



Full wwPDB EM Validation Report ⓘ

Jul 17, 2025 – 10:13 PM JST

PDB ID : 9JMO / pdb_00009jmo
EMDB ID : EMD-61608
Title : Cryo-EM structure of Japan-BatCoV (Vs-CoV-1) S-trimer
Authors : Yuan, H.; Xiong, X.
Deposited on : 2024-09-20
Resolution : 2.80 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

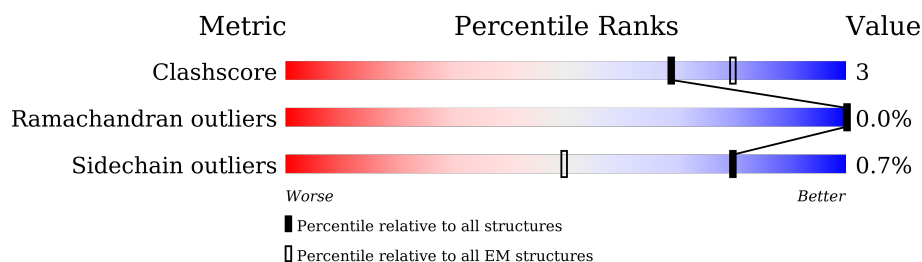
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.80 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	1369	
1	B	1369	
1	C	1369	
2	D	2	
2	G	2	
2	H	2	
2	I	2	
2	J	2	
2	M	2	

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

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 27694 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	1140	Total	C	N	O	S	0	0
			8886	5644	1486	1707	49		
1	B	1140	Total	C	N	O	S	0	0
			8886	5644	1486	1707	49		
1	C	1140	Total	C	N	O	S	0	0
			8886	5644	1486	1707	49		

There are 159 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1291	GLY	-	linker	UNP A0A5H2WTJ3
A	1292	SER	-	linker	UNP A0A5H2WTJ3
A	1314	LEU	PHE	conflict	UNP P10104
A	1320	LEU	-	expression tag	UNP P10104
A	1321	GLU	-	expression tag	UNP P10104
A	1322	VAL	-	expression tag	UNP P10104
A	1323	LEU	-	expression tag	UNP P10104
A	1324	PHE	-	expression tag	UNP P10104
A	1325	GLN	-	expression tag	UNP P10104
A	1326	GLY	-	expression tag	UNP P10104
A	1327	PRO	-	expression tag	UNP P10104
A	1328	GLY	-	expression tag	UNP P10104
A	1329	HIS	-	expression tag	UNP P10104
A	1330	HIS	-	expression tag	UNP P10104
A	1331	HIS	-	expression tag	UNP P10104
A	1332	HIS	-	expression tag	UNP P10104
A	1333	HIS	-	expression tag	UNP P10104
A	1334	HIS	-	expression tag	UNP P10104
A	1335	HIS	-	expression tag	UNP P10104
A	1336	HIS	-	expression tag	UNP P10104
A	1337	SER	-	expression tag	UNP P10104
A	1338	ALA	-	expression tag	UNP P10104
A	1339	TRP	-	expression tag	UNP P10104
A	1340	SER	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1341	HIS	-	expression tag	UNP P10104
A	1342	PRO	-	expression tag	UNP P10104
A	1343	GLN	-	expression tag	UNP P10104
A	1344	PHE	-	expression tag	UNP P10104
A	1345	GLU	-	expression tag	UNP P10104
A	1346	LYS	-	expression tag	UNP P10104
A	1347	GLY	-	expression tag	UNP P10104
A	1348	GLY	-	expression tag	UNP P10104
A	1349	GLY	-	expression tag	UNP P10104
A	1350	SER	-	expression tag	UNP P10104
A	1351	GLY	-	expression tag	UNP P10104
A	1352	GLY	-	expression tag	UNP P10104
A	1353	GLY	-	expression tag	UNP P10104
A	1354	GLY	-	expression tag	UNP P10104
A	1355	SER	-	expression tag	UNP P10104
A	1356	GLY	-	expression tag	UNP P10104
A	1357	GLY	-	expression tag	UNP P10104
A	1358	SER	-	expression tag	UNP P10104
A	1359	ALA	-	expression tag	UNP P10104
A	1360	TRP	-	expression tag	UNP P10104
A	1361	SER	-	expression tag	UNP P10104
A	1362	HIS	-	expression tag	UNP P10104
A	1363	PRO	-	expression tag	UNP P10104
A	1364	GLN	-	expression tag	UNP P10104
A	1365	PHE	-	expression tag	UNP P10104
A	1366	GLU	-	expression tag	UNP P10104
A	1367	LYS	-	expression tag	UNP P10104
A	1368	SER	-	expression tag	UNP P10104
A	1369	ALA	-	expression tag	UNP P10104
B	1291	GLY	-	linker	UNP A0A5H2WTJ3
B	1292	SER	-	linker	UNP A0A5H2WTJ3
B	1314	LEU	PHE	conflict	UNP P10104
B	1320	LEU	-	expression tag	UNP P10104
B	1321	GLU	-	expression tag	UNP P10104
B	1322	VAL	-	expression tag	UNP P10104
B	1323	LEU	-	expression tag	UNP P10104
B	1324	PHE	-	expression tag	UNP P10104
B	1325	GLN	-	expression tag	UNP P10104
B	1326	GLY	-	expression tag	UNP P10104
B	1327	PRO	-	expression tag	UNP P10104
B	1328	GLY	-	expression tag	UNP P10104
B	1329	HIS	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1330	HIS	-	expression tag	UNP P10104
B	1331	HIS	-	expression tag	UNP P10104
B	1332	HIS	-	expression tag	UNP P10104
B	1333	HIS	-	expression tag	UNP P10104
B	1334	HIS	-	expression tag	UNP P10104
B	1335	HIS	-	expression tag	UNP P10104
B	1336	HIS	-	expression tag	UNP P10104
B	1337	SER	-	expression tag	UNP P10104
B	1338	ALA	-	expression tag	UNP P10104
B	1339	TRP	-	expression tag	UNP P10104
B	1340	SER	-	expression tag	UNP P10104
B	1341	HIS	-	expression tag	UNP P10104
B	1342	PRO	-	expression tag	UNP P10104
B	1343	GLN	-	expression tag	UNP P10104
B	1344	PHE	-	expression tag	UNP P10104
B	1345	GLU	-	expression tag	UNP P10104
B	1346	LYS	-	expression tag	UNP P10104
B	1347	GLY	-	expression tag	UNP P10104
B	1348	GLY	-	expression tag	UNP P10104
B	1349	GLY	-	expression tag	UNP P10104
B	1350	SER	-	expression tag	UNP P10104
B	1351	GLY	-	expression tag	UNP P10104
B	1352	GLY	-	expression tag	UNP P10104
B	1353	GLY	-	expression tag	UNP P10104
B	1354	GLY	-	expression tag	UNP P10104
B	1355	SER	-	expression tag	UNP P10104
B	1356	GLY	-	expression tag	UNP P10104
B	1357	GLY	-	expression tag	UNP P10104
B	1358	SER	-	expression tag	UNP P10104
B	1359	ALA	-	expression tag	UNP P10104
B	1360	TRP	-	expression tag	UNP P10104
B	1361	SER	-	expression tag	UNP P10104
B	1362	HIS	-	expression tag	UNP P10104
B	1363	PRO	-	expression tag	UNP P10104
B	1364	GLN	-	expression tag	UNP P10104
B	1365	PHE	-	expression tag	UNP P10104
B	1366	GLU	-	expression tag	UNP P10104
B	1367	LYS	-	expression tag	UNP P10104
B	1368	SER	-	expression tag	UNP P10104
B	1369	ALA	-	expression tag	UNP P10104
C	1291	GLY	-	linker	UNP A0A5H2WTJ3
C	1292	SER	-	linker	UNP A0A5H2WTJ3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1314	LEU	PHE	conflict	UNP P10104
C	1320	LEU	-	expression tag	UNP P10104
C	1321	GLU	-	expression tag	UNP P10104
C	1322	VAL	-	expression tag	UNP P10104
C	1323	LEU	-	expression tag	UNP P10104
C	1324	PHE	-	expression tag	UNP P10104
C	1325	GLN	-	expression tag	UNP P10104
C	1326	GLY	-	expression tag	UNP P10104
C	1327	PRO	-	expression tag	UNP P10104
C	1328	GLY	-	expression tag	UNP P10104
C	1329	HIS	-	expression tag	UNP P10104
C	1330	HIS	-	expression tag	UNP P10104
C	1331	HIS	-	expression tag	UNP P10104
C	1332	HIS	-	expression tag	UNP P10104
C	1333	HIS	-	expression tag	UNP P10104
C	1334	HIS	-	expression tag	UNP P10104
C	1335	HIS	-	expression tag	UNP P10104
C	1336	HIS	-	expression tag	UNP P10104
C	1337	SER	-	expression tag	UNP P10104
C	1338	ALA	-	expression tag	UNP P10104
C	1339	TRP	-	expression tag	UNP P10104
C	1340	SER	-	expression tag	UNP P10104
C	1341	HIS	-	expression tag	UNP P10104
C	1342	PRO	-	expression tag	UNP P10104
C	1343	GLN	-	expression tag	UNP P10104
C	1344	PHE	-	expression tag	UNP P10104
C	1345	GLU	-	expression tag	UNP P10104
C	1346	LYS	-	expression tag	UNP P10104
C	1347	GLY	-	expression tag	UNP P10104
C	1348	GLY	-	expression tag	UNP P10104
C	1349	GLY	-	expression tag	UNP P10104
C	1350	SER	-	expression tag	UNP P10104
C	1351	GLY	-	expression tag	UNP P10104
C	1352	GLY	-	expression tag	UNP P10104
C	1353	GLY	-	expression tag	UNP P10104
C	1354	GLY	-	expression tag	UNP P10104
C	1355	SER	-	expression tag	UNP P10104
C	1356	GLY	-	expression tag	UNP P10104
C	1357	GLY	-	expression tag	UNP P10104
C	1358	SER	-	expression tag	UNP P10104
C	1359	ALA	-	expression tag	UNP P10104
C	1360	TRP	-	expression tag	UNP P10104

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1361	SER	-	expression tag	UNP P10104
C	1362	HIS	-	expression tag	UNP P10104
C	1363	PRO	-	expression tag	UNP P10104
C	1364	GLN	-	expression tag	UNP P10104
C	1365	PHE	-	expression tag	UNP P10104
C	1366	GLU	-	expression tag	UNP P10104
C	1367	LYS	-	expression tag	UNP P10104
C	1368	SER	-	expression tag	UNP P10104
C	1369	ALA	-	expression tag	UNP P10104

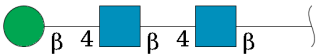
- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

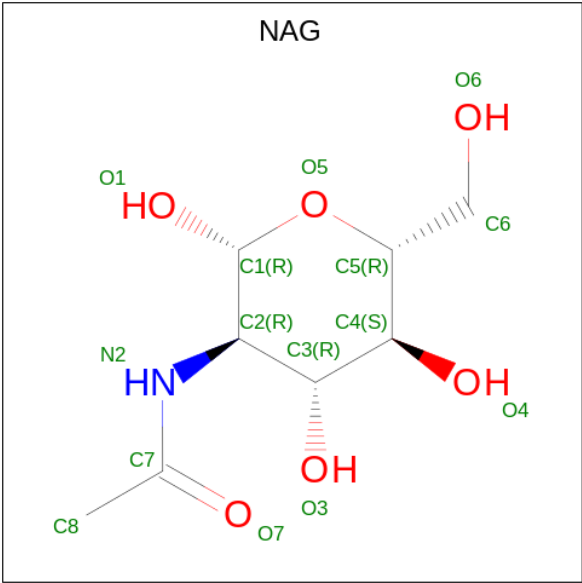
- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-b

eta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	E	3	Total	C	N	O	0	0
			39	22	2	15		
3	F	3	Total	C	N	O	0	0
			39	22	2	15		
3	K	3	Total	C	N	O	0	0
			39	22	2	15		
3	L	3	Total	C	N	O	0	0
			39	22	2	15		
3	P	3	Total	C	N	O	0	0
			39	22	2	15		
3	Q	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (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	

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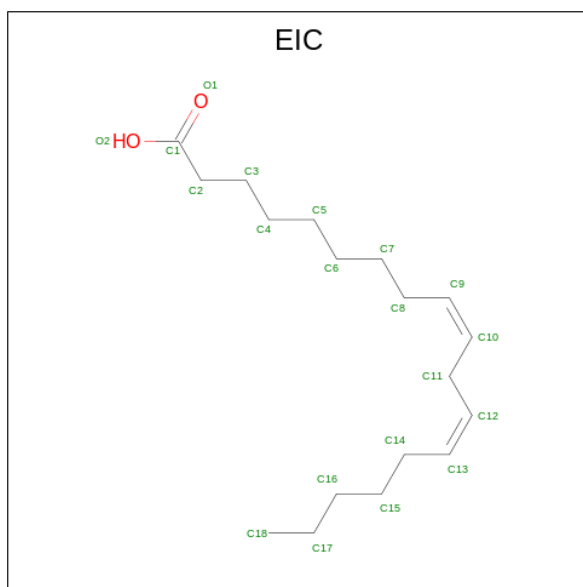
Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	A	1	Total 14	C 8	N 1	O 5	0
4	B	1	Total 14	C 8	N 1	O 5	0
4	B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

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Mol	Chain	Residues	Atoms				AltConf
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 LINOLEIC ACID (CCD ID: EIC) (formula: $C_{18}H_{32}O_2$) (labeled as "Ligand of Interest" by depositor).

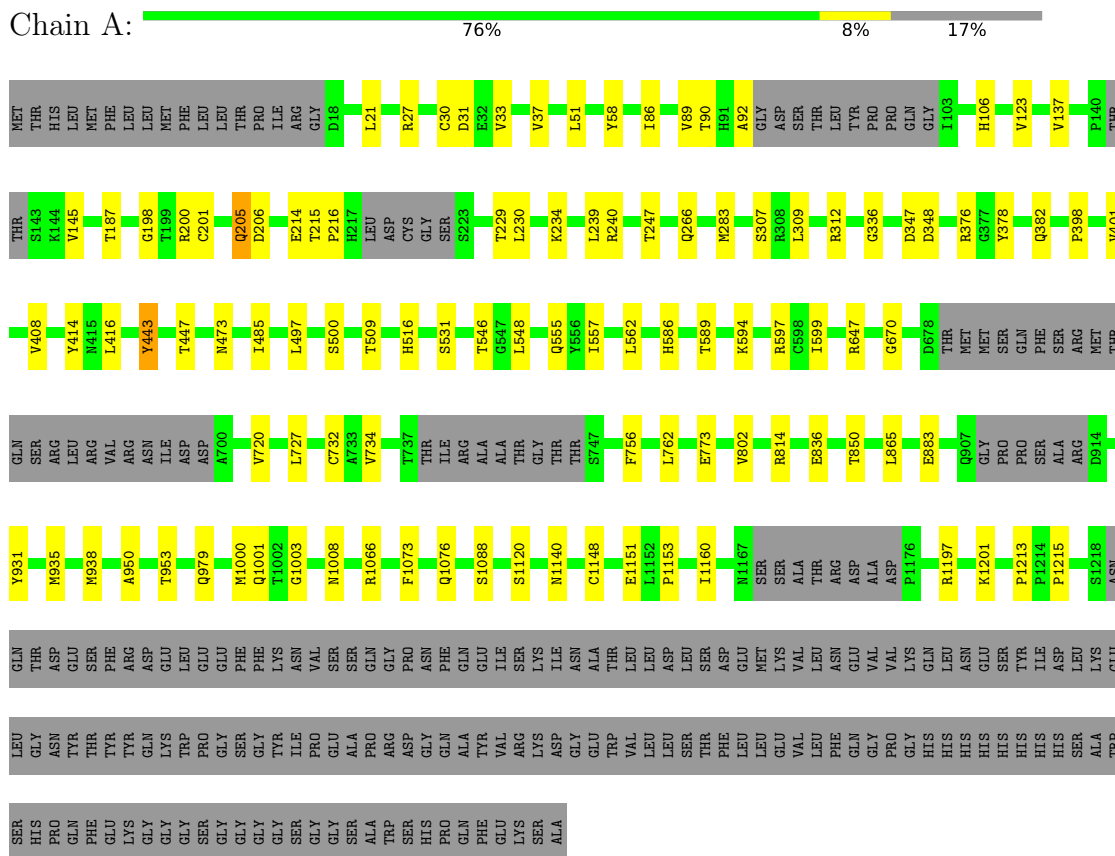


Mol	Chain	Residues	Atoms			AltConf
5	A	1	Total	C	O	0
			20	18	2	
5	B	1	Total	C	O	0
			20	18	2	
5	C	1	Total	C	O	0
			20	18	2	

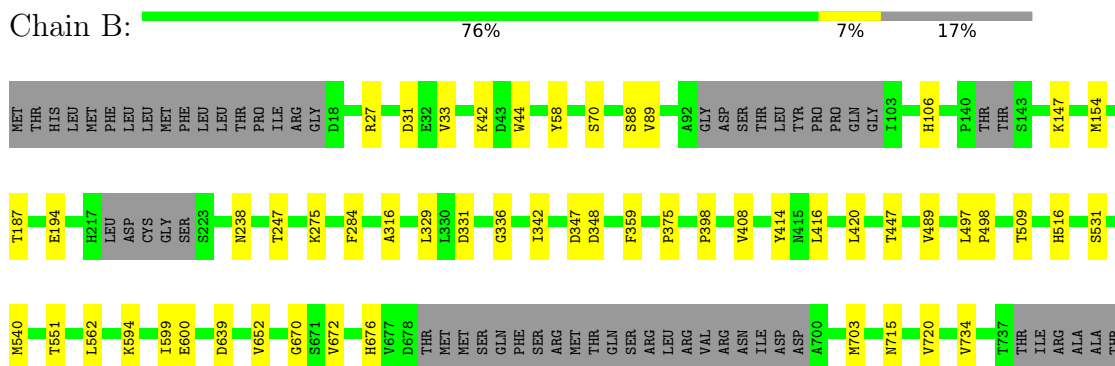
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Spike glycoprotein,Fibrinin



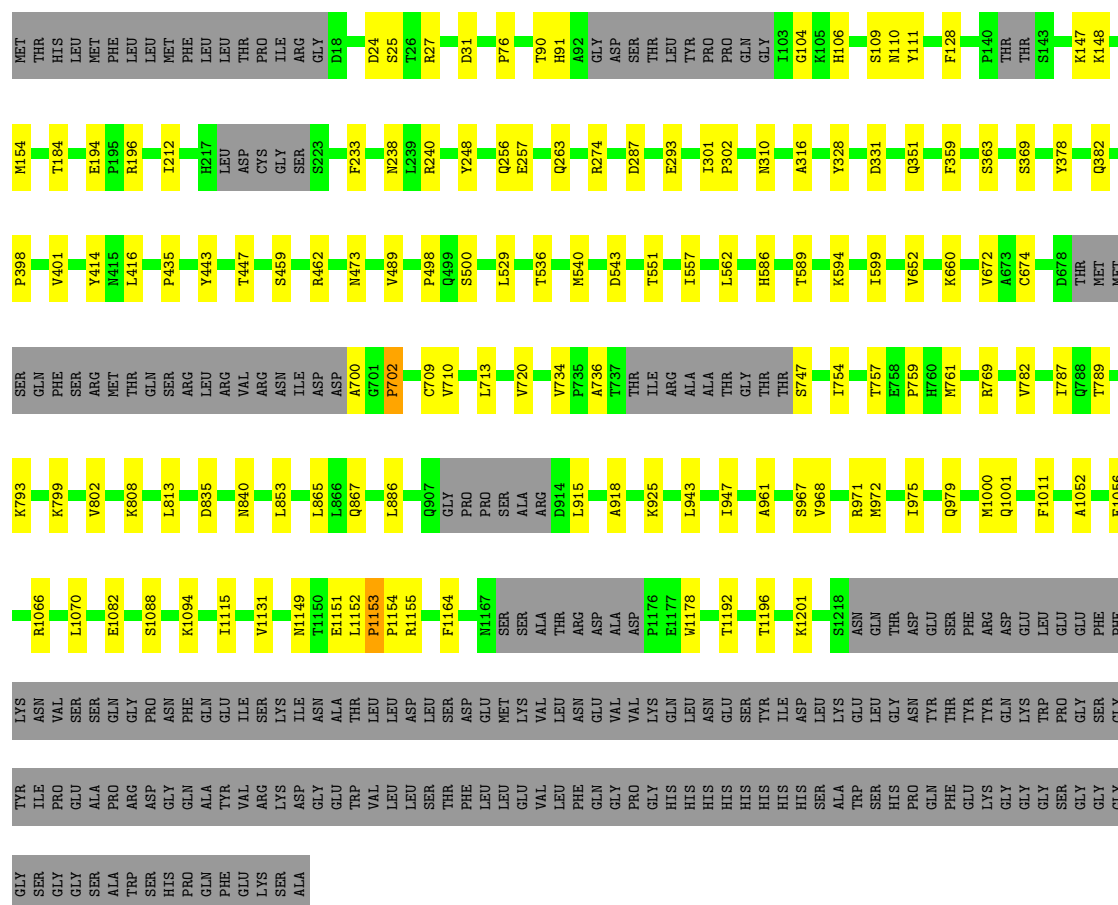
- Molecule 1: Spike glycoprotein,Fibrinin





• Molecule 1: Spike glycoprotein,Fibritin

Chain C: 74% 10% 17%



• 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 G:  100%



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

Chain H:  50% 50%



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

Chain I:  50% 50%



- 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 M:  100%



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

Chain N:  50% 50%



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

Chain O:  100%



- 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 E:  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 F:  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 K:  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 L:  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 P:  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 Q:  100%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	198806	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: NAG, BMA, EIC

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	0.16	0/9100	0.30	0/12385
1	B	0.15	0/9100	0.30	0/12385
1	C	0.16	0/9100	0.32	0/12385
All	All	0.16	0/27300	0.31	0/37155

There are no bond length outliers.

There are no bond angle outliers.

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	8886	0	8530	62	0
1	B	8886	0	8530	57	0
1	C	8886	0	8531	79	0
2	D	28	0	25	0	0
2	G	28	0	25	0	0
2	H	28	0	25	1	0
2	I	28	0	25	0	0
2	J	28	0	25	0	0
2	M	28	0	25	0	0
2	N	28	0	25	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	28	0	25	0	0
2	R	28	0	25	0	0
2	S	28	0	25	0	0
2	T	28	0	25	0	0
3	E	39	0	34	0	0
3	F	39	0	34	0	0
3	K	39	0	34	0	0
3	L	39	0	34	0	0
3	P	39	0	34	0	0
3	Q	39	0	34	0	0
4	A	140	0	130	1	0
4	B	140	0	130	0	0
4	C	154	0	143	1	0
5	A	20	0	31	1	0
5	B	20	0	31	1	0
5	C	20	0	31	1	0
All	All	27694	0	26566	187	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 3.

