



## Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 08:49 AM UTC

PDB ID : 5V8M / pdb\_00005v8m  
EMDB ID : EMD-8644  
Title : BG505 SOSIP.664 trimer in complex with broadly neutralizing HIV antibody 3BNC117  
Authors : Lee, J.H.; Cottrell, C.A.; Ward, A.B.  
Deposited on : 2017-03-22  
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

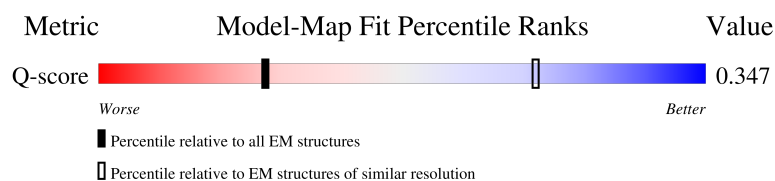
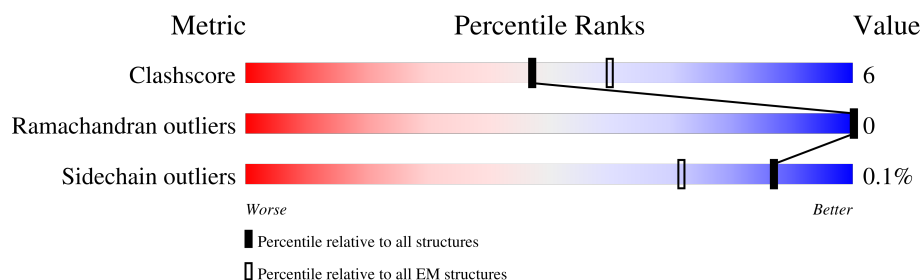
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 4.40 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) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 3132 ( 3.91 - 4.90 )                                     |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 1   | A     | 481    | <br>83% 9% 8%    |
| 1   | F     | 481    | <br>83% 9% 8%    |
| 1   | G     | 481    | <br>83% 9% 8%    |
| 2   | B     | 153    | <br>78% 5% 16%   |

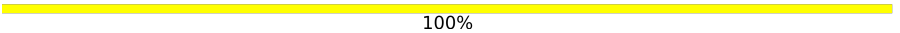
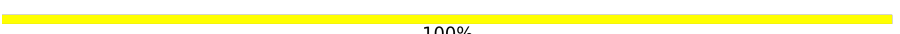
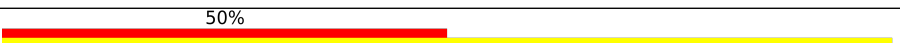
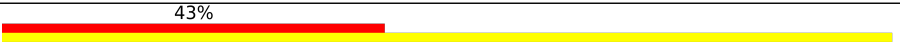
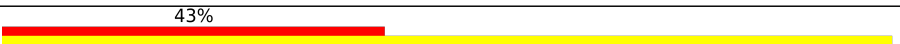
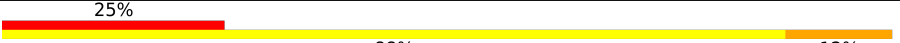
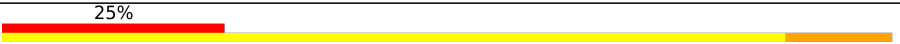
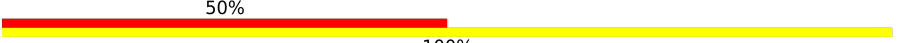
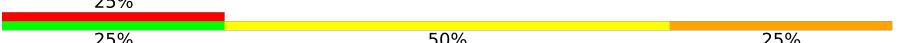
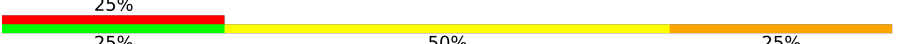
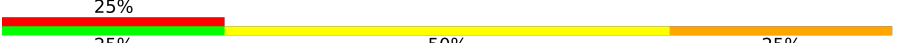
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 2   | I     | 153    |                  |
| 2   | J     | 153    |                  |
| 3   | H     | 226    |                  |
| 3   | R     | 226    |                  |
| 3   | S     | 226    |                  |
| 4   | L     | 206    |                  |
| 4   | T     | 206    |                  |
| 4   | U     | 206    |                  |
| 5   | C     | 3      |                  |
| 5   | Z     | 3      |                  |
| 5   | m     | 3      |                  |
| 6   | D     | 2      |                  |
| 6   | E     | 2      |                  |
| 6   | K     | 2      |                  |
| 6   | O     | 2      |                  |
| 6   | P     | 2      |                  |
| 6   | Q     | 2      |                  |
| 6   | X     | 2      |                  |
| 6   | Y     | 2      |                  |
| 6   | a     | 2      |                  |
| 6   | b     | 2      |                  |
| 6   | c     | 2      |                  |
| 6   | f     | 2      |                  |
| 6   | g     | 2      |                  |
| 6   | h     | 2      |                  |

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| Mol | Chain | Length | Quality of chain                                                                                  |
|-----|-------|--------|---------------------------------------------------------------------------------------------------|
| 6   | k     | 2      |  100%           |
| 6   | l     | 2      |  50%100%        |
| 6   | n     | 2      |  50%100%        |
| 6   | o     | 2      |  50%50%         |
| 6   | p     | 2      |  100%           |
| 6   | s     | 2      |  50%50%         |
| 6   | t     | 2      |  50%100%        |
| 6   | u     | 2      |  50%50%         |
| 6   | x     | 2      |  100%           |
| 6   | y     | 2      |  50%100%        |
| 7   | M     | 7      |  43%100%        |
| 7   | d     | 7      |  43%100%        |
| 7   | q     | 7      |  43%100%      |
| 8   | N     | 8      |  25%88%12%    |
| 8   | e     | 8      |  25%88%12%    |
| 8   | r     | 8      |  25%88%12%    |
| 9   | V     | 6      |  50%100%      |
| 9   | i     | 6      |  50%100%      |
| 9   | v     | 6      |  50%100%      |
| 10  | W     | 4      |  25%25%50%25% |
| 10  | j     | 4      |  25%25%50%25% |
| 10  | w     | 4      |  25%25%50%25% |

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

| Mol | Type | Chain | Res | Chirality | Geometry | Clashes | Electron density |
|-----|------|-------|-----|-----------|----------|---------|------------------|
| 6   | NAG  | O     | 1   | -         | -        | X       | -                |
| 6   | NAG  | f     | 1   | -         | -        | X       | -                |
| 6   | NAG  | s     | 1   | -         | -        | X       | -                |

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 20835 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called gp120.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | A     | 444      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3493  | 2192 | 617 | 656 | 28 |         |       |
| 1   | F     | 444      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3493  | 2192 | 617 | 656 | 28 |         |       |
| 1   | G     | 444      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3493  | 2192 | 617 | 656 | 28 |         |       |

There are 21 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| A     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| A     | 509     | ARG      | -      | expression tag | UNP Q2N0S6 |
| A     | 510     | ARG      | -      | expression tag | UNP Q2N0S6 |
| A     | 511     | ARG      | -      | expression tag | UNP Q2N0S6 |
| A     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |
| A     | 513     | ARG      | -      | expression tag | UNP Q2N0S6 |
| F     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| F     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| F     | 509     | ARG      | -      | expression tag | UNP Q2N0S6 |
| F     | 510     | ARG      | -      | expression tag | UNP Q2N0S6 |
| F     | 511     | ARG      | -      | expression tag | UNP Q2N0S6 |
| F     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |
| F     | 513     | ARG      | -      | expression tag | UNP Q2N0S6 |
| G     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| G     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| G     | 509     | ARG      | -      | expression tag | UNP Q2N0S6 |
| G     | 510     | ARG      | -      | expression tag | UNP Q2N0S6 |
| G     | 511     | ARG      | -      | expression tag | UNP Q2N0S6 |
| G     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |
| G     | 513     | ARG      | -      | expression tag | UNP Q2N0S6 |

- Molecule 2 is a protein called gp41.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | B     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 646 | 177 | 195 | 6 |         |       |
| 2   | I     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 646 | 177 | 195 | 6 |         |       |
| 2   | J     | 129      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1024  | 646 | 177 | 195 | 6 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| B     | 559     | PRO      | ILE    | conflict | UNP Q2N0S6 |
| B     | 605     | CYS      | THR    | conflict | UNP Q2N0S6 |
| I     | 559     | PRO      | ILE    | conflict | UNP Q2N0S6 |
| I     | 605     | CYS      | THR    | conflict | UNP Q2N0S6 |
| J     | 559     | PRO      | ILE    | conflict | UNP Q2N0S6 |
| J     | 605     | CYS      | THR    | conflict | UNP Q2N0S6 |

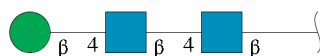
- Molecule 3 is a protein called antibody 3BNC117, heavy chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | H     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 626 | 177 | 179 | 3 |         |       |
| 3   | R     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 626 | 177 | 179 | 3 |         |       |
| 3   | S     | 121      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 985   | 626 | 177 | 179 | 3 |         |       |

- Molecule 4 is a protein called antibody 3BNC117, light chain.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | L     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 783   | 493 | 137 | 150 | 3 |         |       |
| 4   | T     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 783   | 493 | 137 | 150 | 3 |         |       |
| 4   | U     | 98       | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 783   | 493 | 137 | 150 | 3 |         |       |

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 5   | C     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 5   | Z     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 5   | m     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

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



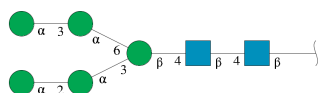
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 6   | D     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | E     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | K     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | O     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | P     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | Q     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | X     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | Y     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | a     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | b     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | c     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | f     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | g     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | h     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

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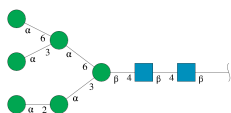
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 6   | k     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | l     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | n     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | o     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | p     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | s     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | t     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | u     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | x     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 6   | y     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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.



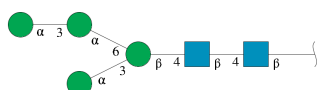
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 7   | M     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |
| 7   | d     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |
| 7   | q     | 7        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 83    | 46 | 2 | 35 |         |       |

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 8   | N     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |
| 8   | e     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |
| 8   | r     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |

- Molecule 9 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



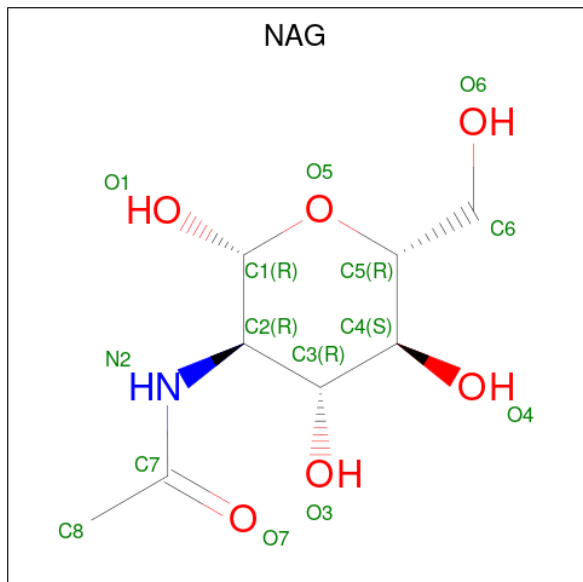
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 9   | V     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 9   | i     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 9   | v     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 10  | W     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 10  | j     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 10  | w     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 11  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | F     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

*Continued on next page...*

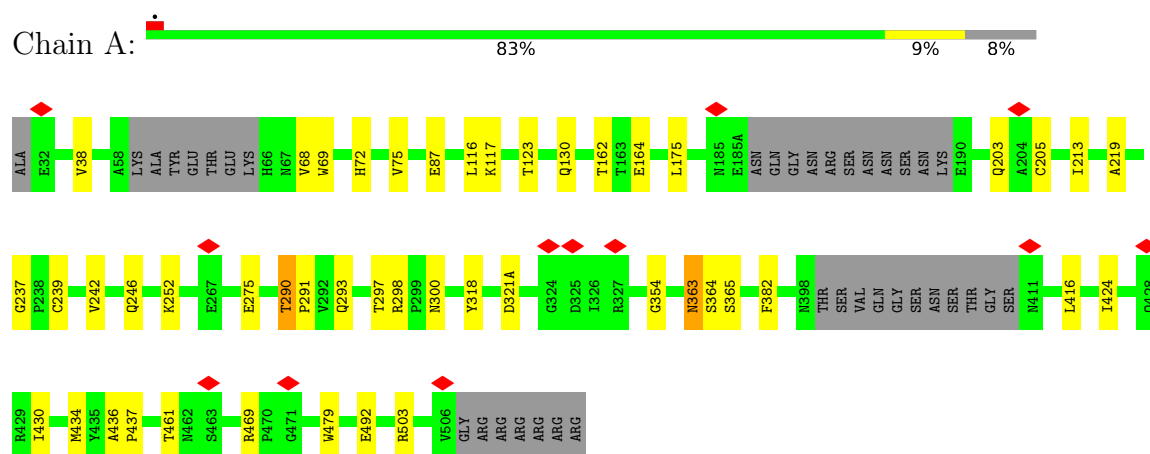
*Continued from previous page...*

| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 11  | I     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | I     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | J     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 11  | J     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

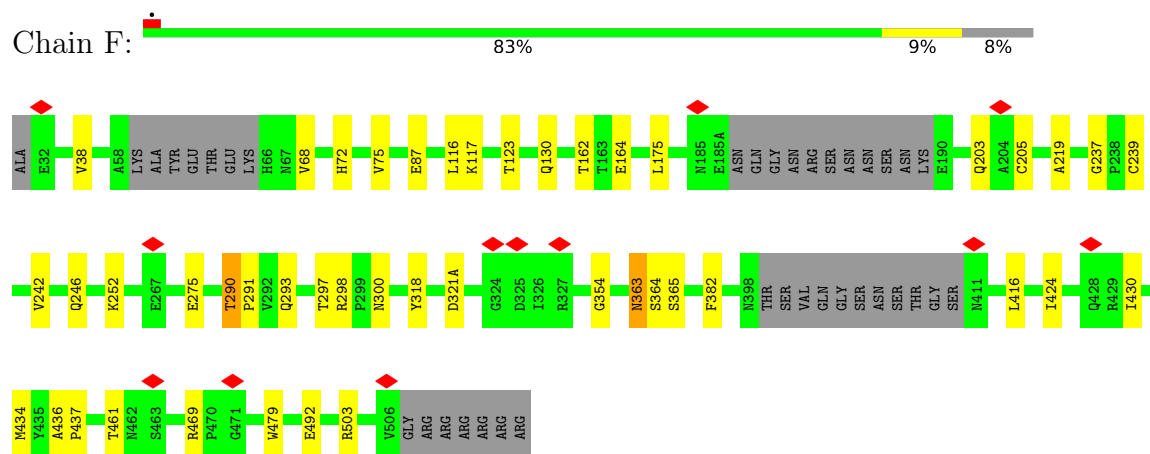
### 3 Residue-property plots

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 and atom inclusion in map density. 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. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

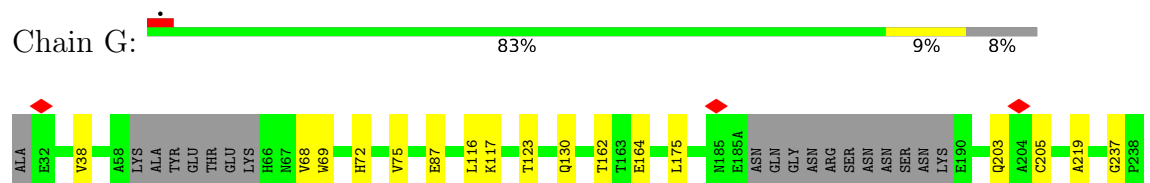
- Molecule 1: gp120



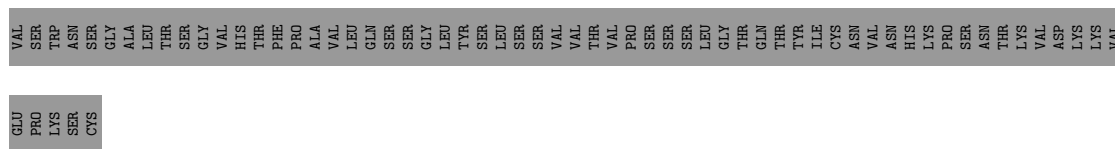
- Molecule 1: gp120



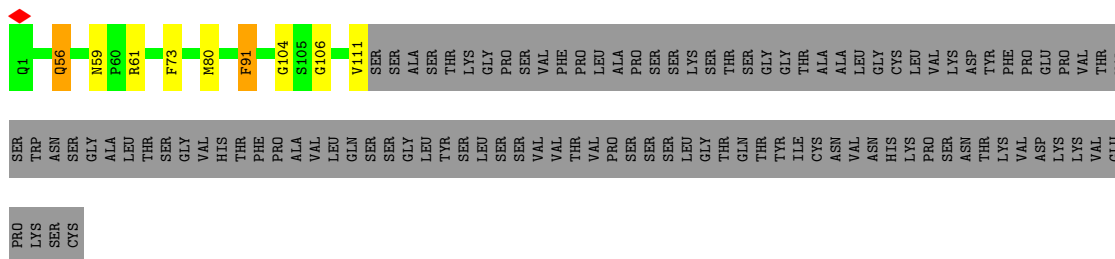
- Molecule 1: gp120



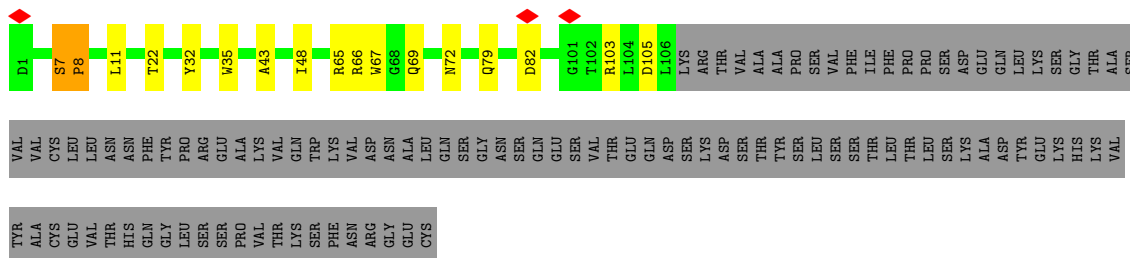
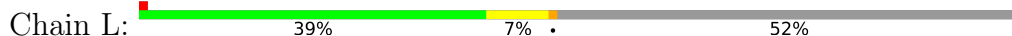




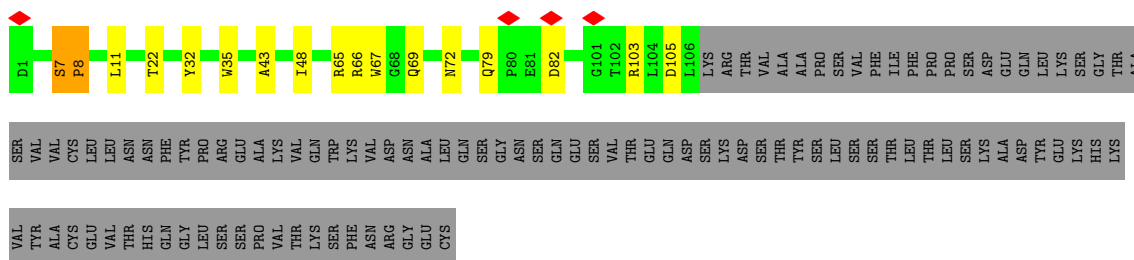
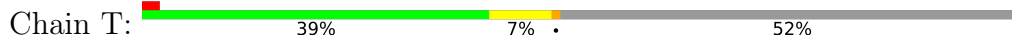
- Molecule 3: antibody 3BNC117, heavy chain



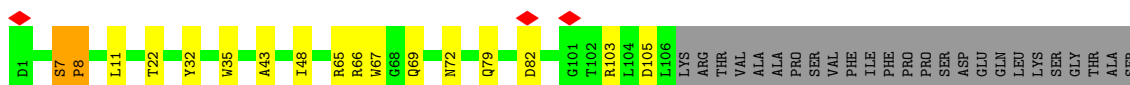
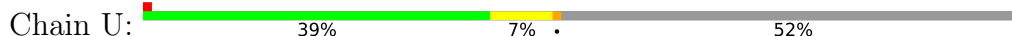
- Molecule 4: antibody 3BNC117, light chain



- Molecule 4: antibody 3BNC117, light chain



- Molecule 4: antibody 3BNC117, light chain



VAL VAL CYS LEU LEU ASN ASN PHE TYR PRO ARG GLU ALA LYS VAL GLN TRP LYS VAL ASP ASN ASN ALA LEU GLN SER GLY ASN SER GLN GLU SER VAL THR GLU GLN ASP SER LYS ASP SER THR TYR SER LEU SER SER THR THR LEU SER LYS ALA ASP TYR GLU LYS HIS LYS VAL

TYR ALA CYS GLU VAL THR HIS GLN TYR GLY LEU SER PRO VAL THR LYS SER PHE ASN ARG GLY CYS

- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



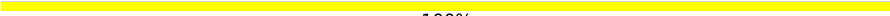
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

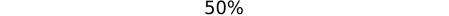


- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  100%

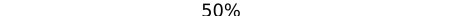
  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:  50%  
 50%

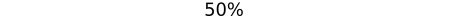
  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain P:  50%  
 100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Q:  50%  
 50%

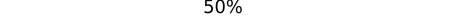
  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X:  100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain Y:  50%  
 100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



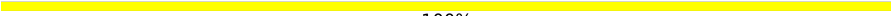
- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain k:  100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain l:  50%  
 100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n:  50%  
 100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain o:  50%  
 50% 50%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain p:  100%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain s:  50%  
 50% 50%

  
NAG1  
NAG2

- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



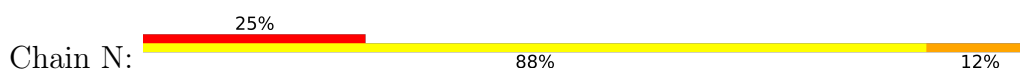
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



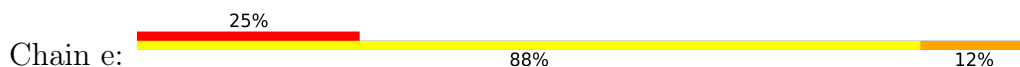
- Molecule 7: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



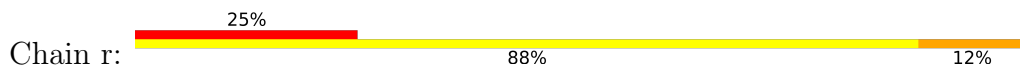
- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 8: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 9: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 10: 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-(1-6)-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-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 22625                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 32                                      | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 0.119                                   | Depositor |
| Minimum map value                    | -0.051                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.035                                   | Depositor |
| Map size (Å)                         | 335.36, 335.36, 335.36                  | wwPDB     |
| Map dimensions                       | 256, 256, 256                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.31, 1.31, 1.31                        | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, BMA, MAN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths |         | Bond angles |                  |
|-----|-------|--------------|---------|-------------|------------------|
|     |       | RMSZ         | # Z  >5 | RMSZ        | # Z  >5          |
| 1   | A     | 0.97         | 0/3565  | 1.33        | 40/4842 (0.8%)   |
| 1   | F     | 0.97         | 0/3565  | 1.34        | 40/4842 (0.8%)   |
| 1   | G     | 0.97         | 0/3565  | 1.34        | 40/4842 (0.8%)   |
| 2   | B     | 1.05         | 0/1041  | 1.16        | 7/1412 (0.5%)    |
| 2   | I     | 1.05         | 0/1041  | 1.16        | 7/1412 (0.5%)    |
| 2   | J     | 1.05         | 0/1041  | 1.16        | 7/1412 (0.5%)    |
| 3   | H     | 1.00         | 0/1017  | 1.26        | 7/1386 (0.5%)    |
| 3   | R     | 1.00         | 0/1017  | 1.26        | 7/1386 (0.5%)    |
| 3   | S     | 1.00         | 0/1017  | 1.26        | 7/1386 (0.5%)    |
| 4   | L     | 0.82         | 0/800   | 1.31        | 9/1086 (0.8%)    |
| 4   | T     | 0.82         | 0/800   | 1.31        | 9/1086 (0.8%)    |
| 4   | U     | 0.82         | 0/800   | 1.31        | 9/1086 (0.8%)    |
| All | All   | 0.97         | 0/19269 | 1.29        | 189/26178 (0.7%) |

There are no bond length outliers.

All (189) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms  | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|-------|-------------|----------|
| 1   | G     | 252 | LYS  | CA-C-N | 10.33 | 131.59      | 120.12   |
| 1   | G     | 252 | LYS  | C-N-CA | 10.33 | 131.59      | 120.12   |
| 1   | A     | 252 | LYS  | CA-C-N | 10.28 | 131.53      | 120.12   |
| 1   | A     | 252 | LYS  | C-N-CA | 10.28 | 131.53      | 120.12   |
| 1   | F     | 252 | LYS  | CA-C-N | 10.27 | 131.52      | 120.12   |
| 1   | F     | 252 | LYS  | C-N-CA | 10.27 | 131.52      | 120.12   |
| 1   | A     | 239 | CYS  | CA-C-N | 9.38  | 129.03      | 119.56   |
| 1   | A     | 239 | CYS  | C-N-CA | 9.38  | 129.03      | 119.56   |
| 1   | F     | 239 | CYS  | CA-C-N | 9.35  | 129.00      | 119.56   |
| 1   | F     | 239 | CYS  | C-N-CA | 9.35  | 129.00      | 119.56   |
| 1   | G     | 239 | CYS  | CA-C-N | 9.34  | 129.00      | 119.56   |
| 1   | G     | 239 | CYS  | C-N-CA | 9.34  | 129.00      | 119.56   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 1   | A     | 436 | ALA  | CA-C-N | 8.99 | 126.22      | 119.66   |
| 1   | A     | 436 | ALA  | C-N-CA | 8.99 | 126.22      | 119.66   |
| 1   | F     | 436 | ALA  | CA-C-N | 8.96 | 126.20      | 119.66   |
| 1   | F     | 436 | ALA  | C-N-CA | 8.96 | 126.20      | 119.66   |
| 1   | G     | 436 | ALA  | CA-C-N | 8.91 | 126.16      | 119.66   |
| 1   | G     | 436 | ALA  | C-N-CA | 8.91 | 126.16      | 119.66   |
| 1   | G     | 237 | GLY  | CA-C-N | 8.56 | 128.60      | 119.78   |
| 1   | G     | 237 | GLY  | C-N-CA | 8.56 | 128.60      | 119.78   |
| 1   | A     | 237 | GLY  | CA-C-N | 8.55 | 128.59      | 119.78   |
| 1   | A     | 237 | GLY  | C-N-CA | 8.55 | 128.59      | 119.78   |
| 1   | F     | 237 | GLY  | CA-C-N | 8.52 | 128.56      | 119.78   |
| 1   | F     | 237 | GLY  | C-N-CA | 8.52 | 128.56      | 119.78   |
| 3   | R     | 56  | GLN  | CA-C-N | 8.46 | 128.39      | 119.85   |
| 3   | R     | 56  | GLN  | C-N-CA | 8.46 | 128.39      | 119.85   |
| 1   | A     | 298 | ARG  | CA-C-N | 8.43 | 128.16      | 119.56   |
| 1   | A     | 298 | ARG  | C-N-CA | 8.43 | 128.16      | 119.56   |
| 3   | H     | 56  | GLN  | CA-C-N | 8.43 | 128.36      | 119.85   |
| 3   | H     | 56  | GLN  | C-N-CA | 8.43 | 128.36      | 119.85   |
| 3   | S     | 56  | GLN  | CA-C-N | 8.43 | 128.37      | 119.85   |
| 3   | S     | 56  | GLN  | C-N-CA | 8.43 | 128.37      | 119.85   |
| 1   | G     | 298 | ARG  | CA-C-N | 8.42 | 128.15      | 119.56   |
| 1   | G     | 298 | ARG  | C-N-CA | 8.42 | 128.15      | 119.56   |
| 1   | F     | 298 | ARG  | CA-C-N | 8.42 | 128.15      | 119.56   |
| 1   | F     | 298 | ARG  | C-N-CA | 8.42 | 128.15      | 119.56   |
| 2   | B     | 608 | VAL  | CA-C-N | 7.90 | 127.83      | 119.85   |
| 2   | B     | 608 | VAL  | C-N-CA | 7.90 | 127.83      | 119.85   |
| 2   | J     | 608 | VAL  | CA-C-N | 7.89 | 127.82      | 119.85   |
| 2   | J     | 608 | VAL  | C-N-CA | 7.89 | 127.82      | 119.85   |
| 2   | I     | 608 | VAL  | CA-C-N | 7.89 | 127.82      | 119.85   |
| 2   | I     | 608 | VAL  | C-N-CA | 7.89 | 127.82      | 119.85   |
| 4   | T     | 43  | ALA  | CA-C-N | 7.74 | 127.75      | 119.78   |
| 4   | T     | 43  | ALA  | C-N-CA | 7.74 | 127.75      | 119.78   |
| 4   | L     | 43  | ALA  | CA-C-N | 7.73 | 127.74      | 119.78   |
| 4   | L     | 43  | ALA  | C-N-CA | 7.73 | 127.74      | 119.78   |
| 4   | U     | 43  | ALA  | CA-C-N | 7.72 | 127.73      | 119.78   |
| 4   | U     | 43  | ALA  | C-N-CA | 7.72 | 127.73      | 119.78   |
| 1   | G     | 416 | LEU  | CA-C-N | 7.69 | 127.61      | 119.85   |
| 1   | G     | 416 | LEU  | C-N-CA | 7.69 | 127.61      | 119.85   |
| 1   | F     | 416 | LEU  | CA-C-N | 7.68 | 127.61      | 119.85   |
| 1   | F     | 416 | LEU  | C-N-CA | 7.68 | 127.61      | 119.85   |
| 1   | A     | 416 | LEU  | CA-C-N | 7.65 | 127.58      | 119.85   |
| 1   | A     | 416 | LEU  | C-N-CA | 7.65 | 127.58      | 119.85   |

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| Mol | Chain | Res | Type | Atoms  | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|--------|------|-------------|----------|
| 3   | H     | 59  | ASN  | CA-C-N | 7.46 | 127.47      | 119.78   |
| 3   | H     | 59  | ASN  | C-N-CA | 7.46 | 127.47      | 119.78   |
| 3   | R     | 59  | ASN  | CA-C-N | 7.43 | 127.44      | 119.78   |
| 3   | R     | 59  | ASN  | C-N-CA | 7.43 | 127.44      | 119.78   |
| 3   | S     | 59  | ASN  | CA-C-N | 7.41 | 127.42      | 119.78   |
| 3   | S     | 59  | ASN  | C-N-CA | 7.41 | 127.42      | 119.78   |
| 1   | G     | 219 | ALA  | CA-C-N | 6.87 | 126.85      | 119.78   |
| 1   | G     | 219 | ALA  | C-N-CA | 6.87 | 126.85      | 119.78   |
| 1   | F     | 219 | ALA  | CA-C-N | 6.84 | 126.82      | 119.78   |
| 1   | F     | 219 | ALA  | C-N-CA | 6.84 | 126.82      | 119.78   |
| 1   | A     | 219 | ALA  | CA-C-N | 6.83 | 126.81      | 119.78   |
| 1   | A     | 219 | ALA  | C-N-CA | 6.83 | 126.81      | 119.78   |
| 1   | G     | 205 | CYS  | CA-C-N | 6.80 | 126.50      | 119.56   |
| 1   | G     | 205 | CYS  | C-N-CA | 6.80 | 126.50      | 119.56   |
| 1   | G     | 492 | GLU  | CA-C-N | 6.77 | 126.73      | 119.28   |
| 1   | G     | 492 | GLU  | C-N-CA | 6.77 | 126.73      | 119.28   |
| 1   | A     | 205 | CYS  | CA-C-N | 6.76 | 126.46      | 119.56   |
| 1   | A     | 205 | CYS  | C-N-CA | 6.76 | 126.46      | 119.56   |
| 1   | F     | 205 | CYS  | CA-C-N | 6.75 | 126.45      | 119.56   |
| 1   | F     | 205 | CYS  | C-N-CA | 6.75 | 126.45      | 119.56   |
| 1   | F     | 492 | GLU  | CA-C-N | 6.72 | 126.68      | 119.28   |
| 1   | F     | 492 | GLU  | C-N-CA | 6.72 | 126.68      | 119.28   |
| 1   | A     | 492 | GLU  | CA-C-N | 6.72 | 126.68      | 119.28   |
| 1   | A     | 492 | GLU  | C-N-CA | 6.72 | 126.68      | 119.28   |
| 1   | G     | 437 | PRO  | CA-C-N | 6.70 | 126.61      | 119.85   |
| 1   | G     | 437 | PRO  | C-N-CA | 6.70 | 126.61      | 119.85   |
| 1   | G     | 38  | VAL  | N-CA-C | 6.69 | 118.21      | 109.58   |
| 1   | A     | 437 | PRO  | CA-C-N | 6.66 | 126.58      | 119.85   |
| 1   | A     | 437 | PRO  | C-N-CA | 6.66 | 126.58      | 119.85   |
| 1   | A     | 38  | VAL  | N-CA-C | 6.66 | 118.17      | 109.58   |
| 1   | F     | 38  | VAL  | N-CA-C | 6.65 | 118.16      | 109.58   |
| 1   | F     | 437 | PRO  | CA-C-N | 6.62 | 126.54      | 119.85   |
| 1   | F     | 437 | PRO  | C-N-CA | 6.62 | 126.54      | 119.85   |
| 1   | F     | 75  | VAL  | CA-C-N | 6.58 | 126.50      | 119.85   |
| 1   | F     | 75  | VAL  | C-N-CA | 6.58 | 126.50      | 119.85   |
| 1   | A     | 75  | VAL  | CA-C-N | 6.51 | 126.49      | 119.78   |
| 1   | A     | 75  | VAL  | C-N-CA | 6.51 | 126.49      | 119.78   |
| 1   | G     | 75  | VAL  | CA-C-N | 6.51 | 126.49      | 119.78   |
| 1   | G     | 75  | VAL  | C-N-CA | 6.51 | 126.49      | 119.78   |
| 1   | F     | 290 | THR  | CA-C-N | 6.50 | 126.42      | 119.85   |
| 1   | F     | 290 | THR  | C-N-CA | 6.50 | 126.42      | 119.85   |
| 1   | G     | 290 | THR  | CA-C-N | 6.47 | 126.39      | 119.85   |

