



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 11, 2024 – 10:15 AM EDT

PDB ID : 8TGO  
Title : Crystal structure of the BG505 triple tandem trimer gp140 HIV-1 Env in complex with PGT124 and 35O22  
Authors : Xian, Y.; Yuan, M.; Wilson, I.A.  
Deposited on : 2023-07-12  
Resolution : 5.75 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36.1

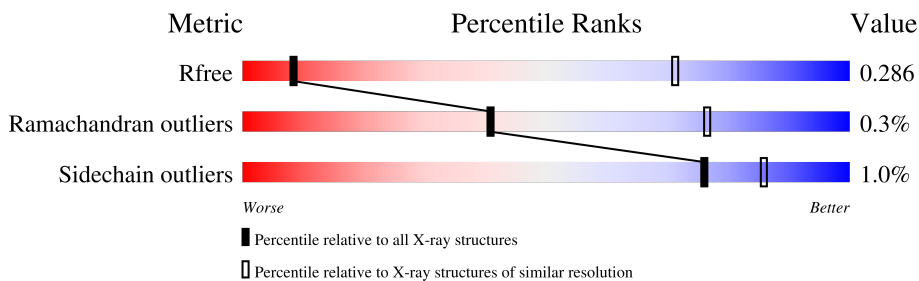
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 5.75 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<br>(#Entries) | Similar resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|---|
| $R_{free}$            | 130704                      | 1007 (7.66-3.86)                                      |
| Ramachandran outliers | 138981                      | 1002 (7.60-3.86)                                      |
| Sidechain outliers    | 138945                      | 1005 (7.70-3.82)                                      |

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

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | B     | 164    |                  |
| 1   | H     | 164    |                  |
| 1   | a     | 164    |                  |
| 2   | D     | 286    |                  |
| 2   | L     | 286    |                  |
| 2   | b     | 286    |                  |
| 3   | C     | 214    |                  |
| 3   | P     | 214    |                  |

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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 3   | c     | 214    | 97%              |
| 4   | G     | 490    | 89%              |
| 4   | R     | 490    | 89%              |
| 4   | e     | 490    | 89%              |
| 5   | O     | 235    | 55%              |
| 5   | S     | 235    | 97%              |
| 5   | f     | 235    | 97%              |
| 6   | A     | 5      | 40%              |
| 7   | F     | 2      | 100%             |
| 7   | K     | 2      | 100%             |
| 7   | M     | 2      | 100%             |
| 7   | T     | 2      | 100%             |
| 7   | U     | 2      | 100%             |
| 7   | W     | 2      | 100%             |
| 7   | X     | 2      | 100%             |
| 7   | g     | 2      | 100%             |
| 7   | h     | 2      | 100%             |
| 7   | j     | 2      | 100%             |
| 7   | l     | 2      | 100%             |
| 7   | o     | 2      | 100%             |
| 7   | p     | 2      | 100%             |
| 7   | r     | 2      | 100%             |
| 8   | I     | 3      | 100%             |
| 8   | J     | 3      | 100%             |
| 8   | Y     | 3      | 100%             |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 8   | Z     | 3      |  100%    |
| 8   | m     | 3      |  100%    |
| 8   | n     | 3      |  100%    |
| 9   | N     | 10     |  10% 90% |
| 9   | i     | 10     |  10% 90% |
| 9   | q     | 10     |  10% 90% |
| 10  | V     | 4      |  50% 50% |
| 10  | k     | 4      |  75% 25% |

## 2 Entry composition i

There are 11 unique types of molecules in this entry. The entry contains 29645 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 |
|-----|-------|----------|-------|-----|-----|-----|---|---------|---------|-------|
|     |       |          | Total | C   | N   | O   | S |         |         |       |
| 1   | B     | 123      | 967   | 609 | 167 | 185 | 6 | 0       | 0       | 0     |
| 1   | H     | 122      | 963   | 607 | 166 | 184 | 6 | 0       | 0       | 0     |
| 1   | a     | 123      | 967   | 609 | 167 | 185 | 6 | 0       | 0       | 0     |

There are 51 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 519     | SER      | PHE    | conflict       | UNP Q2N0S6 |
| B     | 559     | PRO      | ILE    | conflict       | UNP Q2N0S6 |
| B     | 568     | ASP      | LEU    | conflict       | UNP Q2N0S6 |
| B     | 570     | HIS      | VAL    | conflict       | UNP Q2N0S6 |
| B     | 585     | HIS      | ARG    | conflict       | UNP Q2N0S6 |
| B     | 605     | CYS      | THR    | conflict       | UNP Q2N0S6 |
| B     | 665     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 666     | SER      | -      | expression tag | UNP Q2N0S6 |
| B     | 667     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 668     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 669     | SER      | -      | expression tag | UNP Q2N0S6 |
| B     | 670     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 671     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 672     | SER      | -      | expression tag | UNP Q2N0S6 |
| B     | 673     | GLY      | -      | expression tag | UNP Q2N0S6 |
| B     | 674     | SER      | -      | expression tag | UNP Q2N0S6 |
| B     | 675     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 519     | SER      | PHE    | conflict       | UNP Q2N0S6 |
| H     | 559     | PRO      | ILE    | conflict       | UNP Q2N0S6 |
| H     | 568     | ASP      | LEU    | conflict       | UNP Q2N0S6 |
| H     | 570     | HIS      | VAL    | conflict       | UNP Q2N0S6 |
| H     | 585     | HIS      | ARG    | conflict       | UNP Q2N0S6 |
| H     | 605     | CYS      | THR    | conflict       | UNP Q2N0S6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| H     | 665     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 666     | SER      | -      | expression tag | UNP Q2N0S6 |
| H     | 667     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 668     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 669     | SER      | -      | expression tag | UNP Q2N0S6 |
| H     | 670     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 671     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 672     | SER      | -      | expression tag | UNP Q2N0S6 |
| H     | 673     | GLY      | -      | expression tag | UNP Q2N0S6 |
| H     | 674     | SER      | -      | expression tag | UNP Q2N0S6 |
| H     | 675     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 519     | SER      | PHE    | conflict       | UNP Q2N0S6 |
| a     | 559     | PRO      | ILE    | conflict       | UNP Q2N0S6 |
| a     | 568     | ASP      | LEU    | conflict       | UNP Q2N0S6 |
| a     | 570     | HIS      | VAL    | conflict       | UNP Q2N0S6 |
| a     | 585     | HIS      | ARG    | conflict       | UNP Q2N0S6 |
| a     | 605     | CYS      | THR    | conflict       | UNP Q2N0S6 |
| a     | 665     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 666     | SER      | -      | expression tag | UNP Q2N0S6 |
| a     | 667     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 668     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 669     | SER      | -      | expression tag | UNP Q2N0S6 |
| a     | 670     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 671     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 672     | SER      | -      | expression tag | UNP Q2N0S6 |
| a     | 673     | GLY      | -      | expression tag | UNP Q2N0S6 |
| a     | 674     | SER      | -      | expression tag | UNP Q2N0S6 |
| a     | 675     | GLY      | -      | expression tag | UNP Q2N0S6 |

- Molecule 2 is a protein called 35O22 scFv.

| Mol | Chain | Residues | Atoms |      |     |     |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|---------|-------|
| 2   | D     | 236      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1820  | 1148 | 305 | 356 | 11 |         |         |       |
| 2   | L     | 236      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1820  | 1148 | 305 | 356 | 11 |         |         |       |
| 2   | b     | 236      | Total | C    | N   | O   | S  | 0       | 0       | 0     |
|     |       |          | 1820  | 1148 | 305 | 356 | 11 |         |         |       |

- Molecule 3 is a protein called PGT124 light chain.

| Mol | Chain | Residues | Atoms         |           |          |          |        | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|--------|---------|---------|-------|
| 3   | C     | 208      | Total<br>1580 | C<br>997  | N<br>268 | O<br>310 | S<br>5 | 0       | 0       | 0     |
| 3   | P     | 210      | Total<br>1595 | C<br>1005 | N<br>270 | O<br>315 | S<br>5 | 0       | 0       | 0     |
| 3   | c     | 210      | Total<br>1595 | C<br>1005 | N<br>270 | O<br>315 | S<br>5 | 0       | 0       | 0     |

- Molecule 4 is a protein called Envelope glycoprotein gp120.

| Mol | Chain | Residues | Atoms         |           |          |          |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|---------------|-----------|----------|----------|---------|---------|---------|-------|
| 4   | G     | 439      | Total<br>3473 | C<br>2190 | N<br>610 | O<br>646 | S<br>27 | 0       | 0       | 0     |
| 4   | R     | 439      | Total<br>3473 | C<br>2190 | N<br>610 | O<br>646 | S<br>27 | 0       | 0       | 0     |
| 4   | e     | 439      | Total<br>3473 | C<br>2190 | N<br>610 | O<br>646 | S<br>27 | 0       | 0       | 0     |

There are 75 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 64      | LYS      | GLU    | conflict       | UNP Q2N0S6 |
| G     | 106     | GLU      | THR    | conflict       | UNP Q2N0S6 |
| G     | 271     | ILE      | MET    | conflict       | UNP Q2N0S6 |
| G     | 288     | LEU      | PHE    | conflict       | UNP Q2N0S6 |
| G     | 304     | VAL      | ARG    | conflict       | UNP Q2N0S6 |
| G     | 316     | TRP      | ALA    | conflict       | UNP Q2N0S6 |
| G     | 319     | TYR      | ALA    | conflict       | UNP Q2N0S6 |
| G     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| G     | 500     | LYS      | ARG    | conflict       | UNP Q2N0S6 |
| G     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| G     | 508     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 509     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 510     | SER      | -      | expression tag | UNP Q2N0S6 |
| G     | 511     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 512     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 513     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 514     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 515     | SER      | -      | expression tag | UNP Q2N0S6 |
| G     | 516     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 517     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 518     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 519     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 520     | SER      | -      | expression tag | UNP Q2N0S6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| G     | 521     | GLY      | -      | expression tag | UNP Q2N0S6 |
| G     | 522     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 64      | LYS      | GLU    | conflict       | UNP Q2N0S6 |
| R     | 106     | GLU      | THR    | conflict       | UNP Q2N0S6 |
| R     | 271     | ILE      | MET    | conflict       | UNP Q2N0S6 |
| R     | 288     | LEU      | PHE    | conflict       | UNP Q2N0S6 |
| R     | 304     | VAL      | ARG    | conflict       | UNP Q2N0S6 |
| R     | 316     | TRP      | ALA    | conflict       | UNP Q2N0S6 |
| R     | 319     | TYR      | ALA    | conflict       | UNP Q2N0S6 |
| R     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| R     | 500     | LYS      | ARG    | conflict       | UNP Q2N0S6 |
| R     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| R     | 508     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 509     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 510     | SER      | -      | expression tag | UNP Q2N0S6 |
| R     | 511     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 512     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 513     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 514     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 515     | SER      | -      | expression tag | UNP Q2N0S6 |
| R     | 516     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 517     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 518     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 519     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 520     | SER      | -      | expression tag | UNP Q2N0S6 |
| R     | 521     | GLY      | -      | expression tag | UNP Q2N0S6 |
| R     | 522     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 64      | LYS      | GLU    | conflict       | UNP Q2N0S6 |
| e     | 106     | GLU      | THR    | conflict       | UNP Q2N0S6 |
| e     | 271     | ILE      | MET    | conflict       | UNP Q2N0S6 |
| e     | 288     | LEU      | PHE    | conflict       | UNP Q2N0S6 |
| e     | 304     | VAL      | ARG    | conflict       | UNP Q2N0S6 |
| e     | 316     | TRP      | ALA    | conflict       | UNP Q2N0S6 |
| e     | 319     | TYR      | ALA    | conflict       | UNP Q2N0S6 |
| e     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| e     | 500     | LYS      | ARG    | conflict       | UNP Q2N0S6 |
| e     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| e     | 508     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 509     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 510     | SER      | -      | expression tag | UNP Q2N0S6 |
| e     | 511     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 512     | GLY      | -      | expression tag | UNP Q2N0S6 |

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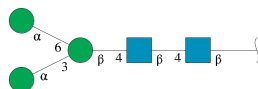
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| e     | 513     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 514     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 515     | SER      | -      | expression tag | UNP Q2N0S6 |
| e     | 516     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 517     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 518     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 519     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 520     | SER      | -      | expression tag | UNP Q2N0S6 |
| e     | 521     | GLY      | -      | expression tag | UNP Q2N0S6 |
| e     | 522     | GLY      | -      | expression tag | UNP Q2N0S6 |

- Molecule 5 is a protein called PGT124 heavy chain.

| Mol | Chain | Residues | Atoms |      |     |     |   | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|---|---------|---------|-------|
| 5   | O     | 130      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1030  | 655  | 175 | 197 | 3 |         |         |       |
| 5   | S     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1750  | 1109 | 292 | 344 | 5 |         |         |       |
| 5   | f     | 230      | Total | C    | N   | O   | S | 0       | 0       | 0     |
|     |       |          | 1750  | 1109 | 292 | 344 | 5 |         |         |       |

- Molecule 6 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.



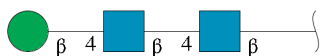
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 6   | A     | 5        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |         |       |

- Molecule 7 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 |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 7   | F     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | K     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | M     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | T     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | U     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | W     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | X     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | g     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | h     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | j     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | l     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | o     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | p     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |
| 7   | r     | 2        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |         |       |

- Molecule 8 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.



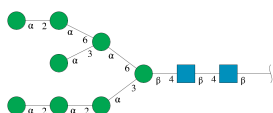
| Mol | Chain | Residues | Atoms |    |   |    | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|---------|-------|
| 8   | I     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |
| 8   | J     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |
| 8   | Y     | 3        | Total | C  | N | O  | 0       | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |         |       |

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| Mol | Chain | Residues | Atoms       |         |        |         | ZeroOcc | AltConf | Trace |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|-------|
|     |       |          | Total       | C       | N      | O       |         |         |       |
| 8   | Z     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0       | 0     |
| 8   | m     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0       | 0     |
| 8   | n     | 3        | Total<br>39 | C<br>22 | N<br>2 | O<br>15 | 0       | 0       | 0     |

- Molecule 9 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 |
|-----|-------|----------|--------------|---------|--------|---------|---------|---------|-------|
|     |       |          | Total        | C       | N      | O       |         |         |       |
| 9   | N     | 10       | Total<br>116 | C<br>64 | N<br>2 | O<br>50 | 0       | 0       | 0     |
| 9   | i     | 10       | Total<br>116 | C<br>64 | N<br>2 | O<br>50 | 0       | 0       | 0     |
| 9   | q     | 10       | Total<br>116 | C<br>64 | N<br>2 | O<br>50 | 0       | 0       | 0     |

- Molecule 10 is an oligosaccharide called 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 |
|-----|-------|----------|-------------|---------|--------|---------|---------|---------|-------|
|     |       |          | Total       | C       | N      | O       |         |         |       |
| 10  | V     | 4        | Total<br>50 | C<br>28 | N<br>2 | O<br>20 | 0       | 0       | 0     |
| 10  | k     | 4        | Total<br>50 | C<br>28 | N<br>2 | O<br>20 | 0       | 0       | 0     |

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



| Mol | Chain | Residues | Atoms |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------|---|---|---|---------|---------|
|     |       |          | Total | C | N | O |         |         |
| 11  | B     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | B     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | B     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | G     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | H     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | H     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |
| 11  | H     | 1        | 14    | 8 | 1 | 5 | 0       | 0       |

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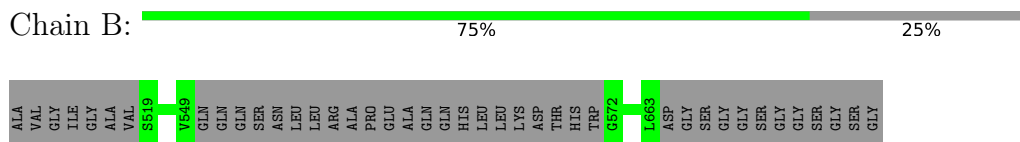
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| Mol | Chain | Residues | Atoms       |   |   |   | ZeroOcc | AltConf |
|-----|-------|----------|-------------|---|---|---|---------|---------|
|     |       |          | Total       | C | N | O |         |         |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | R     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | a     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | a     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | a     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |
| 11  | e     | 1        | Total<br>14 | 8 | 1 | 5 | 0       | 0       |

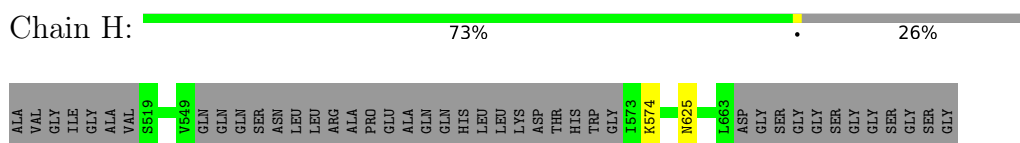
### 3 Residue-property plots [i](#)

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

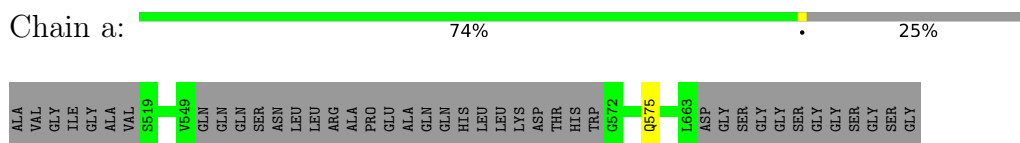
- Molecule 1: Envelope glycoprotein gp41



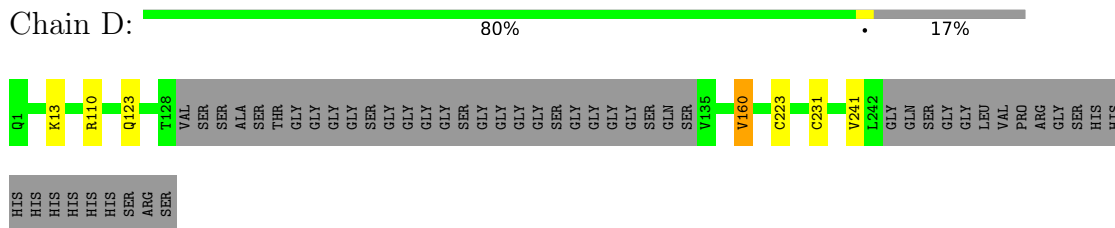
- Molecule 1: Envelope glycoprotein gp41



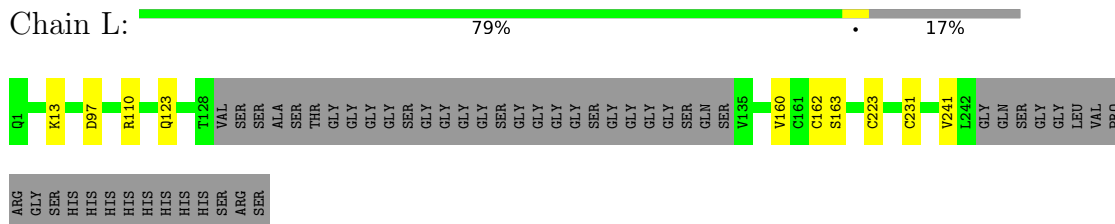
- Molecule 1: Envelope glycoprotein gp41




- Molecule 2: 35O22 scFv

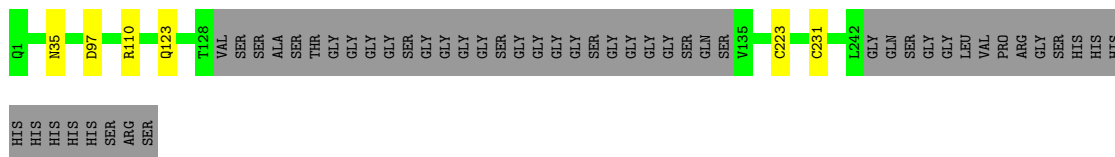


- Molecule 2: 35O22 scFv



- Molecule 2: 35O22 scFv

Chain b:  80% 17%



- Molecule 3: PGT124 light chain

Chain C:  96% ..



- Molecule 3: PGT124 light chain

Chain P:  97% ..



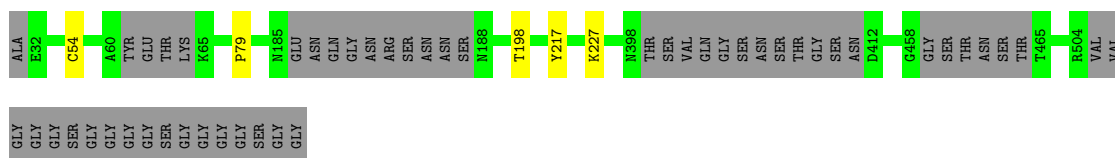
- Molecule 3: PGT124 light chain

Chain c:  97% ..




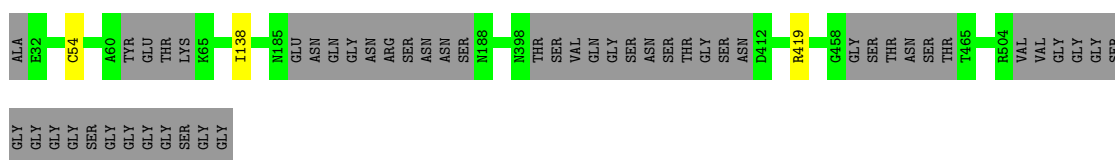
- Molecule 4: Envelope glycoprotein gp120

Chain G:  89% 10%



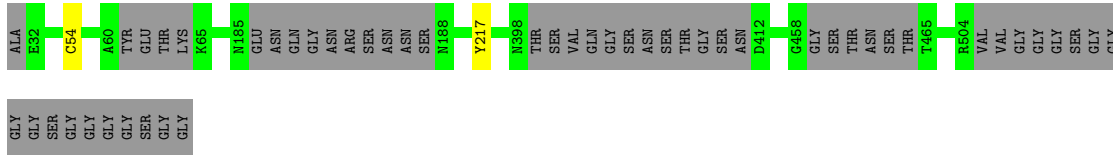
- Molecule 4: Envelope glycoprotein gp120

Chain R:  89% 10%



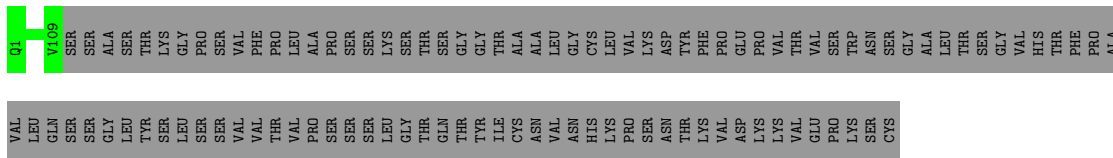
- Molecule 4: Envelope glycoprotein gp120

Chain e:  89%  10%



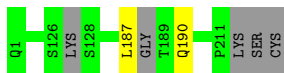
- Molecule 5: PGT124 heavy chain

Chain O:  55%  45%



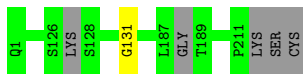
- Molecule 5: PGT124 heavy chain

Chain S:  97%  ..



- Molecule 5: PGT124 heavy chain

Chain f:  97%  .



