



wwPDB EM Validation Summary Report ⓘ

Nov 18, 2024 – 01:07 PM JST

PDB ID : 8XZ8
EMDB ID : EMD-38789
Title : BA.2.86 Spike in complex with bovine ACE2 (bound 1 ACE2)
Authors : Yue, C.; Liu, P.
Deposited on : 2024-01-21
Resolution : 3.65 Å (reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : **FAILED**
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-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

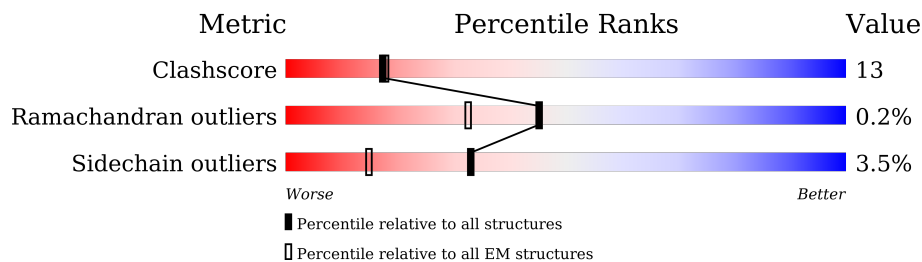
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 Å.

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



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

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1 | A | 804 | 48% 25% • 26% |
| 2 | B | 1206 | 58% 29% • 12% |
| 2 | C | 1206 | 59% 28% • 12% |
| 2 | D | 1206 | 59% 28% • 12% |
| 3 | E | 2 | 100% |
| 3 | F | 2 | 100% |
| 3 | G | 2 | 100% |
| 3 | H | 2 | 100% |
| 3 | I | 2 | 100% |

Continued on next page...

Continued from previous page...

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|---|
| 3 | J | 2 |  100% |
| 3 | K | 2 |  100% |
| 3 | L | 2 |  100% |
| 3 | M | 2 |  100% |
| 3 | N | 2 |  100% |
| 3 | O | 2 |  100% |
| 3 | P | 2 |  100% |
| 3 | Q | 2 |  100% |
| 3 | R | 2 |  100% |
| 3 | S | 2 |  100% |
| 3 | T | 2 |  100% |
| 3 | U | 2 |  100% |

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 30785 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 Angiotensin-converting enzyme.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 1 | A | 596 | 4906 | 3136 | 815 | 925 | 30 | 0 | 0 |

- Molecule 2 is a protein called Spike glycoprotein.

| Mol | Chain | Residues | Atoms | | | | | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| | | | Total | C | N | O | S | | |
| 2 | B | 1063 | 8316 | 5322 | 1383 | 1573 | 38 | 0 | 0 |
| 2 | C | 1063 | 8316 | 5322 | 1383 | 1573 | 38 | 0 | 0 |
| 2 | D | 1063 | 8316 | 5322 | 1383 | 1573 | 38 | 0 | 0 |

There are 219 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | -2 | ALA | - | expression tag | UNP P0DTC2 |
| B | -1 | THR | - | expression tag | UNP P0DTC2 |
| B | 16 | MET | - | insertion | UNP P0DTC2 |
| B | 17 | PRO | - | insertion | UNP P0DTC2 |
| B | 18 | LEU | - | insertion | UNP P0DTC2 |
| B | 19 | PHE | - | insertion | UNP P0DTC2 |
| B | 22 | ILE | THR | conflict | UNP P0DTC2 |
| B | 24 | THR | ARG | conflict | UNP P0DTC2 |
| B | ? | - | LEU | deletion | UNP P0DTC2 |
| B | ? | - | PRO | deletion | UNP P0DTC2 |
| B | ? | - | PRO | deletion | UNP P0DTC2 |
| B | 27 | SER | ALA | variant | UNP P0DTC2 |
| B | 50 | LEU | SER | conflict | UNP P0DTC2 |
| B | ? | - | HIS | deletion | UNP P0DTC2 |
| B | ? | - | VAL | deletion | UNP P0DTC2 |
| B | 127 | PHE | VAL | conflict | UNP P0DTC2 |
| B | 143 | ASP | GLY | variant | UNP P0DTC2 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| B | ? | - | TYR | deletion | UNP P0DTC2 |
| B | 157 | SER | PHE | conflict | UNP P0DTC2 |
| B | 158 | GLY | ARG | conflict | UNP P0DTC2 |
| B | ? | - | ASN | deletion | UNP P0DTC2 |
| B | 212 | ILE | LEU | variant | UNP P0DTC2 |
| B | 213 | GLY | VAL | variant | UNP P0DTC2 |
| B | 216 | PHE | LEU | variant | UNP P0DTC2 |
| B | 245 | ASN | HIS | conflict | UNP P0DTC2 |
| B | 264 | ASP | ALA | conflict | UNP P0DTC2 |
| B | 332 | VAL | ILE | conflict | UNP P0DTC2 |
| B | 339 | HIS | GLY | conflict | UNP P0DTC2 |
| B | 356 | THR | LYS | conflict | UNP P0DTC2 |
| B | 371 | PHE | SER | variant | UNP P0DTC2 |
| B | 373 | PRO | SER | variant | UNP P0DTC2 |
| B | 375 | PHE | SER | variant | UNP P0DTC2 |
| B | 376 | ALA | THR | variant | UNP P0DTC2 |
| B | 403 | LYS | ARG | conflict | UNP P0DTC2 |
| B | 405 | ASN | ASP | variant | UNP P0DTC2 |
| B | 408 | SER | ARG | variant | UNP P0DTC2 |
| B | 417 | ASN | LYS | variant | UNP P0DTC2 |
| B | 440 | LYS | ASN | variant | UNP P0DTC2 |
| B | 445 | HIS | VAL | conflict | UNP P0DTC2 |
| B | 446 | SER | GLY | variant | UNP P0DTC2 |
| B | 450 | ASP | ASN | conflict | UNP P0DTC2 |
| B | 452 | TRP | LEU | conflict | UNP P0DTC2 |
| B | 460 | LYS | ASN | variant | UNP P0DTC2 |
| B | 477 | ASN | SER | variant | UNP P0DTC2 |
| B | 478 | LYS | THR | variant | UNP P0DTC2 |
| B | 481 | LYS | ASN | conflict | UNP P0DTC2 |
| B | ? | - | VAL | deletion | UNP P0DTC2 |
| B | 484 | LYS | GLU | variant | UNP P0DTC2 |
| B | 486 | PRO | PHE | variant | UNP P0DTC2 |
| B | 498 | ARG | GLN | variant | UNP P0DTC2 |
| B | 501 | TYR | ASN | variant | UNP P0DTC2 |
| B | 505 | HIS | TYR | variant | UNP P0DTC2 |
| B | 554 | LYS | GLU | conflict | UNP P0DTC2 |
| B | 570 | VAL | ALA | conflict | UNP P0DTC2 |
| B | 614 | GLY | ASP | variant | UNP P0DTC2 |
| B | 621 | SER | PRO | conflict | UNP P0DTC2 |
| B | 655 | TYR | HIS | variant | UNP P0DTC2 |
| B | 679 | LYS | ASN | variant | UNP P0DTC2 |
| B | 681 | ARG | PRO | variant | UNP P0DTC2 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| B | 683 | ALA | ARG | conflict | UNP P0DTC2 |
| B | 685 | ALA | ARG | conflict | UNP P0DTC2 |
| B | 764 | LYS | ASN | variant | UNP P0DTC2 |
| B | 796 | TYR | ASP | variant | UNP P0DTC2 |
| B | 817 | PRO | PHE | conflict | UNP P0DTC2 |
| B | 892 | PRO | ALA | conflict | UNP P0DTC2 |
| B | 899 | PRO | ALA | conflict | UNP P0DTC2 |
| B | 939 | PHE | SER | conflict | UNP P0DTC2 |
| B | 942 | PRO | ALA | conflict | UNP P0DTC2 |
| B | 954 | HIS | GLN | variant | UNP P0DTC2 |
| B | 969 | LYS | ASN | variant | UNP P0DTC2 |
| B | 986 | PRO | LYS | variant | UNP P0DTC2 |
| B | 987 | PRO | VAL | variant | UNP P0DTC2 |
| B | 1143 | LEU | PRO | conflict | UNP P0DTC2 |
| C | -2 | ALA | - | expression tag | UNP P0DTC2 |
| C | -1 | THR | - | expression tag | UNP P0DTC2 |
| C | 16 | MET | - | insertion | UNP P0DTC2 |
| C | 17 | PRO | - | insertion | UNP P0DTC2 |
| C | 18 | LEU | - | insertion | UNP P0DTC2 |
| C | 19 | PHE | - | insertion | UNP P0DTC2 |
| C | 22 | ILE | THR | conflict | UNP P0DTC2 |
| C | 24 | THR | ARG | conflict | UNP P0DTC2 |
| C | ? | - | LEU | deletion | UNP P0DTC2 |
| C | ? | - | PRO | deletion | UNP P0DTC2 |
| C | ? | - | PRO | deletion | UNP P0DTC2 |
| C | 27 | SER | ALA | variant | UNP P0DTC2 |
| C | 50 | LEU | SER | conflict | UNP P0DTC2 |
| C | ? | - | HIS | deletion | UNP P0DTC2 |
| C | ? | - | VAL | deletion | UNP P0DTC2 |
| C | 127 | PHE | VAL | conflict | UNP P0DTC2 |
| C | 143 | ASP | GLY | variant | UNP P0DTC2 |
| C | ? | - | TYR | deletion | UNP P0DTC2 |
| C | 157 | SER | PHE | conflict | UNP P0DTC2 |
| C | 158 | GLY | ARG | conflict | UNP P0DTC2 |
| C | ? | - | ASN | deletion | UNP P0DTC2 |
| C | 212 | ILE | LEU | variant | UNP P0DTC2 |
| C | 213 | GLY | VAL | variant | UNP P0DTC2 |
| C | 216 | PHE | LEU | variant | UNP P0DTC2 |
| C | 245 | ASN | HIS | conflict | UNP P0DTC2 |
| C | 264 | ASP | ALA | conflict | UNP P0DTC2 |
| C | 332 | VAL | ILE | conflict | UNP P0DTC2 |
| C | 339 | HIS | GLY | conflict | UNP P0DTC2 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| C | 356 | THR | LYS | conflict | UNP P0DTC2 |
| C | 371 | PHE | SER | variant | UNP P0DTC2 |
| C | 373 | PRO | SER | variant | UNP P0DTC2 |
| C | 375 | PHE | SER | variant | UNP P0DTC2 |
| C | 376 | ALA | THR | variant | UNP P0DTC2 |
| C | 403 | LYS | ARG | conflict | UNP P0DTC2 |
| C | 405 | ASN | ASP | variant | UNP P0DTC2 |
| C | 408 | SER | ARG | variant | UNP P0DTC2 |
| C | 417 | ASN | LYS | variant | UNP P0DTC2 |
| C | 440 | LYS | ASN | variant | UNP P0DTC2 |
| C | 445 | HIS | VAL | conflict | UNP P0DTC2 |
| C | 446 | SER | GLY | variant | UNP P0DTC2 |
| C | 450 | ASP | ASN | conflict | UNP P0DTC2 |
| C | 452 | TRP | LEU | conflict | UNP P0DTC2 |
| C | 460 | LYS | ASN | variant | UNP P0DTC2 |
| C | 477 | ASN | SER | variant | UNP P0DTC2 |
| C | 478 | LYS | THR | variant | UNP P0DTC2 |
| C | 481 | LYS | ASN | conflict | UNP P0DTC2 |
| C | ? | - | VAL | deletion | UNP P0DTC2 |
| C | 484 | LYS | GLU | variant | UNP P0DTC2 |
| C | 486 | PRO | PHE | variant | UNP P0DTC2 |
| C | 498 | ARG | GLN | variant | UNP P0DTC2 |
| C | 501 | TYR | ASN | variant | UNP P0DTC2 |
| C | 505 | HIS | TYR | variant | UNP P0DTC2 |
| C | 554 | LYS | GLU | conflict | UNP P0DTC2 |
| C | 570 | VAL | ALA | conflict | UNP P0DTC2 |
| C | 614 | GLY | ASP | variant | UNP P0DTC2 |
| C | 621 | SER | PRO | conflict | UNP P0DTC2 |
| C | 655 | TYR | HIS | variant | UNP P0DTC2 |
| C | 679 | LYS | ASN | variant | UNP P0DTC2 |
| C | 681 | ARG | PRO | variant | UNP P0DTC2 |
| C | 683 | ALA | ARG | conflict | UNP P0DTC2 |
| C | 685 | ALA | ARG | conflict | UNP P0DTC2 |
| C | 764 | LYS | ASN | variant | UNP P0DTC2 |
| C | 796 | TYR | ASP | variant | UNP P0DTC2 |
| C | 817 | PRO | PHE | conflict | UNP P0DTC2 |
| C | 892 | PRO | ALA | conflict | UNP P0DTC2 |
| C | 899 | PRO | ALA | conflict | UNP P0DTC2 |
| C | 939 | PHE | SER | conflict | UNP P0DTC2 |
| C | 942 | PRO | ALA | conflict | UNP P0DTC2 |
| C | 954 | HIS | GLN | variant | UNP P0DTC2 |
| C | 969 | LYS | ASN | variant | UNP P0DTC2 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------------|------------|
| C | 986 | PRO | LYS | variant | UNP P0DTC2 |
| C | 987 | PRO | VAL | variant | UNP P0DTC2 |
| C | 1143 | LEU | PRO | conflict | UNP P0DTC2 |
| D | -2 | ALA | - | expression tag | UNP P0DTC2 |
| D | -1 | THR | - | expression tag | UNP P0DTC2 |
| D | 16 | MET | - | insertion | UNP P0DTC2 |
| D | 17 | PRO | - | insertion | UNP P0DTC2 |
| D | 18 | LEU | - | insertion | UNP P0DTC2 |
| D | 19 | PHE | - | insertion | UNP P0DTC2 |
| D | 22 | ILE | THR | conflict | UNP P0DTC2 |
| D | 24 | THR | ARG | conflict | UNP P0DTC2 |
| D | ? | - | LEU | deletion | UNP P0DTC2 |
| D | ? | - | PRO | deletion | UNP P0DTC2 |
| D | ? | - | PRO | deletion | UNP P0DTC2 |
| D | 27 | SER | ALA | variant | UNP P0DTC2 |
| D | 50 | LEU | SER | conflict | UNP P0DTC2 |
| D | ? | - | HIS | deletion | UNP P0DTC2 |
| D | ? | - | VAL | deletion | UNP P0DTC2 |
| D | 127 | PHE | VAL | conflict | UNP P0DTC2 |
| D | 143 | ASP | GLY | variant | UNP P0DTC2 |
| D | ? | - | TYR | deletion | UNP P0DTC2 |
| D | 157 | SER | PHE | conflict | UNP P0DTC2 |
| D | 158 | GLY | ARG | conflict | UNP P0DTC2 |
| D | ? | - | ASN | deletion | UNP P0DTC2 |
| D | 212 | ILE | LEU | variant | UNP P0DTC2 |
| D | 213 | GLY | VAL | variant | UNP P0DTC2 |
| D | 216 | PHE | LEU | variant | UNP P0DTC2 |
| D | 245 | ASN | HIS | conflict | UNP P0DTC2 |
| D | 264 | ASP | ALA | conflict | UNP P0DTC2 |
| D | 332 | VAL | ILE | conflict | UNP P0DTC2 |
| D | 339 | HIS | GLY | conflict | UNP P0DTC2 |
| D | 356 | THR | LYS | conflict | UNP P0DTC2 |
| D | 371 | PHE | SER | variant | UNP P0DTC2 |
| D | 373 | PRO | SER | variant | UNP P0DTC2 |
| D | 375 | PHE | SER | variant | UNP P0DTC2 |
| D | 376 | ALA | THR | variant | UNP P0DTC2 |
| D | 403 | LYS | ARG | conflict | UNP P0DTC2 |
| D | 405 | ASN | ASP | variant | UNP P0DTC2 |
| D | 408 | SER | ARG | variant | UNP P0DTC2 |
| D | 417 | ASN | LYS | variant | UNP P0DTC2 |
| D | 440 | LYS | ASN | variant | UNP P0DTC2 |
| D | 445 | HIS | VAL | conflict | UNP P0DTC2 |

Continued on next page...

