



Full wwPDB EM Validation Report ⓘ

Jul 14, 2025 – 06:15 PM JST

PDB ID : 9JMI / pdb_00009jmi
EMDB ID : EMD-61603
Title : Cryo-EM structure of CN-HedgehogCoV (HKU31/Erinaceus amurensis/China/2014) S-trimer in a locked-2 conformation
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 3.30 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.44

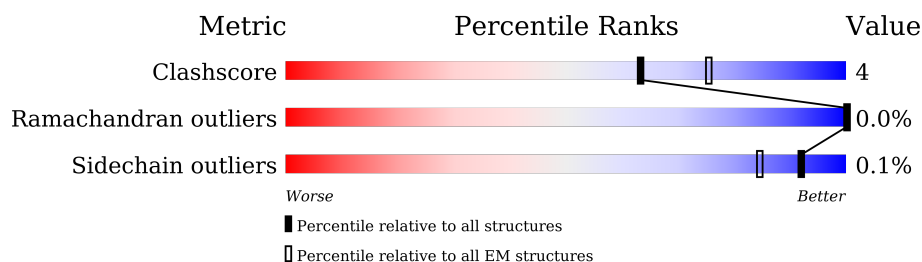
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	1349	74% 9% 16%
1	B	1349	75% 9% 16%
1	C	1349	76% 8% 16%
2	D	2	100%
2	E	2	100%
2	F	2	50% 50%
2	G	2	100%
2	H	2	100%
2	J	2	100%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	K	2	 100%
2	L	2	 100%
2	M	2	 50% 50%
2	N	2	 100%
2	P	2	 100%
2	Q	2	 50% 50%
2	R	2	 100%
2	S	2	 100%
2	T	2	 100%
3	I	3	 67% 33%
3	O	3	 67% 33%
3	U	3	 67% 33%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27732 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,Fibritin.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1131	Total	C	N	O	S	0	0
			8851	5607	1476	1710	58		
1	B	1131	Total	C	N	O	S	0	0
			8851	5607	1476	1710	58		
1	C	1131	Total	C	N	O	S	0	0
			8851	5607	1476	1710	58		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1271	GLY	-	linker	UNP A0A5Q0TVR1
A	1272	SER	-	linker	UNP A0A5Q0TVR1
A	1294	LEU	PHE	conflict	UNP P10104
A	1300	LEU	-	expression tag	UNP P10104
A	1301	GLU	-	expression tag	UNP P10104
A	1302	VAL	-	expression tag	UNP P10104
A	1303	LEU	-	expression tag	UNP P10104
A	1304	PHE	-	expression tag	UNP P10104
A	1305	GLN	-	expression tag	UNP P10104
A	1306	GLY	-	expression tag	UNP P10104
A	1307	PRO	-	expression tag	UNP P10104
A	1308	GLY	-	expression tag	UNP P10104
A	1309	HIS	-	expression tag	UNP P10104
A	1310	HIS	-	expression tag	UNP P10104
A	1311	HIS	-	expression tag	UNP P10104
A	1312	HIS	-	expression tag	UNP P10104
A	1313	HIS	-	expression tag	UNP P10104
A	1314	HIS	-	expression tag	UNP P10104
A	1315	HIS	-	expression tag	UNP P10104
A	1316	HIS	-	expression tag	UNP P10104
A	1317	SER	-	expression tag	UNP P10104
A	1318	ALA	-	expression tag	UNP P10104
A	1319	TRP	-	expression tag	UNP P10104
A	1320	SER	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	1321	HIS	-	expression tag	UNP P10104
A	1322	PRO	-	expression tag	UNP P10104
A	1323	GLN	-	expression tag	UNP P10104
A	1324	PHE	-	expression tag	UNP P10104
A	1325	GLU	-	expression tag	UNP P10104
A	1326	LYS	-	expression tag	UNP P10104
A	1327	GLY	-	expression tag	UNP P10104
A	1328	GLY	-	expression tag	UNP P10104
A	1329	GLY	-	expression tag	UNP P10104
A	1330	SER	-	expression tag	UNP P10104
A	1331	GLY	-	expression tag	UNP P10104
A	1332	GLY	-	expression tag	UNP P10104
A	1333	GLY	-	expression tag	UNP P10104
A	1334	GLY	-	expression tag	UNP P10104
A	1335	SER	-	expression tag	UNP P10104
A	1336	GLY	-	expression tag	UNP P10104
A	1337	GLY	-	expression tag	UNP P10104
A	1338	SER	-	expression tag	UNP P10104
A	1339	ALA	-	expression tag	UNP P10104
A	1340	TRP	-	expression tag	UNP P10104
A	1341	SER	-	expression tag	UNP P10104
A	1342	HIS	-	expression tag	UNP P10104
A	1343	PRO	-	expression tag	UNP P10104
A	1344	GLN	-	expression tag	UNP P10104
A	1345	PHE	-	expression tag	UNP P10104
A	1346	GLU	-	expression tag	UNP P10104
A	1347	LYS	-	expression tag	UNP P10104
A	1348	SER	-	expression tag	UNP P10104
A	1349	ALA	-	expression tag	UNP P10104
B	1271	GLY	-	linker	UNP A0A5Q0TVR1
B	1272	SER	-	linker	UNP A0A5Q0TVR1
B	1294	LEU	PHE	conflict	UNP P10104
B	1300	LEU	-	expression tag	UNP P10104
B	1301	GLU	-	expression tag	UNP P10104
B	1302	VAL	-	expression tag	UNP P10104
B	1303	LEU	-	expression tag	UNP P10104
B	1304	PHE	-	expression tag	UNP P10104
B	1305	GLN	-	expression tag	UNP P10104
B	1306	GLY	-	expression tag	UNP P10104
B	1307	PRO	-	expression tag	UNP P10104
B	1308	GLY	-	expression tag	UNP P10104
B	1309	HIS	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	1310	HIS	-	expression tag	UNP P10104
B	1311	HIS	-	expression tag	UNP P10104
B	1312	HIS	-	expression tag	UNP P10104
B	1313	HIS	-	expression tag	UNP P10104
B	1314	HIS	-	expression tag	UNP P10104
B	1315	HIS	-	expression tag	UNP P10104
B	1316	HIS	-	expression tag	UNP P10104
B	1317	SER	-	expression tag	UNP P10104
B	1318	ALA	-	expression tag	UNP P10104
B	1319	TRP	-	expression tag	UNP P10104
B	1320	SER	-	expression tag	UNP P10104
B	1321	HIS	-	expression tag	UNP P10104
B	1322	PRO	-	expression tag	UNP P10104
B	1323	GLN	-	expression tag	UNP P10104
B	1324	PHE	-	expression tag	UNP P10104
B	1325	GLU	-	expression tag	UNP P10104
B	1326	LYS	-	expression tag	UNP P10104
B	1327	GLY	-	expression tag	UNP P10104
B	1328	GLY	-	expression tag	UNP P10104
B	1329	GLY	-	expression tag	UNP P10104
B	1330	SER	-	expression tag	UNP P10104
B	1331	GLY	-	expression tag	UNP P10104
B	1332	GLY	-	expression tag	UNP P10104
B	1333	GLY	-	expression tag	UNP P10104
B	1334	GLY	-	expression tag	UNP P10104
B	1335	SER	-	expression tag	UNP P10104
B	1336	GLY	-	expression tag	UNP P10104
B	1337	GLY	-	expression tag	UNP P10104
B	1338	SER	-	expression tag	UNP P10104
B	1339	ALA	-	expression tag	UNP P10104
B	1340	TRP	-	expression tag	UNP P10104
B	1341	SER	-	expression tag	UNP P10104
B	1342	HIS	-	expression tag	UNP P10104
B	1343	PRO	-	expression tag	UNP P10104
B	1344	GLN	-	expression tag	UNP P10104
B	1345	PHE	-	expression tag	UNP P10104
B	1346	GLU	-	expression tag	UNP P10104
B	1347	LYS	-	expression tag	UNP P10104
B	1348	SER	-	expression tag	UNP P10104
B	1349	ALA	-	expression tag	UNP P10104
C	1271	GLY	-	linker	UNP A0A5Q0TVR1
C	1272	SER	-	linker	UNP A0A5Q0TVR1

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1294	LEU	PHE	conflict	UNP P10104
C	1300	LEU	-	expression tag	UNP P10104
C	1301	GLU	-	expression tag	UNP P10104
C	1302	VAL	-	expression tag	UNP P10104
C	1303	LEU	-	expression tag	UNP P10104
C	1304	PHE	-	expression tag	UNP P10104
C	1305	GLN	-	expression tag	UNP P10104
C	1306	GLY	-	expression tag	UNP P10104
C	1307	PRO	-	expression tag	UNP P10104
C	1308	GLY	-	expression tag	UNP P10104
C	1309	HIS	-	expression tag	UNP P10104
C	1310	HIS	-	expression tag	UNP P10104
C	1311	HIS	-	expression tag	UNP P10104
C	1312	HIS	-	expression tag	UNP P10104
C	1313	HIS	-	expression tag	UNP P10104
C	1314	HIS	-	expression tag	UNP P10104
C	1315	HIS	-	expression tag	UNP P10104
C	1316	HIS	-	expression tag	UNP P10104
C	1317	SER	-	expression tag	UNP P10104
C	1318	ALA	-	expression tag	UNP P10104
C	1319	TRP	-	expression tag	UNP P10104
C	1320	SER	-	expression tag	UNP P10104
C	1321	HIS	-	expression tag	UNP P10104
C	1322	PRO	-	expression tag	UNP P10104
C	1323	GLN	-	expression tag	UNP P10104
C	1324	PHE	-	expression tag	UNP P10104
C	1325	GLU	-	expression tag	UNP P10104
C	1326	LYS	-	expression tag	UNP P10104
C	1327	GLY	-	expression tag	UNP P10104
C	1328	GLY	-	expression tag	UNP P10104
C	1329	GLY	-	expression tag	UNP P10104
C	1330	SER	-	expression tag	UNP P10104
C	1331	GLY	-	expression tag	UNP P10104
C	1332	GLY	-	expression tag	UNP P10104
C	1333	GLY	-	expression tag	UNP P10104
C	1334	GLY	-	expression tag	UNP P10104
C	1335	SER	-	expression tag	UNP P10104
C	1336	GLY	-	expression tag	UNP P10104
C	1337	GLY	-	expression tag	UNP P10104
C	1338	SER	-	expression tag	UNP P10104
C	1339	ALA	-	expression tag	UNP P10104
C	1340	TRP	-	expression tag	UNP P10104

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	1341	SER	-	expression tag	UNP P10104
C	1342	HIS	-	expression tag	UNP P10104
C	1343	PRO	-	expression tag	UNP P10104
C	1344	GLN	-	expression tag	UNP P10104
C	1345	PHE	-	expression tag	UNP P10104
C	1346	GLU	-	expression tag	UNP P10104
C	1347	LYS	-	expression tag	UNP P10104
C	1348	SER	-	expression tag	UNP P10104
C	1349	ALA	-	expression tag	UNP P10104

- Molecule 2 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
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		
2	F	2	Total	C	N	O	0	0
			28	16	2	10		
2	G	2	Total	C	N	O	0	0
			28	16	2	10		
2	H	2	Total	C	N	O	0	0
			28	16	2	10		
2	J	2	Total	C	N	O	0	0
			28	16	2	10		
2	K	2	Total	C	N	O	0	0
			28	16	2	10		
2	L	2	Total	C	N	O	0	0
			28	16	2	10		
2	M	2	Total	C	N	O	0	0
			28	16	2	10		
2	N	2	Total	C	N	O	0	0
			28	16	2	10		
2	P	2	Total	C	N	O	0	0
			28	16	2	10		
2	Q	2	Total	C	N	O	0	0
			28	16	2	10		

Continued on next page...

Continued from previous page...

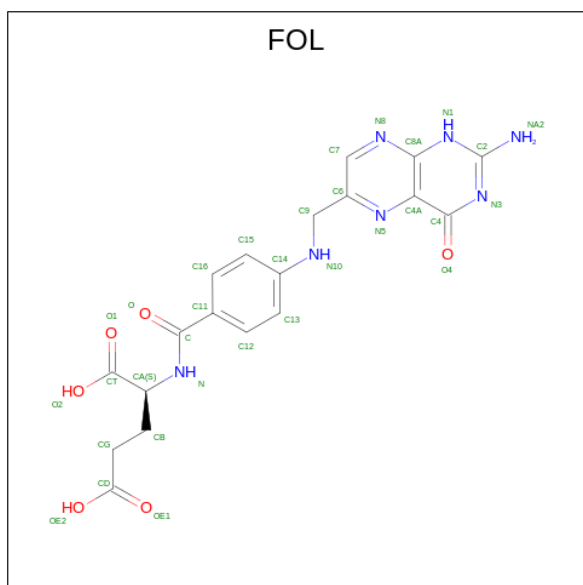
Mol	Chain	Residues	Atoms				AltConf	Trace
2	R	2	Total	C	N	O	0	0
			28	16	2	10		
2	S	2	Total	C	N	O	0	0
			28	16	2	10		
2	T	2	Total	C	N	O	0	0
			28	16	2	10		

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



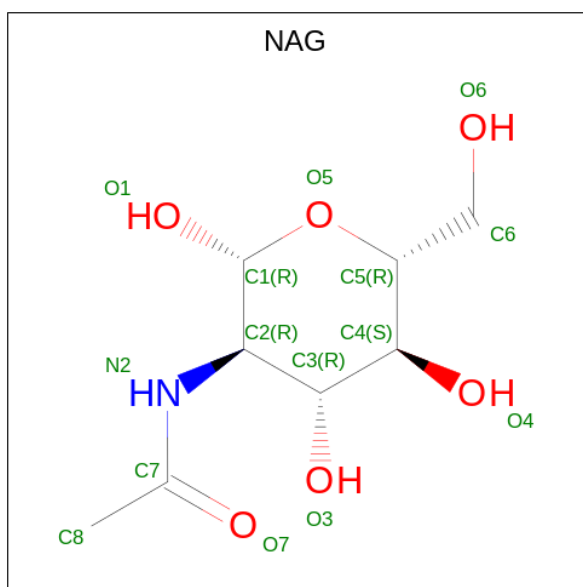
Mol	Chain	Residues	Atoms				AltConf	Trace
3	I	3	Total	C	N	O	0	0
			39	22	2	15		
3	O	3	Total	C	N	O	0	0
			39	22	2	15		
3	U	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			32	19	7	6	
4	B	1	Total	C	N	O	0
			32	19	7	6	
4	C	1	Total	C	N	O	0
			32	19	7	6	

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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	
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	

Continued on next page...

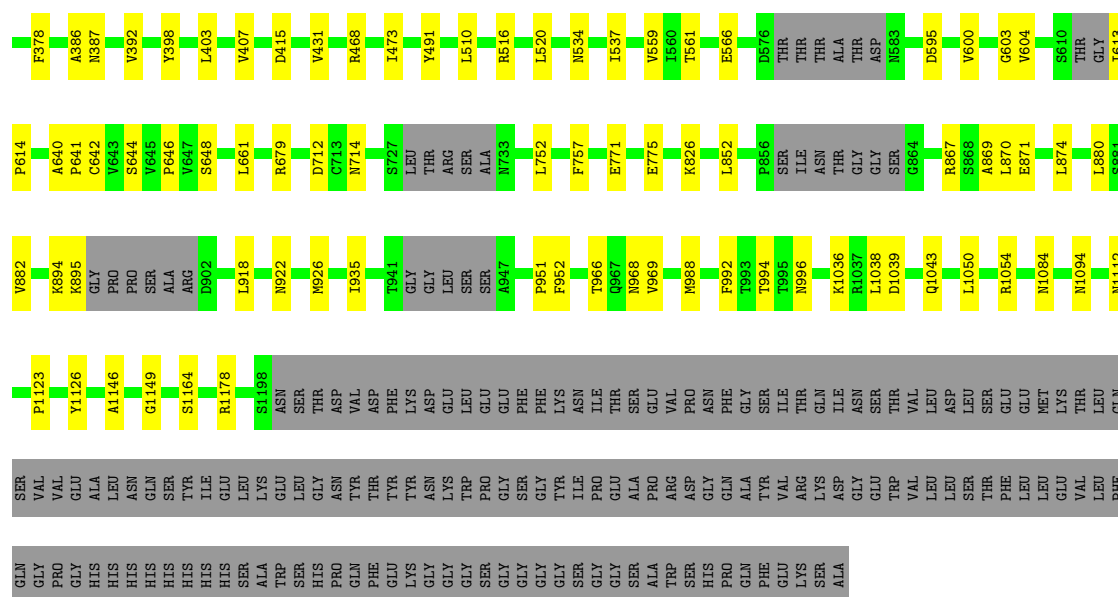
Continued from previous page...

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

Continued on next page...

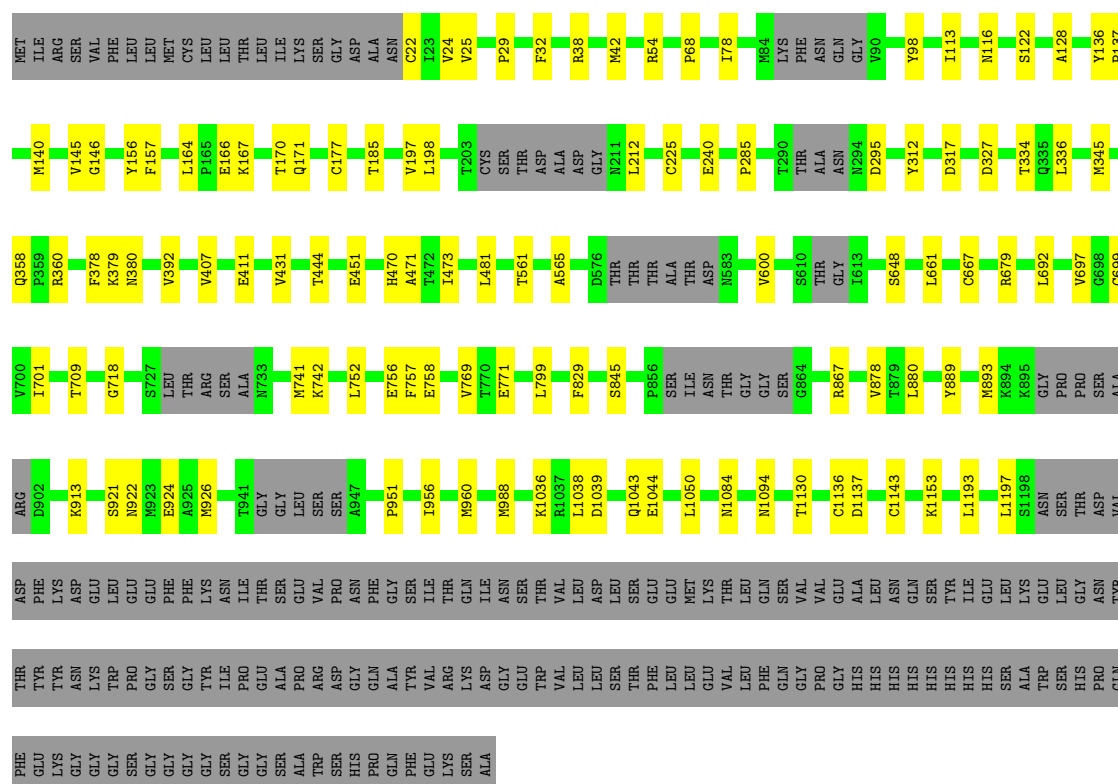
Continued from previous page...

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



• Molecule 1: Spike glycoprotein,Fibrin

Chain C: 76% 8% 16%



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

Chain D: 100%



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

Chain E:  100%



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

Chain F:  50% 50%



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

Chain G:  100%



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

Chain H:  100%



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

Chain J:  100%



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

Chain K:  100%



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

Chain L:  100%



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

Chain M:  50% 50%



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

Chain N:  100%



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

Chain P:  100%



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

Chain Q:  50% 50%



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

Chain R:  100%



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

Chain S:  100%



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

Chain T:  100%



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

Chain I:  67% 33%



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

Chain O:  67% 33%



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

Chain U:  67% 33%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	63700	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, FOL, 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	0.25	1/9043 (0.0%)	0.43	1/12272 (0.0%)
1	B	0.22	0/9043	0.40	0/12272
1	C	0.19	0/9043	0.40	0/12272
All	All	0.22	1/27129 (0.0%)	0.41	1/36816 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	224	ASP	CA-C	-5.63	1.45	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	VAL	N-CA-C	6.19	116.42	108.12

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8851	0	8533	80	0
1	B	8851	0	8533	79	0
1	C	8851	0	8533	70	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	28	0	25	0	0
2	E	28	0	25	0	0
2	F	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	J	28	0	25	0	0
2	K	28	0	25	0	0
2	L	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	0	0
2	P	28	0	25	0	0
2	Q	28	0	25	1	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
3	I	39	0	34	0	0
3	O	39	0	34	0	0
3	U	39	0	34	0	0
4	A	32	0	17	0	0
4	B	32	0	17	1	0
4	C	32	0	17	2	0
5	A	182	0	169	1	0
5	B	182	0	169	1	0
5	C	182	0	169	1	0
All	All	27732	0	26634	215	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 4.

All (215) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:752:LEU:HD13	1:C:757:PHE:HB3	1.71	0.71
1:B:180:GLN:NE2	1:B:223:LYS:HD2	2.05	0.71
1:C:29:PRO:HG2	2:Q:1:NAG:H62	1.75	0.68
1:C:648:SER:HB2	1:C:661:LEU:HB3	1.80	0.62
1:C:198:LEU:HD23	1:C:212:LEU:HD12	1.81	0.62
1:A:513:ILE:HG13	1:A:516:ARG:HH21	1.66	0.61
1:B:752:LEU:HD21	1:C:951:PRO:HD3	1.83	0.61
1:B:752:LEU:HD22	1:B:757:PHE:HB3	1.83	0.61
1:A:81:MET:HE1	1:A:295:ASP:HA	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:MET:HG3	1:A:162:VAL:HG12	1.82	0.60
1:B:95:ILE:HD13	1:B:197:VAL:HB	1.83	0.60
1:C:769:VAL:HG21	1:C:988:MET:HB2	1.84	0.60
1:C:758:GLU:HG2	1:C:1130:THR:HG22	1.83	0.59
1:B:81:MET:HE1	1:B:296:HIS:H	1.67	0.59
1:B:83:HIS:HA	1:B:125:VAL:HG21	1.85	0.59
1:A:410:ASP:OD1	1:A:439:LEU:HD11	2.03	0.59
1:A:752:LEU:HD13	1:A:757:PHE:HB3	1.84	0.58
1:C:166:GLU:HB2	1:C:171:GLN:HB3	1.85	0.57
1:B:566:GLU:N	1:B:566:GLU:OE2	2.36	0.57
1:A:951:PRO:HD3	1:C:752:LEU:HD21	1.87	0.57
1:A:378:PHE:HB3	1:A:481:LEU:HD13	1.87	0.57
1:A:327:ASP:OD2	1:A:679:ARG:NH2	2.36	0.57
1:A:478:SER:HB2	1:A:483:PHE:HB3	1.87	0.56
1:A:516:ARG:NH2	1:B:276:GLU:OE2	2.38	0.56
1:C:709:THR:HB	1:C:742:LYS:HB3	1.87	0.56
1:C:878:VAL:HG13	1:C:880:LEU:HD22	1.88	0.56
1:A:1194:PRO:HD2	1:A:1197:LEU:HD12	1.86	0.56
1:B:117:SER:HA	1:B:132:VAL:HG23	1.88	0.55
1:C:122:SER:H	4:C:1401:FOL:HN1	1.54	0.55
1:A:83:HIS:HA	1:A:125:VAL:HG21	1.89	0.55
1:B:935:ILE:HD11	1:B:952:PHE:HE1	1.71	0.55
1:C:411:GLU:HB3	1:C:470:HIS:HB2	1.89	0.55
1:A:68:PRO:O	1:A:312:TYR:OH	2.24	0.55
1:B:771:GLU:OE2	1:B:996:ASN:ND2	2.39	0.55
5:A:1410:NAG:H81	1:B:894:LYS:HD2	1.90	0.54
1:B:327:ASP:OD2	1:B:679:ARG:NH2	2.41	0.54
1:A:722:CYS:SG	1:A:723:ALA:N	2.80	0.54
1:A:1089:SER:OG	1:A:1090:GLN:N	2.41	0.54
1:C:799:LEU:HD21	1:C:1044:GLU:HA	1.90	0.54
1:B:68:PRO:O	1:B:312:TYR:OH	2.27	0.53
1:C:1136:CYS:HB3	1:C:1143:CYS:HA	1.90	0.53
1:C:1136:CYS:HA	1:C:1197:LEU:HD13	1.91	0.53
1:B:407:VAL:HG12	1:B:473:ILE:HG12	1.91	0.52
1:B:1123:PRO:HB2	1:B:1126:TYR:HE1	1.75	0.52
1:B:510:LEU:HD23	1:B:516:ARG:HH12	1.75	0.52
1:C:358:GLN:OE1	1:C:360:ARG:NH2	2.43	0.52
1:A:144:VAL:HG13	1:A:157:PHE:HB2	1.92	0.52
1:B:132:VAL:HG12	1:B:298:ALA:HB3	1.93	0.51
1:C:22:CYS:N	1:C:185:THR:O	2.42	0.51
1:A:410:ASP:OD2	1:A:439:LEU:HD21	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1038:LEU:O	1:A:1043:GLN:NE2	2.44	0.51
1:A:1094:ASN:O	1:B:1084:ASN:ND2	2.44	0.51
1:C:146:GLY:HA3	1:C:157:PHE:HE2	1.76	0.51
1:A:810:ILE:HD12	1:A:1062:VAL:HG21	1.92	0.51
1:A:407:VAL:HG12	1:A:473:ILE:HG12	1.91	0.51
1:A:697:VAL:HG11	1:A:718:GLY:HA3	1.93	0.51
1:B:40:ILE:HG22	1:B:72:ASP:H	1.75	0.51
1:A:290:THR:HA	1:A:297:MET:HE1	1.93	0.50
1:C:697:VAL:HG11	1:C:718:GLY:HA3	1.93	0.50
1:A:385:ILE:HD13	1:A:453:ILE:HD12	1.93	0.50
1:A:410:ASP:CG	1:A:439:LEU:HD11	2.37	0.50
1:A:1084:ASN:ND2	1:C:1094:ASN:O	2.45	0.50
1:B:223:LYS:HG2	1:B:224:ASP:N	2.27	0.50
1:A:410:ASP:O	1:A:411:GLU:HB2	2.11	0.50
1:A:752:LEU:HD21	1:B:951:PRO:HD3	1.94	0.50
1:A:960:MET:HE1	1:A:977:ILE:HG21	1.93	0.50
1:A:128:ALA:HB3	1:A:295:ASP:HB3	1.93	0.49
1:C:327:ASP:OD2	1:C:679:ARG:NH2	2.41	0.49
1:C:378:PHE:HB3	1:C:481:LEU:HD13	1.92	0.49
1:A:102:THR:HG21	1:A:145:VAL:HG11	1.93	0.49
1:A:392:VAL:HG22	1:A:431:VAL:HG22	1.93	0.49
1:B:566:GLU:HG2	1:C:54:ARG:HD2	1.95	0.49
1:C:98:TYR:HB2	1:C:285:PRO:HG3	1.94	0.49
1:B:966:THR:HG22	1:B:968:ASN:H	1.77	0.49
1:B:201:ASN:HA	1:B:289:LYS:HB3	1.95	0.49
1:B:392:VAL:HG22	1:B:431:VAL:HG22	1.94	0.49
1:B:144:VAL:HG13	1:B:157:PHE:HB2	1.94	0.49
1:C:136:TYR:OH	1:C:240:GLU:OE1	2.29	0.49
1:C:752:LEU:HD23	1:C:752:LEU:H	1.77	0.48
1:C:756:GLU:OE2	1:C:1153:LYS:NZ	2.46	0.48
1:A:156:TYR:HB3	1:A:160:THR:HG21	1.95	0.48
1:B:24:VAL:HB	5:B:1405:NAG:H83	1.94	0.48
1:B:1146:ALA:O	1:B:1178:ARG:NH1	2.47	0.48
1:C:1137:ASP:OD1	1:C:1137:ASP:N	2.42	0.48
1:C:392:VAL:HG22	1:C:431:VAL:HG22	1.95	0.48
1:B:431:VAL:HB	1:B:561:THR:HB	1.96	0.47
1:A:661:LEU:HA	1:A:700:VAL:HG12	1.94	0.47
1:A:1036:LYS:HD3	1:C:600:VAL:HG11	1.95	0.47
1:C:407:VAL:HG12	1:C:473:ILE:HG12	1.95	0.47
1:A:648:SER:HB2	1:A:661:LEU:HB3	1.96	0.47
1:C:1193:LEU:HD12	1:C:1197:LEU:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:874:LEU:HD21	1:B:992:PHE:HZ	1.80	0.47
1:A:1019:GLU:HG3	1:A:1057:SER:HB2	1.97	0.47
1:B:874:LEU:HD21	1:B:992:PHE:CZ	2.50	0.47
1:C:128:ALA:HB1	1:C:295:ASP:HB3	1.96	0.46
1:A:407:VAL:HB	1:A:471:ALA:HB1	1.96	0.46
1:B:1149:GLY:HA2	1:B:1164:SER:HB3	1.95	0.46
1:C:25:VAL:HG11	1:C:197:VAL:HG21	1.98	0.46
1:C:692:LEU:HD23	1:C:701:ILE:HB	1.96	0.46
1:A:364:TYR:HD1	1:A:595:ASP:HB3	1.80	0.46
1:B:364:TYR:HD1	1:B:595:ASP:HB3	1.81	0.46
1:B:966:THR:HB	1:B:969:VAL:HG23	1.98	0.46
1:B:752:LEU:HD22	1:B:757:PHE:CB	2.44	0.46
1:B:1094:ASN:O	1:C:1084:ASN:ND2	2.48	0.46
1:A:38:ARG:O	1:A:305:TYR:OH	2.29	0.46
1:C:444:THR:HG22	1:C:451:GLU:HG3	1.98	0.45
1:A:221:ASP:OD1	1:A:221:ASP:N	2.44	0.45
1:A:1136:CYS:HB3	1:A:1143:CYS:HA	1.99	0.45
1:B:468:ARG:HG3	1:B:559:VAL:HG22	1.98	0.45
1:B:874:LEU:HD23	1:B:992:PHE:HE2	1.82	0.45
1:B:895:LYS:HB2	1:B:895:LYS:HE3	1.78	0.45
1:B:58:ASN:HD22	1:B:318:VAL:HG12	1.80	0.45
1:C:38:ARG:HE	1:C:116:ASN:HD21	1.64	0.45
1:A:769:VAL:HG22	1:A:1119:VAL:HG22	1.99	0.45
1:A:923:MET:HE1	1:C:741:MET:HB3	1.99	0.45
1:A:111:VAL:HG22	1:A:304:ILE:HG12	1.99	0.45
1:A:600:VAL:HG21	1:B:1036:LYS:HD2	1.98	0.45
1:A:123:SER:OG	1:A:125:VAL:O	2.35	0.45
1:C:1039:ASP:OD1	1:C:1039:ASP:N	2.47	0.45
1:B:600:VAL:HG21	1:C:1036:LYS:HD2	2.00	0.44
1:C:68:PRO:O	1:C:312:TYR:OH	2.25	0.44
1:C:431:VAL:HB	1:C:561:THR:HB	1.99	0.44
1:A:852:LEU:HG	1:A:870:LEU:HB2	1.99	0.44
1:A:372:CYS:HB2	1:A:398:TYR:HA	1.99	0.44
1:C:317:ASP:OD1	1:C:317:ASP:C	2.60	0.44
1:C:1038:LEU:O	1:C:1043:GLN:NE2	2.49	0.44
1:C:407:VAL:HB	1:C:471:ALA:HB1	2.00	0.44
1:A:386:ALA:HB2	1:A:491:TYR:HA	1.98	0.44
1:A:549:THR:HG23	1:A:551:GLU:H	1.83	0.44
1:C:692:LEU:HB3	1:C:699:CYS:SG	2.58	0.44
1:A:789:VAL:O	1:A:1054:ARG:NH1	2.51	0.44
1:B:922:ASN:O	1:B:926:MET:HG3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:GLN:NE2	1:B:276:GLU:O	2.42	0.44
1:A:53:GLY:HA2	1:C:565:ALA:HB1	1.99	0.43
1:B:327:ASP:HB3	1:B:330:ALA:HB2	2.00	0.43
1:B:378:PHE:HZ	1:B:403:LEU:HA	1.83	0.43
1:B:386:ALA:HB2	1:B:491:TYR:HA	1.98	0.43
1:A:902:ASP:HB3	1:A:905:CYS:HB2	2.01	0.43
1:B:54:ARG:HG2	1:B:56:TYR:CZ	2.54	0.43
1:A:28:GLN:HB3	1:A:94:PHE:HE1	1.83	0.43
1:B:880:LEU:HB3	1:B:882:VAL:HG23	2.01	0.43
1:C:167:LYS:HB2	1:C:170:THR:HG22	2.01	0.43
1:C:829:PHE:CZ	1:C:924:GLU:HG2	2.53	0.43
1:C:922:ASN:O	1:C:926:MET:HG3	2.18	0.43
1:C:113:ILE:HD13	1:C:137:PRO:HD2	2.00	0.43
1:A:501:LYS:HE2	1:A:501:LYS:HB2	1.82	0.43
1:A:665:VAL:HG22	1:A:666:ALA:H	1.84	0.43
1:C:164:LEU:HD13	1:C:212:LEU:HB3	2.00	0.43
1:A:49:ILE:HD13	1:A:266:MET:HE3	2.00	0.43
1:B:372:CYS:HB2	1:B:398:TYR:HA	2.00	0.43
1:C:177:CYS:HB3	1:C:225:CYS:HA	2.00	0.43
1:C:867:ARG:HH21	1:C:921:SER:HB2	1.83	0.43
1:A:82:TYR:HA	1:A:93:PRO:HA	2.01	0.43
1:A:417:THR:HG23	1:A:465:PRO:HB3	2.00	0.43
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.87	0.42
1:B:712:ASP:OD1	1:B:712:ASP:N	2.52	0.42
1:C:667:CYS:HB2	1:C:699:CYS:HB2	1.67	0.42
1:B:111:VAL:HG22	1:B:304:ILE:HG12	2.01	0.42
1:B:852:LEU:HG	1:B:870:LEU:HB2	2.01	0.42
1:C:956:ILE:O	1:C:960:MET:HG3	2.18	0.42
1:A:956:ILE:HG12	1:A:960:MET:HE2	2.02	0.42
1:B:852:LEU:HA	1:B:869:ALA:HB3	2.01	0.42
1:B:146:GLY:HA3	1:B:157:PHE:HE2	1.84	0.42
1:A:803:TYR:OH	1:A:1052:ASN:ND2	2.48	0.42
1:B:196:TYR:HE1	1:B:284:MET:HG2	1.83	0.42
1:B:775:GLU:HG3	1:B:1112:ASN:HB3	2.02	0.42
1:B:988:MET:HE2	1:B:988:MET:HB3	1.97	0.42
1:A:175:LEU:HB3	1:A:228:GLU:HG3	2.02	0.42
1:A:556:MET:HE3	1:A:556:MET:HB3	1.85	0.42
1:A:263:SER:OG	1:A:264:ASN:N	2.52	0.42
1:B:996:ASN:OD1	1:B:996:ASN:N	2.52	0.42
1:C:140:MET:HG2	1:C:156:TYR:CE2	2.55	0.42
1:A:387:ASN:HB2	1:A:520:LEU:HD11	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ASP:OD1	1:A:622:SER:N	2.51	0.41
1:B:613:ILE:HA	1:B:614:PRO:HD3	1.89	0.41
1:B:867:ARG:HD3	1:B:871:GLU:HB3	2.02	0.41
1:C:379:LYS:HG3	1:C:380:ASN:OD1	2.20	0.41
1:C:845:SER:O	1:C:845:SER:OG	2.34	0.41
1:B:387:ASN:HB2	1:B:520:LEU:HD11	2.03	0.41
1:B:534:ASN:ND2	1:C:145:VAL:O	2.54	0.41
1:B:1039:ASP:N	1:B:1039:ASP:OD1	2.53	0.41
1:A:197:VAL:HG12	1:A:199:VAL:HG13	2.01	0.41
1:A:317:ASP:OD1	1:A:317:ASP:C	2.63	0.41
1:B:648:SER:HB2	1:B:661:LEU:HB3	2.01	0.41
1:C:42:MET:HE1	1:C:334:THR:HG21	2.02	0.41
1:C:889:TYR:CZ	1:C:893:MET:HG3	2.55	0.41
1:A:672:MET:H	1:A:672:MET:HG3	1.66	0.41
1:B:537:ILE:HD13	1:B:537:ILE:HA	1.96	0.41
1:B:646:PRO:HG3	1:C:913:LYS:HD3	2.02	0.41
1:B:1038:LEU:O	1:B:1043:GLN:NE2	2.54	0.41
1:A:742:LYS:HB2	1:A:742:LYS:HE2	1.90	0.41
1:A:1039:ASP:OD1	1:A:1039:ASP:N	2.53	0.41
1:B:297:MET:SD	1:B:297:MET:N	2.94	0.41
1:B:317:ASP:OD1	1:B:317:ASP:C	2.64	0.41
1:B:603:GLY:HA2	1:B:642:CYS:HB2	2.03	0.41
1:C:771:GLU:H	1:C:771:GLU:HG2	1.69	0.41
1:A:264:ASN:N	1:A:264:ASN:OD1	2.46	0.41
1:A:826:LYS:HG3	1:A:918:LEU:HD21	2.02	0.41
1:C:32:PHE:HD2	1:C:78:ILE:HB	1.86	0.41
1:A:587:LEU:HB3	1:A:592:ILE:HG21	2.02	0.41
1:A:1135:LEU:HG	1:A:1151:PHE:CD2	2.56	0.41
4:C:1401:FOL:H15	4:C:1401:FOL:H91	1.87	0.41
1:B:826:LYS:HG3	1:B:918:LEU:HD21	2.03	0.40
1:B:1050:LEU:O	1:B:1054:ARG:HG2	2.21	0.40
1:C:336:LEU:HG	1:C:345:MET:HE3	2.03	0.40
1:A:63:LEU:HD23	1:A:63:LEU:HA	1.92	0.40
1:A:223:LYS:O	1:A:224:ASP:HB3	2.21	0.40
1:B:200:GLU:HG3	1:B:288:ILE:HG23	2.02	0.40
1:B:604:VAL:HG22	1:B:640:ALA:HB3	2.02	0.40
1:B:116:ASN:ND2	4:B:1401:FOL:O4	2.52	0.40
1:A:32:PHE:HA	1:A:78:ILE:HD11	2.03	0.40
1:B:641:PRO:HD2	1:B:644:SER:HB3	2.03	0.40
1:B:714:ASN:OD1	1:B:714:ASN:N	2.53	0.40
1:C:24:VAL:HG23	5:C:1404:NAG:H4	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1050:LEU:HD23	1:C:1050:LEU:HA	1.97	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	1111/1349 (82%)	1059 (95%)	52 (5%)	0	100	100
1	B	1111/1349 (82%)	1062 (96%)	48 (4%)	1 (0%)	48	76
1	C	1111/1349 (82%)	1062 (96%)	49 (4%)	0	100	100
All	All	3333/4047 (82%)	3183 (96%)	149 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	994	THR

