYS
1	C	748	LEU
1	C	767	PHE
1	C	780	GLU
1	C	807	SER
1	C	811	THR
1	C	820	SER
1	C	850	LEU
1	C	863	GLN
1	C	865	VAL
1	C	871	LEU
1	C	872	ASN
1	C	879	VAL
1	C	885	LYS
1	C	894	GLN
1	C	897	SER
1	C	926	THR
1	C	939	SER
1	C	950	LEU
1	C	952	GLU
1	C	953	THR
1	C	964	VAL

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Mol	Chain	Res	Type
1	C	972	SER
1	C	981	LEU
1	C	986	ARG
1	C	1008	PHE
1	C	1042	SER
1	C	1058	LEU
1	C	1066	ASP
1	C	1069	GLU
1	C	1091	GLN
1	C	1096	ILE
1	C	1104	SER
1	C	1118	SER
1	C	1124	CYS
1	C	1131	LEU
1	C	1147	SER
1	C	1154	LYS
1	C	1155	THR
1	C	1156	VAL
1	C	1187	THR
1	C	1208	CYS
1	C	1213	THR
1	C	1217	PHE
1	C	1219	TYR
1	C	1221	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	204	GLN
1	A	291	GLN
1	A	351	ASN
1	A	384	ASN
1	A	402	GLN
1	A	440	ASN
1	A	552	ASN
1	A	595	ASN
1	A	611	ASN
1	A	621	ASN
1	A	630	GLN
1	A	838	ASN
1	A	859	ASN

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Mol	Chain	Res	Type
1	A	876	HIS
1	A	984	GLN
1	A	1001	GLN
1	A	1023	ASN
1	A	1049	ASN
1	A	1091	GLN
1	A	1180	GLN
1	B	73	ASN
1	B	140	GLN
1	B	143	ASN
1	B	152	GLN
1	B	204	GLN
1	B	248	ASN
1	B	269	ASN
1	B	437	ASN
1	B	598	ASN
1	B	605	ASN
1	B	630	GLN
1	B	789	GLN
1	B	876	HIS
1	B	998	ASN
1	B	1000	ASN
1	B	1001	GLN
1	B	1038	GLN
1	B	1086	ASN
1	B	1136	ASN
1	B	1180	GLN
1	B	1201	ASN
1	C	204	GLN
1	C	351	ASN
1	C	395	ASN
1	C	483	ASN
1	C	561	ASN
1	C	587	ASN
1	C	630	GLN
1	C	646	ASN
1	C	863	GLN
1	C	894	GLN
1	C	984	GLN
1	C	1001	GLN
1	C	1038	GLN
1	C	1091	GLN

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Mol	Chain	Res	Type
1	C	1126	ASN
1	C	1136	ASN

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	2,1	14,14,15	0.44	0	17,19,21	0.51	0
2	NAG	D	2	2	14,14,15	0.31	0	17,19,21	0.56	0
2	MAN	D	3	2	11,11,12	1.92	5 (45%)	15,15,17	1.29	1 (6%)
2	MAN	D	4	2	11,11,12	0.73	0	15,15,17	1.25	2 (13%)
2	MAN	D	5	2	11,11,12	1.14	1 (9%)	15,15,17	1.15	1 (6%)
2	MAN	D	6	2	11,11,12	0.70	0	15,15,17	1.17	2 (13%)
3	NAG	E	1	3,1	14,14,15	0.40	0	17,19,21	0.63	0
3	NAG	E	2	3	14,14,15	0.38	0	17,19,21	0.51	0
3	NAG	F	1	3,1	14,14,15	0.28	0	17,19,21	0.53	0
3	NAG	F	2	3	14,14,15	0.23	0	17,19,21	0.50	0
3	NAG	G	1	3,1	14,14,15	0.38	0	17,19,21	0.99	1 (5%)
3	NAG	G	2	3	14,14,15	0.46	0	17,19,21	0.58	0
3	NAG	H	1	3,1	14,14,15	0.33	0	17,19,21	0.62	0
3	NAG	H	2	3	14,14,15	0.40	0	17,19,21	0.58	0
2	NAG	I	1	2,1	14,14,15	0.38	0	17,19,21	0.47	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	2	2	14,14,15	0.25	0	17,19,21	0.63	0
2	MAN	I	3	2	11,11,12	1.71	3 (27%)	15,15,17	1.80	1 (6%)
2	MAN	I	4	2	11,11,12	0.72	0	15,15,17	1.32	2 (13%)
2	MAN	I	5	2	11,11,12	0.86	0	15,15,17	1.14	2 (13%)
2	MAN	I	6	2	11,11,12	1.10	1 (9%)	15,15,17	1.31	1 (6%)
3	NAG	J	1	3,1	14,14,15	0.34	0	17,19,21	0.59	0
3	NAG	J	2	3	14,14,15	0.38	0	17,19,21	0.49	0
3	NAG	K	1	3,1	14,14,15	0.40	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.32	0	17,19,21	0.52	0
3	NAG	L	1	3,1	14,14,15	0.57	0	17,19,21	0.59	0
3	NAG	L	2	3	14,14,15	0.55	0	17,19,21	0.59	0
3	NAG	M	1	3,1	14,14,15	0.20	0	17,19,21	0.51	0
3	NAG	M	2	3	14,14,15	0.27	0	17,19,21	0.49	0
2	NAG	N	1	2,1	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	N	2	2	14,14,15	0.25	0	17,19,21	0.51	0
2	MAN	N	3	2	11,11,12	1.13	1 (9%)	15,15,17	1.19	3 (20%)
2	MAN	N	4	2	11,11,12	0.99	1 (9%)	15,15,17	1.50	3 (20%)
2	MAN	N	5	2	11,11,12	0.94	0	15,15,17	1.03	2 (13%)
2	MAN	N	6	2	11,11,12	1.23	1 (9%)	15,15,17	1.73	3 (20%)
3	NAG	O	1	3,1	14,14,15	0.33	0	17,19,21	0.45	0
3	NAG	O	2	3	14,14,15	0.26	0	17,19,21	0.63	1 (5%)
3	NAG	P	1	3,1	14,14,15	0.22	0	17,19,21	0.58	0
3	NAG	P	2	3	14,14,15	0.51	0	17,19,21	0.54	0
3	NAG	Q	1	3,1	14,14,15	0.52	0	17,19,21	0.50	0
3	NAG	Q	2	3	14,14,15	0.26	0	17,19,21	0.51	0
3	NAG	R	1	3,1	14,14,15	0.32	0	17,19,21	0.46	0
3	NAG	R	2	3	14,14,15	0.27	0	17,19,21	0.64	1 (5%)

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	2,1	-	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	-	2/2/19/22	1/1/1/1
2	MAN	D	4	2	-	2/2/19/22	0/1/1/1
2	MAN	D	5	2	-	2/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	D	6	2	-	1/2/19/22	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	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	NAG	G	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	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	-	2/2/19/22	0/1/1/1
2	MAN	I	5	2	-	1/2/19/22	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	-	0/6/23/26	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	-	2/6/23/26	0/1/1/1
3	NAG	M	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	M	2	3	-	0/6/23/26	0/1/1/1
2	NAG	N	1	2,1	-	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	-	2/2/19/22	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	-	0/2/19/22	0/1/1/1
3	NAG	O	1	3,1	-	0/6/23/26	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	-	1/6/23/26	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

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

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	O5-C5	3.81	1.51	1.43
2	I	3	MAN	C2-C3	3.38	1.57	1.52
2	N	6	MAN	C1-C2	3.10	1.59	1.52
2	I	6	MAN	C1-C2	3.02	1.59	1.52
2	D	3	MAN	C2-C3	2.77	1.56	1.52
2	I	3	MAN	C1-C2	2.61	1.58	1.52
2	I	3	MAN	O5-C5	2.53	1.48	1.43
2	D	5	MAN	C2-C3	2.42	1.56	1.52
2	D	3	MAN	C1-C2	2.24	1.57	1.52
2	D	3	MAN	O5-C1	2.23	1.47	1.43
2	D	3	MAN	C4-C3	2.16	1.57	1.52
2	N	3	MAN	C1-C2	2.14	1.57	1.52
2	N	4	MAN	O5-C5	2.11	1.47	1.43

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	3	MAN	C1-O5-C5	5.43	119.55	112.19
2	N	6	MAN	C1-O5-C5	4.92	118.86	112.19
2	D	3	MAN	C1-O5-C5	3.96	117.55	112.19
2	I	4	MAN	C1-O5-C5	3.91	117.48	112.19
2	N	4	MAN	C1-O5-C5	3.89	117.47	112.19
3	G	1	NAG	C1-O5-C5	3.30	116.66	112.19
2	I	5	MAN	C1-O5-C5	3.28	116.64	112.19
2	D	4	MAN	C1-O5-C5	2.91	116.14	112.19
2	I	6	MAN	C1-O5-C5	2.83	116.03	112.19
2	D	6	MAN	C1-O5-C5	2.81	116.00	112.19
2	N	3	MAN	O2-C2-C3	-2.72	104.69	110.14
2	D	6	MAN	O2-C2-C3	-2.59	104.96	110.14
2	N	3	MAN	C1-O5-C5	2.39	115.43	112.19
2	N	6	MAN	O2-C2-C3	-2.32	105.49	110.14
2	I	5	MAN	O2-C2-C3	-2.30	105.52	110.14
2	D	4	MAN	O2-C2-C3	-2.30	105.53	110.14
2	I	4	MAN	O2-C2-C3	-2.28	105.57	110.14
2	N	5	MAN	O2-C2-C3	-2.25	105.63	110.14
3	R	2	NAG	C1-O5-C5	2.24	115.23	112.19
2	D	5	MAN	C1-C2-C3	2.18	112.35	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	4	MAN	C3-C4-C5	-2.12	106.45	110.24
2	N	6	MAN	O5-C1-C2	2.12	114.05	110.77
2	N	4	MAN	O3-C3-C2	2.11	114.04	109.99
3	O	2	NAG	C1-O5-C5	2.10	115.03	112.19
2	N	5	MAN	C1-O5-C5	2.08	115.01	112.19
2	N	3	MAN	C1-C2-C3	2.04	112.18	109.67

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	Q	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
3	H	2	NAG	C4-C5-C6-O6
2	D	4	MAN	O5-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	N	3	MAN	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	L	2	NAG	O5-C5-C6-O6
3	R	2	NAG	O5-C5-C6-O6
2	N	4	MAN	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
2	I	4	MAN	O5-C5-C6-O6
3	H	1	NAG	O5-C5-C6-O6
2	D	4	MAN	C4-C5-C6-O6
3	Q	2	NAG	C4-C5-C6-O6
3	P	1	NAG	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	L	2	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	I	6	MAN	O5-C5-C6-O6
3	L	1	NAG	O5-C5-C6-O6
2	I	4	MAN	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	H	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	N	3	MAN	O5-C5-C6-O6
2	I	6	MAN	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
2	D	3	MAN	O5-C5-C6-O6
3	R	2	NAG	C4-C5-C6-O6
3	H	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
2	D	5	MAN	C4-C5-C6-O6
2	D	6	MAN	O5-C5-C6-O6
3	G	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	D	5	MAN	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	N	4	MAN	C4-C5-C6-O6
3	R	1	NAG	O5-C5-C6-O6
3	P	1	NAG	C4-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
3	M	1	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	I	3	MAN	C4-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	I	3	MAN	O5-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
2	I	5	MAN	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	J	1	NAG	O5-C5-C6-O6
3	R	1	NAG	C4-C5-C6-O6

All (2) ring outliers are listed below:

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

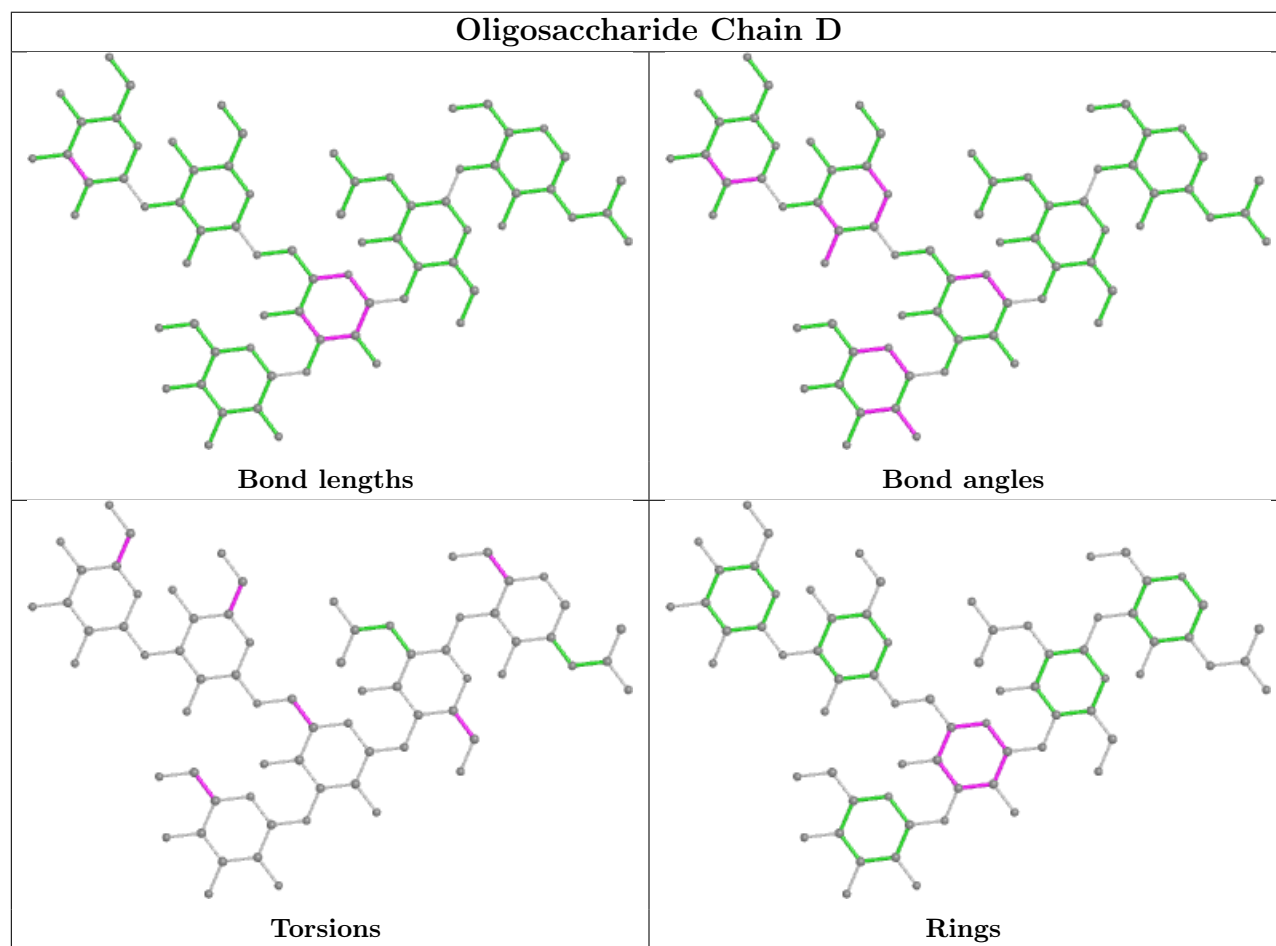
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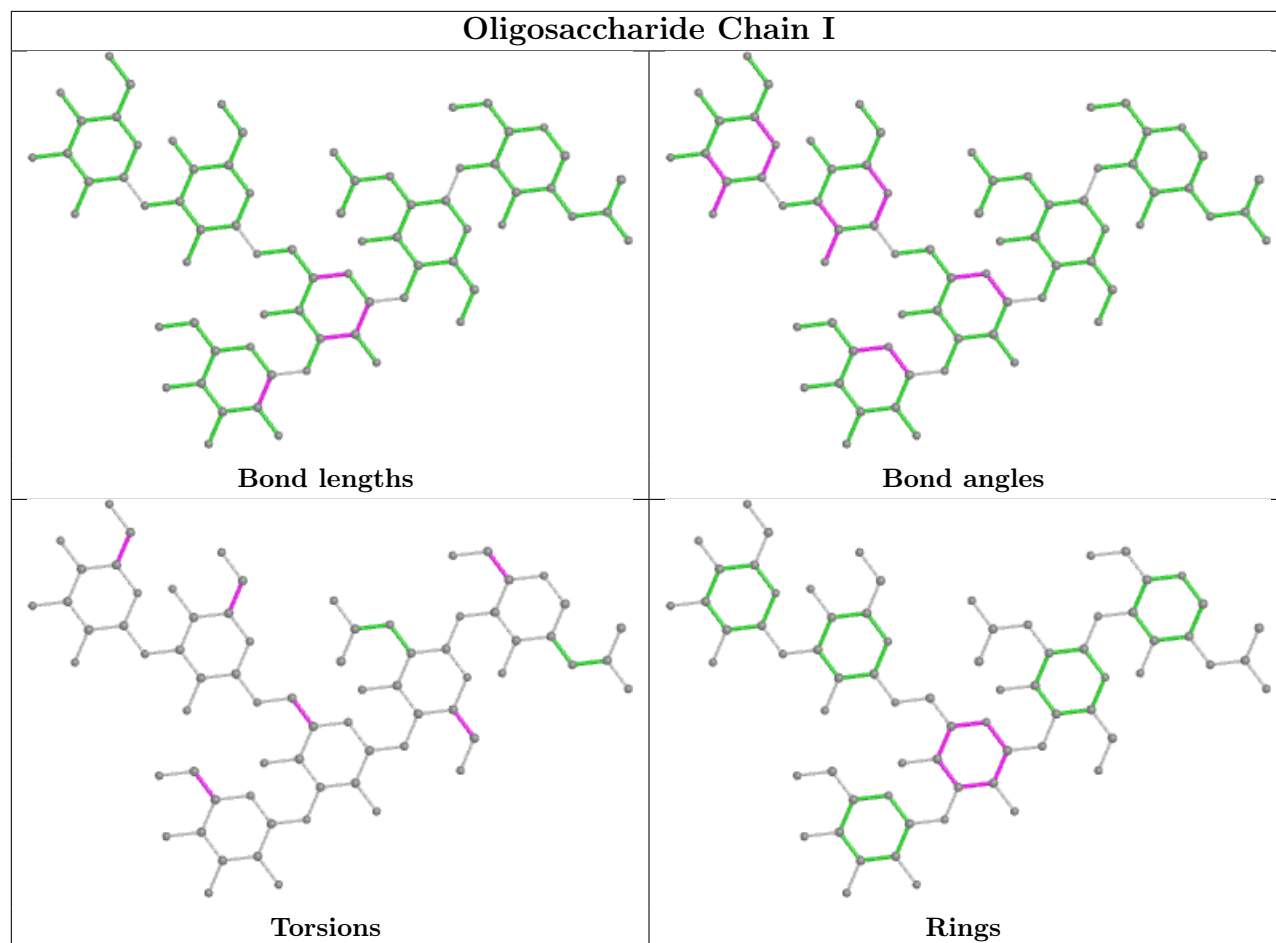
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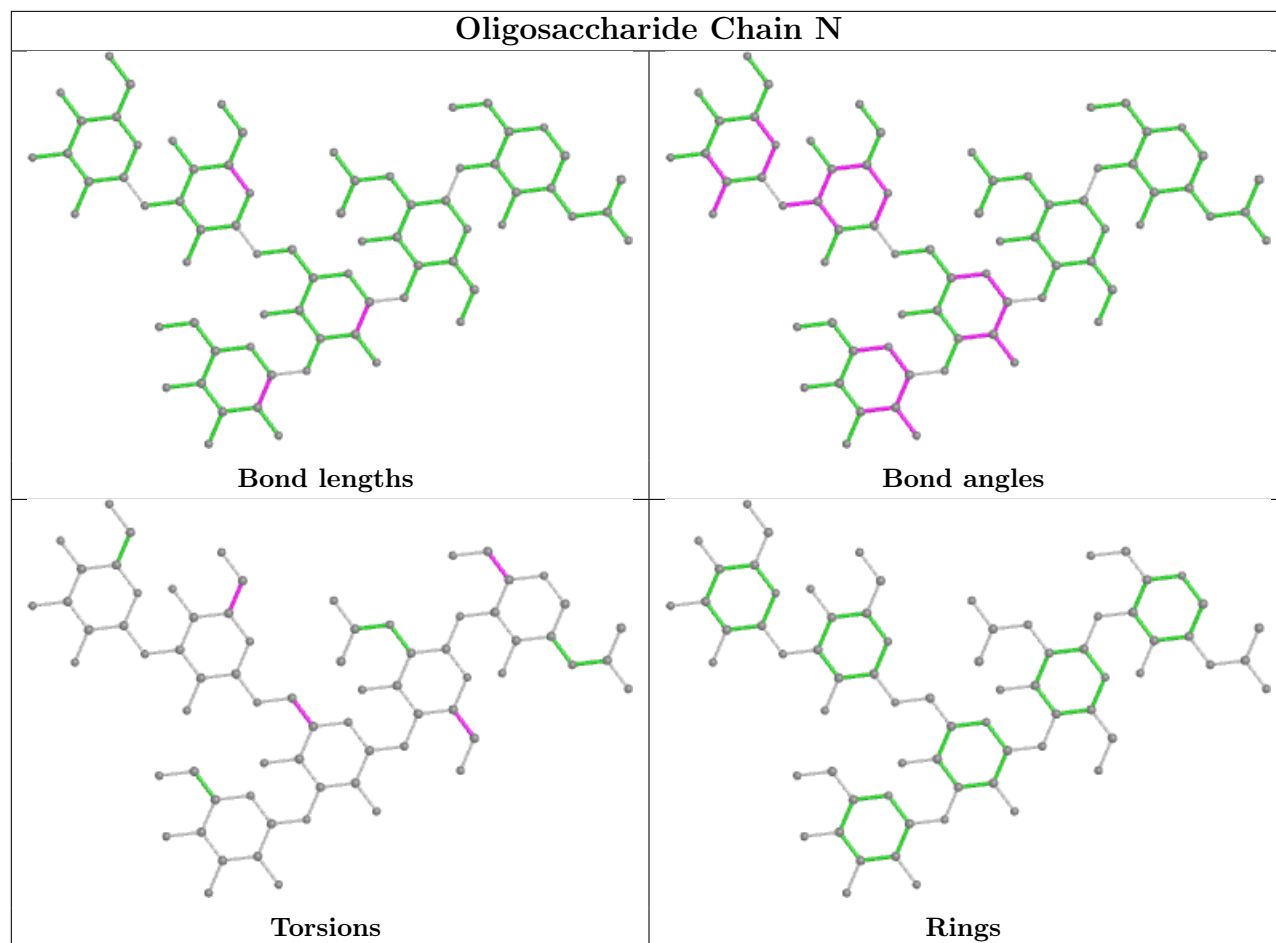
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5

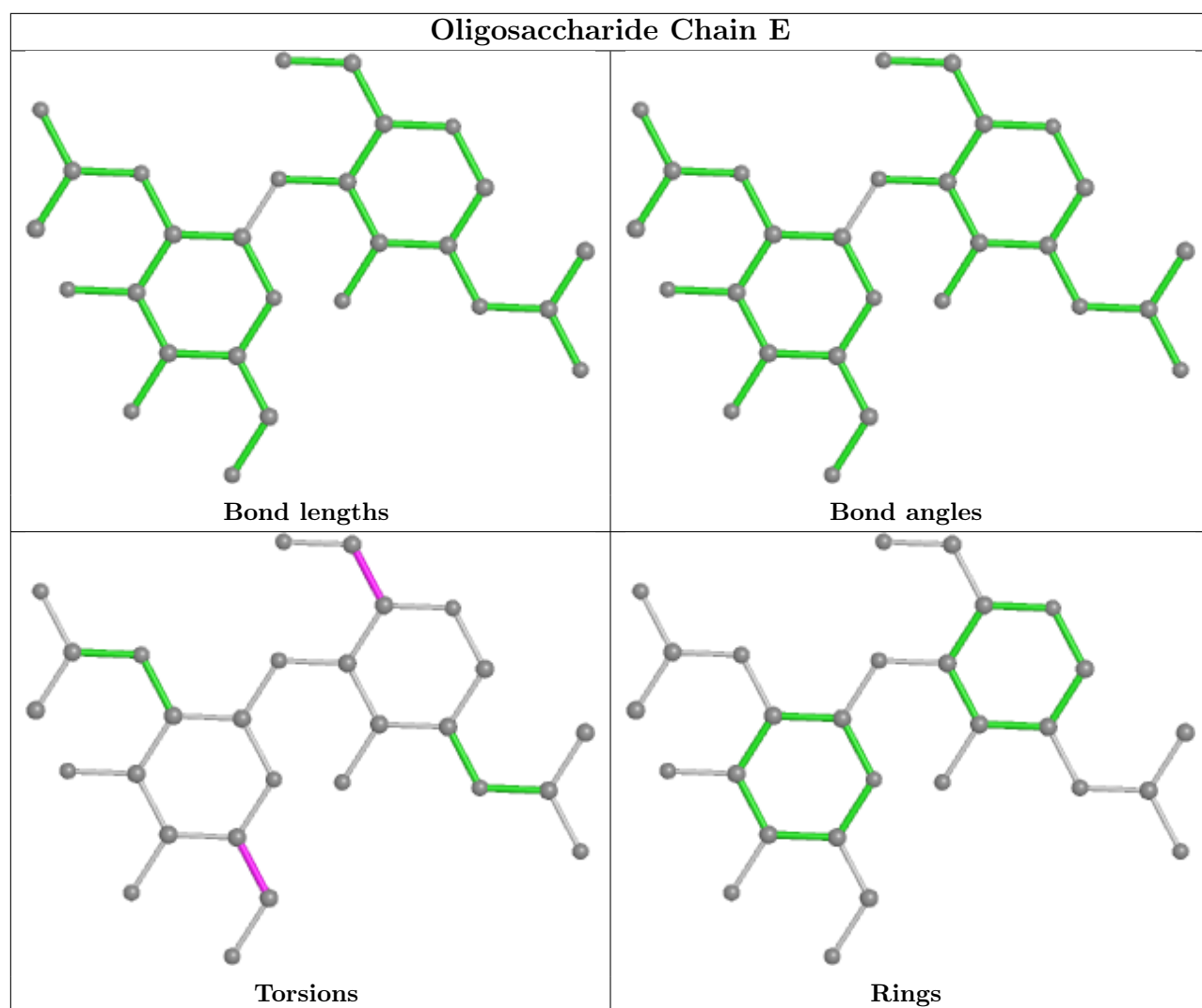
No monomer is involved in short contacts.

