



## Full wwPDB EM Validation Report ⓘ

Oct 16, 2024 – 01:00 AM JST

PDB ID : 8Y1D  
EMDB ID : EMD-38832  
Title : 2up-TM conformation of HKU1-B S protein after incubation of the receptor  
Authors : Xia, L.Y.; Zhang, Y.Y.; Zhou, Q.  
Deposited on : 2024-01-24  
Resolution : 2.70 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](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>.

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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

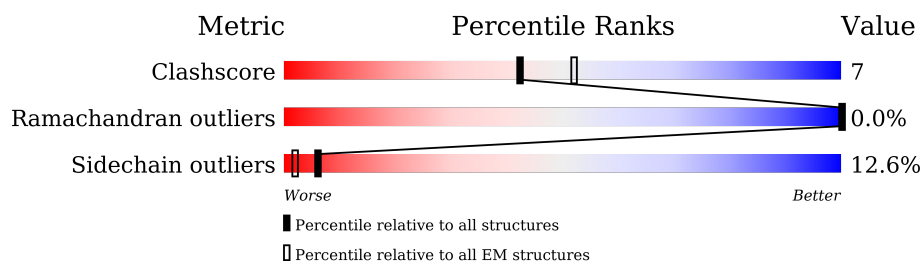
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.70 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	75% 16% • 6%
1	B	1290	73% 18% • 6%
1	C	1290	75% 16% • 6%
2	D	384	54% 29% 6% 10%
2	E	384	55% 29% 5% 10%
3	F	6	33% 50% 17%
3	K	6	17% 83%
3	P	6	17% 83%
4	G	2	100%

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Mol	Chain	Length	Quality of chain
4	H	2	 50% 50%
4	I	2	 50% 50%
4	J	2	 100%
4	L	2	 100%
4	M	2	 50% 50%
4	N	2	 100%
4	O	2	 100%
4	Q	2	 50% 50%
4	R	2	 100%
4	S	2	 100%
4	T	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NAG	B	2001	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 34921 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

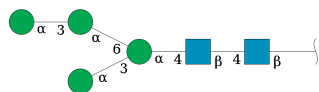
- Molecule 2 is a protein called Transmembrane protease serine 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	345	Total	C	N	O	S	0	0
			2690	1702	467	498	23		
2	E	345	Total	C	N	O	S	0	0
			2690	1702	467	498	23		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	255	GLN	ARG	conflict	UNP O15393
E	255	GLN	ARG	conflict	UNP O15393

- Molecule 3 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
3	F	6	Total	C	N	O	0	0
			72	40	2	30		
3	K	6	Total	C	N	O	0	0
			72	40	2	30		
3	P	6	Total	C	N	O	0	0
			72	40	2	30		

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



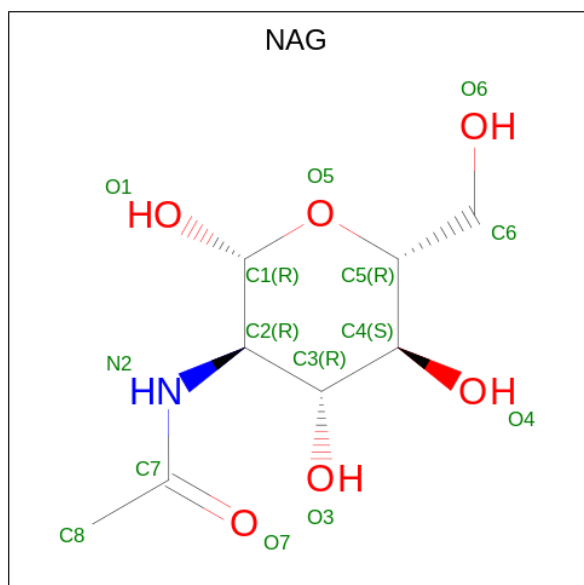
Mol	Chain	Residues	Atoms				AltConf	Trace
4	G	2	Total	C	N	O	0	0
			28	16	2	10		
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		
4	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	N	2	Total	C	N	O	0	0
			28	16	2	10		
4	O	2	Total	C	N	O	0	0
			28	16	2	10		
4	Q	2	Total	C	N	O	0	0
			28	16	2	10		
4	R	2	Total	C	N	O	0	0
			28	16	2	10		
4	S	2	Total	C	N	O	0	0
			28	16	2	10		
4	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 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
5	A	1	Total	C	N	O	0
			14	8	1	5	
5	A	1	Total	C	N	O	0
			14	8	1	5	

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

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

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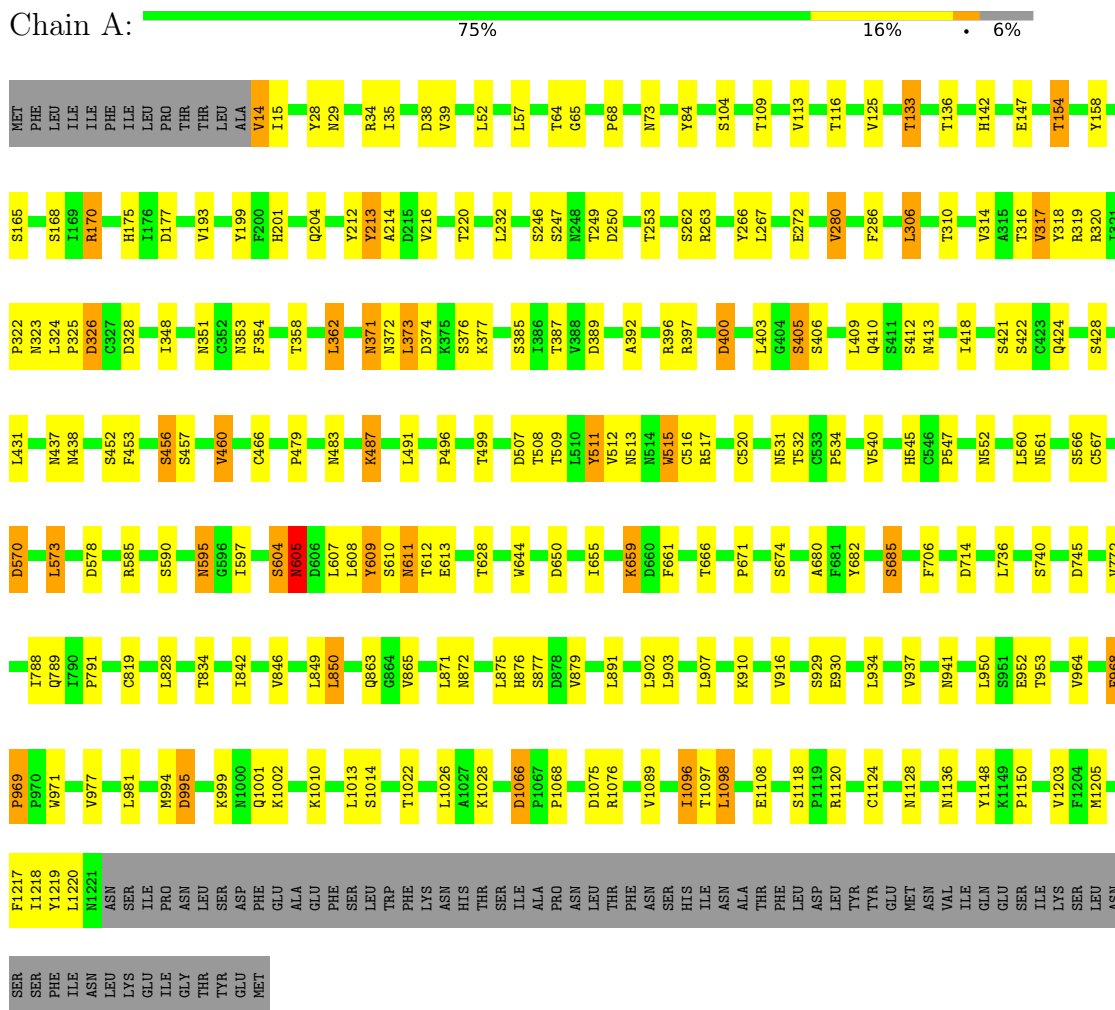
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	

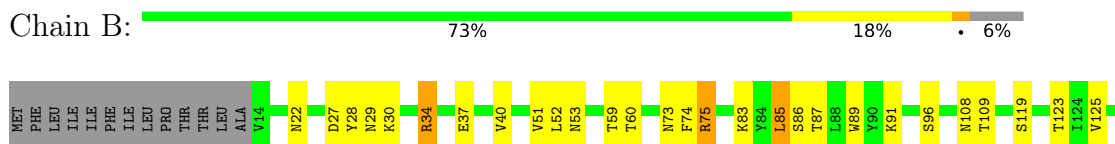
### 3 Residue-property plots

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.

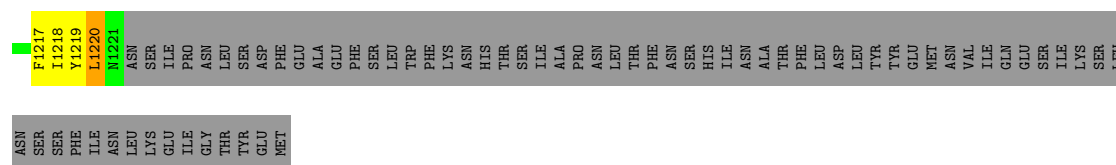
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein

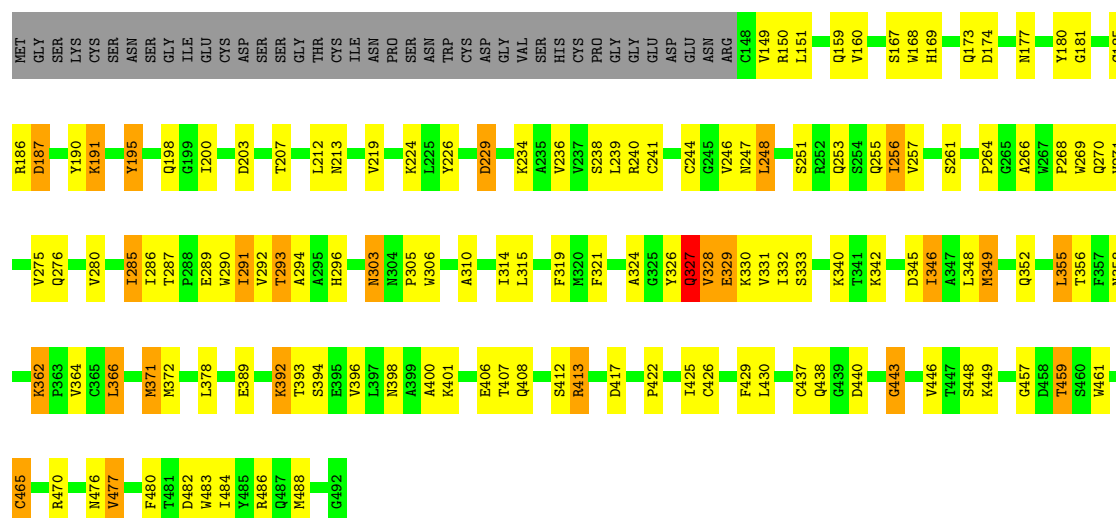






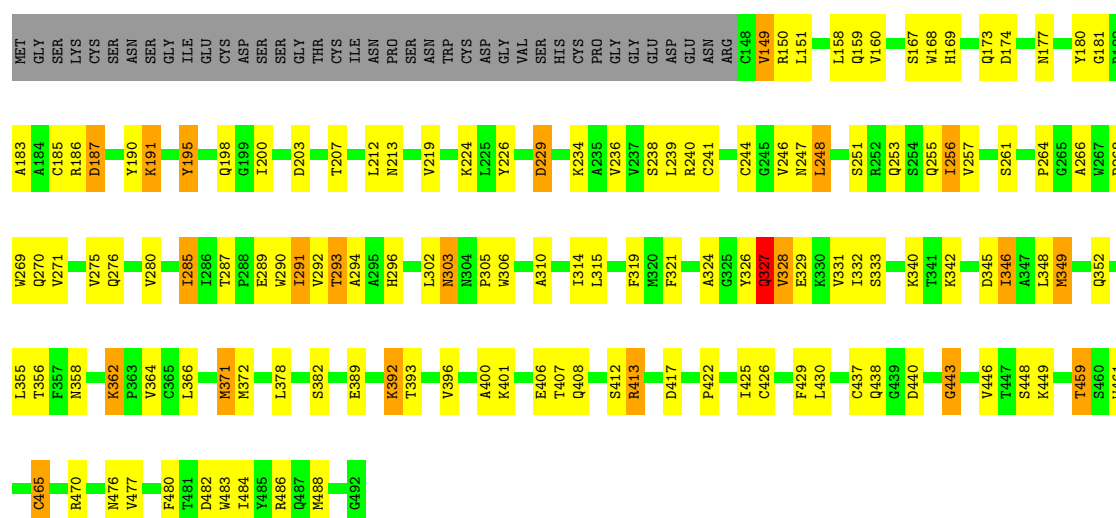
### • Molecule 2: Transmembrane protease serine 2

Chain D:



### • Molecule 2: Transmembrane protease serine 2

Chain E:



### • Molecule 3: 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

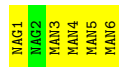
Chain F:

33% 50% 17%



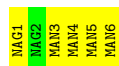
- Molecule 3:  $\alpha$ -D-mannopyranose-(1-3)- $\alpha$ -D-mannopyranose-(1-6)-[ $\alpha$ -D-mannopyranose-(1-3)] $\alpha$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



- Molecule 3:  $\alpha$ -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 P:



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

Chain G:



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

Chain H:



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

Chain I:



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

Chain J:



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain O:  100%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%

MAG1  
MAG2

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

Chain T: 

MAG1  
MAG2

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	408603	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	0.55	0/9653	0.61	0/13146
1	B	0.53	0/9653	0.60	1/13146 (0.0%)
1	C	0.45	0/9653	0.58	0/13146
2	D	0.47	0/2762	0.62	0/3755
2	E	0.47	0/2762	0.62	0/3755
All	All	0.50	0/34483	0.60	1/46948 (0.0%)

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	2
2	D	0	3
2	E	0	3
All	All	0	14

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	604	SER	CB-CA-C	5.78	121.08	110.10

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	819	CYS	Peptide
1	A	929	SER	Peptide
1	A	968	PHE	Peptide
1	A	969	PRO	Peptide
1	B	929	SER	Peptide
1	B	930	GLU	Peptide
1	C	930	GLU	Peptide
1	C	969	PRO	Peptide
2	D	256	ILE	Peptide
2	D	327	GLN	Peptide
2	D	443	GLY	Peptide
2	E	256	ILE	Peptide
2	E	327	GLN	Peptide
2	E	443	GLY	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	9075	97	0
1	B	9425	0	9075	134	0
1	C	9425	0	9075	89	0
2	D	2690	0	2592	71	0
2	E	2690	0	2592	71	0
3	F	72	0	61	1	0
3	K	72	0	61	0	0
3	P	72	0	61	1	0
4	G	28	0	25	0	0
4	H	28	0	25	0	0
4	I	28	0	25	0	0
4	J	28	0	25	0	0
4	L	28	0	25	0	0
4	M	28	0	25	0	0
4	N	28	0	25	2	0
4	O	28	0	25	0	0
4	Q	28	0	25	2	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0
4	T	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	238	0	221	1	0
5	B	238	0	221	11	0
5	C	238	0	221	0	0
All	All	34921	0	33555	446	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 7.

All (446) 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:22:ASN:ND2	5:B:2001:NAG:H5	1.53	1.24
1:C:132:ASN:OD1	1:C:154:THR:HG23	1.42	1.16
1:B:379:PHE:HD1	1:B:606:ASP:HB2	1.04	1.07
1:B:379:PHE:CD1	1:B:606:ASP:HB2	1.96	1.00
1:B:379:PHE:HD1	1:B:606:ASP:CB	1.75	0.98
1:B:22:ASN:HD22	5:B:2001:NAG:H5	1.28	0.91
1:B:22:ASN:HD21	5:B:2001:NAG:H5	1.37	0.90
1:C:186:LYS:HE3	4:Q:1:NAG:H83	1.54	0.90
1:B:22:ASN:ND2	5:B:2001:NAG:C5	2.35	0.89
1:B:354:PHE:CZ	1:B:604:SER:OG	2.26	0.87
1:B:351:ASN:OD1	1:C:183:CYS:HB2	1.77	0.85
1:B:380:GLY:HA2	1:B:607:LEU:HD22	1.59	0.84
1:B:487:LYS:HZ3	1:B:515:TRP:HZ3	1.29	0.79
1:C:132:ASN:OD1	1:C:154:THR:CG2	2.27	0.77
1:B:355:ASN:HB3	1:B:605:ASN:OD1	1.85	0.76
1:A:487:LYS:HZ3	1:A:515:TRP:HZ3	1.32	0.75
1:B:379:PHE:CD1	1:B:606:ASP:CB	2.64	0.74
1:B:354:PHE:CE1	1:B:604:SER:CB	2.70	0.74
1:B:354:PHE:CZ	1:B:604:SER:CB	2.70	0.74
1:A:320:ARG:HG2	1:A:607:LEU:HD13	1.71	0.73
1:B:354:PHE:CE1	1:B:604:SER:HB2	2.25	0.72
1:B:354:PHE:CE2	1:B:604:SER:OG	2.41	0.70
1:B:354:PHE:CZ	1:B:604:SER:HB2	2.26	0.69
2:D:159:GLN:HB3	2:D:168:TRP:HB3	1.75	0.68
2:E:159:GLN:HB3	2:E:168:TRP:HB3	1.75	0.68
1:A:320:ARG:HG2	1:A:607:LEU:CD1	2.24	0.68
1:A:487:LYS:HB2	1:A:515:TRP:HB2	1.78	0.65
1:A:318:TYR:HB3	1:A:609:TYR:O	1.96	0.65
1:A:374:ASP:HB2	1:A:377:LYS:HG2	1.79	0.65
1:B:358:THR:O	1:B:362:LEU:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:THR:O	1:A:362:LEU:HB2	1.96	0.64
1:B:607:LEU:HG	1:B:608:LEU:H	1.62	0.64
1:B:552:ASN:HB2	1:B:573:LEU:HD21	1.79	0.64
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.79	0.64
1:A:552:ASN:HB2	1:A:573:LEU:HD21	1.79	0.64
1:A:428:SER:OG	1:A:585:ARG:NH1	2.30	0.64
1:B:379:PHE:O	1:B:607:LEU:HD23	1.98	0.64
1:B:487:LYS:HB2	1:B:515:TRP:HB2	1.78	0.64
1:B:428:SER:OG	1:B:585:ARG:NH1	2.30	0.63
1:B:374:ASP:HB2	1:B:377:LYS:HG2	1.79	0.63
1:C:494:ILE:HD12	3:F:5:MAN:H62	1.80	0.63
1:B:22:ASN:ND2	5:B:2001:NAG:C4	2.61	0.63
1:B:355:ASN:CB	1:B:605:ASN:OD1	2.47	0.62
1:B:379:PHE:HA	1:B:606:ASP:OD2	1.99	0.62
1:C:135:TYR:HA	1:C:151:CYS:O	2.00	0.61
1:B:22:ASN:HD22	5:B:2001:NAG:C5	2.06	0.61
1:A:318:TYR:O	1:A:610:SER:HA	2.01	0.60
1:C:561:ASN:N	1:C:561:ASN:OD1	2.35	0.60
1:B:379:PHE:O	1:B:607:LEU:CD2	2.49	0.60
1:A:317:VAL:HA	1:A:611:ASN:HD21	1.66	0.60
1:C:459:ASP:HA	1:C:578:ASP:O	2.02	0.59
1:A:487:LYS:NZ	2:D:417:ASP:OD2	2.36	0.58
1:C:88:LEU:HA	1:C:91:LYS:HD3	1.84	0.58
1:A:214:ALA:HB2	1:A:220:THR:HA	1.86	0.58
1:B:487:LYS:NZ	2:E:417:ASP:OD2	2.36	0.58
1:C:319:ARG:NH1	1:C:612:THR:O	2.37	0.58
1:B:213:TYR:HB3	1:B:223:LEU:HD22	1.86	0.57
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.87	0.57
1:B:452:SER:OG	1:B:453:PHE:N	2.38	0.57
1:A:952:GLU:HG3	1:A:1136:ASN:HD21	1.69	0.57
2:D:303:ASN:OD1	2:D:303:ASN:N	2.38	0.57
1:A:1076:ARG:NH2	1:B:1075:ASP:OD2	2.37	0.57
1:A:319:ARG:NH1	1:A:611:ASN:O	2.37	0.57
1:B:1205:MET:HG2	1:C:994:MET:HG2	1.85	0.56
2:D:412:SER:OG	2:D:413:ARG:N	2.38	0.56
1:A:507:ASP:OD2	2:D:470:ARG:NH1	2.38	0.56
1:B:22:ASN:ND2	5:B:2001:NAG:H3	2.21	0.56
1:A:479:PRO:O	1:A:483:ASN:ND2	2.38	0.56
1:B:507:ASP:OD2	2:E:470:ARG:NH1	2.38	0.56
2:E:303:ASN:OD1	2:E:303:ASN:N	2.38	0.56
1:A:611:ASN:HB2	1:A:613:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1018:GLY:O	1:B:1023:ASN:ND2	2.38	0.56
2:E:417:ASP:OD1	2:E:417:ASP:N	2.33	0.56
1:B:108:ASN:HD21	1:B:119:SER:HB3	1.70	0.56
1:B:160:HIS:NE2	1:B:171:ASN:O	2.39	0.56
1:B:479:PRO:O	1:B:483:ASN:ND2	2.38	0.56
1:C:447:ARG:NH2	1:C:473:PHE:O	2.39	0.56
1:C:482:VAL:HG23	1:C:490:PRO:HD2	1.87	0.56
1:A:204:GLN:HE22	1:A:232:LEU:H	1.54	0.55
2:D:314:ILE:HG21	2:D:319:PHE:HB2	1.88	0.55
2:E:314:ILE:HG21	2:E:319:PHE:HB2	1.88	0.55
1:A:508:THR:HG23	1:A:513:ASN:HA	1.89	0.55
1:C:205:GLU:OE2	1:C:206:ARG:NH1	2.40	0.55
1:B:820:SER:OG	1:B:821:ASN:N	2.38	0.55
1:B:409:LEU:HA	1:B:413:ASN:HD22	1.71	0.55
1:B:1108:GLU:OE2	1:B:1120:ARG:NH2	2.40	0.55
1:A:385:SER:OG	1:A:595:ASN:ND2	2.39	0.55
1:B:508:THR:HG23	1:B:513:ASN:HA	1.89	0.55
1:B:1196:PRO:O	1:B:1201:ASN:ND2	2.40	0.55
1:C:301:THR:HG23	1:C:682:TYR:HA	1.88	0.55
2:D:371:MET:O	2:D:449:LYS:NZ	2.39	0.55
1:A:409:LEU:HA	1:A:413:ASN:HD22	1.72	0.55
1:B:22:ASN:HD21	5:B:2001:NAG:C5	2.09	0.55
2:E:306:TRP:HA	2:E:328:VAL:HG21	1.89	0.55
1:A:38:ASP:O	1:A:73:ASN:ND2	2.39	0.55
1:C:396:ARG:NE	1:C:578:ASP:OD2	2.39	0.55
2:E:371:MET:O	2:E:449:LYS:NZ	2.39	0.54
2:E:310:ALA:O	2:E:327:GLN:NE2	2.40	0.54
1:B:246:SER:OG	1:B:247:SER:N	2.40	0.54
1:C:409:LEU:HA	1:C:413:ASN:HD22	1.73	0.54
2:E:177:ASN:O	2:E:181:GLY:N	2.40	0.54
2:D:185:CYS:HB3	2:D:190:TYR:HB2	1.90	0.54
2:D:306:TRP:HA	2:D:328:VAL:HG21	1.89	0.54
2:E:264:PRO:HG3	2:E:315:LEU:HD11	1.90	0.54
1:A:1128:ASN:HB3	1:A:1148:TYR:HB3	1.89	0.54
2:D:264:PRO:HG3	2:D:315:LEU:HD11	1.90	0.54
1:B:570:ASP:OD1	1:B:570:ASP:N	2.32	0.54
1:A:995:ASP:OD1	1:A:995:ASP:N	2.39	0.54
2:D:293:THR:OG1	2:D:294:ALA:N	2.41	0.54
1:A:452:SER:OG	1:A:453:PHE:N	2.38	0.54
1:B:607:LEU:HG	1:B:608:LEU:N	2.21	0.54
2:D:268:PRO:O	2:D:362:LYS:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:185:CYS:HB3	2:E:190:TYR:HB2	1.90	0.54
1:B:405:SER:OG	1:B:406:SER:N	2.41	0.53
2:D:310:ALA:O	2:D:327:GLN:NE2	2.40	0.53
2:D:356:THR:OG1	2:D:358:ASN:ND2	2.42	0.53
2:E:247:ASN:ND2	2:E:266:ALA:O	2.41	0.53
1:A:400:ASP:OD2	1:A:409:LEU:N	2.41	0.53
1:A:405:SER:OG	1:A:406:SER:N	2.41	0.53
1:B:385:SER:OG	1:B:595:ASN:ND2	2.39	0.53
1:A:376:SER:OG	1:A:377:LYS:NZ	2.39	0.53
2:D:417:ASP:OD1	2:D:417:ASP:N	2.33	0.53
1:B:400:ASP:OD2	1:B:409:LEU:N	2.41	0.53
1:A:371:ASN:OD1	1:A:372:ASN:ND2	2.41	0.53
1:B:1098:LEU:HD13	1:C:1097:THR:HG23	1.90	0.53
1:C:1066:ASP:OD1	1:C:1066:ASP:N	2.41	0.53
1:B:187:LYS:HD2	1:B:188:ASN:H	1.74	0.53
1:B:422:SER:OG	1:B:424:GLN:NE2	2.39	0.53
2:E:356:THR:OG1	2:E:358:ASN:ND2	2.42	0.53
1:C:186:LYS:HE3	4:Q:1:NAG:C8	2.34	0.53
1:C:448:TYR:OH	1:C:474:CYS:SG	2.66	0.53
2:D:187:ASP:OD1	2:D:187:ASP:N	2.41	0.53
2:E:150:ARG:NE	2:E:159:GLN:OE1	2.39	0.53
2:E:293:THR:OG1	2:E:294:ALA:N	2.41	0.53
2:E:407:THR:OG1	2:E:408:GLN:NE2	2.38	0.53
1:A:216:VAL:HG22	5:A:2006:NAG:H82	1.90	0.53
1:B:371:ASN:OD1	1:B:372:ASN:ND2	2.41	0.53
2:D:285:ILE:O	2:D:364:VAL:N	2.42	0.53
1:B:376:SER:OG	1:B:377:LYS:NZ	2.39	0.52
2:E:255:GLN:HB2	2:E:261:SER:HA	1.90	0.52
1:A:570:ASP:OD1	1:A:570:ASP:N	2.32	0.52
2:E:448:SER:O	2:E:448:SER:OG	2.27	0.52
1:A:400:ASP:O	1:A:410:GLN:NE2	2.41	0.52
2:D:247:ASN:ND2	2:D:266:ALA:O	2.41	0.52
1:A:353:ASN:HB3	1:A:605:ASN:OD1	2.09	0.52
1:C:110:LYS:HB3	1:C:117:LEU:HD11	1.90	0.52
2:D:255:GLN:HB2	2:D:261:SER:HA	1.90	0.52
2:D:321:PHE:H	2:D:324:ALA:HB3	1.73	0.52
2:E:412:SER:OG	2:E:413:ARG:N	2.38	0.52
1:A:326:ASP:OD1	1:A:326:ASP:N	2.42	0.52
2:D:160:VAL:N	2:D:169:HIS:O	2.42	0.52
2:E:270:GLN:NE2	2:E:271:VAL:O	2.39	0.52
1:A:246:SER:OG	1:A:247:SER:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ALA:HB2	1:B:220:THR:HA	1.91	0.52
1:B:325:PRO:O	1:B:352:CYS:HB2	2.09	0.52
2:D:160:VAL:H	2:D:169:HIS:H	1.57	0.52
1:C:402:GLN:HB2	1:C:405:SER:HB2	1.91	0.52
2:D:177:ASN:O	2:D:181:GLY:N	2.40	0.52
2:E:160:VAL:N	2:E:169:HIS:O	2.43	0.52
1:B:74:PHE:HB3	1:B:257:TRP:HB3	1.92	0.52
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.92	0.52
1:A:496:PRO:O	1:A:499:THR:OG1	2.28	0.52
1:A:1097:THR:HG23	1:C:1098:LEU:HD13	1.92	0.52
1:B:456:SER:OG	1:B:457:SER:N	2.41	0.52
1:C:475:PRO:HB3	1:C:553:GLU:HG3	1.92	0.52
1:B:566:SER:OG	1:B:567:CYS:N	2.43	0.52
1:C:396:ARG:HG3	1:C:397:ARG:HG2	1.92	0.52
1:B:59:THR:OG1	1:B:60:THR:N	2.43	0.51
1:C:735:ASP:OD1	1:C:735:ASP:N	2.42	0.51
1:B:937:VAL:O	1:B:941:ASN:ND2	2.37	0.51
1:C:29:ASN:HD22	1:C:30:LYS:H	1.59	0.51
2:D:256:ILE:HG13	2:D:400:ALA:H	1.75	0.51
2:E:321:PHE:H	2:E:324:ALA:HB3	1.73	0.51
1:A:566:SER:OG	1:A:567:CYS:N	2.43	0.51
1:B:850:LEU:HD13	1:B:1096:ILE:HD11	1.92	0.51
2:E:160:VAL:H	2:E:169:HIS:H	1.57	0.51
2:E:285:ILE:O	2:E:364:VAL:N	2.42	0.51
1:B:348:ILE:HG12	1:B:387:THR:HG23	1.92	0.51
1:B:496:PRO:O	1:B:499:THR:OG1	2.28	0.51
1:B:1207:SER:HB2	1:C:998:ASN:HD22	1.75	0.51
2:E:256:ILE:HG13	2:E:400:ALA:H	1.75	0.51
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.93	0.51
1:A:348:ILE:HG12	1:A:387:THR:HG23	1.92	0.51
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	1.93	0.51
1:B:872:ASN:ND2	1:B:874:ASN:OD1	2.41	0.51
1:B:86:SER:OG	1:B:87:THR:N	2.43	0.51
1:B:994:MET:O	1:B:998:ASN:ND2	2.39	0.51
2:E:151:LEU:HD21	2:E:239:LEU:HD23	1.91	0.51
2:E:268:PRO:O	2:E:362:LYS:N	2.41	0.51
1:B:1126:ASN:ND2	1:B:1127:GLY:O	2.44	0.51
1:C:245:ILE:HG12	1:C:252:GLU:HB2	1.93	0.51
2:E:187:ASP:N	2:E:187:ASP:OD1	2.41	0.51
1:A:650:ASP:OD1	1:A:650:ASP:N	2.42	0.50
1:B:278:ASN:N	1:B:278:ASN:OD1	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:392:ALA:HB3	1:B:460:VAL:HG11	1.93	0.50
1:C:107:LYS:HB2	1:C:255:GLU:HB2	1.93	0.50
1:A:392:ALA:HB3	1:A:460:VAL:HG11	1.93	0.50
1:C:436:ILE:HD13	1:C:460:VAL:HG13	1.93	0.50
2:D:240:ARG:NH2	2:D:244:CYS:SG	2.84	0.50
2:D:150:ARG:NE	2:D:159:GLN:OE1	2.39	0.50
2:E:240:ARG:NH2	2:E:244:CYS:SG	2.84	0.50
1:A:1205:MET:HG2	1:B:994:MET:HG2	1.92	0.50
2:D:151:LEU:HD21	2:D:239:LEU:HD23	1.91	0.50
1:B:27:ASP:OD2	1:B:87:THR:OG1	2.29	0.50
1:C:431:LEU:HD11	1:C:581:ILE:HG12	1.93	0.50
1:A:682:TYR:O	1:A:685:SER:OG	2.29	0.50
1:C:219:PRO:HG2	1:C:276:ILE:HB	1.94	0.49
1:B:320:ARG:NH1	1:B:623:ASP:OD1	2.46	0.49
1:C:332:TRP:O	1:C:390:LYS:NZ	2.45	0.49
1:A:267:LEU:HB3	1:A:280:VAL:HG13	1.93	0.49
1:C:937:VAL:O	1:C:941:ASN:ND2	2.38	0.49
1:C:1055:SER:OG	1:C:1056:SER:N	2.45	0.49
2:D:275:VAL:HG12	2:D:276:GLN:HG3	1.94	0.49
1:B:662:LEU:HD12	4:N:2:NAG:H61	1.93	0.49
1:C:938:GLN:HG3	1:C:1044:LEU:HD22	1.94	0.49
1:A:154:THR:OG1	1:A:177:ASP:OD1	2.27	0.49
1:B:400:ASP:O	1:B:410:GLN:NE2	2.41	0.49
1:B:75:ARG:NH2	1:B:96:SER:OG	2.45	0.49
1:A:872:ASN:H	1:A:876:HIS:CD2	2.31	0.49
1:A:680:ALA:HB1	1:A:736:LEU:HD13	1.94	0.48
1:A:1098:LEU:HD13	1:B:1097:THR:HG23	1.95	0.48
1:C:1091:GLN:HE21	1:C:1091:GLN:HB3	1.53	0.48
1:C:1126:ASN:N	1:C:1126:ASN:OD1	2.45	0.48
2:D:346:ILE:HD11	2:D:484:ILE:HD11	1.95	0.48
2:D:229:ASP:OD1	2:D:229:ASP:N	2.46	0.48
2:D:443:GLY:O	2:D:459:THR:OG1	2.31	0.48
2:E:346:ILE:HD11	2:E:484:ILE:HD11	1.95	0.48
2:D:270:GLN:NE2	2:D:271:VAL:O	2.39	0.48
2:E:443:GLY:O	2:E:459:THR:OG1	2.31	0.48
1:A:456:SER:OG	1:A:457:SER:N	2.41	0.48
1:C:353:ASN:HB3	1:C:605:ASN:HD22	1.79	0.48
1:B:22:ASN:ND2	5:B:2001:NAG:O4	2.47	0.48
1:A:168:SER:OG	1:A:170:ARG:O	2.32	0.48
2:E:275:VAL:HG12	2:E:276:GLN:HG3	1.94	0.48
1:B:161:THR:OG1	1:B:239:PRO:O	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:938:GLN:HG3	1:B:1044:LEU:HD22	1.95	0.47
1:C:151:CYS:HA	1:C:183:CYS:HA	1.97	0.47
2:E:213:ASN:O	2:E:224:LYS:NZ	2.36	0.47
1:A:113:VAL:O	1:A:116:THR:HB	2.15	0.47
1:B:22:ASN:HD22	5:B:2001:NAG:H3	1.79	0.47
1:A:324:LEU:HB3	1:A:325:PRO:HD2	1.97	0.47
2:E:229:ASP:N	2:E:229:ASP:OD1	2.46	0.47
1:A:937:VAL:O	1:A:941:ASN:ND2	2.43	0.47
1:C:139:VAL:HG13	1:C:148:ILE:HG12	1.96	0.47
2:E:389:GLU:HB2	2:E:465:CYS:HB2	1.96	0.47
1:A:1066:ASP:HB3	1:A:1068:PRO:HD2	1.96	0.47
1:B:109:THR:HG21	1:B:254:LEU:HD22	1.96	0.47
1:B:662:LEU:CD1	4:N:2:NAG:H61	2.45	0.47
1:C:142:HIS:N	1:C:145:ILE:O	2.46	0.47
1:C:552:ASN:HB2	1:C:573:LEU:HD11	1.96	0.47
1:C:791:PRO:HB3	1:C:1150:PRO:HB3	1.96	0.47
1:B:791:PRO:HB3	1:B:1150:PRO:HB3	1.96	0.47
1:C:850:LEU:HD13	1:C:1096:ILE:HD11	1.96	0.47
1:C:1182:ASP:N	1:C:1182:ASP:OD1	2.47	0.47
2:D:198:GLN:NE2	2:D:238:SER:OG	2.48	0.47
1:A:515:TRP:HE1	1:A:517:ARG:HH11	1.63	0.47
1:A:1075:ASP:OD2	1:C:1076:ARG:NH2	2.46	0.47
1:C:555:LYS:HB2	1:C:571:ALA:HB2	1.97	0.46
2:D:389:GLU:HB2	2:D:465:CYS:HB2	1.96	0.46
1:B:89:TRP:O	1:B:236:TYR:OH	2.32	0.46
1:B:515:TRP:HE1	1:B:517:ARG:HH11	1.63	0.46
2:E:191:LYS:H	2:E:191:LYS:HG2	1.41	0.46
1:A:396:ARG:NH1	1:A:578:ASP:OD2	2.42	0.46
1:B:642:ASN:ND2	1:B:645:GLN:OE1	2.46	0.46
1:B:912:LYS:HE3	1:B:912:LYS:HB2	1.75	0.46
1:C:902:LEU:HA	1:C:905:ASP:HB2	1.97	0.46
2:D:289:GLU:OE1	2:D:290:TRP:NE1	2.49	0.46
1:A:671:PRO:HB2	1:B:940:PHE:HD2	1.80	0.46
1:B:373:LEU:HG	1:B:421:SER:HB3	1.98	0.46
1:B:402:GLN:O	1:B:410:GLN:NE2	2.36	0.46
2:E:198:GLN:NE2	2:E:238:SER:OG	2.48	0.46
1:C:428:SER:HA	1:C:586:CYS:O	2.16	0.46
1:C:1108:GLU:OE1	1:C:1120:ARG:NH2	2.40	0.46
2:E:289:GLU:OE1	2:E:290:TRP:NE1	2.49	0.46
1:A:373:LEU:HG	1:A:421:SER:HB3	1.98	0.46
2:D:448:SER:O	2:D:448:SER:OG	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1218:ILE:HA	1:A:1220:LEU:HD23	1.98	0.46
1:B:162:VAL:HB	1:B:172:GLU:HB2	1.99	0.46
1:B:249:THR:OG1	1:B:250:ASP:N	2.47	0.46
1:C:505:ASP:N	1:C:505:ASP:OD1	2.49	0.46
1:A:791:PRO:HB3	1:A:1150:PRO:HB3	1.98	0.45
2:E:287:THR:OG1	2:E:290:TRP:N	2.37	0.45
1:C:340:SER:OG	1:C:343:ASN:OD1	2.31	0.45
1:A:354:PHE:CZ	1:A:604:SER:HB2	2.51	0.45
2:D:191:LYS:H	2:D:191:LYS:HG2	1.41	0.45
2:D:407:THR:OG1	2:D:408:GLN:NE2	2.39	0.45
2:D:326:TYR:O	2:D:327:GLN:NE2	2.50	0.45
1:C:141:PRO:O	1:C:142:HIS:ND1	2.50	0.45
2:D:342:LYS:HD2	2:D:461:TRP:CD1	2.52	0.45
2:E:326:TYR:O	2:E:327:GLN:NE2	2.50	0.45
1:C:118:TYR:HA	1:C:143:ASN:HD21	1.82	0.45
1:C:142:HIS:HB2	1:C:145:ILE:HG22	1.97	0.45
2:D:484:ILE:O	2:D:488:MET:N	2.50	0.45
1:A:422:SER:OG	1:A:424:GLN:NE2	2.39	0.45
2:D:203:ASP:OD1	2:D:203:ASP:N	2.50	0.45
2:D:296:HIS:ND1	2:D:345:ASP:OD2	2.49	0.45
1:B:842:ILE:HG21	1:B:1089:VAL:HG13	1.99	0.44
1:C:214:ALA:HB2	1:C:220:THR:HA	1.99	0.44
2:E:484:ILE:O	2:E:488:MET:N	2.50	0.44
2:D:296:HIS:N	2:D:345:ASP:OD1	2.50	0.44
2:E:342:LYS:HD2	2:E:461:TRP:CD1	2.52	0.44
1:A:322:PRO:HD2	1:A:661:PHE:HE2	1.83	0.44
1:A:659:LYS:HG2	1:A:666:THR:HG22	1.99	0.44
1:A:969:PRO:HA	1:A:971:TRP:CE2	2.53	0.44
1:B:379:PHE:HA	1:B:606:ASP:CG	2.37	0.44
1:C:65:GLY:O	1:C:263:ARG:HA	2.17	0.44
1:C:127:GLY:HA2	1:C:232:LEU:HD22	1.99	0.44
2:E:167:SER:OG	2:E:169:HIS:NE2	2.37	0.44
1:B:828:LEU:HD23	1:B:828:LEU:HA	1.88	0.44
1:A:1108:GLU:OE2	1:A:1120:ARG:NH2	2.46	0.44
1:B:801:GLU:OE2	1:B:1109:LYS:NZ	2.38	0.44
1:B:150:ALA:HB3	1:B:185:PHE:HB3	1.99	0.44
2:E:203:ASP:OD1	2:E:203:ASP:N	2.50	0.44
1:A:142:HIS:NE2	1:A:147:GLU:OE1	2.42	0.44
2:D:195:TYR:HB3	2:D:240:ARG:HB2	2.00	0.44
1:A:604:SER:O	1:A:604:SER:OG	2.24	0.44
1:B:1002:LYS:HA	1:B:1002:LYS:HD2	1.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:952:GLU:HG3	1:C:1136:ASN:HD21	1.82	0.44
2:E:296:HIS:ND1	2:E:345:ASP:OD2	2.49	0.44
1:C:124:ILE:HG23	1:C:139:VAL:HB	2.00	0.43
1:C:140:GLN:NE2	1:C:172:GLU:OE2	2.48	0.43
1:C:1218:ILE:HG23	1:C:1220:LEU:HD22	2.00	0.43
2:E:296:HIS:N	2:E:345:ASP:OD1	2.50	0.43
1:B:53:ASN:OD1	1:B:53:ASN:N	2.51	0.43
1:B:85:LEU:HD12	1:B:158:TYR:HB3	1.99	0.43
2:D:348:LEU:HD11	2:D:484:ILE:HG12	1.99	0.43
1:A:286:PHE:HD1	1:A:306:LEU:HD23	1.82	0.43
2:E:392:LYS:H	2:E:392:LYS:HG2	1.64	0.43
2:D:305:PRO:HB3	2:D:331:VAL:HG23	2.00	0.43
2:E:177:ASN:OD1	2:E:180:TYR:N	2.52	0.43
2:E:195:TYR:HB3	2:E:240:ARG:HB2	2.00	0.43
2:E:348:LEU:HD11	2:E:484:ILE:HG12	1.99	0.43
1:A:968:PHE:HA	1:A:969:PRO:HD3	1.82	0.43
2:D:287:THR:OG1	2:D:290:TRP:N	2.37	0.43
2:E:302:LEU:HD23	2:E:302:LEU:HA	1.82	0.43
1:A:511:TYR:HE1	2:D:340:LYS:O	2.02	0.43
1:B:511:TYR:HE1	2:E:340:LYS:O	2.02	0.43
1:C:1184:TRP:HB2	1:C:1218:ILE:HD11	2.00	0.43
2:D:422:PRO:O	2:D:476:ASN:ND2	2.51	0.43
2:E:248:LEU:H	2:E:248:LEU:HG	1.55	0.43
1:A:910:LYS:HD2	1:A:1026:LEU:HD11	2.01	0.43
1:C:849:LEU:HD23	1:C:1096:ILE:HD12	2.00	0.43
1:C:1196:PRO:O	1:C:1201:ASN:ND2	2.52	0.43
2:D:291:ILE:HG23	2:D:349:MET:HB2	2.01	0.43
1:A:14:VAL:HB	1:A:15:ILE:H	1.66	0.43
1:A:373:LEU:HD23	1:A:373:LEU:HA	1.88	0.43
1:A:740:SER:O	1:A:740:SER:OG	2.34	0.43
1:A:1001:GLN:HE21	1:A:1001:GLN:HB2	1.55	0.43
1:A:872:ASN:H	1:A:876:HIS:HD2	1.67	0.43
1:B:509:THR:OG1	1:B:512:VAL:N	2.52	0.43
2:D:248:LEU:H	2:D:248:LEU:HG	1.56	0.43
1:A:487:LYS:HB3	1:A:487:LYS:HE2	1.78	0.43
1:C:403:LEU:HD23	1:C:403:LEU:HA	1.92	0.43
2:E:200:ILE:HG13	2:E:236:VAL:HG23	2.01	0.43
2:E:305:PRO:HB3	2:E:331:VAL:HG23	2.00	0.43
1:C:370:CYS:HA	1:C:423:CYS:HA	2.01	0.42
2:E:287:THR:HG1	2:E:290:TRP:H	1.61	0.42
1:C:45:GLY:O	1:C:48:THR:OG1	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:392:LYS:H	2:D:392:LYS:HG2	1.64	0.42
2:E:285:ILE:H	2:E:285:ILE:HG13	1.46	0.42
2:D:177:ASN:OD1	2:D:180:TYR:N	2.52	0.42
1:A:520:CYS:SG	1:A:534:PRO:HD2	2.59	0.42
1:B:354:PHE:O	1:B:604:SER:HA	2.19	0.42
1:B:520:CYS:SG	1:B:534:PRO:HD2	2.59	0.42
1:C:164:LYS:H	1:C:164:LYS:HG2	1.72	0.42
1:B:34:ARG:H	1:B:34:ARG:HG3	1.54	0.42
2:D:483:TRP:HE3	2:D:484:ILE:HG13	1.84	0.42
1:A:14:VAL:HG11	1:A:158:TYR:HE1	1.84	0.42
1:C:872:ASN:H	1:C:876:HIS:HD2	1.67	0.42
2:E:422:PRO:O	2:E:476:ASN:ND2	2.51	0.42
1:C:871:LEU:HD23	1:C:871:LEU:HA	1.90	0.42
2:D:355:LEU:H	2:D:355:LEU:HG	1.63	0.42
2:E:186:ARG:HG2	2:E:191:LYS:HA	2.02	0.42
1:A:133:THR:O	1:A:133:THR:OG1	2.36	0.42
1:B:907:LEU:HD11	1:B:1142:LEU:HD22	2.02	0.42
1:B:1100:LYS:HE2	1:B:1100:LYS:HB3	1.91	0.42
1:C:402:GLN:O	1:C:410:GLN:NE2	2.52	0.42
2:E:407:THR:HG1	2:E:408:GLN:HE21	1.61	0.42
1:B:354:PHE:CE1	1:B:604:SER:OG	2.60	0.42
1:B:354:PHE:O	1:B:605:ASN:OD1	2.37	0.42
1:B:429:LEU:HD23	1:B:429:LEU:HA	1.83	0.42
1:B:22:ASN:ND2	5:B:2001:NAG:C3	2.82	0.41
1:B:83:LYS:HB3	1:B:83:LYS:HE2	1.87	0.41
1:B:466:CYS:HB3	1:B:547:PRO:HD2	2.02	0.41
1:C:18:PHE:CE2	3:P:1:NAG:H4	2.55	0.41
1:C:103:PHE:HB2	1:C:261:LEU:HD21	2.02	0.41
2:E:213:ASN:HB3	2:E:224:LYS:HG2	2.02	0.41
2:E:291:ILE:HG23	2:E:349:MET:HB2	2.01	0.41
1:A:509:THR:OG1	1:A:512:VAL:N	2.52	0.41
2:D:200:ILE:HG13	2:D:236:VAL:HG23	2.01	0.41
2:D:285:ILE:H	2:D:285:ILE:HG13	1.46	0.41
2:E:287:THR:HG21	2:E:290:TRP:HD1	1.85	0.41
2:E:378:LEU:HD11	2:E:401:LYS:HD2	2.01	0.41
2:E:483:TRP:HE3	2:E:484:ILE:HG13	1.84	0.41
2:D:213:ASN:HB3	2:D:224:LYS:HG2	2.02	0.41
2:D:378:LEU:HD11	2:D:401:LYS:HD2	2.01	0.41
2:D:394:SER:OG	2:D:398:ASN:ND2	2.51	0.41
1:A:65:GLY:O	1:A:263:ARG:HA	2.21	0.41
1:A:850:LEU:HD13	1:A:1096:ILE:HD11	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:444:TRP:NE1	1:C:547:PRO:O	2.52	0.41
1:B:269:ASN:HB2	1:B:297:PHE:CE1	2.55	0.41
1:B:396:ARG:NH1	1:B:578:ASP:OD2	2.42	0.41
1:B:521:LEU:HD23	1:B:521:LEU:HA	1.94	0.41
1:C:368:PHE:HE2	1:C:375:LYS:HD3	1.86	0.41
1:C:969:PRO:HA	1:C:971:TRP:CE2	2.56	0.41
1:A:68:PRO:O	1:A:266:TYR:OH	2.38	0.41
1:B:380:GLY:CA	1:B:607:LEU:HD22	2.39	0.41
2:D:287:THR:HG21	2:D:290:TRP:HD1	1.86	0.41
2:E:247:ASN:HB2	2:E:266:ALA:HA	2.02	0.41
2:E:270:GLN:OE1	2:E:382:SER:OG	2.36	0.41
1:A:466:CYS:HB3	1:A:547:PRO:HD2	2.02	0.41
1:B:709:GLN:HG3	1:B:721:LEU:HD13	2.01	0.41
1:C:935:LEU:HD23	1:C:935:LEU:HA	1.93	0.41
2:D:186:ARG:HG2	2:D:191:LYS:HA	2.02	0.41
2:D:268:PRO:HB2	2:D:362:LYS:HB2	2.03	0.41
2:E:173:GLN:NE2	2:E:198:GLN:O	2.54	0.41
1:A:38:ASP:OD1	1:A:39:VAL:N	2.49	0.41
1:B:487:LYS:HB3	1:B:487:LYS:HE2	1.78	0.41
1:B:1173:LYS:HD3	1:B:1203:VAL:HG12	2.03	0.41
2:D:167:SER:OG	2:D:169:HIS:NE2	2.37	0.41
2:D:329:GLU:OE1	2:D:330:LYS:N	2.50	0.41
2:D:457:GLY:HA2	2:D:477:VAL:HG23	2.03	0.41
2:E:149:VAL:HB	2:E:158:LEU:HD11	2.02	0.41
1:A:113:VAL:HG21	1:A:165:SER:HB2	2.03	0.41
1:A:199:TYR:O	1:A:213:TYR:HA	2.21	0.41
1:C:448:TYR:CE2	1:C:475:PRO:HD2	2.55	0.41
1:C:642:ASN:ND2	1:C:645:GLN:OE1	2.41	0.41
1:B:376:SER:HA	1:B:379:PHE:HD2	1.86	0.40
1:B:546:CYS:HA	1:B:547:PRO:HD3	1.90	0.40
1:B:604:SER:O	1:B:607:LEU:HD23	2.21	0.40
2:D:247:ASN:HB2	2:D:266:ALA:HA	2.03	0.40
2:D:286:ILE:HG21	2:D:366:LEU:HG	2.03	0.40
2:E:183:ALA:O	2:E:186:ARG:NH2	2.47	0.40
1:B:267:LEU:O	1:B:279:ALA:HA	2.20	0.40
1:C:326:ASP:OD1	1:C:326:ASP:N	2.55	0.40
1:C:968:PHE:HA	1:C:969:PRO:HD3	1.85	0.40
2:D:173:GLN:NE2	2:D:198:GLN:O	2.54	0.40
1:A:246:SER:N	1:A:249:THR:OG1	2.54	0.40
1:A:842:ILE:HG21	1:A:1089:VAL:HG13	2.04	0.40
1:B:396:ARG:NH1	1:B:577:PHE:O	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1066:ASP:HB3	1:B:1068:PRO:HD2	2.03	0.40
1:C:525:ILE:HD11	1:C:573:LEU:HB2	2.03	0.40
1:C:533:CYS:HA	1:C:534:PRO:HD3	1.94	0.40
1:A:907:LEU:HA	1:A:907:LEU:HD23	1.91	0.40
1:B:310:THR:HG22	1:B:704:ILE:HG23	2.03	0.40
2:D:286:ILE:HG13	2:D:287:THR:HG23	2.03	0.40

