# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2023 – 02:51 PM EDT

| | | |
|---|---|---|
| PDB ID | : | 6NNF |
| Title | : | Crystal Structure of HIV-1 BG505 SOSIP.664 Prefusion Env Trimer Bound to VRC01 FR3-03 scFv in Complex with Crystallization Chaperones 3H109L Fab and 35O22 scFv at 3.5 Angstrom |
| Authors | : | Lai, Y.-T.; Kwong, P.D. |
| Deposited on | : | 2019-01-14 |
| Resolution | : | 2.76 Å(reported) |

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
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:

| | | |
|---|---|---|
| MolProbity | : | FAILED |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.76 Å.

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

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

## 2 Entry composition (i)

There are 14 unique types of molecules in this entry. The entry contains 11926 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Envelope glycoprotein gp41.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | B | 130 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1030 | 655 | 177 | 192 | 6 | | | |

There are 2 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| B | 559 | PRO | ILE | engineered mutation | UNP Q2N0S6 |
| B | 605 | CYS | THR | engineered mutation | UNP Q2N0S6 |

- Molecule 2 is a protein called 35O22 scFv heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 2 | D | 128 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 994 | 628 | 169 | 192 | 5 | | | |

- Molecule 3 is a protein called 35O22 scFv light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 3 | E | 112 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 851 | 533 | 141 | 171 | 6 | | | |

- Molecule 4 is a protein called Envelope glycoprotein gp120.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 4 | G | 431 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 3400 | 2140 | 601 | 632 | 27 | | | |

There are 8 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 137 | ALA | ASN | engineered mutation | UNP Q2N0S6 |
| G | 332 | ASN | THR | engineered mutation | UNP Q2N0S6 |

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| Chain | Residue | Modelled | Actual | Comment | Reference |
|---|---|---|---|---|---|
| G | 501 | CYS | ALA | engineered mutation | UNP Q2N0S6 |
| G | 509 | ARG | - | expression tag | UNP Q2N0S6 |
| G | 510 | ARG | - | expression tag | UNP Q2N0S6 |
| G | 511 | ARG | - | expression tag | UNP Q2N0S6 |
| G | 512 | ARG | - | expression tag | UNP Q2N0S6 |
| G | 513 | ARG | - | expression tag | UNP Q2N0S6 |

- Molecule 5 is a protein called 3H109L Fab heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 5 | H | 227 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1721 | 1096 | 279 | 340 | 6 | | | |

- Molecule 6 is a protein called 3H109L Fab light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 6 | L | 211 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1604 | 1009 | 276 | 312 | 7 | | | |

- Molecule 7 is a protein called VRC01 FR3-03 heavy chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 7 | U | 126 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 1010 | 636 | 183 | 183 | 8 | | | |

- Molecule 8 is a protein called VRC01 FR3-03 light chain.

| Mol | Chain | Residues | Atoms | | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|---|
| 8 | V | 97 | Total | C | N | O | S | 0 | 0 | 0 |
| | | | 751 | 474 | 129 | 146 | 2 | | | |

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]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 | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 9 | A | 6 | Total | C | N | O | 0 | 0 | 0 |
| | | | 72 | 40 | 2 | 30 | | | |

- Molecule 10 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 10 | C | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | I | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | K | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | M | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | N | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | P | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |
| 10 | Q | 2 | Total | C | N | O | 0 | 0 | 0 |
| | | | 28 | 16 | 2 | 10 | | | |

- Molecule 11 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 11 | F | 5 | Total | C | N | O | 0 | 0 | 0 |
| | | | 61 | 34 | 2 | 25 | | | |

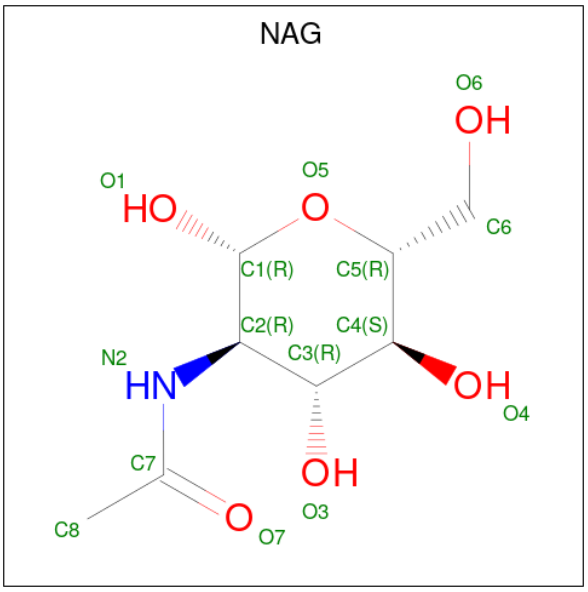
- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

| Mol | Chain | Residues | Atoms | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 12 | J | 4 | Total | C | N | O | 0 | 0 | 0 |
| | | | 50 | 28 | 2 | 20 | | | |

- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]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 | | | | ZeroOcc | AltConf | Trace |
|---|---|---|---|---|---|---|---|---|---|
| 13 | O | 10 | Total | C | N | O | 0 | 0 | 0 |
| | | | 116 | 64 | 2 | 50 | | | |

- Molecule 14 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).




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

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

# 3 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 63 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 130.87Å 130.87Å 315.19Å<br>90.00° 90.00° 120.00° | Depositor |
| Resolution (Å) | 42.84 – 2.76 | Depositor |
| % Data completeness<br>(in resolution range) | 34.8 (42.84-2.76) | Depositor |
| $R_{merge}$ | 0.05 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 2.90 (at 2.69Å) | Xtriage |
| Refinement program | PHENIX 1.14_3260 | Depositor |
| R, $R_{free}$ | 0.242 , 0.298 | Depositor |
| Wilson B-factor (Å$^2$) | 33.4 | Xtriage |
| Anisotropy | 0.018 | Xtriage |
| L-test for twinning[2] | $< \|L\| > = 0.47$, $< L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | 0.089 for h,-h-k,-l | Xtriage |
| Total number of atoms | 11926 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 69.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 4 Model quality

