



## wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 03:00 PM JST

PDB ID : 8WLU  
EMDB ID : EMD-37632  
Title : Cryo-EM structure of bat RsSHC014 spike glycoprotein  
Authors : Wang, X.; Qiao, S.  
Deposited on : 2023-10-01  
Resolution : 2.87 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

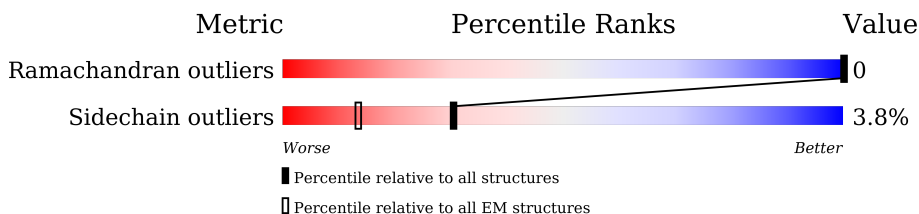
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.87 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.




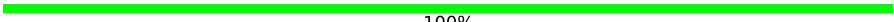
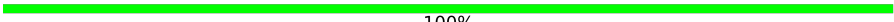
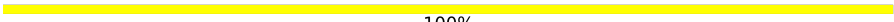
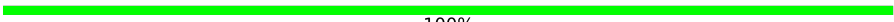

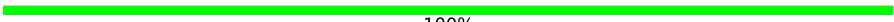

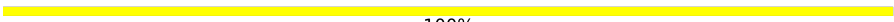




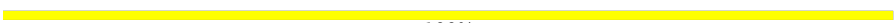











| Metric                | Whole archive (#Entries) | EM structures (#Entries) |
|-----------------------|--------------------------|--------------------------|
| Ramachandran outliers | 207382                   | 16835                    |
| Sidechain outliers    | 206894                   | 16415                    |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 1271   | 84% . 13%        |
| 1   | B     | 1271   | 84% . 13%        |
| 1   | C     | 1271   | 85% . 13%        |
| 2   | D     | 2      | 100%             |
| 2   | J     | 2      | 100%             |
| 2   | K     | 2      | 100%             |
| 2   | L     | 2      | 100%             |
| 2   | N     | 2      | 50% 50%          |
| 2   | O     | 2      | 100%             |
| 2   | P     | 2      | 100%             |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 2   | Q     | 2      |  100%      |
| 2   | R     | 2      |  100%      |
| 2   | S     | 2      |  100%      |
| 2   | T     | 2      |  100%      |
| 2   | Z     | 2      |  100%      |
| 2   | a     | 2      |  100%      |
| 2   | b     | 2      |  100%      |
| 2   | d     | 2      |  50% 50%   |
| 2   | e     | 2      |  100%      |
| 2   | f     | 2      |  100%      |
| 2   | g     | 2      |  100%      |
| 2   | h     | 2      |  100%      |
| 2   | i     | 2      |  100%    |
| 2   | j     | 2      |  100%    |
| 2   | p     | 2      |  100%    |
| 2   | q     | 2      |  100%    |
| 2   | r     | 2      |  100%    |
| 2   | t     | 2      |  50% 50% |
| 2   | u     | 2      |  100%    |
| 2   | v     | 2      |  100%    |
| 2   | w     | 2      |  100%    |
| 2   | x     | 2      |  100%    |
| 2   | y     | 2      |  100%    |
| 3   | E     | 3      |  100%    |
| 3   | F     | 3      |  100%    |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | G     | 3      |  100%      |
| 3   | H     | 3      |  100%      |
| 3   | I     | 3      |  67% 33%   |
| 3   | M     | 3      |  33% 67%   |
| 3   | U     | 3      |  100%      |
| 3   | V     | 3      |  100%      |
| 3   | W     | 3      |  100%      |
| 3   | X     | 3      |  100%      |
| 3   | Y     | 3      |  67% 33%   |
| 3   | c     | 3      |  33% 67%   |
| 3   | k     | 3      |  100%      |
| 3   | l     | 3      |  100%      |
| 3   | m     | 3      |  100%    |
| 3   | n     | 3      |  100%    |
| 3   | o     | 3      |  33% 67% |
| 3   | s     | 3      |  33% 67% |

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 27438 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 |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
|     |       |          | Total | C    | N    | O    | S  |         |       |
| 1   | A     | 1106     | 8604  | 5477 | 1439 | 1644 | 44 | 0       | 0     |
| 1   | C     | 1106     | 8604  | 5477 | 1439 | 1644 | 44 | 0       | 0     |
| 1   | B     | 1106     | 8604  | 5477 | 1439 | 1644 | 44 | 0       | 0     |

There are 168 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 969     | PRO      | LYS    | conflict       | UNP U5WLK5     |
| A     | 970     | PRO      | VAL    | conflict       | UNP U5WLK5     |
| A     | 1192    | GLY      | -      | linker         | UNP U5WLK5     |
| A     | 1193    | SER      | -      | linker         | UNP U5WLK5     |
| A     | 1220    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1221    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1222    | ARG      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1223    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1224    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1225    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1226    | VAL      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1227    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1228    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1229    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1230    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1231    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1232    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1233    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1234    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1235    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1236    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1237    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1238    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1239    | HIS      | -      | expression tag | UNP A0A346FJN8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| A     | 1240    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1241    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1242    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1243    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1244    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1245    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1246    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1247    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1248    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1249    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1250    | LYS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1251    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1252    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1253    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1254    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1255    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1256    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1257    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1258    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1259    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1260    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1261    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1262    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1263    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1264    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1265    | SER      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1266    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1267    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1268    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1269    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1270    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| A     | 1271    | LYS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 969     | PRO      | LYS    | conflict       | UNP U5WLK5     |
| C     | 970     | PRO      | VAL    | conflict       | UNP U5WLK5     |
| C     | 1192    | GLY      | -      | linker         | UNP U5WLK5     |
| C     | 1193    | SER      | -      | linker         | UNP U5WLK5     |
| C     | 1220    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1221    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1222    | ARG      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1223    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1224    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1225    | GLU      | -      | expression tag | UNP A0A346FJN8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| C     | 1226    | VAL      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1227    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1228    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1229    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1230    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1231    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1232    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1233    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1234    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1235    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1236    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1237    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1238    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1239    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1240    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1241    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1242    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1243    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1244    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1245    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1246    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1247    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1248    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1249    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1250    | LYS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1251    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1252    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1253    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1254    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1255    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1256    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1257    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1258    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1259    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1260    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1261    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1262    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1263    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1264    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1265    | SER      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1266    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1267    | PRO      | -      | expression tag | UNP A0A346FJN8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| C     | 1268    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1269    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1270    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| C     | 1271    | LYS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 969     | PRO      | LYS    | conflict       | UNP U5WLK5     |
| B     | 970     | PRO      | VAL    | conflict       | UNP U5WLK5     |
| B     | 1192    | GLY      | -      | linker         | UNP U5WLK5     |
| B     | 1193    | SER      | -      | linker         | UNP U5WLK5     |
| B     | 1220    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1221    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1222    | ARG      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1223    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1224    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1225    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1226    | VAL      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1227    | LEU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1228    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1229    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1230    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1231    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1232    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1233    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1234    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1235    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1236    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1237    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1238    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1239    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1240    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1241    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1242    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1243    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1244    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1245    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1246    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1247    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1248    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1249    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1250    | LYS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1251    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1252    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1253    | GLY      | -      | expression tag | UNP A0A346FJN8 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference      |
|-------|---------|----------|--------|----------------|----------------|
| B     | 1254    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1255    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1256    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1257    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1258    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1259    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1260    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1261    | GLY      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1262    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1263    | ALA      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1264    | TRP      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1265    | SER      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1266    | HIS      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1267    | PRO      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1268    | GLN      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1269    | PHE      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1270    | GLU      | -      | expression tag | UNP A0A346FJN8 |
| B     | 1271    | LYS      | -      | expression tag | UNP A0A346FJN8 |

- 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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
|     |       |          | Total | C  | N | O  |         |       |
| 2   | D     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | J     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | K     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | L     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | N     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | O     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | P     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
|     |       |          | Total | C  | N | O  |         |       |
| 2   | Q     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | R     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | S     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | T     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | Z     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | a     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | b     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | d     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | e     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | f     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | g     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | h     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | i     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | j     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | p     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | q     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | r     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | t     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | u     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | v     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | w     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |

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| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
|     |       |          | Total | C  | N | O  |         |       |
| 2   | x     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |
| 2   | y     | 2        | 28    | 16 | 2 | 10 | 0       | 0     |

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



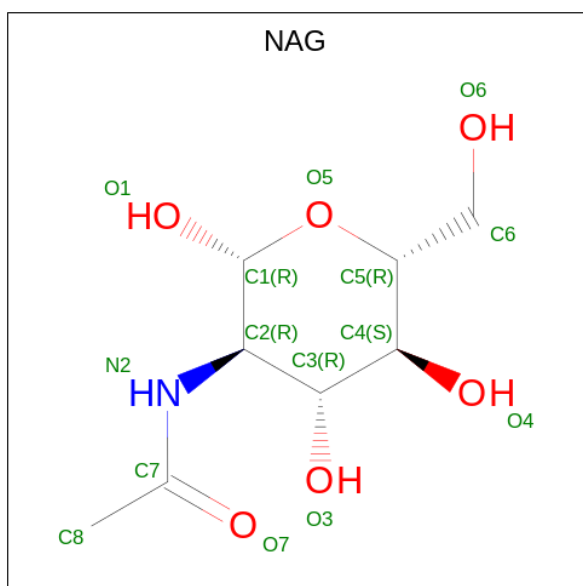
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
|     |       |          | Total | C  | N | O  |         |       |
| 3   | E     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | F     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | G     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | H     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | I     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | M     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | U     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | V     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | W     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | X     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | Y     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | c     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | k     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | l     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |
| 3   | m     | 3        | 39    | 22 | 2 | 15 | 0       | 0     |

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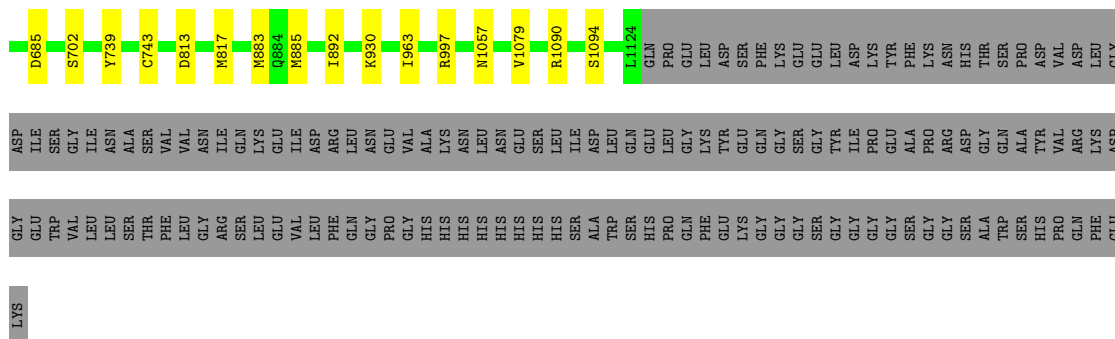
| Mol | Chain | Residues | Atoms       |         |        |         | AltConf | Trace |
|-----|-------|----------|-------------|---------|--------|---------|---------|-------|
|     |       |          | Total       | C       | N      | O       |         |       |
| 3   | n     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0     |
| 3   | o     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0     |
| 3   | s     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0     |

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms       |        |        |        | AltConf |
|-----|-------|----------|-------------|--------|--------|--------|---------|
|     |       |          | Total       | C      | N      | O      |         |
| 4   | A     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | A     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | C     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |
| 4   | B     | 1        | Total<br>14 | C<br>8 | N<br>1 | O<br>5 | 0       |





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

Chain D: 100%

MAG1  
MAG2

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

Chain J: 100%

MAG1  
MAG2

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

Chain K: 100%

MAG1  
MAG2

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

Chain L: 100%

MAG1  
MAG2

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

Chain N: 50% 50%

MAG1  
MAG2

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

Chain O:  100%

MAG1  
MAG2

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

Chain P:  100%

MAG1  
MAG2

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

Chain Q:  100%

MAG1  
MAG2

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

Chain R:  100%


MAG1  
MAG2

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

Chain S:  100%

MAG1  
MAG2

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

Chain T:  100%

MAG1  
MAG2

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

Chain Z:  100%

MAG1  
MAG2

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

Chain a:  100%MAG1  
MAG2

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

Chain b:  100%MAG1  
MAG2

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

Chain d:  50% 50%MAG1  
MAG2

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

Chain e:  100%MAG1  
MAG2

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

Chain f:  100%MAG1  
MAG2

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

Chain g:  100%MAG1  
MAG2



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

Chain h:  100%


MAG1  
MAG2

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

Chain i:  100%

MAG1  
MAG2

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

Chain j:  100%

MAG1  
MAG2

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

Chain p:  100%

MAG1  
MAG2

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

Chain q:  100%

MAG1  
MAG2

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

Chain r:  100%

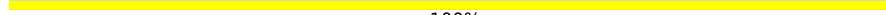
MAG1  
MAG2

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

Chain t:  50% 50%

MAG1  
MAG2

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

Chain u:  100%

MAG1  
MAG2

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

Chain v:  100%

MAG1  
MAG2

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

Chain w:  100%

MAG1  
MAG2

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

Chain x:  100%

MAG1  
MAG2

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

Chain y:  100%

MAG1  
MAG2

- 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:  100%

MAG1  
MAG2  
EMAG3

- 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%

MAG1  
MAG2  
BMA3

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

Chain G:  100%

MAG1  
MAG2  
BMA3

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

Chain H:  100%

MAG1  
MAG2  
BMA3

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

Chain I:  67% 33%

MAG1  
MAG2  
BMA3

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

Chain M:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain U:  100%

MAG1  
MAG2  
BMA3

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

Chain V:  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 W:  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 X:  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 Y:  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 c:  33% 67%



- 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:  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 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 m:  100%


MAG1  
MAG2  
BMA3

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

Chain n:  100%


MAG1  
MAG2  
BMA3

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

Chain o:  33% 67%

MAG1  
MAG2  
BMA3

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

Chain s:  33% 67%

MAG1  
MAG2  
BMA3

## 4 Experimental information

| Property                             | Value               | Source    |
|--------------------------------------|---------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE     | Depositor |
| Imposed symmetry                     | POINT, Not provided |           |
| Number of particles used             | 250439              | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF   | Depositor |
| CTF correction method                | NONE                | Depositor |
| Microscope                           | FEI TITAN KRIOS     | Depositor |
| Voltage (kV)                         | 300                 | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                  | Depositor |
| Minimum defocus (nm)                 | 1500                | Depositor |
| Maximum defocus (nm)                 | 1800                | 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

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     | 0.27         | 0/8810  | 0.51        | 0/11997 |
| 1   | B     | 0.27         | 0/8810  | 0.50        | 0/11997 |
| 1   | C     | 0.27         | 0/8810  | 0.51        | 0/11997 |
| All | All   | 0.27         | 0/26430 | 0.51        | 0/35991 |

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](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

### 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     | 1104/1271 (87%) | 1074 (97%) | 30 (3%) | 0        | 100         | 100 |
| 1   | B     | 1104/1271 (87%) | 1078 (98%) | 26 (2%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | C     | 1104/1271 (87%) | 1077 (98%) | 27 (2%) | 0        | 100         | 100 |
| All | All   | 3312/3813 (87%) | 3229 (98%) | 83 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 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     | 960/1099 (87%)  | 921 (96%)  | 39 (4%)  | 26          | 57 |
| 1   | B     | 960/1099 (87%)  | 922 (96%)  | 38 (4%)  | 27          | 58 |
| 1   | C     | 960/1099 (87%)  | 928 (97%)  | 32 (3%)  | 33          | 65 |
| All | All   | 2880/3297 (87%) | 2771 (96%) | 109 (4%) | 30          | 60 |

5 of 109 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | C     | 561 | ASP  |
| 1   | B     | 57  | GLN  |
| 1   | B     | 883 | MET  |
| 1   | C     | 575 | SER  |
| 1   | C     | 892 | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 948 | GLN  |
| 1   | C     | 722 | ASN  |
| 1   | C     | 948 | GLN  |
| 1   | B     | 940 | GLN  |
| 1   | B     | 948 | GLN  |



### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

114 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   | 2,1  | 14,14,15     | 0.73 | 0           | 17,19,21    | 1.12 | 2 (11%)     |
| 2   | NAG  | D     | 2   | 2    | 14,14,15     | 0.18 | 0           | 17,19,21    | 0.67 | 1 (5%)      |
| 3   | NAG  | E     | 1   | 1,3  | 14,14,15     | 0.24 | 0           | 17,19,21    | 0.50 | 0           |
| 3   | NAG  | E     | 2   | 3    | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.40 | 0           |
| 3   | BMA  | E     | 3   | 3    | 11,11,12     | 0.59 | 0           | 15,15,17    | 0.76 | 0           |
| 3   | NAG  | F     | 1   | 1,3  | 14,14,15     | 0.18 | 0           | 17,19,21    | 0.43 | 0           |
| 3   | NAG  | F     | 2   | 3    | 14,14,15     | 0.19 | 0           | 17,19,21    | 0.51 | 0           |
| 3   | BMA  | F     | 3   | 3    | 11,11,12     | 0.51 | 0           | 15,15,17    | 0.76 | 0           |
| 3   | NAG  | G     | 1   | 1,3  | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.45 | 0           |
| 3   | NAG  | G     | 2   | 3    | 14,14,15     | 0.17 | 0           | 17,19,21    | 0.47 | 0           |
| 3   | BMA  | G     | 3   | 3    | 11,11,12     | 0.69 | 0           | 15,15,17    | 0.70 | 0           |
| 3   | NAG  | H     | 1   | 1,3  | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.47 | 0           |
| 3   | NAG  | H     | 2   | 3    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.40 | 0           |
| 3   | BMA  | H     | 3   | 3    | 11,11,12     | 0.55 | 0           | 15,15,17    | 0.73 | 0           |
| 3   | NAG  | I     | 1   | 1,3  | 14,14,15     | 0.44 | 0           | 17,19,21    | 0.45 | 0           |
| 3   | NAG  | I     | 2   | 3    | 14,14,15     | 0.65 | 1 (7%)      | 17,19,21    | 0.82 | 0           |
| 3   | BMA  | I     | 3   | 3    | 11,11,12     | 0.70 | 0           | 15,15,17    | 1.00 | 0           |
| 2   | NAG  | J     | 1   | 2,1  | 14,14,15     | 0.16 | 0           | 17,19,21    | 0.53 | 0           |
| 2   | NAG  | J     | 2   | 2    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.34 | 0           |
| 2   | NAG  | K     | 1   | 2,1  | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.39 | 0           |
| 2   | NAG  | K     | 2   | 2    | 14,14,15     | 0.20 | 0           | 17,19,21    | 0.40 | 0           |
| 2   | NAG  | L     | 1   | 2,1  | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.39 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | L     | 2   | 2    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.43 | 0        |
| 3   | NAG  | M     | 1   | 1,3  | 14,14,15     | 0.37 | 0        | 17,19,21    | 1.29 | 2 (11%)  |
| 3   | NAG  | M     | 2   | 3    | 14,14,15     | 0.67 | 1 (7%)   | 17,19,21    | 0.97 | 2 (11%)  |
| 3   | BMA  | M     | 3   | 3    | 11,11,12     | 0.76 | 0        | 15,15,17    | 0.91 | 0        |
| 2   | NAG  | N     | 1   | 2,1  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 2   | NAG  | N     | 2   | 2    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.50 | 0        |
| 2   | NAG  | O     | 1   | 2,1  | 14,14,15     | 0.55 | 0        | 17,19,21    | 1.40 | 2 (11%)  |
| 2   | NAG  | O     | 2   | 2    | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.79 | 1 (5%)   |
| 2   | NAG  | P     | 1   | 2,1  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.34 | 0        |
| 2   | NAG  | P     | 2   | 2    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.49 | 0        |
| 2   | NAG  | Q     | 1   | 2,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.33 | 0        |
| 2   | NAG  | Q     | 2   | 2    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.41 | 0        |
| 2   | NAG  | R     | 1   | 2,1  | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.53 | 0        |
| 2   | NAG  | R     | 2   | 2    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.43 | 0        |
| 2   | NAG  | S     | 1   | 2,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.41 | 0        |
| 2   | NAG  | S     | 2   | 2    | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.43 | 0        |
| 2   | NAG  | T     | 1   | 2,1  | 14,14,15     | 0.77 | 1 (7%)   | 17,19,21    | 1.13 | 2 (11%)  |
| 2   | NAG  | T     | 2   | 2    | 14,14,15     | 0.16 | 0        | 17,19,21    | 0.68 | 1 (5%)   |
| 3   | NAG  | U     | 1   | 1,3  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | U     | 2   | 3    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.39 | 0        |
| 3   | BMA  | U     | 3   | 3    | 11,11,12     | 0.58 | 0        | 15,15,17    | 0.74 | 0        |
| 3   | NAG  | V     | 1   | 1,3  | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.41 | 0        |
| 3   | NAG  | V     | 2   | 3    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.51 | 0        |
| 3   | BMA  | V     | 3   | 3    | 11,11,12     | 0.51 | 0        | 15,15,17    | 0.75 | 0        |
| 3   | NAG  | W     | 1   | 1,3  | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | W     | 2   | 3    | 14,14,15     | 0.16 | 0        | 17,19,21    | 0.49 | 0        |
| 3   | BMA  | W     | 3   | 3    | 11,11,12     | 0.69 | 0        | 15,15,17    | 0.68 | 0        |
| 3   | NAG  | X     | 1   | 1,3  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.52 | 0        |
| 3   | NAG  | X     | 2   | 3    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.40 | 0        |
| 3   | BMA  | X     | 3   | 3    | 11,11,12     | 0.54 | 0        | 15,15,17    | 0.76 | 0        |
| 3   | NAG  | Y     | 1   | 1,3  | 14,14,15     | 0.52 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | NAG  | Y     | 2   | 3    | 14,14,15     | 0.65 | 1 (7%)   | 17,19,21    | 0.84 | 0        |
| 3   | BMA  | Y     | 3   | 3    | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.00 | 0        |
| 2   | NAG  | Z     | 1   | 2,1  | 14,14,15     | 0.17 | 0        | 17,19,21    | 0.50 | 0        |
| 2   | NAG  | Z     | 2   | 2    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.35 | 0        |
| 2   | NAG  | a     | 1   | 2,1  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.40 | 0        |
| 2   | NAG  | a     | 2   | 2    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.39 | 0        |
| 2   | NAG  | b     | 1   | 2,1  | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.41 | 0        |
| 2   | NAG  | b     | 2   | 2    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.42 | 0        |
| 3   | NAG  | c     | 1   | 1,3  | 14,14,15     | 0.37 | 0        | 17,19,21    | 1.30 | 2 (11%)  |
| 3   | NAG  | c     | 2   | 3    | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 0.98 | 2 (11%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | BMA  | c     | 3   | 3    | 11,11,12     | 0.74 | 0        | 15,15,17    | 0.92 | 0        |
| 2   | NAG  | d     | 1   | 2,1  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 2   | NAG  | d     | 2   | 2    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.47 | 0        |
| 2   | NAG  | e     | 1   | 2,1  | 14,14,15     | 0.55 | 0        | 17,19,21    | 1.40 | 2 (11%)  |
| 2   | NAG  | e     | 2   | 2    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.82 | 1 (5%)   |
| 2   | NAG  | f     | 1   | 2,1  | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.35 | 0        |
| 2   | NAG  | f     | 2   | 2    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.54 | 0        |
| 2   | NAG  | g     | 1   | 2,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.33 | 0        |
| 2   | NAG  | g     | 2   | 2    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | h     | 1   | 2,1  | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.52 | 0        |
| 2   | NAG  | h     | 2   | 2    | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.45 | 0        |
| 2   | NAG  | i     | 1   | 2,1  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | i     | 2   | 2    | 14,14,15     | 0.15 | 0        | 17,19,21    | 0.43 | 0        |
| 2   | NAG  | j     | 1   | 2,1  | 14,14,15     | 0.74 | 0        | 17,19,21    | 1.12 | 2 (11%)  |
| 2   | NAG  | j     | 2   | 2    | 14,14,15     | 0.15 | 0        | 17,19,21    | 0.70 | 1 (5%)   |
| 3   | NAG  | k     | 1   | 1,3  | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.54 | 0        |
| 3   | NAG  | k     | 2   | 3    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.40 | 0        |
| 3   | BMA  | k     | 3   | 3    | 11,11,12     | 0.58 | 0        | 15,15,17    | 0.74 | 0        |
| 3   | NAG  | l     | 1   | 1,3  | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | l     | 2   | 3    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.48 | 0        |
| 3   | BMA  | l     | 3   | 3    | 11,11,12     | 0.49 | 0        | 15,15,17    | 0.77 | 0        |
| 3   | NAG  | m     | 1   | 1,3  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.46 | 0        |
| 3   | NAG  | m     | 2   | 3    | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.45 | 0        |
| 3   | BMA  | m     | 3   | 3    | 11,11,12     | 0.69 | 0        | 15,15,17    | 0.69 | 0        |
| 3   | NAG  | n     | 1   | 1,3  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.51 | 0        |
| 3   | NAG  | n     | 2   | 3    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.40 | 0        |
| 3   | BMA  | n     | 3   | 3    | 11,11,12     | 0.55 | 0        | 15,15,17    | 0.74 | 0        |
| 3   | NAG  | o     | 1   | 1,3  | 14,14,15     | 0.69 | 1 (7%)   | 17,19,21    | 0.63 | 0        |
| 3   | NAG  | o     | 2   | 3    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.92 | 1 (5%)   |
| 3   | BMA  | o     | 3   | 3    | 11,11,12     | 0.73 | 0        | 15,15,17    | 0.96 | 0        |
| 2   | NAG  | p     | 1   | 2,1  | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.51 | 0        |
| 2   | NAG  | p     | 2   | 2    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.35 | 0        |
| 2   | NAG  | q     | 1   | 2,1  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.41 | 0        |
| 2   | NAG  | q     | 2   | 2    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.39 | 0        |
| 2   | NAG  | r     | 1   | 2,1  | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.38 | 0        |
| 2   | NAG  | r     | 2   | 2    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.41 | 0        |
| 3   | NAG  | s     | 1   | 1,3  | 14,14,15     | 0.38 | 0        | 17,19,21    | 1.31 | 2 (11%)  |
| 3   | NAG  | s     | 2   | 3    | 14,14,15     | 0.64 | 1 (7%)   | 17,19,21    | 0.98 | 2 (11%)  |
| 3   | BMA  | s     | 3   | 3    | 11,11,12     | 0.73 | 0        | 15,15,17    | 0.90 | 0        |
| 2   | NAG  | t     | 1   | 2,1  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.71 | 1 (5%)   |
| 2   | NAG  | t     | 2   | 2    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.49 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 2   | NAG  | u     | 1   | 2,1  | 14,14,15     | 0.55 | 0        | 17,19,21    | 1.40 | 2 (11%)  |
| 2   | NAG  | u     | 2   | 2    | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.80 | 1 (5%)   |
| 2   | NAG  | v     | 1   | 2,1  | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.35 | 0        |
| 2   | NAG  | v     | 2   | 2    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.53 | 0        |
| 2   | NAG  | w     | 1   | 2,1  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.33 | 0        |
| 2   | NAG  | w     | 2   | 2    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.42 | 0        |
| 2   | NAG  | x     | 1   | 2,1  | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.52 | 0        |
| 2   | NAG  | x     | 2   | 2    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.43 | 0        |
| 2   | NAG  | y     | 1   | 2,1  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.45 | 0        |
| 2   | NAG  | y     | 2   | 2    | 14,14,15     | 0.16 | 0        | 17,19,21    | 0.42 | 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   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 2   | 3    | -       | 0/6/23/26 | 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    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | G     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | G     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | H     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | H     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | H     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | I     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | I     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | NAG  | J     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | J     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | K     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | K     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | L     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | L     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | M     | 1   | 1,3  | -       | 5/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | BMA  | M     | 3   | 3    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | NAG  | N     | 1   | 2,1  | -       | 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   | 2,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 2   | NAG  | O     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | P     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | P     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | Q     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | Q     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | R     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | R     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | S     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | S     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | T     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | T     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | U     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | U     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | U     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | V     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | V     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | V     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | W     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | W     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | W     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | X     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | X     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | X     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | Y     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Y     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | Y     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | NAG  | Z     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | Z     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | a     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | a     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | b     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | b     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | c     | 1   | 1,3  | -       | 5/6/23/26 | 0/1/1/1 |
| 3   | NAG  | c     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | BMA  | c     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | NAG  | d     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | d     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | e     | 1   | 2,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 2   | NAG  | e     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | f     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | f     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | g     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | g     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | h     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | h     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | i     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | i     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | j     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | j     | 2   | 2    | -       | 4/6/23/26 | 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  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | l     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | l     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 3   | NAG  | m     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | m     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | m     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | n     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | n     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | BMA  | n     | 3   | 3    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | o     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | o     | 2   | 3    | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | BMA  | o     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | NAG  | p     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | p     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | q     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | q     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | r     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | r     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | s     | 1   | 1,3  | -       | 5/6/23/26 | 0/1/1/1 |
| 3   | NAG  | s     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | BMA  | s     | 3   | 3    | -       | 2/2/19/22 | 0/1/1/1 |
| 2   | NAG  | t     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | t     | 2   | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | u     | 1   | 2,1  | -       | 3/6/23/26 | 0/1/1/1 |
| 2   | NAG  | u     | 2   | 2    | -       | 4/6/23/26 | 0/1/1/1 |
| 2   | NAG  | v     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | v     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | w     | 1   | 2,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | w     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | x     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | x     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 2   | NAG  | y     | 1   | 2,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 2   | NAG  | y     | 2   | 2    | -       | 0/6/23/26 | 0/1/1/1 |