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	985/1165 (84%)	983 (100%)	2 (0%)	92	95
1	B	985/1165 (84%)	983 (100%)	2 (0%)	92	95

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	985/1165 (84%)	985 (100%)	0	100	100
All	All	2955/3495 (84%)	2951 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	672	MET
1	A	891	GLU
1	B	221	ASP
1	B	415	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	107	ASN
1	A	211	ASN
1	A	308	HIS
1	A	524	ASN
1	A	779	GLN
1	A	798	GLN
1	A	811	ASN
1	A	907	GLN
1	A	997	GLN
1	A	1046	GLN
1	A	1109	ASN
1	B	159	HIS
1	B	180	GLN
1	B	311	ASN
1	B	524	ASN
1	B	532	ASN
1	B	570	ASN
1	B	625	ASN
1	B	791	ASN
1	B	798	GLN
1	B	974	GLN
1	B	989	GLN
1	B	1052	ASN
1	B	1077	GLN
1	B	1084	ASN
1	B	1109	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1174	ASN
1	B	1192	ASN
1	C	107	ASN
1	C	159	HIS
1	C	190	HIS
1	C	384	GLN
1	C	512	ASN
1	C	524	ASN
1	C	563	ASN
1	C	569	ASN
1	C	798	GLN
1	C	1052	ASN
1	C	1084	ASN
1	C	1112	ASN
1	C	1140	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

39 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	D	1	1,2	14,14,15	0.29	0	17,19,21	0.49	0
2	NAG	D	2	2	14,14,15	0.26	0	17,19,21	0.46	0
2	NAG	E	1	1,2	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	E	2	2	14,14,15	0.30	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	F	1	1,2	14,14,15	0.30	0	17,19,21	0.90	1 (5%)
2	NAG	F	2	2	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	G	1	1,2	14,14,15	0.30	0	17,19,21	0.59	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.45	0
2	NAG	H	1	1,2	14,14,15	0.26	0	17,19,21	0.43	0
2	NAG	H	2	2	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	I	1	3,1	14,14,15	0.25	0	17,19,21	0.50	0
3	NAG	I	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	I	3	3	11,11,12	0.58	0	15,15,17	0.91	1 (6%)
2	NAG	J	1	1,2	14,14,15	0.27	0	17,19,21	0.51	0
2	NAG	J	2	2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	K	1	1,2	14,14,15	0.26	0	17,19,21	0.44	0
2	NAG	K	2	2	14,14,15	0.26	0	17,19,21	0.53	0
2	NAG	L	1	1,2	14,14,15	0.23	0	17,19,21	0.55	0
2	NAG	L	2	2	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	M	1	1,2	14,14,15	0.30	0	17,19,21	0.68	1 (5%)
2	NAG	M	2	2	14,14,15	0.31	0	17,19,21	0.43	0
2	NAG	N	1	1,2	14,14,15	0.27	0	17,19,21	0.43	0
2	NAG	N	2	2	14,14,15	0.22	0	17,19,21	0.49	0
3	NAG	O	1	3,1	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	O	2	3	14,14,15	0.20	0	17,19,21	0.43	0
3	BMA	O	3	3	11,11,12	0.56	0	15,15,17	0.96	1 (6%)
2	NAG	P	1	1,2	14,14,15	0.30	0	17,19,21	0.51	0
2	NAG	P	2	2	14,14,15	0.26	0	17,19,21	0.45	0
2	NAG	Q	1	1,2	14,14,15	0.23	0	17,19,21	0.45	0
2	NAG	Q	2	2	14,14,15	0.43	0	17,19,21	0.50	0
2	NAG	R	1	1,2	14,14,15	0.25	0	17,19,21	0.56	0
2	NAG	R	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	S	1	1,2	14,14,15	0.30	0	17,19,21	0.58	0
2	NAG	S	2	2	14,14,15	0.27	0	17,19,21	0.43	0
2	NAG	T	1	1,2	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	T	2	2	14,14,15	0.25	0	17,19,21	0.47	0
3	NAG	U	1	3,1	14,14,15	0.24	0	17,19,21	0.48	0
3	NAG	U	2	3	14,14,15	0.21	0	17,19,21	0.44	0
3	BMA	U	3	3	11,11,12	0.61	0	15,15,17	0.87	1 (6%)

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

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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	U	2	3	-	2/6/23/26	0/1/1/1
3	BMA	U	3	3	-	1/2/19/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	2.51	126.47	122.90
3	O	3	BMA	C1-O5-C5	2.33	115.35	112.19
2	M	1	NAG	C1-O5-C5	2.21	115.19	112.19
3	I	3	BMA	C1-O5-C5	2.15	115.10	112.19
3	U	3	BMA	C1-O5-C5	2.11	115.05	112.19

There are no chirality outliers.

All (60) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	F	2	NAG	C4-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	N	1	NAG	O5-C5-C6-O6
2	L	1	NAG	O5-C5-C6-O6
2	T	1	NAG	O5-C5-C6-O6
2	F	2	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	2	NAG	O5-C5-C6-O6
2	N	2	NAG	O5-C5-C6-O6
2	R	2	NAG	O5-C5-C6-O6
2	L	1	NAG	C4-C5-C6-O6
2	T	1	NAG	C4-C5-C6-O6
2	N	1	NAG	C4-C5-C6-O6
2	K	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

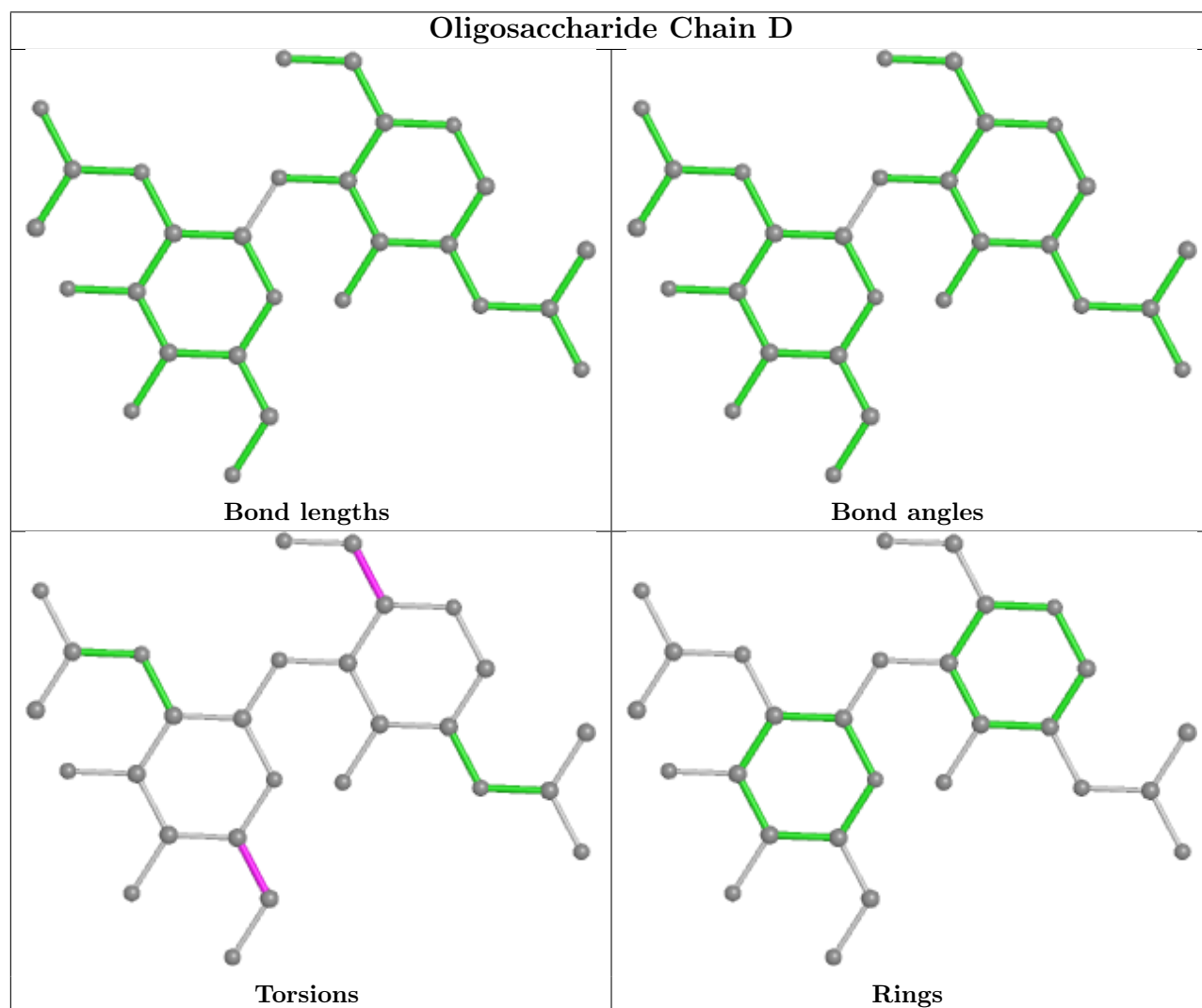
Mol	Chain	Res	Type	Atoms
3	O	3	BMA	O5-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
2	M	1	NAG	C8-C7-N2-C2
2	M	1	NAG	O7-C7-N2-C2
2	Q	1	NAG	C8-C7-N2-C2
2	Q	1	NAG	O7-C7-N2-C2
2	J	1	NAG	O5-C5-C6-O6
3	O	1	NAG	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	P	1	NAG	O5-C5-C6-O6
2	J	1	NAG	C4-C5-C6-O6
3	O	1	NAG	C4-C5-C6-O6
2	Q	2	NAG	O5-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	P	1	NAG	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
3	U	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
2	P	2	NAG	C4-C5-C6-O6
2	P	2	NAG	O5-C5-C6-O6
3	O	2	NAG	C4-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	J	2	NAG	O5-C5-C6-O6
3	U	2	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
2	L	2	NAG	O5-C5-C6-O6
2	M	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
3	O	2	NAG	O5-C5-C6-O6
2	Q	1	NAG	C4-C5-C6-O6
3	I	3	BMA	O5-C5-C6-O6
2	Q	1	NAG	O5-C5-C6-O6
3	U	3	BMA	O5-C5-C6-O6
2	F	1	NAG	C3-C2-N2-C7
3	O	3	BMA	C4-C5-C6-O6

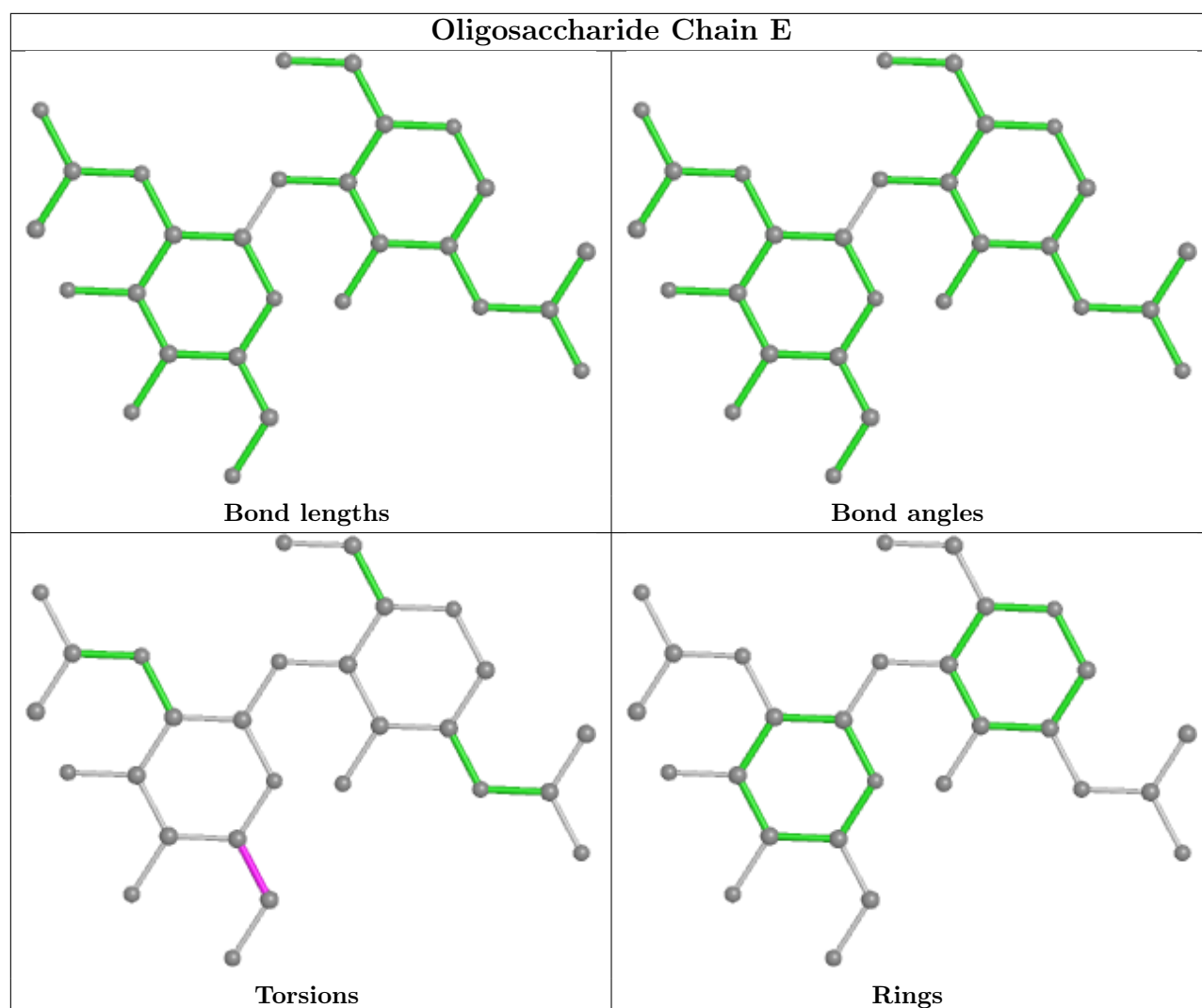
There are no ring outliers.

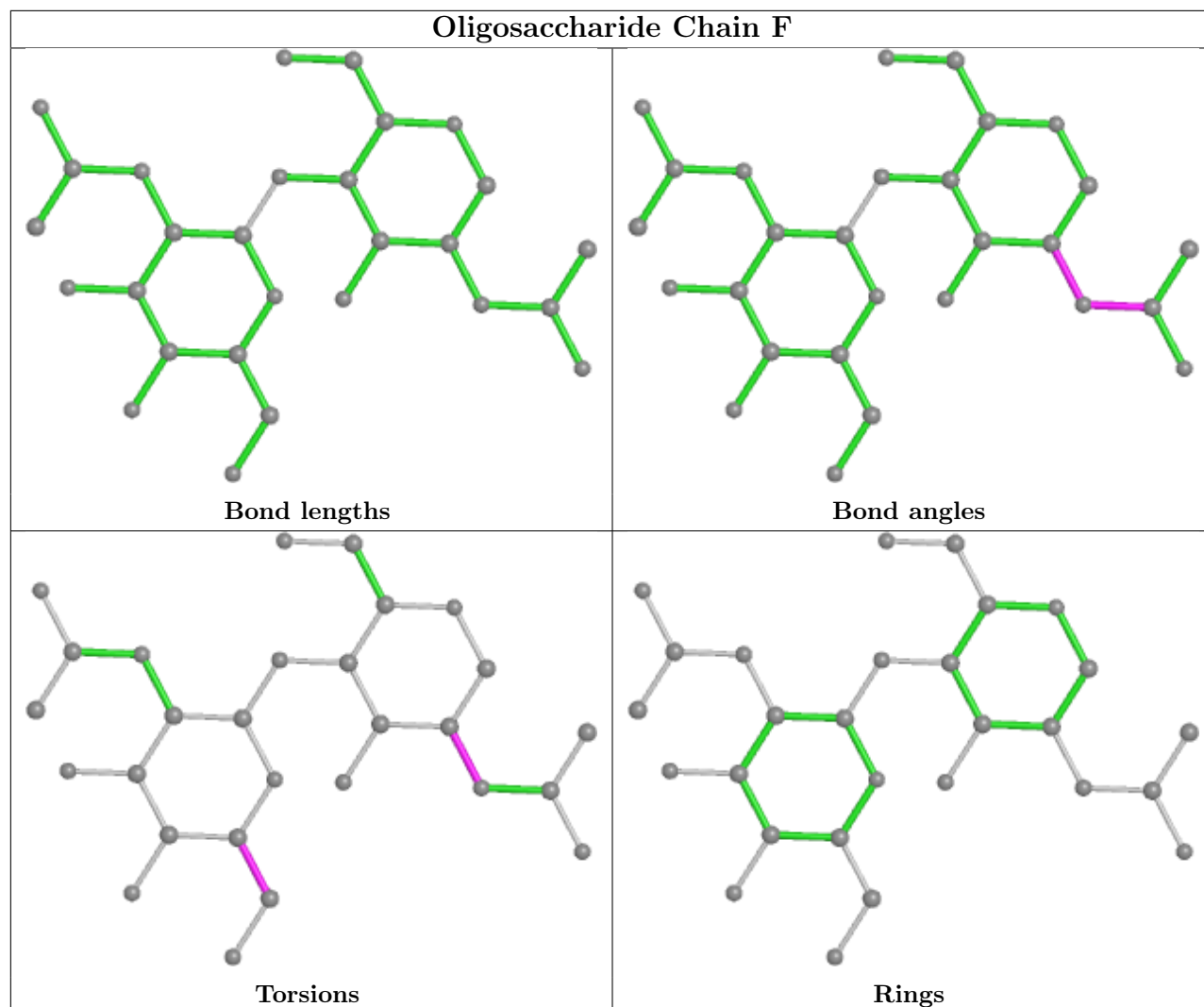
1 monomer is involved in 1 short contact:

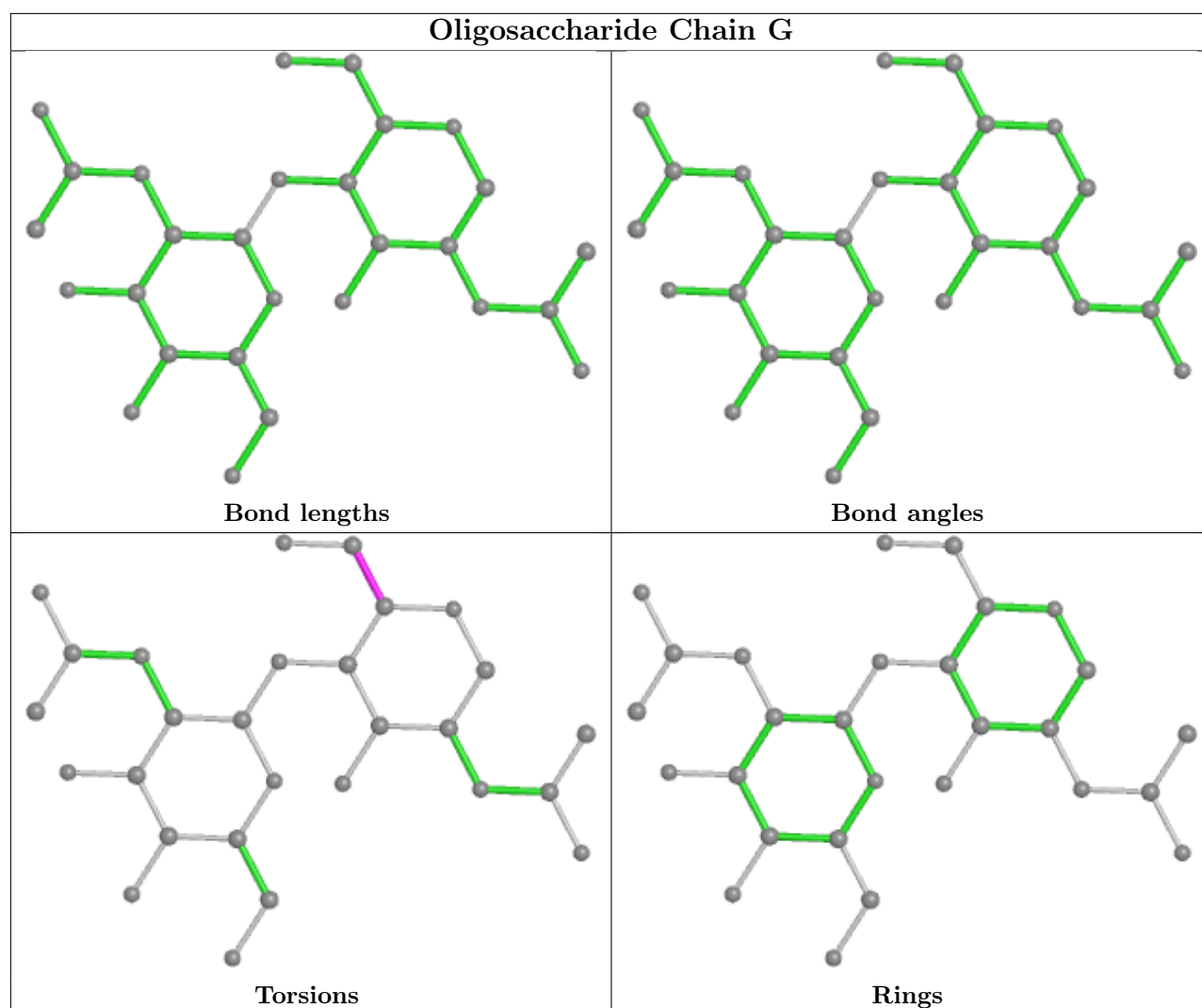
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	Q	1	NAG	1	0

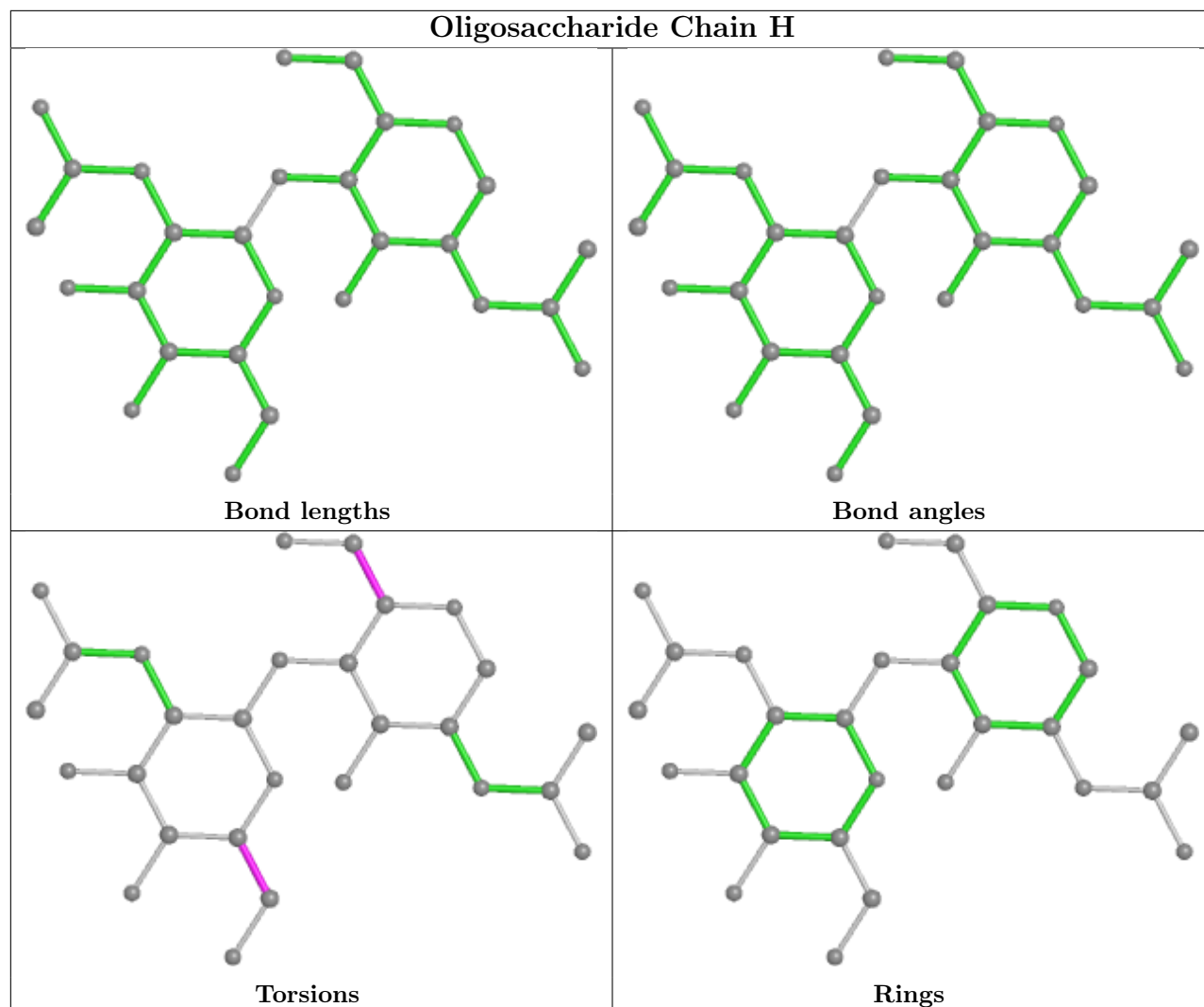
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

