



## Full wwPDB EM Validation Report ⓘ

Nov 13, 2024 – 10:39 AM JST

PDB ID : 8Y1E  
EMDB ID : EMD-38833  
Title : 3up-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

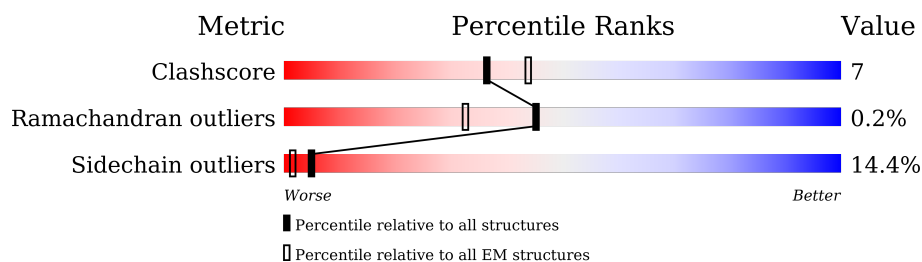
# 1 Overall quality at a glance

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	71% 20% 6%
1	B	1290	73% 18% 6%
1	C	1290	73% 17% 6%
2	D	384	54% 30% 6% 10%
2	E	384	55% 29% 5% 10%
2	F	384	54% 30% 6% 10%
3	G	6	17% 83%
3	L	6	33% 50% 17%
3	Q	6	17% 67% 17%

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

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37611 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

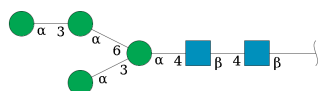
- Molecule 2 is a protein called Transmembrane protease serine 2.

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		
2	F	345	Total	C	N	O	S	0	0
			2690	1702	467	498	23		

There are 3 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
F	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	G	6	Total	C	N	O	0	0
			72	40	2	30		
3	L	6	Total	C	N	O	0	0
			72	40	2	30		
3	Q	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.



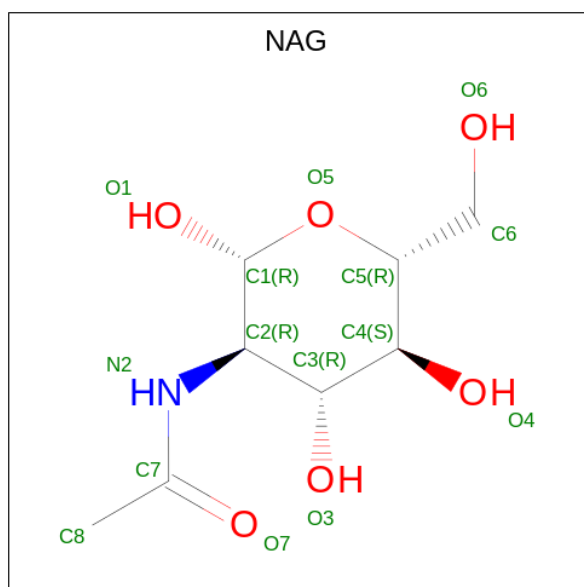
Mol	Chain	Residues	Atoms				AltConf	Trace
4	H	2	Total	C	N	O	0	0
			28	16	2	10		
4	I	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
4	J	2	Total	C	N	O	0	0
			28	16	2	10		
4	K	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	P	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		
4	U	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	

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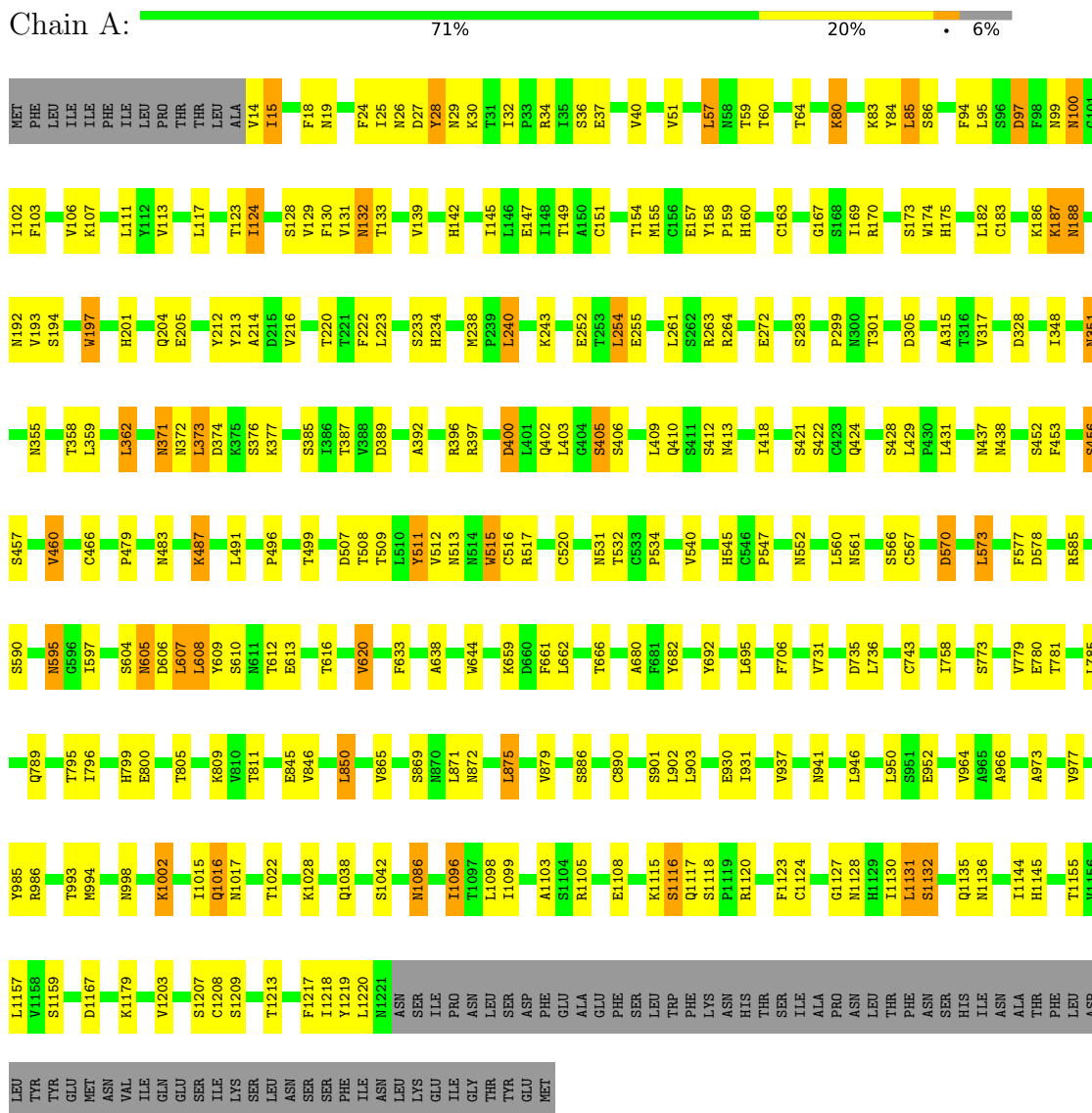
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Mol	Chain	Residues	Atoms				AltConf
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C	N	O	0
			14	8	1	5	
5	C	1	Total	C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

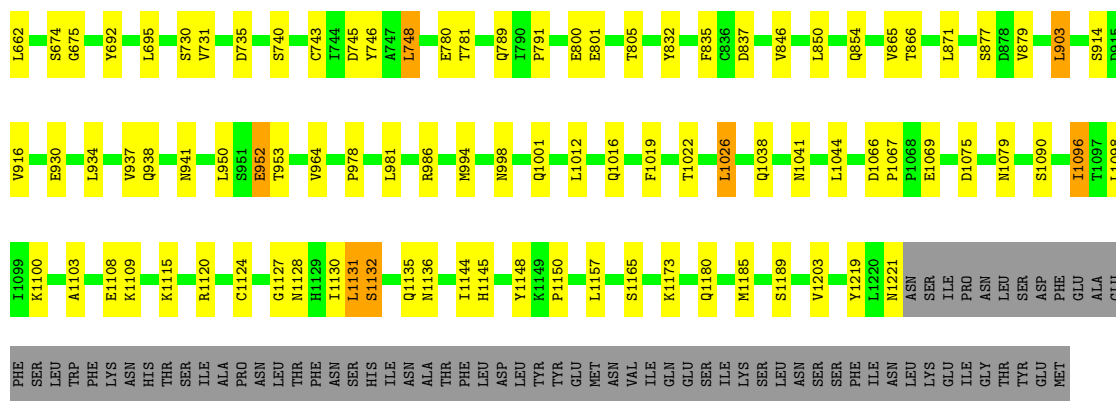
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein

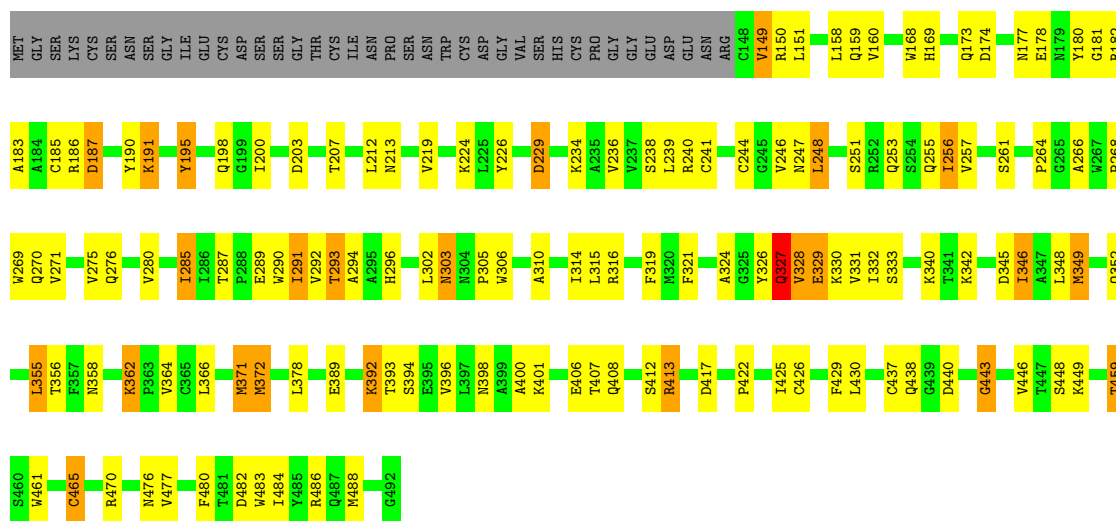






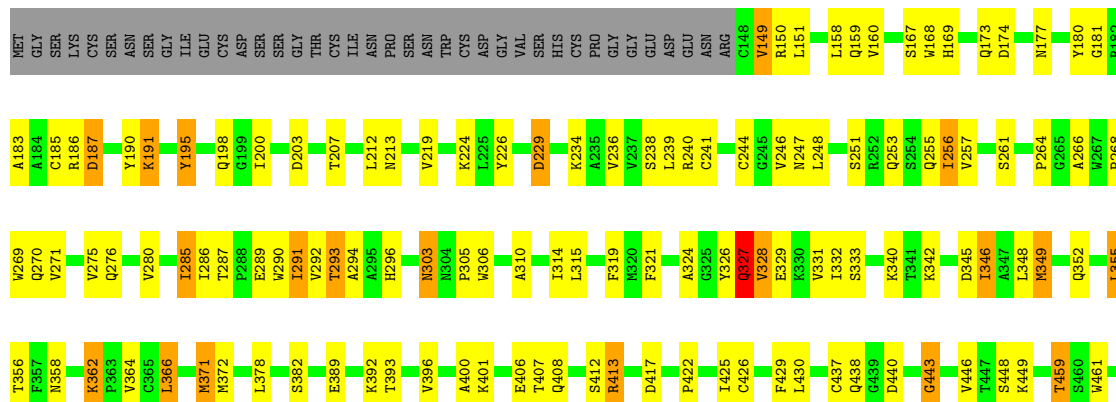
• Molecule 2: Transmembrane protease serine 2

Chain D: 54% 30% 6% 10%



• Molecule 2: Transmembrane protease serine 2

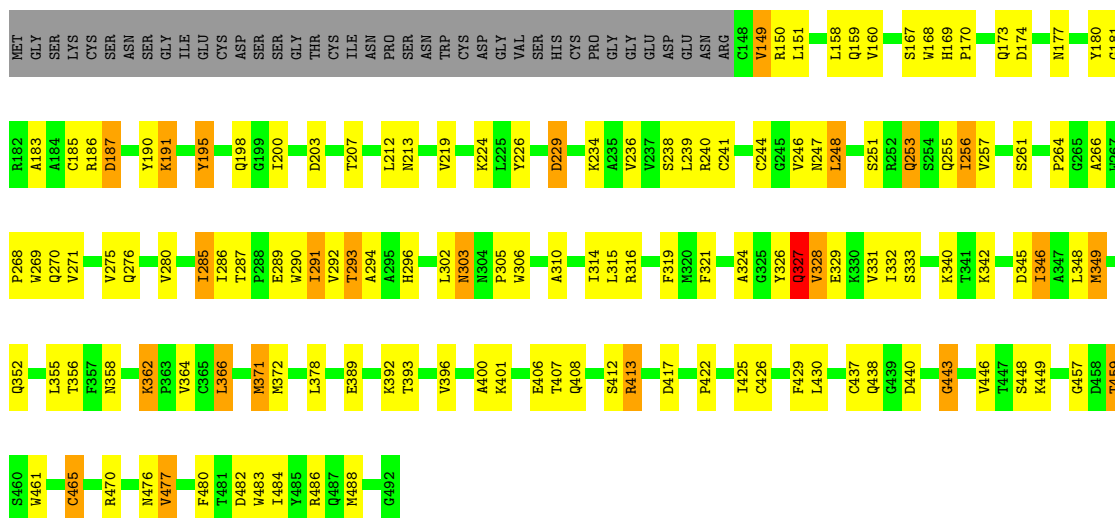
Chain E: 55% 29% 5% 10%





- Molecule 2: Transmembrane protease serine 2

Chain F: 54% 30% 6% 10%



- 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 G: 17% 83%



- 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 L: 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 Q: 17% 67% 17%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



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

Chain J:  50% 50%



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

Chain K:  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:  50% 50%



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

Chain O:  50% 50%



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

Chain P:  100%



- 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:  50% 50%



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

Chain T:  50% 50%



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

Chain U:  100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	366277	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	0.48	0/9653	0.60	0/13146
1	B	0.51	0/9653	0.60	1/13146 (0.0%)
1	C	0.49	0/9653	0.59	0/13146
2	D	0.47	0/2762	0.62	0/3755
2	E	0.47	0/2762	0.62	0/3755
2	F	0.47	0/2762	0.62	0/3755
All	All	0.49	0/37245	0.60	1/50703 (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	1
1	B	0	3
1	C	0	2
2	D	0	3
2	E	0	3
2	F	0	3
All	All	0	15

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	902	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1127	GLY	Peptide
1	B	1127	GLY	Peptide
1	B	51	VAL	Peptide
1	B	930	GLU	Peptide
1	C	1127	GLY	Peptide
1	C	930	GLU	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
2	F	256	ILE	Peptide
2	F	327	GLN	Peptide
2	F	443	GLY	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	9073	125	0
1	B	9425	0	9073	121	0
1	C	9425	0	9074	98	0
2	D	2690	0	2592	79	0
2	E	2690	0	2592	71	0
2	F	2690	0	2592	78	0
3	G	72	0	61	0	0
3	L	72	0	61	3	0
3	Q	72	0	61	2	0
4	H	28	0	25	2	0
4	I	28	0	25	0	0
4	J	28	0	25	5	0
4	K	28	0	25	0	0
4	M	28	0	25	2	0
4	N	28	0	25	0	0
4	O	28	0	25	0	0
4	P	28	0	25	0	0
4	R	28	0	25	0	0
4	S	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	T	28	0	25	0	0
4	U	28	0	25	0	0
5	A	238	0	221	6	0
5	B	238	0	221	4	0
5	C	238	0	221	2	0
All	All	37611	0	36142	552	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 (552) 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:609:TYR:CE2	1:B:611:ASN:HB3	1.50	1.44
1:B:380:GLY:HA2	1:B:607:LEU:CD1	1.55	1.35
1:B:380:GLY:HA2	1:B:607:LEU:HD13	1.15	1.13
1:B:380:GLY:CA	1:B:607:LEU:HD13	1.79	1.11
1:B:609:TYR:CE2	1:B:611:ASN:CB	2.40	1.05
1:B:380:GLY:CA	1:B:607:LEU:CD1	2.36	1.04
1:B:380:GLY:HA2	1:B:607:LEU:HD11	1.41	0.99
1:B:609:TYR:HE2	1:B:611:ASN:CB	1.74	0.99
1:A:145:ILE:HD13	4:H:1:NAG:O6	1.65	0.95
1:A:606:ASP:HB2	4:J:1:NAG:O7	1.68	0.92
1:B:379:PHE:O	1:B:607:LEU:HD22	1.69	0.90
1:A:351:ASN:OD1	1:B:183:CYS:HB2	1.72	0.90
2:D:319:PHE:CD1	2:F:321:PHE:HZ	1.93	0.86
1:A:606:ASP:CB	4:J:1:NAG:O7	2.27	0.82
1:B:487:LYS:HZ3	1:B:515:TRP:HZ3	1.29	0.80
1:A:487:LYS:HZ3	1:A:515:TRP:HZ3	1.30	0.78
2:D:319:PHE:HD1	2:F:321:PHE:HZ	1.31	0.77
1:A:355:ASN:HD22	1:A:606:ASP:HB3	1.49	0.77
1:C:51:VAL:O	1:C:54:ARG:HG3	1.86	0.76
1:B:609:TYR:HE2	1:B:611:ASN:HB3	0.97	0.75
1:B:188:ASN:OD1	4:M:1:NAG:C7	2.34	0.74
1:C:487:LYS:HZ3	1:C:515:TRP:HZ3	1.35	0.72
2:D:159:GLN:HB3	2:D:168:TRP:HB3	1.74	0.69
1:B:380:GLY:CA	1:B:607:LEU:HD11	2.15	0.69
2:E:159:GLN:HB3	2:E:168:TRP:HB3	1.75	0.69
2:F:159:GLN:HB3	2:F:168:TRP:HB3	1.75	0.68
1:B:351:ASN:OD1	1:C:183:CYS:HB2	1.95	0.67
1:A:158:TYR:CE1	5:A:2001:NAG:H82	2.30	0.66

