



## Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:42 PM UTC

PDB ID : 6OSY / pdb\_00006osy  
EMDB ID : EMD-20189  
Title : Cryo-EM structure of vaccine-elicited antibody 0PV-a.01 in complex with HIV-1 Env BG505 DS-SOSIP and antibodies VRC03 and PGT122  
Authors : Gorman, J.; Kwong, P.D.  
Deposited on : 2019-05-02  
Resolution : 4.30 Å(reported)  
Based on initial model : 6CDI

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

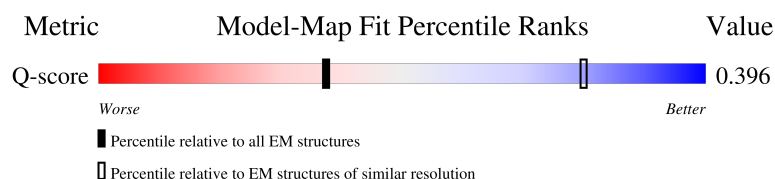
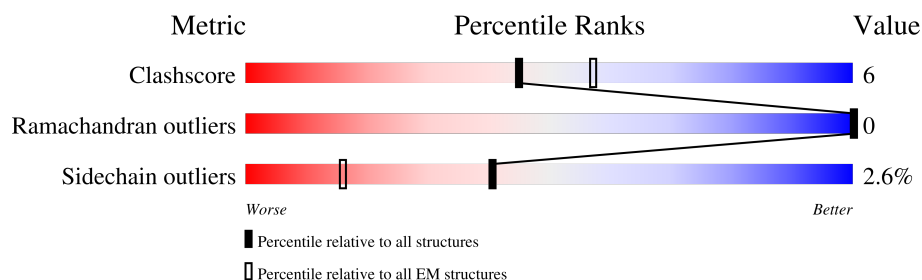
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ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

# 1 Overall quality at a glance

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

The reported resolution of this entry is 4.30 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.



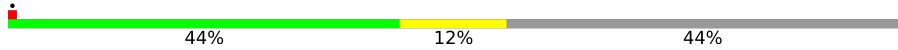
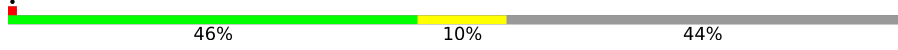
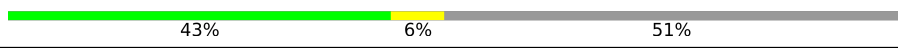
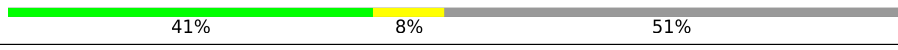
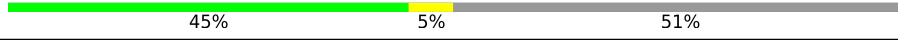
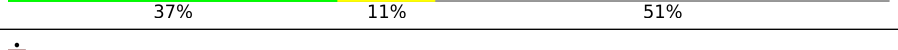
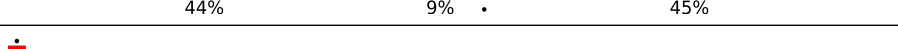
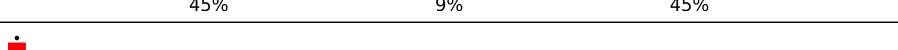
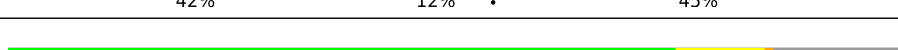
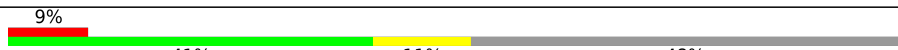
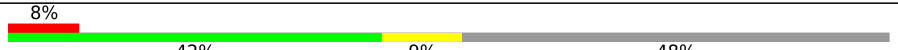
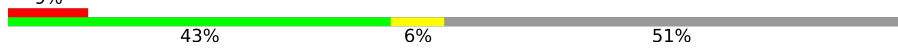
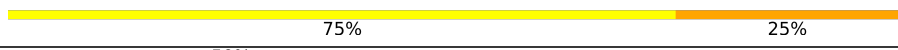
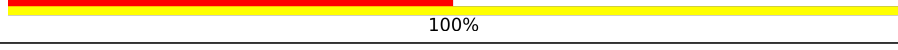
| Metric                | Whole archive<br>(#Entries) | EM structures<br>(#Entries) | Similar EM resolution<br>(#Entries, resolution range(Å)) |
|-----------------------|-----------------------------|-----------------------------|----------------------------------------------------------|
| Clashscore            | 229148                      | 23984                       | -                                                        |
| Ramachandran outliers | 224038                      | 23583                       | -                                                        |
| Sidechain outliers    | 223484                      | 23102                       | -                                                        |
| Q-score               | -                           | 25397                       | 4585 ( 3.80 - 4.80 )                                     |