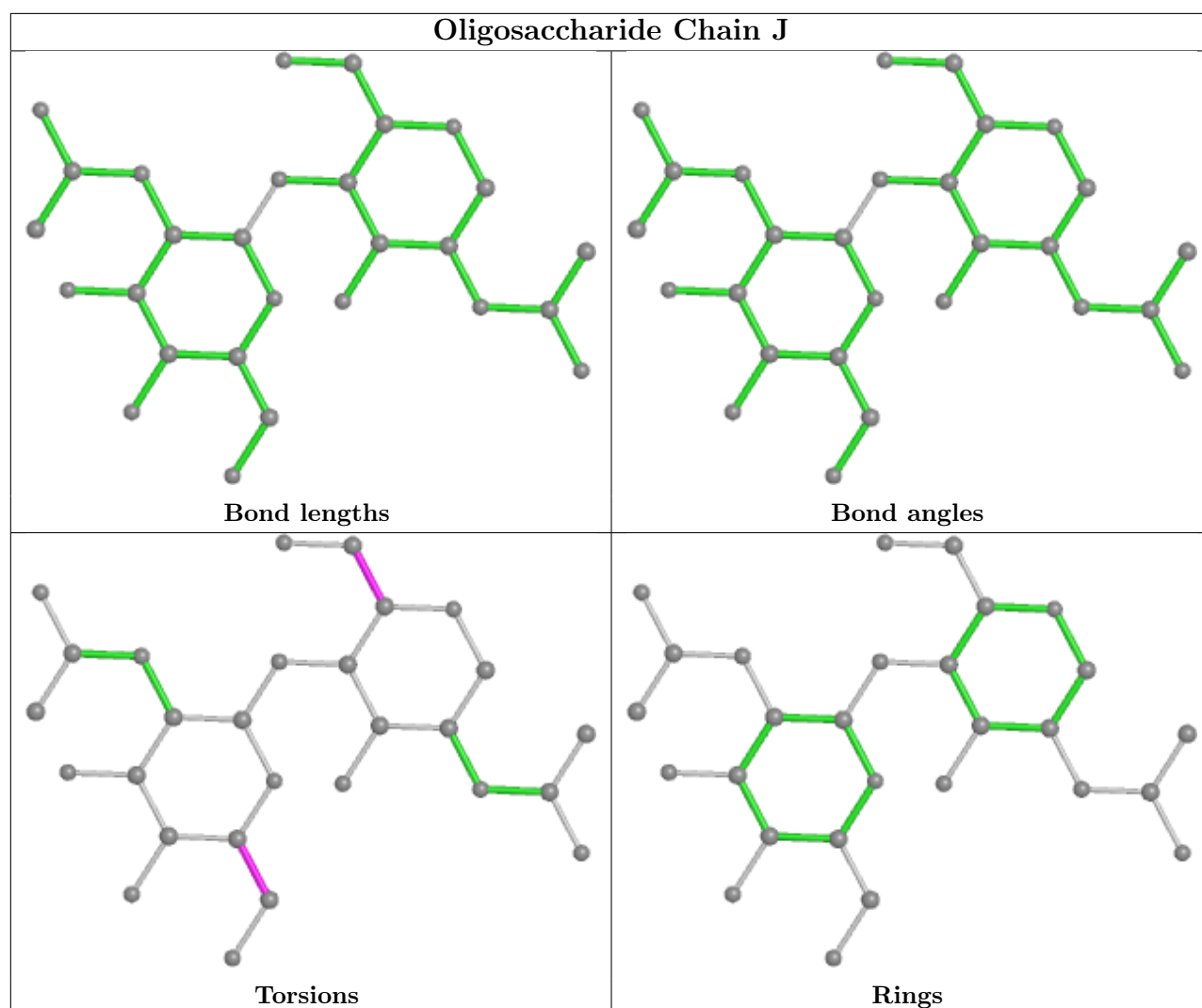


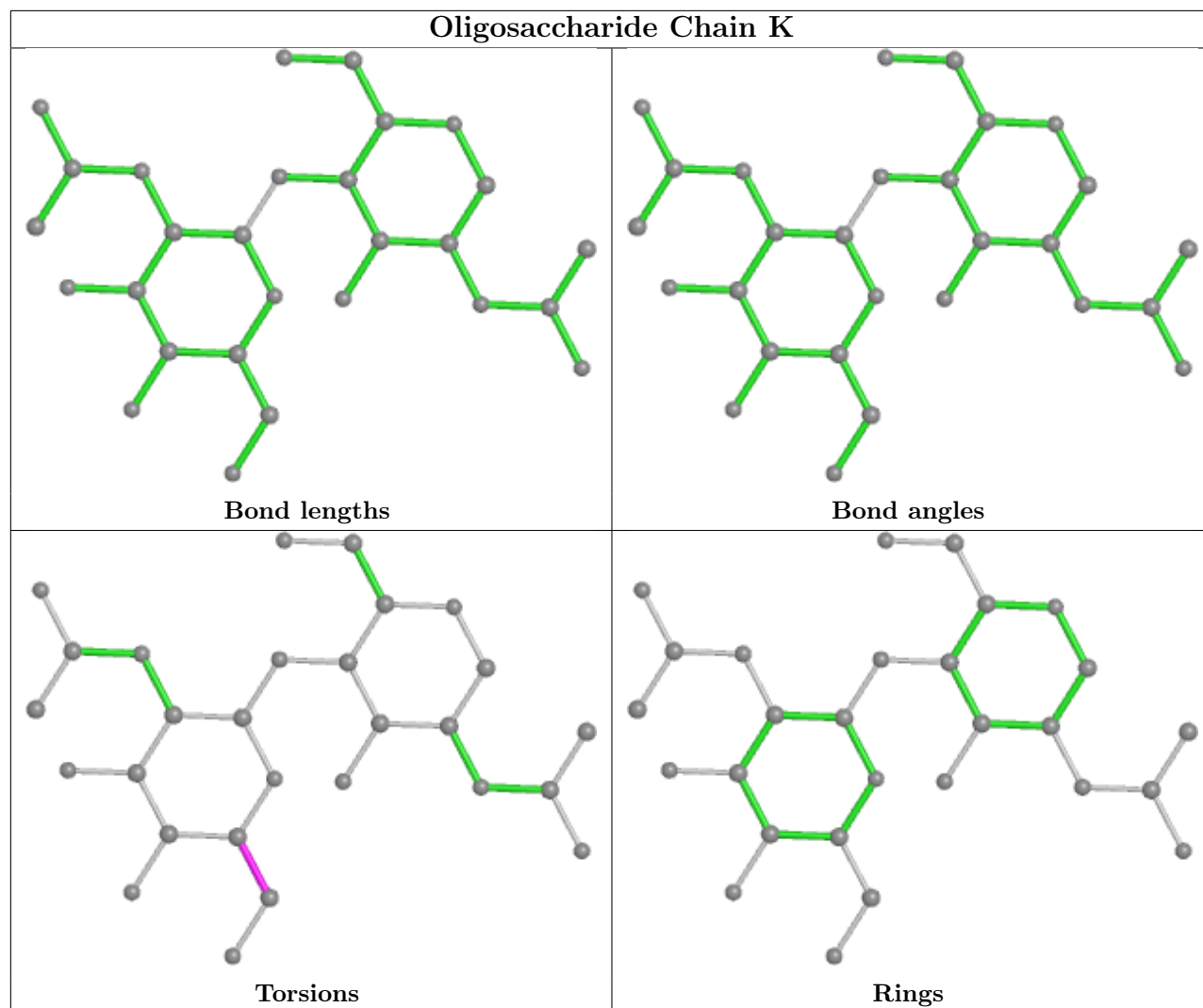


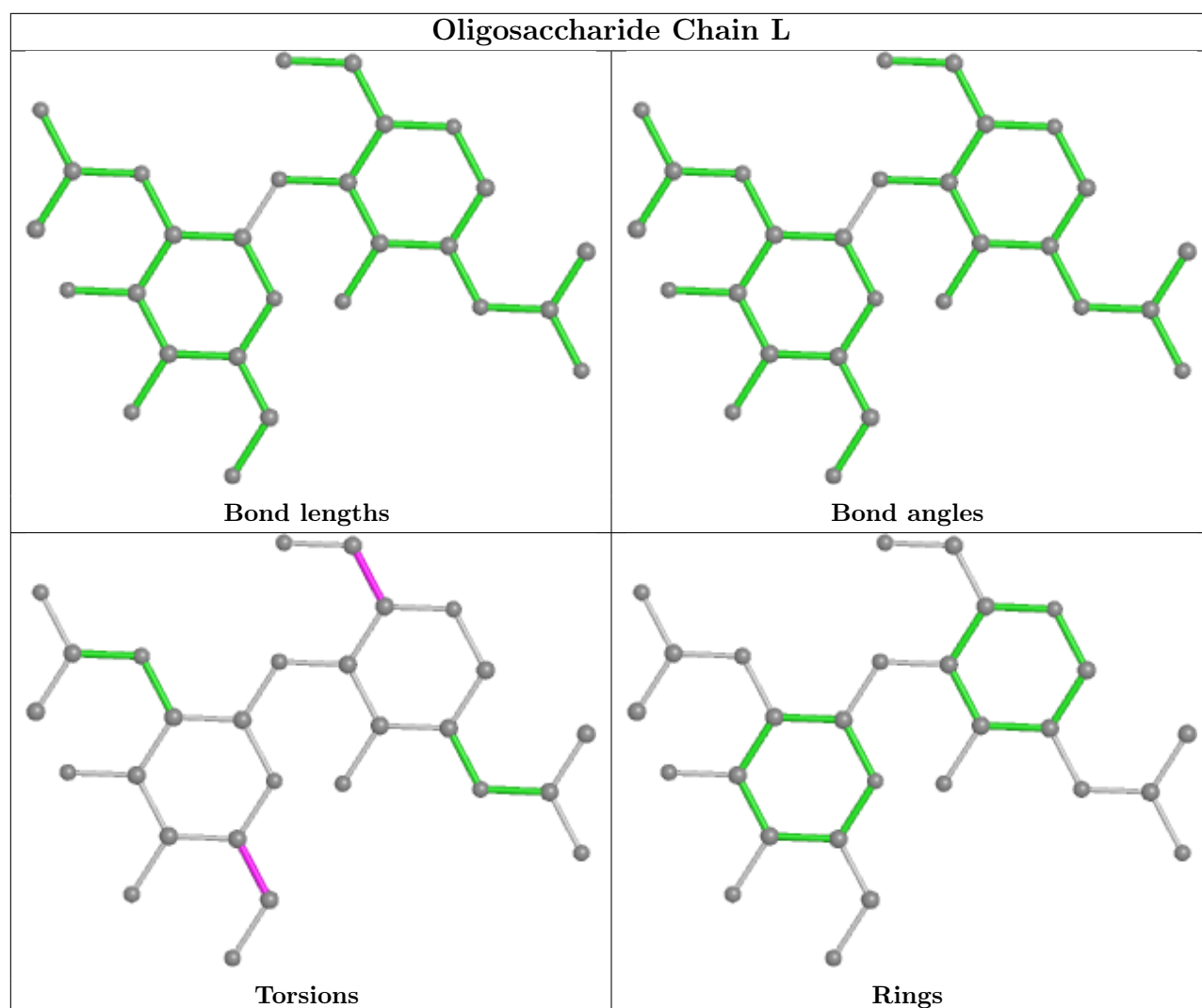


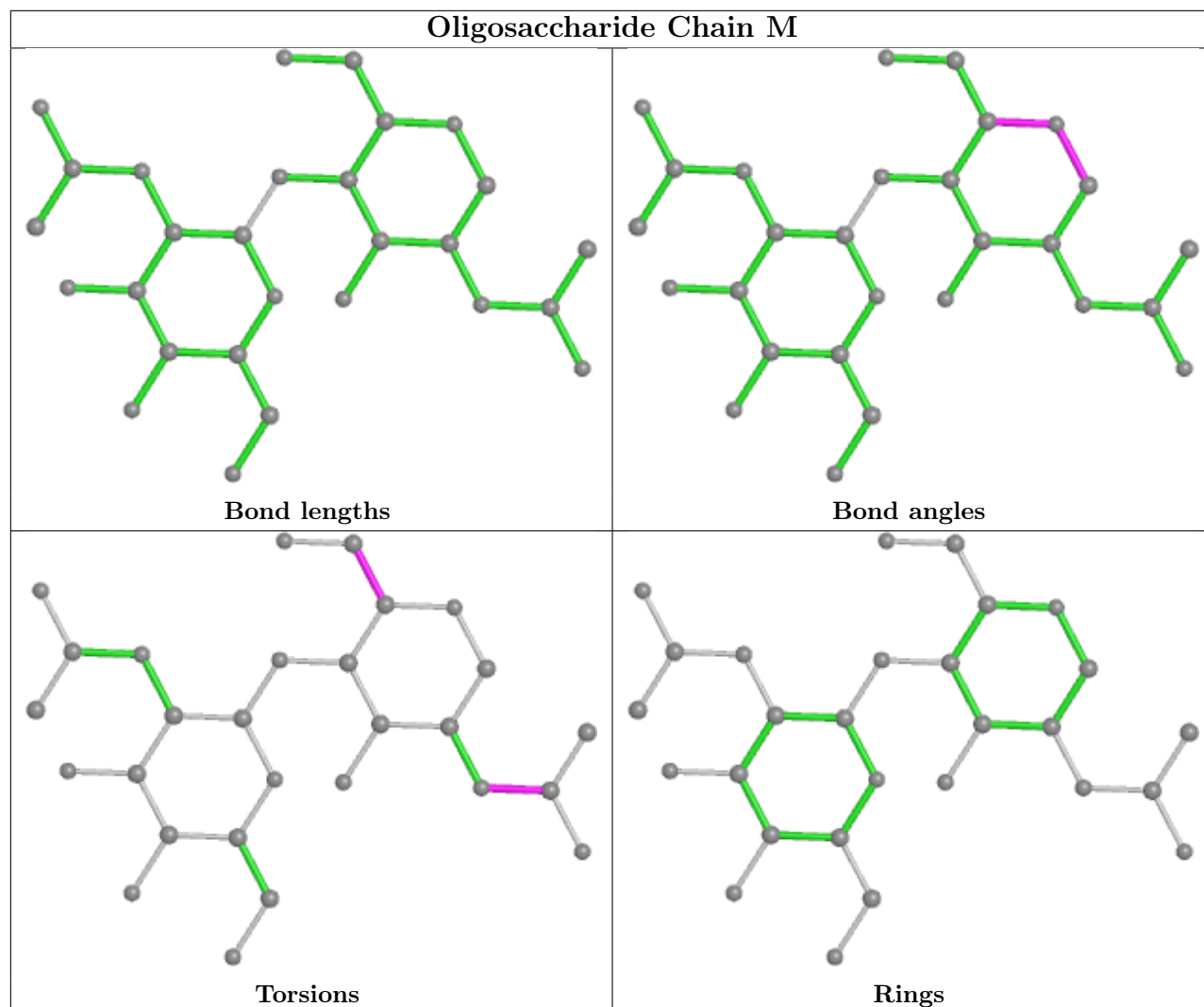


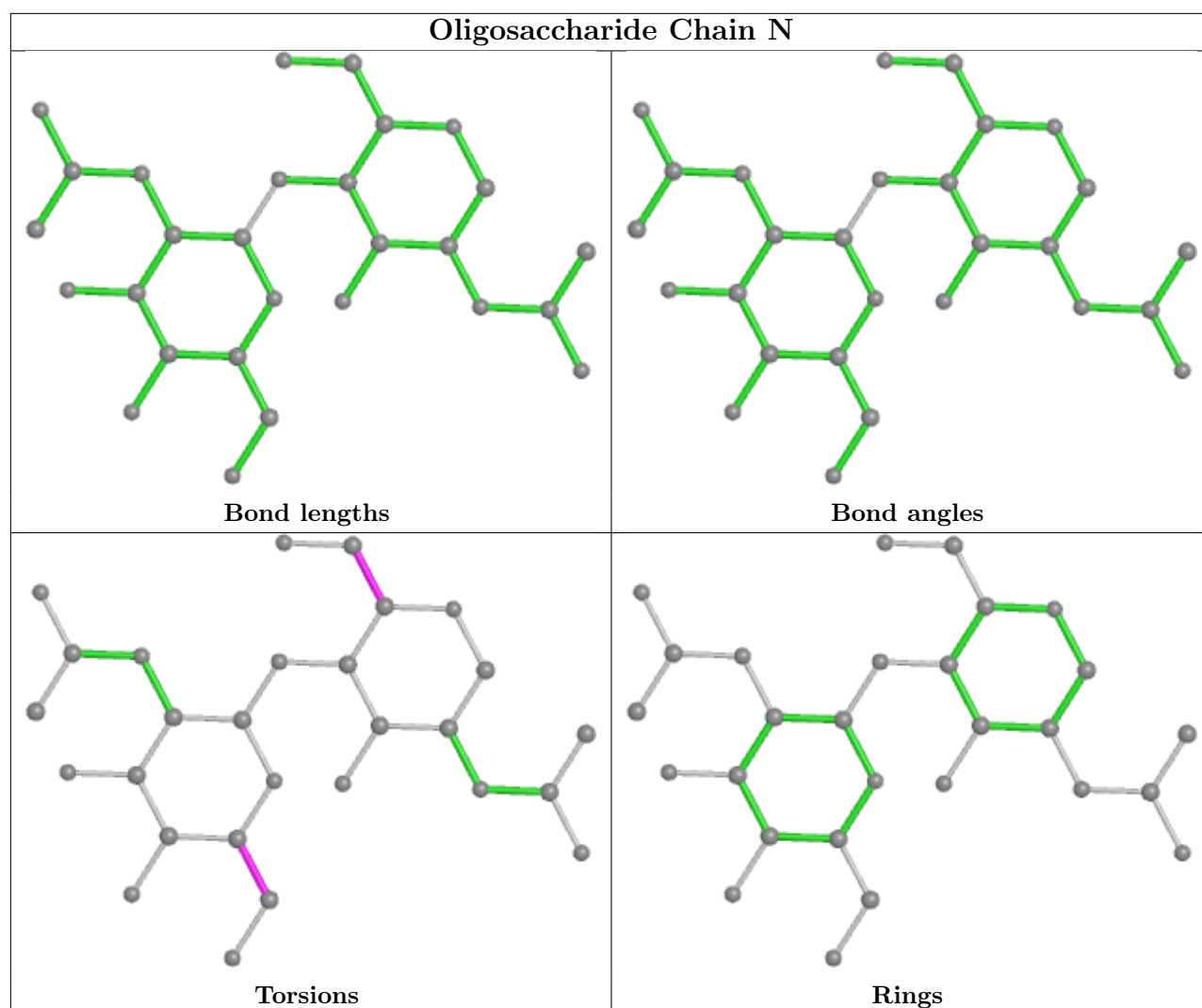


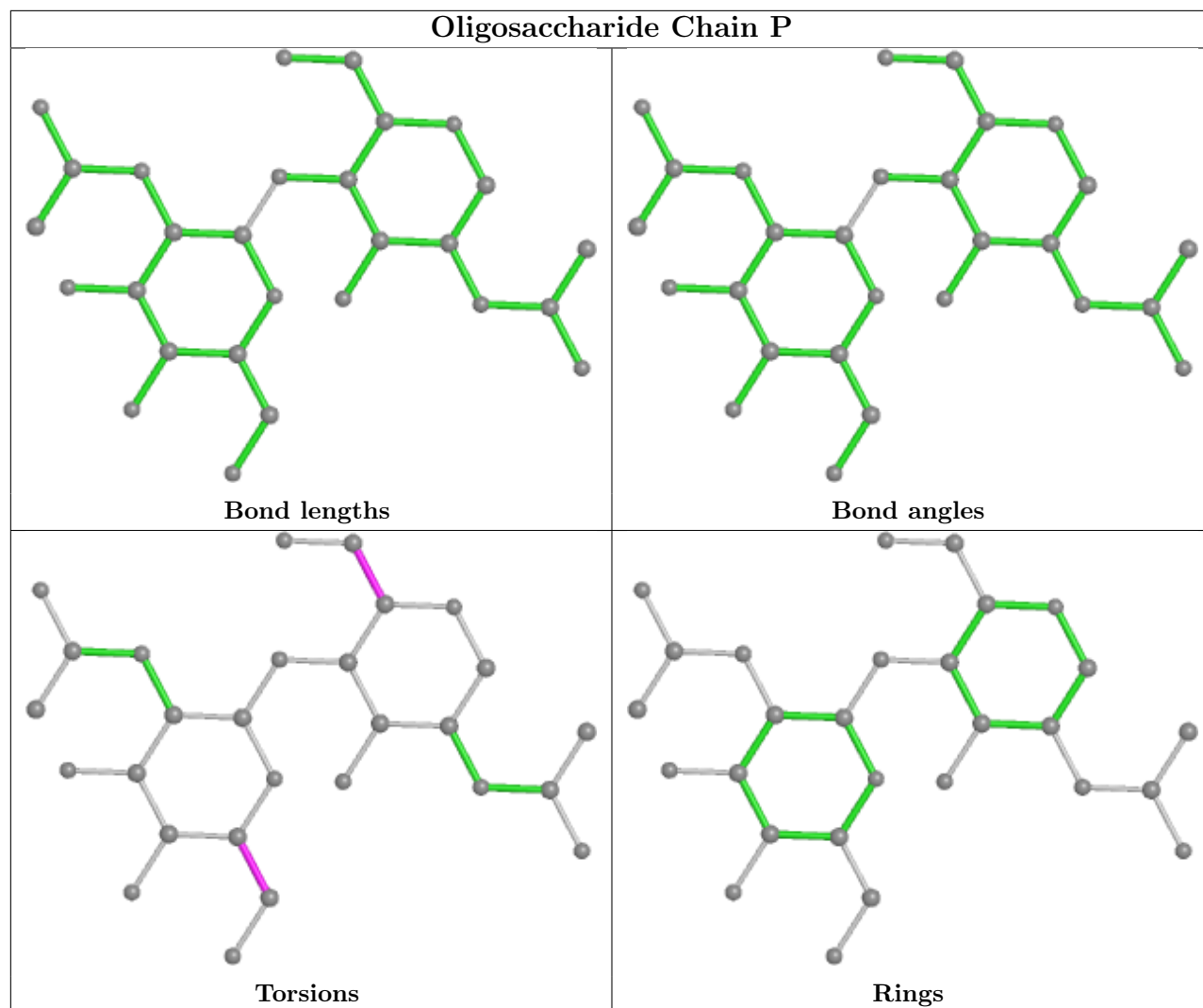


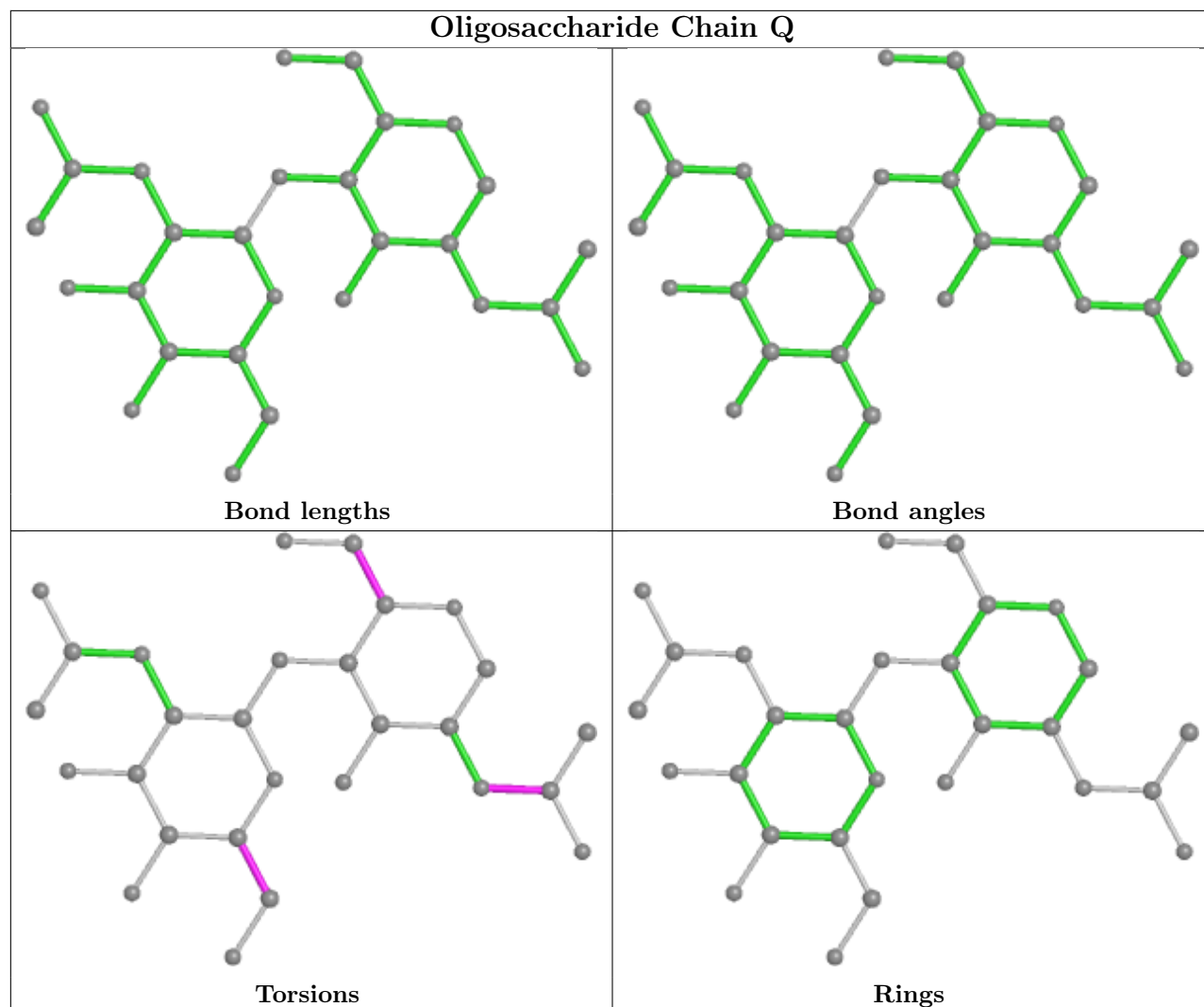


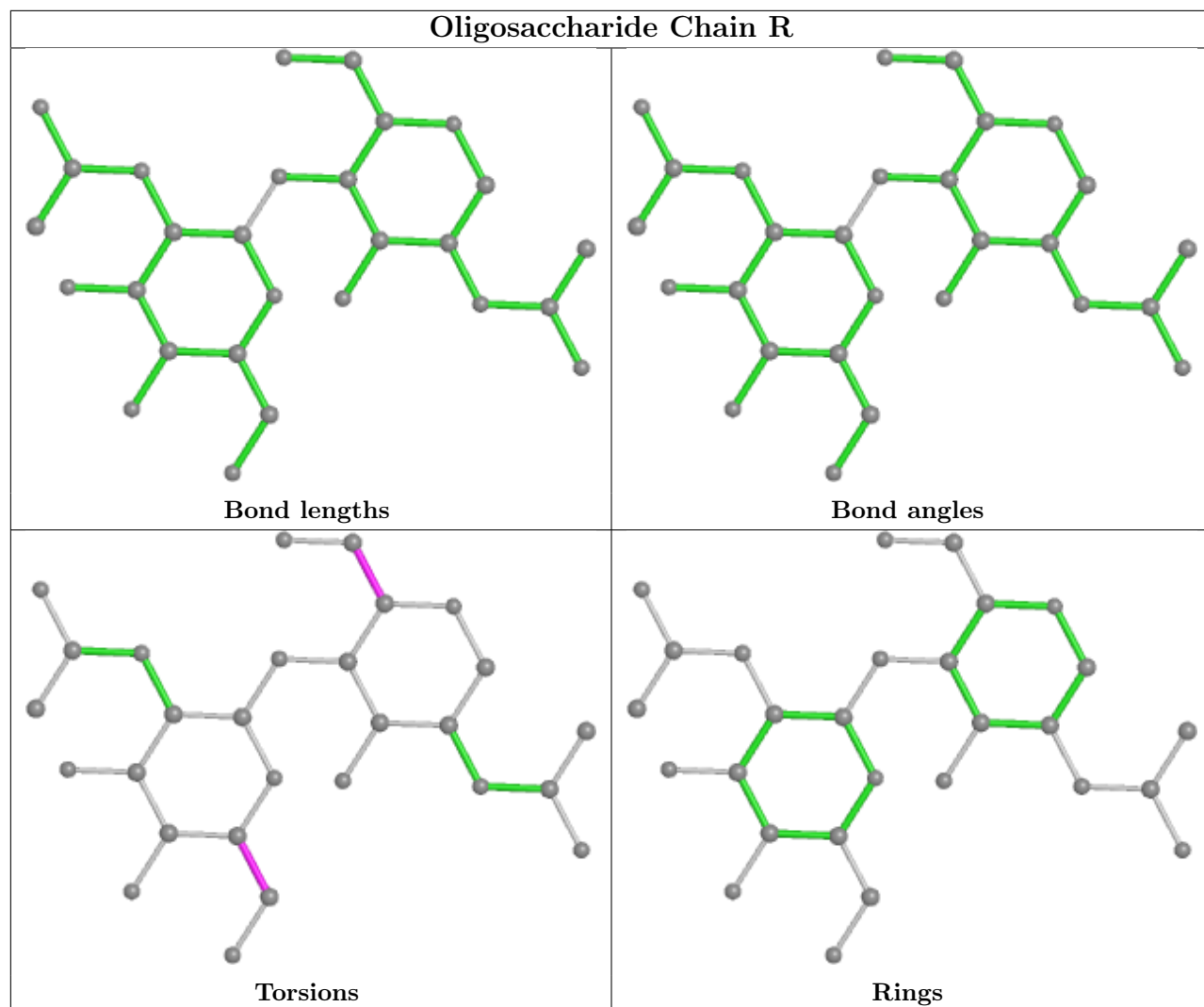


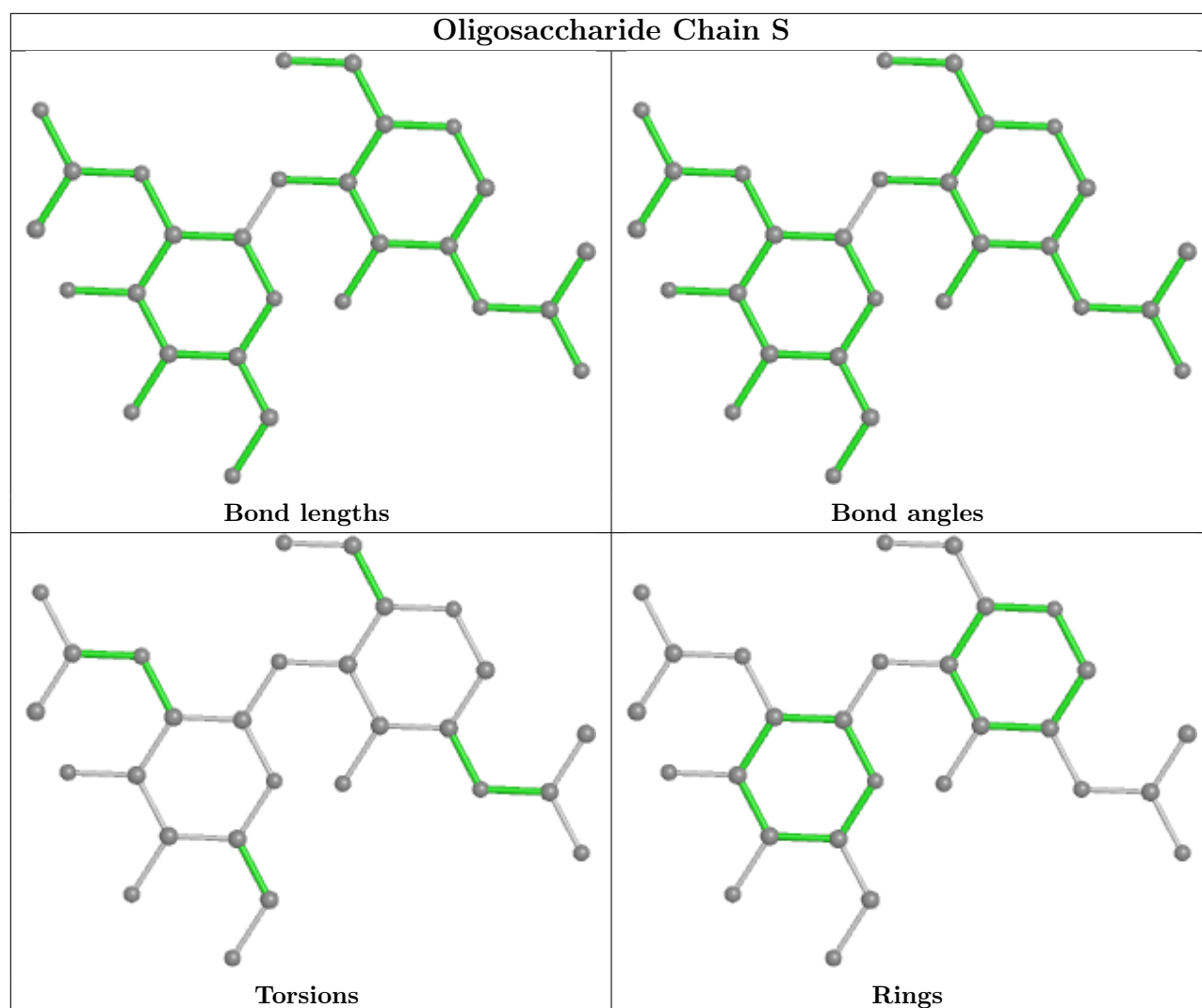


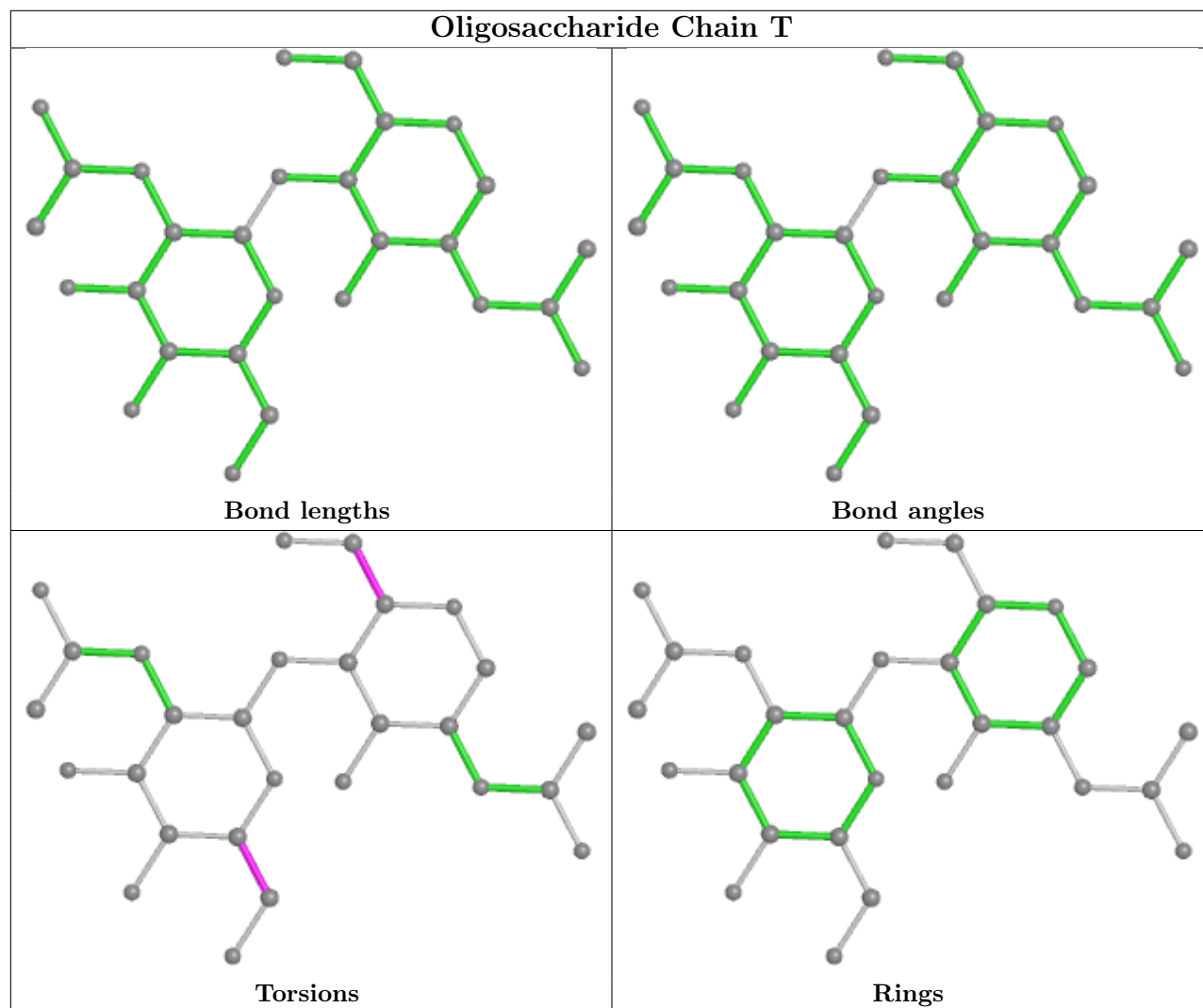


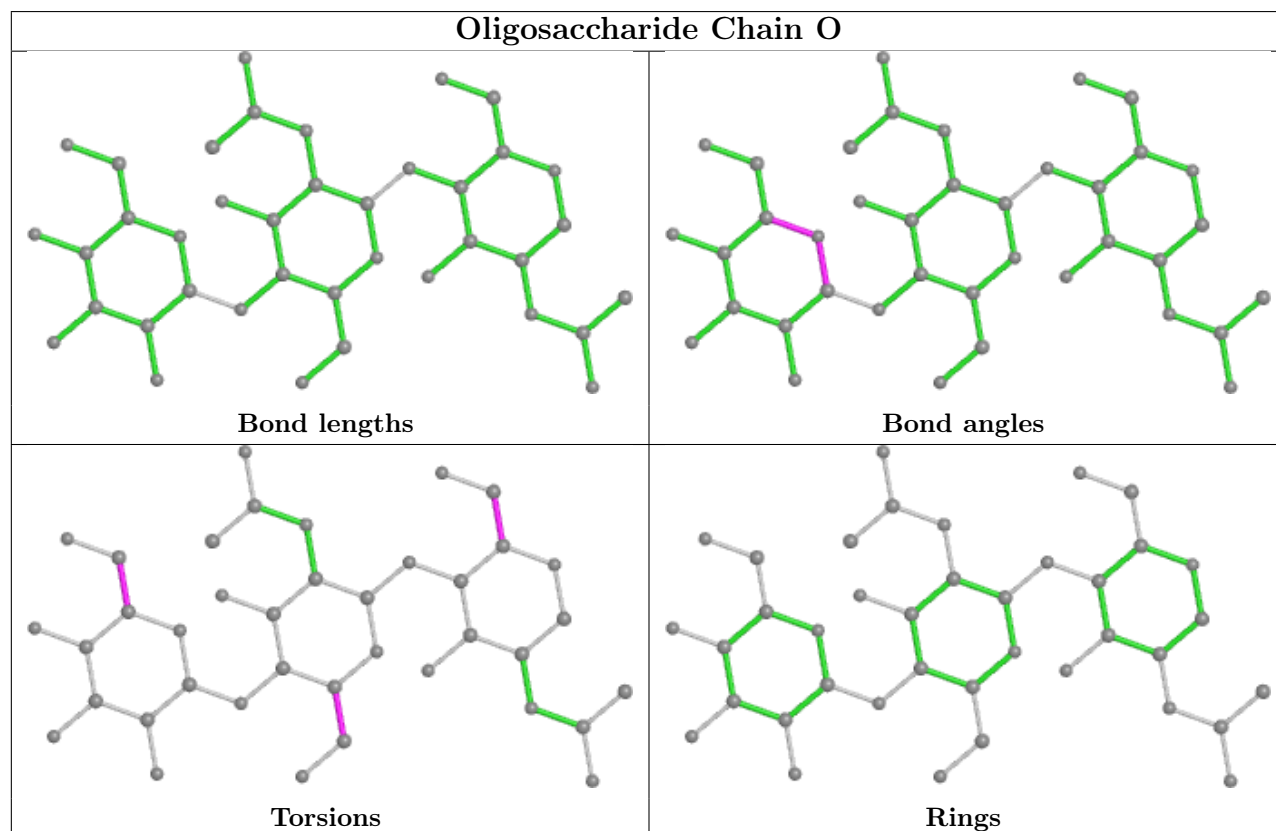
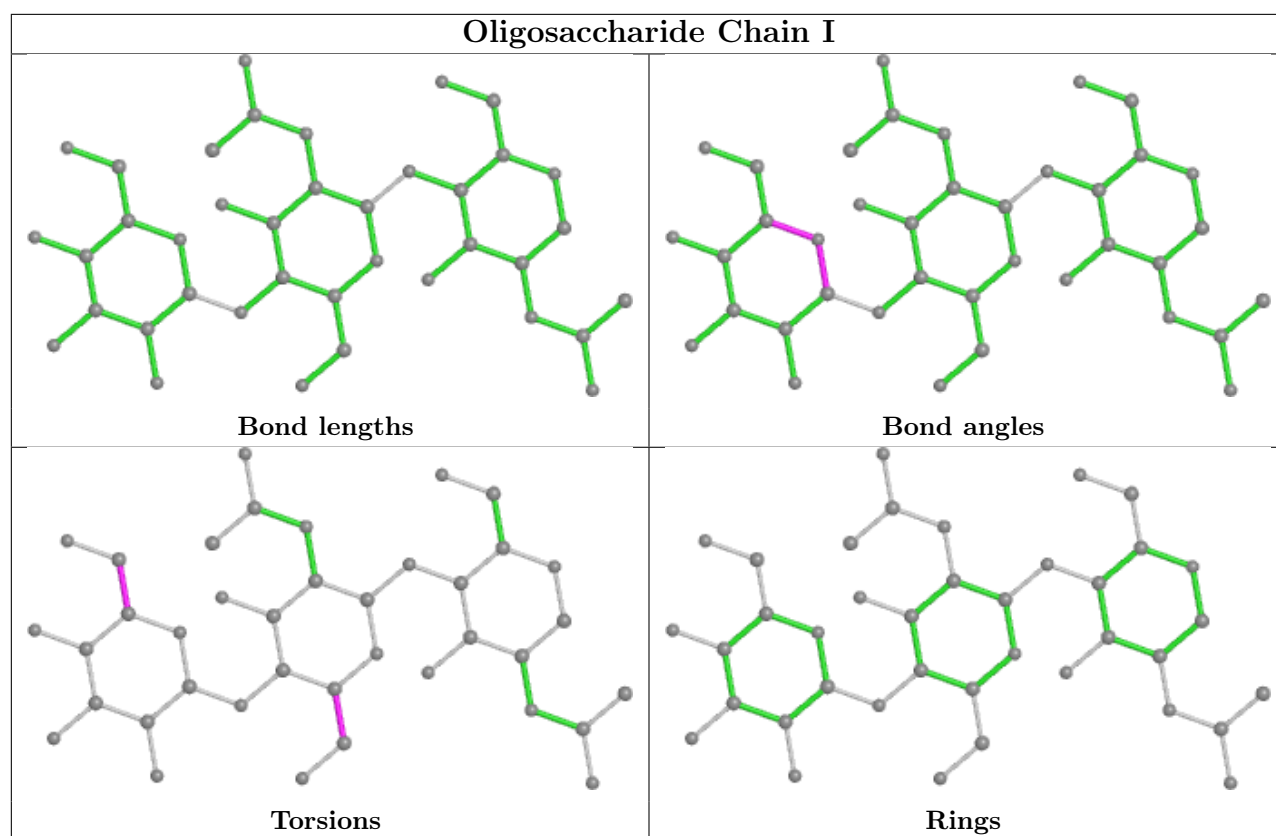


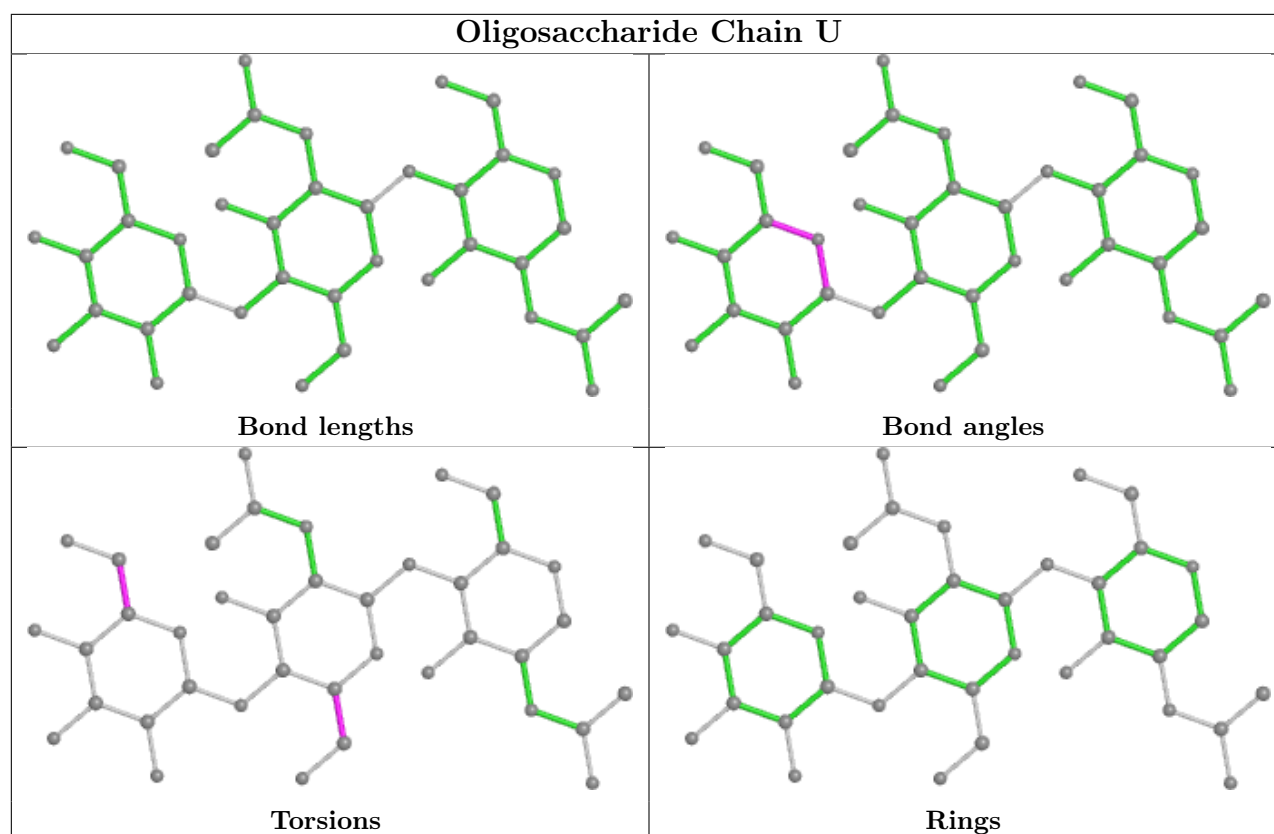












5.6 Ligand geometry [i](#)

42 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	1403	1	14,14,15	0.29	0	17,19,21	0.47	0
5	NAG	B	1411	1	14,14,15	0.26	0	17,19,21	0.43	0
5	NAG	B	1403	1	14,14,15	0.29	0	17,19,21	0.49	0
5	NAG	B	1412	1	14,14,15	0.23	0	17,19,21	0.52	0
5	NAG	B	1409	1	14,14,15	0.28	0	17,19,21	0.41	0
5	NAG	A	1410	1	14,14,15	0.31	0	17,19,21	0.47	0
5	NAG	B	1402	1	14,14,15	0.23	0	17,19,21	0.41	0
4	FOL	B	1401	-	34,34,34	1.24	2 (5%)	44,47,47	2.03	9 (20%)
5	NAG	A	1404	1	14,14,15	0.24	0	17,19,21	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FOL	A	1401	-	34,34,34	1.23	2 (5%)	44,47,47	2.03	9 (20%)
5	NAG	A	1407	1	14,14,15	0.27	0	17,19,21	0.42	0
5	NAG	B	1413	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	B	1404	1	14,14,15	0.22	0	17,19,21	0.48	0
5	NAG	C	1409	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	A	1409	1	14,14,15	0.32	0	17,19,21	0.42	0
5	NAG	A	1405	1	14,14,15	0.28	0	17,19,21	0.46	0
5	NAG	C	1407	1	14,14,15	0.25	0	17,19,21	0.44	0
5	NAG	C	1414	1	14,14,15	0.25	0	17,19,21	0.43	0
5	NAG	B	1408	1	14,14,15	0.26	0	17,19,21	0.42	0
5	NAG	C	1411	1	14,14,15	0.24	0	17,19,21	0.54	0
5	NAG	B	1410	1	14,14,15	0.31	0	17,19,21	0.48	0
5	NAG	B	1407	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	A	1413	1	14,14,15	0.22	0	17,19,21	0.47	0
5	NAG	C	1408	1	14,14,15	0.29	0	17,19,21	0.44	0
5	NAG	C	1405	1	14,14,15	0.29	0	17,19,21	0.50	0
5	NAG	B	1405	1	14,14,15	0.35	0	17,19,21	0.59	0
5	NAG	B	1406	1	14,14,15	0.25	0	17,19,21	0.45	0
5	NAG	A	1411	1	14,14,15	0.24	0	17,19,21	0.43	0
5	NAG	A	1406	1	14,14,15	0.28	0	17,19,21	0.47	0
5	NAG	C	1406	1	14,14,15	0.26	0	17,19,21	0.45	0
5	NAG	A	1414	1	14,14,15	0.25	0	17,19,21	0.49	0
5	NAG	A	1412	1	14,14,15	0.25	0	17,19,21	0.52	0
5	NAG	A	1408	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	A	1402	1	14,14,15	0.59	0	17,19,21	1.02	2 (11%)
5	NAG	B	1414	1	14,14,15	0.26	0	17,19,21	0.52	0
5	NAG	C	1413	1	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	C	1412	1	14,14,15	0.21	0	17,19,21	0.46	0
4	FOL	C	1401	-	34,34,34	1.24	2 (5%)	44,47,47	2.02	9 (20%)
5	NAG	C	1402	1	14,14,15	0.21	0	17,19,21	0.44	0
5	NAG	C	1410	1	14,14,15	0.23	0	17,19,21	0.42	0
5	NAG	C	1404	1	14,14,15	0.26	0	17,19,21	0.44	0
5	NAG	C	1403	1	14,14,15	0.24	0	17,19,21	0.48	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	A	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1411	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1409	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	FOL	B	1401	-	-	4/22/22/22	0/3/3/3
5	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	FOL	A	1401	-	-	2/22/22/22	0/3/3/3
5	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
5	NAG	B	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1409	1	-	3/6/23/26	0/1/1/1
5	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1414	1	-	0/6/23/26	0/1/1/1
5	NAG	B	1408	1	-	0/6/23/26	0/1/1/1
5	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	B	1407	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1408	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1405	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1405	1	-	4/6/23/26	0/1/1/1
5	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1414	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1412	1	-	2/6/23/26	0/1/1/1
5	NAG	A	1408	1	-	1/6/23/26	0/1/1/1
5	NAG	A	1402	1	-	3/6/23/26	0/1/1/1
5	NAG	B	1414	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1413	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1412	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FOL	C	1401	-	-	6/22/22/22	0/3/3/3
5	NAG	C	1402	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1410	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
5	NAG	C	1403	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1401	FOL	C4A-C4	4.04	1.48	1.41