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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	0.66
1:A:487:LYS:HB2	1:A:515:TRP:HB2	1.78	0.66
1:C:358:THR:O	1:C:362:LEU:HB2	1.96	0.66
1:A:201:HIS:HB2	1:A:212:TYR:HB2	1.78	0.66
1:B:487:LYS:HB2	1:B:515:TRP:HB2	1.78	0.65
1:B:358:THR:O	1:B:362:LEU:HB2	1.96	0.65
1:C:487:LYS:HB2	1:C:515:TRP:HB2	1.78	0.65
1:A:428:SER:OG	1:A:585:ARG:NH1	2.30	0.65
1:A:552:ASN:HB2	1:A:573:LEU:HD21	1.79	0.65
1:B:428:SER:OG	1:B:585:ARG:NH1	2.30	0.64
1:C:326:ASP:OD1	1:C:326:ASP:N	2.27	0.64
1:B:552:ASN:HB2	1:B:573:LEU:HD21	1.79	0.64
1:C:428:SER:OG	1:C:585:ARG:NH1	2.30	0.64
1:B:902:LEU:O	1:B:902:LEU:HD12	1.96	0.64
1:B:315:ALA:H	1:B:620:VAL:HG12	1.64	0.63
1:C:552:ASN:HB2	1:C:573:LEU:HD21	1.79	0.63
1:A:374:ASP:HB2	1:A:377:LYS:HG2	1.79	0.63
1:C:374:ASP:HB2	1:C:377:LYS:HG2	1.79	0.63
2:D:319:PHE:HD1	2:F:321:PHE:CZ	2.15	0.63
1:A:692:TYR:HB3	1:A:695:LEU:HD12	1.81	0.63
1:B:374:ASP:HB2	1:B:377:LYS:HG2	1.79	0.63
2:D:316:ARG:HH12	2:F:319:PHE:HZ	1.44	0.63
1:A:80:LYS:HG2	1:A:254:LEU:HD23	1.81	0.62
1:B:606:ASP:C	1:B:608:LEU:H	2.02	0.62
1:B:902:LEU:HD12	1:B:902:LEU:C	2.19	0.62
1:B:1108:GLU:OE2	1:B:1120:ARG:NH2	2.31	0.62
1:A:607:LEU:C	1:A:607:LEU:HD23	2.20	0.61
1:A:132:ASN:N	1:A:132:ASN:OD1	2.31	0.61
5:B:2001:NAG:H4	3:L:6:MAN:O4	2.01	0.61
1:A:1132:SER:HA	1:A:1144:ILE:O	2.01	0.59
1:C:1132:SER:HA	1:C:1144:ILE:O	2.02	0.59
2:D:319:PHE:CD1	2:F:321:PHE:CZ	2.83	0.59
1:A:106:VAL:O	1:A:197:TRP:HA	2.03	0.59
1:C:1128:ASN:HB3	1:C:1148:TYR:HB3	1.83	0.59
1:C:201:HIS:HB2	1:C:212:TYR:HB2	1.84	0.59
1:A:966:ALA:HB2	1:A:973:ALA:HB3	1.84	0.58
1:A:994:MET:O	1:A:998:ASN:ND2	2.32	0.58
1:B:607:LEU:H	1:B:607:LEU:CD2	2.16	0.58
1:A:145:ILE:CD1	4:H:1:NAG:O6	2.46	0.58
1:B:487:LYS:NZ	2:E:417:ASP:OD2	2.36	0.58
1:B:325:PRO:O	1:B:352:CYS:CB	2.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:773:SER:HB2	1:C:866:THR:HG23	1.86	0.58
1:A:1108:GLU:OE2	1:A:1120:ARG:NH2	2.37	0.58
1:B:937:VAL:O	1:B:941:ASN:ND2	2.34	0.58
1:C:487:LYS:NZ	2:F:417:ASP:OD2	2.36	0.58
1:B:607:LEU:N	1:B:607:LEU:HD23	2.19	0.57
1:C:846:VAL:HG13	1:C:1096:ILE:HG13	1.85	0.57
1:B:201:HIS:HB2	1:B:212:TYR:HB2	1.86	0.57
1:A:301:THR:HG23	1:A:682:TYR:HA	1.87	0.57
1:C:479:PRO:O	1:C:483:ASN:ND2	2.38	0.57
2:F:412:SER:OG	2:F:413:ARG:N	2.38	0.57
1:A:487:LYS:NZ	2:D:417:ASP:OD2	2.36	0.57
1:A:507:ASP:OD2	2:D:470:ARG:NH1	2.38	0.57
1:A:805:THR:HG22	1:A:1103:ALA:HA	1.86	0.57
2:F:303:ASN:OD1	2:F:303:ASN:N	2.38	0.57
2:D:412:SER:OG	2:D:413:ARG:N	2.38	0.56
1:A:355:ASN:ND2	1:A:606:ASP:HB3	2.20	0.56
1:A:452:SER:OG	1:A:453:PHE:N	2.38	0.56
1:B:170:ARG:HA	5:B:2005:NAG:H82	1.88	0.56
1:B:479:PRO:O	1:B:483:ASN:ND2	2.38	0.56
1:B:507:ASP:OD2	2:E:470:ARG:NH1	2.38	0.56
1:C:937:VAL:O	1:C:941:ASN:ND2	2.38	0.56
1:A:1159:SER:HG	1:A:1213:THR:HG1	1.53	0.56
2:D:371:MET:O	2:D:449:LYS:NZ	2.39	0.56
1:A:100:ASN:ND2	1:A:261:LEU:O	2.38	0.56
1:A:169:ILE:HG22	5:A:2005:NAG:H83	1.86	0.56
1:A:937:VAL:O	1:A:941:ASN:ND2	2.38	0.56
1:A:479:PRO:O	1:A:483:ASN:ND2	2.38	0.56
1:C:123:THR:HG21	1:C:140:GLN:HE21	1.71	0.56
2:D:314:ILE:HG21	2:D:319:PHE:HB2	1.88	0.56
1:A:1016:GLN:NE2	1:A:1017:ASN:OD1	2.39	0.56
1:C:507:ASP:OD2	2:F:470:ARG:NH1	2.38	0.56
1:B:452:SER:OG	1:B:453:PHE:N	2.38	0.55
2:D:303:ASN:OD1	2:D:303:ASN:N	2.38	0.55
1:A:124:ILE:HG23	1:A:139:VAL:HB	1.88	0.55
2:E:371:MET:O	2:E:449:LYS:NZ	2.39	0.55
1:B:385:SER:OG	1:B:595:ASN:ND2	2.39	0.55
2:E:417:ASP:OD1	2:E:417:ASP:N	2.33	0.55
2:F:371:MET:O	2:F:449:LYS:NZ	2.39	0.55
1:B:409:LEU:HA	1:B:413:ASN:HD22	1.71	0.55
2:D:310:ALA:O	2:D:327:GLN:NE2	2.40	0.55
1:A:409:LEU:HA	1:A:413:ASN:HD22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:ASP:OD1	1:C:570:ASP:N	2.32	0.55
2:E:310:ALA:O	2:E:327:GLN:NE2	2.40	0.55
1:A:952:GLU:HG3	1:A:1136:ASN:HD21	1.72	0.55
1:B:354:PHE:O	1:B:605:ASN:OD1	2.24	0.55
1:C:379:PHE:CD1	1:C:606:ASP:OD2	2.59	0.55
1:C:385:SER:OG	1:C:595:ASN:ND2	2.39	0.55
1:C:452:SER:OG	1:C:453:PHE:N	2.38	0.55
2:E:412:SER:OG	2:E:413:ARG:N	2.38	0.55
2:E:306:TRP:HA	2:E:328:VAL:HG21	1.89	0.55
2:F:314:ILE:HG21	2:F:319:PHE:HB2	1.88	0.55
2:D:185:CYS:HB3	2:D:190:TYR:HB2	1.90	0.54
2:E:177:ASN:O	2:E:181:GLY:N	2.40	0.54
2:E:270:GLN:NE2	2:E:271:VAL:O	2.39	0.54
1:C:409:LEU:HA	1:C:413:ASN:HD22	1.72	0.54
1:A:385:SER:OG	1:A:595:ASN:ND2	2.39	0.54
1:A:508:THR:HG23	1:A:513:ASN:HA	1.89	0.54
1:A:606:ASP:HB2	4:J:1:NAG:C7	2.38	0.54
1:C:310:THR:HG21	1:C:675:GLY:H	1.72	0.54
1:C:400:ASP:OD2	1:C:409:LEU:N	2.41	0.54
2:D:255:GLN:HB2	2:D:261:SER:HA	1.90	0.54
2:E:264:PRO:HG3	2:E:315:LEU:HD11	1.90	0.54
1:A:886:SER:O	1:A:901:SER:OG	2.26	0.54
5:B:2001:NAG:C4	3:L:6:MAN:O4	2.55	0.54
1:C:371:ASN:OD1	1:C:372:ASN:ND2	2.41	0.54
1:C:508:THR:HG23	1:C:513:ASN:HA	1.89	0.54
2:E:303:ASN:OD1	2:E:303:ASN:N	2.37	0.54
2:F:264:PRO:HG3	2:F:315:LEU:HD11	1.90	0.54
2:F:310:ALA:O	2:F:327:GLN:NE2	2.40	0.54
1:B:376:SER:OG	1:B:377:LYS:NZ	2.39	0.54
2:E:314:ILE:HG21	2:E:319:PHE:HB2	1.88	0.54
1:A:606:ASP:HA	4:J:1:NAG:O7	2.07	0.54
1:B:371:ASN:OD1	1:B:372:ASN:ND2	2.41	0.54
2:E:255:GLN:HB2	2:E:261:SER:HA	1.90	0.54
1:C:30:LYS:HB3	1:C:88:LEU:HD23	1.89	0.54
2:D:268:PRO:O	2:D:362:LYS:N	2.41	0.54
2:D:321:PHE:H	2:D:324:ALA:HB3	1.73	0.54
2:D:356:THR:OG1	2:D:358:ASN:ND2	2.41	0.54
2:E:293:THR:OG1	2:E:294:ALA:N	2.41	0.54
2:F:293:THR:OG1	2:F:294:ALA:N	2.41	0.54
1:B:205:GLU:OE2	1:B:206:ARG:NH1	2.38	0.53
1:B:1162:LEU:HD12	1:B:1170:ILE:HD11	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:247:ASN:ND2	2:E:266:ALA:O	2.41	0.53
2:E:356:THR:OG1	2:E:358:ASN:ND2	2.42	0.53
2:F:321:PHE:H	2:F:324:ALA:HB3	1.73	0.53
1:A:371:ASN:OD1	1:A:372:ASN:ND2	2.41	0.53
1:B:400:ASP:OD2	1:B:409:LEU:N	2.41	0.53
1:C:151:CYS:HA	1:C:183:CYS:HA	1.90	0.53
2:D:293:THR:OG1	2:D:294:ALA:N	2.41	0.53
2:F:185:CYS:HB3	2:F:190:TYR:HB2	1.90	0.53
2:F:187:ASP:OD1	2:F:187:ASP:N	2.41	0.53
1:B:508:THR:HG23	1:B:513:ASN:HA	1.89	0.53
1:B:952:GLU:HG3	1:B:1136:ASN:HD21	1.74	0.53
1:C:456:SER:OG	1:C:457:SER:N	2.41	0.53
2:D:177:ASN:O	2:D:181:GLY:N	2.40	0.53
1:A:872:ASN:HB3	1:A:875:LEU:HB2	1.89	0.53
1:C:952:GLU:HG3	1:C:1136:ASN:HD21	1.73	0.53
2:D:264:PRO:HG3	2:D:315:LEU:HD11	1.90	0.53
2:E:185:CYS:HB3	2:E:190:TYR:HB2	1.90	0.53
2:F:448:SER:OG	2:F:448:SER:O	2.27	0.53
1:A:158:TYR:OH	5:A:2001:NAG:C8	2.57	0.53
1:A:846:VAL:HG13	1:A:1096:ILE:HG13	1.89	0.53
1:B:1132:SER:HA	1:B:1144:ILE:O	2.08	0.53
2:D:150:ARG:NE	2:D:159:GLN:OE1	2.39	0.53
2:F:177:ASN:O	2:F:181:GLY:N	2.40	0.53
2:F:306:TRP:HA	2:F:328:VAL:HG21	1.89	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:C:355:ASN:HB3	1:C:605:ASN:O	2.09	0.53
1:C:994:MET:O	1:C:998:ASN:ND2	2.37	0.53
2:F:151:LEU:HD21	2:F:239:LEU:HD23	1.91	0.53
1:C:405:SER:OG	1:C:406:SER:N	2.41	0.53
2:E:321:PHE:H	2:E:324:ALA:HB3	1.73	0.53
1:B:311:VAL:HG21	1:B:672:CYS:HB3	1.91	0.53
2:F:268:PRO:O	2:F:362:LYS:N	2.41	0.53
1:A:496:PRO:O	1:A:499:THR:OG1	2.28	0.52
2:D:285:ILE:O	2:D:364:VAL:N	2.42	0.52
2:D:306:TRP:HA	2:D:328:VAL:HG21	1.89	0.52
2:F:160:VAL:N	2:F:169:HIS:O	2.42	0.52
2:F:356:THR:OG1	2:F:358:ASN:ND2	2.42	0.52
1:B:456:SER:OG	1:B:457:SER:N	2.41	0.52
1:C:376:SER:OG	1:C:377:LYS:NZ	2.40	0.52
2:E:187:ASP:N	2:E:187:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:247:ASN:ND2	2:F:266:ALA:O	2.41	0.52
2:F:255:GLN:HB2	2:F:261:SER:HA	1.90	0.52
2:D:160:VAL:N	2:D:169:HIS:O	2.42	0.52
2:F:285:ILE:O	2:F:364:VAL:N	2.42	0.52
1:C:400:ASP:O	1:C:410:GLN:NE2	2.41	0.52
1:C:938:GLN:NE2	1:C:1041:ASN:OD1	2.42	0.52
5:C:2001:NAG:H61	3:Q:6:MAN:O4	2.08	0.52
2:E:160:VAL:H	2:E:169:HIS:H	1.57	0.52
1:B:566:SER:OG	1:B:567:CYS:N	2.43	0.52
2:D:151:LEU:HD21	2:D:239:LEU:HD23	1.91	0.52
2:D:187:ASP:OD1	2:D:187:ASP:N	2.41	0.52
2:E:268:PRO:O	2:E:362:LYS:N	2.41	0.52
1:C:74:PHE:HB3	1:C:257:TRP:HB3	1.91	0.52
2:E:151:LEU:HD21	2:E:239:LEU:HD23	1.91	0.52
1:B:422:SER:OG	1:B:424:GLN:NE2	2.39	0.52
1:C:348:ILE:HG12	1:C:387:THR:HG23	1.92	0.52
1:A:799:HIS:HA	1:A:1015:ILE:HD11	1.92	0.52
2:D:270:GLN:NE2	2:D:271:VAL:O	2.39	0.52
2:D:247:ASN:ND2	2:D:266:ALA:O	2.41	0.52
2:F:256:ILE:HG13	2:F:400:ALA:H	1.75	0.52
1:A:400:ASP:O	1:A:410:GLN:NE2	2.41	0.51
1:C:566:SER:OG	1:C:567:CYS:N	2.43	0.51
2:E:160:VAL:N	2:E:169:HIS:O	2.42	0.51
1:B:1018:GLY:O	1:B:1023:ASN:ND2	2.43	0.51
1:C:213:TYR:HB3	1:C:223:LEU:HD22	1.92	0.51
2:E:256:ILE:HG13	2:E:400:ALA:H	1.75	0.51
2:F:160:VAL:H	2:F:169:HIS:H	1.57	0.51
1:A:809:LYS:HG3	1:A:850:LEU:HD23	1.92	0.51
1:B:496:PRO:O	1:B:499:THR:OG1	2.28	0.51
1:C:142:HIS:HB2	1:C:145:ILE:HG22	1.91	0.51
2:E:150:ARG:NE	2:E:159:GLN:OE1	2.39	0.51
1:A:24:PHE:HB3	1:A:84:TYR:HA	1.92	0.51
1:A:376:SER:OG	1:A:377:LYS:NZ	2.40	0.51
1:A:456:SER:OG	1:A:457:SER:N	2.41	0.51
1:A:566:SER:OG	1:A:567:CYS:N	2.43	0.51
2:F:417:ASP:OD1	2:F:417:ASP:N	2.33	0.51
1:A:606:ASP:CA	4:J:1:NAG:O7	2.59	0.51
2:D:160:VAL:H	2:D:169:HIS:H	1.57	0.51
2:F:270:GLN:NE2	2:F:271:VAL:O	2.39	0.51
1:B:319:ARG:O	1:B:320:ARG:NH1	2.44	0.51
2:D:240:ARG:NH2	2:D:244:CYS:SG	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ALA:HB1	1:B:249:THR:HG21	1.93	0.51
2:F:240:ARG:NH2	2:F:244:CYS:SG	2.84	0.51
1:A:59:THR:OG1	1:A:60:THR:N	2.44	0.50
1:B:392:ALA:HB3	1:B:460:VAL:HG11	1.93	0.50
1:B:405:SER:OG	1:B:406:SER:N	2.41	0.50
1:B:348:ILE:HG12	1:B:387:THR:HG23	1.92	0.50
2:D:407:THR:OG1	2:D:408:GLN:NE2	2.38	0.50
1:A:348:ILE:HG12	1:A:387:THR:HG23	1.92	0.50
1:A:607:LEU:HD23	1:A:608:LEU:N	2.27	0.50
1:B:846:VAL:HG13	1:B:1096:ILE:HG13	1.92	0.50
1:C:422:SER:OG	1:C:424:GLN:NE2	2.39	0.50
1:B:607:LEU:CD2	1:B:607:LEU:N	2.72	0.50
2:E:285:ILE:O	2:E:364:VAL:N	2.42	0.50
2:E:407:THR:OG1	2:E:408:GLN:NE2	2.39	0.50
1:A:264:ARG:HH22	1:A:283:SER:HB2	1.77	0.50
1:B:400:ASP:O	1:B:410:GLN:NE2	2.41	0.50
1:C:1173:LYS:HG3	1:C:1203:VAL:HG12	1.93	0.50
2:D:448:SER:O	2:D:448:SER:OG	2.27	0.50
1:A:214:ALA:HB2	1:A:220:THR:HA	1.93	0.50
1:B:310:THR:HG21	1:B:675:GLY:H	1.76	0.50
2:D:256:ILE:HG13	2:D:400:ALA:H	1.75	0.50
2:E:448:SER:O	2:E:448:SER:OG	2.27	0.50
1:B:149:THR:HG22	1:B:186:LYS:HG3	1.93	0.50
1:C:168:SER:OG	1:C:169:ILE:N	2.42	0.50
1:B:1218:ILE:HA	1:B:1220:LEU:HD22	1.94	0.50
1:C:496:PRO:O	1:C:499:THR:OG1	2.28	0.50
2:E:240:ARG:NH2	2:E:244:CYS:SG	2.84	0.50
1:A:158:TYR:HE1	5:A:2001:NAG:H82	1.73	0.49
1:C:392:ALA:HB3	1:C:460:VAL:HG11	1.93	0.49
1:A:85:LEU:HB2	1:A:170:ARG:HH12	1.77	0.49
1:B:86:SER:OG	1:B:87:THR:N	2.45	0.49
2:F:275:VAL:HG12	2:F:276:GLN:HG3	1.94	0.49
2:D:443:GLY:O	2:D:459:THR:OG1	2.31	0.49
2:E:443:GLY:O	2:E:459:THR:OG1	2.31	0.49
1:A:392:ALA:HB3	1:A:460:VAL:HG11	1.93	0.49
1:C:621:ASN:OD1	1:C:621:ASN:N	2.44	0.49
1:C:1108:GLU:OE2	1:C:1120:ARG:NH2	2.43	0.49
1:C:805:THR:HG22	1:C:1103:ALA:HA	1.95	0.49
2:E:275:VAL:HG12	2:E:276:GLN:HG3	1.94	0.49
1:A:158:TYR:OH	5:A:2001:NAG:H83	2.12	0.49
1:B:570:ASP:OD1	1:B:570:ASP:N	2.32	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:ASP:OD1	2:D:229:ASP:N	2.46	0.48
2:E:167:SER:OG	2:E:169:HIS:NE2	2.37	0.48
2:E:346:ILE:HD11	2:E:484:ILE:HD11	1.95	0.48
2:F:346:ILE:HD11	2:F:484:ILE:HD11	1.95	0.48
1:A:159:PRO:HA	1:A:174:TRP:HA	1.95	0.48
2:E:229:ASP:N	2:E:229:ASP:OD1	2.46	0.48
1:A:422:SER:OG	1:A:424:GLN:NE2	2.39	0.48
1:A:1116:SER:OG	1:A:1117:GLN:N	2.46	0.48
2:F:443:GLY:O	2:F:459:THR:OG1	2.31	0.48
1:A:317:VAL:HG21	1:A:633:PHE:HE2	1.78	0.48
1:C:320:ARG:HH22	1:C:626:GLY:HA2	1.79	0.48
1:A:1130:ILE:HG22	1:A:1131:LEU:HD23	1.95	0.48
2:D:346:ILE:HD11	2:D:484:ILE:HD11	1.95	0.48
2:F:389:GLU:HB2	2:F:465:CYS:HB2	1.96	0.48
2:E:389:GLU:HB2	2:E:465:CYS:HB2	1.96	0.47
2:F:150:ARG:NE	2:F:159:GLN:OE1	2.39	0.47
1:B:168:SER:HA	1:B:243:LYS:HB2	1.96	0.47
2:D:275:VAL:HG12	2:D:276:GLN:HG3	1.94	0.47
1:B:609:TYR:CE2	1:B:611:ASN:CG	2.88	0.47
1:C:315:ALA:H	1:C:620:VAL:HG12	1.79	0.47
2:D:389:GLU:HB2	2:D:465:CYS:HB2	1.96	0.47
1:A:103:PHE:HB2	1:A:261:LEU:HD21	1.97	0.47
1:A:158:TYR:O	1:A:160:HIS:ND1	2.44	0.47
1:A:1132:SER:OG	1:A:1145:HIS:ND1	2.40	0.47
1:C:166:LYS:HB2	1:C:243:LYS:HD2	1.97	0.47
2:F:229:ASP:OD1	2:F:229:ASP:N	2.46	0.47
1:C:938:GLN:HG3	1:C:1044:LEU:HD22	1.97	0.47
2:D:198:GLN:NE2	2:D:238:SER:OG	2.48	0.47
2:D:316:ARG:HH11	2:F:316:ARG:HH22	1.63	0.47
1:B:326:ASP:OD1	1:B:326:ASP:N	2.48	0.47
1:A:850:LEU:HD13	1:A:1096:ILE:HD11	1.97	0.47
5:B:2001:NAG:O4	3:L:6:MAN:O4	2.31	0.47
1:A:163:CYS:HB3	1:A:240:LEU:HD11	1.97	0.46
1:C:607:LEU:HD23	1:C:608:LEU:HD23	1.96	0.46
2:D:287:THR:HG1	2:D:290:TRP:H	1.61	0.46
1:B:325:PRO:O	1:B:352:CYS:HB2	2.16	0.46
1:C:515:TRP:HE1	1:C:517:ARG:HH11	1.63	0.46
2:D:289:GLU:OE1	2:D:290:TRP:NE1	2.49	0.46
2:E:289:GLU:OE1	2:E:290:TRP:NE1	2.49	0.46
2:F:289:GLU:OE1	2:F:290:TRP:NE1	2.49	0.46
1:A:515:TRP:HE1	1:A:517:ARG:HH11	1.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:832:TYR:OH	1:C:1079:ASN:ND2	2.49	0.46
2:E:198:GLN:NE2	2:E:238:SER:OG	2.48	0.46
2:F:407:THR:OG1	2:F:408:GLN:NE2	2.38	0.46
1:A:355:ASN:CB	1:A:606:ASP:HB3	2.46	0.46
1:B:373:LEU:HG	1:B:421:SER:HB3	1.98	0.46
1:C:1019:PHE:HB3	1:C:1026:LEU:HD12	1.97	0.46
1:C:1132:SER:OG	1:C:1145:HIS:ND1	2.48	0.46
2:F:198:GLN:NE2	2:F:238:SER:OG	2.48	0.46
1:B:515:TRP:HE1	1:B:517:ARG:HH11	1.63	0.46
2:E:319:PHE:CE1	2:F:319:PHE:CE1	3.03	0.46
1:C:214:ALA:HB2	1:C:220:THR:HA	1.98	0.46
2:E:319:PHE:HE1	2:F:319:PHE:CE1	2.34	0.46
1:A:377:LYS:HA	1:A:377:LYS:HD3	1.79	0.45
1:A:901:SER:OG	1:A:902:LEU:N	2.49	0.45
1:A:1209:SER:OG	1:B:998:ASN:OD1	2.28	0.45
2:D:183:ALA:O	2:D:186:ARG:NH2	2.47	0.45
1:C:396:ARG:NH1	1:C:578:ASP:OD2	2.42	0.45
1:C:429:LEU:HD23	1:C:429:LEU:HA	1.83	0.45
1:A:97:ASP:O	1:A:99:ASN:ND2	2.49	0.45
1:C:373:LEU:HG	1:C:421:SER:HB3	1.98	0.45
2:D:302:LEU:HD23	2:D:302:LEU:HA	1.82	0.45
2:E:191:LYS:H	2:E:191:LYS:HG2	1.41	0.45
1:A:402:GLN:O	1:A:410:GLN:NE2	2.36	0.45
1:C:141:PRO:O	1:C:142:HIS:ND1	2.49	0.45
2:D:417:ASP:OD1	2:D:417:ASP:N	2.33	0.45
1:A:785:LEU:HB2	1:A:1157:LEU:HD23	1.99	0.45
1:B:74:PHE:HB3	1:B:257:TRP:HB3	1.98	0.45
1:C:746:TYR:HE2	1:C:748:LEU:HD23	1.81	0.45
2:E:287:THR:OG1	2:E:290:TRP:N	2.37	0.45
1:B:380:GLY:N	1:B:607:LEU:HD13	2.30	0.45
1:A:373:LEU:HG	1:A:421:SER:HB3	1.98	0.45
2:D:285:ILE:H	2:D:285:ILE:HG13	1.46	0.45
2:D:326:TYR:O	2:D:327:GLN:NE2	2.50	0.45
2:E:326:TYR:O	2:E:327:GLN:NE2	2.50	0.45
2:F:484:ILE:O	2:F:488:MET:N	2.50	0.45
1:B:380:GLY:HA3	1:B:607:LEU:CD1	2.41	0.45
1:B:850:LEU:HD13	1:B:1096:ILE:HD11	1.98	0.45
2:D:348:LEU:HD11	2:D:484:ILE:HG12	1.99	0.45
1:B:126:ILE:HG22	1:B:232:LEU:HD22	1.98	0.45
1:B:319:ARG:HD2	1:B:319:ARG:HA	1.82	0.45
1:B:785:LEU:HD22	1:B:1159:SER:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:692:TYR:HB3	1:C:695:LEU:HD12	1.99	0.45
2:E:203:ASP:OD1	2:E:203:ASP:N	2.50	0.44
1:A:223:LEU:HD12	1:A:223:LEU:HA	1.84	0.44
1:B:98:PHE:HE1	1:B:204:GLN:HG2	1.81	0.44
1:C:149:THR:HG22	1:C:186:LYS:HG3	1.99	0.44
2:F:348:LEU:HD11	2:F:484:ILE:HG12	1.99	0.44
2:D:195:TYR:HB3	2:D:240:ARG:HB2	2.00	0.44
2:E:484:ILE:O	2:E:488:MET:N	2.50	0.44
2:F:326:TYR:O	2:F:327:GLN:NE2	2.50	0.44
1:B:607:LEU:O	1:B:607:LEU:HG	2.17	0.44
1:C:107:LYS:HB2	1:C:255:GLU:HB2	2.00	0.44
1:A:1218:ILE:HD13	1:A:1220:LEU:HD23	2.00	0.44
1:B:966:ALA:HB2	1:B:973:ALA:HB3	2.00	0.44
1:C:978:PRO:HD2	1:C:981:LEU:HD12	1.98	0.44
2:E:348:LEU:HD11	2:E:484:ILE:HG12	2.00	0.44
1:B:609:TYR:CD2	1:B:611:ASN:CB	2.98	0.44
1:B:630:GLN:HE21	1:B:630:GLN:HB2	1.59	0.44
2:D:342:LYS:HD2	2:D:461:TRP:CD1	2.52	0.44
2:F:422:PRO:O	2:F:476:ASN:ND2	2.51	0.44
1:A:570:ASP:OD1	1:A:570:ASP:N	2.32	0.44
1:A:795:THR:OG1	1:A:796:ILE:N	2.50	0.44
2:D:248:LEU:H	2:D:248:LEU:HG	1.55	0.44
2:D:305:PRO:HB3	2:D:331:VAL:HG23	2.00	0.44
2:E:287:THR:HG1	2:E:290:TRP:H	1.62	0.44
2:E:213:ASN:O	2:E:224:LYS:NZ	2.36	0.44
1:A:117:LEU:HD21	1:A:194:SER:HA	1.99	0.44
1:A:182:LEU:CD2	1:C:351:ASN:HD21	2.31	0.44
1:B:1173:LYS:HE2	1:B:1173:LYS:HB3	1.89	0.44
1:C:114:ASN:OD1	1:C:114:ASN:N	2.51	0.44
1:A:18:PHE:HB2	1:A:154:THR:HG22	2.00	0.43
1:A:151:CYS:HA	1:A:183:CYS:HA	2.00	0.43
1:B:809:LYS:HG3	1:B:850:LEU:HD23	2.00	0.43
1:C:223:LEU:HA	1:C:223:LEU:HD12	1.81	0.43
2:E:305:PRO:HB3	2:E:331:VAL:HG23	2.00	0.43
2:F:195:TYR:HB3	2:F:240:ARG:HB2	2.00	0.43
2:F:305:PRO:HB3	2:F:331:VAL:HG23	2.00	0.43
1:A:26:ASN:HD21	1:A:28:TYR:HB3	1.84	0.43
2:D:296:HIS:N	2:D:345:ASP:OD1	2.50	0.43
2:D:372:MET:O	2:D:449:LYS:NZ	2.51	0.43
2:E:183:ALA:O	2:E:186:ARG:NH2	2.47	0.43
2:E:342:LYS:HD2	2:E:461:TRP:CD1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:342:LYS:HD2	2:F:461:TRP:CD1	2.52	0.43
1:A:1015:ILE:HD13	1:A:1015:ILE:HA	1.84	0.43
1:B:1130:ILE:HG22	1:B:1131:LEU:HD23	2.00	0.43
1:C:402:GLN:O	1:C:410:GLN:NE2	2.36	0.43
2:D:422:PRO:O	2:D:476:ASN:ND2	2.51	0.43
2:D:484:ILE:O	2:D:488:MET:N	2.50	0.43
2:D:203:ASP:OD1	2:D:203:ASP:N	2.50	0.43
2:F:213:ASN:O	2:F:224:LYS:NZ	2.36	0.43
1:B:1201:ASN:OD1	1:B:1201:ASN:N	2.49	0.43
2:E:177:ASN:OD1	2:E:180:TYR:N	2.52	0.43
2:E:422:PRO:O	2:E:476:ASN:ND2	2.51	0.43
2:F:177:ASN:OD1	2:F:180:TYR:N	2.52	0.43
1:A:15:ILE:H	1:A:15:ILE:HG12	1.63	0.43
1:A:511:TYR:HE1	2:D:340:LYS:O	2.02	0.43
1:A:1086:ASN:HD22	1:A:1086:ASN:HA	1.71	0.43
2:D:291:ILE:HG23	2:D:349:MET:HB2	2.01	0.43
2:E:195:TYR:HB3	2:E:240:ARG:HB2	2.00	0.43
2:F:203:ASP:OD1	2:F:203:ASP:N	2.50	0.43
1:A:509:THR:OG1	1:A:512:VAL:N	2.52	0.43
1:A:680:ALA:HB1	1:A:736:LEU:HD13	2.00	0.43
1:C:45:GLY:O	1:C:48:THR:OG1	2.34	0.43
1:C:791:PRO:HG3	1:C:1150:PRO:HB3	2.00	0.43
2:E:296:HIS:N	2:E:345:ASP:OD1	2.50	0.43
2:F:378:LEU:HD11	2:F:401:LYS:HD2	2.01	0.43
1:B:396:ARG:NH1	1:B:578:ASP:OD2	2.42	0.43
1:C:124:ILE:HG23	1:C:139:VAL:HB	2.01	0.43
1:C:267:LEU:O	1:C:279:ALA:HA	2.19	0.43
1:C:903:LEU:HD11	1:C:1016:GLN:HA	2.00	0.43
2:E:378:LEU:HD11	2:E:401:LYS:HD2	2.01	0.43
2:F:291:ILE:HG23	2:F:349:MET:HB2	2.01	0.43
1:A:83:LYS:HB3	1:A:83:LYS:HE2	1.89	0.43
1:A:128:SER:O	1:A:233:SER:OG	2.36	0.43
1:A:608:LEU:HD13	1:A:608:LEU:HA	1.81	0.43
1:B:214:ALA:HB2	1:B:220:THR:HA	2.00	0.43
2:E:483:TRP:HE3	2:E:484:ILE:HG13	1.84	0.43
1:A:130:PHE:HE1	1:A:234:HIS:HB2	1.84	0.42
1:B:162:VAL:HB	1:B:172:GLU:HB2	2.00	0.42
1:B:402:GLN:O	1:B:410:GLN:NE2	2.36	0.42
1:B:1019:PHE:HA	1:B:1023:ASN:HD22	1.84	0.42
1:C:509:THR:OG1	1:C:512:VAL:N	2.52	0.42
2:D:177:ASN:OD1	2:D:180:TYR:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:ARG:HG2	2:D:191:LYS:HA	2.01	0.42
1:B:185:PHE:CE2	1:B:187:LYS:HB2	2.55	0.42
1:B:509:THR:OG1	1:B:512:VAL:N	2.52	0.42
1:B:511:TYR:HE1	2:E:340:LYS:O	2.02	0.42
1:C:511:TYR:HE1	2:F:340:LYS:O	2.02	0.42
1:C:801:GLU:OE2	1:C:1109:LYS:NZ	2.45	0.42
2:D:200:ILE:HG13	2:D:236:VAL:HG23	2.01	0.42
2:D:483:TRP:HE3	2:D:484:ILE:HG13	1.84	0.42
2:F:167:SER:OG	2:F:169:HIS:NE2	2.37	0.42
1:A:520:CYS:SG	1:A:534:PRO:HD2	2.59	0.42
1:B:204:GLN:HE21	1:B:204:GLN:HB2	1.51	0.42
1:B:1008:PHE:HZ	1:B:1131:LEU:HD11	1.84	0.42
1:C:1130:ILE:HG22	1:C:1131:LEU:HD23	2.01	0.42
2:E:270:GLN:OE1	2:E:382:SER:OG	2.36	0.42
1:B:188:ASN:OD1	4:M:1:NAG:O7	2.37	0.42
1:B:836:CYS:O	1:B:840:ASN:ND2	2.52	0.42
1:C:520:CYS:SG	1:C:534:PRO:HD2	2.59	0.42
1:A:57:LEU:HD12	1:A:57:LEU:HA	1.90	0.42
1:B:1076:ARG:NH2	1:C:1075:ASP:OD2	2.53	0.42
2:D:191:LYS:H	2:D:191:LYS:HG2	1.41	0.42
2:E:186:ARG:HG2	2:E:191:LYS:HA	2.01	0.42
1:A:167:GLY:O	1:A:243:LYS:NZ	2.53	0.42
1:B:373:LEU:HD23	1:B:373:LEU:HA	1.88	0.42
1:B:520:CYS:SG	1:B:534:PRO:HD2	2.59	0.42
2:D:392:LYS:H	2:D:392:LYS:HG2	1.64	0.42
2:E:355:LEU:H	2:E:355:LEU:HG	1.63	0.42
2:F:213:ASN:HB3	2:F:224:LYS:HG2	2.02	0.42
2:F:296:HIS:N	2:F:345:ASP:OD1	2.50	0.42
1:A:977:VAL:HG11	1:A:985:TYR:HE2	1.85	0.42
1:C:246:SER:OG	1:C:247:SER:N	2.52	0.42
2:E:200:ILE:HG13	2:E:236:VAL:HG23	2.01	0.42
1:B:907:LEU:HD23	1:B:907:LEU:HA	1.89	0.42
1:C:326:ASP:C	1:C:352:CYS:HB2	2.40	0.42
1:A:142:HIS:NE2	1:A:147:GLU:OE1	2.36	0.42
1:C:377:LYS:HA	1:C:377:LYS:HD3	1.79	0.42
1:A:36:SER:OG	1:A:37:GLU:N	2.52	0.42
1:A:192:ASN:HD22	5:A:2006:NAG:C7	2.32	0.42
1:A:638:ALA:HB3	1:A:666:THR:HG21	2.02	0.42
1:B:75:ARG:HH21	1:B:77:LEU:HD21	1.85	0.42
1:B:466:CYS:HB3	1:B:547:PRO:HD2	2.02	0.42
1:B:606:ASP:C	1:B:608:LEU:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:378:LEU:HD11	2:D:401:LYS:HD2	2.01	0.42
2:F:296:HIS:ND1	2:F:345:ASP:OD2	2.49	0.42
1:C:1180:GLN:HB3	1:C:1185:MET:HG3	2.02	0.41
2:F:186:ARG:HG2	2:F:191:LYS:HA	2.02	0.41
2:D:355:LEU:H	2:D:355:LEU:HG	1.63	0.41
2:E:247:ASN:HB2	2:E:266:ALA:HA	2.03	0.41
1:B:805:THR:HG22	1:B:1103:ALA:HA	2.03	0.41
2:D:296:HIS:ND1	2:D:345:ASP:OD2	2.49	0.41
1:A:466:CYS:HB3	1:A:547:PRO:HD2	2.02	0.41
1:A:604:SER:O	1:A:605:ASN:HB3	2.20	0.41
1:B:838:ASN:OD1	1:B:838:ASN:N	2.53	0.41
2:D:268:PRO:HB2	2:D:362:LYS:HB2	2.02	0.41
2:F:173:GLN:NE2	2:F:198:GLN:O	2.54	0.41
1:A:429:LEU:HD23	1:A:429:LEU:HA	1.83	0.41
1:A:1120:ARG:HD2	1:A:1123:PHE:HB2	2.02	0.41
1:C:26:ASN:HB3	1:C:84:TYR:HB3	2.02	0.41
2:D:247:ASN:HB2	2:D:266:ALA:HA	2.03	0.41
2:E:268:PRO:HB2	2:E:362:LYS:HB2	2.02	0.41
2:F:149:VAL:HB	2:F:158:LEU:HD11	2.02	0.41
2:F:483:TRP:HE3	2:F:484:ILE:HG13	1.84	0.41
1:A:396:ARG:NH1	1:A:578:ASP:OD2	2.42	0.41
1:C:396:ARG:NH1	1:C:577:PHE:O	2.53	0.41
2:E:287:THR:HG21	2:E:290:TRP:HD1	1.85	0.41
2:F:200:ILE:HG13	2:F:236:VAL:HG23	2.01	0.41
2:F:287:THR:HG21	2:F:290:TRP:HD1	1.86	0.41
1:B:913:LEU:HD23	1:B:913:LEU:HA	1.89	0.41
2:D:213:ASN:HB3	2:D:224:LYS:HG2	2.02	0.41
2:F:302:LEU:HD23	2:F:302:LEU:HA	1.82	0.41
1:A:315:ALA:H	1:A:620:VAL:HG12	1.84	0.41
1:B:1120:ARG:HD2	1:B:1123:PHE:HB2	2.03	0.41
1:C:184:LEU:HD23	1:C:184:LEU:HA	1.91	0.41
1:C:487:LYS:HE2	1:C:487:LYS:HB3	1.78	0.41
2:D:394:SER:OG	2:D:398:ASN:ND2	2.52	0.41
2:E:291:ILE:HG23	2:E:349:MET:HB2	2.01	0.41
2:F:169:HIS:HA	2:F:170:PRO:HD3	1.92	0.41
2:F:248:LEU:H	2:F:248:LEU:HG	1.56	0.41
1:A:149:THR:HG22	1:A:186:LYS:HG3	2.03	0.41
1:A:187:LYS:HD2	1:A:188:ASN:H	1.85	0.41
1:A:359:LEU:HA	1:A:359:LEU:HD12	1.91	0.41
1:A:396:ARG:NH1	1:A:577:PHE:O	2.53	0.41
1:B:901:SER:OG	1:B:902:LEU:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:213:ASN:HB3	2:E:224:LYS:HG2	2.02	0.41
2:F:286:ILE:HG13	2:F:287:THR:HG23	2.03	0.41
1:B:477:ALA:HB3	1:B:492:SER:HB3	2.03	0.41
1:B:608:LEU:HD23	1:B:608:LEU:HA	1.76	0.41
1:B:1182:ASP:N	1:B:1182:ASP:OD1	2.53	0.41
1:C:376:SER:HA	1:C:379:PHE:HD2	1.86	0.41
2:D:319:PHE:CE1	2:F:321:PHE:CZ	3.09	0.41
2:F:457:GLY:HA2	2:F:477:VAL:HG23	2.03	0.41
1:A:351:ASN:OD1	1:B:183:CYS:CB	2.57	0.40
1:A:1002:LYS:HD2	1:A:1002:LYS:HA	1.84	0.40
1:B:396:ARG:NH1	1:B:577:PHE:O	2.53	0.40
1:C:403:LEU:H	1:C:403:LEU:HG	1.66	0.40
5:C:2001:NAG:C6	3:Q:6:MAN:O4	2.69	0.40
2:D:173:GLN:NE2	2:D:198:GLN:O	2.54	0.40
2:D:287:THR:OG1	2:D:290:TRP:N	2.37	0.40
2:F:183:ALA:O	2:F:186:ARG:NH2	2.47	0.40
2:F:253:GLN:H	2:F:253:GLN:HG2	1.63	0.40
1:B:83:LYS:HB3	1:B:83:LYS:HE2	1.84	0.40
1:B:376:SER:HA	1:B:379:PHE:HD2	1.86	0.40
2:E:286:ILE:HG21	2:E:366:LEU:HG	2.03	0.40
2:F:191:LYS:H	2:F:191:LYS:HG2	1.41	0.40
1:B:560:LEU:H	1:B:560:LEU:HG	1.72	0.40
1:C:1066:ASP:HA	1:C:1067:PRO:HD3	1.91	0.40
2:D:149:VAL:HB	2:D:158:LEU:HD11	2.03	0.40
1:C:466:CYS:HB3	1:C:547:PRO:HD2	2.02	0.40
2:D:329:GLU:OE1	2:D:330:LYS:N	2.50	0.40
2:E:149:VAL:HB	2:E:158:LEU:HD11	2.02	0.40
2:E:173:GLN:NE2	2:E:198:GLN:O	2.54	0.40
2:F:286:ILE:HG21	2:F:366:LEU:HG	2.03	0.40
1:C:1100:LYS:HE2	1:C:1100:LYS:HB3	1.88	0.40
2:D:178:GLU:O	2:D:182:ARG:N	2.54	0.40
2:E:286:ILE:HG13	2:E:287:THR:HG23	2.03	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%)	1101 (91%)	102 (8%)	3 (0%)	44	68
1	B	1206/1290 (94%)	1088 (90%)	115 (10%)	3 (0%)	44	68
1	C	1206/1290 (94%)	1096 (91%)	109 (9%)	1 (0%)	48	73
2	D	343/384 (89%)	277 (81%)	66 (19%)	0	100	100
2	E	343/384 (89%)	277 (81%)	66 (19%)	0	100	100
2	F	343/384 (89%)	277 (81%)	66 (19%)	0	100	100
All	All	4647/5022 (92%)	4116 (89%)	524 (11%)	7 (0%)	45	68

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	325	PRO
1	A	1128	ASN
1	B	609	TYR
1	A	605	ASN
1	B	52	LEU
1	B	326	ASP
1	A	51	VAL

### 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%)	931 (86%)	151 (14%)	3	7
1	B	1082/1159 (93%)	941 (87%)	141 (13%)	3	8
1	C	1082/1159 (93%)	946 (87%)	136 (13%)	3	9
2	D	293/326 (90%)	237 (81%)	56 (19%)	1	3
2	E	293/326 (90%)	237 (81%)	56 (19%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	293/326 (90%)	237 (81%)	56 (19%)	1	3
All	All	4125/4455 (93%)	3529 (86%)	596 (14%)	5	7

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	15	ILE
1	A	19	ASN
1	A	25	ILE
1	A	27	ASP
1	A	28	TYR
1	A	29	ASN
1	A	30	LYS
1	A	32	ILE
1	A	34	ARG
1	A	40	VAL
1	A	57	LEU
1	A	64	THR
1	A	80	LYS
1	A	85	LEU
1	A	86	SER
1	A	94	PHE
1	A	95	LEU
1	A	97	ASP
1	A	100	ASN
1	A	102	ILE
1	A	107	LYS
1	A	111	LEU
1	A	113	VAL
1	A	123	THR
1	A	124	ILE
1	A	129	VAL
1	A	131	VAL
1	A	132	ASN
1	A	133	THR
1	A	155	MET
1	A	157	GLU
1	A	173	SER
1	A	175	HIS
1	A	187	LYS
1	A	188	ASN

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Mol	Chain	Res	Type
1	A	193	VAL
1	A	197	TRP
1	A	204	GLN
1	A	205	GLU
1	A	213	TYR
1	A	216	VAL
1	A	222	PHE
1	A	238	MET
1	A	240	LEU
1	A	252	GLU
1	A	254	LEU
1	A	255	GLU
1	A	263	ARG
1	A	272	GLU
1	A	299	PRO
1	A	305	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

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Mol	Chain	Res	Type
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	607	LEU
1	A	608	LEU
1	A	609	TYR
1	A	610	SER
1	A	612	THR
1	A	613	GLU
1	A	616	THR
1	A	620	VAL
1	A	644	TRP
1	A	659	LYS
1	A	661	PHE
1	A	662	LEU
1	A	706	PHE
1	A	731	VAL
1	A	735	ASP
1	A	743	CYS
1	A	758	ILE
1	A	773	SER
1	A	779	VAL
1	A	780	GLU
1	A	781	THR
1	A	789	GLN
1	A	800	GLU
1	A	811	THR
1	A	845	GLU
1	A	850	LEU
1	A	865	VAL
1	A	869	SER
1	A	871	LEU
1	A	875	LEU
1	A	879	VAL
1	A	890	CYS
1	A	903	LEU
1	A	930	GLU
1	A	931	ILE

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Mol	Chain	Res	Type
1	A	946	LEU
1	A	950	LEU
1	A	964	VAL
1	A	986	ARG
1	A	993	THR
1	A	1002	LYS
1	A	1016	GLN
1	A	1022	THR
1	A	1028	LYS
1	A	1038	GLN
1	A	1042	SER
1	A	1086	ASN
1	A	1096	ILE
1	A	1098	LEU
1	A	1099	ILE
1	A	1105	ARG
1	A	1115	LYS
1	A	1116	SER
1	A	1118	SER
1	A	1124	CYS
1	A	1131	LEU
1	A	1132	SER
1	A	1135	GLN
1	A	1155	THR
1	A	1167	ASP
1	A	1179	LYS
1	A	1203	VAL
1	A	1207	SER
1	A	1208	CYS
1	A	1217	PHE
1	A	1219	TYR
1	B	22	ASN
1	B	29	ASN
1	B	30	LYS
1	B	32	ILE
1	B	34	ARG
1	B	40	VAL
1	B	43	SER
1	B	52	LEU
1	B	57	LEU
1	B	58	ASN
1	B	80	LYS

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Mol	Chain	Res	Type
1	B	85	LEU
1	B	91	LYS
1	B	109	THR
1	B	120	GLU
1	B	123	THR
1	B	129	VAL
1	B	132	ASN
1	B	136	THR
1	B	152	GLN
1	B	166	LYS
1	B	175	HIS
1	B	177	ASP
1	B	187	LYS
1	B	204	GLN
1	B	213	TYR
1	B	215	ASP
1	B	216	VAL
1	B	223	LEU
1	B	230	THR
1	B	232	LEU
1	B	245	ILE
1	B	253	THR
1	B	254	LEU
1	B	262	SER
1	B	263	ARG
1	B	284	SER
1	B	305	ASP
1	B	320	ARG
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

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Mol	Chain	Res	Type
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
1	B	607	LEU
1	B	608	LEU
1	B	612	THR
1	B	620	VAL
1	B	630	GLN
1	B	640	TYR
1	B	644	TRP
1	B	651	SER
1	B	659	LYS
1	B	661	PHE
1	B	662	LEU
1	B	668	THR
1	B	687	SER
1	B	707	ILE
1	B	714	ASP
1	B	731	VAL
1	B	735	ASP
1	B	737	ARG
1	B	743	CYS
1	B	745	ASP
1	B	748	LEU
1	B	779	VAL

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Mol	Chain	Res	Type
1	B	787	GLU
1	B	789	GLN
1	B	828	LEU
1	B	845	GLU
1	B	850	LEU
1	B	852	ILE
1	B	865	VAL
1	B	872	ASN
1	B	879	VAL
1	B	886	SER
1	B	890	CYS
1	B	894	GLN
1	B	900	ARG
1	B	901	SER
1	B	902	LEU
1	B	930	GLU
1	B	931	ILE
1	B	946	LEU
1	B	947	PRO
1	B	950	LEU
1	B	951	SER
1	B	964	VAL
1	B	972	SER
1	B	986	ARG
1	B	993	THR
1	B	1012	LEU
1	B	1022	THR
1	B	1030	GLN
1	B	1042	SER
1	B	1086	ASN
1	B	1089	VAL
1	B	1096	ILE
1	B	1098	LEU
1	B	1115	LYS
1	B	1124	CYS
1	B	1131	LEU
1	B	1135	GLN
1	B	1151	THR
1	B	1165	SER
1	B	1201	ASN
1	B	1208	CYS
1	B	1210	VAL

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Mol	Chain	Res	Type
1	B	1212	PHE
1	B	1213	THR
1	B	1219	TYR
1	B	1220	LEU
1	C	14	VAL
1	C	29	ASN
1	C	32	ILE
1	C	34	ARG
1	C	38	ASP
1	C	40	VAL
1	C	54	ARG
1	C	57	LEU
1	C	88	LEU
1	C	91	LYS
1	C	96	SER
1	C	102	ILE
1	C	114	ASN
1	C	116	THR
1	C	123	THR
1	C	124	ILE
1	C	129	VAL
1	C	131	VAL
1	C	132	ASN
1	C	145	ILE
1	C	162	VAL
1	C	166	LYS
1	C	168	SER
1	C	175	HIS
1	C	180	GLU
1	C	187	LYS
1	C	204	GLN
1	C	205	GLU
1	C	213	TYR
1	C	215	ASP
1	C	223	LEU
1	C	230	THR
1	C	245	ILE
1	C	249	THR
1	C	253	THR
1	C	259	THR
1	C	262	SER
1	C	263	ARG

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Mol	Chain	Res	Type
1	C	284	SER
1	C	310	THR
1	C	311	VAL
1	C	319	ARG
1	C	320	ARG
1	C	324	LEU
1	C	326	ASP
1	C	328	ASP
1	C	351	ASN
1	C	362	LEU
1	C	371	ASN
1	C	373	LEU
1	C	389	ASP
1	C	397	ARG
1	C	400	ASP
1	C	403	LEU
1	C	405	SER
1	C	412	SER
1	C	418	ILE
1	C	431	LEU
1	C	437	ASN
1	C	438	ASN
1	C	456	SER
1	C	460	VAL
1	C	487	LYS
1	C	491	LEU
1	C	511	TYR
1	C	515	TRP
1	C	516	CYS
1	C	531	ASN
1	C	532	THR
1	C	540	VAL
1	C	545	HIS
1	C	560	LEU
1	C	561	ASN
1	C	570	ASP
1	C	573	LEU
1	C	590	SER
1	C	595	ASN
1	C	597	ILE
1	C	607	LEU
1	C	609	TYR

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Mol	Chain	Res	Type
1	C	612	THR
1	C	618	VAL
1	C	621	ASN
1	C	636	VAL
1	C	655	ILE
1	C	658	PHE
1	C	661	PHE
1	C	662	LEU
1	C	674	SER
1	C	730	SER
1	C	731	VAL
1	C	735	ASP
1	C	740	SER
1	C	743	CYS
1	C	745	ASP
1	C	748	LEU
1	C	780	GLU
1	C	781	THR
1	C	789	GLN
1	C	800	GLU
1	C	835	PHE
1	C	837	ASP
1	C	850	LEU
1	C	854	GLN
1	C	865	VAL
1	C	871	LEU
1	C	877	SER
1	C	879	VAL
1	C	903	LEU
1	C	914	SER
1	C	916	VAL
1	C	934	LEU
1	C	950	LEU
1	C	952	GLU
1	C	953	THR
1	C	964	VAL
1	C	986	ARG
1	C	1001	GLN
1	C	1012	LEU
1	C	1022	THR
1	C	1026	LEU
1	C	1038	GLN

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Mol	Chain	Res	Type
1	C	1069	GLU
1	C	1090	SER
1	C	1096	ILE
1	C	1098	LEU
1	C	1115	LYS
1	C	1124	CYS
1	C	1131	LEU
1	C	1132	SER
1	C	1135	GLN
1	C	1157	LEU
1	C	1165	SER
1	C	1189	SER
1	C	1219	TYR
1	C	1221	ASN
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
2	F	149	VAL
2	F	174	ASP
2	F	187	ASP
2	F	191	LYS
2	F	195	TYR
2	F	207	THR
2	F	212	LEU
2	F	219	VAL
2	F	226	TYR
2	F	229	ASP
2	F	234	LYS
2	F	241	CYS
2	F	246	VAL
2	F	248	LEU
2	F	251	SER
2	F	253	GLN
2	F	257	VAL
2	F	269	TRP
2	F	280	VAL
2	F	285	ILE
2	F	291	ILE
2	F	292	VAL
2	F	293	THR
2	F	303	ASN
2	F	327	GLN
2	F	328	VAL
2	F	329	GLU
2	F	332	ILE
2	F	333	SER
2	F	346	ILE
2	F	349	MET
2	F	352	GLN
2	F	355	LEU
2	F	362	LYS
2	F	366	LEU
2	F	371	MET
2	F	372	MET
2	F	392	LYS
2	F	393	THR
2	F	396	VAL
2	F	406	GLU
2	F	413	ARG

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Mol	Chain	Res	Type
2	F	425	ILE
2	F	426	CYS
2	F	429	PHE
2	F	430	LEU
2	F	437	CYS
2	F	438	GLN
2	F	440	ASP
2	F	446	VAL
2	F	459	THR
2	F	465	CYS
2	F	477	VAL
2	F	480	PHE
2	F	482	ASP
2	F	486	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	ASN
1	A	323	ASN
1	A	371	ASN
1	A	372	ASN
1	A	413	ASN
1	A	437	ASN
1	A	559	GLN
1	A	595	ASN
1	A	630	GLN
1	A	646	ASN
1	A	984	GLN
1	A	1038	GLN
1	A	1086	ASN
1	A	1091	GLN
1	A	1136	ASN
1	B	26	ASN
1	B	204	GLN
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	630	GLN

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Mol	Chain	Res	Type
1	B	840	ASN
1	B	876	HIS
1	B	1001	GLN
1	B	1023	ASN
1	B	1038	GLN
1	B	1045	GLN
1	B	1079	ASN
1	B	1086	ASN
1	B	1091	GLN
1	B	1122	ASN
1	B	1136	ASN
1	C	140	GLN
1	C	351	ASN
1	C	371	ASN
1	C	372	ASN
1	C	413	ASN
1	C	437	ASN
1	C	559	GLN
1	C	595	ASN
1	C	646	ASN
1	C	938	GLN
1	C	984	GLN
1	C	1038	GLN
1	C	1079	ASN
1	C	1091	GLN
1	C	1136	ASN
1	C	1221	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
2	F	198	GLN
2	F	253	GLN
2	F	327	GLN
2	F	408	GLN
2	F	438	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

42 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	NAG	G	1	1,3	14,14,15	0.33	0	17,19,21	0.62	1 (5%)
3	NAG	G	2	3	14,14,15	0.22	0	17,19,21	0.55	0
3	MAN	G	3	3	11,11,12	1.39	3 (27%)	15,15,17	1.81	3 (20%)
3	MAN	G	4	3	11,11,12	0.84	0	15,15,17	1.14	2 (13%)
3	MAN	G	5	3	11,11,12	0.78	0	15,15,17	1.06	2 (13%)
3	MAN	G	6	3	11,11,12	0.72	0	15,15,17	1.26	2 (13%)
4	NAG	H	1	1,4	14,14,15	0.18	0	17,19,21	0.53	0
4	NAG	H	2	4	14,14,15	0.26	0	17,19,21	0.49	0
4	NAG	I	1	1,4	14,14,15	0.47	0	17,19,21	0.71	0
4	NAG	I	2	4	14,14,15	0.41	0	17,19,21	0.74	1 (5%)
4	NAG	J	1	1,4	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	J	2	4	14,14,15	0.56	0	17,19,21	0.54	0
4	NAG	K	1	1,4	14,14,15	0.23	0	17,19,21	0.51	0
4	NAG	K	2	4	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	L	1	1,3	14,14,15	0.33	0	17,19,21	0.62	0
3	NAG	L	2	3	14,14,15	0.22	0	17,19,21	0.54	0
3	MAN	L	3	3	11,11,12	1.38	3 (27%)	15,15,17	1.80	3 (20%)
3	MAN	L	4	3	11,11,12	0.82	0	15,15,17	1.15	2 (13%)
3	MAN	L	5	3	11,11,12	0.81	0	15,15,17	1.05	2 (13%)
3	MAN	L	6	3	11,11,12	0.74	0	15,15,17	1.27	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	M	1	4	14,14,15	0.74	1 (7%)	17,19,21	0.49	0
4	NAG	M	2	4	14,14,15	0.23	0	17,19,21	0.66	1 (5%)
4	NAG	N	1	1,4	14,14,15	0.47	0	17,19,21	0.71	0
4	NAG	N	2	4	14,14,15	0.42	0	17,19,21	0.74	1 (5%)
4	NAG	O	1	1,4	14,14,15	1.05	1 (7%)	17,19,21	0.87	0
4	NAG	O	2	4	14,14,15	0.57	0	17,19,21	0.53	0
4	NAG	P	1	1,4	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	P	2	4	14,14,15	0.30	0	17,19,21	0.53	0
3	NAG	Q	1	1,3	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
3	NAG	Q	2	3	14,14,15	0.23	0	17,19,21	0.54	0
3	MAN	Q	3	3	11,11,12	1.39	3 (27%)	15,15,17	1.81	3 (20%)
3	MAN	Q	4	3	11,11,12	0.82	0	15,15,17	1.15	2 (13%)
3	MAN	Q	5	3	11,11,12	0.79	0	15,15,17	1.05	2 (13%)
3	MAN	Q	6	3	11,11,12	0.73	0	15,15,17	1.27	2 (13%)
4	NAG	R	1	1,4	14,14,15	0.31	0	17,19,21	0.40	0
4	NAG	R	2	4	14,14,15	0.24	0	17,19,21	0.58	0
4	NAG	S	1	1,4	14,14,15	0.48	0	17,19,21	0.71	0
4	NAG	S	2	4	14,14,15	0.41	0	17,19,21	0.73	1 (5%)
4	NAG	T	1	1,4	14,14,15	1.05	1 (7%)	17,19,21	0.88	0
4	NAG	T	2	4	14,14,15	0.55	0	17,19,21	0.54	0
4	NAG	U	1	1,4	14,14,15	0.23	0	17,19,21	0.50	0
4	NAG	U	2	4	14,14,15	0.31	0	17,19,21	0.54	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	G	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	MAN	G	3	3	-	2/2/19/22	1/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	MAN	G	5	3	-	0/2/19/22	0/1/1/1
3	MAN	G	6	3	-	2/2/19/22	0/1/1/1
4	NAG	H	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	NAG	I	1	1,4	-	2/6/23/26	0/1/1/1

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

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	T	1	NAG	O5-C1	-3.71	1.37	1.43
4	O	1	NAG	O5-C1	-3.70	1.37	1.43
4	M	1	NAG	O5-C1	-2.63	1.39	1.43
3	L	3	MAN	O5-C5	2.58	1.48	1.43
3	G	3	MAN	O5-C5	2.56	1.48	1.43
3	Q	3	MAN	O5-C5	2.56	1.48	1.43
3	Q	3	MAN	C2-C3	2.43	1.56	1.52
3	G	3	MAN	C2-C3	2.40	1.56	1.52
3	L	3	MAN	C2-C3	2.38	1.56	1.52
3	G	3	MAN	C1-C2	2.05	1.56	1.52
3	L	3	MAN	C1-C2	2.03	1.56	1.52
3	Q	3	MAN	C1-C2	2.02	1.56	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	C1-O5-C5	5.47	119.60	112.19
3	Q	3	MAN	C1-O5-C5	5.45	119.58	112.19
3	L	3	MAN	C1-O5-C5	5.43	119.55	112.19
3	Q	6	MAN	C1-O5-C5	3.85	117.40	112.19
3	L	6	MAN	C1-O5-C5	3.83	117.38	112.19
3	G	6	MAN	C1-O5-C5	3.81	117.36	112.19
3	Q	4	MAN	C1-O5-C5	3.16	116.48	112.19
3	L	4	MAN	C1-O5-C5	3.16	116.48	112.19
3	G	4	MAN	C1-O5-C5	3.16	116.47	112.19
3	L	5	MAN	C1-O5-C5	2.84	116.03	112.19
3	G	5	MAN	C1-O5-C5	2.83	116.03	112.19
3	Q	5	MAN	C1-O5-C5	2.78	115.95	112.19
4	N	2	NAG	C1-O5-C5	2.70	115.85	112.19
4	I	2	NAG	C1-O5-C5	2.70	115.85	112.19
4	S	2	NAG	C1-O5-C5	2.69	115.84	112.19
3	Q	3	MAN	C1-C2-C3	2.58	112.84	109.67
3	L	3	MAN	C1-C2-C3	2.57	112.82	109.67
3	G	3	MAN	C1-C2-C3	2.53	112.78	109.67
4	M	2	NAG	C1-O5-C5	2.36	115.38	112.19
3	Q	6	MAN	O2-C2-C3	-2.30	105.54	110.14
3	L	6	MAN	O2-C2-C3	-2.29	105.56	110.14
3	G	6	MAN	O2-C2-C3	-2.28	105.56	110.14
3	Q	3	MAN	O2-C2-C3	-2.24	105.66	110.14
3	L	3	MAN	O2-C2-C3	-2.23	105.66	110.14
3	L	4	MAN	O2-C2-C3	-2.21	105.70	110.14
3	Q	4	MAN	O2-C2-C3	-2.21	105.70	110.14
3	G	4	MAN	O2-C2-C3	-2.20	105.72	110.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3	MAN	O2-C2-C3	-2.20	105.73	110.14
3	G	5	MAN	O2-C2-C3	-2.19	105.76	110.14
3	Q	5	MAN	O2-C2-C3	-2.17	105.79	110.14
3	L	5	MAN	O2-C2-C3	-2.15	105.82	110.14
3	Q	1	NAG	C1-O5-C5	2.03	114.95	112.19
3	G	1	NAG	C1-O5-C5	2.02	114.92	112.19

There are no chirality outliers.