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   | 2     | 480    |                  |
| 1   | B     | 480    |                  |
| 1   | K     | 480    |                  |
| 2   | 5     | 235    |                  |

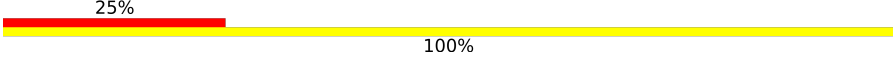
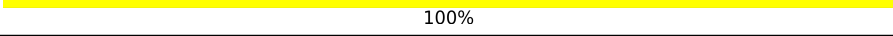
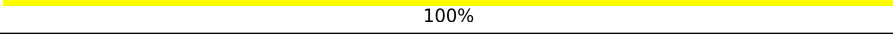
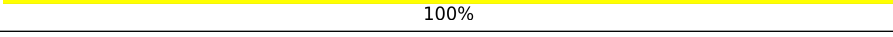
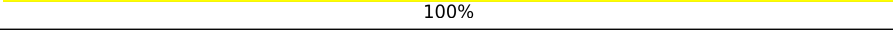
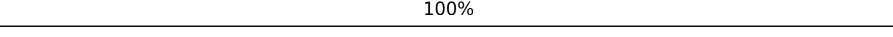
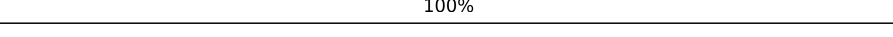
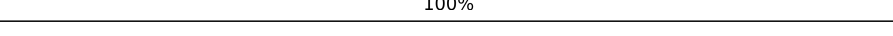
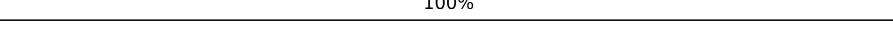
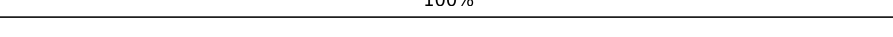
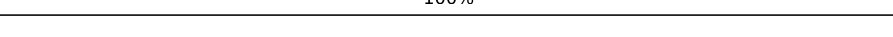
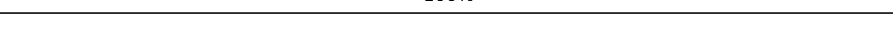
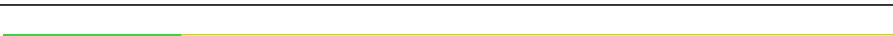
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 2   | C     | 235    |    |
| 2   | M     | 235    |    |
| 3   | 6     | 213    |    |
| 3   | D     | 213    |    |
| 3   | N     | 213    |    |
| 4   | 7     | 209    |    |
| 4   | E     | 209    |    |
| 4   | O     | 209    |    |
| 5   | 8     | 233    |    |
| 5   | F     | 233    |    |
| 5   | P     | 233    |    |
| 6   | A     | 153    |  |
| 6   | G     | 153    |  |
| 6   | Q     | 153    |  |
| 7   | H     | 235    |  |
| 7   | I     | 235    |  |
| 7   | R     | 235    |  |
| 8   | J     | 213    |  |
| 8   | L     | 213    |  |
| 8   | S     | 213    |  |
| 9   | 1     | 4      |  |
| 9   | JA    | 4      |  |
| 9   | T     | 4      |  |
| 9   | V     | 4      |  |
| 9   | i     | 4      |  |