- Molecule 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

Chain A:  40%  60%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%



- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



Chain K:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain T:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain U:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain W:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g:  100%

IMAGE  
IMAGE

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain h:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain j:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

MAG1  
MAG2

- Molecule 7: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain r:  100%

MAG1  
MAG2

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:  100%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:  100%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  100%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Z:  100%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain m:  100%

MAG1  
MAG2  
BMA3

- Molecule 8: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  100%

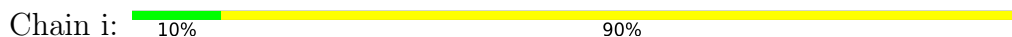
MAG1  
MAG2  
BMA3

- Molecule 9: 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

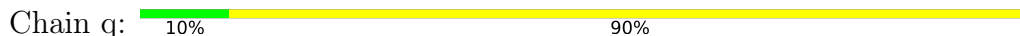
Chain N:  10% 90%



- Molecule 9: 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



- Molecule 9: 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



- Molecule 10: 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



- Molecule 10: 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



## 4 Data and refinement statistics i

| Property  | Value  | Source           |
|---|--|------------------|
| Space group   | C 1 2 1  | Depositor        |
| Cell constants<br>a, b, c, $\alpha$ , $\beta$ , $\gamma$                | 357.59Å 212.04Å 207.71Å<br>90.00° 125.07° 90.00°   | Depositor        |
| Resolution (Å)  | 41.08 – 5.75<br>41.08 – 5.75   | Depositor<br>EDS |
| % Data completeness<br>(in resolution range)                            | 92.3 (41.08-5.75)<br>92.3 (41.08-5.75)   | Depositor<br>EDS |
| $R_{merge}$   | 0.22   | Depositor        |
| $R_{sym}$   | (Not available)  | Depositor        |
| $\langle I/\sigma(I) \rangle$ <sup>1</sup>                              | 2.57 (at 5.72Å)  | Xtriage          |
| Refinement program  | PHENIX (1.19.2_4158: ???)  | Depositor        |
| R, $R_{free}$   | 0.242 , 0.292<br>0.239 , 0.286   | Depositor<br>DCC |
| $R_{free}$ test set   | 1551 reflections (4.64%)   | wwPDB-VP         |
| Wilson B-factor (Å <sup>2</sup> )                                       | 213.2  | Xtriage          |
| Anisotropy  | 0.909  | Xtriage          |
| Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> ) | 0.24 , 414.1   | EDS              |
| L-test for twinning <sup>2</sup>  | $\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.21$  | Xtriage          |
| Estimated twinning fraction   | 0.039 for $-1/2^*h+3/2^*k-1, 1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k$<br>0.047 for $1/2^*h-1/2^*k+2^*l, -1/2^*h+1/2^*k, -1/2^*h-1/2^*k-1$<br>0.034 for $-h-k-1, l, k$<br>0.049 for $-h+k-1, -l, -k$<br>0.035 for $-1/2^*h-3/2^*k-1, -1/2^*h+1/2^*k-1, 1/2^*h+1/2^*k$<br>0.030 for $1/2^*h+1/2^*k+2^*l, 1/2^*h+1/2^*k, -1/2^*h+1/2^*k-1$<br>0.048 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$<br>0.035 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$<br>0.327 for $1/2^*h-3/2^*k, -1/2^*h-1/2^*k, -1/2^*h+1/2^*k-1$<br>0.327 for $1/2^*h+3/2^*k, 1/2^*h-1/2^*k, -1/2^*h-1/2^*k-1$<br>0.038 for $-h-2^*l, -k, l$ | Xtriage          |
| $F_o, F_c$ correlation  | 0.88   | EDS              |
| Total number of atoms   | 29645  | wwPDB-VP         |
| Average B, all atoms (Å <sup>2</sup> )                                  | 359.0  | wwPDB-VP         |

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% of the height of the origin peak. No significant pseudotranslation is detected.*

## 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: BMA, MAN, NAG

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   | B     | 0.24         | 0/983   | 0.44        | 0/1332         |
| 1   | H     | 0.23         | 0/979   | 0.45        | 0/1327         |
| 1   | a     | 0.24         | 0/983   | 0.45        | 0/1332         |
| 2   | D     | 0.27         | 0/1871  | 0.51        | 0/2552         |
| 2   | L     | 0.28         | 0/1871  | 0.52        | 0/2552         |
| 2   | b     | 0.25         | 0/1871  | 0.51        | 0/2552         |
| 3   | C     | 0.25         | 0/1622  | 0.50        | 1/2215 (0.0%)  |
| 3   | P     | 0.25         | 0/1638  | 0.51        | 1/2238 (0.0%)  |
| 3   | c     | 0.25         | 0/1638  | 0.50        | 1/2238 (0.0%)  |
| 4   | G     | 0.26         | 0/3546  | 0.52        | 0/4813         |
| 4   | R     | 0.25         | 0/3546  | 0.51        | 0/4813         |
| 4   | e     | 0.25         | 0/3546  | 0.50        | 0/4813         |
| 5   | O     | 0.25         | 0/1055  | 0.52        | 0/1436         |
| 5   | S     | 0.28         | 0/1792  | 0.52        | 0/2445         |
| 5   | f     | 0.26         | 0/1792  | 0.52        | 0/2445         |
| All | All   | 0.26         | 0/28733 | 0.50        | 3/39103 (0.0%) |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|----------|------|------------------------|---------------------|
| 3   | P     | 46  | LEU  | CA-CB-CG | 5.67 | 128.34                 | 115.30              |
| 3   | c     | 46  | LEU  | CA-CB-CG | 5.63 | 128.26                 | 115.30              |
| 3   | C     | 46  | LEU  | CA-CB-CG | 5.36 | 127.63                 | 115.30              |

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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   | B     | 119/164 (73%)   | 114 (96%)  | 5 (4%)   | 0        | 100         | 100 |
| 1   | H     | 118/164 (72%)   | 112 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 1   | a     | 119/164 (73%)   | 113 (95%)  | 6 (5%)   | 0        | 100         | 100 |
| 2   | D     | 232/286 (81%)   | 213 (92%)  | 17 (7%)  | 2 (1%)   | 17          | 56  |
| 2   | L     | 232/286 (81%)   | 210 (90%)  | 18 (8%)  | 4 (2%)   | 9           | 42  |
| 2   | b     | 232/286 (81%)   | 214 (92%)  | 18 (8%)  | 0        | 100         | 100 |
| 3   | C     | 204/214 (95%)   | 193 (95%)  | 10 (5%)  | 1 (0%)   | 29          | 69  |
| 3   | P     | 208/214 (97%)   | 197 (95%)  | 10 (5%)  | 1 (0%)   | 29          | 69  |
| 3   | c     | 208/214 (97%)   | 197 (95%)  | 10 (5%)  | 1 (0%)   | 29          | 69  |
| 4   | G     | 429/490 (88%)   | 405 (94%)  | 23 (5%)  | 1 (0%)   | 47          | 81  |
| 4   | R     | 429/490 (88%)   | 405 (94%)  | 23 (5%)  | 1 (0%)   | 47          | 81  |
| 4   | e     | 429/490 (88%)   | 405 (94%)  | 24 (6%)  | 0        | 100         | 100 |
| 5   | O     | 128/235 (54%)   | 124 (97%)  | 4 (3%)   | 0        | 100         | 100 |
| 5   | S     | 224/235 (95%)   | 216 (96%)  | 8 (4%)   | 0        | 100         | 100 |
| 5   | f     | 224/235 (95%)   | 215 (96%)  | 8 (4%)   | 1 (0%)   | 34          | 72  |
| All | All   | 3535/4167 (85%) | 3333 (94%) | 190 (5%) | 12 (0%)  | 41          | 76  |

5 of 12 Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 160 | VAL  |
| 2   | L     | 241 | VAL  |
| 2   | D     | 241 | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | C     | 152 | ASP  |
| 2   | L     | 162 | CYS  |

### 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 X-ray entries followed by that with respect to entries of similar resolution.

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   | B     | 105/133 (79%)   | 105 (100%) | 0        | 100         | 100 |
| 1   | H     | 105/133 (79%)   | 103 (98%)  | 2 (2%)   | 57          | 75  |
| 1   | a     | 105/133 (79%)   | 104 (99%)  | 1 (1%)   | 76          | 86  |
| 2   | D     | 202/231 (87%)   | 196 (97%)  | 6 (3%)   | 41          | 63  |
| 2   | L     | 202/231 (87%)   | 196 (97%)  | 6 (3%)   | 41          | 63  |
| 2   | b     | 202/231 (87%)   | 196 (97%)  | 6 (3%)   | 41          | 63  |
| 3   | C     | 174/180 (97%)   | 174 (100%) | 0        | 100         | 100 |
| 3   | P     | 176/180 (98%)   | 176 (100%) | 0        | 100         | 100 |
| 3   | c     | 176/180 (98%)   | 176 (100%) | 0        | 100         | 100 |
| 4   | G     | 394/427 (92%)   | 390 (99%)  | 4 (1%)   | 76          | 86  |
| 4   | R     | 394/427 (92%)   | 392 (100%) | 2 (0%)   | 88          | 93  |
| 4   | e     | 394/427 (92%)   | 392 (100%) | 2 (0%)   | 88          | 93  |
| 5   | O     | 112/203 (55%)   | 112 (100%) | 0        | 100         | 100 |
| 5   | S     | 199/203 (98%)   | 197 (99%)  | 2 (1%)   | 76          | 86  |
| 5   | f     | 199/203 (98%)   | 199 (100%) | 0        | 100         | 100 |
| All | All   | 3139/3522 (89%) | 3108 (99%) | 31 (1%)  | 76          | 86  |

5 of 31 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | L     | 110 | ARG  |
| 2   | b     | 223 | CYS  |
| 2   | L     | 231 | CYS  |
| 4   | e     | 54  | CYS  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 2   | b     | 97  | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | P     | 170 | ASN  |
| 4   | R     | 105 | HIS  |
| 4   | e     | 105 | HIS  |

### 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](#)

89 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 |
| 6   | NAG  | A     | 1   | 6,4  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.33 | 0        |
| 6   | NAG  | A     | 2   | 6    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.51 | 0        |
| 6   | BMA  | A     | 3   | 6    | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 0.95 | 1 (6%)   |
| 6   | MAN  | A     | 4   | 6    | 11,11,12     | 0.59 | 0        | 15,15,17    | 1.00 | 2 (13%)  |
| 6   | MAN  | A     | 5   | 6    | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 1.47 | 3 (20%)  |
| 7   | NAG  | F     | 1   | 2,7  | 14,14,15     | 0.17 | 0        | 17,19,21    | 0.40 | 0        |
| 7   | NAG  | F     | 2   | 7    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.55 | 0        |
| 8   | NAG  | I     | 1   | 8,4  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.45 | 0        |
| 8   | NAG  | I     | 2   | 8    | 14,14,15     | 0.24 | 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   | BMA  | I     | 3   | 8    | 11,11,12     | 0.67 | 0        | 15,15,17    | 0.74 | 0        |
| 8   | NAG  | J     | 1   | 8,4  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.48 | 0        |
| 8   | NAG  | J     | 2   | 8    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.42 | 0        |
| 8   | BMA  | J     | 3   | 8    | 11,11,12     | 0.66 | 0        | 15,15,17    | 0.78 | 0        |
| 7   | NAG  | K     | 1   | 4,7  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.44 | 0        |
| 7   | NAG  | K     | 2   | 7    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.45 | 0        |
| 7   | NAG  | M     | 1   | 4,7  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.40 | 0        |
| 7   | NAG  | M     | 2   | 7    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.50 | 0        |
| 9   | NAG  | N     | 1   | 9,4  | 14,14,15     | 0.73 | 1 (7%)   | 17,19,21    | 1.40 | 2 (11%)  |
| 9   | MAN  | N     | 10  | 9    | 11,11,12     | 0.94 | 0        | 15,15,17    | 1.17 | 2 (13%)  |
| 9   | NAG  | N     | 2   | 9    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.41 | 0        |
| 9   | BMA  | N     | 3   | 9    | 11,11,12     | 1.04 | 0        | 15,15,17    | 0.99 | 1 (6%)   |
| 9   | MAN  | N     | 4   | 9    | 11,11,12     | 1.06 | 1 (9%)   | 15,15,17    | 1.35 | 2 (13%)  |
| 9   | MAN  | N     | 5   | 9    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.12 | 2 (13%)  |
| 9   | MAN  | N     | 6   | 9    | 11,11,12     | 0.78 | 0        | 15,15,17    | 0.98 | 2 (13%)  |
| 9   | MAN  | N     | 7   | 9    | 11,11,12     | 0.80 | 0        | 15,15,17    | 1.01 | 2 (13%)  |
| 9   | MAN  | N     | 8   | 9    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.18 | 2 (13%)  |
| 9   | MAN  | N     | 9   | 9    | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 7   | NAG  | T     | 1   | 4,7  | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.53 | 0        |
| 7   | NAG  | T     | 2   | 7    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.41 | 0        |
| 7   | NAG  | U     | 1   | 4,7  | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.48 | 0        |
| 7   | NAG  | U     | 2   | 7    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.45 | 0        |
| 10  | NAG  | V     | 1   | 10,4 | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.33 | 0        |
| 10  | NAG  | V     | 2   | 10   | 14,14,15     | 0.52 | 0        | 17,19,21    | 0.60 | 0        |
| 10  | BMA  | V     | 3   | 10   | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 1.03 | 1 (6%)   |
| 10  | MAN  | V     | 4   | 10   | 11,11,12     | 0.70 | 0        | 15,15,17    | 2.78 | 4 (26%)  |
| 7   | NAG  | W     | 1   | 4,7  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.59 | 0        |
| 7   | NAG  | W     | 2   | 7    | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.58 | 0        |
| 7   | NAG  | X     | 1   | 2,7  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.40 | 0        |
| 7   | NAG  | X     | 2   | 7    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.55 | 0        |
| 8   | NAG  | Y     | 1   | 8,4  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.46 | 0        |
| 8   | NAG  | Y     | 2   | 8    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.43 | 0        |
| 8   | BMA  | Y     | 3   | 8    | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.75 | 0        |
| 8   | NAG  | Z     | 1   | 8,4  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.49 | 0        |
| 8   | NAG  | Z     | 2   | 8    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.43 | 0        |
| 8   | BMA  | Z     | 3   | 8    | 11,11,12     | 0.68 | 0        | 15,15,17    | 0.80 | 0        |
| 7   | NAG  | g     | 1   | 4,7  | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.45 | 0        |
| 7   | NAG  | g     | 2   | 7    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.44 | 0        |
| 7   | NAG  | h     | 1   | 4,7  | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.39 | 0        |
| 7   | NAG  | h     | 2   | 7    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.49 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | NAG  | i     | 1   | 9,4  | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 1.40 | 2 (11%)  |
| 9   | MAN  | i     | 10  | 9    | 11,11,12     | 0.89 | 0        | 15,15,17    | 1.15 | 1 (6%)   |
| 9   | NAG  | i     | 2   | 9    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.41 | 0        |
| 9   | BMA  | i     | 3   | 9    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.02 | 1 (6%)   |
| 9   | MAN  | i     | 4   | 9    | 11,11,12     | 1.07 | 1 (9%)   | 15,15,17    | 1.37 | 2 (13%)  |
| 9   | MAN  | i     | 5   | 9    | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 9   | MAN  | i     | 6   | 9    | 11,11,12     | 0.78 | 0        | 15,15,17    | 0.97 | 2 (13%)  |
| 9   | MAN  | i     | 7   | 9    | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.00 | 2 (13%)  |
| 9   | MAN  | i     | 8   | 9    | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.13 | 2 (13%)  |
| 9   | MAN  | i     | 9   | 9    | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 7   | NAG  | j     | 1   | 4,7  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.48 | 0        |
| 7   | NAG  | j     | 2   | 7    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.40 | 0        |
| 10  | NAG  | k     | 1   | 10,4 | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.36 | 0        |
| 10  | NAG  | k     | 2   | 10   | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.58 | 0        |
| 10  | BMA  | k     | 3   | 10   | 11,11,12     | 0.68 | 0        | 15,15,17    | 0.76 | 0        |
| 10  | MAN  | k     | 4   | 10   | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.57 | 4 (26%)  |
| 7   | NAG  | l     | 1   | 2,7  | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.41 | 0        |
| 7   | NAG  | l     | 2   | 7    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.54 | 0        |
| 8   | NAG  | m     | 1   | 8    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.45 | 0        |
| 8   | NAG  | m     | 2   | 8    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.40 | 0        |
| 8   | BMA  | m     | 3   | 8    | 11,11,12     | 0.64 | 0        | 15,15,17    | 0.73 | 0        |
| 8   | NAG  | n     | 1   | 8,4  | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.45 | 0        |
| 8   | NAG  | n     | 2   | 8    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.42 | 0        |
| 8   | BMA  | n     | 3   | 8    | 11,11,12     | 0.63 | 0        | 15,15,17    | 0.76 | 0        |
| 7   | NAG  | o     | 1   | 4,7  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.48 | 0        |
| 7   | NAG  | o     | 2   | 7    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.47 | 0        |
| 7   | NAG  | p     | 1   | 4,7  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.41 | 0        |
| 7   | NAG  | p     | 2   | 7    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.50 | 0        |
| 9   | NAG  | q     | 1   | 9,4  | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 1.43 | 2 (11%)  |
| 9   | MAN  | q     | 10  | 9    | 11,11,12     | 0.90 | 0        | 15,15,17    | 1.15 | 1 (6%)   |
| 9   | NAG  | q     | 2   | 9    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.38 | 0        |
| 9   | BMA  | q     | 3   | 9    | 11,11,12     | 0.97 | 0        | 15,15,17    | 0.98 | 1 (6%)   |
| 9   | MAN  | q     | 4   | 9    | 11,11,12     | 1.08 | 1 (9%)   | 15,15,17    | 1.36 | 4 (26%)  |
| 9   | MAN  | q     | 5   | 9    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.19 | 2 (13%)  |
| 9   | MAN  | q     | 6   | 9    | 11,11,12     | 0.79 | 0        | 15,15,17    | 0.98 | 2 (13%)  |
| 9   | MAN  | q     | 7   | 9    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.02 | 2 (13%)  |
| 9   | MAN  | q     | 8   | 9    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.06 | 1 (6%)   |
| 9   | MAN  | q     | 9   | 9    | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.30 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | NAG  | r     | 1   | 4,7  | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.47 | 0        |
| 7   | NAG  | r     | 2   | 7    | 14,14,15     | 0.34 | 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. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 6   | NAG  | A     | 1   | 6,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | A     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | A     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | MAN  | A     | 4   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | MAN  | A     | 5   | 6    | -       | 2/2/19/22 | 1/1/1/1 |
| 7   | NAG  | F     | 1   | 2,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | F     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | I     | 1   | 8,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | I     | 2   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | I     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | J     | 1   | 8,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | J     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | J     | 3   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | K     | 1   | 4,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | K     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | N     | 1   | 9,4  | -       | 5/6/23/26 | 0/1/1/1 |
| 9   | MAN  | N     | 10  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | N     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | N     | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 5   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | N     | 9   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | T     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | T     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | U     | 1   | 4,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | U     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 10  | NAG  | V     | 1   | 10,4 | -       | 1/6/23/26 | 0/1/1/1 |
| 10  | NAG  | V     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | BMA  | V     | 3   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | V     | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | W     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | W     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | X     | 1   | 2,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | X     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | Y     | 1   | 8,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | Y     | 2   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | Y     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | Z     | 1   | 8,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | Z     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | Z     | 3   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | g     | 1   | 4,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | g     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | h     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | h     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | i     | 1   | 9,4  | -       | 5/6/23/26 | 0/1/1/1 |
| 9   | MAN  | i     | 10  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | i     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | i     | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 5   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | i     | 9   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | j     | 1   | 4,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | j     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | NAG  | k     | 1   | 10,4 | -       | 1/6/23/26 | 0/1/1/1 |
| 10  | NAG  | k     | 2   | 10   | -       | 1/6/23/26 | 0/1/1/1 |
| 10  | BMA  | k     | 3   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | k     | 4   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | l     | 1   | 2,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | l     | 2   | 7    | -       | 3/6/23/26 | 0/1/1/1 |
| 8   | NAG  | m     | 1   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | m     | 2   | 8    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | BMA  | m     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | n     | 1   | 8,4  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | n     | 2   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | n     | 3   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | o     | 1   | 4,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | o     | 2   | 7    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | p     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | p     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | q     | 1   | 9,4  | -       | 4/6/23/26 | 0/1/1/1 |
| 9   | MAN  | q     | 10  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | q     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | q     | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 5   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | q     | 9   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | r     | 1   | 4,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | r     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |

The worst 5 of 10 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | N     | 4   | MAN  | C1-C2 | 3.10  | 1.59        | 1.52     |
| 9   | i     | 4   | MAN  | C1-C2 | 3.10  | 1.59        | 1.52     |
| 9   | q     | 4   | MAN  | C1-C2 | 2.96  | 1.58        | 1.52     |
| 9   | N     | 1   | NAG  | O5-C1 | -2.59 | 1.39        | 1.43     |
| 9   | q     | 1   | NAG  | O5-C1 | -2.56 | 1.39        | 1.43     |

The worst 5 of 65 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 10  | V     | 4   | MAN  | C1-O5-C5 | 8.41 | 123.59      | 112.19   |
| 10  | V     | 4   | MAN  | O5-C1-C2 | 4.85 | 118.26      | 110.77   |
| 9   | q     | 1   | NAG  | C2-N2-C7 | 4.46 | 129.25      | 122.90   |
| 9   | N     | 1   | NAG  | C2-N2-C7 | 4.40 | 129.16      | 122.90   |
| 9   | i     | 1   | NAG  | C2-N2-C7 | 4.38 | 129.14      | 122.90   |

There are no chirality outliers.

5 of 91 torsion outliers are listed below:

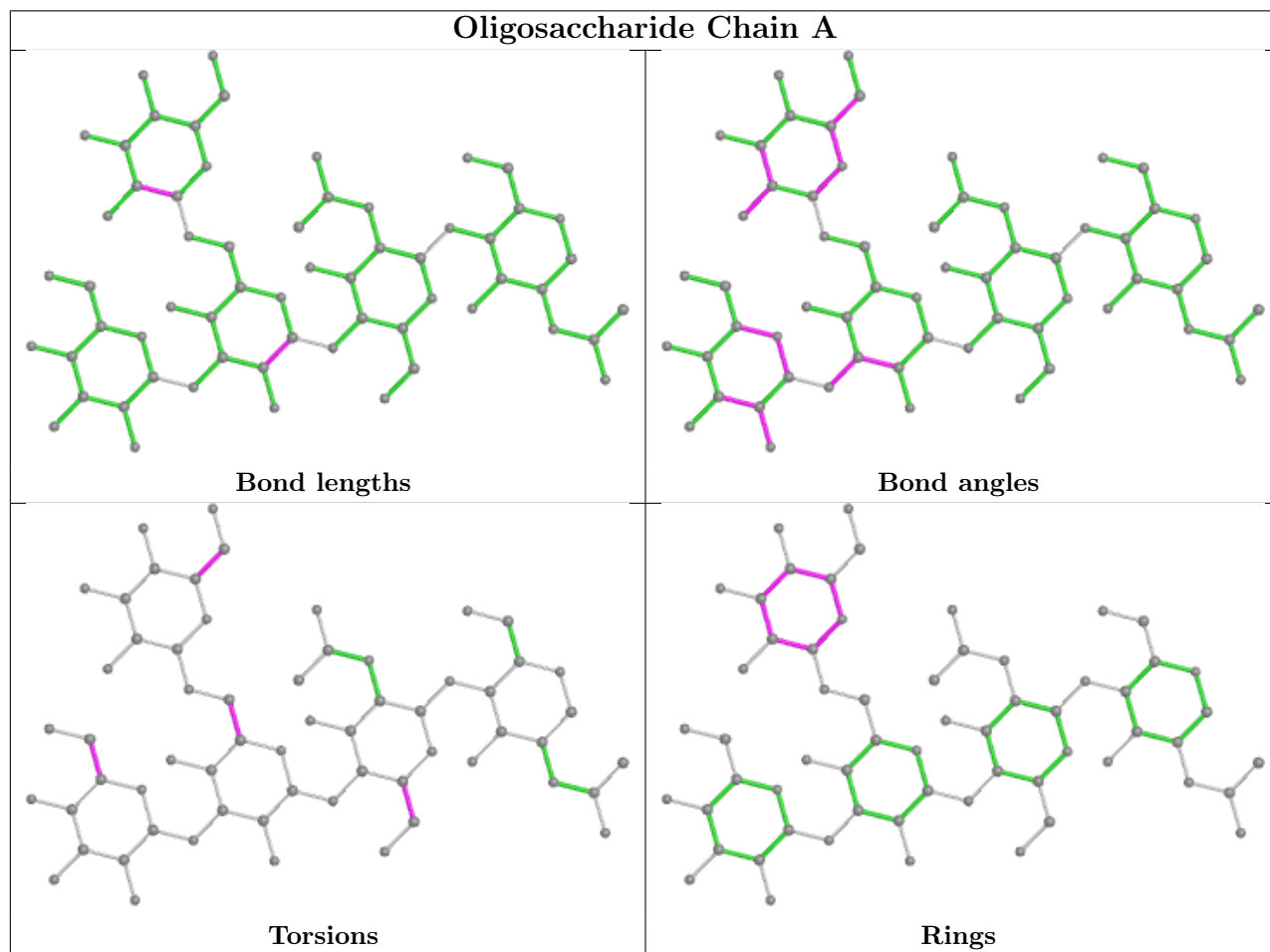
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | J     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | A     | 3   | BMA  | O5-C5-C6-O6 |
| 7   | K     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | g     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | A     | 5   | MAN  | C4-C5-C6-O6 |

All (1) ring outliers are listed below:

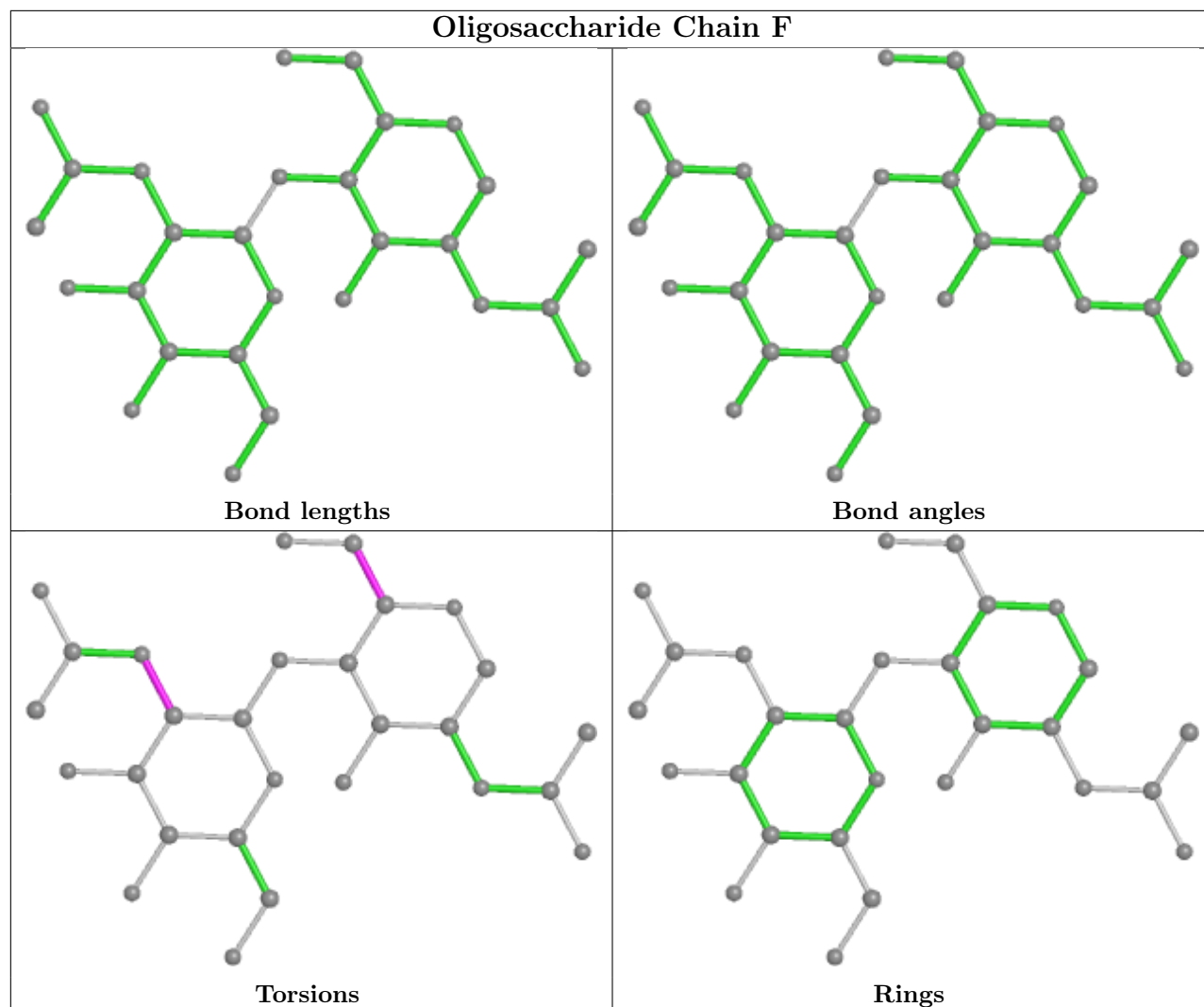
| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 6   | A     | 5   | MAN  | C1-C2-C3-C4-C5-O5 |

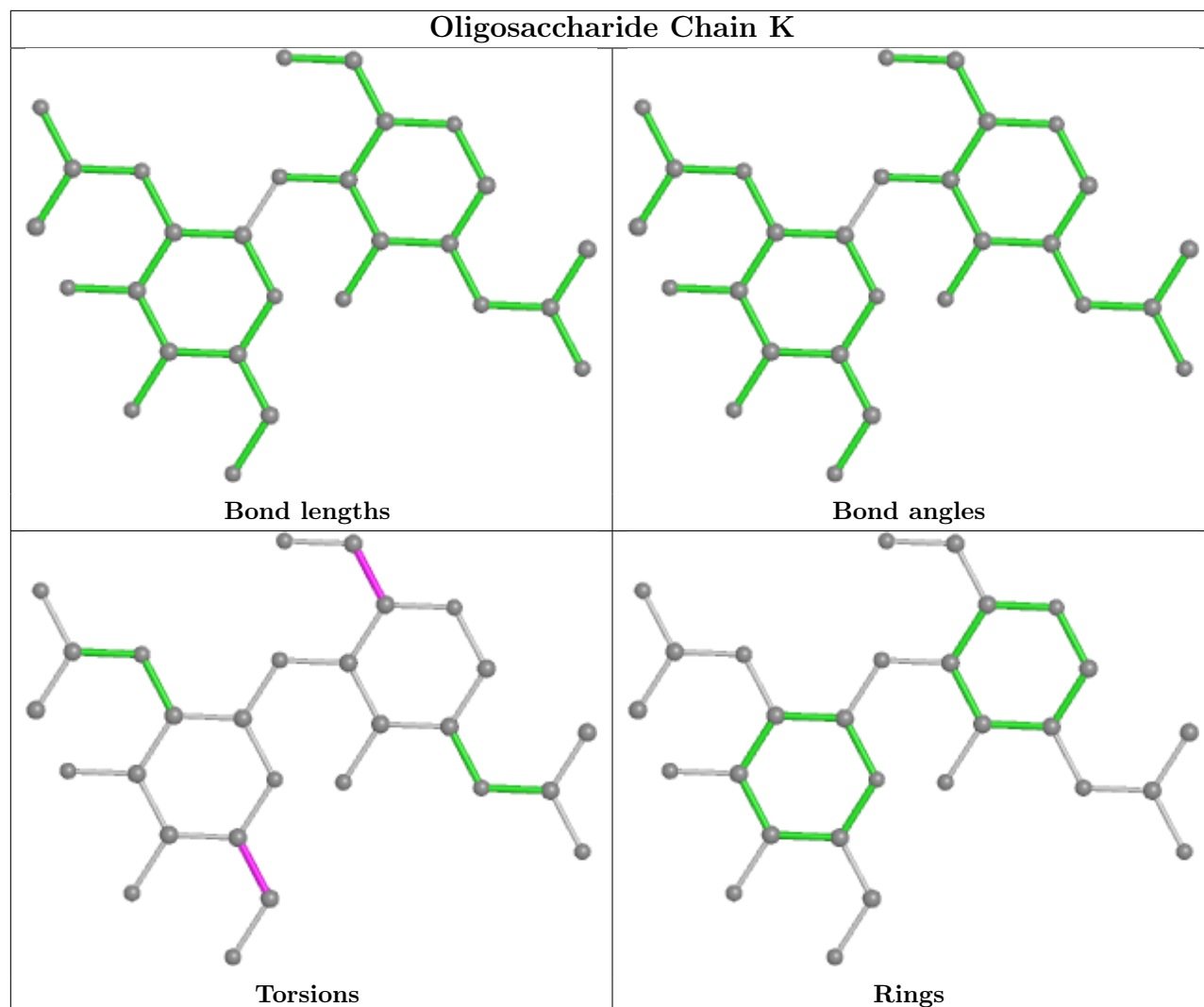
No monomer is involved in short contacts.

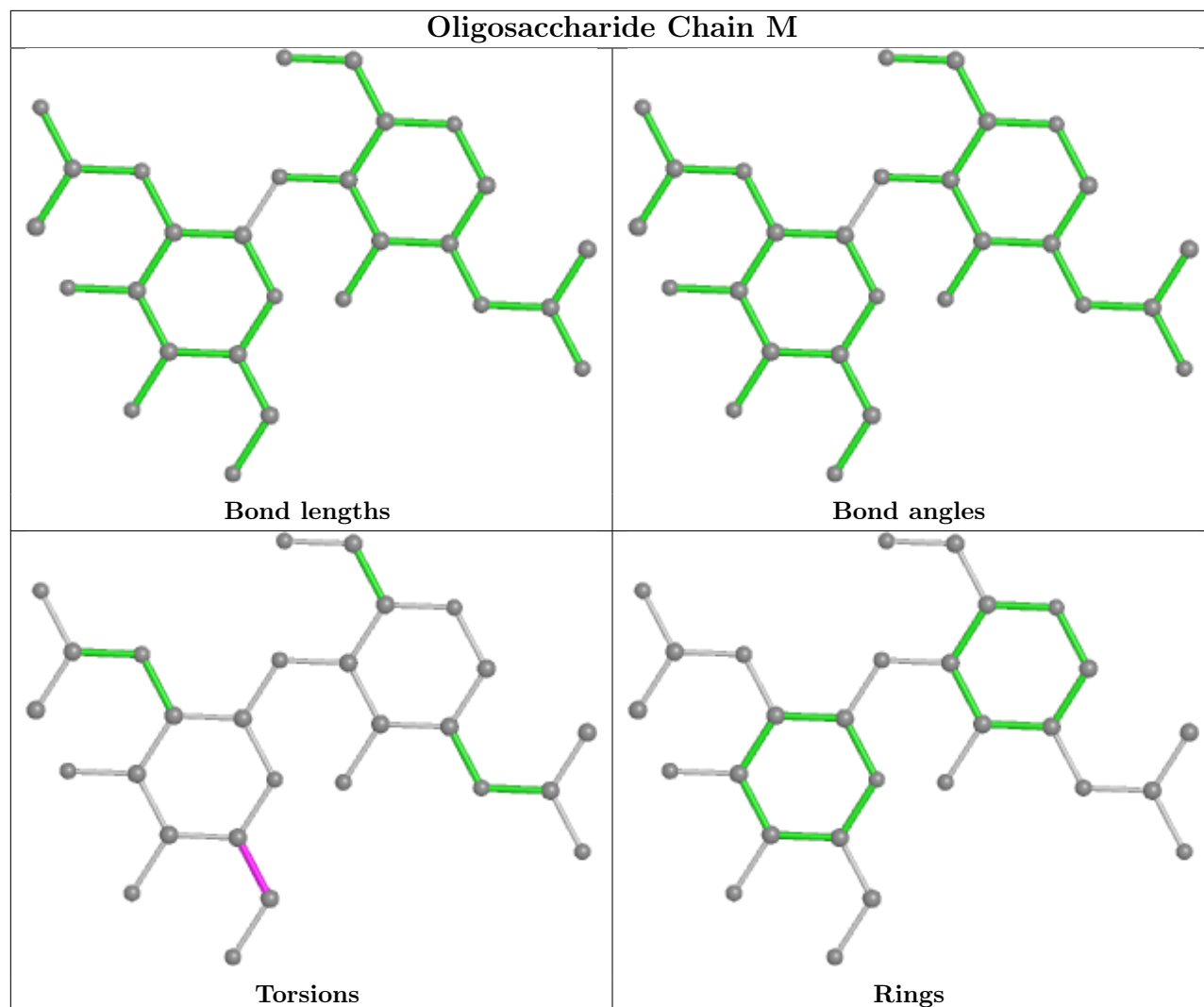
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