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

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | o     | 2   | NAG  | O5-C1 | -2.59 | 1.39        | 1.43     |
| 3   | c     | 2   | NAG  | O5-C1 | -2.41 | 1.39        | 1.43     |
| 3   | o     | 1   | NAG  | O5-C1 | -2.41 | 1.39        | 1.43     |
| 3   | M     | 2   | NAG  | O5-C1 | -2.28 | 1.40        | 1.43     |
| 3   | Y     | 2   | NAG  | O5-C1 | -2.27 | 1.40        | 1.43     |

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

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3   | s     | 1   | NAG  | C2-N2-C7 | 4.32 | 129.05      | 122.90   |
| 3   | c     | 1   | NAG  | C2-N2-C7 | 4.31 | 129.03      | 122.90   |
| 3   | M     | 1   | NAG  | C2-N2-C7 | 4.29 | 129.01      | 122.90   |
| 2   | e     | 1   | NAG  | C2-N2-C7 | 4.23 | 128.93      | 122.90   |
| 2   | u     | 1   | NAG  | C2-N2-C7 | 4.23 | 128.92      | 122.90   |

There are no chirality outliers.

5 of 148 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | M     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | c     | 1   | NAG  | O5-C5-C6-O6 |

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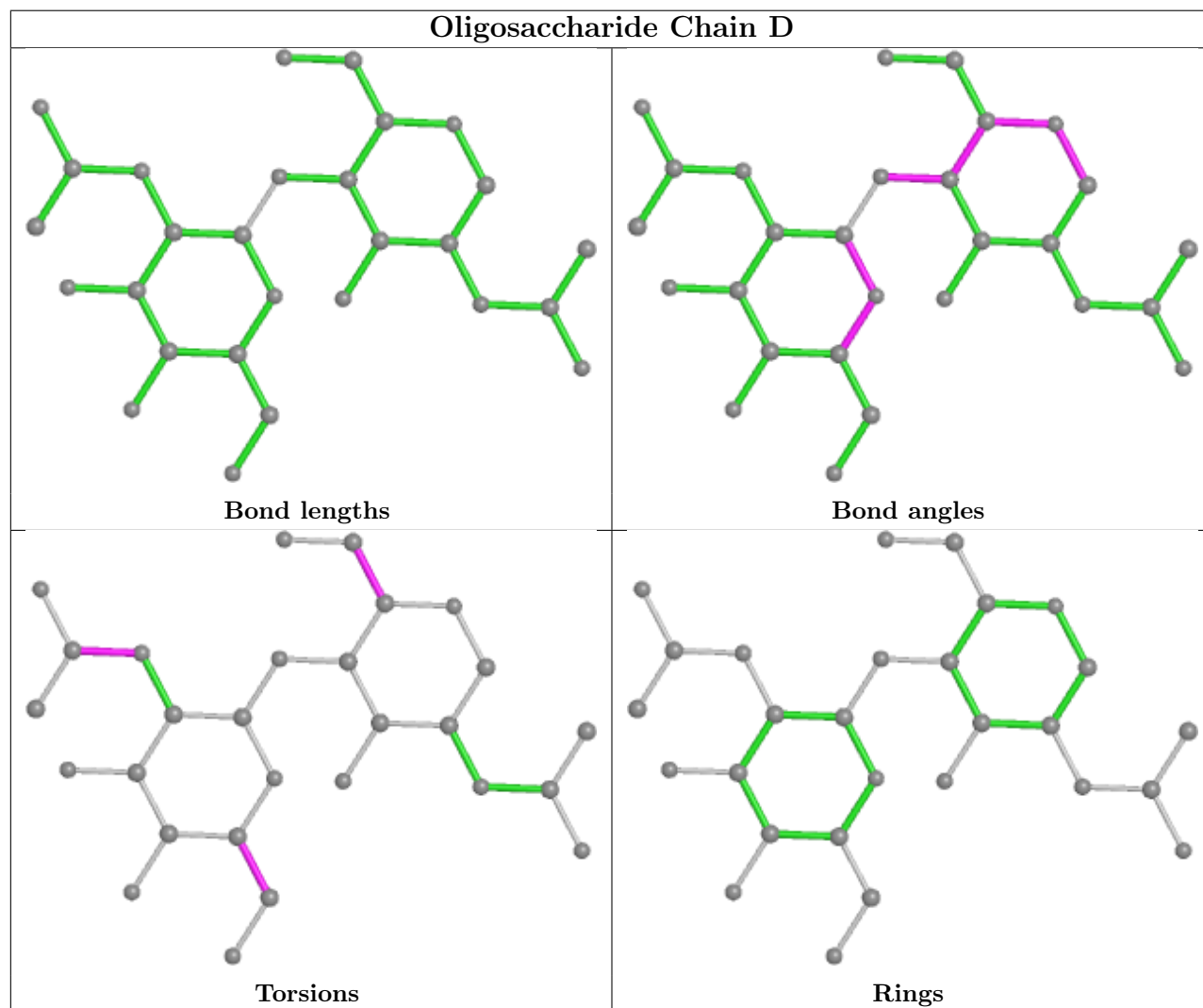
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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | s     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | o     | 3   | BMA  | C4-C5-C6-O6 |

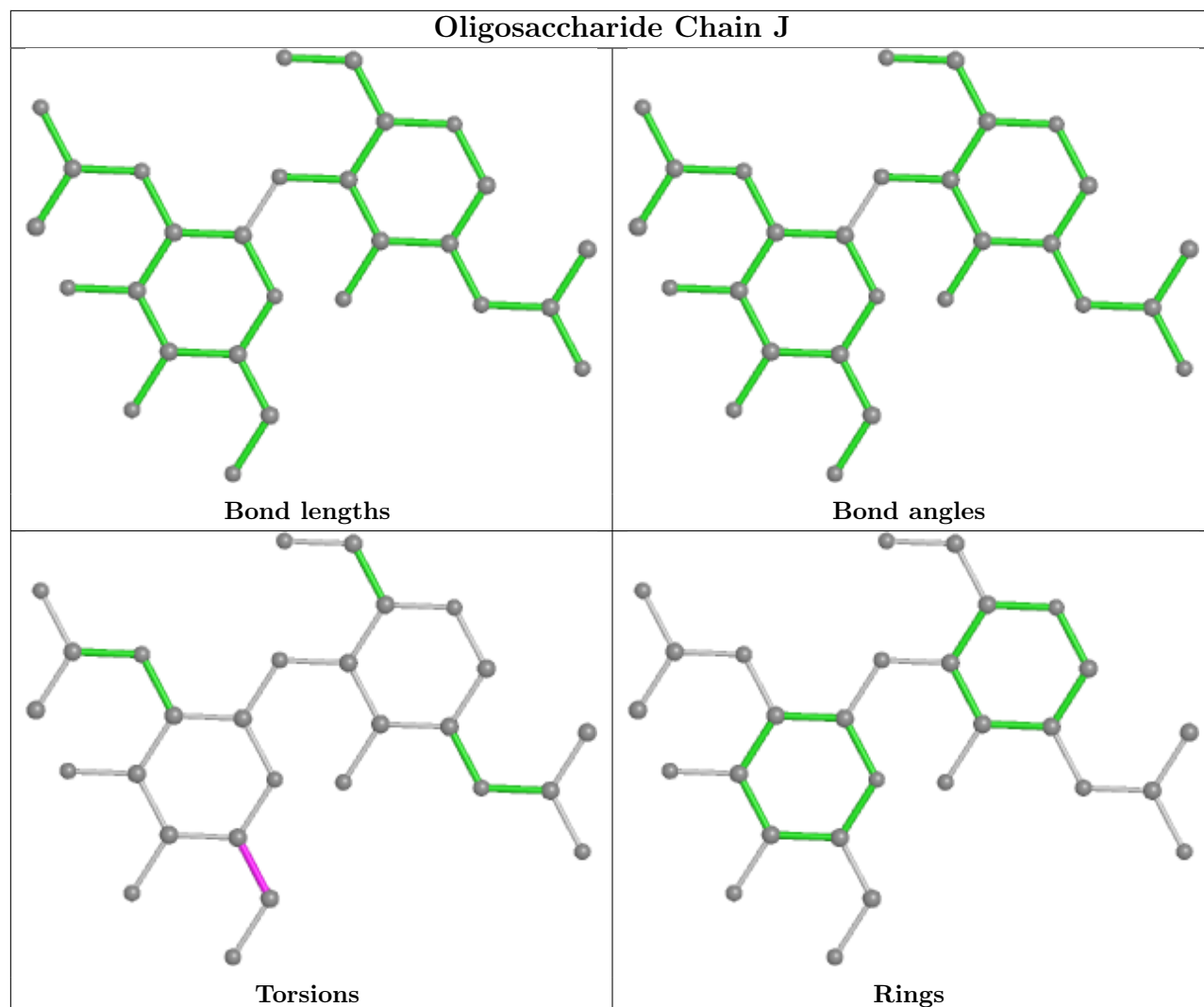
There are no ring outliers.

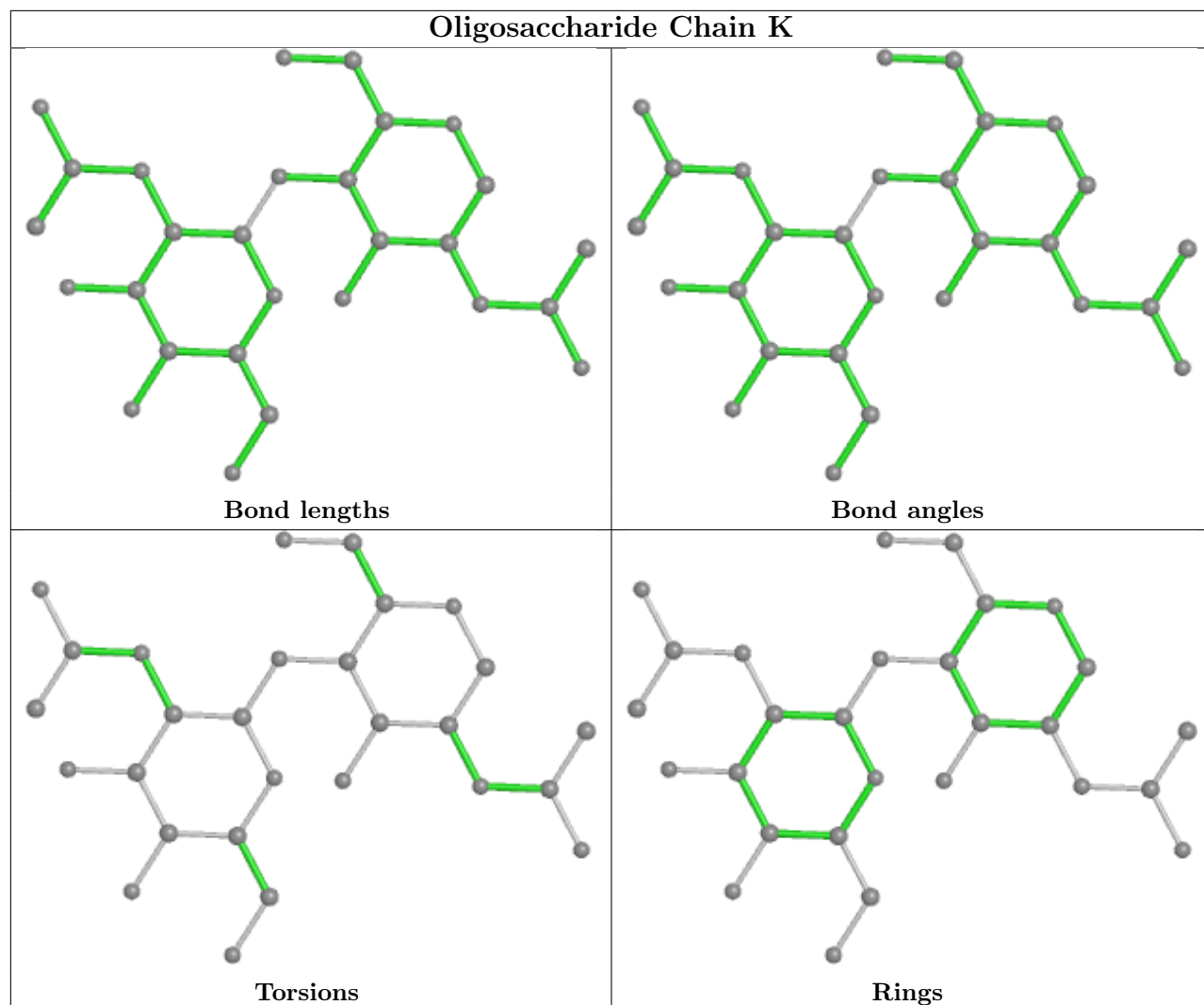
No monomer is involved in short contacts.

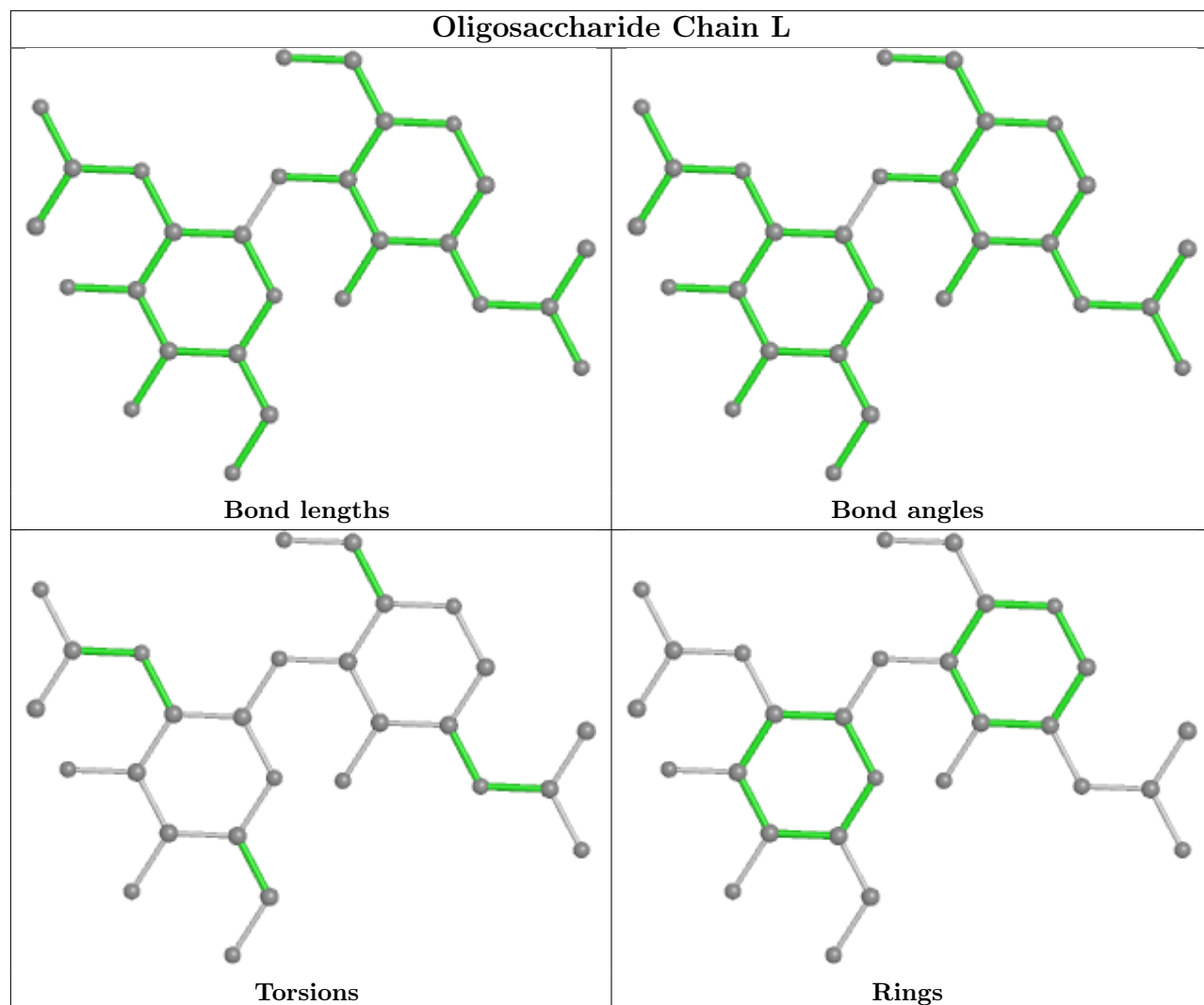
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