Continued from previous page...

| Chain | Residue | Modelled | Actual | Comment | Reference |
|-------|---------|----------|--------|----------|------------|
| D | 446 | SER | GLY | variant | UNP P0DTC2 |
| D | 450 | ASP | ASN | conflict | UNP P0DTC2 |
| D | 452 | TRP | LEU | conflict | UNP P0DTC2 |
| D | 460 | LYS | ASN | variant | UNP P0DTC2 |
| D | 477 | ASN | SER | variant | UNP P0DTC2 |
| D | 478 | LYS | THR | variant | UNP P0DTC2 |
| D | 481 | LYS | ASN | conflict | UNP P0DTC2 |
| D | ? | - | VAL | deletion | UNP P0DTC2 |
| D | 484 | LYS | GLU | variant | UNP P0DTC2 |
| D | 486 | PRO | PHE | variant | UNP P0DTC2 |
| D | 498 | ARG | GLN | variant | UNP P0DTC2 |
| D | 501 | TYR | ASN | variant | UNP P0DTC2 |
| D | 505 | HIS | TYR | variant | UNP P0DTC2 |
| D | 554 | LYS | GLU | conflict | UNP P0DTC2 |
| D | 570 | VAL | ALA | conflict | UNP P0DTC2 |
| D | 614 | GLY | ASP | variant | UNP P0DTC2 |
| D | 621 | SER | PRO | conflict | UNP P0DTC2 |
| D | 655 | TYR | HIS | variant | UNP P0DTC2 |
| D | 679 | LYS | ASN | variant | UNP P0DTC2 |
| D | 681 | ARG | PRO | variant | UNP P0DTC2 |
| D | 683 | ALA | ARG | conflict | UNP P0DTC2 |
| D | 685 | ALA | ARG | conflict | UNP P0DTC2 |
| D | 764 | LYS | ASN | variant | UNP P0DTC2 |
| D | 796 | TYR | ASP | variant | UNP P0DTC2 |
| D | 817 | PRO | PHE | conflict | UNP P0DTC2 |
| D | 892 | PRO | ALA | conflict | UNP P0DTC2 |
| D | 899 | PRO | ALA | conflict | UNP P0DTC2 |
| D | 939 | PHE | SER | conflict | UNP P0DTC2 |
| D | 942 | PRO | ALA | conflict | UNP P0DTC2 |
| D | 954 | HIS | GLN | variant | UNP P0DTC2 |
| D | 969 | LYS | ASN | variant | UNP P0DTC2 |
| D | 986 | PRO | LYS | variant | UNP P0DTC2 |
| D | 987 | PRO | VAL | variant | UNP P0DTC2 |
| D | 1143 | LEU | PRO | conflict | UNP P0DTC2 |

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



| Mol | Chain | Residues | Atoms | | | | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 3 | E | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | F | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | G | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | H | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | I | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | J | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | K | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | L | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | M | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | N | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | O | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | P | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | Q | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | R | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | S | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | T | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |
| 3 | U | 2 | Total | C | N | O | 0 | 0 |
| | | | 25 | 14 | 1 | 10 | | |

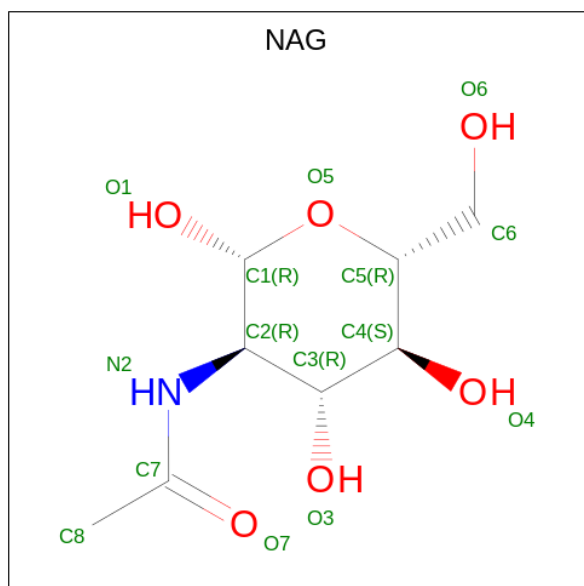
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

| Mol | Chain | Residues | Atoms | | AltConf |
|-----|-------|----------|-------|----|---------|
| 4 | A | 1 | Total | Zn | 0 |
| | | | 1 | 1 | |

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-----------------|---------|
| 5 | A | 1 | Total Cl 1 1 | 0 |

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



| Mol | Chain | Residues | Atoms | AltConf |
|-----|-------|----------|-------------------------|---------|
| 6 | A | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | A | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | A | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | A | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | A | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | B | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | B | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | B | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | B | 1 | Total C N O 14 8 1 5 | 0 |
| 6 | B | 1 | Total C N O 14 8 1 5 | 0 |

Continued on next page...

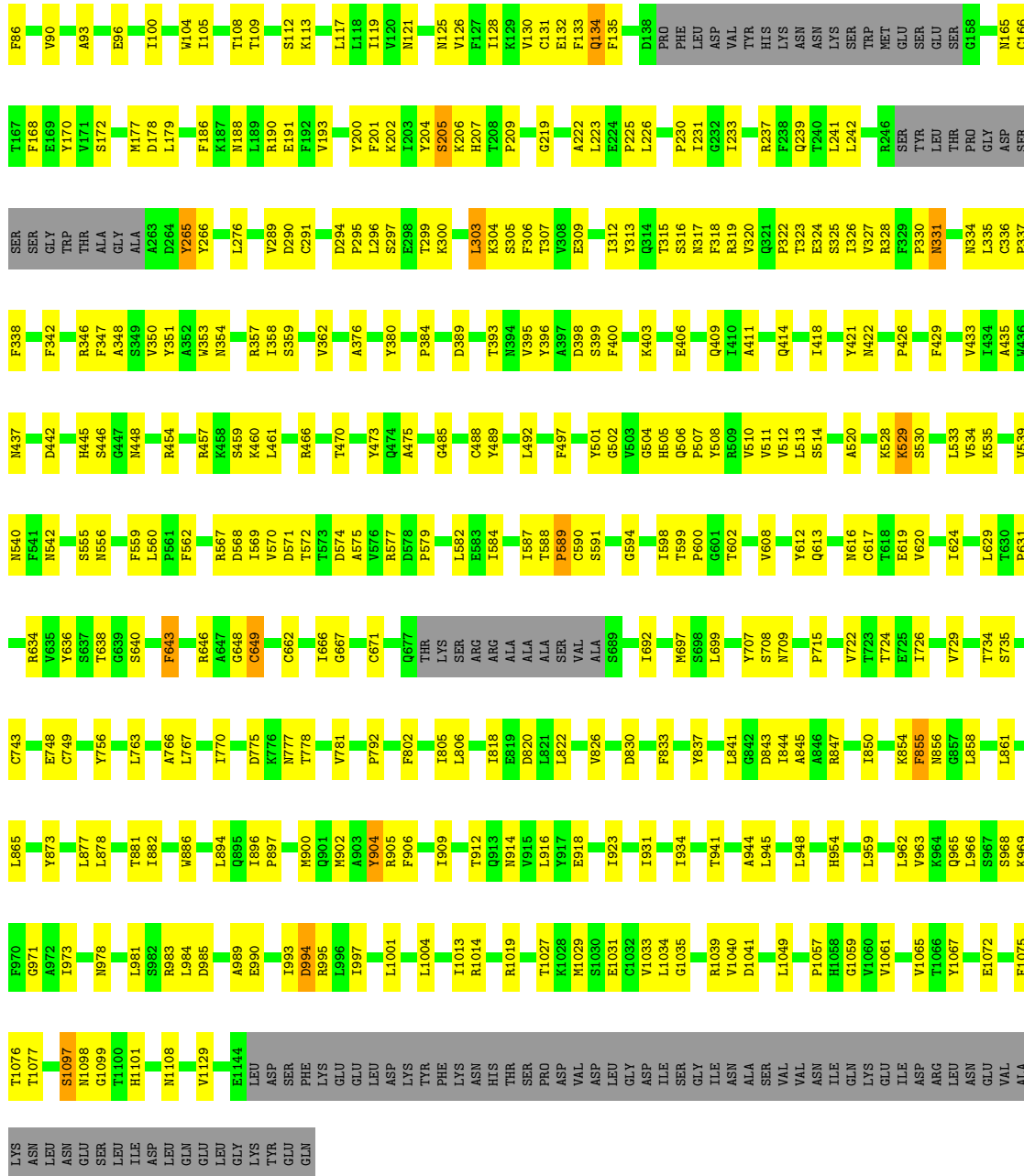
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---|---|---|---------|
| | | | Total | C | N | O | |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | B | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | C | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |

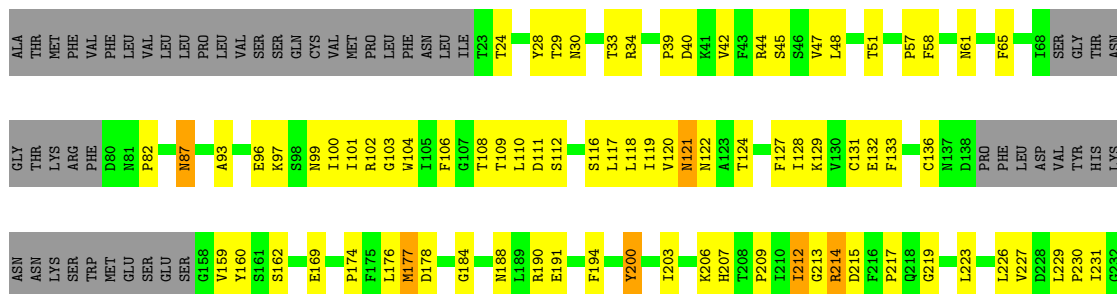
Continued on next page...

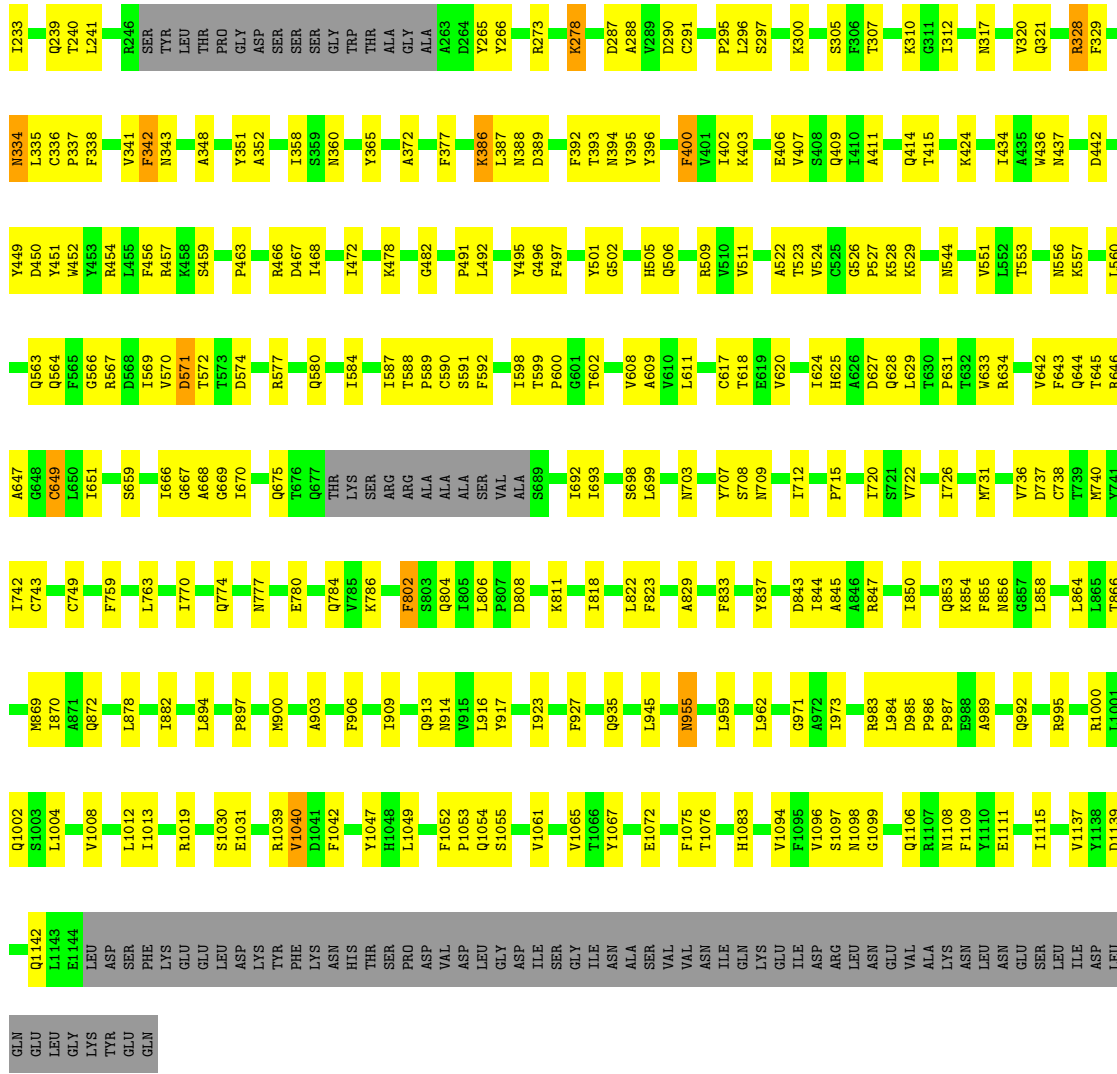
Continued from previous page...