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%)	1101 (91%)	103 (8%)	2 (0%)	44	68
1	B	1206/1290 (94%)	1099 (91%)	107 (9%)	0	100	100
1	C	1206/1290 (94%)	1117 (93%)	89 (7%)	0	100	100
2	D	343/384 (89%)	277 (81%)	66 (19%)	0	100	100
2	E	343/384 (89%)	277 (81%)	66 (19%)	0	100	100
All	All	4304/4638 (93%)	3871 (90%)	431 (10%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ASN
1	A	605	ASN

### 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%)	963 (89%)	119 (11%)	5	12
1	B	1082/1159 (93%)	954 (88%)	128 (12%)	4	10
1	C	1082/1159 (93%)	959 (89%)	123 (11%)	4	11
2	D	293/326 (90%)	237 (81%)	56 (19%)	1	3
2	E	293/326 (90%)	237 (81%)	56 (19%)	1	3
All	All	3832/4129 (93%)	3350 (87%)	482 (13%)	6	9

All (482) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	28	TYR
1	A	29	ASN
1	A	34	ARG
1	A	35	ILE
1	A	52	LEU
1	A	57	LEU
1	A	64	THR
1	A	84	TYR
1	A	104	SER
1	A	109	THR
1	A	125	VAL
1	A	133	THR
1	A	136	THR
1	A	154	THR
1	A	170	ARG
1	A	175	HIS
1	A	193	VAL
1	A	213	TYR
1	A	250	ASP
1	A	253	THR
1	A	262	SER
1	A	272	GLU
1	A	280	VAL
1	A	306	LEU
1	A	310	THR
1	A	314	VAL
1	A	316	THR

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Mol	Chain	Res	Type
1	A	317	VAL
1	A	326	ASP
1	A	328	ASP
1	A	351	ASN
1	A	362	LEU
1	A	371	ASN
1	A	373	LEU
1	A	389	ASP
1	A	397	ARG
1	A	400	ASP
1	A	403	LEU
1	A	405	SER
1	A	412	SER
1	A	418	ILE
1	A	431	LEU
1	A	437	ASN
1	A	438	ASN
1	A	456	SER
1	A	460	VAL
1	A	487	LYS
1	A	491	LEU
1	A	511	TYR
1	A	515	TRP
1	A	516	CYS
1	A	531	ASN
1	A	532	THR
1	A	540	VAL
1	A	545	HIS
1	A	560	LEU
1	A	561	ASN
1	A	570	ASP
1	A	573	LEU
1	A	590	SER
1	A	595	ASN
1	A	597	ILE
1	A	604	SER
1	A	605	ASN
1	A	608	LEU
1	A	609	TYR
1	A	611	ASN
1	A	612	THR
1	A	628	THR

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Mol	Chain	Res	Type
1	A	644	TRP
1	A	655	ILE
1	A	659	LYS
1	A	674	SER
1	A	685	SER
1	A	706	PHE
1	A	714	ASP
1	A	745	ASP
1	A	772	VAL
1	A	788	ILE
1	A	789	GLN
1	A	828	LEU
1	A	834	THR
1	A	849	LEU
1	A	850	LEU
1	A	863	GLN
1	A	865	VAL
1	A	871	LEU
1	A	875	LEU
1	A	877	SER
1	A	879	VAL
1	A	891	LEU
1	A	902	LEU
1	A	903	LEU
1	A	916	VAL
1	A	930	GLU
1	A	934	LEU
1	A	950	LEU
1	A	953	THR
1	A	964	VAL
1	A	977	VAL
1	A	981	LEU
1	A	994	MET
1	A	995	ASP
1	A	999	LYS
1	A	1002	LYS
1	A	1010	LYS
1	A	1013	LEU
1	A	1014	SER
1	A	1022	THR
1	A	1028	LYS
1	A	1066	ASP

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Mol	Chain	Res	Type
1	A	1096	ILE
1	A	1098	LEU
1	A	1118	SER
1	A	1124	CYS
1	A	1203	VAL
1	A	1217	PHE
1	A	1219	TYR
1	B	28	TYR
1	B	29	ASN
1	B	30	LYS
1	B	34	ARG
1	B	37	GLU
1	B	40	VAL
1	B	51	VAL
1	B	52	LEU
1	B	73	ASN
1	B	75	ARG
1	B	85	LEU
1	B	91	LYS
1	B	123	THR
1	B	125	VAL
1	B	129	VAL
1	B	131	VAL
1	B	132	ASN
1	B	136	THR
1	B	152	GLN
1	B	164	LYS
1	B	166	LYS
1	B	175	HIS
1	B	177	ASP
1	B	182	LEU
1	B	187	LYS
1	B	204	GLN
1	B	205	GLU
1	B	213	TYR
1	B	230	THR
1	B	233	SER
1	B	243	LYS
1	B	245	ILE
1	B	248	ASN
1	B	249	THR
1	B	254	LEU

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Mol	Chain	Res	Type
1	B	263	ARG
1	B	264	ARG
1	B	272	GLU
1	B	284	SER
1	B	316	THR
1	B	320	ARG
1	B	321	ILE
1	B	324	LEU
1	B	326	ASP
1	B	328	ASP
1	B	351	ASN
1	B	362	LEU
1	B	371	ASN
1	B	373	LEU
1	B	389	ASP
1	B	397	ARG
1	B	400	ASP
1	B	403	LEU
1	B	405	SER
1	B	412	SER
1	B	418	ILE
1	B	431	LEU
1	B	437	ASN
1	B	438	ASN
1	B	456	SER
1	B	460	VAL
1	B	487	LYS
1	B	491	LEU
1	B	511	TYR
1	B	515	TRP
1	B	516	CYS
1	B	531	ASN
1	B	532	THR
1	B	540	VAL
1	B	545	HIS
1	B	560	LEU
1	B	561	ASN
1	B	570	ASP
1	B	573	LEU
1	B	590	SER
1	B	595	ASN
1	B	597	ILE

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Mol	Chain	Res	Type
1	B	604	SER
1	B	606	ASP
1	B	607	LEU
1	B	609	TYR
1	B	612	THR
1	B	613	GLU
1	B	630	GLN
1	B	640	TYR
1	B	662	LEU
1	B	666	THR
1	B	730	SER
1	B	731	VAL
1	B	732	SER
1	B	735	ASP
1	B	743	CYS
1	B	745	ASP
1	B	772	VAL
1	B	778	SER
1	B	800	GLU
1	B	807	SER
1	B	811	THR
1	B	835	PHE
1	B	850	LEU
1	B	865	VAL
1	B	872	ASN
1	B	879	VAL
1	B	890	CYS
1	B	899	SER
1	B	906	LEU
1	B	946	LEU
1	B	950	LEU
1	B	964	VAL
1	B	972	SER
1	B	986	ARG
1	B	1012	LEU
1	B	1028	LYS
1	B	1054	ILE
1	B	1089	VAL
1	B	1091	GLN
1	B	1096	ILE
1	B	1098	LEU
1	B	1115	LYS

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Mol	Chain	Res	Type
1	B	1118	SER
1	B	1124	CYS
1	B	1135	GLN
1	B	1173	LYS
1	B	1183	SER
1	B	1205	MET
1	B	1208	CYS
1	B	1217	PHE
1	B	1219	TYR
1	C	14	VAL
1	C	17	ASP
1	C	19	ASN
1	C	25	ILE
1	C	29	ASN
1	C	30	LYS
1	C	32	ILE
1	C	34	ARG
1	C	40	VAL
1	C	43	SER
1	C	52	LEU
1	C	57	LEU
1	C	58	ASN
1	C	85	LEU
1	C	91	LYS
1	C	111	LEU
1	C	119	SER
1	C	123	THR
1	C	124	ILE
1	C	125	VAL
1	C	129	VAL
1	C	131	VAL
1	C	132	ASN
1	C	145	ILE
1	C	149	THR
1	C	162	VAL
1	C	164	LYS
1	C	166	LYS
1	C	169	ILE
1	C	184	LEU
1	C	187	LYS
1	C	198	LEU
1	C	204	GLN

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Mol	Chain	Res	Type
1	C	205	GLU
1	C	213	TYR
1	C	216	VAL
1	C	223	LEU
1	C	249	THR
1	C	252	GLU
1	C	253	THR
1	C	259	THR
1	C	263	ARG
1	C	264	ARG
1	C	311	VAL
1	C	324	LEU
1	C	326	ASP
1	C	342	LEU
1	C	351	ASN
1	C	366	ASP
1	C	373	LEU
1	C	374	ASP
1	C	431	LEU
1	C	453	PHE
1	C	460	VAL
1	C	481	VAL
1	C	486	VAL
1	C	487	LYS
1	C	502	ARG
1	C	505	ASP
1	C	513	ASN
1	C	517	ARG
1	C	525	ILE
1	C	540	VAL
1	C	559	GLN
1	C	560	LEU
1	C	561	ASN
1	C	562	HIS
1	C	570	ASP
1	C	575	TRP
1	C	579	SER
1	C	584	ASN
1	C	601	THR
1	C	604	SER
1	C	618	VAL
1	C	621	ASN

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Mol	Chain	Res	Type
1	C	640	TYR
1	C	644	TRP
1	C	659	LYS
1	C	665	LYS
1	C	676	ARG
1	C	706	PHE
1	C	714	ASP
1	C	756	ARG
1	C	763	ARG
1	C	788	ILE
1	C	800	GLU
1	C	830	SER
1	C	834	THR
1	C	850	LEU
1	C	865	VAL
1	C	879	VAL
1	C	885	LYS
1	C	890	CYS
1	C	894	GLN
1	C	898	SER
1	C	931	ILE
1	C	934	LEU
1	C	950	LEU
1	C	964	VAL
1	C	981	LEU
1	C	986	ARG
1	C	995	ASP
1	C	1001	GLN
1	C	1022	THR
1	C	1026	LEU
1	C	1042	SER
1	C	1066	ASP
1	C	1089	VAL
1	C	1090	SER
1	C	1091	GLN
1	C	1096	ILE
1	C	1098	LEU
1	C	1115	LYS
1	C	1118	SER
1	C	1124	CYS
1	C	1126	ASN
1	C	1156	VAL

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Mol	Chain	Res	Type
1	C	1157	LEU
1	C	1159	SER
1	C	1182	ASP
1	C	1217	PHE
1	C	1219	TYR
1	C	1220	LEU
2	D	149	VAL
2	D	174	ASP
2	D	187	ASP
2	D	191	LYS
2	D	195	TYR
2	D	207	THR
2	D	212	LEU
2	D	219	VAL
2	D	226	TYR
2	D	229	ASP
2	D	234	LYS
2	D	241	CYS
2	D	246	VAL
2	D	248	LEU
2	D	251	SER
2	D	253	GLN
2	D	257	VAL
2	D	269	TRP
2	D	280	VAL
2	D	285	ILE
2	D	291	ILE
2	D	292	VAL
2	D	293	THR
2	D	303	ASN
2	D	327	GLN
2	D	328	VAL
2	D	329	GLU
2	D	332	ILE
2	D	333	SER
2	D	346	ILE
2	D	349	MET
2	D	352	GLN
2	D	355	LEU
2	D	362	LYS
2	D	366	LEU
2	D	371	MET

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Mol	Chain	Res	Type
2	D	372	MET
2	D	392	LYS
2	D	393	THR
2	D	396	VAL
2	D	406	GLU
2	D	413	ARG
2	D	425	ILE
2	D	426	CYS
2	D	429	PHE
2	D	430	LEU
2	D	437	CYS
2	D	438	GLN
2	D	440	ASP
2	D	446	VAL
2	D	459	THR
2	D	465	CYS
2	D	477	VAL
2	D	480	PHE
2	D	482	ASP
2	D	486	ARG
2	E	149	VAL
2	E	174	ASP
2	E	187	ASP
2	E	191	LYS
2	E	195	TYR
2	E	207	THR
2	E	212	LEU
2	E	219	VAL
2	E	226	TYR
2	E	229	ASP
2	E	234	LYS
2	E	241	CYS
2	E	246	VAL
2	E	248	LEU
2	E	251	SER
2	E	253	GLN
2	E	257	VAL
2	E	269	TRP
2	E	280	VAL
2	E	285	ILE
2	E	291	ILE
2	E	292	VAL

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Mol	Chain	Res	Type
2	E	293	THR
2	E	303	ASN
2	E	327	GLN
2	E	328	VAL
2	E	329	GLU
2	E	332	ILE
2	E	333	SER
2	E	346	ILE
2	E	349	MET
2	E	352	GLN
2	E	355	LEU
2	E	362	LYS
2	E	366	LEU
2	E	371	MET
2	E	372	MET
2	E	392	LYS
2	E	393	THR
2	E	396	VAL
2	E	406	GLU
2	E	413	ARG
2	E	425	ILE
2	E	426	CYS
2	E	429	PHE
2	E	430	LEU
2	E	437	CYS
2	E	438	GLN
2	E	440	ASP
2	E	446	VAL
2	E	459	THR
2	E	465	CYS
2	E	477	VAL
2	E	480	PHE
2	E	482	ASP
2	E	486	ARG

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	204	GLN
1	A	351	ASN
1	A	371	ASN
1	A	372	ASN

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Mol	Chain	Res	Type
1	A	413	ASN
1	A	437	ASN
1	A	559	GLN
1	A	595	ASN
1	A	611	ASN
1	A	630	GLN
1	A	654	ASN
1	A	872	ASN
1	A	876	HIS
1	A	1001	GLN
1	A	1023	ASN
1	A	1079	ASN
1	A	1136	ASN
1	A	1180	GLN
1	B	22	ASN
1	B	73	ASN
1	B	108	ASN
1	B	204	GLN
1	B	323	ASN
1	B	371	ASN
1	B	372	ASN
1	B	413	ASN
1	B	437	ASN
1	B	559	GLN
1	B	595	ASN
1	B	621	ASN
1	B	840	ASN
1	B	876	HIS
1	B	984	GLN
1	B	1041	ASN
1	B	1122	ASN
1	B	1126	ASN
1	C	351	ASN
1	C	562	HIS
1	C	621	ASN
1	C	630	GLN
1	C	789	GLN
1	C	863	GLN
1	C	876	HIS
1	C	938	GLN
1	C	998	ASN
1	C	1001	GLN

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Mol	Chain	Res	Type
1	C	1091	GLN
1	C	1122	ASN
2	D	198	GLN
2	D	253	GLN
2	D	327	GLN
2	D	408	GLN
2	D	438	GLN
2	E	198	GLN
2	E	253	GLN
2	E	327	GLN
2	E	408	GLN
2	E	438	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

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	$\# Z  > 2$
3	NAG	F	1	3,1	14,14,15	0.52	0	17,19,21	0.57	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.49	0
3	MAN	F	3	3	11,11,12	1.06	1 (9%)	15,15,17	1.46	2 (13%)
3	MAN	F	4	3	11,11,12	0.97	0	15,15,17	1.21	2 (13%)
3	MAN	F	5	3	11,11,12	0.85	1 (9%)	15,15,17	1.25	2 (13%)
3	MAN	F	6	3	11,11,12	0.95	1 (9%)	15,15,17	1.44	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	G	1	4,1	14,14,15	0.42	0	17,19,21	0.51	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.45	0
4	NAG	H	1	4,1	14,14,15	0.47	0	17,19,21	0.71	0
4	NAG	H	2	4	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	NAG	I	1	4,1	14,14,15	1.06	1 (7%)	17,19,21	0.88	0
4	NAG	I	2	4	14,14,15	0.54	0	17,19,21	0.54	0
4	NAG	J	1	4,1	14,14,15	0.26	0	17,19,21	0.50	0
4	NAG	J	2	4	14,14,15	0.29	0	17,19,21	0.51	0
3	NAG	K	1	3,1	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
3	NAG	K	2	3	14,14,15	0.22	0	17,19,21	0.55	0
3	MAN	K	3	3	11,11,12	1.40	3 (27%)	15,15,17	1.80	3 (20%)
3	MAN	K	4	3	11,11,12	0.82	0	15,15,17	1.14	2 (13%)
3	MAN	K	5	3	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
3	MAN	K	6	3	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
4	NAG	L	1	4,1	14,14,15	0.29	0	17,19,21	0.53	0
4	NAG	L	2	4	14,14,15	0.30	0	17,19,21	0.51	0
4	NAG	M	1	4,1	14,14,15	0.48	0	17,19,21	0.71	0
4	NAG	M	2	4	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
4	NAG	N	1	4,1	14,14,15	1.06	1 (7%)	17,19,21	0.87	0
4	NAG	N	2	4	14,14,15	0.54	0	17,19,21	0.54	0
4	NAG	O	1	4,1	14,14,15	0.26	0	17,19,21	0.59	0
4	NAG	O	2	4	14,14,15	0.34	0	17,19,21	0.47	0
3	NAG	P	1	3,1	14,14,15	0.32	0	17,19,21	0.62	0
3	NAG	P	2	3	14,14,15	0.21	0	17,19,21	0.54	0
3	MAN	P	3	3	11,11,12	1.38	3 (27%)	15,15,17	1.81	3 (20%)
3	MAN	P	4	3	11,11,12	0.82	0	15,15,17	1.15	2 (13%)
3	MAN	P	5	3	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
3	MAN	P	6	3	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
4	NAG	Q	1	4,1	14,14,15	0.27	0	17,19,21	0.52	0
4	NAG	Q	2	4	14,14,15	0.31	0	17,19,21	0.52	0
4	NAG	R	1	4,1	14,14,15	0.35	0	17,19,21	0.51	0
4	NAG	R	2	4	14,14,15	0.38	0	17,19,21	0.48	0
4	NAG	S	1	4,1	14,14,15	0.42	0	17,19,21	0.52	0
4	NAG	S	2	4	14,14,15	0.25	0	17,19,21	0.60	0
4	NAG	T	1	4,1	14,14,15	0.38	0	17,19,21	0.83	1 (5%)
4	NAG	T	2	4	14,14,15	0.30	0	17,19,21	0.52	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	1/2/19/22	1/1/1/1
3	MAN	F	4	3	-	1/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1
3	MAN	F	6	3	-	0/2/19/22	0/1/1/1
4	NAG	G	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	G	2	4	-	2/6/23/26	0/1/1/1
4	NAG	H	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	1/6/23/26	0/1/1/1
4	NAG	I	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	I	2	4	-	2/6/23/26	0/1/1/1
4	NAG	J	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	J	2	4	-	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	MAN	K	3	3	-	2/2/19/22	1/1/1/1
3	MAN	K	4	3	-	2/2/19/22	0/1/1/1
3	MAN	K	5	3	-	0/2/19/22	0/1/1/1
3	MAN	K	6	3	-	2/2/19/22	0/1/1/1
4	NAG	L	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	L	2	4	-	0/6/23/26	0/1/1/1
4	NAG	M	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	M	2	4	-	1/6/23/26	0/1/1/1
4	NAG	N	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	N	2	4	-	2/6/23/26	0/1/1/1
4	NAG	O	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	O	2	4	-	0/6/23/26	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	MAN	P	3	3	-	2/2/19/22	1/1/1/1
3	MAN	P	4	3	-	2/2/19/22	0/1/1/1
3	MAN	P	5	3	-	0/2/19/22	0/1/1/1
3	MAN	P	6	3	-	2/2/19/22	0/1/1/1
4	NAG	Q	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	Q	2	4	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	R	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	R	2	4	-	2/6/23/26	0/1/1/1
4	NAG	S	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	S	2	4	-	2/6/23/26	0/1/1/1
4	NAG	T	1	4,1	-	1/6/23/26	0/1/1/1
4	NAG	T	2	4	-	1/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	1	NAG	O5-C1	-3.72	1.37	1.43
4	N	1	NAG	O5-C1	-3.72	1.37	1.43
3	P	3	MAN	O5-C5	2.59	1.48	1.43
3	K	3	MAN	O5-C5	2.59	1.48	1.43
3	K	3	MAN	C2-C3	2.41	1.56	1.52
3	P	3	MAN	C2-C3	2.36	1.56	1.52
3	F	3	MAN	O5-C5	2.34	1.48	1.43
3	F	5	MAN	C1-C2	2.26	1.57	1.52
3	F	6	MAN	O5-C5	2.17	1.47	1.43
3	K	3	MAN	C1-C2	2.05	1.56	1.52
3	P	3	MAN	C1-C2	2.03	1.56	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	3	MAN	C1-O5-C5	5.44	119.57	112.19
3	K	3	MAN	C1-O5-C5	5.43	119.56	112.19
3	F	6	MAN	C1-O5-C5	4.63	118.46	112.19
3	F	3	MAN	C1-O5-C5	4.24	117.94	112.19
3	P	6	MAN	C1-O5-C5	3.86	117.42	112.19
3	K	6	MAN	C1-O5-C5	3.85	117.40	112.19
3	F	4	MAN	C1-O5-C5	3.22	116.55	112.19
3	P	4	MAN	C1-O5-C5	3.18	116.50	112.19
3	F	5	MAN	C1-O5-C5	3.17	116.49	112.19
3	K	4	MAN	C1-O5-C5	3.15	116.46	112.19
3	P	5	MAN	C1-O5-C5	2.82	116.01	112.19
3	K	5	MAN	C1-O5-C5	2.77	115.94	112.19
4	M	2	NAG	C1-O5-C5	2.71	115.86	112.19
4	H	2	NAG	C1-O5-C5	2.68	115.82	112.19
3	P	3	MAN	C1-C2-C3	2.58	112.84	109.67
3	K	3	MAN	C1-C2-C3	2.54	112.78	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	MAN	O2-C2-C3	-2.51	105.12	110.14
3	P	6	MAN	O2-C2-C3	-2.30	105.54	110.14
3	K	6	MAN	O2-C2-C3	-2.29	105.55	110.14
3	P	3	MAN	O2-C2-C3	-2.25	105.64	110.14
3	K	3	MAN	O2-C2-C3	-2.22	105.68	110.14
3	P	4	MAN	O2-C2-C3	-2.21	105.70	110.14
4	T	1	NAG	C1-O5-C5	2.21	115.18	112.19
3	K	4	MAN	O2-C2-C3	-2.21	105.72	110.14
3	K	5	MAN	O2-C2-C3	-2.19	105.75	110.14
3	F	5	MAN	O2-C2-C3	-2.18	105.77	110.14
3	F	4	MAN	O2-C2-C3	-2.17	105.78	110.14
3	P	5	MAN	O2-C2-C3	-2.16	105.81	110.14
3	F	6	MAN	O2-C2-C3	-2.10	105.94	110.14
3	K	1	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	S	2	NAG	C4-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
4	S	1	NAG	C4-C5-C6-O6
4	S	1	NAG	O5-C5-C6-O6
4	I	2	NAG	C4-C5-C6-O6
4	N	2	NAG	C4-C5-C6-O6
3	K	4	MAN	O5-C5-C6-O6
3	P	4	MAN	O5-C5-C6-O6
3	K	2	NAG	C4-C5-C6-O6
3	P	2	NAG	C4-C5-C6-O6
4	H	1	NAG	C4-C5-C6-O6
4	M	1	NAG	C4-C5-C6-O6
4	S	2	NAG	O5-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
4	I	1	NAG	O5-C5-C6-O6
4	N	1	NAG	O5-C5-C6-O6
3	K	2	NAG	O5-C5-C6-O6
3	P	2	NAG	O5-C5-C6-O6
4	G	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
4	I	2	NAG	O5-C5-C6-O6
4	N	2	NAG	O5-C5-C6-O6

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

All (3) ring outliers are listed below:

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

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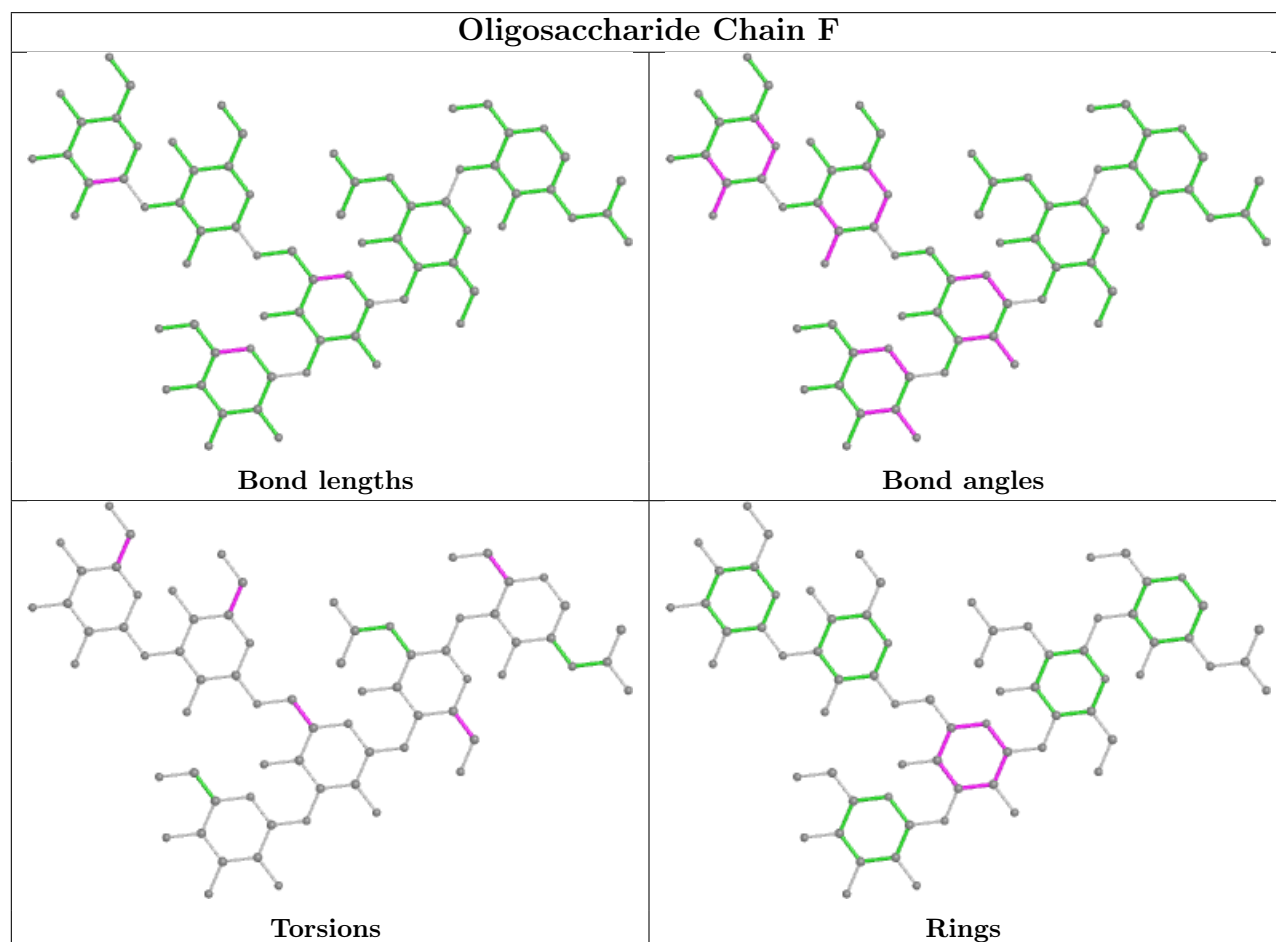
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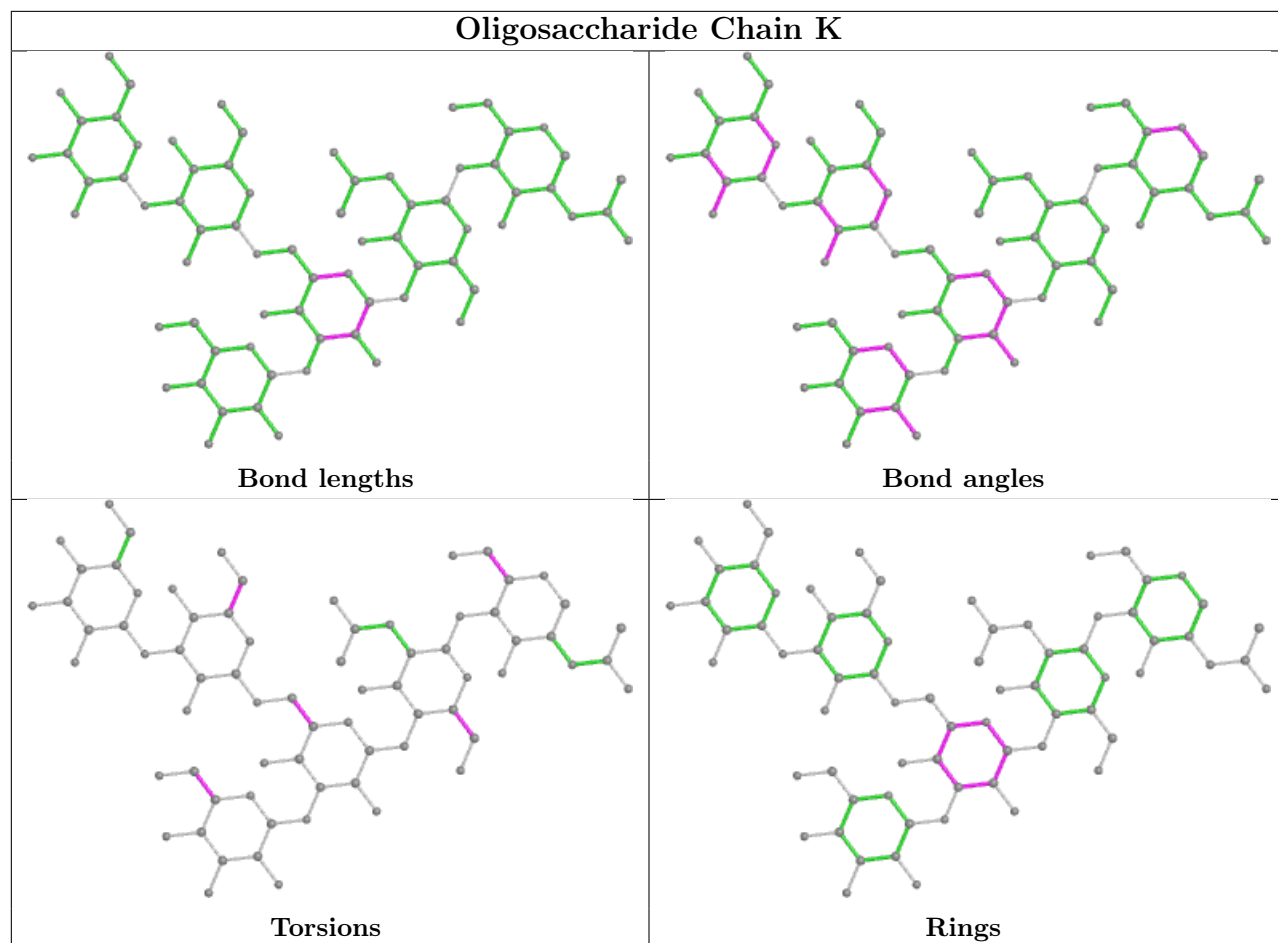
Mol	Chain	Res	Type	Atoms
3	P	3	MAN	C1-C2-C3-C4-C5-O5
3	F	3	MAN	C1-C2-C3-C4-C5-O5

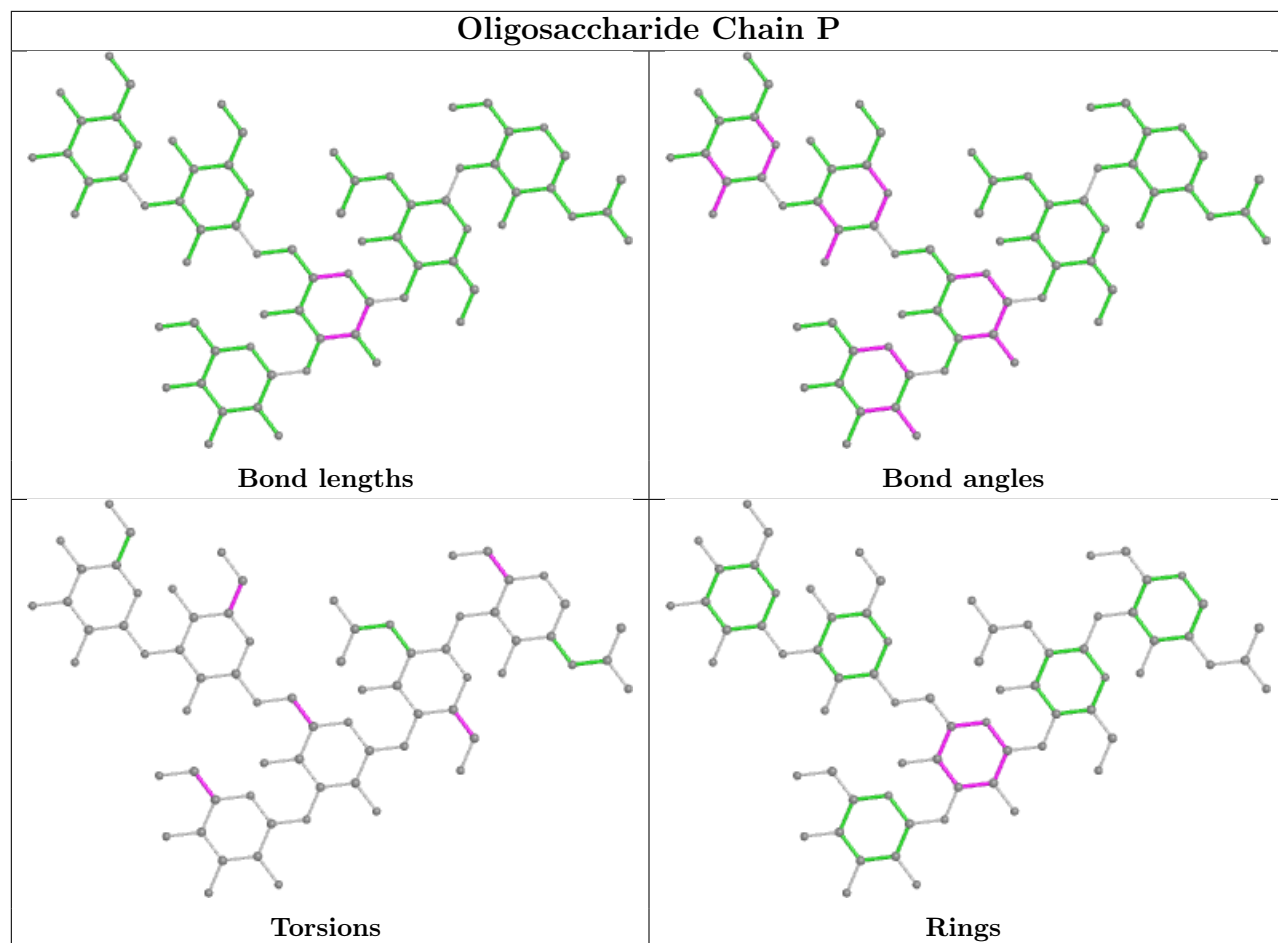
4 monomers are involved in 6 short contacts:

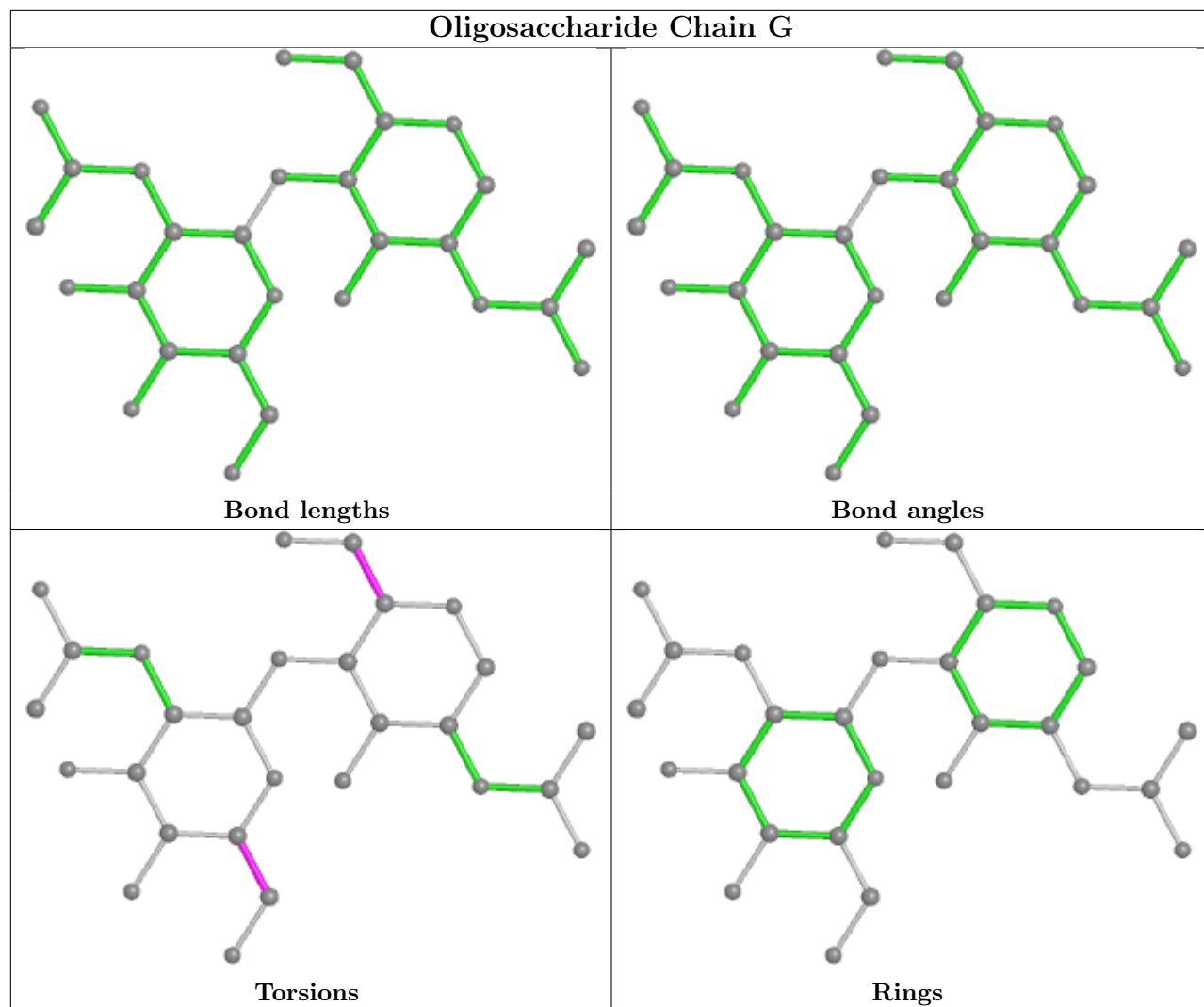
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	Q	1	NAG	2	0
4	N	2	NAG	2	0
3	F	5	MAN	1	0
3	P	1	NAG	1	0

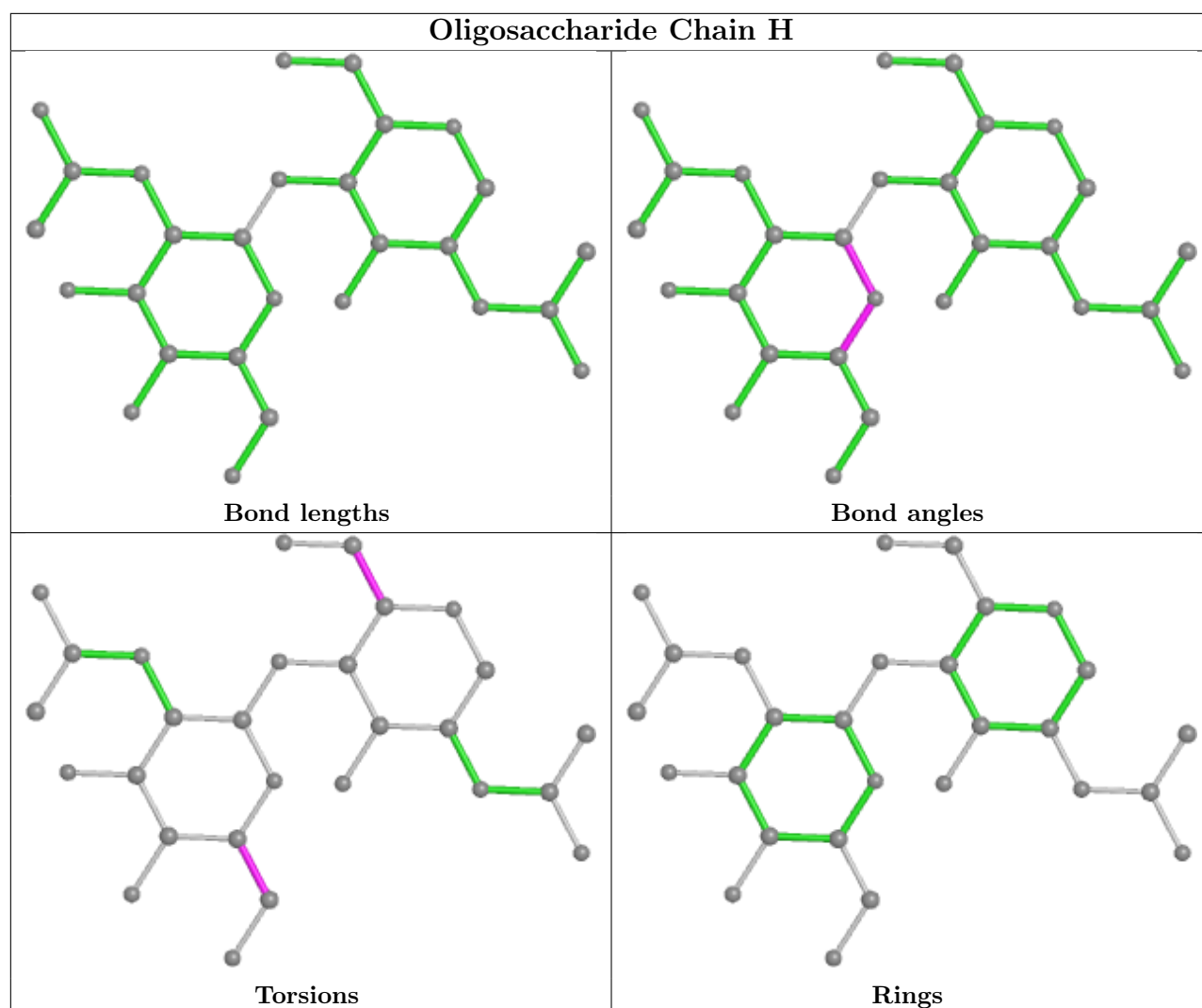
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