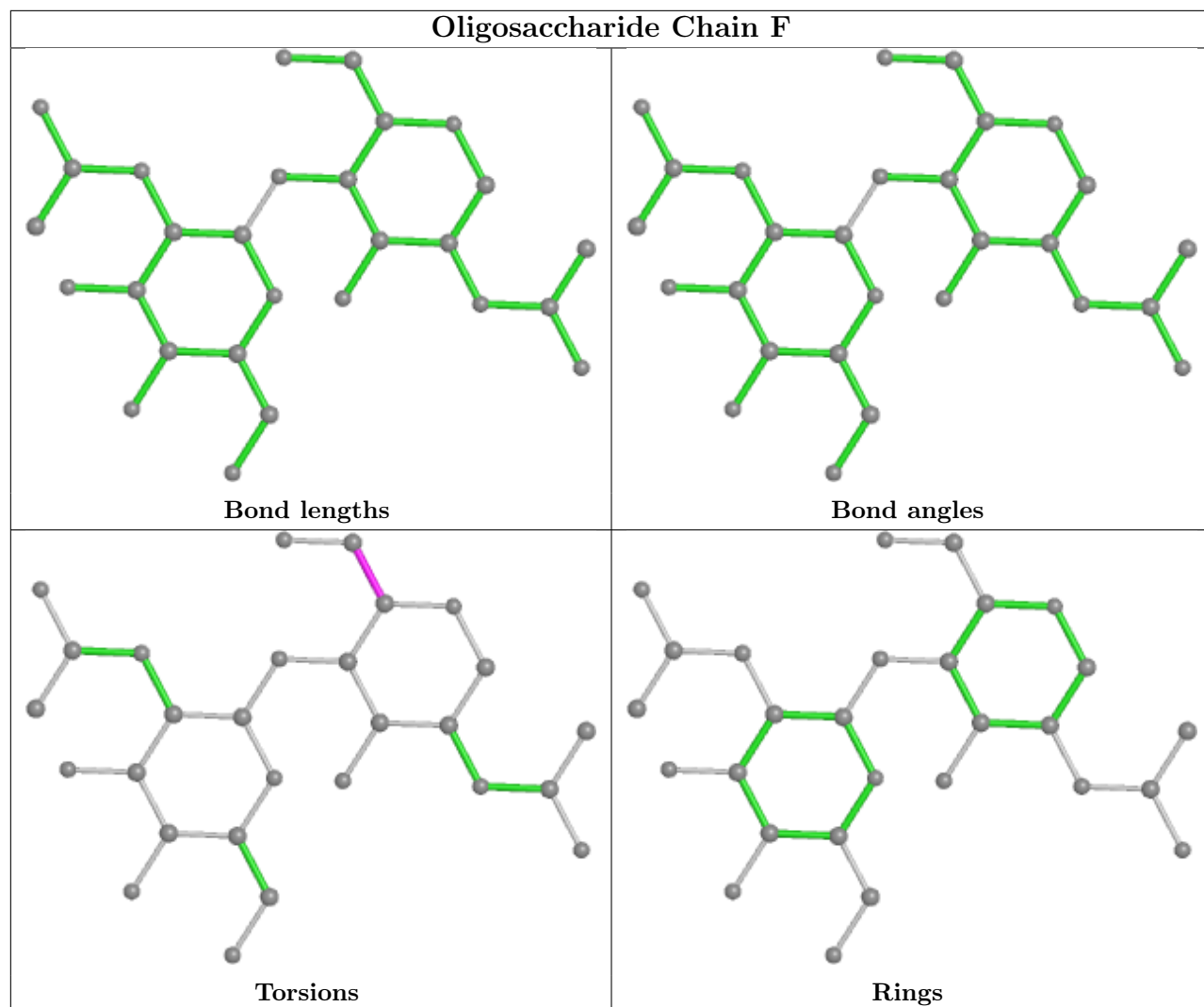
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