## 4.1 Standard geometry

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

## 4.2 Too-close contacts

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

## 4.3 Torsion angles

### 4.3.1 Protein backbone

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

### 4.3.2 Protein sidechains

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

### 4.3.3 RNA

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

## 4.4 Non-standard residues in protein, DNA, RNA chains

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

## 4.5 Carbohydrates

39 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|---|---|---|---|---|---|---|---|---|---|---|
| | | | | | Counts | RMSZ | $\#\|Z\|>2$ | Counts | RMSZ | $\#\|Z\|>2$ |
| 9 | NAG | A | 1 | 9,4 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.47 | 0 |
| 9 | NAG | A | 2 | 9 | 14,14,15 | 0.41 | 0 | 17,19,21 | 1.27 | 1 (5%) |
| 9 | BMA | A | 3 | 9 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.68 | 0 |
| 9 | MAN | A | 4 | 9 | 11,11,12 | 1.07 | 1 (9%) | 15,15,17 | 1.09 | 1 (6%) |
| 9 | MAN | A | 5 | 9 | 11,11,12 | 1.62 | 2 (18%) | 15,15,17 | 1.97 | 4 (26%) |
| 9 | MAN | A | 6 | 9 | 11,11,12 | 0.63 | 0 | 15,15,17 | 0.98 | 2 (13%) |
| 10 | NAG | C | 1 | 10,4 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.45 | 0 |
| 10 | NAG | C | 2 | 10 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.43 | 0 |
| 11 | NAG | F | 1 | 11,4 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.41 | 0 |
| 11 | NAG | F | 2 | 11 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.38 | 0 |
| 11 | BMA | F | 3 | 11 | 11,11,12 | 0.61 | 0 | 15,15,17 | 0.73 | 0 |
| 11 | MAN | F | 4 | 11 | 11,11,12 | 0.76 | 1 (9%) | 15,15,17 | 1.13 | 2 (13%) |
| 11 | MAN | F | 5 | 11 | 11,11,12 | 0.69 | 0 | 15,15,17 | 1.04 | 2 (13%) |
| 10 | NAG | I | 1 | 10,4 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.46 | 0 |
| 10 | NAG | I | 2 | 10 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.39 | 0 |
| 12 | NAG | J | 1 | 12,4 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.46 | 0 |
| 12 | NAG | J | 2 | 12 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.50 | 0 |
| 12 | BMA | J | 3 | 12 | 11,11,12 | 1.11 | 2 (18%) | 15,15,17 | 1.18 | 1 (6%) |
| 12 | MAN | J | 4 | 12 | 11,11,12 | 0.63 | 0 | 15,15,17 | 1.04 | 2 (13%) |
| 10 | NAG | K | 1 | 10,4 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.39 | 0 |
| 10 | NAG | K | 2 | 10 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.46 | 0 |
| 10 | NAG | M | 1 | 10,4 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.44 | 0 |
| 10 | NAG | M | 2 | 10 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.41 | 0 |
| 10 | NAG | N | 1 | 10,4 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.44 | 0 |
| 10 | NAG | N | 2 | 10 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.50 | 0 |
| 13 | NAG | O | 1 | 13,4 | 14,14,15 | 0.43 | 0 | 17,19,21 | 1.41 | 2 (11%) |
| 13 | MAN | O | 10 | 13 | 11,11,12 | 1.06 | 0 | 15,15,17 | 1.17 | 2 (13%) |
| 13 | NAG | O | 2 | 13 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.44 | 0 |
| 13 | BMA | O | 3 | 13 | 11,11,12 | 0.92 | 0 | 15,15,17 | 0.92 | 0 |
| 13 | MAN | O | 4 | 13 | 11,11,12 | 0.82 | 1 (9%) | 15,15,17 | 1.40 | 2 (13%) |
| 13 | MAN | O | 5 | 13 | 11,11,12 | 0.73 | 0 | 15,15,17 | 0.93 | 1 (6%) |
| 13 | MAN | O | 6 | 13 | 11,11,12 | 0.65 | 0 | 15,15,17 | 0.88 | 1 (6%) |
| 13 | MAN | O | 7 | 13 | 11,11,12 | 0.70 | 0 | 15,15,17 | 1.06 | 2 (13%) |
| 13 | MAN | O | 8 | 13 | 11,11,12 | 0.74 | 0 | 15,15,17 | 1.00 | 1 (6%) |
| 13 | MAN | O | 9 | 13 | 11,11,12 | 0.82 | 1 (9%) | 15,15,17 | 1.34 | 2 (13%) |
| 10 | NAG | P | 1 | 10,4 | 14,14,15 | 0.33 | 0 | 17,19,21 | 0.46 | 0 |
| 10 | NAG | P | 2 | 10 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.50 | 0 |
| 10 | NAG | Q | 1 | 10,4 | 14,14,15 | 0.96 | 1 (7%) | 17,19,21 | 1.60 | 1 (5%) |
| 10 | NAG | Q | 2 | 10 | 14,14,15 | 0.22 | 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 |
|---|---|---|---|---|---|---|---|
| 9 | NAG | A | 1 | 9,4 | - | 0/6/23/26 | 0/1/1/1 |
| 9 | NAG | A | 2 | 9 | - | 5/6/23/26 | 0/1/1/1 |
| 9 | BMA | A | 3 | 9 | - | 2/2/19/22 | 0/1/1/1 |
| 9 | MAN | A | 4 | 9 | - | 2/2/19/22 | 0/1/1/1 |
| 9 | MAN | A | 5 | 9 | - | 1/2/19/22 | 0/1/1/1 |
| 9 | MAN | A | 6 | 9 | - | 0/2/19/22 | 0/1/1/1 |
| 10 | NAG | C | 1 | 10,4 | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NAG | C | 2 | 10 | - | 2/6/23/26 | 0/1/1/1 |
| 11 | NAG | F | 1 | 11,4 | - | 1/6/23/26 | 0/1/1/1 |
| 11 | NAG | F | 2 | 11 | - | 0/6/23/26 | 0/1/1/1 |
| 11 | BMA | F | 3 | 11 | - | 2/2/19/22 | 0/1/1/1 |
| 11 | MAN | F | 4 | 11 | - | 0/2/19/22 | 0/1/1/1 |
| 11 | MAN | F | 5 | 11 | - | 2/2/19/22 | 0/1/1/1 |
| 10 | NAG | I | 1 | 10,4 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NAG | I | 2 | 10 | - | 2/6/23/26 | 0/1/1/1 |
| 12 | NAG | J | 1 | 12,4 | - | 2/6/23/26 | 0/1/1/1 |
| 12 | NAG | J | 2 | 12 | - | 2/6/23/26 | 0/1/1/1 |
| 12 | BMA | J | 3 | 12 | - | 0/2/19/22 | 0/1/1/1 |
| 12 | MAN | J | 4 | 12 | - | 2/2/19/22 | 0/1/1/1 |
| 10 | NAG | K | 1 | 10,4 | - | 1/6/23/26 | 0/1/1/1 |
| 10 | NAG | K | 2 | 10 | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NAG | M | 1 | 10,4 | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NAG | M | 2 | 10 | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NAG | N | 1 | 10,4 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NAG | N | 2 | 10 | - | 2/6/23/26 | 0/1/1/1 |
| 13 | NAG | O | 1 | 13,4 | - | 3/6/23/26 | 0/1/1/1 |
| 13 | MAN | O | 10 | 13 | - | 2/2/19/22 | 0/1/1/1 |
| 13 | NAG | O | 2 | 13 | - | 2/6/23/26 | 0/1/1/1 |
| 13 | BMA | O | 3 | 13 | - | 0/2/19/22 | 0/1/1/1 |
| 13 | MAN | O | 4 | 13 | - | 2/2/19/22 | 0/1/1/1 |
| 13 | MAN | O | 5 | 13 | - | 2/2/19/22 | 0/1/1/1 |
| 13 | MAN | O | 6 | 13 | - | 0/2/19/22 | 0/1/1/1 |
| 13 | MAN | O | 7 | 13 | - | 0/2/19/22 | 0/1/1/1 |
| 13 | MAN | O | 8 | 13 | - | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|---|---|---|---|---|---|---|---|
| 13 | MAN | O | 9 | 13 | - | 2/2/19/22 | 0/1/1/1 |
| 10 | NAG | P | 1 | 10,4 | - | 2/6/23/26 | 0/1/1/1 |
| 10 | NAG | P | 2 | 10 | - | 0/6/23/26 | 0/1/1/1 |
| 10 | NAG | Q | 1 | 10,4 | - | 4/6/23/26 | 0/1/1/1 |
| 10 | NAG | Q | 2 | 10 | - | 0/6/23/26 | 0/1/1/1 |

All (9) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|---|---|---|---|---|---|---|---|
| 9 | A | 5 | MAN | C1-C2 | 4.60 | 1.62 | 1.52 |
| 10 | Q | 1 | NAG | O5-C1 | 3.45 | 1.49 | 1.43 |
| 13 | O | 4 | MAN | C1-C2 | 2.52 | 1.58 | 1.52 |
| 13 | O | 9 | MAN | C1-C2 | 2.35 | 1.57 | 1.52 |
| 9 | A | 4 | MAN | O5-C1 | -2.26 | 1.40 | 1.43 |
| 9 | A | 5 | MAN | O5-C1 | 2.12 | 1.47 | 1.43 |
| 11 | F | 4 | MAN | C1-C2 | 2.11 | 1.57 | 1.52 |
| 12 | J | 3 | BMA | C4-C3 | 2.08 | 1.57 | 1.52 |
| 12 | J | 3 | BMA | C2-C3 | 2.00 | 1.55 | 1.52 |

All (29) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 10 | Q | 1 | NAG | C1-O5-C5 | 6.23 | 120.63 | 112.19 |
| 13 | O | 1 | NAG | C2-N2-C7 | 4.51 | 129.32 | 122.90 |
| 9 | A | 5 | MAN | C1-O5-C5 | 4.48 | 118.26 | 112.19 |
| 9 | A | 5 | MAN | C1-C2-C3 | 4.36 | 115.03 | 109.67 |
| 9 | A | 2 | NAG | C2-N2-C7 | 4.33 | 129.07 | 122.90 |
| 13 | O | 9 | MAN | C1-O5-C5 | 3.80 | 117.34 | 112.19 |
| 13 | O | 4 | MAN | C1-O5-C5 | 3.62 | 117.09 | 112.19 |
| 13 | O | 8 | MAN | C1-O5-C5 | 2.70 | 115.85 | 112.19 |
| 12 | J | 3 | BMA | C2-C3-C4 | 2.69 | 115.56 | 110.89 |
| 9 | A | 5 | MAN | O5-C1-C2 | 2.64 | 114.84 | 110.77 |
| 11 | F | 4 | MAN | C1-O5-C5 | 2.62 | 115.74 | 112.19 |
| 13 | O | 4 | MAN | O2-C2-C3 | -2.52 | 105.09 | 110.14 |
| 12 | J | 4 | MAN | C1-O5-C5 | 2.51 | 115.59 | 112.19 |
| 13 | O | 7 | MAN | C1-O5-C5 | 2.51 | 115.59 | 112.19 |
| 9 | A | 6 | MAN | C1-O5-C5 | 2.45 | 115.52 | 112.19 |
| 11 | F | 5 | MAN | C1-O5-C5 | 2.45 | 115.51 | 112.19 |
| 13 | O | 10 | MAN | O2-C2-C3 | -2.36 | 105.42 | 110.14 |
| 13 | O | 1 | NAG | C1-C2-N2 | 2.31 | 114.44 | 110.49 |
| 13 | O | 5 | MAN | O2-C2-C3 | -2.30 | 105.53 | 110.14 |

