



## Full wwPDB EM Validation Report ⓘ

May 4, 2025 – 12:20 AM JST

PDB ID : 8ZDW / pdb\_00008zdw  
EMDB ID : EMD-60015  
Title : The cryoEM structure of H5N1 HA split from symmetric filament in conformation A  
Authors : Li, R.; Gao, J.; Wang, L.; Gui, M.; Xiang, Y.  
Deposited on : 2024-05-03  
Resolution : 3.45 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : **FAILED**  
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) : 2.43.1

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.45 Å.

There are no overall percentile quality scores available for this entry.

MolProbity failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 22602 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 Hemagglutinin.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 321      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |       |
| 1   | C     | 321      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |       |
| 1   | H     | 321      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2549  | 1611 | 440 | 483 | 15 |         |       |

- Molecule 2 is a protein called Hemagglutinin.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1412  | 878 | 245 | 281 | 8 |         |       |
| 2   | D     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1412  | 878 | 245 | 281 | 8 |         |       |
| 2   | I     | 174      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1412  | 878 | 245 | 281 | 8 |         |       |

- Molecule 3 is a protein called H5M9 Fab, light chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 3   | R     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1683  | 1044 | 291 | 342 | 6 |         |       |
| 3   | E     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1683  | 1044 | 291 | 342 | 6 |         |       |
| 3   | J     | 217      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1683  | 1044 | 291 | 342 | 6 |         |       |

- Molecule 4 is a protein called Anti-H5N1 hemagglutinin monoclonal antibody H5M9 heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | U     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1062 | 277 | 334 | 9 |         |       |

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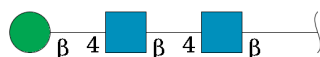
| Mol | Chain | Residues | Atoms |      |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|-------|
| 4   | F     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1062 | 277 | 334 | 9 |         |       |
| 4   | L     | 222      | Total | C    | N   | O   | S | 0       | 0     |
|     |       |          | 1682  | 1062 | 277 | 334 | 9 |         |       |

- Molecule 5 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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 5   | G     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 5   | N     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 5   | Q     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

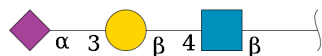
- Molecule 6 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 6   | K     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | M     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | O     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | P     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | S     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 6   | T     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

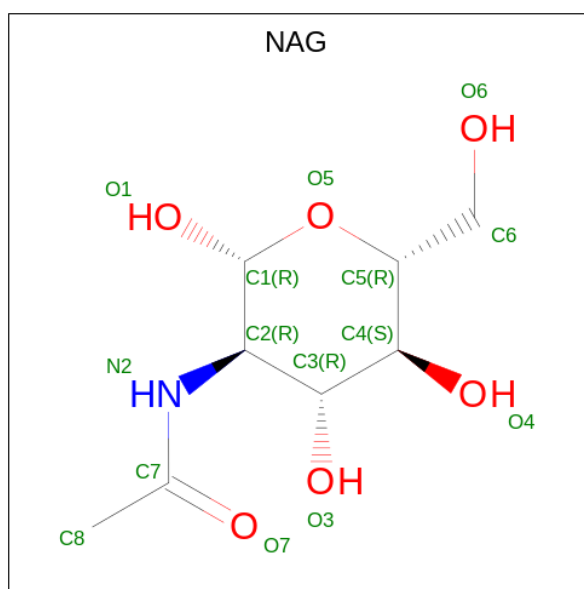
- Molecule 7 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galacto

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



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 7   | V     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 46    | 25 | 2 | 19 |         |       |
| 7   | W     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 46    | 25 | 2 | 19 |         |       |
| 7   | X     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 46    | 25 | 2 | 19 |         |       |

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

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| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 8   | I     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | E     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | J     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | H     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 8   | H     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

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### 3 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 216514                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 2000                                    | Depositor |
| Maximum defocus (nm)                 | 3000                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |

## 4 Model quality [i](#)

### 4.1 Standard geometry [i](#)

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### 4.2 Too-close contacts [i](#)

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section is therefore empty.

#### 4.3.3 RNA [i](#)

MolProbity failed to run properly - this section is therefore empty.

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

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

### 4.5 Carbohydrates [i](#)

33 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 |
| 5   | NAG  | G     | 1   | 1,5  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.56 | 0        |
| 5   | NAG  | G     | 2   | 5    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.42 | 0        |
| 6   | NAG  | K     | 1   | 6,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.46 | 0        |
| 6   | NAG  | K     | 2   | 6    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.64 | 1 (5%)   |
| 6   | BMA  | K     | 3   | 6    | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.81 | 0        |
| 6   | NAG  | M     | 1   | 6,1  | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.54 | 0        |
| 6   | NAG  | M     | 2   | 6    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.58 | 0        |
| 6   | BMA  | M     | 3   | 6    | 11,11,12     | 0.59 | 0        | 15,15,17    | 0.74 | 0        |
| 5   | NAG  | N     | 1   | 1,5  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.56 | 0        |
| 5   | NAG  | N     | 2   | 5    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.43 | 0        |
| 6   | NAG  | O     | 1   | 6,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.46 | 0        |
| 6   | NAG  | O     | 2   | 6    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.63 | 1 (5%)   |
| 6   | BMA  | O     | 3   | 6    | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.82 | 0        |
| 6   | NAG  | P     | 1   | 6,1  | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.54 | 0        |
| 6   | NAG  | P     | 2   | 6    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.58 | 0        |
| 6   | BMA  | P     | 3   | 6    | 11,11,12     | 0.59 | 0        | 15,15,17    | 0.74 | 0        |
| 5   | NAG  | Q     | 1   | 1,5  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.56 | 0        |
| 5   | NAG  | Q     | 2   | 5    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.42 | 0        |
| 6   | NAG  | S     | 1   | 6,1  | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.45 | 0        |
| 6   | NAG  | S     | 2   | 6    | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.63 | 1 (5%)   |
| 6   | BMA  | S     | 3   | 6    | 11,11,12     | 0.57 | 0        | 15,15,17    | 0.81 | 0        |
| 6   | NAG  | T     | 1   | 6,1  | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.54 | 0        |
| 6   | NAG  | T     | 2   | 6    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.58 | 0        |
| 6   | BMA  | T     | 3   | 6    | 11,11,12     | 0.59 | 0        | 15,15,17    | 0.74 | 0        |
| 7   | NAG  | V     | 1   | 7    | 15,15,15     | 0.41 | 0        | 21,21,21    | 0.87 | 1 (4%)   |
| 7   | GAL  | V     | 2   | 7    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.52 | 4 (26%)  |
| 7   | SIA  | V     | 3   | 7    | 20,20,21     | 0.92 | 1 (5%)   | 24,28,31    | 1.12 | 3 (12%)  |
| 7   | NAG  | W     | 1   | 7    | 15,15,15     | 0.41 | 0        | 21,21,21    | 0.87 | 1 (4%)   |
| 7   | GAL  | W     | 2   | 7    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.53 | 4 (26%)  |
| 7   | SIA  | W     | 3   | 7    | 20,20,21     | 0.91 | 1 (5%)   | 24,28,31    | 1.12 | 3 (12%)  |
| 7   | NAG  | X     | 1   | 7    | 15,15,15     | 0.41 | 0        | 21,21,21    | 0.89 | 1 (4%)   |
| 7   | GAL  | X     | 2   | 7    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.53 | 4 (26%)  |
| 7   | SIA  | X     | 3   | 7    | 20,20,21     | 0.91 | 1 (5%)   | 24,28,31    | 1.12 | 3 (12%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions   | Rings   |
|-----|------|-------|-----|------|---------|------------|---------|
| 5   | NAG  | G     | 1   | 1,5  | -       | 1/6/23/26  | 0/1/1/1 |
| 5   | NAG  | G     | 2   | 5    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | NAG  | K     | 1   | 6,1  | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | NAG  | K     | 2   | 6    | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | BMA  | K     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 6   | NAG  | M     | 1   | 6,1  | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | NAG  | M     | 2   | 6    | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | BMA  | M     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 5   | NAG  | N     | 1   | 1,5  | -       | 1/6/23/26  | 0/1/1/1 |
| 5   | NAG  | N     | 2   | 5    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | NAG  | O     | 1   | 6,1  | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | NAG  | O     | 2   | 6    | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | BMA  | O     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 6   | NAG  | P     | 1   | 6,1  | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | NAG  | P     | 2   | 6    | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | BMA  | P     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 5   | NAG  | Q     | 1   | 1,5  | -       | 1/6/23/26  | 0/1/1/1 |
| 5   | NAG  | Q     | 2   | 5    | -       | 0/6/23/26  | 0/1/1/1 |
| 6   | NAG  | S     | 1   | 6,1  | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | NAG  | S     | 2   | 6    | -       | 2/6/23/26  | 0/1/1/1 |
| 6   | BMA  | S     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 6   | NAG  | T     | 1   | 6,1  | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | NAG  | T     | 2   | 6    | -       | 1/6/23/26  | 0/1/1/1 |
| 6   | BMA  | T     | 3   | 6    | -       | 0/2/19/22  | 0/1/1/1 |
| 7   | NAG  | V     | 1   | 7    | -       | 4/6/26/26  | 0/1/1/1 |
| 7   | GAL  | V     | 2   | 7    | -       | 1/2/19/22  | 0/1/1/1 |
| 7   | SIA  | V     | 3   | 7    | -       | 4/18/34/38 | 0/1/1/1 |
| 7   | NAG  | W     | 1   | 7    | -       | 4/6/26/26  | 0/1/1/1 |
| 7   | GAL  | W     | 2   | 7    | -       | 1/2/19/22  | 0/1/1/1 |
| 7   | SIA  | W     | 3   | 7    | -       | 4/18/34/38 | 0/1/1/1 |
| 7   | NAG  | X     | 1   | 7    | -       | 4/6/26/26  | 0/1/1/1 |
| 7   | GAL  | X     | 2   | 7    | -       | 1/2/19/22  | 0/1/1/1 |
| 7   | SIA  | X     | 3   | 7    | -       | 4/18/34/38 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 7   | X     | 3   | SIA  | O1B-C1 | -3.23 | 1.20        | 1.30     |
| 7   | V     | 3   | SIA  | O1B-C1 | -3.23 | 1.20        | 1.30     |
| 7   | W     | 3   | SIA  | O1B-C1 | -3.21 | 1.20        | 1.30     |

All (27) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 7   | W     | 2   | GAL  | O5-C5-C6  | 3.02  | 111.93      | 107.20   |
| 7   | X     | 2   | GAL  | O5-C5-C6  | 2.99  | 111.90      | 107.20   |
| 7   | V     | 2   | GAL  | O5-C5-C6  | 2.97  | 111.86      | 107.20   |
| 7   | V     | 3   | SIA  | O1B-C1-C2 | 2.96  | 121.49      | 113.03   |
| 7   | X     | 3   | SIA  | O1B-C1-C2 | 2.96  | 121.48      | 113.03   |
| 7   | W     | 3   | SIA  | O1B-C1-C2 | 2.96  | 121.47      | 113.03   |
| 7   | W     | 3   | SIA  | C3-C4-C5  | -2.76 | 108.12      | 111.46   |
| 7   | V     | 3   | SIA  | C3-C4-C5  | -2.75 | 108.13      | 111.46   |
| 7   | X     | 3   | SIA  | C3-C4-C5  | -2.75 | 108.14      | 111.46   |
| 7   | X     | 2   | GAL  | C1-C2-C3  | 2.29  | 112.49      | 109.67   |
| 7   | V     | 2   | GAL  | O5-C5-C4  | -2.29 | 105.25      | 110.83   |
| 7   | W     | 2   | GAL  | C1-C2-C3  | 2.29  | 112.48      | 109.67   |
| 7   | V     | 2   | GAL  | C1-C2-C3  | 2.29  | 112.48      | 109.67   |
| 7   | X     | 2   | GAL  | O5-C5-C4  | -2.29 | 105.26      | 110.83   |
| 7   | W     | 2   | GAL  | O5-C5-C4  | -2.28 | 105.27      | 110.83   |
| 7   | X     | 1   | NAG  | C4-C3-C2  | -2.23 | 107.07      | 110.34   |
| 7   | V     | 1   | NAG  | C4-C3-C2  | -2.21 | 107.10      | 110.34   |
| 7   | W     | 1   | NAG  | C4-C3-C2  | -2.21 | 107.11      | 110.34   |
| 7   | W     | 2   | GAL  | C1-O5-C5  | 2.14  | 115.10      | 112.19   |
| 7   | W     | 3   | SIA  | O1A-C1-C2 | -2.12 | 117.56      | 122.57   |
| 7   | X     | 2   | GAL  | C1-O5-C5  | 2.12  | 115.06      | 112.19   |
| 7   | V     | 3   | SIA  | O1A-C1-C2 | -2.11 | 117.58      | 122.57   |
| 7   | X     | 3   | SIA  | O1A-C1-C2 | -2.11 | 117.58      | 122.57   |
| 7   | V     | 2   | GAL  | C1-O5-C5  | 2.10  | 115.04      | 112.19   |
| 6   | K     | 2   | NAG  | C1-O5-C5  | 2.08  | 115.00      | 112.19   |
| 6   | O     | 2   | NAG  | C1-O5-C5  | 2.06  | 114.99      | 112.19   |
| 6   | S     | 2   | NAG  | C1-O5-C5  | 2.06  | 114.98      | 112.19   |

There are no chirality outliers.