All (73) torsion outliers are listed below:

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

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

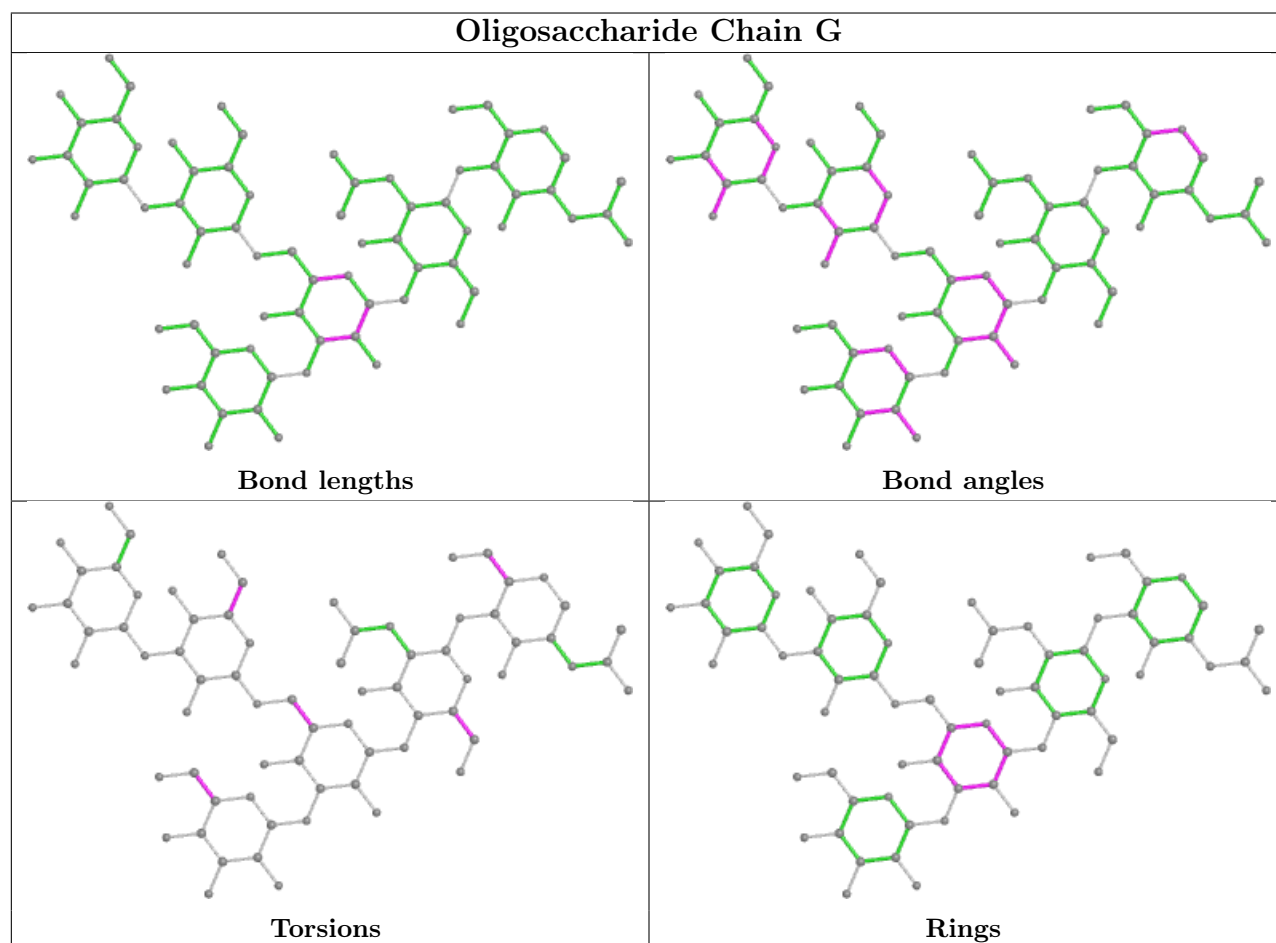
All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	3	MAN	C1-C2-C3-C4-C5-O5
3	Q	3	MAN	C1-C2-C3-C4-C5-O5
3	L	3	MAN	C1-C2-C3-C4-C5-O5

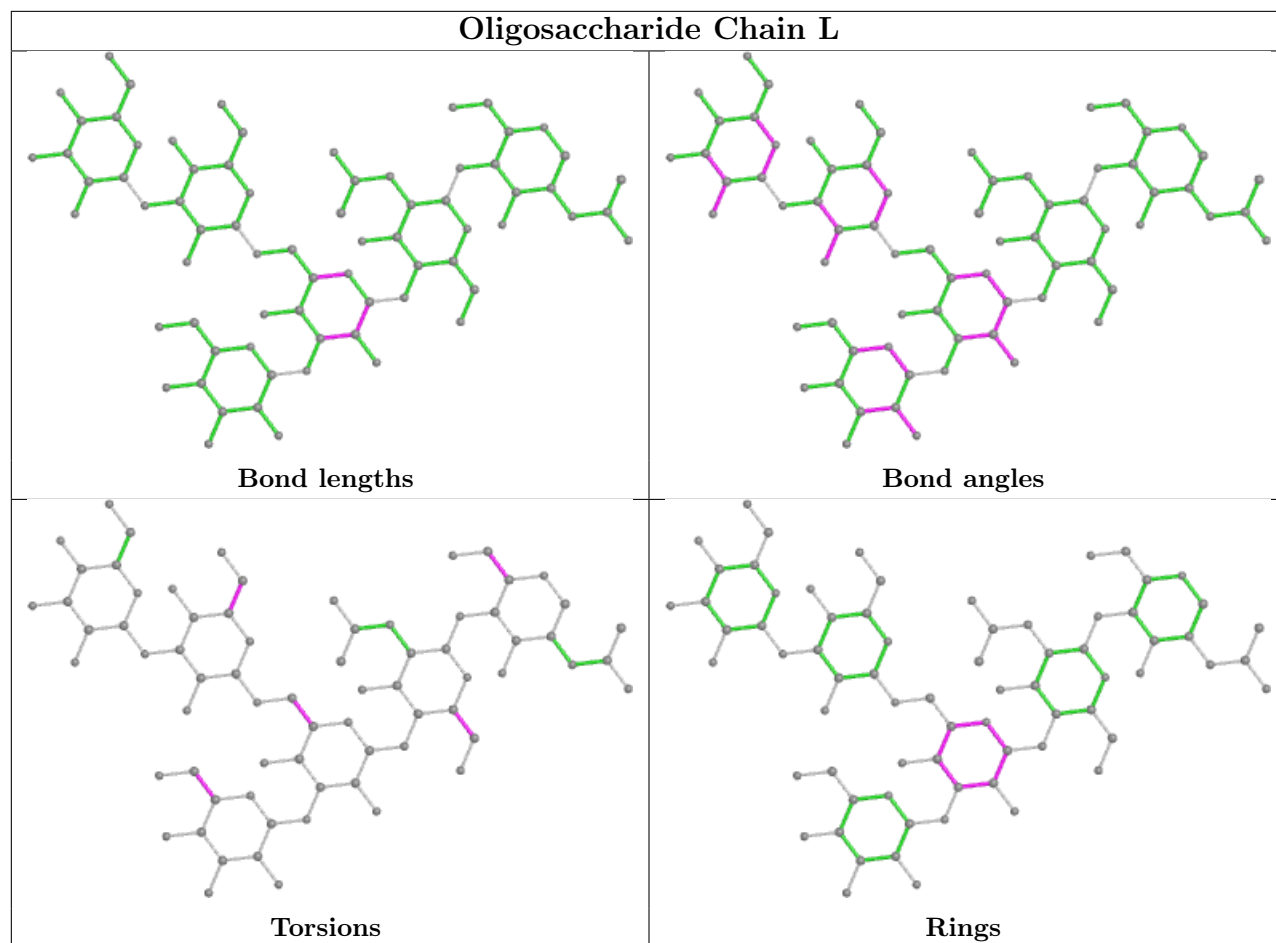
5 monomers are involved in 14 short contacts:

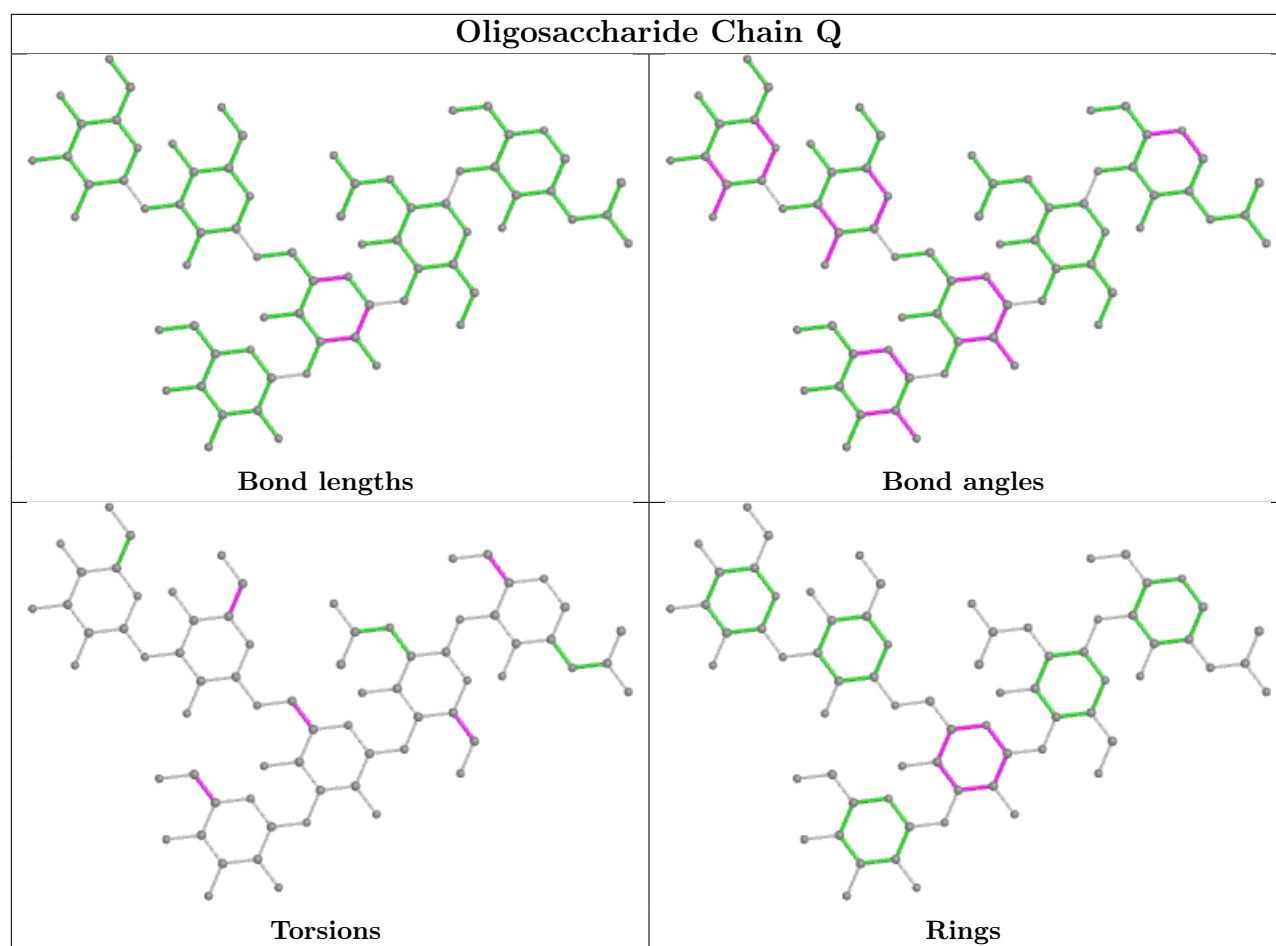
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	6	MAN	3	0
3	Q	6	MAN	2	0
4	H	1	NAG	2	0
4	M	1	NAG	2	0
4	J	1	NAG	5	0

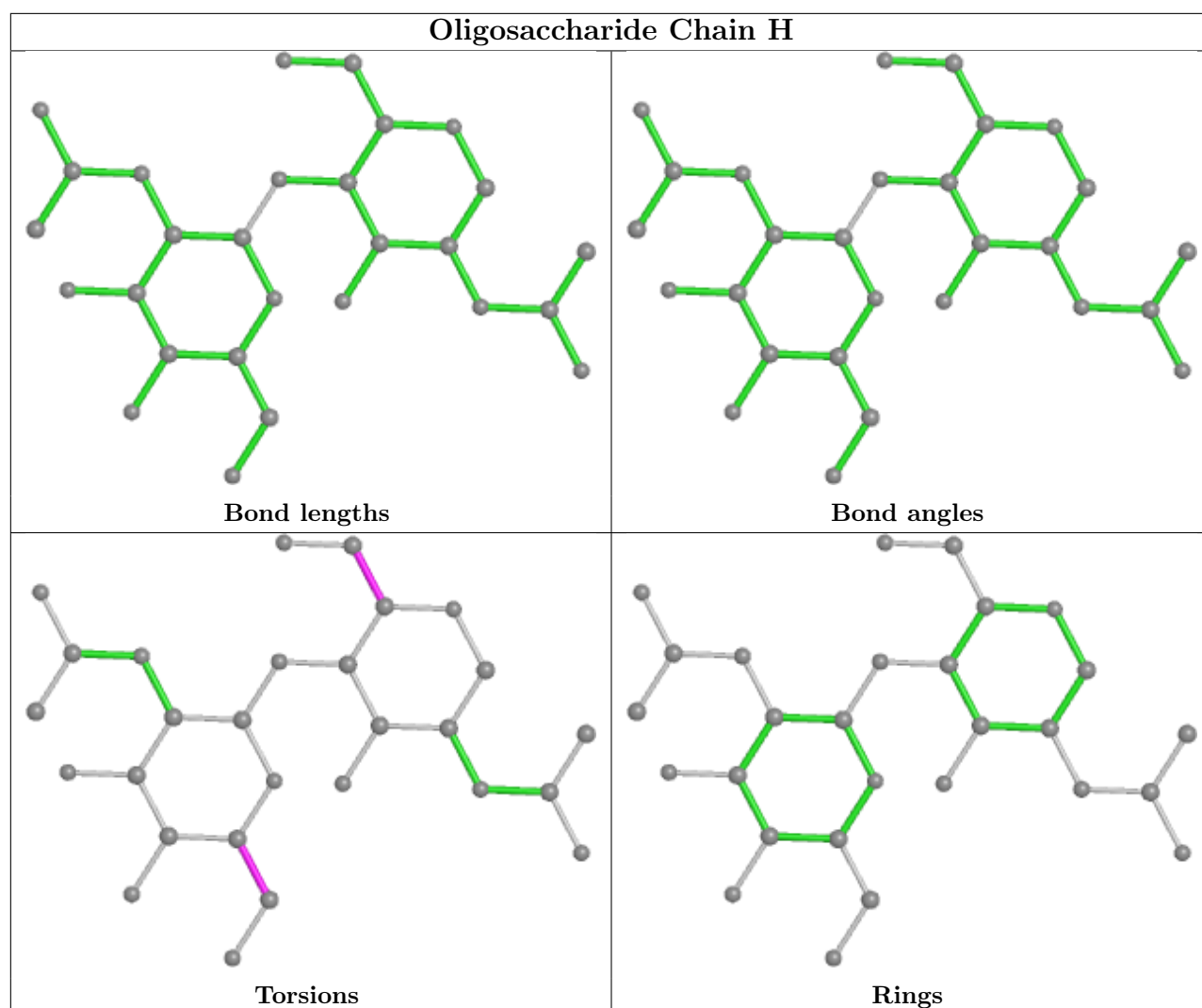
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