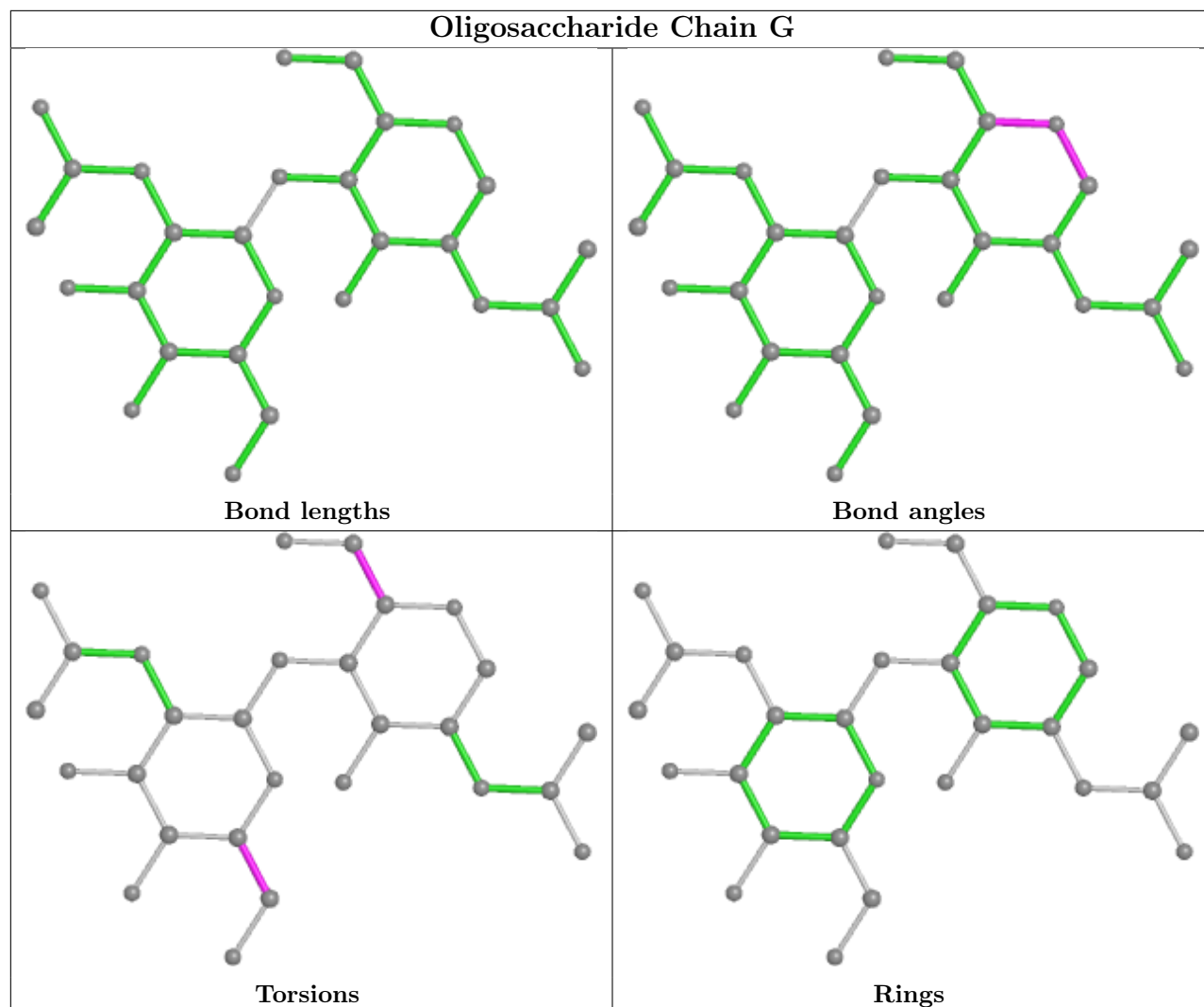


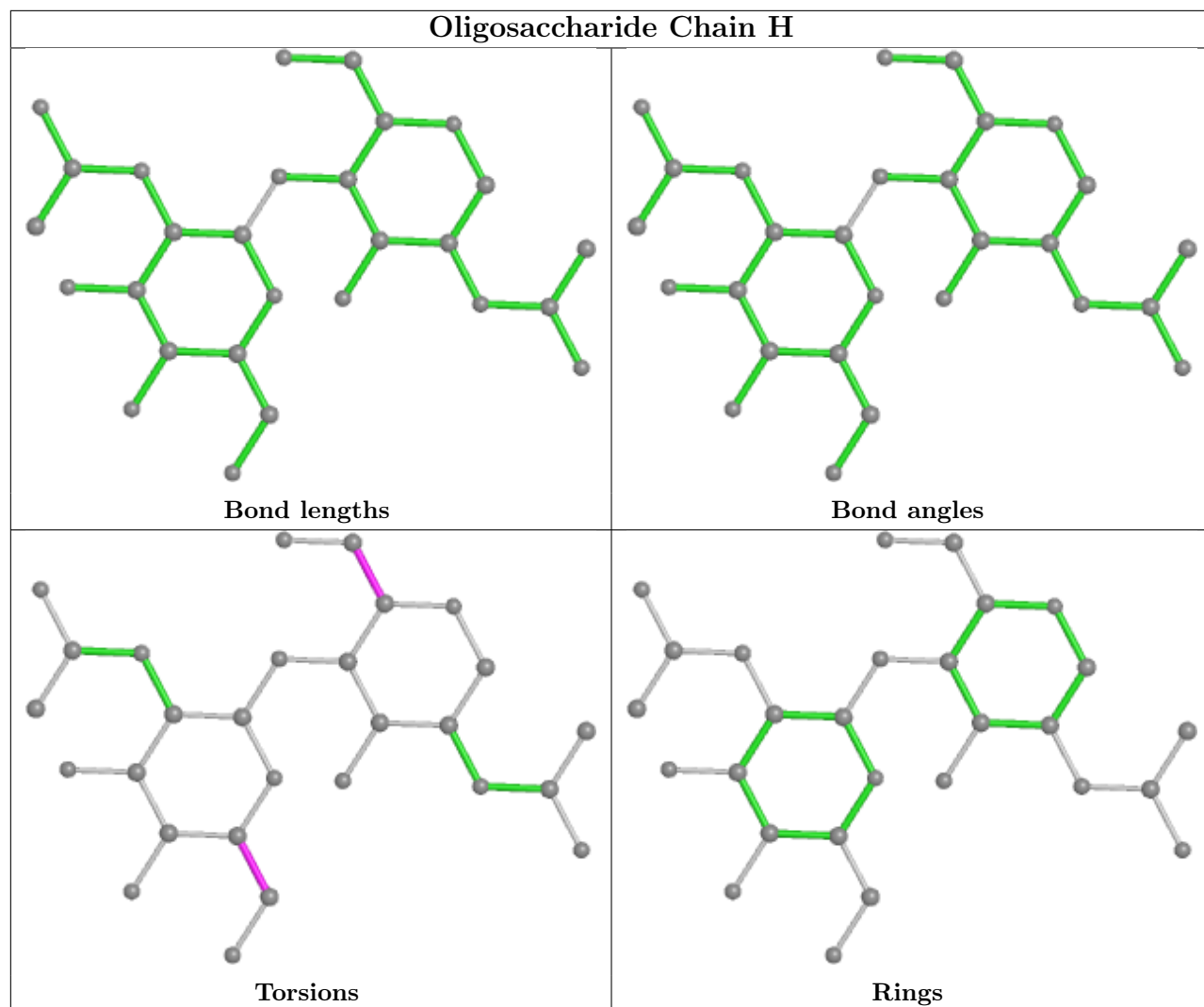


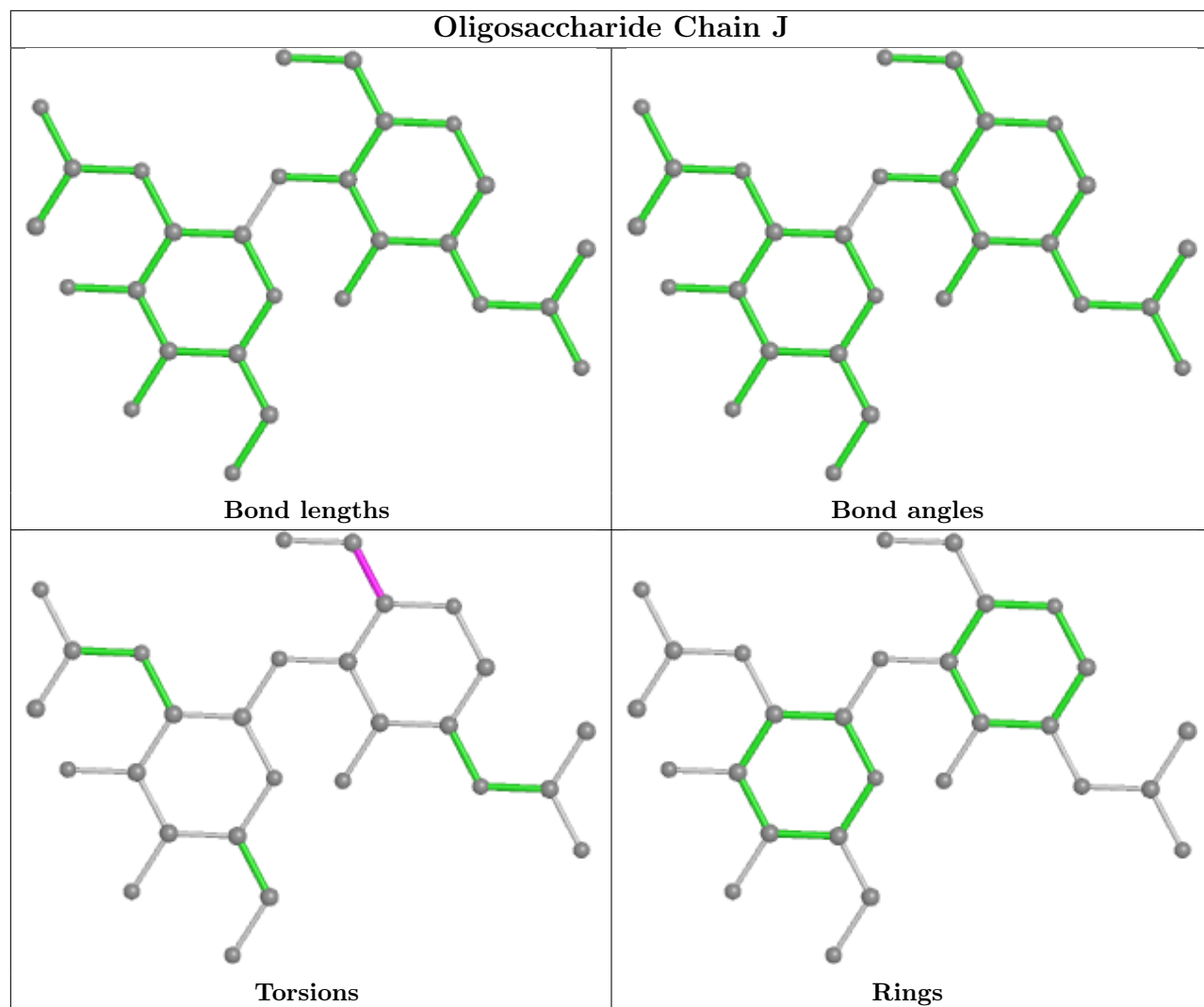


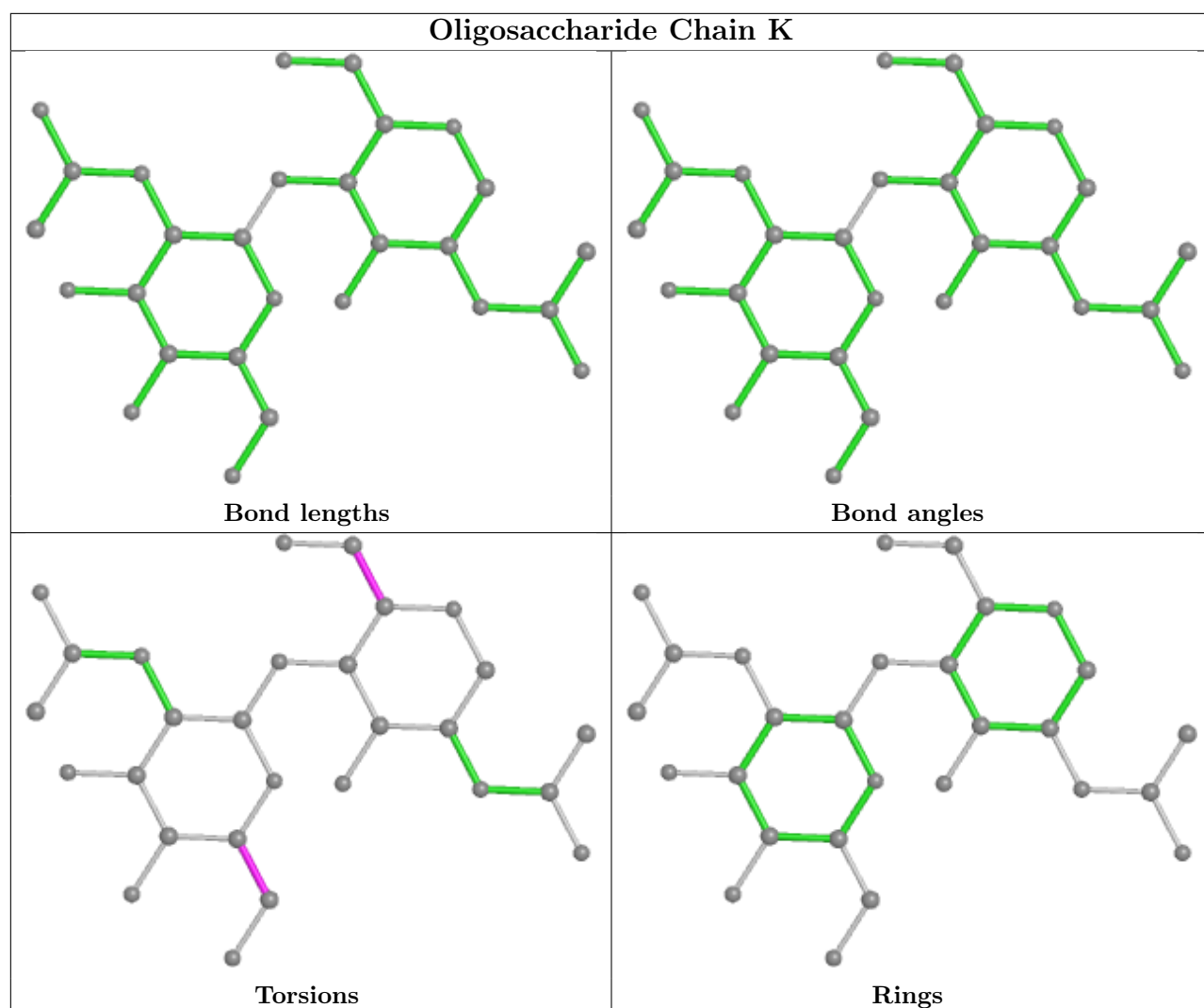


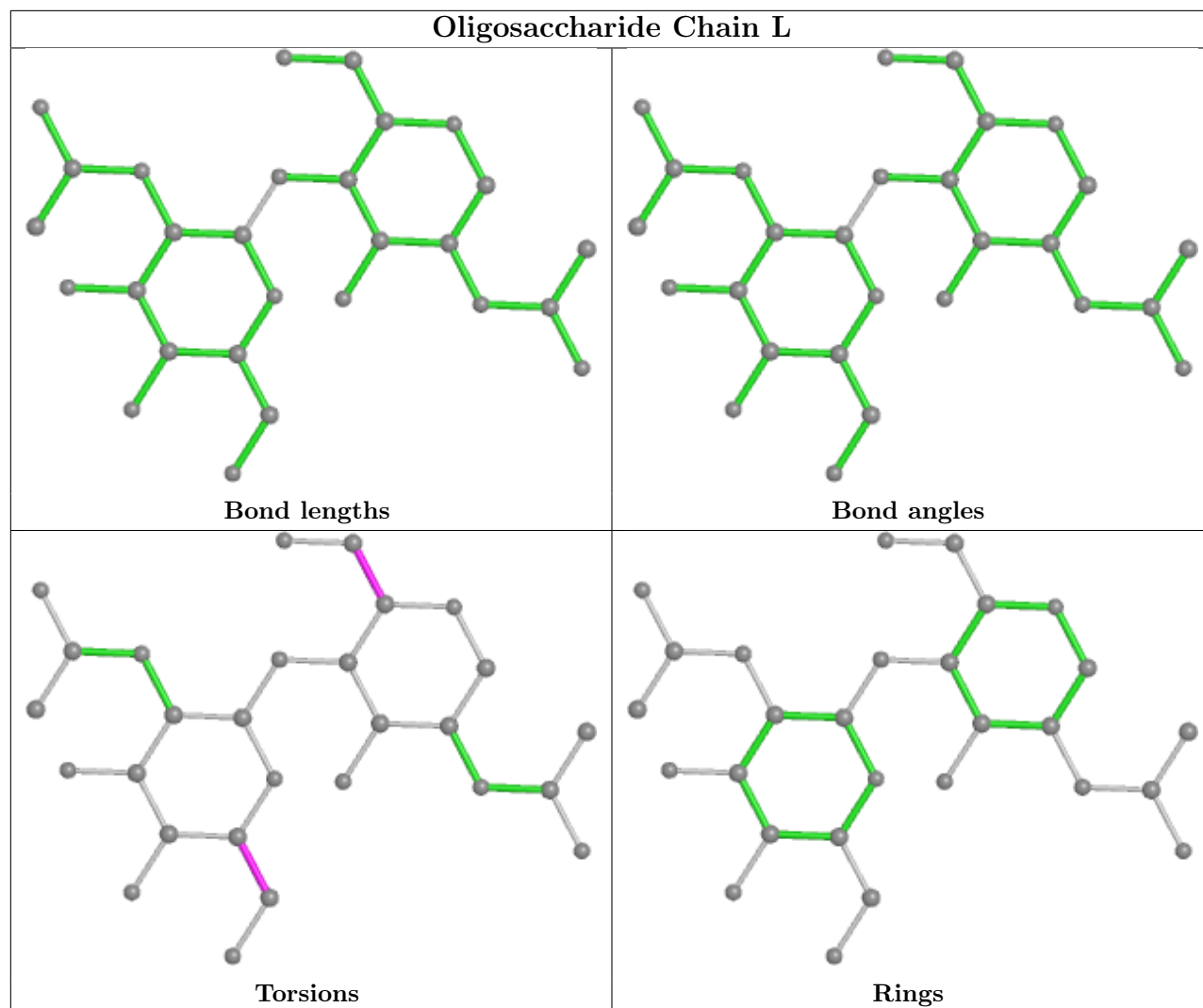


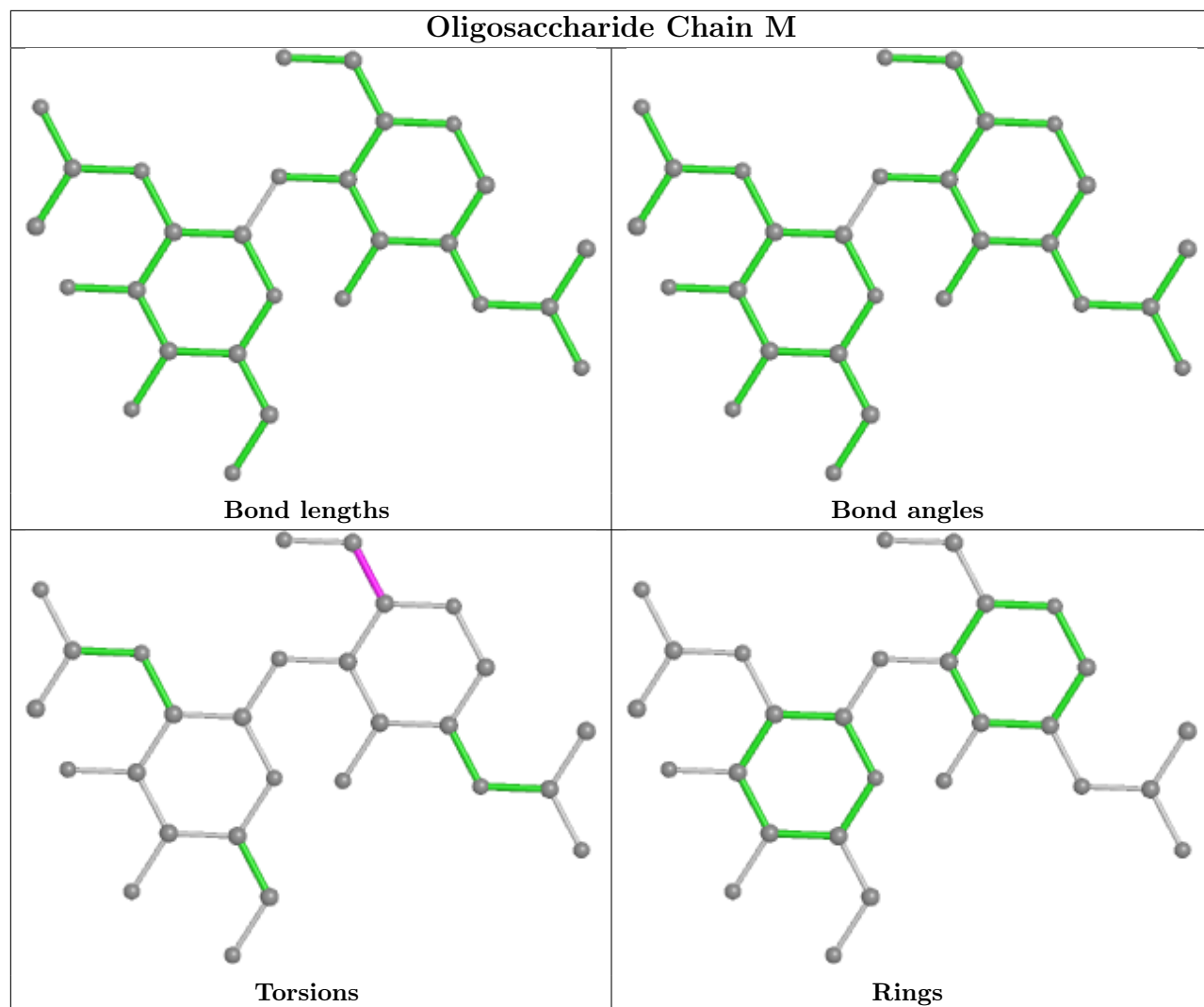


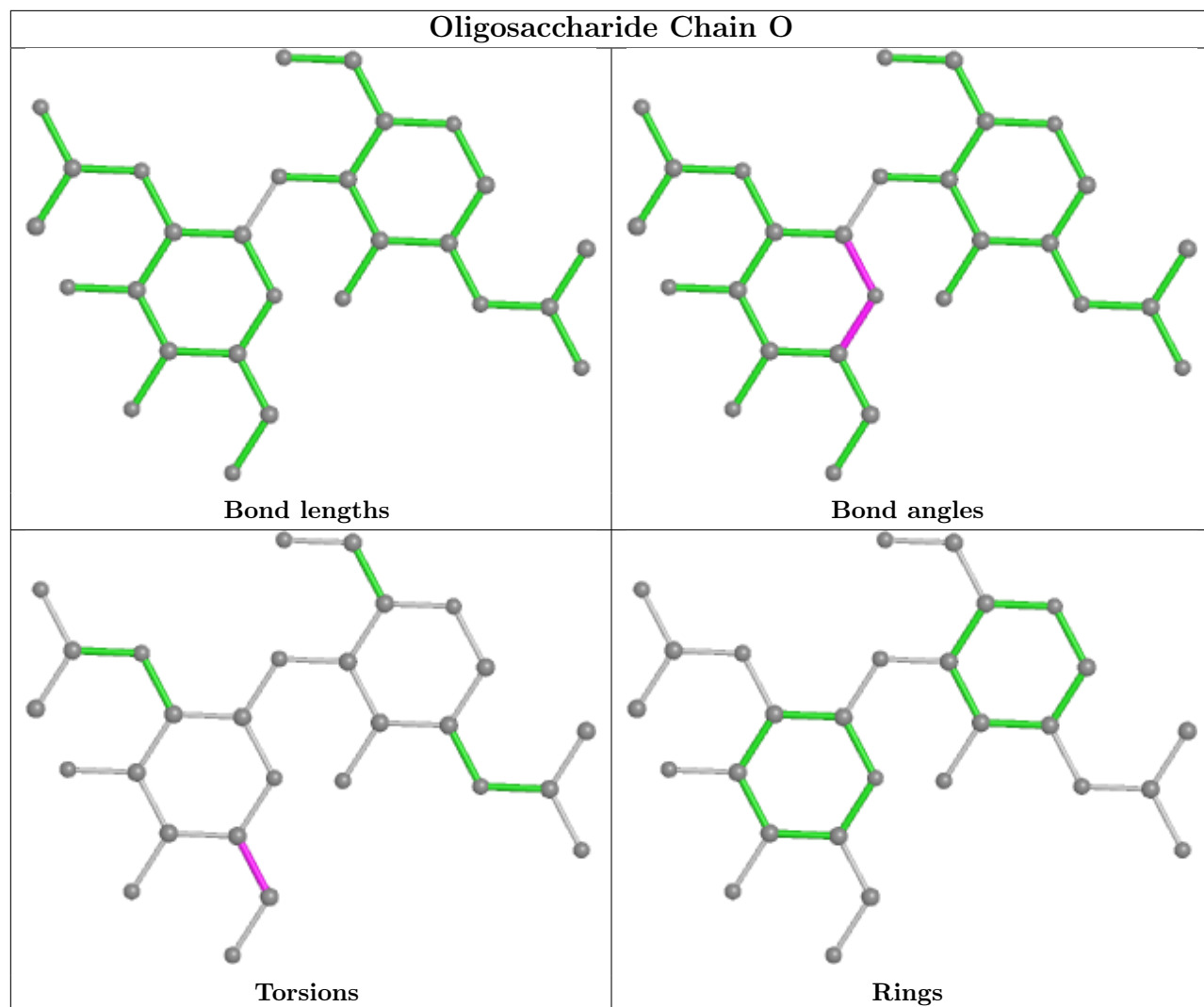


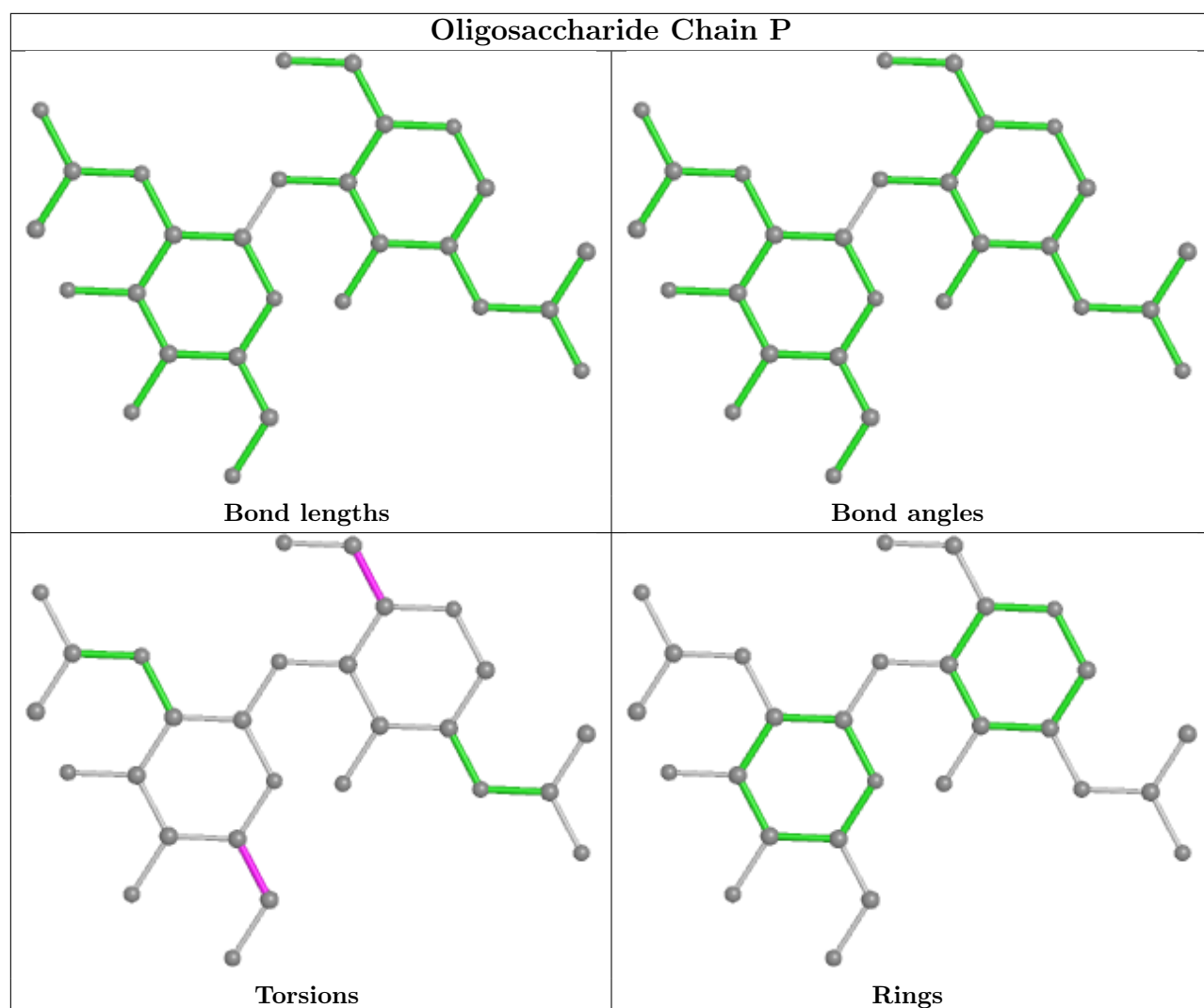


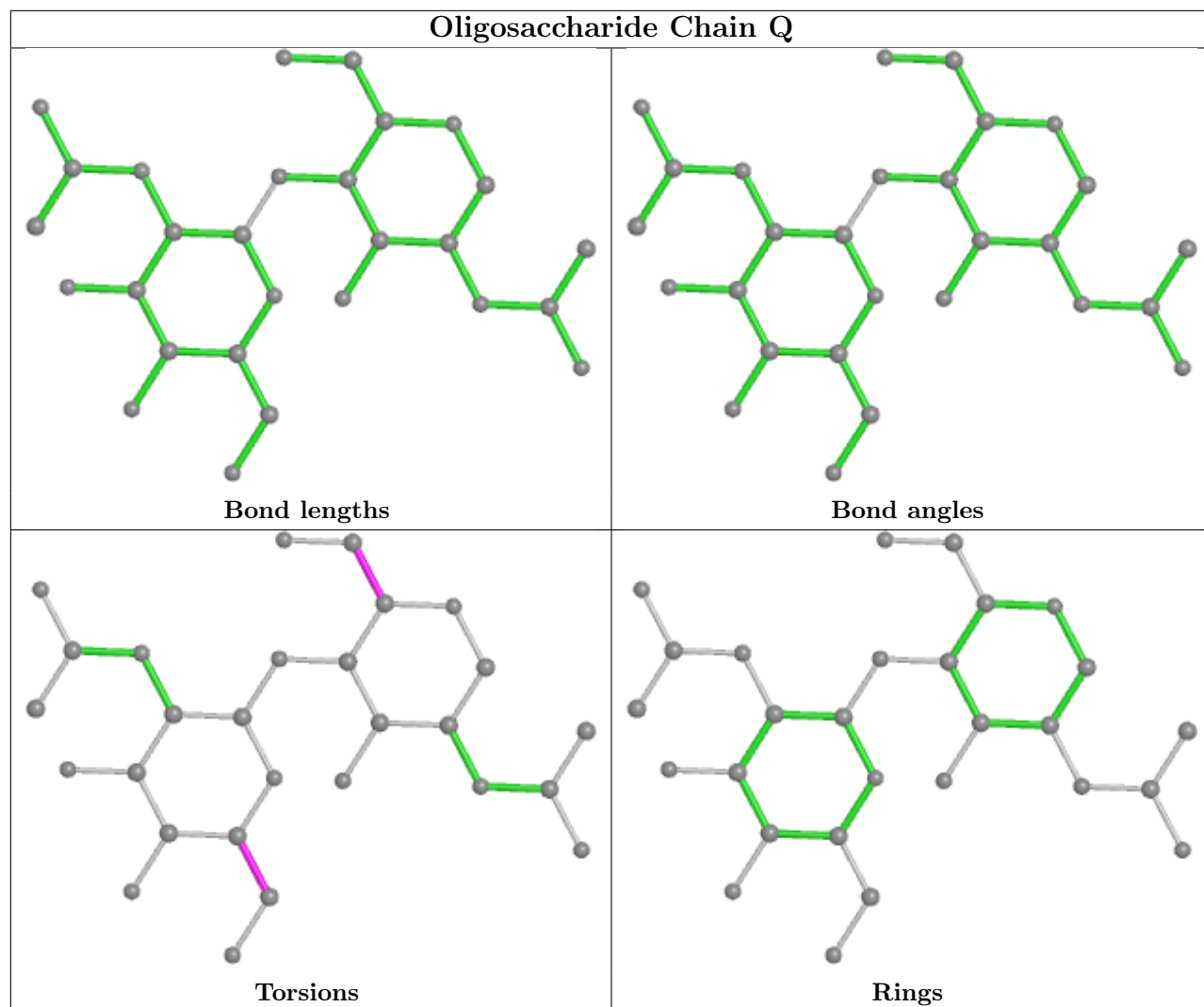


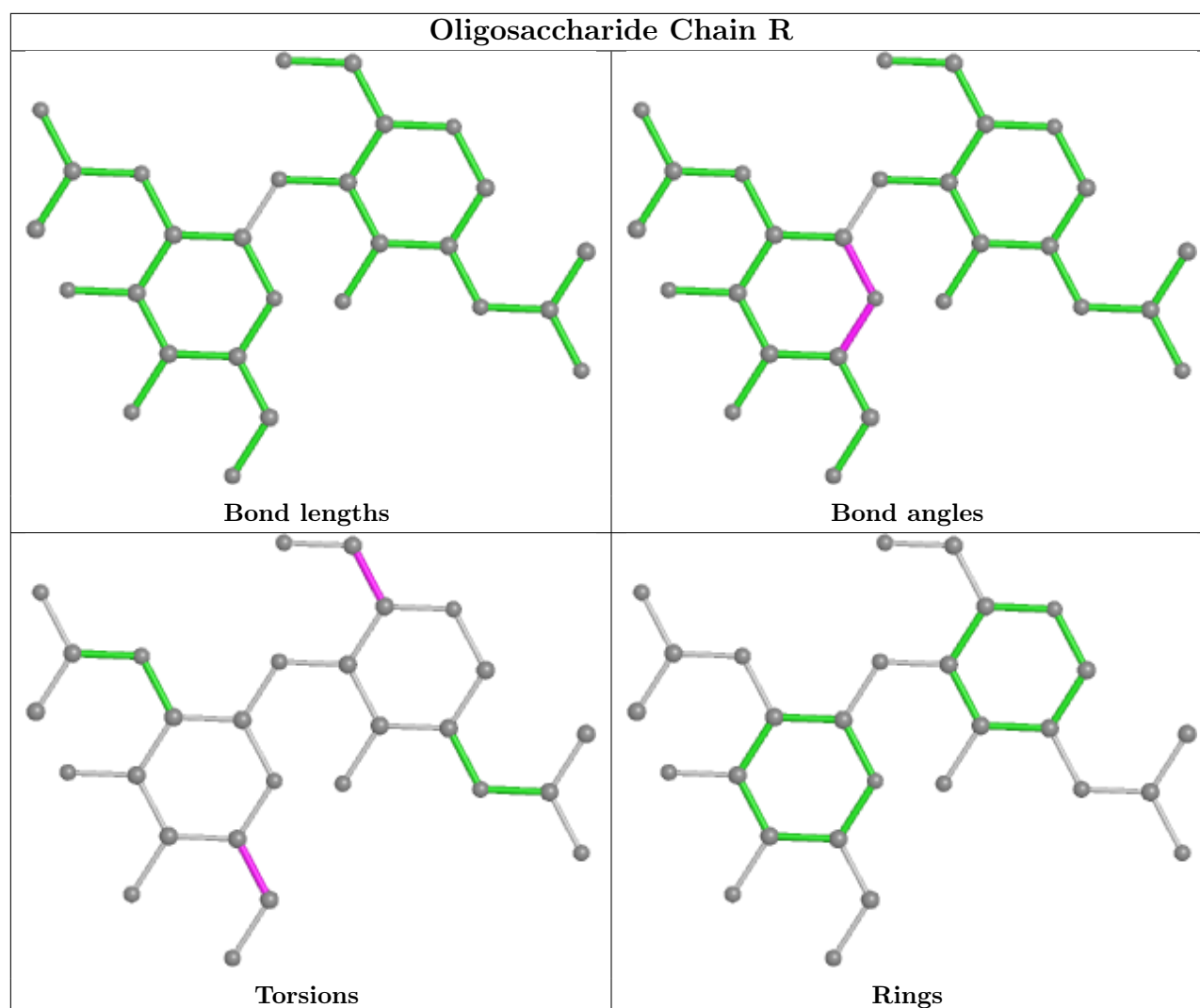












5.6 Ligand geometry [i](#)

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	2001	1	14,14,15	0.22	0	17,19,21	0.49	0
4	NAG	A	2012	1	14,14,15	0.29	0	17,19,21	0.83	1 (5%)
4	NAG	A	2008	1	14,14,15	0.43	0	17,19,21	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2005	1	14,14,15	0.36	0	17,19,21	0.52	0
4	NAG	C	2014	1	14,14,15	0.48	0	17,19,21	0.59	0
4	NAG	C	2010	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	A	2004	1	14,14,15	0.53	0	17,19,21	0.66	1 (5%)
4	NAG	B	2013	1	14,14,15	0.29	0	17,19,21	0.42	0
4	NAG	A	2007	1	14,14,15	0.41	0	17,19,21	0.54	0
4	NAG	C	2016	1	14,14,15	0.53	0	17,19,21	0.64	1 (5%)
4	NAG	B	2005	1	14,14,15	0.42	0	17,19,21	0.63	1 (5%)
4	NAG	C	2008	1	14,14,15	0.54	0	17,19,21	0.57	0
4	NAG	C	2015	1	14,14,15	0.48	0	17,19,21	0.69	1 (5%)
4	NAG	A	2014	1	14,14,15	0.52	0	17,19,21	0.53	0
4	NAG	B	2006	1	14,14,15	0.34	0	17,19,21	0.44	0
4	NAG	C	2006	1	14,14,15	0.35	0	17,19,21	0.44	0
4	NAG	A	2010	1	14,14,15	0.52	0	17,19,21	0.42	0
4	NAG	A	2005	1	14,14,15	0.24	0	17,19,21	0.59	1 (5%)
4	NAG	A	2015	1	14,14,15	0.20	0	17,19,21	0.62	1 (5%)
4	NAG	B	2004	1	14,14,15	0.33	0	17,19,21	0.52	0
4	NAG	A	2002	1	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
4	NAG	B	2008	1	14,14,15	0.57	0	17,19,21	0.60	1 (5%)
4	NAG	B	2014	1	14,14,15	0.54	0	17,19,21	0.56	0
4	NAG	A	2003	1	14,14,15	0.23	0	17,19,21	0.34	0
4	NAG	B	2016	1	14,14,15	0.25	0	17,19,21	0.68	1 (5%)
4	NAG	A	2009	1	14,14,15	0.44	0	17,19,21	0.63	1 (5%)
4	NAG	C	2011	1	14,14,15	0.23	0	17,19,21	0.74	1 (5%)
4	NAG	B	2002	1	14,14,15	0.33	0	17,19,21	0.50	0
4	NAG	A	2006	1	14,14,15	0.23	0	17,19,21	0.54	0
4	NAG	B	2007	1	14,14,15	0.39	0	17,19,21	0.48	0
4	NAG	B	2010	1	14,14,15	0.56	0	17,19,21	0.66	1 (5%)
4	NAG	B	2009	1	14,14,15	0.30	0	17,19,21	0.49	0
4	NAG	B	2011	1	14,14,15	0.39	0	17,19,21	0.64	1 (5%)
4	NAG	C	2002	1	14,14,15	0.24	0	17,19,21	0.43	0
4	NAG	C	2009	1	14,14,15	0.32	0	17,19,21	0.45	0
4	NAG	A	2017	1	14,14,15	0.26	0	17,19,21	0.64	0
4	NAG	B	2003	1	14,14,15	0.31	0	17,19,21	0.44	0
4	NAG	B	2015	1	14,14,15	0.28	0	17,19,21	0.63	1 (5%)
4	NAG	C	2007	1	14,14,15	0.54	0	17,19,21	0.60	0
4	NAG	C	2003	1	14,14,15	0.31	0	17,19,21	0.41	0
4	NAG	B	2012	1	14,14,15	0.33	0	17,19,21	0.59	0
4	NAG	C	2012	1	14,14,15	0.28	0	17,19,21	0.62	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	2013	1	14,14,15	0.28	0	17,19,21	0.49	0
4	NAG	C	2017	1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
4	NAG	A	2001	1	14,14,15	0.45	0	17,19,21	0.69	1 (5%)
4	NAG	B	2001	1	14,14,15	0.44	0	17,19,21	0.48	0
4	NAG	B	2017	1	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	A	2011	1	14,14,15	0.34	0	17,19,21	0.53	0
4	NAG	A	2013	1	14,14,15	0.33	0	17,19,21	0.40	0
4	NAG	A	2016	1	14,14,15	0.48	0	17,19,21	0.80	1 (5%)
4	NAG	C	2004	1	14,14,15	0.20	0	17,19,21	0.62	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	2001	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	2008	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2005	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	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2007	1	-	1/6/23/26	0/1/1/1
4	NAG	C	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2008	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2015	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	2006	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	2010	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2015	1	-	0/6/23/26	0/1/1/1
4	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2008	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2009	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2011	1	-	1/6/23/26	0/1/1/1
4	NAG	B	2002	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2007	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2009	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	2002	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2015	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	2003	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2012	1	-	0/6/23/26	0/1/1/1
4	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2017	1	-	0/6/23/26	0/1/1/1
4	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
4	NAG	B	2017	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2011	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2013	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2016	1	-	2/6/23/26	0/1/1/1
4	NAG	C	2004	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2012	NAG	C1-O5-C5	2.97	116.21	112.19
4	A	2016	NAG	C1-O5-C5	2.77	115.95	112.19
4	C	2017	NAG	C1-O5-C5	2.50	115.58	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2001	NAG	C1-O5-C5	2.45	115.51	112.19
4	C	2011	NAG	C1-O5-C5	2.44	115.50	112.19
4	B	2010	NAG	C1-O5-C5	2.42	115.47	112.19
4	B	2016	NAG	C1-O5-C5	2.40	115.44	112.19
4	C	2015	NAG	C1-O5-C5	2.35	115.38	112.19
4	A	2002	NAG	C1-O5-C5	2.30	115.30	112.19
4	A	2004	NAG	C1-O5-C5	2.22	115.20	112.19
4	B	2015	NAG	C1-O5-C5	2.21	115.18	112.19
4	B	2005	NAG	C1-O5-C5	2.17	115.14	112.19
4	B	2011	NAG	C1-O5-C5	2.17	115.13	112.19
4	C	2012	NAG	C1-O5-C5	2.10	115.03	112.19
4	A	2009	NAG	C1-O5-C5	2.07	115.00	112.19
4	A	2005	NAG	C1-O5-C5	2.06	114.99	112.19
4	C	2016	NAG	C1-O5-C5	2.03	114.94	112.19
4	B	2008	NAG	C1-O5-C5	2.03	114.94	112.19
4	A	2015	NAG	C1-O5-C5	2.01	114.92	112.19

There are no chirality outliers.

All (81) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	2002	NAG	C4-C5-C6-O6
4	B	2003	NAG	C4-C5-C6-O6
4	C	2003	NAG	C4-C5-C6-O6
4	B	2004	NAG	O5-C5-C6-O6
4	C	2014	NAG	O5-C5-C6-O6
4	C	2001	NAG	O5-C5-C6-O6
4	B	2003	NAG	O5-C5-C6-O6
4	B	2002	NAG	O5-C5-C6-O6
4	C	2016	NAG	O5-C5-C6-O6
4	C	2015	NAG	C4-C5-C6-O6
4	A	2008	NAG	C4-C5-C6-O6
4	B	2006	NAG	O5-C5-C6-O6
4	B	2009	NAG	O5-C5-C6-O6
4	B	2012	NAG	O5-C5-C6-O6
4	A	2002	NAG	O5-C5-C6-O6
4	A	2011	NAG	O5-C5-C6-O6
4	B	2011	NAG	O5-C5-C6-O6
4	C	2003	NAG	O5-C5-C6-O6
4	A	2003	NAG	O5-C5-C6-O6
4	C	2004	NAG	O5-C5-C6-O6
4	C	2005	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	2014	NAG	O5-C5-C6-O6
4	C	2010	NAG	O5-C5-C6-O6
4	B	2004	NAG	C4-C5-C6-O6
4	B	2014	NAG	O5-C5-C6-O6
4	C	2009	NAG	O5-C5-C6-O6
4	C	2015	NAG	O5-C5-C6-O6
4	A	2002	NAG	C4-C5-C6-O6
4	C	2014	NAG	C4-C5-C6-O6
4	A	2001	NAG	O5-C5-C6-O6
4	C	2007	NAG	O5-C5-C6-O6
4	C	2001	NAG	C4-C5-C6-O6
4	B	2016	NAG	O5-C5-C6-O6
4	A	2005	NAG	C4-C5-C6-O6
4	B	2001	NAG	C4-C5-C6-O6
4	C	2005	NAG	C4-C5-C6-O6
4	A	2014	NAG	C4-C5-C6-O6
4	C	2007	NAG	C4-C5-C6-O6
4	C	2009	NAG	C4-C5-C6-O6
4	A	2006	NAG	O5-C5-C6-O6
4	B	2006	NAG	C4-C5-C6-O6
4	B	2009	NAG	C4-C5-C6-O6
4	B	2012	NAG	C4-C5-C6-O6
4	C	2004	NAG	C4-C5-C6-O6
4	C	2016	NAG	C4-C5-C6-O6
4	A	2006	NAG	C4-C5-C6-O6
4	B	2014	NAG	C4-C5-C6-O6
4	B	2007	NAG	O5-C5-C6-O6
4	B	2016	NAG	C4-C5-C6-O6
4	A	2001	NAG	C4-C5-C6-O6
4	A	2011	NAG	C4-C5-C6-O6
4	B	2011	NAG	C4-C5-C6-O6
4	B	2001	NAG	O5-C5-C6-O6
4	A	2008	NAG	O5-C5-C6-O6
4	A	2003	NAG	C4-C5-C6-O6
4	C	2013	NAG	C4-C5-C6-O6
4	A	2016	NAG	O5-C5-C6-O6
4	B	2015	NAG	O5-C5-C6-O6
4	B	2015	NAG	C4-C5-C6-O6
4	C	2006	NAG	O5-C5-C6-O6
4	A	2005	NAG	O5-C5-C6-O6
4	B	2017	NAG	O5-C5-C6-O6
4	C	2006	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	C	2010	NAG	C4-C5-C6-O6
4	C	2011	NAG	O5-C5-C6-O6
4	C	2013	NAG	O5-C5-C6-O6
4	A	2017	NAG	C4-C5-C6-O6
4	B	2013	NAG	O5-C5-C6-O6
4	A	2007	NAG	O5-C5-C6-O6
4	B	2010	NAG	C4-C5-C6-O6
4	A	2013	NAG	O5-C5-C6-O6
4	A	2017	NAG	O5-C5-C6-O6
4	B	2008	NAG	O5-C5-C6-O6
4	A	2016	NAG	C4-C5-C6-O6
4	B	2010	NAG	O5-C5-C6-O6
4	A	2010	NAG	C4-C5-C6-O6
4	A	2004	NAG	O5-C5-C6-O6
4	A	2004	NAG	C4-C5-C6-O6
4	B	2007	NAG	C4-C5-C6-O6
4	A	2012	NAG	C4-C5-C6-O6
4	A	2012	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

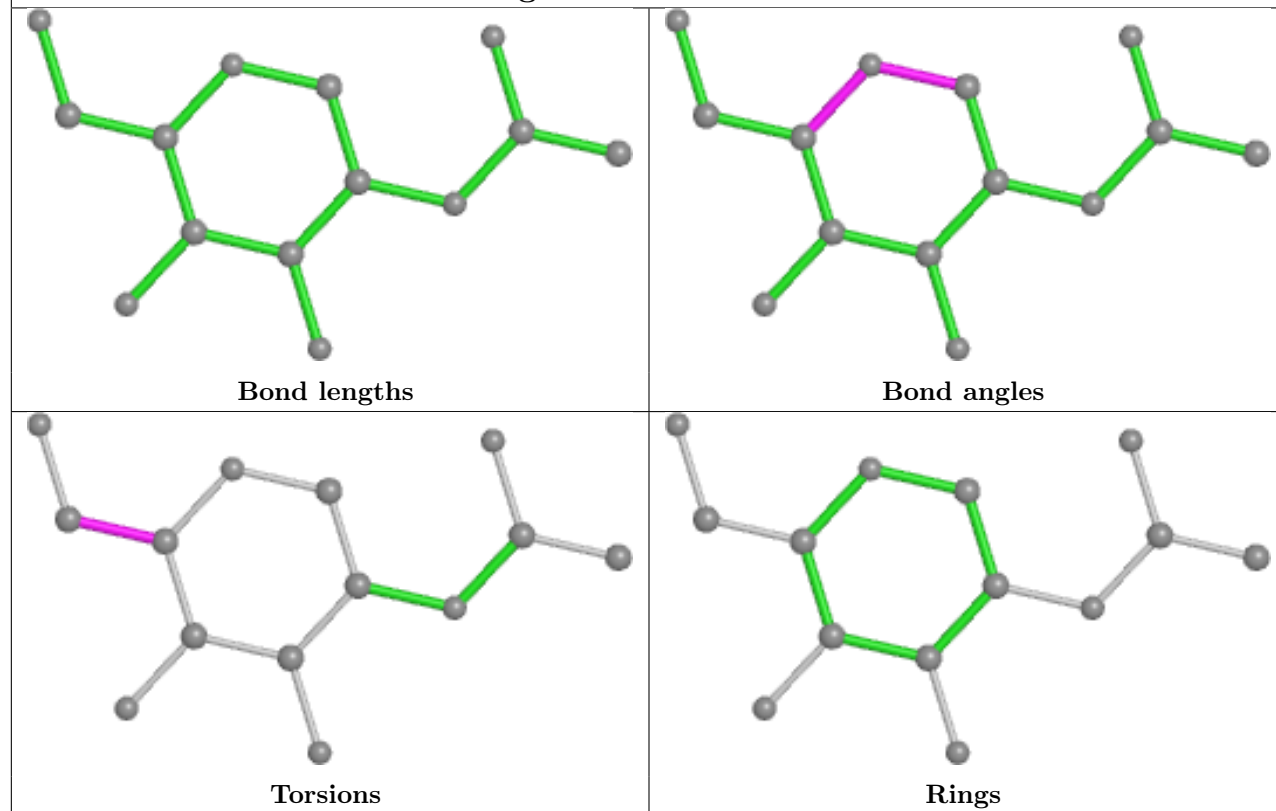
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	2011	NAG	1	0

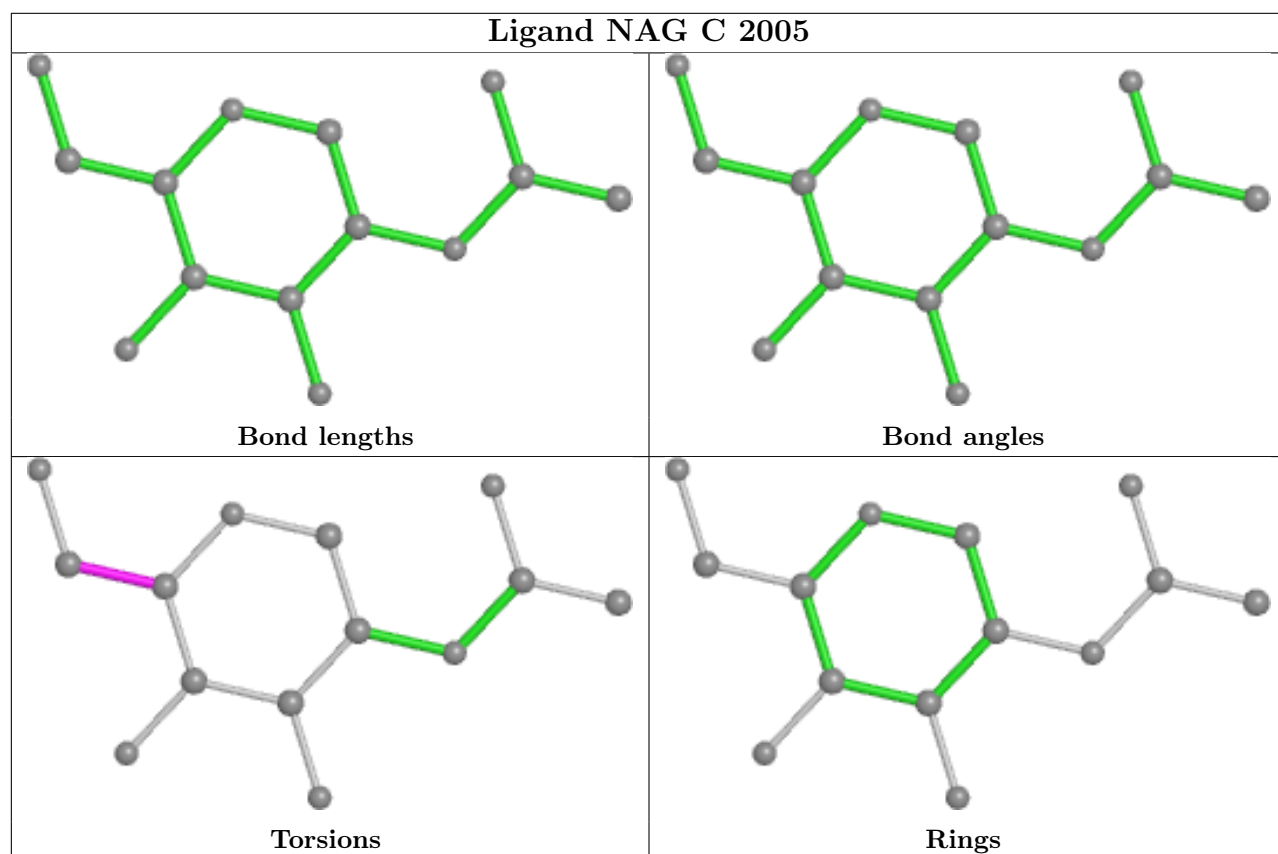
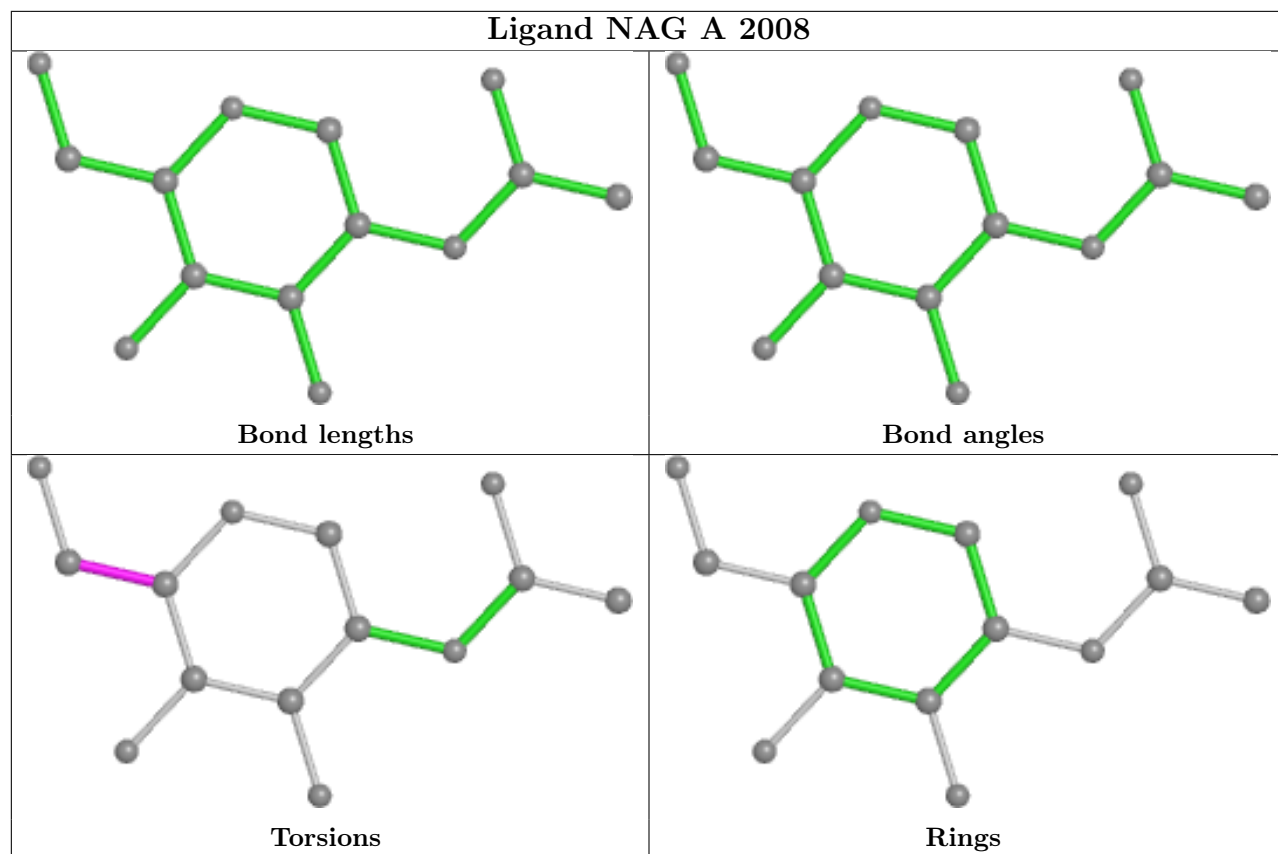
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

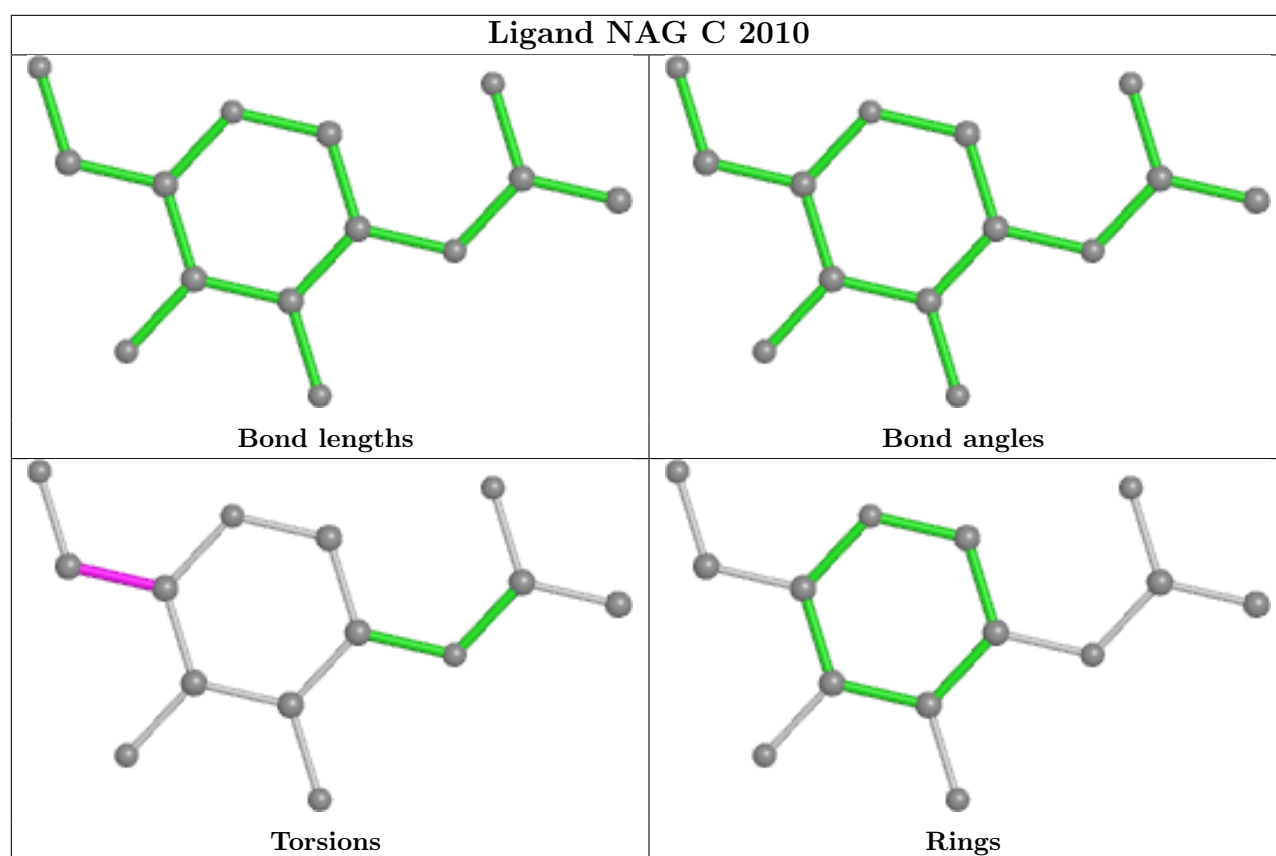
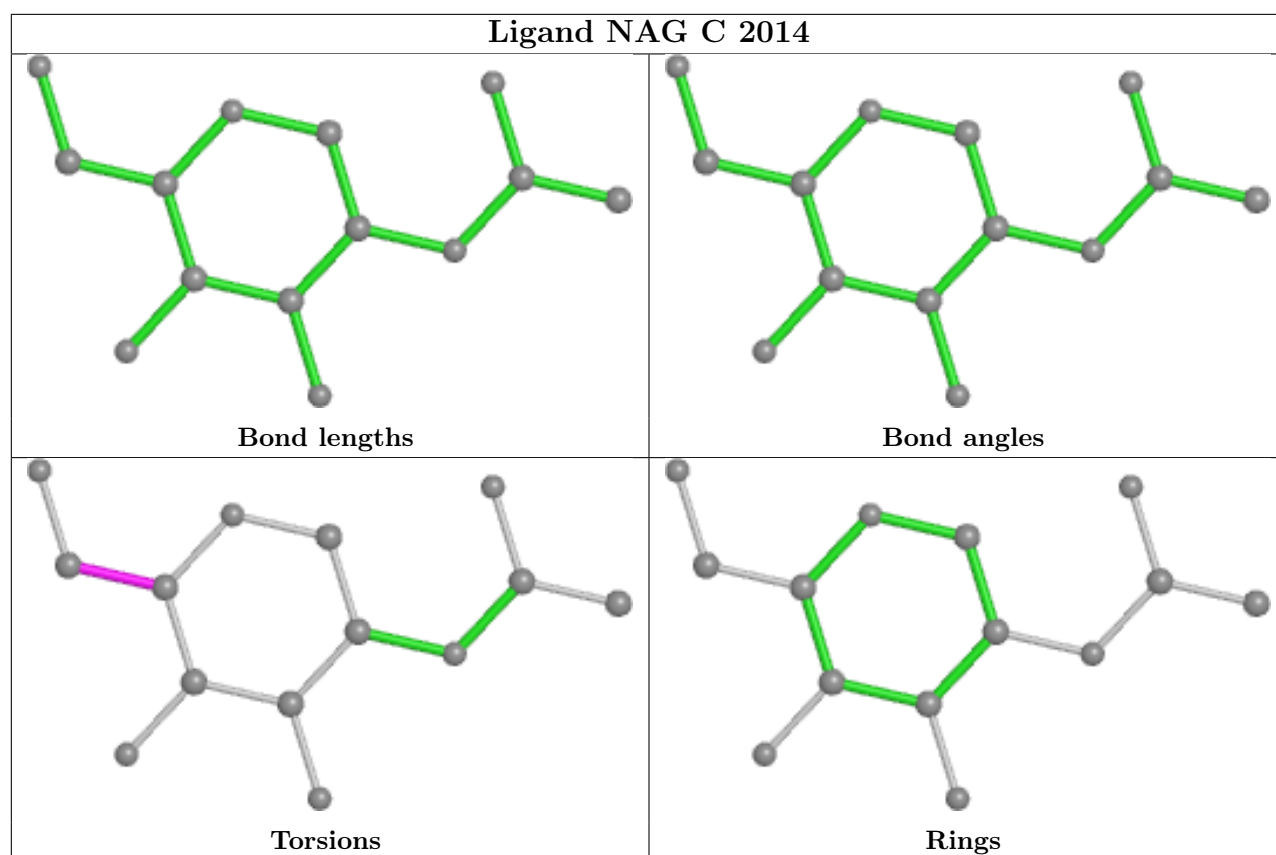
Ligand NAG C 2001

