



## wwPDB EM Validation Summary Report ⓘ

Jul 4, 2026 – 12:40 PM JST

PDB ID : 9UFE / pdb\_00009ufe  
EMDB ID : EMD-64106  
Title : Cryo-EM structure of the tubular mastigoneme (the central tube) from golden algae 2.17 angstrom resolution  
Authors : Huang, J.; Tao, H.; Chen, S.; Cui, Y.; Xu, Y.; Yan, C.; Yan, N.  
Deposited on : 2025-04-10  
Resolution : 2.17 Å(reported)

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

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

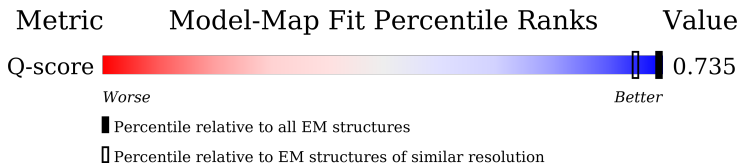
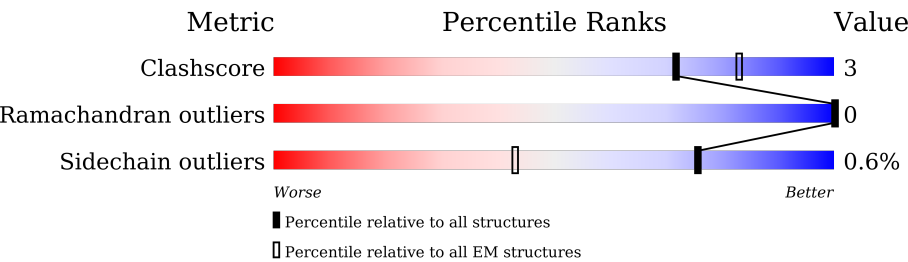
EMDB validation analysis : 0.0.1.dev133  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.50

# 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 2.17 Å.

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



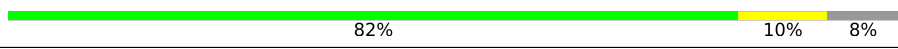
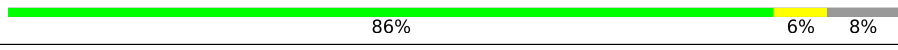
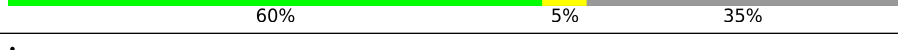
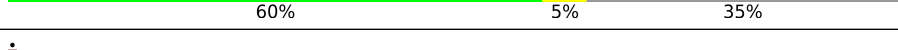
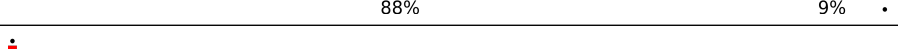
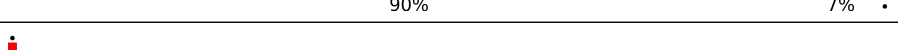
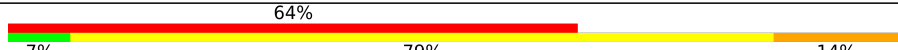
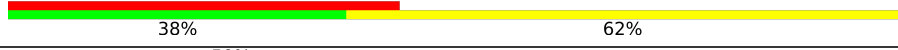
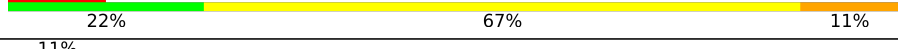
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 2651 ( 1.67 - 2.67 )                                     |

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   | EA    | 368    |                  |
| 1   | EB    | 368    |                  |
| 1   | EC    | 368    |                  |
| 2   | FA    | 723    |                  |

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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | FB    | 723    |    |
| 2   | FC    | 723    |    |
| 3   | DA    | 209    |    |
| 3   | DB    | 209    |    |
| 3   | DC    | 209    |    |
| 4   | CA    | 349    |    |
| 4   | CB    | 349    |    |
| 4   | CC    | 349    |    |
| 5   | AA    | 748    |    |
| 5   | AB    | 748    |    |
| 5   | AC    | 748    |    |
| 6   | BA    | 366    |  |
| 6   | BB    | 366    |  |
| 6   | BC    | 366    |  |
| 7   | aA    | 14     |  |
| 7   | aF    | 14     |  |
| 7   | aK    | 14     |  |
| 8   | aB    | 16     |  |
| 8   | aG    | 16     |  |
| 8   | aL    | 16     |  |
| 9   | aC    | 16     |  |
| 9   | aH    | 16     |  |
| 9   | aM    | 16     |  |
| 10  | aD    | 9      |  |
| 10  | aI    | 9      |  |

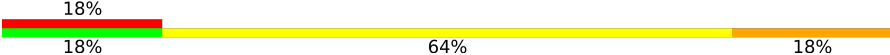
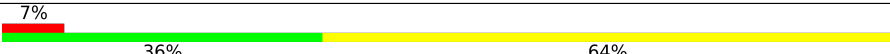
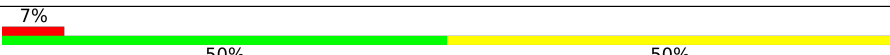
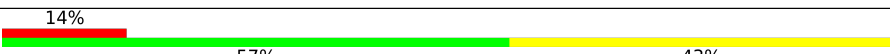
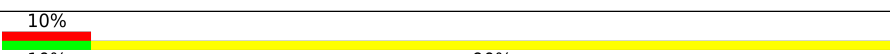
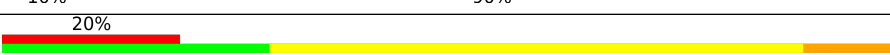
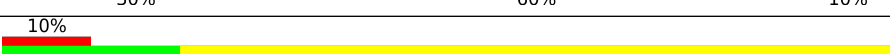
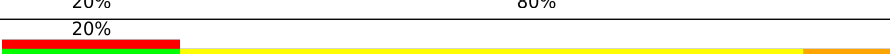
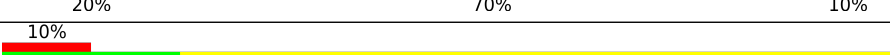
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| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|------------------|
| 10  | aN    | 9      |                  |
| 11  | aE    | 15     |                  |
| 11  | aJ    | 15     |                  |
| 11  | aO    | 15     |                  |
| 12  | bA    | 9      |                  |
| 12  | bD    | 9      |                  |
| 12  | bG    | 9      |                  |
| 13  | bB    | 5      |                  |
| 13  | bE    | 5      |                  |
| 13  | bH    | 5      |                  |
| 14  | bC    | 10     |                  |
| 14  | bF    | 10     |                  |
| 14  | bI    | 10     |                  |
| 15  | cA    | 4      |                  |
| 15  | cB    | 4      |                  |
| 15  | cC    | 4      |                  |
| 16  | dA    | 7      |                  |
| 16  | dB    | 7      |                  |
| 16  | dC    | 7      |                  |
| 17  | eA    | 11     |                  |
| 17  | eC    | 11     |                  |
| 17  | eE    | 11     |                  |
| 17  | fC    | 11     |                  |
| 17  | fD    | 11     |                  |
| 17  | fH    | 11     |                  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 17  | fI    | 11     |  27%64%9%      |
| 17  | fM    | 11     |  18%18%64%     |
| 17  | fN    | 11     |  9%91%         |
| 18  | eB    | 14     |  7%36%64%      |
| 18  | eD    | 14     |  7%50%50%      |
| 18  | eF    | 14     |  14%57%43%     |
| 19  | fB    | 10     |  10%10%90%     |
| 19  | fE    | 10     |  20%30%60%10%  |
| 19  | fG    | 10     |  10%20%80%     |
| 19  | fJ    | 10     |  20%20%70%10%  |
| 19  | fL    | 10     |  10%20%80%     |
| 19  | fO    | 10     |  20%30%60%10%  |
| 20  | fF    | 14     |  57%36%64%    |
| 20  | fK    | 14     |  57%36%57%7% |
| 20  | fP    | 14     |  57%43%57%   |

## 2 Entry composition [i](#)

There are 25 unique types of molecules in this entry. The entry contains 71986 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 OCM5.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | EA    | 351      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2672  | 1651 | 460 | 532 | 29 |         |       |
| 1   | EB    | 351      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2672  | 1651 | 460 | 532 | 29 |         |       |
| 1   | EC    | 351      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2672  | 1651 | 460 | 532 | 29 |         |       |

- Molecule 2 is a protein called OCM6.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 2   | FA    | 699      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5350  | 3333 | 898 | 1078 | 41 |         |       |
| 2   | FB    | 699      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5350  | 3333 | 898 | 1078 | 41 |         |       |
| 2   | FC    | 699      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5350  | 3333 | 898 | 1078 | 41 |         |       |

- Molecule 3 is a protein called Tubular mastigoneme protein.

| Mol | Chain | Residues | Atoms |     |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|----|---------|-------|
| 3   | DA    | 192      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1409  | 850 | 251 | 284 | 24 |         |       |
| 3   | DB    | 192      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1409  | 850 | 251 | 284 | 24 |         |       |
| 3   | DC    | 192      | Total | C   | N   | O   | S  | 0       | 0     |
|     |       |          | 1409  | 850 | 251 | 284 | 24 |         |       |

There are 3 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| DA    | 106     | SER      | PRO    | conflict | UNP C4B7Q8 |
| DB    | 106     | SER      | PRO    | conflict | UNP C4B7Q8 |
| DC    | 106     | SER      | PRO    | conflict | UNP C4B7Q8 |

- Molecule 4 is a protein called OCM3.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 4   | CA    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1728  | 1047 | 313 | 343 | 25 |         |       |
| 4   | CB    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1728  | 1047 | 313 | 343 | 25 |         |       |
| 4   | CC    | 227      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 1728  | 1047 | 313 | 343 | 25 |         |       |

- Molecule 5 is a protein called Tubular mastigoneme protein.

| Mol | Chain | Residues | Atoms |      |     |      |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|------|----|---------|-------|
| 5   | AA    | 727      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5689  | 3561 | 936 | 1150 | 42 |         |       |
| 5   | AB    | 727      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5689  | 3561 | 936 | 1150 | 42 |         |       |
| 5   | AC    | 727      | Total | C    | N   | O    | S  | 0       | 0     |
|     |       |          | 5689  | 3561 | 936 | 1150 | 42 |         |       |

- Molecule 6 is a protein called Tubular mastigoneme protein.

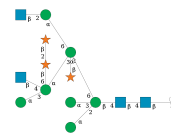
| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 6   | BA    | 348      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2725  | 1678 | 462 | 558 | 27 |         |       |
| 6   | BB    | 348      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2725  | 1678 | 462 | 558 | 27 |         |       |
| 6   | BC    | 348      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 2725  | 1678 | 462 | 558 | 27 |         |       |

There are 6 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment  | Reference  |
|-------|---------|----------|--------|----------|------------|
| BA    | 72      | GLY      | VAL    | conflict | UNP C4B7Q7 |
| BA    | 112     | ASP      | ALA    | conflict | UNP C4B7Q7 |
| BB    | 72      | GLY      | VAL    | conflict | UNP C4B7Q7 |
| BB    | 112     | ASP      | ALA    | conflict | UNP C4B7Q7 |
| BC    | 72      | GLY      | VAL    | conflict | UNP C4B7Q7 |
| BC    | 112     | ASP      | ALA    | conflict | UNP C4B7Q7 |

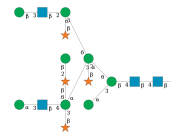
- Molecule 7 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyra

nose-(1-2)][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.



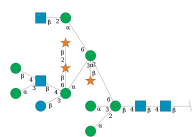
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 7   | aA    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 160   | 89 | 4 | 67 |         |       |
| 7   | aF    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 160   | 89 | 4 | 67 |         |       |
| 7   | aK    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 160   | 89 | 4 | 67 |         |       |

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



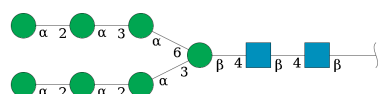
| Mol | Chain | Residues | Atoms |     |   |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|---------|-------|
| 8   | aB    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 180   | 100 | 4 | 76 |         |       |
| 8   | aG    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 180   | 100 | 4 | 76 |         |       |
| 8   | aL    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 180   | 100 | 4 | 76 |         |       |

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



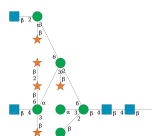
| Mol | Chain | Residues | Atoms |     |   |    | AltConf | Trace |
|-----|-------|----------|-------|-----|---|----|---------|-------|
| 9   | aC    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 182   | 101 | 4 | 77 |         |       |
| 9   | aH    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 182   | 101 | 4 | 77 |         |       |
| 9   | aM    | 16       | Total | C   | N | O  | 0       | 0     |
|     |       |          | 182   | 101 | 4 | 77 |         |       |

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-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.



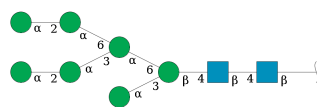
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 10  | aD    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 10  | aI    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 10  | aN    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |

- Molecule 11 is an oligosaccharide called beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][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.



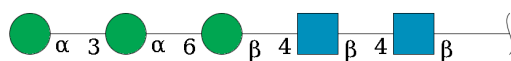
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 11  | aE    | 15       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 167   | 93 | 4 | 70 |         |       |
| 11  | aJ    | 15       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 167   | 93 | 4 | 70 |         |       |
| 11  | aO    | 15       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 167   | 93 | 4 | 70 |         |       |

- Molecule 12 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 12  | bA    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 12  | bD    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 12  | bG    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |

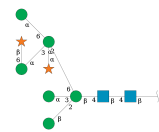
- Molecule 13 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 13  | bB    | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 13  | bE    | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 13  | bH    | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |

- Molecule 14 is an oligosaccharide called beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][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.



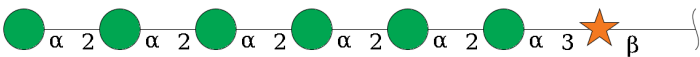
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 14  | bC    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 112   | 62 | 2 | 48 |         |       |
| 14  | bF    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 112   | 62 | 2 | 48 |         |       |
| 14  | bI    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 112   | 62 | 2 | 48 |         |       |

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



| Mol | Chain | Residues | Atoms |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|-------|
| 15  | cA    | 4        | Total | C  | O  | 0       | 0     |
|     |       |          | 42    | 23 | 19 |         |       |
| 15  | cB    | 4        | Total | C  | O  | 0       | 0     |
|     |       |          | 42    | 23 | 19 |         |       |
| 15  | cC    | 4        | Total | C  | O  | 0       | 0     |
|     |       |          | 42    | 23 | 19 |         |       |

- Molecule 16 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose.



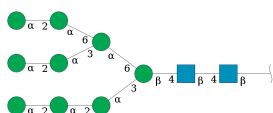
| Mol | Chain | Residues | Atoms |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|-------|
| 16  | dA    | 7        | Total | C  | O  | 0       | 0     |
|     |       |          | 75    | 41 | 34 |         |       |
| 16  | dB    | 7        | Total | C  | O  | 0       | 0     |
|     |       |          | 75    | 41 | 34 |         |       |

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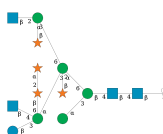
| Mol | Chain | Residues | Atoms |    |    | AltConf | Trace |
|-----|-------|----------|-------|----|----|---------|-------|
| 16  | dC    | 7        | Total | C  | O  | 0       | 0     |
|     |       |          | 75    | 41 | 34 |         |       |

- Molecule 17 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



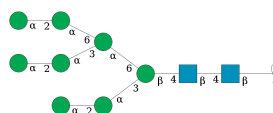
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 17  | eA    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fC    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fD    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | eC    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fH    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fI    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | eE    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fM    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |
| 17  | fN    | 11       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 127   | 70 | 2 | 55 |         |       |

- Molecule 18 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



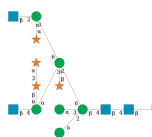
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 18  | eB    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |
| 18  | eD    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |
| 18  | eF    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |

- Molecule 19 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 19  | fB    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |
| 19  | fE    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |
| 19  | fG    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |
| 19  | fJ    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |
| 19  | fL    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |
| 19  | fO    | 10       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 116   | 64 | 2 | 50 |         |       |

- Molecule 20 is an oligosaccharide called alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)]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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 20  | fF    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |
| 20  | fK    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |
| 20  | fP    | 14       | Total | C  | N | O  | 0       | 0     |
|     |       |          | 158   | 88 | 4 | 66 |         |       |

- Molecule 21 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

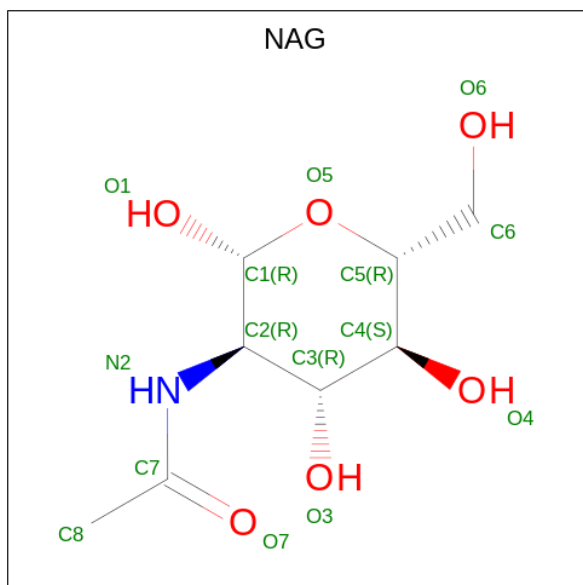
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | EA    | 2        | Total | Ca | 0       |
|     |       |          | 2     | 2  |         |
| 21  | FA    | 6        | Total | Ca | 0       |
|     |       |          | 6     | 6  |         |
| 21  | CA    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 21  | AA    | 7        | Total | Ca | 0       |
|     |       |          | 7     | 7  |         |
| 21  | BA    | 3        | Total | Ca | 0       |
|     |       |          | 3     | 3  |         |
| 21  | EB    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 21  | FB    | 6        | Total | Ca | 0       |
|     |       |          | 6     | 6  |         |
| 21  | CB    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 21  | AB    | 7        | Total | Ca | 0       |
|     |       |          | 7     | 7  |         |
| 21  | BB    | 3        | Total | Ca | 0       |
|     |       |          | 3     | 3  |         |
| 21  | EC    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 21  | FC    | 6        | Total | Ca | 0       |
|     |       |          | 6     | 6  |         |
| 21  | CC    | 1        | Total | Ca | 0       |
|     |       |          | 1     | 1  |         |
| 21  | AC    | 7        | Total | Ca | 0       |
|     |       |          | 7     | 7  |         |

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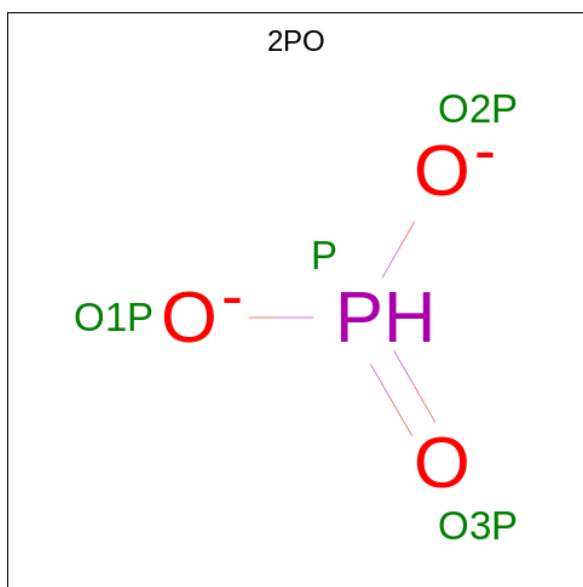
| Mol | Chain | Residues | Atoms |    | AltConf |
|-----|-------|----------|-------|----|---------|
| 21  | BC    | 3        | Total | Ca | 0       |
|     |       |          | 3     | 3  |         |

- Molecule 22 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 22  | EA    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 22  | FA    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 22  | EB    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 22  | FB    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 22  | EC    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 22  | FC    | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

- Molecule 23 is PHOSPHONATE (CCD ID: 2PO) (formula:  $HO_3P$ ).



| Mol | Chain | Residues | Atoms |   |   | AltConf |
|-----|-------|----------|-------|---|---|---------|
| 23  | EA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | FA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | BA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | BA    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | EB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | FB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | AB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | BB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |
| 23  | BB    | 1        | Total | O | P | 0       |
|     |       |          | 4     | 3 | 1 |         |

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| Mol | Chain | Residues | Atoms      |        |        | AltConf |
|-----|-------|----------|------------|--------|--------|---------|
| 23  | EC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | FC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | AC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | AC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | AC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | BC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |
| 23  | BC    | 1        | Total<br>4 | O<br>3 | P<br>1 | 0       |

- Molecule 24 is CHLORIDE ION (CCD ID: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

| Mol | Chain | Residues | Atoms      |         | AltConf |
|-----|-------|----------|------------|---------|---------|
| 24  | DA    | 1        | Total<br>1 | Cl<br>1 | 0       |
| 24  | DB    | 1        | Total<br>1 | Cl<br>1 | 0       |
| 24  | DC    | 1        | Total<br>1 | Cl<br>1 | 0       |

- Molecule 25 is water.

| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 25  | EA    | 293      | Total<br>293 | O<br>293 | 0       |
| 25  | FA    | 632      | Total<br>632 | O<br>632 | 0       |
| 25  | DA    | 167      | Total<br>167 | O<br>167 | 0       |
| 25  | CA    | 219      | Total<br>219 | O<br>219 | 0       |
| 25  | AA    | 610      | Total<br>610 | O<br>610 | 0       |
| 25  | BA    | 275      | Total<br>275 | O<br>275 | 0       |
| 25  | EB    | 294      | Total<br>294 | O<br>294 | 0       |

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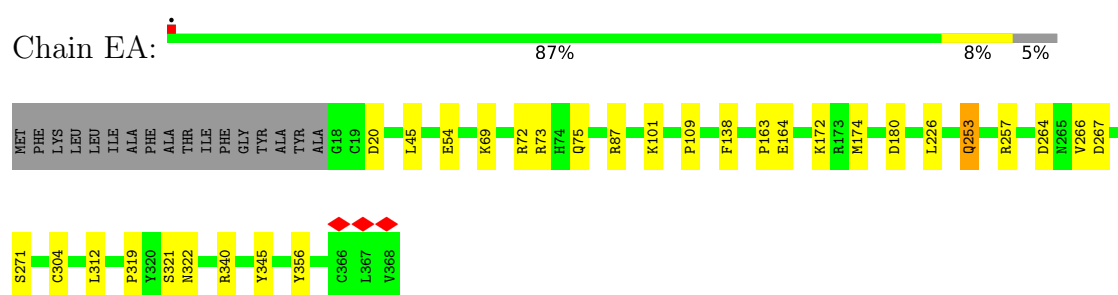
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| Mol | Chain | Residues | Atoms        |          | AltConf |
|-----|-------|----------|--------------|----------|---------|
| 25  | FB    | 635      | Total<br>635 | O<br>635 | 0       |
| 25  | DB    | 169      | Total<br>169 | O<br>169 | 0       |
| 25  | CB    | 217      | Total<br>217 | O<br>217 | 0       |
| 25  | AB    | 619      | Total<br>619 | O<br>619 | 0       |
| 25  | BB    | 300      | Total<br>300 | O<br>300 | 0       |
| 25  | EC    | 324      | Total<br>324 | O<br>324 | 0       |
| 25  | FC    | 636      | Total<br>636 | O<br>636 | 0       |
| 25  | DC    | 170      | Total<br>170 | O<br>170 | 0       |
| 25  | CC    | 209      | Total<br>209 | O<br>209 | 0       |
| 25  | AC    | 617      | Total<br>617 | O<br>617 | 0       |
| 25  | BC    | 301      | Total<br>301 | O<br>301 | 0       |

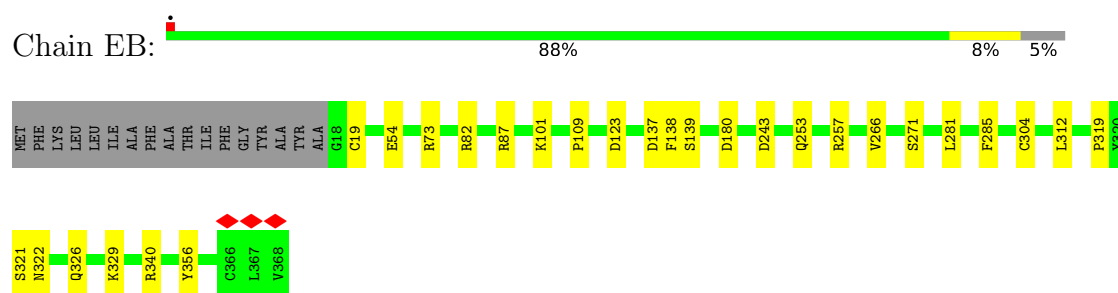
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

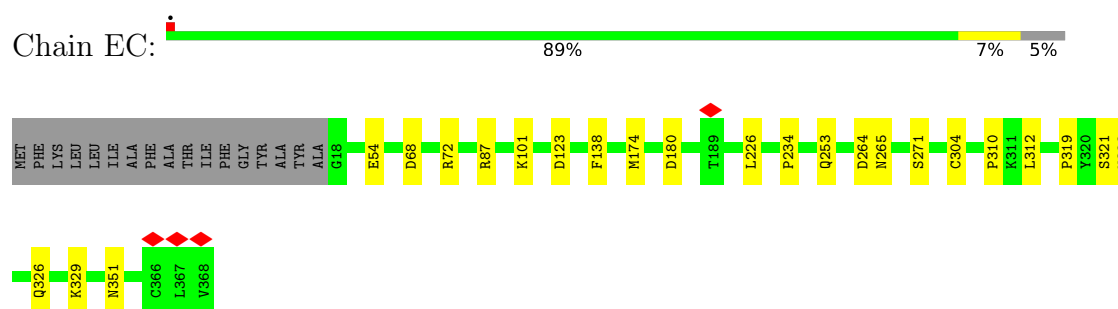
- Molecule 1: OCM5



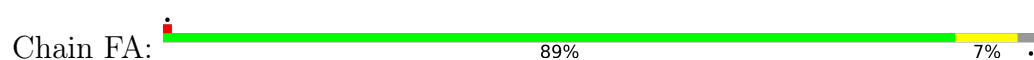
- Molecule 1: OCM5

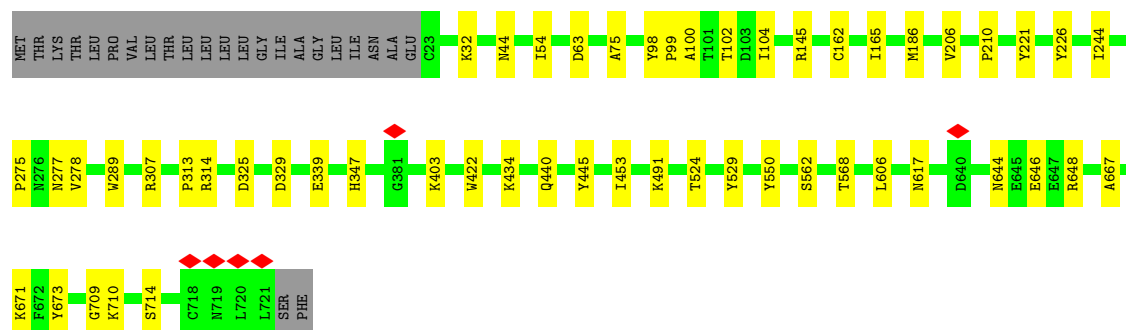


- Molecule 1: OCM5



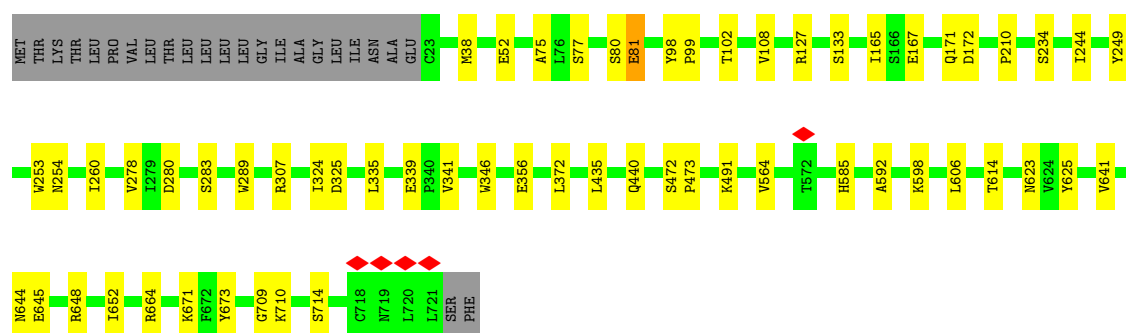
- Molecule 2: OCM6





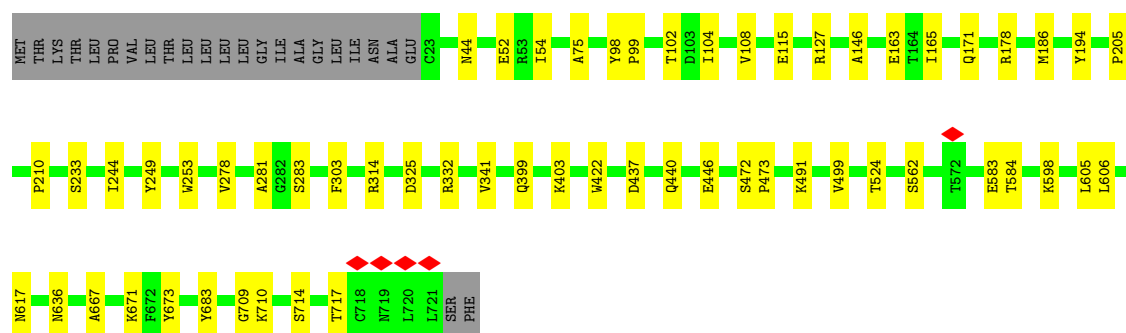
- Molecule 2: OCM6

Chain FB: 88% 8%



- Molecule 2: OCM6

Chain FC: 89% 8%



- Molecule 3: Tubular mastigoneme protein

Chain DA: 82% 10% 8%

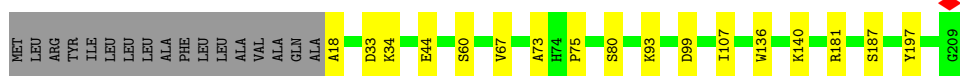
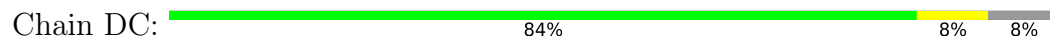


- Molecule 3: Tubular mastigoneme protein

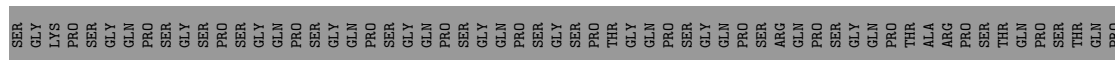
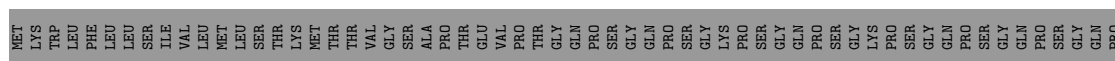
Chain DB: 86% 6% 8%



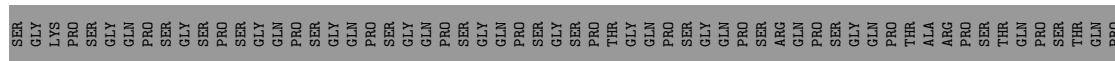
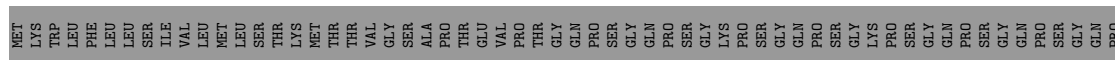
• Molecule 3: Tubular mastigoneme protein



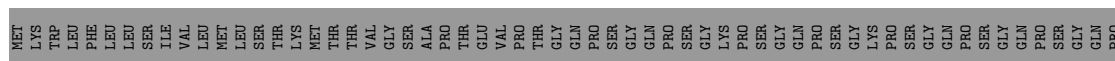
• Molecule 4: OCM3



• Molecule 4: OCM3

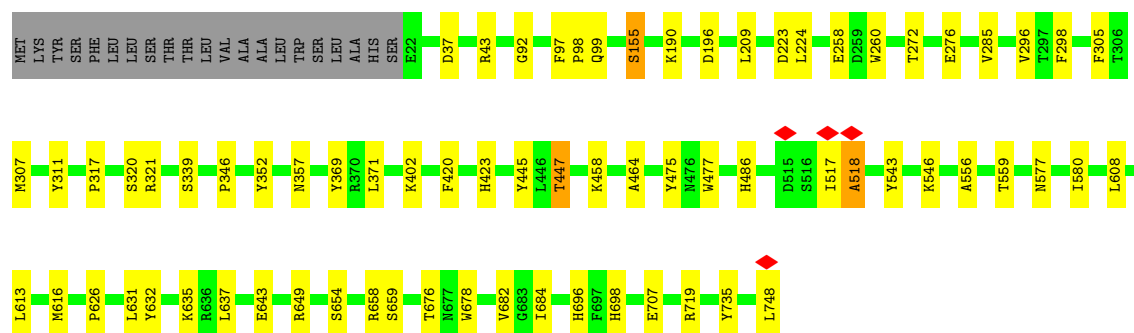


• Molecule 4: OCM3



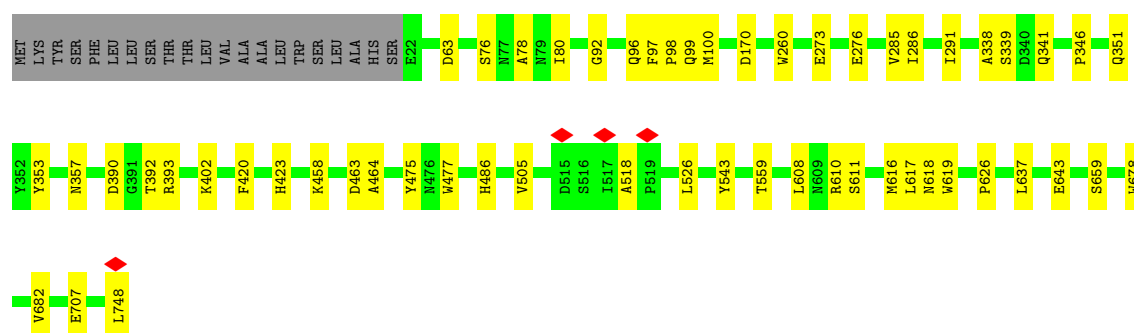
• Molecule 5: Tubular mastigoneme protein

Chain AA:  88% 9%



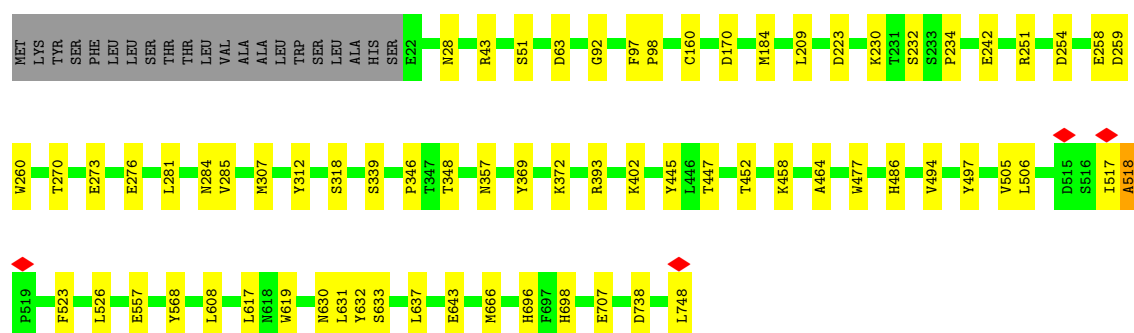
• Molecule 5: Tubular mastigoneme protein

Chain AB:  90% 7%



• Molecule 5: Tubular mastigoneme protein

Chain AC:  88% 9%



• Molecule 6: Tubular mastigoneme protein

Chain BA:  88% 7% 5%





- Molecule 6: Tubular mastigoneme protein

Chain BB: 88% 7% 5%



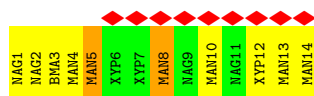
- Molecule 6: Tubular mastigoneme protein

Chain BC: 87% 8% 5%



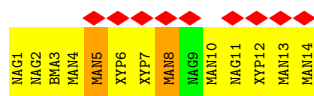
- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta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

Chain aA: 29% 64% 57% 14%

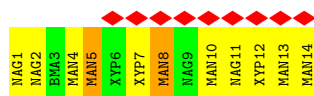


- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta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

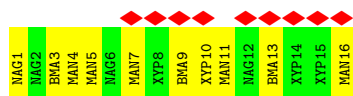
Chain aF: 7% 64% 79% 14%



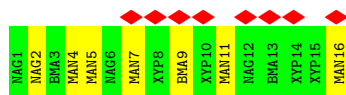
- Molecule 7: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)][2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta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



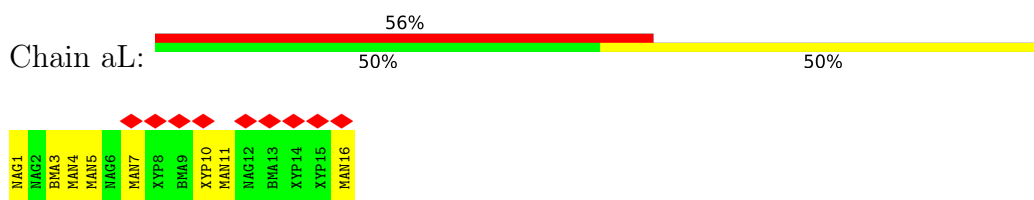
- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-m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



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



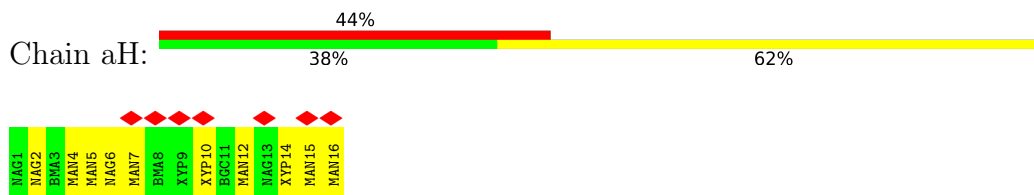
- Molecule 8: alpha-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-mannopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-m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



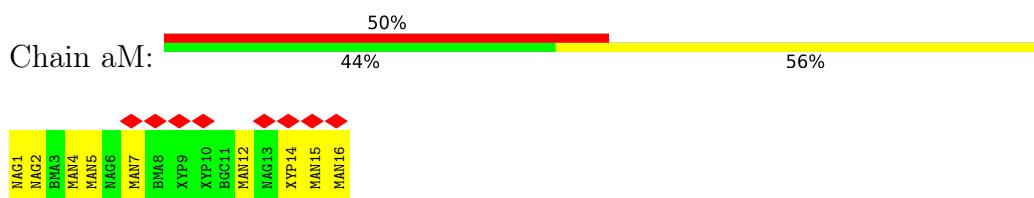
• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-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



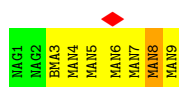
• Molecule 9: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-4)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)][beta-D-glucopyranose-(1-3)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-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



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



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[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



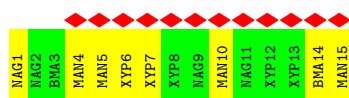
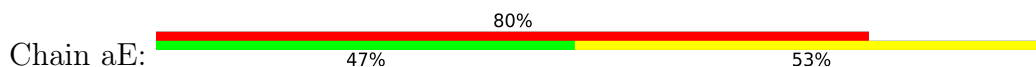
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



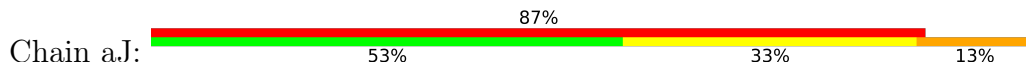
- Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

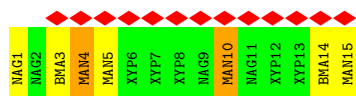


- Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

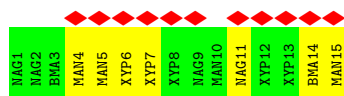
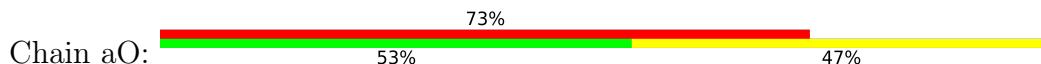


- Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)]alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose





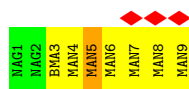
- Molecule 11: beta-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-xylopyranose-(1-3)]|2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)]|alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



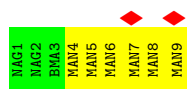
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



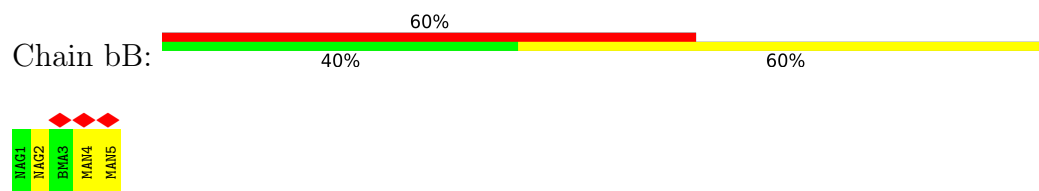
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



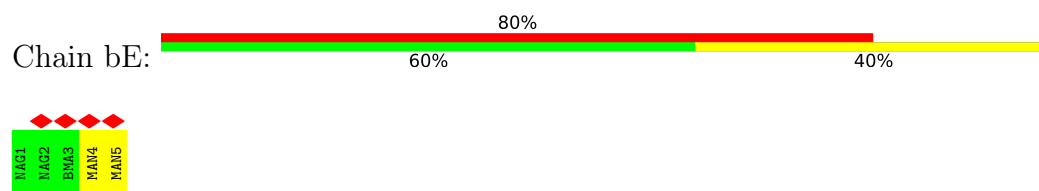
- Molecule 12: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



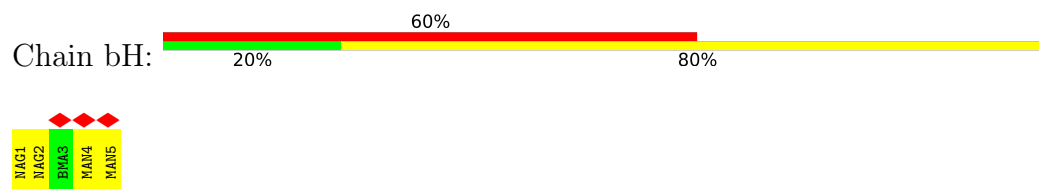
- Molecule 13: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



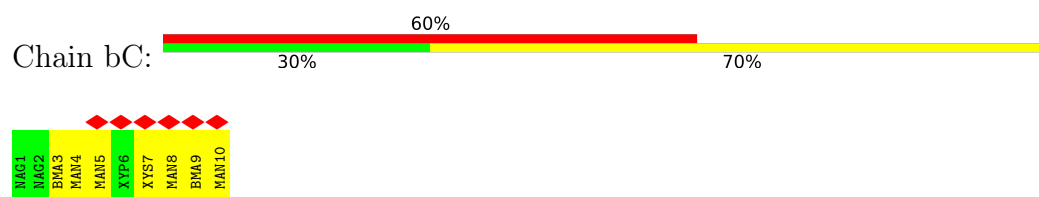
- Molecule 13: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



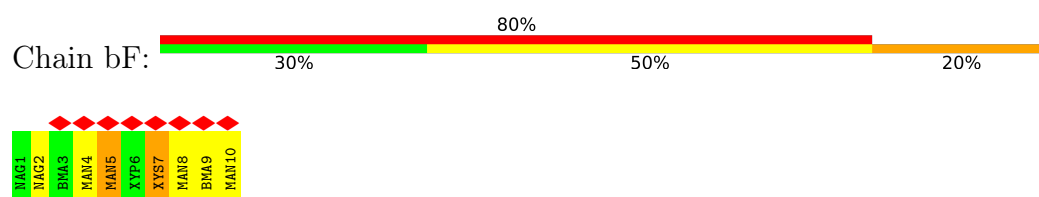
- Molecule 13: alpha-D-mannopyranose-(1-3)-alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



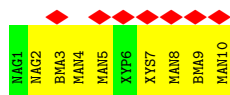
- Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][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 14: beta-D-xylopyranose-(1-6)-alpha-D-mannopyranose-(1-3)-[alpha-D-xylopyranose-(1-2)][alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[beta-D-mannopyranose-(1-2)][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 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose





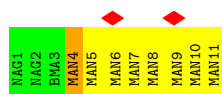
- Molecule 16: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-xylopyranose



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

se-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e



• Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranos e



- Molecule 17: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



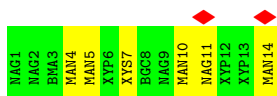
- Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)]|[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



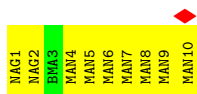
- Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)]|[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 18: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[beta-D-glucopyranose-(1-3)]|[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[beta-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)]|[beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



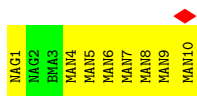
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



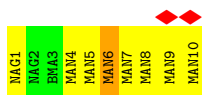
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



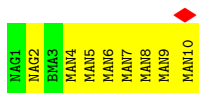
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



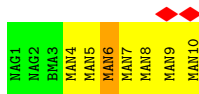
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



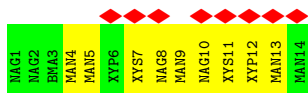
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



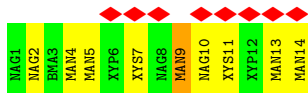
- Molecule 19: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][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

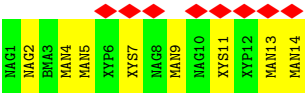


- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 20: alpha-D-xylopyranose-(1-2)-beta-D-xylopyranose-(1-6)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)]alpha-D-mannopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][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

e-(1-2)-[alpha-D-xylopyranose-(1-3)]alpha-D-mannopyranose-(1-6)][beta-D-xylopyranose-(1-2)]alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-2)][alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, Not provided                     |           |
| Number of particles used             | 104125                                  | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | TFS KRIOS                               | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 50                                      | Depositor |
| Minimum defocus (nm)                 | 600                                     | Depositor |
| Maximum defocus (nm)                 | 1200                                    | Depositor |
| Magnification                        | Not provided                            |           |
| Image detector                       | FEI FALCON IV (4k x 4k)                 | Depositor |
| Maximum map value                    | 1.519                                   | Depositor |
| Minimum map value                    | -0.995                                  | Depositor |
| Average map value                    | 0.001                                   | Depositor |
| Map value standard deviation         | 0.055                                   | Depositor |
| Recommended contour level            | 0.2                                     | Depositor |
| Map size (Å)                         | 460.00128, 460.00128, 460.00128         | wwPDB     |
| Map dimensions                       | 512, 512, 512                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 0.89844, 0.89844, 0.89844               | Depositor |

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 2PO, MAN, XYS, CL, NAG, CA, BGC, BMA, XYP

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   | EA    | 0.24         | 0/2733  | 0.41        | 0/3708         |
| 1   | EB    | 0.24         | 0/2733  | 0.42        | 0/3708         |
| 1   | EC    | 0.23         | 0/2733  | 0.43        | 0/3708         |
| 2   | FA    | 0.22         | 0/5484  | 0.40        | 0/7488         |
| 2   | FB    | 0.23         | 0/5484  | 0.42        | 0/7488         |
| 2   | FC    | 0.24         | 0/5484  | 0.43        | 0/7488         |
| 3   | DA    | 0.25         | 0/1439  | 0.45        | 0/1947         |
| 3   | DB    | 0.27         | 0/1439  | 0.46        | 0/1947         |
| 3   | DC    | 0.25         | 0/1439  | 0.47        | 0/1947         |
| 4   | CA    | 0.24         | 0/1776  | 0.41        | 0/2413         |
| 4   | CB    | 0.24         | 0/1776  | 0.45        | 0/2413         |
| 4   | CC    | 0.26         | 0/1776  | 0.44        | 0/2413         |
| 5   | AA    | 0.23         | 0/5841  | 0.40        | 0/7967         |
| 5   | AB    | 0.24         | 0/5841  | 0.43        | 0/7967         |
| 5   | AC    | 0.24         | 0/5841  | 0.43        | 2/7967 (0.0%)  |
| 6   | BA    | 0.23         | 0/2782  | 0.42        | 0/3781         |
| 6   | BB    | 0.25         | 0/2782  | 0.44        | 0/3781         |
| 6   | BC    | 0.25         | 0/2782  | 0.44        | 0/3781         |
| All | All   | 0.24         | 0/60165 | 0.42        | 2/81912 (0.0%) |

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

| Mol | Chain | #Chirality outliers | #Planarity outliers |
|-----|-------|---------------------|---------------------|
| 5   | AA    | 0                   | 1                   |
| 5   | AB    | 0                   | 1                   |
| 5   | AC    | 0                   | 1                   |
| All | All   | 0                   | 3                   |

There are no bond length outliers.

All (2) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms   | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5   | AC    | 234 | PRO  | N-CD-CG | -8.23 | 93.92       | 103.80   |
| 5   | AC    | 234 | PRO  | CA-N-CD | -5.62 | 103.62      | 111.50   |

There are no chirality outliers.