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| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 1   | G     | 290 | THR  | C-N-CA  | 6.47  | 126.39      | 119.85   |
| 1   | A     | 290 | THR  | CA-C-N  | 6.47  | 126.39      | 119.85   |
| 1   | A     | 290 | THR  | C-N-CA  | 6.47  | 126.39      | 119.85   |
| 1   | G     | 68  | VAL  | CB-CA-C | -6.43 | 103.46      | 112.14   |
| 1   | A     | 68  | VAL  | CB-CA-C | -6.40 | 103.50      | 112.14   |
| 1   | F     | 68  | VAL  | CB-CA-C | -6.39 | 103.51      | 112.14   |
| 1   | G     | 275 | GLU  | CB-CA-C | -6.28 | 107.55      | 116.34   |
| 1   | F     | 275 | GLU  | CB-CA-C | -6.26 | 107.58      | 116.34   |
| 1   | A     | 275 | GLU  | CB-CA-C | -6.25 | 107.58      | 116.34   |
| 3   | R     | 91  | PHE  | N-CA-C  | 6.21  | 118.51      | 109.07   |
| 4   | U     | 103 | ARG  | N-CA-C  | 6.21  | 118.74      | 108.99   |
| 4   | L     | 103 | ARG  | N-CA-C  | 6.21  | 118.73      | 108.99   |
| 3   | H     | 91  | PHE  | N-CA-C  | 6.20  | 118.50      | 109.07   |
| 3   | S     | 91  | PHE  | N-CA-C  | 6.20  | 118.50      | 109.07   |
| 4   | T     | 103 | ARG  | N-CA-C  | 6.19  | 118.71      | 108.99   |
| 1   | G     | 162 | THR  | N-CA-C  | 6.18  | 118.76      | 110.35   |
| 1   | F     | 162 | THR  | N-CA-C  | 6.17  | 118.75      | 110.35   |
| 1   | A     | 162 | THR  | N-CA-C  | 6.17  | 118.74      | 110.35   |
| 1   | G     | 117 | LYS  | CA-C-N  | 6.13  | 125.75      | 119.56   |
| 1   | G     | 117 | LYS  | C-N-CA  | 6.13  | 125.75      | 119.56   |
| 1   | A     | 117 | LYS  | CA-C-N  | 6.12  | 125.74      | 119.56   |
| 1   | A     | 117 | LYS  | C-N-CA  | 6.12  | 125.74      | 119.56   |
| 2   | I     | 608 | VAL  | N-CA-C  | 6.09  | 113.91      | 107.76   |
| 1   | F     | 117 | LYS  | CA-C-N  | 6.06  | 125.69      | 119.56   |
| 1   | F     | 117 | LYS  | C-N-CA  | 6.06  | 125.69      | 119.56   |
| 2   | J     | 608 | VAL  | N-CA-C  | 6.06  | 113.88      | 107.76   |
| 2   | B     | 608 | VAL  | N-CA-C  | 6.04  | 113.87      | 107.76   |
| 4   | U     | 79  | GLN  | CA-C-N  | 5.90  | 125.77      | 119.28   |
| 4   | U     | 79  | GLN  | C-N-CA  | 5.90  | 125.77      | 119.28   |
| 4   | T     | 79  | GLN  | CA-C-N  | 5.88  | 125.74      | 119.28   |
| 4   | T     | 79  | GLN  | C-N-CA  | 5.88  | 125.74      | 119.28   |
| 4   | L     | 79  | GLN  | CA-C-N  | 5.86  | 125.72      | 119.28   |
| 4   | L     | 79  | GLN  | C-N-CA  | 5.86  | 125.72      | 119.28   |
| 1   | G     | 469 | ARG  | CA-C-N  | 5.65  | 125.60      | 119.78   |
| 1   | G     | 469 | ARG  | C-N-CA  | 5.65  | 125.60      | 119.78   |
| 1   | F     | 469 | ARG  | CA-C-N  | 5.64  | 125.58      | 119.78   |
| 1   | F     | 469 | ARG  | C-N-CA  | 5.64  | 125.58      | 119.78   |
| 2   | B     | 546 | SER  | N-CA-C  | 5.63  | 118.43      | 110.50   |
| 2   | I     | 546 | SER  | N-CA-C  | 5.62  | 118.43      | 110.50   |
| 1   | A     | 469 | ARG  | CA-C-N  | 5.61  | 125.55      | 119.78   |
| 1   | A     | 469 | ARG  | C-N-CA  | 5.61  | 125.55      | 119.78   |
| 2   | J     | 546 | SER  | N-CA-C  | 5.60  | 118.40      | 110.50   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | A     | 382 | PHE  | CA-CB-CG | -5.53 | 108.27      | 113.80   |
| 1   | G     | 382 | PHE  | CA-CB-CG | -5.52 | 108.28      | 113.80   |
| 1   | F     | 382 | PHE  | CA-CB-CG | -5.50 | 108.30      | 113.80   |
| 1   | G     | 354 | GLY  | N-CA-C   | -5.38 | 105.20      | 112.14   |
| 1   | F     | 354 | GLY  | N-CA-C   | -5.37 | 105.21      | 112.14   |
| 1   | A     | 354 | GLY  | N-CA-C   | -5.35 | 105.24      | 112.14   |
| 2   | B     | 607 | ASN  | CA-C-N   | -5.34 | 118.74      | 122.59   |
| 2   | B     | 607 | ASN  | C-N-CA   | -5.34 | 118.74      | 122.59   |
| 2   | J     | 607 | ASN  | CA-C-N   | -5.33 | 118.75      | 122.59   |
| 2   | J     | 607 | ASN  | C-N-CA   | -5.33 | 118.75      | 122.59   |
| 2   | I     | 607 | ASN  | CA-C-N   | -5.33 | 118.76      | 122.59   |
| 2   | I     | 607 | ASN  | C-N-CA   | -5.33 | 118.76      | 122.59   |
| 1   | A     | 424 | ILE  | N-CA-C   | 5.30  | 115.73      | 107.99   |
| 1   | F     | 424 | ILE  | N-CA-C   | 5.29  | 115.71      | 107.99   |
| 1   | G     | 424 | ILE  | N-CA-C   | 5.28  | 115.69      | 107.99   |
| 1   | F     | 242 | VAL  | N-CA-C   | 5.27  | 117.22      | 109.63   |
| 1   | A     | 242 | VAL  | N-CA-C   | 5.24  | 117.18      | 109.63   |
| 3   | H     | 73  | PHE  | CA-CB-CG | -5.24 | 108.56      | 113.80   |
| 1   | G     | 242 | VAL  | N-CA-C   | 5.23  | 117.16      | 109.63   |
| 3   | S     | 73  | PHE  | CA-CB-CG | -5.23 | 108.57      | 113.80   |
| 3   | R     | 73  | PHE  | CA-CB-CG | -5.22 | 108.58      | 113.80   |
| 4   | L     | 82  | ASP  | CA-C-N   | -5.15 | 114.58      | 121.80   |
| 4   | L     | 82  | ASP  | C-N-CA   | -5.15 | 114.58      | 121.80   |
| 4   | U     | 82  | ASP  | CA-C-N   | -5.15 | 114.59      | 121.80   |
| 4   | U     | 82  | ASP  | C-N-CA   | -5.15 | 114.59      | 121.80   |
| 1   | A     | 300 | ASN  | CA-CB-CG | -5.15 | 107.45      | 112.60   |
| 4   | T     | 82  | ASP  | CA-C-N   | -5.15 | 114.59      | 121.80   |
| 4   | T     | 82  | ASP  | C-N-CA   | -5.15 | 114.59      | 121.80   |
| 1   | G     | 300 | ASN  | CA-CB-CG | -5.13 | 107.47      | 112.60   |
| 1   | F     | 300 | ASN  | CA-CB-CG | -5.13 | 107.47      | 112.60   |
| 3   | H     | 104 | GLY  | N-CA-C   | -5.09 | 106.03      | 112.54   |
| 2   | J     | 636 | SER  | N-CA-C   | 5.08  | 118.95      | 112.34   |
| 3   | S     | 104 | GLY  | N-CA-C   | -5.07 | 106.05      | 112.54   |
| 1   | G     | 123 | THR  | CA-C-N   | 5.07  | 124.73      | 119.56   |
| 1   | G     | 123 | THR  | C-N-CA   | 5.07  | 124.73      | 119.56   |
| 4   | U     | 8   | PRO  | N-CA-C   | 5.07  | 120.49      | 113.65   |
| 3   | R     | 104 | GLY  | N-CA-C   | -5.06 | 106.06      | 112.54   |
| 2   | B     | 636 | SER  | N-CA-C   | 5.06  | 118.92      | 112.34   |
| 4   | L     | 8   | PRO  | N-CA-C   | 5.06  | 120.48      | 113.65   |
| 4   | T     | 8   | PRO  | N-CA-C   | 5.06  | 120.48      | 113.65   |
| 1   | A     | 123 | THR  | CA-C-N   | 5.04  | 124.71      | 119.56   |
| 1   | A     | 123 | THR  | C-N-CA   | 5.04  | 124.71      | 119.56   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1   | G     | 318 | TYR  | CA-CB-CG | -5.04 | 104.83      | 113.90   |
| 2   | I     | 636 | SER  | N-CA-C   | 5.03  | 118.88      | 112.34   |
| 1   | A     | 318 | TYR  | CA-CB-CG | -5.03 | 104.84      | 113.90   |
| 1   | F     | 318 | TYR  | CA-CB-CG | -5.03 | 104.85      | 113.90   |
| 1   | F     | 123 | THR  | CA-C-N   | 5.02  | 124.68      | 119.56   |
| 1   | F     | 123 | THR  | C-N-CA   | 5.02  | 124.68      | 119.56   |
| 4   | U     | 7   | SER  | N-CA-C   | 5.02  | 120.90      | 109.81   |
| 4   | L     | 7   | SER  | N-CA-C   | 5.01  | 120.89      | 109.81   |
| 4   | T     | 7   | SER  | N-CA-C   | 5.01  | 120.89      | 109.81   |

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | A     | 3493  | 0        | 3420     | 50      | 0            |
| 1   | F     | 3493  | 0        | 3420     | 48      | 0            |
| 1   | G     | 3493  | 0        | 3420     | 49      | 0            |
| 2   | B     | 1024  | 0        | 1005     | 9       | 0            |
| 2   | I     | 1024  | 0        | 1005     | 10      | 0            |
| 2   | J     | 1024  | 0        | 1005     | 11      | 0            |
| 3   | H     | 985   | 0        | 919      | 4       | 0            |
| 3   | R     | 985   | 0        | 919      | 6       | 0            |
| 3   | S     | 985   | 0        | 919      | 5       | 0            |
| 4   | L     | 783   | 0        | 763      | 14      | 0            |
| 4   | T     | 783   | 0        | 763      | 13      | 0            |
| 4   | U     | 783   | 0        | 763      | 13      | 0            |
| 5   | C     | 39    | 0        | 34       | 3       | 0            |
| 5   | Z     | 39    | 0        | 34       | 3       | 0            |
| 5   | m     | 39    | 0        | 34       | 3       | 0            |
| 6   | D     | 28    | 0        | 25       | 6       | 0            |
| 6   | E     | 28    | 0        | 25       | 6       | 0            |
| 6   | K     | 28    | 0        | 25       | 0       | 0            |
| 6   | O     | 28    | 0        | 25       | 13      | 0            |
| 6   | P     | 28    | 0        | 25       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 6   | Q     | 28    | 0        | 25       | 5       | 0            |
| 6   | X     | 28    | 0        | 25       | 2       | 0            |
| 6   | Y     | 28    | 0        | 25       | 0       | 0            |
| 6   | a     | 28    | 0        | 25       | 6       | 0            |
| 6   | b     | 28    | 0        | 25       | 6       | 0            |
| 6   | c     | 28    | 0        | 25       | 0       | 0            |
| 6   | f     | 28    | 0        | 25       | 13      | 0            |
| 6   | g     | 28    | 0        | 25       | 1       | 0            |
| 6   | h     | 28    | 0        | 25       | 5       | 0            |
| 6   | k     | 28    | 0        | 25       | 2       | 0            |
| 6   | l     | 28    | 0        | 25       | 0       | 0            |
| 6   | n     | 28    | 0        | 25       | 6       | 0            |
| 6   | o     | 28    | 0        | 25       | 6       | 0            |
| 6   | p     | 28    | 0        | 25       | 0       | 0            |
| 6   | s     | 28    | 0        | 25       | 13      | 0            |
| 6   | t     | 28    | 0        | 25       | 1       | 0            |
| 6   | u     | 28    | 0        | 25       | 5       | 0            |
| 6   | x     | 28    | 0        | 25       | 2       | 0            |
| 6   | y     | 28    | 0        | 25       | 0       | 0            |
| 7   | M     | 83    | 0        | 70       | 0       | 0            |
| 7   | d     | 83    | 0        | 70       | 0       | 0            |
| 7   | q     | 83    | 0        | 70       | 0       | 0            |
| 8   | N     | 94    | 0        | 79       | 4       | 0            |
| 8   | e     | 94    | 0        | 79       | 4       | 0            |
| 8   | r     | 94    | 0        | 79       | 4       | 0            |
| 9   | V     | 72    | 0        | 61       | 1       | 0            |
| 9   | i     | 72    | 0        | 61       | 1       | 0            |
| 9   | v     | 72    | 0        | 61       | 1       | 0            |
| 10  | W     | 50    | 0        | 43       | 1       | 0            |
| 10  | j     | 50    | 0        | 43       | 1       | 0            |
| 10  | w     | 50    | 0        | 43       | 1       | 0            |
| 11  | A     | 70    | 0        | 65       | 0       | 0            |
| 11  | B     | 28    | 0        | 26       | 6       | 0            |
| 11  | F     | 70    | 0        | 65       | 0       | 0            |
| 11  | G     | 70    | 0        | 65       | 0       | 0            |
| 11  | I     | 28    | 0        | 26       | 6       | 0            |
| 11  | J     | 28    | 0        | 26       | 6       | 0            |
| All | All   | 20835 | 0        | 20055    | 238     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (238) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 1:F:130:GLN:HG2   | 6:b:1:NAG:C8     | 1.79                     | 1.12              |
| 1:A:130:GLN:HG2   | 6:E:1:NAG:C8     | 1.79                     | 1.11              |
| 1:G:130:GLN:HG2   | 6:o:1:NAG:C8     | 1.79                     | 1.11              |
| 1:A:130:GLN:HG2   | 6:E:1:NAG:H81    | 1.05                     | 1.04              |
| 1:F:130:GLN:CG    | 6:b:1:NAG:H81    | 1.88                     | 1.04              |
| 1:A:130:GLN:CG    | 6:E:1:NAG:H81    | 1.88                     | 1.03              |
| 1:F:87:GLU:OE1    | 5:Z:1:NAG:H81    | 1.59                     | 1.03              |
| 1:G:87:GLU:OE1    | 5:m:1:NAG:H81    | 1.59                     | 1.03              |
| 1:F:130:GLN:HG2   | 6:b:1:NAG:H81    | 1.04                     | 1.02              |
| 1:A:87:GLU:OE1    | 5:C:1:NAG:H81    | 1.59                     | 1.02              |
| 1:G:130:GLN:CG    | 6:o:1:NAG:H81    | 1.89                     | 1.02              |
| 1:A:293:GLN:CD    | 6:O:1:NAG:HN2    | 1.67                     | 1.02              |
| 1:G:293:GLN:CD    | 6:s:1:NAG:HN2    | 1.67                     | 1.01              |
| 1:G:130:GLN:HG2   | 6:o:1:NAG:H81    | 1.05                     | 1.01              |
| 1:A:203:GLN:OE1   | 1:A:434:MET:HE3  | 1.60                     | 1.01              |
| 1:F:293:GLN:CD    | 6:f:1:NAG:HN2    | 1.68                     | 1.00              |
| 1:A:293:GLN:HE22  | 6:O:1:NAG:H3     | 1.26                     | 1.00              |
| 1:G:203:GLN:OE1   | 1:G:434:MET:HE3  | 1.60                     | 0.99              |
| 1:F:293:GLN:HE22  | 6:f:1:NAG:H3     | 1.26                     | 0.99              |
| 1:F:203:GLN:OE1   | 1:F:434:MET:HE3  | 1.60                     | 0.99              |
| 1:G:293:GLN:HE22  | 6:s:1:NAG:H3     | 1.26                     | 0.98              |
| 1:F:130:GLN:CG    | 6:b:1:NAG:C8     | 2.43                     | 0.97              |
| 1:A:130:GLN:CG    | 6:E:1:NAG:C8     | 2.43                     | 0.96              |
| 1:G:130:GLN:CG    | 6:o:1:NAG:C8     | 2.43                     | 0.94              |
| 4:T:66:ARG:O      | 4:T:67:TRP:CD1   | 2.21                     | 0.93              |
| 4:L:66:ARG:O      | 4:L:67:TRP:CD1   | 2.21                     | 0.93              |
| 4:T:66:ARG:O      | 4:T:67:TRP:HD1   | 1.51                     | 0.93              |
| 4:U:66:ARG:O      | 4:U:67:TRP:HD1   | 1.51                     | 0.93              |
| 4:U:66:ARG:O      | 4:U:67:TRP:CD1   | 2.21                     | 0.92              |
| 4:L:66:ARG:O      | 4:L:67:TRP:HD1   | 1.51                     | 0.92              |
| 6:x:1:NAG:H61     | 6:x:2:NAG:HN2    | 1.43                     | 0.83              |
| 2:I:633:LYS:O     | 11:I:702:NAG:H82 | 1.79                     | 0.83              |
| 6:k:1:NAG:H61     | 6:k:2:NAG:HN2    | 1.43                     | 0.83              |
| 2:J:633:LYS:O     | 11:J:702:NAG:H82 | 1.79                     | 0.82              |
| 1:G:321(A):ASP:CG | 6:n:1:NAG:H83    | 2.05                     | 0.82              |
| 2:B:633:LYS:O     | 11:B:702:NAG:H82 | 1.79                     | 0.82              |
| 6:X:1:NAG:H61     | 6:X:2:NAG:HN2    | 1.43                     | 0.82              |
| 1:A:321(A):ASP:CG | 6:D:1:NAG:H83    | 2.05                     | 0.81              |
| 1:F:321(A):ASP:CG | 6:a:1:NAG:H83    | 2.05                     | 0.81              |
| 1:F:130:GLN:HG3   | 6:b:1:NAG:H83    | 1.65                     | 0.79              |
| 1:G:130:GLN:HG3   | 6:o:1:NAG:H83    | 1.65                     | 0.79              |
| 1:A:130:GLN:HG3   | 6:E:1:NAG:H83    | 1.65                     | 0.78              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:130:GLN:CG     | 6:b:1:NAG:H83    | 2.19                     | 0.73              |
| 1:A:293:GLN:NE2    | 6:O:1:NAG:H3     | 2.04                     | 0.72              |
| 3:S:111:VAL:HG12   | 3:S:111:VAL:O    | 1.90                     | 0.72              |
| 1:G:130:GLN:CG     | 6:o:1:NAG:H83    | 2.19                     | 0.72              |
| 3:H:111:VAL:HG12   | 3:H:111:VAL:O    | 1.90                     | 0.72              |
| 3:R:111:VAL:O      | 3:R:111:VAL:HG12 | 1.90                     | 0.71              |
| 1:A:130:GLN:CG     | 6:E:1:NAG:H83    | 2.19                     | 0.71              |
| 1:F:293:GLN:NE2    | 6:f:1:NAG:H3     | 2.04                     | 0.71              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:H3     | 2.04                     | 0.70              |
| 1:A:293:GLN:NE2    | 6:O:1:NAG:HN2    | 1.91                     | 0.69              |
| 4:L:32:TYR:OH      | 8:N:1:NAG:H4     | 1.94                     | 0.68              |
| 4:U:32:TYR:OH      | 8:r:1:NAG:H4     | 1.94                     | 0.68              |
| 1:F:293:GLN:NE2    | 6:f:1:NAG:HN2    | 1.92                     | 0.67              |
| 4:T:32:TYR:OH      | 8:e:1:NAG:H4     | 1.94                     | 0.67              |
| 1:F:363:ASN:OD1    | 1:F:364:SER:O    | 2.12                     | 0.67              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:HN2    | 1.91                     | 0.67              |
| 1:G:203:GLN:OE1    | 1:G:434:MET:CE   | 2.40                     | 0.67              |
| 1:A:363:ASN:OD1    | 1:A:364:SER:O    | 2.12                     | 0.67              |
| 1:G:363:ASN:OD1    | 1:G:364:SER:O    | 2.12                     | 0.66              |
| 4:T:66:ARG:NH1     | 8:e:2:NAG:O7     | 2.30                     | 0.65              |
| 1:G:293:GLN:HE22   | 6:s:1:NAG:C3     | 2.06                     | 0.65              |
| 4:U:66:ARG:NH1     | 8:r:2:NAG:O7     | 2.30                     | 0.65              |
| 1:A:203:GLN:OE1    | 1:A:434:MET:CE   | 2.41                     | 0.65              |
| 1:F:203:GLN:OE1    | 1:F:434:MET:CE   | 2.40                     | 0.65              |
| 4:L:32:TYR:CZ      | 8:N:1:NAG:H4     | 2.33                     | 0.64              |
| 4:T:32:TYR:CZ      | 8:e:1:NAG:H4     | 2.33                     | 0.64              |
| 4:L:66:ARG:NH1     | 8:N:2:NAG:O7     | 2.30                     | 0.64              |
| 4:U:32:TYR:CZ      | 8:r:1:NAG:H4     | 2.33                     | 0.63              |
| 1:F:72:HIS:CD2     | 1:F:72:HIS:N     | 2.67                     | 0.62              |
| 1:A:293:GLN:HE22   | 6:O:1:NAG:C3     | 2.06                     | 0.62              |
| 1:F:293:GLN:HE22   | 6:f:1:NAG:C3     | 2.06                     | 0.62              |
| 1:F:293:GLN:NE2    | 6:f:1:NAG:N2     | 2.48                     | 0.62              |
| 1:A:72:HIS:N       | 1:A:72:HIS:CD2   | 2.67                     | 0.61              |
| 1:A:293:GLN:NE2    | 6:O:1:NAG:N2     | 2.48                     | 0.61              |
| 1:F:293:GLN:CD     | 6:f:1:NAG:N2     | 2.51                     | 0.61              |
| 1:G:321(A):ASP:OD1 | 6:n:1:NAG:H82    | 2.01                     | 0.61              |
| 4:L:65:ARG:NH2     | 4:L:67:TRP:HZ2   | 1.99                     | 0.61              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:N2     | 2.48                     | 0.61              |
| 1:F:321(A):ASP:OD1 | 6:a:1:NAG:H82    | 2.01                     | 0.60              |
| 1:G:321(A):ASP:OD1 | 6:n:1:NAG:C8     | 2.50                     | 0.60              |
| 1:A:321(A):ASP:OD1 | 6:D:1:NAG:H82    | 2.01                     | 0.60              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:F:321(A):ASP:CG  | 6:a:1:NAG:C8     | 2.75                     | 0.60              |
| 1:F:321(A):ASP:OD1 | 6:a:1:NAG:C8     | 2.50                     | 0.60              |
| 1:G:293:GLN:CD     | 6:s:1:NAG:N2     | 2.51                     | 0.60              |
| 4:U:65:ARG:NH2     | 4:U:67:TRP:HZ2   | 1.99                     | 0.60              |
| 4:U:65:ARG:NH2     | 4:U:67:TRP:CZ2   | 2.70                     | 0.60              |
| 4:T:65:ARG:NH2     | 4:T:67:TRP:HZ2   | 1.99                     | 0.59              |
| 4:T:65:ARG:NH2     | 4:T:67:TRP:CZ2   | 2.70                     | 0.59              |
| 1:G:72:HIS:CD2     | 1:G:72:HIS:N     | 2.67                     | 0.59              |
| 1:A:293:GLN:HB3    | 6:O:1:NAG:C8     | 2.33                     | 0.59              |
| 1:F:87:GLU:CD      | 5:Z:1:NAG:H81    | 2.27                     | 0.59              |
| 1:A:321(A):ASP:OD1 | 6:D:1:NAG:C8     | 2.50                     | 0.59              |
| 1:A:175:LEU:HD21   | 6:D:1:NAG:H82    | 1.85                     | 0.59              |
| 1:G:175:LEU:HD21   | 6:n:1:NAG:H82    | 1.85                     | 0.59              |
| 1:G:293:GLN:HB3    | 6:s:1:NAG:C8     | 2.33                     | 0.58              |
| 1:A:321(A):ASP:CG  | 6:D:1:NAG:C8     | 2.75                     | 0.58              |
| 1:F:293:GLN:HB3    | 6:f:1:NAG:C8     | 2.33                     | 0.58              |
| 1:G:87:GLU:CD      | 5:m:1:NAG:H81    | 2.27                     | 0.58              |
| 4:L:65:ARG:NH2     | 4:L:67:TRP:CZ2   | 2.70                     | 0.58              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:C2     | 2.66                     | 0.58              |
| 1:A:87:GLU:CD      | 5:C:1:NAG:H81    | 2.27                     | 0.58              |
| 1:A:293:GLN:NE2    | 6:O:1:NAG:C2     | 2.66                     | 0.58              |
| 1:F:175:LEU:HD21   | 6:a:1:NAG:H82    | 1.85                     | 0.58              |
| 1:F:293:GLN:NE2    | 6:f:1:NAG:C2     | 2.66                     | 0.58              |
| 4:L:69:GLN:OE1     | 4:L:69:GLN:N     | 2.31                     | 0.57              |
| 1:G:321(A):ASP:CG  | 6:n:1:NAG:C8     | 2.75                     | 0.57              |
| 4:U:69:GLN:OE1     | 4:U:69:GLN:N     | 2.31                     | 0.57              |
| 2:B:633:LYS:O      | 11:B:702:NAG:C8  | 2.53                     | 0.57              |
| 1:G:461:THR:OG1    | 3:S:61:ARG:NH2   | 2.38                     | 0.57              |
| 2:J:634:GLU:O      | 11:J:702:NAG:H81 | 2.05                     | 0.57              |
| 2:I:634:GLU:O      | 11:I:702:NAG:H81 | 2.05                     | 0.56              |
| 1:F:461:THR:OG1    | 3:R:61:ARG:NH2   | 2.38                     | 0.56              |
| 1:A:461:THR:OG1    | 3:H:61:ARG:NH2   | 2.38                     | 0.56              |
| 2:J:634:GLU:HA     | 11:J:702:NAG:H81 | 1.87                     | 0.56              |
| 2:J:633:LYS:O      | 11:J:702:NAG:C8  | 2.53                     | 0.56              |
| 2:I:634:GLU:HA     | 11:I:702:NAG:H81 | 1.87                     | 0.56              |
| 2:B:634:GLU:O      | 11:B:702:NAG:H81 | 2.05                     | 0.56              |
| 1:F:293:GLN:NE2    | 6:f:1:NAG:C1     | 2.69                     | 0.56              |
| 1:F:297:THR:CG2    | 6:h:1:NAG:H83    | 2.36                     | 0.56              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:C1     | 2.69                     | 0.56              |
| 2:B:634:GLU:HA     | 11:B:702:NAG:H81 | 1.87                     | 0.55              |
| 1:A:293:GLN:NE2    | 6:O:1:NAG:C1     | 2.69                     | 0.55              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:G:297:THR:CG2  | 6:u:1:NAG:H83   | 2.36                     | 0.55              |
| 2:I:633:LYS:O    | 11:I:702:NAG:C8 | 2.53                     | 0.55              |
| 1:A:297:THR:CG2  | 6:Q:1:NAG:H83   | 2.36                     | 0.54              |
| 4:T:69:GLN:OE1   | 4:T:69:GLN:N    | 2.31                     | 0.54              |
| 1:F:293:GLN:HB3  | 6:f:1:NAG:H82   | 1.90                     | 0.54              |
| 1:G:293:GLN:HB3  | 6:s:1:NAG:H82   | 1.90                     | 0.54              |
| 2:I:611:ASN:ND2  | 11:I:701:NAG:O7 | 2.42                     | 0.53              |
| 1:A:293:GLN:HB3  | 6:O:1:NAG:H82   | 1.90                     | 0.53              |
| 1:G:297:THR:CG2  | 6:u:1:NAG:C8    | 2.87                     | 0.52              |
| 2:B:611:ASN:ND2  | 11:B:701:NAG:O7 | 2.42                     | 0.52              |
| 4:L:7:SER:N      | 4:L:8:PRO:CD    | 2.73                     | 0.52              |
| 1:A:293:GLN:CD   | 6:O:1:NAG:N2    | 2.51                     | 0.52              |
| 2:J:611:ASN:ND2  | 11:J:701:NAG:O7 | 2.42                     | 0.52              |
| 2:I:634:GLU:HA   | 11:I:702:NAG:C8 | 2.40                     | 0.52              |
| 2:J:634:GLU:HA   | 11:J:702:NAG:C8 | 2.40                     | 0.52              |
| 1:A:297:THR:CG2  | 6:Q:1:NAG:C8    | 2.87                     | 0.52              |
| 4:T:7:SER:N      | 4:T:8:PRO:CD    | 2.73                     | 0.52              |
| 1:F:297:THR:CG2  | 6:h:1:NAG:C8    | 2.88                     | 0.51              |
| 4:U:7:SER:N      | 4:U:8:PRO:CD    | 2.73                     | 0.51              |
| 2:B:634:GLU:HA   | 11:B:702:NAG:C8 | 2.40                     | 0.51              |
| 5:C:2:NAG:H83    | 5:C:2:NAG:H3    | 1.92                     | 0.51              |
| 5:Z:2:NAG:H3     | 5:Z:2:NAG:H83   | 1.92                     | 0.50              |
| 1:F:365:SER:OG   | 3:R:56:GLN:NE2  | 2.44                     | 0.50              |
| 1:G:365:SER:OG   | 3:S:56:GLN:NE2  | 2.44                     | 0.50              |
| 1:A:297:THR:HG22 | 6:Q:1:NAG:H82   | 1.94                     | 0.50              |
| 1:F:246:GLN:OE1  | 1:F:246:GLN:N   | 2.36                     | 0.50              |
| 5:m:2:NAG:H3     | 5:m:2:NAG:H83   | 1.92                     | 0.50              |
| 1:A:365:SER:OG   | 3:H:56:GLN:NE2  | 2.44                     | 0.49              |
| 1:F:363:ASN:OD1  | 1:F:363:ASN:C   | 2.55                     | 0.49              |
| 1:A:293:GLN:NE2  | 6:O:1:NAG:C3    | 2.71                     | 0.49              |
| 1:F:297:THR:HG22 | 6:h:1:NAG:H82   | 1.94                     | 0.49              |
| 1:G:164:GLU:OE1  | 1:G:164:GLU:N   | 2.36                     | 0.48              |
| 1:G:297:THR:HG22 | 6:u:1:NAG:C8    | 2.43                     | 0.48              |
| 1:G:297:THR:HG22 | 6:u:1:NAG:H82   | 1.94                     | 0.48              |
| 1:G:363:ASN:OD1  | 1:G:363:ASN:C   | 2.56                     | 0.48              |
| 1:F:293:GLN:NE2  | 6:f:1:NAG:C3    | 2.71                     | 0.48              |
| 1:G:246:GLN:OE1  | 1:G:246:GLN:N   | 2.36                     | 0.48              |
| 1:A:363:ASN:OD1  | 1:A:363:ASN:C   | 2.56                     | 0.48              |
| 1:F:297:THR:HG22 | 6:h:1:NAG:C8    | 2.43                     | 0.47              |
| 1:A:479:TRP:HA   | 1:A:479:TRP:CE3 | 2.49                     | 0.47              |
| 1:F:164:GLU:OE1  | 1:F:164:GLU:N   | 2.36                     | 0.47              |

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| Atom-1             | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|--------------------|------------------|--------------------------|-------------------|
| 1:G:479:TRP:HA     | 1:G:479:TRP:CE3  | 2.50                     | 0.47              |
| 1:G:293:GLN:NE2    | 6:s:1:NAG:C3     | 2.71                     | 0.47              |
| 1:F:479:TRP:HE3    | 1:F:479:TRP:HA   | 1.80                     | 0.47              |
| 1:G:479:TRP:HA     | 1:G:479:TRP:HE3  | 1.80                     | 0.47              |
| 2:J:635:ILE:HG13   | 2:J:635:ILE:O    | 2.15                     | 0.47              |
| 1:A:297:THR:HG22   | 6:Q:1:NAG:C8     | 2.43                     | 0.46              |
| 1:F:479:TRP:HA     | 1:F:479:TRP:CE3  | 2.49                     | 0.46              |
| 1:F:430:ILE:HD12   | 1:F:430:ILE:C    | 2.41                     | 0.46              |
| 1:A:479:TRP:HA     | 1:A:479:TRP:HE3  | 1.80                     | 0.46              |
| 1:A:321(A):ASP:OD2 | 6:D:1:NAG:H83    | 2.16                     | 0.46              |
| 2:B:635:ILE:HG13   | 2:B:635:ILE:O    | 2.15                     | 0.46              |
| 1:A:246:GLN:OE1    | 1:A:246:GLN:N    | 2.36                     | 0.46              |
| 1:A:293:GLN:HB3    | 6:O:1:NAG:H83    | 1.98                     | 0.45              |
| 1:A:430:ILE:C      | 1:A:430:ILE:HD12 | 2.41                     | 0.45              |
| 1:G:293:GLN:HB3    | 6:s:1:NAG:H83    | 1.98                     | 0.45              |
| 1:A:297:THR:HG21   | 6:Q:1:NAG:H83    | 1.97                     | 0.45              |
| 1:G:430:ILE:C      | 1:G:430:ILE:HD12 | 2.41                     | 0.45              |
| 4:L:11:LEU:O       | 4:L:105:ASP:N    | 2.50                     | 0.45              |
| 1:G:321(A):ASP:OD2 | 6:n:1:NAG:H83    | 2.16                     | 0.45              |
| 4:T:11:LEU:O       | 4:T:105:ASP:N    | 2.50                     | 0.45              |
| 1:G:297:THR:HG21   | 6:u:1:NAG:H83    | 1.97                     | 0.45              |
| 9:i:1:NAG:H2       | 10:j:1:NAG:H5    | 1.99                     | 0.45              |
| 6:P:1:NAG:H61      | 6:P:2:NAG:N2     | 2.32                     | 0.45              |
| 1:F:297:THR:HG21   | 6:h:1:NAG:H83    | 1.97                     | 0.45              |
| 6:t:1:NAG:H61      | 6:t:2:NAG:N2     | 2.32                     | 0.45              |
| 4:L:22:THR:HG22    | 4:L:72:ASN:OD1   | 2.17                     | 0.44              |
| 1:F:293:GLN:HB3    | 6:f:1:NAG:H83    | 1.98                     | 0.44              |
| 6:x:1:NAG:H61      | 6:x:2:NAG:N2     | 2.22                     | 0.44              |
| 9:V:1:NAG:H2       | 10:W:1:NAG:H5    | 1.99                     | 0.44              |
| 4:T:22:THR:HG22    | 4:T:72:ASN:OD1   | 2.17                     | 0.44              |
| 3:H:91:PHE:HB3     | 3:H:106:GLY:HA2  | 1.99                     | 0.44              |
| 2:I:635:ILE:HG13   | 2:I:635:ILE:O    | 2.15                     | 0.44              |
| 6:g:1:NAG:H61      | 6:g:2:NAG:N2     | 2.32                     | 0.44              |
| 1:F:321(A):ASP:OD2 | 6:a:1:NAG:H83    | 2.16                     | 0.44              |
| 6:X:1:NAG:H61      | 6:X:2:NAG:N2     | 2.22                     | 0.44              |
| 4:U:22:THR:HG22    | 4:U:72:ASN:OD1   | 2.17                     | 0.43              |
| 9:v:1:NAG:H2       | 10:w:1:NAG:H5    | 1.99                     | 0.43              |
| 3:R:91:PHE:HB3     | 3:R:106:GLY:HA2  | 1.99                     | 0.43              |
| 4:U:11:LEU:O       | 4:U:105:ASP:N    | 2.50                     | 0.43              |
| 2:B:614:TRP:CD1    | 2:B:614:TRP:N    | 2.85                     | 0.43              |
| 3:S:91:PHE:HB3     | 3:S:106:GLY:HA2  | 1.99                     | 0.43              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:I:614:TRP:CD1  | 2:I:614:TRP:N    | 2.85                     | 0.42              |
| 4:L:66:ARG:C     | 4:L:67:TRP:CD1   | 2.96                     | 0.42              |
| 2:J:614:TRP:N    | 2:J:614:TRP:CD1  | 2.85                     | 0.42              |
| 1:F:290:THR:HB   | 1:F:291:PRO:HD2  | 2.02                     | 0.42              |
| 1:G:290:THR:HB   | 1:G:291:PRO:HD2  | 2.02                     | 0.42              |
| 1:F:479:TRP:CE3  | 1:F:479:TRP:CA   | 3.03                     | 0.42              |
| 1:A:290:THR:HB   | 1:A:291:PRO:HD2  | 2.02                     | 0.42              |
| 1:A:164:GLU:OE1  | 1:A:164:GLU:N    | 2.36                     | 0.42              |
| 1:F:503:ARG:HB3  | 2:I:607:ASN:HB2  | 2.02                     | 0.41              |
| 4:T:66:ARG:CZ    | 8:e:2:NAG:H81    | 2.50                     | 0.41              |
| 1:A:69:TRP:HA    | 1:A:69:TRP:CE3   | 2.56                     | 0.41              |
| 1:G:116:LEU:HD11 | 1:G:434:MET:SD   | 2.60                     | 0.41              |
| 4:U:66:ARG:CZ    | 8:r:2:NAG:H81    | 2.50                     | 0.41              |
| 1:A:116:LEU:HD11 | 1:A:434:MET:SD   | 2.60                     | 0.41              |
| 1:A:479:TRP:CE3  | 1:A:479:TRP:CA   | 3.03                     | 0.41              |
| 4:L:66:ARG:CZ    | 8:N:2:NAG:H81    | 2.50                     | 0.41              |
| 1:F:116:LEU:HD11 | 1:F:434:MET:SD   | 2.60                     | 0.41              |
| 1:G:479:TRP:CE3  | 1:G:479:TRP:CA   | 3.03                     | 0.41              |
| 4:L:35:TRP:HB2   | 4:L:48:ILE:HG22  | 2.03                     | 0.41              |
| 1:G:503:ARG:HB3  | 2:J:607:ASN:HB2  | 2.02                     | 0.41              |
| 2:I:570:VAL:O    | 2:I:571:TRP:HB2  | 2.21                     | 0.41              |
| 1:A:213:ILE:O    | 1:A:213:ILE:HG23 | 2.21                     | 0.41              |
| 4:T:35:TRP:HB2   | 4:T:48:ILE:HG22  | 2.03                     | 0.41              |
| 1:A:503:ARG:HB3  | 2:B:607:ASN:HB2  | 2.02                     | 0.40              |
| 2:J:530:MET:HG2  | 2:J:628:TRP:HA   | 2.04                     | 0.40              |
| 3:S:80:MET:SD    | 3:S:80:MET:C     | 3.05                     | 0.40              |
| 2:J:570:VAL:O    | 2:J:571:TRP:HB2  | 2.21                     | 0.40              |
| 3:R:80:MET:SD    | 3:R:80:MET:C     | 3.05                     | 0.40              |
| 4:U:35:TRP:HB2   | 4:U:48:ILE:HG22  | 2.03                     | 0.40              |
| 6:k:1:NAG:H61    | 6:k:2:NAG:N2     | 2.22                     | 0.40              |
| 3:R:56:GLN:HA    | 3:R:57:PRO:HD2   | 1.92                     | 0.40              |
| 1:G:69:TRP:CE3   | 1:G:69:TRP:HA    | 2.56                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

entries.