All (48) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | V     | 1   | NAG  | C1-C2-N2-C7 |
| 7   | V     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | V     | 1   | NAG  | C8-C7-N2-C2 |
| 7   | V     | 1   | NAG  | O7-C7-N2-C2 |
| 7   | V     | 3   | SIA  | C7-C8-C9-O9 |
| 7   | V     | 3   | SIA  | O8-C8-C9-O9 |
| 7   | W     | 1   | NAG  | C1-C2-N2-C7 |
| 7   | W     | 1   | NAG  | C3-C2-N2-C7 |
| 7   | W     | 1   | NAG  | C8-C7-N2-C2 |

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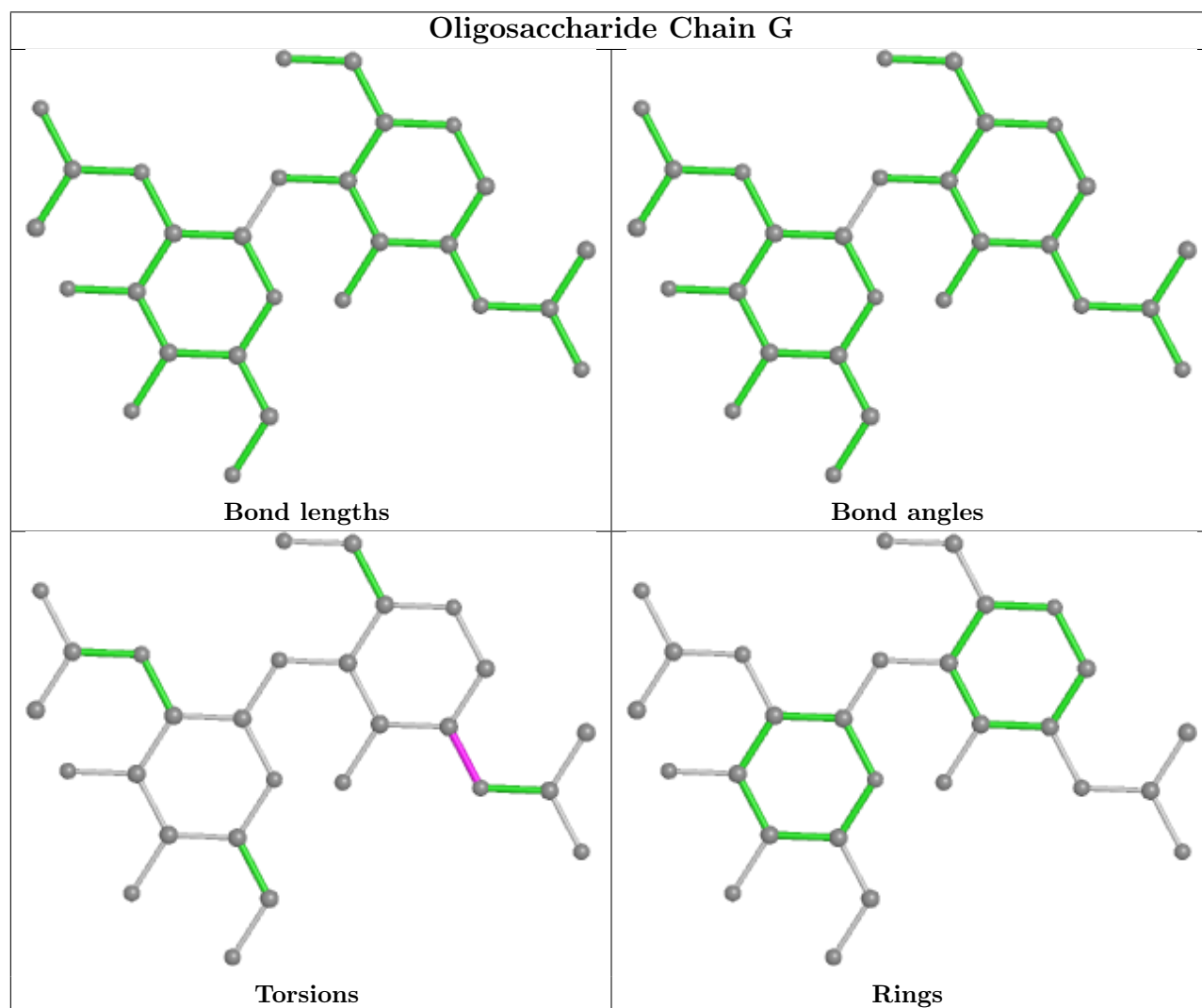
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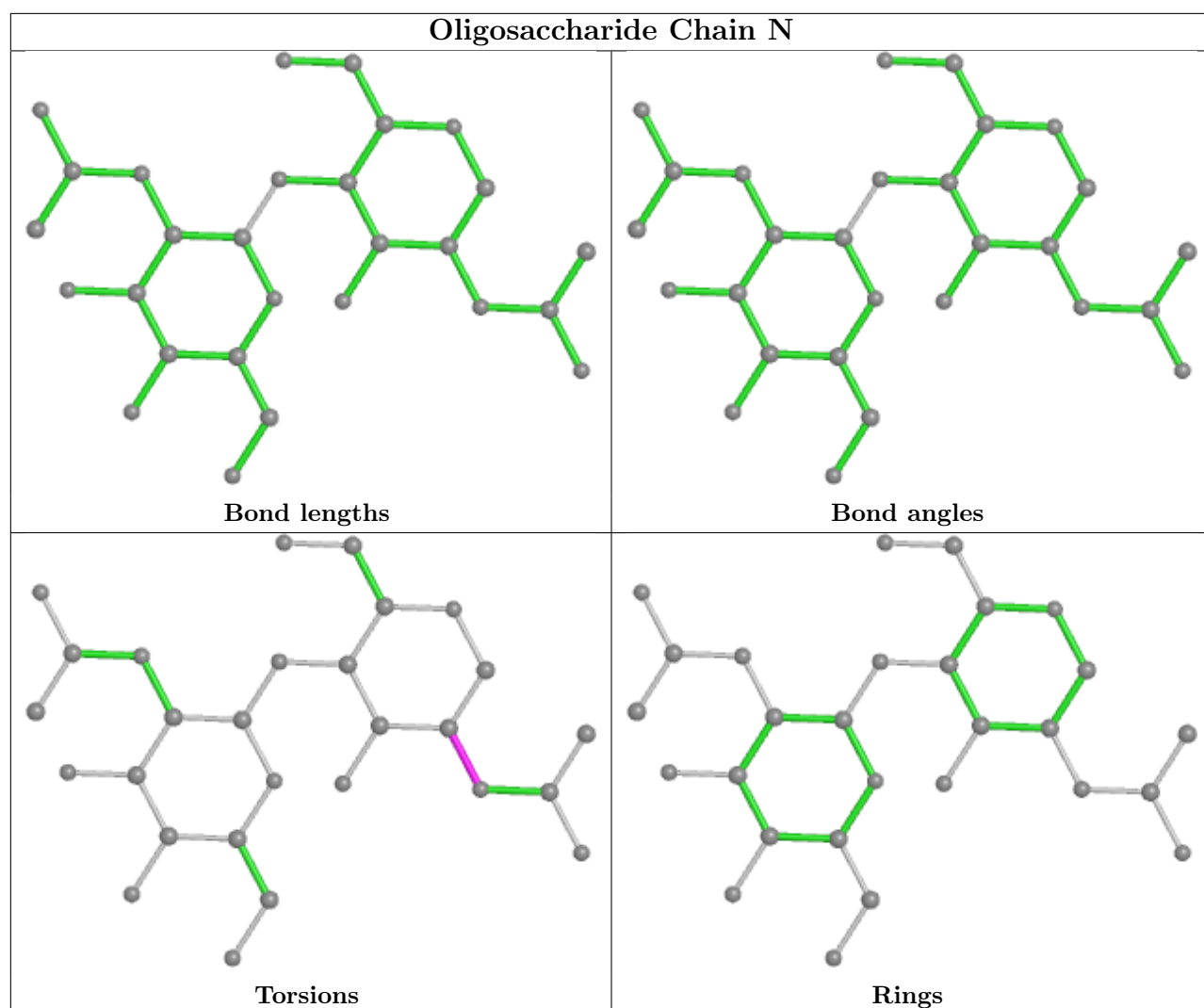
| Mol | Chain | Res | Type | Atoms         |
|-----|-------|-----|------|---------------|
| 7   | W     | 1   | NAG  | O7-C7-N2-C2   |
| 7   | W     | 3   | SIA  | C7-C8-C9-O9   |
| 7   | W     | 3   | SIA  | O8-C8-C9-O9   |
| 7   | X     | 1   | NAG  | C1-C2-N2-C7   |
| 7   | X     | 1   | NAG  | C3-C2-N2-C7   |
| 7   | X     | 1   | NAG  | C8-C7-N2-C2   |
| 7   | X     | 1   | NAG  | O7-C7-N2-C2   |
| 7   | X     | 3   | SIA  | C7-C8-C9-O9   |
| 7   | X     | 3   | SIA  | O8-C8-C9-O9   |
| 6   | K     | 1   | NAG  | O5-C5-C6-O6   |
| 6   | O     | 1   | NAG  | O5-C5-C6-O6   |
| 6   | S     | 1   | NAG  | O5-C5-C6-O6   |
| 6   | K     | 1   | NAG  | C4-C5-C6-O6   |
| 6   | O     | 1   | NAG  | C4-C5-C6-O6   |
| 6   | S     | 1   | NAG  | C4-C5-C6-O6   |
| 6   | K     | 2   | NAG  | C8-C7-N2-C2   |
| 6   | K     | 2   | NAG  | O7-C7-N2-C2   |
| 6   | O     | 2   | NAG  | C8-C7-N2-C2   |
| 6   | O     | 2   | NAG  | O7-C7-N2-C2   |
| 6   | S     | 2   | NAG  | C8-C7-N2-C2   |
| 6   | S     | 2   | NAG  | O7-C7-N2-C2   |
| 7   | V     | 3   | SIA  | C11-C10-N5-C5 |
| 7   | W     | 3   | SIA  | C11-C10-N5-C5 |
| 7   | X     | 3   | SIA  | C11-C10-N5-C5 |
| 7   | V     | 3   | SIA  | O10-C10-N5-C5 |
| 7   | W     | 3   | SIA  | O10-C10-N5-C5 |
| 7   | X     | 3   | SIA  | O10-C10-N5-C5 |
| 7   | V     | 2   | GAL  | C4-C5-C6-O6   |
| 7   | W     | 2   | GAL  | C4-C5-C6-O6   |
| 7   | X     | 2   | GAL  | C4-C5-C6-O6   |
| 5   | G     | 1   | NAG  | C3-C2-N2-C7   |
| 5   | N     | 1   | NAG  | C3-C2-N2-C7   |
| 5   | Q     | 1   | NAG  | C3-C2-N2-C7   |
| 6   | M     | 2   | NAG  | C3-C2-N2-C7   |
| 6   | P     | 2   | NAG  | C3-C2-N2-C7   |
| 6   | T     | 2   | NAG  | C3-C2-N2-C7   |
| 6   | M     | 1   | NAG  | C3-C2-N2-C7   |
| 6   | P     | 1   | NAG  | C3-C2-N2-C7   |
| 6   | T     | 1   | NAG  | C3-C2-N2-C7   |