| Mol | Chain | Residues | Atoms | | | | AltConf |
|-----|-------|----------|-------------|---|---|---|---------|
| | | | Total | C | N | O | |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |
| 6 | D | 1 | Total 14 | 8 | 1 | 5 | 0 |

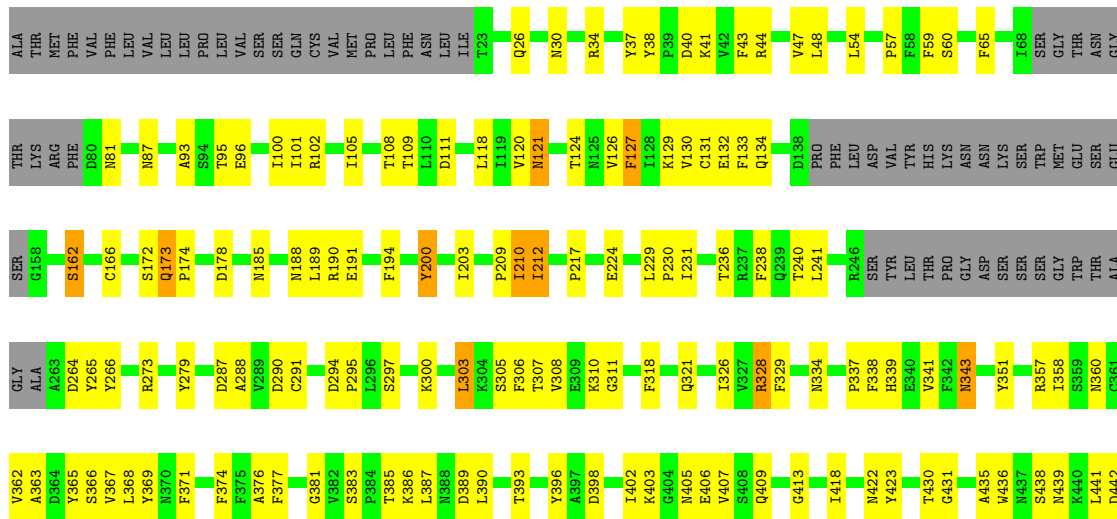
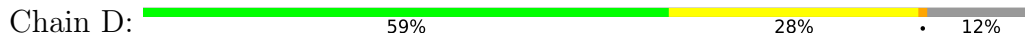


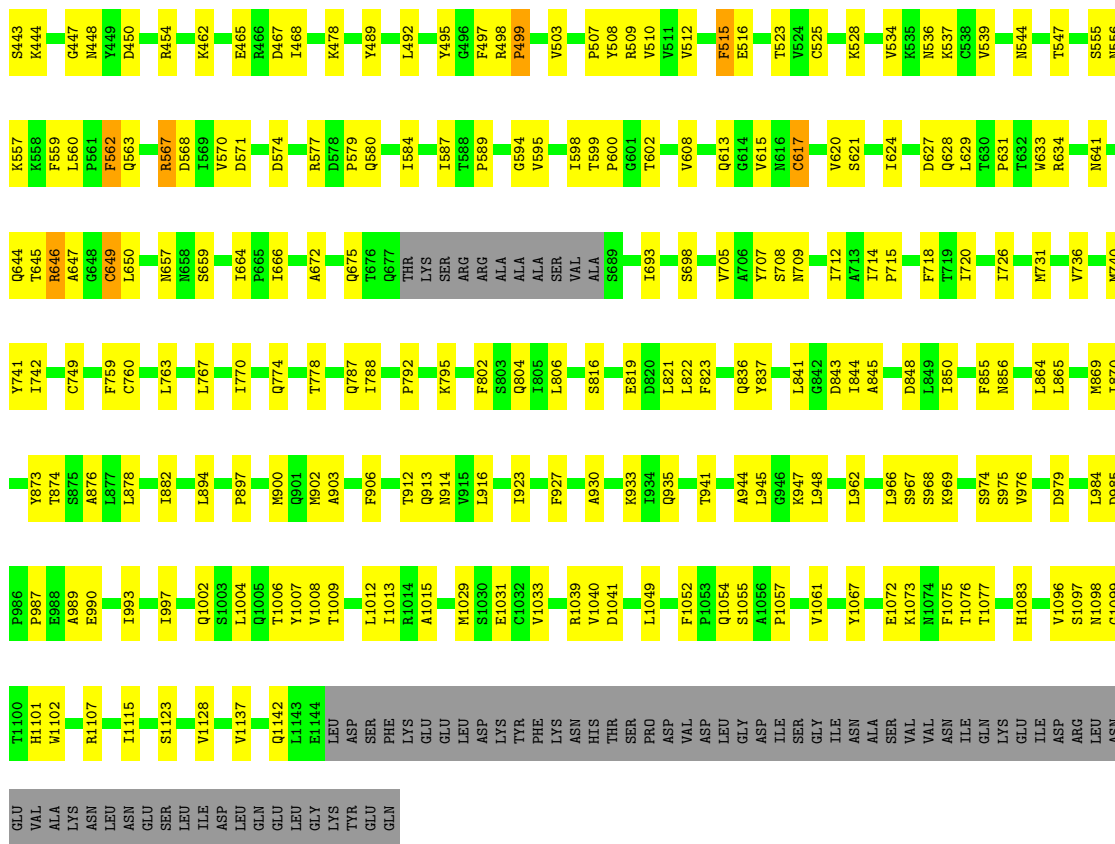
● Molecule 2: Spike glycoprotein





• Molecule 2: Spike glycoprotein





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

Chain E: 100%

MAG1
BMA2

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

Chain F: 100%

MAG1
BMA2

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

Chain G: 100%

MAG1
BMA2


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

Chain H: 100%



MAG1
BM42

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

Chain I:  100%



MAG1
BM42

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

Chain J:  100%



MAG1
BM42

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

Chain K:  100%



MAG1
BM42

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

Chain L:  100%



MAG1
BM42

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

Chain M:  100%



MAG1
BM42

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

Chain N:  100%



MAG1
BM42

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

Chain O:  100%



MAG1
BM42

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

Chain P:  100%

NA01
BM02

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

Chain Q:  100%

NA01
BM02

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

Chain R:  100%

NA01
BM02

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

Chain S:  100%

NA01
BM02

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

Chain T:  100%

NA01
BM02

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

Chain U:  100%

NA01
BM02

4 Experimental information

| Property | Value | Source |
|--------------------------------------|---------------------------|-----------|
| EM reconstruction method | SINGLE PARTICLE | Depositor |
| Imposed symmetry | POINT, Not provided | |
| Number of particles used | 89392 | Depositor |
| Resolution determination method | FSC 0.143 CUT-OFF | Depositor |
| CTF correction method | PHASE FLIPPING ONLY | Depositor |
| Microscope | FEI TALOS ARCTICA | Depositor |
| Voltage (kV) | 200 | Depositor |
| Electron dose ($e^-/\text{\AA}^2$) | 60 | Depositor |
| Minimum defocus (nm) | 1200 | Depositor |
| Maximum defocus (nm) | 2000 | Depositor |
| Magnification | Not provided | |
| Image detector | GATAN K2 SUMMIT (4k 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, ZN, BMA, CL

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 | 0/5043 | 0.52 | 0/6838 |
| 2 | B | 0.27 | 0/8516 | 0.50 | 0/11591 |
| 2 | C | 0.26 | 0/8516 | 0.50 | 0/11591 |
| 2 | D | 0.26 | 0/8516 | 0.50 | 0/11591 |
| All | All | 0.26 | 0/30591 | 0.50 | 0/41611 |

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1 | A | 4906 | 0 | 4691 | 134 | 0 |
| 2 | B | 8316 | 0 | 8103 | 240 | 0 |
| 2 | C | 8316 | 0 | 8104 | 246 | 0 |
| 2 | D | 8316 | 0 | 8104 | 261 | 0 |
| 3 | E | 25 | 0 | 22 | 0 | 0 |
| 3 | F | 25 | 0 | 22 | 0 | 0 |
| 3 | G | 25 | 0 | 22 | 0 | 0 |
| 3 | H | 25 | 0 | 22 | 0 | 0 |
| 3 | I | 25 | 0 | 22 | 0 | 0 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 3 | J | 25 | 0 | 22 | 0 | 0 |
| 3 | K | 25 | 0 | 22 | 0 | 0 |
| 3 | L | 25 | 0 | 22 | 0 | 0 |
| 3 | M | 25 | 0 | 22 | 0 | 0 |
| 3 | N | 25 | 0 | 22 | 0 | 0 |
| 3 | O | 25 | 0 | 22 | 0 | 0 |
| 3 | P | 25 | 0 | 22 | 0 | 0 |
| 3 | Q | 25 | 0 | 22 | 0 | 0 |
| 3 | R | 25 | 0 | 22 | 0 | 0 |
| 3 | S | 25 | 0 | 22 | 0 | 0 |
| 3 | T | 25 | 0 | 22 | 0 | 0 |
| 3 | U | 25 | 0 | 22 | 0 | 0 |
| 4 | A | 1 | 0 | 0 | 0 | 0 |
| 5 | A | 1 | 0 | 0 | 0 | 0 |
| 6 | A | 70 | 0 | 65 | 0 | 0 |
| 6 | B | 154 | 0 | 140 | 1 | 0 |
| 6 | C | 140 | 0 | 130 | 1 | 0 |
| 6 | D | 140 | 0 | 130 | 3 | 0 |
| All | All | 30785 | 0 | 29841 | 812 | 0 |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

The worst 5 of 812 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:B:334:ASN:OD1 | 2:B:362:VAL:HG13 | 1.58 | 1.00 |
| 2:D:617:CYS:HA | 2:D:620:VAL:HG12 | 1.56 | 0.88 |
| 2:C:212:ILE:HG22 | 2:C:213:GLY:H | 1.39 | 0.87 |
| 2:C:777:ASN:HD21 | 2:C:1019:ARG:HA | 1.45 | 0.82 |
| 2:C:352:ALA:HA | 2:C:466:ARG:HD2 | 1.59 | 0.82 |

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

| Mol | Chain | Analysed | Favoured | Allowed | Outliers | Percentiles | |
|-----|-------|-----------------|------------|----------|----------|-------------|----|
| 1 | A | 594/804 (74%) | 570 (96%) | 21 (4%) | 3 (0%) | 25 | 57 |
| 2 | B | 1053/1206 (87%) | 969 (92%) | 82 (8%) | 2 (0%) | 44 | 72 |
| 2 | C | 1053/1206 (87%) | 965 (92%) | 87 (8%) | 1 (0%) | 48 | 78 |
| 2 | D | 1053/1206 (87%) | 978 (93%) | 73 (7%) | 2 (0%) | 44 | 72 |
| All | All | 3753/4422 (85%) | 3482 (93%) | 263 (7%) | 8 (0%) | 45 | 72 |

5 of 8 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 212 | ILE |
| 2 | D | 210 | ILE |
| 2 | D | 499 | PRO |
| 1 | A | 147 | LEU |
| 2 | B | 331 | ASN |

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 | 525/711 (74%) | 505 (96%) | 20 (4%) | 28 | 53 |
| 2 | B | 925/1054 (88%) | 892 (96%) | 33 (4%) | 30 | 54 |
| 2 | C | 925/1054 (88%) | 893 (96%) | 32 (4%) | 31 | 55 |
| 2 | D | 925/1054 (88%) | 894 (97%) | 31 (3%) | 32 | 55 |
| All | All | 3300/3873 (85%) | 3184 (96%) | 116 (4%) | 33 | 55 |

5 of 116 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 177 | MET |
| 2 | D | 649 | CYS |
| 2 | C | 400 | PHE |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | D | 646 | ARG |
| 2 | D | 377 | PHE |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2 | C | 321 | GLN |
| 2 | C | 437 | ASN |
| 2 | D | 207 | HIS |
| 2 | D | 173 | GLN |
| 2 | B | 777 | ASN |

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

34 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 | $\# Z > 2$ |
| 3 | NAG | E | 1 | 3,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | BMA | E | 2 | 3 | 11,11,12 | 0.60 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | F | 1 | 3,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | BMA | F | 2 | 3 | 11,11,12 | 0.60 | 0 | 15,15,17 | 0.77 | 0 |
| 3 | NAG | G | 1 | 3,2 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.49 | 0 |
| 3 | BMA | G | 2 | 3 | 11,11,12 | 0.60 | 0 | 15,15,17 | 0.70 | 0 |

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 3 | NAG | H | 1 | 3,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 3 | BMA | H | 2 | 3 | 11,11,12 | 0.61 | 0 | 15,15,17 | 0.75 | 0 |
| 3 | NAG | I | 1 | 3,2 | 14,14,15 | 0.90 | 1 (7%) | 17,19,21 | 0.90 | 1 (5%) |
| 3 | BMA | I | 2 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 1.24 | 2 (13%) |
| 3 | NAG | J | 1 | 3,2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | BMA | J | 2 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.82 | 0 |
| 3 | NAG | K | 1 | 3,2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | BMA | K | 2 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.69 | 0 |
| 3 | NAG | L | 1 | 3,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.43 | 0 |
| 3 | BMA | L | 2 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.74 | 0 |
| 3 | NAG | M | 1 | 3,2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | BMA | M | 2 | 3 | 11,11,12 | 0.61 | 0 | 15,15,17 | 0.68 | 0 |
| 3 | NAG | N | 1 | 3,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.46 | 0 |
| 3 | BMA | N | 2 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.71 | 0 |
| 3 | NAG | O | 1 | 3,2 | 14,14,15 | 0.94 | 1 (7%) | 17,19,21 | 0.94 | 1 (5%) |
| 3 | BMA | O | 2 | 3 | 11,11,12 | 0.55 | 0 | 15,15,17 | 1.10 | 1 (6%) |
| 3 | NAG | P | 1 | 3,2 | 14,14,15 | 0.27 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | BMA | P | 2 | 3 | 11,11,12 | 0.58 | 0 | 15,15,17 | 0.76 | 0 |
| 3 | NAG | Q | 1 | 3,2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.39 | 0 |
| 3 | BMA | Q | 2 | 3 | 11,11,12 | 0.57 | 0 | 15,15,17 | 0.72 | 0 |
| 3 | NAG | R | 1 | 3,2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.41 | 0 |
| 3 | BMA | R | 2 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.79 | 0 |
| 3 | NAG | S | 1 | 3,2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.47 | 0 |
| 3 | BMA | S | 2 | 3 | 11,11,12 | 0.59 | 0 | 15,15,17 | 0.73 | 0 |
| 3 | NAG | T | 1 | 3,2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.45 | 0 |
| 3 | BMA | T | 2 | 3 | 11,11,12 | 0.62 | 0 | 15,15,17 | 0.74 | 0 |
| 3 | NAG | U | 1 | 3,2 | 14,14,15 | 1.25 | 1 (7%) | 17,19,21 | 1.23 | 1 (5%) |
| 3 | BMA | U | 2 | 3 | 11,11,12 | 0.61 | 0 | 15,15,17 | 1.26 | 3 (20%) |

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 |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3 | NAG | E | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | E | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | F | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | F | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | G | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | G | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |

Continued on next page...