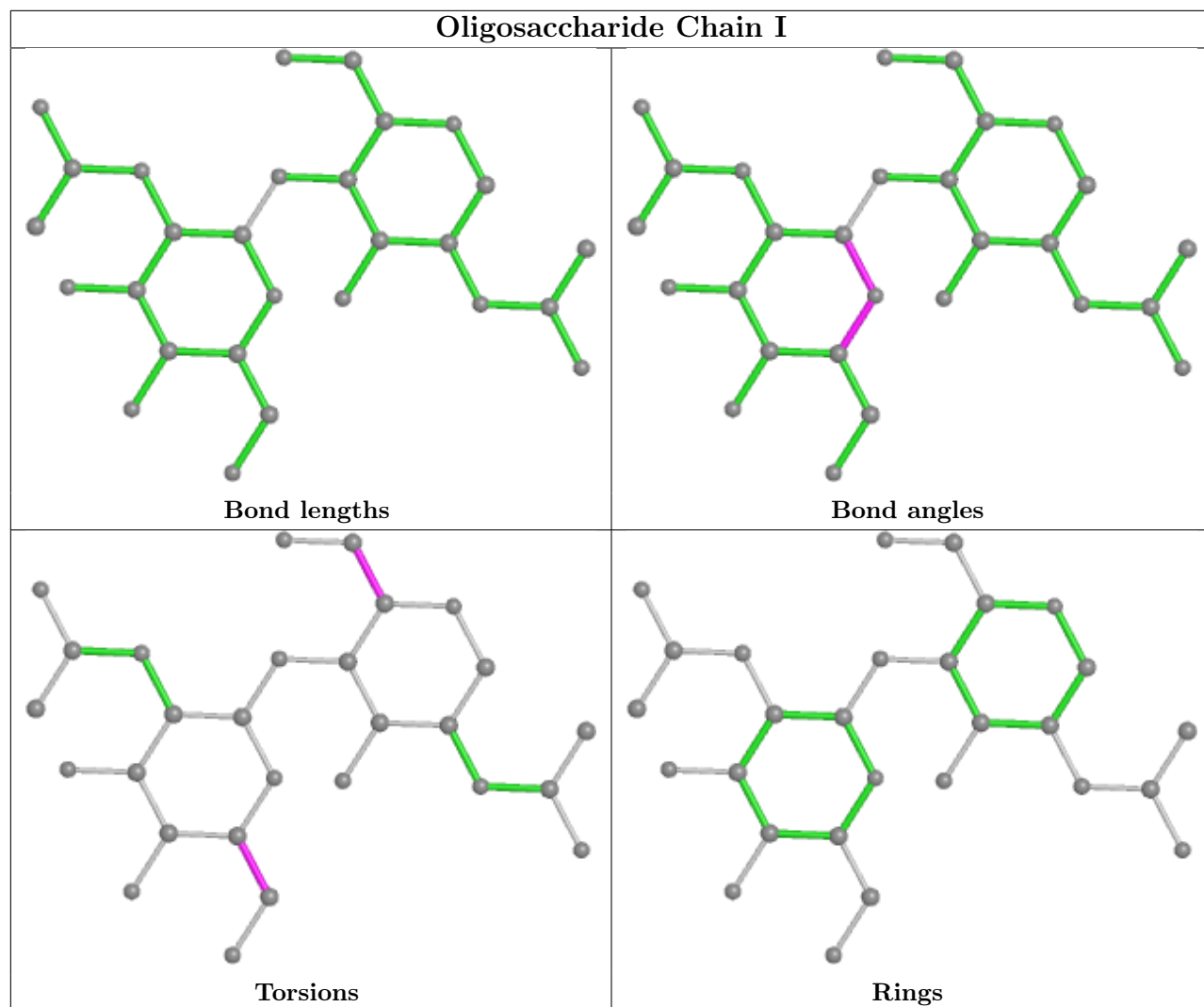


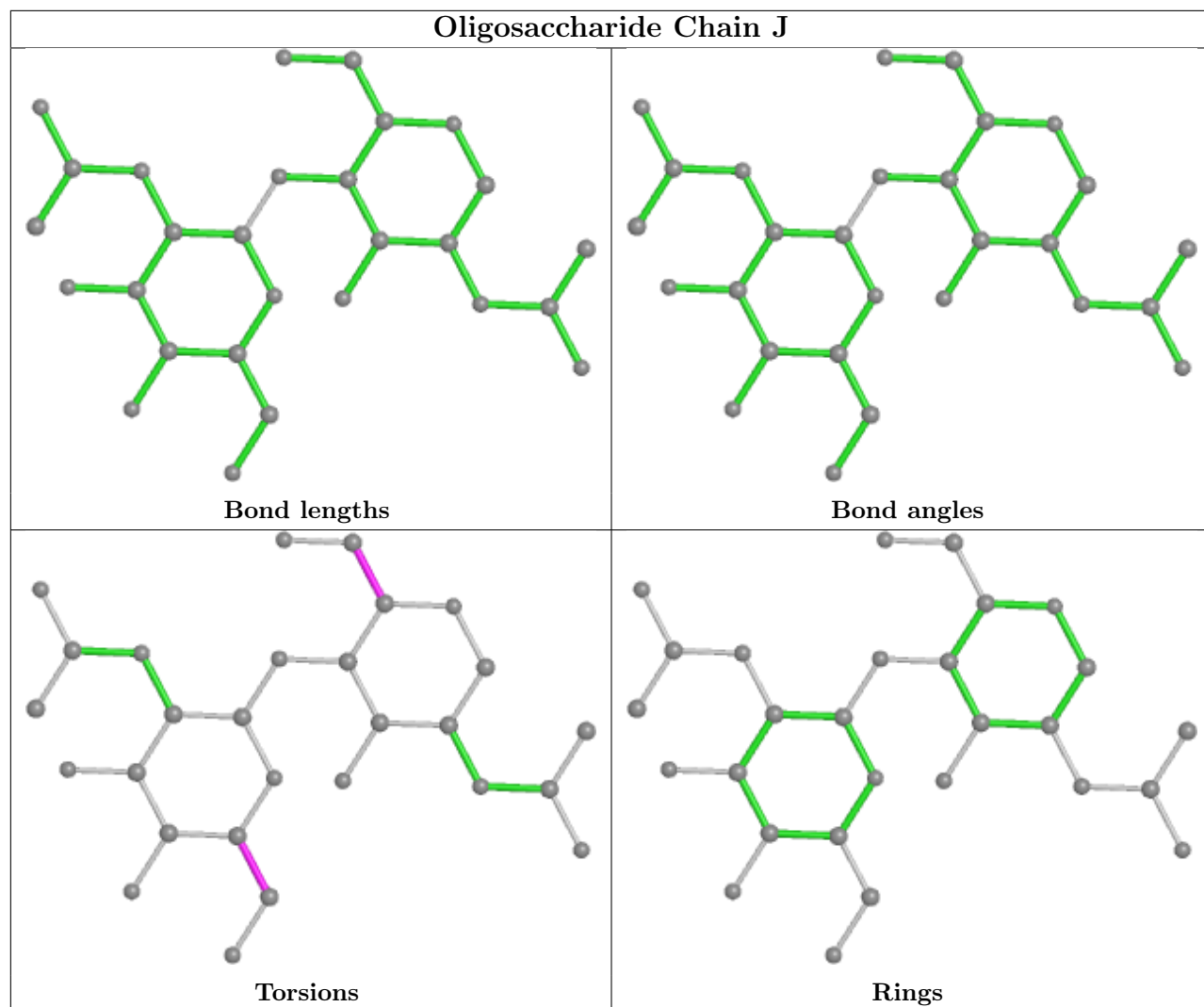


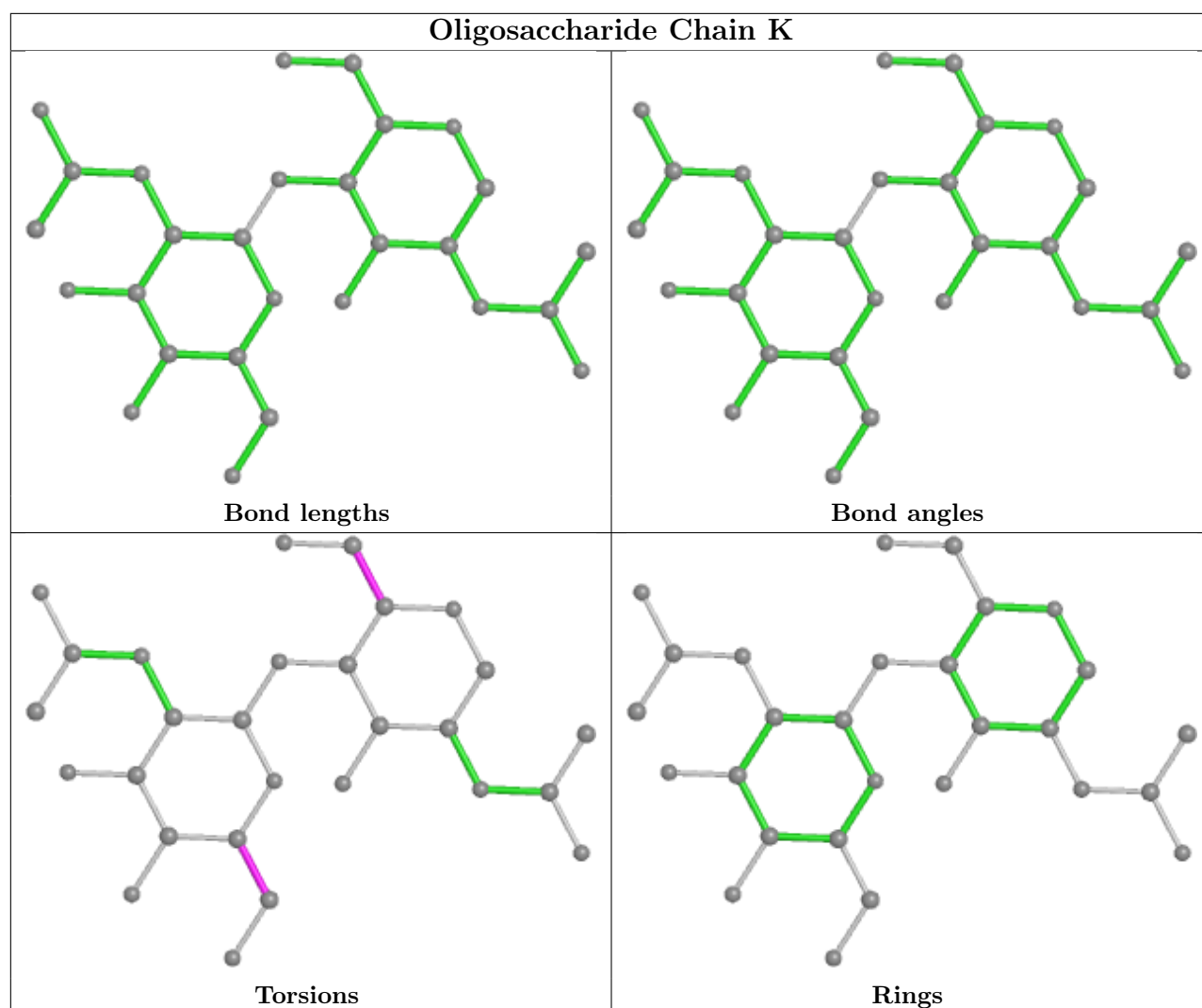


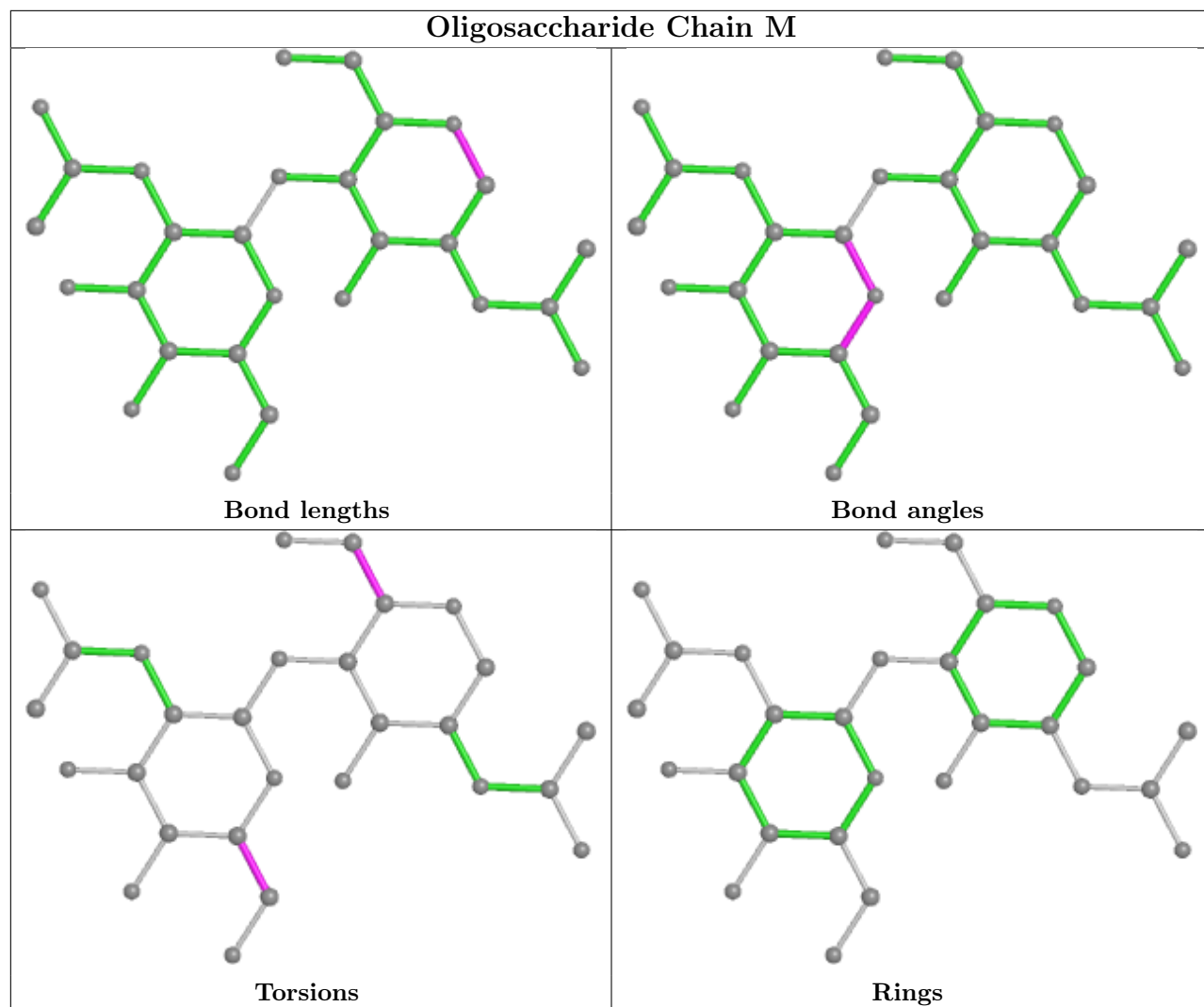


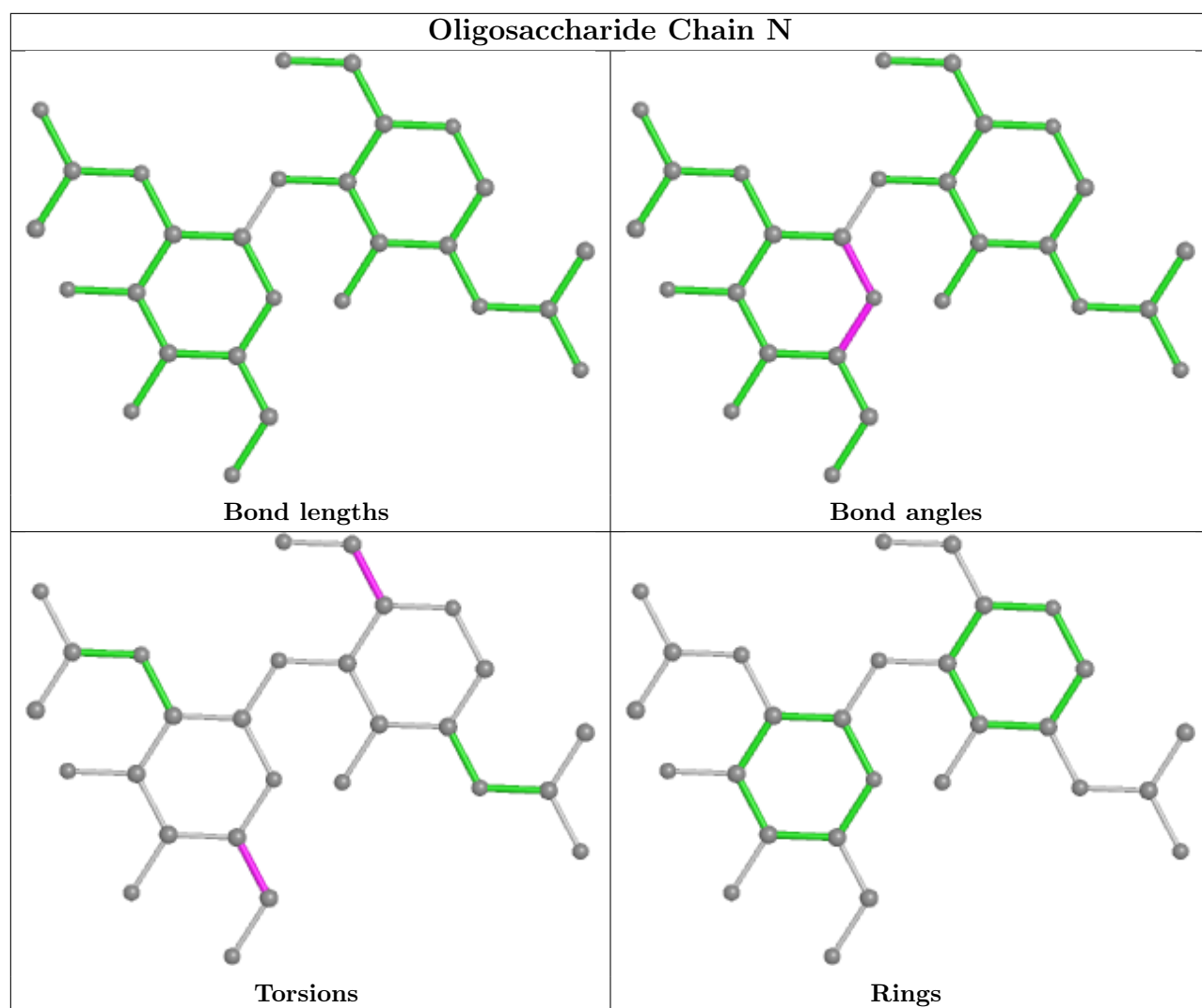




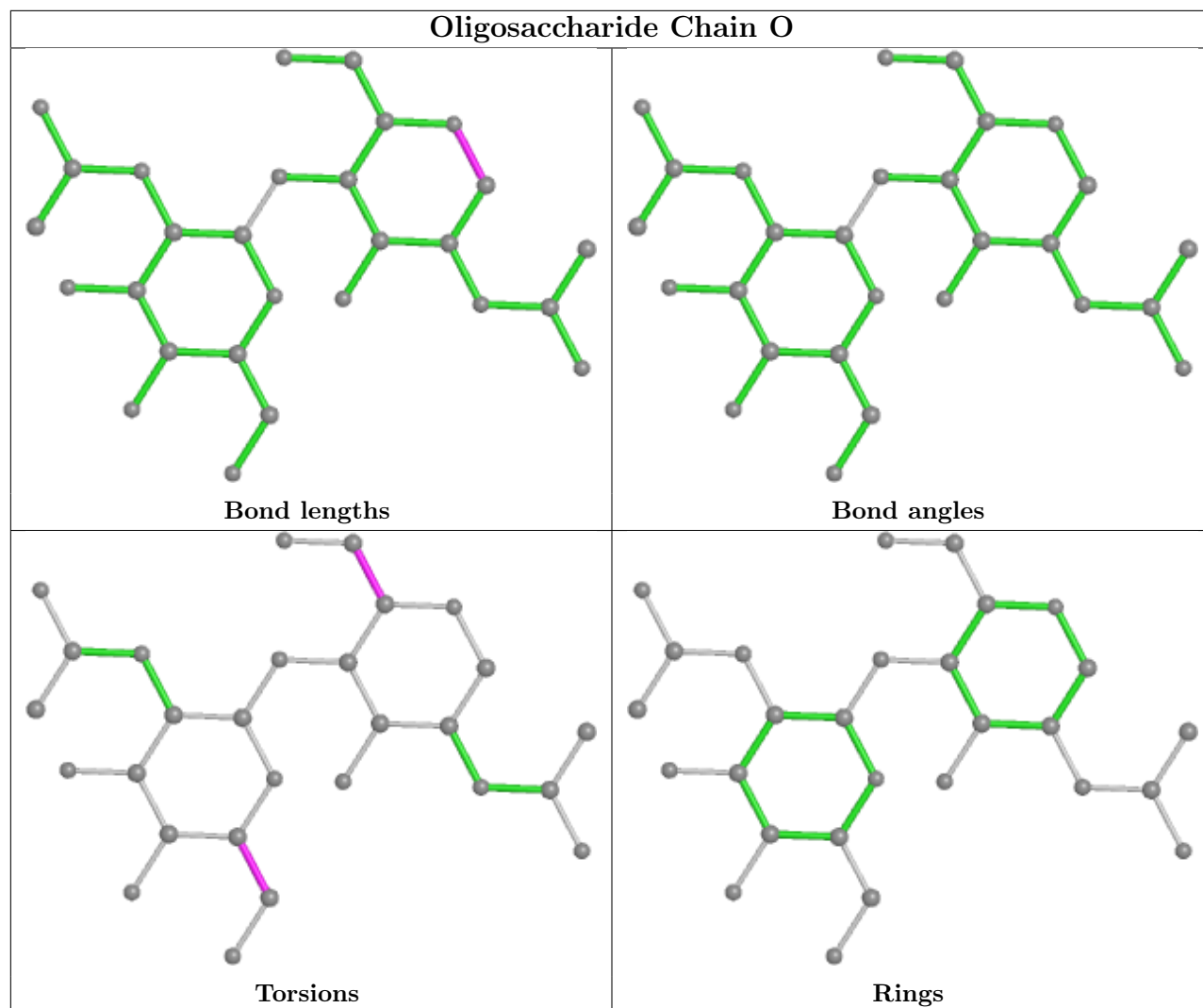


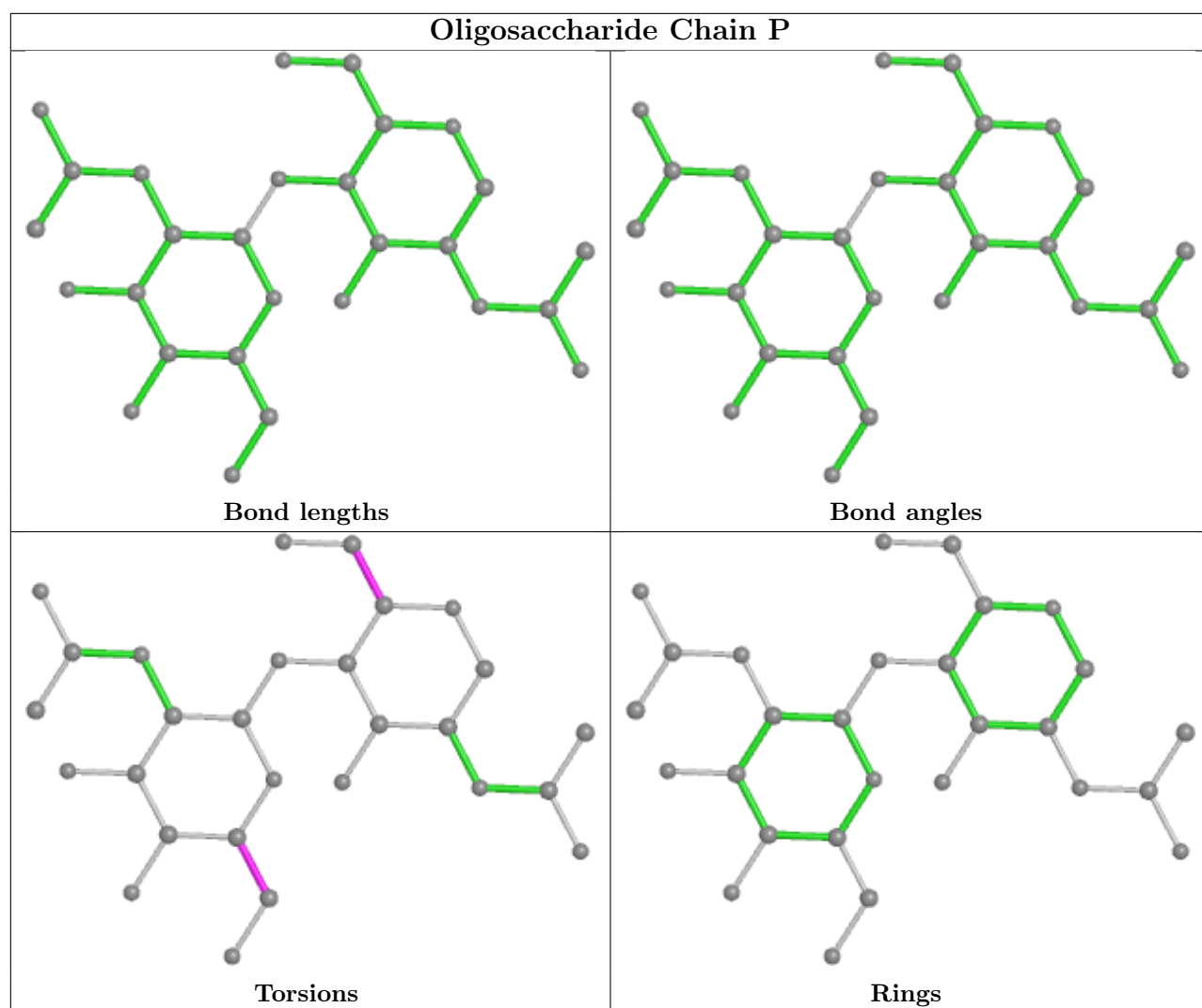


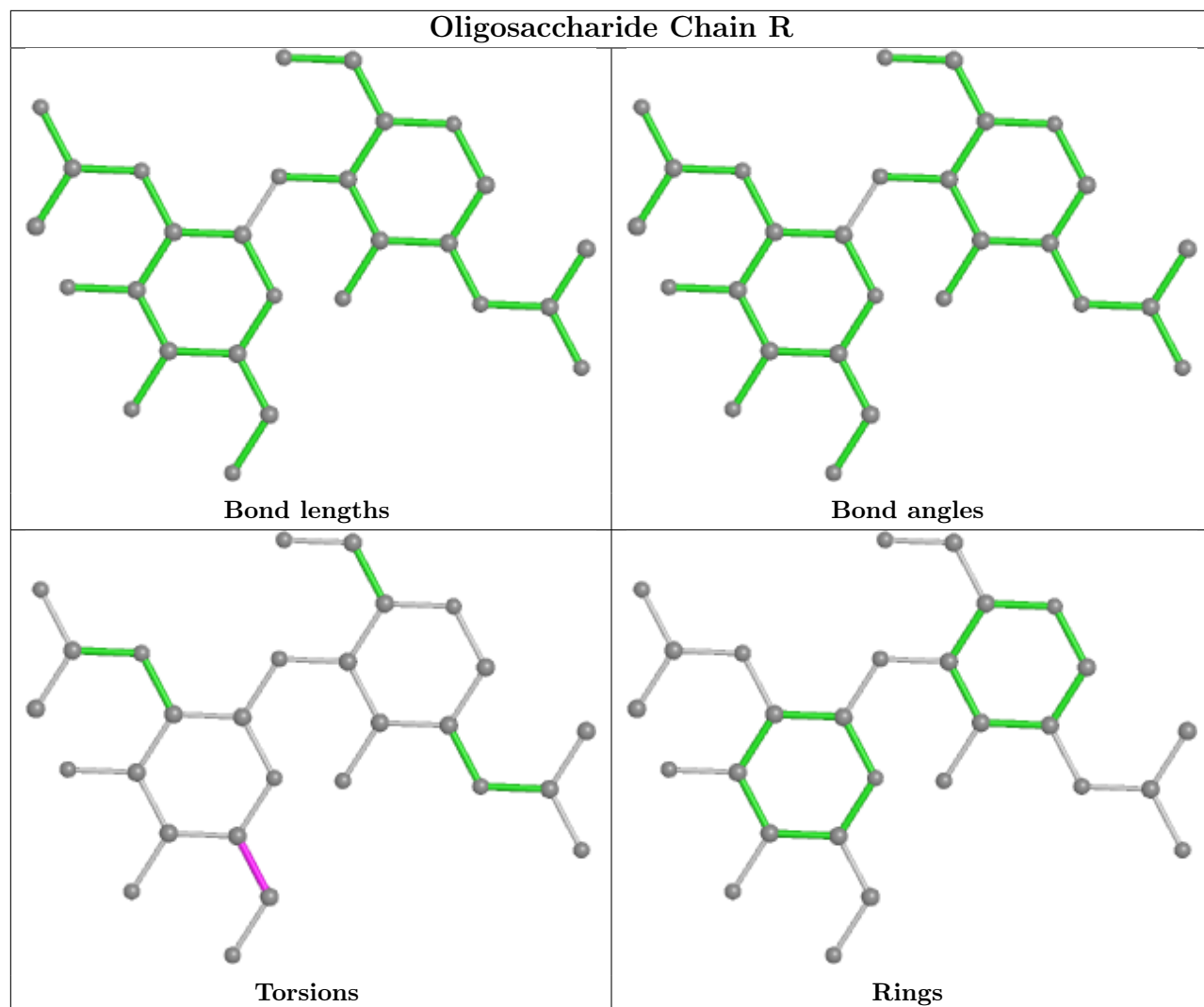


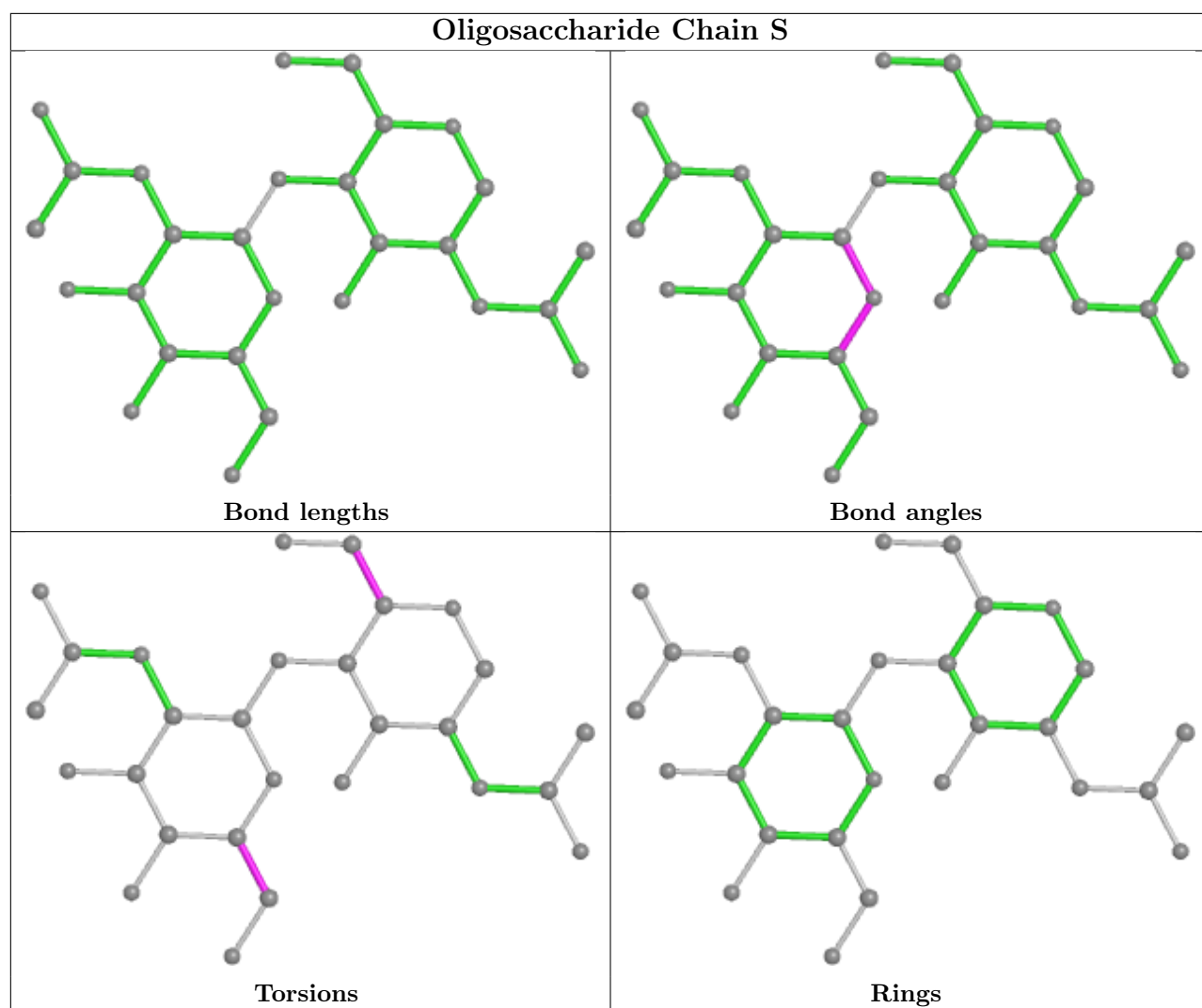


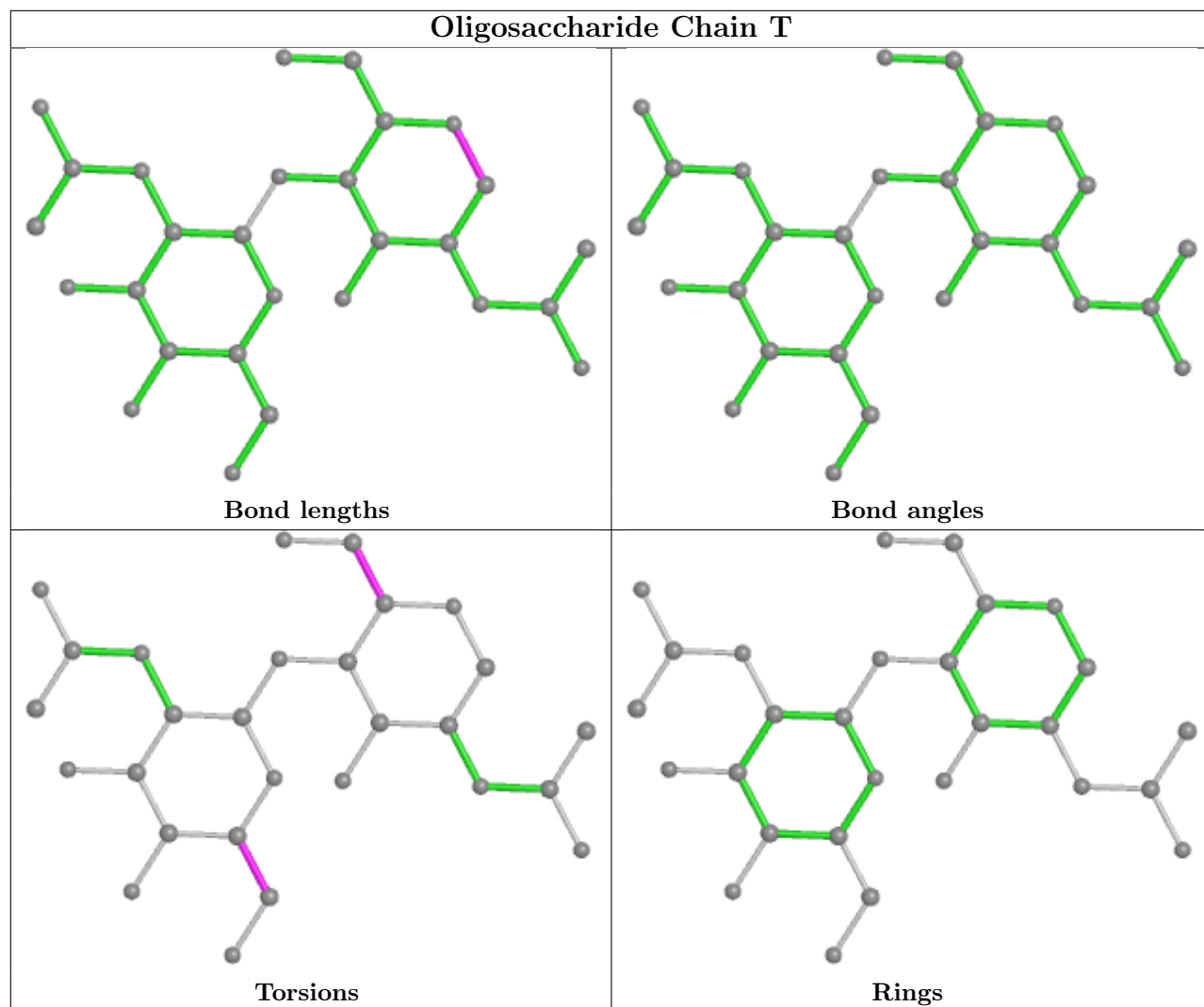


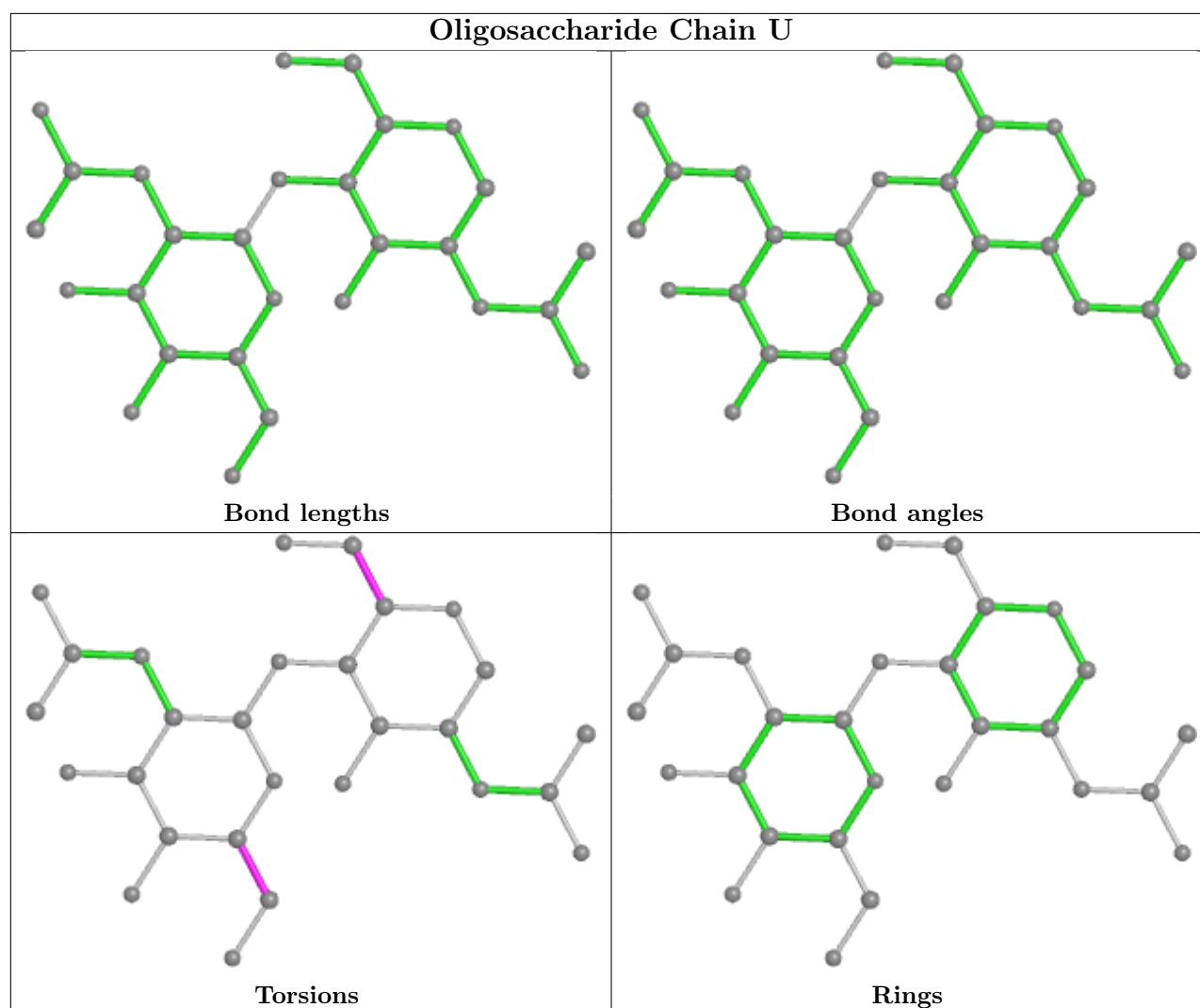












## 5.6 Ligand geometry [i](#)

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	B	2010	1	14,14,15	0.44	0	17,19,21	0.50	0
5	NAG	A	2015	1	14,14,15	0.45	0	17,19,21	0.65	1 (5%)
5	NAG	B	2011	1	14,14,15	0.30	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	2015	1	14,14,15	0.22	0	17,19,21	0.55	0
5	NAG	C	2013	1	14,14,15	0.25	0	17,19,21	0.62	1 (5%)
5	NAG	B	2017	1	14,14,15	0.40	0	17,19,21	0.56	0
5	NAG	C	2004	1	14,14,15	0.26	0	17,19,21	0.51	0
5	NAG	B	2008	1	14,14,15	0.58	0	17,19,21	0.77	1 (5%)
5	NAG	A	2003	1	14,14,15	0.27	0	17,19,21	0.66	1 (5%)
5	NAG	C	2011	1	14,14,15	0.31	0	17,19,21	0.49	0
5	NAG	C	2001	1	14,14,15	0.33	0	17,19,21	0.63	1 (5%)
5	NAG	A	2011	1	14,14,15	0.34	0	17,19,21	0.43	0
5	NAG	B	2001	1	14,14,15	0.40	0	17,19,21	1.17	2 (11%)
5	NAG	A	2001	1	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	A	2007	1	14,14,15	0.30	0	17,19,21	0.50	0
5	NAG	B	2007	1	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	B	2009	1	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
5	NAG	C	2015	1	14,14,15	0.39	0	17,19,21	0.47	0
5	NAG	C	2006	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	A	2006	1	14,14,15	0.43	0	17,19,21	0.41	0
5	NAG	A	2016	1	14,14,15	0.26	0	17,19,21	0.54	0
5	NAG	C	2017	1	14,14,15	0.25	0	17,19,21	0.50	0
5	NAG	C	2009	1	14,14,15	0.35	0	17,19,21	0.94	1 (5%)
5	NAG	C	2007	1	14,14,15	0.45	0	17,19,21	0.45	0
5	NAG	B	2016	1	14,14,15	0.48	0	17,19,21	0.57	0
5	NAG	B	2006	1	14,14,15	0.38	0	17,19,21	0.61	1 (5%)
5	NAG	C	2003	1	14,14,15	0.32	0	17,19,21	0.35	0
5	NAG	A	2005	1	14,14,15	0.45	0	17,19,21	0.39	0
5	NAG	B	2005	1	14,14,15	0.19	0	17,19,21	0.60	0
5	NAG	C	2002	1	14,14,15	0.39	0	17,19,21	0.67	1 (5%)
5	NAG	C	2010	1	14,14,15	0.29	0	17,19,21	0.48	0
5	NAG	A	2009	1	14,14,15	0.36	0	17,19,21	0.94	1 (5%)
5	NAG	B	2012	1	14,14,15	0.36	0	17,19,21	0.82	1 (5%)
5	NAG	C	2014	1	14,14,15	0.46	0	17,19,21	0.64	1 (5%)
5	NAG	A	2008	1	14,14,15	0.57	0	17,19,21	0.77	1 (5%)
5	NAG	A	2002	1	14,14,15	0.36	0	17,19,21	0.60	1 (5%)
5	NAG	C	2005	1	14,14,15	0.24	0	17,19,21	0.47	0
5	NAG	A	2013	1	14,14,15	0.40	0	17,19,21	0.42	0
5	NAG	C	2012	1	14,14,15	0.22	0	17,19,21	0.67	1 (5%)
5	NAG	A	2014	1	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	A	2004	1	14,14,15	0.37	0	17,19,21	0.53	0
5	NAG	B	2014	1	14,14,15	0.32	0	17,19,21	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	B	2003	1	14,14,15	0.46	0	17,19,21	0.36	0
5	NAG	C	2016	1	14,14,15	0.34	0	17,19,21	0.65	1 (5%)
5	NAG	C	2008	1	14,14,15	0.57	0	17,19,21	0.77	1 (5%)
5	NAG	B	2002	1	14,14,15	0.36	0	17,19,21	0.54	0
5	NAG	A	2010	1	14,14,15	0.50	0	17,19,21	0.44	0
5	NAG	B	2013	1	14,14,15	0.49	0	17,19,21	0.49	0
5	NAG	A	2012	1	14,14,15	0.21	0	17,19,21	0.74	1 (5%)
5	NAG	B	2004	1	14,14,15	0.29	0	17,19,21	0.46	0
5	NAG	A	2017	1	14,14,15	0.35	0	17,19,21	0.47	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
5	NAG	B	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2015	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2011	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2015	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2013	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2017	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2008	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	2011	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2001	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	2001	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2001	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	2007	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2009	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2015	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2006	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2006	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2016	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2017	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	C	2009	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2007	1	-	0/6/23/26	0/1/1/1
5	NAG	B	2016	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2006	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2005	1	-	0/6/23/26	0/1/1/1
5	NAG	C	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2009	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	2014	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2008	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2002	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2005	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2013	1	-	1/6/23/26	0/1/1/1
5	NAG	C	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	A	2004	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2014	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2003	1	-	2/6/23/26	0/1/1/1
5	NAG	C	2016	1	-	0/6/23/26	0/1/1/1
5	NAG	C	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	A	2010	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2013	1	-	1/6/23/26	0/1/1/1
5	NAG	A	2012	1	-	2/6/23/26	0/1/1/1
5	NAG	B	2004	1	-	0/6/23/26	0/1/1/1
5	NAG	A	2017	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2009	NAG	C1-O5-C5	3.34	116.72	112.19
5	B	2009	NAG	C1-O5-C5	3.34	116.71	112.19
5	C	2009	NAG	C1-O5-C5	3.32	116.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2012	NAG	C1-O5-C5	2.92	116.16	112.19
5	A	2008	NAG	C1-O5-C5	2.73	115.89	112.19
5	C	2008	NAG	C1-O5-C5	2.73	115.89	112.19
5	B	2008	NAG	C1-O5-C5	2.72	115.88	112.19
5	A	2012	NAG	C1-O5-C5	2.54	115.64	112.19
5	C	2012	NAG	C1-O5-C5	2.38	115.42	112.19
5	C	2016	NAG	C1-O5-C5	2.32	115.34	112.19
5	B	2001	NAG	C8-C7-N2	2.32	120.03	116.10
5	C	2014	NAG	C1-O5-C5	2.30	115.31	112.19
5	A	2015	NAG	C1-O5-C5	2.21	115.19	112.19
5	C	2002	NAG	C1-O5-C5	2.18	115.14	112.19
5	C	2013	NAG	C1-O5-C5	2.17	115.13	112.19
5	C	2001	NAG	C1-O5-C5	2.15	115.10	112.19
5	A	2003	NAG	C1-O5-C5	2.14	115.09	112.19
5	A	2002	NAG	C1-O5-C5	2.14	115.09	112.19
5	B	2006	NAG	C1-O5-C5	2.07	114.99	112.19
5	B	2001	NAG	C2-N2-C7	-2.00	120.05	122.90

There are no chirality outliers.

All (76) torsion outliers are listed below:

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

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

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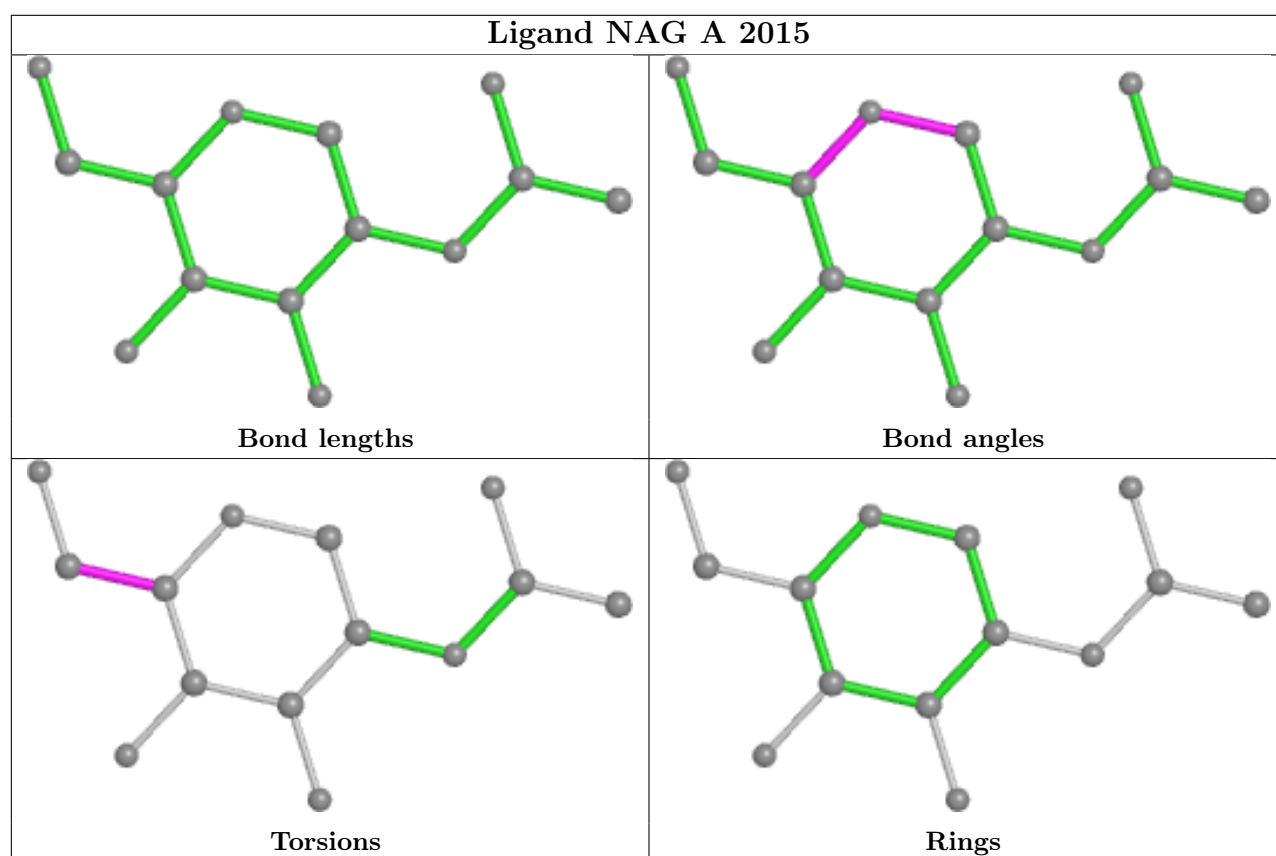
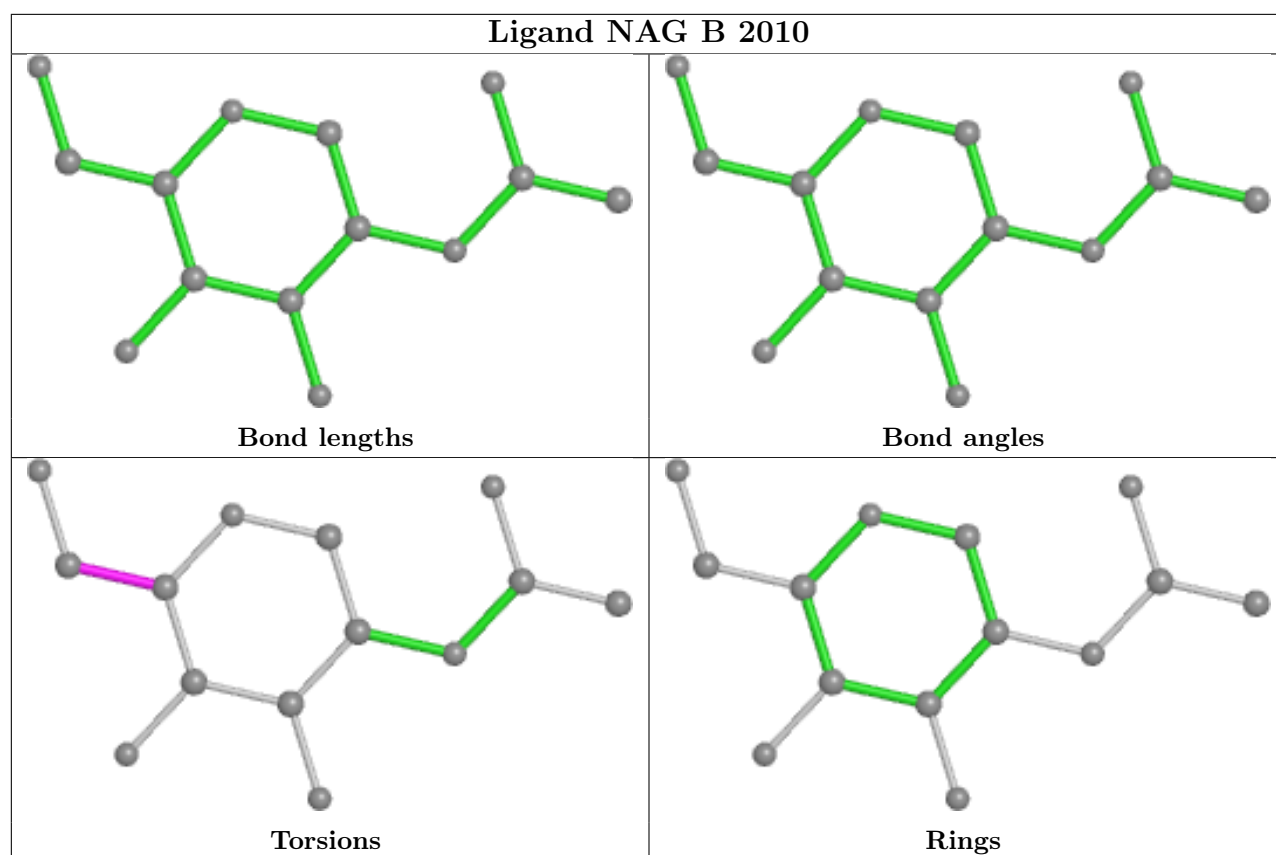
Mol	Chain	Res	Type	Atoms
5	A	2002	NAG	O5-C5-C6-O6
5	A	2014	NAG	C4-C5-C6-O6
5	A	2009	NAG	C4-C5-C6-O6
5	B	2009	NAG	C4-C5-C6-O6
5	C	2009	NAG	C4-C5-C6-O6
5	B	2015	NAG	O5-C5-C6-O6
5	A	2003	NAG	O5-C5-C6-O6
5	B	2015	NAG	C4-C5-C6-O6
5	A	2004	NAG	O5-C5-C6-O6
5	A	2013	NAG	O5-C5-C6-O6
5	A	2002	NAG	C4-C5-C6-O6
5	A	2006	NAG	C4-C5-C6-O6
5	B	2013	NAG	C4-C5-C6-O6
5	A	2017	NAG	C4-C5-C6-O6

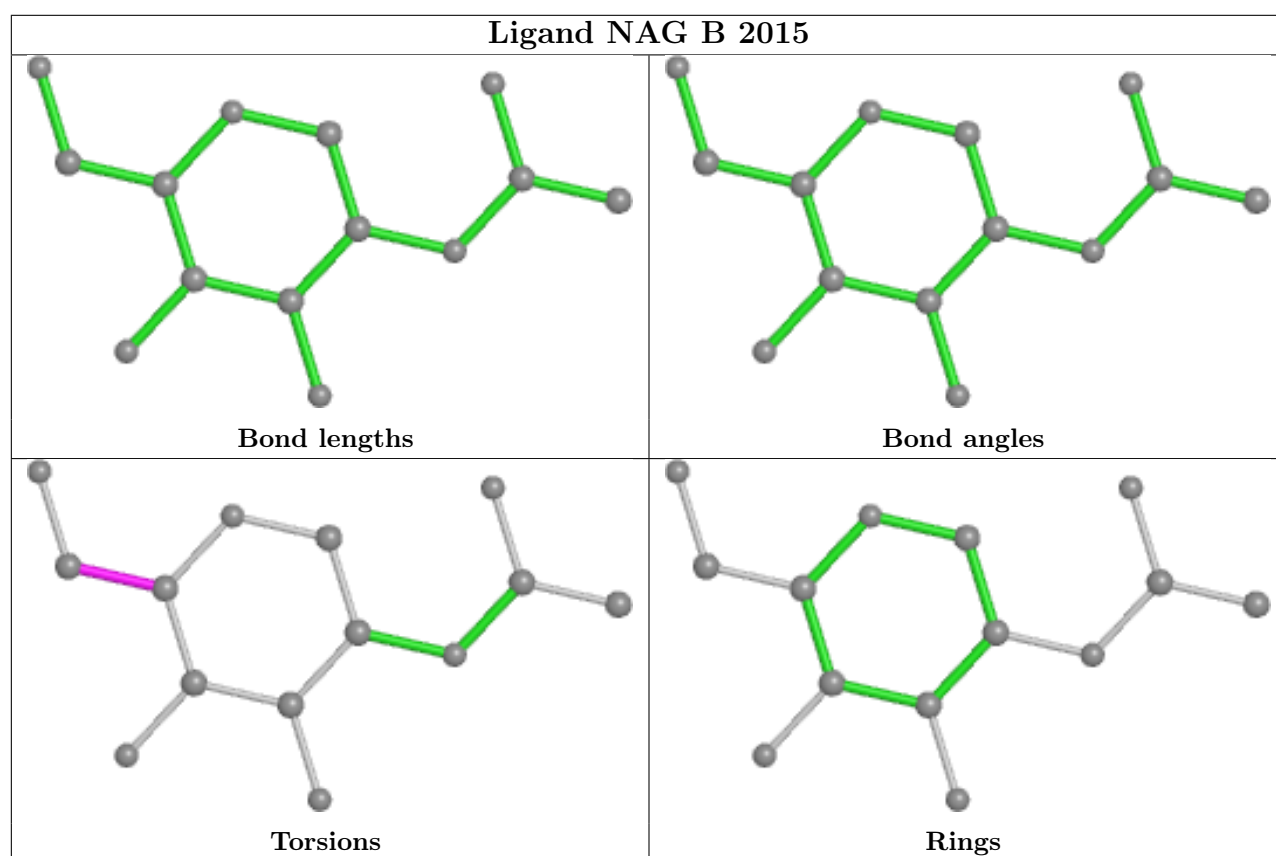
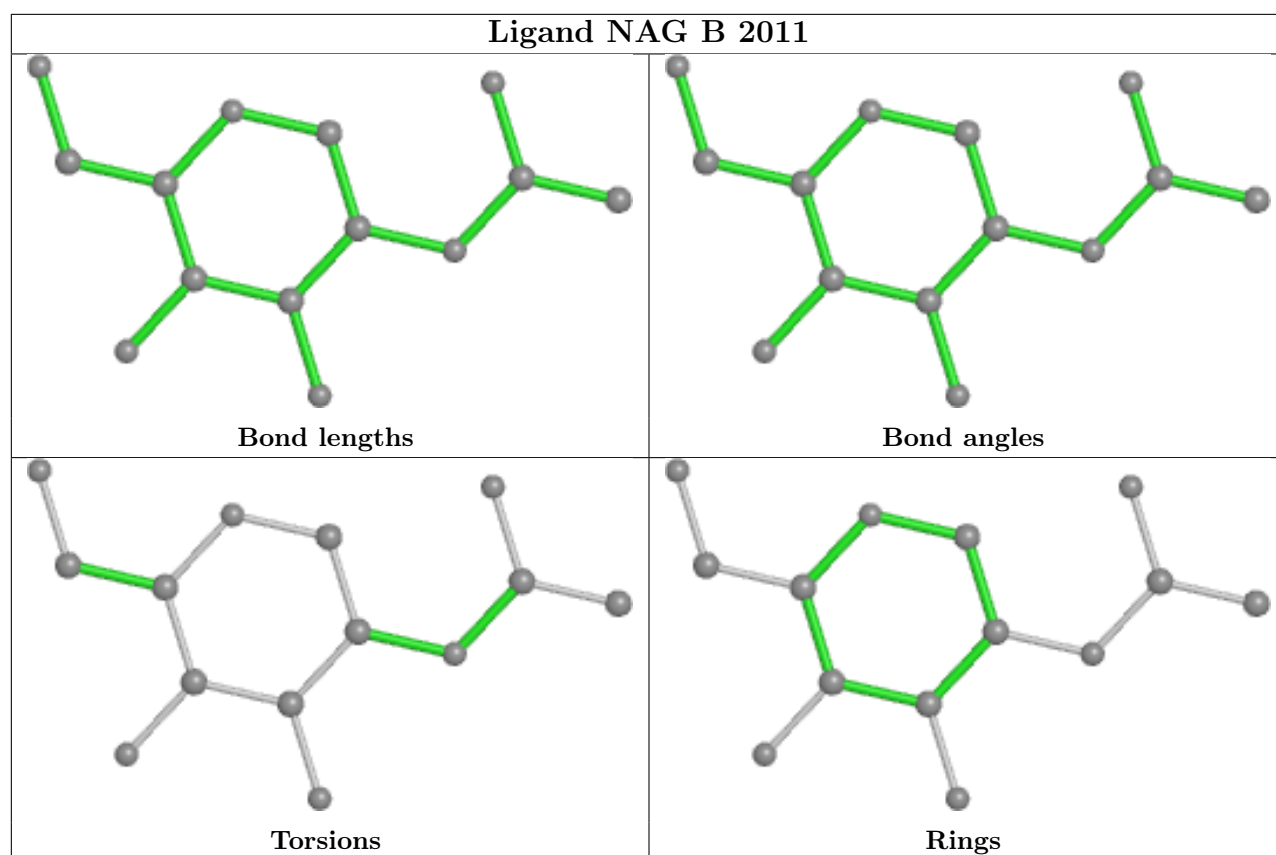
There are no ring outliers.