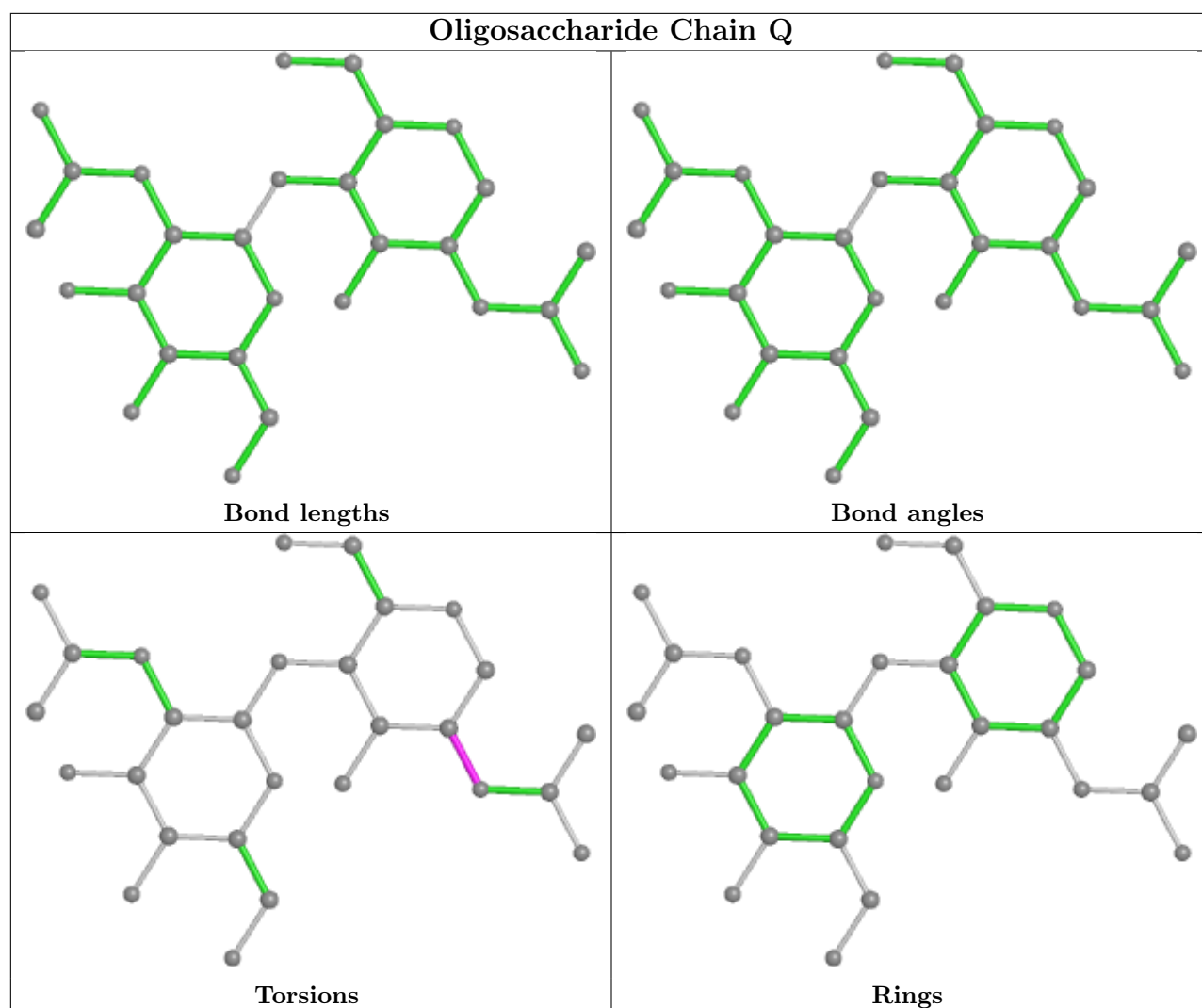
There are no ring outliers.

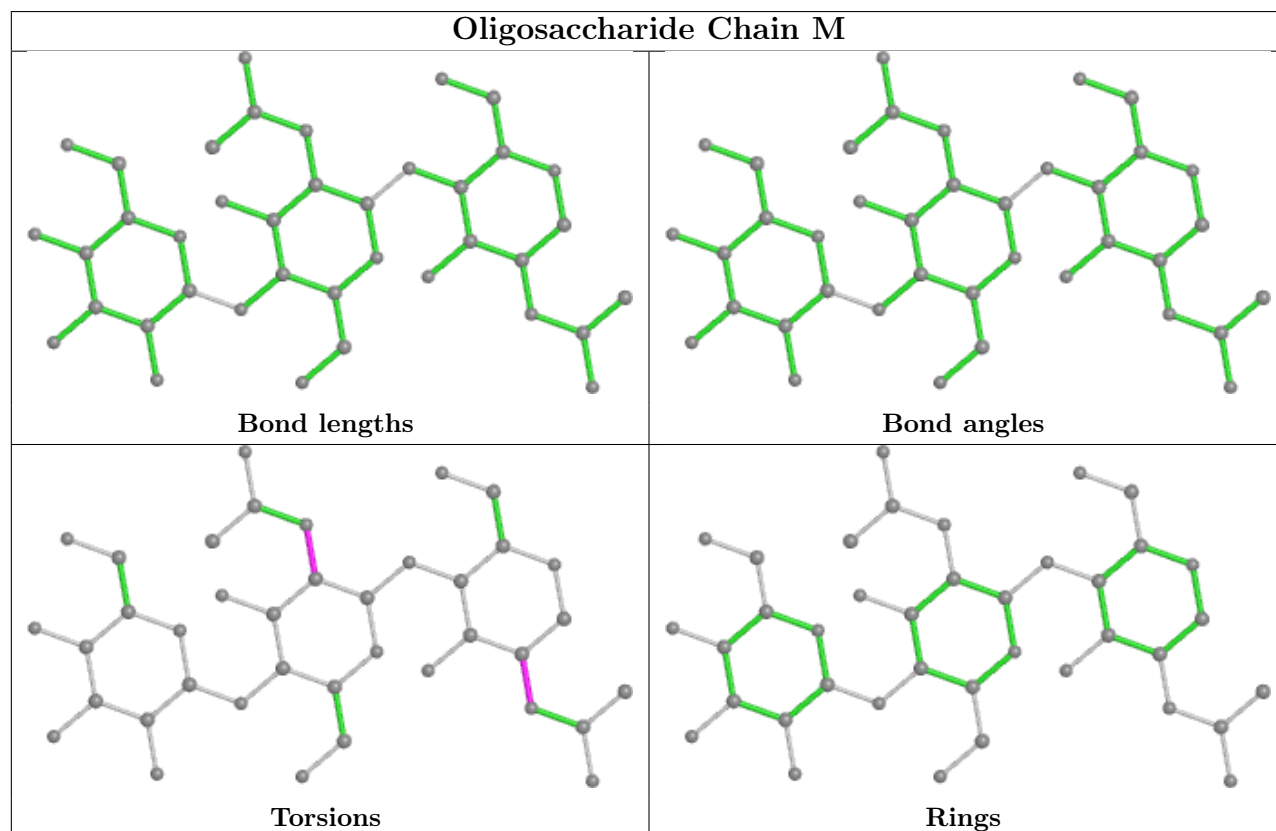
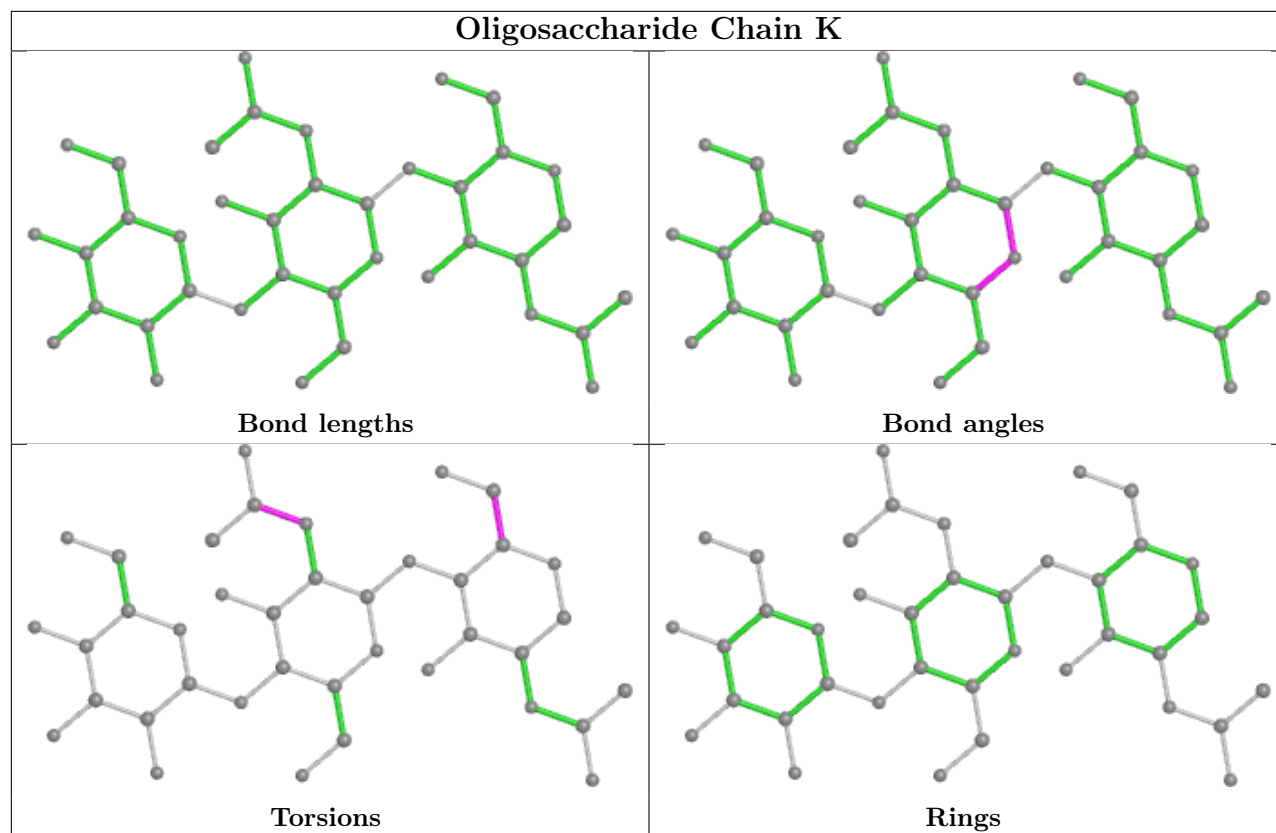
No monomer is involved in short contacts.

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

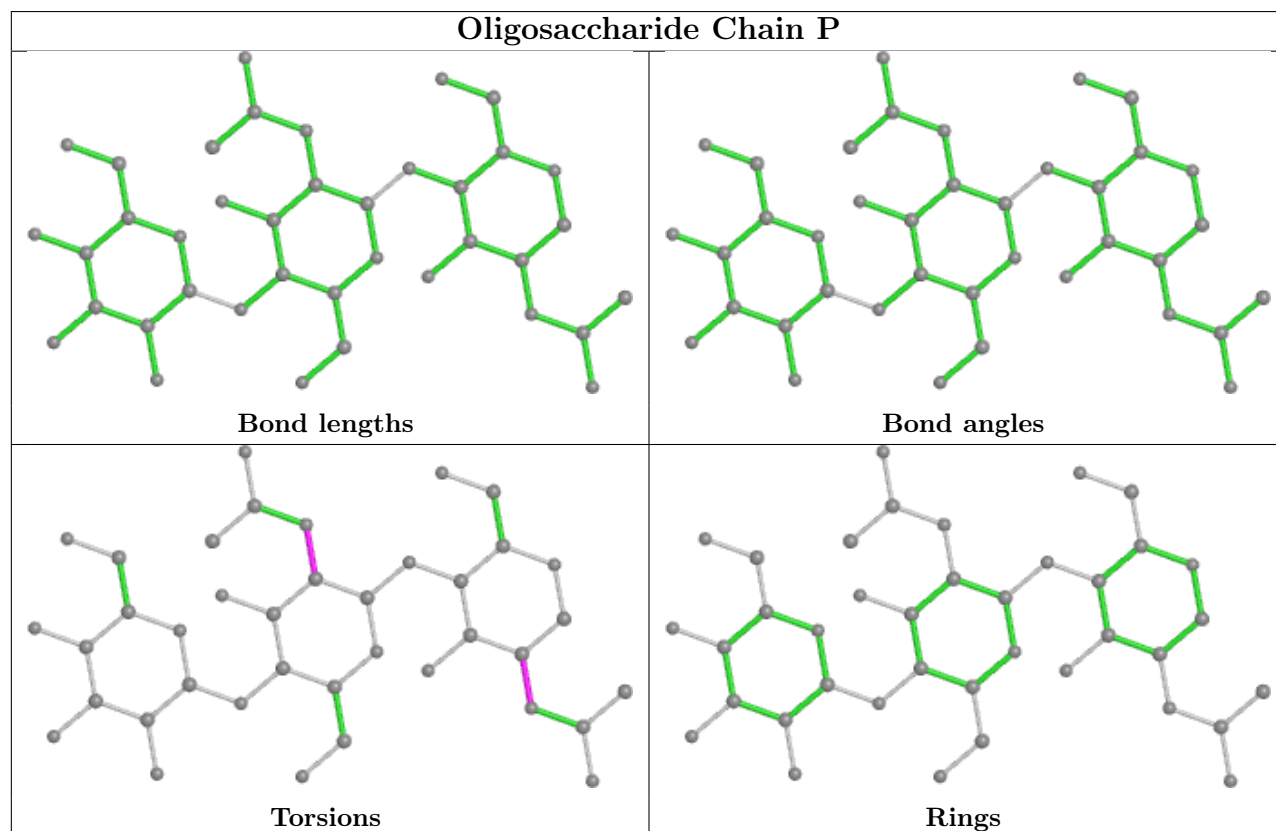
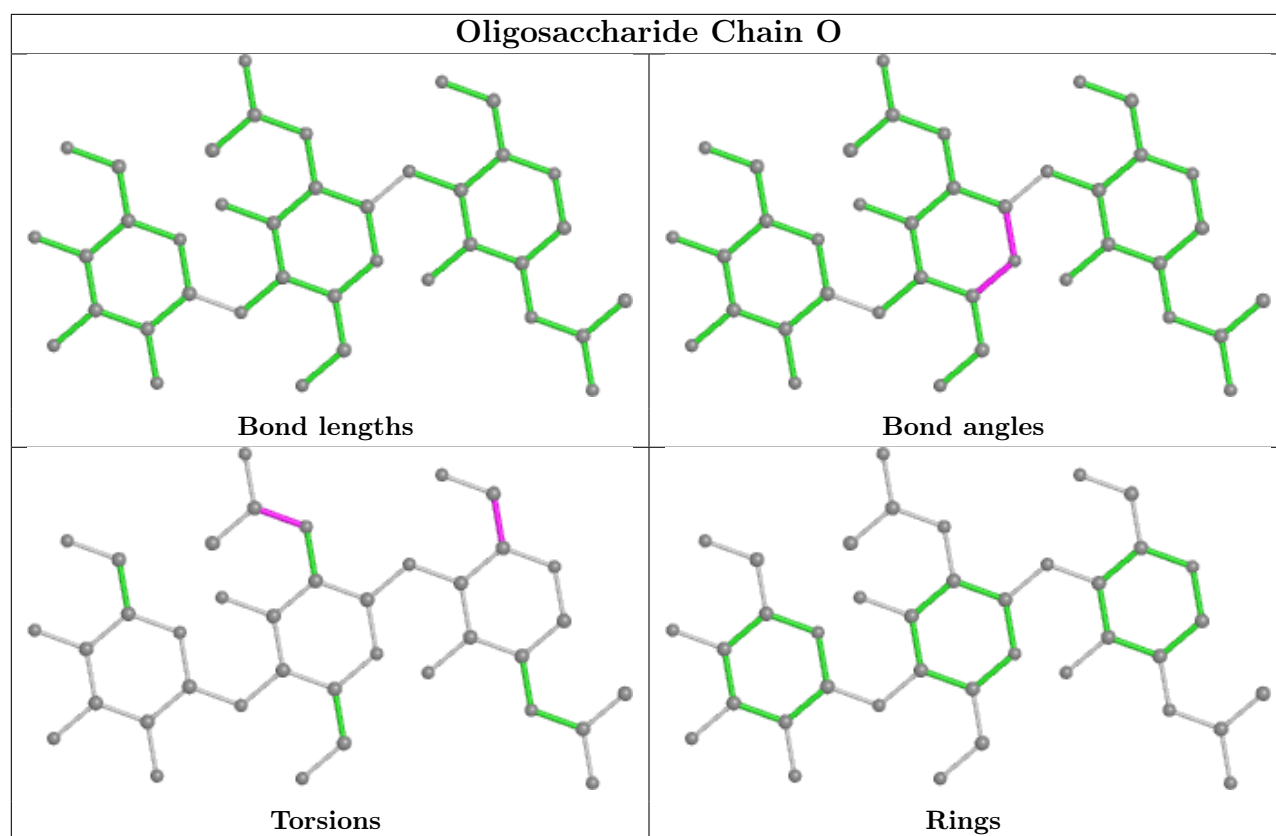