4	A	1401	FOL	C4A-C4	3.94	1.48	1.41
4	B	1401	FOL	C4A-C4	3.93	1.48	1.41
4	B	1401	FOL	C4A-C8A	3.73	1.47	1.40
4	A	1401	FOL	C4A-C8A	3.66	1.47	1.40
4	C	1401	FOL	C4A-C8A	3.63	1.47	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1401	FOL	N8-C8A-N1	5.94	122.60	115.82
4	A	1401	FOL	N8-C8A-N1	5.75	122.38	115.82
4	C	1401	FOL	C2-N1-C8A	5.65	121.81	115.36
4	A	1401	FOL	C2-N1-C8A	5.58	121.73	115.36
4	B	1401	FOL	N8-C8A-N1	5.57	122.18	115.82
4	B	1401	FOL	C2-N1-C8A	5.32	121.43	115.36
4	B	1401	FOL	C4A-C4-N3	-4.31	117.53	123.43
4	B	1401	FOL	C8A-C4A-C4	-4.25	117.14	119.95
4	A	1401	FOL	C8A-C4A-C4	-4.23	117.15	119.95
4	C	1401	FOL	C4A-C4-N3	-4.11	117.81	123.43
4	A	1401	FOL	C4A-C4-N3	-4.08	117.86	123.43
4	C	1401	FOL	C8A-C4A-C4	-4.00	117.30	119.95
4	A	1401	FOL	C4-C4A-N5	3.90	123.05	118.60
4	B	1401	FOL	C2-N3-C4	3.84	122.03	115.93
4	C	1401	FOL	C4-C4A-N5	3.83	122.98	118.60
4	B	1401	FOL	C4-C4A-N5	3.77	122.90	118.60
4	A	1401	FOL	C2-N3-C4	3.64	121.72	115.93
4	C	1401	FOL	C2-N3-C4	3.61	121.67	115.93
4	A	1401	FOL	N1-C2-N3	-3.32	122.80	127.22
4	B	1401	FOL	N1-C2-N3	-3.28	122.85	127.22
4	C	1401	FOL	N1-C2-N3	-3.28	122.85	127.22
4	C	1401	FOL	C7-N8-C8A	3.04	119.75	116.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1401	FOL	C7-N8-C8A	2.95	119.66	116.69
4	B	1401	FOL	C7-N8-C8A	2.86	119.57	116.69
5	A	1402	NAG	C1-O5-C5	2.77	115.95	112.19
5	A	1402	NAG	C2-N2-C7	2.40	126.32	122.90
4	C	1401	FOL	C8A-C4A-N5	-2.30	119.72	122.33
4	A	1401	FOL	C8A-C4A-N5	-2.24	119.80	122.33
4	B	1401	FOL	C8A-C4A-N5	-2.09	119.96	122.33

There are no chirality outliers.

All (90) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1404	NAG	O5-C5-C6-O6
5	B	1404	NAG	O5-C5-C6-O6
5	B	1413	NAG	O5-C5-C6-O6
5	C	1408	NAG	C4-C5-C6-O6
5	C	1409	NAG	C4-C5-C6-O6
5	B	1403	NAG	O5-C5-C6-O6
5	B	1405	NAG	O5-C5-C6-O6
5	B	1407	NAG	O5-C5-C6-O6
5	B	1414	NAG	O5-C5-C6-O6
5	C	1402	NAG	O5-C5-C6-O6
5	C	1403	NAG	O5-C5-C6-O6
5	B	1404	NAG	C4-C5-C6-O6
5	C	1404	NAG	O5-C5-C6-O6
5	C	1410	NAG	O5-C5-C6-O6
5	A	1405	NAG	O5-C5-C6-O6
5	C	1406	NAG	O5-C5-C6-O6
5	B	1413	NAG	C4-C5-C6-O6
5	B	1406	NAG	O5-C5-C6-O6
5	C	1402	NAG	C4-C5-C6-O6
5	A	1403	NAG	O5-C5-C6-O6
5	A	1406	NAG	O5-C5-C6-O6
5	A	1413	NAG	O5-C5-C6-O6
5	B	1410	NAG	O5-C5-C6-O6
5	C	1405	NAG	O5-C5-C6-O6
5	B	1403	NAG	C4-C5-C6-O6
5	C	1403	NAG	C4-C5-C6-O6
4	B	1401	FOL	C13-C14-N10-C9
5	B	1411	NAG	O5-C5-C6-O6
5	C	1408	NAG	O5-C5-C6-O6
5	B	1402	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	1404	NAG	C4-C5-C6-O6
5	B	1409	NAG	C4-C5-C6-O6
5	A	1405	NAG	C4-C5-C6-O6
5	A	1406	NAG	C4-C5-C6-O6
5	A	1413	NAG	C4-C5-C6-O6
5	B	1406	NAG	C4-C5-C6-O6
5	B	1411	NAG	C4-C5-C6-O6
5	C	1405	NAG	C4-C5-C6-O6
5	C	1406	NAG	C4-C5-C6-O6
5	A	1411	NAG	O5-C5-C6-O6
5	C	1412	NAG	O5-C5-C6-O6
5	B	1405	NAG	C4-C5-C6-O6
5	B	1407	NAG	C4-C5-C6-O6
5	B	1410	NAG	C4-C5-C6-O6
5	B	1414	NAG	C4-C5-C6-O6
5	A	1409	NAG	C8-C7-N2-C2
5	A	1409	NAG	O7-C7-N2-C2
5	B	1405	NAG	C8-C7-N2-C2
5	B	1405	NAG	O7-C7-N2-C2
5	B	1409	NAG	C8-C7-N2-C2
5	B	1409	NAG	O7-C7-N2-C2
5	C	1405	NAG	C8-C7-N2-C2
5	C	1405	NAG	O7-C7-N2-C2
5	B	1402	NAG	O5-C5-C6-O6
5	C	1410	NAG	C4-C5-C6-O6
5	A	1402	NAG	O5-C5-C6-O6
5	A	1410	NAG	O5-C5-C6-O6
5	A	1403	NAG	C4-C5-C6-O6
5	B	1412	NAG	O5-C5-C6-O6
5	C	1404	NAG	C4-C5-C6-O6
5	B	1409	NAG	O5-C5-C6-O6
5	C	1409	NAG	O5-C5-C6-O6
5	A	1411	NAG	C4-C5-C6-O6
4	B	1401	FOL	C15-C14-N10-C9
5	A	1410	NAG	C4-C5-C6-O6
5	A	1402	NAG	C4-C5-C6-O6
5	B	1412	NAG	C4-C5-C6-O6
5	C	1412	NAG	C4-C5-C6-O6
5	A	1409	NAG	O5-C5-C6-O6
5	C	1413	NAG	O5-C5-C6-O6
4	A	1401	FOL	C11-C-N-CA
5	C	1413	NAG	C4-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	1401	FOL	O-C-N-CA
5	A	1414	NAG	C4-C5-C6-O6
5	A	1414	NAG	O5-C5-C6-O6
5	C	1411	NAG	C4-C5-C6-O6
5	C	1411	NAG	O5-C5-C6-O6
5	A	1412	NAG	C4-C5-C6-O6
5	A	1412	NAG	O5-C5-C6-O6
4	C	1401	FOL	CB-CA-CT-O2
4	C	1401	FOL	C11-C-N-CA
4	C	1401	FOL	CB-CA-CT-O1
4	C	1401	FOL	O-C-N-CA
5	A	1402	NAG	C3-C2-N2-C7
4	C	1401	FOL	OE2-CD-CG-CB
4	C	1401	FOL	OE1-CD-CG-CB
4	B	1401	FOL	OE1-CD-CG-CB
4	B	1401	FOL	OE2-CD-CG-CB
5	A	1407	NAG	O5-C5-C6-O6
5	A	1408	NAG	C4-C5-C6-O6

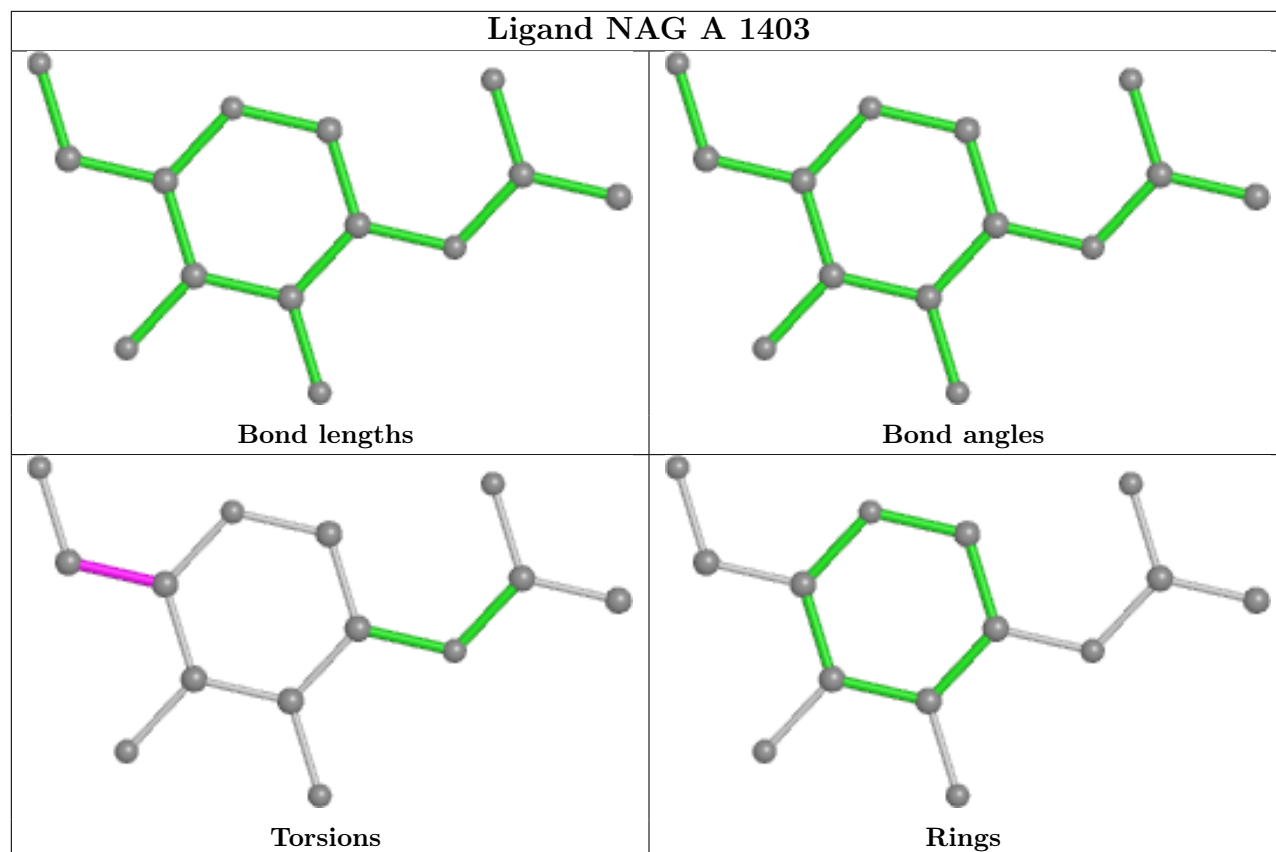
There are no ring outliers.

5 monomers are involved in 6 short contacts:

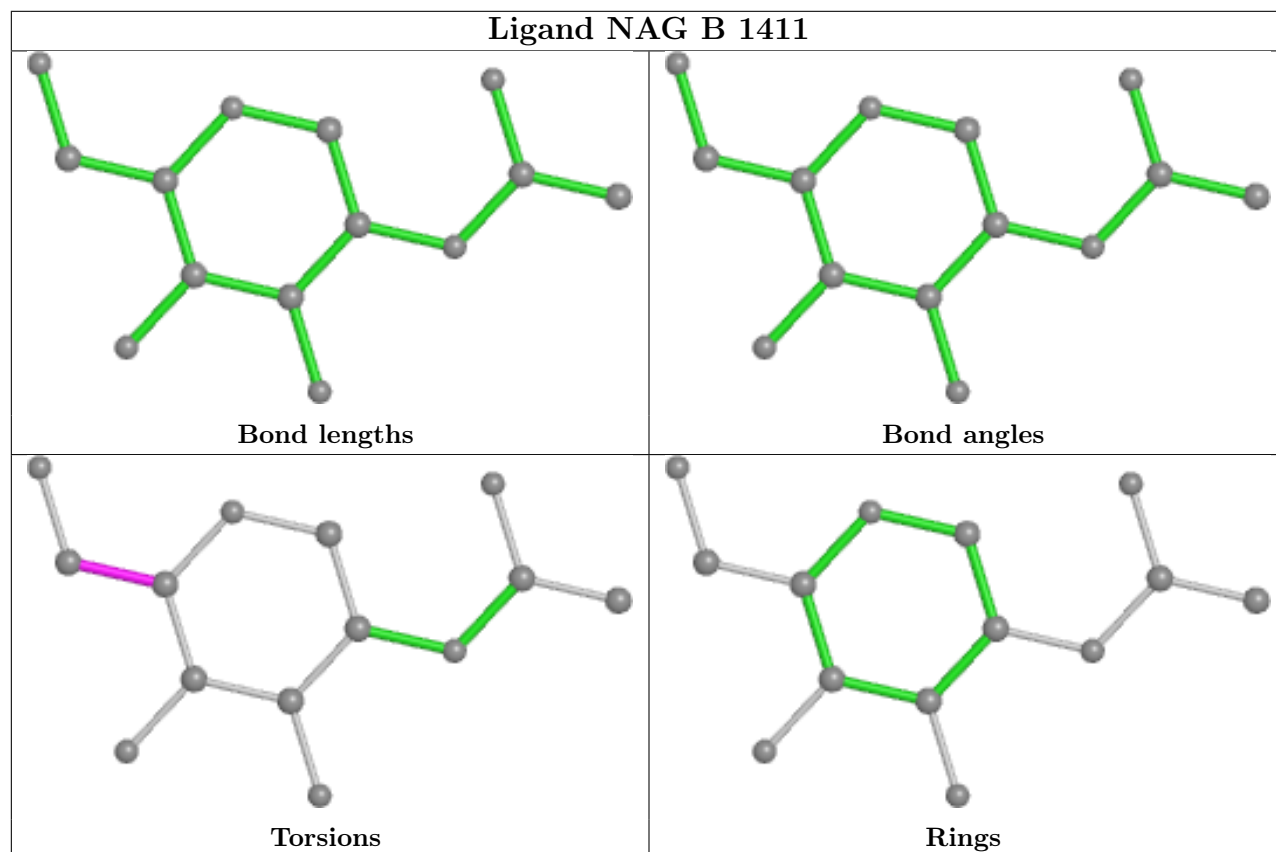
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1410	NAG	1	0
4	B	1401	FOL	1	0
5	B	1405	NAG	1	0
4	C	1401	FOL	2	0
5	C	1404	NAG	1	0