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

| Mol | Chain | Analysed        | Favoured   | Allowed | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|---------|----------|-------------|-----|
| 1   | A     | 436/481 (91%)   | 427 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 1   | F     | 436/481 (91%)   | 427 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 1   | G     | 436/481 (91%)   | 427 (98%)  | 9 (2%)  | 0        | 100         | 100 |
| 2   | B     | 125/153 (82%)   | 123 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 2   | I     | 125/153 (82%)   | 123 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 2   | J     | 125/153 (82%)   | 122 (98%)  | 3 (2%)  | 0        | 100         | 100 |
| 3   | H     | 119/226 (53%)   | 117 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 3   | R     | 119/226 (53%)   | 117 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 3   | S     | 119/226 (53%)   | 117 (98%)  | 2 (2%)  | 0        | 100         | 100 |
| 4   | L     | 96/206 (47%)    | 91 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 4   | T     | 96/206 (47%)    | 91 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| 4   | U     | 96/206 (47%)    | 91 (95%)   | 5 (5%)  | 0        | 100         | 100 |
| All | All   | 2328/3198 (73%) | 2273 (98%) | 55 (2%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

| Mol | Chain | Analysed      | Rotameric  | Outliers | Percentiles |     |
|-----|-------|---------------|------------|----------|-------------|-----|
| 1   | A     | 397/428 (93%) | 396 (100%) | 1 (0%)   | 86          | 84  |
| 1   | F     | 397/428 (93%) | 396 (100%) | 1 (0%)   | 86          | 84  |
| 1   | G     | 397/428 (93%) | 396 (100%) | 1 (0%)   | 86          | 84  |
| 2   | B     | 111/129 (86%) | 111 (100%) | 0        | 100         | 100 |
| 2   | I     | 111/129 (86%) | 111 (100%) | 0        | 100         | 100 |
| 2   | J     | 111/129 (86%) | 111 (100%) | 0        | 100         | 100 |

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| Mol | Chain | Analysed        | Rotameric   | Outliers | Percentiles |     |
|-----|-------|-----------------|-------------|----------|-------------|-----|
| 3   | H     | 102/193 (53%)   | 102 (100%)  | 0        | 100         | 100 |
| 3   | R     | 102/193 (53%)   | 102 (100%)  | 0        | 100         | 100 |
| 3   | S     | 102/193 (53%)   | 102 (100%)  | 0        | 100         | 100 |
| 4   | L     | 86/183 (47%)    | 86 (100%)   | 0        | 100         | 100 |
| 4   | T     | 86/183 (47%)    | 86 (100%)   | 0        | 100         | 100 |
| 4   | U     | 86/183 (47%)    | 86 (100%)   | 0        | 100         | 100 |
| All | All   | 2088/2799 (75%) | 2085 (100%) | 3 (0%)   | 87          | 88  |

All (3) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 363 | ASN  |
| 1   | F     | 363 | ASN  |
| 1   | G     | 363 | ASN  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 66  | HIS  |
| 1   | A     | 293 | GLN  |
| 1   | A     | 428 | GLN  |
| 2   | B     | 640 | GLN  |
| 3   | H     | 39  | GLN  |
| 4   | L     | 38  | GLN  |
| 4   | L     | 76  | ASN  |
| 1   | F     | 66  | HIS  |
| 1   | F     | 293 | GLN  |
| 1   | F     | 428 | GLN  |
| 3   | R     | 39  | GLN  |
| 4   | T     | 38  | GLN  |
| 4   | T     | 76  | ASN  |
| 1   | G     | 66  | HIS  |
| 1   | G     | 293 | GLN  |
| 1   | G     | 428 | GLN  |
| 2   | J     | 640 | GLN  |
| 3   | S     | 39  | GLN  |
| 4   | U     | 38  | GLN  |
| 4   | U     | 76  | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

132 monosaccharides are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 5   | NAG  | C     | 1   | 1,5  | 14,14,15     | 0.79 | 1 (7%)      | 17,19,21    | 0.92 | 1 (5%)      |
| 5   | NAG  | C     | 2   | 5    | 14,14,15     | 0.45 | 0           | 17,19,21    | 1.56 | 3 (17%)     |
| 5   | BMA  | C     | 3   | 5    | 11,11,12     | 1.15 | 1 (9%)      | 15,15,17    | 1.40 | 1 (6%)      |
| 6   | NAG  | D     | 1   | 1,6  | 14,14,15     | 0.26 | 0           | 17,19,21    | 0.55 | 0           |
| 6   | NAG  | D     | 2   | 6    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.67 | 1 (5%)      |
| 6   | NAG  | E     | 1   | 1,6  | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.47 | 0           |
| 6   | NAG  | E     | 2   | 6    | 14,14,15     | 0.29 | 0           | 17,19,21    | 0.51 | 0           |
| 6   | NAG  | K     | 1   | 1,6  | 14,14,15     | 0.50 | 0           | 17,19,21    | 2.27 | 3 (17%)     |
| 6   | NAG  | K     | 2   | 6    | 14,14,15     | 0.52 | 0           | 17,19,21    | 1.33 | 3 (17%)     |
| 7   | NAG  | M     | 1   | 1,7  | 14,14,15     | 0.51 | 0           | 17,19,21    | 2.27 | 3 (17%)     |
| 7   | NAG  | M     | 2   | 7    | 14,14,15     | 0.50 | 0           | 17,19,21    | 1.33 | 3 (17%)     |
| 7   | BMA  | M     | 3   | 7    | 11,11,12     | 0.66 | 0           | 15,15,17    | 1.43 | 3 (20%)     |
| 7   | MAN  | M     | 4   | 7    | 11,11,12     | 0.57 | 0           | 15,15,17    | 1.50 | 2 (13%)     |
| 7   | MAN  | M     | 5   | 7    | 11,11,12     | 0.59 | 0           | 15,15,17    | 2.30 | 5 (33%)     |
| 7   | MAN  | M     | 6   | 7    | 11,11,12     | 0.59 | 0           | 15,15,17    | 2.22 | 3 (20%)     |
| 7   | MAN  | M     | 7   | 7    | 11,11,12     | 0.55 | 0           | 15,15,17    | 1.92 | 5 (33%)     |
| 8   | NAG  | N     | 1   | 1,8  | 14,14,15     | 0.77 | 1 (7%)      | 17,19,21    | 0.69 | 0           |
| 8   | NAG  | N     | 2   | 8    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.47 | 0           |
| 8   | BMA  | N     | 3   | 8    | 11,11,12     | 1.65 | 4 (36%)     | 15,15,17    | 1.80 | 2 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | MAN  | N     | 4   | 8    | 11,11,12     | 1.66 | 3 (27%)  | 15,15,17    | 1.28 | 2 (13%)  |
| 8   | MAN  | N     | 5   | 8    | 11,11,12     | 2.28 | 4 (36%)  | 15,15,17    | 1.68 | 3 (20%)  |
| 8   | MAN  | N     | 6   | 8    | 11,11,12     | 0.60 | 0        | 15,15,17    | 2.21 | 3 (20%)  |
| 8   | MAN  | N     | 7   | 8    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.92 | 5 (33%)  |
| 8   | MAN  | N     | 8   | 8    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.26 | 7 (46%)  |
| 6   | NAG  | O     | 1   | 1,6  | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.73 | 0        |
| 6   | NAG  | O     | 2   | 6    | 14,14,15     | 0.67 | 0        | 17,19,21    | 0.54 | 0        |
| 6   | NAG  | P     | 1   | 1,6  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.43 | 0        |
| 6   | NAG  | P     | 2   | 6    | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | Q     | 1   | 1,6  | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.76 | 1 (5%)   |
| 6   | NAG  | Q     | 2   | 6    | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.55 | 0        |
| 9   | NAG  | V     | 1   | 1,9  | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.59 | 0        |
| 9   | NAG  | V     | 2   | 9    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.84 | 1 (5%)   |
| 9   | BMA  | V     | 3   | 9    | 11,11,12     | 0.65 | 0        | 15,15,17    | 1.44 | 3 (20%)  |
| 9   | MAN  | V     | 4   | 9    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.20 | 3 (20%)  |
| 9   | MAN  | V     | 5   | 9    | 11,11,12     | 0.55 | 0        | 15,15,17    | 1.93 | 5 (33%)  |
| 9   | MAN  | V     | 6   | 9    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.47 | 2 (13%)  |
| 10  | NAG  | W     | 1   | 1,10 | 14,14,15     | 0.97 | 1 (7%)   | 17,19,21    | 1.06 | 1 (5%)   |
| 10  | NAG  | W     | 2   | 10   | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.56 | 0        |
| 10  | BMA  | W     | 3   | 10   | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.42 | 3 (20%)  |
| 10  | MAN  | W     | 4   | 10   | 11,11,12     | 0.60 | 0        | 15,15,17    | 2.22 | 3 (20%)  |
| 6   | NAG  | X     | 1   | 1,6  | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | X     | 2   | 6    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.45 | 0        |
| 6   | NAG  | Y     | 1   | 4,6  | 14,14,15     | 0.50 | 0        | 17,19,21    | 2.28 | 3 (17%)  |
| 6   | NAG  | Y     | 2   | 6    | 14,14,15     | 0.51 | 0        | 17,19,21    | 1.33 | 3 (17%)  |
| 5   | NAG  | Z     | 1   | 1,5  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 0.92 | 2 (11%)  |
| 5   | NAG  | Z     | 2   | 5    | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.56 | 3 (17%)  |
| 5   | BMA  | Z     | 3   | 5    | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 1.40 | 1 (6%)   |
| 6   | NAG  | a     | 1   | 1,6  | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.55 | 0        |
| 6   | NAG  | a     | 2   | 6    | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.67 | 1 (5%)   |
| 6   | NAG  | b     | 1   | 1,6  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.48 | 0        |
| 6   | NAG  | b     | 2   | 6    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.51 | 0        |
| 6   | NAG  | c     | 1   | 1,6  | 14,14,15     | 0.49 | 0        | 17,19,21    | 2.27 | 3 (17%)  |
| 6   | NAG  | c     | 2   | 6    | 14,14,15     | 0.52 | 0        | 17,19,21    | 1.33 | 3 (17%)  |
| 7   | NAG  | d     | 1   | 1,7  | 14,14,15     | 0.51 | 0        | 17,19,21    | 2.27 | 3 (17%)  |
| 7   | NAG  | d     | 2   | 7    | 14,14,15     | 0.49 | 0        | 17,19,21    | 1.33 | 3 (17%)  |
| 7   | BMA  | d     | 3   | 7    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.43 | 3 (20%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | MAN  | d     | 4   | 7    | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.50 | 2 (13%)  |
| 7   | MAN  | d     | 5   | 7    | 11,11,12     | 0.59 | 0        | 15,15,17    | 2.30 | 5 (33%)  |
| 7   | MAN  | d     | 6   | 7    | 11,11,12     | 0.59 | 0        | 15,15,17    | 2.22 | 3 (20%)  |
| 7   | MAN  | d     | 7   | 7    | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.93 | 5 (33%)  |
| 8   | NAG  | e     | 1   | 1,8  | 14,14,15     | 0.76 | 1 (7%)   | 17,19,21    | 0.68 | 0        |
| 8   | NAG  | e     | 2   | 8    | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.47 | 0        |
| 8   | BMA  | e     | 3   | 8    | 11,11,12     | 1.66 | 4 (36%)  | 15,15,17    | 1.79 | 2 (13%)  |
| 8   | MAN  | e     | 4   | 8    | 11,11,12     | 1.66 | 3 (27%)  | 15,15,17    | 1.28 | 2 (13%)  |
| 8   | MAN  | e     | 5   | 8    | 11,11,12     | 2.27 | 4 (36%)  | 15,15,17    | 1.68 | 3 (20%)  |
| 8   | MAN  | e     | 6   | 8    | 11,11,12     | 0.59 | 0        | 15,15,17    | 2.21 | 3 (20%)  |
| 8   | MAN  | e     | 7   | 8    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.92 | 5 (33%)  |
| 8   | MAN  | e     | 8   | 8    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.27 | 7 (46%)  |
| 6   | NAG  | f     | 1   | 1,6  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.73 | 0        |
| 6   | NAG  | f     | 2   | 6    | 14,14,15     | 0.68 | 0        | 17,19,21    | 0.55 | 0        |
| 6   | NAG  | g     | 1   | 1,6  | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.43 | 0        |
| 6   | NAG  | g     | 2   | 6    | 14,14,15     | 0.62 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | h     | 1   | 1,6  | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.75 | 1 (5%)   |
| 6   | NAG  | h     | 2   | 6    | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.55 | 0        |
| 9   | NAG  | i     | 1   | 1,9  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.59 | 0        |
| 9   | NAG  | i     | 2   | 9    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.83 | 1 (5%)   |
| 9   | BMA  | i     | 3   | 9    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.45 | 3 (20%)  |
| 9   | MAN  | i     | 4   | 9    | 11,11,12     | 0.62 | 0        | 15,15,17    | 2.20 | 3 (20%)  |
| 9   | MAN  | i     | 5   | 9    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.93 | 5 (33%)  |
| 9   | MAN  | i     | 6   | 9    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.47 | 2 (13%)  |
| 10  | NAG  | j     | 1   | 1,10 | 14,14,15     | 0.97 | 1 (7%)   | 17,19,21    | 1.05 | 1 (5%)   |
| 10  | NAG  | j     | 2   | 10   | 14,14,15     | 0.49 | 0        | 17,19,21    | 0.56 | 0        |
| 10  | BMA  | j     | 3   | 10   | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.42 | 3 (20%)  |
| 10  | MAN  | j     | 4   | 10   | 11,11,12     | 0.60 | 0        | 15,15,17    | 2.21 | 3 (20%)  |
| 6   | NAG  | k     | 1   | 1,6  | 14,14,15     | 0.49 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | k     | 2   | 6    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.45 | 0        |
| 6   | NAG  | l     | 1   | 4,6  | 14,14,15     | 0.49 | 0        | 17,19,21    | 2.28 | 3 (17%)  |
| 6   | NAG  | l     | 2   | 6    | 14,14,15     | 0.52 | 0        | 17,19,21    | 1.32 | 3 (17%)  |
| 5   | NAG  | m     | 1   | 1,5  | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 0.92 | 2 (11%)  |
| 5   | NAG  | m     | 2   | 5    | 14,14,15     | 0.45 | 0        | 17,19,21    | 1.55 | 3 (17%)  |
| 5   | BMA  | m     | 3   | 5    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.40 | 1 (6%)   |
| 6   | NAG  | n     | 1   | 1,6  | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.56 | 0        |
| 6   | NAG  | n     | 2   | 6    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.66 | 1 (5%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | NAG  | o     | 1   | 1,6  | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.47 | 0        |
| 6   | NAG  | o     | 2   | 6    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.51 | 0        |
| 6   | NAG  | p     | 1   | 1,6  | 14,14,15     | 0.49 | 0        | 17,19,21    | 2.27 | 3 (17%)  |
| 6   | NAG  | p     | 2   | 6    | 14,14,15     | 0.52 | 0        | 17,19,21    | 1.33 | 3 (17%)  |
| 7   | NAG  | q     | 1   | 1,7  | 14,14,15     | 0.51 | 0        | 17,19,21    | 2.27 | 3 (17%)  |
| 7   | NAG  | q     | 2   | 7    | 14,14,15     | 0.49 | 0        | 17,19,21    | 1.34 | 3 (17%)  |
| 7   | BMA  | q     | 3   | 7    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.43 | 3 (20%)  |
| 7   | MAN  | q     | 4   | 7    | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.50 | 2 (13%)  |
| 7   | MAN  | q     | 5   | 7    | 11,11,12     | 0.60 | 0        | 15,15,17    | 2.30 | 5 (33%)  |
| 7   | MAN  | q     | 6   | 7    | 11,11,12     | 0.59 | 0        | 15,15,17    | 2.21 | 3 (20%)  |
| 7   | MAN  | q     | 7   | 7    | 11,11,12     | 0.55 | 0        | 15,15,17    | 1.92 | 5 (33%)  |
| 8   | NAG  | r     | 1   | 1,8  | 14,14,15     | 0.77 | 1 (7%)   | 17,19,21    | 0.69 | 0        |
| 8   | NAG  | r     | 2   | 8    | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.47 | 0        |
| 8   | BMA  | r     | 3   | 8    | 11,11,12     | 1.65 | 4 (36%)  | 15,15,17    | 1.79 | 2 (13%)  |
| 8   | MAN  | r     | 4   | 8    | 11,11,12     | 1.66 | 3 (27%)  | 15,15,17    | 1.27 | 2 (13%)  |
| 8   | MAN  | r     | 5   | 8    | 11,11,12     | 2.27 | 4 (36%)  | 15,15,17    | 1.68 | 3 (20%)  |
| 8   | MAN  | r     | 6   | 8    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.22 | 3 (20%)  |
| 8   | MAN  | r     | 7   | 8    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.93 | 5 (33%)  |
| 8   | MAN  | r     | 8   | 8    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.26 | 7 (46%)  |
| 6   | NAG  | s     | 1   | 1,6  | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.73 | 0        |
| 6   | NAG  | s     | 2   | 6    | 14,14,15     | 0.67 | 0        | 17,19,21    | 0.54 | 0        |
| 6   | NAG  | t     | 1   | 1,6  | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.43 | 0        |
| 6   | NAG  | t     | 2   | 6    | 14,14,15     | 0.62 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | u     | 1   | 1,6  | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.76 | 1 (5%)   |
| 6   | NAG  | u     | 2   | 6    | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.55 | 0        |
| 9   | NAG  | v     | 1   | 1,9  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.59 | 0        |
| 9   | NAG  | v     | 2   | 9    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.84 | 1 (5%)   |
| 9   | BMA  | v     | 3   | 9    | 11,11,12     | 0.65 | 0        | 15,15,17    | 1.45 | 3 (20%)  |
| 9   | MAN  | v     | 4   | 9    | 11,11,12     | 0.61 | 0        | 15,15,17    | 2.20 | 3 (20%)  |
| 9   | MAN  | v     | 5   | 9    | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.93 | 5 (33%)  |
| 9   | MAN  | v     | 6   | 9    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.47 | 2 (13%)  |
| 10  | NAG  | w     | 1   | 1,10 | 14,14,15     | 0.96 | 1 (7%)   | 17,19,21    | 1.06 | 1 (5%)   |
| 10  | NAG  | w     | 2   | 10   | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.56 | 0        |
| 10  | BMA  | w     | 3   | 10   | 11,11,12     | 0.65 | 0        | 15,15,17    | 1.42 | 3 (20%)  |
| 10  | MAN  | w     | 4   | 10   | 11,11,12     | 0.62 | 0        | 15,15,17    | 2.21 | 3 (20%)  |
| 6   | NAG  | x     | 1   | 1,6  | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.57 | 0        |
| 6   | NAG  | x     | 2   | 6    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.45 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | NAG  | y     | 1   | 4,6  | 14,14,15     | 0.49 | 0        | 17,19,21    | 2.29 | 3 (17%)  |
| 6   | NAG  | y     | 2   | 6    | 14,14,15     | 0.51 | 0        | 17,19,21    | 1.33 | 3 (17%)  |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 5   | NAG  | C     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | C     | 2   | 5    | -       | 6/6/23/26 | 0/1/1/1 |
| 5   | BMA  | C     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | NAG  | D     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | D     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | E     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | E     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | M     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | M     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | M     | 4   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | M     | 5   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | M     | 6   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | M     | 7   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | N     | 1   | 1,8  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | N     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | N     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 4   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 6   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 7   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 8   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | O     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | O     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | P     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | P     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | Q     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | Q     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 9   | NAG  | V     | 1   | 1,9  | -       | 3/6/23/26 | 0/1/1/1 |
| 9   | NAG  | V     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | V     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | V     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | V     | 5   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | V     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | NAG  | W     | 1   | 1,10 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | W     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | BMA  | W     | 3   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | W     | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | X     | 1   | 1,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | X     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | Y     | 1   | 4,6  | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | Y     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 5   | NAG  | Z     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | Z     | 2   | 5    | -       | 6/6/23/26 | 0/1/1/1 |
| 5   | BMA  | Z     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | NAG  | a     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | a     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | b     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | b     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | c     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | c     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | d     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | d     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | d     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | d     | 4   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | d     | 5   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | d     | 6   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | d     | 7   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | e     | 1   | 1,8  | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | NAG  | e     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | e     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | e     | 4   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | e     | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | e     | 6   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | e     | 7   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | e     | 8   | 8    | -       | 0/2/19/22 | 0/1/1/1 |

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

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | r     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | r     | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | r     | 4   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | r     | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | r     | 6   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | r     | 7   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | r     | 8   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | s     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | s     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | t     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | t     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | u     | 1   | 1,6  | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | u     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | v     | 1   | 1,9  | -       | 3/6/23/26 | 0/1/1/1 |
| 9   | NAG  | v     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | v     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | v     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | v     | 5   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | v     | 6   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | NAG  | w     | 1   | 1,10 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | w     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | BMA  | w     | 3   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | w     | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | NAG  | x     | 1   | 1,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 6   | NAG  | x     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | NAG  | y     | 1   | 4,6  | -       | 3/6/23/26 | 0/1/1/1 |
| 6   | NAG  | y     | 2   | 6    | -       | 0/6/23/26 | 0/1/1/1 |

All (45) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 8   | N     | 5   | MAN  | C4-C5 | 4.34 | 1.62        | 1.53     |
| 8   | r     | 5   | MAN  | C4-C5 | 4.33 | 1.62        | 1.53     |
| 8   | e     | 5   | MAN  | C4-C5 | 4.32 | 1.62        | 1.53     |
| 8   | e     | 5   | MAN  | C4-C3 | 3.69 | 1.61        | 1.52     |
| 8   | N     | 5   | MAN  | C4-C3 | 3.69 | 1.61        | 1.52     |
| 8   | r     | 5   | MAN  | C4-C3 | 3.66 | 1.61        | 1.52     |
| 10  | j     | 1   | NAG  | O5-C1 | 3.42 | 1.49        | 1.43     |
| 10  | W     | 1   | NAG  | O5-C1 | 3.41 | 1.49        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10  | w     | 1   | NAG  | O5-C1 | 3.38  | 1.49        | 1.43     |
| 8   | N     | 4   | MAN  | O5-C5 | 3.18  | 1.49        | 1.43     |
| 8   | r     | 4   | MAN  | O5-C5 | 3.17  | 1.49        | 1.43     |
| 8   | e     | 4   | MAN  | O5-C5 | 3.14  | 1.49        | 1.43     |
| 8   | r     | 5   | MAN  | C2-C3 | 2.89  | 1.56        | 1.52     |
| 8   | N     | 5   | MAN  | C2-C3 | 2.88  | 1.56        | 1.52     |
| 8   | e     | 5   | MAN  | C2-C3 | 2.85  | 1.56        | 1.52     |
| 8   | e     | 4   | MAN  | C4-C3 | 2.47  | 1.58        | 1.52     |
| 8   | N     | 4   | MAN  | C4-C5 | 2.46  | 1.58        | 1.53     |
| 8   | e     | 4   | MAN  | C4-C5 | 2.45  | 1.58        | 1.53     |
| 8   | r     | 4   | MAN  | C4-C5 | 2.45  | 1.58        | 1.53     |
| 8   | N     | 4   | MAN  | C4-C3 | 2.44  | 1.58        | 1.52     |
| 8   | r     | 4   | MAN  | C4-C3 | 2.43  | 1.58        | 1.52     |
| 8   | N     | 3   | BMA  | O5-C5 | 2.43  | 1.48        | 1.43     |
| 8   | r     | 3   | BMA  | O5-C5 | 2.43  | 1.48        | 1.43     |
| 8   | e     | 3   | BMA  | O5-C5 | 2.42  | 1.48        | 1.43     |
| 8   | e     | 3   | BMA  | C2-C3 | 2.41  | 1.56        | 1.52     |
| 8   | N     | 3   | BMA  | C2-C3 | 2.40  | 1.56        | 1.52     |
| 8   | r     | 3   | BMA  | C2-C3 | 2.38  | 1.56        | 1.52     |
| 5   | m     | 3   | BMA  | C1-C2 | 2.33  | 1.57        | 1.52     |
| 5   | C     | 3   | BMA  | C1-C2 | 2.33  | 1.57        | 1.52     |
| 5   | Z     | 3   | BMA  | C1-C2 | 2.32  | 1.57        | 1.52     |
| 8   | r     | 5   | MAN  | O5-C5 | 2.32  | 1.48        | 1.43     |
| 8   | r     | 1   | NAG  | O5-C1 | -2.32 | 1.39        | 1.43     |
| 8   | e     | 1   | NAG  | O5-C1 | -2.30 | 1.39        | 1.43     |
| 8   | N     | 5   | MAN  | O5-C5 | 2.30  | 1.47        | 1.43     |
| 8   | N     | 1   | NAG  | O5-C1 | -2.29 | 1.39        | 1.43     |
| 8   | e     | 5   | MAN  | O5-C5 | 2.27  | 1.47        | 1.43     |
| 5   | Z     | 1   | NAG  | O5-C1 | -2.24 | 1.39        | 1.43     |
| 8   | N     | 3   | BMA  | C4-C5 | 2.20  | 1.57        | 1.53     |
| 8   | e     | 3   | BMA  | C4-C5 | 2.20  | 1.57        | 1.53     |
| 8   | r     | 3   | BMA  | C4-C5 | 2.20  | 1.57        | 1.53     |
| 5   | C     | 1   | NAG  | O5-C1 | -2.19 | 1.40        | 1.43     |
| 5   | m     | 1   | NAG  | O5-C1 | -2.19 | 1.40        | 1.43     |
| 8   | e     | 3   | BMA  | O2-C2 | 2.04  | 1.47        | 1.43     |
| 8   | N     | 3   | BMA  | O2-C2 | 2.03  | 1.47        | 1.43     |
| 8   | r     | 3   | BMA  | O2-C2 | 2.01  | 1.47        | 1.43     |

All (260) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | q     | 1   | NAG  | O5-C1-C2 | -7.52 | 99.65       | 111.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | y     | 1   | NAG  | O5-C1-C2 | -7.52 | 99.65       | 111.29   |
| 7   | M     | 1   | NAG  | O5-C1-C2 | -7.51 | 99.68       | 111.29   |
| 7   | d     | 1   | NAG  | O5-C1-C2 | -7.50 | 99.68       | 111.29   |
| 6   | c     | 1   | NAG  | O5-C1-C2 | -7.50 | 99.68       | 111.29   |
| 6   | Y     | 1   | NAG  | O5-C1-C2 | -7.50 | 99.69       | 111.29   |
| 6   | l     | 1   | NAG  | O5-C1-C2 | -7.50 | 99.69       | 111.29   |
| 6   | K     | 1   | NAG  | O5-C1-C2 | -7.49 | 99.70       | 111.29   |
| 6   | p     | 1   | NAG  | O5-C1-C2 | -7.48 | 99.72       | 111.29   |
| 8   | r     | 6   | MAN  | C1-C2-C3 | 5.91  | 118.25      | 109.64   |
| 10  | W     | 4   | MAN  | C1-C2-C3 | 5.91  | 118.25      | 109.64   |
| 8   | N     | 6   | MAN  | C1-C2-C3 | 5.90  | 118.23      | 109.64   |
| 7   | d     | 6   | MAN  | C1-C2-C3 | 5.90  | 118.23      | 109.64   |
| 10  | j     | 4   | MAN  | C1-C2-C3 | 5.90  | 118.23      | 109.64   |
| 7   | M     | 6   | MAN  | C1-C2-C3 | 5.90  | 118.23      | 109.64   |
| 10  | w     | 4   | MAN  | C1-C2-C3 | 5.89  | 118.22      | 109.64   |
| 8   | e     | 6   | MAN  | C1-C2-C3 | 5.89  | 118.22      | 109.64   |
| 7   | q     | 6   | MAN  | C1-C2-C3 | 5.87  | 118.19      | 109.64   |
| 9   | V     | 4   | MAN  | C1-C2-C3 | 5.85  | 118.17      | 109.64   |
| 9   | v     | 4   | MAN  | C1-C2-C3 | 5.85  | 118.17      | 109.64   |
| 9   | i     | 4   | MAN  | C1-C2-C3 | 5.84  | 118.15      | 109.64   |
| 8   | N     | 3   | BMA  | C1-O5-C5 | 5.74  | 119.88      | 112.19   |
| 8   | e     | 3   | BMA  | C1-O5-C5 | 5.73  | 119.86      | 112.19   |
| 8   | r     | 3   | BMA  | C1-O5-C5 | 5.69  | 119.81      | 112.19   |
| 7   | d     | 5   | MAN  | C1-O5-C5 | 4.85  | 118.69      | 112.19   |
| 8   | e     | 8   | MAN  | C6-C5-C4 | -4.82 | 101.17      | 113.02   |
| 7   | M     | 5   | MAN  | C1-O5-C5 | 4.82  | 118.65      | 112.19   |
| 8   | N     | 8   | MAN  | C6-C5-C4 | -4.82 | 101.18      | 113.02   |
| 8   | r     | 8   | MAN  | C6-C5-C4 | -4.82 | 101.19      | 113.02   |
| 7   | q     | 5   | MAN  | C1-O5-C5 | 4.79  | 118.61      | 112.19   |
| 5   | Z     | 2   | NAG  | C2-N2-C7 | 4.79  | 129.31      | 122.90   |
| 5   | C     | 2   | NAG  | C2-N2-C7 | 4.77  | 129.29      | 122.90   |
| 5   | m     | 2   | NAG  | C2-N2-C7 | 4.73  | 129.24      | 122.90   |
| 7   | q     | 5   | MAN  | O2-C2-C1 | 4.46  | 119.43      | 109.22   |
| 7   | M     | 5   | MAN  | O2-C2-C1 | 4.45  | 119.41      | 109.22   |
| 7   | d     | 5   | MAN  | O2-C2-C1 | 4.45  | 119.40      | 109.22   |
| 7   | M     | 6   | MAN  | C2-C3-C4 | -4.06 | 103.72      | 110.86   |
| 7   | d     | 6   | MAN  | C2-C3-C4 | -4.06 | 103.72      | 110.86   |
| 7   | q     | 6   | MAN  | C2-C3-C4 | -4.05 | 103.74      | 110.86   |
| 5   | C     | 3   | BMA  | C1-O5-C5 | 4.04  | 117.60      | 112.19   |
| 5   | m     | 3   | BMA  | C1-O5-C5 | 4.04  | 117.59      | 112.19   |
| 8   | e     | 6   | MAN  | C2-C3-C4 | -4.03 | 103.77      | 110.86   |
| 10  | w     | 4   | MAN  | C2-C3-C4 | -4.03 | 103.77      | 110.86   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 5   | Z     | 3   | BMA  | C1-O5-C5 | 4.03  | 117.58      | 112.19   |
| 8   | N     | 6   | MAN  | C2-C3-C4 | -4.03 | 103.78      | 110.86   |
| 10  | W     | 4   | MAN  | C2-C3-C4 | -4.02 | 103.78      | 110.86   |
| 8   | r     | 6   | MAN  | C2-C3-C4 | -4.01 | 103.80      | 110.86   |
| 10  | j     | 4   | MAN  | C2-C3-C4 | -3.99 | 103.84      | 110.86   |
| 9   | i     | 4   | MAN  | C2-C3-C4 | -3.99 | 103.85      | 110.86   |
| 9   | v     | 4   | MAN  | C2-C3-C4 | -3.98 | 103.86      | 110.86   |
| 7   | q     | 5   | MAN  | O2-C2-C3 | -3.96 | 101.94      | 110.15   |
| 9   | V     | 4   | MAN  | C2-C3-C4 | -3.96 | 103.90      | 110.86   |
| 7   | M     | 5   | MAN  | O2-C2-C3 | -3.95 | 101.97      | 110.15   |
| 8   | e     | 5   | MAN  | C1-O5-C5 | 3.94  | 117.47      | 112.19   |
| 8   | r     | 5   | MAN  | C1-O5-C5 | 3.94  | 117.46      | 112.19   |
| 7   | d     | 5   | MAN  | O2-C2-C3 | -3.94 | 102.00      | 110.15   |
| 9   | i     | 5   | MAN  | O4-C4-C3 | -3.93 | 101.11      | 110.38   |
| 9   | V     | 5   | MAN  | O4-C4-C3 | -3.92 | 101.13      | 110.38   |
| 8   | N     | 5   | MAN  | C1-O5-C5 | 3.92  | 117.44      | 112.19   |
| 9   | v     | 5   | MAN  | O4-C4-C3 | -3.91 | 101.15      | 110.38   |
| 7   | M     | 7   | MAN  | O4-C4-C3 | -3.87 | 101.24      | 110.38   |
| 7   | d     | 7   | MAN  | O4-C4-C3 | -3.87 | 101.26      | 110.38   |
| 7   | q     | 7   | MAN  | O4-C4-C3 | -3.86 | 101.27      | 110.38   |
| 8   | e     | 7   | MAN  | O4-C4-C3 | -3.85 | 101.29      | 110.38   |
| 8   | r     | 7   | MAN  | O4-C4-C3 | -3.85 | 101.30      | 110.38   |
| 8   | N     | 7   | MAN  | O4-C4-C3 | -3.85 | 101.31      | 110.38   |
| 8   | e     | 4   | MAN  | C1-O5-C5 | 3.81  | 117.29      | 112.19   |
| 8   | N     | 4   | MAN  | C1-O5-C5 | 3.78  | 117.26      | 112.19   |
| 8   | r     | 4   | MAN  | C1-O5-C5 | 3.77  | 117.23      | 112.19   |
| 8   | r     | 8   | MAN  | O4-C4-C3 | -3.54 | 102.04      | 110.38   |
| 8   | N     | 8   | MAN  | O4-C4-C3 | -3.52 | 102.07      | 110.38   |
| 8   | e     | 8   | MAN  | O4-C4-C3 | -3.52 | 102.09      | 110.38   |
| 7   | d     | 7   | MAN  | O4-C4-C5 | 3.26  | 117.36      | 109.32   |
| 8   | r     | 7   | MAN  | O4-C4-C5 | 3.24  | 117.31      | 109.32   |
| 7   | M     | 7   | MAN  | O4-C4-C5 | 3.24  | 117.31      | 109.32   |
| 7   | q     | 7   | MAN  | O4-C4-C5 | 3.24  | 117.31      | 109.32   |
| 9   | v     | 5   | MAN  | O4-C4-C5 | 3.24  | 117.30      | 109.32   |
| 8   | N     | 7   | MAN  | O4-C4-C5 | 3.22  | 117.25      | 109.32   |
| 9   | V     | 5   | MAN  | O4-C4-C5 | 3.22  | 117.25      | 109.32   |
| 9   | i     | 5   | MAN  | O4-C4-C5 | 3.22  | 117.25      | 109.32   |
| 8   | e     | 7   | MAN  | O4-C4-C5 | 3.21  | 117.22      | 109.32   |
| 10  | W     | 1   | NAG  | C1-O5-C5 | 3.17  | 116.43      | 112.19   |
| 10  | w     | 1   | NAG  | C1-O5-C5 | 3.16  | 116.43      | 112.19   |
| 10  | j     | 1   | NAG  | C1-O5-C5 | 3.15  | 116.41      | 112.19   |
| 7   | q     | 2   | NAG  | O5-C5-C6 | -3.13 | 101.56      | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | d     | 2   | NAG  | O5-C5-C6 | -3.13 | 101.58      | 107.66   |
| 7   | M     | 2   | NAG  | O5-C5-C6 | -3.12 | 101.59      | 107.66   |
| 8   | e     | 8   | MAN  | C3-C4-C5 | -3.11 | 104.60      | 110.23   |
| 6   | Y     | 2   | NAG  | O5-C5-C6 | -3.10 | 101.63      | 107.66   |
| 8   | N     | 8   | MAN  | C3-C4-C5 | -3.09 | 104.62      | 110.23   |
| 6   | l     | 2   | NAG  | O5-C5-C6 | -3.08 | 101.67      | 107.66   |
| 6   | y     | 2   | NAG  | O5-C5-C6 | -3.08 | 101.67      | 107.66   |
| 8   | r     | 8   | MAN  | C3-C4-C5 | -3.07 | 104.66      | 110.23   |
| 6   | K     | 2   | NAG  | O5-C5-C6 | -3.03 | 101.76      | 107.66   |
| 6   | p     | 2   | NAG  | O5-C5-C6 | -3.03 | 101.77      | 107.66   |
| 6   | c     | 2   | NAG  | O5-C5-C6 | -3.03 | 101.77      | 107.66   |
| 9   | v     | 3   | BMA  | O2-C2-C3 | 2.96  | 116.28      | 110.15   |
| 7   | q     | 3   | BMA  | O2-C2-C3 | 2.94  | 116.25      | 110.15   |
| 9   | i     | 3   | BMA  | O2-C2-C3 | 2.94  | 116.25      | 110.15   |
| 7   | d     | 3   | BMA  | O2-C2-C3 | 2.94  | 116.24      | 110.15   |
| 7   | M     | 3   | BMA  | O2-C2-C3 | 2.93  | 116.22      | 110.15   |
| 9   | V     | 3   | BMA  | O2-C2-C3 | 2.93  | 116.22      | 110.15   |
| 6   | Y     | 1   | NAG  | O7-C7-C8 | -2.92 | 116.85      | 122.05   |
| 6   | y     | 1   | NAG  | O7-C7-C8 | -2.92 | 116.85      | 122.05   |
| 6   | l     | 1   | NAG  | O7-C7-C8 | -2.90 | 116.89      | 122.05   |
| 7   | M     | 1   | NAG  | O7-C7-C8 | -2.87 | 116.95      | 122.05   |
| 8   | e     | 8   | MAN  | O2-C2-C3 | -2.86 | 104.23      | 110.15   |
| 10  | j     | 3   | BMA  | O2-C2-C3 | 2.86  | 116.07      | 110.15   |
| 7   | d     | 1   | NAG  | O7-C7-C8 | -2.86 | 116.97      | 122.05   |
| 7   | q     | 1   | NAG  | O7-C7-C8 | -2.86 | 116.97      | 122.05   |
| 8   | N     | 8   | MAN  | O2-C2-C3 | -2.85 | 104.24      | 110.15   |
| 10  | W     | 3   | BMA  | O2-C2-C3 | 2.85  | 116.06      | 110.15   |
| 10  | w     | 3   | BMA  | O2-C2-C3 | 2.85  | 116.06      | 110.15   |
| 8   | r     | 8   | MAN  | O2-C2-C3 | -2.85 | 104.25      | 110.15   |
| 6   | K     | 1   | NAG  | O7-C7-C8 | -2.83 | 117.01      | 122.05   |
| 6   | p     | 1   | NAG  | O7-C7-C8 | -2.82 | 117.03      | 122.05   |
| 6   | c     | 1   | NAG  | O7-C7-C8 | -2.82 | 117.03      | 122.05   |
| 8   | e     | 5   | MAN  | C1-C2-C3 | -2.78 | 105.60      | 109.64   |
| 8   | N     | 5   | MAN  | C1-C2-C3 | -2.77 | 105.61      | 109.64   |
| 8   | r     | 5   | MAN  | C1-C2-C3 | -2.76 | 105.62      | 109.64   |
| 6   | y     | 1   | NAG  | C4-C3-C2 | -2.76 | 106.98      | 111.02   |
| 6   | l     | 1   | NAG  | C4-C3-C2 | -2.72 | 107.04      | 111.02   |
| 6   | Y     | 1   | NAG  | C4-C3-C2 | -2.71 | 107.04      | 111.02   |
| 6   | K     | 1   | NAG  | C4-C3-C2 | -2.70 | 107.06      | 111.02   |
| 6   | p     | 1   | NAG  | C4-C3-C2 | -2.69 | 107.08      | 111.02   |
| 6   | c     | 1   | NAG  | C4-C3-C2 | -2.68 | 107.09      | 111.02   |
| 7   | M     | 5   | MAN  | O4-C4-C3 | -2.68 | 104.06      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | v     | 3   | BMA  | O4-C4-C5 | -2.68 | 102.72      | 109.32   |
| 9   | i     | 3   | BMA  | O4-C4-C5 | -2.68 | 102.73      | 109.32   |
| 7   | d     | 5   | MAN  | O4-C4-C3 | -2.68 | 104.07      | 110.38   |
| 7   | q     | 5   | MAN  | O4-C4-C3 | -2.67 | 104.09      | 110.38   |
| 9   | V     | 3   | BMA  | O4-C4-C5 | -2.66 | 102.77      | 109.32   |
| 7   | d     | 1   | NAG  | C4-C3-C2 | -2.65 | 107.14      | 111.02   |
| 7   | M     | 1   | NAG  | C4-C3-C2 | -2.65 | 107.14      | 111.02   |
| 10  | j     | 3   | BMA  | O4-C4-C5 | -2.65 | 102.81      | 109.32   |
| 5   | m     | 2   | NAG  | C1-C2-N2 | 2.64  | 114.60      | 110.43   |
| 10  | W     | 3   | BMA  | O4-C4-C5 | -2.64 | 102.82      | 109.32   |
| 7   | d     | 3   | BMA  | O4-C4-C5 | -2.63 | 102.84      | 109.32   |
| 10  | w     | 3   | BMA  | O4-C4-C5 | -2.63 | 102.84      | 109.32   |
| 7   | M     | 3   | BMA  | O4-C4-C5 | -2.63 | 102.86      | 109.32   |
| 7   | q     | 1   | NAG  | C4-C3-C2 | -2.62 | 107.17      | 111.02   |
| 7   | q     | 3   | BMA  | O4-C4-C5 | -2.62 | 102.87      | 109.32   |
| 5   | C     | 2   | NAG  | C1-C2-N2 | 2.62  | 114.56      | 110.43   |
| 5   | Z     | 2   | NAG  | C1-C2-N2 | 2.59  | 114.51      | 110.43   |
| 8   | e     | 7   | MAN  | O5-C5-C6 | -2.54 | 102.72      | 107.66   |
| 8   | N     | 7   | MAN  | O5-C5-C6 | -2.53 | 102.74      | 107.66   |
| 9   | i     | 5   | MAN  | O5-C5-C6 | -2.53 | 102.74      | 107.66   |
| 7   | d     | 4   | MAN  | O5-C5-C6 | 2.53  | 112.58      | 107.66   |
| 8   | r     | 8   | MAN  | O5-C5-C6 | 2.53  | 112.58      | 107.66   |
| 7   | d     | 7   | MAN  | O5-C5-C6 | -2.52 | 102.75      | 107.66   |
| 7   | q     | 7   | MAN  | O5-C5-C6 | -2.52 | 102.75      | 107.66   |
| 7   | M     | 7   | MAN  | O5-C5-C6 | -2.52 | 102.76      | 107.66   |
| 7   | M     | 4   | MAN  | O5-C5-C6 | 2.51  | 112.56      | 107.66   |
| 9   | v     | 5   | MAN  | O5-C5-C6 | -2.51 | 102.77      | 107.66   |
| 9   | V     | 5   | MAN  | O5-C5-C6 | -2.51 | 102.78      | 107.66   |
| 8   | r     | 7   | MAN  | O5-C5-C6 | -2.50 | 102.79      | 107.66   |
| 7   | q     | 4   | MAN  | O5-C5-C6 | 2.50  | 112.53      | 107.66   |
| 8   | N     | 8   | MAN  | O5-C5-C6 | 2.50  | 112.53      | 107.66   |
| 8   | e     | 8   | MAN  | O5-C5-C6 | 2.49  | 112.51      | 107.66   |
| 9   | V     | 6   | MAN  | O5-C5-C6 | 2.43  | 112.39      | 107.66   |
| 9   | v     | 6   | MAN  | O5-C5-C6 | 2.42  | 112.37      | 107.66   |
| 9   | i     | 6   | MAN  | O5-C5-C6 | 2.42  | 112.36      | 107.66   |
| 6   | c     | 2   | NAG  | O5-C1-C2 | -2.37 | 107.63      | 111.29   |
| 7   | d     | 3   | BMA  | C6-C5-C4 | -2.36 | 107.23      | 113.02   |
| 7   | M     | 3   | BMA  | C6-C5-C4 | -2.35 | 107.25      | 113.02   |
| 6   | p     | 2   | NAG  | O5-C1-C2 | -2.34 | 107.67      | 111.29   |
| 7   | q     | 3   | BMA  | C6-C5-C4 | -2.34 | 107.27      | 113.02   |
| 6   | K     | 2   | NAG  | O5-C1-C2 | -2.34 | 107.67      | 111.29   |
| 10  | w     | 3   | BMA  | C6-C5-C4 | -2.33 | 107.30      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | r     | 5   | MAN  | O3-C3-C4 | 2.32  | 115.86      | 110.38   |
| 10  | j     | 3   | BMA  | C6-C5-C4 | -2.32 | 107.31      | 113.02   |
| 8   | e     | 5   | MAN  | O3-C3-C4 | 2.32  | 115.85      | 110.38   |
| 8   | N     | 5   | MAN  | O3-C3-C4 | 2.32  | 115.85      | 110.38   |
| 7   | q     | 2   | NAG  | O5-C1-C2 | -2.32 | 107.70      | 111.29   |
| 7   | M     | 2   | NAG  | O5-C1-C2 | -2.32 | 107.70      | 111.29   |
| 10  | W     | 3   | BMA  | C6-C5-C4 | -2.31 | 107.34      | 113.02   |
| 9   | i     | 3   | BMA  | C6-C5-C4 | -2.31 | 107.36      | 113.02   |
| 7   | d     | 2   | NAG  | O5-C1-C2 | -2.29 | 107.74      | 111.29   |
| 9   | V     | 5   | MAN  | C1-O5-C5 | 2.29  | 115.26      | 112.19   |
| 9   | V     | 3   | BMA  | C6-C5-C4 | -2.29 | 107.39      | 113.02   |
| 6   | y     | 2   | NAG  | O5-C1-C2 | -2.29 | 107.75      | 111.29   |
| 9   | v     | 3   | BMA  | C6-C5-C4 | -2.29 | 107.40      | 113.02   |
| 6   | Y     | 2   | NAG  | O5-C1-C2 | -2.29 | 107.75      | 111.29   |
| 9   | v     | 5   | MAN  | C1-O5-C5 | 2.29  | 115.25      | 112.19   |
| 5   | m     | 1   | NAG  | C3-C4-C5 | 2.28  | 114.37      | 110.23   |
| 7   | M     | 5   | MAN  | O6-C6-C5 | 2.28  | 119.10      | 111.33   |
| 9   | i     | 5   | MAN  | C1-O5-C5 | 2.28  | 115.24      | 112.19   |
| 9   | V     | 2   | NAG  | C1-O5-C5 | 2.27  | 115.23      | 112.19   |
| 8   | r     | 7   | MAN  | C1-O5-C5 | 2.27  | 115.23      | 112.19   |
| 5   | C     | 1   | NAG  | C3-C4-C5 | 2.27  | 114.35      | 110.23   |
| 7   | q     | 5   | MAN  | O6-C6-C5 | 2.27  | 119.06      | 111.33   |
| 9   | v     | 2   | NAG  | C1-O5-C5 | 2.27  | 115.22      | 112.19   |
| 7   | d     | 5   | MAN  | O6-C6-C5 | 2.27  | 119.05      | 111.33   |
| 5   | Z     | 1   | NAG  | C3-C4-C5 | 2.26  | 114.33      | 110.23   |
| 6   | l     | 2   | NAG  | O5-C1-C2 | -2.26 | 107.79      | 111.29   |
| 7   | d     | 6   | MAN  | O5-C1-C2 | -2.25 | 105.41      | 110.79   |
| 8   | N     | 7   | MAN  | C1-O5-C5 | 2.25  | 115.20      | 112.19   |
| 8   | e     | 7   | MAN  | C1-O5-C5 | 2.25  | 115.20      | 112.19   |
| 7   | q     | 6   | MAN  | O5-C1-C2 | -2.24 | 105.45      | 110.79   |
| 7   | d     | 7   | MAN  | C1-O5-C5 | 2.24  | 115.19      | 112.19   |
| 7   | M     | 6   | MAN  | O5-C1-C2 | -2.24 | 105.45      | 110.79   |
| 8   | r     | 6   | MAN  | O5-C1-C2 | -2.23 | 105.47      | 110.79   |
| 8   | e     | 6   | MAN  | O5-C1-C2 | -2.22 | 105.49      | 110.79   |
| 10  | W     | 4   | MAN  | O5-C1-C2 | -2.22 | 105.50      | 110.79   |
| 7   | M     | 7   | MAN  | C1-O5-C5 | 2.22  | 115.16      | 112.19   |
| 9   | i     | 2   | NAG  | C1-O5-C5 | 2.22  | 115.16      | 112.19   |
| 8   | N     | 6   | MAN  | O5-C1-C2 | -2.21 | 105.51      | 110.79   |
| 10  | w     | 4   | MAN  | O5-C1-C2 | -2.21 | 105.51      | 110.79   |
| 6   | Y     | 2   | NAG  | C4-C3-C2 | -2.21 | 107.78      | 111.02   |
| 8   | N     | 3   | BMA  | O2-C2-C1 | 2.20  | 114.27      | 109.22   |
| 8   | r     | 3   | BMA  | O2-C2-C1 | 2.20  | 114.27      | 109.22   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | e     | 3   | BMA  | O2-C2-C1 | 2.20  | 114.27      | 109.22   |
| 5   | Z     | 2   | NAG  | O4-C4-C5 | -2.20 | 103.91      | 109.32   |
| 10  | j     | 4   | MAN  | O5-C1-C2 | -2.20 | 105.55      | 110.79   |
| 5   | C     | 2   | NAG  | O4-C4-C5 | -2.20 | 103.91      | 109.32   |
| 6   | K     | 2   | NAG  | C4-C3-C2 | -2.20 | 107.80      | 111.02   |
| 6   | c     | 2   | NAG  | C4-C3-C2 | -2.20 | 107.80      | 111.02   |
| 7   | M     | 2   | NAG  | C4-C3-C2 | -2.20 | 107.80      | 111.02   |
| 9   | v     | 4   | MAN  | O5-C1-C2 | -2.19 | 105.56      | 110.79   |
| 9   | V     | 4   | MAN  | O5-C1-C2 | -2.19 | 105.56      | 110.79   |
| 6   | y     | 2   | NAG  | C4-C3-C2 | -2.19 | 107.81      | 111.02   |
| 7   | d     | 2   | NAG  | C4-C3-C2 | -2.19 | 107.81      | 111.02   |
| 5   | m     | 2   | NAG  | O4-C4-C5 | -2.19 | 103.94      | 109.32   |
| 7   | q     | 2   | NAG  | C4-C3-C2 | -2.18 | 107.82      | 111.02   |
| 9   | i     | 4   | MAN  | O5-C1-C2 | -2.18 | 105.58      | 110.79   |
| 8   | e     | 4   | MAN  | O2-C2-C3 | -2.18 | 105.64      | 110.15   |
| 6   | l     | 2   | NAG  | C4-C3-C2 | -2.18 | 107.83      | 111.02   |
| 7   | q     | 7   | MAN  | C1-O5-C5 | 2.18  | 115.11      | 112.19   |
| 8   | r     | 4   | MAN  | O2-C2-C3 | -2.18 | 105.64      | 110.15   |
| 8   | N     | 4   | MAN  | O2-C2-C3 | -2.17 | 105.65      | 110.15   |
| 7   | q     | 7   | MAN  | O3-C3-C2 | -2.17 | 105.63      | 110.05   |
| 6   | Q     | 1   | NAG  | O4-C4-C5 | -2.17 | 103.98      | 109.32   |
| 6   | p     | 2   | NAG  | C4-C3-C2 | -2.17 | 107.84      | 111.02   |
| 7   | d     | 7   | MAN  | O3-C3-C2 | -2.16 | 105.64      | 110.05   |
| 6   | u     | 1   | NAG  | O4-C4-C5 | -2.16 | 104.00      | 109.32   |
| 6   | h     | 1   | NAG  | O4-C4-C5 | -2.16 | 104.01      | 109.32   |
| 8   | N     | 8   | MAN  | O2-C2-C1 | 2.15  | 114.15      | 109.22   |
| 8   | r     | 8   | MAN  | O2-C2-C1 | 2.15  | 114.15      | 109.22   |
| 9   | i     | 5   | MAN  | O3-C3-C2 | -2.15 | 105.67      | 110.05   |
| 7   | M     | 7   | MAN  | O3-C3-C2 | -2.15 | 105.67      | 110.05   |
| 8   | e     | 8   | MAN  | O2-C2-C1 | 2.14  | 114.13      | 109.22   |
| 9   | V     | 5   | MAN  | O3-C3-C2 | -2.14 | 105.69      | 110.05   |
| 8   | N     | 7   | MAN  | O3-C3-C2 | -2.13 | 105.70      | 110.05   |
| 9   | v     | 5   | MAN  | O3-C3-C2 | -2.13 | 105.72      | 110.05   |
| 8   | r     | 7   | MAN  | O3-C3-C2 | -2.13 | 105.72      | 110.05   |
| 8   | e     | 7   | MAN  | O3-C3-C2 | -2.12 | 105.72      | 110.05   |
| 7   | q     | 4   | MAN  | O3-C3-C4 | 2.12  | 115.38      | 110.38   |
| 7   | M     | 4   | MAN  | O3-C3-C4 | 2.11  | 115.36      | 110.38   |
| 7   | d     | 4   | MAN  | O3-C3-C4 | 2.10  | 115.34      | 110.38   |
| 9   | V     | 6   | MAN  | O3-C3-C4 | 2.09  | 115.30      | 110.38   |
| 9   | i     | 6   | MAN  | O3-C3-C4 | 2.09  | 115.30      | 110.38   |
| 9   | v     | 6   | MAN  | O3-C3-C4 | 2.08  | 115.29      | 110.38   |
| 6   | D     | 2   | NAG  | C1-O5-C5 | 2.07  | 114.96      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | a     | 2   | NAG  | C1-O5-C5 | 2.06  | 114.94      | 112.19   |
| 6   | n     | 2   | NAG  | C1-O5-C5 | 2.04  | 114.92      | 112.19   |
| 8   | e     | 8   | MAN  | C2-C3-C4 | 2.03  | 114.43      | 110.86   |
| 8   | N     | 8   | MAN  | C2-C3-C4 | 2.02  | 114.41      | 110.86   |
| 5   | Z     | 1   | NAG  | O4-C4-C5 | -2.00 | 104.39      | 109.32   |
| 8   | r     | 8   | MAN  | C2-C3-C4 | 2.00  | 114.38      | 110.86   |
| 5   | m     | 1   | NAG  | O4-C4-C5 | -2.00 | 104.39      | 109.32   |