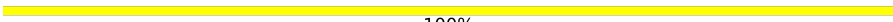
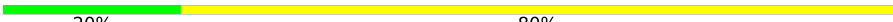
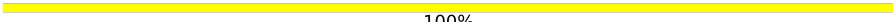
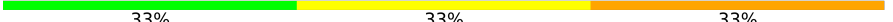
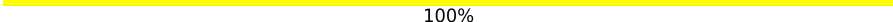
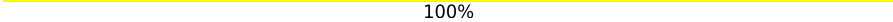
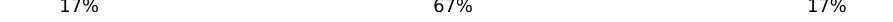
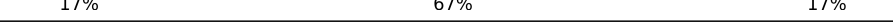
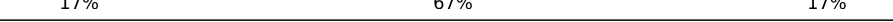
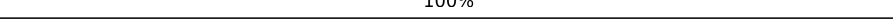
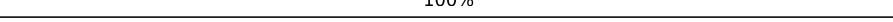
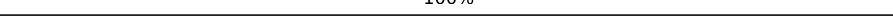
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| Mol | Chain | Length | Quality of chain                                                                     |
|-----|-------|--------|--------------------------------------------------------------------------------------|
| 9   | j     | 4      |    |
| 9   | l     | 4      |    |
| 9   | y     | 4      |    |
| 9   | z     | 4      |    |
| 10  | 0     | 2      |    |
| 10  | AA    | 2      |    |
| 10  | CA    | 2      |    |
| 10  | DA    | 2      |    |
| 10  | GA    | 2      |    |
| 10  | IA    | 2      |    |
| 10  | U     | 2      |    |
| 10  | Z     | 2      |   |
| 10  | b     | 2      |  |
| 10  | c     | 2      |  |
| 10  | f     | 2      |  |
| 10  | h     | 2      |  |
| 10  | k     | 2      |  |
| 10  | p     | 2      |  |
| 10  | r     | 2      |  |
| 10  | s     | 2      |  |
| 10  | v     | 2      |  |
| 10  | x     | 2      |  |
| 11  | 3     | 5      |  |
| 11  | FA    | 5      |  |
| 11  | W     | 5      |  |

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| Mol | Chain | Length | Quality of chain                                                                                 |
|-----|-------|--------|--------------------------------------------------------------------------------------------------|
| 11  | e     | 5      |  100%          |
| 11  | m     | 5      |  20% 80%       |
| 11  | u     | 5      |  100%          |
| 12  | 4     | 3      |  33% 33% 33%   |
| 12  | EA    | 3      |  100%          |
| 12  | X     | 3      |  100%          |
| 12  | d     | 3      |  100%          |
| 12  | n     | 3      |  67% 33%       |
| 12  | t     | 3      |  100%          |
| 13  | 9     | 4      |  25% 75% 25%   |
| 13  | Y     | 4      |  50% 75% 25%   |
| 13  | o     | 4      |  25% 75% 25%  |
| 14  | BA    | 6      |  17% 67% 17% |
| 14  | a     | 6      |  17% 67% 17% |
| 14  | q     | 6      |  17% 67% 17% |
| 15  | HA    | 9      |  100%        |
| 15  | g     | 9      |  100%        |
| 15  | w     | 9      |  100%        |

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 32463 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 BG505 gp120.