All (187) 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:33:VAL:HG12	1:B:106:HIS:HB2	1.71	0.73
1:A:33:VAL:HG12	1:A:106:HIS:HB2	1.72	0.72
1:B:594:LYS:HB3	1:B:599:ILE:HG21	1.73	0.70
1:B:509:THR:HG1	1:B:516:HIS:HE2	1.42	0.65
1:C:652:VAL:HG13	1:C:672:VAL:HG21	1.76	0.65
1:A:509:THR:HG1	1:A:516:HIS:HE2	1.43	0.64
1:B:1151:GLU:HG3	1:B:1153:PRO:HD2	1.78	0.64
1:C:351:GLN:HE22	1:C:369:SER:H	1.45	0.64
1:C:865:LEU:HD23	1:C:1000:MET:HE2	1.80	0.64
1:B:652:VAL:HG13	1:B:672:VAL:HG21	1.80	0.63
1:B:720:VAL:HG11	1:B:734:VAL:HG21	1.80	0.63
1:B:1148:CYS:HB3	1:B:1156:CYS:HA	1.81	0.62
1:B:1201:LYS:O	1:C:979:GLN:NE2	2.34	0.61
1:C:865:LEU:HD11	1:C:1001:GLN:HG3	1.81	0.61
1:B:194:GLU:HB3	1:B:238:ASN:HB2	1.83	0.61
1:A:594:LYS:HB3	1:A:599:ILE:HG21	1.83	0.60
1:A:865:LEU:HD23	1:A:1000:MET:HE2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:HA	1:A:312:ARG:HD3	1.85	0.59
1:B:1037:GLY:HA3	1:B:1061:ARG:HH21	1.68	0.58
5:B:1411:EIC:H52	1:C:435:PRO:HB3	1.84	0.57
1:C:27:ARG:NH2	1:C:31:ASP:OD1	2.37	0.57
1:A:187:THR:HG22	1:A:247:THR:HG22	1.86	0.56
1:A:398:PRO:HG3	1:A:562:LEU:HD21	1.87	0.56
1:B:973:ASN:ND2	1:B:977:ILE:O	2.35	0.56
1:A:720:VAL:HG11	1:A:734:VAL:HG21	1.88	0.56
1:B:187:THR:HG22	1:B:247:THR:HG22	1.87	0.56
1:C:720:VAL:HG11	1:C:734:VAL:HG21	1.88	0.56
1:C:1152:LEU:HB3	1:C:1153:PRO:HD3	1.88	0.55
1:B:808:LYS:HZ1	1:B:1056:GLU:HG2	1.70	0.55
1:A:92:ALA:HB3	1:A:312:ARG:HH11	1.71	0.55
1:B:898:MET:HG2	1:B:899:GLN:HG3	1.89	0.55
1:C:398:PRO:HG3	1:C:562:LEU:HD21	1.88	0.55
1:A:21:LEU:HD23	1:A:239:LEU:HD23	1.89	0.54
1:B:398:PRO:HG2	1:B:562:LEU:HD21	1.89	0.54
1:C:382:GLN:NE2	1:C:586:HIS:O	2.34	0.54
1:A:216:PRO:HG2	1:A:307:SER:HB3	1.89	0.53
1:A:1003:GLY:O	1:A:1008:ASN:ND2	2.41	0.53
1:B:497:LEU:HD22	1:B:562:LEU:HB2	1.89	0.53
1:A:123:VAL:HG12	1:A:283:MET:HE1	1.89	0.53
1:C:24:ASP:OD2	1:C:240:ARG:NH2	2.42	0.53
1:A:89:VAL:HG11	1:A:312:ARG:HG2	1.91	0.52
1:C:25:SER:O	1:C:196:ARG:NH2	2.39	0.52
1:C:540:MET:HG3	1:C:551:THR:HG22	1.91	0.52
1:A:647:ARG:NH2	1:B:904:CYS:O	2.43	0.52
1:C:194:GLU:HB3	1:C:238:ASN:HB2	1.91	0.52
1:C:1151:GLU:HG2	1:C:1154:PRO:HA	1.92	0.52
1:C:594:LYS:HB3	1:C:599:ILE:HG21	1.92	0.52
1:C:1152:LEU:C	1:C:1154:PRO:HD3	2.35	0.52
1:B:811:GLN:OE1	1:B:814:ARG:NH2	2.44	0.51
1:B:1078:LEU:O	1:B:1082:GLU:HG2	2.10	0.51
1:A:1201:LYS:O	1:B:979:GLN:NE2	2.45	0.50
1:B:27:ARG:NH2	1:B:31:ASP:OD1	2.44	0.50
1:C:802:VAL:O	1:C:1066:ARG:NH1	2.40	0.50
1:C:787:ILE:HD11	1:C:1094:LYS:HD2	1.93	0.50
1:A:382:GLN:NE2	1:A:586:HIS:O	2.35	0.49
1:A:531:SER:HB3	2:H:1:NAG:H81	1.94	0.49
1:C:414:TYR:HE2	1:C:416:LEU:HD13	1.78	0.49
1:A:670:GLY:HA3	1:B:925:LYS:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1152:LEU:O	1:C:1154:PRO:HD3	2.12	0.49
1:C:736:ALA:HB3	1:C:747:SER:HB2	1.94	0.48
1:C:128:PHE:HA	1:C:256:GLN:HG3	1.94	0.48
1:C:378:TYR:O	1:C:589:THR:OG1	2.26	0.48
1:C:310:ASN:OD1	1:C:310:ASN:N	2.46	0.48
1:A:931:TYR:HE1	1:C:754:ILE:HG21	1.78	0.48
1:A:935:MET:HA	1:A:938:MET:HE2	1.96	0.48
1:B:793:LYS:NZ	1:B:835:ASP:OD1	2.41	0.48
1:B:1149:ASN:HB3	1:B:1212:LEU:HD21	1.95	0.48
1:A:414:TYR:OH	1:A:443:TYR:OH	2.32	0.48
1:A:37:VAL:HG11	4:A:1401:NAG:H62	1.95	0.48
1:C:459:SER:HA	1:C:462:ARG:HG3	1.95	0.48
1:A:230:LEU:HG	1:A:234:LYS:HE3	1.96	0.48
1:B:540:MET:HG3	1:B:551:THR:HG22	1.95	0.48
1:C:248:TYR:OH	1:C:287:ASP:OD2	2.30	0.48
1:C:90:THR:HG22	1:C:106:HIS:HA	1.96	0.47
1:C:757:THR:HA	4:C:1406:NAG:H62	1.96	0.47
1:A:979:GLN:NE2	1:C:1201:LYS:O	2.47	0.47
1:C:529:LEU:HD21	1:C:543:ASP:HB2	1.96	0.47
1:A:376:ARG:HG3	1:A:597:ARG:HH12	1.80	0.47
1:A:802:VAL:O	1:A:1066:ARG:NH1	2.42	0.47
1:C:971:ARG:NH1	1:C:1115:ILE:O	2.41	0.47
1:B:1160:ILE:HD11	1:B:1197:ARG:HB3	1.97	0.47
1:A:850:THR:HG23	1:C:759:PRO:HB2	1.95	0.46
1:B:42:LYS:HE2	1:B:44:TRP:HE1	1.80	0.46
1:B:147:LYS:O	1:B:316:ALA:N	2.45	0.46
1:C:968:VAL:O	1:C:972:MET:HG3	2.14	0.46
1:A:30:CYS:O	1:A:200:ARG:NE	2.39	0.46
1:B:865:LEU:HD23	1:B:1000:MET:HE2	1.97	0.46
1:C:853:LEU:O	1:C:867:GLN:NE2	2.48	0.46
1:C:500:SER:HA	1:C:557:ILE:HG13	1.97	0.46
1:C:769:ARG:HD3	1:C:1178:TRP:HH2	1.80	0.46
1:A:198:GLY:H	1:A:201:CYS:HB2	1.81	0.46
1:B:348:ASP:OD1	1:B:348:ASP:N	2.49	0.46
1:B:531:SER:HB3	2:N:1:NAG:H81	1.97	0.46
1:C:212:ILE:HD11	1:C:233:PHE:HD1	1.81	0.46
1:A:756:PHE:HB2	1:B:935:MET:HE3	1.97	0.46
1:B:398:PRO:HD2	1:B:498:PRO:HD3	1.98	0.46
1:A:200:ARG:HA	1:A:206:ASP:O	2.15	0.46
1:B:822:LYS:HA	1:B:822:LYS:HD3	1.72	0.46
1:B:932:ASP:N	1:B:932:ASP:OD1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:782:VAL:HG22	1:C:1131:VAL:HG22	1.97	0.46
1:B:275:LYS:HB3	1:B:284:PHE:HB2	1.98	0.45
1:C:91:HIS:HB2	1:C:104:GLY:HA3	1.98	0.45
1:C:700:ALA:HB3	1:C:713:LEU:O	2.16	0.45
1:C:808:LYS:NZ	1:C:1056:GLU:OE1	2.47	0.45
1:A:1140:ASN:OD1	1:A:1140:ASN:N	2.45	0.45
1:C:975:ILE:HD13	1:C:1115:ILE:HD11	1.99	0.45
1:B:154:MET:HE3	1:B:154:MET:HB2	1.77	0.44
1:C:710:VAL:HG21	1:C:713:LEU:HD12	1.98	0.44
1:A:485:ILE:HG21	5:C:1401:EIC:H183	1.99	0.44
1:C:184:THR:O	1:C:184:THR:OG1	2.33	0.44
1:B:58:TYR:OH	1:B:336:GLY:O	2.31	0.44
1:C:194:GLU:OE1	1:C:238:ASN:ND2	2.47	0.44
1:B:1045:ASP:HA	1:B:1048:LYS:HG2	1.99	0.44
1:B:88:SER:OG	1:B:89:VAL:N	2.51	0.44
1:B:799:LYS:HB3	1:B:799:LYS:HE2	1.78	0.44
1:B:347:ASP:OD1	1:B:347:ASP:N	2.50	0.43
1:B:771:ILE:HG13	1:C:961:ALA:HB3	2.00	0.43
1:B:670:GLY:HA3	1:C:925:LYS:HE3	1.99	0.43
1:B:854:ASP:OD1	1:B:854:ASP:N	2.50	0.43
1:C:1149:ASN:HD21	1:C:1155:ARG:HB2	1.84	0.43
1:B:782:VAL:HG22	1:B:1131:VAL:HG22	2.00	0.43
1:A:1151:GLU:HG3	1:A:1153:PRO:HD2	2.00	0.43
1:B:331:ASP:HB2	1:B:359:PHE:CE1	2.53	0.43
1:B:414:TYR:HE2	1:B:416:LEU:HD13	1.82	0.43
1:A:214:GLU:OE2	1:A:229:THR:OG1	2.37	0.43
1:A:546:THR:HG23	1:A:548:LEU:H	1.83	0.43
1:C:109:SER:OG	1:C:110:ASN:N	2.52	0.43
1:C:257:GLU:OE2	1:C:274:ARG:NH1	2.47	0.43
1:C:1070:LEU:HD23	1:C:1070:LEU:HA	1.92	0.43
1:B:1003:GLY:O	1:B:1008:ASN:ND2	2.47	0.43
1:A:1213:PRO:HB2	1:A:1215:PRO:HD2	2.00	0.43
1:C:111:TYR:HB2	1:C:302:PRO:HG3	2.01	0.43
1:A:58:TYR:OH	1:A:336:GLY:O	2.36	0.42
1:A:950:ALA:HB3	1:A:953:THR:HG23	2.01	0.42
1:C:865:LEU:HD21	1:C:1001:GLN:HB2	2.01	0.42
1:C:886:LEU:HD23	1:C:1011:PHE:HE1	1.84	0.42
1:A:414:TYR:HE2	1:A:416:LEU:HD13	1.84	0.42
1:A:500:SER:HB2	1:A:555:GLN:O	2.20	0.42
1:C:331:ASP:HB2	1:C:359:PHE:CE1	2.54	0.42
1:A:27:ARG:NH2	1:A:31:ASP:OD1	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG22	1:A:106:HIS:HA	2.01	0.42
1:A:205:GLN:H	1:A:205:GLN:HG2	1.40	0.42
1:A:814:ARG:HH11	1:A:814:ARG:HG3	1.84	0.42
1:C:263:GLN:NE2	1:C:293:GLU:O	2.40	0.42
1:C:761:MET:HE2	1:C:761:MET:HB2	1.87	0.42
1:A:240:ARG:HD3	1:A:240:ARG:HA	1.85	0.42
1:C:148:LYS:NZ	1:C:257:GLU:OE2	2.50	0.42
1:C:154:MET:HB2	1:C:301:ILE:HD11	2.01	0.42
1:A:953:THR:O	1:A:953:THR:OG1	2.36	0.42
5:A:1411:EIC:H172	1:B:420:LEU:HD23	2.01	0.42
1:C:789:THR:O	1:C:1088:SER:OG	2.38	0.42
1:A:408:VAL:HG22	1:A:447:THR:HG23	2.02	0.42
1:C:793:LYS:NZ	1:C:835:ASP:OD1	2.43	0.42
1:A:497:LEU:HD12	1:A:557:ILE:HG21	2.02	0.42
1:B:807:GLU:OE1	1:B:807:GLU:N	2.39	0.42
1:C:947:ILE:HD12	1:C:961:ALA:HA	2.01	0.42
1:A:266:GLN:OE1	1:C:447:THR:OG1	2.37	0.41
1:C:398:PRO:HD2	1:C:498:PRO:HD3	2.03	0.41
1:C:363:SER:HG	1:C:660:LYS:H	1.65	0.41
1:A:378:TYR:O	1:A:589:THR:OG1	2.29	0.41
1:C:674:CYS:SG	1:C:702:PRO:HB3	2.60	0.41
1:C:799:LYS:HG3	1:C:813:LEU:HD23	2.02	0.41
1:C:915:LEU:HA	1:C:918:ALA:HB3	2.02	0.41
1:A:347:ASP:N	1:A:347:ASP:OD1	2.53	0.41
1:C:943:LEU:HA	1:C:943:LEU:HD23	1.84	0.41
1:B:375:PRO:HB2	1:B:600:GLU:HG2	2.02	0.41
1:A:86:ILE:HG21	1:A:137:VAL:HG21	2.02	0.41
1:A:348:ASP:OD1	1:A:348:ASP:N	2.50	0.41
1:A:865:LEU:HD21	1:A:1001:GLN:HB2	2.03	0.41
1:B:827:LEU:HD23	1:B:827:LEU:HA	1.94	0.41
1:C:147:LYS:O	1:C:316:ALA:N	2.49	0.41
1:A:727:LEU:HG	1:A:732:CYS:HA	2.02	0.41
1:C:540:MET:HE2	1:C:540:MET:HB3	1.90	0.41
1:B:639:ASP:OD1	1:B:639:ASP:N	2.52	0.40
1:B:703:MET:HE1	1:B:715:ASN:HB2	2.03	0.40
1:C:1052:ALA:O	1:C:1056:GLU:HG2	2.21	0.40
1:A:1073:PHE:HA	1:A:1076:GLN:HG2	2.02	0.40
1:A:762:LEU:HD11	1:A:773:GLU:HG3	2.02	0.40
1:C:76:PRO:O	1:C:328:TYR:OH	2.32	0.40
1:C:401:VAL:HG22	1:C:473:ASN:HB3	2.03	0.40
1:C:967:SER:O	1:C:971:ARG:HG2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1164:PHE:HZ	1:C:1196:THR:HG22	1.86	0.40
1:A:1160:ILE:HD11	1:A:1197:ARG:HB3	2.03	0.40
1:B:329:LEU:HB3	1:B:342:ILE:HB	2.04	0.40
1:B:408:VAL:HG22	1:B:447:THR:HG23	2.02	0.40
1:A:401:VAL:HG22	1:A:473:ASN:HB3	2.02	0.40
1:A:883:GLU:HG3	1:A:1120:SER:HB2	2.02	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	1124/1369 (82%)	1102 (98%)	22 (2%)	0	100	100
1	B	1124/1369 (82%)	1095 (97%)	29 (3%)	0	100	100
1	C	1124/1369 (82%)	1097 (98%)	26 (2%)	1 (0%)	48	77
All	All	3372/4107 (82%)	3294 (98%)	77 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1153	PRO

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	985/1180 (84%)	977 (99%)	8 (1%)	79	93
1	B	985/1180 (84%)	980 (100%)	5 (0%)	86	95
1	C	985/1180 (84%)	977 (99%)	8 (1%)	79	93
All	All	2955/3540 (84%)	2934 (99%)	21 (1%)	80	94

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	LEU
1	A	145	VAL
1	A	205	GLN
1	A	215	THR
1	A	443	TYR
1	A	836	GLU
1	A	1088	SER
1	A	1148	CYS
1	B	70	SER
1	B	489	VAL
1	B	676	HIS
1	B	857	LEU
1	B	875	GLN
1	C	443	TYR
1	C	489	VAL
1	C	536	THR
1	C	702	PRO
1	C	709	CYS
1	C	840	ASN
1	C	1082	GLU
1	C	1192	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	729	GLN
1	A	804	ASN
1	A	840	ASN
1	A	985	ASN
1	A	986	GLN
1	A	1113	ASN
1	A	1206	GLN
1	B	41	GLN

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Mol	Chain	Res	Type
1	B	310	ASN
1	B	431	HIS
1	B	840	ASN
1	B	899	GLN
1	B	934	ASN
1	B	986	GLN
1	B	1187	ASN
1	C	41	GLN
1	C	164	HIS
1	C	351	GLN
1	C	424	GLN
1	C	613	GLN
1	C	632	ASN
1	C	729	GLN
1	C	750	GLN
1	C	966	GLN
1	C	986	GLN
1	C	1055	GLN
1	C	1064	ASN
1	C	1089	GLN
1	C	1106	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](#)

40 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	0.24	0	17,19,21	0.48	0
2	NAG	D	2	2	14,14,15	0.27	0	17,19,21	0.42	0
3	NAG	E	1	1,3	14,14,15	0.25	0	17,19,21	0.46	0
3	NAG	E	2	3	14,14,15	0.22	0	17,19,21	0.44	0
3	BMA	E	3	3	11,11,12	0.54	0	15,15,17	1.01	1 (6%)
3	NAG	F	1	1,3	14,14,15	0.28	0	17,19,21	0.47	0
3	NAG	F	2	3	14,14,15	0.24	0	17,19,21	0.41	0
3	BMA	F	3	3	11,11,12	0.54	0	15,15,17	0.81	0
2	NAG	G	1	1,2	14,14,15	0.26	0	17,19,21	0.40	0
2	NAG	G	2	2	14,14,15	0.23	0	17,19,21	0.41	0
2	NAG	H	1	1,2	14,14,15	0.32	0	17,19,21	0.47	0
2	NAG	H	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	I	1	1,2	14,14,15	0.30	0	17,19,21	0.53	0
2	NAG	I	2	2	14,14,15	0.32	0	17,19,21	0.68	1 (5%)
2	NAG	J	1	1,2	14,14,15	0.20	0	17,19,21	0.47	0
2	NAG	J	2	2	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	K	1	1,3	14,14,15	0.23	0	17,19,21	0.44	0
3	NAG	K	2	3	14,14,15	0.21	0	17,19,21	0.42	0
3	BMA	K	3	3	11,11,12	0.71	0	15,15,17	1.15	1 (6%)
3	NAG	L	1	1,3	14,14,15	0.28	0	17,19,21	0.48	0
3	NAG	L	2	3	14,14,15	0.25	0	17,19,21	0.42	0
3	BMA	L	3	3	11,11,12	0.55	0	15,15,17	0.82	0
2	NAG	M	1	1,2	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	M	2	2	14,14,15	0.22	0	17,19,21	0.45	0
2	NAG	N	1	1,2	14,14,15	0.30	0	17,19,21	0.46	0
2	NAG	N	2	2	14,14,15	0.21	0	17,19,21	0.48	0
2	NAG	O	1	1,2	14,14,15	0.29	0	17,19,21	0.59	0
2	NAG	O	2	2	14,14,15	0.26	0	17,19,21	0.37	0
3	NAG	P	1	1,3	14,14,15	0.25	0	17,19,21	0.43	0
3	NAG	P	2	3	14,14,15	0.23	0	17,19,21	0.44	0
3	BMA	P	3	3	11,11,12	0.62	0	15,15,17	1.05	1 (6%)
3	NAG	Q	1	3	14,14,15	0.33	0	17,19,21	0.42	0
3	NAG	Q	2	3	14,14,15	0.26	0	17,19,21	0.41	0
3	BMA	Q	3	3	11,11,12	0.59	0	15,15,17	0.76	0
2	NAG	R	1	1,2	14,14,15	0.30	0	17,19,21	0.44	0
2	NAG	R	2	2	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	S	1	1,2	14,14,15	0.28	0	17,19,21	0.73	0
2	NAG	S	2	2	14,14,15	0.22	0	17,19,21	0.46	0
2	NAG	T	1	1,2	14,14,15	0.24	0	17,19,21	0.41	0
2	NAG	T	2	2	14,14,15	0.23	0	17,19,21	0.43	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	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
3	NAG	E	1	1,3	-	4/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	BMA	E	3	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	0/6/23/26	0/1/1/1
3	BMA	F	3	3	-	0/2/19/22	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	2/6/23/26	0/1/1/1
2	NAG	I	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	I	2	2	-	3/6/23/26	0/1/1/1
2	NAG	J	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	J	2	2	-	2/6/23/26	0/1/1/1
3	NAG	K	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	BMA	K	3	3	-	0/2/19/22	0/1/1/1
3	NAG	L	1	1,3	-	1/6/23/26	0/1/1/1
3	NAG	L	2	3	-	0/6/23/26	0/1/1/1
3	BMA	L	3	3	-	0/2/19/22	0/1/1/1
2	NAG	M	1	1,2	-	1/6/23/26	0/1/1/1
2	NAG	M	2	2	-	4/6/23/26	0/1/1/1
2	NAG	N	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	N	2	2	-	2/6/23/26	0/1/1/1
2	NAG	O	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	O	2	2	-	2/6/23/26	0/1/1/1
3	NAG	P	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	P	2	3	-	0/6/23/26	0/1/1/1
3	BMA	P	3	3	-	0/2/19/22	0/1/1/1
3	NAG	Q	1	3	-	2/6/23/26	0/1/1/1
3	NAG	Q	2	3	-	1/6/23/26	0/1/1/1
3	BMA	Q	3	3	-	0/2/19/22	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

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	3	BMA	C1-O5-C5	2.28	115.28	112.19
3	K	3	BMA	C1-O5-C5	2.25	115.23	112.19
3	P	3	BMA	C1-O5-C5	2.22	115.20	112.19
2	I	2	NAG	C2-N2-C7	2.01	125.77	122.90

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	D	2	NAG	O5-C5-C6-O6
2	O	2	NAG	O5-C5-C6-O6
2	S	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	Q	1	NAG	O5-C5-C6-O6
2	R	2	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	N	2	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
2	J	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	Q	1	NAG	C4-C5-C6-O6
2	O	2	NAG	C4-C5-C6-O6
2	R	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C8-C7-N2-C2
2	G	2	NAG	O7-C7-N2-C2
2	M	2	NAG	C8-C7-N2-C2
2	M	2	NAG	O7-C7-N2-C2
3	E	1	NAG	C8-C7-N2-C2

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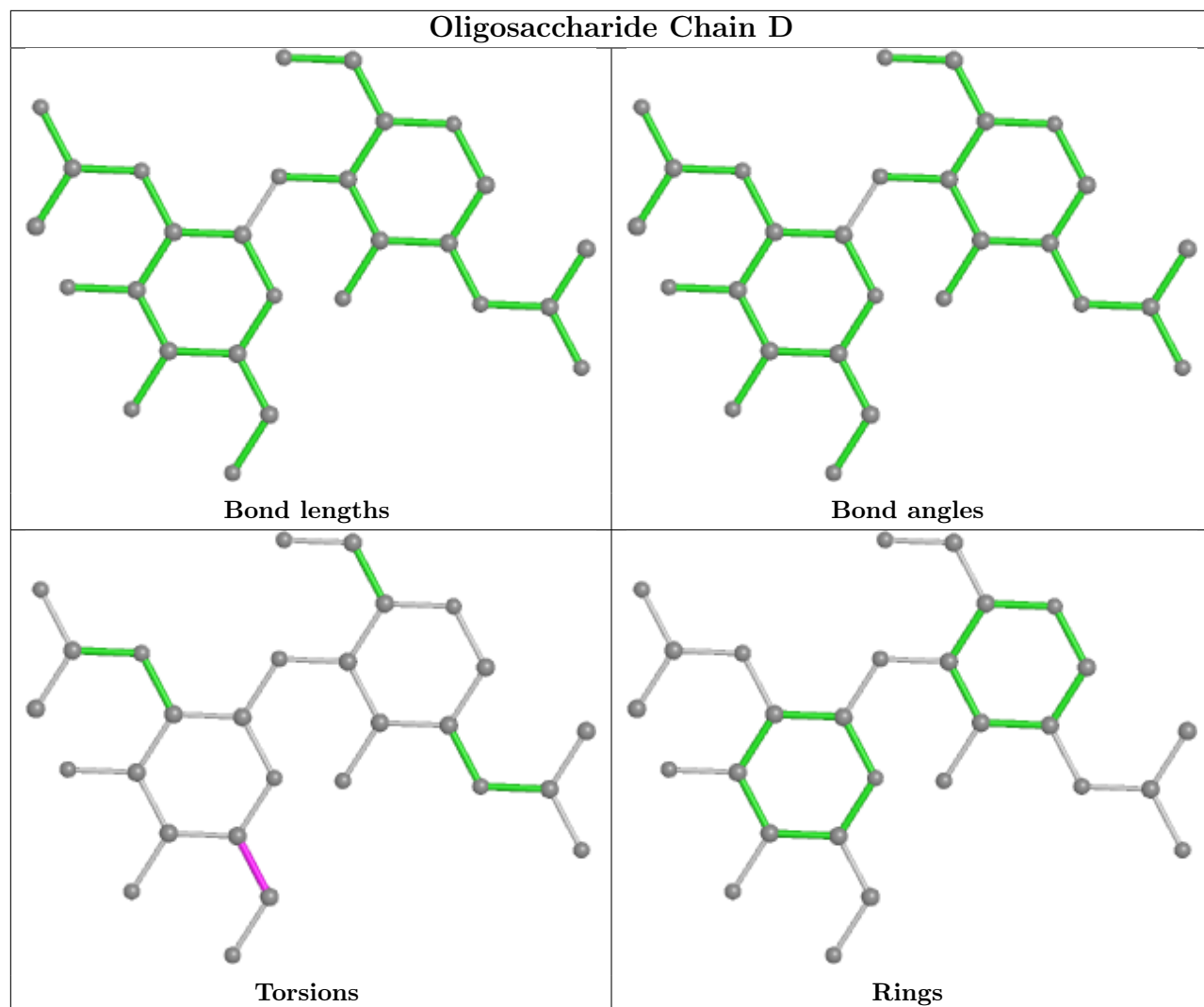
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O7-C7-N2-C2
2	J	2	NAG	O5-C5-C6-O6
2	S	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
2	R	1	NAG	C4-C5-C6-O6
2	M	2	NAG	O5-C5-C6-O6
2	T	2	NAG	O5-C5-C6-O6
2	M	2	NAG	C4-C5-C6-O6
2	T	2	NAG	C4-C5-C6-O6
3	E	1	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6
3	Q	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C3-C2-N2-C7
2	S	1	NAG	C3-C2-N2-C7
2	I	1	NAG	C4-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
2	M	1	NAG	C4-C5-C6-O6

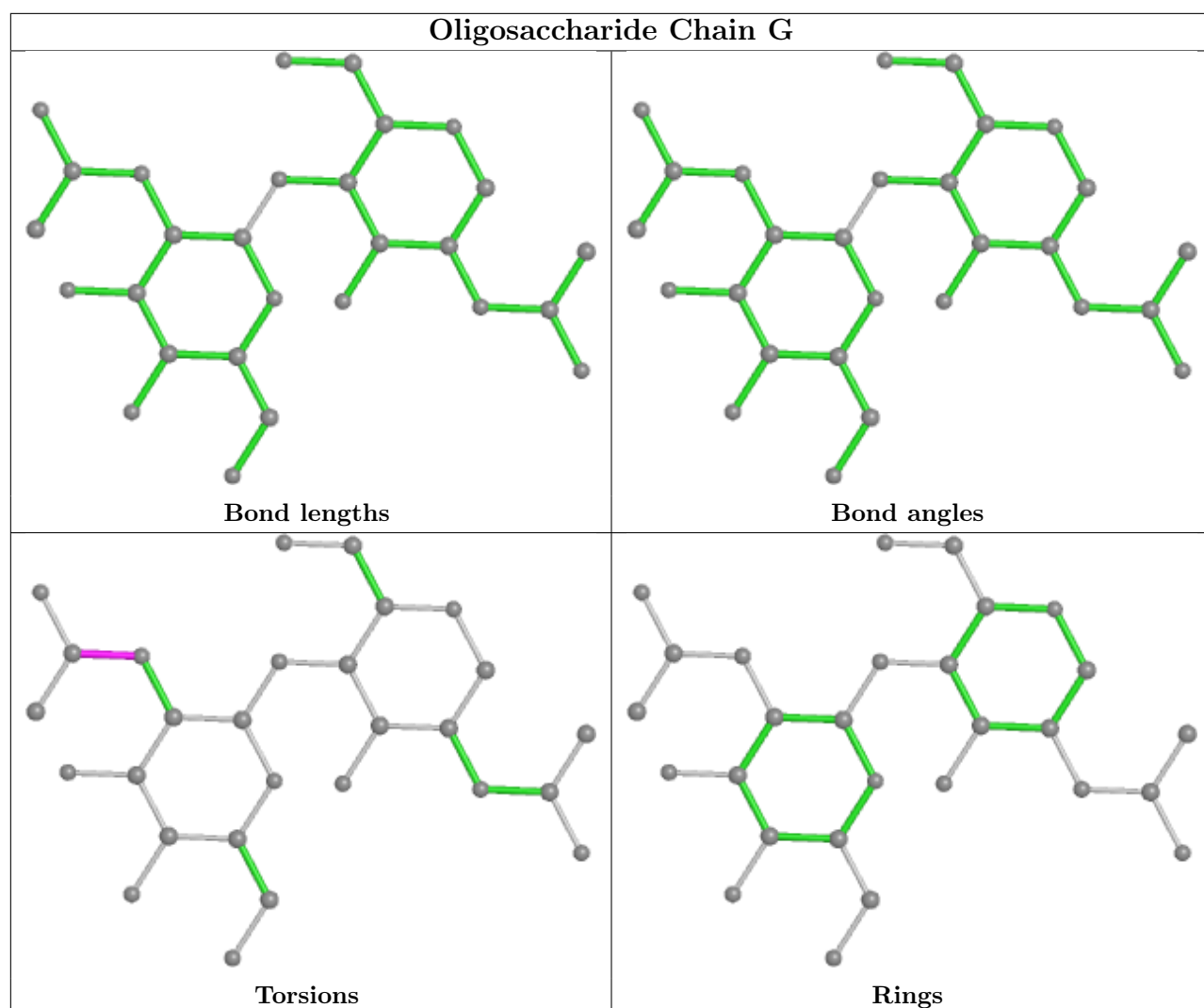
There are no ring outliers.

