



## Full wwPDB EM Validation Report ⓘ

Nov 9, 2024 – 11:30 AM EST

PDB ID : 5SZS  
EMDB ID : EMD-8331  
Title : Glycan shield and epitope masking of a coronavirus spike protein observed by cryo-electron microscopy  
Authors : Walls, A.C.; Tortorici, M.A.; Frenz, B.; Snijder, J.; Li, W.; Rey, F.A.; DiMaio, F.; Bosch, B.J.; Veisler, D.  
Deposited on : 2016-08-15  
Resolution : 3.40 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:

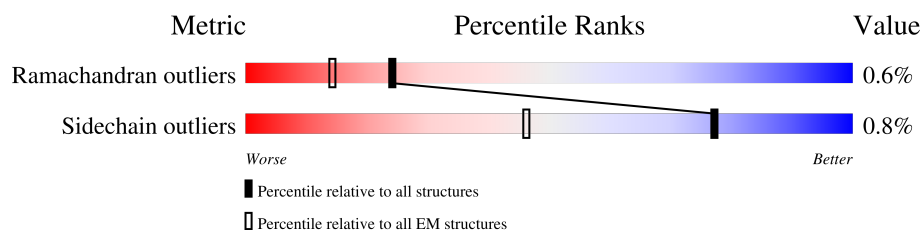
EMDB validation analysis : 0.0.1.dev113  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:  
*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 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.



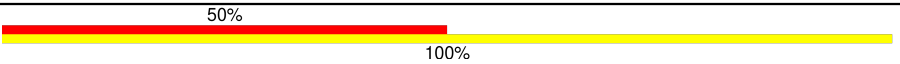
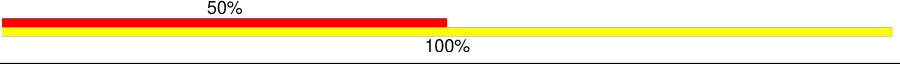
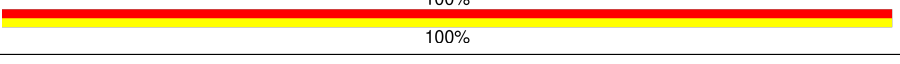
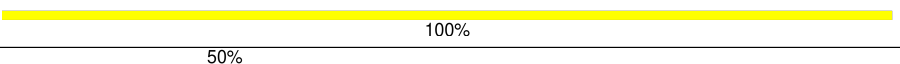
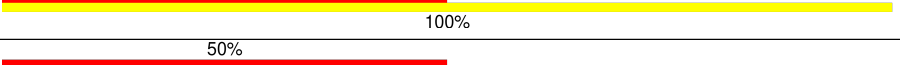
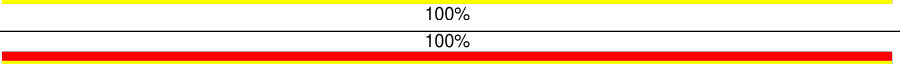
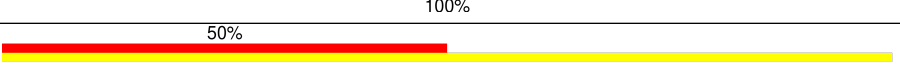
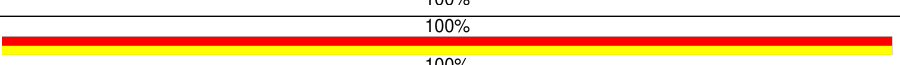
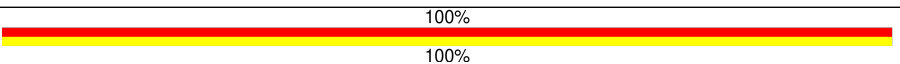

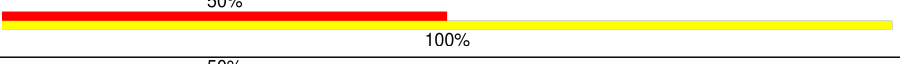
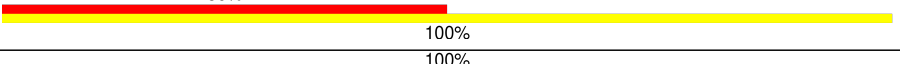
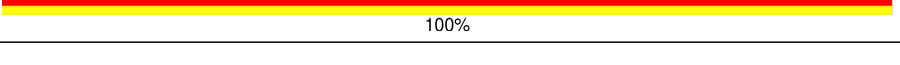
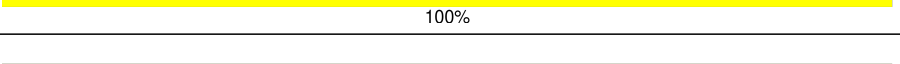
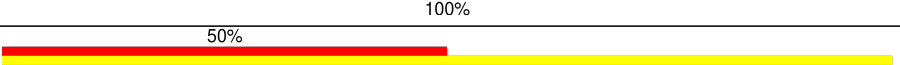
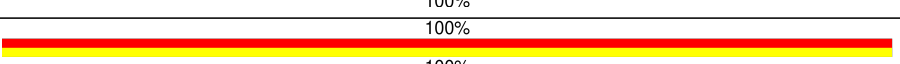
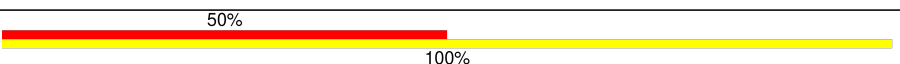
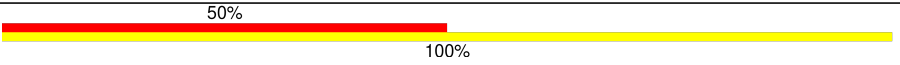
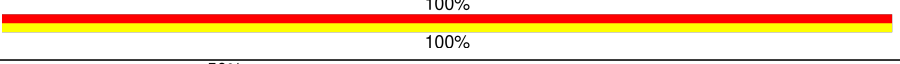
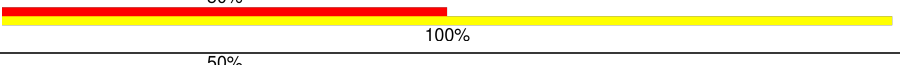
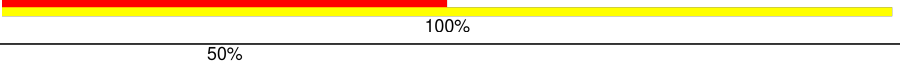

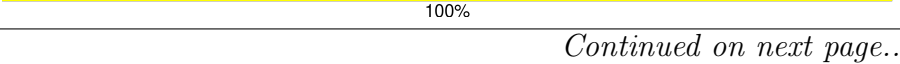


| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) |
|-----------------------|-----------------------------|-----------------------------|
| Ramachandran outliers | 207382                      | 16835                       |
| Sidechain outliers    | 206894                      | 16415                       |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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     | 1325   | <br>5% 86% 11%   |
| 1   | B     | 1325   | <br>5% 86% 11%   |
| 1   | C     | 1325   | <br>5% 86% 11%   |
| 2   | D     | 6      | <br>17% 100%     |
| 2   | Y     | 6      | <br>17% 100%     |
| 2   | t     | 6      | <br>17% 100%     |
| 3   | 2     | 2      | <br>50% 100%     |
| 3   | 5     | 2      | <br>100% 100%    |
| 3   | 6     | 2      | <br>50% 100%     |

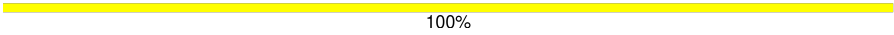


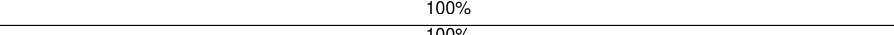
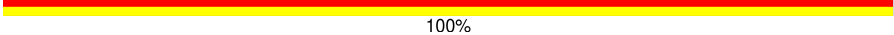

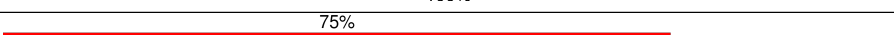
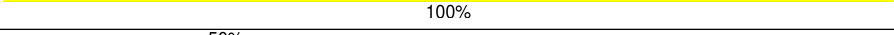


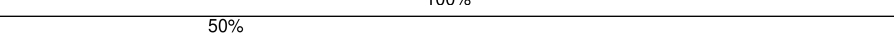
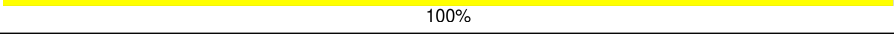


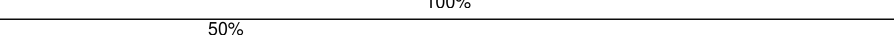
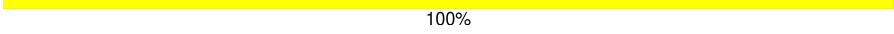


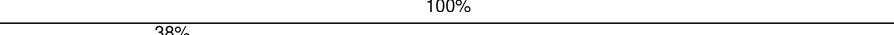
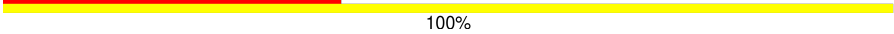

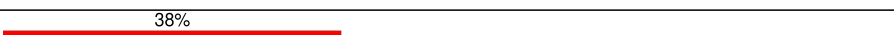
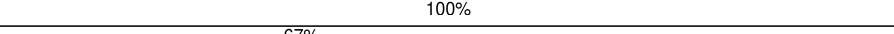


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| Mol | Chain | Length | Quality of chain   |  |
|-----|-------|--------|--|--|
| 3   | 7     | 2      |    |  |
| 3   | 8     | 2      |    |  |
| 3   | 9     | 2      |    |  |
| 3   | CA    | 2      |    |  |
| 3   | E     | 2      |    |  |
| 3   | G     | 2      |    |  |
| 3   | I     | 2      |    |  |
| 3   | J     | 2      |    |  |
| 3   | M     | 2      |    |  |
| 3   | P     | 2      |    |  |
| 3   | Q     | 2      |   |  |
| 3   | R     | 2      |  |  |
| 3   | S     | 2      |  |  |
| 3   | T     | 2      |  |  |
| 3   | W     | 2      |  |  |
| 3   | Z     | 2      |  |  |
| 3   | b     | 2      |  |  |
| 3   | d     | 2      |  |  |
| 3   | e     | 2      |  |  |
| 3   | h     | 2      |  |  |
| 3   | k     | 2      |  |  |
| 3   | l     | 2      |  |  |
| 3   | m     | 2      |  |  |
| 3   | n     | 2      |  |  |
| 3   | o     | 2      |  |  |

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| Mol | Chain | Length | Quality of chain   |
|-----|-------|--------|--|
| 3   | r     | 2      |  100%      |
| 3   | u     | 2      |  50%100%   |
| 3   | w     | 2      |  50%100%   |
| 3   | y     | 2      |  100%100%  |
| 3   | z     | 2      |  50%100%   |
| 4   | AA    | 4      |  75%100%   |
| 4   | F     | 4      |  50%100%   |
| 4   | U     | 4      |  75%100%   |
| 4   | a     | 4      |  50%100%   |
| 4   | p     | 4      |  75%100%   |
| 4   | v     | 4      |  50%100%   |
| 5   | H     | 4      |  50%100%   |
| 5   | c     | 4      |  50%100%   |
| 5   | x     | 4      |  50%100%   |
| 6   | 0     | 8      |  38%100%   |
| 6   | K     | 8      |  38%100%  |
| 6   | f     | 8      |  38%100% |
| 7   | 1     | 3      |  67%100% |
| 7   | 4     | 3      |  67%100% |
| 7   | DA    | 3      |  67%100% |
| 7   | L     | 3      |  67%100% |
| 7   | O     | 3      |  67%100% |
| 7   | X     | 3      |  67%100% |
| 7   | g     | 3      |  67%100% |
| 7   | j     | 3      |  67%100% |

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| Mol | Chain | Length | Quality of chain                         |
|-----|-------|--------|--|
| 7   | s     | 3      | <div><div>67%</div><div>100%</div></div> |
| 8   | 3     | 5      | <div><div>80%</div><div>100%</div></div> |
| 8   | BA    | 5      | <div><div>80%</div><div>100%</div></div> |
| 8   | N     | 5      | <div><div>80%</div><div>100%</div></div> |
| 8   | V     | 5      | <div><div>80%</div><div>100%</div></div> |
| 8   | i     | 5      | <div><div>80%</div><div>100%</div></div> |
| 8   | q     | 5      | <div><div>80%</div><div>100%</div></div> |

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 30306 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 Spike glycoprotein.

| Mol | Chain | Residues | Atoms |      |      |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|------|------|----|---------|-------|
| 1   | A     | 1177     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9141  | 5821 | 1532 | 1745 | 43 |         |       |
| 1   | B     | 1177     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9141  | 5821 | 1532 | 1745 | 43 |         |       |
| 1   | C     | 1177     | Total | C    | N    | O    | S  | 0       | 0     |
|     |       |          | 9141  | 5821 | 1532 | 1745 | 43 |         |       |

There are 147 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1292    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1293    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1294    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1295    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1296    | MET      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1297    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1298    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1299    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1300    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1301    | ASP      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1302    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1303    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1304    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1305    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1306    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1307    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1308    | SER      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1309    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1310    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1311    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1312    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1313    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1314    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1315    | ASN      | -      | expression tag | UNP Q6Q1S2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| A     | 1316    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1317    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1318    | ALA      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1319    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1320    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1321    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1322    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1323    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1324    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1325    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1326    | VAL      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1327    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1328    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1329    | GLY      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1330    | SER      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1331    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1332    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1333    | TRP      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1334    | SER      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1335    | HIS      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1336    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1337    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1338    | PHE      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1339    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| A     | 1340    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1292    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1293    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1294    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1295    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1296    | MET      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1297    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1298    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1299    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1300    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1301    | ASP      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1302    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1303    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1304    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1305    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1306    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1307    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1308    | SER      | -      | expression tag | UNP Q6Q1S2 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| B     | 1309    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1310    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1311    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1312    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1313    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1314    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1315    | ASN      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1316    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1317    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1318    | ALA      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1319    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1320    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1321    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1322    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1323    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1324    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1325    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1326    | VAL      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1327    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1328    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1329    | GLY      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1330    | SER      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1331    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1332    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1333    | TRP      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1334    | SER      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1335    | HIS      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1336    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1337    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1338    | PHE      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1339    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| B     | 1340    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1292    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1293    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1294    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1295    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1296    | MET      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1297    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1298    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1299    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1300    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1301    | ASP      | -      | expression tag | UNP Q6Q1S2 |

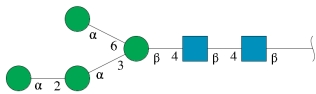
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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| C     | 1302    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1303    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1304    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1305    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1306    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1307    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1308    | SER      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1309    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1310    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1311    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1312    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1313    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1314    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1315    | ASN      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1316    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1317    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1318    | ALA      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1319    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1320    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1321    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1322    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1323    | ILE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1324    | LYS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1325    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1326    | VAL      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1327    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1328    | ARG      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1329    | GLY      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1330    | SER      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1331    | LEU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1332    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1333    | TRP      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1334    | SER      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1335    | HIS      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1336    | PRO      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1337    | GLN      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1338    | PHE      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1339    | GLU      | -      | expression tag | UNP Q6Q1S2 |
| C     | 1340    | LYS      | -      | expression tag | UNP Q6Q1S2 |

- Molecule 2 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 2   | D     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 2   | Y     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 2   | t     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |

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



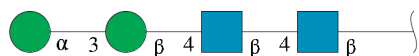
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 3   | E     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | G     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | I     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | J     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | M     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | P     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | Q     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | R     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | S     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | T     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | W     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | Z     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

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| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 3   | b     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | d     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | e     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | h     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | k     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | l     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | m     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | n     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | o     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | r     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | u     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | w     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | y     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | z     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 2     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 5     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 6     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 7     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 8     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | 9     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 3   | CA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

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



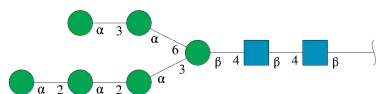
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 4   | F     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 4   | U     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 4   | a     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 4   | p     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 4   | v     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 4   | AA    | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |

- Molecule 5 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.



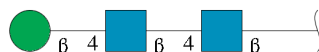
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 5   | H     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 5   | c     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 5   | x     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-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.



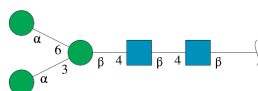
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 6   | K     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |
| 6   | f     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |
| 6   | 0     | 8        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 94    | 52 | 2 | 40 |         |       |

- Molecule 7 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.



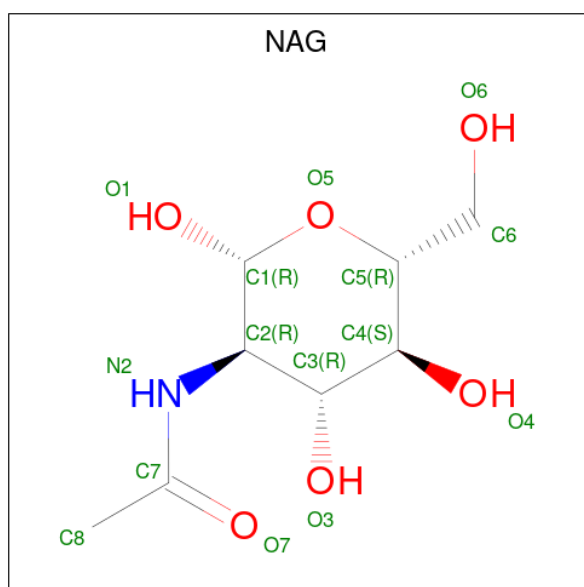
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 7   | L     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | O     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | X     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | g     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | j     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | s     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | 1     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | 4     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 7   | DA    | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

- Molecule 8 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 8   | N     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 8   | V     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 8   | i     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 8   | q     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 8   | 3     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 8   | BA    | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

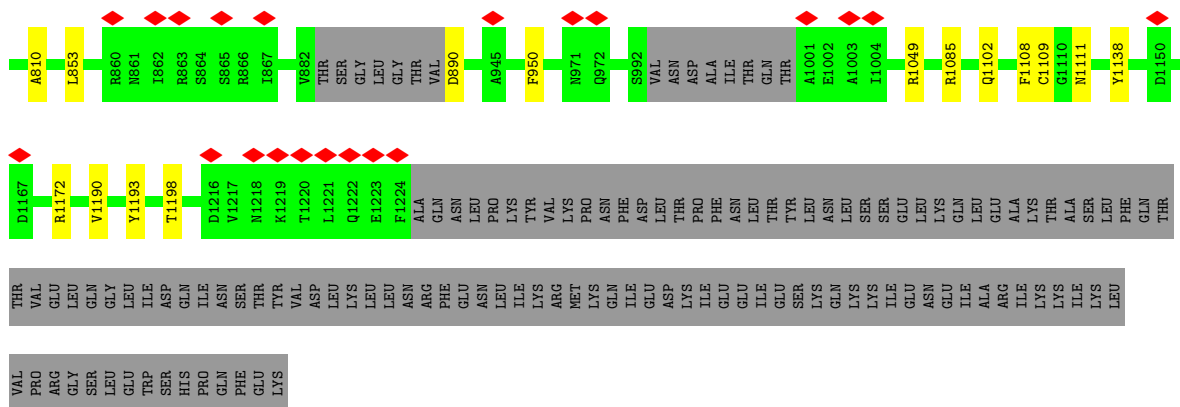
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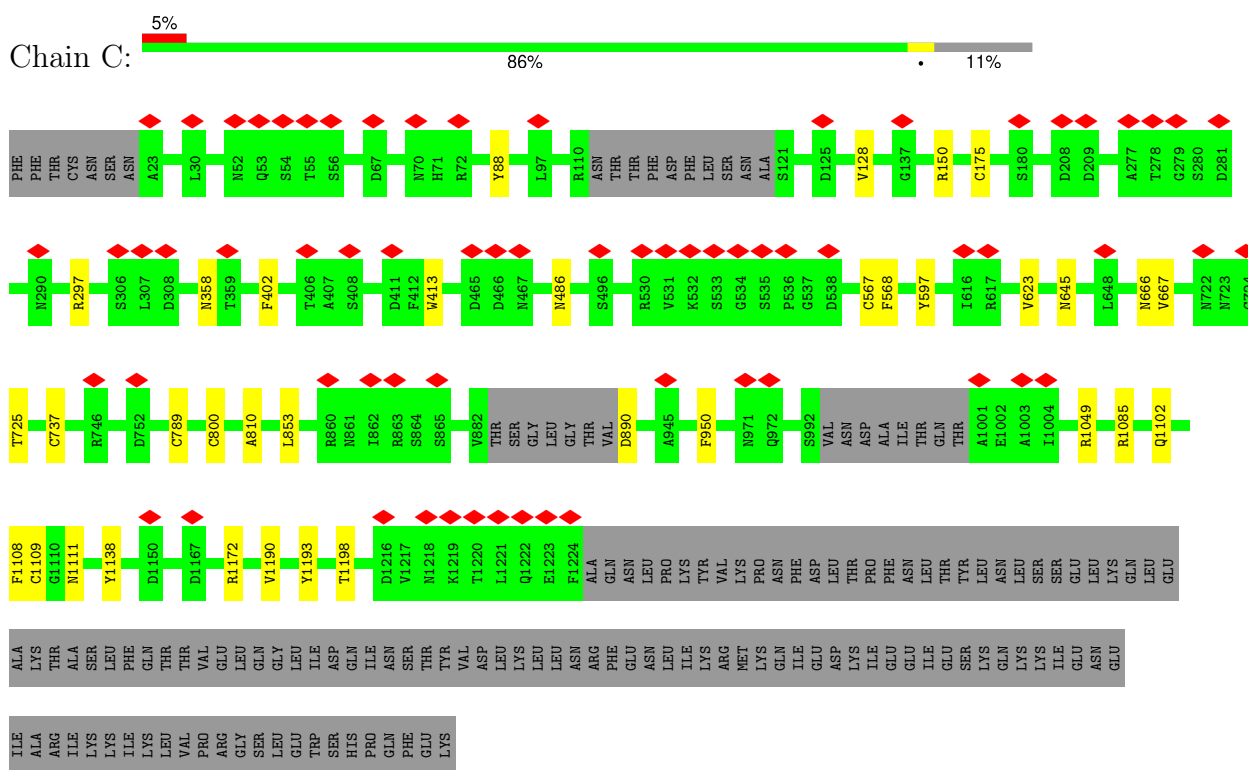
| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 9   | C     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |







- Molecule 1: Spike glycoprotein



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



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



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



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



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



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



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



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



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



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





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

Chain W:  100%



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

Chain Z:  100%



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

Chain b:  50%  
100%



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

Chain d:  100%  
100%



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

Chain e:  50%  
100%



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

Chain h:  50%  
100%



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



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



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



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



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



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

Chain r:  100%

MAG1  
MAG2

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

Chain u:  50%  
 100%

MAG1  
MAG2

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

Chain w:  50%  
 100%

MAG1  
MAG2

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

Chain y:  100%  
 100%

MAG1  
MAG2

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

Chain z:  50%  
 100%

MAG1  
MAG2

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

Chain 2:  50%  
 100%

MAG1  
MAG2

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



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



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



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



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



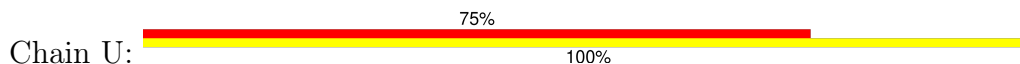
- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



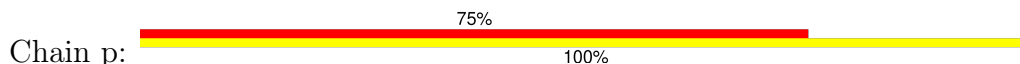
- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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



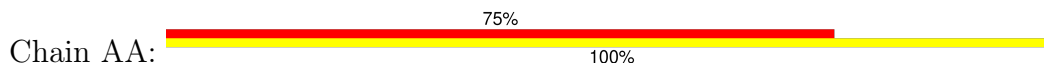
- Molecule 4: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 4: 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 4: 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 5: 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 5: 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 5: 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 6: alpha-D-mannopyranose-(1-2)-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 6: alpha-D-mannopyranose-(1-2)-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 6: alpha-D-mannopyranose-(1-2)-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

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



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



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



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



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



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





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



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



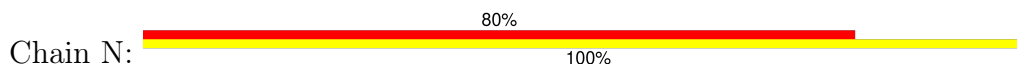
- Molecule 7: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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

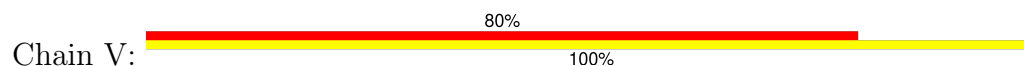


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

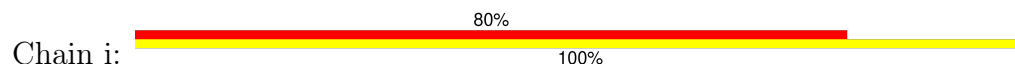


- Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

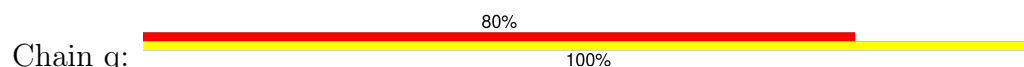
nose



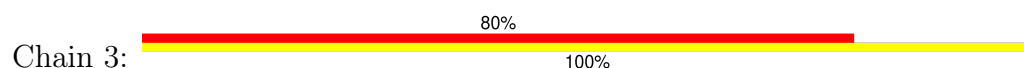
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



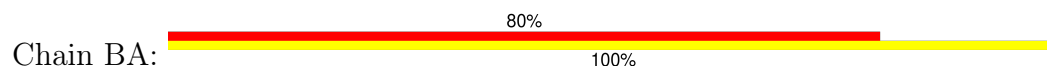
• Molecule 8: alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 8: alpha-D-mannopyranose-(1-3)-[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-(1-3)-[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



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|---|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 79667                                   | 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 ( $e^-/\text{\AA}^2$ ) | 48                                      | 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                    | 0.299                                   | Depositor |
| Minimum map value                    | -0.139                                  | Depositor |
| Average map value                    | 0.000                                   | Depositor |
| Map value standard deviation         | 0.006                                   | Depositor |
| Recommended contour level            | 0.055                                   | Depositor |
| Map size (Å)                         | 435.2, 435.2, 435.2                     | wwPDB     |
| Map dimensions                       | 320, 320, 320                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.36, 1.36, 1.36                        | Depositor |

## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, 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     | 0.95         | 10/9345 (0.1%)  | 0.82        | 12/12747 (0.1%) |
| 1   | B     | 0.95         | 10/9345 (0.1%)  | 0.82        | 12/12747 (0.1%) |
| 1   | C     | 0.95         | 10/9345 (0.1%)  | 0.82        | 12/12747 (0.1%) |
| All | All   | 0.95         | 30/28035 (0.1%) | 0.82        | 36/38241 (0.1%) |

All (30) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms  | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|--------|-------|-------------|----------|
| 1   | A     | 737  | CYS  | CB-SG  | -8.38 | 1.68        | 1.82     |
| 1   | C     | 737  | CYS  | CB-SG  | -8.37 | 1.68        | 1.82     |
| 1   | B     | 737  | CYS  | CB-SG  | -8.34 | 1.68        | 1.82     |
| 1   | C     | 800  | CYS  | CB-SG  | -7.71 | 1.69        | 1.82     |
| 1   | A     | 800  | CYS  | CB-SG  | -7.70 | 1.69        | 1.82     |
| 1   | B     | 800  | CYS  | CB-SG  | -7.69 | 1.69        | 1.82     |
| 1   | C     | 1193 | TYR  | CB-CG  | -6.75 | 1.41        | 1.51     |
| 1   | A     | 1193 | TYR  | CB-CG  | -6.69 | 1.41        | 1.51     |
| 1   | B     | 1193 | TYR  | CB-CG  | -6.65 | 1.41        | 1.51     |
| 1   | B     | 1190 | VAL  | C-N    | 5.62  | 1.47        | 1.34     |
| 1   | B     | 666  | ASN  | CB-CG  | 5.61  | 1.64        | 1.51     |
| 1   | C     | 666  | ASN  | CB-CG  | 5.61  | 1.64        | 1.51     |
| 1   | A     | 666  | ASN  | CB-CG  | 5.61  | 1.64        | 1.51     |
| 1   | A     | 1190 | VAL  | C-N    | 5.61  | 1.47        | 1.34     |
| 1   | C     | 1190 | VAL  | C-N    | 5.61  | 1.47        | 1.34     |
| 1   | C     | 128  | VAL  | CB-CG2 | -5.58 | 1.41        | 1.52     |
| 1   | A     | 128  | VAL  | CB-CG2 | -5.58 | 1.41        | 1.52     |
| 1   | B     | 128  | VAL  | CB-CG2 | -5.56 | 1.41        | 1.52     |
| 1   | A     | 950  | PHE  | CB-CG  | -5.39 | 1.42        | 1.51     |
| 1   | C     | 950  | PHE  | CB-CG  | -5.38 | 1.42        | 1.51     |
| 1   | B     | 950  | PHE  | CB-CG  | -5.37 | 1.42        | 1.51     |
| 1   | B     | 568  | PHE  | CB-CG  | -5.33 | 1.42        | 1.51     |
| 1   | C     | 568  | PHE  | CB-CG  | -5.31 | 1.42        | 1.51     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 1   | A     | 568 | PHE  | CB-CG | -5.31 | 1.42        | 1.51     |
| 1   | C     | 413 | TRP  | CB-CG | -5.22 | 1.40        | 1.50     |
| 1   | A     | 413 | TRP  | CB-CG | -5.21 | 1.40        | 1.50     |
| 1   | C     | 597 | TYR  | CB-CG | -5.19 | 1.43        | 1.51     |
| 1   | B     | 413 | TRP  | CB-CG | -5.18 | 1.41        | 1.50     |
| 1   | B     | 597 | TYR  | CB-CG | -5.17 | 1.43        | 1.51     |
| 1   | A     | 597 | TYR  | CB-CG | -5.16 | 1.44        | 1.51     |

All (36) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|-----------|-------|-------------|----------|
| 1   | A     | 297  | ARG  | NE-CZ-NH2 | -8.77 | 115.92      | 120.30   |
| 1   | C     | 297  | ARG  | NE-CZ-NH2 | -8.74 | 115.93      | 120.30   |
| 1   | B     | 297  | ARG  | NE-CZ-NH2 | -8.71 | 115.94      | 120.30   |
| 1   | C     | 1172 | ARG  | NE-CZ-NH2 | -8.55 | 116.02      | 120.30   |
| 1   | B     | 1172 | ARG  | NE-CZ-NH2 | -8.53 | 116.04      | 120.30   |
| 1   | B     | 810  | ALA  | CB-CA-C   | 8.49  | 122.84      | 110.10   |
| 1   | A     | 1172 | ARG  | NE-CZ-NH2 | -8.49 | 116.06      | 120.30   |
| 1   | C     | 810  | ALA  | CB-CA-C   | 8.48  | 122.83      | 110.10   |
| 1   | A     | 810  | ALA  | CB-CA-C   | 8.46  | 122.79      | 110.10   |
| 1   | A     | 1193 | TYR  | CB-CG-CD2 | -8.06 | 116.16      | 121.00   |
| 1   | B     | 1193 | TYR  | CB-CG-CD2 | -8.06 | 116.17      | 121.00   |
| 1   | C     | 1193 | TYR  | CB-CG-CD2 | -8.01 | 116.20      | 121.00   |
| 1   | B     | 1085 | ARG  | NE-CZ-NH2 | -7.52 | 116.54      | 120.30   |
| 1   | C     | 1085 | ARG  | NE-CZ-NH2 | -7.47 | 116.57      | 120.30   |
| 1   | A     | 1085 | ARG  | NE-CZ-NH2 | -7.43 | 116.59      | 120.30   |
| 1   | C     | 1198 | THR  | C-N-CA    | 7.10  | 139.45      | 121.70   |
| 1   | A     | 1198 | THR  | C-N-CA    | 7.09  | 139.42      | 121.70   |
| 1   | B     | 1198 | THR  | C-N-CA    | 7.08  | 139.40      | 121.70   |
| 1   | B     | 297  | ARG  | NE-CZ-NH1 | 6.24  | 123.42      | 120.30   |
| 1   | C     | 297  | ARG  | NE-CZ-NH1 | 6.24  | 123.42      | 120.30   |
| 1   | A     | 297  | ARG  | NE-CZ-NH1 | 6.21  | 123.40      | 120.30   |
| 1   | B     | 1049 | ARG  | NE-CZ-NH2 | -6.12 | 117.24      | 120.30   |
| 1   | A     | 1049 | ARG  | NE-CZ-NH2 | -6.11 | 117.25      | 120.30   |
| 1   | C     | 1049 | ARG  | NE-CZ-NH2 | -6.10 | 117.25      | 120.30   |
| 1   | C     | 88   | TYR  | CB-CG-CD2 | -6.01 | 117.39      | 121.00   |
| 1   | B     | 88   | TYR  | CB-CG-CD2 | -6.00 | 117.40      | 121.00   |
| 1   | A     | 88   | TYR  | CB-CG-CD2 | -5.99 | 117.41      | 121.00   |
| 1   | A     | 623  | VAL  | O-C-N     | 5.50  | 131.50      | 122.70   |
| 1   | C     | 623  | VAL  | O-C-N     | 5.50  | 131.51      | 122.70   |
| 1   | B     | 623  | VAL  | O-C-N     | 5.50  | 131.50      | 122.70   |
| 1   | B     | 150  | ARG  | NE-CZ-NH2 | -5.38 | 117.61      | 120.30   |

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| Mol | Chain | Res | Type | Atoms     | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-----------|-------|-------------|----------|
| 1   | A     | 150 | ARG  | NE-CZ-NH2 | -5.35 | 117.62      | 120.30   |
| 1   | C     | 150 | ARG  | NE-CZ-NH2 | -5.29 | 117.66      | 120.30   |
| 1   | B     | 890 | ASP  | CB-CG-OD2 | 5.23  | 123.01      | 118.30   |
| 1   | C     | 890 | ASP  | CB-CG-OD2 | 5.23  | 123.00      | 118.30   |
| 1   | A     | 890 | ASP  | CB-CG-OD2 | 5.22  | 123.00      | 118.30   |

There are no chirality outliers.

There are no planarity outliers.

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

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

## 5.3 Torsion angles [i](#)

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

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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     | 1169/1325 (88%) | 1095 (94%) | 67 (6%)  | 7 (1%)   | 22          | 50 |  |
| 1   | B     | 1169/1325 (88%) | 1096 (94%) | 66 (6%)  | 7 (1%)   | 22          | 50 |  |
| 1   | C     | 1169/1325 (88%) | 1095 (94%) | 67 (6%)  | 7 (1%)   | 22          | 50 |  |
| All | All   | 3507/3975 (88%) | 3286 (94%) | 200 (6%) | 21 (1%)  | 24          | 50 |  |

All (21) Ramachandran outliers are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 667 | VAL  |
| 1   | A     | 853 | LEU  |
| 1   | B     | 667 | VAL  |
| 1   | B     | 853 | LEU  |
| 1   | C     | 667 | VAL  |
| 1   | C     | 853 | LEU  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 567  | CYS  |
| 1   | A     | 725  | THR  |
| 1   | A     | 1102 | GLN  |
| 1   | B     | 567  | CYS  |
| 1   | B     | 725  | THR  |
| 1   | B     | 1102 | GLN  |
| 1   | C     | 567  | CYS  |
| 1   | C     | 725  | THR  |
| 1   | C     | 1102 | GLN  |
| 1   | A     | 1109 | CYS  |
| 1   | B     | 1109 | CYS  |
| 1   | C     | 1109 | CYS  |
| 1   | A     | 1108 | PHE  |
| 1   | B     | 1108 | PHE  |
| 1   | C     | 1108 | PHE  |

### 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     | 1031/1169 (88%) | 1023 (99%) | 8 (1%)   | 79          | 87 |
| 1   | B     | 1031/1169 (88%) | 1023 (99%) | 8 (1%)   | 79          | 87 |
| 1   | C     | 1031/1169 (88%) | 1023 (99%) | 8 (1%)   | 79          | 87 |
| All | All   | 3093/3507 (88%) | 3069 (99%) | 24 (1%)  | 77          | 87 |

All (24) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 175  | CYS  |
| 1   | A     | 358  | ASN  |
| 1   | A     | 402  | PHE  |
| 1   | A     | 486  | ASN  |
| 1   | A     | 645  | ASN  |
| 1   | A     | 789  | CYS  |
| 1   | A     | 1111 | ASN  |

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| Mol | Chain | Res  | Type |
|-----|-------|------|------|
| 1   | A     | 1138 | TYR  |
| 1   | B     | 175  | CYS  |
| 1   | B     | 358  | ASN  |
| 1   | B     | 402  | PHE  |
| 1   | B     | 486  | ASN  |
| 1   | B     | 645  | ASN  |
| 1   | B     | 789  | CYS  |
| 1   | B     | 1111 | ASN  |
| 1   | B     | 1138 | TYR  |
| 1   | C     | 175  | CYS  |
| 1   | C     | 358  | ASN  |
| 1   | C     | 402  | PHE  |
| 1   | C     | 486  | ASN  |
| 1   | C     | 645  | ASN  |
| 1   | C     | 789  | CYS  |
| 1   | C     | 1111 | ASN  |
| 1   | C     | 1138 | TYR  |

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

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | A     | 660 | ASN  |
| 1   | B     | 660 | ASN  |
| 1   | C     | 660 | ASN  |

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

201 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | NAG  | 0     | 1   | 1,6  | 14,14,15     | 2.69 | 3 (21%)  | 17,19,21    | 3.96 | 6 (35%)  |
| 6   | NAG  | 0     | 2   | 6    | 14,14,15     | 2.81 | 4 (28%)  | 17,19,21    | 3.54 | 5 (29%)  |
| 6   | BMA  | 0     | 3   | 6    | 11,11,12     | 1.84 | 2 (18%)  | 15,15,17    | 5.50 | 6 (40%)  |
| 6   | MAN  | 0     | 4   | 6    | 11,11,12     | 1.69 | 2 (18%)  | 15,15,17    | 8.19 | 6 (40%)  |
| 6   | MAN  | 0     | 5   | 6    | 11,11,12     | 1.69 | 3 (27%)  | 15,15,17    | 4.22 | 5 (33%)  |
| 6   | MAN  | 0     | 6   | 6    | 11,11,12     | 1.97 | 3 (27%)  | 15,15,17    | 2.47 | 1 (6%)   |
| 6   | MAN  | 0     | 7   | 6    | 11,11,12     | 1.93 | 4 (36%)  | 15,15,17    | 5.07 | 6 (40%)  |
| 6   | MAN  | 0     | 8   | 6    | 11,11,12     | 2.57 | 6 (54%)  | 15,15,17    | 3.75 | 6 (40%)  |
| 7   | NAG  | 1     | 1   | 1,7  | 14,14,15     | 3.23 | 4 (28%)  | 17,19,21    | 5.61 | 6 (35%)  |
| 7   | NAG  | 1     | 2   | 7    | 14,14,15     | 2.96 | 4 (28%)  | 17,19,21    | 2.72 | 7 (41%)  |
| 7   | BMA  | 1     | 3   | 7    | 11,11,12     | 2.06 | 5 (45%)  | 15,15,17    | 3.60 | 5 (33%)  |
| 3   | NAG  | 2     | 1   | 1,3  | 14,14,15     | 2.80 | 3 (21%)  | 17,19,21    | 4.13 | 6 (35%)  |
| 3   | NAG  | 2     | 2   | 3    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 2.10 | 3 (17%)  |
| 8   | NAG  | 3     | 1   | 1,8  | 14,14,15     | 2.62 | 3 (21%)  | 17,19,21    | 3.21 | 6 (35%)  |
| 8   | NAG  | 3     | 2   | 8    | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 6.10 | 7 (41%)  |
| 8   | BMA  | 3     | 3   | 8    | 11,11,12     | 1.86 | 3 (27%)  | 15,15,17    | 2.98 | 5 (33%)  |
| 8   | MAN  | 3     | 4   | 8    | 11,11,12     | 2.08 | 5 (45%)  | 15,15,17    | 2.73 | 6 (40%)  |
| 8   | MAN  | 3     | 5   | 8    | 11,11,12     | 1.96 | 4 (36%)  | 15,15,17    | 3.02 | 5 (33%)  |
| 7   | NAG  | 4     | 1   | 1,7  | 14,14,15     | 2.85 | 3 (21%)  | 17,19,21    | 3.06 | 5 (29%)  |
| 7   | NAG  | 4     | 2   | 7    | 14,14,15     | 2.91 | 4 (28%)  | 17,19,21    | 4.01 | 8 (47%)  |
| 7   | BMA  | 4     | 3   | 7    | 11,11,12     | 1.95 | 3 (27%)  | 15,15,17    | 3.81 | 5 (33%)  |
| 3   | NAG  | 5     | 1   | 1,3  | 14,14,15     | 2.77 | 3 (21%)  | 17,19,21    | 3.46 | 5 (29%)  |
| 3   | NAG  | 5     | 2   | 3    | 14,14,15     | 2.78 | 4 (28%)  | 17,19,21    | 2.60 | 6 (35%)  |
| 3   | NAG  | 6     | 1   | 1,3  | 14,14,15     | 2.77 | 4 (28%)  | 17,19,21    | 4.60 | 7 (41%)  |
| 3   | NAG  | 6     | 2   | 3    | 14,14,15     | 2.79 | 2 (14%)  | 17,19,21    | 2.88 | 3 (17%)  |
| 3   | NAG  | 7     | 1   | 1,3  | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 3.79 | 6 (35%)  |
| 3   | NAG  | 7     | 2   | 3    | 14,14,15     | 2.92 | 3 (21%)  | 17,19,21    | 3.64 | 4 (23%)  |
| 3   | NAG  | 8     | 1   | 1,3  | 14,14,15     | 2.77 | 3 (21%)  | 17,19,21    | 3.83 | 4 (23%)  |
| 3   | NAG  | 8     | 2   | 3    | 14,14,15     | 2.68 | 4 (28%)  | 17,19,21    | 2.26 | 2 (11%)  |
| 3   | NAG  | 9     | 1   | 1,3  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.09 | 3 (17%)  |
| 3   | NAG  | 9     | 2   | 3    | 14,14,15     | 2.90 | 3 (21%)  | 17,19,21    | 3.23 | 4 (23%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | NAG  | AA    | 1   | 1,4  | 14,14,15     | 2.63 | 3 (21%)  | 17,19,21    | 5.21 | 5 (29%)  |
| 4   | NAG  | AA    | 2   | 4    | 14,14,15     | 2.86 | 3 (21%)  | 17,19,21    | 3.32 | 6 (35%)  |
| 4   | BMA  | AA    | 3   | 4    | 11,11,12     | 1.82 | 1 (9%)   | 15,15,17    | 4.26 | 4 (26%)  |
| 4   | MAN  | AA    | 4   | 4    | 11,11,12     | 2.00 | 3 (27%)  | 15,15,17    | 3.43 | 6 (40%)  |
| 8   | NAG  | BA    | 1   | 1,8  | 14,14,15     | 2.69 | 3 (21%)  | 17,19,21    | 4.18 | 7 (41%)  |
| 8   | NAG  | BA    | 2   | 8    | 14,14,15     | 2.75 | 4 (28%)  | 17,19,21    | 5.47 | 8 (47%)  |
| 8   | BMA  | BA    | 3   | 8    | 11,11,12     | 1.85 | 3 (27%)  | 15,15,17    | 4.41 | 6 (40%)  |
| 8   | MAN  | BA    | 4   | 8    | 11,11,12     | 2.06 | 4 (36%)  | 15,15,17    | 2.91 | 5 (33%)  |
| 8   | MAN  | BA    | 5   | 8    | 11,11,12     | 2.02 | 4 (36%)  | 15,15,17    | 3.74 | 4 (26%)  |
| 3   | NAG  | CA    | 1   | 1,3  | 14,14,15     | 2.86 | 4 (28%)  | 17,19,21    | 5.69 | 7 (41%)  |
| 3   | NAG  | CA    | 2   | 3    | 14,14,15     | 2.90 | 2 (14%)  | 17,19,21    | 1.63 | 3 (17%)  |
| 2   | NAG  | D     | 1   | 1,2  | 14,14,15     | 2.66 | 3 (21%)  | 17,19,21    | 3.24 | 5 (29%)  |
| 2   | NAG  | D     | 2   | 2    | 14,14,15     | 2.81 | 4 (28%)  | 17,19,21    | 5.15 | 8 (47%)  |
| 2   | BMA  | D     | 3   | 2    | 11,11,12     | 1.98 | 4 (36%)  | 15,15,17    | 3.11 | 5 (33%)  |
| 2   | MAN  | D     | 4   | 2    | 11,11,12     | 1.93 | 4 (36%)  | 15,15,17    | 4.11 | 5 (33%)  |
| 2   | MAN  | D     | 5   | 2    | 11,11,12     | 2.66 | 6 (54%)  | 15,15,17    | 2.54 | 6 (40%)  |
| 2   | MAN  | D     | 6   | 2    | 11,11,12     | 2.58 | 6 (54%)  | 15,15,17    | 3.27 | 5 (33%)  |
| 7   | NAG  | DA    | 1   | 1,7  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.54 | 6 (35%)  |
| 7   | NAG  | DA    | 2   | 7    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 5.78 | 9 (52%)  |
| 7   | BMA  | DA    | 3   | 7    | 11,11,12     | 2.03 | 3 (27%)  | 15,15,17    | 3.22 | 5 (33%)  |
| 3   | NAG  | E     | 1   | 1,3  | 14,14,15     | 2.88 | 3 (21%)  | 17,19,21    | 3.89 | 7 (41%)  |
| 3   | NAG  | E     | 2   | 3    | 14,14,15     | 3.20 | 6 (42%)  | 17,19,21    | 3.74 | 6 (35%)  |
| 4   | NAG  | F     | 1   | 1,4  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 5.68 | 6 (35%)  |
| 4   | NAG  | F     | 2   | 4    | 14,14,15     | 2.74 | 3 (21%)  | 17,19,21    | 7.16 | 6 (35%)  |
| 4   | BMA  | F     | 3   | 4    | 11,11,12     | 1.84 | 3 (27%)  | 15,15,17    | 2.78 | 4 (26%)  |
| 4   | MAN  | F     | 4   | 4    | 11,11,12     | 2.01 | 3 (27%)  | 15,15,17    | 3.46 | 5 (33%)  |
| 3   | NAG  | G     | 1   | 1,3  | 14,14,15     | 2.76 | 3 (21%)  | 17,19,21    | 2.43 | 5 (29%)  |
| 3   | NAG  | G     | 2   | 3    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 4.44 | 4 (23%)  |
| 5   | NAG  | H     | 1   | 1,5  | 14,14,15     | 2.70 | 3 (21%)  | 17,19,21    | 2.90 | 5 (29%)  |
| 5   | NAG  | H     | 2   | 5    | 14,14,15     | 2.95 | 3 (21%)  | 17,19,21    | 4.86 | 8 (47%)  |
| 5   | BMA  | H     | 3   | 5    | 11,11,12     | 1.88 | 3 (27%)  | 15,15,17    | 3.45 | 4 (26%)  |
| 5   | MAN  | H     | 4   | 5    | 11,11,12     | 1.91 | 3 (27%)  | 15,15,17    | 3.41 | 5 (33%)  |
| 3   | NAG  | I     | 1   | 1,3  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.44 | 6 (35%)  |
| 3   | NAG  | I     | 2   | 3    | 14,14,15     | 2.90 | 4 (28%)  | 17,19,21    | 2.11 | 3 (17%)  |
| 3   | NAG  | J     | 1   | 1,3  | 14,14,15     | 2.58 | 3 (21%)  | 17,19,21    | 5.00 | 6 (35%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 3   | NAG  | J     | 2   | 3    | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 2.10 | 4 (23%)  |
| 6   | NAG  | K     | 1   | 1,6  | 14,14,15     | 2.69 | 3 (21%)  | 17,19,21    | 3.96 | 6 (35%)  |
| 6   | NAG  | K     | 2   | 6    | 14,14,15     | 2.82 | 4 (28%)  | 17,19,21    | 3.54 | 5 (29%)  |
| 6   | BMA  | K     | 3   | 6    | 11,11,12     | 1.84 | 2 (18%)  | 15,15,17    | 5.49 | 6 (40%)  |
| 6   | MAN  | K     | 4   | 6    | 11,11,12     | 1.70 | 2 (18%)  | 15,15,17    | 8.19 | 6 (40%)  |
| 6   | MAN  | K     | 5   | 6    | 11,11,12     | 1.70 | 3 (27%)  | 15,15,17    | 4.22 | 5 (33%)  |
| 6   | MAN  | K     | 6   | 6    | 11,11,12     | 1.96 | 3 (27%)  | 15,15,17    | 2.47 | 1 (6%)   |
| 6   | MAN  | K     | 7   | 6    | 11,11,12     | 1.93 | 4 (36%)  | 15,15,17    | 5.07 | 6 (40%)  |
| 6   | MAN  | K     | 8   | 6    | 11,11,12     | 2.57 | 6 (54%)  | 15,15,17    | 3.74 | 6 (40%)  |
| 7   | NAG  | L     | 1   | 1,7  | 14,14,15     | 3.23 | 4 (28%)  | 17,19,21    | 5.61 | 6 (35%)  |
| 7   | NAG  | L     | 2   | 7    | 14,14,15     | 2.97 | 4 (28%)  | 17,19,21    | 2.73 | 7 (41%)  |
| 7   | BMA  | L     | 3   | 7    | 11,11,12     | 2.07 | 5 (45%)  | 15,15,17    | 3.60 | 5 (33%)  |
| 3   | NAG  | M     | 1   | 1,3  | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 4.14 | 6 (35%)  |
| 3   | NAG  | M     | 2   | 3    | 14,14,15     | 2.82 | 3 (21%)  | 17,19,21    | 2.09 | 3 (17%)  |
| 8   | NAG  | N     | 1   | 1,8  | 14,14,15     | 2.62 | 3 (21%)  | 17,19,21    | 3.21 | 6 (35%)  |
| 8   | NAG  | N     | 2   | 8    | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 6.11 | 7 (41%)  |
| 8   | BMA  | N     | 3   | 8    | 11,11,12     | 1.87 | 3 (27%)  | 15,15,17    | 2.98 | 5 (33%)  |
| 8   | MAN  | N     | 4   | 8    | 11,11,12     | 2.07 | 5 (45%)  | 15,15,17    | 2.73 | 6 (40%)  |
| 8   | MAN  | N     | 5   | 8    | 11,11,12     | 1.96 | 4 (36%)  | 15,15,17    | 3.02 | 5 (33%)  |
| 7   | NAG  | O     | 1   | 1,7  | 14,14,15     | 2.86 | 3 (21%)  | 17,19,21    | 3.06 | 5 (29%)  |
| 7   | NAG  | O     | 2   | 7    | 14,14,15     | 2.91 | 4 (28%)  | 17,19,21    | 4.01 | 8 (47%)  |
| 7   | BMA  | O     | 3   | 7    | 11,11,12     | 1.95 | 3 (27%)  | 15,15,17    | 3.81 | 5 (33%)  |
| 3   | NAG  | P     | 1   | 1,3  | 14,14,15     | 2.78 | 3 (21%)  | 17,19,21    | 3.47 | 5 (29%)  |
| 3   | NAG  | P     | 2   | 3    | 14,14,15     | 2.78 | 4 (28%)  | 17,19,21    | 2.60 | 6 (35%)  |
| 3   | NAG  | Q     | 1   | 1,3  | 14,14,15     | 2.77 | 4 (28%)  | 17,19,21    | 4.60 | 7 (41%)  |
| 3   | NAG  | Q     | 2   | 3    | 14,14,15     | 2.79 | 2 (14%)  | 17,19,21    | 2.88 | 3 (17%)  |
| 3   | NAG  | R     | 1   | 1,3  | 14,14,15     | 2.67 | 3 (21%)  | 17,19,21    | 3.79 | 6 (35%)  |
| 3   | NAG  | R     | 2   | 3    | 14,14,15     | 2.93 | 3 (21%)  | 17,19,21    | 3.64 | 4 (23%)  |
| 3   | NAG  | S     | 1   | 1,3  | 14,14,15     | 2.76 | 3 (21%)  | 17,19,21    | 3.83 | 4 (23%)  |
| 3   | NAG  | S     | 2   | 3    | 14,14,15     | 2.68 | 4 (28%)  | 17,19,21    | 2.27 | 2 (11%)  |
| 3   | NAG  | T     | 1   | 1,3  | 14,14,15     | 2.72 | 3 (21%)  | 17,19,21    | 4.09 | 3 (17%)  |
| 3   | NAG  | T     | 2   | 3    | 14,14,15     | 2.89 | 3 (21%)  | 17,19,21    | 3.23 | 4 (23%)  |
| 4   | NAG  | U     | 1   | 1,4  | 14,14,15     | 2.64 | 3 (21%)  | 17,19,21    | 5.21 | 5 (29%)  |
| 4   | NAG  | U     | 2   | 4    | 14,14,15     | 2.86 | 3 (21%)  | 17,19,21    | 3.32 | 6 (35%)  |
| 4   | BMA  | U     | 3   | 4    | 11,11,12     | 1.82 | 2 (18%)  | 15,15,17    | 4.26 | 4 (26%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 4   | MAN  | U     | 4   | 4    | 11,11,12     | 2.01 | 3 (27%)  | 15,15,17    | 3.43 | 6 (40%)  |
| 8   | NAG  | V     | 1   | 1,8  | 14,14,15     | 2.69 | 3 (21%)  | 17,19,21    | 4.18 | 7 (41%)  |
| 8   | NAG  | V     | 2   | 8    | 14,14,15     | 2.75 | 4 (28%)  | 17,19,21    | 5.47 | 8 (47%)  |
| 8   | BMA  | V     | 3   | 8    | 11,11,12     | 1.85 | 2 (18%)  | 15,15,17    | 4.41 | 6 (40%)  |
| 8   | MAN  | V     | 4   | 8    | 11,11,12     | 2.05 | 4 (36%)  | 15,15,17    | 2.91 | 5 (33%)  |
| 8   | MAN  | V     | 5   | 8    | 11,11,12     | 2.02 | 4 (36%)  | 15,15,17    | 3.74 | 4 (26%)  |
| 3   | NAG  | W     | 1   | 1,3  | 14,14,15     | 2.87 | 4 (28%)  | 17,19,21    | 5.69 | 7 (41%)  |
| 3   | NAG  | W     | 2   | 3    | 14,14,15     | 2.90 | 2 (14%)  | 17,19,21    | 1.63 | 3 (17%)  |
| 7   | NAG  | X     | 1   | 1,7  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.54 | 6 (35%)  |
| 7   | NAG  | X     | 2   | 7    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 5.78 | 9 (52%)  |
| 7   | BMA  | X     | 3   | 7    | 11,11,12     | 2.04 | 3 (27%)  | 15,15,17    | 3.22 | 5 (33%)  |
| 2   | NAG  | Y     | 1   | 1,2  | 14,14,15     | 2.67 | 3 (21%)  | 17,19,21    | 3.24 | 5 (29%)  |
| 2   | NAG  | Y     | 2   | 2    | 14,14,15     | 2.81 | 4 (28%)  | 17,19,21    | 5.15 | 8 (47%)  |
| 2   | BMA  | Y     | 3   | 2    | 11,11,12     | 1.99 | 4 (36%)  | 15,15,17    | 3.11 | 5 (33%)  |
| 2   | MAN  | Y     | 4   | 2    | 11,11,12     | 1.93 | 4 (36%)  | 15,15,17    | 4.11 | 5 (33%)  |
| 2   | MAN  | Y     | 5   | 2    | 11,11,12     | 2.65 | 6 (54%)  | 15,15,17    | 2.54 | 6 (40%)  |
| 2   | MAN  | Y     | 6   | 2    | 11,11,12     | 2.58 | 6 (54%)  | 15,15,17    | 3.27 | 5 (33%)  |
| 3   | NAG  | Z     | 1   | 1,3  | 14,14,15     | 2.88 | 3 (21%)  | 17,19,21    | 3.90 | 7 (41%)  |
| 3   | NAG  | Z     | 2   | 3    | 14,14,15     | 3.20 | 6 (42%)  | 17,19,21    | 3.74 | 6 (35%)  |
| 4   | NAG  | a     | 1   | 1,4  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 5.68 | 6 (35%)  |
| 4   | NAG  | a     | 2   | 4    | 14,14,15     | 2.74 | 3 (21%)  | 17,19,21    | 7.16 | 6 (35%)  |
| 4   | BMA  | a     | 3   | 4    | 11,11,12     | 1.84 | 3 (27%)  | 15,15,17    | 2.78 | 4 (26%)  |
| 4   | MAN  | a     | 4   | 4    | 11,11,12     | 2.00 | 3 (27%)  | 15,15,17    | 3.46 | 5 (33%)  |
| 3   | NAG  | b     | 1   | 1,3  | 14,14,15     | 2.76 | 3 (21%)  | 17,19,21    | 2.43 | 5 (29%)  |
| 3   | NAG  | b     | 2   | 3    | 14,14,15     | 2.80 | 3 (21%)  | 17,19,21    | 4.44 | 4 (23%)  |
| 5   | NAG  | c     | 1   | 1,5  | 14,14,15     | 2.70 | 3 (21%)  | 17,19,21    | 2.90 | 5 (29%)  |
| 5   | NAG  | c     | 2   | 5    | 14,14,15     | 2.94 | 3 (21%)  | 17,19,21    | 4.85 | 8 (47%)  |
| 5   | BMA  | c     | 3   | 5    | 11,11,12     | 1.87 | 3 (27%)  | 15,15,17    | 3.45 | 4 (26%)  |
| 5   | MAN  | c     | 4   | 5    | 11,11,12     | 1.92 | 3 (27%)  | 15,15,17    | 3.41 | 5 (33%)  |
| 3   | NAG  | d     | 1   | 1,3  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.44 | 6 (35%)  |
| 3   | NAG  | d     | 2   | 3    | 14,14,15     | 2.90 | 4 (28%)  | 17,19,21    | 2.10 | 3 (17%)  |
| 3   | NAG  | e     | 1   | 1,3  | 14,14,15     | 2.58 | 3 (21%)  | 17,19,21    | 5.00 | 6 (35%)  |
| 3   | NAG  | e     | 2   | 3    | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 2.10 | 4 (23%)  |
| 6   | NAG  | f     | 1   | 1,6  | 14,14,15     | 2.69 | 3 (21%)  | 17,19,21    | 3.96 | 6 (35%)  |
| 6   | NAG  | f     | 2   | 6    | 14,14,15     | 2.82 | 4 (28%)  | 17,19,21    | 3.54 | 5 (29%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 6   | BMA  | f     | 3   | 6    | 11,11,12     | 1.83 | 2 (18%)  | 15,15,17    | 5.49 | 6 (40%)  |
| 6   | MAN  | f     | 4   | 6    | 11,11,12     | 1.70 | 2 (18%)  | 15,15,17    | 8.19 | 6 (40%)  |
| 6   | MAN  | f     | 5   | 6    | 11,11,12     | 1.70 | 3 (27%)  | 15,15,17    | 4.22 | 5 (33%)  |
| 6   | MAN  | f     | 6   | 6    | 11,11,12     | 1.96 | 3 (27%)  | 15,15,17    | 2.47 | 1 (6%)   |
| 6   | MAN  | f     | 7   | 6    | 11,11,12     | 1.92 | 4 (36%)  | 15,15,17    | 5.08 | 6 (40%)  |
| 6   | MAN  | f     | 8   | 6    | 11,11,12     | 2.57 | 6 (54%)  | 15,15,17    | 3.74 | 6 (40%)  |
| 7   | NAG  | g     | 1   | 1,7  | 14,14,15     | 3.22 | 4 (28%)  | 17,19,21    | 5.61 | 6 (35%)  |
| 7   | NAG  | g     | 2   | 7    | 14,14,15     | 2.98 | 4 (28%)  | 17,19,21    | 2.73 | 7 (41%)  |
| 7   | BMA  | g     | 3   | 7    | 11,11,12     | 2.07 | 5 (45%)  | 15,15,17    | 3.60 | 5 (33%)  |
| 3   | NAG  | h     | 1   | 1,3  | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 4.13 | 6 (35%)  |
| 3   | NAG  | h     | 2   | 3    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 2.09 | 3 (17%)  |
| 8   | NAG  | i     | 1   | 1,8  | 14,14,15     | 2.61 | 3 (21%)  | 17,19,21    | 3.21 | 6 (35%)  |
| 8   | NAG  | i     | 2   | 8    | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 6.11 | 7 (41%)  |
| 8   | BMA  | i     | 3   | 8    | 11,11,12     | 1.86 | 3 (27%)  | 15,15,17    | 2.98 | 5 (33%)  |
| 8   | MAN  | i     | 4   | 8    | 11,11,12     | 2.08 | 5 (45%)  | 15,15,17    | 2.73 | 6 (40%)  |
| 8   | MAN  | i     | 5   | 8    | 11,11,12     | 1.96 | 4 (36%)  | 15,15,17    | 3.02 | 5 (33%)  |
| 7   | NAG  | j     | 1   | 1,7  | 14,14,15     | 2.85 | 3 (21%)  | 17,19,21    | 3.06 | 5 (29%)  |
| 7   | NAG  | j     | 2   | 7    | 14,14,15     | 2.91 | 4 (28%)  | 17,19,21    | 4.01 | 8 (47%)  |
| 7   | BMA  | j     | 3   | 7    | 11,11,12     | 1.95 | 3 (27%)  | 15,15,17    | 3.80 | 5 (33%)  |
| 3   | NAG  | k     | 1   | 1,3  | 14,14,15     | 2.77 | 3 (21%)  | 17,19,21    | 3.47 | 5 (29%)  |
| 3   | NAG  | k     | 2   | 3    | 14,14,15     | 2.78 | 4 (28%)  | 17,19,21    | 2.60 | 6 (35%)  |
| 3   | NAG  | l     | 1   | 1,3  | 14,14,15     | 2.77 | 4 (28%)  | 17,19,21    | 4.60 | 7 (41%)  |
| 3   | NAG  | l     | 2   | 3    | 14,14,15     | 2.79 | 2 (14%)  | 17,19,21    | 2.88 | 3 (17%)  |
| 3   | NAG  | m     | 1   | 1,3  | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 3.79 | 6 (35%)  |
| 3   | NAG  | m     | 2   | 3    | 14,14,15     | 2.93 | 3 (21%)  | 17,19,21    | 3.64 | 4 (23%)  |
| 3   | NAG  | n     | 1   | 1,3  | 14,14,15     | 2.76 | 3 (21%)  | 17,19,21    | 3.83 | 4 (23%)  |
| 3   | NAG  | n     | 2   | 3    | 14,14,15     | 2.68 | 4 (28%)  | 17,19,21    | 2.27 | 2 (11%)  |
| 3   | NAG  | o     | 1   | 1,3  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.09 | 3 (17%)  |
| 3   | NAG  | o     | 2   | 3    | 14,14,15     | 2.89 | 4 (28%)  | 17,19,21    | 3.23 | 4 (23%)  |
| 4   | NAG  | p     | 1   | 1,4  | 14,14,15     | 2.64 | 3 (21%)  | 17,19,21    | 5.22 | 5 (29%)  |
| 4   | NAG  | p     | 2   | 4    | 14,14,15     | 2.87 | 3 (21%)  | 17,19,21    | 3.32 | 6 (35%)  |
| 4   | BMA  | p     | 3   | 4    | 11,11,12     | 1.82 | 1 (9%)   | 15,15,17    | 4.26 | 4 (26%)  |
| 4   | MAN  | p     | 4   | 4    | 11,11,12     | 2.00 | 3 (27%)  | 15,15,17    | 3.43 | 6 (40%)  |
| 8   | NAG  | q     | 1   | 1,8  | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 4.18 | 7 (41%)  |
| 8   | NAG  | q     | 2   | 8    | 14,14,15     | 2.74 | 4 (28%)  | 17,19,21    | 5.47 | 8 (47%)  |



| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | BMA  | q     | 3   | 8    | 11,11,12     | 1.85 | 3 (27%)  | 15,15,17    | 4.41 | 6 (40%)  |
| 8   | MAN  | q     | 4   | 8    | 11,11,12     | 2.05 | 4 (36%)  | 15,15,17    | 2.91 | 5 (33%)  |
| 8   | MAN  | q     | 5   | 8    | 11,11,12     | 2.03 | 4 (36%)  | 15,15,17    | 3.74 | 4 (26%)  |
| 3   | NAG  | r     | 1   | 1,3  | 14,14,15     | 2.88 | 4 (28%)  | 17,19,21    | 5.69 | 7 (41%)  |
| 3   | NAG  | r     | 2   | 3    | 14,14,15     | 2.89 | 2 (14%)  | 17,19,21    | 1.63 | 3 (17%)  |
| 7   | NAG  | s     | 1   | 1,7  | 14,14,15     | 2.72 | 3 (21%)  | 17,19,21    | 4.55 | 6 (35%)  |
| 7   | NAG  | s     | 2   | 7    | 14,14,15     | 2.82 | 3 (21%)  | 17,19,21    | 5.78 | 9 (52%)  |
| 7   | BMA  | s     | 3   | 7    | 11,11,12     | 2.04 | 3 (27%)  | 15,15,17    | 3.23 | 5 (33%)  |
| 2   | NAG  | t     | 1   | 1,2  | 14,14,15     | 2.67 | 3 (21%)  | 17,19,21    | 3.24 | 5 (29%)  |
| 2   | NAG  | t     | 2   | 2    | 14,14,15     | 2.81 | 4 (28%)  | 17,19,21    | 5.15 | 8 (47%)  |
| 2   | BMA  | t     | 3   | 2    | 11,11,12     | 1.99 | 4 (36%)  | 15,15,17    | 3.10 | 5 (33%)  |
| 2   | MAN  | t     | 4   | 2    | 11,11,12     | 1.94 | 4 (36%)  | 15,15,17    | 4.12 | 5 (33%)  |
| 2   | MAN  | t     | 5   | 2    | 11,11,12     | 2.66 | 6 (54%)  | 15,15,17    | 2.53 | 6 (40%)  |
| 2   | MAN  | t     | 6   | 2    | 11,11,12     | 2.57 | 6 (54%)  | 15,15,17    | 3.27 | 5 (33%)  |
| 3   | NAG  | u     | 1   | 1,3  | 14,14,15     | 2.87 | 3 (21%)  | 17,19,21    | 3.90 | 7 (41%)  |
| 3   | NAG  | u     | 2   | 3    | 14,14,15     | 3.20 | 6 (42%)  | 17,19,21    | 3.74 | 6 (35%)  |
| 4   | NAG  | v     | 1   | 1,4  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 5.68 | 6 (35%)  |
| 4   | NAG  | v     | 2   | 4    | 14,14,15     | 2.74 | 3 (21%)  | 17,19,21    | 7.16 | 6 (35%)  |
| 4   | BMA  | v     | 3   | 4    | 11,11,12     | 1.84 | 3 (27%)  | 15,15,17    | 2.78 | 4 (26%)  |
| 4   | MAN  | v     | 4   | 4    | 11,11,12     | 2.01 | 3 (27%)  | 15,15,17    | 3.46 | 5 (33%)  |
| 3   | NAG  | w     | 1   | 1,3  | 14,14,15     | 2.76 | 3 (21%)  | 17,19,21    | 2.43 | 5 (29%)  |
| 3   | NAG  | w     | 2   | 3    | 14,14,15     | 2.81 | 3 (21%)  | 17,19,21    | 4.44 | 4 (23%)  |
| 5   | NAG  | x     | 1   | 1,5  | 14,14,15     | 2.71 | 3 (21%)  | 17,19,21    | 2.90 | 5 (29%)  |
| 5   | NAG  | x     | 2   | 5    | 14,14,15     | 2.94 | 3 (21%)  | 17,19,21    | 4.86 | 8 (47%)  |
| 5   | BMA  | x     | 3   | 5    | 11,11,12     | 1.87 | 3 (27%)  | 15,15,17    | 3.45 | 4 (26%)  |
| 5   | MAN  | x     | 4   | 5    | 11,11,12     | 1.91 | 3 (27%)  | 15,15,17    | 3.41 | 5 (33%)  |
| 3   | NAG  | y     | 1   | 1,3  | 14,14,15     | 2.73 | 3 (21%)  | 17,19,21    | 4.44 | 6 (35%)  |
| 3   | NAG  | y     | 2   | 3    | 14,14,15     | 2.90 | 4 (28%)  | 17,19,21    | 2.11 | 3 (17%)  |
| 3   | NAG  | z     | 1   | 1,3  | 14,14,15     | 2.59 | 3 (21%)  | 17,19,21    | 5.00 | 6 (35%)  |
| 3   | NAG  | z     | 2   | 3    | 14,14,15     | 2.68 | 3 (21%)  | 17,19,21    | 2.10 | 4 (23%)  |