Continued from previous page...

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3 | NAG | H | 1 | 3,2 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | BMA | H | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | I | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | I | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | J | 1 | 3,2 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | BMA | J | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | K | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | K | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | L | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | L | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | M | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | M | 2 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | NAG | N | 1 | 3,2 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | BMA | N | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | O | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | O | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | P | 1 | 3,2 | - | 1/6/23/26 | 0/1/1/1 |
| 3 | BMA | P | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | Q | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | Q | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | R | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | R | 2 | 3 | - | 1/2/19/22 | 0/1/1/1 |
| 3 | NAG | S | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | S | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | T | 1 | 3,2 | - | 0/6/23/26 | 0/1/1/1 |
| 3 | BMA | T | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |
| 3 | NAG | U | 1 | 3,2 | - | 2/6/23/26 | 0/1/1/1 |
| 3 | BMA | U | 2 | 3 | - | 0/2/19/22 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3 | U | 1 | NAG | O5-C1 | -4.32 | 1.36 | 1.43 |
| 3 | O | 1 | NAG | O5-C1 | -3.29 | 1.38 | 1.43 |
| 3 | I | 1 | NAG | O5-C1 | -3.13 | 1.38 | 1.43 |

The worst 5 of 9 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | U | 1 | NAG | C3-C4-C5 | 3.52 | 116.52 | 110.24 |

Continued on next page...

Continued from previous page...

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 3 | U | 2 | BMA | C1-O5-C5 | 2.75 | 115.91 | 112.19 |
| 3 | I | 2 | BMA | C1-O5-C5 | 2.73 | 115.89 | 112.19 |
| 3 | O | 2 | BMA | C1-O5-C5 | 2.52 | 115.61 | 112.19 |
| 3 | O | 1 | NAG | C3-C4-C5 | 2.47 | 114.64 | 110.24 |

There are no chirality outliers.

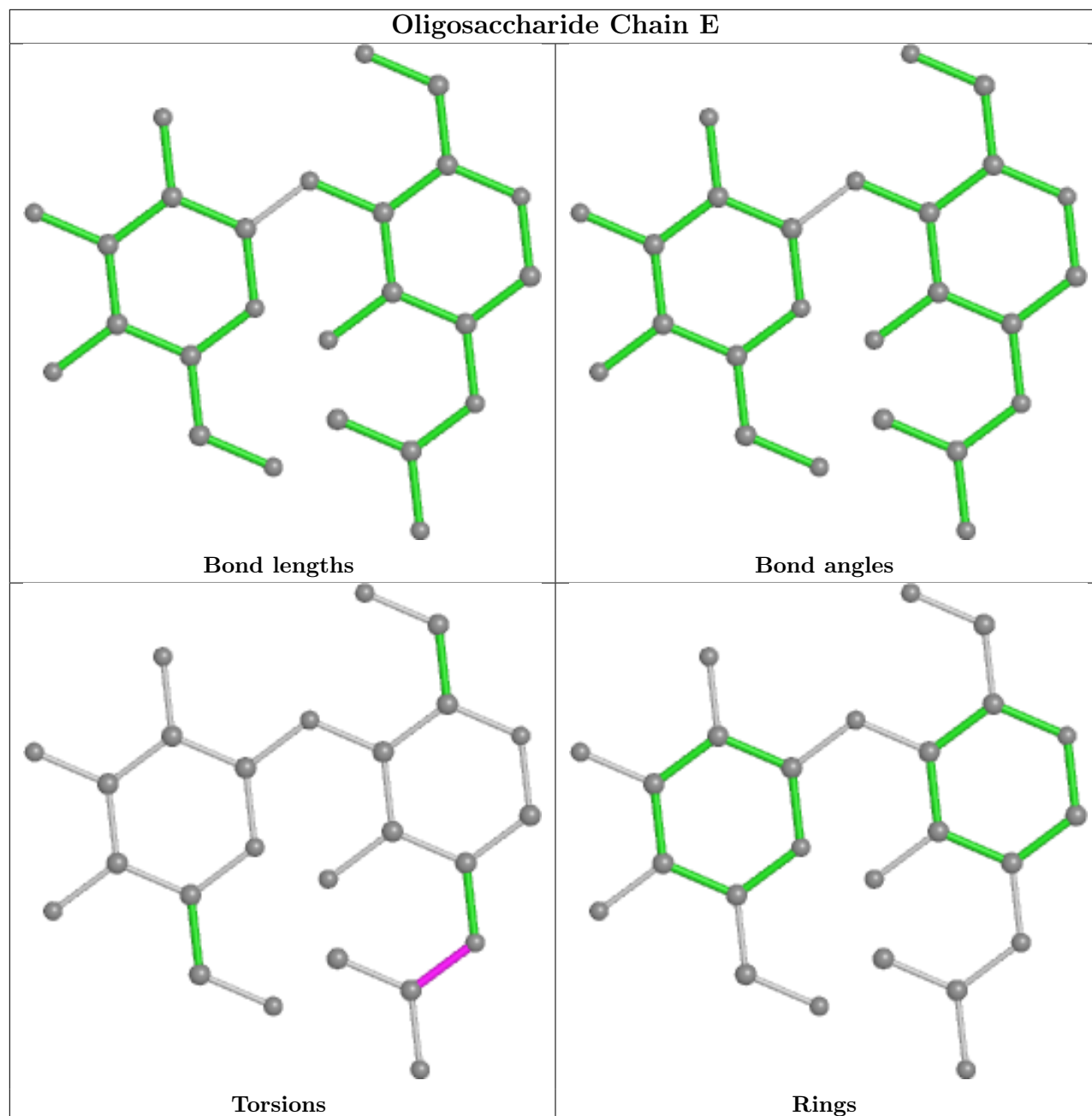
5 of 29 torsion outliers are listed below:

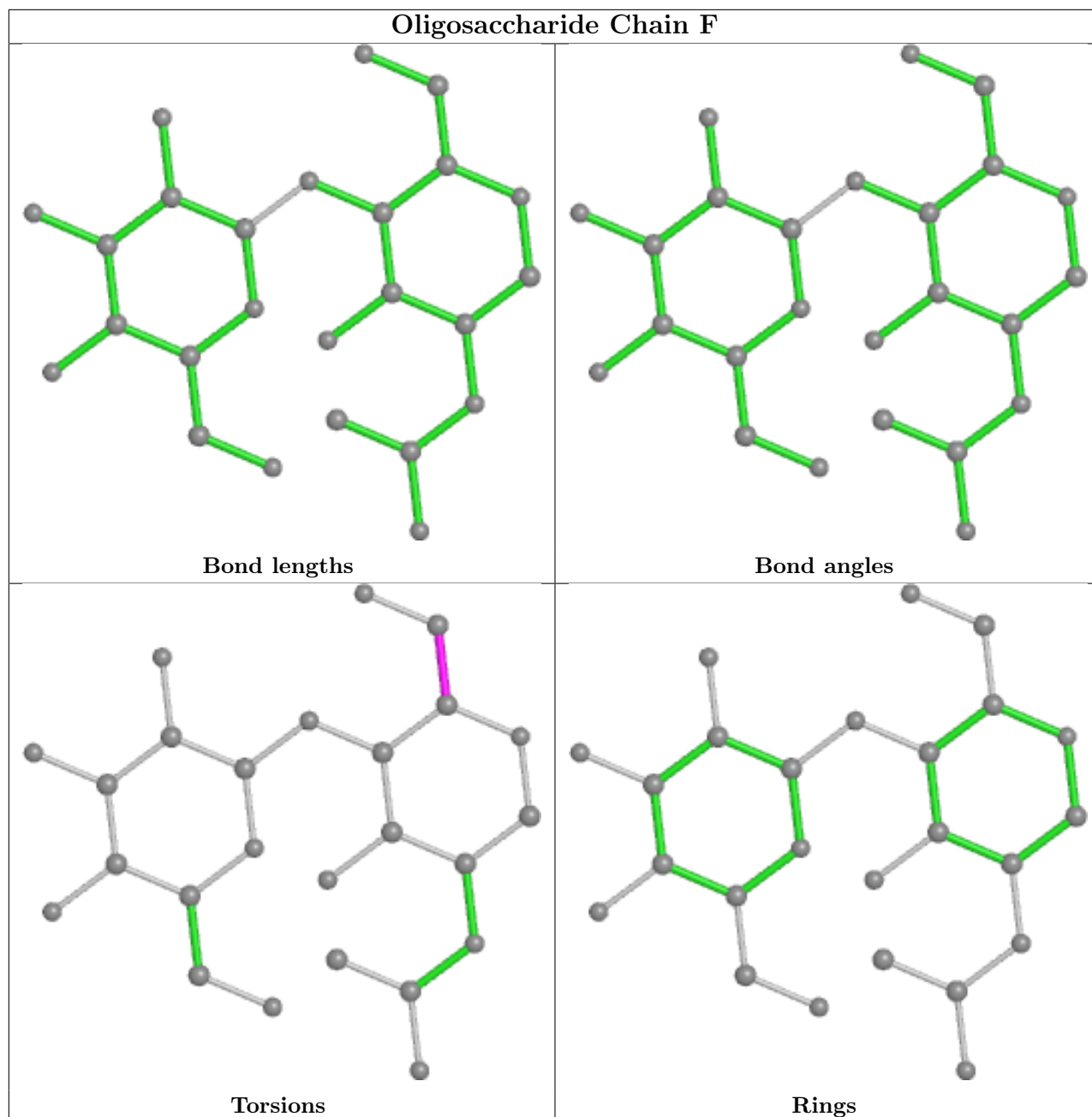
| Mol | Chain | Res | Type | Atoms |
|-----|-------|-----|------|-------------|
| 3 | L | 1 | NAG | O5-C5-C6-O6 |
| 3 | R | 1 | NAG | O5-C5-C6-O6 |
| 3 | S | 1 | NAG | O5-C5-C6-O6 |
| 3 | U | 1 | NAG | C4-C5-C6-O6 |
| 3 | M | 1 | NAG | O5-C5-C6-O6 |

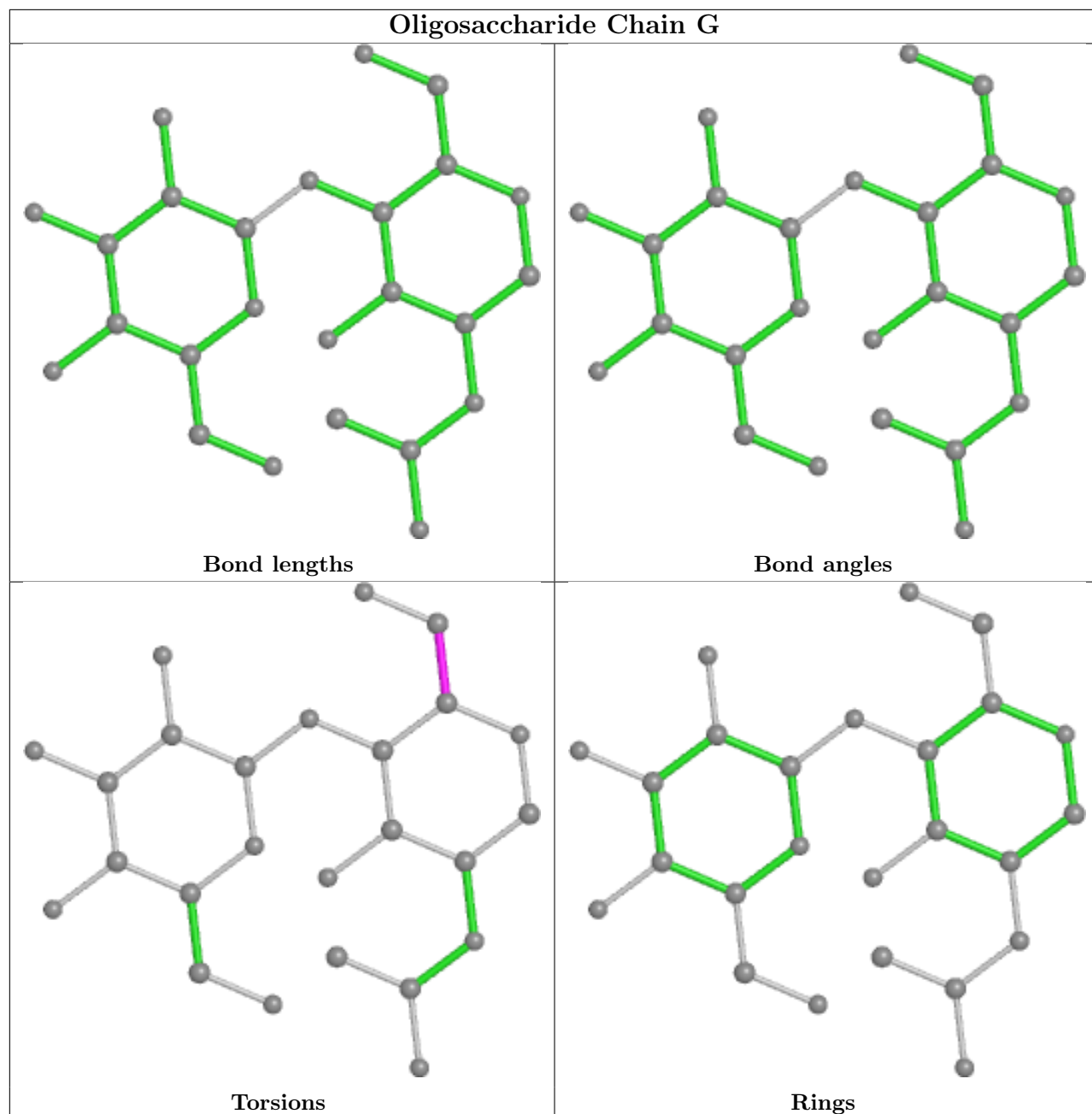
There are no ring outliers.