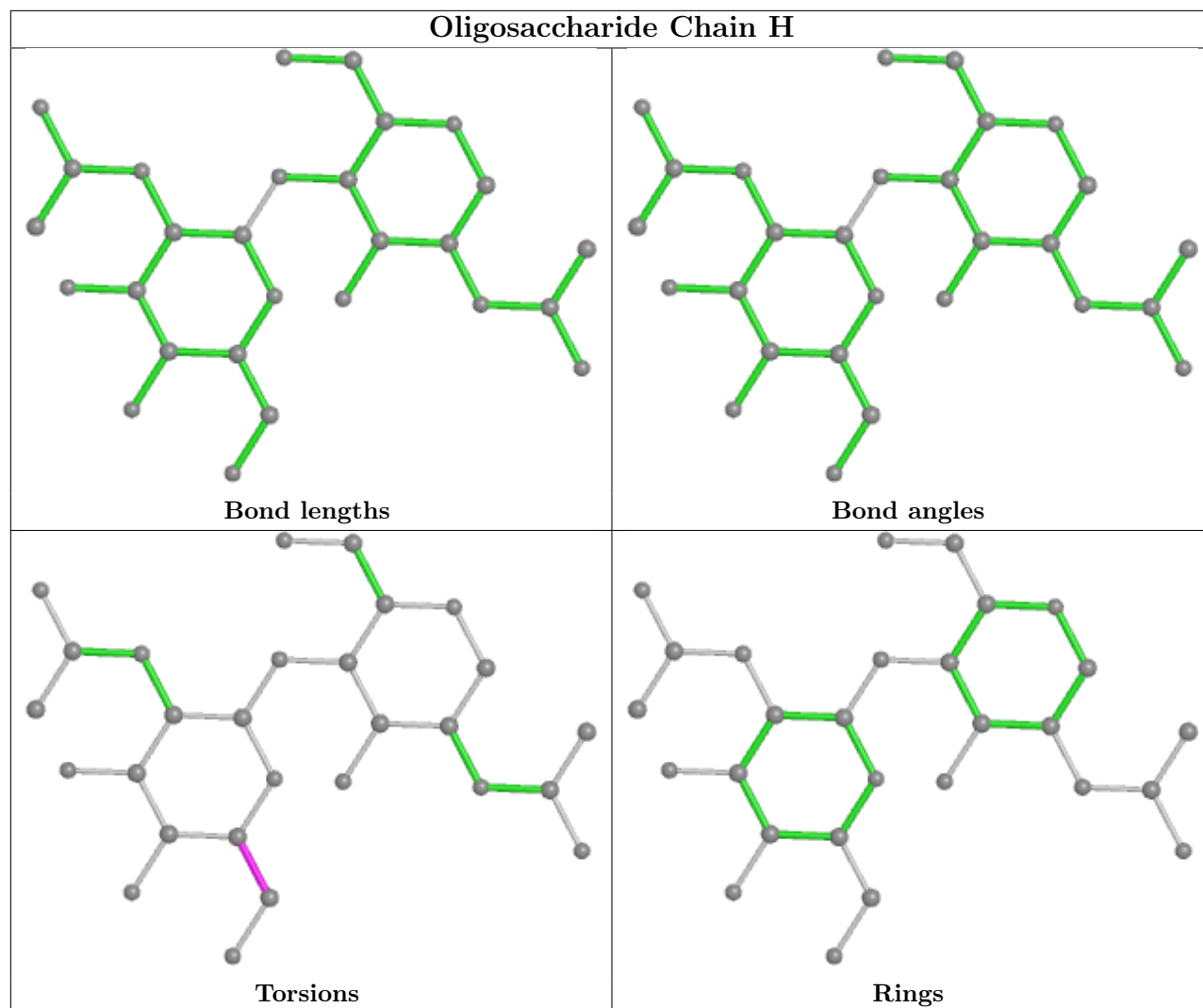
2 monomers are involved in 2 short contacts:

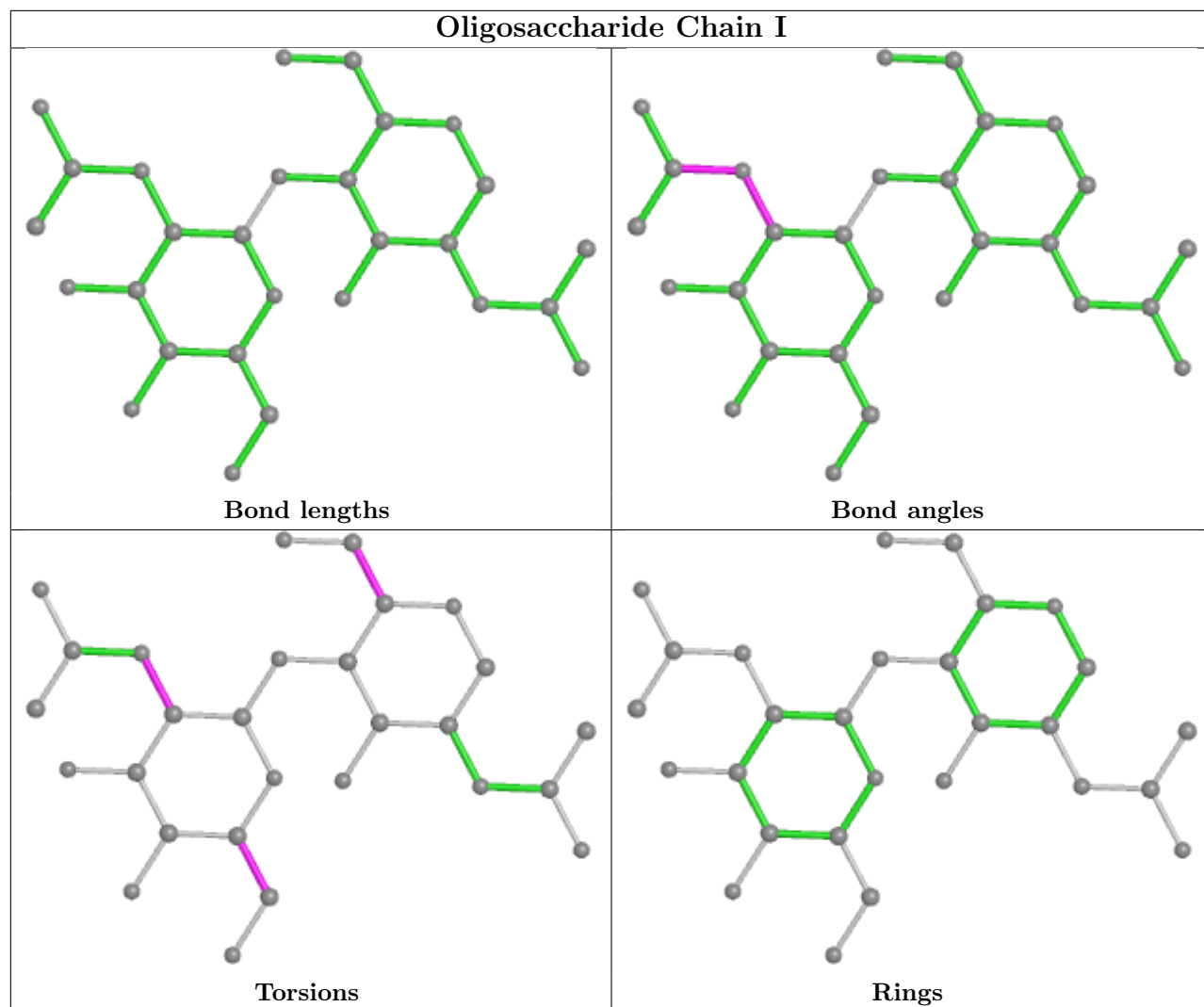
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	H	1	NAG	1	0
2	N	1	NAG	1	0

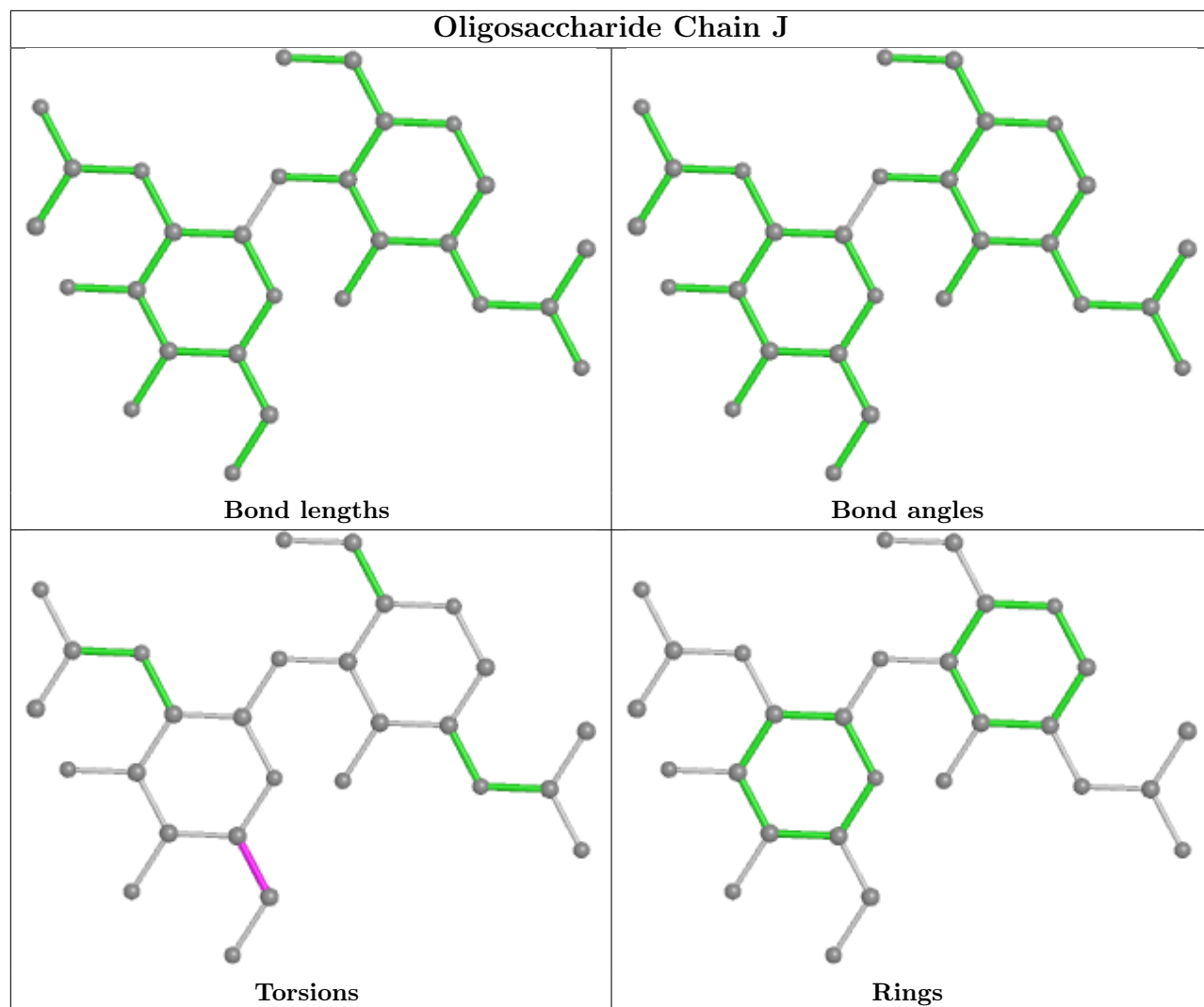
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