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



| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 6   | NAG  | 0     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | 0     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | 0     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | MAN  | 0     | 4   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | 0     | 5   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | 0     | 6   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | 0     | 7   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | MAN  | 0     | 8   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | 1     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | 1     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | 1     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | 2     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 2     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | 3     | 1   | 1,8  | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | 3     | 2   | 8    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | BMA  | 3     | 3   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | 3     | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | 3     | 5   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | 4     | 1   | 1,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | 4     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | 4     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | 5     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 5     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 6     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 6     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 7     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 7     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 8     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 8     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 9     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | 9     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | AA    | 1   | 1,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | AA    | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | BMA  | AA    | 3   | 4    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | MAN  | AA    | 4   | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | BA    | 1   | 1,8  | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | BA    | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | BA    | 3   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | BA    | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | BA    | 5   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | CA    | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 3   | NAG  | CA    | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | D     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | BMA  | D     | 3   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 4   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 5   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | D     | 6   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | DA    | 1   | 1,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | DA    | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | BMA  | DA    | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | E     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | E     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | F     | 1   | 1,4  | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | F     | 2   | 4    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | BMA  | F     | 3   | 4    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | MAN  | F     | 4   | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | G     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | G     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | NAG  | H     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | H     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | BMA  | H     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | H     | 4   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | I     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | I     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | J     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | K     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | K     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | MAN  | K     | 4   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | K     | 5   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | K     | 6   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | K     | 7   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | MAN  | K     | 8   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | L     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | L     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | L     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | M     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | M     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | N     | 1   | 1,8  | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | NAG  | N     | 2   | 8    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | BMA  | N     | 3   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | N     | 5   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | O     | 1   | 1,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | O     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | O     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | P     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | P     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Q     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Q     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | R     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | R     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | S     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | S     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | T     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | T     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | U     | 1   | 1,4  | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | U     | 2   | 4    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | BMA  | U     | 3   | 4    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | MAN  | U     | 4   | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | V     | 1   | 1,8  | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | V     | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | V     | 3   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | V     | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | V     | 5   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | W     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | W     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | X     | 1   | 1,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | NAG  | X     | 2   | 7    | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | BMA  | X     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 2   | NAG  | Y     | 1   | 1,2  | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | NAG  | Y     | 2   | 2    | -       | 1/6/23/26 | 0/1/1/1 |
| 2   | BMA  | Y     | 3   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | Y     | 4   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | Y     | 5   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 2   | MAN  | Y     | 6   | 2    | -       | 1/2/19/22 | 0/1/1/1 |
| 3   | NAG  | Z     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | Z     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 4   | NAG  | a     | 1   | 1,4  | -       | 1/6/23/26 | 0/1/1/1 |
| 4   | NAG  | a     | 2   | 4    | -       | 1/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 4   | BMA  | a     | 3   | 4    | -       | 1/2/19/22 | 0/1/1/1 |
| 4   | MAN  | a     | 4   | 4    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | b     | 1   | 1,3  | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | b     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 5   | NAG  | c     | 1   | 1,5  | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | NAG  | c     | 2   | 5    | -       | 2/6/23/26 | 0/1/1/1 |
| 5   | BMA  | c     | 3   | 5    | -       | 2/2/19/22 | 0/1/1/1 |
| 5   | MAN  | c     | 4   | 5    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | d     | 1   | 1,3  | -       | 4/6/23/26 | 0/1/1/1 |
| 3   | NAG  | d     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | e     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | e     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | f     | 1   | 1,6  | -       | 1/6/23/26 | 0/1/1/1 |
| 6   | NAG  | f     | 2   | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 6   | BMA  | f     | 3   | 6    | -       | 2/2/19/22 | 0/1/1/1 |
| 6   | MAN  | f     | 4   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | f     | 5   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | f     | 6   | 6    | -       | 0/2/19/22 | 0/1/1/1 |
| 6   | MAN  | f     | 7   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 6   | MAN  | f     | 8   | 6    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | g     | 1   | 1,7  | -       | 1/6/23/26 | 0/1/1/1 |
| 7   | NAG  | g     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | g     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | h     | 1   | 1,3  | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | h     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | i     | 1   | 1,8  | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | NAG  | i     | 2   | 8    | -       | 1/6/23/26 | 0/1/1/1 |
| 8   | BMA  | i     | 3   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | MAN  | i     | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | i     | 5   | 8    | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | j     | 1   | 1,7  | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | j     | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | j     | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 3   | NAG  | k     | 1   | 1,3  | -       | 1/6/23/26 | 0/1/1/1 |
| 3   | NAG  | k     | 2   | 3    | -       | 0/6/23/26 | 0/1/1/1 |
| 3   | NAG  | l     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | l     | 2   | 3    | -       | 2/6/23/26 | 0/1/1/1 |
| 3   | NAG  | m     | 1   | 1,3  | -       | 3/6/23/26 | 0/1/1/1 |
| 3   | NAG  | m     | 2   | 3    | -       | 1/6/23/26 | 0/1/1/1 |

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

All (685) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | E     | 2   | NAG  | O5-C1 | 8.80  | 1.58        | 1.43     |
| 3   | u     | 2   | NAG  | O5-C1 | 8.79  | 1.58        | 1.43     |
| 3   | Z     | 2   | NAG  | O5-C1 | 8.79  | 1.58        | 1.43     |
| 7   | 1     | 1   | NAG  | O5-C1 | 8.54  | 1.58        | 1.43     |
| 7   | L     | 1   | NAG  | O5-C1 | 8.52  | 1.58        | 1.43     |
| 7   | g     | 1   | NAG  | O5-C1 | 8.50  | 1.58        | 1.43     |
| 7   | g     | 2   | NAG  | O5-C1 | 8.35  | 1.57        | 1.43     |
| 7   | L     | 2   | NAG  | O5-C1 | 8.34  | 1.57        | 1.43     |
| 7   | 1     | 2   | NAG  | O5-C1 | 8.31  | 1.57        | 1.43     |
| 3   | I     | 2   | NAG  | O5-C1 | 8.07  | 1.57        | 1.43     |
| 3   | y     | 2   | NAG  | O5-C1 | 8.05  | 1.57        | 1.43     |
| 3   | d     | 2   | NAG  | O5-C1 | 8.04  | 1.57        | 1.43     |
| 3   | m     | 2   | NAG  | O5-C1 | 7.83  | 1.56        | 1.43     |
| 3   | 7     | 2   | NAG  | O5-C1 | 7.80  | 1.56        | 1.43     |
| 3   | R     | 2   | NAG  | O5-C1 | 7.79  | 1.56        | 1.43     |
| 3   | 6     | 2   | NAG  | O5-C1 | 7.77  | 1.56        | 1.43     |
| 3   | 2     | 2   | NAG  | O5-C1 | 7.76  | 1.56        | 1.43     |
| 3   | Q     | 2   | NAG  | O5-C1 | 7.76  | 1.56        | 1.43     |
| 3   | l     | 2   | NAG  | O5-C1 | 7.76  | 1.56        | 1.43     |
| 3   | M     | 2   | NAG  | O5-C1 | 7.74  | 1.56        | 1.43     |
| 3   | h     | 2   | NAG  | O5-C1 | 7.72  | 1.56        | 1.43     |
| 3   | CA    | 2   | NAG  | C2-N2 | -7.64 | 1.33        | 1.46     |
| 3   | W     | 2   | NAG  | C2-N2 | -7.62 | 1.33        | 1.46     |
| 3   | r     | 2   | NAG  | C2-N2 | -7.59 | 1.33        | 1.46     |
| 3   | r     | 1   | NAG  | C2-N2 | -7.58 | 1.33        | 1.46     |
| 3   | o     | 2   | NAG  | O5-C1 | 7.57  | 1.56        | 1.43     |
| 3   | 9     | 2   | NAG  | O5-C1 | 7.57  | 1.56        | 1.43     |
| 3   | T     | 2   | NAG  | O5-C1 | 7.57  | 1.56        | 1.43     |
| 3   | W     | 1   | NAG  | C2-N2 | -7.55 | 1.33        | 1.46     |
| 3   | CA    | 1   | NAG  | C2-N2 | -7.53 | 1.33        | 1.46     |
| 3   | w     | 2   | NAG  | O5-C1 | 7.51  | 1.56        | 1.43     |
| 3   | G     | 2   | NAG  | O5-C1 | 7.47  | 1.56        | 1.43     |
| 3   | P     | 2   | NAG  | O5-C1 | 7.46  | 1.56        | 1.43     |
| 3   | b     | 2   | NAG  | O5-C1 | 7.46  | 1.56        | 1.43     |
| 3   | k     | 2   | NAG  | O5-C1 | 7.43  | 1.56        | 1.43     |
| 3   | z     | 2   | NAG  | O5-C1 | 7.43  | 1.56        | 1.43     |
| 3   | J     | 2   | NAG  | O5-C1 | 7.42  | 1.56        | 1.43     |
| 3   | 5     | 2   | NAG  | O5-C1 | 7.41  | 1.56        | 1.43     |
| 3   | e     | 2   | NAG  | O5-C1 | 7.41  | 1.56        | 1.43     |
| 7   | O     | 2   | NAG  | O5-C1 | 7.40  | 1.56        | 1.43     |
| 7   | j     | 2   | NAG  | O5-C1 | 7.40  | 1.56        | 1.43     |
| 7   | 4     | 2   | NAG  | O5-C1 | 7.38  | 1.56        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 2   | Y     | 2   | NAG  | O5-C1 | 7.29  | 1.55        | 1.43     |
| 2   | t     | 2   | NAG  | O5-C1 | 7.29  | 1.55        | 1.43     |
| 2   | D     | 2   | NAG  | O5-C1 | 7.27  | 1.55        | 1.43     |
| 5   | H     | 2   | NAG  | C2-N2 | -7.22 | 1.34        | 1.46     |
| 5   | c     | 2   | NAG  | C2-N2 | -7.21 | 1.34        | 1.46     |
| 3   | Z     | 1   | NAG  | C2-N2 | -7.21 | 1.34        | 1.46     |
| 3   | E     | 1   | NAG  | C2-N2 | -7.20 | 1.34        | 1.46     |
| 5   | x     | 2   | NAG  | C2-N2 | -7.20 | 1.34        | 1.46     |
| 3   | u     | 1   | NAG  | C2-N2 | -7.18 | 1.34        | 1.46     |
| 4   | p     | 2   | NAG  | O5-C1 | 7.17  | 1.55        | 1.43     |
| 7   | O     | 1   | NAG  | C2-N2 | -7.16 | 1.34        | 1.46     |
| 4   | U     | 2   | NAG  | O5-C1 | 7.16  | 1.55        | 1.43     |
| 7   | 4     | 1   | NAG  | C2-N2 | -7.15 | 1.34        | 1.46     |
| 7   | j     | 1   | NAG  | C2-N2 | -7.15 | 1.34        | 1.46     |
| 6   | K     | 2   | NAG  | O5-C1 | 7.14  | 1.55        | 1.43     |
| 5   | H     | 2   | NAG  | O5-C1 | 7.14  | 1.55        | 1.43     |
| 4   | AA    | 2   | NAG  | O5-C1 | 7.13  | 1.55        | 1.43     |
| 5   | x     | 2   | NAG  | O5-C1 | 7.13  | 1.55        | 1.43     |
| 5   | c     | 2   | NAG  | O5-C1 | 7.12  | 1.55        | 1.43     |
| 6   | f     | 2   | NAG  | O5-C1 | 7.12  | 1.55        | 1.43     |
| 6   | 0     | 2   | NAG  | O5-C1 | 7.12  | 1.55        | 1.43     |
| 3   | l     | 1   | NAG  | O5-C1 | 6.98  | 1.55        | 1.43     |
| 3   | Q     | 1   | NAG  | O5-C1 | 6.98  | 1.55        | 1.43     |
| 3   | 6     | 1   | NAG  | O5-C1 | 6.98  | 1.55        | 1.43     |
| 3   | b     | 1   | NAG  | O5-C1 | 6.97  | 1.55        | 1.43     |
| 3   | w     | 1   | NAG  | O5-C1 | 6.96  | 1.55        | 1.43     |
| 3   | G     | 1   | NAG  | O5-C1 | 6.95  | 1.55        | 1.43     |
| 3   | k     | 1   | NAG  | O5-C1 | 6.94  | 1.55        | 1.43     |
| 3   | u     | 1   | NAG  | O5-C1 | 6.94  | 1.55        | 1.43     |
| 3   | P     | 1   | NAG  | O5-C1 | 6.94  | 1.55        | 1.43     |
| 3   | E     | 1   | NAG  | O5-C1 | 6.93  | 1.55        | 1.43     |
| 3   | Z     | 1   | NAG  | O5-C1 | 6.93  | 1.55        | 1.43     |
| 3   | 5     | 1   | NAG  | O5-C1 | 6.93  | 1.55        | 1.43     |
| 7   | s     | 2   | NAG  | O5-C1 | 6.92  | 1.55        | 1.43     |
| 3   | 2     | 1   | NAG  | O5-C1 | 6.92  | 1.55        | 1.43     |
| 7   | X     | 1   | NAG  | O5-C1 | 6.91  | 1.55        | 1.43     |
| 3   | 9     | 1   | NAG  | O5-C1 | 6.90  | 1.55        | 1.43     |
| 4   | p     | 2   | NAG  | C2-N2 | -6.90 | 1.34        | 1.46     |
| 3   | M     | 1   | NAG  | O5-C1 | 6.89  | 1.55        | 1.43     |
| 7   | DA    | 2   | NAG  | O5-C1 | 6.89  | 1.55        | 1.43     |
| 3   | h     | 1   | NAG  | O5-C1 | 6.89  | 1.55        | 1.43     |
| 7   | X     | 2   | NAG  | O5-C1 | 6.89  | 1.55        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | DA    | 1   | NAG  | O5-C1 | 6.89  | 1.55        | 1.43     |
| 7   | s     | 1   | NAG  | O5-C1 | 6.88  | 1.55        | 1.43     |
| 4   | AA    | 2   | NAG  | C2-N2 | -6.87 | 1.34        | 1.46     |
| 4   | U     | 2   | NAG  | C2-N2 | -6.87 | 1.34        | 1.46     |
| 3   | T     | 1   | NAG  | O5-C1 | 6.86  | 1.55        | 1.43     |
| 8   | BA    | 2   | NAG  | O5-C1 | 6.86  | 1.55        | 1.43     |
| 3   | o     | 1   | NAG  | O5-C1 | 6.85  | 1.55        | 1.43     |
| 8   | V     | 2   | NAG  | O5-C1 | 6.85  | 1.55        | 1.43     |
| 3   | m     | 1   | NAG  | O5-C1 | 6.83  | 1.55        | 1.43     |
| 8   | q     | 2   | NAG  | O5-C1 | 6.83  | 1.55        | 1.43     |
| 7   | O     | 2   | NAG  | C2-N2 | -6.81 | 1.35        | 1.46     |
| 6   | 0     | 1   | NAG  | O5-C1 | 6.81  | 1.55        | 1.43     |
| 3   | 8     | 1   | NAG  | C2-N2 | -6.81 | 1.35        | 1.46     |
| 7   | j     | 2   | NAG  | C2-N2 | -6.81 | 1.35        | 1.46     |
| 3   | 7     | 1   | NAG  | O5-C1 | 6.81  | 1.55        | 1.43     |
| 7   | 4     | 2   | NAG  | C2-N2 | -6.81 | 1.35        | 1.46     |
| 7   | O     | 1   | NAG  | O5-C1 | 6.81  | 1.55        | 1.43     |
| 3   | R     | 1   | NAG  | O5-C1 | 6.81  | 1.55        | 1.43     |
| 6   | K     | 1   | NAG  | O5-C1 | 6.81  | 1.55        | 1.43     |
| 8   | N     | 2   | NAG  | O5-C1 | 6.80  | 1.55        | 1.43     |
| 3   | S     | 1   | NAG  | C2-N2 | -6.80 | 1.35        | 1.46     |
| 7   | 4     | 1   | NAG  | O5-C1 | 6.80  | 1.55        | 1.43     |
| 3   | n     | 1   | NAG  | C2-N2 | -6.80 | 1.35        | 1.46     |
| 8   | 3     | 2   | NAG  | O5-C1 | 6.79  | 1.55        | 1.43     |
| 7   | j     | 1   | NAG  | O5-C1 | 6.79  | 1.55        | 1.43     |
| 6   | f     | 1   | NAG  | O5-C1 | 6.77  | 1.55        | 1.43     |
| 8   | i     | 2   | NAG  | O5-C1 | 6.77  | 1.55        | 1.43     |
| 3   | 2     | 1   | NAG  | C2-N2 | -6.77 | 1.35        | 1.46     |
| 3   | M     | 1   | NAG  | C2-N2 | -6.76 | 1.35        | 1.46     |
| 3   | h     | 1   | NAG  | C2-N2 | -6.76 | 1.35        | 1.46     |
| 3   | n     | 2   | NAG  | O5-C1 | 6.75  | 1.55        | 1.43     |
| 3   | S     | 2   | NAG  | O5-C1 | 6.74  | 1.55        | 1.43     |
| 3   | I     | 1   | NAG  | O5-C1 | 6.73  | 1.55        | 1.43     |
| 7   | s     | 2   | NAG  | C2-N2 | -6.73 | 1.35        | 1.46     |
| 3   | y     | 1   | NAG  | O5-C1 | 6.73  | 1.55        | 1.43     |
| 8   | 3     | 2   | NAG  | C2-N2 | -6.73 | 1.35        | 1.46     |
| 3   | d     | 1   | NAG  | O5-C1 | 6.72  | 1.55        | 1.43     |
| 8   | i     | 2   | NAG  | C2-N2 | -6.72 | 1.35        | 1.46     |
| 8   | V     | 1   | NAG  | O5-C1 | 6.72  | 1.55        | 1.43     |
| 7   | X     | 2   | NAG  | C2-N2 | -6.71 | 1.35        | 1.46     |
| 3   | 8     | 2   | NAG  | O5-C1 | 6.71  | 1.55        | 1.43     |
| 4   | F     | 1   | NAG  | C2-N2 | -6.70 | 1.35        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | q     | 1   | NAG  | O5-C1 | 6.70  | 1.54        | 1.43     |
| 8   | N     | 2   | NAG  | C2-N2 | -6.70 | 1.35        | 1.46     |
| 4   | a     | 1   | NAG  | C2-N2 | -6.69 | 1.35        | 1.46     |
| 7   | DA    | 2   | NAG  | C2-N2 | -6.69 | 1.35        | 1.46     |
| 8   | BA    | 1   | NAG  | O5-C1 | 6.69  | 1.54        | 1.43     |
| 4   | v     | 1   | NAG  | C2-N2 | -6.69 | 1.35        | 1.46     |
| 5   | c     | 1   | NAG  | O5-C1 | 6.67  | 1.54        | 1.43     |
| 5   | x     | 1   | NAG  | O5-C1 | 6.67  | 1.54        | 1.43     |
| 2   | Y     | 1   | NAG  | O5-C1 | 6.66  | 1.54        | 1.43     |
| 3   | 8     | 1   | NAG  | O5-C1 | 6.66  | 1.54        | 1.43     |
| 3   | CA    | 2   | NAG  | O5-C1 | 6.65  | 1.54        | 1.43     |
| 4   | v     | 2   | NAG  | O5-C1 | 6.65  | 1.54        | 1.43     |
| 5   | H     | 1   | NAG  | O5-C1 | 6.65  | 1.54        | 1.43     |
| 4   | F     | 1   | NAG  | O5-C1 | 6.64  | 1.54        | 1.43     |
| 4   | a     | 2   | NAG  | C2-N2 | -6.64 | 1.35        | 1.46     |
| 4   | a     | 1   | NAG  | O5-C1 | 6.64  | 1.54        | 1.43     |
| 4   | v     | 1   | NAG  | O5-C1 | 6.64  | 1.54        | 1.43     |
| 4   | F     | 2   | NAG  | C2-N2 | -6.63 | 1.35        | 1.46     |
| 3   | W     | 2   | NAG  | O5-C1 | 6.63  | 1.54        | 1.43     |
| 4   | F     | 2   | NAG  | O5-C1 | 6.63  | 1.54        | 1.43     |
| 2   | D     | 1   | NAG  | O5-C1 | 6.62  | 1.54        | 1.43     |
| 4   | v     | 2   | NAG  | C2-N2 | -6.62 | 1.35        | 1.46     |
| 3   | S     | 1   | NAG  | O5-C1 | 6.62  | 1.54        | 1.43     |
| 3   | r     | 2   | NAG  | O5-C1 | 6.62  | 1.54        | 1.43     |
| 4   | a     | 2   | NAG  | O5-C1 | 6.62  | 1.54        | 1.43     |
| 3   | n     | 1   | NAG  | O5-C1 | 6.61  | 1.54        | 1.43     |
| 3   | R     | 2   | NAG  | C2-N2 | -6.60 | 1.35        | 1.46     |
| 2   | t     | 1   | NAG  | O5-C1 | 6.59  | 1.54        | 1.43     |
| 3   | 9     | 2   | NAG  | C2-N2 | -6.59 | 1.35        | 1.46     |
| 3   | m     | 2   | NAG  | C2-N2 | -6.58 | 1.35        | 1.46     |
| 3   | d     | 1   | NAG  | C2-N2 | -6.58 | 1.35        | 1.46     |
| 3   | P     | 1   | NAG  | C2-N2 | -6.58 | 1.35        | 1.46     |
| 3   | T     | 2   | NAG  | C2-N2 | -6.57 | 1.35        | 1.46     |
| 3   | o     | 2   | NAG  | C2-N2 | -6.57 | 1.35        | 1.46     |
| 3   | I     | 1   | NAG  | C2-N2 | -6.56 | 1.35        | 1.46     |
| 3   | 7     | 2   | NAG  | C2-N2 | -6.56 | 1.35        | 1.46     |
| 3   | y     | 1   | NAG  | C2-N2 | -6.55 | 1.35        | 1.46     |
| 3   | 5     | 1   | NAG  | C2-N2 | -6.55 | 1.35        | 1.46     |
| 3   | w     | 1   | NAG  | C2-N2 | -6.55 | 1.35        | 1.46     |
| 8   | N     | 1   | NAG  | O5-C1 | 6.54  | 1.54        | 1.43     |
| 7   | L     | 1   | NAG  | C2-N2 | -6.54 | 1.35        | 1.46     |
| 8   | 3     | 1   | NAG  | O5-C1 | 6.53  | 1.54        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | k     | 1   | NAG  | C2-N2 | -6.53 | 1.35        | 1.46     |
| 7   | l     | 1   | NAG  | C2-N2 | -6.53 | 1.35        | 1.46     |
| 3   | G     | 1   | NAG  | C2-N2 | -6.53 | 1.35        | 1.46     |
| 3   | 6     | 1   | NAG  | C2-N2 | -6.53 | 1.35        | 1.46     |
| 7   | DA    | 1   | NAG  | C2-N2 | -6.52 | 1.35        | 1.46     |
| 7   | X     | 1   | NAG  | C2-N2 | -6.51 | 1.35        | 1.46     |
| 7   | g     | 1   | NAG  | C2-N2 | -6.51 | 1.35        | 1.46     |
| 3   | l     | 1   | NAG  | C2-N2 | -6.51 | 1.35        | 1.46     |
| 3   | Q     | 1   | NAG  | C2-N2 | -6.50 | 1.35        | 1.46     |
| 3   | b     | 1   | NAG  | C2-N2 | -6.50 | 1.35        | 1.46     |
| 8   | i     | 1   | NAG  | O5-C1 | 6.50  | 1.54        | 1.43     |
| 6   | f     | 2   | NAG  | C2-N2 | -6.49 | 1.35        | 1.46     |
| 7   | s     | 1   | NAG  | C2-N2 | -6.49 | 1.35        | 1.46     |
| 6   | K     | 2   | NAG  | C2-N2 | -6.48 | 1.35        | 1.46     |
| 5   | x     | 1   | NAG  | C2-N2 | -6.47 | 1.35        | 1.46     |
| 5   | H     | 1   | NAG  | C2-N2 | -6.46 | 1.35        | 1.46     |
| 6   | 0     | 2   | NAG  | C2-N2 | -6.46 | 1.35        | 1.46     |
| 2   | t     | 1   | NAG  | C2-N2 | -6.45 | 1.35        | 1.46     |
| 5   | c     | 1   | NAG  | C2-N2 | -6.43 | 1.35        | 1.46     |
| 2   | D     | 1   | NAG  | C2-N2 | -6.43 | 1.35        | 1.46     |
| 4   | p     | 1   | NAG  | O5-C1 | 6.42  | 1.54        | 1.43     |
| 4   | U     | 1   | NAG  | O5-C1 | 6.41  | 1.54        | 1.43     |
| 8   | BA    | 1   | NAG  | C2-N2 | -6.39 | 1.35        | 1.46     |
| 2   | Y     | 1   | NAG  | C2-N2 | -6.39 | 1.35        | 1.46     |
| 4   | AA    | 1   | NAG  | O5-C1 | 6.38  | 1.54        | 1.43     |
| 8   | V     | 1   | NAG  | C2-N2 | -6.38 | 1.35        | 1.46     |
| 8   | q     | 1   | NAG  | C2-N2 | -6.38 | 1.35        | 1.46     |
| 3   | o     | 1   | NAG  | C2-N2 | -6.37 | 1.35        | 1.46     |
| 4   | U     | 1   | NAG  | C2-N2 | -6.34 | 1.35        | 1.46     |
| 4   | AA    | 1   | NAG  | C2-N2 | -6.34 | 1.35        | 1.46     |
| 8   | V     | 2   | NAG  | C2-N2 | -6.34 | 1.35        | 1.46     |
| 3   | z     | 1   | NAG  | O5-C1 | 6.33  | 1.54        | 1.43     |
| 4   | p     | 1   | NAG  | C2-N2 | -6.33 | 1.35        | 1.46     |
| 8   | 3     | 1   | NAG  | C2-N2 | -6.32 | 1.35        | 1.46     |
| 8   | N     | 1   | NAG  | C2-N2 | -6.32 | 1.35        | 1.46     |
| 8   | BA    | 2   | NAG  | C2-N2 | -6.31 | 1.35        | 1.46     |
| 3   | J     | 1   | NAG  | O5-C1 | 6.31  | 1.54        | 1.43     |
| 8   | i     | 1   | NAG  | C2-N2 | -6.31 | 1.35        | 1.46     |
| 3   | 9     | 1   | NAG  | C2-N2 | -6.31 | 1.35        | 1.46     |
| 3   | T     | 1   | NAG  | C2-N2 | -6.31 | 1.35        | 1.46     |
| 8   | q     | 2   | NAG  | C2-N2 | -6.30 | 1.35        | 1.46     |
| 6   | f     | 1   | NAG  | C2-N2 | -6.30 | 1.35        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | K     | 1   | NAG  | C2-N2 | -6.29 | 1.35        | 1.46     |
| 3   | e     | 1   | NAG  | O5-C1 | 6.28  | 1.54        | 1.43     |
| 3   | z     | 1   | NAG  | C2-N2 | -6.27 | 1.35        | 1.46     |
| 6   | 0     | 1   | NAG  | C2-N2 | -6.27 | 1.35        | 1.46     |
| 3   | e     | 1   | NAG  | C2-N2 | -6.25 | 1.35        | 1.46     |
| 3   | J     | 1   | NAG  | C2-N2 | -6.24 | 1.35        | 1.46     |
| 3   | r     | 1   | NAG  | O5-C1 | 6.22  | 1.54        | 1.43     |
| 3   | S     | 2   | NAG  | C2-N2 | -6.22 | 1.36        | 1.46     |
| 3   | 8     | 2   | NAG  | C2-N2 | -6.21 | 1.36        | 1.46     |
| 3   | n     | 2   | NAG  | C2-N2 | -6.21 | 1.36        | 1.46     |
| 3   | W     | 1   | NAG  | O5-C1 | 6.21  | 1.54        | 1.43     |
| 3   | 7     | 1   | NAG  | C2-N2 | -6.20 | 1.36        | 1.46     |
| 3   | R     | 1   | NAG  | C2-N2 | -6.20 | 1.36        | 1.46     |
| 3   | m     | 1   | NAG  | C2-N2 | -6.19 | 1.36        | 1.46     |
| 3   | CA    | 1   | NAG  | O5-C1 | 6.17  | 1.54        | 1.43     |
| 3   | G     | 2   | NAG  | C2-N2 | -6.13 | 1.36        | 1.46     |
| 3   | b     | 2   | NAG  | C2-N2 | -6.12 | 1.36        | 1.46     |
| 3   | w     | 2   | NAG  | C2-N2 | -6.10 | 1.36        | 1.46     |
| 3   | 5     | 2   | NAG  | C2-N2 | -6.10 | 1.36        | 1.46     |
| 3   | k     | 2   | NAG  | C2-N2 | -6.09 | 1.36        | 1.46     |
| 3   | P     | 2   | NAG  | C2-N2 | -6.08 | 1.36        | 1.46     |
| 3   | h     | 2   | NAG  | C2-N2 | -6.04 | 1.36        | 1.46     |
| 3   | M     | 2   | NAG  | C2-N2 | -6.03 | 1.36        | 1.46     |
| 3   | 2     | 2   | NAG  | C2-N2 | -5.98 | 1.36        | 1.46     |
| 3   | d     | 2   | NAG  | C2-N2 | -5.94 | 1.36        | 1.46     |
| 3   | I     | 2   | NAG  | C2-N2 | -5.94 | 1.36        | 1.46     |
| 3   | y     | 2   | NAG  | C2-N2 | -5.93 | 1.36        | 1.46     |
| 3   | 6     | 2   | NAG  | C2-N2 | -5.77 | 1.36        | 1.46     |
| 3   | Q     | 2   | NAG  | C2-N2 | -5.77 | 1.36        | 1.46     |
| 3   | l     | 2   | NAG  | C2-N2 | -5.76 | 1.36        | 1.46     |
| 2   | Y     | 2   | NAG  | C2-N2 | -5.75 | 1.36        | 1.46     |
| 2   | D     | 2   | NAG  | C2-N2 | -5.73 | 1.36        | 1.46     |
| 2   | t     | 2   | NAG  | C2-N2 | -5.72 | 1.36        | 1.46     |
| 3   | z     | 2   | NAG  | C2-N2 | -5.61 | 1.37        | 1.46     |
| 3   | J     | 2   | NAG  | C2-N2 | -5.61 | 1.37        | 1.46     |
| 3   | e     | 2   | NAG  | C2-N2 | -5.60 | 1.37        | 1.46     |
| 7   | g     | 2   | NAG  | C2-N2 | -5.59 | 1.37        | 1.46     |
| 7   | L     | 2   | NAG  | C2-N2 | -5.56 | 1.37        | 1.46     |
| 7   | 1     | 2   | NAG  | C2-N2 | -5.55 | 1.37        | 1.46     |
| 3   | Z     | 2   | NAG  | C2-N2 | -4.99 | 1.38        | 1.46     |
| 3   | E     | 2   | NAG  | C2-N2 | -4.98 | 1.38        | 1.46     |
| 3   | u     | 2   | NAG  | C2-N2 | -4.97 | 1.38        | 1.46     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | 0     | 3   | BMA  | O2-C2 | -4.30 | 1.34        | 1.43     |
| 6   | K     | 3   | BMA  | O2-C2 | -4.29 | 1.34        | 1.43     |
| 6   | f     | 3   | BMA  | O2-C2 | -4.23 | 1.34        | 1.43     |
| 8   | q     | 5   | MAN  | O2-C2 | -4.23 | 1.34        | 1.43     |
| 8   | V     | 5   | MAN  | O2-C2 | -4.23 | 1.34        | 1.43     |
| 7   | s     | 3   | BMA  | O2-C2 | -4.21 | 1.34        | 1.43     |
| 7   | X     | 3   | BMA  | O2-C2 | -4.21 | 1.34        | 1.43     |
| 8   | BA    | 5   | MAN  | O2-C2 | -4.21 | 1.34        | 1.43     |
| 7   | DA    | 3   | BMA  | O2-C2 | -4.18 | 1.34        | 1.43     |
| 4   | v     | 4   | MAN  | O2-C2 | -4.18 | 1.34        | 1.43     |
| 4   | F     | 4   | MAN  | O2-C2 | -4.17 | 1.34        | 1.43     |
| 4   | a     | 4   | MAN  | O2-C2 | -4.15 | 1.34        | 1.43     |
| 6   | 0     | 6   | MAN  | O2-C2 | -4.13 | 1.34        | 1.43     |
| 6   | f     | 6   | MAN  | O2-C2 | -4.12 | 1.34        | 1.43     |
| 6   | K     | 6   | MAN  | O2-C2 | -4.11 | 1.34        | 1.43     |
| 7   | 4     | 3   | BMA  | O2-C2 | -4.11 | 1.34        | 1.43     |
| 8   | V     | 3   | BMA  | O2-C2 | -4.10 | 1.34        | 1.43     |
| 8   | q     | 3   | BMA  | O2-C2 | -4.10 | 1.34        | 1.43     |
| 7   | O     | 3   | BMA  | O2-C2 | -4.09 | 1.34        | 1.43     |
| 8   | BA    | 3   | BMA  | O2-C2 | -4.08 | 1.34        | 1.43     |
| 7   | j     | 3   | BMA  | O2-C2 | -4.08 | 1.34        | 1.43     |
| 4   | p     | 4   | MAN  | O2-C2 | -4.07 | 1.34        | 1.43     |
| 4   | U     | 4   | MAN  | O2-C2 | -4.07 | 1.34        | 1.43     |
| 2   | Y     | 3   | BMA  | O2-C2 | -4.06 | 1.34        | 1.43     |
| 4   | AA    | 4   | MAN  | O2-C2 | -4.06 | 1.34        | 1.43     |
| 2   | t     | 6   | MAN  | C4-C5 | 4.05  | 1.61        | 1.53     |
| 8   | 3     | 3   | BMA  | O2-C2 | -4.04 | 1.34        | 1.43     |
| 2   | Y     | 5   | MAN  | C4-C5 | 4.04  | 1.61        | 1.53     |
| 6   | 0     | 8   | MAN  | O5-C1 | 4.04  | 1.50        | 1.43     |
| 2   | t     | 5   | MAN  | C4-C5 | 4.04  | 1.61        | 1.53     |
| 6   | K     | 8   | MAN  | O5-C1 | 4.03  | 1.50        | 1.43     |
| 2   | Y     | 6   | MAN  | C4-C5 | 4.03  | 1.61        | 1.53     |
| 6   | f     | 8   | MAN  | O5-C1 | 4.03  | 1.50        | 1.43     |
| 8   | N     | 3   | BMA  | O2-C2 | -4.03 | 1.34        | 1.43     |
| 8   | i     | 3   | BMA  | O2-C2 | -4.03 | 1.34        | 1.43     |
| 2   | t     | 3   | BMA  | O2-C2 | -4.02 | 1.34        | 1.43     |
| 2   | D     | 6   | MAN  | C4-C5 | 4.02  | 1.61        | 1.53     |
| 2   | D     | 3   | BMA  | O2-C2 | -4.02 | 1.34        | 1.43     |
| 2   | D     | 5   | MAN  | C4-C5 | 4.01  | 1.61        | 1.53     |
| 7   | 1     | 3   | BMA  | O2-C2 | -4.00 | 1.35        | 1.43     |
| 2   | t     | 5   | MAN  | O5-C1 | 4.00  | 1.50        | 1.43     |
| 7   | L     | 3   | BMA  | O2-C2 | -4.00 | 1.35        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 5   | H     | 4   | MAN  | O2-C2 | -4.00 | 1.35        | 1.43     |
| 5   | c     | 4   | MAN  | O2-C2 | -3.99 | 1.35        | 1.43     |
| 7   | g     | 3   | BMA  | O2-C2 | -3.99 | 1.35        | 1.43     |
| 2   | D     | 5   | MAN  | O5-C1 | 3.99  | 1.50        | 1.43     |
| 5   | H     | 3   | BMA  | O2-C2 | -3.99 | 1.35        | 1.43     |
| 5   | c     | 3   | BMA  | O2-C2 | -3.98 | 1.35        | 1.43     |
| 5   | x     | 4   | MAN  | O2-C2 | -3.98 | 1.35        | 1.43     |
| 5   | x     | 3   | BMA  | O2-C2 | -3.98 | 1.35        | 1.43     |
| 8   | 3     | 4   | MAN  | O2-C2 | -3.97 | 1.35        | 1.43     |
| 8   | N     | 4   | MAN  | O2-C2 | -3.97 | 1.35        | 1.43     |
| 8   | i     | 4   | MAN  | O2-C2 | -3.96 | 1.35        | 1.43     |
| 8   | BA    | 4   | MAN  | O2-C2 | -3.96 | 1.35        | 1.43     |
| 4   | a     | 3   | BMA  | O2-C2 | -3.95 | 1.35        | 1.43     |
| 8   | i     | 5   | MAN  | O2-C2 | -3.94 | 1.35        | 1.43     |
| 4   | p     | 3   | BMA  | O2-C2 | -3.94 | 1.35        | 1.43     |
| 8   | N     | 5   | MAN  | O2-C2 | -3.94 | 1.35        | 1.43     |
| 4   | F     | 3   | BMA  | O2-C2 | -3.94 | 1.35        | 1.43     |
| 8   | V     | 4   | MAN  | O2-C2 | -3.94 | 1.35        | 1.43     |
| 4   | v     | 3   | BMA  | O2-C2 | -3.93 | 1.35        | 1.43     |
| 2   | Y     | 5   | MAN  | O5-C1 | 3.93  | 1.50        | 1.43     |
| 6   | f     | 8   | MAN  | O2-C2 | -3.92 | 1.35        | 1.43     |
| 8   | 3     | 5   | MAN  | O2-C2 | -3.92 | 1.35        | 1.43     |
| 8   | q     | 4   | MAN  | O2-C2 | -3.92 | 1.35        | 1.43     |
| 4   | U     | 3   | BMA  | O2-C2 | -3.92 | 1.35        | 1.43     |
| 4   | AA    | 3   | BMA  | O2-C2 | -3.91 | 1.35        | 1.43     |
| 6   | 0     | 8   | MAN  | O2-C2 | -3.91 | 1.35        | 1.43     |
| 6   | K     | 8   | MAN  | O2-C2 | -3.90 | 1.35        | 1.43     |
| 2   | D     | 6   | MAN  | O2-C2 | -3.83 | 1.35        | 1.43     |
| 2   | Y     | 6   | MAN  | O2-C2 | -3.83 | 1.35        | 1.43     |
| 2   | Y     | 5   | MAN  | O2-C2 | -3.82 | 1.35        | 1.43     |
| 2   | D     | 5   | MAN  | O2-C2 | -3.82 | 1.35        | 1.43     |
| 2   | t     | 5   | MAN  | O2-C2 | -3.81 | 1.35        | 1.43     |
| 2   | t     | 6   | MAN  | O2-C2 | -3.78 | 1.35        | 1.43     |
| 7   | 1     | 1   | NAG  | C4-C3 | 3.76  | 1.62        | 1.52     |
| 7   | L     | 1   | NAG  | C4-C3 | 3.74  | 1.62        | 1.52     |
| 7   | g     | 1   | NAG  | C4-C3 | 3.73  | 1.62        | 1.52     |
| 6   | 0     | 7   | MAN  | O2-C2 | -3.71 | 1.35        | 1.43     |
| 6   | 0     | 8   | MAN  | C4-C5 | 3.70  | 1.60        | 1.53     |
| 6   | K     | 7   | MAN  | O2-C2 | -3.70 | 1.35        | 1.43     |
| 6   | f     | 7   | MAN  | O2-C2 | -3.70 | 1.35        | 1.43     |
| 6   | f     | 8   | MAN  | C4-C5 | 3.69  | 1.60        | 1.53     |
| 6   | K     | 8   | MAN  | C4-C5 | 3.69  | 1.60        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 3   | E     | 2   | NAG  | C4-C5 | 3.40  | 1.60        | 1.53     |
| 3   | u     | 2   | NAG  | C4-C5 | 3.40  | 1.60        | 1.53     |
| 3   | Z     | 2   | NAG  | C4-C5 | 3.40  | 1.60        | 1.53     |
| 2   | D     | 6   | MAN  | O5-C1 | 3.40  | 1.49        | 1.43     |
| 2   | t     | 6   | MAN  | O5-C1 | 3.36  | 1.49        | 1.43     |
| 2   | Y     | 6   | MAN  | O5-C1 | 3.36  | 1.49        | 1.43     |
| 7   | g     | 3   | BMA  | O5-C1 | 3.35  | 1.49        | 1.43     |
| 7   | L     | 3   | BMA  | O5-C1 | 3.34  | 1.49        | 1.43     |
| 7   | l     | 3   | BMA  | O5-C1 | 3.31  | 1.49        | 1.43     |
| 3   | u     | 2   | NAG  | C4-C3 | 3.22  | 1.60        | 1.52     |
| 3   | Z     | 2   | NAG  | C4-C3 | 3.21  | 1.60        | 1.52     |
| 8   | 3     | 4   | MAN  | O5-C1 | 3.21  | 1.49        | 1.43     |
| 2   | D     | 2   | NAG  | C4-C3 | 3.20  | 1.60        | 1.52     |
| 3   | E     | 2   | NAG  | C4-C3 | 3.20  | 1.60        | 1.52     |
| 8   | N     | 4   | MAN  | O5-C1 | 3.20  | 1.49        | 1.43     |
| 6   | K     | 4   | MAN  | O2-C2 | -3.20 | 1.36        | 1.43     |
| 8   | i     | 4   | MAN  | O5-C1 | 3.19  | 1.49        | 1.43     |
| 2   | Y     | 2   | NAG  | C4-C3 | 3.19  | 1.60        | 1.52     |
| 6   | f     | 4   | MAN  | O2-C2 | -3.19 | 1.36        | 1.43     |
| 2   | t     | 2   | NAG  | C4-C3 | 3.18  | 1.60        | 1.52     |
| 6   | 0     | 4   | MAN  | O2-C2 | -3.18 | 1.36        | 1.43     |
| 8   | BA    | 4   | MAN  | O5-C1 | 3.17  | 1.49        | 1.43     |
| 2   | t     | 5   | MAN  | O5-C5 | 3.17  | 1.49        | 1.43     |
| 8   | V     | 4   | MAN  | O5-C1 | 3.16  | 1.49        | 1.43     |
| 8   | q     | 4   | MAN  | O5-C1 | 3.15  | 1.49        | 1.43     |
| 2   | D     | 5   | MAN  | O5-C5 | 3.12  | 1.49        | 1.43     |
| 2   | Y     | 5   | MAN  | O5-C5 | 3.12  | 1.49        | 1.43     |
| 2   | t     | 4   | MAN  | O5-C1 | 3.09  | 1.48        | 1.43     |
| 2   | D     | 4   | MAN  | O5-C1 | 3.09  | 1.48        | 1.43     |
| 2   | Y     | 6   | MAN  | O5-C5 | 3.07  | 1.49        | 1.43     |
| 2   | t     | 4   | MAN  | O2-C2 | -3.07 | 1.36        | 1.43     |
| 2   | D     | 6   | MAN  | O5-C5 | 3.07  | 1.49        | 1.43     |
| 2   | Y     | 4   | MAN  | O2-C2 | -3.06 | 1.36        | 1.43     |
| 4   | F     | 4   | MAN  | O5-C1 | 3.05  | 1.48        | 1.43     |
| 6   | f     | 8   | MAN  | O5-C5 | 3.05  | 1.49        | 1.43     |
| 2   | t     | 6   | MAN  | O5-C5 | 3.04  | 1.49        | 1.43     |
| 4   | v     | 4   | MAN  | O5-C1 | 3.04  | 1.48        | 1.43     |
| 4   | a     | 4   | MAN  | O5-C1 | 3.04  | 1.48        | 1.43     |
| 6   | K     | 8   | MAN  | O5-C5 | 3.04  | 1.49        | 1.43     |
| 2   | Y     | 4   | MAN  | O5-C1 | 3.03  | 1.48        | 1.43     |
| 6   | 0     | 8   | MAN  | O5-C5 | 3.03  | 1.49        | 1.43     |
| 2   | D     | 4   | MAN  | O2-C2 | -3.02 | 1.37        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 7   | DA    | 2   | NAG  | C4-C3 | 3.01  | 1.60        | 1.52     |
| 6   | 0     | 6   | MAN  | O5-C1 | 3.00  | 1.48        | 1.43     |
| 6   | f     | 5   | MAN  | O2-C2 | -3.00 | 1.37        | 1.43     |
| 7   | s     | 2   | NAG  | C4-C3 | 3.00  | 1.60        | 1.52     |
| 6   | K     | 5   | MAN  | O2-C2 | -2.99 | 1.37        | 1.43     |
| 7   | X     | 2   | NAG  | C4-C3 | 2.99  | 1.60        | 1.52     |
| 6   | K     | 6   | MAN  | O5-C1 | 2.98  | 1.48        | 1.43     |
| 6   | 0     | 5   | MAN  | O2-C2 | -2.98 | 1.37        | 1.43     |
| 6   | f     | 6   | MAN  | O5-C1 | 2.97  | 1.48        | 1.43     |
| 7   | j     | 3   | BMA  | O5-C1 | 2.90  | 1.48        | 1.43     |
| 7   | O     | 3   | BMA  | O5-C1 | 2.89  | 1.48        | 1.43     |
| 7   | 1     | 2   | NAG  | C4-C5 | 2.86  | 1.59        | 1.53     |
| 7   | L     | 2   | NAG  | C4-C5 | 2.86  | 1.59        | 1.53     |
| 7   | g     | 2   | NAG  | C4-C5 | 2.85  | 1.59        | 1.53     |
| 7   | 4     | 3   | BMA  | O5-C1 | 2.85  | 1.48        | 1.43     |
| 7   | s     | 3   | BMA  | O5-C1 | 2.83  | 1.48        | 1.43     |
| 7   | DA    | 3   | BMA  | O5-C1 | 2.83  | 1.48        | 1.43     |
| 4   | p     | 4   | MAN  | O5-C1 | 2.81  | 1.48        | 1.43     |
| 7   | X     | 3   | BMA  | O5-C1 | 2.80  | 1.48        | 1.43     |
| 4   | U     | 4   | MAN  | O5-C1 | 2.80  | 1.48        | 1.43     |
| 4   | AA    | 4   | MAN  | O5-C1 | 2.80  | 1.48        | 1.43     |
| 8   | q     | 2   | NAG  | C4-C3 | 2.80  | 1.59        | 1.52     |
| 8   | V     | 2   | NAG  | C4-C3 | 2.78  | 1.59        | 1.52     |
| 2   | D     | 2   | NAG  | C4-C5 | 2.77  | 1.58        | 1.53     |
| 2   | Y     | 4   | MAN  | C4-C5 | 2.77  | 1.58        | 1.53     |
| 2   | t     | 6   | MAN  | C1-C2 | 2.76  | 1.58        | 1.52     |
| 8   | BA    | 2   | NAG  | C4-C3 | 2.76  | 1.59        | 1.52     |
| 2   | t     | 2   | NAG  | C4-C5 | 2.75  | 1.58        | 1.53     |
| 2   | Y     | 2   | NAG  | C4-C5 | 2.75  | 1.58        | 1.53     |
| 2   | Y     | 6   | MAN  | C1-C2 | 2.74  | 1.58        | 1.52     |
| 5   | H     | 2   | NAG  | C4-C3 | 2.74  | 1.59        | 1.52     |
| 5   | c     | 2   | NAG  | C4-C3 | 2.74  | 1.59        | 1.52     |
| 2   | D     | 4   | MAN  | C4-C5 | 2.74  | 1.58        | 1.53     |
| 5   | x     | 2   | NAG  | C4-C3 | 2.74  | 1.59        | 1.52     |
| 2   | D     | 6   | MAN  | C1-C2 | 2.74  | 1.58        | 1.52     |
| 2   | t     | 4   | MAN  | C4-C5 | 2.72  | 1.58        | 1.53     |
| 3   | W     | 1   | NAG  | C1-C2 | -2.66 | 1.48        | 1.52     |
| 3   | CA    | 1   | NAG  | C1-C2 | -2.65 | 1.48        | 1.52     |
| 3   | r     | 1   | NAG  | C1-C2 | -2.65 | 1.48        | 1.52     |
| 3   | Q     | 1   | NAG  | C4-C3 | 2.64  | 1.59        | 1.52     |
| 7   | 1     | 2   | NAG  | C4-C3 | 2.64  | 1.59        | 1.52     |
| 7   | L     | 2   | NAG  | C4-C3 | 2.63  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 7   | g     | 2   | NAG  | C4-C3 | 2.63 | 1.59        | 1.52     |
| 3   | 6     | 1   | NAG  | C4-C3 | 2.63 | 1.59        | 1.52     |
| 3   | l     | 1   | NAG  | C4-C3 | 2.63 | 1.59        | 1.52     |
| 3   | E     | 2   | NAG  | C1-C2 | 2.61 | 1.55        | 1.52     |
| 3   | u     | 2   | NAG  | C1-C2 | 2.61 | 1.55        | 1.52     |
| 3   | Z     | 2   | NAG  | C1-C2 | 2.60 | 1.55        | 1.52     |
| 2   | t     | 5   | MAN  | C1-C2 | 2.60 | 1.58        | 1.52     |
| 2   | D     | 5   | MAN  | C1-C2 | 2.59 | 1.58        | 1.52     |
| 2   | Y     | 5   | MAN  | C1-C2 | 2.59 | 1.58        | 1.52     |
| 3   | 8     | 2   | NAG  | C4-C3 | 2.58 | 1.59        | 1.52     |
| 6   | f     | 7   | MAN  | O5-C1 | 2.57 | 1.48        | 1.43     |
| 8   | BA    | 5   | MAN  | O5-C1 | 2.57 | 1.48        | 1.43     |
| 3   | S     | 2   | NAG  | C4-C3 | 2.56 | 1.59        | 1.52     |
| 3   | b     | 2   | NAG  | C4-C3 | 2.55 | 1.59        | 1.52     |
| 6   | 0     | 7   | MAN  | O5-C1 | 2.55 | 1.48        | 1.43     |
| 6   | K     | 7   | MAN  | O5-C1 | 2.55 | 1.48        | 1.43     |
| 3   | G     | 2   | NAG  | C4-C3 | 2.55 | 1.59        | 1.52     |
| 3   | w     | 2   | NAG  | C4-C3 | 2.55 | 1.58        | 1.52     |
| 3   | n     | 2   | NAG  | C4-C3 | 2.54 | 1.58        | 1.52     |
| 5   | c     | 4   | MAN  | O5-C1 | 2.53 | 1.47        | 1.43     |
| 8   | q     | 5   | MAN  | O5-C1 | 2.52 | 1.47        | 1.43     |
| 8   | V     | 5   | MAN  | O5-C1 | 2.52 | 1.47        | 1.43     |
| 2   | D     | 3   | BMA  | O5-C1 | 2.51 | 1.47        | 1.43     |
| 2   | t     | 3   | BMA  | O5-C1 | 2.51 | 1.47        | 1.43     |
| 5   | H     | 4   | MAN  | O5-C1 | 2.51 | 1.47        | 1.43     |
| 8   | V     | 5   | MAN  | C4-C5 | 2.50 | 1.58        | 1.53     |
| 7   | L     | 1   | NAG  | C4-C5 | 2.50 | 1.58        | 1.53     |
| 5   | x     | 4   | MAN  | O5-C1 | 2.49 | 1.47        | 1.43     |
| 4   | F     | 2   | NAG  | C4-C3 | 2.49 | 1.58        | 1.52     |
| 7   | 1     | 1   | NAG  | C4-C5 | 2.49 | 1.58        | 1.53     |
| 8   | 3     | 5   | MAN  | C4-C5 | 2.49 | 1.58        | 1.53     |
| 4   | v     | 2   | NAG  | C4-C3 | 2.49 | 1.58        | 1.52     |
| 7   | g     | 1   | NAG  | C4-C5 | 2.48 | 1.58        | 1.53     |
| 4   | a     | 2   | NAG  | C4-C3 | 2.47 | 1.58        | 1.52     |
| 2   | Y     | 3   | BMA  | O5-C1 | 2.47 | 1.47        | 1.43     |
| 3   | m     | 2   | NAG  | C4-C3 | 2.47 | 1.58        | 1.52     |
| 8   | 3     | 5   | MAN  | O5-C1 | 2.47 | 1.47        | 1.43     |
| 8   | i     | 5   | MAN  | O5-C1 | 2.47 | 1.47        | 1.43     |
| 8   | BA    | 5   | MAN  | C4-C5 | 2.46 | 1.58        | 1.53     |
| 8   | N     | 5   | MAN  | C4-C5 | 2.46 | 1.58        | 1.53     |
| 3   | 7     | 2   | NAG  | C4-C3 | 2.46 | 1.58        | 1.52     |
| 8   | q     | 5   | MAN  | C4-C5 | 2.46 | 1.58        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | R     | 2   | NAG  | C4-C3 | 2.45 | 1.58        | 1.52     |
| 8   | i     | 5   | MAN  | C4-C5 | 2.45 | 1.58        | 1.53     |
| 7   | O     | 2   | NAG  | C4-C3 | 2.45 | 1.58        | 1.52     |
| 3   | e     | 1   | NAG  | C4-C3 | 2.44 | 1.58        | 1.52     |
| 3   | z     | 1   | NAG  | C4-C3 | 2.44 | 1.58        | 1.52     |
| 7   | 4     | 2   | NAG  | C4-C3 | 2.44 | 1.58        | 1.52     |
| 8   | N     | 5   | MAN  | O5-C1 | 2.43 | 1.47        | 1.43     |
| 3   | J     | 1   | NAG  | C4-C3 | 2.43 | 1.58        | 1.52     |
| 4   | AA    | 4   | MAN  | C4-C5 | 2.42 | 1.58        | 1.53     |
| 8   | i     | 2   | NAG  | C4-C3 | 2.42 | 1.58        | 1.52     |
| 7   | j     | 2   | NAG  | C4-C3 | 2.42 | 1.58        | 1.52     |
| 4   | U     | 4   | MAN  | C4-C5 | 2.42 | 1.58        | 1.53     |
| 6   | K     | 1   | NAG  | C4-C3 | 2.41 | 1.58        | 1.52     |
| 8   | i     | 4   | MAN  | C4-C5 | 2.41 | 1.58        | 1.53     |
| 6   | f     | 1   | NAG  | C4-C3 | 2.40 | 1.58        | 1.52     |
| 6   | 0     | 1   | NAG  | C4-C3 | 2.40 | 1.58        | 1.52     |
| 3   | T     | 2   | NAG  | C4-C3 | 2.40 | 1.58        | 1.52     |
| 8   | 3     | 4   | MAN  | C4-C5 | 2.40 | 1.58        | 1.53     |
| 3   | 9     | 2   | NAG  | C4-C3 | 2.40 | 1.58        | 1.52     |
| 4   | p     | 4   | MAN  | C4-C5 | 2.40 | 1.58        | 1.53     |
| 3   | o     | 2   | NAG  | C4-C3 | 2.40 | 1.58        | 1.52     |
| 8   | N     | 4   | MAN  | C4-C5 | 2.40 | 1.58        | 1.53     |
| 6   | K     | 7   | MAN  | C4-C5 | 2.39 | 1.58        | 1.53     |
| 8   | N     | 2   | NAG  | C4-C3 | 2.38 | 1.58        | 1.52     |
| 6   | 0     | 7   | MAN  | C4-C5 | 2.38 | 1.58        | 1.53     |
| 3   | I     | 2   | NAG  | C4-C3 | 2.38 | 1.58        | 1.52     |
| 3   | y     | 2   | NAG  | C4-C3 | 2.38 | 1.58        | 1.52     |
| 3   | d     | 2   | NAG  | C4-C3 | 2.38 | 1.58        | 1.52     |
| 6   | f     | 7   | MAN  | C4-C5 | 2.36 | 1.58        | 1.53     |
| 8   | BA    | 1   | NAG  | C4-C3 | 2.36 | 1.58        | 1.52     |
| 8   | 3     | 2   | NAG  | C4-C3 | 2.36 | 1.58        | 1.52     |
| 2   | t     | 3   | BMA  | C4-C5 | 2.36 | 1.58        | 1.53     |
| 6   | K     | 2   | NAG  | C4-C3 | 2.35 | 1.58        | 1.52     |
| 8   | V     | 4   | MAN  | C4-C5 | 2.34 | 1.58        | 1.53     |
| 2   | D     | 3   | BMA  | C4-C5 | 2.34 | 1.58        | 1.53     |
| 8   | V     | 1   | NAG  | C4-C3 | 2.34 | 1.58        | 1.52     |
| 8   | q     | 4   | MAN  | C4-C5 | 2.34 | 1.58        | 1.53     |
| 6   | f     | 2   | NAG  | C4-C3 | 2.34 | 1.58        | 1.52     |
| 6   | 0     | 2   | NAG  | C4-C3 | 2.34 | 1.58        | 1.52     |
| 8   | q     | 1   | NAG  | C4-C3 | 2.33 | 1.58        | 1.52     |
| 2   | Y     | 3   | BMA  | C4-C5 | 2.33 | 1.58        | 1.53     |
| 3   | 8     | 1   | NAG  | C4-C3 | 2.33 | 1.58        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 3   | k     | 1   | NAG  | C4-C3 | 2.33 | 1.58        | 1.52     |
| 3   | 5     | 1   | NAG  | C4-C3 | 2.33 | 1.58        | 1.52     |
| 2   | Y     | 5   | MAN  | C6-C5 | 2.32 | 1.59        | 1.51     |
| 3   | P     | 1   | NAG  | C4-C3 | 2.32 | 1.58        | 1.52     |
| 3   | E     | 1   | NAG  | C4-C3 | 2.31 | 1.58        | 1.52     |
| 2   | D     | 5   | MAN  | C6-C5 | 2.31 | 1.59        | 1.51     |
| 3   | S     | 1   | NAG  | C4-C3 | 2.31 | 1.58        | 1.52     |
| 3   | n     | 1   | NAG  | C4-C3 | 2.31 | 1.58        | 1.52     |
| 2   | t     | 5   | MAN  | C6-C5 | 2.31 | 1.59        | 1.51     |
| 8   | BA    | 4   | MAN  | C4-C5 | 2.31 | 1.57        | 1.53     |
| 3   | Z     | 1   | NAG  | C4-C3 | 2.31 | 1.58        | 1.52     |
| 3   | 5     | 2   | NAG  | C4-C3 | 2.31 | 1.58        | 1.52     |
| 3   | u     | 1   | NAG  | C4-C3 | 2.30 | 1.58        | 1.52     |
| 4   | U     | 1   | NAG  | C4-C3 | 2.30 | 1.58        | 1.52     |
| 3   | k     | 2   | NAG  | C4-C3 | 2.30 | 1.58        | 1.52     |
| 7   | X     | 1   | NAG  | C4-C3 | 2.30 | 1.58        | 1.52     |
| 3   | P     | 2   | NAG  | C4-C3 | 2.30 | 1.58        | 1.52     |
| 4   | AA    | 1   | NAG  | C4-C3 | 2.29 | 1.58        | 1.52     |
| 3   | M     | 1   | NAG  | C4-C3 | 2.29 | 1.58        | 1.52     |
| 3   | 2     | 1   | NAG  | C4-C3 | 2.29 | 1.58        | 1.52     |
| 4   | p     | 1   | NAG  | C4-C3 | 2.29 | 1.58        | 1.52     |
| 3   | 9     | 1   | NAG  | C4-C3 | 2.29 | 1.58        | 1.52     |
| 3   | h     | 1   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | o     | 1   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | I     | 1   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | z     | 2   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | J     | 2   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 7   | s     | 1   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | T     | 1   | NAG  | C4-C3 | 2.28 | 1.58        | 1.52     |
| 3   | e     | 2   | NAG  | C4-C3 | 2.27 | 1.58        | 1.52     |
| 3   | d     | 1   | NAG  | C4-C3 | 2.27 | 1.58        | 1.52     |
| 7   | DA    | 1   | NAG  | C4-C3 | 2.27 | 1.58        | 1.52     |
| 3   | y     | 1   | NAG  | C4-C3 | 2.27 | 1.58        | 1.52     |
| 3   | m     | 1   | NAG  | C4-C3 | 2.27 | 1.58        | 1.52     |
| 6   | 0     | 8   | MAN  | C6-C5 | 2.27 | 1.59        | 1.51     |
| 2   | Y     | 6   | MAN  | C6-C5 | 2.26 | 1.59        | 1.51     |
| 6   | K     | 8   | MAN  | C6-C5 | 2.26 | 1.59        | 1.51     |
| 6   | f     | 8   | MAN  | C6-C5 | 2.26 | 1.59        | 1.51     |
| 8   | BA    | 4   | MAN  | C6-C5 | 2.26 | 1.59        | 1.51     |
| 8   | q     | 4   | MAN  | C6-C5 | 2.25 | 1.59        | 1.51     |
| 5   | x     | 4   | MAN  | C4-C5 | 2.25 | 1.57        | 1.53     |
| 3   | M     | 2   | NAG  | C4-C3 | 2.25 | 1.58        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2   | D     | 6   | MAN  | C6-C5 | 2.25 | 1.59        | 1.51     |
| 8   | V     | 4   | MAN  | C6-C5 | 2.25 | 1.59        | 1.51     |
| 5   | c     | 4   | MAN  | C4-C5 | 2.25 | 1.57        | 1.53     |
| 5   | H     | 4   | MAN  | C4-C5 | 2.24 | 1.57        | 1.53     |
| 3   | R     | 1   | NAG  | C4-C3 | 2.24 | 1.58        | 1.52     |
| 3   | 7     | 1   | NAG  | C4-C3 | 2.24 | 1.58        | 1.52     |
| 4   | a     | 4   | MAN  | C4-C5 | 2.23 | 1.57        | 1.53     |
| 2   | t     | 6   | MAN  | C6-C5 | 2.23 | 1.59        | 1.51     |
| 3   | 2     | 2   | NAG  | C4-C3 | 2.23 | 1.58        | 1.52     |
| 4   | F     | 4   | MAN  | C4-C5 | 2.23 | 1.57        | 1.53     |
| 4   | v     | 4   | MAN  | C4-C5 | 2.22 | 1.57        | 1.53     |
| 3   | h     | 2   | NAG  | C4-C3 | 2.22 | 1.58        | 1.52     |
| 4   | a     | 3   | BMA  | O5-C1 | 2.22 | 1.47        | 1.43     |
| 4   | F     | 3   | BMA  | O5-C1 | 2.21 | 1.47        | 1.43     |
| 4   | AA    | 2   | NAG  | C4-C3 | 2.21 | 1.58        | 1.52     |
| 4   | v     | 3   | BMA  | O5-C1 | 2.20 | 1.47        | 1.43     |
| 6   | 0     | 4   | MAN  | O5-C1 | 2.20 | 1.47        | 1.43     |
| 4   | p     | 2   | NAG  | C4-C3 | 2.20 | 1.58        | 1.52     |
| 3   | n     | 2   | NAG  | C4-C5 | 2.20 | 1.57        | 1.53     |
| 7   | DA    | 3   | BMA  | C4-C5 | 2.20 | 1.57        | 1.53     |
| 7   | s     | 3   | BMA  | C4-C5 | 2.19 | 1.57        | 1.53     |
| 4   | U     | 2   | NAG  | C4-C3 | 2.19 | 1.58        | 1.52     |
| 3   | S     | 2   | NAG  | C4-C5 | 2.19 | 1.57        | 1.53     |
| 7   | X     | 3   | BMA  | C4-C5 | 2.19 | 1.57        | 1.53     |
| 7   | g     | 3   | BMA  | C4-C5 | 2.18 | 1.57        | 1.53     |
| 3   | 8     | 2   | NAG  | C4-C5 | 2.18 | 1.57        | 1.53     |
| 6   | K     | 4   | MAN  | O5-C1 | 2.18 | 1.47        | 1.43     |
| 6   | f     | 4   | MAN  | O5-C1 | 2.18 | 1.47        | 1.43     |
| 4   | F     | 1   | NAG  | C4-C3 | 2.18 | 1.58        | 1.52     |
| 7   | L     | 3   | BMA  | C4-C5 | 2.17 | 1.57        | 1.53     |
| 6   | 0     | 6   | MAN  | C4-C5 | 2.17 | 1.57        | 1.53     |
| 6   | K     | 6   | MAN  | C4-C5 | 2.17 | 1.57        | 1.53     |
| 4   | v     | 1   | NAG  | C4-C3 | 2.17 | 1.58        | 1.52     |
| 4   | a     | 1   | NAG  | C4-C3 | 2.16 | 1.58        | 1.52     |
| 7   | 1     | 3   | BMA  | C4-C5 | 2.16 | 1.57        | 1.53     |
| 7   | 1     | 3   | BMA  | C6-C5 | 2.16 | 1.59        | 1.51     |
| 7   | L     | 3   | BMA  | C6-C5 | 2.15 | 1.59        | 1.51     |
| 7   | g     | 3   | BMA  | C6-C5 | 2.15 | 1.59        | 1.51     |
| 6   | f     | 6   | MAN  | C4-C5 | 2.14 | 1.57        | 1.53     |
| 2   | Y     | 1   | NAG  | C4-C3 | 2.14 | 1.57        | 1.52     |
| 5   | x     | 1   | NAG  | C4-C3 | 2.13 | 1.57        | 1.52     |
| 6   | f     | 2   | NAG  | C4-C5 | 2.13 | 1.57        | 1.53     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | K     | 7   | MAN  | C6-C5 | 2.13  | 1.59        | 1.51     |
| 2   | t     | 1   | NAG  | C4-C3 | 2.13  | 1.57        | 1.52     |
| 5   | H     | 1   | NAG  | C4-C3 | 2.13  | 1.57        | 1.52     |
| 6   | 0     | 7   | MAN  | C6-C5 | 2.12  | 1.58        | 1.51     |
| 6   | K     | 2   | NAG  | C4-C5 | 2.12  | 1.57        | 1.53     |
| 5   | c     | 1   | NAG  | C4-C3 | 2.12  | 1.57        | 1.52     |
| 5   | H     | 3   | BMA  | C6-C5 | 2.12  | 1.58        | 1.51     |
| 6   | f     | 5   | MAN  | C6-C5 | 2.12  | 1.58        | 1.51     |
| 2   | D     | 1   | NAG  | C4-C3 | 2.11  | 1.57        | 1.52     |
| 3   | CA    | 1   | NAG  | C3-C2 | -2.11 | 1.48        | 1.52     |
| 2   | t     | 4   | MAN  | C6-C5 | 2.11  | 1.58        | 1.51     |
| 3   | G     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 2   | Y     | 4   | MAN  | C6-C5 | 2.10  | 1.58        | 1.51     |
| 7   | 4     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 5   | c     | 3   | BMA  | C6-C5 | 2.10  | 1.58        | 1.51     |
| 7   | O     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 3   | w     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 6   | 0     | 2   | NAG  | C4-C5 | 2.10  | 1.57        | 1.53     |
| 6   | K     | 5   | MAN  | C6-C5 | 2.10  | 1.58        | 1.51     |
| 6   | f     | 7   | MAN  | C6-C5 | 2.10  | 1.58        | 1.51     |
| 7   | j     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 3   | W     | 1   | NAG  | C3-C2 | -2.10 | 1.48        | 1.52     |
| 6   | 0     | 5   | MAN  | C6-C5 | 2.10  | 1.58        | 1.51     |
| 3   | b     | 1   | NAG  | C4-C3 | 2.10  | 1.57        | 1.52     |
| 3   | r     | 1   | NAG  | C3-C2 | -2.10 | 1.48        | 1.52     |
| 5   | x     | 3   | BMA  | C6-C5 | 2.09  | 1.58        | 1.51     |
| 2   | D     | 4   | MAN  | C6-C5 | 2.09  | 1.58        | 1.51     |
| 5   | c     | 3   | BMA  | O5-C1 | 2.09  | 1.47        | 1.43     |
| 5   | H     | 3   | BMA  | O5-C1 | 2.09  | 1.47        | 1.43     |
| 8   | BA    | 2   | NAG  | C4-C5 | 2.09  | 1.57        | 1.53     |
| 3   | 6     | 1   | NAG  | C4-C5 | 2.09  | 1.57        | 1.53     |
| 6   | K     | 8   | MAN  | C1-C2 | 2.08  | 1.57        | 1.52     |
| 5   | x     | 3   | BMA  | O5-C1 | 2.08  | 1.47        | 1.43     |
| 8   | i     | 3   | BMA  | C2-C3 | -2.08 | 1.49        | 1.52     |
| 8   | 3     | 1   | NAG  | C4-C3 | 2.08  | 1.57        | 1.52     |
| 3   | Q     | 1   | NAG  | C4-C5 | 2.08  | 1.57        | 1.53     |
| 6   | f     | 8   | MAN  | C1-C2 | 2.07  | 1.57        | 1.52     |
| 8   | i     | 4   | MAN  | O5-C5 | 2.07  | 1.47        | 1.43     |
| 8   | V     | 2   | NAG  | C4-C5 | 2.07  | 1.57        | 1.53     |
| 6   | 0     | 8   | MAN  | C1-C2 | 2.07  | 1.57        | 1.52     |
| 8   | N     | 3   | BMA  | C2-C3 | -2.07 | 1.49        | 1.52     |
| 3   | Z     | 2   | NAG  | O5-C5 | 2.07  | 1.47        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 8   | N     | 4   | MAN  | C6-C5 | 2.07  | 1.58        | 1.51     |
| 8   | 3     | 3   | BMA  | C2-C3 | -2.07 | 1.49        | 1.52     |
| 3   | I     | 2   | NAG  | C4-C5 | 2.07  | 1.57        | 1.53     |
| 3   | l     | 1   | NAG  | C4-C5 | 2.07  | 1.57        | 1.53     |
| 8   | i     | 4   | MAN  | C6-C5 | 2.06  | 1.58        | 1.51     |
| 3   | d     | 2   | NAG  | C4-C5 | 2.06  | 1.57        | 1.53     |
| 8   | N     | 1   | NAG  | C4-C3 | 2.06  | 1.57        | 1.52     |
| 3   | y     | 2   | NAG  | C4-C5 | 2.06  | 1.57        | 1.53     |
| 8   | 3     | 4   | MAN  | C6-C5 | 2.06  | 1.58        | 1.51     |
| 8   | q     | 2   | NAG  | C4-C5 | 2.06  | 1.57        | 1.53     |
| 8   | i     | 1   | NAG  | C4-C3 | 2.05  | 1.57        | 1.52     |
| 4   | a     | 3   | BMA  | C6-C5 | 2.05  | 1.58        | 1.51     |
| 8   | BA    | 3   | BMA  | C6-C5 | 2.05  | 1.58        | 1.51     |
| 7   | j     | 2   | NAG  | C4-C5 | 2.05  | 1.57        | 1.53     |
| 8   | q     | 3   | BMA  | C6-C5 | 2.05  | 1.58        | 1.51     |
| 6   | f     | 5   | MAN  | O5-C1 | 2.05  | 1.47        | 1.43     |
| 6   | K     | 5   | MAN  | O5-C1 | 2.05  | 1.47        | 1.43     |
| 8   | V     | 3   | BMA  | C6-C5 | 2.05  | 1.58        | 1.51     |
| 8   | N     | 4   | MAN  | O5-C5 | 2.04  | 1.47        | 1.43     |
| 4   | F     | 3   | BMA  | C6-C5 | 2.04  | 1.58        | 1.51     |
| 8   | 3     | 4   | MAN  | O5-C5 | 2.04  | 1.47        | 1.43     |
| 7   | O     | 2   | NAG  | C4-C5 | 2.04  | 1.57        | 1.53     |
| 2   | t     | 3   | BMA  | C6-C5 | 2.04  | 1.58        | 1.51     |
| 7   | 4     | 2   | NAG  | C4-C5 | 2.04  | 1.57        | 1.53     |
| 8   | i     | 5   | MAN  | C6-C5 | 2.04  | 1.58        | 1.51     |
| 3   | k     | 2   | NAG  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 3   | E     | 2   | NAG  | O5-C5 | 2.03  | 1.47        | 1.43     |
| 7   | O     | 3   | BMA  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 8   | q     | 5   | MAN  | C6-C5 | 2.03  | 1.58        | 1.51     |
| 3   | 5     | 2   | NAG  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 7   | j     | 3   | BMA  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 4   | v     | 3   | BMA  | C6-C5 | 2.03  | 1.58        | 1.51     |
| 8   | N     | 5   | MAN  | C6-C5 | 2.03  | 1.58        | 1.51     |
| 2   | D     | 3   | BMA  | C6-C5 | 2.03  | 1.58        | 1.51     |
| 7   | 1     | 3   | BMA  | O5-C5 | 2.03  | 1.47        | 1.43     |
| 3   | P     | 2   | NAG  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 3   | u     | 2   | NAG  | O5-C5 | 2.03  | 1.47        | 1.43     |
| 7   | 4     | 3   | BMA  | C4-C5 | 2.03  | 1.57        | 1.53     |
| 7   | L     | 3   | BMA  | O5-C5 | 2.02  | 1.47        | 1.43     |
| 8   | N     | 3   | BMA  | C6-C5 | 2.02  | 1.58        | 1.51     |
| 6   | 0     | 5   | MAN  | O5-C1 | 2.02  | 1.47        | 1.43     |
| 7   | g     | 3   | BMA  | O5-C5 | 2.01  | 1.47        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 6   | K     | 3   | BMA  | C4-C5 | 2.01  | 1.57        | 1.53     |
| 8   | BA    | 5   | MAN  | C6-C5 | 2.01  | 1.58        | 1.51     |
| 6   | f     | 3   | BMA  | C4-C5 | 2.01  | 1.57        | 1.53     |
| 8   | 3     | 5   | MAN  | C6-C5 | 2.01  | 1.58        | 1.51     |
| 8   | V     | 5   | MAN  | C6-C5 | 2.01  | 1.58        | 1.51     |
| 2   | Y     | 3   | BMA  | C6-C5 | 2.01  | 1.58        | 1.51     |
| 4   | U     | 3   | BMA  | O5-C1 | 2.01  | 1.47        | 1.43     |
| 8   | 3     | 3   | BMA  | C6-C5 | 2.00  | 1.58        | 1.51     |
| 8   | BA    | 3   | BMA  | C2-C3 | -2.00 | 1.49        | 1.52     |
| 6   | 0     | 3   | BMA  | C4-C5 | 2.00  | 1.57        | 1.53     |
| 8   | q     | 3   | BMA  | C2-C3 | -2.00 | 1.49        | 1.52     |
| 8   | i     | 3   | BMA  | C6-C5 | 2.00  | 1.58        | 1.51     |
| 3   | o     | 2   | NAG  | C4-C5 | 2.00  | 1.57        | 1.53     |