All (3) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 5   | AA    | 518 | ALA  | Peptide |
| 5   | AB    | 518 | ALA  | Peptide |
| 5   | AC    | 518 | ALA  | Peptide |

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

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

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | EA    | 2672  | 0        | 2469     | 24      | 0            |
| 1   | EB    | 2672  | 0        | 2470     | 20      | 0            |
| 1   | EC    | 2672  | 0        | 2470     | 18      | 0            |
| 2   | FA    | 5350  | 0        | 4914     | 35      | 0            |
| 2   | FB    | 5350  | 0        | 4914     | 35      | 0            |
| 2   | FC    | 5350  | 0        | 4913     | 41      | 0            |
| 3   | DA    | 1409  | 0        | 1268     | 17      | 0            |
| 3   | DB    | 1409  | 0        | 1268     | 11      | 0            |
| 3   | DC    | 1409  | 0        | 1268     | 14      | 0            |
| 4   | CA    | 1728  | 0        | 1530     | 12      | 0            |
| 4   | CB    | 1728  | 0        | 1530     | 11      | 0            |
| 4   | CC    | 1728  | 0        | 1530     | 9       | 0            |
| 5   | AA    | 5689  | 0        | 5214     | 43      | 0            |
| 5   | AB    | 5689  | 0        | 5214     | 36      | 0            |
| 5   | AC    | 5689  | 0        | 5214     | 44      | 0            |
| 6   | BA    | 2725  | 0        | 2484     | 16      | 0            |
| 6   | BB    | 2725  | 0        | 2486     | 22      | 0            |
| 6   | BC    | 2725  | 0        | 2485     | 22      | 0            |
| 7   | aA    | 160   | 0        | 109      | 2       | 0            |
| 7   | aF    | 160   | 0        | 109      | 1       | 0            |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 7   | aK    | 160   | 0        | 109      | 2       | 0            |
| 8   | aB    | 180   | 0        | 117      | 0       | 0            |
| 8   | aG    | 180   | 0        | 117      | 0       | 0            |
| 8   | aL    | 180   | 0        | 117      | 1       | 0            |
| 9   | aC    | 182   | 0        | 127      | 1       | 0            |
| 9   | aH    | 182   | 0        | 127      | 0       | 0            |
| 9   | aM    | 182   | 0        | 127      | 1       | 0            |
| 10  | aD    | 105   | 0        | 88       | 1       | 0            |
| 10  | aI    | 105   | 0        | 88       | 1       | 0            |
| 10  | aN    | 105   | 0        | 88       | 1       | 0            |
| 11  | aE    | 167   | 0        | 98       | 2       | 0            |
| 11  | aJ    | 167   | 0        | 98       | 2       | 0            |
| 11  | aO    | 167   | 0        | 98       | 1       | 0            |
| 12  | bA    | 105   | 0        | 88       | 0       | 0            |
| 12  | bD    | 105   | 0        | 88       | 1       | 0            |
| 12  | bG    | 105   | 0        | 88       | 0       | 0            |
| 13  | bB    | 61    | 0        | 52       | 0       | 0            |
| 13  | bE    | 61    | 0        | 52       | 0       | 0            |
| 13  | bH    | 61    | 0        | 52       | 0       | 0            |
| 14  | bC    | 112   | 0        | 84       | 0       | 0            |
| 14  | bF    | 112   | 0        | 84       | 1       | 0            |
| 14  | bI    | 112   | 0        | 84       | 0       | 0            |
| 15  | cA    | 42    | 0        | 28       | 0       | 0            |
| 15  | cB    | 42    | 0        | 28       | 0       | 0            |
| 15  | cC    | 42    | 0        | 28       | 0       | 0            |
| 16  | dA    | 75    | 0        | 55       | 0       | 0            |
| 16  | dB    | 75    | 0        | 55       | 0       | 0            |
| 16  | dC    | 75    | 0        | 55       | 1       | 0            |
| 17  | eA    | 127   | 0        | 106      | 0       | 0            |
| 17  | eC    | 127   | 0        | 106      | 2       | 0            |
| 17  | eE    | 127   | 0        | 106      | 0       | 0            |
| 17  | fC    | 127   | 0        | 106      | 1       | 0            |
| 17  | fD    | 127   | 0        | 106      | 0       | 0            |
| 17  | fH    | 127   | 0        | 106      | 0       | 0            |
| 17  | fI    | 127   | 0        | 106      | 1       | 0            |
| 17  | fM    | 127   | 0        | 106      | 3       | 0            |
| 17  | fN    | 127   | 0        | 106      | 1       | 0            |
| 18  | eB    | 158   | 0        | 107      | 1       | 0            |
| 18  | eD    | 158   | 0        | 107      | 0       | 0            |
| 18  | eF    | 158   | 0        | 107      | 0       | 0            |
| 19  | fB    | 116   | 0        | 97       | 0       | 0            |
| 19  | fE    | 116   | 0        | 97       | 1       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 19  | fG    | 116   | 0        | 97       | 0       | 0            |
| 19  | fJ    | 116   | 0        | 97       | 1       | 0            |
| 19  | fL    | 116   | 0        | 97       | 0       | 0            |
| 19  | fO    | 116   | 0        | 97       | 1       | 0            |
| 20  | fF    | 158   | 0        | 115      | 2       | 0            |
| 20  | fK    | 158   | 0        | 115      | 1       | 0            |
| 20  | fP    | 158   | 0        | 115      | 0       | 0            |
| 21  | AA    | 7     | 0        | 0        | 0       | 0            |
| 21  | AB    | 7     | 0        | 0        | 0       | 0            |
| 21  | AC    | 7     | 0        | 0        | 0       | 0            |
| 21  | BA    | 3     | 0        | 0        | 0       | 0            |
| 21  | BB    | 3     | 0        | 0        | 1       | 0            |
| 21  | BC    | 3     | 0        | 0        | 0       | 0            |
| 21  | CA    | 1     | 0        | 0        | 0       | 0            |
| 21  | CB    | 1     | 0        | 0        | 0       | 0            |
| 21  | CC    | 1     | 0        | 0        | 0       | 0            |
| 21  | EA    | 2     | 0        | 0        | 1       | 0            |
| 21  | EB    | 1     | 0        | 0        | 0       | 0            |
| 21  | EC    | 1     | 0        | 0        | 0       | 0            |
| 21  | FA    | 6     | 0        | 0        | 0       | 0            |
| 21  | FB    | 6     | 0        | 0        | 0       | 0            |
| 21  | FC    | 6     | 0        | 0        | 0       | 0            |
| 22  | EA    | 14    | 0        | 13       | 1       | 0            |
| 22  | EB    | 14    | 0        | 13       | 1       | 0            |
| 22  | EC    | 14    | 0        | 13       | 1       | 0            |
| 22  | FA    | 14    | 0        | 13       | 0       | 0            |
| 22  | FB    | 14    | 0        | 13       | 0       | 0            |
| 22  | FC    | 14    | 0        | 13       | 0       | 0            |
| 23  | AA    | 12    | 0        | 0        | 0       | 0            |
| 23  | AB    | 12    | 0        | 0        | 0       | 0            |
| 23  | AC    | 12    | 0        | 0        | 0       | 0            |
| 23  | BA    | 8     | 0        | 0        | 0       | 0            |
| 23  | BB    | 8     | 0        | 0        | 0       | 0            |
| 23  | BC    | 8     | 0        | 0        | 0       | 0            |
| 23  | EA    | 4     | 0        | 0        | 0       | 0            |
| 23  | EB    | 4     | 0        | 0        | 0       | 0            |
| 23  | EC    | 4     | 0        | 0        | 0       | 0            |
| 23  | FA    | 4     | 0        | 0        | 0       | 0            |
| 23  | FB    | 4     | 0        | 0        | 0       | 0            |
| 23  | FC    | 4     | 0        | 0        | 0       | 0            |
| 24  | DA    | 1     | 0        | 0        | 0       | 0            |
| 24  | DB    | 1     | 0        | 0        | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 24  | DC    | 1     | 0        | 0        | 0       | 0            |
| 25  | AA    | 610   | 0        | 0        | 8       | 0            |
| 25  | AB    | 619   | 0        | 0        | 8       | 0            |
| 25  | AC    | 617   | 0        | 0        | 8       | 0            |
| 25  | BA    | 275   | 0        | 0        | 1       | 0            |
| 25  | BB    | 300   | 0        | 0        | 6       | 0            |
| 25  | BC    | 301   | 0        | 0        | 9       | 0            |
| 25  | CA    | 219   | 0        | 0        | 2       | 0            |
| 25  | CB    | 217   | 0        | 0        | 2       | 0            |
| 25  | CC    | 209   | 0        | 0        | 1       | 0            |
| 25  | DA    | 167   | 0        | 0        | 5       | 0            |
| 25  | DB    | 169   | 0        | 0        | 2       | 0            |
| 25  | DC    | 170   | 0        | 0        | 3       | 0            |
| 25  | EA    | 293   | 0        | 0        | 8       | 0            |
| 25  | EB    | 294   | 0        | 0        | 7       | 0            |
| 25  | EC    | 324   | 0        | 0        | 7       | 0            |
| 25  | FA    | 632   | 0        | 0        | 4       | 0            |
| 25  | FB    | 635   | 0        | 0        | 7       | 0            |
| 25  | FC    | 636   | 0        | 0        | 14      | 0            |
| All | All   | 71986 | 0        | 58459    | 415     | 0            |

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

The worst 5 of 415 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 2:FC:440:GLN:NE2 | 2:FC:491:LYS:O  | 2.05                     | 0.89              |
| 2:FC:524:THR:HG1 | 17:fM:4:MAN:HO4 | 1.17                     | 0.87              |
| 4:CB:17:HIS:ND1  | 25:AB:902:HOH:O | 2.09                     | 0.85              |
| 2:FB:440:GLN:NE2 | 2:FB:491:LYS:O  | 2.11                     | 0.83              |
| 2:FA:524:THR:HG1 | 17:fC:4:MAN:HO4 | 1.25                     | 0.80              |

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|----------|-------------|-----|
| 1   | EA    | 349/368 (95%)   | 345 (99%)  | 4 (1%)   | 0        | 100         | 100 |
| 1   | EB    | 349/368 (95%)   | 343 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 1   | EC    | 349/368 (95%)   | 343 (98%)  | 6 (2%)   | 0        | 100         | 100 |
| 2   | FA    | 697/723 (96%)   | 677 (97%)  | 20 (3%)  | 0        | 100         | 100 |
| 2   | FB    | 697/723 (96%)   | 674 (97%)  | 23 (3%)  | 0        | 100         | 100 |
| 2   | FC    | 697/723 (96%)   | 681 (98%)  | 16 (2%)  | 0        | 100         | 100 |
| 3   | DA    | 190/209 (91%)   | 181 (95%)  | 9 (5%)   | 0        | 100         | 100 |
| 3   | DB    | 190/209 (91%)   | 184 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 3   | DC    | 190/209 (91%)   | 184 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 4   | CA    | 225/349 (64%)   | 218 (97%)  | 7 (3%)   | 0        | 100         | 100 |
| 4   | CB    | 225/349 (64%)   | 220 (98%)  | 5 (2%)   | 0        | 100         | 100 |
| 4   | CC    | 225/349 (64%)   | 219 (97%)  | 6 (3%)   | 0        | 100         | 100 |
| 5   | AA    | 725/748 (97%)   | 705 (97%)  | 20 (3%)  | 0        | 100         | 100 |
| 5   | AB    | 725/748 (97%)   | 700 (97%)  | 25 (3%)  | 0        | 100         | 100 |
| 5   | AC    | 725/748 (97%)   | 708 (98%)  | 17 (2%)  | 0        | 100         | 100 |
| 6   | BA    | 346/366 (94%)   | 332 (96%)  | 14 (4%)  | 0        | 100         | 100 |
| 6   | BB    | 346/366 (94%)   | 334 (96%)  | 12 (4%)  | 0        | 100         | 100 |
| 6   | BC    | 346/366 (94%)   | 336 (97%)  | 10 (3%)  | 0        | 100         | 100 |
| All | All   | 7596/8289 (92%) | 7384 (97%) | 212 (3%) | 0        | 100         | 100 |

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|----------|-------------|-----|
| 1   | EA    | 294/306 (96%)   | 291 (99%)  | 3 (1%)   | 68          | 79  |
| 1   | EB    | 294/306 (96%)   | 292 (99%)  | 2 (1%)   | 76          | 86  |
| 1   | EC    | 294/306 (96%)   | 293 (100%) | 1 (0%)   | 86          | 92  |
| 2   | FA    | 582/602 (97%)   | 580 (100%) | 2 (0%)   | 86          | 92  |
| 2   | FB    | 582/602 (97%)   | 578 (99%)  | 4 (1%)   | 76          | 86  |
| 2   | FC    | 582/602 (97%)   | 580 (100%) | 2 (0%)   | 86          | 92  |
| 3   | DA    | 152/165 (92%)   | 152 (100%) | 0        | 100         | 100 |
| 3   | DB    | 152/165 (92%)   | 152 (100%) | 0        | 100         | 100 |
| 3   | DC    | 152/165 (92%)   | 151 (99%)  | 1 (1%)   | 76          | 86  |
| 4   | CA    | 187/287 (65%)   | 186 (100%) | 1 (0%)   | 81          | 89  |
| 4   | CB    | 187/287 (65%)   | 186 (100%) | 1 (0%)   | 81          | 89  |
| 4   | CC    | 187/287 (65%)   | 187 (100%) | 0        | 100         | 100 |
| 5   | AA    | 628/646 (97%)   | 623 (99%)  | 5 (1%)   | 73          | 83  |
| 5   | AB    | 628/646 (97%)   | 625 (100%) | 3 (0%)   | 81          | 89  |
| 5   | AC    | 628/646 (97%)   | 623 (99%)  | 5 (1%)   | 73          | 83  |
| 6   | BA    | 306/319 (96%)   | 305 (100%) | 1 (0%)   | 86          | 92  |
| 6   | BB    | 306/319 (96%)   | 303 (99%)  | 3 (1%)   | 68          | 79  |
| 6   | BC    | 306/319 (96%)   | 303 (99%)  | 3 (1%)   | 68          | 79  |
| All | All   | 6447/6975 (92%) | 6410 (99%) | 37 (1%)  | 76          | 87  |

5 of 37 residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 3   | DC    | 187 | SER  |
| 6   | BC    | 298 | CYS  |
| 5   | AC    | 357 | ASN  |
| 5   | AC    | 696 | HIS  |
| 1   | EB    | 243 | ASP  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AC    | 46  | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | AC    | 157 | HIS  |
| 6   | BC    | 153 | ASN  |
| 2   | FB    | 492 | GLN  |
| 2   | FB    | 315 | ASN  |