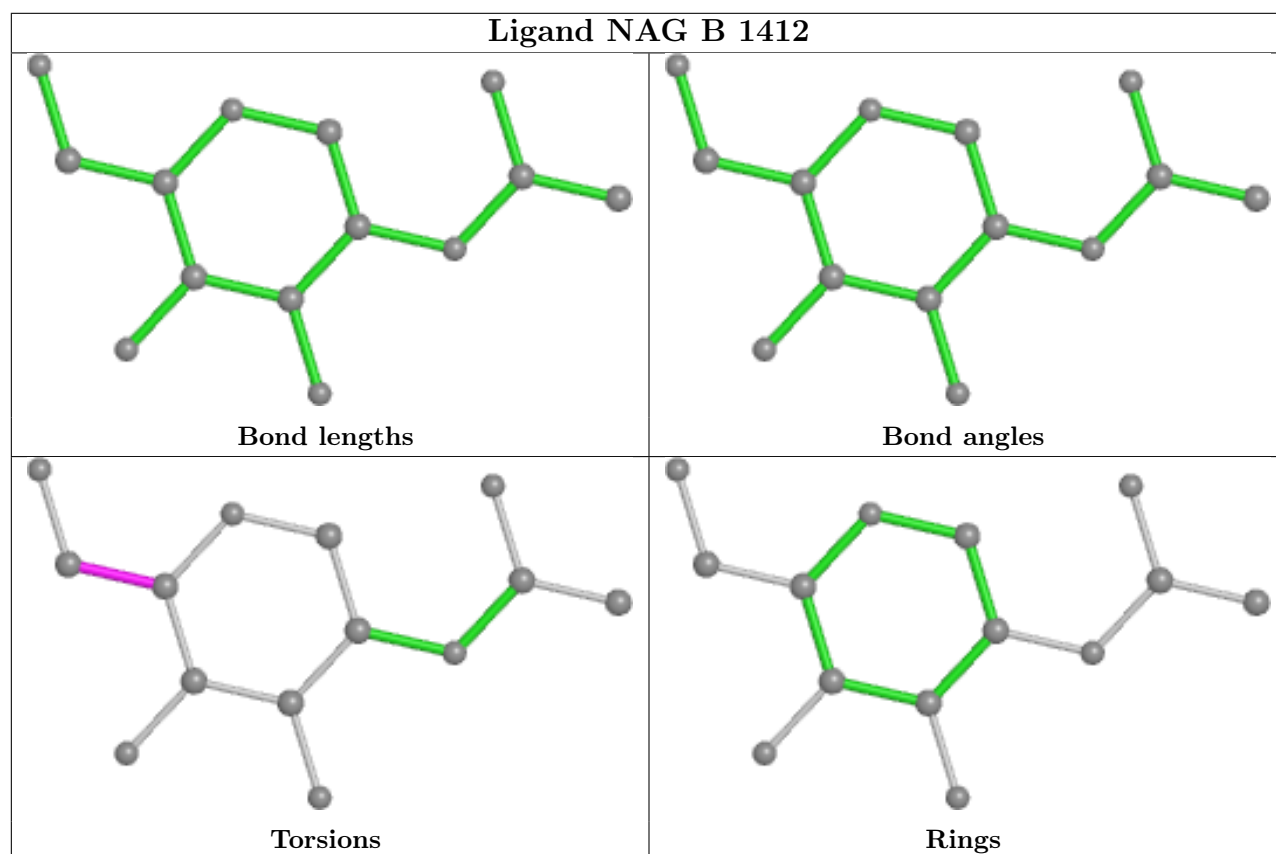
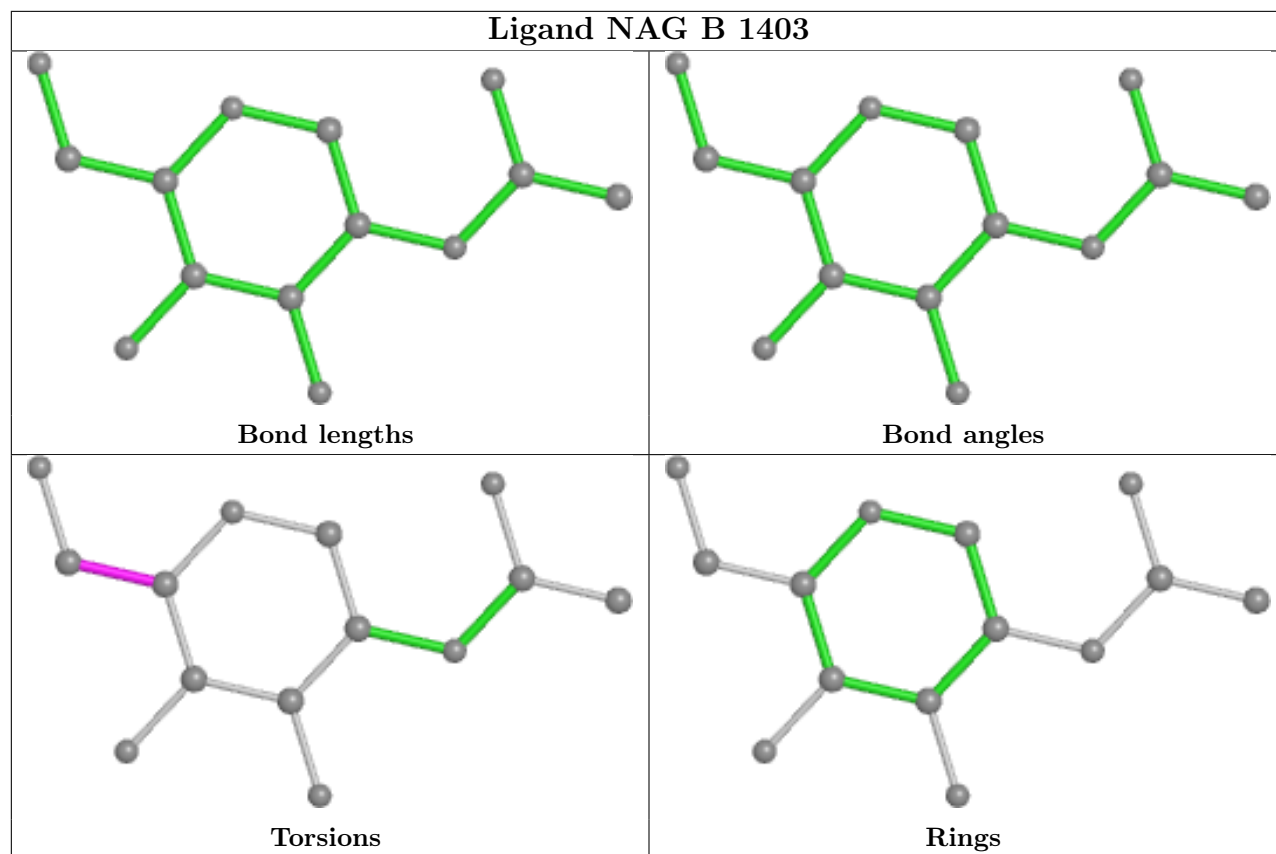
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 1403