6 monomers are involved in 12 short contacts:

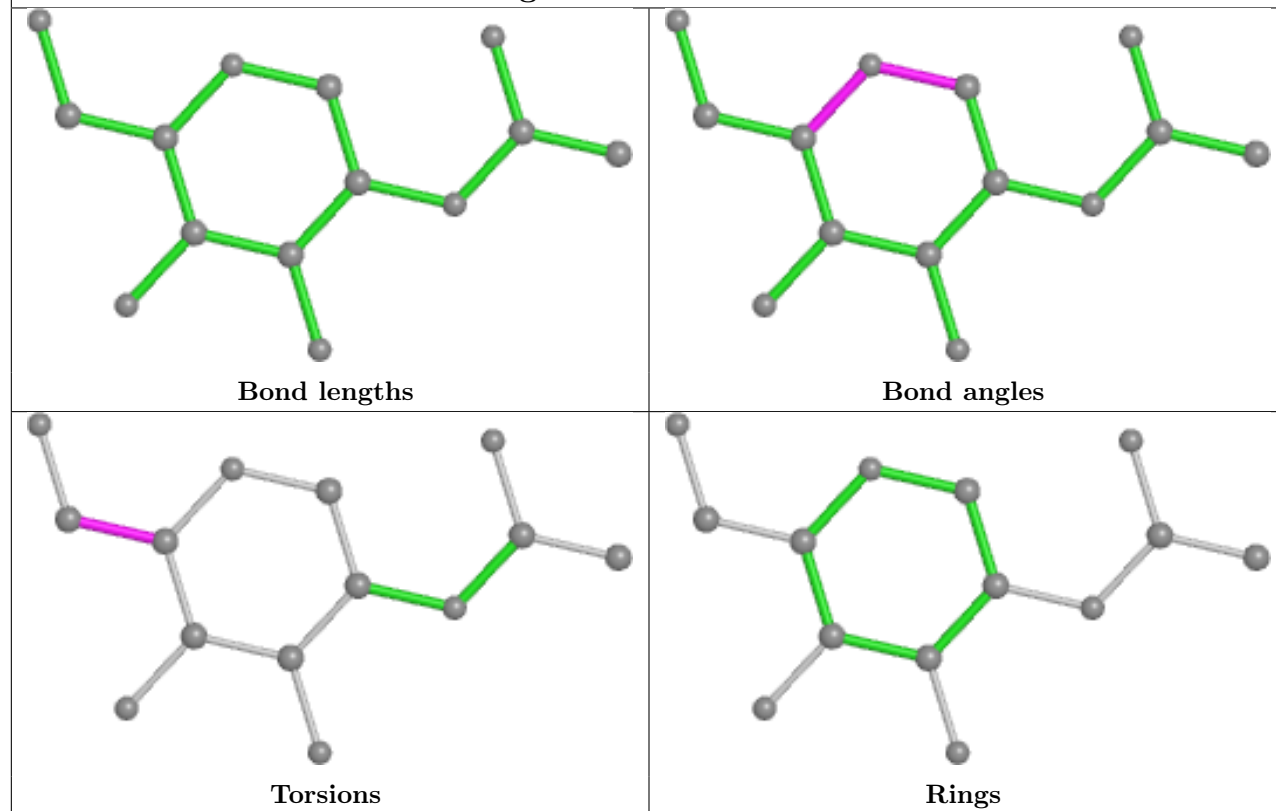
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	NAG	2	0
5	B	2001	NAG	3	0
5	A	2001	NAG	4	0
5	A	2006	NAG	1	0
5	A	2005	NAG	1	0
5	B	2005	NAG	1	0

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.

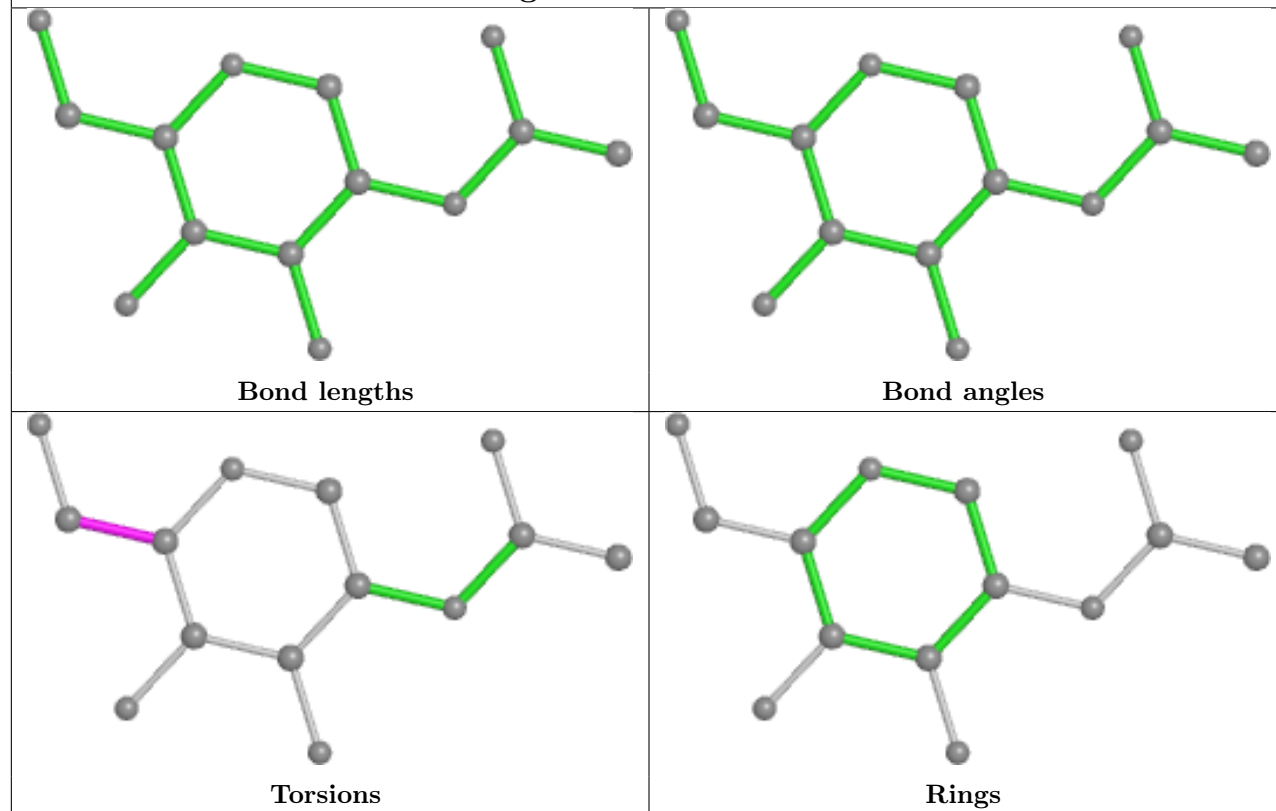


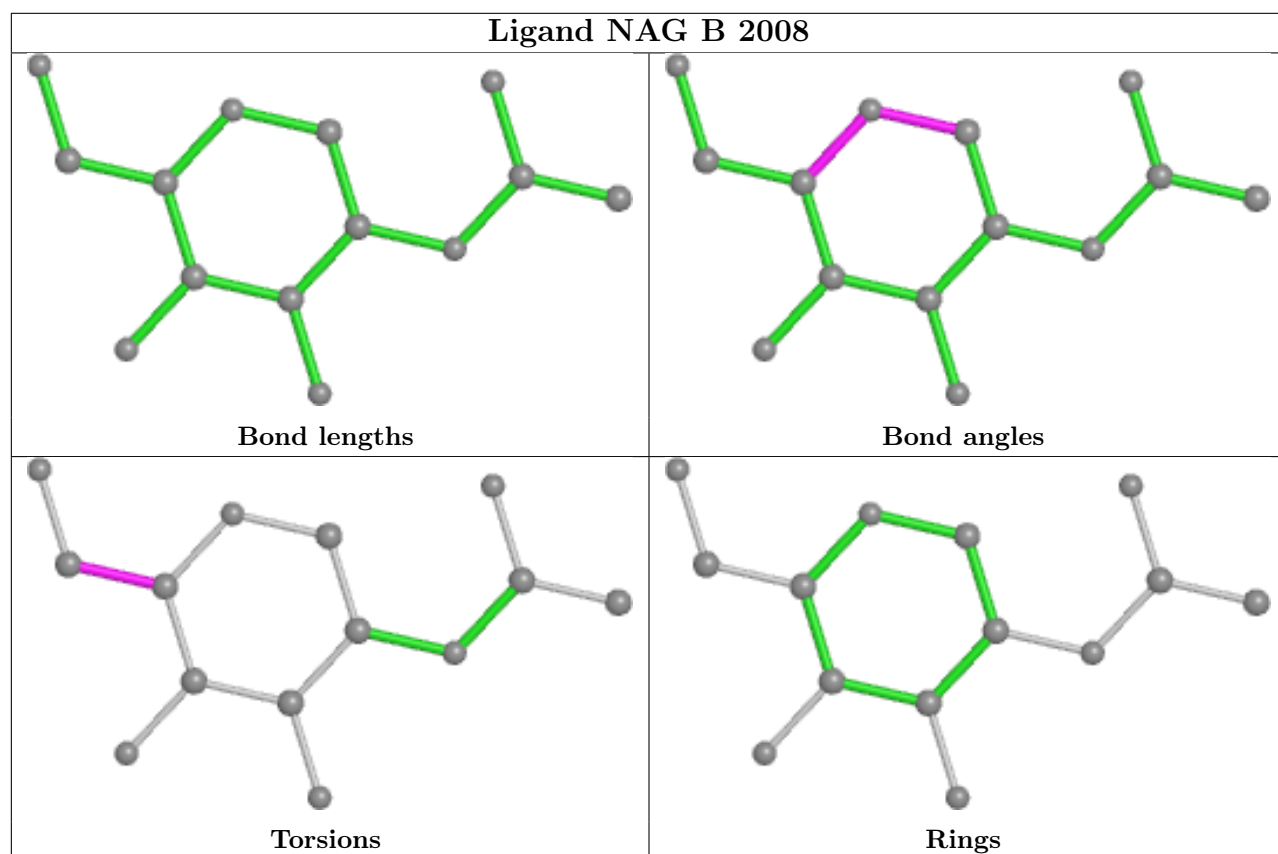
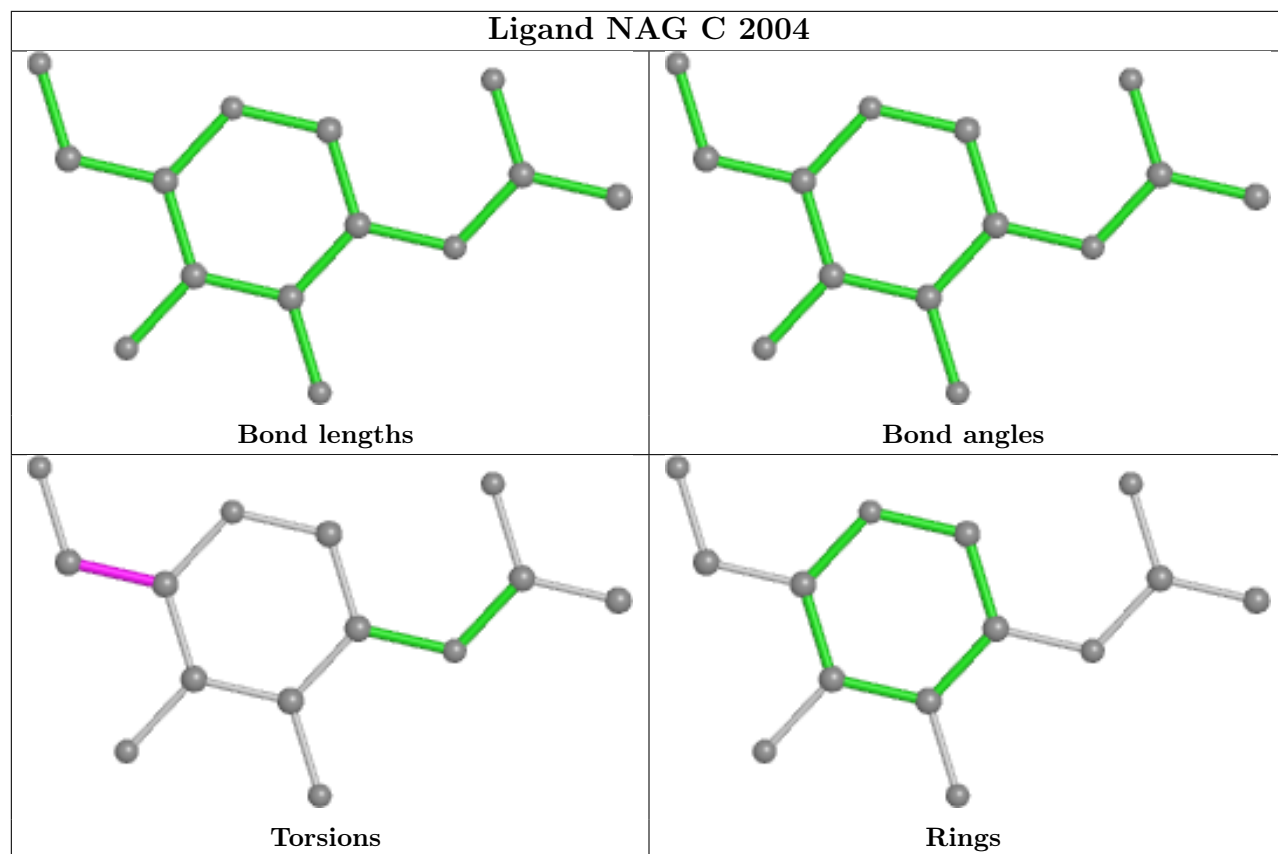


## Ligand NAG C 2013

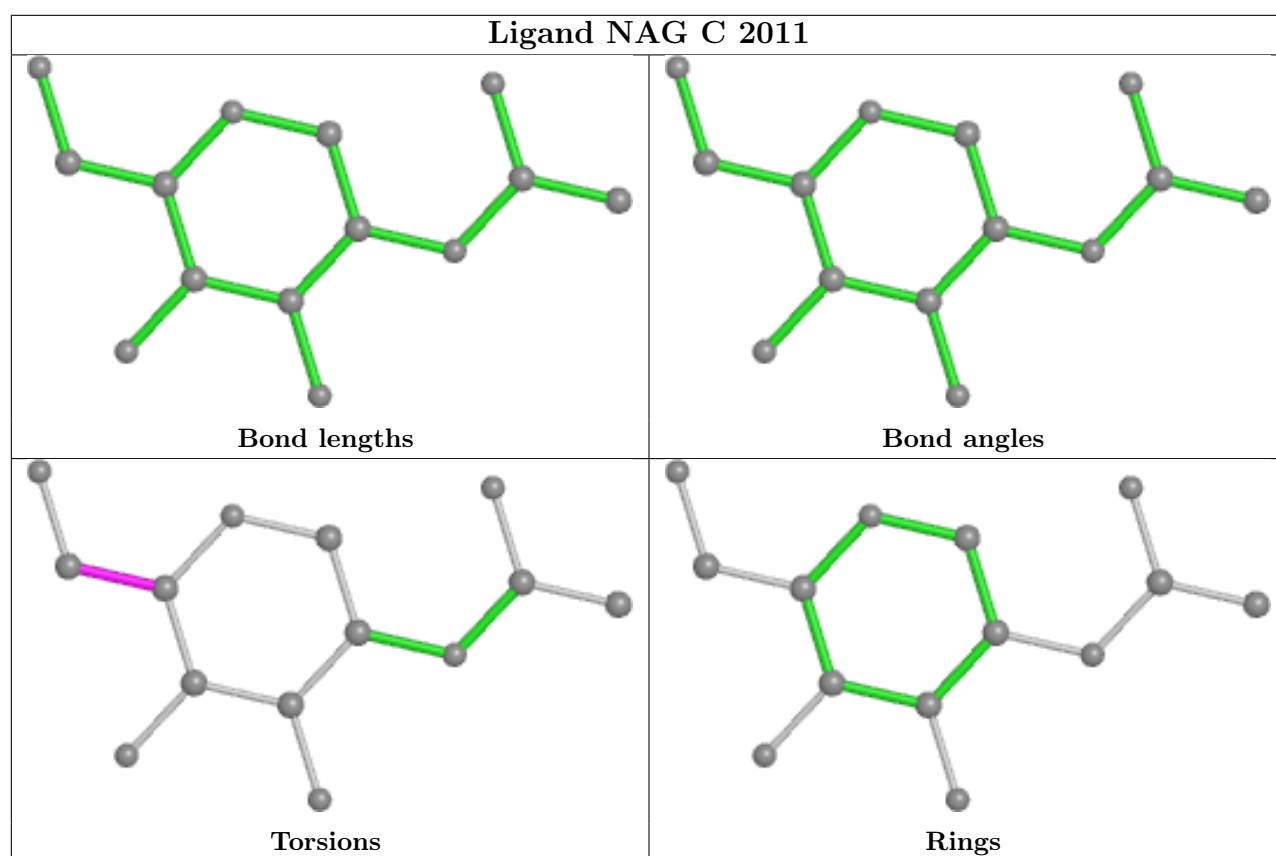
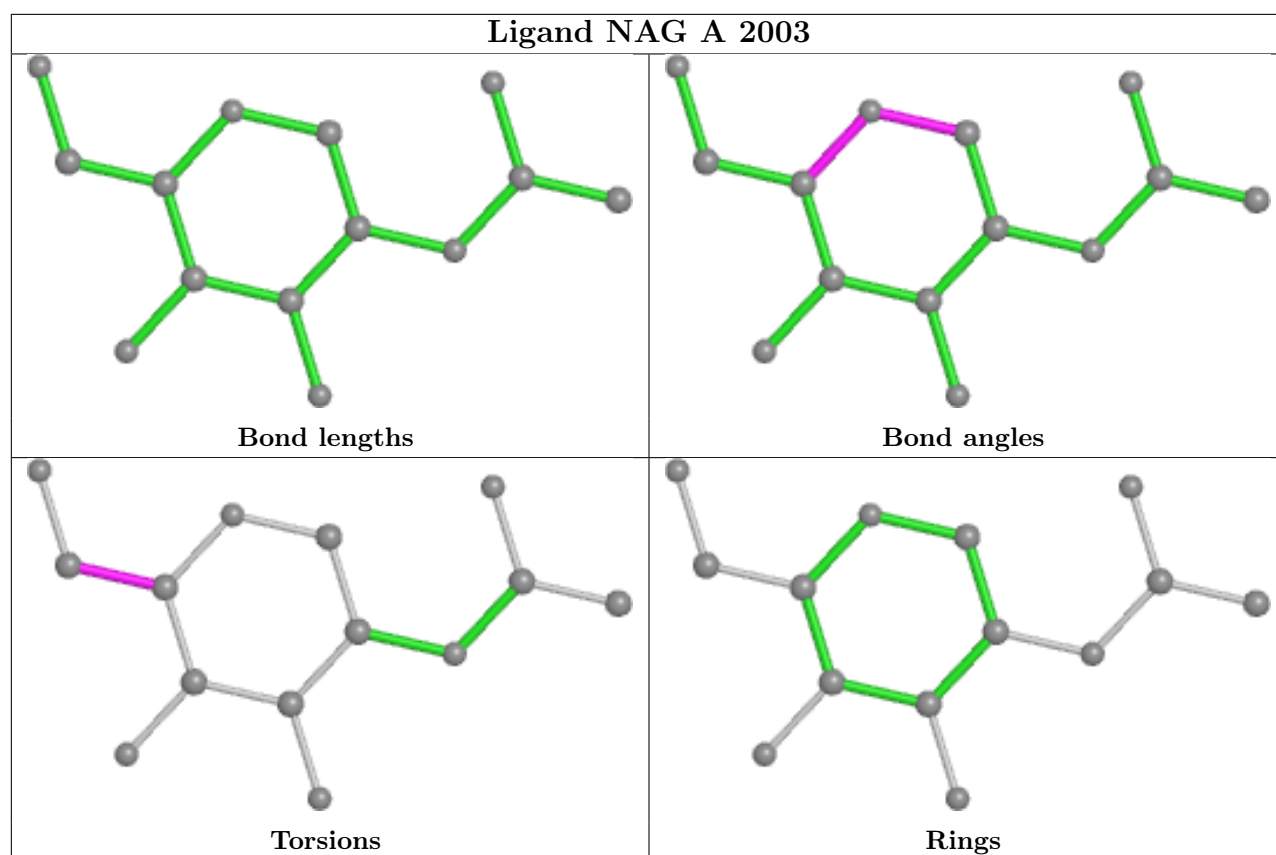


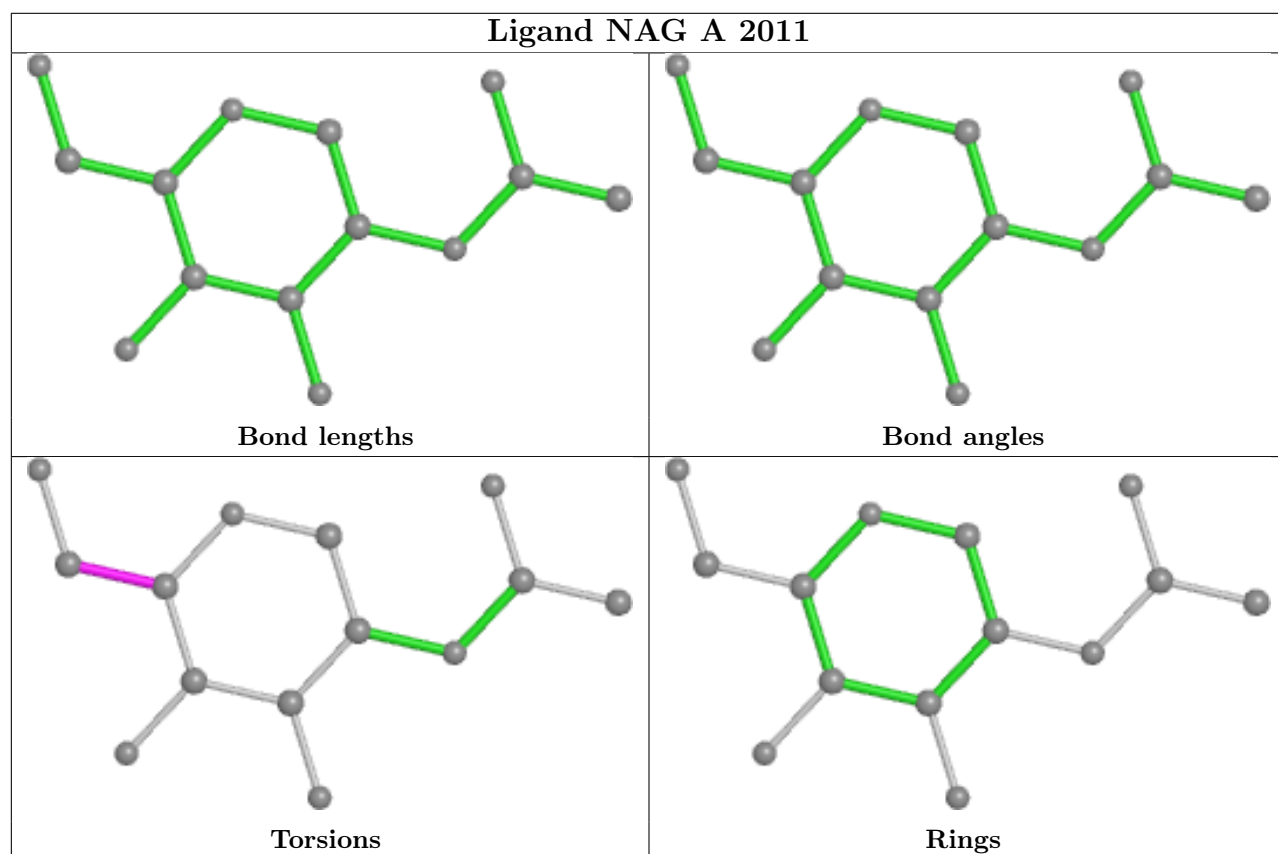
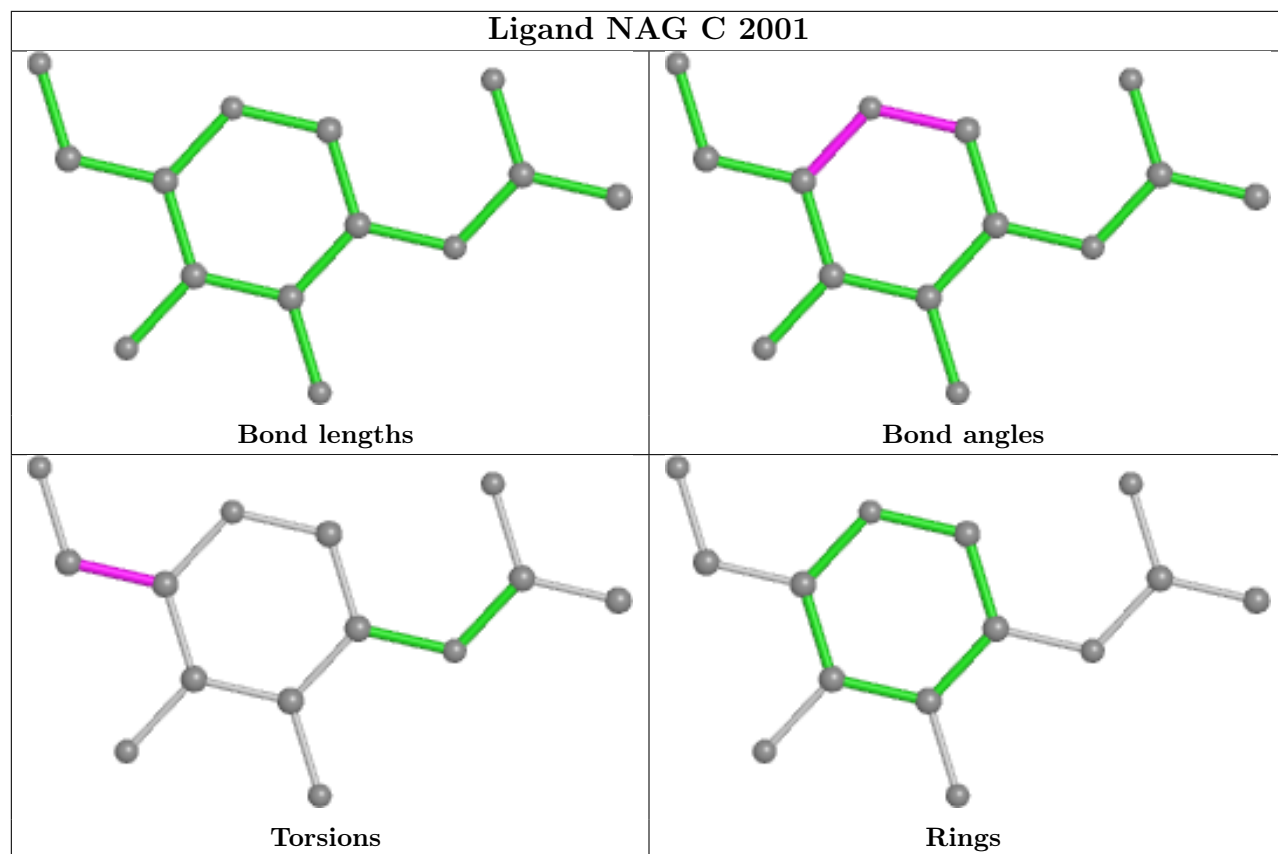
## Ligand NAG B 2017

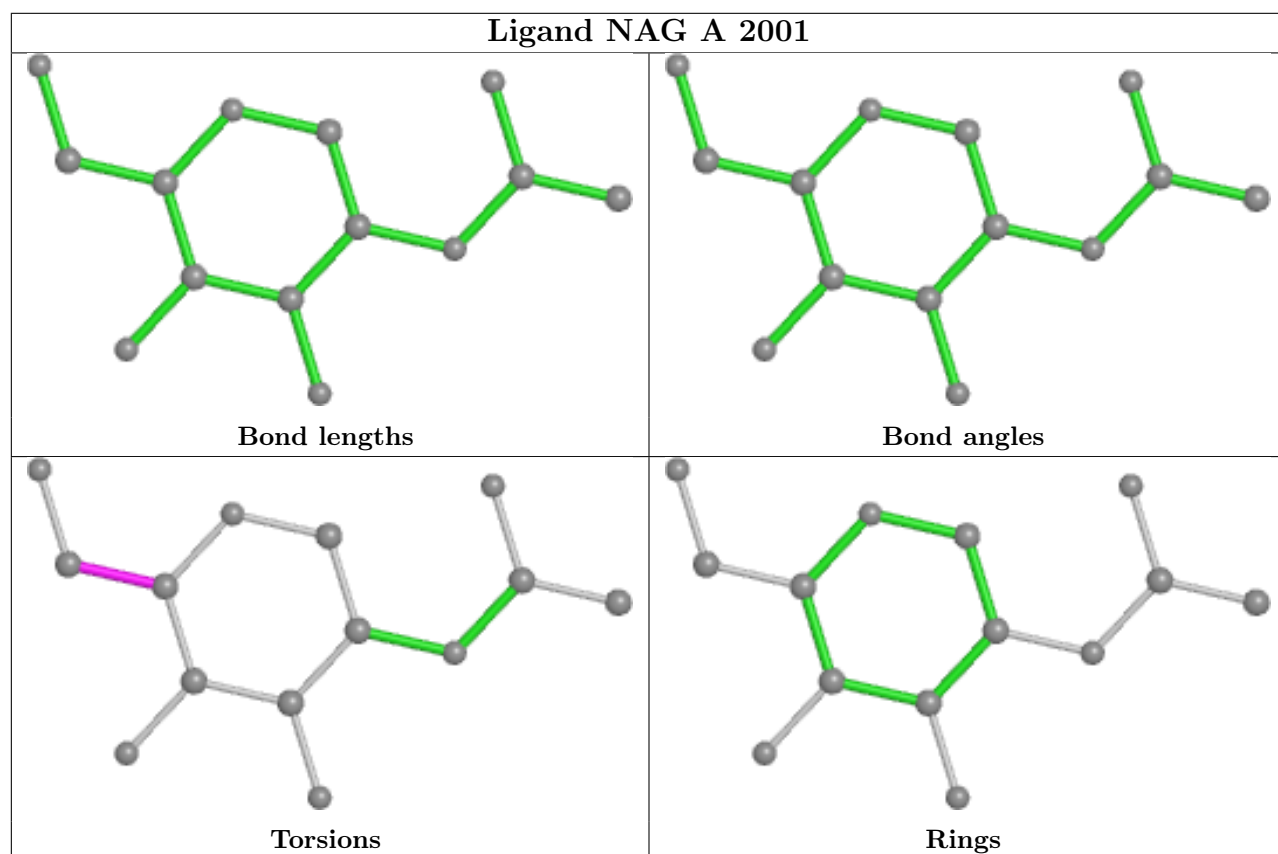
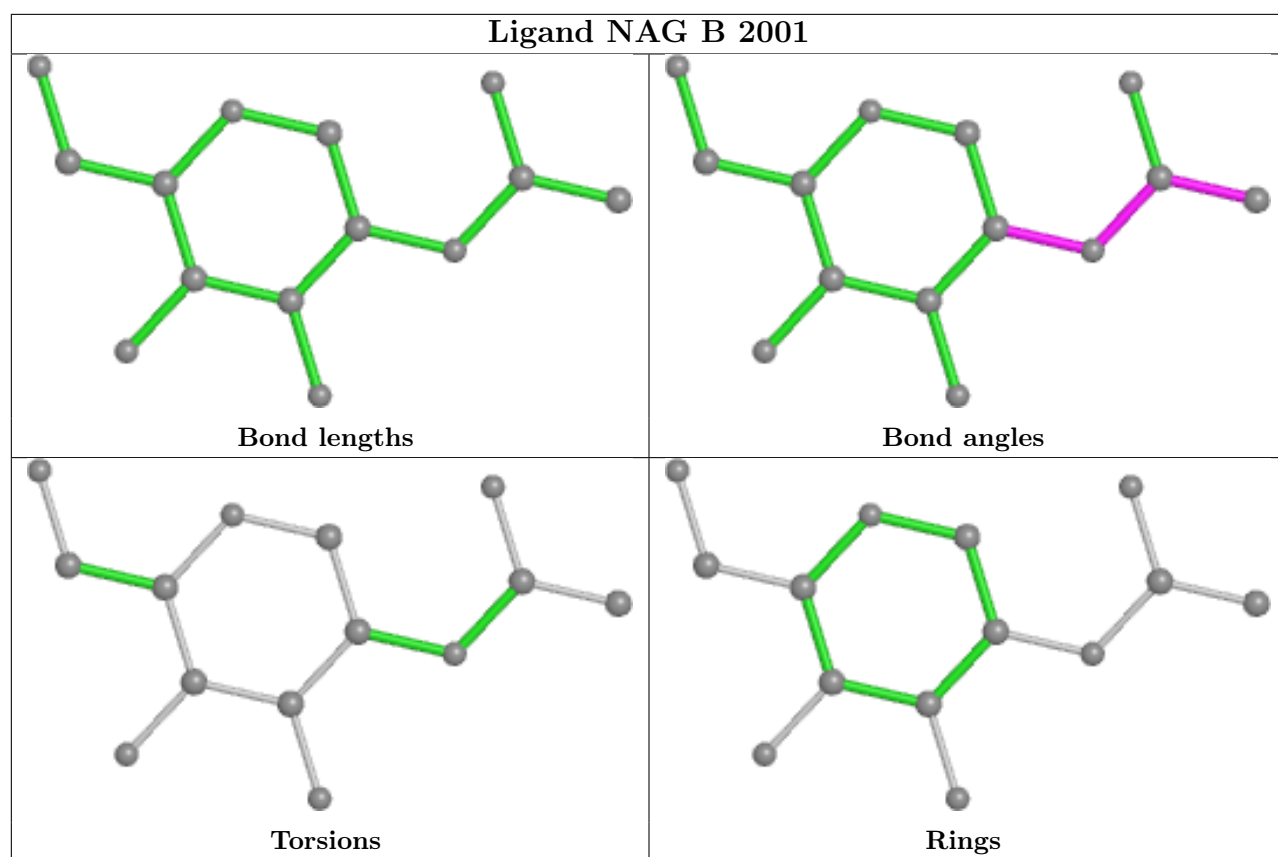


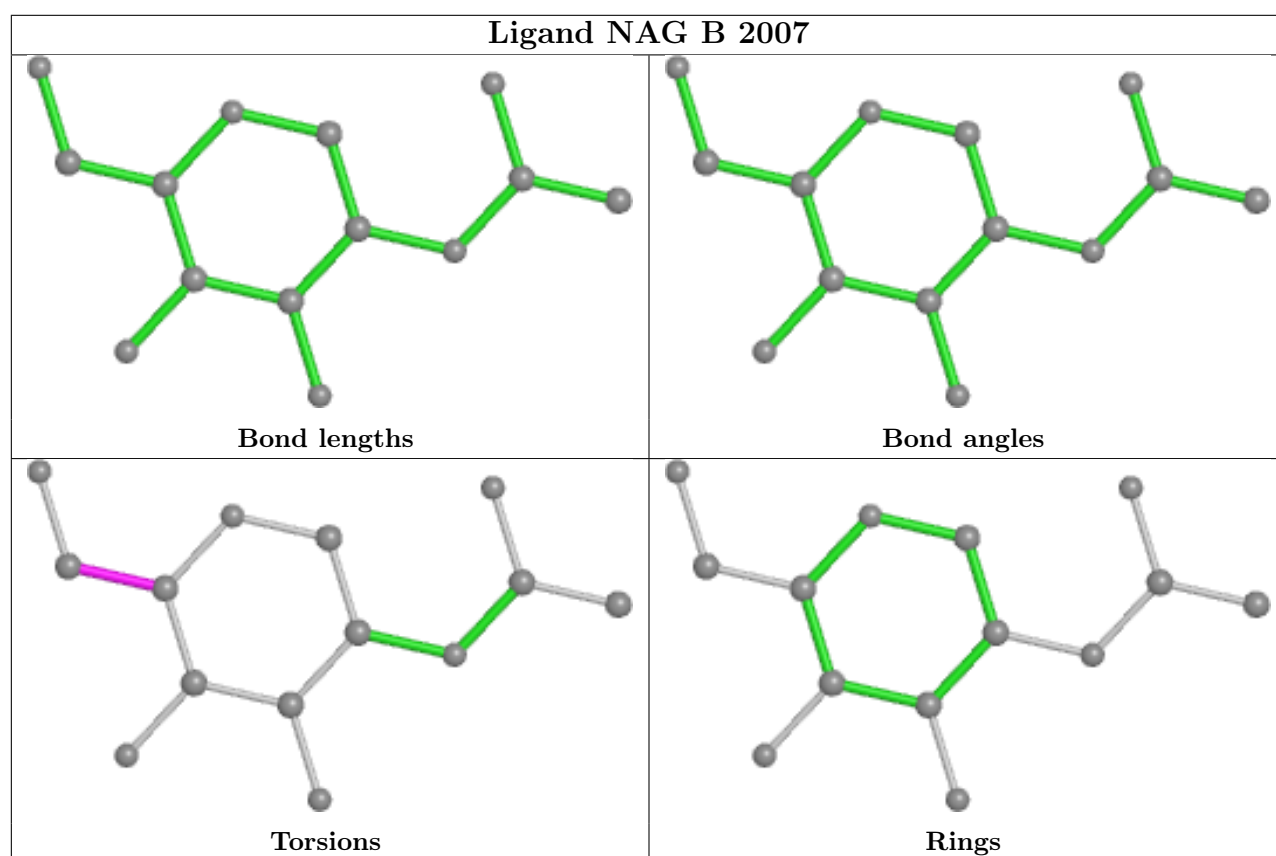
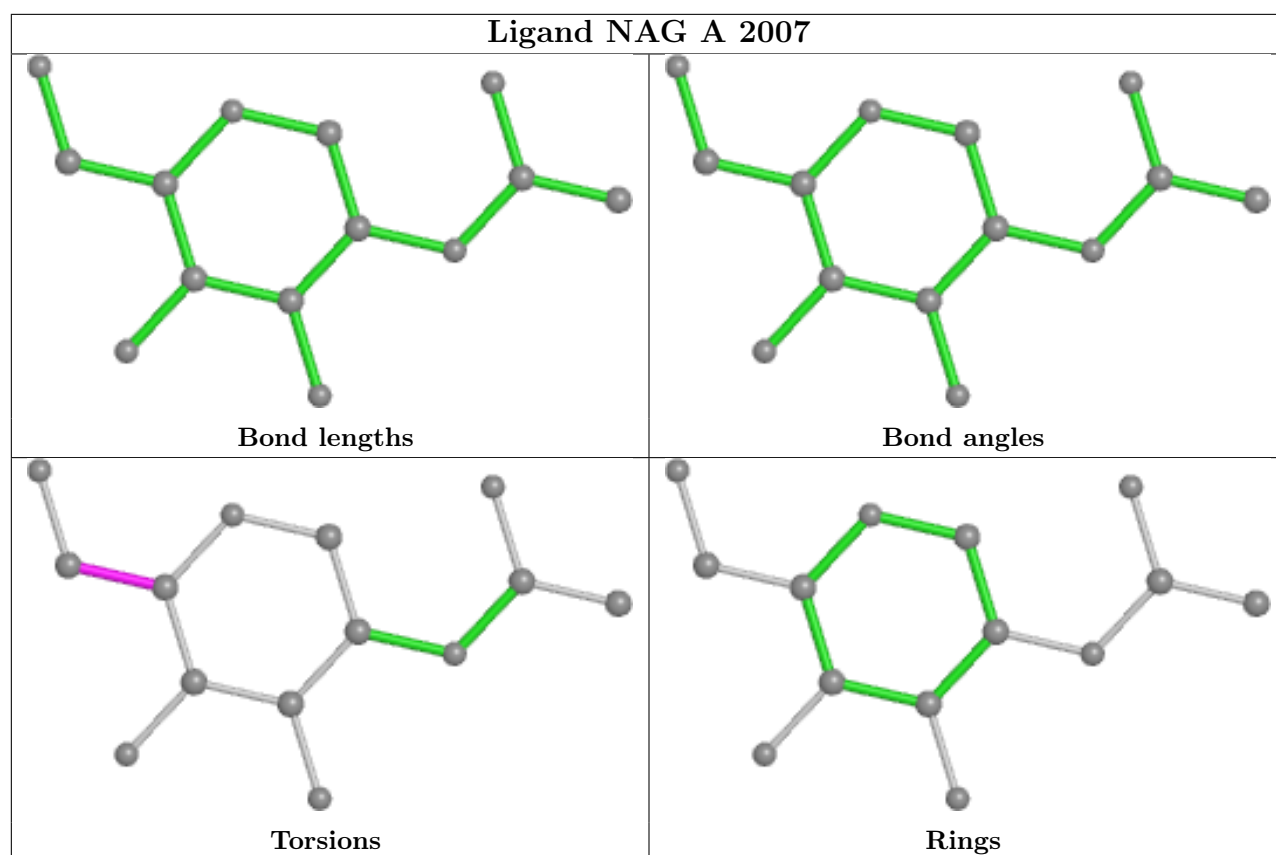