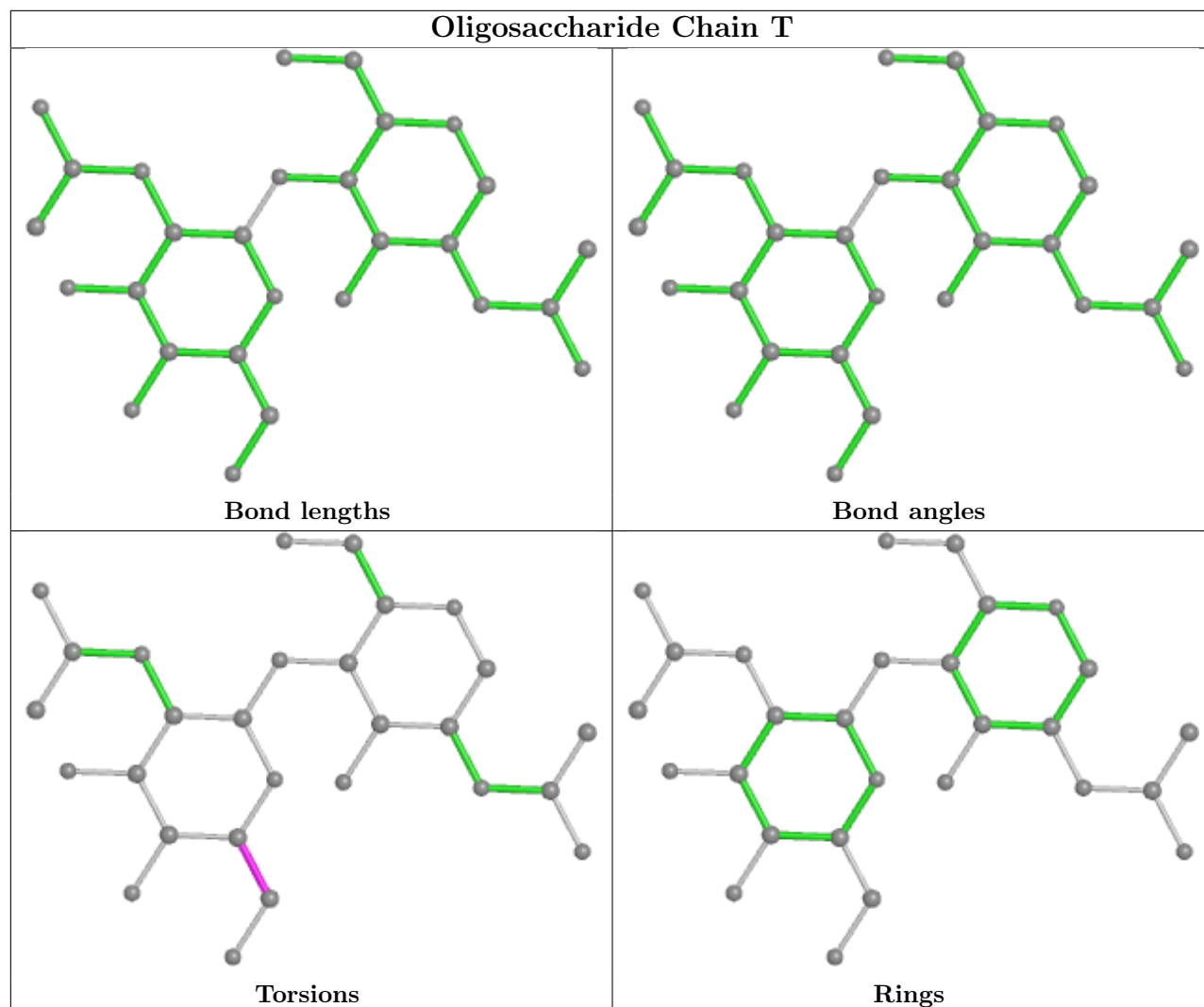


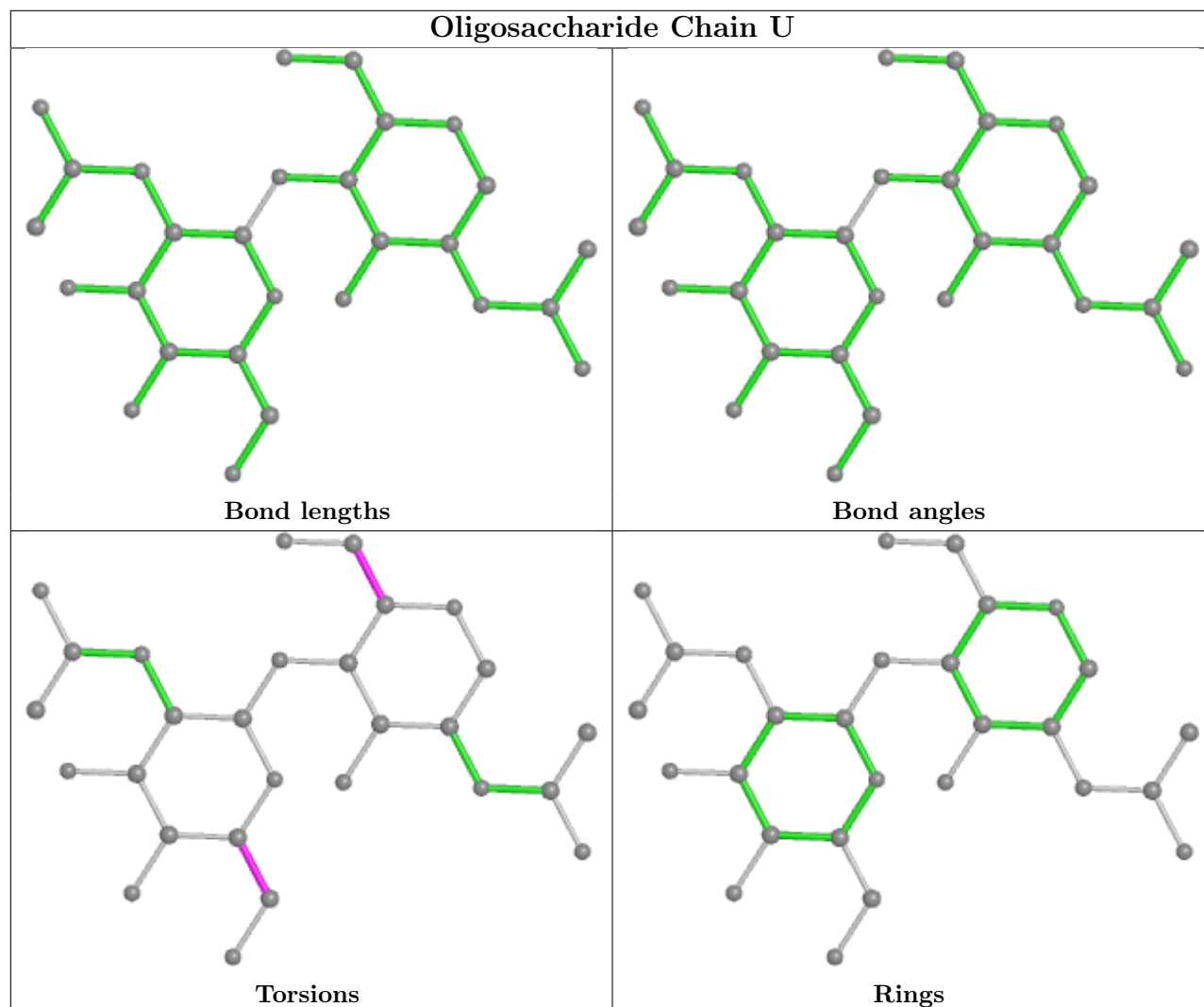


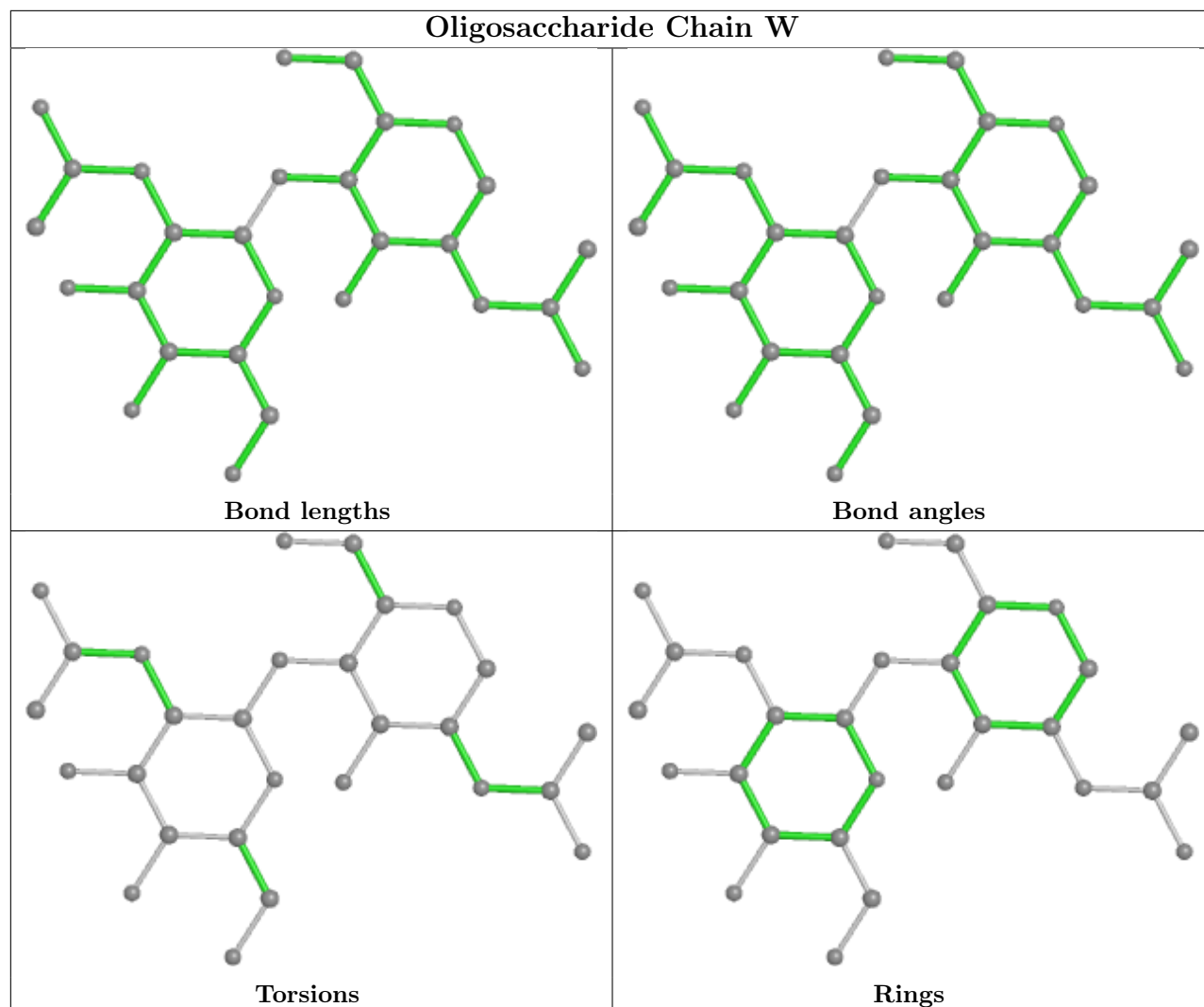


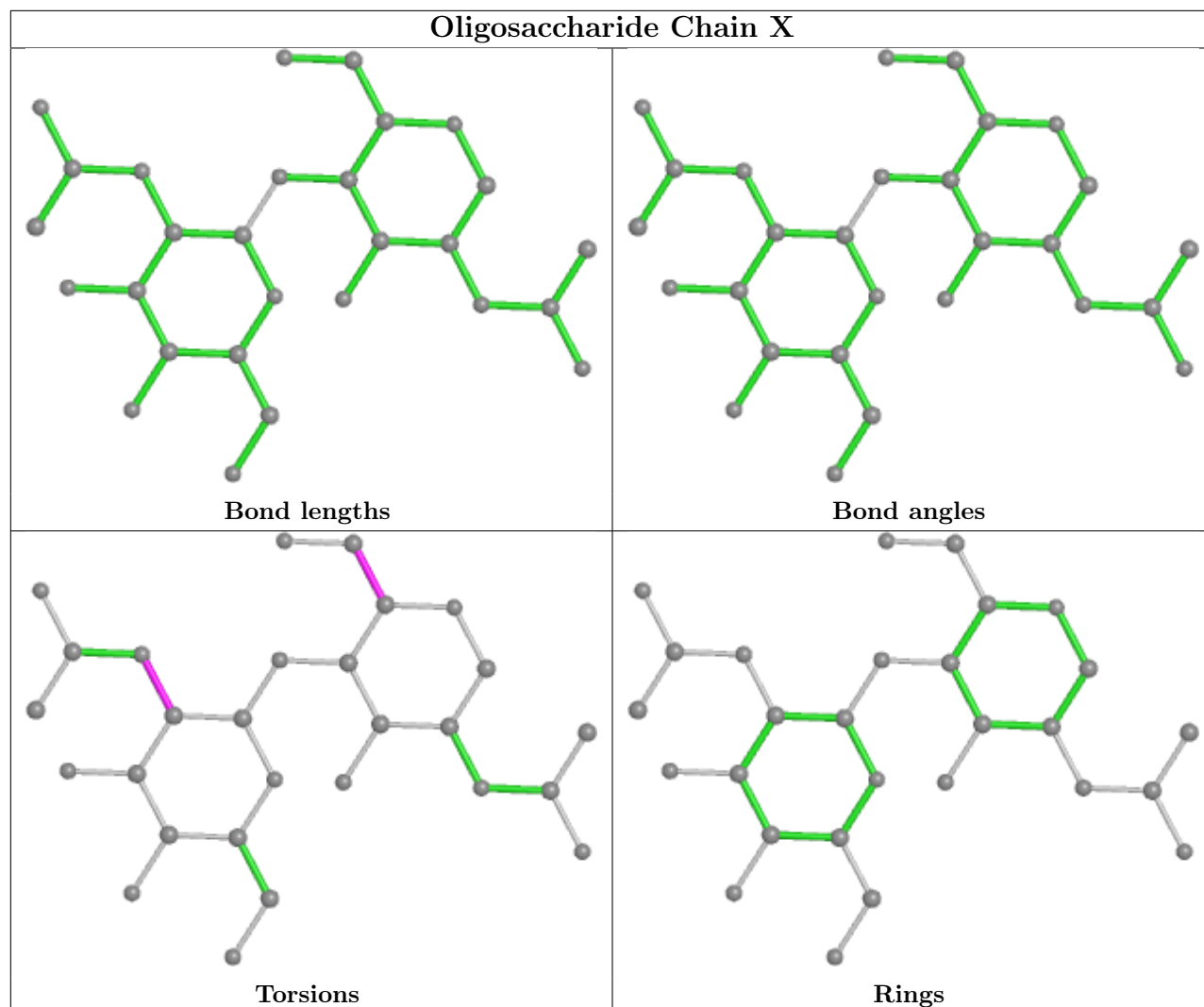


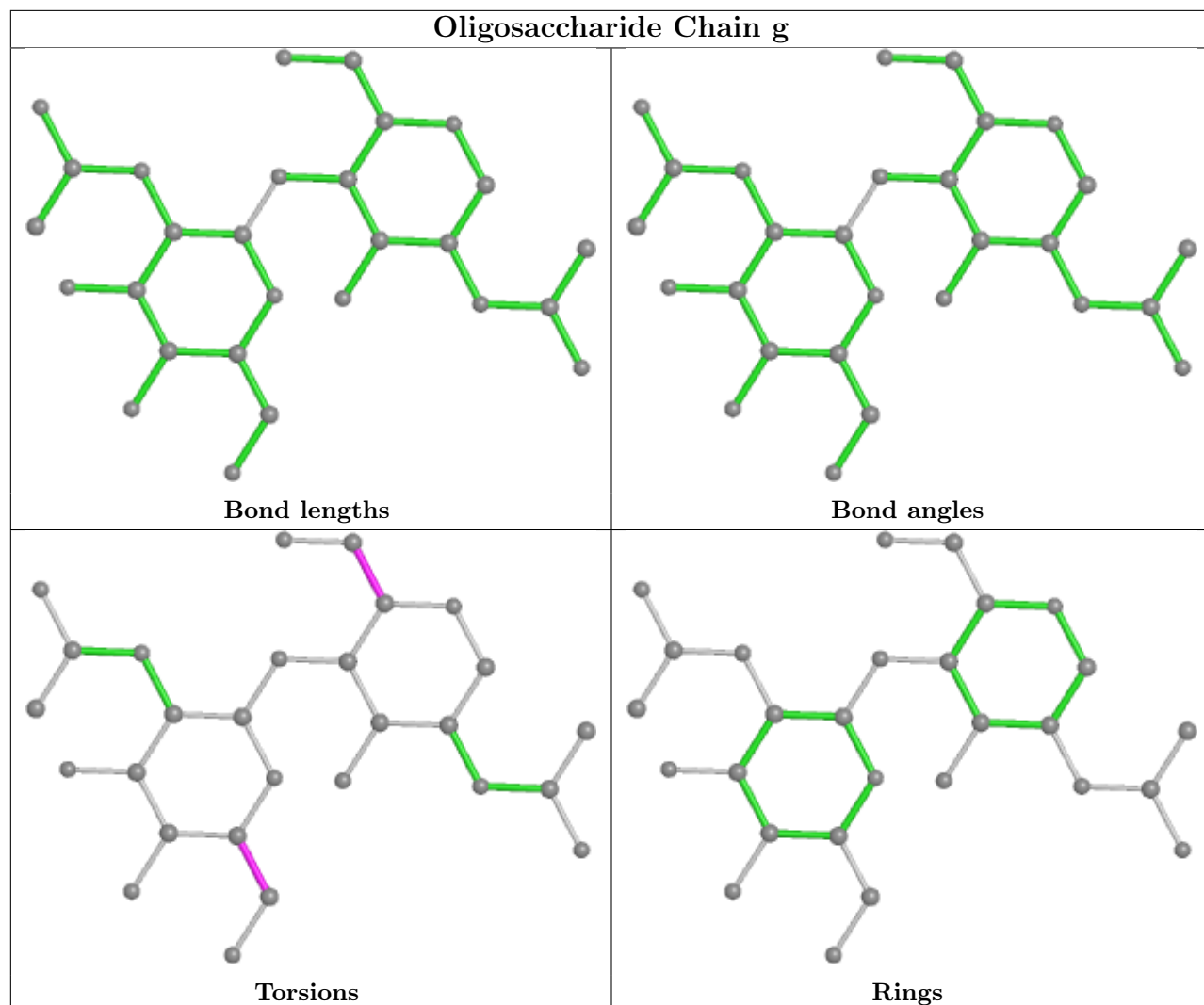




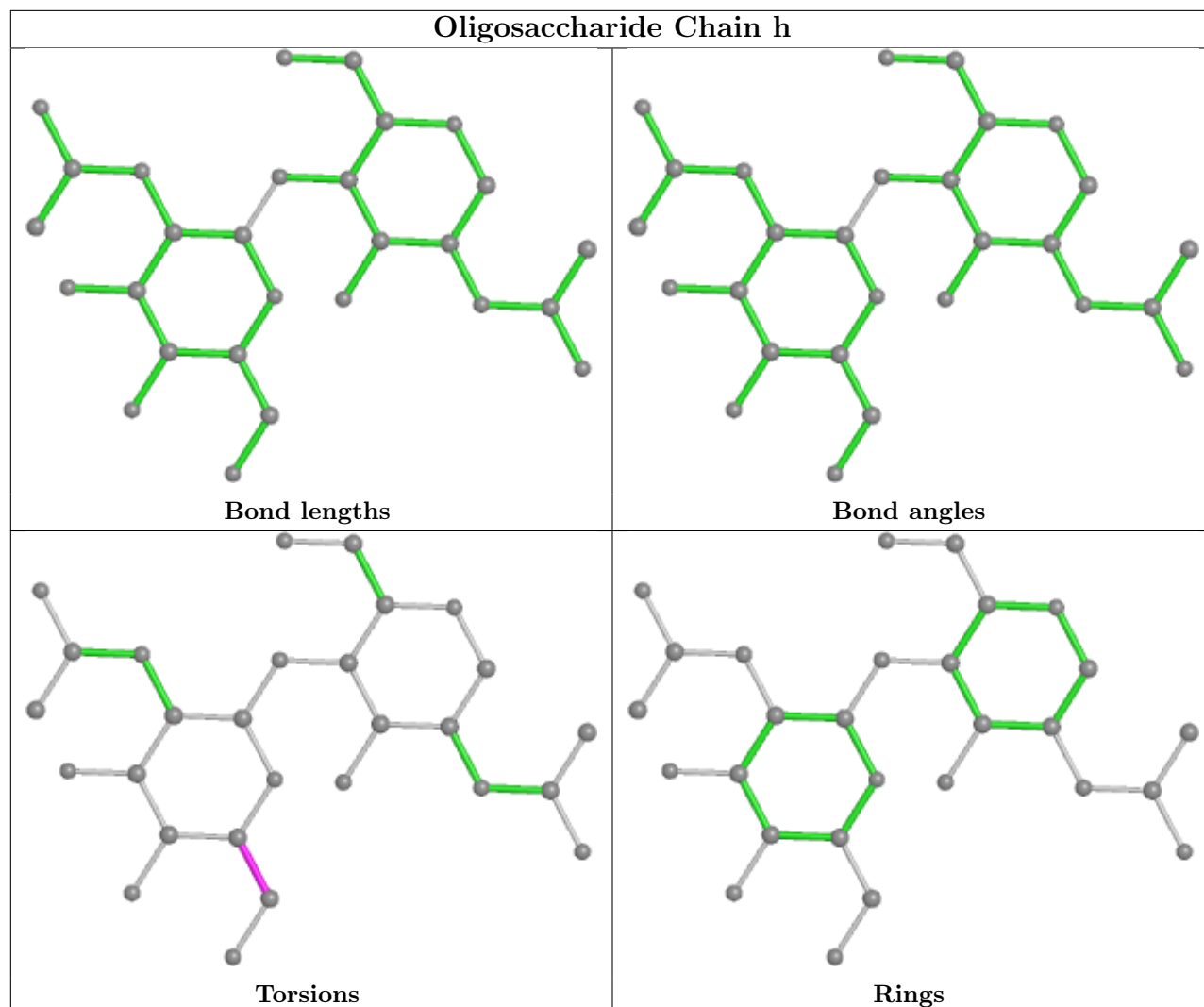


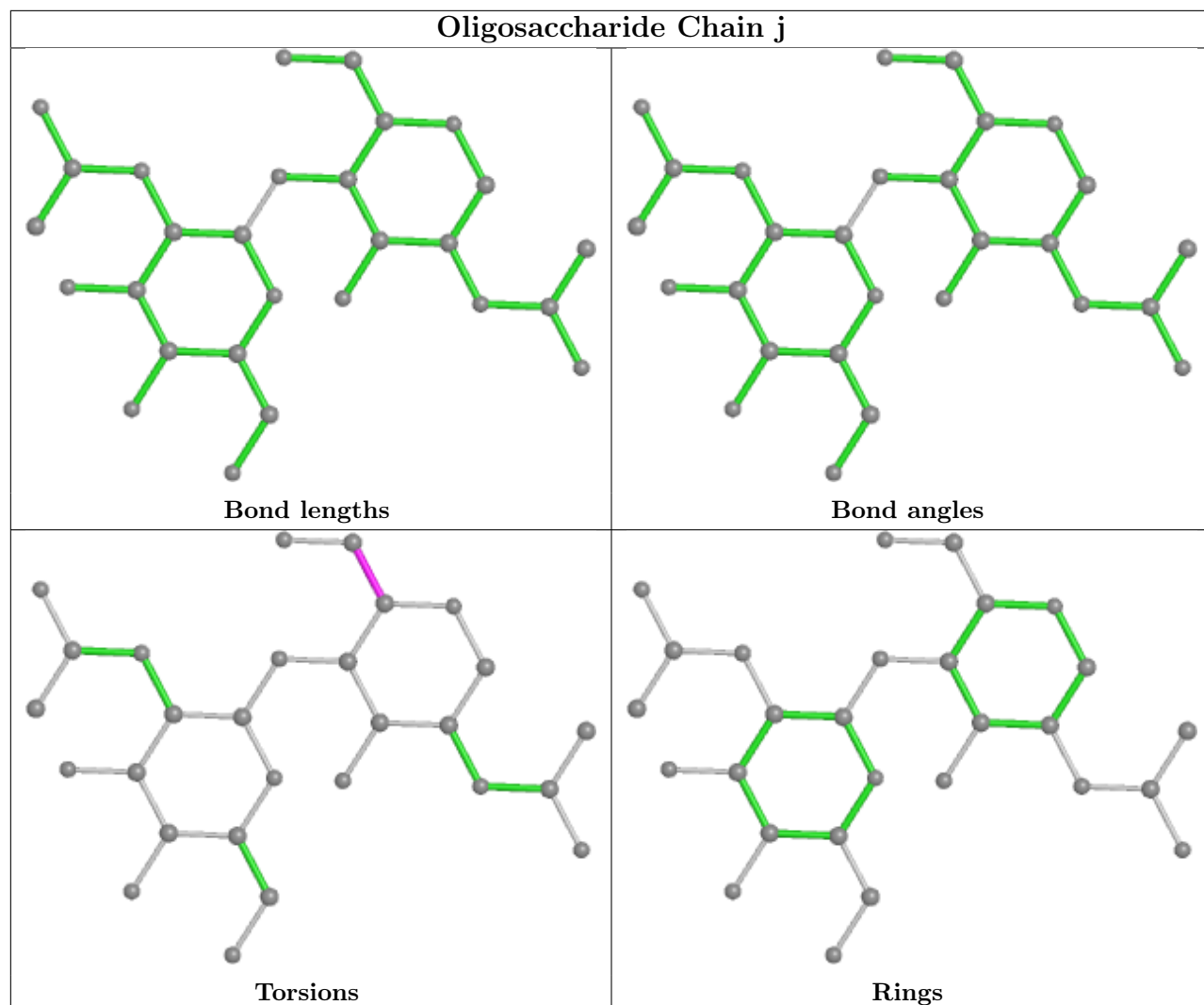


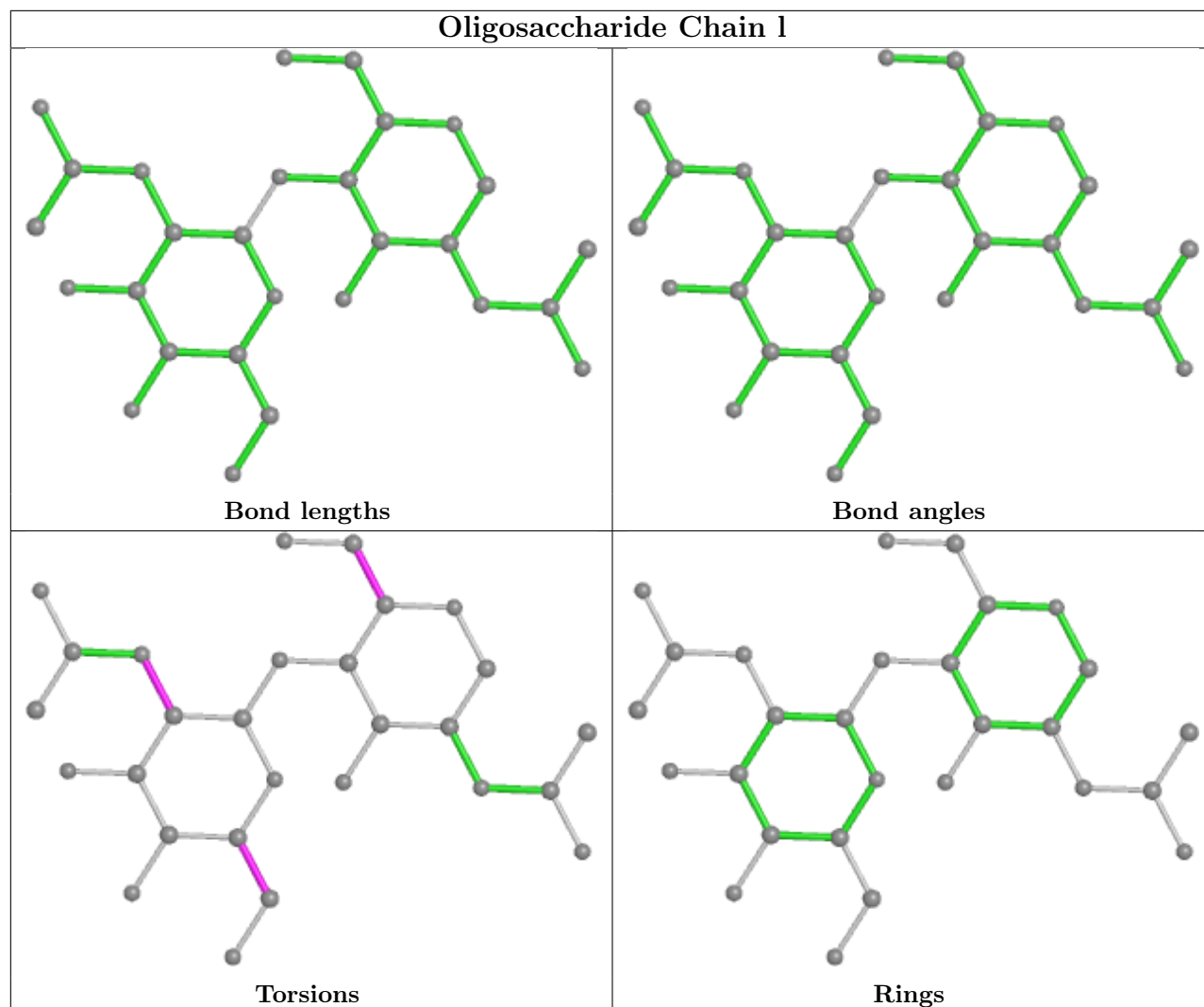