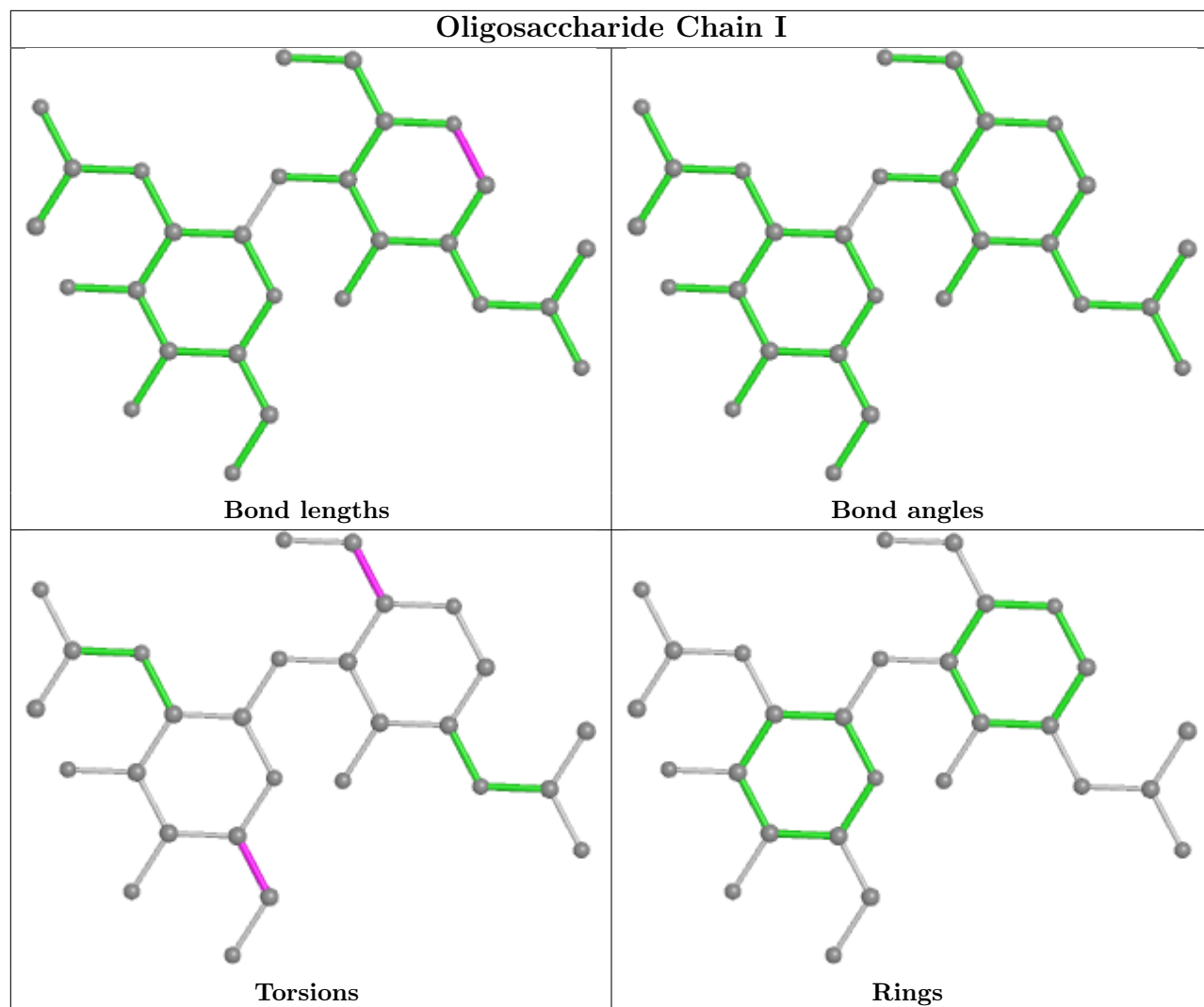


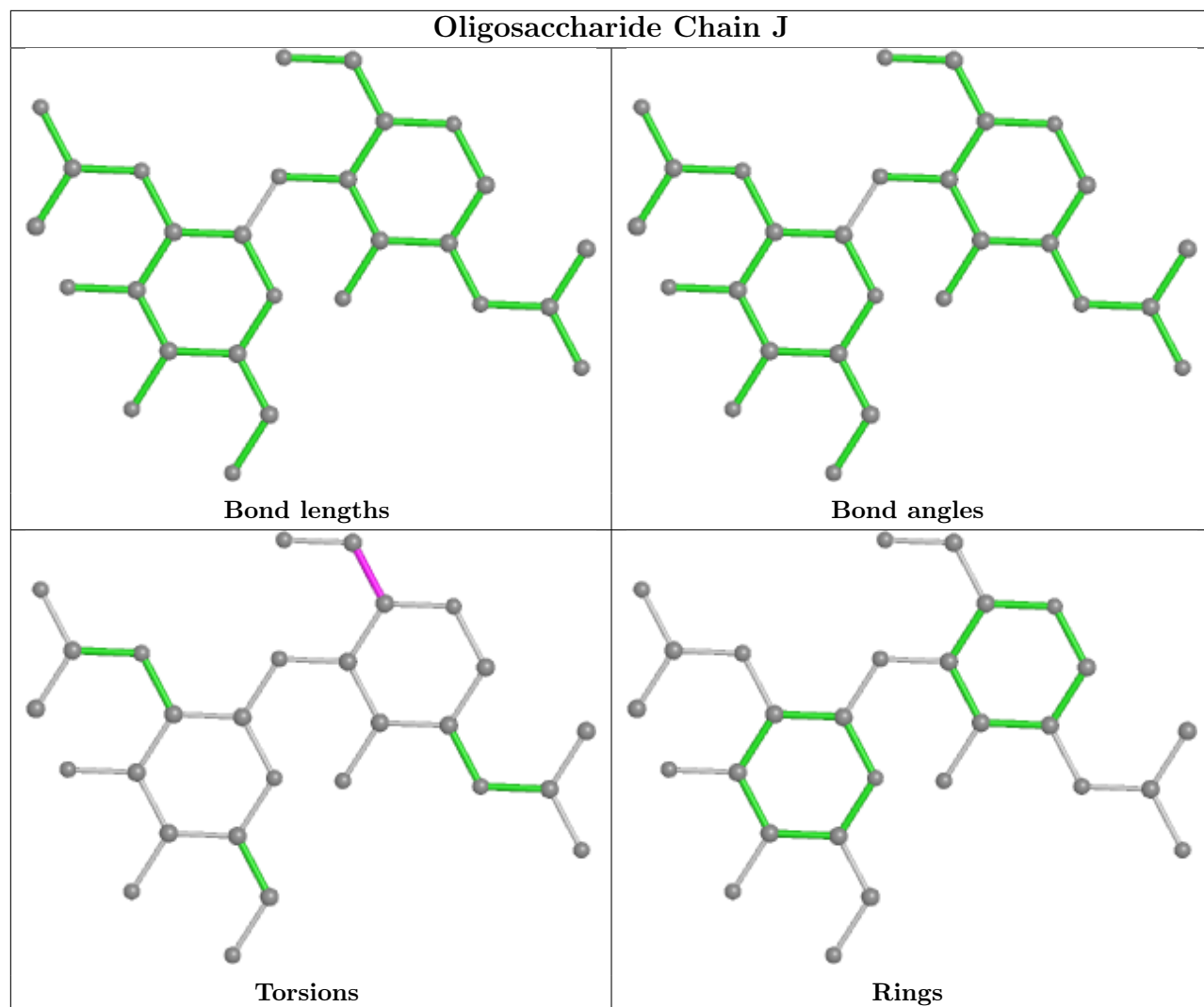




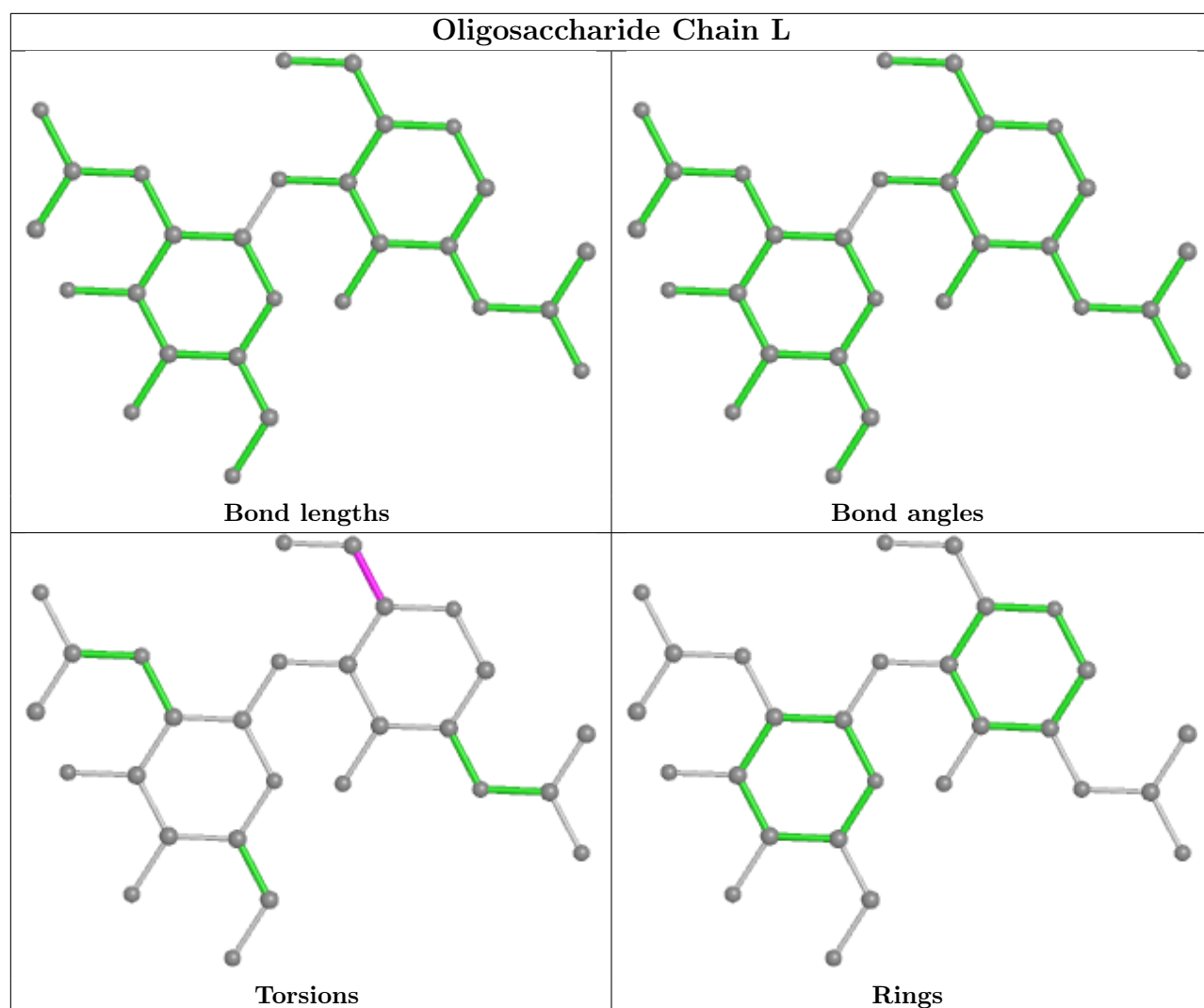


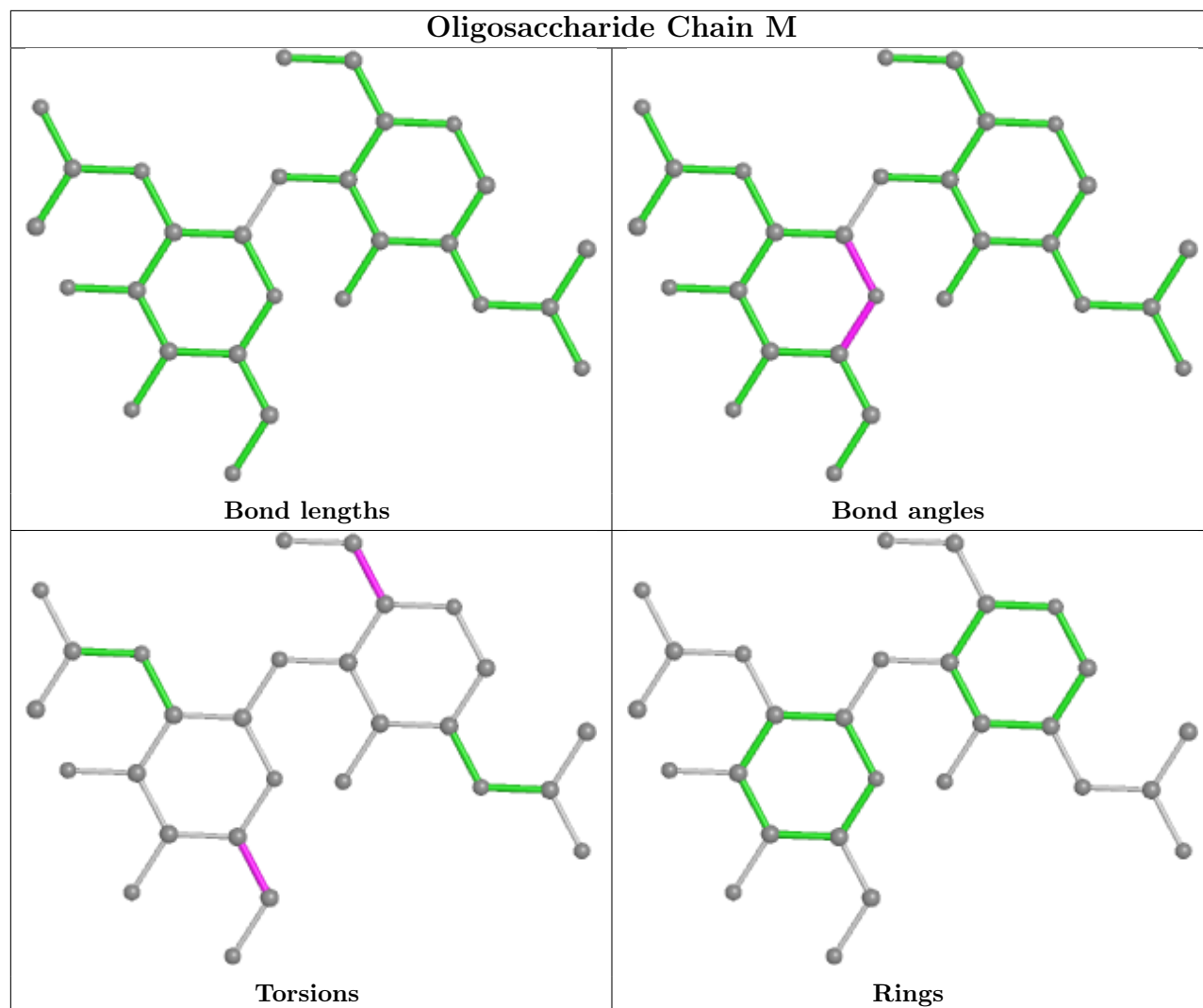


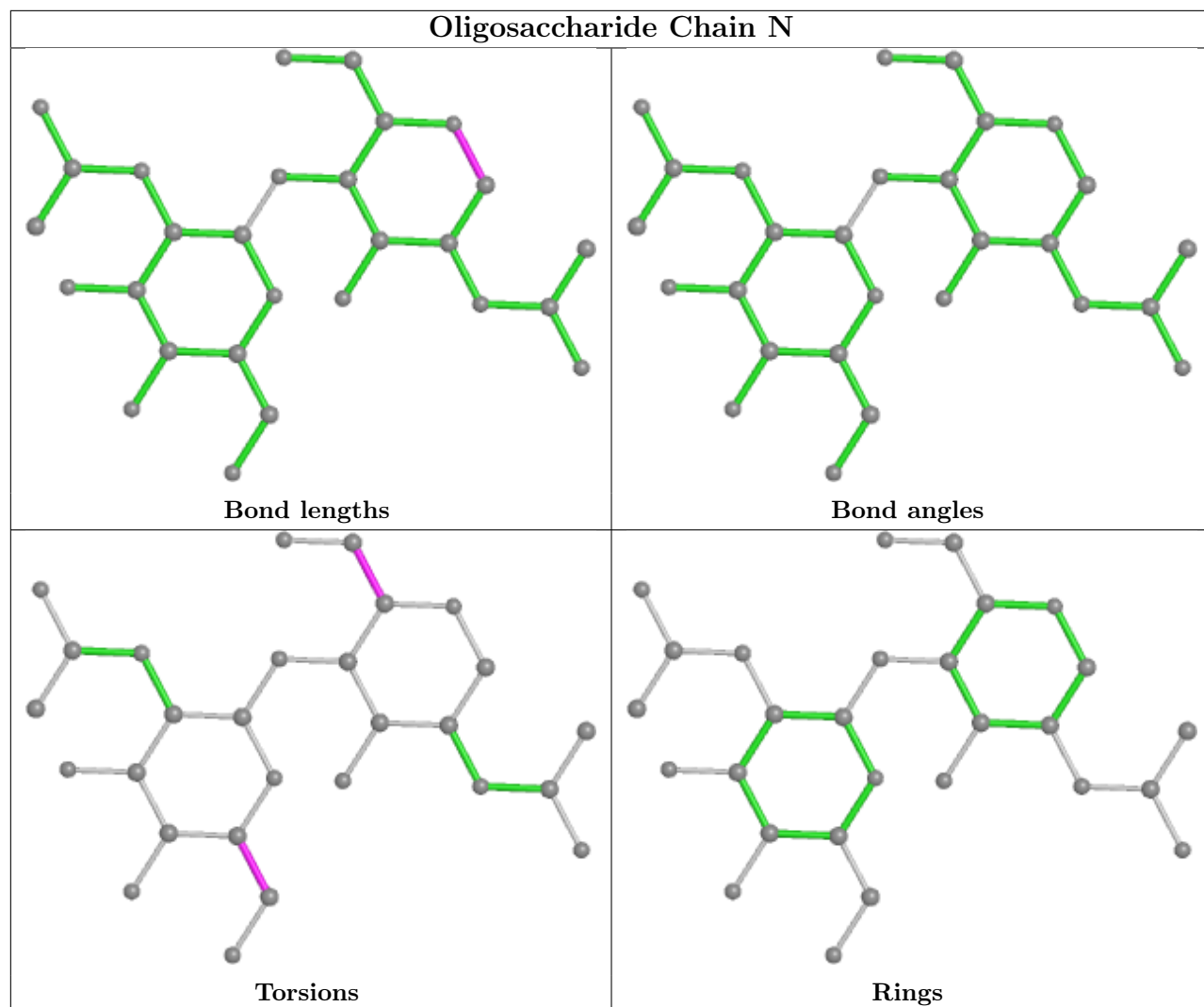


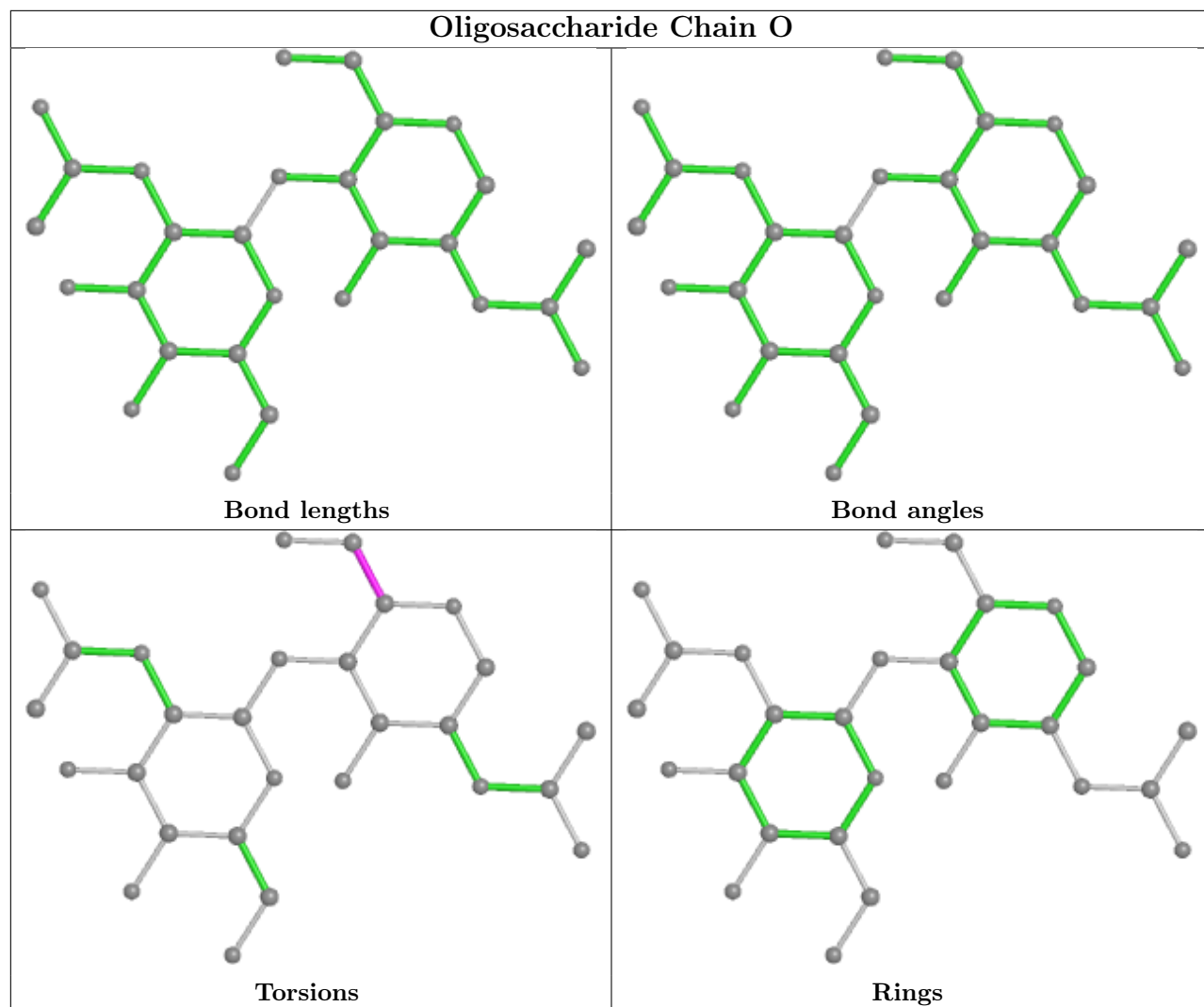


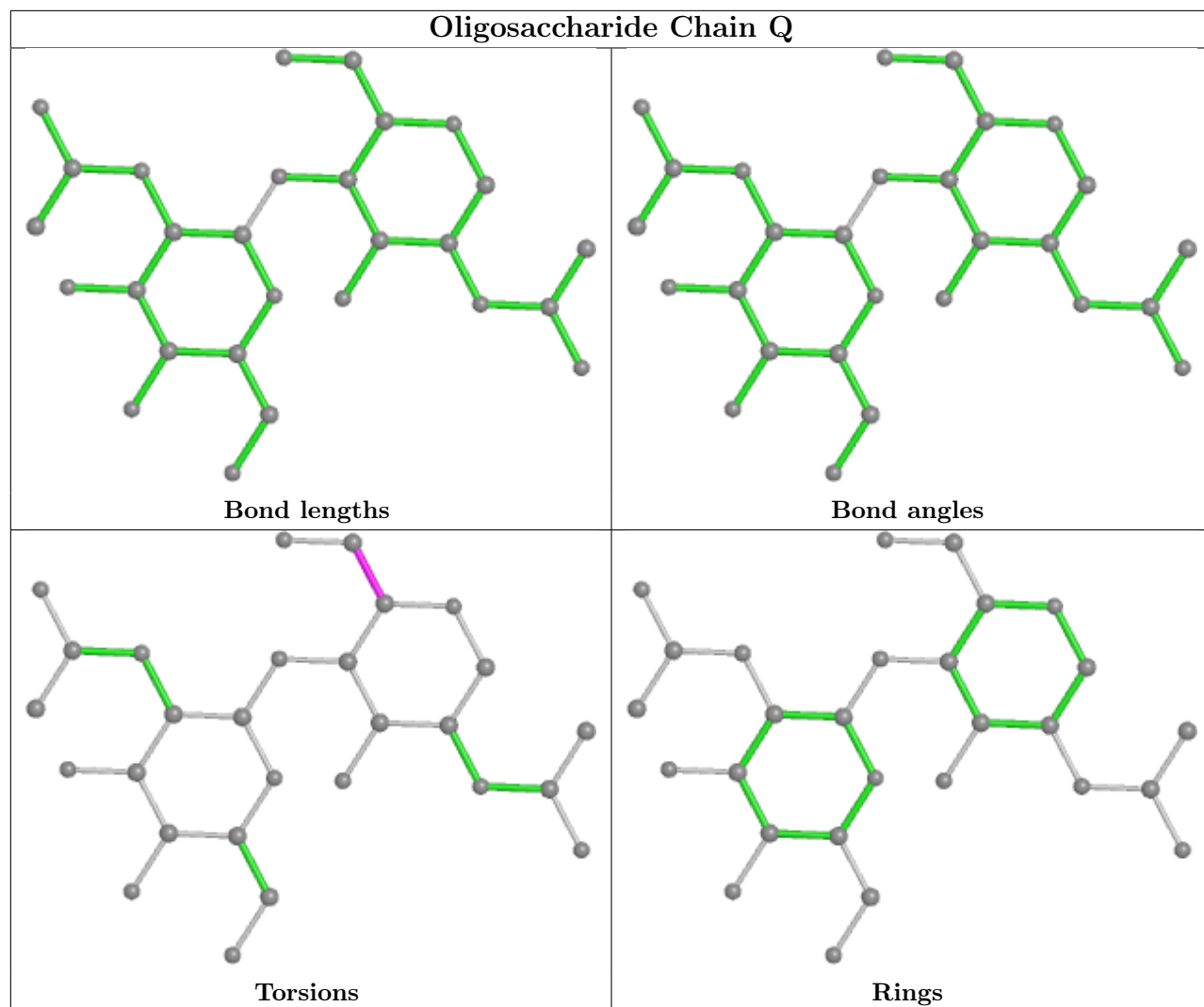


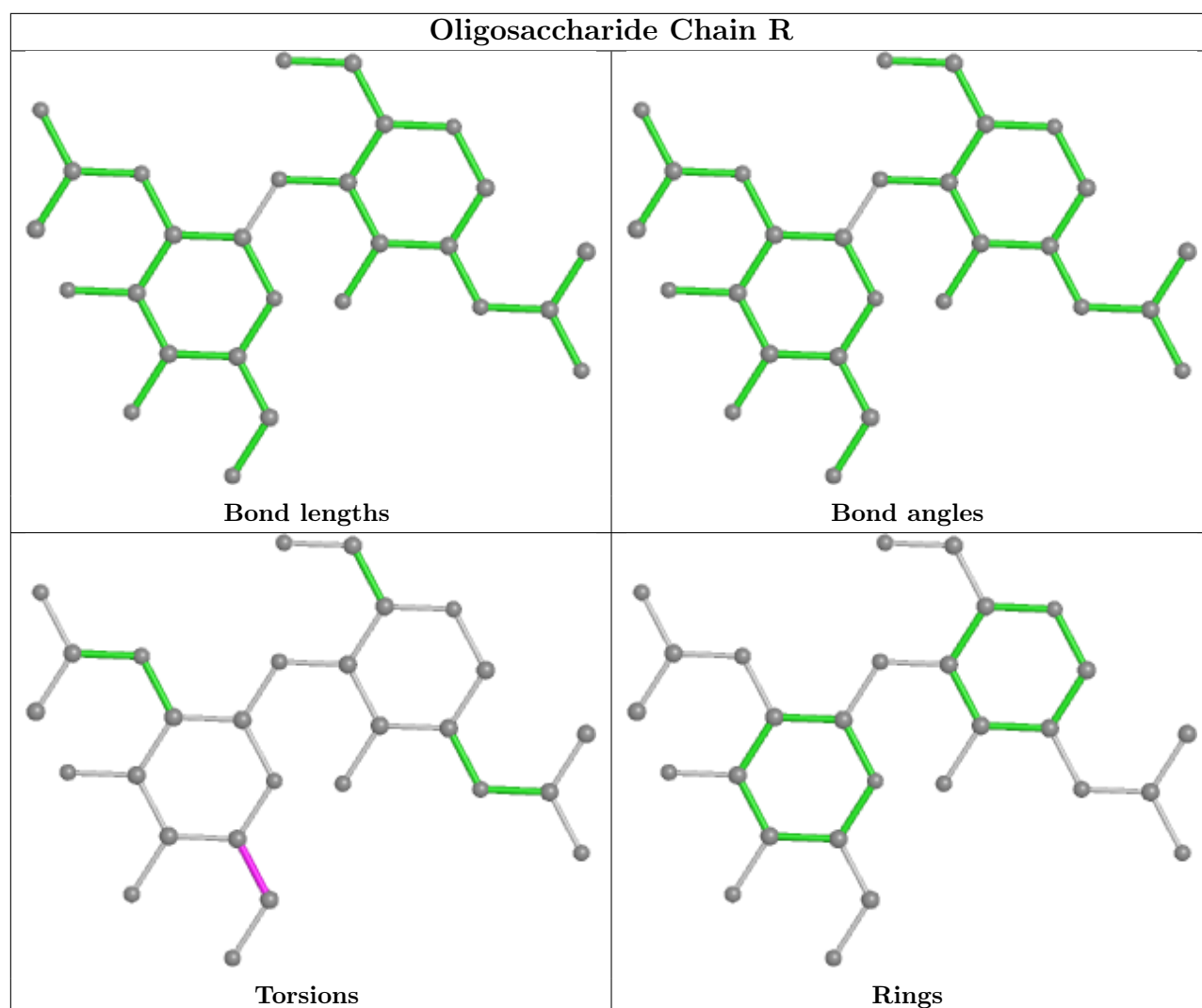


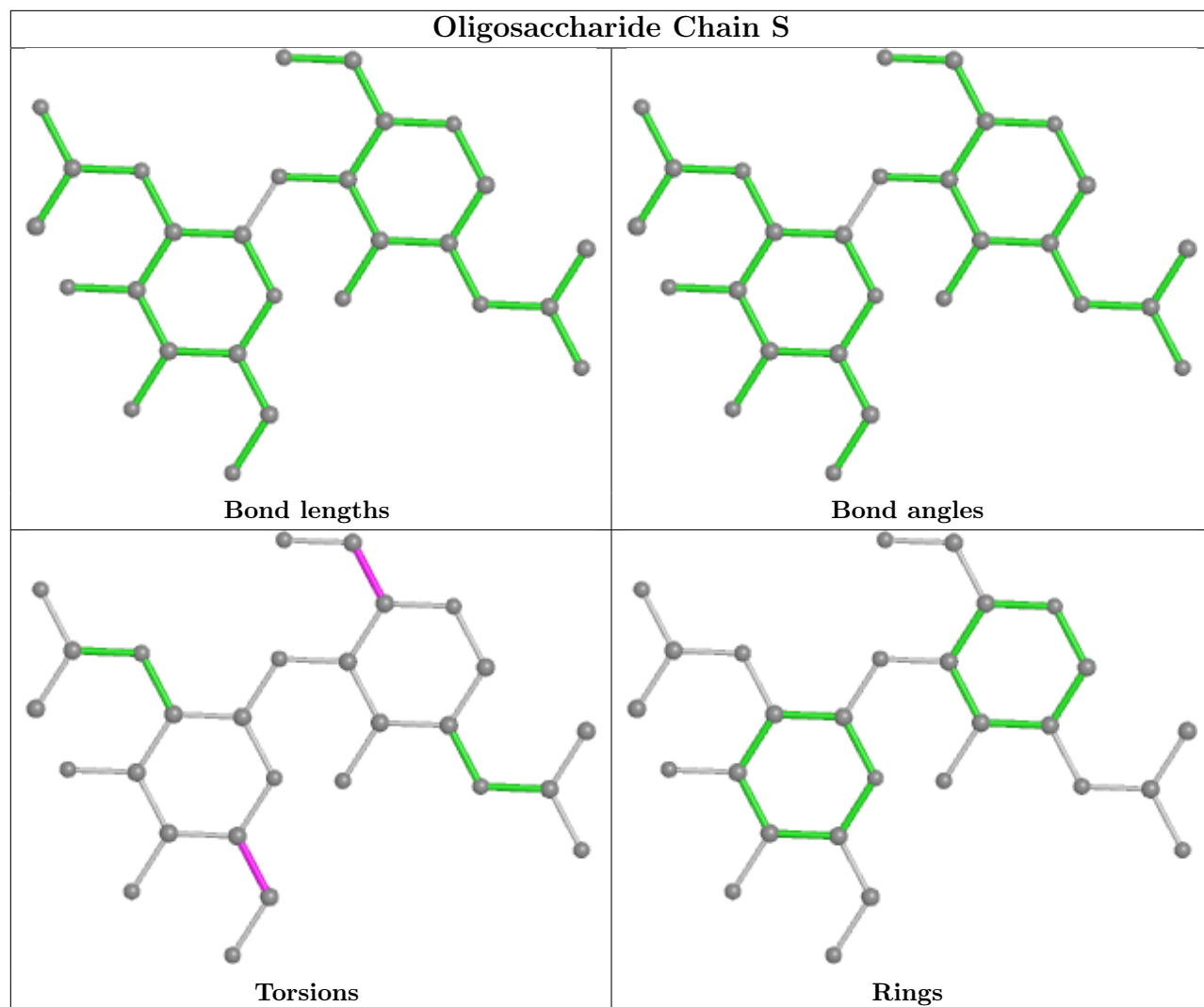


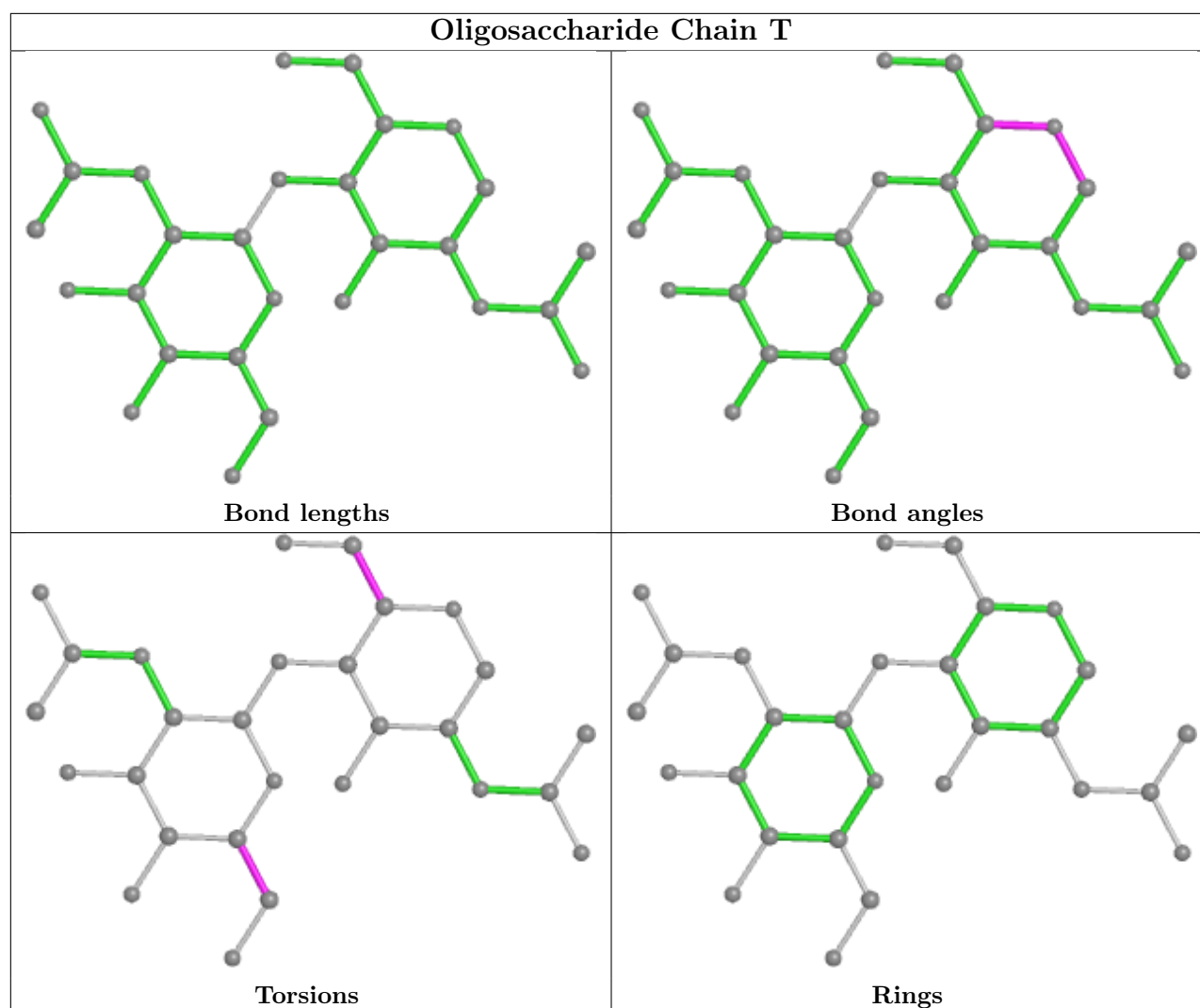












## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
5	NAG	A	2004	1	14,14,15	0.32	0	17,19,21	0.49	0
5	NAG	C	2010	1	14,14,15	0.23	0	17,19,21	0.54	0
5	NAG	A	2002	1	14,14,15	0.29	0	17,19,21	0.51	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	2009	1	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
5	NAG	B	2013	1	14,14,15	0.28	0	17,19,21	0.57	0
5	NAG	B	2012	1	14,14,15	0.22	0	17,19,21	0.66	1 (5%)
5	NAG	C	2011	1	14,14,15	0.47	0	17,19,21	0.75	1 (5%)
5	NAG	C	2007	1	14,14,15	0.41	0	17,19,21	0.48	0
5	NAG	B	2014	1	14,14,15	0.34	0	17,19,21	0.73	1 (5%)
5	NAG	C	2009	1	14,14,15	0.43	0	17,19,21	0.79	1 (5%)
5	NAG	A	2007	1	14,14,15	0.45	0	17,19,21	0.50	0
5	NAG	B	2006	1	14,14,15	0.42	0	17,19,21	0.58	0
5	NAG	B	2017	1	14,14,15	0.61	0	17,19,21	0.56	0
5	NAG	A	2017	1	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	A	2009	1	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
5	NAG	A	2011	1	14,14,15	0.27	0	17,19,21	0.56	0
5	NAG	B	2008	1	14,14,15	0.58	0	17,19,21	0.76	1 (5%)
5	NAG	B	2016	1	14,14,15	0.51	0	17,19,21	0.43	0
5	NAG	B	2001	1	14,14,15	0.34	0	17,19,21	0.49	0
5	NAG	B	2005	1	14,14,15	0.35	0	17,19,21	0.52	0
5	NAG	B	2010	1	14,14,15	0.36	0	17,19,21	0.41	0
5	NAG	C	2013	1	14,14,15	0.60	0	17,19,21	0.43	0
5	NAG	A	2016	1	14,14,15	0.40	0	17,19,21	0.55	0
5	NAG	B	2011	1	14,14,15	0.36	0	17,19,21	0.55	0
5	NAG	A	2001	1	14,14,15	0.30	0	17,19,21	0.55	0
5	NAG	B	2007	1	14,14,15	0.29	0	17,19,21	0.52	0
5	NAG	C	2004	1	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	A	2013	1	14,14,15	0.59	0	17,19,21	0.55	0
5	NAG	A	2005	1	14,14,15	0.28	0	17,19,21	0.71	1 (5%)
5	NAG	A	2015	1	14,14,15	0.27	0	17,19,21	0.61	0
5	NAG	C	2017	1	14,14,15	0.25	0	17,19,21	0.59	0
5	NAG	A	2012	1	14,14,15	0.28	0	17,19,21	0.56	0
5	NAG	C	2015	1	14,14,15	0.41	0	17,19,21	0.55	0
5	NAG	A	2008	1	14,14,15	0.58	0	17,19,21	0.76	1 (5%)
5	NAG	B	2002	1	14,14,15	0.51	0	17,19,21	0.67	1 (5%)
5	NAG	C	2001	1	14,14,15	0.32	0	17,19,21	0.50	0
5	NAG	C	2003	1	14,14,15	0.36	0	17,19,21	0.40	0
5	NAG	C	2005	1	14,14,15	0.37	0	17,19,21	0.52	0
5	NAG	A	2010	1	14,14,15	0.35	0	17,19,21	0.51	0
5	NAG	A	2003	1	14,14,15	0.34	0	17,19,21	0.40	0
5	NAG	C	2014	1	14,14,15	0.27	0	17,19,21	0.35	0
5	NAG	B	2004	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	2006	1	14,14,15	0.44	0	17,19,21	0.41	0
5	NAG	C	2016	1	14,14,15	0.35	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	C	2008	1	14,14,15	0.22	0	17,19,21	0.45	0
5	NAG	C	2002	1	14,14,15	0.37	0	17,19,21	0.62	1 (5%)
5	NAG	A	2014	1	14,14,15	0.37	0	17,19,21	0.43	0
5	NAG	C	2012	1	14,14,15	0.28	0	17,19,21	0.79	1 (5%)
5	NAG	A	2006	1	14,14,15	0.24	0	17,19,21	0.53	0
5	NAG	B	2003	1	14,14,15	0.34	0	17,19,21	0.33	0
5	NAG	B	2015	1	14,14,15	0.30	0	17,19,21	0.62	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
5	NAG	A	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2011	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2007	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2007	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2017	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2009	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2011	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2016	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2016	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	2011	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2007	1	-	1/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2017	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2015	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2002	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2001	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2016	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2003	1	-	1/6/23/26	0/1/1/1
5	NAG	B	2015	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2009	NAG	C1-O5-C5	3.30	116.66	112.19
5	B	2009	NAG	C1-O5-C5	3.25	116.60	112.19
5	C	2009	NAG	C1-O5-C5	2.93	116.16	112.19
5	C	2012	NAG	C1-O5-C5	2.74	115.91	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2008	NAG	C1-O5-C5	2.71	115.86	112.19
5	B	2008	NAG	C1-O5-C5	2.71	115.86	112.19
5	C	2011	NAG	C1-O5-C5	2.70	115.84	112.19
5	B	2014	NAG	C1-O5-C5	2.64	115.78	112.19
5	A	2005	NAG	C1-O5-C5	2.56	115.66	112.19
5	B	2002	NAG	C1-O5-C5	2.31	115.33	112.19
5	B	2012	NAG	C1-O5-C5	2.24	115.22	112.19
5	C	2002	NAG	C1-O5-C5	2.10	115.04	112.19
5	B	2015	NAG	C1-O5-C5	2.03	114.94	112.19

There are no chirality outliers.

All (81) torsion outliers are listed below:

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

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

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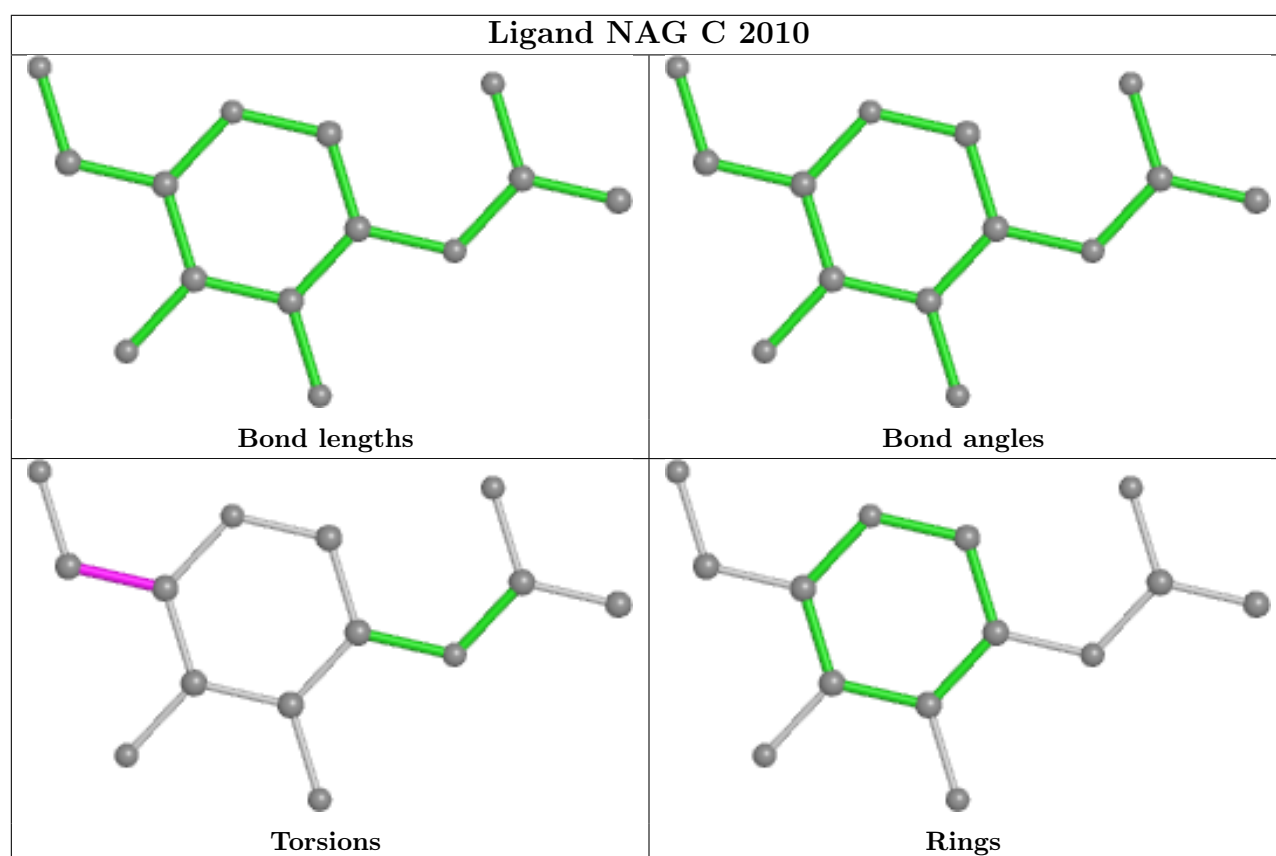
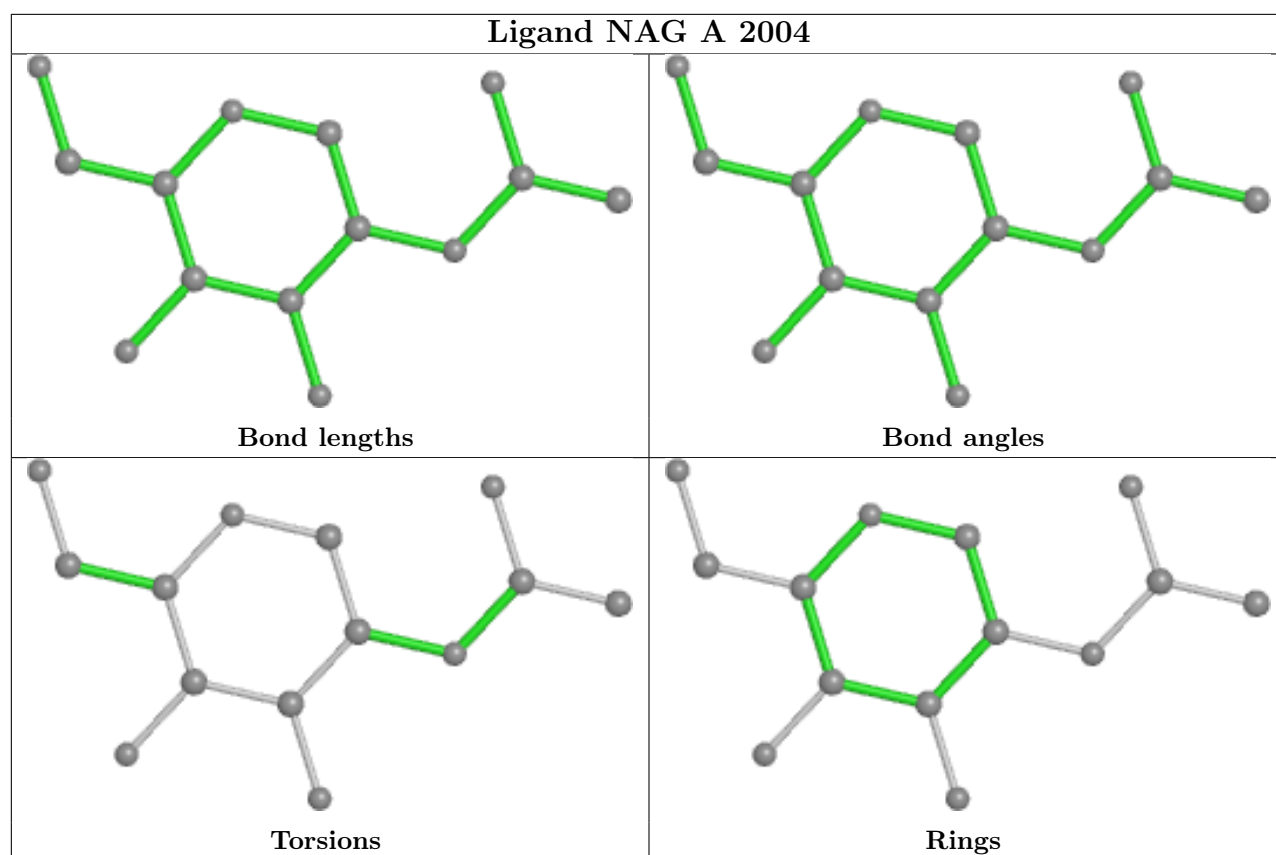
Mol	Chain	Res	Type	Atoms
5	C	2016	NAG	O5-C5-C6-O6
5	C	2008	NAG	C4-C5-C6-O6
5	B	2010	NAG	C4-C5-C6-O6
5	C	2008	NAG	O5-C5-C6-O6
5	A	2011	NAG	O5-C5-C6-O6
5	A	2005	NAG	C4-C5-C6-O6
5	C	2006	NAG	C4-C5-C6-O6
5	C	2009	NAG	C4-C5-C6-O6
5	C	2003	NAG	C4-C5-C6-O6
5	C	2009	NAG	O5-C5-C6-O6
5	C	2013	NAG	C4-C5-C6-O6

There are no ring outliers.

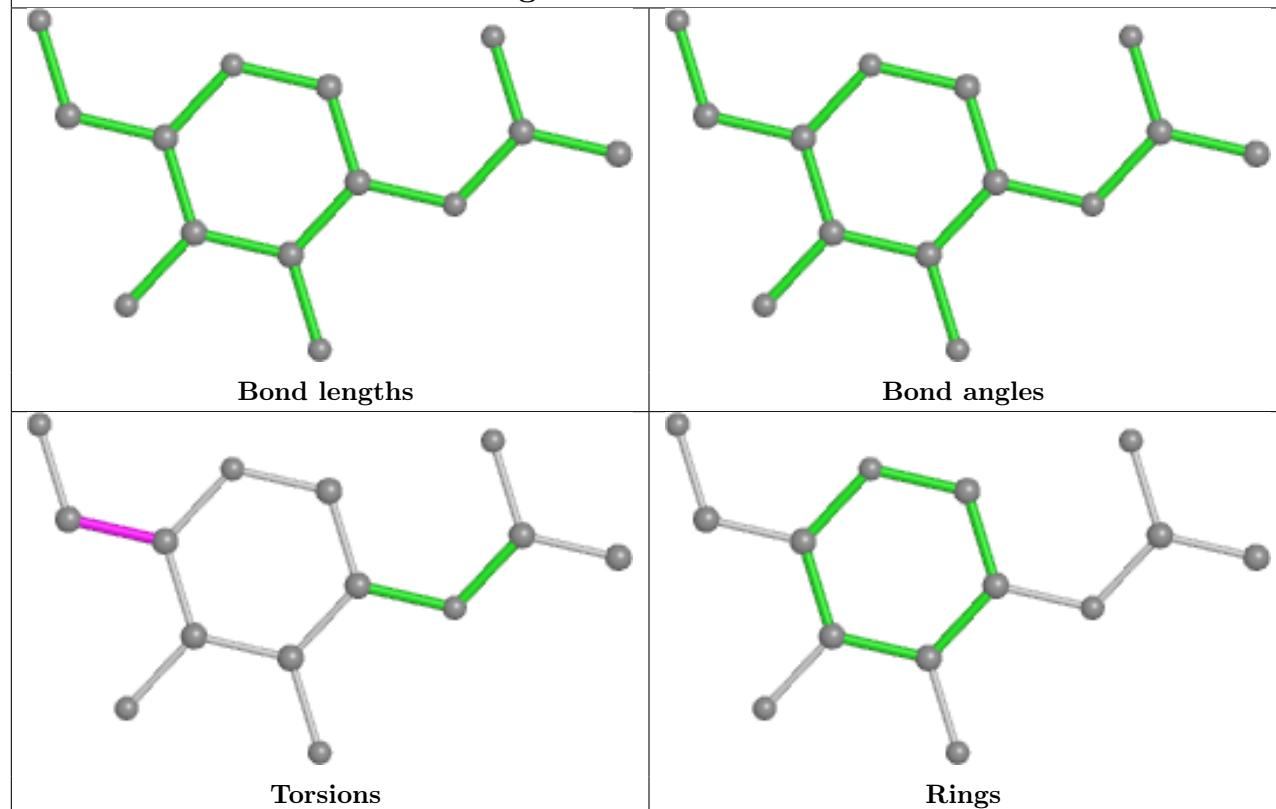
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2001	NAG	11	0
5	A	2006	NAG	1	0

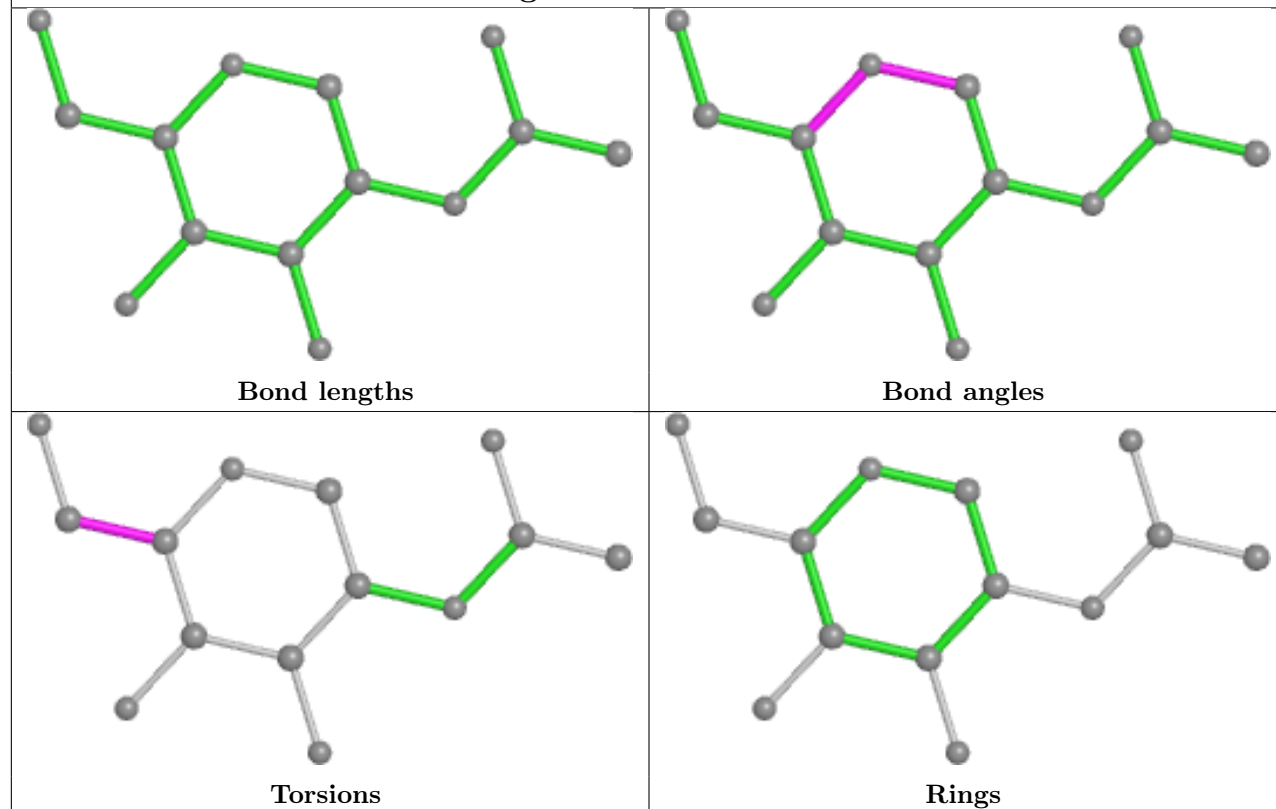
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



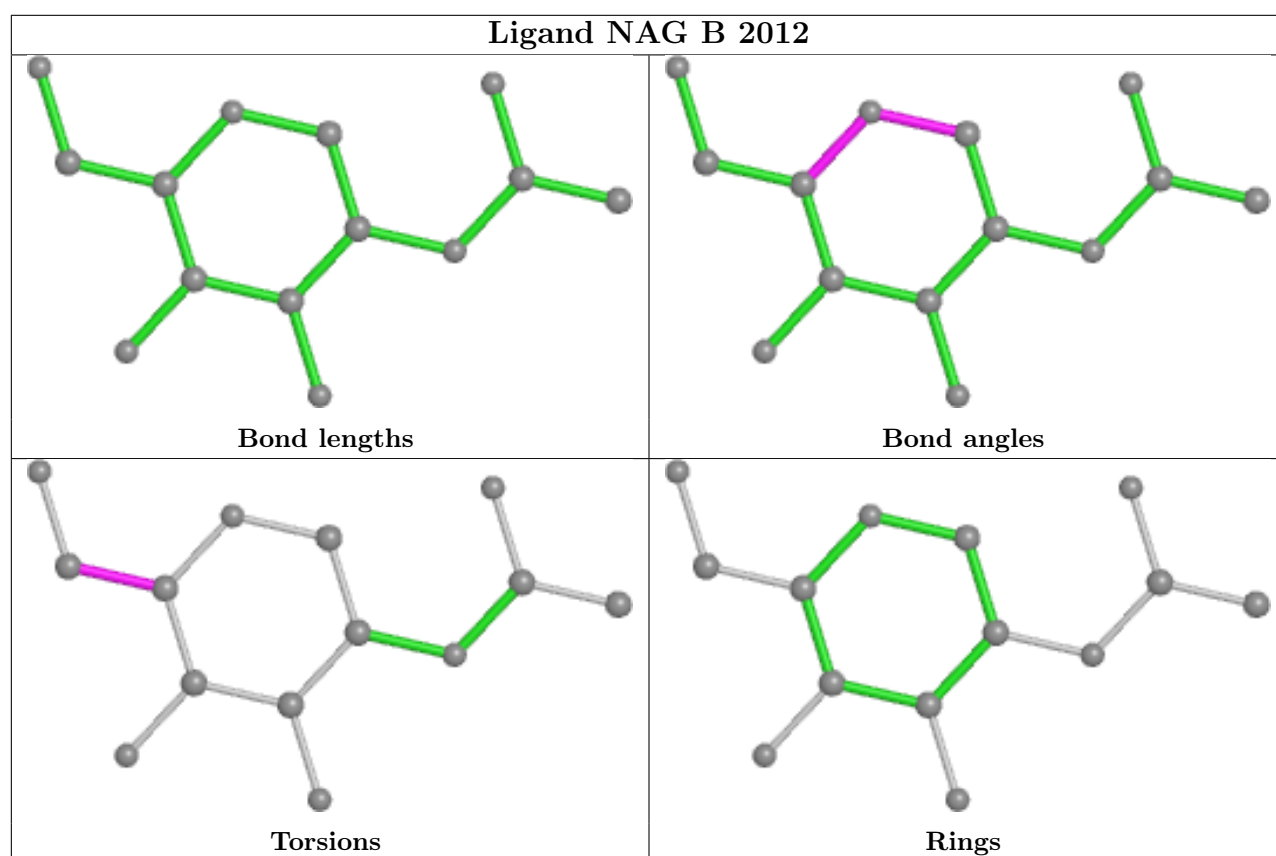
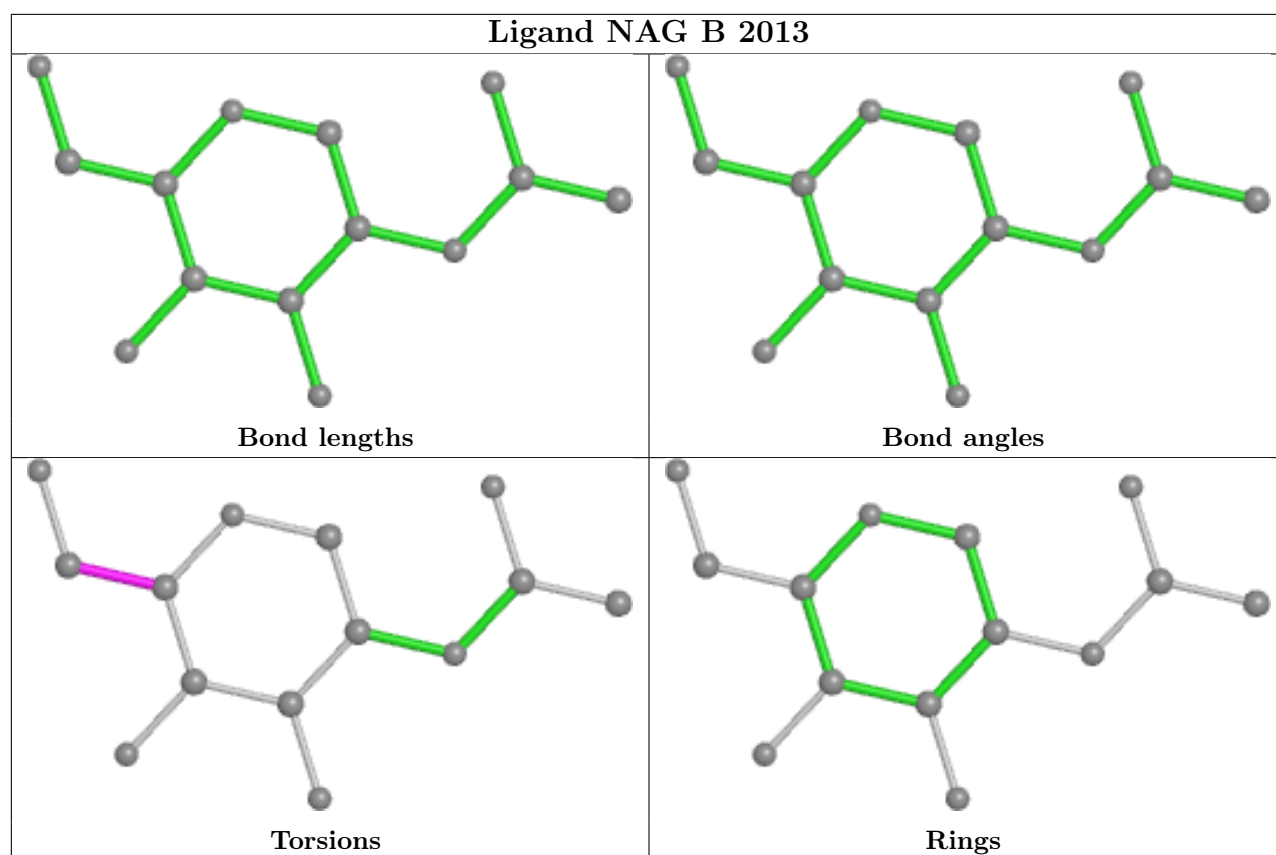
## Ligand NAG A 2002

