



wwPDB EM Validation Summary Report ⓘ

Jul 17, 2025 – 10:18 PM JST

PDB ID : 9JMN / pdb_00009jmn
EMDB ID : EMD-61607
Title : Cryo-EM structure of CN-HedgehogCoV (HKU31/Erinaceus amurensis/China/2014) S-trimer in a locked-1 conformation
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 3.80 Å(reported)

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

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

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

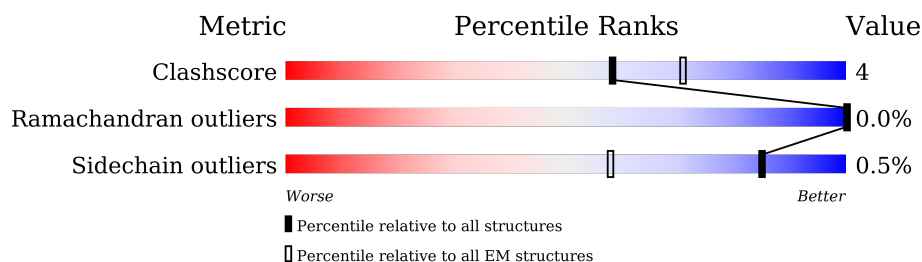
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	73% 9% 18%
1	B	1349	73% 10% 18%
1	C	1349	72% 10% 18%
2	D	3	67% 33%
2	E	3	100%
2	F	3	100%
2	H	3	100%
2	I	3	33% 67%
2	K	3	100%

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Mol	Chain	Length	Quality of chain
3	G	2	<div><div></div><div>50%</div><div>50%</div></div>
3	J	2	<div><div></div><div>50%</div><div>50%</div></div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 26833 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	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		
1	B	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		
1	C	1110	Total	C	N	O	S	0	0
			8679	5501	1444	1677	57		

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

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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

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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

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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

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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 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
2	D	3	Total	C	N	O	0	0
			39	22	2	15		
2	E	3	Total	C	N	O	0	0
			39	22	2	15		
2	F	3	Total	C	N	O	0	0
			39	22	2	15		
2	H	3	Total	C	N	O	0	0
			39	22	2	15		
2	I	3	Total	C	N	O	0	0
			39	22	2	15		
2	K	3	Total	C	N	O	0	0
			39	22	2	15		

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



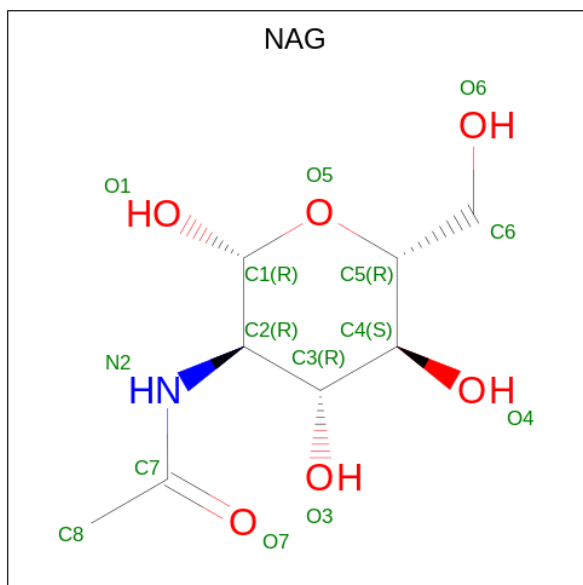
Mol	Chain	Residues	Atoms				AltConf	Trace
3	G	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				AltConf	Trace
3	J	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 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
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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

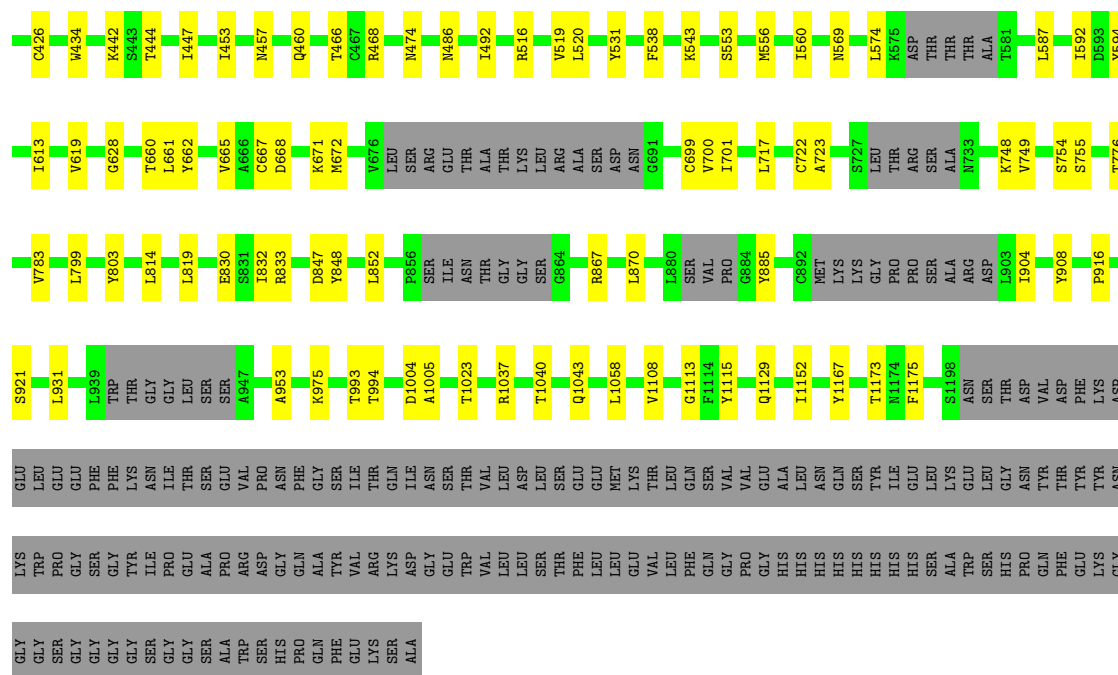
- Molecule 5 is FOLIC ACID (CCD ID: FOL) (formula: C₁₉H₁₉N₇O₆) (labeled as "Ligand of Interest" by depositor).



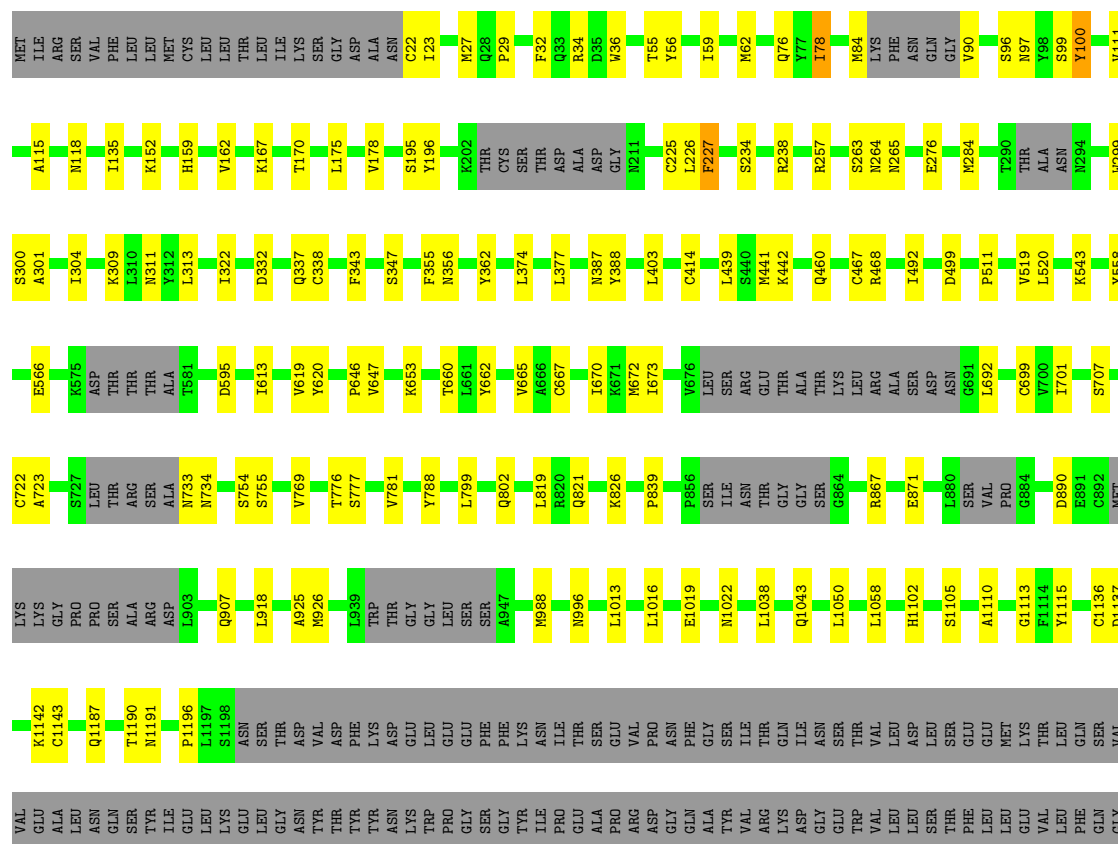
- Molecule 6 is LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
6	A	1	Total 20	C 18	O 2	0
6	A	1	Total 20	C 18	O 2	0
6	B	1	Total 20	C 18	O 2	0



● Molecule 1: Spike glycoprotein,Fibrin



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

Chain D: 67% 33%

NAG1
NAG2
BMA3

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

Chain E:  100%

NAG1
NAG2
BMA3

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

Chain F: 100%

NAG1
NAG2
BMA3

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

Chain H: 100%

NAG1
NAG2
BMA3

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

Chain I:  33% 67%

NAG1
NAG2
BMA3

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

Chain K: 100%

NAG1
NAG2
BMA3

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

Chain G:  50% 50%

MAG1
MAG2

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

Chain J:  50% 50%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	23410	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: FOL, NAG, EIC, BMA

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	0.17	0/8867	0.39	0/12033
1	B	0.17	0/8867	0.37	0/12033
1	C	0.18	0/8867	0.38	1/12033 (0.0%)
All	All	0.18	0/26601	0.38	1/36099 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	100	TYR	N-CA-C	-6.79	103.17	113.89

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	8679	0	8363	78	0
1	B	8679	0	8362	79	0
1	C	8679	0	8362	90	0
2	D	39	0	34	1	0
2	E	39	0	34	0	0
2	F	39	0	34	0	0
2	H	39	0	34	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	39	0	34	1	0
2	K	39	0	34	0	0
3	G	28	0	25	1	0
3	J	28	0	25	1	0
4	A	126	0	117	0	0
4	B	112	0	104	1	0
4	C	112	0	104	1	0
5	A	32	0	17	1	0
5	B	32	0	17	1	0
5	C	32	0	17	1	0
6	A	40	0	62	7	0
6	B	20	0	31	0	0
All	All	26833	0	25810	237	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.

The worst 5 of 237 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:1040:THR:HA	1:B:1043:GLN:HE21	1.52	0.74
1:B:82:TYR:HE1	1:B:289:LYS:HA	1.59	0.68
1:A:487:ASN:OD1	1:A:488:ASN:ND2	2.28	0.67
1:B:587:LEU:HD13	1:B:592:ILE:HG13	1.76	0.66
1:A:55:THR:HG21	1:C:613:ILE:H	1.61	0.65

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	1088/1349 (81%)	1032 (95%)	56 (5%)	0	100	100
1	B	1088/1349 (81%)	1042 (96%)	46 (4%)	0	100	100
1	C	1088/1349 (81%)	1046 (96%)	41 (4%)	1 (0%)	48	79
All	All	3264/4047 (81%)	3120 (96%)	143 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	PHE

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	965/1165 (83%)	962 (100%)	3 (0%)	91	92
1	B	965/1165 (83%)	959 (99%)	6 (1%)	84	88
1	C	965/1165 (83%)	959 (99%)	6 (1%)	84	88
All	All	2895/3495 (83%)	2880 (100%)	15 (0%)	85	90

5 of 15 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	749	VAL
1	C	692	LEU
1	B	814	LEU
1	C	907	GLN
1	C	225	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 50 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1077	GLN
1	C	91	ASN

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Mol	Chain	Res	Type
1	C	1192	ASN
1	B	1084	ASN
1	B	1112	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

22 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	0.65	1 (7%)	17,19,21	0.83	0
2	NAG	D	2	2	14,14,15	0.18	0	17,19,21	0.64	1 (5%)
2	BMA	D	3	2	11,11,12	0.58	0	15,15,17	1.14	2 (13%)
2	NAG	E	1	1,2	14,14,15	0.40	0	17,19,21	0.55	0
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.62	0
2	BMA	E	3	2	11,11,12	0.80	0	15,15,17	0.86	0
2	NAG	F	1	1,2	14,14,15	0.62	0	17,19,21	1.97	2 (11%)
2	NAG	F	2	2	14,14,15	0.28	0	17,19,21	0.87	1 (5%)
2	BMA	F	3	2	11,11,12	1.01	1 (9%)	15,15,17	1.02	1 (6%)
3	NAG	G	1	1,3	14,14,15	0.21	0	17,19,21	0.43	0
3	NAG	G	2	3	14,14,15	0.20	0	17,19,21	0.53	0
2	NAG	H	1	1,2	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.22	0	17,19,21	0.47	0
2	BMA	H	3	2	11,11,12	0.56	0	15,15,17	0.84	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	I	1	1,2	14,14,15	0.32	0	17,19,21	0.52	0
2	NAG	I	2	2	14,14,15	0.28	0	17,19,21	0.57	0
2	BMA	I	3	2	11,11,12	0.54	0	15,15,17	0.91	1 (6%)
3	NAG	J	1	1,3	14,14,15	0.21	0	17,19,21	0.50	0
3	NAG	J	2	3	14,14,15	0.21	0	17,19,21	0.52	0
2	NAG	K	1	1,2	14,14,15	0.21	0	17,19,21	0.62	0
2	NAG	K	2	2	14,14,15	0.20	0	17,19,21	0.47	0
2	BMA	K	3	2	11,11,12	0.53	0	15,15,17	0.84	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	D	1	1,2	-	3/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	BMA	D	3	2	-	1/2/19/22	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
2	BMA	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	F	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	F	2	2	-	2/6/23/26	0/1/1/1
2	BMA	F	3	2	-	1/2/19/22	0/1/1/1
3	NAG	G	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	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
2	BMA	H	3	2	-	0/2/19/22	0/1/1/1
2	NAG	I	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	1/6/23/26	0/1/1/1
2	BMA	I	3	2	-	1/2/19/22	0/1/1/1
3	NAG	J	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
2	NAG	K	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	K	2	2	-	2/6/23/26	0/1/1/1
2	BMA	K	3	2	-	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	3	BMA	C1-C2	2.63	1.58	1.52
2	D	1	NAG	O5-C1	-2.22	1.40	1.43

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAG	C2-N2-C7	6.91	132.74	122.90
2	F	1	NAG	C1-C2-N2	3.23	116.01	110.49
2	D	3	BMA	C1-O5-C5	2.79	115.98	112.19
2	D	3	BMA	O2-C2-C3	-2.43	105.27	110.14
2	F	2	NAG	C2-N2-C7	2.39	126.30	122.90

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

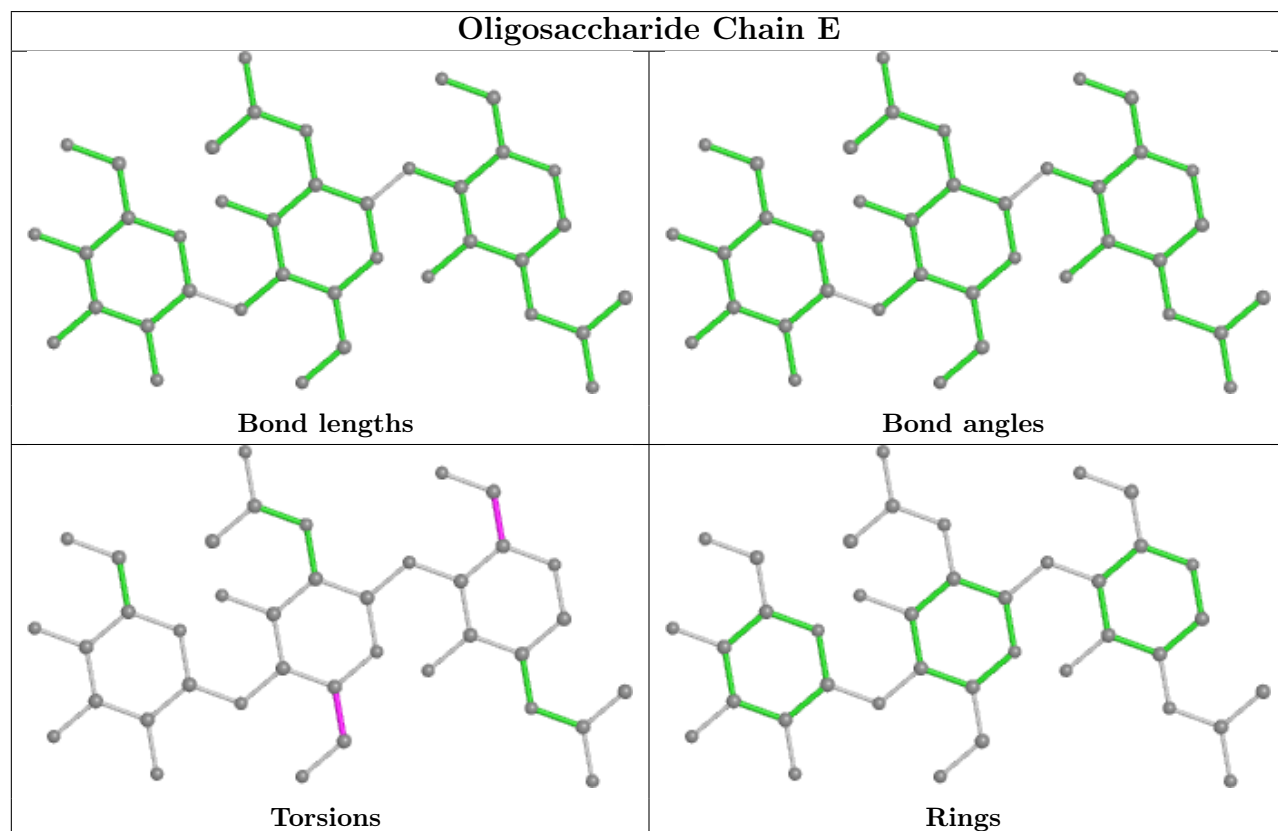
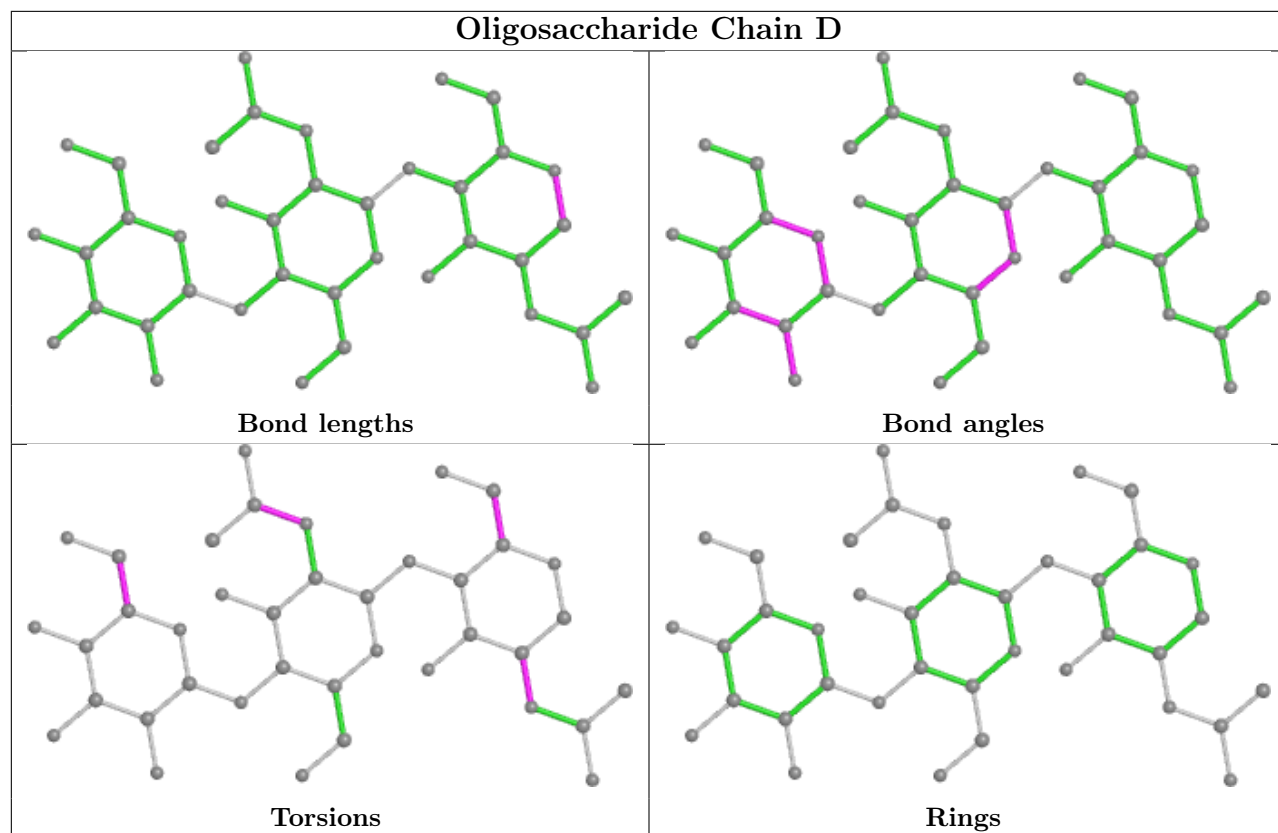
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	O5-C5-C6-O6
2	K	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6