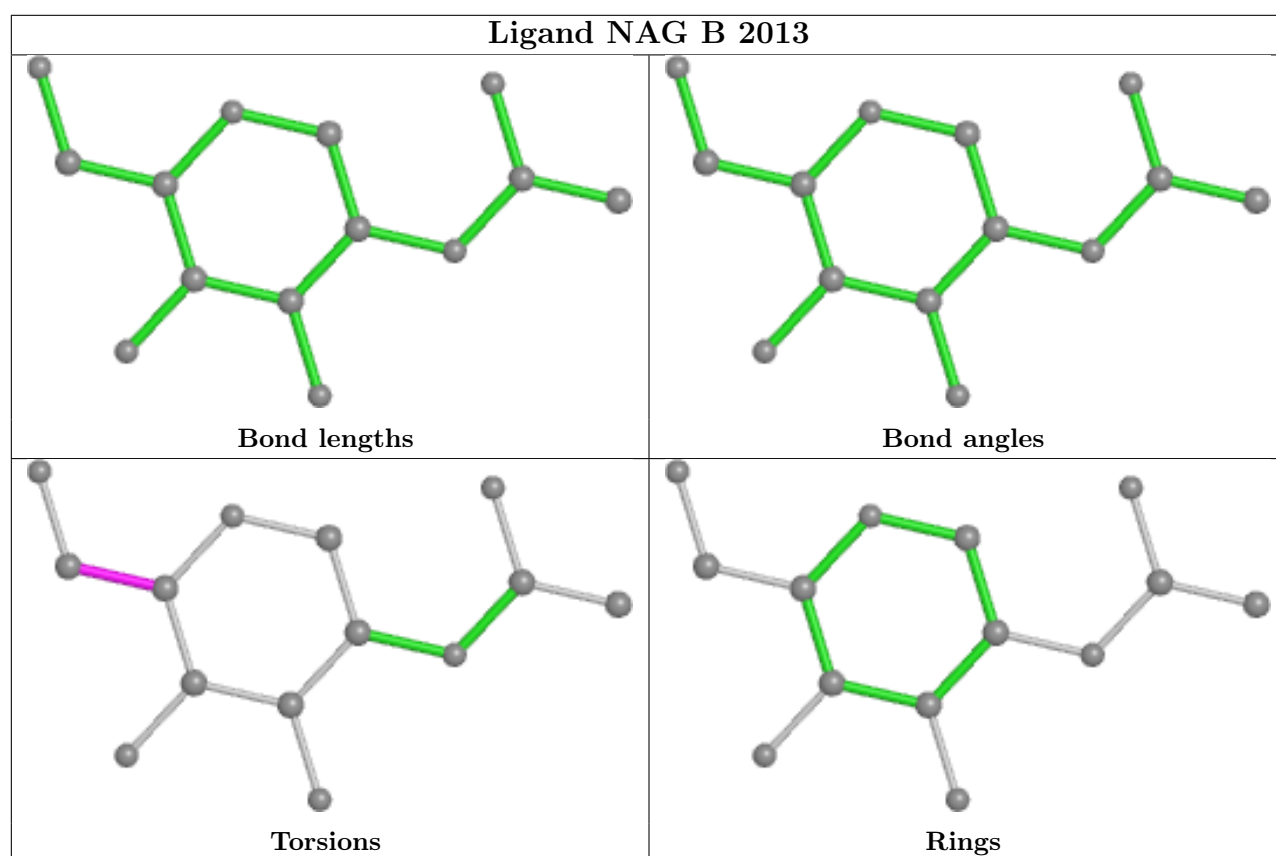
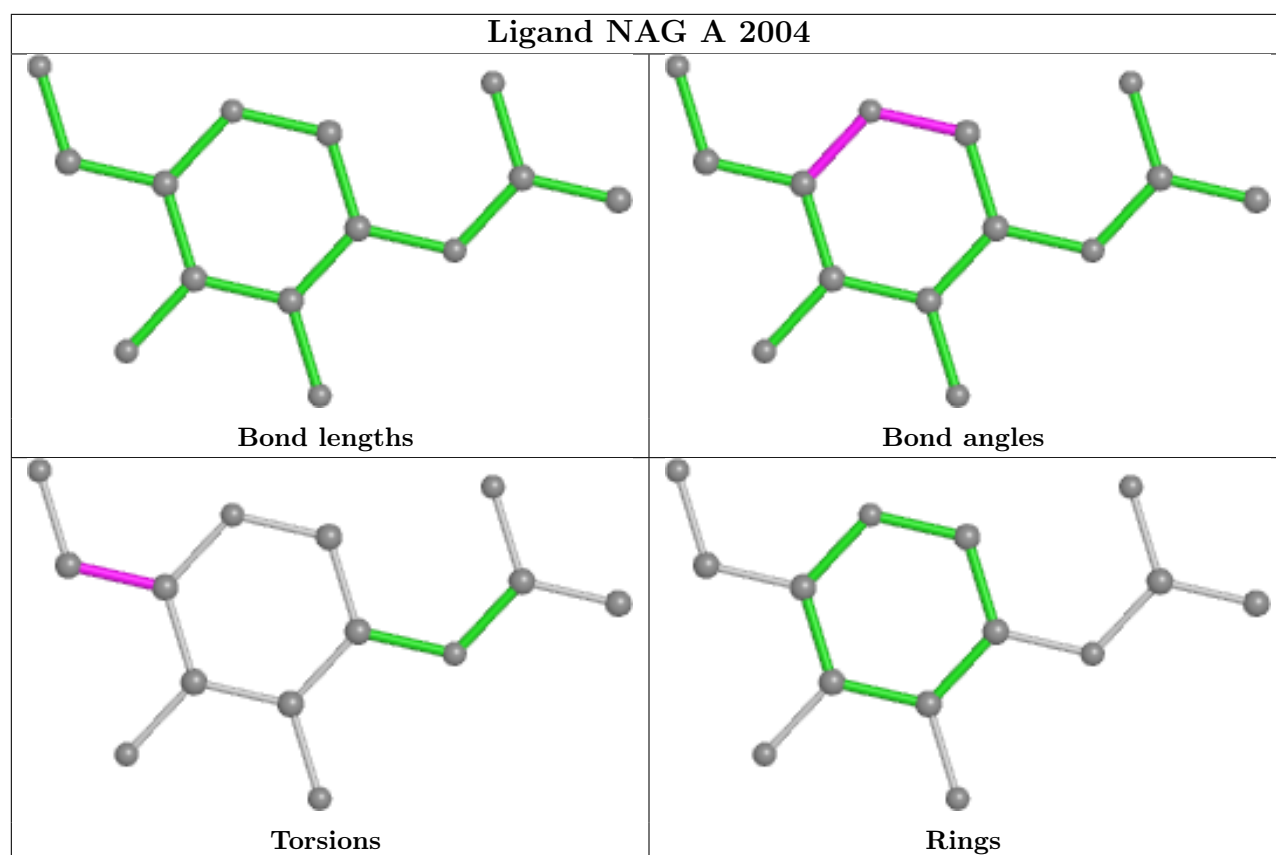


Ligand NAG A 2012

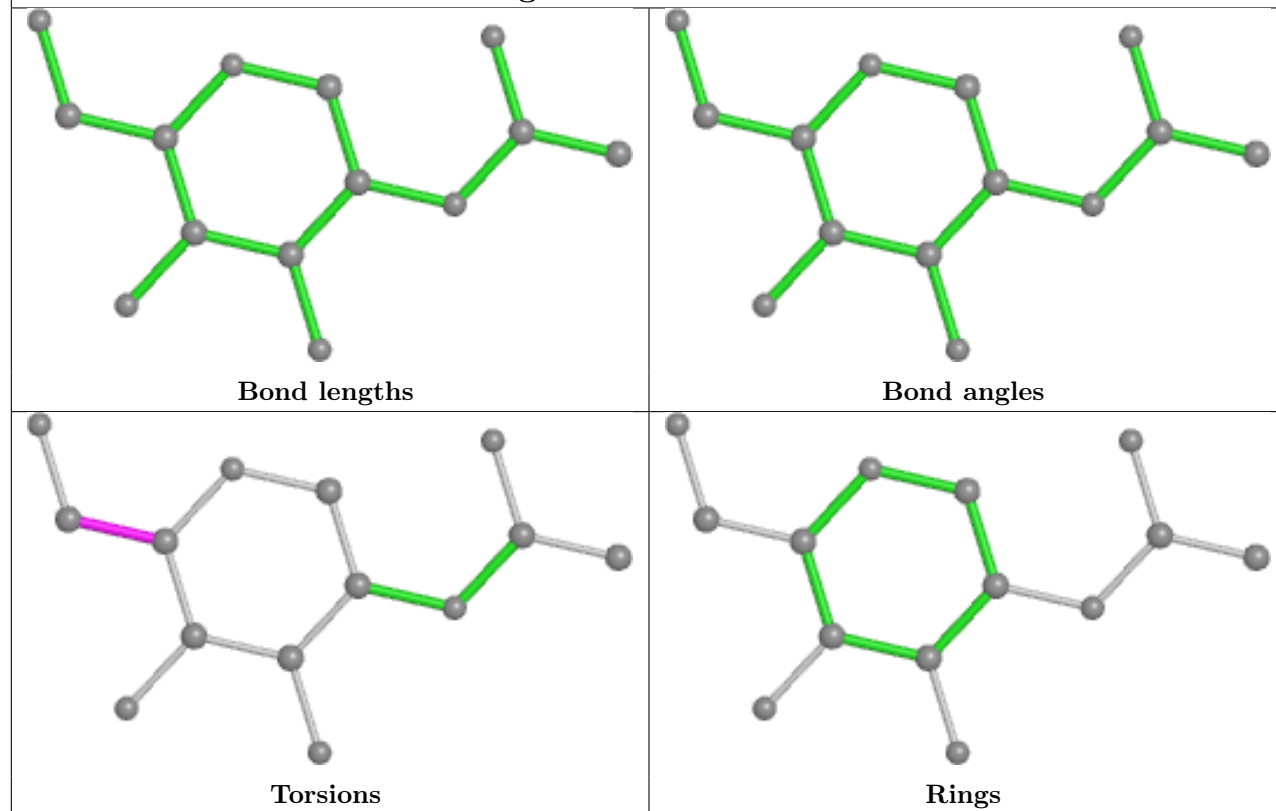




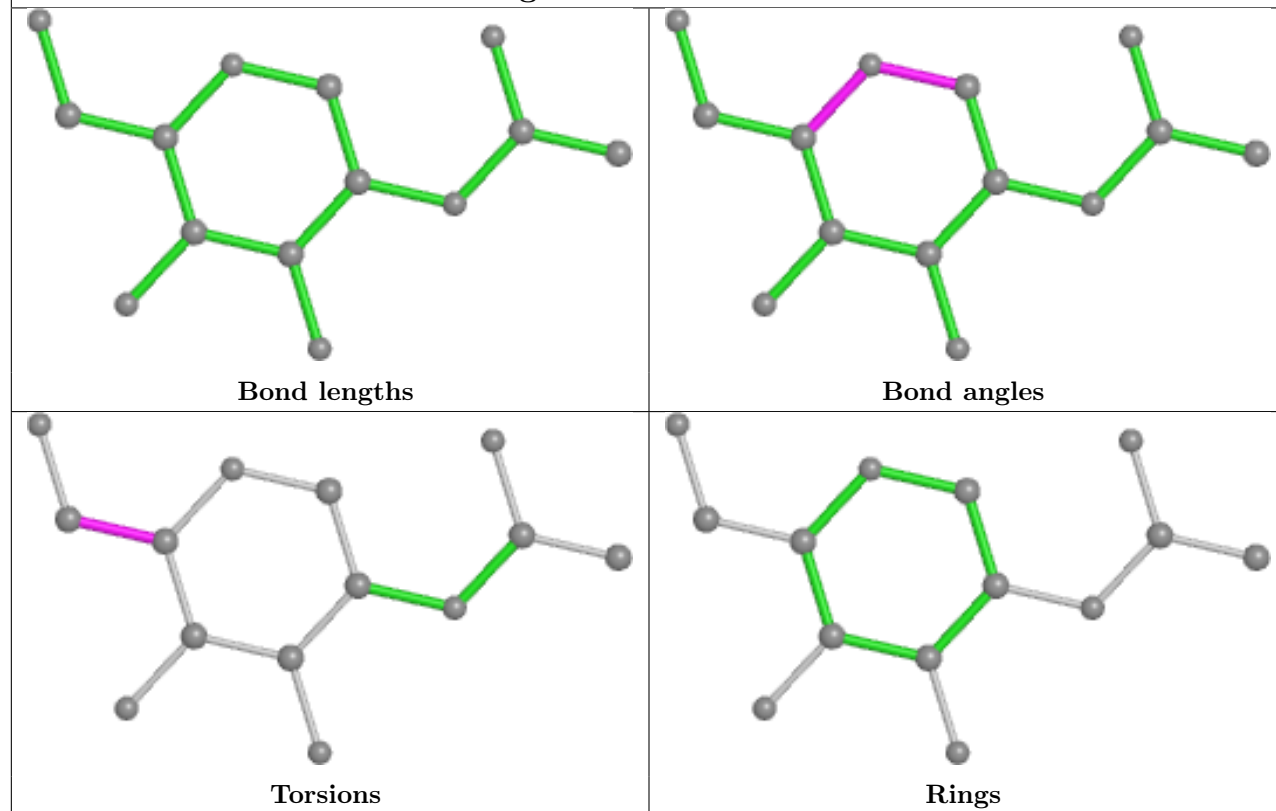


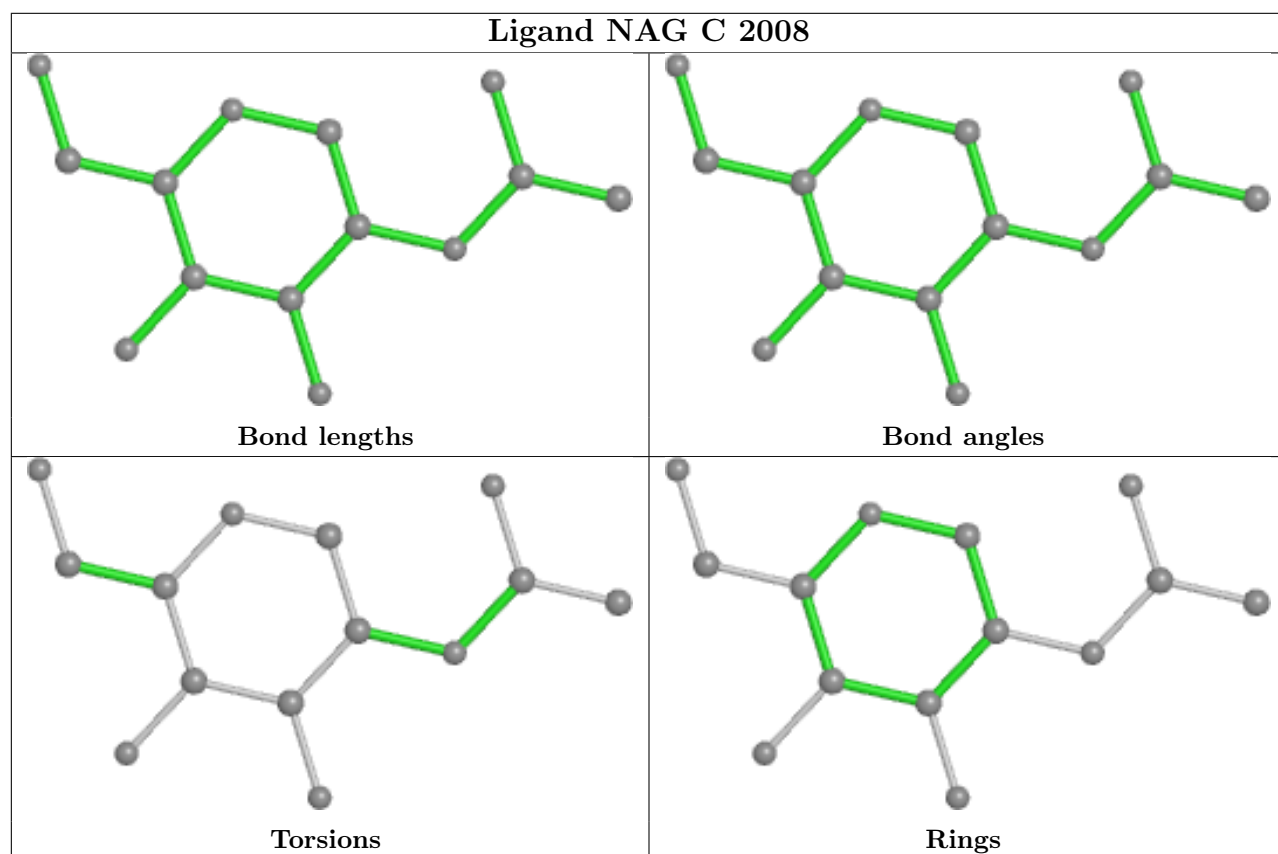
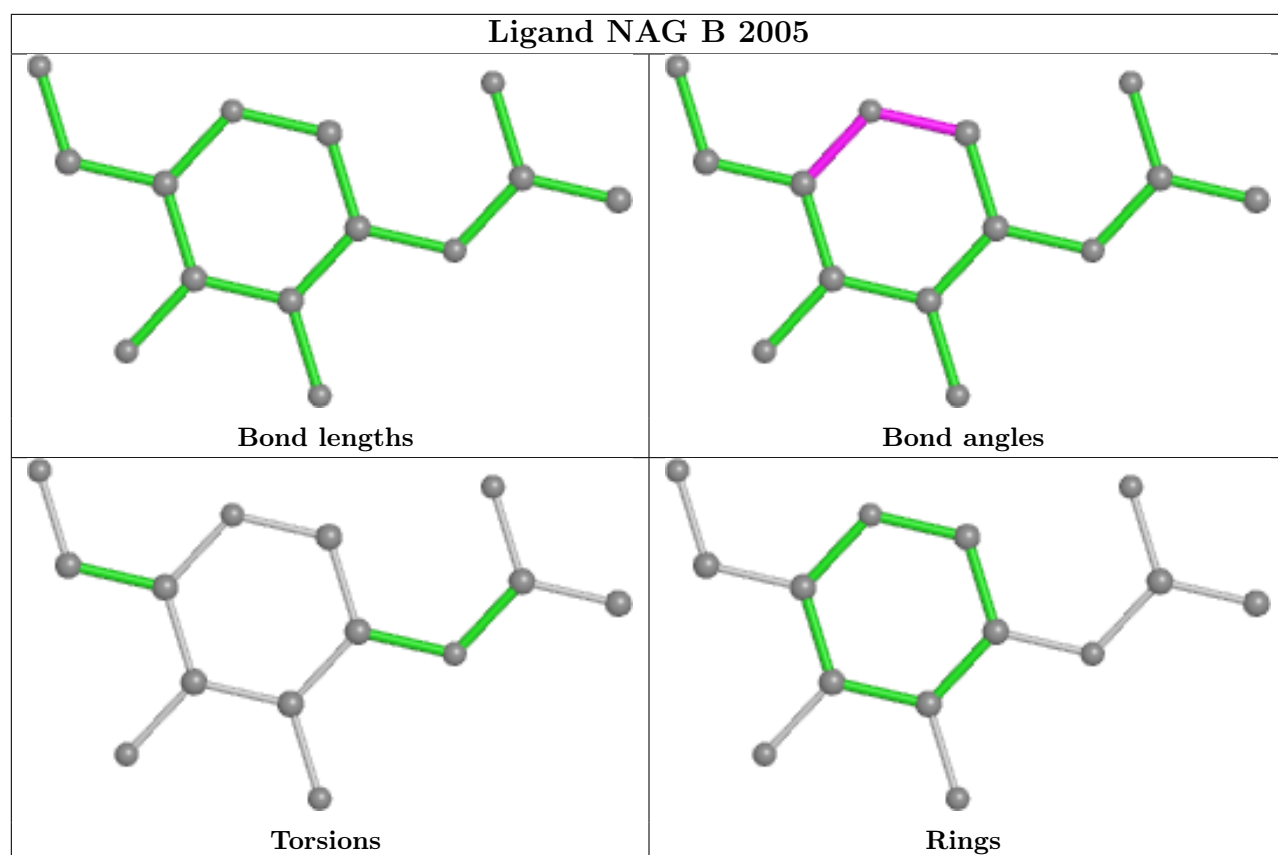


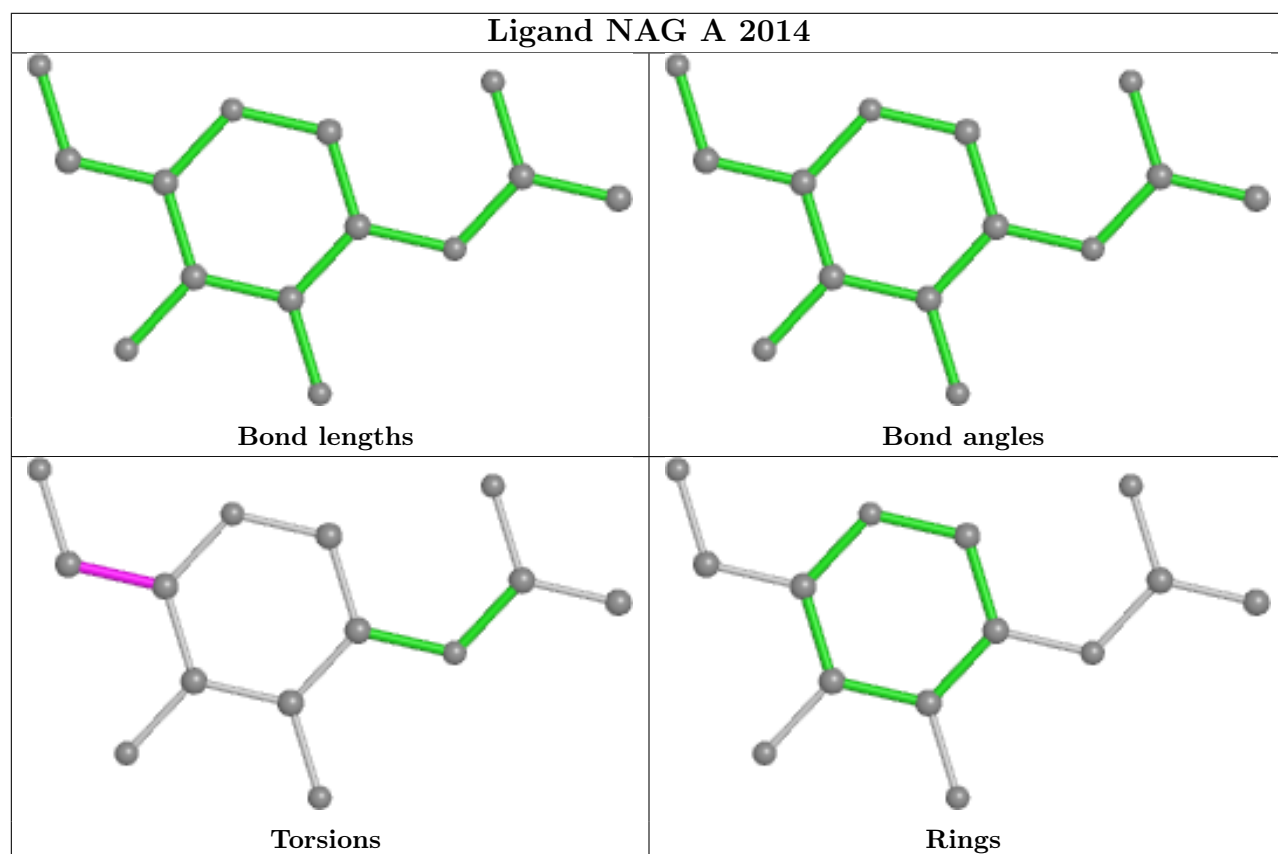
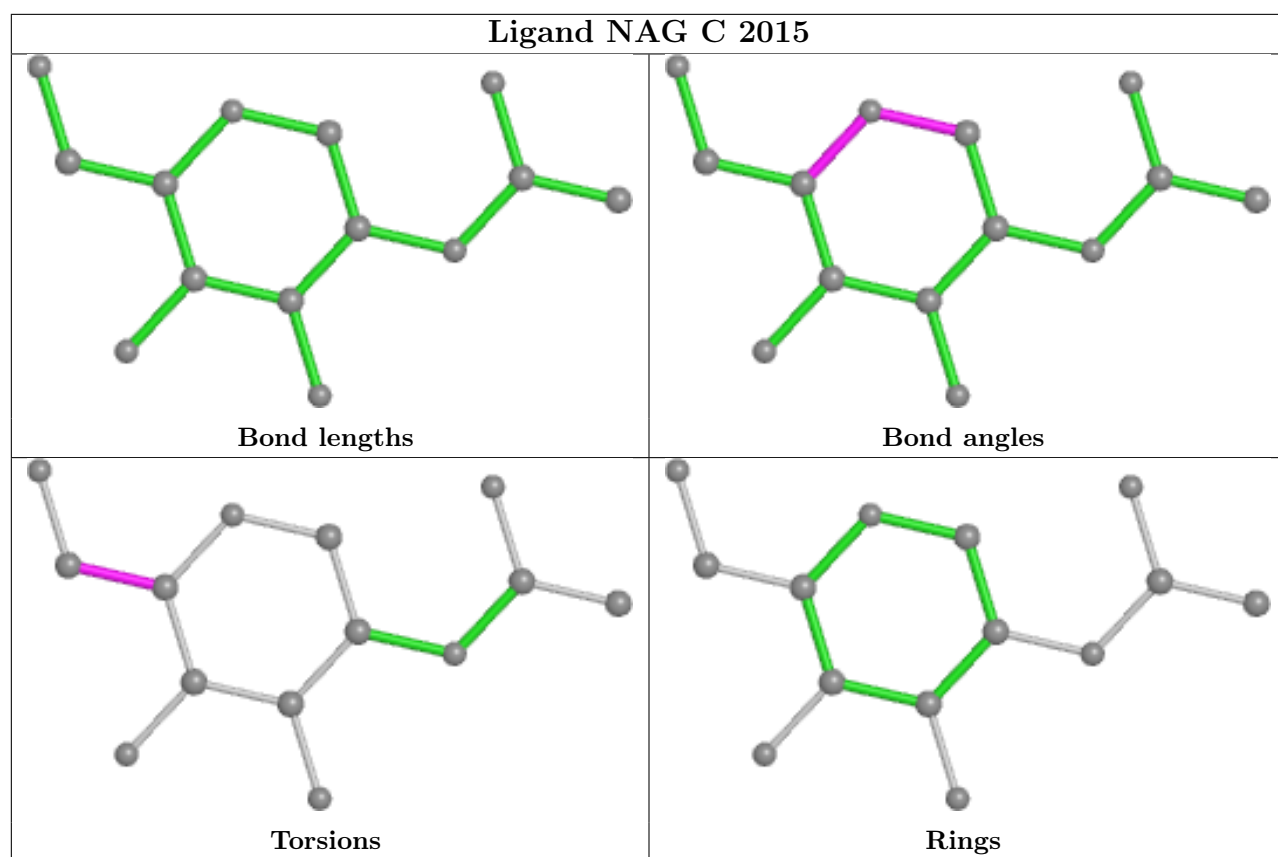
Ligand NAG A 2007