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

558 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 | $\# Z  > 2$ |
| 7   | NAG  | aA    | 1   | 5,7  | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.81 | 0           |
| 7   | MAN  | aA    | 10  | 23,7 | 11,11,12     | 0.66 | 0           | 15,15,17    | 1.04 | 2 (13%)     |
| 7   | NAG  | aA    | 11  | 7    | 14,14,15     | 0.28 | 0           | 17,19,21    | 0.66 | 0           |
| 7   | XYP  | aA    | 12  | 7    | 9,9,10       | 1.89 | 3 (33%)     | 10,12,14    | 0.91 | 0           |
| 7   | MAN  | aA    | 13  | 7    | 11,11,12     | 0.67 | 1 (9%)      | 15,15,17    | 1.06 | 1 (6%)      |
| 7   | MAN  | aA    | 14  | 7    | 11,11,12     | 0.69 | 0           | 15,15,17    | 1.27 | 3 (20%)     |
| 7   | NAG  | aA    | 2   | 7    | 14,14,15     | 0.38 | 0           | 17,19,21    | 0.96 | 1 (5%)      |
| 7   | BMA  | aA    | 3   | 7    | 11,11,12     | 0.24 | 0           | 15,15,17    | 0.96 | 1 (6%)      |
| 7   | MAN  | aA    | 4   | 7    | 11,11,12     | 1.08 | 1 (9%)      | 15,15,17    | 1.29 | 3 (20%)     |
| 7   | MAN  | aA    | 5   | 7    | 11,11,12     | 0.64 | 0           | 15,15,17    | 1.33 | 3 (20%)     |
| 7   | XYP  | aA    | 6   | 7    | 9,9,10       | 0.19 | 0           | 10,12,14    | 0.90 | 0           |
| 7   | XYP  | aA    | 7   | 7    | 9,9,10       | 0.18 | 0           | 10,12,14    | 0.65 | 0           |
| 7   | MAN  | aA    | 8   | 7    | 11,11,12     | 0.79 | 1 (9%)      | 15,15,17    | 1.18 | 2 (13%)     |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 7   | NAG  | aA    | 9   | 7    | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.65 | 0        |
| 8   | NAG  | aB    | 1   | 5,8  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.69 | 1 (5%)   |
| 8   | XYP  | aB    | 10  | 8    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.73 | 1 (10%)  |
| 8   | MAN  | aB    | 11  | 8    | 11,11,12     | 0.76 | 1 (9%)   | 15,15,17    | 1.04 | 1 (6%)   |
| 8   | NAG  | aB    | 12  | 8    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.81 | 0        |
| 8   | BMA  | aB    | 13  | 8    | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.72 | 1 (6%)   |
| 8   | XYP  | aB    | 14  | 8    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.66 | 0        |
| 8   | XYP  | aB    | 15  | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.61 | 0        |
| 8   | MAN  | aB    | 16  | 8    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.08 | 2 (13%)  |
| 8   | NAG  | aB    | 2   | 8    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.74 | 0        |
| 8   | BMA  | aB    | 3   | 8    | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.93 | 1 (6%)   |
| 8   | MAN  | aB    | 4   | 8    | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.13 | 2 (13%)  |
| 8   | MAN  | aB    | 5   | 8    | 11,11,12     | 0.59 | 0        | 15,15,17    | 1.48 | 3 (20%)  |
| 8   | NAG  | aB    | 6   | 8    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.48 | 0        |
| 8   | MAN  | aB    | 7   | 8    | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.04 | 2 (13%)  |
| 8   | XYP  | aB    | 8   | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.66 | 0        |
| 8   | BMA  | aB    | 9   | 8    | 11,11,12     | 0.28 | 0        | 15,15,17    | 1.35 | 2 (13%)  |
| 9   | NAG  | aC    | 1   | 5,9  | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.78 | 0        |
| 9   | XYP  | aC    | 10  | 9    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.68 | 0        |
| 9   | BGC  | aC    | 11  | 9    | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.59 | 0        |
| 9   | MAN  | aC    | 12  | 23,9 | 11,11,12     | 0.88 | 1 (9%)   | 15,15,17    | 1.28 | 2 (13%)  |
| 9   | NAG  | aC    | 13  | 9    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 9   | XYP  | aC    | 14  | 9    | 9,9,10       | 1.78 | 3 (33%)  | 10,12,14    | 1.90 | 3 (30%)  |
| 9   | MAN  | aC    | 15  | 9    | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.21 | 3 (20%)  |
| 9   | MAN  | aC    | 16  | 9    | 11,11,12     | 0.80 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 9   | NAG  | aC    | 2   | 9    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.78 | 0        |
| 9   | BMA  | aC    | 3   | 9    | 11,11,12     | 0.27 | 0        | 15,15,17    | 0.61 | 0        |
| 9   | MAN  | aC    | 4   | 9    | 11,11,12     | 0.94 | 1 (9%)   | 15,15,17    | 1.20 | 1 (6%)   |
| 9   | MAN  | aC    | 5   | 9    | 11,11,12     | 0.91 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 9   | NAG  | aC    | 6   | 9    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 9   | MAN  | aC    | 7   | 9    | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.34 | 3 (20%)  |
| 9   | BMA  | aC    | 8   | 9    | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.80 | 0        |
| 9   | XYP  | aC    | 9   | 9    | 9,9,10       | 0.15 | 0        | 10,12,14    | 0.59 | 0        |
| 10  | NAG  | aD    | 1   | 10,5 | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.61 | 0        |
| 10  | NAG  | aD    | 2   | 10   | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.78 | 0        |
| 10  | BMA  | aD    | 3   | 10   | 11,11,12     | 0.21 | 0        | 15,15,17    | 0.91 | 1 (6%)   |
| 10  | MAN  | aD    | 4   | 10   | 11,11,12     | 0.91 | 1 (9%)   | 15,15,17    | 1.16 | 1 (6%)   |
| 10  | MAN  | aD    | 5   | 10   | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 10  | MAN  | aD    | 6   | 10    | 11,11,12     | 0.83 | 0        | 15,15,17    | 1.13 | 2 (13%)  |
| 10  | MAN  | aD    | 7   | 10    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.29 | 3 (20%)  |
| 10  | MAN  | aD    | 8   | 10    | 11,11,12     | 0.91 | 1 (9%)   | 15,15,17    | 1.17 | 2 (13%)  |
| 10  | MAN  | aD    | 9   | 10    | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.31 | 2 (13%)  |
| 11  | NAG  | aE    | 1   | 5,11  | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.67 | 0        |
| 11  | MAN  | aE    | 10  | 23,11 | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 0.93 | 1 (6%)   |
| 11  | NAG  | aE    | 11  | 11    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.89 | 0        |
| 11  | XYP  | aE    | 12  | 11    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.67 | 0        |
| 11  | XYP  | aE    | 13  | 11    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.62 | 0        |
| 11  | BMA  | aE    | 14  | 11    | 11,11,12     | 0.88 | 1 (9%)   | 15,15,17    | 1.15 | 2 (13%)  |
| 11  | MAN  | aE    | 15  | 11    | 11,11,12     | 0.76 | 0        | 15,15,17    | 0.99 | 1 (6%)   |
| 11  | NAG  | aE    | 2   | 11    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.76 | 0        |
| 11  | BMA  | aE    | 3   | 11    | 11,11,12     | 0.36 | 0        | 15,15,17    | 0.95 | 0        |
| 11  | MAN  | aE    | 4   | 11    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.03 | 1 (6%)   |
| 11  | MAN  | aE    | 5   | 11    | 11,11,12     | 0.60 | 0        | 15,15,17    | 1.56 | 3 (20%)  |
| 11  | XYP  | aE    | 6   | 11    | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.70 | 0        |
| 11  | XYP  | aE    | 7   | 11    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.60 | 0        |
| 11  | XYP  | aE    | 8   | 11    | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.64 | 0        |
| 11  | NAG  | aE    | 9   | 11    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.75 | 0        |
| 7   | NAG  | aF    | 1   | 5,7   | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 7   | MAN  | aF    | 10  | 23,7  | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.01 | 1 (6%)   |
| 7   | NAG  | aF    | 11  | 7     | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.83 | 1 (5%)   |
| 7   | XYP  | aF    | 12  | 7     | 9,9,10       | 1.86 | 3 (33%)  | 10,12,14    | 0.92 | 1 (10%)  |
| 7   | MAN  | aF    | 13  | 7     | 11,11,12     | 0.60 | 0        | 15,15,17    | 1.08 | 2 (13%)  |
| 7   | MAN  | aF    | 14  | 7     | 11,11,12     | 0.81 | 0        | 15,15,17    | 1.19 | 2 (13%)  |
| 7   | NAG  | aF    | 2   | 7     | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.81 | 1 (5%)   |
| 7   | BMA  | aF    | 3   | 7     | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.81 | 1 (6%)   |
| 7   | MAN  | aF    | 4   | 7     | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 1.15 | 1 (6%)   |
| 7   | MAN  | aF    | 5   | 7     | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.44 | 3 (20%)  |
| 7   | XYP  | aF    | 6   | 7     | 9,9,10       | 0.19 | 0        | 10,12,14    | 1.00 | 1 (10%)  |
| 7   | XYP  | aF    | 7   | 7     | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.72 | 1 (10%)  |
| 7   | MAN  | aF    | 8   | 7     | 11,11,12     | 0.81 | 1 (9%)   | 15,15,17    | 1.00 | 2 (13%)  |
| 7   | NAG  | aF    | 9   | 7     | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.72 | 0        |
| 8   | NAG  | aG    | 1   | 5,8   | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.79 | 0        |
| 8   | XYP  | aG    | 10  | 8     | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.65 | 0        |
| 8   | MAN  | aG    | 11  | 8     | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.25 | 1 (6%)   |
| 8   | NAG  | aG    | 12  | 8     | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.75 | 0        |
| 8   | BMA  | aG    | 13  | 8     | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.65 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | XYP  | aG    | 14  | 8    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.68 | 0        |
| 8   | XYP  | aG    | 15  | 8    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.58 | 0        |
| 8   | MAN  | aG    | 16  | 8    | 11,11,12     | 0.86 | 1 (9%)   | 15,15,17    | 1.03 | 1 (6%)   |
| 8   | NAG  | aG    | 2   | 8    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.92 | 1 (5%)   |
| 8   | BMA  | aG    | 3   | 8    | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.91 | 0        |
| 8   | MAN  | aG    | 4   | 8    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 8   | MAN  | aG    | 5   | 8    | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.53 | 3 (20%)  |
| 8   | NAG  | aG    | 6   | 8    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.49 | 0        |
| 8   | MAN  | aG    | 7   | 8    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 8   | XYP  | aG    | 8   | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.63 | 0        |
| 8   | BMA  | aG    | 9   | 8    | 11,11,12     | 0.27 | 0        | 15,15,17    | 1.30 | 3 (20%)  |
| 9   | NAG  | aH    | 1   | 5,9  | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.79 | 0        |
| 9   | XYP  | aH    | 10  | 9    | 9,9,10       | 0.13 | 0        | 10,12,14    | 0.73 | 1 (10%)  |
| 9   | BGC  | aH    | 11  | 9    | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.56 | 0        |
| 9   | MAN  | aH    | 12  | 9    | 11,11,12     | 1.07 | 1 (9%)   | 15,15,17    | 1.27 | 3 (20%)  |
| 9   | NAG  | aH    | 13  | 9    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.67 | 0        |
| 9   | XYP  | aH    | 14  | 9    | 9,9,10       | 1.94 | 4 (44%)  | 10,12,14    | 0.86 | 1 (10%)  |
| 9   | MAN  | aH    | 15  | 9    | 11,11,12     | 0.54 | 0        | 15,15,17    | 1.26 | 3 (20%)  |
| 9   | MAN  | aH    | 16  | 9    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 0.89 | 1 (6%)   |
| 9   | NAG  | aH    | 2   | 9    | 14,14,15     | 0.34 | 0        | 17,19,21    | 1.04 | 1 (5%)   |
| 9   | BMA  | aH    | 3   | 9    | 11,11,12     | 0.26 | 0        | 15,15,17    | 0.66 | 0        |
| 9   | MAN  | aH    | 4   | 9    | 11,11,12     | 1.43 | 1 (9%)   | 15,15,17    | 1.32 | 3 (20%)  |
| 9   | MAN  | aH    | 5   | 9    | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 1.18 | 2 (13%)  |
| 9   | NAG  | aH    | 6   | 9    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.80 | 1 (5%)   |
| 9   | MAN  | aH    | 7   | 9    | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.30 | 3 (20%)  |
| 9   | BMA  | aH    | 8   | 9    | 11,11,12     | 0.23 | 0        | 15,15,17    | 0.95 | 0        |
| 9   | XYP  | aH    | 9   | 9    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.67 | 0        |
| 10  | NAG  | aI    | 1   | 10,5 | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.73 | 0        |
| 10  | NAG  | aI    | 2   | 10   | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.75 | 0        |
| 10  | BMA  | aI    | 3   | 10   | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.79 | 0        |
| 10  | MAN  | aI    | 4   | 10   | 11,11,12     | 0.83 | 1 (9%)   | 15,15,17    | 1.26 | 2 (13%)  |
| 10  | MAN  | aI    | 5   | 10   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.09 | 2 (13%)  |
| 10  | MAN  | aI    | 6   | 10   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.17 | 1 (6%)   |
| 10  | MAN  | aI    | 7   | 10   | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.31 | 3 (20%)  |
| 10  | MAN  | aI    | 8   | 10   | 11,11,12     | 0.86 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 10  | MAN  | aI    | 9   | 10   | 11,11,12     | 0.81 | 0        | 15,15,17    | 1.25 | 2 (13%)  |
| 11  | NAG  | aJ    | 1   | 5,11 | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.75 | 0        |
| 11  | MAN  | aJ    | 10  | 11   | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.09 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | NAG  | aJ    | 11  | 11   | 14,14,15     | 0.27 | 0        | 17,19,21    | 0.72 | 0        |
| 11  | XYP  | aJ    | 12  | 11   | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.61 | 0        |
| 11  | XYP  | aJ    | 13  | 11   | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.67 | 0        |
| 11  | BMA  | aJ    | 14  | 11   | 11,11,12     | 0.94 | 1 (9%)   | 15,15,17    | 0.99 | 2 (13%)  |
| 11  | MAN  | aJ    | 15  | 11   | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.03 | 1 (6%)   |
| 11  | NAG  | aJ    | 2   | 11   | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.62 | 0        |
| 11  | BMA  | aJ    | 3   | 11   | 11,11,12     | 0.33 | 0        | 15,15,17    | 0.92 | 1 (6%)   |
| 11  | MAN  | aJ    | 4   | 11   | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.08 | 2 (13%)  |
| 11  | MAN  | aJ    | 5   | 11   | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.42 | 2 (13%)  |
| 11  | XYP  | aJ    | 6   | 11   | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.62 | 0        |
| 11  | XYP  | aJ    | 7   | 11   | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.58 | 0        |
| 11  | XYP  | aJ    | 8   | 11   | 9,9,10       | 0.21 | 0        | 10,12,14    | 0.62 | 0        |
| 11  | NAG  | aJ    | 9   | 11   | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.75 | 0        |
| 7   | NAG  | aK    | 1   | 5,7  | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.72 | 0        |
| 7   | MAN  | aK    | 10  | 23,7 | 11,11,12     | 0.60 | 0        | 15,15,17    | 1.28 | 2 (13%)  |
| 7   | NAG  | aK    | 11  | 7    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.84 | 1 (5%)   |
| 7   | XYP  | aK    | 12  | 7    | 9,9,10       | 1.93 | 3 (33%)  | 10,12,14    | 1.13 | 1 (10%)  |
| 7   | MAN  | aK    | 13  | 7    | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.04 | 2 (13%)  |
| 7   | MAN  | aK    | 14  | 7    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.08 | 2 (13%)  |
| 7   | NAG  | aK    | 2   | 7    | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.80 | 1 (5%)   |
| 7   | BMA  | aK    | 3   | 7    | 11,11,12     | 0.19 | 0        | 15,15,17    | 0.72 | 0        |
| 7   | MAN  | aK    | 4   | 7    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.08 | 1 (6%)   |
| 7   | MAN  | aK    | 5   | 7    | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.26 | 2 (13%)  |
| 7   | XYP  | aK    | 6   | 7    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.94 | 0        |
| 7   | XYP  | aK    | 7   | 7    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.79 | 1 (10%)  |
| 7   | MAN  | aK    | 8   | 7    | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.17 | 3 (20%)  |
| 7   | NAG  | aK    | 9   | 7    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.72 | 0        |
| 8   | NAG  | aL    | 1   | 5,8  | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.73 | 0        |
| 8   | XYP  | aL    | 10  | 8    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.73 | 1 (10%)  |
| 8   | MAN  | aL    | 11  | 23,8 | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.21 | 2 (13%)  |
| 8   | NAG  | aL    | 12  | 8    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.84 | 0        |
| 8   | BMA  | aL    | 13  | 8    | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.65 | 0        |
| 8   | XYP  | aL    | 14  | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.68 | 0        |
| 8   | XYP  | aL    | 15  | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.60 | 0        |
| 8   | MAN  | aL    | 16  | 8    | 11,11,12     | 0.73 | 1 (9%)   | 15,15,17    | 0.98 | 1 (6%)   |
| 8   | NAG  | aL    | 2   | 8    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.59 | 0        |
| 8   | BMA  | aL    | 3   | 8    | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.97 | 1 (6%)   |
| 8   | MAN  | aL    | 4   | 8    | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.31 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 8   | MAN  | aL    | 5   | 8    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.46 | 2 (13%)  |
| 8   | NAG  | aL    | 6   | 8    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.71 | 0        |
| 8   | MAN  | aL    | 7   | 8    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.36 | 3 (20%)  |
| 8   | XYP  | aL    | 8   | 8    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.61 | 0        |
| 8   | BMA  | aL    | 9   | 8    | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.84 | 0        |
| 9   | NAG  | aM    | 1   | 5,9  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.68 | 0        |
| 9   | XYP  | aM    | 10  | 9    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.62 | 0        |
| 9   | BGC  | aM    | 11  | 9    | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.56 | 0        |
| 9   | MAN  | aM    | 12  | 23,9 | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.19 | 2 (13%)  |
| 9   | NAG  | aM    | 13  | 9    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.67 | 0        |
| 9   | XYP  | aM    | 14  | 9    | 9,9,10       | 1.85 | 3 (33%)  | 10,12,14    | 1.02 | 1 (10%)  |
| 9   | MAN  | aM    | 15  | 9    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 9   | MAN  | aM    | 16  | 9    | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 0.83 | 0        |
| 9   | NAG  | aM    | 2   | 9    | 14,14,15     | 0.26 | 0        | 17,19,21    | 0.77 | 0        |
| 9   | BMA  | aM    | 3   | 9    | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.62 | 0        |
| 9   | MAN  | aM    | 4   | 9    | 11,11,12     | 0.87 | 0        | 15,15,17    | 1.23 | 1 (6%)   |
| 9   | MAN  | aM    | 5   | 9    | 11,11,12     | 1.10 | 1 (9%)   | 15,15,17    | 1.25 | 3 (20%)  |
| 9   | NAG  | aM    | 6   | 9    | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.52 | 0        |
| 9   | MAN  | aM    | 7   | 9    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.30 | 3 (20%)  |
| 9   | BMA  | aM    | 8   | 9    | 11,11,12     | 0.23 | 0        | 15,15,17    | 0.61 | 0        |
| 9   | XYP  | aM    | 9   | 9    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.51 | 0        |
| 10  | NAG  | aN    | 1   | 10,5 | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.64 | 0        |
| 10  | NAG  | aN    | 2   | 10   | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.91 | 0        |
| 10  | BMA  | aN    | 3   | 10   | 11,11,12     | 0.23 | 0        | 15,15,17    | 0.72 | 0        |
| 10  | MAN  | aN    | 4   | 10   | 11,11,12     | 0.88 | 0        | 15,15,17    | 1.06 | 2 (13%)  |
| 10  | MAN  | aN    | 5   | 10   | 11,11,12     | 0.89 | 1 (9%)   | 15,15,17    | 1.10 | 2 (13%)  |
| 10  | MAN  | aN    | 6   | 10   | 11,11,12     | 0.91 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 10  | MAN  | aN    | 7   | 10   | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.34 | 2 (13%)  |
| 10  | MAN  | aN    | 8   | 10   | 11,11,12     | 0.88 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 10  | MAN  | aN    | 9   | 10   | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.21 | 2 (13%)  |
| 11  | NAG  | aO    | 1   | 5,11 | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.80 | 0        |
| 11  | MAN  | aO    | 10  | 11   | 11,11,12     | 0.75 | 0        | 15,15,17    | 0.87 | 0        |
| 11  | NAG  | aO    | 11  | 11   | 14,14,15     | 0.31 | 0        | 17,19,21    | 1.07 | 1 (5%)   |
| 11  | XYP  | aO    | 12  | 11   | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.62 | 0        |
| 11  | XYP  | aO    | 13  | 11   | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.62 | 0        |
| 11  | BMA  | aO    | 14  | 11   | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.05 | 1 (6%)   |
| 11  | MAN  | aO    | 15  | 11   | 11,11,12     | 0.90 | 1 (9%)   | 15,15,17    | 1.08 | 2 (13%)  |
| 11  | NAG  | aO    | 2   | 11   | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.62 | 0        |
| 11  | BMA  | aO    | 3   | 11   | 11,11,12     | 0.29 | 0        | 15,15,17    | 0.98 | 0        |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | MAN  | aO    | 4   | 11    | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 1.05 | 1 (6%)   |
| 11  | MAN  | aO    | 5   | 11    | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.37 | 2 (13%)  |
| 11  | XYP  | aO    | 6   | 11    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.63 | 0        |
| 11  | XYP  | aO    | 7   | 11    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.61 | 0        |
| 11  | XYP  | aO    | 8   | 11    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.67 | 0        |
| 11  | NAG  | aO    | 9   | 11    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.64 | 0        |
| 12  | NAG  | bA    | 1   | 6,12  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.73 | 0        |
| 12  | NAG  | bA    | 2   | 12    | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.92 | 0        |
| 12  | BMA  | bA    | 3   | 12    | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.79 | 1 (6%)   |
| 12  | MAN  | bA    | 4   | 12    | 11,11,12     | 0.89 | 1 (9%)   | 15,15,17    | 1.11 | 1 (6%)   |
| 12  | MAN  | bA    | 5   | 12    | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.30 | 3 (20%)  |
| 12  | MAN  | bA    | 6   | 12    | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.12 | 1 (6%)   |
| 12  | MAN  | bA    | 7   | 12    | 11,11,12     | 0.73 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 12  | MAN  | bA    | 8   | 12    | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 12  | MAN  | bA    | 9   | 12    | 11,11,12     | 0.73 | 0        | 15,15,17    | 0.98 | 0        |
| 13  | NAG  | bB    | 1   | 13,6  | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.50 | 0        |
| 13  | NAG  | bB    | 2   | 13    | 14,14,15     | 0.28 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 13  | BMA  | bB    | 3   | 13    | 11,11,12     | 0.18 | 0        | 15,15,17    | 0.57 | 0        |
| 13  | MAN  | bB    | 4   | 13    | 11,11,12     | 0.78 | 0        | 15,15,17    | 1.24 | 2 (13%)  |
| 13  | MAN  | bB    | 5   | 13    | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.26 | 3 (20%)  |
| 14  | NAG  | bC    | 1   | 6,14  | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.61 | 0        |
| 14  | MAN  | bC    | 10  | 14    | 11,11,12     | 0.79 | 1 (9%)   | 15,15,17    | 0.91 | 1 (6%)   |
| 14  | NAG  | bC    | 2   | 14    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.69 | 0        |
| 14  | BMA  | bC    | 3   | 14    | 11,11,12     | 0.23 | 0        | 15,15,17    | 1.13 | 2 (13%)  |
| 14  | MAN  | bC    | 4   | 14    | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 1.27 | 2 (13%)  |
| 14  | MAN  | bC    | 5   | 14    | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.35 | 2 (13%)  |
| 14  | XYP  | bC    | 6   | 14    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.59 | 0        |
| 14  | XYS  | bC    | 7   | 14    | 9,9,10       | 1.93 | 3 (33%)  | 10,12,14    | 0.91 | 1 (10%)  |
| 14  | MAN  | bC    | 8   | 14,23 | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 0.92 | 1 (6%)   |
| 14  | BMA  | bC    | 9   | 14    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.07 | 2 (13%)  |
| 12  | NAG  | bD    | 1   | 6,12  | 14,14,15     | 0.48 | 0        | 17,19,21    | 0.65 | 0        |
| 12  | NAG  | bD    | 2   | 12    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.84 | 0        |
| 12  | BMA  | bD    | 3   | 12    | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.79 | 1 (6%)   |
| 12  | MAN  | bD    | 4   | 12    | 11,11,12     | 0.96 | 1 (9%)   | 15,15,17    | 1.17 | 1 (6%)   |
| 12  | MAN  | bD    | 5   | 12    | 11,11,12     | 1.03 | 1 (9%)   | 15,15,17    | 1.23 | 2 (13%)  |
| 12  | MAN  | bD    | 6   | 12    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.19 | 2 (13%)  |
| 12  | MAN  | bD    | 7   | 12    | 11,11,12     | 0.79 | 1 (9%)   | 15,15,17    | 1.05 | 2 (13%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | MAN  | bD    | 8   | 12    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 12  | MAN  | bD    | 9   | 12    | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.12 | 1 (6%)   |
| 13  | NAG  | bE    | 1   | 13,6  | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.54 | 0        |
| 13  | NAG  | bE    | 2   | 13    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.68 | 0        |
| 13  | BMA  | bE    | 3   | 13    | 11,11,12     | 0.20 | 0        | 15,15,17    | 0.61 | 0        |
| 13  | MAN  | bE    | 4   | 13    | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.18 | 2 (13%)  |
| 13  | MAN  | bE    | 5   | 13    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.18 | 2 (13%)  |
| 14  | NAG  | bF    | 1   | 6,14  | 14,14,15     | 0.43 | 0        | 17,19,21    | 0.63 | 0        |
| 14  | MAN  | bF    | 10  | 14    | 11,11,12     | 0.90 | 1 (9%)   | 15,15,17    | 0.95 | 1 (6%)   |
| 14  | NAG  | bF    | 2   | 14    | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.91 | 1 (5%)   |
| 14  | BMA  | bF    | 3   | 14    | 11,11,12     | 0.35 | 0        | 15,15,17    | 0.80 | 0        |
| 14  | MAN  | bF    | 4   | 14    | 11,11,12     | 0.83 | 1 (9%)   | 15,15,17    | 1.05 | 2 (13%)  |
| 14  | MAN  | bF    | 5   | 14    | 11,11,12     | 0.89 | 0        | 15,15,17    | 1.46 | 2 (13%)  |
| 14  | XYP  | bF    | 6   | 14    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.61 | 0        |
| 14  | XYS  | bF    | 7   | 14    | 9,9,10       | 1.93 | 3 (33%)  | 10,12,14    | 1.03 | 1 (10%)  |
| 14  | MAN  | bF    | 8   | 14,23 | 11,11,12     | 0.79 | 1 (9%)   | 15,15,17    | 1.04 | 2 (13%)  |
| 14  | BMA  | bF    | 9   | 14    | 11,11,12     | 1.09 | 1 (9%)   | 15,15,17    | 1.03 | 2 (13%)  |
| 12  | NAG  | bG    | 1   | 6,12  | 14,14,15     | 0.45 | 0        | 17,19,21    | 0.75 | 0        |
| 12  | NAG  | bG    | 2   | 12    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.81 | 0        |
| 12  | BMA  | bG    | 3   | 12    | 11,11,12     | 0.37 | 0        | 15,15,17    | 0.69 | 0        |
| 12  | MAN  | bG    | 4   | 12    | 11,11,12     | 0.81 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 12  | MAN  | bG    | 5   | 12    | 11,11,12     | 0.87 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 12  | MAN  | bG    | 6   | 12    | 11,11,12     | 0.79 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 12  | MAN  | bG    | 7   | 12    | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.13 | 2 (13%)  |
| 12  | MAN  | bG    | 8   | 12    | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.16 | 2 (13%)  |
| 12  | MAN  | bG    | 9   | 12    | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 0.93 | 1 (6%)   |
| 13  | NAG  | bH    | 1   | 13,6  | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.60 | 1 (5%)   |
| 13  | NAG  | bH    | 2   | 13    | 14,14,15     | 0.29 | 0        | 17,19,21    | 0.79 | 1 (5%)   |
| 13  | BMA  | bH    | 3   | 13    | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.49 | 0        |
| 13  | MAN  | bH    | 4   | 13    | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 13  | MAN  | bH    | 5   | 13    | 11,11,12     | 0.62 | 0        | 15,15,17    | 1.48 | 3 (20%)  |
| 14  | NAG  | bI    | 1   | 6,14  | 14,14,15     | 0.42 | 0        | 17,19,21    | 0.67 | 0        |
| 14  | MAN  | bI    | 10  | 14    | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.07 | 2 (13%)  |
| 14  | NAG  | bI    | 2   | 14    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.98 | 1 (5%)   |
| 14  | BMA  | bI    | 3   | 14    | 11,11,12     | 0.42 | 0        | 15,15,17    | 1.30 | 1 (6%)   |
| 14  | MAN  | bI    | 4   | 14    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.32 | 2 (13%)  |
| 14  | MAN  | bI    | 5   | 14    | 11,11,12     | 0.53 | 0        | 15,15,17    | 1.51 | 3 (20%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 14  | XYP  | bI    | 6   | 14    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.58 | 0        |
| 14  | XYS  | bI    | 7   | 14    | 9,9,10       | 1.92 | 3 (33%)  | 10,12,14    | 1.37 | 1 (10%)  |
| 14  | MAN  | bI    | 8   | 14,23 | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 0.92 | 1 (6%)   |
| 14  | BMA  | bI    | 9   | 14    | 11,11,12     | 1.01 | 1 (9%)   | 15,15,17    | 0.99 | 1 (6%)   |
| 15  | XYP  | cA    | 1   | 15    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.63 | 0        |
| 15  | MAN  | cA    | 2   | 15    | 11,11,12     | 0.80 | 0        | 15,15,17    | 1.49 | 2 (13%)  |
| 15  | MAN  | cA    | 3   | 15    | 11,11,12     | 0.96 | 1 (9%)   | 15,15,17    | 1.09 | 2 (13%)  |
| 15  | MAN  | cA    | 4   | 15    | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.39 | 3 (20%)  |
| 15  | XYP  | cB    | 1   | 15    | 9,9,10       | 0.21 | 0        | 10,12,14    | 0.71 | 0        |
| 15  | MAN  | cB    | 2   | 15    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.09 | 1 (6%)   |
| 15  | MAN  | cB    | 3   | 15    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.16 | 2 (13%)  |
| 15  | MAN  | cB    | 4   | 15    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.35 | 2 (13%)  |
| 15  | XYP  | cC    | 1   | 15    | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.63 | 0        |
| 15  | MAN  | cC    | 2   | 15    | 11,11,12     | 0.78 | 0        | 15,15,17    | 1.43 | 2 (13%)  |
| 15  | MAN  | cC    | 3   | 15    | 11,11,12     | 0.85 | 0        | 15,15,17    | 1.24 | 2 (13%)  |
| 15  | MAN  | cC    | 4   | 15    | 11,11,12     | 0.78 | 0        | 15,15,17    | 1.44 | 3 (20%)  |
| 16  | XYP  | dA    | 1   | 16    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.74 | 0        |
| 16  | MAN  | dA    | 2   | 16    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.27 | 3 (20%)  |
| 16  | MAN  | dA    | 3   | 16    | 11,11,12     | 1.21 | 1 (9%)   | 15,15,17    | 1.25 | 2 (13%)  |
| 16  | MAN  | dA    | 4   | 16    | 11,11,12     | 1.08 | 1 (9%)   | 15,15,17    | 1.27 | 2 (13%)  |
| 16  | MAN  | dA    | 5   | 16    | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.22 | 2 (13%)  |
| 16  | MAN  | dA    | 6   | 16    | 11,11,12     | 0.94 | 1 (9%)   | 15,15,17    | 1.05 | 2 (13%)  |
| 16  | MAN  | dA    | 7   | 16    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.27 | 3 (20%)  |
| 16  | XYP  | dB    | 1   | 16    | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.67 | 0        |
| 16  | MAN  | dB    | 2   | 16    | 11,11,12     | 0.96 | 1 (9%)   | 15,15,17    | 1.18 | 2 (13%)  |
| 16  | MAN  | dB    | 3   | 16    | 11,11,12     | 1.06 | 1 (9%)   | 15,15,17    | 1.31 | 2 (13%)  |
| 16  | MAN  | dB    | 4   | 16    | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.31 | 2 (13%)  |
| 16  | MAN  | dB    | 5   | 16    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 16  | MAN  | dB    | 6   | 16    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.01 | 1 (6%)   |
| 16  | MAN  | dB    | 7   | 16    | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 16  | XYP  | dC    | 1   | 16    | 9,9,10       | 0.15 | 0        | 10,12,14    | 0.65 | 0        |
| 16  | MAN  | dC    | 2   | 16    | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 16  | MAN  | dC    | 3   | 16    | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 1.24 | 2 (13%)  |
| 16  | MAN  | dC    | 4   | 16    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.35 | 3 (20%)  |
| 16  | MAN  | dC    | 5   | 16    | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 16  | MAN  | dC    | 6   | 16    | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 1.12 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | MAN  | dC    | 7   | 16   | 11,11,12     | 0.86 | 1 (9%)   | 15,15,17    | 1.07 | 1 (6%)   |
| 17  | NAG  | eA    | 1   | 17,1 | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.81 | 1 (5%)   |
| 17  | MAN  | eA    | 10  | 17   | 11,11,12     | 0.77 | 1 (9%)   | 15,15,17    | 1.13 | 2 (13%)  |
| 17  | MAN  | eA    | 11  | 17   | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.20 | 2 (13%)  |
| 17  | NAG  | eA    | 2   | 17   | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.72 | 0        |
| 17  | BMA  | eA    | 3   | 17   | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.72 | 0        |
| 17  | MAN  | eA    | 4   | 17   | 11,11,12     | 0.57 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 17  | MAN  | eA    | 5   | 17   | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.02 | 1 (6%)   |
| 17  | MAN  | eA    | 6   | 17   | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.00 | 2 (13%)  |
| 17  | MAN  | eA    | 7   | 17   | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.30 | 3 (20%)  |
| 17  | MAN  | eA    | 8   | 17   | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 1.03 | 2 (13%)  |
| 17  | MAN  | eA    | 9   | 17   | 11,11,12     | 0.83 | 0        | 15,15,17    | 1.20 | 2 (13%)  |
| 18  | NAG  | eB    | 1   | 18,1 | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.80 | 1 (5%)   |
| 18  | MAN  | eB    | 10  | 18   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.10 | 2 (13%)  |
| 18  | NAG  | eB    | 11  | 18   | 14,14,15     | 0.33 | 0        | 17,19,21    | 1.12 | 2 (11%)  |
| 18  | XYP  | eB    | 12  | 18   | 9,9,10       | 0.18 | 0        | 10,12,14    | 0.66 | 0        |
| 18  | XYP  | eB    | 13  | 18   | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.63 | 0        |
| 18  | MAN  | eB    | 14  | 18   | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.14 | 2 (13%)  |
| 18  | NAG  | eB    | 2   | 18   | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.76 | 0        |
| 18  | BMA  | eB    | 3   | 18   | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.69 | 0        |
| 18  | MAN  | eB    | 4   | 18   | 11,11,12     | 0.98 | 0        | 15,15,17    | 1.25 | 1 (6%)   |
| 18  | MAN  | eB    | 5   | 18   | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 1.19 | 2 (13%)  |
| 18  | XYP  | eB    | 6   | 18   | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.65 | 0        |
| 18  | XYS  | eB    | 7   | 18   | 9,9,10       | 1.85 | 3 (33%)  | 10,12,14    | 0.93 | 1 (10%)  |
| 18  | BGC  | eB    | 8   | 18   | 11,11,12     | 0.42 | 0        | 15,15,17    | 0.67 | 0        |
| 18  | NAG  | eB    | 9   | 18   | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.61 | 0        |
| 17  | NAG  | eC    | 1   | 17,1 | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.62 | 0        |
| 17  | MAN  | eC    | 10  | 17   | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.19 | 3 (20%)  |
| 17  | MAN  | eC    | 11  | 17   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.08 | 1 (6%)   |
| 17  | NAG  | eC    | 2   | 17   | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.71 | 0        |
| 17  | BMA  | eC    | 3   | 17   | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.92 | 1 (6%)   |
| 17  | MAN  | eC    | 4   | 17   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.13 | 2 (13%)  |
| 17  | MAN  | eC    | 5   | 17   | 11,11,12     | 0.97 | 1 (9%)   | 15,15,17    | 1.02 | 2 (13%)  |
| 17  | MAN  | eC    | 6   | 17   | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.37 | 3 (20%)  |
| 17  | MAN  | eC    | 7   | 17   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.33 | 3 (20%)  |
| 17  | MAN  | eC    | 8   | 17   | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 1.07 | 2 (13%)  |
| 17  | MAN  | eC    | 9   | 17   | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.19 | 2 (13%)  |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | NAG  | eD    | 1   | 18,1  | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.59 | 0        |
| 18  | MAN  | eD    | 10  | 18,23 | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.15 | 2 (13%)  |
| 18  | NAG  | eD    | 11  | 18    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.93 | 1 (5%)   |
| 18  | XYP  | eD    | 12  | 18    | 9,9,10       | 0.15 | 0        | 10,12,14    | 0.64 | 0        |
| 18  | XYP  | eD    | 13  | 18    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.61 | 0        |
| 18  | MAN  | eD    | 14  | 18    | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.08 | 2 (13%)  |
| 18  | NAG  | eD    | 2   | 18    | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.68 | 0        |
| 18  | BMA  | eD    | 3   | 18    | 11,11,12     | 0.21 | 0        | 15,15,17    | 0.77 | 0        |
| 18  | MAN  | eD    | 4   | 18    | 11,11,12     | 0.89 | 0        | 15,15,17    | 1.52 | 3 (20%)  |
| 18  | MAN  | eD    | 5   | 18    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.32 | 3 (20%)  |
| 18  | XYP  | eD    | 6   | 18    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.61 | 0        |
| 18  | XYS  | eD    | 7   | 18    | 9,9,10       | 1.84 | 3 (33%)  | 10,12,14    | 0.99 | 0        |
| 18  | BGC  | eD    | 8   | 18    | 11,11,12     | 0.23 | 0        | 15,15,17    | 0.73 | 1 (6%)   |
| 18  | NAG  | eD    | 9   | 18    | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.56 | 0        |
| 17  | NAG  | eE    | 1   | 17,1  | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.65 | 0        |
| 17  | MAN  | eE    | 10  | 17    | 11,11,12     | 0.80 | 0        | 15,15,17    | 1.05 | 1 (6%)   |
| 17  | MAN  | eE    | 11  | 17    | 11,11,12     | 0.80 | 1 (9%)   | 15,15,17    | 1.06 | 2 (13%)  |
| 17  | NAG  | eE    | 2   | 17    | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.74 | 0        |
| 17  | BMA  | eE    | 3   | 17    | 11,11,12     | 0.29 | 0        | 15,15,17    | 0.89 | 1 (6%)   |
| 17  | MAN  | eE    | 4   | 17    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 17  | MAN  | eE    | 5   | 17    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.10 | 2 (13%)  |
| 17  | MAN  | eE    | 6   | 17    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.09 | 2 (13%)  |
| 17  | MAN  | eE    | 7   | 17    | 11,11,12     | 0.71 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 17  | MAN  | eE    | 8   | 17    | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 0.99 | 1 (6%)   |
| 17  | MAN  | eE    | 9   | 17    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.15 | 2 (13%)  |
| 18  | NAG  | eF    | 1   | 18,1  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.62 | 0        |
| 18  | MAN  | eF    | 10  | 18    | 11,11,12     | 0.66 | 0        | 15,15,17    | 1.14 | 2 (13%)  |
| 18  | NAG  | eF    | 11  | 18    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.92 | 1 (5%)   |
| 18  | XYP  | eF    | 12  | 18    | 9,9,10       | 0.19 | 0        | 10,12,14    | 0.64 | 0        |
| 18  | XYP  | eF    | 13  | 18    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.63 | 0        |
| 18  | MAN  | eF    | 14  | 18    | 11,11,12     | 0.81 | 1 (9%)   | 15,15,17    | 1.03 | 2 (13%)  |
| 18  | NAG  | eF    | 2   | 18    | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.56 | 0        |
| 18  | BMA  | eF    | 3   | 18    | 11,11,12     | 0.20 | 0        | 15,15,17    | 0.68 | 0        |
| 18  | MAN  | eF    | 4   | 18    | 11,11,12     | 0.91 | 0        | 15,15,17    | 1.54 | 3 (20%)  |
| 18  | MAN  | eF    | 5   | 18    | 11,11,12     | 1.02 | 1 (9%)   | 15,15,17    | 1.23 | 2 (13%)  |
| 18  | XYP  | eF    | 6   | 18    | 9,9,10       | 0.16 | 0        | 10,12,14    | 0.60 | 0        |
| 18  | XYS  | eF    | 7   | 18    | 9,9,10       | 1.93 | 3 (33%)  | 10,12,14    | 0.77 | 0        |
| 18  | BGC  | eF    | 8   | 18    | 11,11,12     | 0.29 | 0        | 15,15,17    | 0.72 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 18  | NAG  | eF    | 9   | 18   | 14,14,15     | 0.30 | 0        | 17,19,21    | 0.58 | 0        |
| 19  | NAG  | fB    | 1   | 19,2 | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.75 | 1 (5%)   |
| 19  | MAN  | fB    | 10  | 19   | 11,11,12     | 0.76 | 1 (9%)   | 15,15,17    | 0.98 | 2 (13%)  |
| 19  | NAG  | fB    | 2   | 19   | 14,14,15     | 0.31 | 0        | 17,19,21    | 1.24 | 1 (5%)   |
| 19  | BMA  | fB    | 3   | 19   | 11,11,12     | 0.25 | 0        | 15,15,17    | 0.73 | 0        |
| 19  | MAN  | fB    | 4   | 19   | 11,11,12     | 0.97 | 1 (9%)   | 15,15,17    | 1.08 | 2 (13%)  |
| 19  | MAN  | fB    | 5   | 19   | 11,11,12     | 0.79 | 0        | 15,15,17    | 1.07 | 1 (6%)   |
| 19  | MAN  | fB    | 6   | 19   | 11,11,12     | 0.78 | 0        | 15,15,17    | 1.20 | 2 (13%)  |
| 19  | MAN  | fB    | 7   | 19   | 11,11,12     | 0.81 | 1 (9%)   | 15,15,17    | 1.33 | 2 (13%)  |
| 19  | MAN  | fB    | 8   | 19   | 11,11,12     | 0.83 | 1 (9%)   | 15,15,17    | 1.25 | 3 (20%)  |
| 19  | MAN  | fB    | 9   | 19   | 11,11,12     | 0.81 | 1 (9%)   | 15,15,17    | 1.07 | 2 (13%)  |
| 17  | NAG  | fC    | 1   | 17,2 | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.75 | 0        |
| 17  | MAN  | fC    | 10  | 17   | 11,11,12     | 0.91 | 1 (9%)   | 15,15,17    | 1.07 | 2 (13%)  |
| 17  | MAN  | fC    | 11  | 17   | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.05 | 2 (13%)  |
| 17  | NAG  | fC    | 2   | 17   | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.81 | 0        |
| 17  | BMA  | fC    | 3   | 17   | 11,11,12     | 0.26 | 0        | 15,15,17    | 0.96 | 0        |
| 17  | MAN  | fC    | 4   | 17   | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.46 | 2 (13%)  |
| 17  | MAN  | fC    | 5   | 17   | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.10 | 1 (6%)   |
| 17  | MAN  | fC    | 6   | 17   | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.02 | 2 (13%)  |
| 17  | MAN  | fC    | 7   | 17   | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.08 | 1 (6%)   |
| 17  | MAN  | fC    | 8   | 17   | 11,11,12     | 0.79 | 1 (9%)   | 15,15,17    | 1.12 | 2 (13%)  |
| 17  | MAN  | fC    | 9   | 17   | 11,11,12     | 0.61 | 0        | 15,15,17    | 1.26 | 3 (20%)  |
| 17  | NAG  | fD    | 1   | 17,2 | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.81 | 0        |
| 17  | MAN  | fD    | 10  | 17   | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.21 | 2 (13%)  |
| 17  | MAN  | fD    | 11  | 17   | 11,11,12     | 0.96 | 1 (9%)   | 15,15,17    | 1.25 | 1 (6%)   |
| 17  | NAG  | fD    | 2   | 17   | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.57 | 0        |
| 17  | BMA  | fD    | 3   | 17   | 11,11,12     | 0.27 | 0        | 15,15,17    | 0.75 | 0        |
| 17  | MAN  | fD    | 4   | 17   | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.32 | 3 (20%)  |
| 17  | MAN  | fD    | 5   | 17   | 11,11,12     | 0.76 | 0        | 15,15,17    | 0.96 | 1 (6%)   |
| 17  | MAN  | fD    | 6   | 17   | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.25 | 1 (6%)   |
| 17  | MAN  | fD    | 7   | 17   | 11,11,12     | 1.08 | 2 (18%)  | 15,15,17    | 1.11 | 1 (6%)   |
| 17  | MAN  | fD    | 8   | 17   | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.20 | 2 (13%)  |
| 17  | MAN  | fD    | 9   | 17   | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.16 | 3 (20%)  |
| 19  | NAG  | fE    | 1   | 19,2 | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.57 | 0        |
| 19  | MAN  | fE    | 10  | 19   | 11,11,12     | 0.79 | 1 (9%)   | 15,15,17    | 0.97 | 1 (6%)   |
| 19  | NAG  | fE    | 2   | 19   | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.58 | 0        |
| 19  | BMA  | fE    | 3   | 19   | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.82 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | MAN  | fE    | 4   | 19   | 11,11,12     | 0.86 | 0        | 15,15,17    | 1.31 | 3 (20%)  |
| 19  | MAN  | fE    | 5   | 19   | 11,11,12     | 0.89 | 1 (9%)   | 15,15,17    | 1.22 | 2 (13%)  |
| 19  | MAN  | fE    | 6   | 19   | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 1.02 | 2 (13%)  |
| 19  | MAN  | fE    | 7   | 19   | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.25 | 2 (13%)  |
| 19  | MAN  | fE    | 8   | 19   | 11,11,12     | 0.81 | 1 (9%)   | 15,15,17    | 1.26 | 2 (13%)  |
| 19  | MAN  | fE    | 9   | 19   | 11,11,12     | 0.80 | 0        | 15,15,17    | 1.01 | 1 (6%)   |
| 20  | NAG  | fF    | 1   | 20,2 | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.68 | 0        |
| 20  | NAG  | fF    | 10  | 20   | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.75 | 0        |
| 20  | XYS  | fF    | 11  | 20   | 9,9,10       | 2.09 | 4 (44%)  | 10,12,14    | 1.04 | 1 (10%)  |
| 20  | XYP  | fF    | 12  | 20   | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.65 | 0        |
| 20  | MAN  | fF    | 13  | 20   | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.03 | 2 (13%)  |
| 20  | MAN  | fF    | 14  | 20   | 11,11,12     | 0.73 | 0        | 15,15,17    | 0.92 | 0        |
| 20  | NAG  | fF    | 2   | 20   | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.89 | 0        |
| 20  | BMA  | fF    | 3   | 20   | 11,11,12     | 0.16 | 0        | 15,15,17    | 0.88 | 0        |
| 20  | MAN  | fF    | 4   | 20   | 11,11,12     | 0.77 | 0        | 15,15,17    | 1.18 | 2 (13%)  |
| 20  | MAN  | fF    | 5   | 20   | 11,11,12     | 0.69 | 0        | 15,15,17    | 1.22 | 2 (13%)  |
| 20  | XYP  | fF    | 6   | 20   | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.64 | 0        |
| 20  | XYS  | fF    | 7   | 20   | 9,9,10       | 1.89 | 3 (33%)  | 10,12,14    | 1.47 | 1 (10%)  |
| 20  | NAG  | fF    | 8   | 20   | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.48 | 0        |
| 20  | MAN  | fF    | 9   | 20   | 11,11,12     | 0.80 | 1 (9%)   | 15,15,17    | 1.02 | 1 (6%)   |
| 19  | NAG  | fG    | 1   | 19,2 | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.73 | 1 (5%)   |
| 19  | MAN  | fG    | 10  | 19   | 11,11,12     | 0.77 | 1 (9%)   | 15,15,17    | 1.04 | 1 (6%)   |
| 19  | NAG  | fG    | 2   | 19   | 14,14,15     | 0.33 | 0        | 17,19,21    | 0.93 | 0        |
| 19  | BMA  | fG    | 3   | 19   | 11,11,12     | 0.29 | 0        | 15,15,17    | 0.72 | 0        |
| 19  | MAN  | fG    | 4   | 19   | 11,11,12     | 0.91 | 1 (9%)   | 15,15,17    | 1.16 | 1 (6%)   |
| 19  | MAN  | fG    | 5   | 19   | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.29 | 1 (6%)   |
| 19  | MAN  | fG    | 6   | 19   | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.23 | 2 (13%)  |
| 19  | MAN  | fG    | 7   | 19   | 11,11,12     | 0.89 | 1 (9%)   | 15,15,17    | 1.32 | 3 (20%)  |
| 19  | MAN  | fG    | 8   | 19   | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 1.14 | 2 (13%)  |
| 19  | MAN  | fG    | 9   | 19   | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.03 | 1 (6%)   |
| 17  | NAG  | fH    | 1   | 17,2 | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.93 | 0        |
| 17  | MAN  | fH    | 10  | 17   | 11,11,12     | 0.90 | 1 (9%)   | 15,15,17    | 1.10 | 1 (6%)   |
| 17  | MAN  | fH    | 11  | 17   | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.09 | 2 (13%)  |
| 17  | NAG  | fH    | 2   | 17   | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.53 | 0        |
| 17  | BMA  | fH    | 3   | 17   | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.75 | 0        |
| 17  | MAN  | fH    | 4   | 17   | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.24 | 2 (13%)  |
| 17  | MAN  | fH    | 5   | 17   | 11,11,12     | 1.12 | 1 (9%)   | 15,15,17    | 1.01 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 17  | MAN  | fH    | 6   | 17   | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.19 | 2 (13%)  |
| 17  | MAN  | fH    | 7   | 17   | 11,11,12     | 1.03 | 1 (9%)   | 15,15,17    | 1.11 | 1 (6%)   |
| 17  | MAN  | fH    | 8   | 17   | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.10 | 2 (13%)  |
| 17  | MAN  | fH    | 9   | 17   | 11,11,12     | 0.56 | 0        | 15,15,17    | 1.21 | 2 (13%)  |
| 17  | NAG  | fI    | 1   | 17,2 | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.79 | 0        |
| 17  | MAN  | fI    | 10  | 17   | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.15 | 2 (13%)  |
| 17  | MAN  | fI    | 11  | 17   | 11,11,12     | 1.04 | 1 (9%)   | 15,15,17    | 1.04 | 2 (13%)  |
| 17  | NAG  | fI    | 2   | 17   | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.48 | 0        |
| 17  | BMA  | fI    | 3   | 17   | 11,11,12     | 0.28 | 0        | 15,15,17    | 0.79 | 0        |
| 17  | MAN  | fI    | 4   | 17   | 11,11,12     | 0.72 | 0        | 15,15,17    | 1.24 | 3 (20%)  |
| 17  | MAN  | fI    | 5   | 17   | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.04 | 1 (6%)   |
| 17  | MAN  | fI    | 6   | 17   | 11,11,12     | 0.64 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 17  | MAN  | fI    | 7   | 17   | 11,11,12     | 0.90 | 0        | 15,15,17    | 1.44 | 2 (13%)  |
| 17  | MAN  | fI    | 8   | 17   | 11,11,12     | 0.86 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 17  | MAN  | fI    | 9   | 17   | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.04 | 2 (13%)  |
| 19  | NAG  | fJ    | 1   | 19,2 | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.67 | 1 (5%)   |
| 19  | MAN  | fJ    | 10  | 19   | 11,11,12     | 0.92 | 1 (9%)   | 15,15,17    | 0.99 | 1 (6%)   |
| 19  | NAG  | fJ    | 2   | 19   | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.51 | 0        |
| 19  | BMA  | fJ    | 3   | 19   | 11,11,12     | 0.24 | 0        | 15,15,17    | 0.80 | 0        |
| 19  | MAN  | fJ    | 4   | 19   | 11,11,12     | 0.85 | 0        | 15,15,17    | 1.31 | 2 (13%)  |
| 19  | MAN  | fJ    | 5   | 19   | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 1.12 | 2 (13%)  |
| 19  | MAN  | fJ    | 6   | 19   | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.14 | 2 (13%)  |
| 19  | MAN  | fJ    | 7   | 19   | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.28 | 1 (6%)   |
| 19  | MAN  | fJ    | 8   | 19   | 11,11,12     | 0.90 | 1 (9%)   | 15,15,17    | 1.12 | 1 (6%)   |
| 19  | MAN  | fJ    | 9   | 19   | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.09 | 1 (6%)   |
| 20  | NAG  | fK    | 1   | 20,2 | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.78 | 0        |
| 20  | NAG  | fK    | 10  | 20   | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 20  | XYS  | fK    | 11  | 20   | 9,9,10       | 1.99 | 4 (44%)  | 10,12,14    | 1.59 | 1 (10%)  |
| 20  | XYP  | fK    | 12  | 20   | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.66 | 0        |
| 20  | MAN  | fK    | 13  | 20   | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.15 | 2 (13%)  |
| 20  | MAN  | fK    | 14  | 20   | 11,11,12     | 0.66 | 0        | 15,15,17    | 0.98 | 2 (13%)  |
| 20  | NAG  | fK    | 2   | 20   | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.97 | 1 (5%)   |
| 20  | BMA  | fK    | 3   | 20   | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.75 | 0        |
| 20  | MAN  | fK    | 4   | 20   | 11,11,12     | 0.89 | 1 (9%)   | 15,15,17    | 1.12 | 2 (13%)  |
| 20  | MAN  | fK    | 5   | 20   | 11,11,12     | 0.55 | 0        | 15,15,17    | 1.16 | 1 (6%)   |
| 20  | XYP  | fK    | 6   | 20   | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.64 | 0        |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 20  | XYX  | fK    | 7   | 20    | 9,9,10       | 1.94 | 3 (33%)  | 10,12,14    | 1.20 | 1 (10%)  |
| 20  | NAG  | fK    | 8   | 20    | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.59 | 0        |
| 20  | MAN  | fK    | 9   | 20,23 | 11,11,12     | 0.70 | 0        | 15,15,17    | 1.11 | 1 (6%)   |
| 19  | NAG  | fL    | 1   | 19,2  | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.57 | 0        |
| 19  | MAN  | fL    | 10  | 19    | 11,11,12     | 0.75 | 0        | 15,15,17    | 1.00 | 2 (13%)  |
| 19  | NAG  | fL    | 2   | 19    | 14,14,15     | 0.34 | 0        | 17,19,21    | 1.16 | 1 (5%)   |
| 19  | BMA  | fL    | 3   | 19    | 11,11,12     | 0.21 | 0        | 15,15,17    | 0.62 | 0        |
| 19  | MAN  | fL    | 4   | 19    | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.33 | 2 (13%)  |
| 19  | MAN  | fL    | 5   | 19    | 11,11,12     | 0.94 | 1 (9%)   | 15,15,17    | 1.19 | 1 (6%)   |
| 19  | MAN  | fL    | 6   | 19    | 11,11,12     | 0.80 | 0        | 15,15,17    | 1.34 | 2 (13%)  |
| 19  | MAN  | fL    | 7   | 19    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.44 | 3 (20%)  |
| 19  | MAN  | fL    | 8   | 19    | 11,11,12     | 1.14 | 1 (9%)   | 15,15,17    | 1.19 | 2 (13%)  |
| 19  | MAN  | fL    | 9   | 19    | 11,11,12     | 0.83 | 1 (9%)   | 15,15,17    | 1.03 | 1 (6%)   |
| 17  | NAG  | fM    | 1   | 17,2  | 14,14,15     | 0.55 | 0        | 17,19,21    | 0.83 | 0        |
| 17  | MAN  | fM    | 10  | 17    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.45 | 3 (20%)  |
| 17  | MAN  | fM    | 11  | 17    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.17 | 2 (13%)  |
| 17  | NAG  | fM    | 2   | 17    | 14,14,15     | 0.37 | 0        | 17,19,21    | 1.03 | 1 (5%)   |
| 17  | BMA  | fM    | 3   | 17    | 11,11,12     | 0.29 | 0        | 15,15,17    | 0.85 | 0        |
| 17  | MAN  | fM    | 4   | 17    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.48 | 3 (20%)  |
| 17  | MAN  | fM    | 5   | 17    | 11,11,12     | 0.85 | 1 (9%)   | 15,15,17    | 1.16 | 1 (6%)   |
| 17  | MAN  | fM    | 6   | 17    | 11,11,12     | 0.58 | 0        | 15,15,17    | 1.26 | 2 (13%)  |
| 17  | MAN  | fM    | 7   | 17    | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 17  | MAN  | fM    | 8   | 17    | 11,11,12     | 0.86 | 1 (9%)   | 15,15,17    | 1.13 | 1 (6%)   |
| 17  | MAN  | fM    | 9   | 17    | 11,11,12     | 0.73 | 0        | 15,15,17    | 1.12 | 2 (13%)  |
| 17  | NAG  | fN    | 1   | 17,2  | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.86 | 0        |
| 17  | MAN  | fN    | 10  | 17    | 11,11,12     | 0.76 | 0        | 15,15,17    | 1.20 | 2 (13%)  |
| 17  | MAN  | fN    | 11  | 17    | 11,11,12     | 0.95 | 1 (9%)   | 15,15,17    | 1.23 | 2 (13%)  |
| 17  | NAG  | fN    | 2   | 17    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.67 | 0        |
| 17  | BMA  | fN    | 3   | 17    | 11,11,12     | 0.27 | 0        | 15,15,17    | 0.85 | 1 (6%)   |
| 17  | MAN  | fN    | 4   | 17    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.21 | 2 (13%)  |
| 17  | MAN  | fN    | 5   | 17    | 11,11,12     | 0.78 | 0        | 15,15,17    | 1.05 | 2 (13%)  |
| 17  | MAN  | fN    | 6   | 17    | 11,11,12     | 0.68 | 0        | 15,15,17    | 1.19 | 1 (6%)   |
| 17  | MAN  | fN    | 7   | 17    | 11,11,12     | 0.86 | 0        | 15,15,17    | 1.30 | 2 (13%)  |
| 17  | MAN  | fN    | 8   | 17    | 11,11,12     | 0.85 | 0        | 15,15,17    | 1.27 | 2 (13%)  |
| 17  | MAN  | fN    | 9   | 17    | 11,11,12     | 0.75 | 1 (9%)   | 15,15,17    | 1.08 | 2 (13%)  |
| 19  | NAG  | fO    | 1   | 19,2  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.48 | 0        |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 19  | MAN  | fO    | 10  | 19    | 11,11,12     | 0.83 | 1 (9%)   | 15,15,17    | 1.04 | 2 (13%)  |
| 19  | NAG  | fO    | 2   | 19    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.65 | 0        |
| 19  | BMA  | fO    | 3   | 19    | 11,11,12     | 0.32 | 0        | 15,15,17    | 0.73 | 0        |
| 19  | MAN  | fO    | 4   | 19    | 11,11,12     | 0.90 | 0        | 15,15,17    | 1.29 | 3 (20%)  |
| 19  | MAN  | fO    | 5   | 19    | 11,11,12     | 1.05 | 1 (9%)   | 15,15,17    | 1.11 | 2 (13%)  |
| 19  | MAN  | fO    | 6   | 19    | 11,11,12     | 0.91 | 1 (9%)   | 15,15,17    | 1.15 | 2 (13%)  |
| 19  | MAN  | fO    | 7   | 19    | 11,11,12     | 0.82 | 1 (9%)   | 15,15,17    | 1.27 | 2 (13%)  |
| 19  | MAN  | fO    | 8   | 19    | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.18 | 2 (13%)  |
| 19  | MAN  | fO    | 9   | 19    | 11,11,12     | 0.84 | 1 (9%)   | 15,15,17    | 1.02 | 1 (6%)   |
| 20  | NAG  | fP    | 1   | 20,2  | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.67 | 0        |
| 20  | NAG  | fP    | 10  | 20    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.80 | 0        |
| 20  | XYS  | fP    | 11  | 20    | 9,9,10       | 1.99 | 3 (33%)  | 10,12,14    | 1.27 | 2 (20%)  |
| 20  | XYP  | fP    | 12  | 20    | 9,9,10       | 0.20 | 0        | 10,12,14    | 0.66 | 0        |
| 20  | MAN  | fP    | 13  | 20    | 11,11,12     | 0.77 | 1 (9%)   | 15,15,17    | 1.07 | 1 (6%)   |
| 20  | MAN  | fP    | 14  | 20    | 11,11,12     | 0.71 | 1 (9%)   | 15,15,17    | 0.99 | 1 (6%)   |
| 20  | NAG  | fP    | 2   | 20    | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.79 | 1 (5%)   |
| 20  | BMA  | fP    | 3   | 20    | 11,11,12     | 0.22 | 0        | 15,15,17    | 0.87 | 0        |
| 20  | MAN  | fP    | 4   | 20    | 11,11,12     | 0.74 | 0        | 15,15,17    | 1.17 | 3 (20%)  |
| 20  | MAN  | fP    | 5   | 20    | 11,11,12     | 0.63 | 0        | 15,15,17    | 1.33 | 3 (20%)  |
| 20  | XYP  | fP    | 6   | 20    | 9,9,10       | 0.17 | 0        | 10,12,14    | 0.62 | 0        |
| 20  | XYS  | fP    | 7   | 20    | 9,9,10       | 1.90 | 3 (33%)  | 10,12,14    | 1.12 | 1 (10%)  |
| 20  | NAG  | fP    | 8   | 20    | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.70 | 0        |
| 20  | MAN  | fP    | 9   | 20,23 | 11,11,12     | 0.67 | 0        | 15,15,17    | 1.09 | 1 (6%)   |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | NAG  | aA    | 1   | 5,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | MAN  | aA    | 10  | 23,7 | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aA    | 11  | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | XYP  | aA    | 12  | 7    | -       | -         | 0/1/1/1 |
| 7   | MAN  | aA    | 13  | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aA    | 14  | 7    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aA    | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | aA    | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aA    | 4   | 7    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 7   | MAN  | aA    | 5   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | XYP  | aA    | 6   | 7    | -       | -         | 0/1/1/1 |
| 7   | XYP  | aA    | 7   | 7    | -       | -         | 0/1/1/1 |
| 7   | MAN  | aA    | 8   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aA    | 9   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | aB    | 1   | 5,8  | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | XYP  | aB    | 10  | 8    | -       | -         | 0/1/1/1 |
| 8   | MAN  | aB    | 11  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aB    | 12  | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aB    | 13  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aB    | 14  | 8    | -       | -         | 0/1/1/1 |
| 8   | XYP  | aB    | 15  | 8    | -       | -         | 0/1/1/1 |
| 8   | MAN  | aB    | 16  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aB    | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aB    | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aB    | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aB    | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aB    | 6   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | MAN  | aB    | 7   | 8    | -       | 2/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aB    | 8   | 8    | -       | -         | 0/1/1/1 |
| 8   | BMA  | aB    | 9   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aC    | 1   | 5,9  | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aC    | 10  | 9    | -       | -         | 0/1/1/1 |
| 9   | BGC  | aC    | 11  | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aC    | 12  | 23,9 | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aC    | 13  | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aC    | 14  | 9    | -       | -         | 0/1/1/1 |
| 9   | MAN  | aC    | 15  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aC    | 16  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aC    | 2   | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | BMA  | aC    | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aC    | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aC    | 5   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aC    | 6   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | MAN  | aC    | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | BMA  | aC    | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | XYP  | aC    | 9   | 9    | -       | -         | 0/1/1/1 |
| 10  | NAG  | aD    | 1   | 10,5 | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | NAG  | aD    | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | BMA  | aD    | 3   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aD    | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 10  | MAN  | aD    | 5   | 10    | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aD    | 6   | 10    | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aD    | 7   | 10    | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aD    | 8   | 10    | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aD    | 9   | 10    | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aE    | 1   | 5,11  | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | MAN  | aE    | 10  | 23,11 | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aE    | 11  | 11    | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | XYP  | aE    | 12  | 11    | -       | -         | 0/1/1/1 |
| 11  | XYP  | aE    | 13  | 11    | -       | -         | 0/1/1/1 |
| 11  | BMA  | aE    | 14  | 11    | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aE    | 15  | 11    | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aE    | 2   | 11    | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | aE    | 3   | 11    | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aE    | 4   | 11    | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aE    | 5   | 11    | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | XYP  | aE    | 6   | 11    | -       | -         | 0/1/1/1 |
| 11  | XYP  | aE    | 7   | 11    | -       | -         | 0/1/1/1 |
| 11  | XYP  | aE    | 8   | 11    | -       | -         | 0/1/1/1 |
| 11  | NAG  | aE    | 9   | 11    | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | aF    | 1   | 5,7   | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | MAN  | aF    | 10  | 23,7  | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aF    | 11  | 7     | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | XYP  | aF    | 12  | 7     | -       | -         | 0/1/1/1 |
| 7   | MAN  | aF    | 13  | 7     | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aF    | 14  | 7     | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aF    | 2   | 7     | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | aF    | 3   | 7     | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aF    | 4   | 7     | -       | 1/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aF    | 5   | 7     | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | XYP  | aF    | 6   | 7     | -       | -         | 0/1/1/1 |
| 7   | XYP  | aF    | 7   | 7     | -       | -         | 0/1/1/1 |
| 7   | MAN  | aF    | 8   | 7     | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aF    | 9   | 7     | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | aG    | 1   | 5,8   | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | XYP  | aG    | 10  | 8     | -       | -         | 0/1/1/1 |
| 8   | MAN  | aG    | 11  | 8     | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aG    | 12  | 8     | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aG    | 13  | 8     | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aG    | 14  | 8     | -       | -         | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 8   | XYP  | aG    | 15  | 8    | -       | -         | 0/1/1/1 |
| 8   | MAN  | aG    | 16  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aG    | 2   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aG    | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aG    | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aG    | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aG    | 6   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | MAN  | aG    | 7   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aG    | 8   | 8    | -       | -         | 0/1/1/1 |
| 8   | BMA  | aG    | 9   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aH    | 1   | 5,9  | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aH    | 10  | 9    | -       | -         | 0/1/1/1 |
| 9   | BGC  | aH    | 11  | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aH    | 12  | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aH    | 13  | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aH    | 14  | 9    | -       | -         | 0/1/1/1 |
| 9   | MAN  | aH    | 15  | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aH    | 16  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aH    | 2   | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | BMA  | aH    | 3   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aH    | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aH    | 5   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aH    | 6   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | MAN  | aH    | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | BMA  | aH    | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | XYP  | aH    | 9   | 9    | -       | -         | 0/1/1/1 |
| 10  | NAG  | aI    | 1   | 10,5 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | aI    | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | BMA  | aI    | 3   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 5   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 6   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 7   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 8   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aI    | 9   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aJ    | 1   | 5,11 | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | MAN  | aJ    | 10  | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aJ    | 11  | 11   | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | XYP  | aJ    | 12  | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aJ    | 13  | 11   | -       | -         | 0/1/1/1 |
| 11  | BMA  | aJ    | 14  | 11   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | MAN  | aJ    | 15  | 11   | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aJ    | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | aJ    | 3   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aJ    | 4   | 11   | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aJ    | 5   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | XYP  | aJ    | 6   | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aJ    | 7   | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aJ    | 8   | 11   | -       | -         | 0/1/1/1 |
| 11  | NAG  | aJ    | 9   | 11   | -       | 2/6/23/26 | 0/1/1/1 |
| 7   | NAG  | aK    | 1   | 5,7  | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | MAN  | aK    | 10  | 23,7 | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aK    | 11  | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | XYP  | aK    | 12  | 7    | -       | -         | 0/1/1/1 |
| 7   | MAN  | aK    | 13  | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aK    | 14  | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aK    | 2   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 7   | BMA  | aK    | 3   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aK    | 4   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | MAN  | aK    | 5   | 7    | -       | 2/2/19/22 | 0/1/1/1 |
| 7   | XYP  | aK    | 6   | 7    | -       | -         | 0/1/1/1 |
| 7   | XYP  | aK    | 7   | 7    | -       | -         | 0/1/1/1 |
| 7   | MAN  | aK    | 8   | 7    | -       | 0/2/19/22 | 0/1/1/1 |
| 7   | NAG  | aK    | 9   | 7    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | NAG  | aL    | 1   | 5,8  | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | XYP  | aL    | 10  | 8    | -       | -         | 0/1/1/1 |
| 8   | MAN  | aL    | 11  | 23,8 | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aL    | 12  | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aL    | 13  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aL    | 14  | 8    | -       | -         | 0/1/1/1 |
| 8   | XYP  | aL    | 15  | 8    | -       | -         | 0/1/1/1 |
| 8   | MAN  | aL    | 16  | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aL    | 2   | 8    | -       | 2/6/23/26 | 0/1/1/1 |
| 8   | BMA  | aL    | 3   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aL    | 4   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | MAN  | aL    | 5   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | NAG  | aL    | 6   | 8    | -       | 0/6/23/26 | 0/1/1/1 |
| 8   | MAN  | aL    | 7   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 8   | XYP  | aL    | 8   | 8    | -       | -         | 0/1/1/1 |
| 8   | BMA  | aL    | 9   | 8    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aM    | 1   | 5,9  | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aM    | 10  | 9    | -       | -         | 0/1/1/1 |
| 9   | BGC  | aM    | 11  | 9    | -       | 1/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 9   | MAN  | aM    | 12  | 23,9 | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aM    | 13  | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | XYP  | aM    | 14  | 9    | -       | -         | 0/1/1/1 |
| 9   | MAN  | aM    | 15  | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aM    | 16  | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aM    | 2   | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | BMA  | aM    | 3   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aM    | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | MAN  | aM    | 5   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | NAG  | aM    | 6   | 9    | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | MAN  | aM    | 7   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | BMA  | aM    | 8   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | XYP  | aM    | 9   | 9    | -       | -         | 0/1/1/1 |
| 10  | NAG  | aN    | 1   | 10,5 | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | NAG  | aN    | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 10  | BMA  | aN    | 3   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 4   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 5   | 10   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 6   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 7   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 8   | 10   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | MAN  | aN    | 9   | 10   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aO    | 1   | 5,11 | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | MAN  | aO    | 10  | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aO    | 11  | 11   | -       | 3/6/23/26 | 0/1/1/1 |
| 11  | XYP  | aO    | 12  | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aO    | 13  | 11   | -       | -         | 0/1/1/1 |
| 11  | BMA  | aO    | 14  | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aO    | 15  | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | NAG  | aO    | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | aO    | 3   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aO    | 4   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | aO    | 5   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | XYP  | aO    | 6   | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aO    | 7   | 11   | -       | -         | 0/1/1/1 |
| 11  | XYP  | aO    | 8   | 11   | -       | -         | 0/1/1/1 |
| 11  | NAG  | aO    | 9   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | NAG  | bA    | 1   | 6,12 | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | NAG  | bA    | 2   | 12   | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | bA    | 3   | 12   | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bA    | 4   | 12   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 12  | MAN  | bA    | 5   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bA    | 6   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bA    | 7   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bA    | 8   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bA    | 9   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 13  | NAG  | bB    | 1   | 13,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | NAG  | bB    | 2   | 13    | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | bB    | 3   | 13    | -       | 1/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bB    | 4   | 13    | -       | 1/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bB    | 5   | 13    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bC    | 1   | 6,14  | -       | 0/6/23/26 | 0/1/1/1 |
| 14  | MAN  | bC    | 10  | 14    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bC    | 2   | 14    | -       | 0/6/23/26 | 0/1/1/1 |
| 14  | BMA  | bC    | 3   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bC    | 4   | 14    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bC    | 5   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | XYP  | bC    | 6   | 14    | -       | -         | 0/1/1/1 |
| 14  | XYS  | bC    | 7   | 14    | -       | -         | 0/1/1/1 |
| 14  | MAN  | bC    | 8   | 14,23 | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | BMA  | bC    | 9   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | NAG  | bD    | 1   | 6,12  | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | NAG  | bD    | 2   | 12    | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | bD    | 3   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 4   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 5   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 6   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 7   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 8   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bD    | 9   | 12    | -       | 2/2/19/22 | 0/1/1/1 |
| 13  | NAG  | bE    | 1   | 13,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | NAG  | bE    | 2   | 13    | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | bE    | 3   | 13    | -       | 1/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bE    | 4   | 13    | -       | 2/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bE    | 5   | 13    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bF    | 1   | 6,14  | -       | 0/6/23/26 | 0/1/1/1 |
| 14  | MAN  | bF    | 10  | 14    | -       | 1/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bF    | 2   | 14    | -       | 0/6/23/26 | 0/1/1/1 |
| 14  | BMA  | bF    | 3   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bF    | 4   | 14    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bF    | 5   | 14    | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 14  | XYP  | bF    | 6   | 14    | -       | -         | 0/1/1/1 |
| 14  | XYS  | bF    | 7   | 14    | -       | -         | 0/1/1/1 |
| 14  | MAN  | bF    | 8   | 14,23 | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | BMA  | bF    | 9   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | NAG  | bG    | 1   | 6,12  | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | NAG  | bG    | 2   | 12    | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | bG    | 3   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 4   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 5   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 6   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 7   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 8   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | MAN  | bG    | 9   | 12    | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | NAG  | bH    | 1   | 13,6  | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | NAG  | bH    | 2   | 13    | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | bH    | 3   | 13    | -       | 2/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bH    | 4   | 13    | -       | 1/2/19/22 | 0/1/1/1 |
| 13  | MAN  | bH    | 5   | 13    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bI    | 1   | 6,14  | -       | 0/6/23/26 | 0/1/1/1 |
| 14  | MAN  | bI    | 10  | 14    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | NAG  | bI    | 2   | 14    | -       | 1/6/23/26 | 0/1/1/1 |
| 14  | BMA  | bI    | 3   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bI    | 4   | 14    | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | bI    | 5   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | XYP  | bI    | 6   | 14    | -       | -         | 0/1/1/1 |
| 14  | XYS  | bI    | 7   | 14    | -       | -         | 0/1/1/1 |
| 14  | MAN  | bI    | 8   | 14,23 | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | BMA  | bI    | 9   | 14    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | XYP  | cA    | 1   | 15    | -       | -         | 0/1/1/1 |
| 15  | MAN  | cA    | 2   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cA    | 3   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cA    | 4   | 15    | -       | 2/2/19/22 | 0/1/1/1 |
| 15  | XYP  | cB    | 1   | 15    | -       | -         | 0/1/1/1 |
| 15  | MAN  | cB    | 2   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cB    | 3   | 15    | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cB    | 4   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | XYP  | cC    | 1   | 15    | -       | -         | 0/1/1/1 |
| 15  | MAN  | cC    | 2   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cC    | 3   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | cC    | 4   | 15    | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | XYP  | dA    | 1   | 16    | -       | -         | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 16  | MAN  | dA    | 2   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dA    | 3   | 16   | -       | 1/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dA    | 4   | 16   | -       | 1/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dA    | 5   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dA    | 6   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dA    | 7   | 16   | -       | 1/2/19/22 | 0/1/1/1 |
| 16  | XYP  | dB    | 1   | 16   | -       | -         | 0/1/1/1 |
| 16  | MAN  | dB    | 2   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dB    | 3   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dB    | 4   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dB    | 5   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dB    | 6   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dB    | 7   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | XYP  | dC    | 1   | 16   | -       | -         | 0/1/1/1 |
| 16  | MAN  | dC    | 2   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dC    | 3   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dC    | 4   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dC    | 5   | 16   | -       | 0/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dC    | 6   | 16   | -       | 2/2/19/22 | 0/1/1/1 |
| 16  | MAN  | dC    | 7   | 16   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | NAG  | eA    | 1   | 17,1 | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | MAN  | eA    | 10  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 11  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | eA    | 2   | 17   | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | eA    | 3   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 4   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 5   | 17   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 6   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 7   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 8   | 17   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eA    | 9   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eB    | 1   | 18,1 | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | MAN  | eB    | 10  | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eB    | 11  | 18   | -       | 3/6/23/26 | 0/1/1/1 |
| 18  | XYP  | eB    | 12  | 18   | -       | -         | 0/1/1/1 |
| 18  | XYP  | eB    | 13  | 18   | -       | -         | 0/1/1/1 |
| 18  | MAN  | eB    | 14  | 18   | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eB    | 2   | 18   | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | BMA  | eB    | 3   | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | MAN  | eB    | 4   | 18   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 18  | MAN  | eB    | 5   | 18    | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | XYP  | eB    | 6   | 18    | -       | -         | 0/1/1/1 |
| 18  | XYS  | eB    | 7   | 18    | -       | -         | 0/1/1/1 |
| 18  | BGC  | eB    | 8   | 18    | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eB    | 9   | 18    | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | NAG  | eC    | 1   | 17,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | MAN  | eC    | 10  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 11  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | eC    | 2   | 17    | -       | 2/6/23/26 | 0/1/1/1 |
| 17  | BMA  | eC    | 3   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 4   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 5   | 17    | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 6   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 7   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 8   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eC    | 9   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eD    | 1   | 18,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | MAN  | eD    | 10  | 18,23 | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eD    | 11  | 18    | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | XYP  | eD    | 12  | 18    | -       | -         | 0/1/1/1 |
| 18  | XYP  | eD    | 13  | 18    | -       | -         | 0/1/1/1 |
| 18  | MAN  | eD    | 14  | 18    | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eD    | 2   | 18    | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | BMA  | eD    | 3   | 18    | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | MAN  | eD    | 4   | 18    | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | MAN  | eD    | 5   | 18    | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | XYP  | eD    | 6   | 18    | -       | -         | 0/1/1/1 |
| 18  | XYS  | eD    | 7   | 18    | -       | -         | 0/1/1/1 |
| 18  | BGC  | eD    | 8   | 18    | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eD    | 9   | 18    | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | NAG  | eE    | 1   | 17,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | MAN  | eE    | 10  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 11  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | eE    | 2   | 17    | -       | 1/6/23/26 | 0/1/1/1 |
| 17  | BMA  | eE    | 3   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 4   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 5   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 6   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 7   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 8   | 17    | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | eE    | 9   | 17    | -       | 1/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 18  | NAG  | eF    | 1   | 18,1 | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | MAN  | eF    | 10  | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eF    | 11  | 18   | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | XYP  | eF    | 12  | 18   | -       | -         | 0/1/1/1 |
| 18  | XYP  | eF    | 13  | 18   | -       | -         | 0/1/1/1 |
| 18  | MAN  | eF    | 14  | 18   | -       | 2/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eF    | 2   | 18   | -       | 0/6/23/26 | 0/1/1/1 |
| 18  | BMA  | eF    | 3   | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | MAN  | eF    | 4   | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | MAN  | eF    | 5   | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | XYP  | eF    | 6   | 18   | -       | -         | 0/1/1/1 |
| 18  | XYS  | eF    | 7   | 18   | -       | -         | 0/1/1/1 |
| 18  | BGC  | eF    | 8   | 18   | -       | 0/2/19/22 | 0/1/1/1 |
| 18  | NAG  | eF    | 9   | 18   | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | NAG  | fB    | 1   | 19,2 | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fB    | 10  | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fB    | 2   | 19   | -       | 1/6/23/26 | 0/1/1/1 |
| 19  | BMA  | fB    | 3   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 4   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 5   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 6   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 7   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 8   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fB    | 9   | 19   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fC    | 1   | 17,2 | -       | 1/6/23/26 | 0/1/1/1 |
| 17  | MAN  | fC    | 10  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 11  | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fC    | 2   | 17   | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fC    | 3   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 4   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 5   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 6   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 7   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 8   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fC    | 9   | 17   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fD    | 1   | 17,2 | -       | 2/6/23/26 | 0/1/1/1 |
| 17  | MAN  | fD    | 10  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 11  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fD    | 2   | 17   | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fD    | 3   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 4   | 17   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 17  | MAN  | fD    | 5   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 6   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 7   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 8   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fD    | 9   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fE    | 1   | 19,2 | -       | 2/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fE    | 10  | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fE    | 2   | 19   | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | BMA  | fE    | 3   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 4   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 5   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 6   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 7   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 8   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fE    | 9   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fF    | 1   | 20,2 | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | NAG  | fF    | 10  | 20   | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | XYS  | fF    | 11  | 20   | -       | -         | 0/1/1/1 |
| 20  | XYP  | fF    | 12  | 20   | -       | -         | 0/1/1/1 |
| 20  | MAN  | fF    | 13  | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fF    | 14  | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fF    | 2   | 20   | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | BMA  | fF    | 3   | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fF    | 4   | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fF    | 5   | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | XYP  | fF    | 6   | 20   | -       | -         | 0/1/1/1 |
| 20  | XYS  | fF    | 7   | 20   | -       | -         | 0/1/1/1 |
| 20  | NAG  | fF    | 8   | 20   | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | MAN  | fF    | 9   | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fG    | 1   | 19,2 | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fG    | 10  | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fG    | 2   | 19   | -       | 3/6/23/26 | 0/1/1/1 |
| 19  | BMA  | fG    | 3   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 4   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 5   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 6   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 7   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 8   | 19   | -       | 1/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fG    | 9   | 19   | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fH    | 1   | 17,2 | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 17  | MAN  | fH    | 10  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 11  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fH    | 2   | 17   | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fH    | 3   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 4   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 5   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 6   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 7   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 8   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fH    | 9   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fI    | 1   | 17,2 | -       | 1/6/23/26 | 0/1/1/1 |
| 17  | MAN  | fI    | 10  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 11  | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fI    | 2   | 17   | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fI    | 3   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 4   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 5   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 6   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 7   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 8   | 17   | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fI    | 9   | 17   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fJ    | 1   | 19,2 | -       | 2/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fJ    | 10  | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fJ    | 2   | 19   | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | BMA  | fJ    | 3   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 4   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 5   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 6   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 7   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 8   | 19   | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fJ    | 9   | 19   | -       | 2/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fK    | 1   | 20,2 | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | NAG  | fK    | 10  | 20   | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | XYS  | fK    | 11  | 20   | -       | -         | 0/1/1/1 |
| 20  | XYP  | fK    | 12  | 20   | -       | -         | 0/1/1/1 |
| 20  | MAN  | fK    | 13  | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fK    | 14  | 20   | -       | 1/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fK    | 2   | 20   | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | BMA  | fK    | 3   | 20   | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fK    | 4   | 20   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 20  | MAN  | fK    | 5   | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | XYP  | fK    | 6   | 20    | -       | -         | 0/1/1/1 |
| 20  | XYS  | fK    | 7   | 20    | -       | -         | 0/1/1/1 |
| 20  | NAG  | fK    | 8   | 20    | -       | 2/6/23/26 | 0/1/1/1 |
| 20  | MAN  | fK    | 9   | 20,23 | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fL    | 1   | 19,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fL    | 10  | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fL    | 2   | 19    | -       | 1/6/23/26 | 0/1/1/1 |
| 19  | BMA  | fL    | 3   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 4   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 5   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 6   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 7   | 19    | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 8   | 19    | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fL    | 9   | 19    | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fM    | 1   | 17,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | MAN  | fM    | 10  | 17    | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 11  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fM    | 2   | 17    | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fM    | 3   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 4   | 17    | -       | 1/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 5   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 6   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 7   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 8   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fM    | 9   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fN    | 1   | 17,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 17  | MAN  | fN    | 10  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 11  | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | NAG  | fN    | 2   | 17    | -       | 0/6/23/26 | 0/1/1/1 |
| 17  | BMA  | fN    | 3   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 4   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 5   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 6   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 7   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 8   | 17    | -       | 0/2/19/22 | 0/1/1/1 |
| 17  | MAN  | fN    | 9   | 17    | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fO    | 1   | 19,2  | -       | 2/6/23/26 | 0/1/1/1 |
| 19  | MAN  | fO    | 10  | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | NAG  | fO    | 2   | 19    | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link  | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|-------|---------|-----------|---------|
| 19  | BMA  | fO    | 3   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 4   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 5   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 6   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 7   | 19    | -       | 1/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 8   | 19    | -       | 2/2/19/22 | 0/1/1/1 |
| 19  | MAN  | fO    | 9   | 19    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fP    | 1   | 20,2  | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | NAG  | fP    | 10  | 20    | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | XYS  | fP    | 11  | 20    | -       | -         | 0/1/1/1 |
| 20  | XYP  | fP    | 12  | 20    | -       | -         | 0/1/1/1 |
| 20  | MAN  | fP    | 13  | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fP    | 14  | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | NAG  | fP    | 2   | 20    | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | BMA  | fP    | 3   | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fP    | 4   | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | MAN  | fP    | 5   | 20    | -       | 0/2/19/22 | 0/1/1/1 |
| 20  | XYP  | fP    | 6   | 20    | -       | -         | 0/1/1/1 |
| 20  | XYS  | fP    | 7   | 20    | -       | -         | 0/1/1/1 |
| 20  | NAG  | fP    | 8   | 20    | -       | 0/6/23/26 | 0/1/1/1 |
| 20  | MAN  | fP    | 9   | 20,23 | -       | 0/2/19/22 | 0/1/1/1 |

The worst 5 of 195 bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 20  | fP    | 11  | XYS  | O5-C1 | 4.13  | 1.50        | 1.42     |
| 20  | fF    | 11  | XYS  | O5-C1 | 4.13  | 1.50        | 1.42     |
| 9   | aH    | 4   | MAN  | O5-C1 | -4.07 | 1.37        | 1.43     |
| 20  | fK    | 11  | XYS  | O5-C1 | 4.03  | 1.50        | 1.42     |
| 14  | bF    | 7   | XYS  | O5-C1 | 3.99  | 1.50        | 1.42     |

The worst 5 of 629 bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 15  | cA    | 2   | MAN  | C1-O5-C5 | 4.65 | 118.49      | 112.19   |
| 17  | fC    | 4   | MAN  | C1-O5-C5 | 4.45 | 118.22      | 112.19   |
| 8   | aG    | 5   | MAN  | C1-O5-C5 | 4.32 | 118.04      | 112.19   |
| 8   | aB    | 5   | MAN  | C1-O5-C5 | 4.25 | 117.95      | 112.19   |
| 17  | fM    | 10  | MAN  | C1-O5-C5 | 4.08 | 117.72      | 112.19   |

There are no chirality outliers.

5 of 241 torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | aE    | 11  | NAG  | C8-C7-N2-C2 |
| 11  | aE    | 11  | NAG  | O7-C7-N2-C2 |
| 11  | aJ    | 11  | NAG  | C3-C2-N2-C7 |
| 11  | aJ    | 11  | NAG  | C8-C7-N2-C2 |
| 11  | aJ    | 11  | NAG  | O7-C7-N2-C2 |

There are no ring outliers.