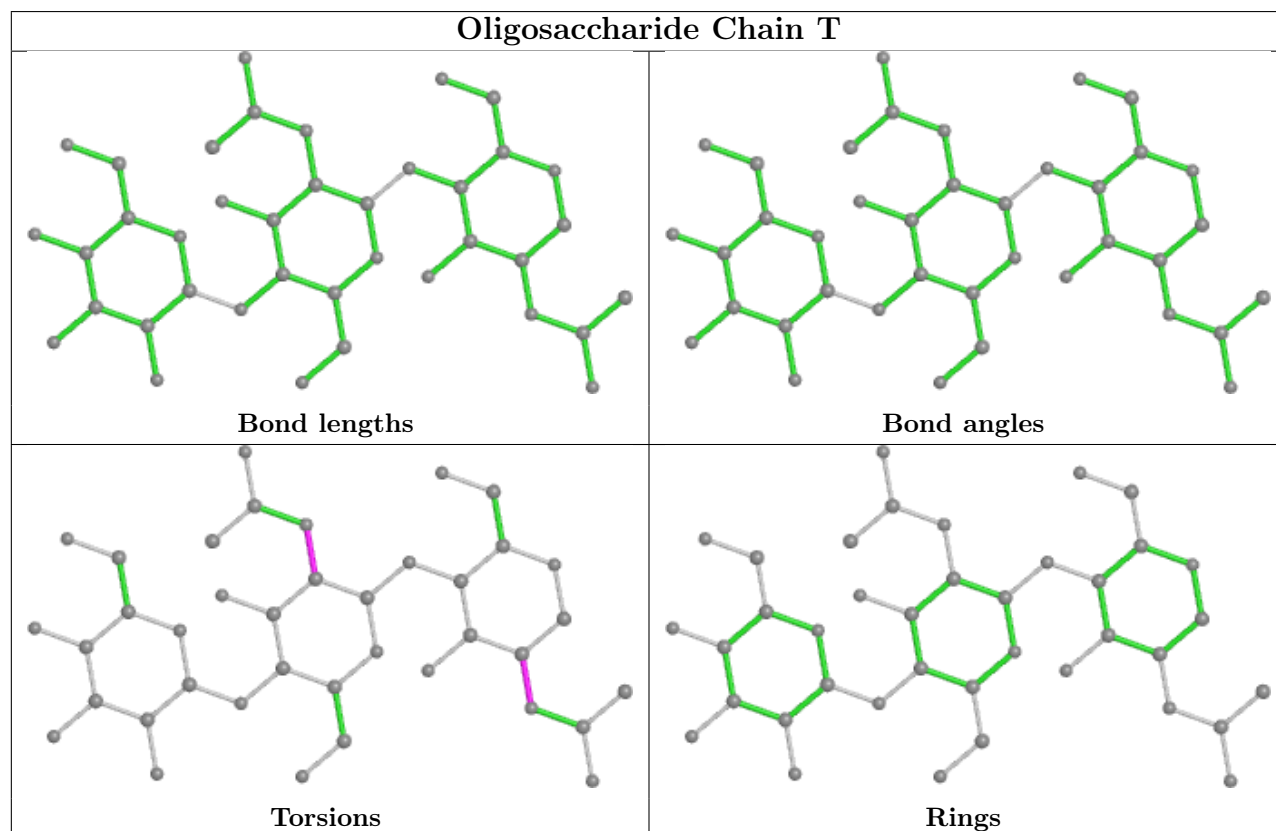
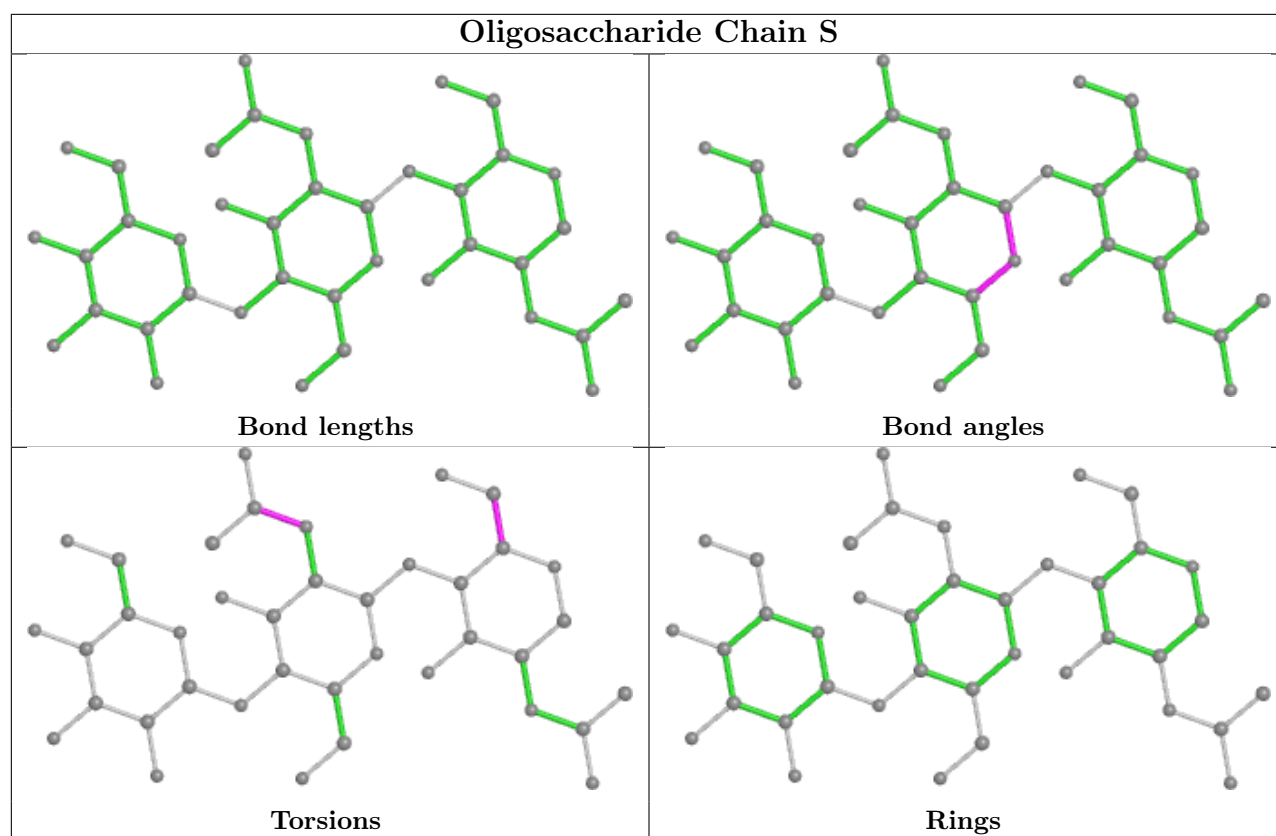