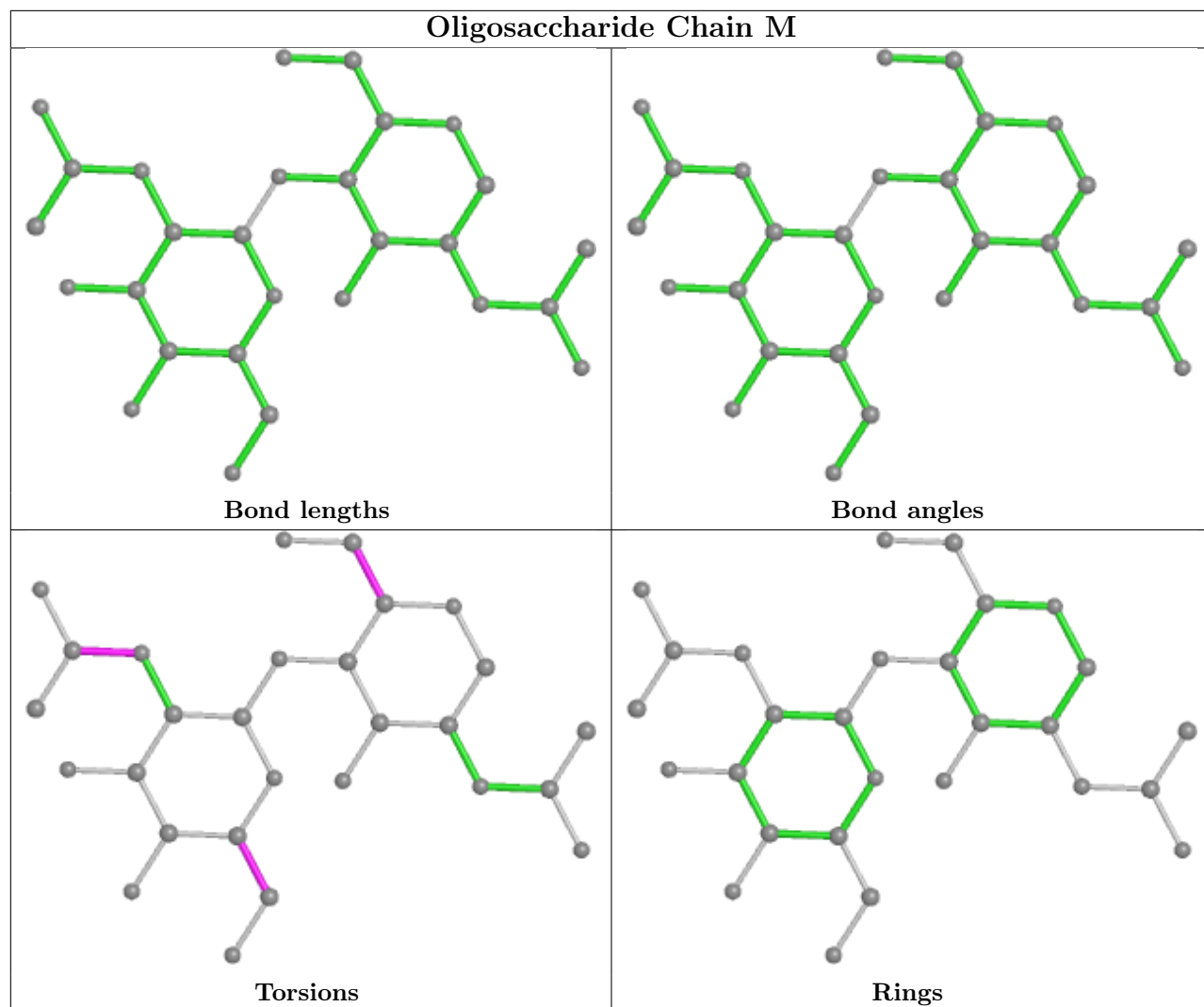


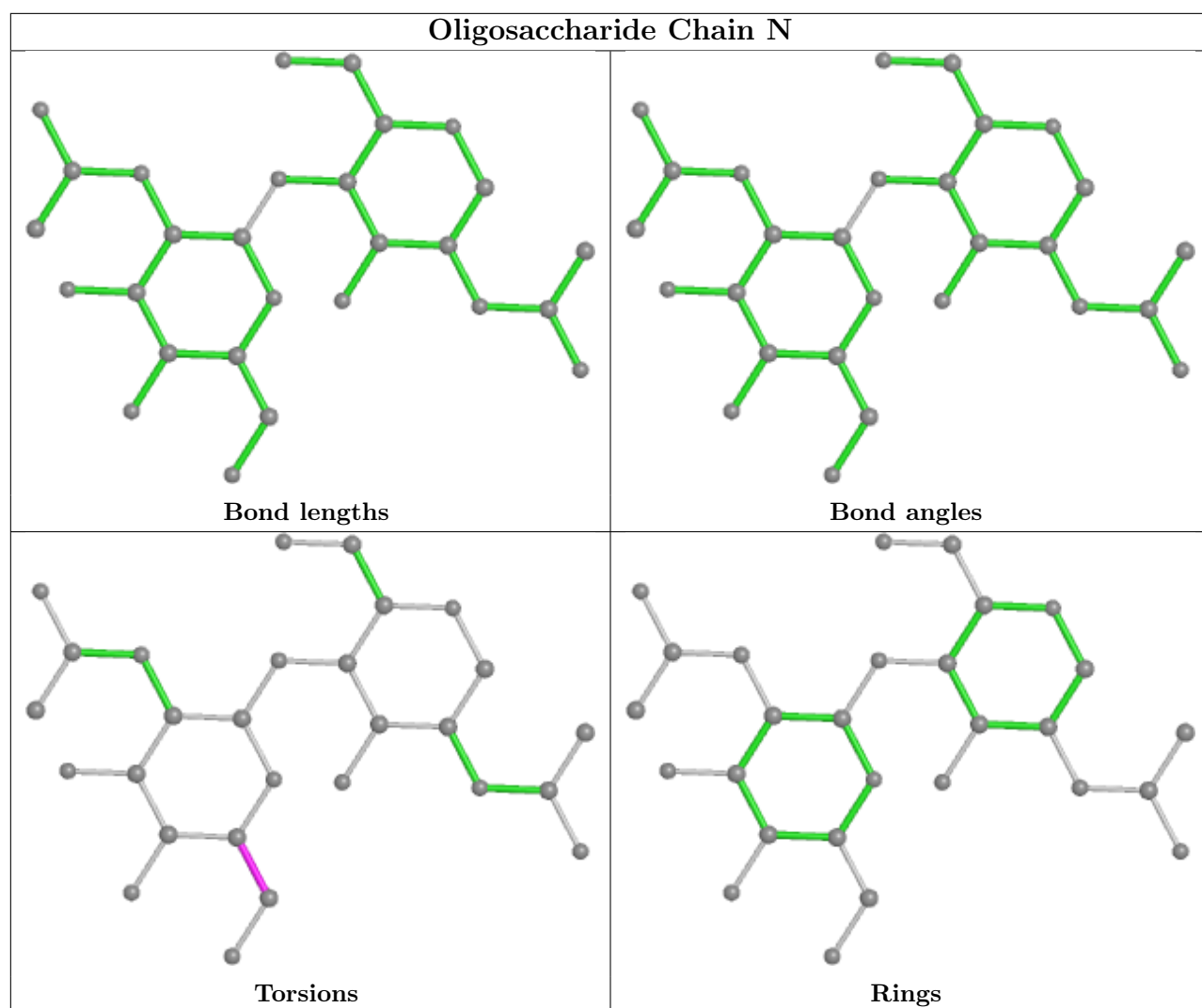


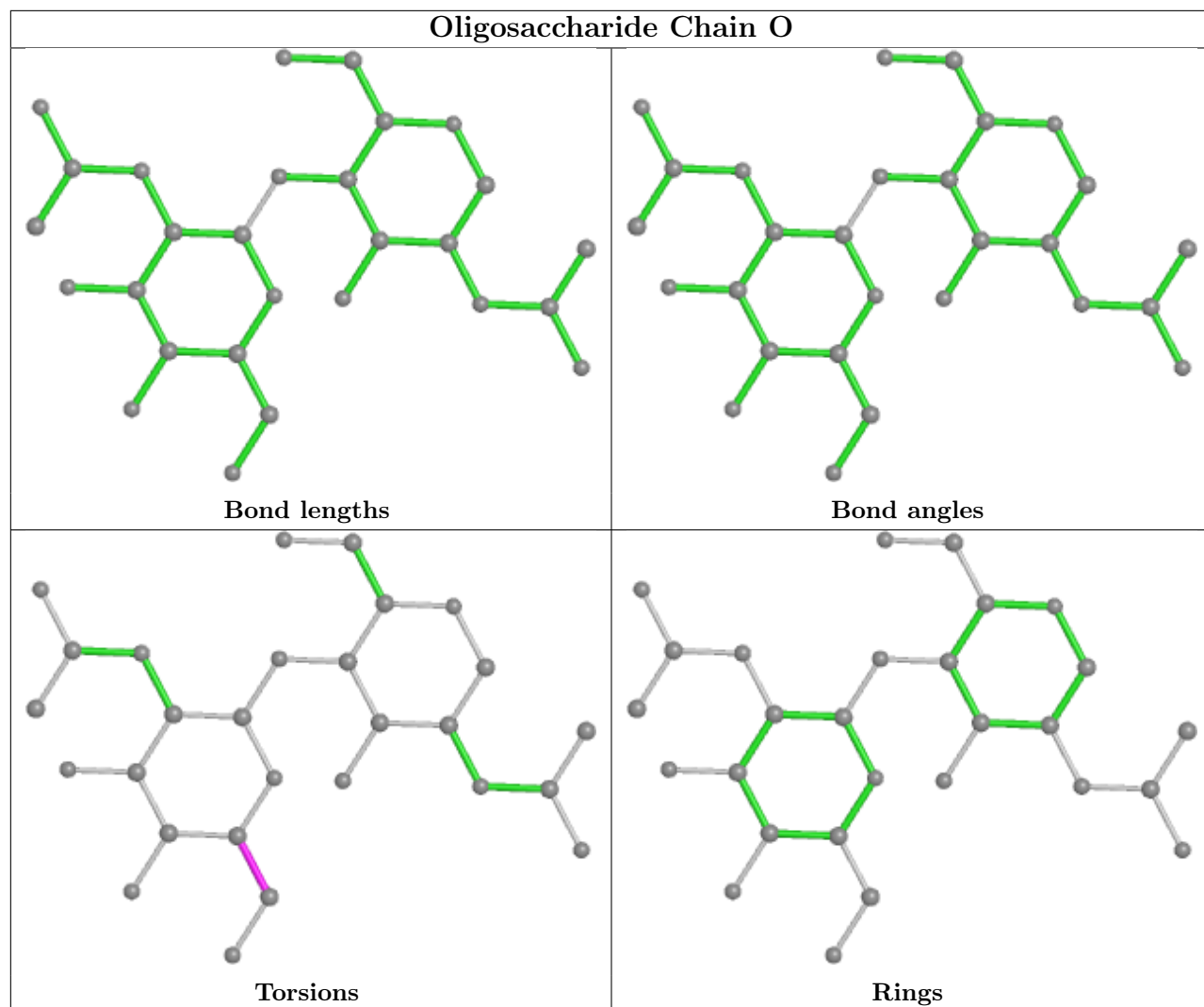


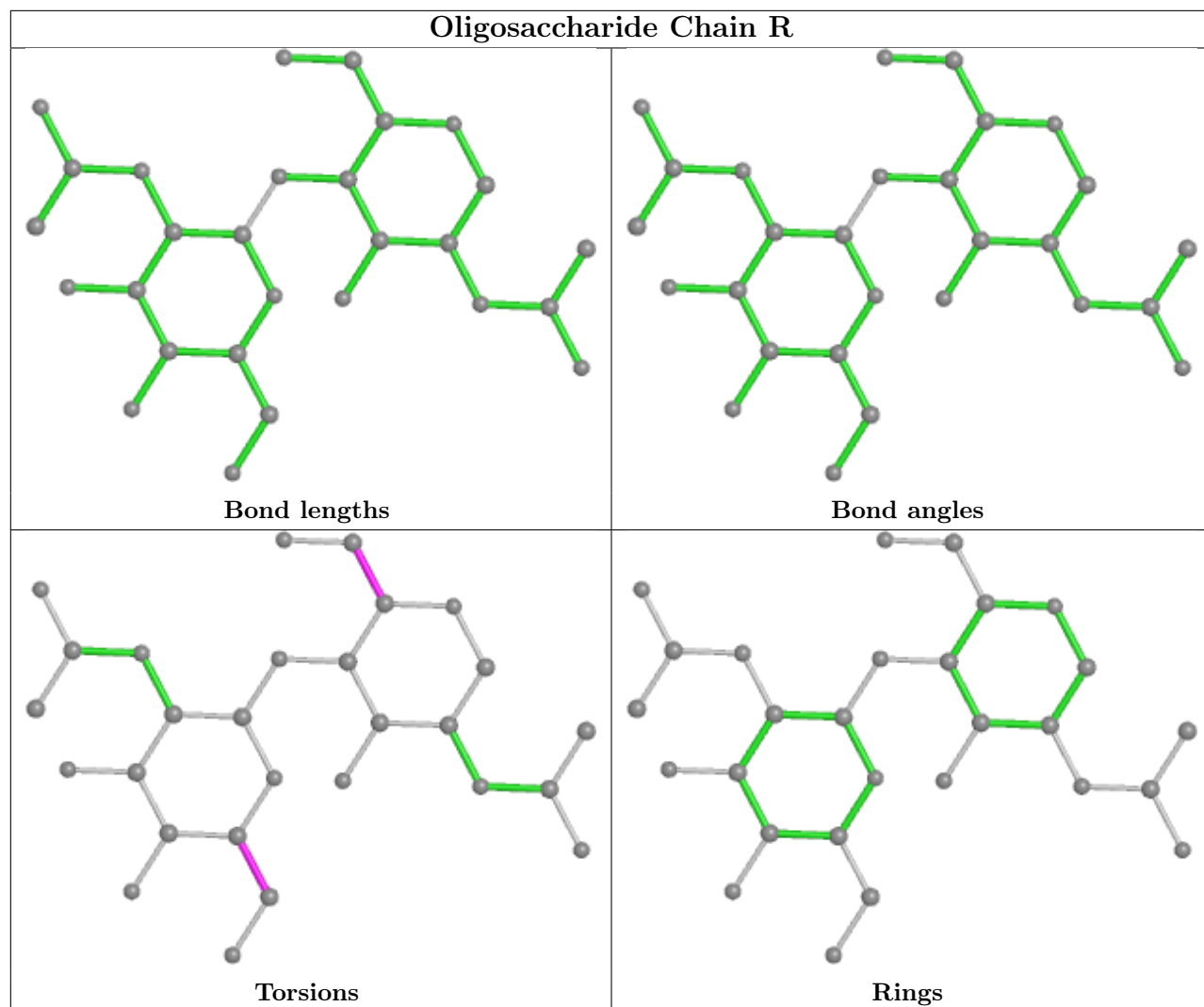


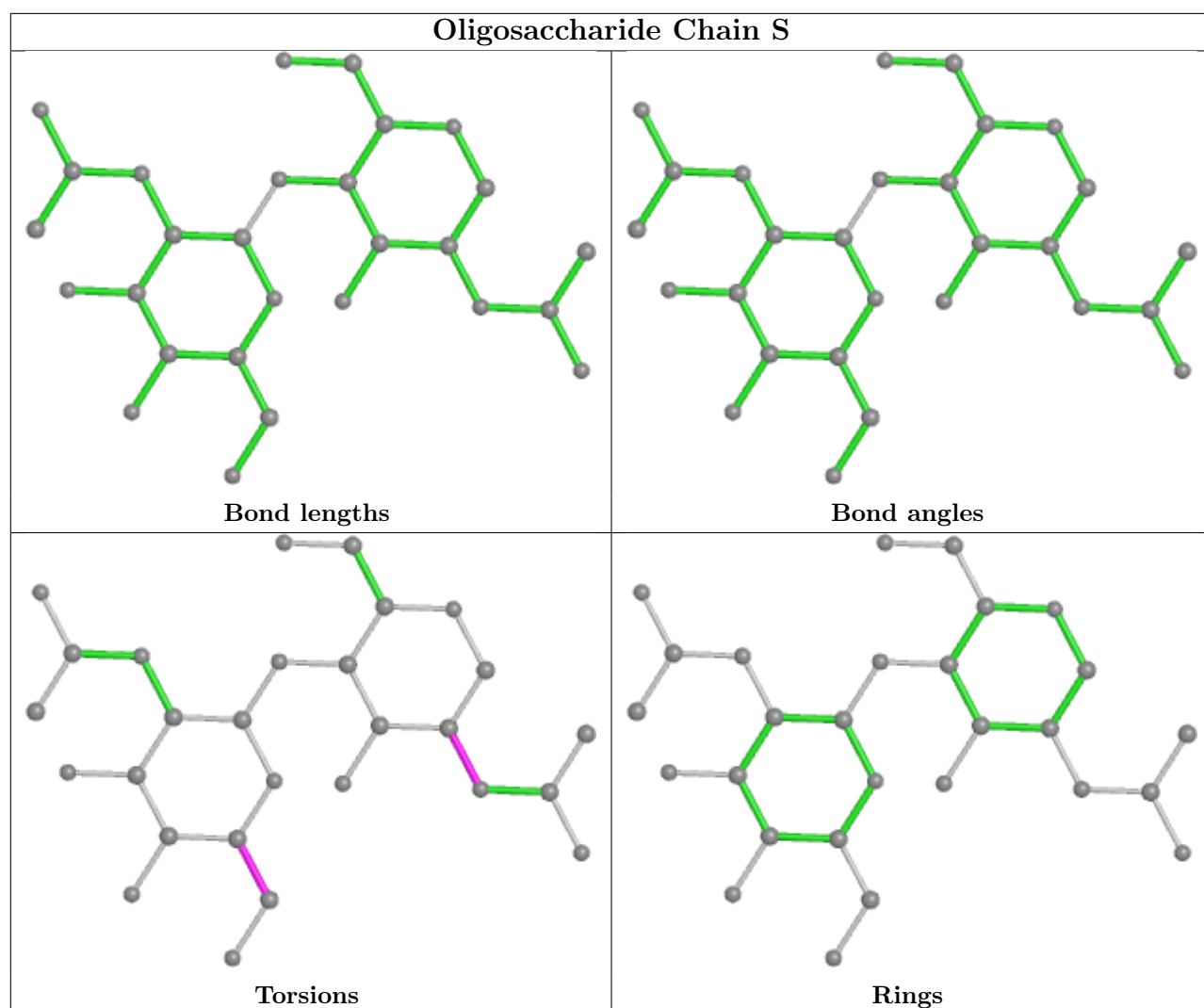


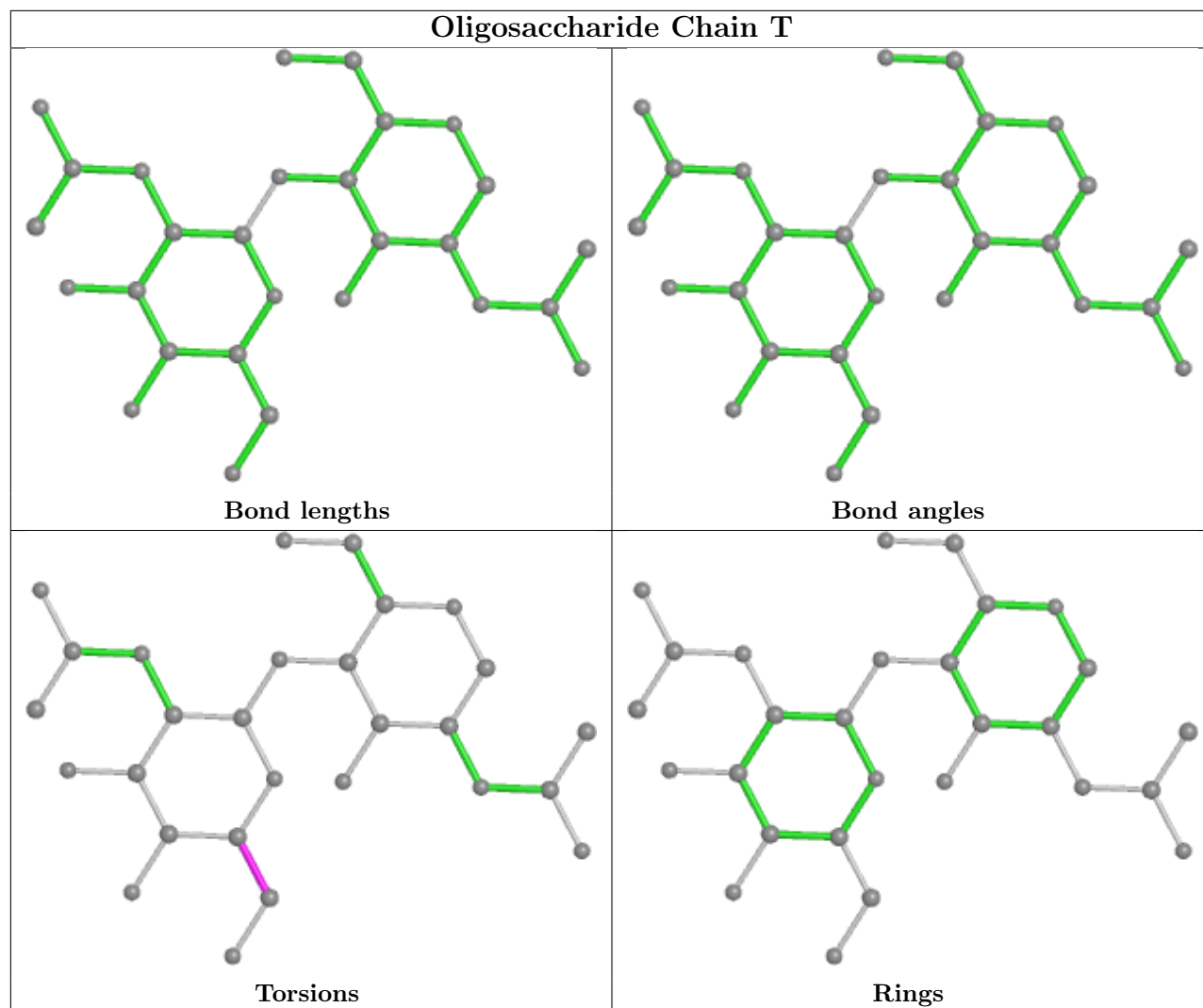


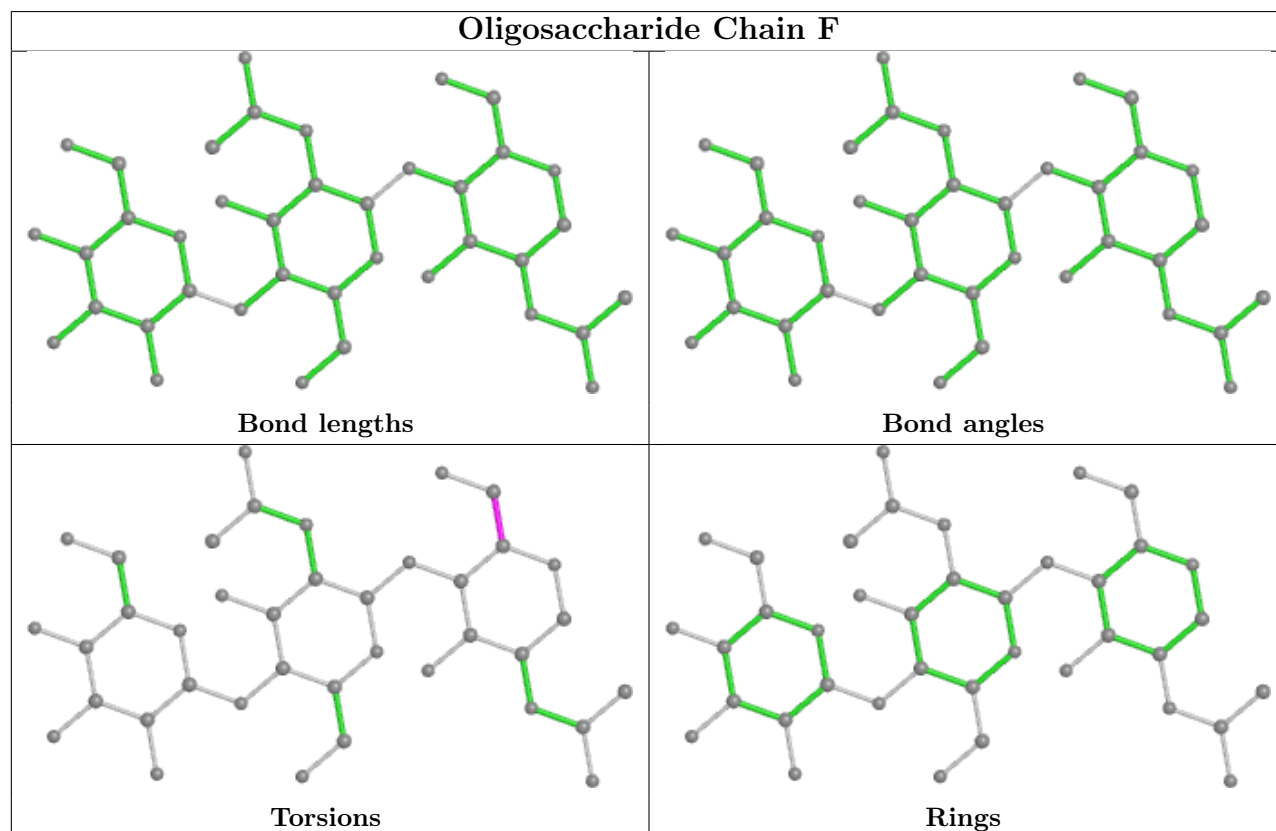
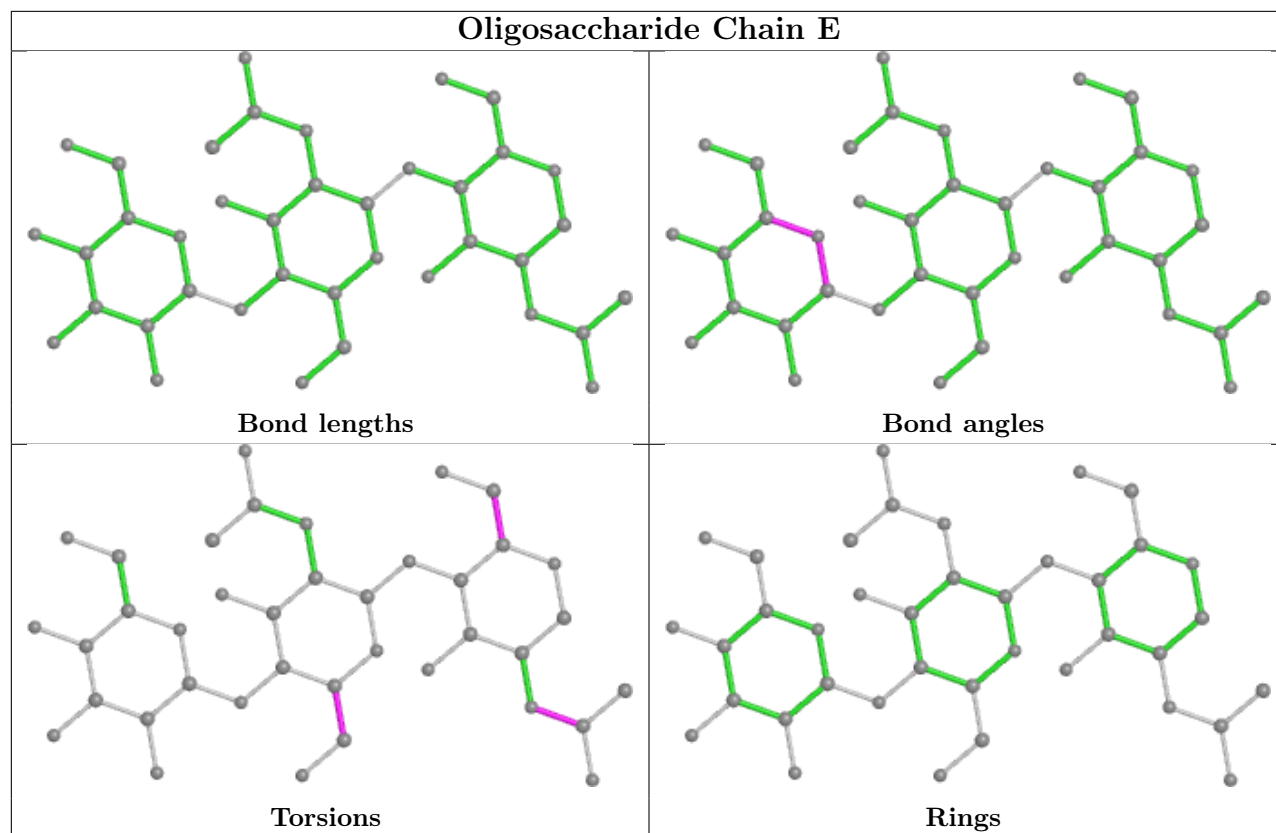


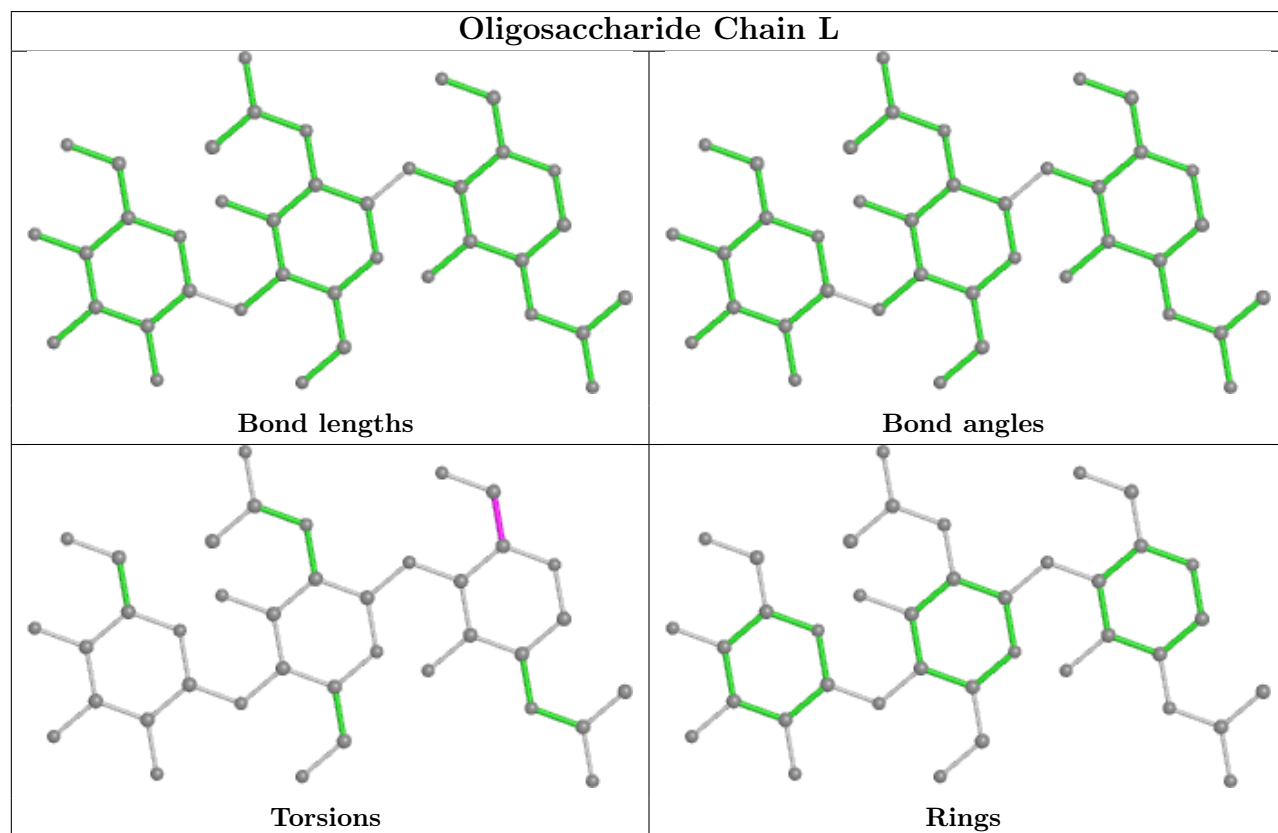
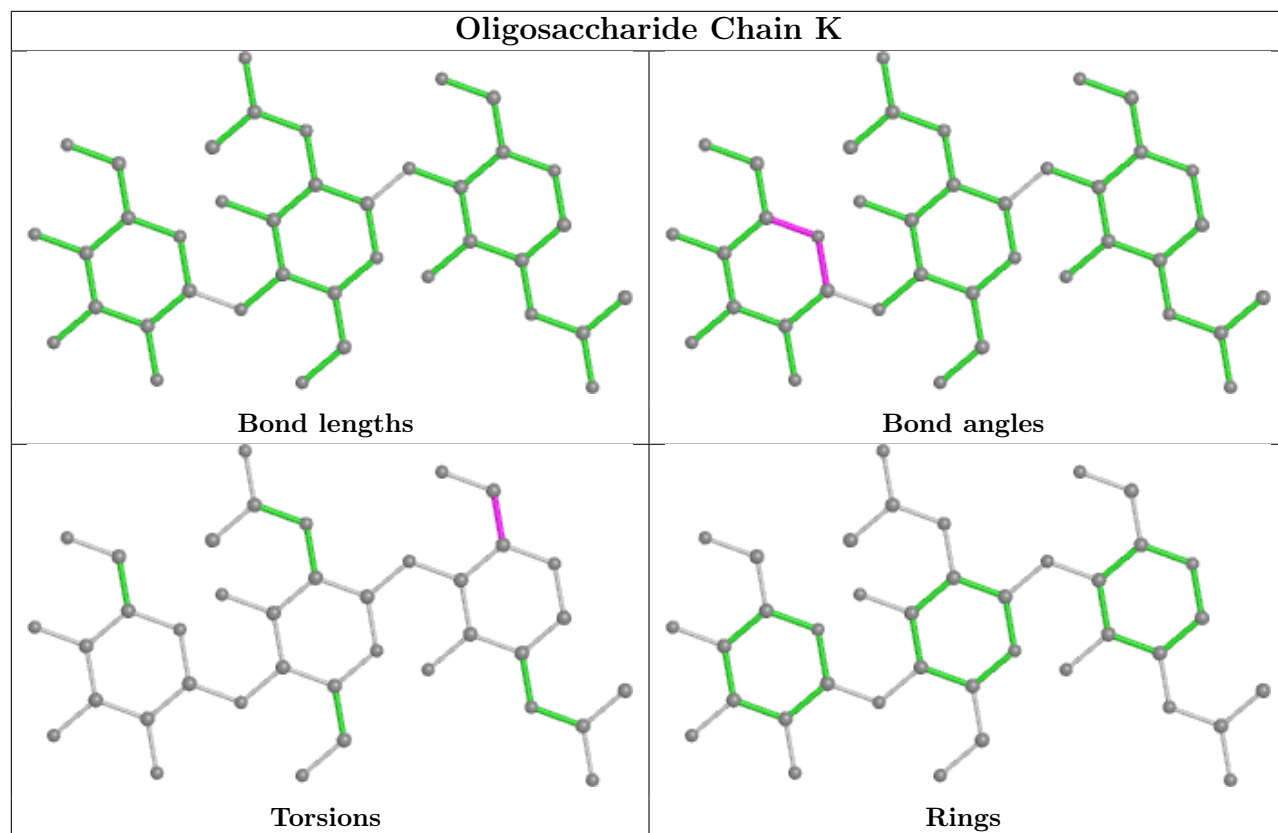


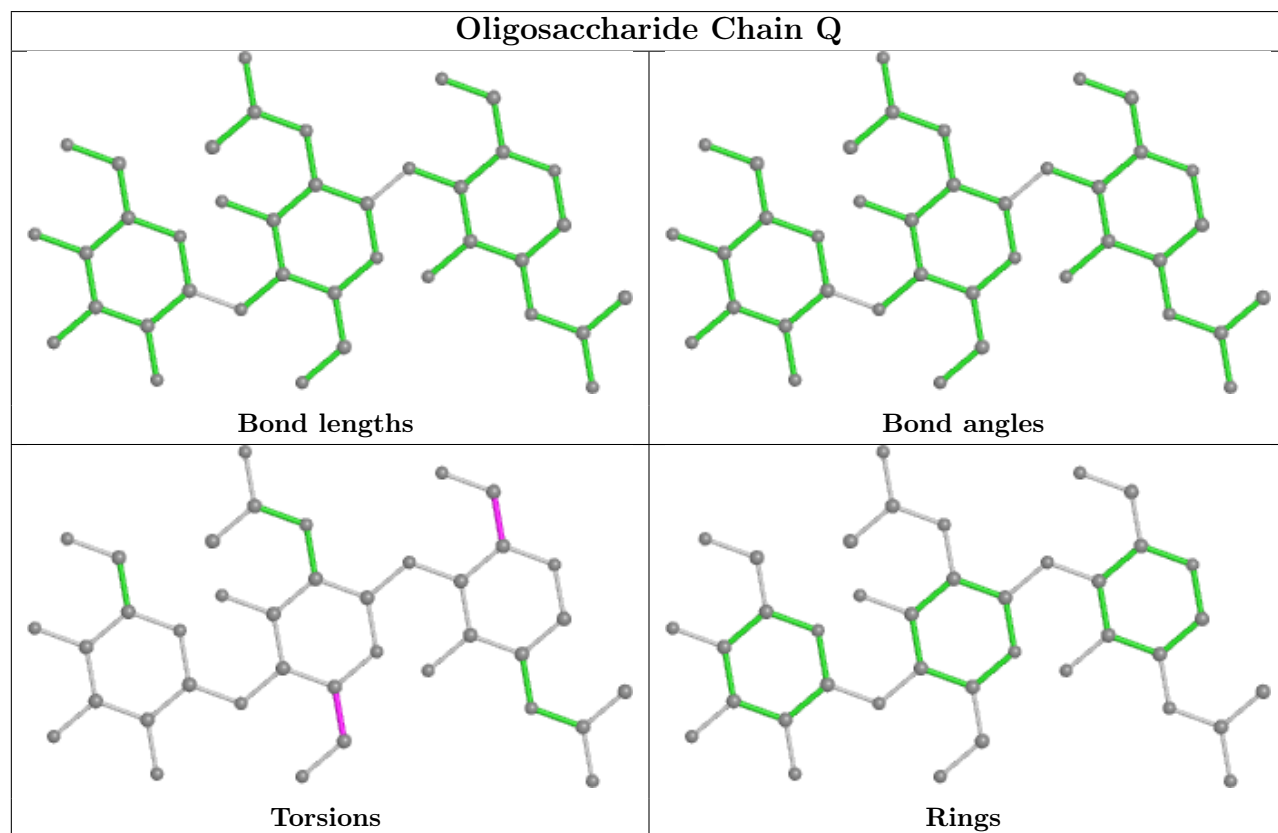
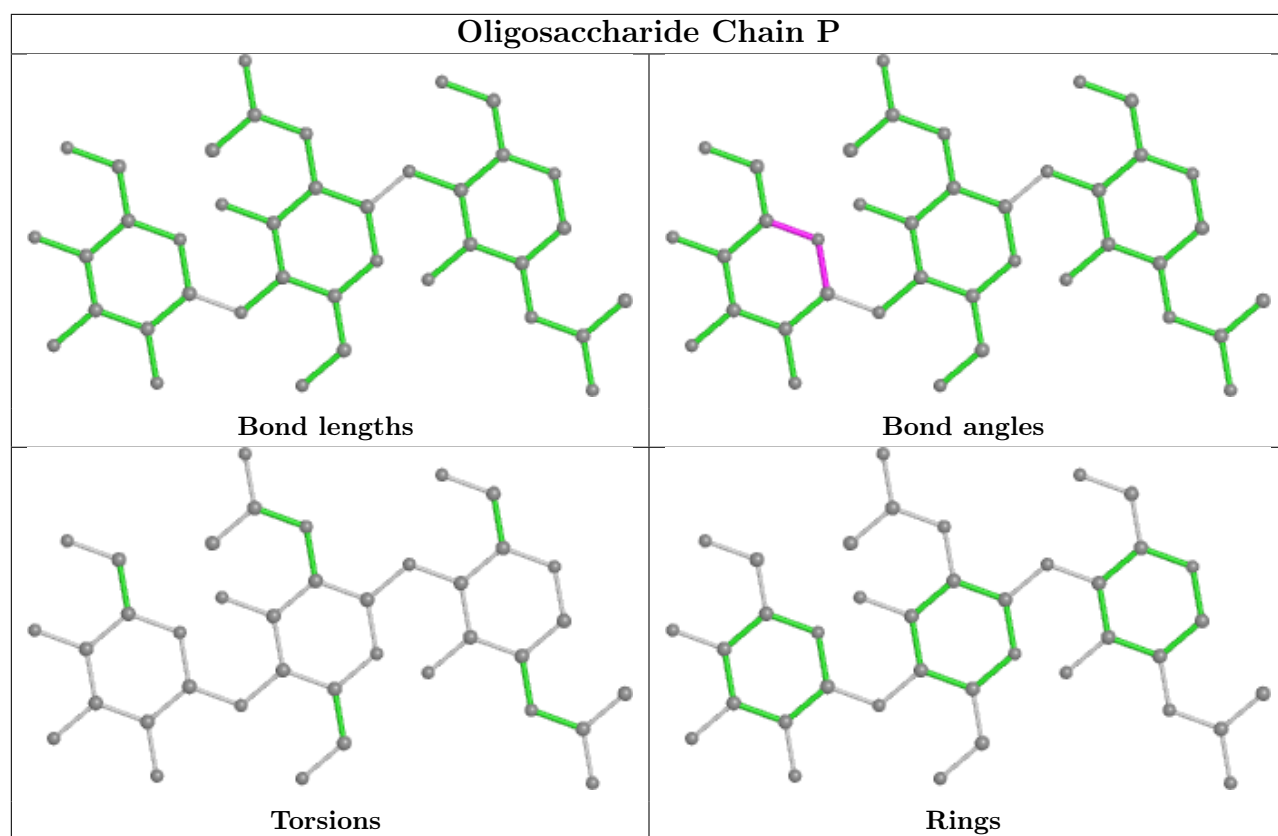