43 monomers are involved in 34 short contacts:

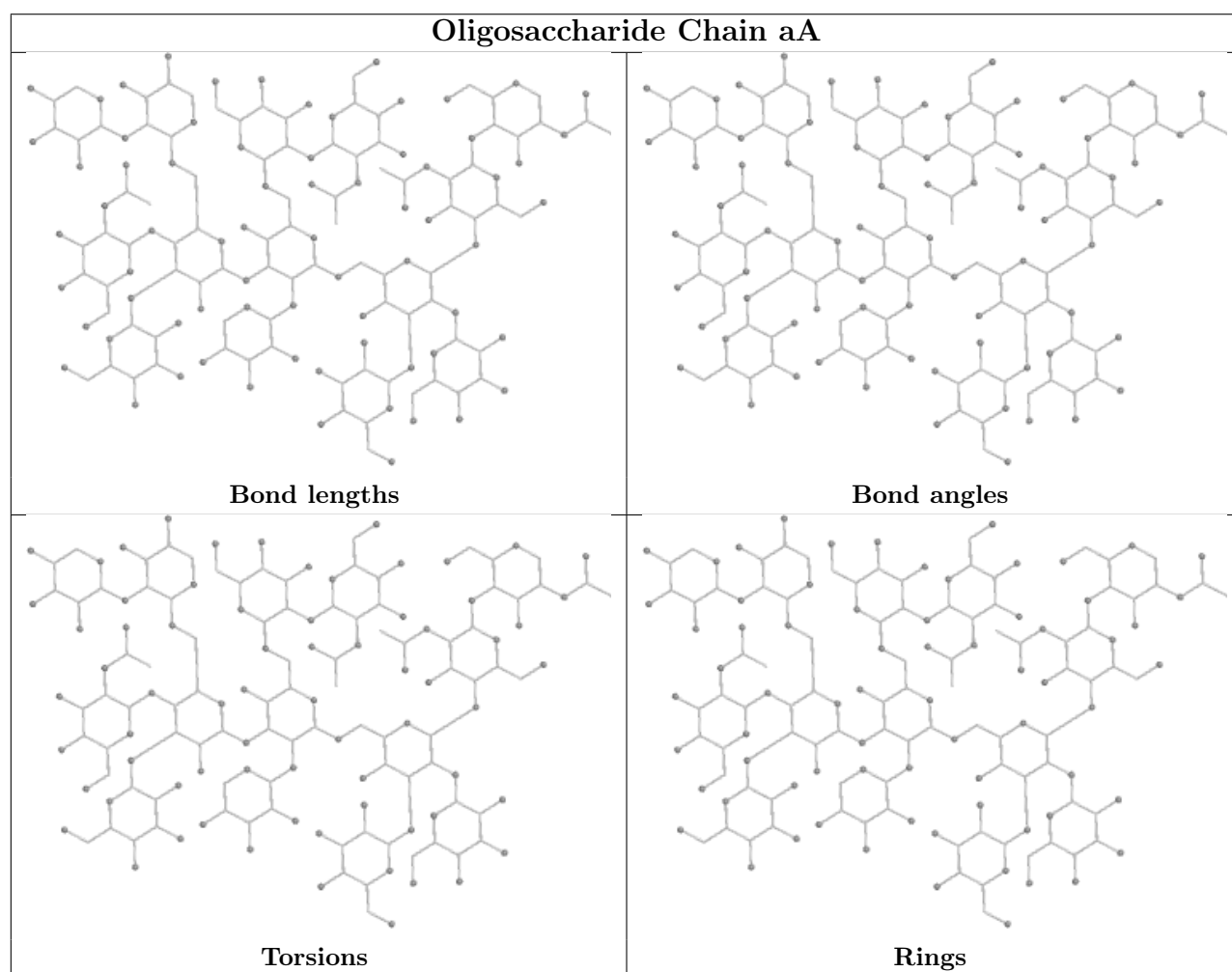
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | aM    | 1   | NAG  | 1       | 0            |
| 8   | aL    | 1   | NAG  | 1       | 0            |
| 20  | fF    | 12  | XYP  | 1       | 0            |
| 11  | aJ    | 1   | NAG  | 1       | 0            |
| 20  | fF    | 10  | NAG  | 1       | 0            |
| 20  | fK    | 9   | MAN  | 1       | 0            |
| 10  | aD    | 8   | MAN  | 1       | 0            |
| 7   | aA    | 8   | MAN  | 1       | 0            |
| 17  | eC    | 11  | MAN  | 2       | 0            |
| 11  | aO    | 7   | XYP  | 1       | 0            |
| 11  | aE    | 6   | XYP  | 1       | 0            |
| 7   | aK    | 8   | MAN  | 1       | 0            |
| 18  | eB    | 8   | BGC  | 1       | 0            |
| 11  | aJ    | 4   | MAN  | 1       | 0            |
| 11  | aO    | 6   | XYP  | 1       | 0            |
| 10  | aN    | 8   | MAN  | 1       | 0            |
| 17  | fN    | 2   | NAG  | 1       | 0            |
| 17  | fM    | 4   | MAN  | 2       | 0            |
| 11  | aE    | 7   | XYP  | 1       | 0            |
| 19  | fO    | 6   | MAN  | 1       | 0            |
| 19  | fE    | 6   | MAN  | 1       | 0            |
| 14  | bF    | 7   | XYS  | 1       | 0            |
| 17  | fI    | 10  | MAN  | 1       | 0            |
| 7   | aF    | 8   | MAN  | 1       | 0            |
| 17  | fM    | 2   | NAG  | 1       | 0            |
| 17  | fC    | 4   | MAN  | 1       | 0            |
| 14  | bF    | 5   | MAN  | 1       | 0            |
| 9   | aC    | 9   | XYP  | 1       | 0            |
| 11  | aJ    | 10  | MAN  | 1       | 0            |
| 9   | aM    | 2   | NAG  | 1       | 0            |
| 10  | aI    | 8   | MAN  | 1       | 0            |
| 18  | eB    | 9   | NAG  | 1       | 0            |
| 16  | dC    | 2   | MAN  | 1       | 0            |

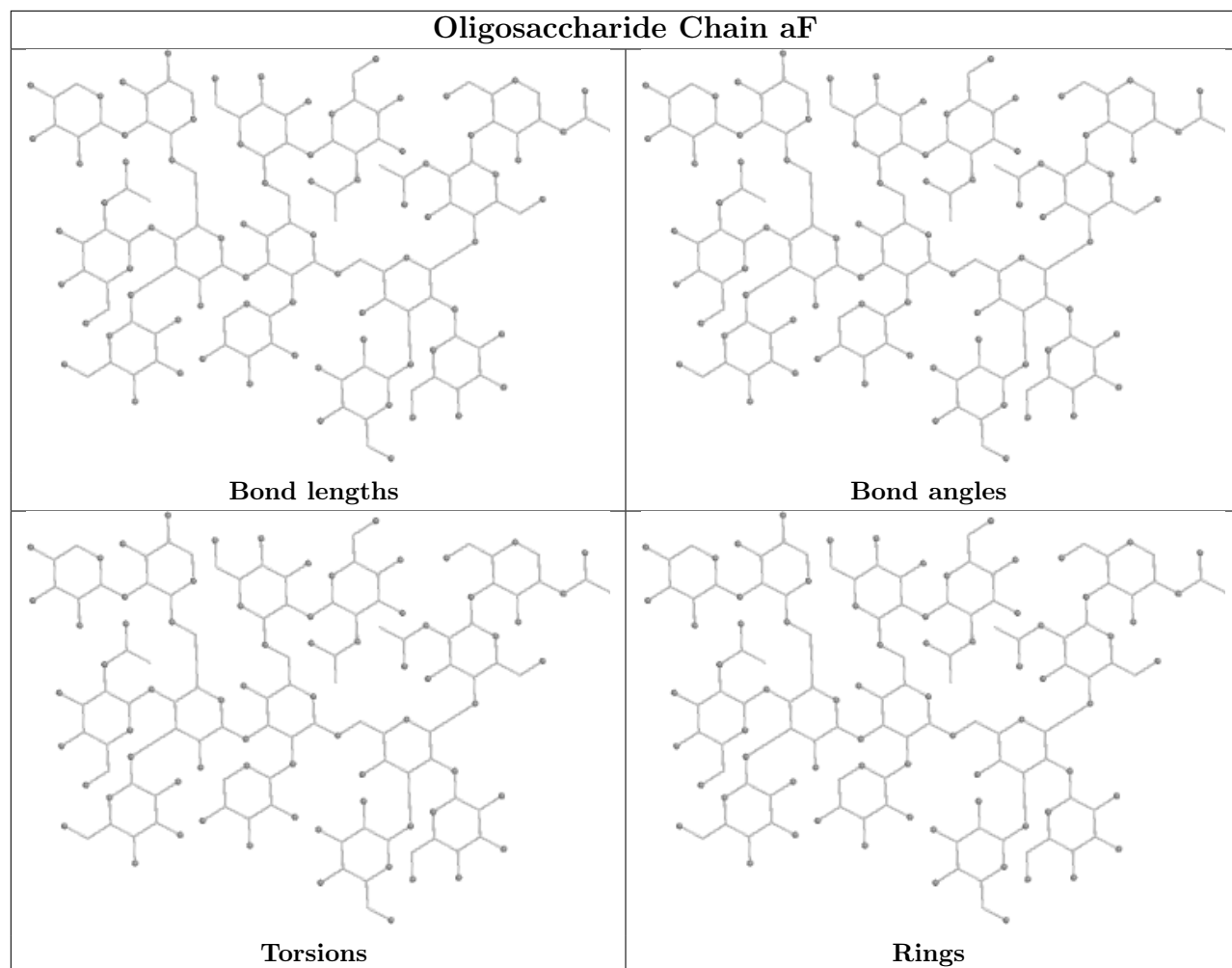
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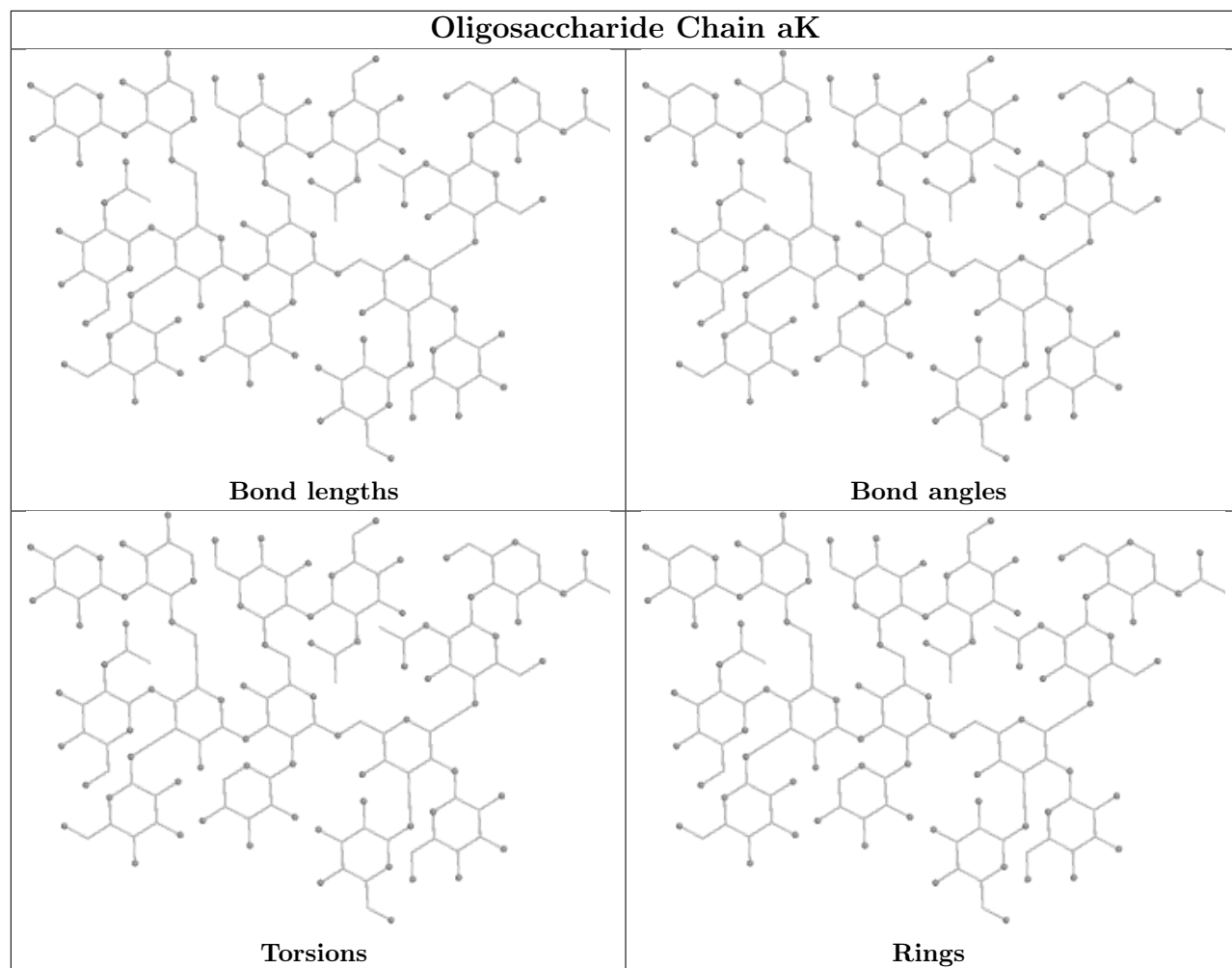
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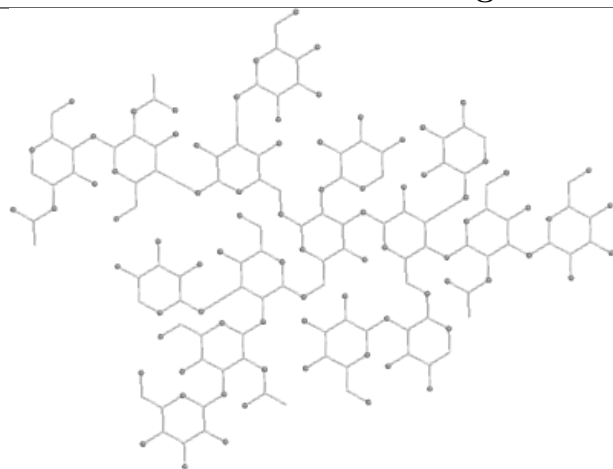
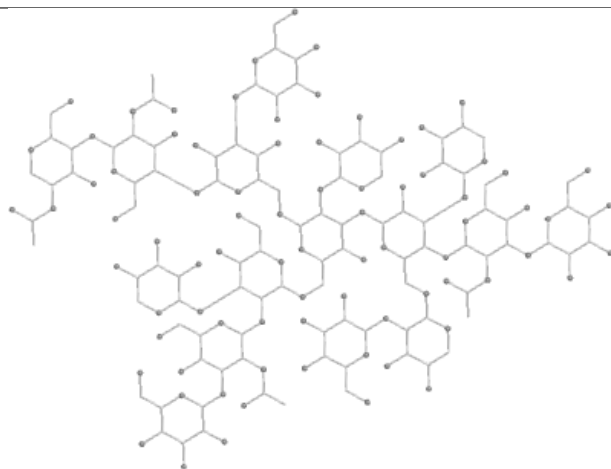
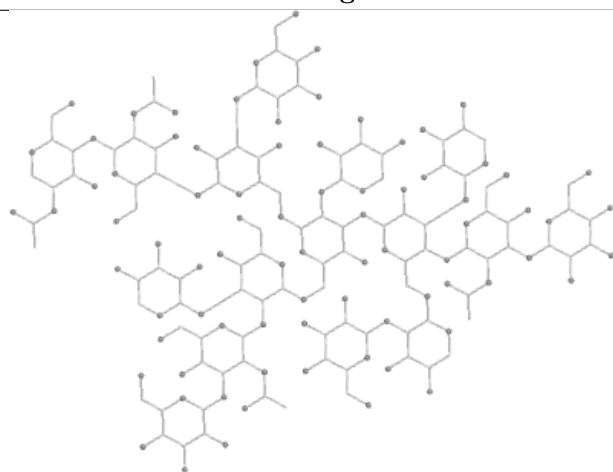
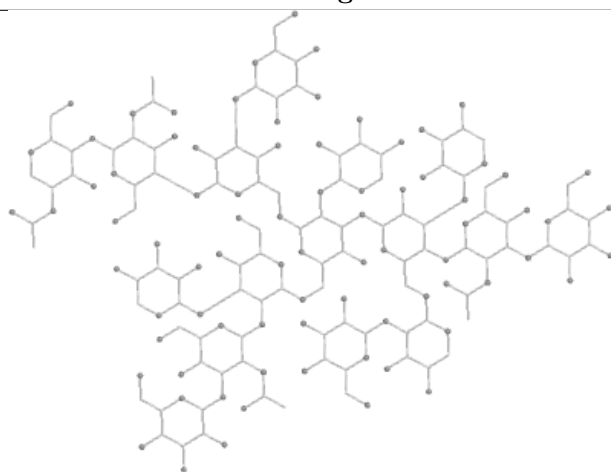
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 12  | bD    | 5   | MAN  | 1       | 0            |
| 7   | aF    | 5   | MAN  | 1       | 0            |
| 7   | aA    | 1   | NAG  | 1       | 0            |
| 20  | fF    | 8   | NAG  | 1       | 0            |
| 7   | aK    | 1   | NAG  | 1       | 0            |
| 9   | aC    | 10  | XYP  | 1       | 0            |
| 7   | aA    | 5   | MAN  | 1       | 0            |
| 19  | fJ    | 6   | MAN  | 1       | 0            |
| 11  | aE    | 1   | NAG  | 1       | 0            |
| 7   | aK    | 5   | MAN  | 1       | 0            |

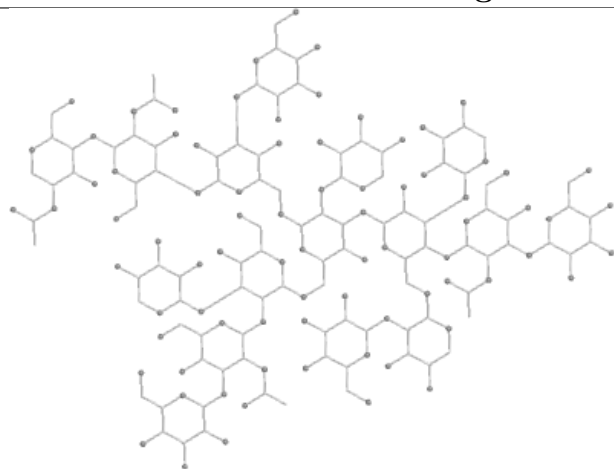
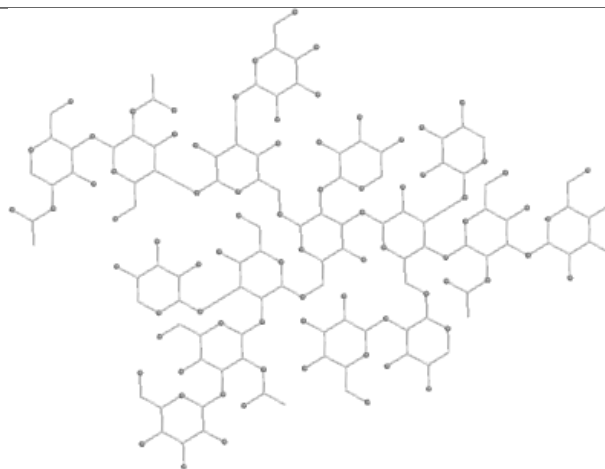
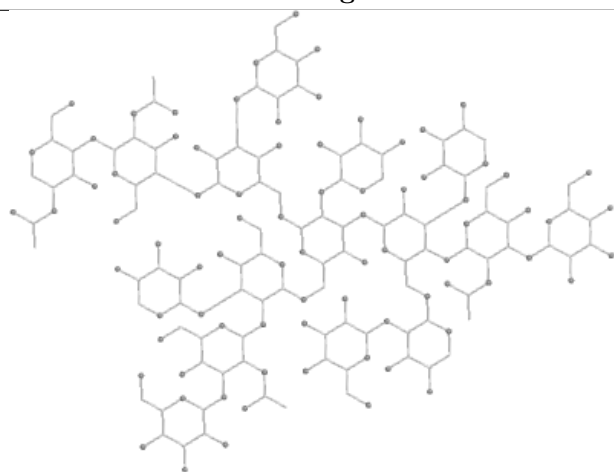
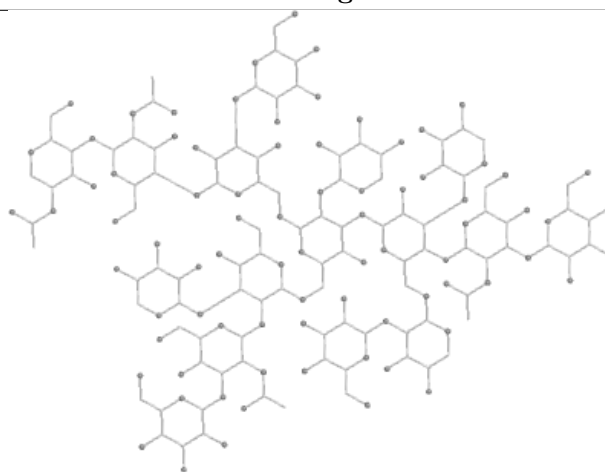
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

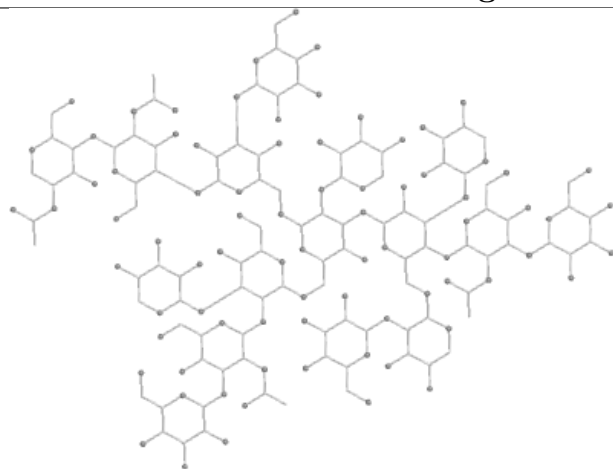
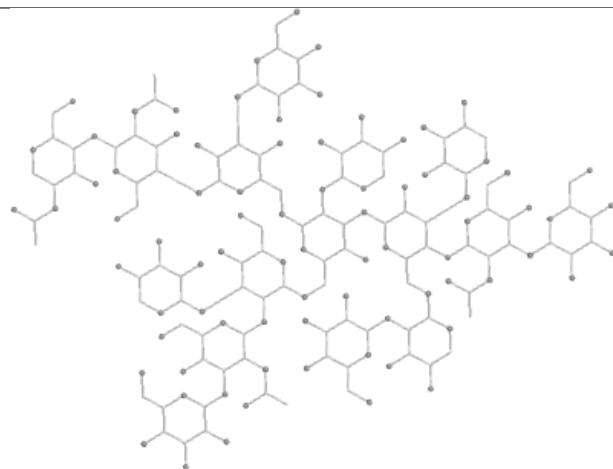
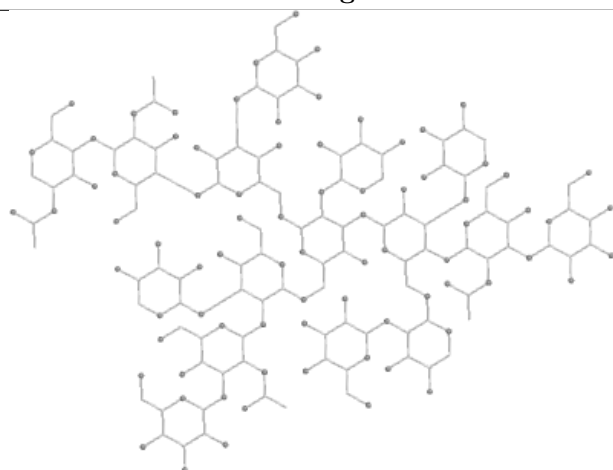
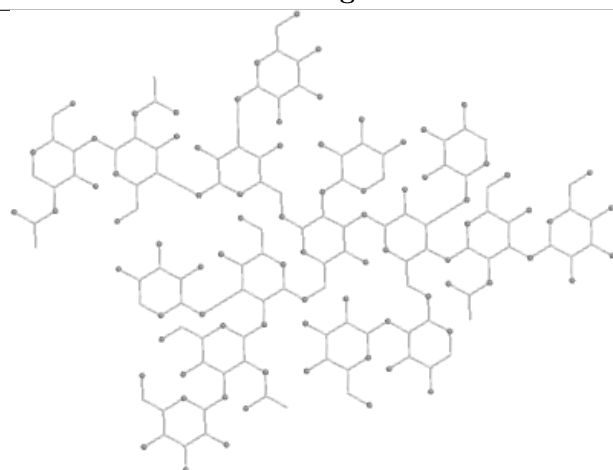


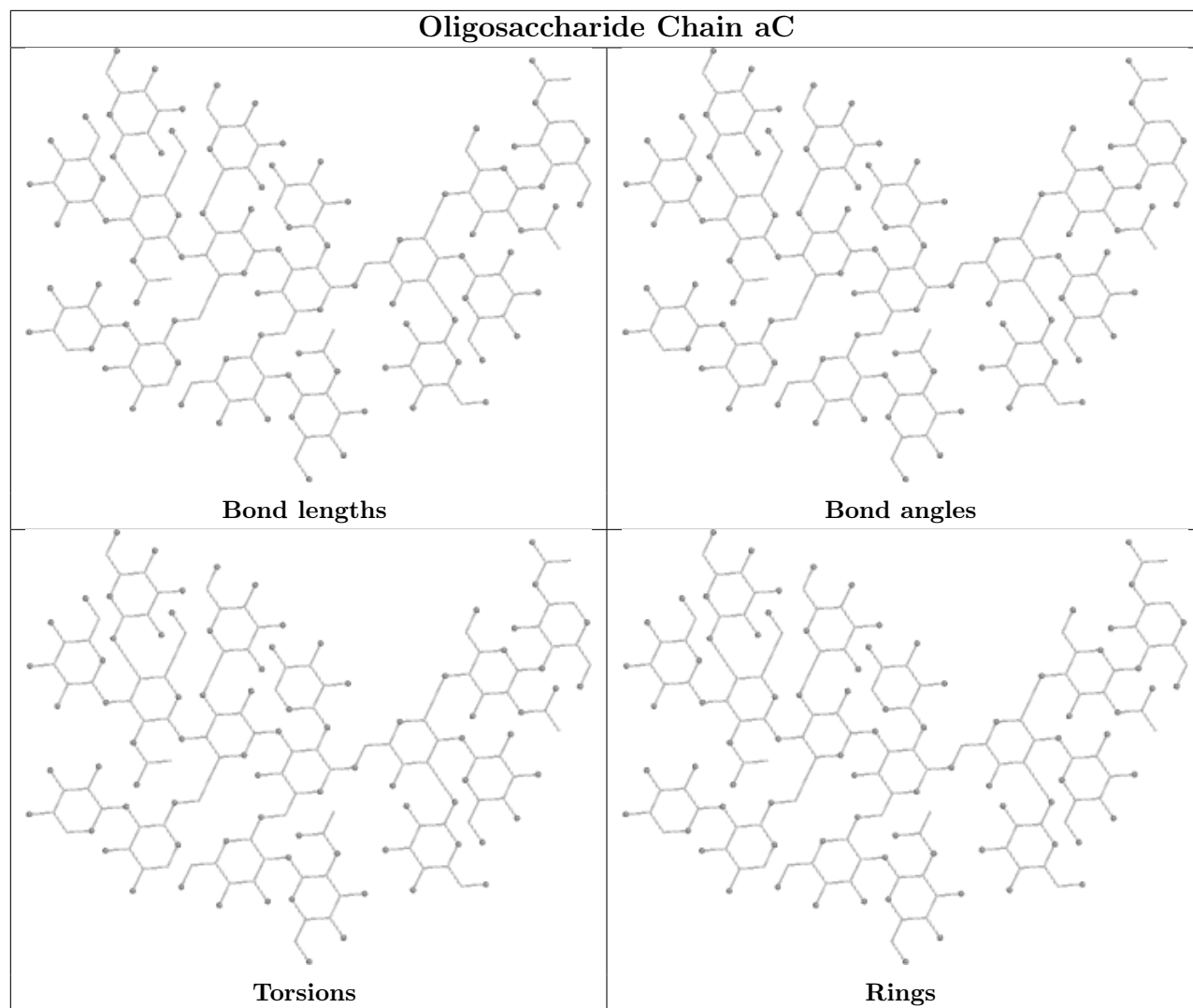


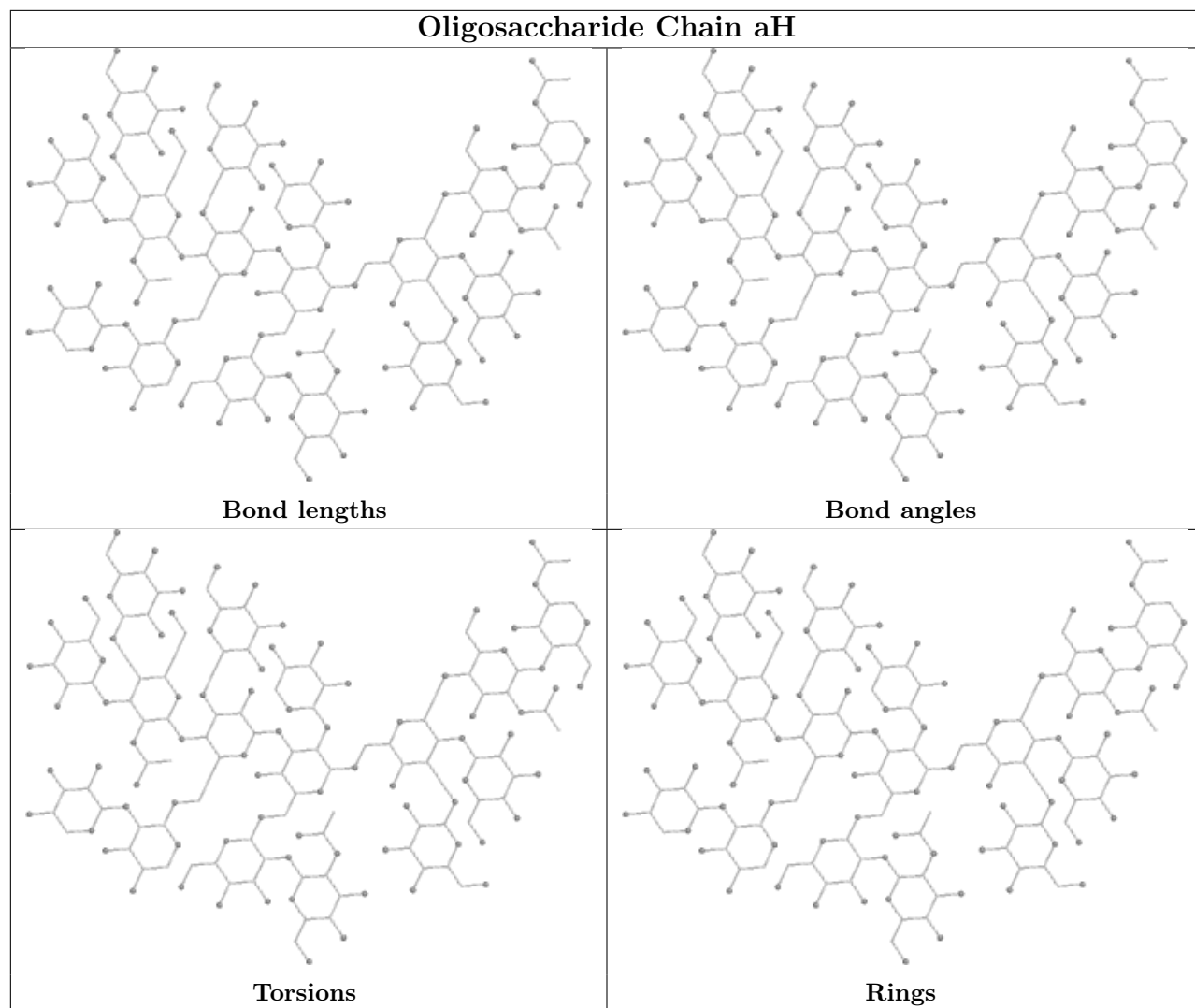


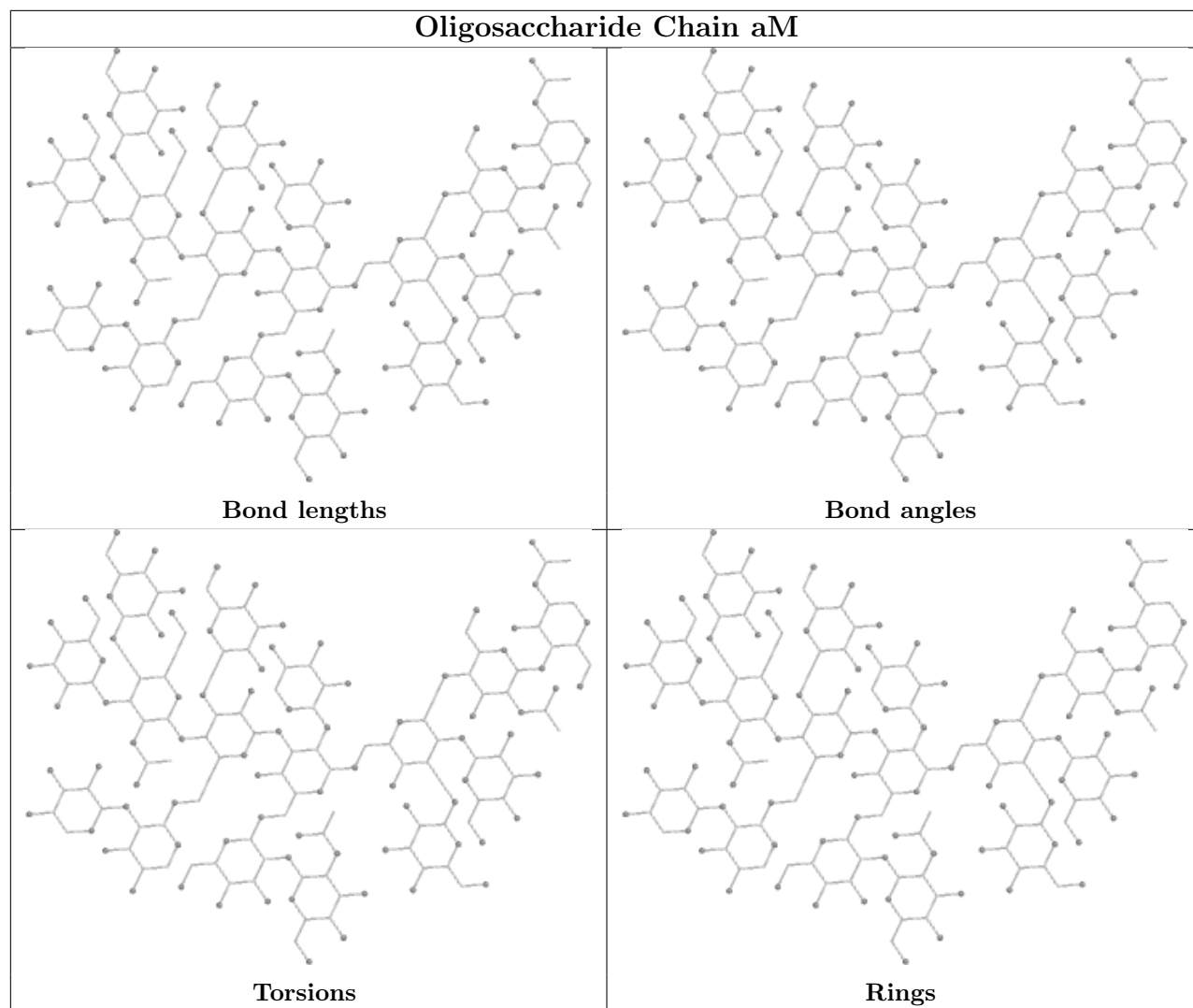
**Oligosaccharide Chain aB****Bond lengths****Bond angles****Torsions****Rings**

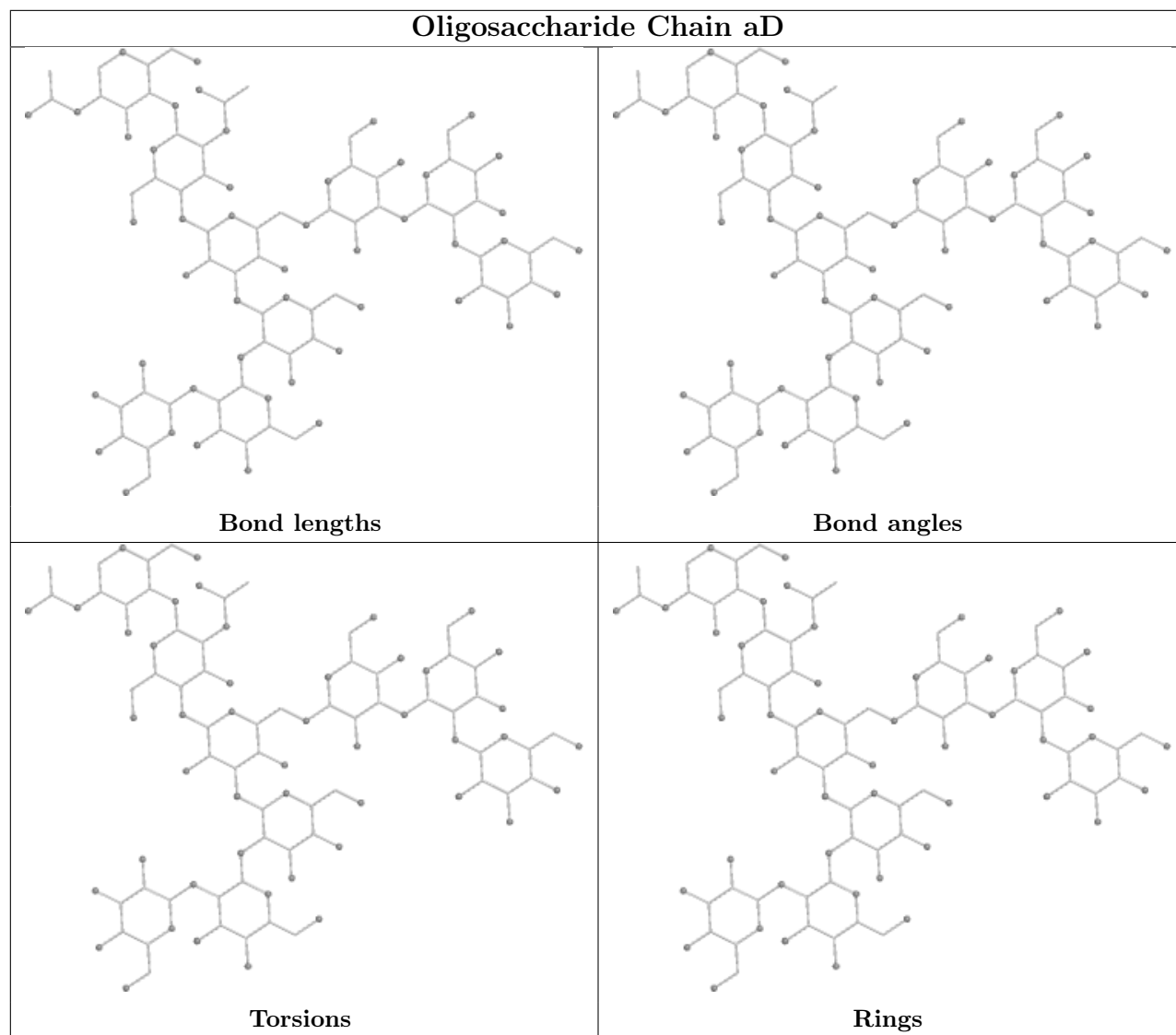
**Oligosaccharide Chain aG****Bond lengths****Bond angles****Torsions****Rings**

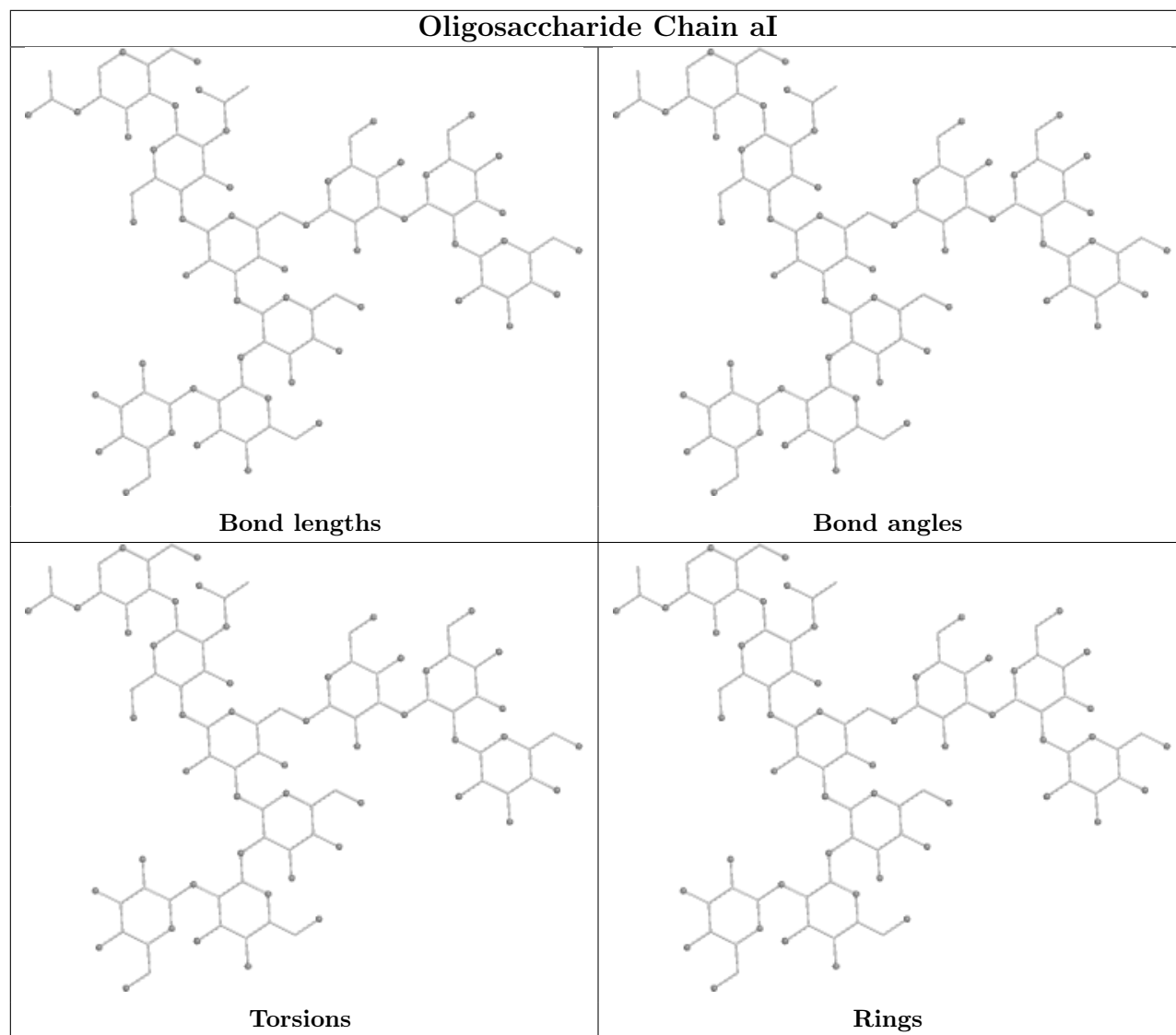
**Oligosaccharide Chain aL****Bond lengths****Bond angles****Torsions****Rings**

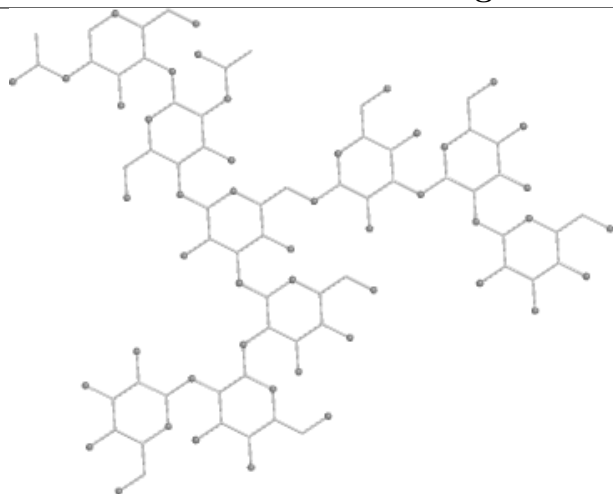
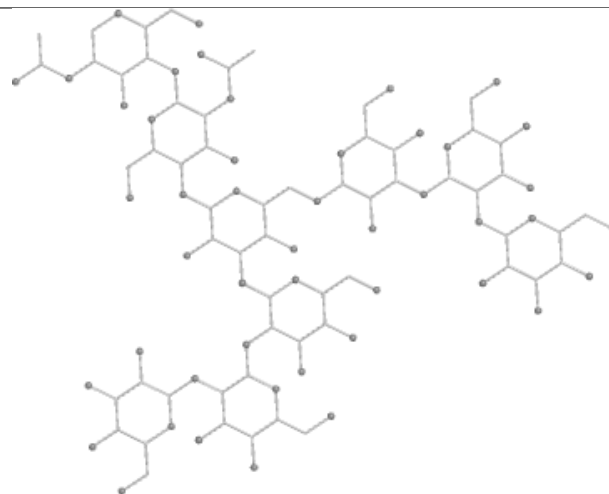
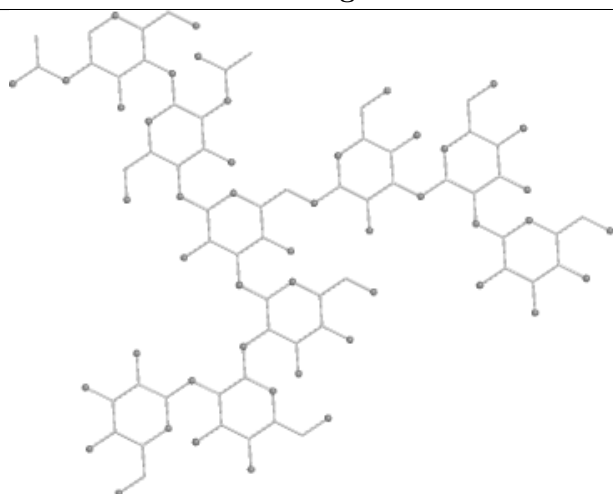
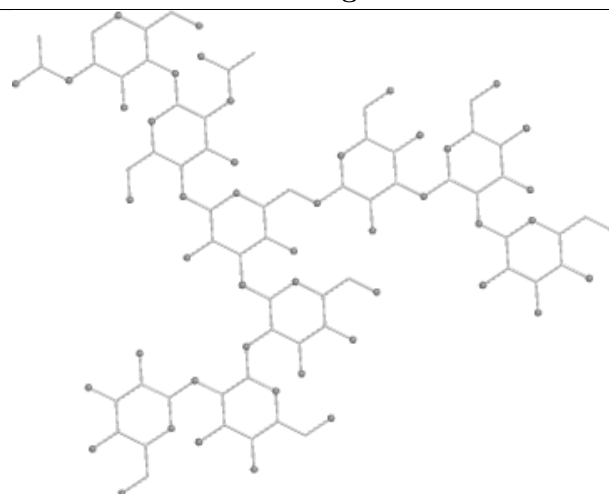


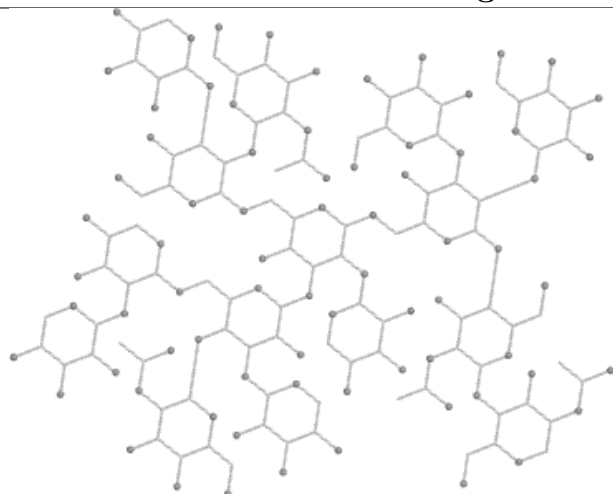
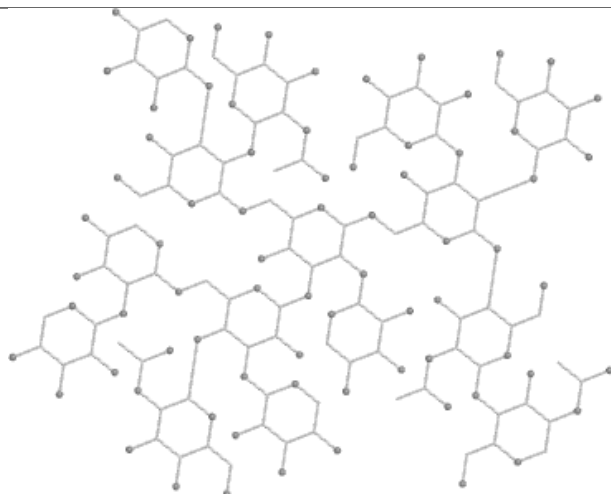
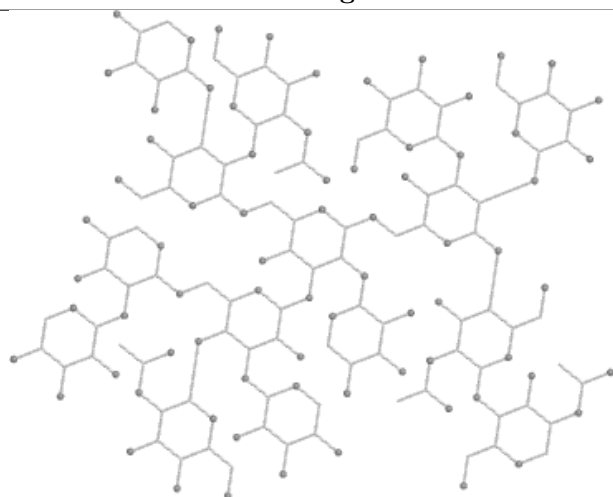
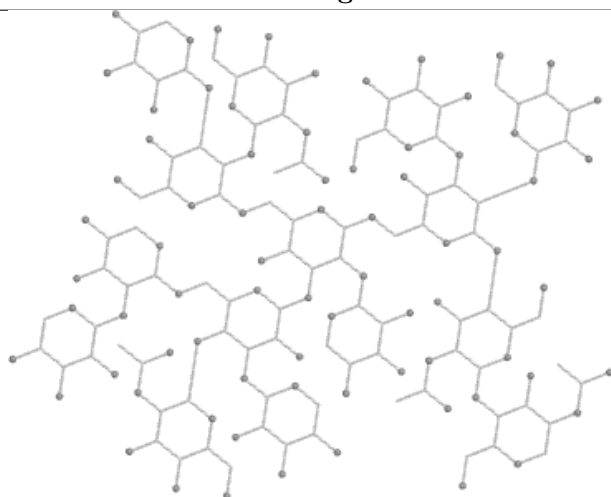


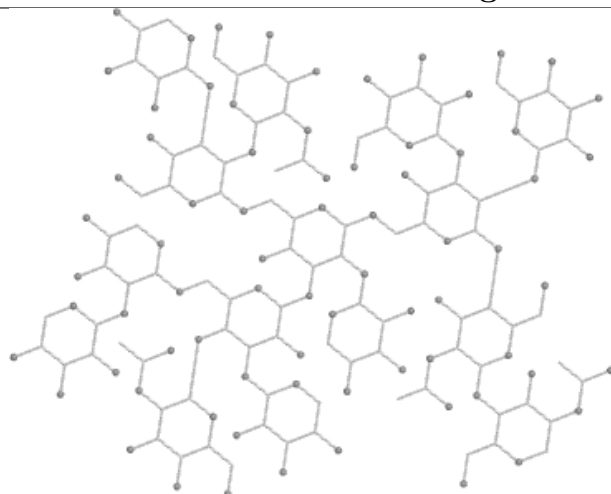
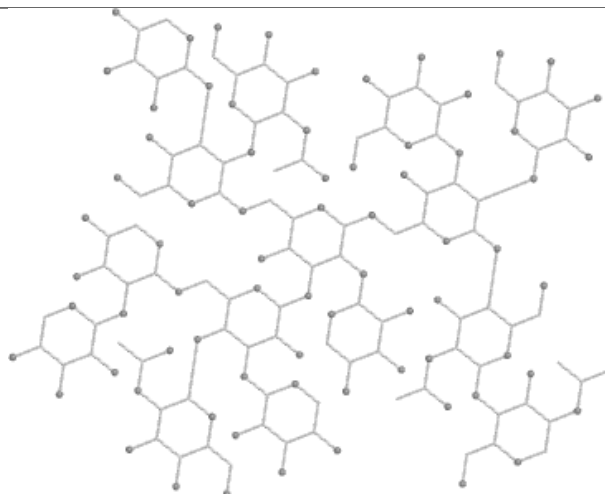
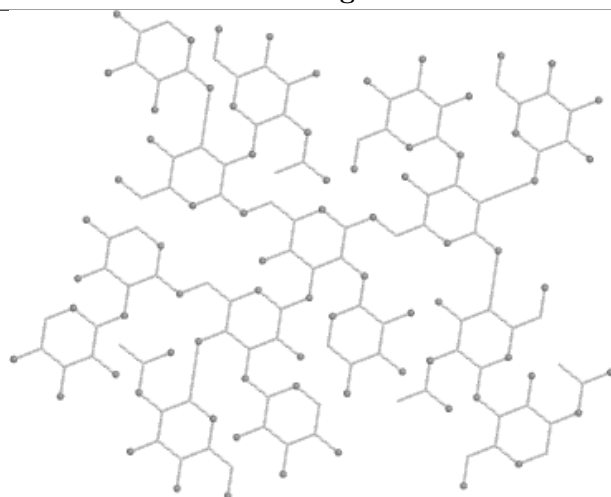
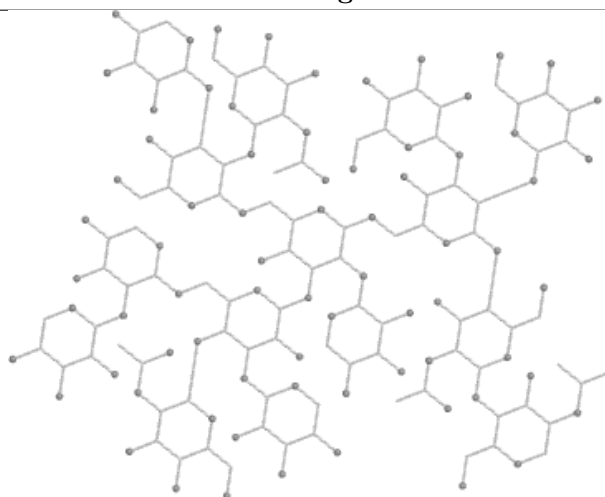