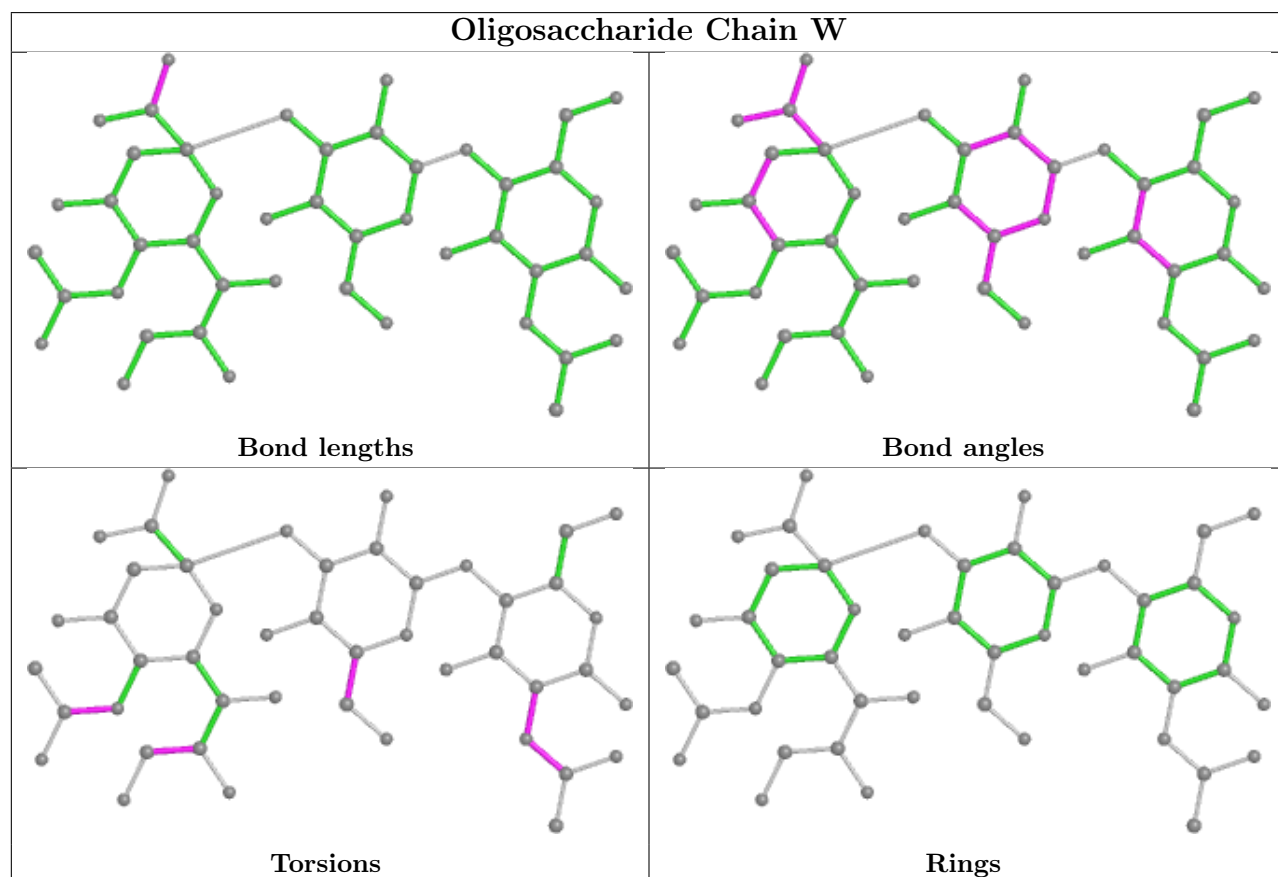
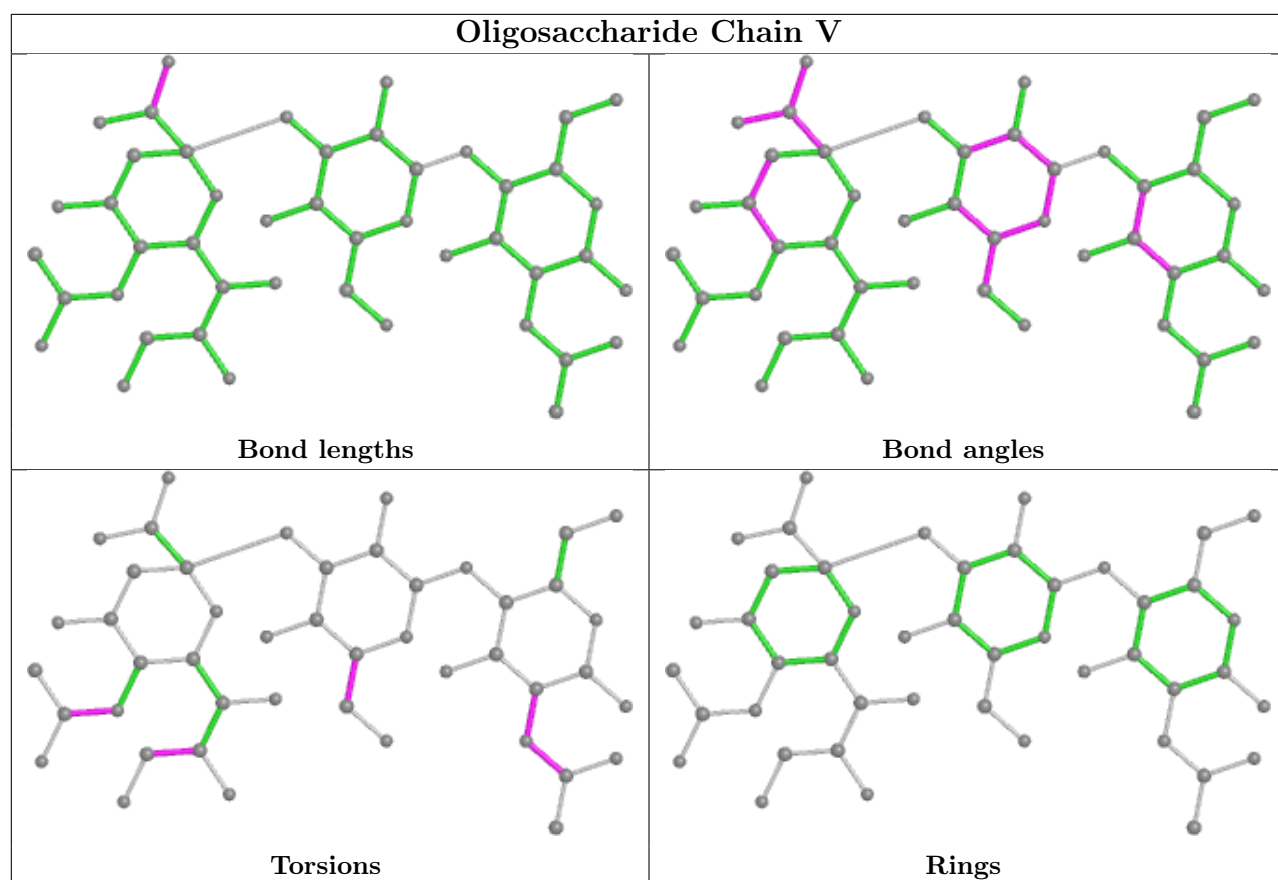


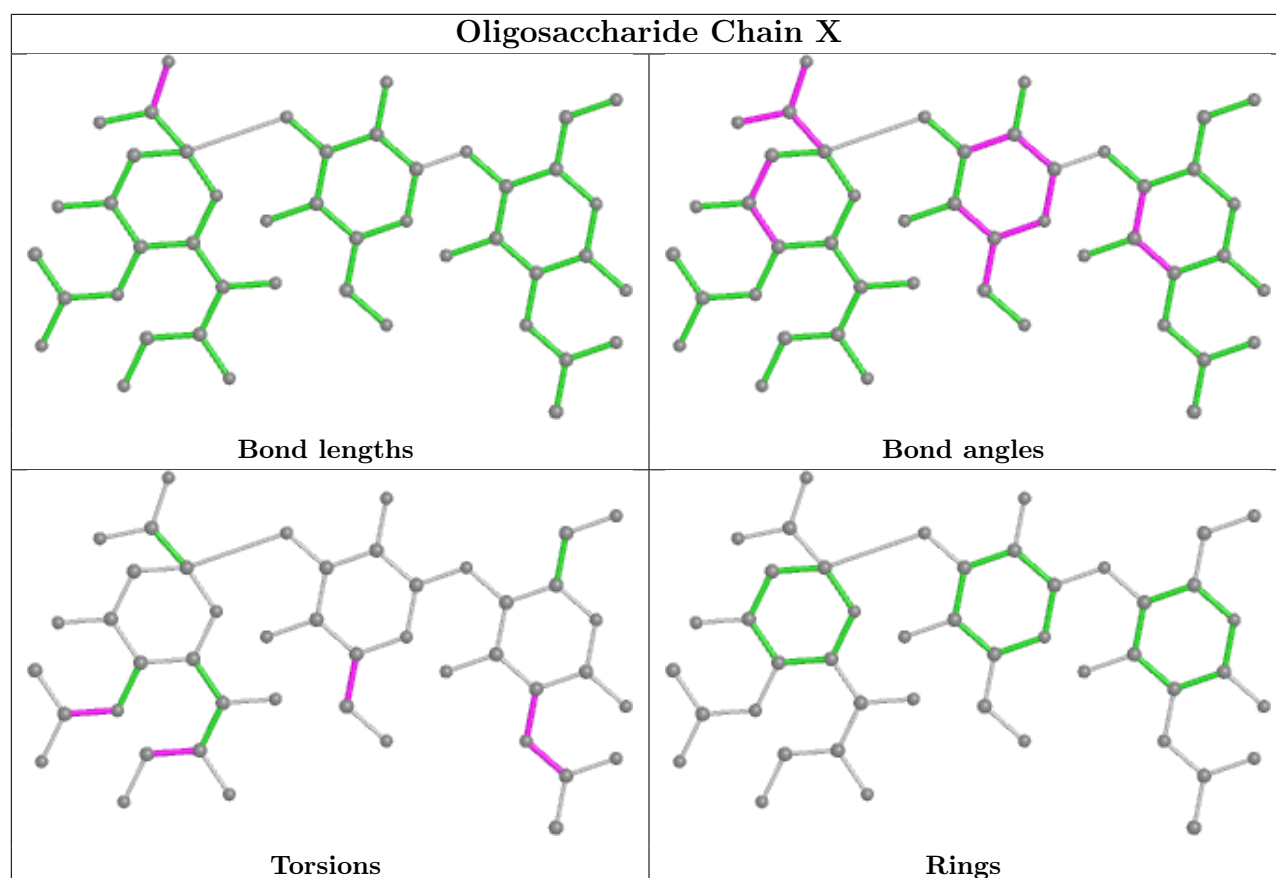












## 4.6 Ligand geometry [i](#)

12 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 | $\# Z  > 2$ |
| 8   | NAG  | D     | 301 | 2    | 14,14,15     | 0.25 | 0           | 17,19,21    | 0.48 | 0           |
| 8   | NAG  | A     | 402 | 1    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.42 | 0           |
| 8   | NAG  | A     | 401 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.40 | 0           |
| 8   | NAG  | B     | 301 | 2    | 14,14,15     | 0.25 | 0           | 17,19,21    | 0.49 | 0           |
| 8   | NAG  | C     | 402 | 1    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.42 | 0           |
| 8   | NAG  | R     | 301 | 3    | 14,14,15     | 0.38 | 0           | 17,19,21    | 0.45 | 0           |
| 8   | NAG  | C     | 401 | 1    | 14,14,15     | 0.22 | 0           | 17,19,21    | 0.41 | 0           |
| 8   | NAG  | H     | 402 | 1    | 14,14,15     | 0.23 | 0           | 17,19,21    | 0.41 | 0           |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | NAG  | H     | 401 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.40 | 0        |
| 8   | NAG  | J     | 301 | 3    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.46 | 0        |
| 8   | NAG  | I     | 301 | 2    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.49 | 0        |
| 8   | NAG  | E     | 301 | 3    | 14,14,15     | 0.38 | 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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | D     | 301 | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | A     | 402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | A     | 401 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | B     | 301 | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | R     | 301 | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | C     | 401 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | H     | 402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | H     | 401 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | J     | 301 | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | I     | 301 | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | E     | 301 | 3    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | R     | 301 | NAG  | O5-C5-C6-O6 |
| 8   | E     | 301 | NAG  | O5-C5-C6-O6 |
| 8   | J     | 301 | NAG  | O5-C5-C6-O6 |
| 8   | R     | 301 | NAG  | C4-C5-C6-O6 |
| 8   | E     | 301 | NAG  | C4-C5-C6-O6 |
| 8   | J     | 301 | NAG  | C4-C5-C6-O6 |
| 8   | A     | 401 | NAG  | O5-C5-C6-O6 |
| 8   | C     | 401 | NAG  | O5-C5-C6-O6 |
| 8   | H     | 401 | NAG  | O5-C5-C6-O6 |
| 8   | B     | 301 | NAG  | O5-C5-C6-O6 |