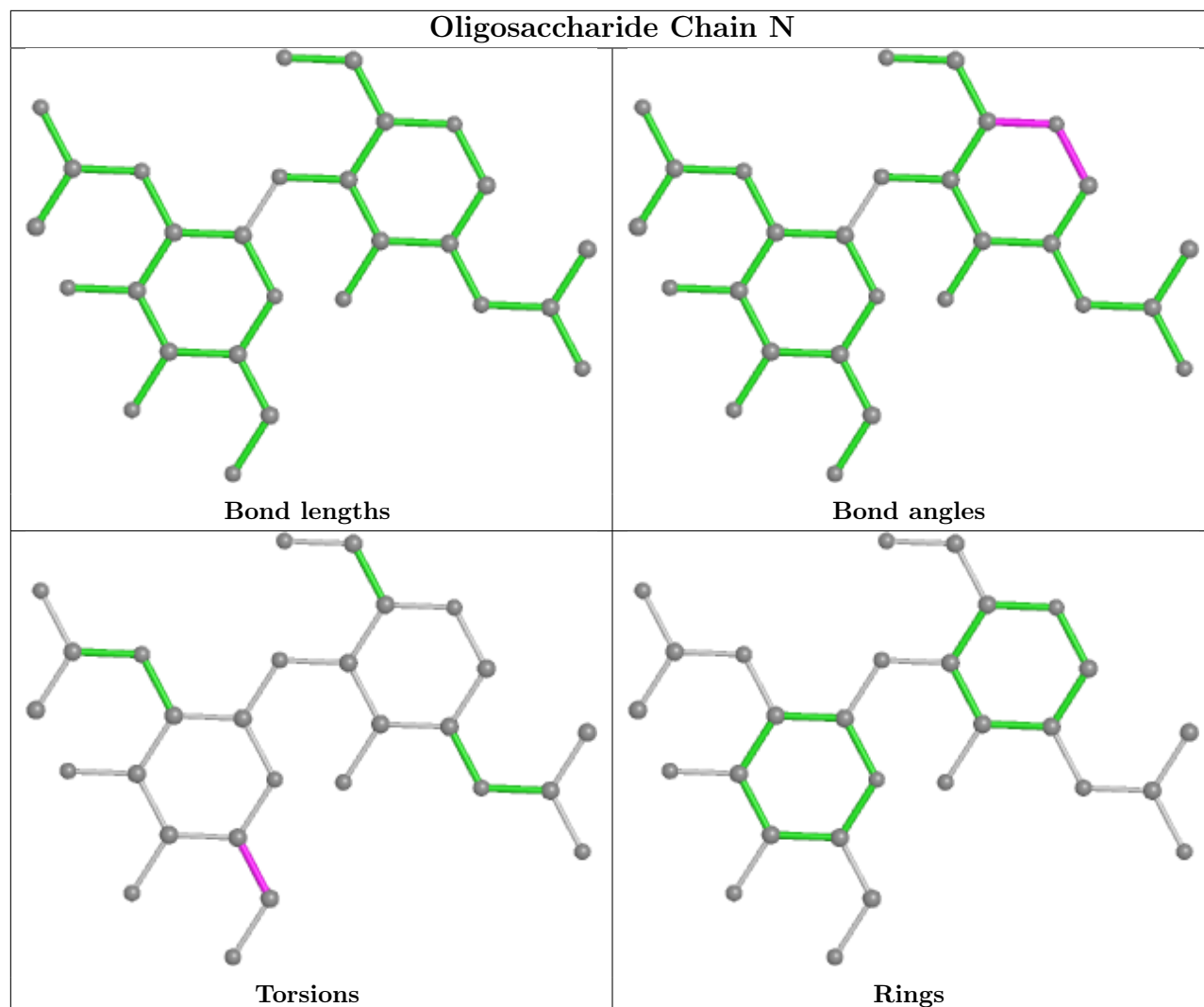


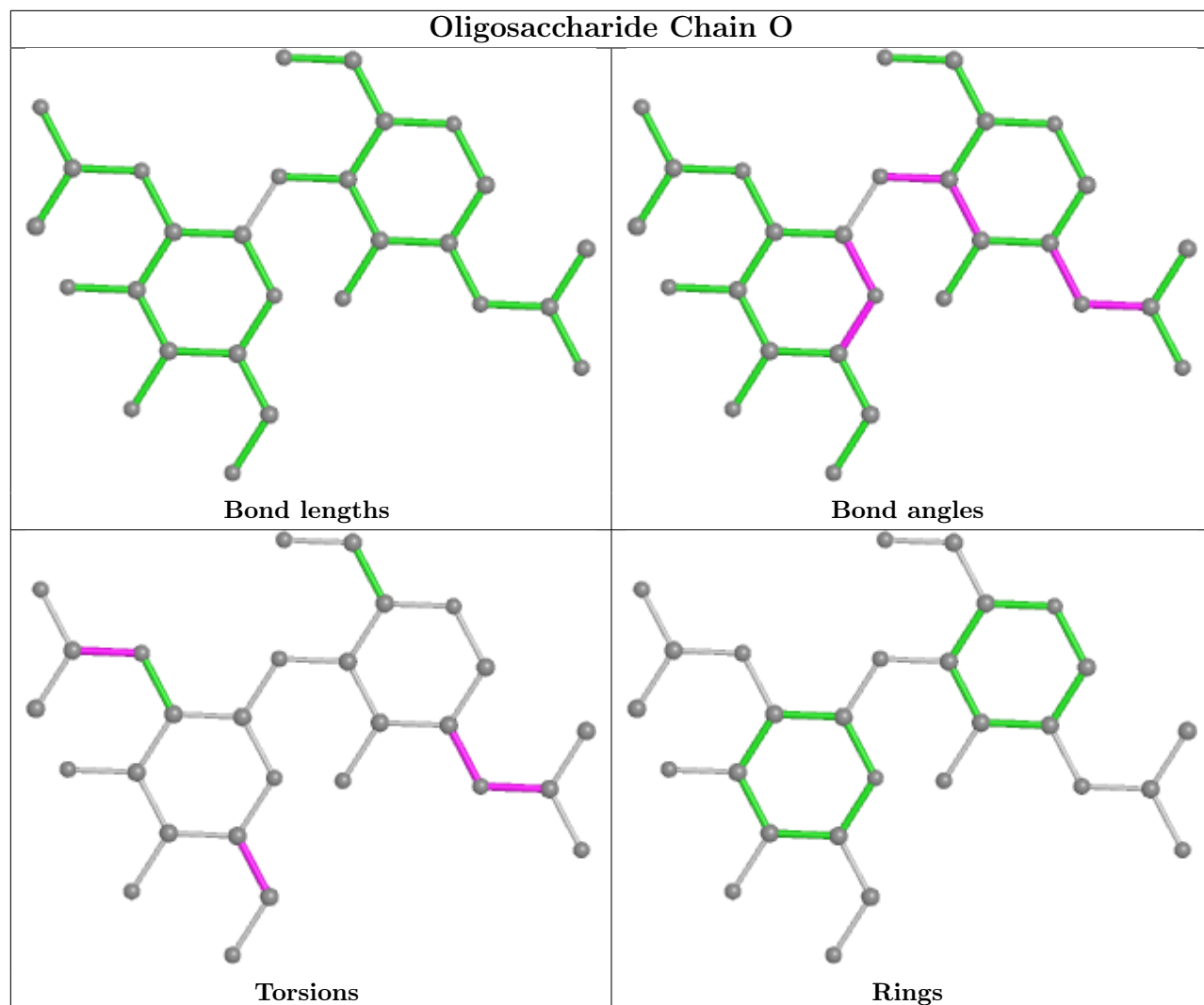


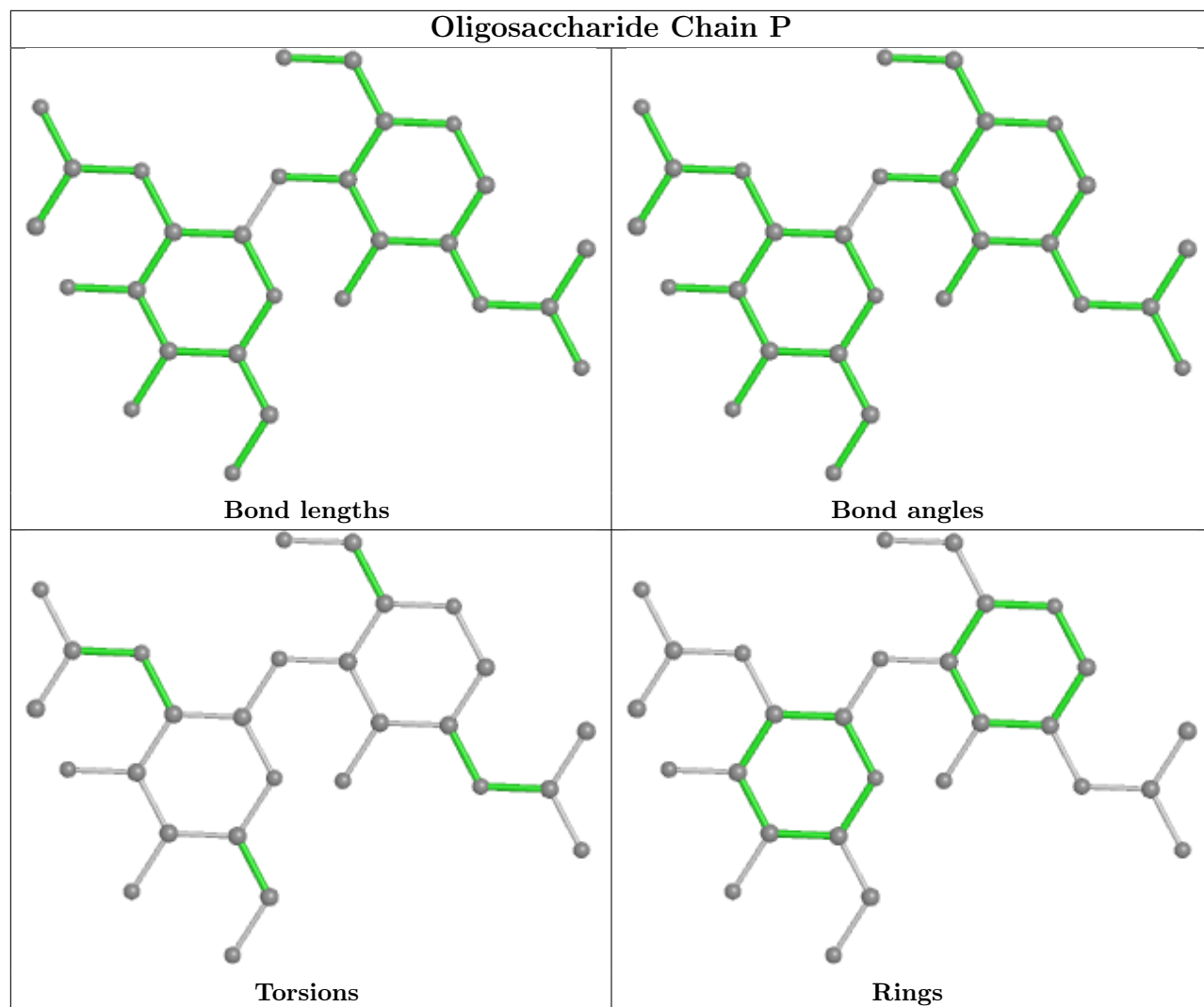


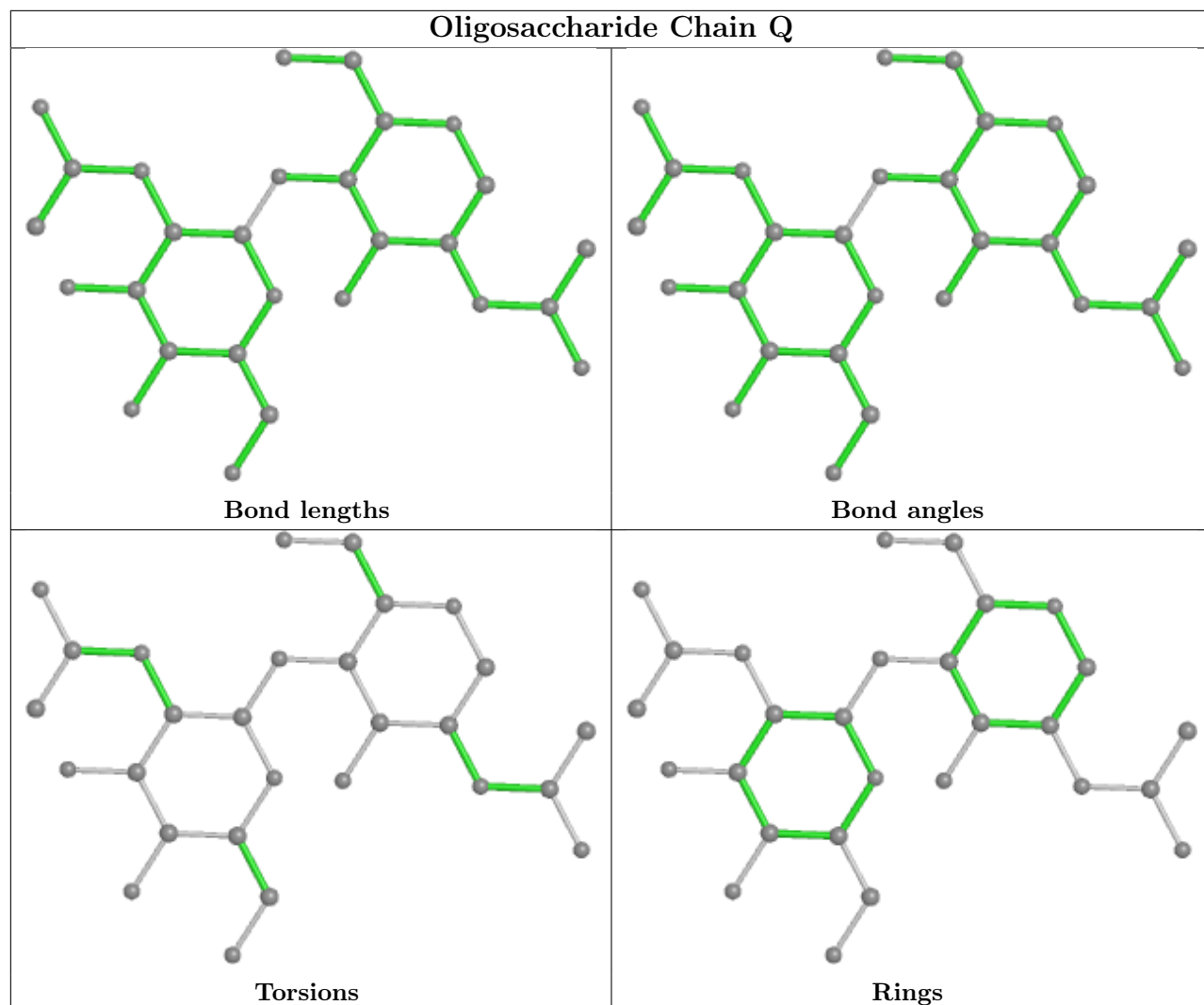


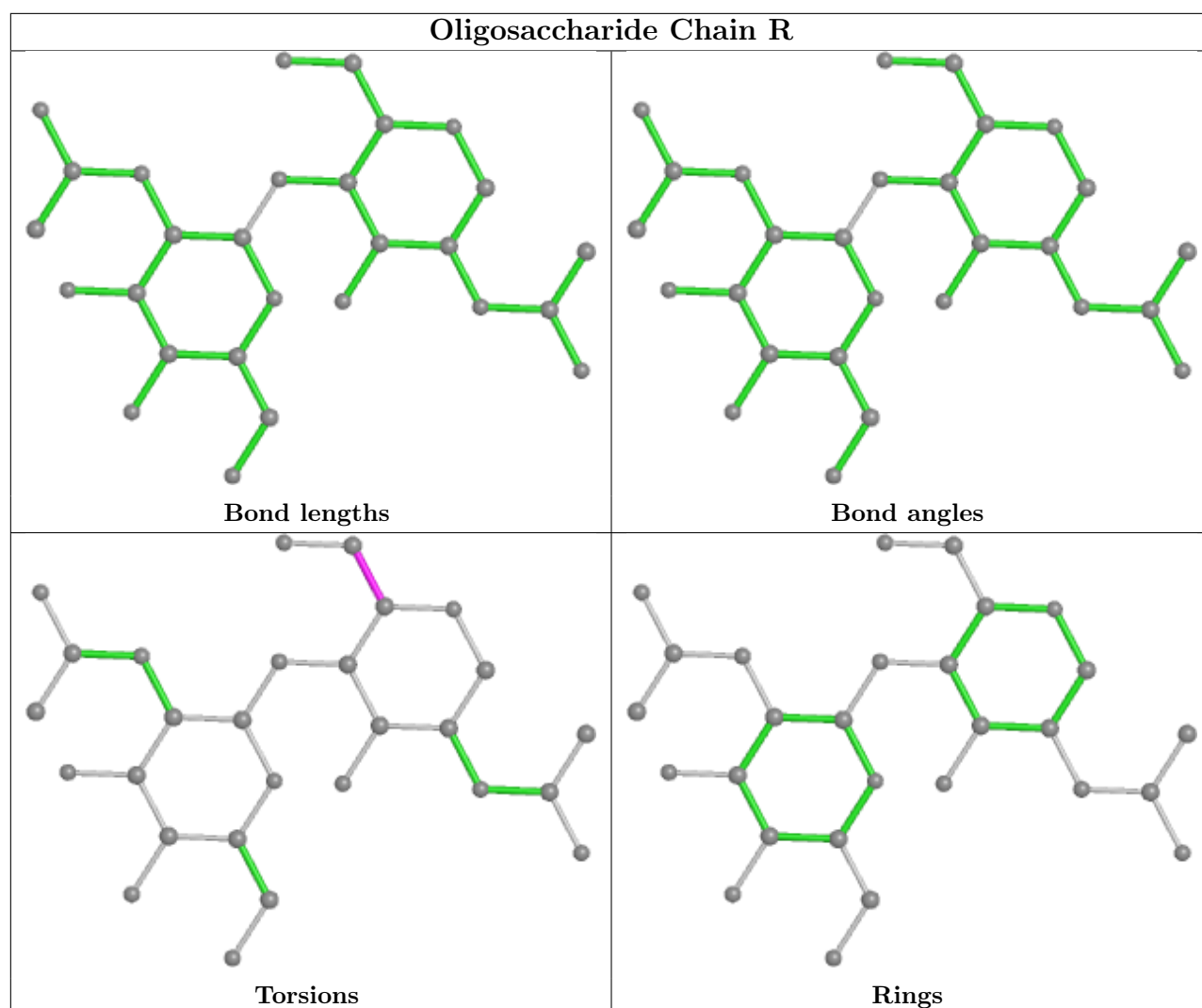




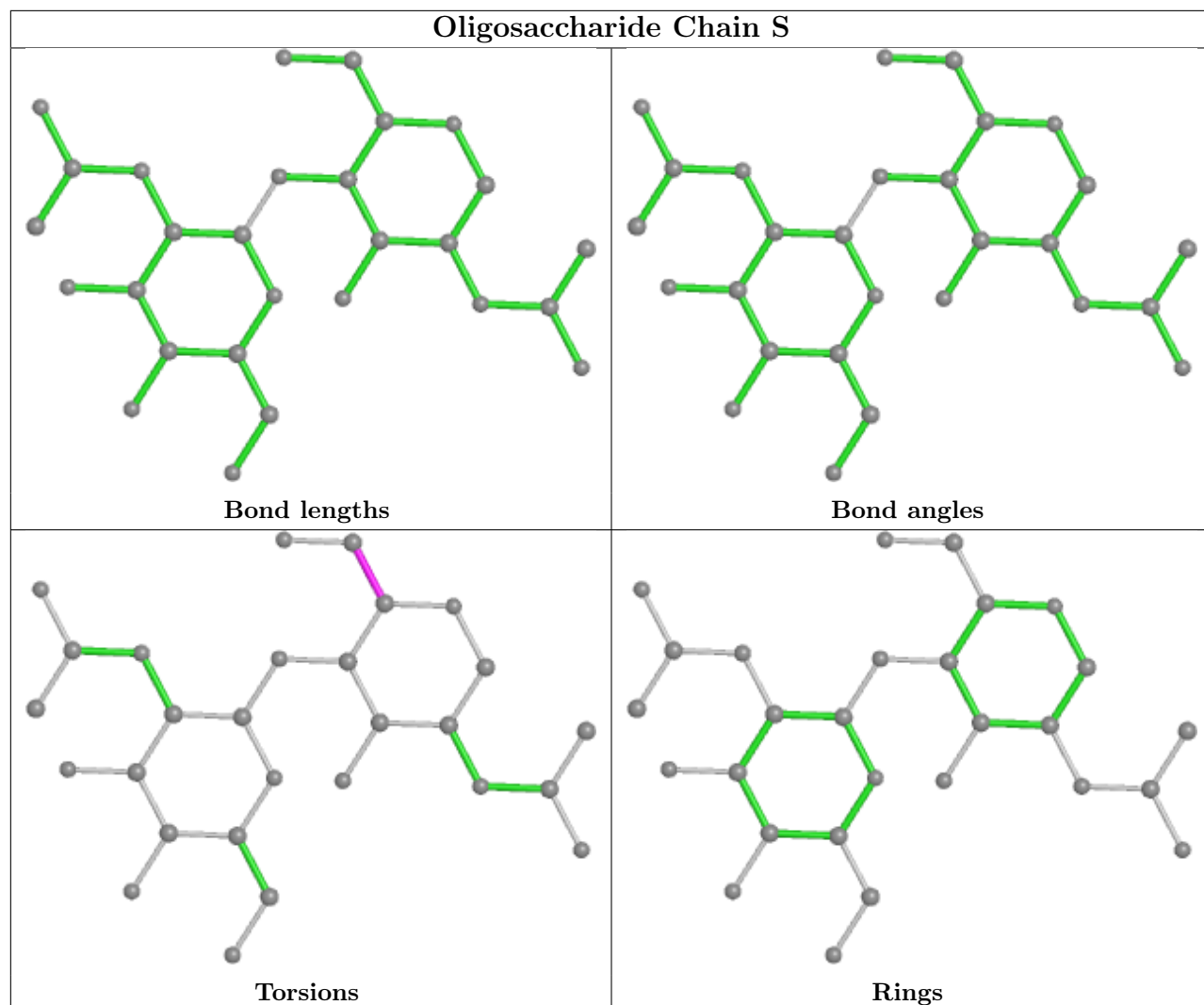


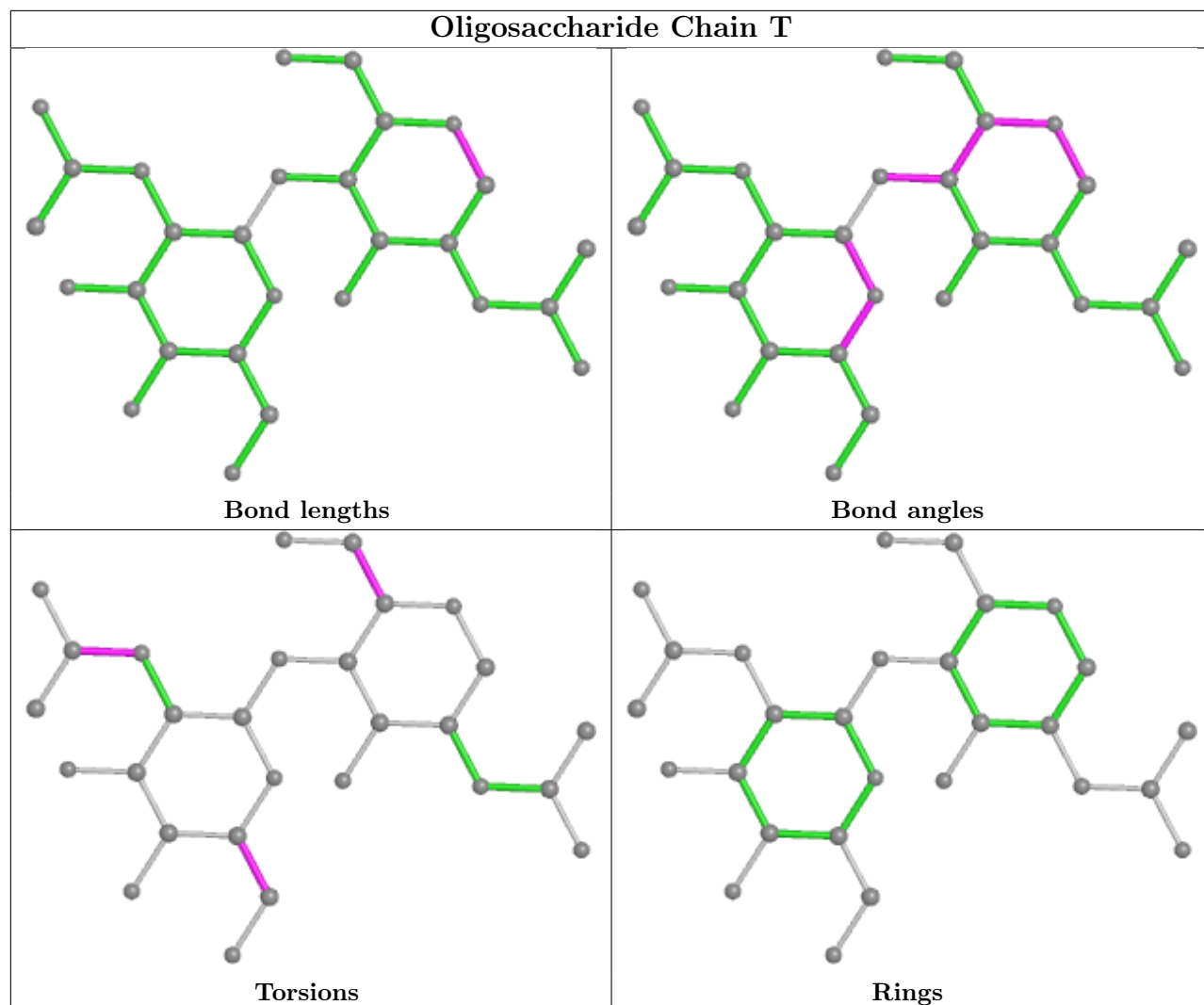