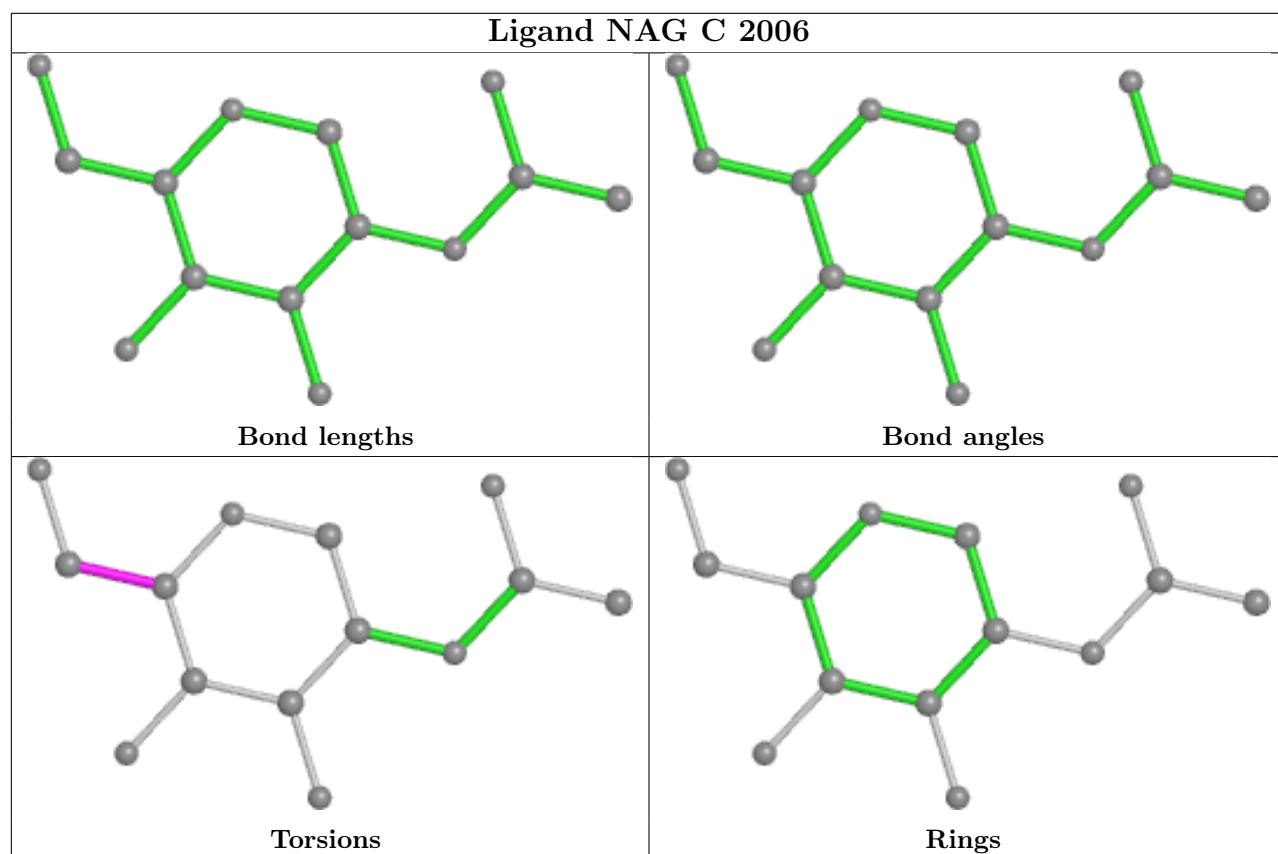
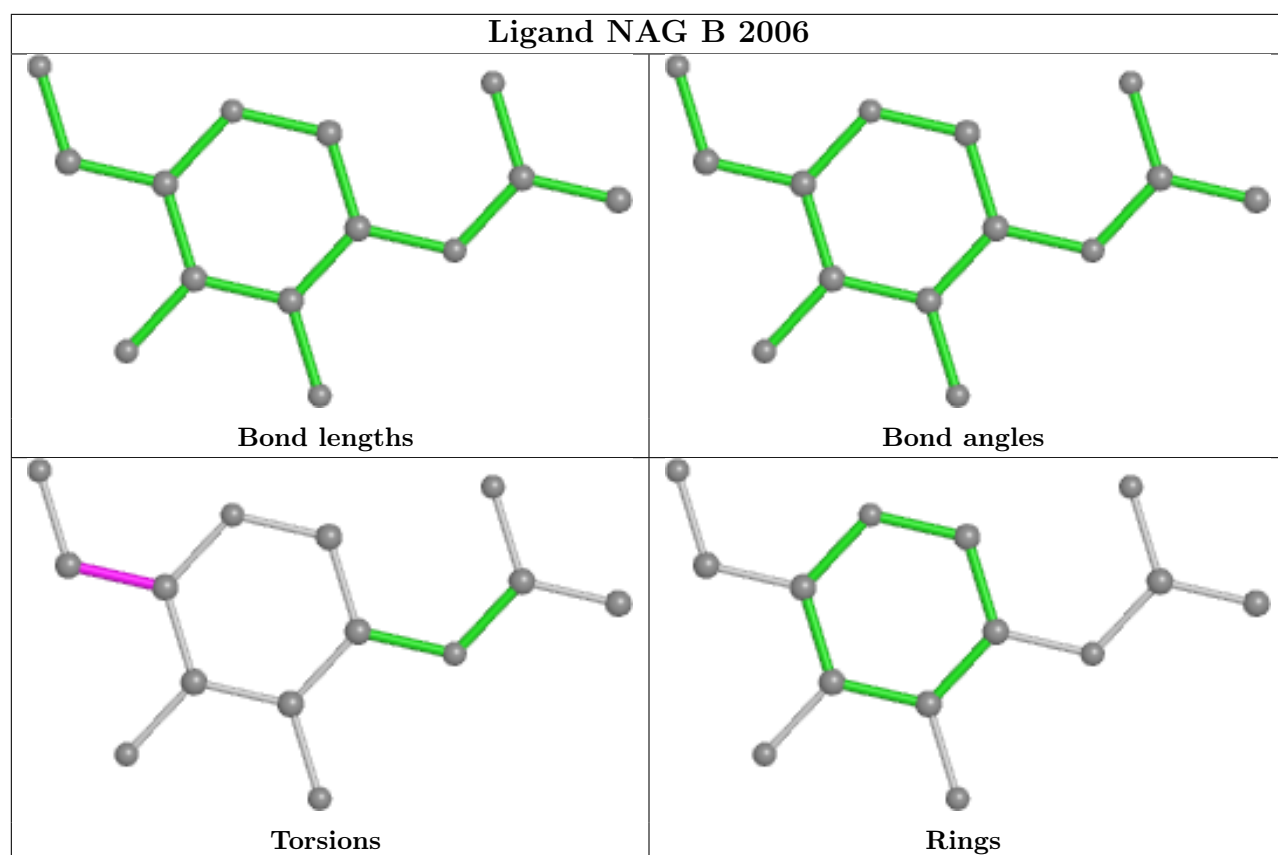


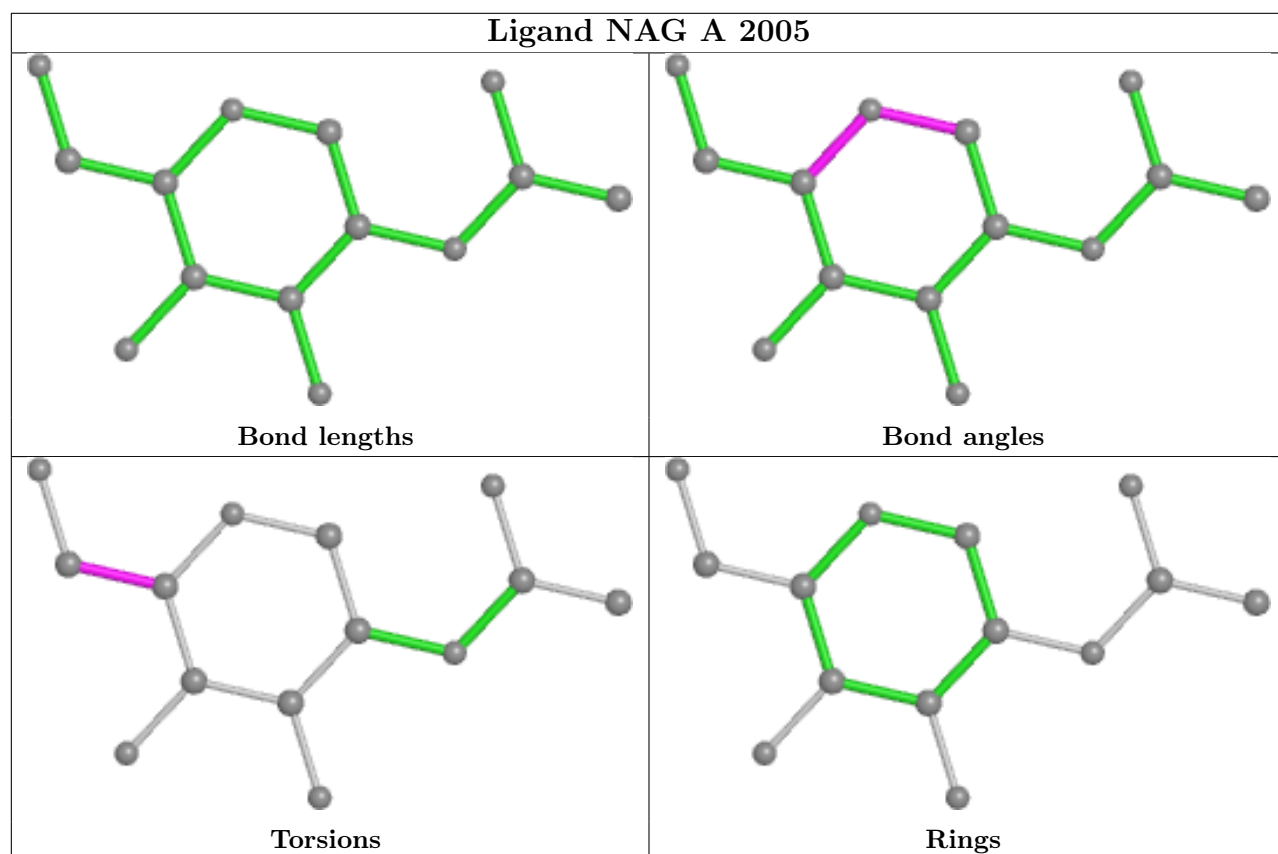
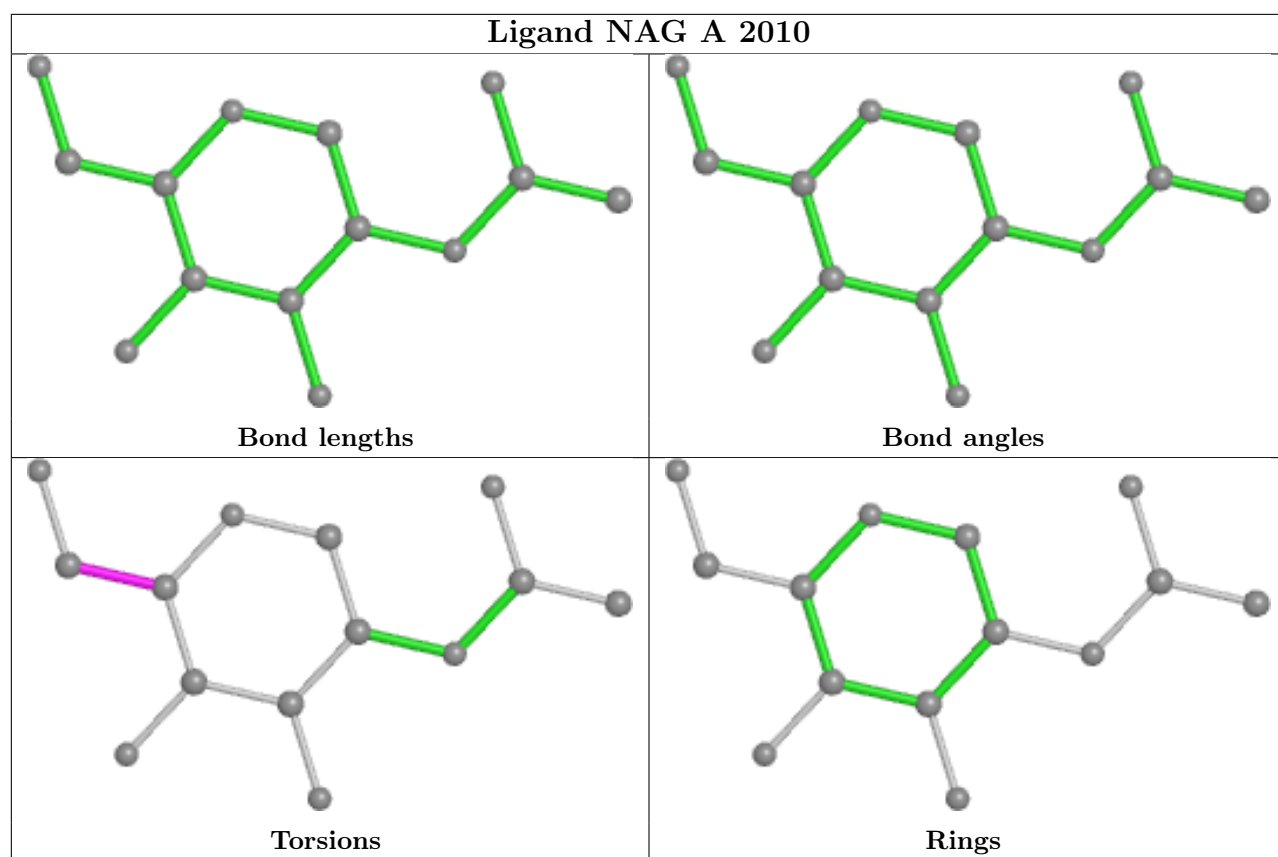
Ligand NAG C 2016

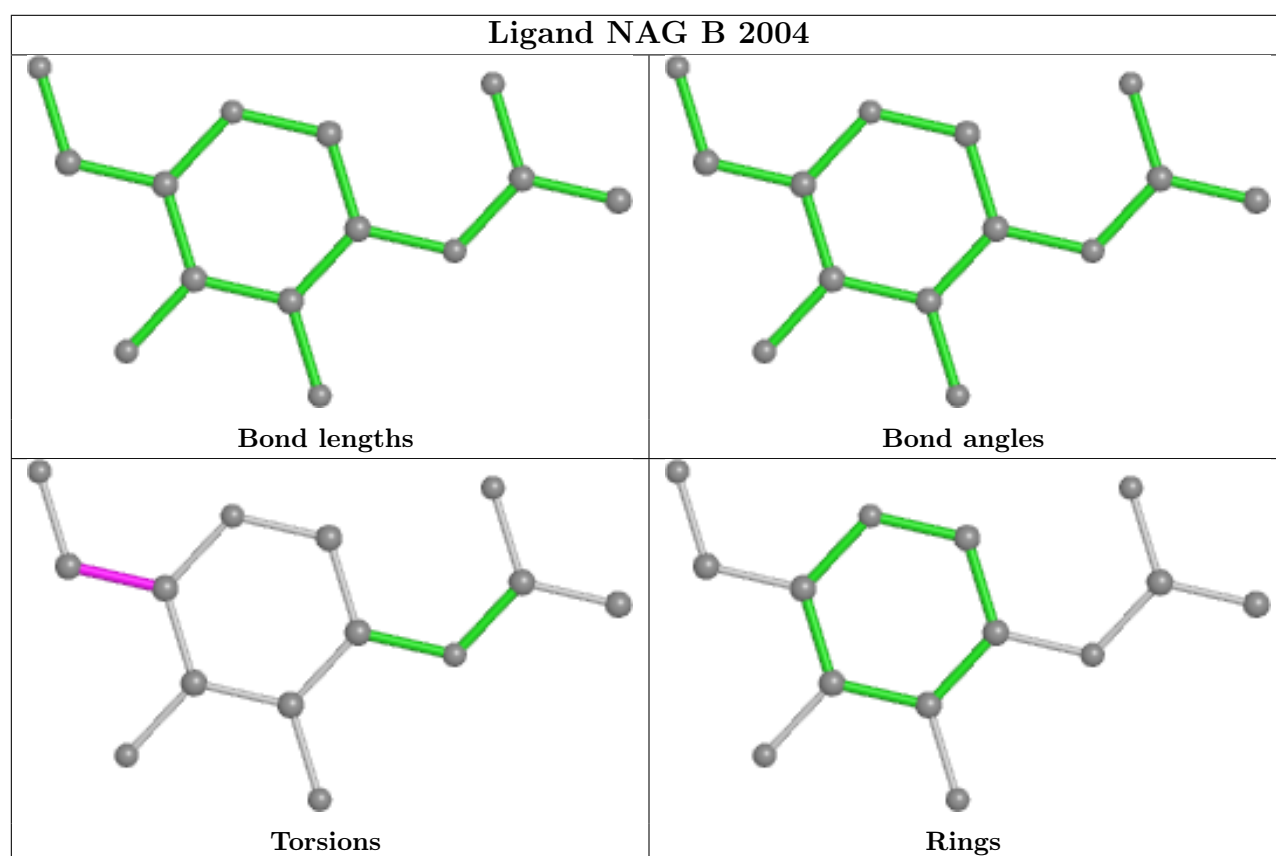
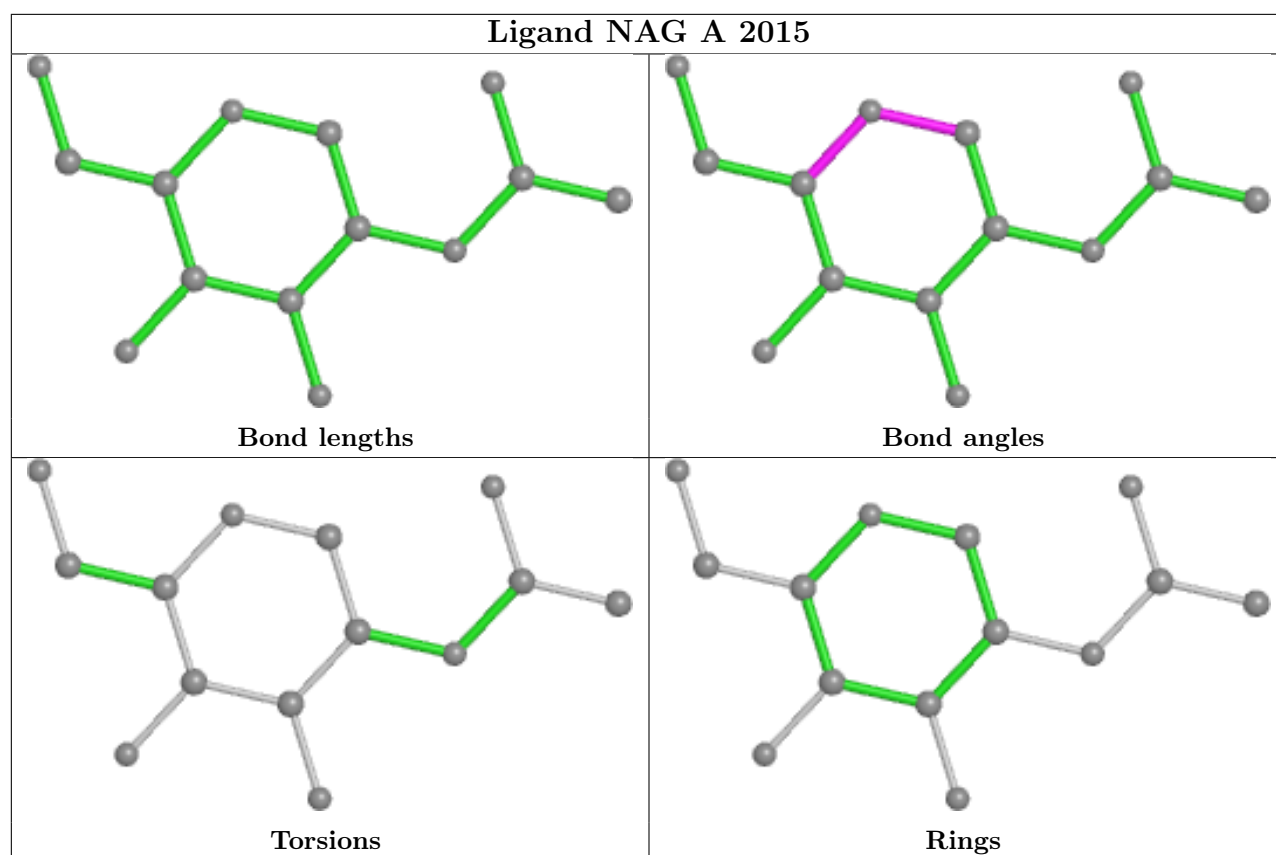


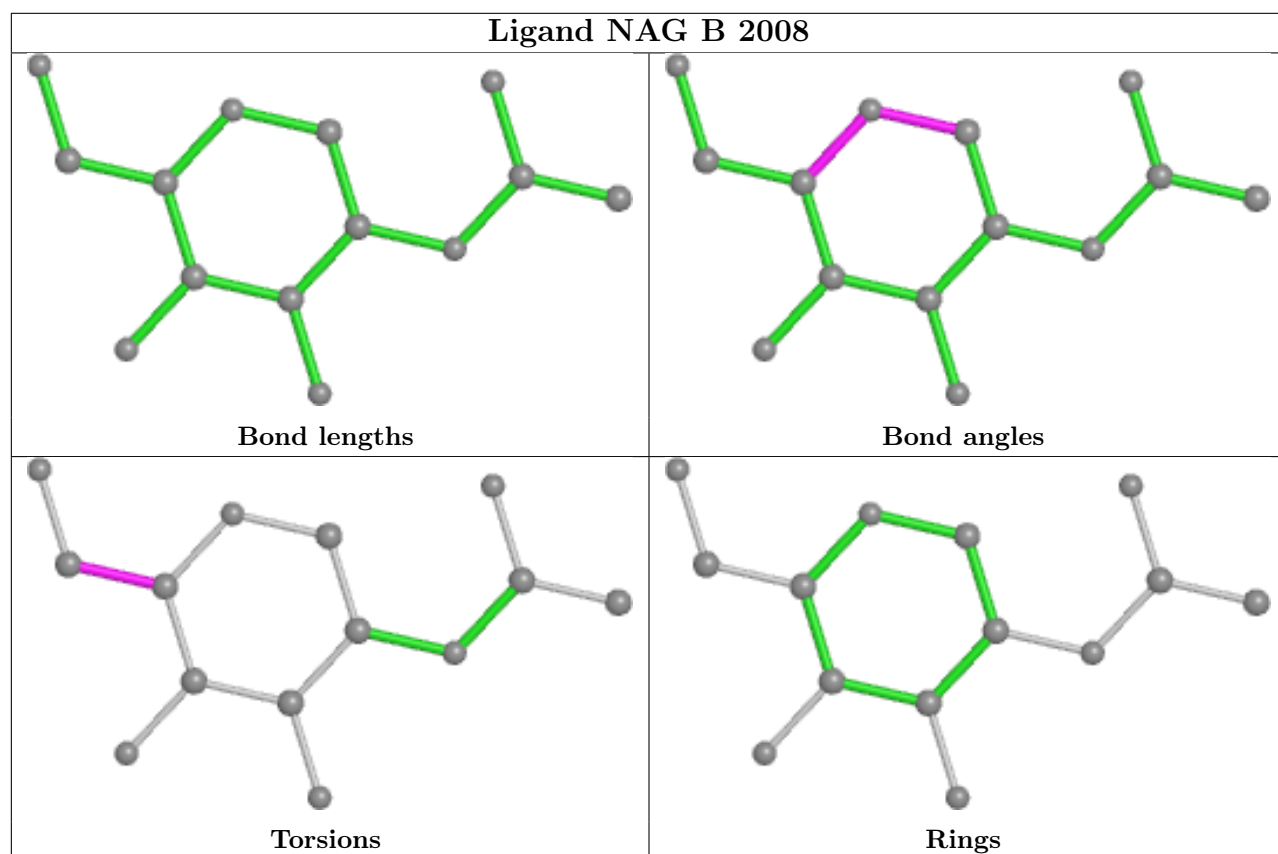
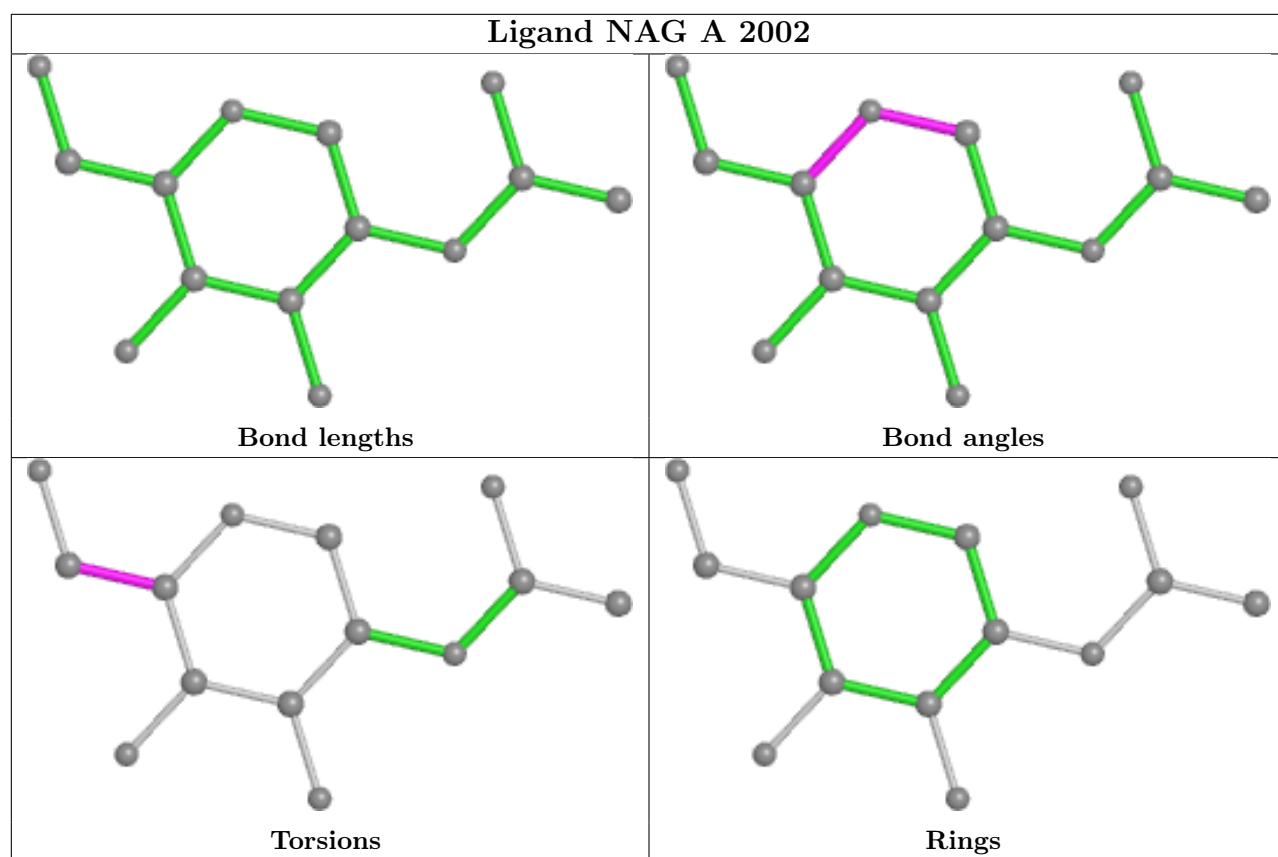