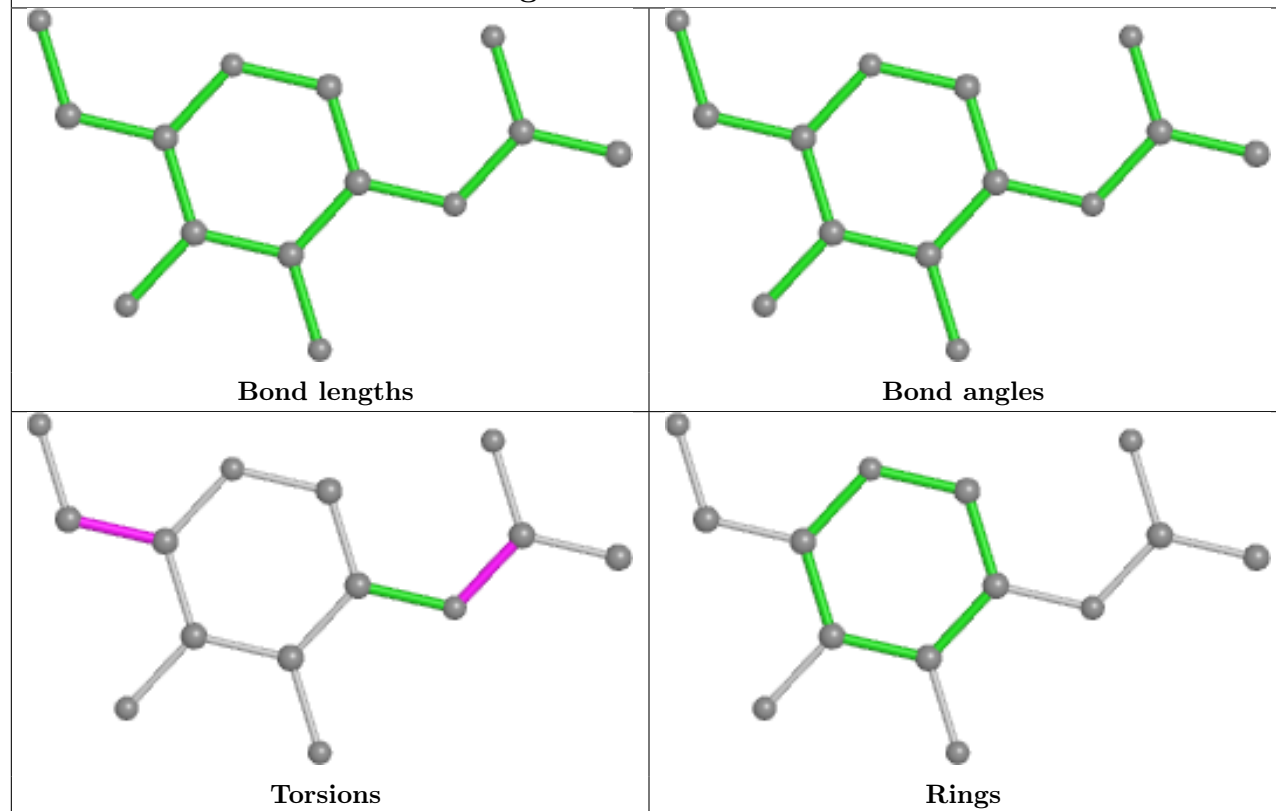


Ligand NAG B 1411

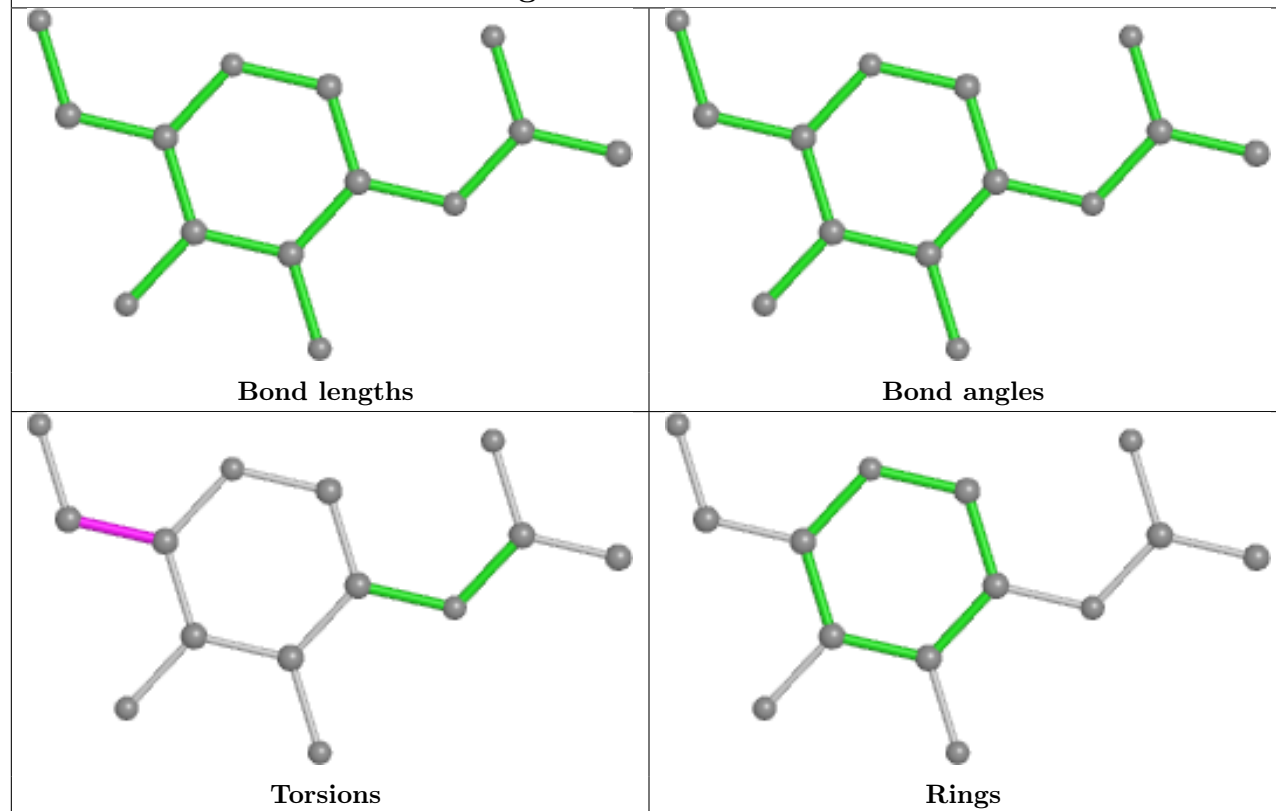




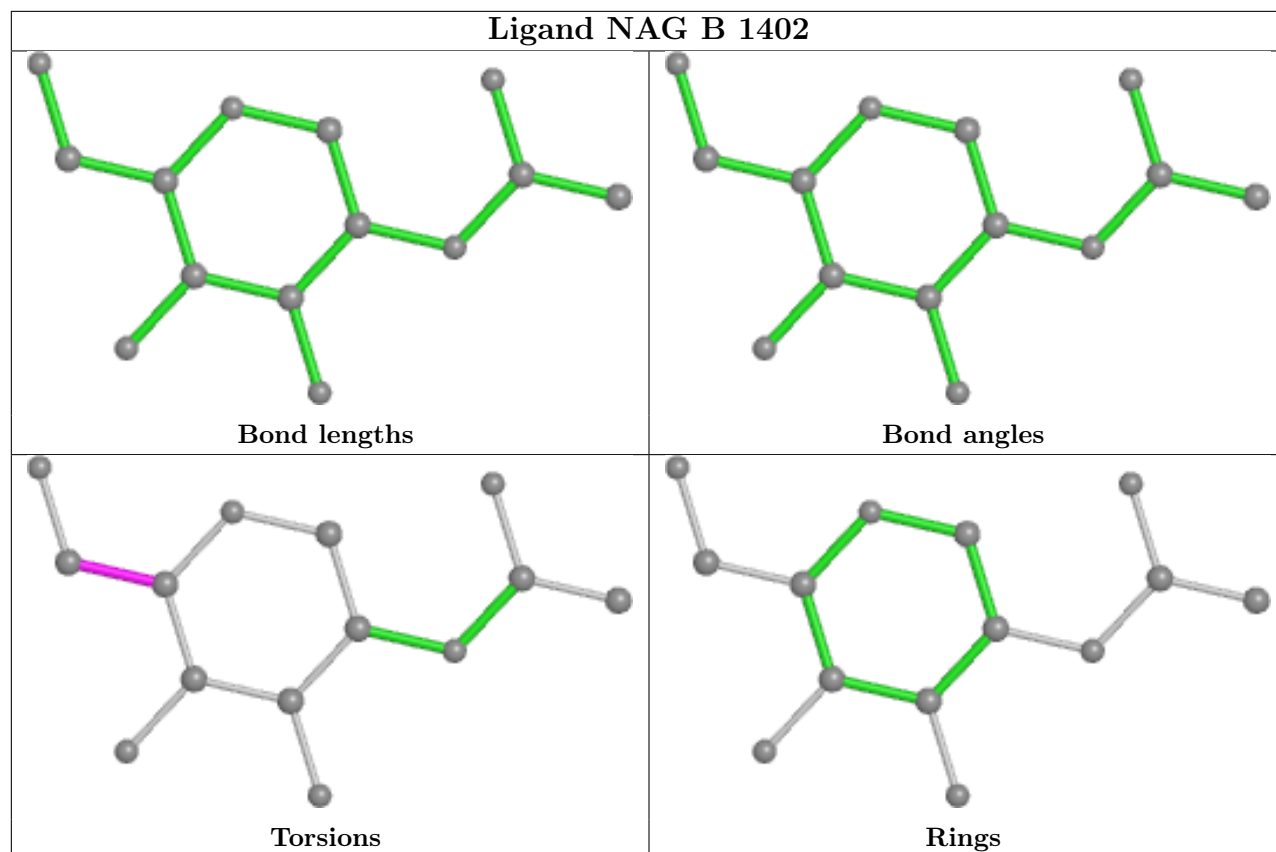
Ligand NAG B 1409



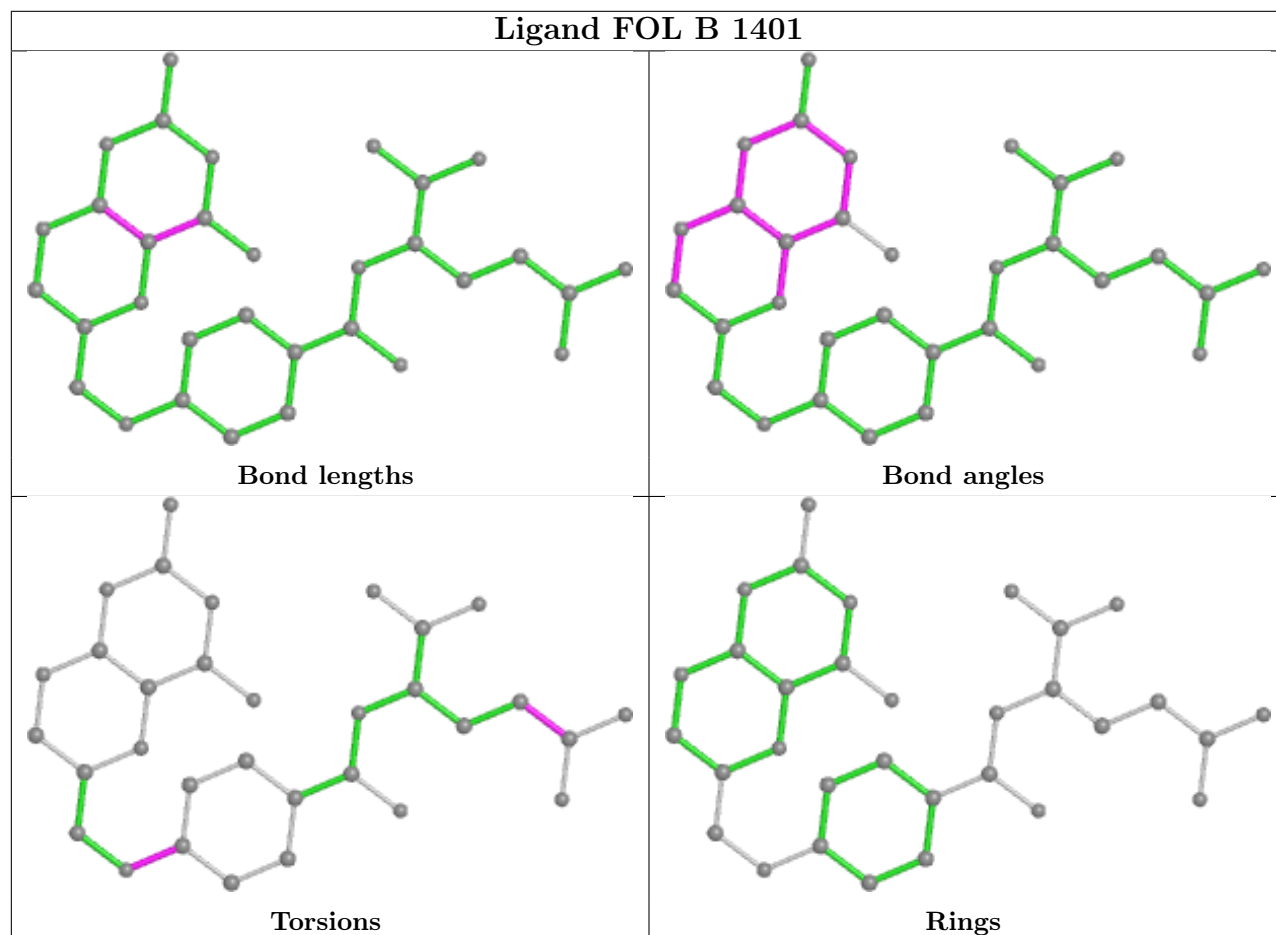
Ligand NAG A 1410



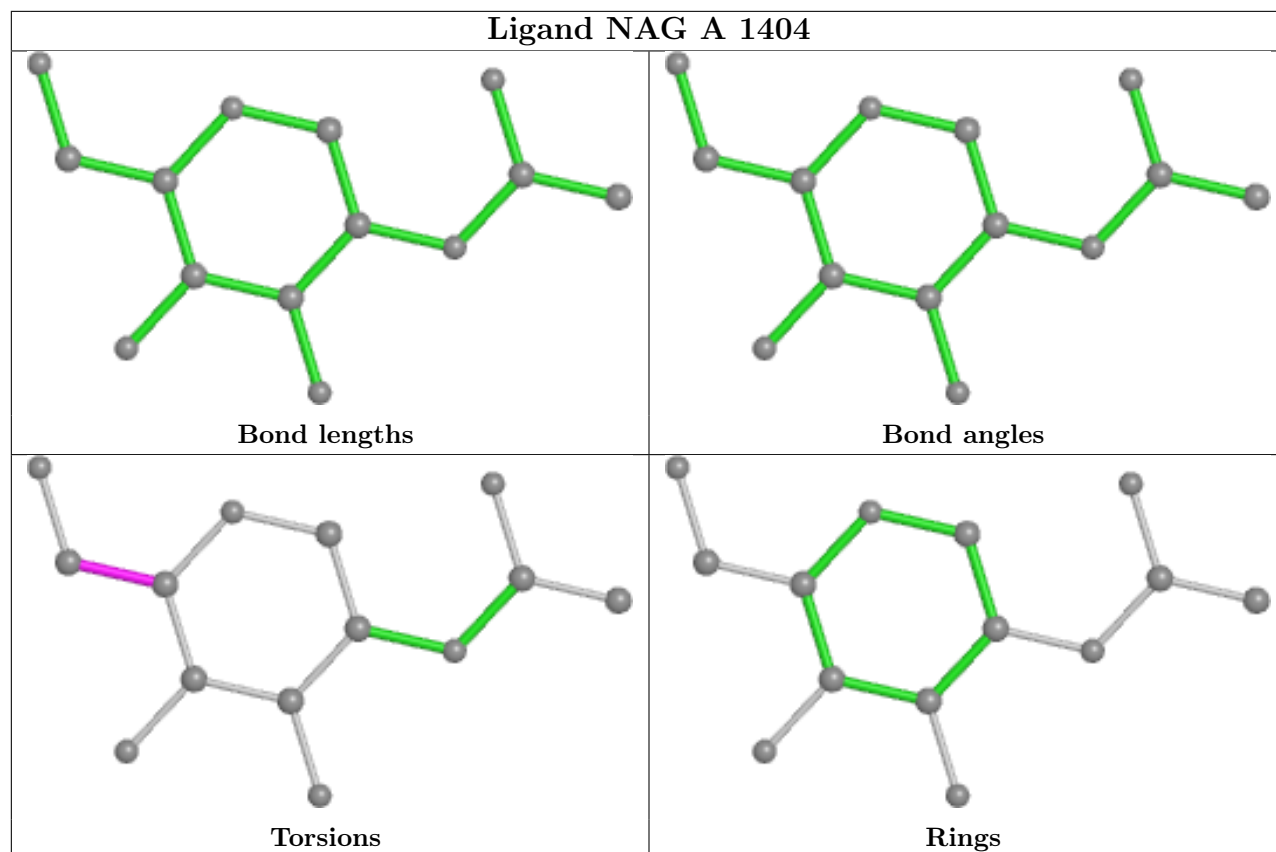
Ligand NAG B 1402



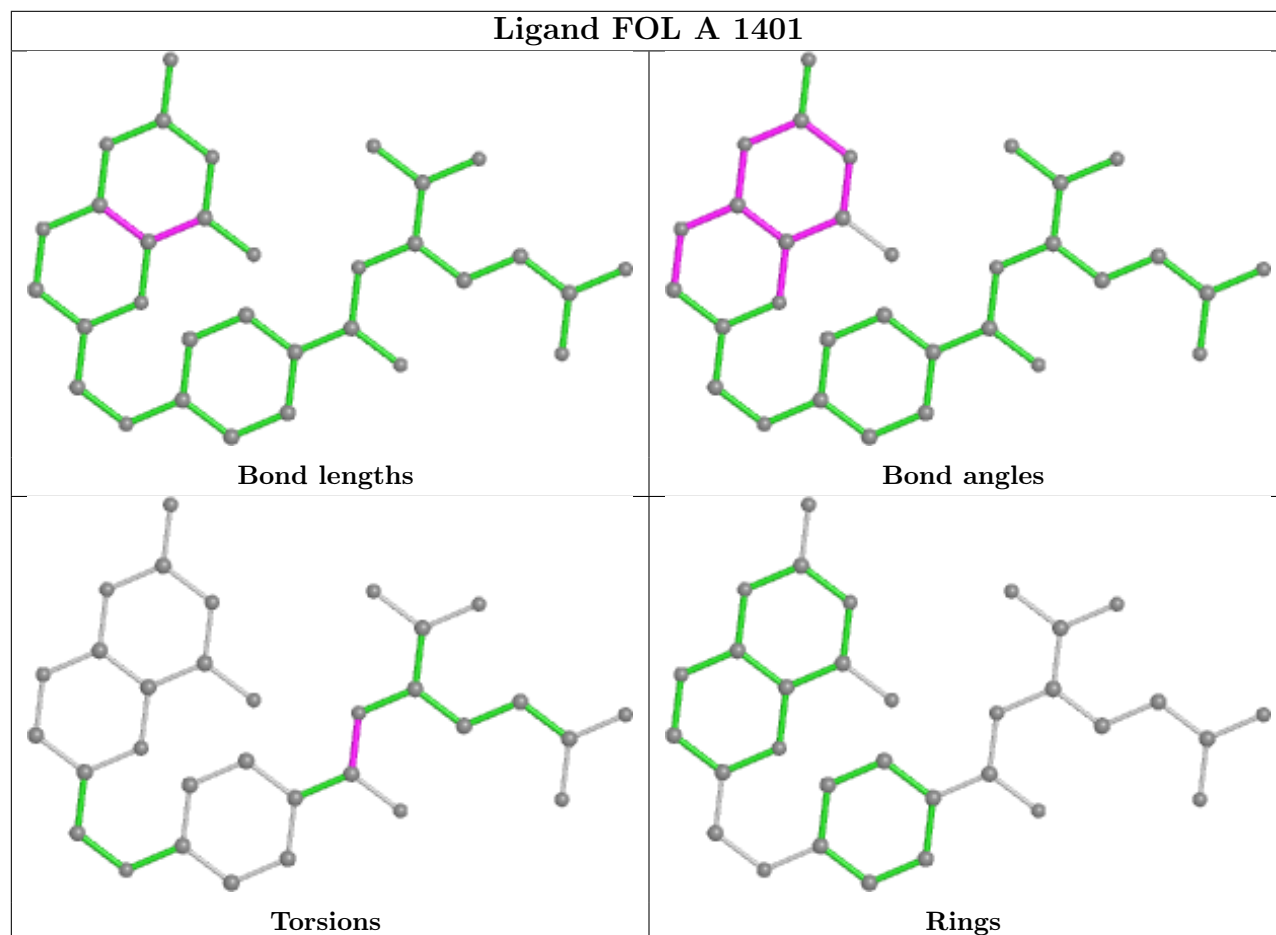
Ligand FOL B 1401



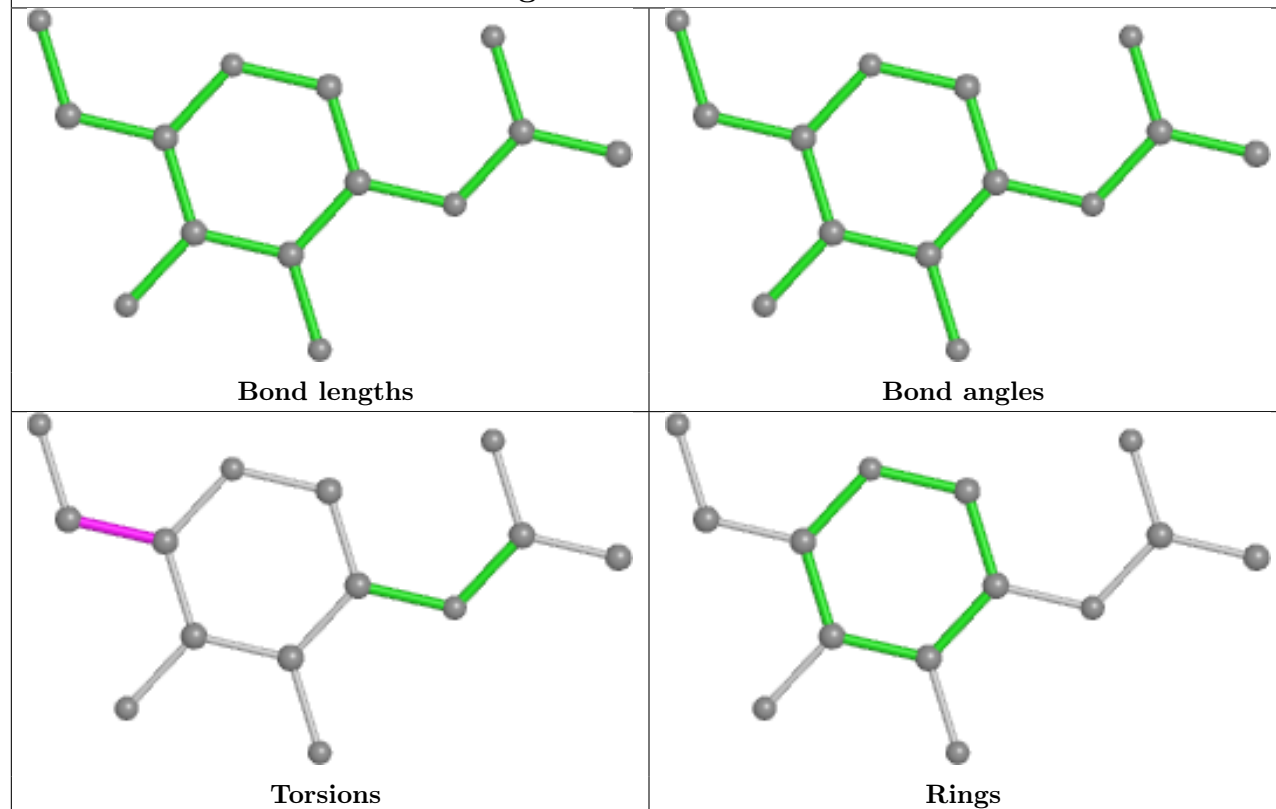
Ligand NAG A 1404



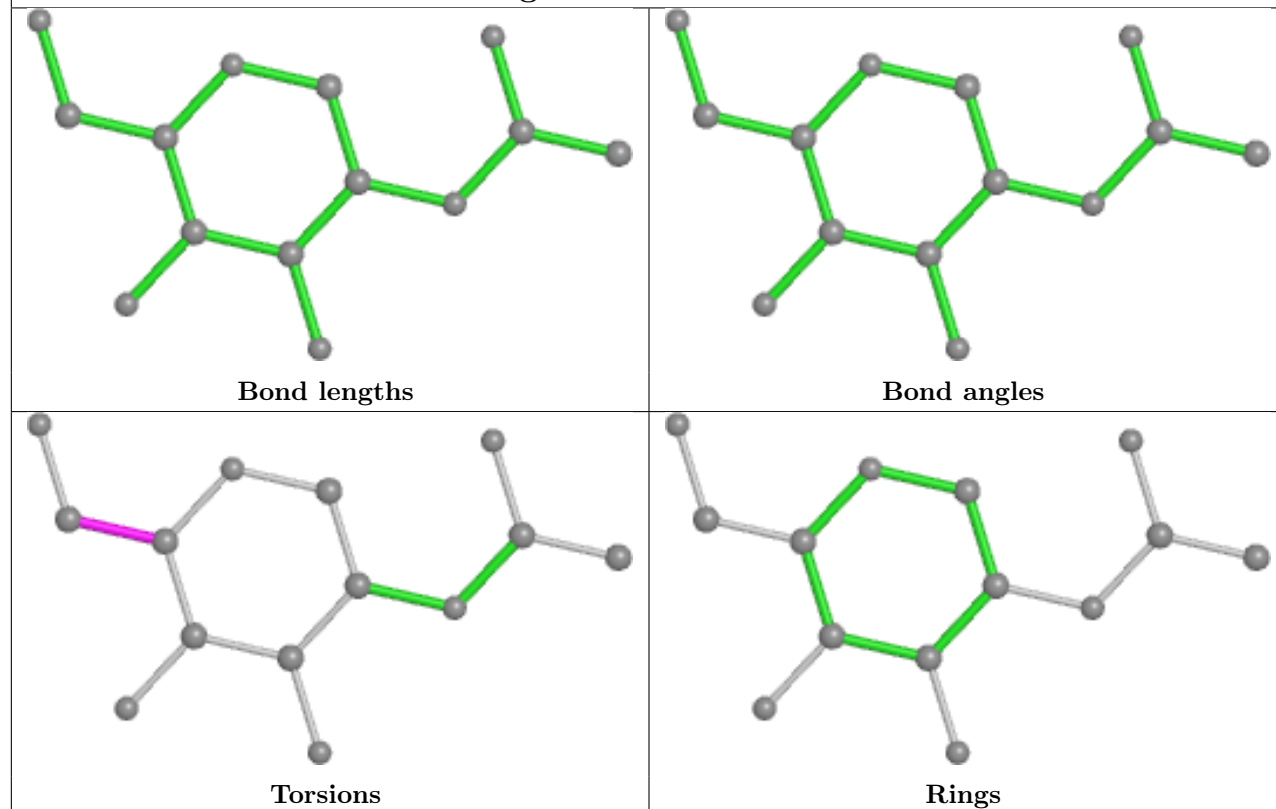
Ligand FOL A 1401



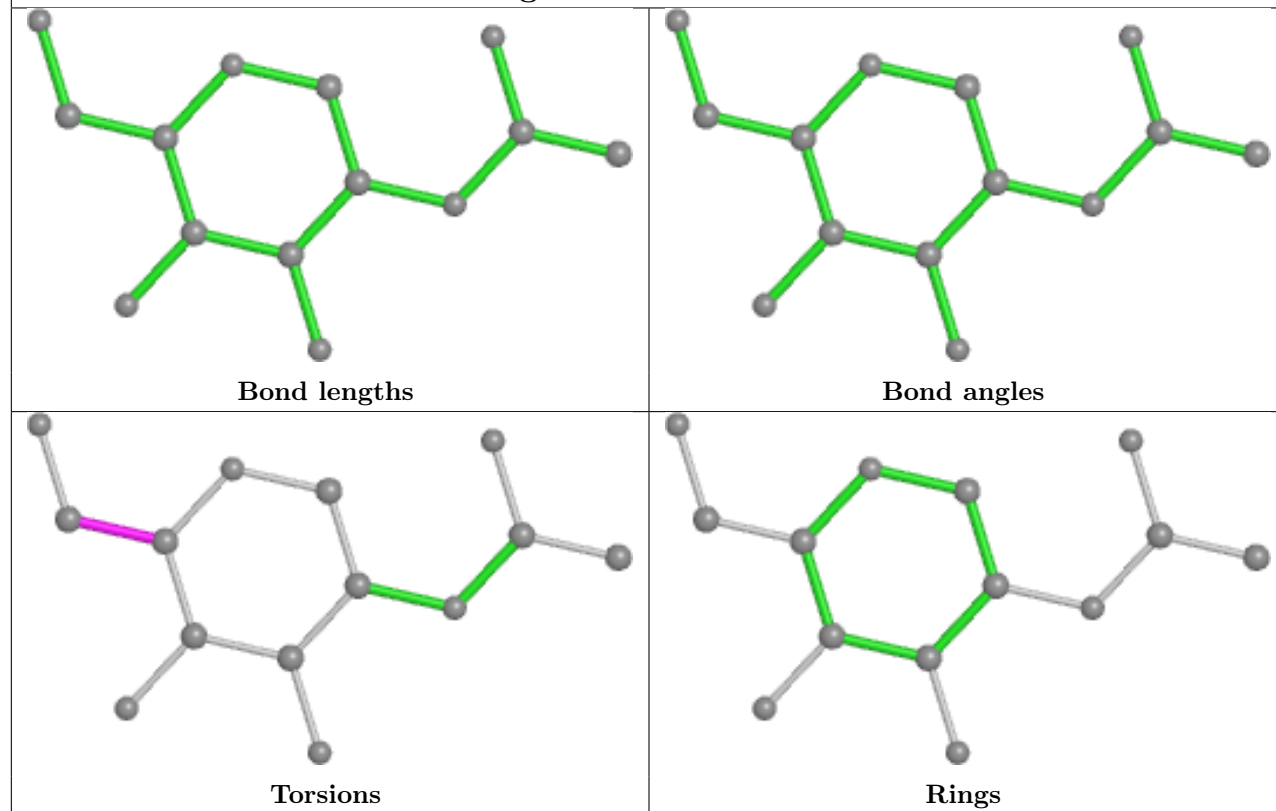
Ligand NAG A 1407



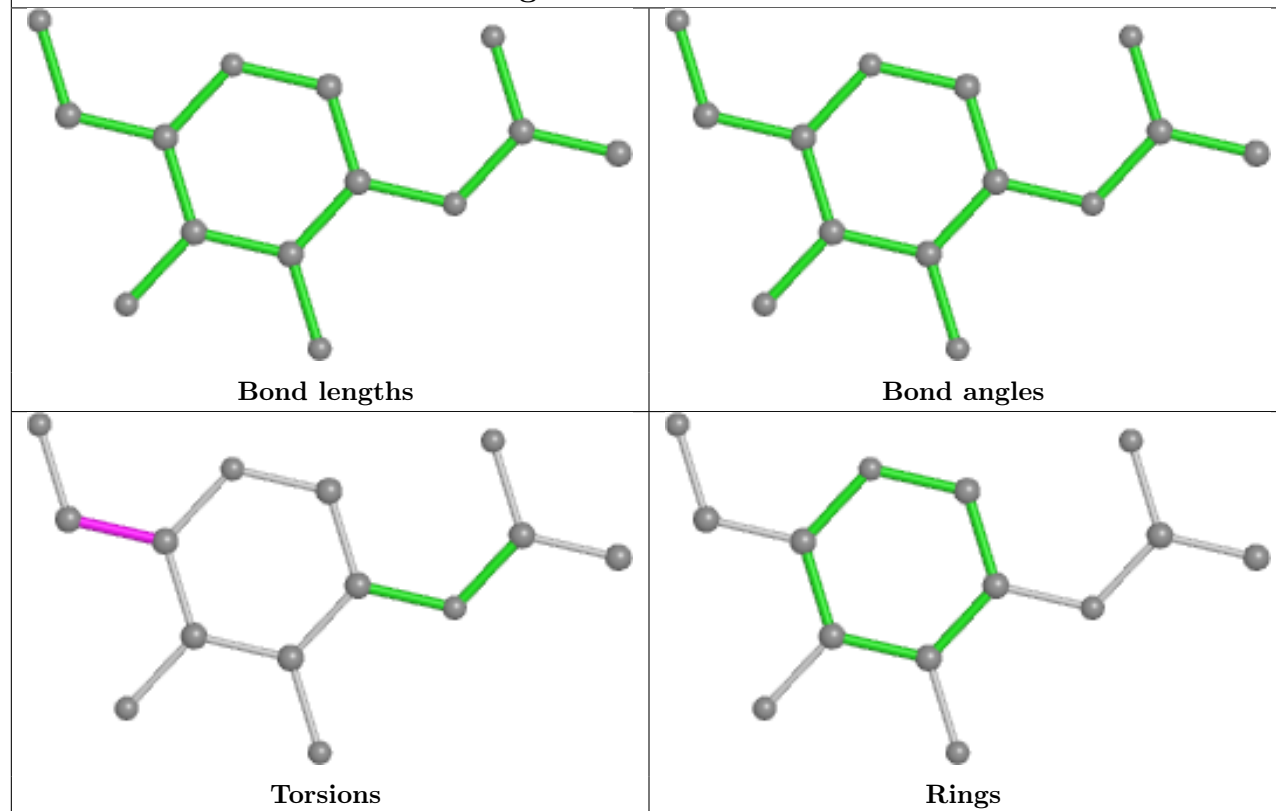
Ligand NAG B 1413



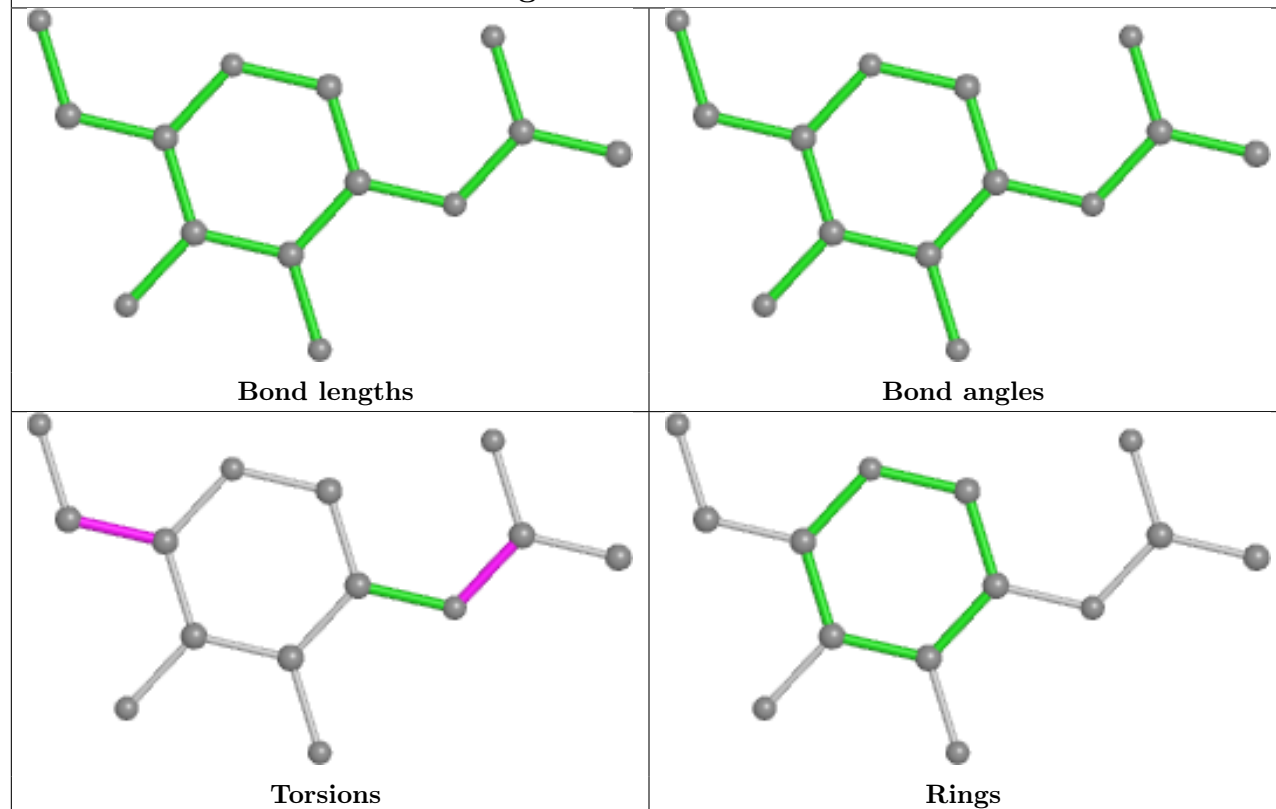
Ligand NAG B 1404



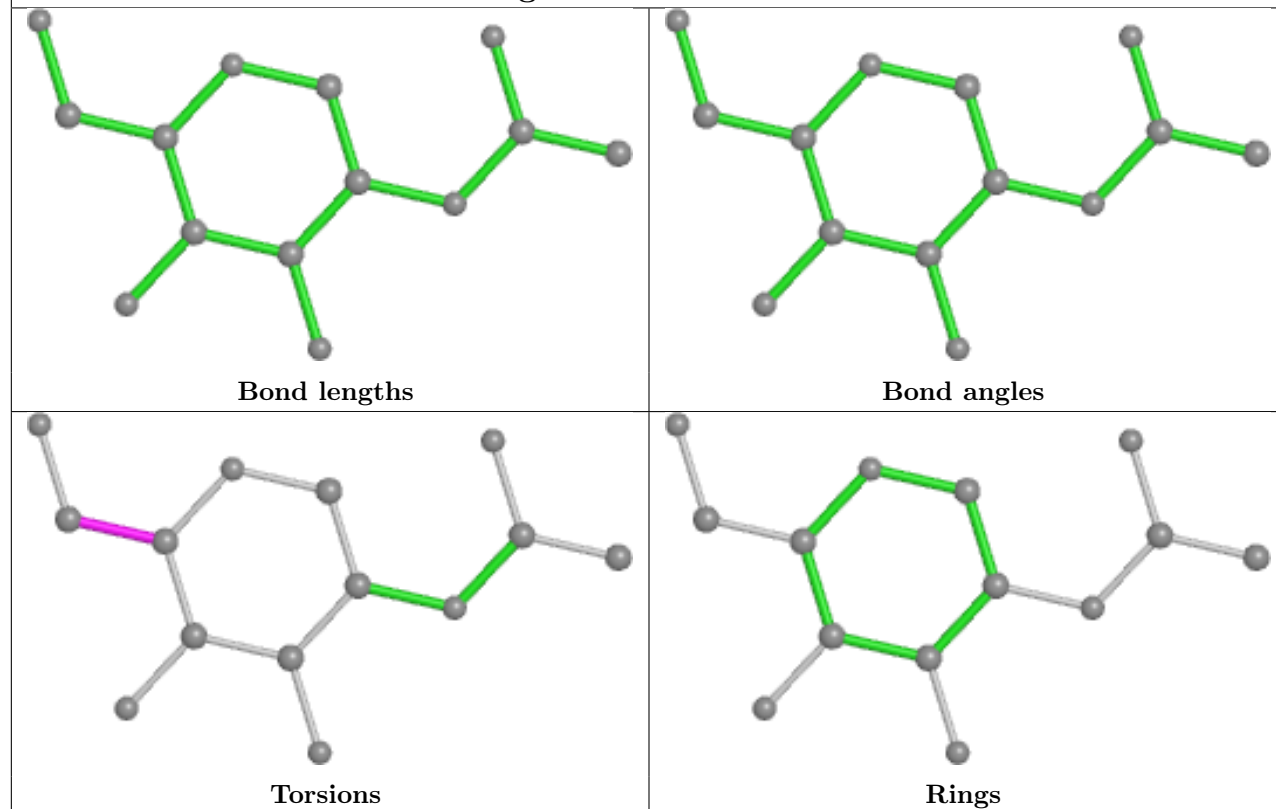
Ligand NAG C 1409



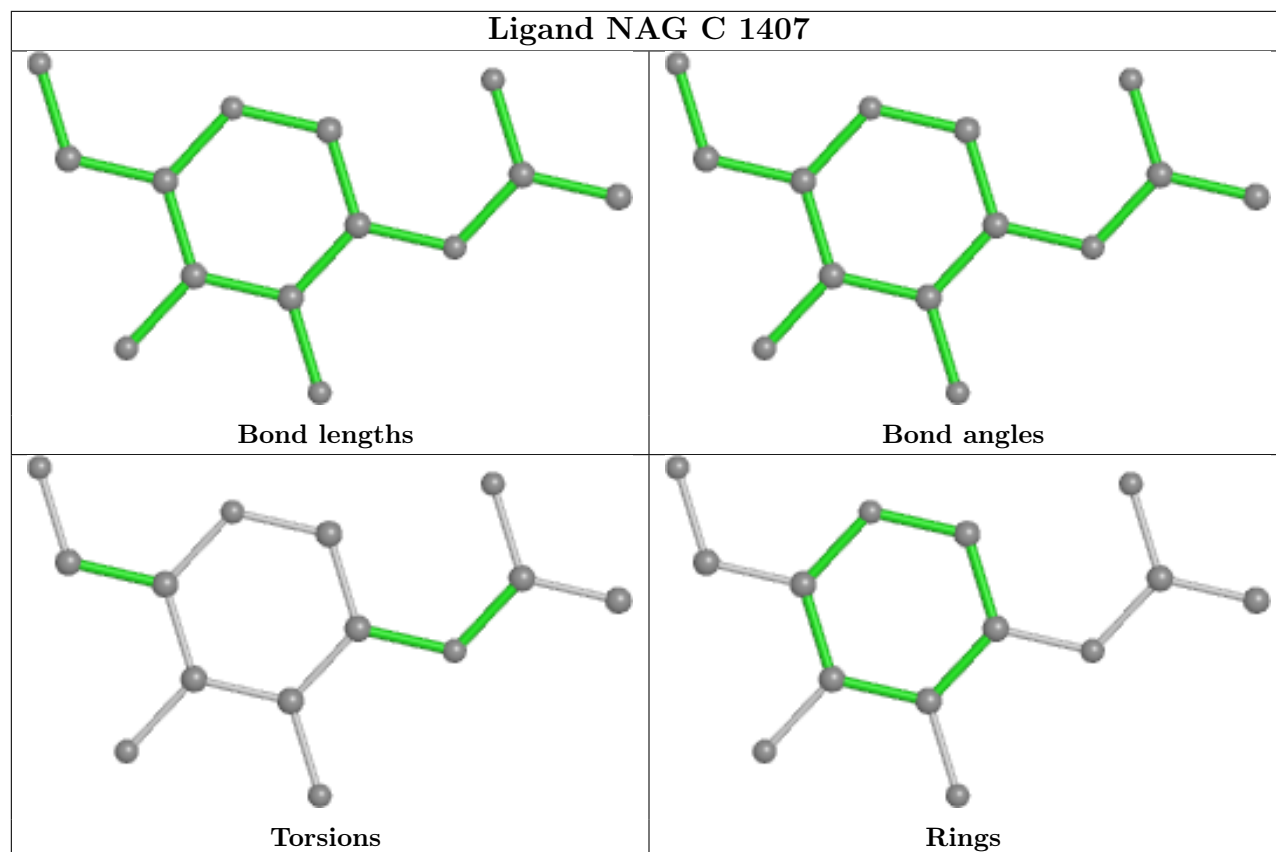
Ligand NAG A 1409



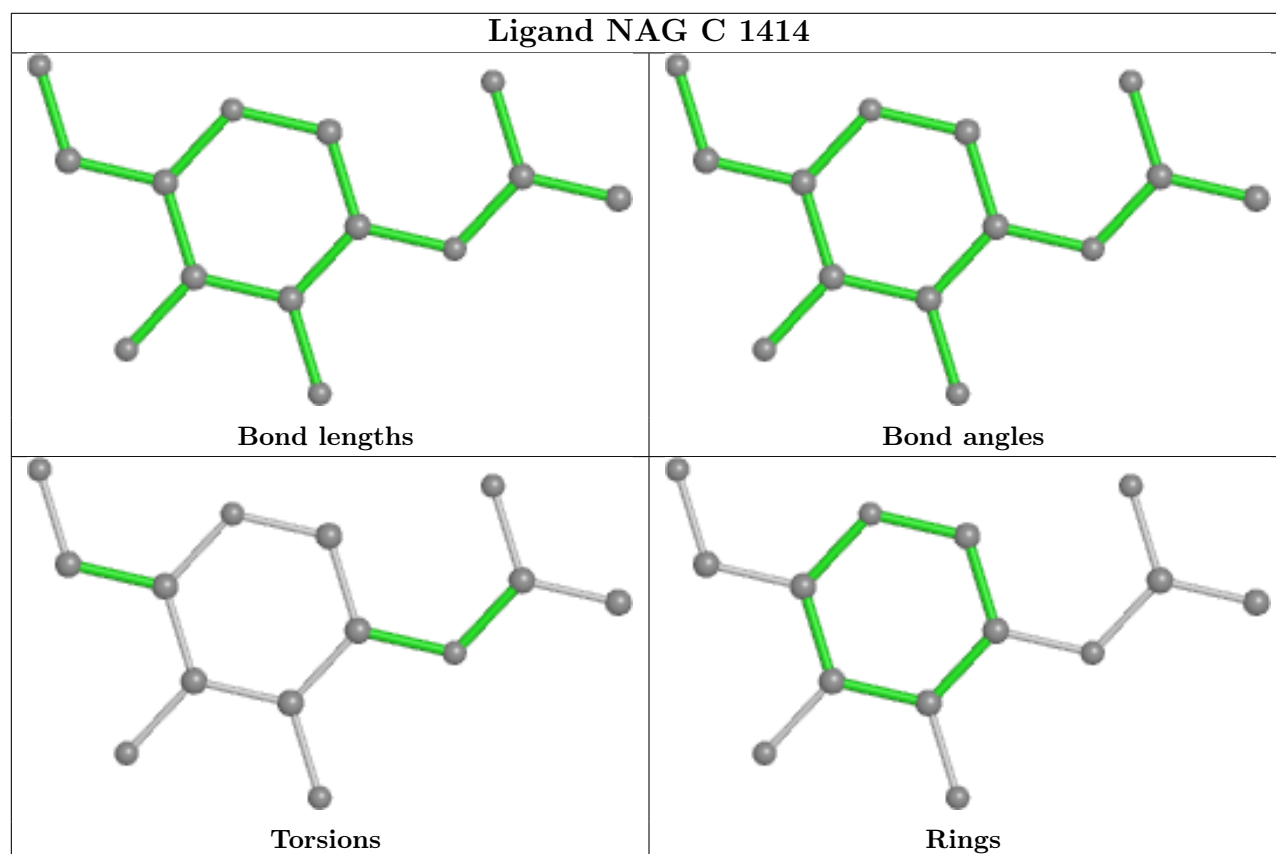
Ligand NAG A 1405

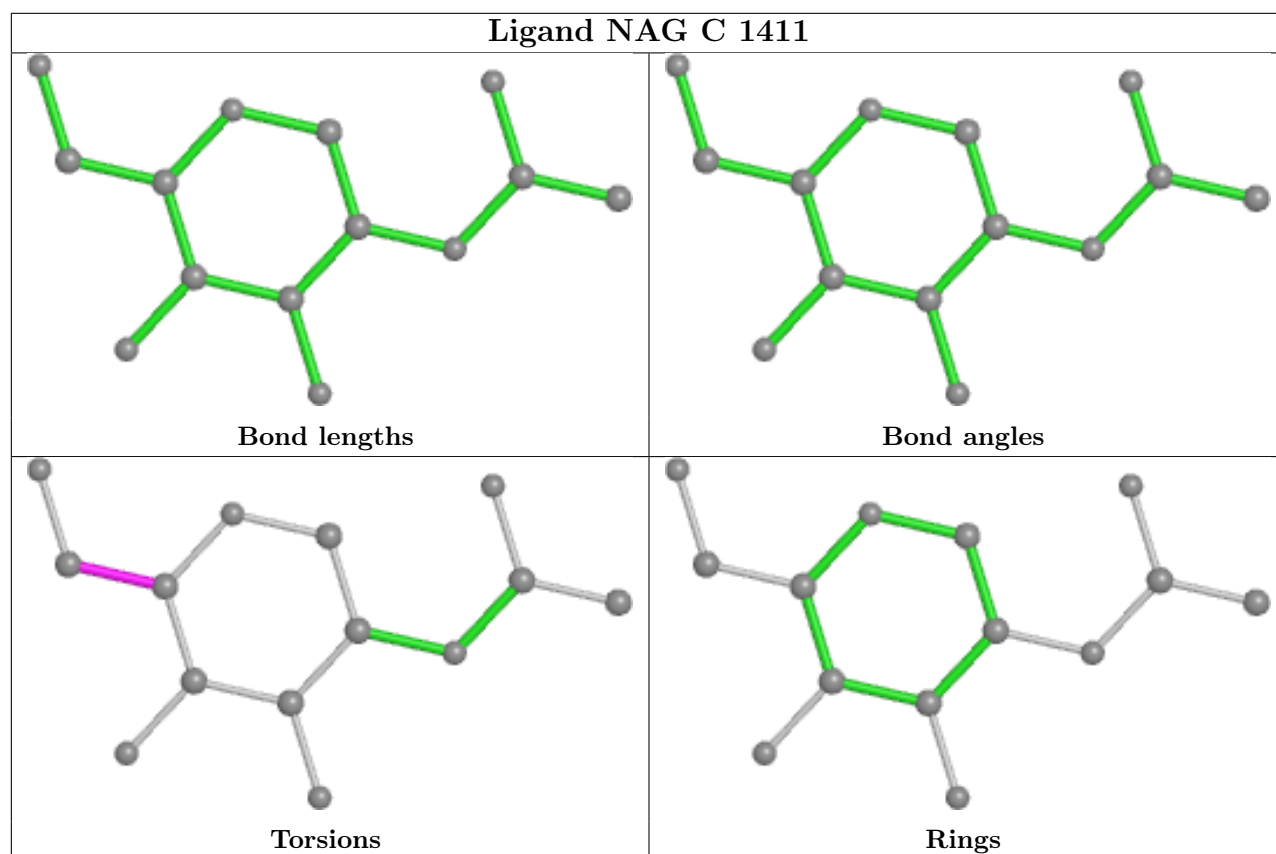
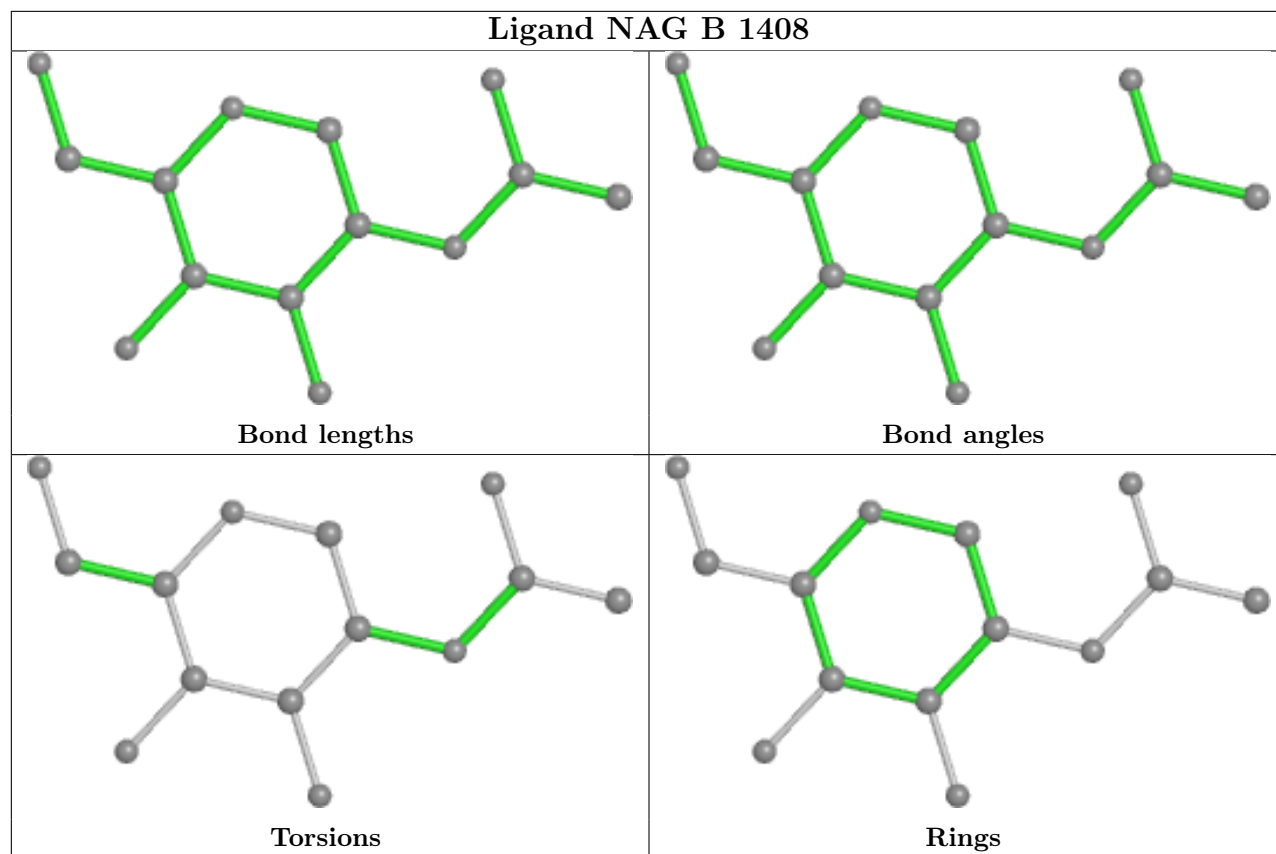


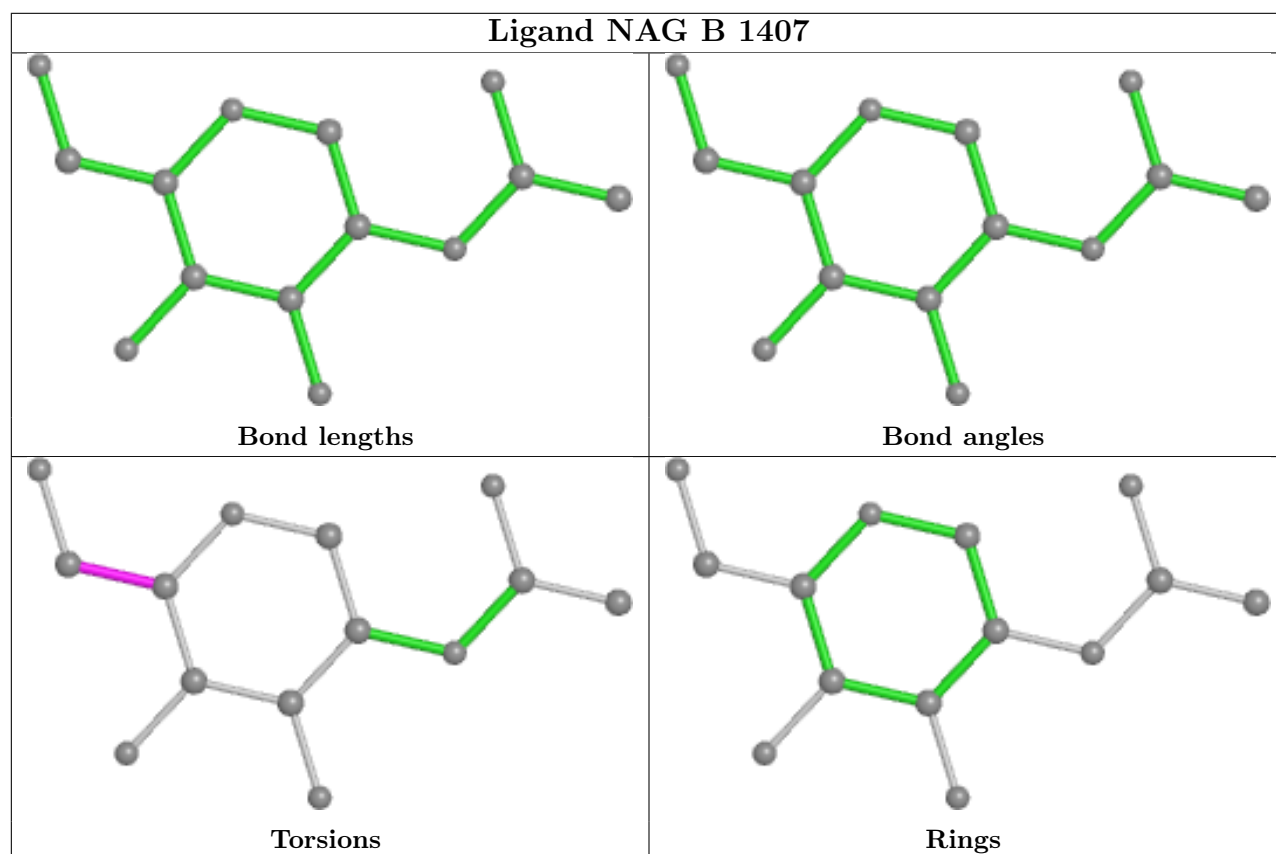
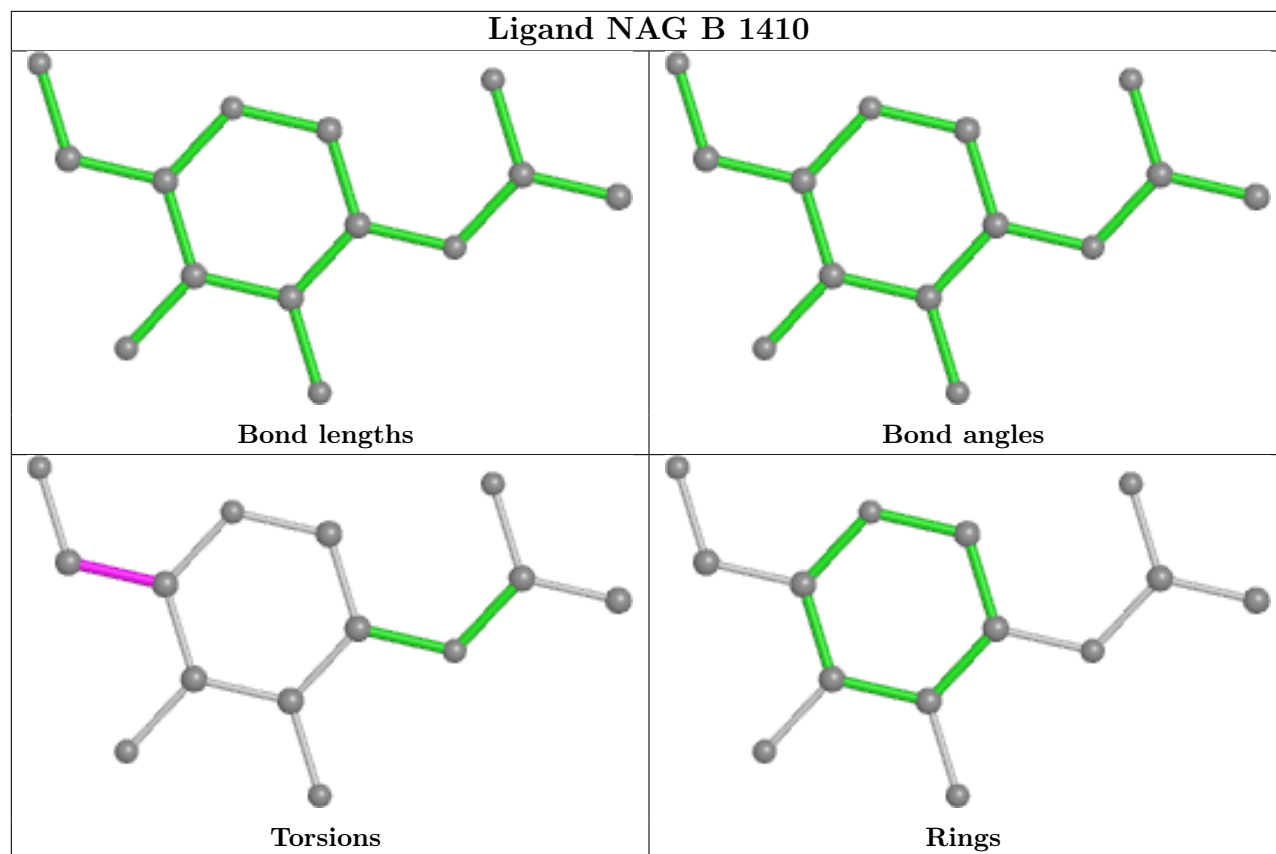
Ligand NAG C 1407