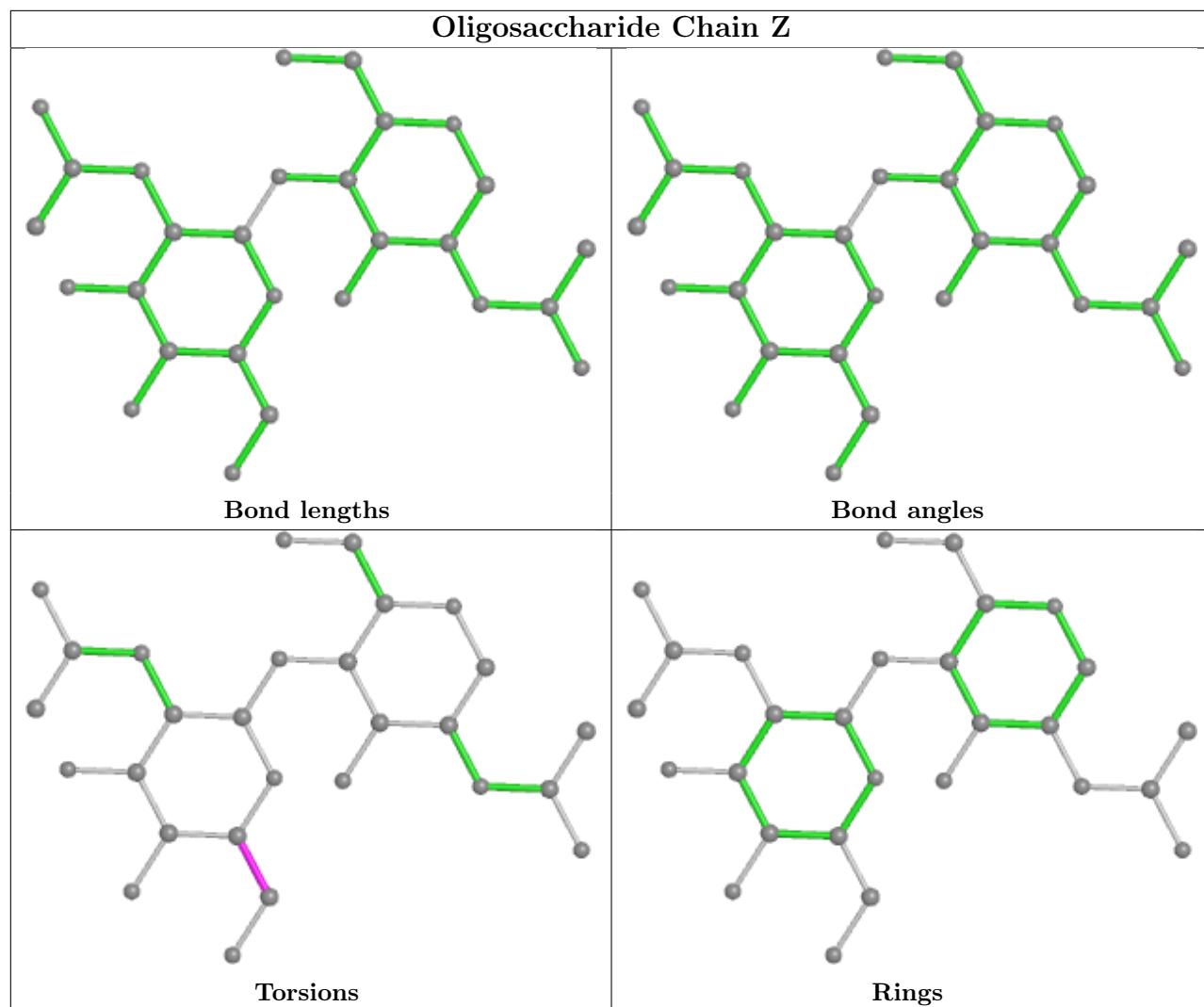


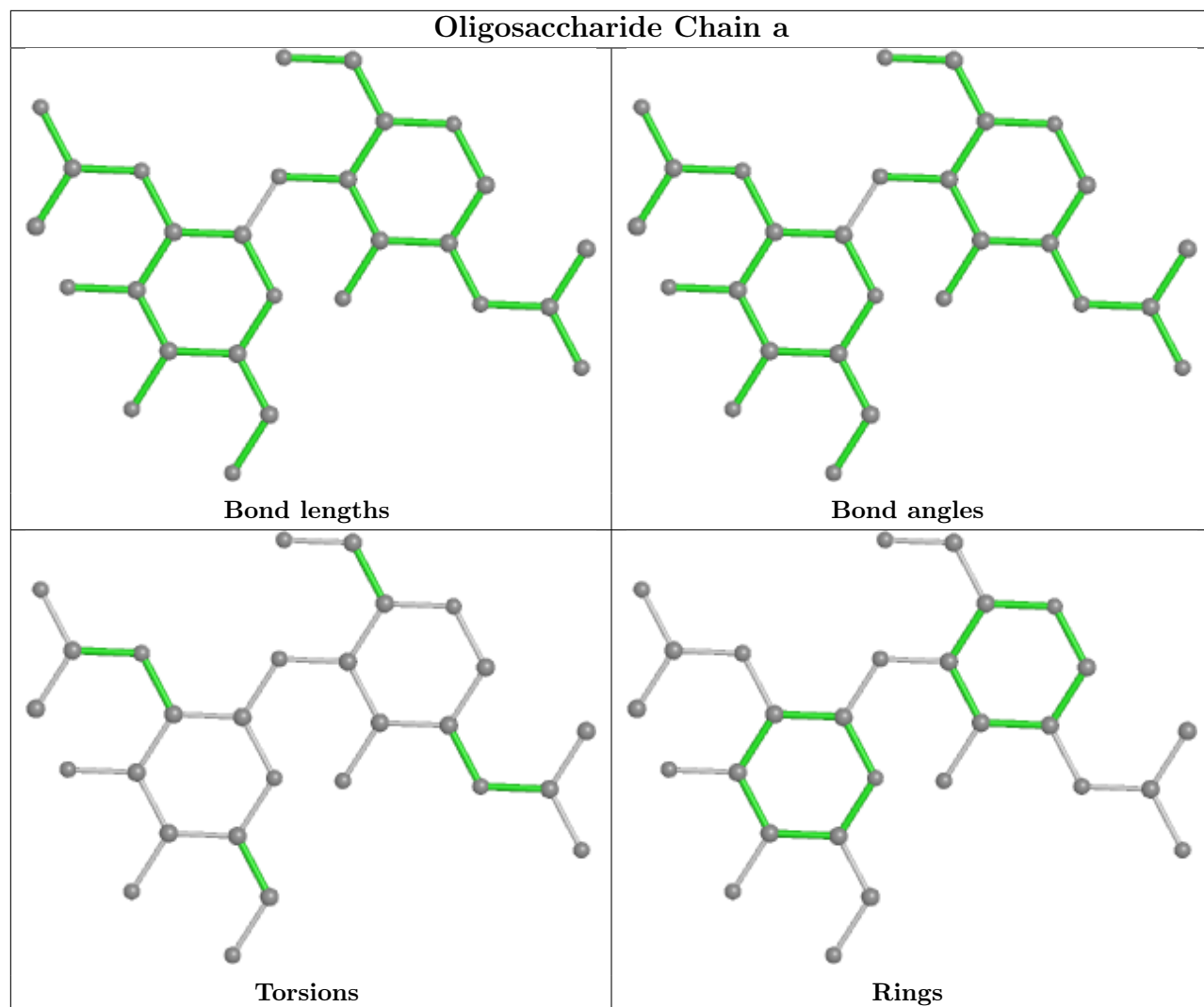


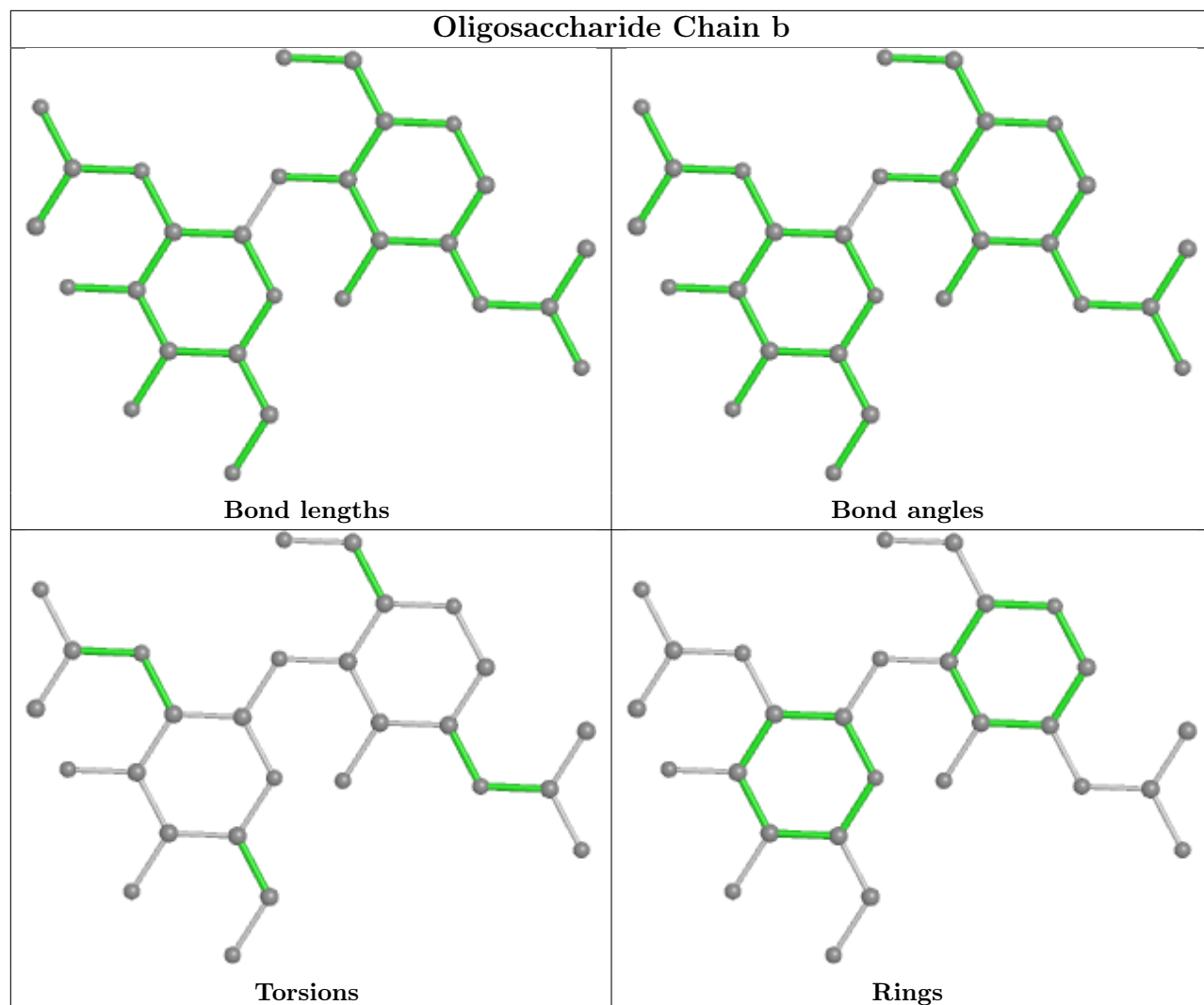


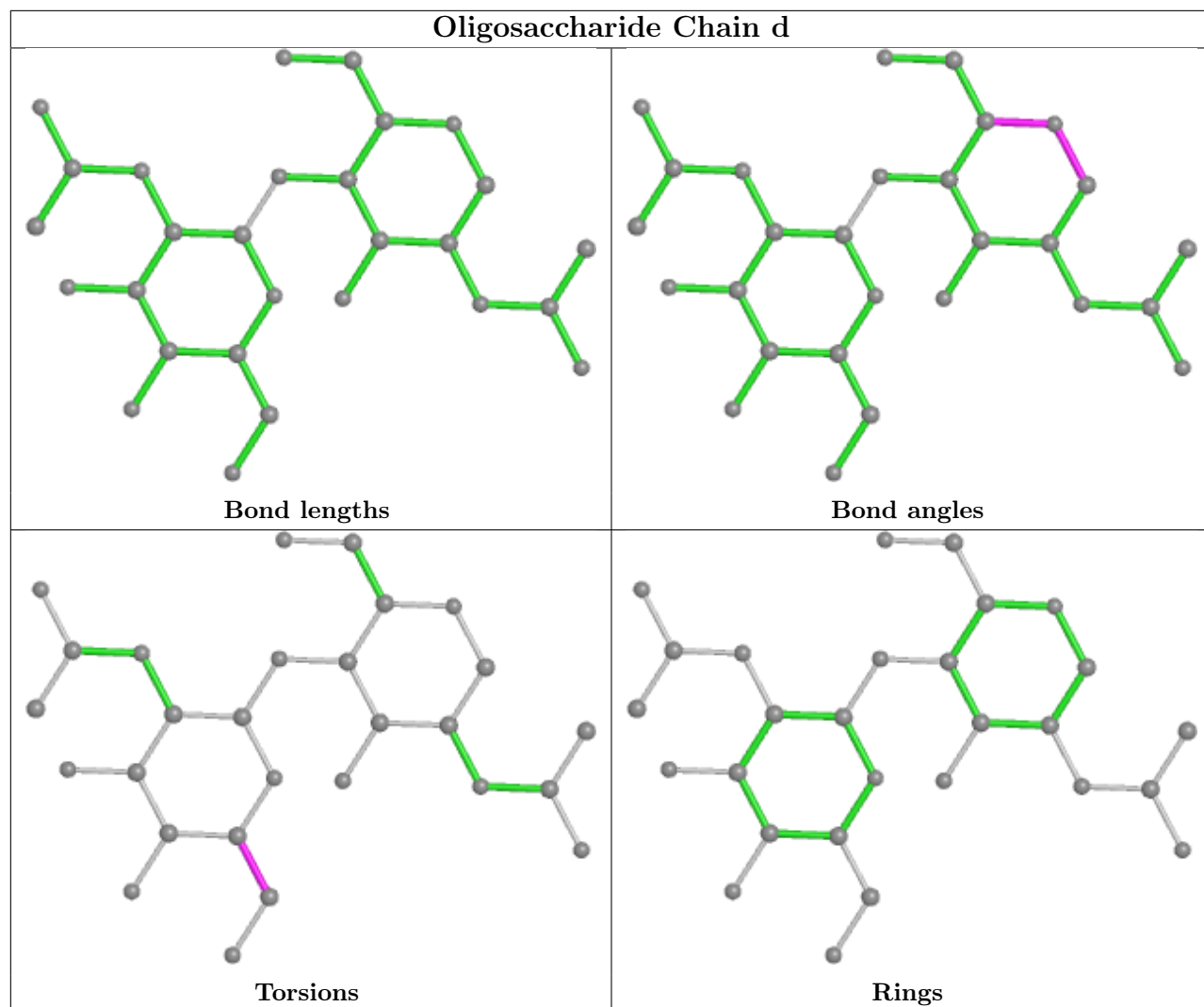


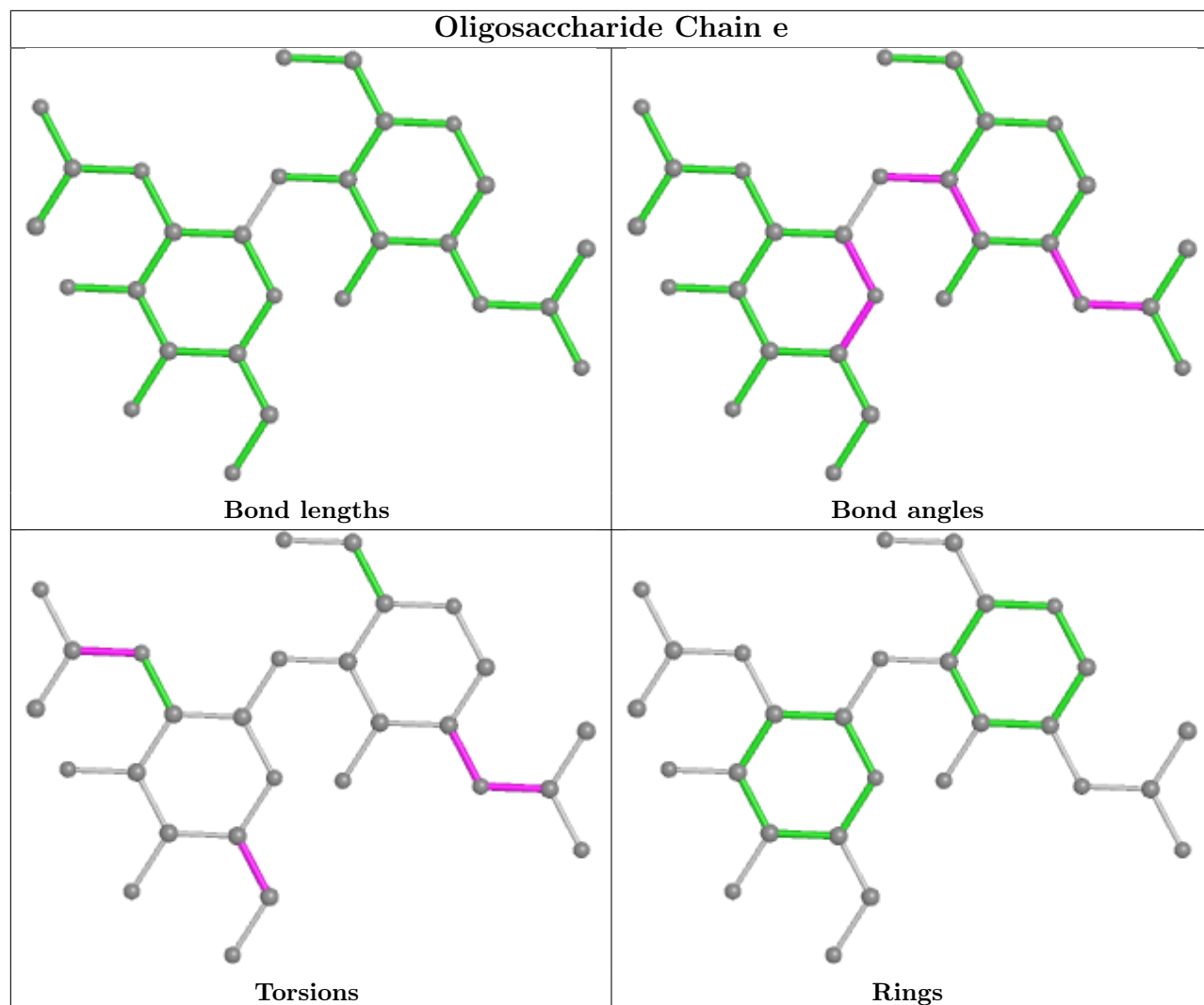


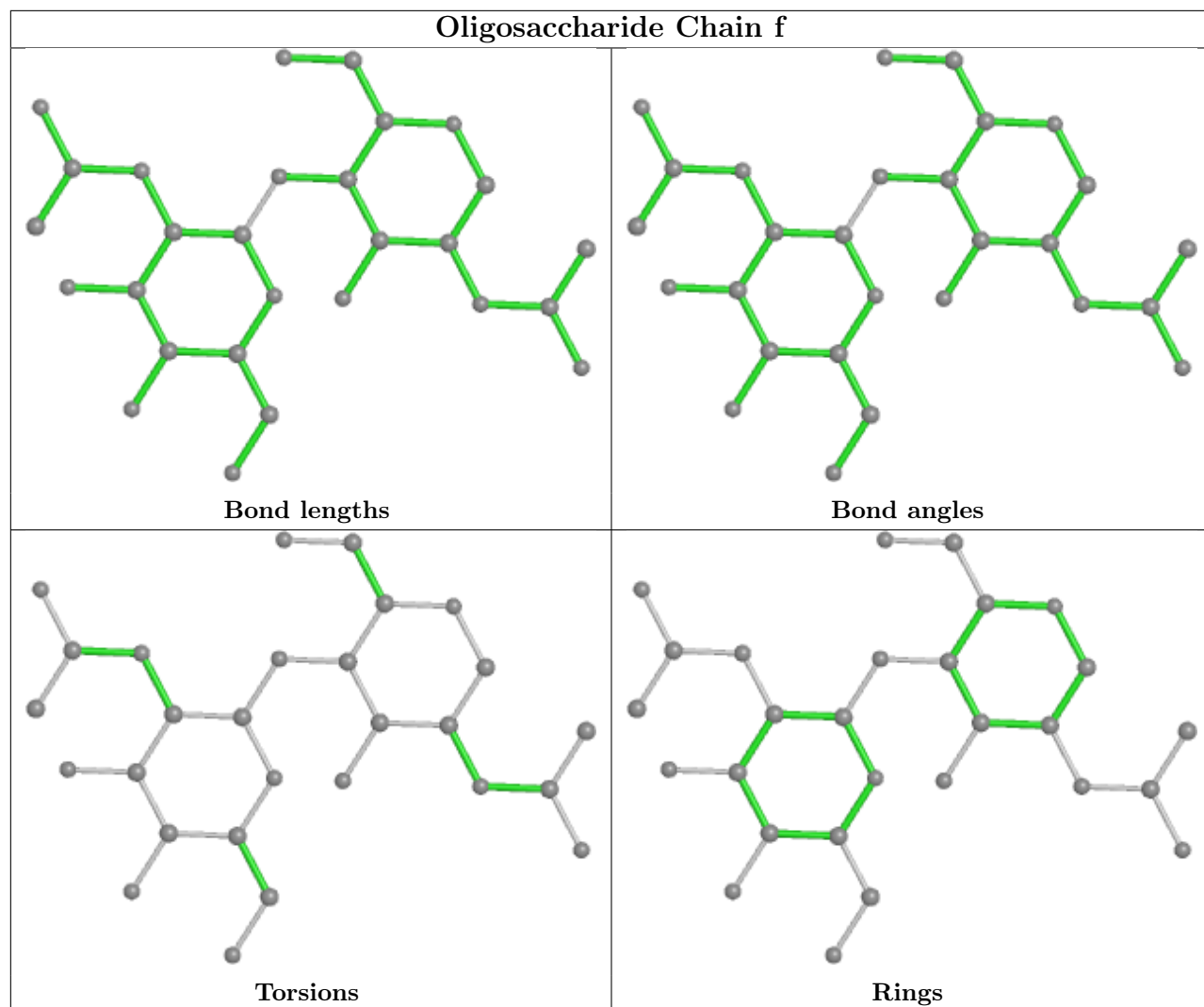




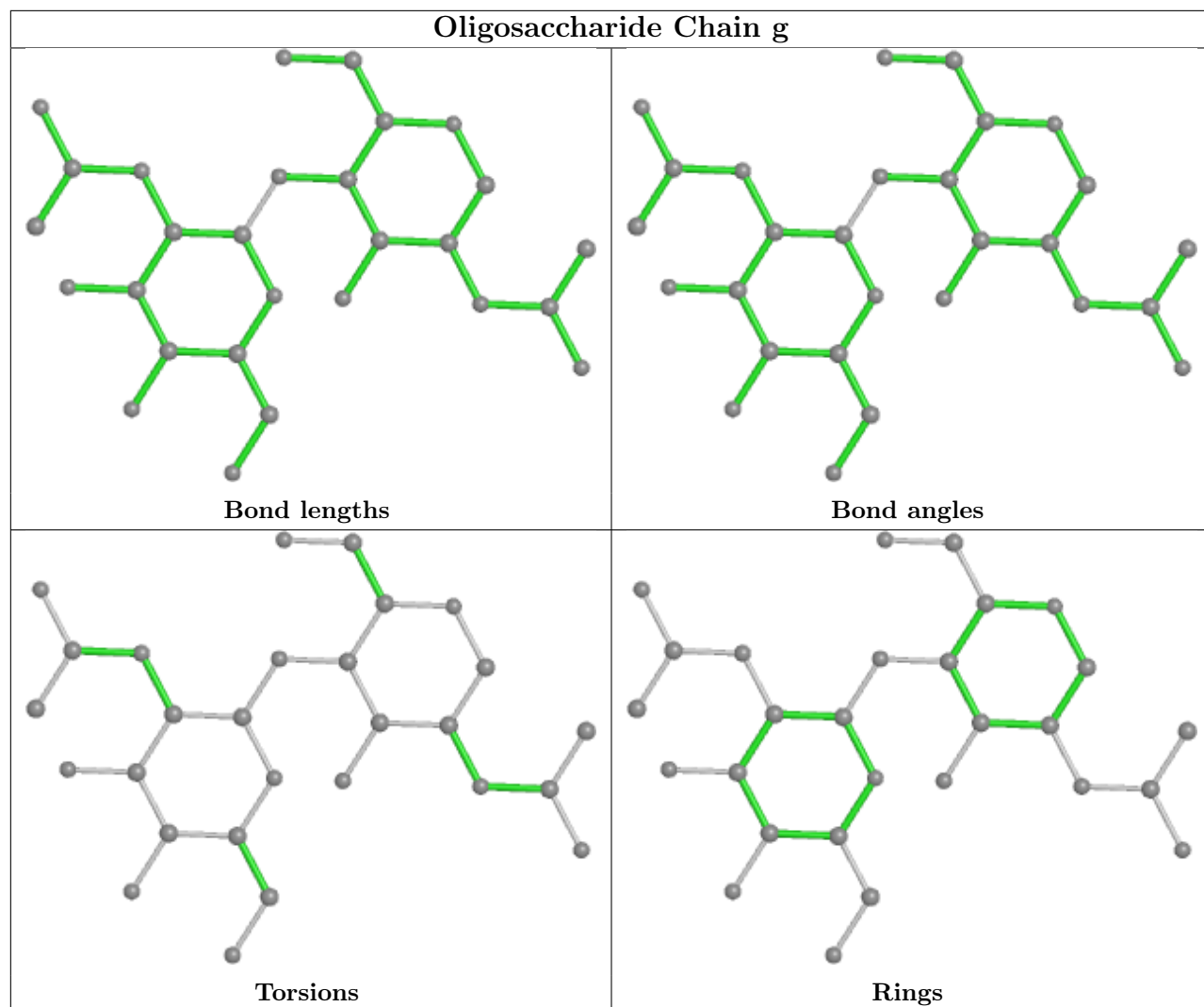


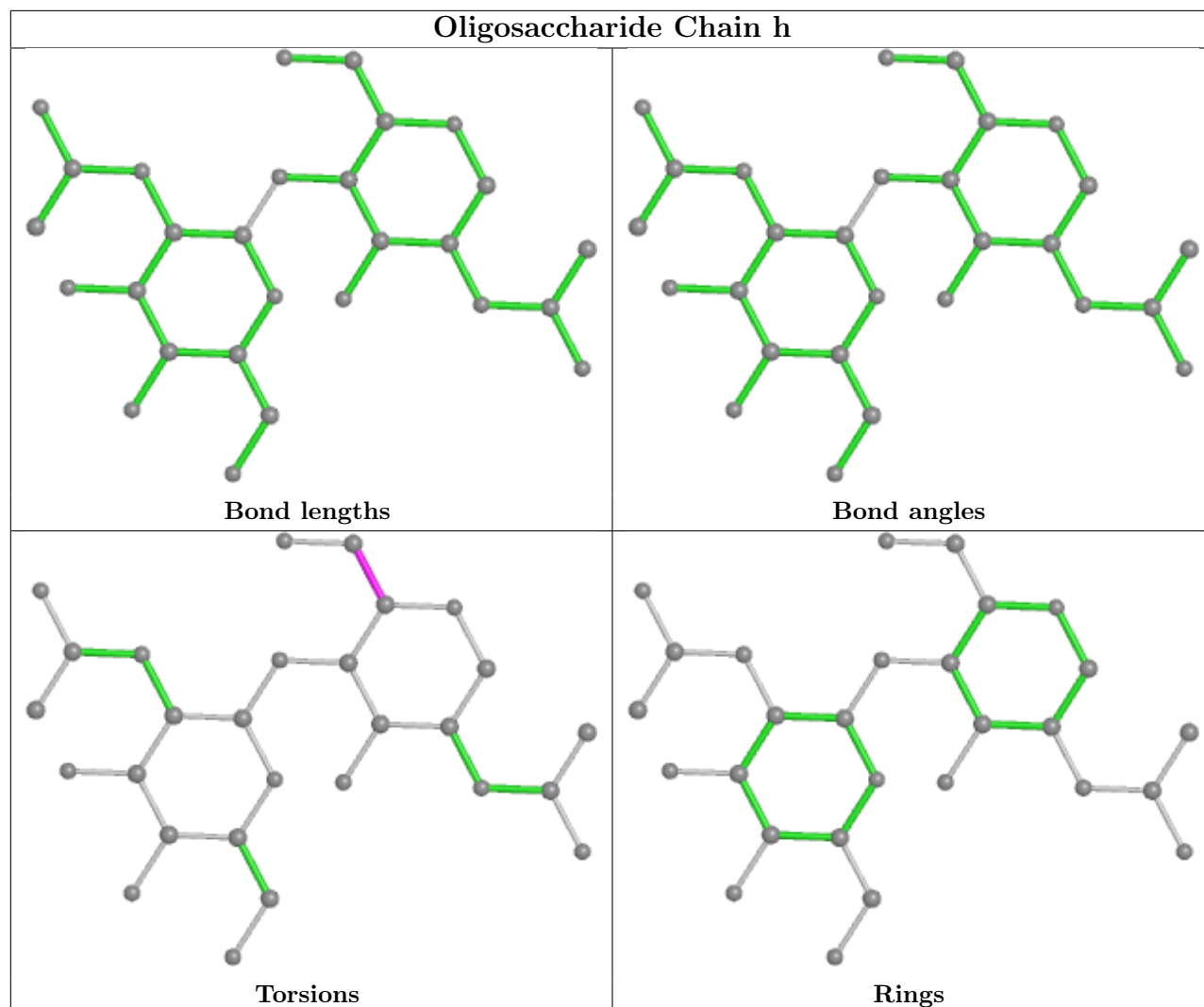