*Continued on next page...*

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| Mol | Chain | Res | Type | Atoms | Z | Observed($^o$) | Ideal($^o$) |
|---|---|---|---|---|---|---|---|
| 13 | O | 7 | MAN | O2-C2-C3 | -2.26 | 105.61 | 110.14 |
| 9 | A | 5 | MAN | O2-C2-C3 | -2.24 | 105.65 | 110.14 |
| 12 | J | 4 | MAN | O2-C2-C3 | -2.23 | 105.67 | 110.14 |
| 13 | O | 9 | MAN | O2-C2-C3 | -2.21 | 105.70 | 110.14 |
| 9 | A | 4 | MAN | O2-C2-C3 | -2.21 | 105.71 | 110.14 |
| 9 | A | 6 | MAN | O2-C2-C3 | -2.19 | 105.75 | 110.14 |
| 11 | F | 5 | MAN | O2-C2-C3 | -2.18 | 105.77 | 110.14 |
| 13 | O | 6 | MAN | O2-C2-C3 | -2.14 | 105.85 | 110.14 |
| 11 | F | 4 | MAN | O2-C2-C3 | -2.13 | 105.88 | 110.14 |
| 13 | O | 10 | MAN | C1-C2-C3 | 2.08 | 112.22 | 109.67 |

There are no chirality outliers.

All (51) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 13 | O | 2 | NAG | O5-C5-C6-O6 |
| 9 | A | 3 | BMA | O5-C5-C6-O6 |
| 11 | F | 3 | BMA | C4-C5-C6-O6 |
| 10 | I | 2 | NAG | O5-C5-C6-O6 |
| 10 | Q | 1 | NAG | O5-C5-C6-O6 |
| 12 | J | 2 | NAG | O5-C5-C6-O6 |
| 13 | O | 2 | NAG | C4-C5-C6-O6 |
| 9 | A | 3 | BMA | C4-C5-C6-O6 |
| 10 | I | 2 | NAG | C4-C5-C6-O6 |
| 13 | O | 9 | MAN | C4-C5-C6-O6 |
| 10 | I | 1 | NAG | O5-C5-C6-O6 |
| 12 | J | 1 | NAG | O5-C5-C6-O6 |
| 12 | J | 4 | MAN | C4-C5-C6-O6 |
| 10 | C | 2 | NAG | O5-C5-C6-O6 |
| 11 | F | 3 | BMA | O5-C5-C6-O6 |
| 13 | O | 9 | MAN | O5-C5-C6-O6 |
| 12 | J | 4 | MAN | O5-C5-C6-O6 |
| 13 | O | 10 | MAN | C4-C5-C6-O6 |
| 10 | C | 2 | NAG | C4-C5-C6-O6 |
| 9 | A | 2 | NAG | C8-C7-N2-C2 |
| 9 | A | 2 | NAG | O7-C7-N2-C2 |
| 10 | Q | 1 | NAG | C8-C7-N2-C2 |
| 10 | Q | 1 | NAG | O7-C7-N2-C2 |
| 13 | O | 1 | NAG | C8-C7-N2-C2 |
| 13 | O | 1 | NAG | O7-C7-N2-C2 |
| 9 | A | 2 | NAG | O5-C5-C6-O6 |
| 13 | O | 4 | MAN | O5-C5-C6-O6 |

*Continued on next page...*

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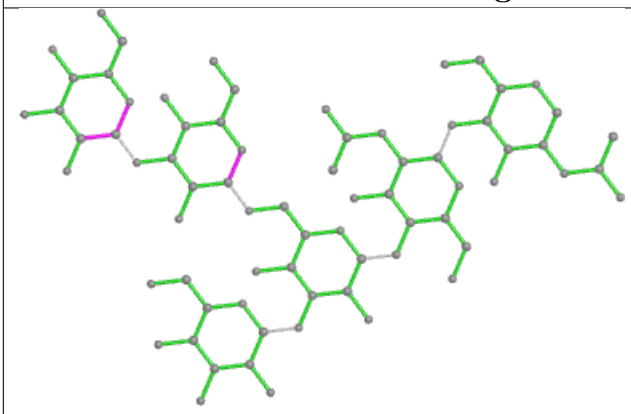
| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 12 | J | 1 | NAG | C4-C5-C6-O6 |
| 10 | N | 2 | NAG | C4-C5-C6-O6 |
| 12 | J | 2 | NAG | C4-C5-C6-O6 |
| 9 | A | 2 | NAG | C4-C5-C6-O6 |
| 10 | P | 1 | NAG | O5-C5-C6-O6 |
| 13 | O | 4 | MAN | C4-C5-C6-O6 |
| 13 | O | 10 | MAN | O5-C5-C6-O6 |
| 10 | N | 1 | NAG | O5-C5-C6-O6 |
| 9 | A | 4 | MAN | O5-C5-C6-O6 |
| 10 | N | 2 | NAG | O5-C5-C6-O6 |
| 9 | A | 4 | MAN | C4-C5-C6-O6 |
| 10 | Q | 1 | NAG | C4-C5-C6-O6 |
| 13 | O | 5 | MAN | O5-C5-C6-O6 |
| 11 | F | 5 | MAN | C4-C5-C6-O6 |
| 13 | O | 5 | MAN | C4-C5-C6-O6 |
| 9 | A | 5 | MAN | O5-C5-C6-O6 |
| 10 | I | 1 | NAG | C4-C5-C6-O6 |
| 11 | F | 5 | MAN | O5-C5-C6-O6 |
| 10 | P | 1 | NAG | C4-C5-C6-O6 |
| 10 | N | 1 | NAG | C4-C5-C6-O6 |
| 10 | K | 1 | NAG | C1-C2-N2-C7 |
| 11 | F | 1 | NAG | C4-C5-C6-O6 |
| 9 | A | 2 | NAG | C3-C2-N2-C7 |
| 13 | O | 1 | NAG | C3-C2-N2-C7 |

There are no ring outliers.

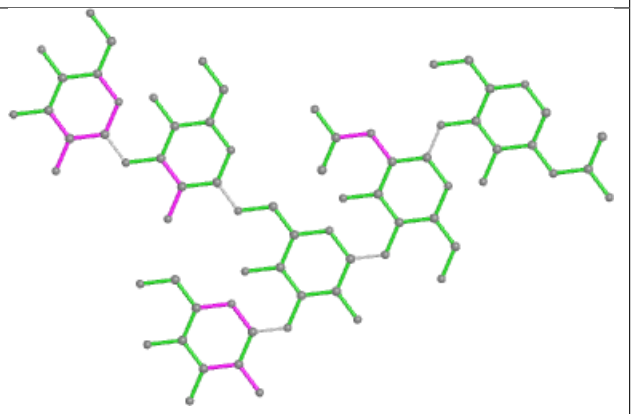
No monomer is involved in short contacts.