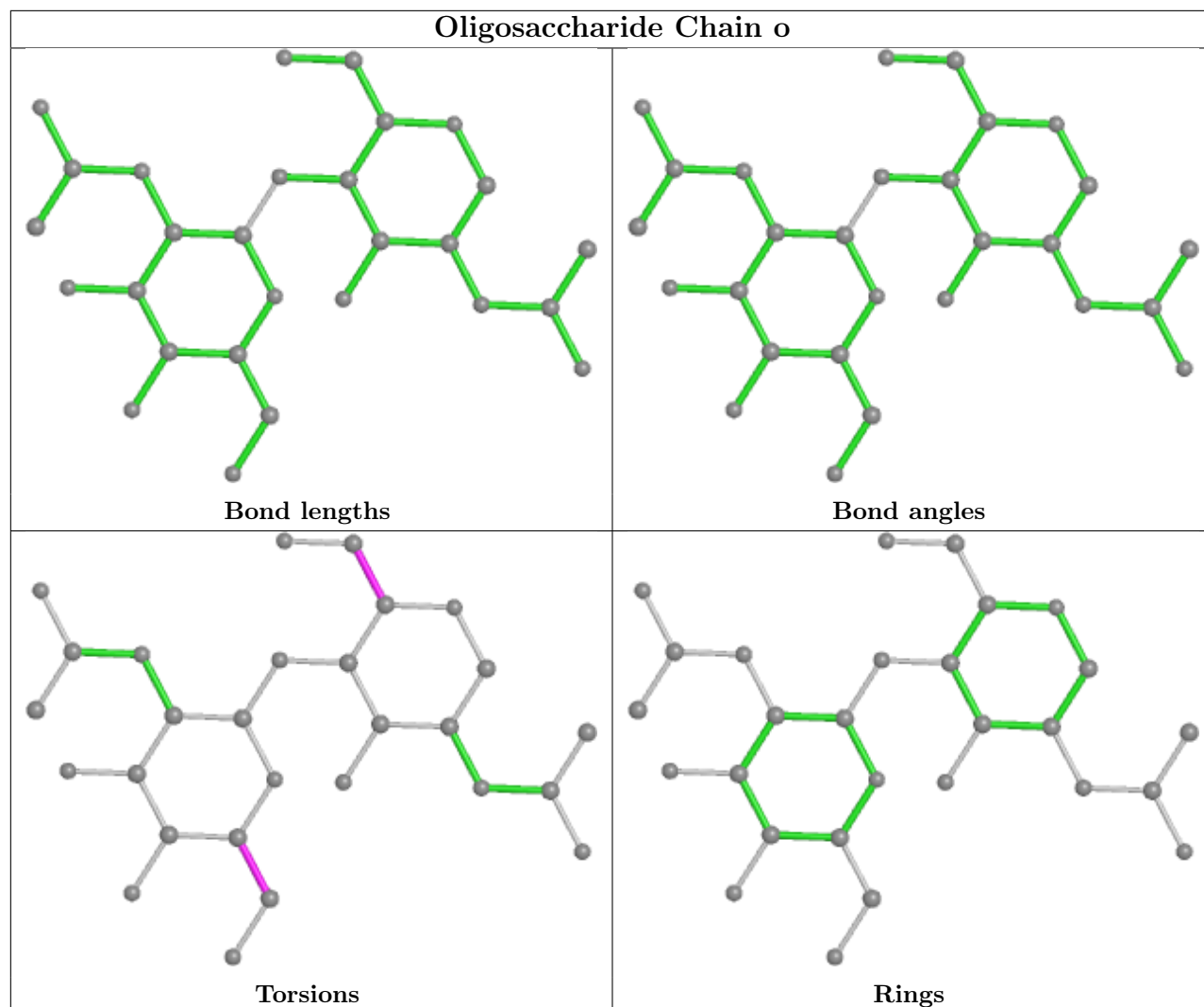


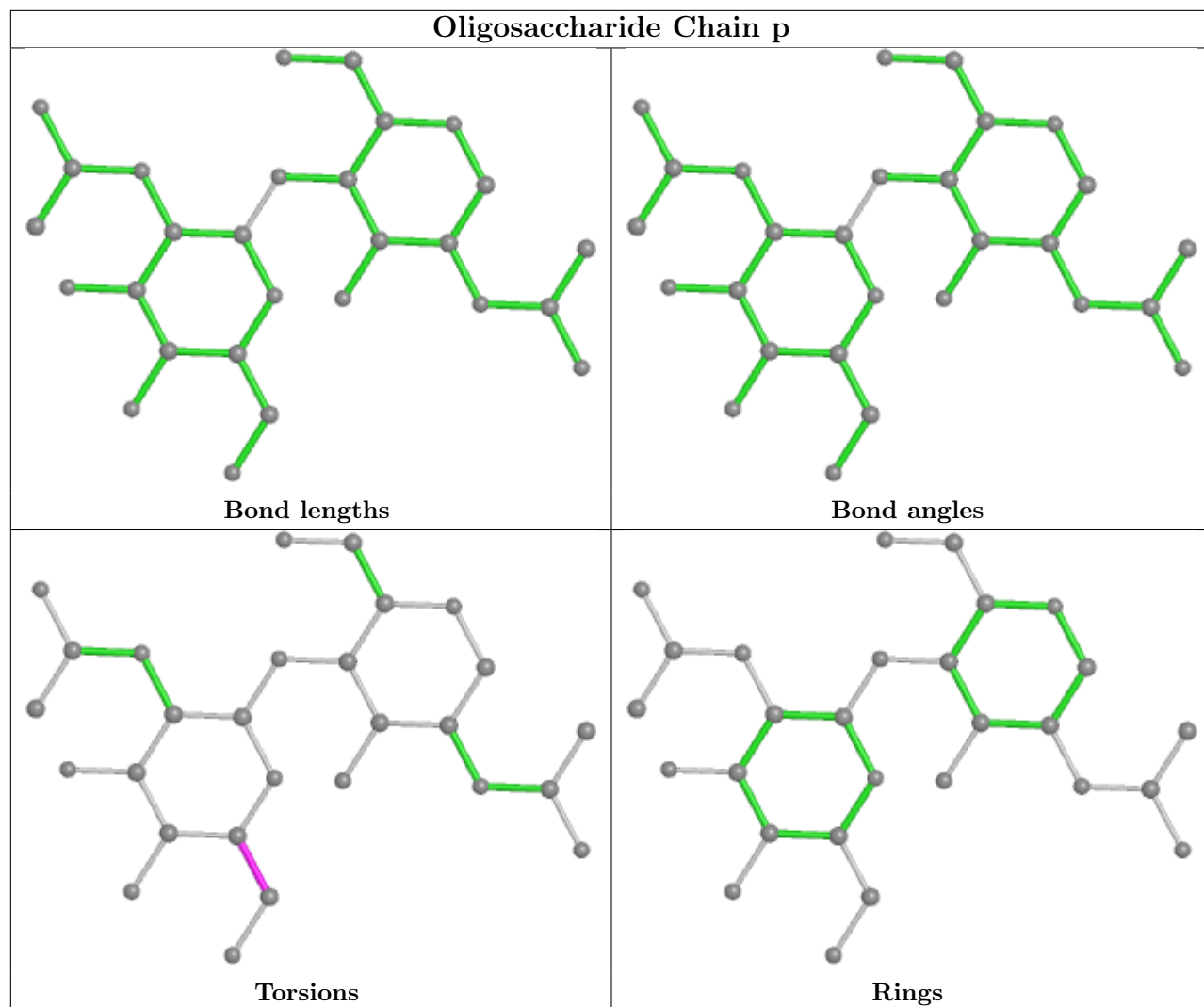


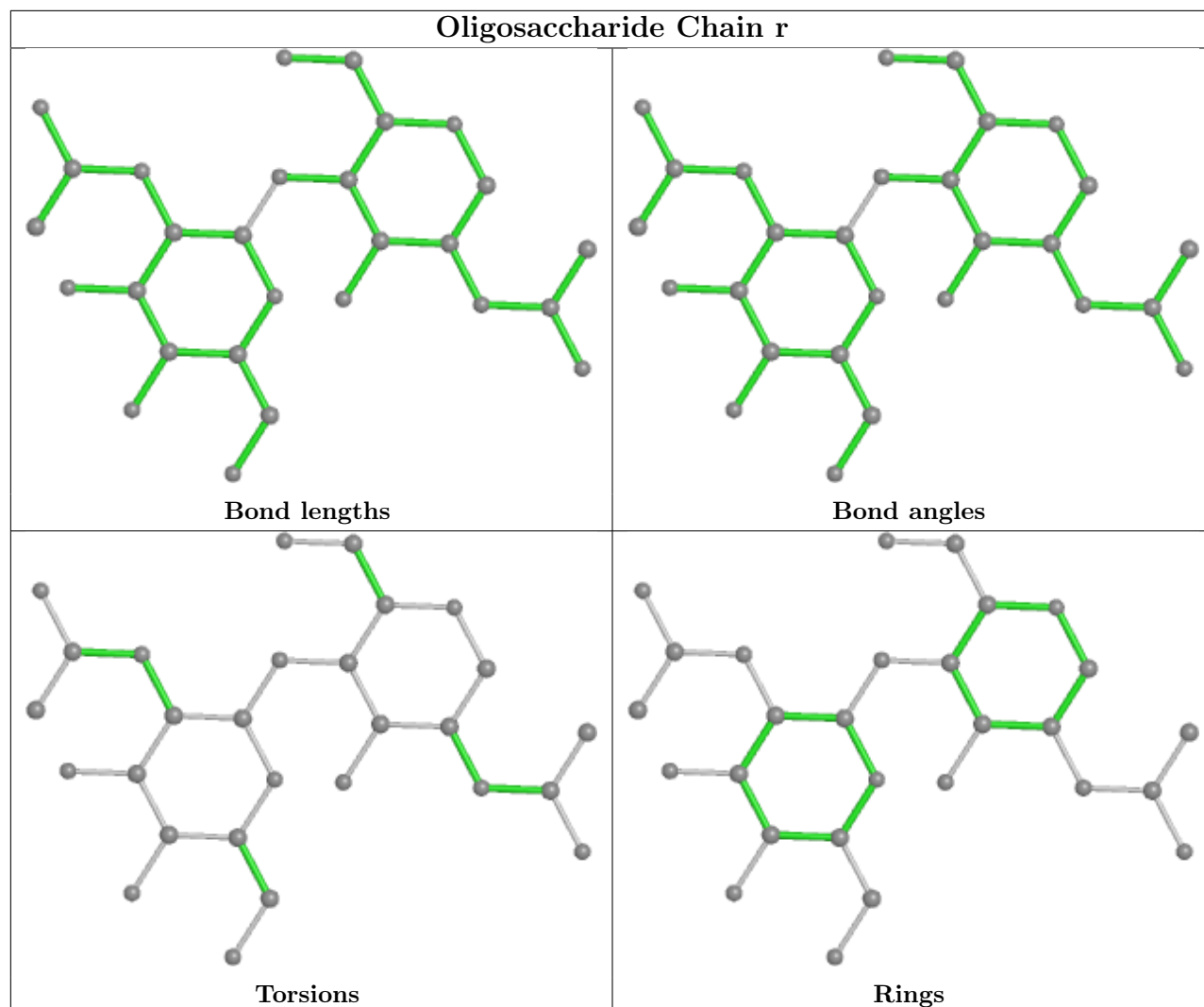


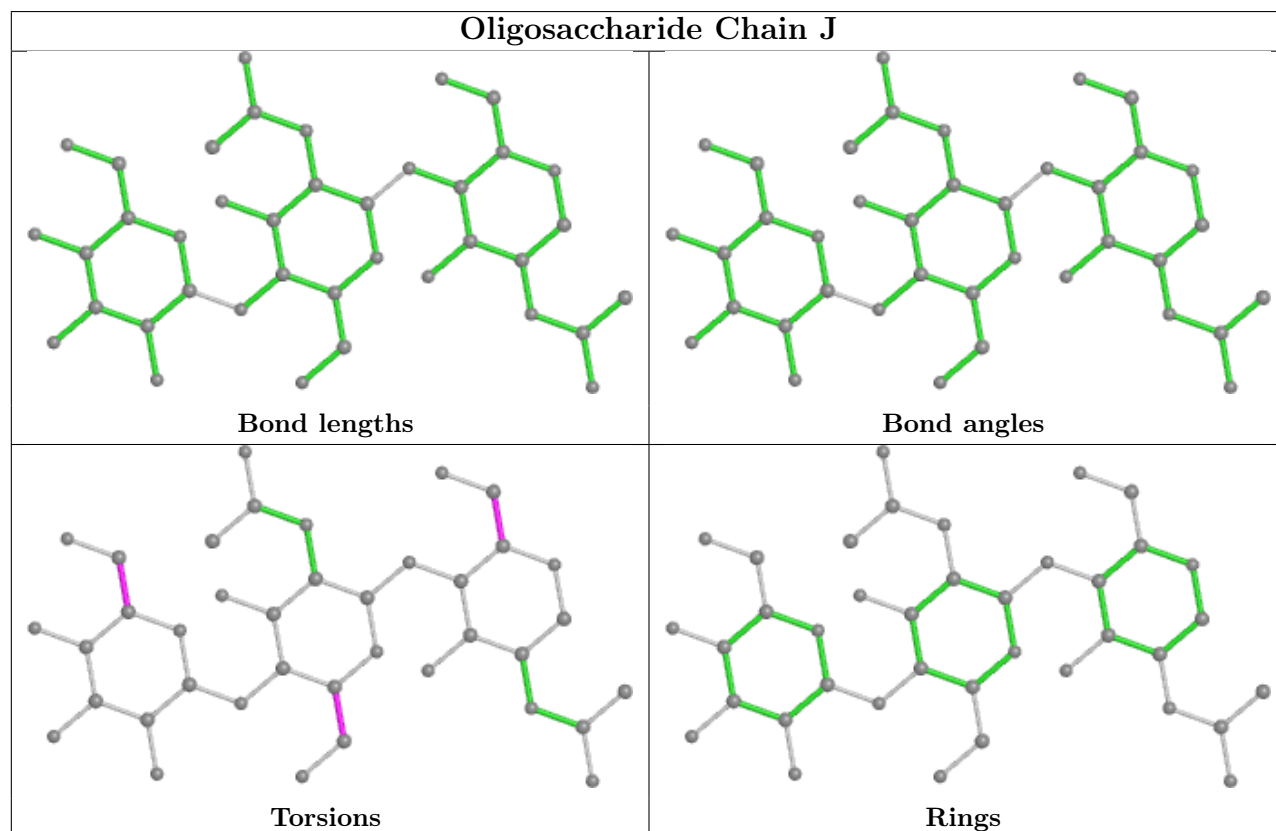
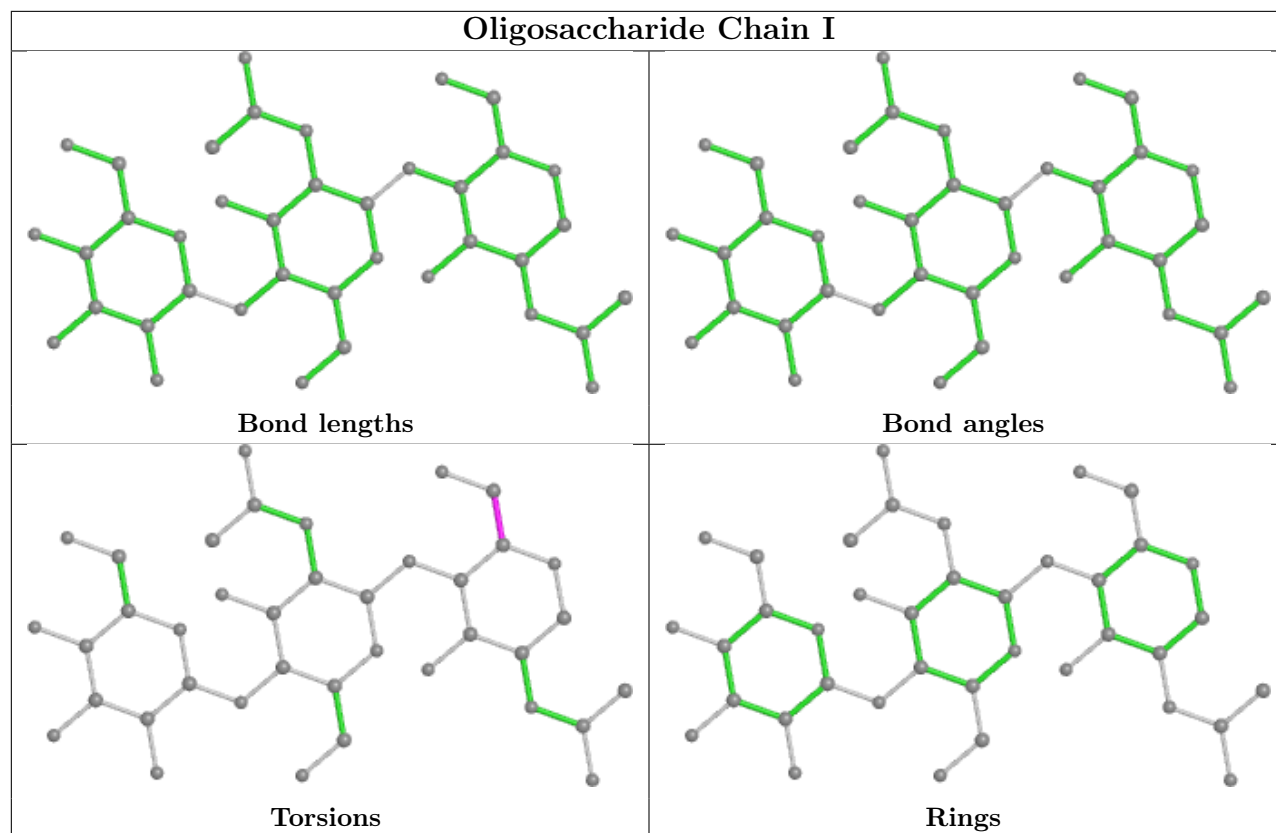


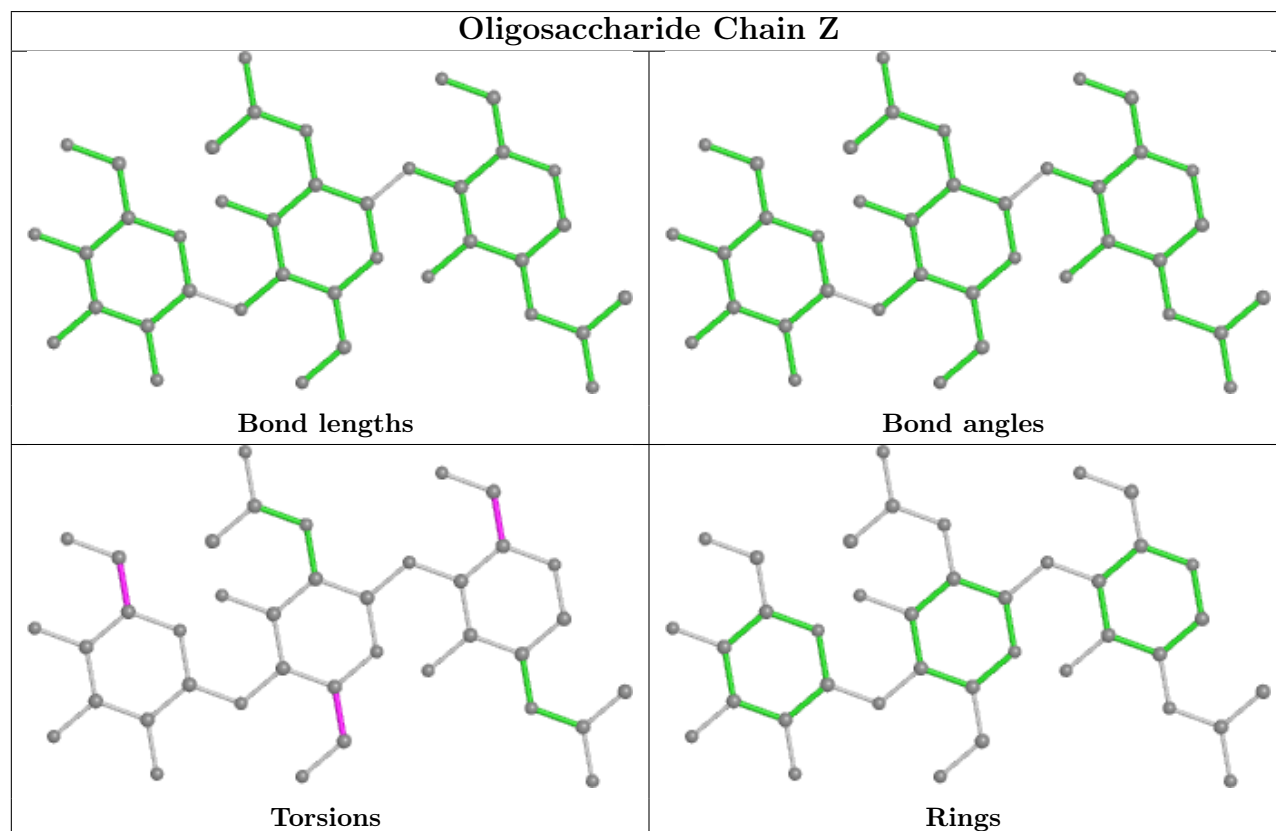
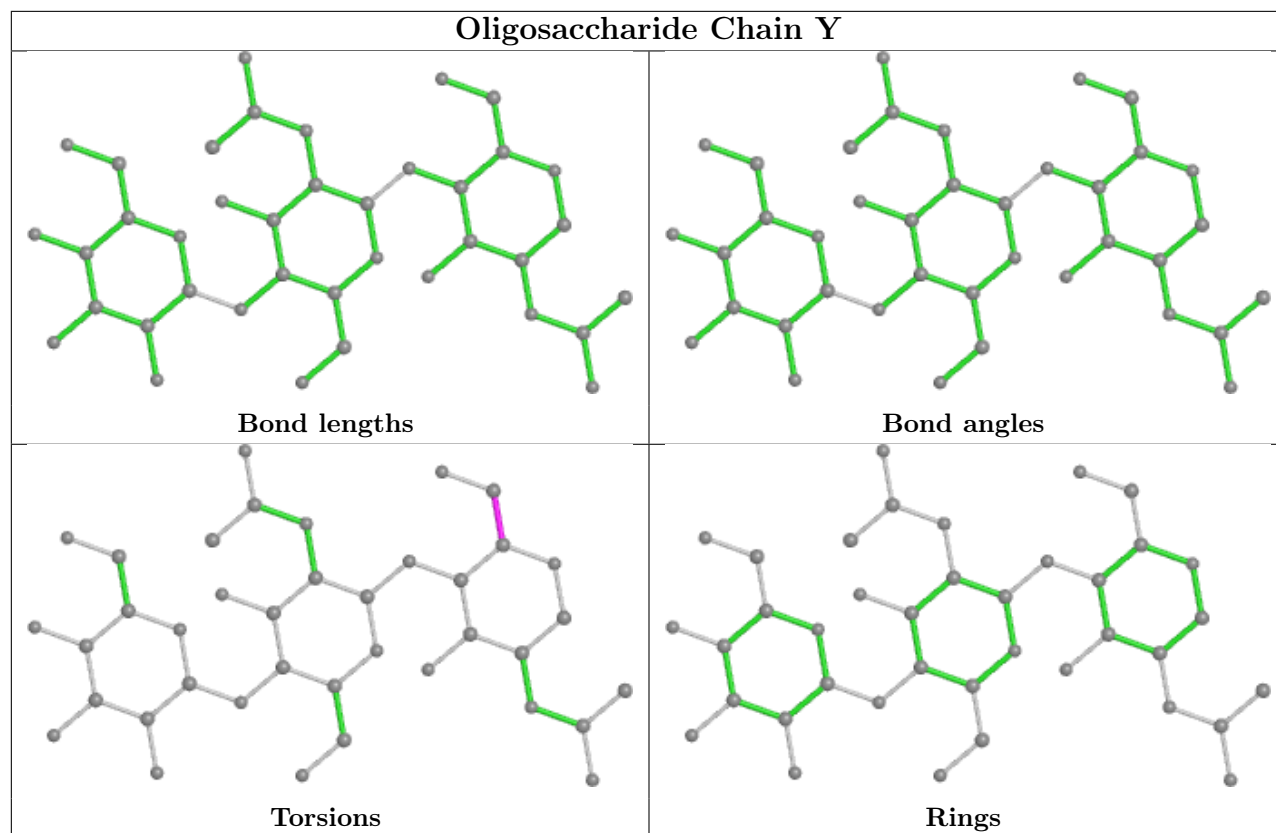




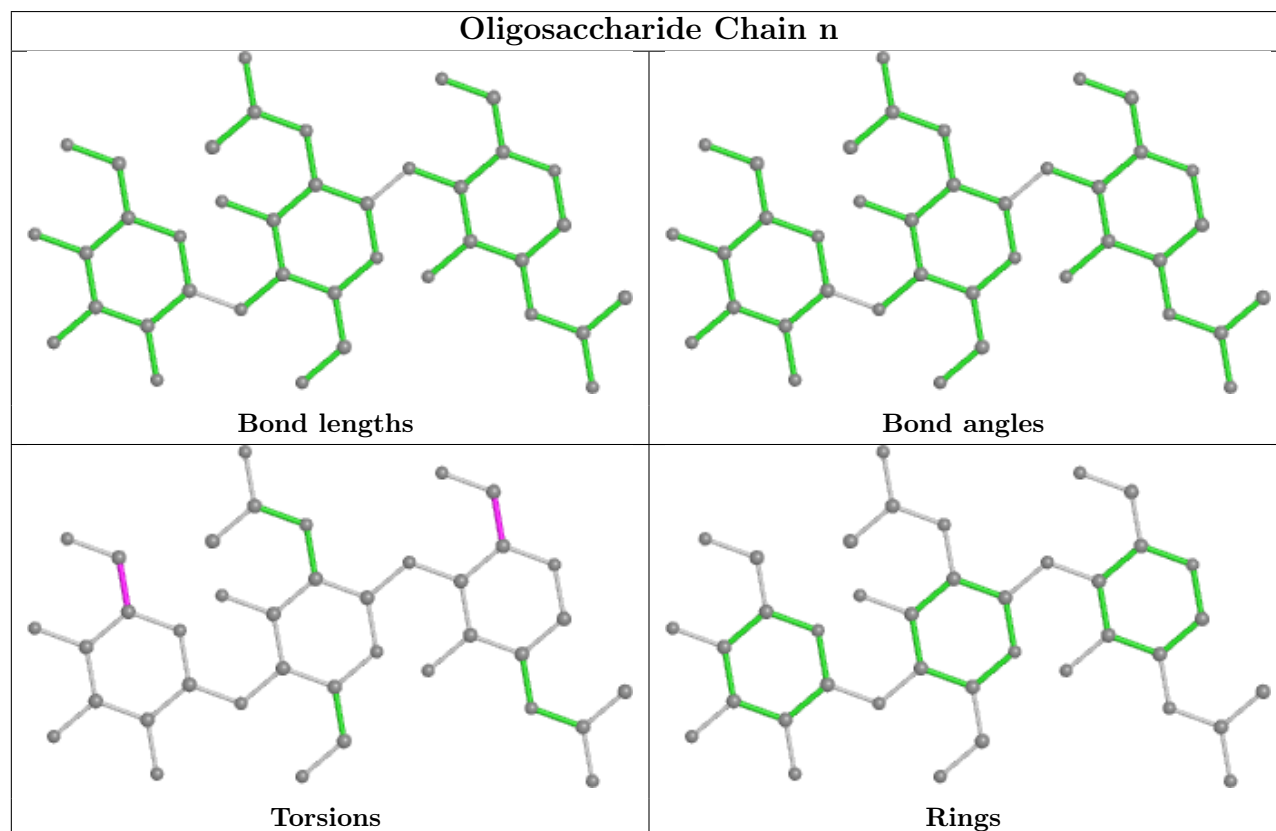
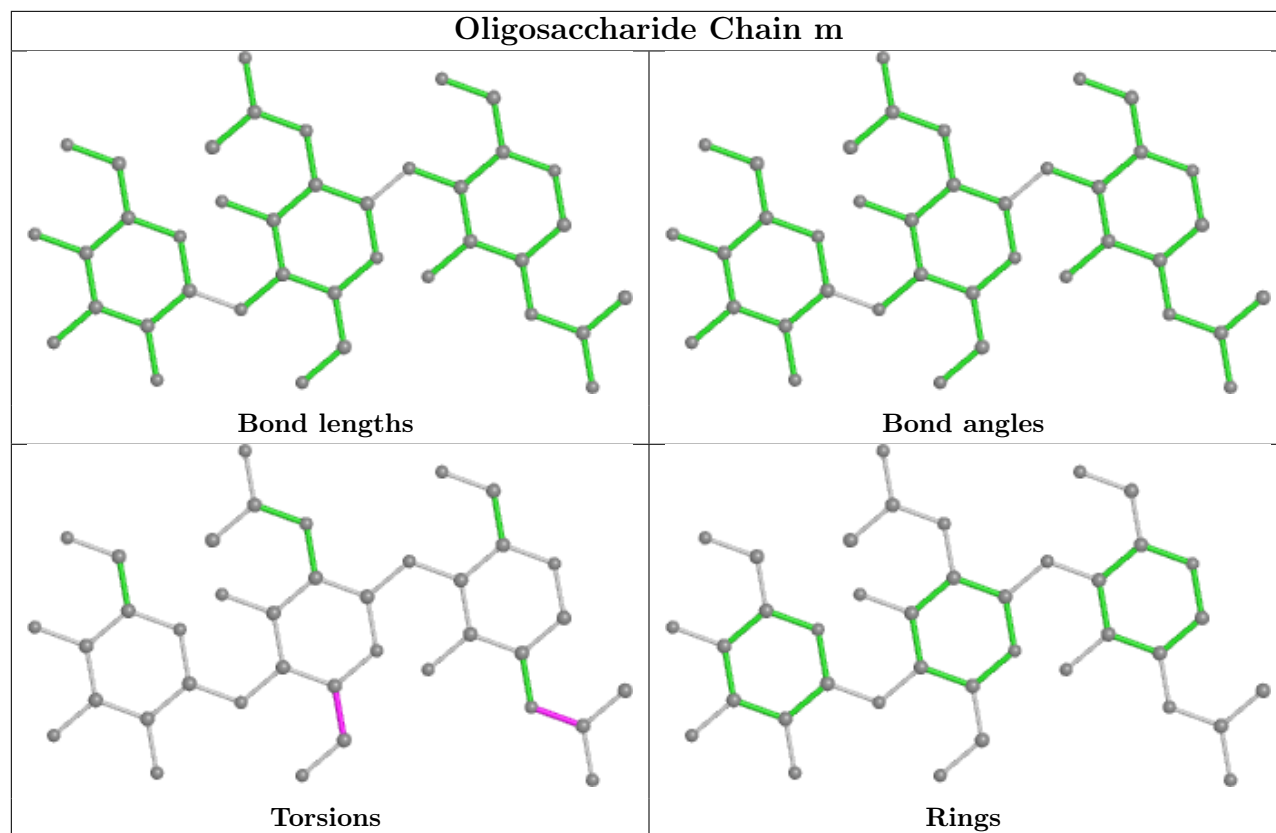