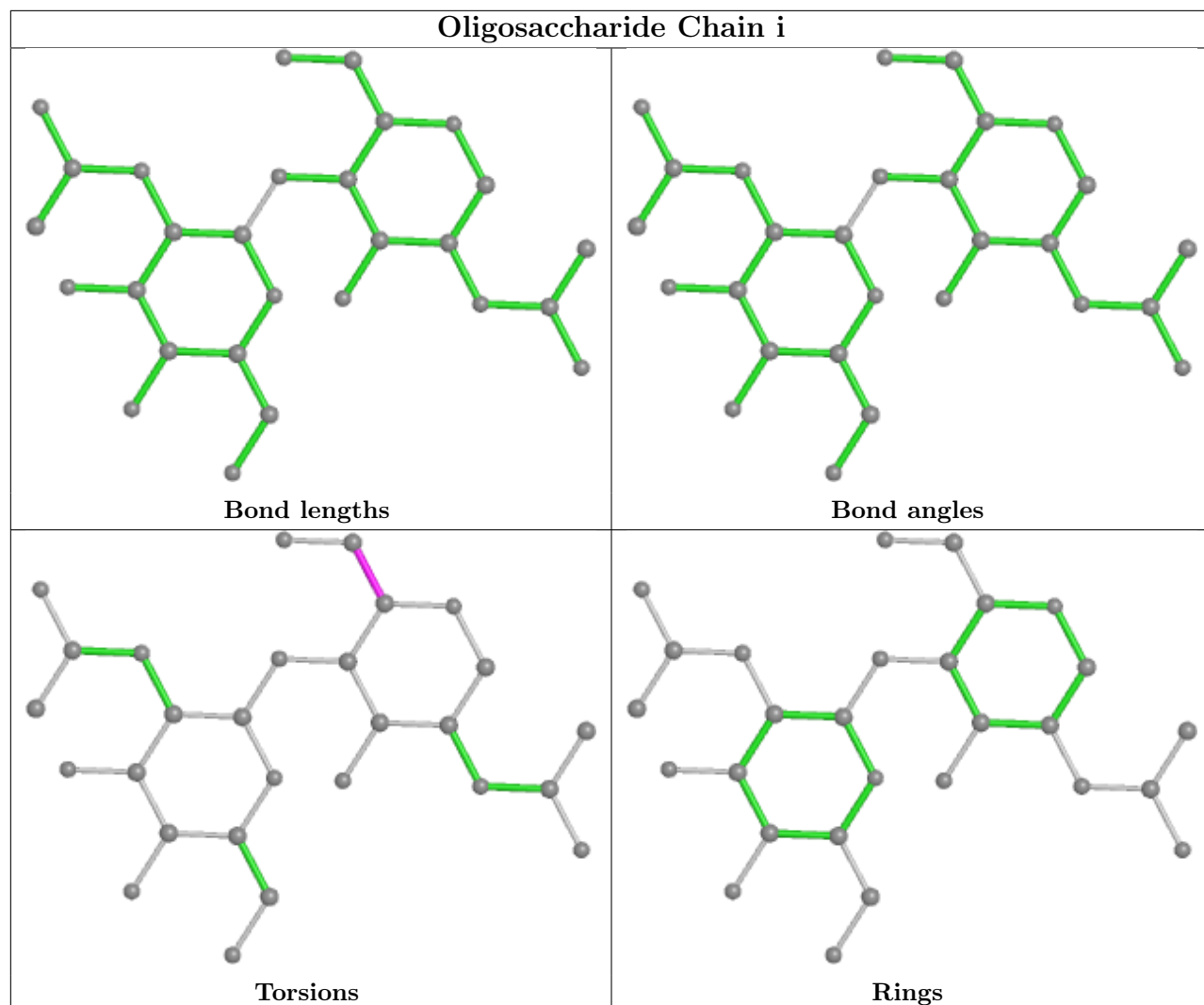


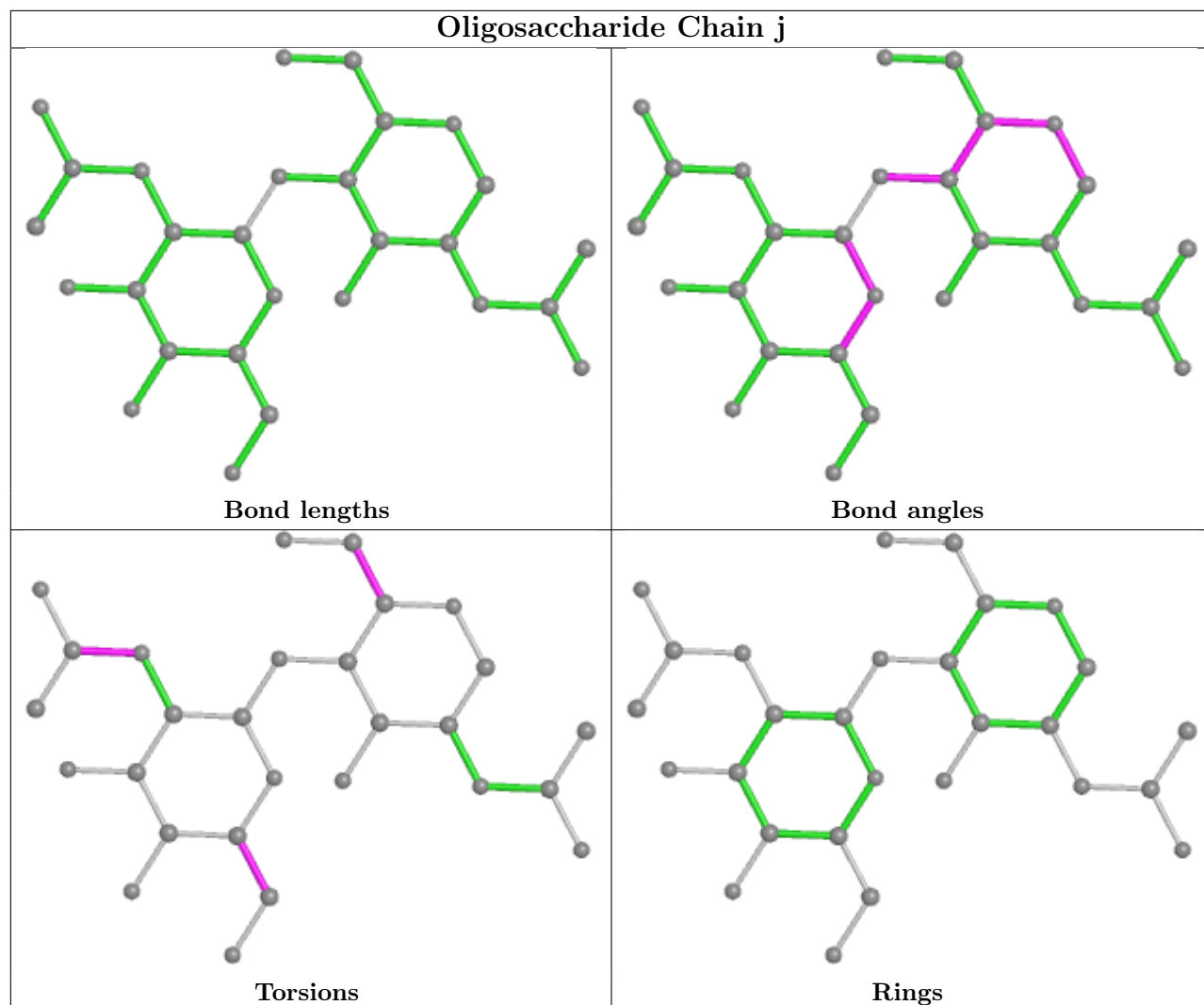


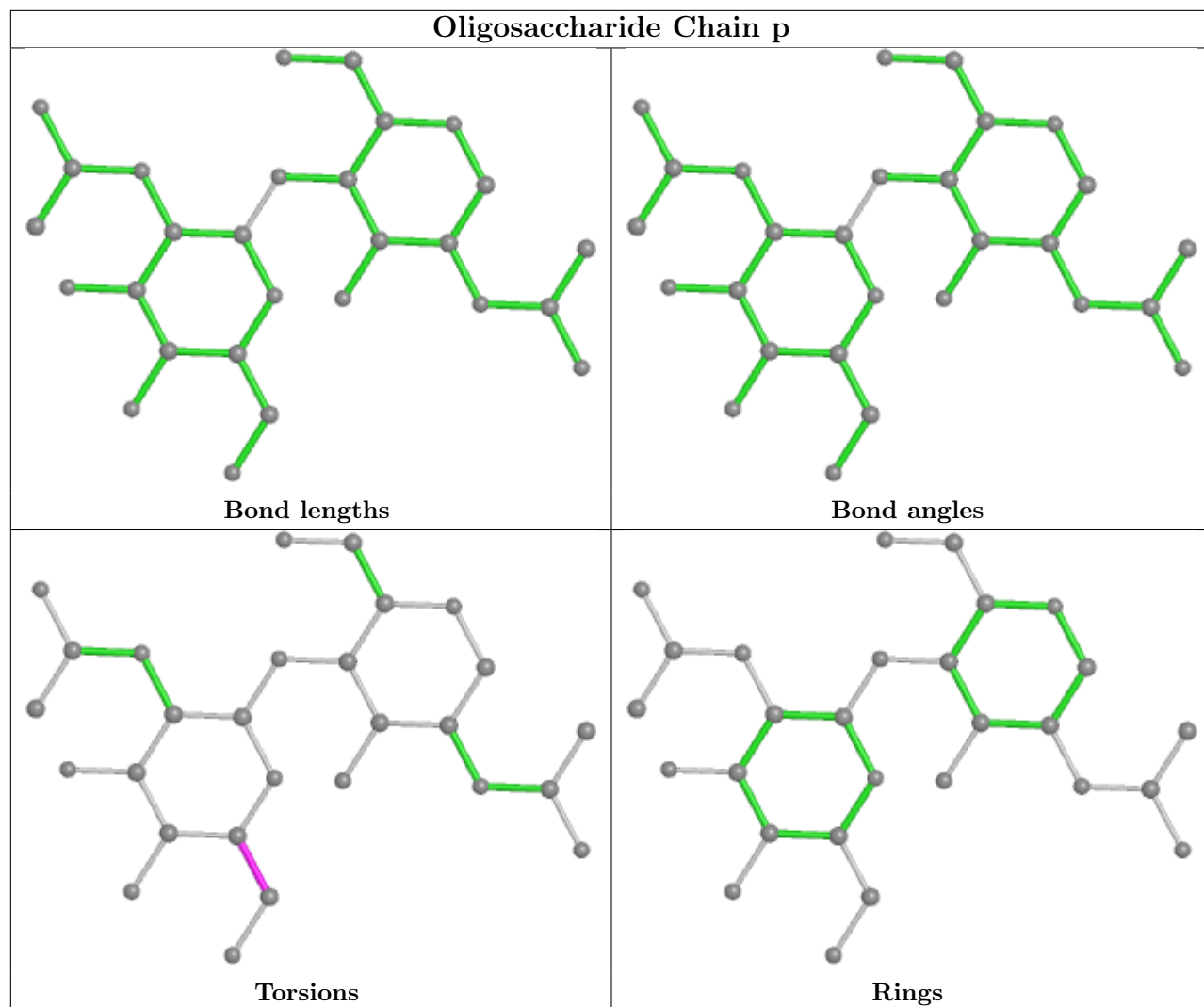


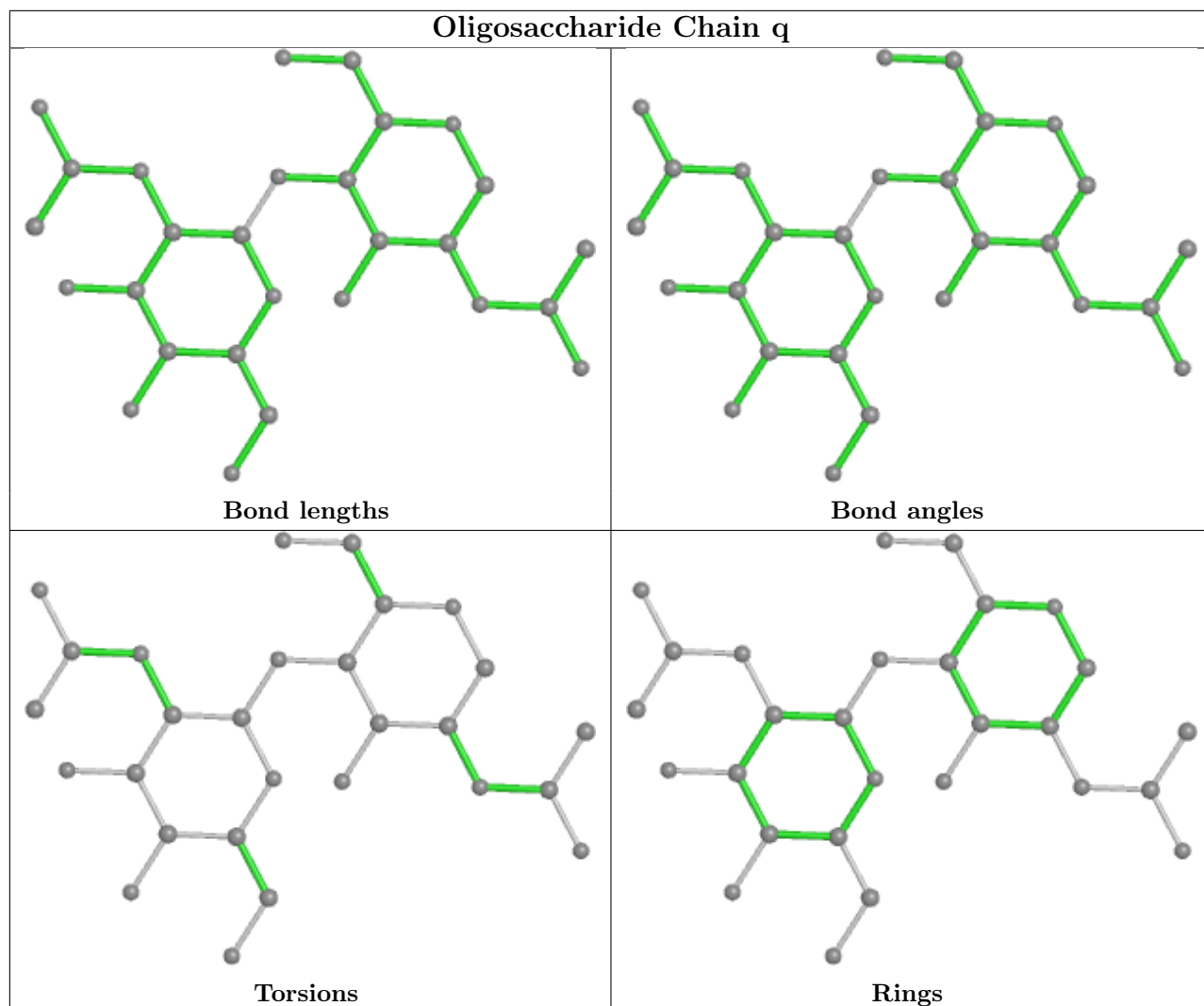


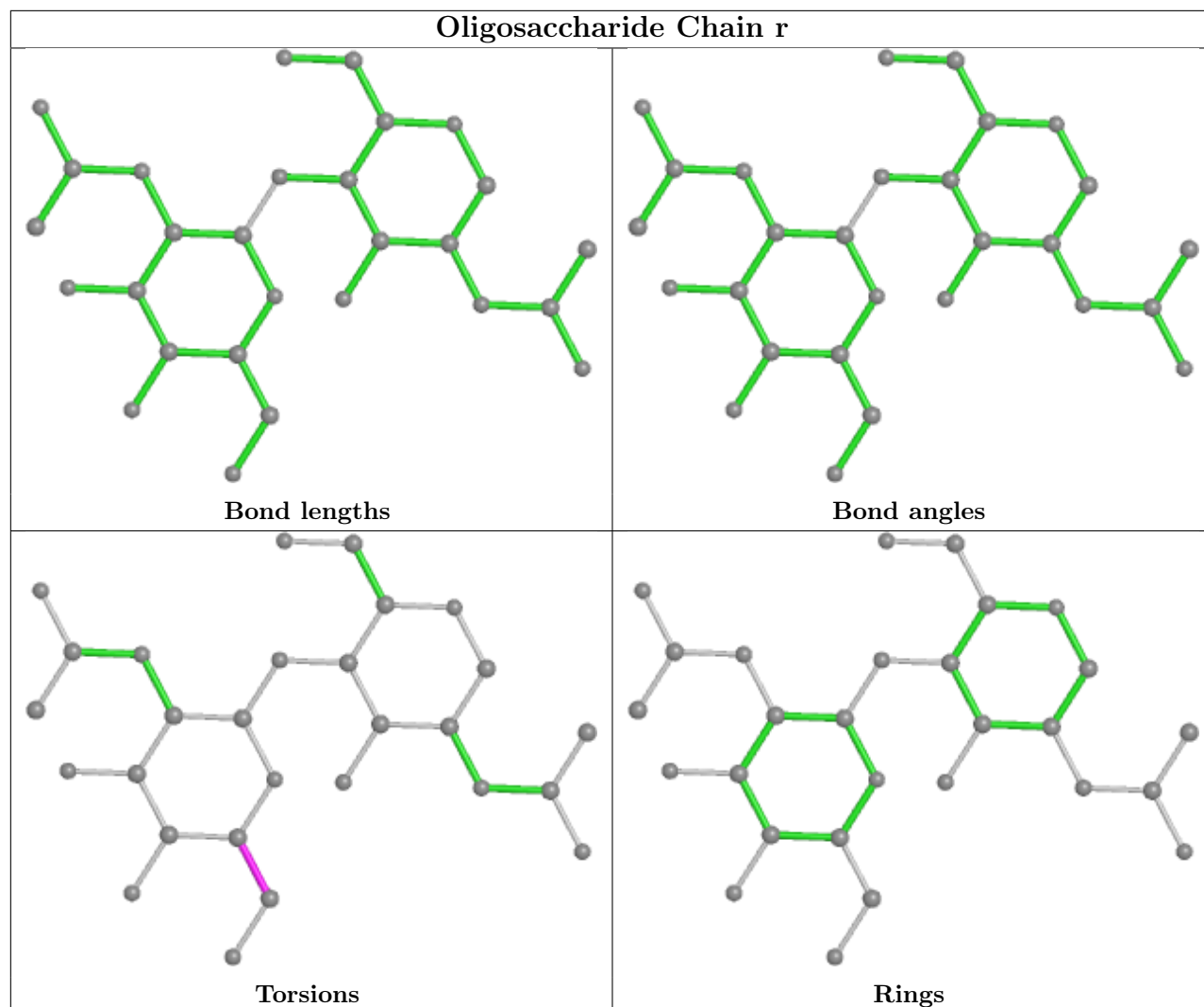


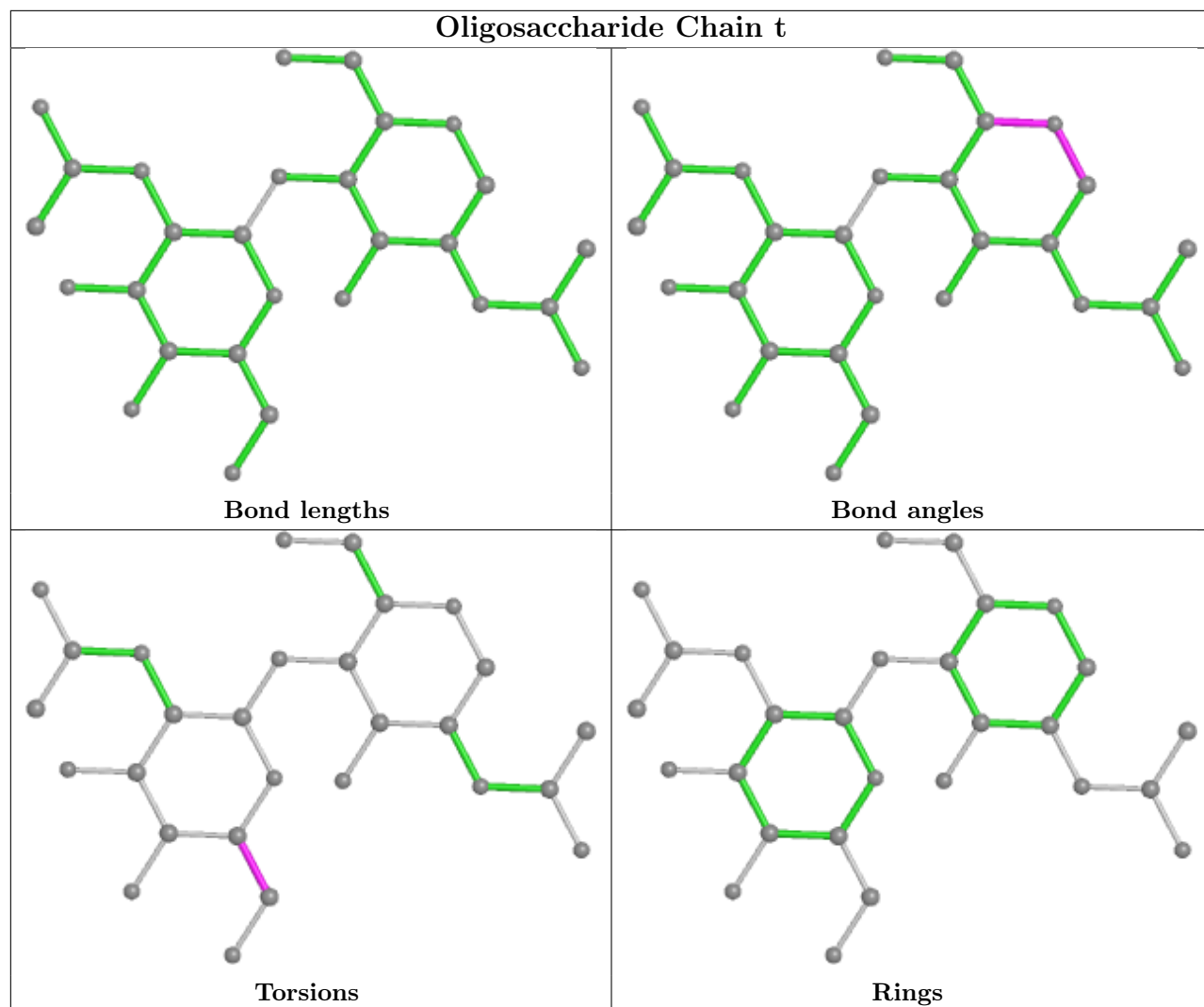




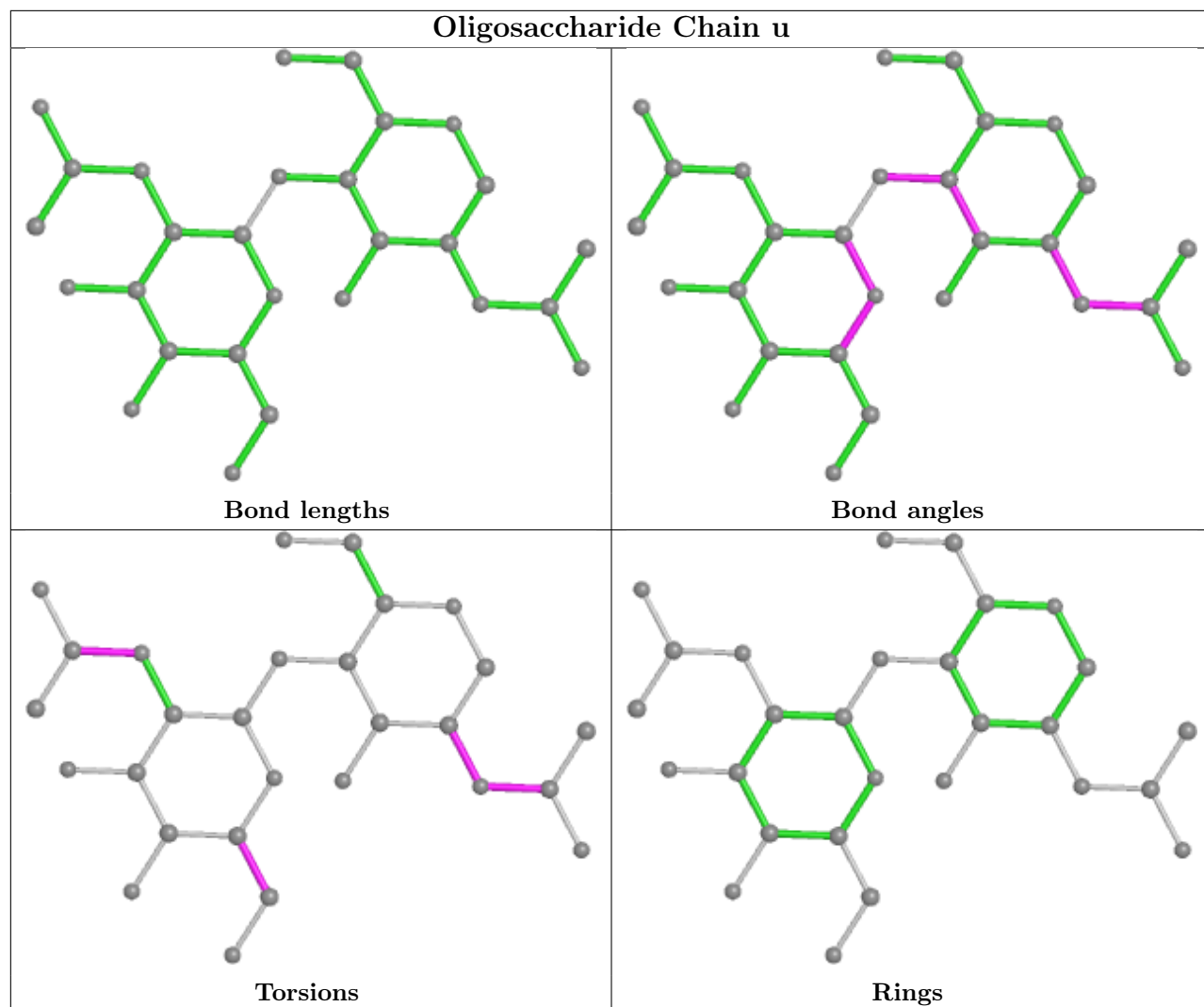