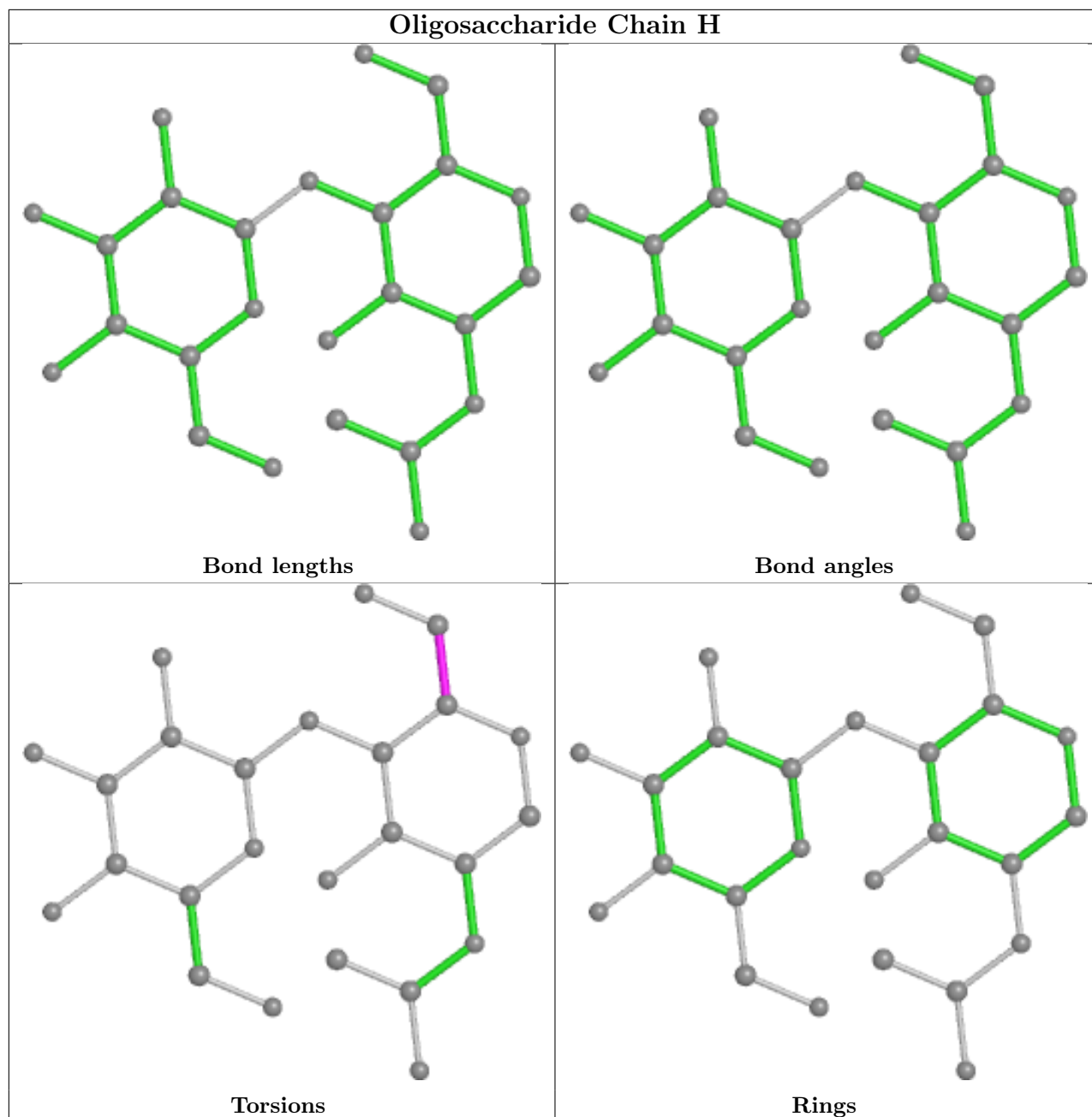
No monomer is involved in short contacts.

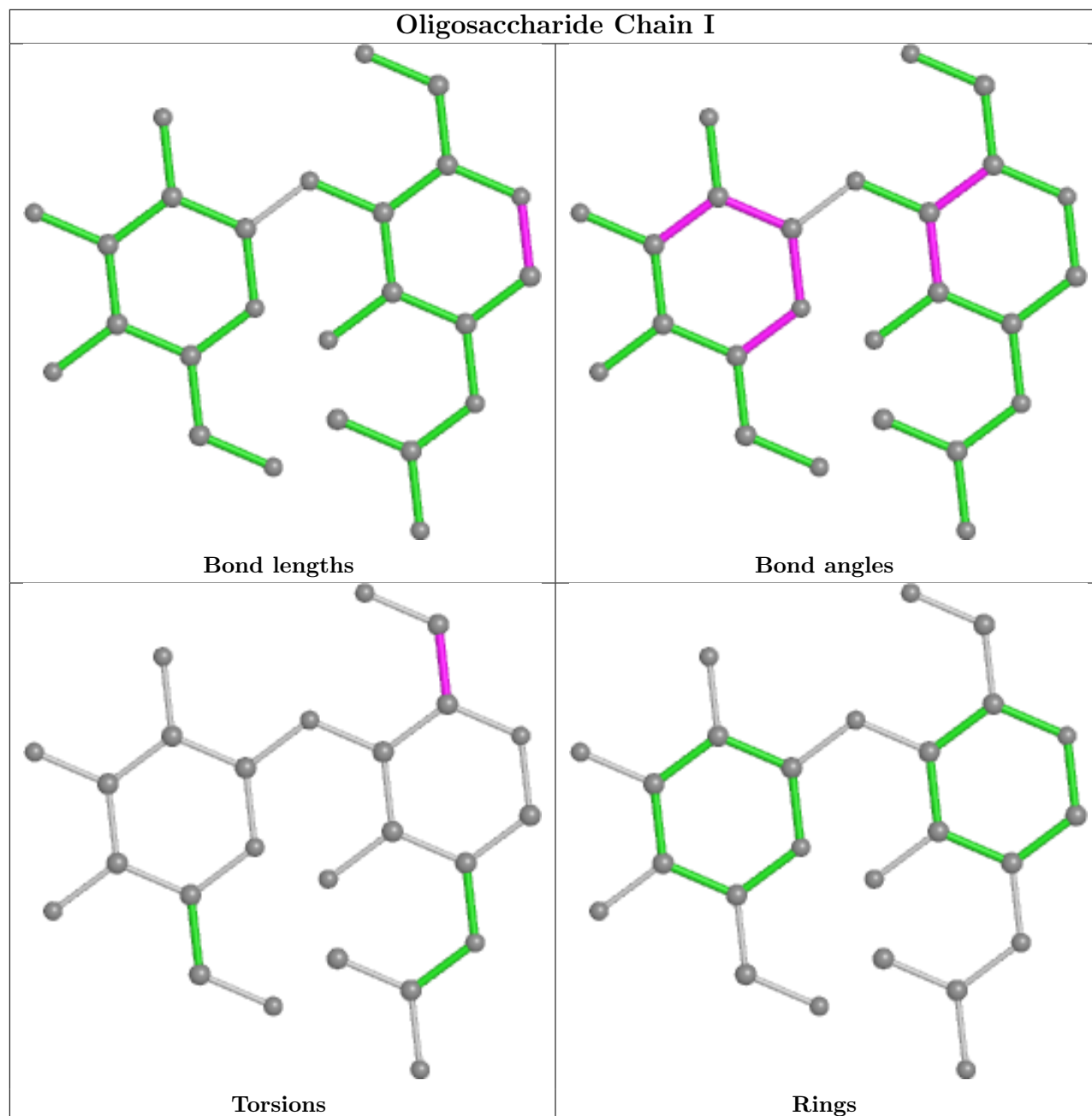
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