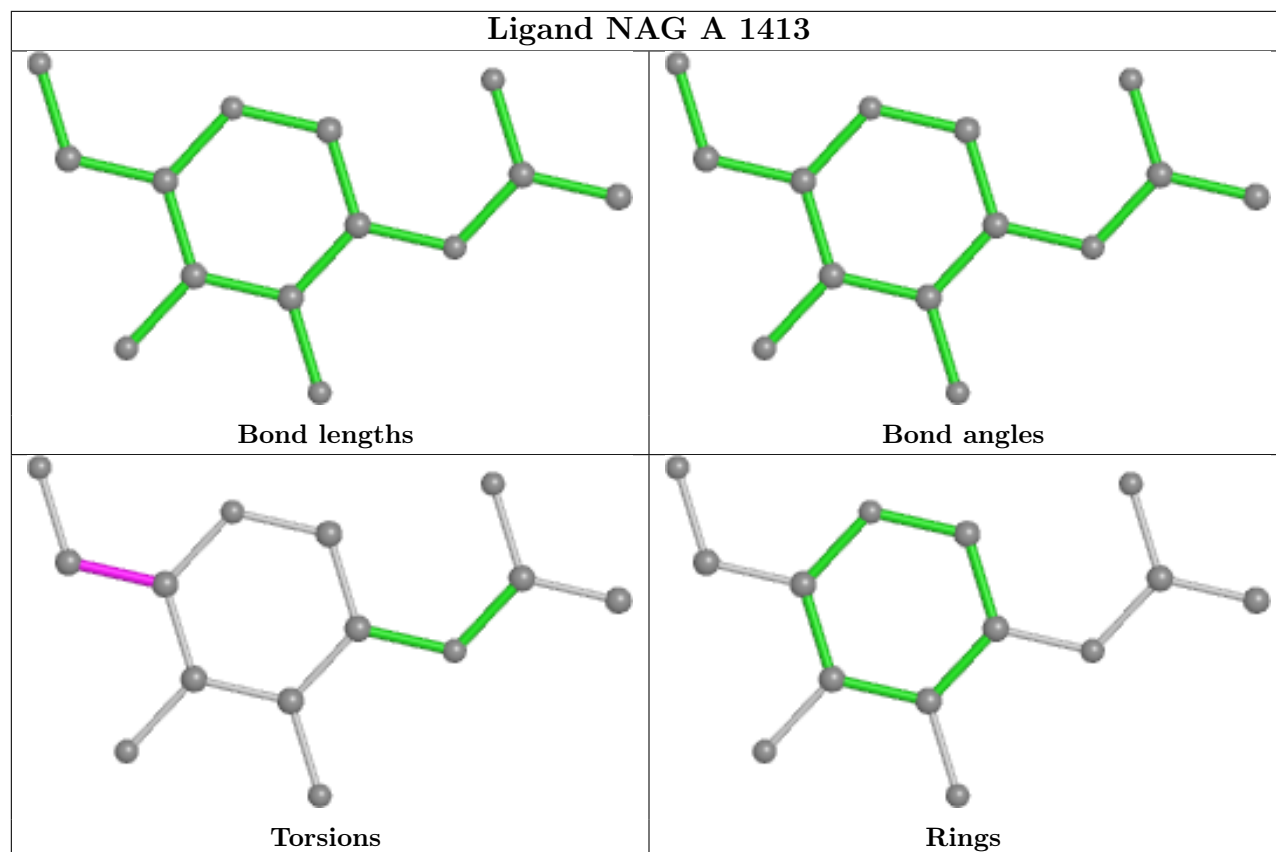
Ligand NAG C 1414



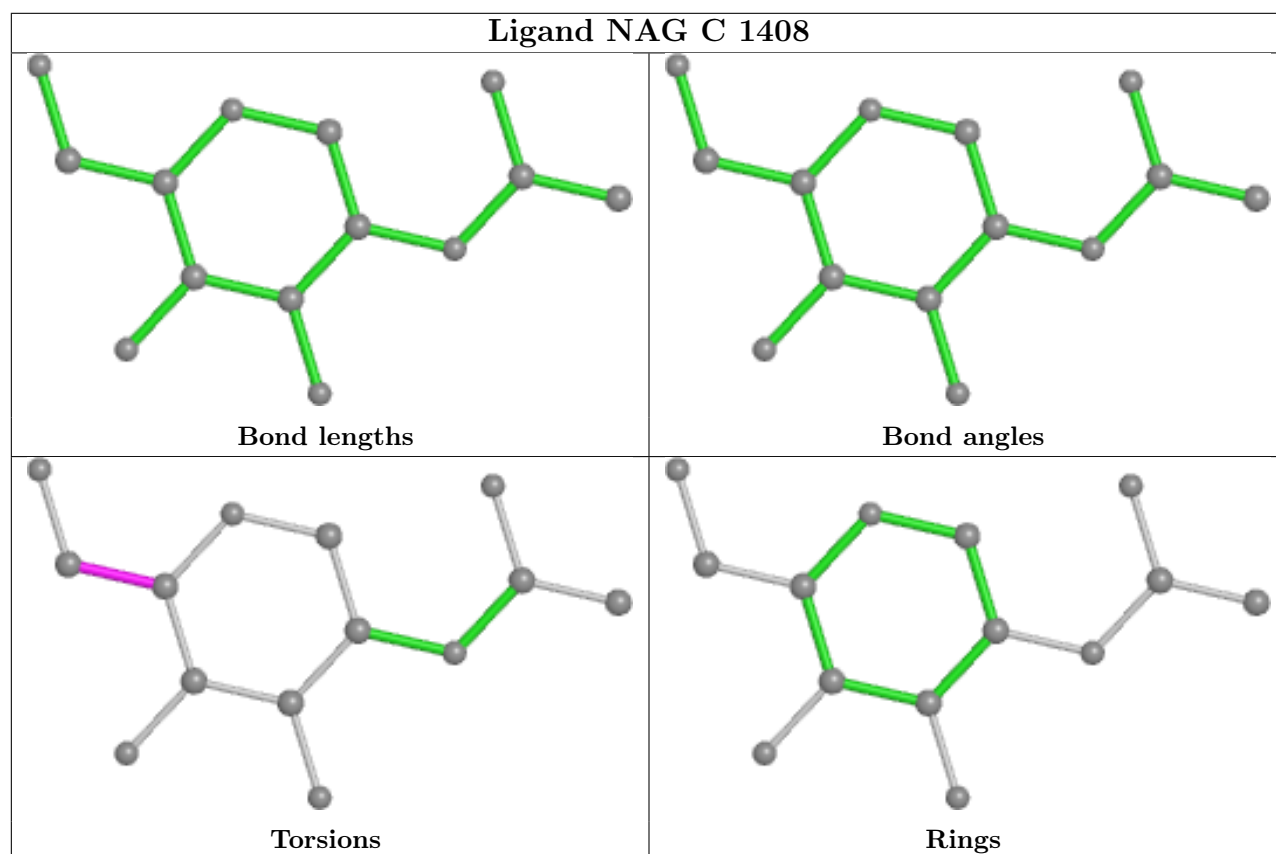


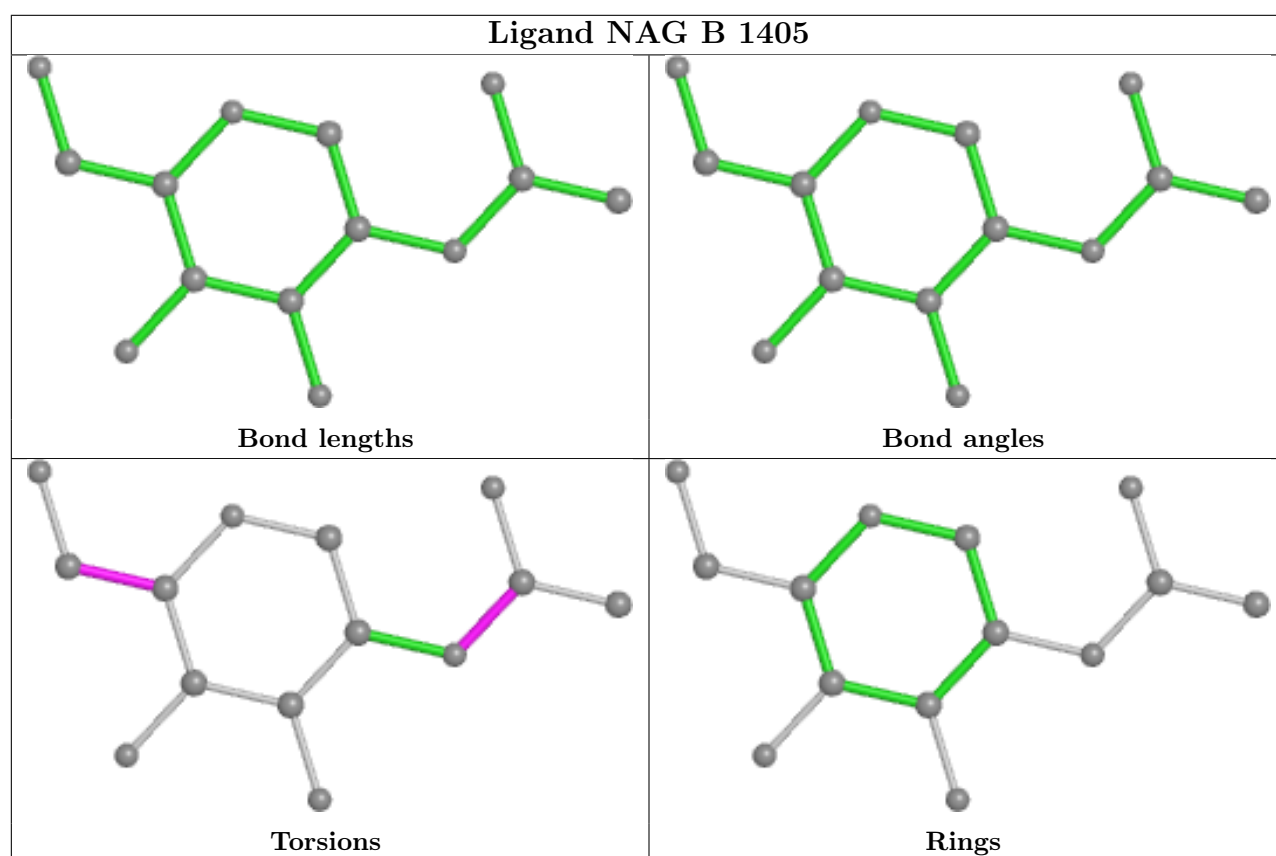
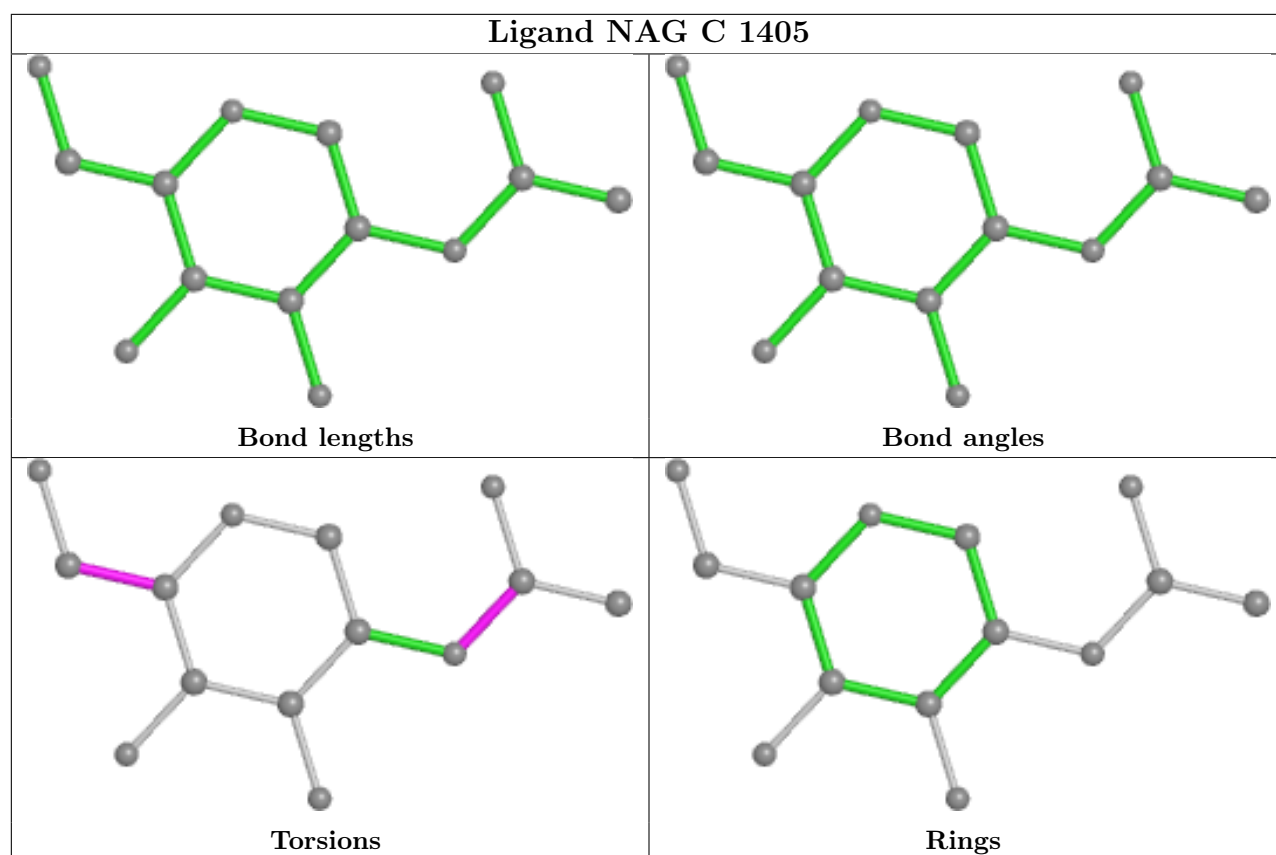


Ligand NAG A 1413

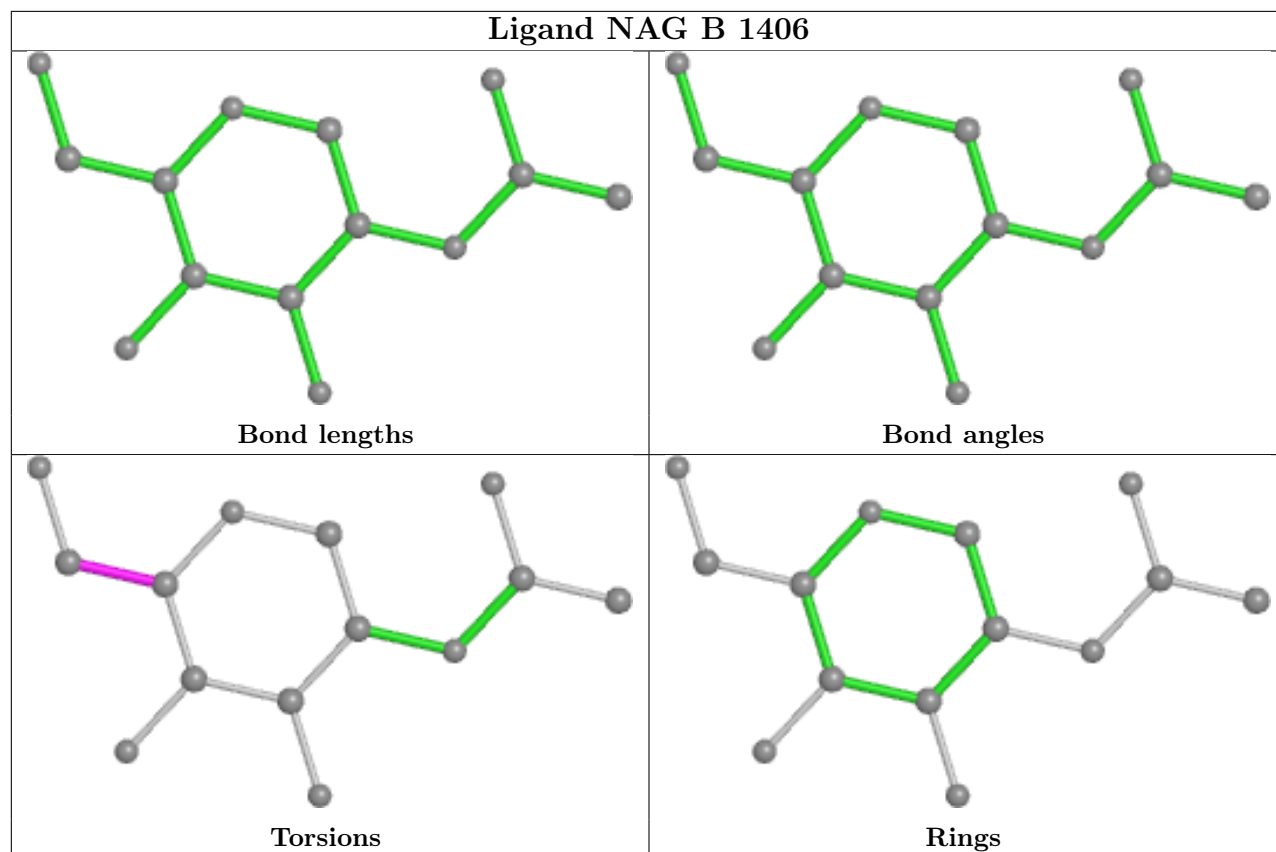


Ligand NAG C 1408

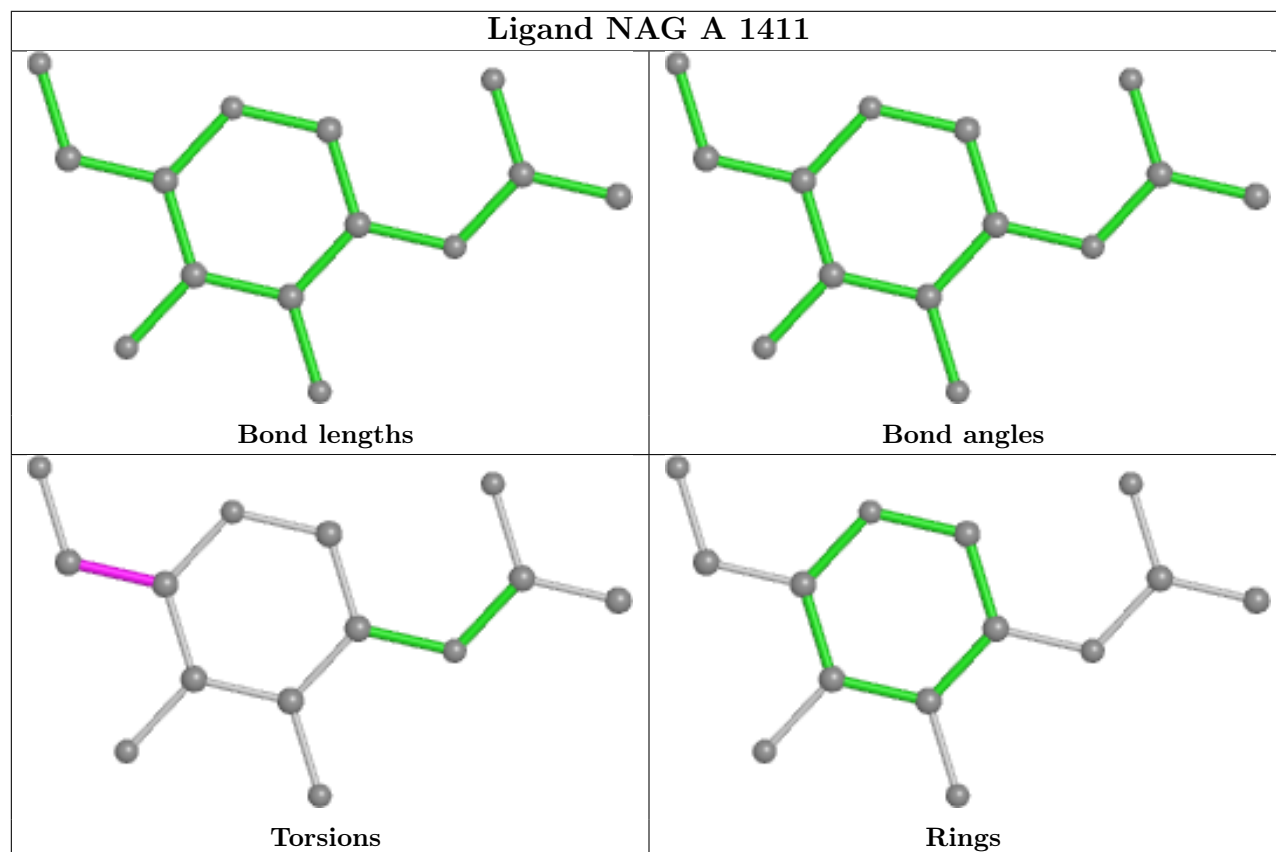




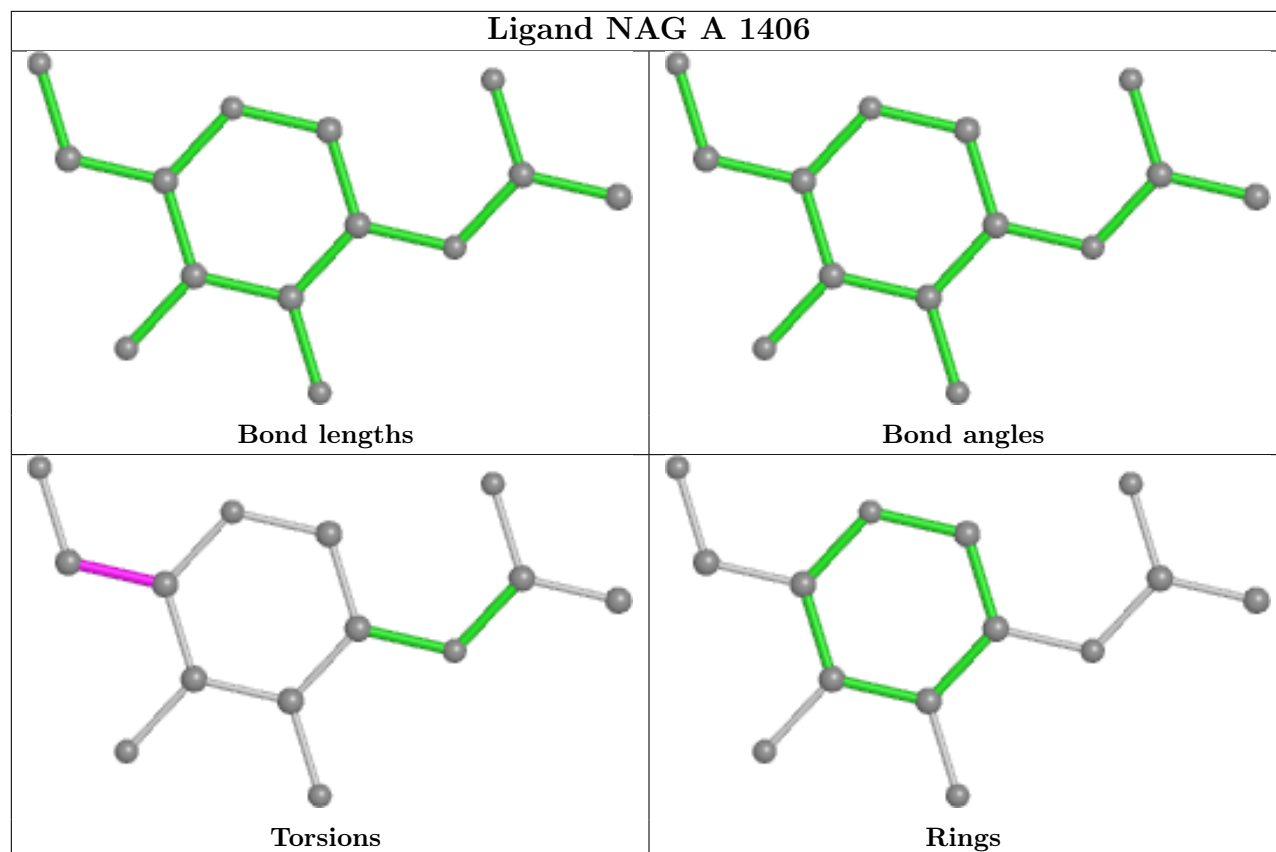
Ligand NAG B 1406



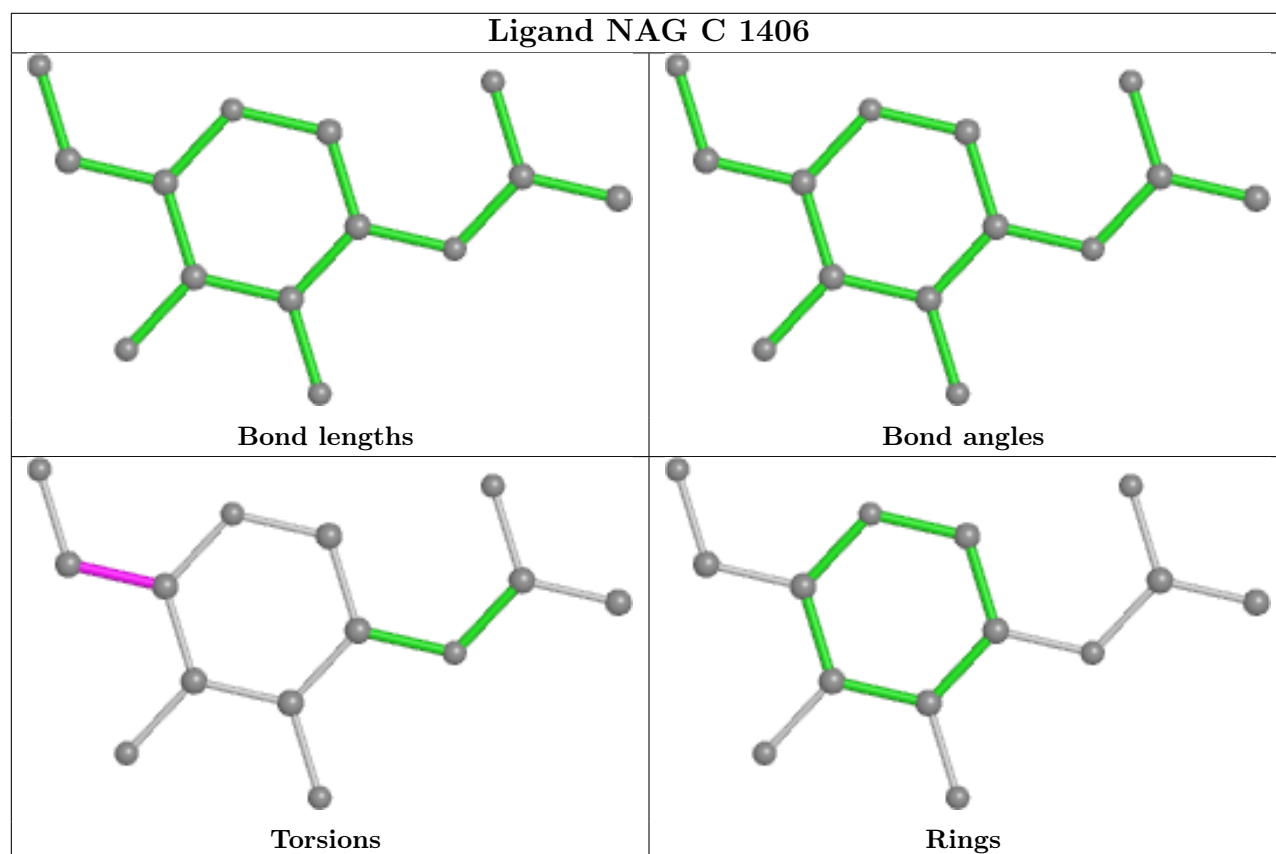
Ligand NAG A 1411

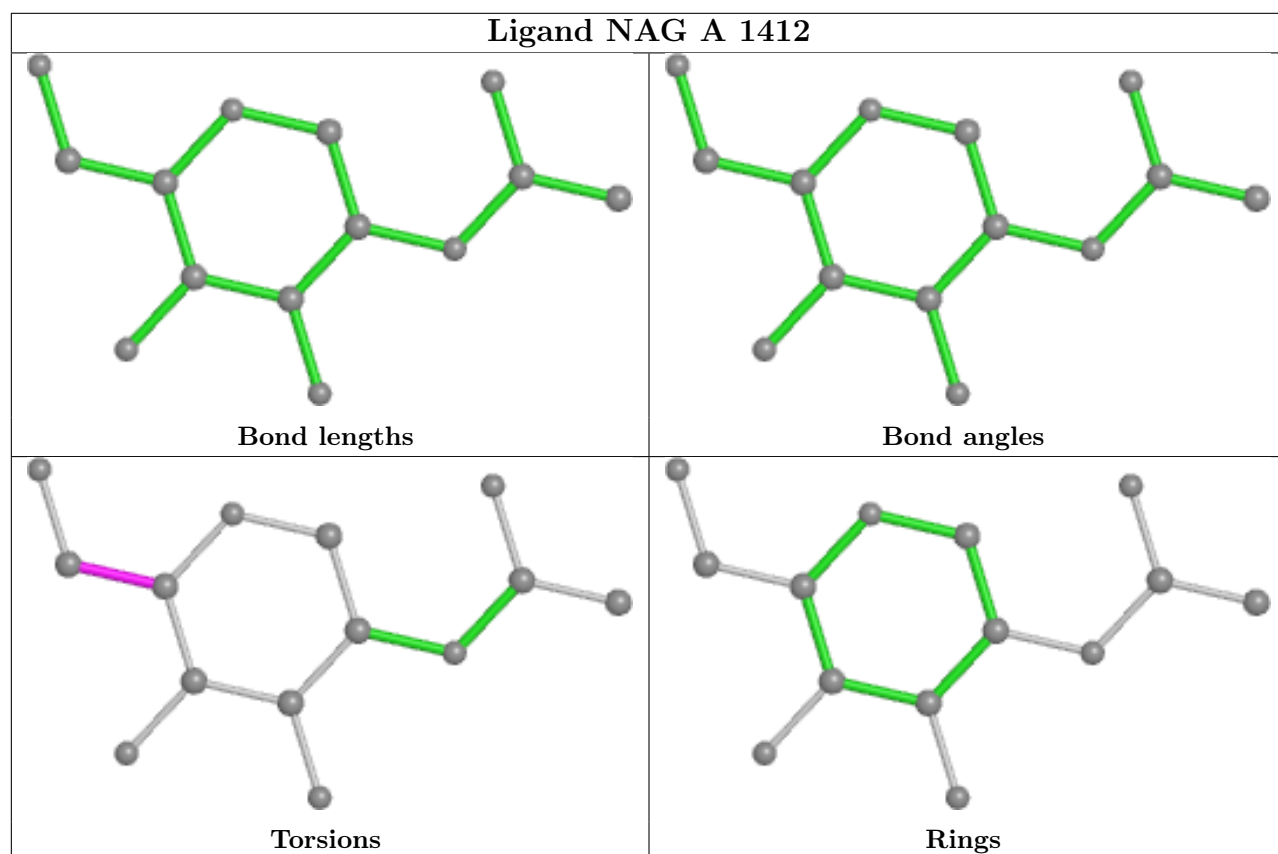
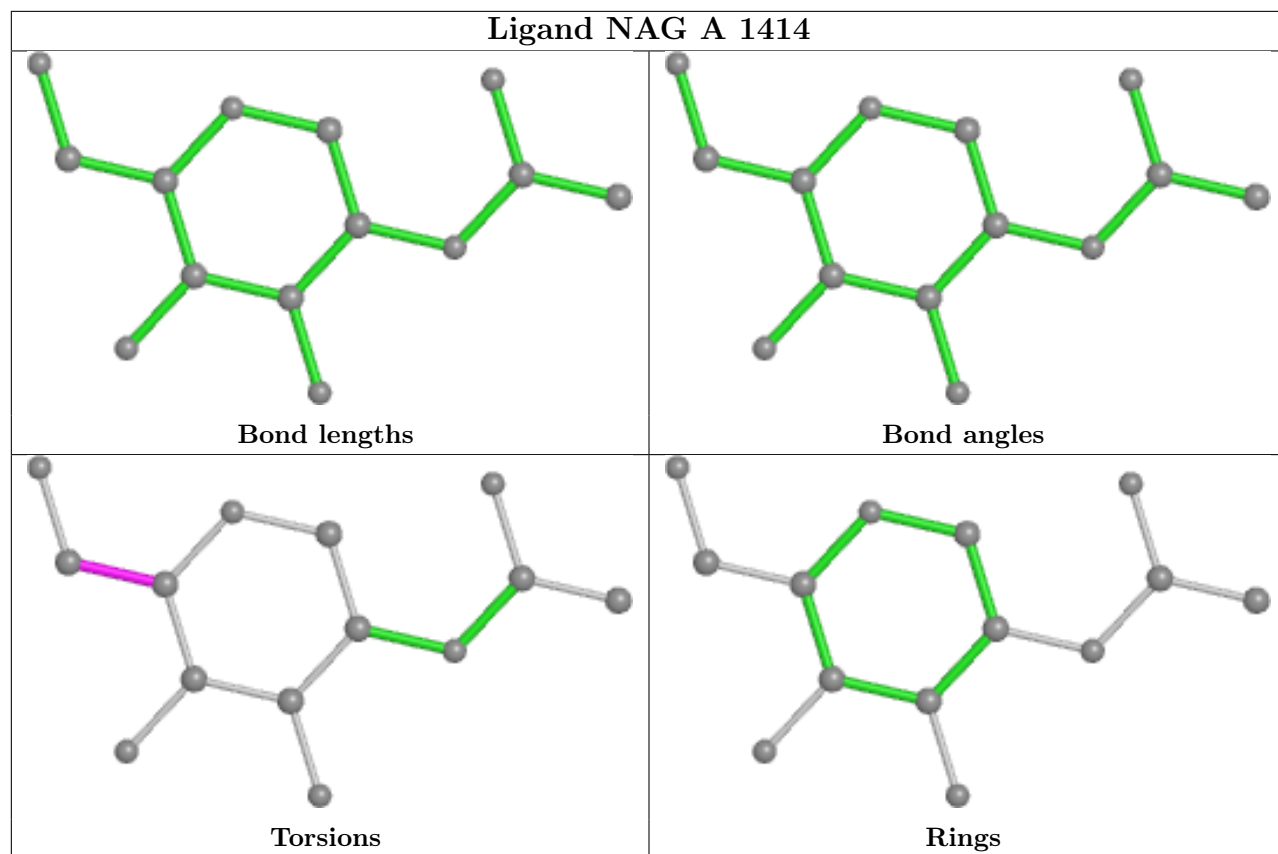