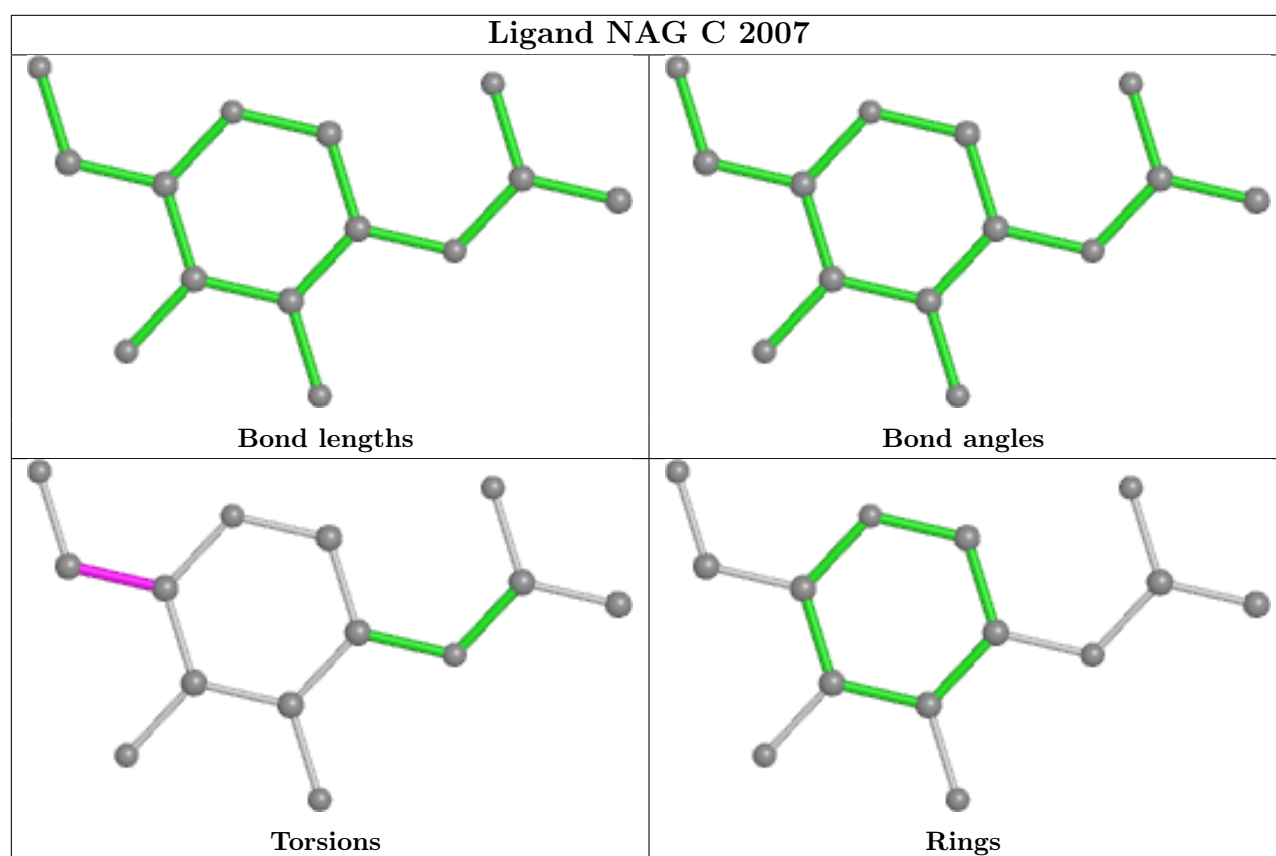
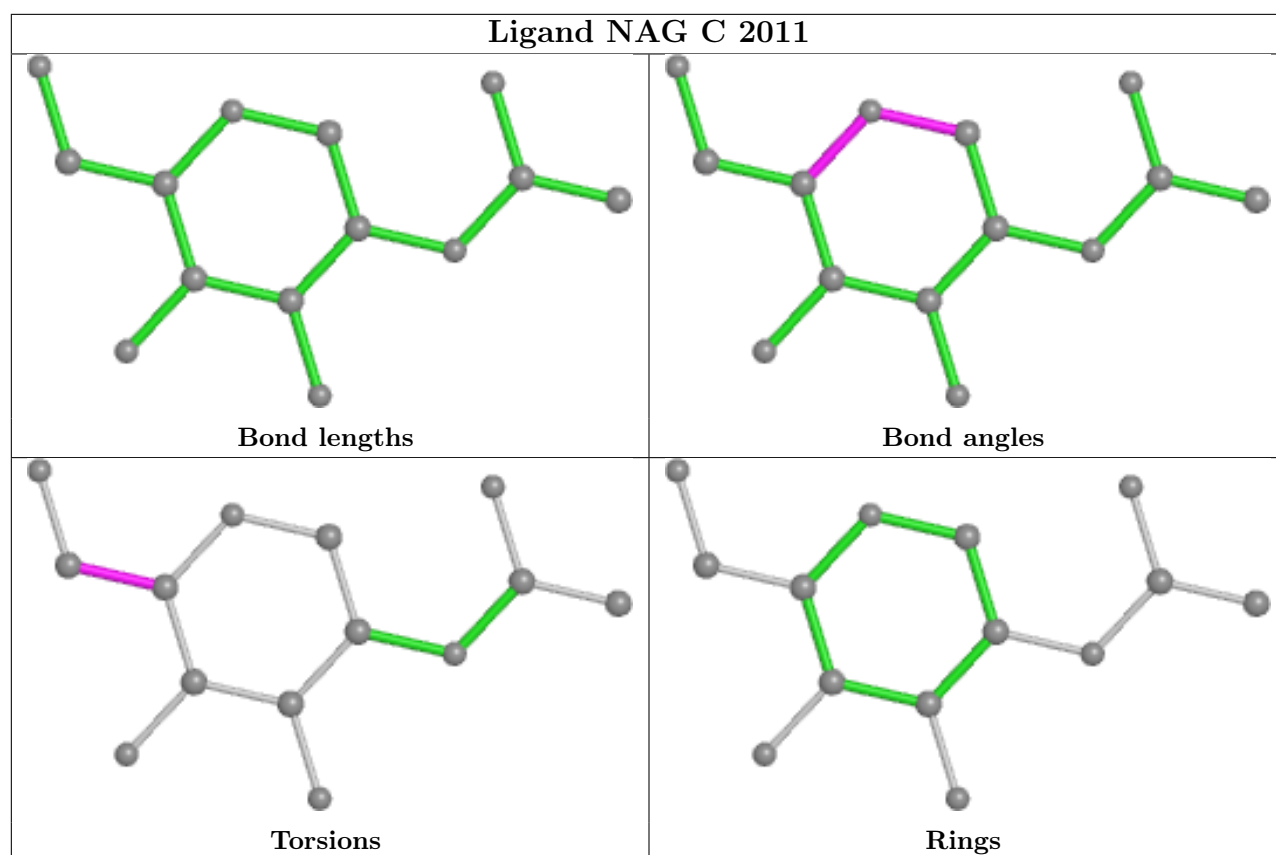


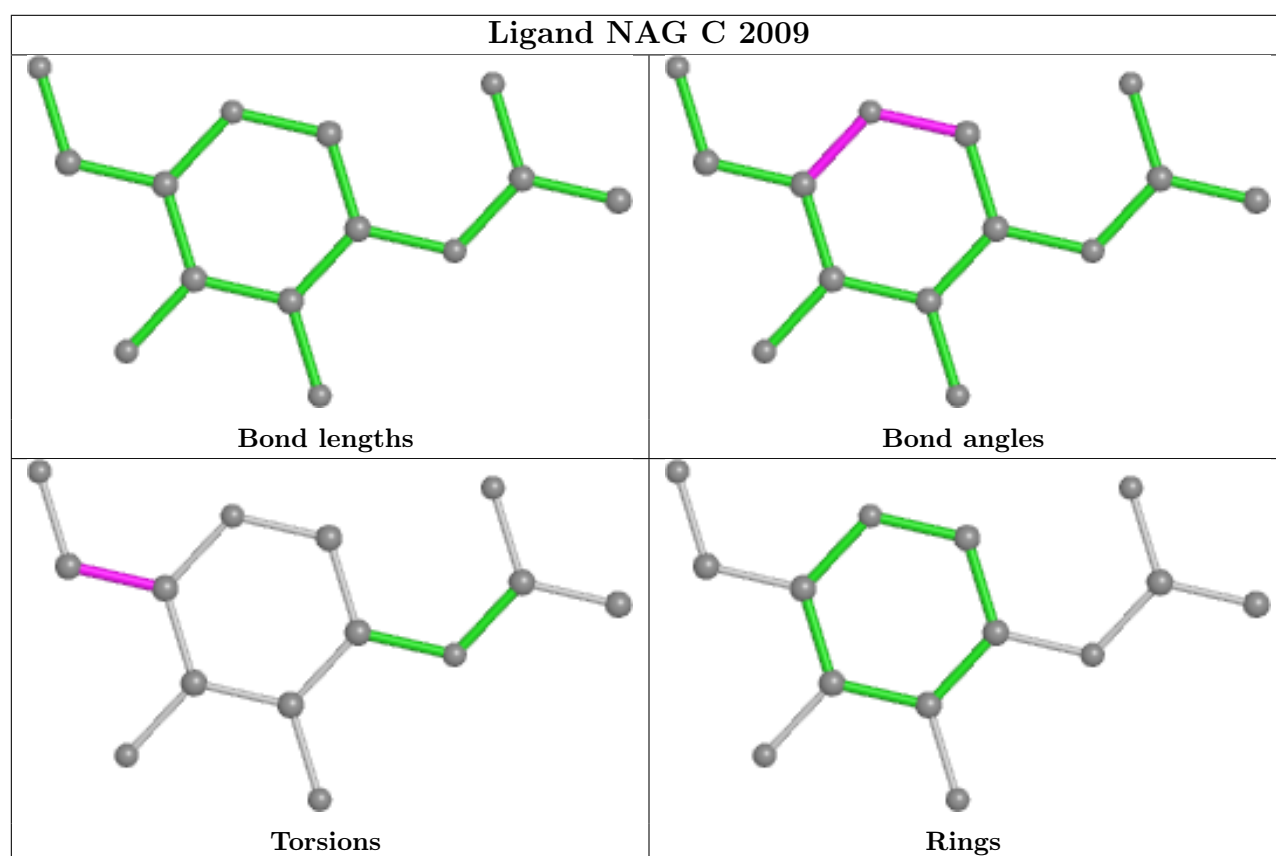
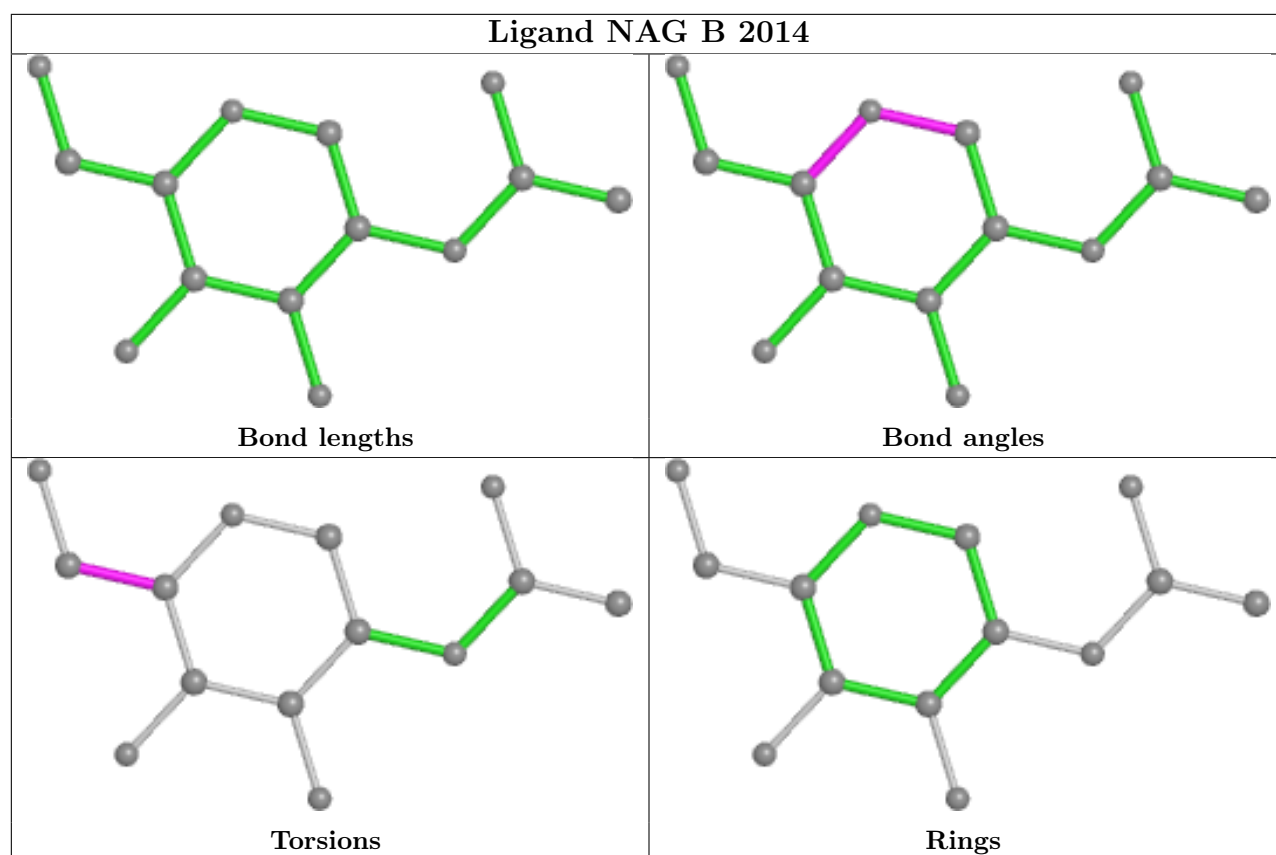
## Ligand NAG B 2009

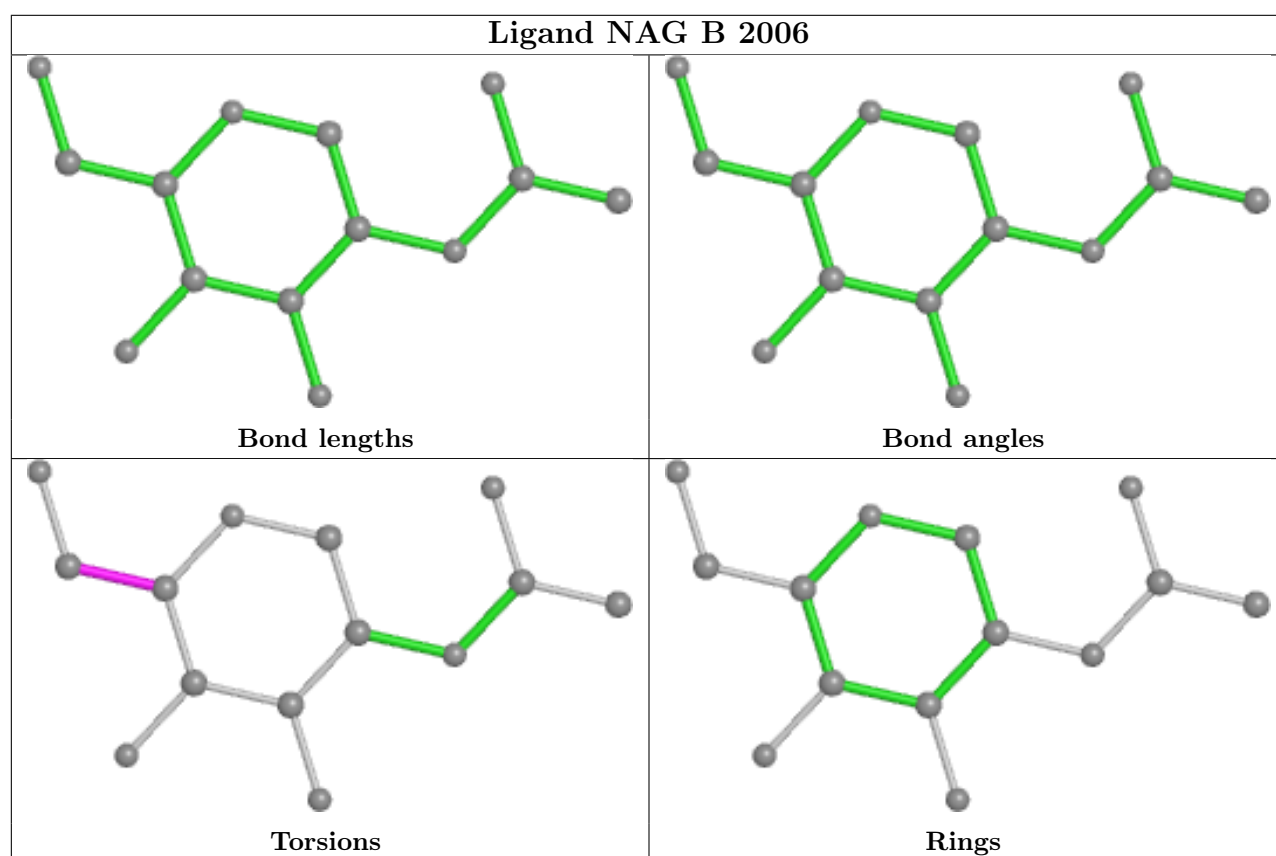
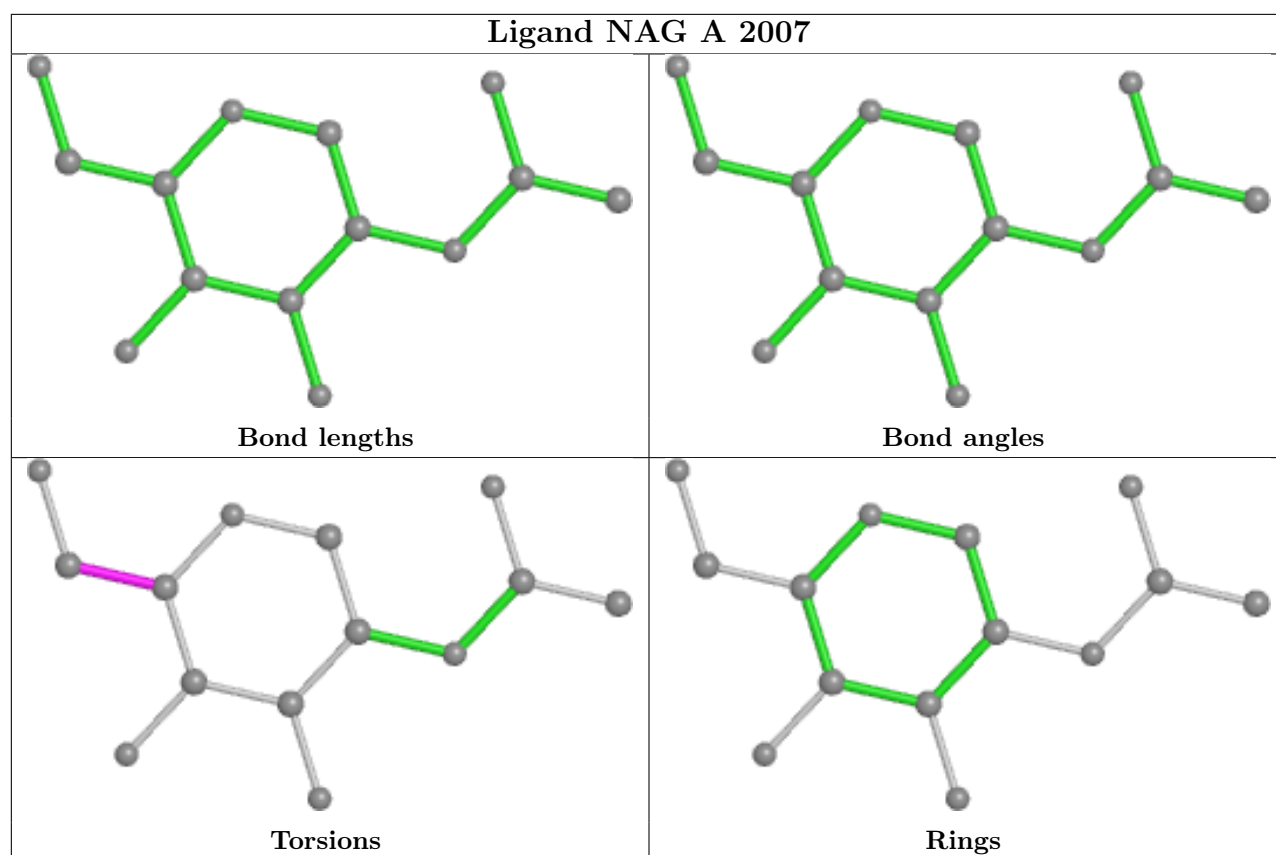


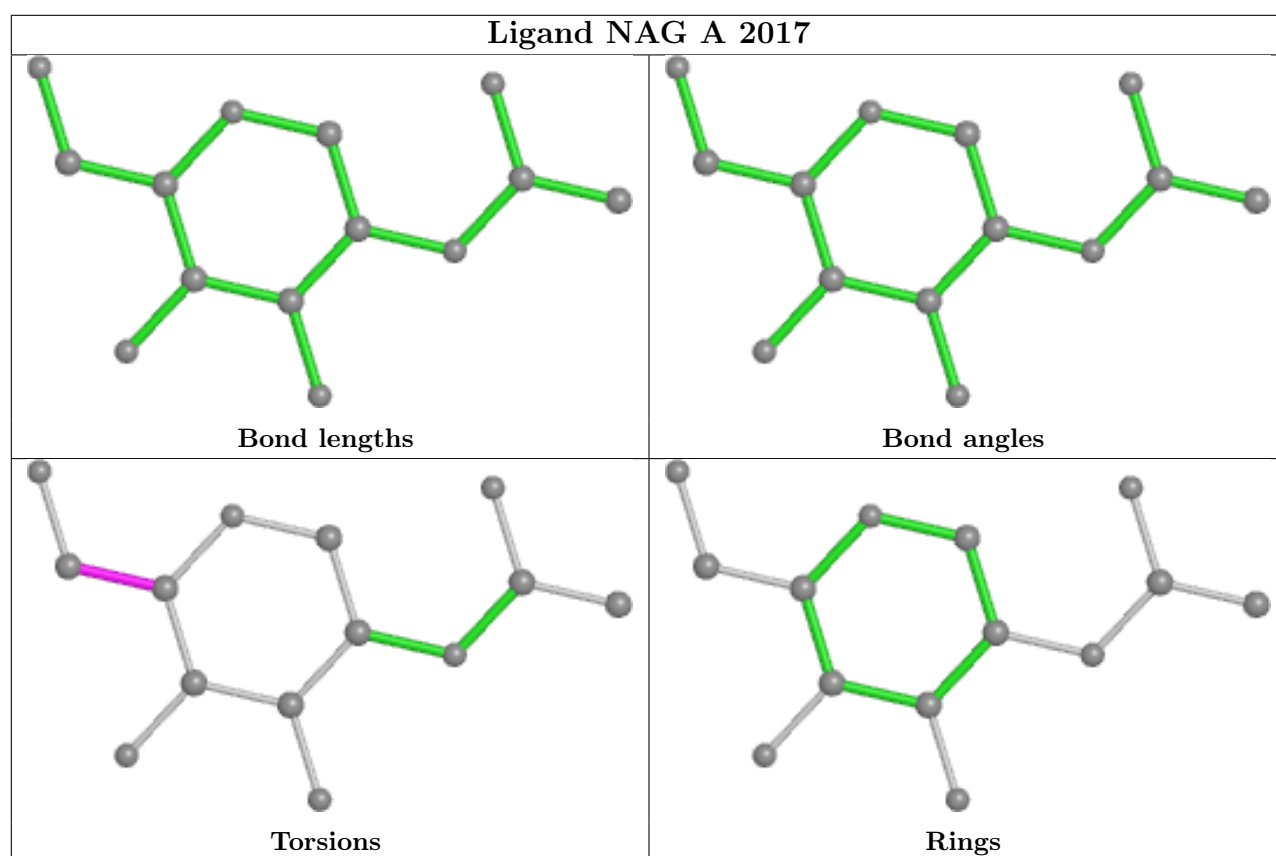
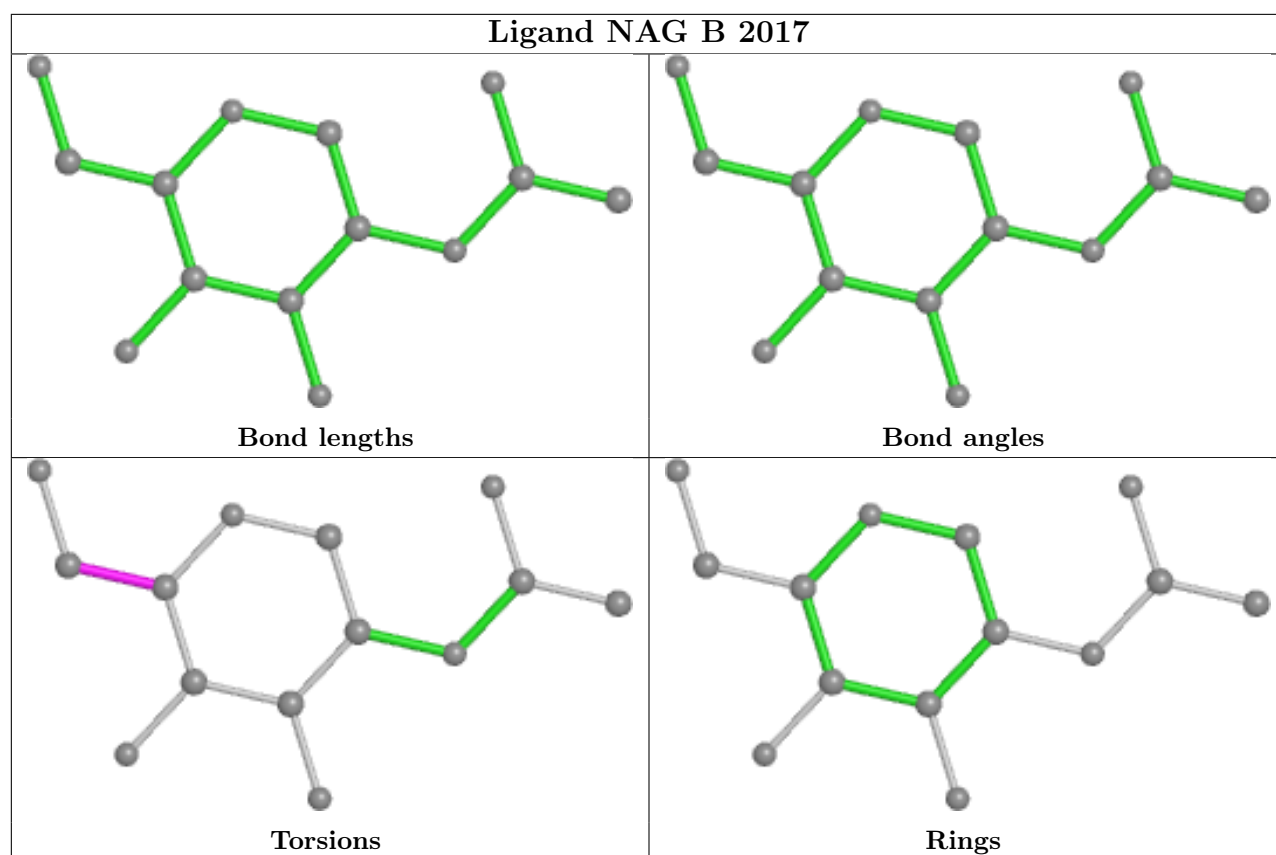


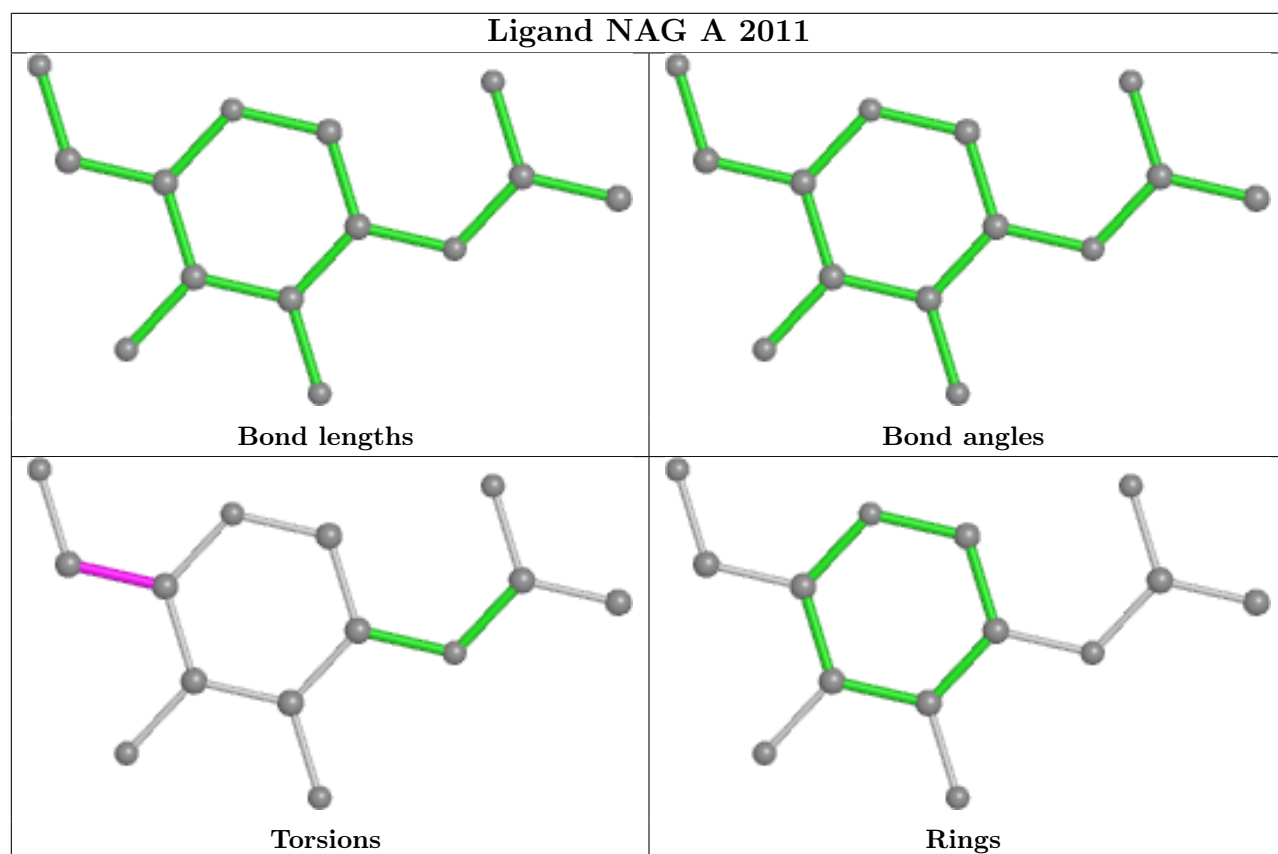
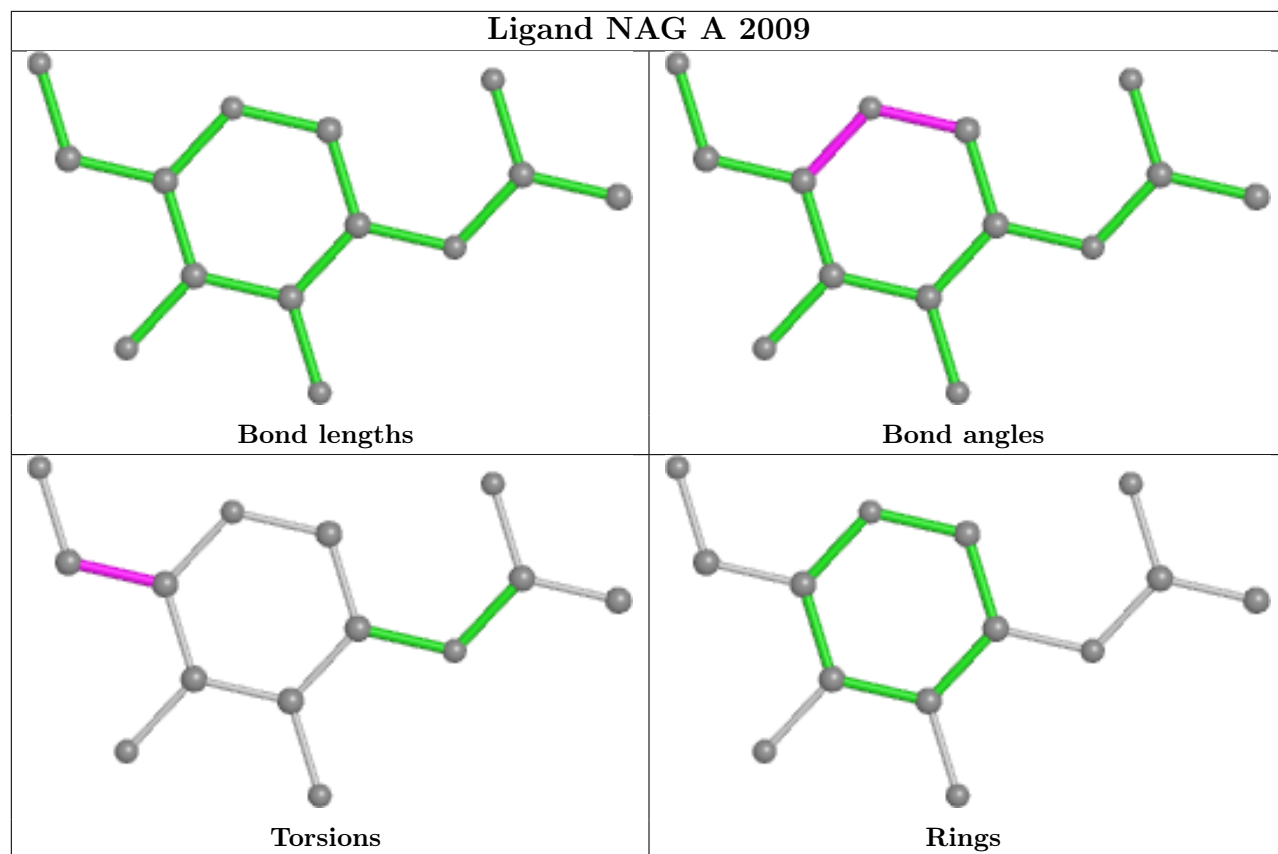