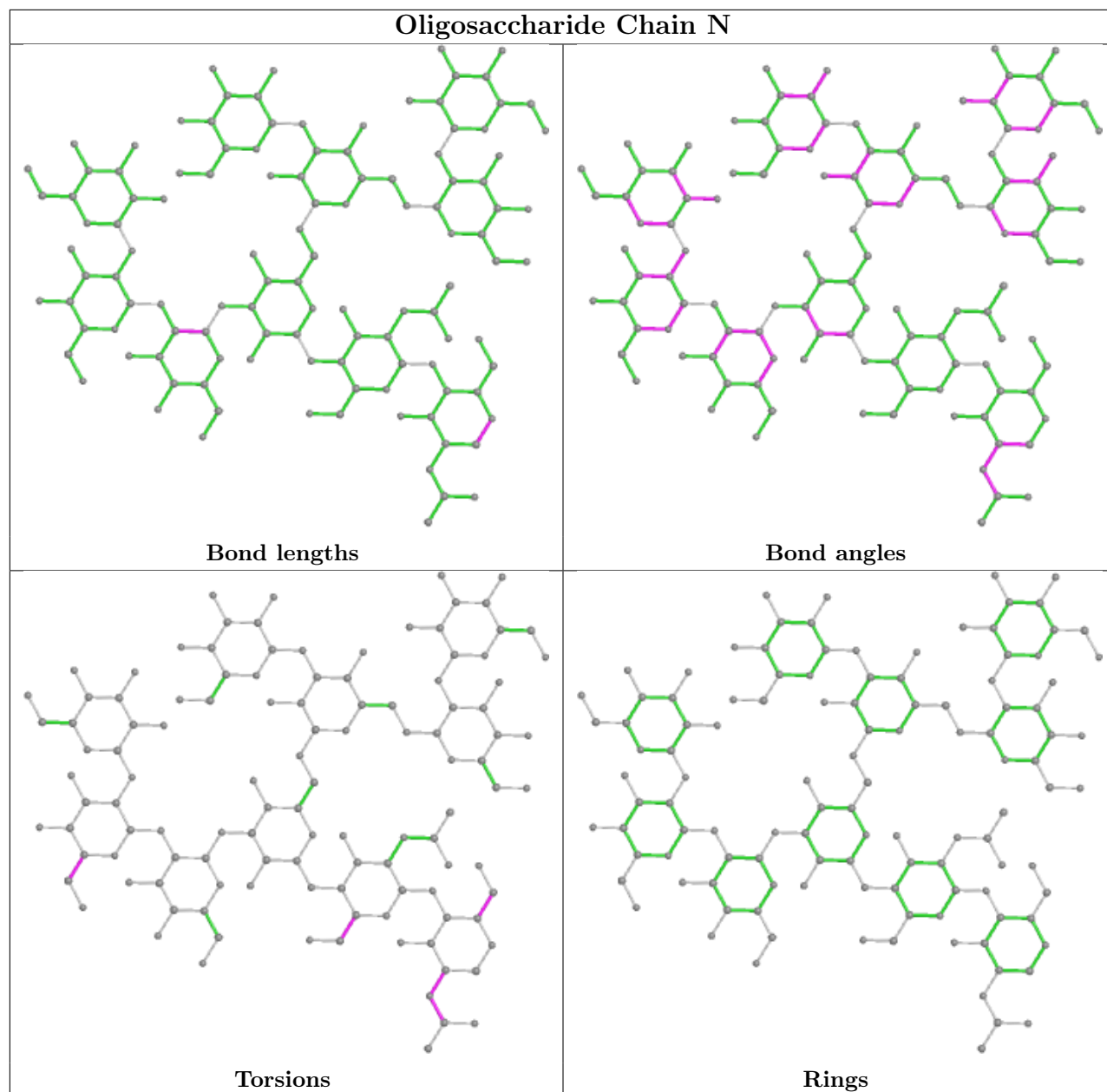


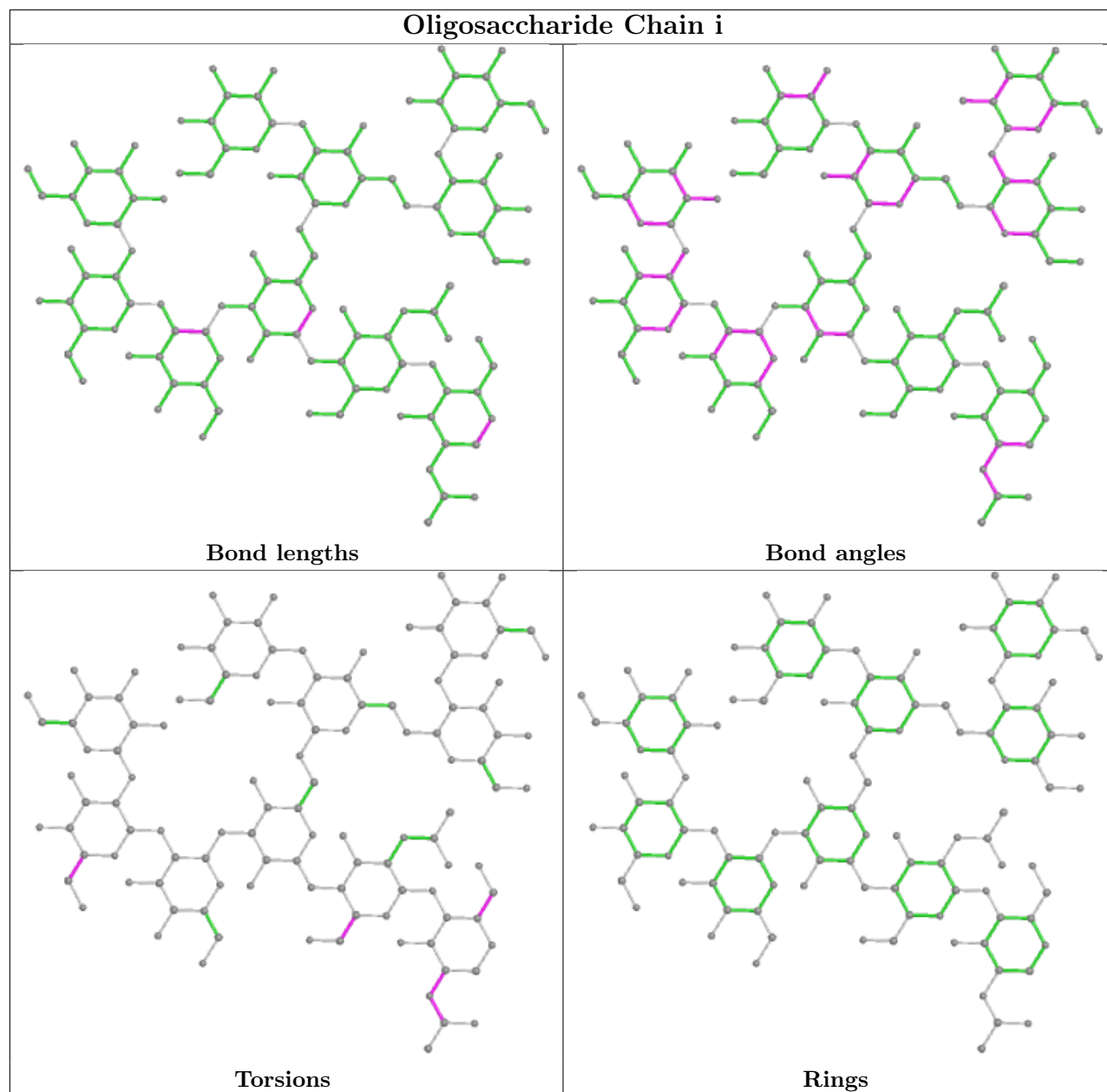


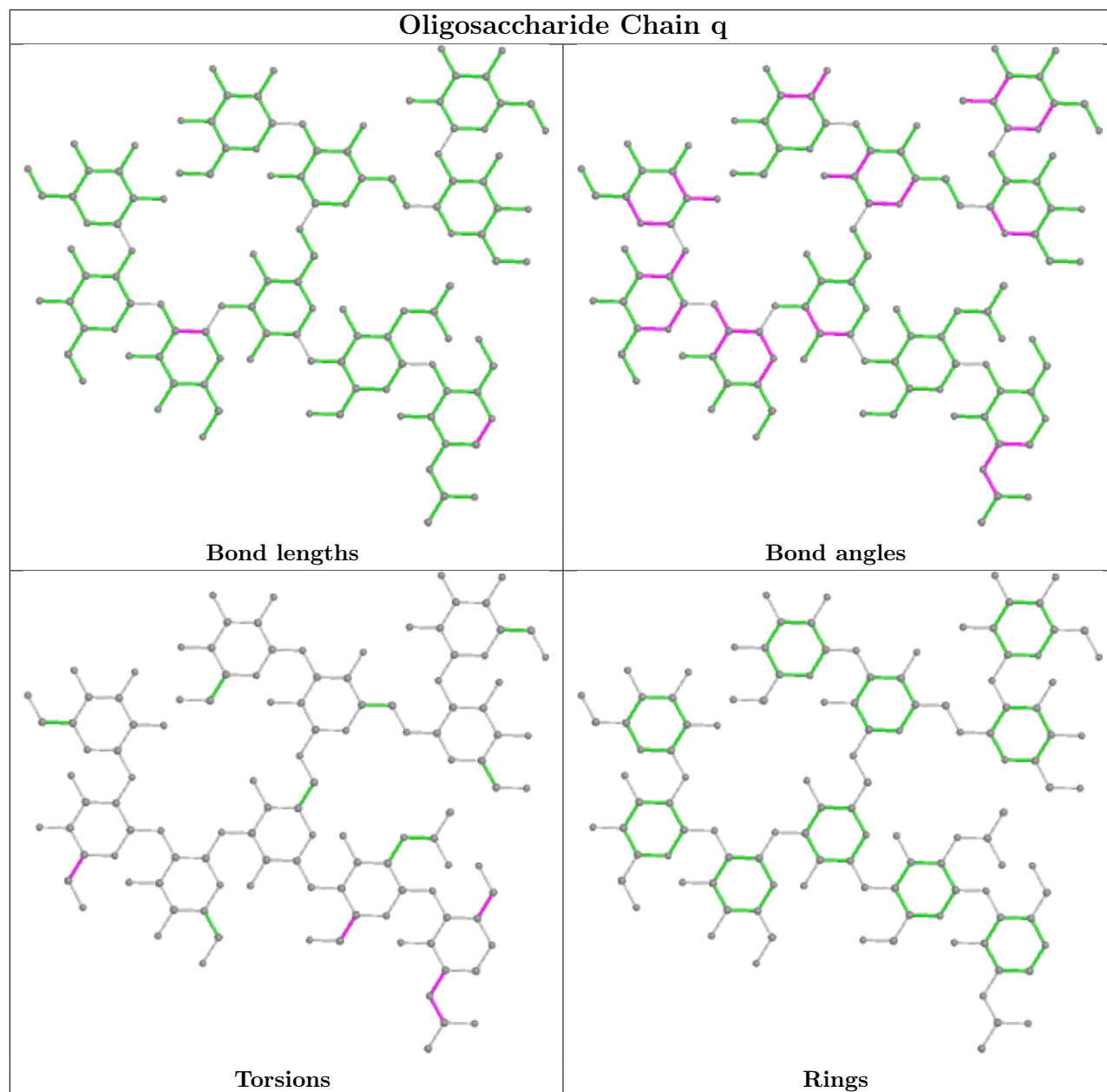


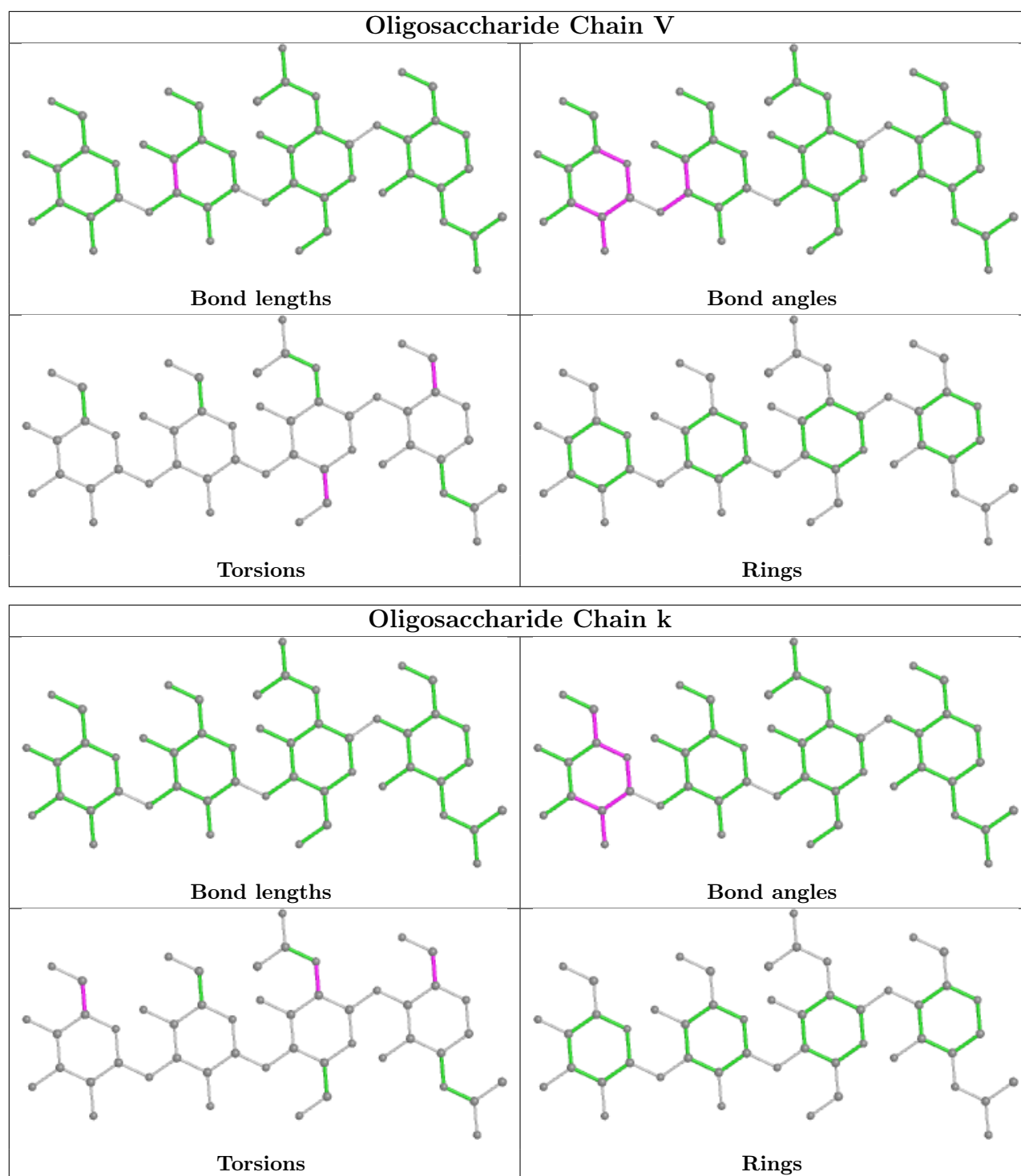












## 5.6 Ligand geometry [i](#)

31 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 |
| 11  | NAG  | G     | 605 | 4    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.44 | 0        |
| 11  | NAG  | e     | 607 | 4    | 14,14,15     | 0.19 | 0        | 17,19,21    | 0.43 | 0        |
| 11  | NAG  | R     | 604 | 4    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.44 | 0        |
| 11  | NAG  | G     | 603 | 4    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.41 | 0        |
| 11  | NAG  | B     | 701 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.46 | 0        |
| 11  | NAG  | e     | 604 | 4    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.49 | 0        |
| 11  | NAG  | H     | 703 | 1    | 14,14,15     | 0.18 | 0        | 17,19,21    | 0.42 | 0        |
| 11  | NAG  | R     | 601 | 4    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.49 | 0        |
| 11  | NAG  | G     | 608 | 4    | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.56 | 0        |
| 11  | NAG  | a     | 701 | 1    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | e     | 603 | 4    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.41 | 0        |
| 11  | NAG  | e     | 606 | 4    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.49 | 0        |
| 11  | NAG  | G     | 607 | 4    | 14,14,15     | 0.21 | 0        | 17,19,21    | 0.44 | 0        |
| 11  | NAG  | R     | 602 | 4    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.41 | 0        |
| 11  | NAG  | R     | 605 | 4    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.49 | 0        |
| 11  | NAG  | B     | 703 | 1    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.43 | 0        |
| 11  | NAG  | e     | 608 | 4    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.49 | 0        |
| 11  | NAG  | e     | 605 | 4    | 14,14,15     | 0.25 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | R     | 603 | 4    | 14,14,15     | 0.23 | 0        | 17,19,21    | 0.50 | 0        |
| 11  | NAG  | a     | 702 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.40 | 0        |
| 11  | NAG  | G     | 606 | 4    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.48 | 0        |
| 11  | NAG  | R     | 606 | 4    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.43 | 0        |
| 11  | NAG  | G     | 602 | 4    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | G     | 604 | 4    | 14,14,15     | 0.24 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | H     | 701 | 1    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | G     | 601 | 4    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.48 | 0        |
| 11  | NAG  | a     | 703 | 1    | 14,14,15     | 0.22 | 0        | 17,19,21    | 0.42 | 0        |
| 11  | NAG  | e     | 602 | 4    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.47 | 0        |
| 11  | NAG  | H     | 702 | 1    | 14,14,15     | 0.28 | 0        | 17,19,21    | 1.51 | 2 (11%)  |
| 11  | NAG  | B     | 702 | 1    | 14,14,15     | 0.20 | 0        | 17,19,21    | 0.53 | 0        |
| 11  | NAG  | e     | 601 | 4    | 14,14,15     | 0.39 | 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. '2' means no outliers of that kind were identified.

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | NAG  | G     | 605 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 607 | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 604 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 603 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | B     | 701 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 604 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | H     | 703 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 601 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 608 | 4    | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | NAG  | a     | 701 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 603 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 606 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 607 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 602 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 605 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | B     | 703 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 608 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 605 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 603 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | a     | 702 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 606 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | R     | 606 | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 602 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 604 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | H     | 701 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 601 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | a     | 703 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 602 | 4    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | H     | 702 | 1    | -       | 4/6/23/26 | 0/1/1/1 |
| 11  | NAG  | B     | 702 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 601 | 4    | -       | 1/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11  | H     | 702 | NAG  | C2-N2-C7 | 5.02 | 130.05      | 122.90   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11  | H     | 702 | NAG  | C1-C2-N2 | 2.85 | 115.36      | 110.49   |

There are no chirality outliers.

5 of 59 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | R     | 603 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 604 | NAG  | O5-C5-C6-O6 |
| 11  | a     | 701 | NAG  | O5-C5-C6-O6 |
| 11  | e     | 603 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 605 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

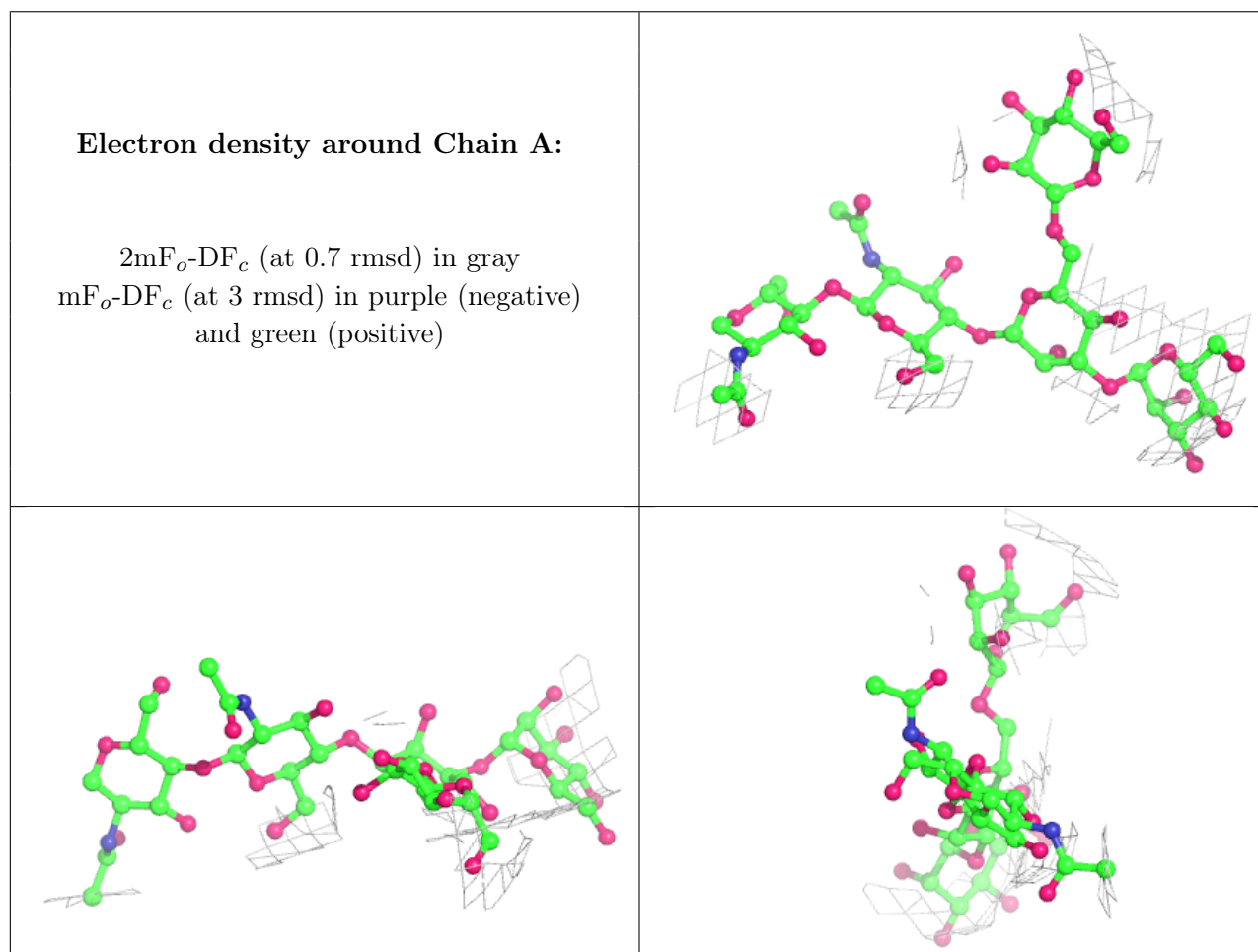
### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

Unable to reproduce the depositors R factor - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

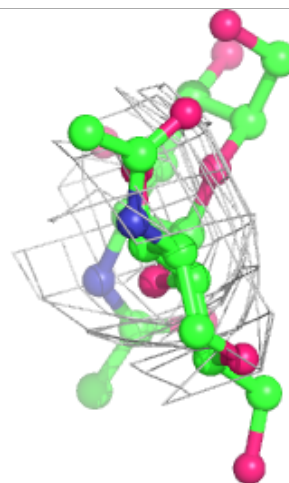
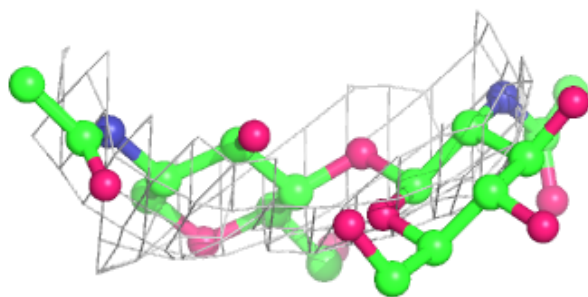
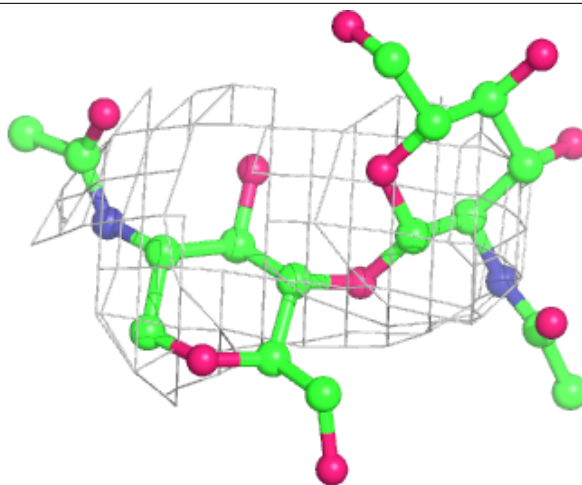
Unable to reproduce the depositors R factor - this section is therefore empty.