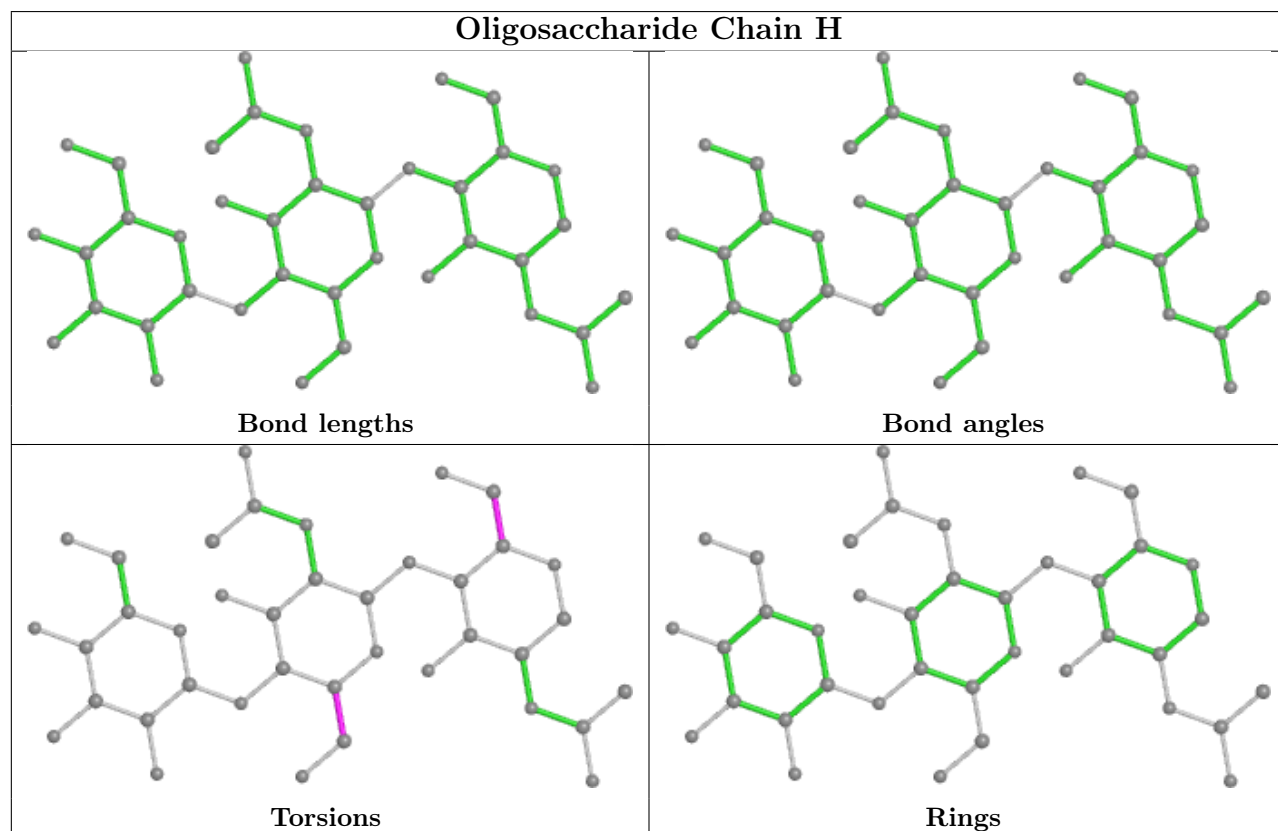
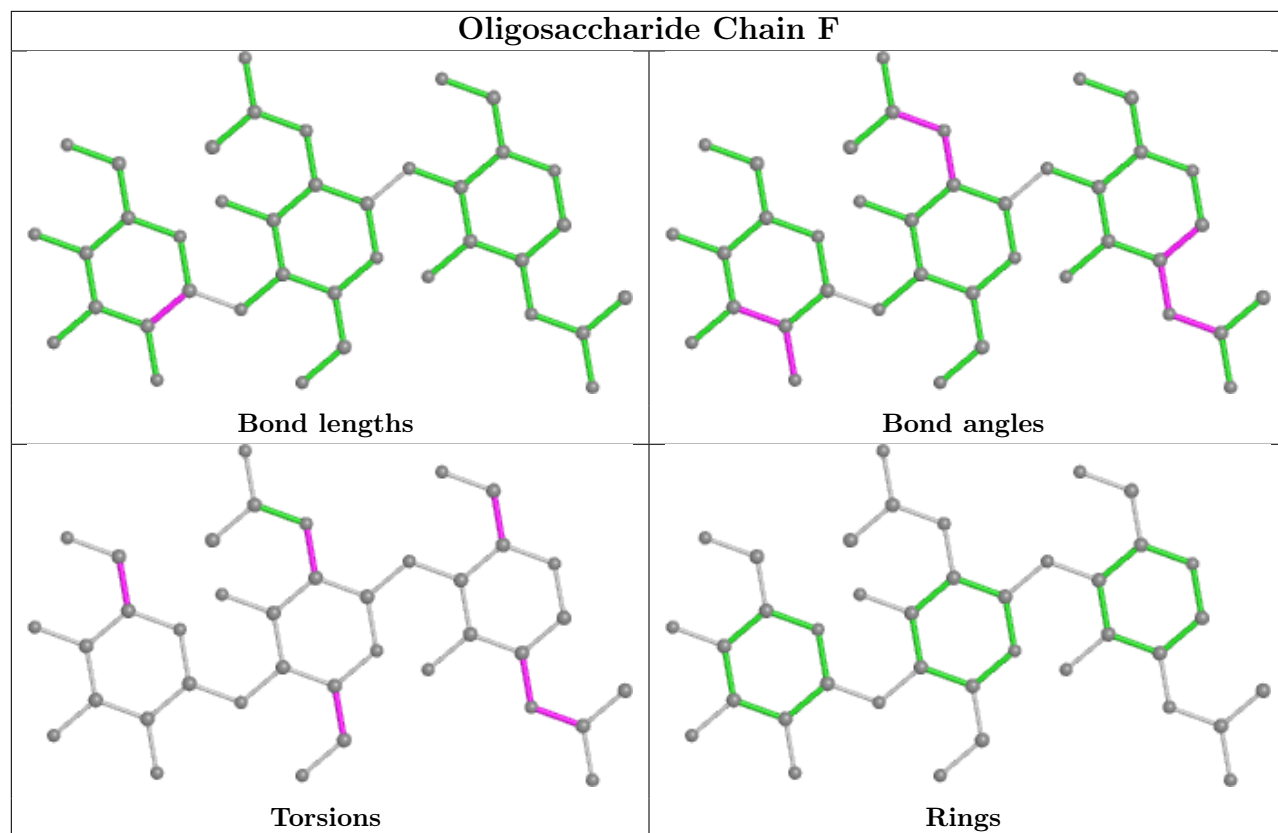
There are no ring outliers.

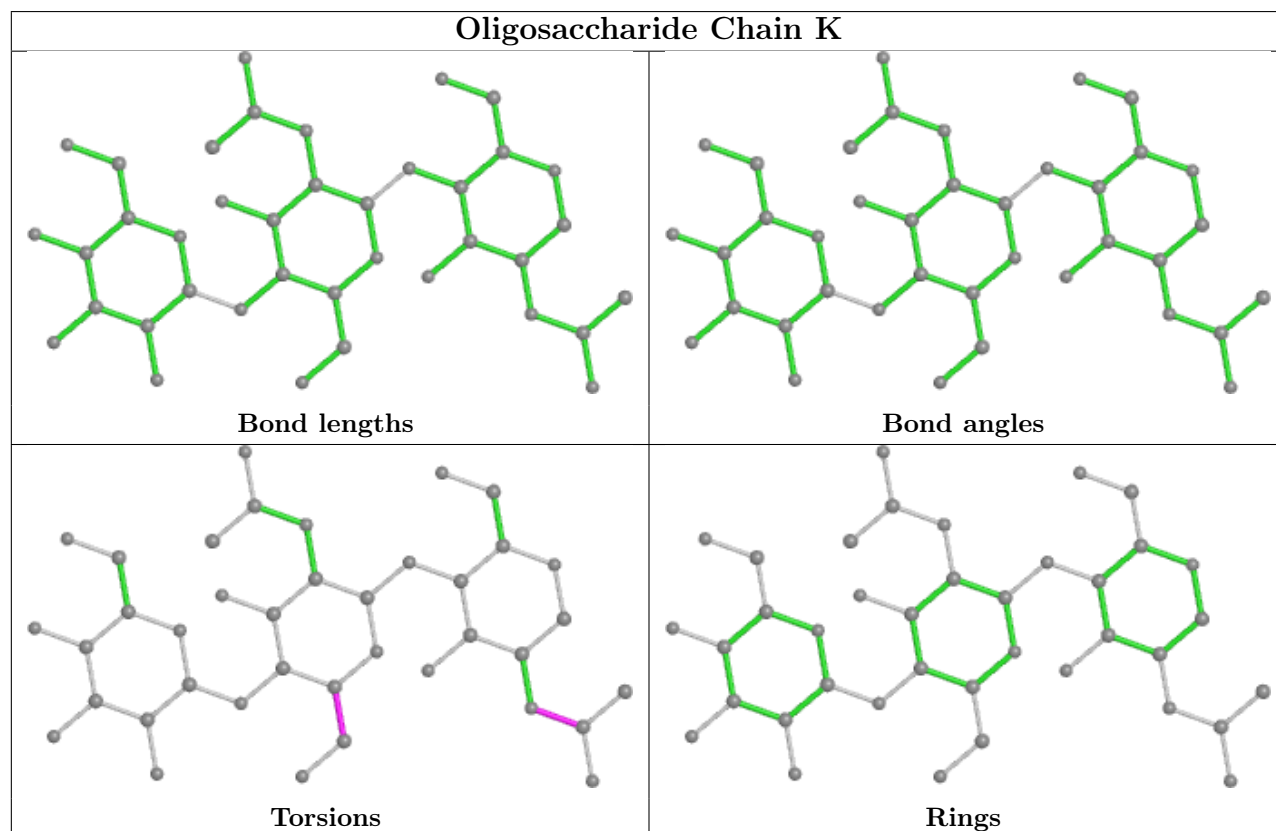
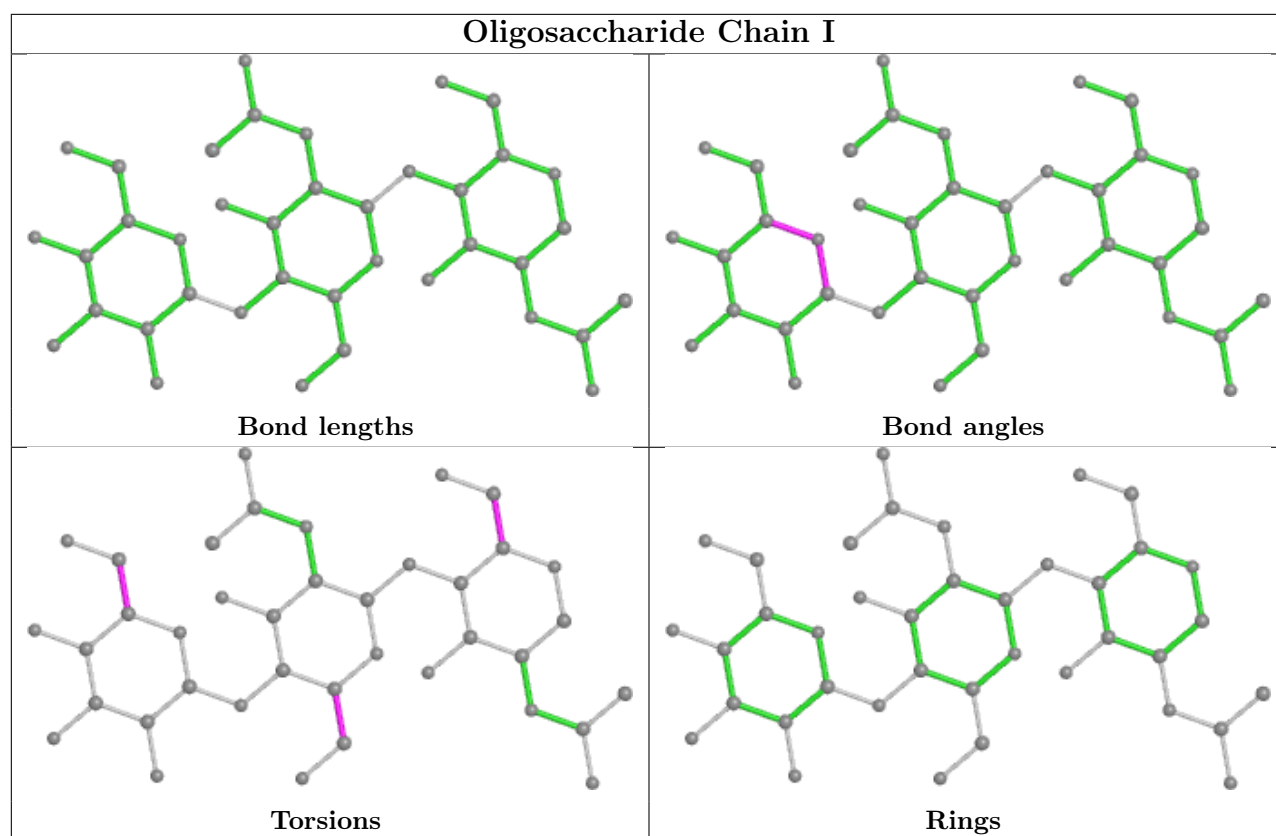
4 monomers are involved in 4 short contacts:

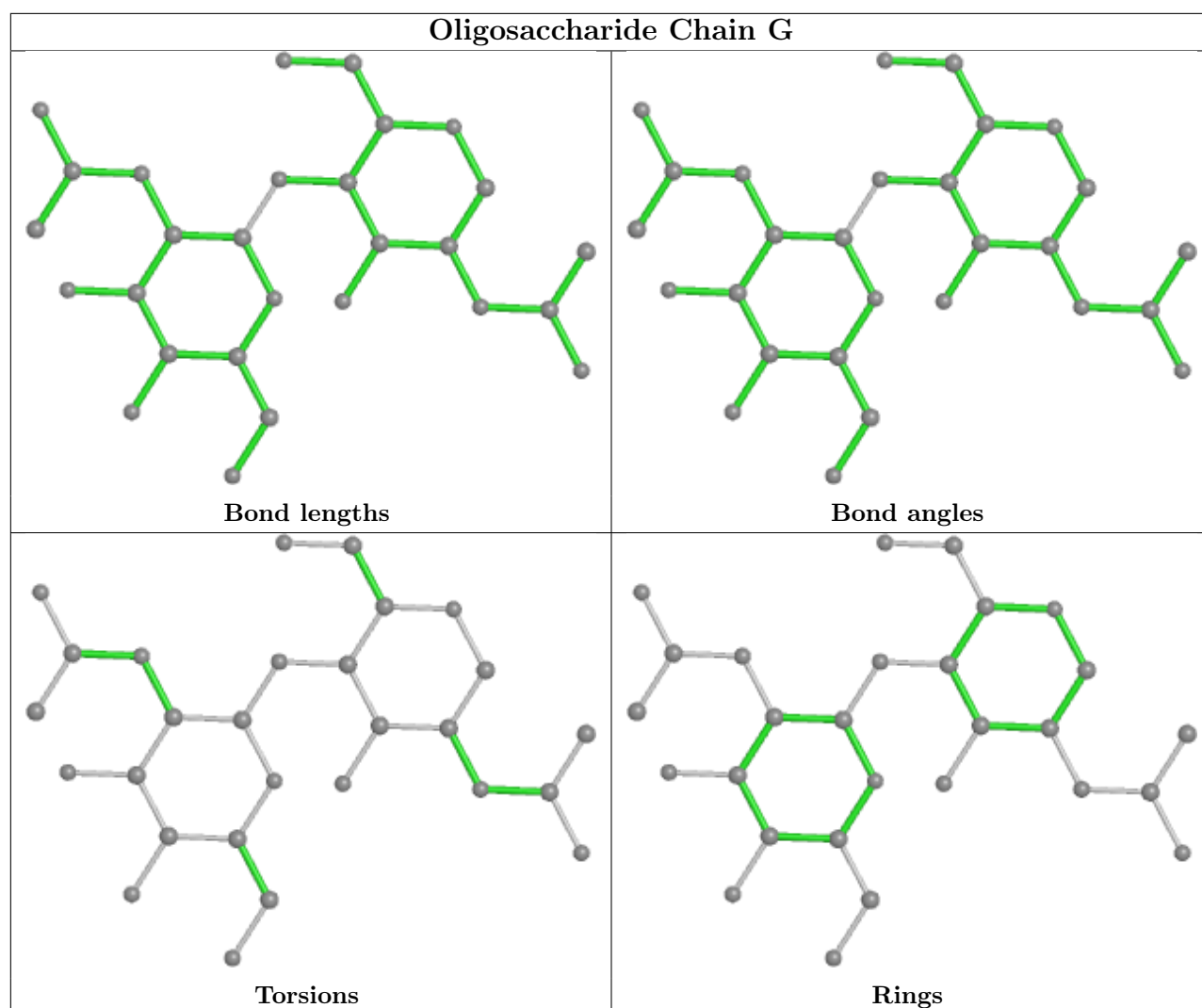
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	2	NAG	1	0
2	D	1	NAG	1	0
3	J	1	NAG	1	0
3	G	1	NAG	1	0

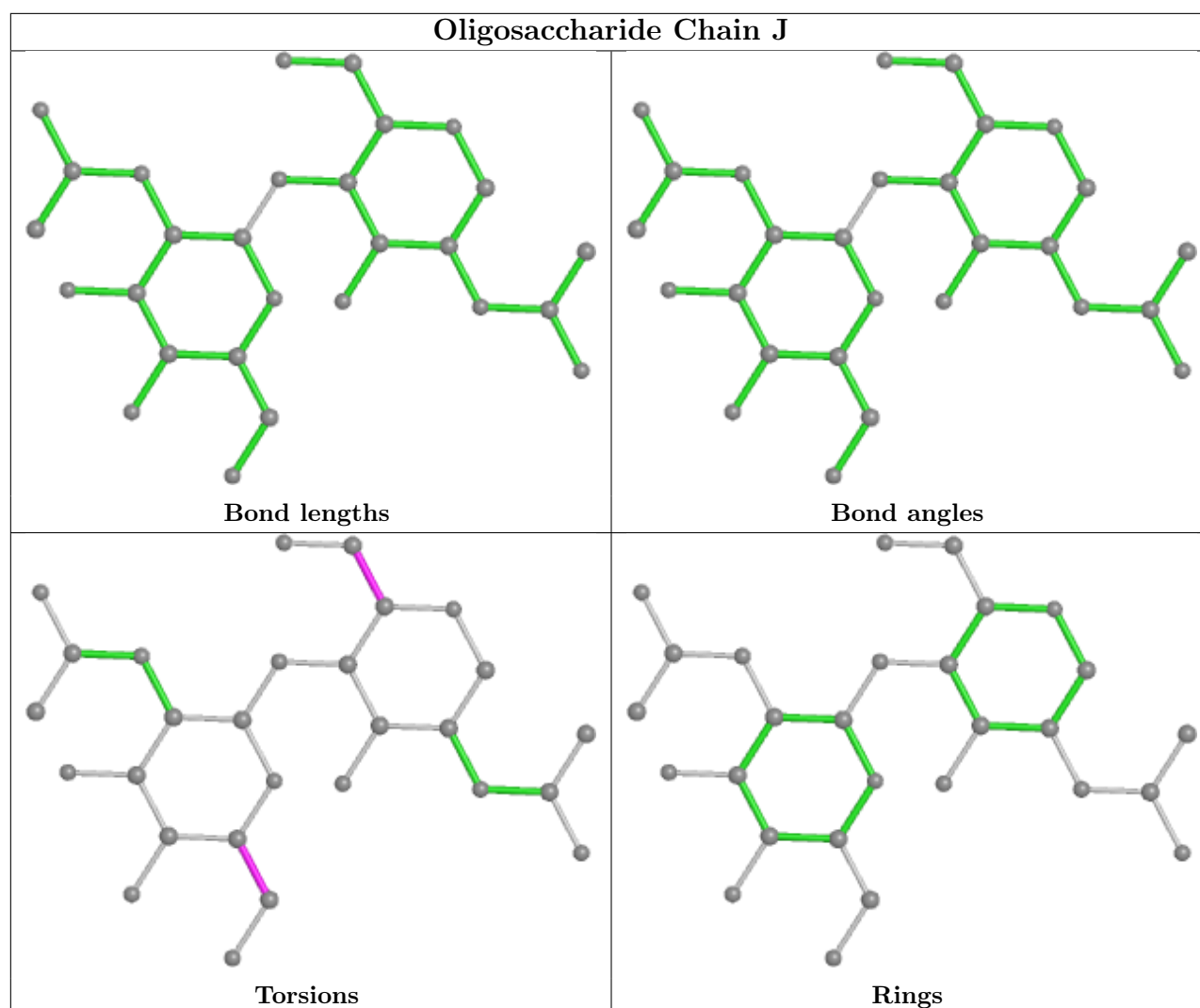
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
6	EIC	A	1411	-	19,19,19	0.56	0	19,19,19	0.58	0
4	NAG	A	1403	1	14,14,15	0.29	0	17,19,21	0.50	0
4	NAG	B	1405	1	14,14,15	0.24	0	17,19,21	0.42	0
4	NAG	C	1404	1	14,14,15	0.29	0	17,19,21	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1401	1	14,14,15	0.23	0	17,19,21	0.52	0
4	NAG	B	1403	1	14,14,15	0.33	0	17,19,21	0.35	0
6	EIC	B	1410	-	19,19,19	0.56	0	19,19,19	0.56	0
4	NAG	C	1403	1	14,14,15	0.31	0	17,19,21	0.45	0
4	NAG	A	1402	1	14,14,15	0.31	0	17,19,21	0.43	0
4	NAG	C	1401	1	14,14,15	0.24	0	17,19,21	0.47	0
6	EIC	A	1412	-	19,19,19	0.55	0	19,19,19	0.61	0
4	NAG	B	1406	1	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	B	1409	1	14,14,15	0.22	0	17,19,21	0.54	0
4	NAG	A	1409	1	14,14,15	0.28	0	17,19,21	0.50	0
4	NAG	C	1409	1	14,14,15	0.23	0	17,19,21	0.46	0
4	NAG	A	1406	1	14,14,15	0.16	0	17,19,21	0.44	0
5	FOL	C	1408	-	34,34,34	1.27	2 (5%)	44,47,47	2.37	12 (27%)
4	NAG	A	1405	1	14,14,15	0.22	0	17,19,21	0.48	0
4	NAG	C	1407	1	14,14,15	0.28	0	17,19,21	0.47	0
4	NAG	A	1408	1	14,14,15	0.21	0	17,19,21	0.48	0
4	NAG	B	1401	1	14,14,15	0.31	0	17,19,21	0.53	0
4	NAG	B	1402	1	14,14,15	0.29	0	17,19,21	0.37	0
4	NAG	A	1404	1	14,14,15	0.32	0	17,19,21	0.52	0
4	NAG	C	1405	1	14,14,15	0.21	0	17,19,21	0.53	0
4	NAG	C	1406	1	14,14,15	0.22	0	17,19,21	0.51	0
4	NAG	C	1402	1	14,14,15	0.70	1 (7%)	17,19,21	1.99	2 (11%)
4	NAG	A	1407	-	14,14,15	0.19	0	17,19,21	0.48	0
4	NAG	B	1408	1	14,14,15	0.26	0	17,19,21	0.39	0
5	FOL	A	1410	-	34,34,34	1.19	2 (5%)	44,47,47	1.98	8 (18%)
5	FOL	B	1407	-	34,34,34	1.23	2 (5%)	44,47,47	2.40	12 (27%)
4	NAG	B	1404	1	14,14,15	0.33	0	17,19,21	0.51	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
6	EIC	A	1411	-	-	5/17/17/17	-
4	NAG	A	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	2/6/23/26	0/1/1/1
6	EIC	B	1410	-	-	5/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	1403	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1401	1	-	2/6/23/26	0/1/1/1
6	EIC	A	1412	-	-	7/17/17/17	-
4	NAG	B	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1409	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	4/6/23/26	0/1/1/1
5	FOL	C	1408	-	-	17/22/22/22	0/3/3/3
4	NAG	A	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1407	-	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	3/6/23/26	0/1/1/1
5	FOL	A	1410	-	-	13/22/22/22	0/3/3/3
5	FOL	B	1407	-	-	17/22/22/22	0/3/3/3
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	1408	FOL	C4A-C4	4.08	1.48	1.41
5	B	1407	FOL	C4A-C4	3.87	1.48	1.41
5	C	1408	FOL	C4A-C8A	3.77	1.47	1.40
5	B	1407	FOL	C4A-C8A	3.72	1.47	1.40
5	A	1410	FOL	C4A-C8A	3.60	1.47	1.40

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1407	FOL	CB-CA-N	6.98	124.99	110.88
5	C	1408	FOL	CB-CA-N	6.92	124.87	110.88
4	C	1402	NAG	C2-N2-C7	6.90	132.72	122.90
5	A	1410	FOL	N8-C8A-N1	6.12	122.81	115.82
5	A	1410	FOL	C2-N1-C8A	5.51	121.65	115.36

There are no chirality outliers.

5 of 119 torsion outliers are listed below:

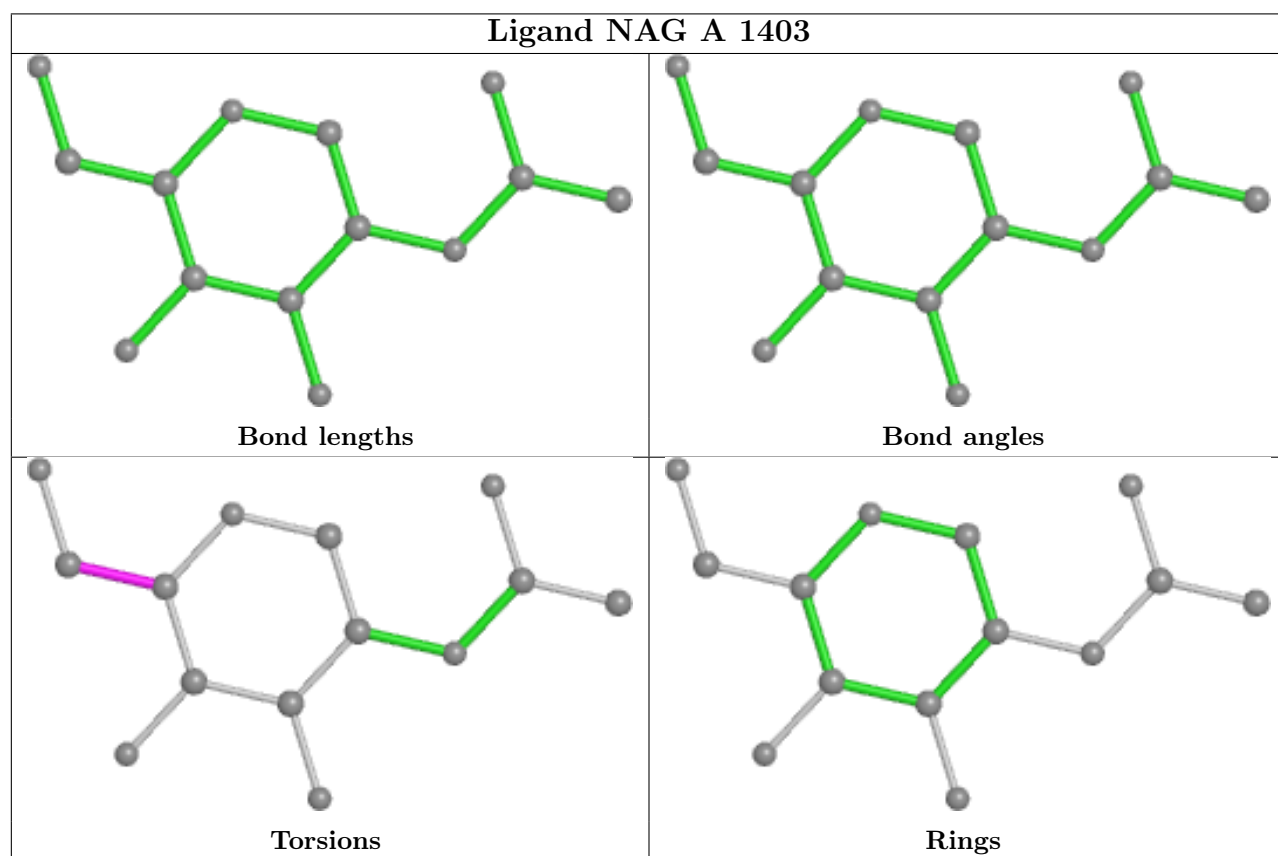
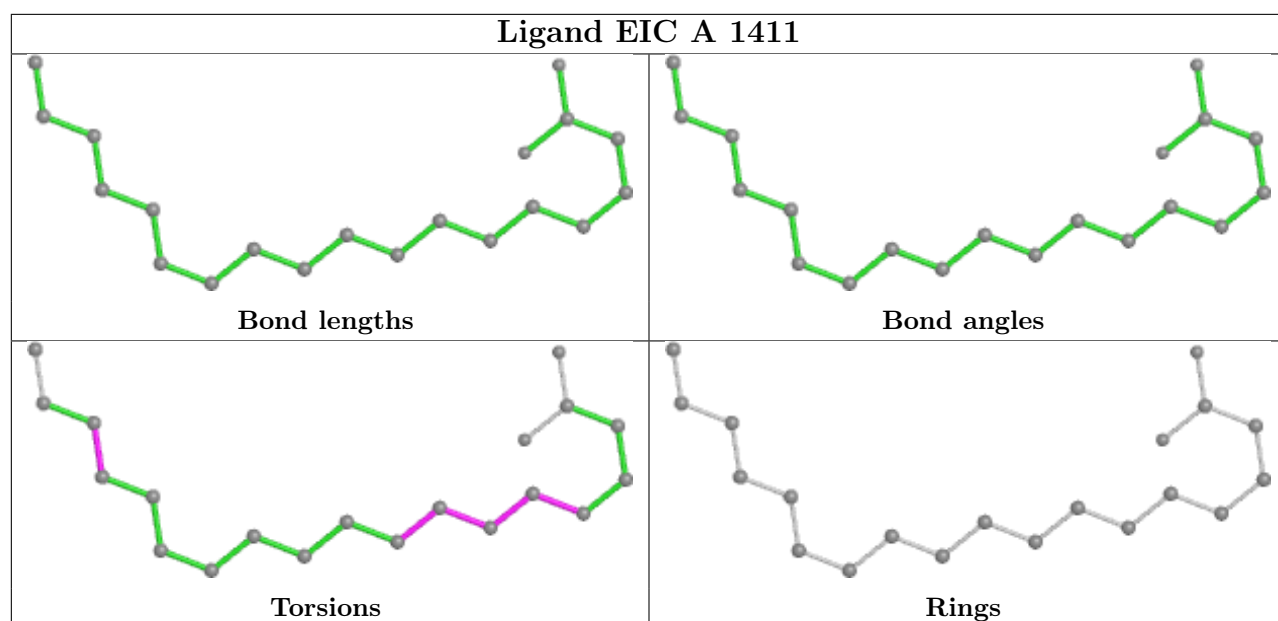
Mol	Chain	Res	Type	Atoms
5	A	1410	FOL	C6-C9-N10-C14
5	A	1410	FOL	O-C-N-CA
5	B	1407	FOL	N-CA-CB-CG
5	C	1408	FOL	C6-C9-N10-C14
6	A	1412	EIC	C10-C11-C12-C13