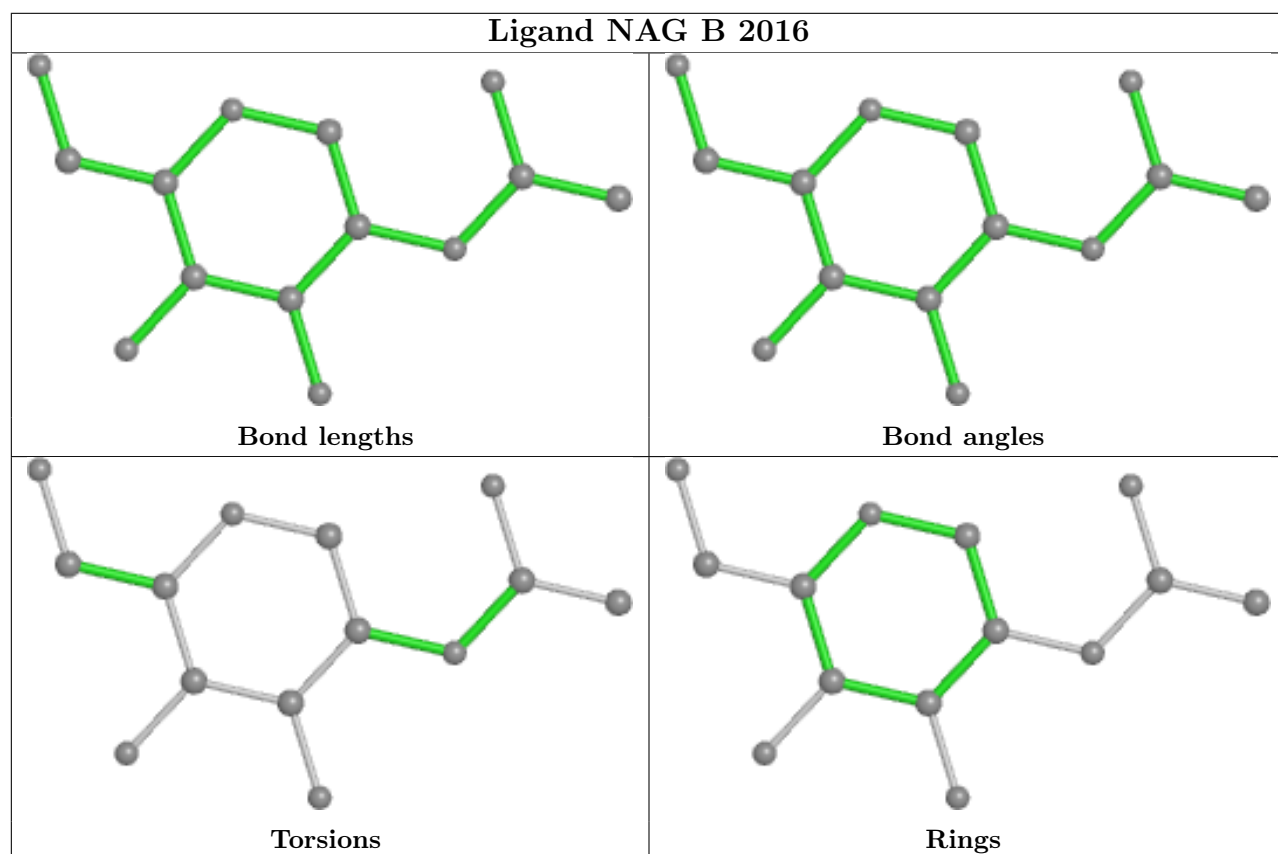
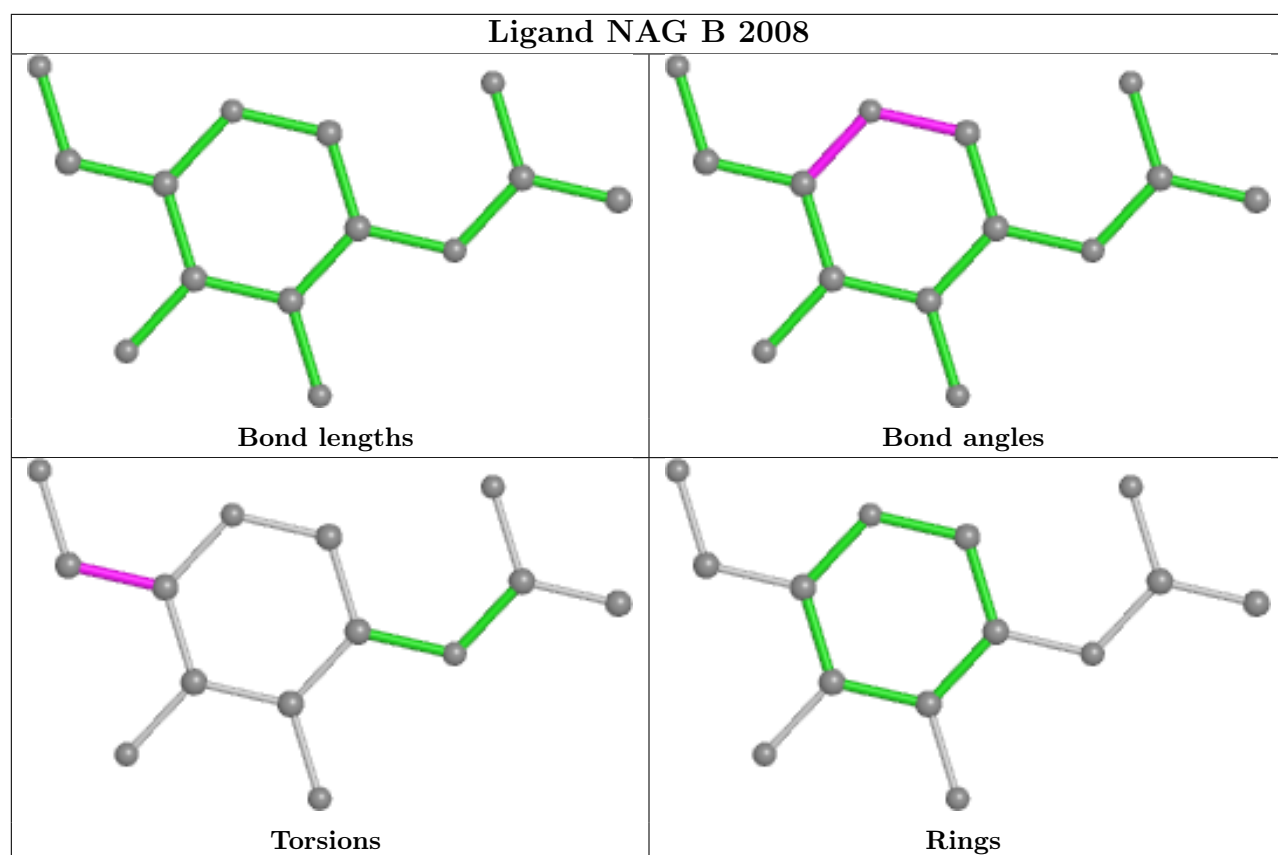


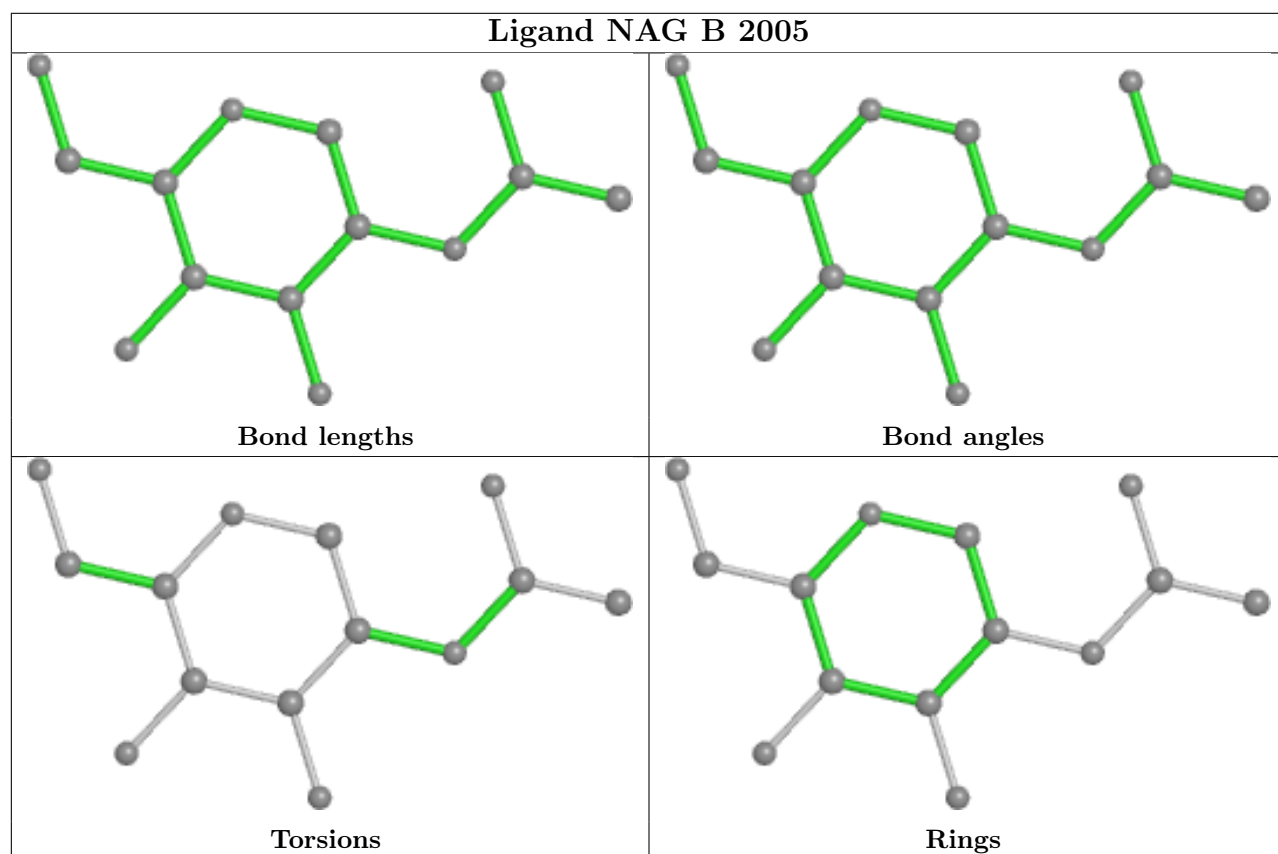
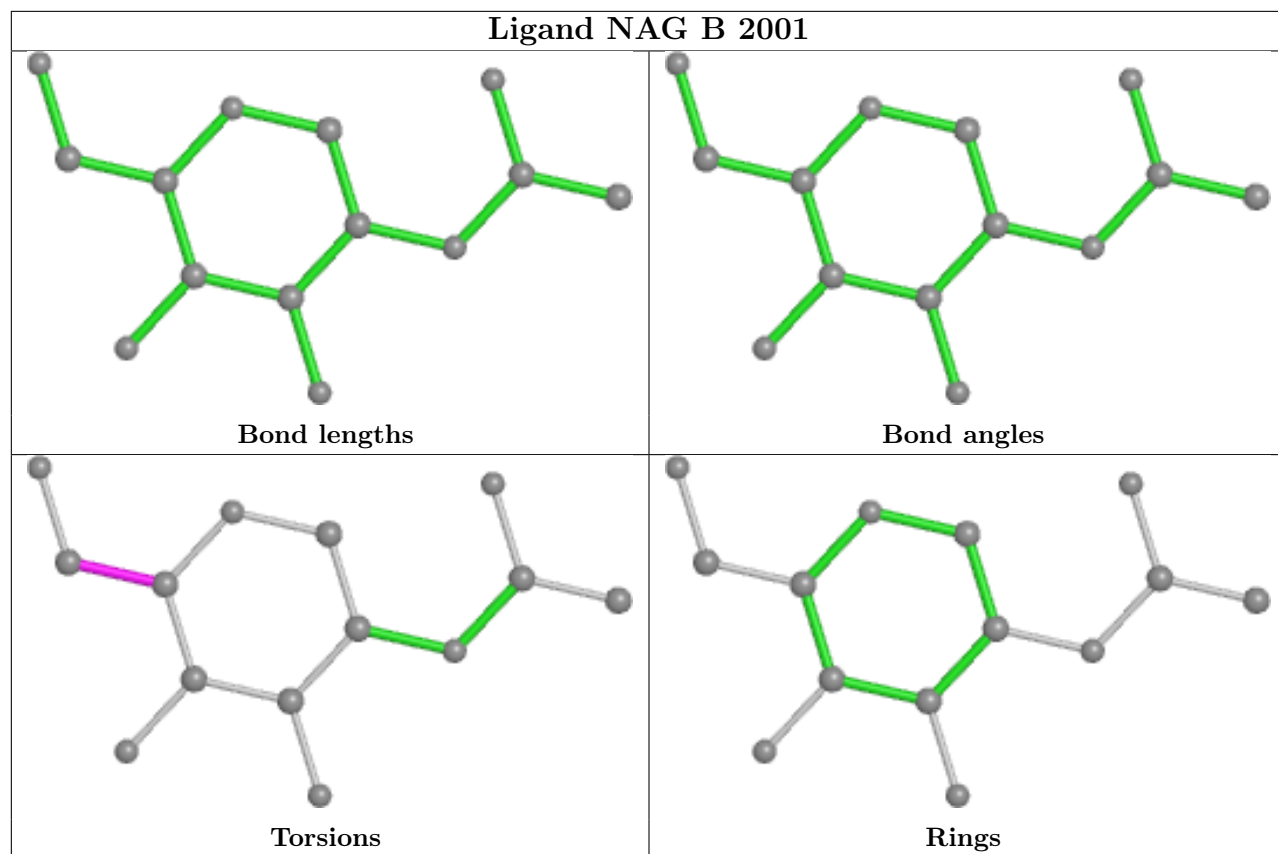




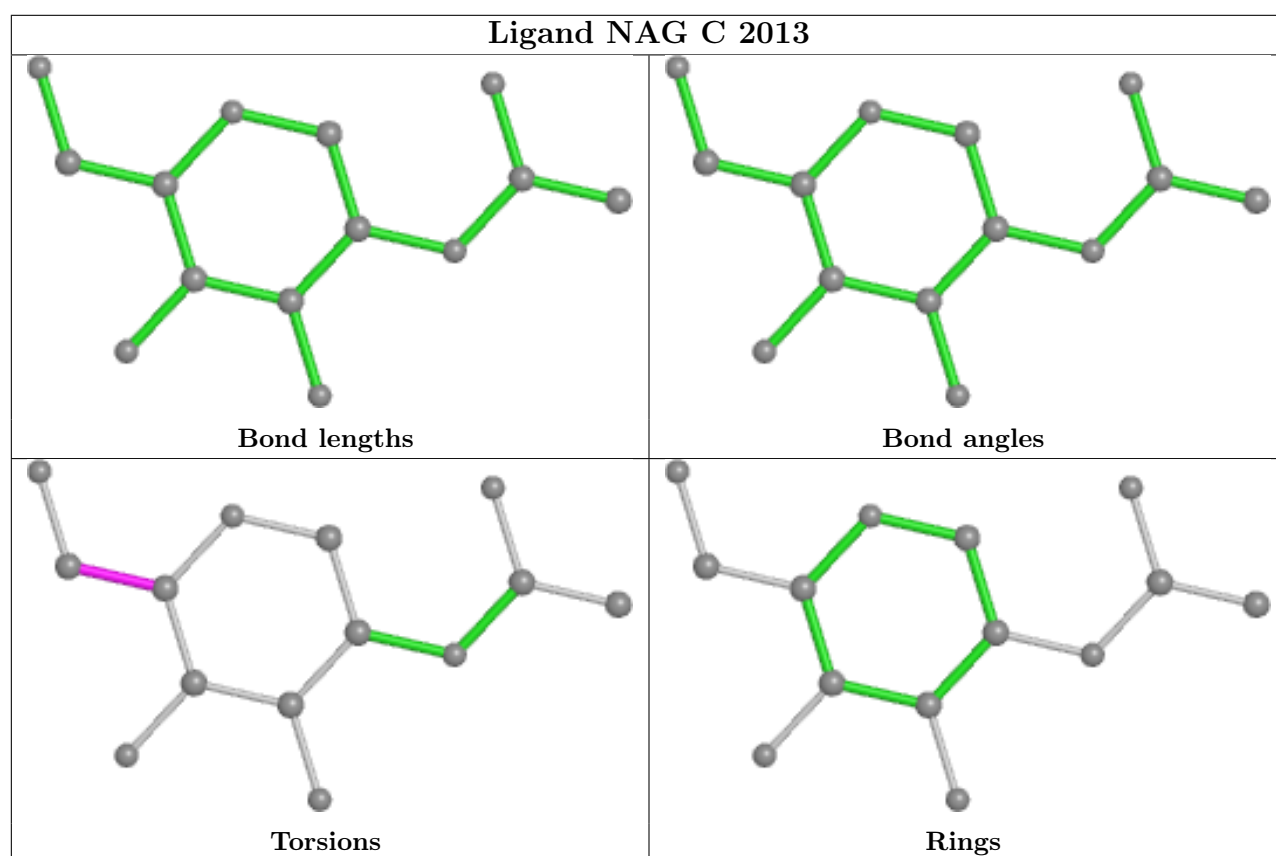
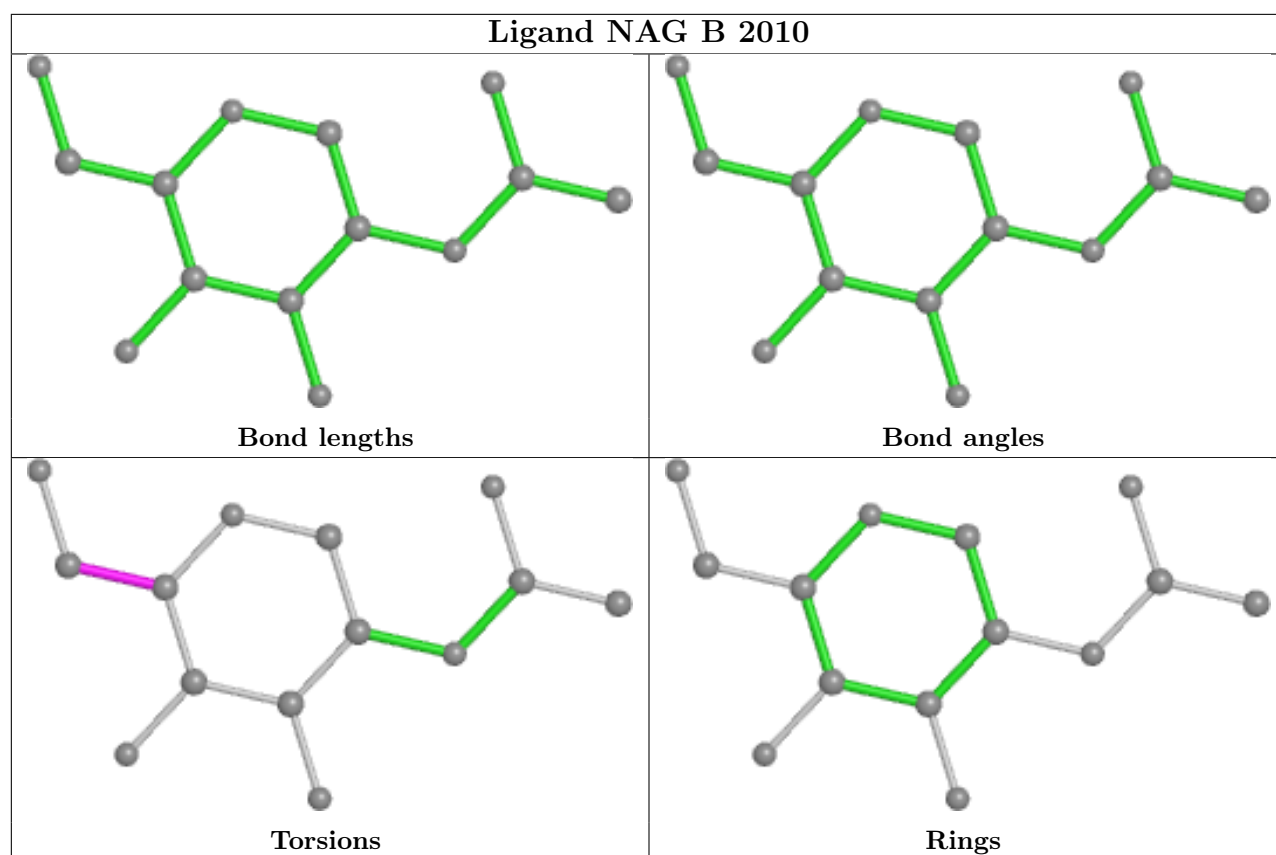


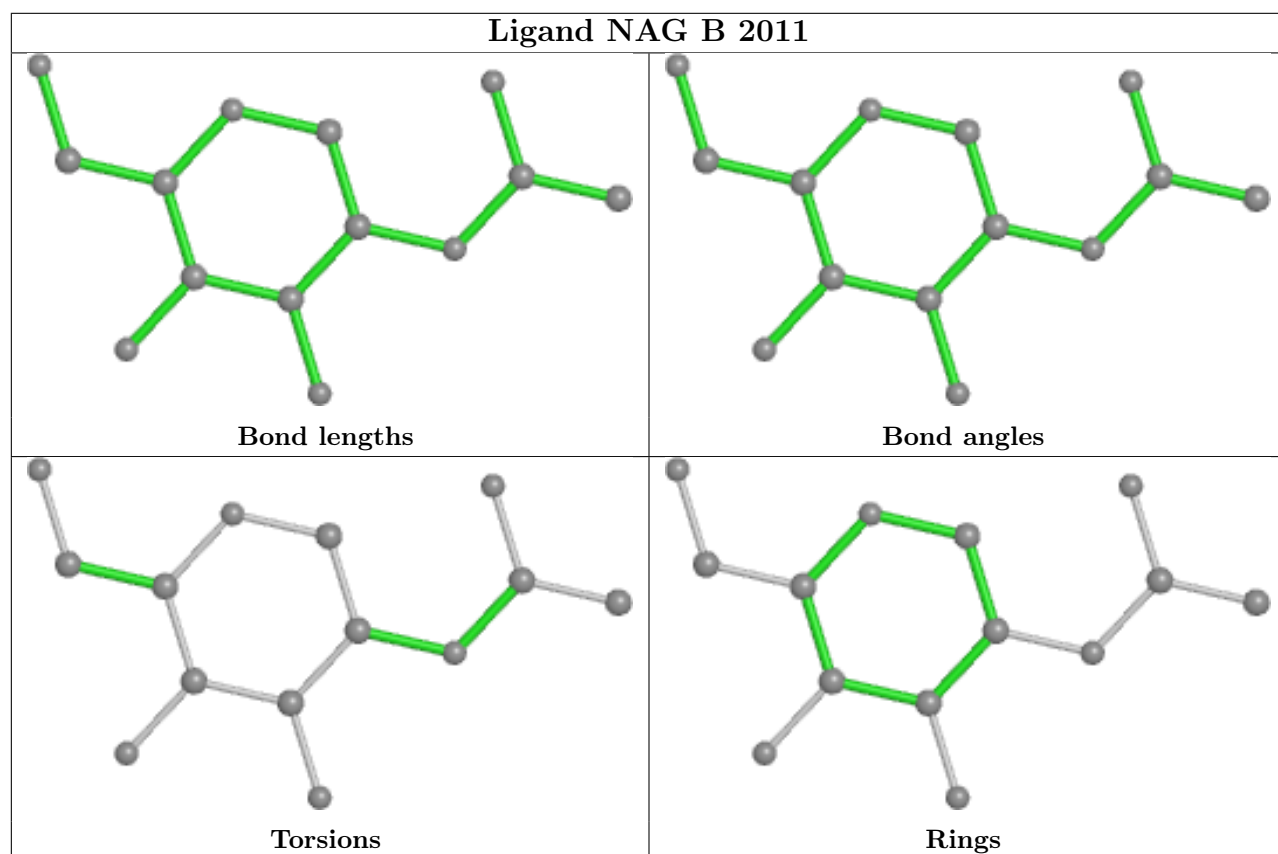
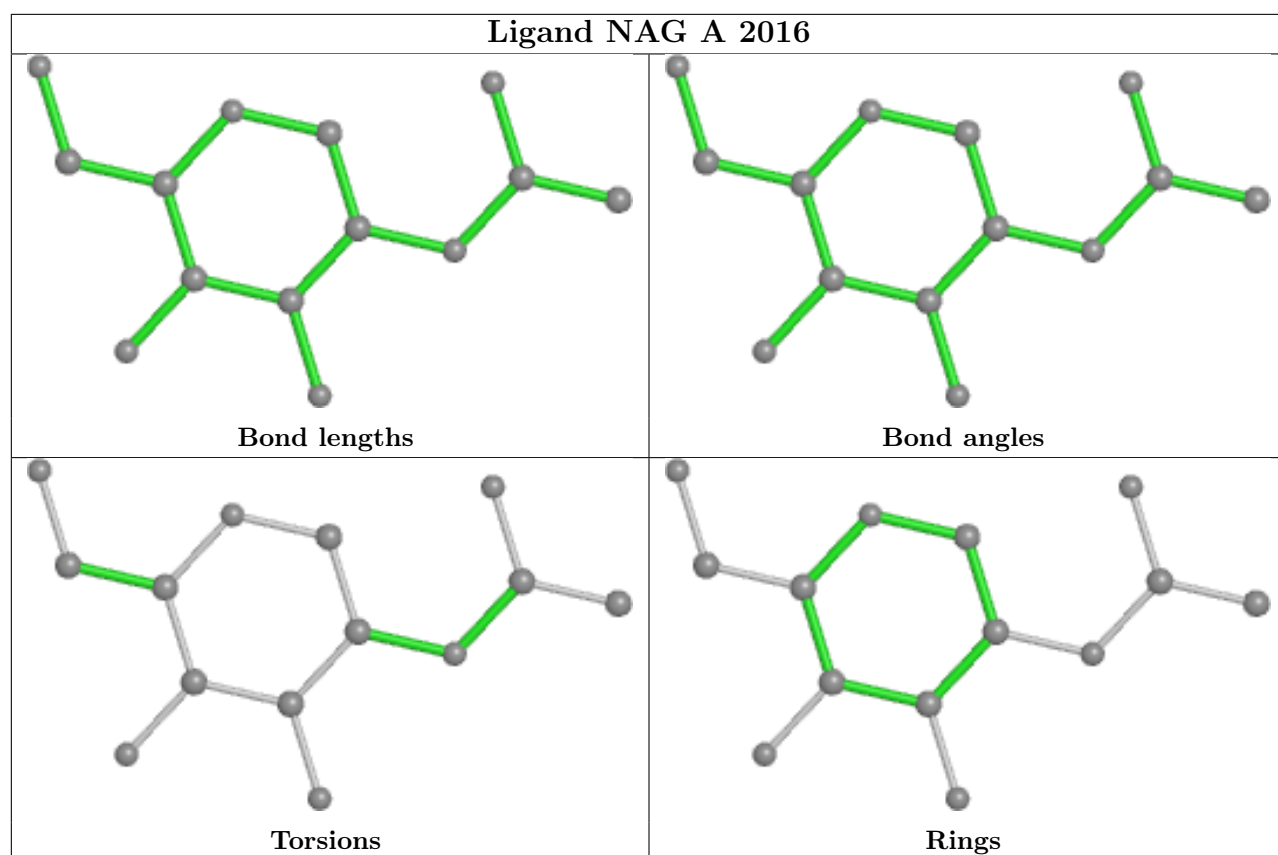


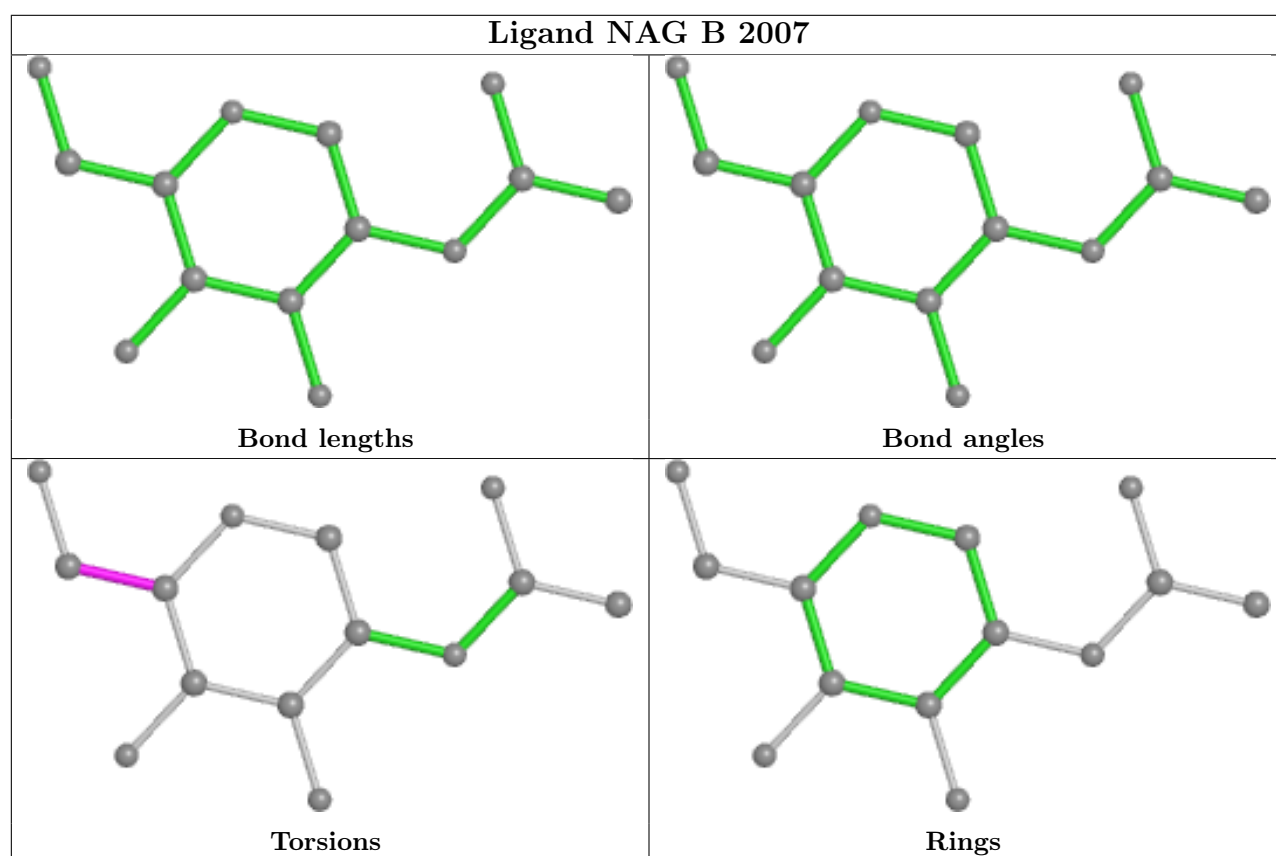
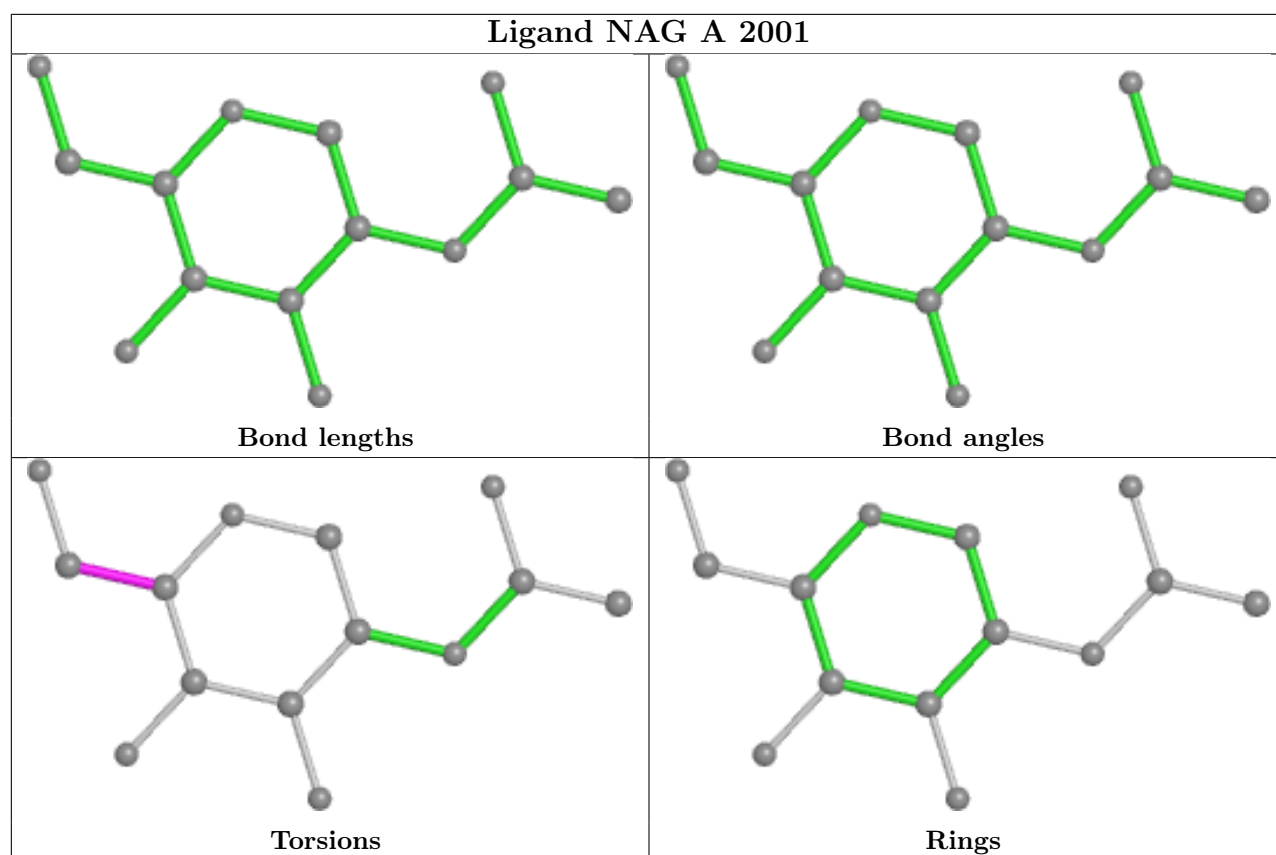


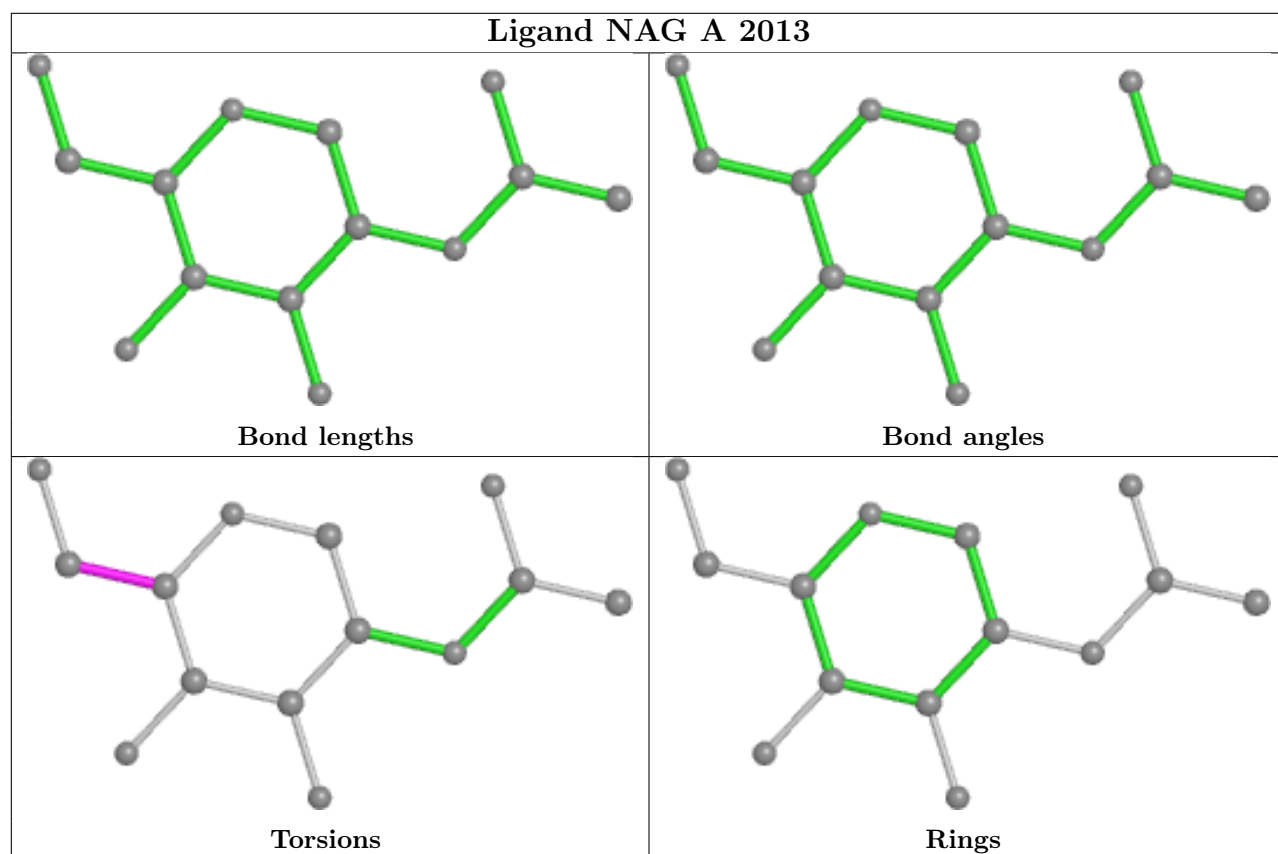
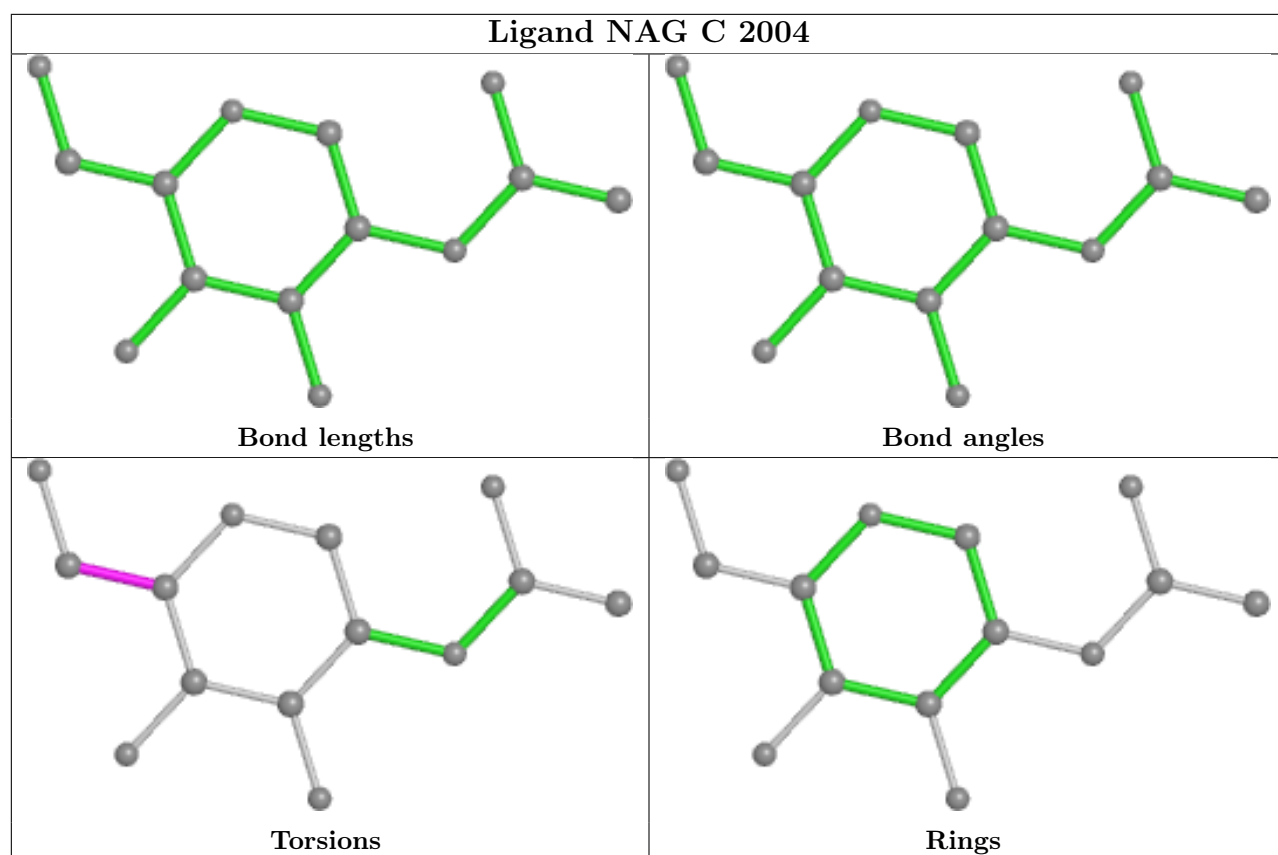