All (1074) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 6   | 0     | 4   | MAN  | O3-C3-C2 | 20.43  | 151.74      | 110.05   |
| 6   | f     | 4   | MAN  | O3-C3-C2 | 20.42  | 151.73      | 110.05   |
| 6   | K     | 4   | MAN  | O3-C3-C2 | 20.41  | 151.70      | 110.05   |
| 4   | v     | 1   | NAG  | C1-C2-N2 | 20.35  | 142.51      | 110.43   |
| 4   | F     | 1   | NAG  | C1-C2-N2 | 20.35  | 142.50      | 110.43   |
| 4   | a     | 1   | NAG  | C1-C2-N2 | 20.34  | 142.49      | 110.43   |
| 3   | e     | 1   | NAG  | O5-C5-C6 | -18.70 | 71.26       | 107.66   |
| 3   | z     | 1   | NAG  | O5-C5-C6 | -18.70 | 71.27       | 107.66   |
| 3   | J     | 1   | NAG  | O5-C5-C6 | -18.70 | 71.27       | 107.66   |
| 7   | L     | 1   | NAG  | O4-C4-C3 | -17.40 | 69.36       | 110.38   |
| 7   | g     | 1   | NAG  | O4-C4-C3 | -17.40 | 69.37       | 110.38   |
| 7   | 1     | 1   | NAG  | O4-C4-C3 | -17.39 | 69.37       | 110.38   |
| 6   | f     | 4   | MAN  | O3-C3-C4 | -16.91 | 70.52       | 110.38   |
| 6   | 0     | 4   | MAN  | O3-C3-C4 | -16.91 | 70.53       | 110.38   |
| 6   | K     | 4   | MAN  | O3-C3-C4 | -16.90 | 70.54       | 110.38   |
| 4   | F     | 2   | NAG  | O5-C5-C6 | -16.82 | 74.93       | 107.66   |
| 4   | a     | 2   | NAG  | O5-C5-C6 | -16.82 | 74.94       | 107.66   |
| 4   | v     | 2   | NAG  | O5-C5-C6 | -16.80 | 74.97       | 107.66   |
| 8   | i     | 2   | NAG  | O5-C5-C6 | -16.71 | 75.13       | 107.66   |
| 8   | N     | 2   | NAG  | O5-C5-C6 | -16.71 | 75.14       | 107.66   |
| 8   | 3     | 2   | NAG  | O5-C5-C6 | -16.71 | 75.15       | 107.66   |
| 3   | W     | 1   | NAG  | O5-C5-C6 | -16.21 | 76.11       | 107.66   |
| 3   | r     | 1   | NAG  | O5-C5-C6 | -16.21 | 76.12       | 107.66   |
| 3   | CA    | 1   | NAG  | O5-C5-C6 | -16.21 | 76.12       | 107.66   |
| 7   | s     | 2   | NAG  | O5-C5-C6 | -16.16 | 76.21       | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 7   | DA    | 2   | NAG  | O5-C5-C6 | -16.16 | 76.21       | 107.66   |
| 7   | X     | 2   | NAG  | O5-C5-C6 | -16.15 | 76.23       | 107.66   |
| 4   | p     | 1   | NAG  | O5-C5-C6 | -15.85 | 76.82       | 107.66   |
| 4   | U     | 1   | NAG  | O5-C5-C6 | -15.84 | 76.83       | 107.66   |
| 4   | AA    | 1   | NAG  | O5-C5-C6 | -15.82 | 76.86       | 107.66   |
| 3   | I     | 1   | NAG  | O5-C5-C6 | -14.99 | 78.48       | 107.66   |
| 3   | d     | 1   | NAG  | O5-C5-C6 | -14.99 | 78.49       | 107.66   |
| 3   | y     | 1   | NAG  | O5-C5-C6 | -14.98 | 78.52       | 107.66   |
| 3   | W     | 1   | NAG  | C1-C2-N2 | 14.87  | 133.87      | 110.43   |
| 3   | r     | 1   | NAG  | C1-C2-N2 | 14.87  | 133.86      | 110.43   |
| 3   | CA    | 1   | NAG  | C1-C2-N2 | 14.86  | 133.85      | 110.43   |
| 2   | Y     | 2   | NAG  | O5-C5-C6 | -14.85 | 78.77       | 107.66   |
| 2   | D     | 2   | NAG  | O5-C5-C6 | -14.84 | 78.78       | 107.66   |
| 2   | t     | 2   | NAG  | O5-C5-C6 | -14.84 | 78.79       | 107.66   |
| 4   | v     | 2   | NAG  | C6-C5-C4 | 14.73  | 149.18      | 113.02   |
| 4   | F     | 2   | NAG  | C6-C5-C4 | 14.72  | 149.17      | 113.02   |
| 4   | a     | 2   | NAG  | C6-C5-C4 | 14.72  | 149.16      | 113.02   |
| 3   | w     | 2   | NAG  | O5-C5-C6 | -13.25 | 81.87       | 107.66   |
| 3   | G     | 2   | NAG  | O5-C5-C6 | -13.24 | 81.90       | 107.66   |
| 3   | b     | 2   | NAG  | O5-C5-C6 | -13.23 | 81.91       | 107.66   |
| 6   | 0     | 3   | BMA  | O3-C3-C2 | 13.16  | 136.92      | 110.05   |
| 6   | K     | 3   | BMA  | O3-C3-C2 | 13.14  | 136.87      | 110.05   |
| 6   | f     | 3   | BMA  | O3-C3-C2 | 13.13  | 136.85      | 110.05   |
| 3   | M     | 1   | NAG  | O5-C5-C6 | -12.85 | 82.66       | 107.66   |
| 3   | 2     | 1   | NAG  | O5-C5-C6 | -12.85 | 82.66       | 107.66   |
| 3   | h     | 1   | NAG  | O5-C5-C6 | -12.84 | 82.67       | 107.66   |
| 3   | 8     | 1   | NAG  | O4-C4-C3 | -12.79 | 80.22       | 110.38   |
| 3   | n     | 1   | NAG  | O4-C4-C3 | -12.79 | 80.22       | 110.38   |
| 3   | S     | 1   | NAG  | O4-C4-C3 | -12.79 | 80.23       | 110.38   |
| 6   | f     | 7   | MAN  | O3-C3-C2 | -12.59 | 84.36       | 110.05   |
| 6   | K     | 7   | MAN  | O3-C3-C2 | -12.59 | 84.37       | 110.05   |
| 6   | 0     | 7   | MAN  | O3-C3-C2 | -12.58 | 84.38       | 110.05   |
| 4   | AA    | 3   | BMA  | O3-C3-C2 | -12.58 | 84.39       | 110.05   |
| 4   | U     | 3   | BMA  | O3-C3-C2 | -12.57 | 84.40       | 110.05   |
| 4   | p     | 3   | BMA  | O3-C3-C2 | -12.57 | 84.40       | 110.05   |
| 6   | K     | 4   | MAN  | O5-C5-C6 | -12.45 | 83.44       | 107.66   |
| 6   | f     | 4   | MAN  | O5-C5-C6 | -12.44 | 83.44       | 107.66   |
| 6   | 0     | 4   | MAN  | O5-C5-C6 | -12.43 | 83.46       | 107.66   |
| 6   | f     | 7   | MAN  | O5-C5-C6 | -12.11 | 84.10       | 107.66   |
| 6   | 0     | 7   | MAN  | O5-C5-C6 | -12.10 | 84.12       | 107.66   |
| 6   | K     | 7   | MAN  | O5-C5-C6 | -12.09 | 84.12       | 107.66   |
| 3   | T     | 1   | NAG  | O5-C5-C6 | -11.92 | 84.47       | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 3   | 9     | 1   | NAG  | O5-C5-C6 | -11.91 | 84.47       | 107.66   |
| 3   | o     | 1   | NAG  | O5-C5-C6 | -11.90 | 84.50       | 107.66   |
| 6   | f     | 5   | MAN  | O5-C5-C6 | -11.90 | 84.51       | 107.66   |
| 6   | K     | 5   | MAN  | O5-C5-C6 | -11.89 | 84.52       | 107.66   |
| 6   | 0     | 5   | MAN  | O5-C5-C6 | -11.89 | 84.53       | 107.66   |
| 8   | N     | 2   | NAG  | C6-C5-C4 | 11.78  | 141.94      | 113.02   |
| 8   | 3     | 2   | NAG  | C6-C5-C4 | 11.78  | 141.94      | 113.02   |
| 8   | i     | 2   | NAG  | C6-C5-C4 | 11.78  | 141.94      | 113.02   |
| 5   | c     | 2   | NAG  | O5-C5-C6 | -11.61 | 85.07       | 107.66   |
| 5   | H     | 2   | NAG  | O5-C5-C6 | -11.60 | 85.08       | 107.66   |
| 5   | x     | 2   | NAG  | O5-C5-C6 | -11.60 | 85.09       | 107.66   |
| 6   | K     | 3   | BMA  | C6-C5-C4 | 11.52  | 141.30      | 113.02   |
| 6   | 0     | 3   | BMA  | C6-C5-C4 | 11.51  | 141.29      | 113.02   |
| 6   | f     | 3   | BMA  | C6-C5-C4 | 11.51  | 141.28      | 113.02   |
| 3   | Q     | 1   | NAG  | O4-C4-C3 | 11.33  | 137.08      | 110.38   |
| 3   | l     | 1   | NAG  | O4-C4-C3 | 11.32  | 137.07      | 110.38   |
| 3   | 6     | 1   | NAG  | O4-C4-C3 | 11.32  | 137.06      | 110.38   |
| 7   | DA    | 2   | NAG  | O4-C4-C3 | 11.32  | 137.06      | 110.38   |
| 7   | X     | 2   | NAG  | O4-C4-C3 | 11.31  | 137.03      | 110.38   |
| 7   | s     | 2   | NAG  | O4-C4-C3 | 11.30  | 137.01      | 110.38   |
| 4   | a     | 2   | NAG  | O3-C3-C2 | -11.26 | 86.02       | 109.40   |
| 4   | v     | 2   | NAG  | C1-C2-N2 | -11.25 | 92.71       | 110.43   |
| 4   | F     | 2   | NAG  | O3-C3-C2 | -11.24 | 86.04       | 109.40   |
| 4   | v     | 2   | NAG  | O3-C3-C2 | -11.24 | 86.05       | 109.40   |
| 8   | BA    | 2   | NAG  | C1-C2-N2 | -11.24 | 92.72       | 110.43   |
| 8   | V     | 2   | NAG  | C1-C2-N2 | -11.24 | 92.72       | 110.43   |
| 4   | F     | 2   | NAG  | C1-C2-N2 | -11.23 | 92.73       | 110.43   |
| 8   | q     | 2   | NAG  | C1-C2-N2 | -11.23 | 92.74       | 110.43   |
| 4   | a     | 2   | NAG  | C1-C2-N2 | -11.23 | 92.74       | 110.43   |
| 6   | f     | 1   | NAG  | C6-C5-C4 | 11.16  | 140.42      | 113.02   |
| 7   | s     | 2   | NAG  | C1-C2-N2 | -11.15 | 92.86       | 110.43   |
| 6   | K     | 1   | NAG  | C6-C5-C4 | 11.15  | 140.40      | 113.02   |
| 7   | X     | 2   | NAG  | C1-C2-N2 | -11.15 | 92.86       | 110.43   |
| 6   | 0     | 1   | NAG  | C6-C5-C4 | 11.14  | 140.38      | 113.02   |
| 7   | DA    | 2   | NAG  | C1-C2-N2 | -11.14 | 92.88       | 110.43   |
| 3   | l     | 1   | NAG  | O3-C3-C2 | -11.09 | 86.37       | 109.40   |
| 3   | 6     | 1   | NAG  | O3-C3-C2 | -11.08 | 86.39       | 109.40   |
| 3   | Q     | 1   | NAG  | O3-C3-C2 | -11.07 | 86.41       | 109.40   |
| 7   | s     | 1   | NAG  | O4-C4-C3 | -11.06 | 84.30       | 110.38   |
| 7   | X     | 1   | NAG  | O4-C4-C3 | -11.06 | 84.31       | 110.38   |
| 7   | DA    | 1   | NAG  | O4-C4-C3 | -11.05 | 84.33       | 110.38   |
| 8   | BA    | 2   | NAG  | O4-C4-C3 | 10.93  | 136.13      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|--------|-------------|----------|
| 8   | V     | 2   | NAG  | O4-C4-C3 | 10.91  | 136.09      | 110.38   |
| 8   | q     | 2   | NAG  | O4-C4-C3 | 10.90  | 136.07      | 110.38   |
| 3   | 9     | 1   | NAG  | C6-C5-C4 | 10.77  | 139.46      | 113.02   |
| 3   | T     | 1   | NAG  | C6-C5-C4 | 10.76  | 139.45      | 113.02   |
| 3   | o     | 1   | NAG  | C6-C5-C4 | 10.74  | 139.40      | 113.02   |
| 8   | q     | 2   | NAG  | O3-C3-C2 | -10.59 | 87.40       | 109.40   |
| 8   | BA    | 2   | NAG  | O3-C3-C2 | -10.59 | 87.41       | 109.40   |
| 8   | V     | 2   | NAG  | O3-C3-C2 | -10.58 | 87.42       | 109.40   |
| 6   | f     | 2   | NAG  | O4-C4-C3 | 10.55  | 135.25      | 110.38   |
| 6   | K     | 2   | NAG  | O4-C4-C3 | 10.54  | 135.23      | 110.38   |
| 6   | 0     | 2   | NAG  | O4-C4-C3 | 10.52  | 135.18      | 110.38   |
| 2   | t     | 4   | MAN  | O5-C5-C6 | -10.51 | 87.20       | 107.66   |
| 3   | Z     | 2   | NAG  | O5-C5-C6 | -10.51 | 87.21       | 107.66   |
| 3   | E     | 2   | NAG  | O5-C5-C6 | -10.50 | 87.23       | 107.66   |
| 8   | BA    | 5   | MAN  | O5-C5-C6 | -10.50 | 87.23       | 107.66   |
| 2   | D     | 4   | MAN  | O5-C5-C6 | -10.49 | 87.25       | 107.66   |
| 2   | Y     | 4   | MAN  | O5-C5-C6 | -10.48 | 87.26       | 107.66   |
| 8   | q     | 5   | MAN  | O5-C5-C6 | -10.48 | 87.26       | 107.66   |
| 3   | u     | 2   | NAG  | O5-C5-C6 | -10.48 | 87.27       | 107.66   |
| 8   | V     | 5   | MAN  | O5-C5-C6 | -10.47 | 87.28       | 107.66   |
| 5   | c     | 4   | MAN  | O5-C5-C6 | -10.40 | 87.43       | 107.66   |
| 5   | H     | 4   | MAN  | O5-C5-C6 | -10.39 | 87.43       | 107.66   |
| 3   | G     | 2   | NAG  | C6-C5-C4 | 10.38  | 138.51      | 113.02   |
| 3   | w     | 2   | NAG  | C6-C5-C4 | 10.38  | 138.50      | 113.02   |
| 5   | x     | 4   | MAN  | O5-C5-C6 | -10.38 | 87.47       | 107.66   |
| 3   | b     | 2   | NAG  | C6-C5-C4 | 10.37  | 138.49      | 113.02   |
| 4   | U     | 2   | NAG  | O5-C5-C6 | -10.22 | 87.76       | 107.66   |
| 4   | AA    | 2   | NAG  | O5-C5-C6 | -10.22 | 87.77       | 107.66   |
| 4   | p     | 2   | NAG  | O5-C5-C6 | -10.22 | 87.77       | 107.66   |
| 8   | q     | 1   | NAG  | O4-C4-C3 | -10.19 | 86.35       | 110.38   |
| 8   | V     | 1   | NAG  | O4-C4-C3 | -10.19 | 86.36       | 110.38   |
| 8   | BA    | 1   | NAG  | O4-C4-C3 | -10.18 | 86.38       | 110.38   |
| 4   | a     | 2   | NAG  | O4-C4-C3 | 10.14  | 134.28      | 110.38   |
| 4   | v     | 2   | NAG  | O4-C4-C3 | 10.13  | 134.26      | 110.38   |
| 8   | q     | 3   | BMA  | O2-C2-C3 | 10.13  | 131.14      | 110.15   |
| 4   | F     | 2   | NAG  | O4-C4-C3 | 10.13  | 134.25      | 110.38   |
| 8   | BA    | 3   | BMA  | O2-C2-C3 | 10.13  | 131.12      | 110.15   |
| 8   | V     | 3   | BMA  | O2-C2-C3 | 10.12  | 131.12      | 110.15   |
| 3   | R     | 1   | NAG  | C6-C5-C4 | 10.01  | 137.60      | 113.02   |
| 8   | i     | 2   | NAG  | C1-C2-N2 | -10.00 | 94.67       | 110.43   |
| 8   | N     | 2   | NAG  | C1-C2-N2 | -10.00 | 94.68       | 110.43   |
| 3   | m     | 1   | NAG  | C6-C5-C4 | 10.00  | 137.57      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | 3     | 2   | NAG  | C1-C2-N2 | -9.99 | 94.68       | 110.43   |
| 3   | 7     | 1   | NAG  | C6-C5-C4 | 9.99  | 137.55      | 113.02   |
| 2   | Y     | 2   | NAG  | O4-C4-C3 | -9.98 | 86.84       | 110.38   |
| 4   | U     | 1   | NAG  | O4-C4-C3 | -9.98 | 86.85       | 110.38   |
| 2   | D     | 2   | NAG  | O4-C4-C3 | -9.98 | 86.86       | 110.38   |
| 4   | p     | 1   | NAG  | O4-C4-C3 | -9.98 | 86.86       | 110.38   |
| 4   | AA    | 1   | NAG  | O4-C4-C3 | -9.98 | 86.86       | 110.38   |
| 7   | 4     | 2   | NAG  | O4-C4-C3 | 9.97  | 133.88      | 110.38   |
| 3   | R     | 2   | NAG  | O5-C5-C6 | -9.97 | 88.25       | 107.66   |
| 3   | 7     | 2   | NAG  | O5-C5-C6 | -9.97 | 88.26       | 107.66   |
| 2   | t     | 2   | NAG  | O4-C4-C3 | -9.97 | 86.88       | 110.38   |
| 7   | DA    | 1   | NAG  | O3-C3-C2 | -9.97 | 88.70       | 109.40   |
| 3   | m     | 2   | NAG  | O5-C5-C6 | -9.96 | 88.27       | 107.66   |
| 7   | s     | 1   | NAG  | O3-C3-C2 | -9.96 | 88.70       | 109.40   |
| 7   | X     | 1   | NAG  | O3-C3-C2 | -9.96 | 88.71       | 109.40   |
| 7   | O     | 2   | NAG  | O4-C4-C3 | 9.96  | 133.85      | 110.38   |
| 7   | j     | 2   | NAG  | O4-C4-C3 | 9.95  | 133.83      | 110.38   |
| 6   | f     | 3   | BMA  | O5-C5-C6 | -9.89 | 88.40       | 107.66   |
| 6   | K     | 3   | BMA  | O5-C5-C6 | -9.89 | 88.42       | 107.66   |
| 6   | 0     | 3   | BMA  | O5-C5-C6 | -9.88 | 88.43       | 107.66   |
| 2   | Y     | 1   | NAG  | O5-C5-C6 | -9.85 | 88.49       | 107.66   |
| 2   | D     | 1   | NAG  | O5-C5-C6 | -9.85 | 88.49       | 107.66   |
| 2   | t     | 1   | NAG  | O5-C5-C6 | -9.84 | 88.50       | 107.66   |
| 5   | c     | 3   | BMA  | O3-C3-C4 | -9.79 | 87.29       | 110.38   |
| 5   | x     | 3   | BMA  | O3-C3-C4 | -9.78 | 87.31       | 110.38   |
| 5   | H     | 3   | BMA  | O3-C3-C4 | -9.78 | 87.31       | 110.38   |
| 3   | u     | 1   | NAG  | O5-C5-C6 | -9.62 | 88.95       | 107.66   |
| 3   | Z     | 1   | NAG  | O5-C5-C6 | -9.61 | 88.96       | 107.66   |
| 3   | E     | 1   | NAG  | O5-C5-C6 | -9.61 | 88.97       | 107.66   |
| 3   | Z     | 1   | NAG  | O4-C4-C3 | 9.54  | 132.88      | 110.38   |
| 3   | u     | 1   | NAG  | O4-C4-C3 | 9.54  | 132.86      | 110.38   |
| 3   | E     | 1   | NAG  | O4-C4-C3 | 9.52  | 132.83      | 110.38   |
| 8   | N     | 2   | NAG  | O4-C4-C3 | -9.51 | 87.97       | 110.38   |
| 8   | i     | 2   | NAG  | O4-C4-C3 | -9.50 | 87.97       | 110.38   |
| 8   | 3     | 2   | NAG  | O4-C4-C3 | -9.50 | 87.98       | 110.38   |
| 3   | 5     | 1   | NAG  | O4-C4-C3 | -9.49 | 88.00       | 110.38   |
| 3   | k     | 1   | NAG  | O4-C4-C3 | -9.49 | 88.00       | 110.38   |
| 3   | P     | 1   | NAG  | O4-C4-C3 | -9.49 | 88.00       | 110.38   |
| 6   | K     | 8   | MAN  | O5-C5-C6 | -9.44 | 89.30       | 107.66   |
| 6   | f     | 8   | MAN  | O5-C5-C6 | -9.43 | 89.30       | 107.66   |
| 6   | 0     | 8   | MAN  | O5-C5-C6 | -9.43 | 89.31       | 107.66   |
| 8   | q     | 2   | NAG  | O5-C5-C6 | -9.40 | 89.36       | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | V     | 2   | NAG  | O5-C5-C6 | -9.39 | 89.39       | 107.66   |
| 8   | BA    | 2   | NAG  | O5-C5-C6 | -9.39 | 89.39       | 107.66   |
| 7   | 1     | 1   | NAG  | O5-C5-C6 | -9.38 | 89.40       | 107.66   |
| 7   | L     | 1   | NAG  | O5-C5-C6 | -9.38 | 89.41       | 107.66   |
| 7   | g     | 1   | NAG  | O5-C5-C6 | -9.37 | 89.42       | 107.66   |
| 5   | H     | 2   | NAG  | O3-C3-C4 | 9.27  | 132.22      | 110.38   |
| 5   | x     | 2   | NAG  | O3-C3-C4 | 9.26  | 132.21      | 110.38   |
| 5   | c     | 2   | NAG  | O3-C3-C4 | 9.26  | 132.19      | 110.38   |
| 5   | c     | 1   | NAG  | O3-C3-C2 | -9.14 | 90.42       | 109.40   |
| 5   | H     | 1   | NAG  | O3-C3-C2 | -9.14 | 90.42       | 109.40   |
| 5   | x     | 1   | NAG  | O3-C3-C2 | -9.13 | 90.43       | 109.40   |
| 3   | m     | 1   | NAG  | O5-C5-C6 | -9.12 | 89.92       | 107.66   |
| 3   | R     | 1   | NAG  | O5-C5-C6 | -9.11 | 89.93       | 107.66   |
| 3   | 7     | 1   | NAG  | O5-C5-C6 | -9.11 | 89.94       | 107.66   |
| 8   | q     | 1   | NAG  | C6-C5-C4 | 9.10  | 135.36      | 113.02   |
| 8   | V     | 1   | NAG  | C6-C5-C4 | 9.10  | 135.36      | 113.02   |
| 8   | BA    | 1   | NAG  | C6-C5-C4 | 9.10  | 135.36      | 113.02   |
| 7   | s     | 3   | BMA  | O2-C2-C3 | 9.05  | 128.89      | 110.15   |
| 7   | X     | 3   | BMA  | O2-C2-C3 | 9.03  | 128.86      | 110.15   |
| 7   | DA    | 3   | BMA  | O2-C2-C3 | 9.02  | 128.84      | 110.15   |
| 6   | f     | 6   | MAN  | O5-C5-C6 | -8.87 | 90.40       | 107.66   |
| 6   | 0     | 6   | MAN  | O5-C5-C6 | -8.86 | 90.42       | 107.66   |
| 6   | K     | 6   | MAN  | O5-C5-C6 | -8.85 | 90.43       | 107.66   |
| 8   | 3     | 1   | NAG  | O5-C5-C6 | -8.77 | 90.60       | 107.66   |
| 8   | N     | 1   | NAG  | O5-C5-C6 | -8.76 | 90.62       | 107.66   |
| 8   | i     | 1   | NAG  | O5-C5-C6 | -8.75 | 90.64       | 107.66   |
| 7   | O     | 3   | BMA  | O5-C5-C6 | -8.64 | 90.86       | 107.66   |
| 7   | j     | 3   | BMA  | O5-C5-C6 | -8.63 | 90.86       | 107.66   |
| 7   | 4     | 3   | BMA  | O5-C5-C6 | -8.62 | 90.88       | 107.66   |
| 2   | Y     | 6   | MAN  | O5-C5-C6 | -8.57 | 90.99       | 107.66   |
| 2   | D     | 6   | MAN  | O5-C5-C6 | -8.56 | 91.00       | 107.66   |
| 2   | t     | 6   | MAN  | O5-C5-C6 | -8.54 | 91.04       | 107.66   |
| 4   | AA    | 3   | BMA  | O5-C5-C6 | -8.53 | 91.05       | 107.66   |
| 4   | p     | 3   | BMA  | O5-C5-C6 | -8.53 | 91.06       | 107.66   |
| 4   | U     | 3   | BMA  | O5-C5-C6 | -8.53 | 91.06       | 107.66   |
| 7   | 1     | 1   | NAG  | O3-C3-C4 | -8.51 | 90.31       | 110.38   |
| 7   | g     | 1   | NAG  | O3-C3-C4 | -8.49 | 90.35       | 110.38   |
| 7   | L     | 1   | NAG  | O3-C3-C4 | -8.49 | 90.36       | 110.38   |
| 8   | BA    | 3   | BMA  | O2-C2-C1 | -8.47 | 89.82       | 109.22   |
| 8   | q     | 3   | BMA  | O2-C2-C1 | -8.47 | 89.83       | 109.22   |
| 3   | M     | 1   | NAG  | C6-C5-C4 | 8.47  | 133.81      | 113.02   |
| 3   | h     | 1   | NAG  | C6-C5-C4 | 8.47  | 133.81      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | 2     | 1   | NAG  | C6-C5-C4 | 8.46  | 133.79      | 113.02   |
| 8   | V     | 3   | BMA  | O2-C2-C1 | -8.46 | 89.86       | 109.22   |
| 4   | U     | 1   | NAG  | C6-C5-C4 | 8.44  | 133.73      | 113.02   |
| 4   | AA    | 1   | NAG  | C6-C5-C4 | 8.44  | 133.73      | 113.02   |
| 4   | p     | 1   | NAG  | C6-C5-C4 | 8.43  | 133.73      | 113.02   |
| 6   | K     | 4   | MAN  | O4-C4-C5 | -8.42 | 88.58       | 109.32   |
| 6   | f     | 4   | MAN  | O4-C4-C5 | -8.42 | 88.59       | 109.32   |
| 6   | 0     | 4   | MAN  | O4-C4-C5 | -8.41 | 88.61       | 109.32   |
| 8   | i     | 3   | BMA  | O5-C5-C6 | -8.37 | 91.37       | 107.66   |
| 4   | F     | 1   | NAG  | O5-C5-C6 | -8.37 | 91.37       | 107.66   |
| 4   | a     | 1   | NAG  | O5-C5-C6 | -8.37 | 91.37       | 107.66   |
| 8   | N     | 3   | BMA  | O5-C5-C6 | -8.37 | 91.37       | 107.66   |
| 8   | 3     | 3   | BMA  | O5-C5-C6 | -8.37 | 91.37       | 107.66   |
| 4   | v     | 1   | NAG  | O5-C5-C6 | -8.36 | 91.39       | 107.66   |
| 7   | O     | 1   | NAG  | O5-C5-C6 | -8.27 | 91.56       | 107.66   |
| 7   | 4     | 1   | NAG  | O5-C5-C6 | -8.27 | 91.57       | 107.66   |
| 7   | j     | 1   | NAG  | O5-C5-C6 | -8.27 | 91.57       | 107.66   |
| 3   | k     | 1   | NAG  | O5-C5-C6 | -8.17 | 91.77       | 107.66   |
| 3   | P     | 1   | NAG  | O5-C5-C6 | -8.16 | 91.77       | 107.66   |
| 3   | 5     | 1   | NAG  | O5-C5-C6 | -8.15 | 91.79       | 107.66   |
| 4   | v     | 4   | MAN  | O3-C3-C2 | -8.12 | 93.49       | 110.05   |
| 4   | a     | 4   | MAN  | O3-C3-C2 | -8.10 | 93.51       | 110.05   |
| 4   | F     | 4   | MAN  | O3-C3-C2 | -8.10 | 93.52       | 110.05   |
| 5   | c     | 2   | NAG  | O4-C4-C3 | 8.08  | 129.43      | 110.38   |
| 5   | x     | 2   | NAG  | O4-C4-C3 | 8.08  | 129.43      | 110.38   |
| 5   | H     | 2   | NAG  | O4-C4-C3 | 8.08  | 129.42      | 110.38   |
| 3   | l     | 2   | NAG  | C1-C2-N2 | -8.07 | 97.71       | 110.43   |
| 3   | Q     | 2   | NAG  | C1-C2-N2 | -8.06 | 97.74       | 110.43   |
| 3   | 6     | 2   | NAG  | C1-C2-N2 | -8.05 | 97.75       | 110.43   |
| 6   | K     | 5   | MAN  | O3-C3-C4 | -7.94 | 91.65       | 110.38   |
| 6   | 0     | 5   | MAN  | O3-C3-C4 | -7.94 | 91.66       | 110.38   |
| 6   | f     | 5   | MAN  | O3-C3-C4 | -7.93 | 91.69       | 110.38   |
| 3   | o     | 2   | NAG  | O5-C5-C6 | -7.87 | 92.35       | 107.66   |
| 3   | 9     | 2   | NAG  | O5-C5-C6 | -7.87 | 92.35       | 107.66   |
| 3   | T     | 2   | NAG  | O5-C5-C6 | -7.86 | 92.36       | 107.66   |
| 3   | w     | 1   | NAG  | O3-C3-C2 | -7.84 | 93.11       | 109.40   |
| 3   | G     | 1   | NAG  | O3-C3-C2 | -7.83 | 93.14       | 109.40   |
| 3   | b     | 1   | NAG  | O3-C3-C2 | -7.82 | 93.15       | 109.40   |
| 3   | 9     | 2   | NAG  | C1-C2-N2 | -7.82 | 98.11       | 110.43   |
| 3   | P     | 2   | NAG  | O5-C5-C6 | -7.81 | 92.46       | 107.66   |
| 3   | T     | 2   | NAG  | C1-C2-N2 | -7.81 | 98.13       | 110.43   |
| 3   | o     | 2   | NAG  | C1-C2-N2 | -7.80 | 98.14       | 110.43   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | k     | 2   | NAG  | O5-C5-C6 | -7.80 | 92.48       | 107.66   |
| 3   | 5     | 2   | NAG  | O5-C5-C6 | -7.78 | 92.53       | 107.66   |
| 3   | R     | 2   | NAG  | C1-C2-N2 | 7.76  | 122.66      | 110.43   |
| 3   | 7     | 2   | NAG  | C1-C2-N2 | 7.75  | 122.65      | 110.43   |
| 3   | m     | 2   | NAG  | C1-C2-N2 | 7.75  | 122.64      | 110.43   |
| 3   | u     | 2   | NAG  | C1-C2-N2 | -7.68 | 98.33       | 110.43   |
| 3   | Z     | 2   | NAG  | C1-C2-N2 | -7.67 | 98.35       | 110.43   |
| 3   | E     | 2   | NAG  | C1-C2-N2 | -7.66 | 98.36       | 110.43   |
| 7   | 4     | 3   | BMA  | O2-C2-C3 | 7.57  | 125.82      | 110.15   |
| 4   | F     | 4   | MAN  | O5-C5-C6 | -7.56 | 92.95       | 107.66   |
| 4   | a     | 4   | MAN  | O5-C5-C6 | -7.56 | 92.96       | 107.66   |
| 4   | v     | 4   | MAN  | O5-C5-C6 | -7.55 | 92.97       | 107.66   |
| 7   | O     | 3   | BMA  | O2-C2-C3 | 7.54  | 125.76      | 110.15   |
| 7   | j     | 3   | BMA  | O2-C2-C3 | 7.52  | 125.74      | 110.15   |
| 8   | BA    | 1   | NAG  | O5-C5-C6 | -7.48 | 93.11       | 107.66   |
| 8   | V     | 1   | NAG  | O5-C5-C6 | -7.47 | 93.12       | 107.66   |
| 8   | q     | 1   | NAG  | O5-C5-C6 | -7.47 | 93.13       | 107.66   |
| 8   | BA    | 5   | MAN  | C6-C5-C4 | 7.46  | 131.33      | 113.02   |
| 8   | V     | 5   | MAN  | C6-C5-C4 | 7.44  | 131.28      | 113.02   |
| 8   | q     | 5   | MAN  | C6-C5-C4 | 7.42  | 131.25      | 113.02   |
| 4   | a     | 3   | BMA  | O5-C5-C6 | -7.37 | 93.31       | 107.66   |
| 4   | F     | 3   | BMA  | O5-C5-C6 | -7.37 | 93.33       | 107.66   |
| 4   | v     | 3   | BMA  | O5-C5-C6 | -7.36 | 93.34       | 107.66   |
| 7   | X     | 1   | NAG  | O3-C3-C4 | -7.35 | 93.04       | 110.38   |
| 7   | DA    | 1   | NAG  | O3-C3-C4 | -7.35 | 93.06       | 110.38   |
| 7   | s     | 1   | NAG  | O3-C3-C4 | -7.34 | 93.06       | 110.38   |
| 6   | K     | 1   | NAG  | O3-C3-C2 | -7.34 | 94.16       | 109.40   |
| 6   | f     | 1   | NAG  | O3-C3-C2 | -7.33 | 94.19       | 109.40   |
| 6   | 0     | 1   | NAG  | O3-C3-C2 | -7.33 | 94.19       | 109.40   |
| 8   | 3     | 5   | MAN  | O5-C5-C6 | -7.32 | 93.42       | 107.66   |
| 2   | t     | 4   | MAN  | O3-C3-C4 | -7.32 | 93.12       | 110.38   |
| 8   | N     | 5   | MAN  | O5-C5-C6 | -7.32 | 93.42       | 107.66   |
| 2   | Y     | 4   | MAN  | O3-C3-C4 | -7.31 | 93.13       | 110.38   |
| 8   | i     | 5   | MAN  | O5-C5-C6 | -7.31 | 93.43       | 107.66   |
| 7   | j     | 1   | NAG  | O4-C4-C3 | -7.31 | 93.14       | 110.38   |
| 2   | D     | 4   | MAN  | O3-C3-C4 | -7.31 | 93.15       | 110.38   |
| 7   | 4     | 1   | NAG  | O4-C4-C3 | -7.31 | 93.15       | 110.38   |
| 7   | O     | 1   | NAG  | O4-C4-C3 | -7.31 | 93.15       | 110.38   |
| 2   | t     | 2   | NAG  | C1-C2-N2 | -7.29 | 98.95       | 110.43   |
| 2   | D     | 2   | NAG  | C1-C2-N2 | -7.29 | 98.95       | 110.43   |
| 2   | Y     | 2   | NAG  | C1-C2-N2 | -7.28 | 98.97       | 110.43   |
| 5   | x     | 2   | NAG  | C1-C2-N2 | -7.25 | 99.01       | 110.43   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | O     | 2   | NAG  | C1-C2-N2 | -7.24 | 99.02       | 110.43   |
| 2   | t     | 4   | MAN  | O2-C2-C1 | 7.24  | 125.80      | 109.22   |
| 7   | 4     | 2   | NAG  | C1-C2-N2 | -7.24 | 99.03       | 110.43   |
| 5   | H     | 2   | NAG  | C1-C2-N2 | -7.24 | 99.03       | 110.43   |
| 5   | c     | 2   | NAG  | C1-C2-N2 | -7.23 | 99.03       | 110.43   |
| 7   | j     | 2   | NAG  | C1-C2-N2 | -7.22 | 99.06       | 110.43   |
| 4   | p     | 4   | MAN  | O5-C5-C6 | -7.22 | 93.61       | 107.66   |
| 4   | AA    | 4   | MAN  | O5-C5-C6 | -7.21 | 93.63       | 107.66   |
| 4   | U     | 4   | MAN  | O5-C5-C6 | -7.21 | 93.63       | 107.66   |
| 2   | D     | 4   | MAN  | O2-C2-C1 | 7.20  | 125.70      | 109.22   |
| 2   | Y     | 4   | MAN  | O2-C2-C1 | 7.20  | 125.70      | 109.22   |
| 3   | n     | 2   | NAG  | O5-C5-C6 | -7.18 | 93.69       | 107.66   |
| 7   | O     | 2   | NAG  | O5-C5-C6 | -7.17 | 93.71       | 107.66   |
| 3   | S     | 2   | NAG  | O5-C5-C6 | -7.16 | 93.73       | 107.66   |
| 7   | s     | 1   | NAG  | C1-C2-N2 | -7.16 | 99.15       | 110.43   |
| 7   | j     | 2   | NAG  | O5-C5-C6 | -7.15 | 93.74       | 107.66   |
| 7   | X     | 1   | NAG  | C1-C2-N2 | -7.15 | 99.16       | 110.43   |
| 7   | 4     | 2   | NAG  | O5-C5-C6 | -7.15 | 93.74       | 107.66   |
| 8   | V     | 4   | MAN  | O3-C3-C2 | -7.14 | 95.48       | 110.05   |
| 8   | q     | 4   | MAN  | O3-C3-C2 | -7.14 | 95.49       | 110.05   |
| 7   | DA    | 1   | NAG  | C1-C2-N2 | -7.13 | 99.19       | 110.43   |
| 3   | 8     | 2   | NAG  | O5-C5-C6 | -7.13 | 93.78       | 107.66   |
| 8   | BA    | 4   | MAN  | O3-C3-C2 | -7.12 | 95.52       | 110.05   |
| 6   | 0     | 8   | MAN  | O3-C3-C2 | -7.09 | 95.59       | 110.05   |
| 6   | K     | 8   | MAN  | O3-C3-C2 | -7.08 | 95.61       | 110.05   |
| 6   | f     | 8   | MAN  | O3-C3-C2 | -7.06 | 95.65       | 110.05   |
| 7   | 1     | 3   | BMA  | O3-C3-C2 | -6.99 | 95.78       | 110.05   |
| 7   | g     | 3   | BMA  | O3-C3-C2 | -6.99 | 95.79       | 110.05   |
| 7   | L     | 3   | BMA  | O3-C3-C2 | -6.99 | 95.79       | 110.05   |
| 6   | 0     | 2   | NAG  | O3-C3-C4 | 6.96  | 126.77      | 110.38   |
| 6   | K     | 2   | NAG  | O3-C3-C4 | 6.95  | 126.75      | 110.38   |
| 6   | f     | 2   | NAG  | O3-C3-C4 | 6.94  | 126.73      | 110.38   |
| 3   | 8     | 1   | NAG  | O5-C5-C6 | -6.87 | 94.28       | 107.66   |
| 3   | S     | 1   | NAG  | O5-C5-C6 | -6.87 | 94.29       | 107.66   |
| 3   | n     | 1   | NAG  | O5-C5-C6 | -6.86 | 94.30       | 107.66   |
| 7   | 1     | 3   | BMA  | O4-C4-C3 | -6.85 | 94.22       | 110.38   |
| 7   | L     | 3   | BMA  | O4-C4-C3 | -6.84 | 94.24       | 110.38   |
| 7   | g     | 3   | BMA  | O4-C4-C3 | -6.84 | 94.26       | 110.38   |
| 7   | 1     | 1   | NAG  | C1-C2-N2 | 6.81  | 121.17      | 110.43   |
| 7   | g     | 1   | NAG  | C1-C2-N2 | 6.81  | 121.17      | 110.43   |
| 7   | L     | 1   | NAG  | C1-C2-N2 | 6.81  | 121.16      | 110.43   |
| 3   | 6     | 1   | NAG  | O5-C5-C6 | -6.76 | 94.50       | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | Q     | 1   | NAG  | O5-C5-C6 | -6.76 | 94.51       | 107.66   |
| 3   | l     | 1   | NAG  | O5-C5-C6 | -6.75 | 94.52       | 107.66   |
| 8   | i     | 4   | MAN  | O3-C3-C2 | -6.74 | 96.29       | 110.05   |
| 2   | t     | 3   | BMA  | O2-C2-C1 | 6.74  | 124.66      | 109.22   |
| 8   | 3     | 4   | MAN  | O3-C3-C2 | -6.74 | 96.30       | 110.05   |
| 2   | Y     | 3   | BMA  | O2-C2-C1 | 6.74  | 124.65      | 109.22   |
| 8   | N     | 4   | MAN  | O3-C3-C2 | -6.73 | 96.31       | 110.05   |
| 2   | D     | 3   | BMA  | O2-C2-C1 | 6.73  | 124.64      | 109.22   |
| 4   | a     | 3   | BMA  | O2-C2-C3 | 6.65  | 123.92      | 110.15   |
| 4   | F     | 3   | BMA  | O2-C2-C3 | 6.63  | 123.89      | 110.15   |
| 4   | p     | 2   | NAG  | C6-C5-C4 | 6.63  | 129.30      | 113.02   |
| 4   | v     | 3   | BMA  | O2-C2-C3 | 6.63  | 123.88      | 110.15   |
| 4   | AA    | 2   | NAG  | C6-C5-C4 | 6.63  | 129.29      | 113.02   |
| 4   | U     | 2   | NAG  | C6-C5-C4 | 6.62  | 129.27      | 113.02   |
| 6   | f     | 4   | MAN  | O4-C4-C3 | 6.61  | 125.95      | 110.38   |
| 6   | 0     | 4   | MAN  | O4-C4-C3 | 6.60  | 125.94      | 110.38   |
| 6   | K     | 4   | MAN  | O4-C4-C3 | 6.60  | 125.93      | 110.38   |
| 3   | 2     | 2   | NAG  | O5-C5-C6 | -6.57 | 94.87       | 107.66   |
| 3   | M     | 2   | NAG  | O5-C5-C6 | -6.56 | 94.89       | 107.66   |
| 3   | h     | 2   | NAG  | O5-C5-C6 | -6.55 | 94.91       | 107.66   |
| 7   | 1     | 3   | BMA  | O2-C2-C1 | -6.50 | 94.34       | 109.22   |
| 7   | L     | 3   | BMA  | O2-C2-C1 | -6.49 | 94.37       | 109.22   |
| 7   | g     | 3   | BMA  | O2-C2-C1 | -6.47 | 94.40       | 109.22   |
| 8   | q     | 3   | BMA  | O4-C4-C5 | -6.36 | 93.65       | 109.32   |
| 8   | V     | 3   | BMA  | O4-C4-C5 | -6.36 | 93.66       | 109.32   |
| 8   | BA    | 3   | BMA  | O4-C4-C5 | -6.36 | 93.67       | 109.32   |
| 6   | 0     | 1   | NAG  | C1-C2-N2 | -6.29 | 100.52      | 110.43   |
| 6   | f     | 1   | NAG  | C1-C2-N2 | -6.28 | 100.53      | 110.43   |
| 6   | K     | 1   | NAG  | C1-C2-N2 | -6.28 | 100.53      | 110.43   |
| 2   | t     | 3   | BMA  | O5-C5-C6 | -6.25 | 95.49       | 107.66   |
| 2   | D     | 3   | BMA  | O5-C5-C6 | -6.25 | 95.49       | 107.66   |
| 2   | Y     | 3   | BMA  | O5-C5-C6 | -6.25 | 95.49       | 107.66   |
| 3   | R     | 2   | NAG  | O4-C4-C5 | -6.24 | 93.96       | 109.32   |
| 3   | m     | 2   | NAG  | O4-C4-C5 | -6.24 | 93.96       | 109.32   |
| 3   | 7     | 2   | NAG  | O4-C4-C5 | -6.24 | 93.97       | 109.32   |
| 7   | O     | 3   | BMA  | O2-C2-C1 | -6.23 | 94.95       | 109.22   |
| 7   | 4     | 3   | BMA  | O2-C2-C1 | -6.23 | 94.96       | 109.22   |
| 7   | j     | 3   | BMA  | O2-C2-C1 | -6.23 | 94.97       | 109.22   |
| 8   | N     | 1   | NAG  | O4-C4-C3 | -6.16 | 95.86       | 110.38   |
| 3   | y     | 1   | NAG  | C8-C7-N2 | 6.16  | 126.33      | 116.12   |
| 3   | I     | 1   | NAG  | C8-C7-N2 | 6.16  | 126.33      | 116.12   |
| 8   | i     | 1   | NAG  | O4-C4-C3 | -6.15 | 95.87       | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | 3     | 1   | NAG  | O4-C4-C3 | -6.15 | 95.88       | 110.38   |
| 3   | d     | 1   | NAG  | C8-C7-N2 | 6.15  | 126.31      | 116.12   |
| 5   | H     | 3   | BMA  | O3-C3-C2 | 6.04  | 122.38      | 110.05   |
| 5   | c     | 3   | BMA  | O3-C3-C2 | 6.03  | 122.36      | 110.05   |
| 5   | x     | 3   | BMA  | O3-C3-C2 | 6.03  | 122.36      | 110.05   |
| 3   | I     | 2   | NAG  | O4-C4-C3 | -5.98 | 96.29       | 110.38   |
| 3   | d     | 2   | NAG  | O4-C4-C3 | -5.98 | 96.29       | 110.38   |
| 3   | y     | 2   | NAG  | O4-C4-C3 | -5.98 | 96.29       | 110.38   |
| 5   | x     | 2   | NAG  | O3-C3-C2 | -5.92 | 97.10       | 109.40   |
| 5   | H     | 2   | NAG  | O3-C3-C2 | -5.92 | 97.10       | 109.40   |
| 5   | c     | 2   | NAG  | O3-C3-C2 | -5.91 | 97.13       | 109.40   |
| 8   | i     | 4   | MAN  | O5-C5-C6 | -5.83 | 96.31       | 107.66   |
| 8   | 3     | 4   | MAN  | O5-C5-C6 | -5.83 | 96.32       | 107.66   |
| 8   | N     | 4   | MAN  | O5-C5-C6 | -5.82 | 96.33       | 107.66   |
| 3   | Q     | 1   | NAG  | C6-C5-C4 | 5.82  | 127.31      | 113.02   |
| 8   | q     | 3   | BMA  | O5-C5-C6 | -5.82 | 96.34       | 107.66   |
| 3   | 6     | 1   | NAG  | C6-C5-C4 | 5.82  | 127.30      | 113.02   |
| 3   | l     | 1   | NAG  | C6-C5-C4 | 5.82  | 127.30      | 113.02   |
| 8   | V     | 3   | BMA  | O5-C5-C6 | -5.81 | 96.35       | 107.66   |
| 8   | BA    | 3   | BMA  | O5-C5-C6 | -5.81 | 96.36       | 107.66   |
| 4   | U     | 4   | MAN  | O3-C3-C2 | -5.78 | 98.26       | 110.05   |
| 4   | AA    | 4   | MAN  | O3-C3-C2 | -5.78 | 98.26       | 110.05   |
| 4   | p     | 4   | MAN  | O3-C3-C2 | -5.77 | 98.28       | 110.05   |
| 7   | 1     | 3   | BMA  | O2-C2-C3 | 5.76  | 122.09      | 110.15   |
| 7   | L     | 3   | BMA  | O2-C2-C3 | 5.75  | 122.06      | 110.15   |
| 7   | g     | 3   | BMA  | O2-C2-C3 | 5.74  | 122.04      | 110.15   |
| 8   | N     | 5   | MAN  | O3-C3-C2 | -5.68 | 98.46       | 110.05   |
| 8   | i     | 5   | MAN  | O3-C3-C2 | -5.68 | 98.46       | 110.05   |
| 8   | 3     | 5   | MAN  | O3-C3-C2 | -5.67 | 98.48       | 110.05   |
| 8   | q     | 2   | NAG  | C6-C5-C4 | 5.64  | 126.87      | 113.02   |
| 7   | O     | 3   | BMA  | O3-C3-C2 | -5.64 | 98.55       | 110.05   |
| 7   | j     | 3   | BMA  | O3-C3-C2 | -5.64 | 98.55       | 110.05   |
| 8   | V     | 2   | NAG  | C6-C5-C4 | 5.64  | 126.86      | 113.02   |
| 3   | d     | 1   | NAG  | C6-C5-C4 | 5.63  | 126.85      | 113.02   |
| 8   | BA    | 2   | NAG  | C6-C5-C4 | 5.63  | 126.85      | 113.02   |
| 7   | 4     | 3   | BMA  | O3-C3-C2 | -5.62 | 98.58       | 110.05   |
| 3   | I     | 1   | NAG  | C6-C5-C4 | 5.62  | 126.81      | 113.02   |
| 3   | y     | 1   | NAG  | C6-C5-C4 | 5.62  | 126.81      | 113.02   |
| 3   | 6     | 2   | NAG  | C6-C5-C4 | 5.56  | 126.66      | 113.02   |
| 3   | Q     | 2   | NAG  | C6-C5-C4 | 5.55  | 126.64      | 113.02   |
| 3   | l     | 2   | NAG  | C6-C5-C4 | 5.55  | 126.64      | 113.02   |
| 8   | BA    | 4   | MAN  | O5-C5-C6 | -5.53 | 96.90       | 107.66   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | q     | 4   | MAN  | O5-C5-C6 | -5.52 | 96.92       | 107.66   |
| 8   | V     | 4   | MAN  | O5-C5-C6 | -5.52 | 96.93       | 107.66   |
| 6   | K     | 5   | MAN  | C6-C5-C4 | 5.51  | 126.55      | 113.02   |
| 6   | 0     | 5   | MAN  | C6-C5-C4 | 5.51  | 126.54      | 113.02   |
| 7   | L     | 2   | NAG  | O3-C3-C4 | -5.51 | 97.40       | 110.38   |
| 2   | Y     | 5   | MAN  | O3-C3-C2 | -5.51 | 98.82       | 110.05   |
| 7   | g     | 2   | NAG  | O3-C3-C4 | -5.50 | 97.42       | 110.38   |
| 2   | D     | 5   | MAN  | O3-C3-C2 | -5.50 | 98.83       | 110.05   |
| 7   | 1     | 2   | NAG  | O3-C3-C4 | -5.50 | 97.42       | 110.38   |
| 3   | E     | 1   | NAG  | C1-C2-N2 | 5.50  | 119.09      | 110.43   |
| 6   | f     | 5   | MAN  | C6-C5-C4 | 5.50  | 126.51      | 113.02   |
| 2   | t     | 5   | MAN  | O3-C3-C2 | -5.50 | 98.84       | 110.05   |
| 3   | u     | 1   | NAG  | C1-C2-N2 | 5.49  | 119.09      | 110.43   |
| 3   | Z     | 1   | NAG  | C1-C2-N2 | 5.48  | 119.07      | 110.43   |
| 8   | q     | 1   | NAG  | O3-C3-C2 | -5.47 | 98.05       | 109.40   |
| 8   | BA    | 1   | NAG  | O3-C3-C2 | -5.46 | 98.07       | 109.40   |
| 8   | V     | 1   | NAG  | O3-C3-C2 | -5.45 | 98.08       | 109.40   |
| 3   | CA    | 1   | NAG  | O4-C4-C3 | -5.40 | 97.65       | 110.38   |
| 3   | W     | 1   | NAG  | O4-C4-C3 | -5.39 | 97.67       | 110.38   |
| 3   | r     | 1   | NAG  | O4-C4-C3 | -5.39 | 97.68       | 110.38   |
| 3   | w     | 2   | NAG  | C1-C2-N2 | -5.38 | 101.95      | 110.43   |
| 2   | D     | 6   | MAN  | O2-C2-C1 | 5.37  | 121.53      | 109.22   |
| 3   | G     | 2   | NAG  | C1-C2-N2 | -5.37 | 101.98      | 110.43   |
| 2   | Y     | 6   | MAN  | O2-C2-C1 | 5.36  | 121.50      | 109.22   |
| 3   | b     | 2   | NAG  | C1-C2-N2 | -5.36 | 101.98      | 110.43   |
| 2   | t     | 6   | MAN  | O2-C2-C1 | 5.36  | 121.50      | 109.22   |
| 3   | J     | 2   | NAG  | O5-C5-C6 | -5.35 | 97.24       | 107.66   |
| 3   | e     | 2   | NAG  | O5-C5-C6 | -5.35 | 97.25       | 107.66   |
| 2   | D     | 3   | BMA  | C6-C5-C4 | 5.35  | 126.15      | 113.02   |
| 3   | z     | 2   | NAG  | O5-C5-C6 | -5.35 | 97.26       | 107.66   |
| 2   | Y     | 3   | BMA  | C6-C5-C4 | 5.34  | 126.13      | 113.02   |
| 2   | t     | 3   | BMA  | C6-C5-C4 | 5.33  | 126.11      | 113.02   |
| 2   | Y     | 5   | MAN  | C1-O5-C5 | 5.33  | 119.32      | 112.19   |
| 2   | D     | 5   | MAN  | C1-O5-C5 | 5.29  | 119.28      | 112.19   |
| 2   | t     | 5   | MAN  | C1-O5-C5 | 5.29  | 119.28      | 112.19   |
| 6   | f     | 8   | MAN  | C6-C5-C4 | 5.29  | 126.01      | 113.02   |
| 6   | 0     | 8   | MAN  | C6-C5-C4 | 5.29  | 126.00      | 113.02   |
| 6   | K     | 8   | MAN  | C6-C5-C4 | 5.29  | 126.00      | 113.02   |
| 6   | f     | 7   | MAN  | O2-C2-C3 | 5.28  | 121.09      | 110.15   |
| 6   | 0     | 7   | MAN  | O2-C2-C3 | 5.27  | 121.06      | 110.15   |
| 6   | K     | 7   | MAN  | O2-C2-C3 | 5.27  | 121.06      | 110.15   |
| 8   | BA    | 3   | BMA  | O4-C4-C3 | 5.22  | 122.69      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | V     | 3   | BMA  | O4-C4-C3 | 5.22  | 122.68      | 110.38   |
| 3   | Q     | 2   | NAG  | O5-C5-C6 | -5.21 | 97.52       | 107.66   |
| 3   | 6     | 2   | NAG  | O5-C5-C6 | -5.21 | 97.52       | 107.66   |
| 5   | H     | 4   | MAN  | O2-C2-C1 | 5.21  | 121.15      | 109.22   |
| 5   | x     | 4   | MAN  | O2-C2-C1 | 5.21  | 121.15      | 109.22   |
| 5   | c     | 4   | MAN  | O2-C2-C1 | 5.21  | 121.15      | 109.22   |
| 3   | l     | 2   | NAG  | O5-C5-C6 | -5.21 | 97.53       | 107.66   |
| 8   | q     | 3   | BMA  | O4-C4-C3 | 5.20  | 122.64      | 110.38   |
| 4   | p     | 4   | MAN  | O2-C2-C1 | 5.20  | 121.12      | 109.22   |
| 4   | AA    | 4   | MAN  | O2-C2-C1 | 5.20  | 121.12      | 109.22   |
| 4   | U     | 4   | MAN  | O2-C2-C1 | 5.19  | 121.10      | 109.22   |
| 7   | g     | 2   | NAG  | O5-C5-C6 | -5.18 | 97.59       | 107.66   |
| 7   | 1     | 2   | NAG  | O5-C5-C6 | -5.18 | 97.59       | 107.66   |
| 7   | L     | 2   | NAG  | O5-C5-C6 | -5.17 | 97.60       | 107.66   |
| 8   | i     | 5   | MAN  | C6-C5-C4 | 5.17  | 125.71      | 113.02   |
| 8   | N     | 5   | MAN  | C6-C5-C4 | 5.17  | 125.71      | 113.02   |
| 8   | 3     | 5   | MAN  | C6-C5-C4 | 5.17  | 125.70      | 113.02   |
| 4   | a     | 1   | NAG  | O4-C4-C3 | -5.16 | 98.21       | 110.38   |
| 4   | F     | 1   | NAG  | O4-C4-C3 | -5.16 | 98.22       | 110.38   |
| 4   | v     | 1   | NAG  | O4-C4-C3 | -5.15 | 98.24       | 110.38   |
| 2   | t     | 2   | NAG  | C6-C5-C4 | 5.15  | 125.66      | 113.02   |
| 3   | u     | 2   | NAG  | O4-C4-C5 | -5.15 | 96.65       | 109.32   |
| 3   | E     | 2   | NAG  | O4-C4-C5 | -5.15 | 96.65       | 109.32   |
| 2   | Y     | 2   | NAG  | C6-C5-C4 | 5.14  | 125.64      | 113.02   |
| 3   | Z     | 2   | NAG  | O4-C4-C5 | -5.14 | 96.67       | 109.32   |
| 2   | D     | 2   | NAG  | C6-C5-C4 | 5.14  | 125.63      | 113.02   |
| 6   | K     | 4   | MAN  | O2-C2-C1 | 5.13  | 120.98      | 109.22   |
| 6   | f     | 4   | MAN  | O2-C2-C1 | 5.13  | 120.98      | 109.22   |
| 6   | 0     | 4   | MAN  | O2-C2-C1 | 5.13  | 120.97      | 109.22   |
| 2   | Y     | 4   | MAN  | C6-C5-C4 | 5.11  | 125.57      | 113.02   |
| 2   | t     | 4   | MAN  | C6-C5-C4 | 5.10  | 125.55      | 113.02   |
| 7   | s     | 3   | BMA  | O5-C5-C6 | -5.09 | 97.75       | 107.66   |
| 2   | D     | 4   | MAN  | C6-C5-C4 | 5.09  | 125.51      | 113.02   |
| 7   | DA    | 3   | BMA  | O5-C5-C6 | -5.09 | 97.77       | 107.66   |
| 7   | X     | 3   | BMA  | O5-C5-C6 | -5.08 | 97.77       | 107.66   |
| 7   | j     | 2   | NAG  | C6-C5-C4 | 5.07  | 125.47      | 113.02   |
| 7   | 4     | 2   | NAG  | C6-C5-C4 | 5.07  | 125.47      | 113.02   |
| 7   | O     | 2   | NAG  | C6-C5-C4 | 5.06  | 125.45      | 113.02   |
| 8   | 3     | 1   | NAG  | C6-C5-C4 | 5.05  | 125.43      | 113.02   |
| 8   | N     | 1   | NAG  | C6-C5-C4 | 5.05  | 125.42      | 113.02   |
| 8   | i     | 1   | NAG  | C6-C5-C4 | 5.05  | 125.42      | 113.02   |
| 4   | F     | 4   | MAN  | C6-C5-C4 | 5.01  | 125.32      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | a     | 4   | MAN  | C6-C5-C4 | 5.01  | 125.31      | 113.02   |
| 4   | v     | 4   | MAN  | C6-C5-C4 | 5.00  | 125.29      | 113.02   |
| 8   | i     | 3   | BMA  | C6-C5-C4 | 4.90  | 125.04      | 113.02   |
| 8   | 3     | 3   | BMA  | C6-C5-C4 | 4.88  | 125.01      | 113.02   |
| 8   | N     | 3   | BMA  | C6-C5-C4 | 4.88  | 125.00      | 113.02   |
| 3   | e     | 1   | NAG  | O3-C3-C4 | 4.87  | 121.84      | 110.38   |
| 3   | z     | 1   | NAG  | O3-C3-C4 | 4.87  | 121.84      | 110.38   |
| 5   | x     | 1   | NAG  | C6-C5-C4 | 4.86  | 124.96      | 113.02   |
| 5   | H     | 1   | NAG  | C6-C5-C4 | 4.86  | 124.95      | 113.02   |
| 5   | c     | 1   | NAG  | C6-C5-C4 | 4.86  | 124.95      | 113.02   |
| 3   | J     | 1   | NAG  | O3-C3-C4 | 4.86  | 121.83      | 110.38   |
| 6   | f     | 1   | NAG  | O5-C5-C6 | -4.83 | 98.25       | 107.66   |
| 6   | K     | 1   | NAG  | O5-C5-C6 | -4.83 | 98.27       | 107.66   |
| 6   | 0     | 1   | NAG  | O5-C5-C6 | -4.82 | 98.29       | 107.66   |
| 4   | p     | 4   | MAN  | C6-C5-C4 | 4.80  | 124.81      | 113.02   |
| 6   | 0     | 2   | NAG  | C6-C5-C4 | 4.80  | 124.81      | 113.02   |
| 6   | K     | 2   | NAG  | C6-C5-C4 | 4.80  | 124.79      | 113.02   |
| 4   | U     | 4   | MAN  | C6-C5-C4 | 4.79  | 124.79      | 113.02   |
| 2   | D     | 1   | NAG  | O3-C3-C2 | -4.79 | 99.45       | 109.40   |
| 6   | f     | 2   | NAG  | C6-C5-C4 | 4.79  | 124.78      | 113.02   |
| 2   | t     | 1   | NAG  | O3-C3-C2 | -4.79 | 99.45       | 109.40   |
| 4   | AA    | 4   | MAN  | C6-C5-C4 | 4.79  | 124.78      | 113.02   |
| 2   | Y     | 1   | NAG  | O3-C3-C2 | -4.78 | 99.47       | 109.40   |
| 3   | 9     | 2   | NAG  | C6-C5-C4 | 4.74  | 124.66      | 113.02   |
| 3   | o     | 2   | NAG  | C6-C5-C4 | 4.73  | 124.64      | 113.02   |
| 3   | T     | 2   | NAG  | C6-C5-C4 | 4.73  | 124.64      | 113.02   |
| 3   | R     | 1   | NAG  | C1-C2-N2 | 4.71  | 117.86      | 110.43   |
| 3   | m     | 1   | NAG  | C1-C2-N2 | 4.71  | 117.86      | 110.43   |
| 3   | 7     | 1   | NAG  | C1-C2-N2 | 4.69  | 117.82      | 110.43   |
| 6   | f     | 3   | BMA  | O2-C2-C1 | -4.66 | 98.56       | 109.22   |
| 6   | K     | 3   | BMA  | O2-C2-C1 | -4.65 | 98.57       | 109.22   |
| 6   | 0     | 3   | BMA  | O2-C2-C1 | -4.64 | 98.60       | 109.22   |
| 4   | p     | 1   | NAG  | C1-C2-N2 | -4.63 | 103.14      | 110.43   |
| 3   | J     | 2   | NAG  | C1-C2-N2 | 4.61  | 117.70      | 110.43   |
| 3   | e     | 2   | NAG  | C1-C2-N2 | 4.61  | 117.69      | 110.43   |
| 3   | z     | 2   | NAG  | C1-C2-N2 | 4.61  | 117.69      | 110.43   |
| 4   | U     | 1   | NAG  | C1-C2-N2 | -4.60 | 103.18      | 110.43   |
| 4   | AA    | 1   | NAG  | C1-C2-N2 | -4.60 | 103.18      | 110.43   |
| 3   | 9     | 2   | NAG  | O4-C4-C3 | -4.59 | 99.56       | 110.38   |
| 3   | T     | 2   | NAG  | O4-C4-C3 | -4.59 | 99.57       | 110.38   |
| 3   | o     | 2   | NAG  | O4-C4-C3 | -4.58 | 99.58       | 110.38   |
| 3   | n     | 2   | NAG  | O4-C4-C5 | -4.55 | 98.11       | 109.32   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | S     | 2   | NAG  | O4-C4-C5 | -4.53 | 98.17       | 109.32   |
| 3   | 8     | 2   | NAG  | O4-C4-C5 | -4.52 | 98.20       | 109.32   |
| 6   | 0     | 7   | MAN  | C6-C5-C4 | 4.51  | 124.10      | 113.02   |
| 6   | f     | 7   | MAN  | C6-C5-C4 | 4.51  | 124.09      | 113.02   |
| 3   | P     | 1   | NAG  | C6-C5-C4 | 4.50  | 124.07      | 113.02   |
| 3   | 5     | 1   | NAG  | C6-C5-C4 | 4.50  | 124.06      | 113.02   |
| 6   | K     | 7   | MAN  | C6-C5-C4 | 4.50  | 124.06      | 113.02   |
| 3   | k     | 1   | NAG  | C6-C5-C4 | 4.49  | 124.04      | 113.02   |
| 4   | U     | 4   | MAN  | O4-C4-C3 | -4.47 | 99.84       | 110.38   |
| 4   | AA    | 4   | MAN  | O4-C4-C3 | -4.47 | 99.84       | 110.38   |
| 4   | p     | 4   | MAN  | O4-C4-C3 | -4.45 | 99.88       | 110.38   |
| 5   | x     | 3   | BMA  | O2-C2-C3 | 4.45  | 119.36      | 110.15   |
| 5   | H     | 3   | BMA  | O2-C2-C3 | 4.45  | 119.36      | 110.15   |
| 5   | c     | 3   | BMA  | O2-C2-C3 | 4.44  | 119.36      | 110.15   |
| 4   | AA    | 3   | BMA  | O2-C2-C3 | 4.34  | 119.13      | 110.15   |
| 4   | p     | 3   | BMA  | O2-C2-C3 | 4.33  | 119.12      | 110.15   |
| 4   | U     | 3   | BMA  | O2-C2-C3 | 4.33  | 119.12      | 110.15   |
| 2   | Y     | 6   | MAN  | C6-C5-C4 | 4.33  | 123.64      | 113.02   |
| 2   | t     | 6   | MAN  | C6-C5-C4 | 4.33  | 123.64      | 113.02   |
| 2   | D     | 6   | MAN  | C6-C5-C4 | 4.31  | 123.61      | 113.02   |
| 4   | F     | 4   | MAN  | O2-C2-C3 | 4.31  | 119.08      | 110.15   |
| 4   | a     | 4   | MAN  | O2-C2-C3 | 4.31  | 119.07      | 110.15   |
| 4   | v     | 4   | MAN  | O2-C2-C3 | 4.31  | 119.07      | 110.15   |
| 2   | Y     | 1   | NAG  | C6-C5-C4 | 4.27  | 123.50      | 113.02   |
| 2   | t     | 1   | NAG  | C6-C5-C4 | 4.27  | 123.50      | 113.02   |
| 2   | D     | 1   | NAG  | C6-C5-C4 | 4.27  | 123.50      | 113.02   |
| 3   | 5     | 2   | NAG  | C1-C2-N2 | 4.25  | 117.13      | 110.43   |
| 8   | BA    | 5   | MAN  | O2-C2-C3 | 4.23  | 118.92      | 110.15   |
| 3   | P     | 2   | NAG  | C1-C2-N2 | 4.23  | 117.10      | 110.43   |
| 3   | k     | 2   | NAG  | C1-C2-N2 | 4.23  | 117.10      | 110.43   |
| 6   | K     | 7   | MAN  | O4-C4-C5 | -4.23 | 98.91       | 109.32   |
| 6   | 0     | 7   | MAN  | O4-C4-C5 | -4.23 | 98.91       | 109.32   |
| 6   | f     | 7   | MAN  | O4-C4-C5 | -4.23 | 98.92       | 109.32   |
| 8   | q     | 5   | MAN  | O2-C2-C3 | 4.23  | 118.90      | 110.15   |
| 3   | y     | 2   | NAG  | O3-C3-C2 | 4.22  | 118.17      | 109.40   |
| 8   | V     | 5   | MAN  | O2-C2-C3 | 4.22  | 118.89      | 110.15   |
| 3   | I     | 2   | NAG  | O3-C3-C2 | 4.22  | 118.16      | 109.40   |
| 3   | d     | 2   | NAG  | O3-C3-C2 | 4.22  | 118.16      | 109.40   |
| 8   | i     | 3   | BMA  | O2-C2-C3 | 4.19  | 118.83      | 110.15   |
| 8   | 3     | 3   | BMA  | O2-C2-C3 | 4.19  | 118.83      | 110.15   |
| 8   | N     | 3   | BMA  | O2-C2-C3 | 4.19  | 118.83      | 110.15   |
| 2   | t     | 6   | MAN  | C1-O5-C5 | 4.17  | 117.78      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | 1     | 2   | NAG  | O4-C4-C3 | 4.13  | 120.11      | 110.38   |
| 2   | Y     | 6   | MAN  | C1-O5-C5 | 4.13  | 117.72      | 112.19   |
| 7   | L     | 2   | NAG  | O4-C4-C3 | 4.13  | 120.11      | 110.38   |
| 7   | s     | 3   | BMA  | O3-C3-C2 | -4.13 | 101.63      | 110.05   |
| 2   | D     | 6   | MAN  | C1-O5-C5 | 4.12  | 117.71      | 112.19   |
| 7   | DA    | 3   | BMA  | O3-C3-C2 | -4.12 | 101.64      | 110.05   |
| 7   | X     | 3   | BMA  | O3-C3-C2 | -4.12 | 101.64      | 110.05   |
| 7   | g     | 2   | NAG  | O4-C4-C3 | 4.12  | 120.08      | 110.38   |
| 3   | u     | 2   | NAG  | C1-O5-C5 | 4.12  | 117.70      | 112.19   |
| 2   | t     | 1   | NAG  | O4-C4-C3 | -4.11 | 100.68      | 110.38   |
| 2   | D     | 1   | NAG  | O4-C4-C3 | -4.11 | 100.68      | 110.38   |
| 2   | Y     | 1   | NAG  | O4-C4-C3 | -4.11 | 100.68      | 110.38   |
| 3   | E     | 2   | NAG  | C1-O5-C5 | 4.10  | 117.68      | 112.19   |
| 6   | 0     | 8   | MAN  | C1-O5-C5 | 4.10  | 117.68      | 112.19   |
| 6   | f     | 8   | MAN  | C1-O5-C5 | 4.09  | 117.67      | 112.19   |
| 3   | Z     | 2   | NAG  | C1-O5-C5 | 4.09  | 117.67      | 112.19   |
| 6   | K     | 8   | MAN  | C1-O5-C5 | 4.09  | 117.67      | 112.19   |
| 3   | y     | 1   | NAG  | C1-C2-N2 | 4.08  | 116.87      | 110.43   |
| 8   | BA    | 4   | MAN  | O4-C4-C3 | -4.07 | 100.78      | 110.38   |
| 3   | I     | 1   | NAG  | C1-C2-N2 | 4.07  | 116.85      | 110.43   |
| 3   | d     | 1   | NAG  | C1-C2-N2 | 4.07  | 116.85      | 110.43   |
| 8   | q     | 4   | MAN  | O4-C4-C3 | -4.07 | 100.79      | 110.38   |
| 8   | V     | 4   | MAN  | O4-C4-C3 | -4.07 | 100.79      | 110.38   |
| 8   | q     | 5   | MAN  | O3-C3-C2 | -4.06 | 101.77      | 110.05   |
| 8   | V     | 5   | MAN  | O3-C3-C2 | -4.03 | 101.83      | 110.05   |
| 8   | BA    | 5   | MAN  | O3-C3-C2 | -4.02 | 101.85      | 110.05   |
| 5   | H     | 3   | BMA  | O4-C4-C3 | 4.02  | 119.84      | 110.38   |
| 5   | x     | 3   | BMA  | O4-C4-C3 | 4.01  | 119.83      | 110.38   |
| 5   | c     | 3   | BMA  | O4-C4-C3 | 4.01  | 119.83      | 110.38   |
| 4   | U     | 4   | MAN  | O4-C4-C5 | 4.01  | 119.19      | 109.32   |
| 4   | AA    | 4   | MAN  | O4-C4-C5 | 3.99  | 119.16      | 109.32   |
| 4   | p     | 4   | MAN  | O4-C4-C5 | 3.98  | 119.13      | 109.32   |
| 3   | Z     | 1   | NAG  | O3-C3-C4 | -3.96 | 101.05      | 110.38   |
| 3   | u     | 1   | NAG  | O3-C3-C4 | -3.95 | 101.08      | 110.38   |
| 3   | E     | 1   | NAG  | O3-C3-C4 | -3.94 | 101.08      | 110.38   |
| 7   | g     | 3   | BMA  | O4-C4-C5 | 3.93  | 119.00      | 109.32   |
| 7   | L     | 3   | BMA  | O4-C4-C5 | 3.92  | 118.98      | 109.32   |
| 7   | 4     | 2   | NAG  | O3-C3-C2 | -3.92 | 101.26      | 109.40   |
| 7   | 1     | 3   | BMA  | O4-C4-C5 | 3.91  | 118.97      | 109.32   |
| 7   | O     | 2   | NAG  | O3-C3-C2 | -3.91 | 101.27      | 109.40   |
| 7   | j     | 2   | NAG  | O3-C3-C2 | -3.91 | 101.28      | 109.40   |
| 7   | L     | 2   | NAG  | C6-C5-C4 | 3.90  | 122.60      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | g     | 2   | NAG  | C6-C5-C4 | 3.88  | 122.54      | 113.02   |
| 7   | l     | 2   | NAG  | C6-C5-C4 | 3.88  | 122.54      | 113.02   |
| 5   | c     | 4   | MAN  | O3-C3-C2 | -3.88 | 102.14      | 110.05   |
| 5   | H     | 4   | MAN  | O3-C3-C2 | -3.88 | 102.15      | 110.05   |
| 5   | x     | 4   | MAN  | O3-C3-C2 | -3.87 | 102.15      | 110.05   |
| 3   | M     | 1   | NAG  | O3-C3-C2 | 3.85  | 117.39      | 109.40   |
| 3   | 2     | 1   | NAG  | O3-C3-C2 | 3.84  | 117.37      | 109.40   |
| 3   | h     | 1   | NAG  | O3-C3-C2 | 3.83  | 117.36      | 109.40   |
| 6   | 0     | 5   | MAN  | O4-C4-C3 | -3.76 | 101.50      | 110.38   |
| 6   | K     | 5   | MAN  | O4-C4-C3 | -3.76 | 101.51      | 110.38   |
| 6   | f     | 5   | MAN  | O4-C4-C3 | -3.75 | 101.55      | 110.38   |
| 6   | 0     | 2   | NAG  | O5-C5-C6 | -3.73 | 100.39      | 107.66   |
| 6   | K     | 2   | NAG  | O5-C5-C6 | -3.72 | 100.42      | 107.66   |
| 6   | f     | 2   | NAG  | O5-C5-C6 | -3.72 | 100.43      | 107.66   |
| 2   | Y     | 3   | BMA  | O3-C3-C2 | -3.68 | 102.54      | 110.05   |
| 2   | D     | 3   | BMA  | O3-C3-C2 | -3.68 | 102.55      | 110.05   |
| 2   | t     | 3   | BMA  | O3-C3-C2 | -3.68 | 102.55      | 110.05   |
| 7   | X     | 3   | BMA  | O4-C4-C5 | 3.65  | 118.31      | 109.32   |
| 7   | DA    | 3   | BMA  | O4-C4-C5 | 3.65  | 118.31      | 109.32   |
| 7   | s     | 3   | BMA  | O4-C4-C5 | 3.64  | 118.30      | 109.32   |
| 3   | h     | 1   | NAG  | O3-C3-C4 | -3.64 | 101.80      | 110.38   |
| 3   | M     | 1   | NAG  | O3-C3-C4 | -3.63 | 101.81      | 110.38   |
| 3   | 2     | 1   | NAG  | O3-C3-C4 | -3.63 | 101.82      | 110.38   |
| 3   | CA    | 2   | NAG  | O4-C4-C3 | -3.62 | 101.85      | 110.38   |
| 3   | W     | 2   | NAG  | O4-C4-C3 | -3.61 | 101.86      | 110.38   |
| 3   | d     | 1   | NAG  | O7-C7-N2 | -3.61 | 115.60      | 121.98   |
| 3   | y     | 1   | NAG  | O7-C7-N2 | -3.61 | 115.60      | 121.98   |
| 3   | I     | 1   | NAG  | O7-C7-N2 | -3.61 | 115.61      | 121.98   |
| 3   | r     | 2   | NAG  | O4-C4-C3 | -3.61 | 101.87      | 110.38   |
| 3   | z     | 1   | NAG  | O4-C4-C3 | -3.58 | 101.94      | 110.38   |
| 3   | e     | 1   | NAG  | O4-C4-C3 | -3.57 | 101.95      | 110.38   |
| 3   | J     | 1   | NAG  | O4-C4-C3 | -3.57 | 101.97      | 110.38   |
| 5   | H     | 4   | MAN  | C6-C5-C4 | 3.56  | 121.76      | 113.02   |
| 4   | U     | 2   | NAG  | O3-C3-C4 | 3.56  | 118.76      | 110.38   |
| 5   | c     | 4   | MAN  | C6-C5-C4 | 3.56  | 121.75      | 113.02   |
| 3   | 8     | 1   | NAG  | C6-C5-C4 | 3.56  | 121.75      | 113.02   |
| 4   | p     | 2   | NAG  | O3-C3-C4 | 3.55  | 118.75      | 110.38   |
| 5   | x     | 4   | MAN  | C6-C5-C4 | 3.55  | 121.74      | 113.02   |
| 4   | AA    | 2   | NAG  | O3-C3-C4 | 3.54  | 118.73      | 110.38   |
| 3   | S     | 1   | NAG  | C6-C5-C4 | 3.54  | 121.72      | 113.02   |
| 3   | n     | 1   | NAG  | C6-C5-C4 | 3.54  | 121.70      | 113.02   |
| 2   | t     | 2   | NAG  | O3-C3-C2 | -3.54 | 102.06      | 109.40   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 2   | D     | 2   | NAG  | O3-C3-C2 | -3.53 | 102.06      | 109.40   |
| 2   | D     | 5   | MAN  | C6-C5-C4 | 3.53  | 121.69      | 113.02   |
| 2   | Y     | 2   | NAG  | O3-C3-C2 | -3.52 | 102.09      | 109.40   |
| 2   | Y     | 5   | MAN  | C6-C5-C4 | 3.52  | 121.66      | 113.02   |
| 2   | t     | 5   | MAN  | C6-C5-C4 | 3.51  | 121.63      | 113.02   |
| 7   | 4     | 1   | NAG  | O3-C3-C4 | 3.44  | 118.49      | 110.38   |
| 7   | O     | 1   | NAG  | O3-C3-C4 | 3.44  | 118.47      | 110.38   |
| 7   | j     | 1   | NAG  | O3-C3-C4 | 3.43  | 118.47      | 110.38   |
| 3   | h     | 2   | NAG  | C6-C5-C4 | 3.43  | 121.44      | 113.02   |
| 3   | 2     | 2   | NAG  | C6-C5-C4 | 3.43  | 121.43      | 113.02   |
| 3   | M     | 2   | NAG  | C6-C5-C4 | 3.42  | 121.42      | 113.02   |
| 8   | V     | 4   | MAN  | C6-C5-C4 | 3.42  | 121.41      | 113.02   |
| 8   | q     | 4   | MAN  | C6-C5-C4 | 3.41  | 121.40      | 113.02   |
| 8   | N     | 1   | NAG  | O3-C3-C4 | -3.41 | 102.34      | 110.38   |
| 8   | 3     | 1   | NAG  | O3-C3-C4 | -3.41 | 102.34      | 110.38   |
| 8   | BA    | 4   | MAN  | C6-C5-C4 | 3.41  | 121.39      | 113.02   |
| 8   | i     | 1   | NAG  | O3-C3-C4 | -3.41 | 102.34      | 110.38   |
| 3   | R     | 1   | NAG  | O4-C4-C3 | -3.38 | 102.42      | 110.38   |
| 3   | 7     | 1   | NAG  | O4-C4-C3 | -3.37 | 102.42      | 110.38   |
| 3   | m     | 1   | NAG  | O4-C4-C3 | -3.37 | 102.42      | 110.38   |
| 3   | e     | 1   | NAG  | O3-C3-C2 | -3.37 | 102.39      | 109.40   |
| 7   | X     | 2   | NAG  | C6-C5-C4 | 3.37  | 121.30      | 113.02   |
| 7   | 4     | 2   | NAG  | O3-C3-C4 | -3.37 | 102.43      | 110.38   |
| 3   | z     | 1   | NAG  | O3-C3-C2 | -3.37 | 102.40      | 109.40   |
| 7   | DA    | 2   | NAG  | C6-C5-C4 | 3.37  | 121.30      | 113.02   |
| 7   | s     | 2   | NAG  | C6-C5-C4 | 3.37  | 121.29      | 113.02   |
| 3   | J     | 1   | NAG  | O3-C3-C2 | -3.37 | 102.40      | 109.40   |
| 7   | j     | 2   | NAG  | O3-C3-C4 | -3.37 | 102.44      | 110.38   |
| 7   | O     | 2   | NAG  | O3-C3-C4 | -3.37 | 102.44      | 110.38   |
| 2   | Y     | 6   | MAN  | O3-C3-C2 | -3.34 | 103.25      | 110.05   |
| 2   | t     | 6   | MAN  | O3-C3-C2 | -3.31 | 103.31      | 110.05   |
| 7   | X     | 3   | BMA  | O4-C4-C3 | -3.30 | 102.60      | 110.38   |
| 7   | DA    | 3   | BMA  | O4-C4-C3 | -3.30 | 102.61      | 110.38   |
| 2   | D     | 6   | MAN  | O3-C3-C2 | -3.29 | 103.34      | 110.05   |
| 7   | s     | 3   | BMA  | O4-C4-C3 | -3.29 | 102.62      | 110.38   |
| 4   | F     | 1   | NAG  | C8-C7-N2 | 3.28  | 121.56      | 116.12   |
| 4   | v     | 1   | NAG  | C8-C7-N2 | 3.28  | 121.56      | 116.12   |
| 4   | a     | 1   | NAG  | C8-C7-N2 | 3.28  | 121.55      | 116.12   |
| 6   | f     | 5   | MAN  | O3-C3-C2 | 3.26  | 116.71      | 110.05   |
| 5   | c     | 1   | NAG  | O5-C5-C6 | -3.25 | 101.34      | 107.66   |
| 7   | DA    | 2   | NAG  | C2-N2-C7 | -3.25 | 118.55      | 122.90   |
| 3   | u     | 2   | NAG  | O5-C1-C2 | -3.24 | 106.27      | 111.29   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 6   | K     | 5   | MAN  | O3-C3-C2 | 3.24  | 116.67      | 110.05   |
| 7   | X     | 2   | NAG  | C2-N2-C7 | -3.24 | 118.56      | 122.90   |
| 6   | 0     | 5   | MAN  | O3-C3-C2 | 3.24  | 116.67      | 110.05   |
| 7   | s     | 2   | NAG  | C2-N2-C7 | -3.24 | 118.56      | 122.90   |
| 5   | H     | 1   | NAG  | O5-C5-C6 | -3.24 | 101.36      | 107.66   |
| 5   | x     | 1   | NAG  | O5-C5-C6 | -3.23 | 101.37      | 107.66   |
| 3   | Z     | 2   | NAG  | O5-C1-C2 | -3.23 | 106.29      | 111.29   |
| 3   | E     | 2   | NAG  | O5-C1-C2 | -3.23 | 106.29      | 111.29   |
| 3   | k     | 2   | NAG  | O4-C4-C5 | -3.22 | 101.41      | 109.32   |
| 3   | P     | 2   | NAG  | O4-C4-C5 | -3.21 | 101.42      | 109.32   |
| 3   | 5     | 2   | NAG  | O4-C4-C5 | -3.21 | 101.43      | 109.32   |
| 6   | K     | 1   | NAG  | O3-C3-C4 | -3.20 | 102.83      | 110.38   |
| 6   | 0     | 1   | NAG  | O3-C3-C4 | -3.19 | 102.85      | 110.38   |
| 6   | f     | 1   | NAG  | O3-C3-C4 | -3.18 | 102.87      | 110.38   |
| 7   | g     | 2   | NAG  | C1-C2-N2 | 3.18  | 115.44      | 110.43   |
| 7   | L     | 2   | NAG  | C1-C2-N2 | 3.17  | 115.43      | 110.43   |
| 7   | 1     | 2   | NAG  | C1-C2-N2 | 3.16  | 115.42      | 110.43   |
| 2   | Y     | 2   | NAG  | C1-O5-C5 | 3.16  | 116.42      | 112.19   |
| 2   | D     | 2   | NAG  | C1-O5-C5 | 3.15  | 116.41      | 112.19   |
| 2   | t     | 2   | NAG  | C1-O5-C5 | 3.14  | 116.40      | 112.19   |
| 3   | R     | 2   | NAG  | O3-C3-C2 | 3.14  | 115.92      | 109.40   |
| 3   | 7     | 2   | NAG  | O3-C3-C2 | 3.14  | 115.92      | 109.40   |
| 3   | m     | 2   | NAG  | O3-C3-C2 | 3.14  | 115.92      | 109.40   |
| 8   | i     | 3   | BMA  | O2-C2-C1 | 3.09  | 116.29      | 109.22   |
| 8   | N     | 3   | BMA  | O2-C2-C1 | 3.09  | 116.29      | 109.22   |
| 8   | 3     | 3   | BMA  | O2-C2-C1 | 3.08  | 116.28      | 109.22   |
| 3   | w     | 1   | NAG  | C6-C5-C4 | 3.07  | 120.57      | 113.02   |
| 3   | b     | 1   | NAG  | C6-C5-C4 | 3.06  | 120.54      | 113.02   |
| 3   | G     | 1   | NAG  | C6-C5-C4 | 3.05  | 120.51      | 113.02   |
| 8   | q     | 2   | NAG  | O3-C3-C4 | 3.05  | 117.57      | 110.38   |
| 8   | V     | 2   | NAG  | O3-C3-C4 | 3.05  | 117.56      | 110.38   |
| 8   | BA    | 2   | NAG  | O3-C3-C4 | 3.04  | 117.55      | 110.38   |
| 3   | r     | 2   | NAG  | O5-C1-C2 | -3.04 | 106.59      | 111.29   |
| 3   | b     | 1   | NAG  | O5-C5-C6 | 3.03  | 113.56      | 107.66   |
| 3   | W     | 2   | NAG  | O5-C1-C2 | -3.03 | 106.60      | 111.29   |
| 3   | CA    | 2   | NAG  | O5-C1-C2 | -3.03 | 106.60      | 111.29   |
| 3   | w     | 1   | NAG  | O5-C5-C6 | 3.02  | 113.55      | 107.66   |
| 3   | G     | 1   | NAG  | O5-C5-C6 | 3.02  | 113.55      | 107.66   |
| 8   | 3     | 5   | MAN  | O2-C2-C1 | 3.02  | 116.13      | 109.22   |
| 8   | N     | 5   | MAN  | O2-C2-C1 | 3.02  | 116.13      | 109.22   |
| 2   | D     | 2   | NAG  | O3-C3-C4 | -3.01 | 103.27      | 110.38   |
| 4   | p     | 3   | BMA  | O4-C4-C3 | -3.01 | 103.28      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 8   | i     | 5   | MAN  | O2-C2-C1 | 3.01  | 116.12      | 109.22   |
| 3   | 8     | 1   | NAG  | O3-C3-C4 | -3.01 | 103.29      | 110.38   |
| 4   | U     | 3   | BMA  | O4-C4-C3 | -3.01 | 103.29      | 110.38   |
| 4   | AA    | 3   | BMA  | O4-C4-C3 | -3.01 | 103.29      | 110.38   |
| 2   | t     | 2   | NAG  | O3-C3-C4 | -3.00 | 103.30      | 110.38   |
| 2   | Y     | 2   | NAG  | O3-C3-C4 | -3.00 | 103.30      | 110.38   |
| 3   | S     | 1   | NAG  | O3-C3-C4 | -3.00 | 103.31      | 110.38   |
| 3   | 7     | 1   | NAG  | O3-C3-C2 | -3.00 | 103.17      | 109.40   |
| 3   | n     | 1   | NAG  | O3-C3-C4 | -2.99 | 103.33      | 110.38   |
| 6   | 0     | 3   | BMA  | O2-C2-C3 | 2.99  | 116.34      | 110.15   |
| 3   | R     | 1   | NAG  | O3-C3-C2 | -2.98 | 103.22      | 109.40   |
| 3   | m     | 1   | NAG  | O3-C3-C2 | -2.97 | 103.22      | 109.40   |
| 6   | K     | 3   | BMA  | O2-C2-C3 | 2.97  | 116.30      | 110.15   |
| 5   | x     | 2   | NAG  | C2-N2-C7 | -2.96 | 118.93      | 122.90   |
| 3   | CA    | 1   | NAG  | O3-C3-C4 | -2.96 | 103.40      | 110.38   |
| 3   | r     | 1   | NAG  | O3-C3-C4 | -2.96 | 103.41      | 110.38   |
| 6   | f     | 3   | BMA  | O2-C2-C3 | 2.95  | 116.26      | 110.15   |
| 3   | P     | 2   | NAG  | C6-C5-C4 | 2.95  | 120.26      | 113.02   |
| 5   | H     | 2   | NAG  | C2-N2-C7 | -2.95 | 118.95      | 122.90   |
| 3   | k     | 2   | NAG  | C6-C5-C4 | 2.95  | 120.25      | 113.02   |
| 3   | 5     | 2   | NAG  | C6-C5-C4 | 2.95  | 120.25      | 113.02   |
| 3   | W     | 1   | NAG  | O3-C3-C4 | -2.94 | 103.44      | 110.38   |
| 5   | c     | 2   | NAG  | C2-N2-C7 | -2.94 | 118.96      | 122.90   |
| 8   | BA    | 3   | BMA  | O3-C3-C2 | -2.94 | 104.06      | 110.05   |
| 8   | V     | 3   | BMA  | O3-C3-C2 | -2.94 | 104.06      | 110.05   |
| 8   | q     | 3   | BMA  | O3-C3-C2 | -2.94 | 104.06      | 110.05   |
| 3   | r     | 1   | NAG  | C6-C5-C4 | -2.93 | 105.81      | 113.02   |
| 3   | CA    | 1   | NAG  | C6-C5-C4 | -2.93 | 105.82      | 113.02   |
| 3   | W     | 1   | NAG  | C6-C5-C4 | -2.93 | 105.84      | 113.02   |
| 8   | N     | 4   | MAN  | C6-C5-C4 | 2.91  | 120.17      | 113.02   |
| 7   | s     | 2   | NAG  | O3-C3-C2 | -2.91 | 103.36      | 109.40   |
| 8   | 3     | 4   | MAN  | C6-C5-C4 | 2.91  | 120.16      | 113.02   |
| 7   | X     | 2   | NAG  | O3-C3-C2 | -2.91 | 103.36      | 109.40   |
| 8   | i     | 4   | MAN  | C6-C5-C4 | 2.90  | 120.15      | 113.02   |
| 7   | DA    | 2   | NAG  | O3-C3-C2 | -2.90 | 103.38      | 109.40   |
| 6   | 0     | 8   | MAN  | O2-C2-C3 | 2.89  | 116.14      | 110.15   |
| 6   | K     | 8   | MAN  | O2-C2-C3 | 2.88  | 116.13      | 110.15   |
| 6   | f     | 8   | MAN  | O2-C2-C3 | 2.87  | 116.10      | 110.15   |
| 6   | 0     | 3   | BMA  | C2-C3-C4 | -2.84 | 105.86      | 110.86   |
| 4   | a     | 1   | NAG  | C2-N2-C7 | -2.84 | 119.10      | 122.90   |
| 4   | F     | 1   | NAG  | C2-N2-C7 | -2.83 | 119.10      | 122.90   |
| 7   | X     | 2   | NAG  | C8-C7-N2 | 2.83  | 120.81      | 116.12   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | s     | 2   | NAG  | C8-C7-N2 | 2.83  | 120.81      | 116.12   |
| 4   | v     | 1   | NAG  | C2-N2-C7 | -2.83 | 119.11      | 122.90   |
| 2   | Y     | 3   | BMA  | O2-C2-C3 | 2.82  | 116.00      | 110.15   |
| 6   | K     | 3   | BMA  | C2-C3-C4 | -2.82 | 105.91      | 110.86   |
| 7   | DA    | 2   | NAG  | C8-C7-N2 | 2.81  | 120.78      | 116.12   |
| 2   | D     | 3   | BMA  | O2-C2-C3 | 2.81  | 115.97      | 110.15   |
| 2   | t     | 3   | BMA  | O2-C2-C3 | 2.81  | 115.96      | 110.15   |
| 6   | f     | 3   | BMA  | C2-C3-C4 | -2.80 | 105.94      | 110.86   |
| 8   | BA    | 2   | NAG  | C8-C7-N2 | 2.80  | 120.76      | 116.12   |
| 8   | q     | 2   | NAG  | C8-C7-N2 | 2.80  | 120.76      | 116.12   |
| 8   | V     | 2   | NAG  | C8-C7-N2 | 2.80  | 120.75      | 116.12   |
| 7   | 1     | 1   | NAG  | C1-O5-C5 | 2.77  | 115.89      | 112.19   |
| 2   | Y     | 5   | MAN  | O2-C2-C3 | 2.76  | 115.87      | 110.15   |
| 7   | L     | 1   | NAG  | C1-O5-C5 | 2.76  | 115.89      | 112.19   |
| 2   | D     | 5   | MAN  | O2-C2-C3 | 2.76  | 115.86      | 110.15   |
| 3   | E     | 1   | NAG  | C8-C7-N2 | 2.76  | 120.69      | 116.12   |
| 3   | J     | 1   | NAG  | C8-C7-N2 | 2.76  | 120.69      | 116.12   |
| 3   | z     | 1   | NAG  | C8-C7-N2 | 2.76  | 120.69      | 116.12   |
| 2   | D     | 5   | MAN  | O5-C5-C6 | -2.75 | 102.30      | 107.66   |
| 3   | e     | 1   | NAG  | C8-C7-N2 | 2.75  | 120.68      | 116.12   |
| 2   | t     | 5   | MAN  | O2-C2-C3 | 2.75  | 115.85      | 110.15   |
| 3   | u     | 1   | NAG  | C8-C7-N2 | 2.75  | 120.68      | 116.12   |
| 3   | M     | 1   | NAG  | C8-C7-N2 | 2.74  | 120.67      | 116.12   |
| 2   | t     | 5   | MAN  | O5-C5-C6 | -2.74 | 102.33      | 107.66   |
| 7   | g     | 1   | NAG  | C1-O5-C5 | 2.74  | 115.86      | 112.19   |
| 3   | Z     | 1   | NAG  | C8-C7-N2 | 2.73  | 120.65      | 116.12   |
| 8   | i     | 4   | MAN  | O4-C4-C3 | -2.73 | 103.94      | 110.38   |
| 3   | h     | 1   | NAG  | C8-C7-N2 | 2.73  | 120.64      | 116.12   |
| 8   | 3     | 4   | MAN  | O4-C4-C3 | -2.73 | 103.94      | 110.38   |
| 3   | T     | 1   | NAG  | C8-C7-N2 | 2.73  | 120.64      | 116.12   |
| 3   | 2     | 1   | NAG  | C8-C7-N2 | 2.73  | 120.64      | 116.12   |
| 3   | o     | 1   | NAG  | C8-C7-N2 | 2.73  | 120.64      | 116.12   |
| 8   | N     | 4   | MAN  | O4-C4-C3 | -2.72 | 103.96      | 110.38   |
| 5   | c     | 1   | NAG  | C8-C7-N2 | 2.72  | 120.63      | 116.12   |
| 2   | Y     | 5   | MAN  | O5-C5-C6 | -2.72 | 102.38      | 107.66   |
| 5   | H     | 1   | NAG  | C8-C7-N2 | 2.72  | 120.62      | 116.12   |
| 3   | 9     | 1   | NAG  | C8-C7-N2 | 2.71  | 120.61      | 116.12   |
| 3   | 5     | 1   | NAG  | O3-C3-C4 | 2.71  | 116.76      | 110.38   |
| 7   | X     | 1   | NAG  | C6-C5-C4 | 2.70  | 119.64      | 113.02   |
| 3   | k     | 1   | NAG  | O3-C3-C4 | 2.70  | 116.73      | 110.38   |
| 5   | x     | 1   | NAG  | C8-C7-N2 | 2.69  | 120.59      | 116.12   |
| 3   | P     | 1   | NAG  | O3-C3-C4 | 2.69  | 116.72      | 110.38   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | s     | 1   | NAG  | C6-C5-C4 | 2.69  | 119.62      | 113.02   |
| 8   | 3     | 1   | NAG  | C8-C7-N2 | 2.69  | 120.58      | 116.12   |
| 7   | DA    | 1   | NAG  | C6-C5-C4 | 2.69  | 119.62      | 113.02   |
| 8   | N     | 1   | NAG  | C8-C7-N2 | 2.67  | 120.55      | 116.12   |
| 8   | i     | 1   | NAG  | C8-C7-N2 | 2.67  | 120.54      | 116.12   |
| 6   | f     | 7   | MAN  | C1-O5-C5 | 2.66  | 115.75      | 112.19   |
| 7   | DA    | 1   | NAG  | C8-C7-N2 | 2.66  | 120.53      | 116.12   |
| 6   | K     | 7   | MAN  | C1-O5-C5 | 2.66  | 115.75      | 112.19   |
| 3   | m     | 1   | NAG  | C8-C7-N2 | 2.64  | 120.50      | 116.12   |
| 3   | I     | 2   | NAG  | O4-C4-C5 | 2.64  | 115.83      | 109.32   |
| 3   | d     | 2   | NAG  | O4-C4-C5 | 2.64  | 115.83      | 109.32   |
| 3   | y     | 2   | NAG  | O4-C4-C5 | 2.64  | 115.83      | 109.32   |
| 6   | 0     | 7   | MAN  | C1-O5-C5 | 2.64  | 115.72      | 112.19   |
| 3   | R     | 1   | NAG  | C8-C7-N2 | 2.64  | 120.49      | 116.12   |
| 3   | 7     | 1   | NAG  | C8-C7-N2 | 2.64  | 120.49      | 116.12   |
| 7   | X     | 1   | NAG  | C8-C7-N2 | 2.63  | 120.48      | 116.12   |
| 3   | J     | 1   | NAG  | C6-C5-C4 | 2.63  | 119.47      | 113.02   |
| 3   | e     | 1   | NAG  | C6-C5-C4 | 2.62  | 119.46      | 113.02   |
| 3   | z     | 1   | NAG  | C6-C5-C4 | 2.62  | 119.45      | 113.02   |
| 7   | s     | 1   | NAG  | C8-C7-N2 | 2.62  | 120.46      | 116.12   |
| 7   | j     | 3   | BMA  | C6-C5-C4 | 2.60  | 119.41      | 113.02   |
| 7   | O     | 3   | BMA  | C6-C5-C4 | 2.60  | 119.40      | 113.02   |
| 7   | 4     | 3   | BMA  | C6-C5-C4 | 2.60  | 119.39      | 113.02   |
| 3   | 2     | 2   | NAG  | O3-C3-C2 | -2.59 | 104.01      | 109.40   |
| 3   | h     | 2   | NAG  | O3-C3-C2 | -2.58 | 104.04      | 109.40   |
| 3   | M     | 2   | NAG  | O3-C3-C2 | -2.58 | 104.05      | 109.40   |
| 4   | a     | 4   | MAN  | O4-C4-C5 | -2.58 | 102.98      | 109.32   |
| 4   | v     | 4   | MAN  | O4-C4-C5 | -2.57 | 102.99      | 109.32   |
| 4   | F     | 4   | MAN  | O4-C4-C5 | -2.57 | 102.99      | 109.32   |
| 3   | Z     | 1   | NAG  | C2-N2-C7 | -2.57 | 119.45      | 122.90   |
| 4   | v     | 1   | NAG  | C6-C5-C4 | 2.57  | 119.33      | 113.02   |
| 3   | u     | 1   | NAG  | C2-N2-C7 | -2.57 | 119.46      | 122.90   |
| 3   | CA    | 1   | NAG  | C3-C4-C5 | -2.56 | 105.59      | 110.23   |
| 8   | BA    | 4   | MAN  | O2-C2-C1 | 2.55  | 115.07      | 109.22   |
| 4   | a     | 1   | NAG  | C6-C5-C4 | 2.55  | 119.29      | 113.02   |
| 4   | F     | 1   | NAG  | C6-C5-C4 | 2.55  | 119.29      | 113.02   |
| 3   | E     | 1   | NAG  | C2-N2-C7 | -2.55 | 119.48      | 122.90   |
| 3   | r     | 1   | NAG  | C3-C4-C5 | -2.55 | 105.61      | 110.23   |
| 8   | V     | 4   | MAN  | O2-C2-C1 | 2.54  | 115.04      | 109.22   |
| 3   | W     | 1   | NAG  | C3-C4-C5 | -2.53 | 105.64      | 110.23   |
| 8   | q     | 4   | MAN  | O2-C2-C1 | 2.52  | 114.99      | 109.22   |
| 7   | O     | 1   | NAG  | C6-C5-C4 | 2.51  | 119.18      | 113.02   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | j     | 1   | NAG  | C6-C5-C4 | 2.51  | 119.18      | 113.02   |
| 8   | i     | 4   | MAN  | O2-C2-C1 | 2.51  | 114.96      | 109.22   |
| 7   | 4     | 1   | NAG  | C6-C5-C4 | 2.50  | 119.16      | 113.02   |
| 8   | N     | 4   | MAN  | O2-C2-C1 | 2.50  | 114.94      | 109.22   |
| 8   | 3     | 4   | MAN  | O2-C2-C1 | 2.50  | 114.94      | 109.22   |
| 3   | w     | 2   | NAG  | O4-C4-C5 | -2.49 | 103.19      | 109.32   |
| 3   | G     | 2   | NAG  | O4-C4-C5 | -2.48 | 103.20      | 109.32   |
| 3   | b     | 2   | NAG  | O4-C4-C5 | -2.48 | 103.21      | 109.32   |
| 3   | z     | 2   | NAG  | O4-C4-C5 | -2.48 | 103.22      | 109.32   |
| 3   | e     | 2   | NAG  | O4-C4-C5 | -2.47 | 103.23      | 109.32   |
| 3   | J     | 2   | NAG  | O4-C4-C5 | -2.47 | 103.25      | 109.32   |
| 7   | g     | 2   | NAG  | C1-O5-C5 | 2.45  | 115.47      | 112.19   |
| 7   | L     | 2   | NAG  | C1-O5-C5 | 2.45  | 115.47      | 112.19   |
| 3   | 6     | 1   | NAG  | C3-C4-C5 | -2.45 | 105.79      | 110.23   |
| 3   | Q     | 1   | NAG  | C3-C4-C5 | -2.44 | 105.80      | 110.23   |
| 3   | l     | 1   | NAG  | C3-C4-C5 | -2.44 | 105.81      | 110.23   |
| 7   | s     | 2   | NAG  | O3-C3-C4 | 2.44  | 116.13      | 110.38   |
| 7   | X     | 2   | NAG  | O3-C3-C4 | 2.44  | 116.12      | 110.38   |
| 2   | t     | 1   | NAG  | C1-C2-N2 | 2.43  | 114.27      | 110.43   |
| 7   | 1     | 2   | NAG  | C1-O5-C5 | 2.43  | 115.45      | 112.19   |
| 7   | DA    | 2   | NAG  | O3-C3-C4 | 2.43  | 116.11      | 110.38   |
| 3   | 6     | 1   | NAG  | C8-C7-N2 | 2.43  | 120.15      | 116.12   |
| 6   | 0     | 1   | NAG  | C8-C7-N2 | 2.43  | 120.14      | 116.12   |
| 7   | 4     | 2   | NAG  | C2-N2-C7 | -2.43 | 119.65      | 122.90   |
| 6   | K     | 1   | NAG  | C8-C7-N2 | 2.43  | 120.14      | 116.12   |
| 4   | AA    | 1   | NAG  | C8-C7-N2 | 2.42  | 120.14      | 116.12   |
| 3   | l     | 1   | NAG  | C8-C7-N2 | 2.42  | 120.13      | 116.12   |
| 6   | f     | 1   | NAG  | C8-C7-N2 | 2.42  | 120.13      | 116.12   |
| 8   | N     | 2   | NAG  | C2-N2-C7 | -2.42 | 119.66      | 122.90   |
| 3   | Q     | 1   | NAG  | C8-C7-N2 | 2.42  | 120.13      | 116.12   |
| 4   | U     | 1   | NAG  | C8-C7-N2 | 2.42  | 120.13      | 116.12   |
| 8   | i     | 2   | NAG  | C2-N2-C7 | -2.42 | 119.66      | 122.90   |
| 4   | p     | 1   | NAG  | C8-C7-N2 | 2.41  | 120.12      | 116.12   |
| 8   | 3     | 2   | NAG  | C2-N2-C7 | -2.41 | 119.67      | 122.90   |
| 2   | D     | 1   | NAG  | C1-C2-N2 | 2.41  | 114.23      | 110.43   |
| 3   | CA    | 2   | NAG  | O5-C5-C6 | -2.41 | 102.98      | 107.66   |
| 7   | O     | 2   | NAG  | C2-N2-C7 | -2.40 | 119.68      | 122.90   |
| 3   | 6     | 1   | NAG  | C1-C2-N2 | 2.40  | 114.21      | 110.43   |
| 3   | W     | 2   | NAG  | O5-C5-C6 | -2.39 | 103.00      | 107.66   |
| 3   | Q     | 1   | NAG  | C1-C2-N2 | 2.39  | 114.20      | 110.43   |
| 2   | Y     | 1   | NAG  | C1-C2-N2 | 2.39  | 114.19      | 110.43   |
| 7   | j     | 2   | NAG  | C2-N2-C7 | -2.38 | 119.70      | 122.90   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 3   | l     | 1   | NAG  | C1-C2-N2 | 2.38  | 114.19      | 110.43   |
| 4   | a     | 3   | BMA  | O3-C3-C2 | 2.38  | 114.92      | 110.05   |
| 8   | 3     | 3   | BMA  | O4-C4-C5 | 2.38  | 115.18      | 109.32   |
| 4   | F     | 3   | BMA  | O3-C3-C2 | 2.38  | 114.91      | 110.05   |
| 4   | v     | 3   | BMA  | O3-C3-C2 | 2.37  | 114.90      | 110.05   |
| 3   | r     | 2   | NAG  | O5-C5-C6 | -2.37 | 103.04      | 107.66   |
| 8   | N     | 3   | BMA  | O4-C4-C5 | 2.36  | 115.15      | 109.32   |
| 7   | 1     | 2   | NAG  | O5-C1-C2 | -2.36 | 107.65      | 111.29   |
| 6   | 0     | 8   | MAN  | O2-C2-C1 | 2.35  | 114.61      | 109.22   |
| 8   | i     | 3   | BMA  | O4-C4-C5 | 2.35  | 115.10      | 109.32   |
| 5   | x     | 2   | NAG  | C8-C7-N2 | 2.35  | 120.01      | 116.12   |
| 5   | c     | 2   | NAG  | C8-C7-N2 | 2.34  | 120.01      | 116.12   |
| 5   | H     | 2   | NAG  | C8-C7-N2 | 2.34  | 120.00      | 116.12   |
| 3   | w     | 1   | NAG  | C8-C7-N2 | 2.34  | 120.00      | 116.12   |
| 7   | g     | 2   | NAG  | O5-C1-C2 | -2.34 | 107.67      | 111.29   |
| 6   | f     | 8   | MAN  | O2-C2-C1 | 2.34  | 114.58      | 109.22   |
| 6   | K     | 8   | MAN  | O2-C2-C1 | 2.34  | 114.57      | 109.22   |
| 7   | L     | 2   | NAG  | O5-C1-C2 | -2.34 | 107.67      | 111.29   |
| 8   | N     | 1   | NAG  | C1-C2-N2 | -2.34 | 106.75      | 110.43   |
| 3   | b     | 1   | NAG  | C8-C7-N2 | 2.33  | 119.99      | 116.12   |
| 8   | 3     | 1   | NAG  | C1-C2-N2 | -2.33 | 106.76      | 110.43   |
| 3   | G     | 1   | NAG  | C8-C7-N2 | 2.33  | 119.98      | 116.12   |
| 3   | h     | 1   | NAG  | C2-N2-C7 | -2.33 | 119.78      | 122.90   |
| 8   | q     | 1   | NAG  | C1-C2-N2 | -2.33 | 106.77      | 110.43   |
| 8   | i     | 1   | NAG  | C1-C2-N2 | -2.32 | 106.77      | 110.43   |
| 5   | x     | 4   | MAN  | O4-C4-C3 | -2.32 | 104.91      | 110.38   |
| 5   | c     | 4   | MAN  | O4-C4-C3 | -2.32 | 104.91      | 110.38   |
| 5   | H     | 4   | MAN  | O4-C4-C3 | -2.32 | 104.92      | 110.38   |
| 8   | BA    | 1   | NAG  | C1-C2-N2 | -2.31 | 106.79      | 110.43   |
| 8   | V     | 1   | NAG  | C1-C2-N2 | -2.31 | 106.80      | 110.43   |
| 2   | Y     | 4   | MAN  | C1-O5-C5 | 2.30  | 115.27      | 112.19   |
| 3   | 2     | 1   | NAG  | C2-N2-C7 | -2.30 | 119.82      | 122.90   |
| 3   | M     | 1   | NAG  | C2-N2-C7 | -2.29 | 119.83      | 122.90   |
| 2   | t     | 4   | MAN  | C1-O5-C5 | 2.27  | 115.23      | 112.19   |
| 7   | DA    | 2   | NAG  | C3-C4-C5 | -2.27 | 106.12      | 110.23   |
| 8   | 3     | 2   | NAG  | C8-C7-N2 | 2.27  | 119.88      | 116.12   |
| 2   | t     | 5   | MAN  | O5-C5-C4 | -2.26 | 105.33      | 110.83   |
| 8   | i     | 2   | NAG  | C8-C7-N2 | 2.26  | 119.87      | 116.12   |
| 7   | s     | 2   | NAG  | C3-C4-C5 | -2.25 | 106.14      | 110.23   |
| 8   | N     | 2   | NAG  | C8-C7-N2 | 2.25  | 119.86      | 116.12   |
| 2   | Y     | 5   | MAN  | O5-C5-C4 | -2.25 | 105.35      | 110.83   |
| 3   | P     | 1   | NAG  | C8-C7-N2 | 2.25  | 119.85      | 116.12   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 7   | X     | 2   | NAG  | C3-C4-C5 | -2.25 | 106.15      | 110.23   |
| 2   | D     | 4   | MAN  | C1-O5-C5 | 2.25  | 115.20      | 112.19   |
| 3   | 5     | 1   | NAG  | C8-C7-N2 | 2.25  | 119.85      | 116.12   |
| 3   | I     | 1   | NAG  | O7-C7-C8 | -2.24 | 118.06      | 122.05   |
| 3   | y     | 1   | NAG  | O7-C7-C8 | -2.24 | 118.07      | 122.05   |
| 2   | D     | 5   | MAN  | O5-C5-C4 | -2.24 | 105.38      | 110.83   |
| 7   | 1     | 1   | NAG  | O7-C7-C8 | -2.23 | 118.08      | 122.05   |
| 3   | d     | 1   | NAG  | O7-C7-C8 | -2.23 | 118.09      | 122.05   |
| 7   | L     | 1   | NAG  | O7-C7-C8 | -2.23 | 118.09      | 122.05   |
| 3   | Z     | 2   | NAG  | C2-N2-C7 | 2.23  | 125.88      | 122.90   |
| 3   | k     | 1   | NAG  | C8-C7-N2 | 2.22  | 119.80      | 116.12   |
| 4   | U     | 2   | NAG  | C8-C7-N2 | 2.22  | 119.80      | 116.12   |
| 4   | p     | 2   | NAG  | C8-C7-N2 | 2.22  | 119.80      | 116.12   |
| 4   | AA    | 2   | NAG  | C8-C7-N2 | 2.22  | 119.79      | 116.12   |
| 7   | g     | 1   | NAG  | O7-C7-C8 | -2.21 | 118.11      | 122.05   |
| 3   | u     | 2   | NAG  | C2-N2-C7 | 2.21  | 125.86      | 122.90   |
| 3   | E     | 2   | NAG  | C2-N2-C7 | 2.20  | 125.85      | 122.90   |
| 8   | q     | 1   | NAG  | O3-C3-C4 | 2.15  | 115.45      | 110.38   |
| 8   | BA    | 1   | NAG  | O3-C3-C4 | 2.15  | 115.44      | 110.38   |
| 7   | j     | 2   | NAG  | C8-C7-N2 | 2.15  | 119.68      | 116.12   |
| 8   | V     | 1   | NAG  | O3-C3-C4 | 2.15  | 115.44      | 110.38   |
| 7   | O     | 2   | NAG  | C8-C7-N2 | 2.14  | 119.67      | 116.12   |
| 3   | J     | 2   | NAG  | C8-C7-N2 | 2.13  | 119.66      | 116.12   |
| 7   | 4     | 2   | NAG  | C8-C7-N2 | 2.13  | 119.65      | 116.12   |
| 4   | AA    | 2   | NAG  | O3-C3-C2 | -2.13 | 104.98      | 109.40   |
| 8   | i     | 2   | NAG  | O3-C3-C4 | -2.12 | 105.37      | 110.38   |
| 3   | e     | 2   | NAG  | C8-C7-N2 | 2.12  | 119.63      | 116.12   |
| 8   | N     | 2   | NAG  | O3-C3-C4 | -2.12 | 105.39      | 110.38   |
| 3   | W     | 1   | NAG  | C2-N2-C7 | -2.11 | 120.07      | 122.90   |
| 8   | 3     | 2   | NAG  | O3-C3-C4 | -2.11 | 105.40      | 110.38   |
| 3   | z     | 2   | NAG  | C8-C7-N2 | 2.11  | 119.62      | 116.12   |
| 3   | r     | 1   | NAG  | C2-N2-C7 | -2.11 | 120.07      | 122.90   |
| 4   | AA    | 2   | NAG  | C2-N2-C7 | -2.11 | 120.07      | 122.90   |
| 4   | U     | 2   | NAG  | O3-C3-C2 | -2.11 | 105.02      | 109.40   |
| 6   | K     | 2   | NAG  | C2-N2-C7 | -2.11 | 120.07      | 122.90   |
| 8   | i     | 5   | MAN  | O4-C4-C5 | 2.11  | 114.51      | 109.32   |
| 5   | c     | 1   | NAG  | O7-C7-C8 | -2.10 | 118.31      | 122.05   |
| 3   | G     | 1   | NAG  | C1-C2-N2 | 2.10  | 113.75      | 110.43   |
| 4   | p     | 2   | NAG  | O3-C3-C2 | -2.10 | 105.03      | 109.40   |
| 3   | CA    | 1   | NAG  | C2-N2-C7 | -2.10 | 120.09      | 122.90   |
| 4   | p     | 2   | NAG  | C2-N2-C7 | -2.10 | 120.09      | 122.90   |
| 4   | v     | 2   | NAG  | C8-C7-N2 | 2.10  | 119.59      | 116.12   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 4   | U     | 2   | NAG  | C2-N2-C7 | -2.09 | 120.09      | 122.90   |
| 5   | H     | 1   | NAG  | O7-C7-C8 | -2.09 | 118.33      | 122.05   |
| 8   | N     | 5   | MAN  | O4-C4-C5 | 2.09  | 114.47      | 109.32   |
| 4   | v     | 3   | BMA  | O2-C2-C1 | -2.09 | 104.44      | 109.22   |
| 4   | F     | 2   | NAG  | C8-C7-N2 | 2.09  | 119.58      | 116.12   |
| 4   | a     | 2   | NAG  | C8-C7-N2 | 2.09  | 119.58      | 116.12   |
| 4   | F     | 3   | BMA  | O2-C2-C1 | -2.09 | 104.44      | 109.22   |
| 8   | BA    | 2   | NAG  | C3-C4-C5 | -2.09 | 106.45      | 110.23   |
| 6   | 0     | 2   | NAG  | C2-N2-C7 | -2.08 | 120.11      | 122.90   |
| 3   | P     | 2   | NAG  | O5-C1-C2 | -2.08 | 108.07      | 111.29   |
| 5   | x     | 1   | NAG  | O7-C7-C8 | -2.08 | 118.35      | 122.05   |
| 7   | 4     | 1   | NAG  | C1-C2-N2 | 2.08  | 113.70      | 110.43   |
| 8   | V     | 2   | NAG  | C3-C4-C5 | -2.07 | 106.47      | 110.23   |
| 6   | f     | 2   | NAG  | C2-N2-C7 | -2.07 | 120.12      | 122.90   |
| 4   | a     | 3   | BMA  | O2-C2-C1 | -2.07 | 104.48      | 109.22   |
| 8   | 3     | 5   | MAN  | O4-C4-C5 | 2.07  | 114.43      | 109.32   |
| 3   | P     | 2   | NAG  | O7-C7-C8 | -2.07 | 118.36      | 122.05   |
| 3   | k     | 2   | NAG  | O5-C1-C2 | -2.07 | 108.09      | 111.29   |
| 5   | H     | 2   | NAG  | C3-C4-C5 | -2.07 | 106.48      | 110.23   |
| 3   | w     | 1   | NAG  | C1-C2-N2 | 2.07  | 113.69      | 110.43   |
| 3   | 5     | 2   | NAG  | O7-C7-C8 | -2.07 | 118.38      | 122.05   |
| 5   | x     | 2   | NAG  | C3-C4-C5 | -2.06 | 106.49      | 110.23   |
| 3   | b     | 1   | NAG  | C1-C2-N2 | 2.06  | 113.69      | 110.43   |
| 8   | q     | 2   | NAG  | C3-C4-C5 | -2.06 | 106.50      | 110.23   |
| 3   | k     | 2   | NAG  | O7-C7-C8 | -2.06 | 118.39      | 122.05   |
| 8   | BA    | 1   | NAG  | C8-C7-N2 | 2.06  | 119.53      | 116.12   |
| 7   | O     | 1   | NAG  | C1-C2-N2 | 2.06  | 113.67      | 110.43   |
| 3   | 5     | 2   | NAG  | O5-C1-C2 | -2.05 | 108.11      | 111.29   |
| 7   | j     | 1   | NAG  | C1-C2-N2 | 2.05  | 113.67      | 110.43   |
| 5   | c     | 2   | NAG  | C3-C4-C5 | -2.05 | 106.51      | 110.23   |
| 8   | V     | 1   | NAG  | C8-C7-N2 | 2.05  | 119.52      | 116.12   |
| 8   | q     | 1   | NAG  | C8-C7-N2 | 2.04  | 119.50      | 116.12   |
| 8   | i     | 4   | MAN  | O2-C2-C3 | 2.03  | 114.35      | 110.15   |
| 8   | N     | 4   | MAN  | O2-C2-C3 | 2.03  | 114.35      | 110.15   |
| 2   | Y     | 2   | NAG  | C8-C7-N2 | 2.03  | 119.48      | 116.12   |
| 8   | 3     | 4   | MAN  | O2-C2-C3 | 2.03  | 114.35      | 110.15   |
| 2   | D     | 2   | NAG  | C8-C7-N2 | 2.02  | 119.47      | 116.12   |
| 3   | E     | 1   | NAG  | O3-C3-C2 | 2.02  | 113.59      | 109.40   |
| 3   | u     | 1   | NAG  | O3-C3-C2 | 2.01  | 113.58      | 109.40   |
| 2   | t     | 2   | NAG  | C8-C7-N2 | 2.01  | 119.44      | 116.12   |
| 3   | Z     | 1   | NAG  | O3-C3-C2 | 2.00  | 113.56      | 109.40   |