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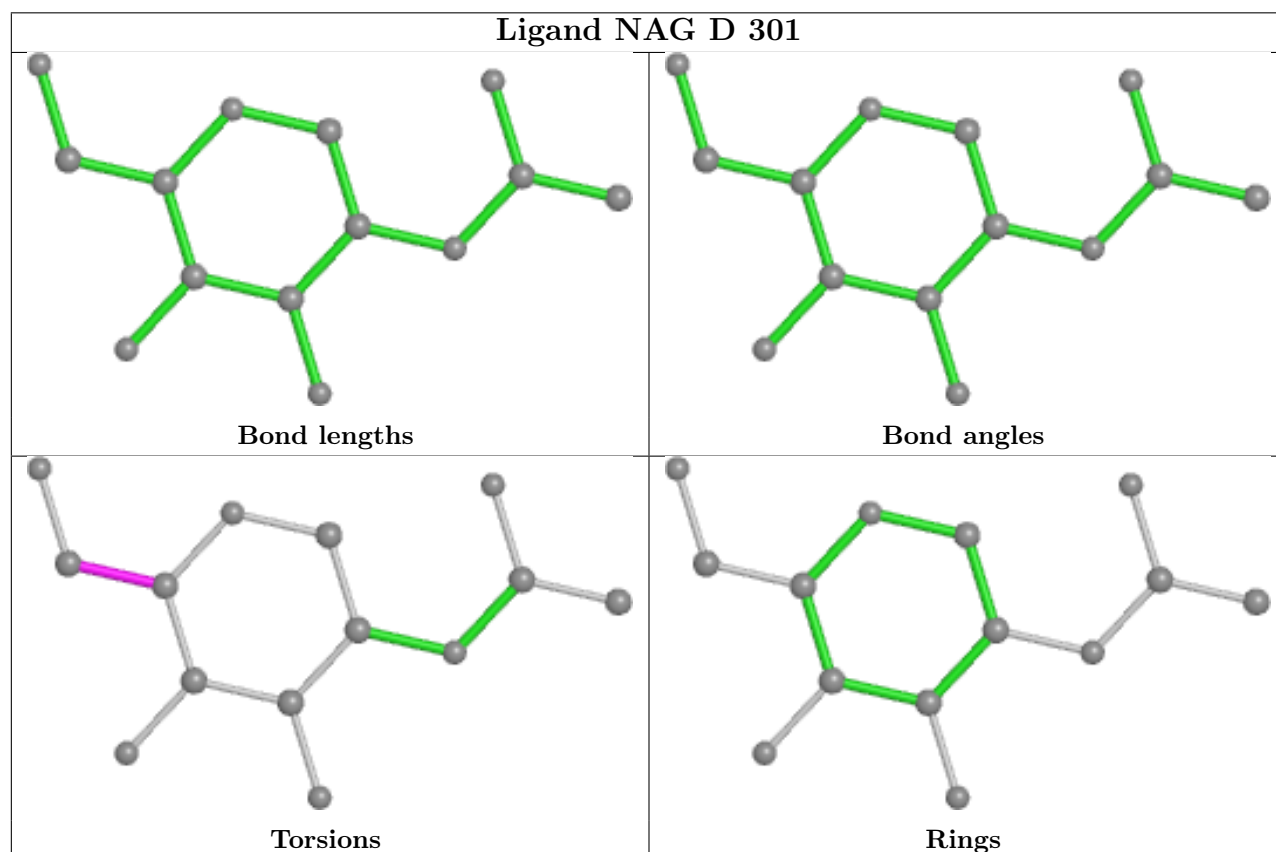
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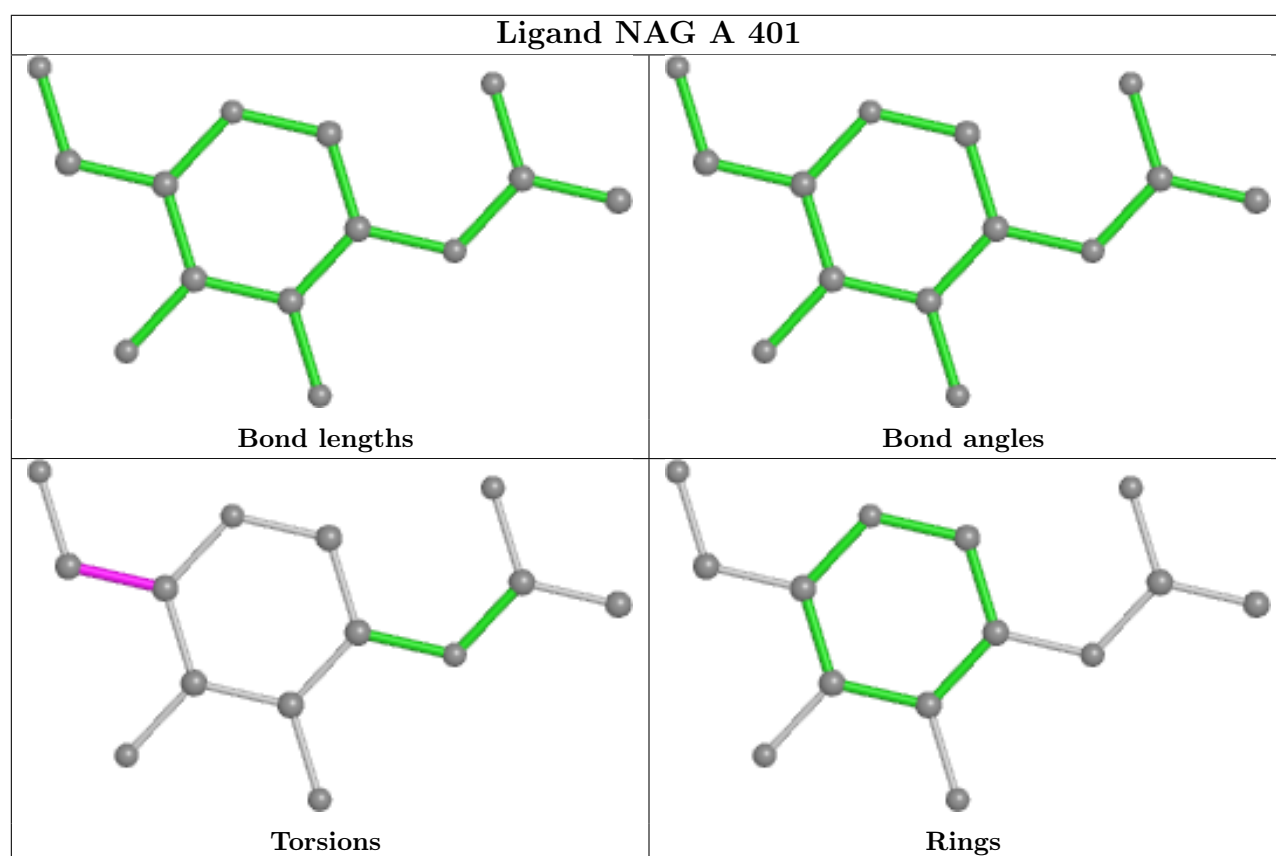
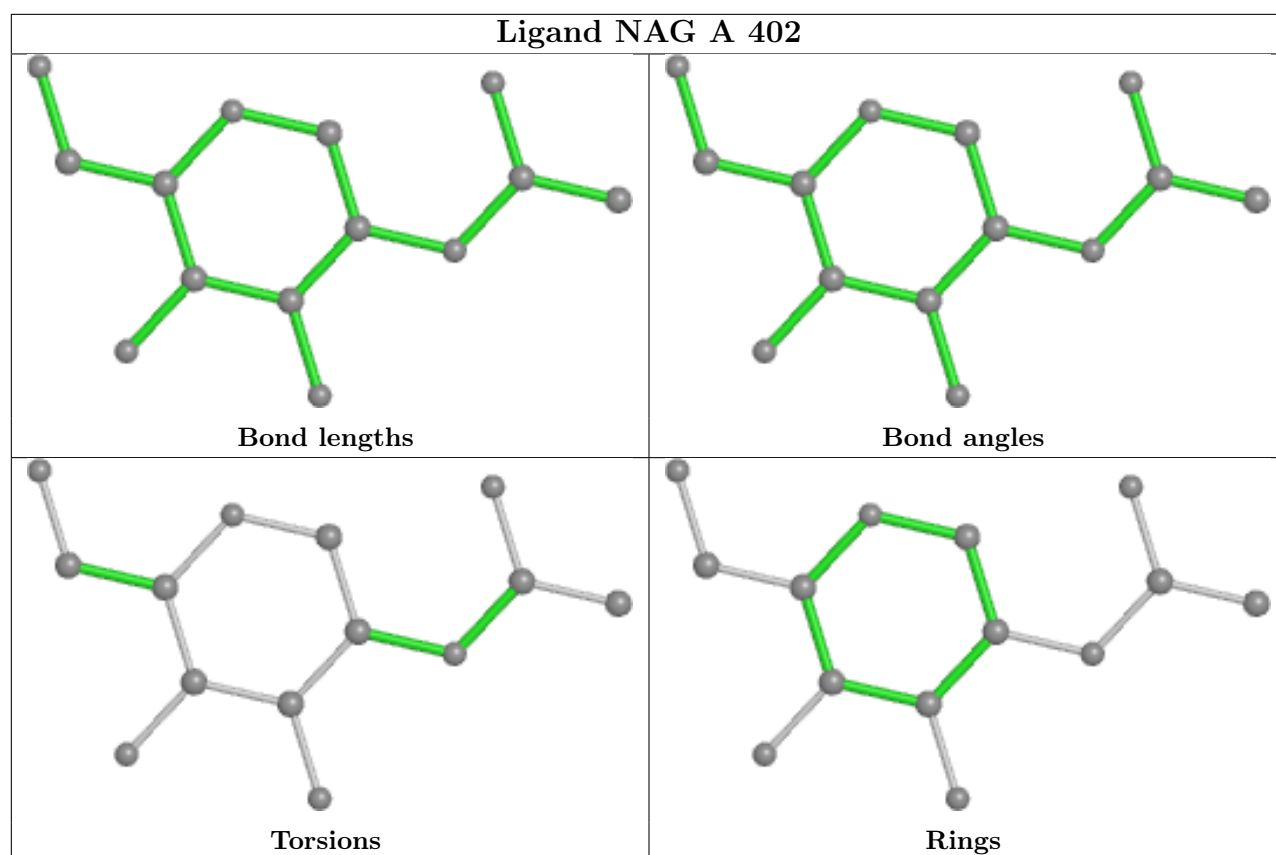
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | D     | 301 | NAG  | O5-C5-C6-O6 |
| 8   | I     | 301 | NAG  | O5-C5-C6-O6 |

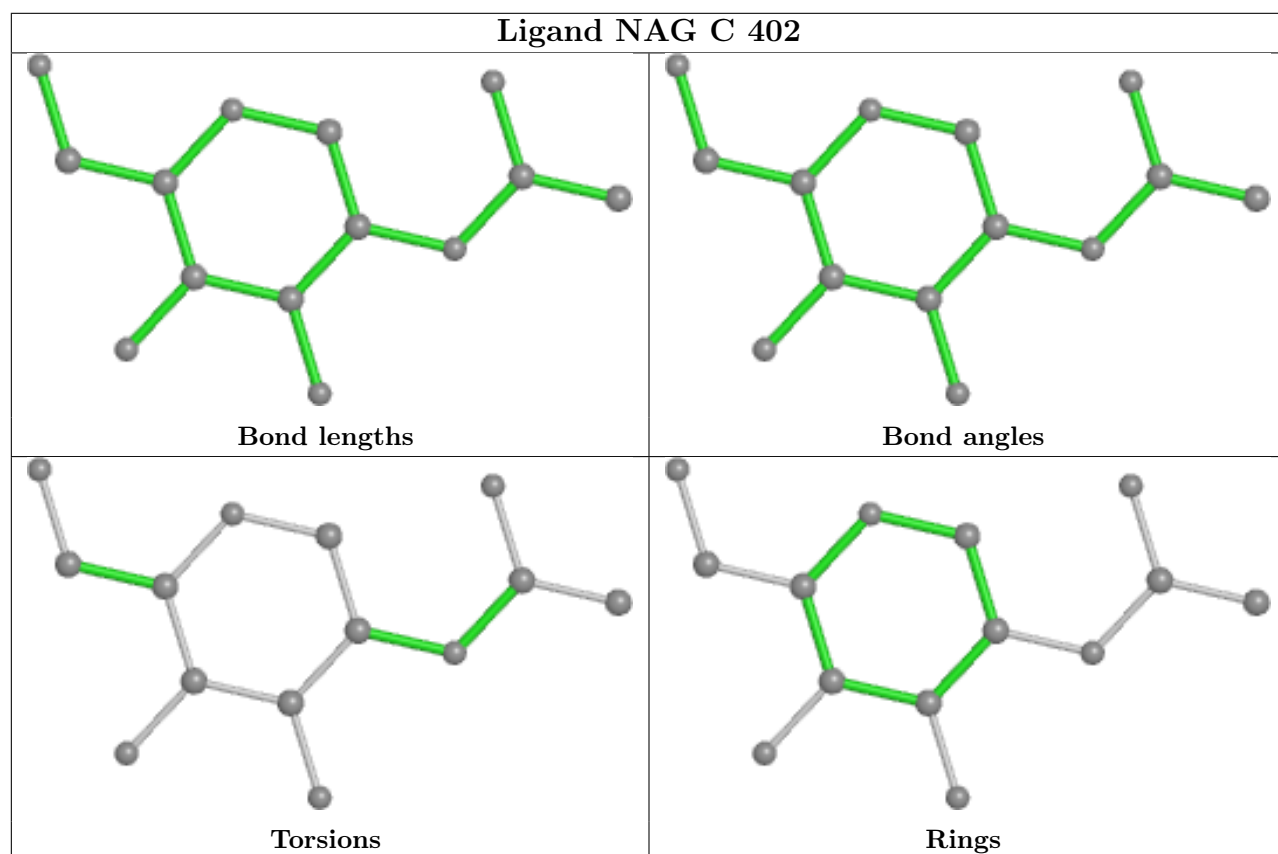
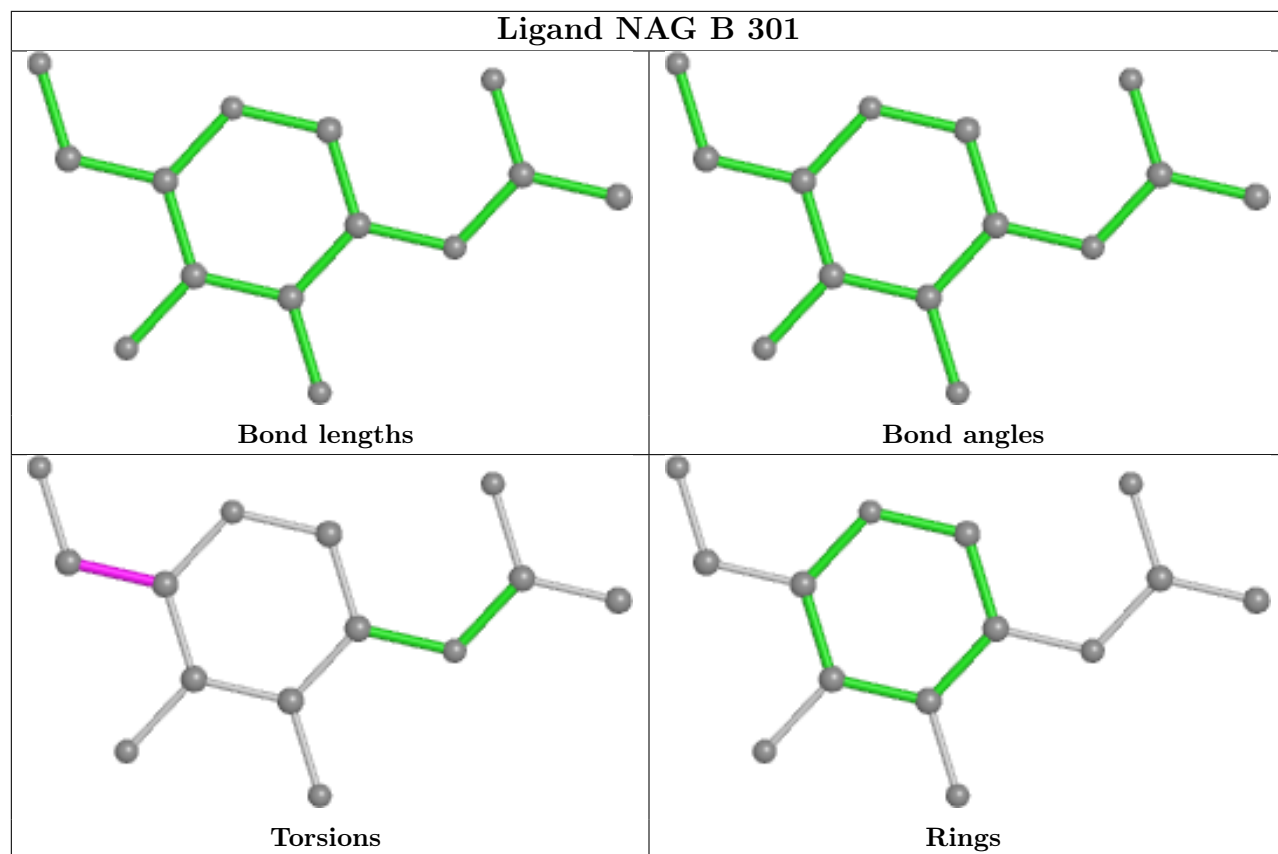
There are no ring outliers.