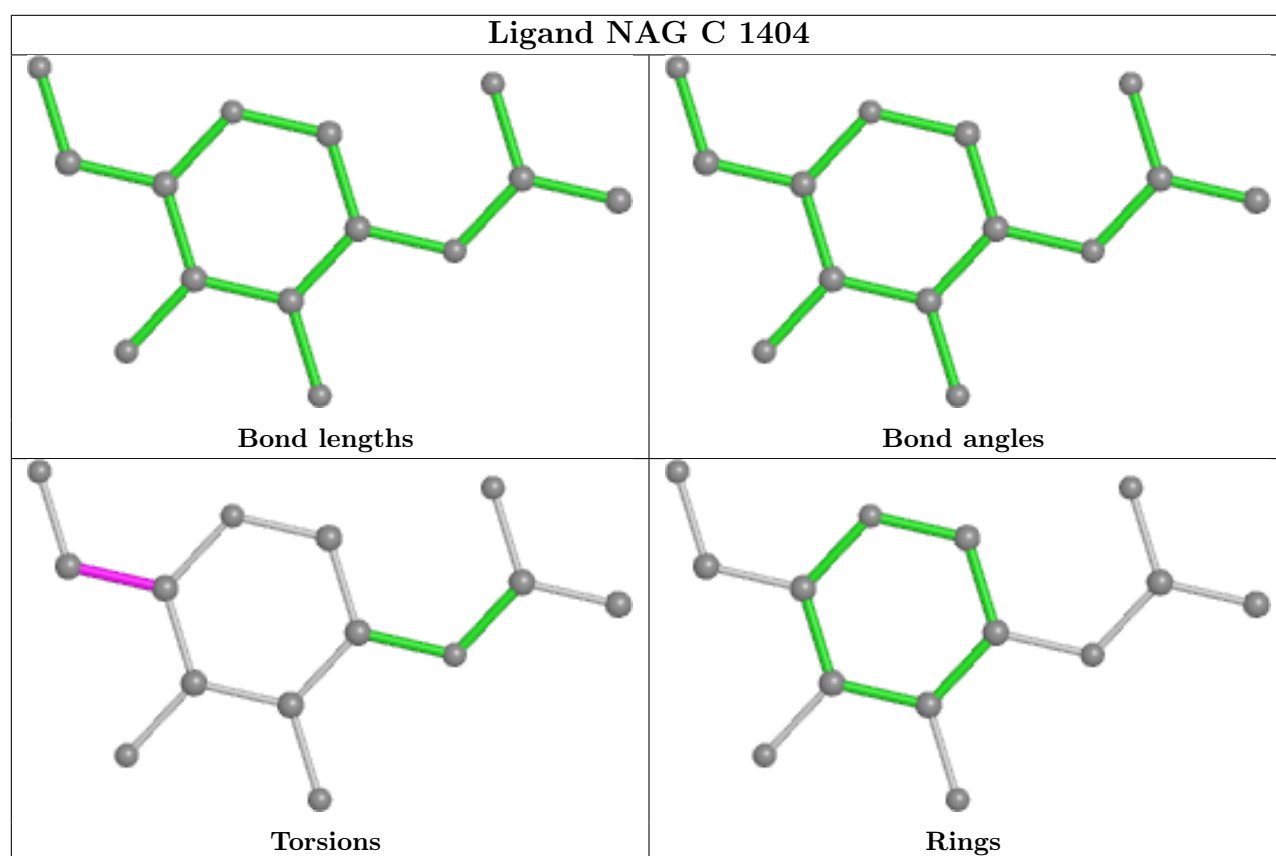
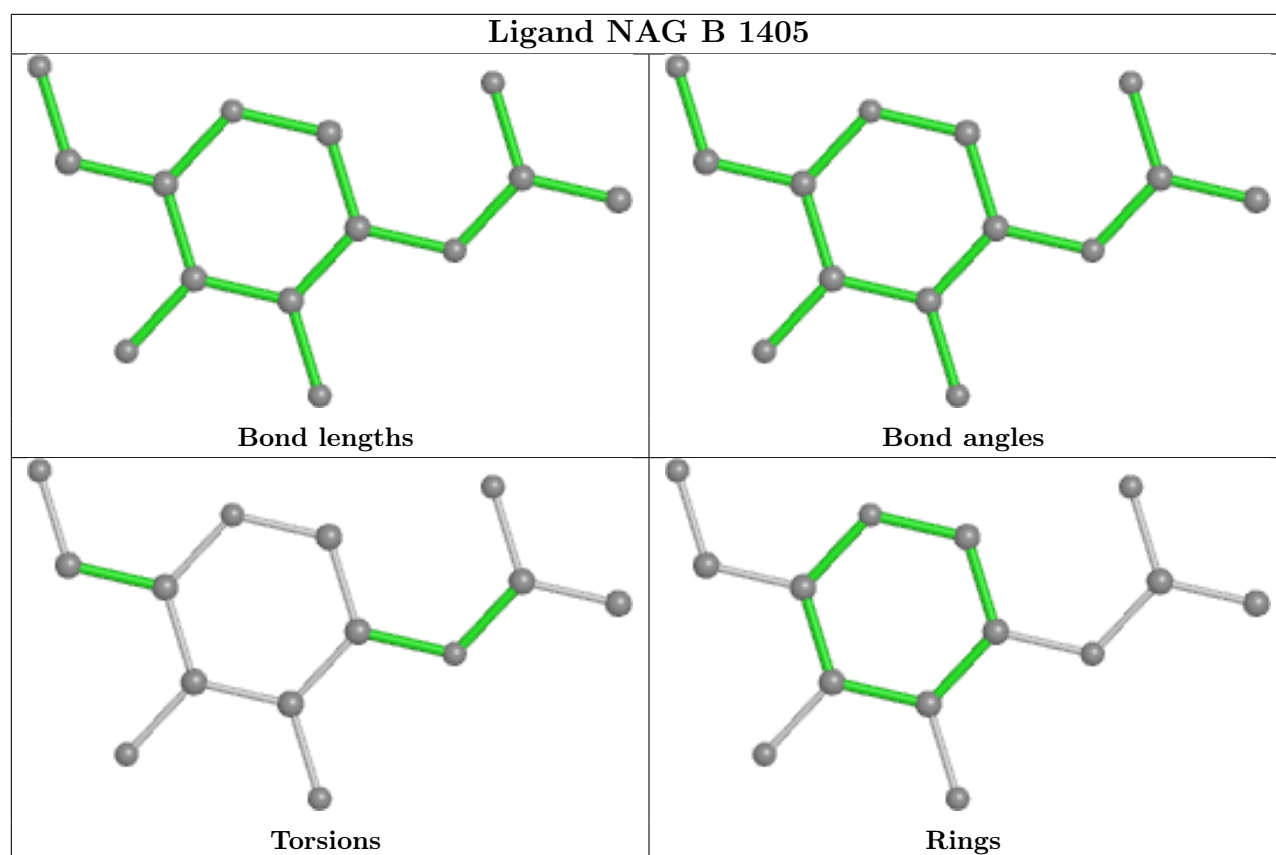
There are no ring outliers.

7 monomers are involved in 12 short contacts:

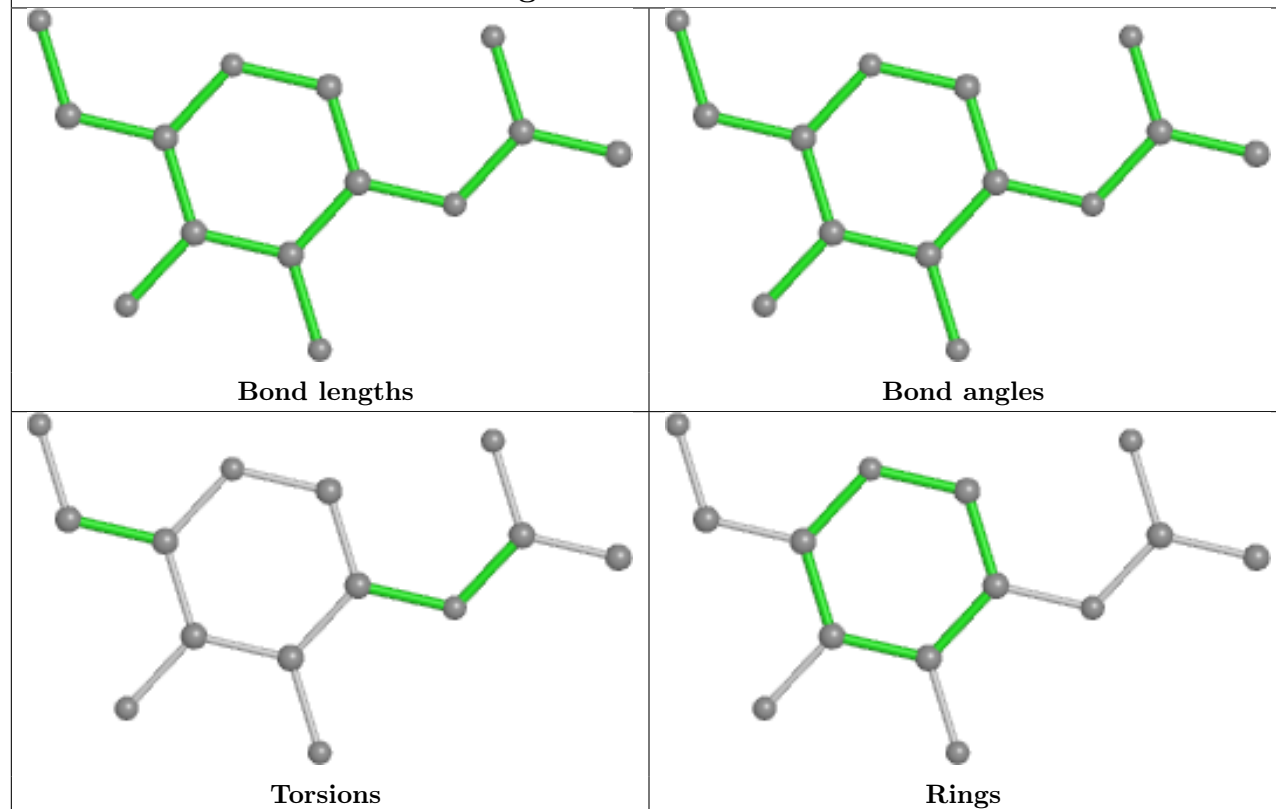
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1411	EIC	3	0
4	B	1403	NAG	1	0
6	A	1412	EIC	4	0
5	C	1408	FOL	1	0
4	C	1407	NAG	1	0
5	A	1410	FOL	1	0
5	B	1407	FOL	1	0

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.

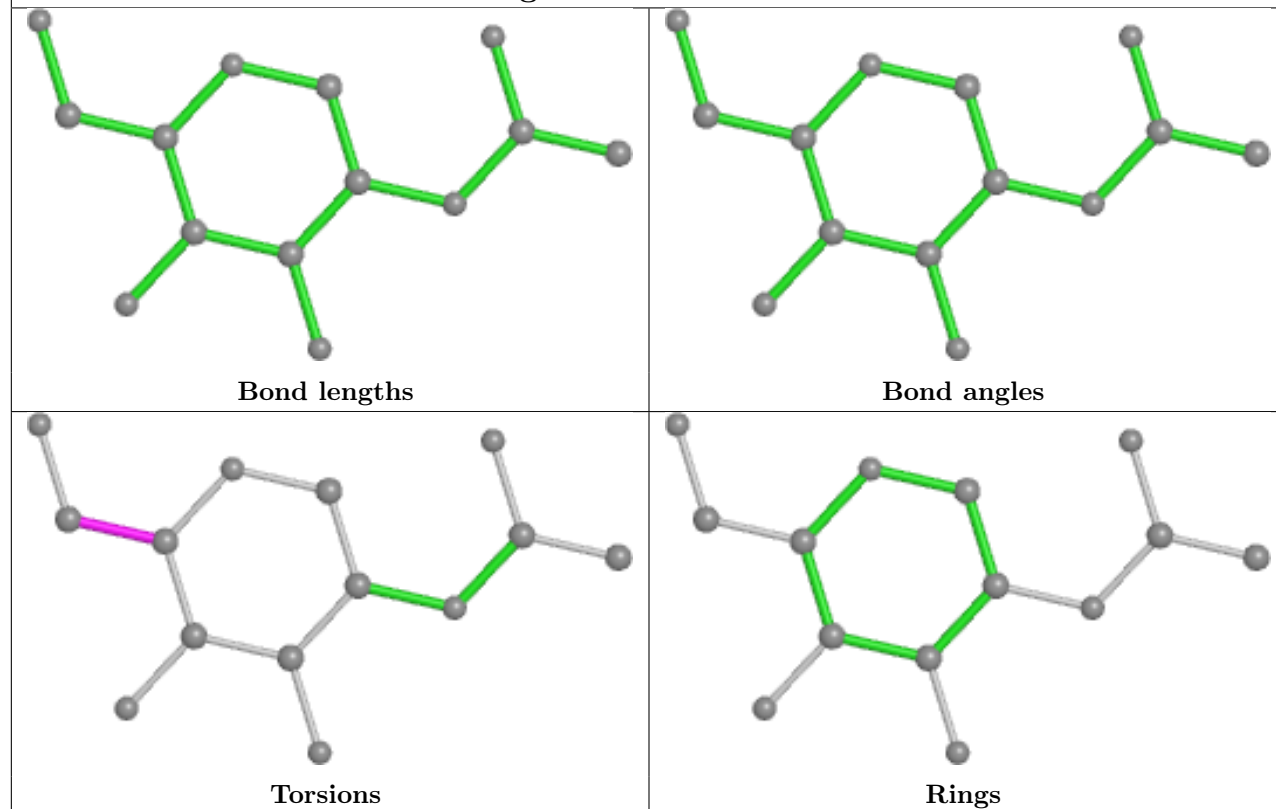


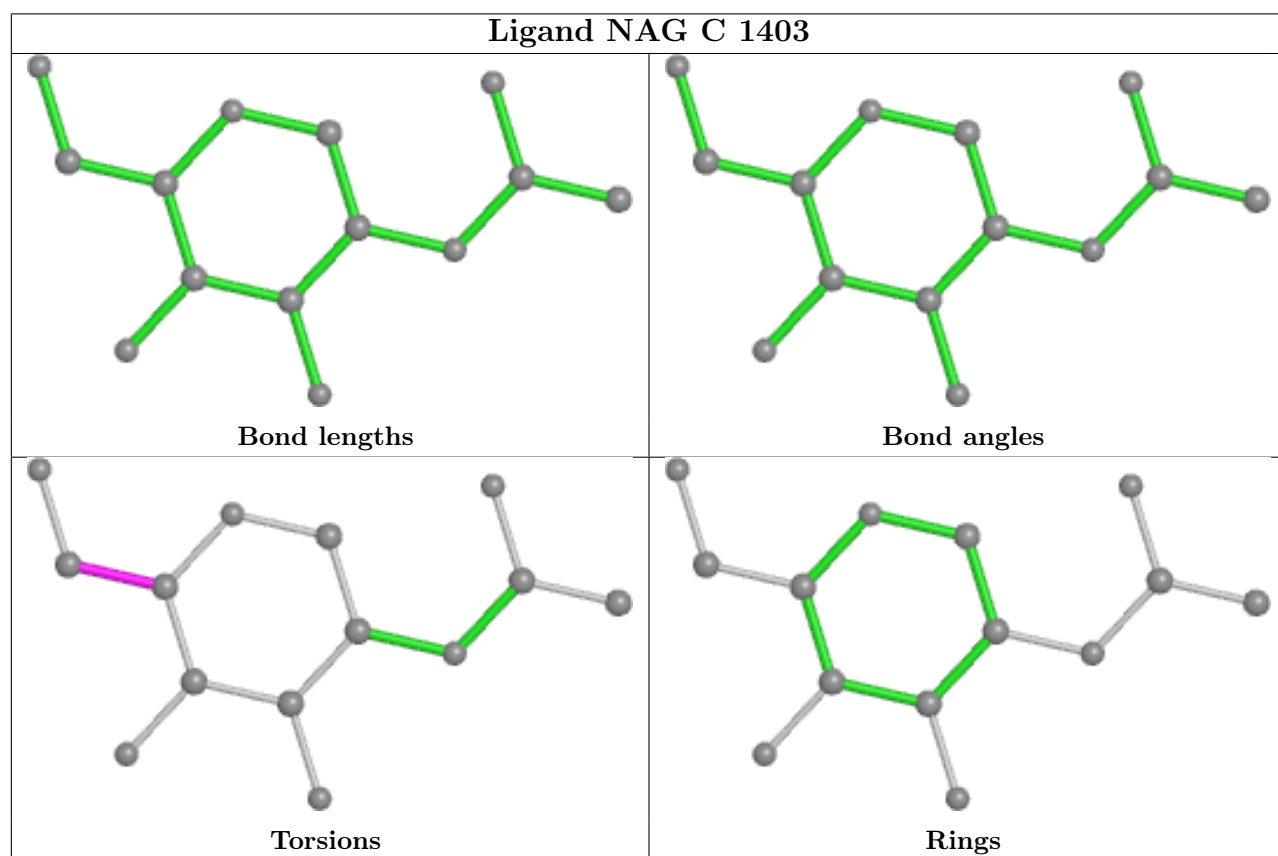
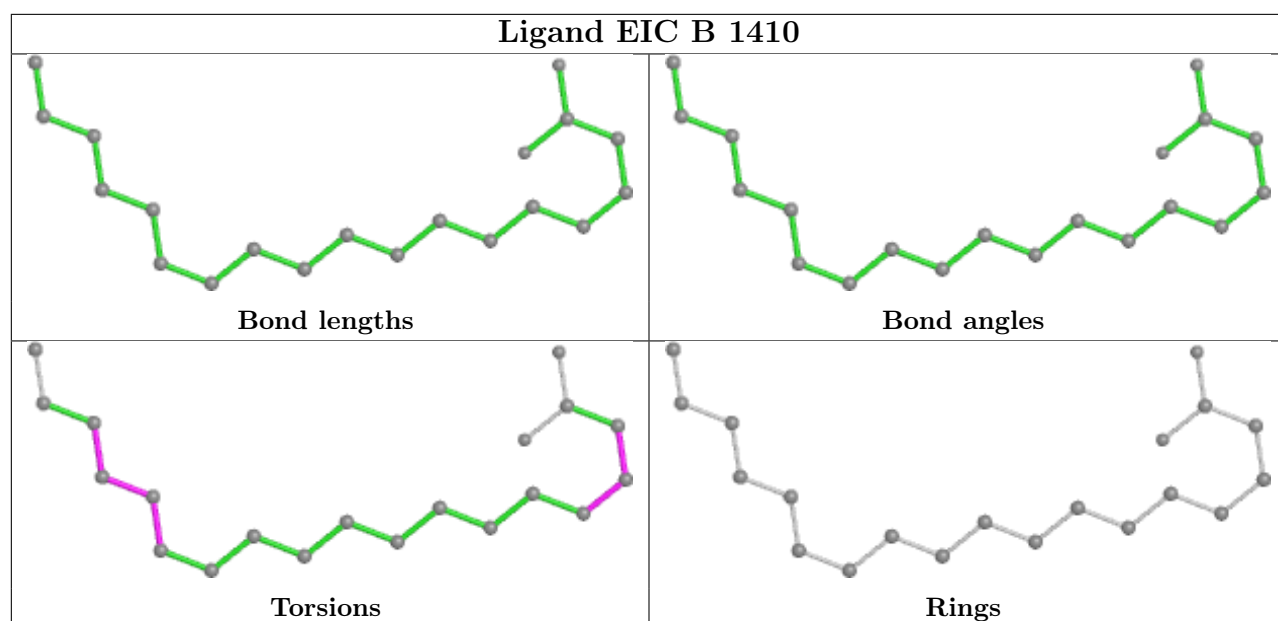