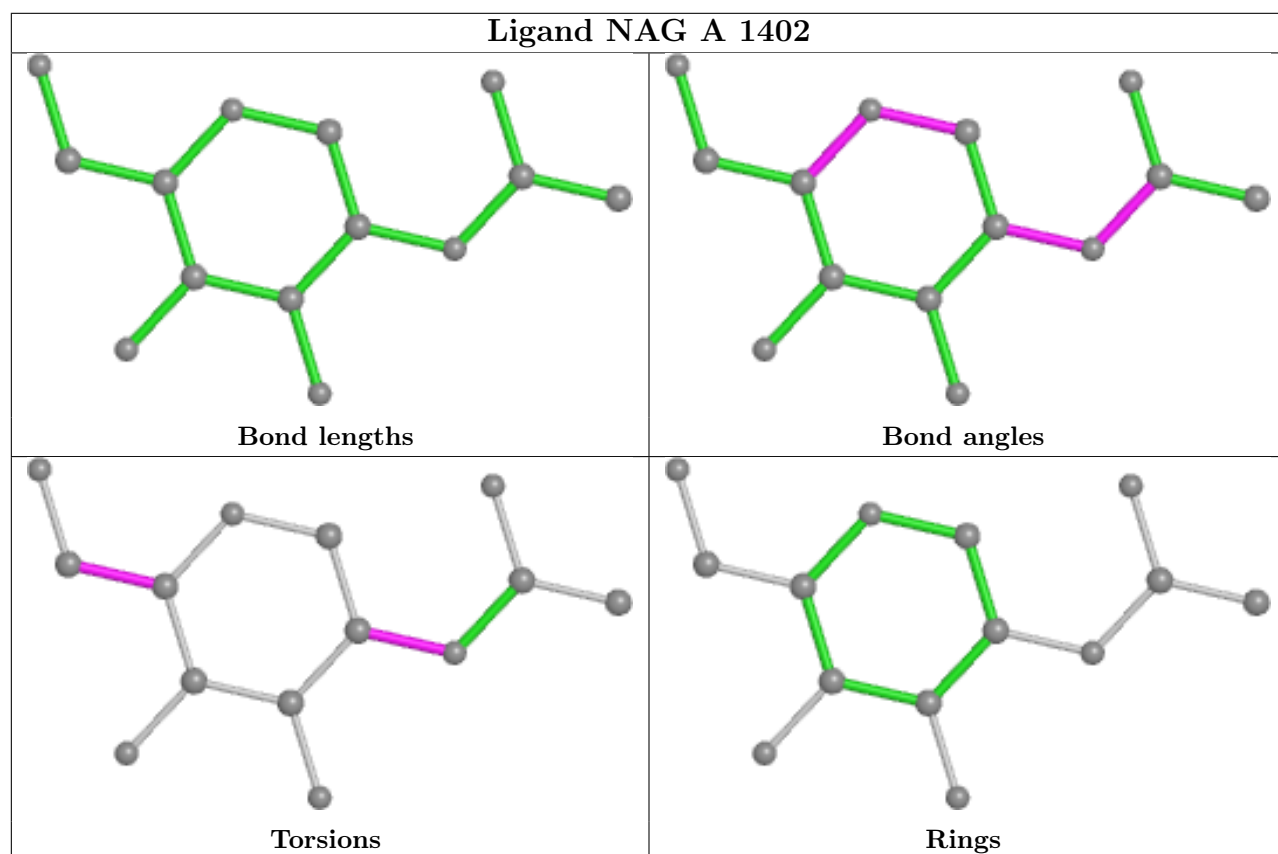
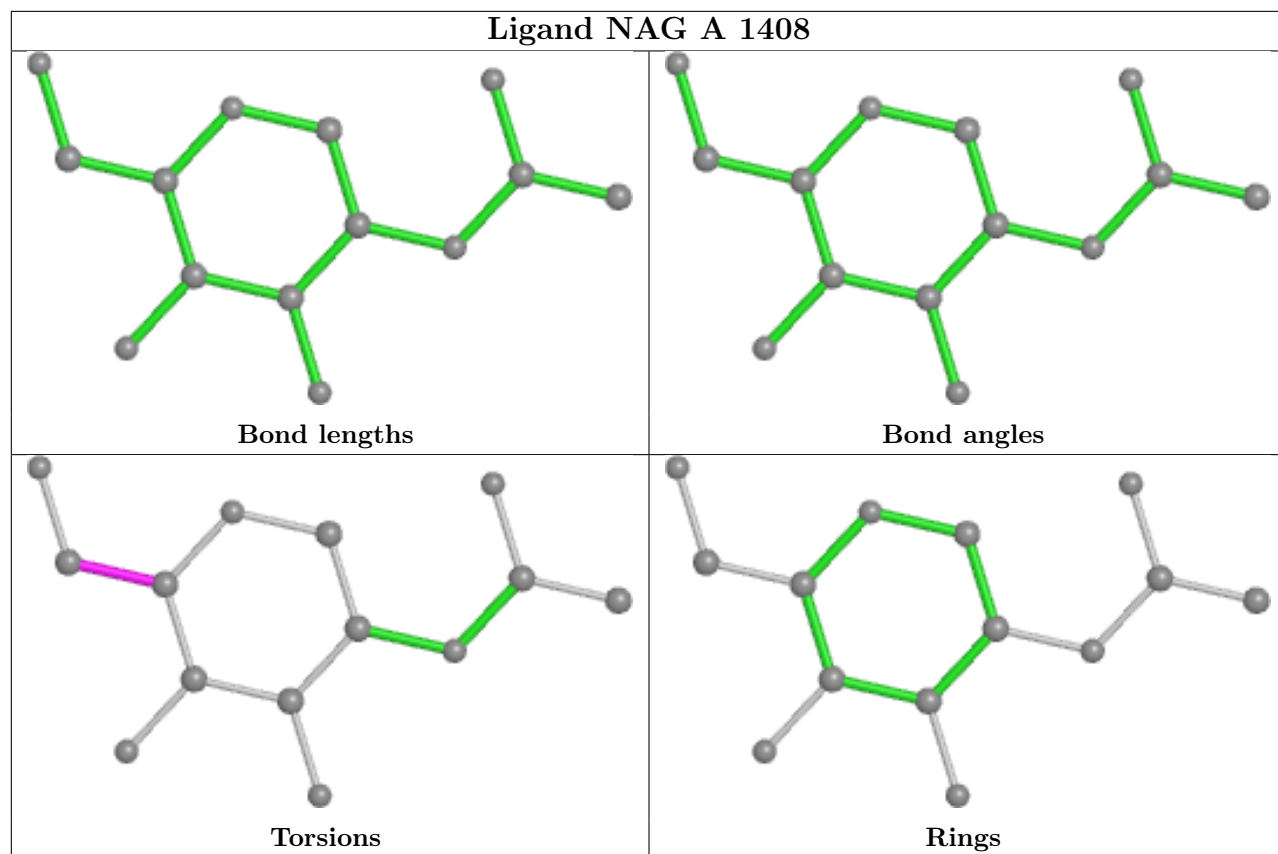
Ligand NAG A 1406



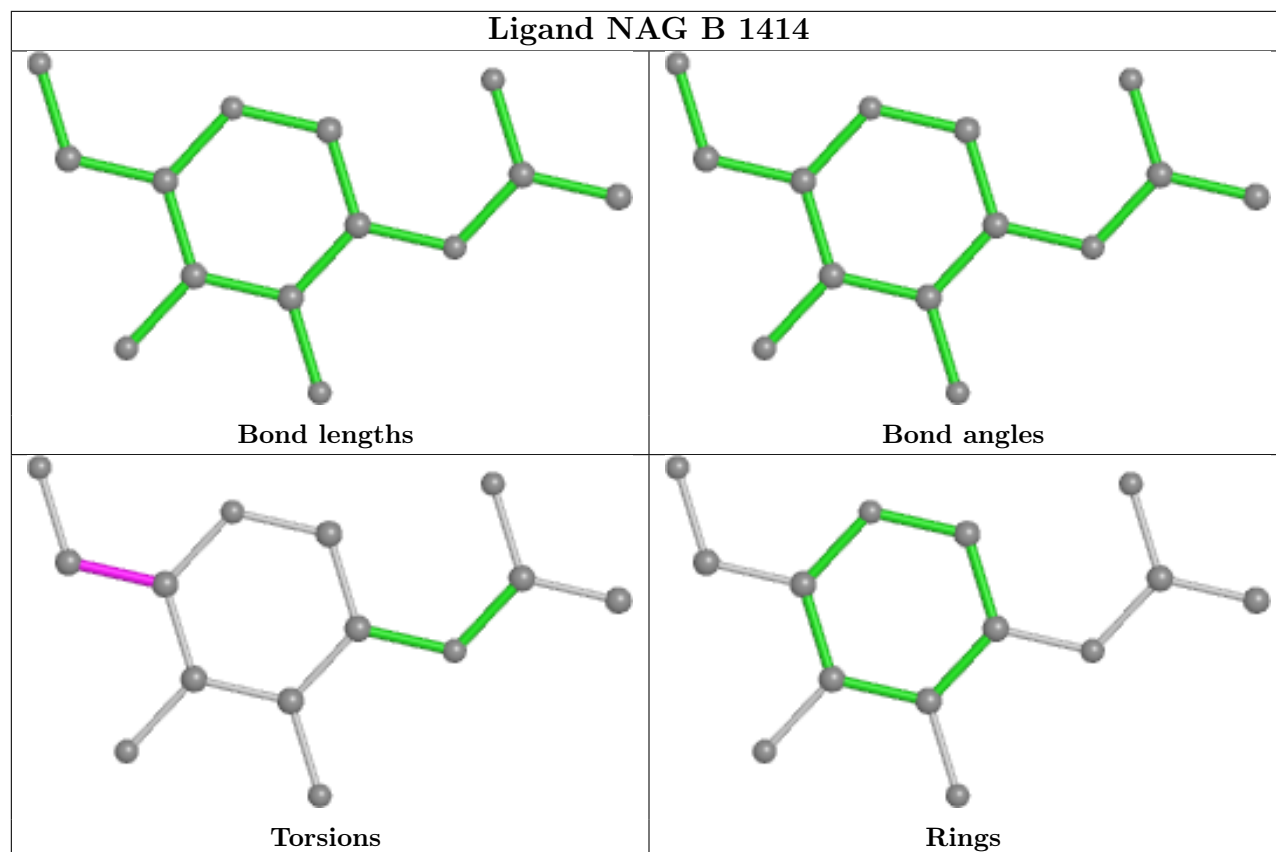
Ligand NAG C 1406



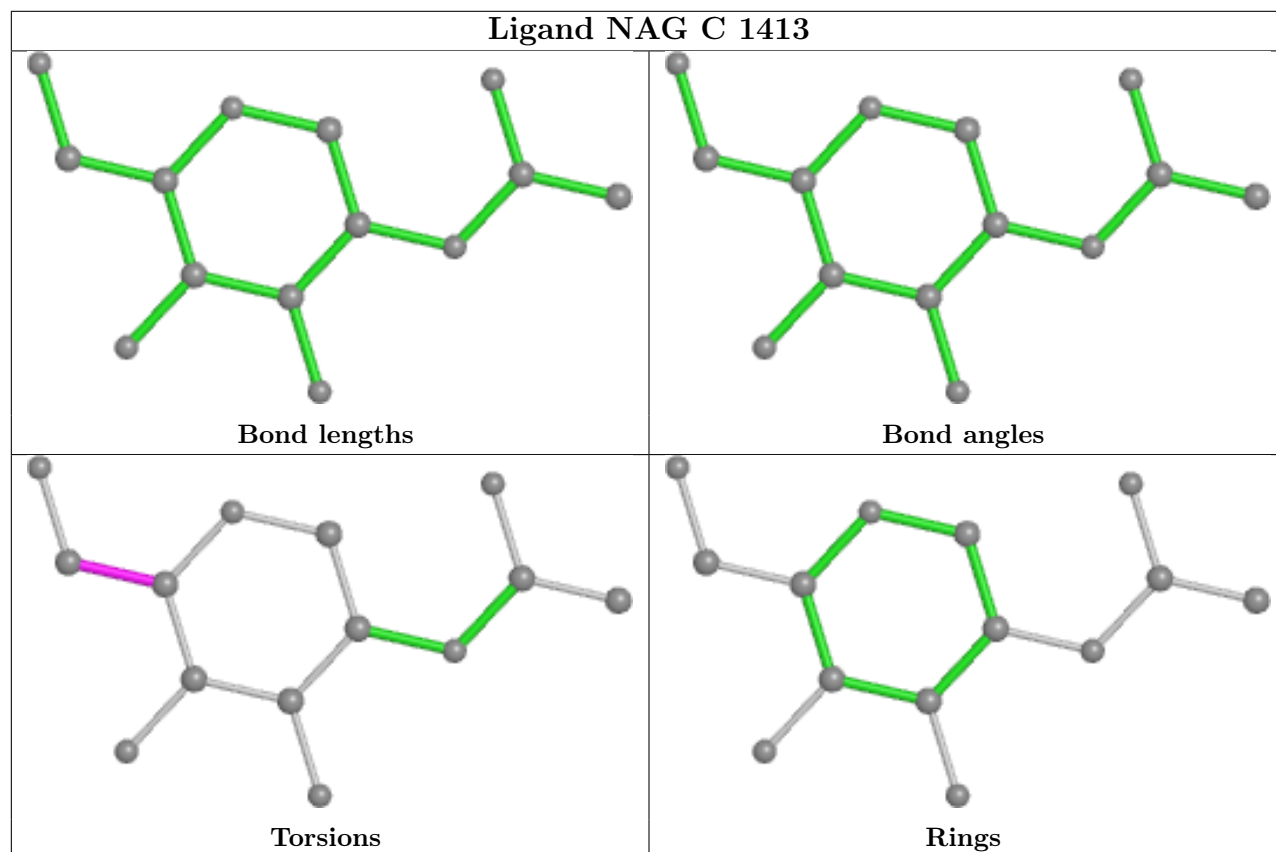




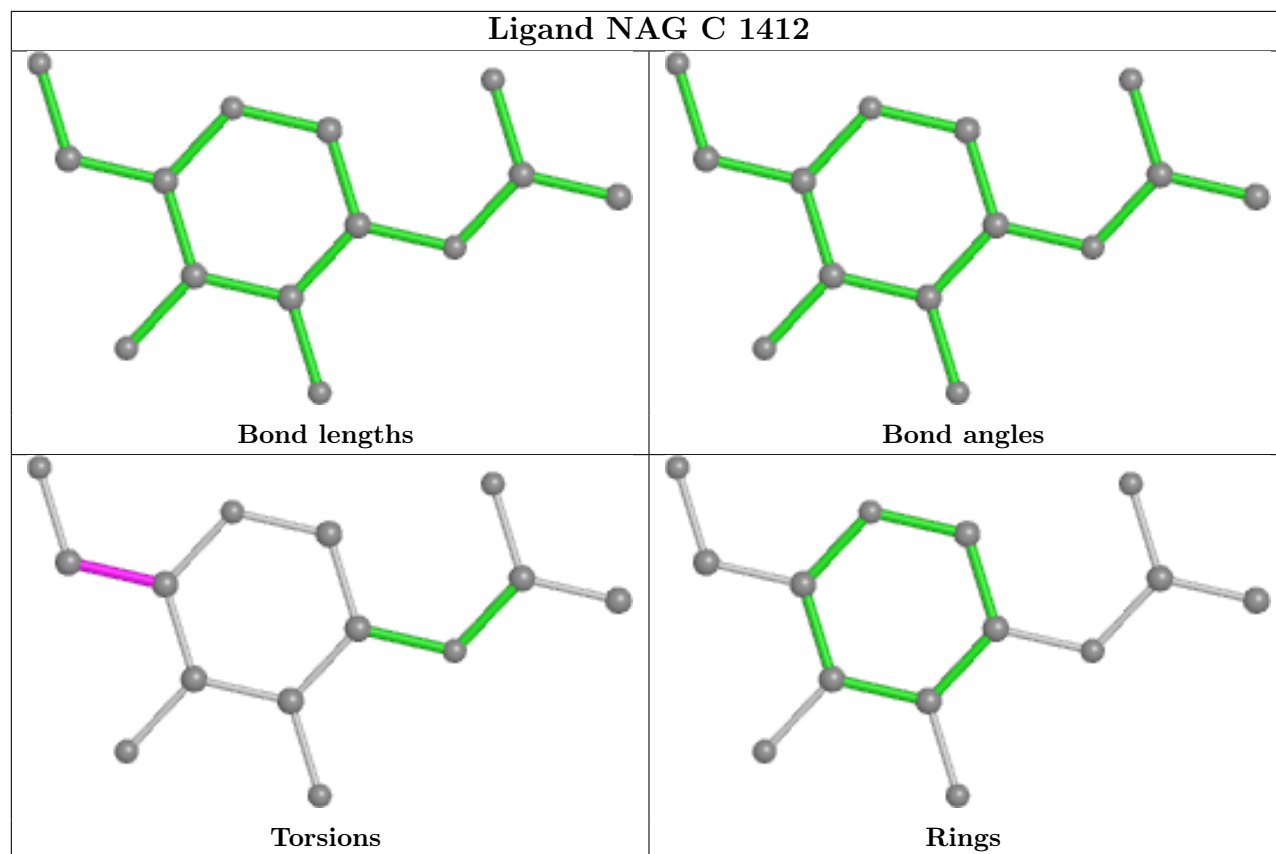
Ligand NAG B 1414



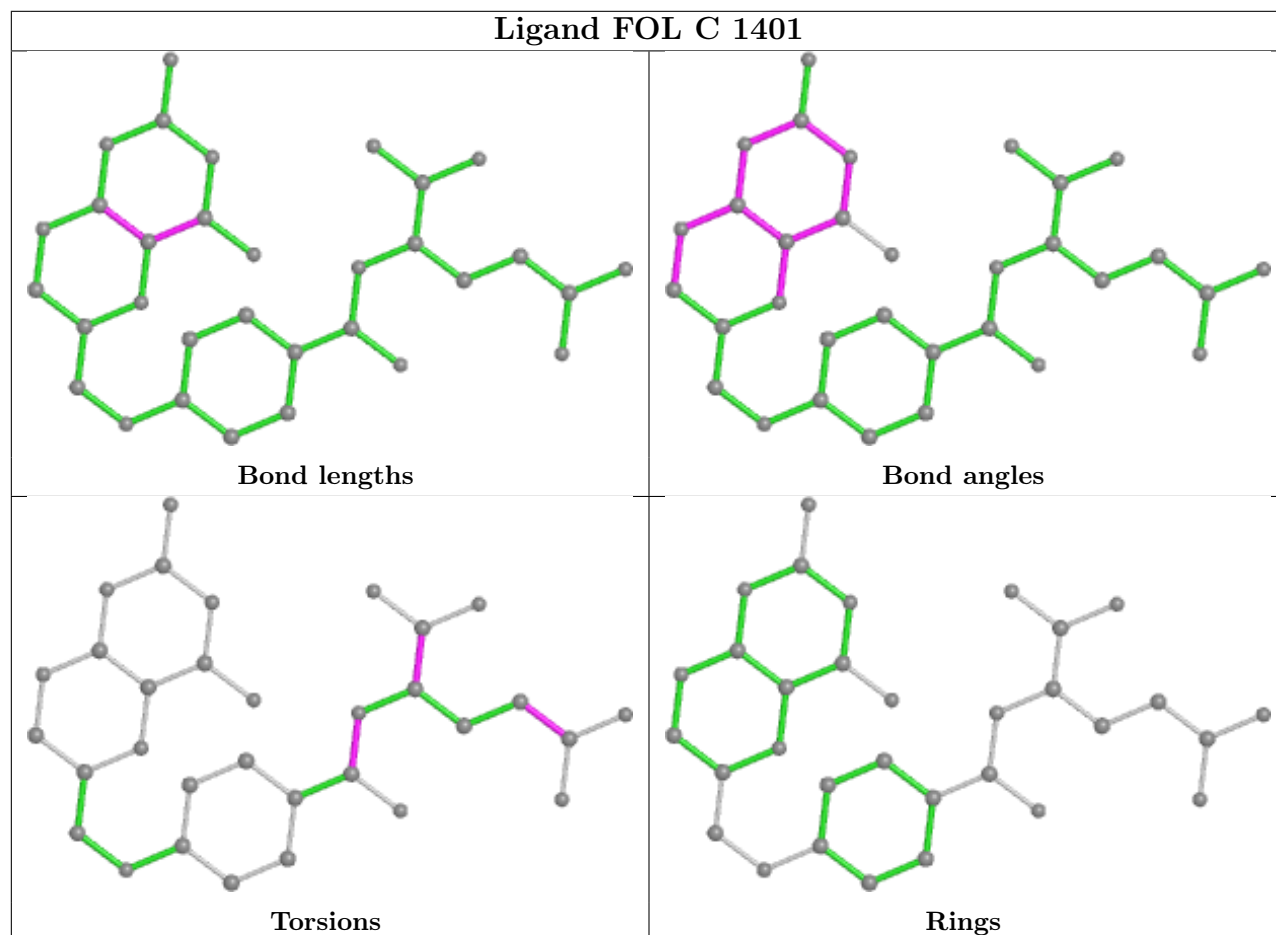
Ligand NAG C 1413



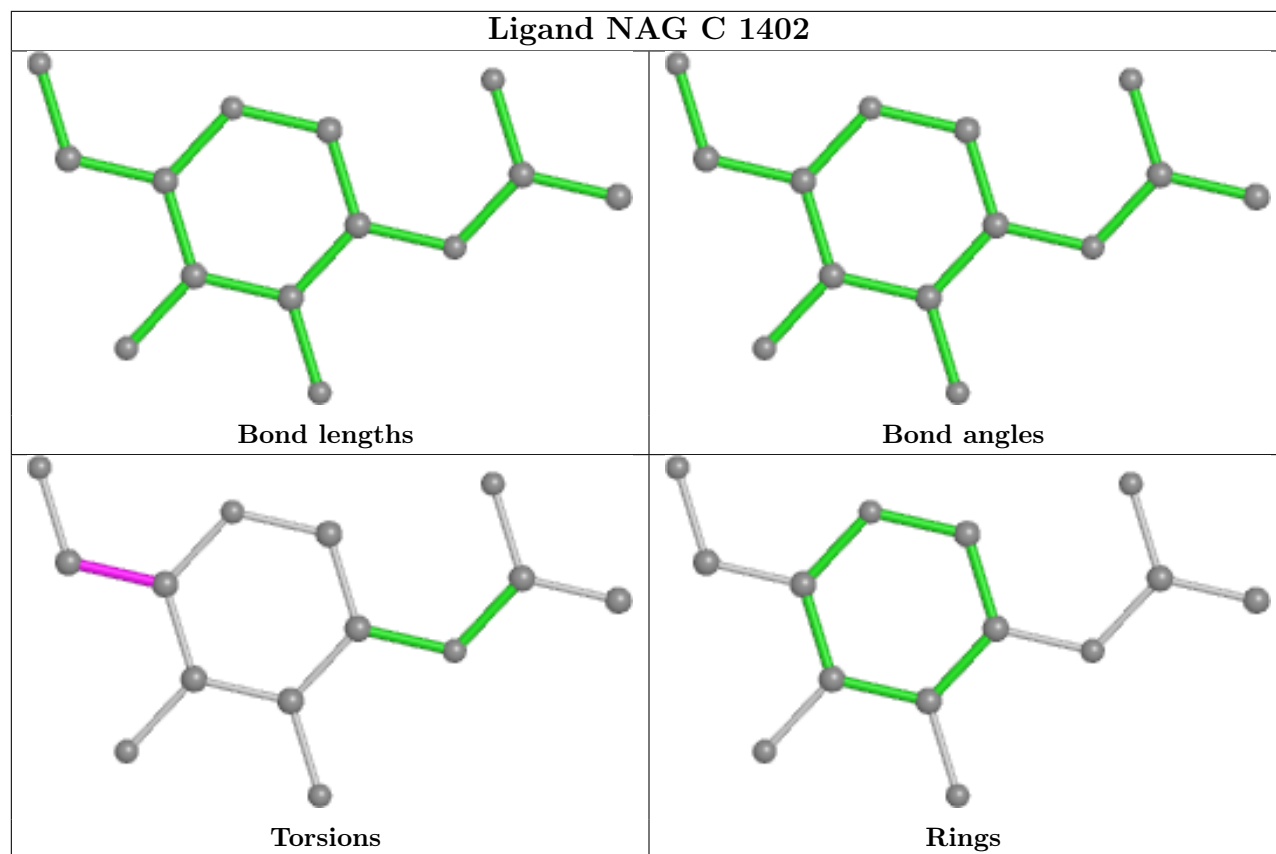
Ligand NAG C 1412



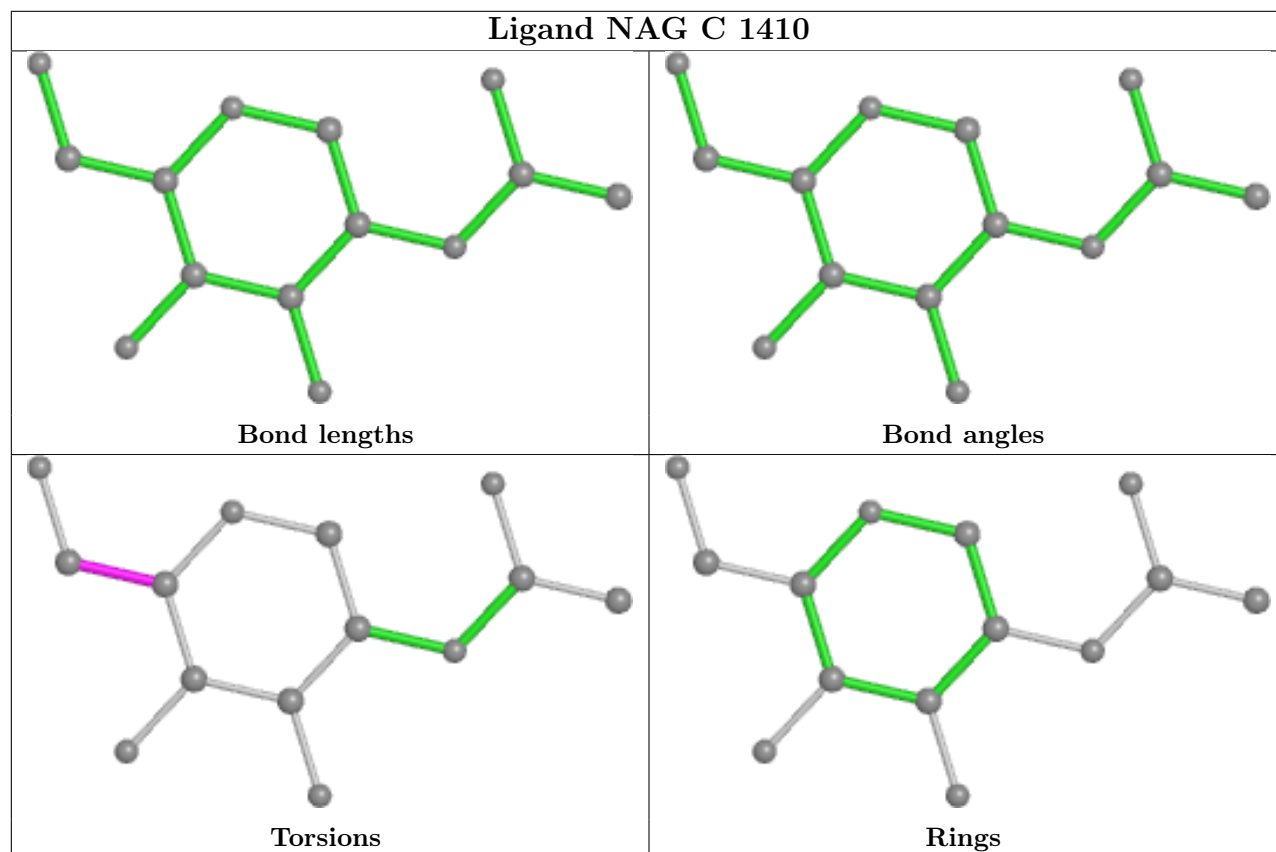
Ligand FOL C 1401

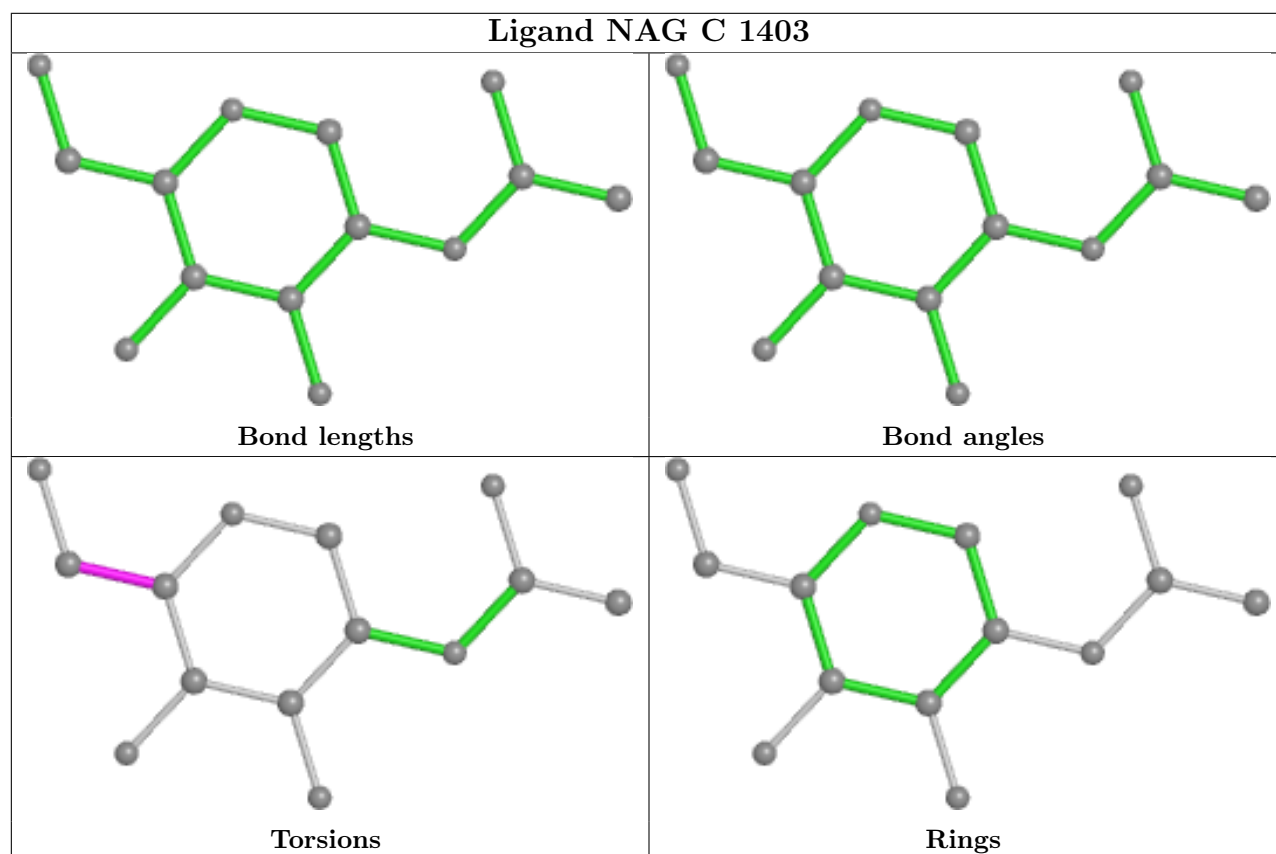
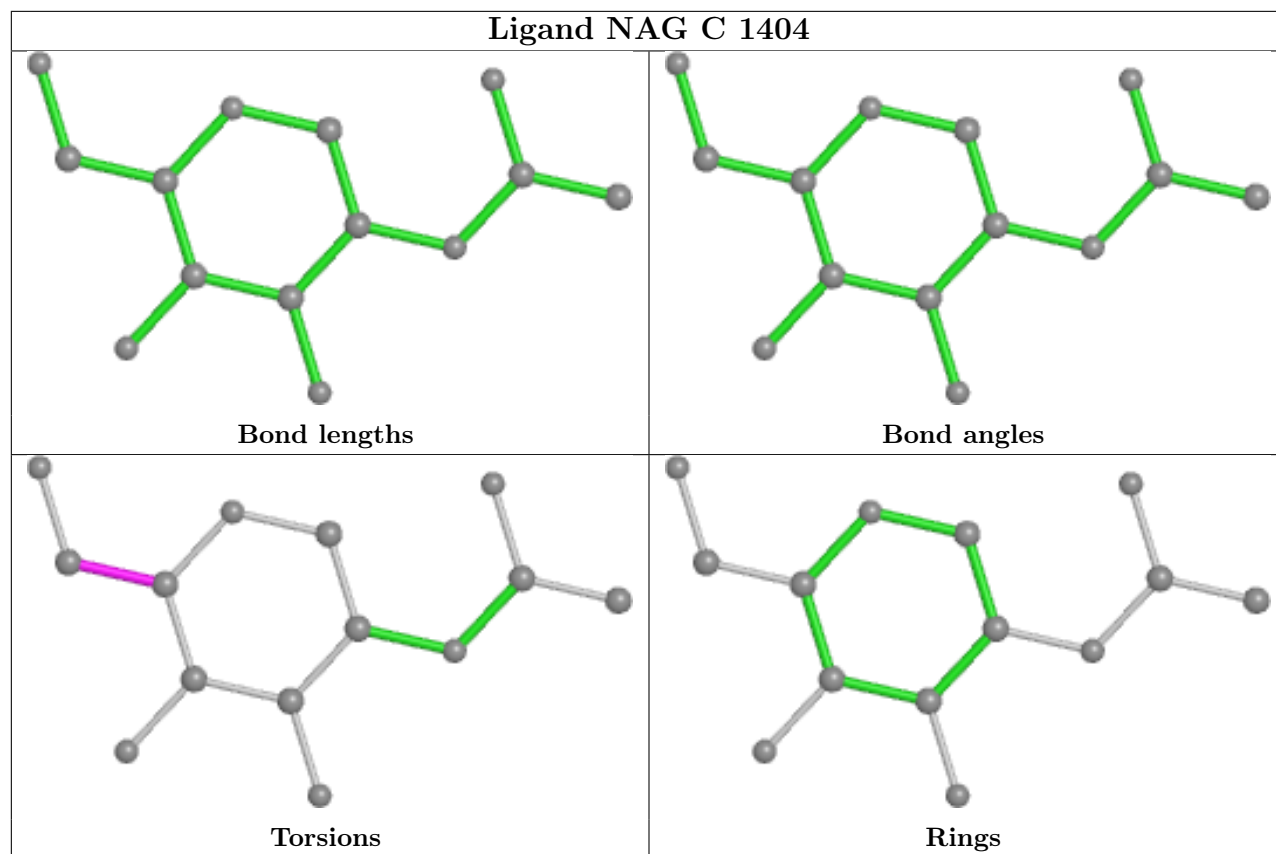


Ligand NAG C 1402



Ligand NAG C 1410





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.