There are no chirality outliers.



All (189) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | W     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | r     | 1   | NAG  | C1-C2-N2-C7 |
| 3   | CA    | 1   | NAG  | C1-C2-N2-C7 |
| 5   | H     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | c     | 1   | NAG  | C4-C5-C6-O6 |
| 5   | x     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | V     | 3   | BMA  | C4-C5-C6-O6 |
| 8   | q     | 3   | BMA  | C4-C5-C6-O6 |
| 8   | BA    | 3   | BMA  | C4-C5-C6-O6 |
| 5   | H     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | c     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | x     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | f     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | 0     | 3   | BMA  | C4-C5-C6-O6 |
| 6   | K     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | f     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | 0     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | d     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | y     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | V     | 3   | BMA  | O5-C5-C6-O6 |
| 8   | q     | 3   | BMA  | O5-C5-C6-O6 |
| 8   | BA    | 3   | BMA  | O5-C5-C6-O6 |
| 6   | K     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | f     | 2   | NAG  | C4-C5-C6-O6 |
| 6   | 0     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | H     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | c     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | x     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | Q     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | l     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | 6     | 1   | NAG  | C4-C5-C6-O6 |
| 8   | V     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | q     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | BA    | 2   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | d     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | y     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | V     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | q     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | BA    | 2   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 5   | x     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | H     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | c     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | Q     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | l     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | 6     | 2   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 3   | BMA  | O5-C5-C6-O6 |
| 6   | f     | 3   | BMA  | O5-C5-C6-O6 |
| 6   | 0     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | I     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | I     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | d     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | d     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | y     | 1   | NAG  | C8-C7-N2-C2 |
| 3   | y     | 1   | NAG  | O7-C7-N2-C2 |
| 3   | G     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | b     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | w     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | R     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | m     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | 7     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | Q     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | l     | 2   | NAG  | C4-C5-C6-O6 |
| 3   | 6     | 2   | NAG  | C4-C5-C6-O6 |
| 5   | H     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | c     | 3   | BMA  | C4-C5-C6-O6 |
| 5   | x     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | Q     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | l     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | 6     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | Y     | 2   | NAG  | O5-C5-C6-O6 |
| 2   | t     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | N     | 3   | BMA  | O5-C5-C6-O6 |
| 8   | i     | 3   | BMA  | O5-C5-C6-O6 |
| 8   | 3     | 3   | BMA  | O5-C5-C6-O6 |
| 6   | K     | 7   | MAN  | O5-C5-C6-O6 |
| 6   | f     | 7   | MAN  | O5-C5-C6-O6 |
| 6   | 0     | 7   | MAN  | O5-C5-C6-O6 |
| 3   | I     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | d     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | y     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 7   | O     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | 4     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | j     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | K     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | f     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | 0     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | N     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | i     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | 3     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | J     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | e     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | z     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | S     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | T     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | n     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | o     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | 8     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | 9     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | i     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | N     | 2   | NAG  | C4-C5-C6-O6 |
| 8   | 3     | 2   | NAG  | C4-C5-C6-O6 |
| 2   | D     | 5   | MAN  | O5-C5-C6-O6 |
| 2   | Y     | 5   | MAN  | O5-C5-C6-O6 |
| 2   | t     | 5   | MAN  | O5-C5-C6-O6 |
| 4   | F     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | a     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | v     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | U     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | p     | 3   | BMA  | O5-C5-C6-O6 |
| 4   | AA    | 3   | BMA  | O5-C5-C6-O6 |
| 8   | N     | 3   | BMA  | C4-C5-C6-O6 |
| 8   | i     | 3   | BMA  | C4-C5-C6-O6 |
| 8   | 3     | 3   | BMA  | C4-C5-C6-O6 |
| 3   | T     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | o     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | 9     | 1   | NAG  | O5-C5-C6-O6 |
| 5   | x     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | R     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | m     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | 7     | 2   | NAG  | O5-C5-C6-O6 |
| 5   | H     | 3   | BMA  | O5-C5-C6-O6 |
| 5   | c     | 3   | BMA  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 2   | D     | 3   | BMA  | O5-C5-C6-O6 |
| 2   | Y     | 3   | BMA  | O5-C5-C6-O6 |
| 2   | t     | 3   | BMA  | O5-C5-C6-O6 |
| 3   | W     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | r     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | CA    | 2   | NAG  | O5-C5-C6-O6 |
| 8   | N     | 5   | MAN  | O5-C5-C6-O6 |
| 8   | i     | 5   | MAN  | O5-C5-C6-O6 |
| 8   | 3     | 5   | MAN  | O5-C5-C6-O6 |
| 8   | V     | 1   | NAG  | C3-C2-N2-C7 |
| 8   | q     | 1   | NAG  | C3-C2-N2-C7 |
| 8   | BA    | 1   | NAG  | C3-C2-N2-C7 |
| 2   | D     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | Y     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | t     | 1   | NAG  | O5-C5-C6-O6 |
| 2   | D     | 4   | MAN  | O5-C5-C6-O6 |
| 2   | Y     | 4   | MAN  | O5-C5-C6-O6 |
| 2   | t     | 4   | MAN  | O5-C5-C6-O6 |
| 3   | m     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | 7     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | R     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | P     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | k     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | 5     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | O     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | j     | 1   | NAG  | C4-C5-C6-O6 |
| 7   | 4     | 1   | NAG  | C4-C5-C6-O6 |
| 3   | G     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | Q     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | b     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | l     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | w     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | 6     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | G     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | b     | 2   | NAG  | O5-C5-C6-O6 |
| 3   | w     | 2   | NAG  | O5-C5-C6-O6 |
| 8   | q     | 5   | MAN  | O5-C5-C6-O6 |
| 7   | L     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | g     | 1   | NAG  | O5-C5-C6-O6 |
| 7   | 1     | 1   | NAG  | O5-C5-C6-O6 |
| 8   | V     | 5   | MAN  | O5-C5-C6-O6 |
| 8   | BA    | 5   | MAN  | O5-C5-C6-O6 |

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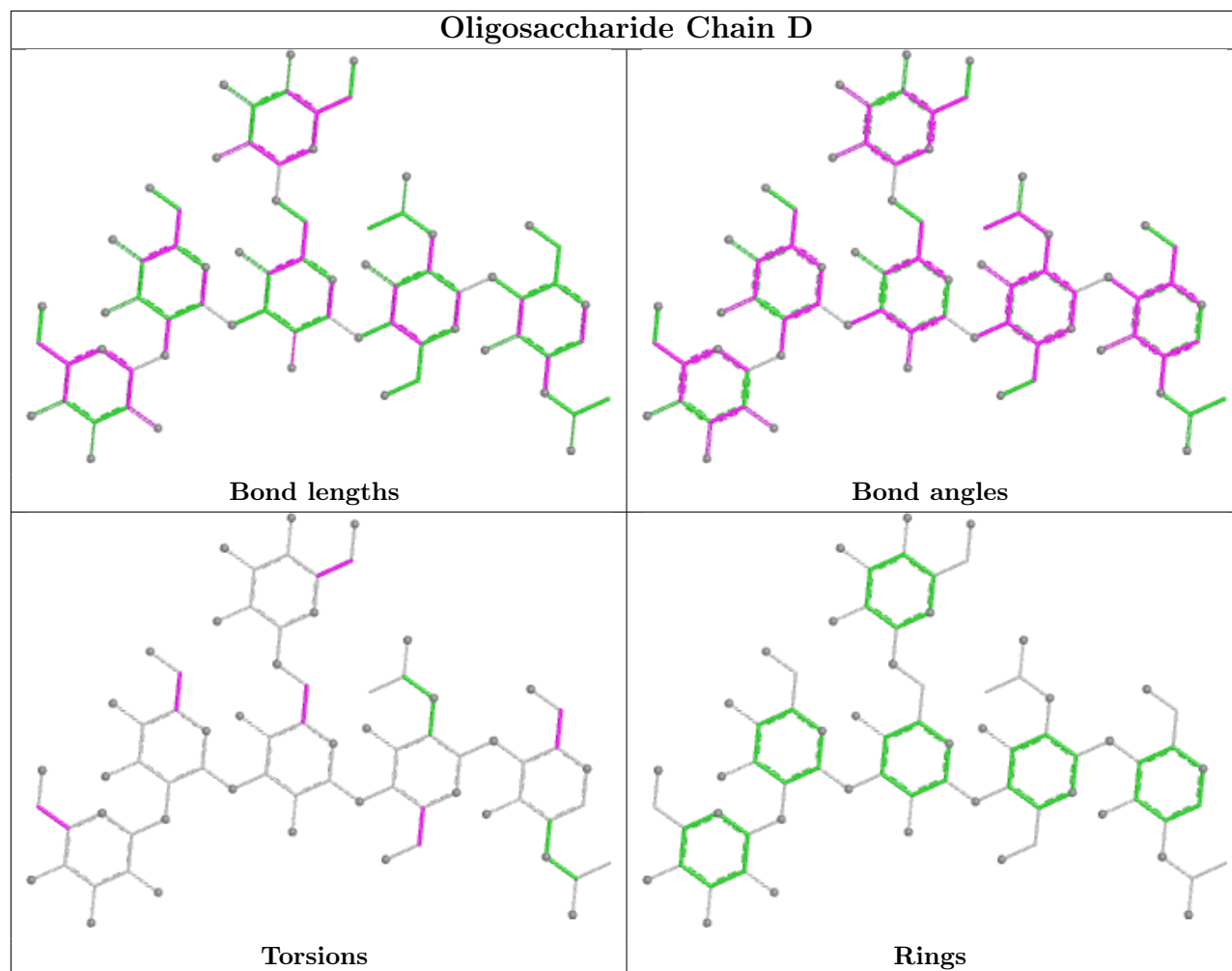
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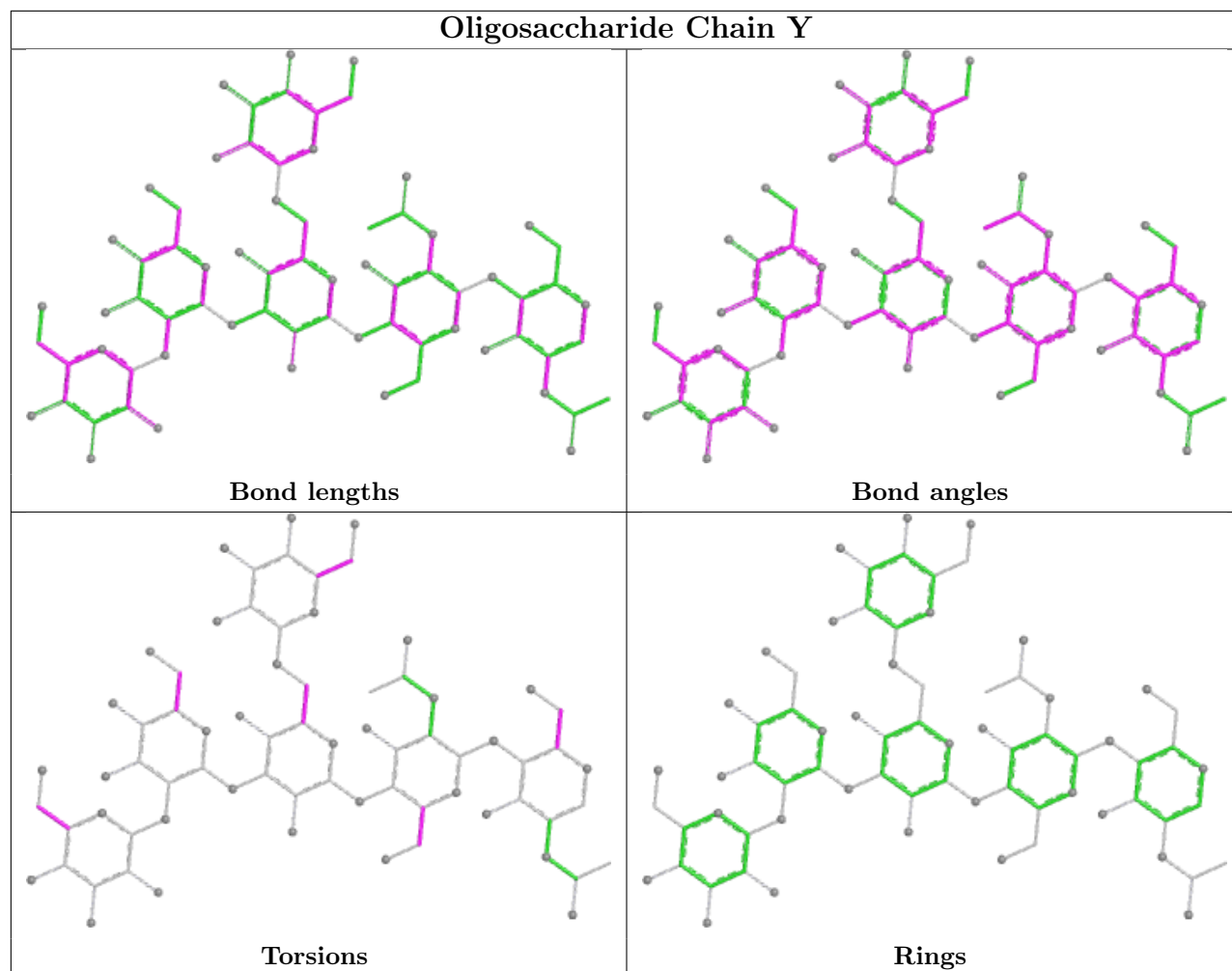
| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 3   | d     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | I     | 1   | NAG  | O5-C5-C6-O6 |
| 3   | y     | 1   | NAG  | O5-C5-C6-O6 |
| 6   | f     | 8   | MAN  | O5-C5-C6-O6 |
| 6   | K     | 8   | MAN  | O5-C5-C6-O6 |
| 6   | 0     | 8   | MAN  | O5-C5-C6-O6 |
| 4   | F     | 1   | NAG  | C1-C2-N2-C7 |
| 4   | a     | 1   | NAG  | C1-C2-N2-C7 |
| 4   | v     | 1   | NAG  | C1-C2-N2-C7 |
| 7   | X     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | s     | 2   | NAG  | O5-C5-C6-O6 |
| 7   | DA    | 2   | NAG  | O5-C5-C6-O6 |
| 3   | R     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | m     | 1   | NAG  | C3-C2-N2-C7 |
| 3   | 7     | 1   | NAG  | C3-C2-N2-C7 |
| 2   | D     | 6   | MAN  | O5-C5-C6-O6 |
| 2   | t     | 6   | MAN  | O5-C5-C6-O6 |
| 2   | Y     | 6   | MAN  | O5-C5-C6-O6 |
| 4   | v     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | F     | 2   | NAG  | O5-C5-C6-O6 |
| 4   | a     | 2   | NAG  | O5-C5-C6-O6 |

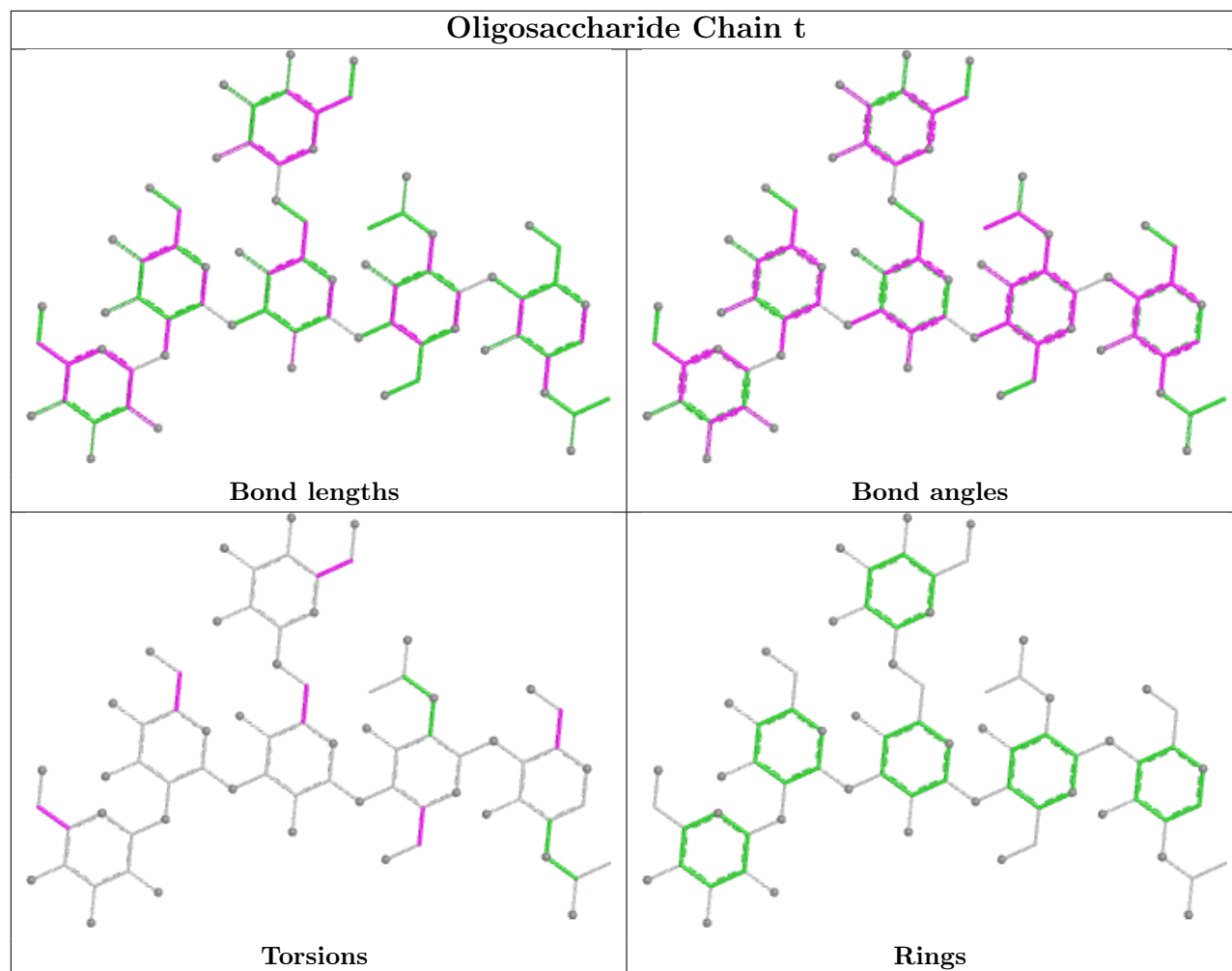
There are no ring outliers.