Ligand NAG A 1401

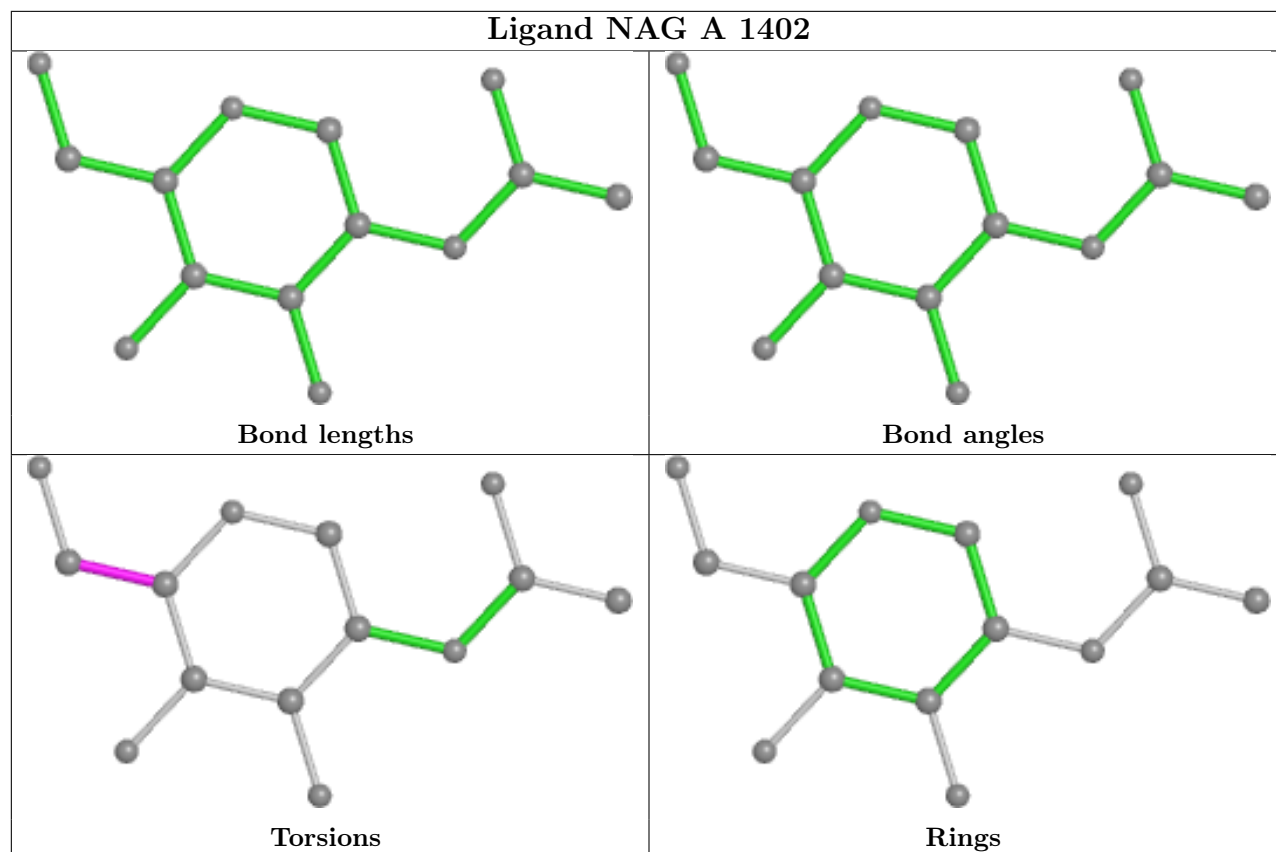


Ligand NAG B 1403

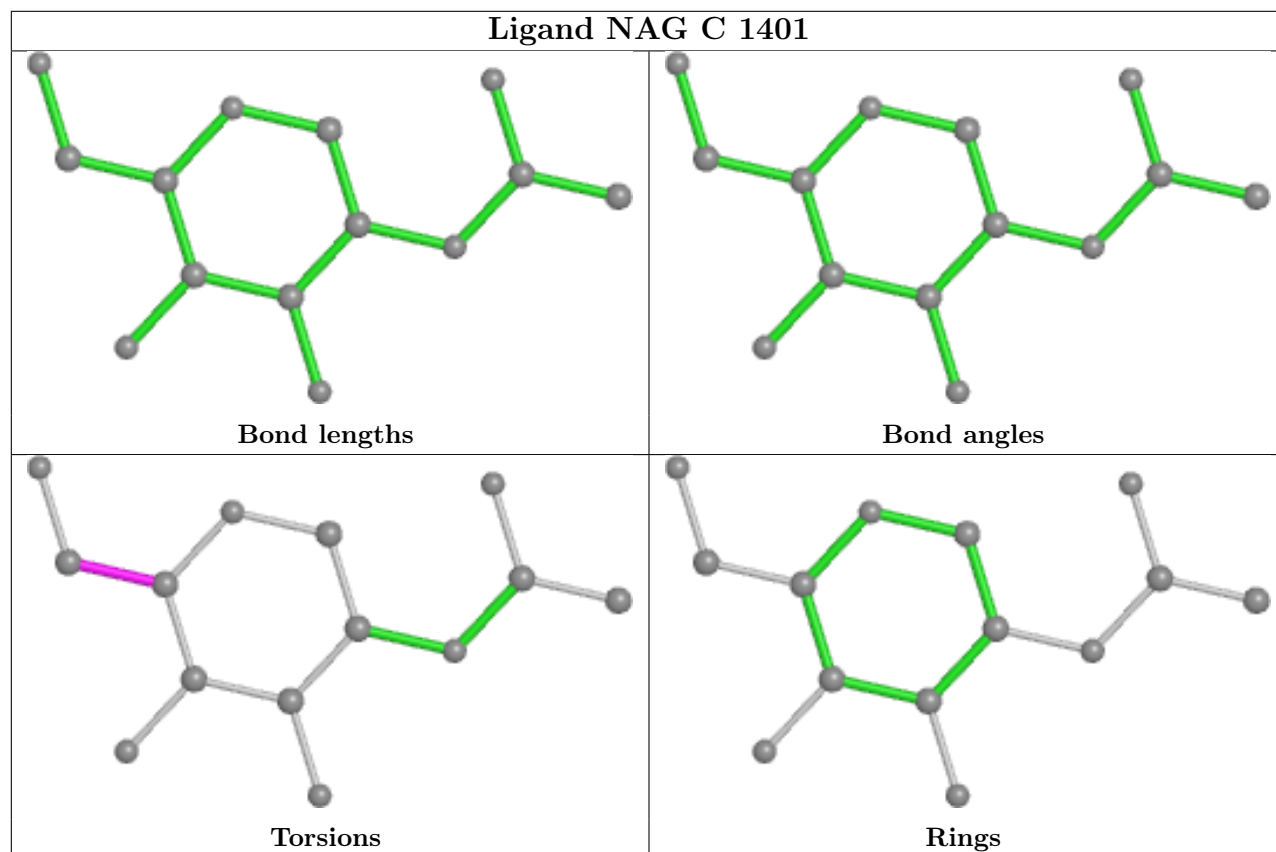


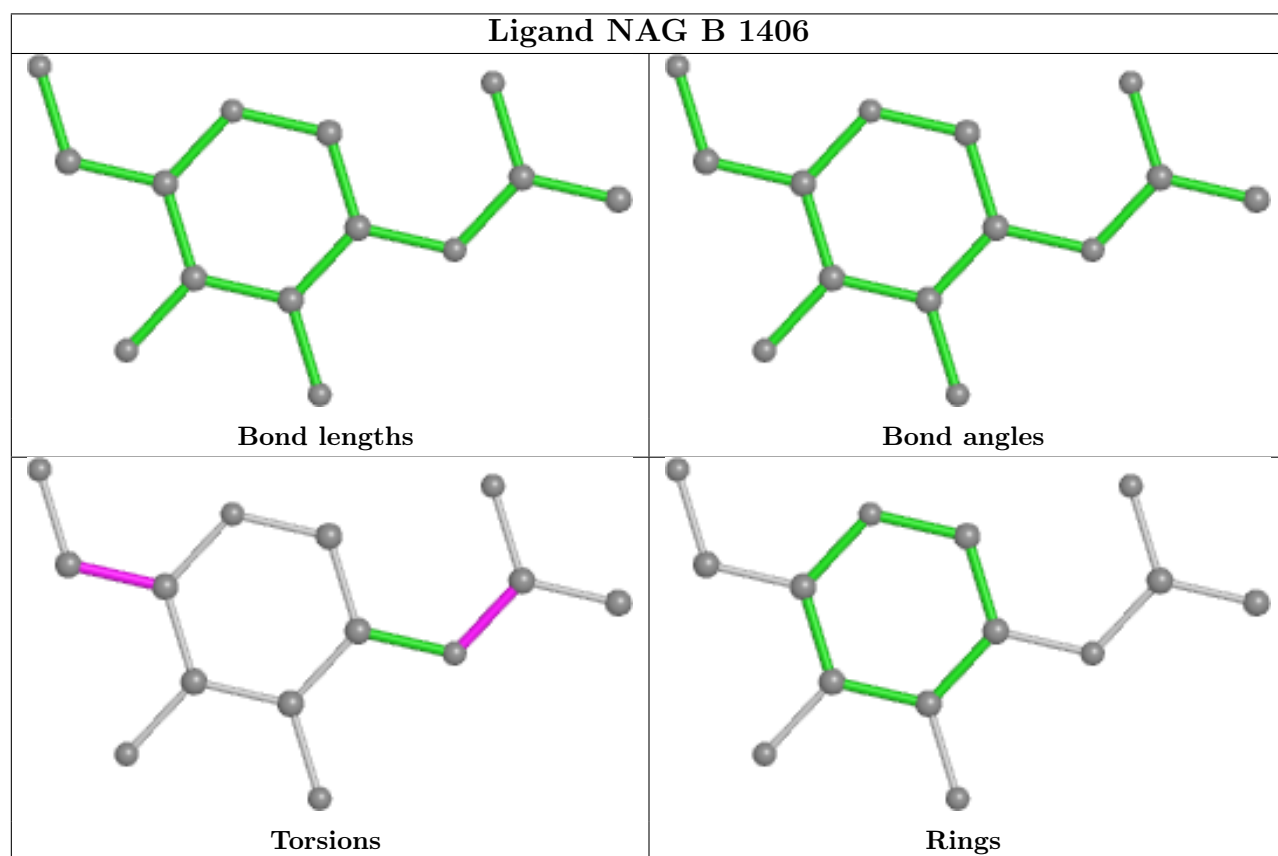
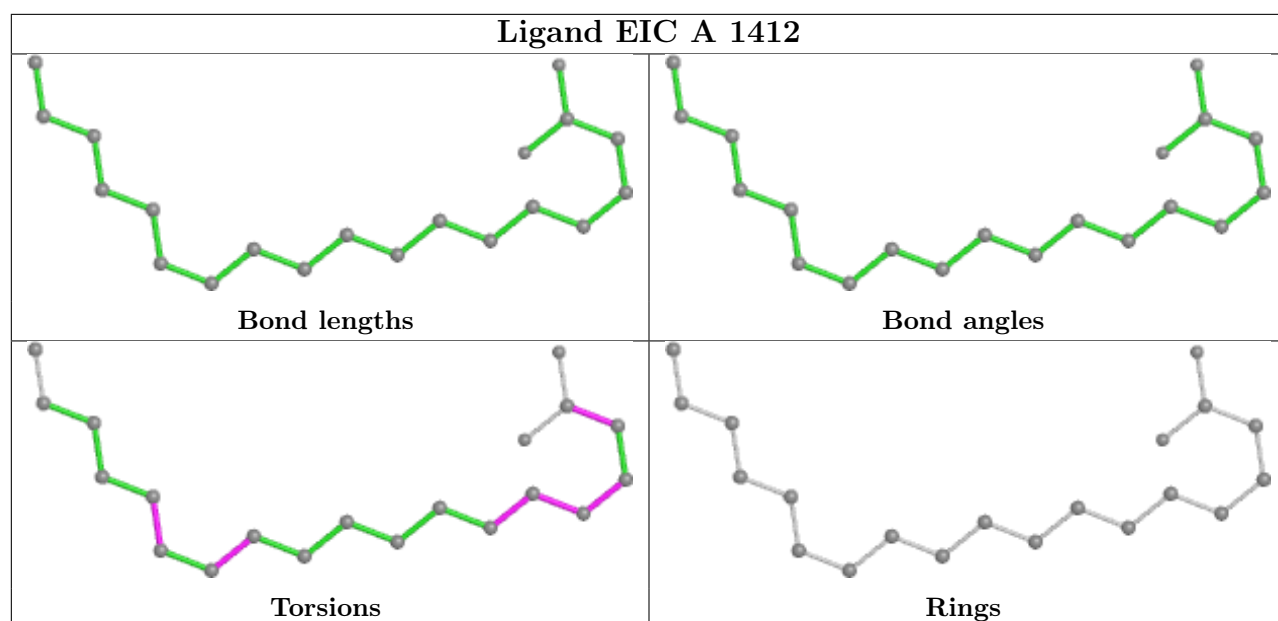


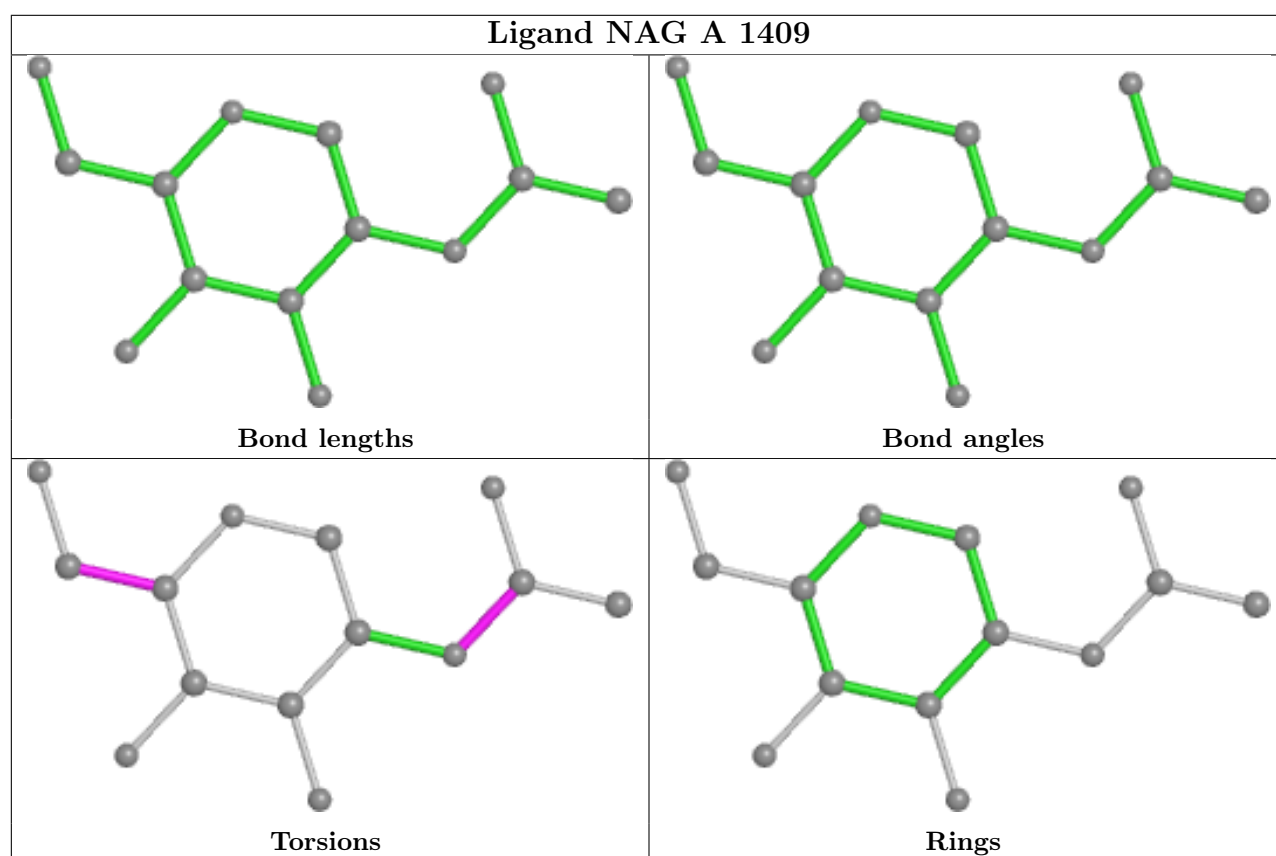
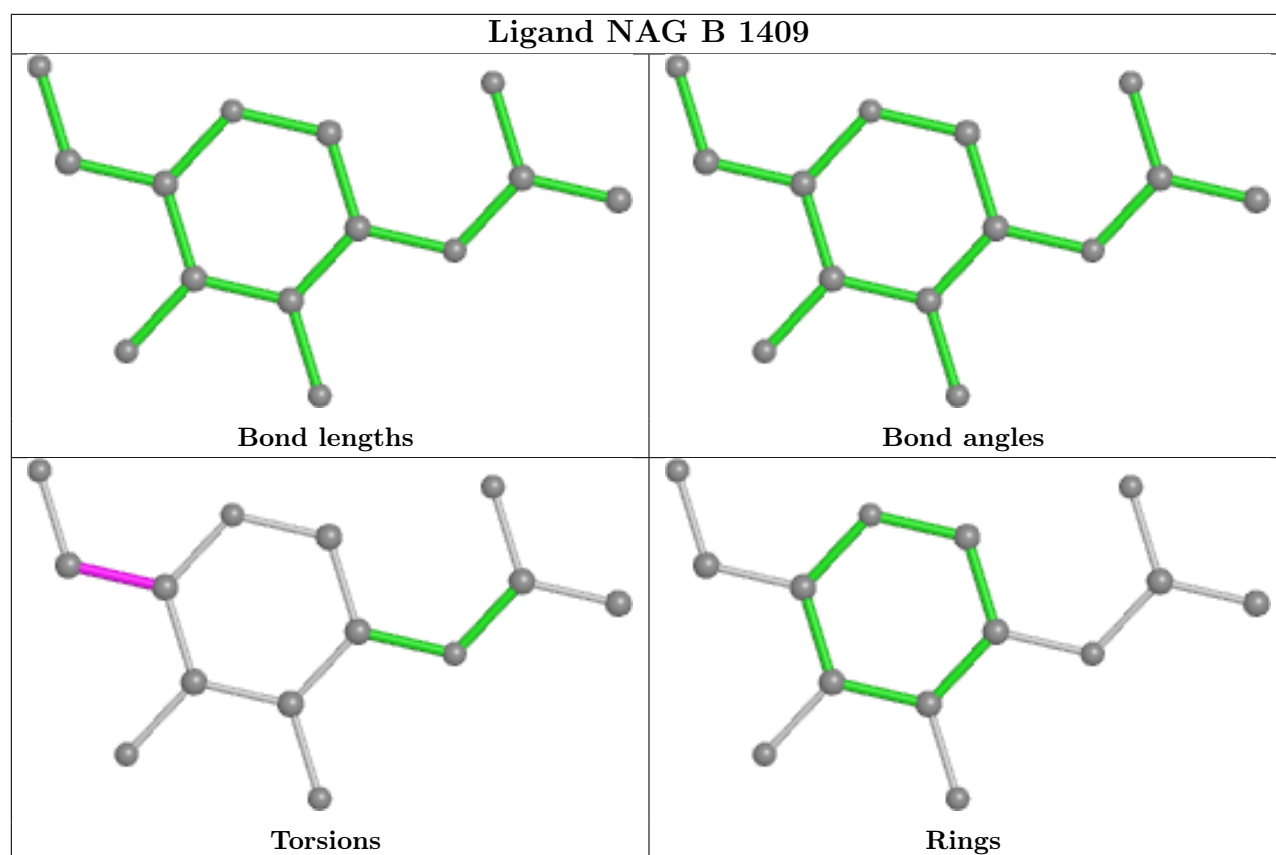
Ligand NAG A 1402