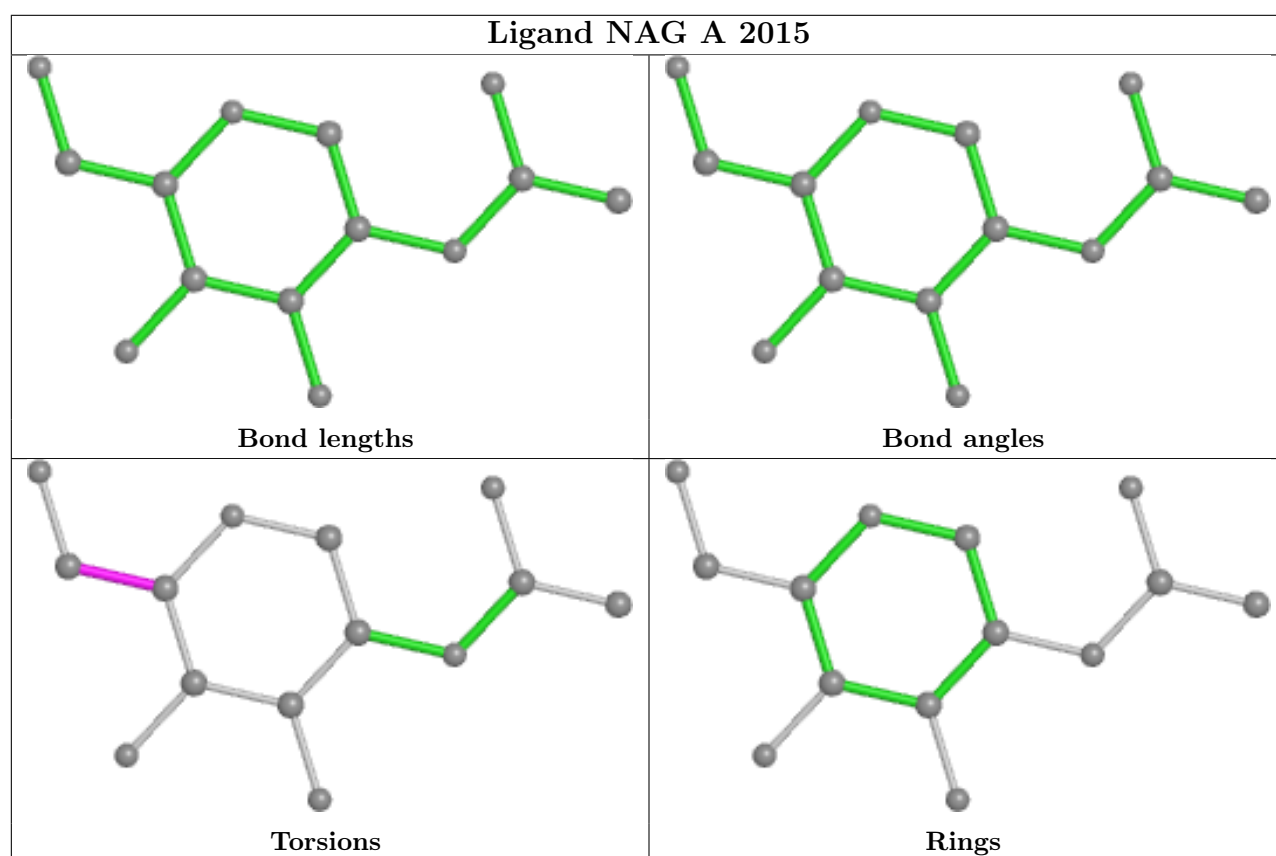
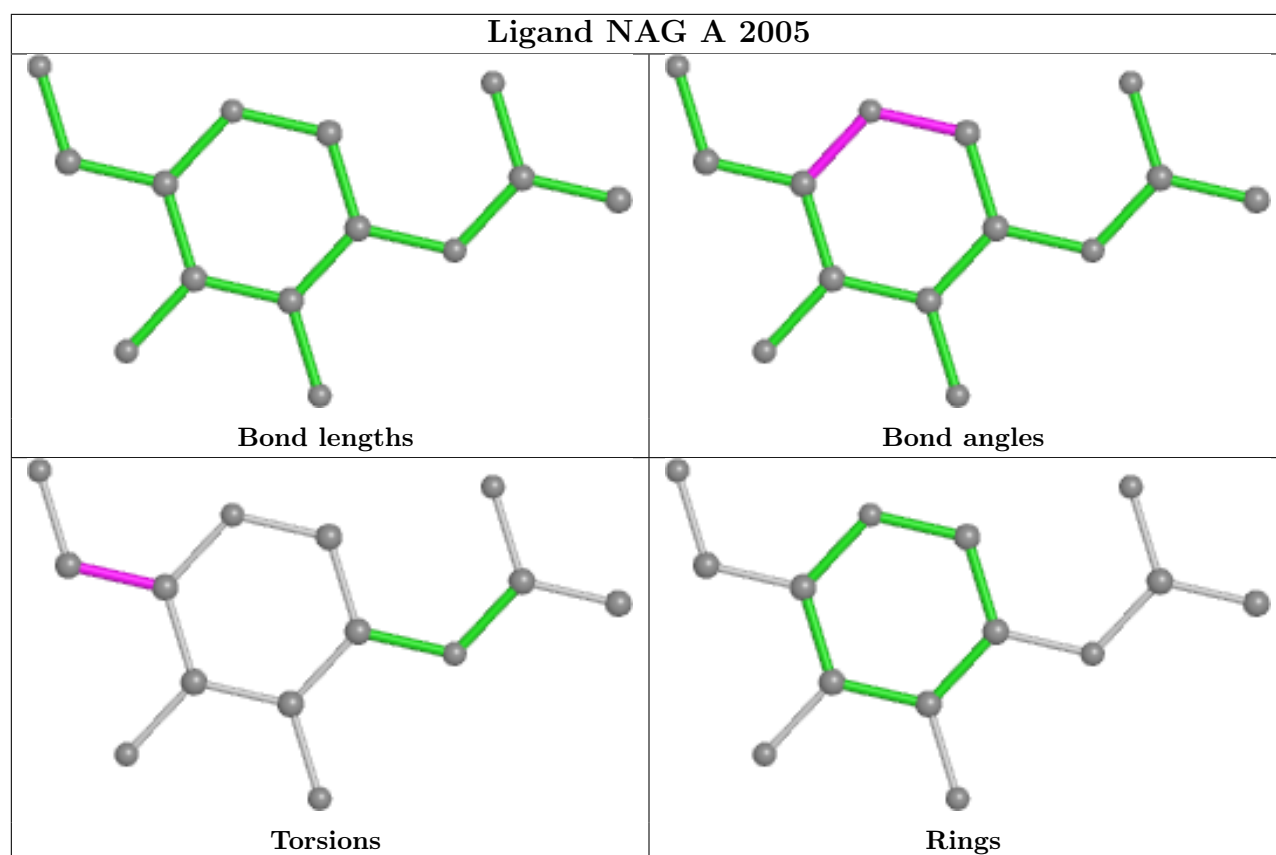


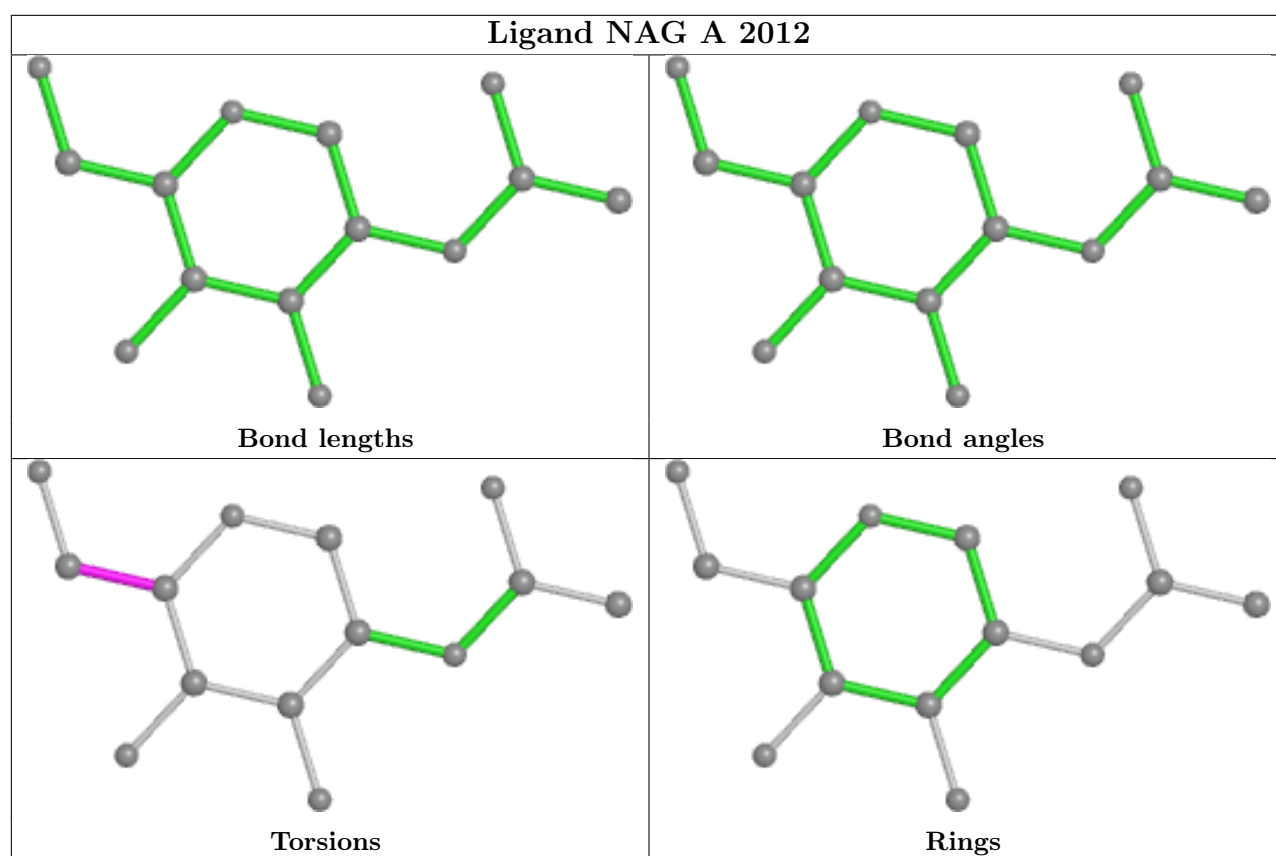
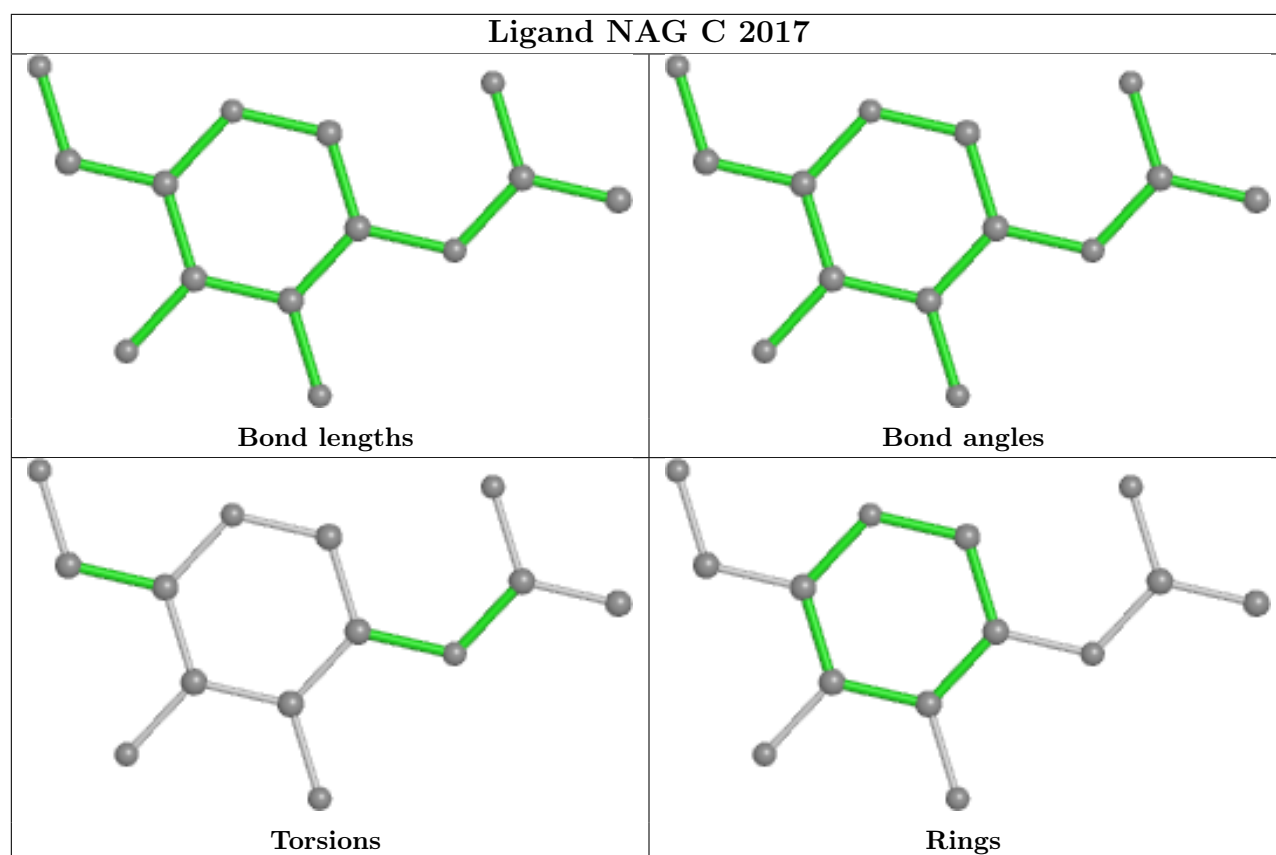




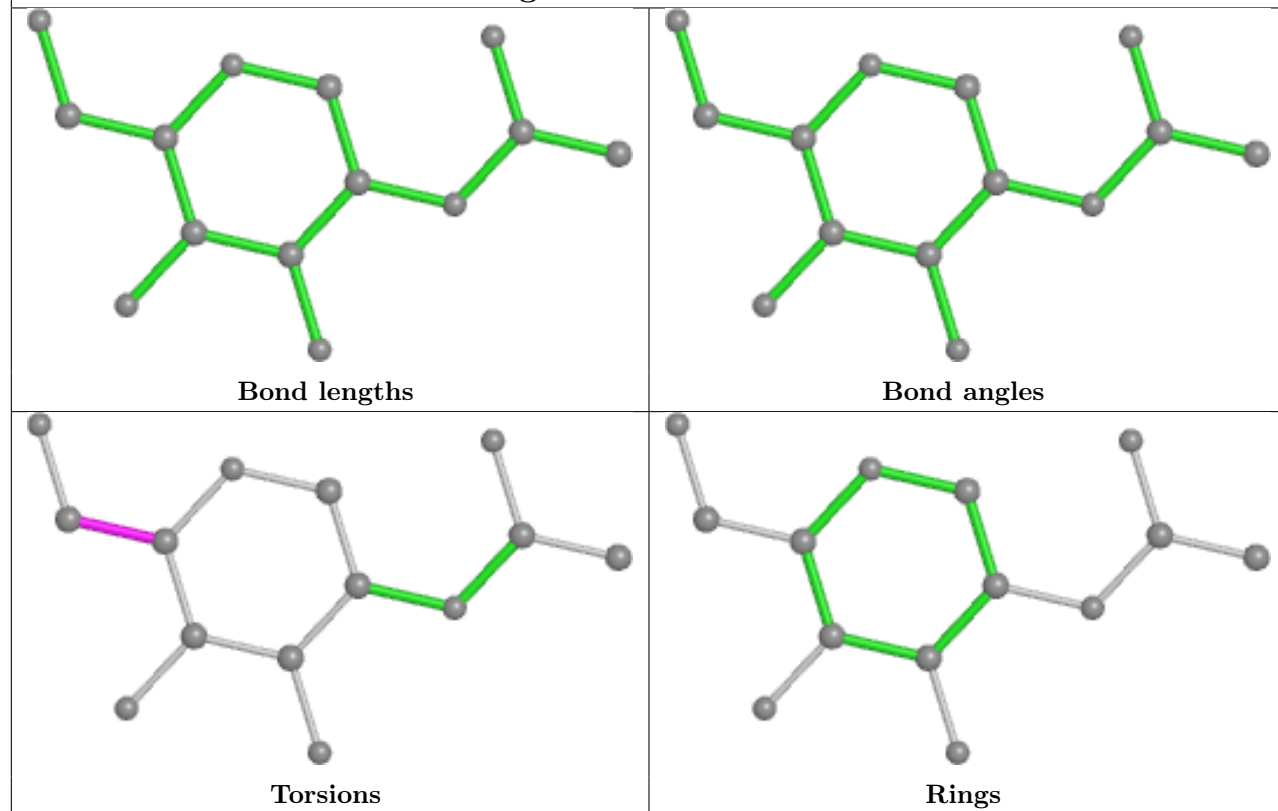




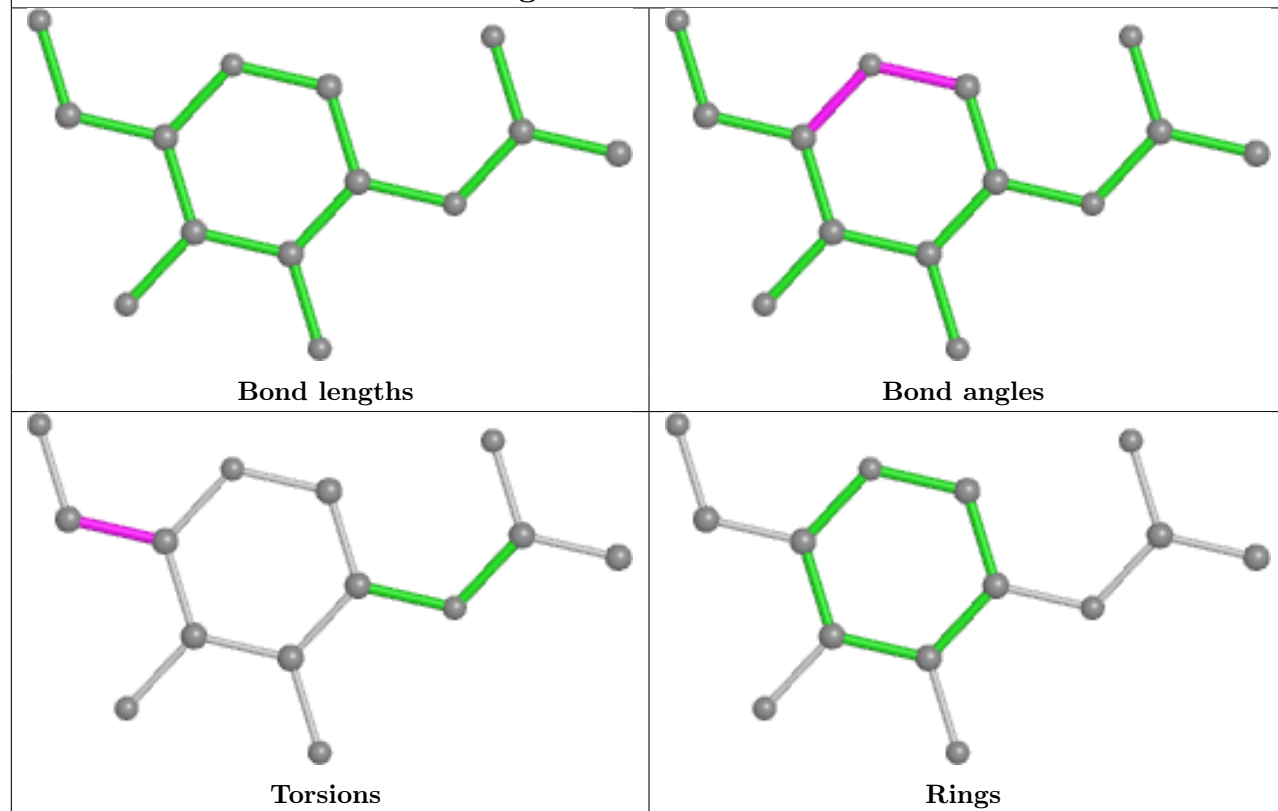


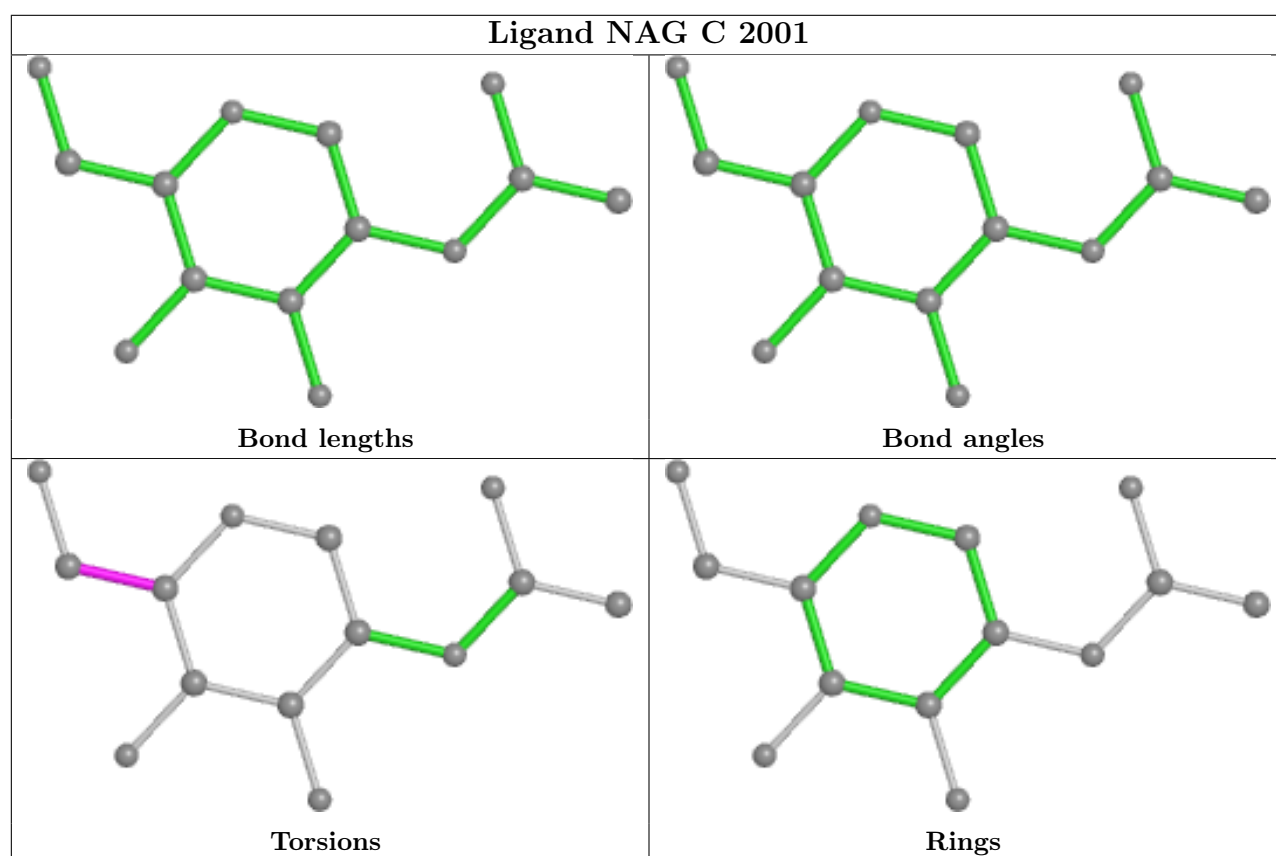
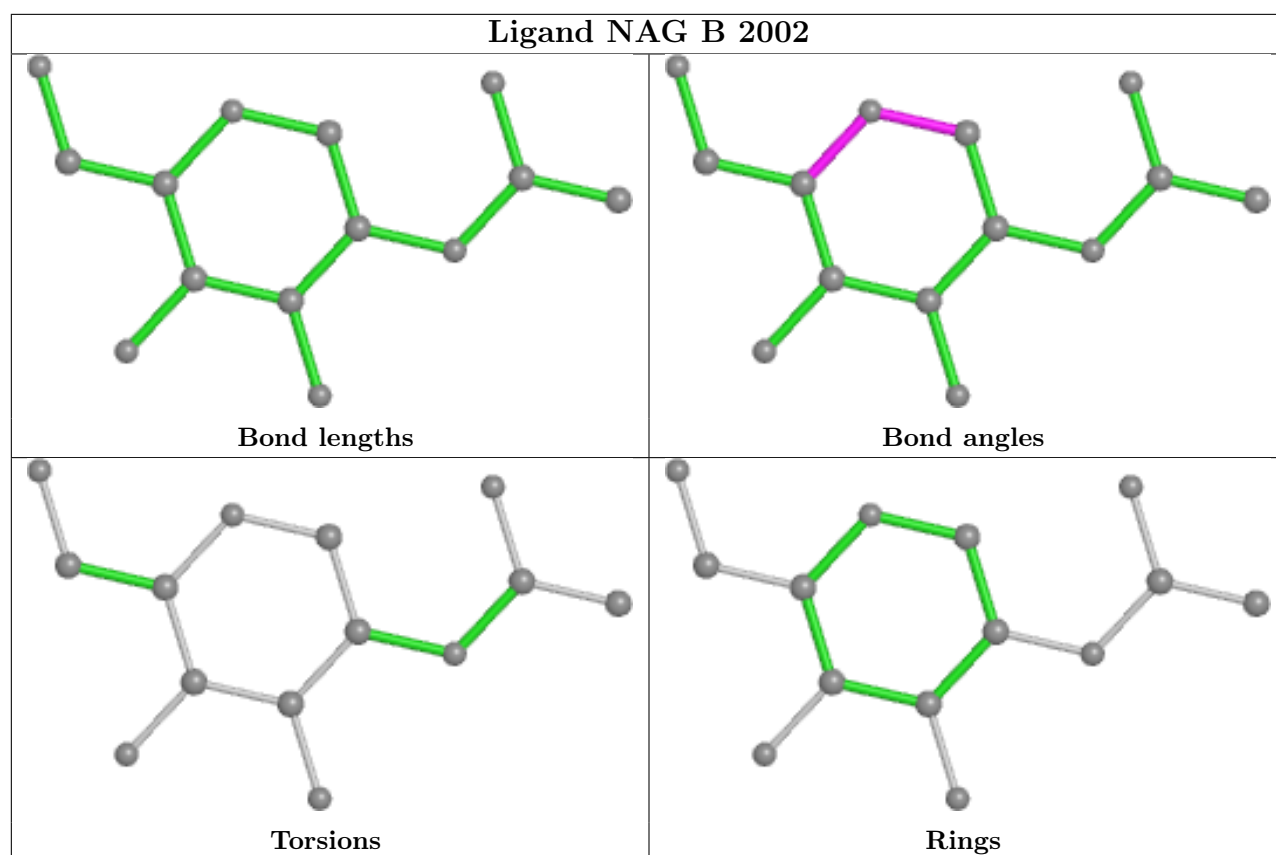


## Ligand NAG C 2015

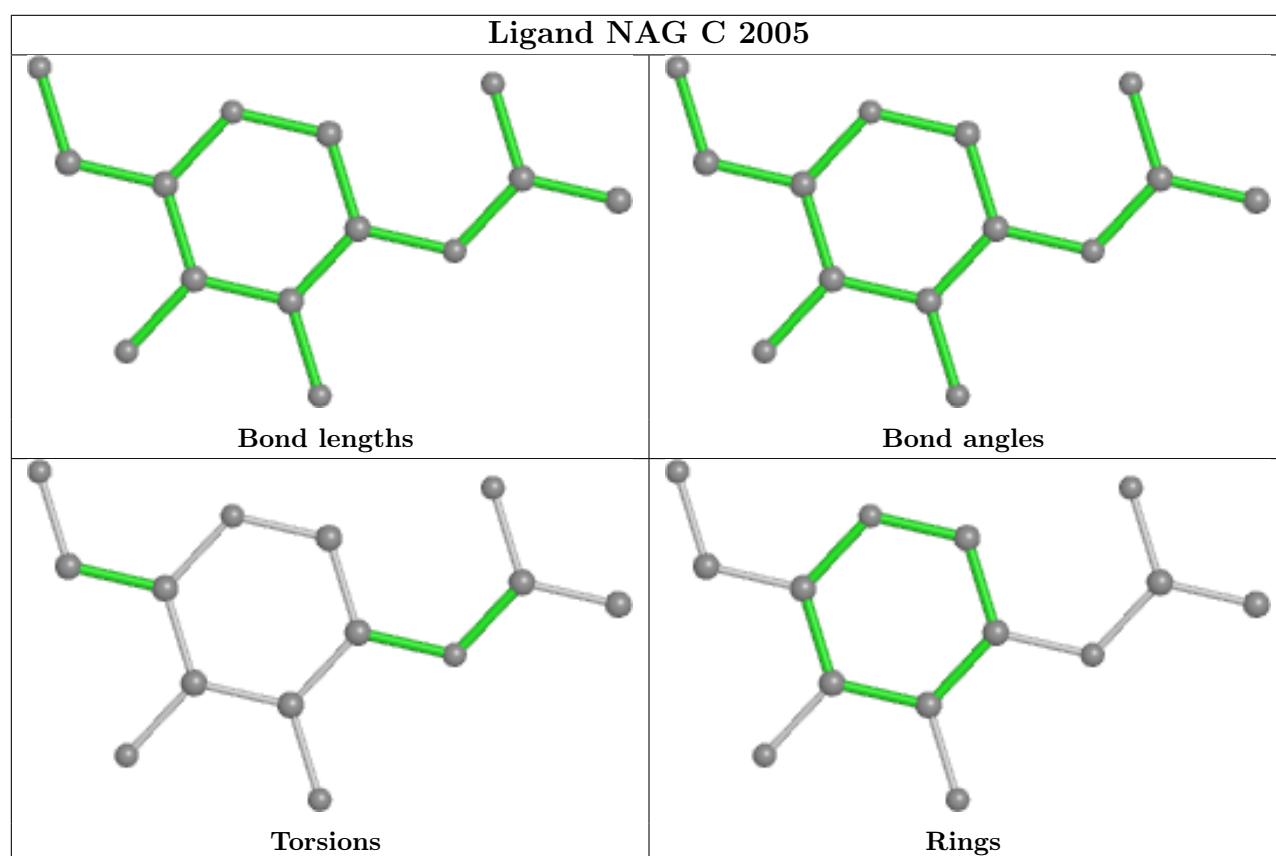
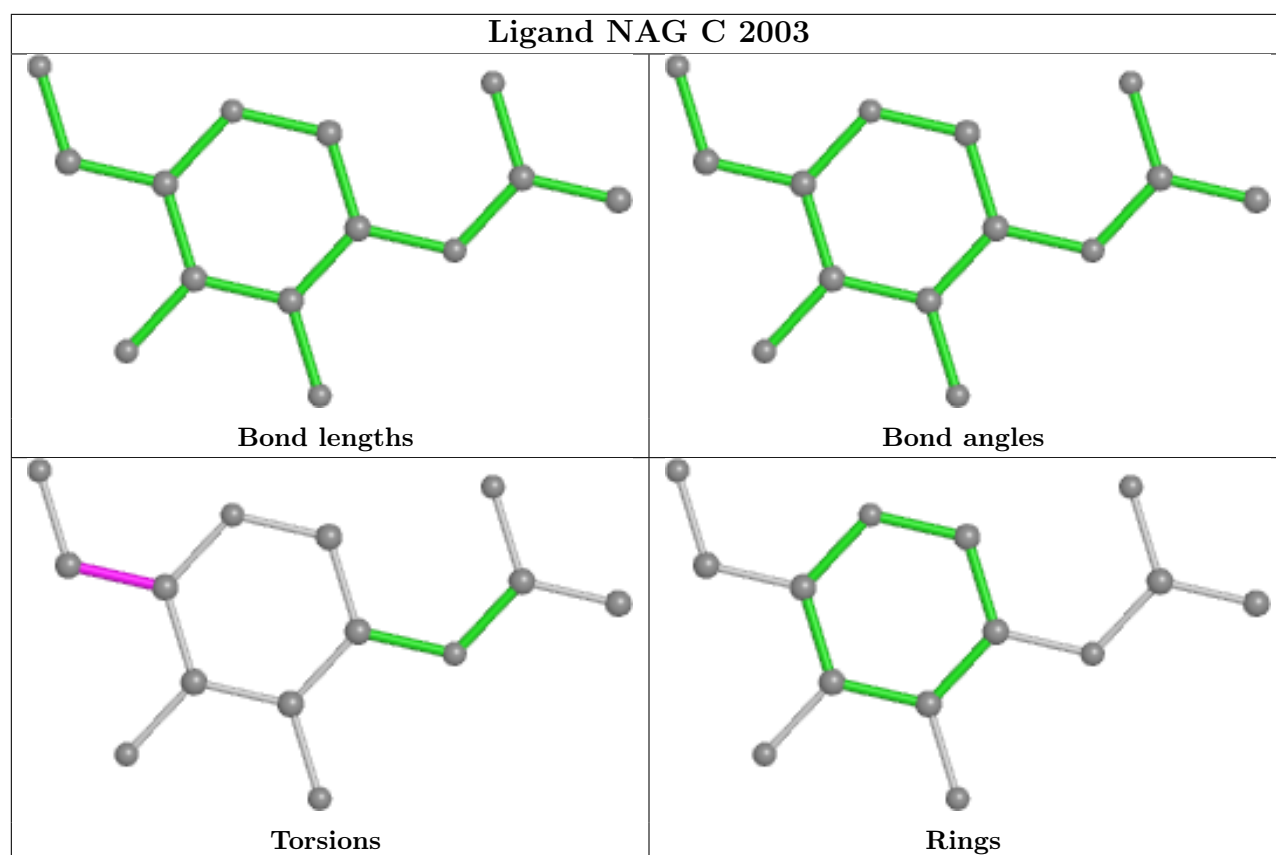


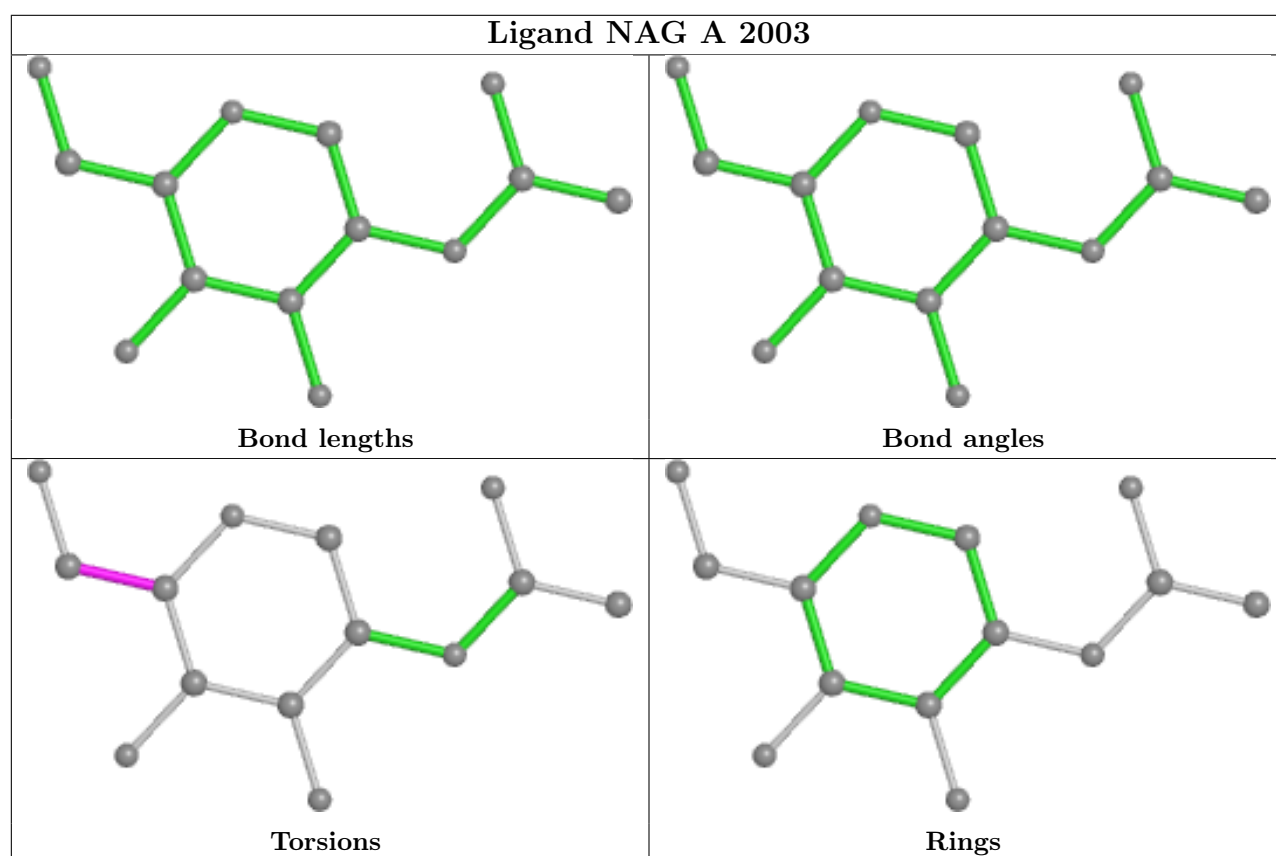
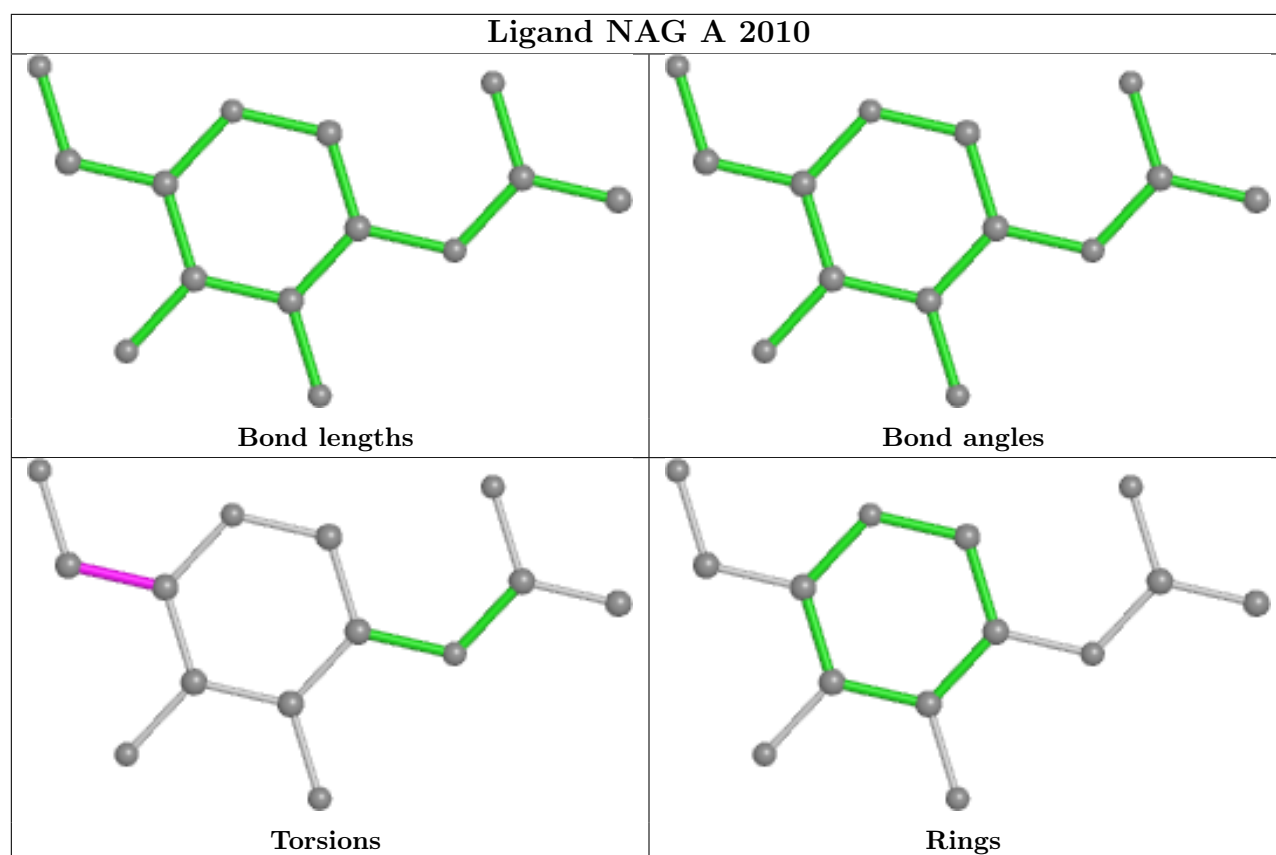
## Ligand NAG A 2008