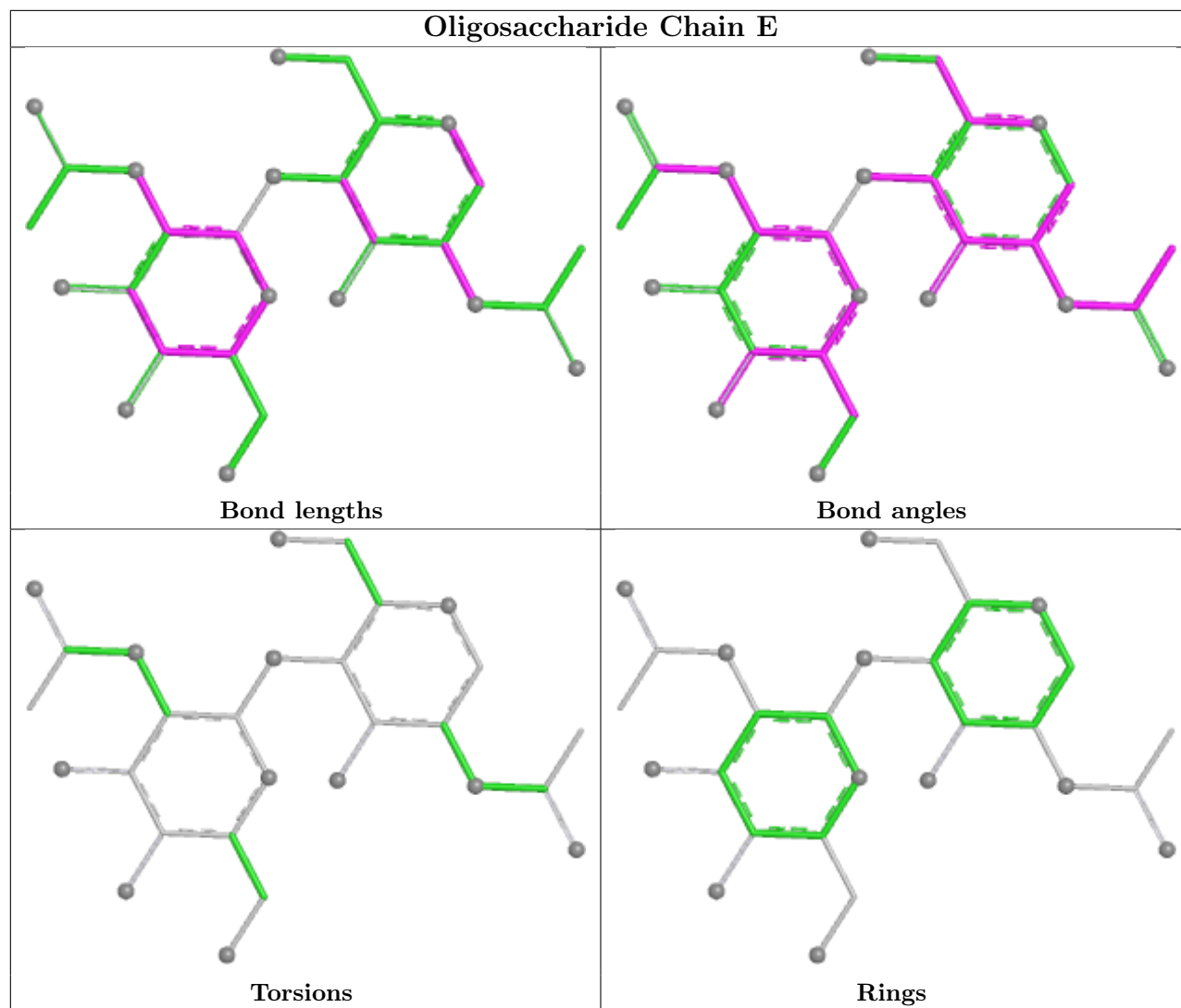
No monomer is involved in short contacts.