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



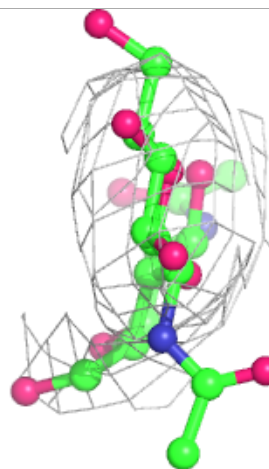
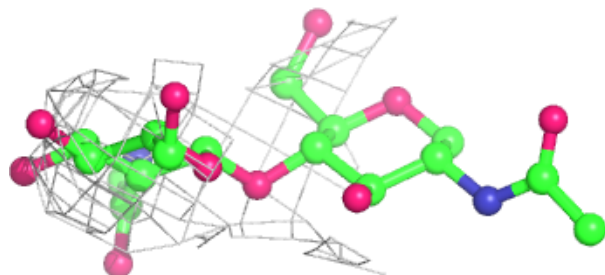
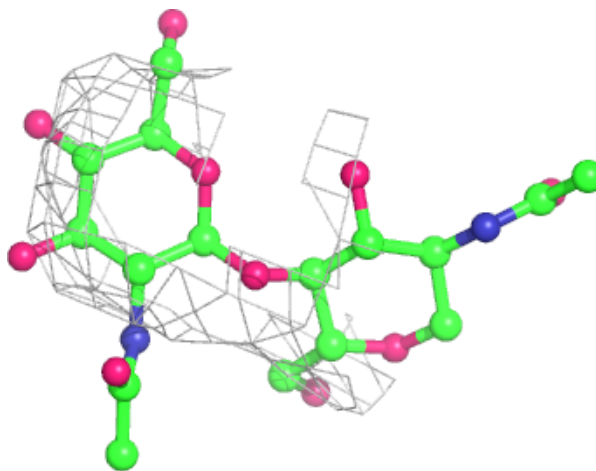
**Electron density around Chain F:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



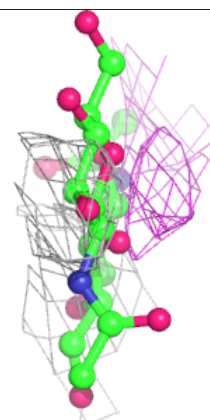
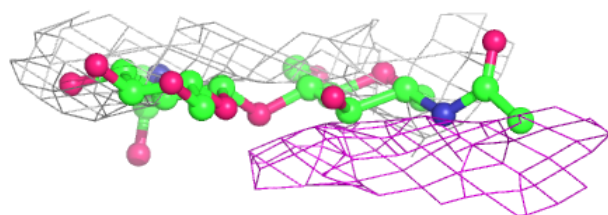
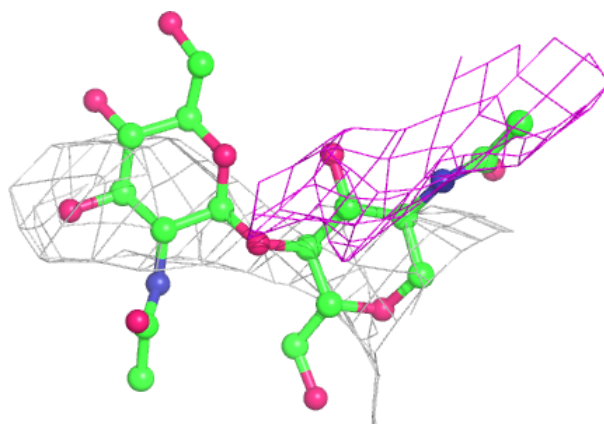
**Electron density around Chain K:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

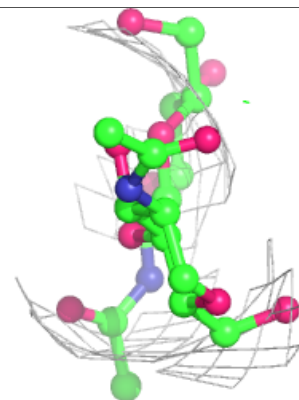
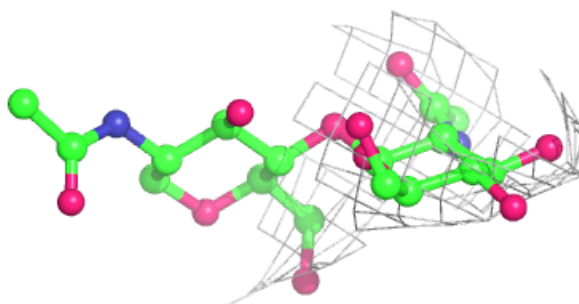
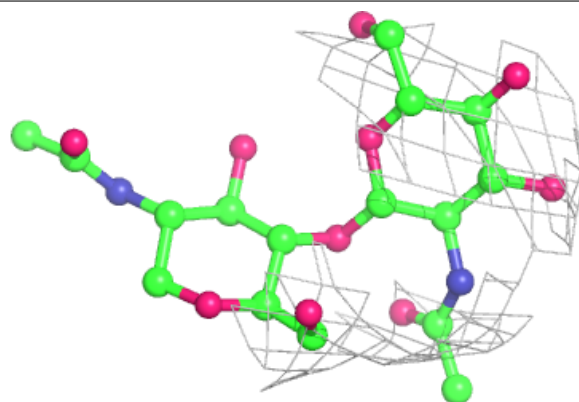


**Electron density around Chain M:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

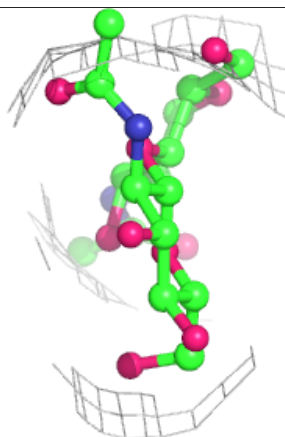
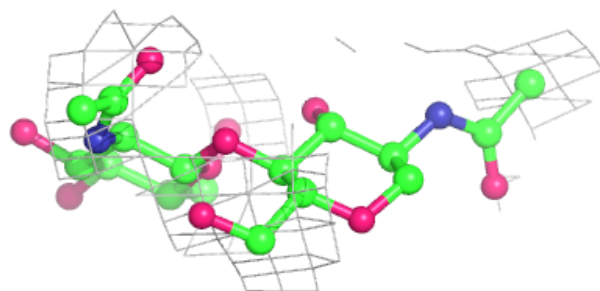
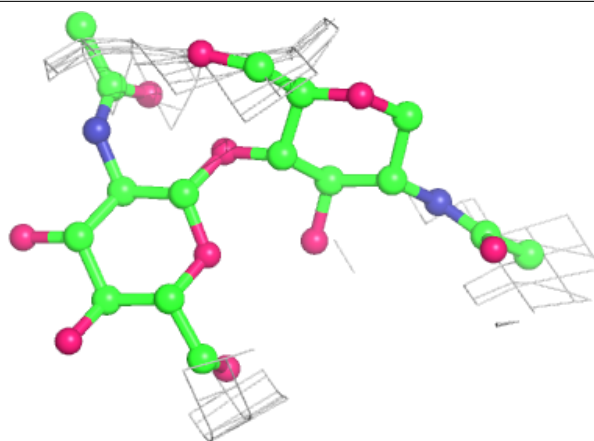
**Electron density around Chain T:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



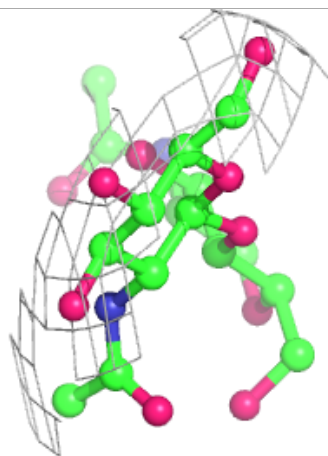
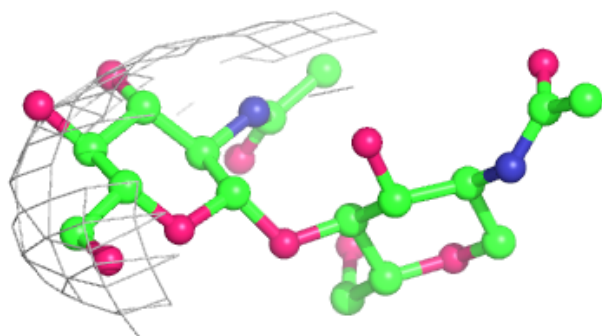
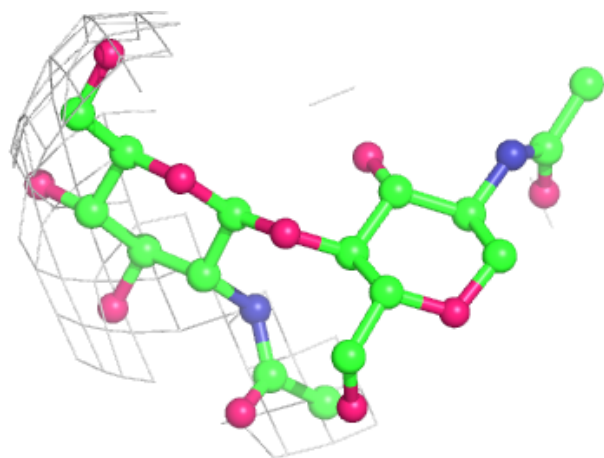
**Electron density around Chain U:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



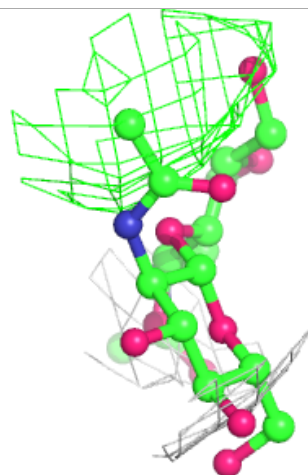
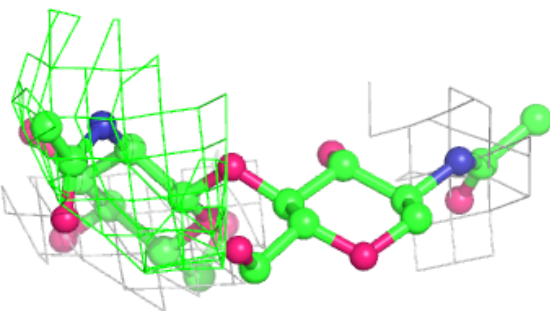
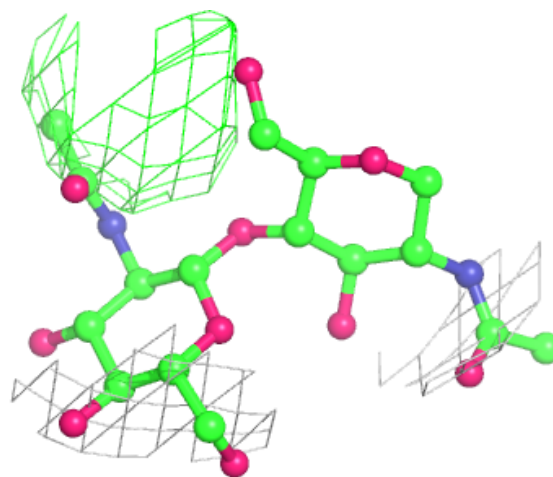
**Electron density around Chain W:**

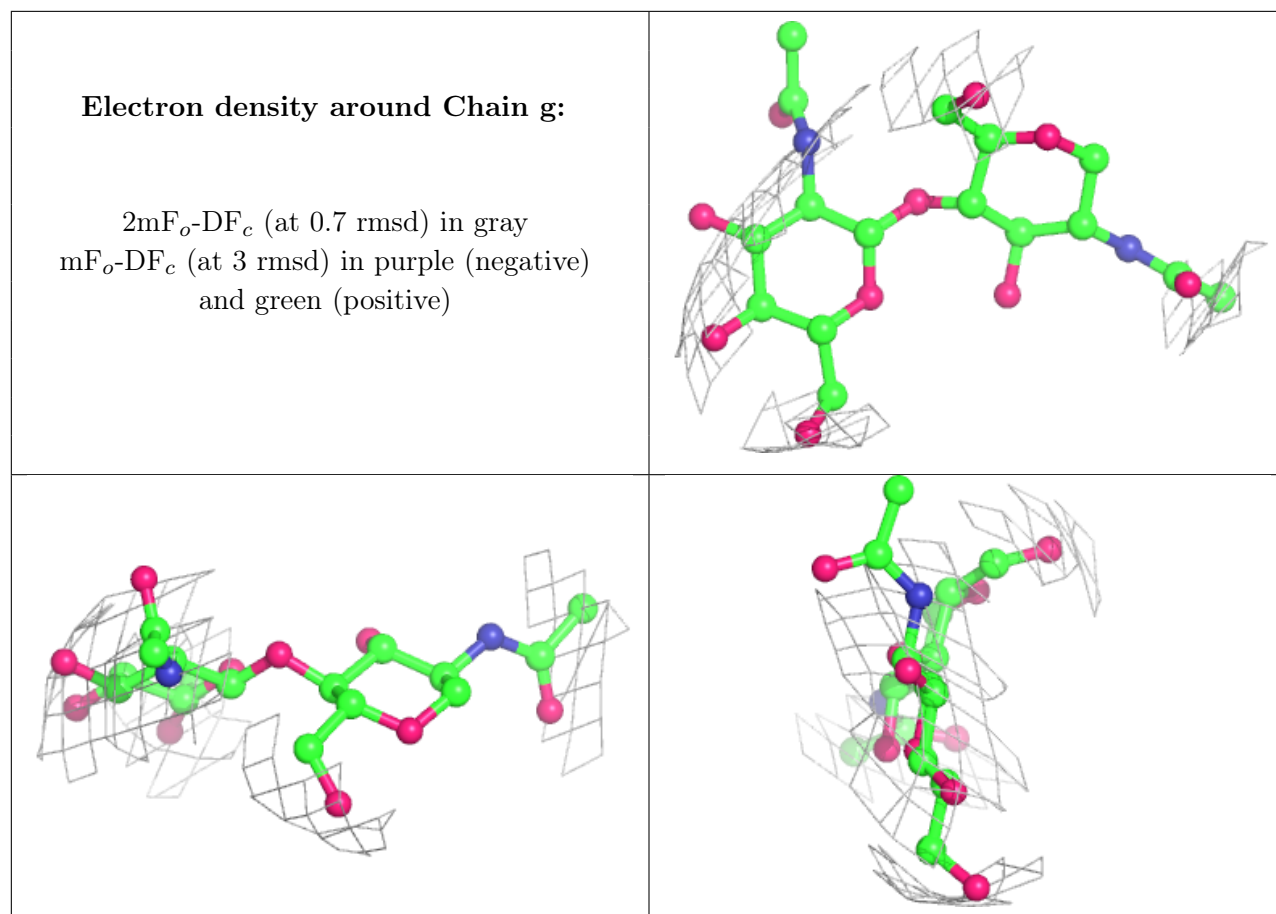
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around Chain X:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

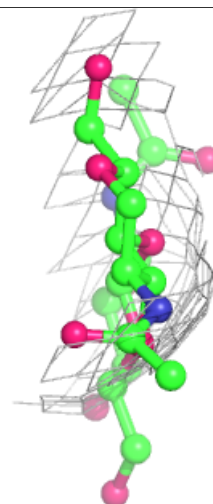
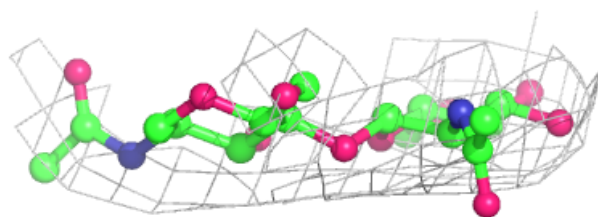
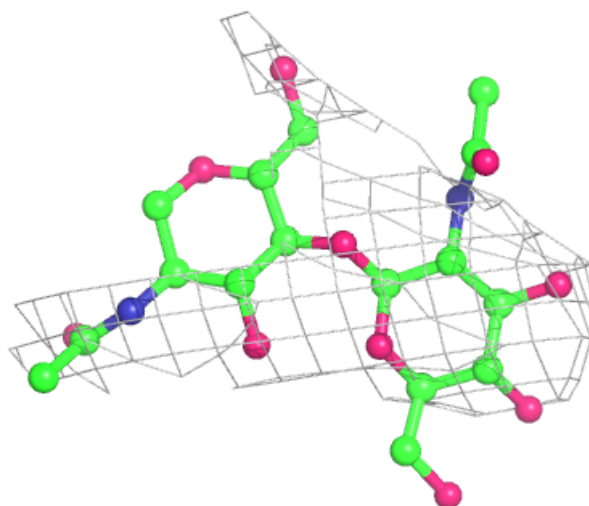


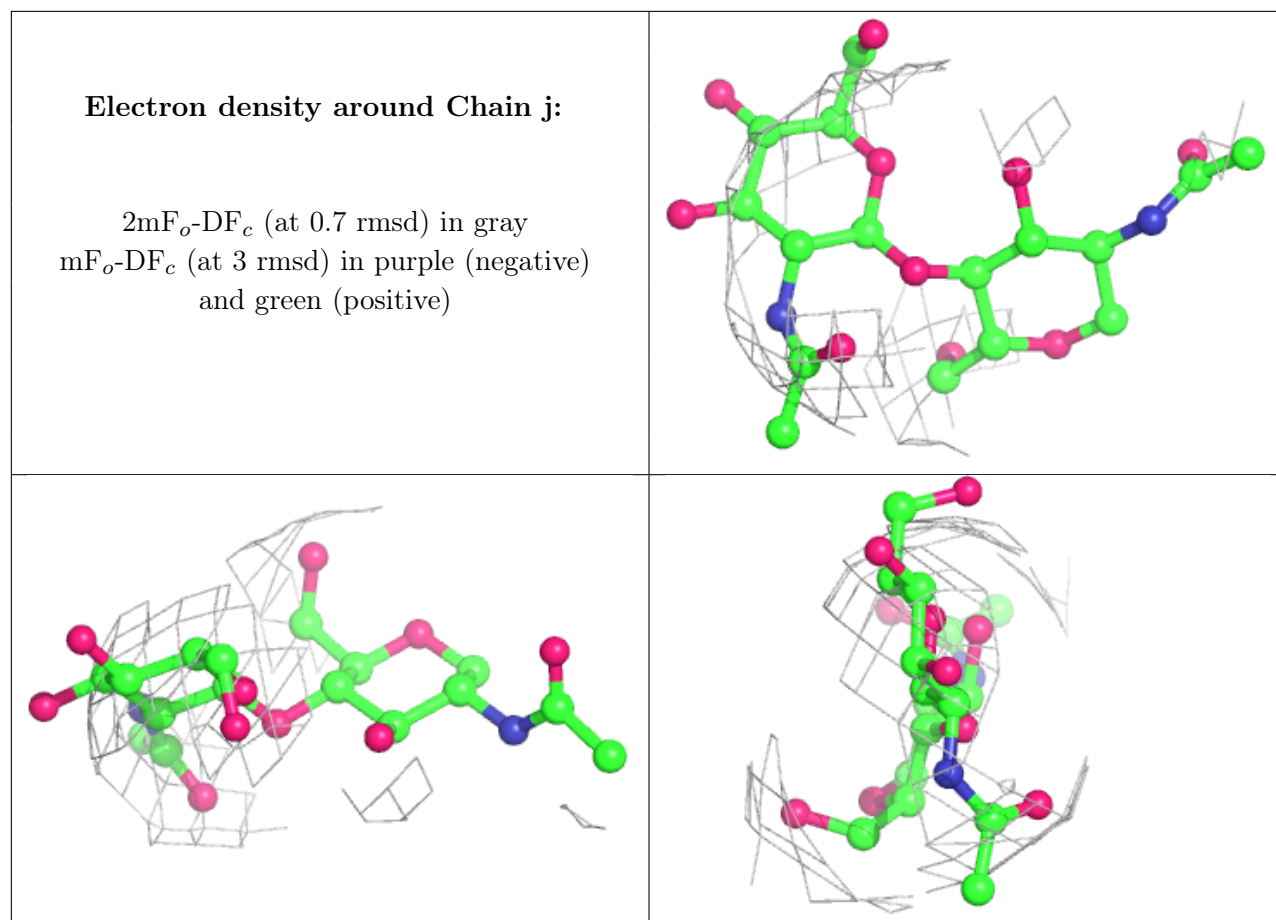


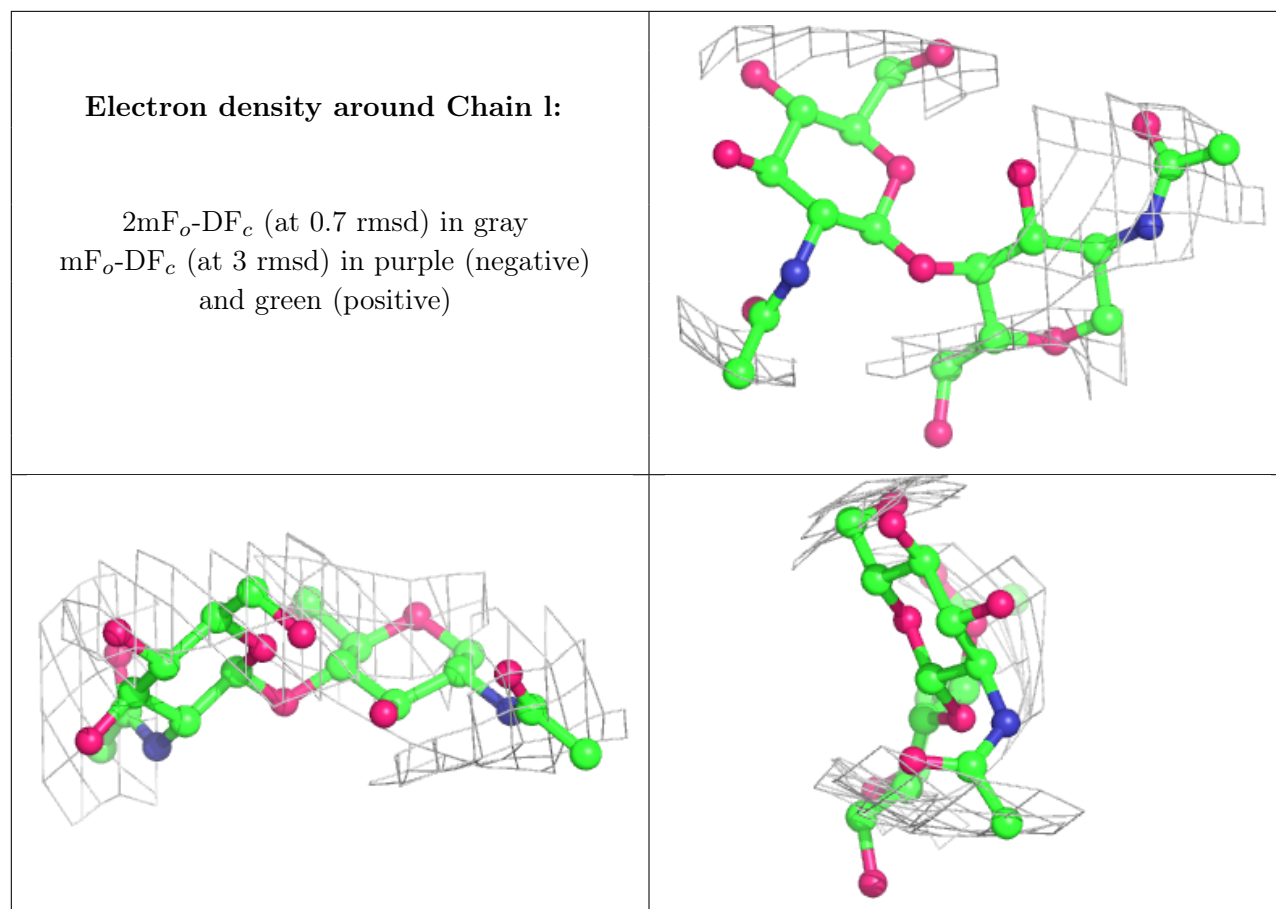


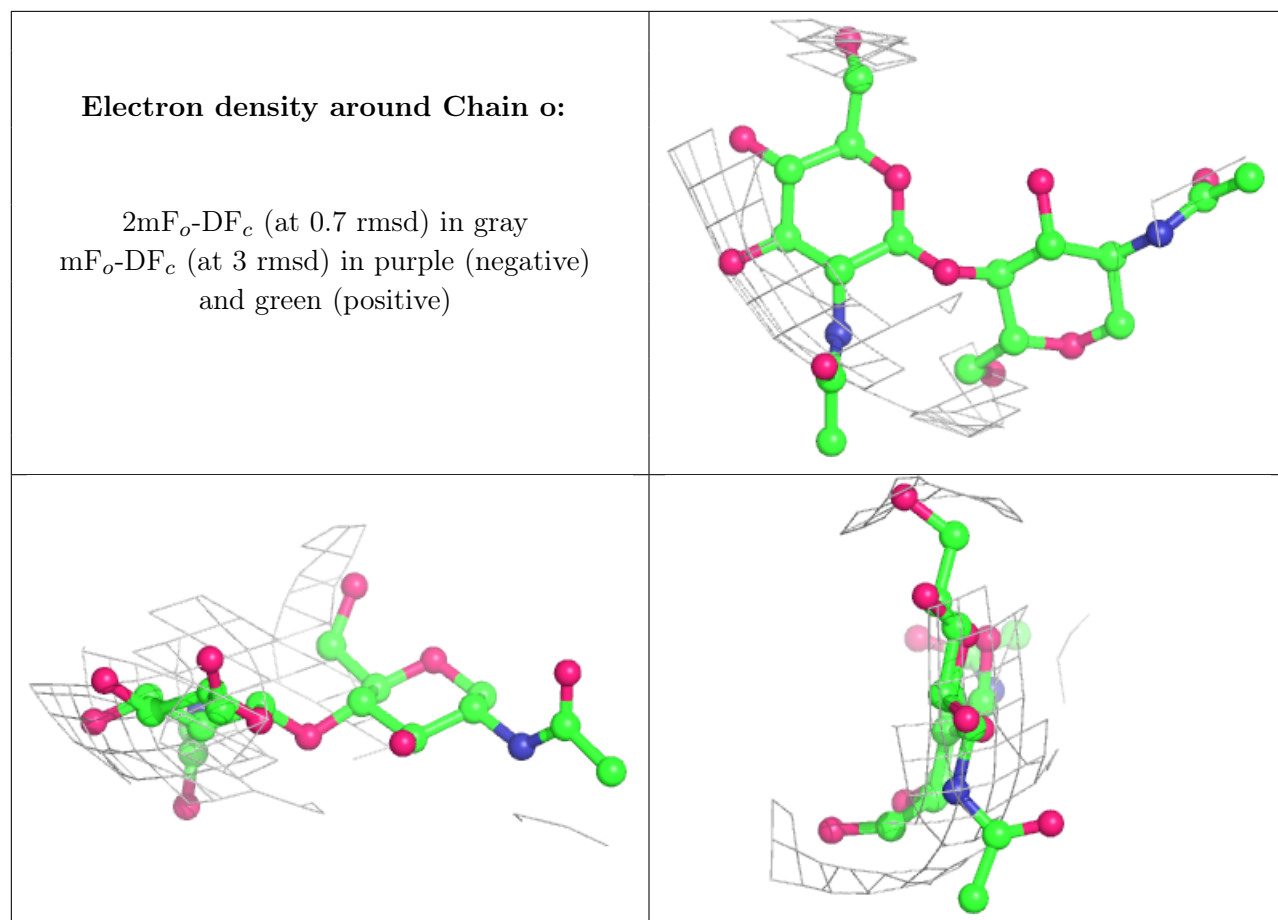
**Electron density around Chain h:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