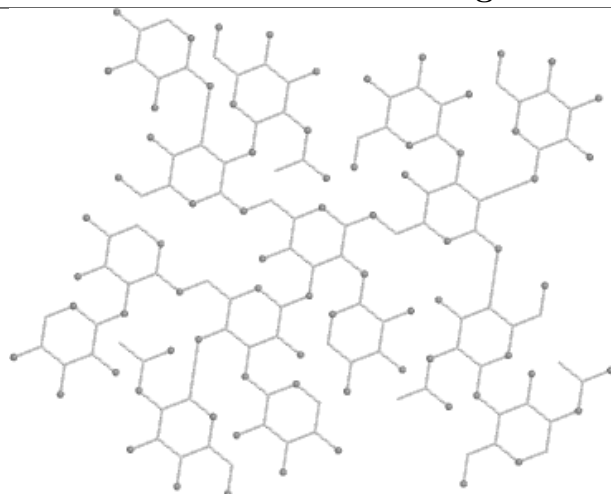
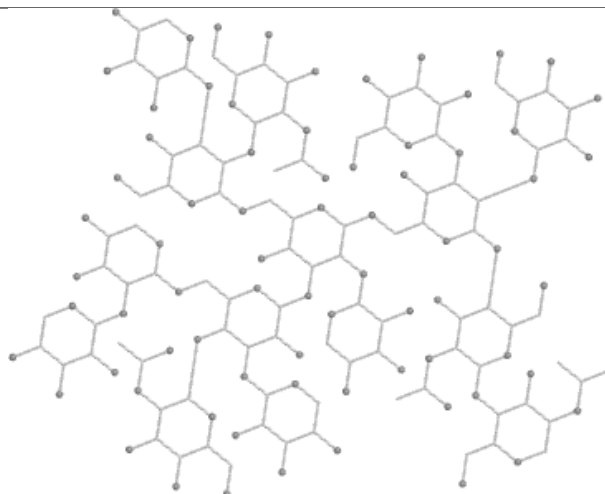
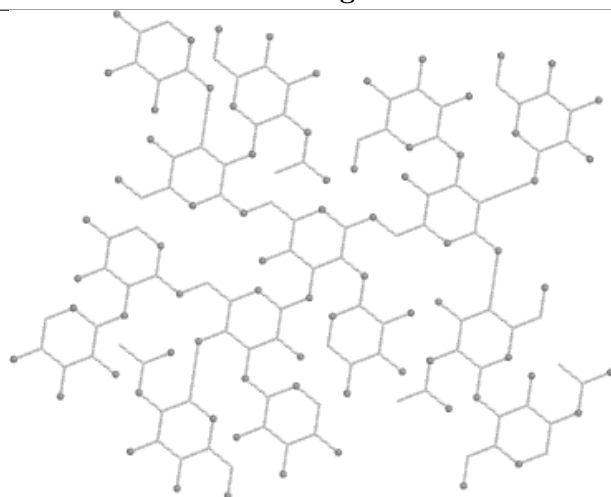
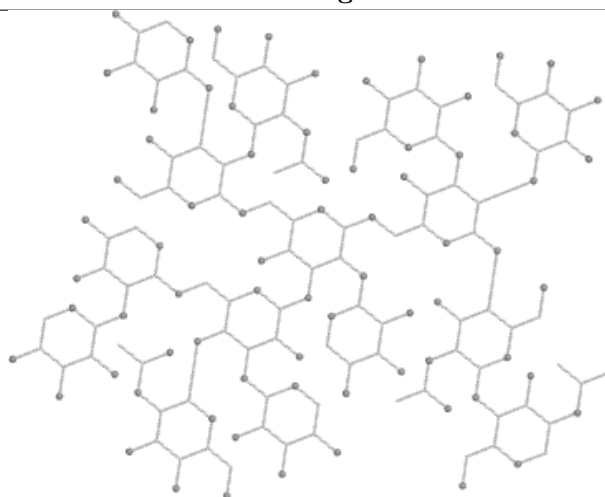


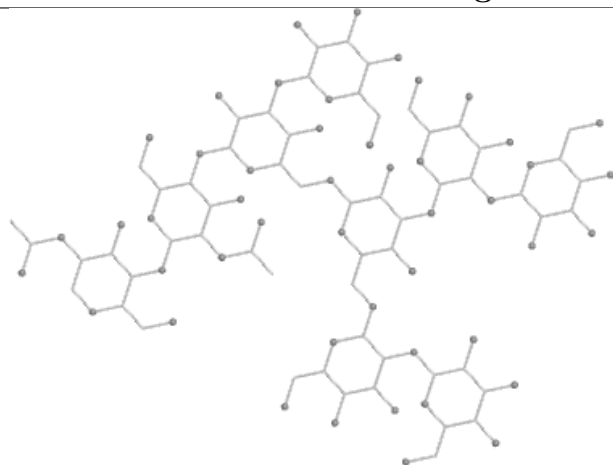
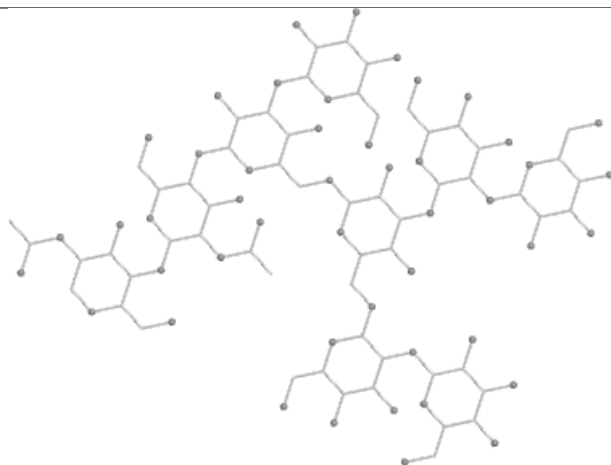
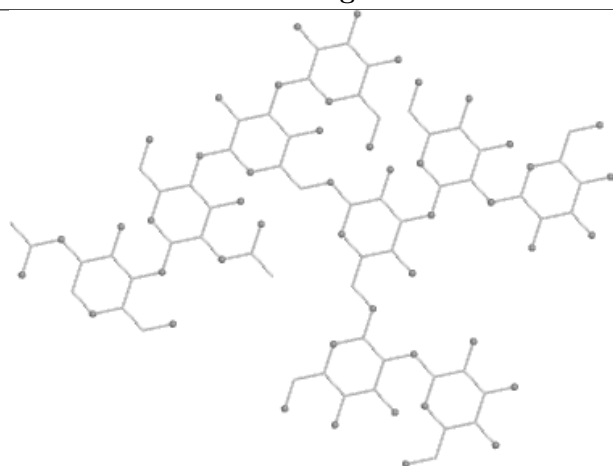
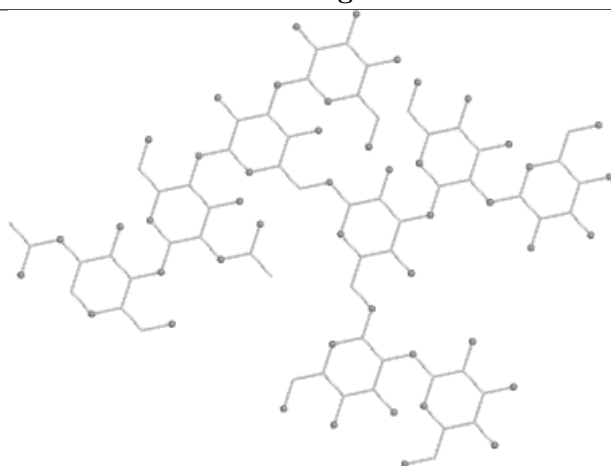


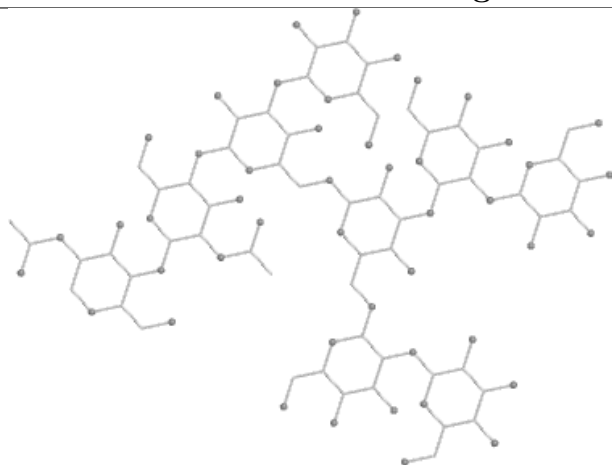
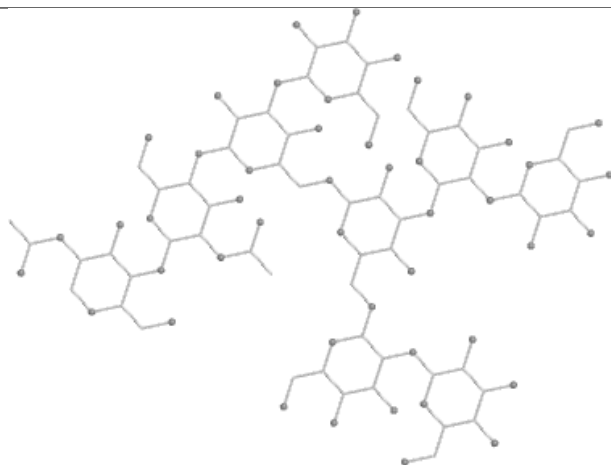
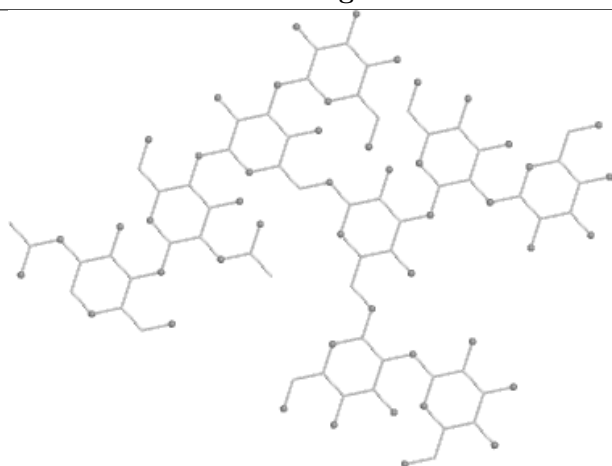
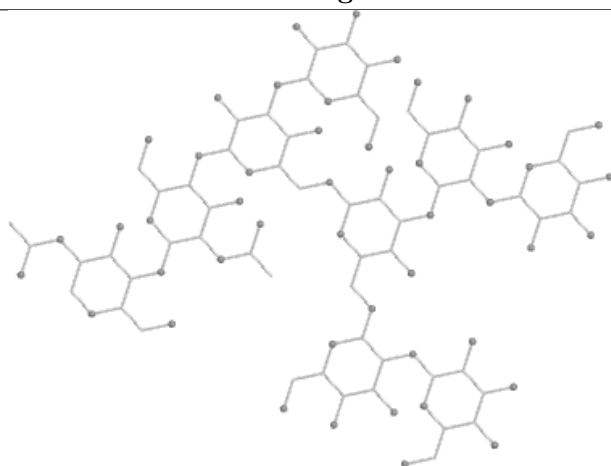
**Oligosaccharide Chain aN****Bond lengths****Bond angles****Torsions****Rings**

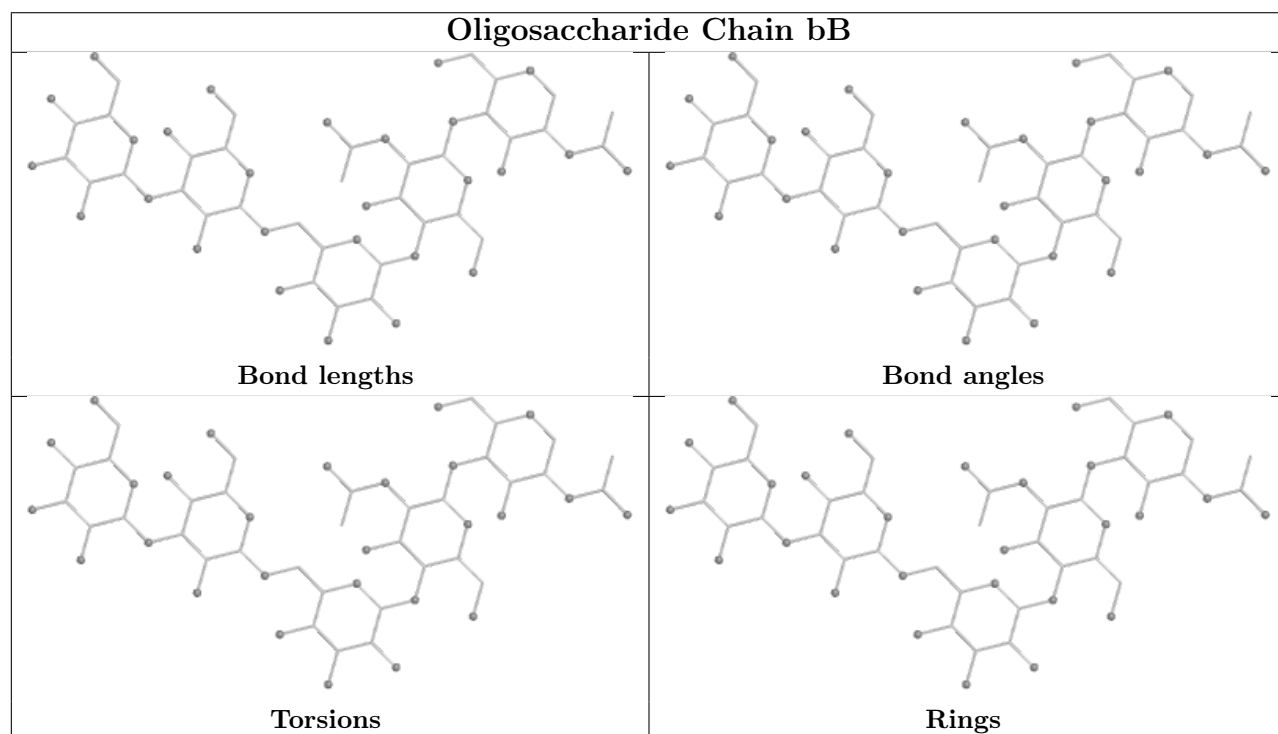
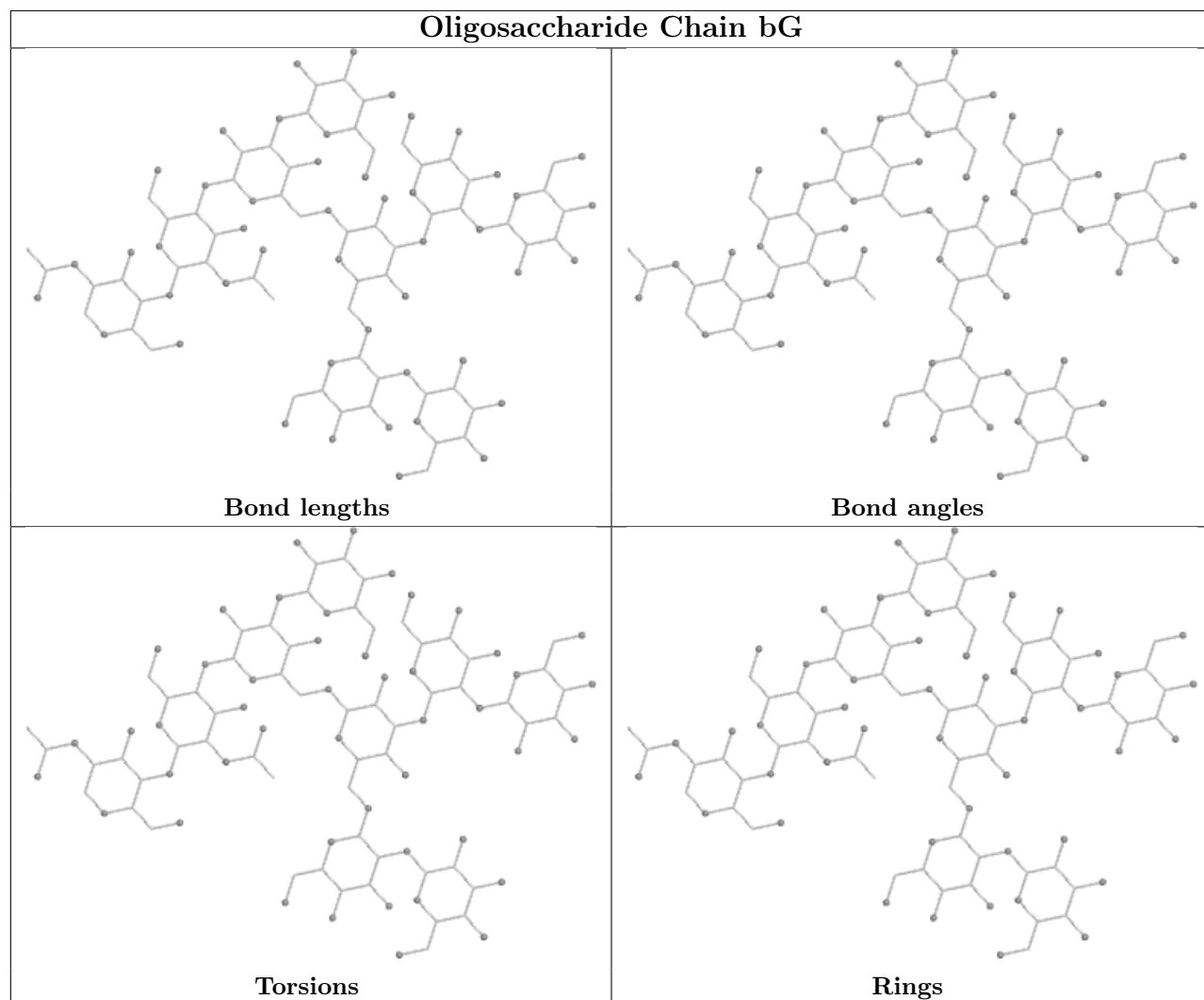
**Oligosaccharide Chain aE****Bond lengths****Bond angles****Torsions****Rings**

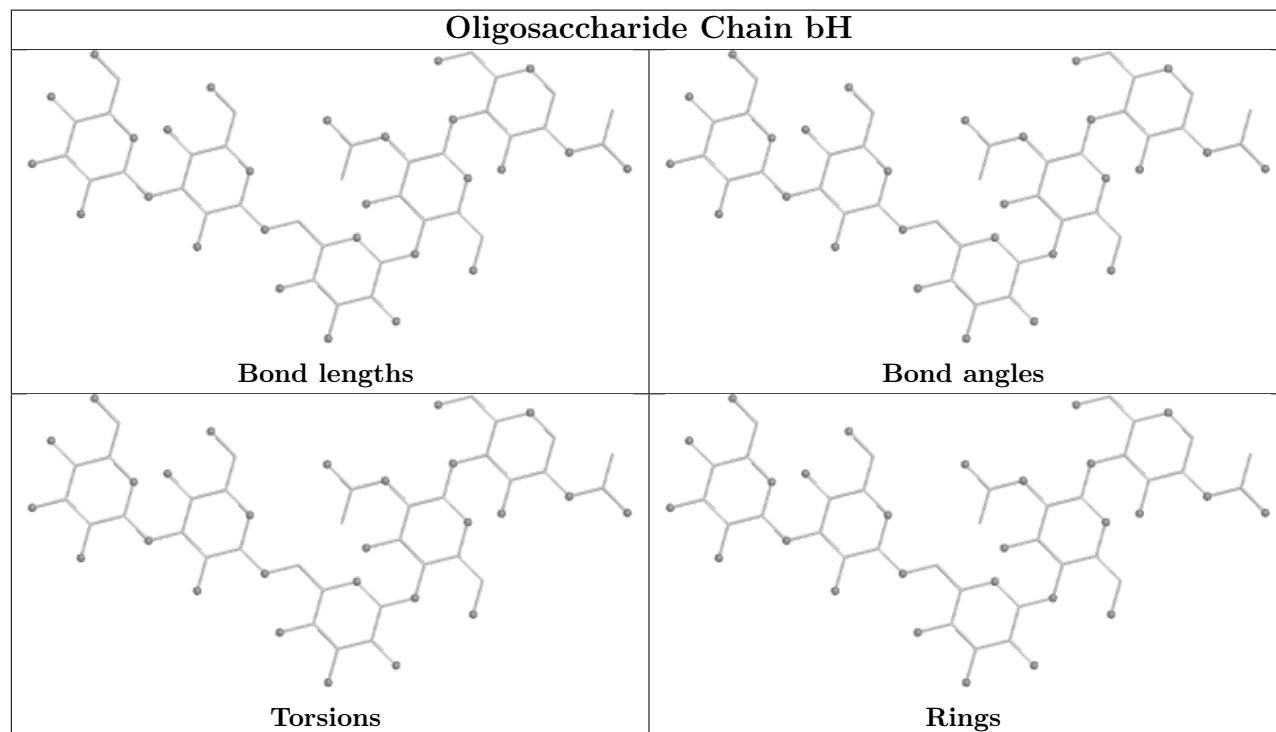
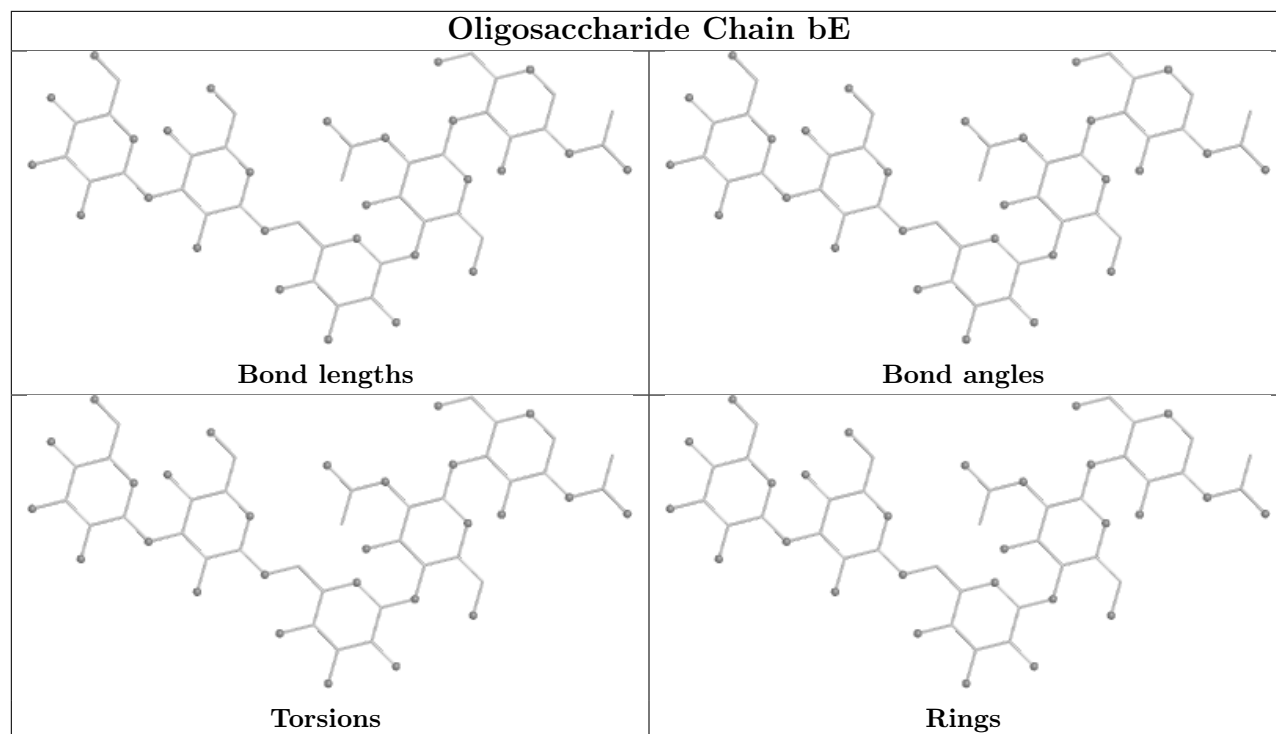
**Oligosaccharide Chain aJ****Bond lengths****Bond angles****Torsions****Rings**

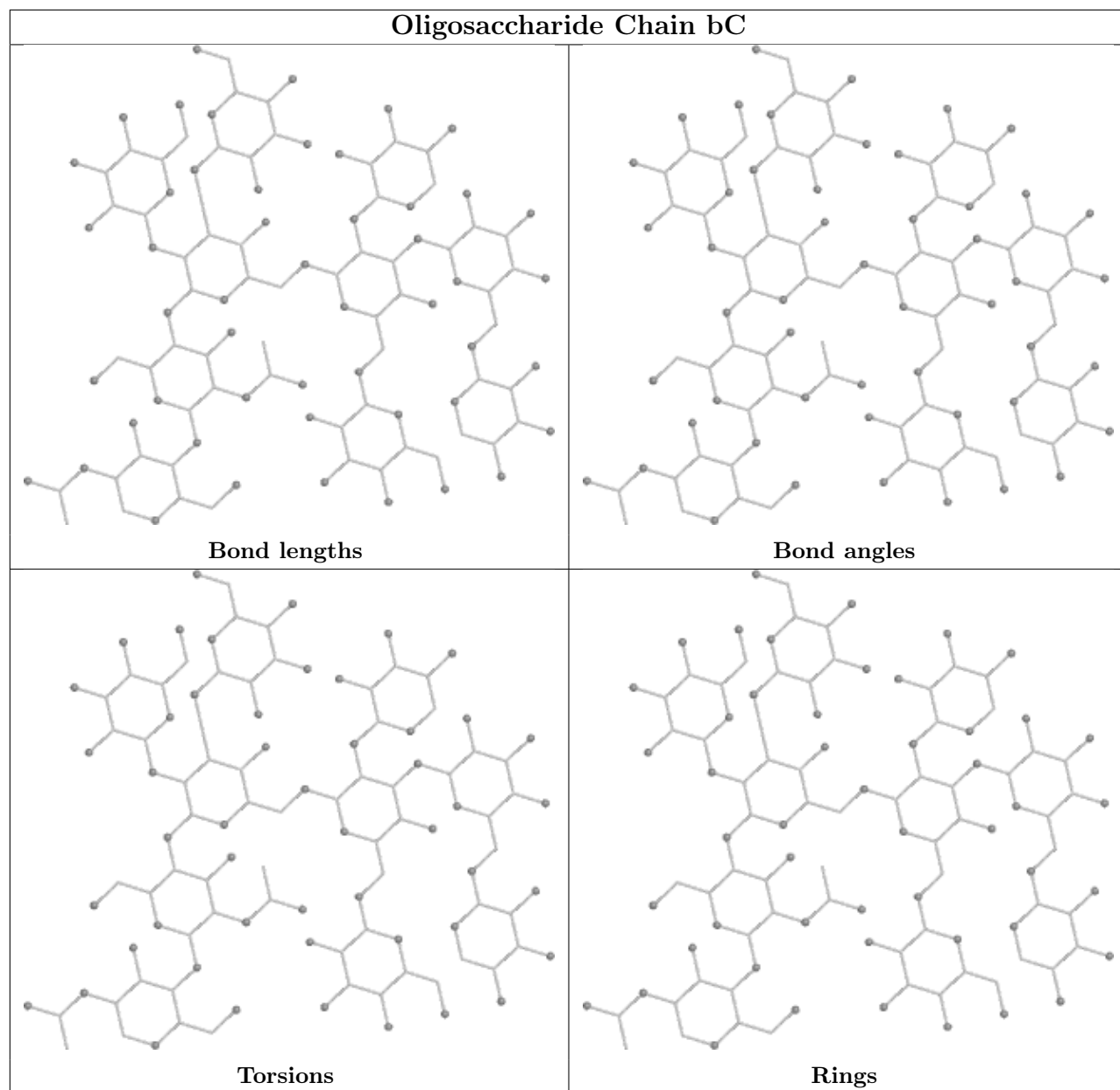
**Oligosaccharide Chain aO****Bond lengths****Bond angles****Torsions****Rings**

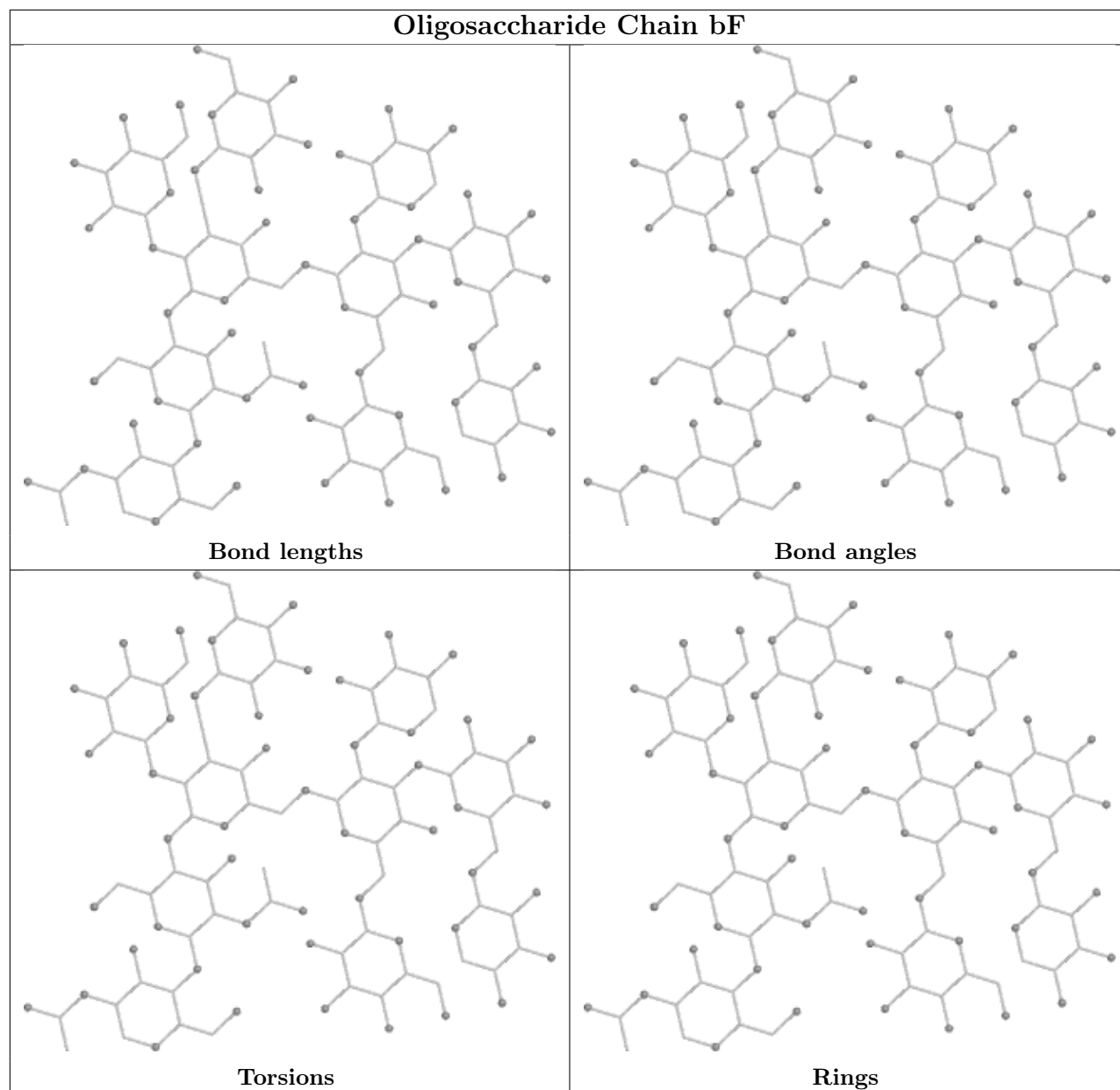
**Oligosaccharide Chain bA****Bond lengths****Bond angles****Torsions****Rings**

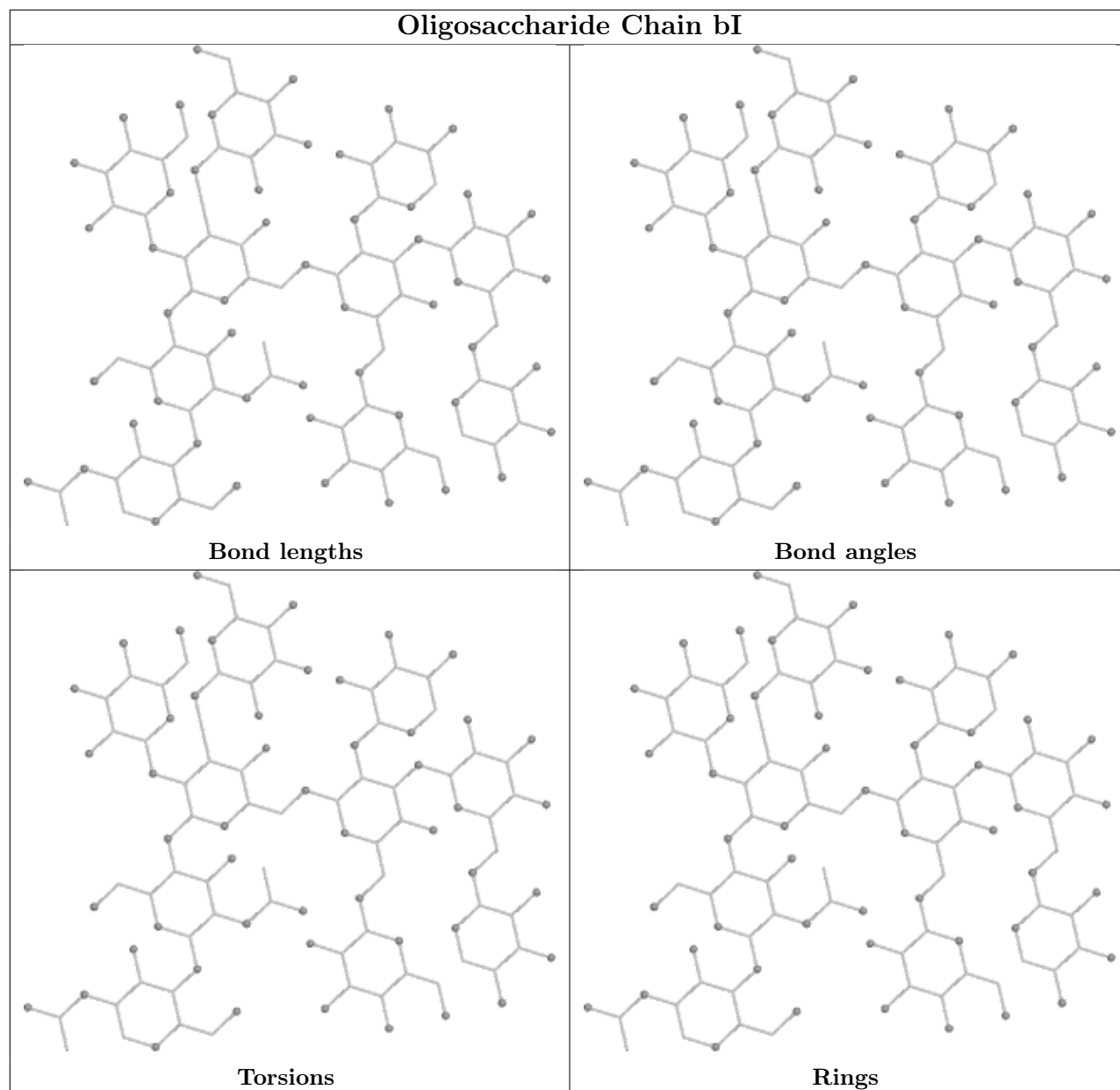
**Oligosaccharide Chain bD****Bond lengths****Bond angles****Torsions****Rings**

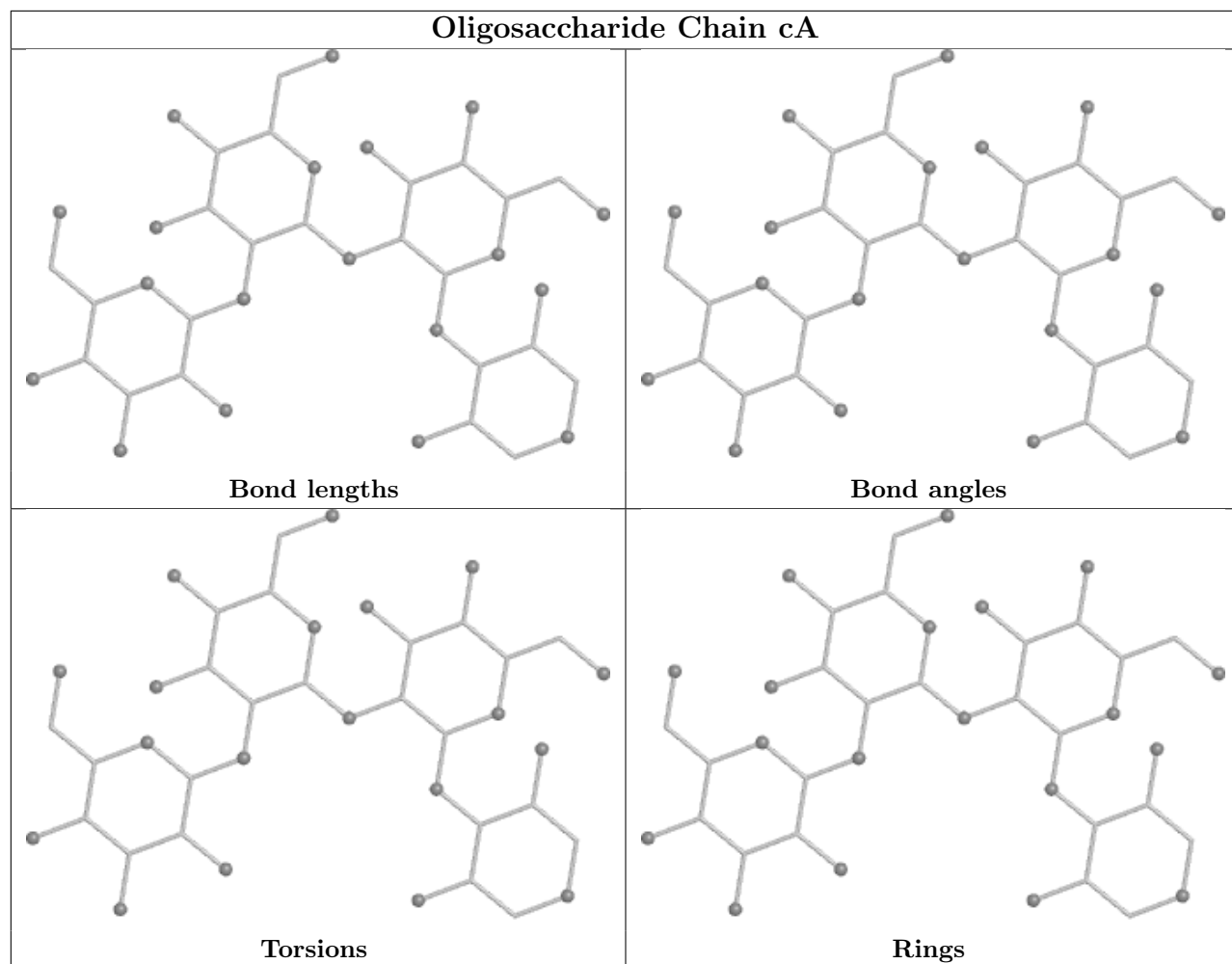


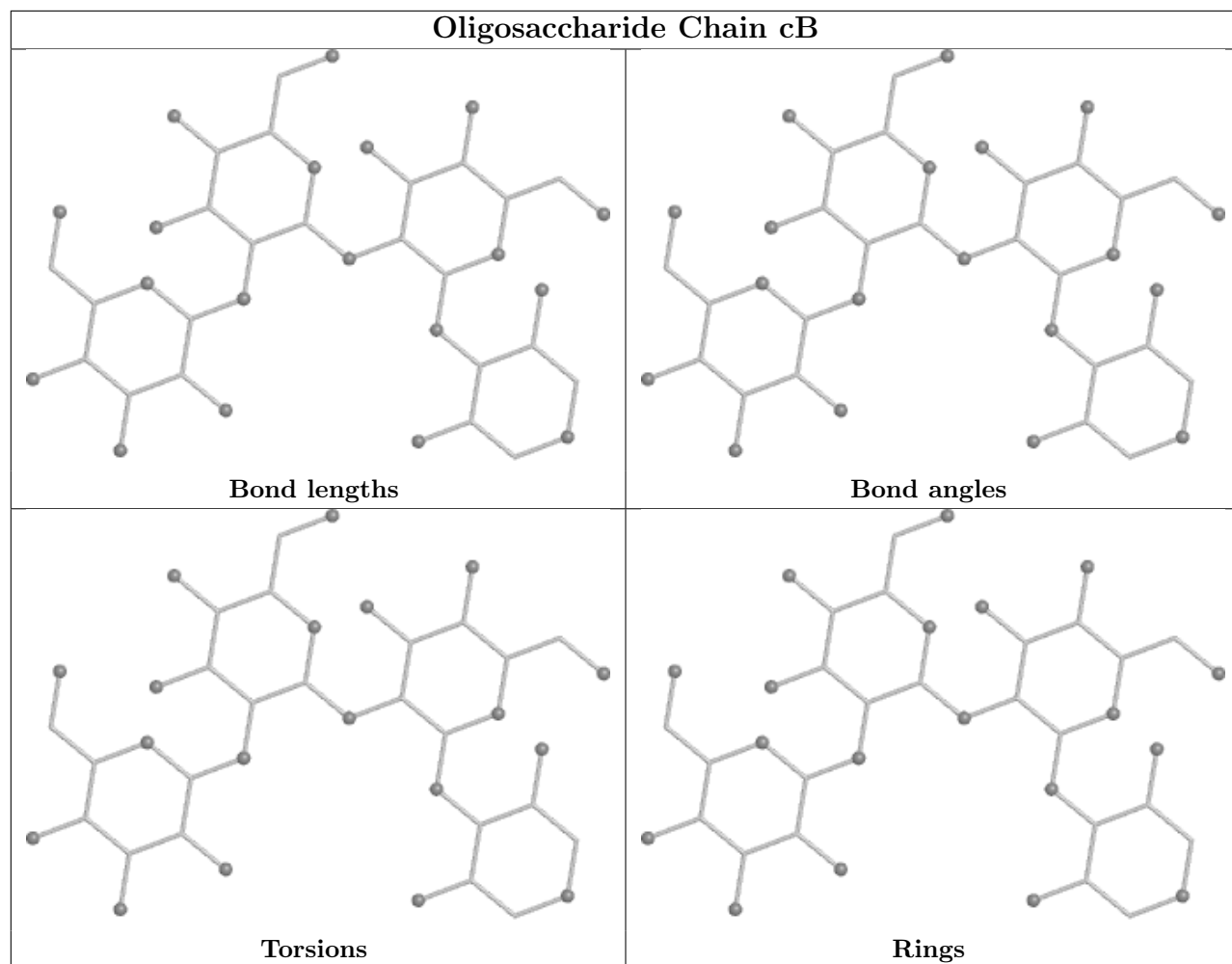


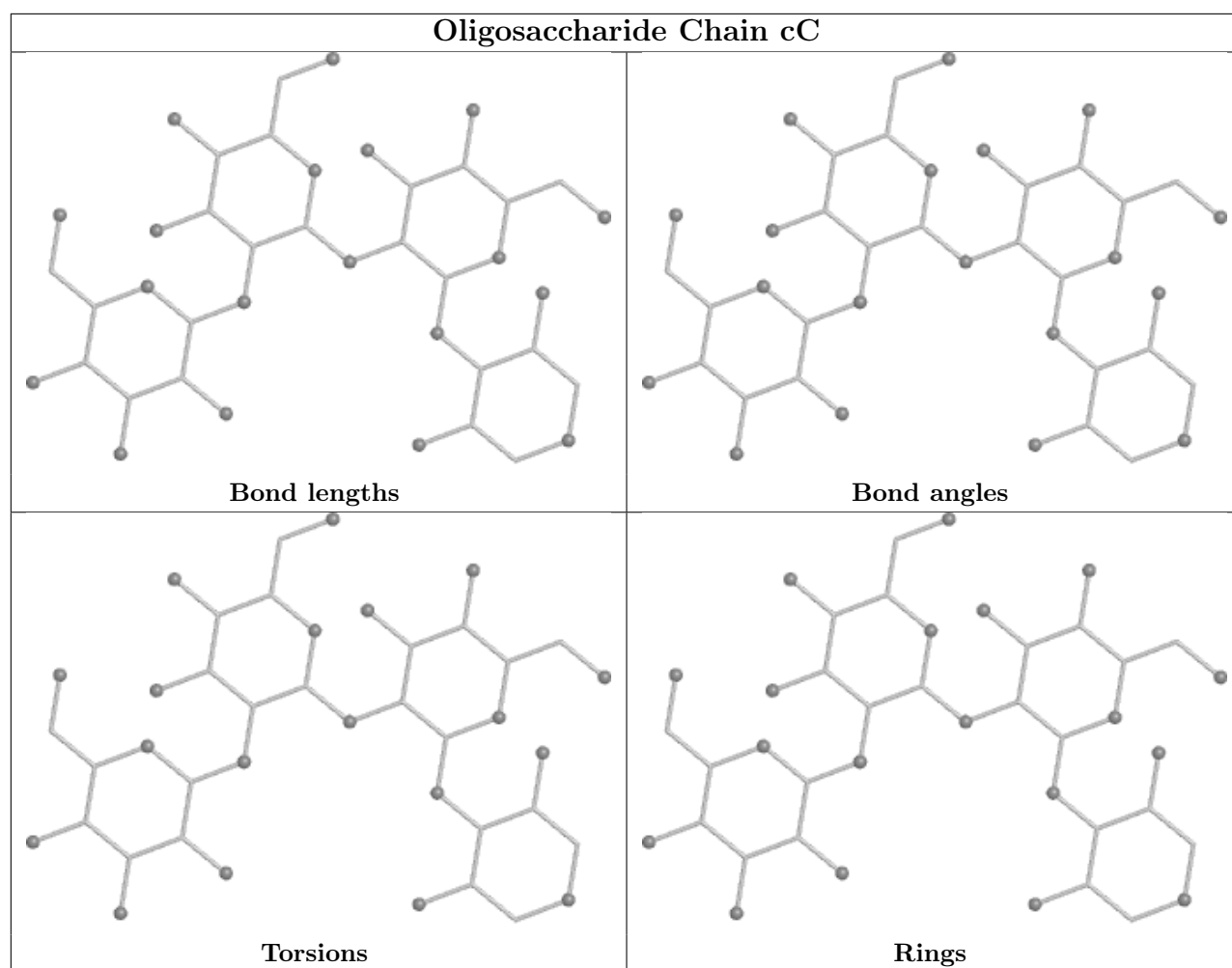


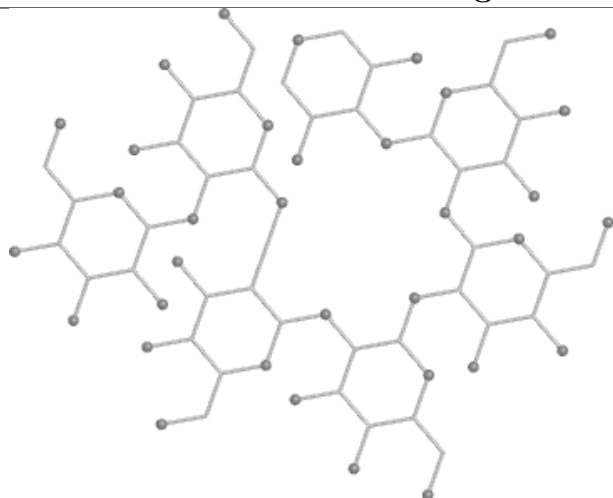
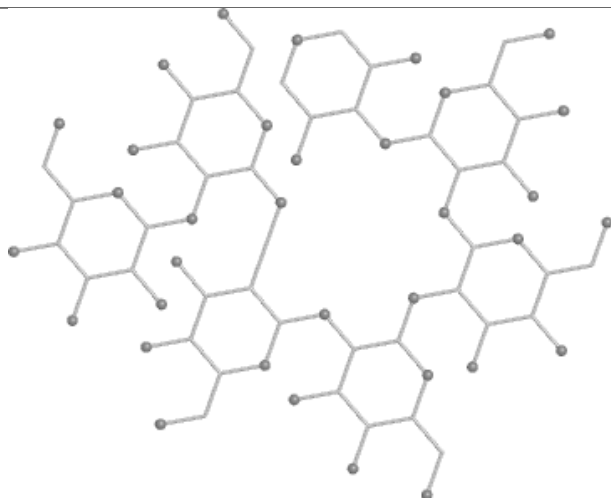
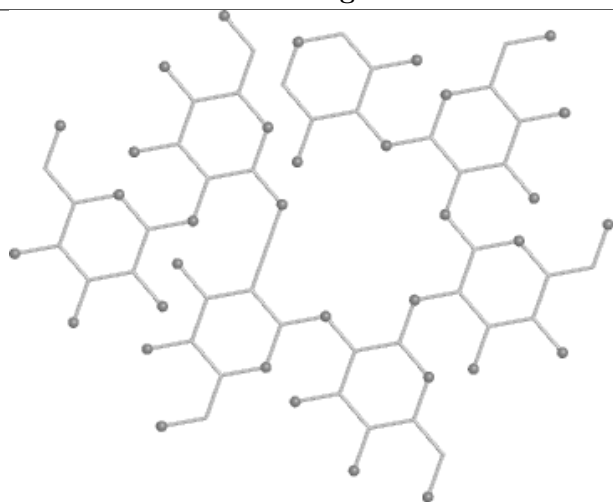
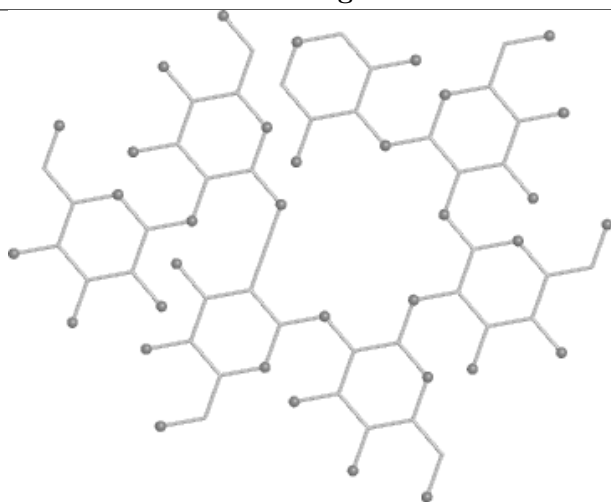