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

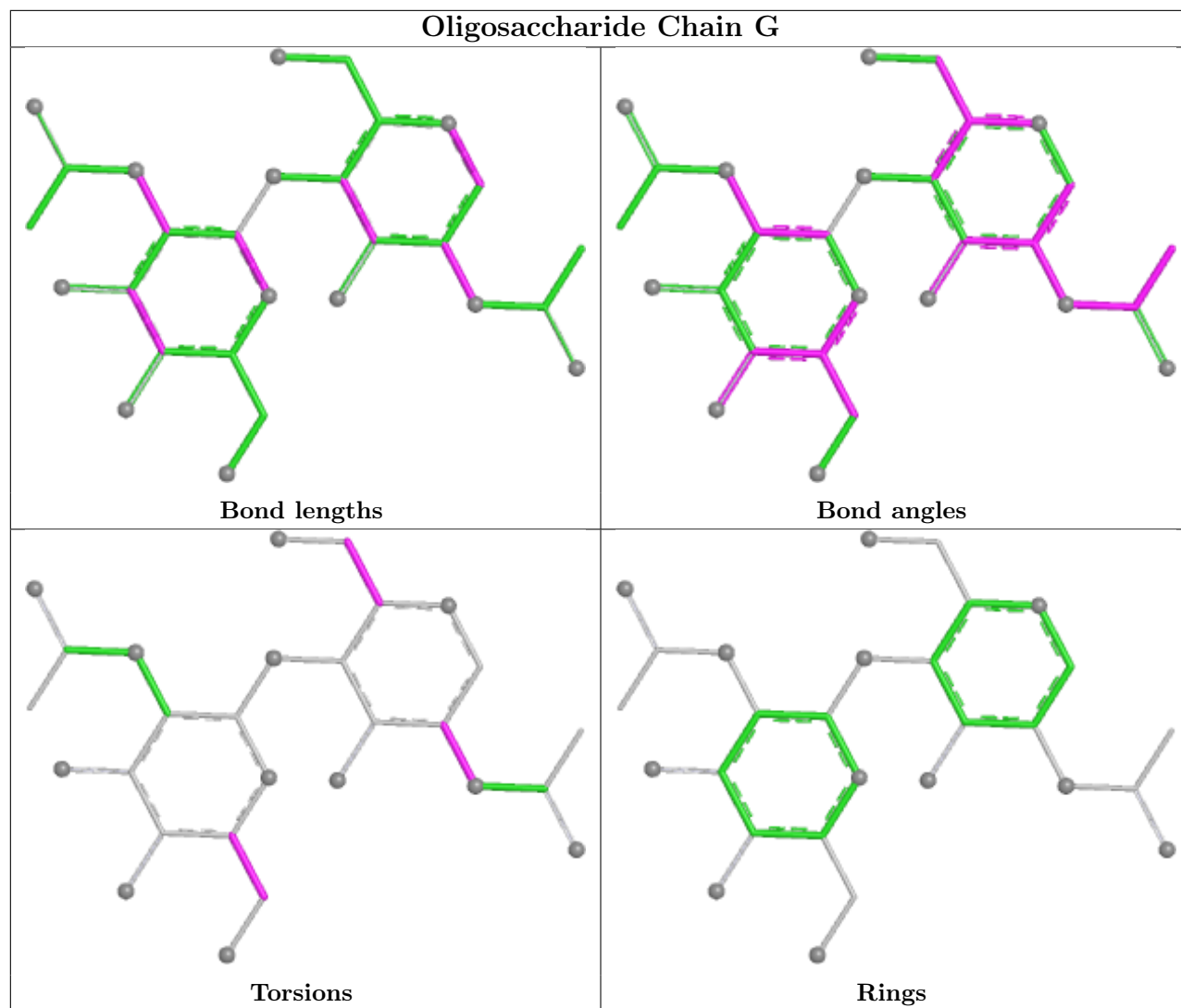


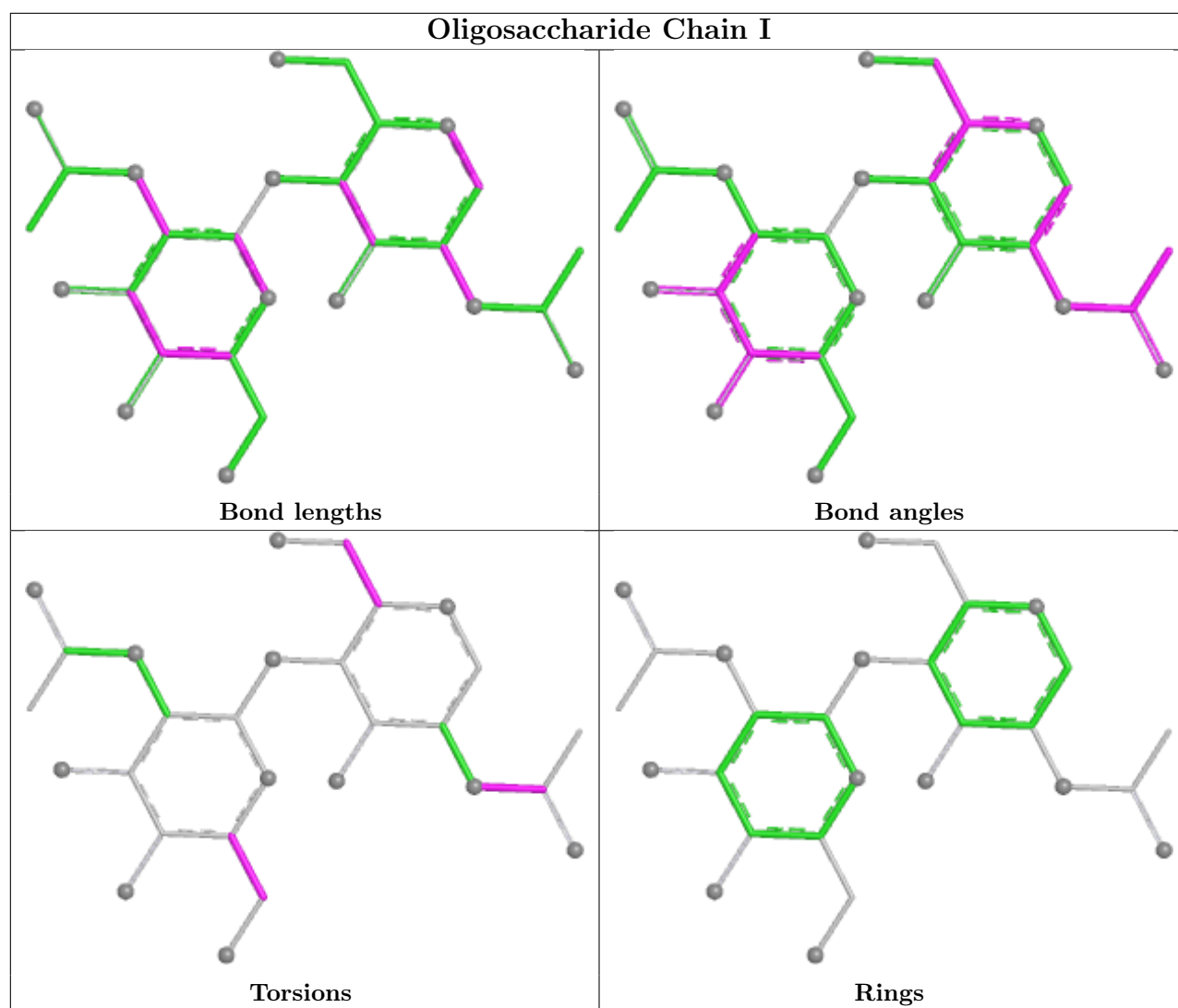


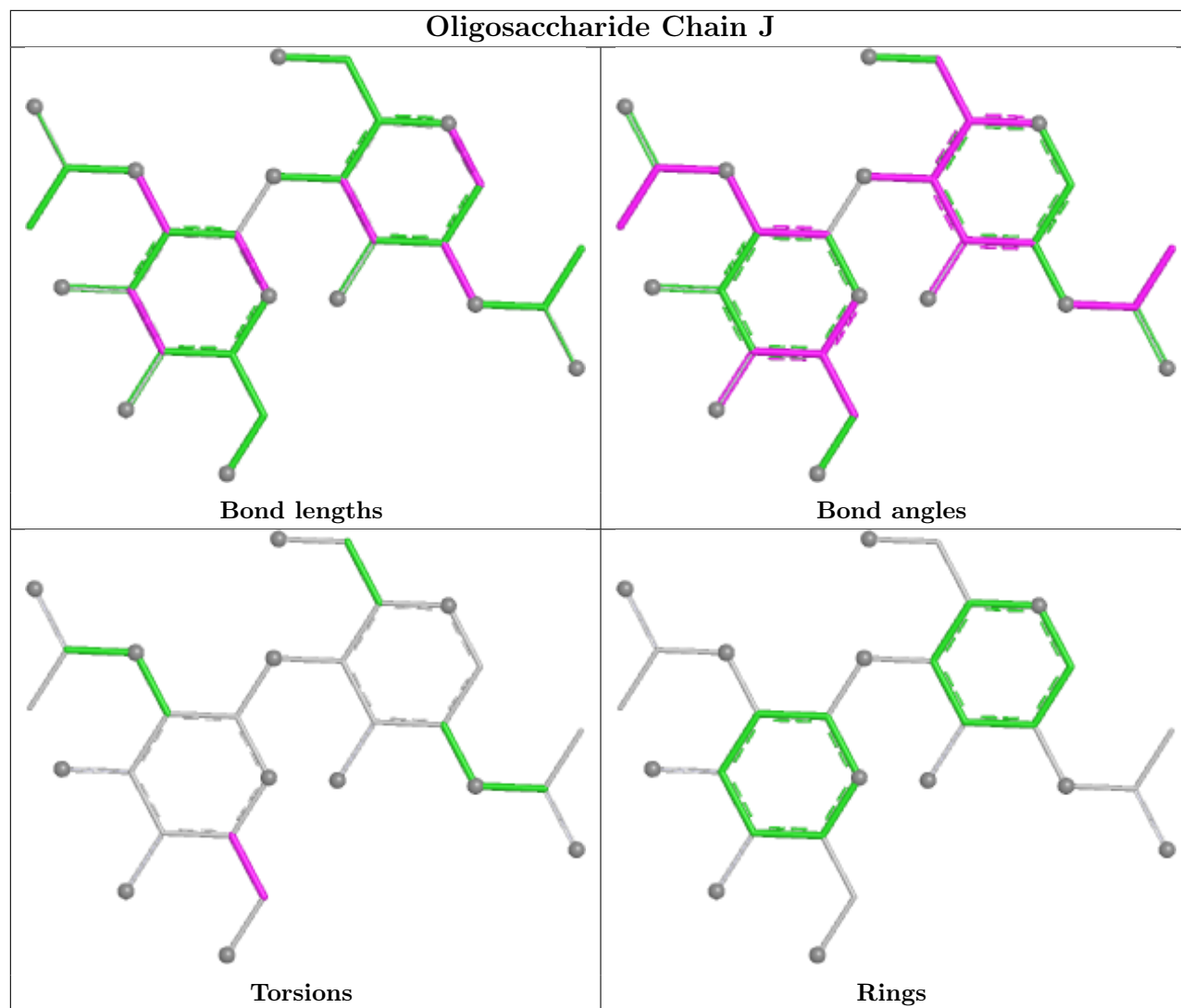


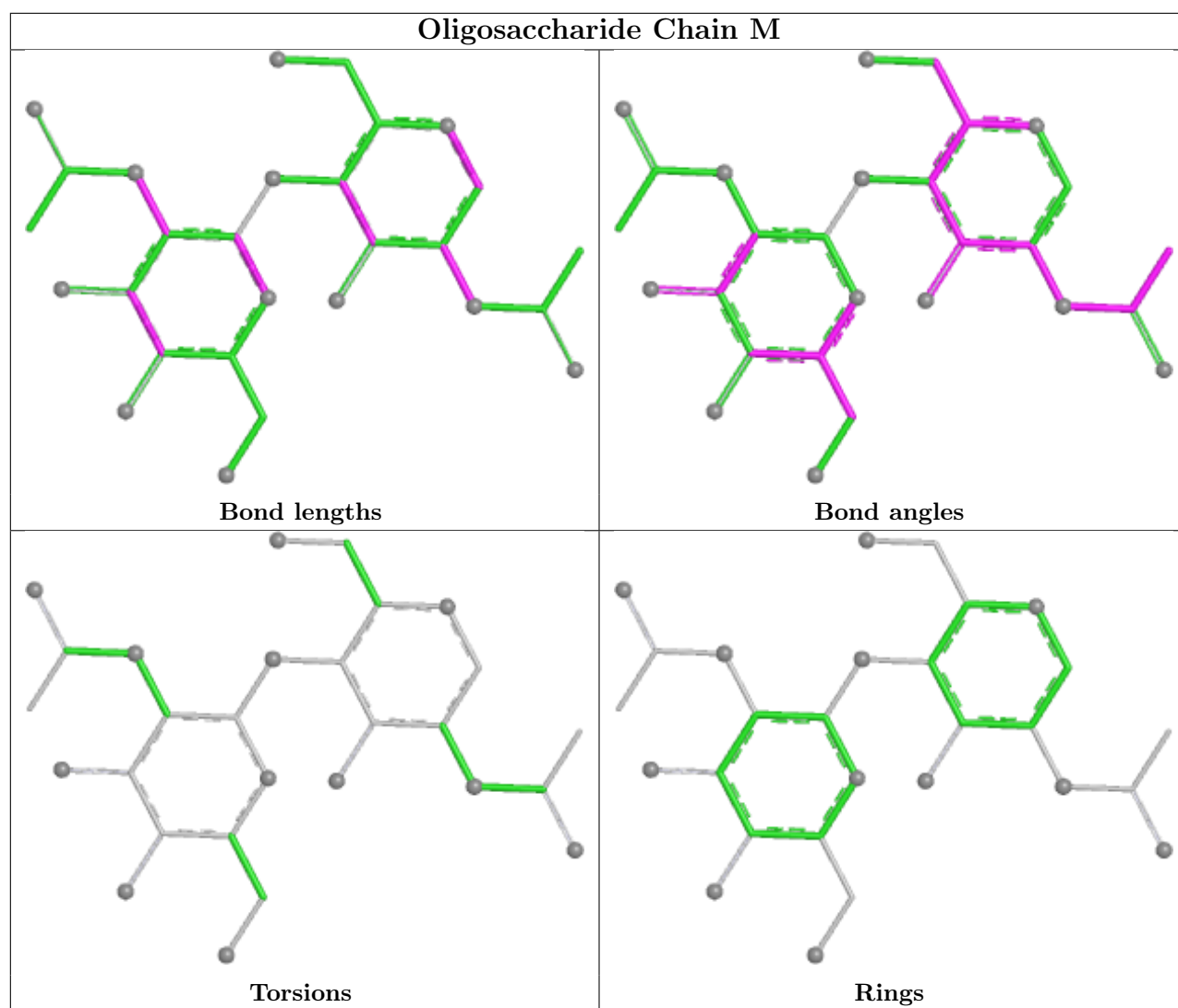


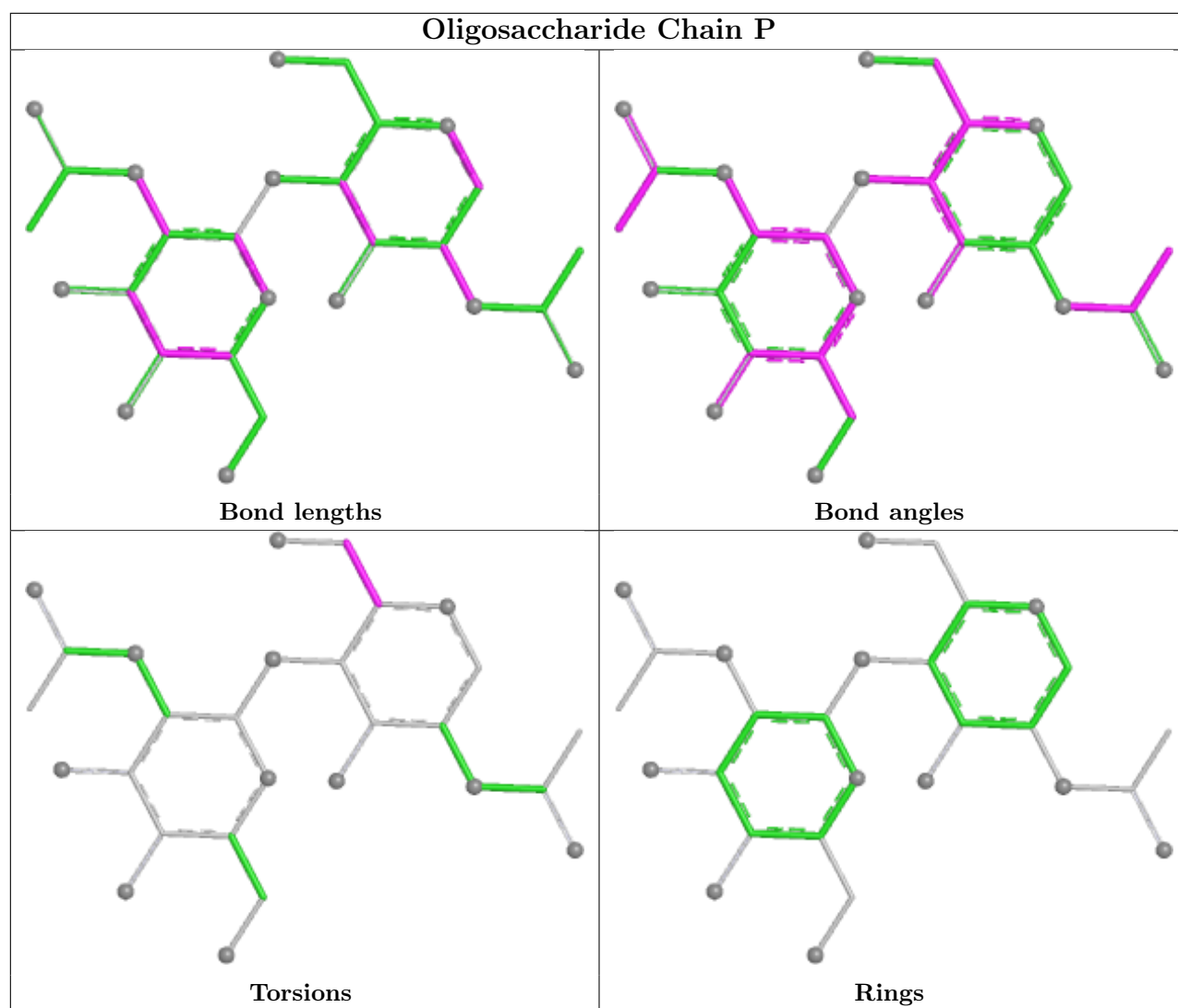


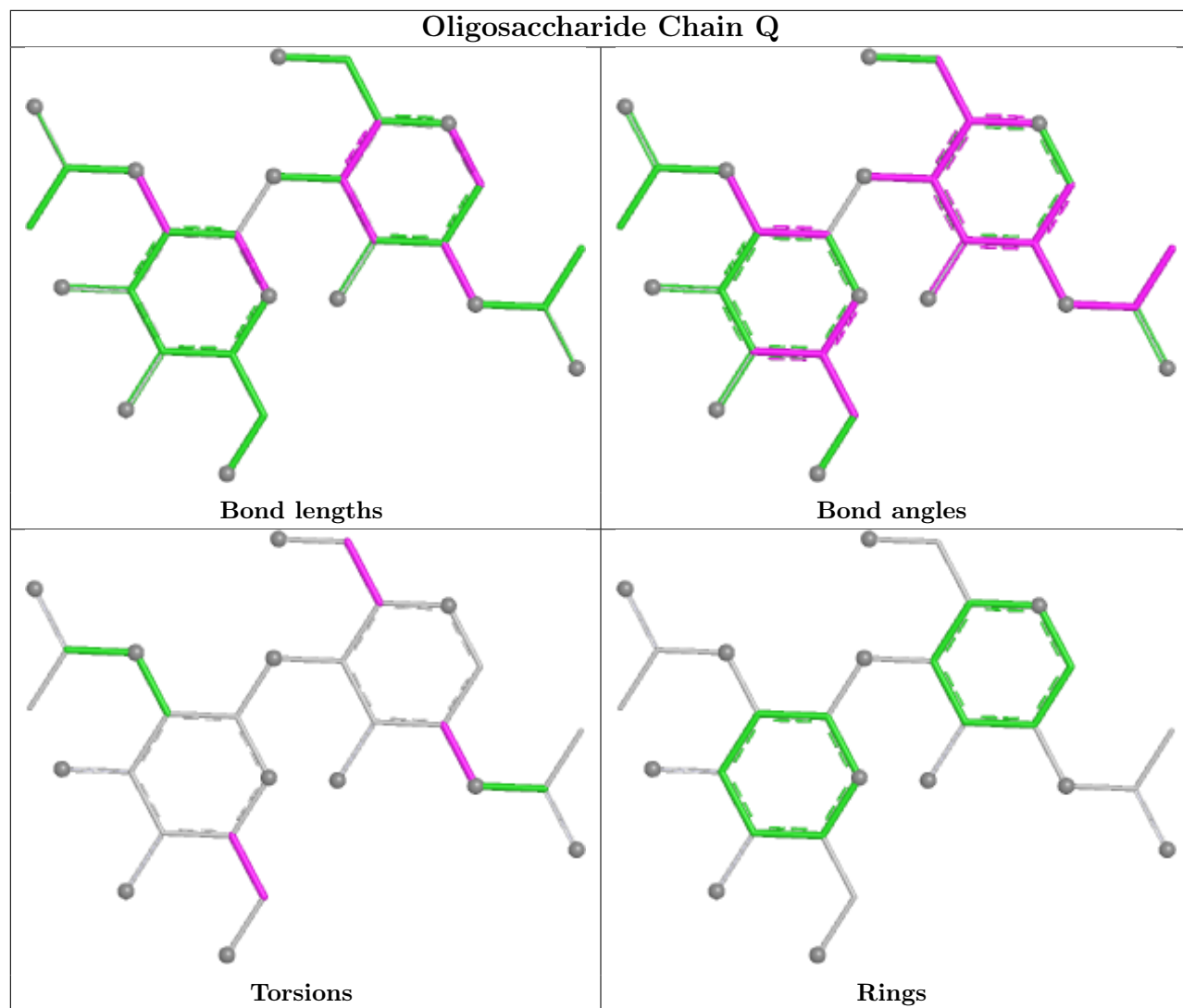


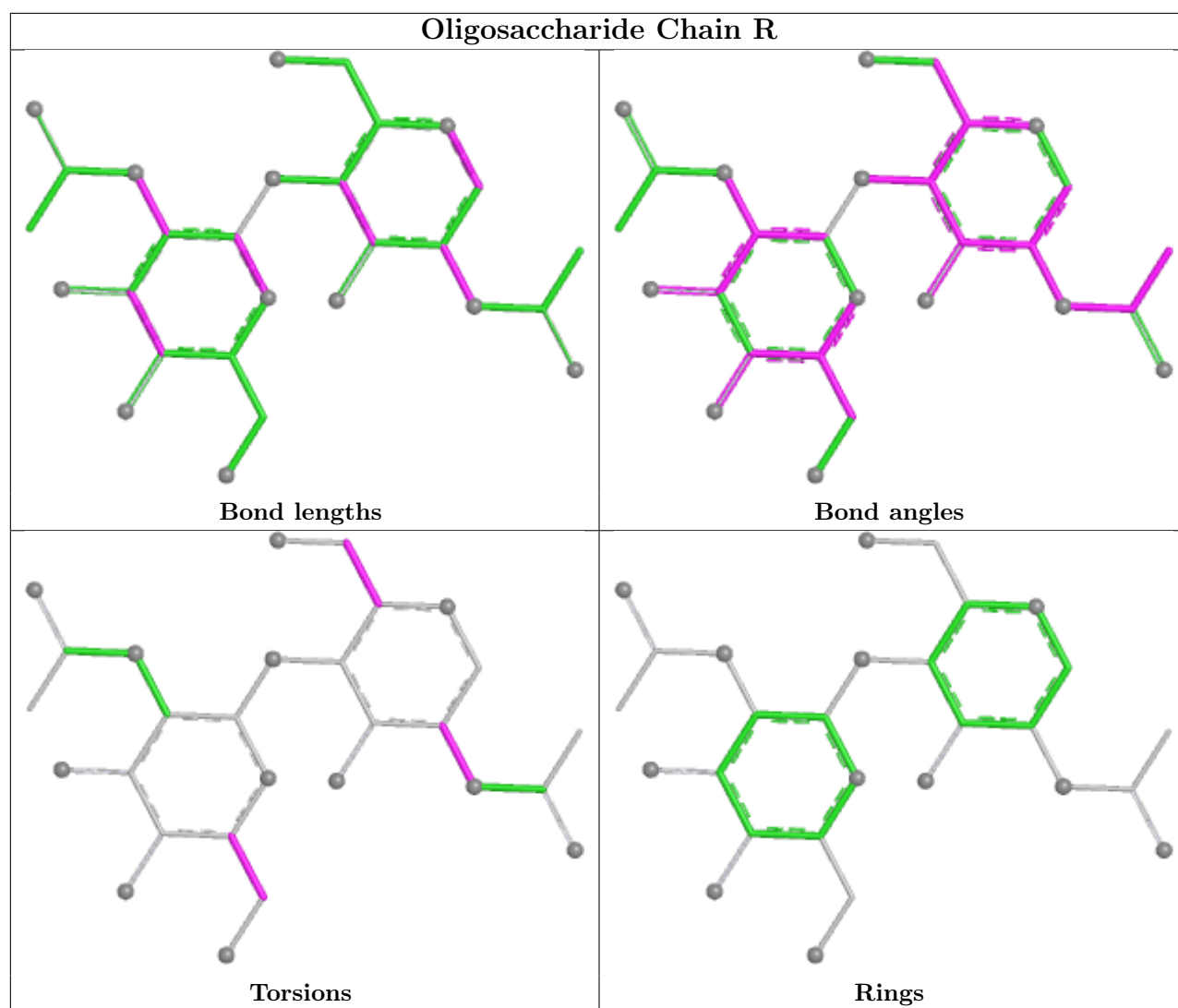


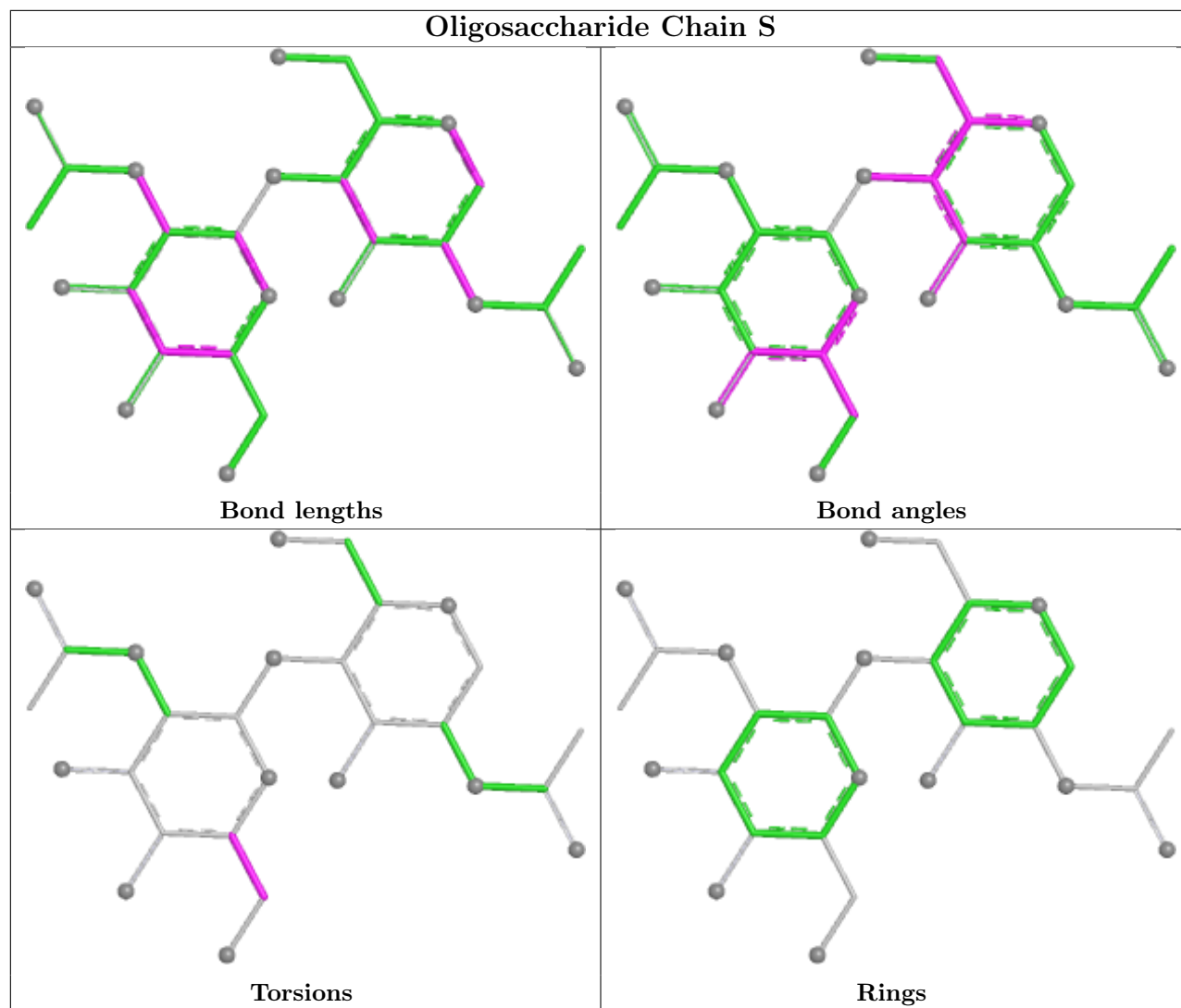




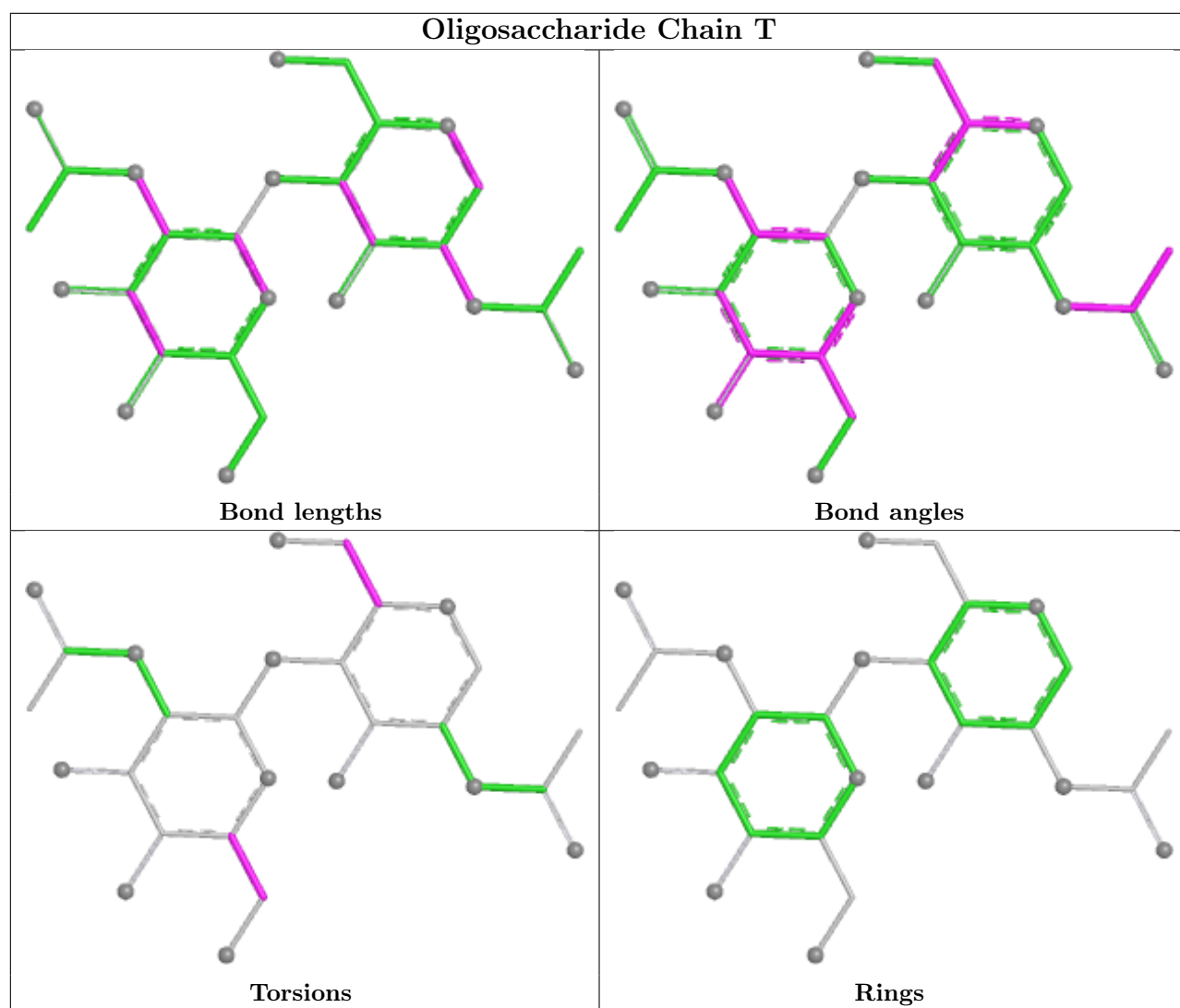


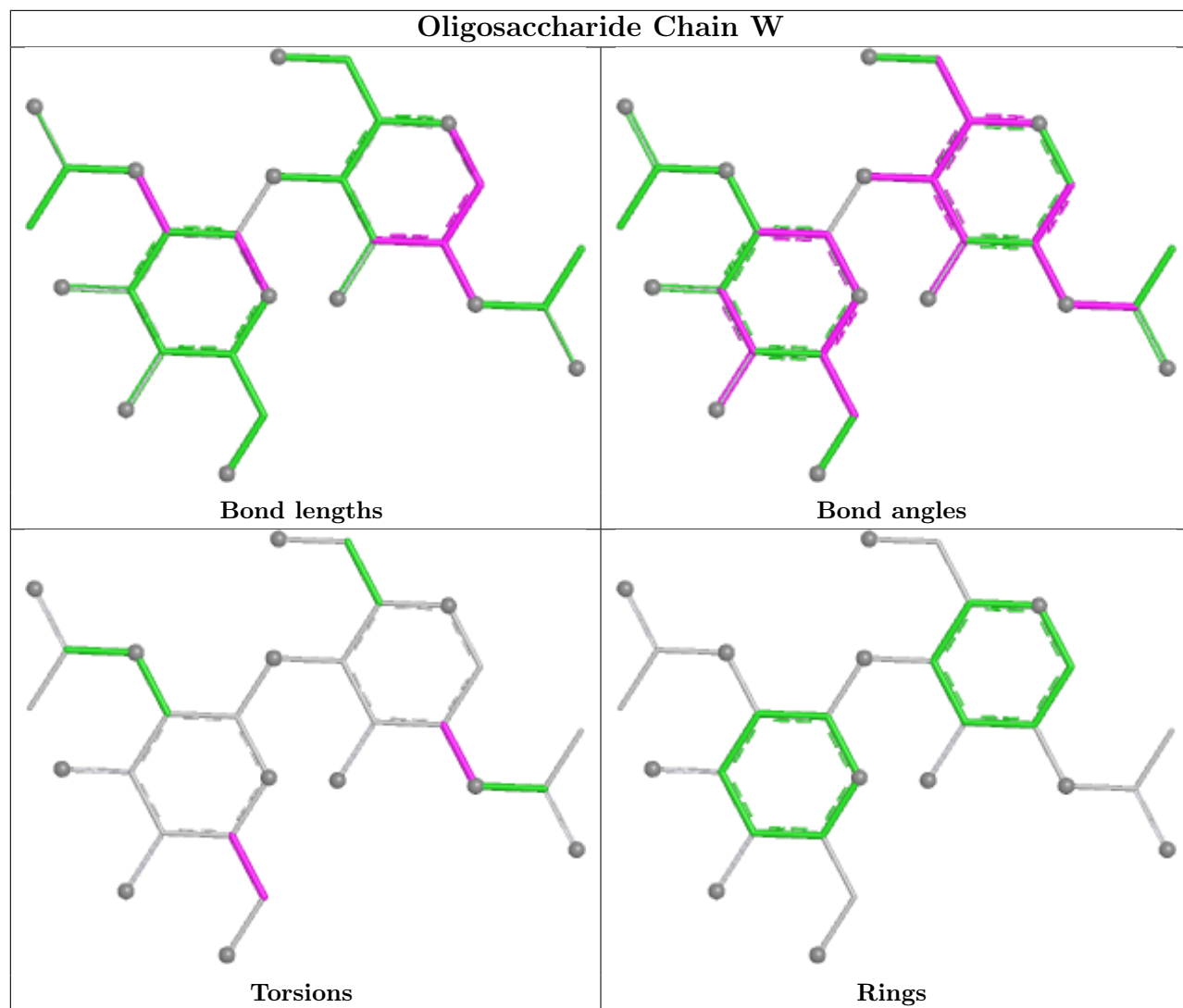


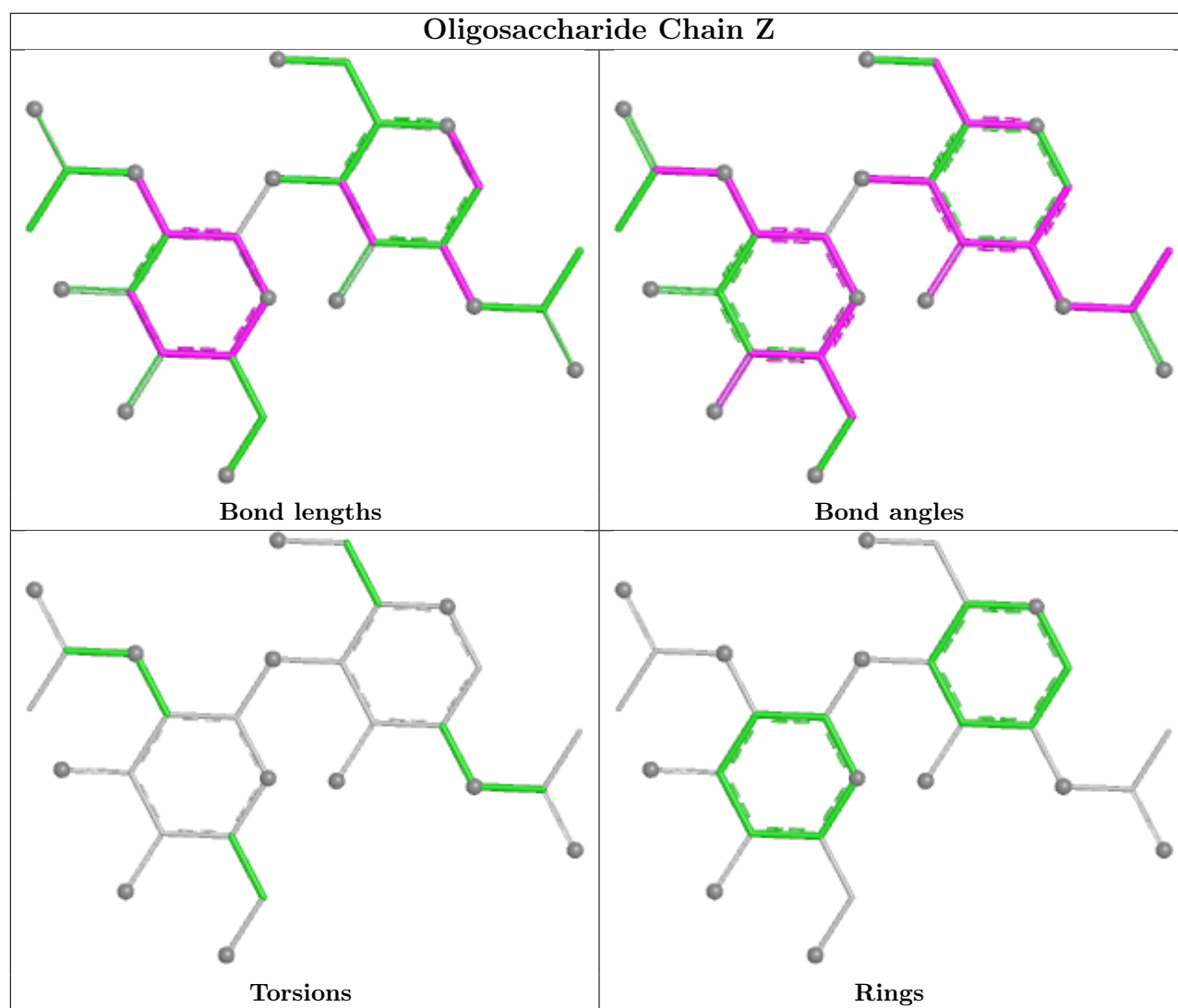


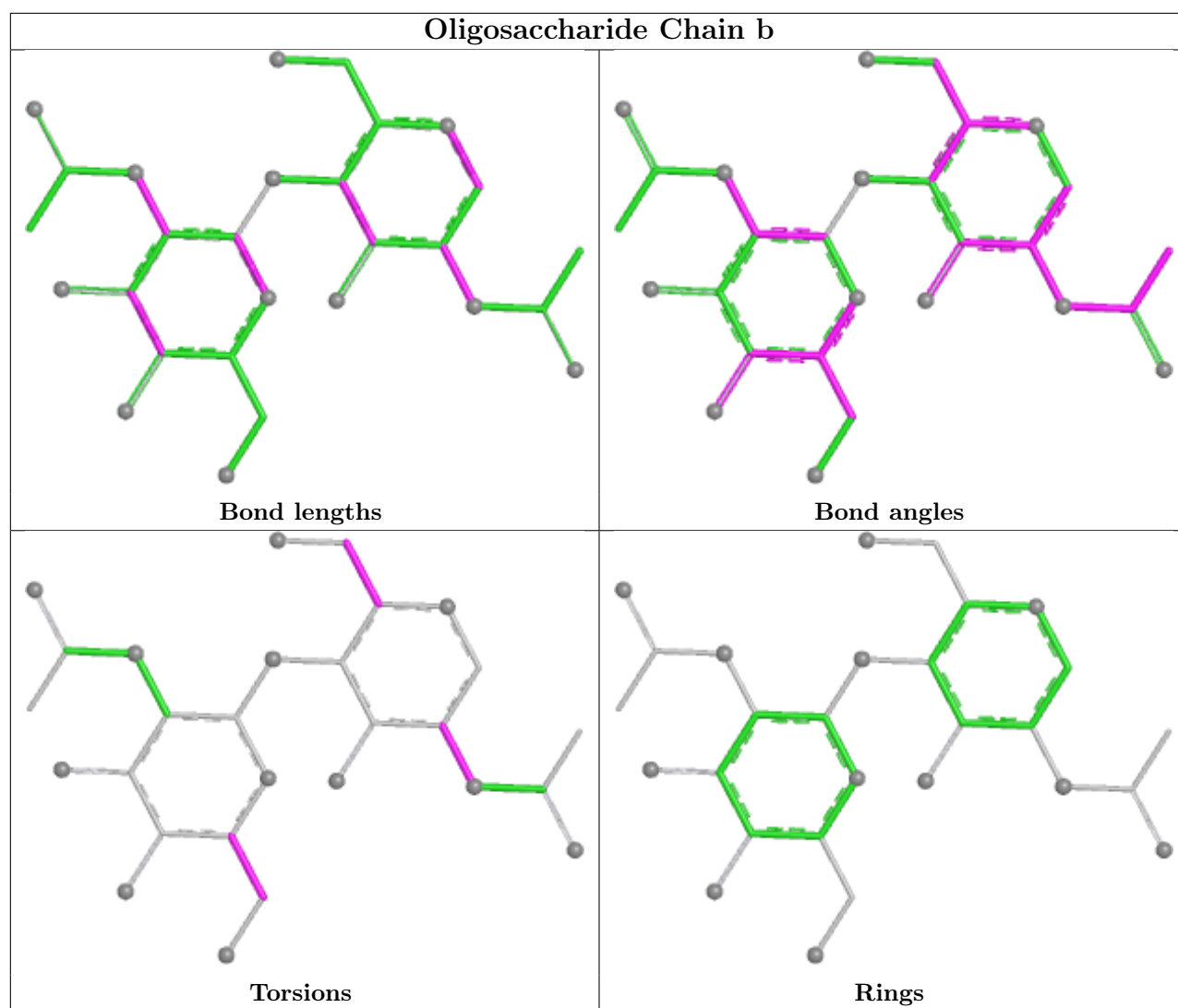


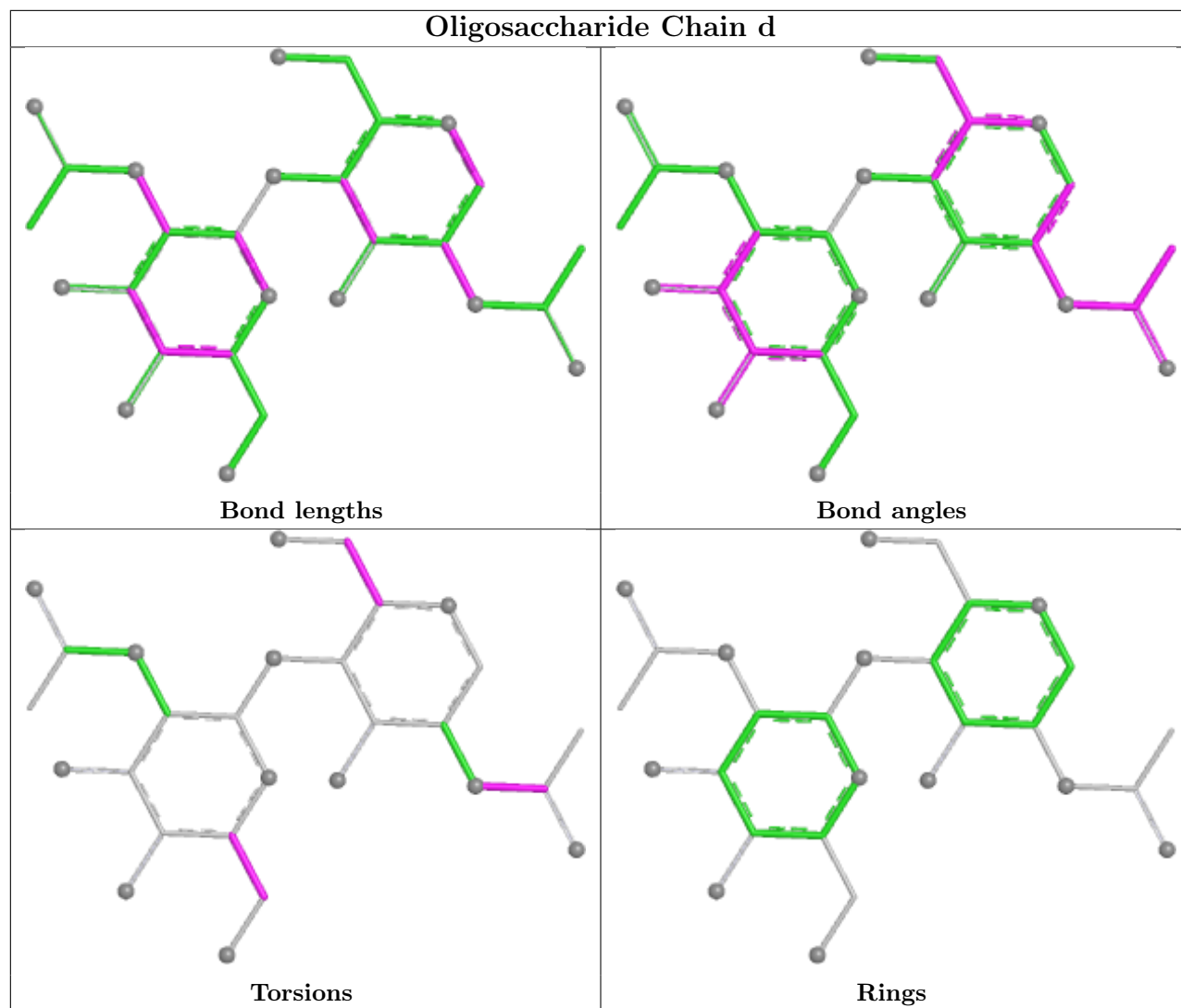


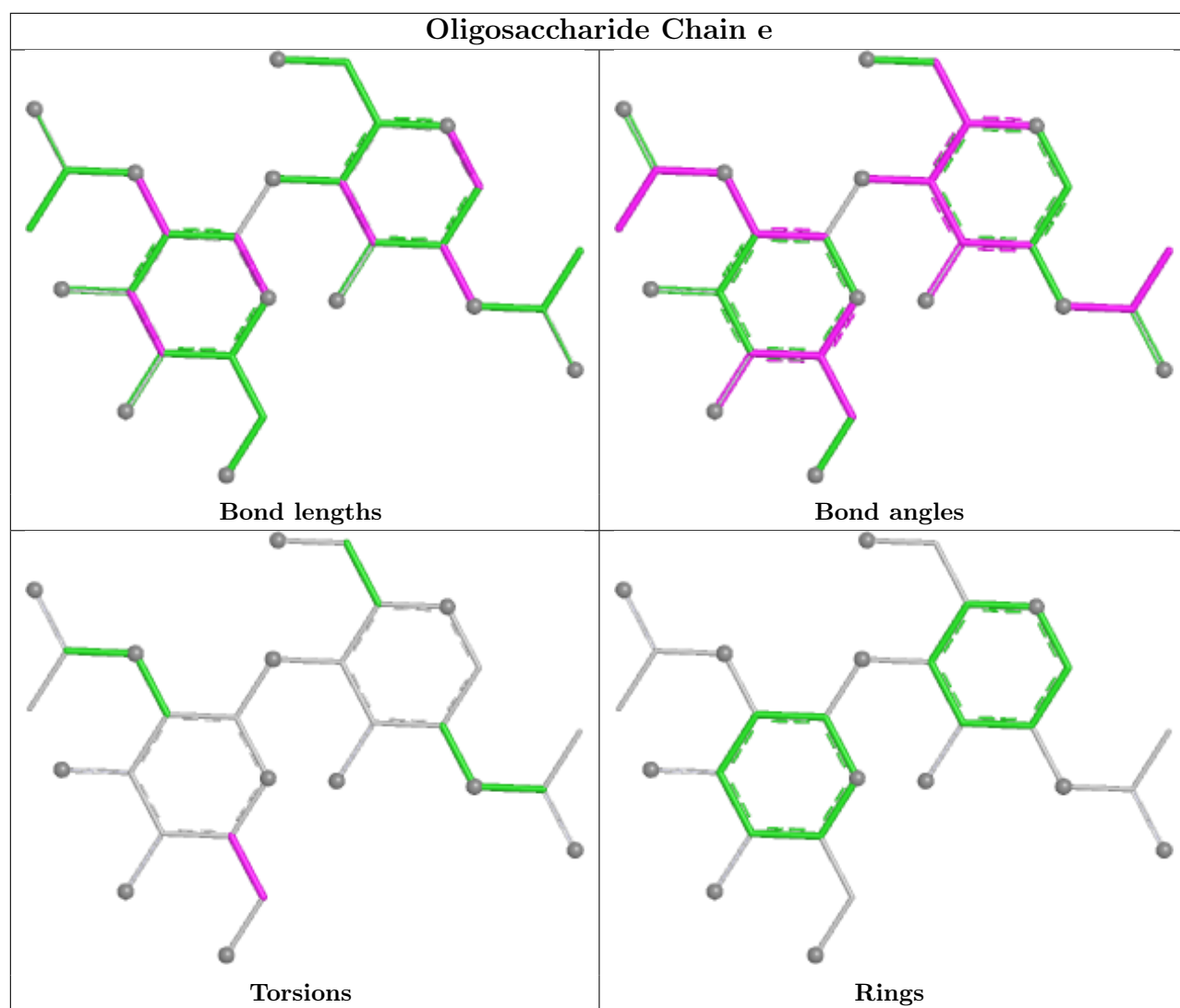


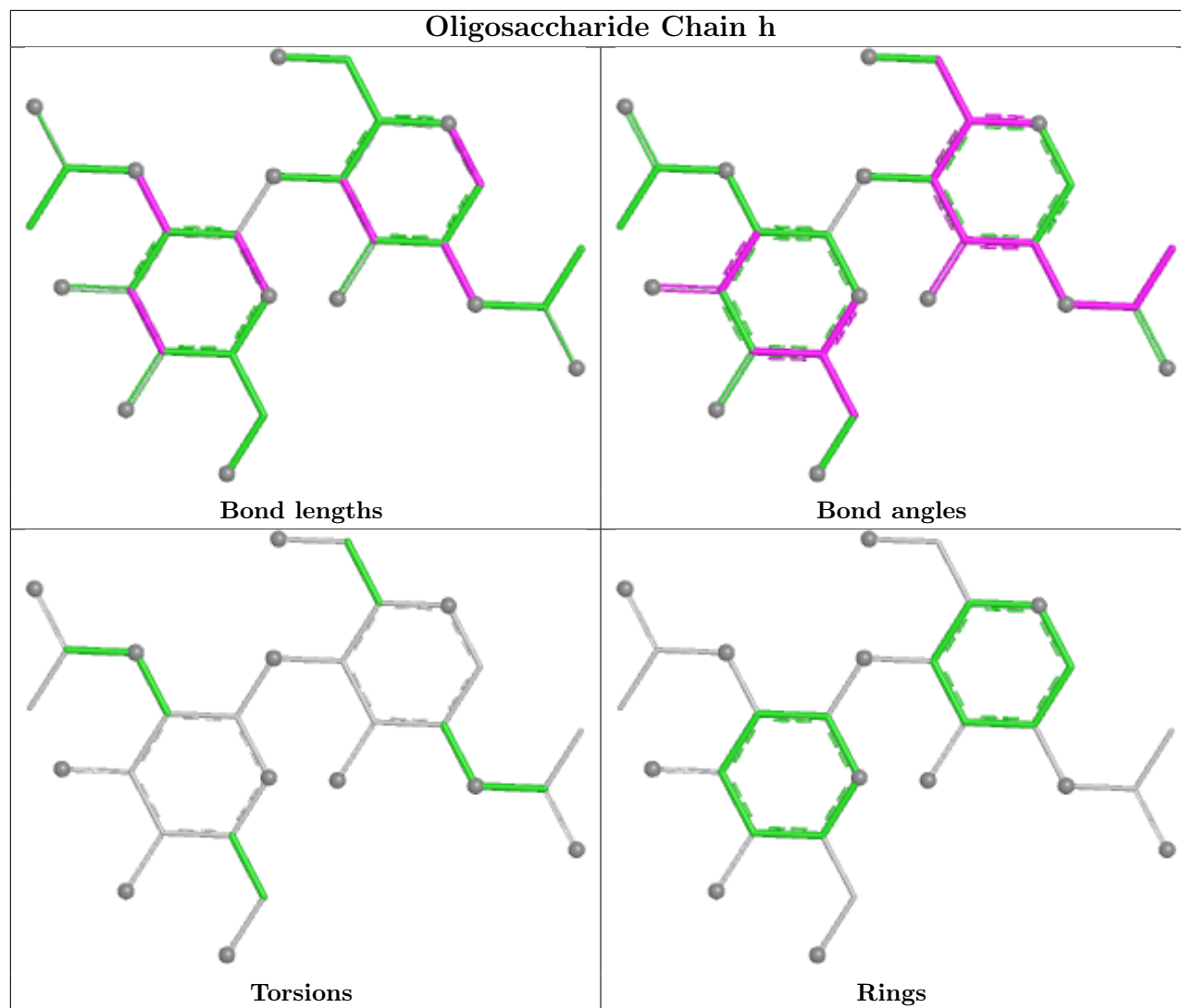


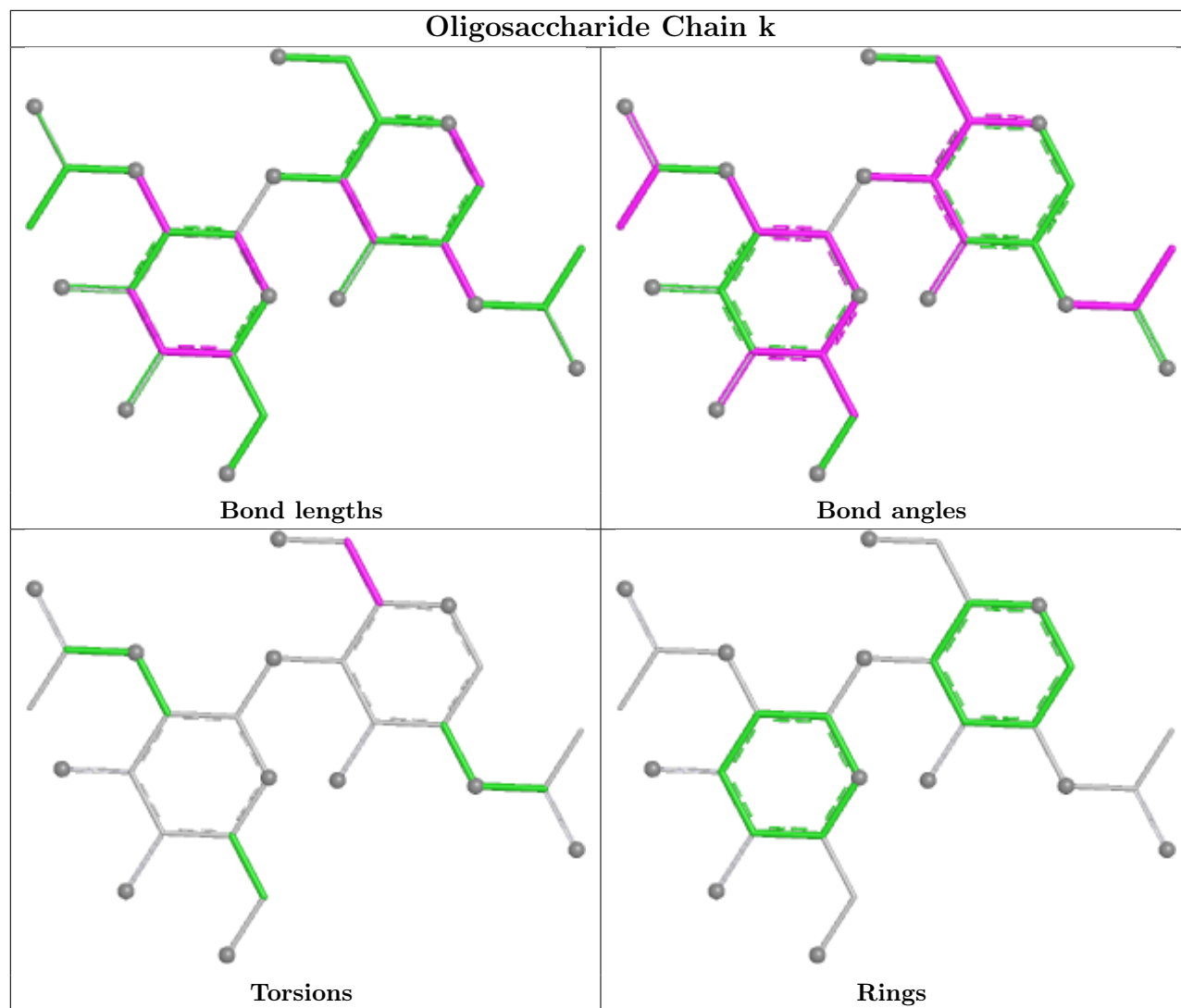




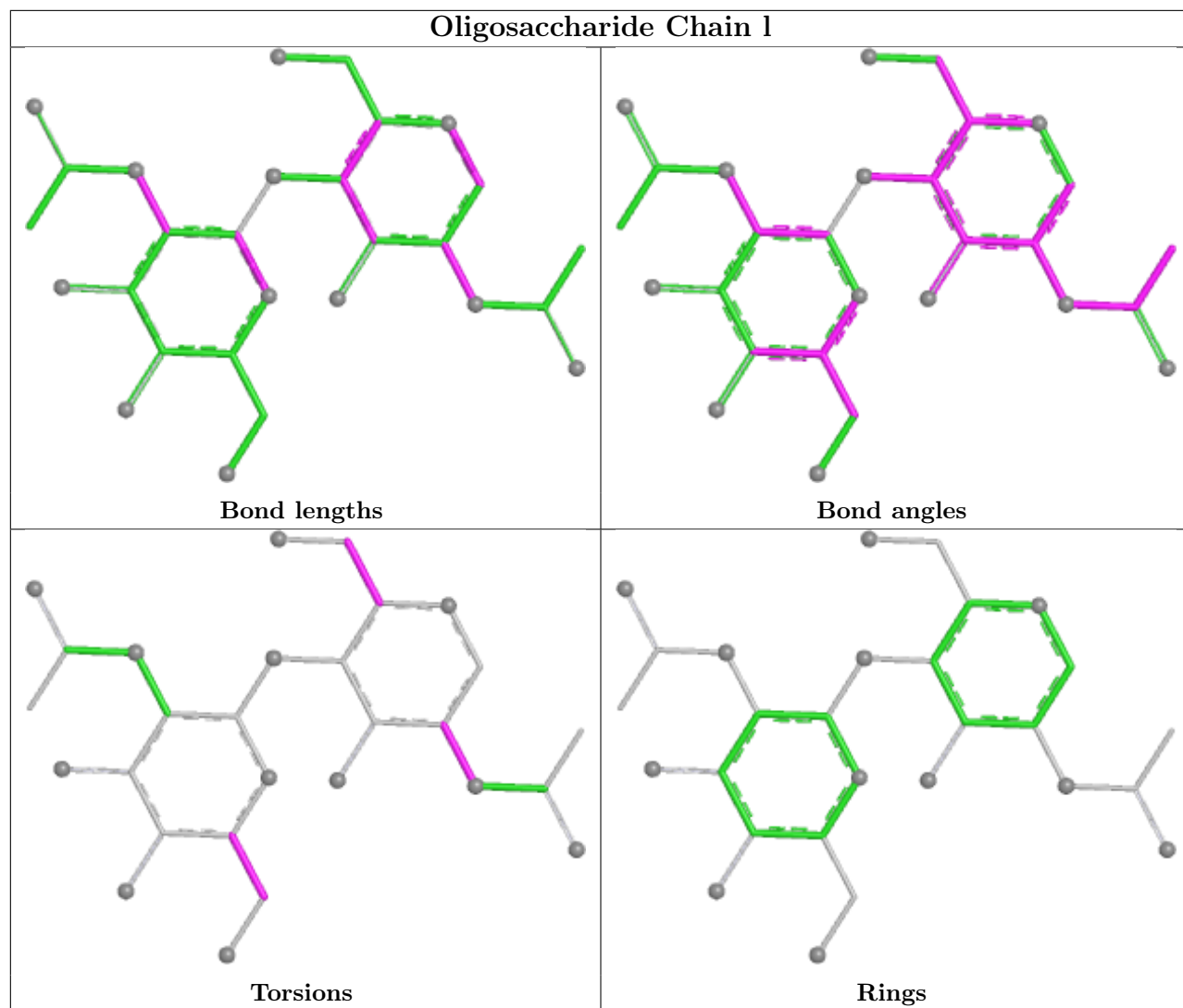


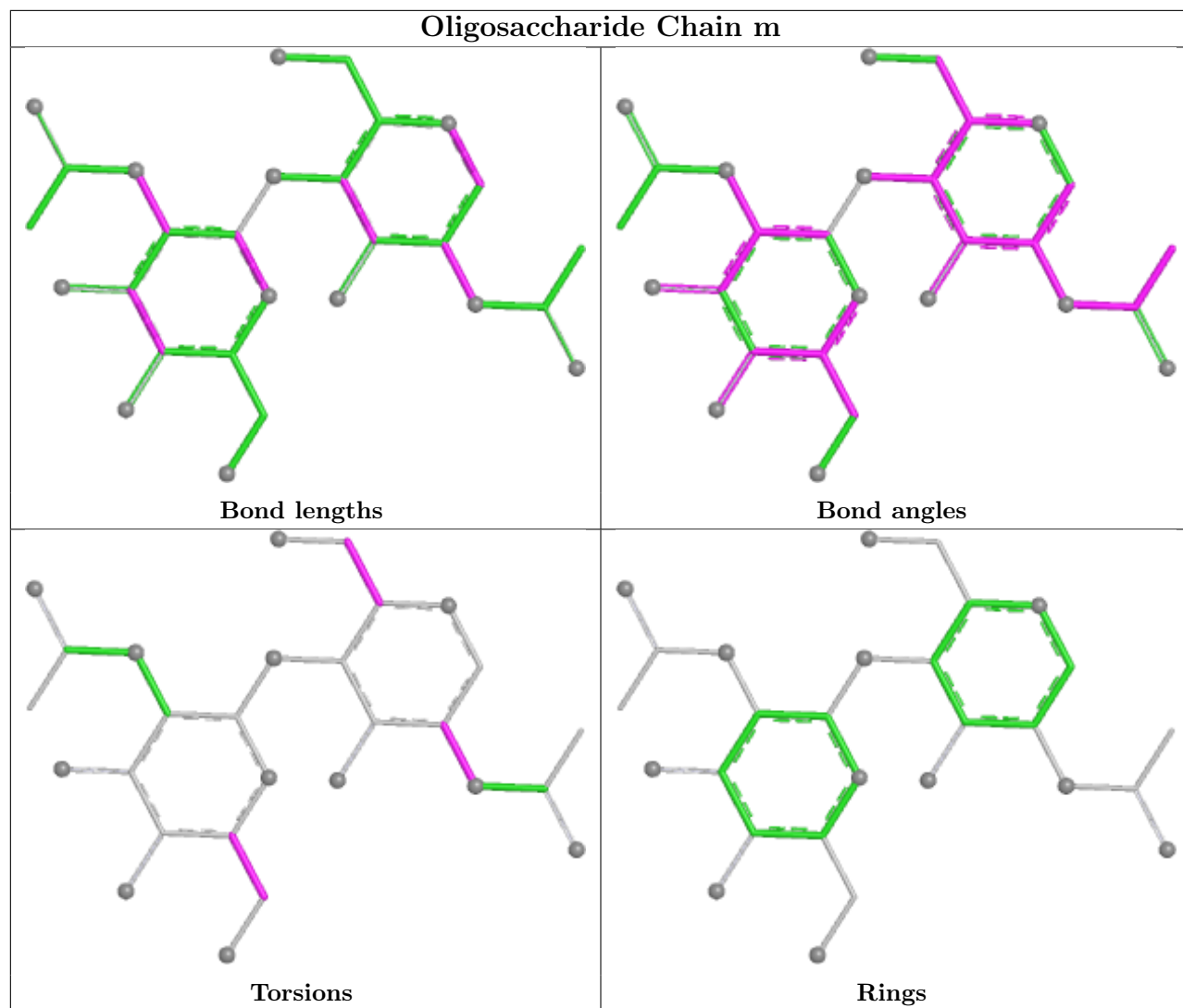


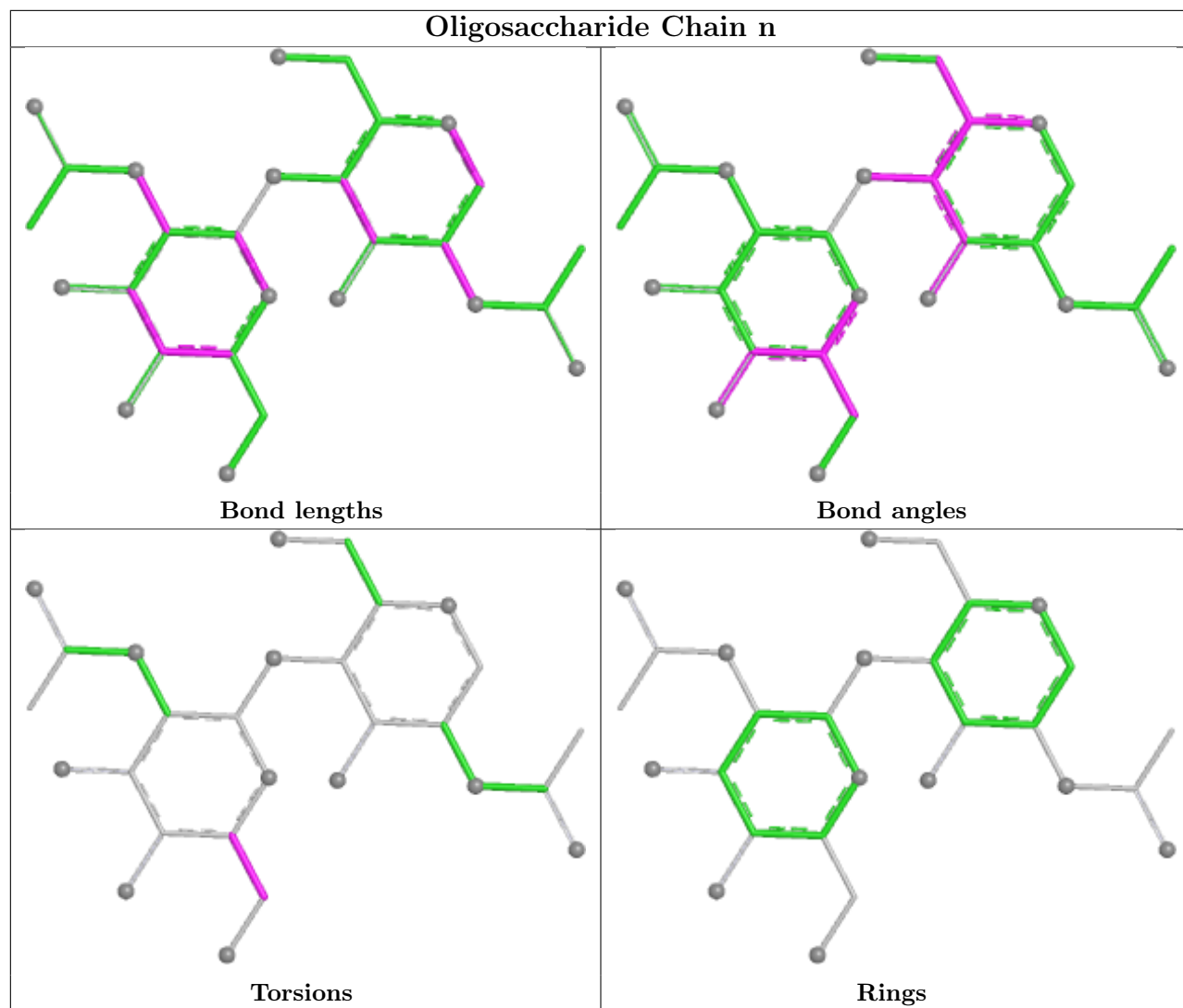


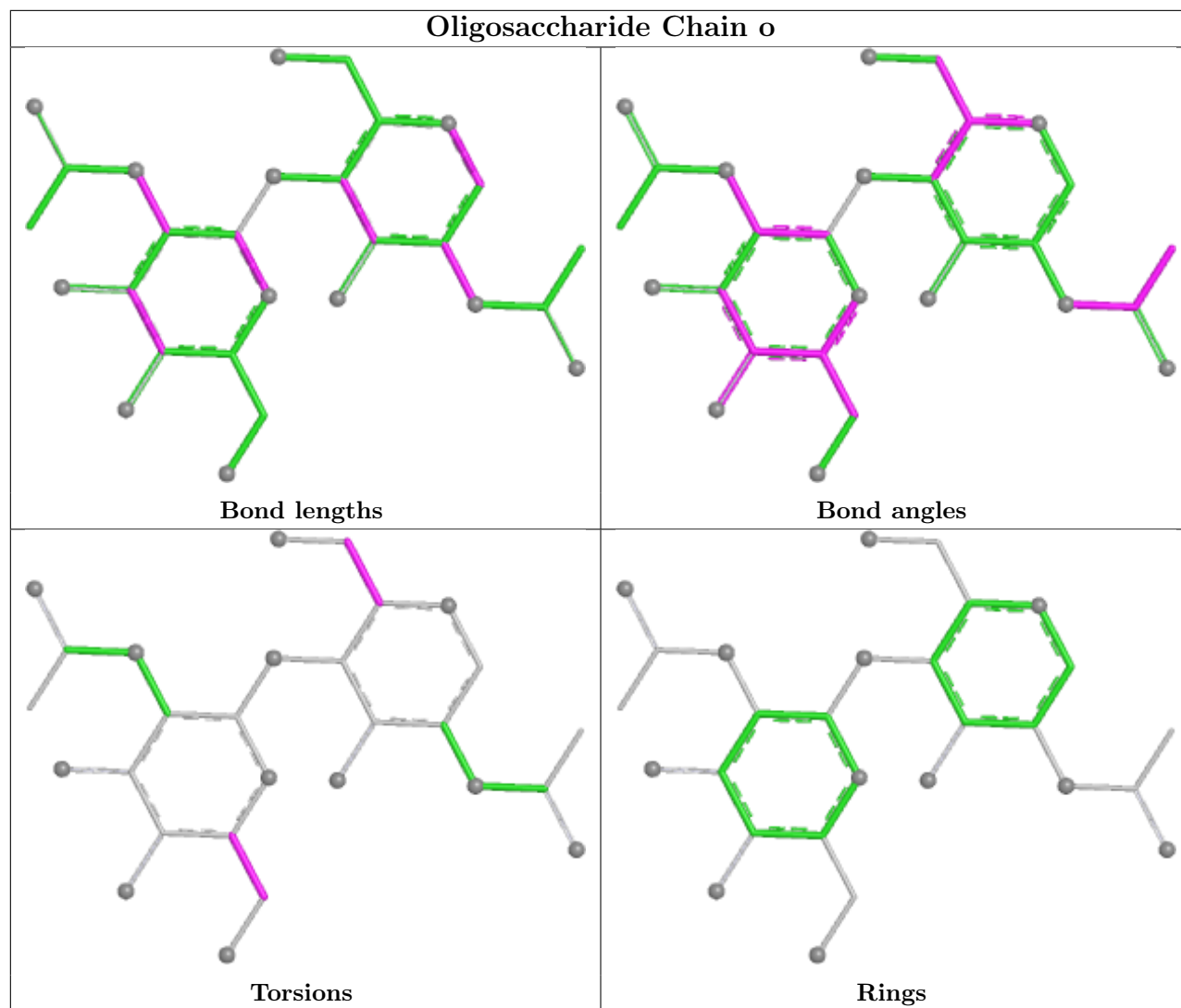


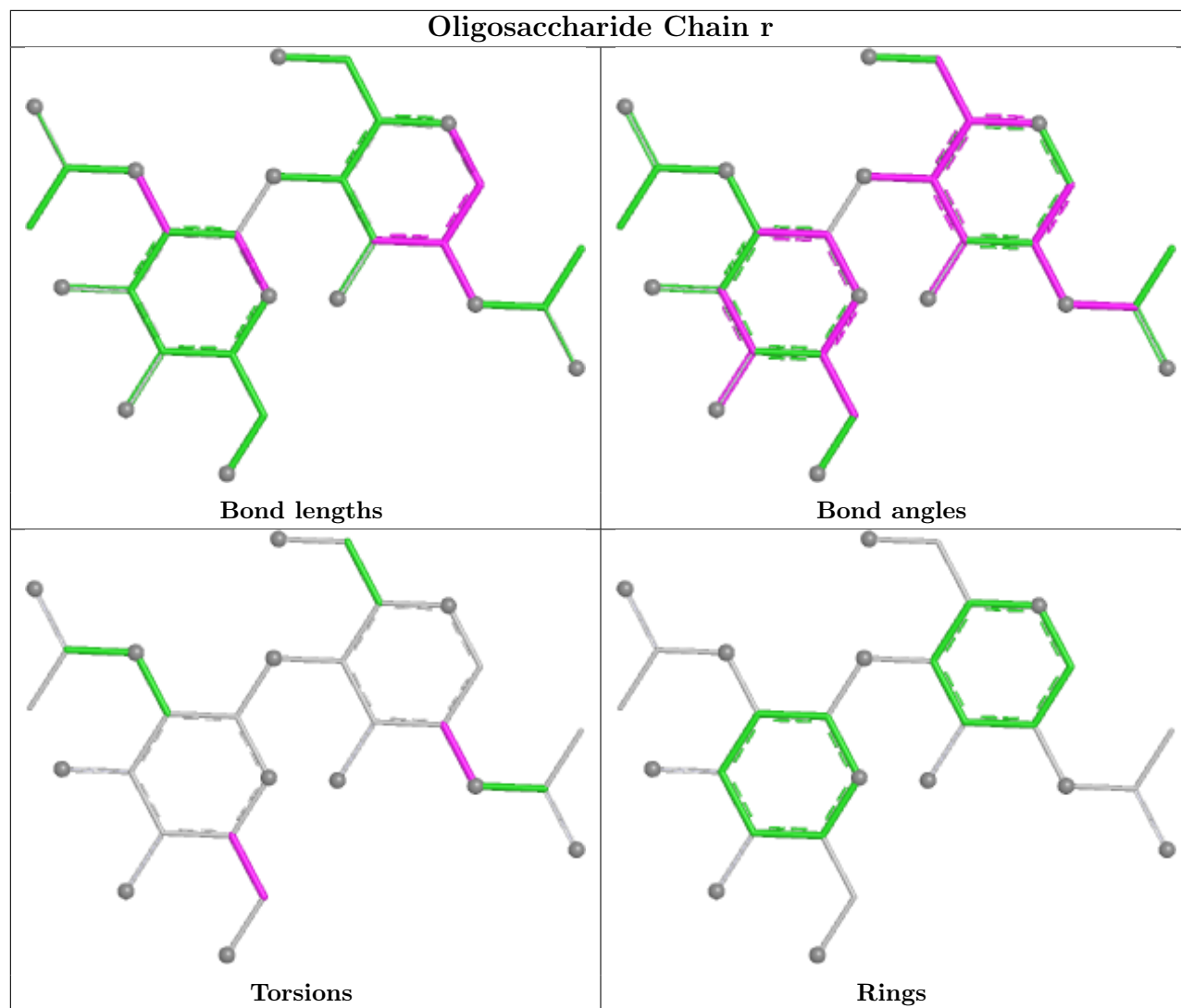


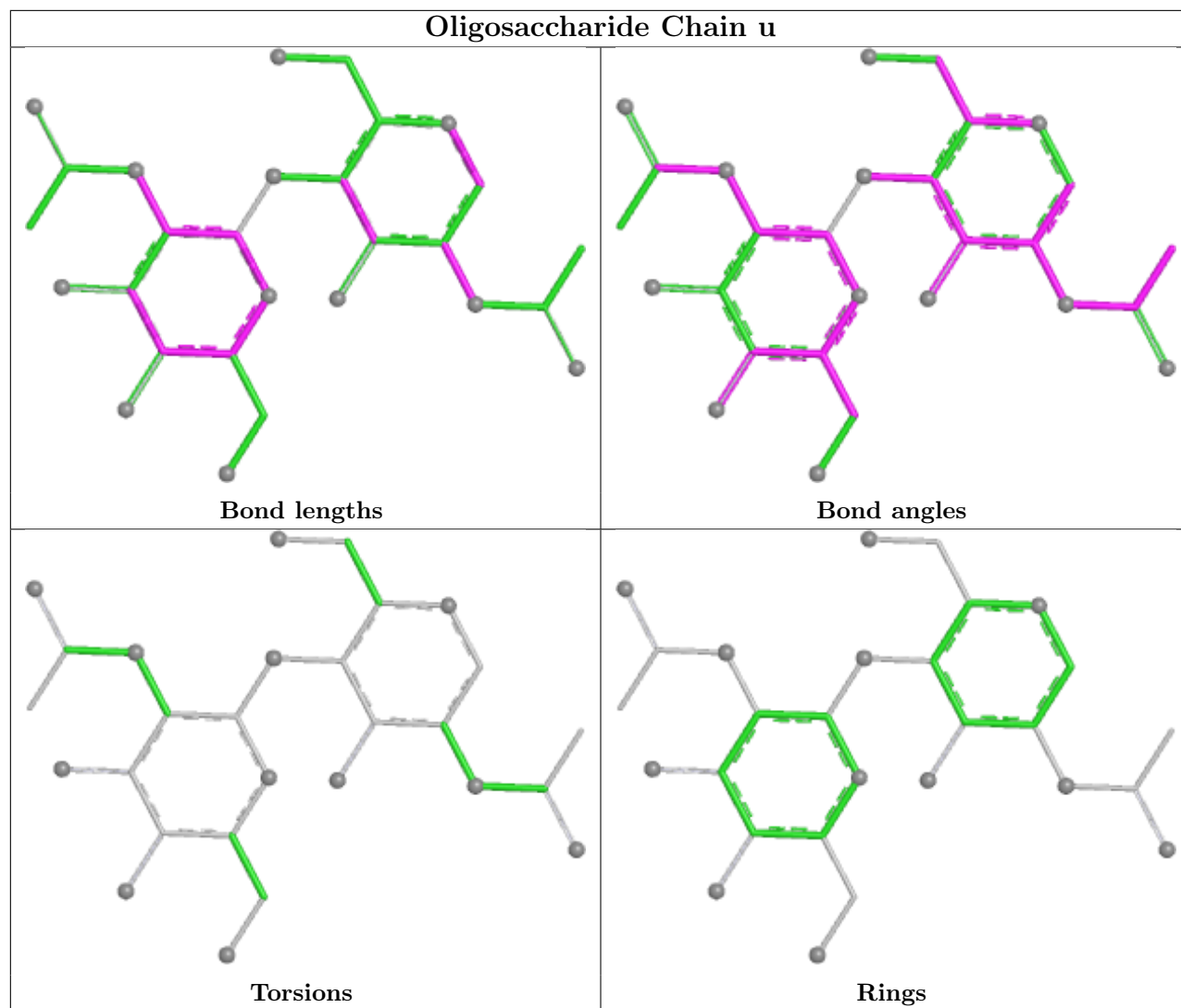


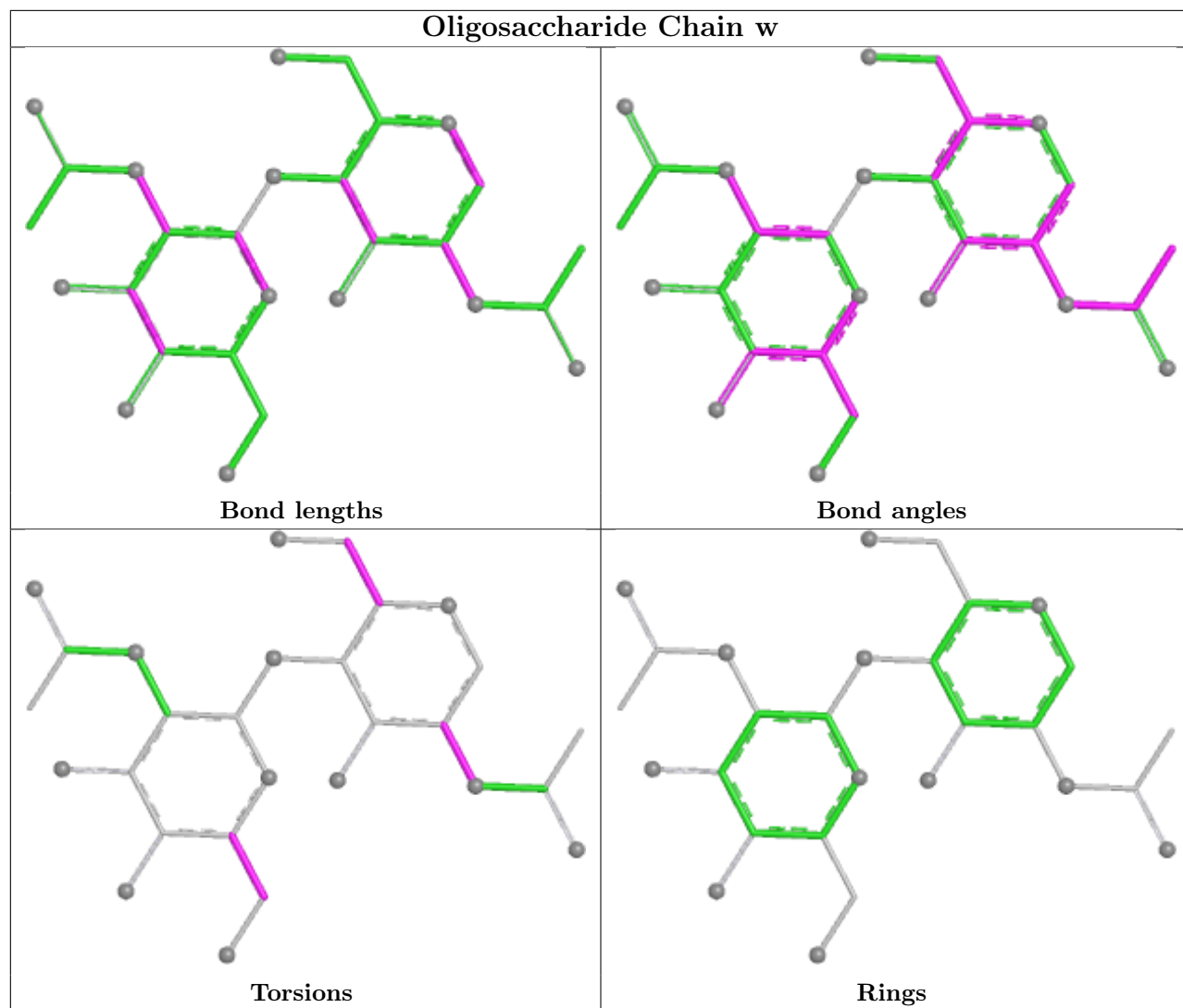


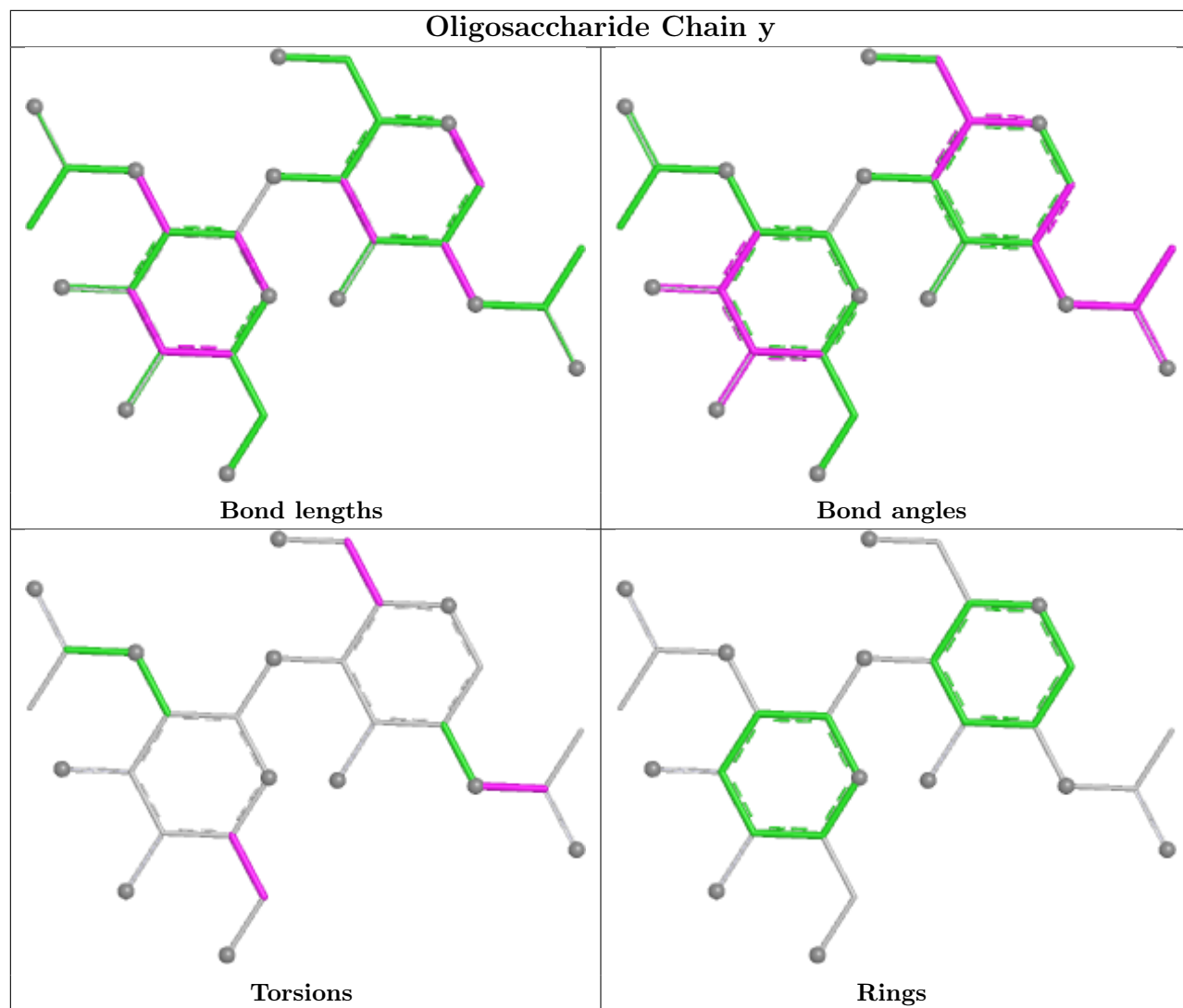




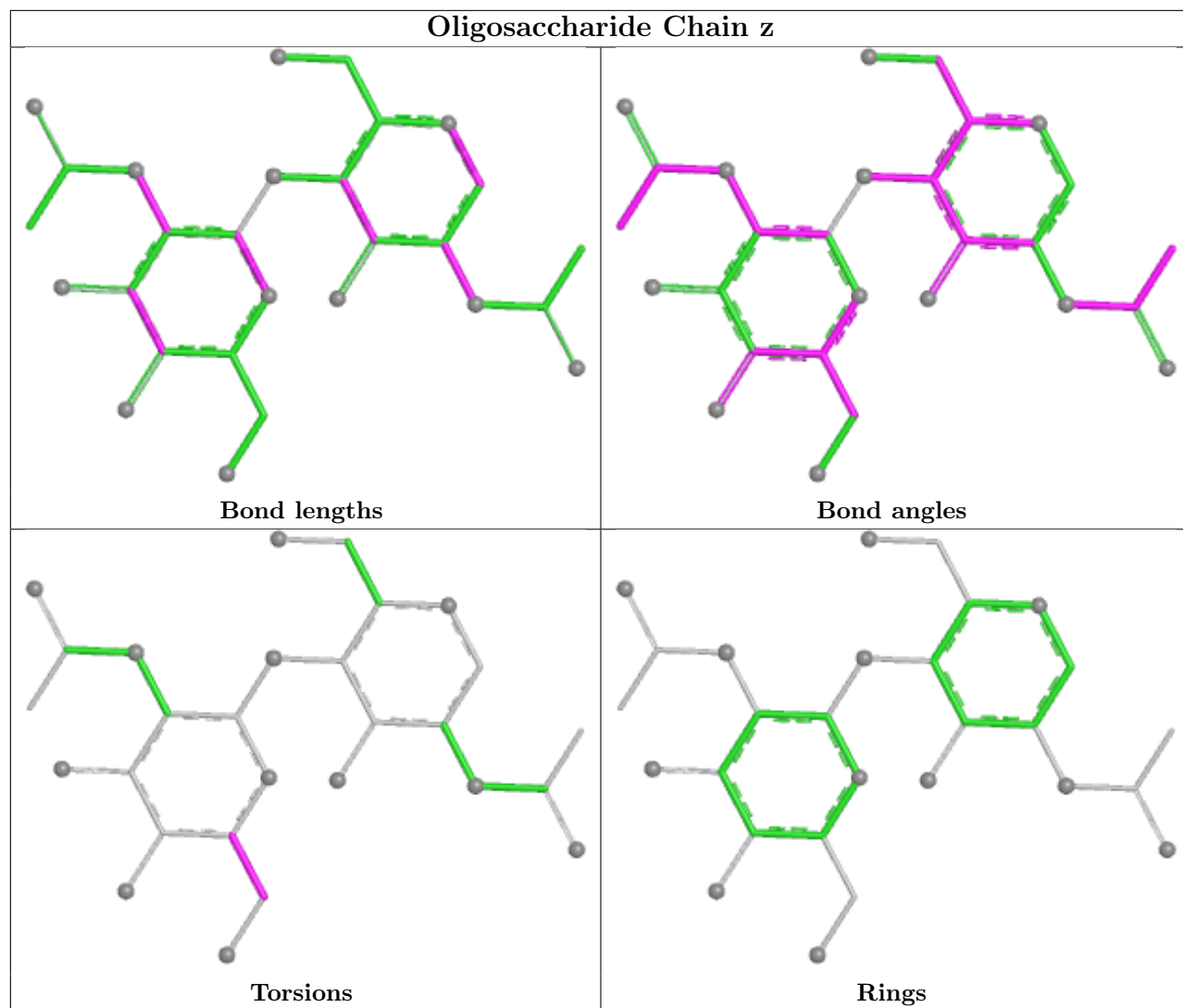


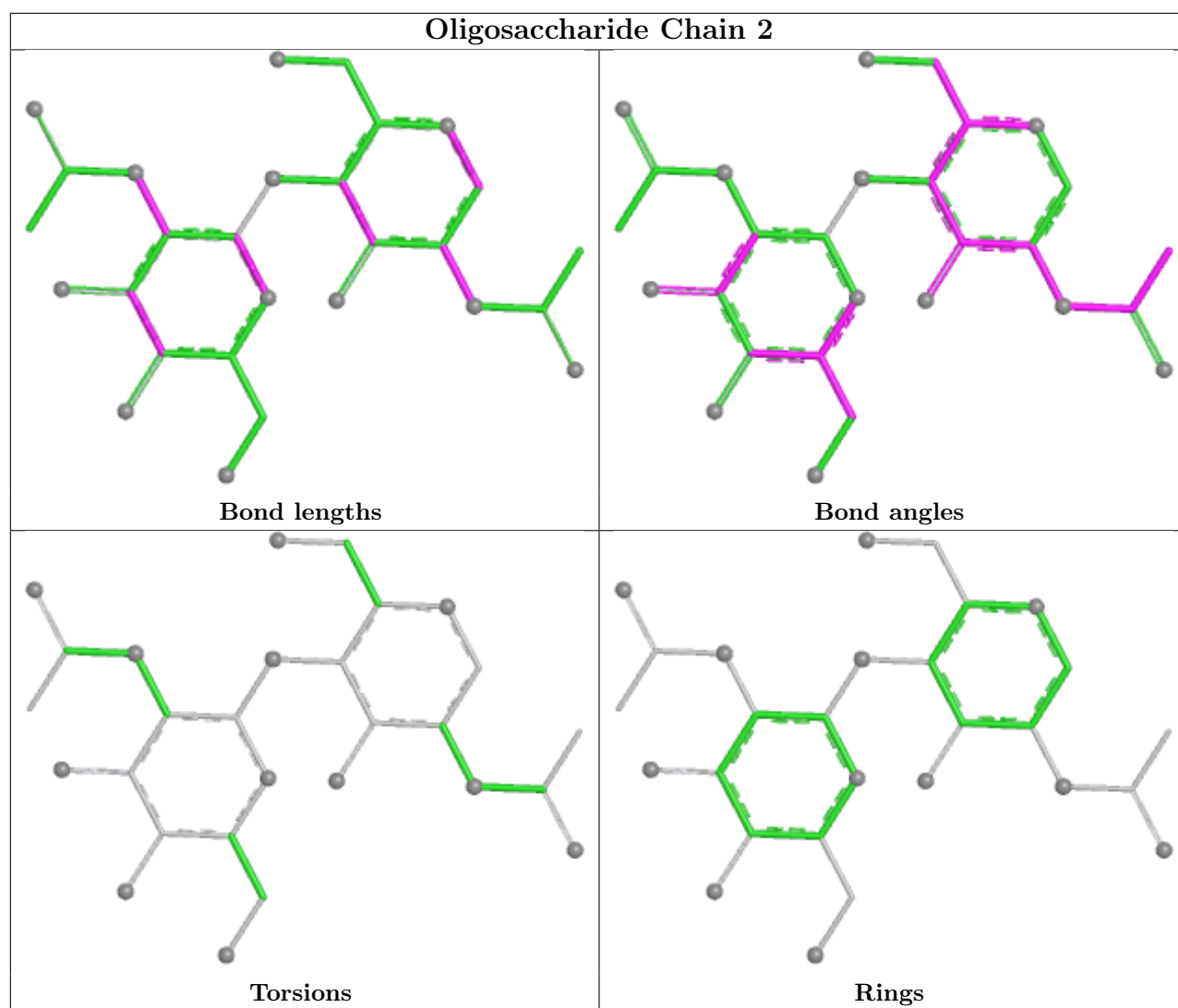


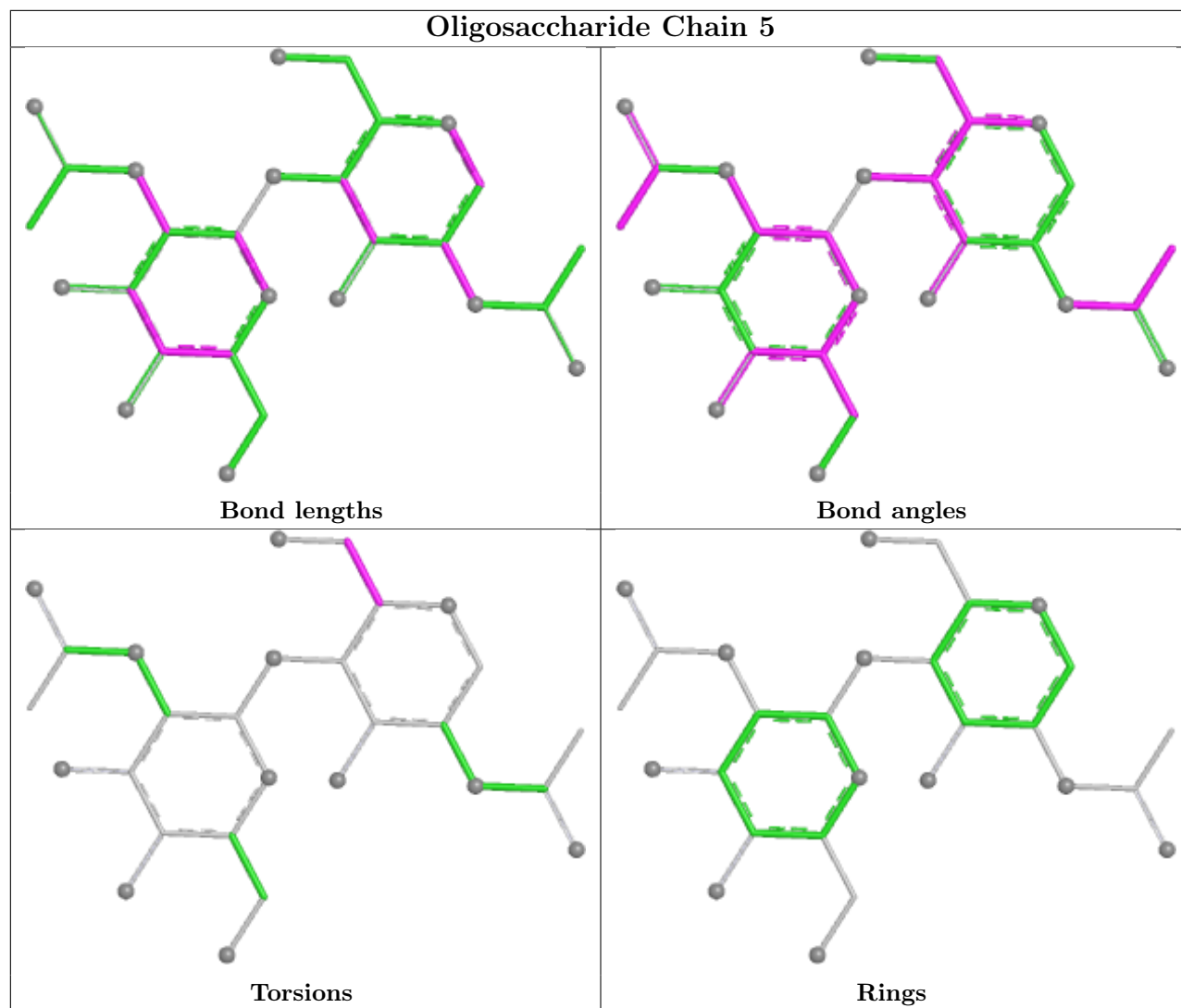


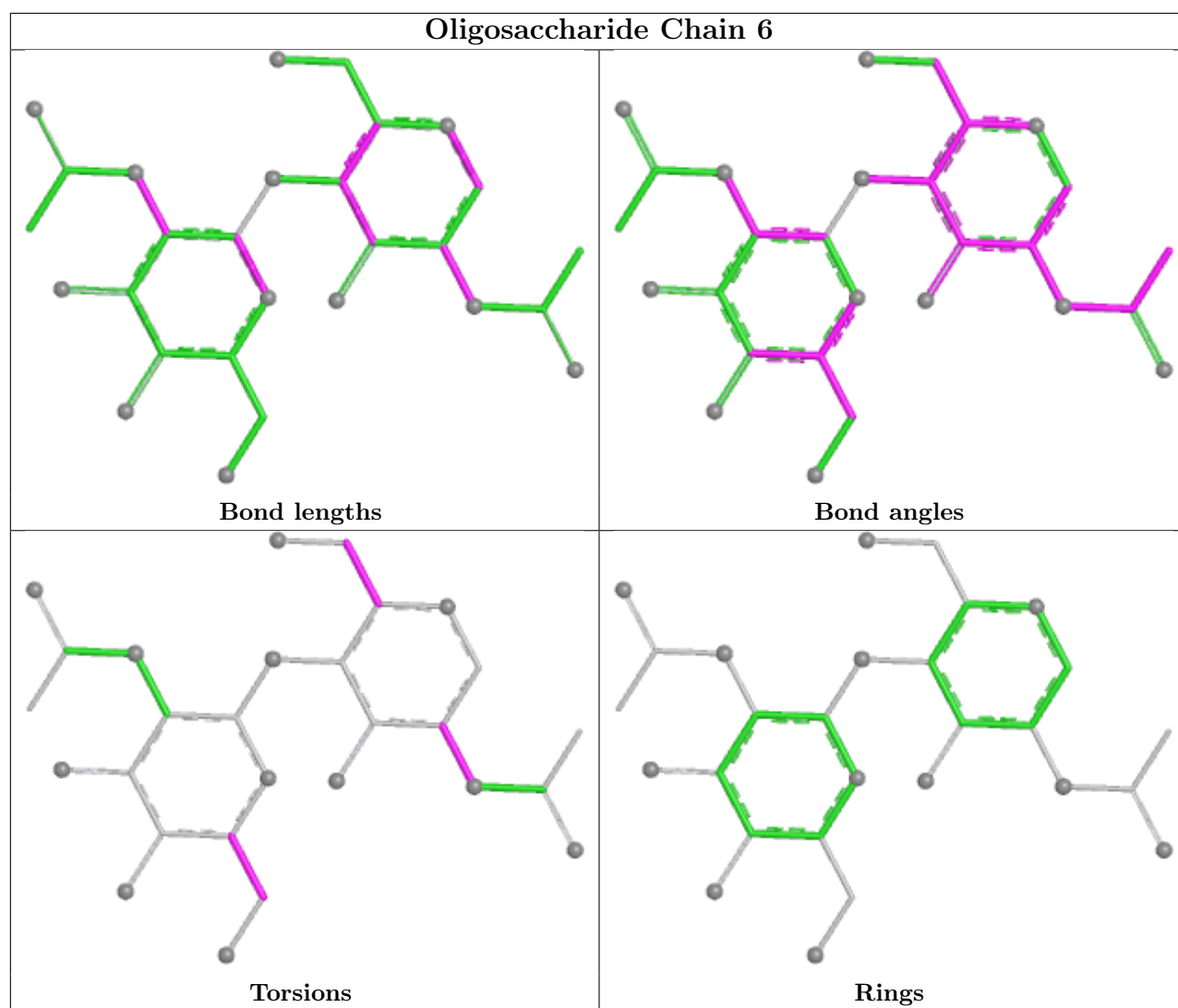


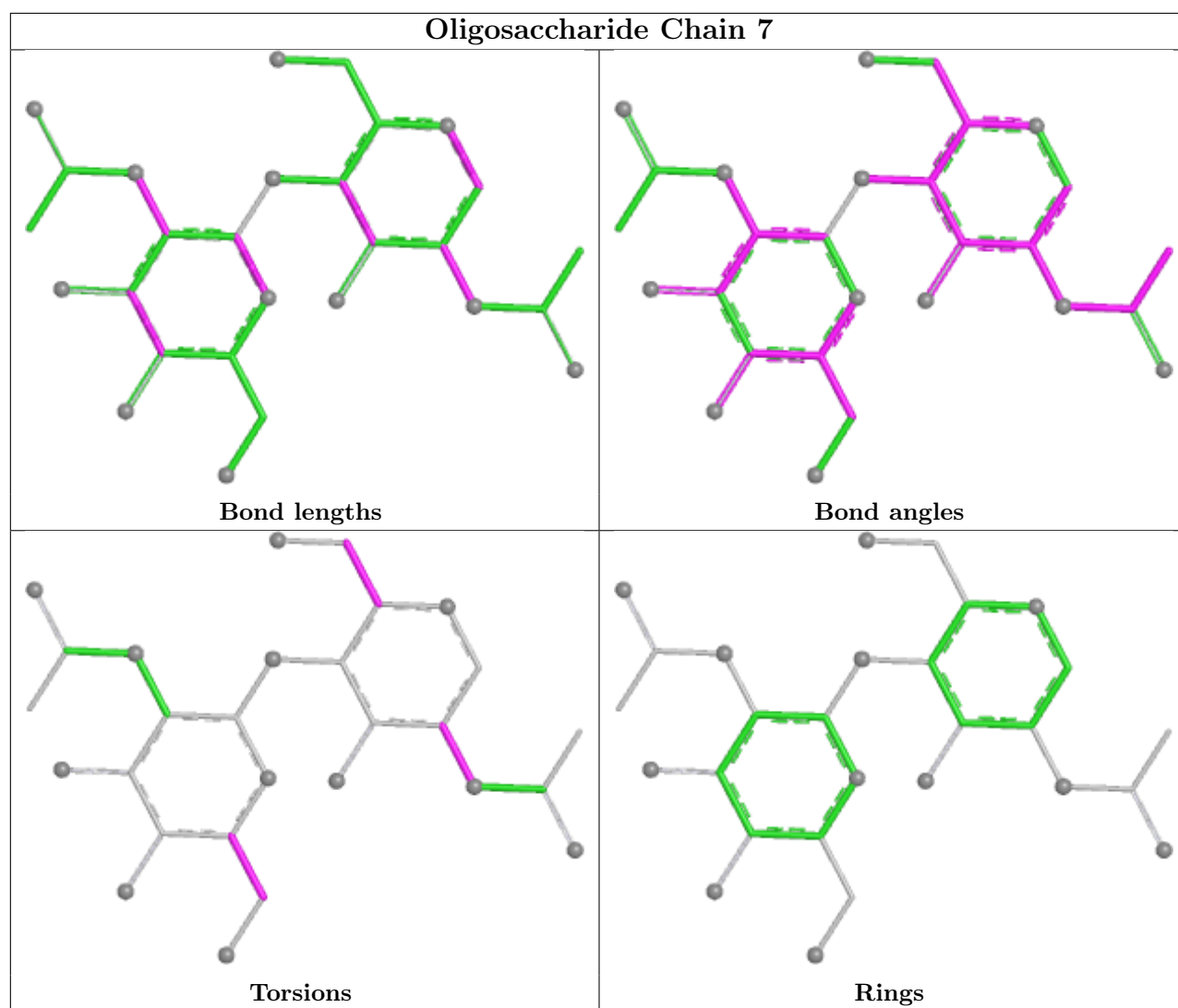


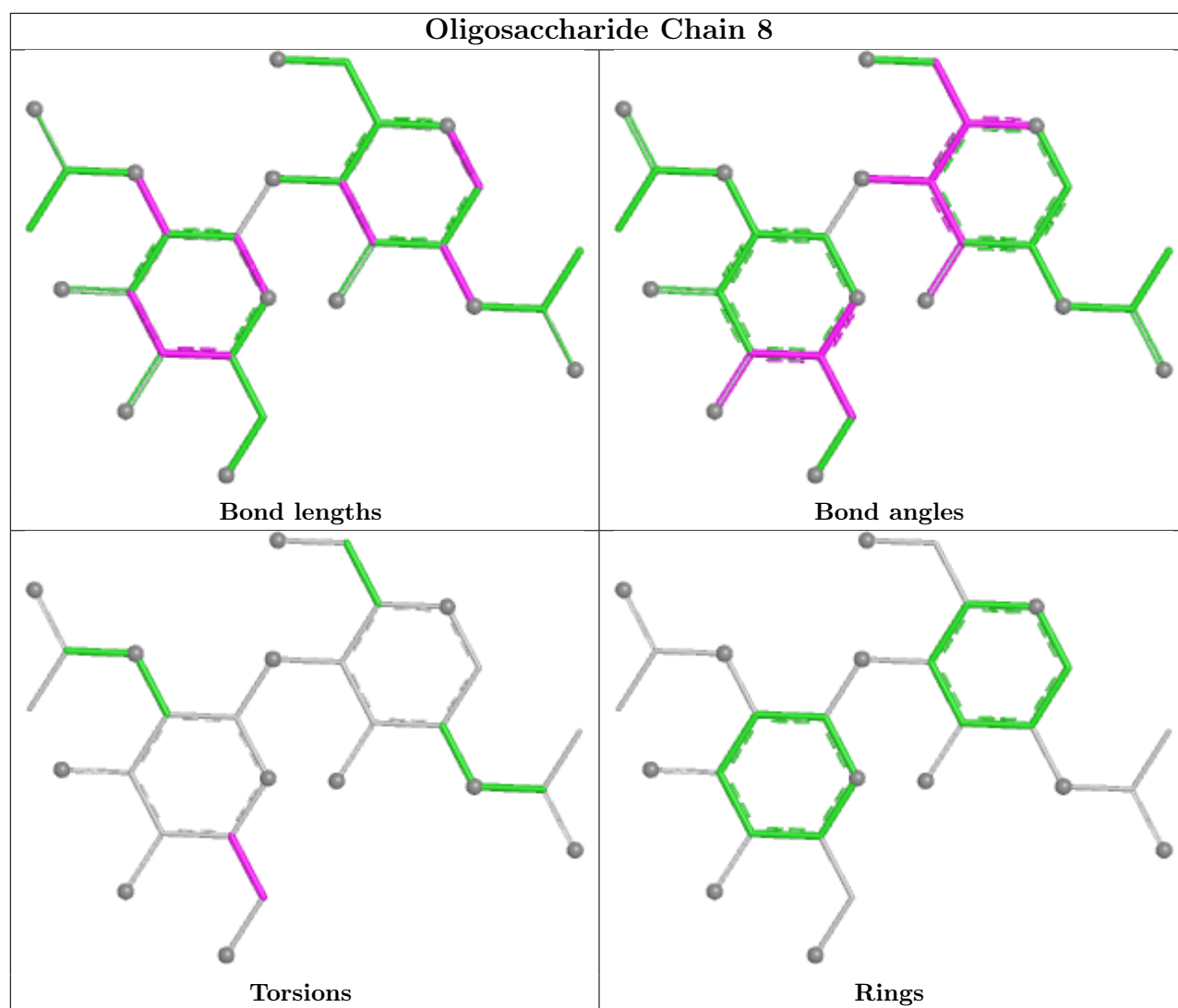


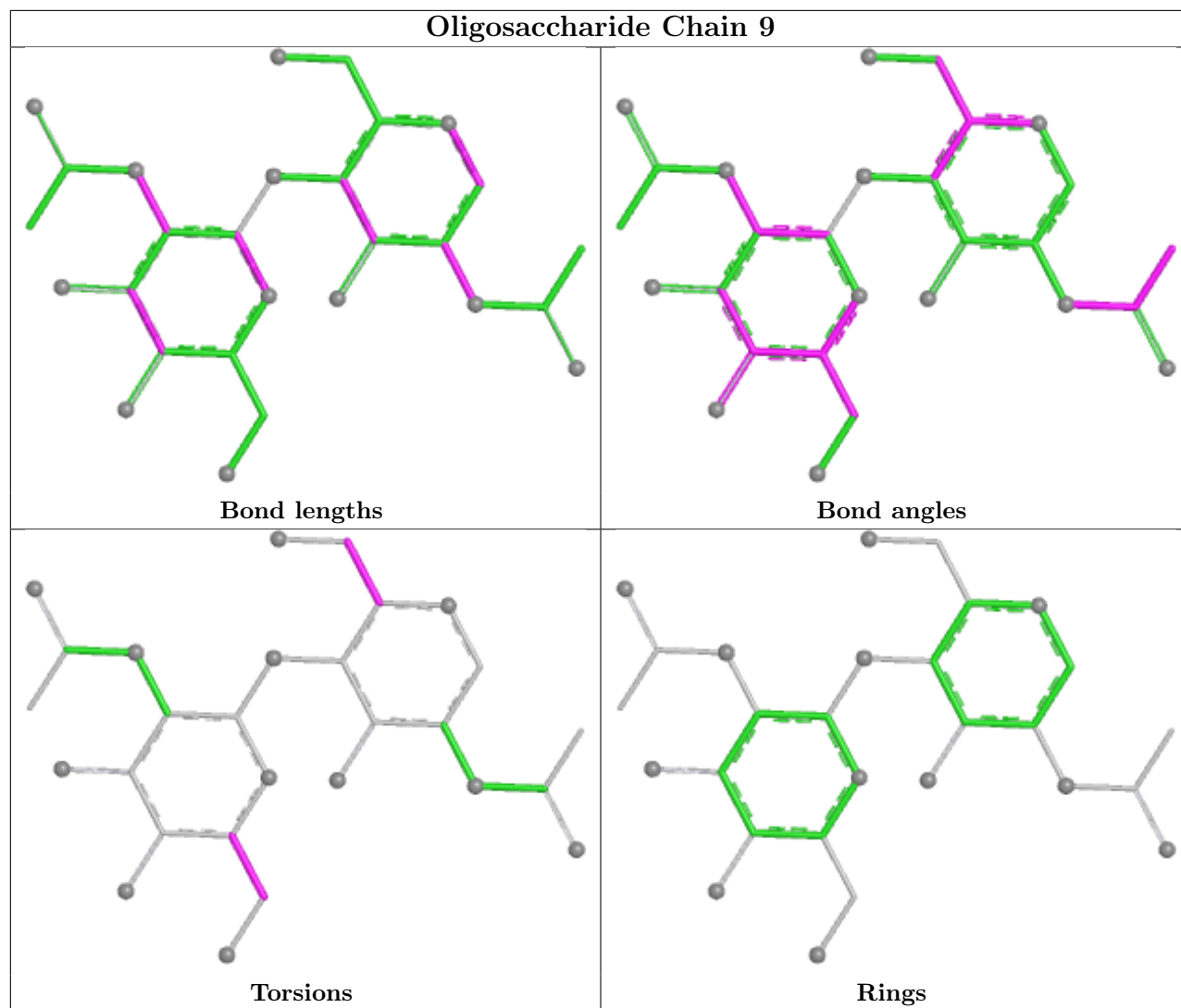


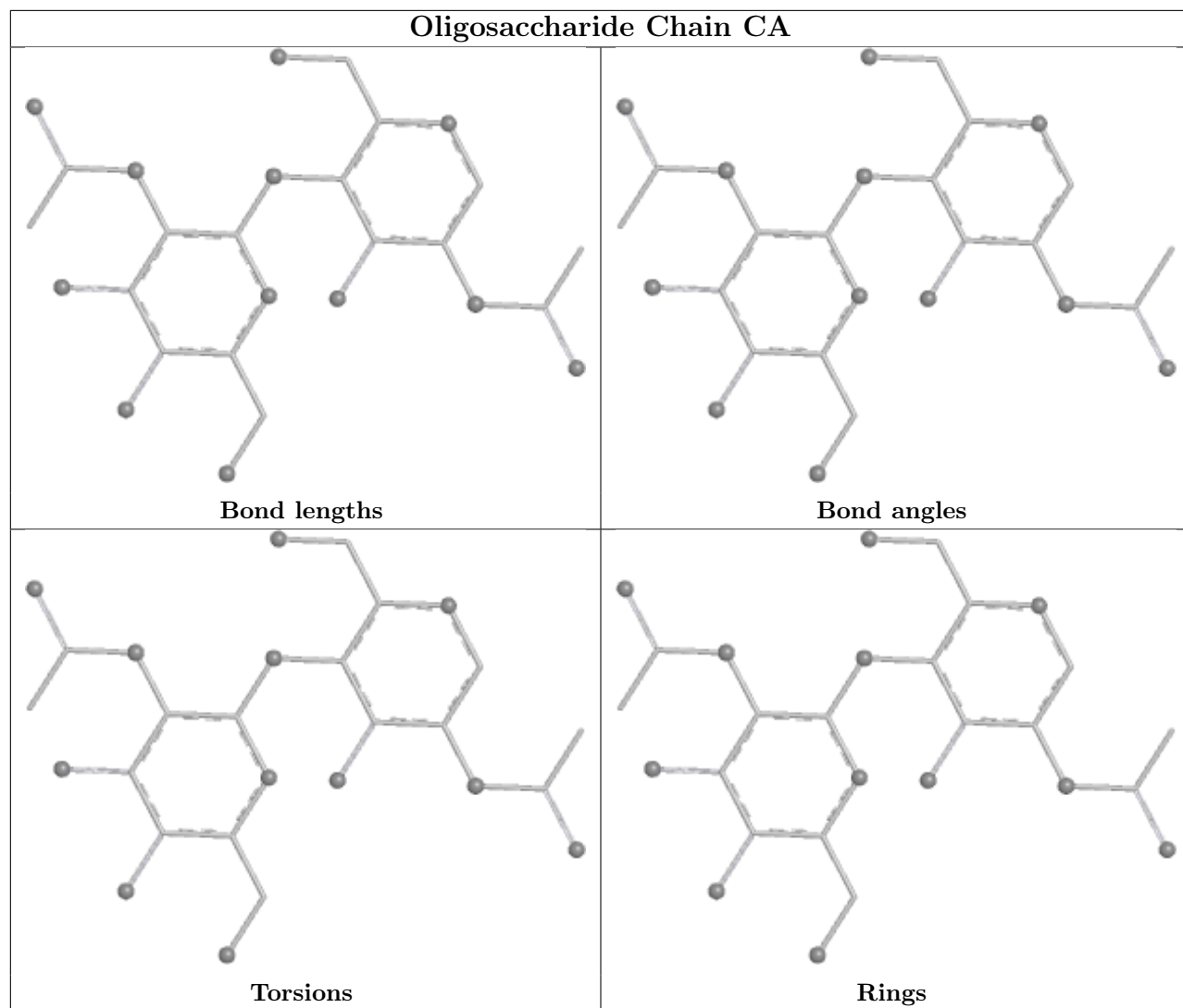




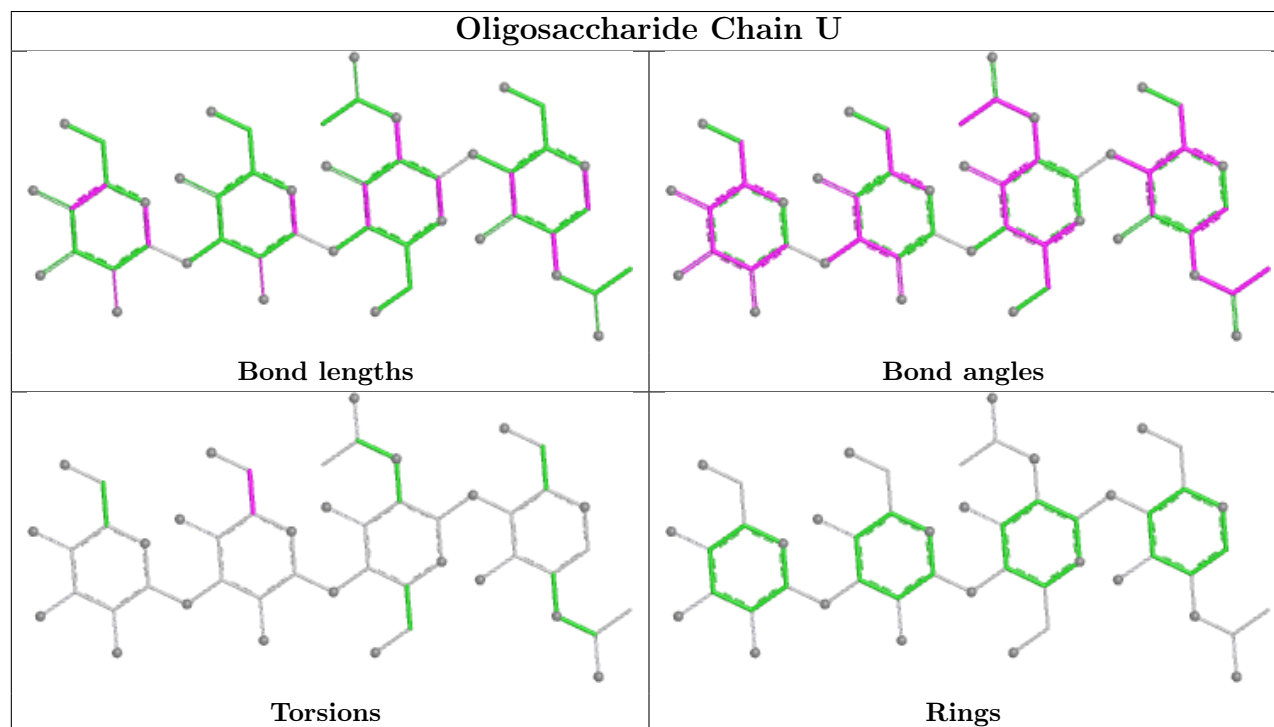
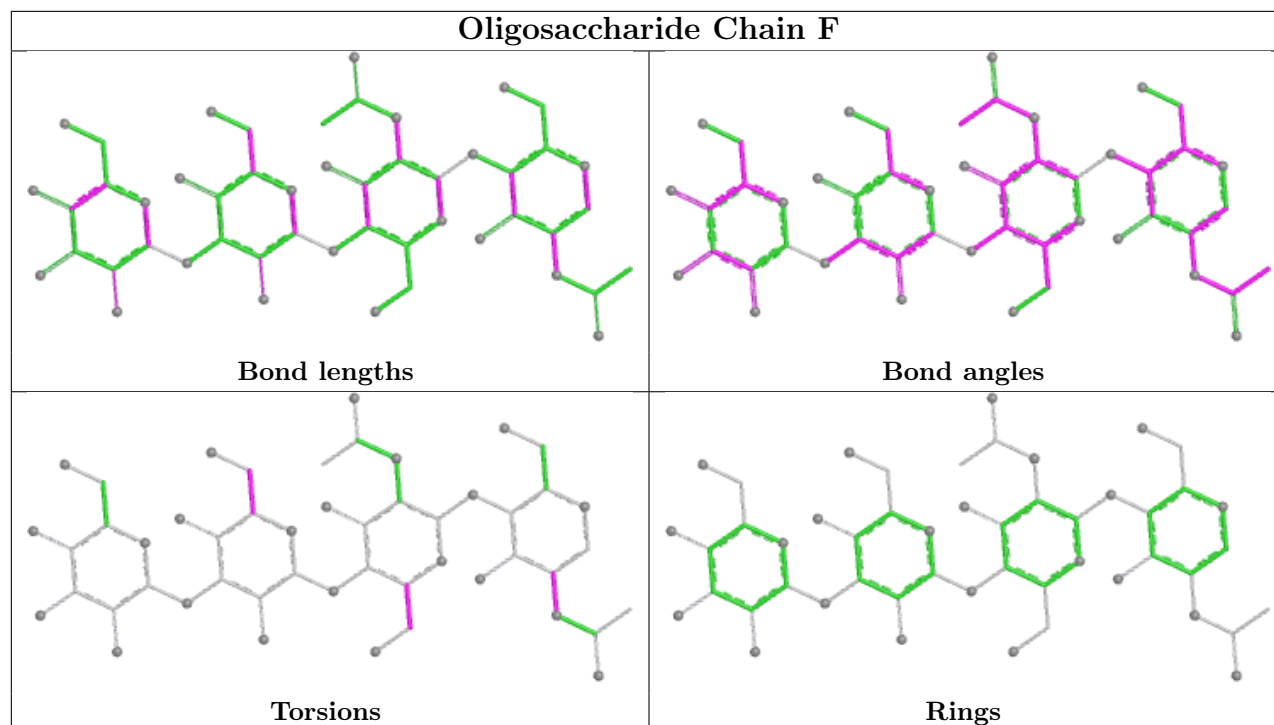