No monomer is involved in short contacts.

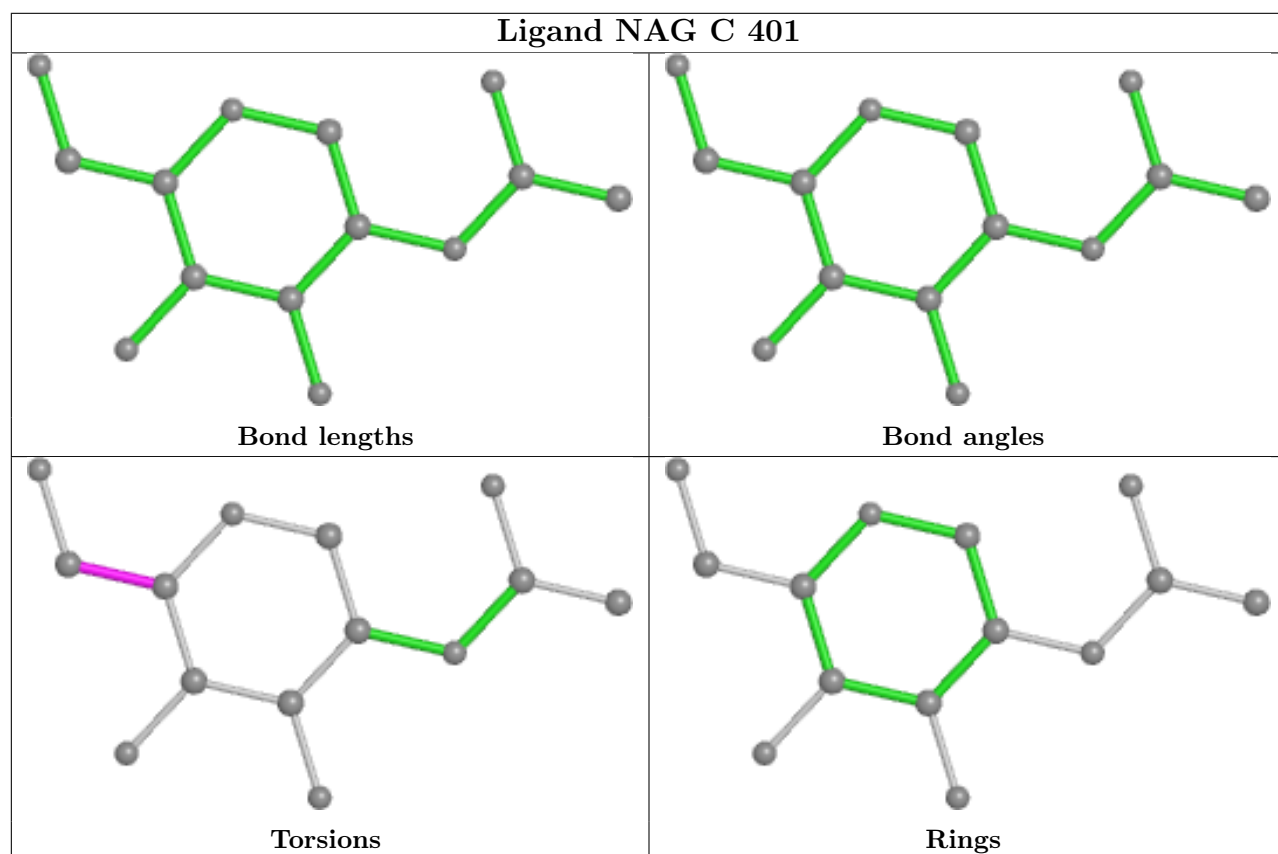
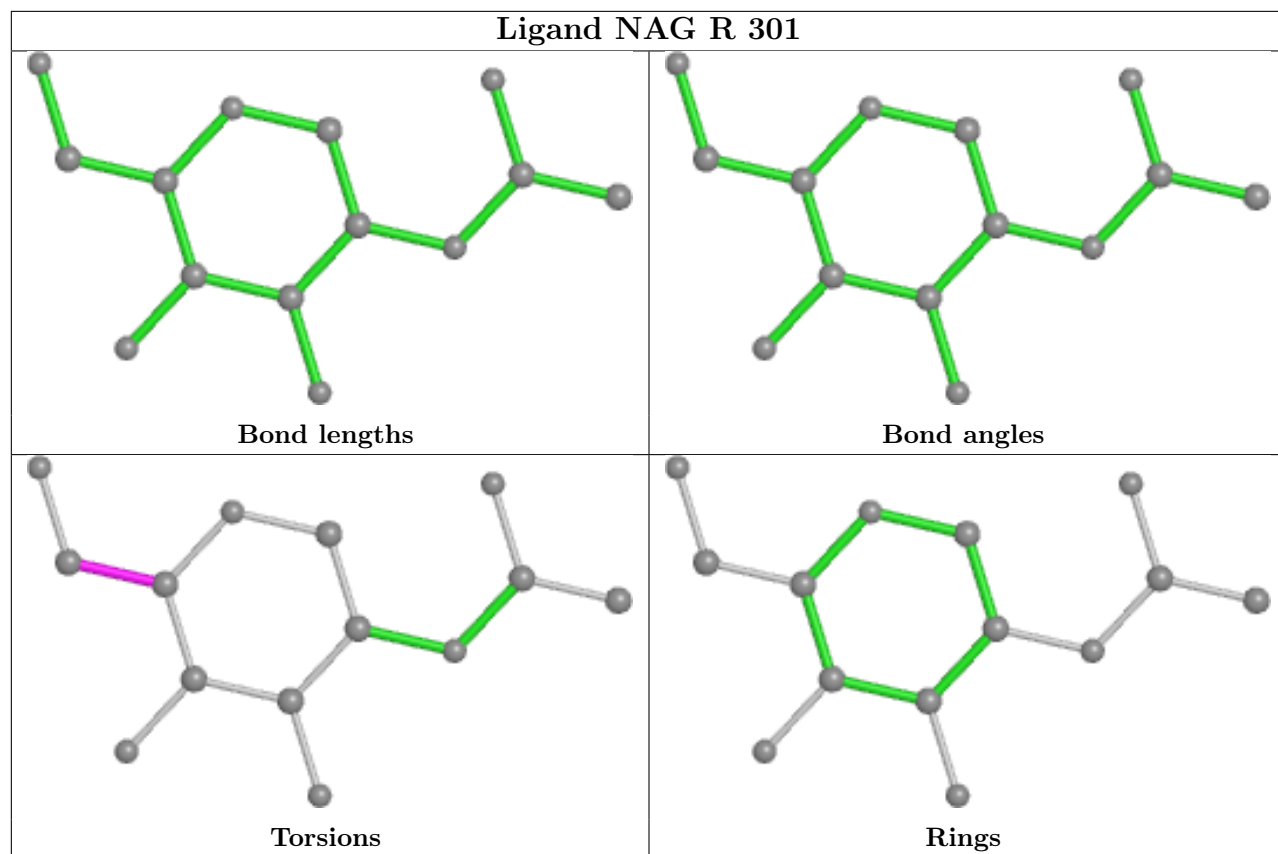
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

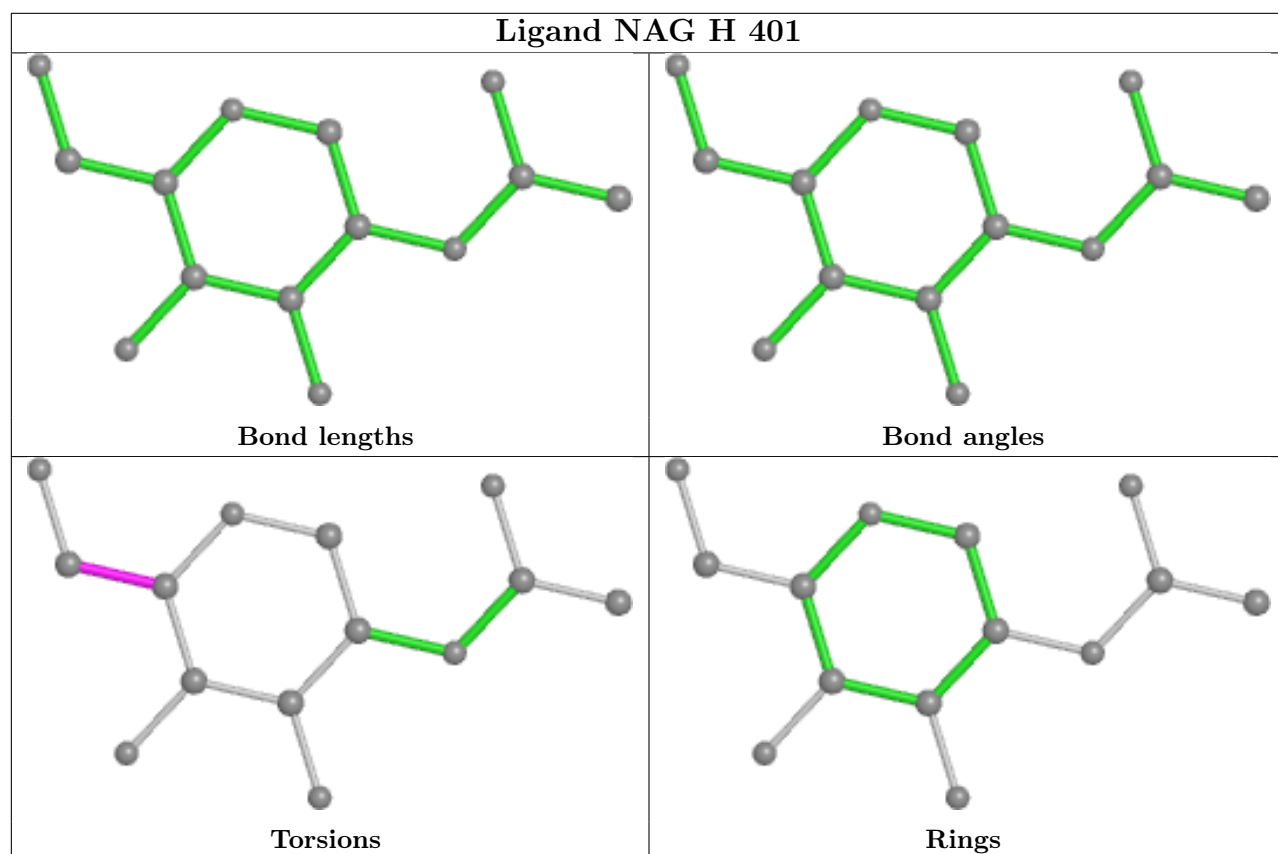
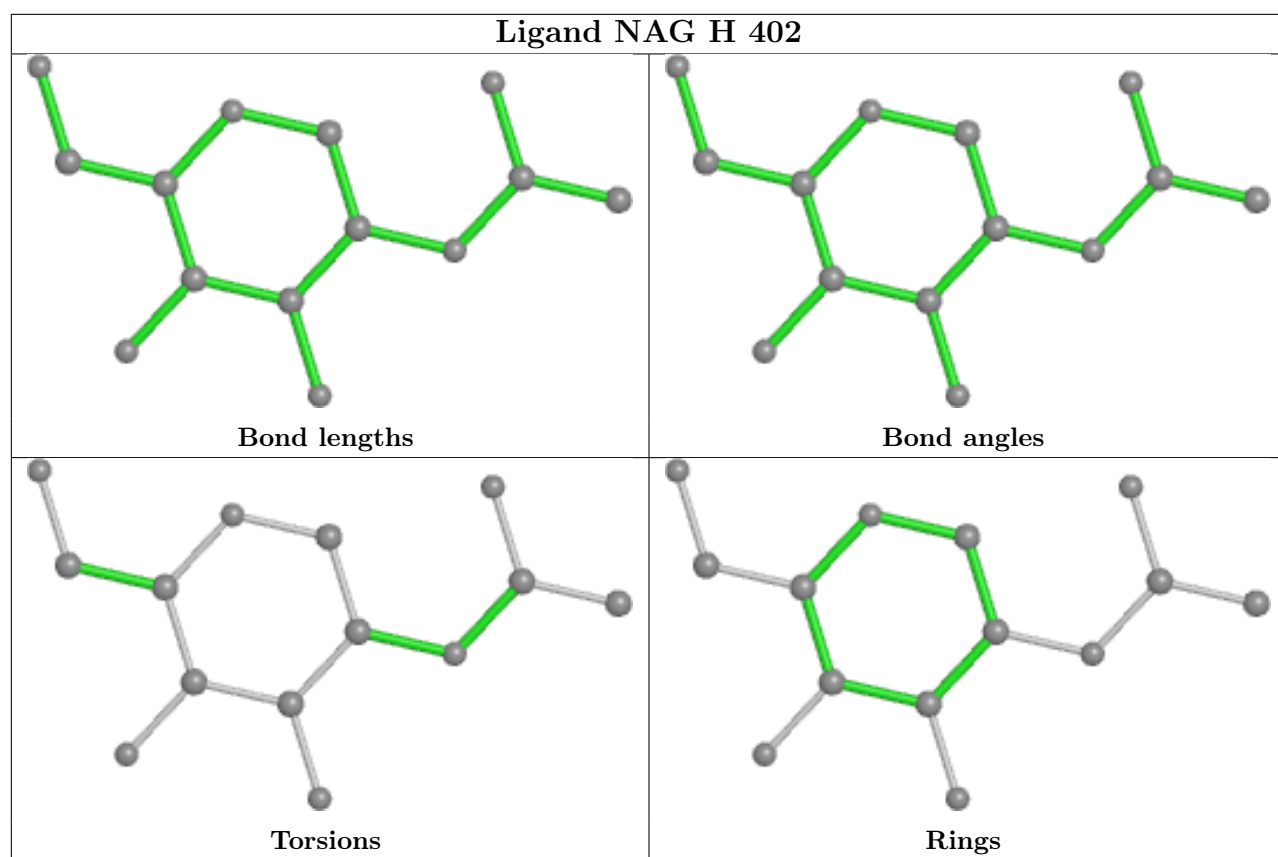