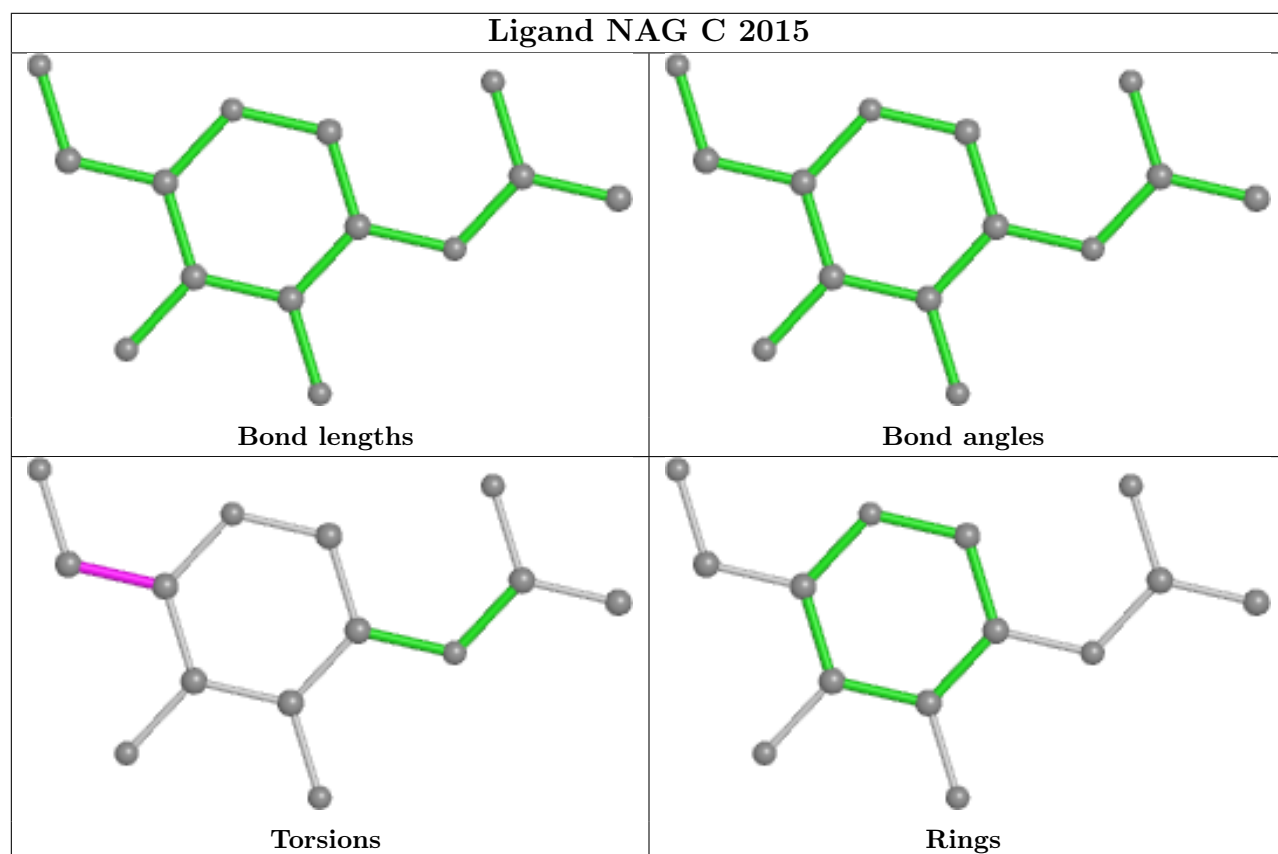
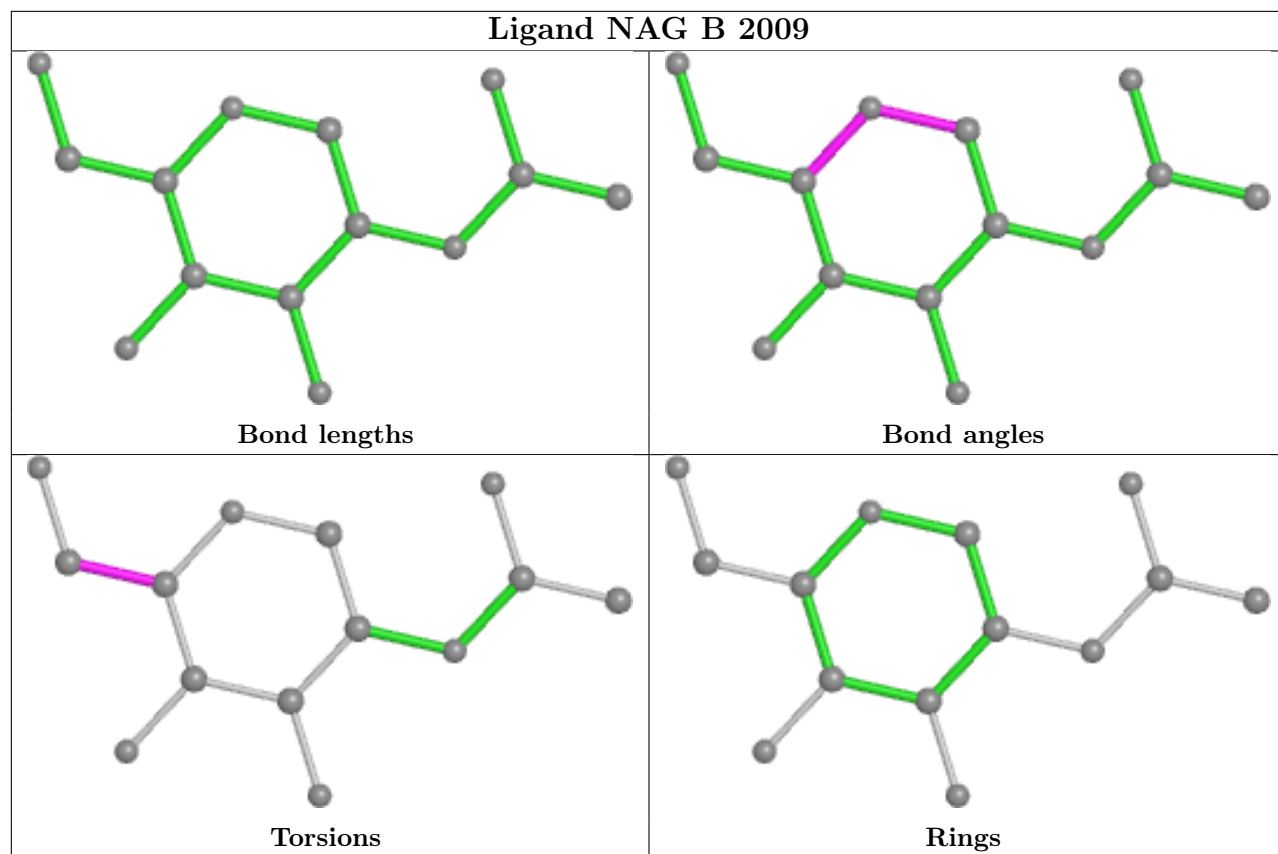


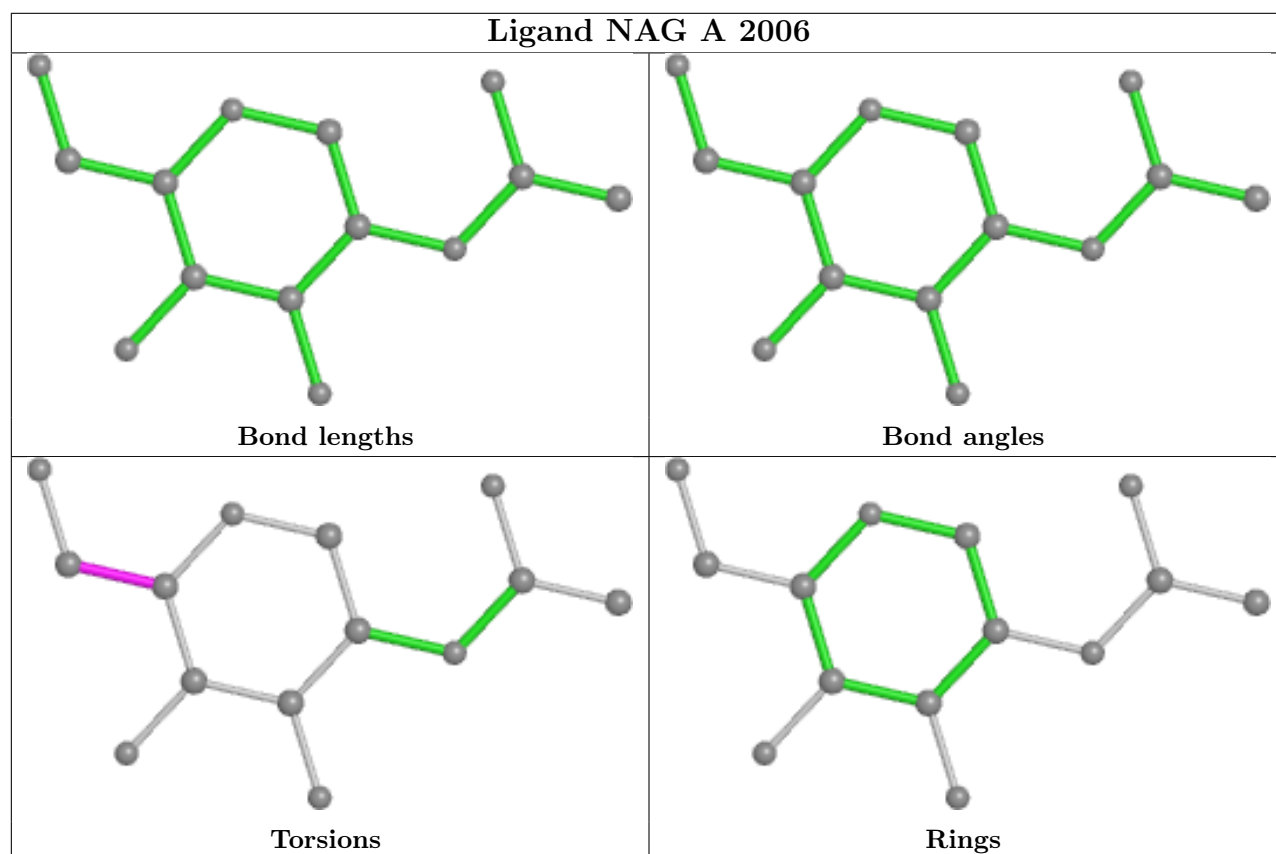
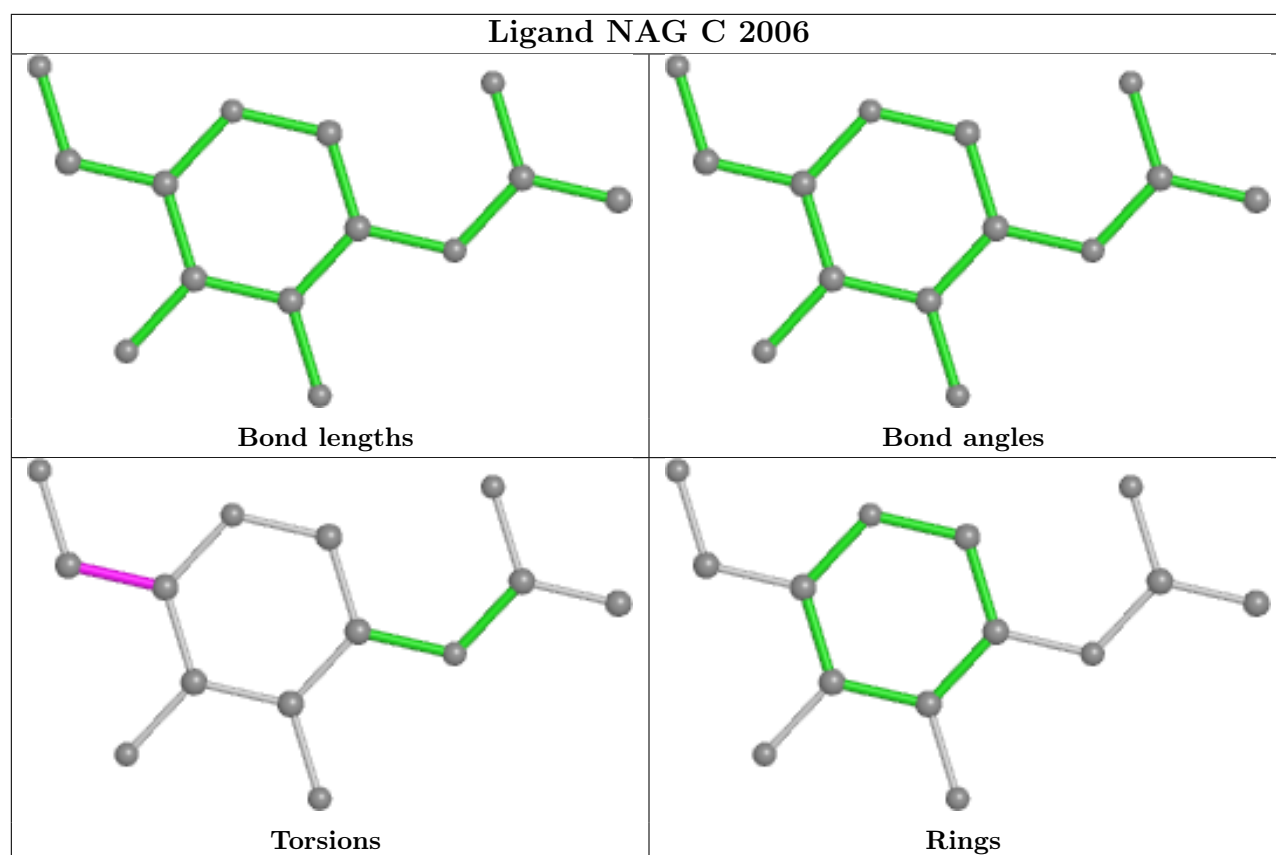


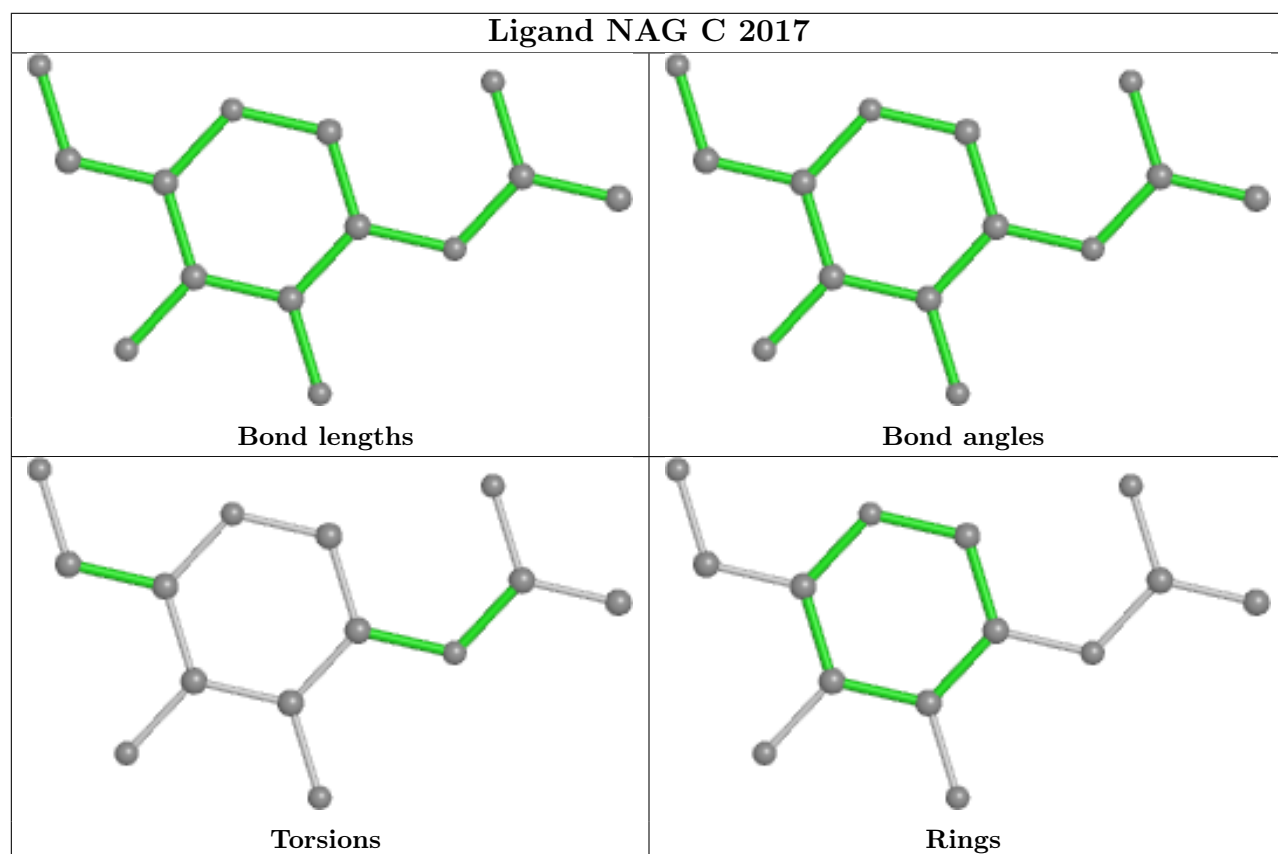
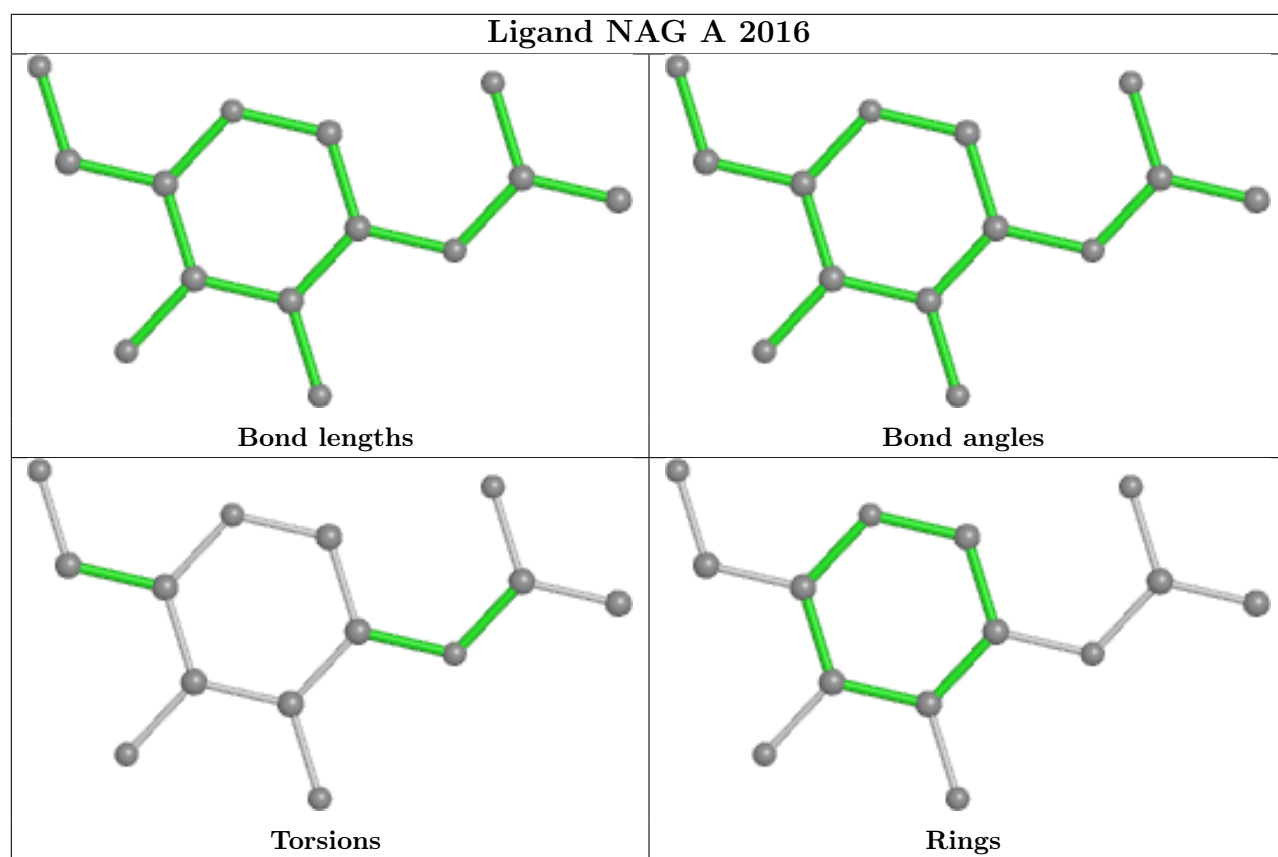


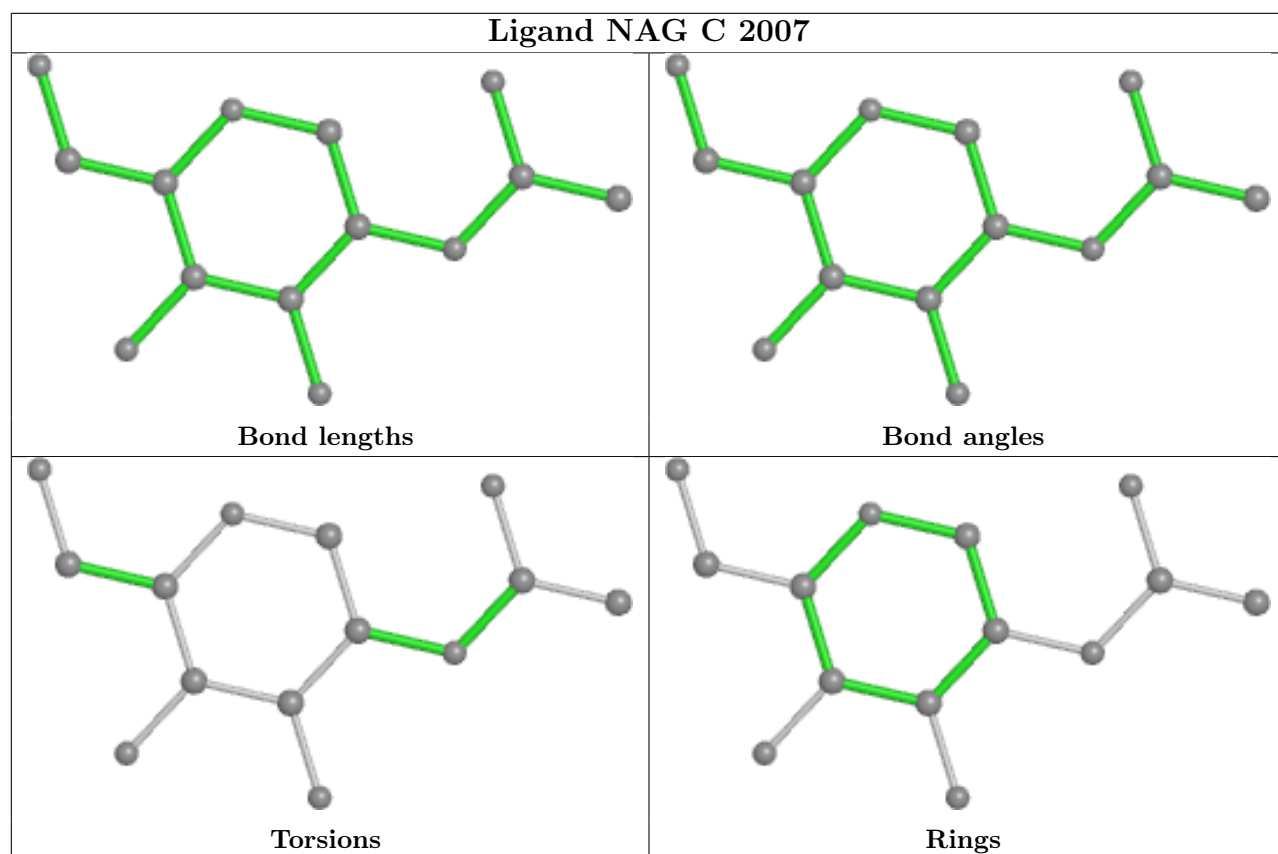
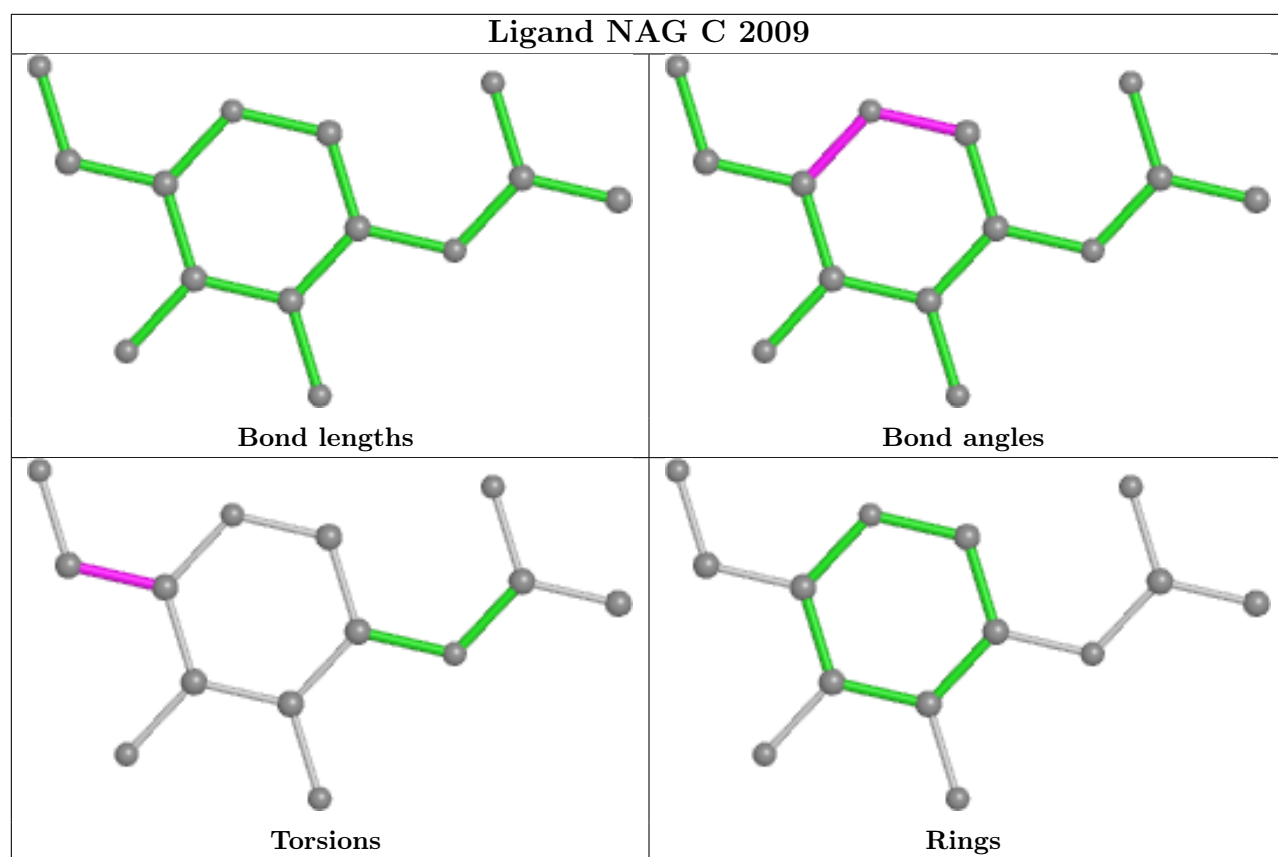




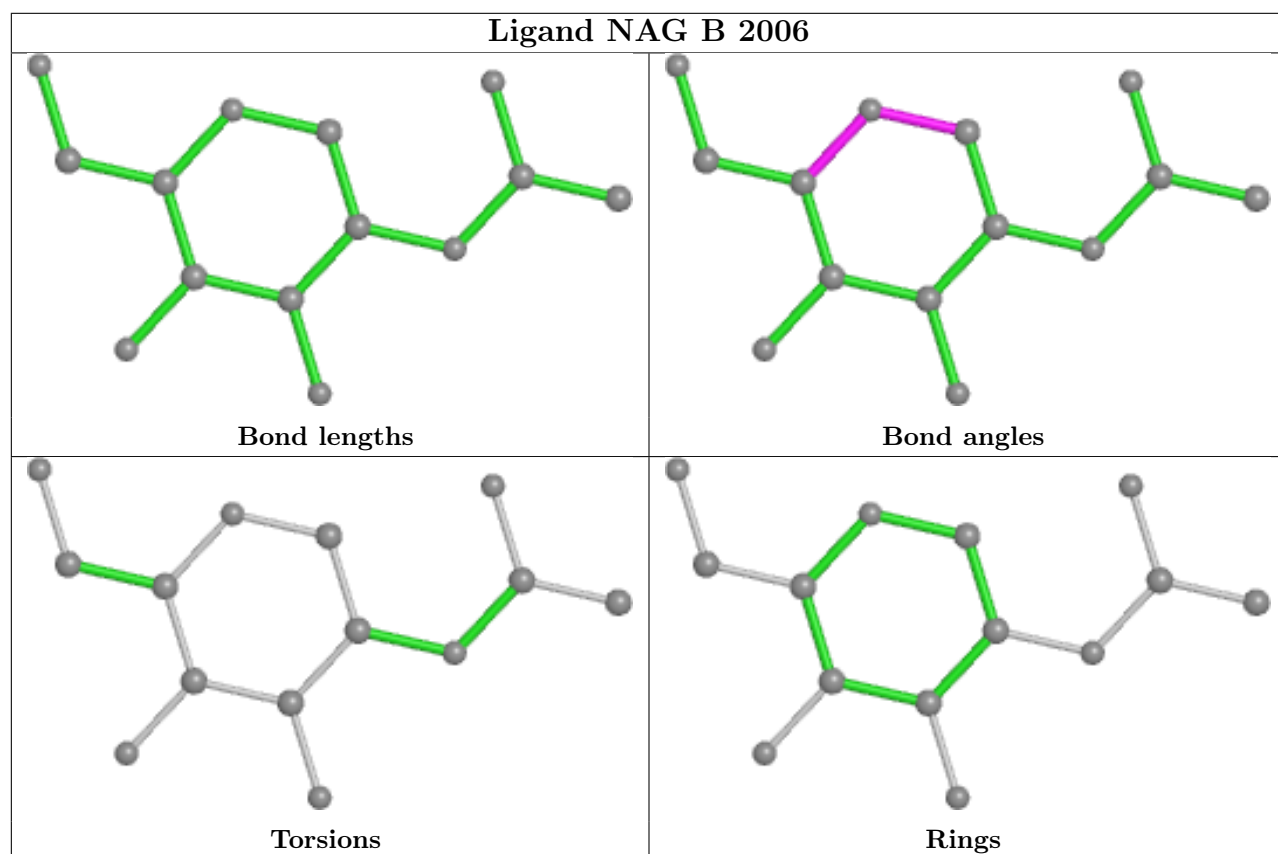
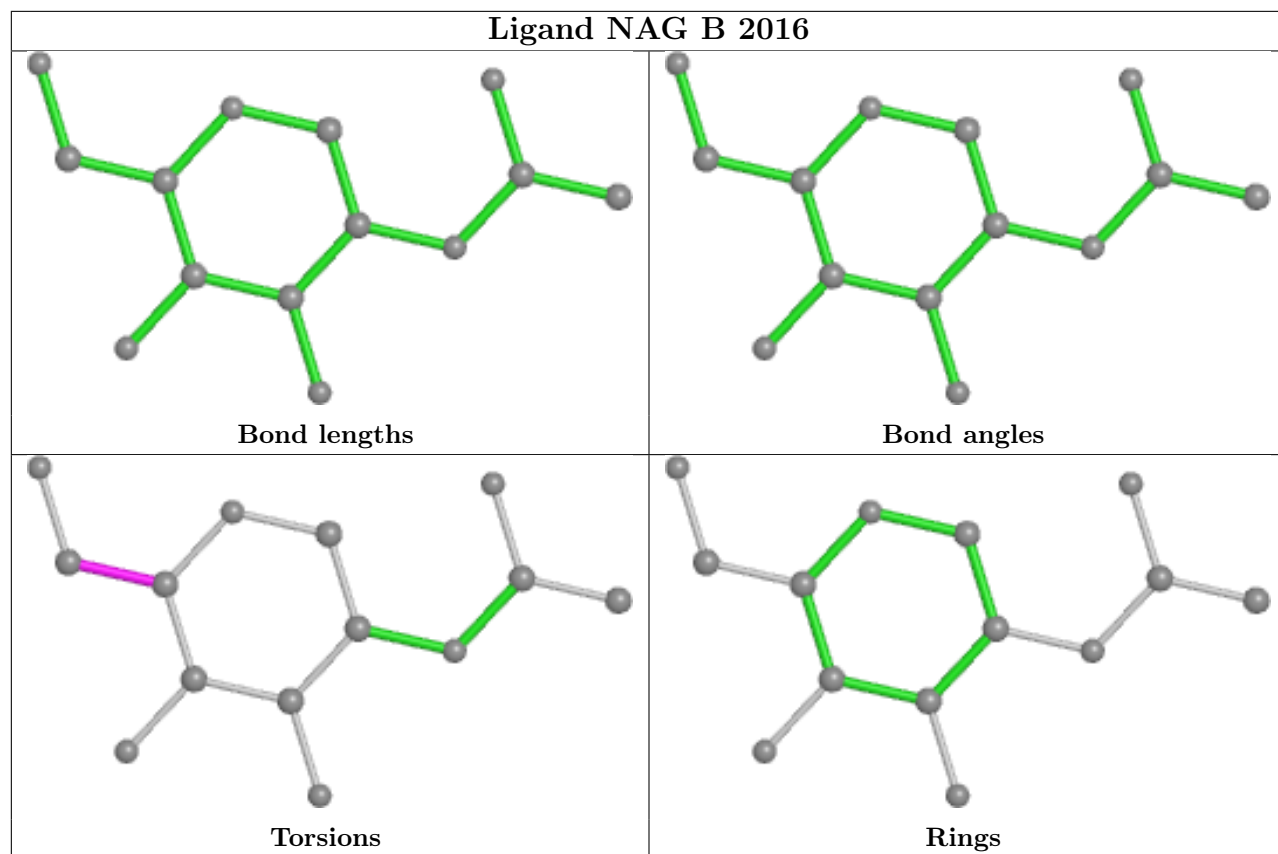