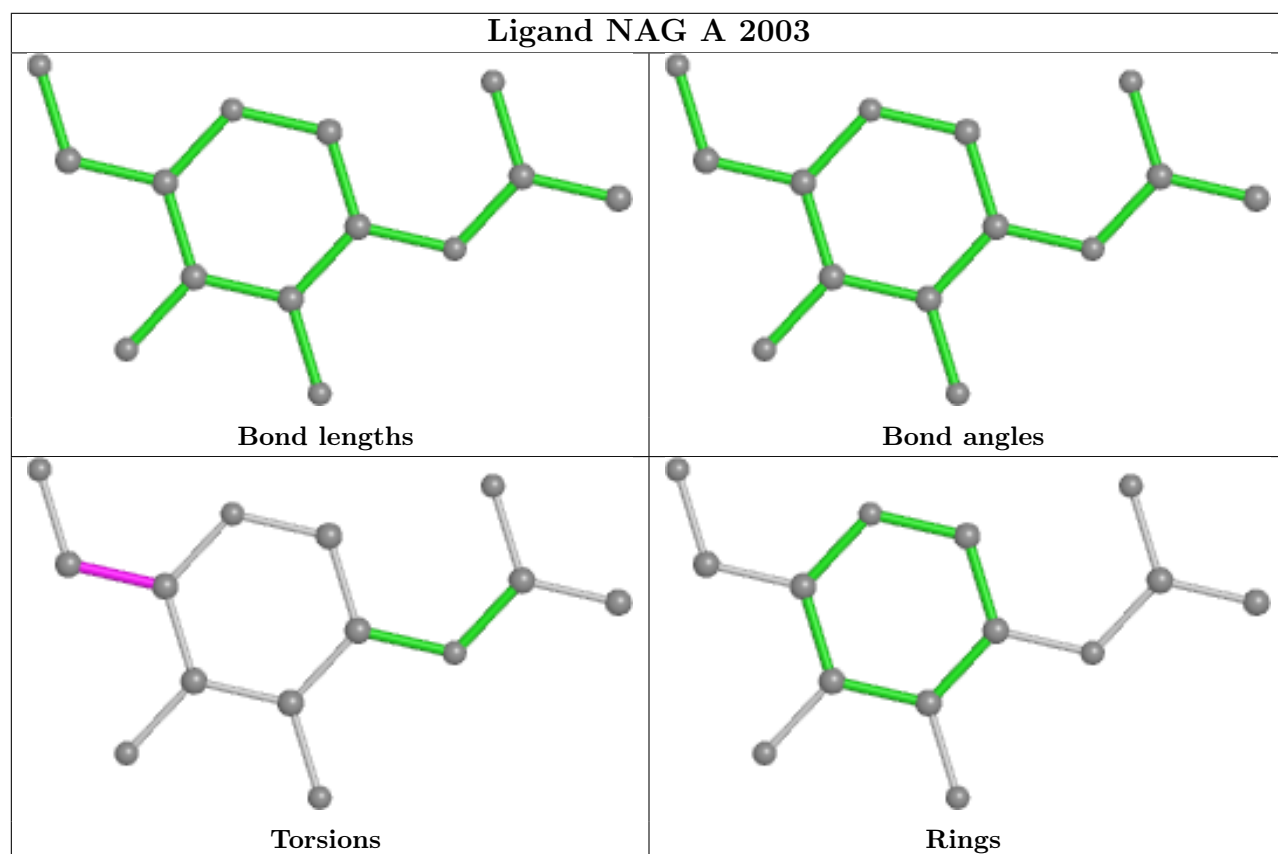
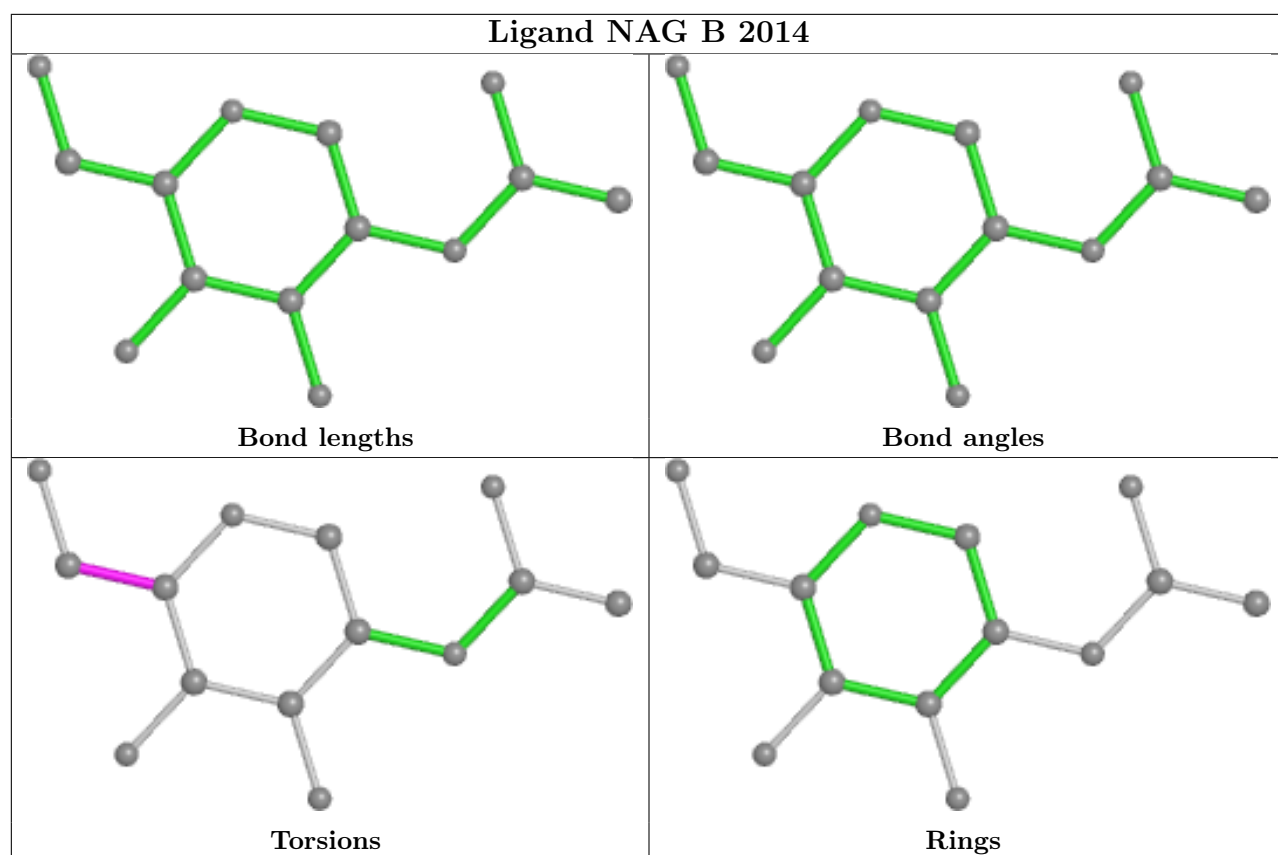


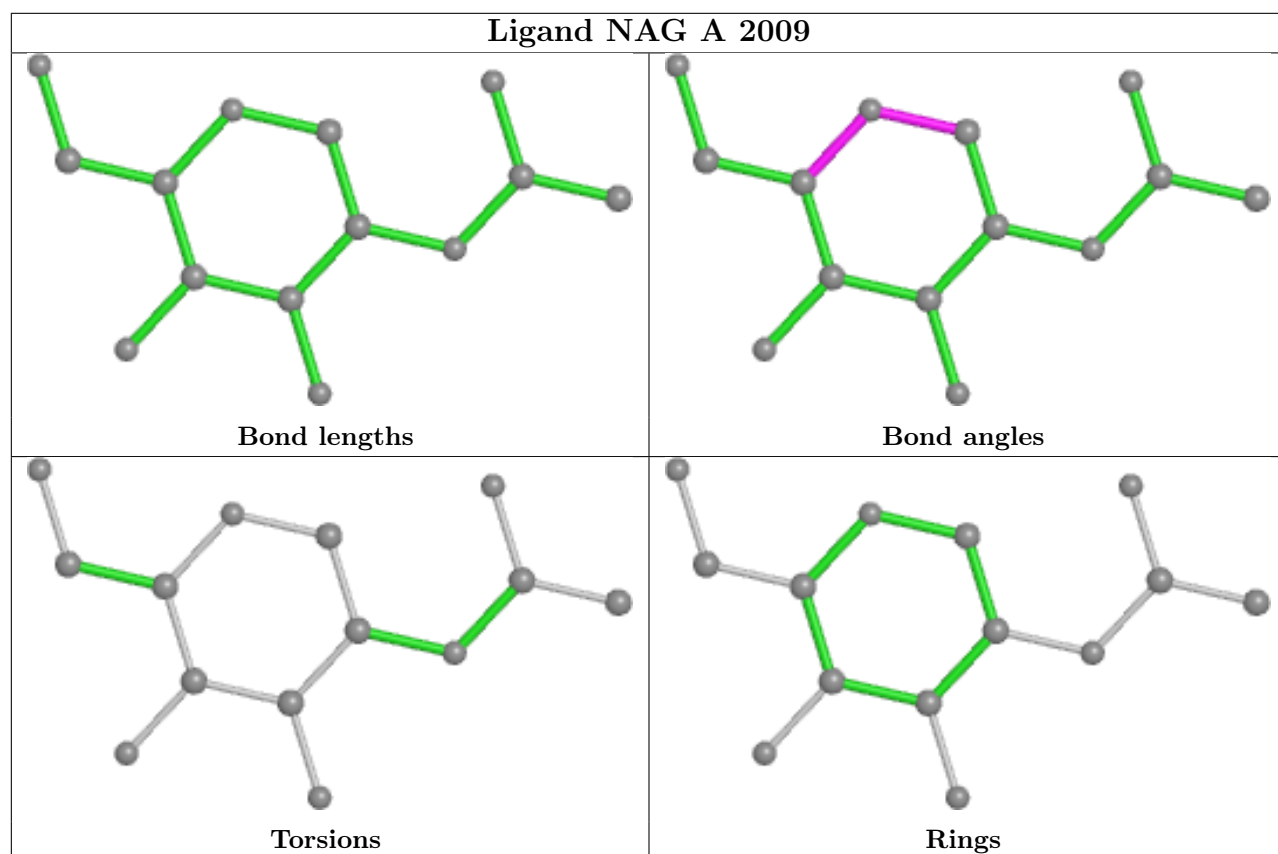
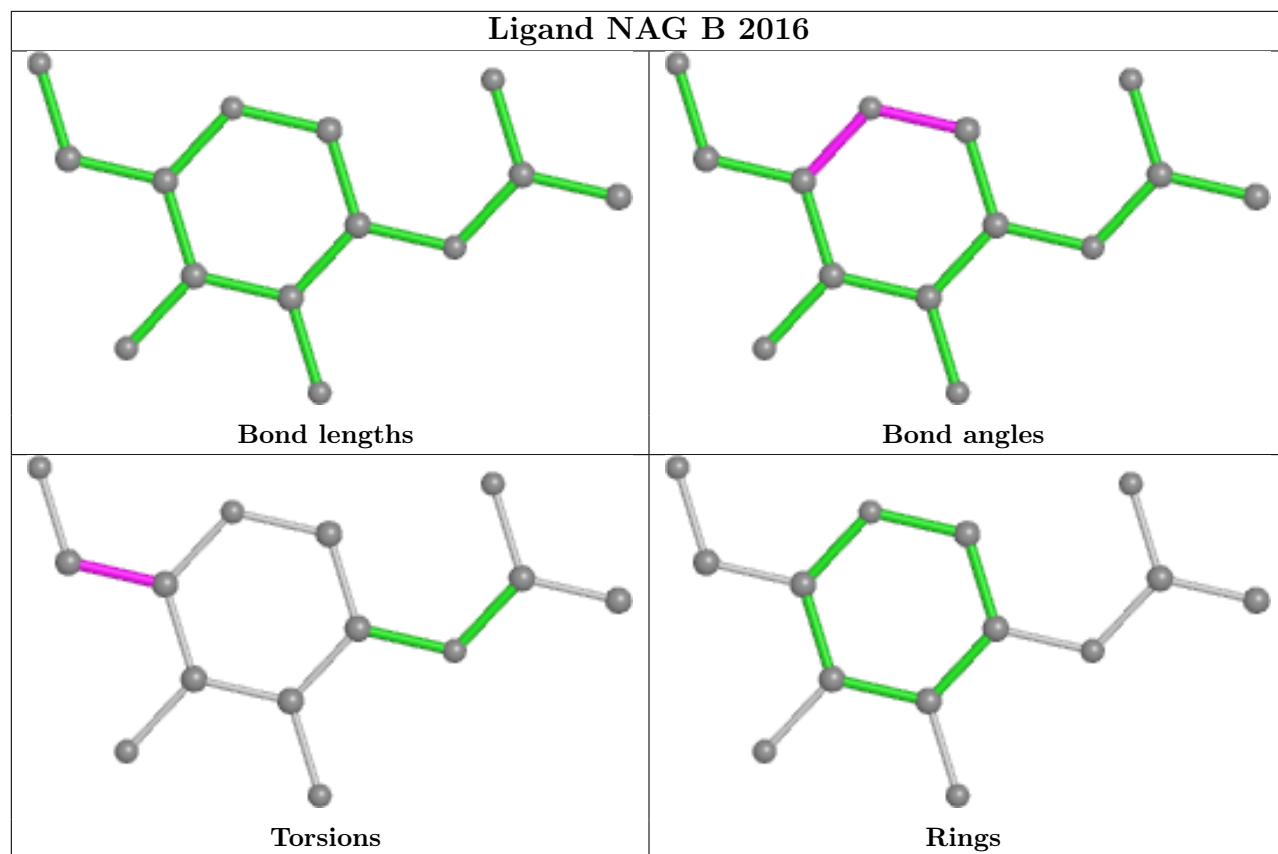




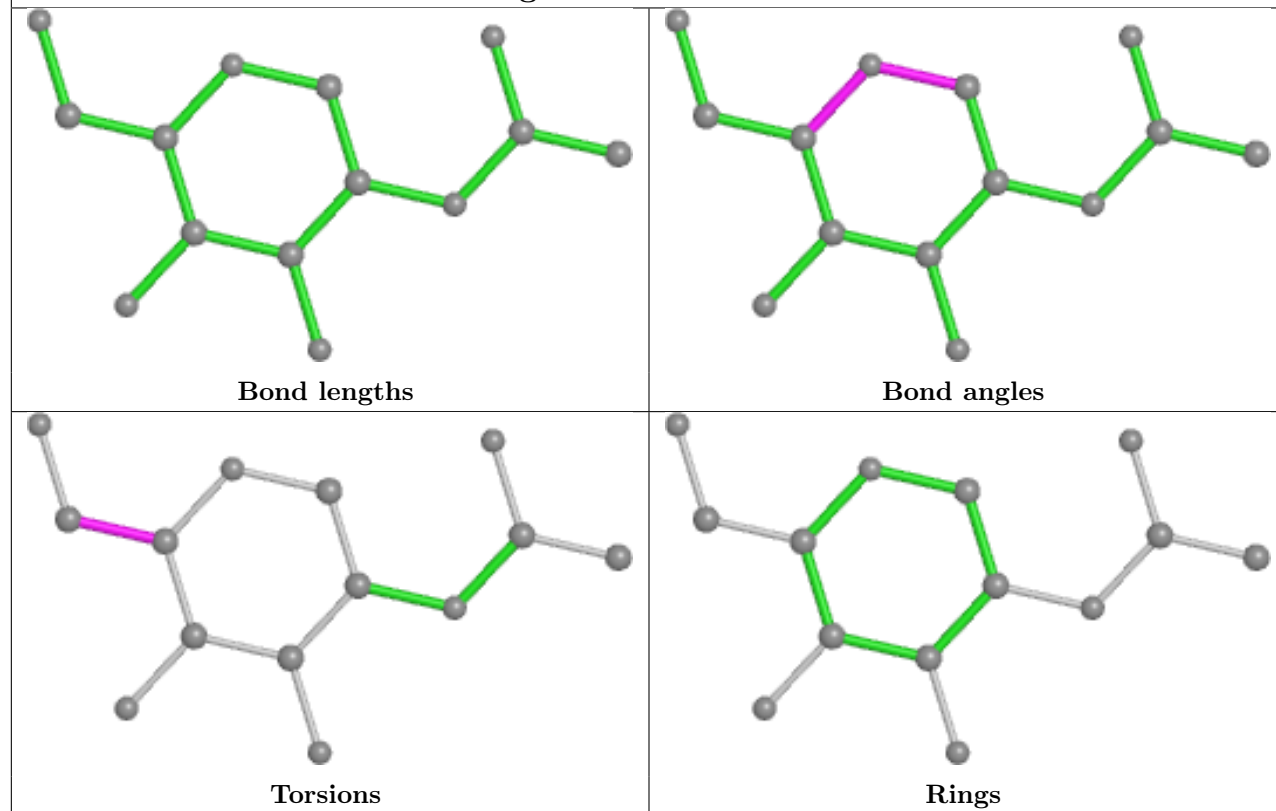




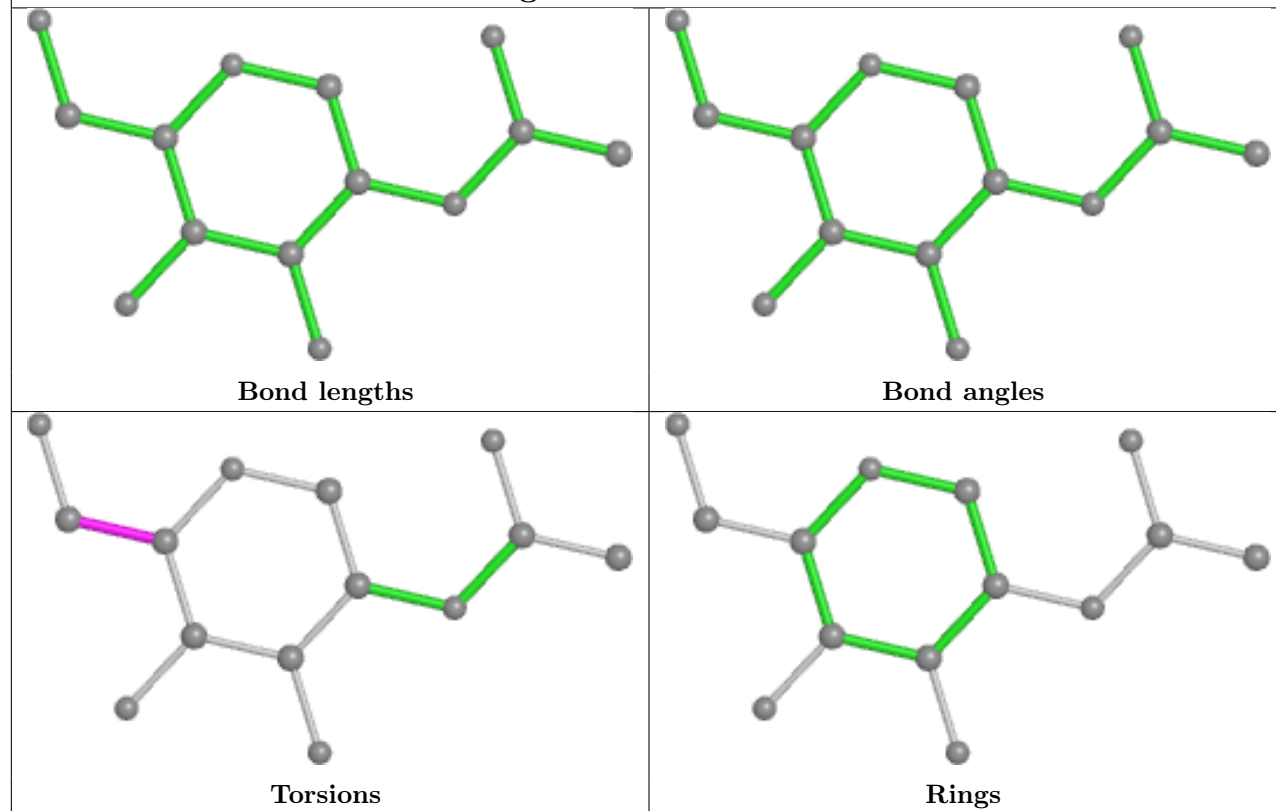


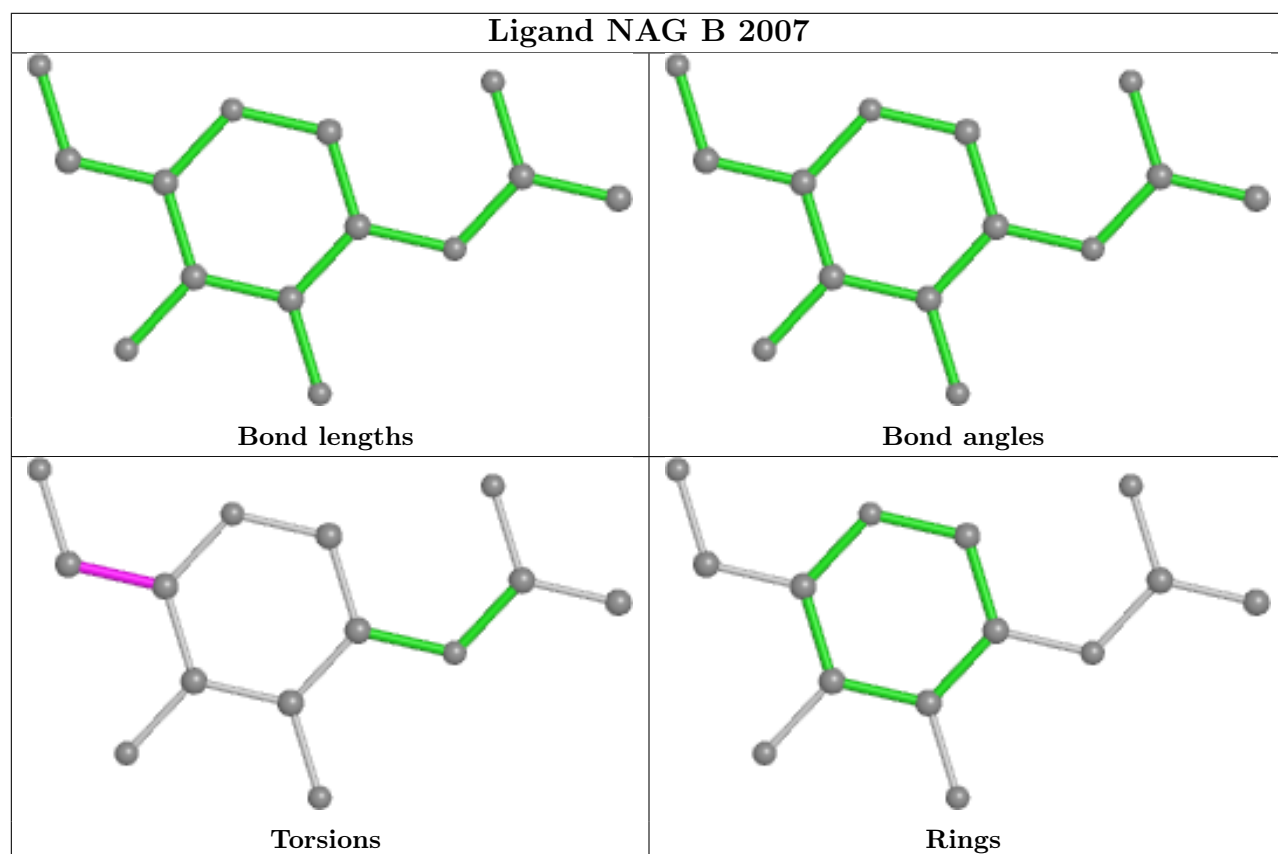
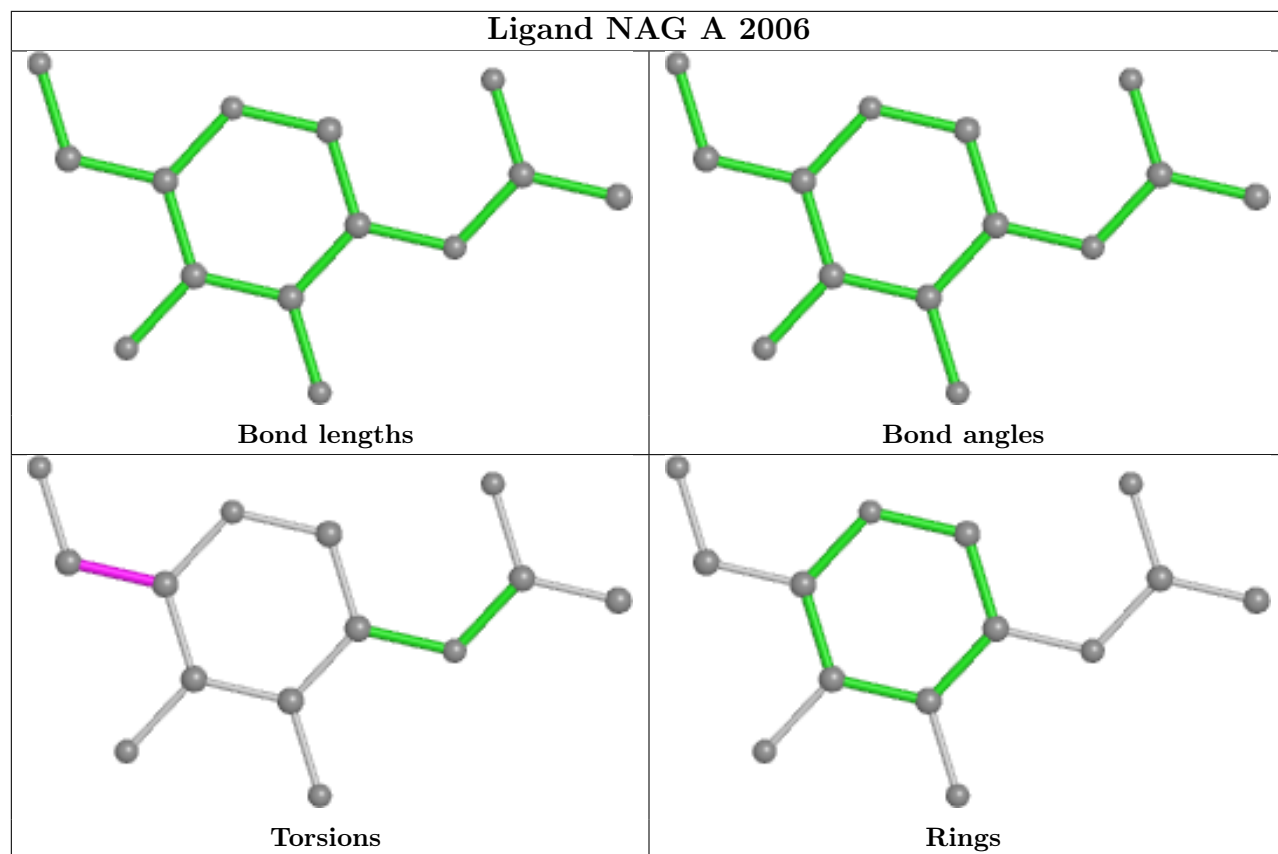


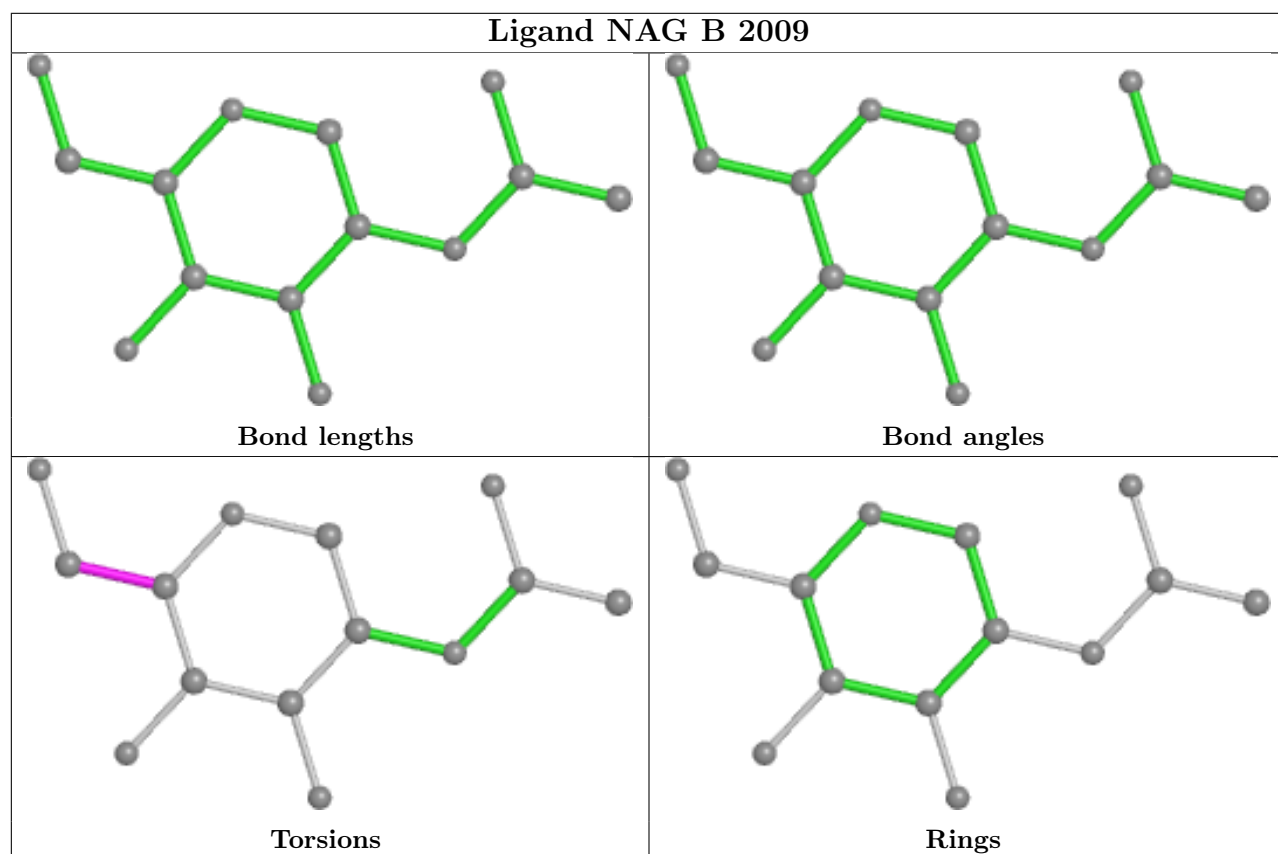
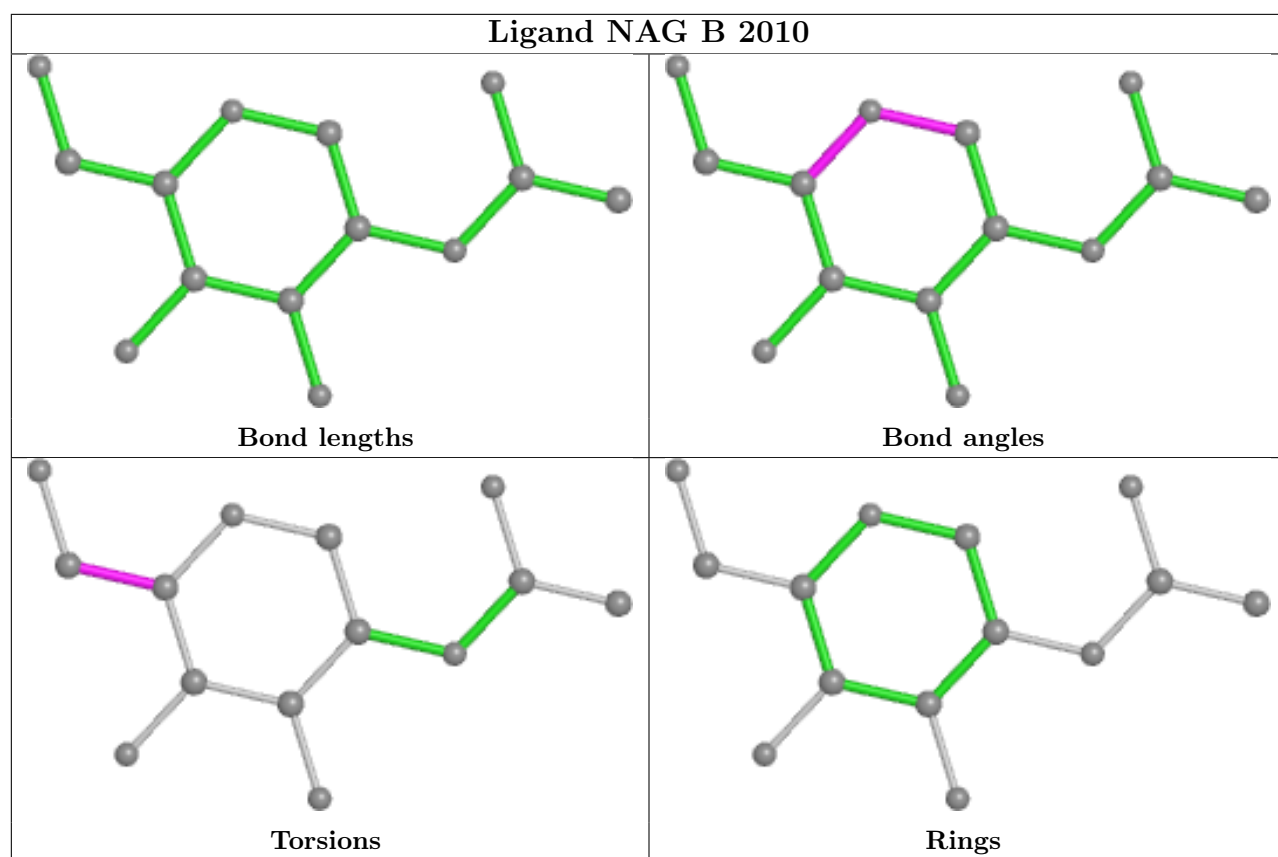
Ligand NAG C 2011