| Mol | Chain | Residues | Atoms |      |     |     |    | AltConf | Trace |
|-----|-------|----------|-------|------|-----|-----|----|---------|-------|
| 1   | 2     | 453      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3564  | 2233 | 630 | 671 | 30 |         |       |
| 1   | B     | 453      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3564  | 2233 | 630 | 671 | 30 |         |       |
| 1   | K     | 453      | Total | C    | N   | O   | S  | 0       | 0     |
|     |       |          | 3564  | 2233 | 630 | 671 | 30 |         |       |

There are 27 discrepancies between the modelled and reference sequences:

| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| 2     | 201     | CYS      | ILE    | conflict       | UNP Q2N0S6 |
| 2     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| 2     | 433     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| 2     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| 2     | 506     | GLY      | VAL    | conflict       | UNP Q2N0S6 |
| 2     | 507     | ARG      | GLY    | conflict       | UNP Q2N0S6 |
| 2     | 509     | ARG      | GLU    | conflict       | UNP Q2N0S6 |
| 2     | 510     | ARG      | LYS    | conflict       | UNP Q2N0S6 |
| 2     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |
| B     | 201     | CYS      | ILE    | conflict       | UNP Q2N0S6 |
| B     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| B     | 433     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| B     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| B     | 506     | GLY      | VAL    | conflict       | UNP Q2N0S6 |
| B     | 507     | ARG      | GLY    | conflict       | UNP Q2N0S6 |
| B     | 509     | ARG      | GLU    | conflict       | UNP Q2N0S6 |
| B     | 510     | ARG      | LYS    | conflict       | UNP Q2N0S6 |
| B     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |
| K     | 201     | CYS      | ILE    | conflict       | UNP Q2N0S6 |
| K     | 332     | ASN      | THR    | conflict       | UNP Q2N0S6 |
| K     | 433     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| K     | 501     | CYS      | ALA    | conflict       | UNP Q2N0S6 |
| K     | 506     | GLY      | VAL    | conflict       | UNP Q2N0S6 |
| K     | 507     | ARG      | GLY    | conflict       | UNP Q2N0S6 |

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| Chain | Residue | Modelled | Actual | Comment        | Reference  |
|-------|---------|----------|--------|----------------|------------|
| K     | 509     | ARG      | GLU    | conflict       | UNP Q2N0S6 |
| K     | 510     | ARG      | LYS    | conflict       | UNP Q2N0S6 |
| K     | 512     | ARG      | -      | expression tag | UNP Q2N0S6 |

- Molecule 2 is a protein called PGT122 Heavy.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 2   | 5     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 669 | 180 | 195 | 3 |         |       |
| 2   | C     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 669 | 180 | 195 | 3 |         |       |
| 2   | M     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1047  | 669 | 180 | 195 | 3 |         |       |

- Molecule 3 is a protein called PGT122 Light.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 3   | 6     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 504 | 139 | 160 | 2 |         |       |
| 3   | D     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 504 | 139 | 160 | 2 |         |       |
| 3   | N     | 105      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 805   | 504 | 139 | 160 | 2 |         |       |

- Molecule 4 is a protein called VRC03 Light.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 4   | 7     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 510 | 137 | 152 | 3 |         |       |
| 4   | E     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 510 | 137 | 152 | 3 |         |       |
| 4   | O     | 102      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 510 | 137 | 152 | 3 |         |       |

- Molecule 5 is a protein called VRC03 Heavy.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | 8     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 657 | 175 | 185 | 6 |         |       |
| 5   | F     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 657 | 175 | 185 | 6 |         |       |

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| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 5   | P     | 128      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1023  | 657 | 175 | 185 | 6 |         |       |

- Molecule 6 is a protein called BG505 gp41.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 6   | A     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 654 | 178 | 196 | 6 |         |       |
| 6   | G     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 654 | 178 | 196 | 6 |         |       |
| 6   | Q     | 132      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 1034  | 654 | 178 | 196 | 6 |         |       |

- Molecule 7 is a protein called 0PV-a.01 Heavy.

| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 7   | H     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 609 | 160 | 184 | 4 |         |       |
| 7   | I     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 609 | 160 | 184 | 4 |         |       |
| 7   | R     | 122      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 957   | 609 | 160 | 184 | 4 |         |       |

- Molecule 8 is a protein called 0PV-a.01 Light.