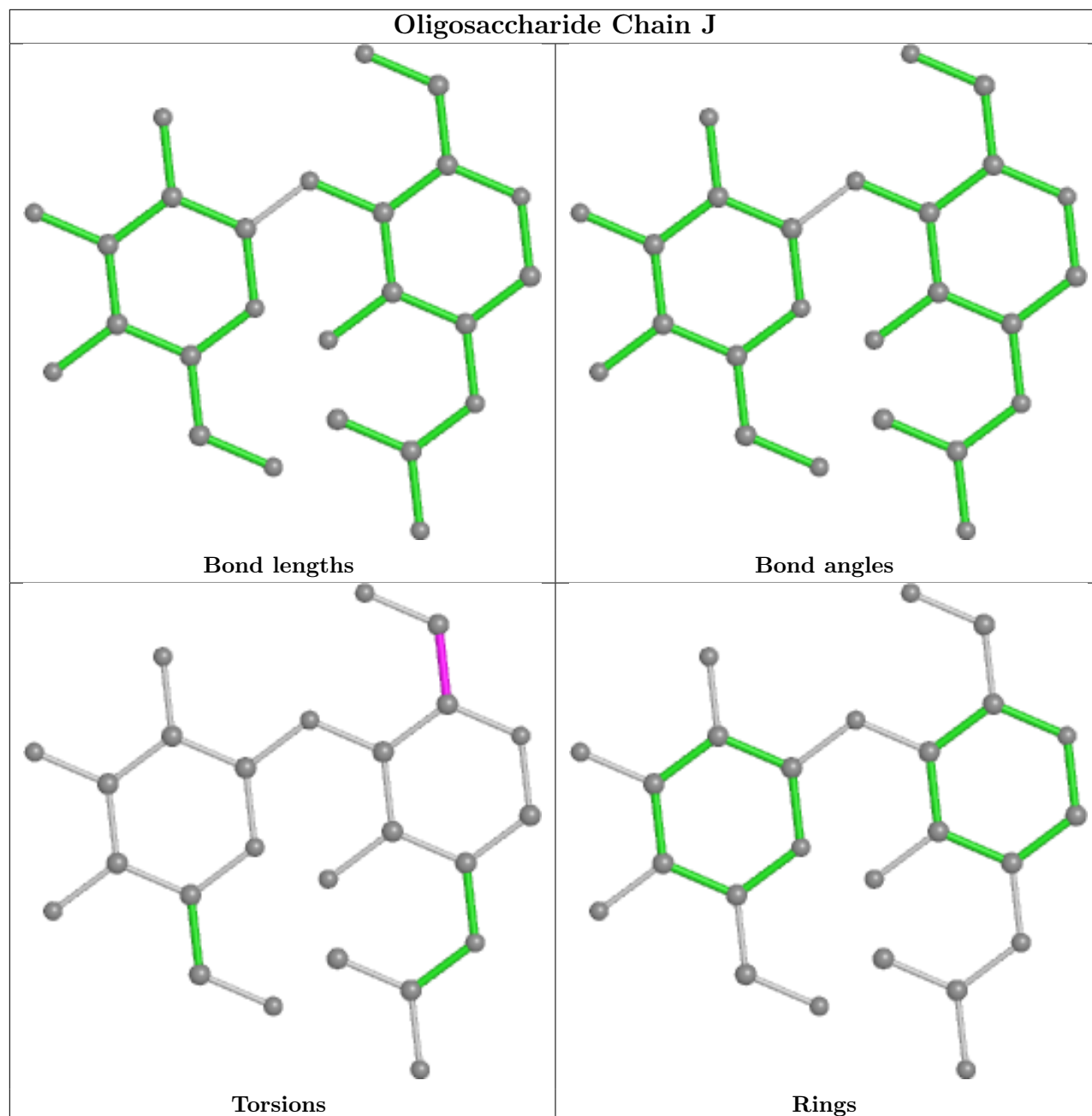


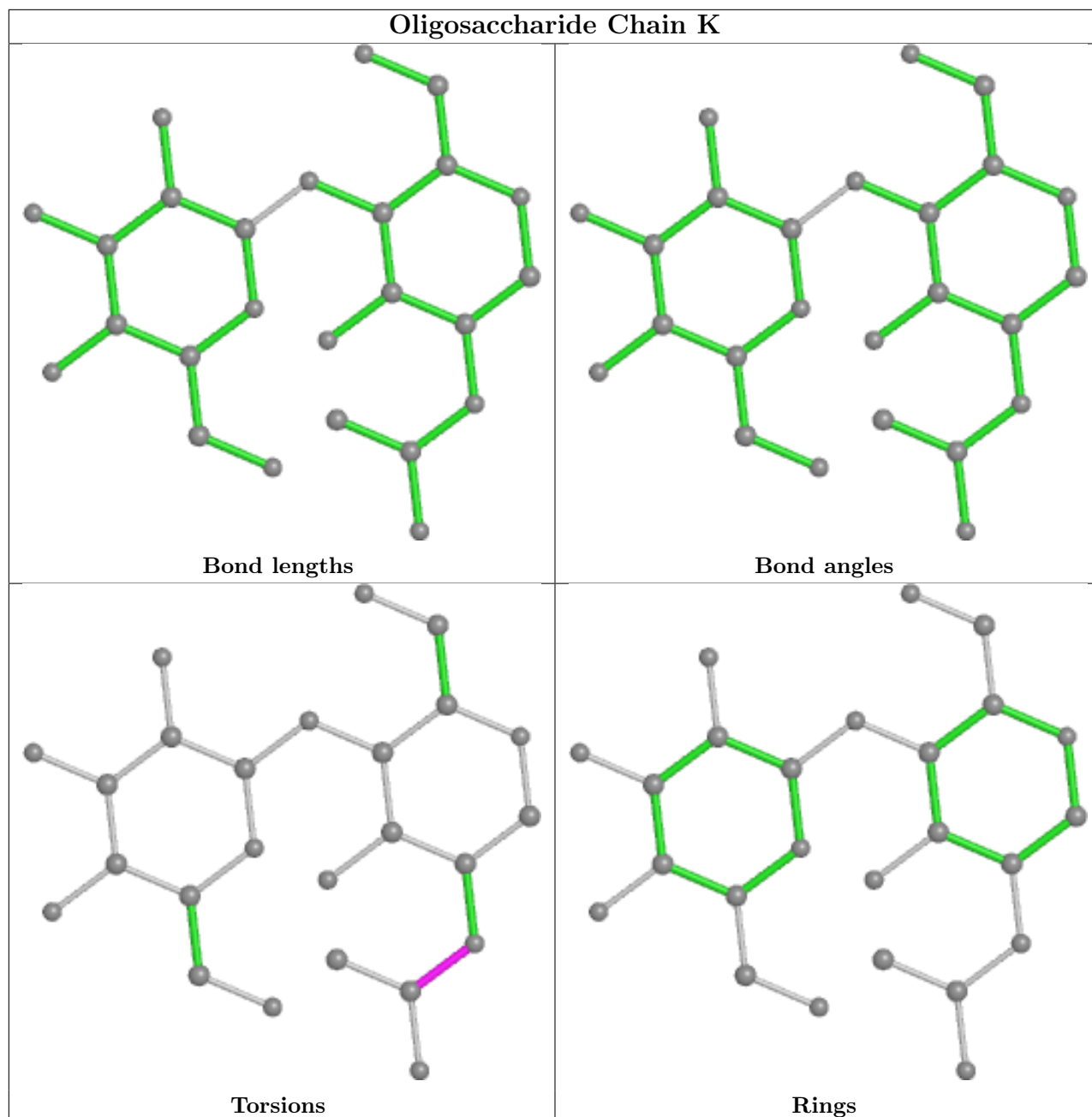


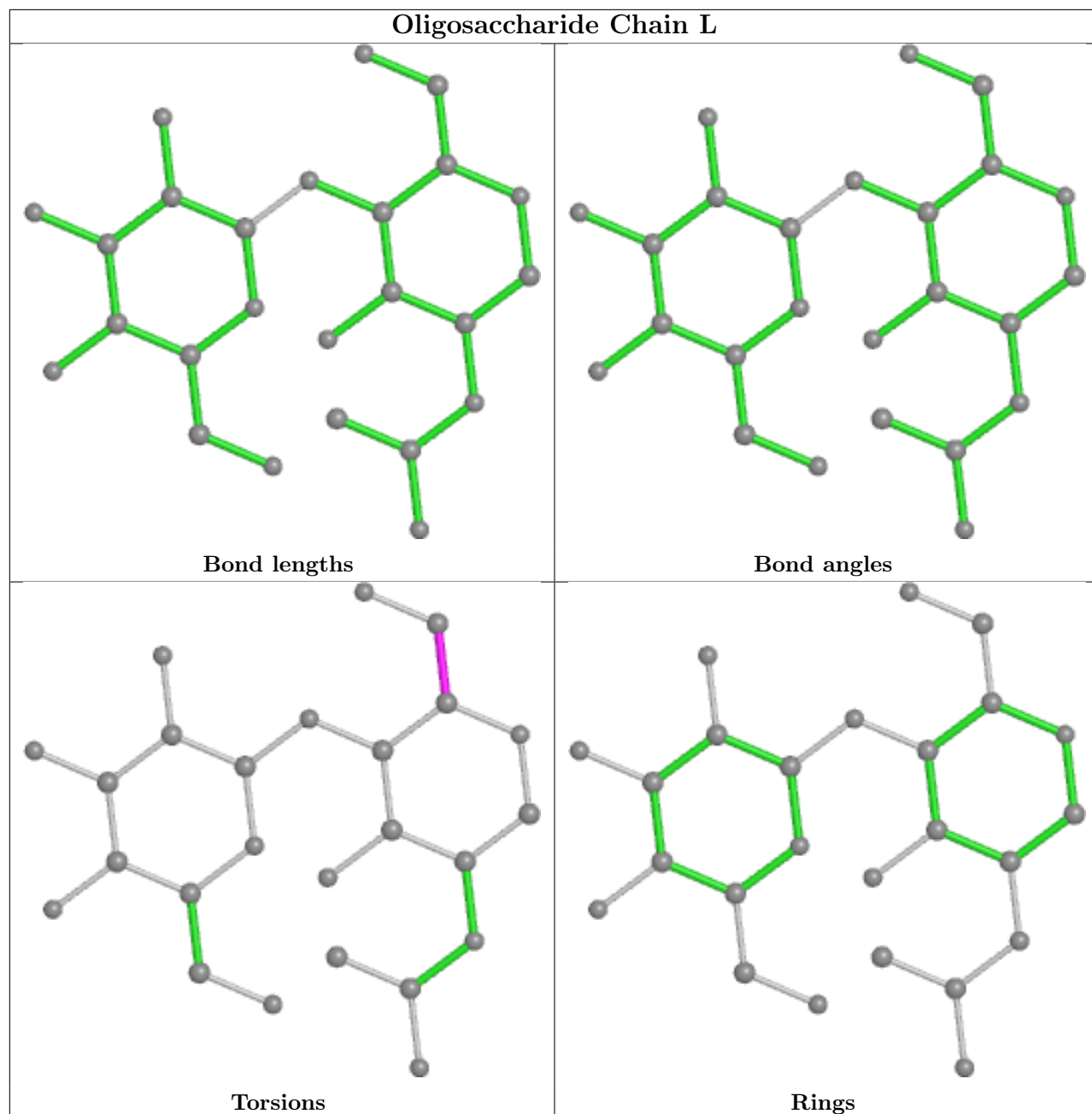


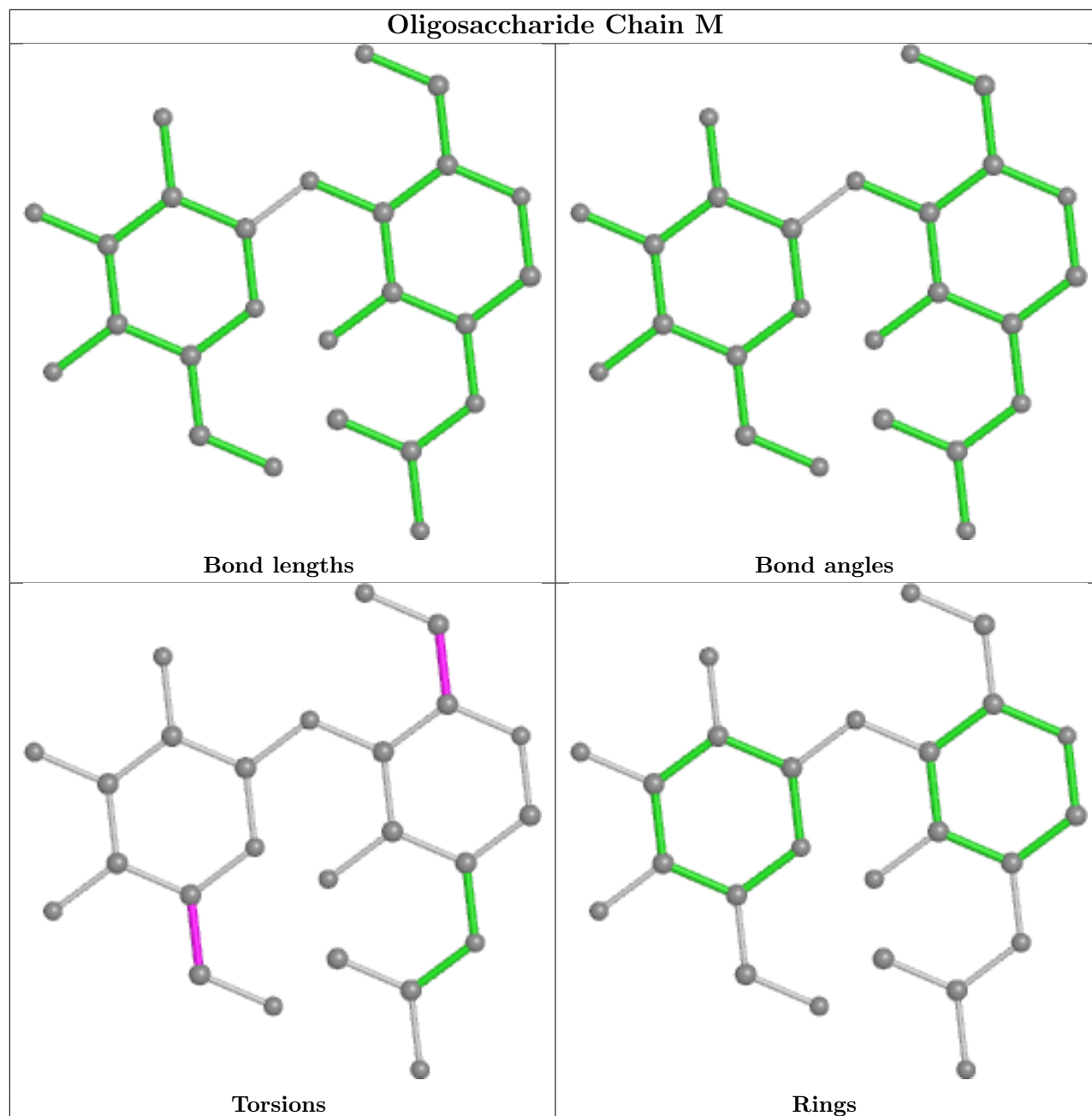


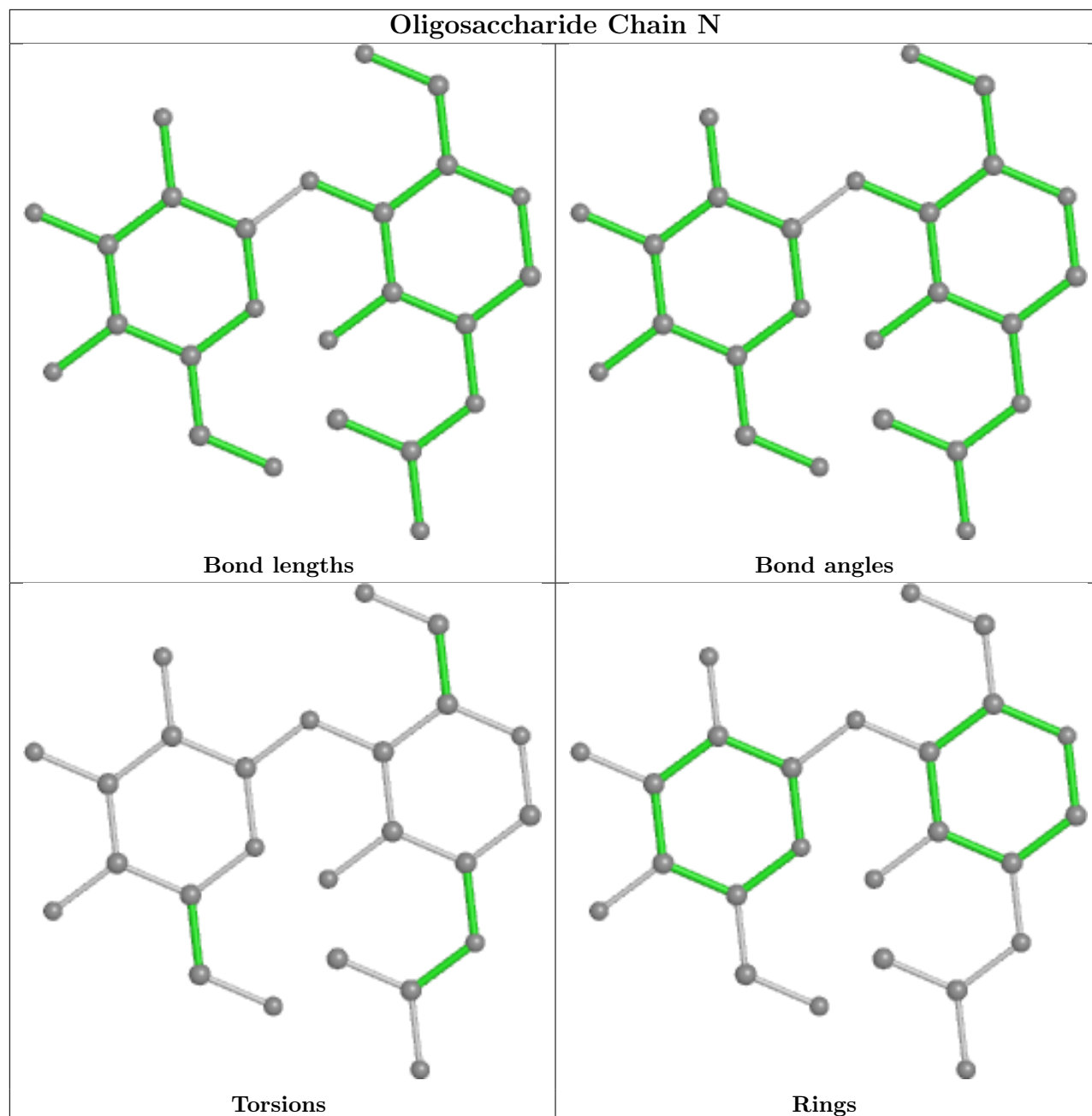


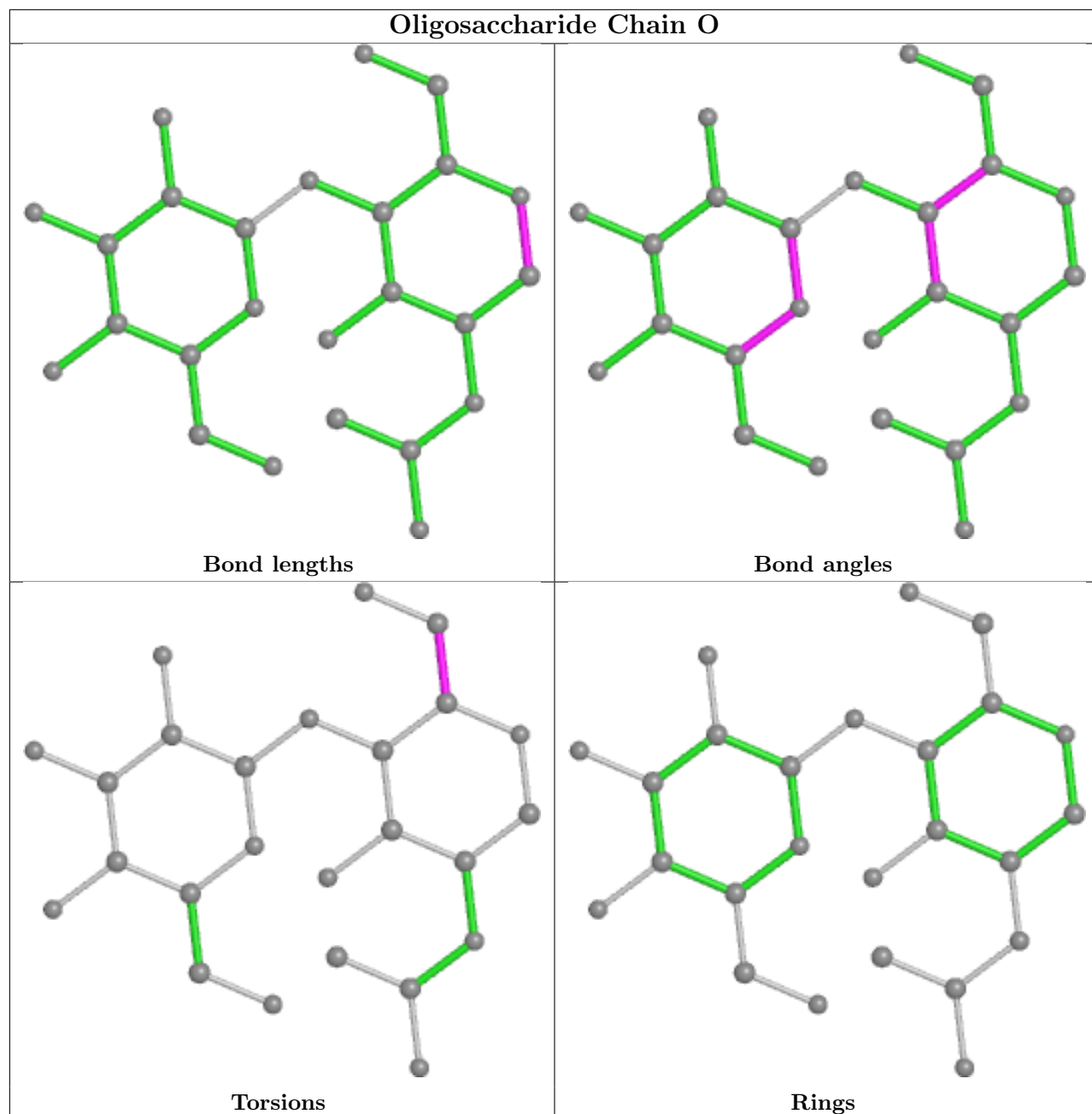


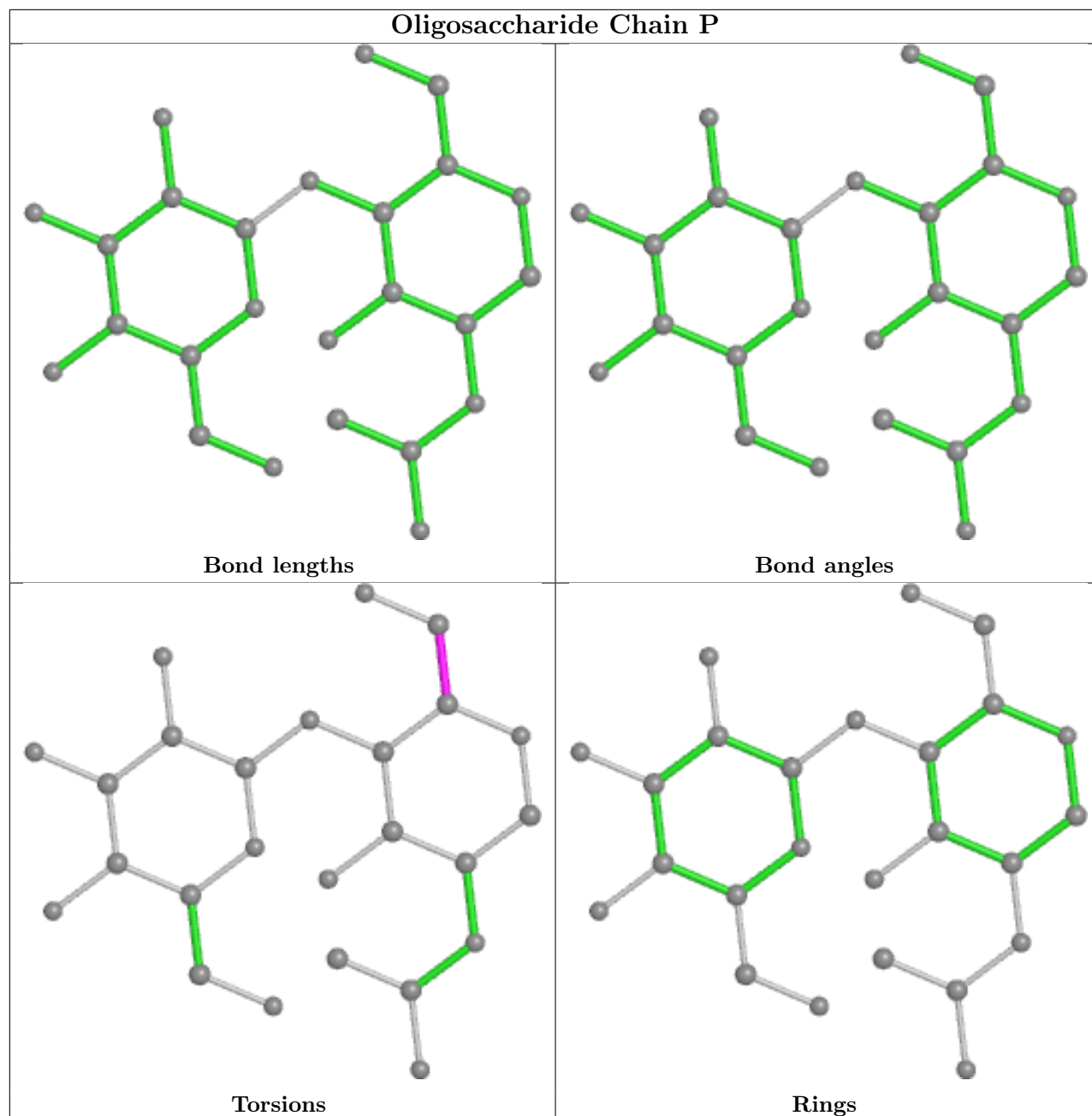


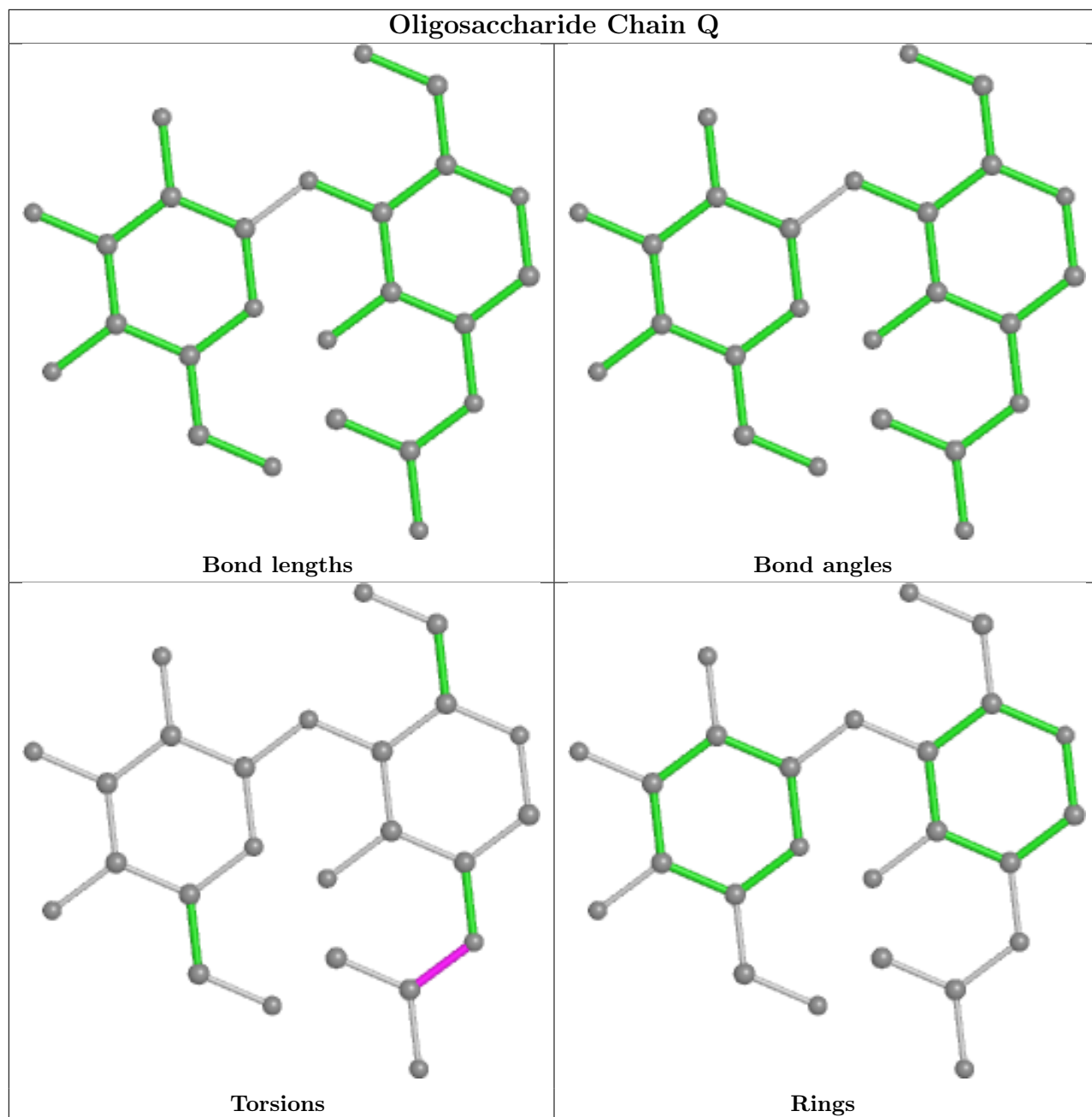


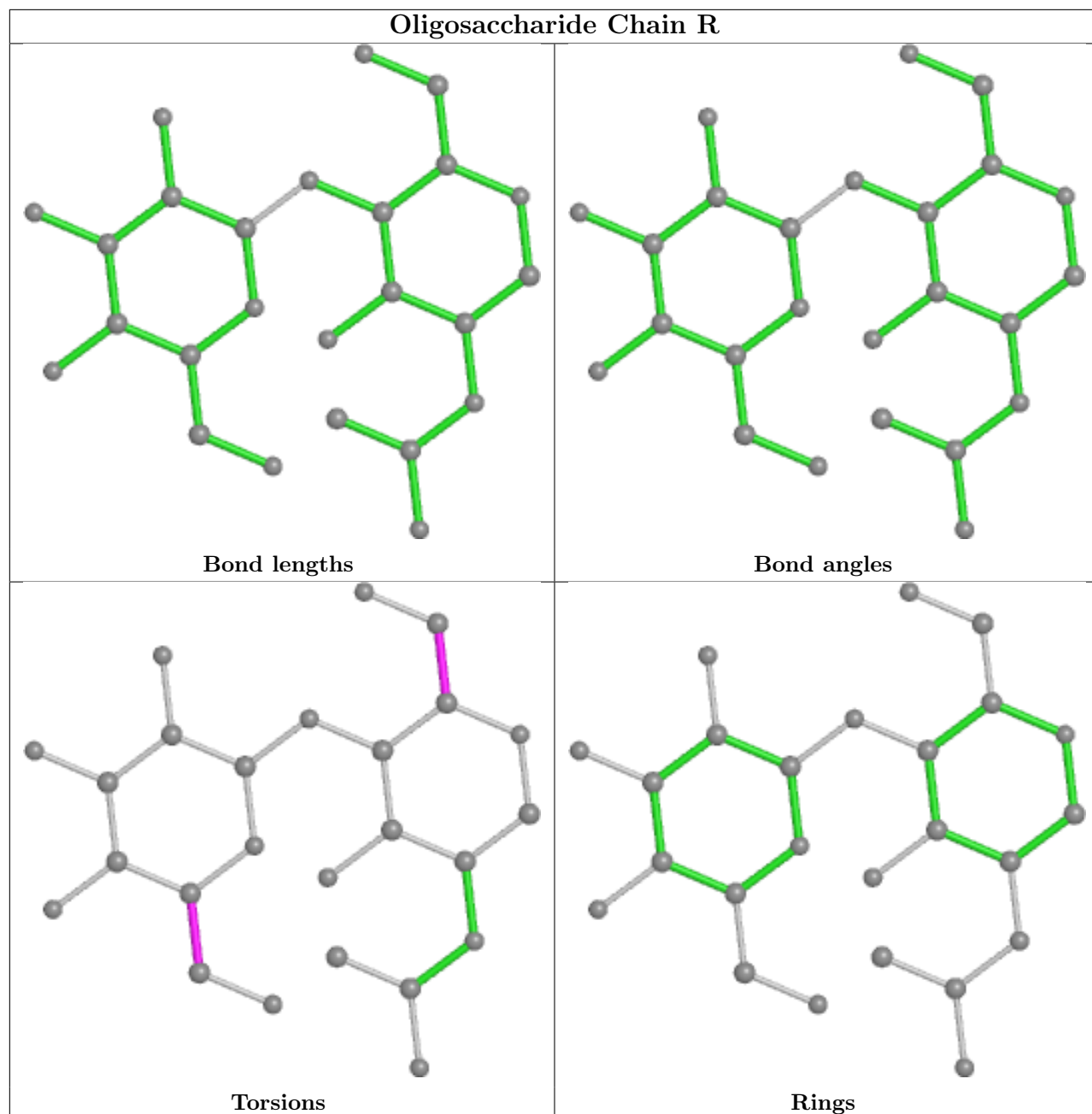


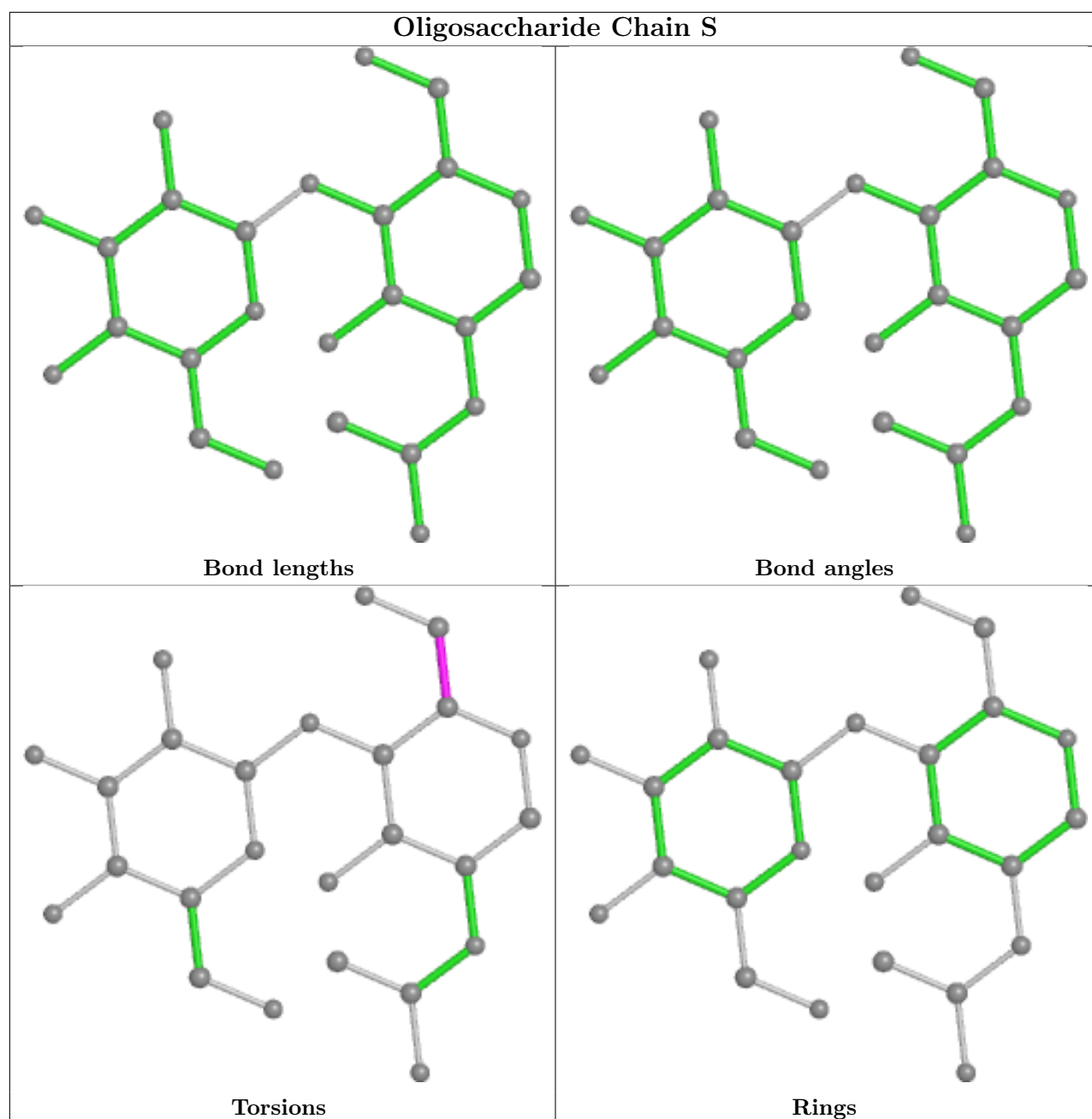


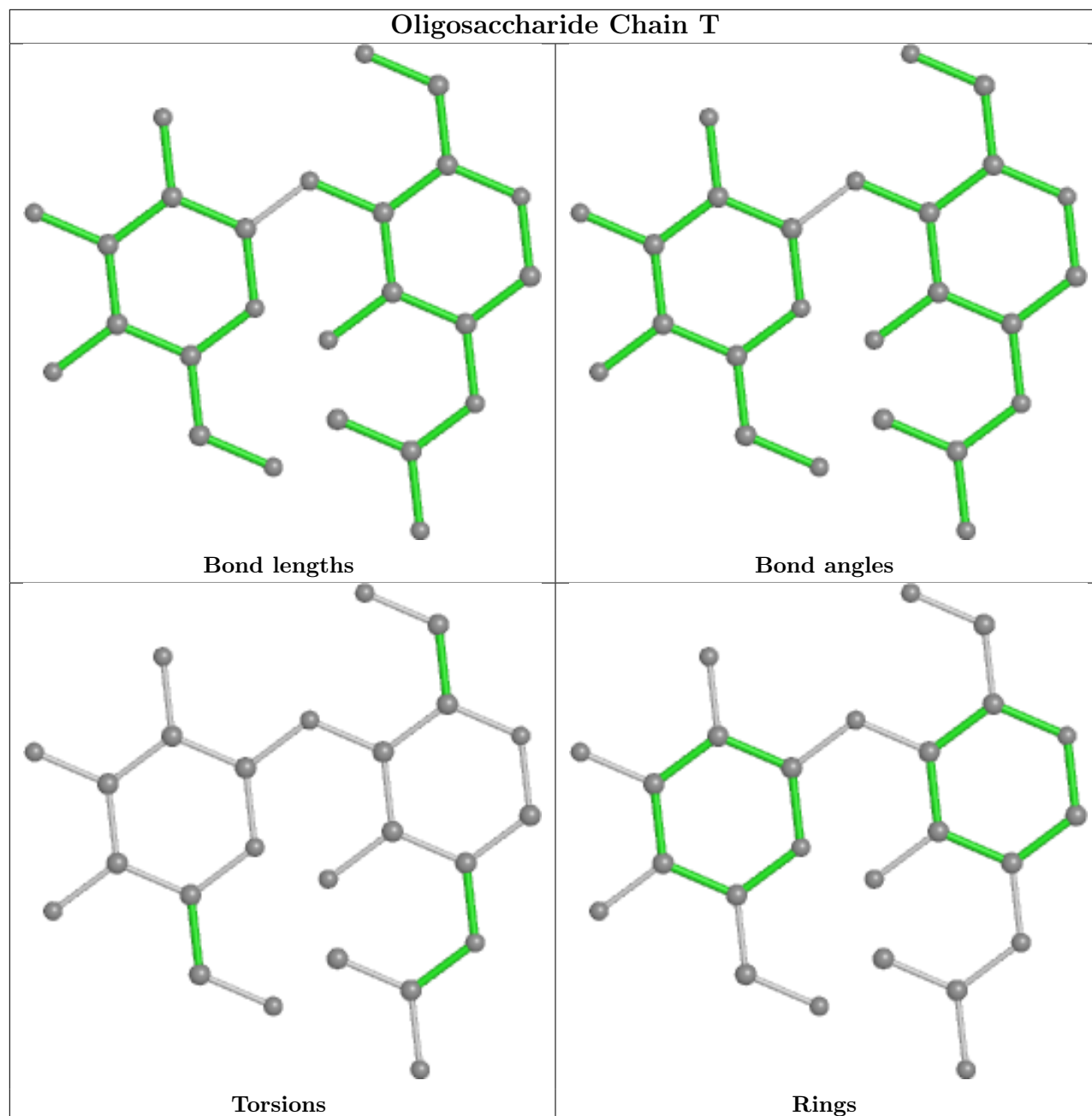


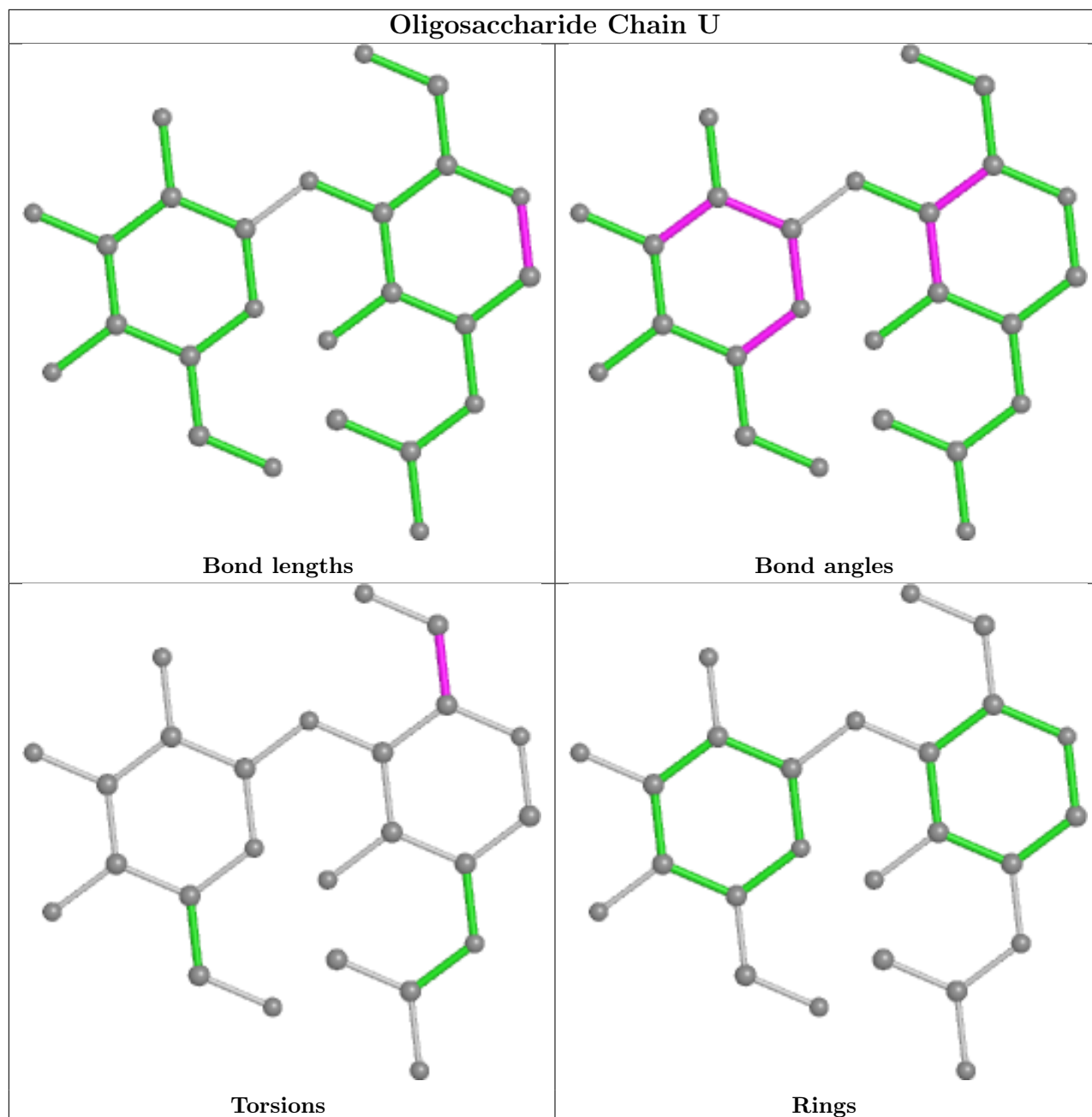












5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 2 are monoatomic - leaving 36 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths | | | Bond angles | | |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
| | | | | | Counts | RMSZ | # Z > 2 | Counts | RMSZ | # Z > 2 |
| 6 | NAG | C | 1303 | 2 | 14,14,15 | 1.05 | 2 (14%) | 17,19,21 | 0.87 | 1 (5%) |
| 6 | NAG | B | 1311 | 2 | 14,14,15 | 0.29 | 0 | 17,19,21 | 0.48 | 0 |
| 6 | NAG | C | 1310 | 2 | 14,14,15 | 0.42 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | D | 1301 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.56 | 0 |
| 6 | NAG | C | 1309 | 2 | 14,14,15 | 0.19 | 0 | 17,19,21 | 0.42 | 0 |
| 6 | NAG | B | 1301 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.53 | 0 |
| 6 | NAG | D | 1303 | 2 | 14,14,15 | 0.40 | 0 | 17,19,21 | 0.49 | 0 |
| 6 | NAG | D | 1302 | 2 | 14,14,15 | 0.26 | 0 | 17,19,21 | 0.43 | 0 |
| 6 | NAG | B | 1304 | 2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.38 | 0 |
| 6 | NAG | C | 1307 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.44 | 0 |
| 6 | NAG | D | 1306 | 2 | 14,14,15 | 0.36 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | D | 1310 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.38 | 0 |
| 6 | NAG | B | 1308 | 2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.42 | 0 |
| 6 | NAG | B | 1303 | 2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.45 | 0 |
| 6 | NAG | C | 1302 | 2 | 14,14,15 | 0.21 | 0 | 17,19,21 | 0.37 | 0 |
| 6 | NAG | A | 905 | 1 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.49 | 0 |
| 6 | NAG | C | 1304 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.37 | 0 |
| 6 | NAG | C | 1306 | 2 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | D | 1305 | 2 | 14,14,15 | 0.30 | 0 | 17,19,21 | 1.39 | 2 (11%) |
| 6 | NAG | A | 904 | 1 | 14,14,15 | 0.81 | 1 (7%) | 17,19,21 | 1.48 | 3 (17%) |