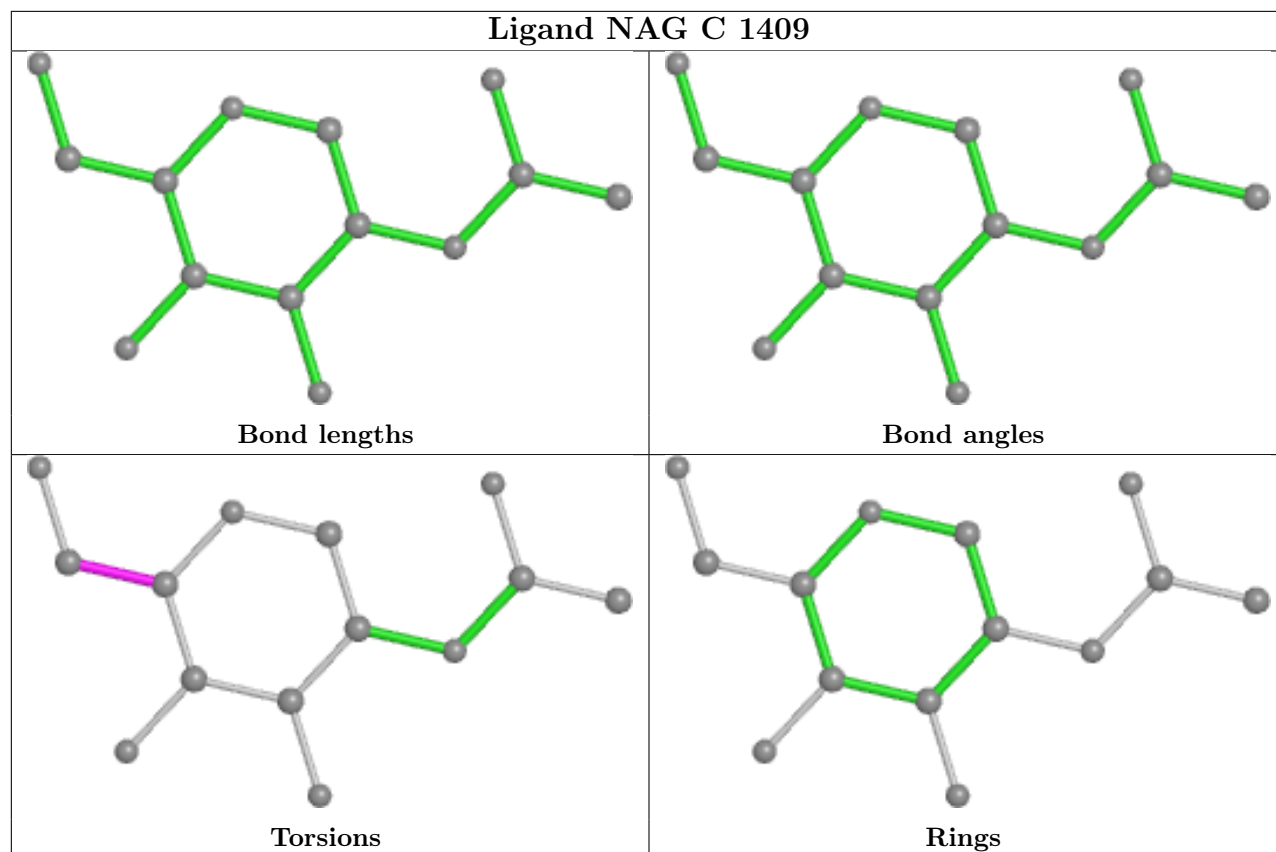
Ligand NAG C 1401



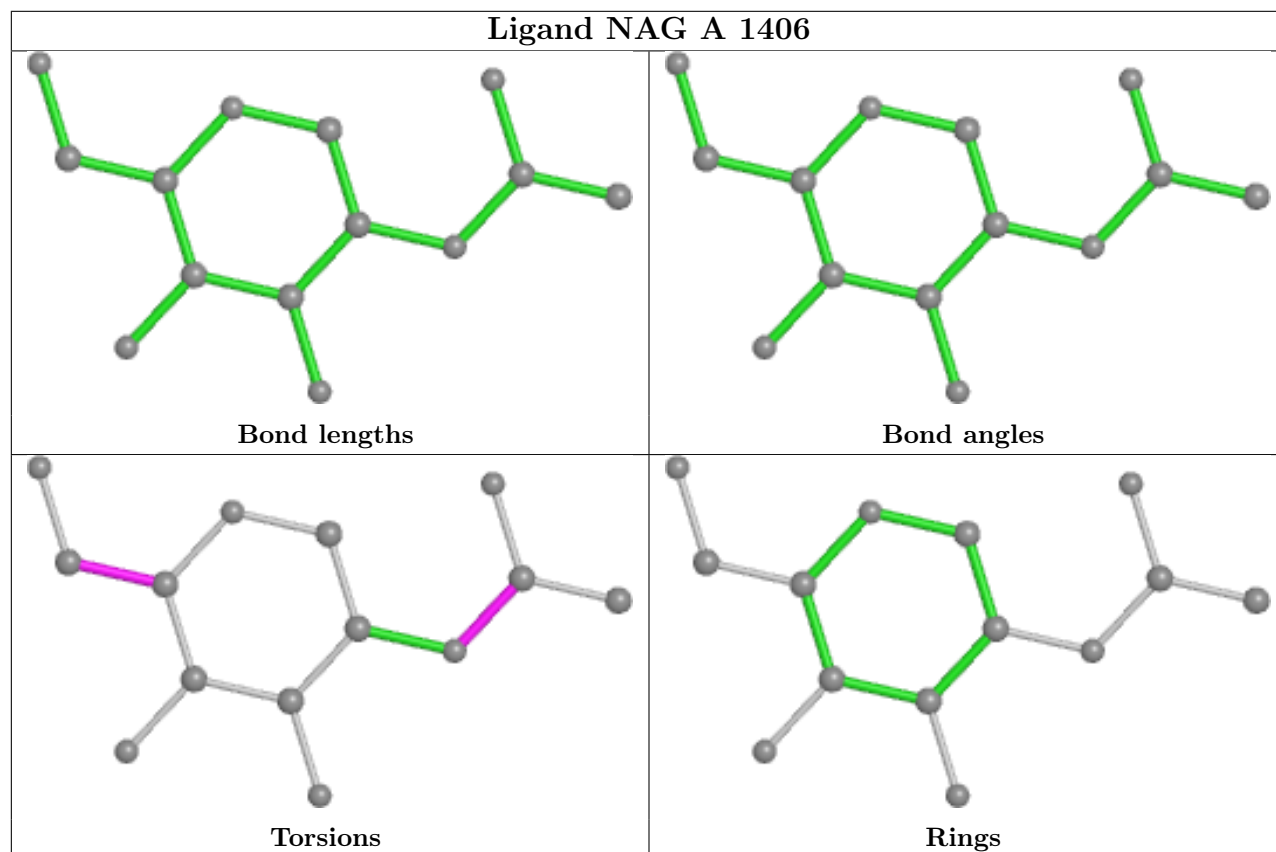




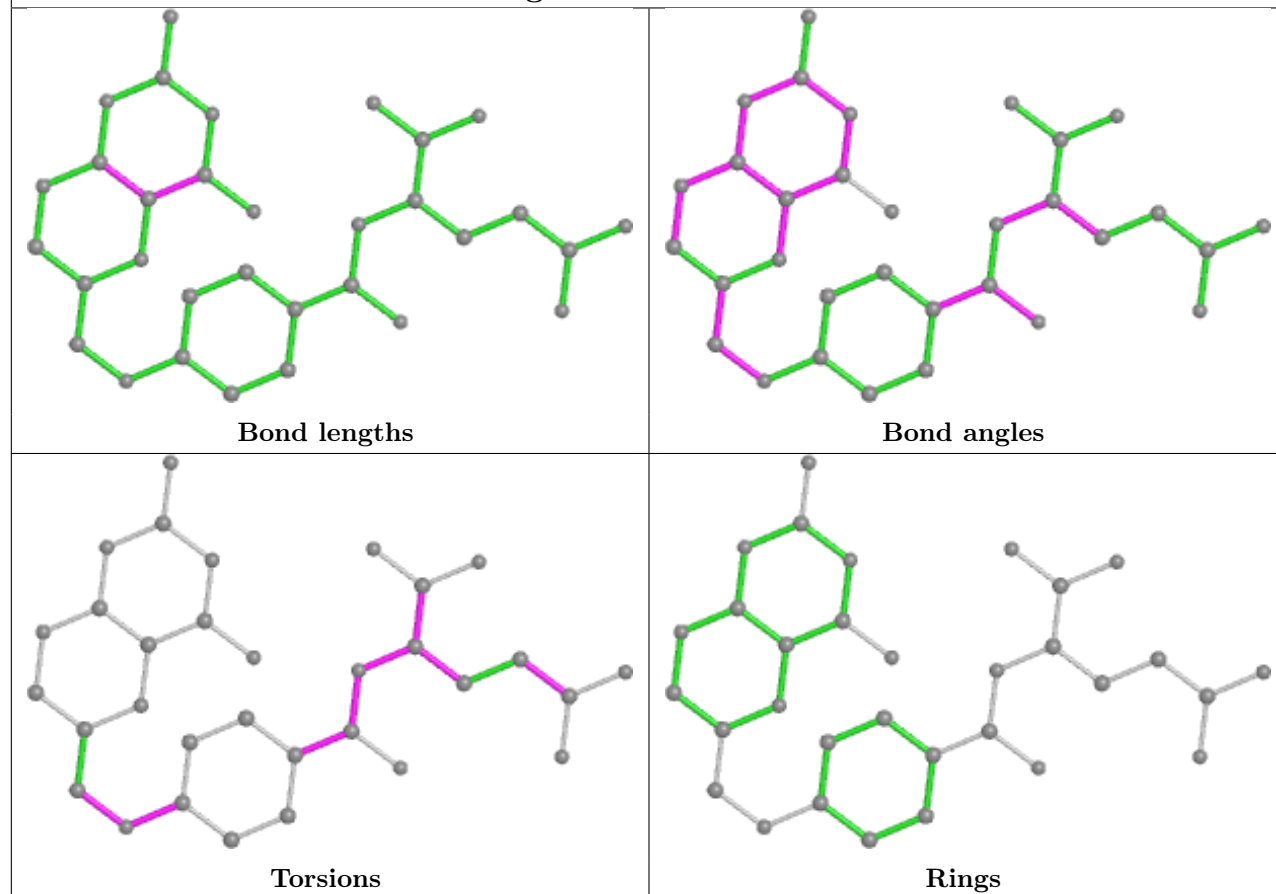
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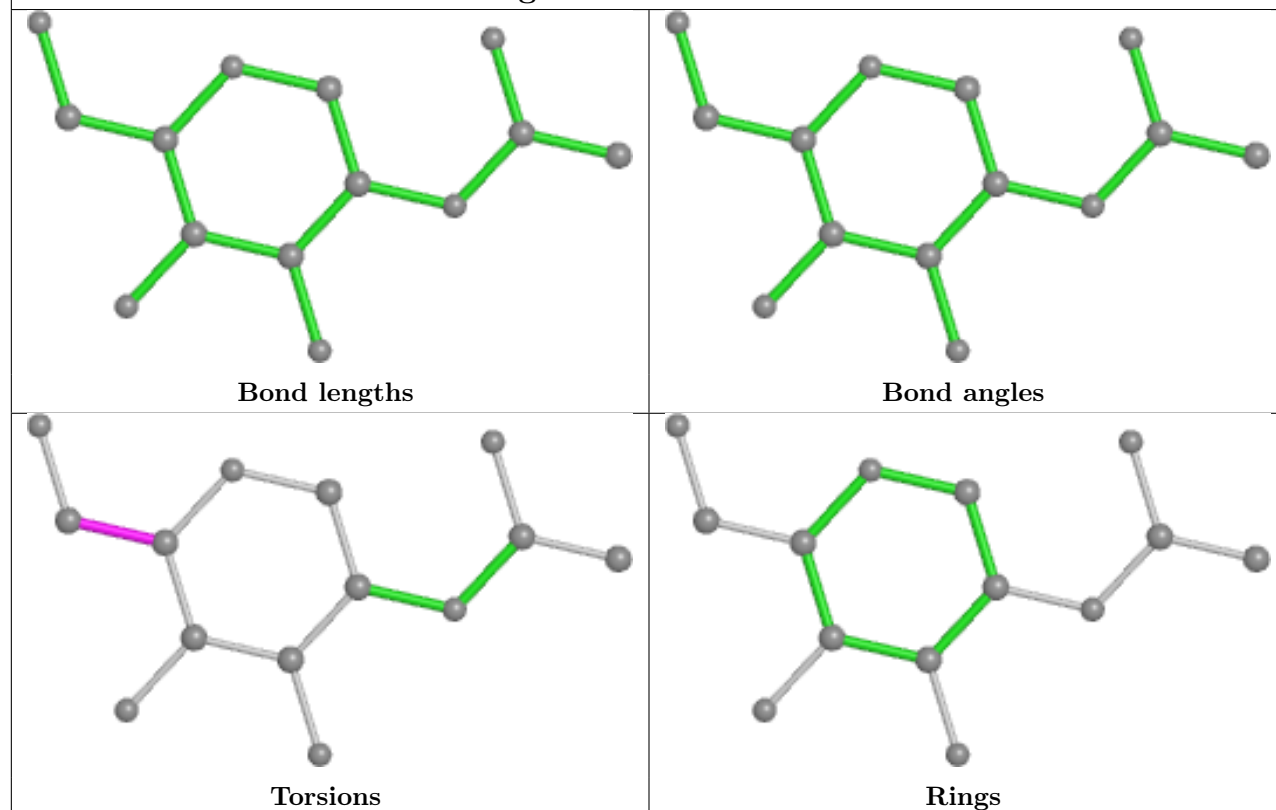
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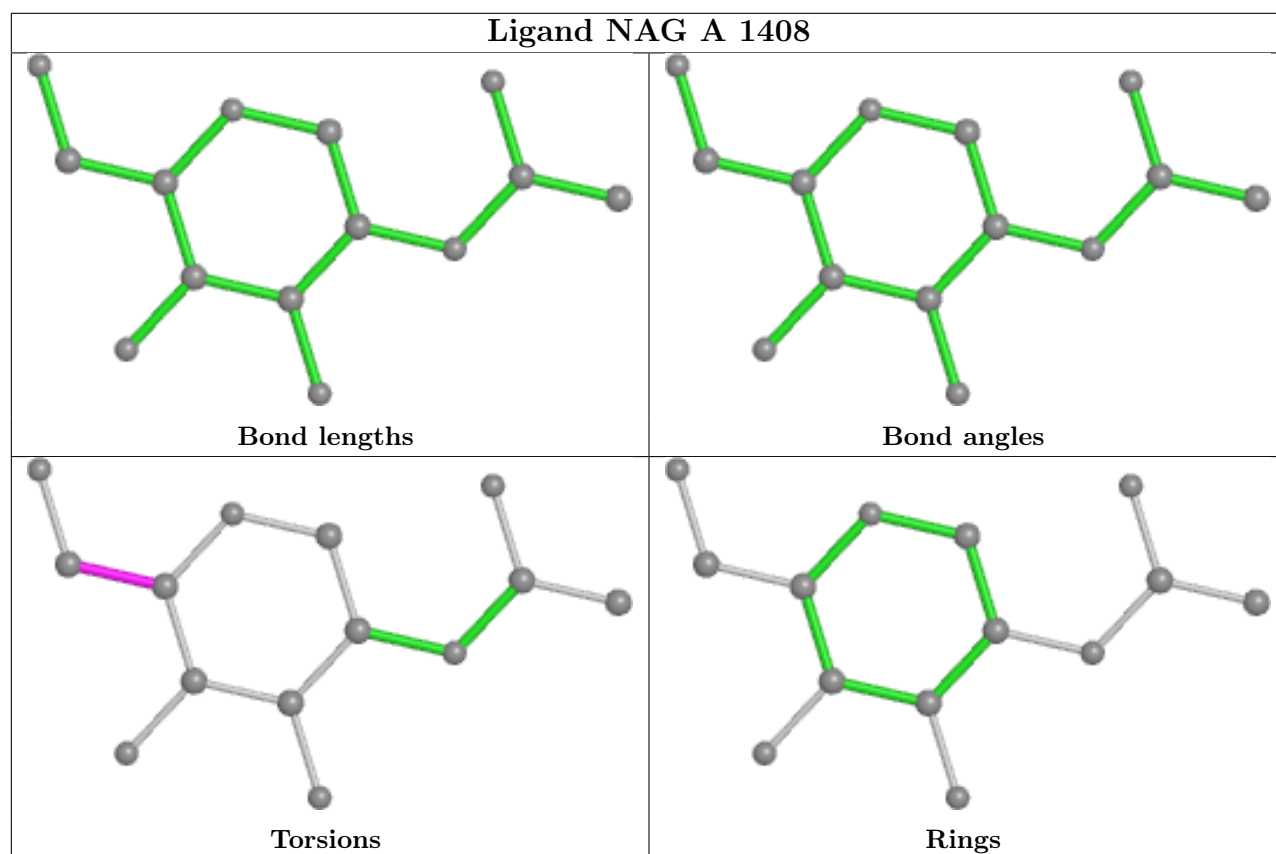
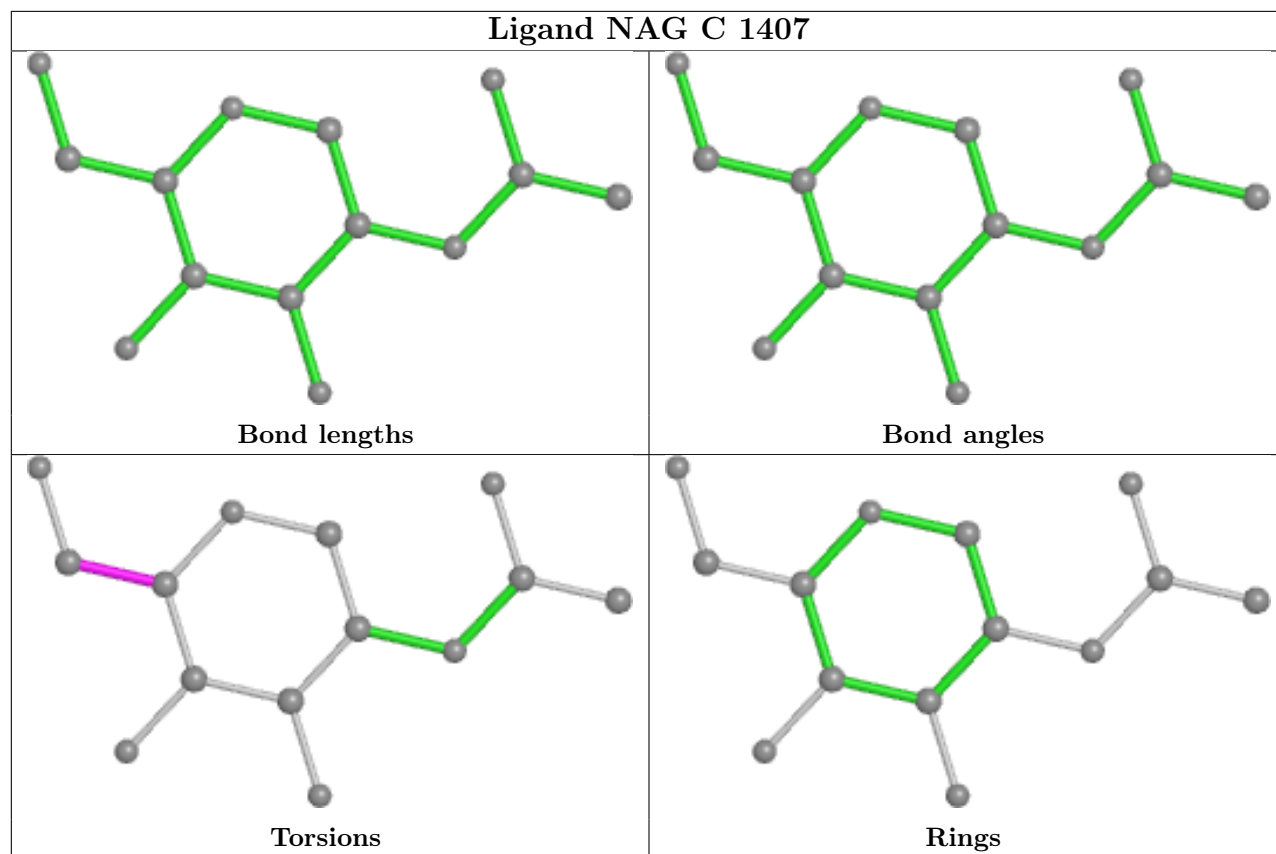