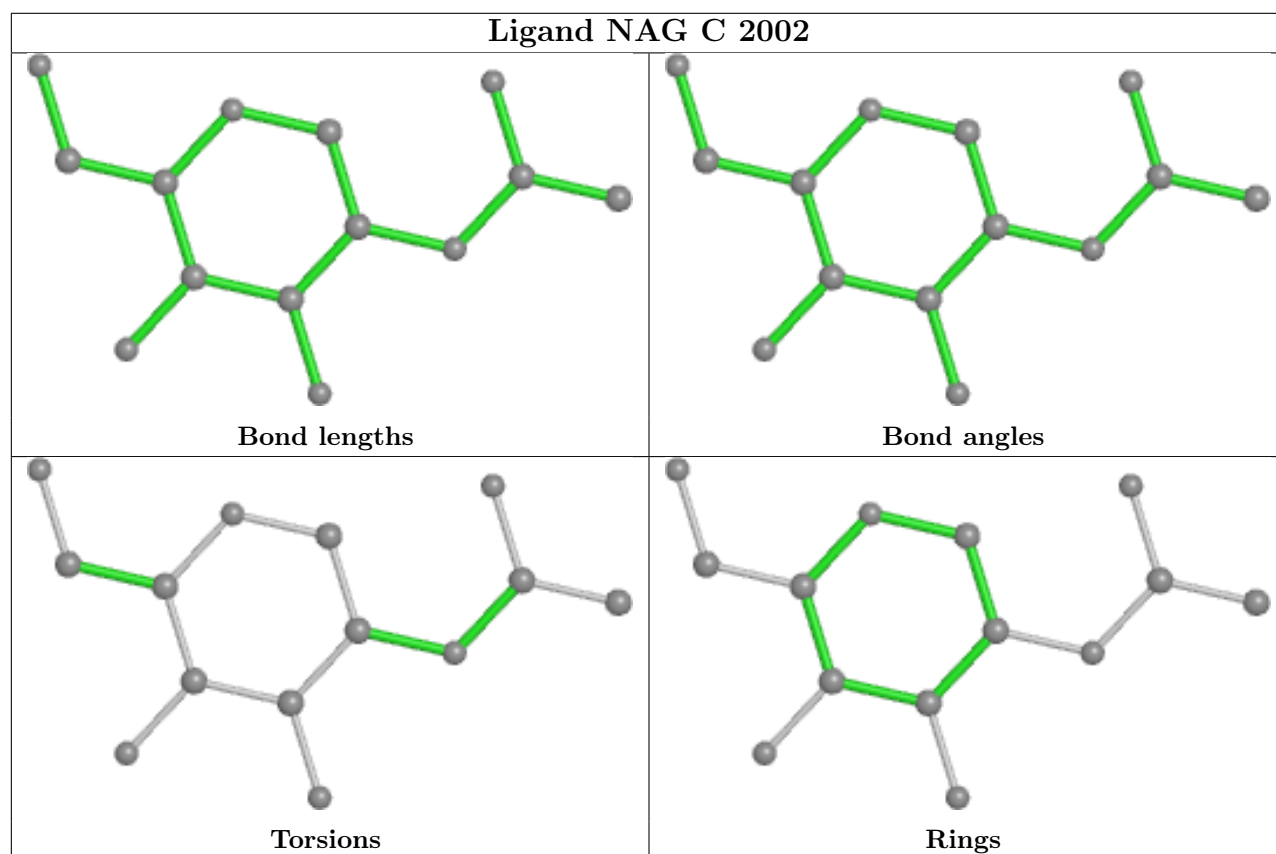
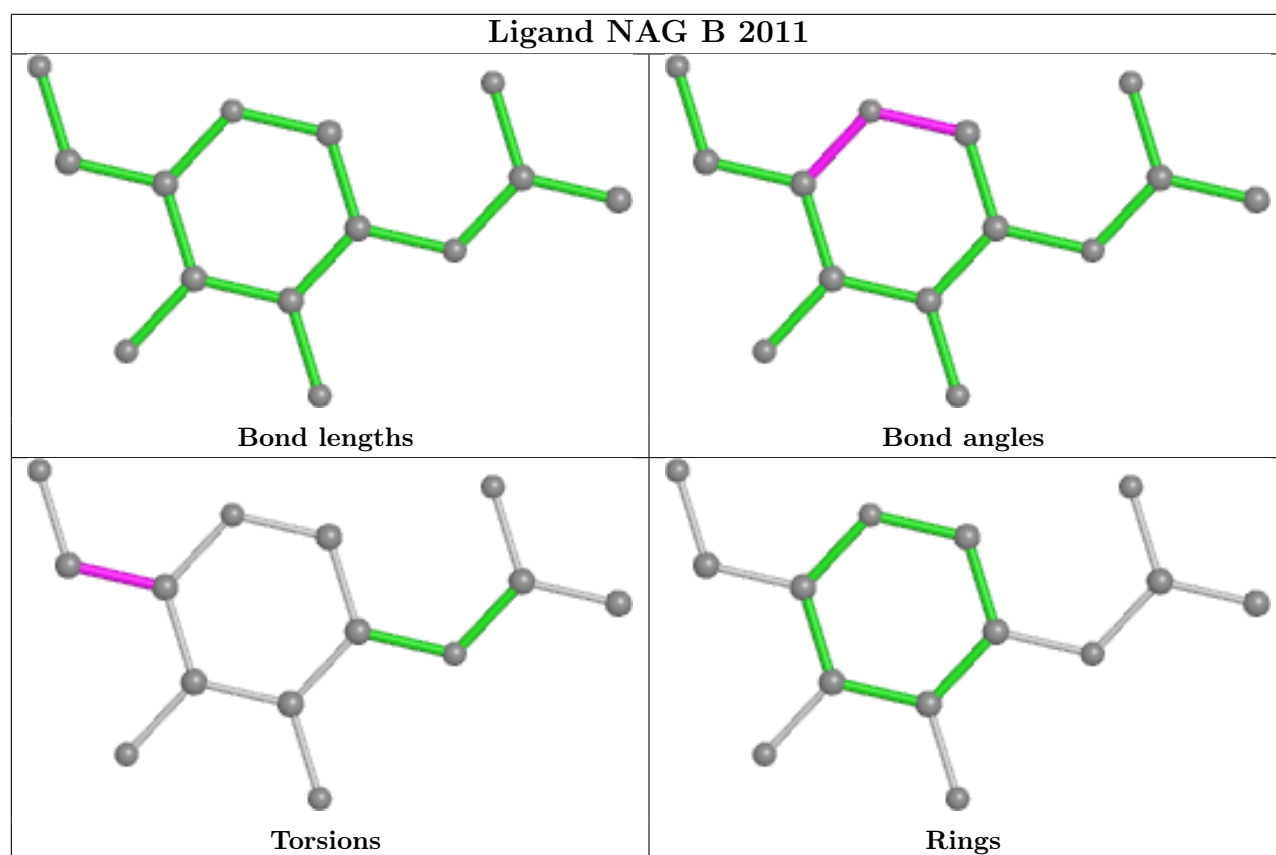


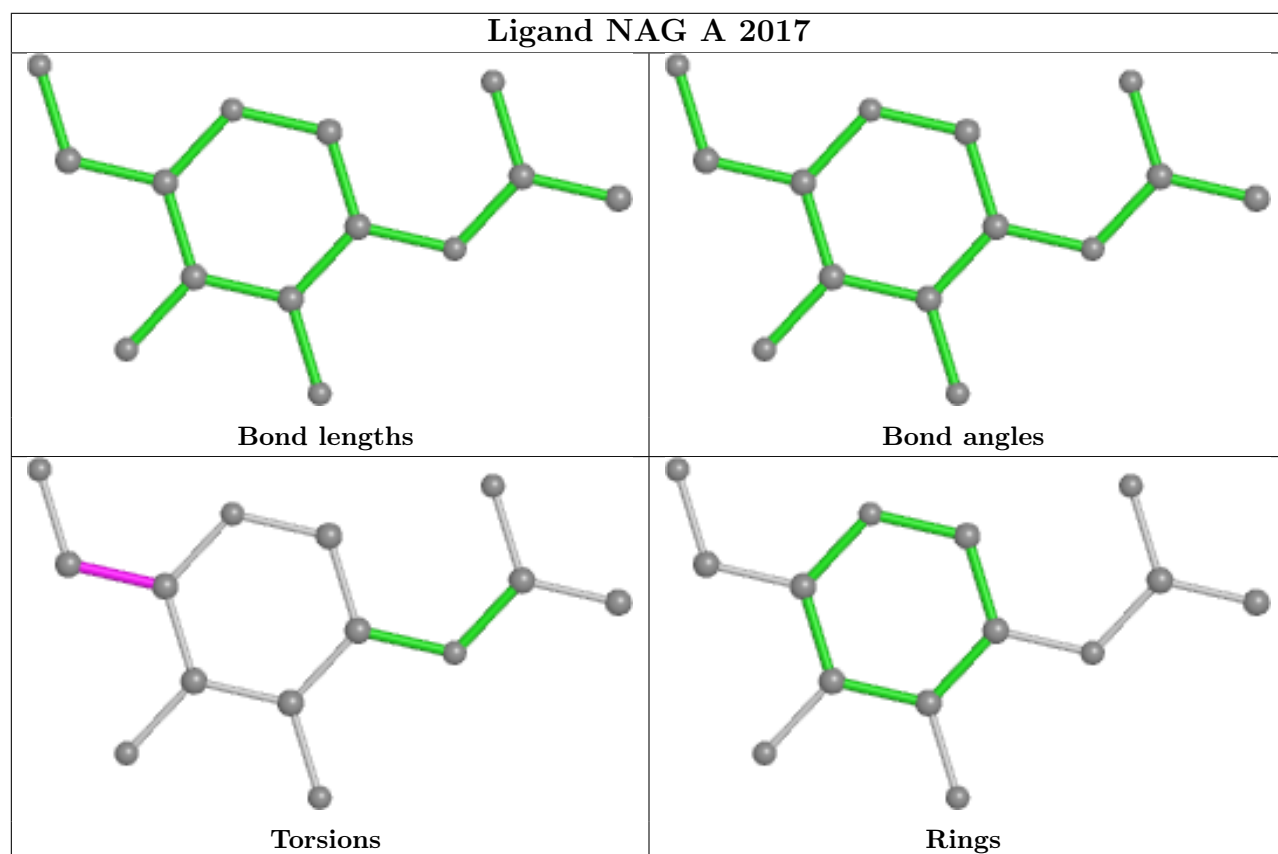
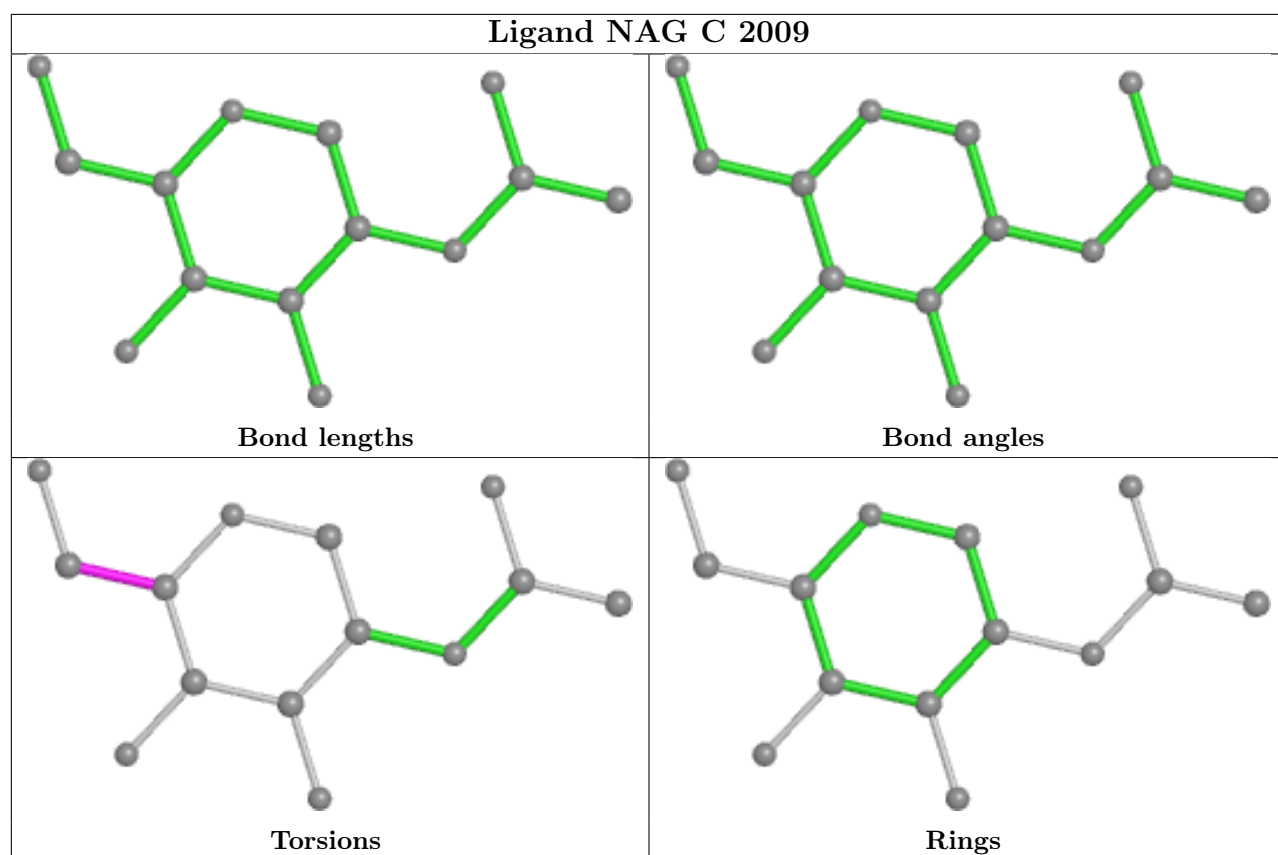
Ligand NAG B 2002

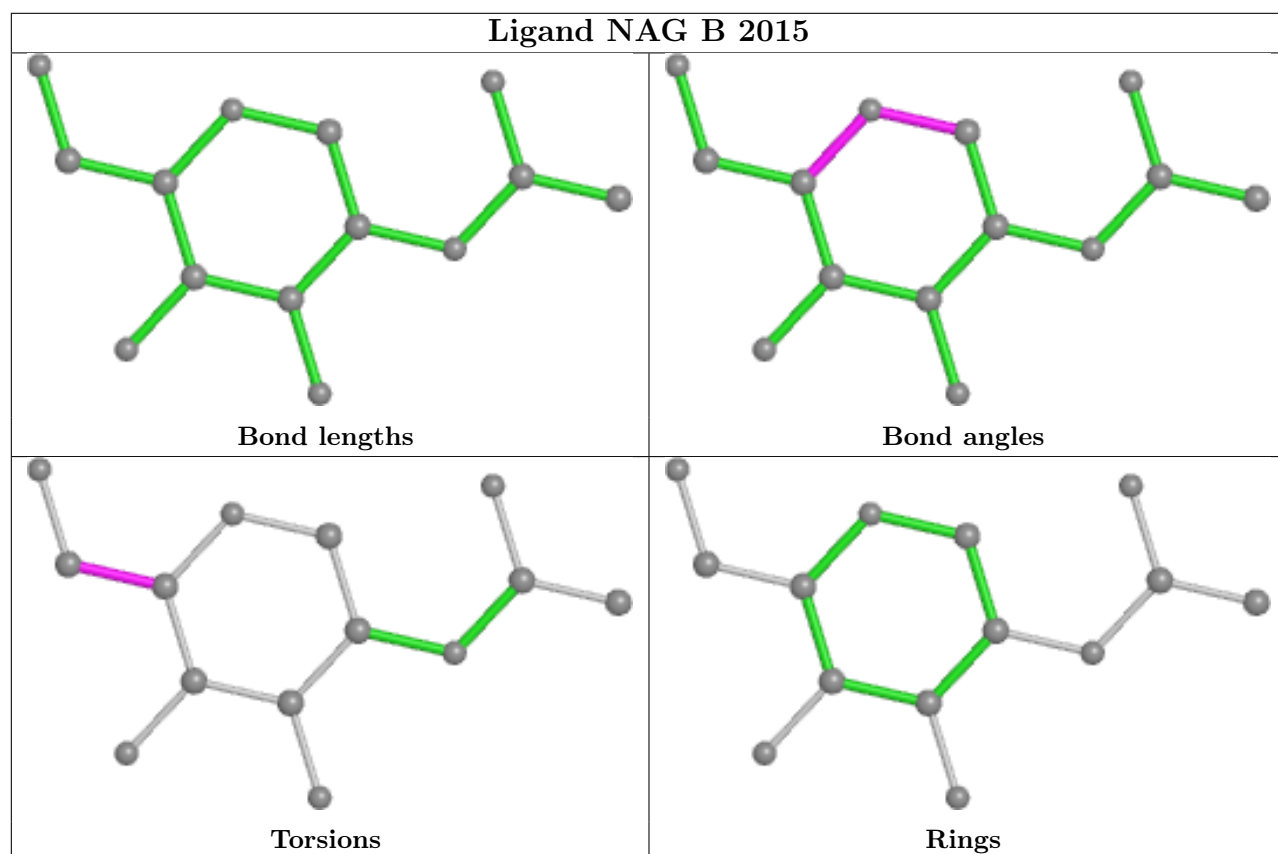
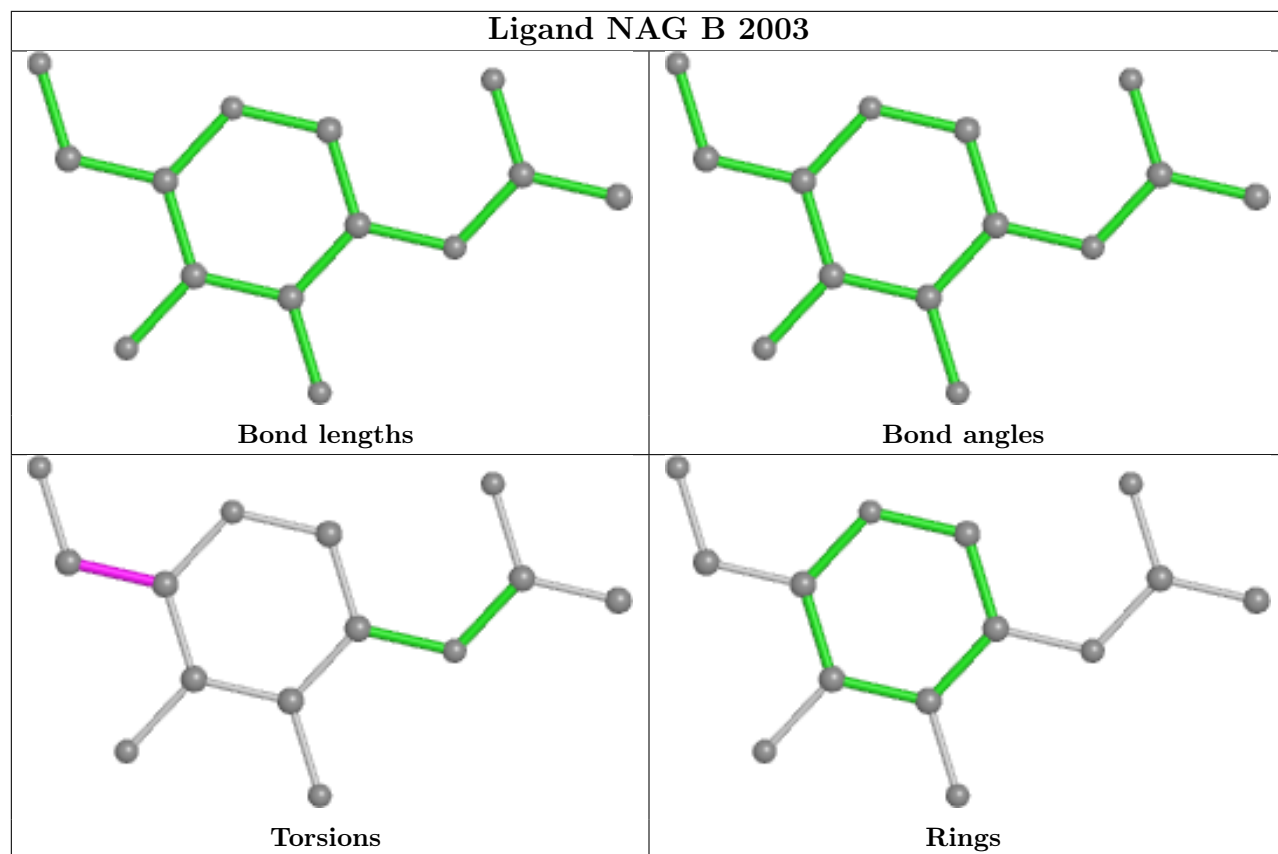


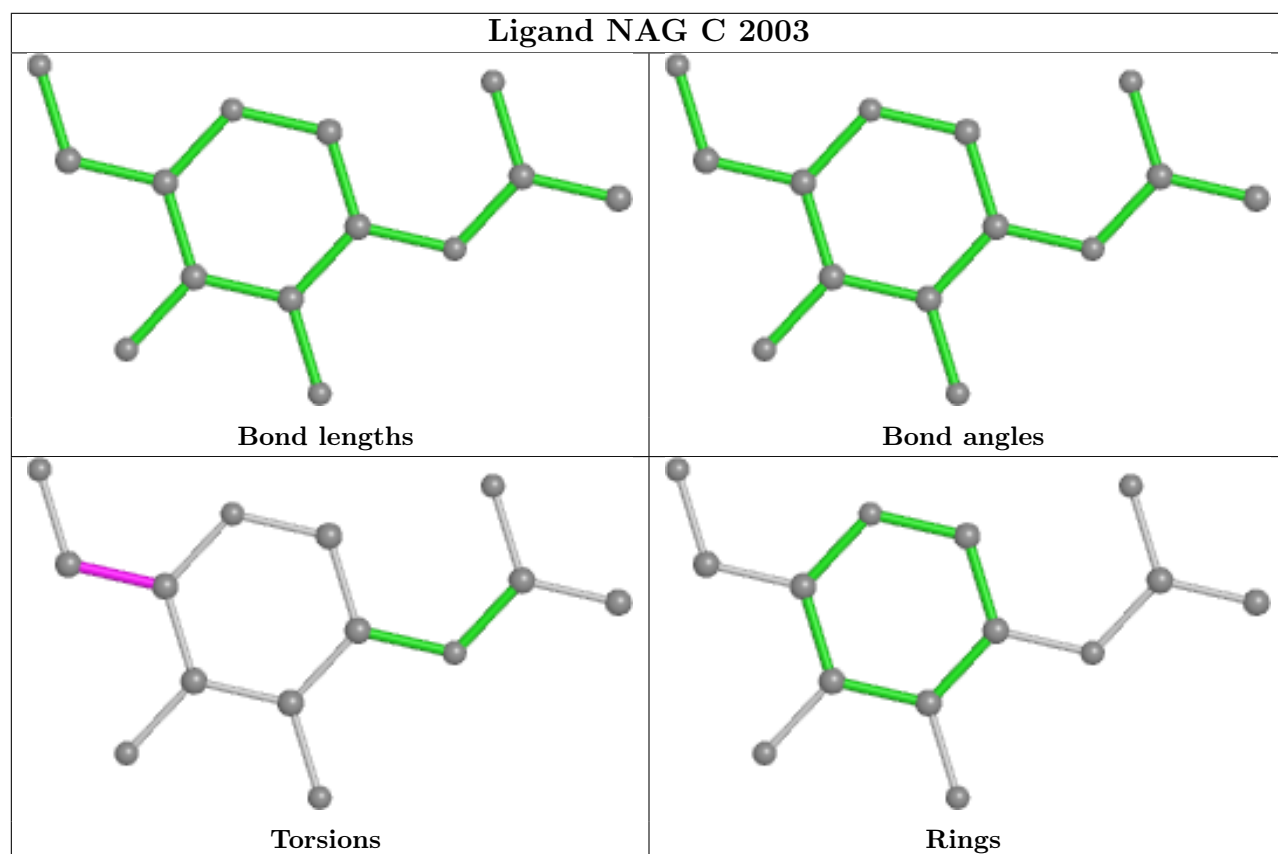
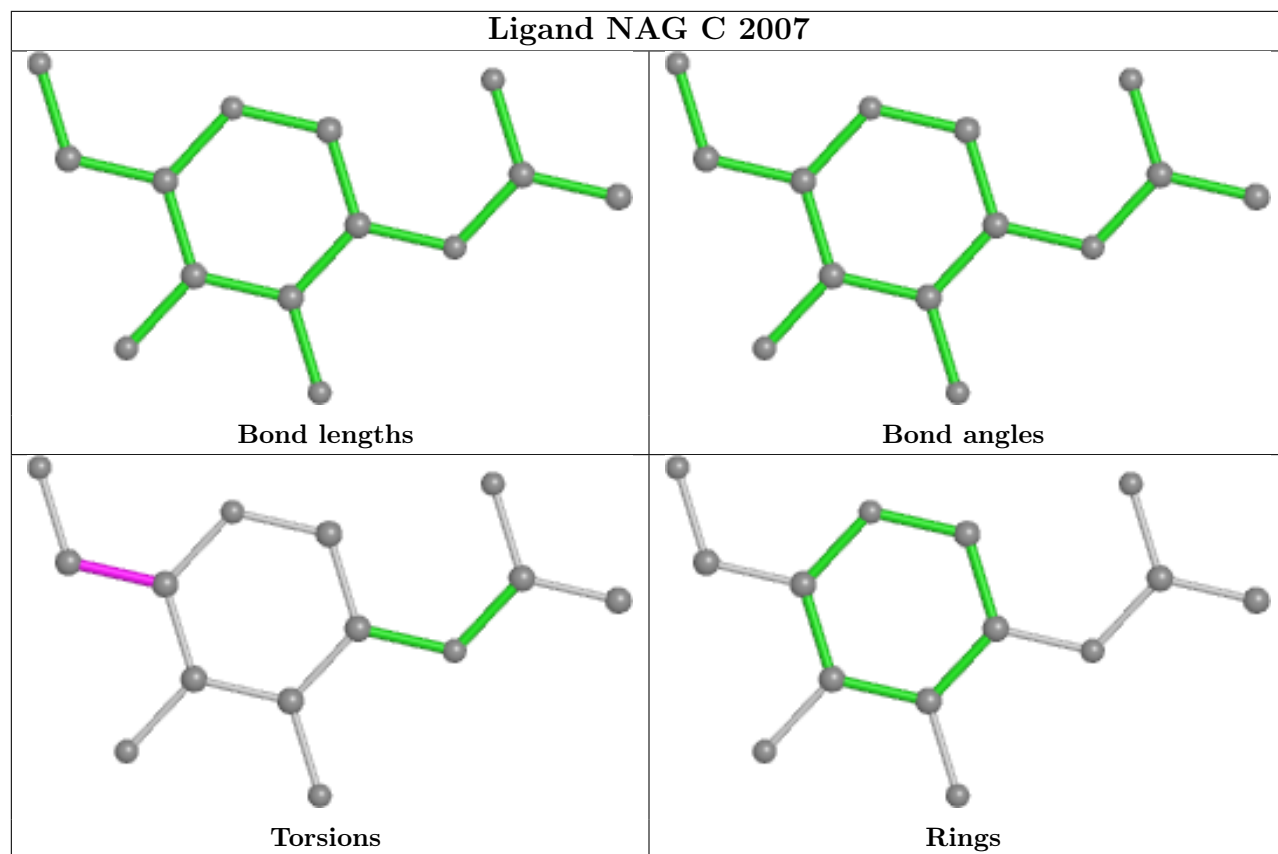