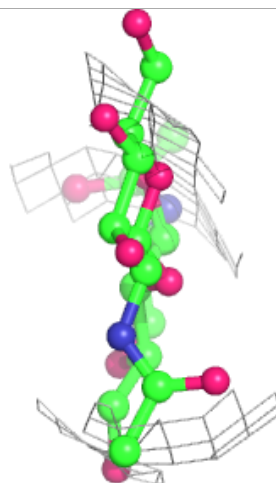
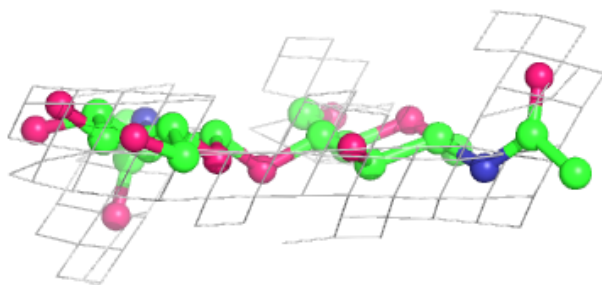
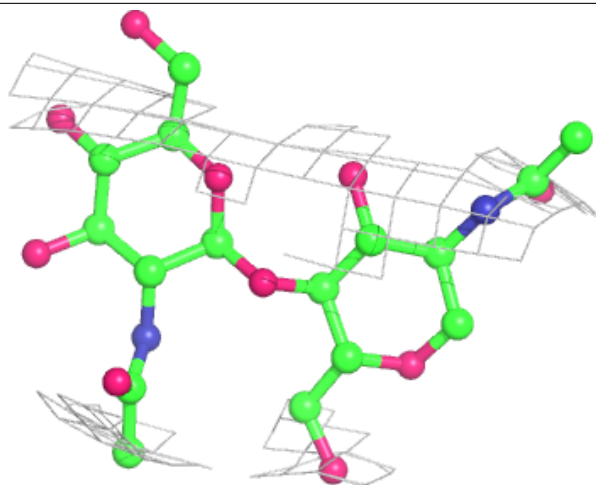






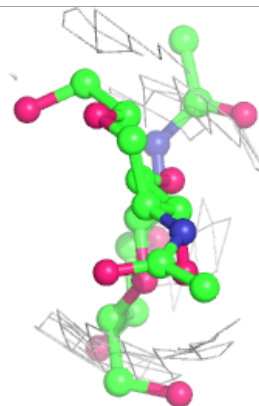
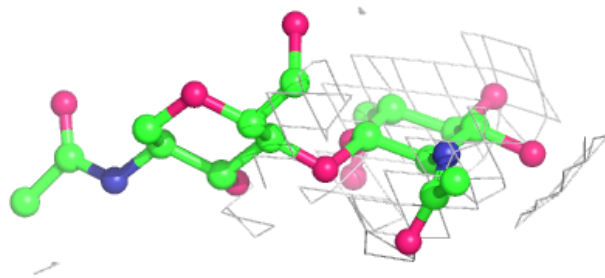
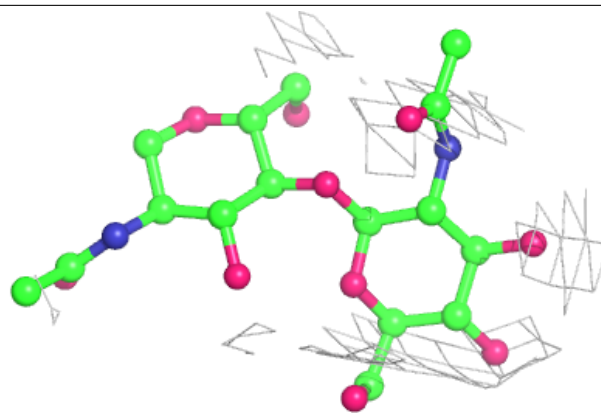
**Electron density around Chain p:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

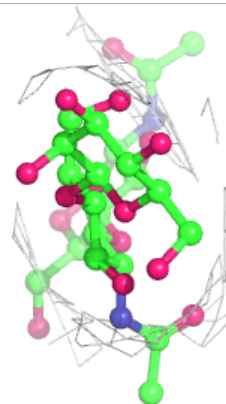
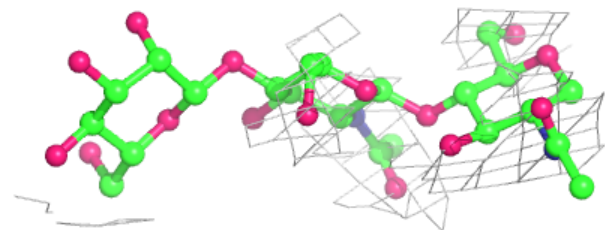
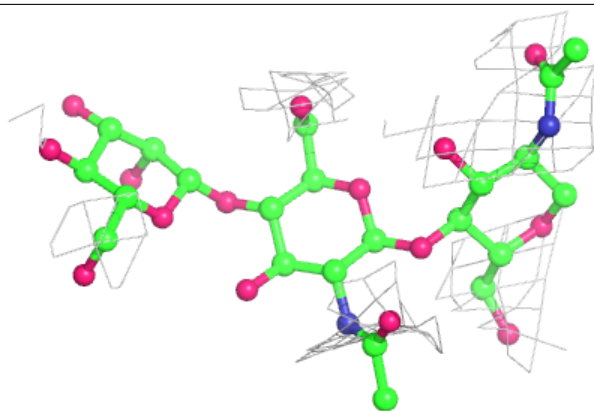


**Electron density around Chain r:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

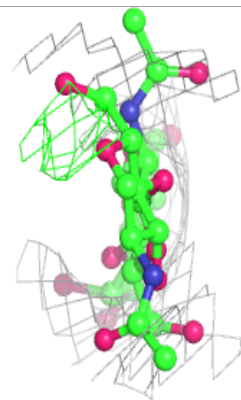
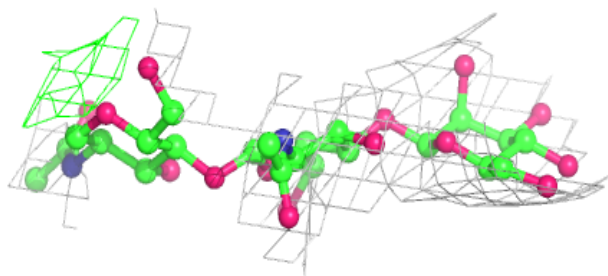
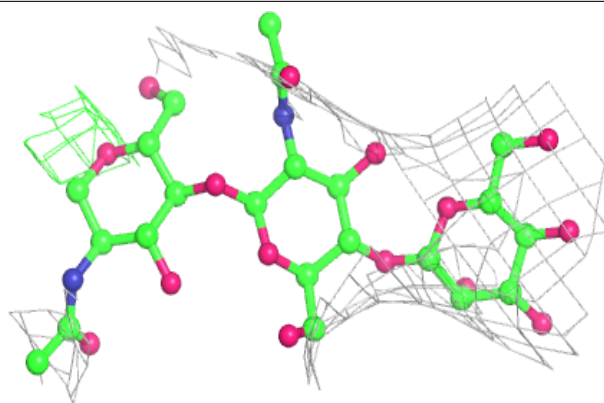
**Electron density around Chain I:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

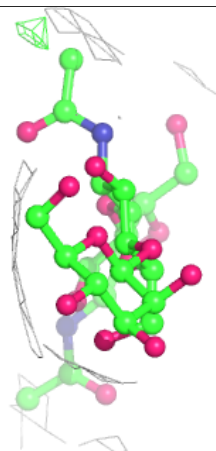
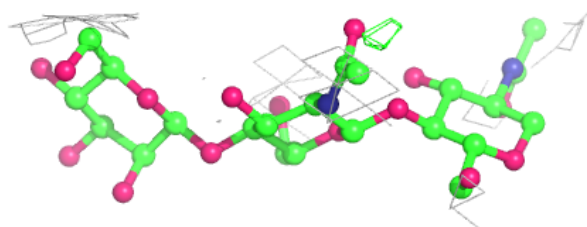
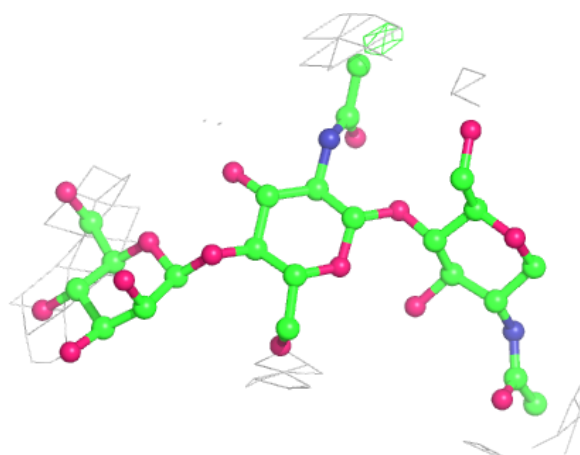


**Electron density around Chain J:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

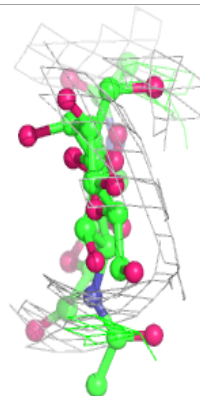
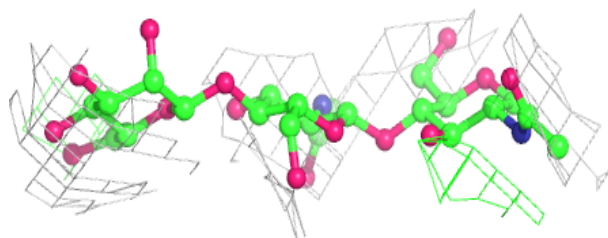
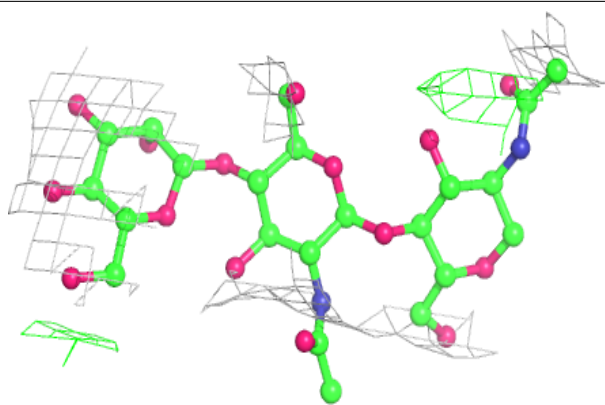
**Electron density around Chain Y:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

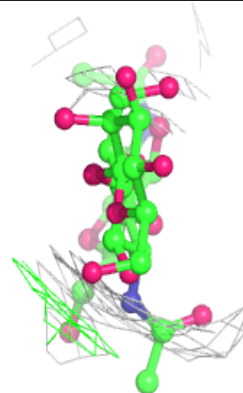
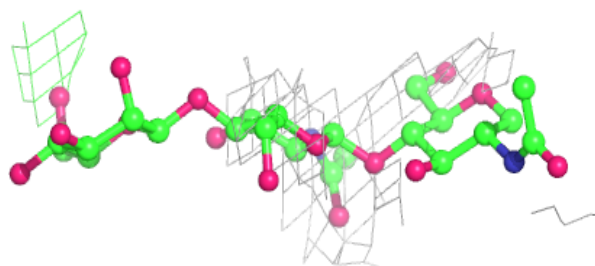
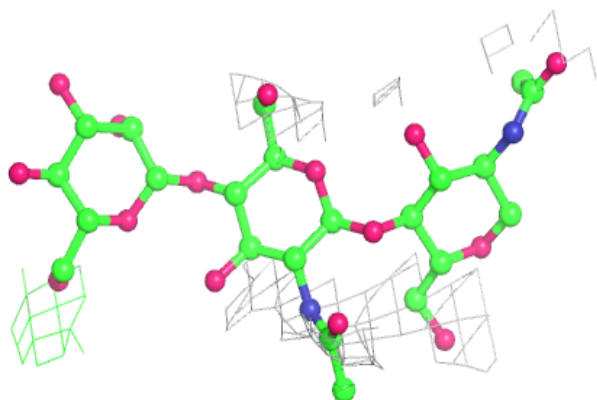


**Electron density around Chain Z:**

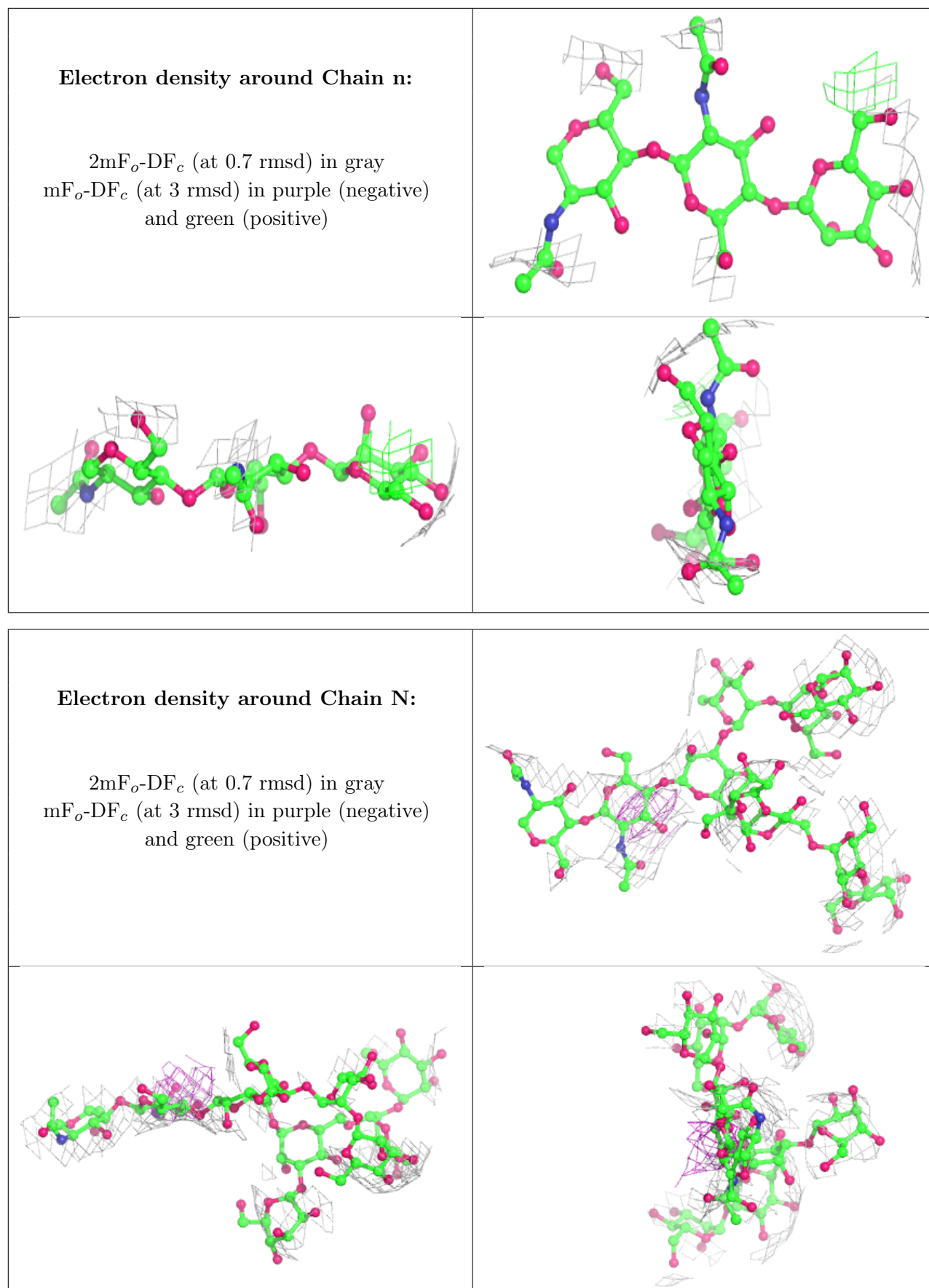
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain m:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

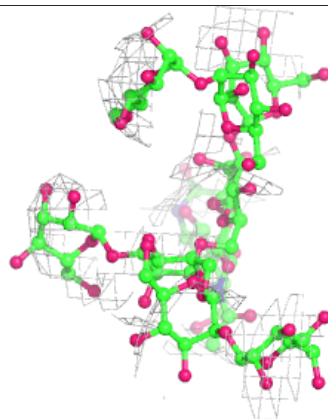
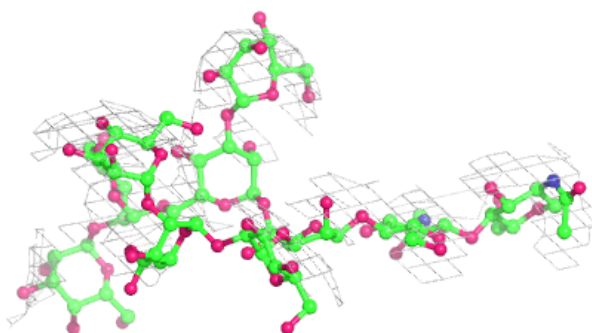
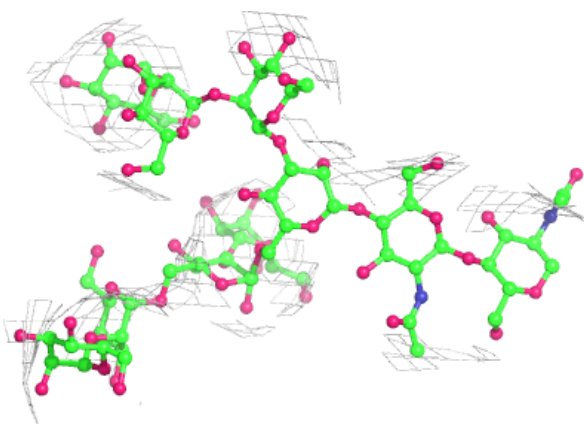




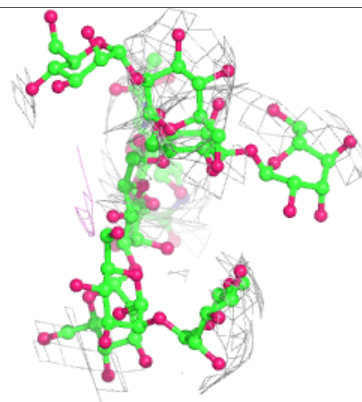
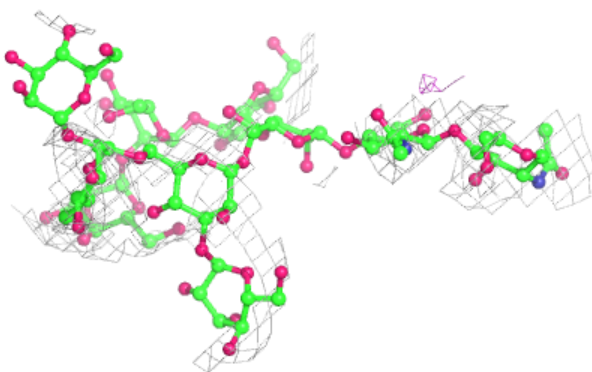
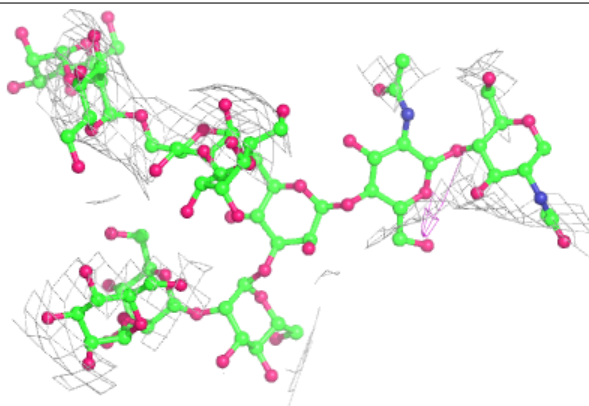


**Electron density around Chain i:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

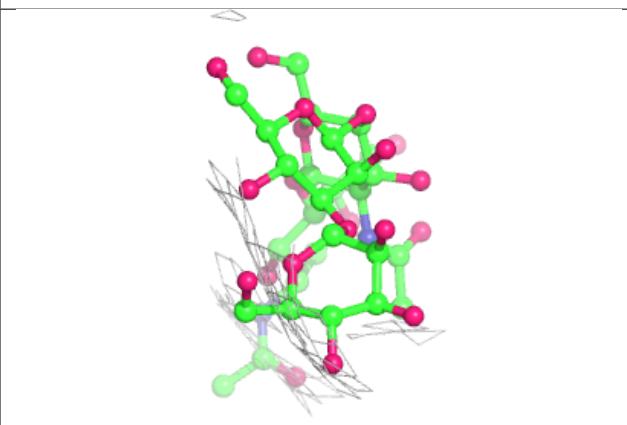
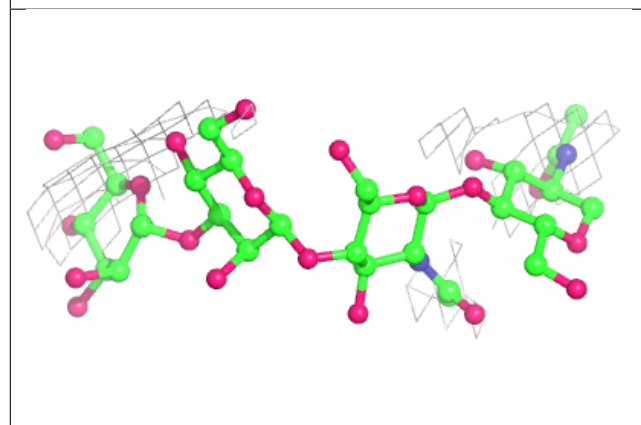
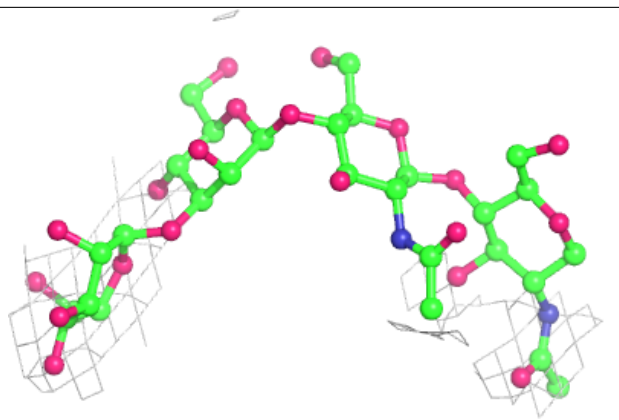
**Electron density around Chain q:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

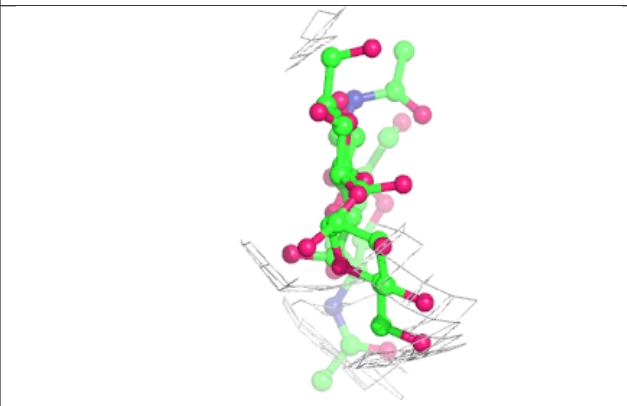
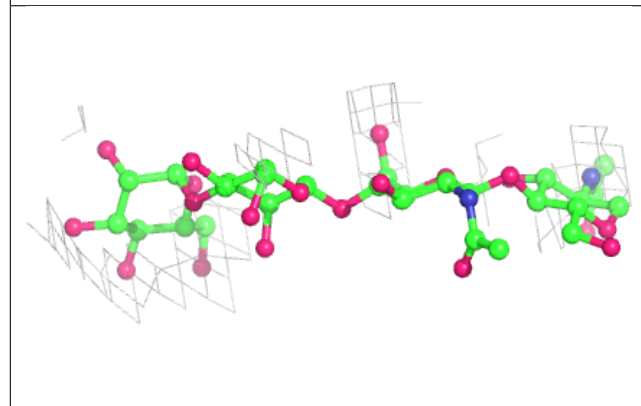
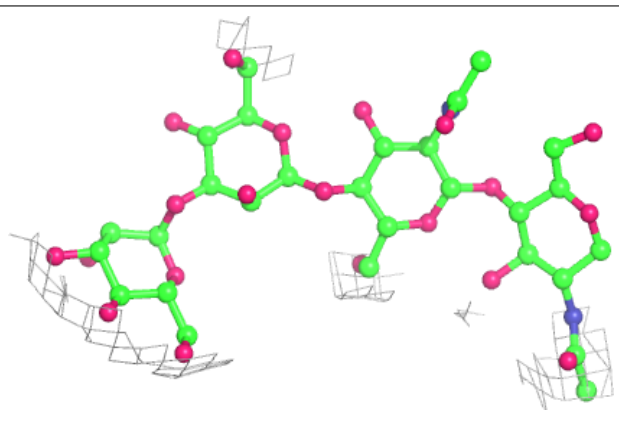


**Electron density around Chain V:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Chain k:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

## 6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.