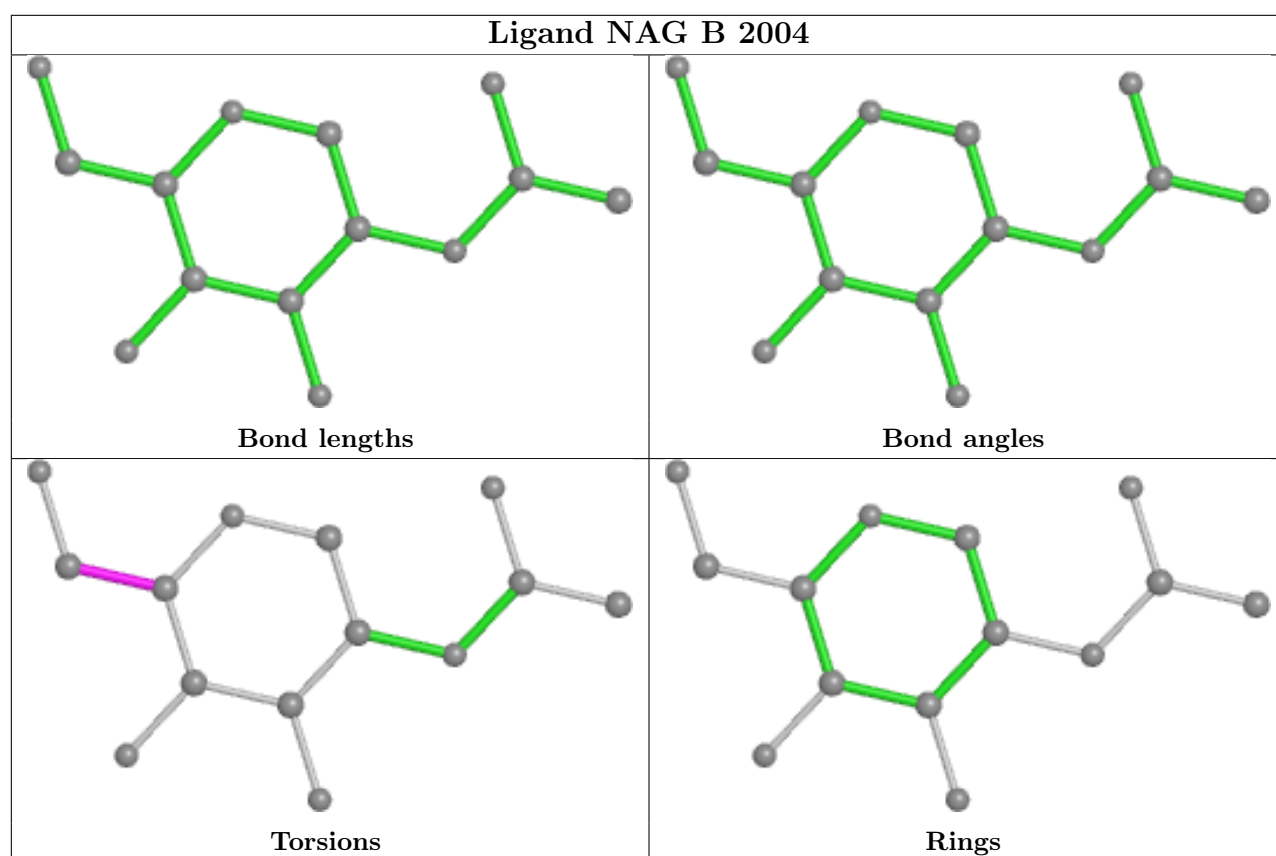
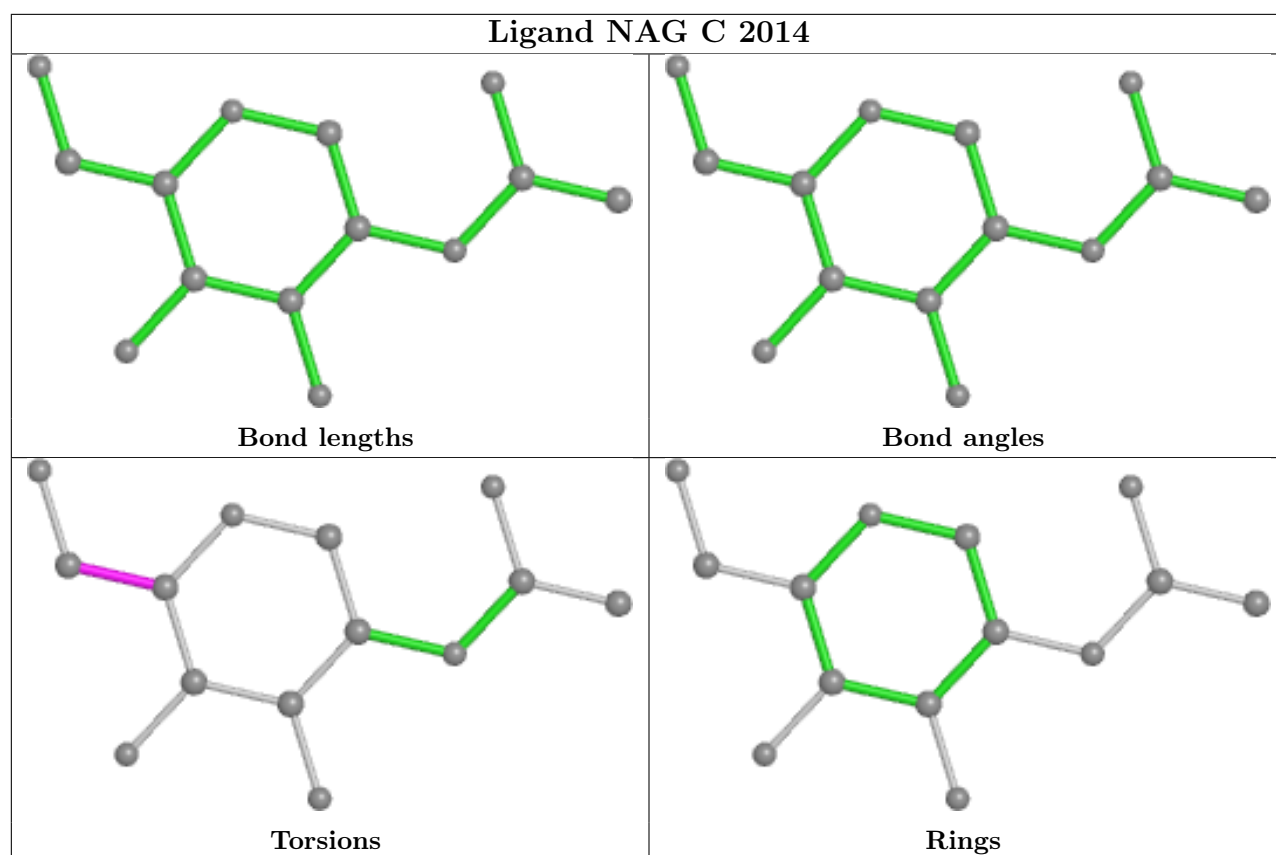


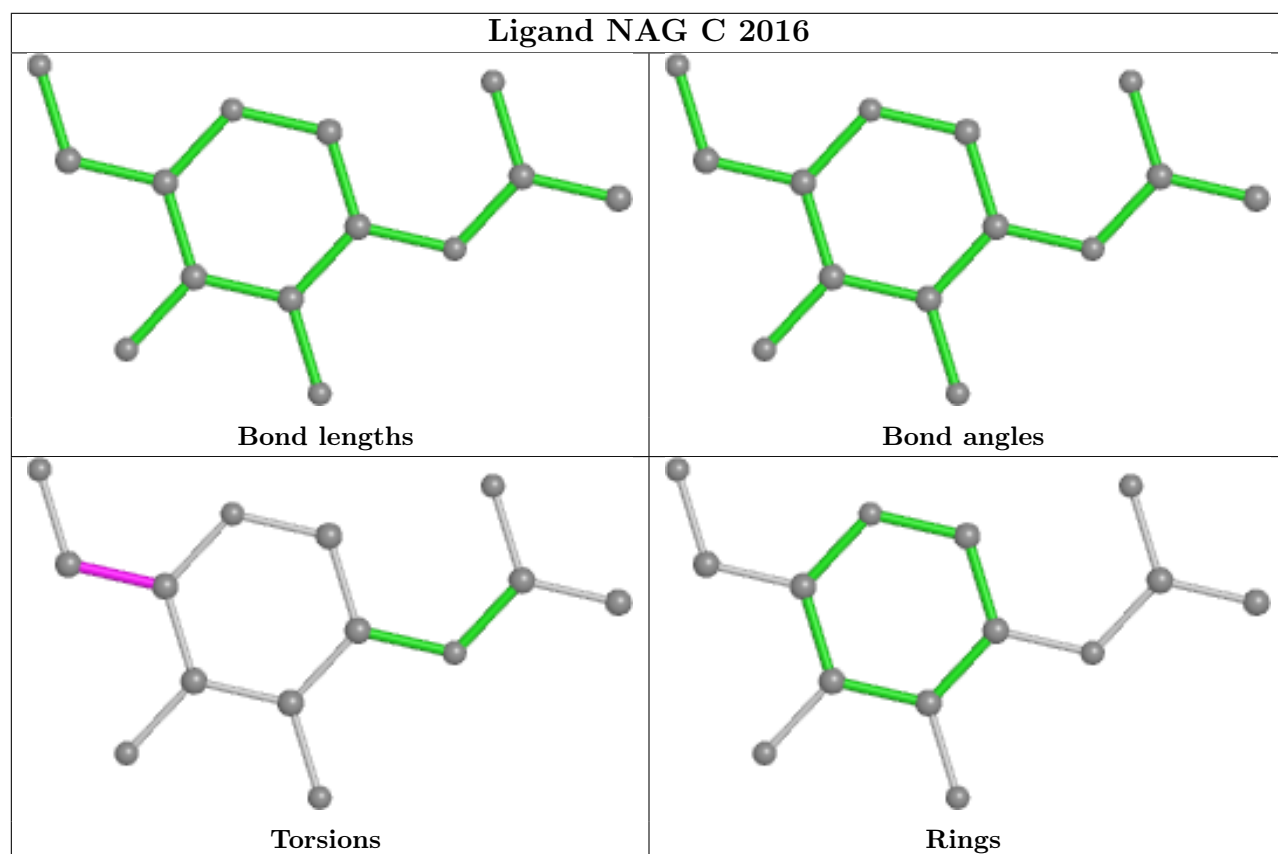
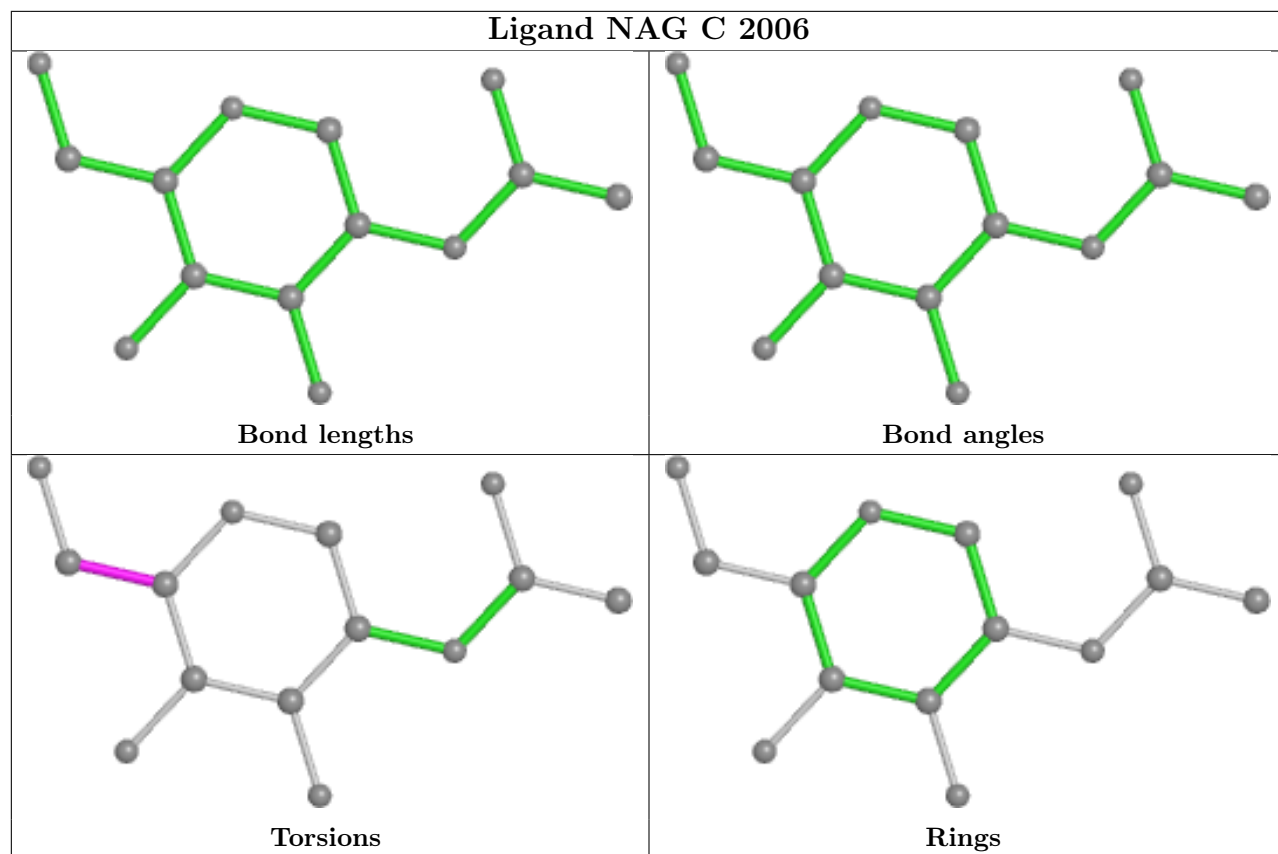


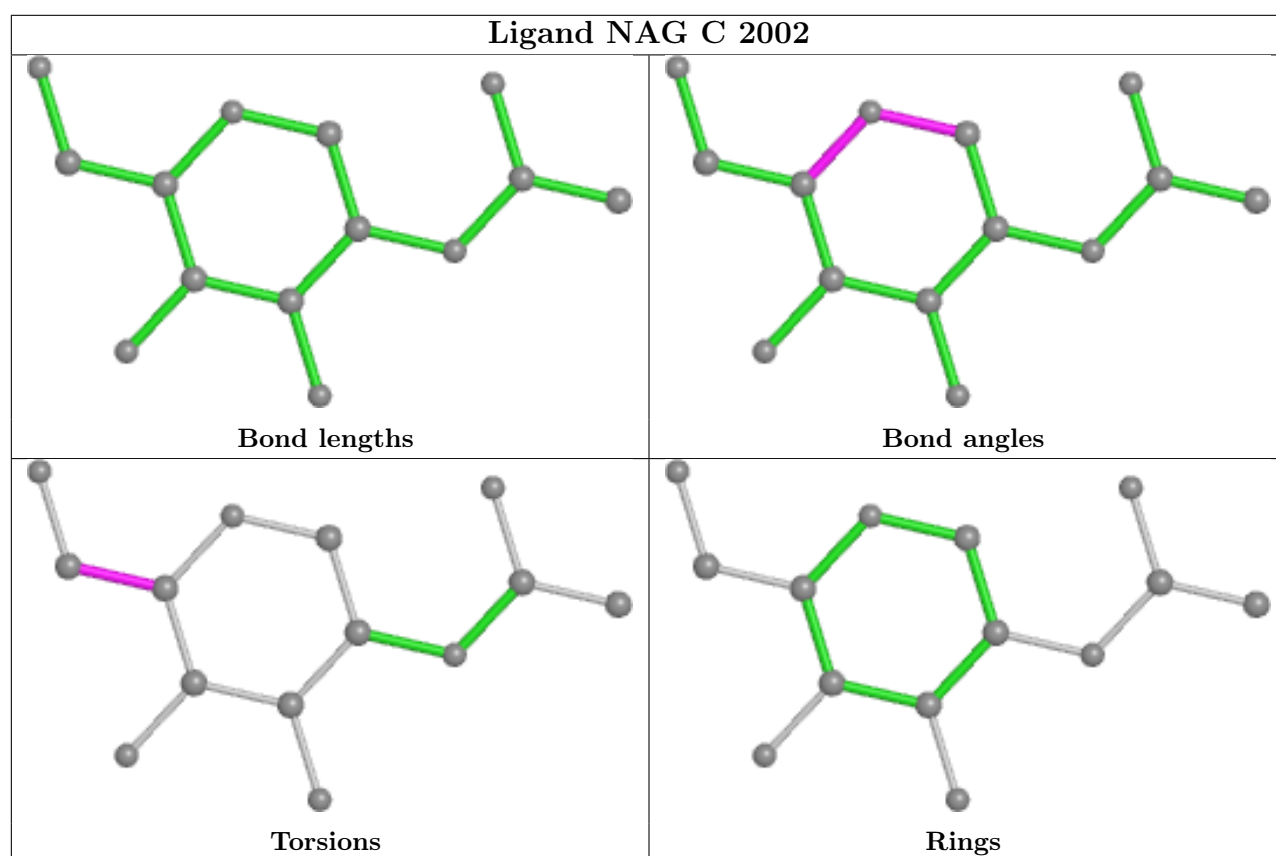
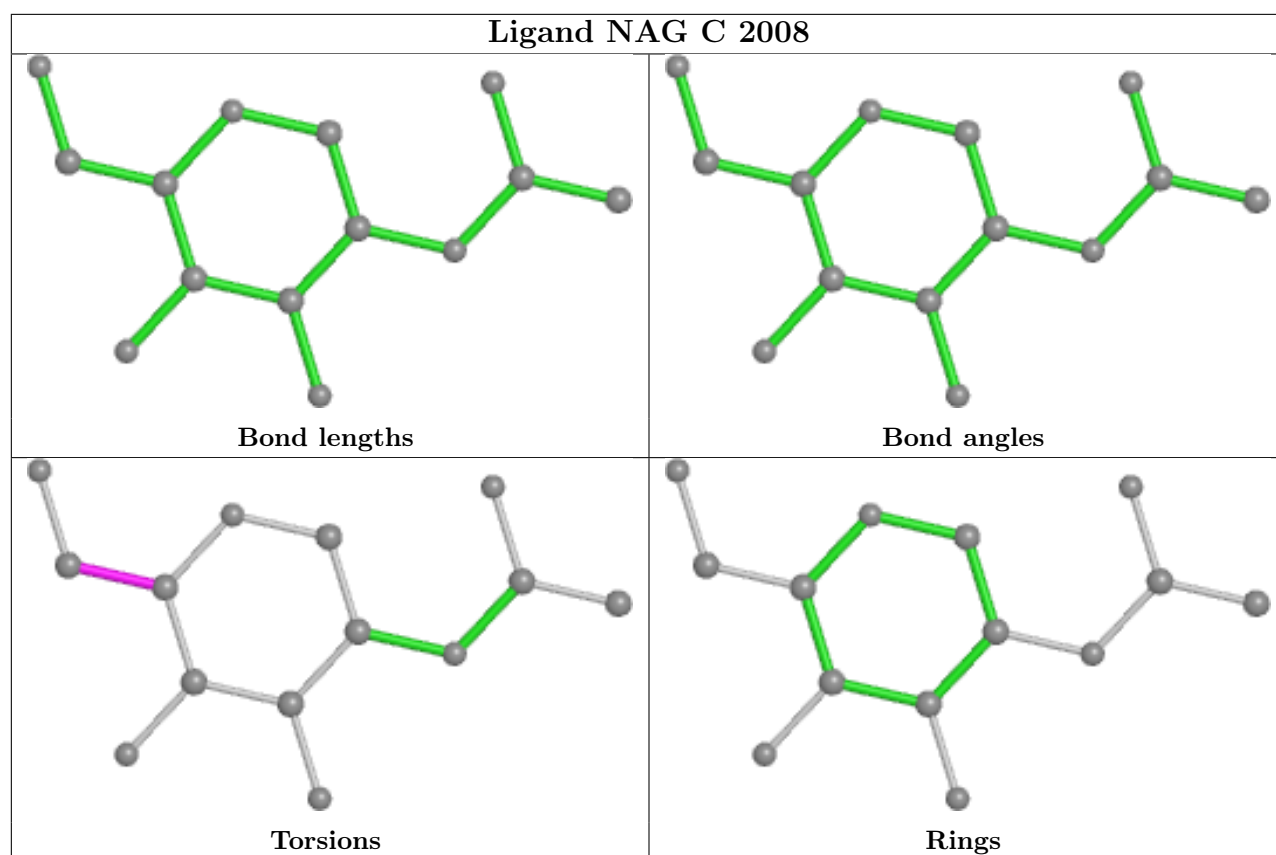


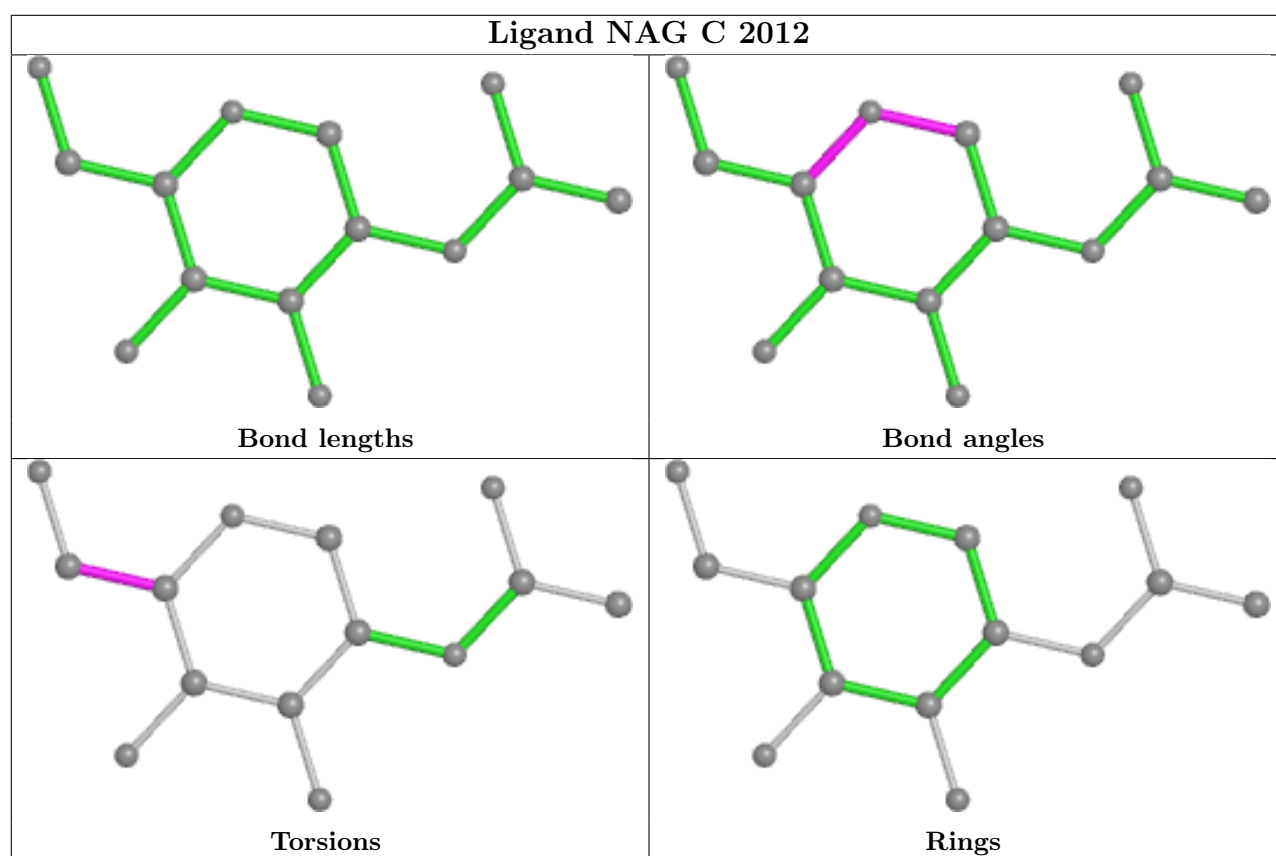
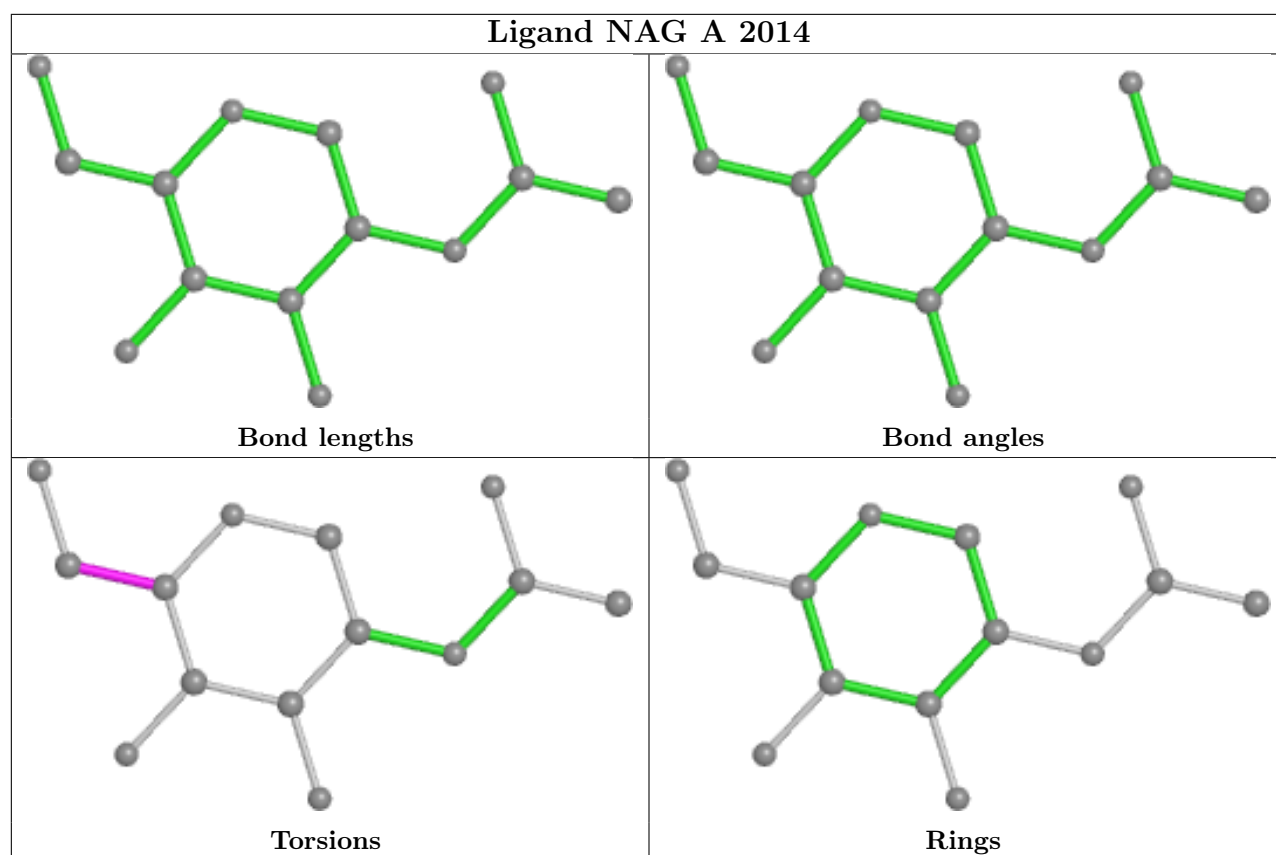


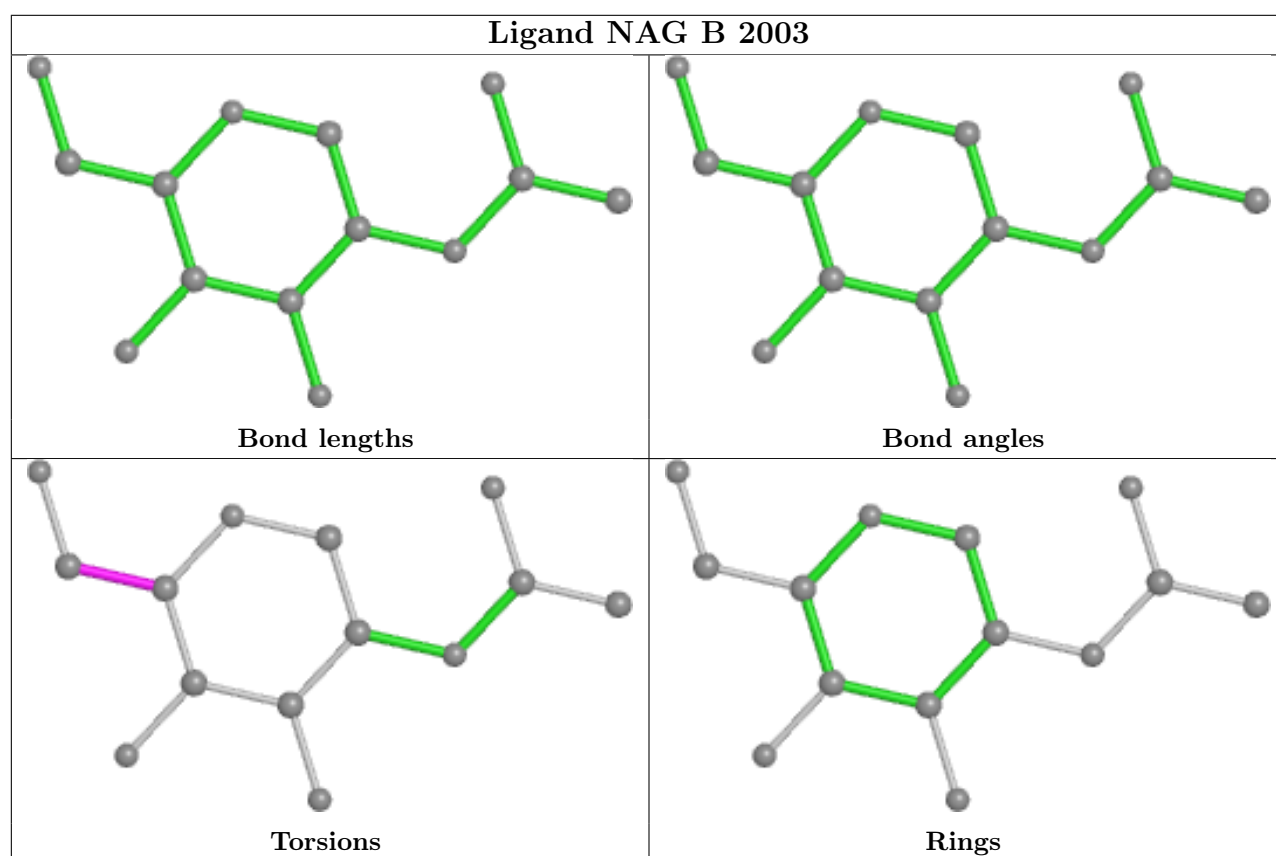
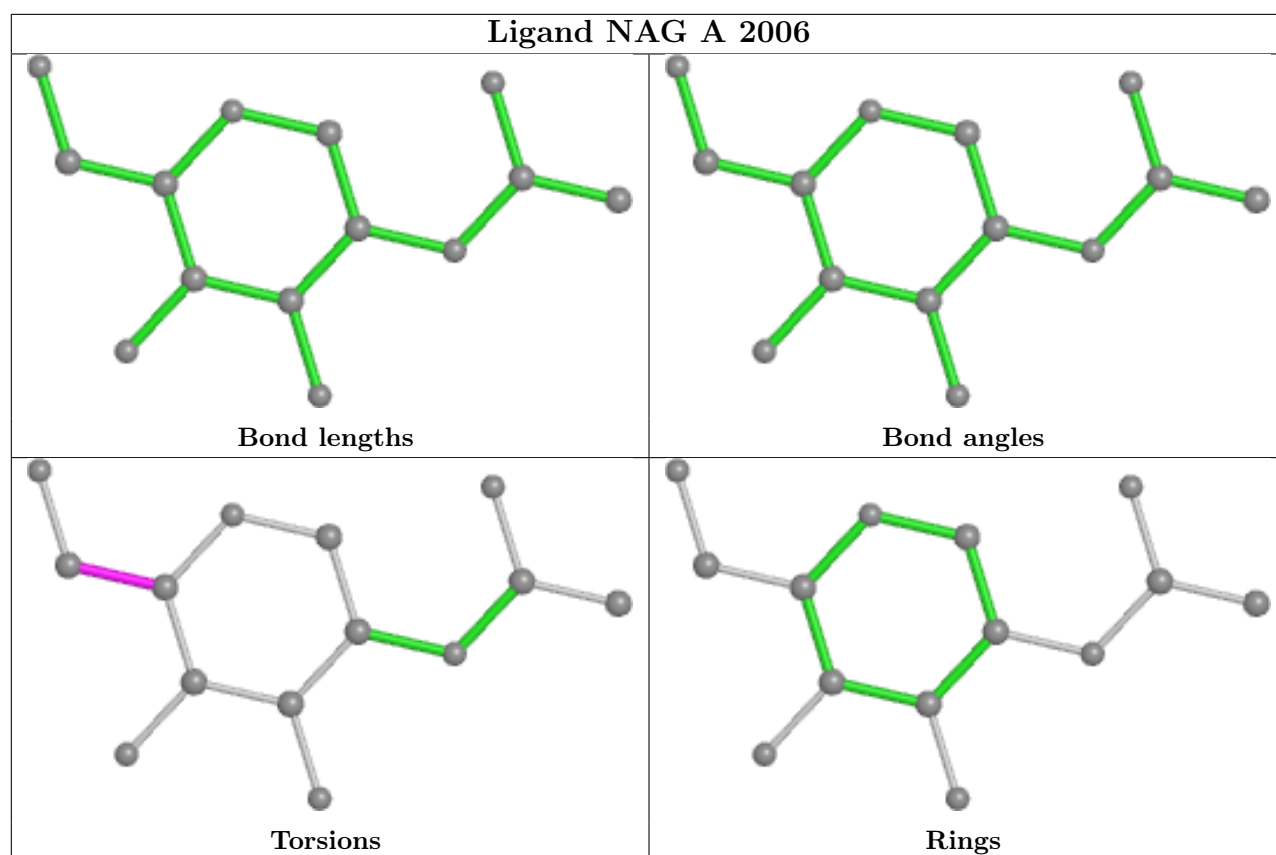


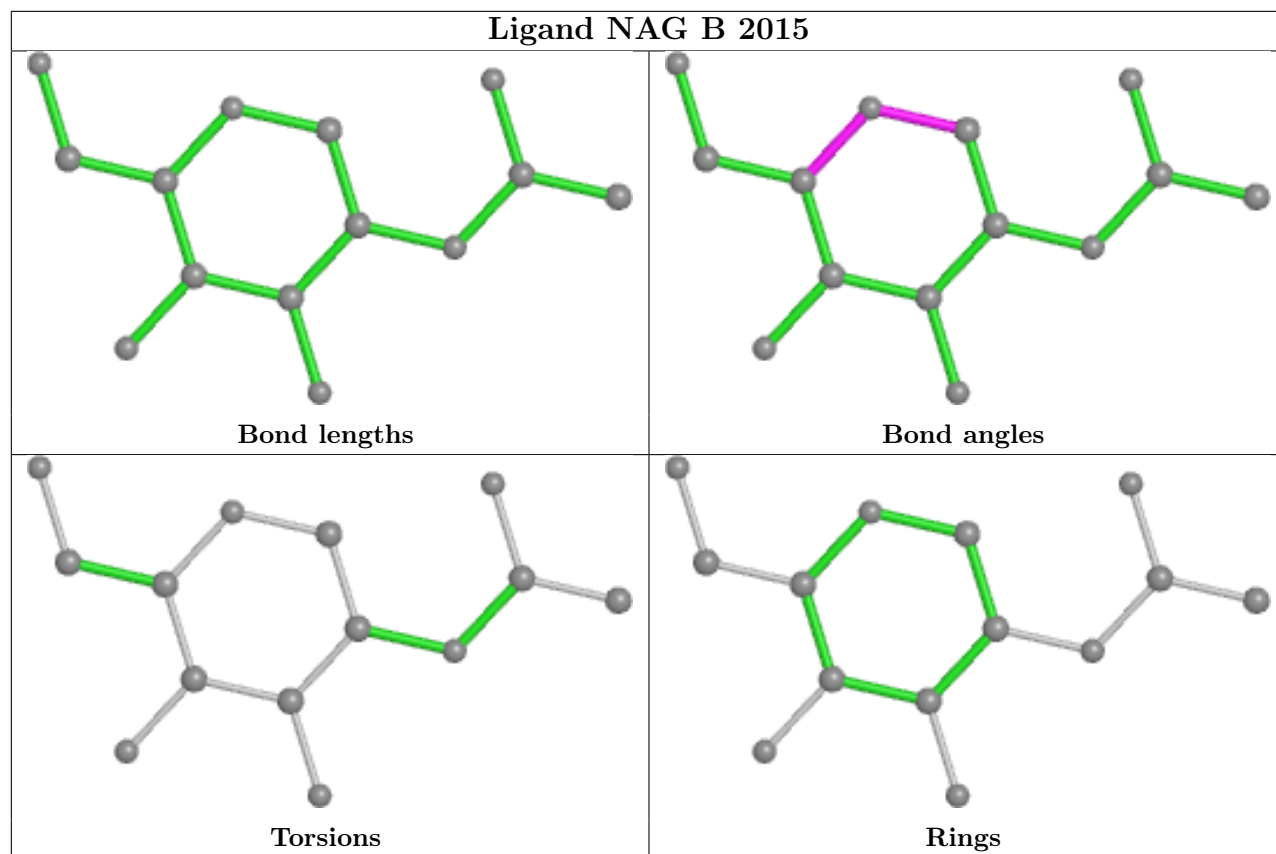












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.