There are no chirality outliers.

All (159) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | C     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | Z     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | m     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | O     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | f     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | s     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | P     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | g     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | t     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | E     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | b     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | o     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | C     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | Z     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | m     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | C     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | Z     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | m     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | Q     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | h     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | u     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | E     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | b     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | o     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | Q     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | h     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | u     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | N     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | e     | 2   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 8   | r     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | P     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | f     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | g     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | s     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | t     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | e     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | r     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | C     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | Z     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | m     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | D     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | a     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | n     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | V     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | v     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | P     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | g     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | t     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | Q     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | u     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | i     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | v     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | C     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | Z     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | m     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | h     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | e     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | r     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | P     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | Q     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | g     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | h     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | t     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | u     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 4   | MAN  | O5-C5-C6-O6 |
| 8   | e     | 4   | MAN  | O5-C5-C6-O6 |
| 8   | r     | 4   | MAN  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | D     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | a     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | n     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | V     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | v     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | C     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | Z     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | m     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | i     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | v     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | C     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | C     | 2   | NAG  | O7-C7-N2-C2 |
| 5   | Z     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | Z     | 2   | NAG  | O7-C7-N2-C2 |
| 5   | m     | 2   | NAG  | C8-C7-N2-C2 |
| 5   | m     | 2   | NAG  | O7-C7-N2-C2 |
| 6   | X     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | k     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | x     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | V     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | i     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | v     | 3   | BMA  | O5-C5-C6-O6 |
| 6   | Y     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | l     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | y     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | D     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | a     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | n     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | i     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | v     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | X     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | k     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | x     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | e     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | r     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | W     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | j     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | w     | 1   | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | a     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | D     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | n     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | Y     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | l     | 1   | NAG  | C4-C5-C6-O6 |
| 6   | y     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 4   | MAN  | C4-C5-C6-O6 |
| 8   | r     | 4   | MAN  | C4-C5-C6-O6 |
| 8   | e     | 4   | MAN  | C4-C5-C6-O6 |
| 6   | E     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | b     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | o     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | W     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | j     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | w     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | w     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | W     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | j     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | W     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | w     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | j     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | W     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | j     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | w     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | W     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | j     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | w     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | C     | 2   | NAG  | C1-C2-N2-C7 |
| 5   | Z     | 2   | NAG  | C1-C2-N2-C7 |
| 5   | m     | 2   | NAG  | C1-C2-N2-C7 |
| 5   | C     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | Z     | 2   | NAG  | C3-C2-N2-C7 |
| 5   | m     | 2   | NAG  | C3-C2-N2-C7 |
| 9   | V     | 1   | NAG  | C3-C2-N2-C7 |
| 9   | i     | 1   | NAG  | C3-C2-N2-C7 |
| 9   | v     | 1   | NAG  | C3-C2-N2-C7 |
| 6   | K     | 1   | NAG  | O7-C7-N2-C2 |
| 7   | M     | 1   | NAG  | O7-C7-N2-C2 |
| 7   | d     | 1   | NAG  | O7-C7-N2-C2 |
| 7   | q     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | Y     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | c     | 1   | NAG  | O7-C7-N2-C2 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 6   | l     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | p     | 1   | NAG  | O7-C7-N2-C2 |
| 6   | y     | 1   | NAG  | O7-C7-N2-C2 |

There are no ring outliers.

42 monomers are involved in 123 short contacts:

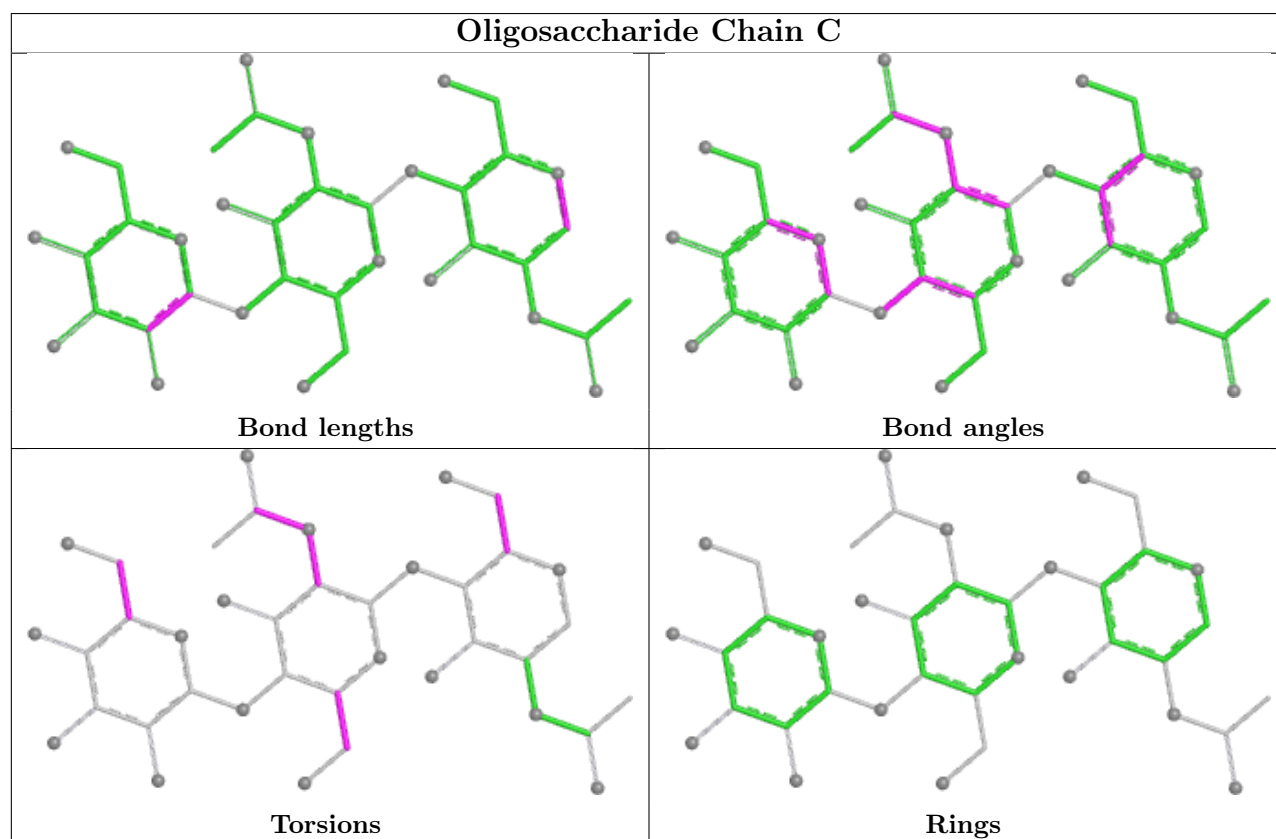
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | h     | 1   | NAG  | 5       | 0            |
| 8   | N     | 2   | NAG  | 2       | 0            |
| 6   | g     | 2   | NAG  | 1       | 0            |
| 5   | C     | 2   | NAG  | 1       | 0            |
| 6   | o     | 1   | NAG  | 6       | 0            |
| 6   | O     | 1   | NAG  | 13      | 0            |
| 6   | P     | 2   | NAG  | 1       | 0            |
| 6   | a     | 1   | NAG  | 6       | 0            |
| 5   | Z     | 2   | NAG  | 1       | 0            |
| 6   | Q     | 1   | NAG  | 5       | 0            |
| 6   | b     | 1   | NAG  | 6       | 0            |
| 6   | g     | 1   | NAG  | 1       | 0            |
| 8   | e     | 1   | NAG  | 2       | 0            |
| 6   | k     | 1   | NAG  | 2       | 0            |
| 8   | e     | 2   | NAG  | 2       | 0            |
| 10  | W     | 1   | NAG  | 1       | 0            |
| 6   | E     | 1   | NAG  | 6       | 0            |
| 6   | P     | 1   | NAG  | 1       | 0            |
| 6   | X     | 2   | NAG  | 2       | 0            |
| 5   | Z     | 1   | NAG  | 2       | 0            |
| 6   | n     | 1   | NAG  | 6       | 0            |
| 9   | V     | 1   | NAG  | 1       | 0            |
| 9   | i     | 1   | NAG  | 1       | 0            |
| 10  | j     | 1   | NAG  | 1       | 0            |
| 6   | x     | 2   | NAG  | 2       | 0            |
| 8   | r     | 2   | NAG  | 2       | 0            |
| 5   | m     | 2   | NAG  | 1       | 0            |
| 8   | N     | 1   | NAG  | 2       | 0            |
| 10  | w     | 1   | NAG  | 1       | 0            |
| 6   | f     | 1   | NAG  | 13      | 0            |
| 5   | C     | 1   | NAG  | 2       | 0            |
| 6   | D     | 1   | NAG  | 6       | 0            |
| 6   | X     | 1   | NAG  | 2       | 0            |
| 6   | s     | 1   | NAG  | 13      | 0            |

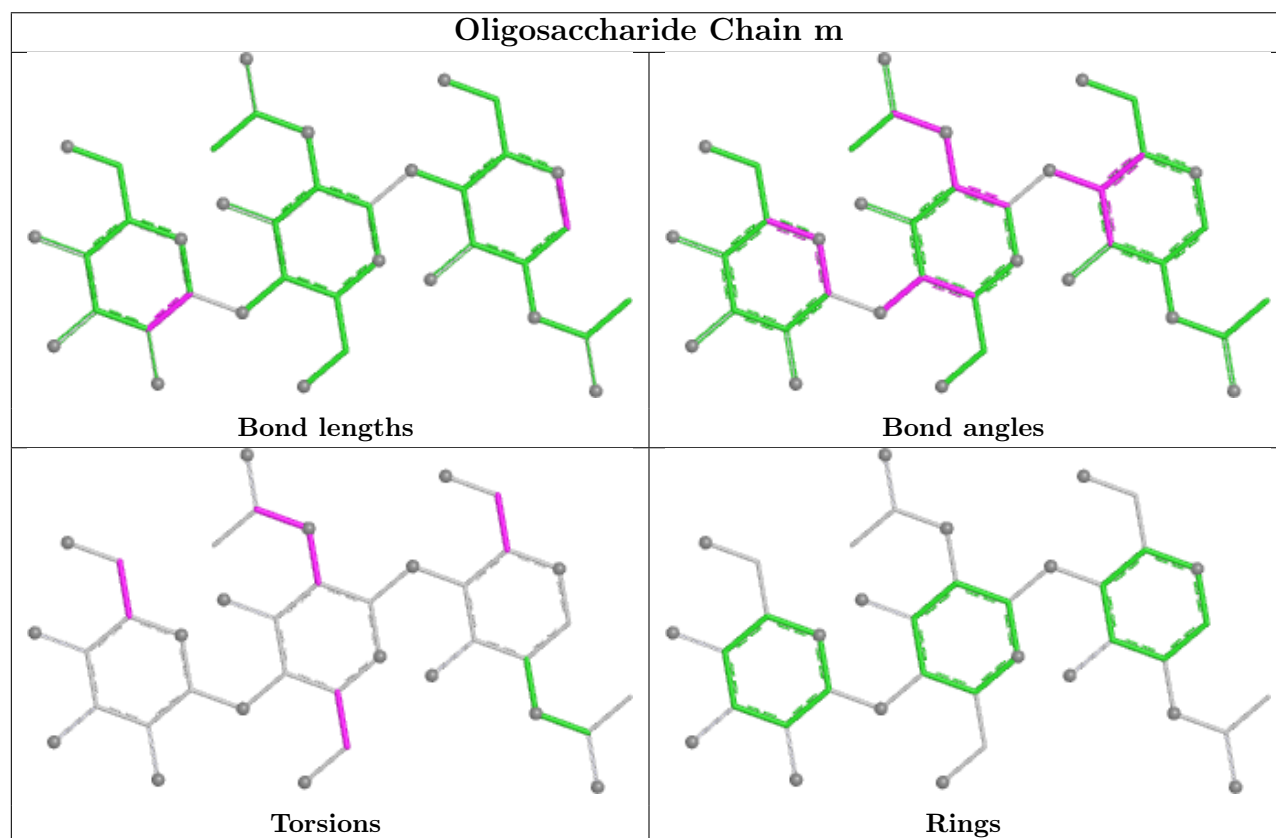
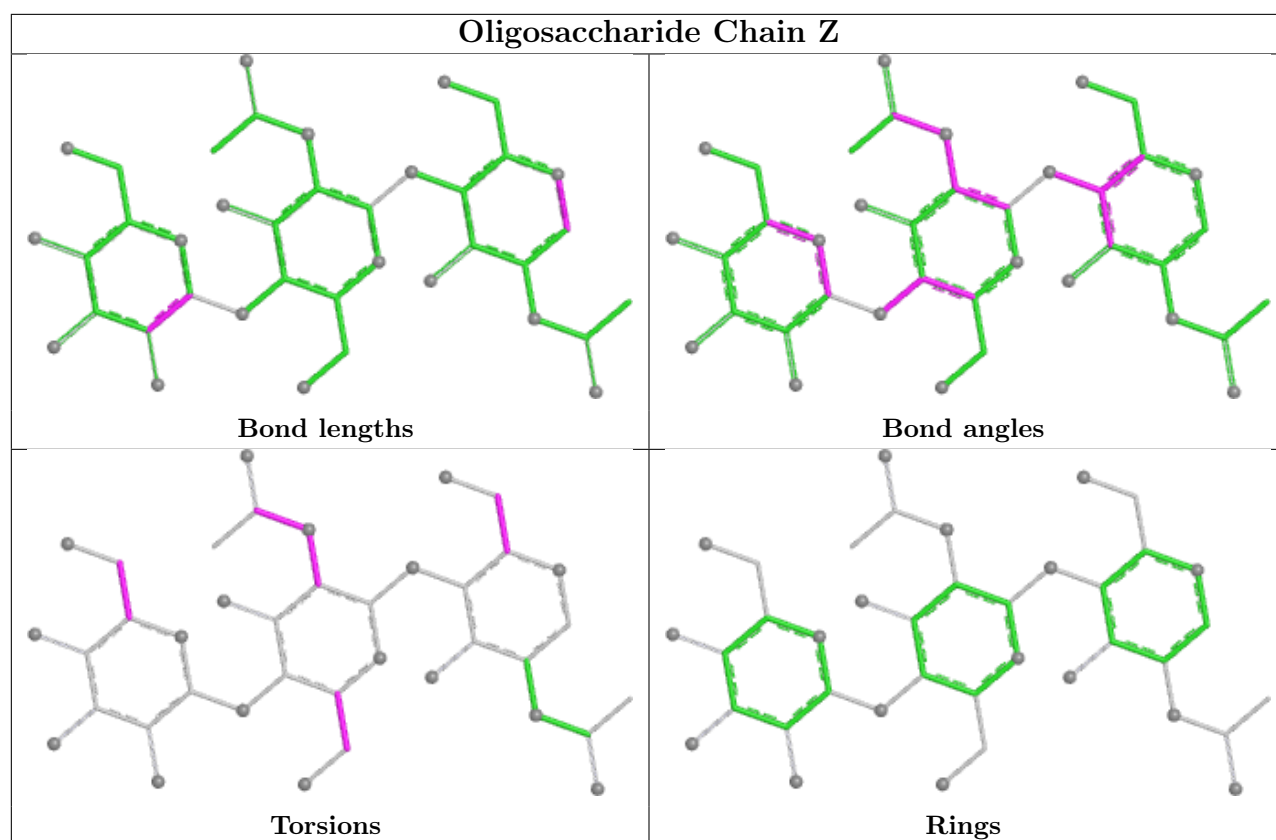
*Continued on next page...*

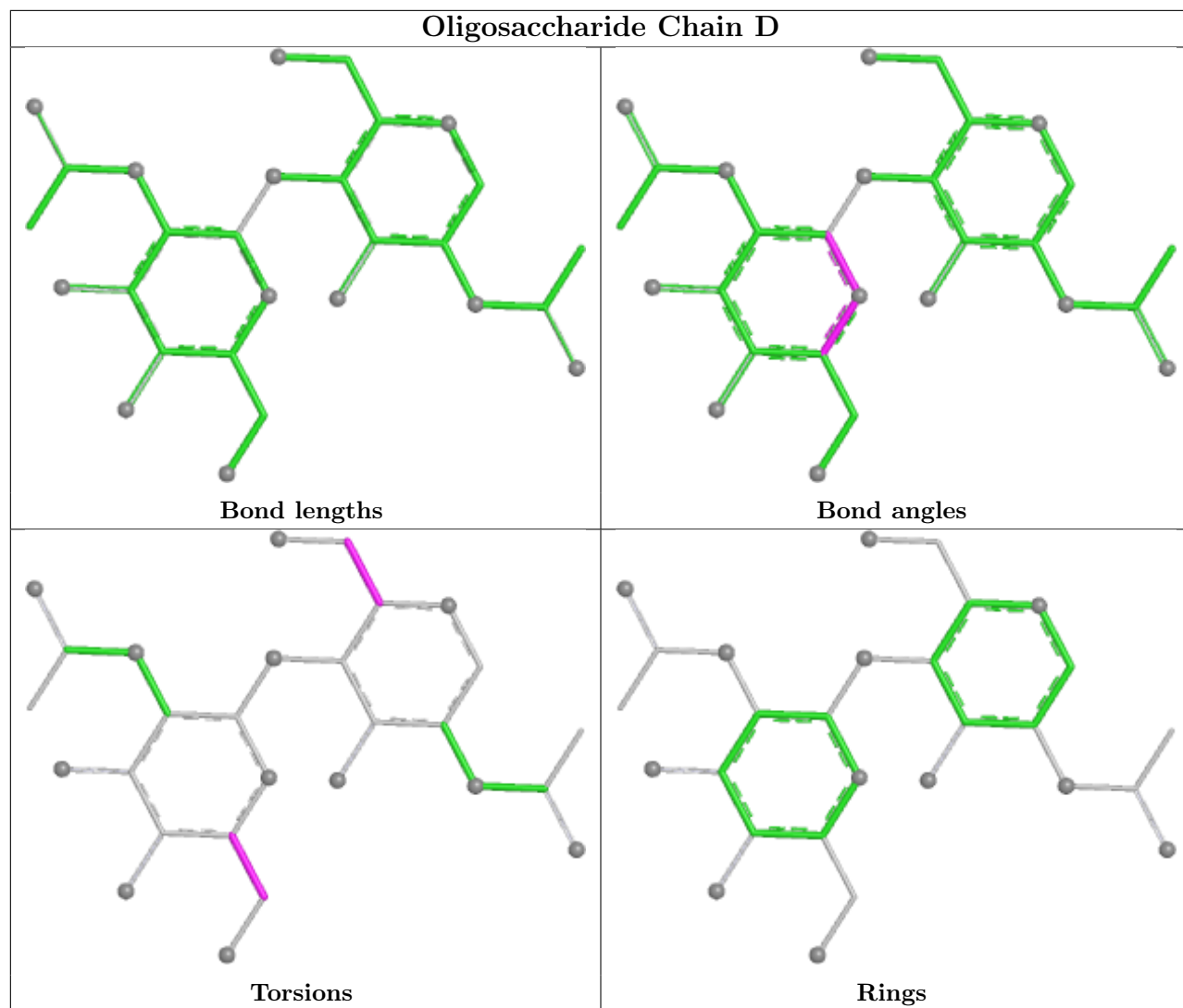
*Continued from previous page...*

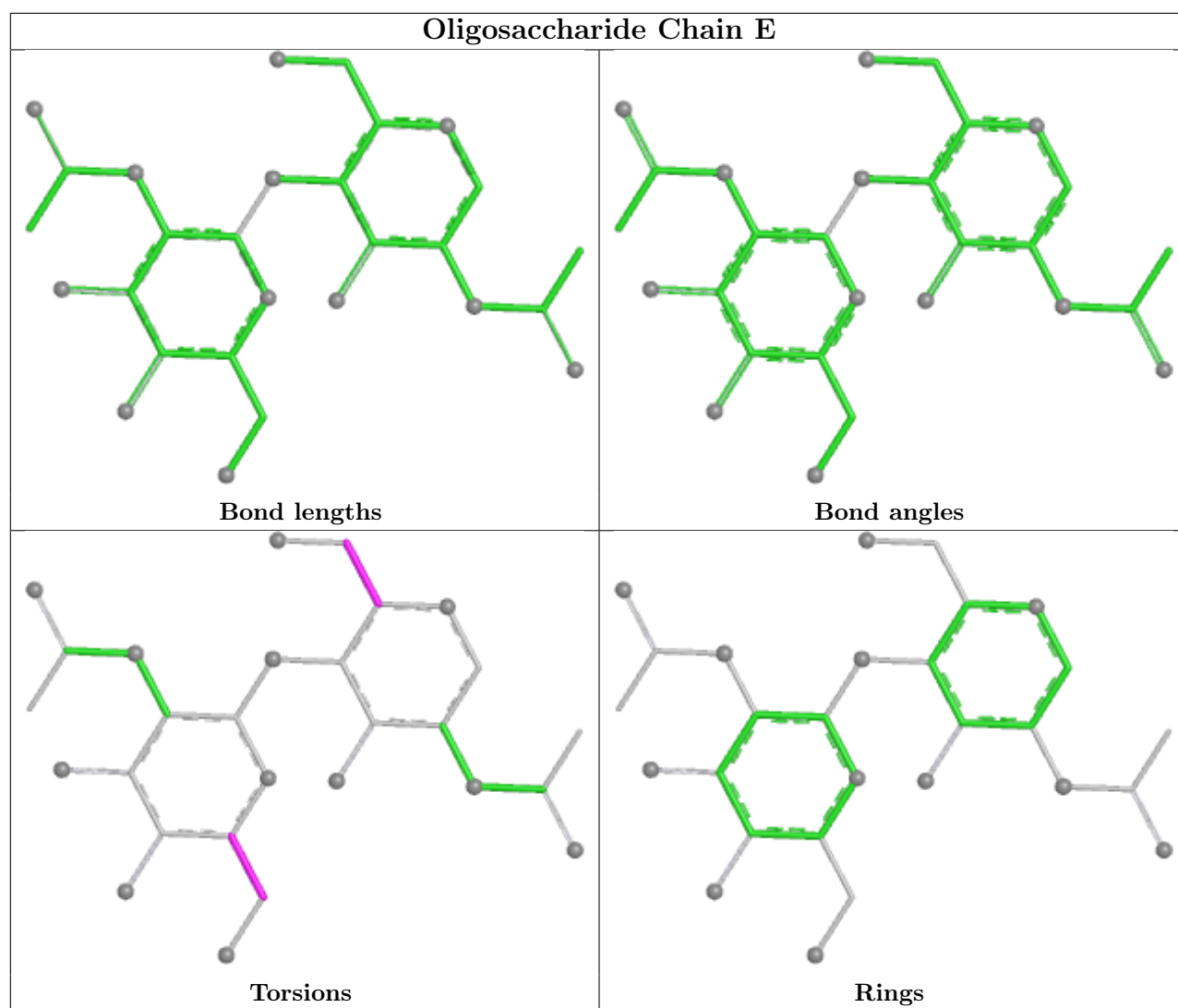
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 6   | k     | 2   | NAG  | 2       | 0            |
| 6   | x     | 1   | NAG  | 2       | 0            |
| 6   | u     | 1   | NAG  | 5       | 0            |
| 8   | r     | 1   | NAG  | 2       | 0            |
| 6   | t     | 2   | NAG  | 1       | 0            |
| 5   | m     | 1   | NAG  | 2       | 0            |
| 9   | v     | 1   | NAG  | 1       | 0            |
| 6   | t     | 1   | NAG  | 1       | 0            |

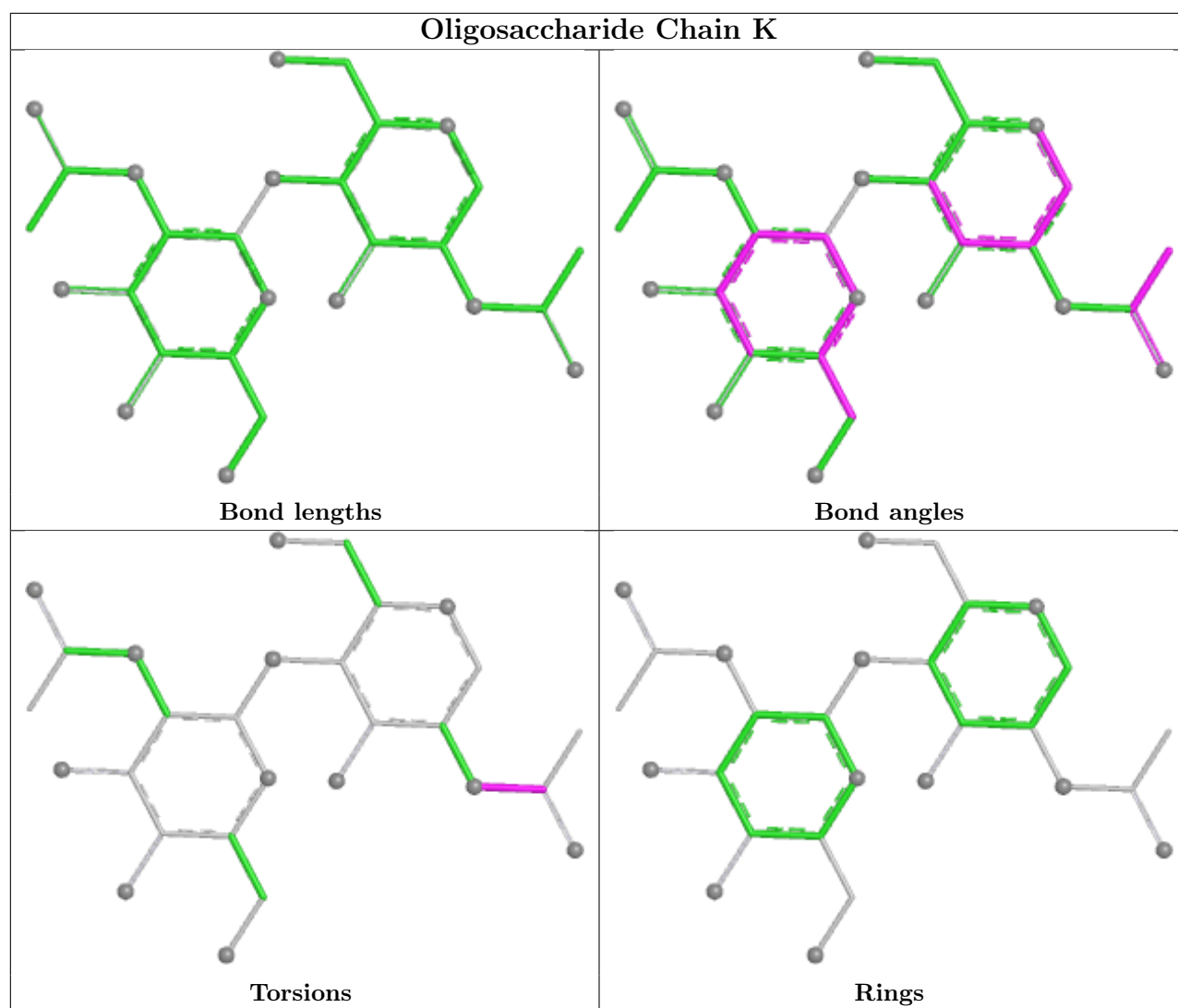
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