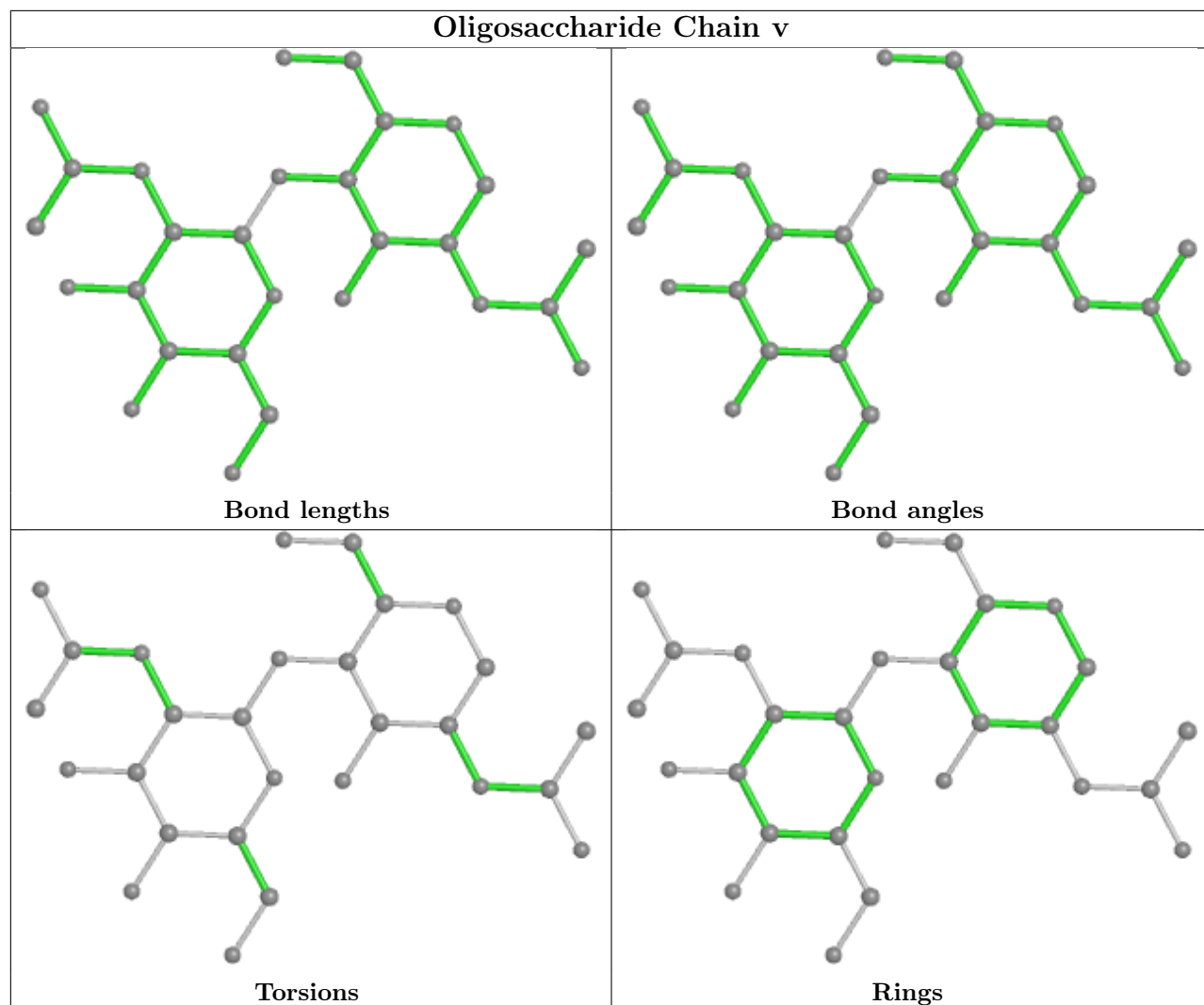


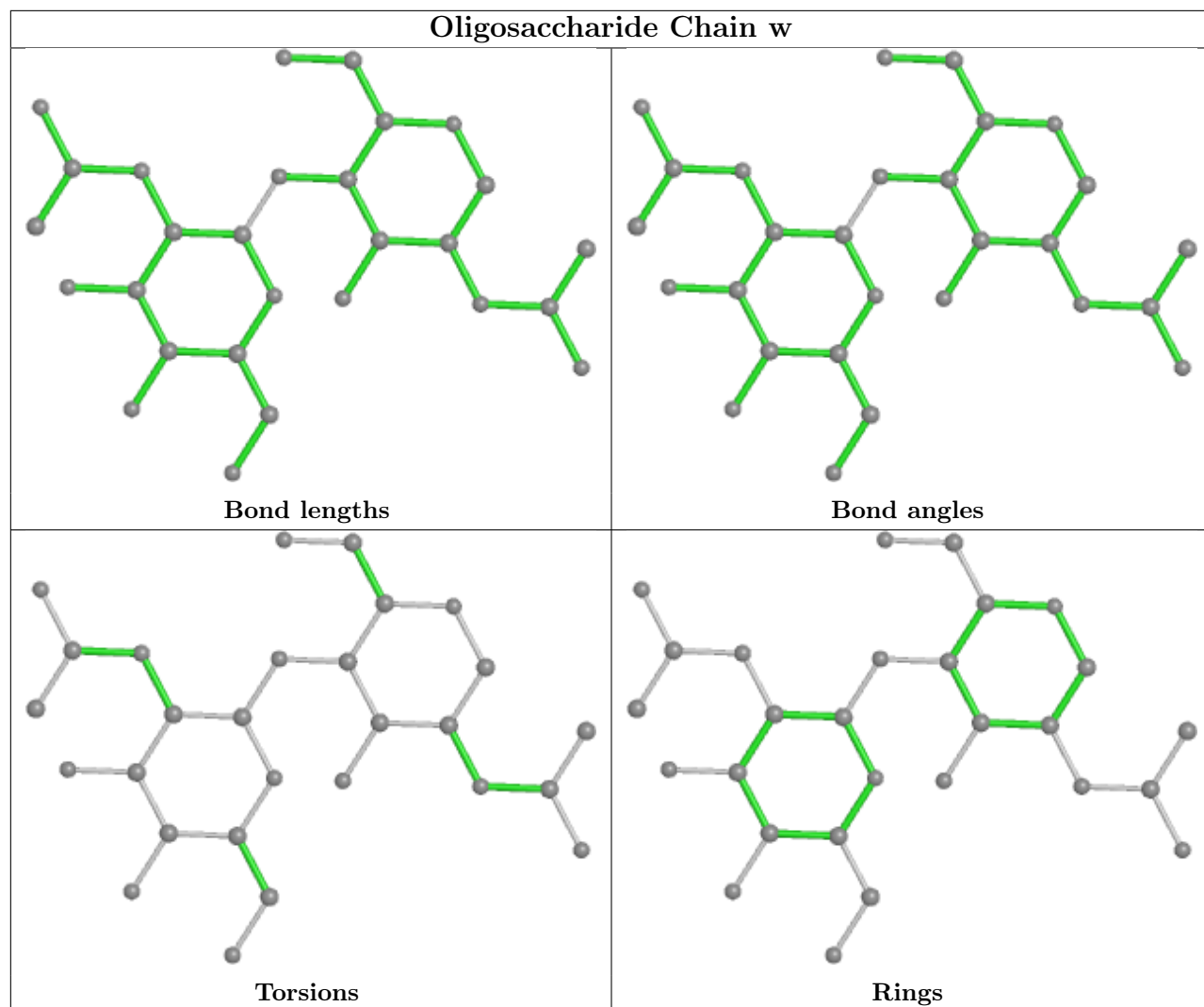


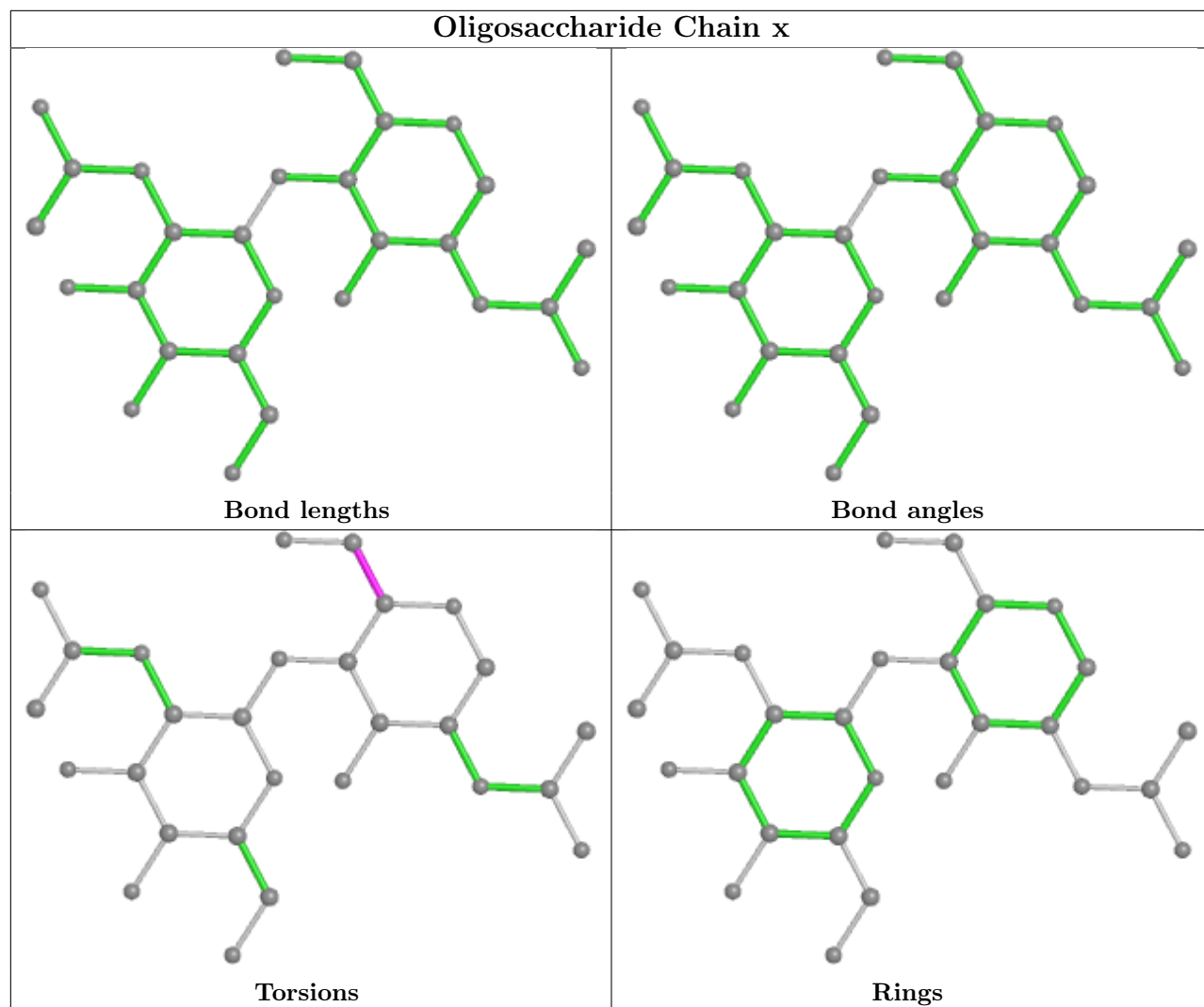


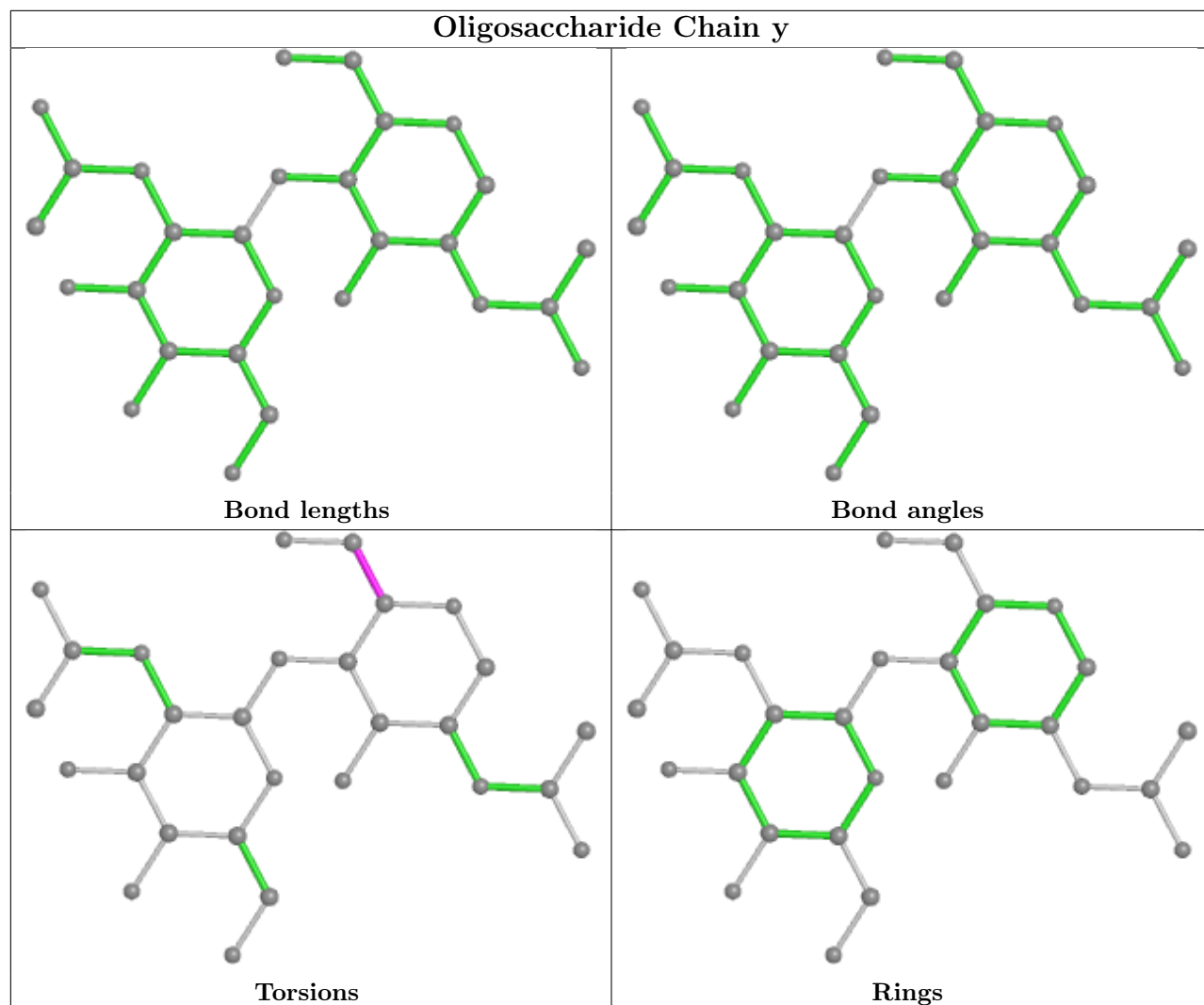


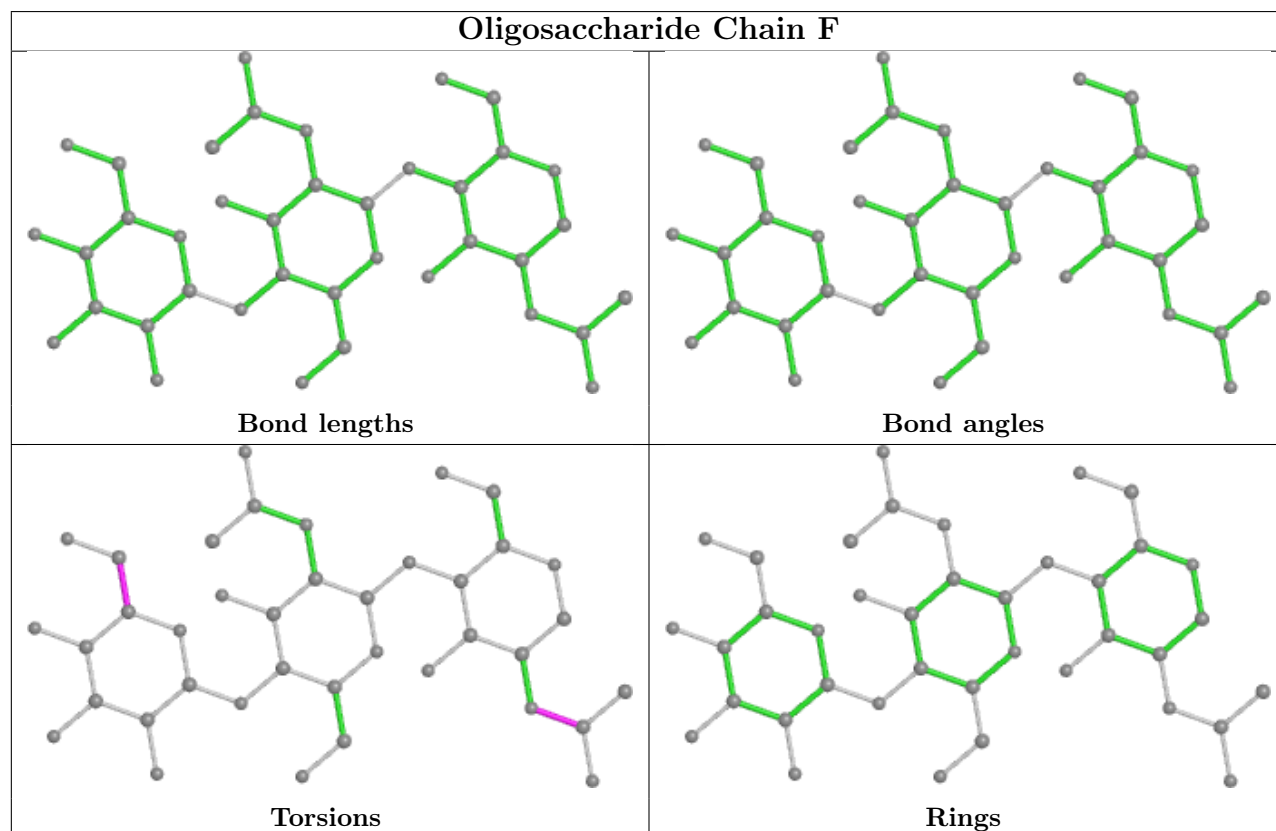
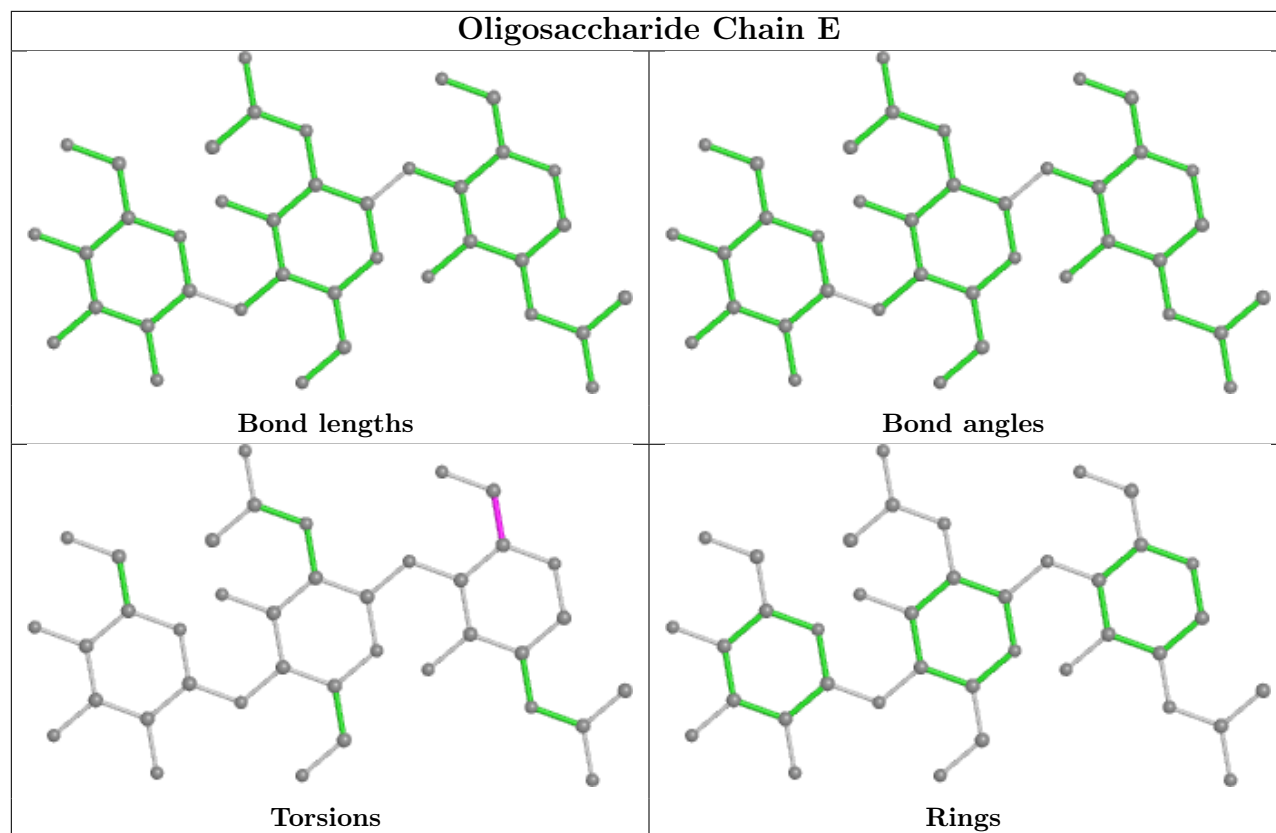


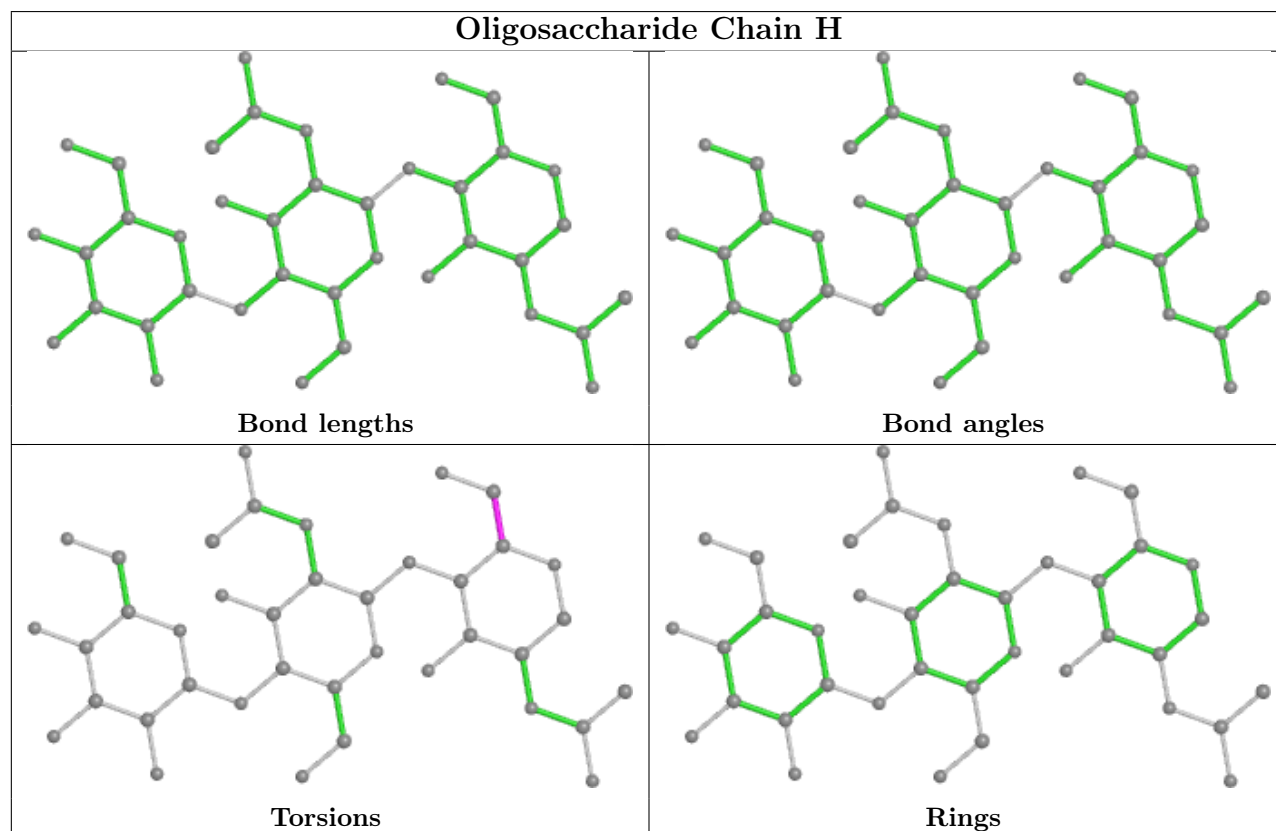
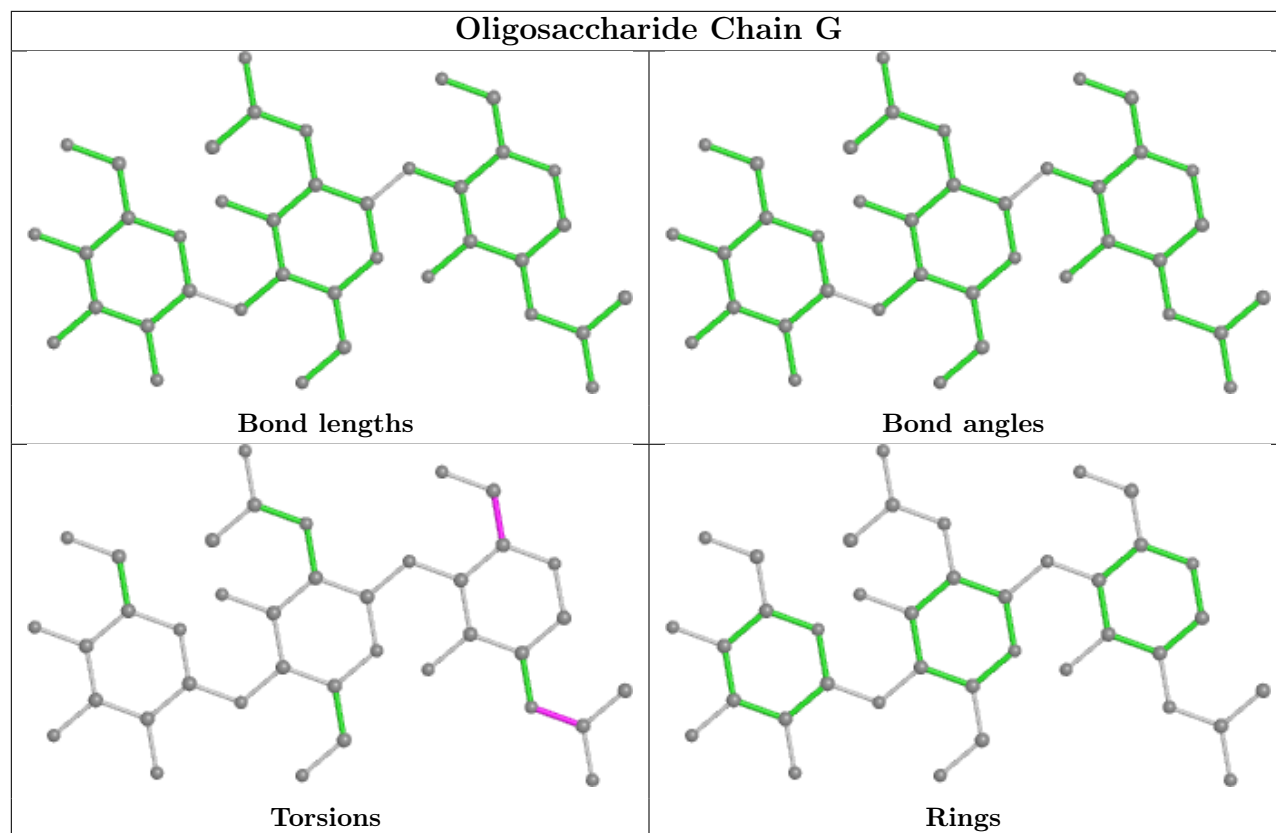