5.6 Ligand geometry

34 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	A	1409	1	14,14,15	0.23	0	17,19,21	0.41	0
4	NAG	B	1405	1	14,14,15	0.25	0	17,19,21	0.38	0
4	NAG	C	1412	1	14,14,15	0.29	0	17,19,21	0.72	0
4	NAG	C	1407	1	14,14,15	0.22	0	17,19,21	0.44	0
4	NAG	C	1405	1	14,14,15	0.21	0	17,19,21	0.44	0
4	NAG	A	1410	1	14,14,15	0.22	0	17,19,21	0.47	0
4	NAG	B	1404	1	14,14,15	0.22	0	17,19,21	0.45	0
4	NAG	B	1408	1	14,14,15	0.20	0	17,19,21	0.43	0
4	NAG	C	1404	1	14,14,15	0.26	0	17,19,21	0.42	0
4	NAG	B	1410	1	14,14,15	0.27	0	17,19,21	0.72	0
4	NAG	C	1411	1	14,14,15	0.23	0	17,19,21	0.42	0
5	EIC	B	1411	-	19,19,19	0.59	0	19,19,19	0.60	0
4	NAG	C	1410	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	B	1401	1	14,14,15	0.26	0	17,19,21	0.43	0
4	NAG	C	1409	1	14,14,15	0.21	0	17,19,21	0.46	0
4	NAG	C	1406	1	14,14,15	0.24	0	17,19,21	0.44	0
4	NAG	A	1406	1	14,14,15	0.22	0	17,19,21	0.41	0
4	NAG	C	1408	1	14,14,15	0.20	0	17,19,21	0.46	0
4	NAG	B	1406	1	14,14,15	0.24	0	17,19,21	0.46	0
4	NAG	A	1405	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	A	1407	1	14,14,15	0.22	0	17,19,21	0.43	0
4	NAG	B	1407	1	14,14,15	0.23	0	17,19,21	0.45	0
4	NAG	A	1403	1	14,14,15	0.19	0	17,19,21	0.43	0
4	NAG	A	1404	1	14,14,15	0.21	0	17,19,21	0.45	0
4	NAG	B	1403	1	14,14,15	0.25	0	17,19,21	0.44	0
4	NAG	A	1402	1	14,14,15	0.36	0	17,19,21	0.66	0
4	NAG	B	1402	1	14,14,15	0.19	0	17,19,21	0.44	0
4	NAG	C	1402	1	14,14,15	0.24	0	17,19,21	0.50	0
4	NAG	B	1409	1	14,14,15	0.22	0	17,19,21	0.42	0
5	EIC	C	1401	-	19,19,19	0.58	0	19,19,19	0.57	0
5	EIC	A	1411	-	19,19,19	0.59	0	19,19,19	0.57	0
4	NAG	A	1401	1	14,14,15	0.21	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	1403	1	14,14,15	0.22	0	17,19,21	0.42	0
4	NAG	A	1408	1	14,14,15	0.23	0	17,19,21	0.45	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1405	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1412	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1404	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1410	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1411	1	-	2/6/23/26	0/1/1/1
5	EIC	B	1411	-	-	6/17/17/17	-
4	NAG	C	1410	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1401	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1409	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1408	1	-	4/6/23/26	0/1/1/1
4	NAG	B	1406	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1405	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1407	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1407	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1404	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1403	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1402	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1402	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1409	1	-	2/6/23/26	0/1/1/1
5	EIC	C	1401	-	-	5/17/17/17	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EIC	A	1411	-	-	5/17/17/17	-
4	NAG	A	1401	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1403	1	-	1/6/23/26	0/1/1/1
4	NAG	A	1408	1	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	1406	NAG	C4-C5-C6-O6
4	A	1406	NAG	O5-C5-C6-O6
4	B	1406	NAG	O5-C5-C6-O6
4	C	1406	NAG	O5-C5-C6-O6
4	C	1404	NAG	C4-C5-C6-O6
4	C	1411	NAG	C4-C5-C6-O6
4	A	1409	NAG	O5-C5-C6-O6
4	C	1411	NAG	O5-C5-C6-O6
4	C	1404	NAG	O5-C5-C6-O6
4	B	1406	NAG	C4-C5-C6-O6
4	A	1406	NAG	C4-C5-C6-O6
4	B	1409	NAG	C4-C5-C6-O6
4	B	1405	NAG	C4-C5-C6-O6
4	A	1401	NAG	C4-C5-C6-O6
4	B	1408	NAG	C8-C7-N2-C2
4	B	1408	NAG	O7-C7-N2-C2
4	C	1408	NAG	C8-C7-N2-C2
4	C	1408	NAG	O7-C7-N2-C2
4	B	1409	NAG	O5-C5-C6-O6
4	B	1408	NAG	O5-C5-C6-O6
4	B	1405	NAG	O5-C5-C6-O6
4	B	1408	NAG	C4-C5-C6-O6
4	C	1408	NAG	O5-C5-C6-O6
4	C	1408	NAG	C4-C5-C6-O6
4	A	1401	NAG	O5-C5-C6-O6
4	C	1409	NAG	O5-C5-C6-O6
5	A	1411	EIC	C3-C4-C5-C6
5	C	1401	EIC	C3-C4-C5-C6
4	C	1409	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	B	1411	EIC	C2-C3-C4-C5
4	A	1408	NAG	O5-C5-C6-O6
5	B	1411	EIC	C4-C5-C6-C7
5	A	1411	EIC	C10-C11-C12-C13
5	B	1411	EIC	C10-C11-C12-C13
4	A	1409	NAG	C4-C5-C6-O6
5	C	1401	EIC	C13-C14-C15-C16
4	B	1404	NAG	C4-C5-C6-O6
4	A	1402	NAG	C3-C2-N2-C7
4	B	1410	NAG	C3-C2-N2-C7
4	C	1412	NAG	C3-C2-N2-C7
5	A	1411	EIC	C1-C2-C3-C4
5	B	1411	EIC	O2-C1-C2-C3
4	C	1403	NAG	C4-C5-C6-O6
4	B	1404	NAG	O5-C5-C6-O6
5	A	1411	EIC	C7-C8-C9-C10
5	B	1411	EIC	O1-C1-C2-C3
5	C	1401	EIC	C14-C15-C16-C17
5	C	1401	EIC	C10-C11-C12-C13
5	C	1401	EIC	C7-C8-C9-C10
5	A	1411	EIC	C6-C7-C8-C9
4	A	1407	NAG	O5-C5-C6-O6
5	B	1411	EIC	C3-C4-C5-C6

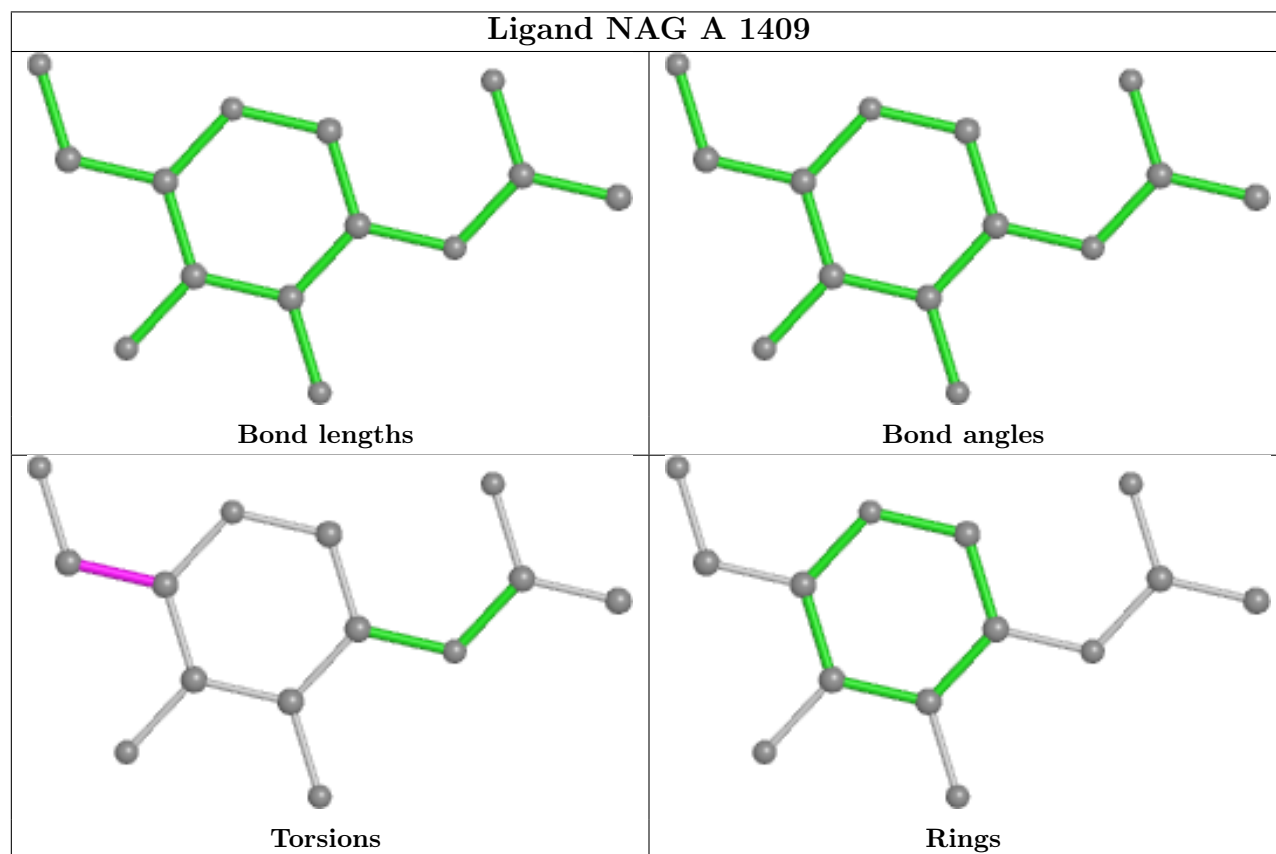
There are no ring outliers.

5 monomers are involved in 5 short contacts:

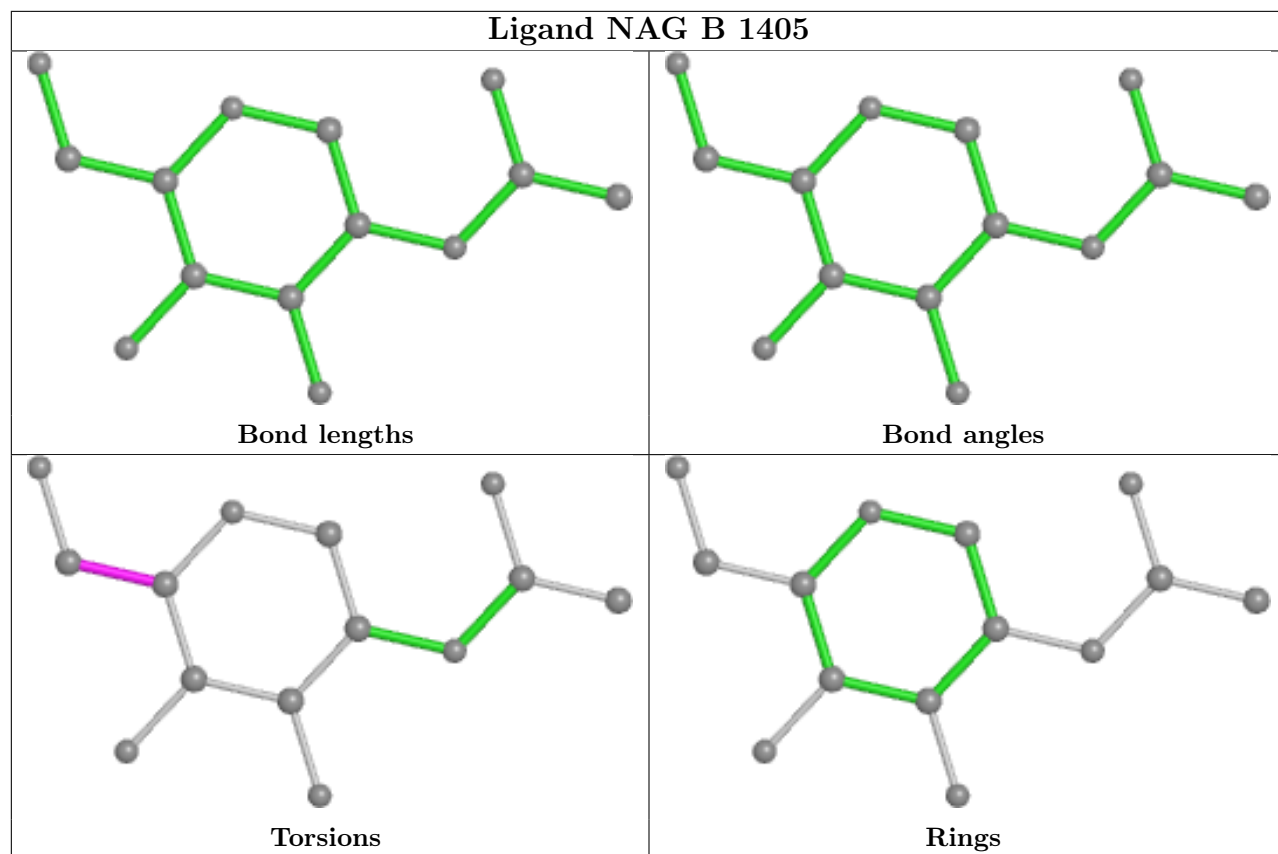
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1411	EIC	1	0
4	C	1406	NAG	1	0
5	C	1401	EIC	1	0
5	A	1411	EIC	1	0
4	A	1401	NAG	1	0

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

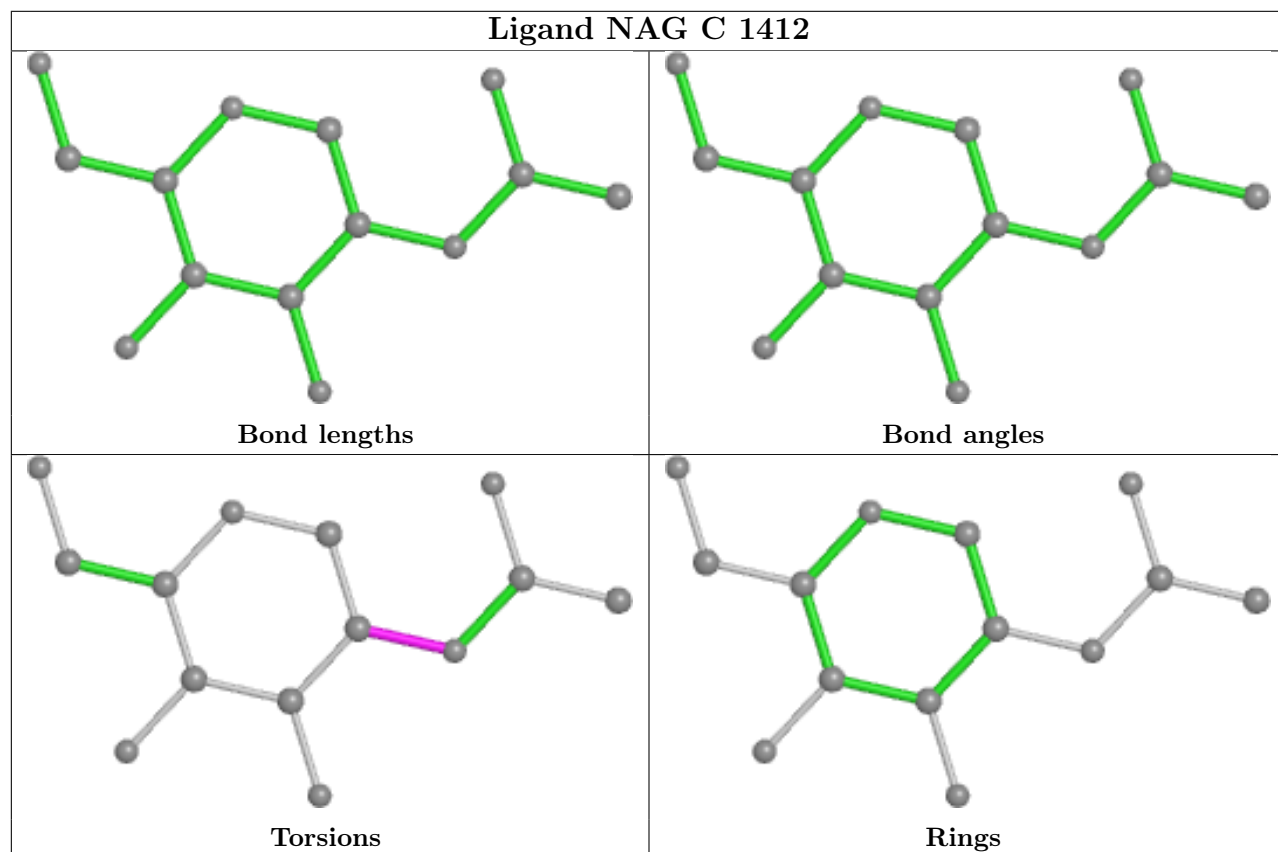
average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