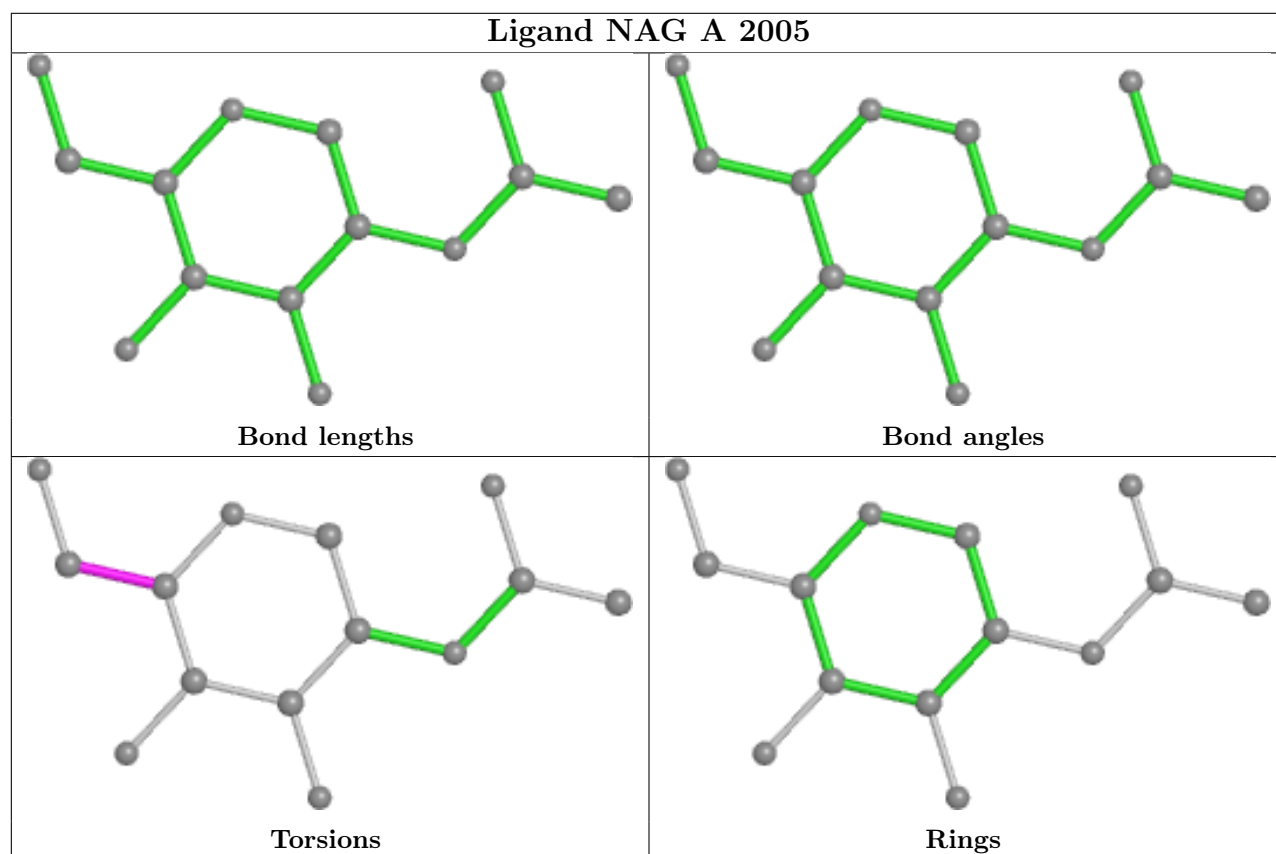
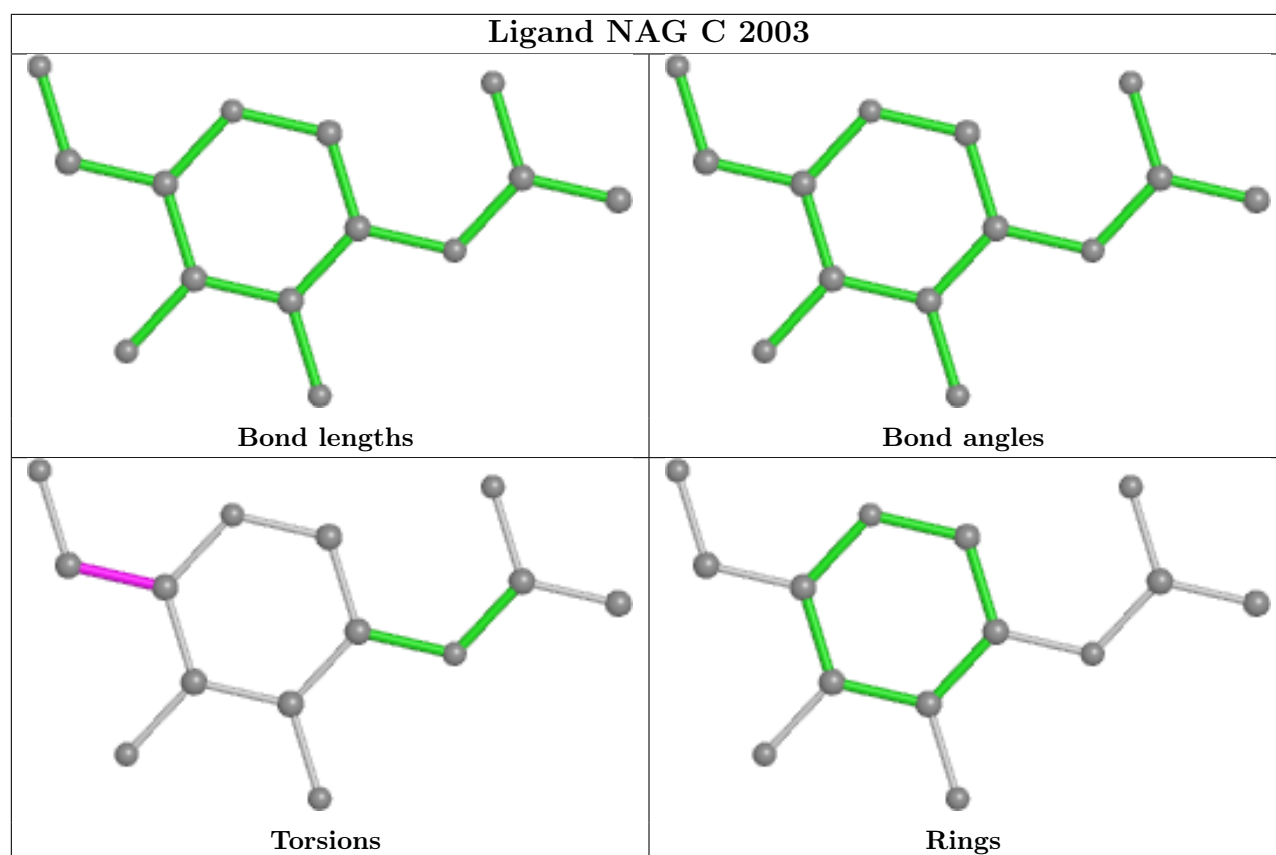


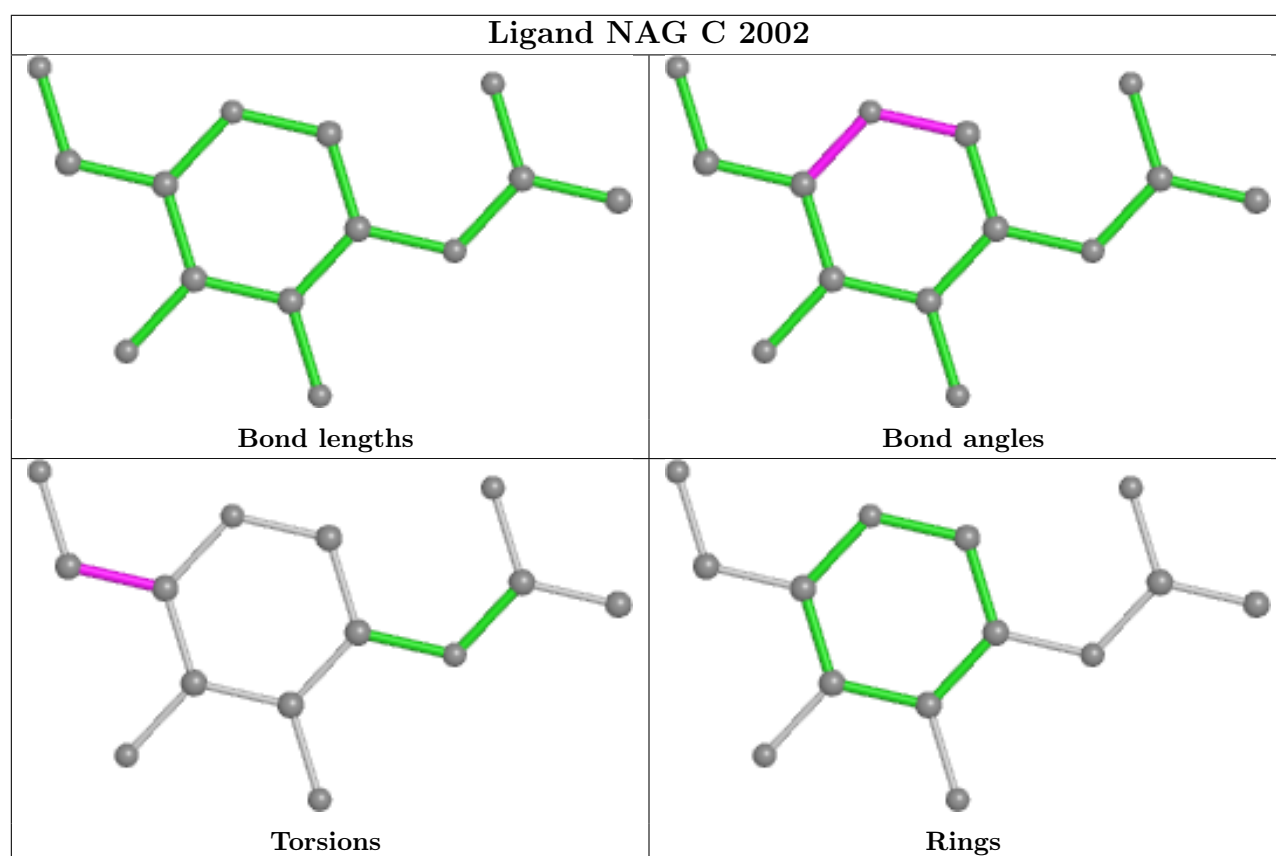
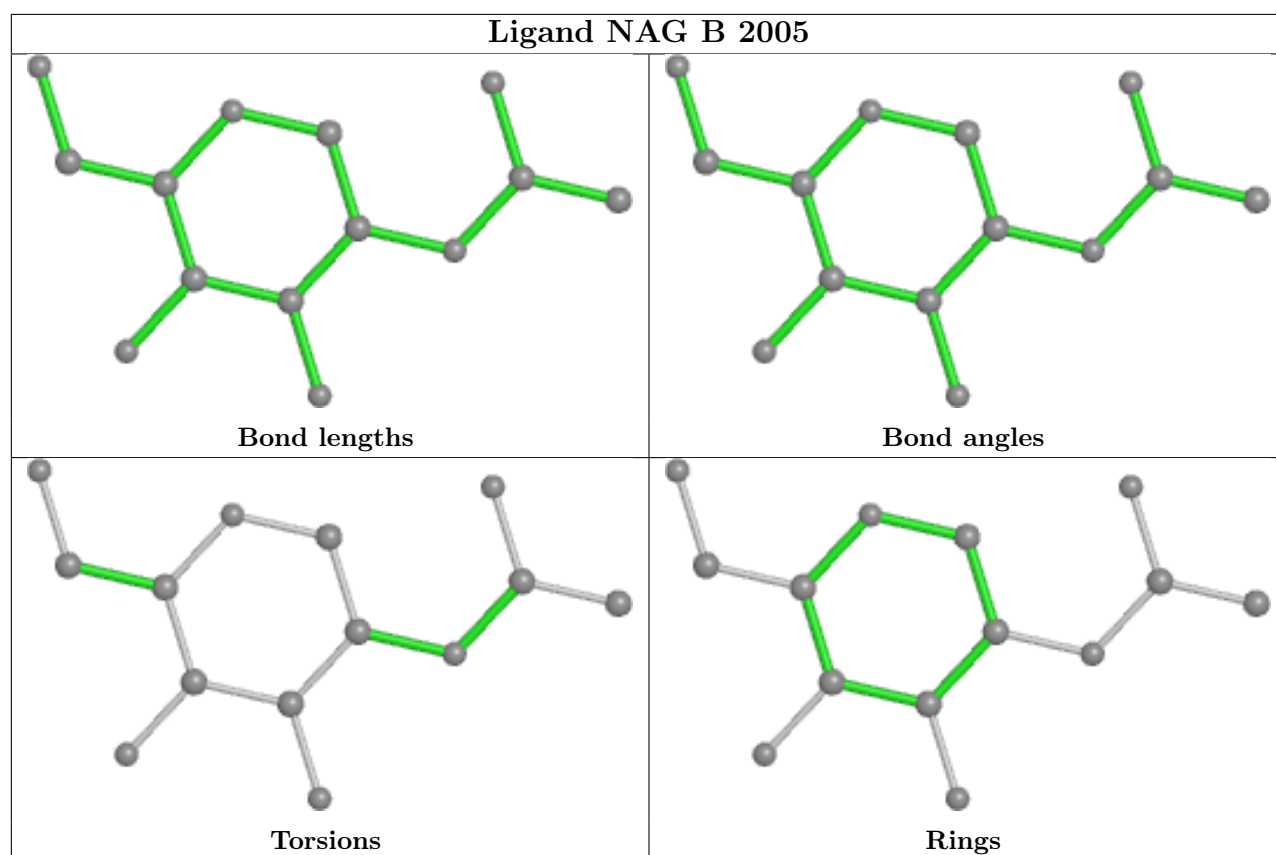




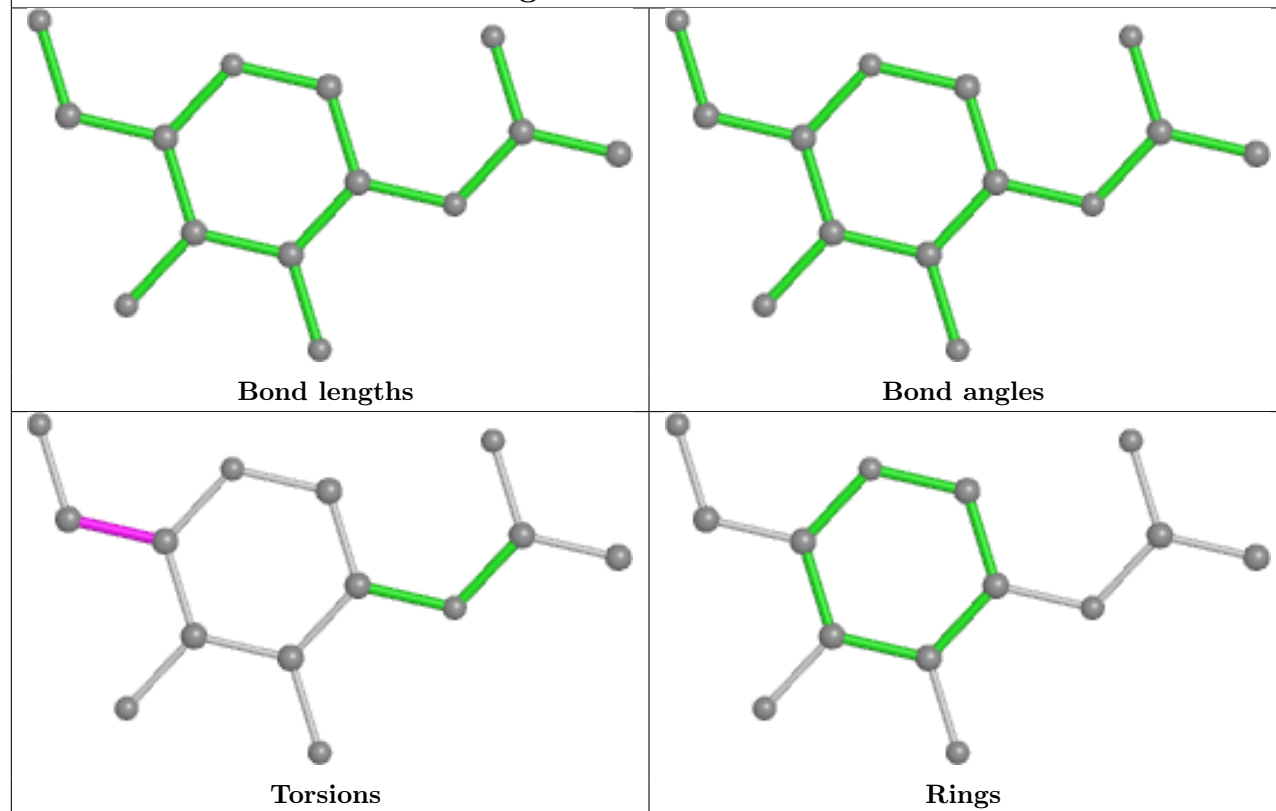




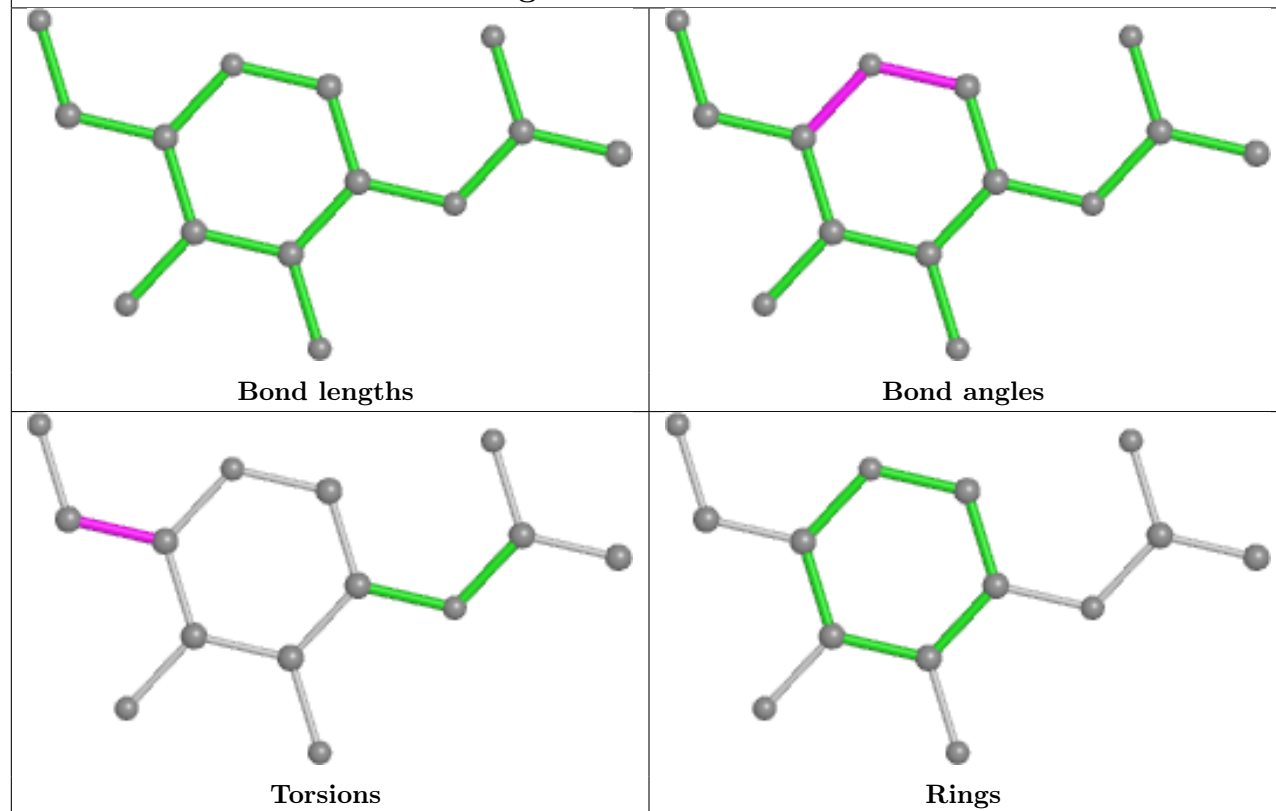




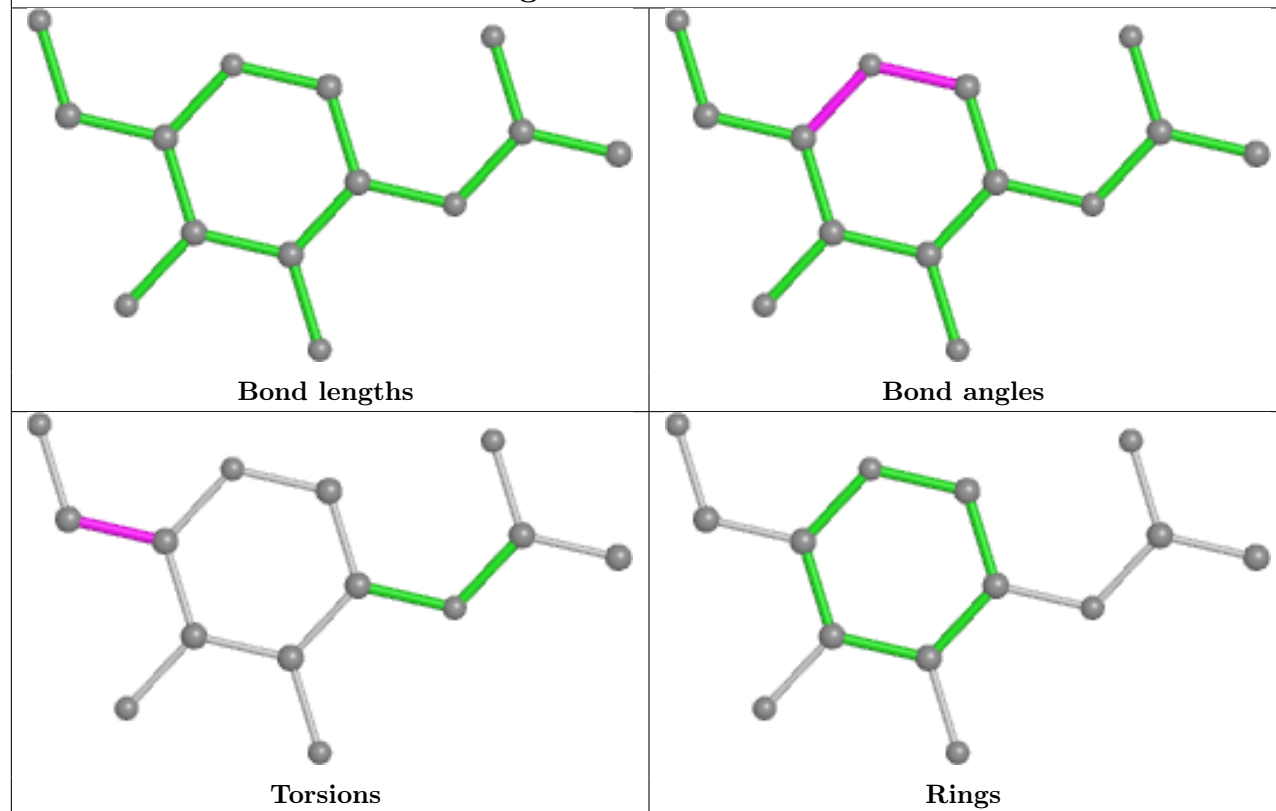
## Ligand NAG C 2010



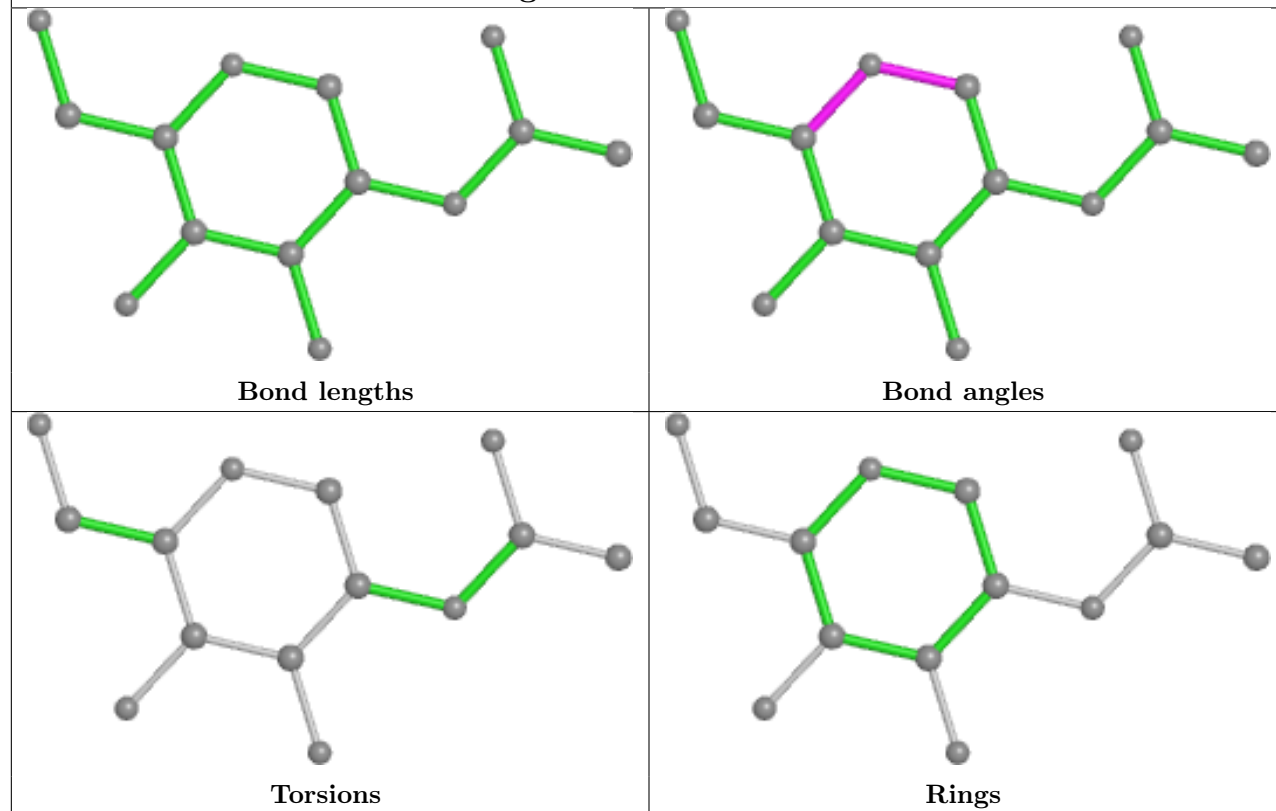
## Ligand NAG A 2009

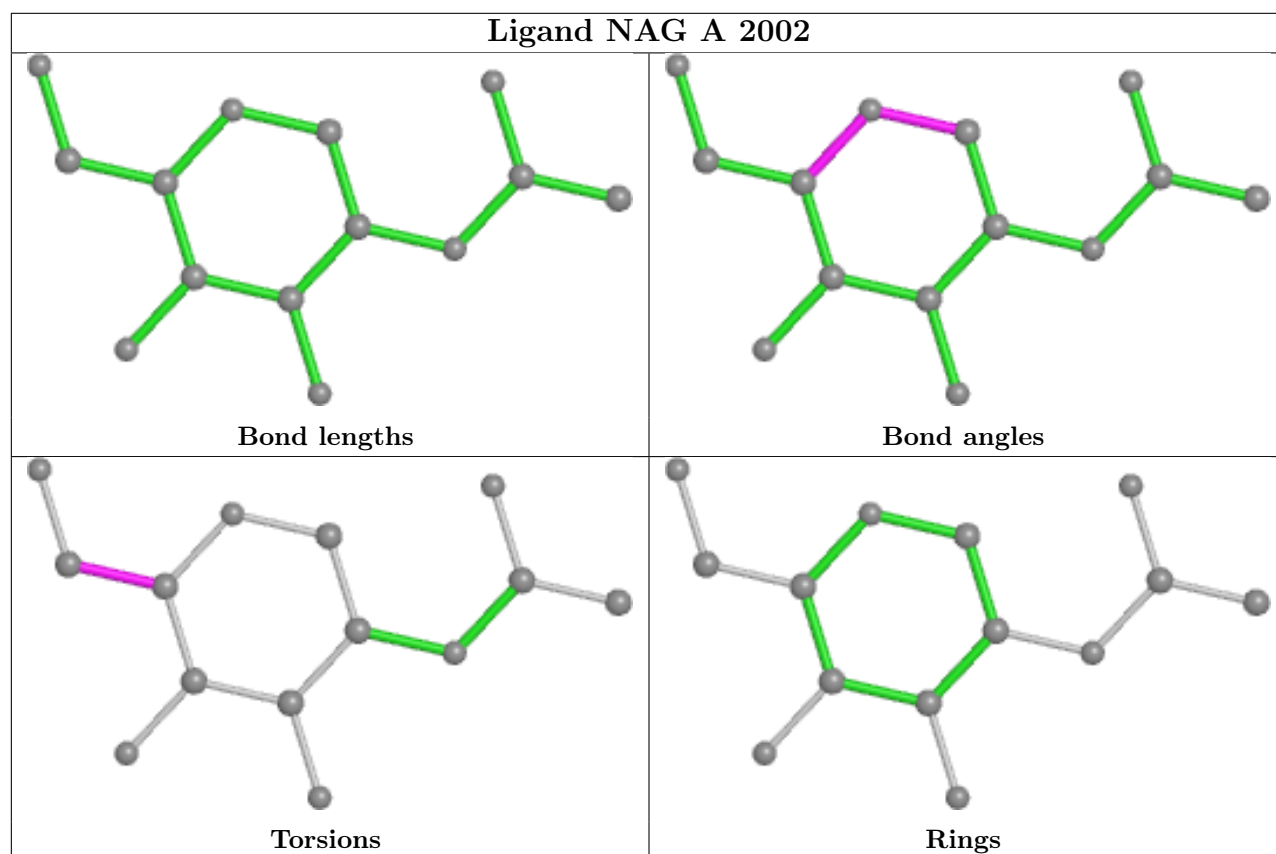
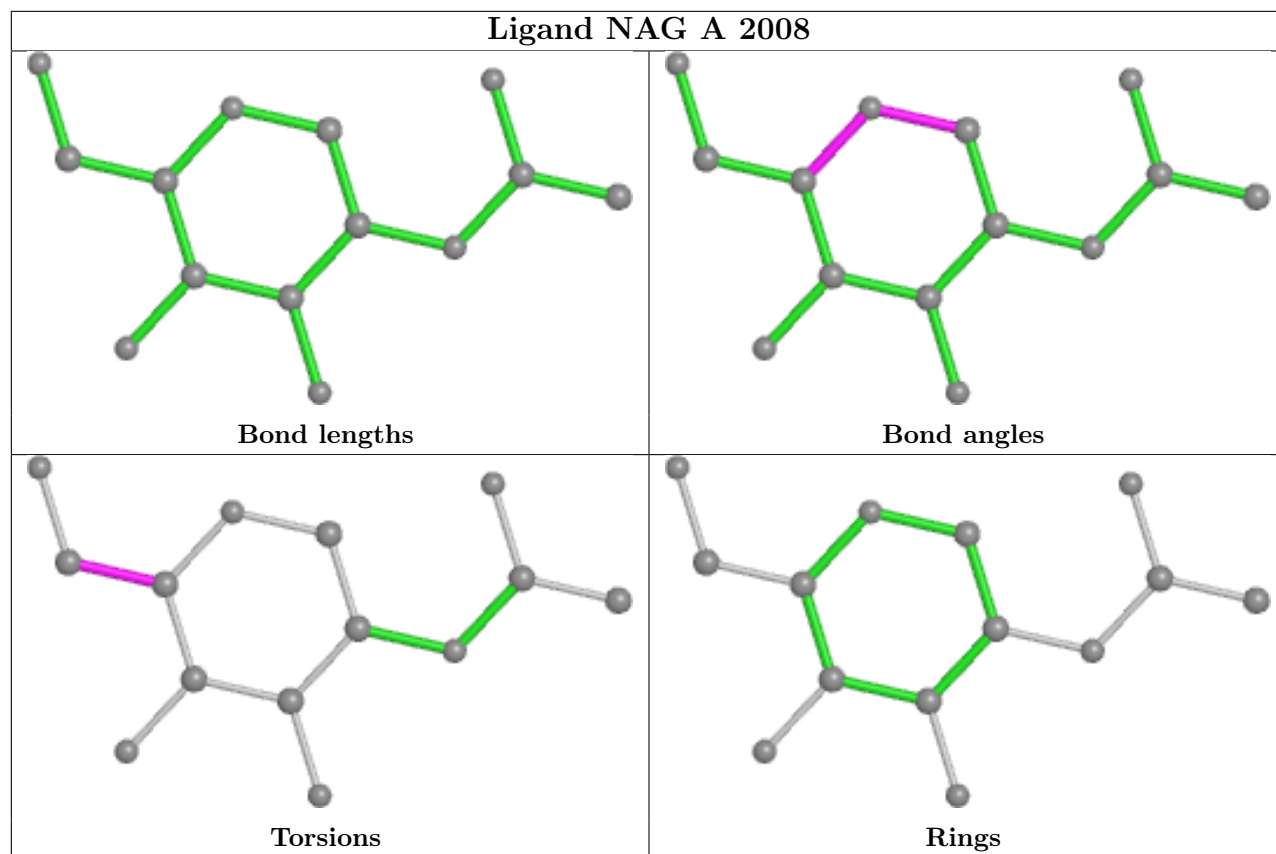