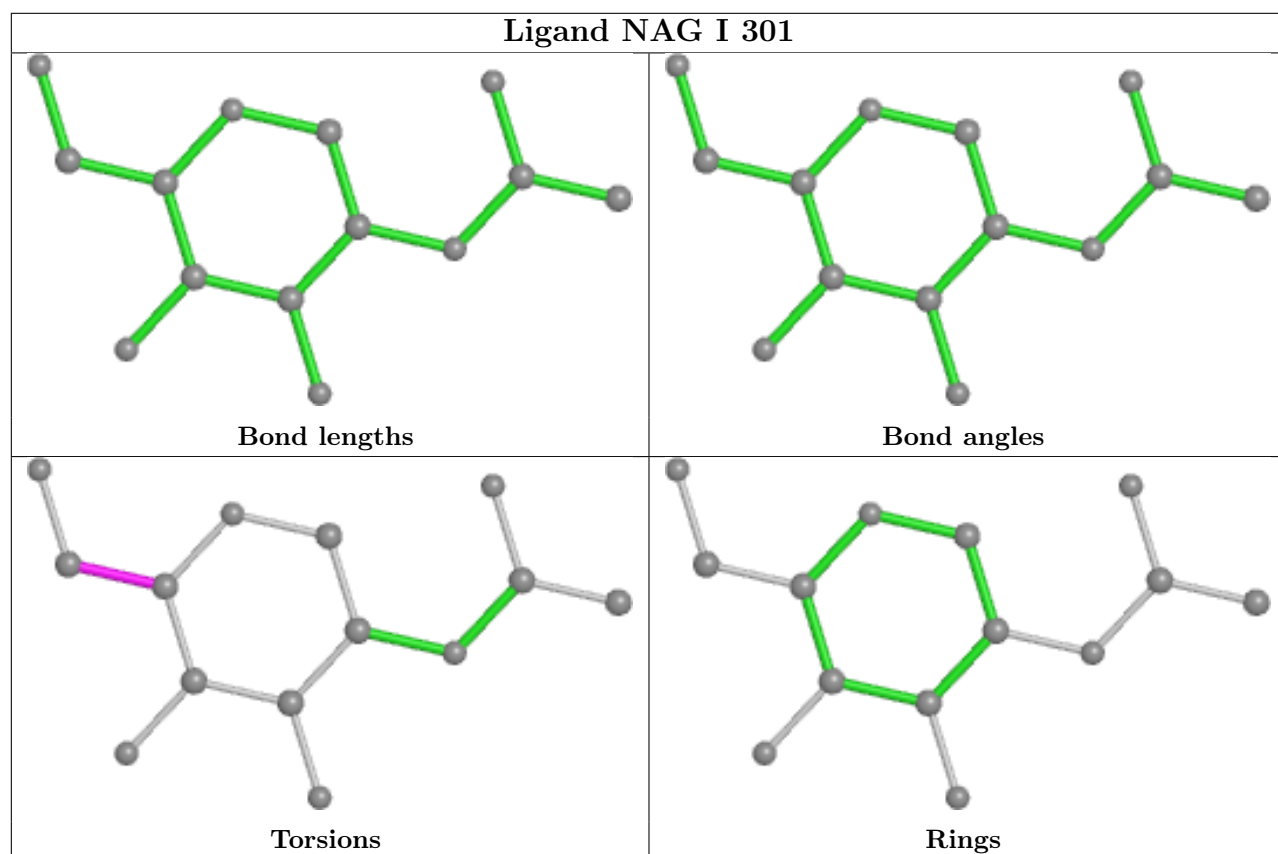
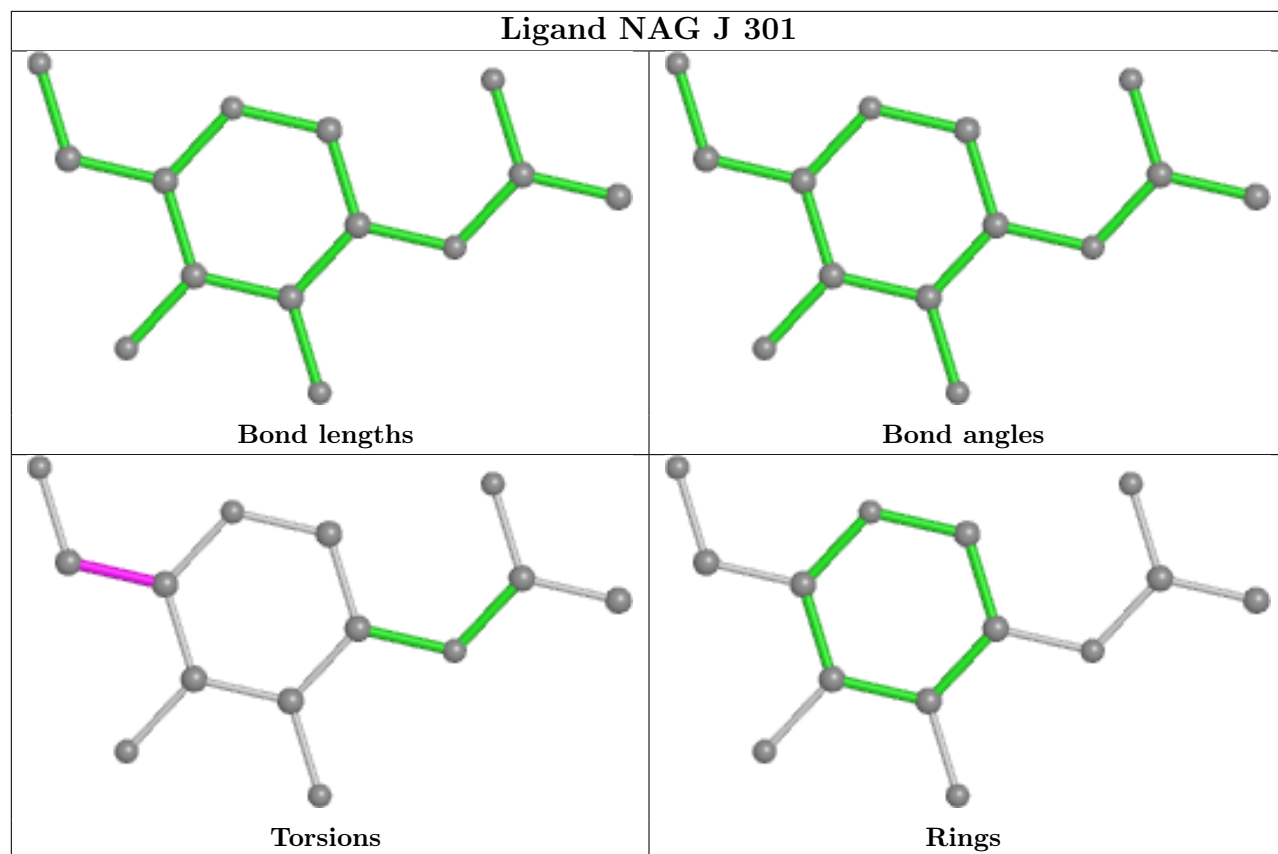


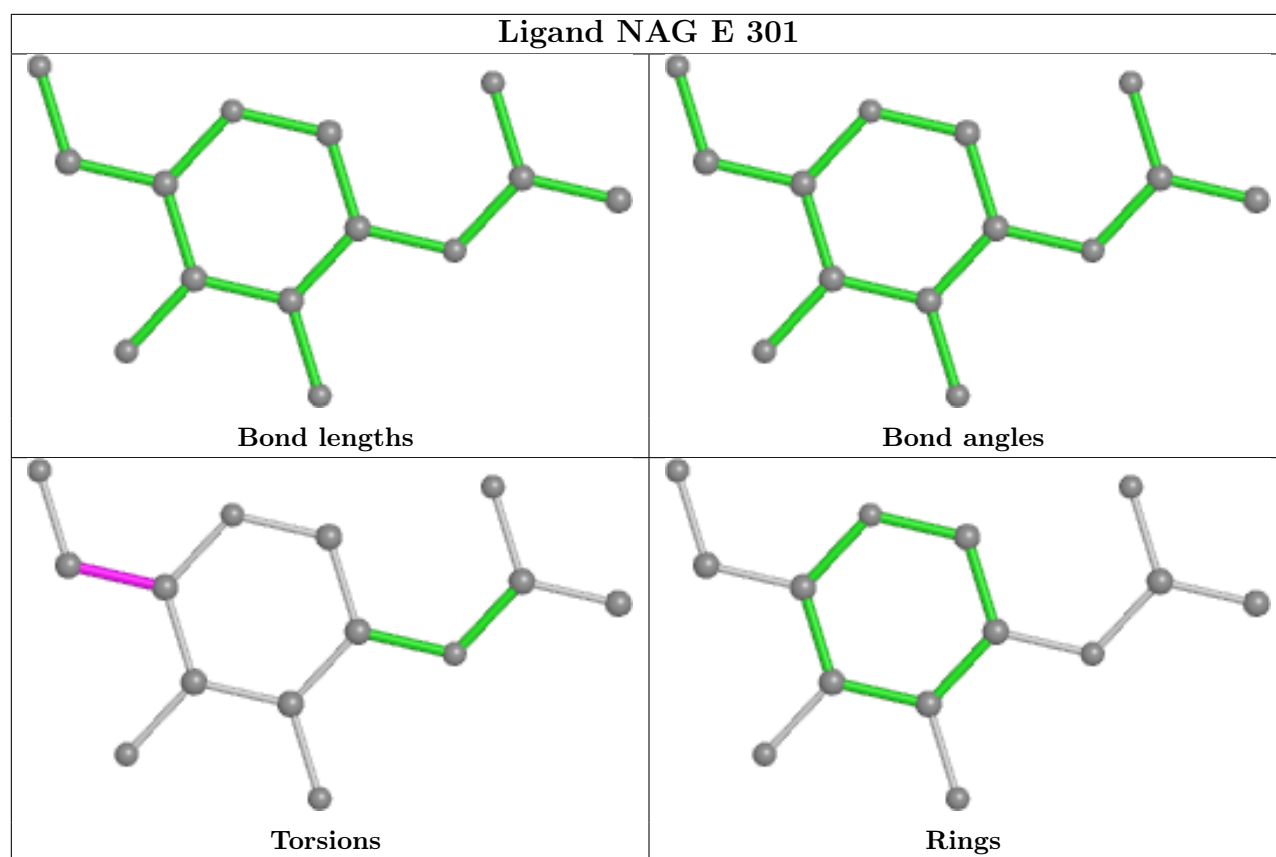












#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.