| 6 | NAG | D | 1307 | 2 | 14,14,15 | 0.20 | 0 | 17,19,21 | 0.44 | 0 |
| 6 | NAG | A | 902 | 1 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.36 | 0 |
| 6 | NAG | B | 1306 | 2 | 14,14,15 | 0.35 | 0 | 17,19,21 | 1.35 | 1 (5%) |
| 6 | NAG | B | 1305 | 2 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 6 | NAG | D | 1309 | 2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | B | 1309 | 2 | 14,14,15 | 0.34 | 0 | 17,19,21 | 0.60 | 1 (5%) |
| 6 | NAG | B | 1302 | 2 | 14,14,15 | 0.23 | 0 | 17,19,21 | 0.38 | 0 |
| 6 | NAG | B | 1307 | 2 | 14,14,15 | 0.39 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | D | 1304 | 2 | 14,14,15 | 0.24 | 0 | 17,19,21 | 0.34 | 0 |
| 6 | NAG | B | 1310 | - | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.42 | 0 |
| 6 | NAG | C | 1301 | 2 | 14,14,15 | 0.25 | 0 | 17,19,21 | 0.54 | 0 |
| 6 | NAG | A | 906 | 1 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | A | 903 | 1 | 14,14,15 | 0.22 | 0 | 17,19,21 | 0.40 | 0 |
| 6 | NAG | C | 1305 | 2 | 14,14,15 | 0.29 | 0 | 17,19,21 | 1.36 | 2 (11%) |
| 6 | NAG | C | 1308 | 2 | 14,14,15 | 0.28 | 0 | 17,19,21 | 0.60 | 1 (5%) |
| 6 | NAG | D | 1308 | 2 | 14,14,15 | 0.32 | 0 | 17,19,21 | 0.60 | 1 (5%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|------|------|---------|-----------|---------|
| 6 | NAG | C | 1303 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1311 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1310 | 2 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1301 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1309 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1301 | 2 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1303 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1302 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1304 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1307 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1306 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1310 | 2 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1308 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1303 | 2 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1302 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 905 | 1 | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1304 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1306 