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

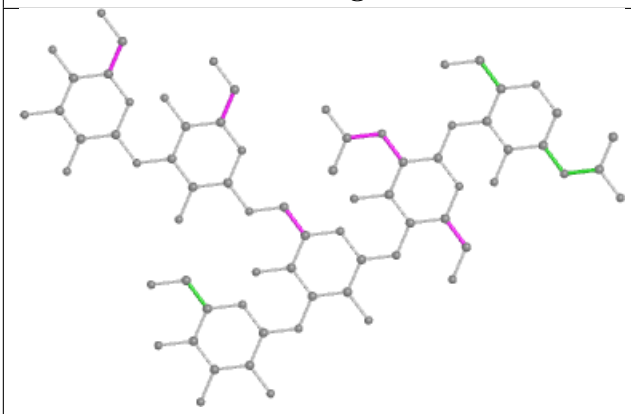
**Oligosaccharide Chain A**



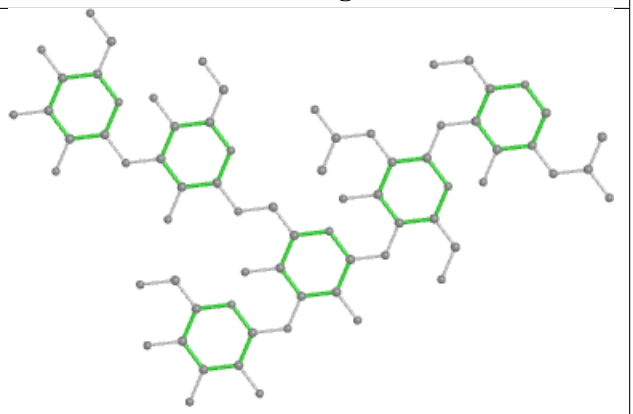
**Bond lengths**



**Bond angles**

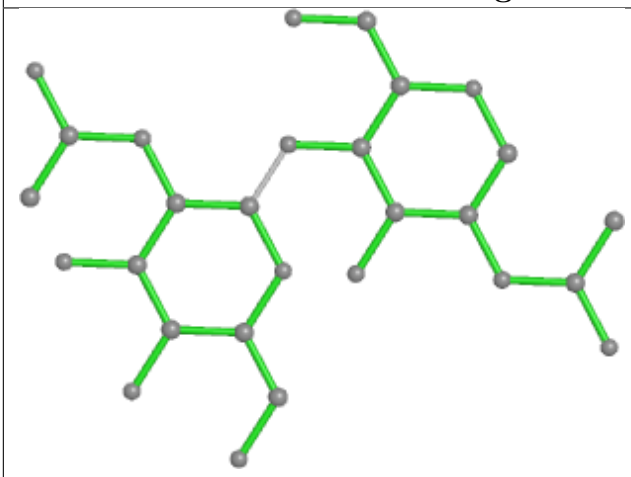


**Torsions**

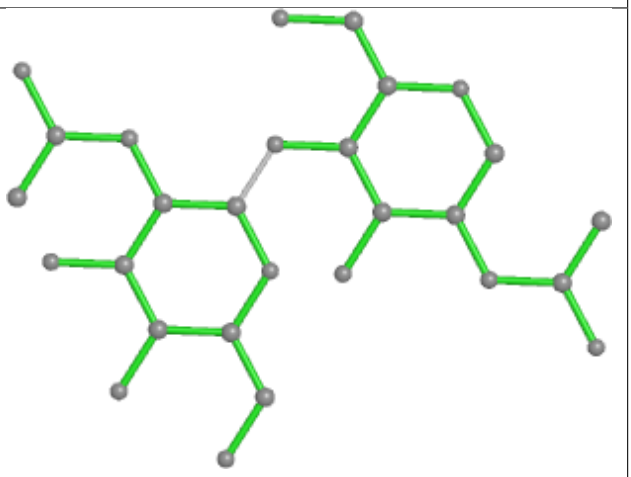


**Rings**

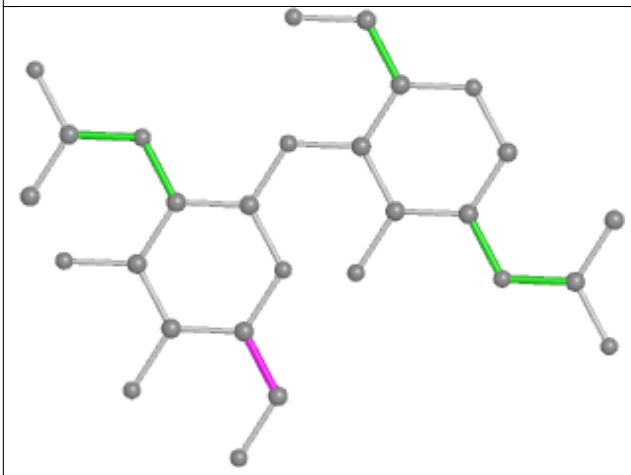
**Oligosaccharide Chain C**



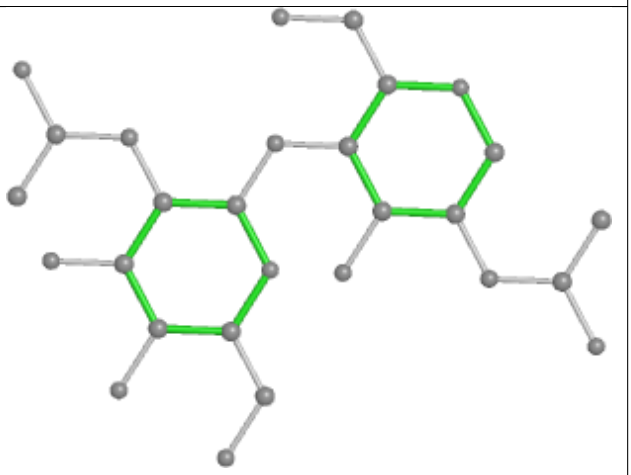
**Bond lengths**



**Bond angles**

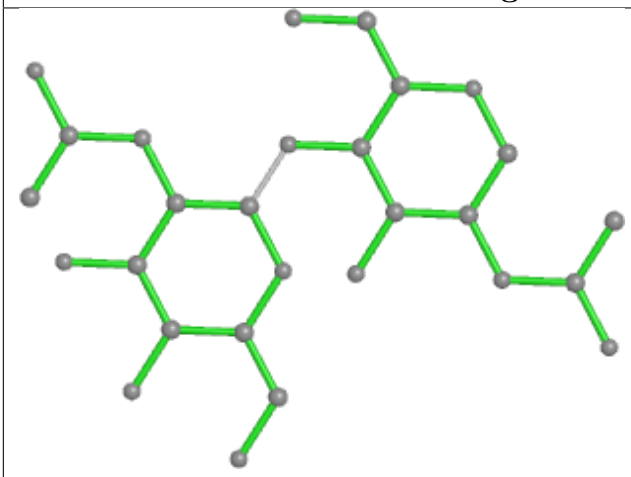


**Torsions**

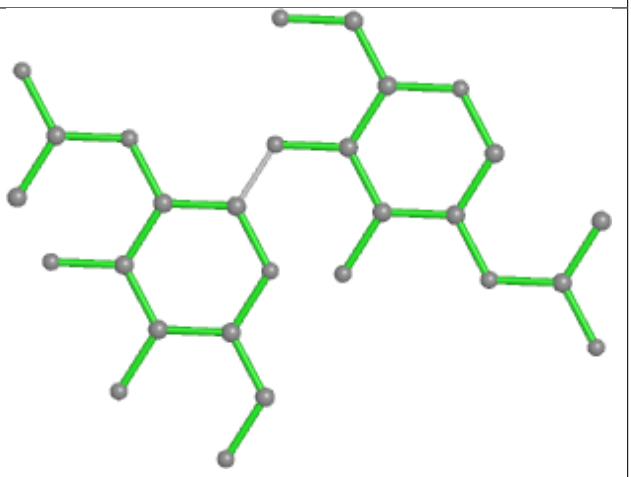


**Rings**

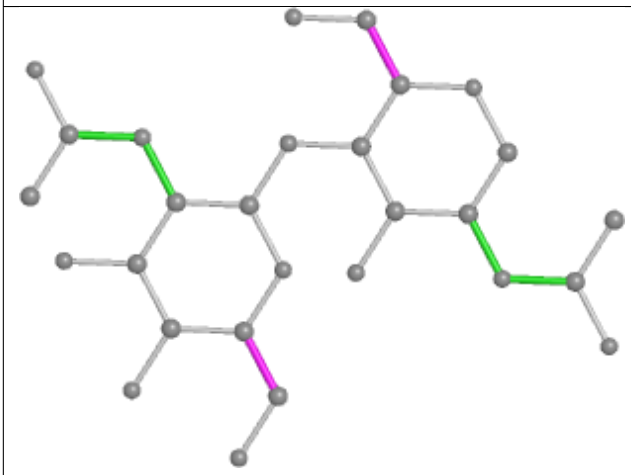
**Oligosaccharide Chain I**



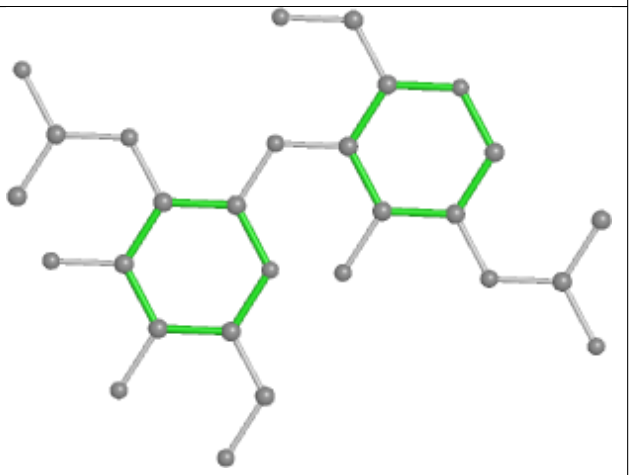
**Bond lengths**



**Bond angles**

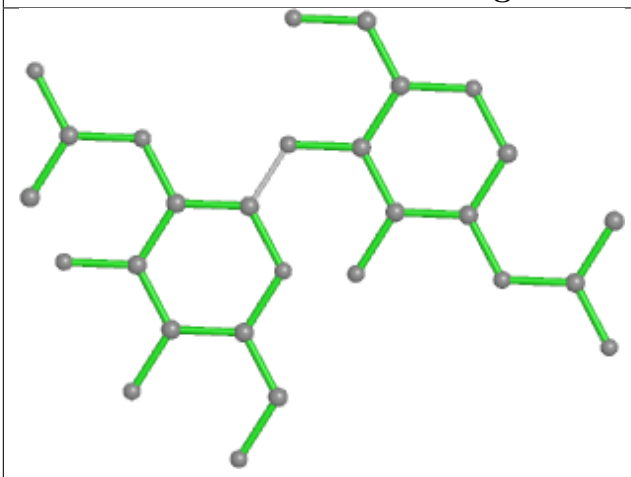


**Torsions**

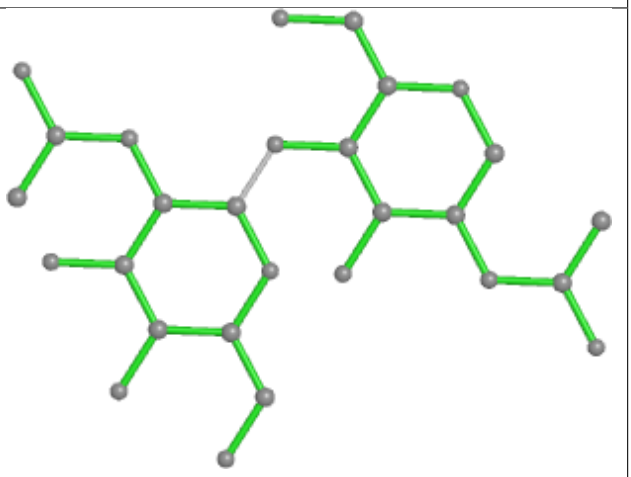