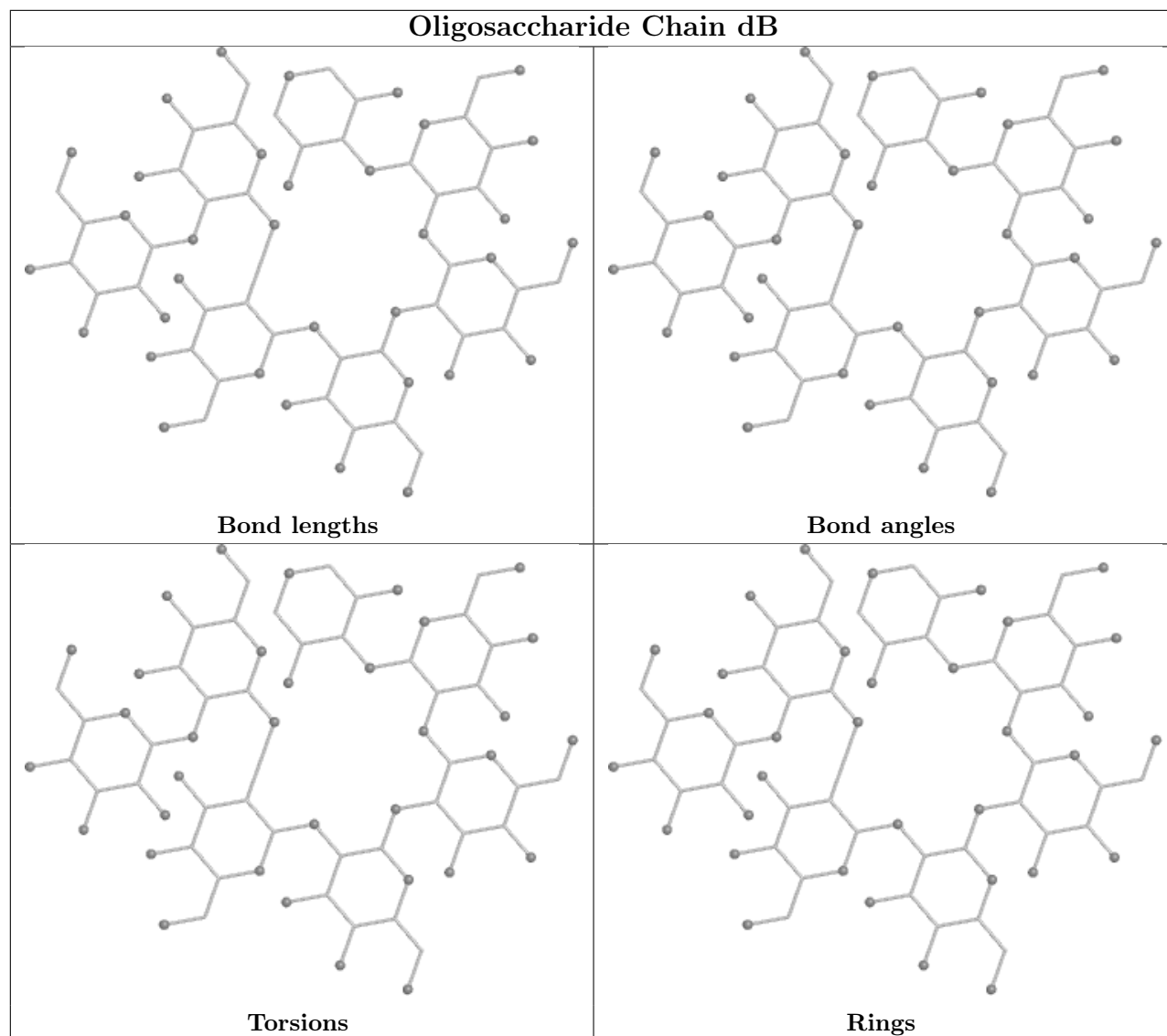


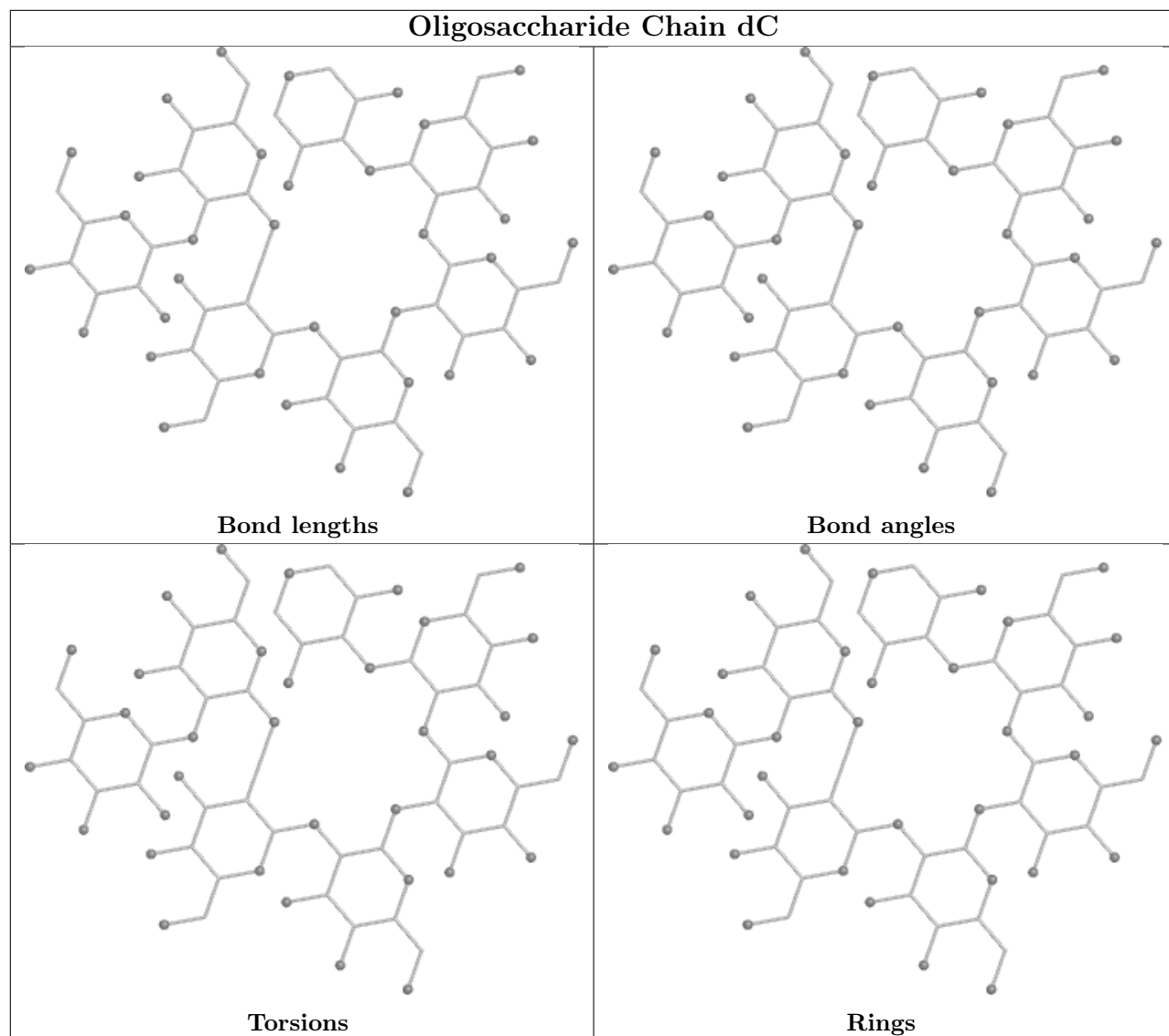


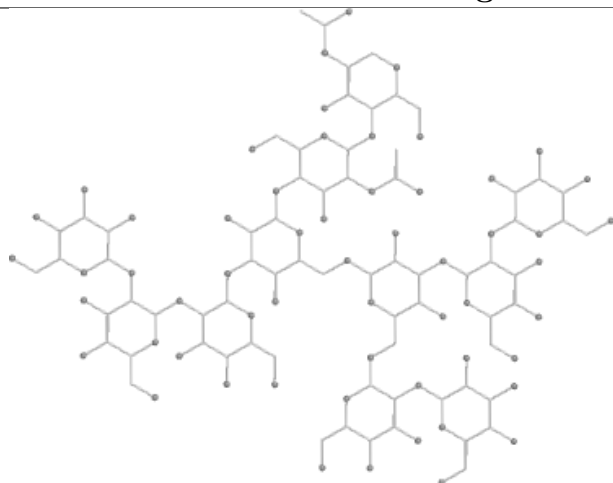
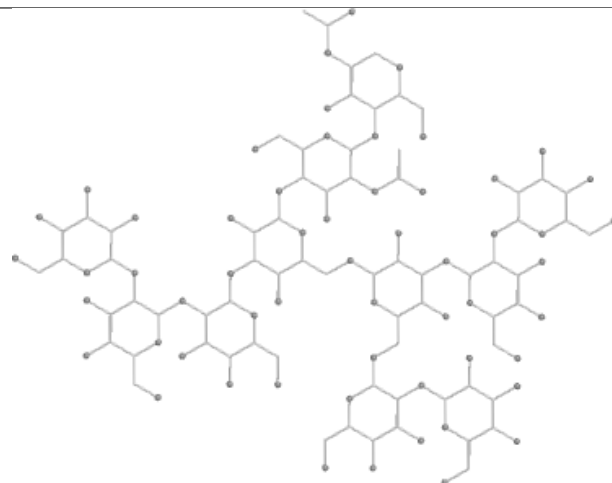
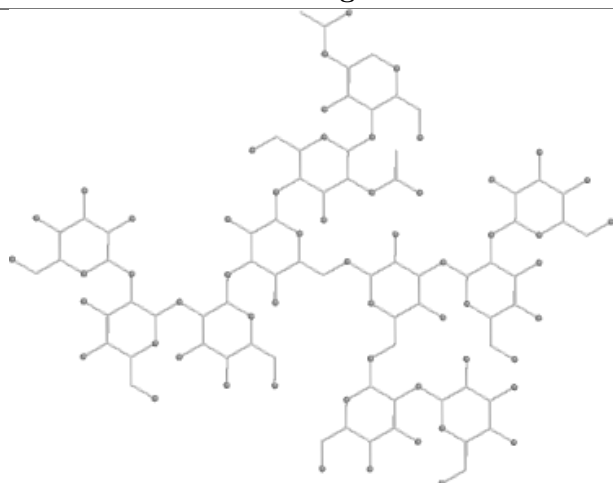
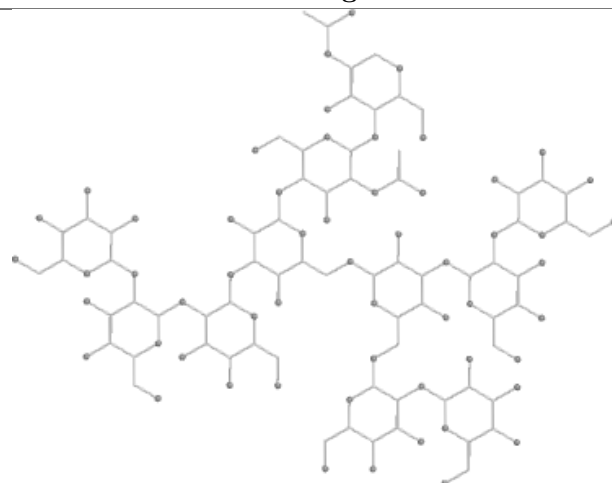


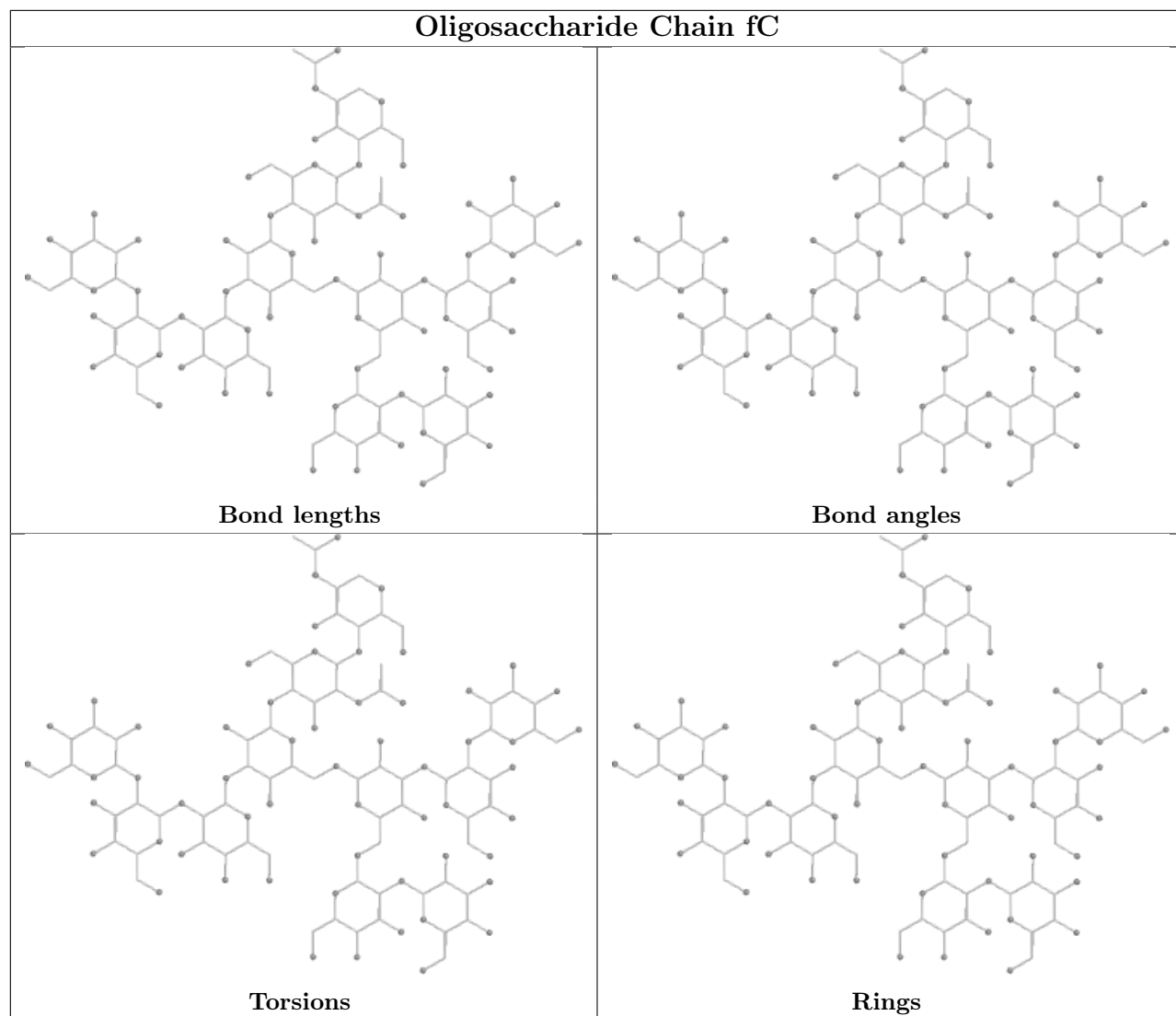


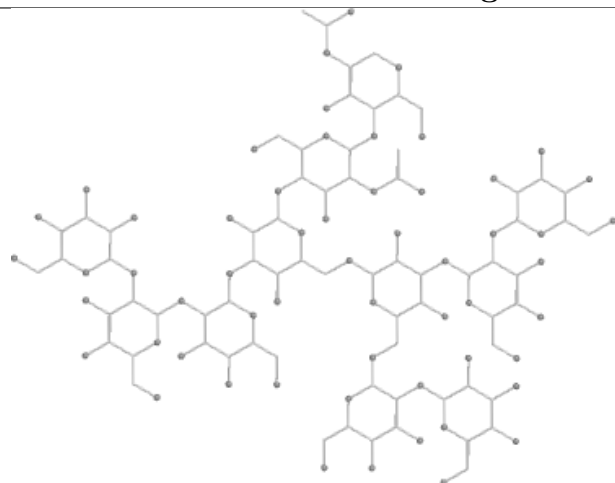
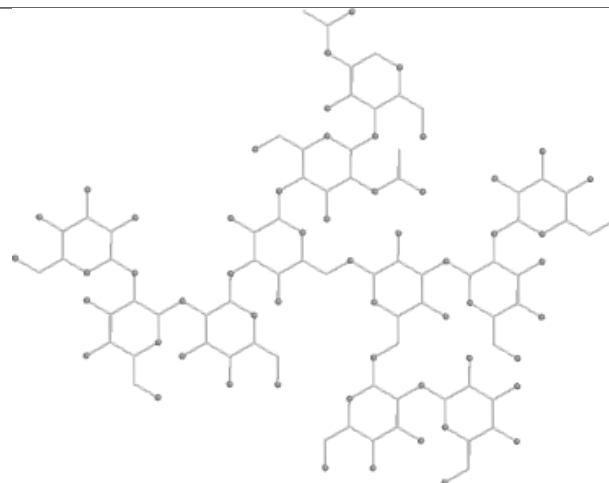
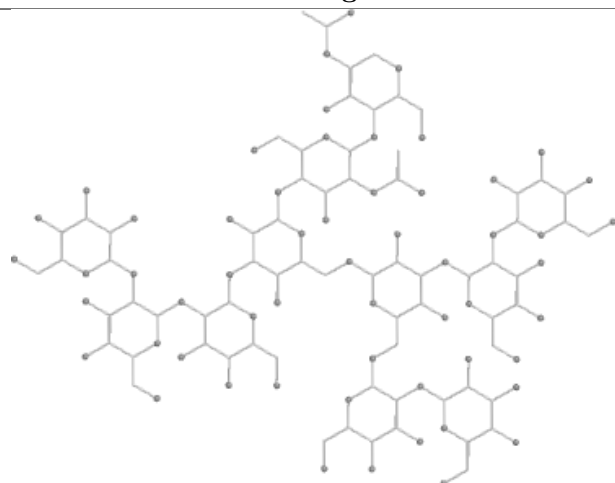
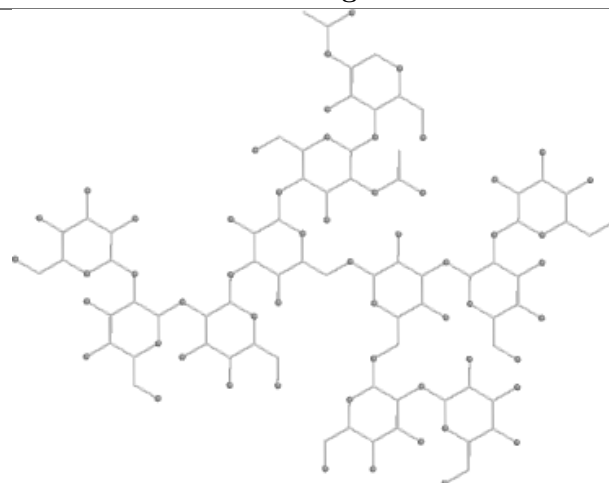
**Oligosaccharide Chain dA****Bond lengths****Bond angles****Torsions****Rings**

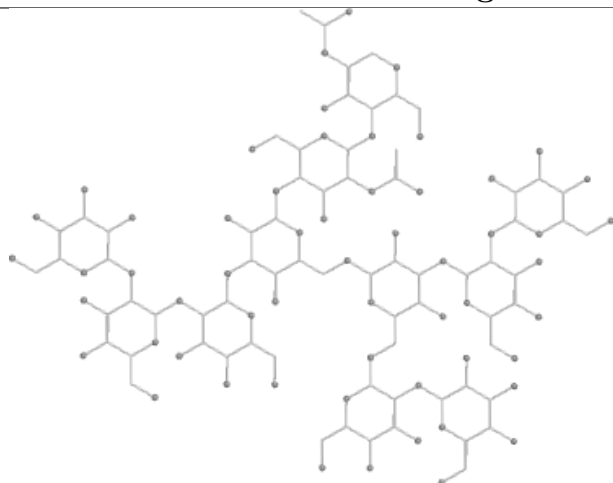
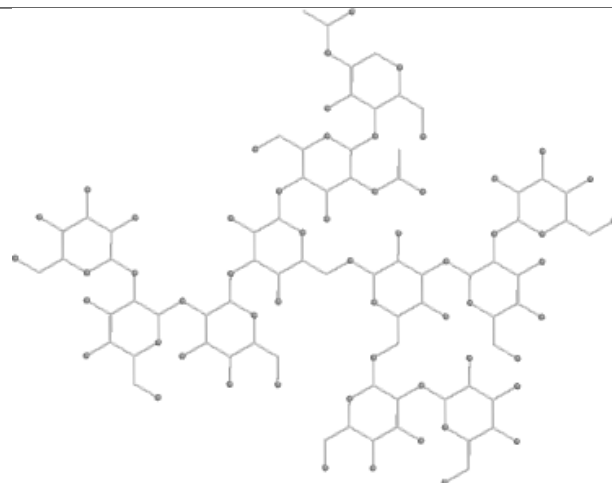
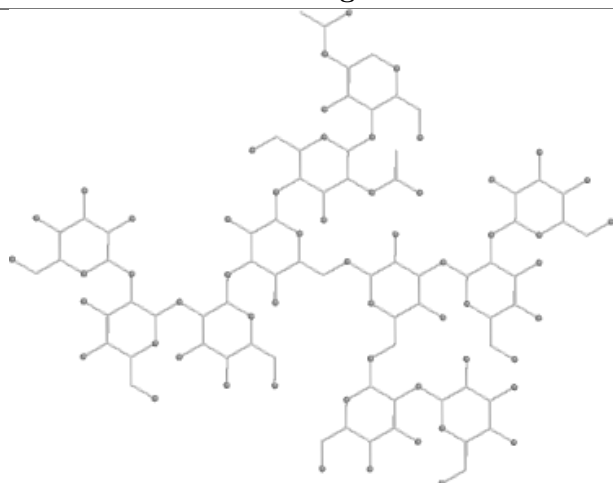
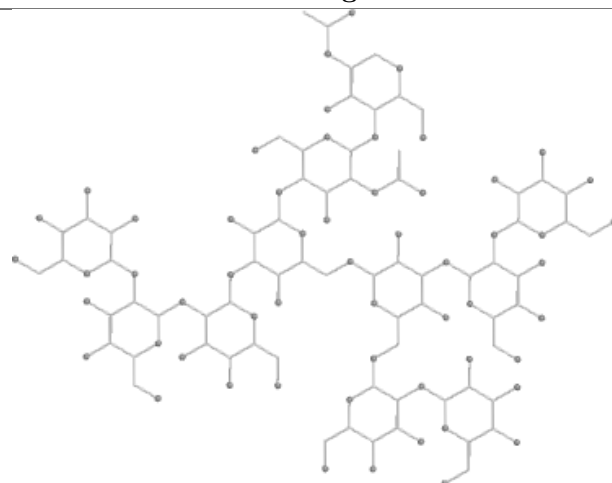


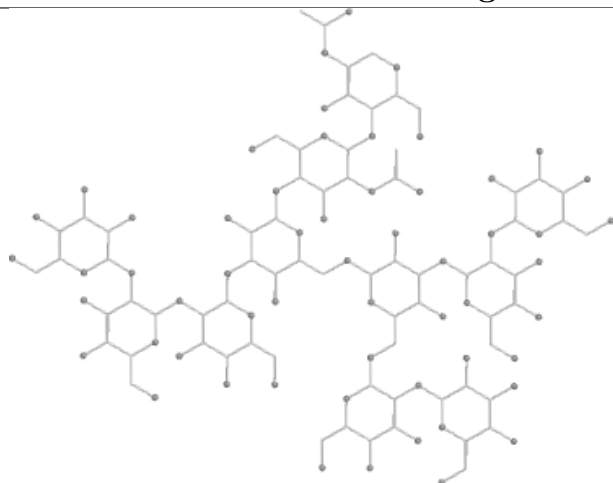
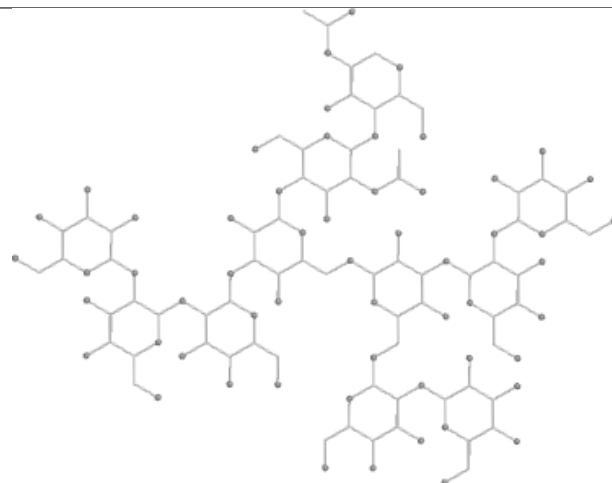
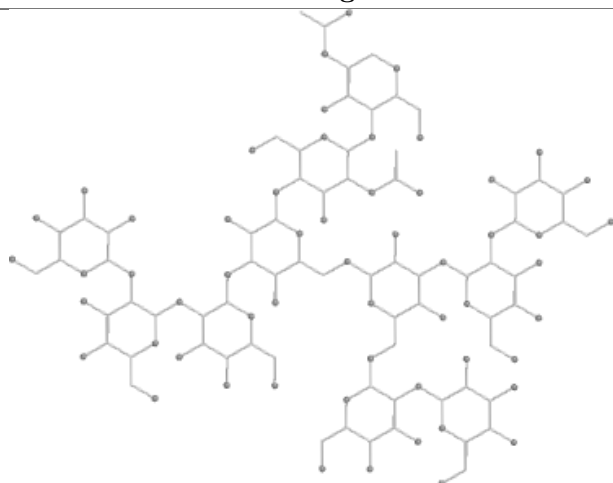
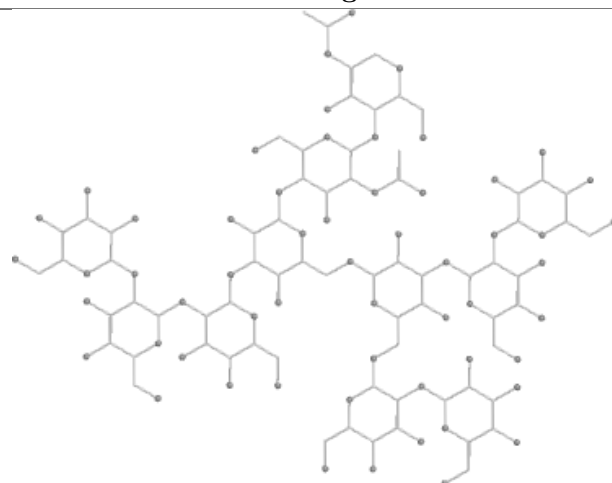


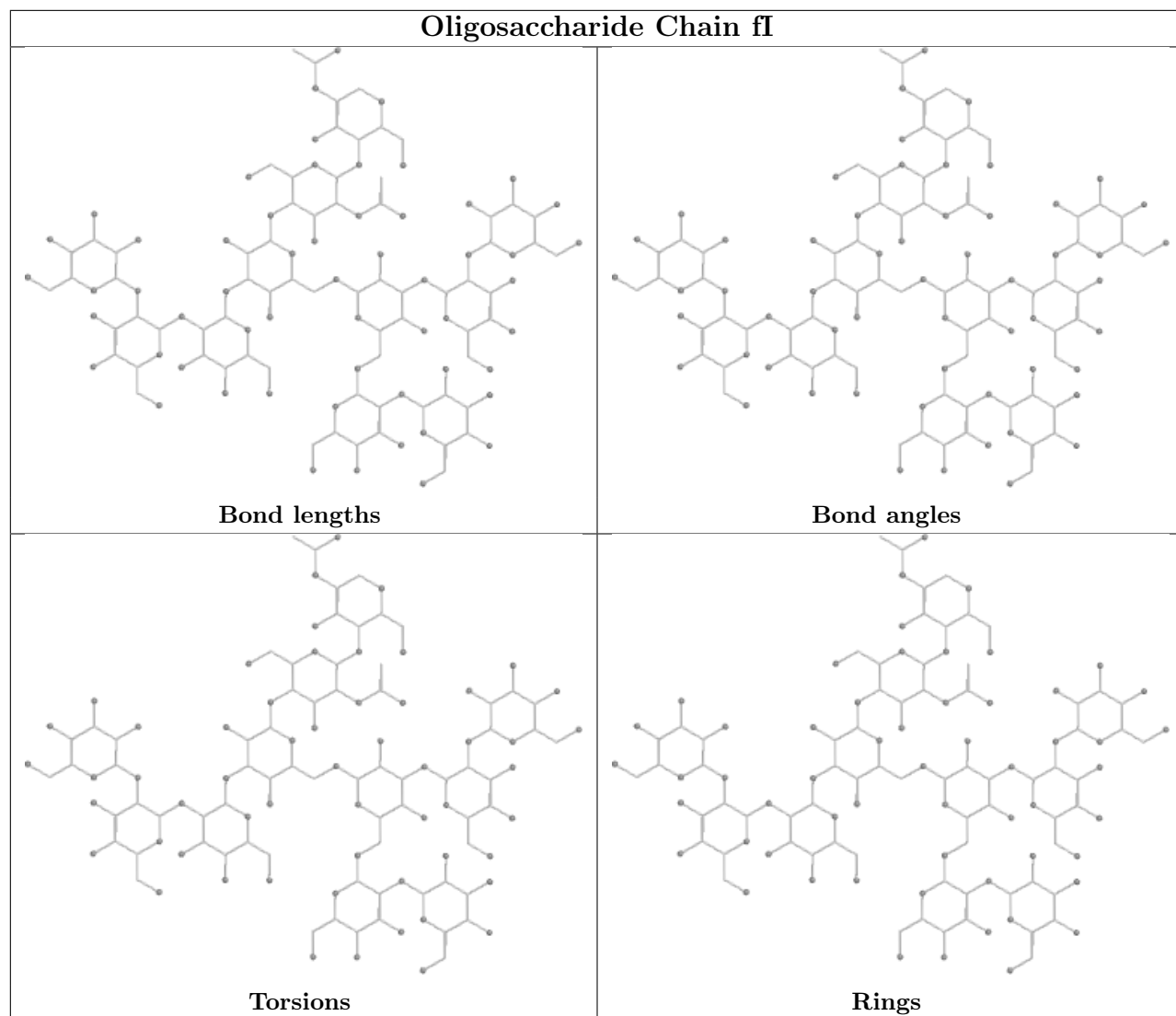
**Oligosaccharide Chain eA****Bond lengths****Bond angles****Torsions****Rings**

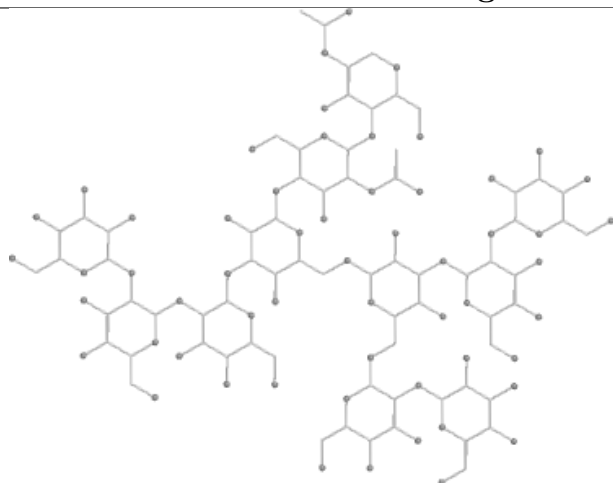
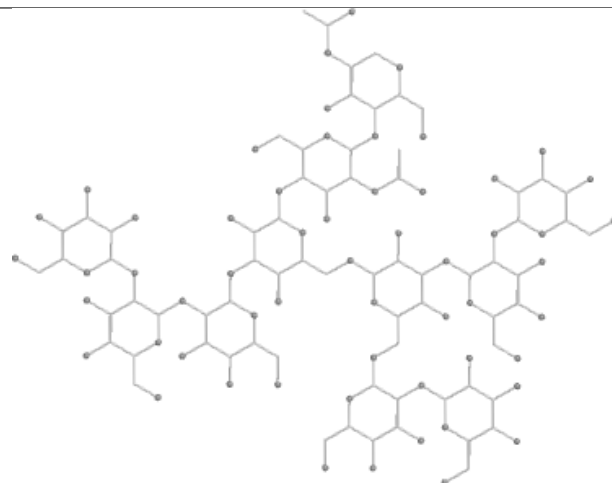
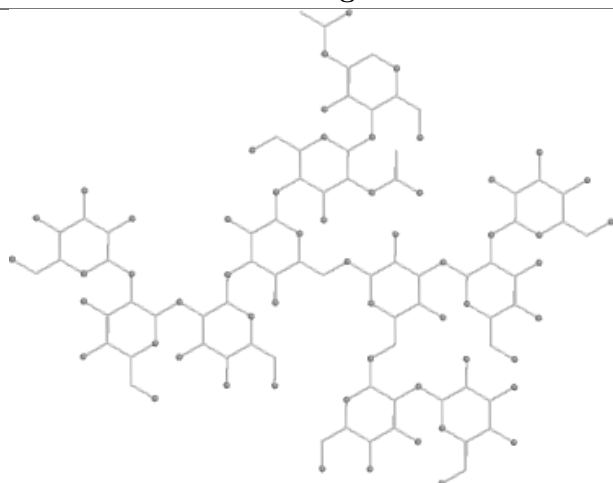
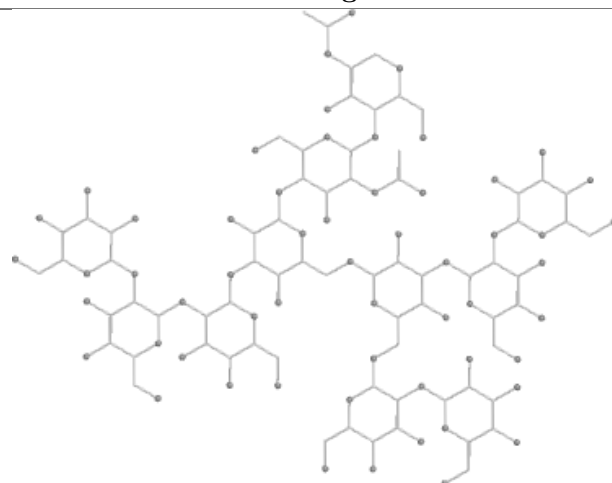


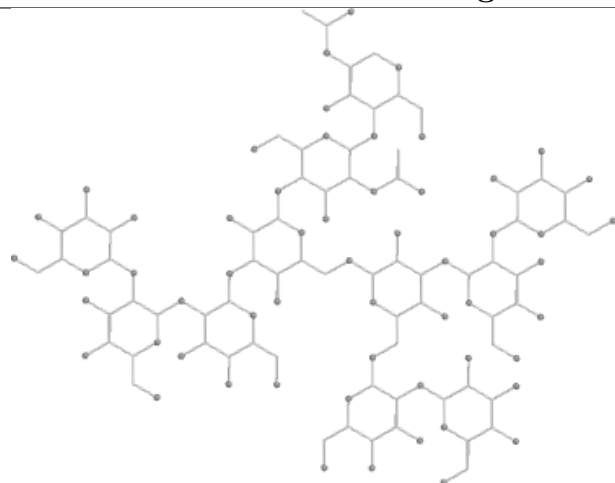
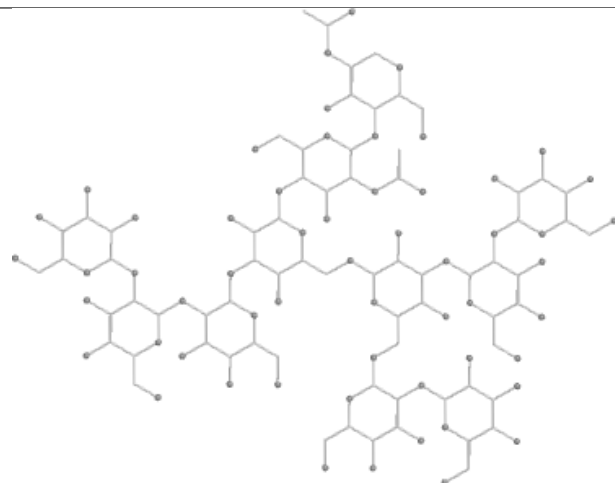
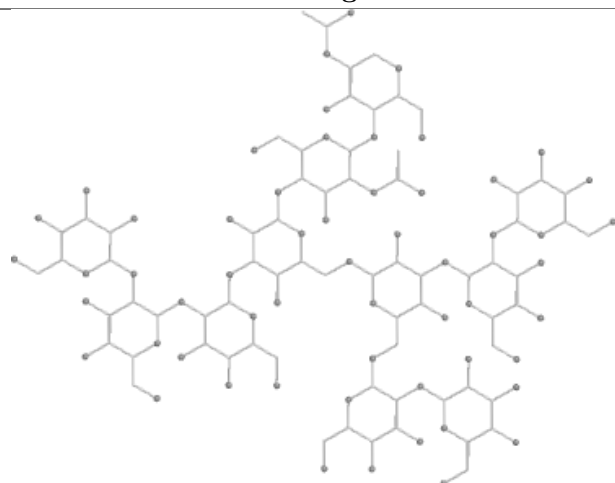
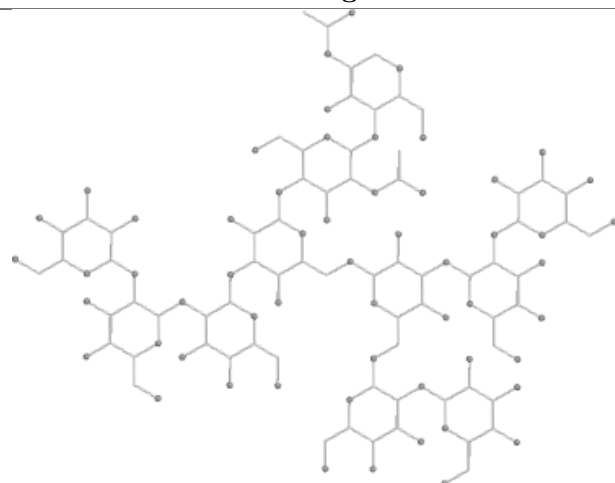
**Oligosaccharide Chain fD****Bond lengths****Bond angles****Torsions****Rings**

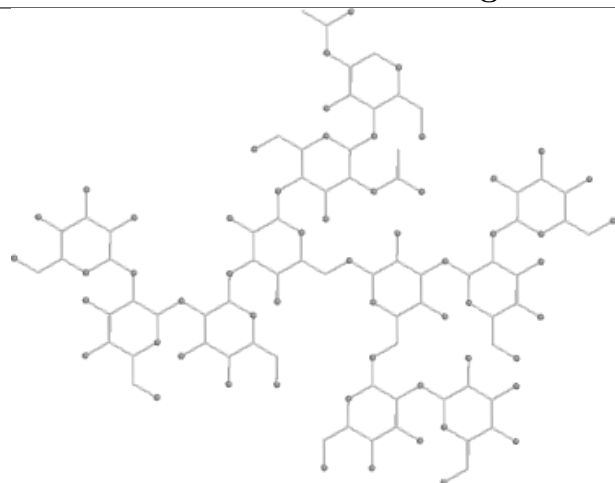
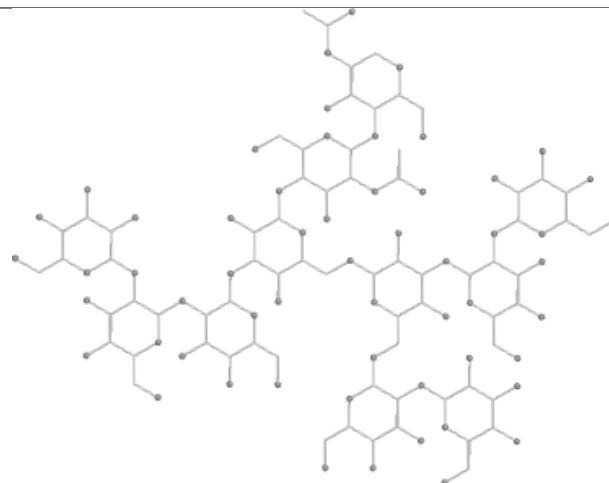
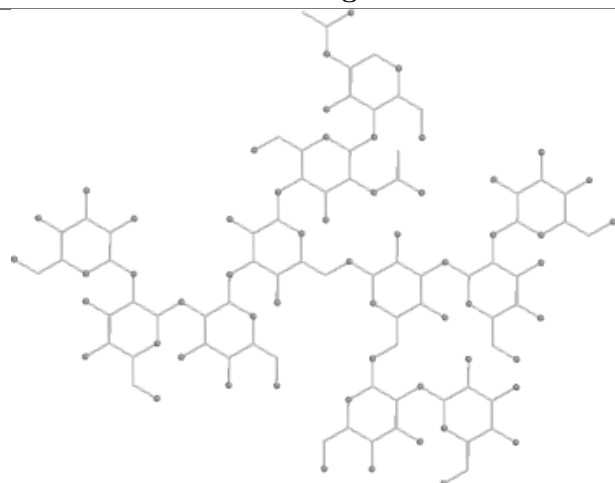
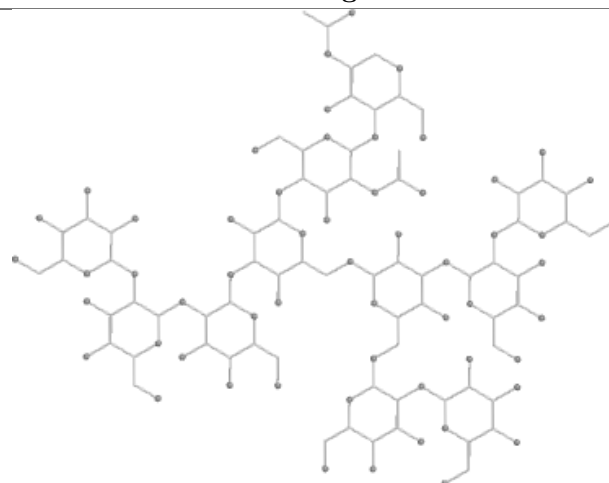
**Oligosaccharide Chain eC****Bond lengths****Bond angles****Torsions****Rings**

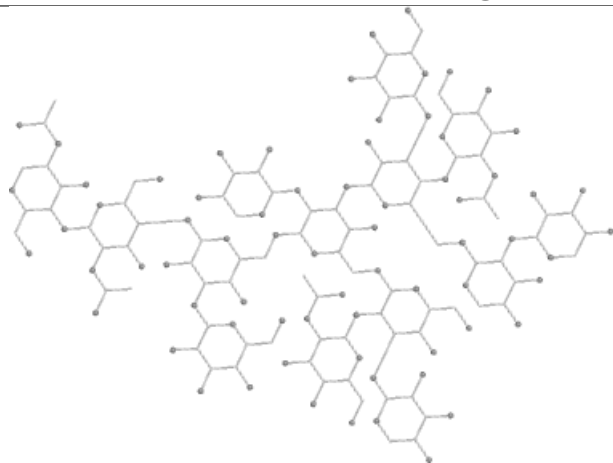
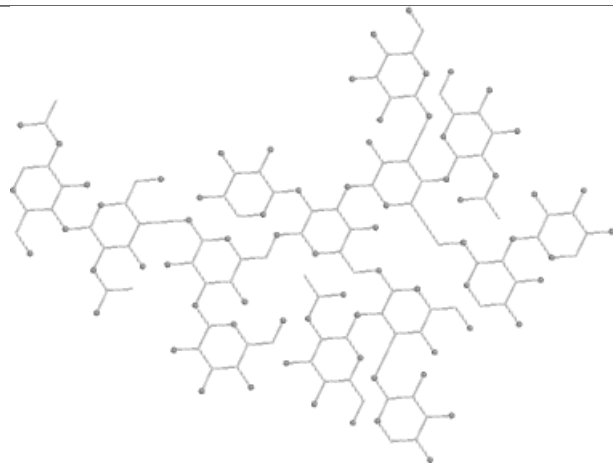
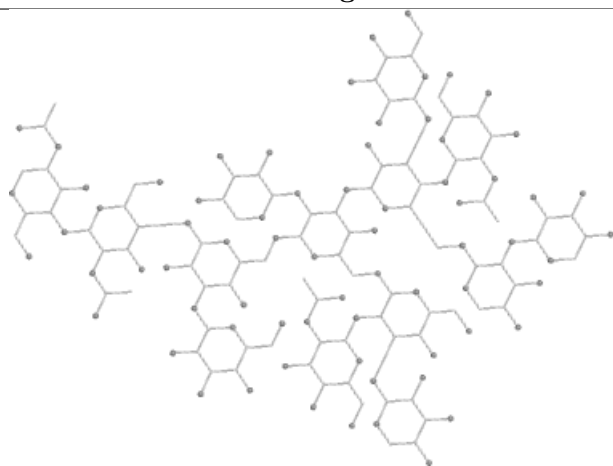
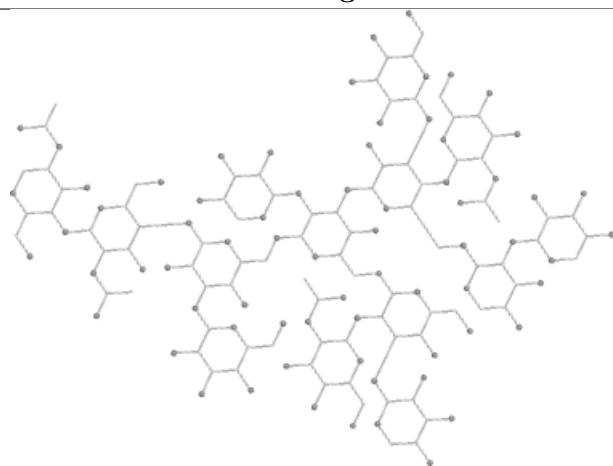
**Oligosaccharide Chain fH****Bond lengths****Bond angles****Torsions****Rings**

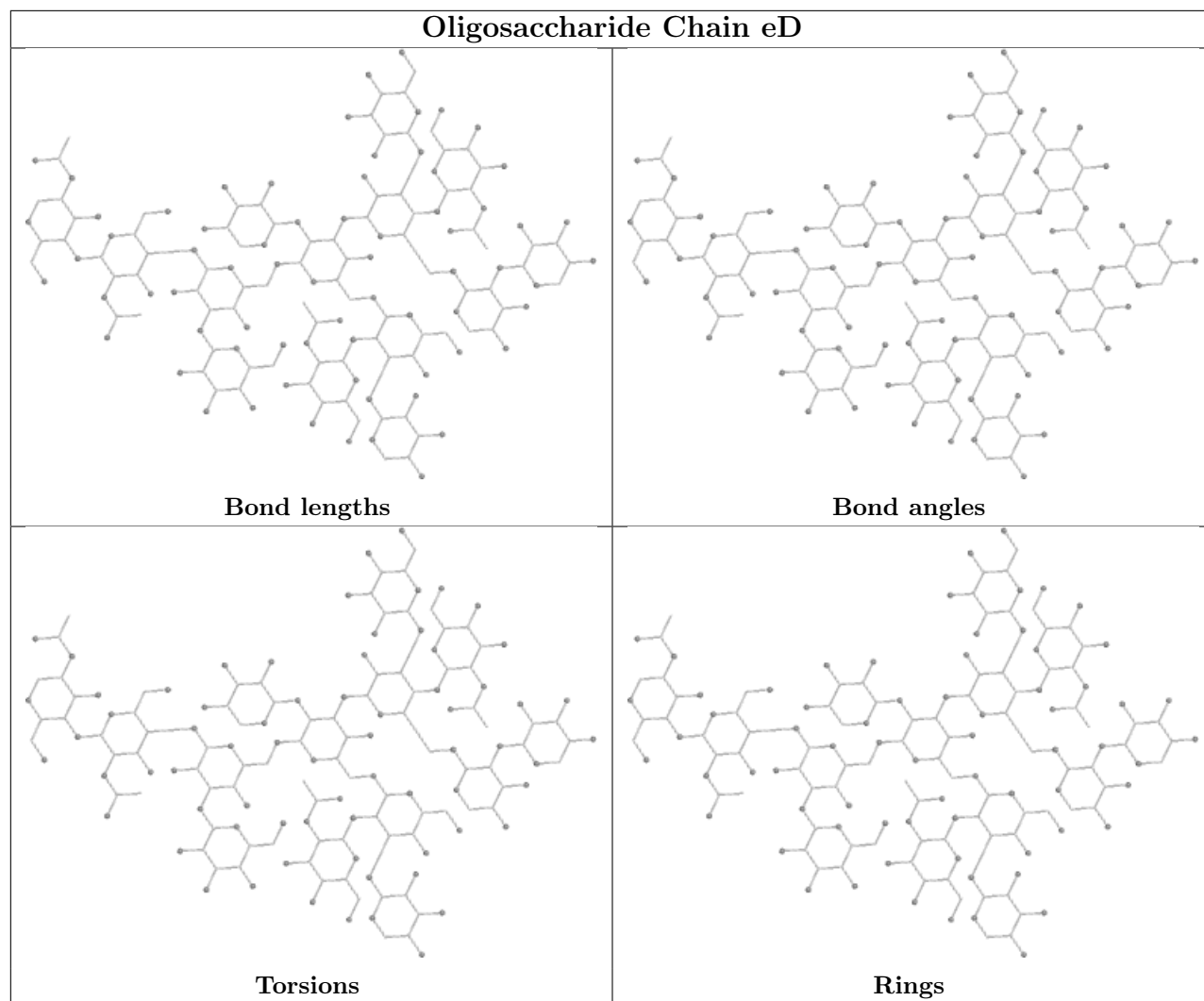


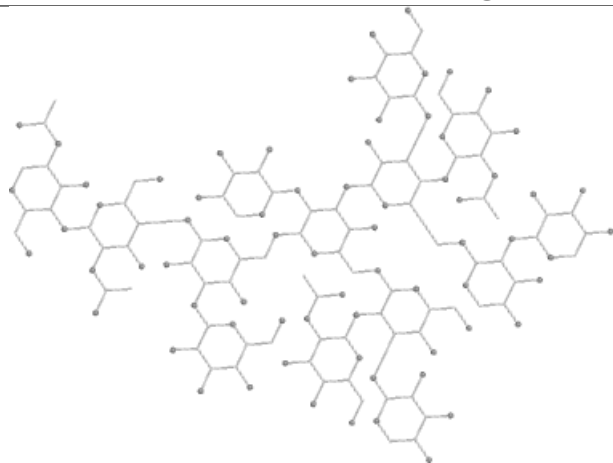
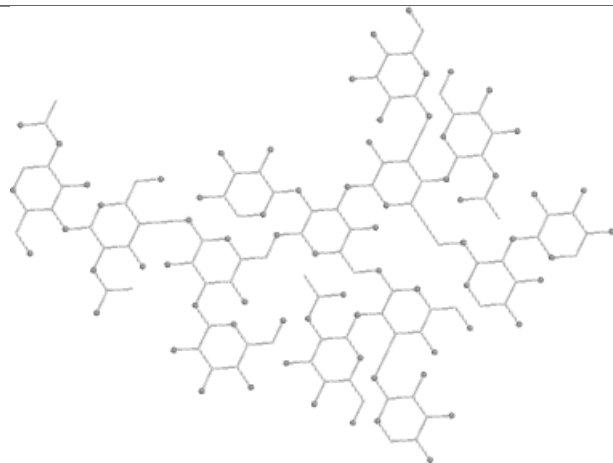
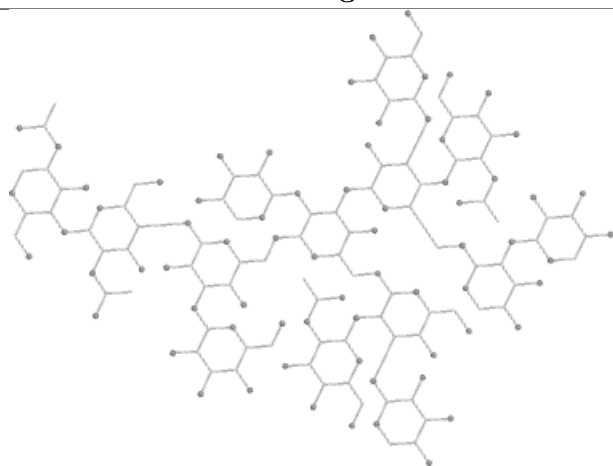
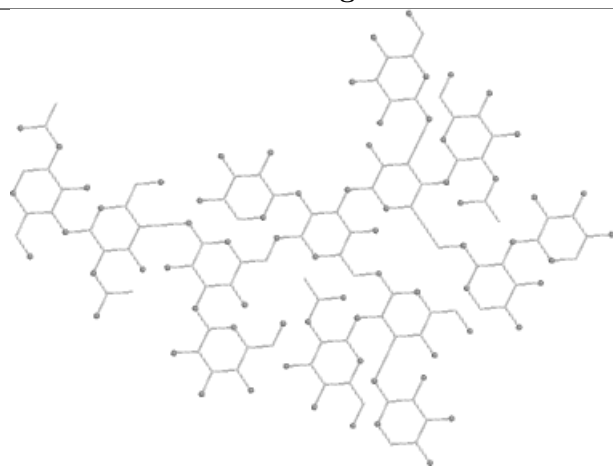
**Oligosaccharide Chain eE****Bond lengths****Bond angles****Torsions****Rings**