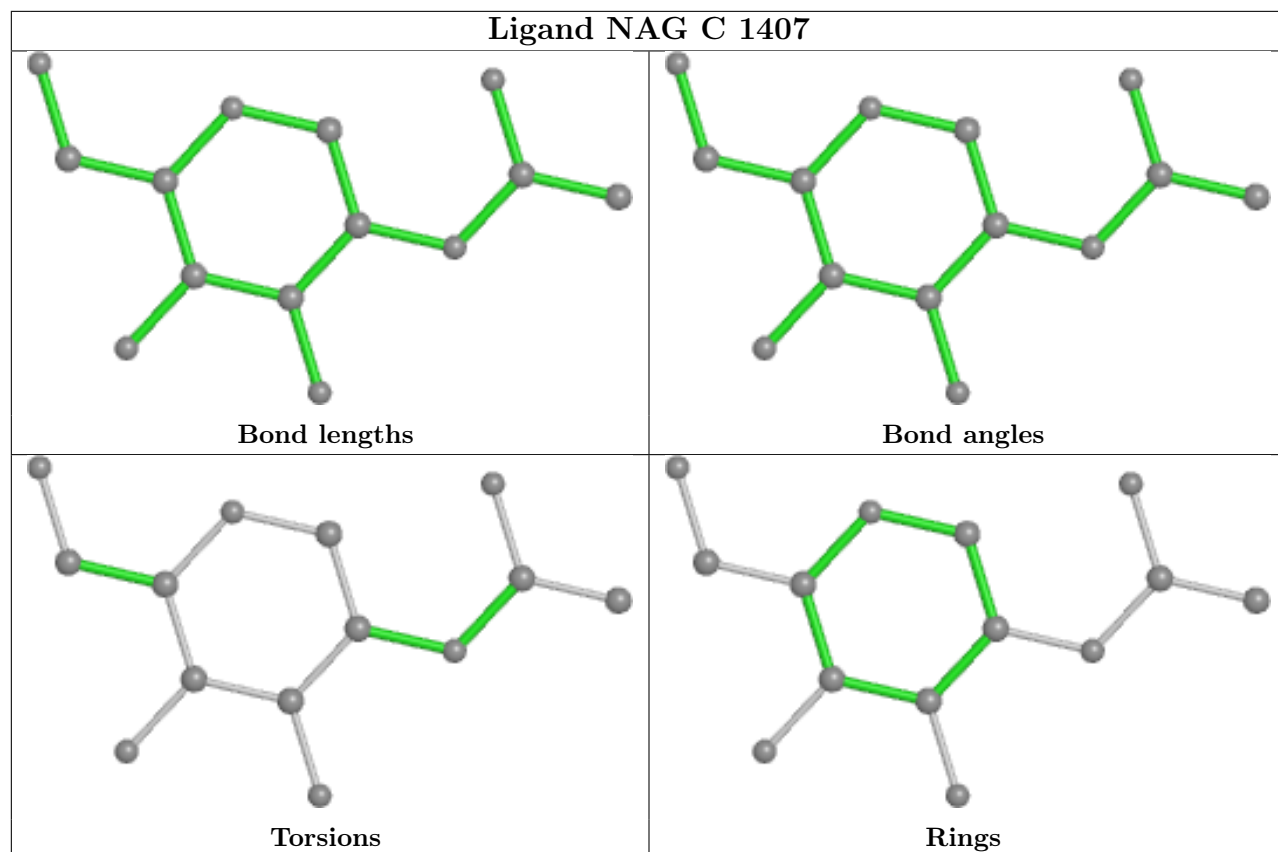
Ligand NAG B 1405



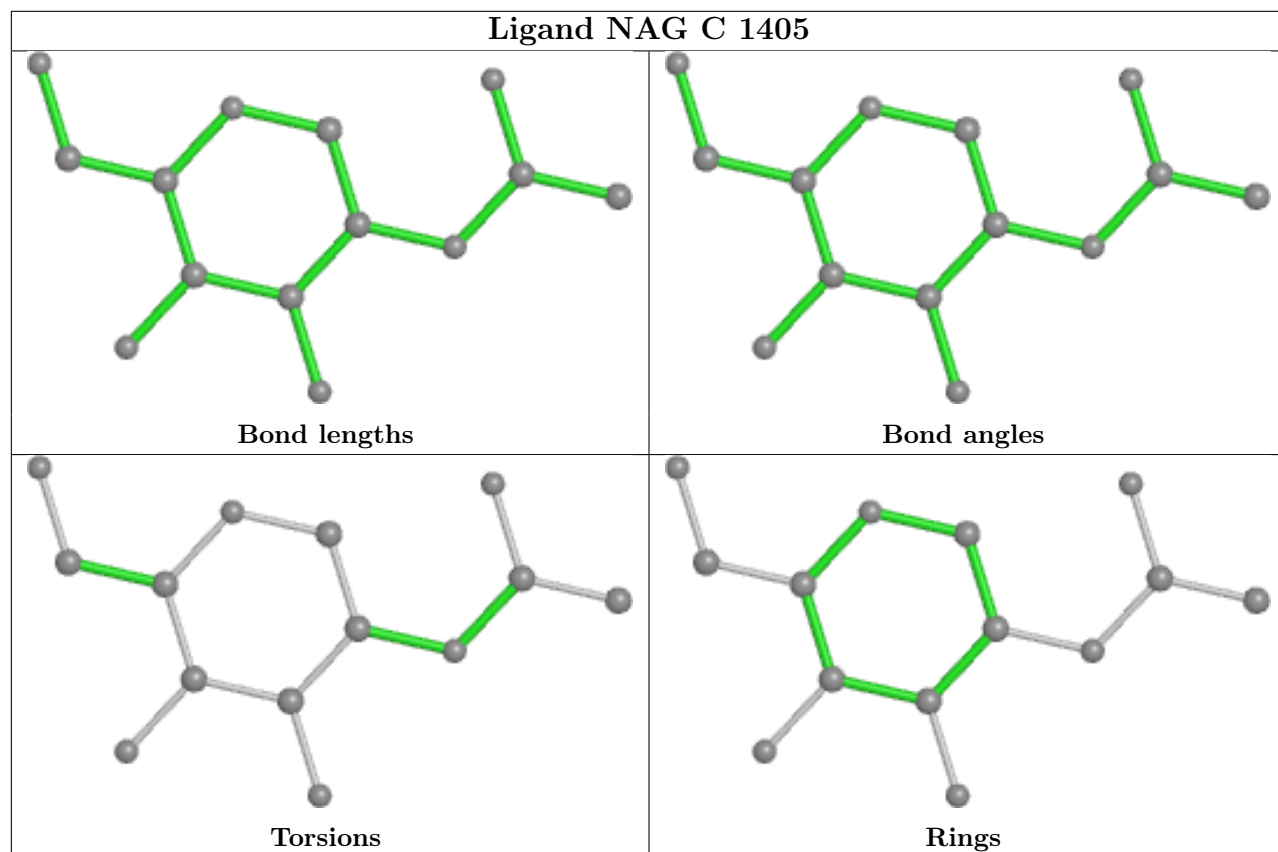
Ligand NAG C 1412



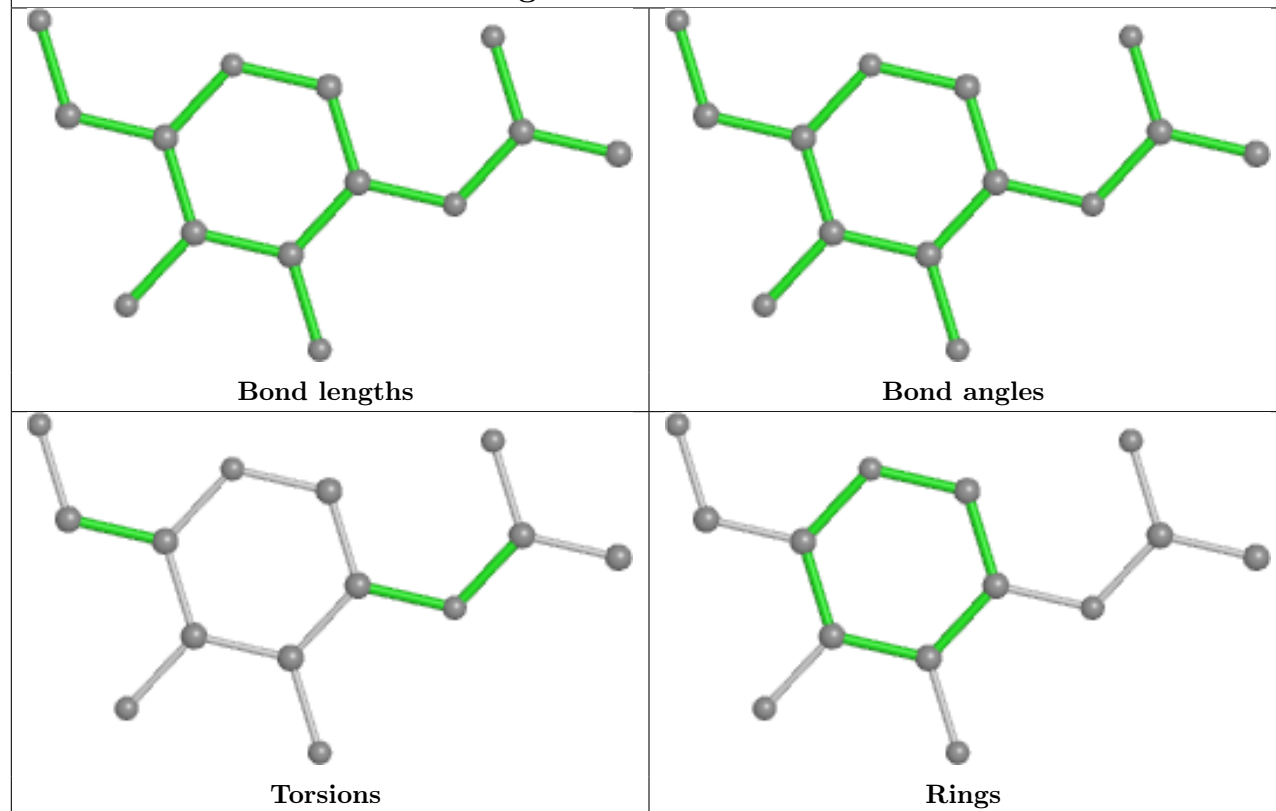
Ligand NAG C 1407



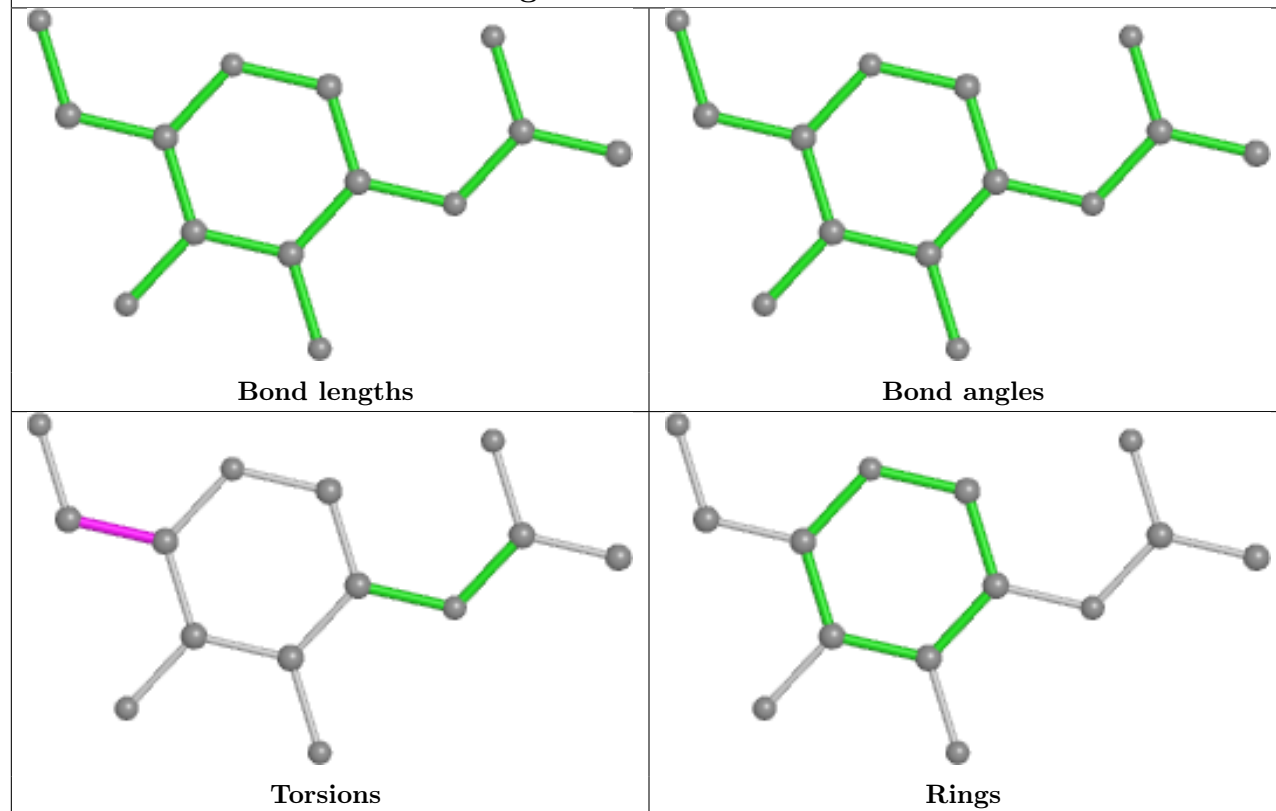
Ligand NAG C 1405



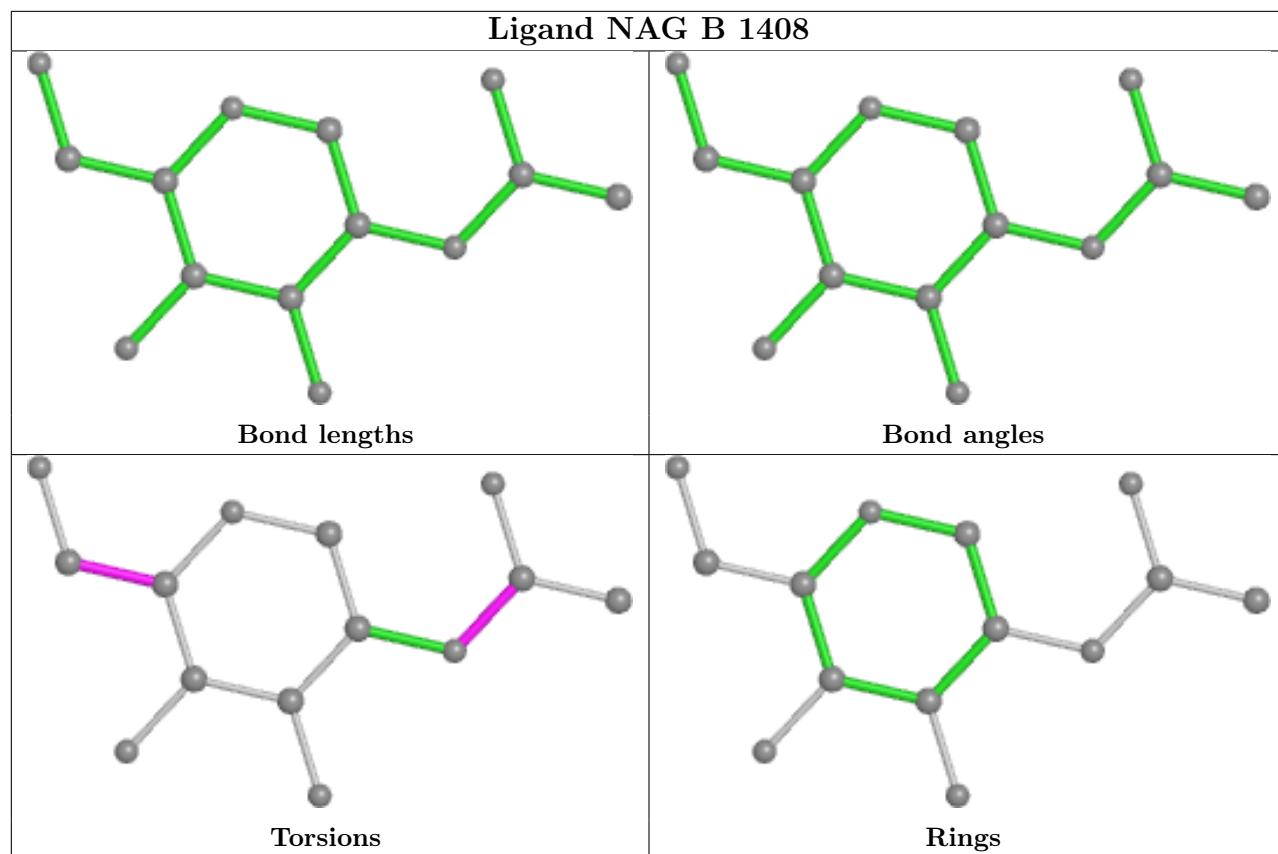
Ligand NAG A 1410



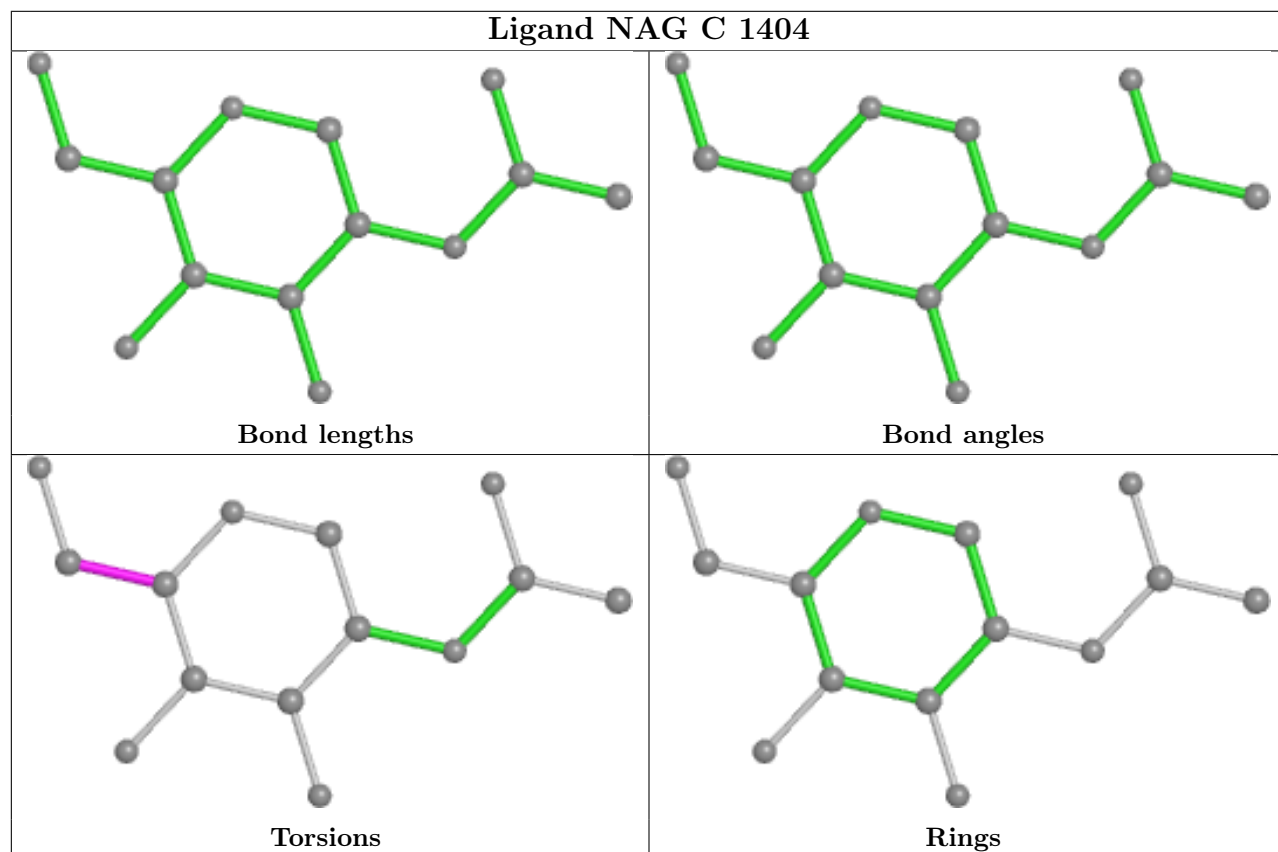
Ligand NAG B 1404

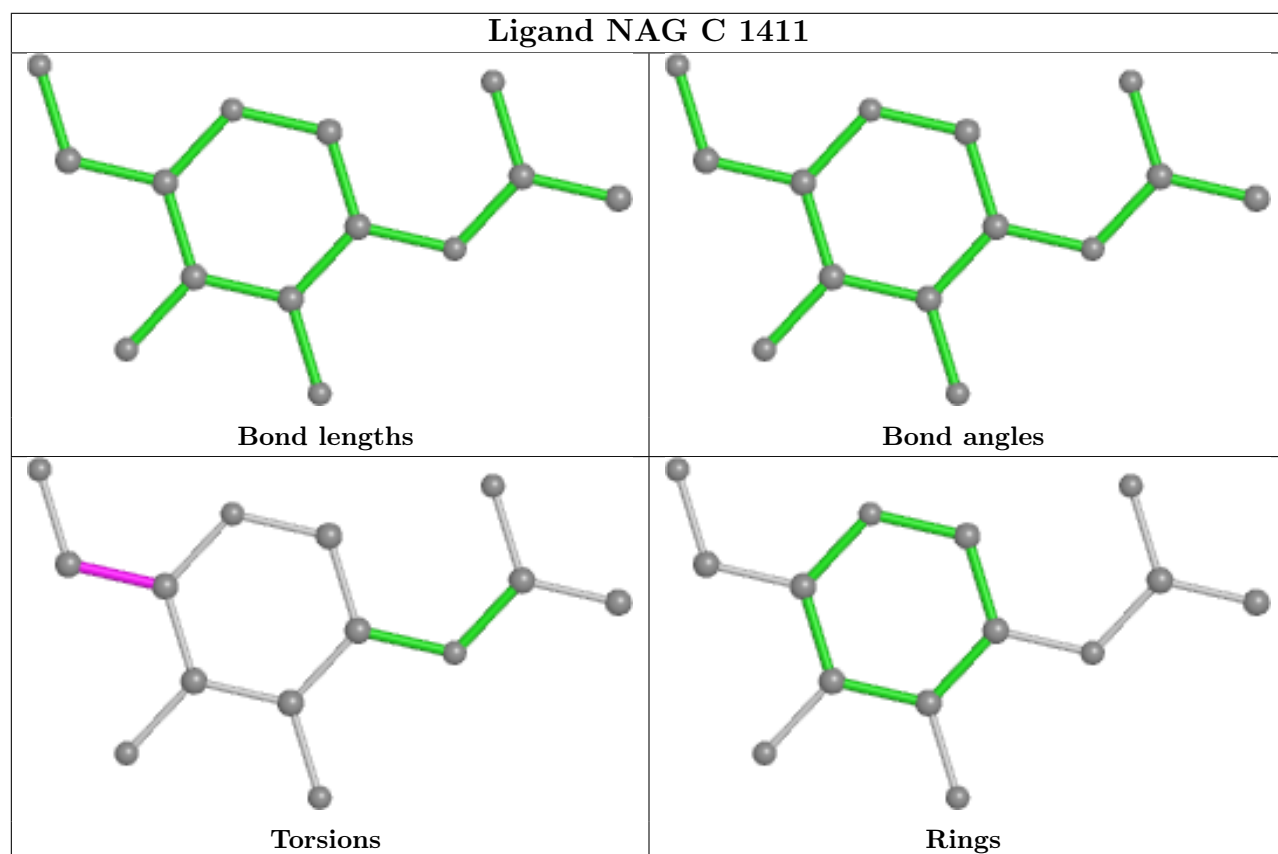
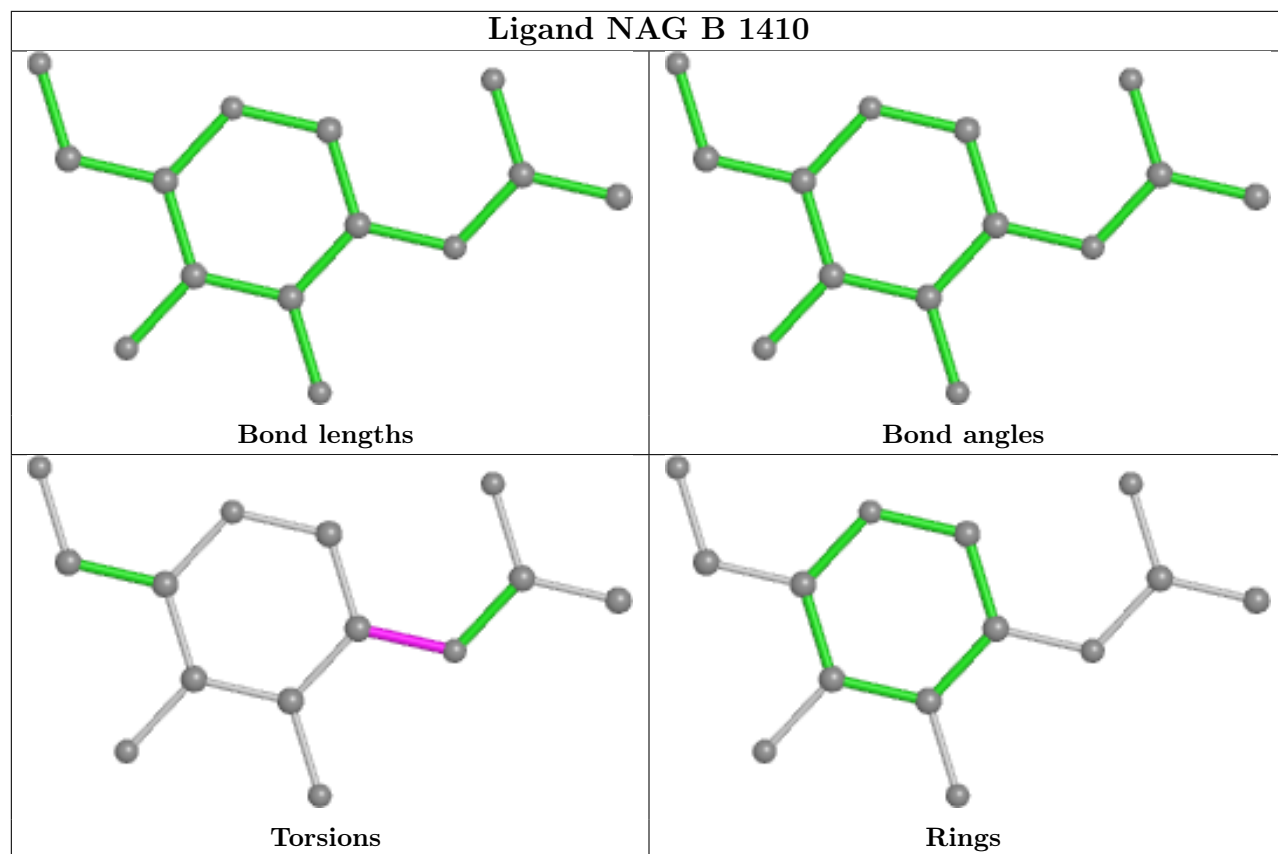


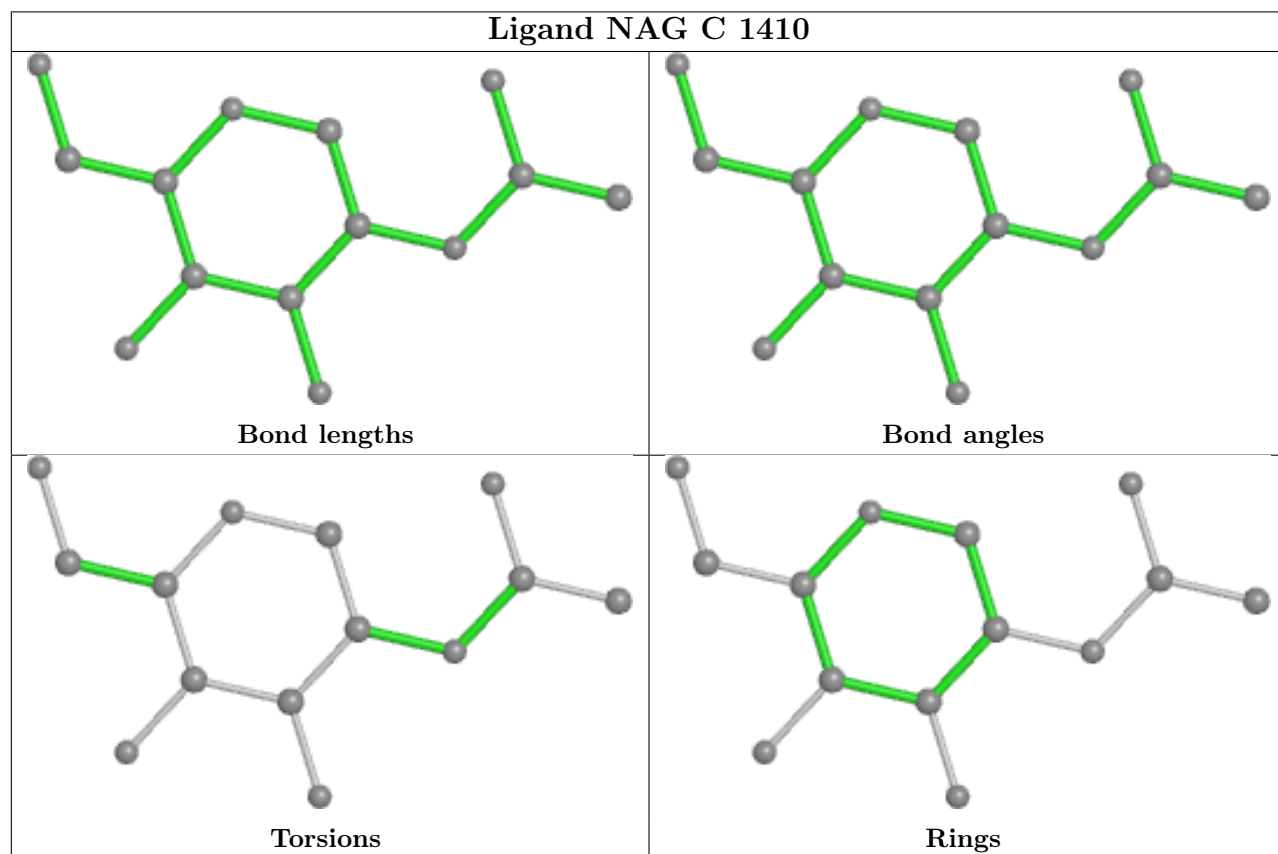
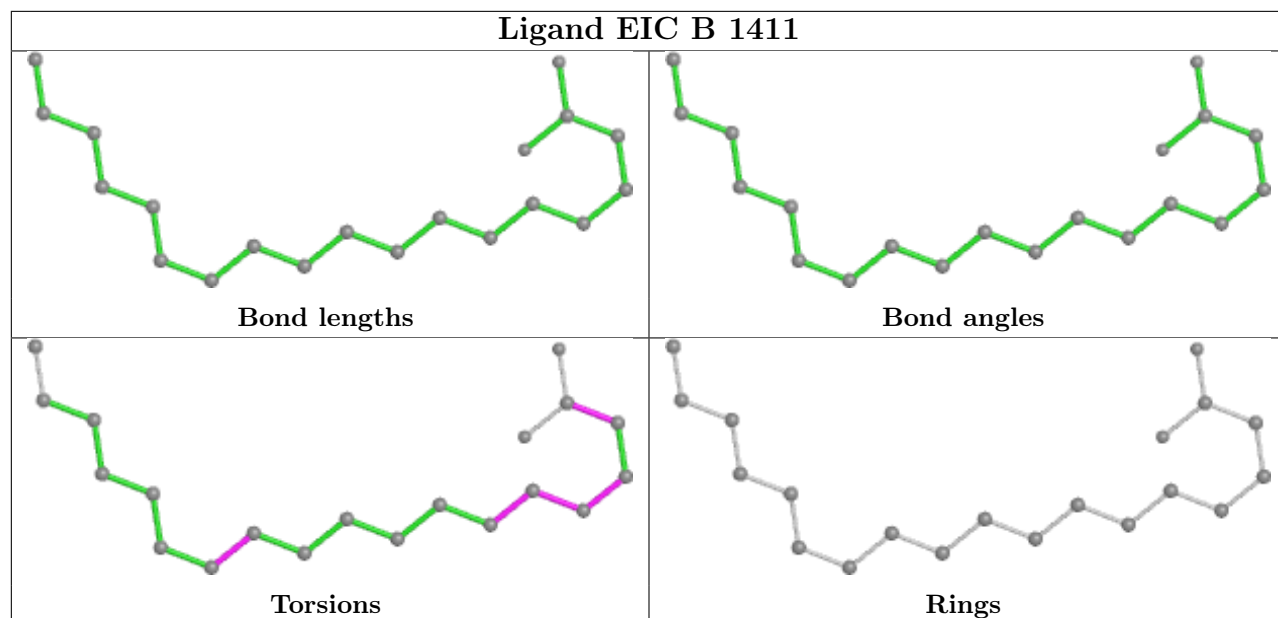
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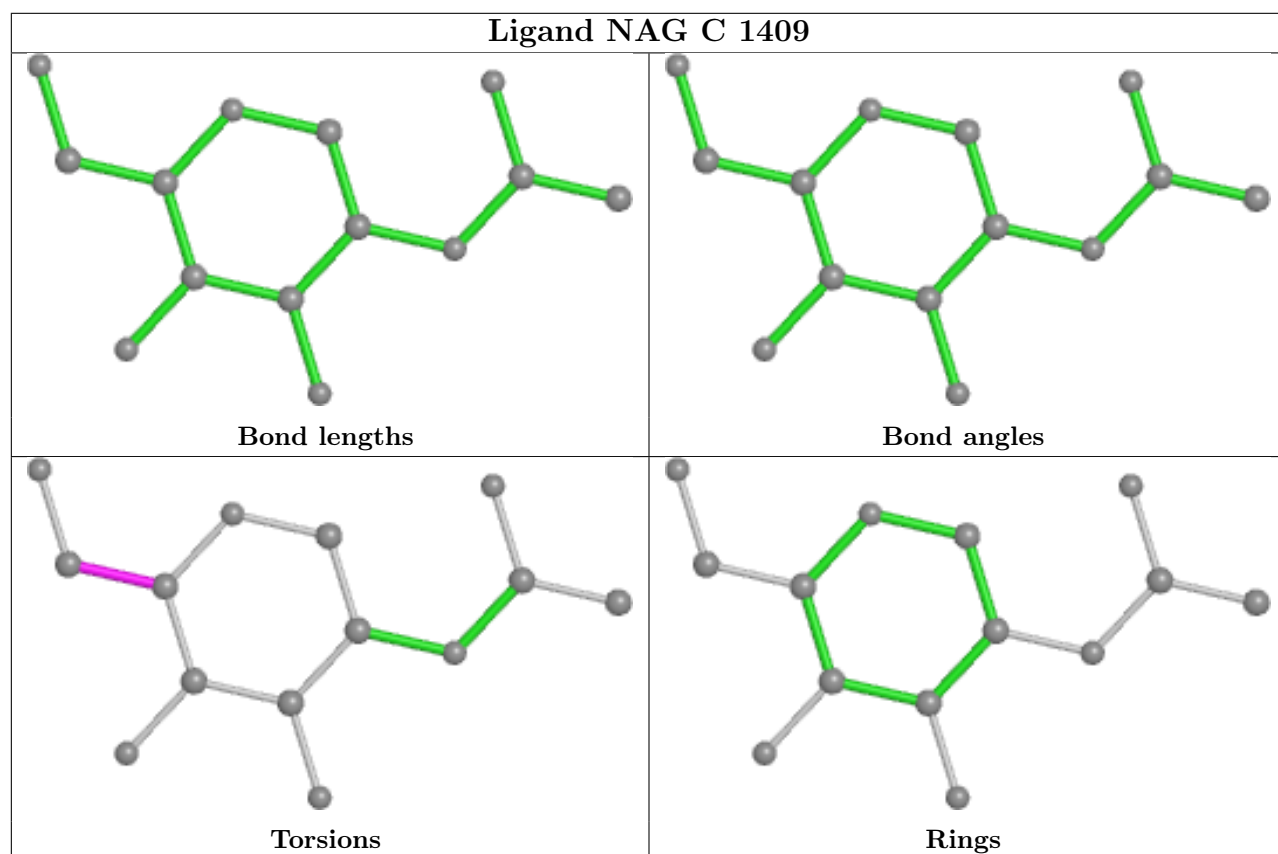
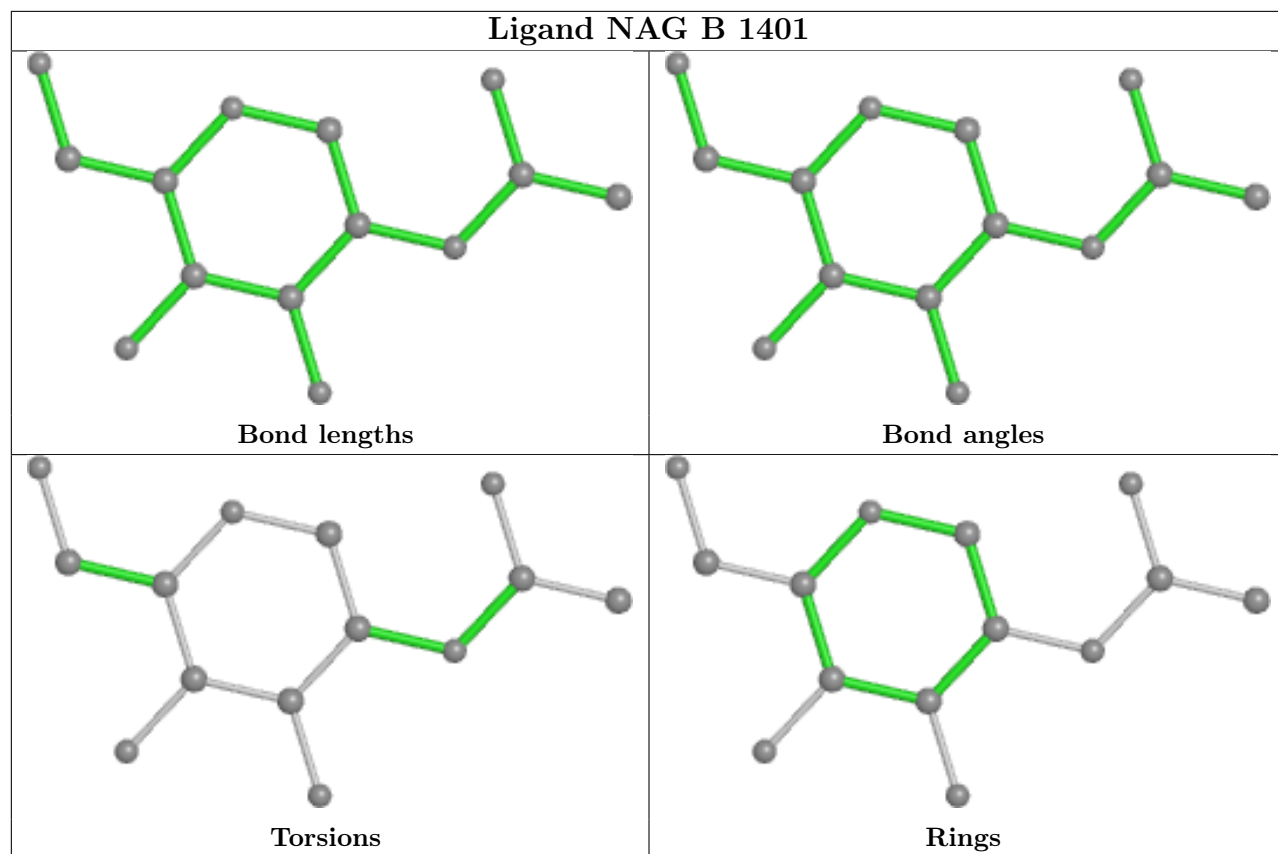