**Rings**

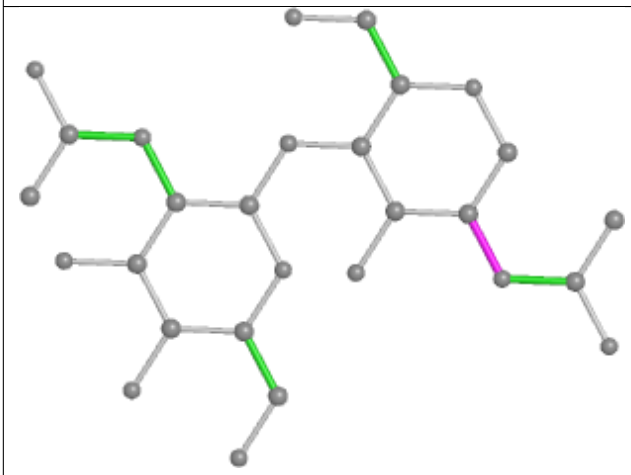
**Oligosaccharide Chain K**



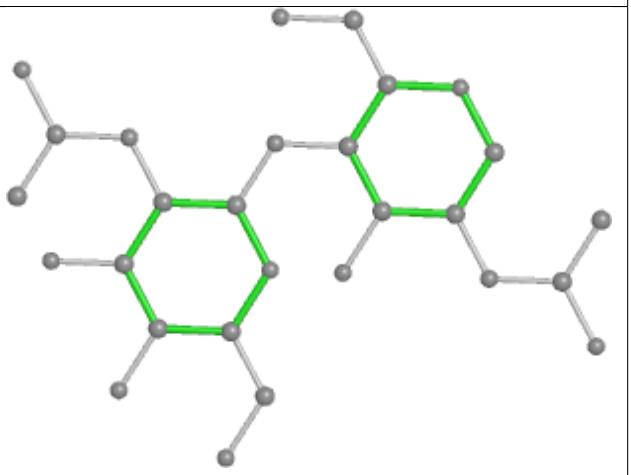
**Bond lengths**



**Bond angles**

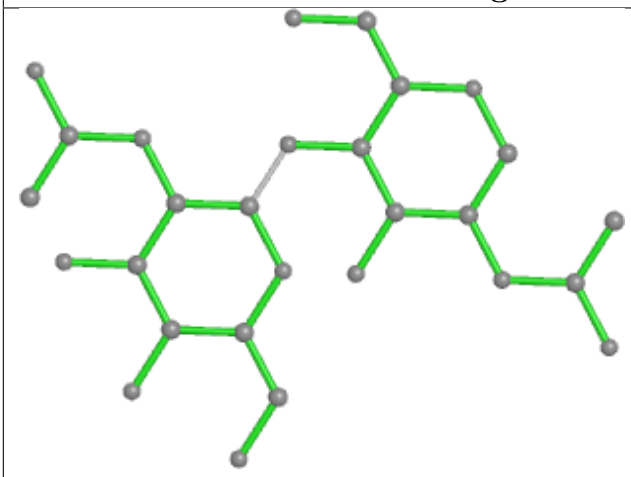


**Torsions**

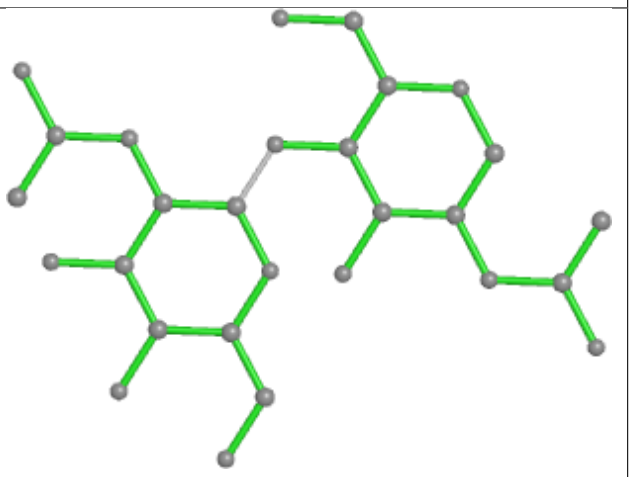


**Rings**

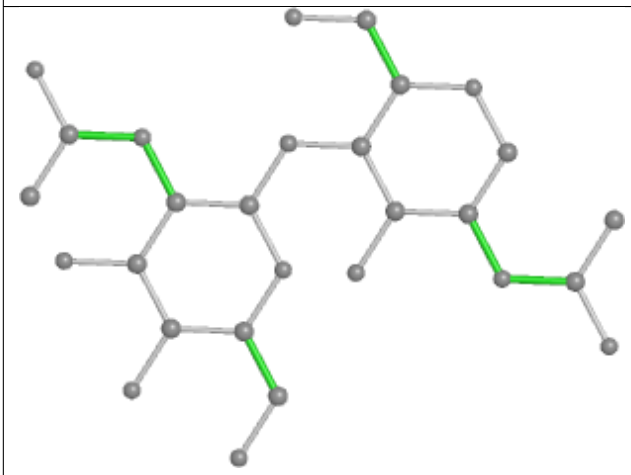
**Oligosaccharide Chain M**



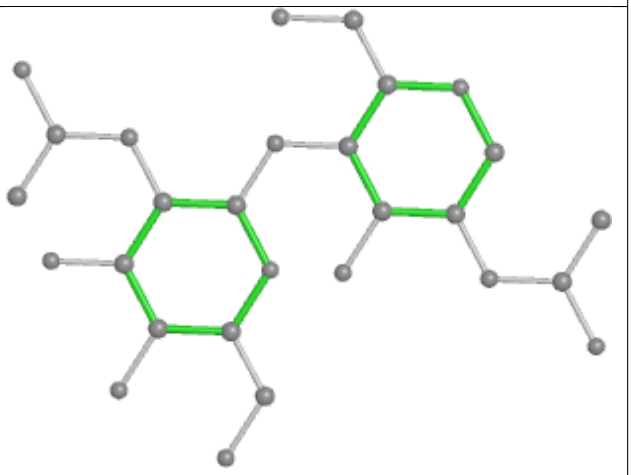
**Bond lengths**



**Bond angles**

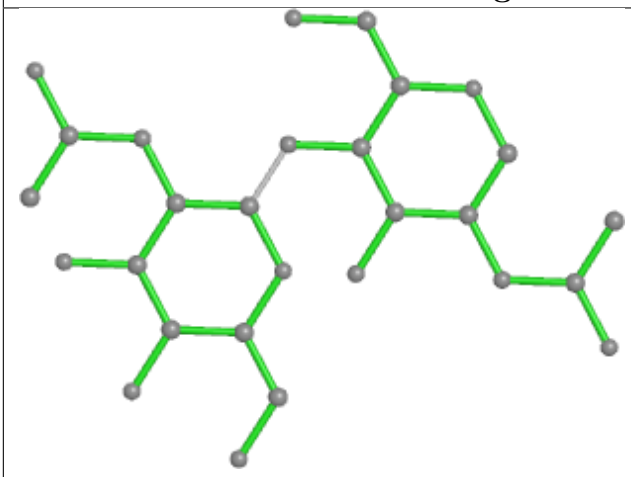


**Torsions**

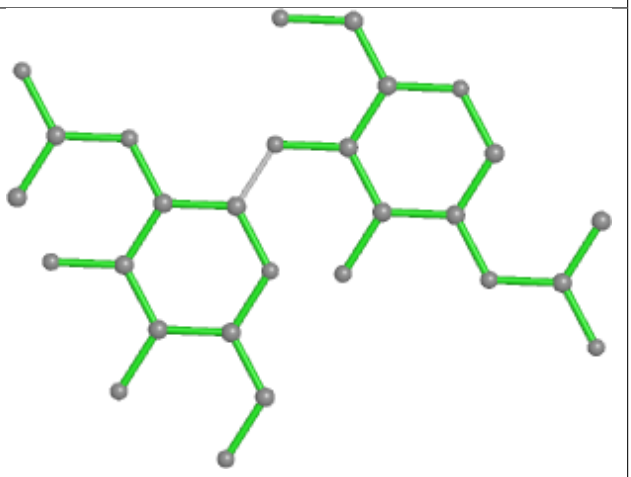


**Rings**

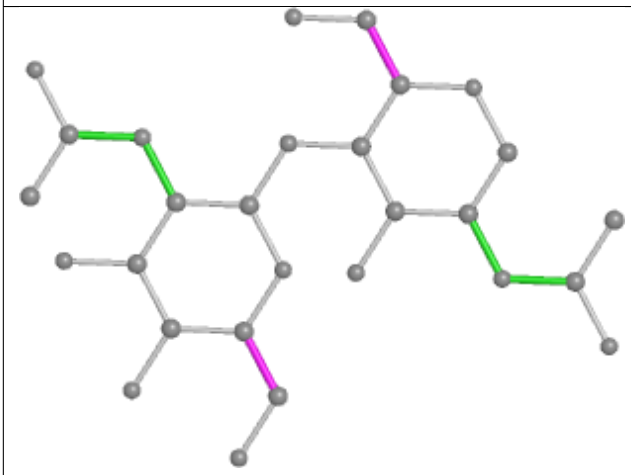
**Oligosaccharide Chain N**



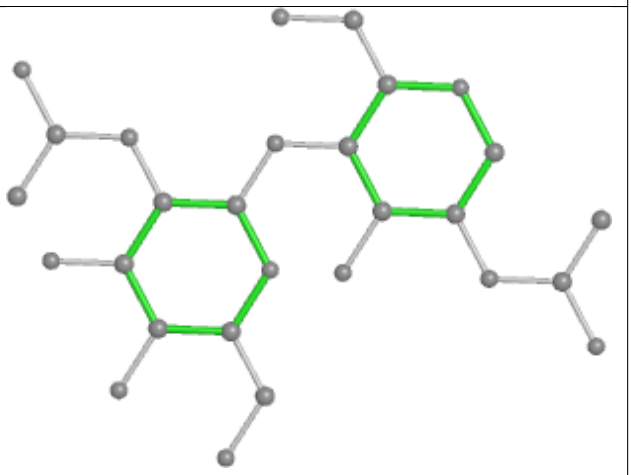
**Bond lengths**



**Bond angles**

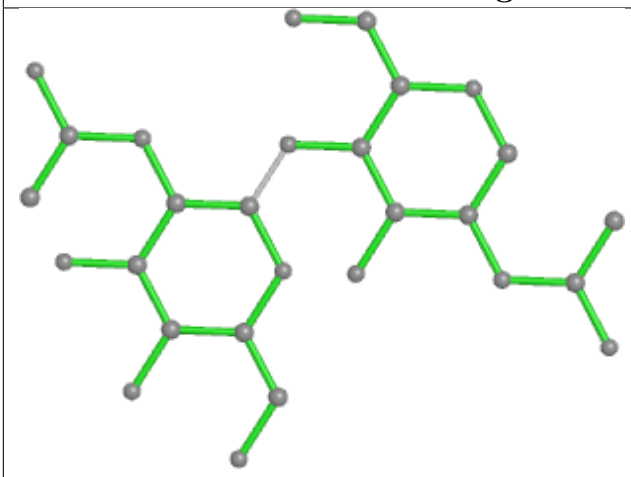


**Torsions**

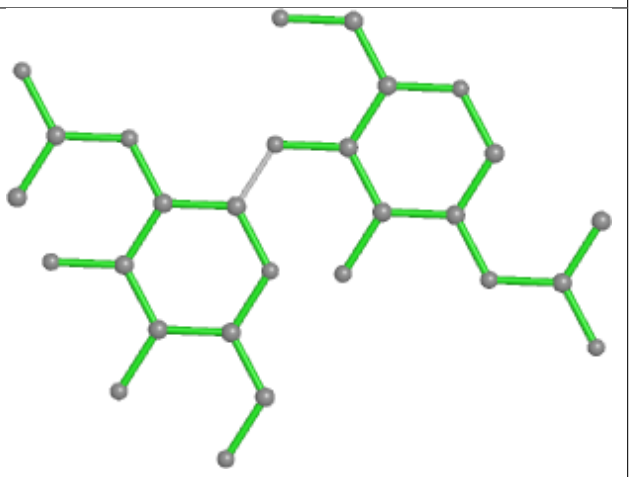


**Rings**

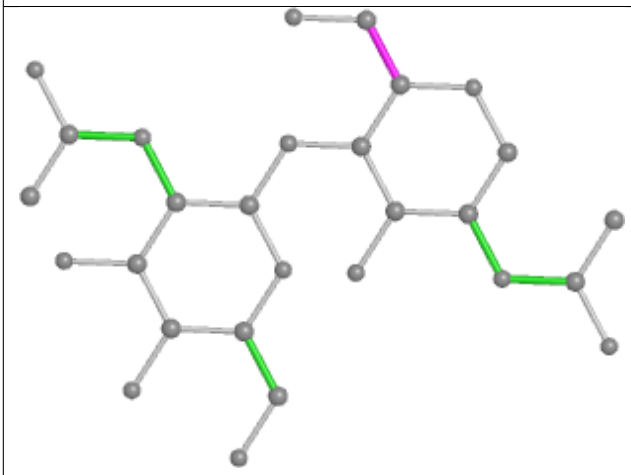