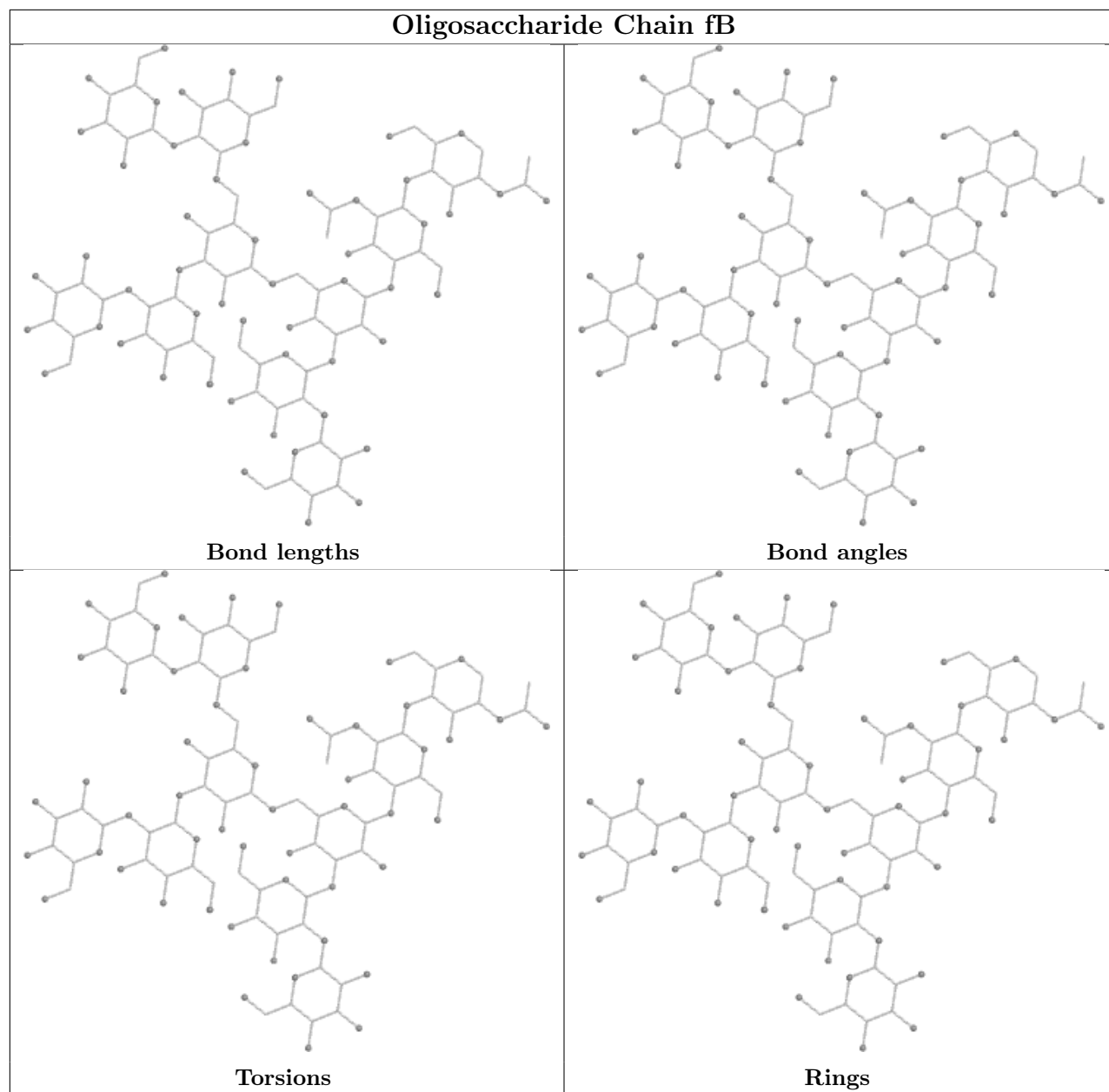
**Oligosaccharide Chain fM****Bond lengths****Bond angles****Torsions****Rings**

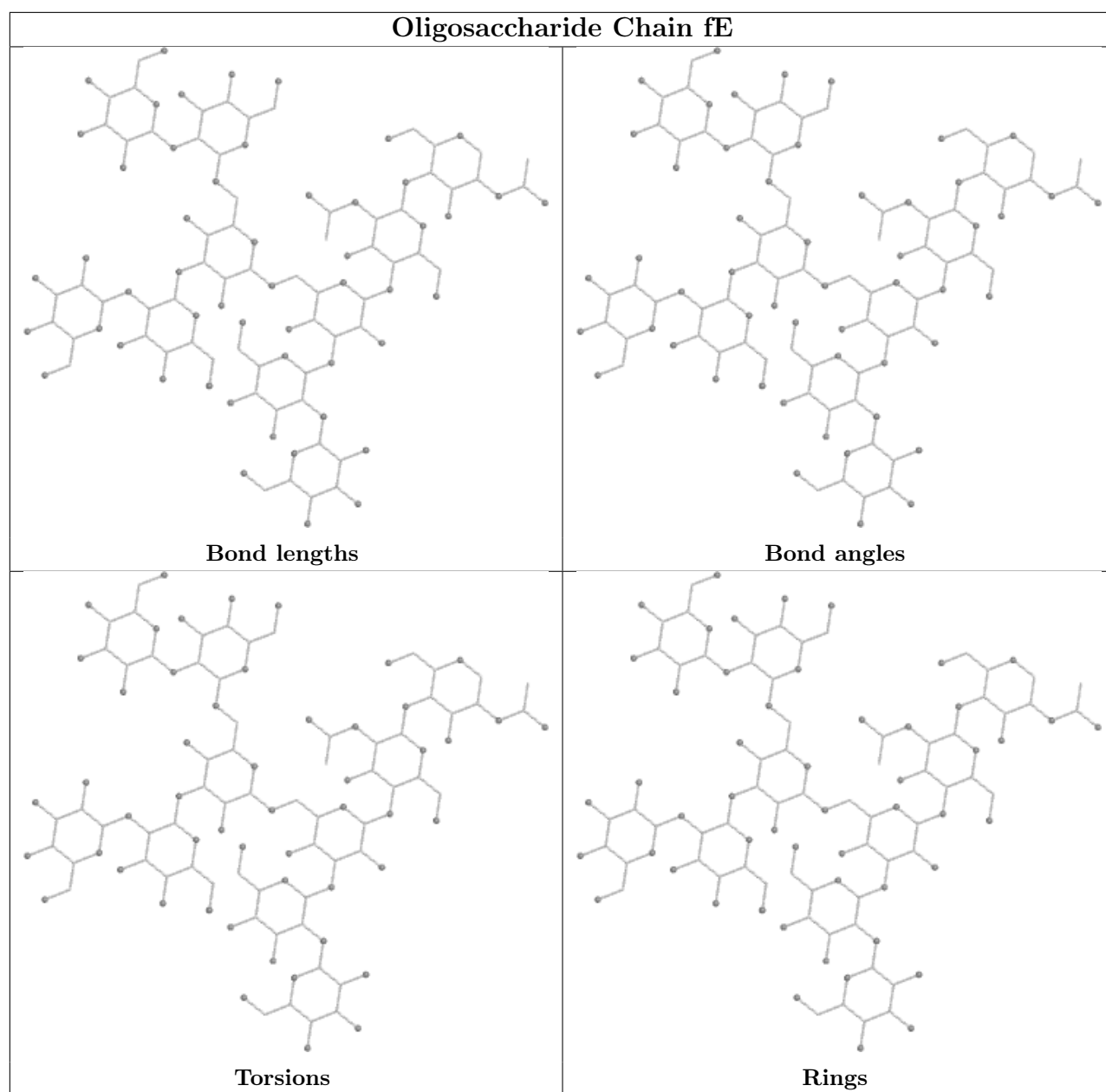
**Oligosaccharide Chain fN****Bond lengths****Bond angles****Torsions****Rings**

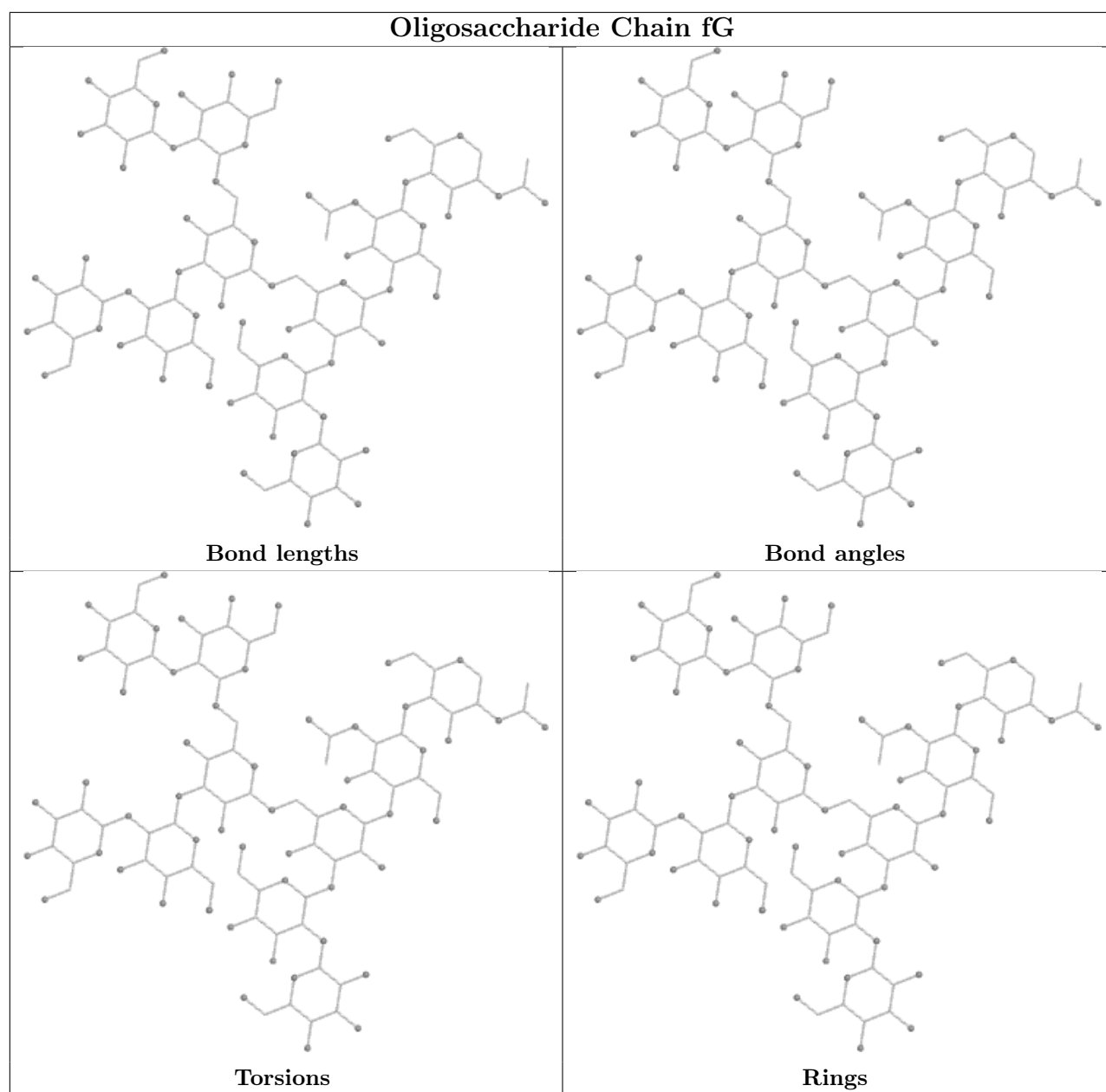
**Oligosaccharide Chain eB****Bond lengths****Bond angles****Torsions****Rings**

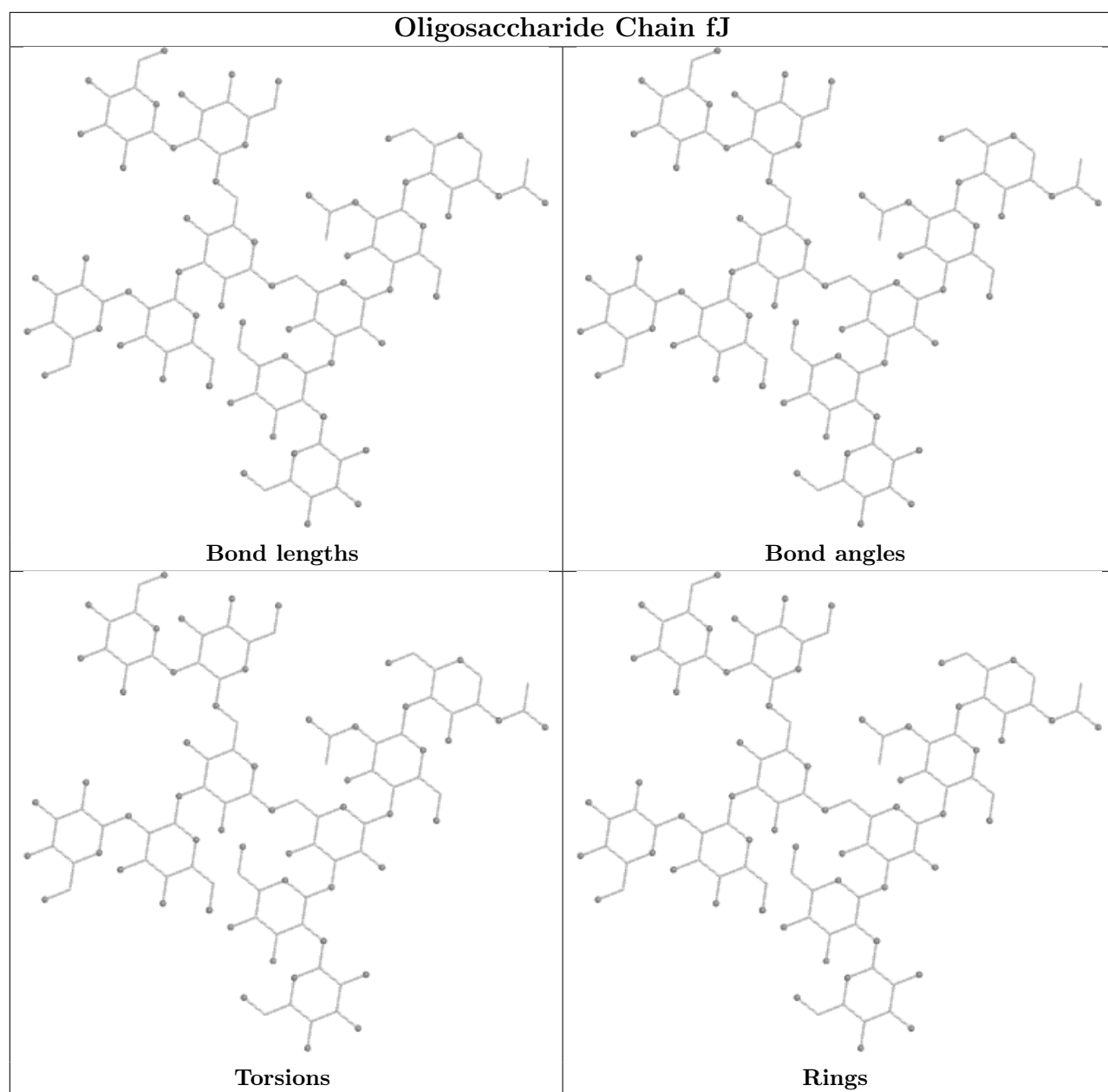


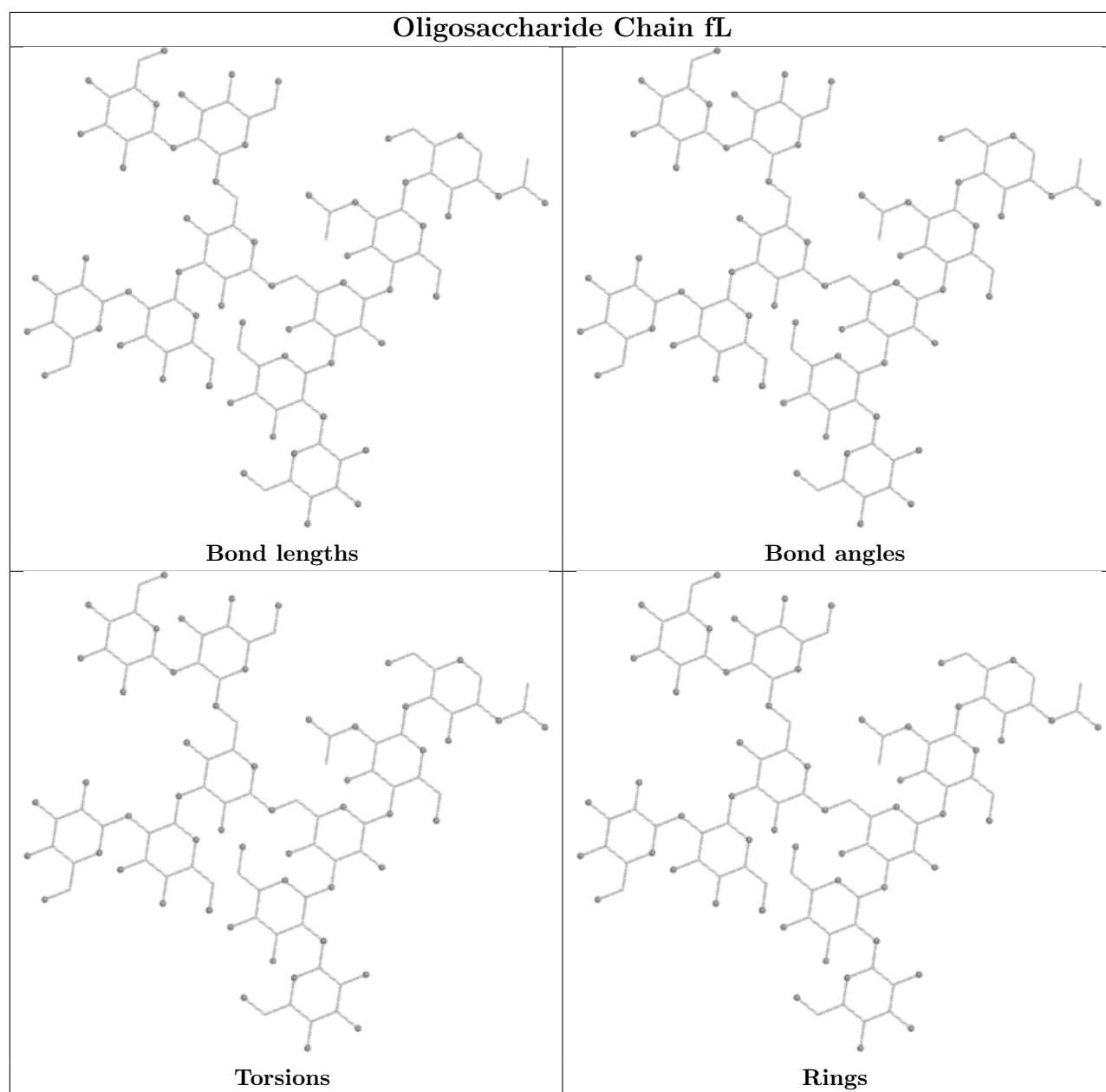
**Oligosaccharide Chain eF****Bond lengths****Bond angles****Torsions****Rings**

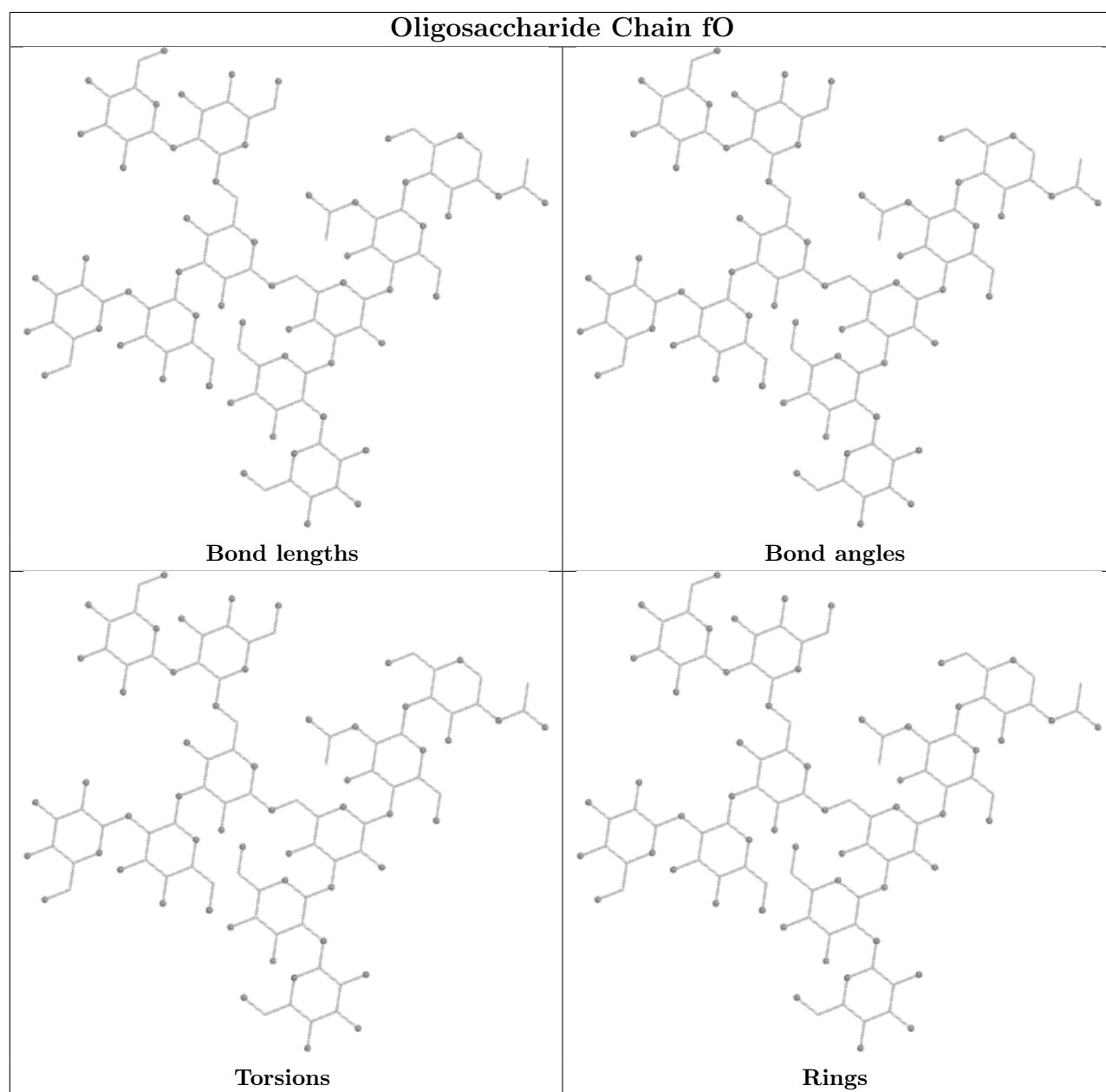


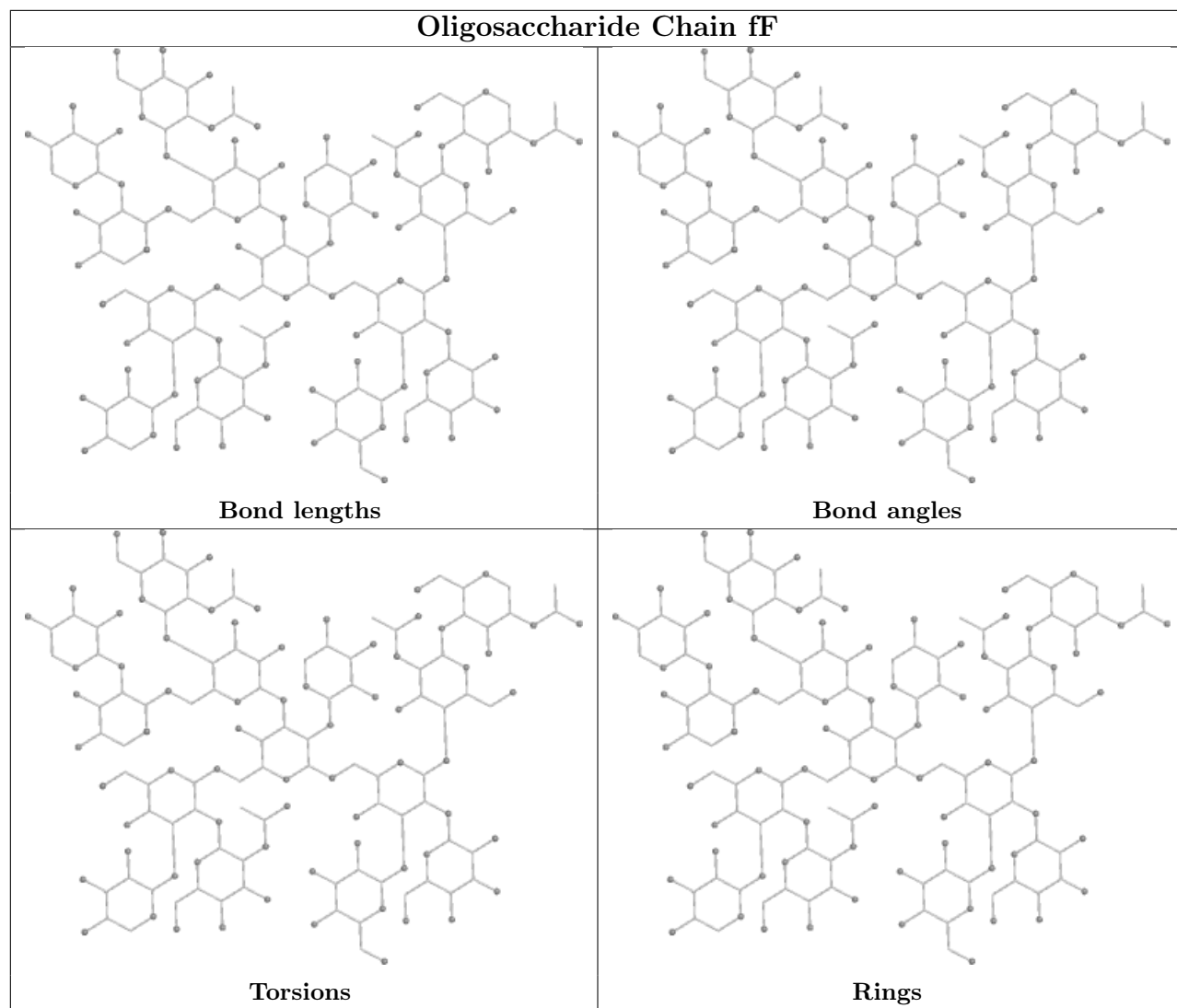


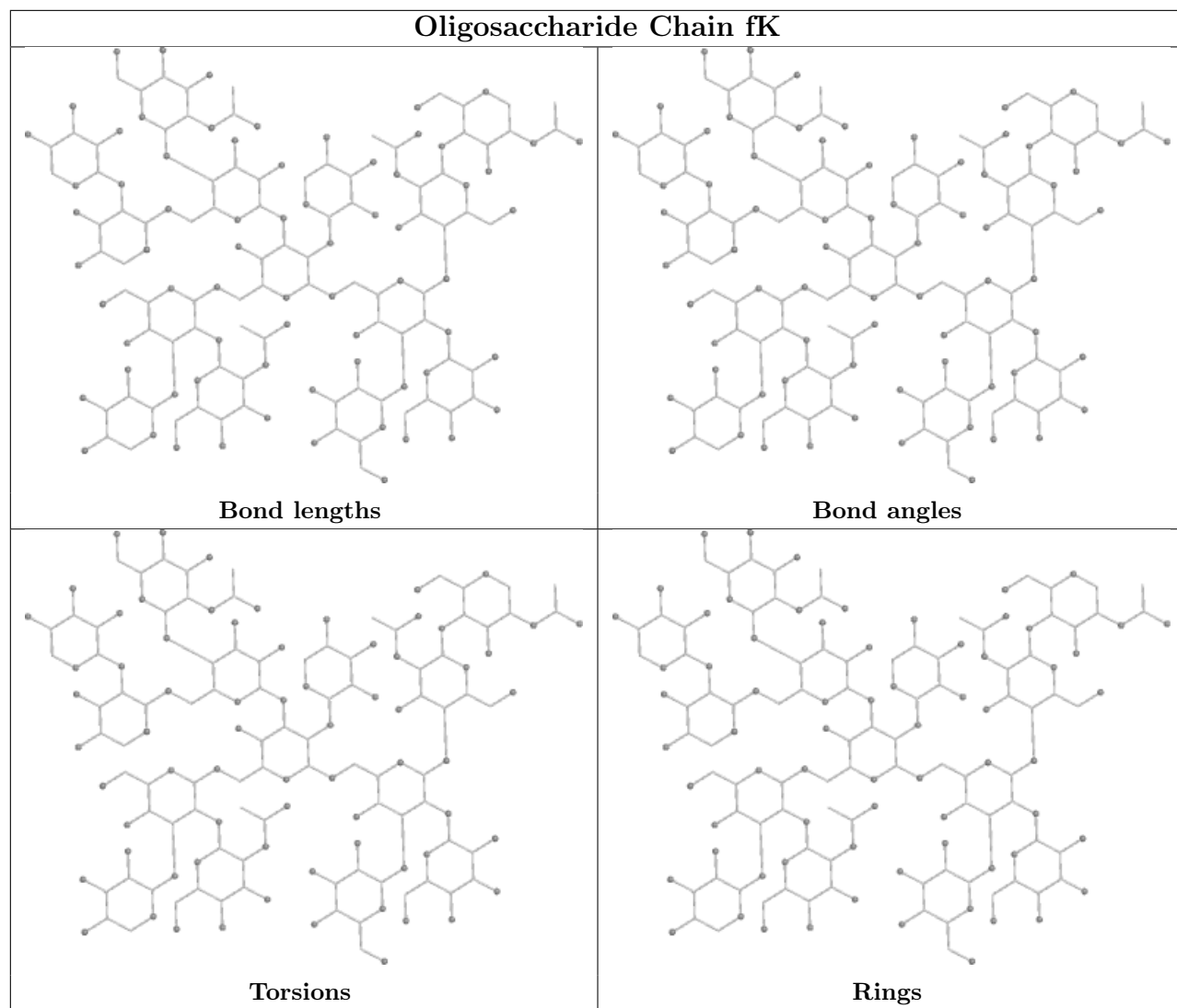


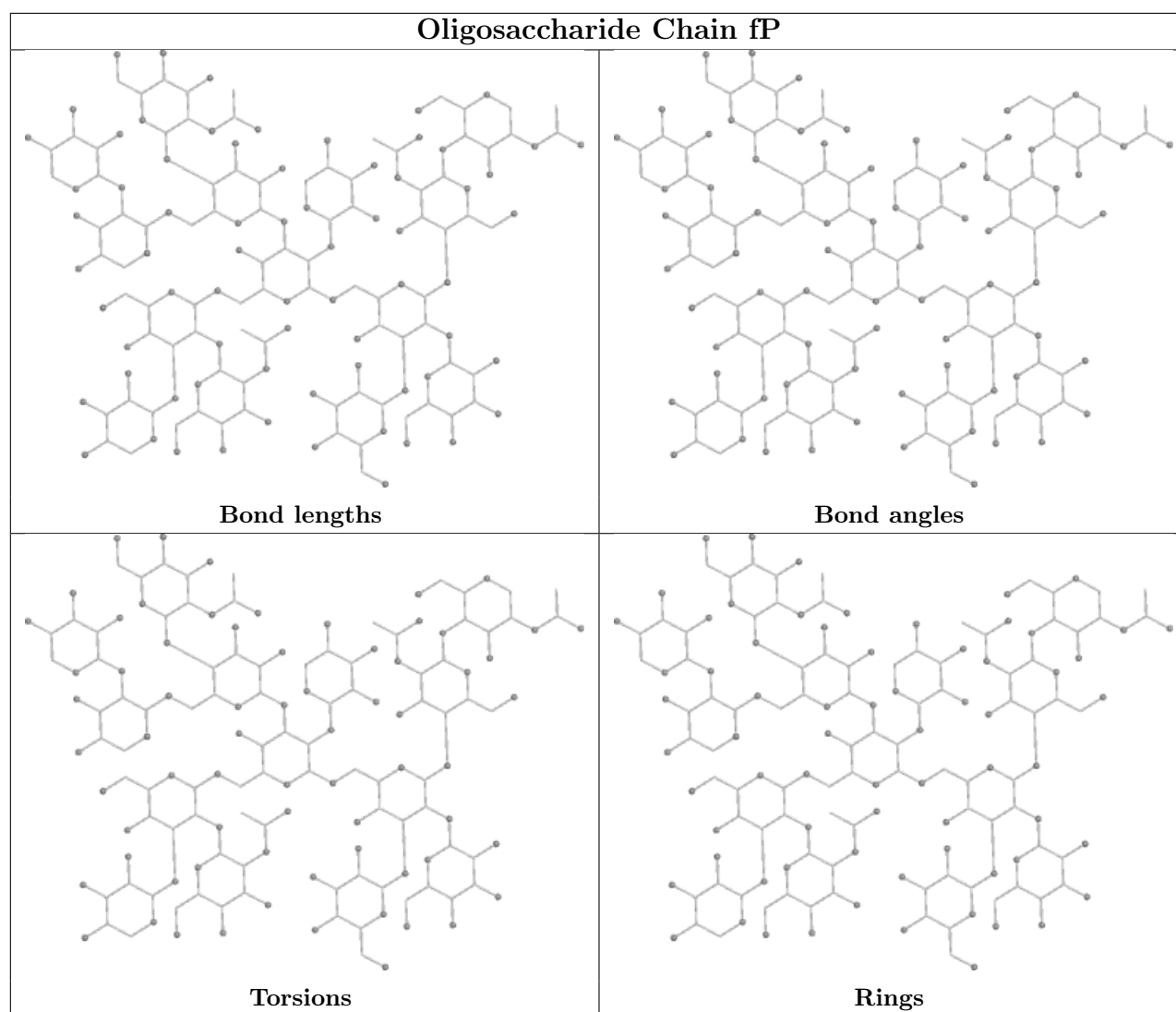












## 5.6 Ligand geometry [i](#)

Of 85 ligands modelled in this entry, 58 are monoatomic - leaving 27 for Mogul analysis.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 22  | NAG  | FA    | 801 | 2    | 14,14,15     | 0.37 | 0           | 17,19,21    | 0.63 | 0           |
| 22  | NAG  | FB    | 801 | 2    | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.81 | 0           |
| 23  | 2PO  | FC    | 802 | 20   | 0,3,3        | -    | -           | 0,3,3       | -    | -           |

| Mol | Type | Chain | Res | Link  | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|-------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |       | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 23  | 2PO  | FB    | 802 | 20    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 22  | NAG  | FC    | 801 | 2     | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.64 | 0        |
| 23  | 2PO  | AC    | 802 | 8     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | EA    | 403 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BA    | 401 | 21,11 | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BC    | 401 | 21    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BA    | 402 | 14    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AC    | 803 | 9     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 22  | NAG  | EA    | 402 | 1     | 14,14,15     | 0.39 | 0        | 17,19,21    | 1.04 | 1 (5%)   |
| 23  | 2PO  | EC    | 402 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | EB    | 402 | 18    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 22  | NAG  | EB    | 401 | 1     | 14,14,15     | 0.34 | 0        | 17,19,21    | 1.03 | 1 (5%)   |
| 23  | 2PO  | AA    | 803 | 9     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 22  | NAG  | EC    | 401 | 1     | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.88 | 1 (5%)   |
| 23  | 2PO  | AC    | 801 | 7     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BB    | 401 | 21    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AB    | 802 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BC    | 402 | 14    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | FA    | 802 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AB    | 803 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AA    | 801 | 7     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | BB    | 402 | 14    | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AA    | 802 | -     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |
| 23  | 2PO  | AB    | 801 | 7     | 0,3,3        | -    | -        | 0,3,3       | -    | -        |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 22  | NAG  | EB    | 401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 22  | NAG  | FA    | 801 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 22  | NAG  | FB    | 801 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 22  | NAG  | FC    | 801 | 2    | -       | 0/6/23/26 | 0/1/1/1 |
| 22  | NAG  | EA    | 402 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 22  | NAG  | EC    | 401 | 1    | -       | 0/6/23/26 | 0/1/1/1 |

There are no bond length outliers.

All (3) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed( $^{\circ}$ ) | Ideal( $^{\circ}$ ) |
|-----|-------|-----|------|----------|------|------------------------|---------------------|
| 22  | EA    | 402 | NAG  | C1-O5-C5 | 3.44 | 116.85                 | 112.19              |
| 22  | EB    | 401 | NAG  | C1-O5-C5 | 2.96 | 116.20                 | 112.19              |
| 22  | EC    | 401 | NAG  | C1-O5-C5 | 2.72 | 115.88                 | 112.19              |

There are no chirality outliers.

All (1) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 22  | EA    | 402 | NAG  | C4-C5-C6-O6 |

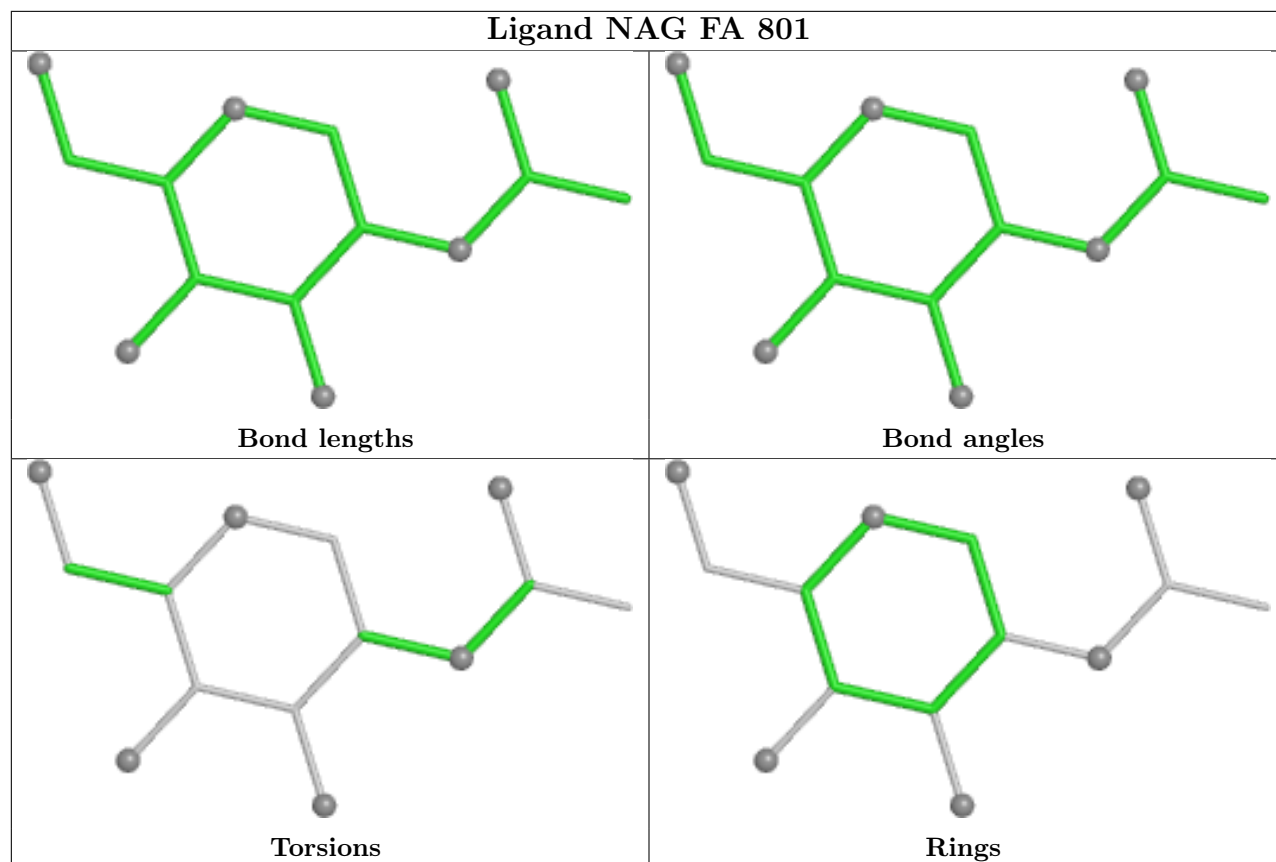
There are no ring outliers.

3 monomers are involved in 3 short contacts:

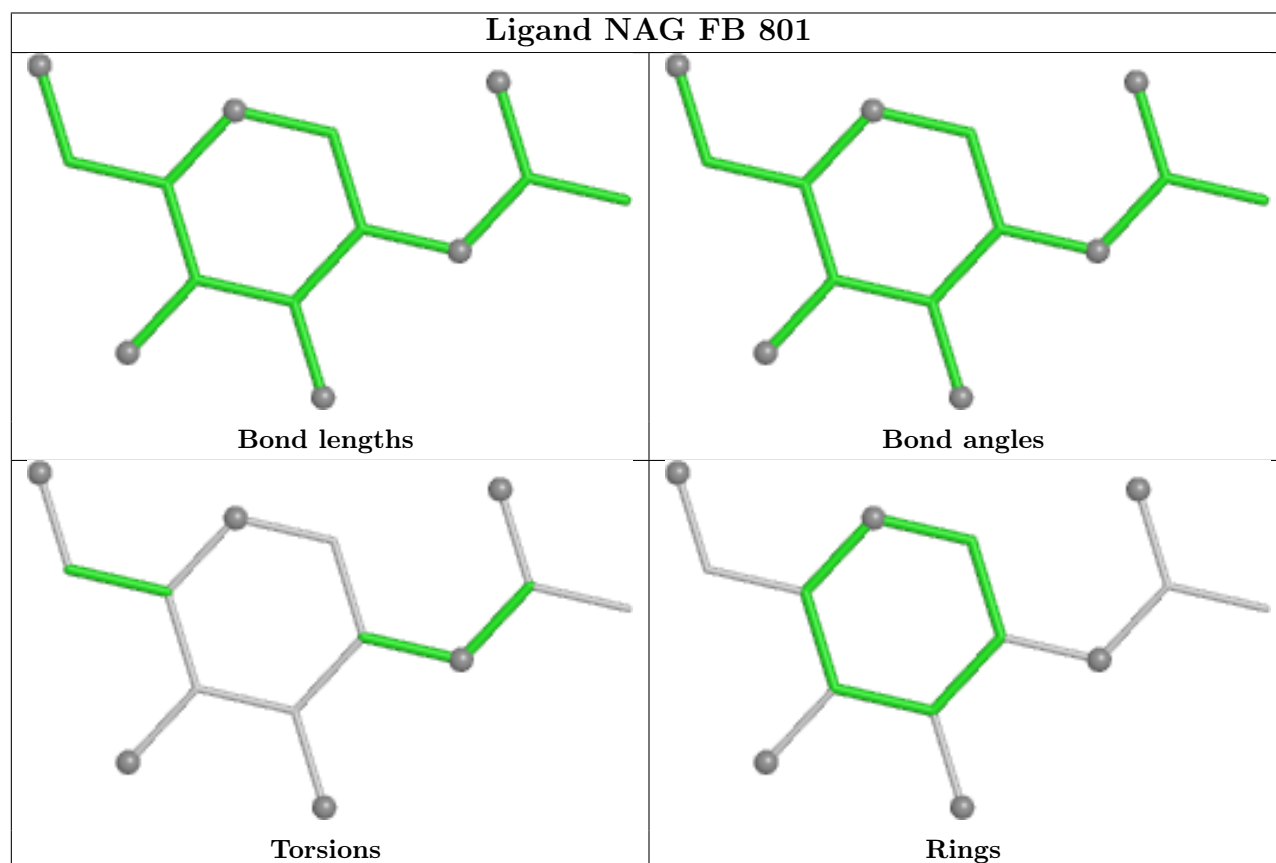
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 22  | EA    | 402 | NAG  | 1       | 0            |
| 22  | EB    | 401 | NAG  | 1       | 0            |
| 22  | EC    | 401 | NAG  | 1       | 0            |

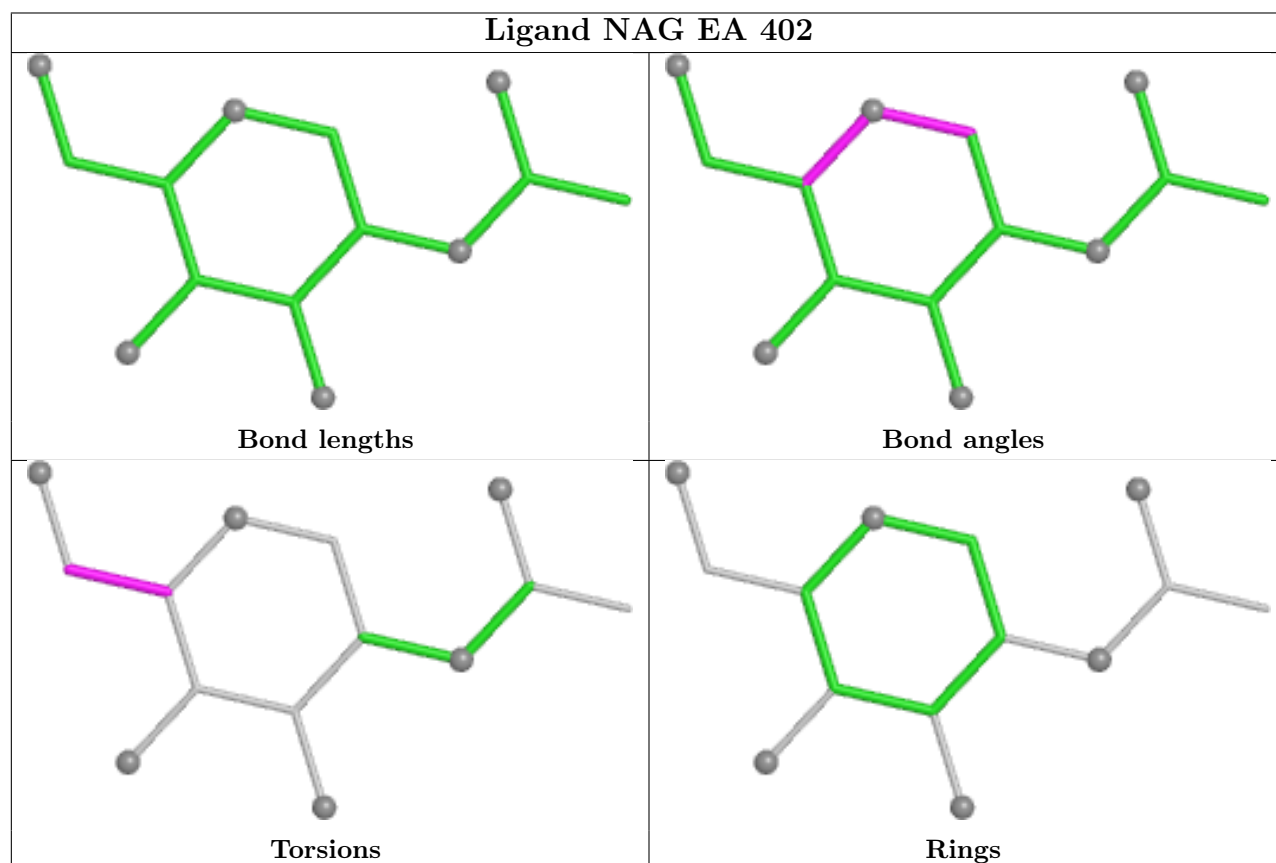
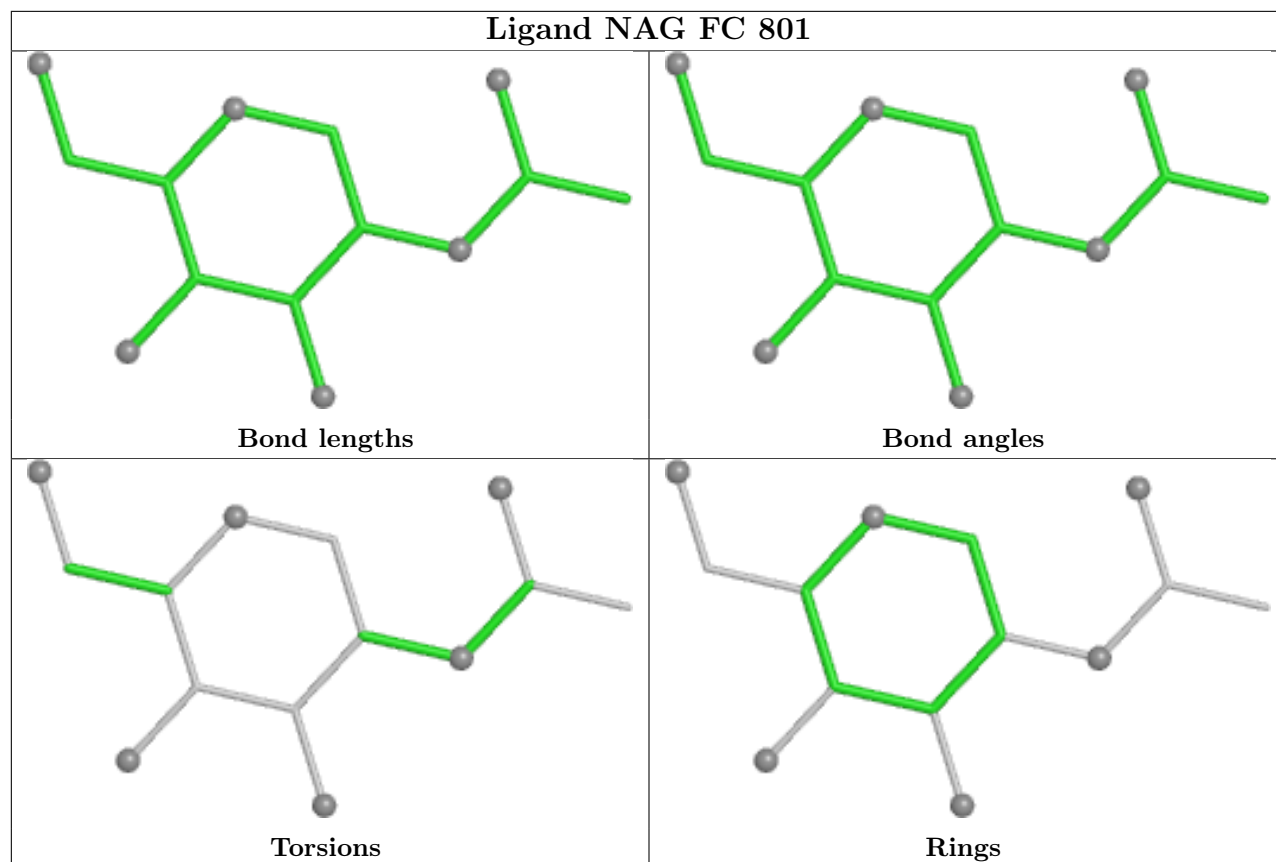
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

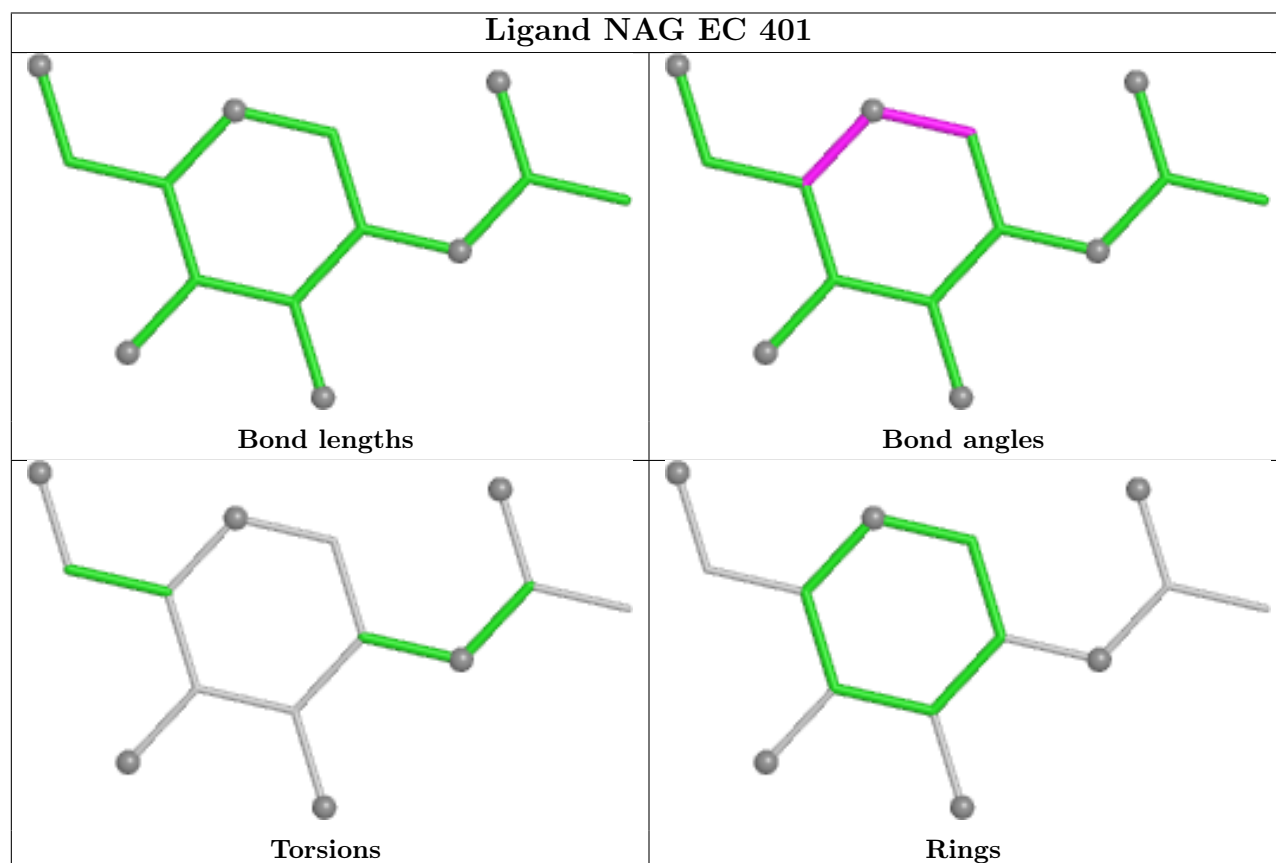
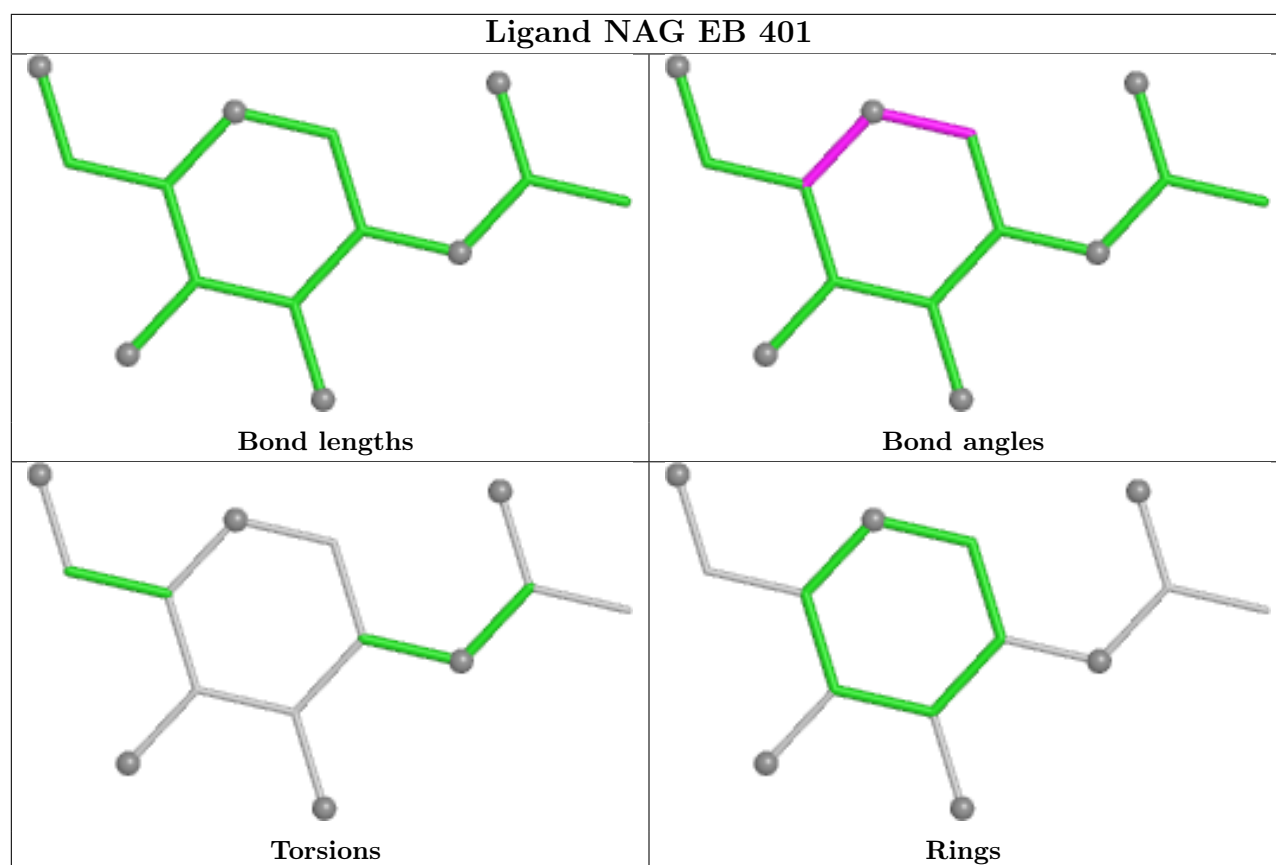
## Ligand NAG FA 801



## Ligand NAG FB 801







## 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.

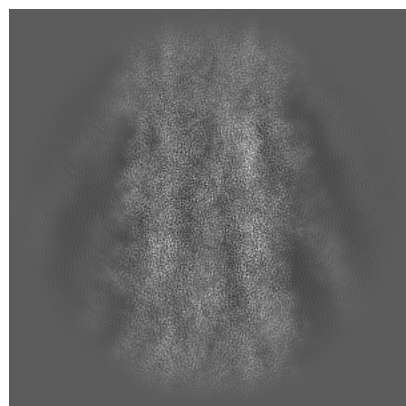
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-64106. These allow visual inspection of the internal detail of the map and identification of artifacts.