Ligand NAG C 1404

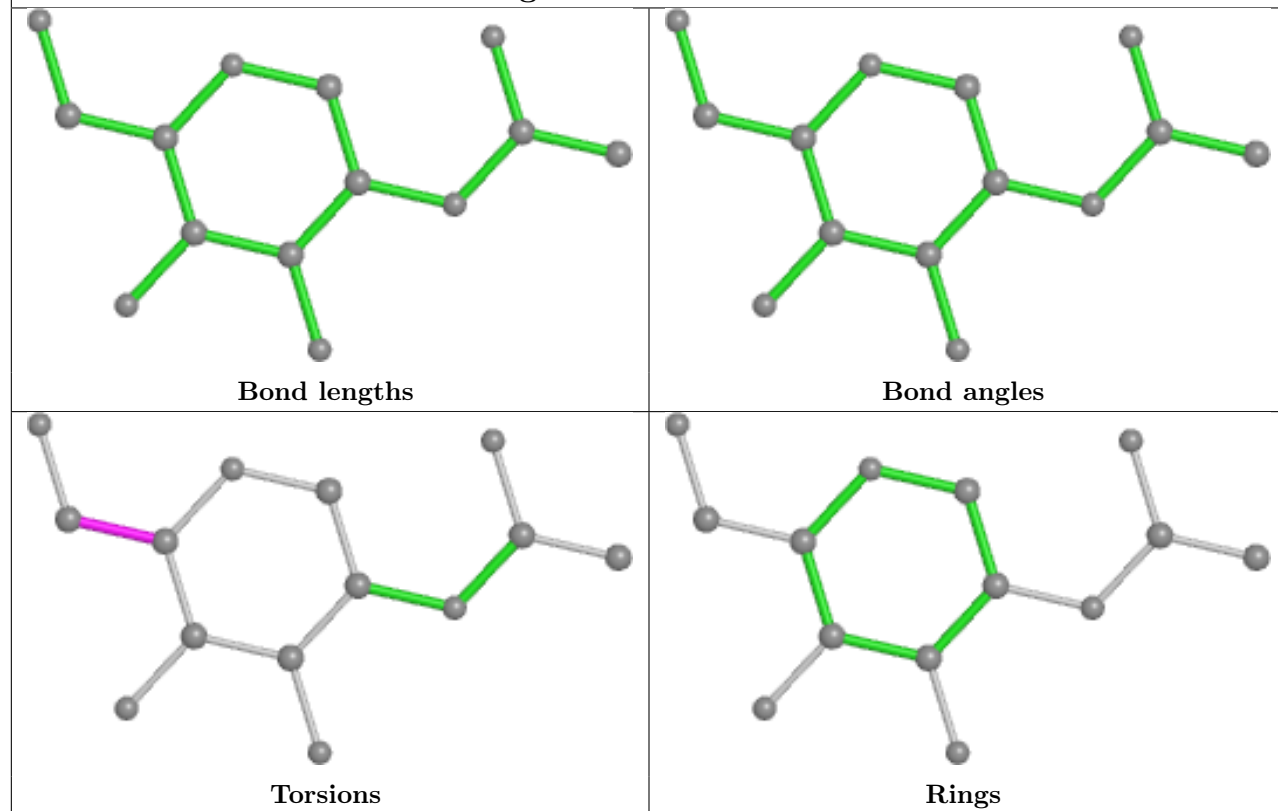




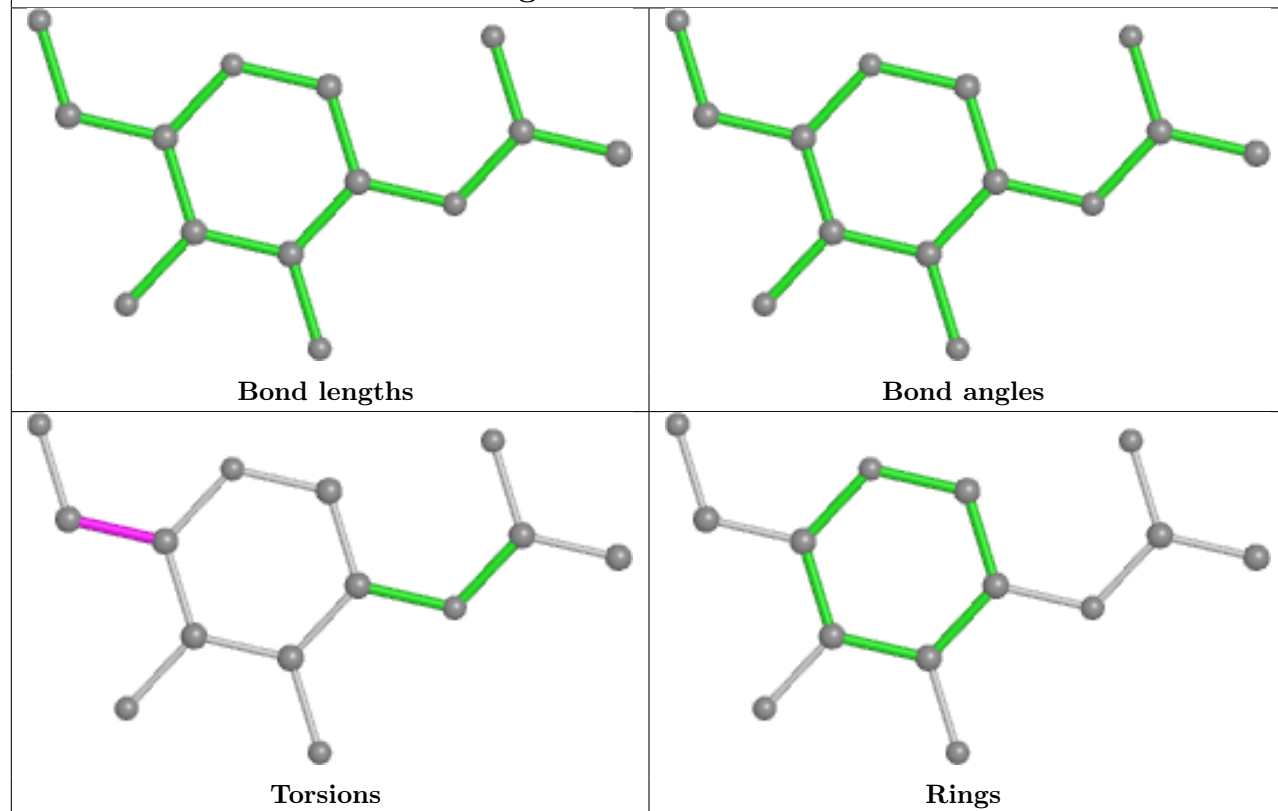




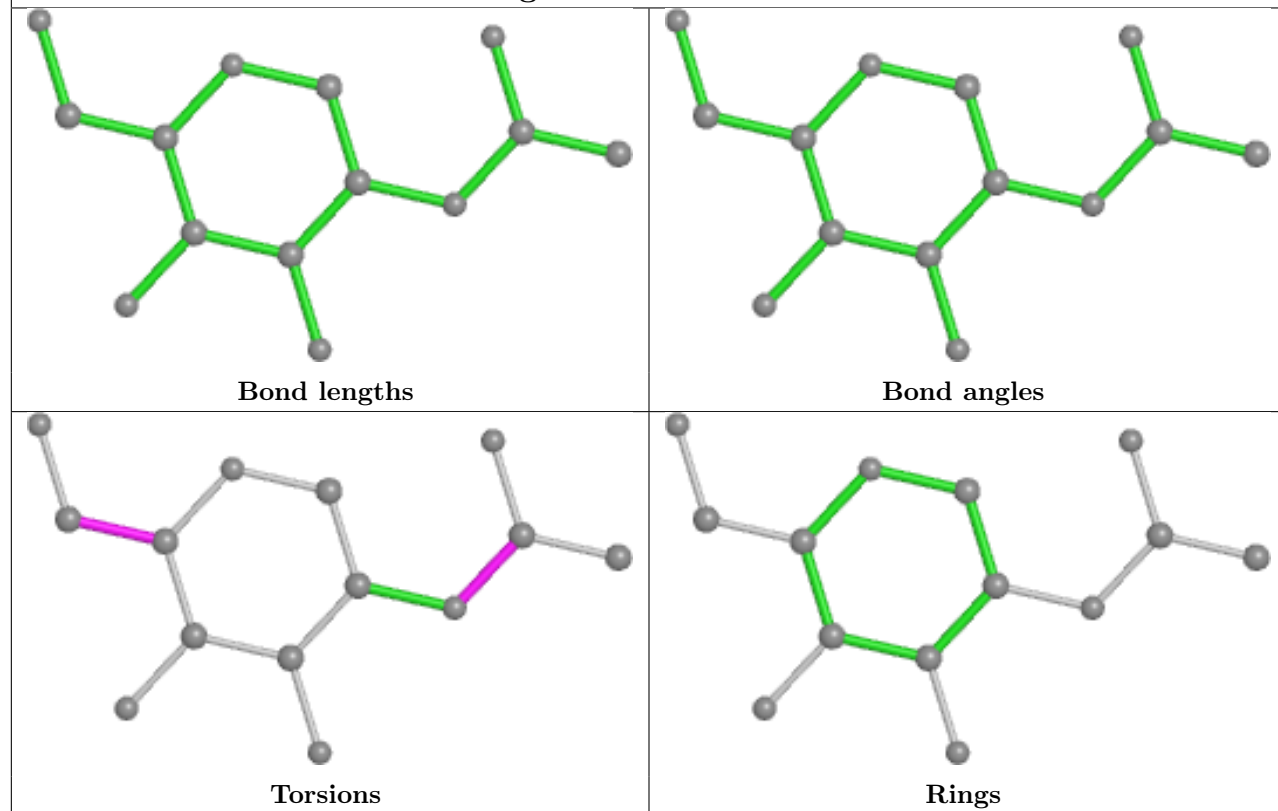
Ligand NAG C 1406



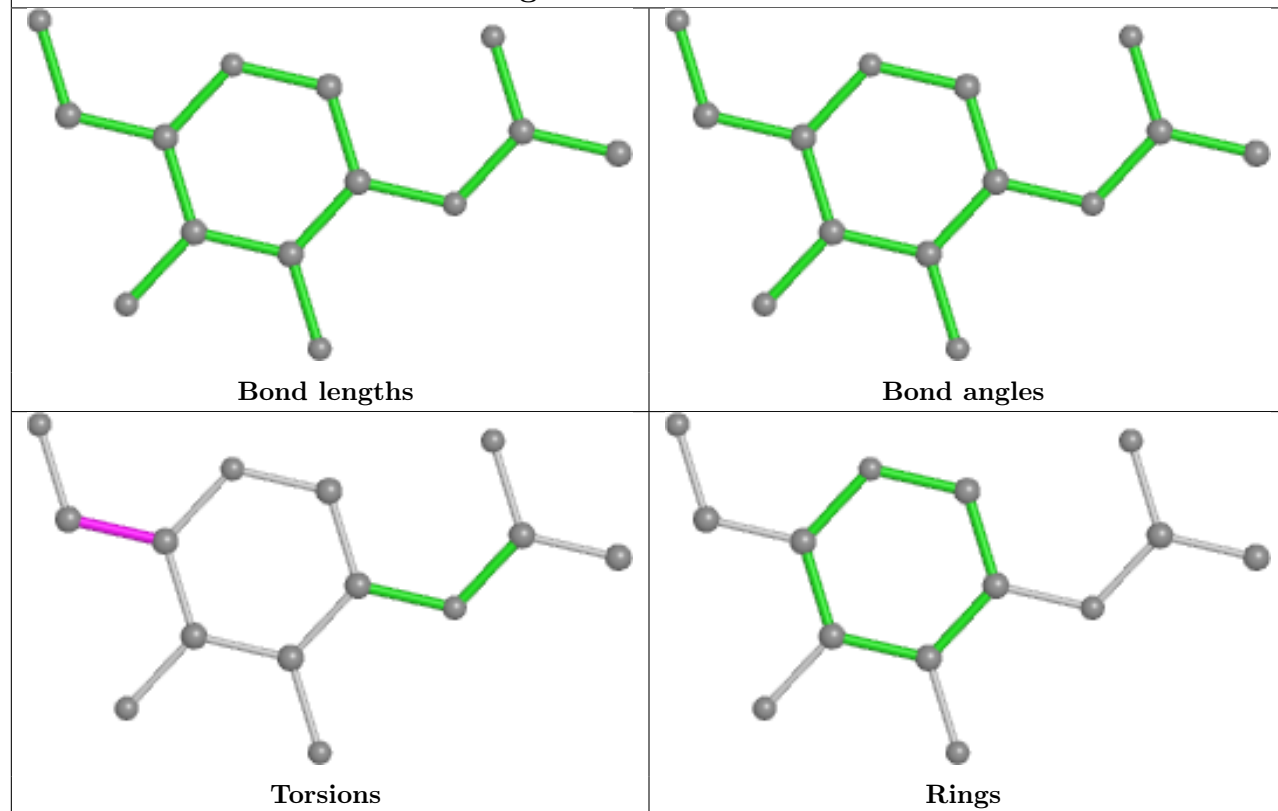
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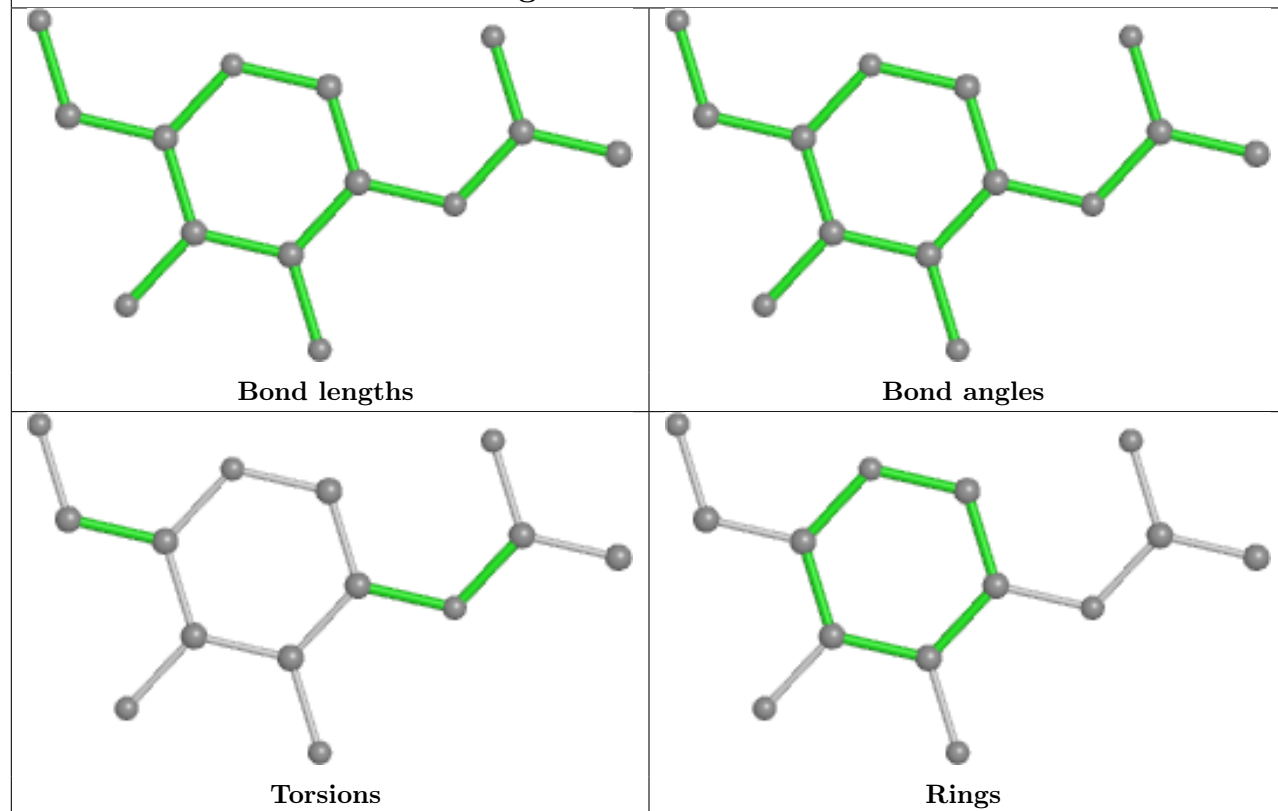
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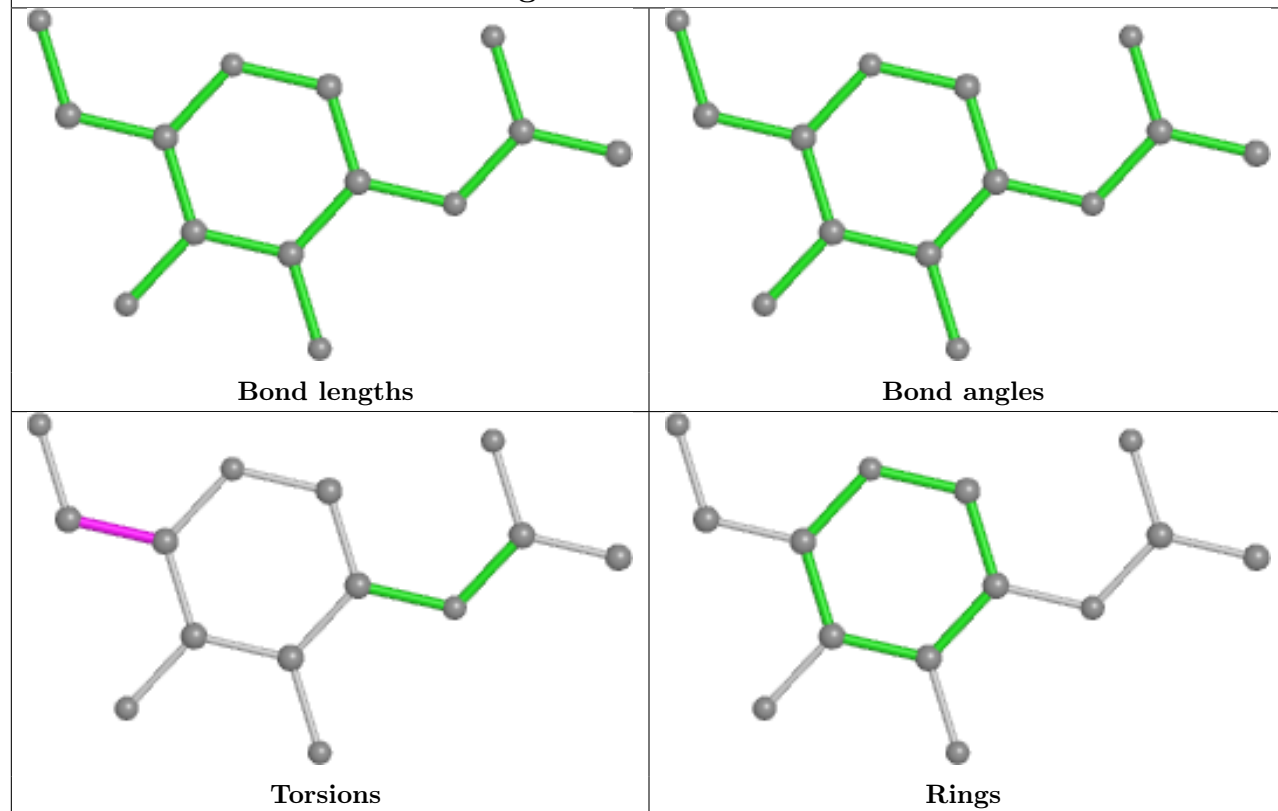
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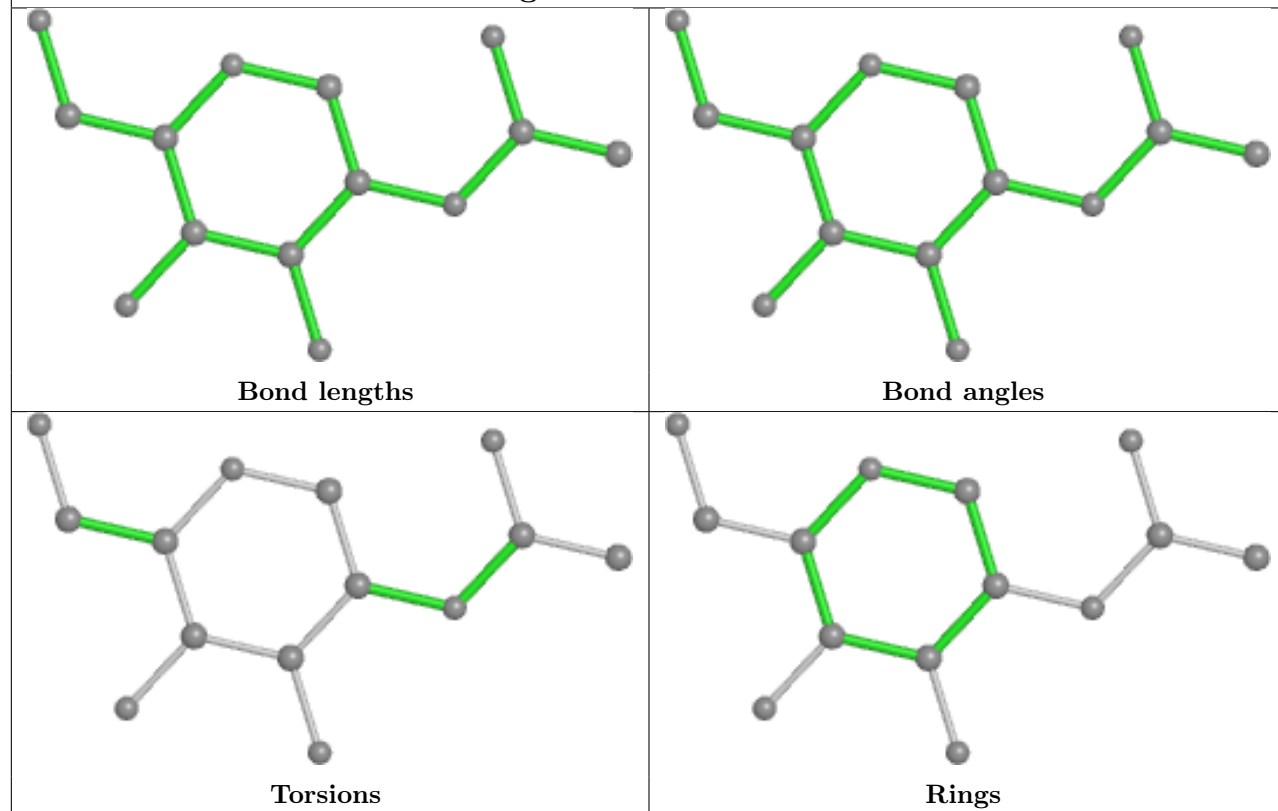
Ligand NAG A 1405



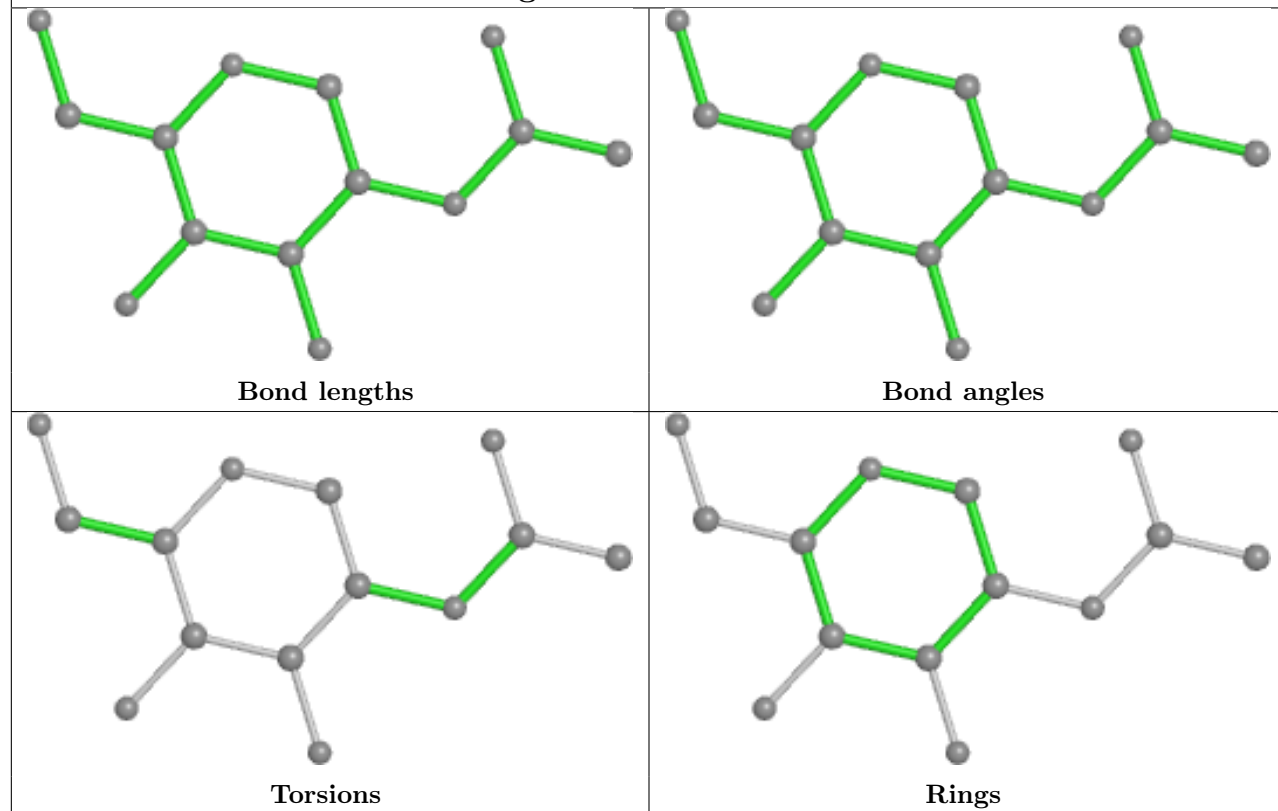
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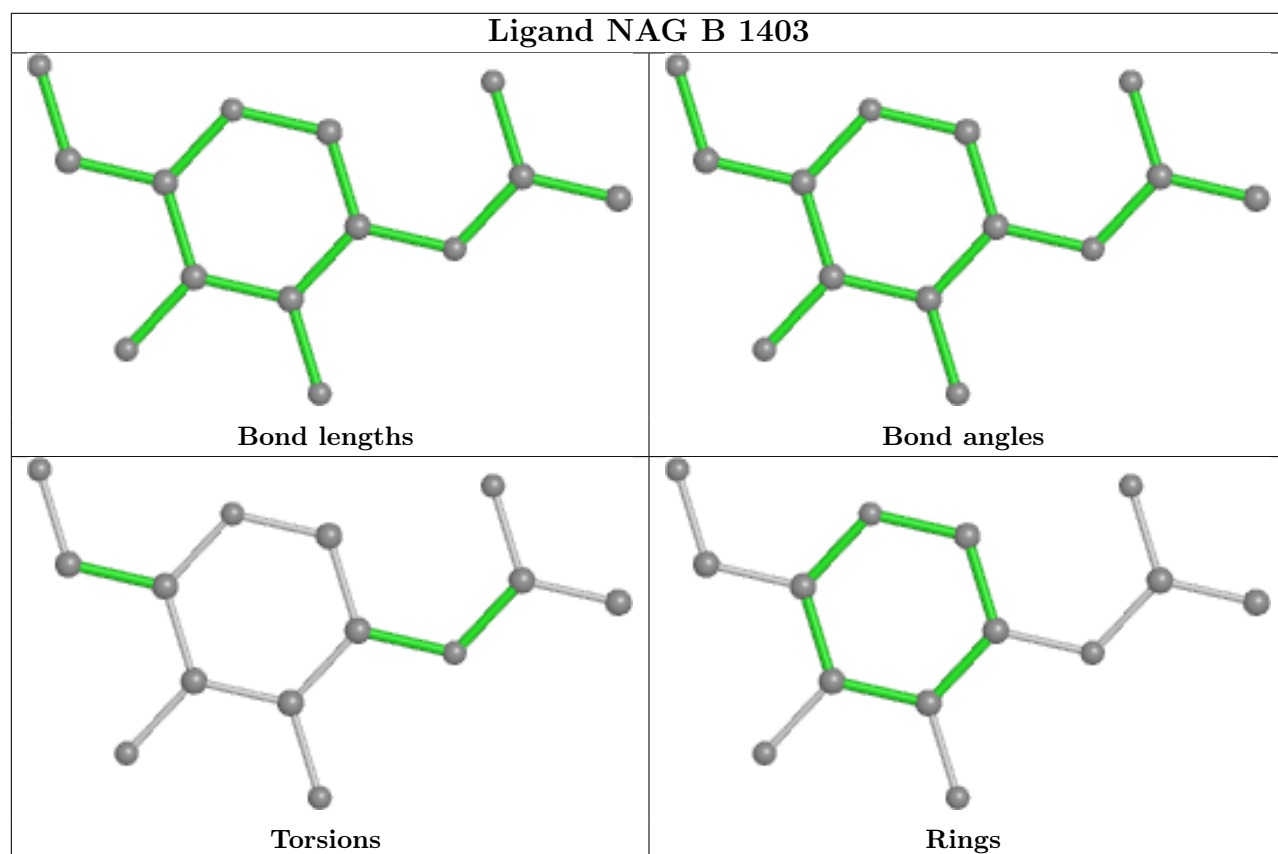
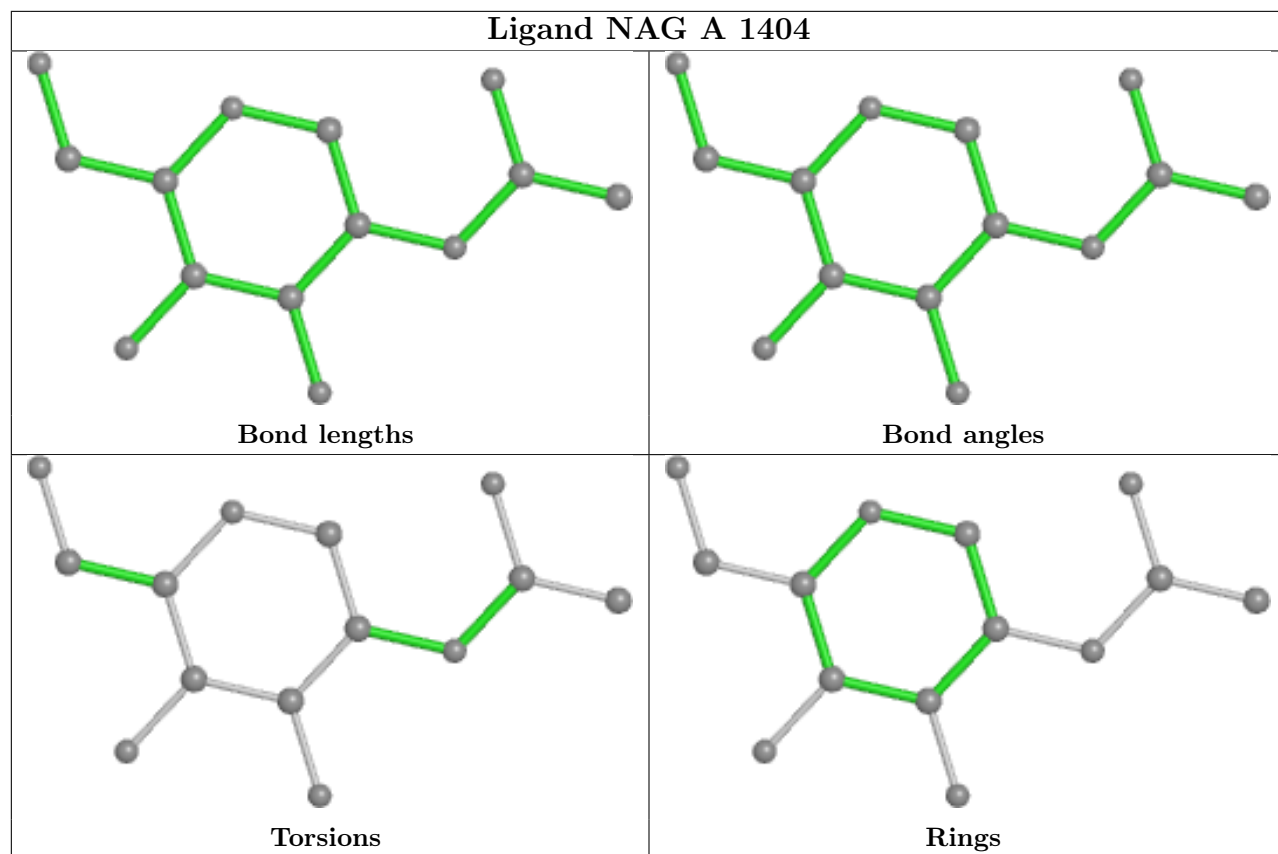