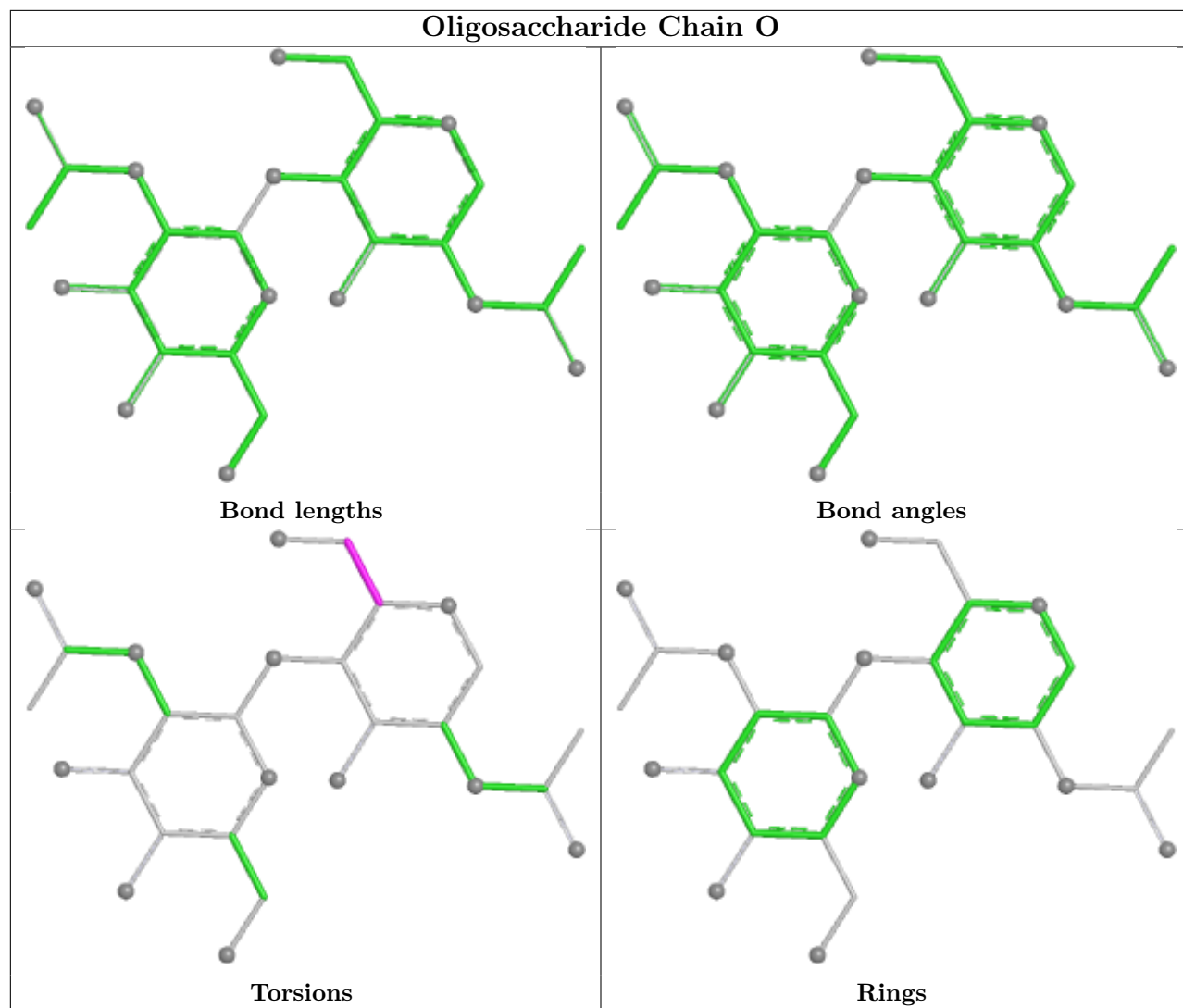


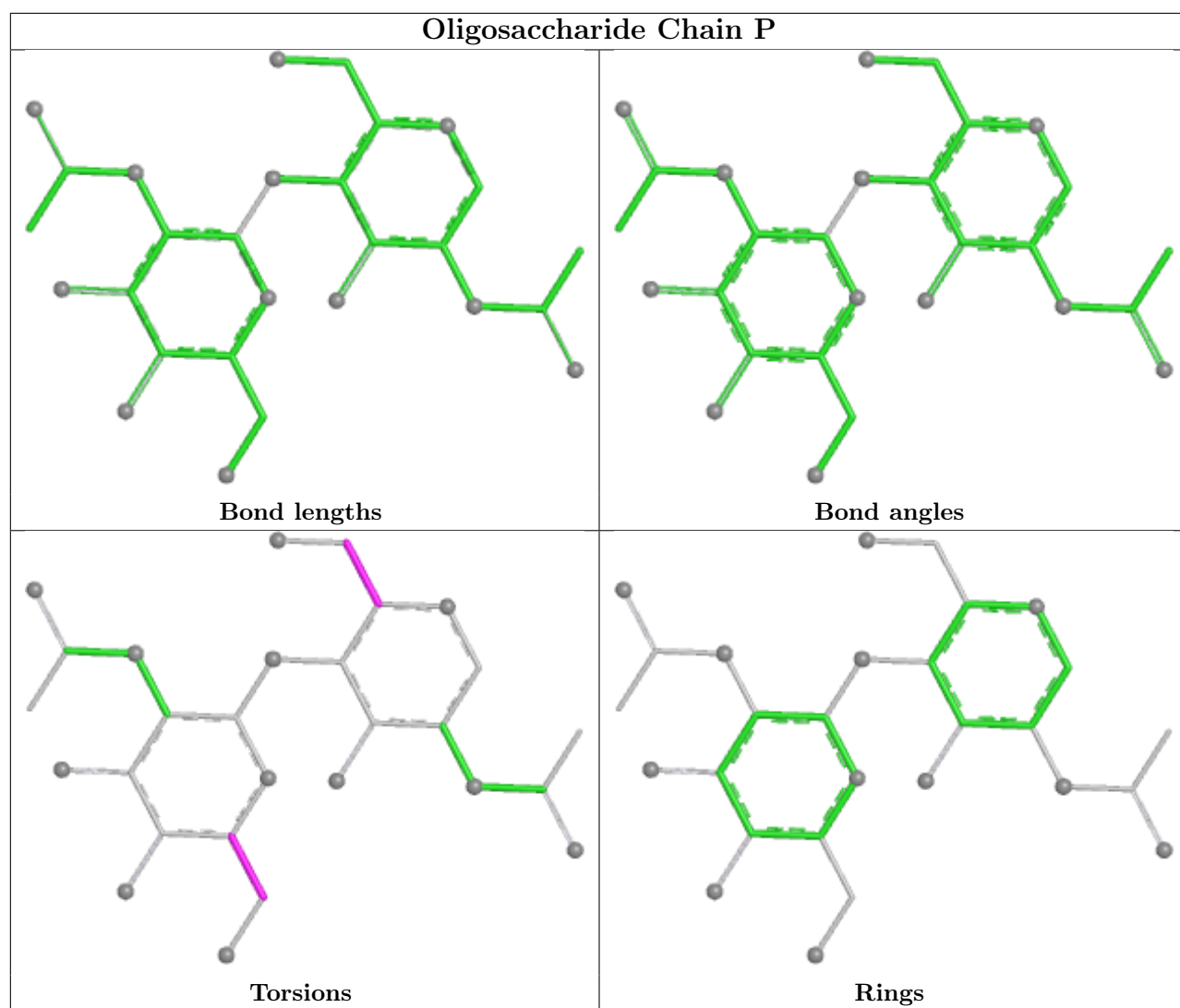


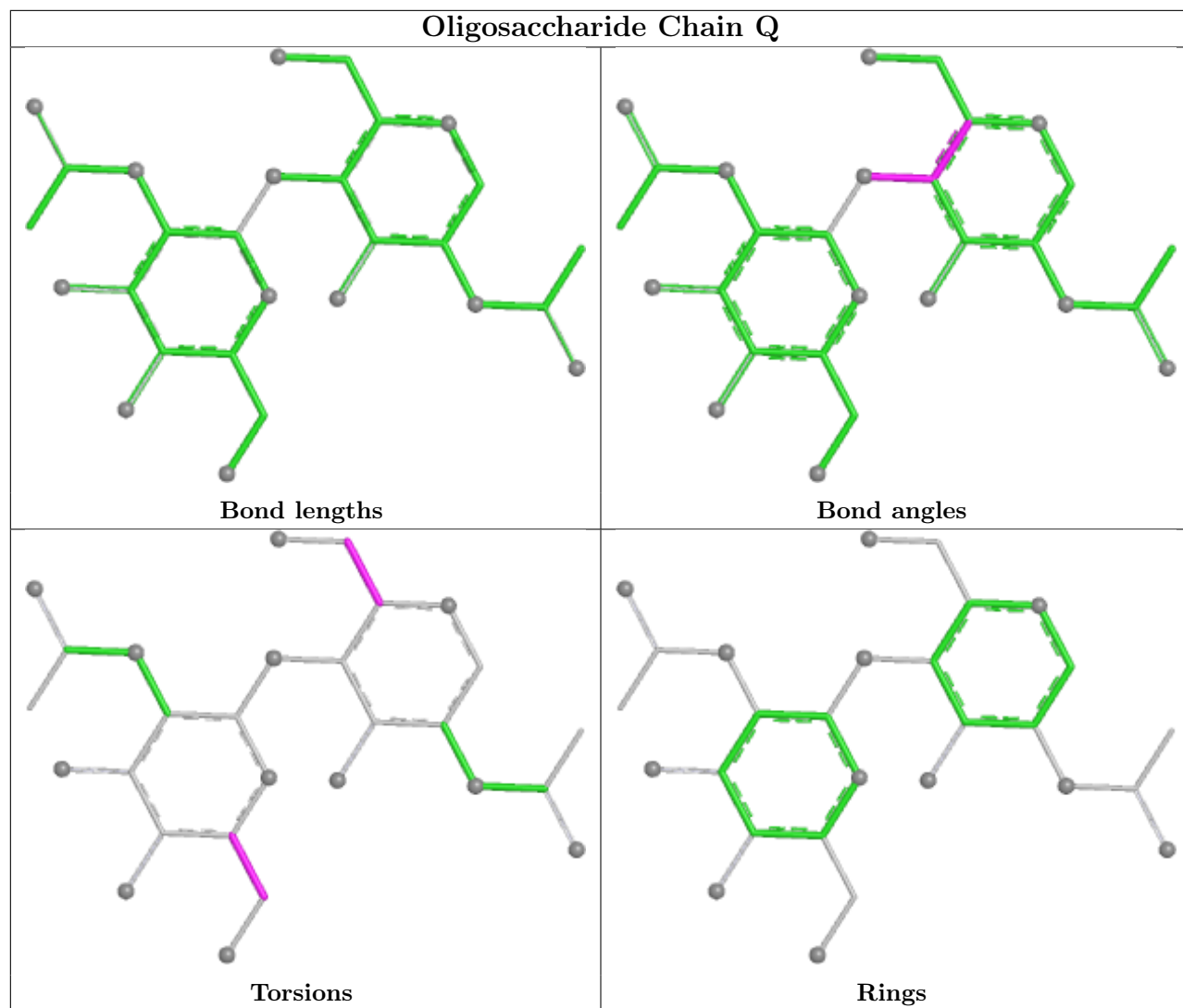


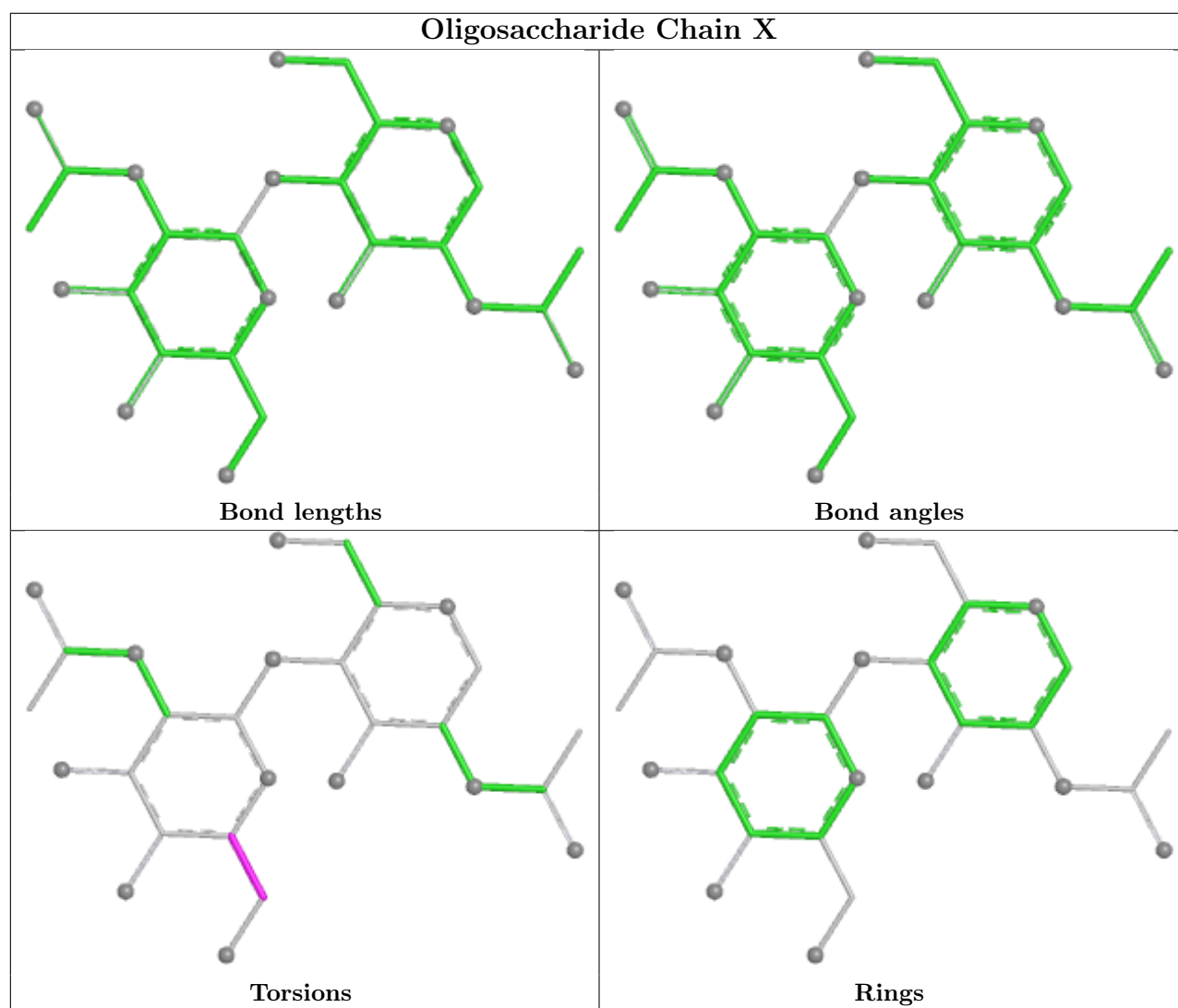


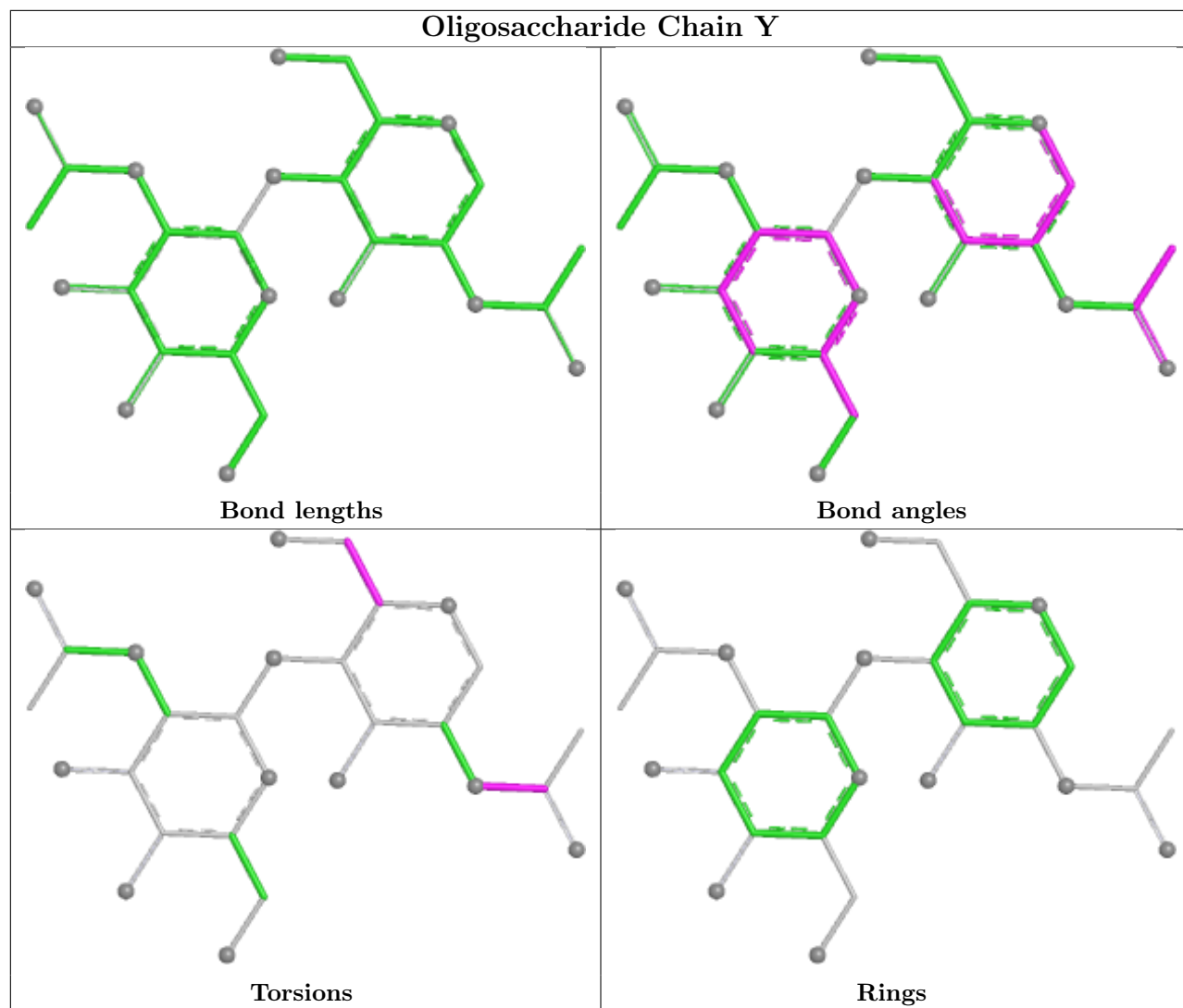


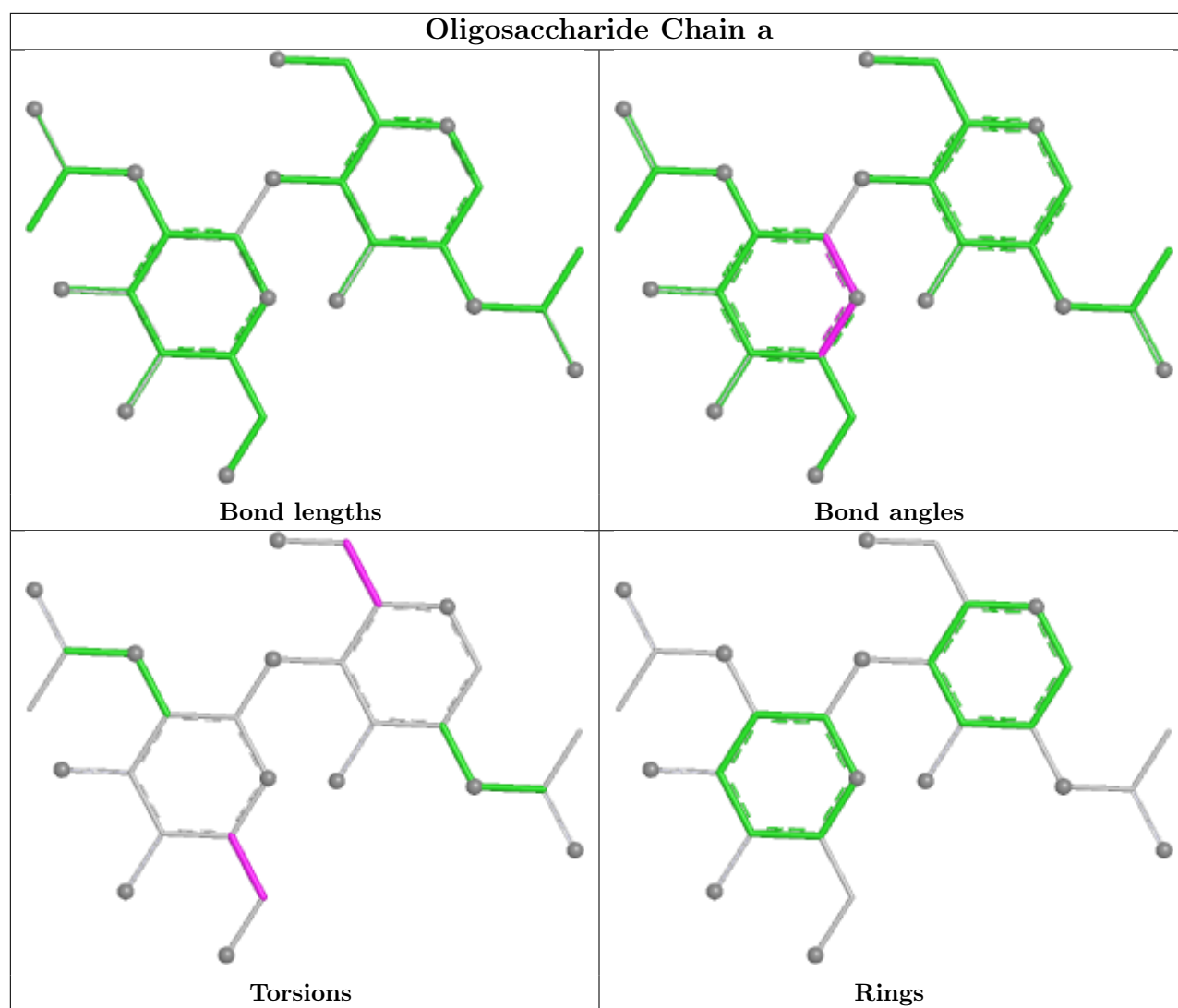


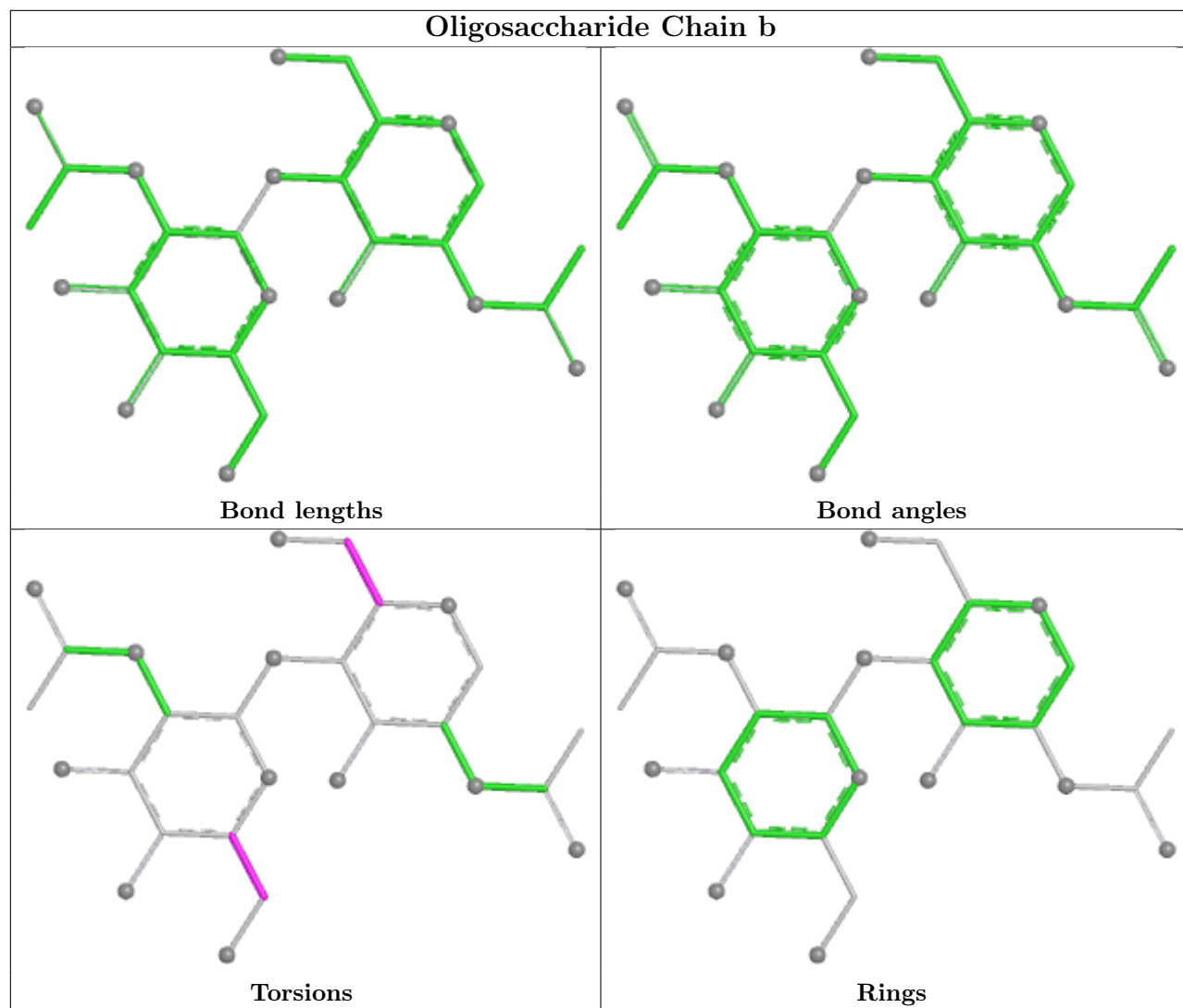


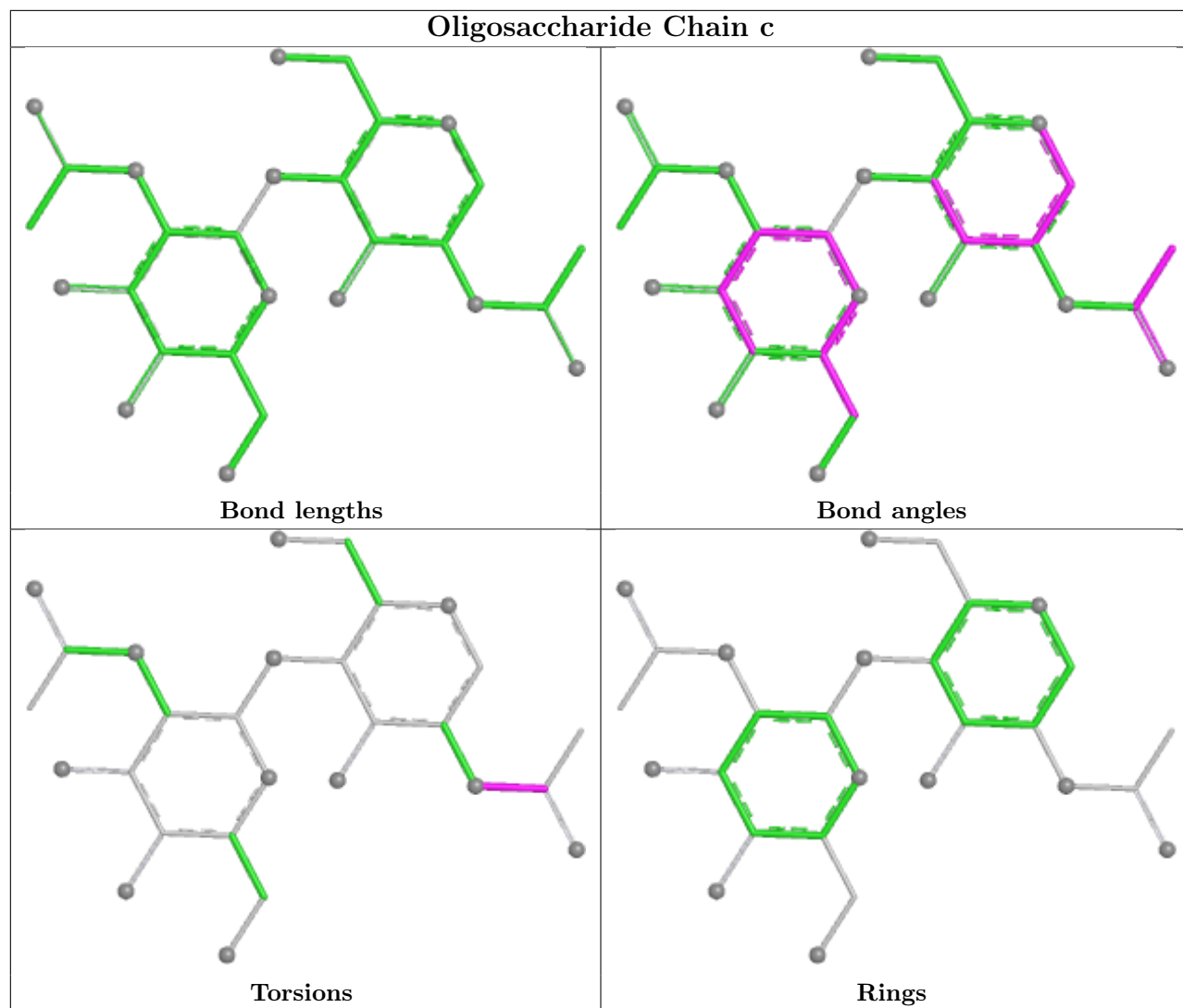


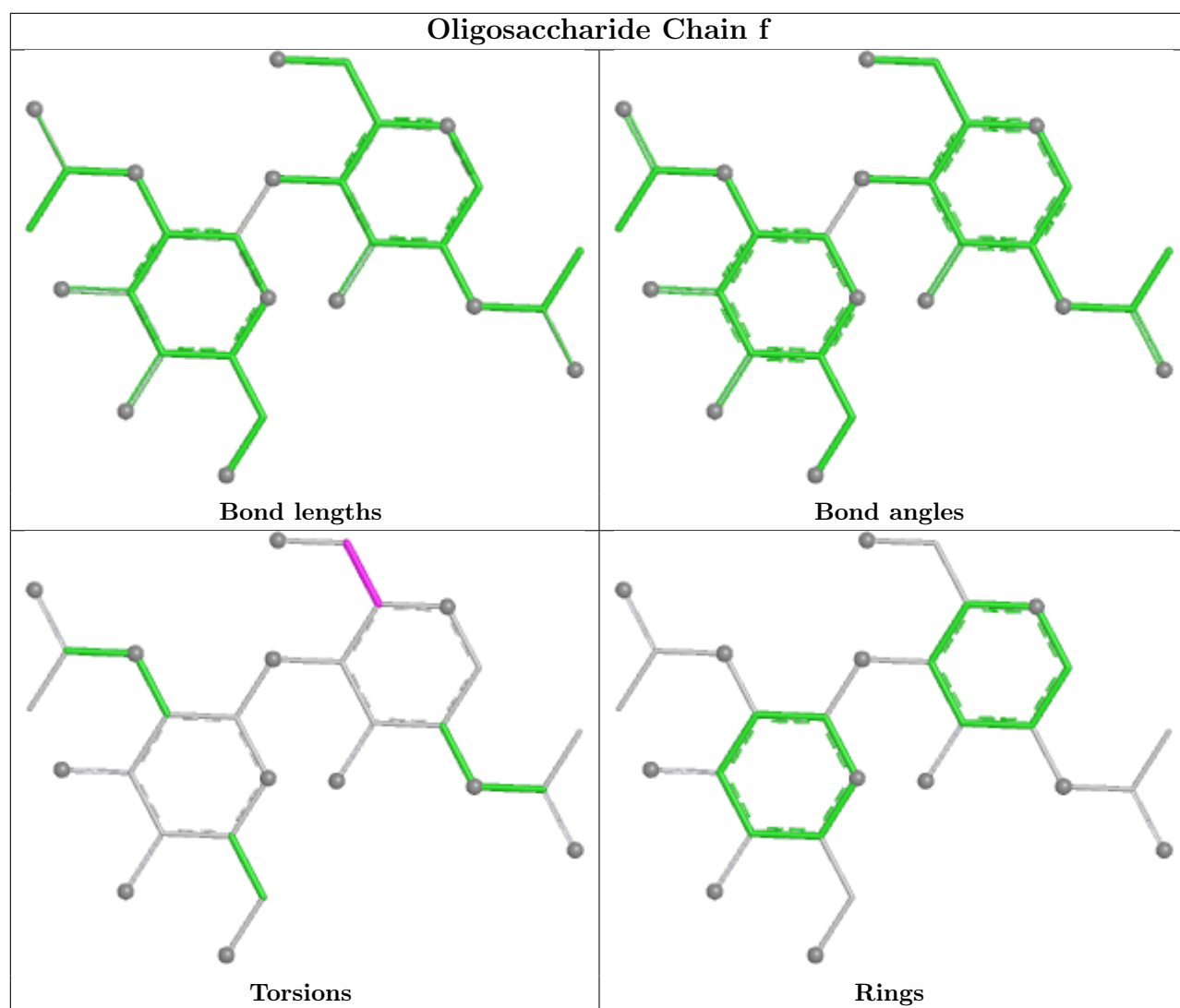


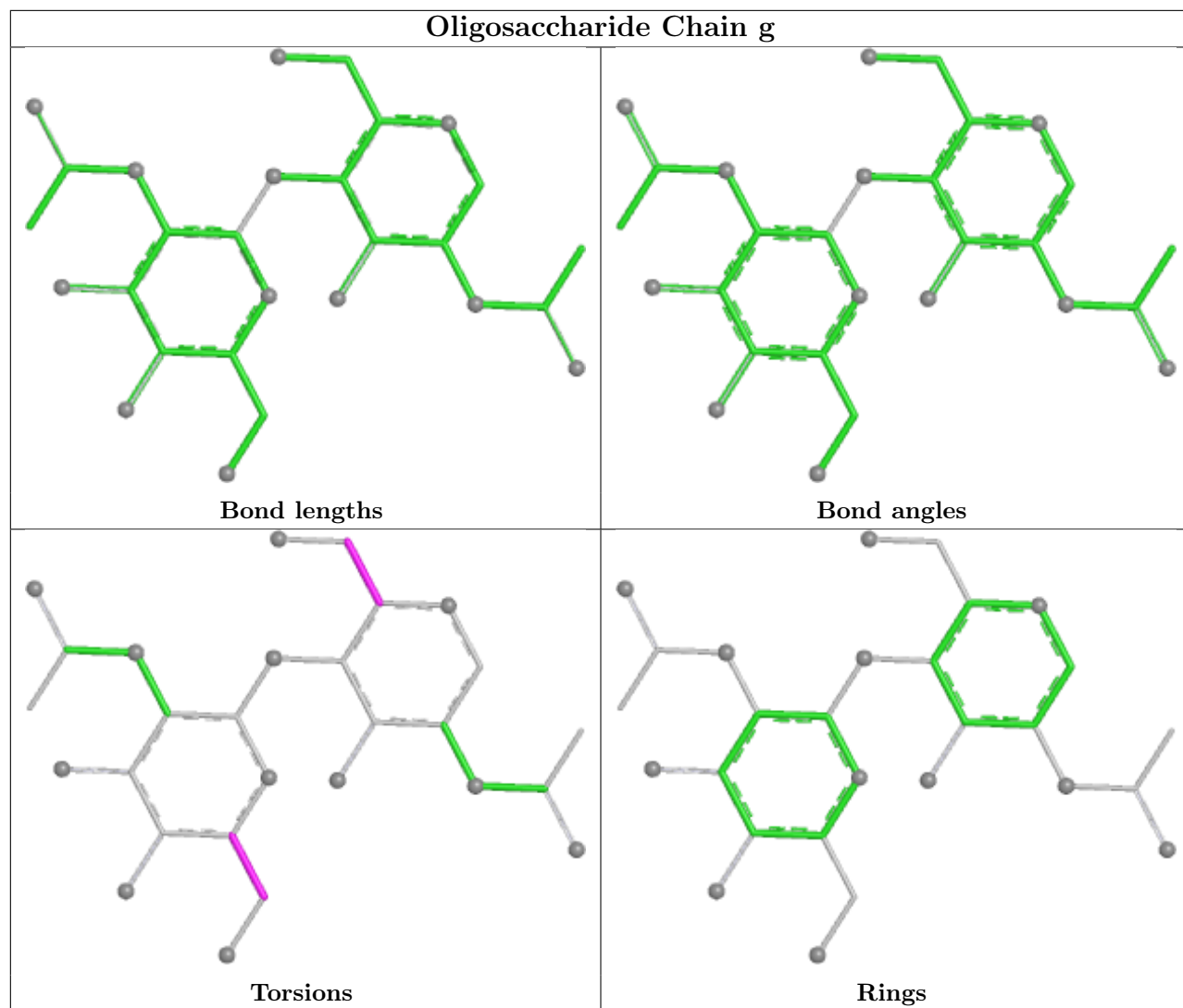


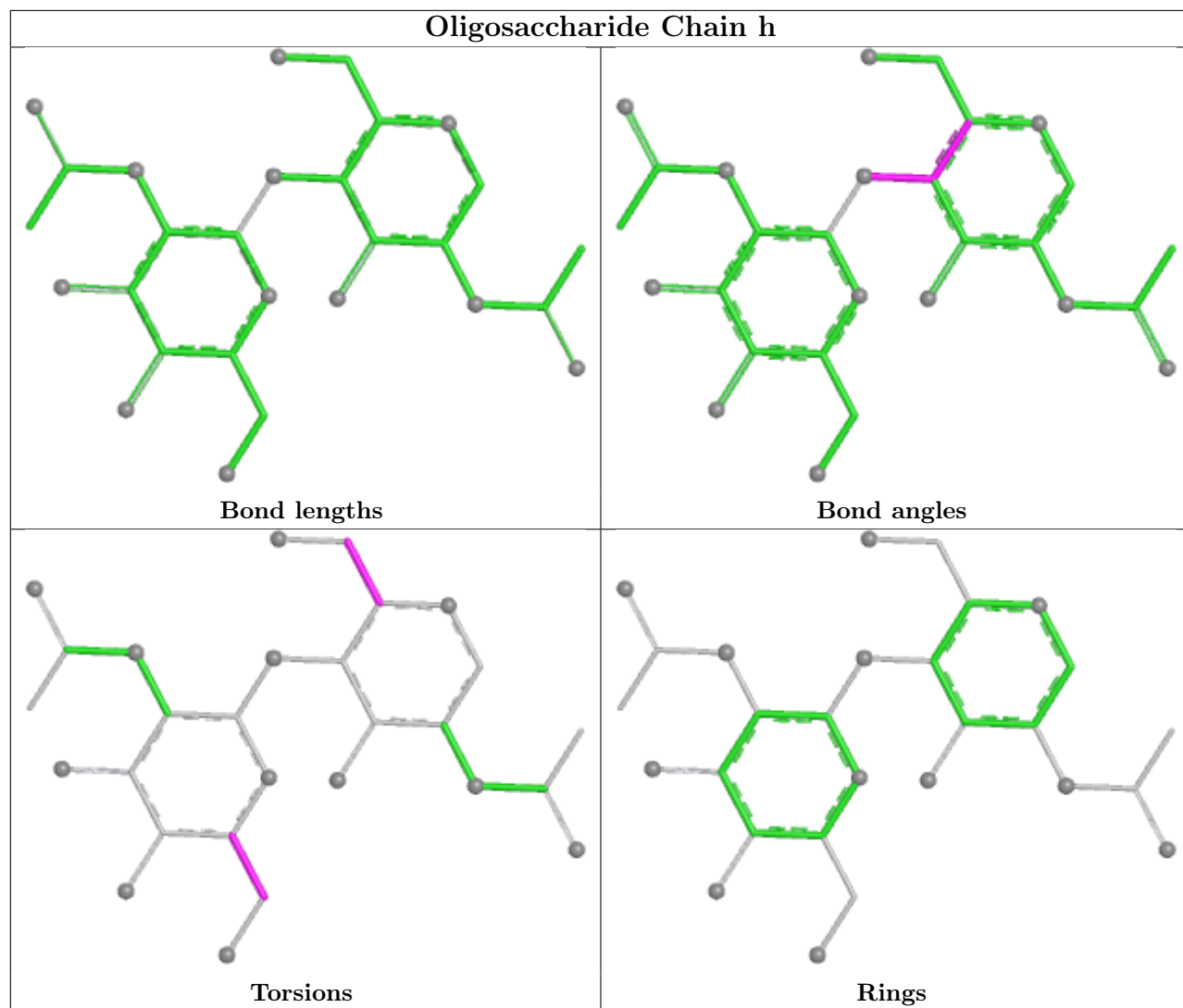


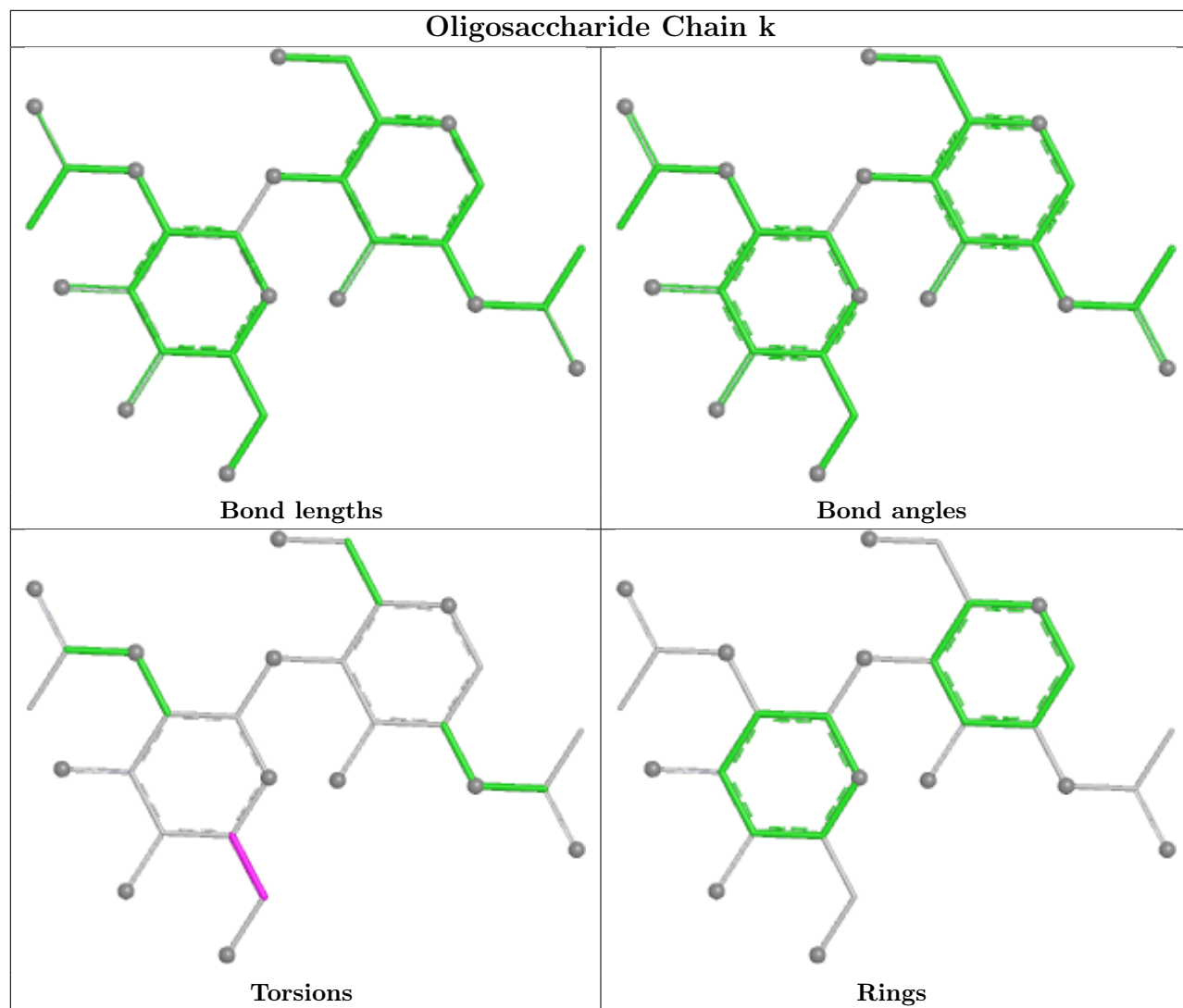


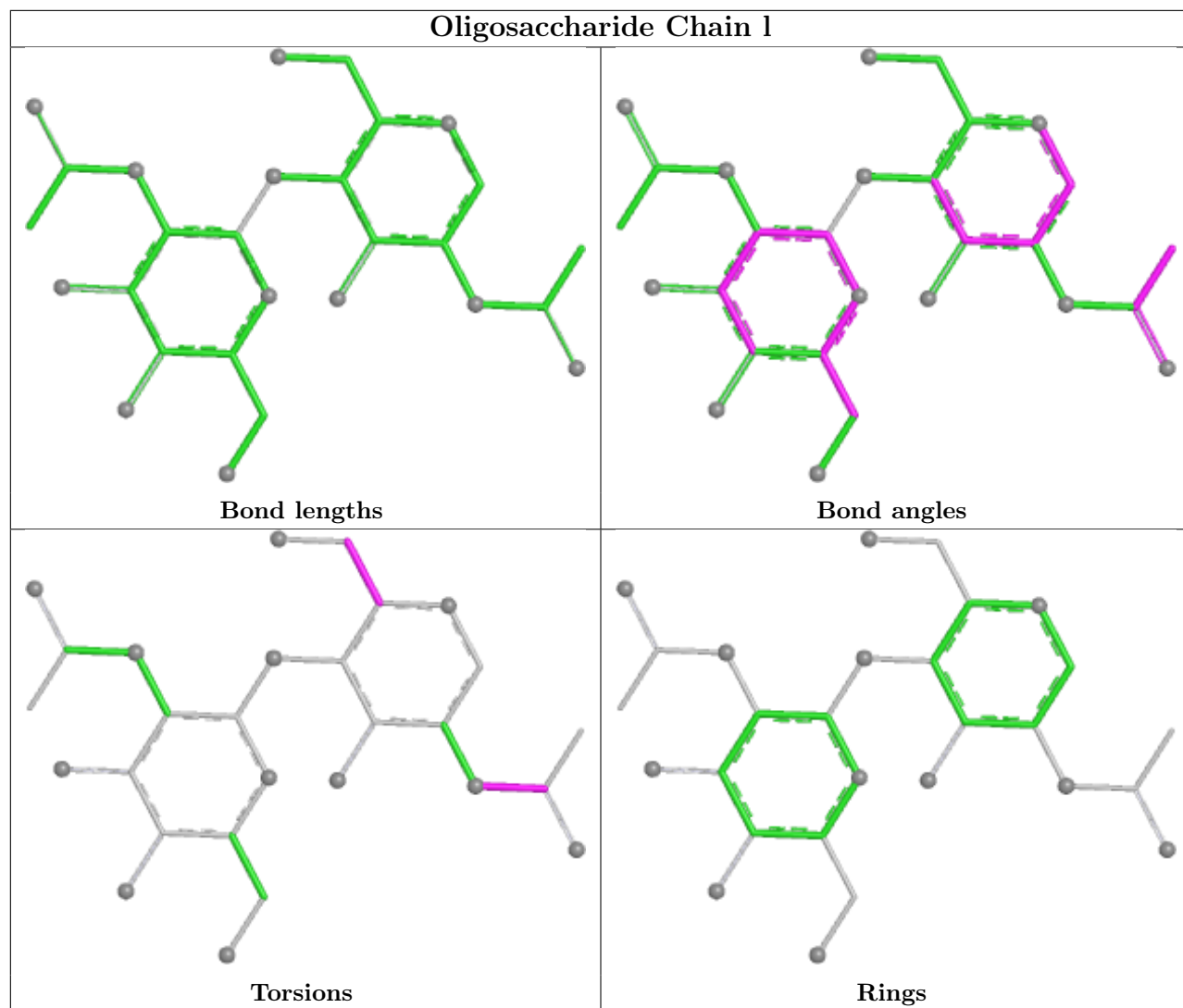


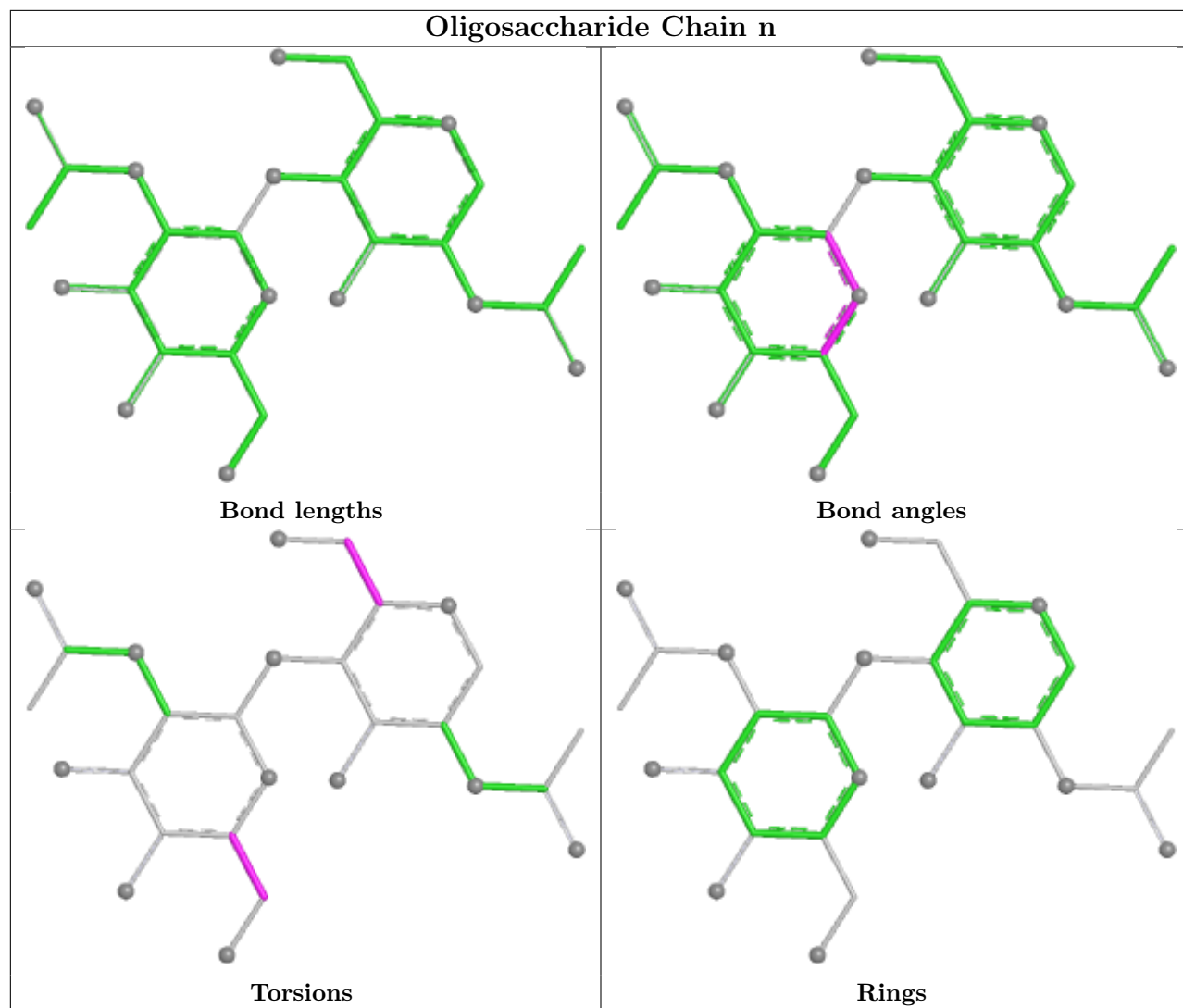


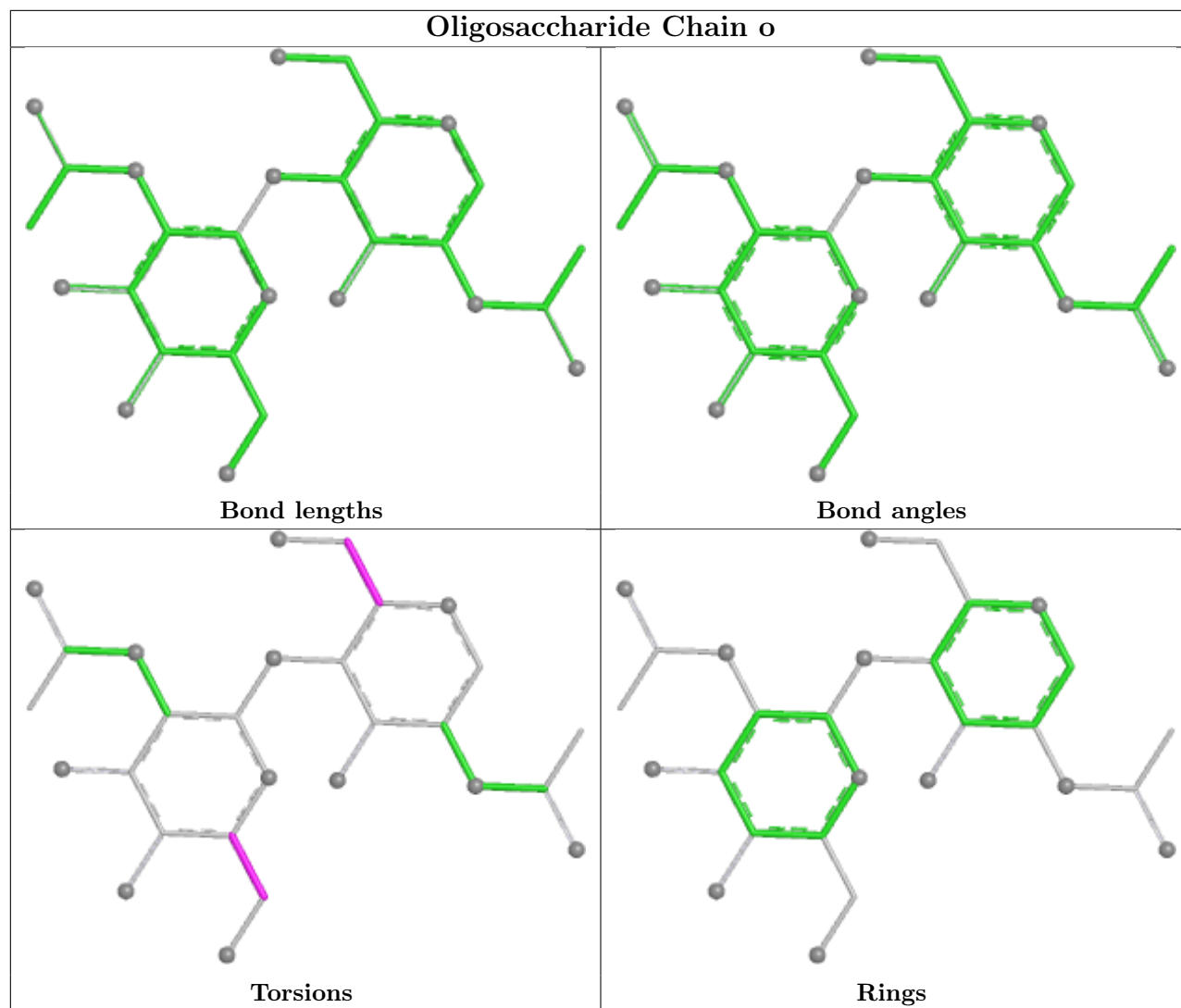


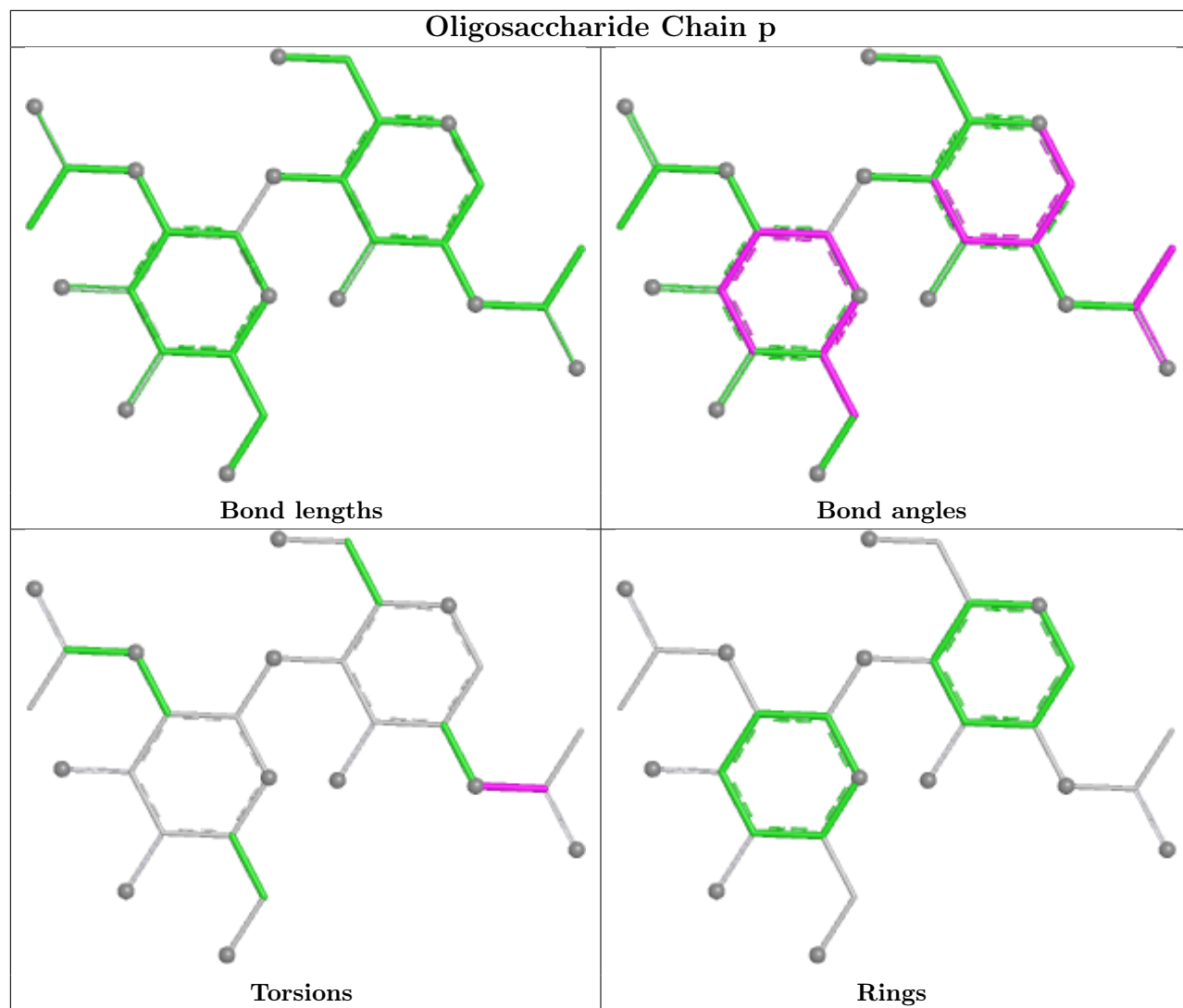


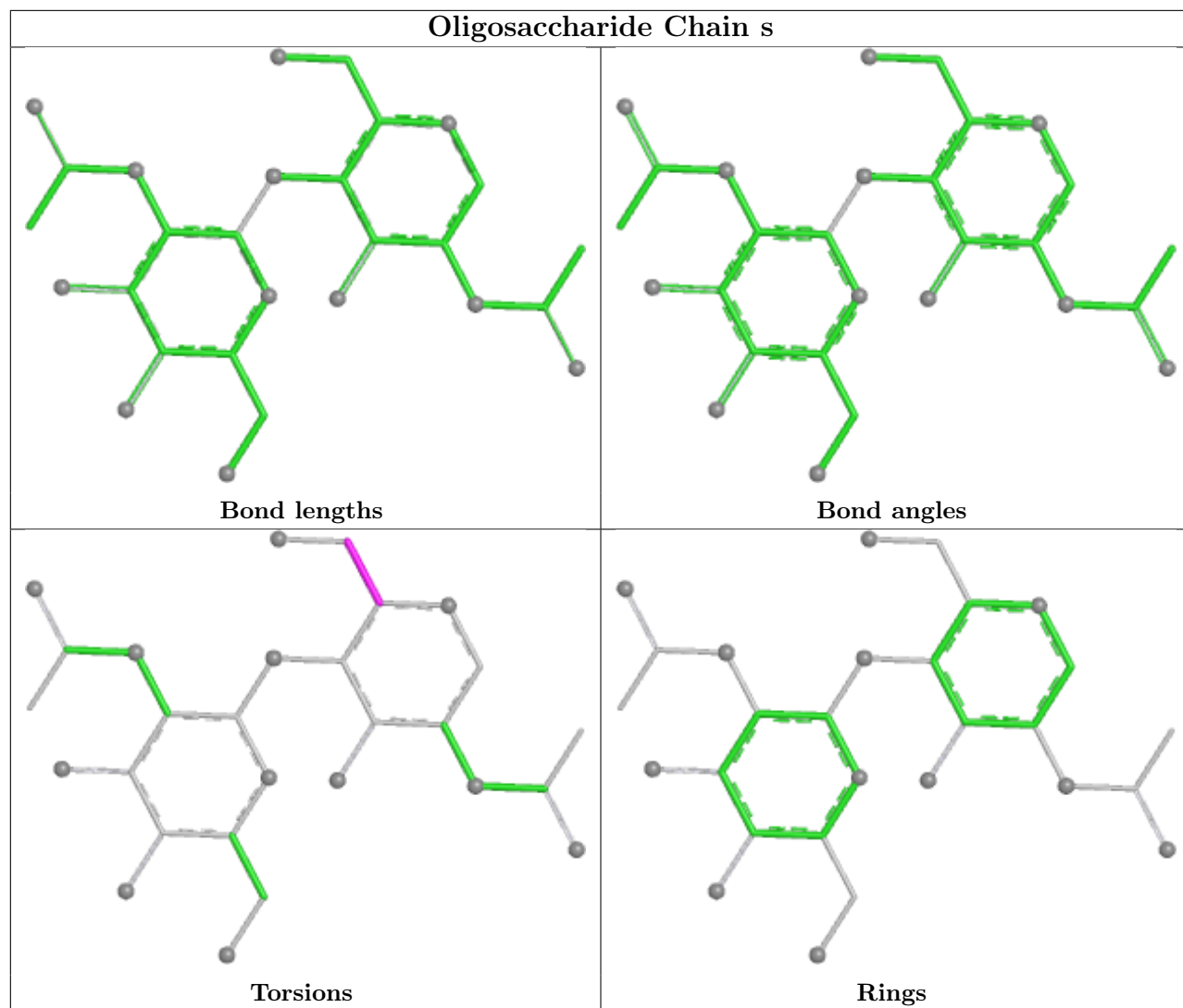


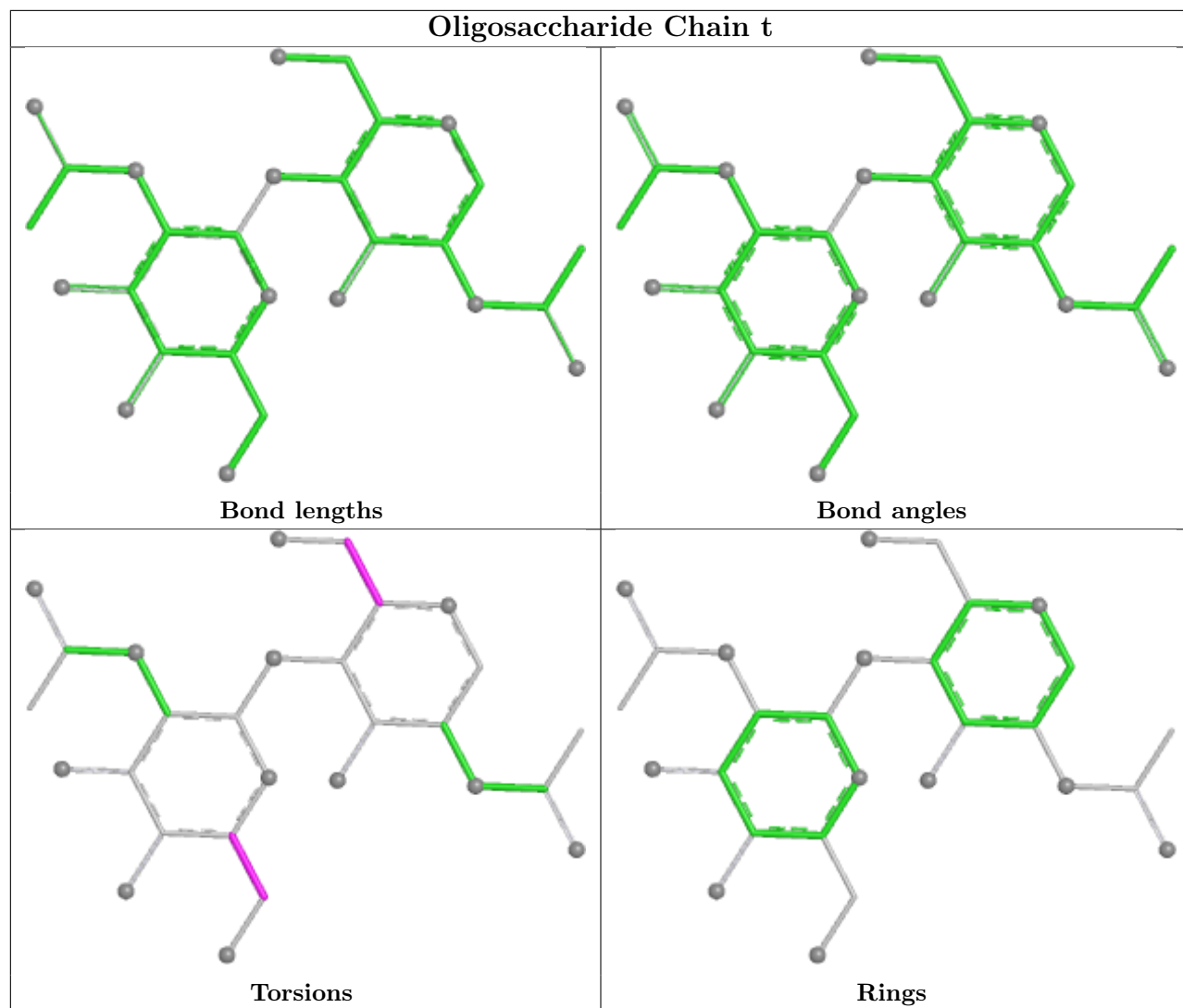


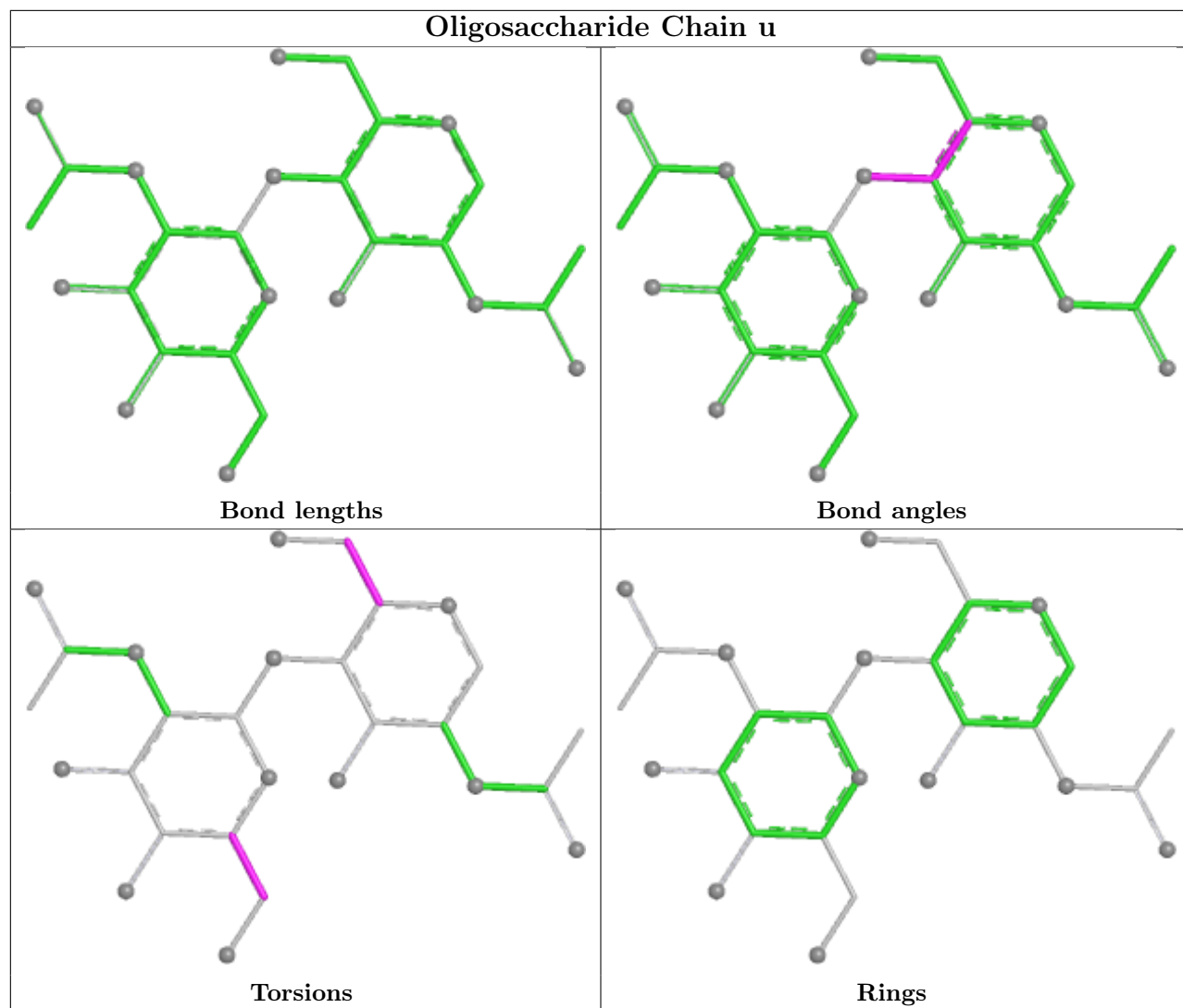


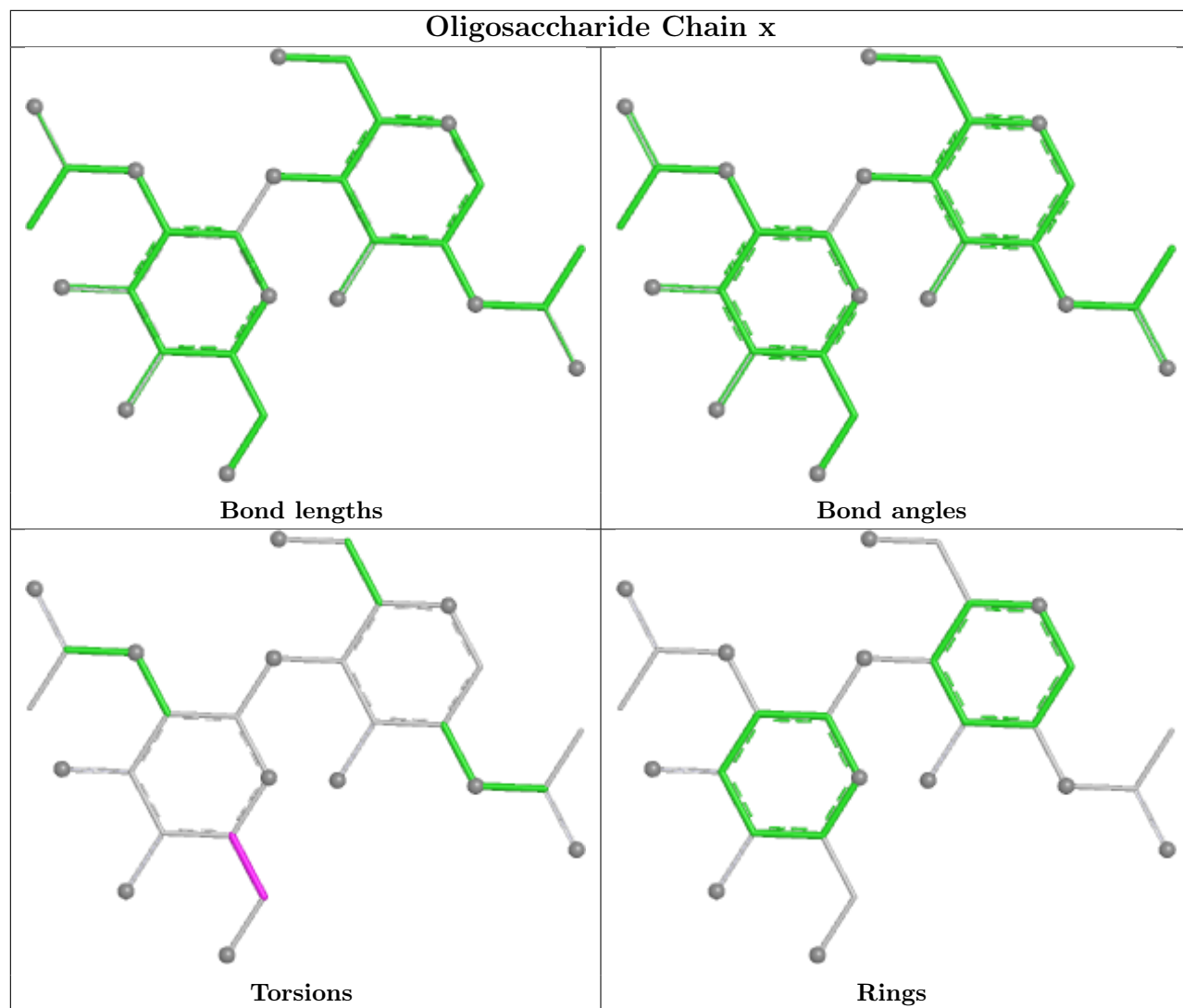


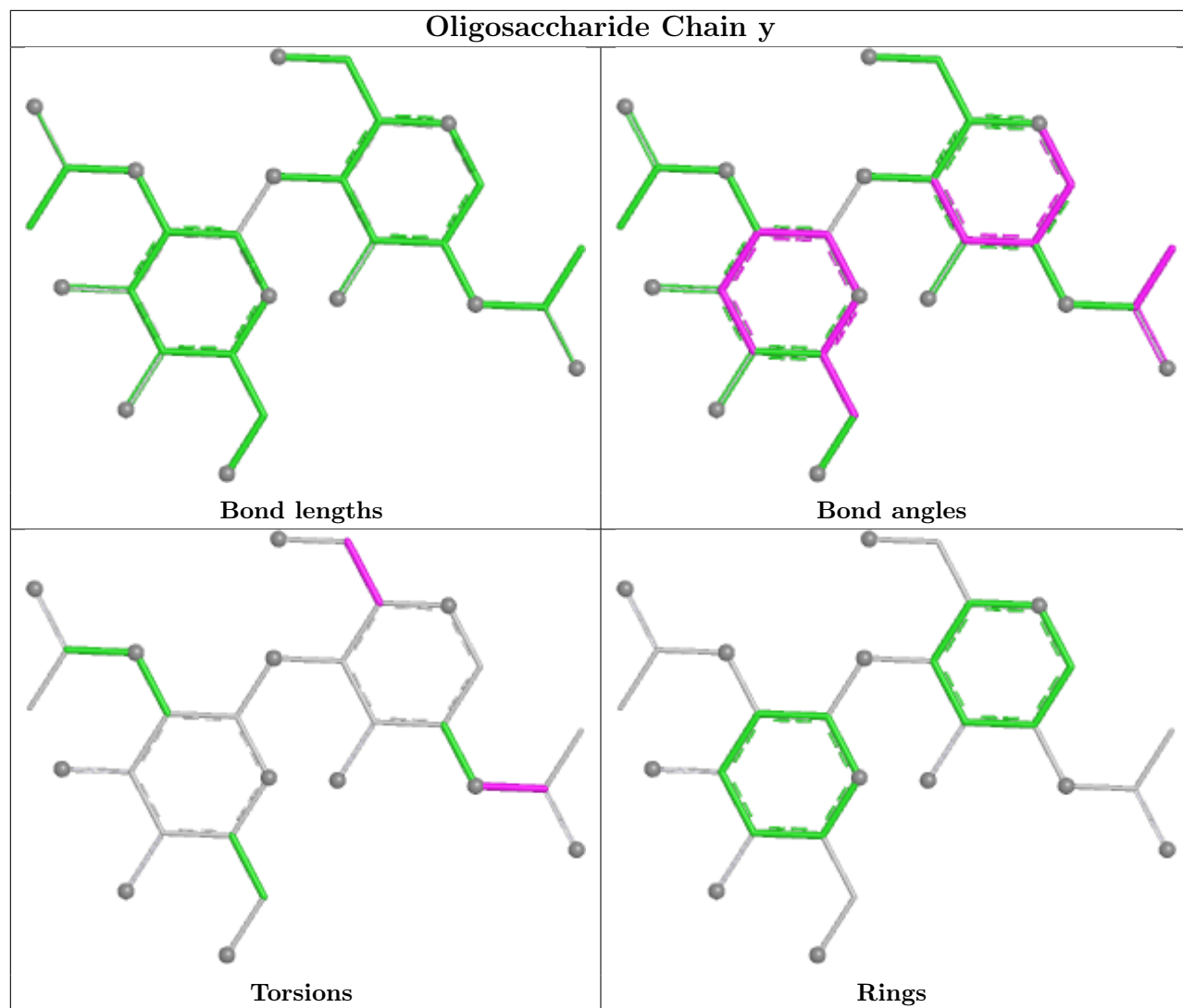


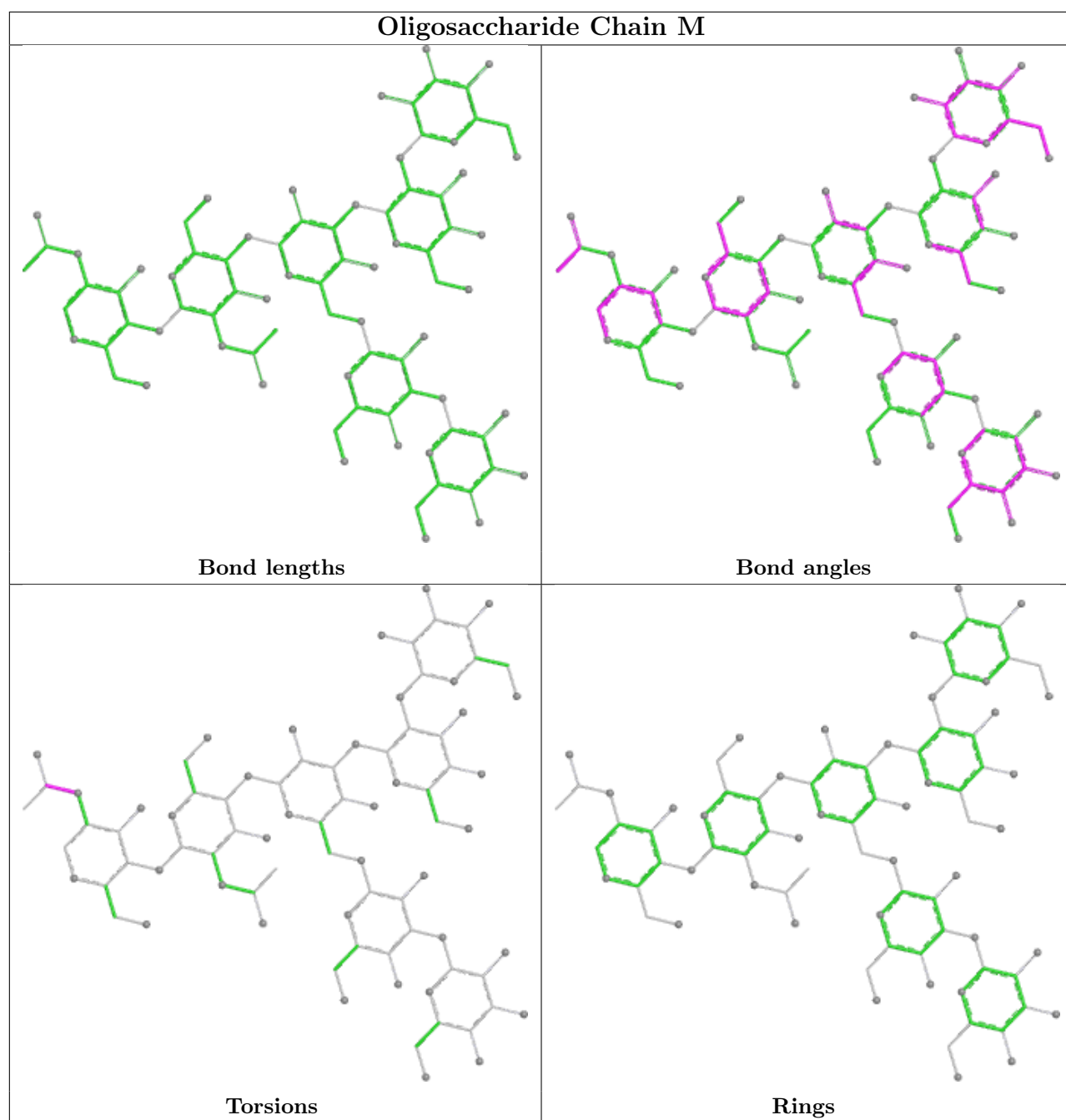


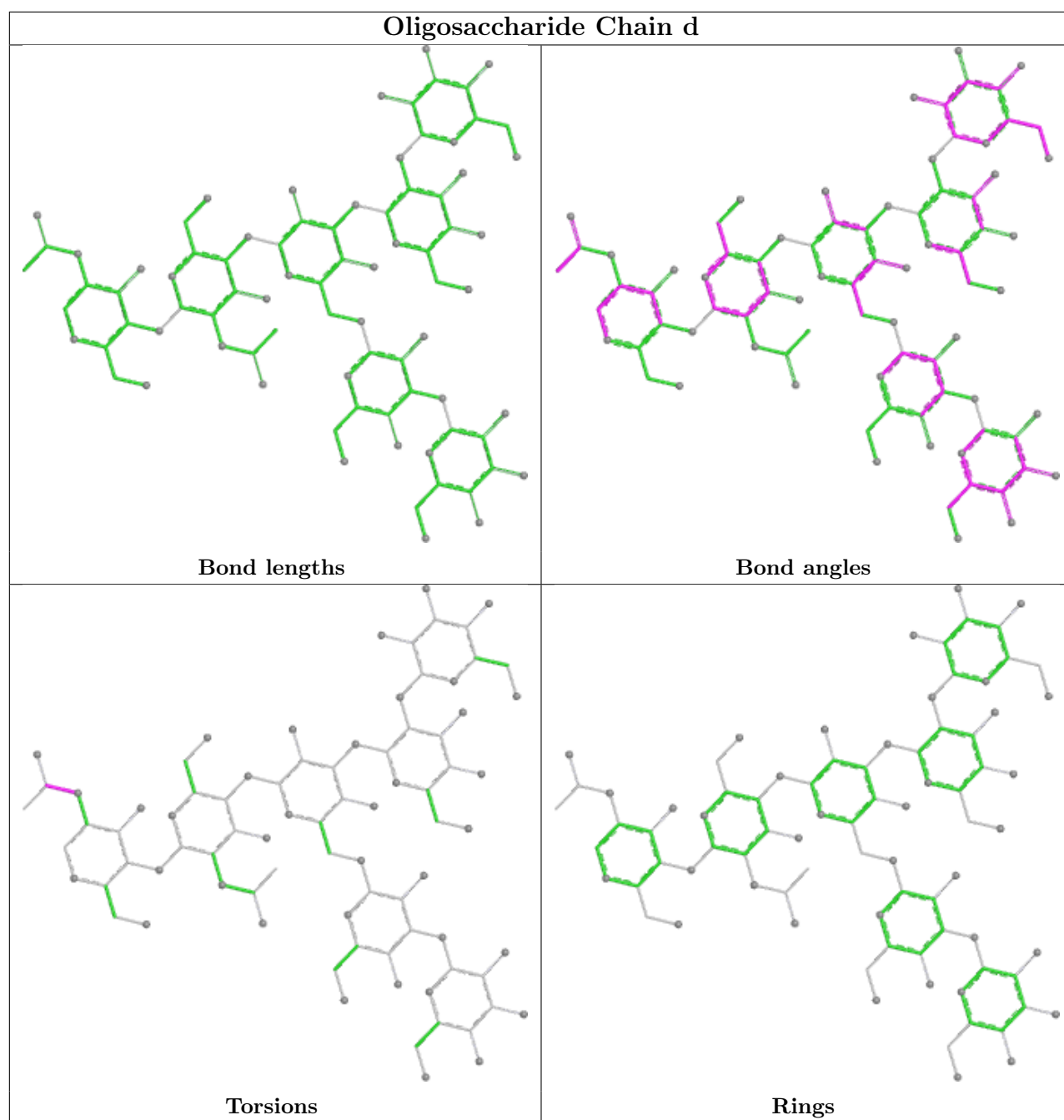


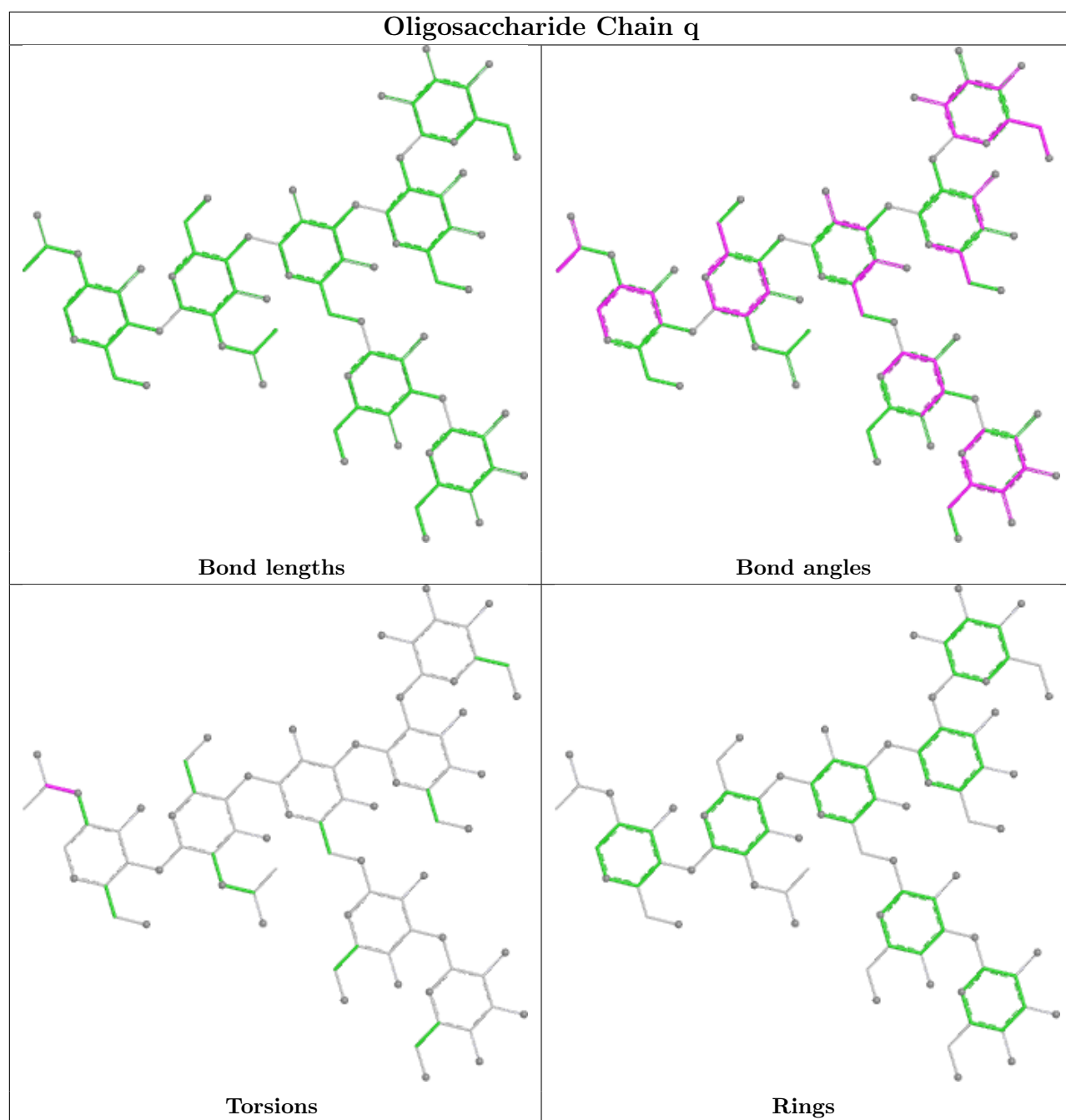


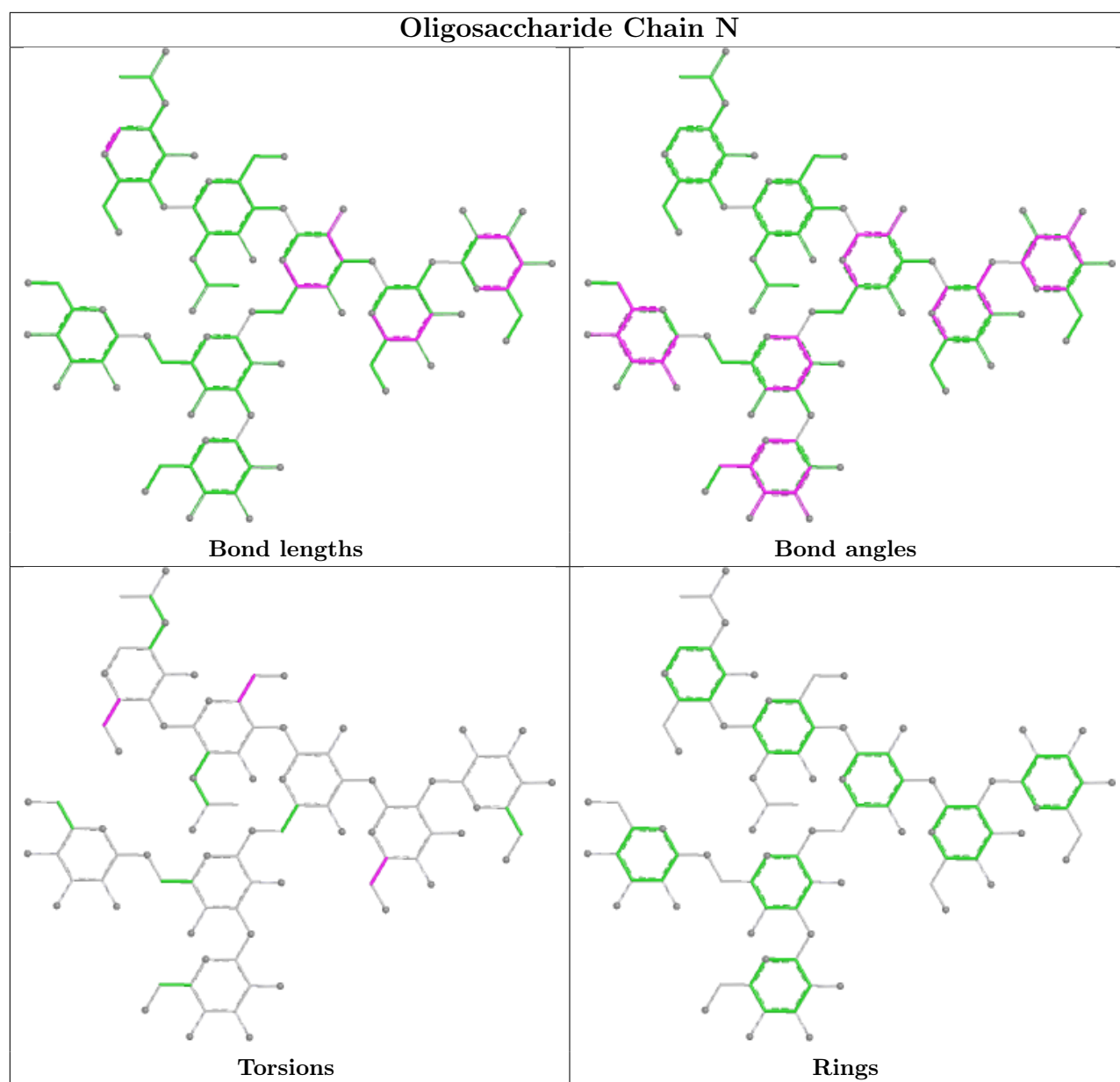


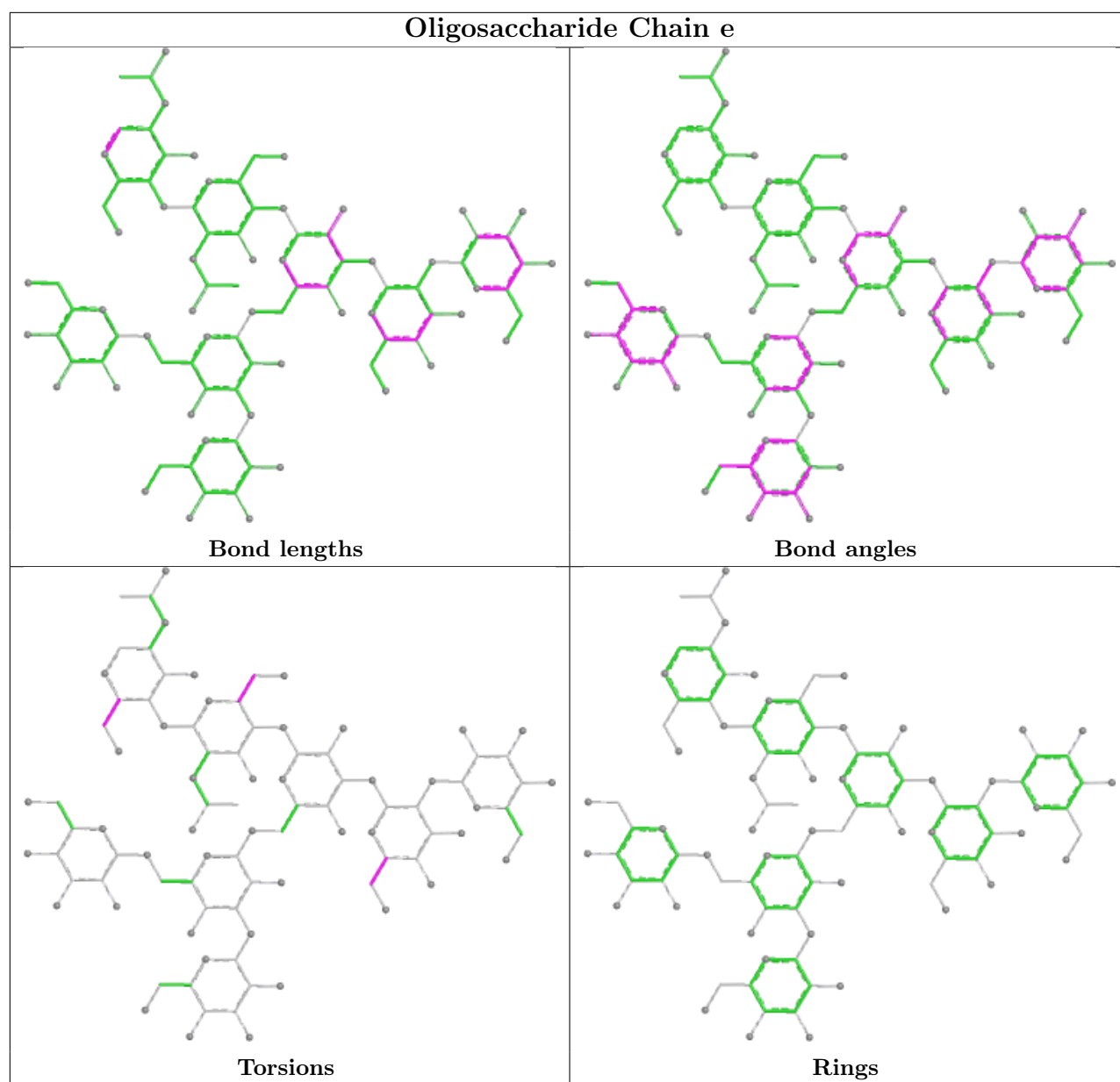


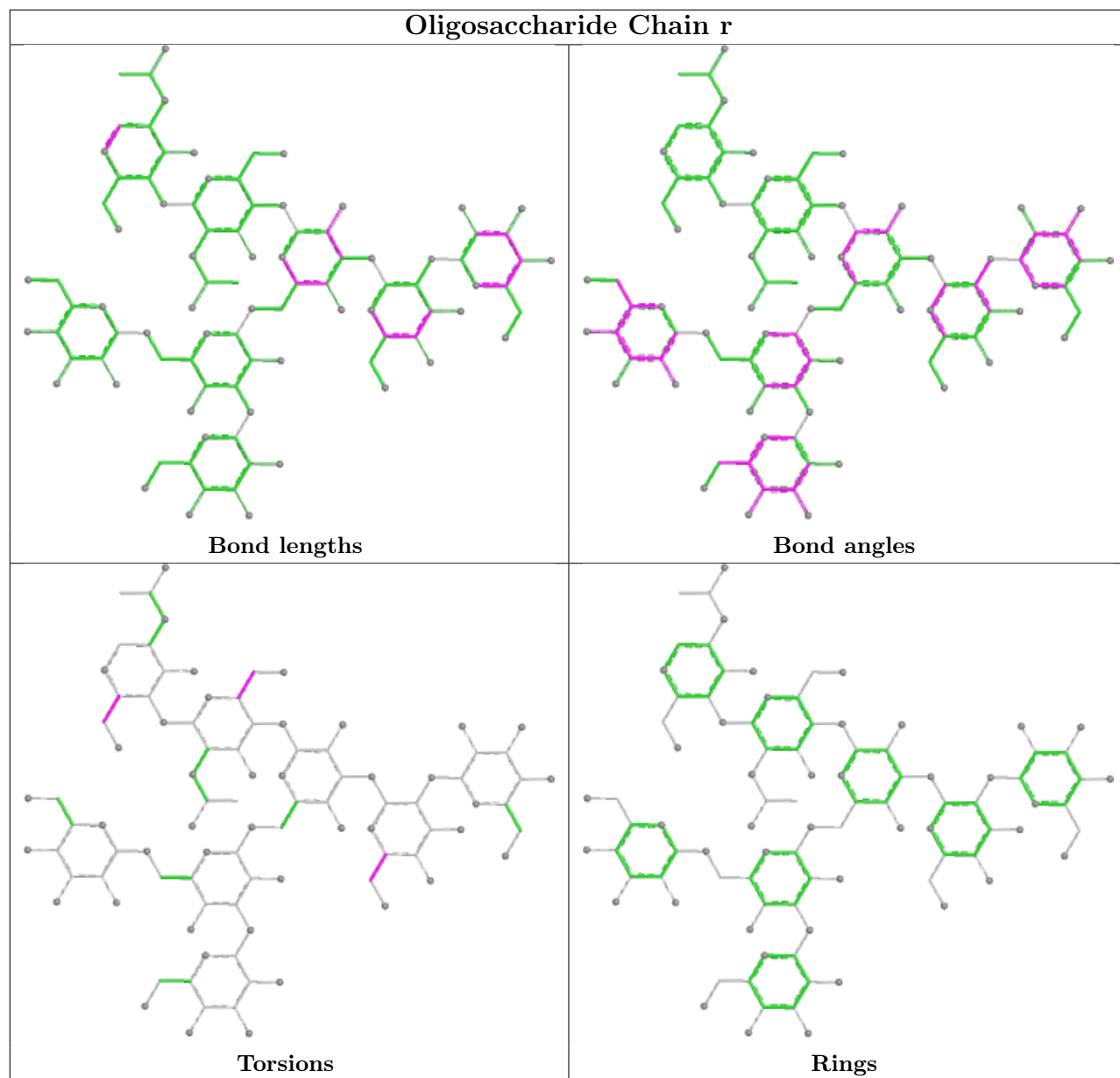


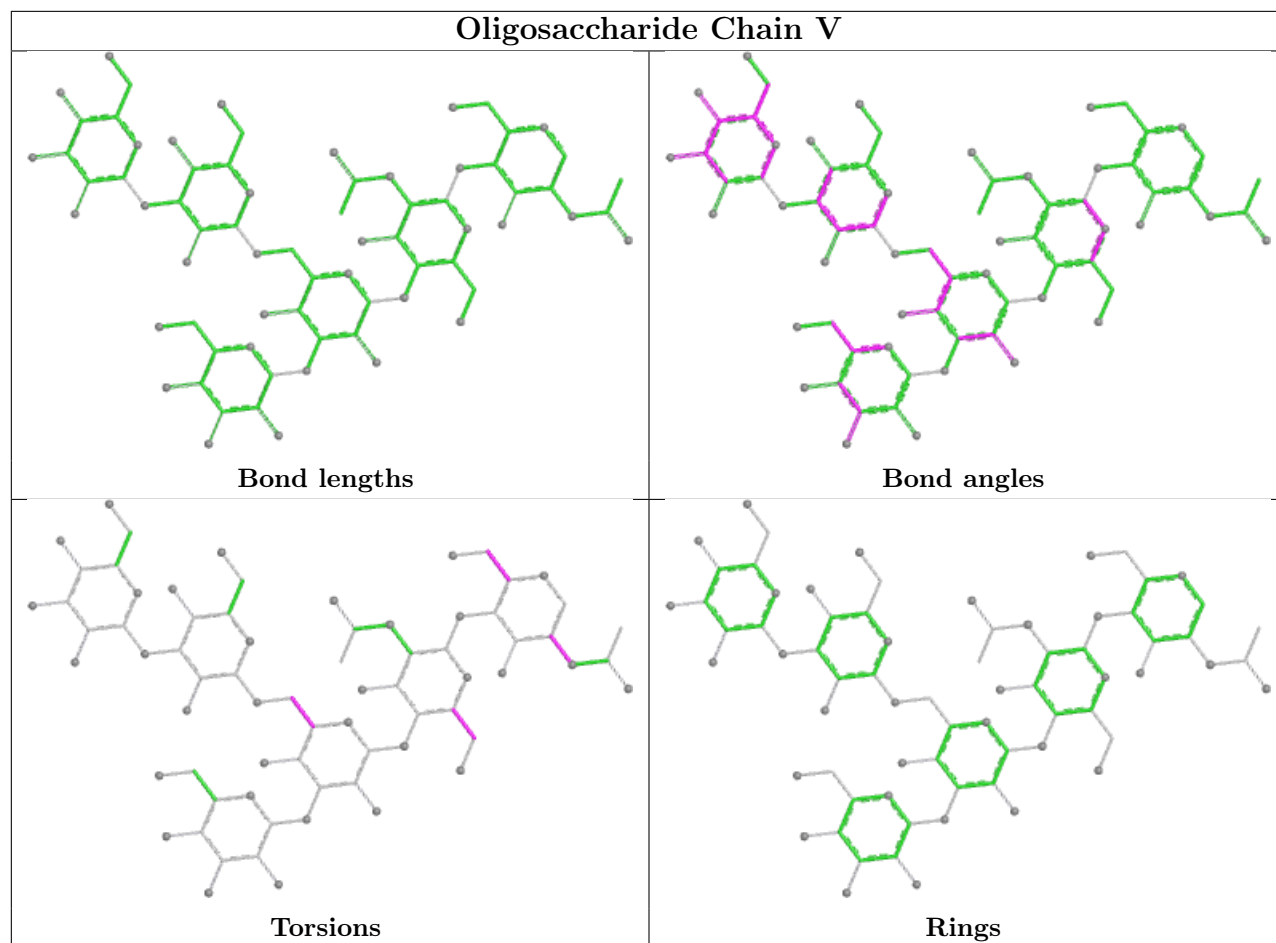


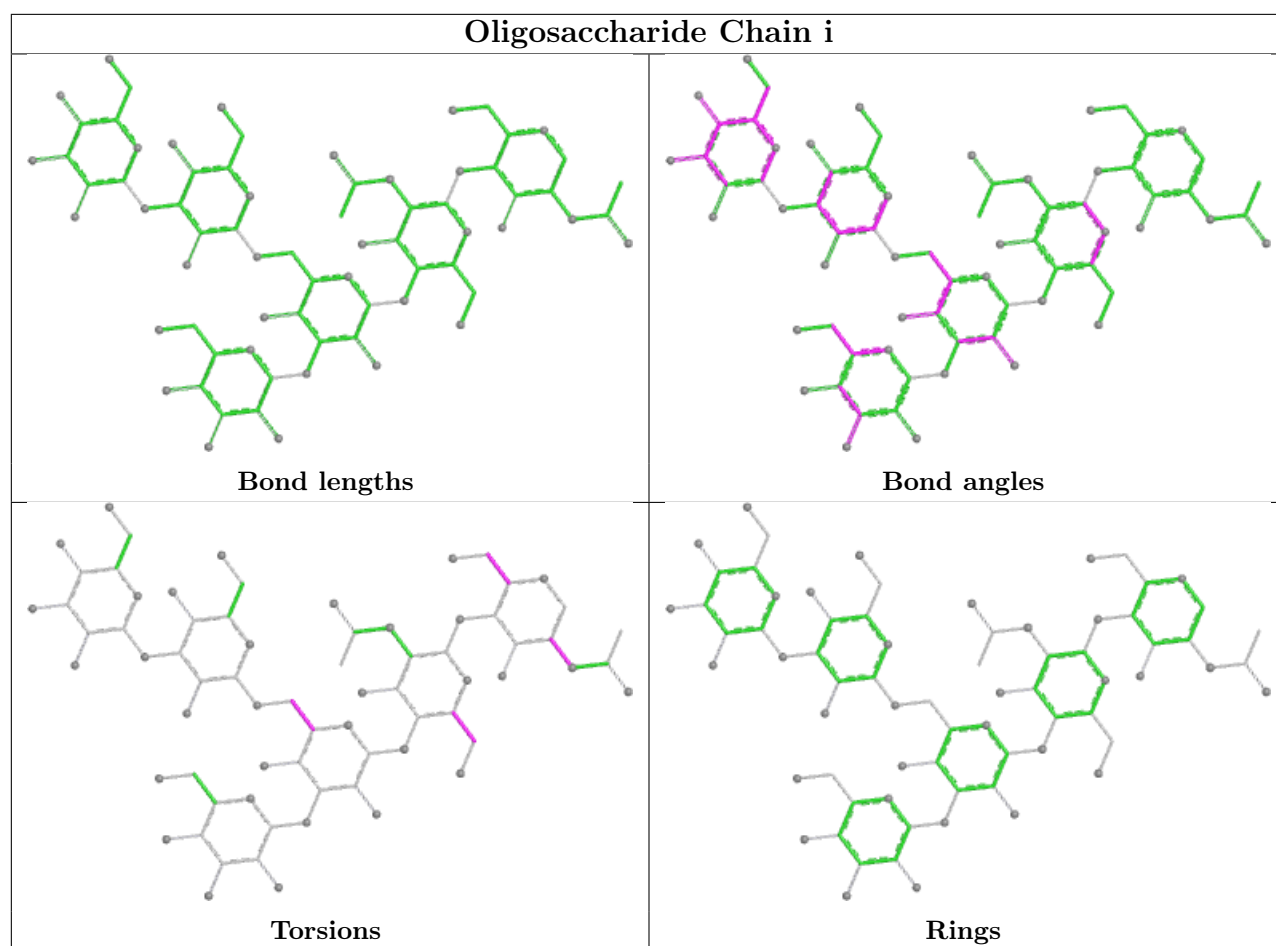


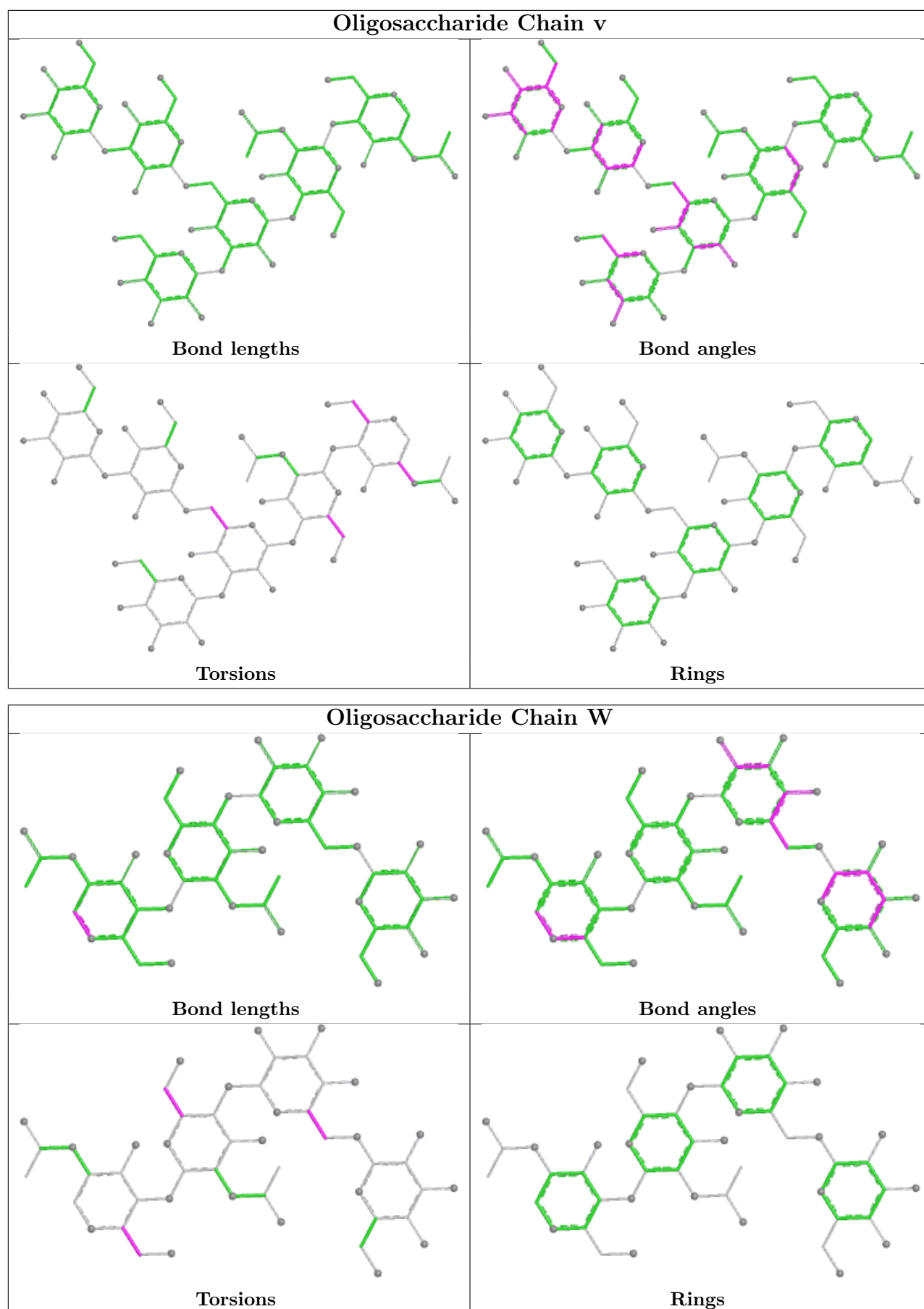


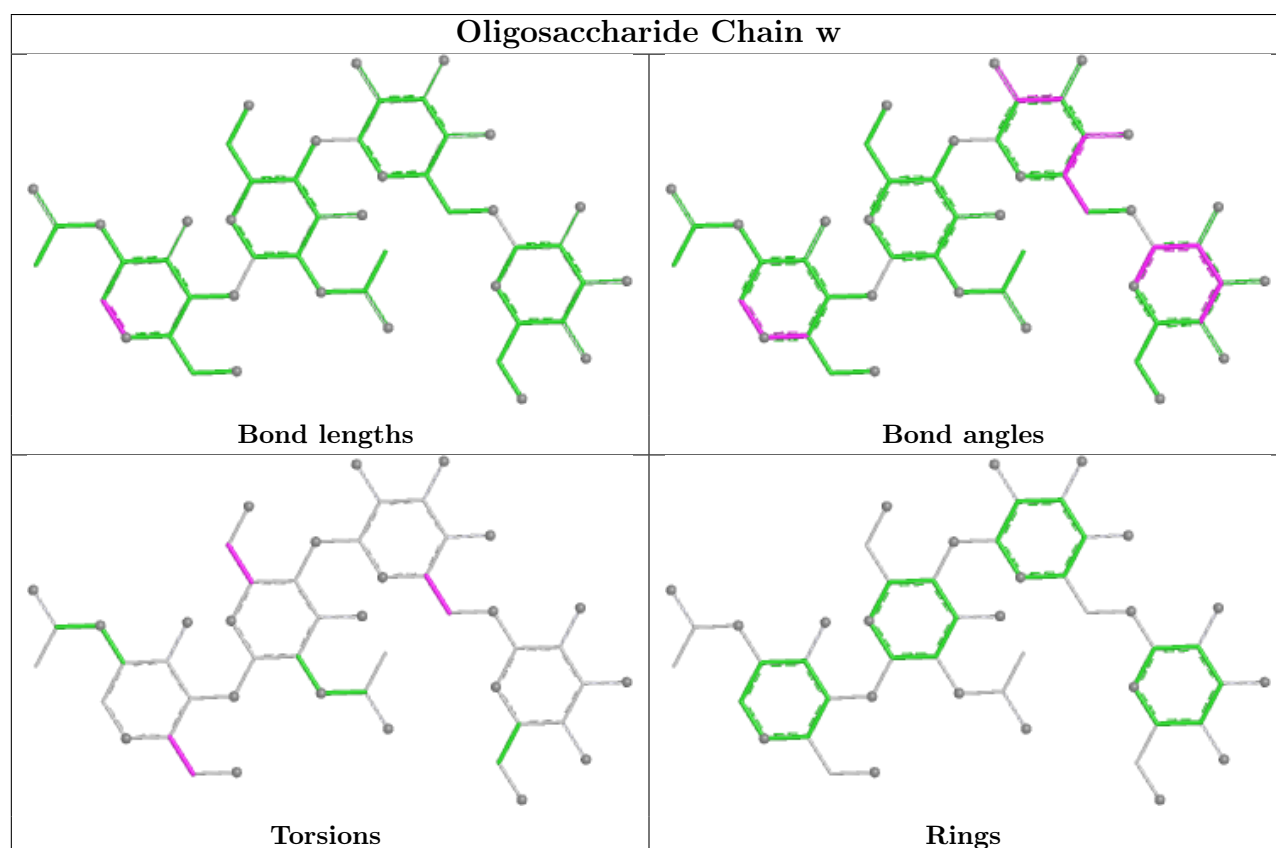
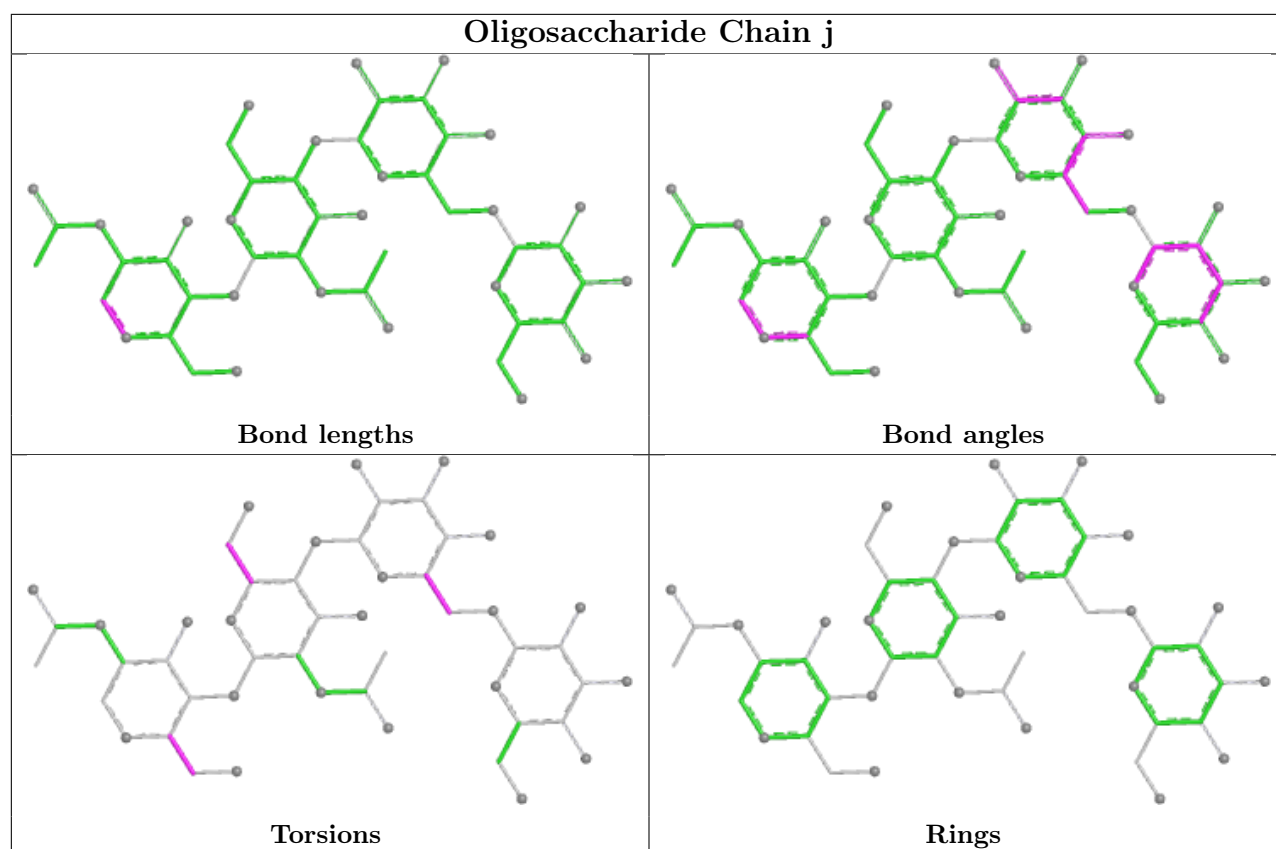












## 5.6 Ligand geometry

21 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  | F     | 611 | 1    | 14,14,15     | 0.52 | 0           | 17,19,21    | 0.51 | 0           |
| 11  | NAG  | F     | 645 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.56 | 0           |
| 11  | NAG  | I     | 701 | 2    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.61 | 0           |