**Oligosaccharide Chain P**



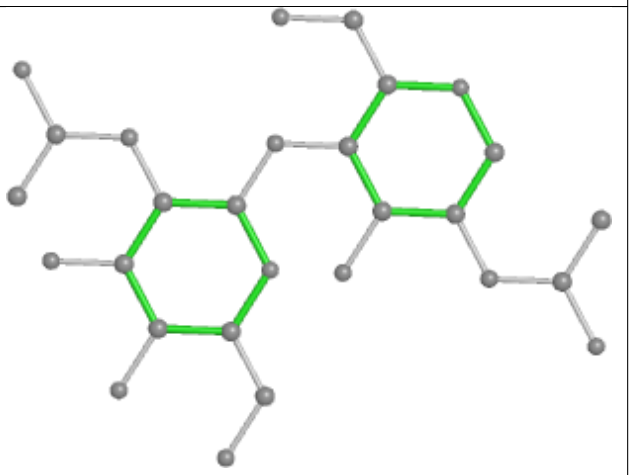
**Bond lengths**



**Bond angles**

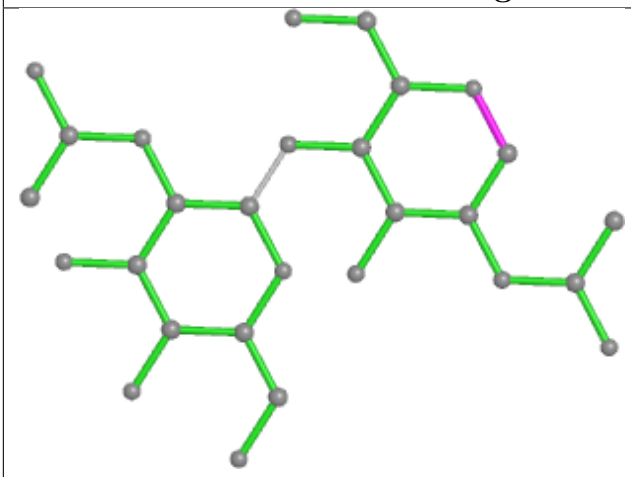


**Torsions**

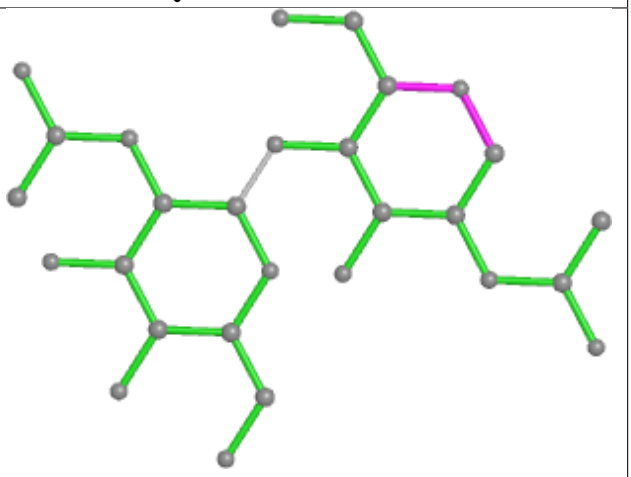


**Rings**

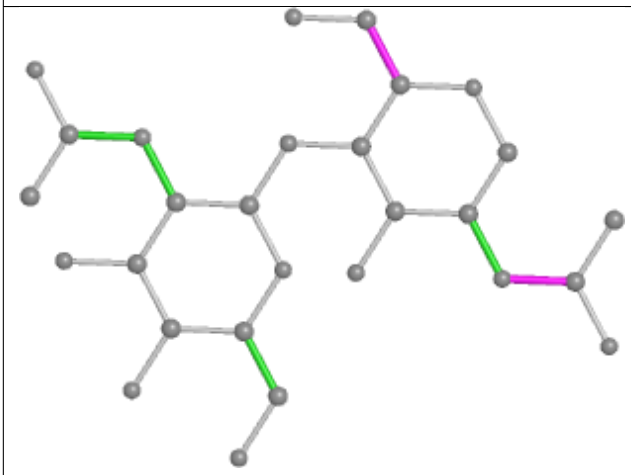
**Oligosaccharide Chain Q**



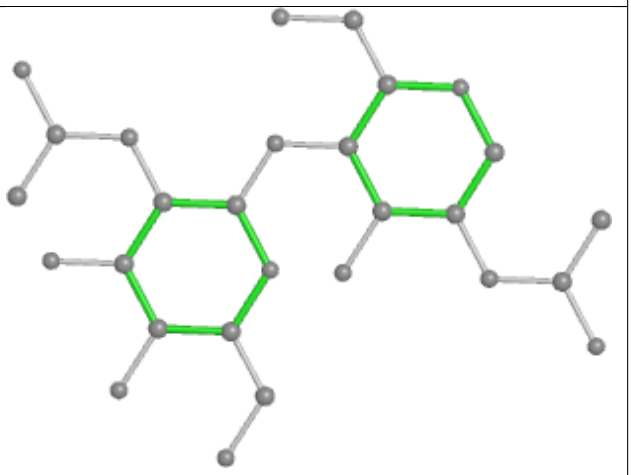
**Bond lengths**



**Bond angles**

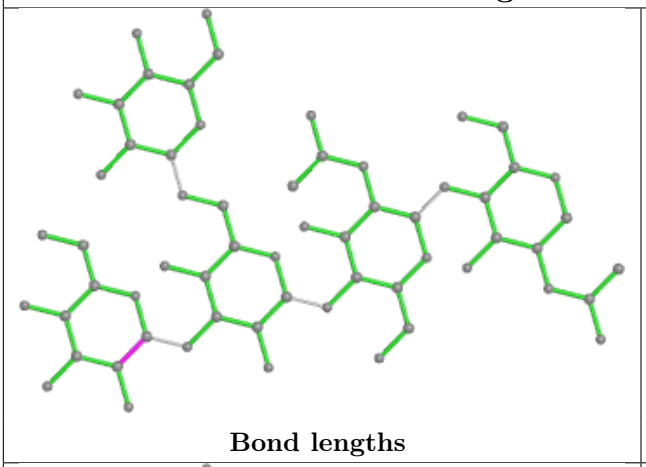


**Torsions**

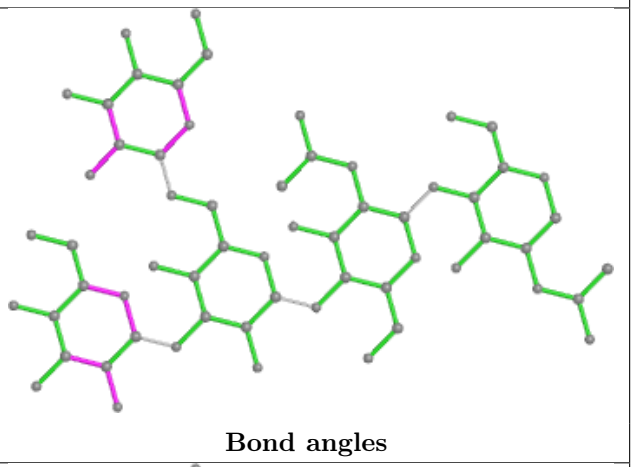


**Rings**

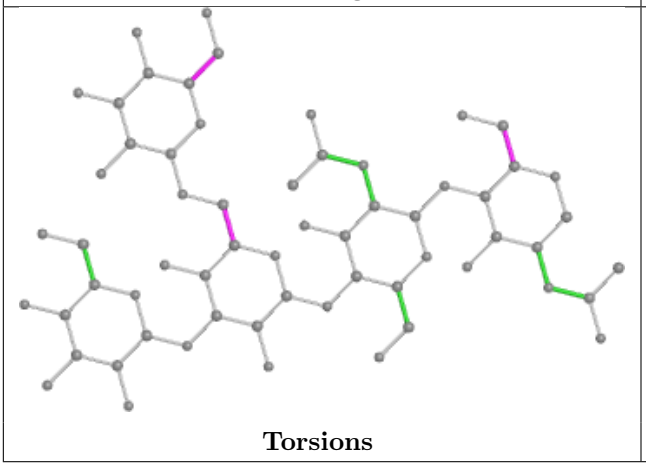
## Oligosaccharide Chain F



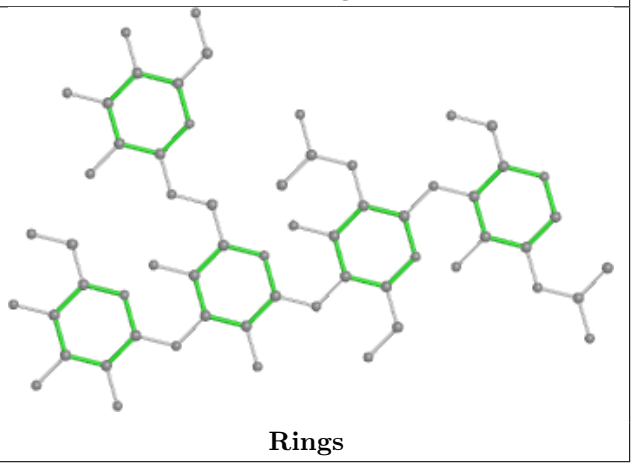
Bond lengths



Bond angles

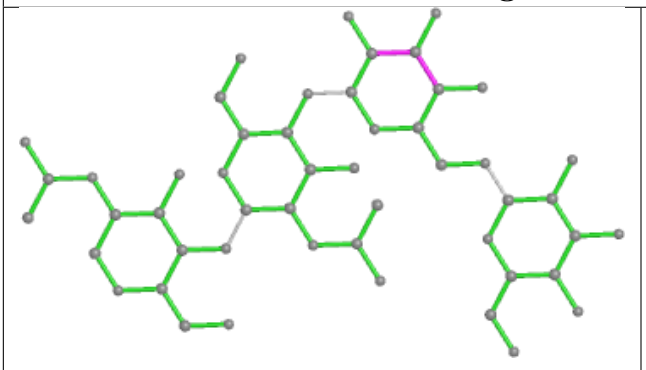


Torsions

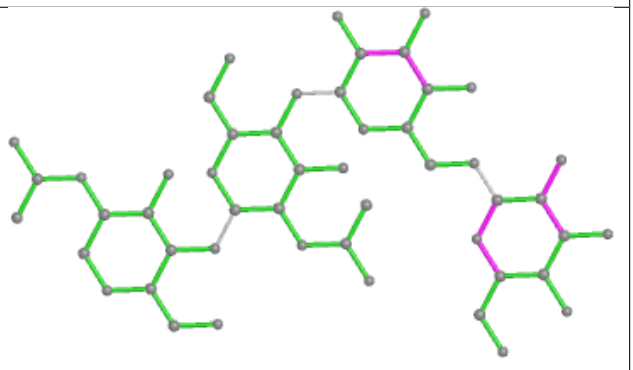


Rings

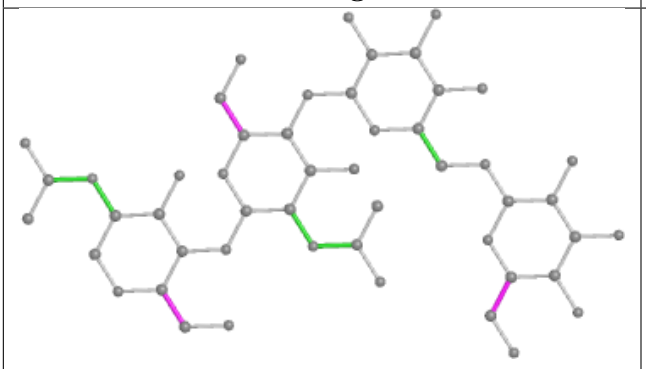
## Oligosaccharide Chain J



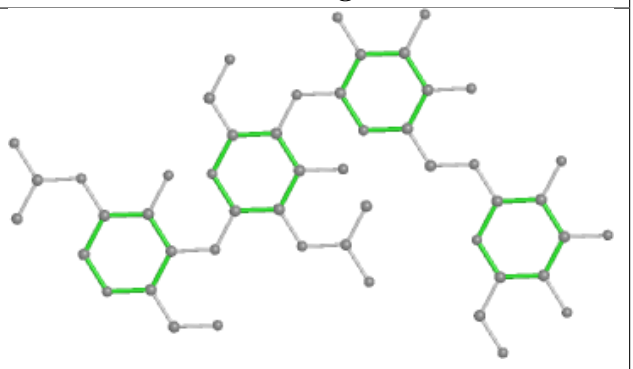
Bond lengths



Bond angles