Ligand FOL C 1408

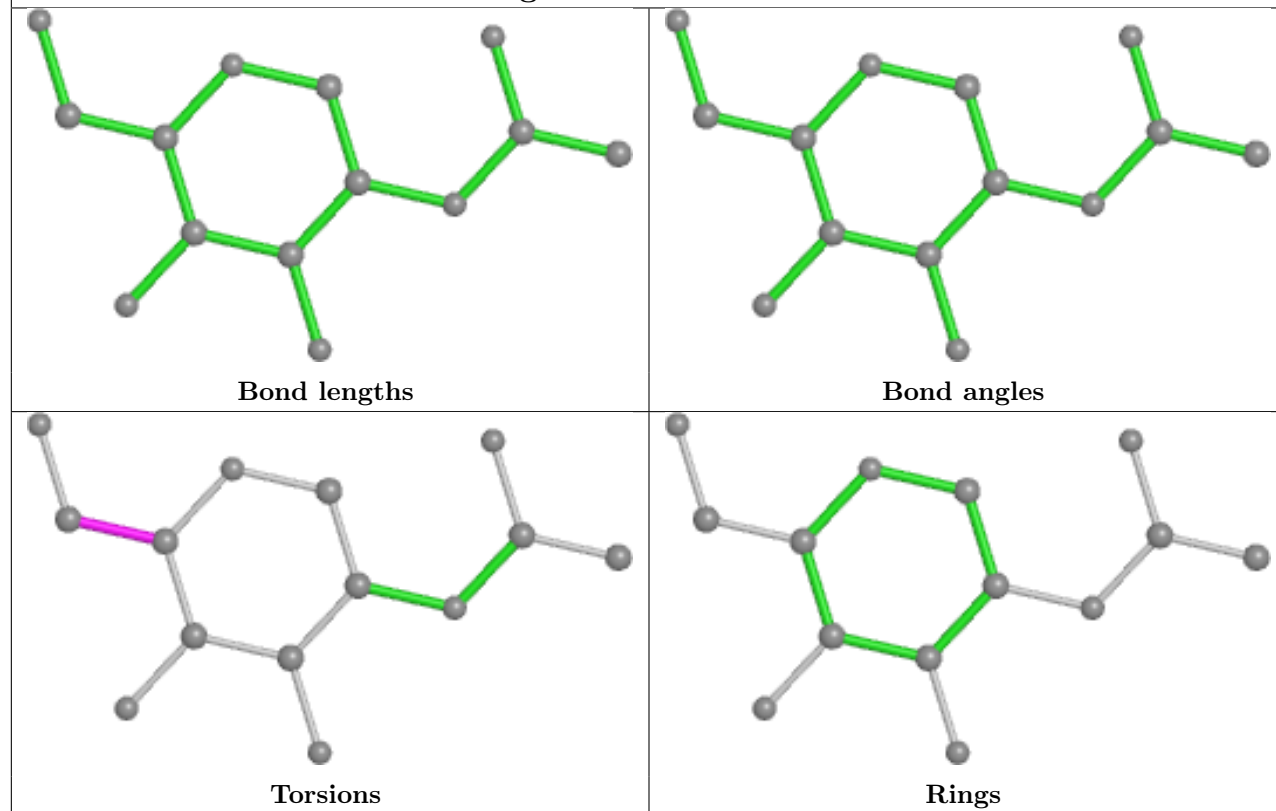


Ligand NAG A 1405

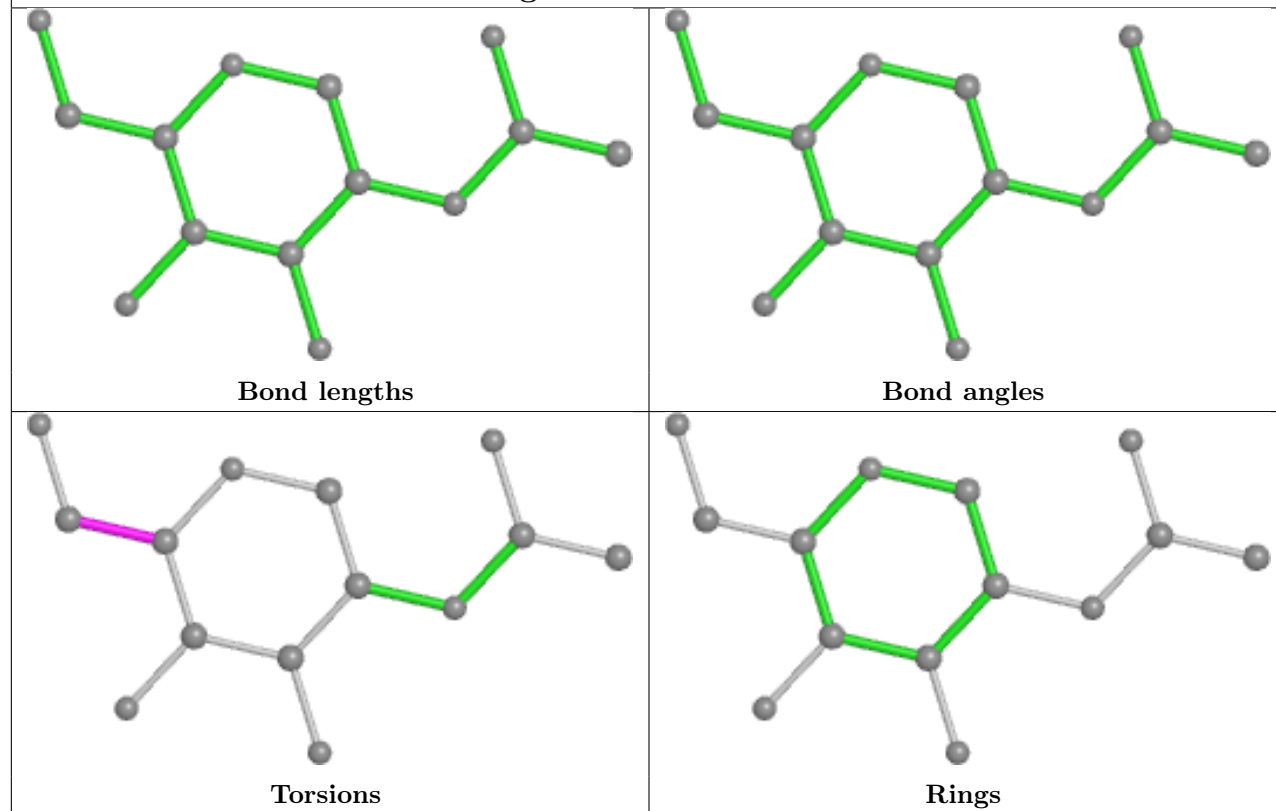




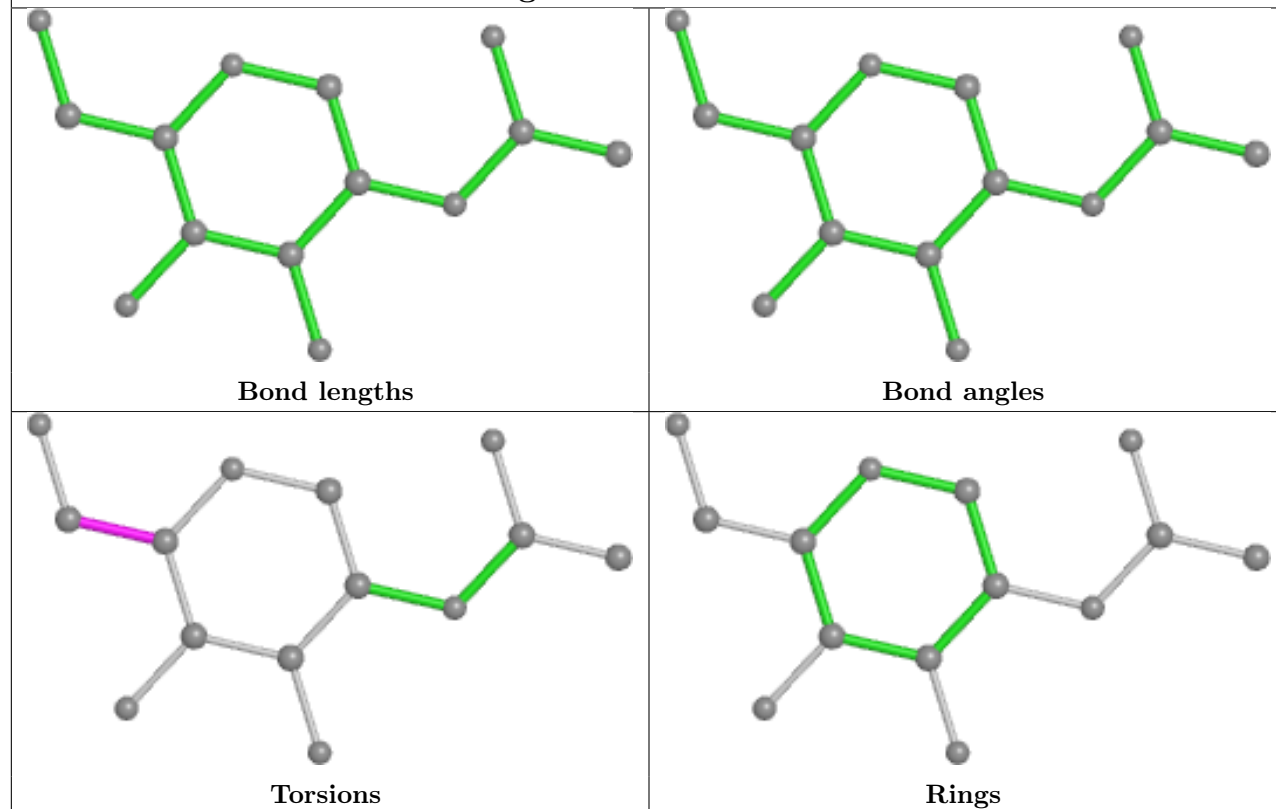
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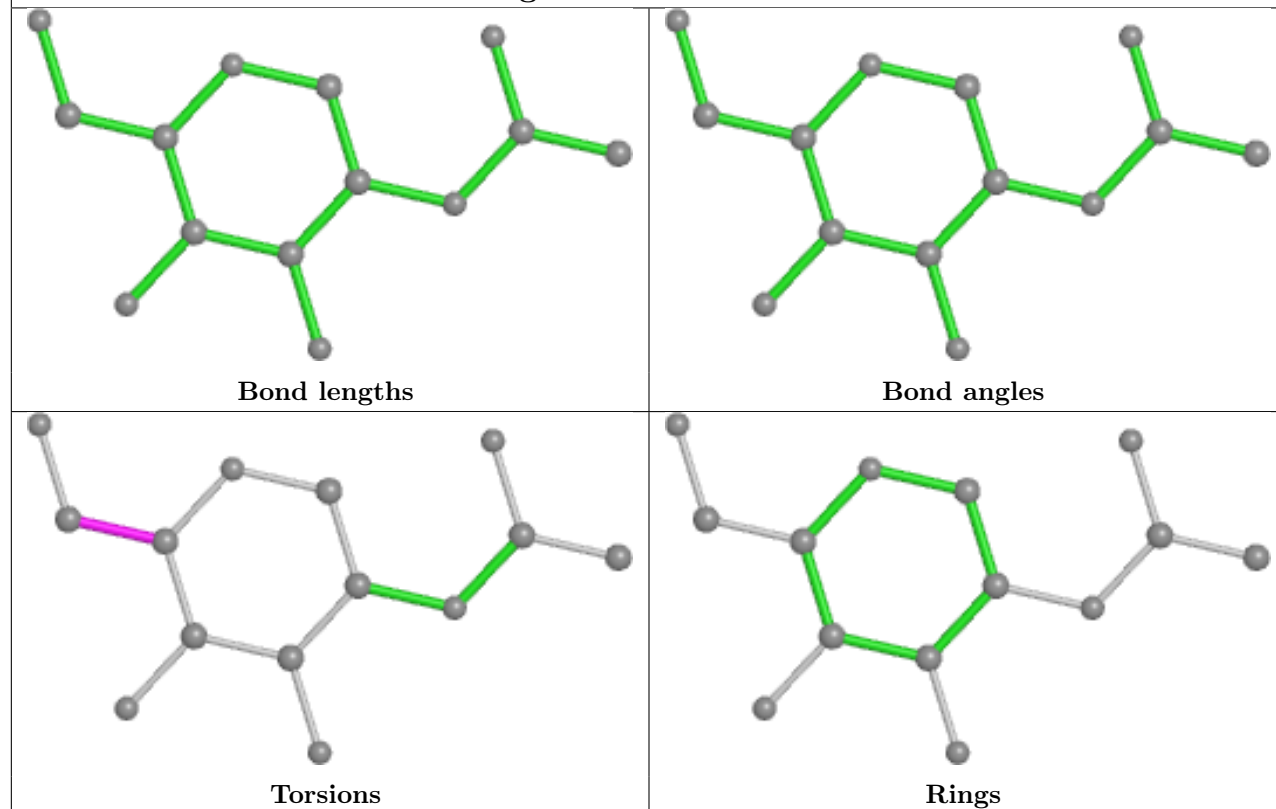
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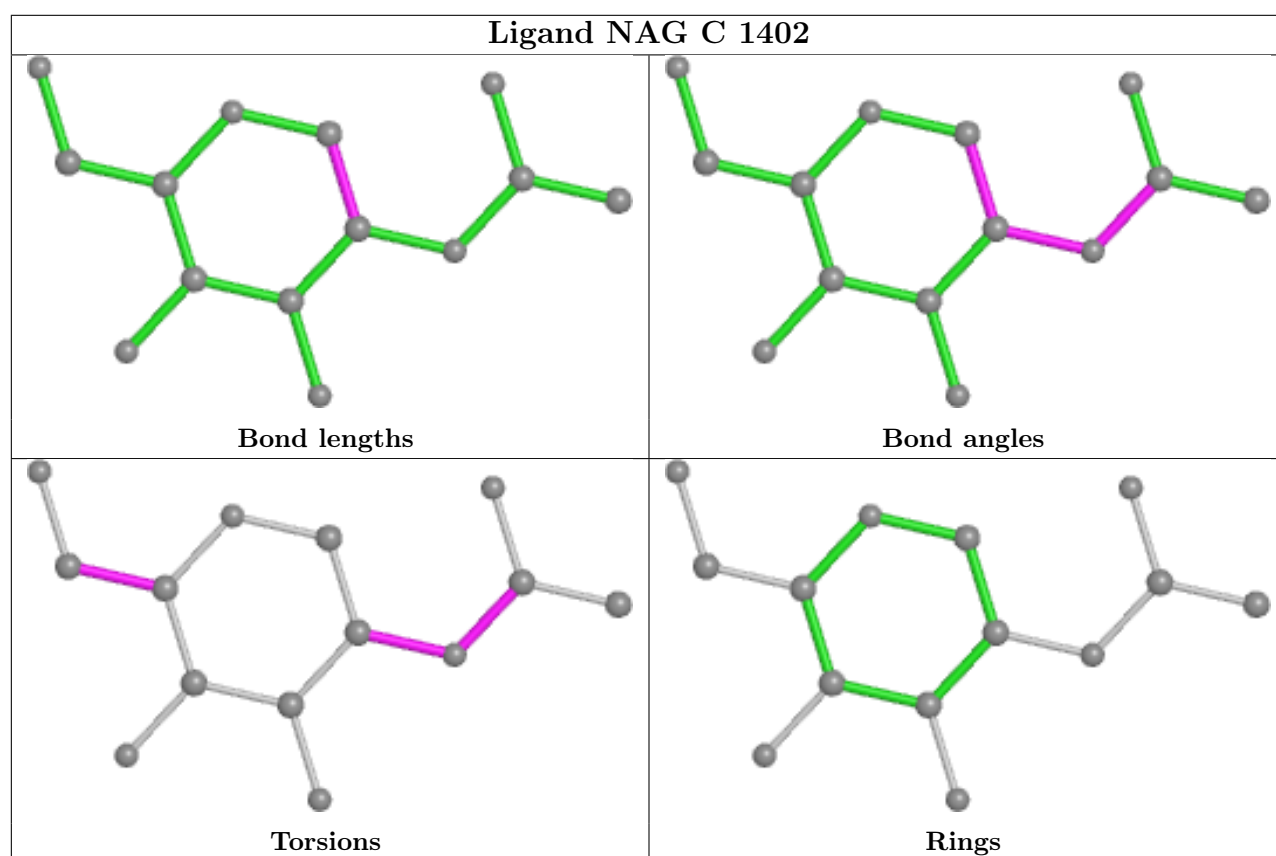
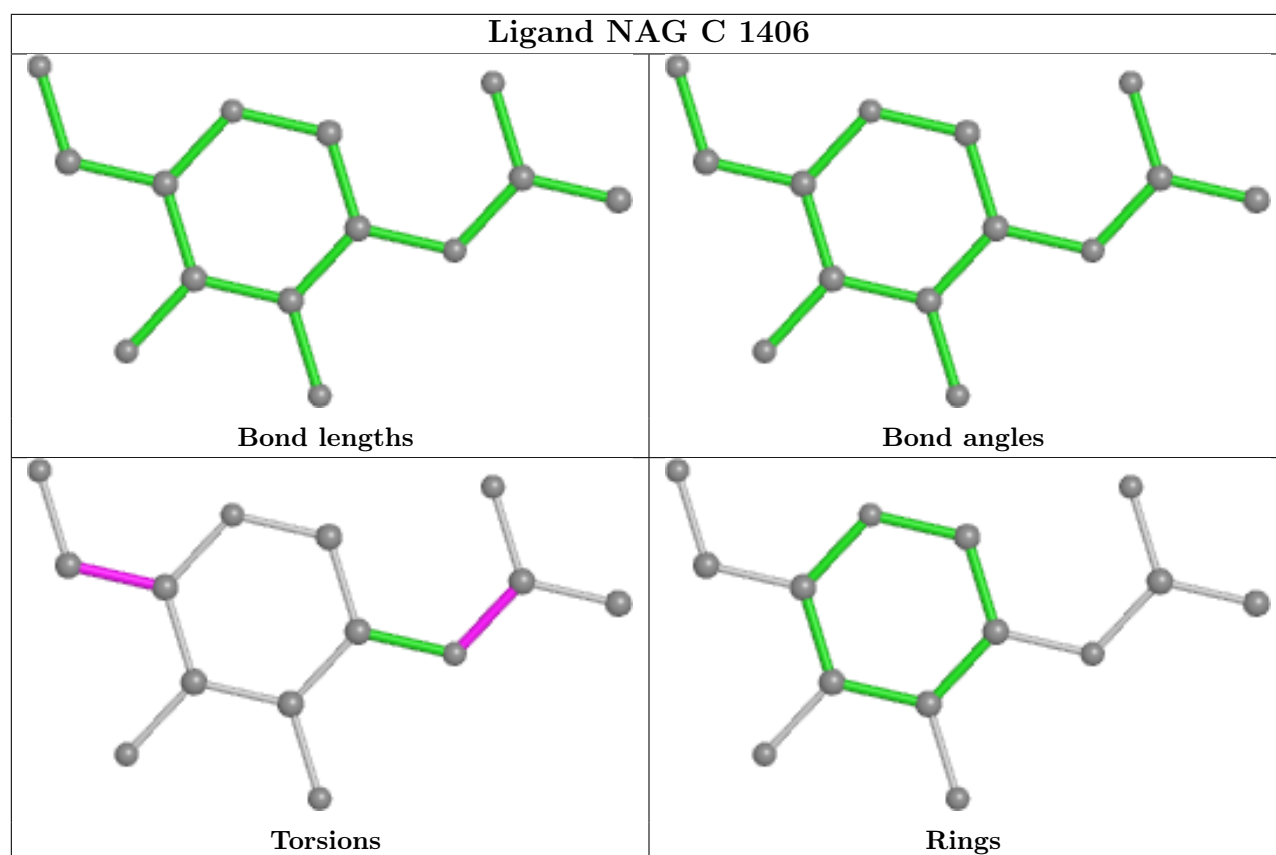