| 11  | NAG  | G     | 611 | 1    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.51 | 0           |
| 11  | NAG  | I     | 702 | 2    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.54 | 0           |
| 11  | NAG  | A     | 645 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.56 | 0           |
| 11  | NAG  | A     | 633 | 1    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.40 | 0           |
| 11  | NAG  | B     | 701 | 2    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.62 | 0           |
| 11  | NAG  | G     | 633 | 1    | 14,14,15     | 0.33 | 0           | 17,19,21    | 0.41 | 0           |
| 11  | NAG  | G     | 634 | 1    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.42 | 0           |
| 11  | NAG  | A     | 634 | 1    | 14,14,15     | 0.50 | 0           | 17,19,21    | 0.42 | 0           |
| 11  | NAG  | A     | 604 | 1    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.65 | 1 (5%)      |
| 11  | NAG  | J     | 701 | 2    | 14,14,15     | 0.35 | 0           | 17,19,21    | 0.61 | 0           |
| 11  | NAG  | G     | 645 | 1    | 14,14,15     | 0.47 | 0           | 17,19,21    | 0.56 | 0           |
| 11  | NAG  | J     | 702 | 2    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.53 | 0           |
| 11  | NAG  | A     | 611 | 1    | 14,14,15     | 0.52 | 0           | 17,19,21    | 0.51 | 0           |
| 11  | NAG  | G     | 604 | 1    | 14,14,15     | 0.42 | 0           | 17,19,21    | 0.65 | 1 (5%)      |
| 11  | NAG  | B     | 702 | 2    | 14,14,15     | 0.53 | 0           | 17,19,21    | 0.54 | 0           |
| 11  | NAG  | F     | 604 | 1    | 14,14,15     | 0.41 | 0           | 17,19,21    | 0.65 | 1 (5%)      |
| 11  | NAG  | F     | 634 | 1    | 14,14,15     | 0.32 | 0           | 17,19,21    | 0.40 | 0           |
| 11  | NAG  | F     | 631 | 1    | 14,14,15     | 0.51 | 0           | 17,19,21    | 0.41 | 0           |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | NAG  | F     | 611 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | F     | 645 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | NAG  | I     | 701 | 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 611 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | I     | 702 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 645 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 633 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | B     | 701 | 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 633 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 634 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 634 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 604 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | J     | 701 | 2    | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 645 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | NAG  | J     | 702 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | A     | 611 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | G     | 604 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | B     | 702 | 2    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | F     | 604 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | F     | 634 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | F     | 631 | 1    | -       | 2/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 11  | A     | 604 | NAG  | C1-O5-C5 | 2.07 | 114.97      | 112.19   |
| 11  | F     | 604 | NAG  | C1-O5-C5 | 2.07 | 114.96      | 112.19   |
| 11  | G     | 604 | NAG  | C1-O5-C5 | 2.07 | 114.96      | 112.19   |

There are no chirality outliers.