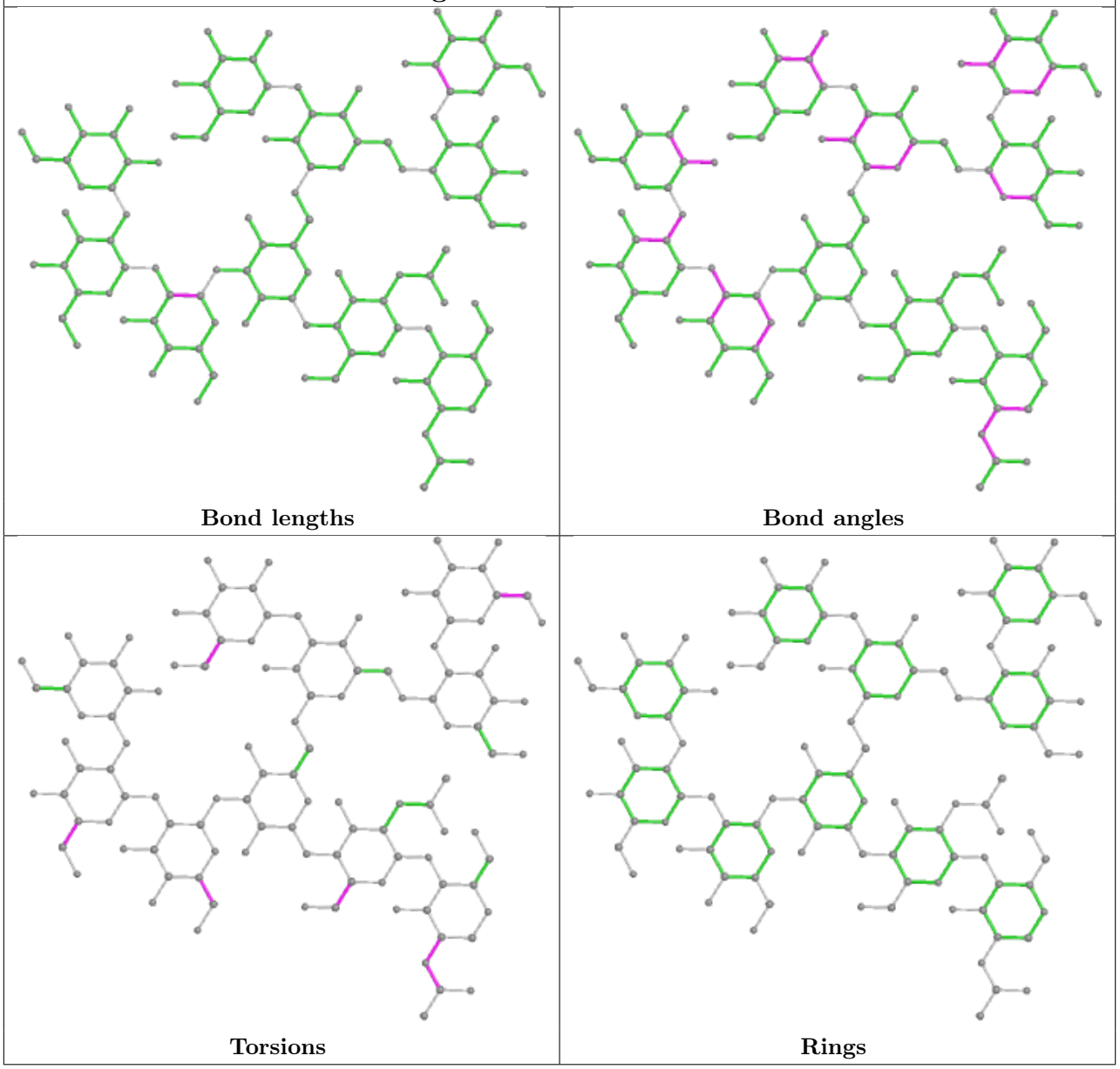


Torsions



Rings

**Oligosaccharide Chain O**




## 4.6 Ligand geometry (i)

5 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 | $\#\|Z\|>2$ |
| 14 | NAG | B | 702 | 1 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.45 | 0 |
| 14 | NAG | G | 617 | 4 | 14,14,15 | 0.31 | 0 | 17,19,21 | 0.45 | 0 |
| 14 | NAG | B | 701 | 1 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.54 | 0 |
| 14 | NAG | G | 614 | 4 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.44 | 0 |
| 14 | NAG | G | 638 | 4 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.44 | 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 |
|---|---|---|---|---|---|---|---|
| 14 | NAG | B | 702 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 14 | NAG | G | 617 | 4 | - | 2/6/23/26 | 0/1/1/1 |
| 14 | NAG | B | 701 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 14 | NAG | G | 614 | 4 | - | 1/6/23/26 | 0/1/1/1 |
| 14 | NAG | G | 638 | 4 | - | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|---|---|---|---|---|
| 14 | G | 617 | NAG | O5-C5-C6-O6 |
| 14 | G | 617 | NAG | C4-C5-C6-O6 |
| 14 | B | 702 | NAG | O5-C5-C6-O6 |
| 14 | G | 614 | NAG | O5-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

# 5 Fit of model and data

## 5.1 Protein, DNA and RNA chains

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

## 5.2 Non-standard residues in protein, DNA, RNA chains

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

## 5.3 Carbohydrates

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

## 5.4 Ligands

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

## 5.5 Other polymers

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