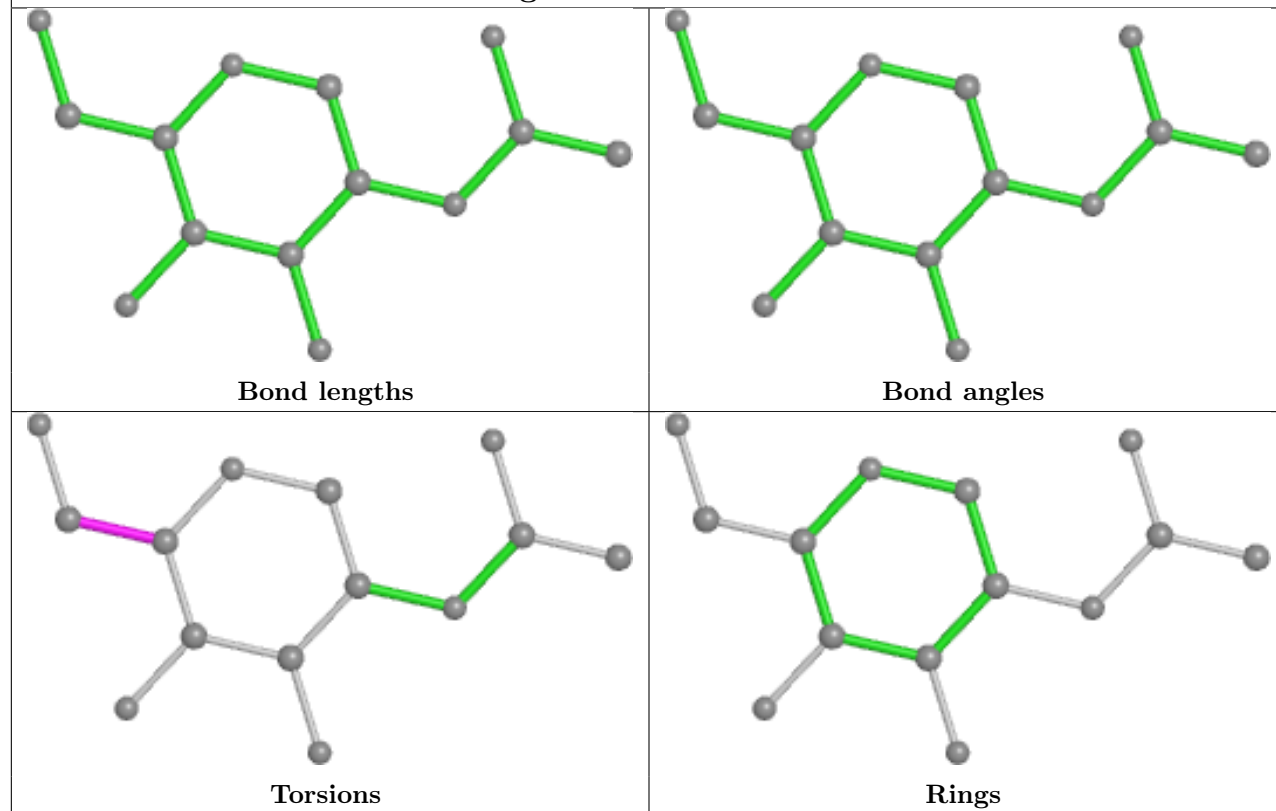




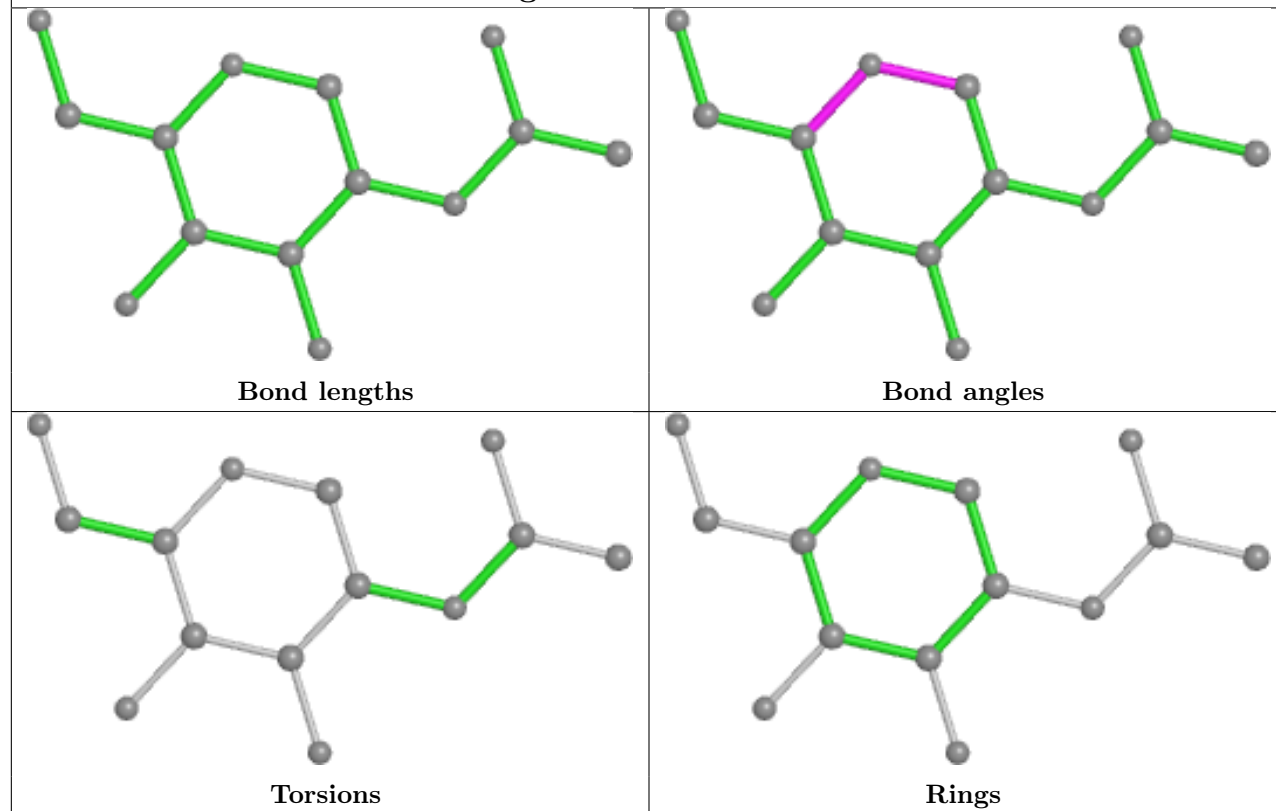


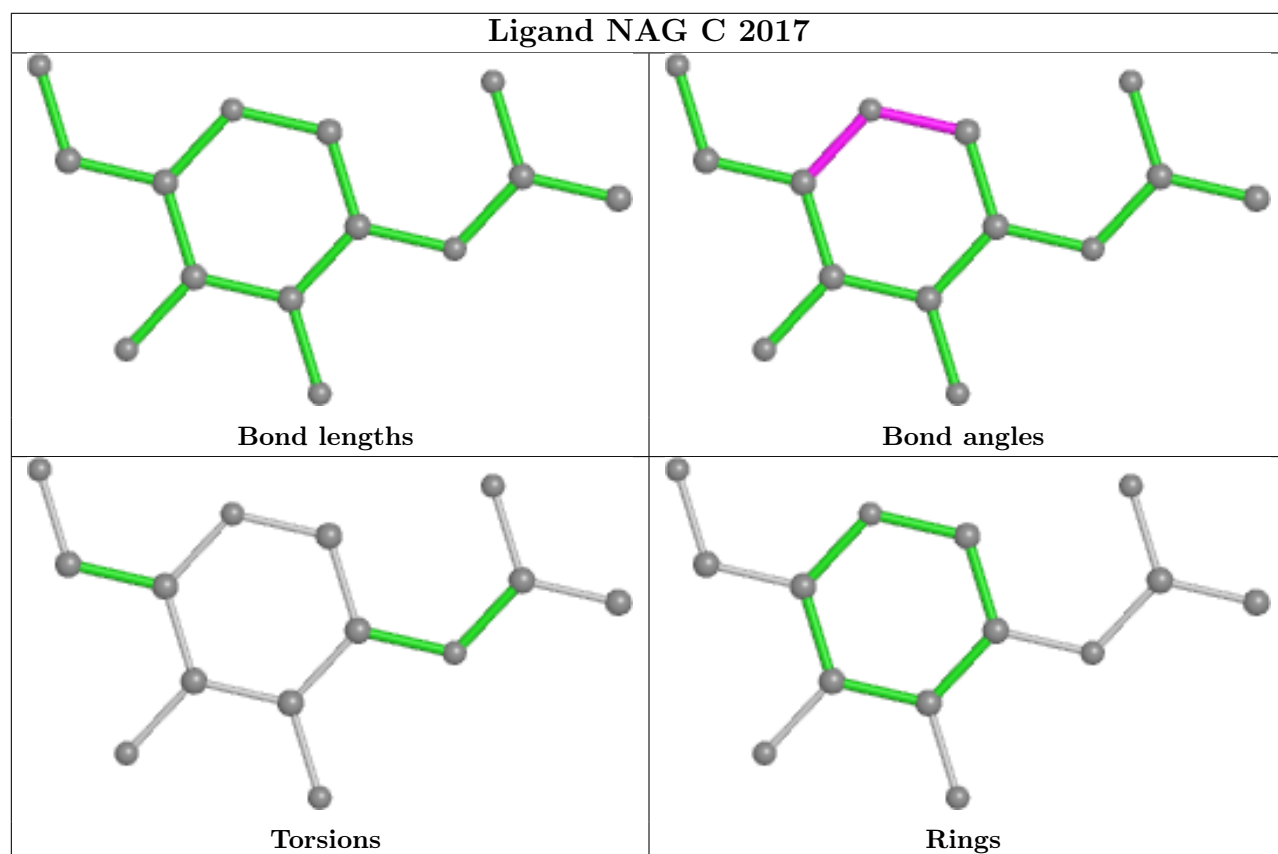
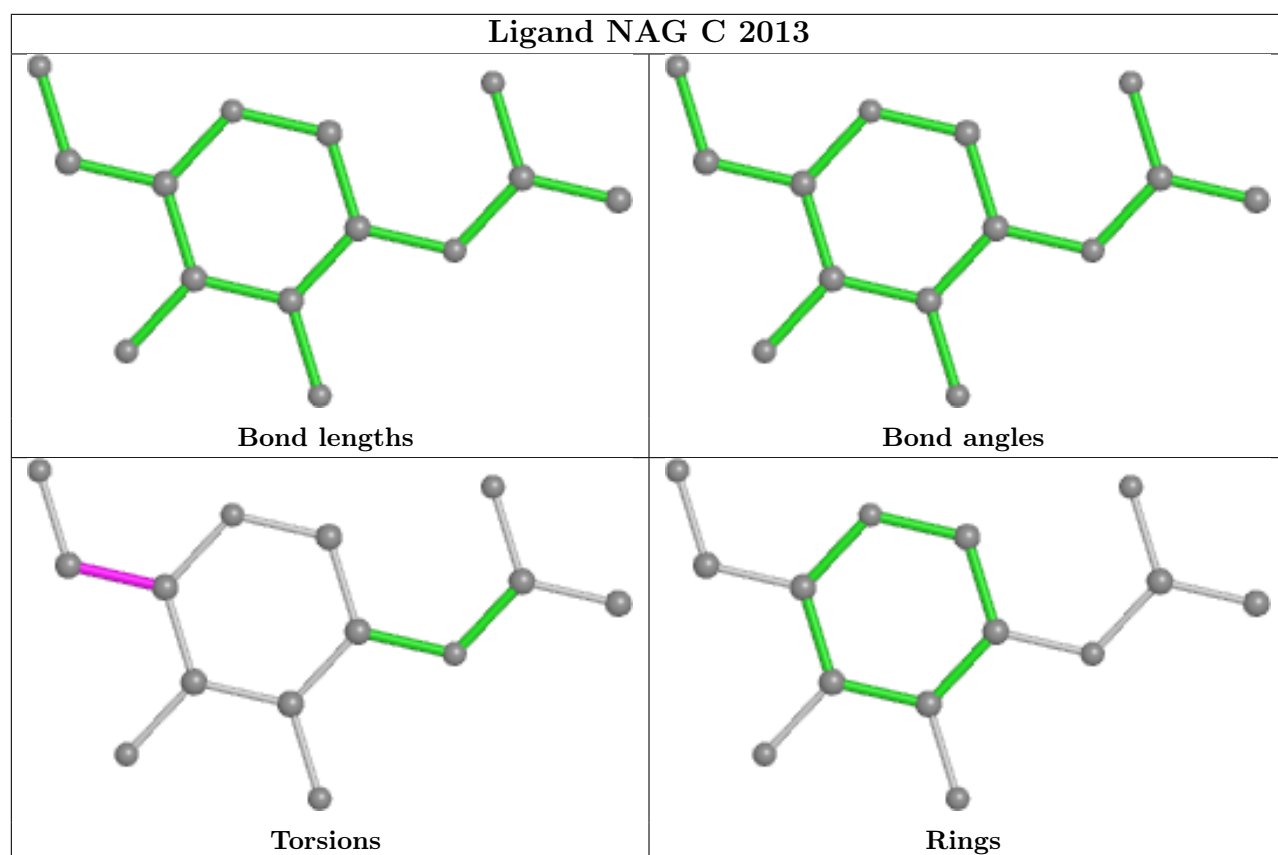


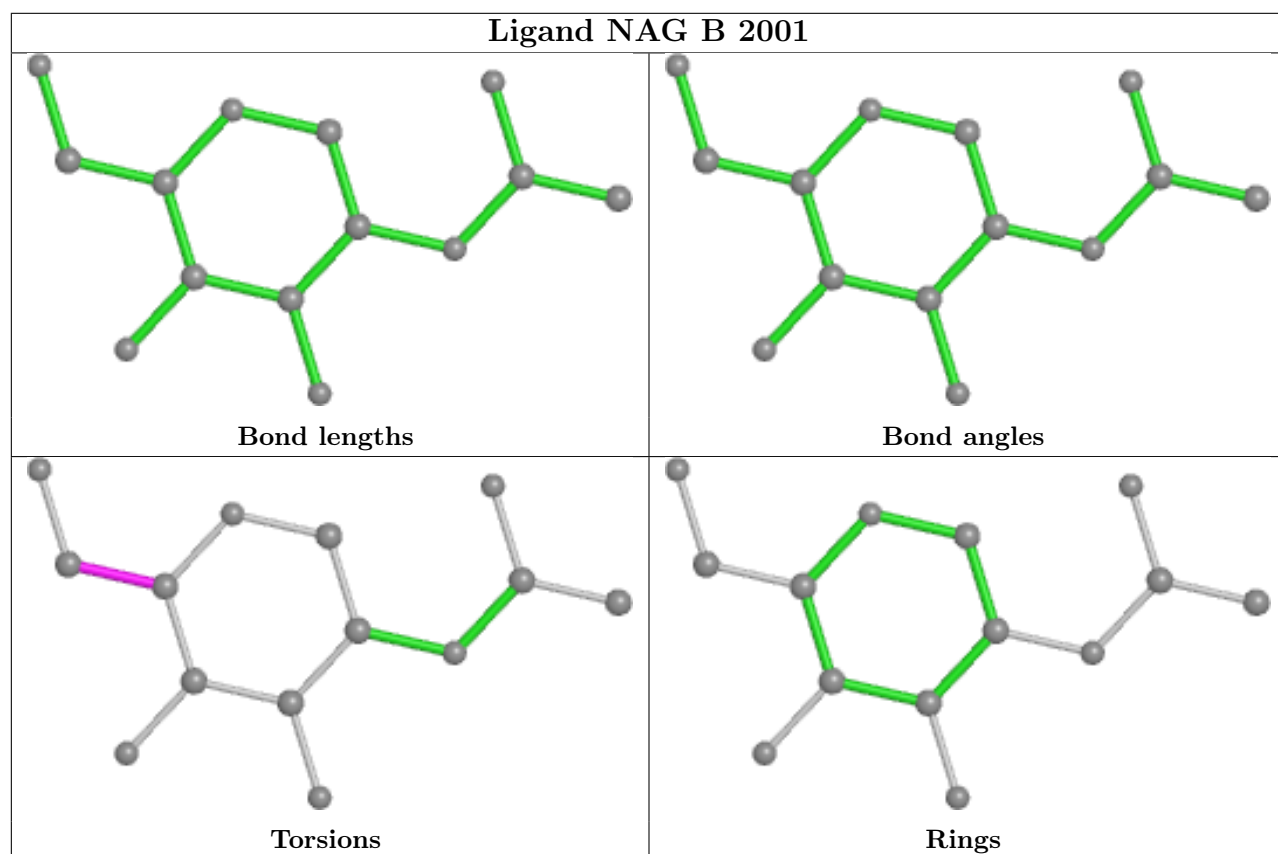
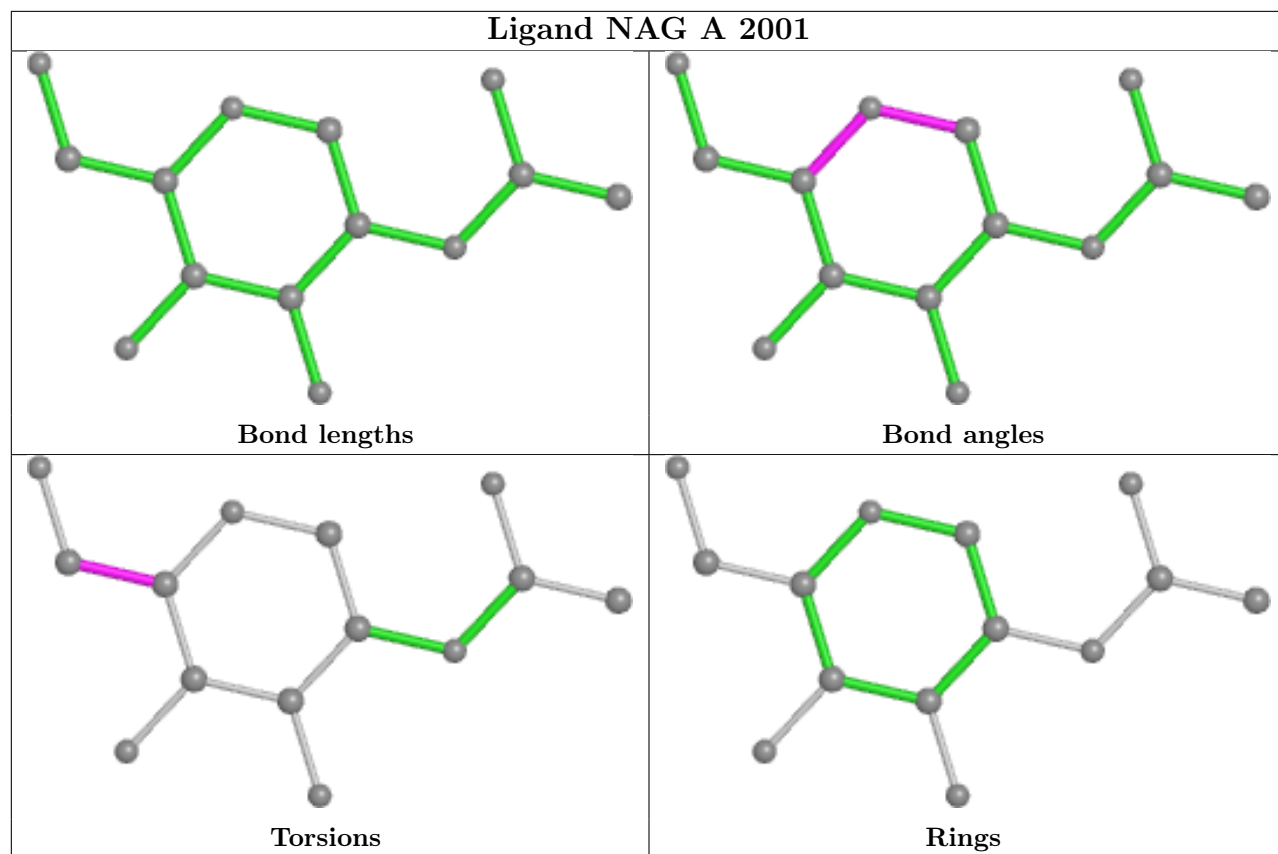
Ligand NAG B 2012

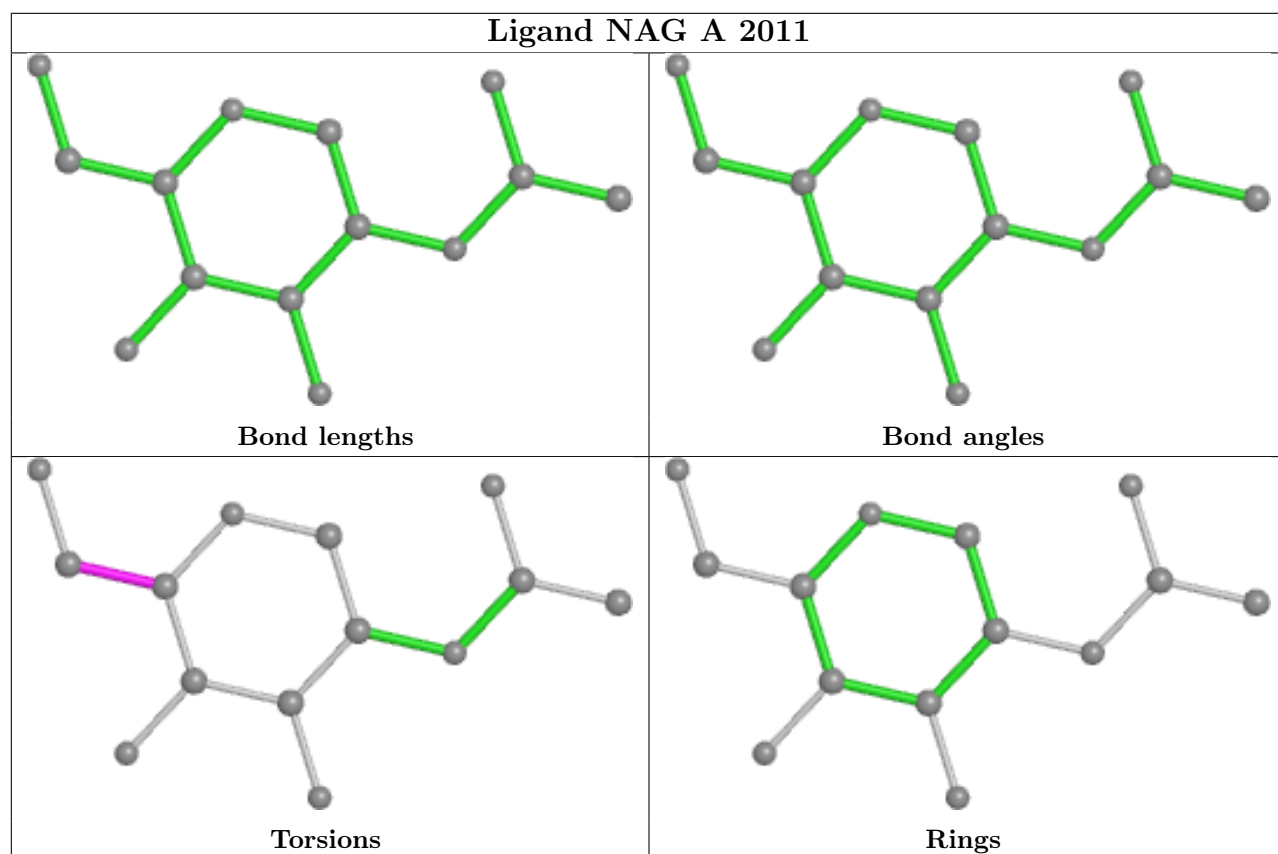
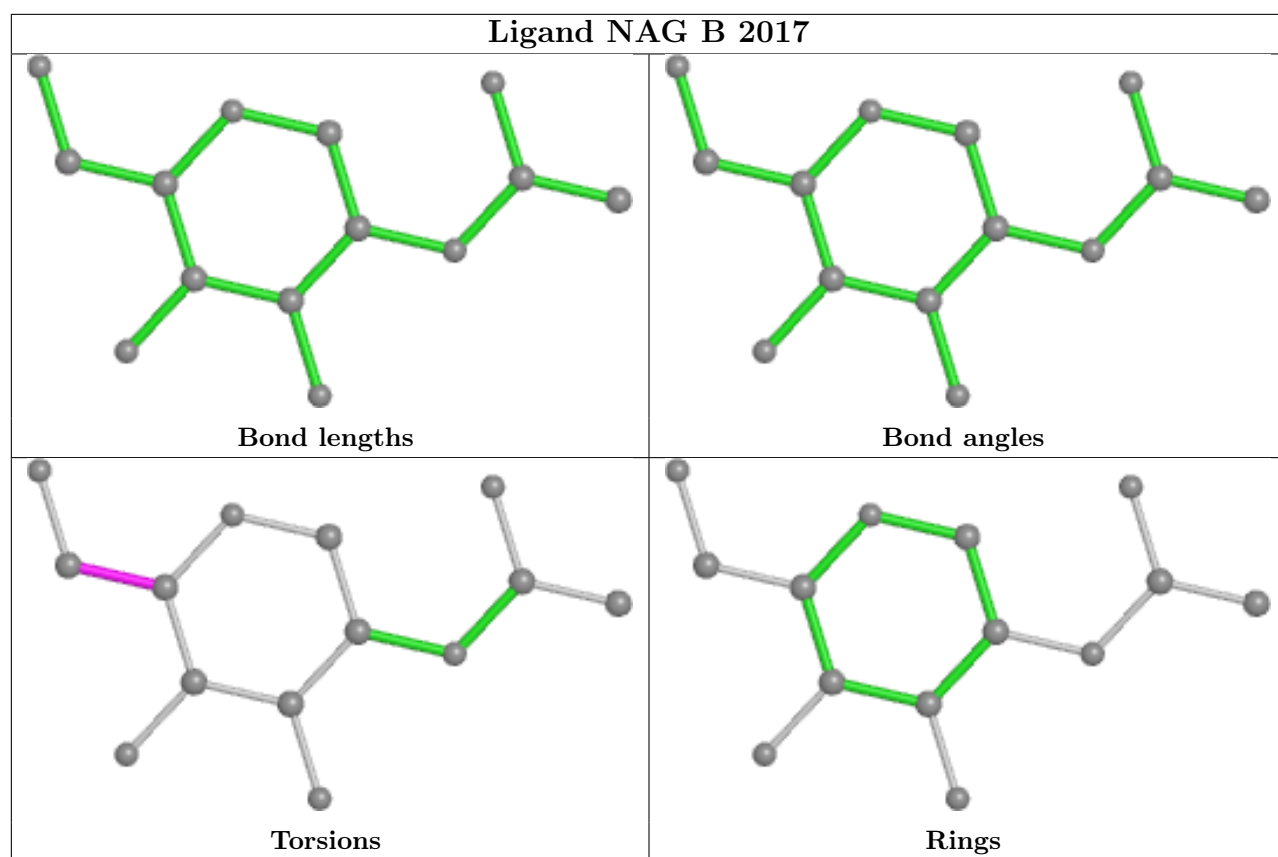


Ligand NAG C 2012





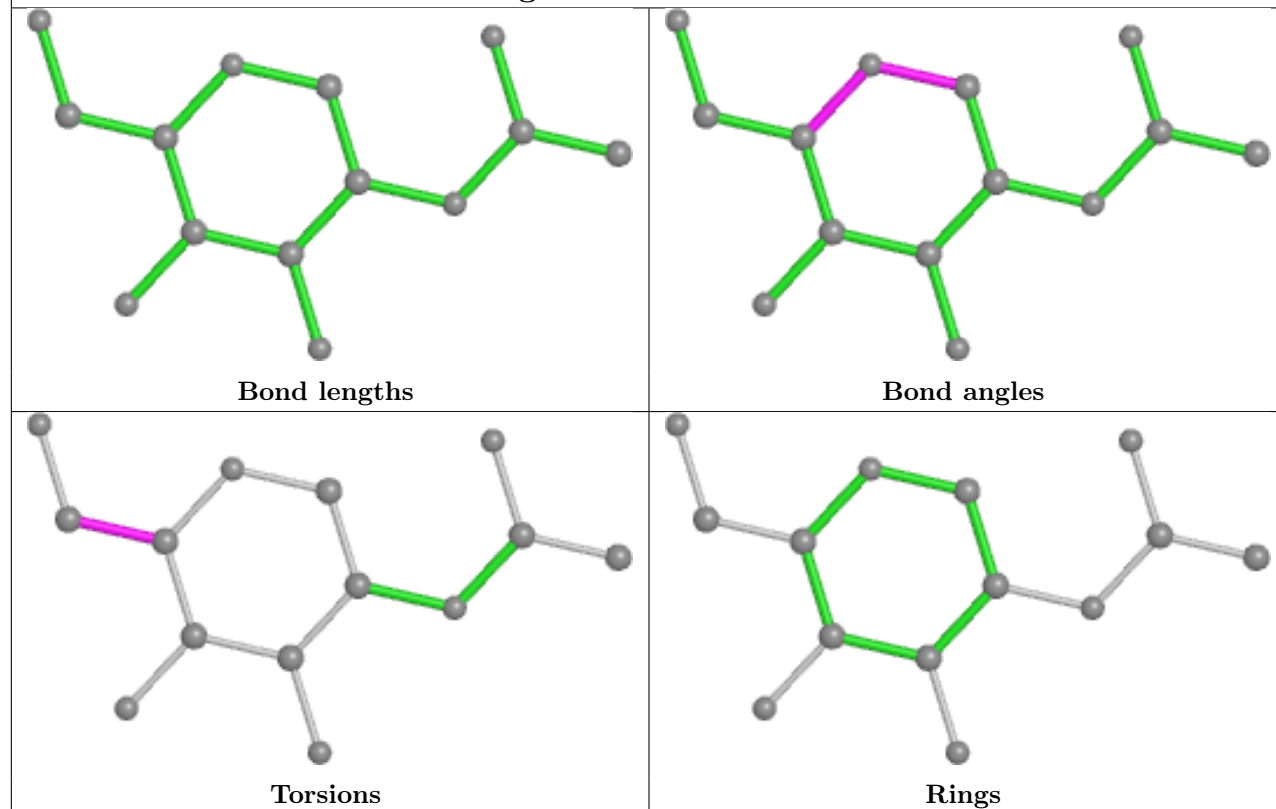


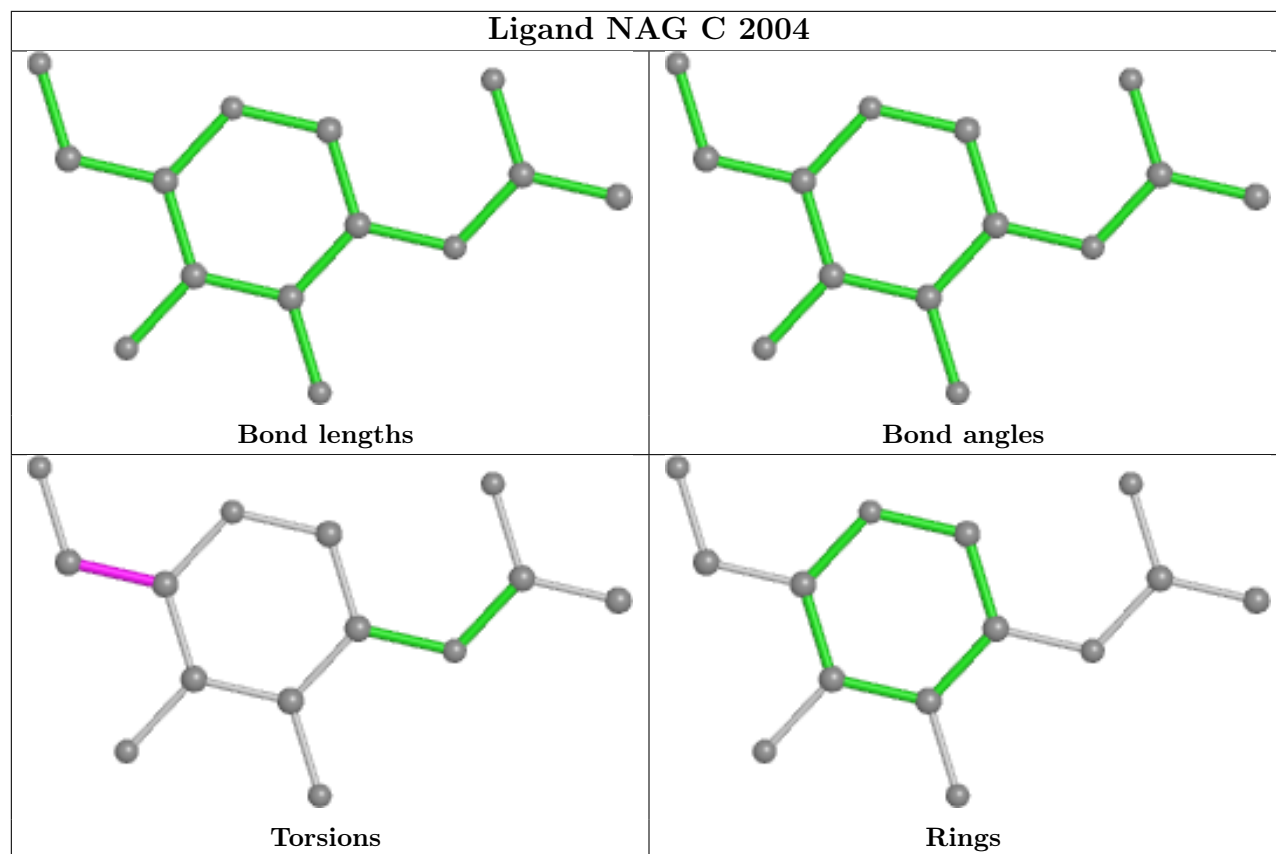


Ligand NAG A 2013



Ligand NAG A 2016





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.