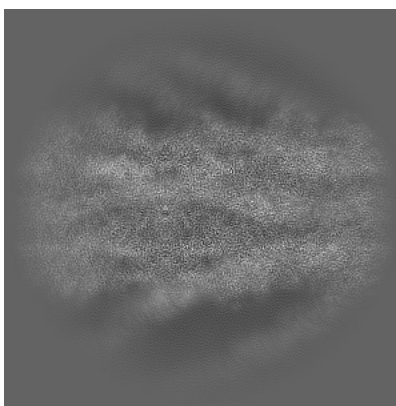
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

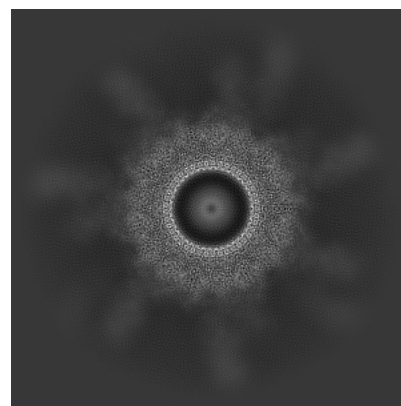
#### 6.1.1 Primary map



X

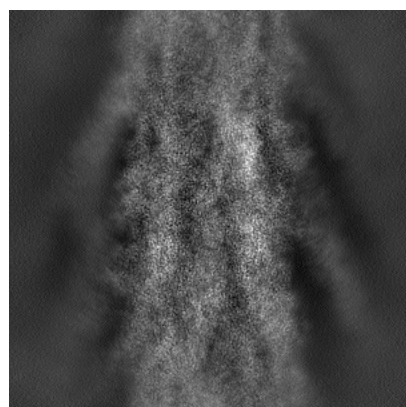


Y

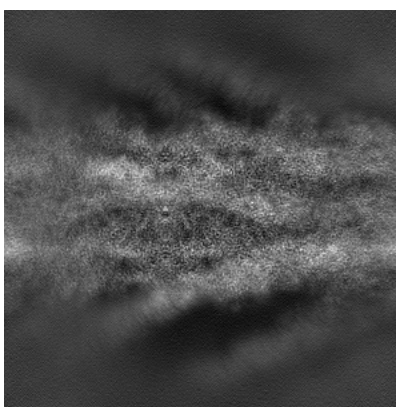


Z

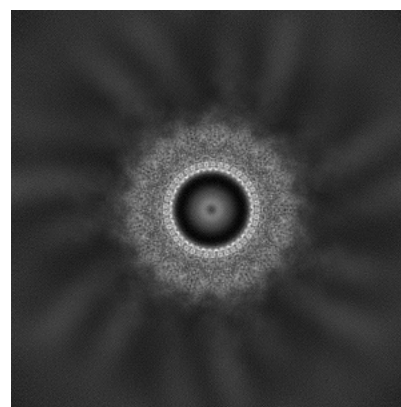
#### 6.1.2 Raw map



X



Y

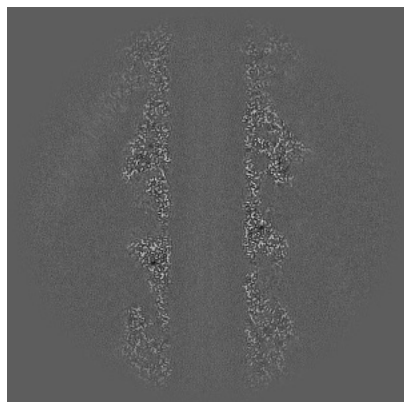


Z

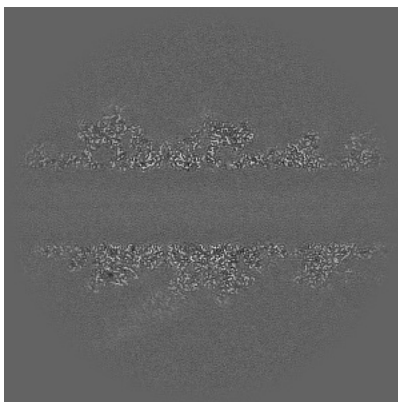
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

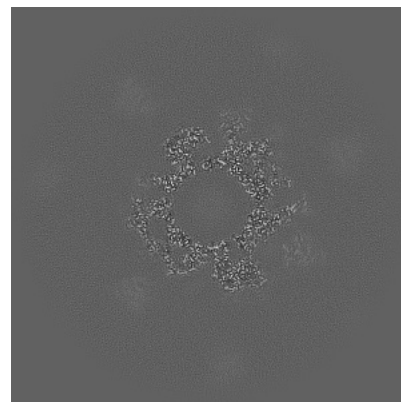
### 6.2.1 Primary map



X Index: 256

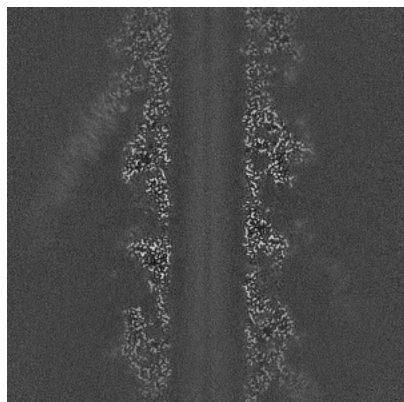


Y Index: 256

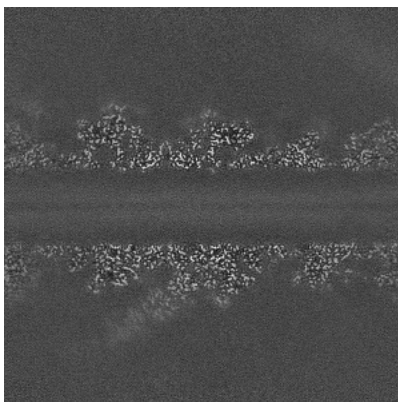


Z Index: 256

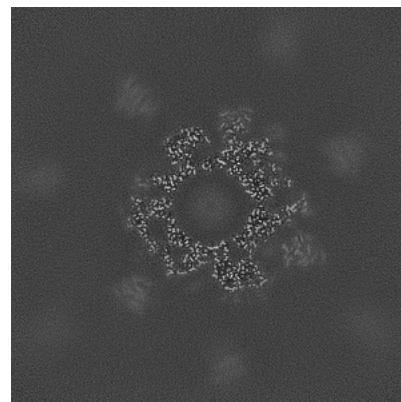
### 6.2.2 Raw map



X Index: 256



Y Index: 256

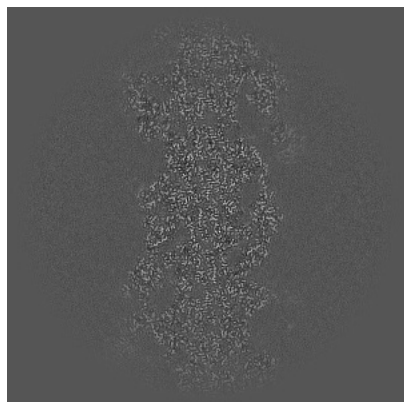


Z Index: 256

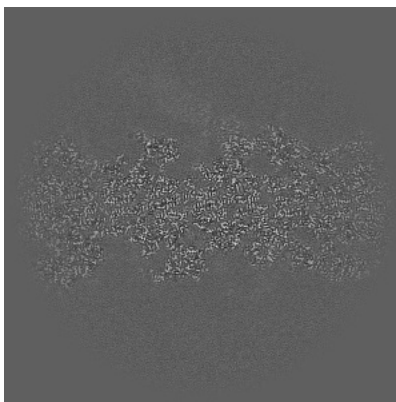
The images above show central slices of the map in three orthogonal directions.

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

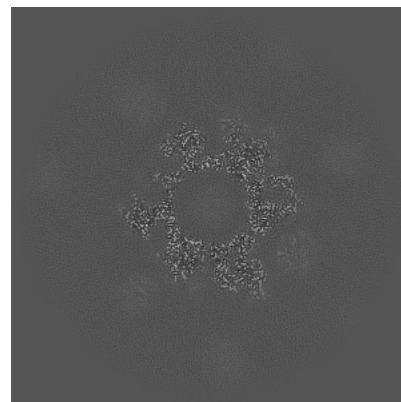
### 6.3.1 Primary map



X Index: 204

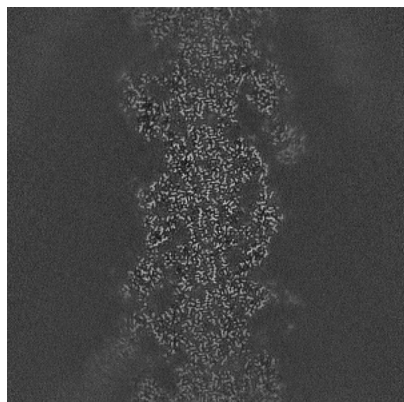


Y Index: 204

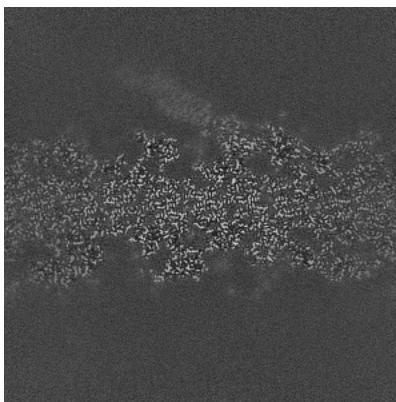


Z Index: 266

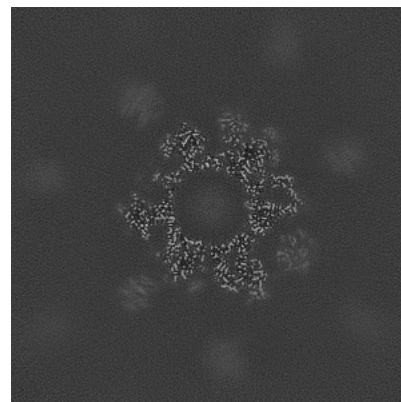
### 6.3.2 Raw map



X Index: 204



Y Index: 204

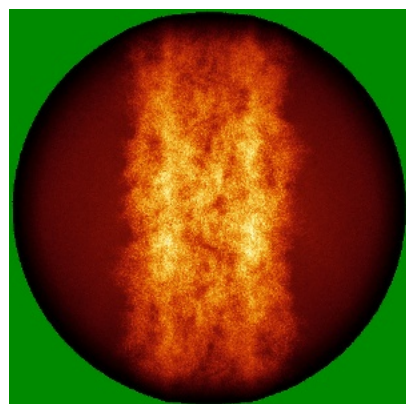


Z Index: 266

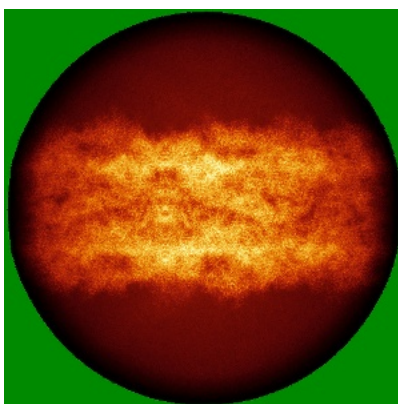
The images above show the largest variance slices of the map in three orthogonal directions.

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

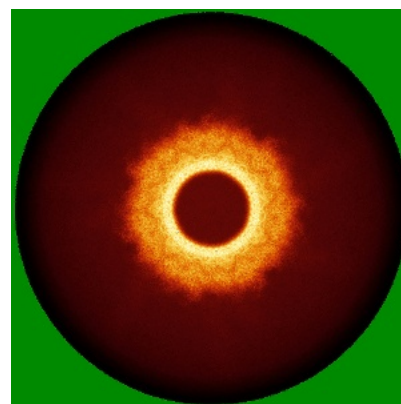
### 6.4.1 Primary map



X

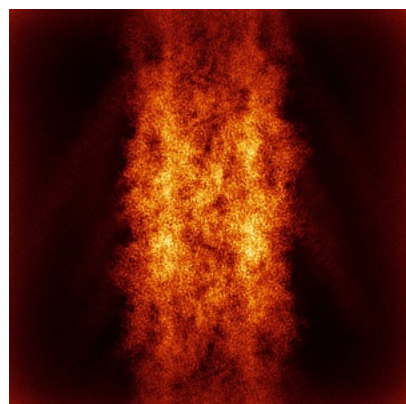


Y

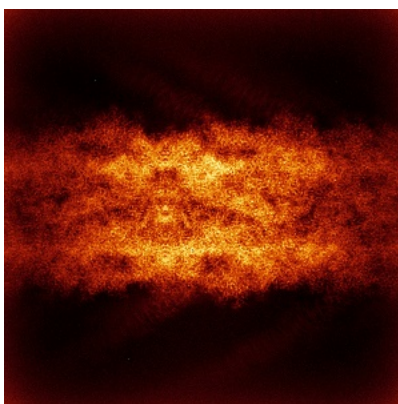


Z

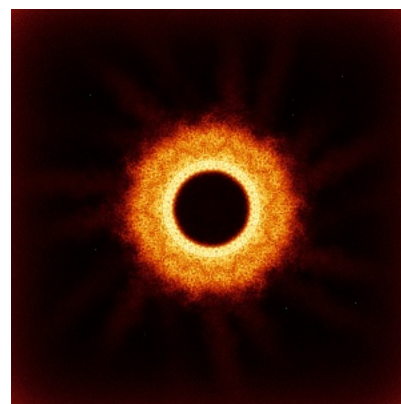
### 6.4.2 Raw map



X



Y

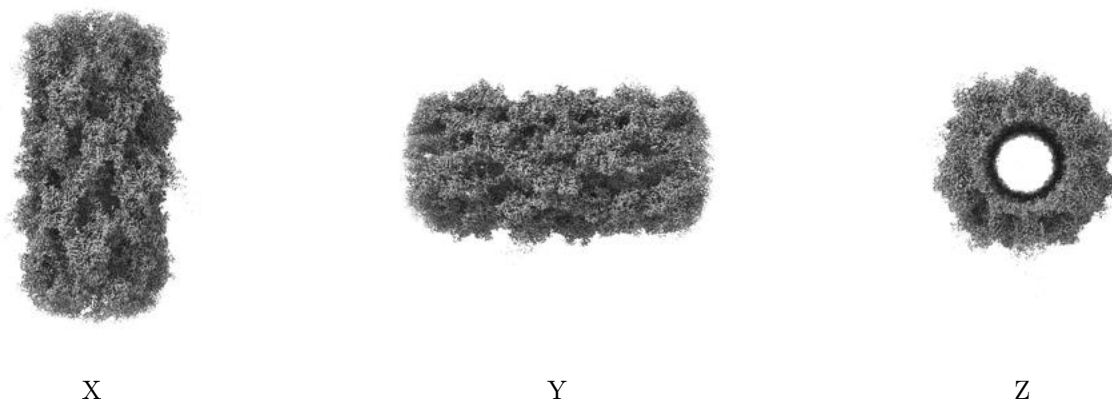


Z

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.

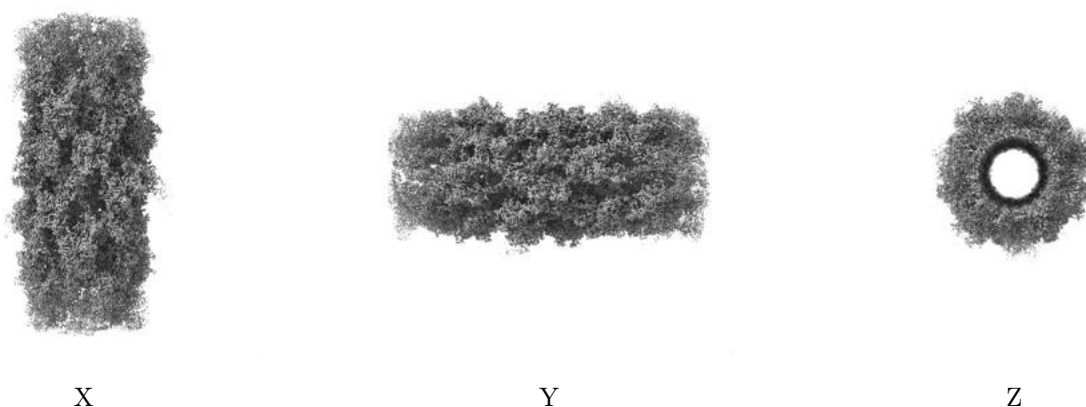
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

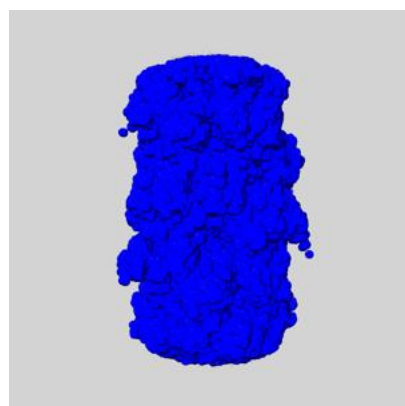
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

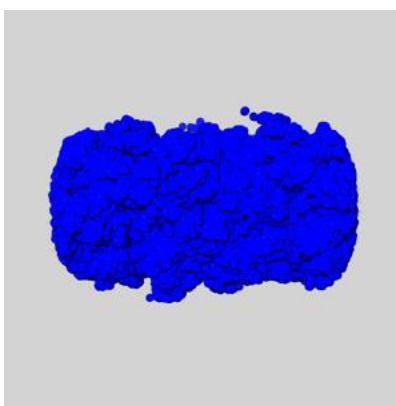
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

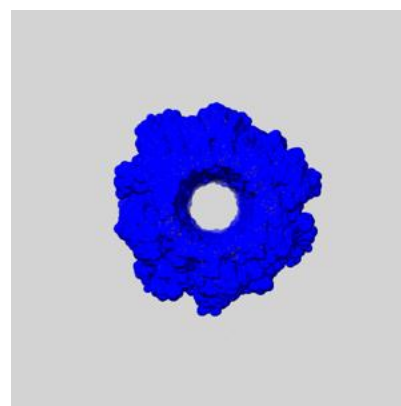
### 6.6.1 emd\_64106\_msk\_1.map [i](#)



X



Y

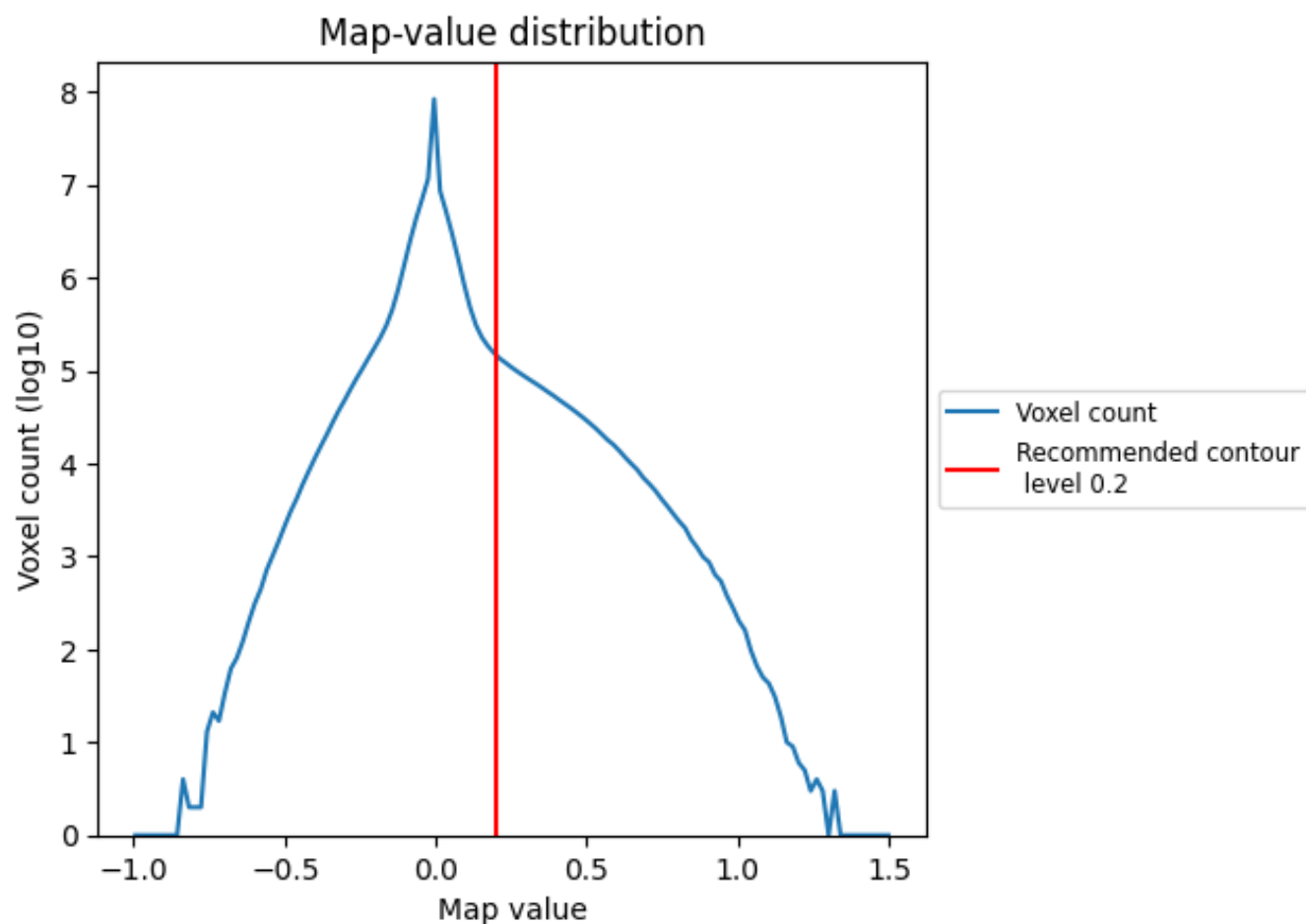


Z

## 7 Map analysis [i](#)

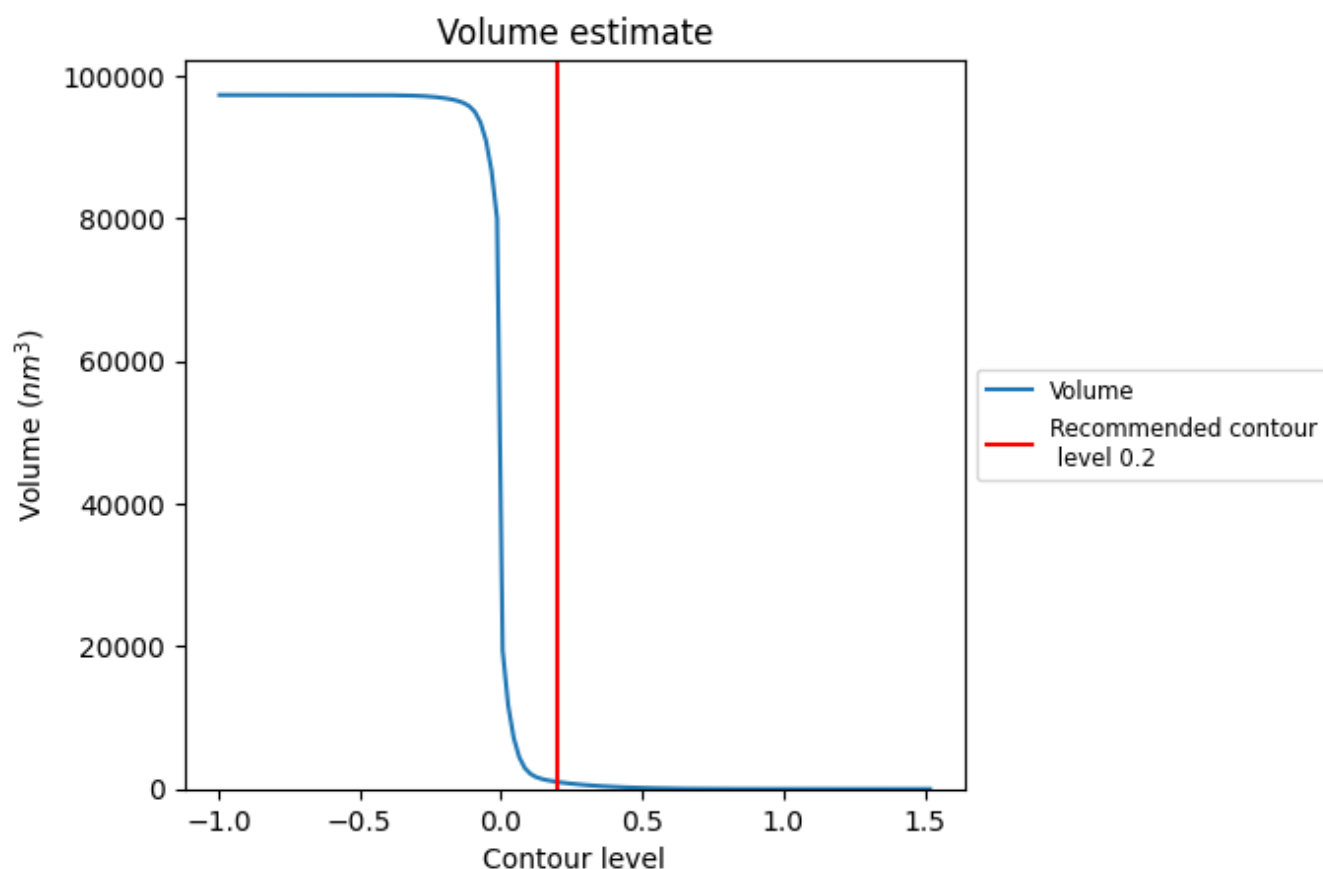
This section contains the results of statistical analysis of the map.

### 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.

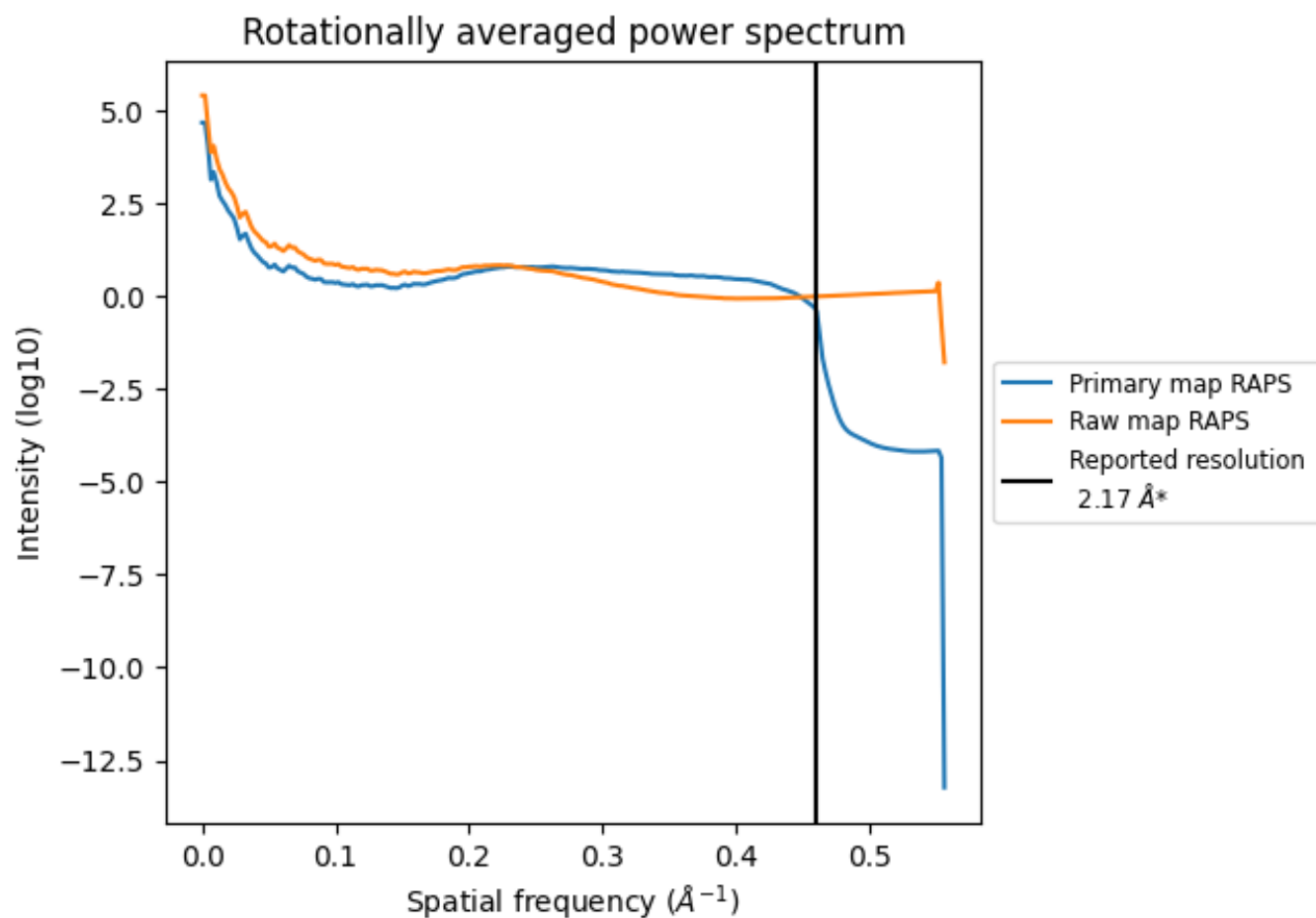
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 984  $\text{nm}^3$ ; this corresponds to an approximate mass of 889 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 ⓘ

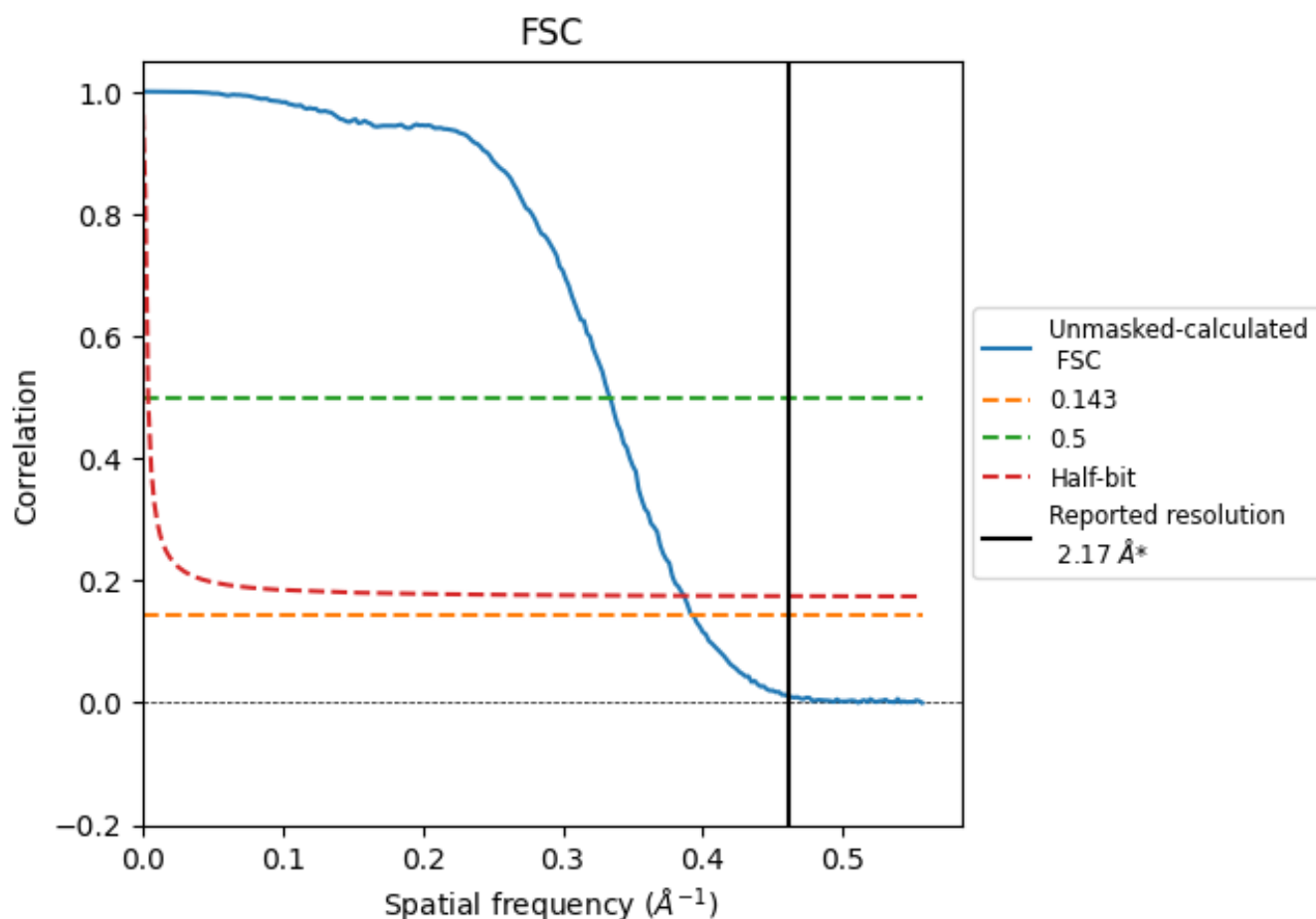


\*Reported resolution corresponds to spatial frequency of 0.461 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.461 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

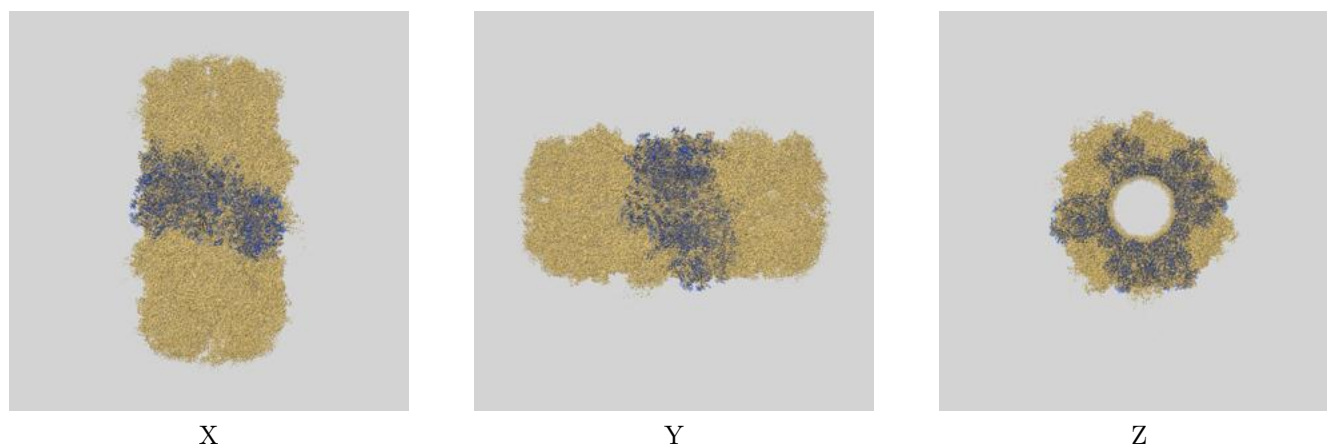
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 2.17                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 2.55                               | 3.00 | 2.59     |

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 2.55 differs from the reported value 2.17 by more than 10 %

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

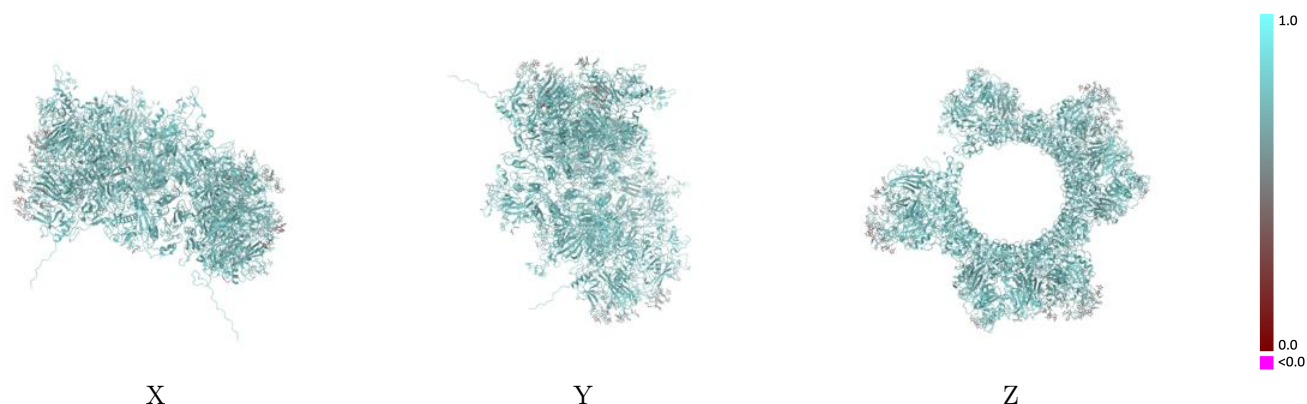
This section contains information regarding the fit between EMDB map EMD-64106 and PDB model 9UFE. Per-residue inclusion information can be found in section [3](#) on page [19](#).

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



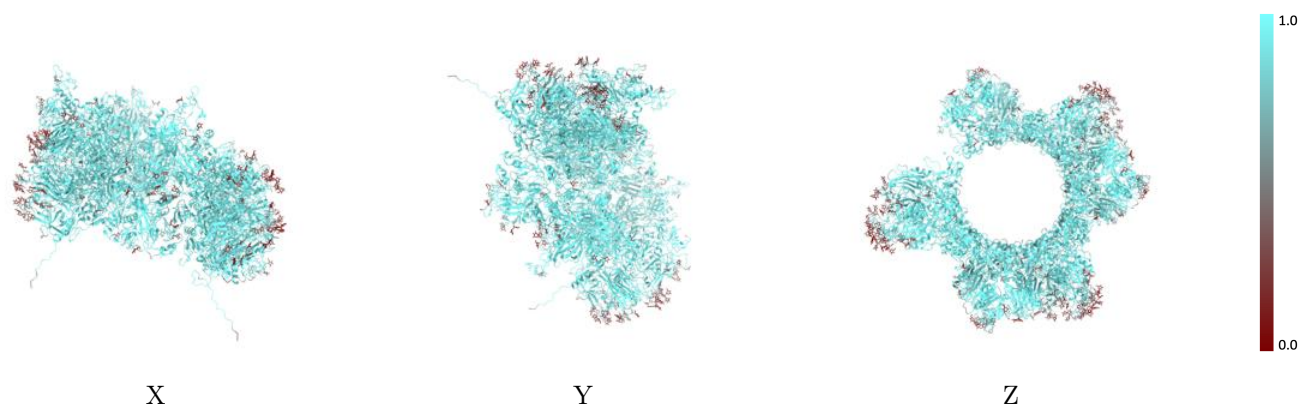
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



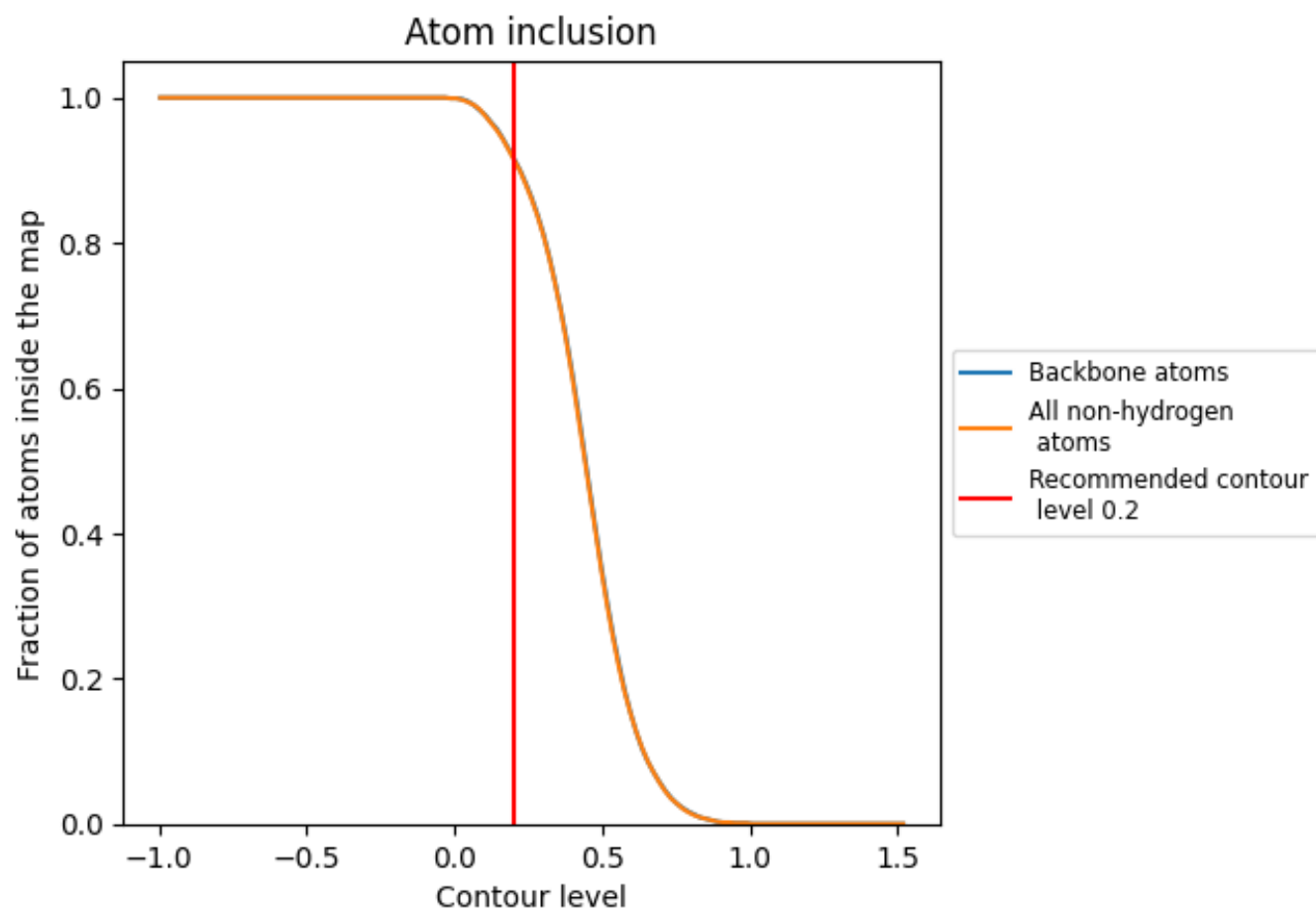
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 92% 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 (0.2) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.9160   |  0.7350   |
| AA    |  0.9580   |  0.7470   |
| AB    |  0.9580   |  0.7460   |
| AC    |  0.9560   |  0.7460   |
| BA    |  0.9550   |  0.7480   |
| BB    |  0.9550   |  0.7510   |
| BC    |  0.9610   |  0.7490   |
| CA    |  0.9540   |  0.7490   |
| CB    |  0.9510   |  0.7480   |
| CC    |  0.9510   |  0.7480   |
| DA    |  0.9630   |  0.7540   |
| DB    |  0.9660   |  0.7520   |
| DC    |  0.9670   |  0.7510   |
| EA    |  0.9490   |  0.7450   |
| EB    |  0.9440  |  0.7420  |
| EC    |  0.9440 |  0.7420 |
| FA    |  0.9460 |  0.7430 |
| FB    |  0.9520 |  0.7420 |
| FC    |  0.9540 |  0.7440 |
| aA    |  0.3940 |  0.5650 |
| aB    |  0.4720 |  0.5700 |
| aC    |  0.4230 |  0.5910 |
| aD    |  0.8670 |  0.7100 |
| aE    |  0.2220 |  0.5220 |
| aF    |  0.3750 |  0.5480 |
| aG    |  0.4610 |  0.5710 |
| aH    |  0.4400 |  0.5930 |
| aI    |  0.8290 |  0.7110 |
| aJ    |  0.2280 |  0.5380 |
| aK    |  0.3500 |  0.5780 |
| aL    |  0.4330 |  0.5560 |
| aM    |  0.4340 |  0.6030 |
| aN    |  0.8380 |  0.7110 |
| aO    |  0.2340 |  0.5270 |
| bA    |  0.7140 |  0.7050 |



*Continued on next page...*

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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| bB    |  0.3280   |  0.6010   |
| bC    |  0.3570   |  0.5770   |
| bD    |  0.7710   |  0.6960   |
| bE    |  0.3280   |  0.5830   |
| bF    |  0.3300   |  0.5670   |
| bG    |  0.7810   |  0.7000   |
| bH    |  0.3440   |  0.6040   |
| bI    |  0.3570   |  0.5410   |
| cA    |  0.9290   |  0.7110   |
| cB    |  0.9290   |  0.7170   |
| cC    |  0.9290   |  0.7220   |
| dA    |  0.7870   |  0.6860   |
| dB    |  0.7730   |  0.6860   |
| dC    |  0.8270   |  0.6990   |
| eA    |  0.7240   |  0.6880   |
| eB    |  0.7470   |  0.6880   |
| eC    |  0.6770   |  0.6950   |
| eD    |  0.7530   |  0.6820   |
| eE    |  0.6610   |  0.6840   |
| eF    |  0.7340  |  0.6770  |
| fB    |  0.8450 |  0.7140 |
| fC    |  0.7320 |  0.6960 |
| fD    |  0.9050 |  0.7250 |
| fE    |  0.7840 |  0.6920 |
| fF    |  0.3990 |  0.5870 |
| fG    |  0.8530 |  0.7040 |
| fH    |  0.7170 |  0.6780 |
| fI    |  0.8660 |  0.7130 |
| fJ    |  0.8100 |  0.6930 |
| fK    |  0.4050 |  0.5960 |
| fL    |  0.8970 |  0.7010 |
| fM    |  0.7790 |  0.6890 |
| fN    |  0.8580 |  0.7180 |
| fO    |  0.7930 |  0.6930 |
| fP    |  0.3730 |  0.6040 |