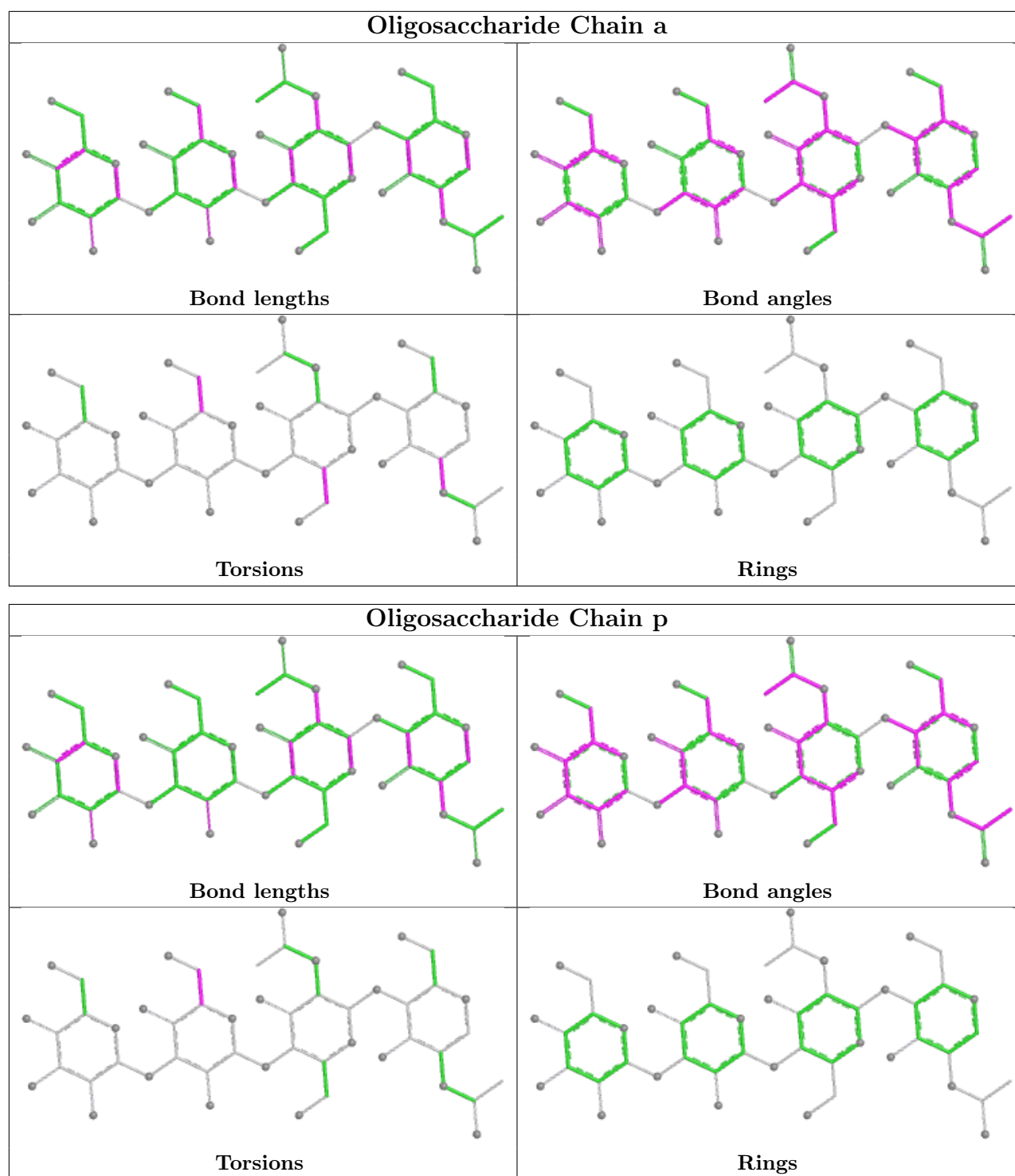


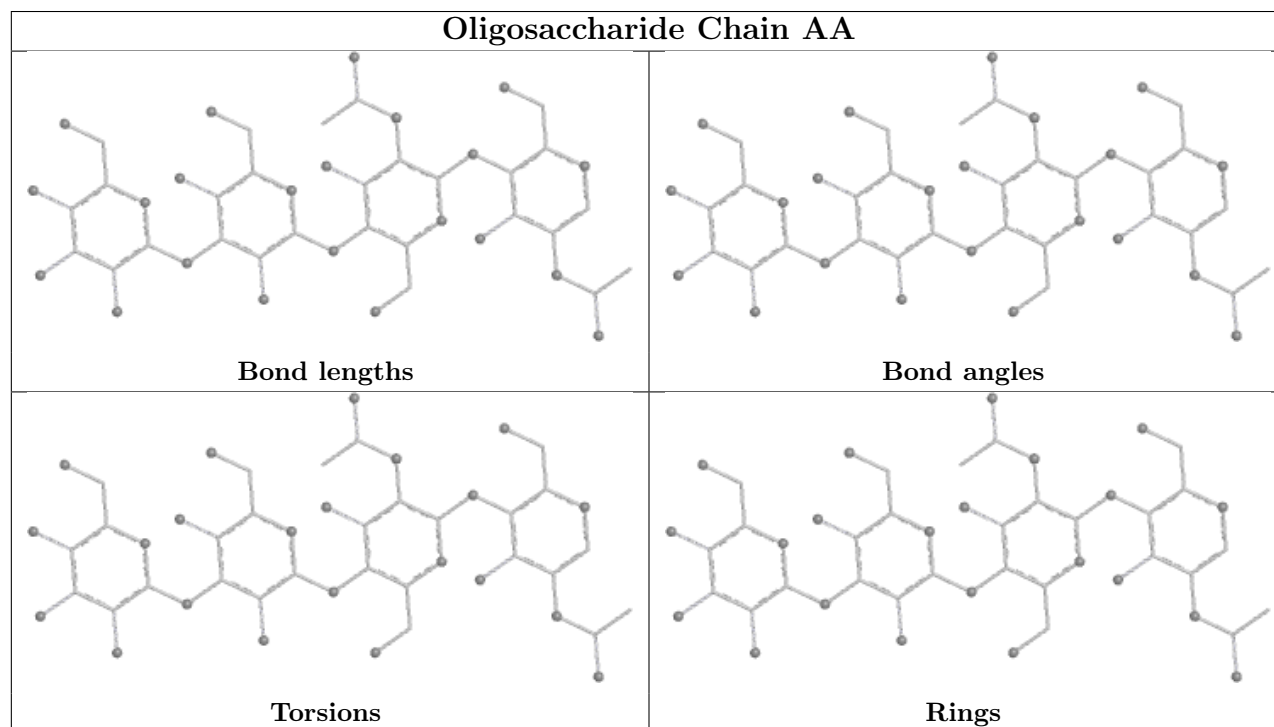
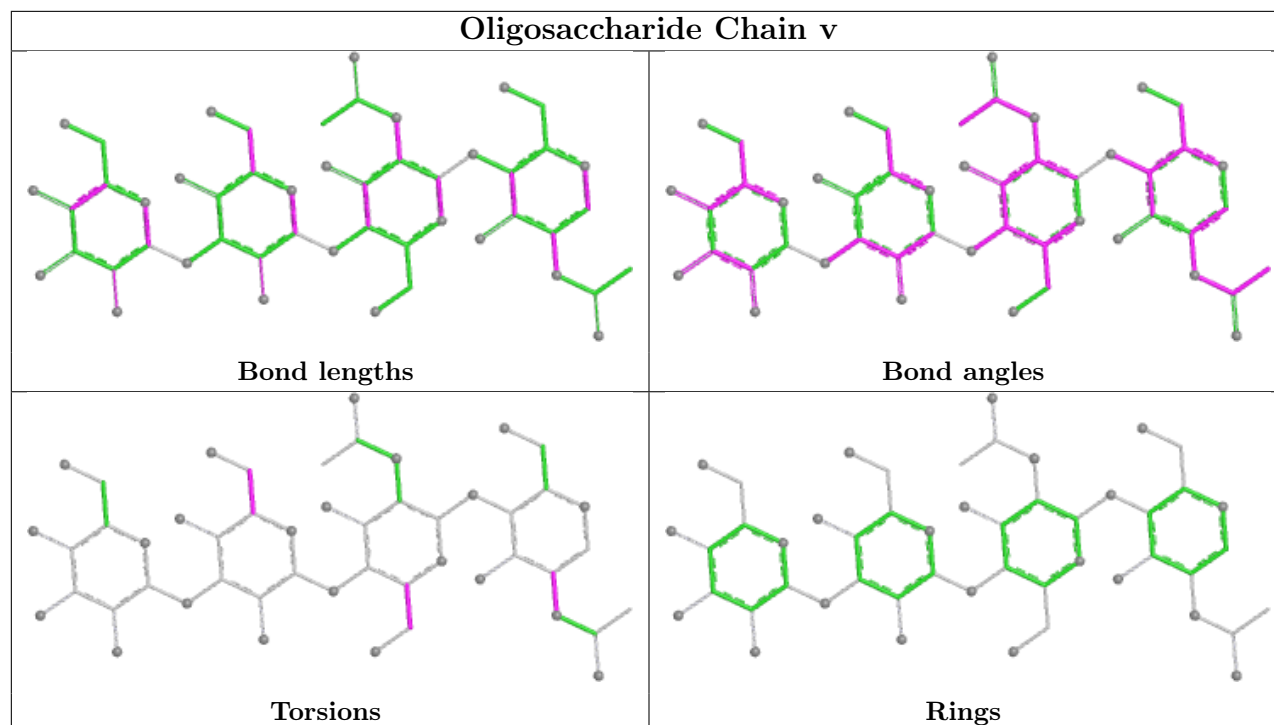


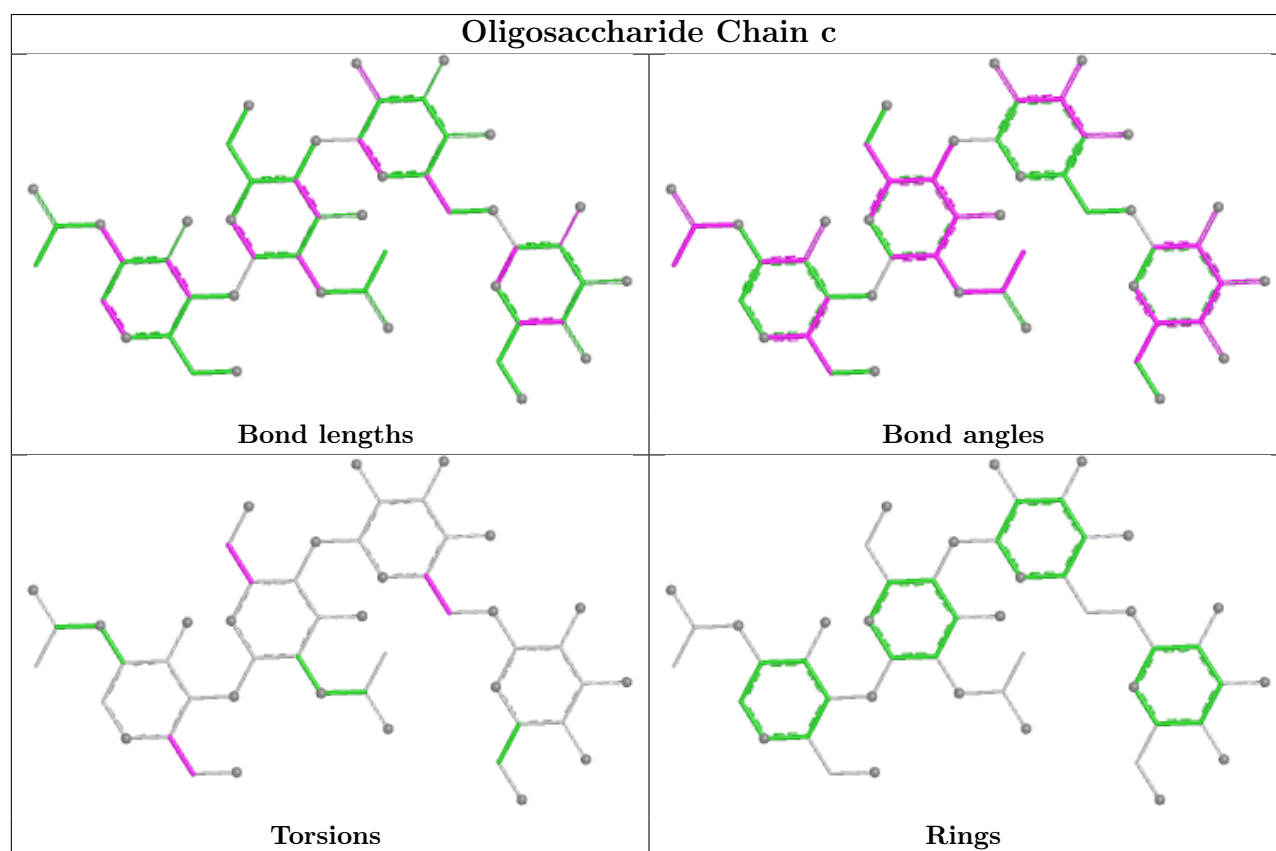
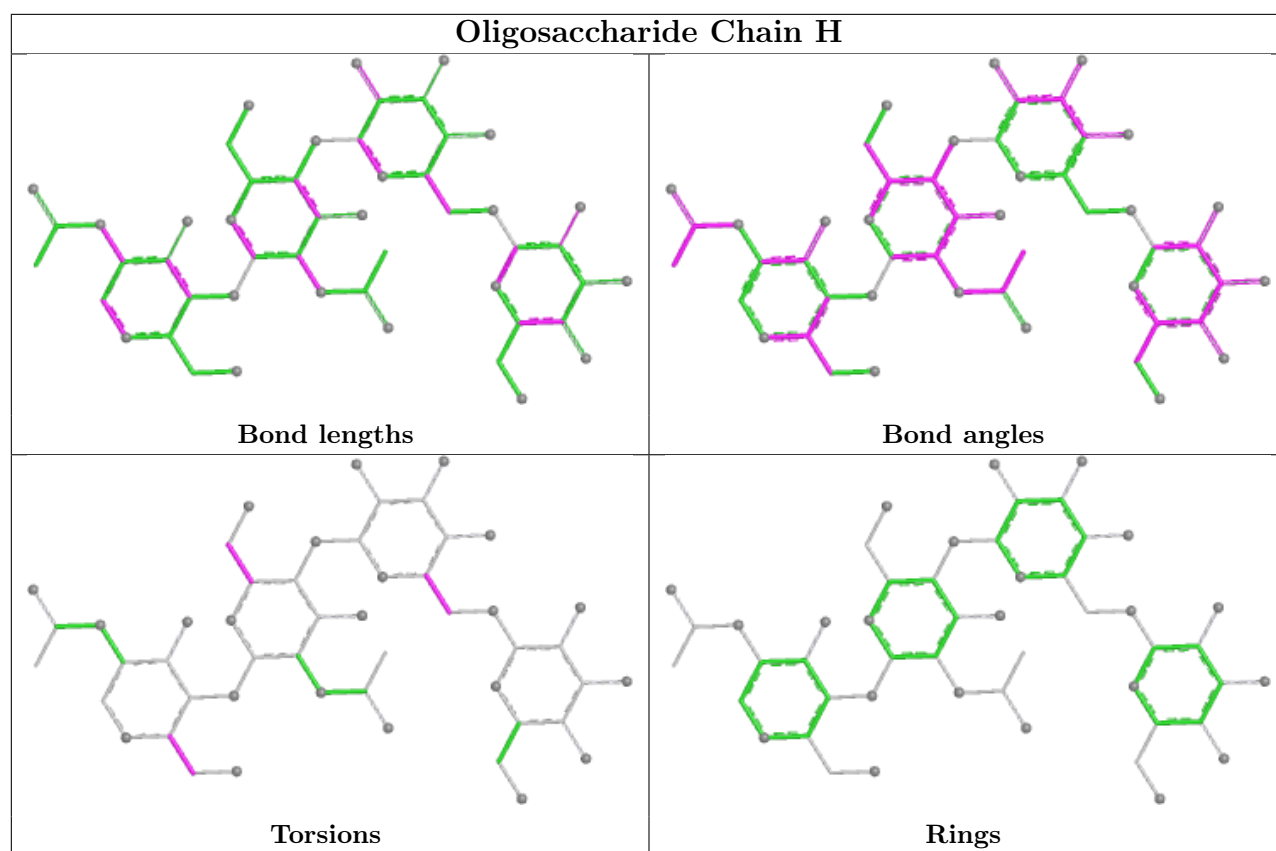


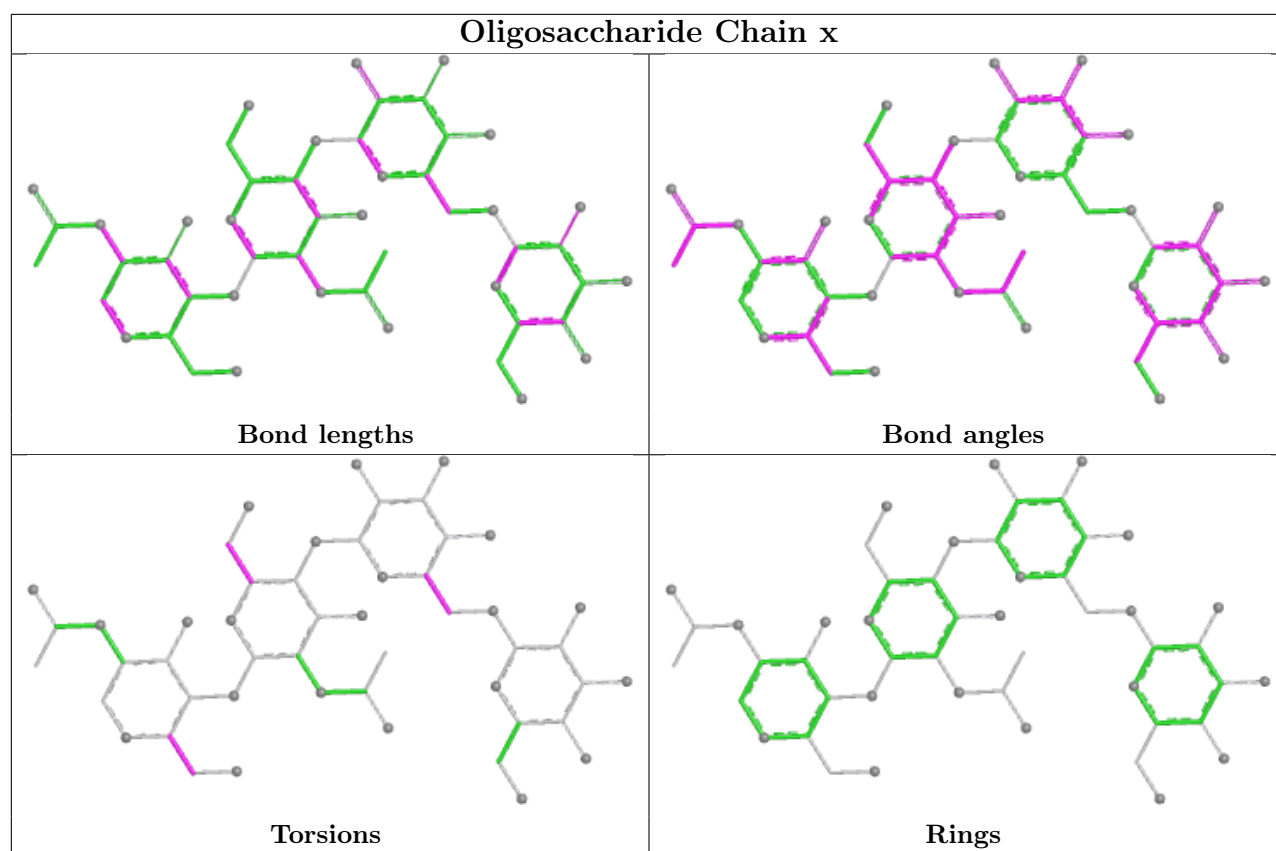


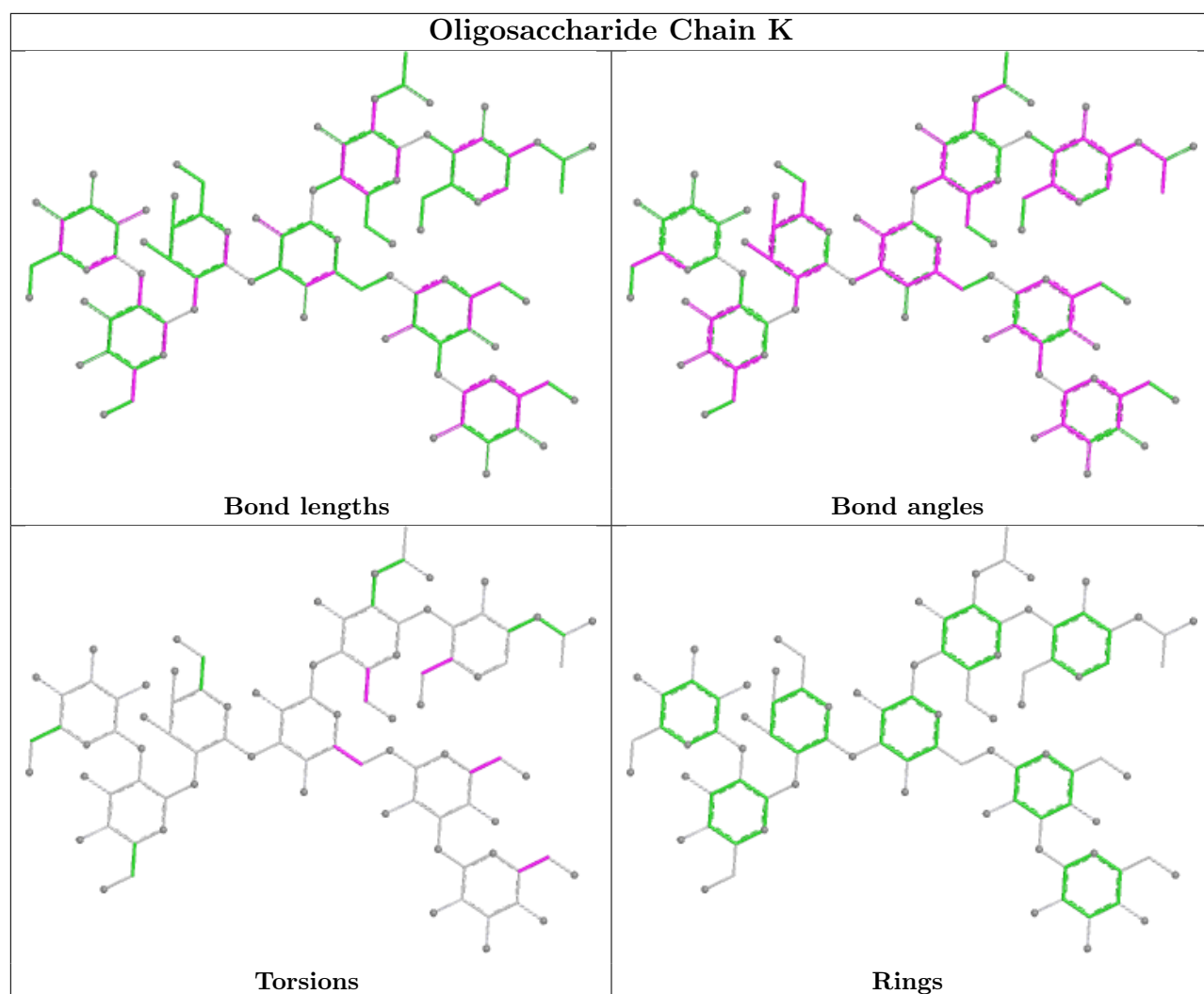


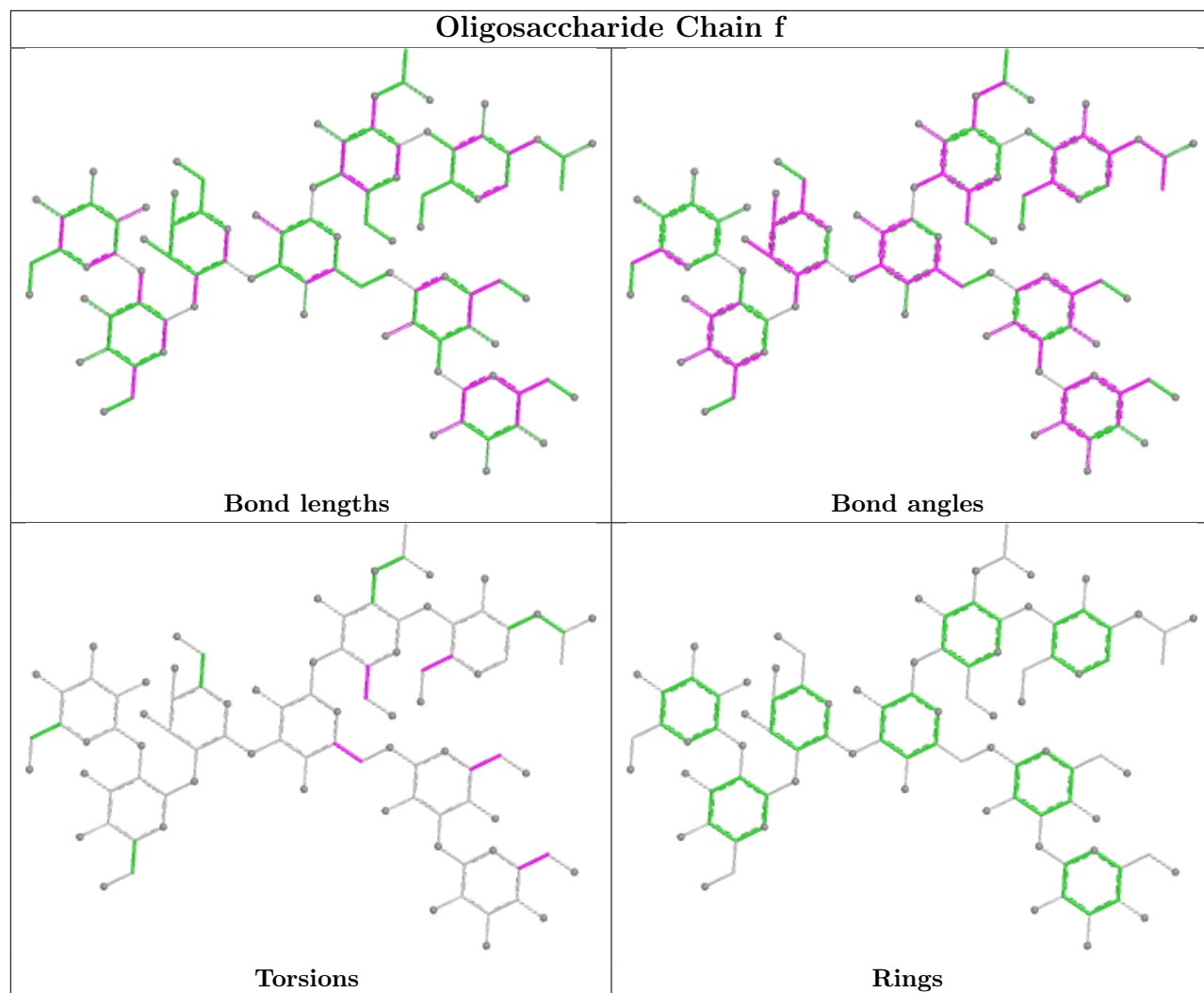


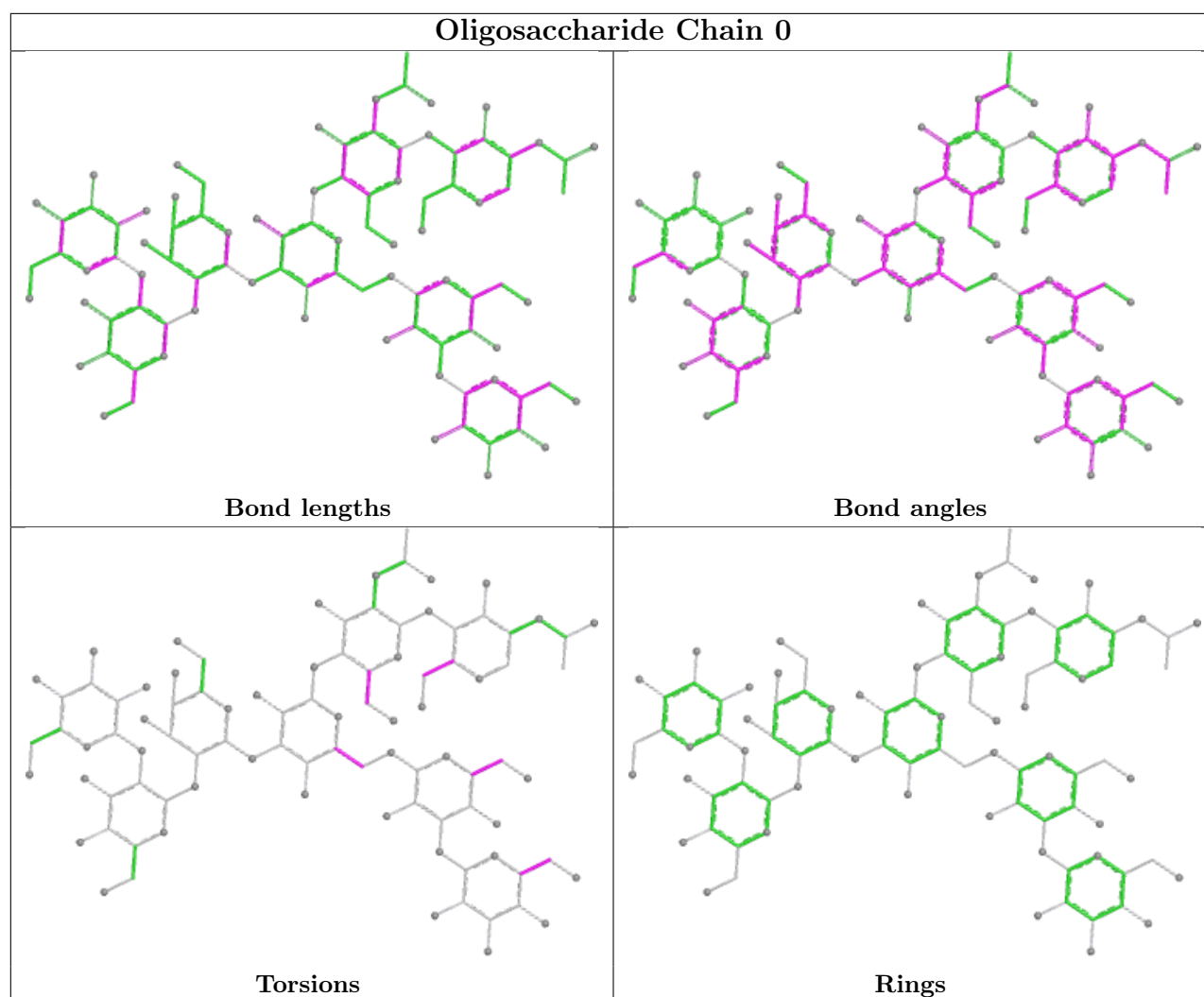




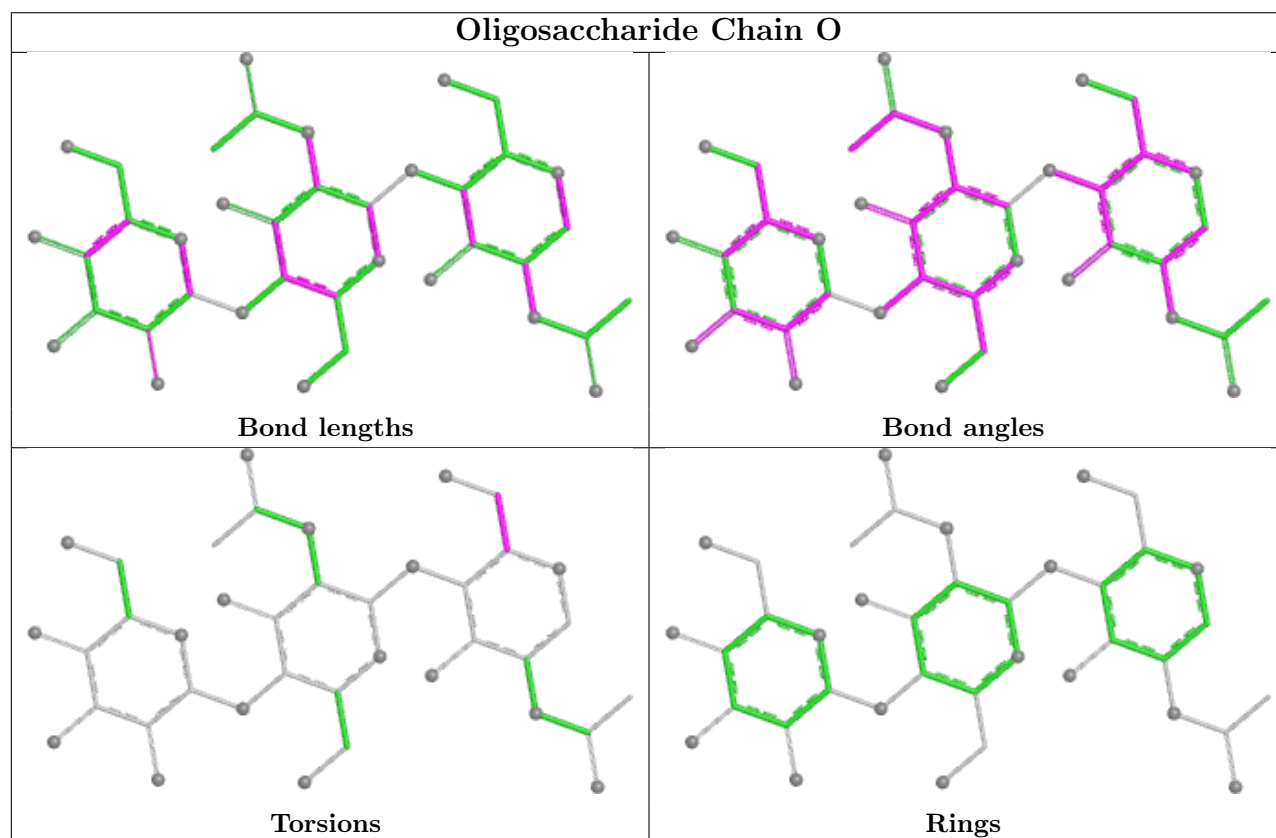
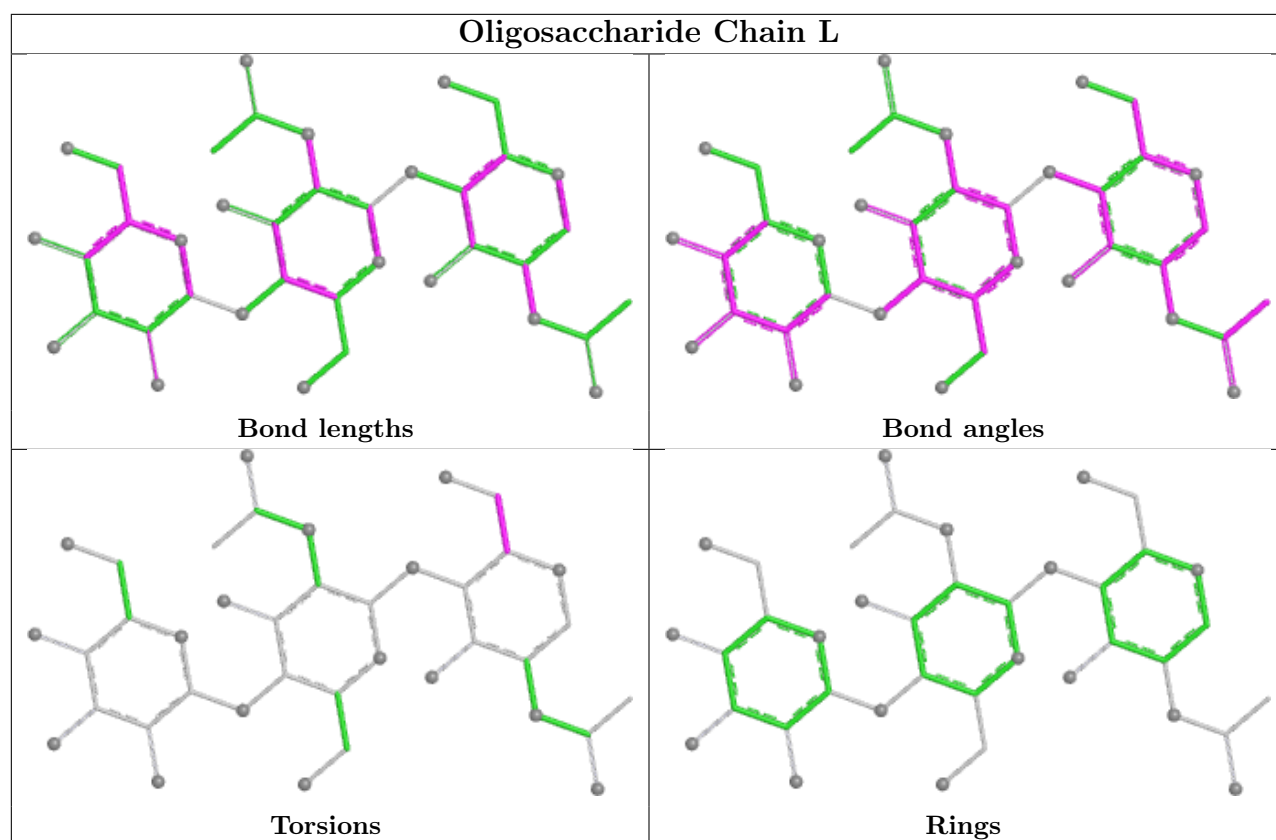


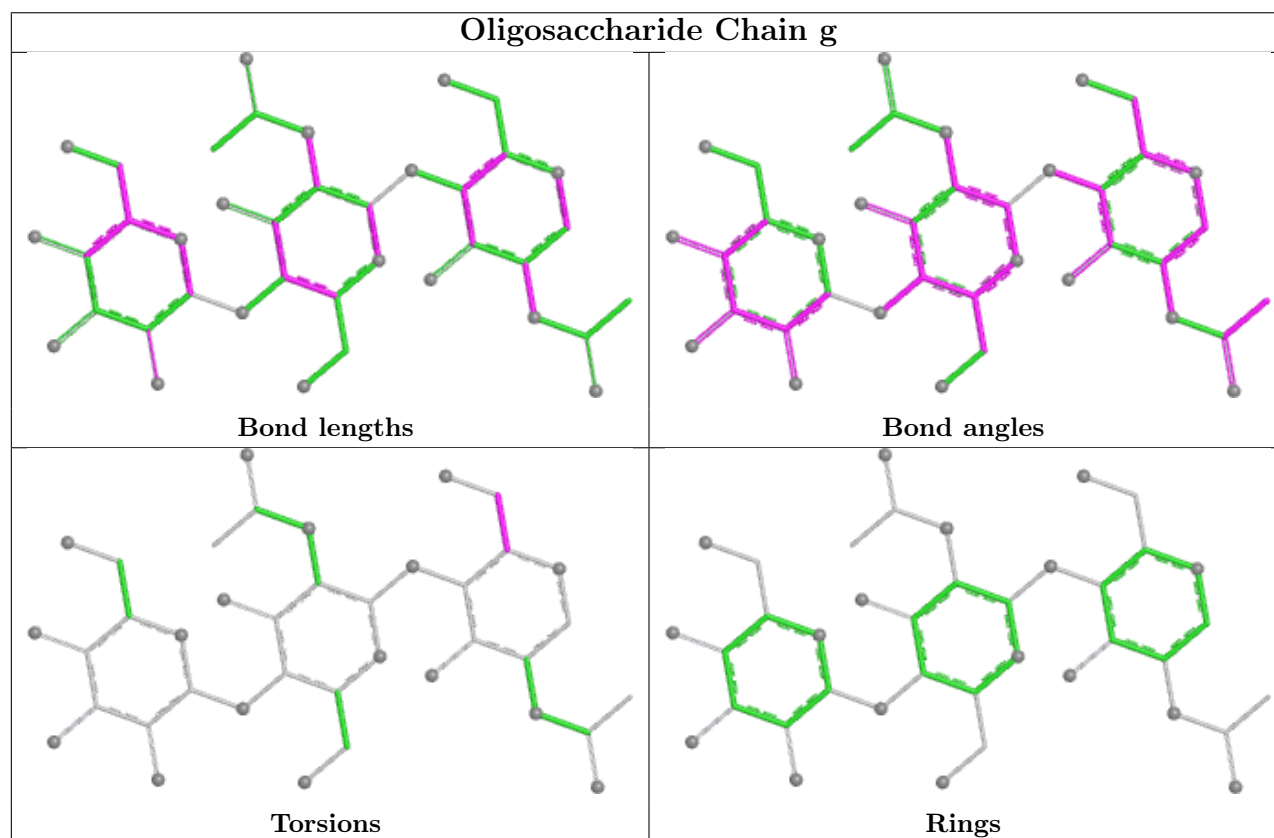
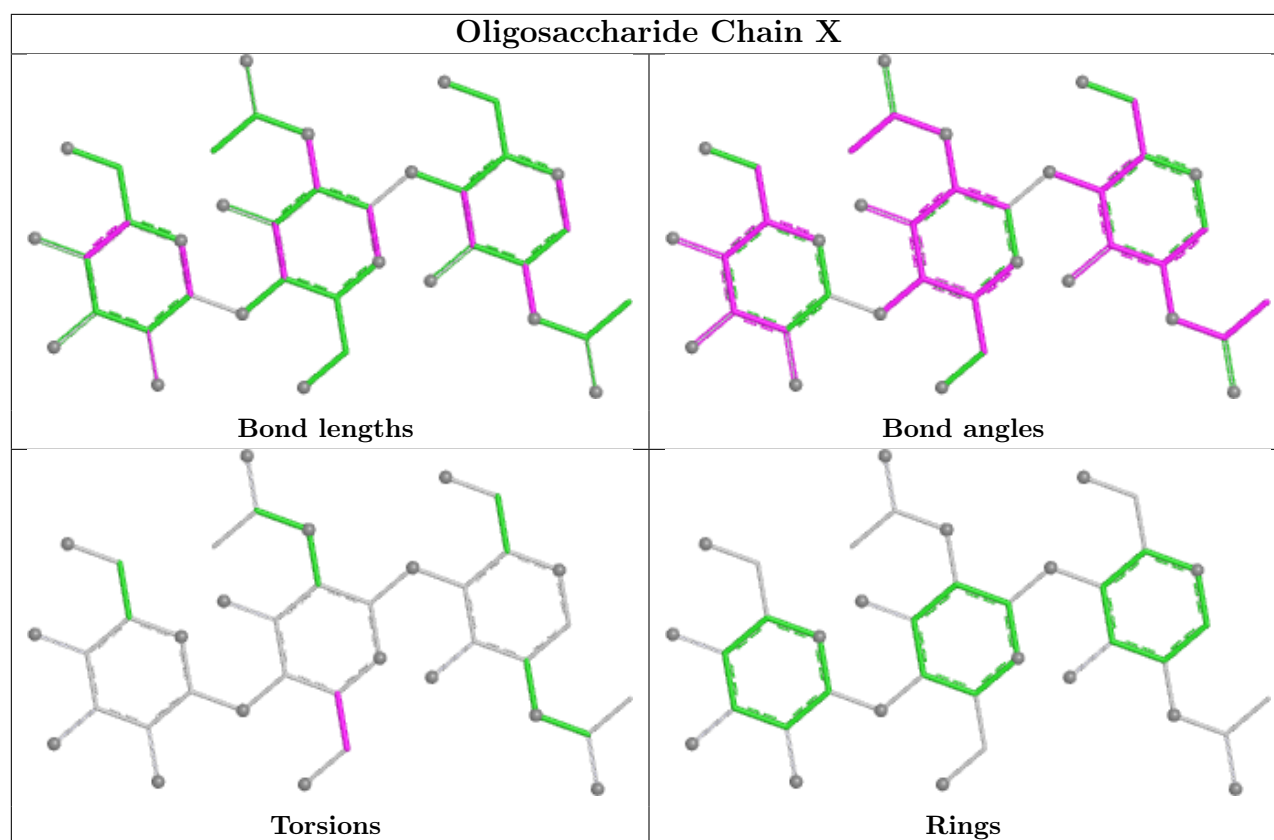


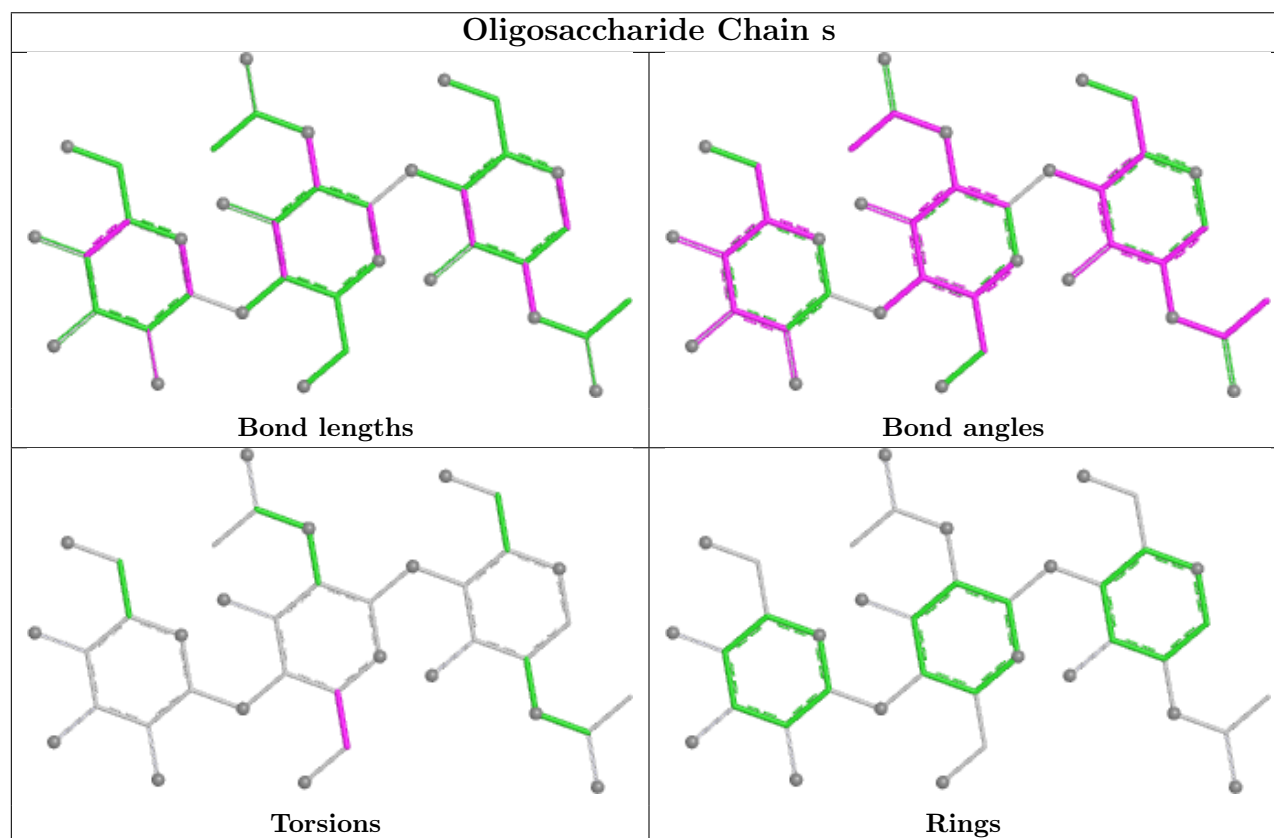
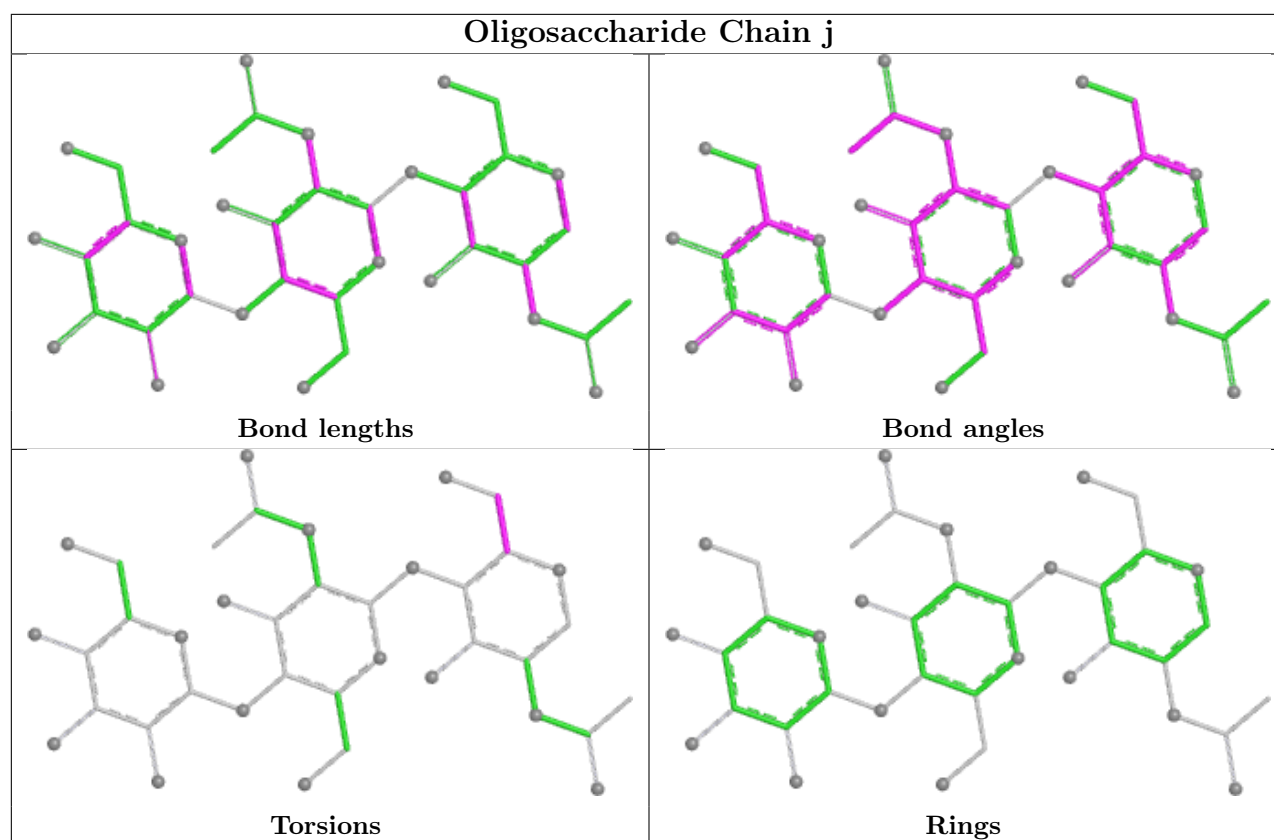


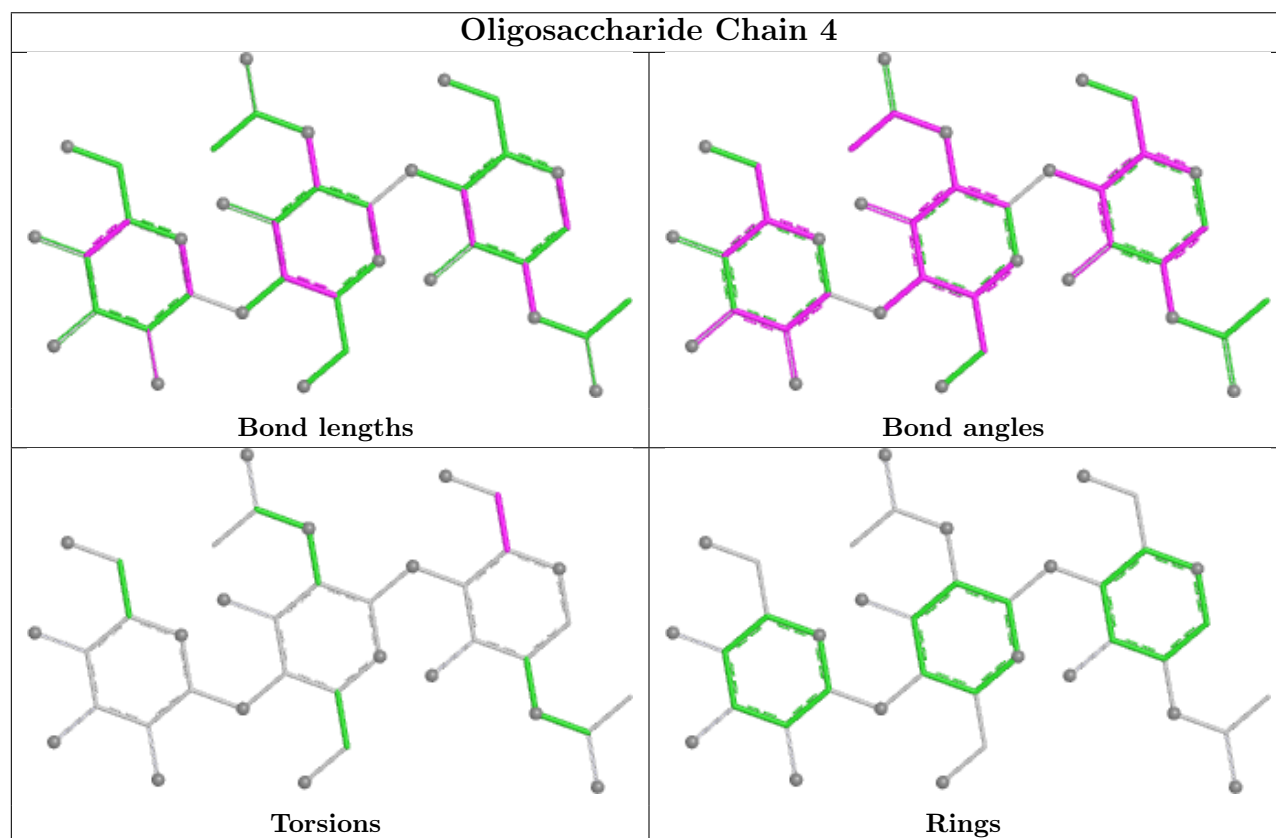
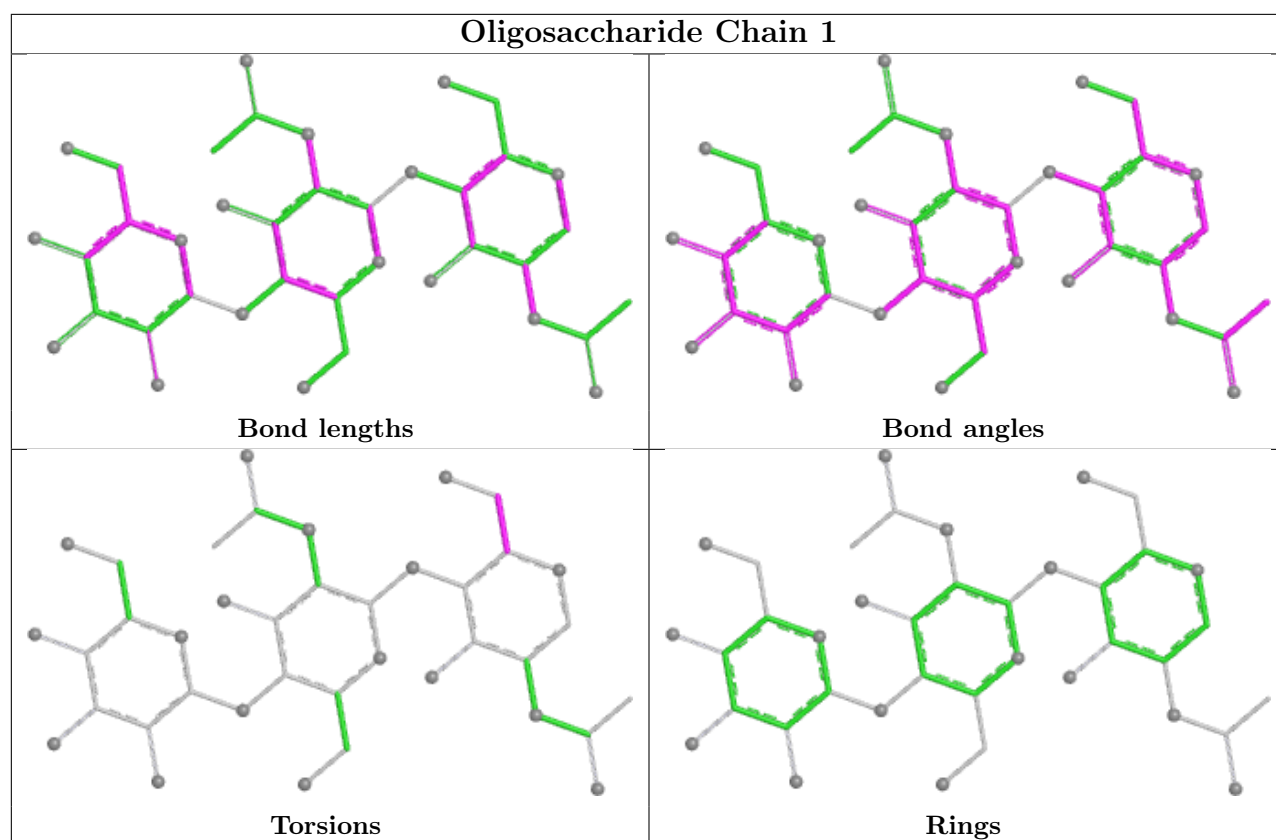