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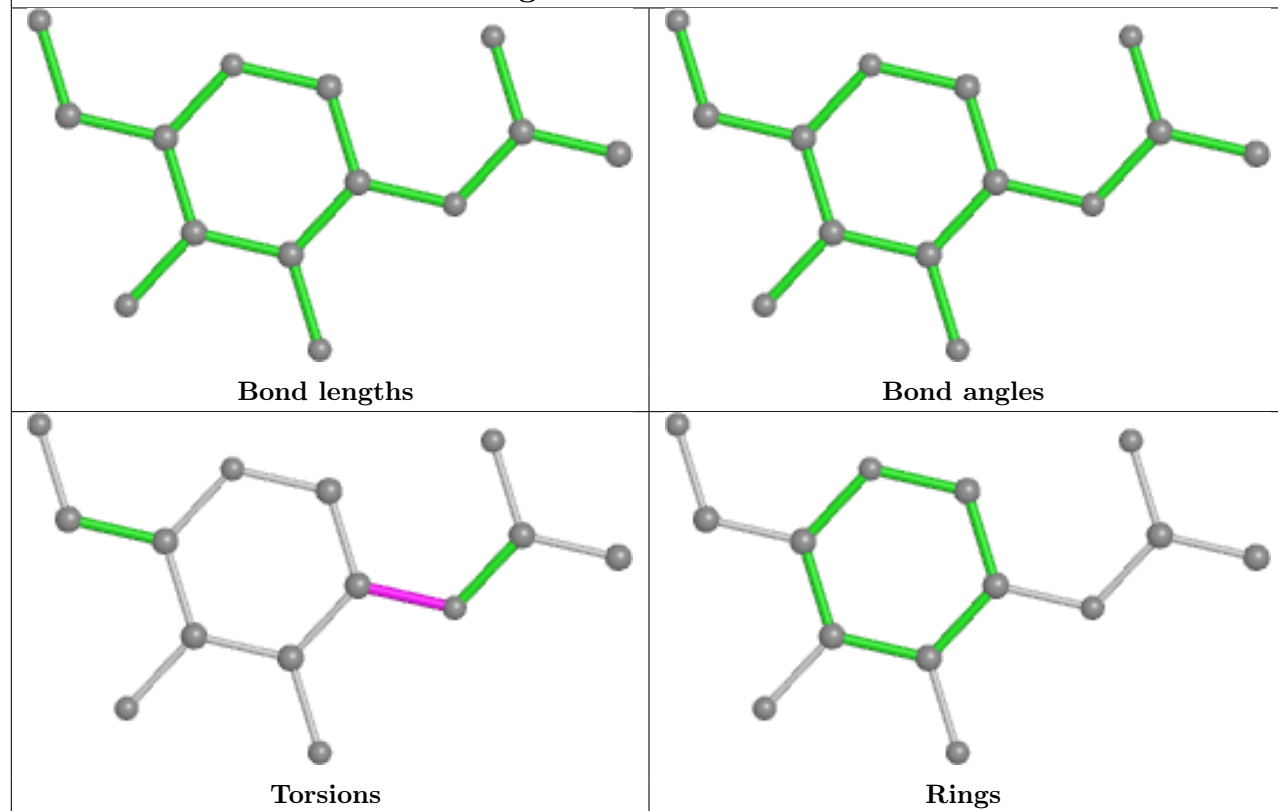


Ligand NAG A 1403

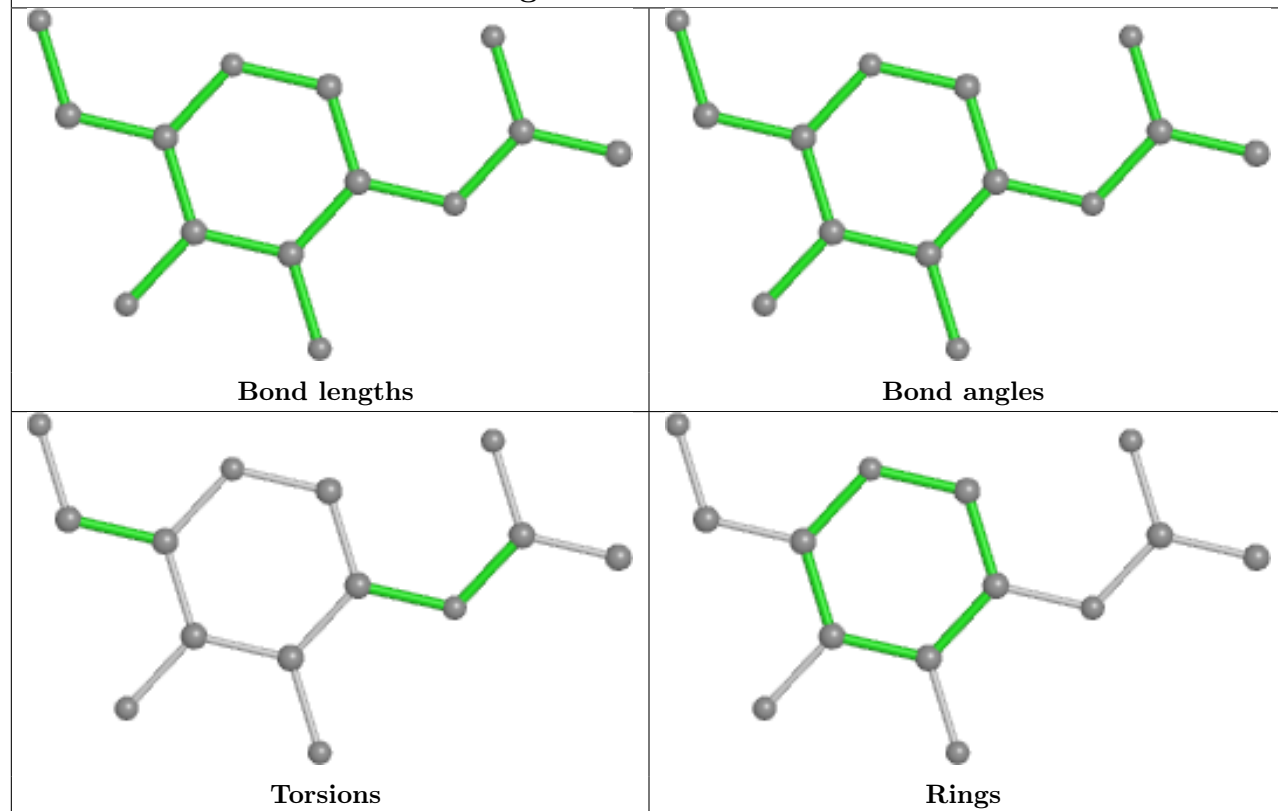


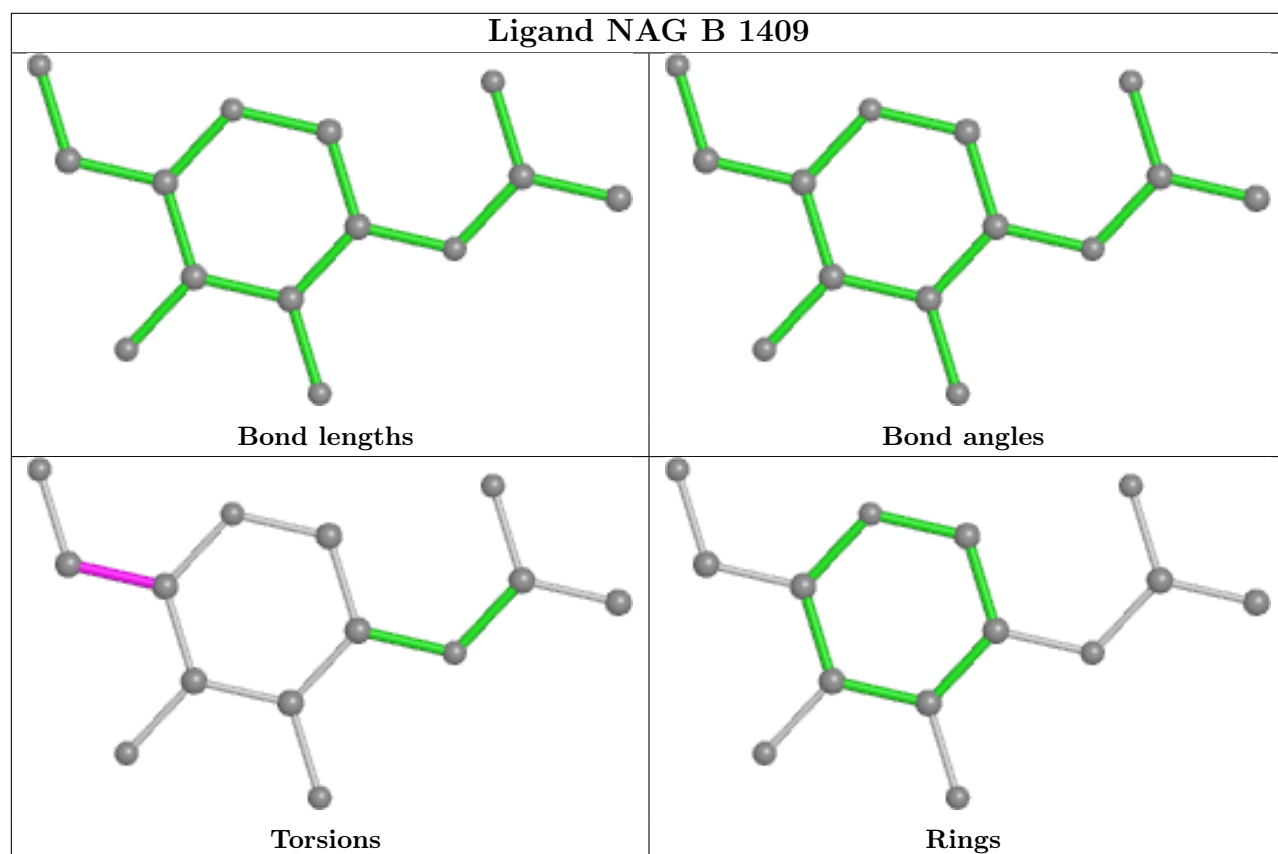
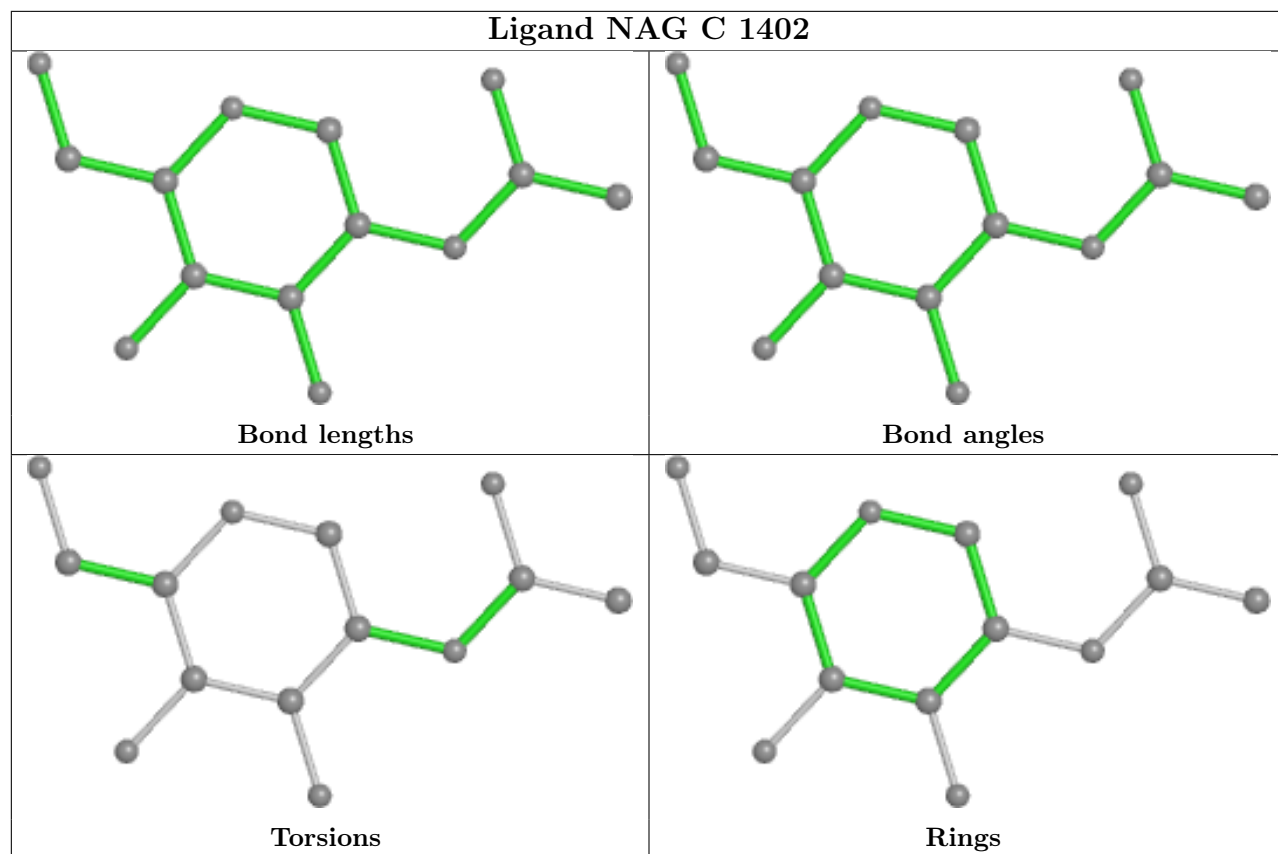


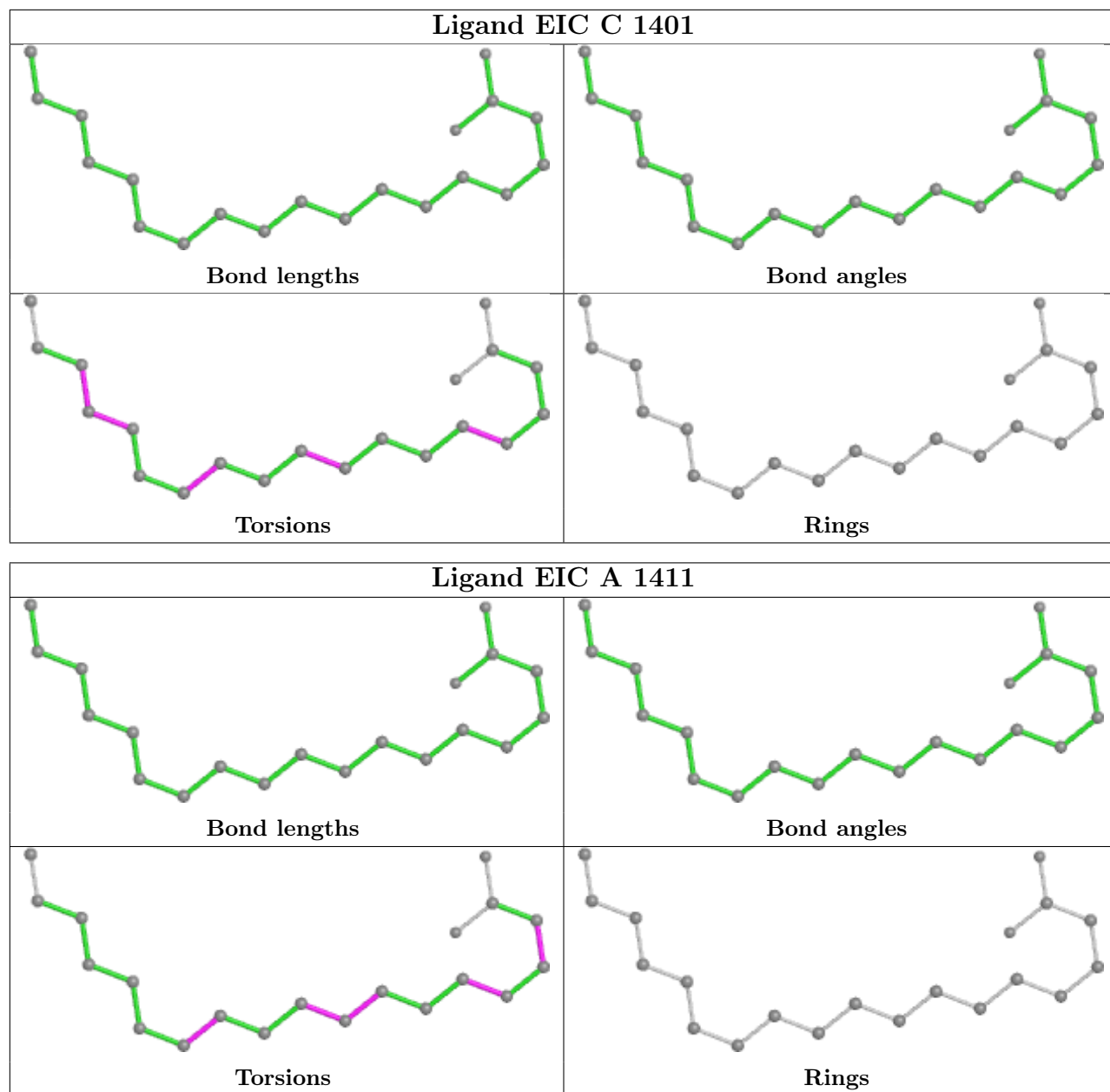
Ligand NAG A 1402



Ligand NAG B 1402



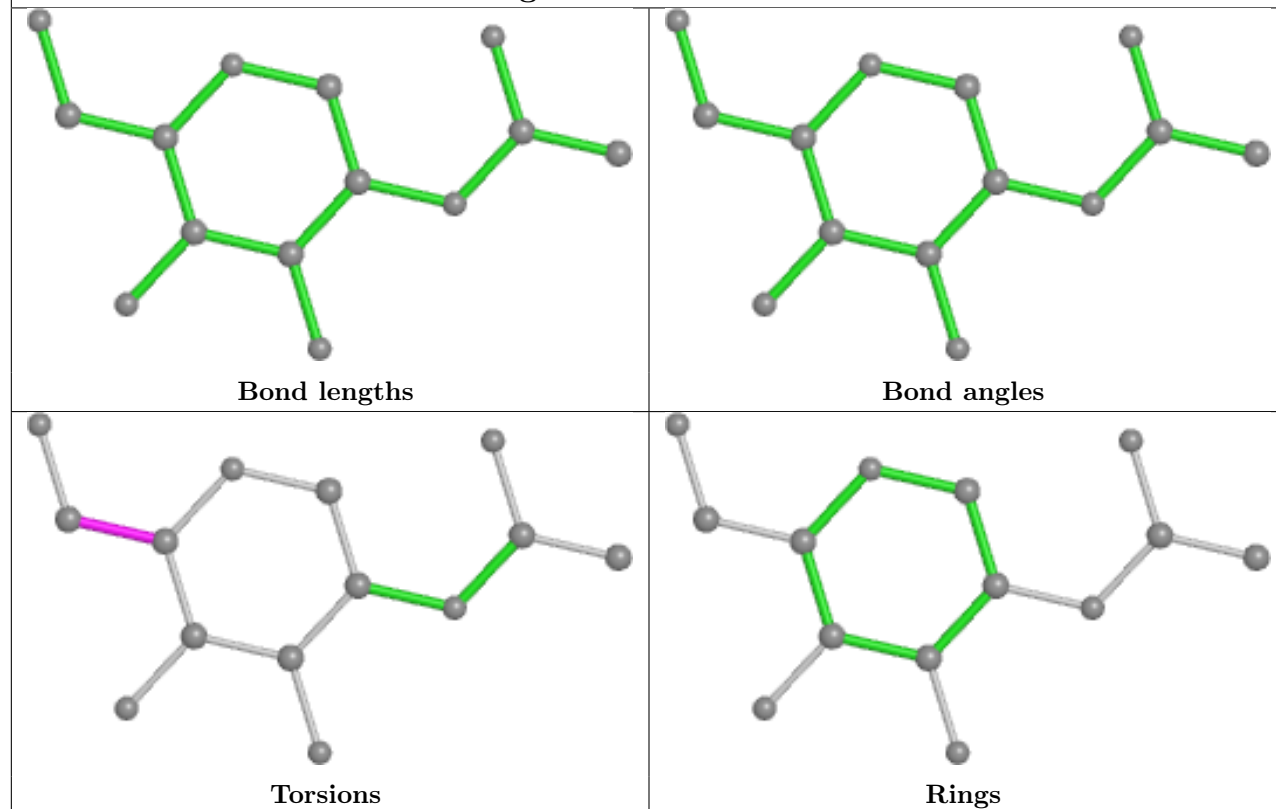


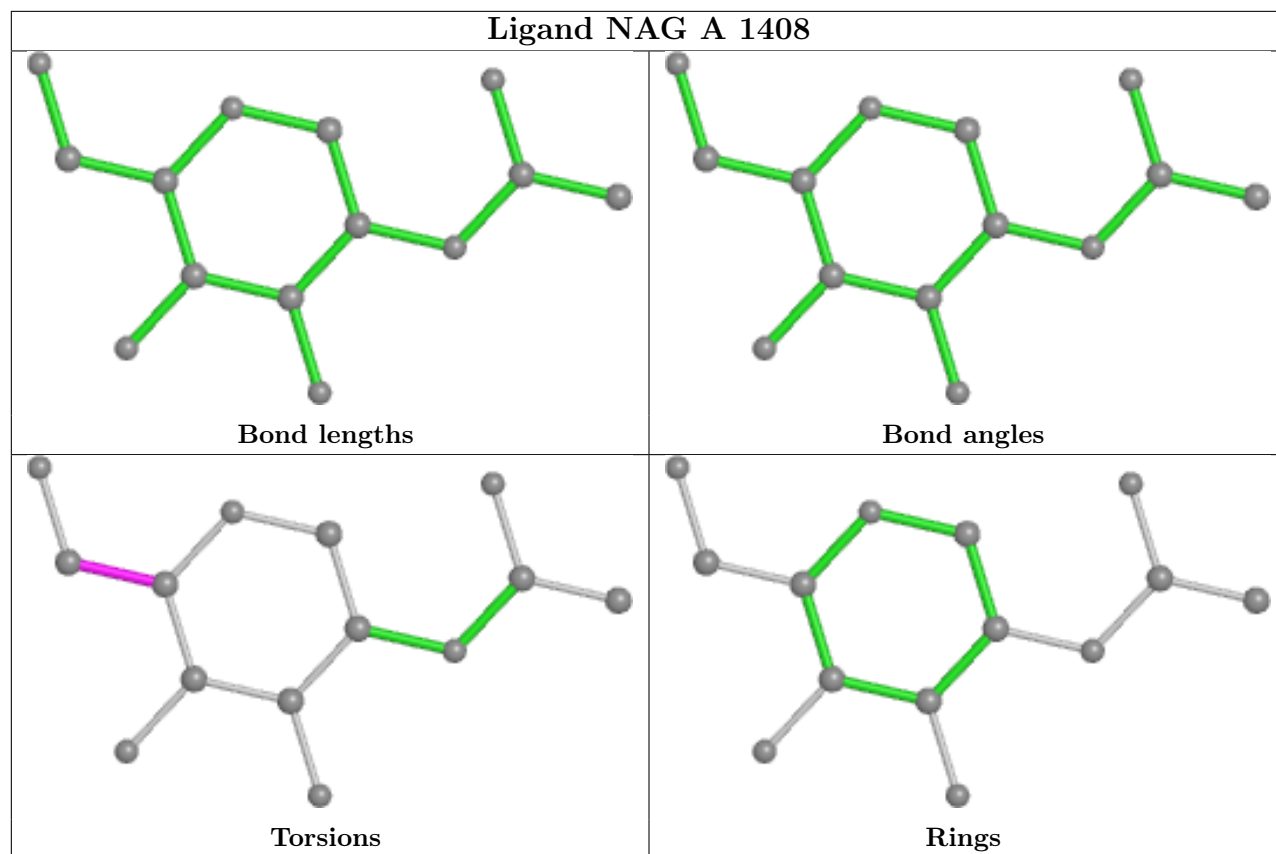


Ligand NAG A 1401



Ligand NAG C 1403





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.