## Ligand NAG B 2012

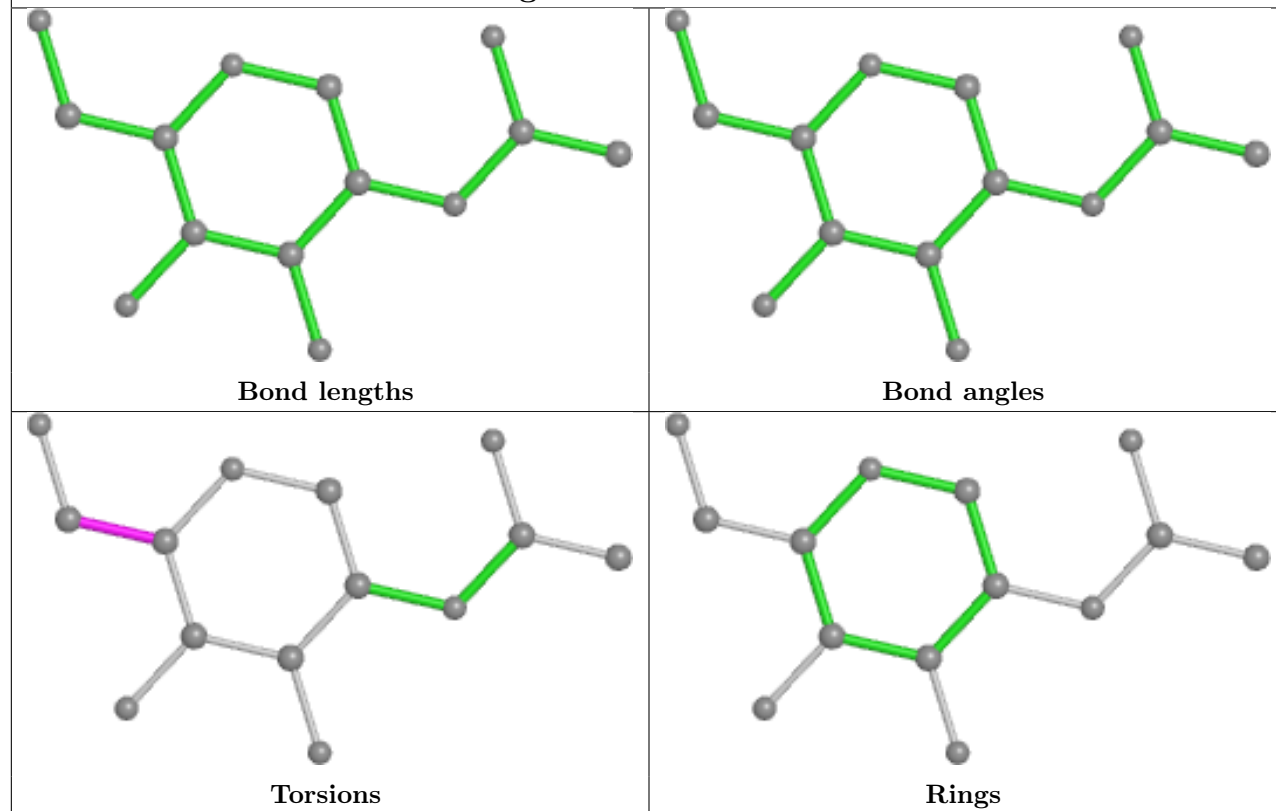


## Ligand NAG C 2014

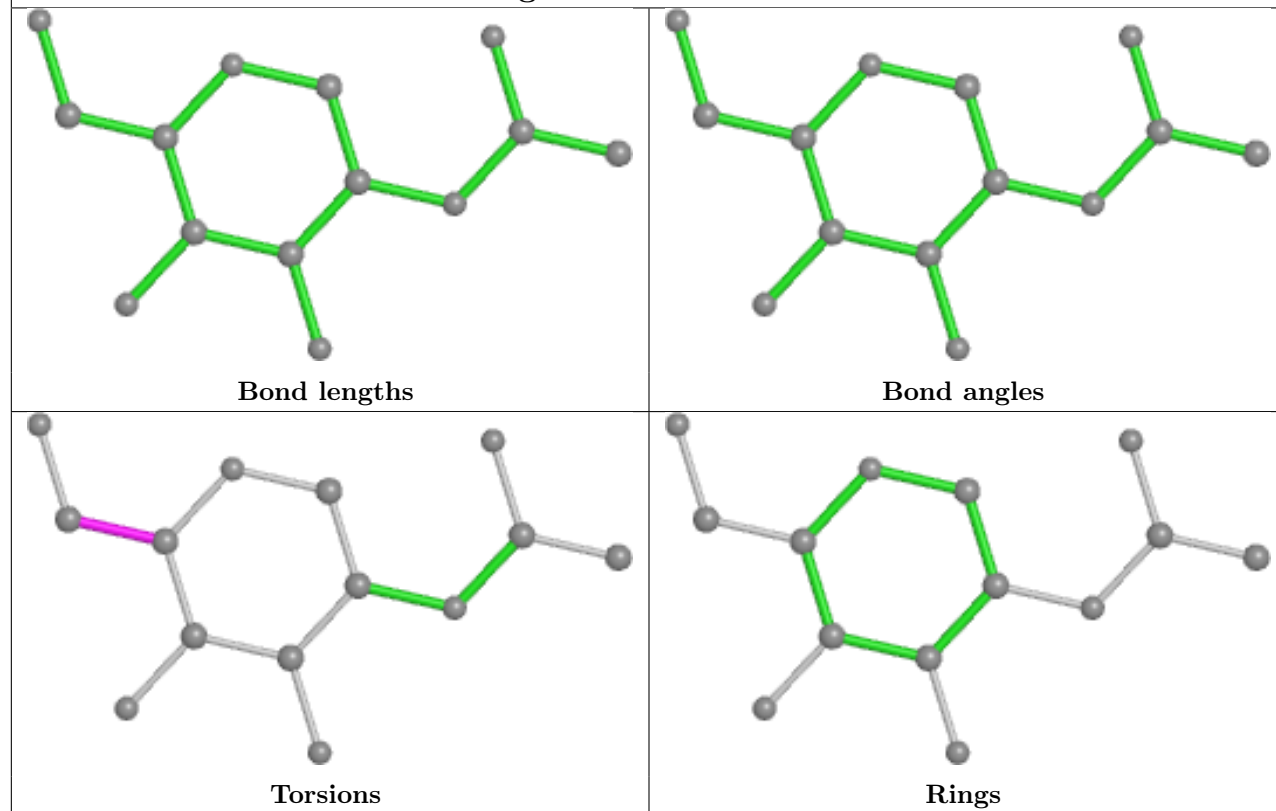




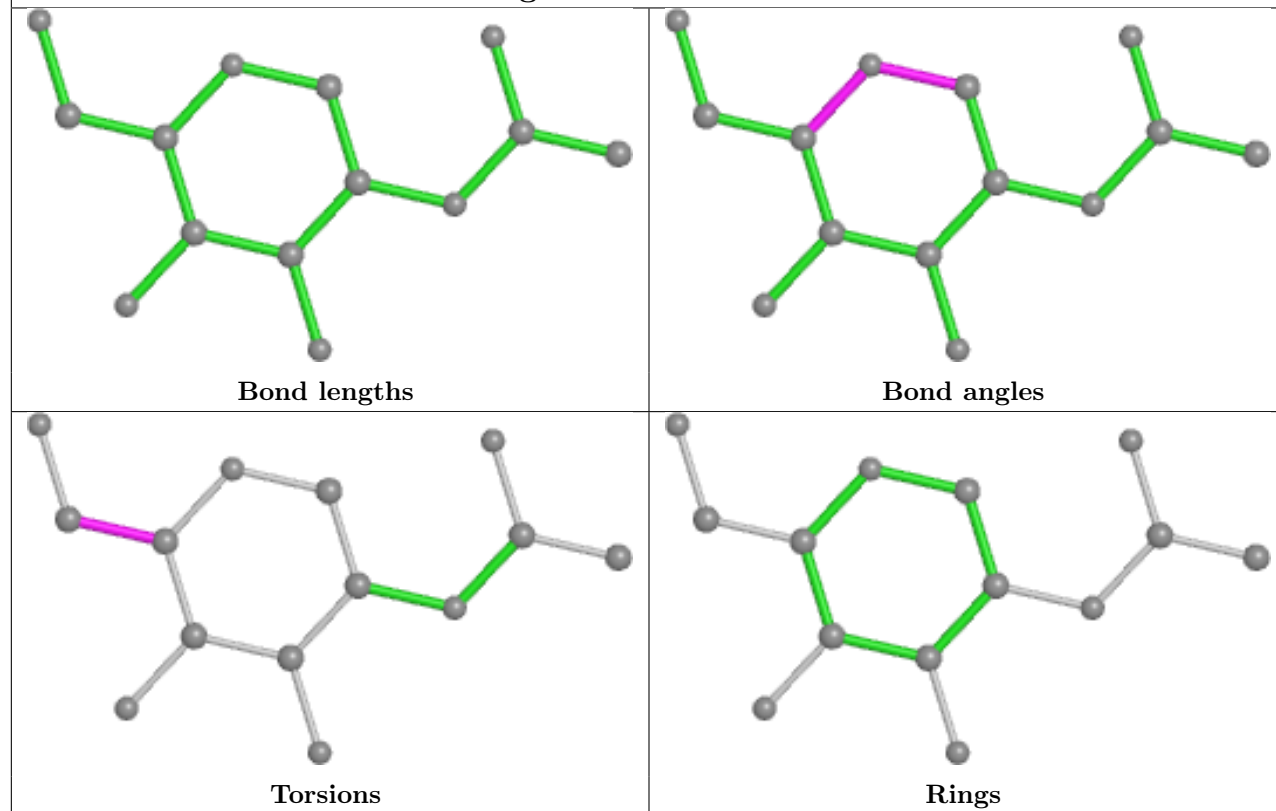
## Ligand NAG C 2005



## Ligand NAG A 2013



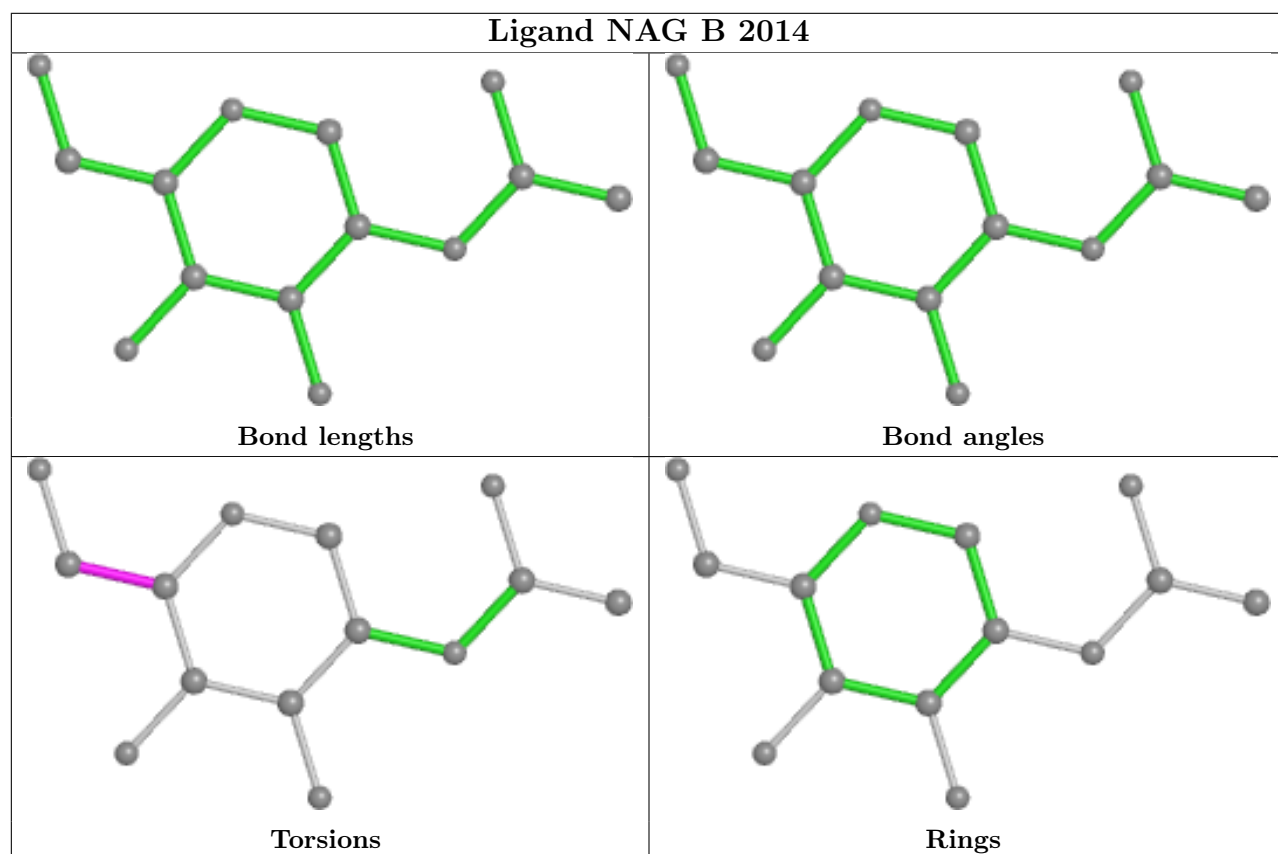
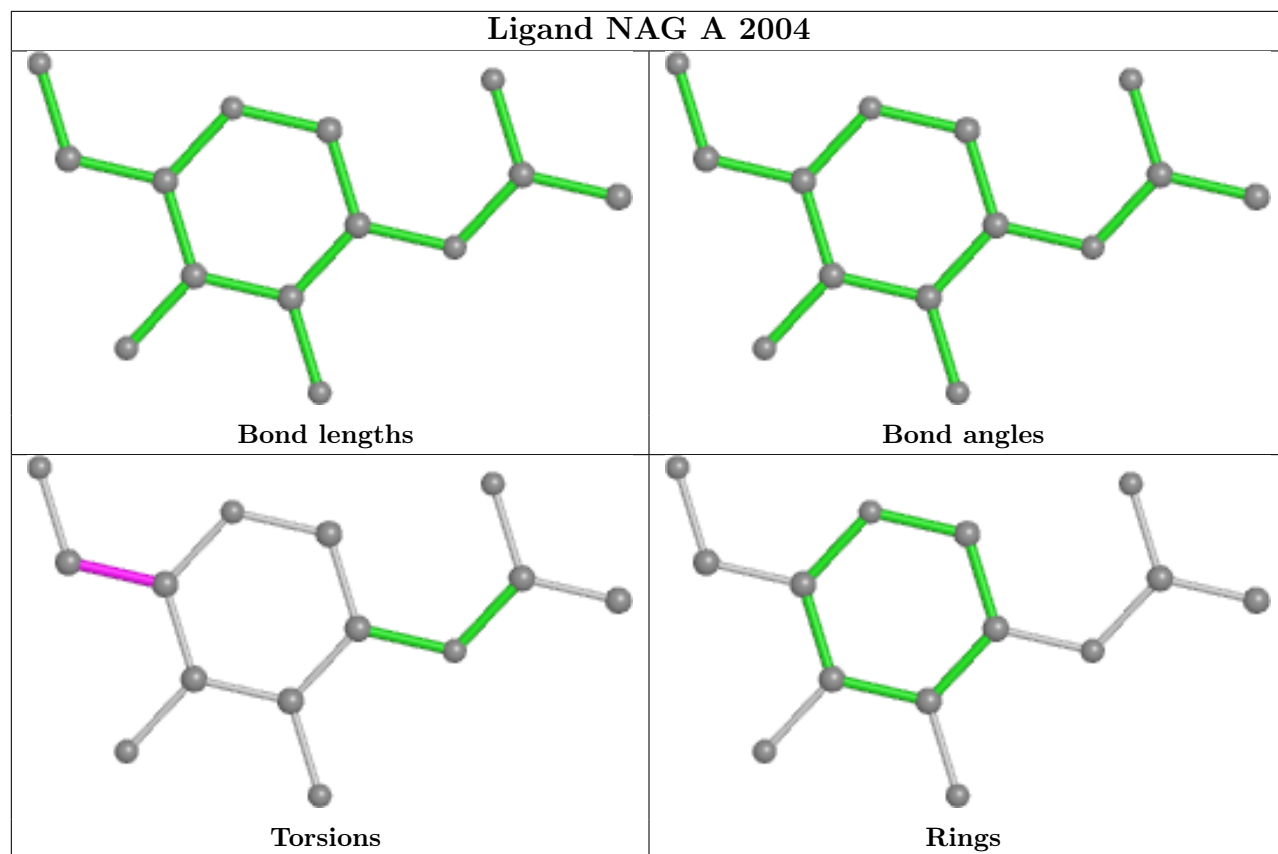
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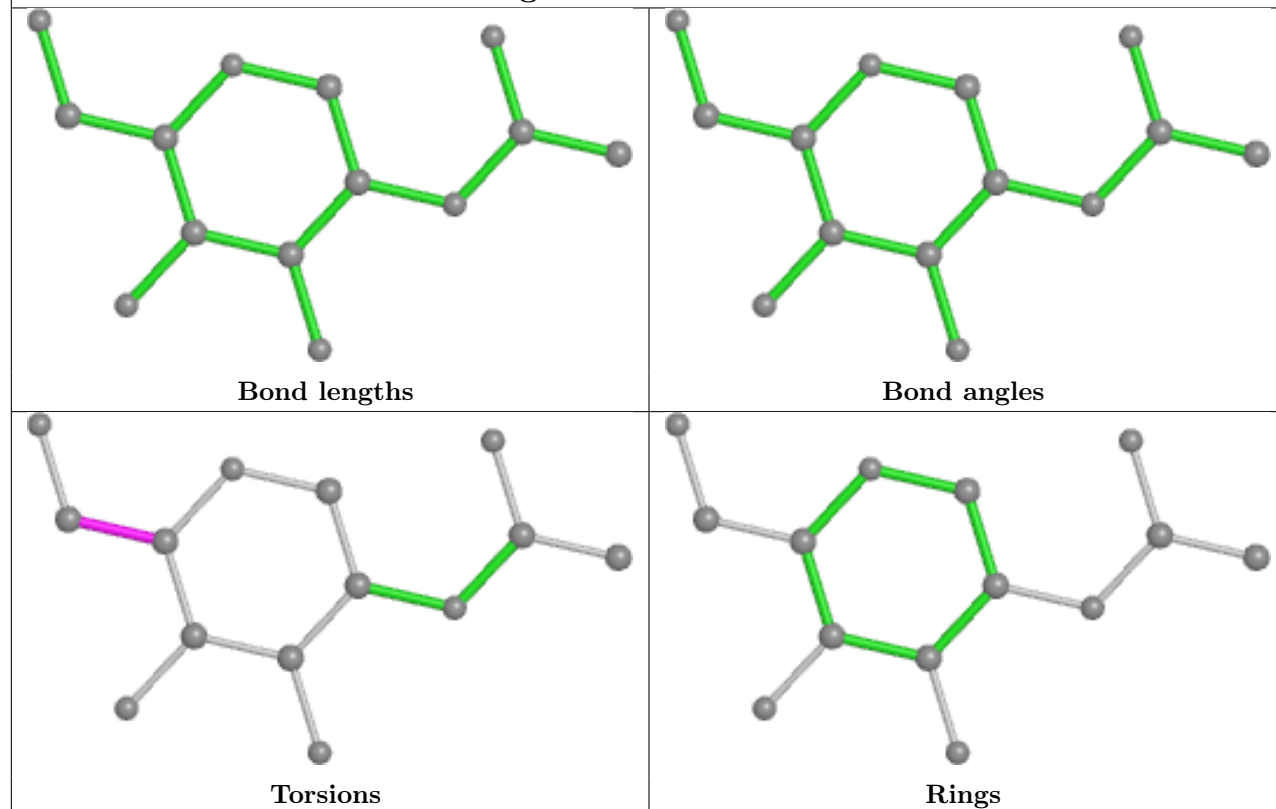
## Ligand NAG A 2014



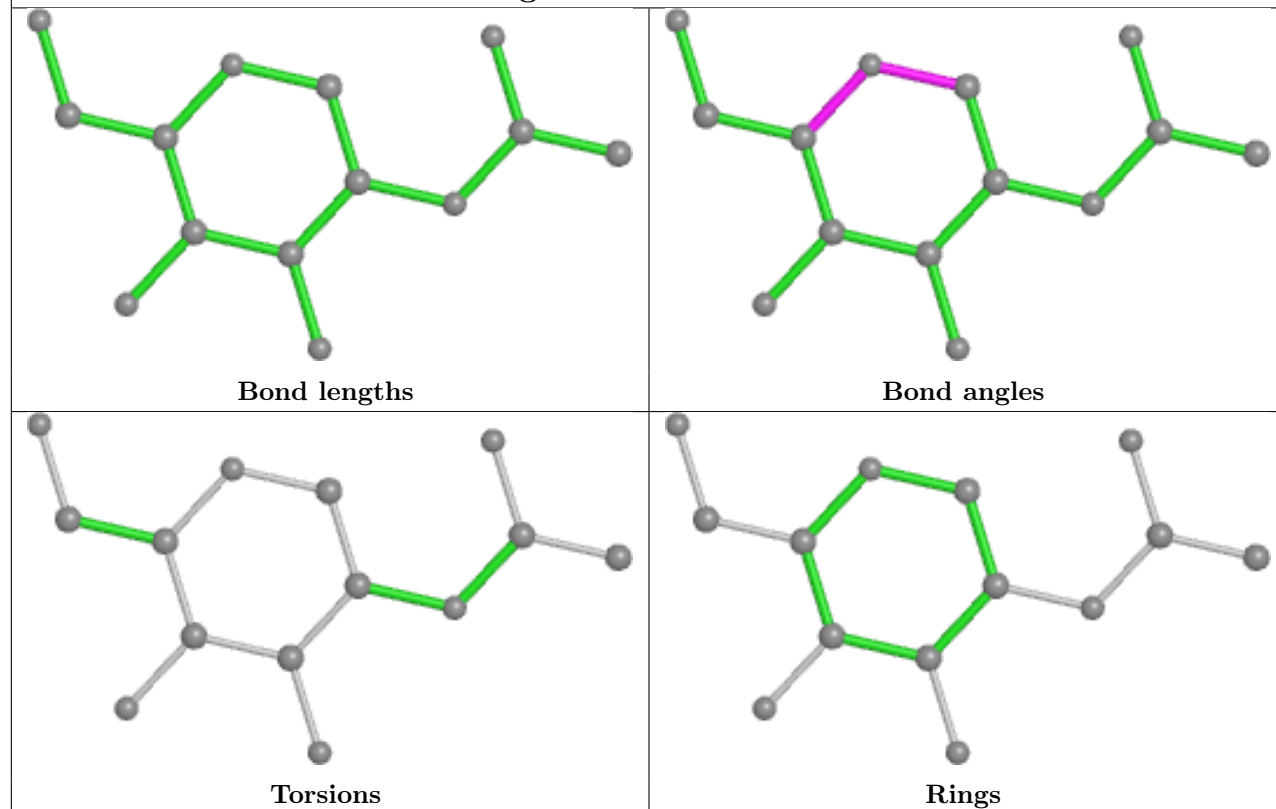


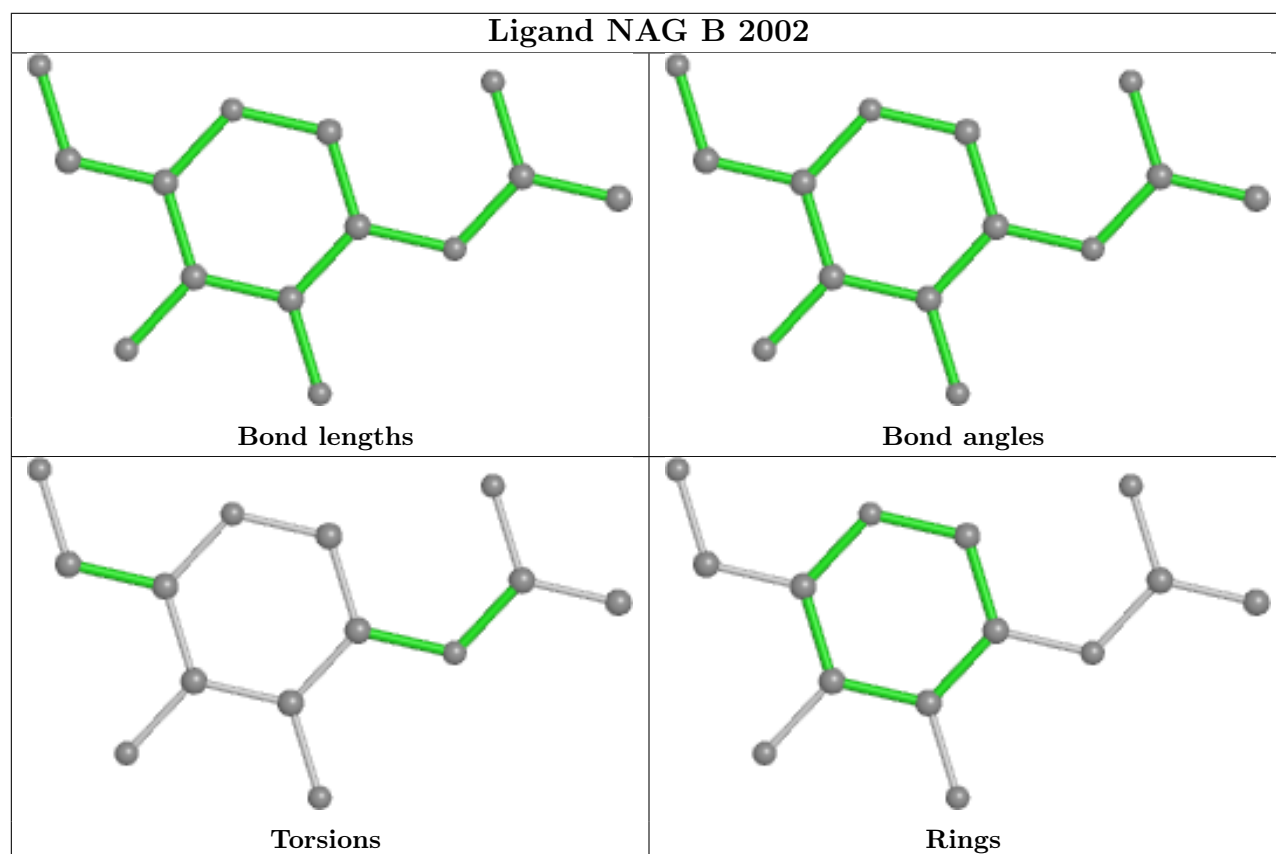
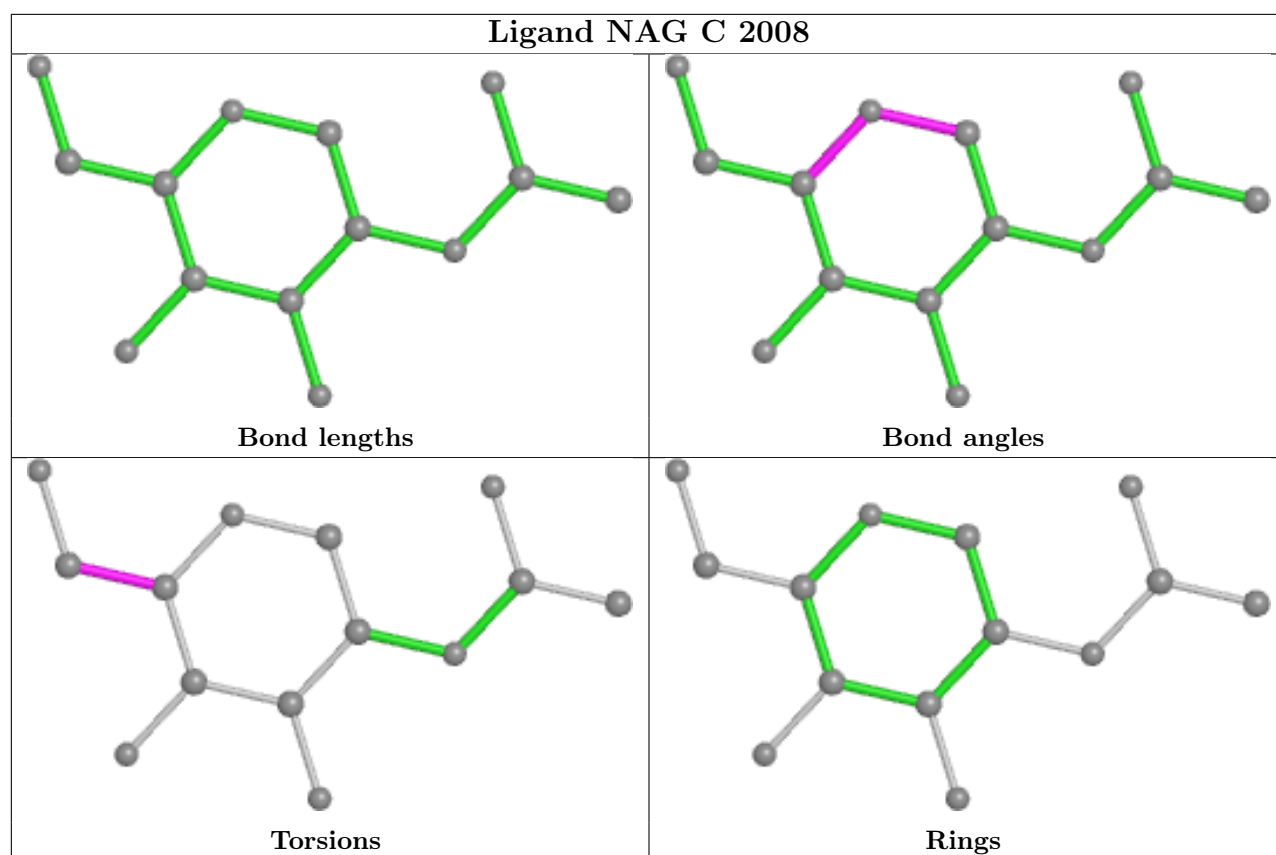


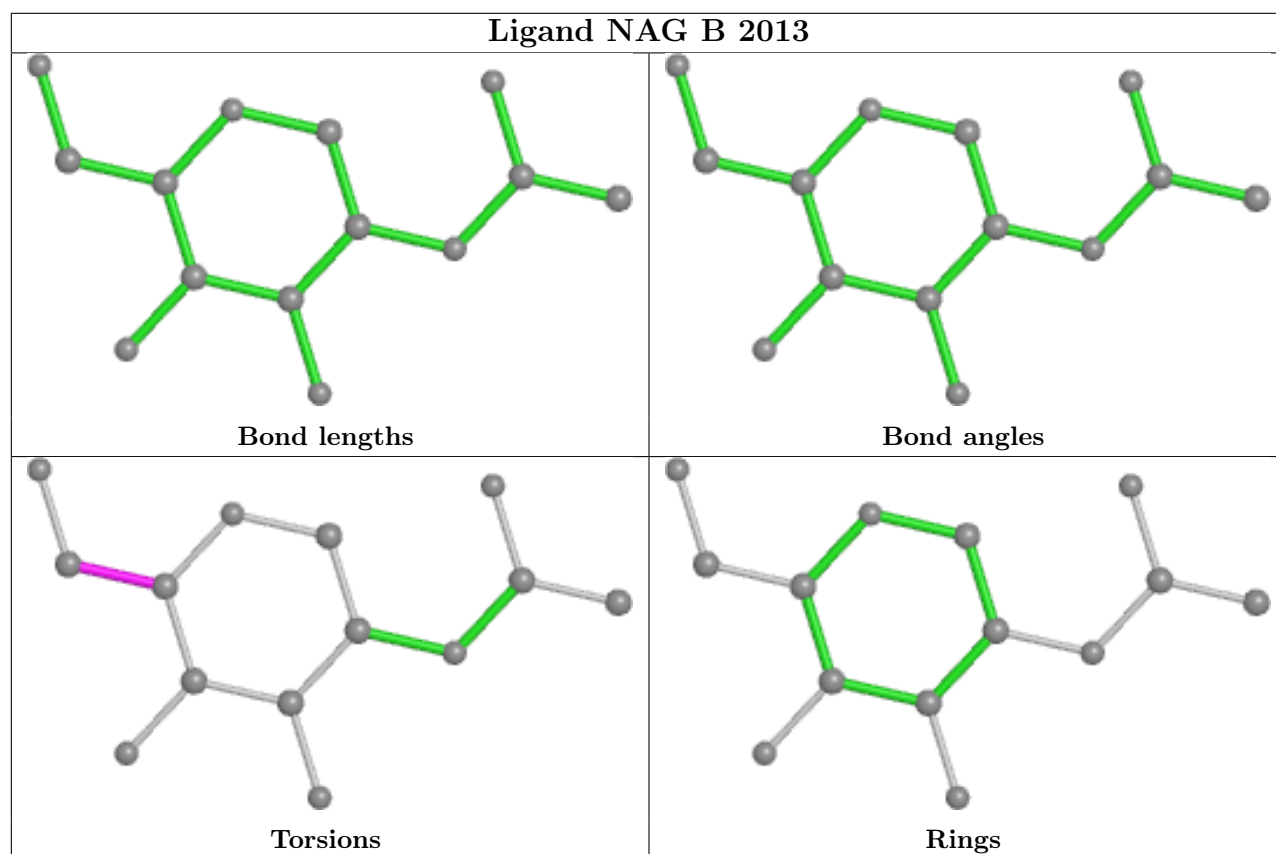
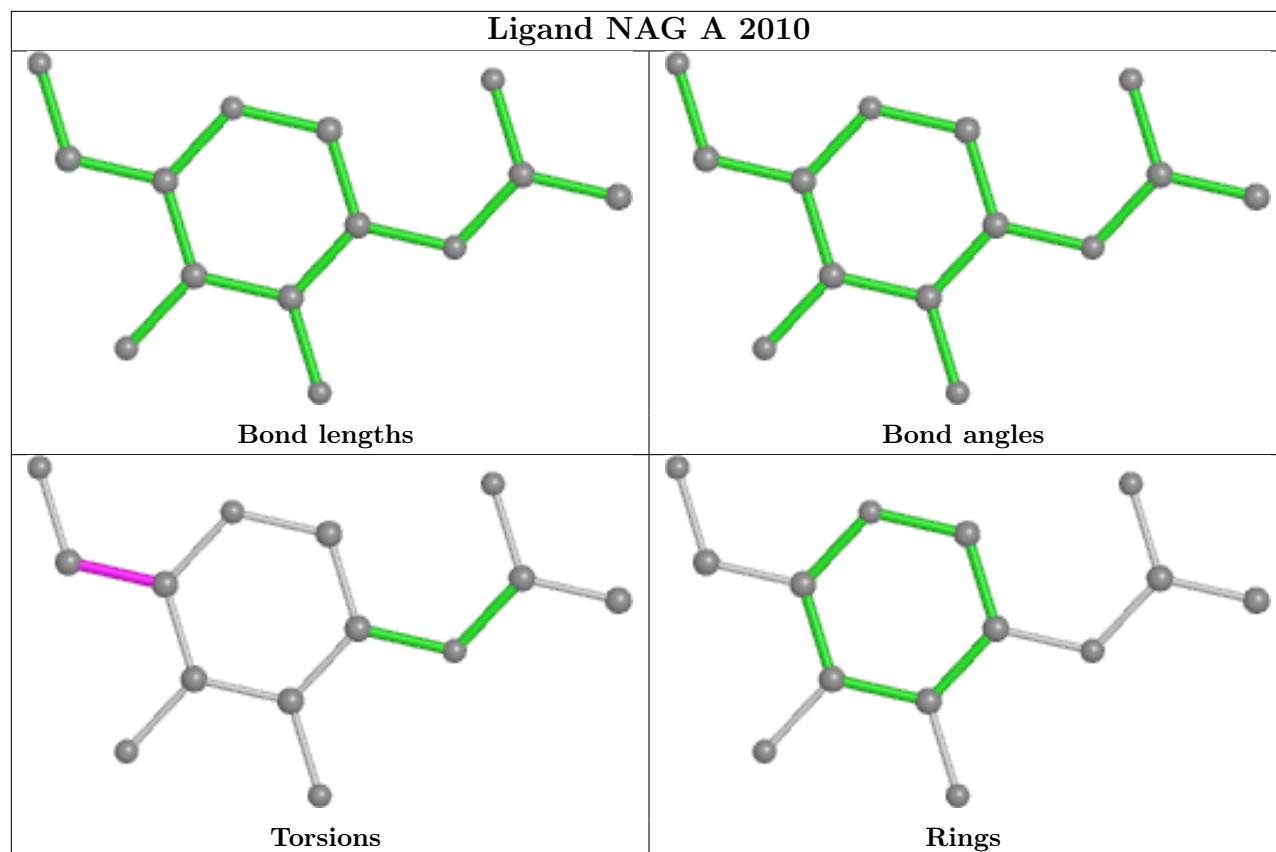
## Ligand NAG B 2003

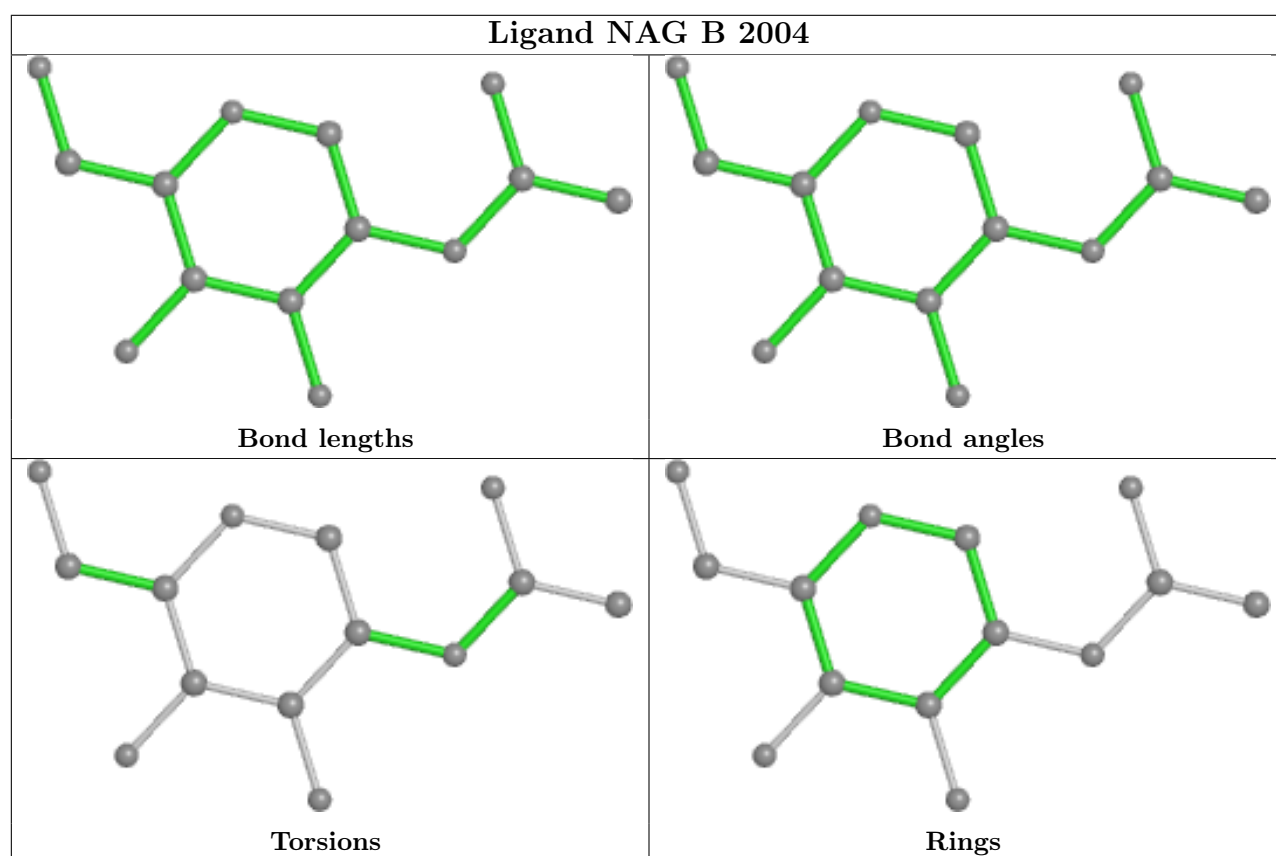
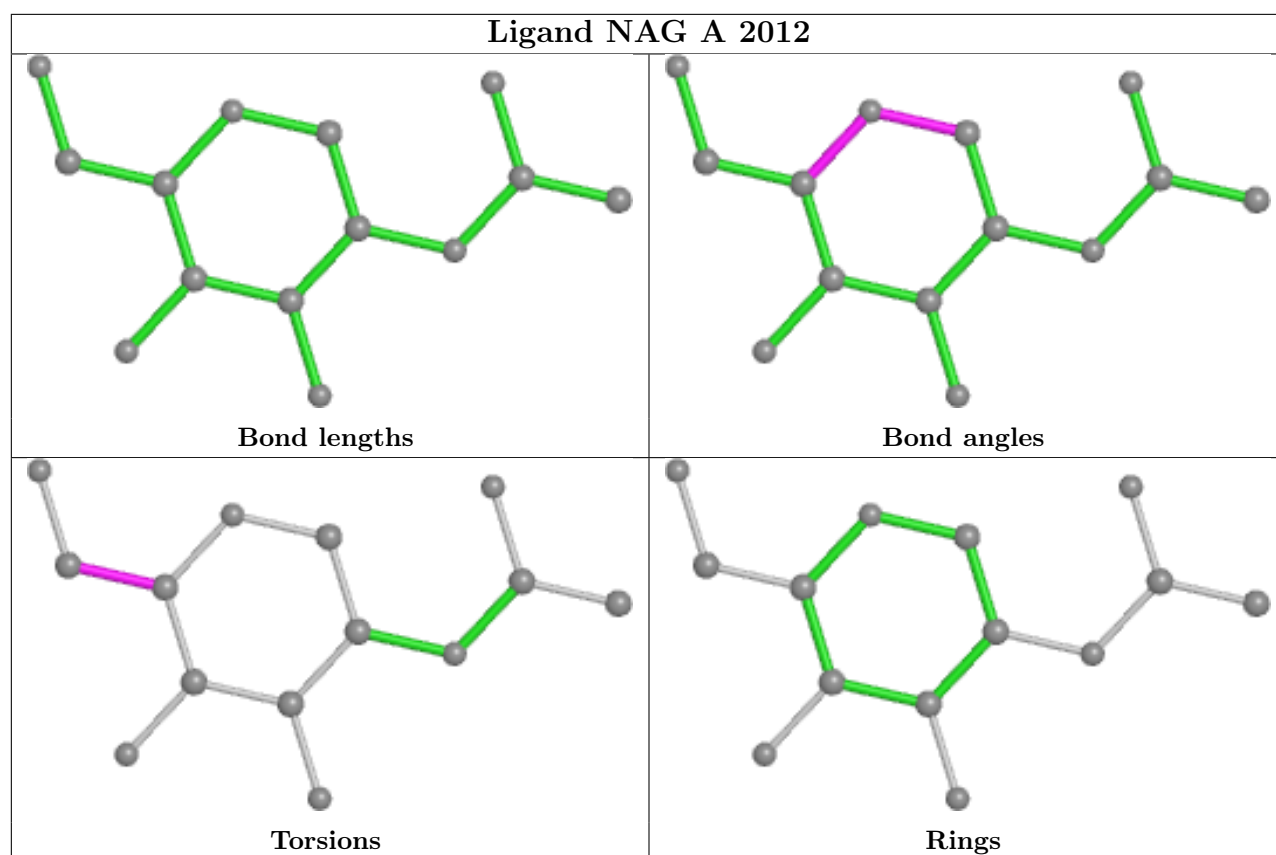


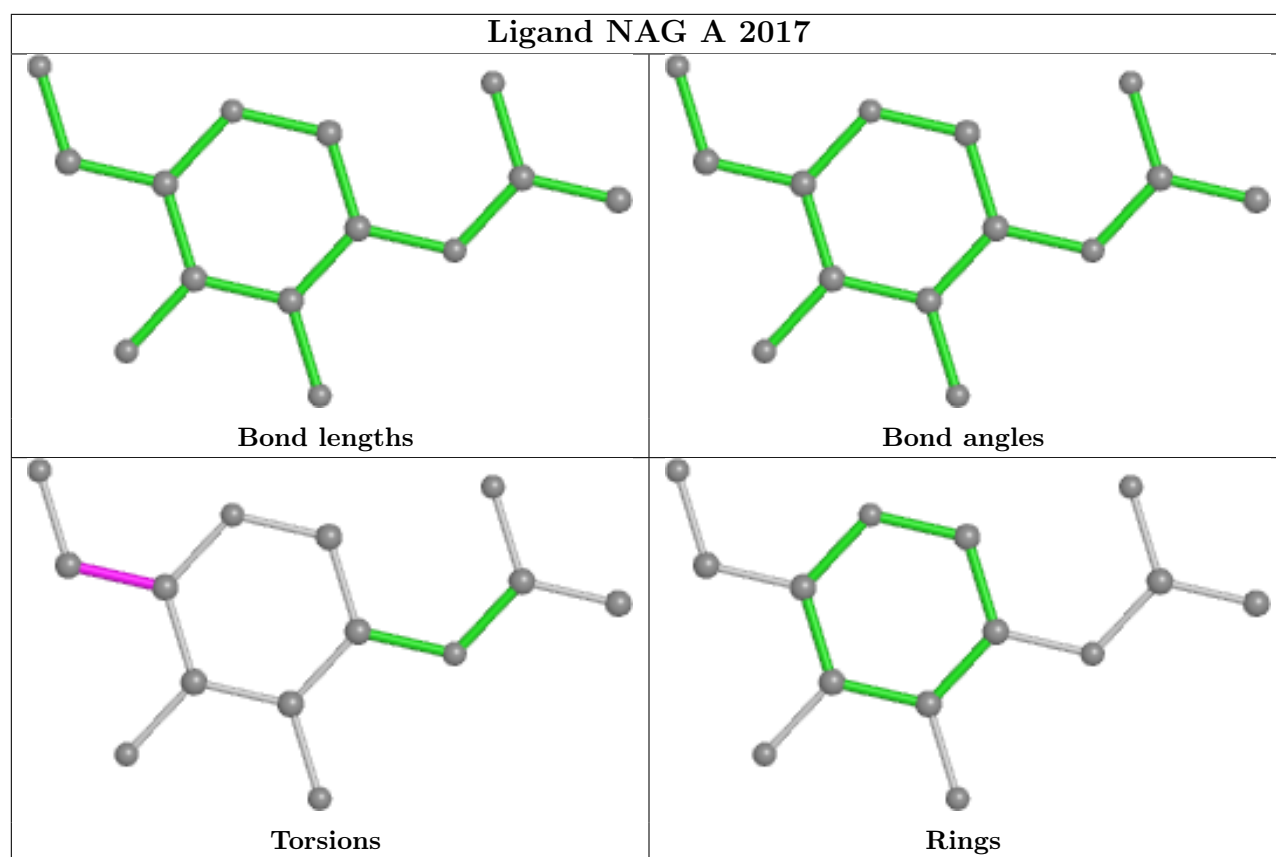
## Ligand NAG C 2016











## 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.