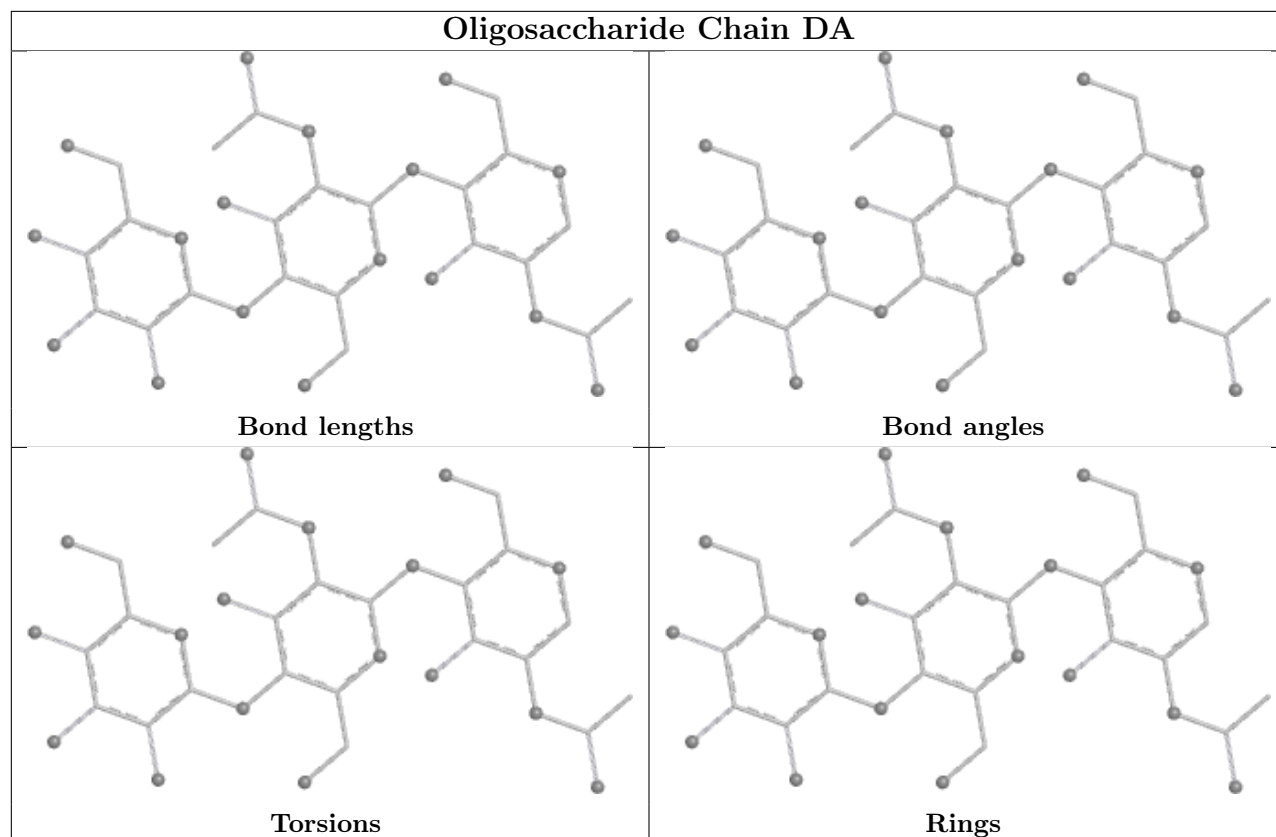




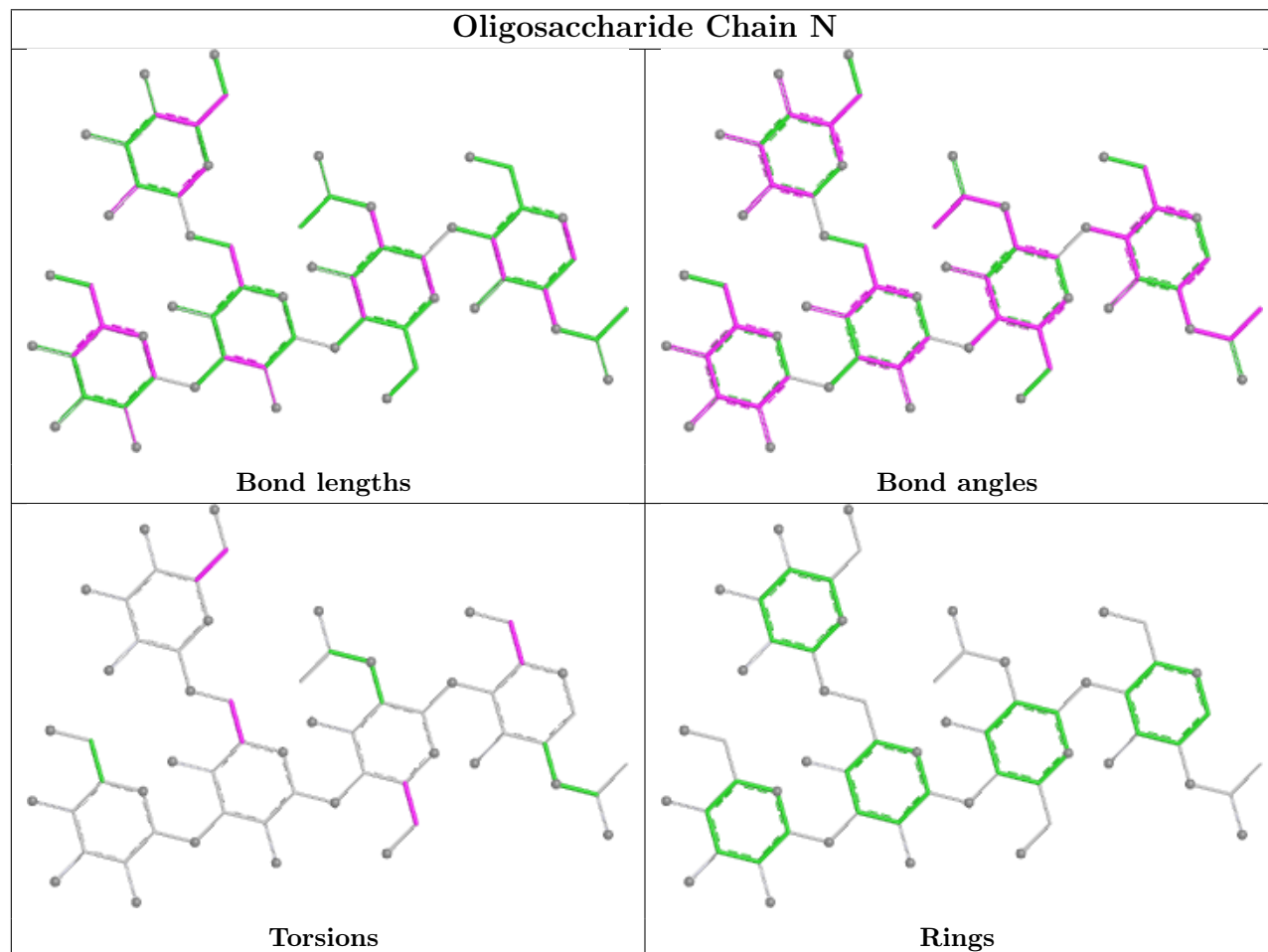


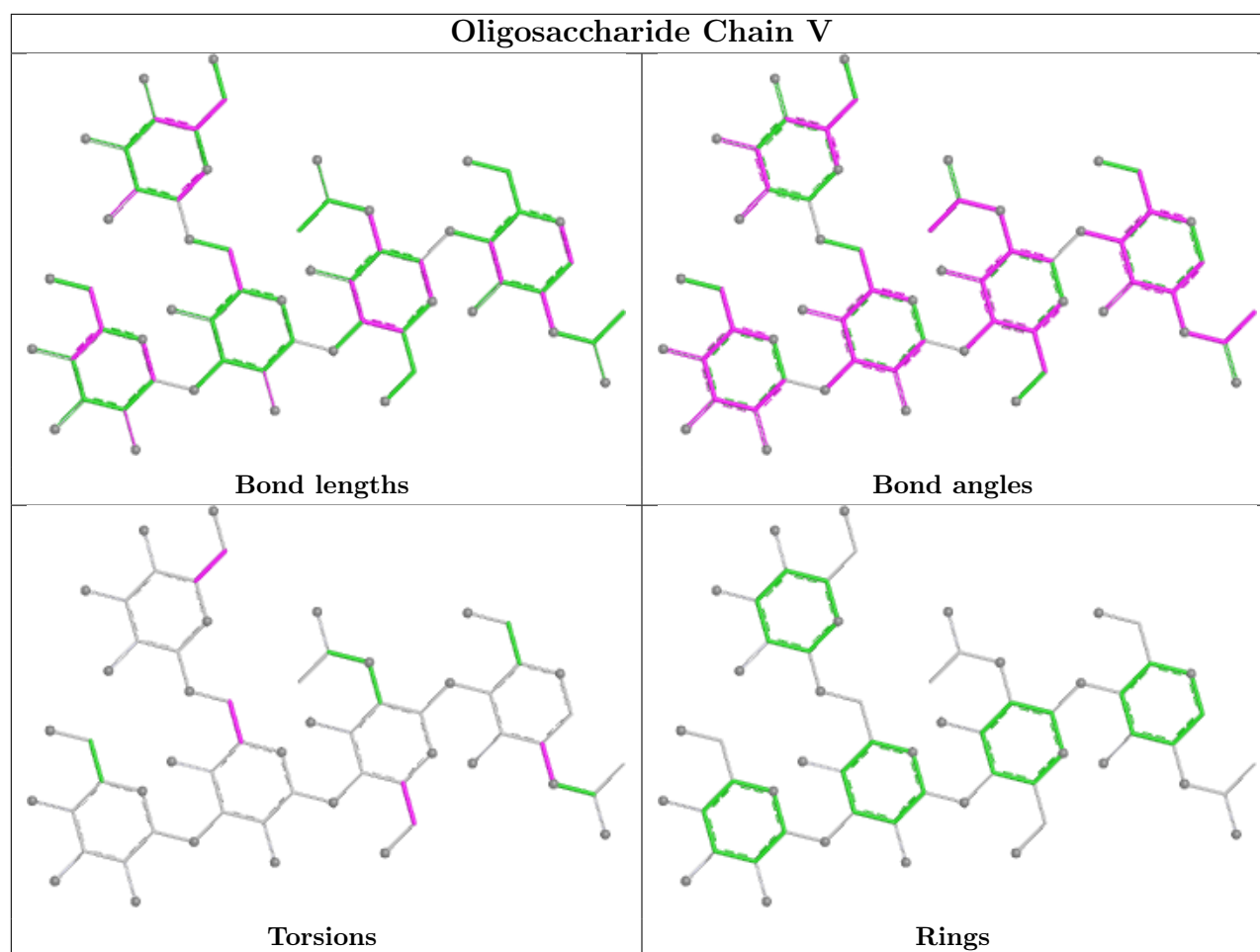


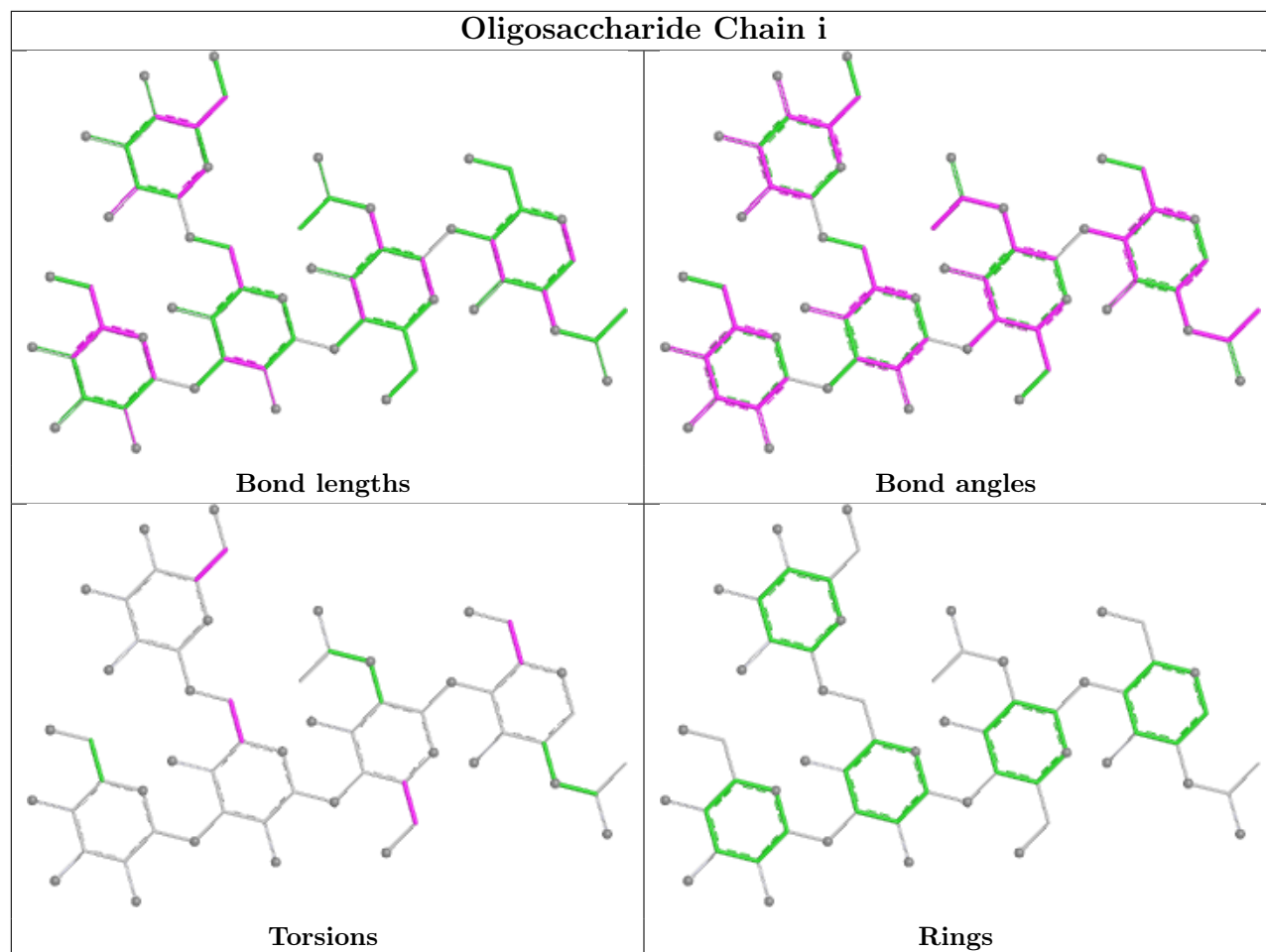
## Oligosaccharide Chain DA

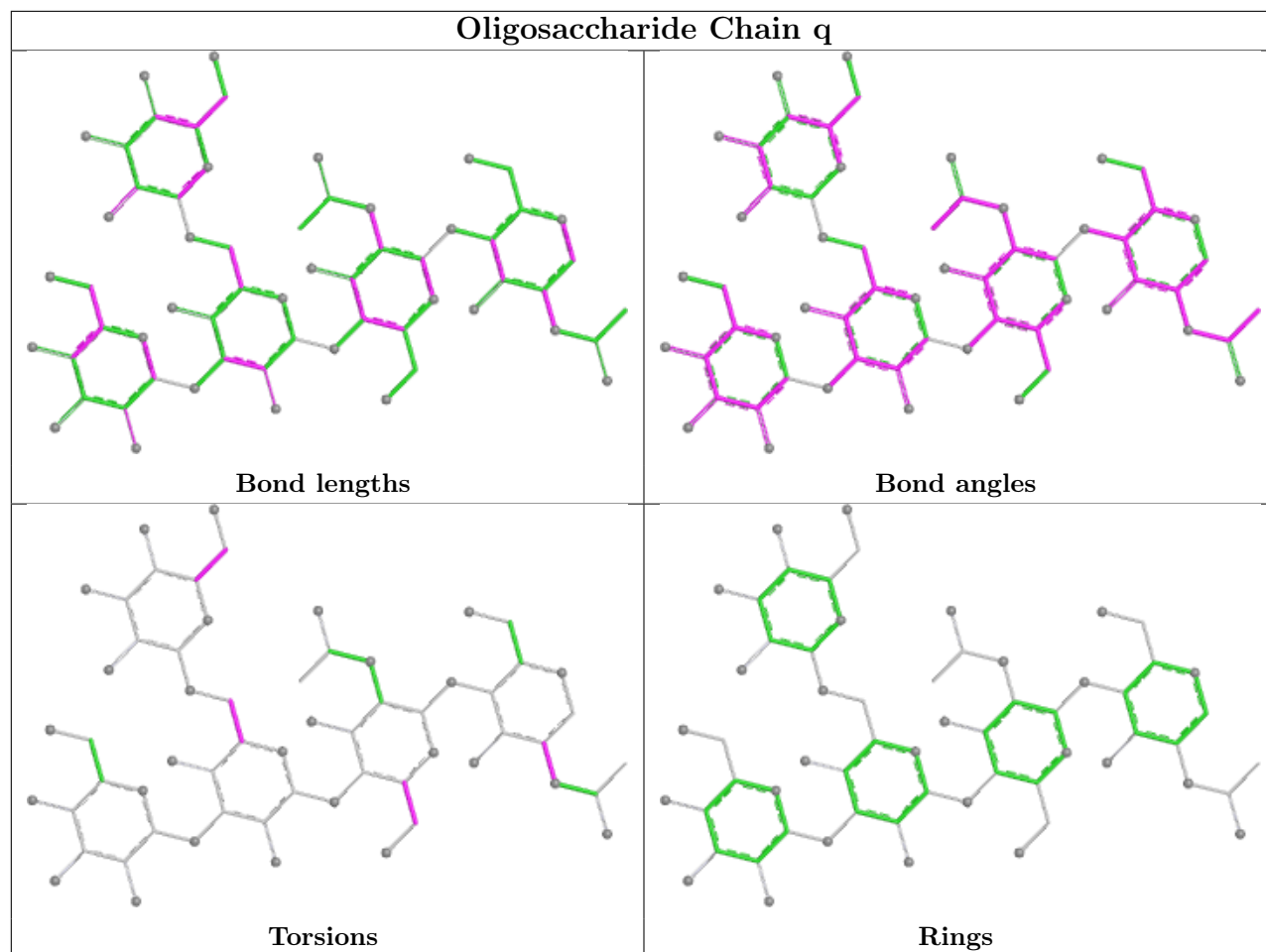


## Oligosaccharide Chain N

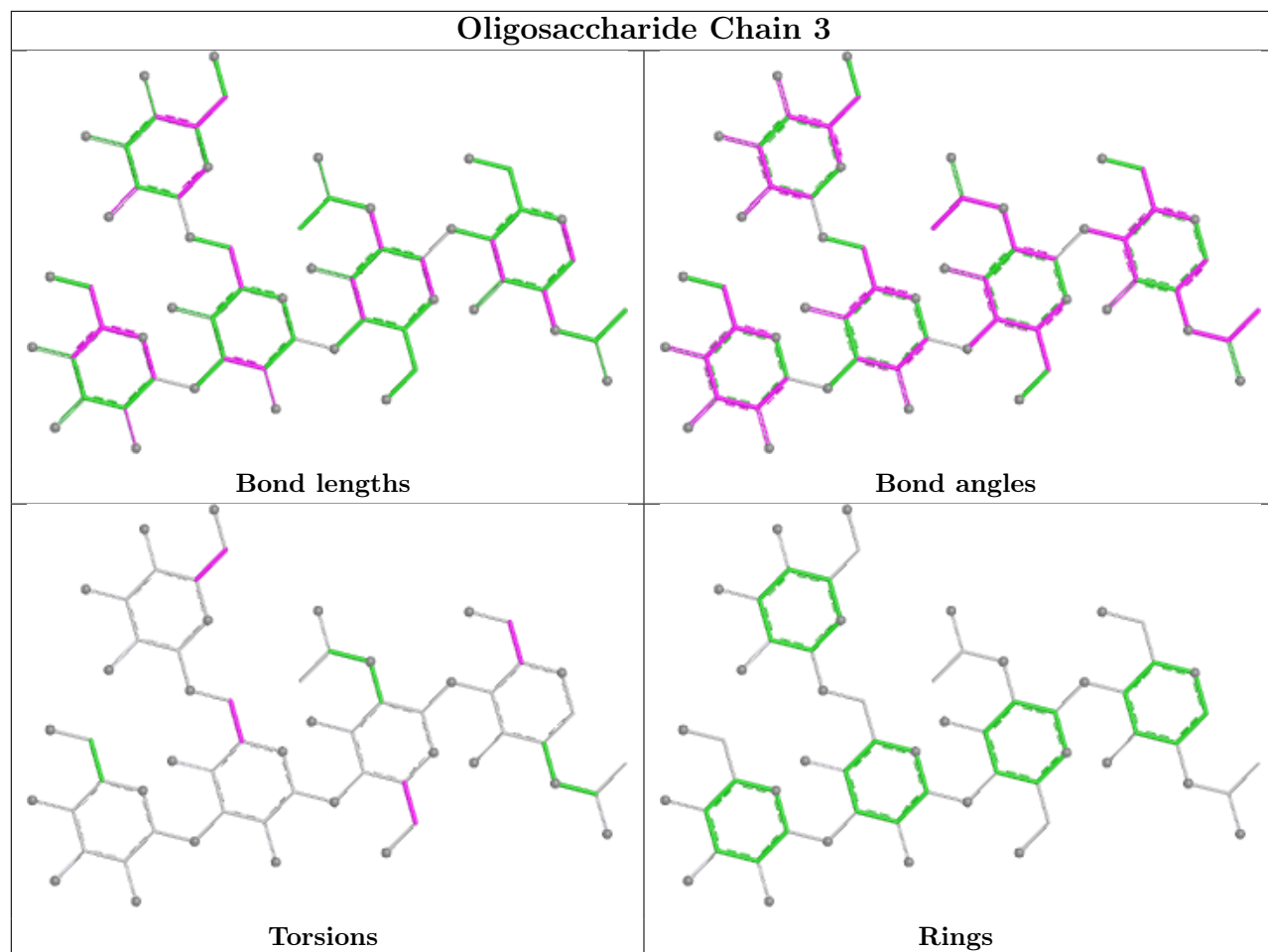


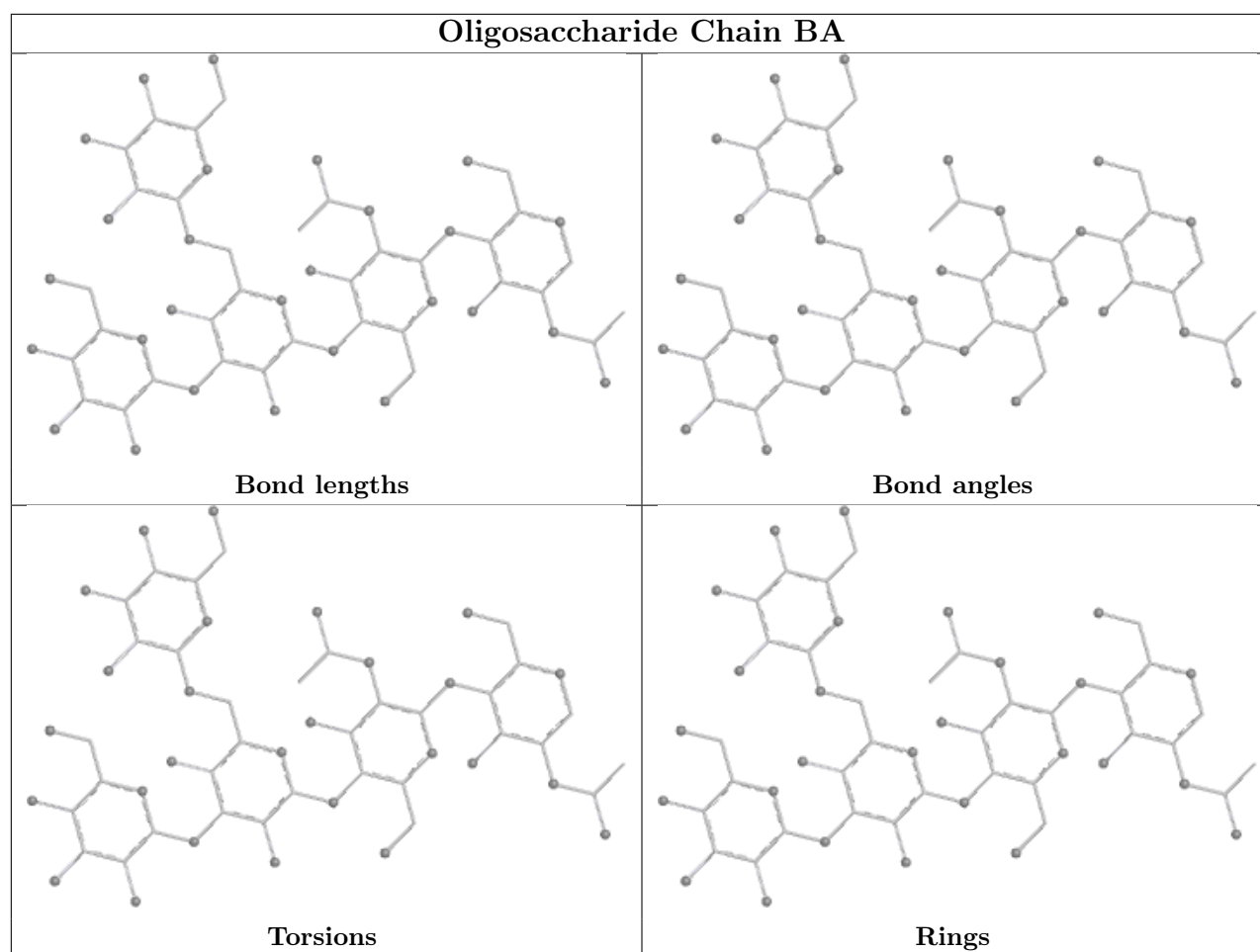












## 5.6 Ligand geometry [i](#)

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 | $\# Z  > 2$ |
| 9   | NAG  | A     | 1440 | 1    | 14,14,15     | 3.55 | 6 (42%)     | 17,19,21    | 3.47 | 8 (47%)     |
| 9   | NAG  | B     | 1440 | 1    | 14,14,15     | 3.56 | 6 (42%)     | 17,19,21    | 3.46 | 8 (47%)     |
| 9   | NAG  | C     | 1474 | 1    | 14,14,15     | 2.78 | 3 (21%)     | 17,19,21    | 3.02 | 4 (23%)     |
| 9   | NAG  | B     | 1401 | 1    | 14,14,15     | 2.82 | 4 (28%)     | 17,19,21    | 2.00 | 3 (17%)     |
| 9   | NAG  | C     | 1440 | 1    | 14,14,15     | 3.55 | 6 (42%)     | 17,19,21    | 3.47 | 8 (47%)     |

| Mol | Type | Chain | Res  | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|------|------|--------------|------|----------|-------------|------|----------|
|     |      |       |      |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | NAG  | A     | 1402 | 1    | 14,14,15     | 2.70 | 4 (28%)  | 17,19,21    | 3.68 | 6 (35%)  |
| 9   | NAG  | B     | 1403 | 1    | 14,14,15     | 2.63 | 3 (21%)  | 17,19,21    | 4.06 | 6 (35%)  |
| 9   | NAG  | B     | 1402 | 1    | 14,14,15     | 2.70 | 4 (28%)  | 17,19,21    | 3.68 | 6 (35%)  |
| 9   | NAG  | C     | 1402 | 1    | 14,14,15     | 2.69 | 4 (28%)  | 17,19,21    | 3.68 | 6 (35%)  |
| 9   | NAG  | C     | 1401 | 1    | 14,14,15     | 2.82 | 4 (28%)  | 17,19,21    | 2.00 | 4 (23%)  |
| 9   | NAG  | A     | 1439 | 1    | 14,14,15     | 2.45 | 3 (21%)  | 17,19,21    | 3.31 | 3 (17%)  |
| 9   | NAG  | B     | 1439 | 1    | 14,14,15     | 2.45 | 3 (21%)  | 17,19,21    | 3.31 | 3 (17%)  |
| 9   | NAG  | A     | 1403 | 1    | 14,14,15     | 2.62 | 3 (21%)  | 17,19,21    | 4.06 | 6 (35%)  |
| 9   | NAG  | C     | 1441 | 1    | 14,14,15     | 2.99 | 4 (28%)  | 17,19,21    | 4.50 | 4 (23%)  |
| 9   | NAG  | C     | 1403 | 1    | 14,14,15     | 2.62 | 3 (21%)  | 17,19,21    | 4.06 | 6 (35%)  |
| 9   | NAG  | A     | 1474 | 1    | 14,14,15     | 2.79 | 3 (21%)  | 17,19,21    | 3.01 | 4 (23%)  |
| 9   | NAG  | A     | 1441 | 1    | 14,14,15     | 3.00 | 4 (28%)  | 17,19,21    | 4.50 | 4 (23%)  |
| 9   | NAG  | C     | 1439 | 1    | 14,14,15     | 2.46 | 3 (21%)  | 17,19,21    | 3.31 | 3 (17%)  |
| 9   | NAG  | B     | 1474 | 1    | 14,14,15     | 2.78 | 3 (21%)  | 17,19,21    | 3.01 | 4 (23%)  |
| 9   | NAG  | B     | 1441 | 1    | 14,14,15     | 3.00 | 4 (28%)  | 17,19,21    | 4.49 | 4 (23%)  |
| 9   | NAG  | A     | 1401 | 1    | 14,14,15     | 2.82 | 4 (28%)  | 17,19,21    | 2.00 | 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   |
|-----|------|-------|------|------|---------|-----------|---------|
| 9   | NAG  | A     | 1440 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1440 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1474 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1440 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | A     | 1402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1403 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1402 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | A     | 1439 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1439 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | A     | 1403 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1441 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1403 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | A     | 1474 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res  | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|------|------|---------|-----------|---------|
| 9   | NAG  | A     | 1441 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | C     | 1439 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1474 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | B     | 1441 | 1    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | A     | 1401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

All (81) bond length outliers are listed below:

| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | C     | 1440 | NAG  | O5-C1 | 8.55  | 1.58        | 1.43     |
| 9   | A     | 1440 | NAG  | O5-C1 | 8.55  | 1.58        | 1.43     |
| 9   | B     | 1440 | NAG  | O5-C1 | 8.54  | 1.58        | 1.43     |
| 9   | A     | 1441 | NAG  | O5-C1 | 7.68  | 1.56        | 1.43     |
| 9   | C     | 1441 | NAG  | O5-C1 | 7.67  | 1.56        | 1.43     |
| 9   | B     | 1441 | NAG  | O5-C1 | 7.66  | 1.56        | 1.43     |
| 9   | C     | 1401 | NAG  | O5-C1 | 7.34  | 1.56        | 1.43     |
| 9   | B     | 1401 | NAG  | O5-C1 | 7.34  | 1.56        | 1.43     |
| 9   | A     | 1401 | NAG  | O5-C1 | 7.33  | 1.56        | 1.43     |
| 9   | C     | 1402 | NAG  | O5-C1 | 7.18  | 1.55        | 1.43     |
| 9   | A     | 1402 | NAG  | O5-C1 | 7.18  | 1.55        | 1.43     |
| 9   | B     | 1402 | NAG  | O5-C1 | 7.16  | 1.55        | 1.43     |
| 9   | A     | 1474 | NAG  | O5-C1 | 7.00  | 1.55        | 1.43     |
| 9   | C     | 1474 | NAG  | O5-C1 | 6.99  | 1.55        | 1.43     |
| 9   | B     | 1474 | NAG  | O5-C1 | 6.94  | 1.55        | 1.43     |
| 9   | B     | 1403 | NAG  | O5-C1 | 6.85  | 1.55        | 1.43     |
| 9   | A     | 1403 | NAG  | O5-C1 | 6.83  | 1.55        | 1.43     |
| 9   | B     | 1441 | NAG  | C2-N2 | -6.82 | 1.35        | 1.46     |
| 9   | A     | 1441 | NAG  | C2-N2 | -6.82 | 1.35        | 1.46     |
| 9   | C     | 1403 | NAG  | O5-C1 | 6.80  | 1.55        | 1.43     |
| 9   | C     | 1441 | NAG  | C2-N2 | -6.76 | 1.35        | 1.46     |
| 9   | B     | 1474 | NAG  | C2-N2 | -6.47 | 1.35        | 1.46     |
| 9   | A     | 1474 | NAG  | C2-N2 | -6.47 | 1.35        | 1.46     |
| 9   | A     | 1439 | NAG  | O5-C1 | 6.47  | 1.54        | 1.43     |
| 9   | B     | 1439 | NAG  | O5-C1 | 6.47  | 1.54        | 1.43     |
| 9   | C     | 1439 | NAG  | O5-C1 | 6.46  | 1.54        | 1.43     |
| 9   | C     | 1474 | NAG  | C2-N2 | -6.43 | 1.35        | 1.46     |
| 9   | A     | 1401 | NAG  | C2-N2 | -6.30 | 1.35        | 1.46     |
| 9   | C     | 1401 | NAG  | C2-N2 | -6.30 | 1.35        | 1.46     |
| 9   | B     | 1401 | NAG  | C2-N2 | -6.27 | 1.35        | 1.46     |
| 9   | B     | 1440 | NAG  | C2-N2 | -5.98 | 1.36        | 1.46     |
| 9   | A     | 1440 | NAG  | C2-N2 | -5.96 | 1.36        | 1.46     |
| 9   | C     | 1440 | NAG  | C2-N2 | -5.95 | 1.36        | 1.46     |

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| Mol | Chain | Res  | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|-------|-------------|----------|
| 9   | B     | 1402 | NAG  | C2-N2 | -5.64 | 1.36        | 1.46     |
| 9   | A     | 1402 | NAG  | C2-N2 | -5.61 | 1.37        | 1.46     |
| 9   | C     | 1402 | NAG  | C2-N2 | -5.61 | 1.37        | 1.46     |
| 9   | B     | 1403 | NAG  | C2-N2 | -5.44 | 1.37        | 1.46     |
| 9   | A     | 1403 | NAG  | C2-N2 | -5.43 | 1.37        | 1.46     |
| 9   | C     | 1403 | NAG  | C2-N2 | -5.42 | 1.37        | 1.46     |
| 9   | C     | 1439 | NAG  | C2-N2 | -5.18 | 1.37        | 1.46     |
| 9   | A     | 1439 | NAG  | C2-N2 | -5.14 | 1.37        | 1.46     |
| 9   | B     | 1439 | NAG  | C2-N2 | -5.12 | 1.37        | 1.46     |
| 9   | B     | 1440 | NAG  | C4-C3 | 4.49  | 1.64        | 1.52     |
| 9   | A     | 1440 | NAG  | C4-C3 | 4.49  | 1.64        | 1.52     |
| 9   | C     | 1440 | NAG  | C4-C3 | 4.49  | 1.64        | 1.52     |
| 9   | A     | 1440 | NAG  | C4-C5 | 4.18  | 1.61        | 1.53     |
| 9   | C     | 1440 | NAG  | C4-C5 | 4.18  | 1.61        | 1.53     |
| 9   | B     | 1440 | NAG  | C4-C5 | 4.17  | 1.61        | 1.53     |
| 9   | B     | 1440 | NAG  | C1-C2 | 3.80  | 1.57        | 1.52     |
| 9   | A     | 1440 | NAG  | C1-C2 | 3.76  | 1.57        | 1.52     |
| 9   | C     | 1440 | NAG  | C1-C2 | 3.75  | 1.57        | 1.52     |
| 9   | A     | 1441 | NAG  | C4-C3 | 2.93  | 1.59        | 1.52     |
| 9   | B     | 1441 | NAG  | C4-C3 | 2.93  | 1.59        | 1.52     |
| 9   | C     | 1441 | NAG  | C4-C3 | 2.92  | 1.59        | 1.52     |
| 9   | C     | 1440 | NAG  | O5-C5 | 2.72  | 1.48        | 1.43     |
| 9   | A     | 1440 | NAG  | O5-C5 | 2.72  | 1.48        | 1.43     |
| 9   | B     | 1440 | NAG  | O5-C5 | 2.72  | 1.48        | 1.43     |
| 9   | A     | 1402 | NAG  | C1-C2 | 2.53  | 1.55        | 1.52     |
| 9   | B     | 1402 | NAG  | C1-C2 | 2.52  | 1.55        | 1.52     |
| 9   | C     | 1402 | NAG  | C1-C2 | 2.52  | 1.55        | 1.52     |
| 9   | A     | 1439 | NAG  | C4-C3 | 2.41  | 1.58        | 1.52     |
| 9   | B     | 1439 | NAG  | C4-C3 | 2.40  | 1.58        | 1.52     |
| 9   | C     | 1439 | NAG  | C4-C3 | 2.40  | 1.58        | 1.52     |
| 9   | B     | 1441 | NAG  | C4-C5 | 2.38  | 1.58        | 1.53     |
| 9   | A     | 1441 | NAG  | C4-C5 | 2.34  | 1.58        | 1.53     |
| 9   | A     | 1401 | NAG  | C4-C3 | 2.33  | 1.58        | 1.52     |
| 9   | B     | 1401 | NAG  | C4-C3 | 2.33  | 1.58        | 1.52     |
| 9   | C     | 1441 | NAG  | C4-C5 | 2.33  | 1.58        | 1.53     |
| 9   | C     | 1401 | NAG  | C4-C3 | 2.31  | 1.58        | 1.52     |
| 9   | C     | 1403 | NAG  | C4-C3 | 2.30  | 1.58        | 1.52     |
| 9   | A     | 1403 | NAG  | C4-C3 | 2.29  | 1.58        | 1.52     |
| 9   | B     | 1403 | NAG  | C4-C3 | 2.27  | 1.58        | 1.52     |
| 9   | A     | 1474 | NAG  | C4-C3 | 2.24  | 1.58        | 1.52     |
| 9   | C     | 1474 | NAG  | C4-C3 | 2.24  | 1.58        | 1.52     |
| 9   | B     | 1474 | NAG  | C4-C3 | 2.21  | 1.58        | 1.52     |

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| Mol | Chain | Res  | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|------|------|-------|------|-------------|----------|
| 9   | B     | 1402 | NAG  | C4-C3 | 2.17 | 1.58        | 1.52     |
| 9   | A     | 1402 | NAG  | C4-C3 | 2.16 | 1.57        | 1.52     |
| 9   | C     | 1402 | NAG  | C4-C3 | 2.14 | 1.57        | 1.52     |
| 9   | A     | 1401 | NAG  | C4-C5 | 2.07 | 1.57        | 1.53     |
| 9   | C     | 1401 | NAG  | C4-C5 | 2.06 | 1.57        | 1.53     |
| 9   | B     | 1401 | NAG  | C4-C5 | 2.06 | 1.57        | 1.53     |

All (103) bond angle outliers are listed below:

| Mol | Chain | Res  | Type | Atoms    | Z      | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|--------|-------------|----------|
| 9   | B     | 1403 | NAG  | O5-C5-C6 | -14.07 | 80.28       | 107.66   |
| 9   | A     | 1403 | NAG  | O5-C5-C6 | -14.06 | 80.29       | 107.66   |
| 9   | C     | 1403 | NAG  | O5-C5-C6 | -14.06 | 80.31       | 107.66   |
| 9   | A     | 1402 | NAG  | O5-C5-C6 | -11.42 | 85.44       | 107.66   |
| 9   | C     | 1402 | NAG  | O5-C5-C6 | -11.42 | 85.44       | 107.66   |
| 9   | B     | 1402 | NAG  | O5-C5-C6 | -11.41 | 85.45       | 107.66   |
| 9   | C     | 1441 | NAG  | O5-C5-C6 | -10.51 | 87.20       | 107.66   |
| 9   | A     | 1441 | NAG  | O5-C5-C6 | -10.50 | 87.22       | 107.66   |
| 9   | B     | 1441 | NAG  | O5-C5-C6 | -10.48 | 87.26       | 107.66   |
| 9   | C     | 1439 | NAG  | O5-C5-C6 | -10.48 | 87.26       | 107.66   |
| 9   | B     | 1439 | NAG  | O5-C5-C6 | -10.48 | 87.27       | 107.66   |
| 9   | A     | 1439 | NAG  | O5-C5-C6 | -10.47 | 87.28       | 107.66   |
| 9   | A     | 1474 | NAG  | O5-C5-C6 | -10.38 | 87.47       | 107.66   |
| 9   | C     | 1474 | NAG  | O5-C5-C6 | -10.37 | 87.48       | 107.66   |
| 9   | B     | 1474 | NAG  | O5-C5-C6 | -10.37 | 87.48       | 107.66   |
| 9   | C     | 1441 | NAG  | C1-C2-N2 | 10.37  | 126.77      | 110.43   |
| 9   | A     | 1441 | NAG  | C1-C2-N2 | 10.37  | 126.77      | 110.43   |
| 9   | B     | 1441 | NAG  | C1-C2-N2 | 10.36  | 126.77      | 110.43   |
| 9   | C     | 1441 | NAG  | C6-C5-C4 | 10.08  | 137.76      | 113.02   |
| 9   | A     | 1441 | NAG  | C6-C5-C4 | 10.06  | 137.73      | 113.02   |
| 9   | B     | 1441 | NAG  | C6-C5-C4 | 10.06  | 137.72      | 113.02   |
| 9   | A     | 1440 | NAG  | O5-C5-C6 | -9.27  | 89.63       | 107.66   |
| 9   | B     | 1440 | NAG  | O5-C5-C6 | -9.26  | 89.63       | 107.66   |
| 9   | C     | 1440 | NAG  | O5-C5-C6 | -9.26  | 89.63       | 107.66   |
| 9   | B     | 1403 | NAG  | O4-C4-C5 | -6.65  | 92.94       | 109.32   |
| 9   | C     | 1440 | NAG  | C1-C2-N2 | 6.65   | 120.91      | 110.43   |
| 9   | A     | 1403 | NAG  | O4-C4-C5 | -6.65  | 92.96       | 109.32   |
| 9   | C     | 1403 | NAG  | O4-C4-C5 | -6.64  | 92.96       | 109.32   |
| 9   | A     | 1440 | NAG  | C1-C2-N2 | 6.63   | 120.89      | 110.43   |
| 9   | B     | 1440 | NAG  | C1-C2-N2 | 6.63   | 120.88      | 110.43   |
| 9   | A     | 1401 | NAG  | O5-C5-C6 | -6.42  | 95.17       | 107.66   |
| 9   | B     | 1401 | NAG  | O5-C5-C6 | -6.41  | 95.18       | 107.66   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | C     | 1401 | NAG  | O5-C5-C6 | -6.41 | 95.19       | 107.66   |
| 9   | C     | 1402 | NAG  | O3-C3-C2 | 6.15  | 122.17      | 109.40   |
| 9   | A     | 1402 | NAG  | O3-C3-C2 | 6.14  | 122.15      | 109.40   |
| 9   | B     | 1402 | NAG  | O3-C3-C2 | 6.13  | 122.13      | 109.40   |
| 9   | B     | 1439 | NAG  | C1-C2-N2 | -6.03 | 100.93      | 110.43   |
| 9   | A     | 1439 | NAG  | C1-C2-N2 | -6.02 | 100.95      | 110.43   |
| 9   | C     | 1439 | NAG  | C1-C2-N2 | -5.99 | 100.99      | 110.43   |
| 9   | C     | 1440 | NAG  | O3-C3-C2 | -5.03 | 98.95       | 109.40   |
| 9   | A     | 1440 | NAG  | O3-C3-C2 | -5.02 | 98.97       | 109.40   |
| 9   | B     | 1440 | NAG  | O3-C3-C2 | -5.01 | 98.99       | 109.40   |
| 9   | C     | 1402 | NAG  | C6-C5-C4 | 4.34  | 123.69      | 113.02   |
| 9   | B     | 1439 | NAG  | O3-C3-C2 | 4.34  | 118.42      | 109.40   |
| 9   | B     | 1402 | NAG  | C6-C5-C4 | 4.34  | 123.67      | 113.02   |
| 9   | A     | 1402 | NAG  | C6-C5-C4 | 4.34  | 123.67      | 113.02   |
| 9   | A     | 1439 | NAG  | O3-C3-C2 | 4.33  | 118.40      | 109.40   |
| 9   | C     | 1439 | NAG  | O3-C3-C2 | 4.32  | 118.37      | 109.40   |
| 9   | C     | 1474 | NAG  | O4-C4-C3 | -4.32 | 100.19      | 110.38   |
| 9   | A     | 1474 | NAG  | O4-C4-C3 | -4.30 | 100.23      | 110.38   |
| 9   | B     | 1474 | NAG  | O4-C4-C3 | -4.30 | 100.24      | 110.38   |
| 9   | B     | 1402 | NAG  | C1-C2-N2 | -3.99 | 104.14      | 110.43   |
| 9   | C     | 1402 | NAG  | C1-C2-N2 | -3.99 | 104.14      | 110.43   |
| 9   | A     | 1402 | NAG  | C1-C2-N2 | -3.98 | 104.15      | 110.43   |
| 9   | A     | 1441 | NAG  | O3-C3-C2 | -3.70 | 101.71      | 109.40   |
| 9   | B     | 1441 | NAG  | O3-C3-C2 | -3.70 | 101.72      | 109.40   |
| 9   | C     | 1441 | NAG  | O3-C3-C2 | -3.69 | 101.74      | 109.40   |
| 9   | B     | 1440 | NAG  | O4-C4-C3 | -3.40 | 102.36      | 110.38   |
| 9   | A     | 1440 | NAG  | O4-C4-C3 | -3.40 | 102.37      | 110.38   |
| 9   | C     | 1440 | NAG  | O4-C4-C3 | -3.40 | 102.37      | 110.38   |
| 9   | C     | 1403 | NAG  | C1-C2-N2 | 3.20  | 115.48      | 110.43   |
| 9   | B     | 1403 | NAG  | C1-C2-N2 | 3.18  | 115.44      | 110.43   |
| 9   | A     | 1403 | NAG  | C1-C2-N2 | 3.18  | 115.44      | 110.43   |
| 9   | B     | 1440 | NAG  | C2-N2-C7 | 3.07  | 127.02      | 122.90   |
| 9   | A     | 1440 | NAG  | C2-N2-C7 | 3.07  | 127.01      | 122.90   |
| 9   | C     | 1440 | NAG  | C2-N2-C7 | 3.06  | 127.00      | 122.90   |
| 9   | B     | 1403 | NAG  | C6-C5-C4 | 3.05  | 120.51      | 113.02   |
| 9   | C     | 1403 | NAG  | C6-C5-C4 | 3.05  | 120.50      | 113.02   |
| 9   | A     | 1403 | NAG  | C6-C5-C4 | 3.04  | 120.49      | 113.02   |
| 9   | A     | 1474 | NAG  | C6-C5-C4 | 3.04  | 120.48      | 113.02   |
| 9   | B     | 1474 | NAG  | C6-C5-C4 | 3.04  | 120.48      | 113.02   |
| 9   | C     | 1474 | NAG  | C6-C5-C4 | 3.04  | 120.47      | 113.02   |
| 9   | C     | 1402 | NAG  | O5-C1-C2 | -2.93 | 106.75      | 111.29   |
| 9   | A     | 1402 | NAG  | O5-C1-C2 | -2.91 | 106.78      | 111.29   |

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| Mol | Chain | Res  | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|------|------|----------|-------|-------------|----------|
| 9   | B     | 1402 | NAG  | O5-C1-C2 | -2.91 | 106.79      | 111.29   |
| 9   | A     | 1440 | NAG  | O4-C4-C5 | -2.53 | 103.09      | 109.32   |
| 9   | C     | 1440 | NAG  | O4-C4-C5 | -2.53 | 103.10      | 109.32   |
| 9   | B     | 1440 | NAG  | O4-C4-C5 | -2.51 | 103.13      | 109.32   |
| 9   | B     | 1403 | NAG  | C8-C7-N2 | 2.48  | 120.24      | 116.12   |
| 9   | A     | 1403 | NAG  | C8-C7-N2 | 2.47  | 120.22      | 116.12   |
| 9   | B     | 1440 | NAG  | C4-C3-C2 | 2.46  | 114.62      | 111.02   |
| 9   | A     | 1440 | NAG  | C4-C3-C2 | 2.46  | 114.62      | 111.02   |
| 9   | C     | 1440 | NAG  | C4-C3-C2 | 2.46  | 114.62      | 111.02   |
| 9   | C     | 1403 | NAG  | C8-C7-N2 | 2.45  | 120.19      | 116.12   |
| 9   | C     | 1401 | NAG  | C1-C2-N2 | 2.43  | 114.26      | 110.43   |
| 9   | A     | 1401 | NAG  | C1-C2-N2 | 2.42  | 114.25      | 110.43   |
| 9   | C     | 1440 | NAG  | C6-C5-C4 | 2.42  | 118.97      | 113.02   |
| 9   | A     | 1403 | NAG  | O7-C7-C8 | -2.42 | 117.75      | 122.05   |
| 9   | A     | 1440 | NAG  | C6-C5-C4 | 2.41  | 118.94      | 113.02   |
| 9   | C     | 1403 | NAG  | O7-C7-C8 | -2.40 | 117.78      | 122.05   |
| 9   | B     | 1403 | NAG  | O7-C7-C8 | -2.40 | 117.78      | 122.05   |
| 9   | B     | 1440 | NAG  | C6-C5-C4 | 2.40  | 118.91      | 113.02   |
| 9   | B     | 1401 | NAG  | C1-C2-N2 | 2.39  | 114.20      | 110.43   |
| 9   | A     | 1474 | NAG  | O3-C3-C2 | 2.32  | 114.22      | 109.40   |
| 9   | C     | 1474 | NAG  | O3-C3-C2 | 2.31  | 114.20      | 109.40   |
| 9   | B     | 1474 | NAG  | O3-C3-C2 | 2.31  | 114.20      | 109.40   |
| 9   | C     | 1401 | NAG  | C6-C5-C4 | 2.18  | 118.37      | 113.02   |
| 9   | A     | 1401 | NAG  | C6-C5-C4 | 2.17  | 118.36      | 113.02   |
| 9   | B     | 1401 | NAG  | C6-C5-C4 | 2.17  | 118.34      | 113.02   |
| 9   | C     | 1402 | NAG  | C4-C3-C2 | -2.14 | 107.89      | 111.02   |
| 9   | A     | 1402 | NAG  | C4-C3-C2 | -2.12 | 107.91      | 111.02   |
| 9   | B     | 1402 | NAG  | C4-C3-C2 | -2.11 | 107.93      | 111.02   |
| 9   | C     | 1401 | NAG  | O7-C7-C8 | -2.00 | 118.49      | 122.05   |

There are no chirality outliers.

All (12) torsion outliers are listed below:

| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 9   | A     | 1441 | NAG  | C1-C2-N2-C7 |
| 9   | B     | 1441 | NAG  | C1-C2-N2-C7 |
| 9   | C     | 1441 | NAG  | C1-C2-N2-C7 |
| 9   | C     | 1439 | NAG  | O5-C5-C6-O6 |
| 9   | A     | 1439 | NAG  | O5-C5-C6-O6 |
| 9   | B     | 1439 | NAG  | O5-C5-C6-O6 |
| 9   | A     | 1441 | NAG  | O5-C5-C6-O6 |
| 9   | B     | 1441 | NAG  | O5-C5-C6-O6 |

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| Mol | Chain | Res  | Type | Atoms       |
|-----|-------|------|------|-------------|
| 9   | C     | 1441 | NAG  | O5-C5-C6-O6 |
| 9   | A     | 1440 | NAG  | C1-C2-N2-C7 |
| 9   | B     | 1440 | NAG  | C1-C2-N2-C7 |
| 9   | C     | 1440 | NAG  | C1-C2-N2-C7 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

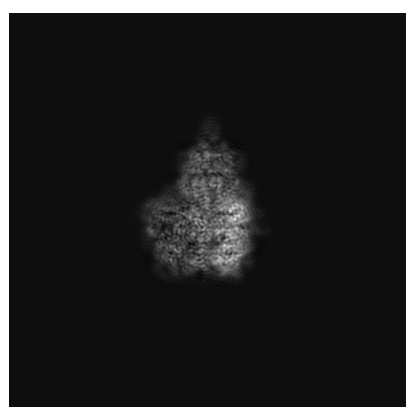
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-8331. These allow visual inspection of the internal detail of the map and identification of artifacts.

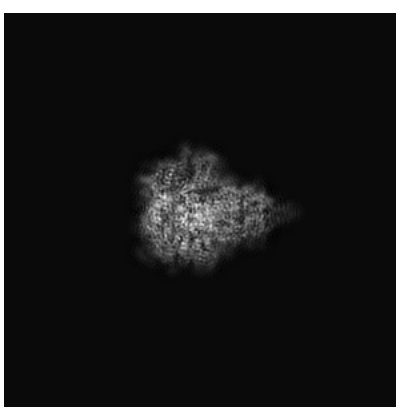
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

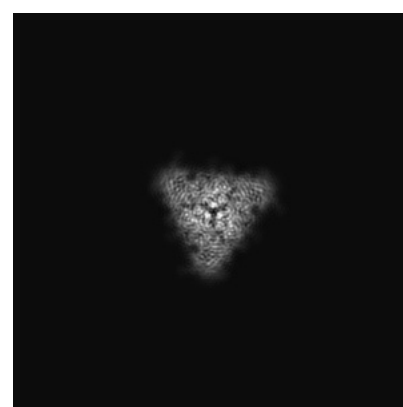
#### 6.1.1 Primary map



X



Y



Z

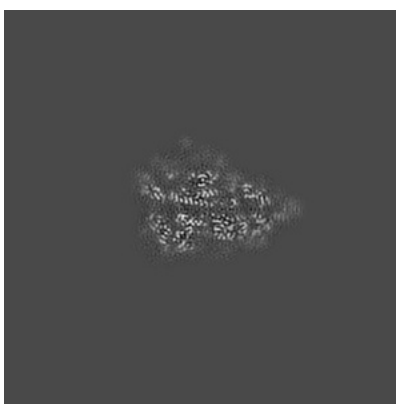
The images above show the map projected in three orthogonal directions.

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

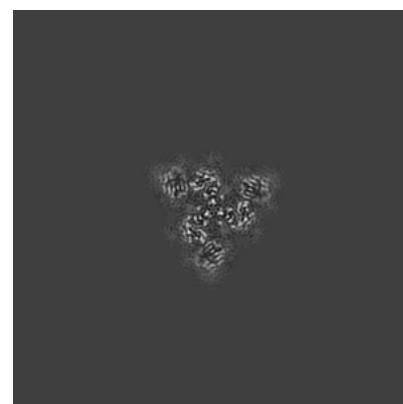
#### 6.2.1 Primary map



X Index: 160



Y Index: 160

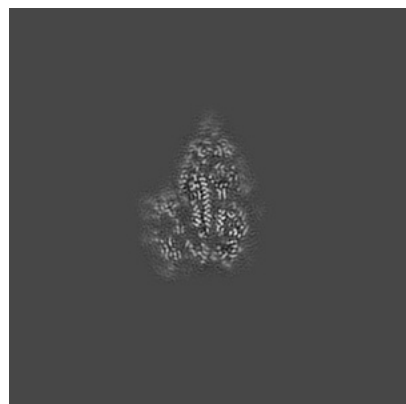


Z Index: 160

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

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

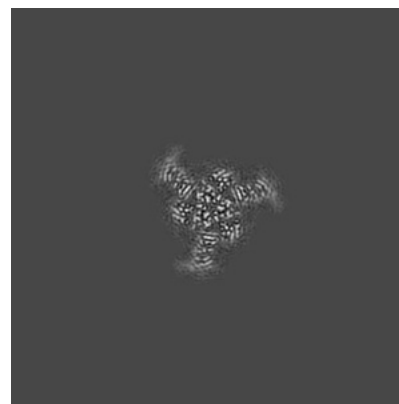
### 6.3.1 Primary map



X Index: 165



Y Index: 168

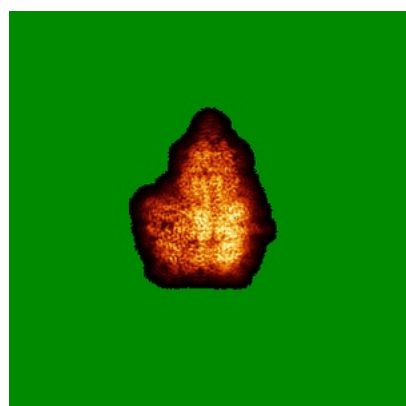


Z Index: 145

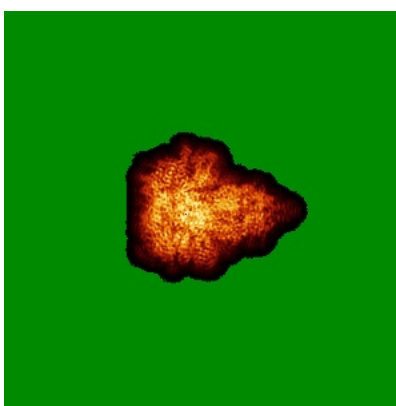
The images above show the largest variance slices of the map in three orthogonal directions.

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

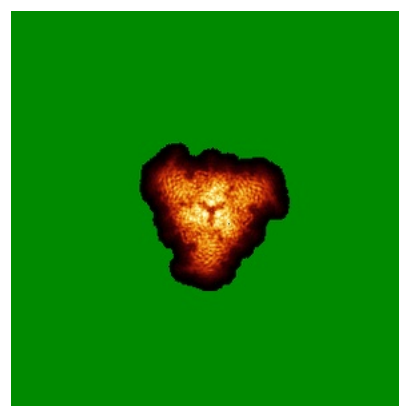
### 6.4.1 Primary map



X



Y

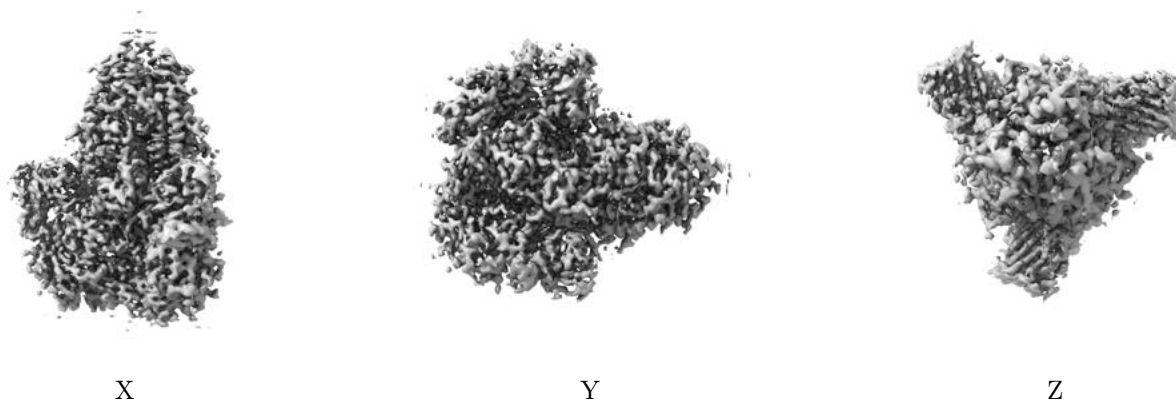


Z

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 0.055. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

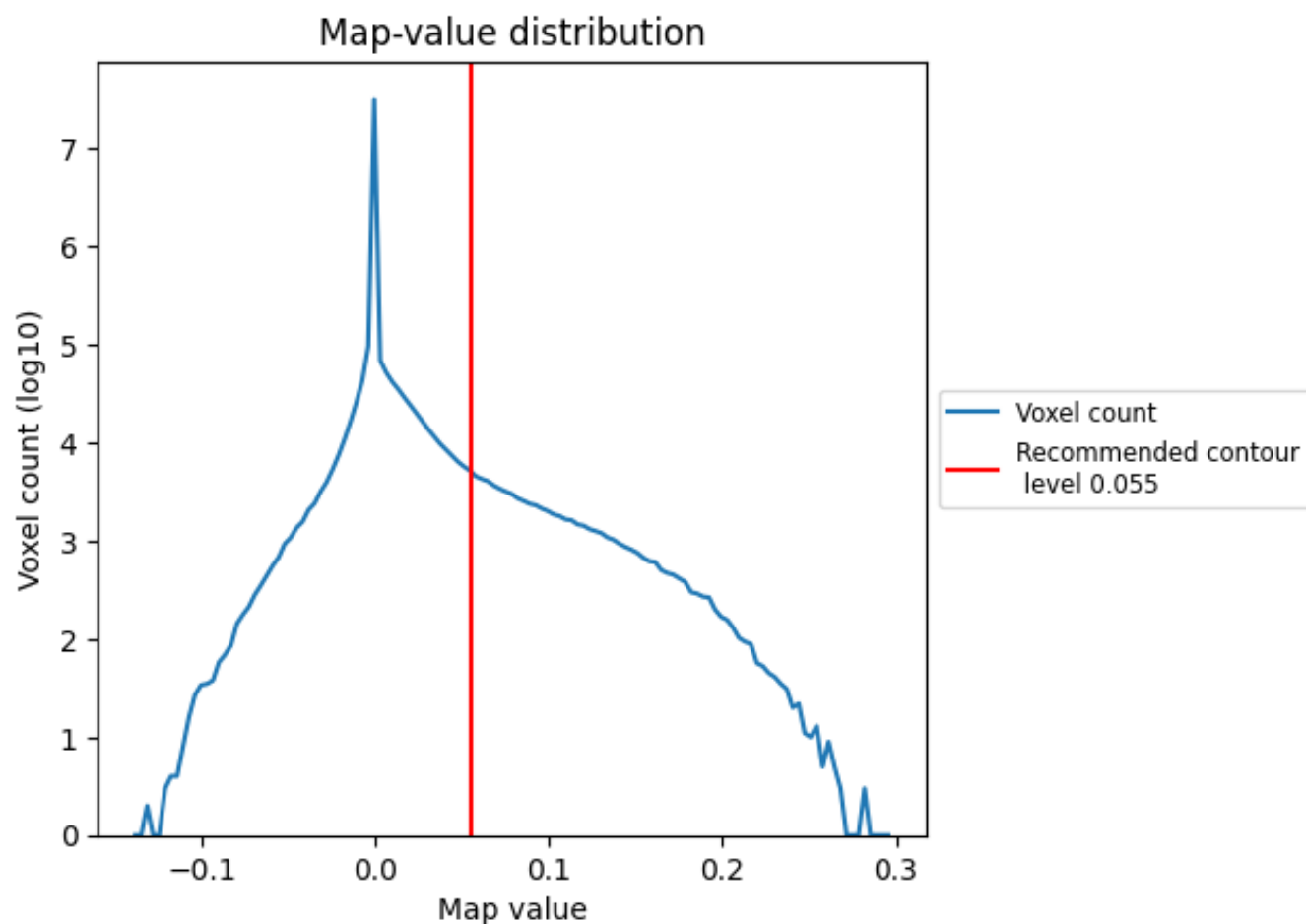
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

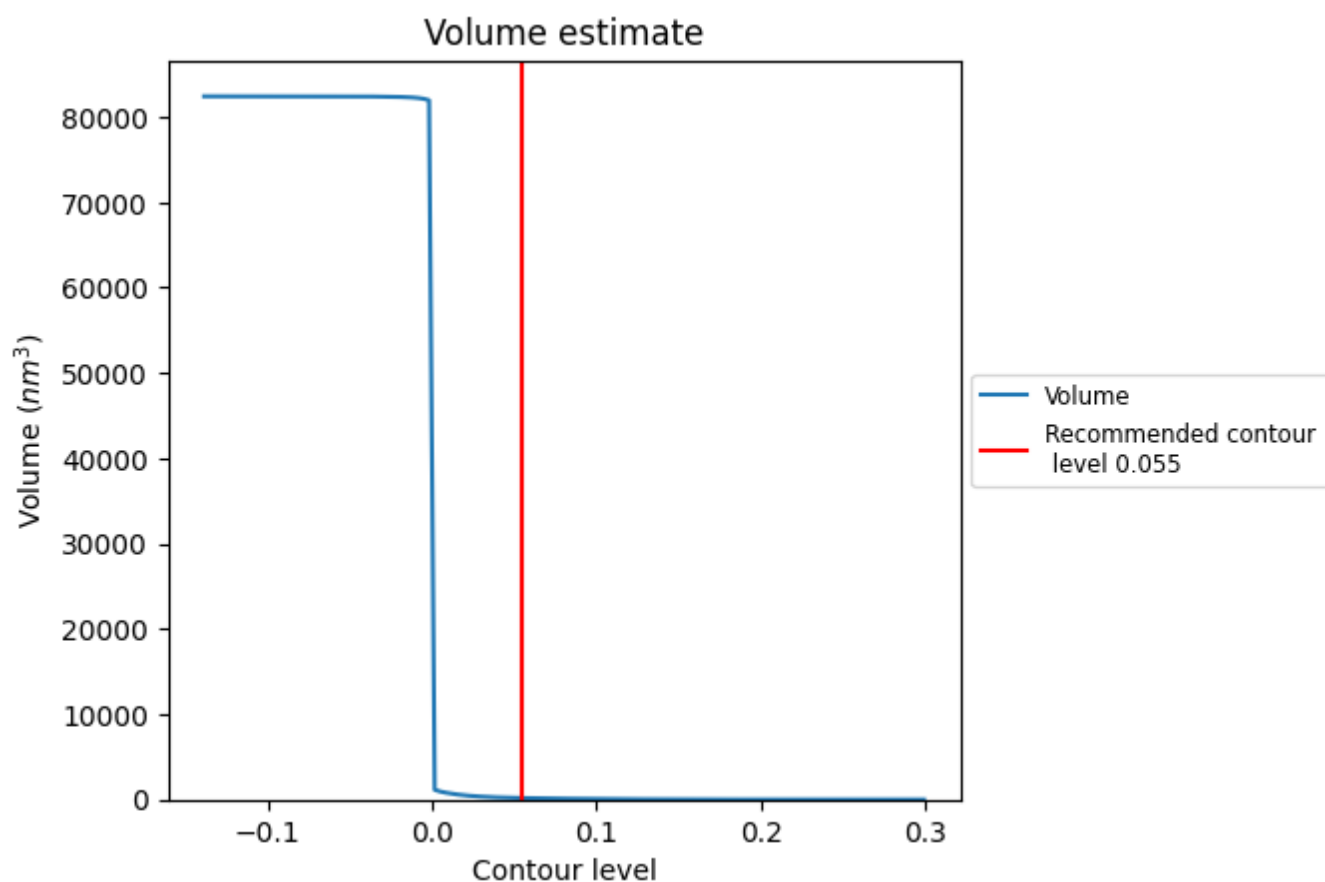
This section contains the results of statistical analysis of the map.

### 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.

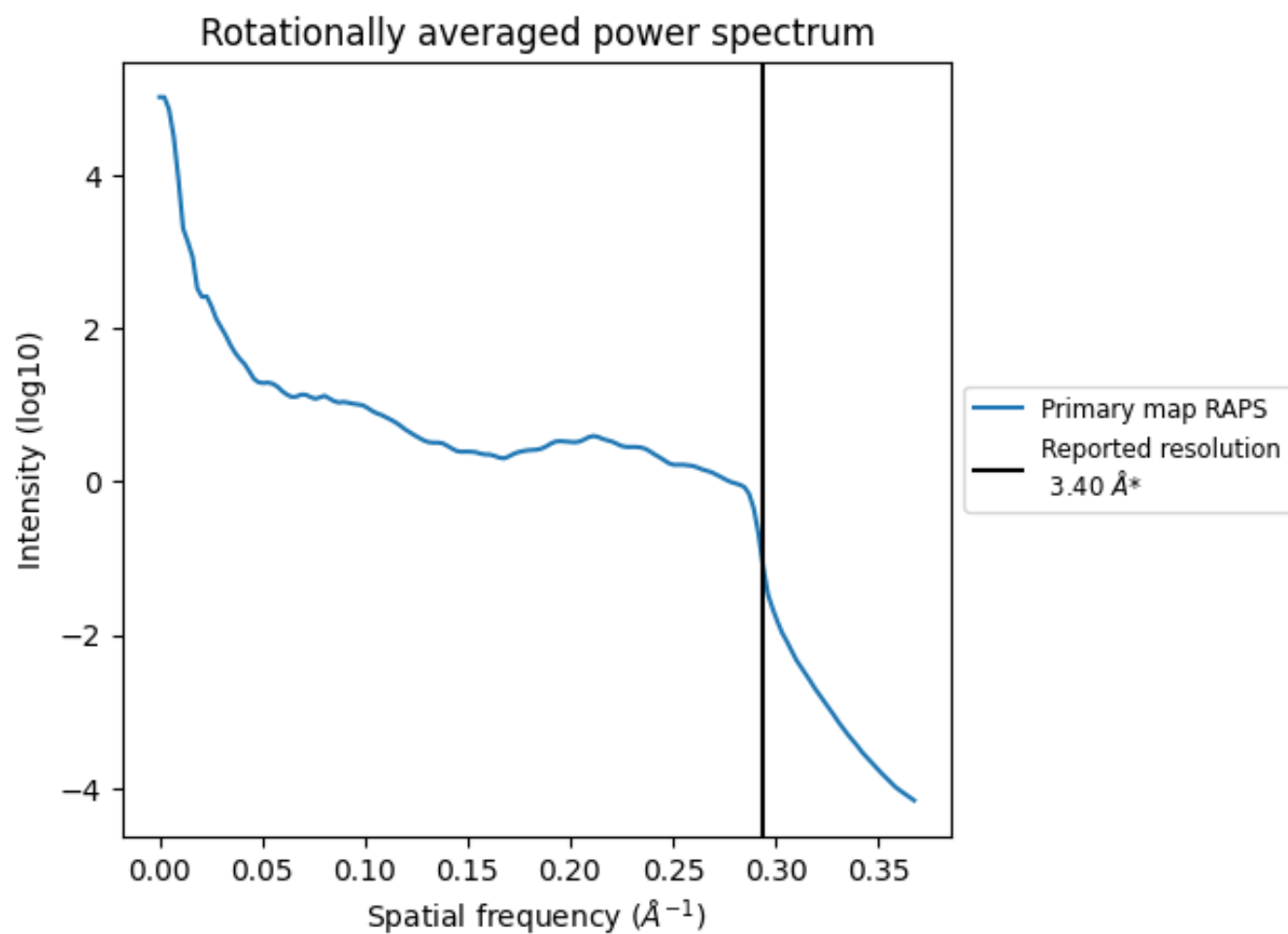
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177  $\text{nm}^3$ ; this corresponds to an approximate mass of 160 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 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation

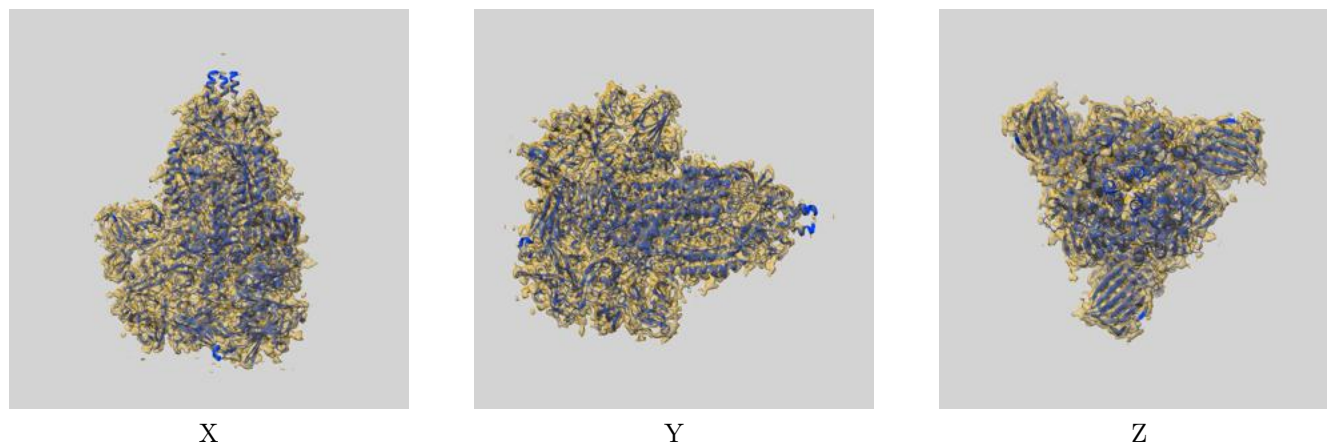
This section was not generated. No FSC curve or half-maps provided.



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

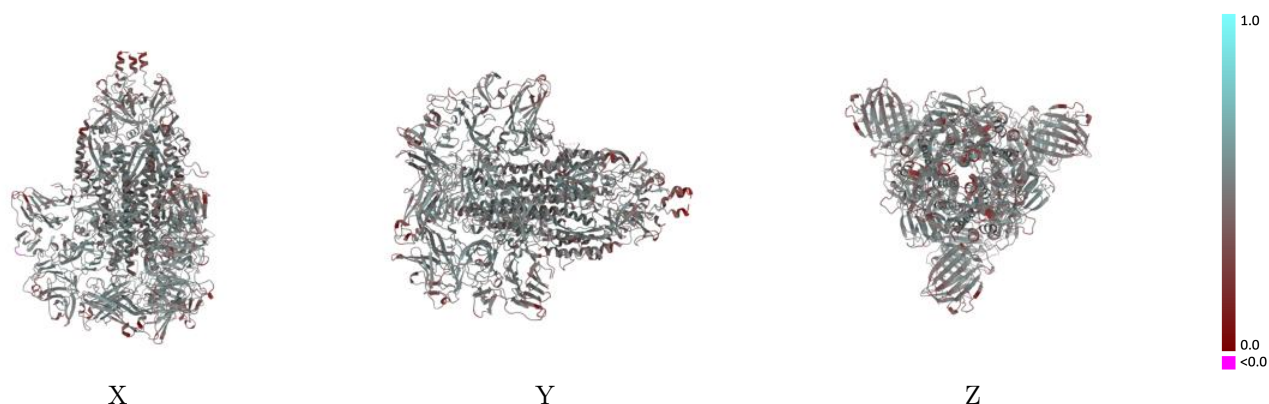
This section contains information regarding the fit between EMDB map EMD-8331 and PDB model 5SZS. Per-residue inclusion information can be found in [section 3](#) on [page 16](#).

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



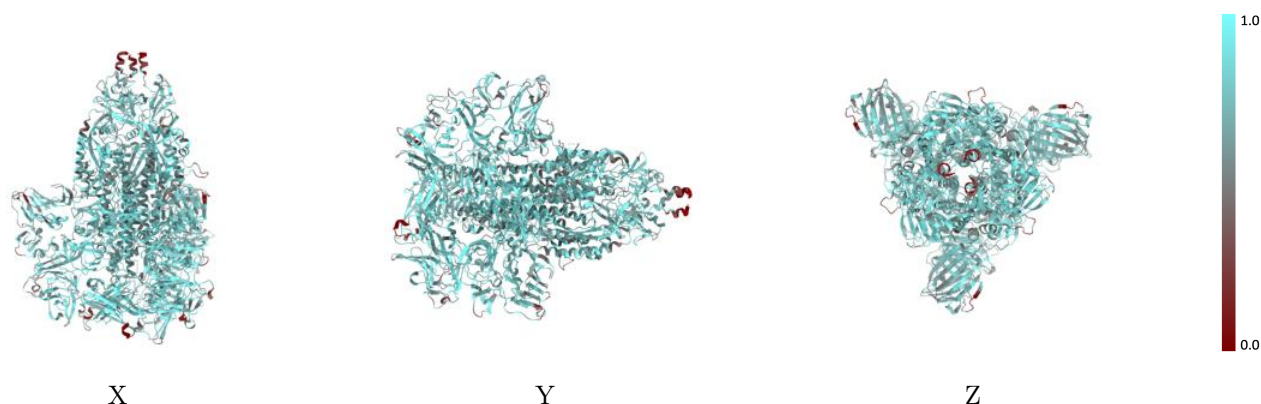
The images above show the 3D surface view of the map at the recommended contour level 0.055 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



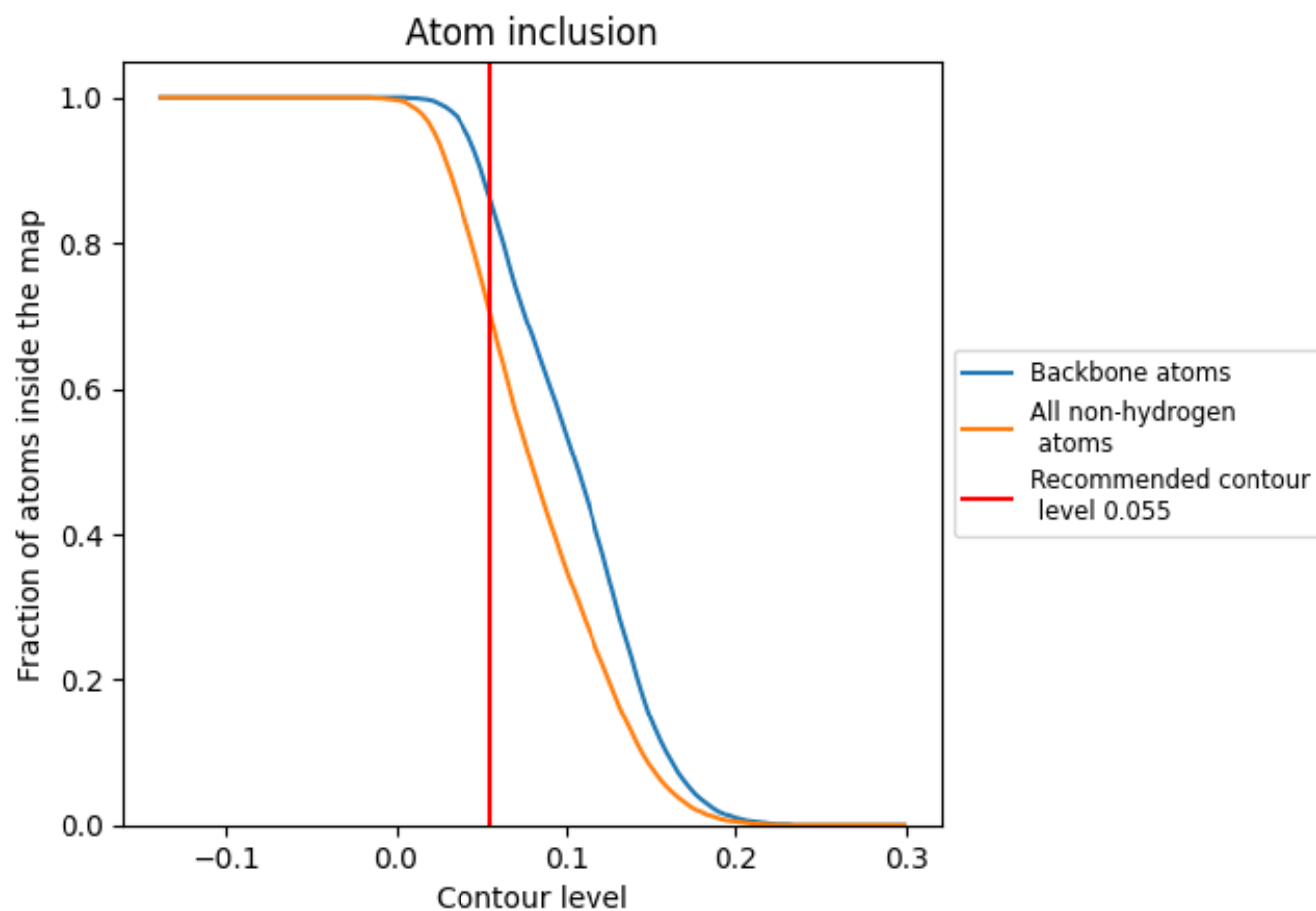
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.055).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 86% of all backbone atoms, 71% 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 (0.055) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| All   |  0.7070   |  0.4500   |
| 0     |  0.4890   |  0.4000   |
| 1     |  0.2820   |  0.2840   |
| 2     |  0.2140   |  0.3660   |
| 3     |  0.1800   |  0.2190   |
| 4     |  0.2560   |  0.3880   |
| 5     |  0.1070   |  0.2770   |
| 6     |  0.2860   |  0.1090   |
| 7     |  0.2860   |  0.2640   |
| 8     |  0.2500   |  0.3100   |
| 9     |  0.1790   |  0.1990   |
| A     |  0.7440   |  0.4630   |
| AA    |  0.2400   |  0.2810   |
| B     |  0.7440   |  0.4620   |
| BA    |  0.2300  |  0.2980  |
| C     |  0.7450 |  0.4630 |
| CA    |  0.5000 |  0.4620 |
| D     |  0.5140 |  0.3610 |
| DA    |  0.2820 |  0.3110 |
| E     |  0.5000 |  0.3390 |
| F     |  0.3400 |  0.3400 |
| G     |  0.2860 |  0.3100 |
| H     |  0.3600 |  0.3390 |
| I     |  0.0360 |  0.1950 |
| J     |  0.2860 |  0.3410 |
| K     |  0.4890 |  0.4060 |
| L     |  0.2820 |  0.2780 |
| M     |  0.1790 |  0.3610 |
| N     |  0.1800 |  0.2230 |
| O     |  0.2560 |  0.3910 |
| P     |  0.1430 |  0.2880 |
| Q     |  0.2500 |  0.1180 |
| R     |  0.2860 |  0.2760 |
| S     |  0.2500 |  0.3170 |
| T     |  0.1790 |  0.2120 |



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| Chain | Atom inclusion   | Q-score  |
|-------|--|--|
| U     |  0.2800   |  0.2650   |
| V     |  0.2460   |  0.2990   |
| W     |  0.5000   |  0.4490   |
| X     |  0.3080   |  0.3330   |
| Y     |  0.5280   |  0.3640   |
| Z     |  0.5000   |  0.3260   |
| a     |  0.3400   |  0.3360   |
| b     |  0.2500   |  0.3020   |
| c     |  0.3400   |  0.3480   |
| d     |  0.0360   |  0.1820   |
| e     |  0.2860   |  0.2960   |
| f     |  0.5110   |  0.4040   |
| g     |  0.2820   |  0.2750   |
| h     |  0.2140   |  0.3580   |
| i     |  0.1640   |  0.2280   |
| j     |  0.2560   |  0.3800   |
| k     |  0.1070   |  0.2850   |
| l     |  0.2140   |  0.1100   |
| m     |  0.2500   |  0.2590   |
| n     |  0.2500  |  0.3110  |
| o     |  0.1790 |  0.1950 |
| p     |  0.2800 |  0.2680 |
| q     |  0.2300 |  0.3000 |
| r     |  0.5000 |  0.4250 |
| s     |  0.2820 |  0.3290 |
| t     |  0.5560 |  0.3710 |
| u     |  0.4640 |  0.3480 |
| v     |  0.3400 |  0.3410 |
| w     |  0.2500 |  0.3140 |
| x     |  0.3800 |  0.3510 |
| y     |  0.0360 |  0.1720 |
| z     |  0.2860 |  0.3160 |