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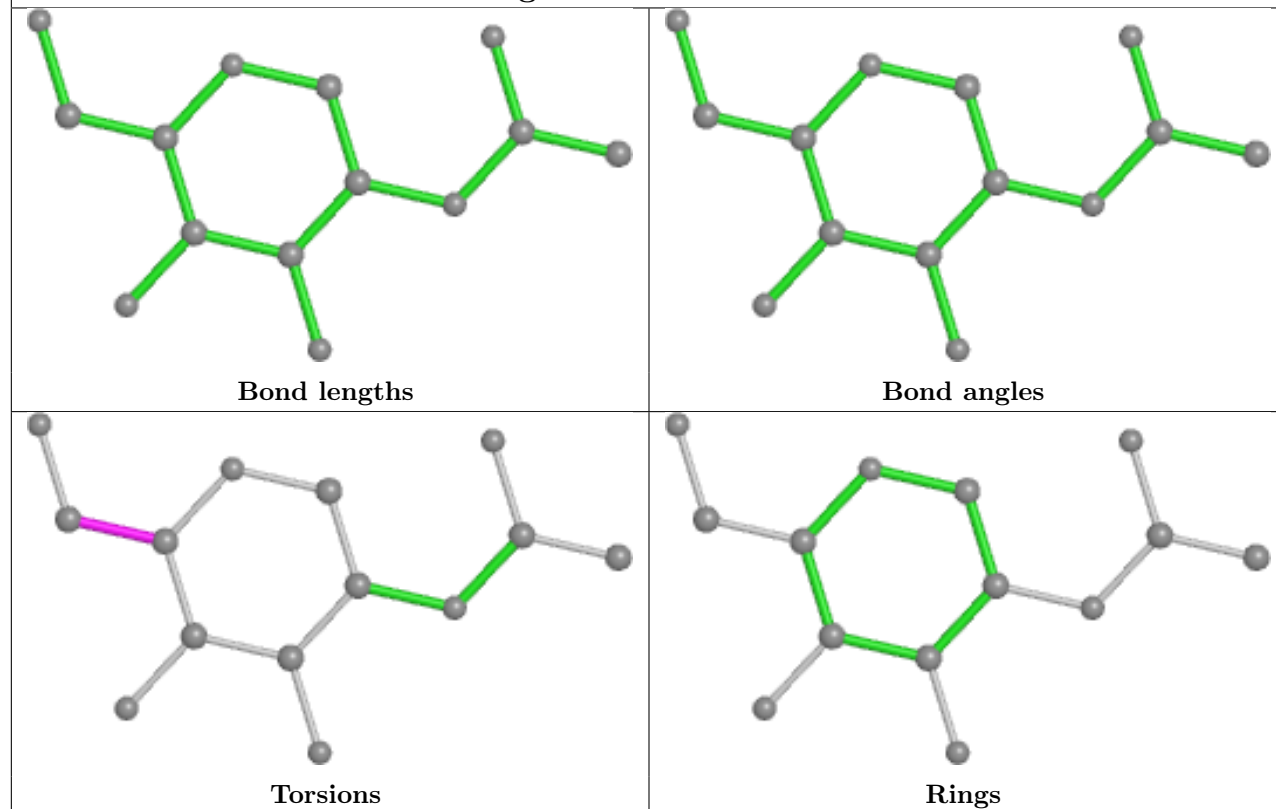


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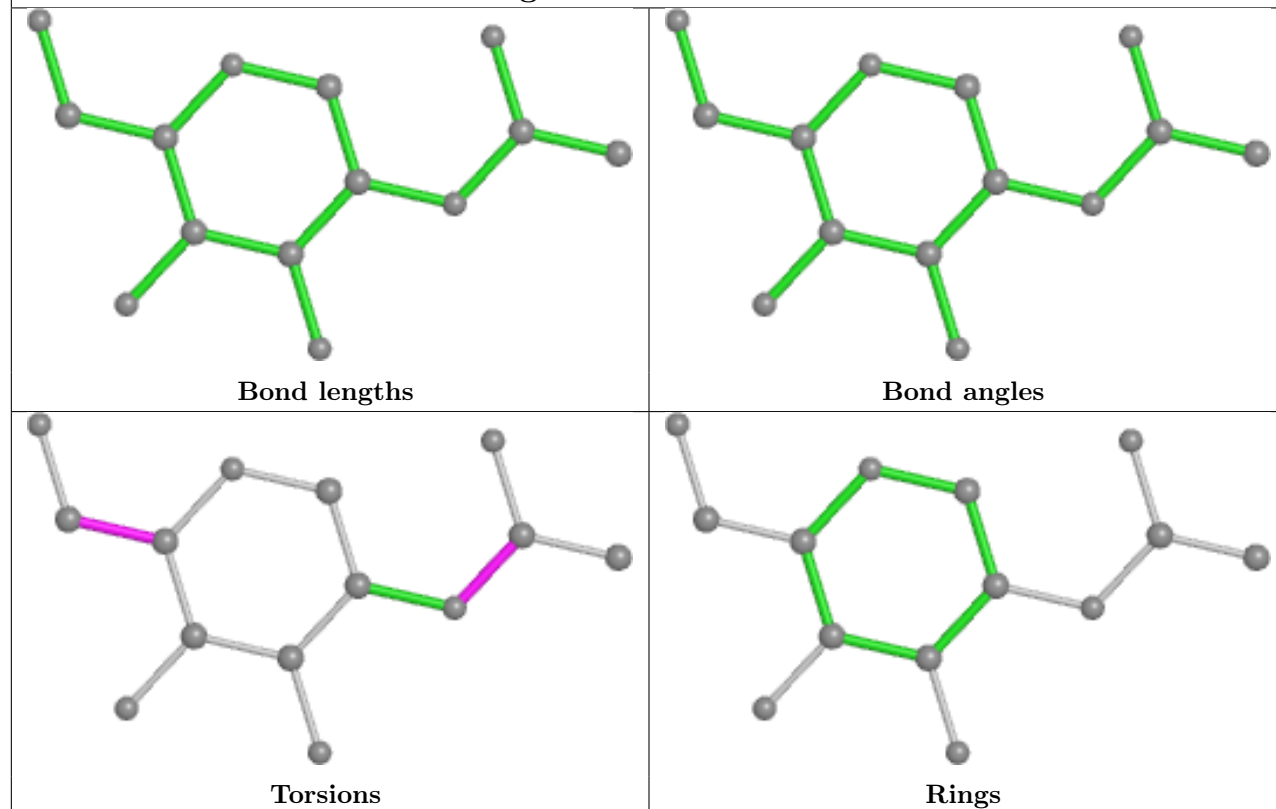


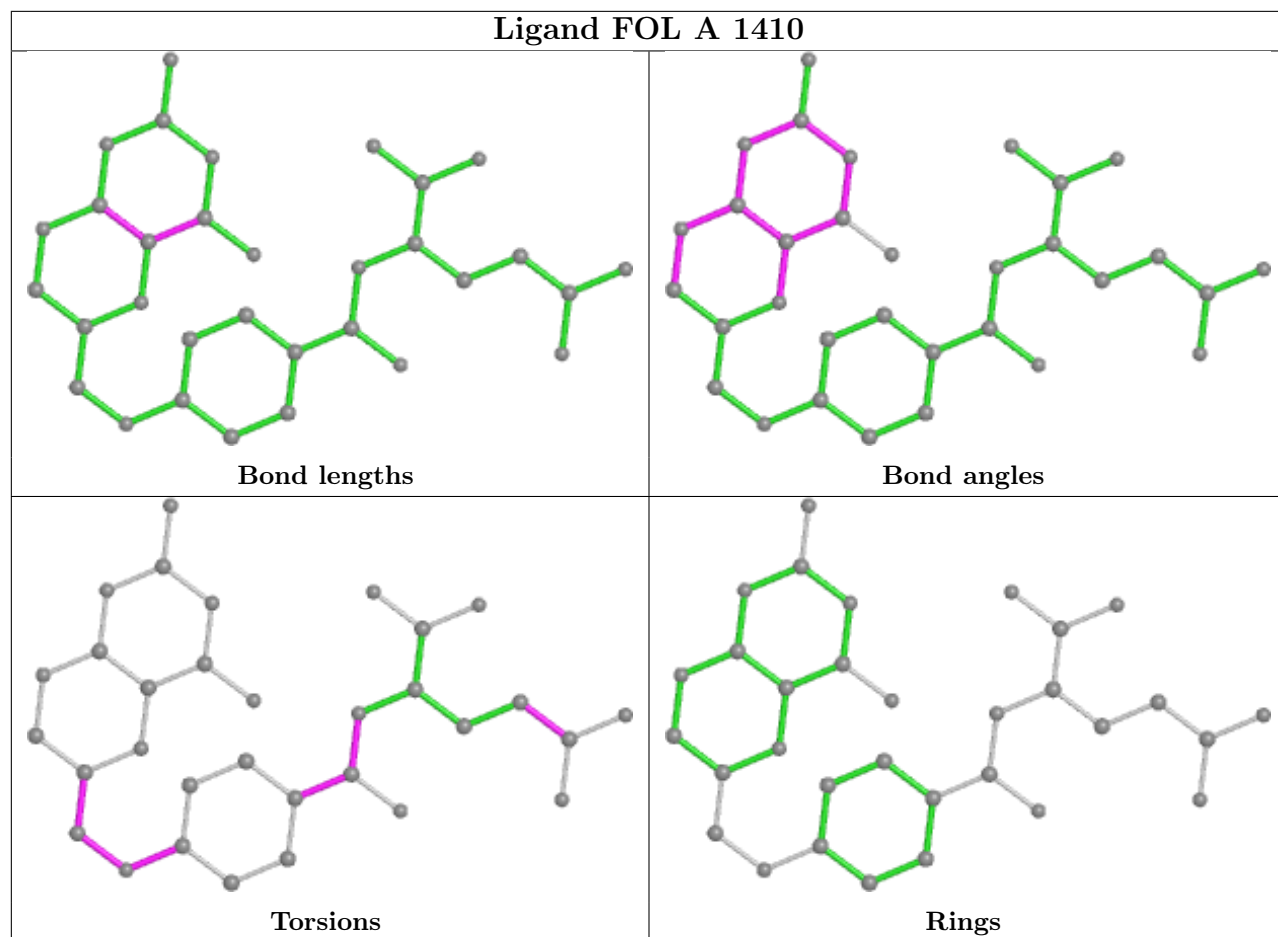


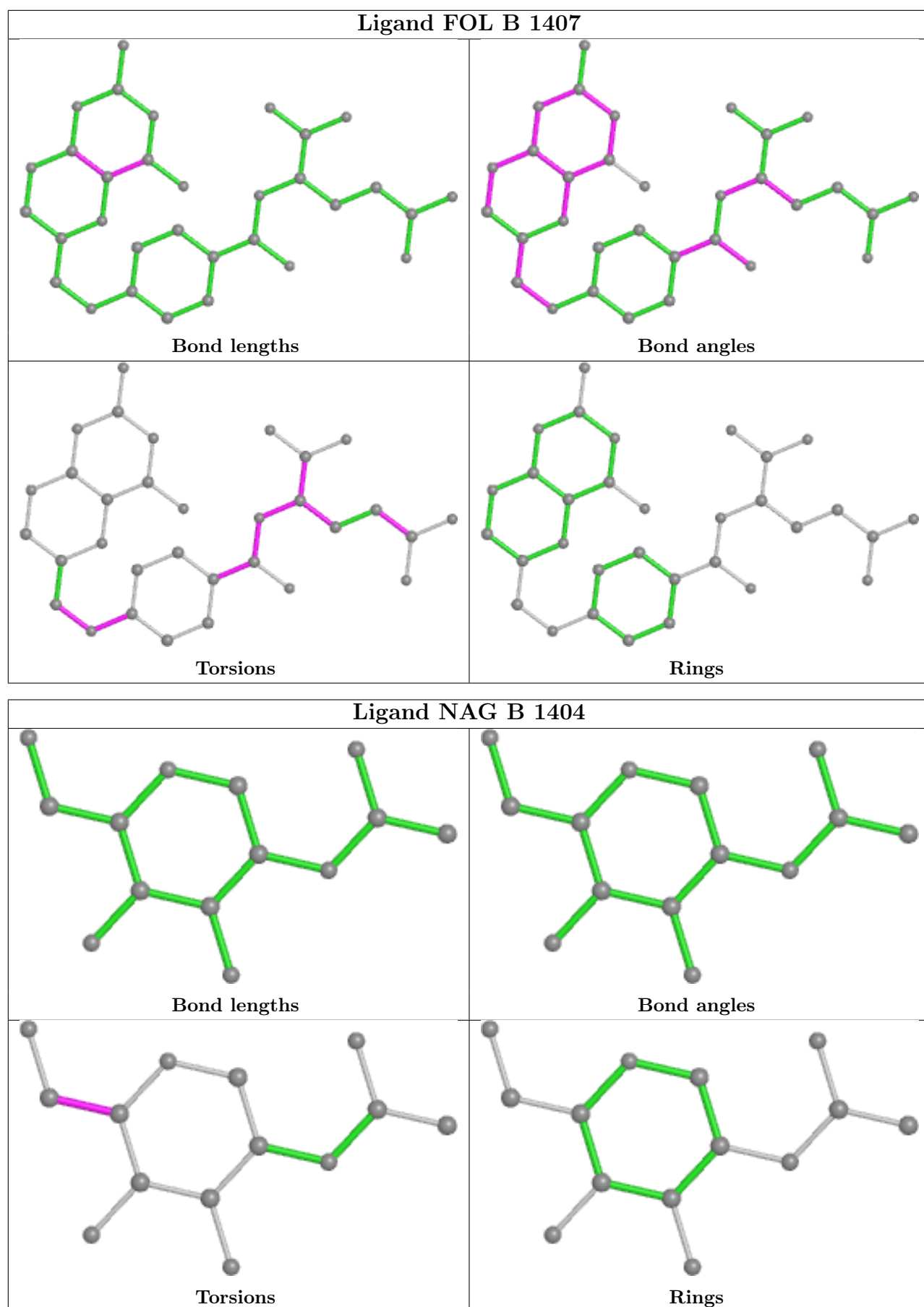
Ligand NAG A 1407



Ligand NAG B 1408







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.