All (39) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | A     | 633 | NAG  | O5-C5-C6-O6 |
| 11  | A     | 634 | NAG  | O5-C5-C6-O6 |
| 11  | F     | 631 | NAG  | O5-C5-C6-O6 |
| 11  | F     | 634 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 633 | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | G     | 634 | NAG  | O5-C5-C6-O6 |
| 11  | B     | 702 | NAG  | O5-C5-C6-O6 |
| 11  | I     | 702 | NAG  | O5-C5-C6-O6 |
| 11  | J     | 702 | NAG  | O5-C5-C6-O6 |
| 11  | B     | 701 | NAG  | O5-C5-C6-O6 |
| 11  | I     | 701 | NAG  | O5-C5-C6-O6 |
| 11  | J     | 701 | NAG  | O5-C5-C6-O6 |
| 11  | A     | 634 | NAG  | C4-C5-C6-O6 |
| 11  | F     | 631 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 634 | NAG  | C4-C5-C6-O6 |
| 11  | B     | 701 | NAG  | C4-C5-C6-O6 |
| 11  | I     | 701 | NAG  | C4-C5-C6-O6 |
| 11  | J     | 701 | NAG  | C4-C5-C6-O6 |
| 11  | A     | 604 | NAG  | O5-C5-C6-O6 |
| 11  | F     | 604 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 604 | NAG  | O5-C5-C6-O6 |
| 11  | A     | 611 | NAG  | O5-C5-C6-O6 |
| 11  | F     | 611 | NAG  | O5-C5-C6-O6 |
| 11  | G     | 611 | NAG  | O5-C5-C6-O6 |
| 11  | A     | 633 | NAG  | C4-C5-C6-O6 |
| 11  | F     | 634 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 633 | NAG  | C4-C5-C6-O6 |
| 11  | B     | 702 | NAG  | C4-C5-C6-O6 |
| 11  | I     | 702 | NAG  | C4-C5-C6-O6 |
| 11  | J     | 702 | NAG  | C4-C5-C6-O6 |
| 11  | A     | 611 | NAG  | C4-C5-C6-O6 |
| 11  | F     | 611 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 611 | NAG  | C4-C5-C6-O6 |
| 11  | A     | 604 | NAG  | C4-C5-C6-O6 |
| 11  | F     | 604 | NAG  | C4-C5-C6-O6 |
| 11  | G     | 604 | NAG  | C4-C5-C6-O6 |
| 11  | B     | 701 | NAG  | C1-C2-N2-C7 |
| 11  | I     | 701 | NAG  | C1-C2-N2-C7 |
| 11  | J     | 701 | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

6 monomers are involved in 18 short contacts:

| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | I     | 701 | NAG  | 1       | 0            |
| 11  | I     | 702 | NAG  | 5       | 0            |
| 11  | B     | 701 | NAG  | 1       | 0            |

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| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 11  | J     | 701 | NAG  | 1       | 0            |
| 11  | J     | 702 | NAG  | 5       | 0            |
| 11  | B     | 702 | NAG  | 5       | 0            |

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

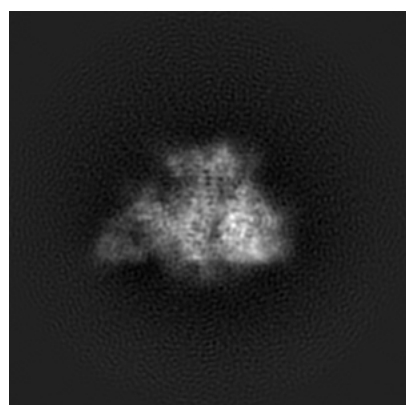
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8644. These allow visual inspection of the internal detail of the map and identification of artifacts.

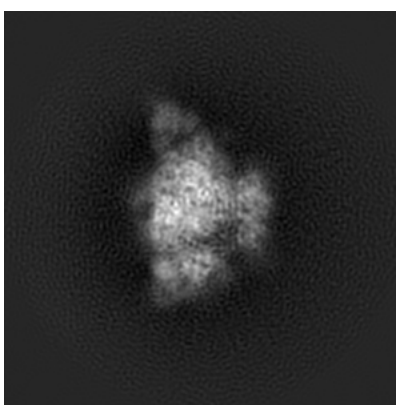
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

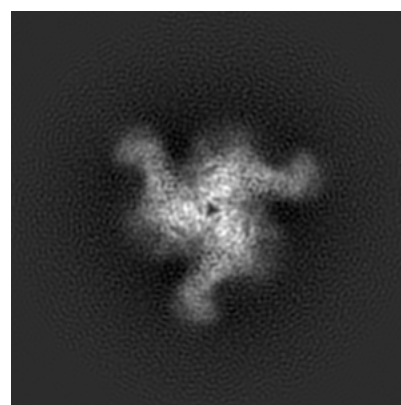
#### 6.1.1 Primary map



X



Y

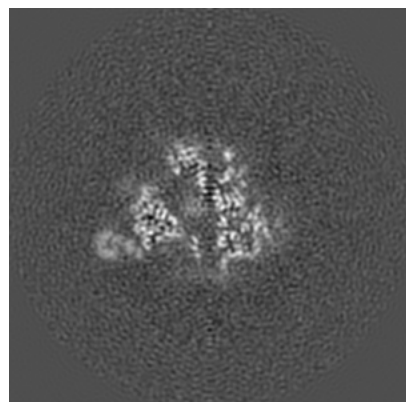


Z

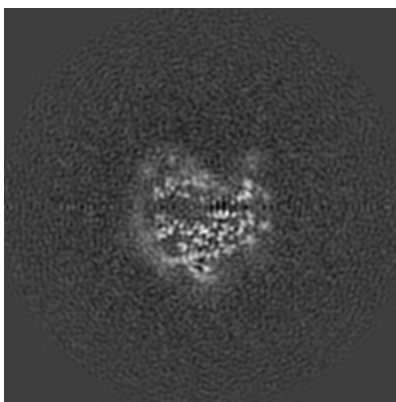
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

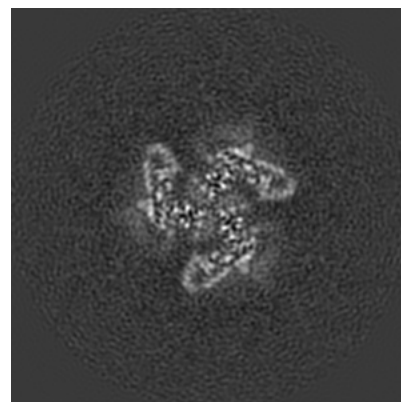
#### 6.2.1 Primary map



X Index: 128



Y Index: 128

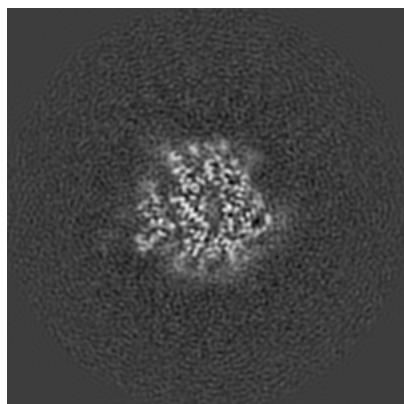


Z Index: 128

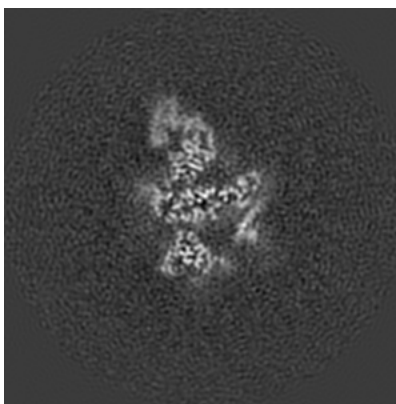
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

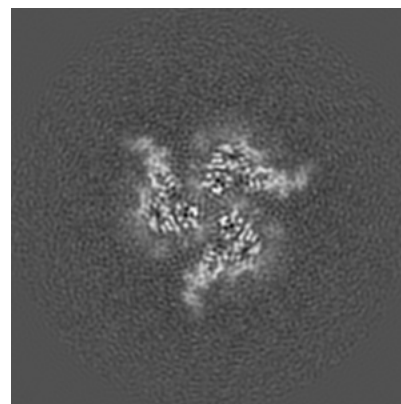
### 6.3.1 Primary map



X Index: 135



Y Index: 142

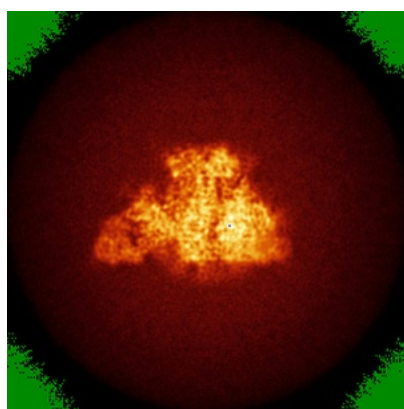


Z Index: 123

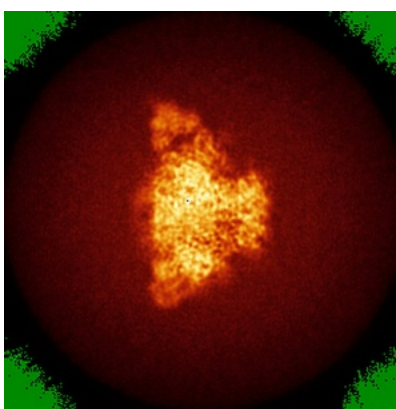
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

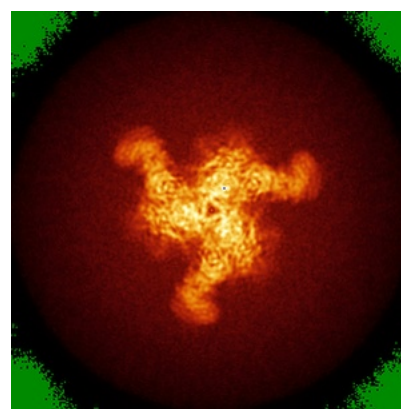
### 6.4.1 Primary map



X



Y

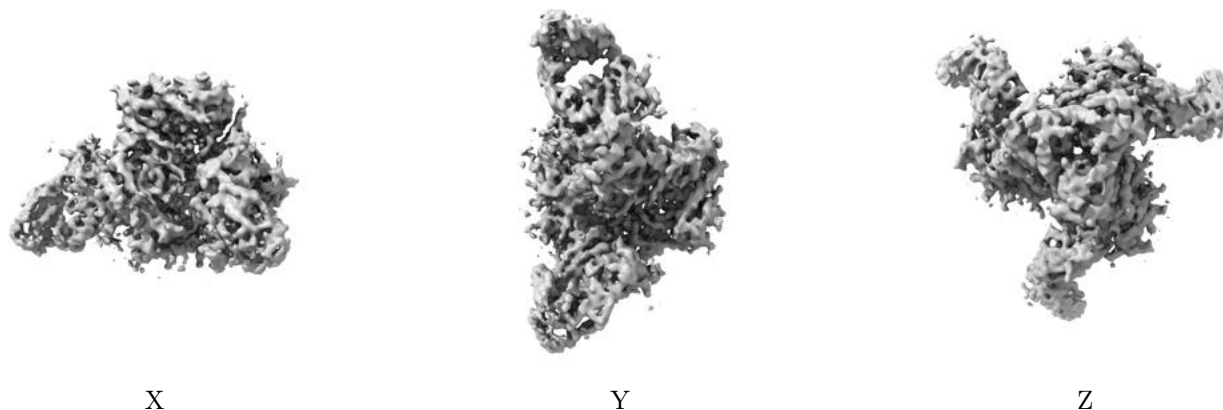


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.035. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

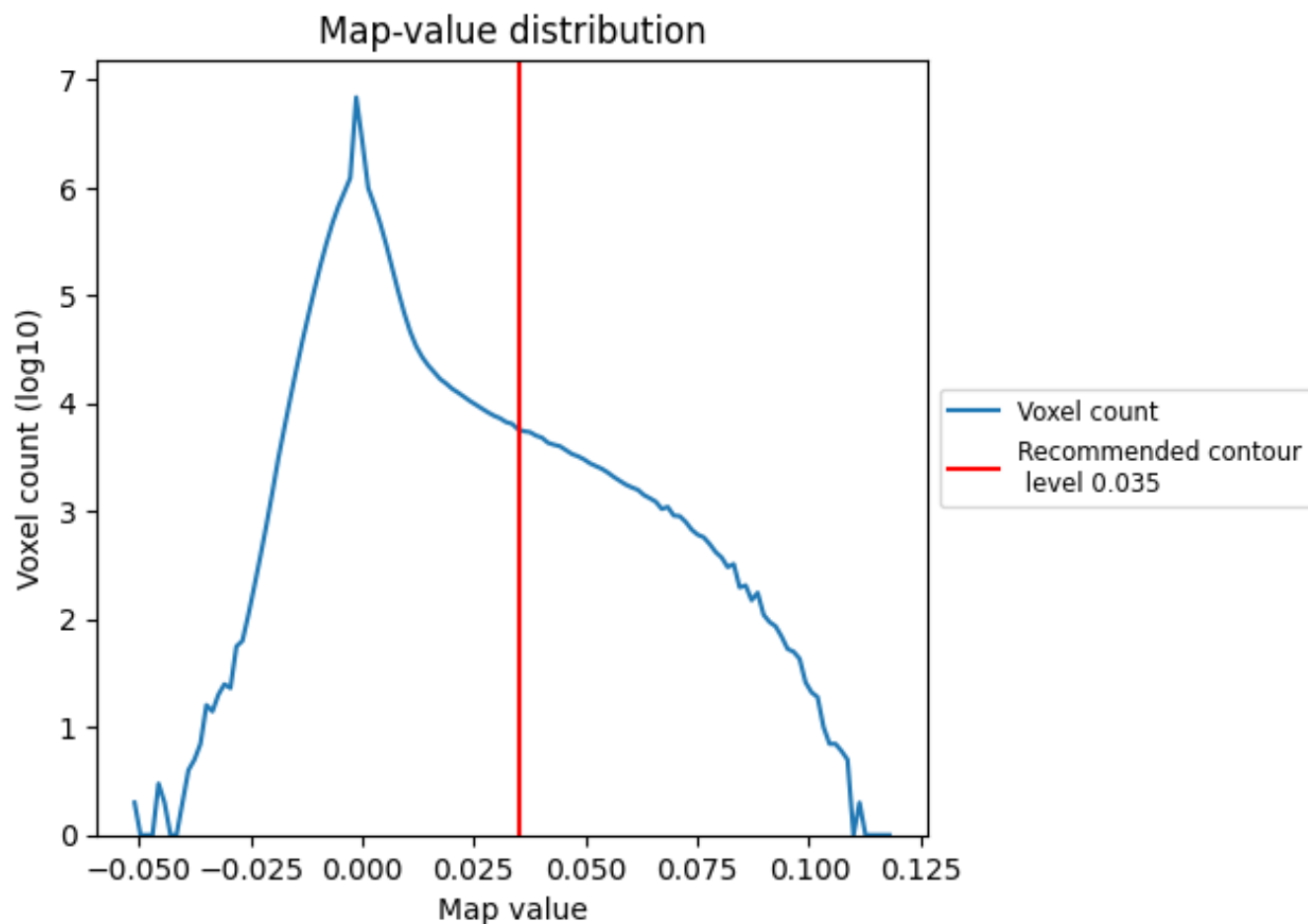
## 6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Map analysis [i](#)

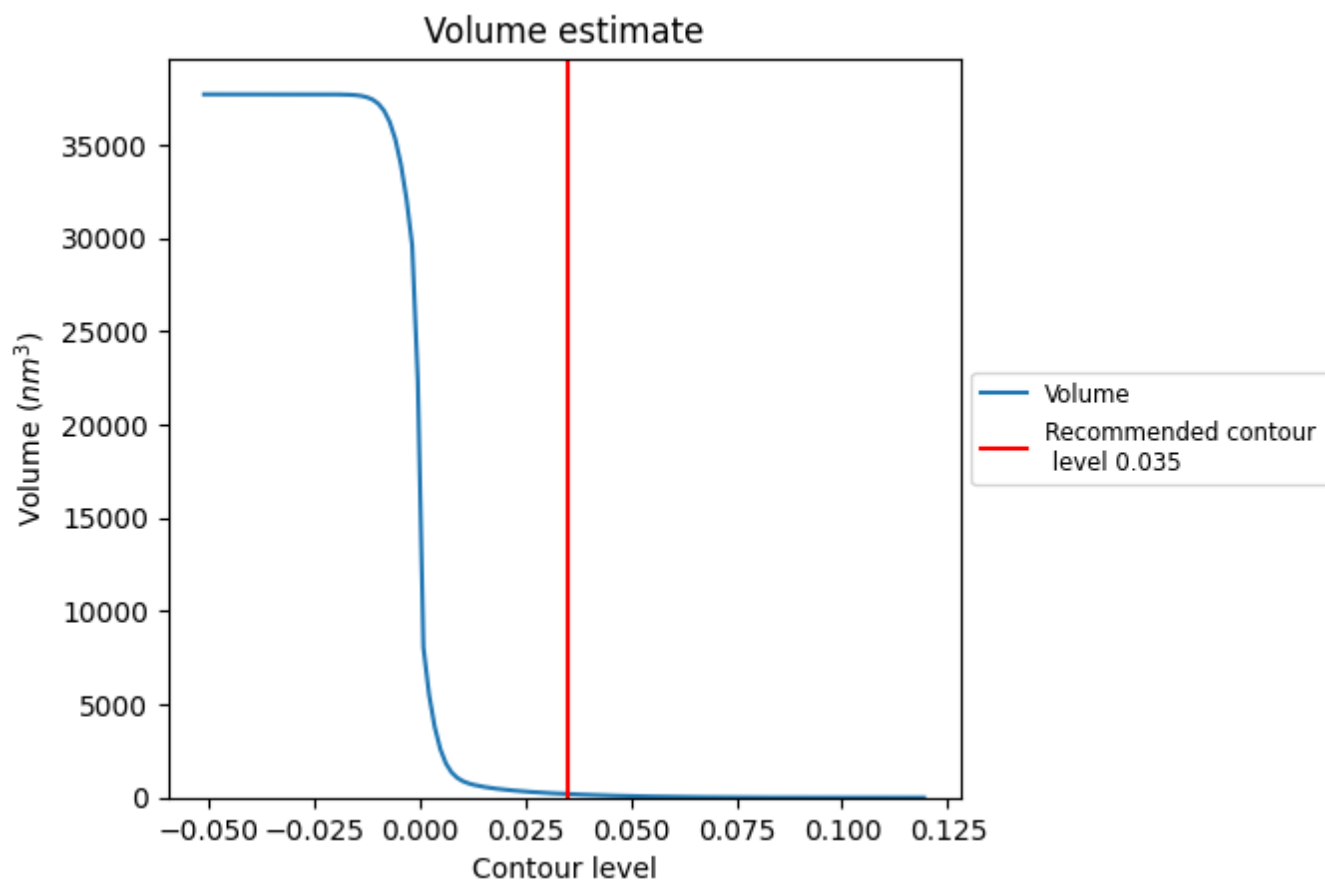
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

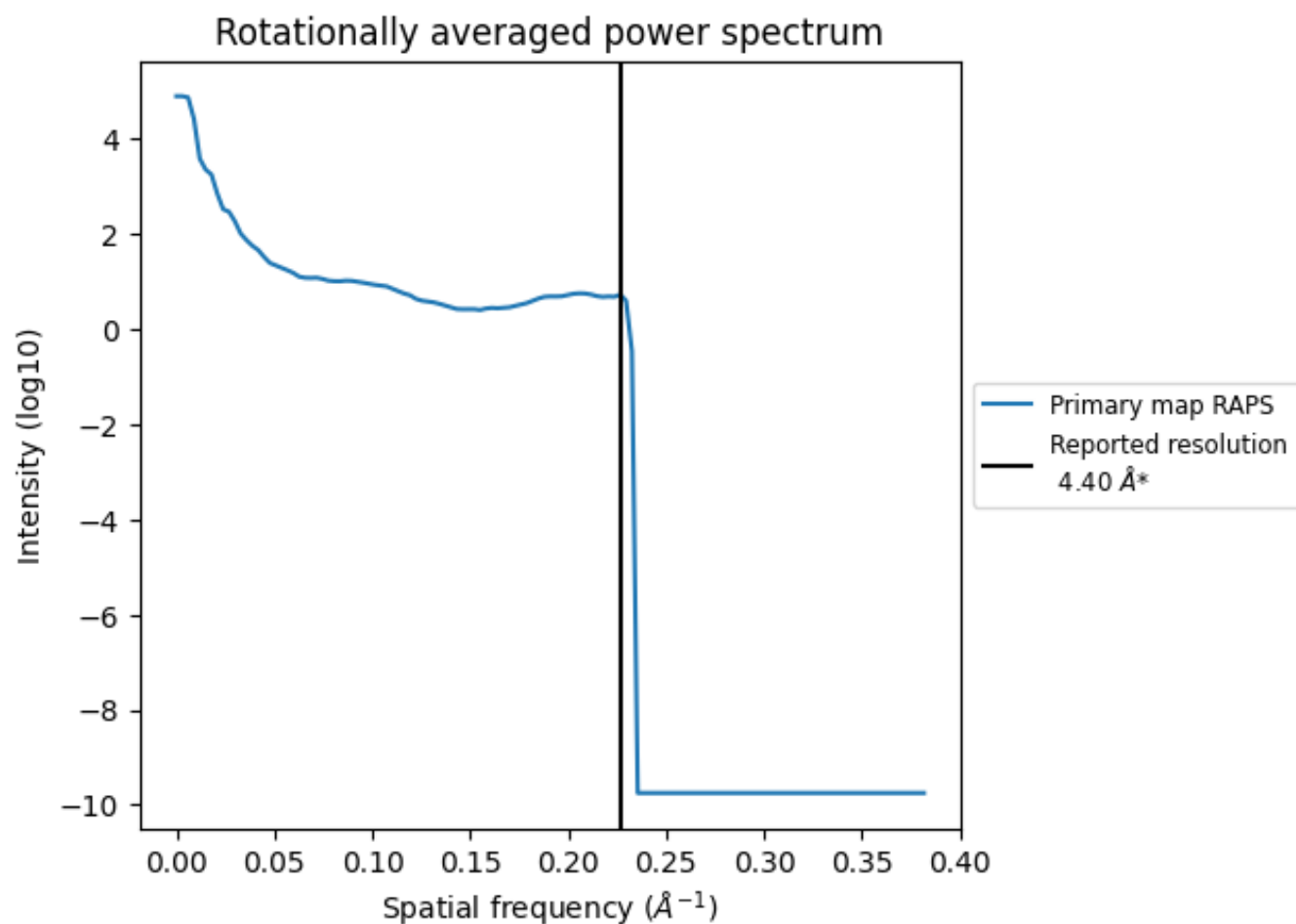
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 191 nm<sup>3</sup>; this corresponds to an approximate mass of 173 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

### 7.3 Rotationally averaged power spectrum ⓘ



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

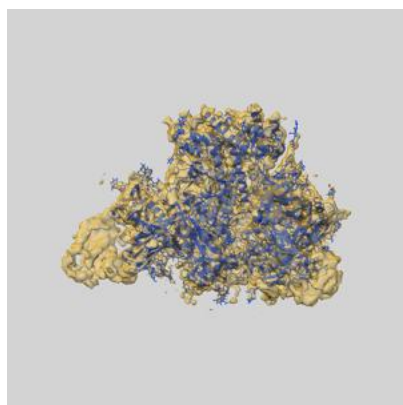
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

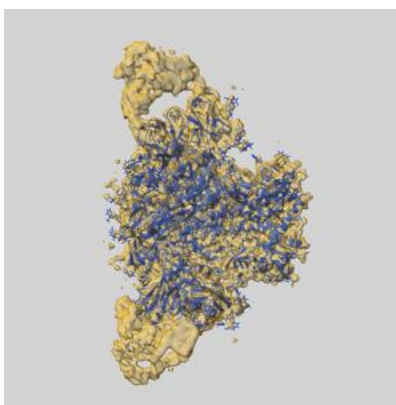
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-8644 and PDB model 5V8M. Per-residue inclusion information can be found in section 3 on page 13.

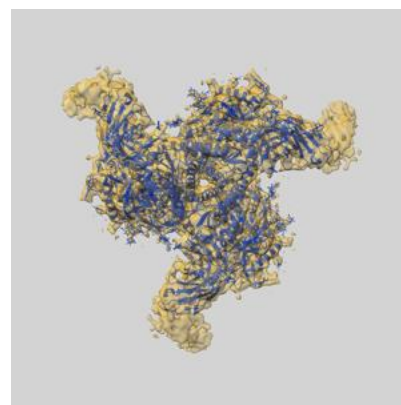
### 9.1 Map-model overlay [i](#)



X



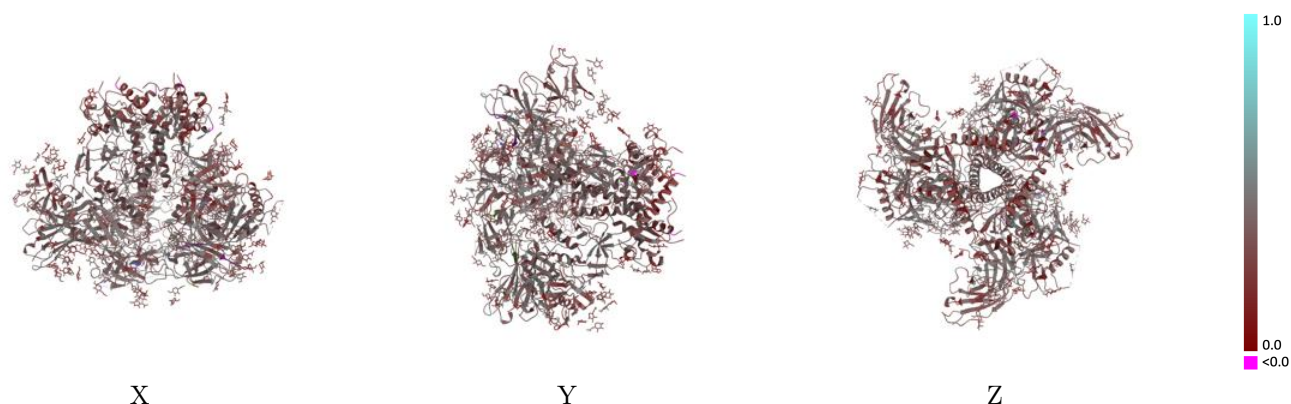
Y



Z

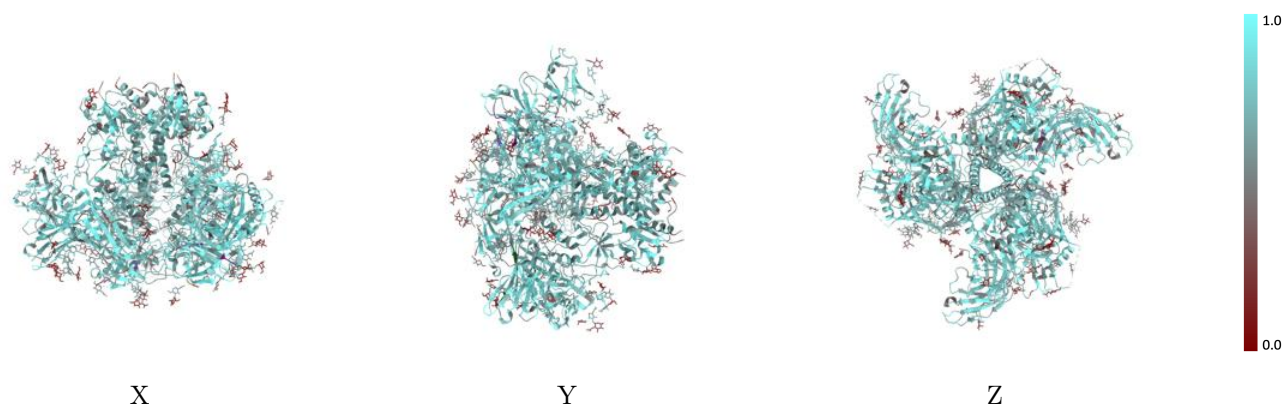
The images above show the 3D surface view of the map at the recommended contour level 0.035 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



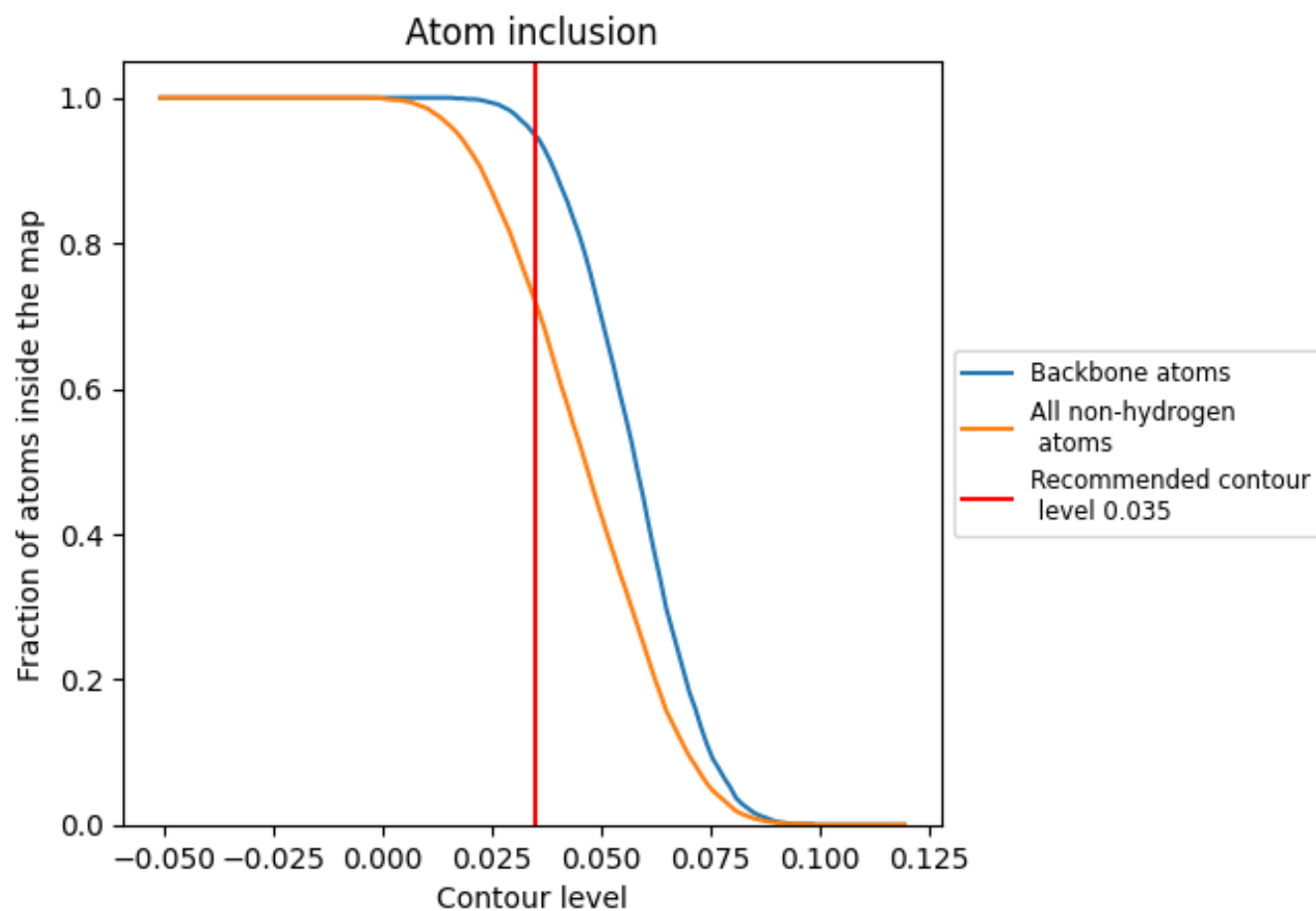
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

## 9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.035).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

## 9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.035) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.7170   |  0.3470   |
| A     |  0.7440   |  0.3680   |
| B     |  0.6890   |  0.2910   |
| C     |  0.2050   |  0.2380   |
| D     |  0.4640   |  0.2370   |
| E     |  0.3570   |  0.3160   |
| F     |  0.7450   |  0.3680   |
| G     |  0.7460   |  0.3690   |
| H     |  0.8070   |  0.3810   |
| I     |  0.6870   |  0.2970   |
| J     |  0.6900   |  0.2930   |
| K     |  0.6790   |  0.3890   |
| L     |  0.7200   |  0.3270   |
| M     |  0.3860   |  0.3000   |
| N     |  0.5530  |  0.3110  |
| O     |  0.3930 |  0.2740 |
| P     |  0.4290 |  0.2910 |
| Q     |  0.4640 |  0.2180 |
| R     |  0.7990 |  0.3780 |
| S     |  0.8030 |  0.3790 |
| T     |  0.7180 |  0.3230 |
| U     |  0.7200 |  0.3230 |
| V     |  0.3890 |  0.2840 |
| W     |  0.5000 |  0.2210 |
| X     |  0.5000 |  0.3160 |
| Y     |  0.4640 |  0.2950 |
| Z     |  0.2310 |  0.2520 |
| a     |  0.5000 |  0.2450 |
| b     |  0.3570 |  0.3210 |
| c     |  0.6430 |  0.4100 |
| d     |  0.3860 |  0.3040 |
| e     |  0.5430 |  0.3190 |
| f     |  0.3930 |  0.2740 |
| g     |  0.4640 |  0.2870 |
| h     |  0.4640 |  0.2360 |



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| Chain | Atom inclusion                                                                           | Q-score                                                                                  |
|-------|------------------------------------------------------------------------------------------|------------------------------------------------------------------------------------------|
| i     |  0.3750 |  0.2850 |
| j     |  0.5000 |  0.2280 |
| k     |  0.5000 |  0.3170 |
| l     |  0.4640 |  0.3340 |
| m     |  0.2310 |  0.2500 |
| n     |  0.4640 |  0.2390 |
| o     |  0.3570 |  0.3280 |
| p     |  0.6430 |  0.3850 |
| q     |  0.3860 |  0.2910 |
| r     |  0.5530 |  0.3240 |
| s     |  0.3570 |  0.2740 |
| t     |  0.4640 |  0.2930 |
| u     |  0.4640 |  0.2080 |
| v     |  0.3750 |  0.2850 |
| w     |  0.5000 |  0.2290 |
| x     |  0.5000 |  0.3130 |
| y     |  0.4640 |  0.3070 |