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1305 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 904 | 1 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1307 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 902 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1306 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1305 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1309 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1309 | 2 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1302 | 2 | - | 1/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1307 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1304 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | B | 1310 | - | - | 3/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1301 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 906 | 1 | - | 4/6/23/26 | 0/1/1/1 |
| 6 | NAG | A | 903 | 1 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1305 | 2 | - | 0/6/23/26 | 0/1/1/1 |
| 6 | NAG | C | 1308 | 2 | - | 2/6/23/26 | 0/1/1/1 |
| 6 | NAG | D | 1308 | 2 | - | 4/6/23/26 | 0/1/1/1 |

All (3) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 6 | C | 1303 | NAG | C1-C2 | 2.93 | 1.56 | 1.52 |
| 6 | C | 1303 | NAG | O5-C1 | 2.52 | 1.47 | 1.43 |
| 6 | A | 904 | NAG | C1-C2 | 2.38 | 1.55 | 1.52 |

The worst 5 of 12 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|------|-------------|----------|
| 6 | D | 1305 | NAG | C1-O5-C5 | 4.98 | 118.94 | 112.19 |
| 6 | B | 1306 | NAG | C1-O5-C5 | 4.92 | 118.86 | 112.19 |
| 6 | C | 1305 | NAG | C1-O5-C5 | 4.90 | 118.83 | 112.19 |
| 6 | A | 904 | NAG | C1-O5-C5 | 4.62 | 118.45 | 112.19 |
| 6 | C | 1303 | NAG | C1-O5-C5 | 3.06 | 116.33 | 112.19 |

There are no chirality outliers.

5 of 70 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms |
|-----|-------|------|------|-------------|
| 6 | A | 906 | NAG | C4-C5-C6-O6 |
| 6 | B | 1301 | NAG | C4-C5-C6-O6 |
| 6 | D | 1310 | NAG | C4-C5-C6-O6 |
| 6 | D | 1307 | NAG | O5-C5-C6-O6 |
| 6 | D | 1308 | NAG | C4-C5-C6-O6 |

There are no ring outliers.

5 monomers are involved in 5 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|------|------|---------|--------------|
| 6 | D | 1301 | NAG | 1 | 0 |
| 6 | D | 1306 | NAG | 1 | 0 |
| 6 | D | 1310 | NAG | 1 | 0 |
| 6 | B | 1310 | NAG | 1 | 0 |
| 6 | C | 1305 | NAG | 1 | 0 |

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.