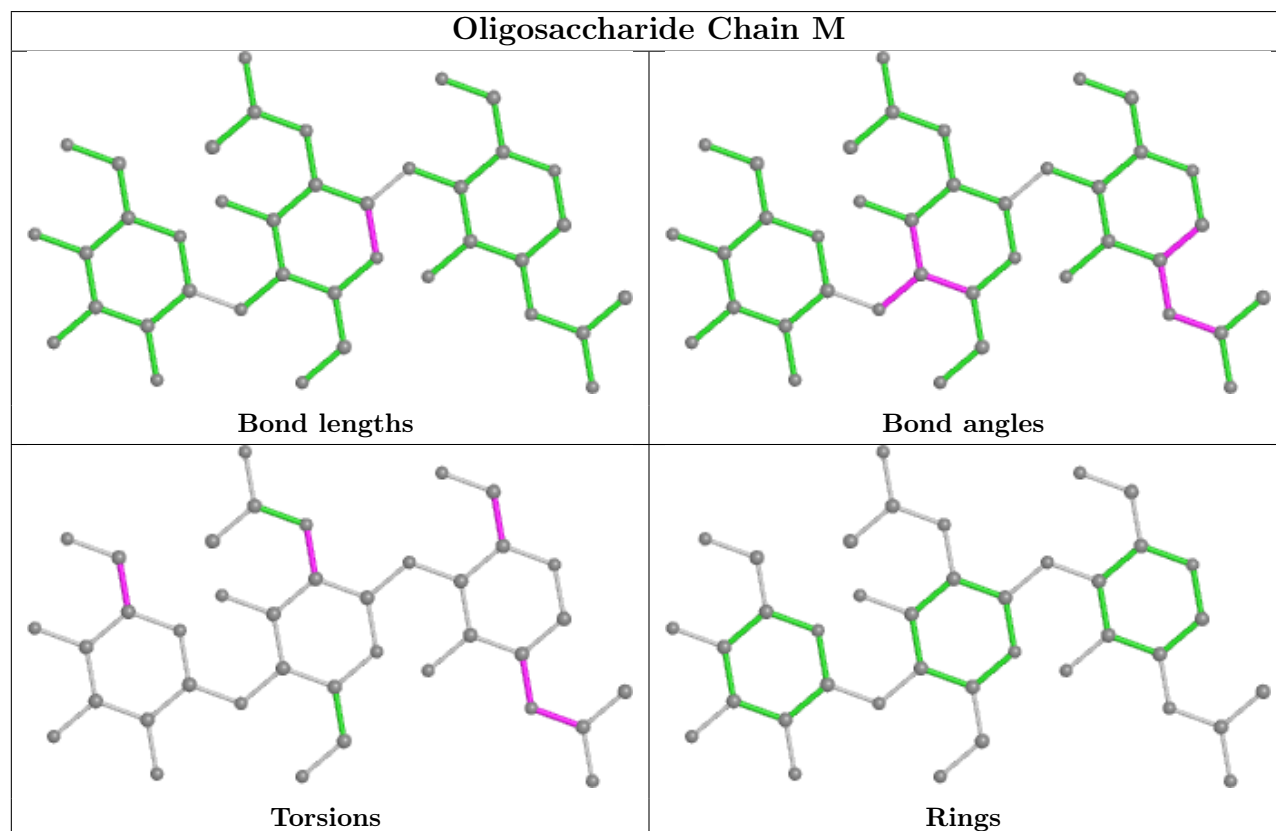
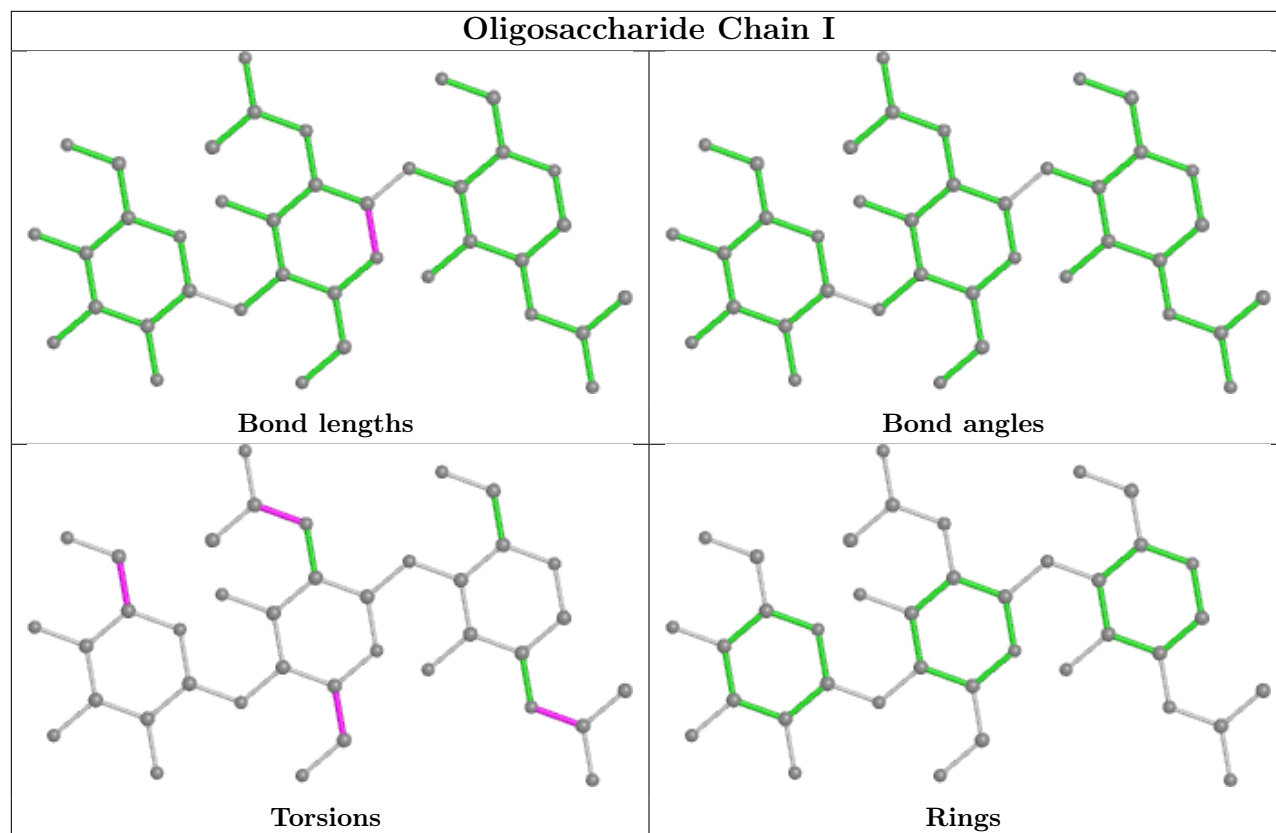




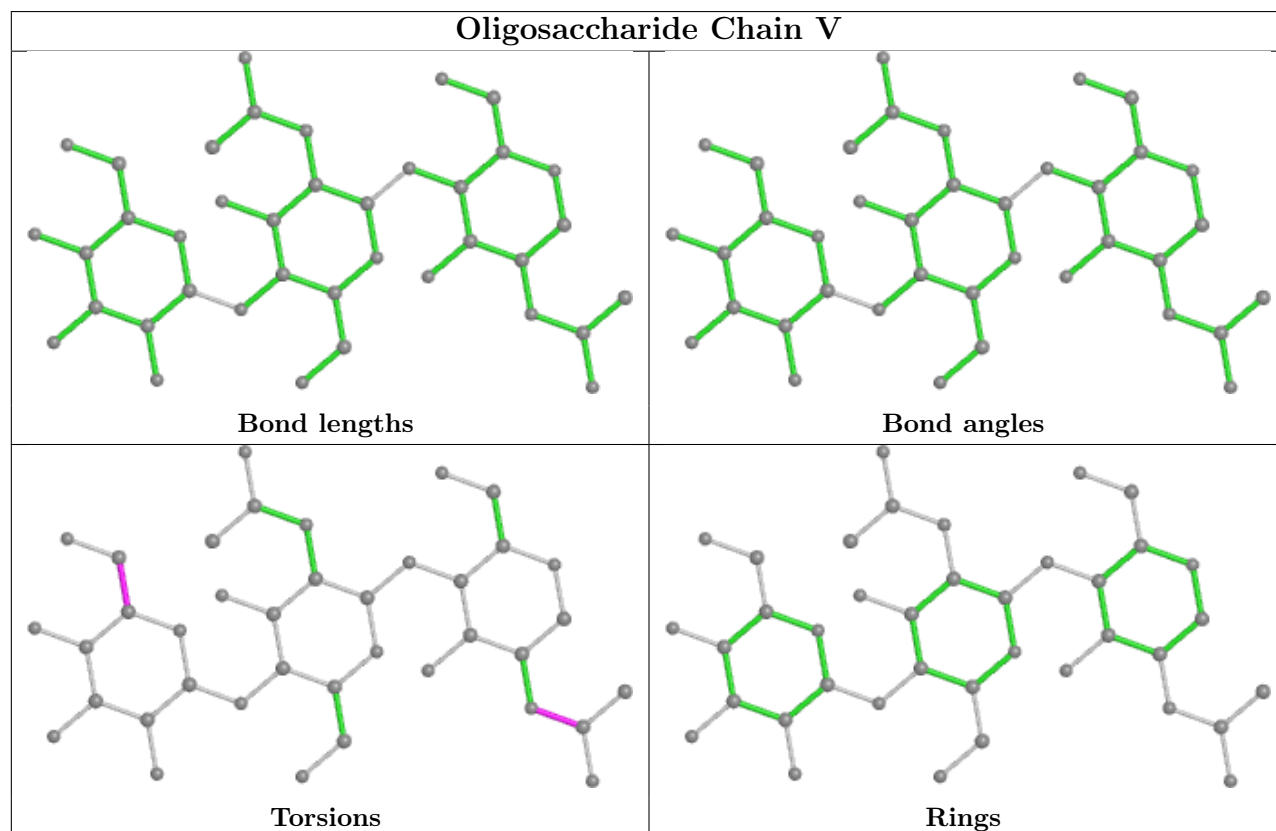
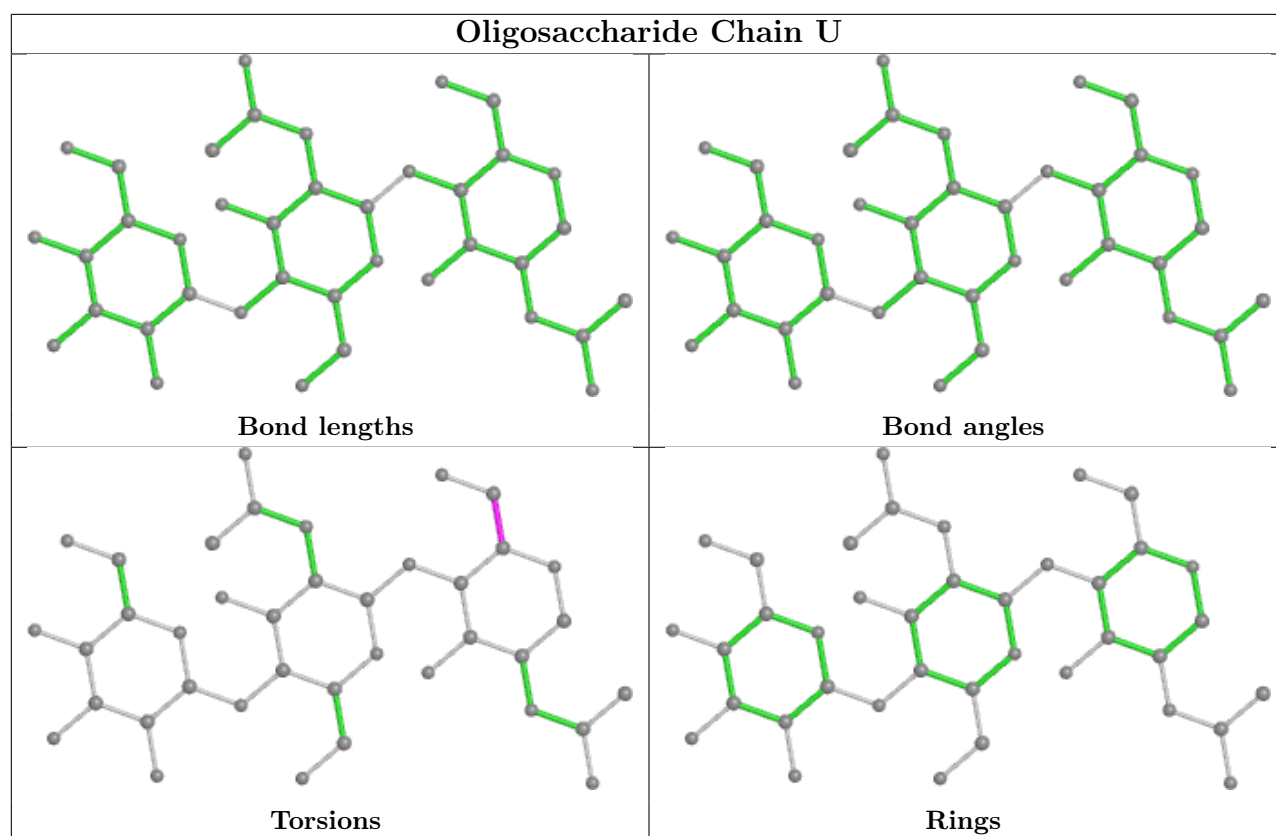


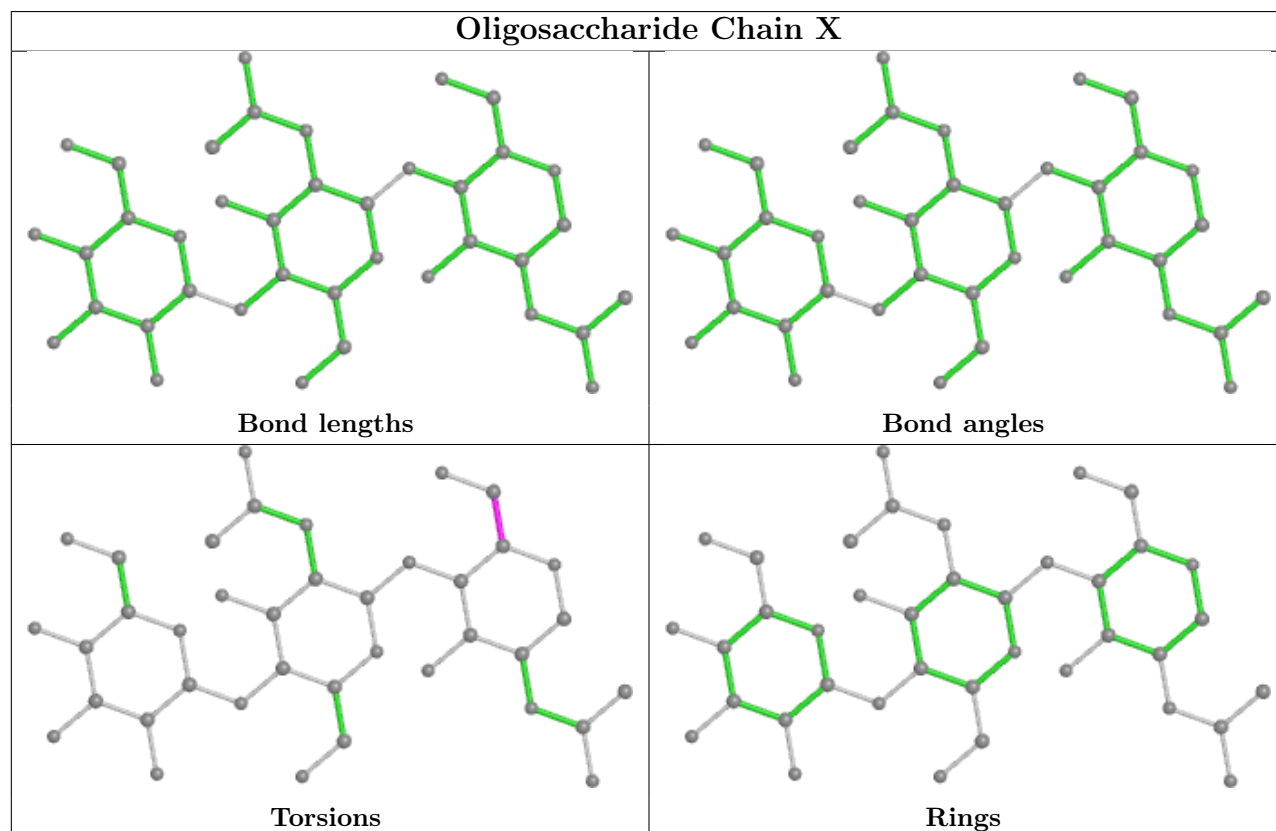
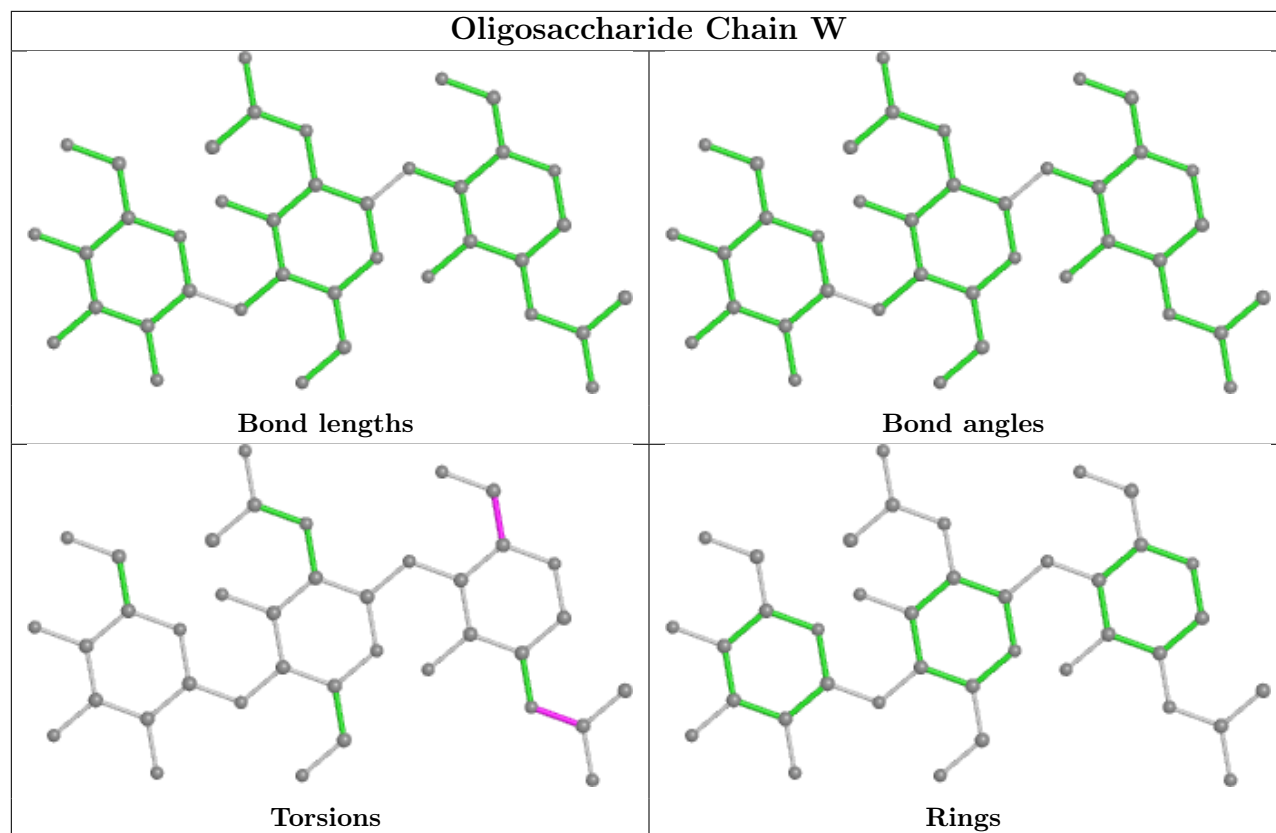


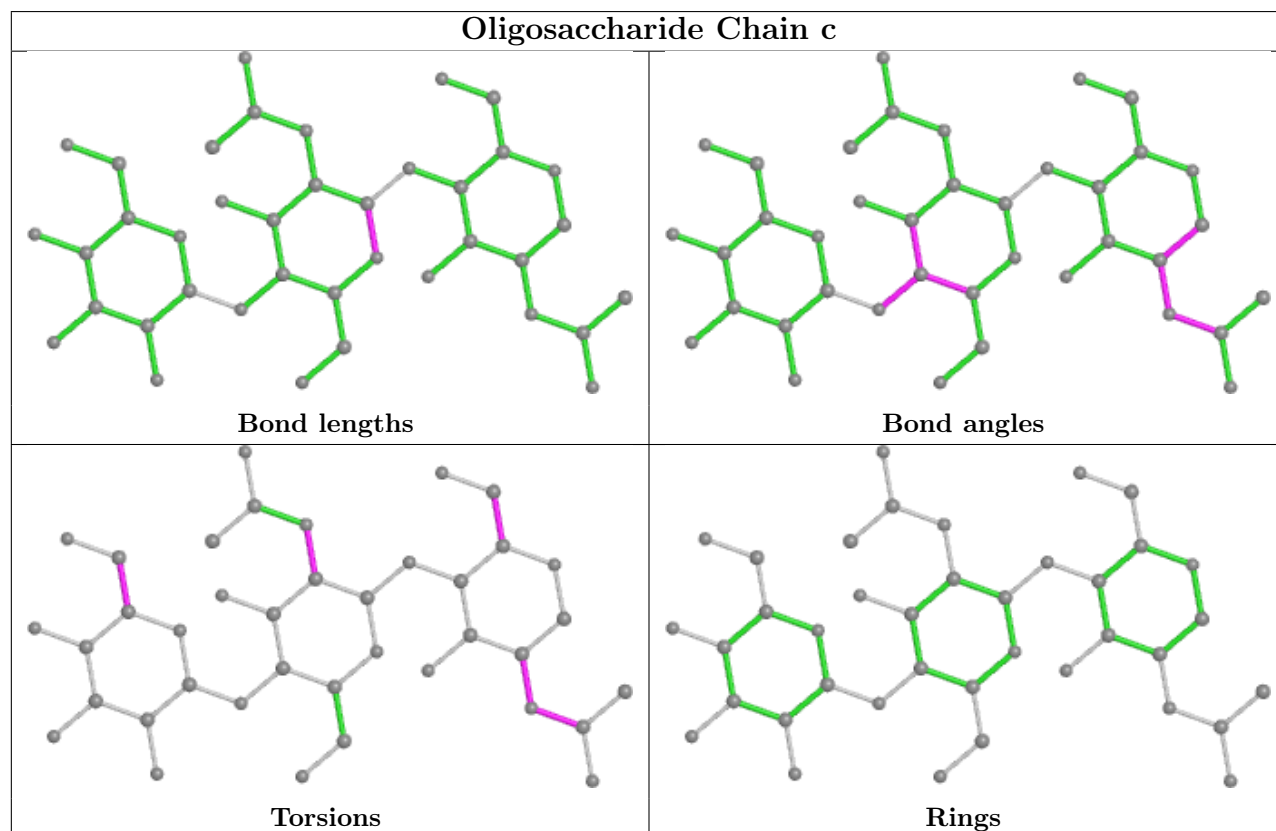
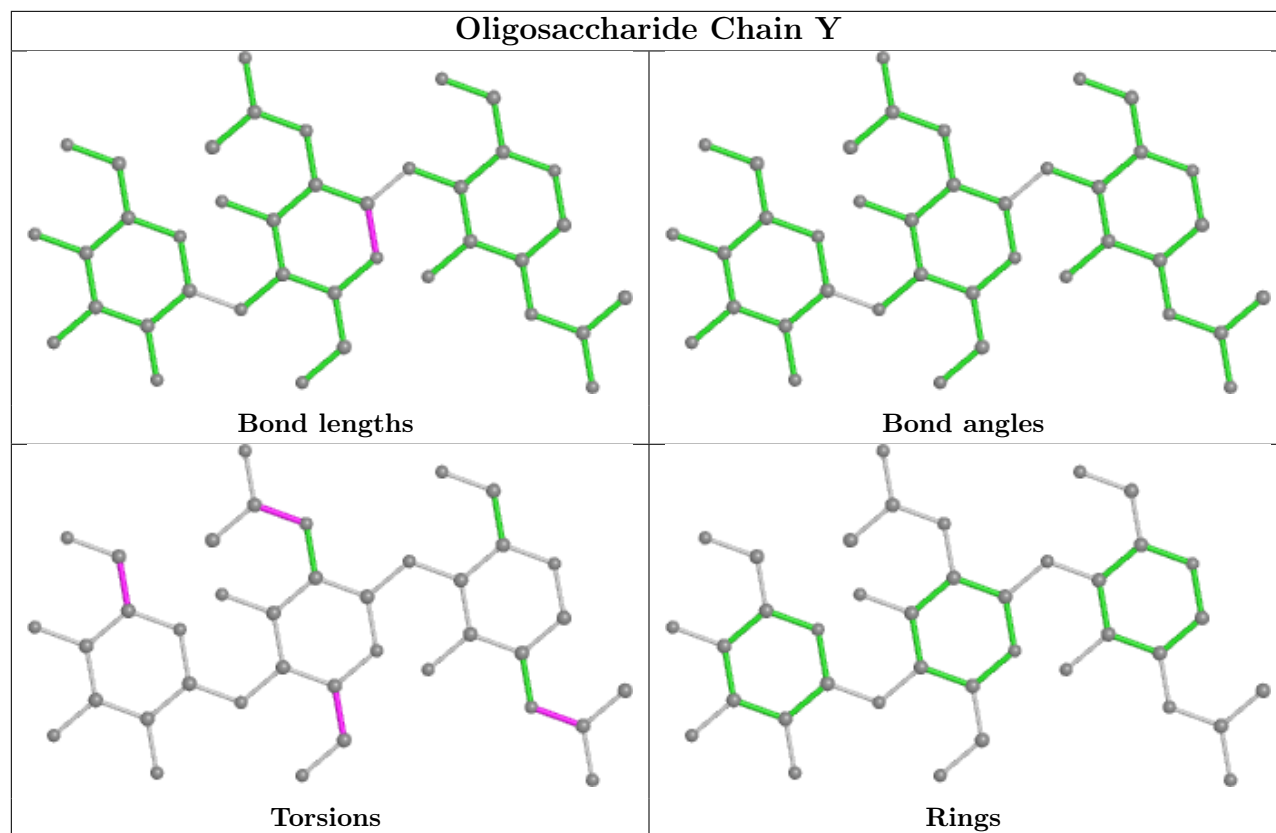


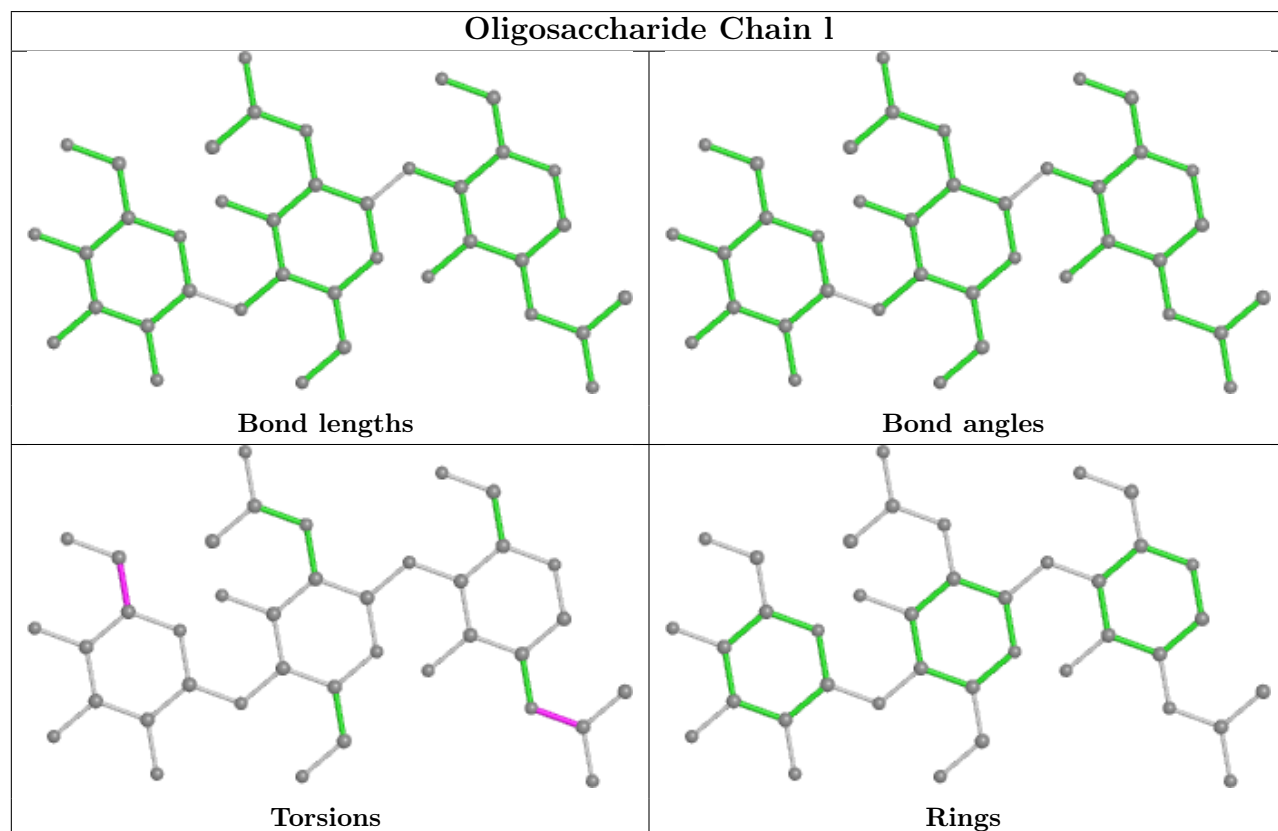
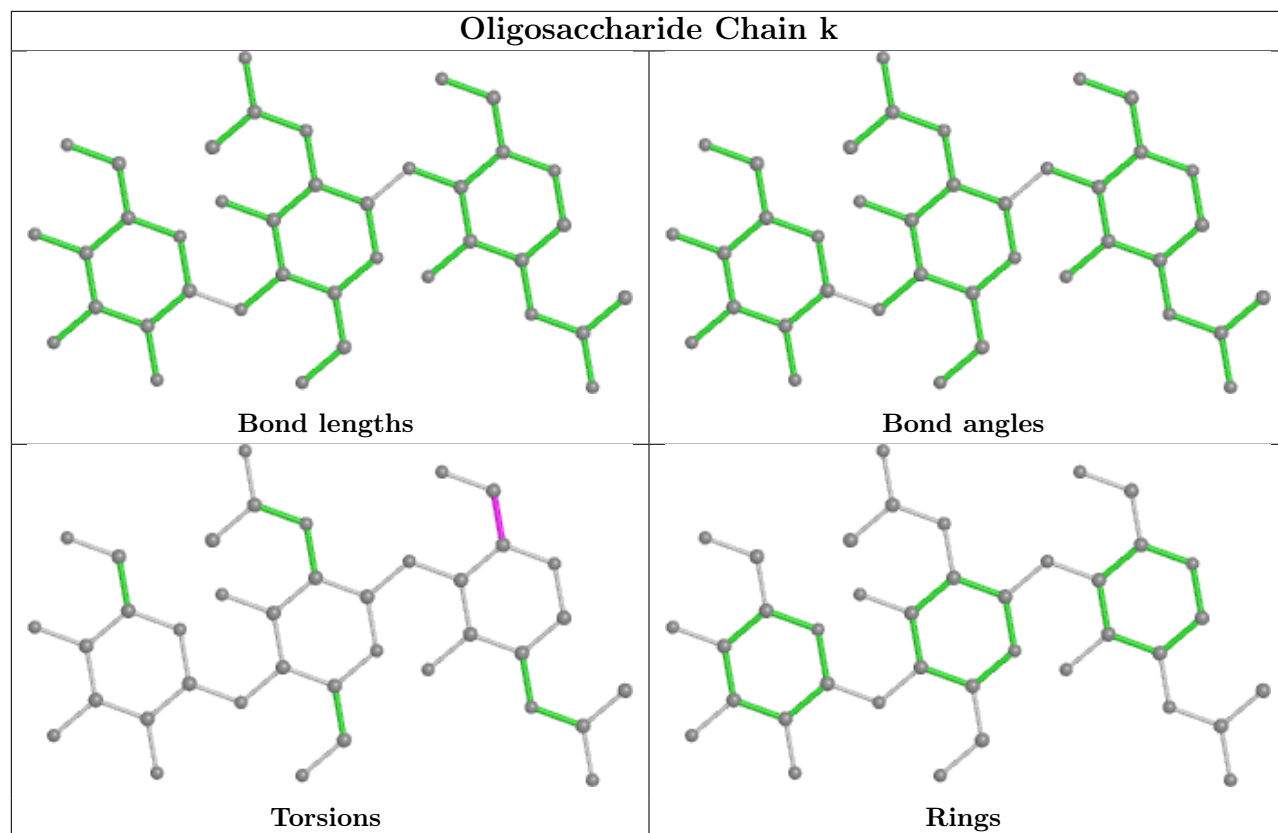


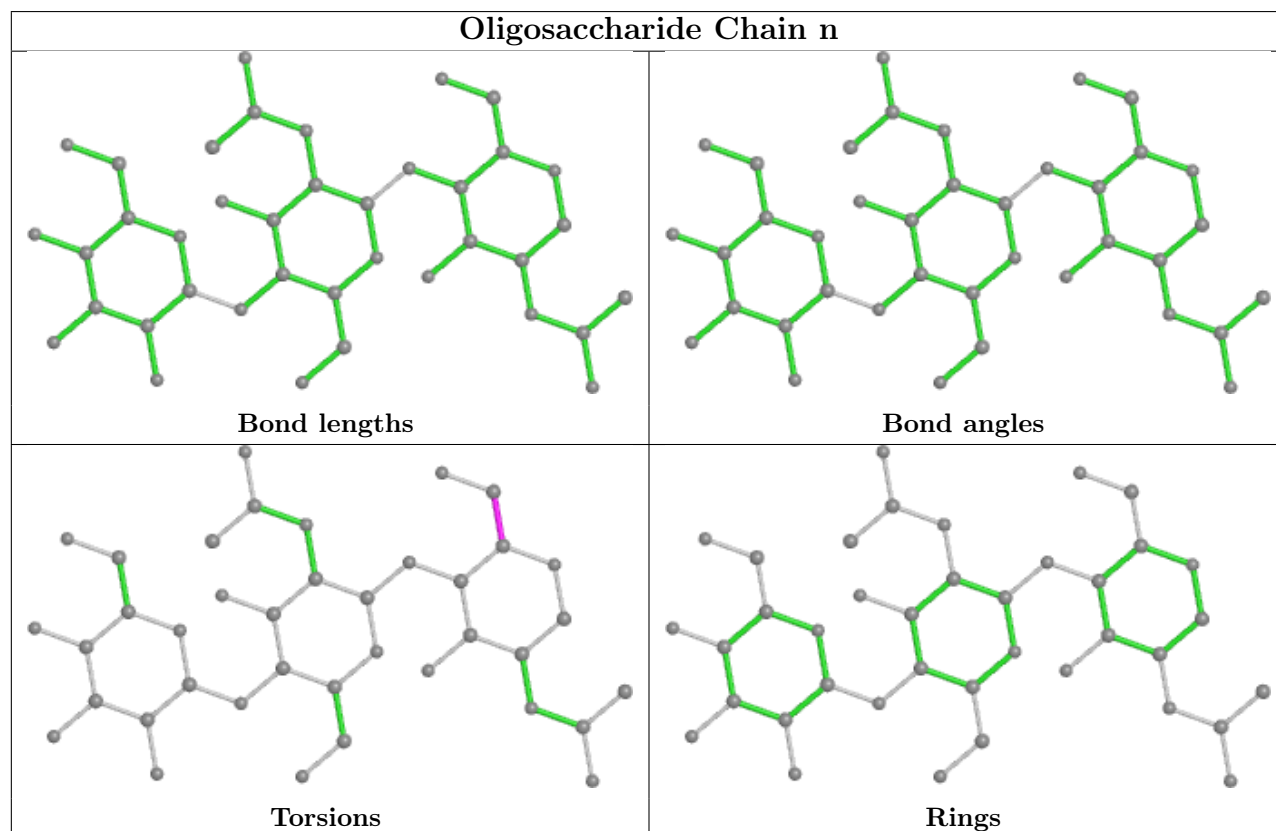
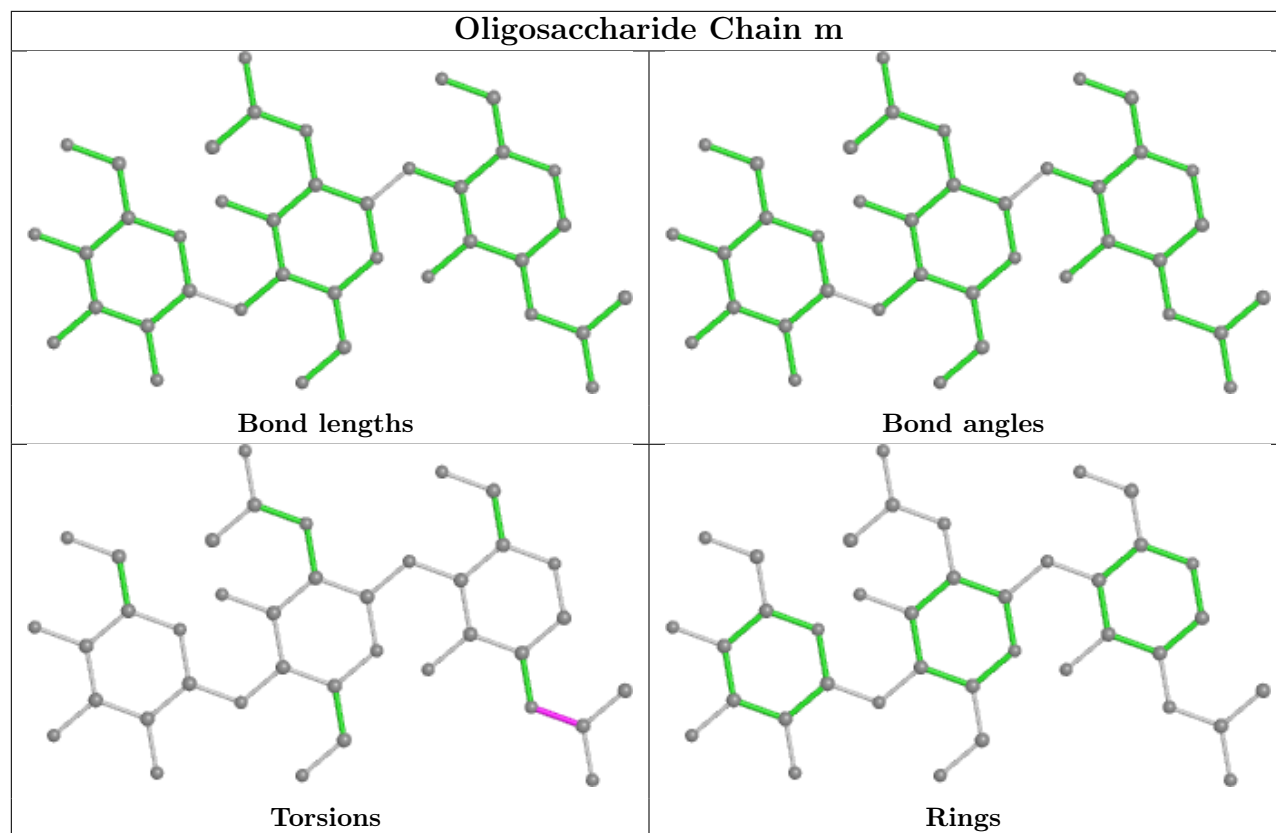


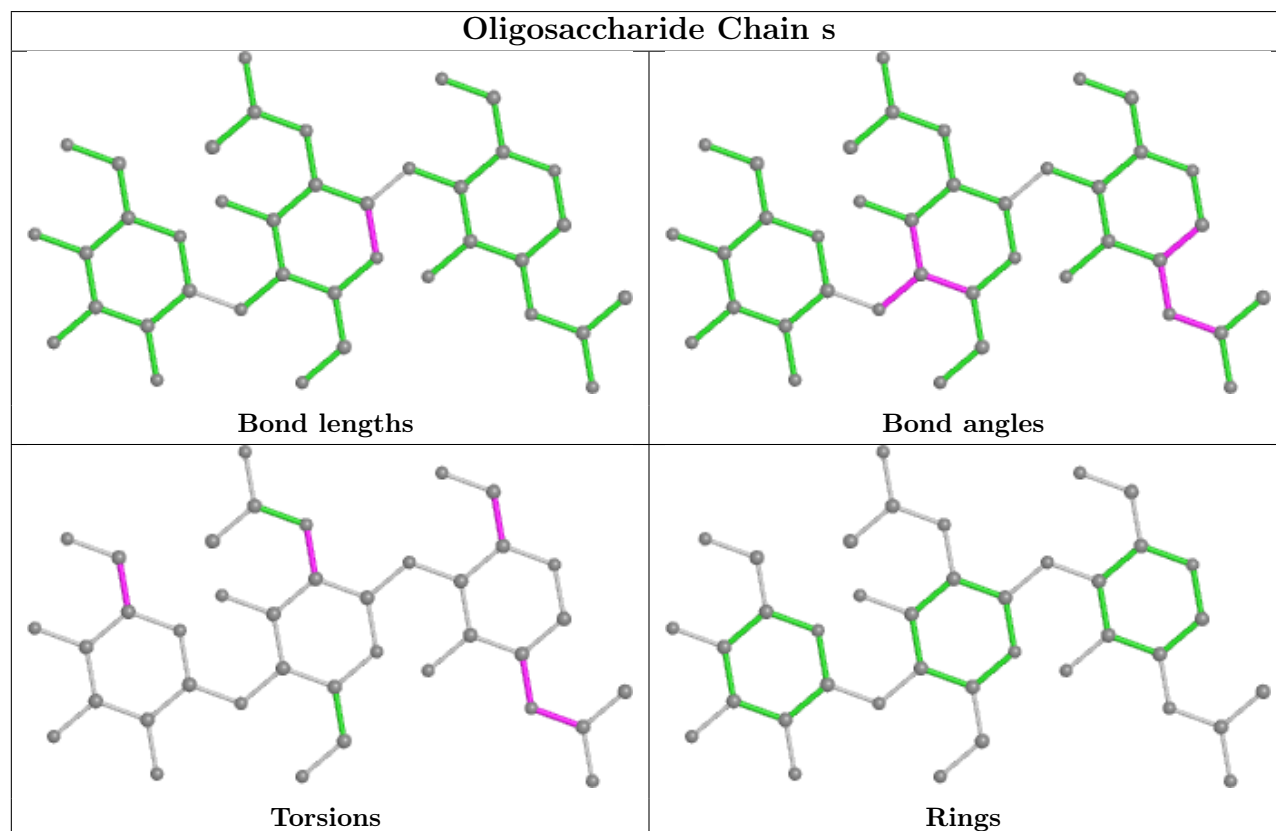
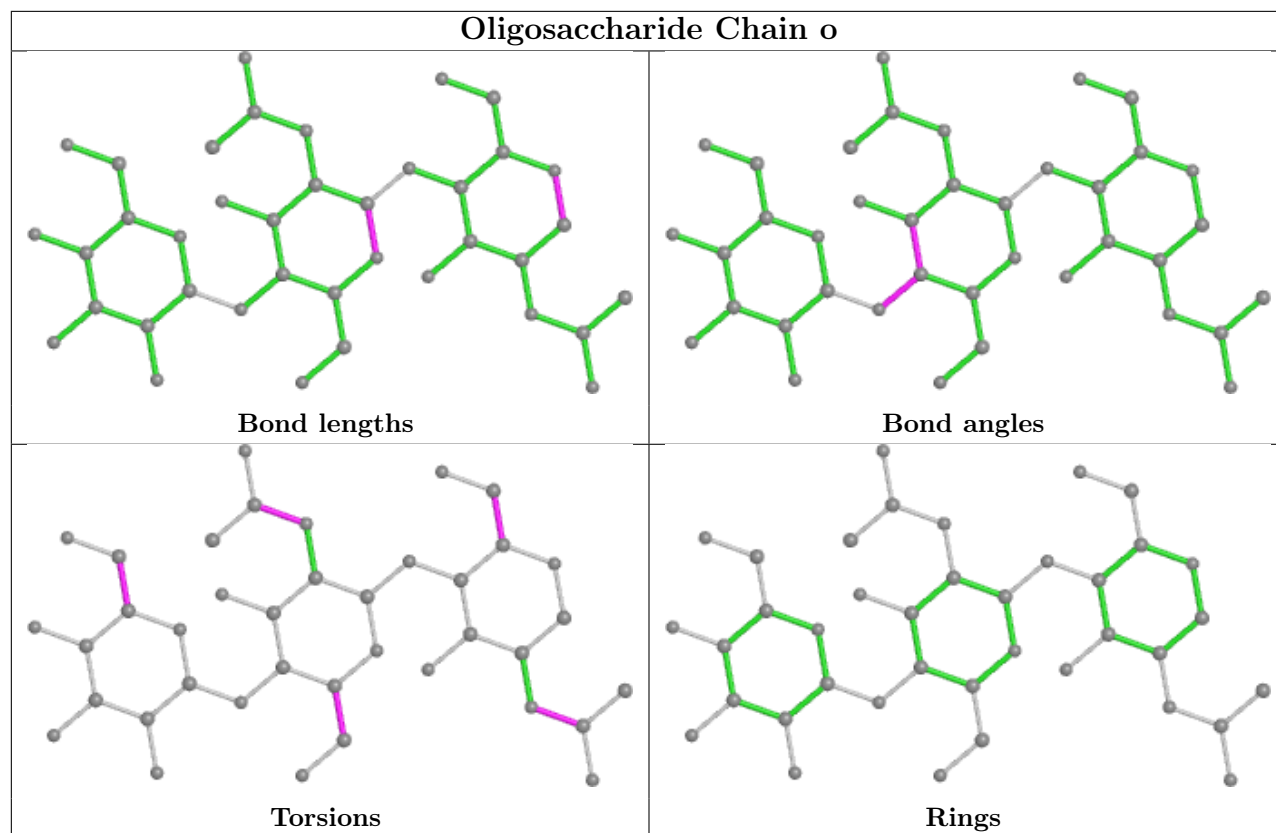












## 5.6 Ligand geometry

6 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     | 1301 | 1    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.34 | 0        |
| 4   | NAG  | A     | 1302 | 1    | 14,14,15     | 0.83 | 1 (7%)   | 17,19,21    | 0.50 | 0        |
| 4   | NAG  | B     | 1302 | 1    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.36 | 0        |
| 4   | NAG  | C     | 1301 | 1    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.35 | 0        |
| 4   | NAG  | C     | 1302 | 1    | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 0.68 | 1 (5%)   |
| 4   | NAG  | B     | 1301 | 1    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.35 | 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     | 1301 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | A     | 1302 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1302 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1301 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 4   | NAG  | C     | 1302 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 4   | NAG  | B     | 1301 | 1    | -       | 4/6/23/26 | 0/1/1/1 |

All (2) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 4   | A     | 1302 | NAG  | C1-C2 | 2.87 | 1.56        | 1.52     |
| 4   | C     | 1302 | NAG  | C1-C2 | 2.49 | 1.56        | 1.52     |

All (1) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|------|------|----------|------|------------------------|---------------------|
| 4   | C     | 1302 | NAG  | C1-O5-C5 | 2.09 | 115.02                 | 112.19              |

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 4   | C     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | B     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1301 | NAG  | C4-C5-C6-O6 |
| 4   | A     | 1302 | NAG  | O5-C5-C6-O6 |
| 4   | A     | 1301 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 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.