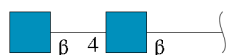
| Mol | Chain | Residues | Atoms |     |     |     |   | AltConf | Trace |
|-----|-------|----------|-------|-----|-----|-----|---|---------|-------|
| 8   | J     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 498 | 138 | 162 | 4 |         |       |
| 8   | L     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 498 | 138 | 162 | 4 |         |       |
| 8   | S     | 104      | Total | C   | N   | O   | S | 0       | 0     |
|     |       |          | 802   | 498 | 138 | 162 | 4 |         |       |

- 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)-2-acetamido-2-deoxy-beta-D-glucopyranose.



| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 9   | T     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | V     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | i     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | j     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | l     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | y     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | z     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | 1     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 9   | JA    | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |

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



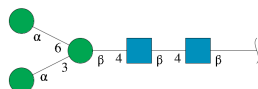
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 10  | U     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | Z     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | b     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | c     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | f     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | h     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | k     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | p     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

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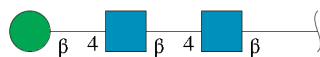
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 10  | r     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | s     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | v     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | x     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | 0     | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | AA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | CA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | DA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | GA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |
| 10  | IA    | 2        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 28    | 16 | 2 | 10 |         |       |

- Molecule 11 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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 11  | W     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 11  | e     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 11  | m     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 11  | u     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 11  | 3     | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |
| 11  | FA    | 5        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 61    | 34 | 2 | 25 |         |       |

- Molecule 12 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



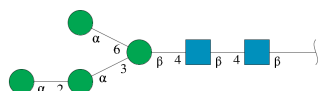
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 12  | X     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 12  | d     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 12  | n     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 12  | t     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 12  | 4     | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |
| 12  | EA    | 3        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 39    | 22 | 2 | 15 |         |       |

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



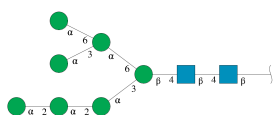
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 13  | Y     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 13  | o     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |
| 13  | 9     | 4        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 50    | 28 | 2 | 20 |         |       |

- Molecule 14 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



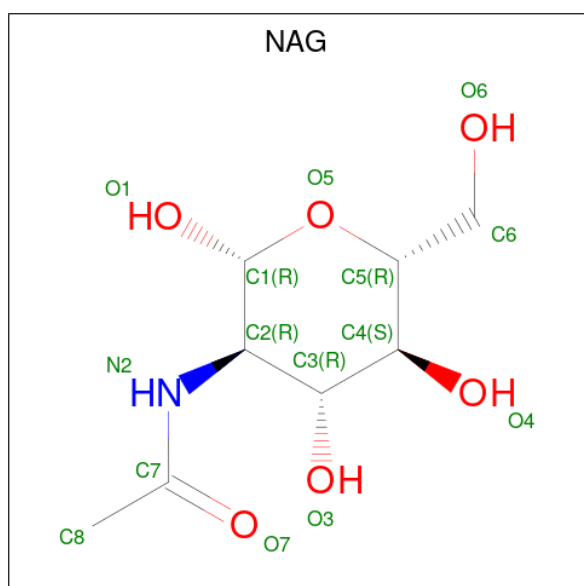
| Mol | Chain | Residues | Atoms |    |   |    | AltConf | Trace |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 14  | a     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 14  | q     | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |
| 14  | BA    | 6        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 72    | 40 | 2 | 30 |         |       |

- Molecule 15 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]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 |
|-----|-------|----------|-------|----|---|----|---------|-------|
| 15  | g     | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 15  | w     | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |
| 15  | HA    | 9        | Total | C  | N | O  | 0       | 0     |
|     |       |          | 105   | 58 | 2 | 45 |         |       |

- Molecule 16 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).

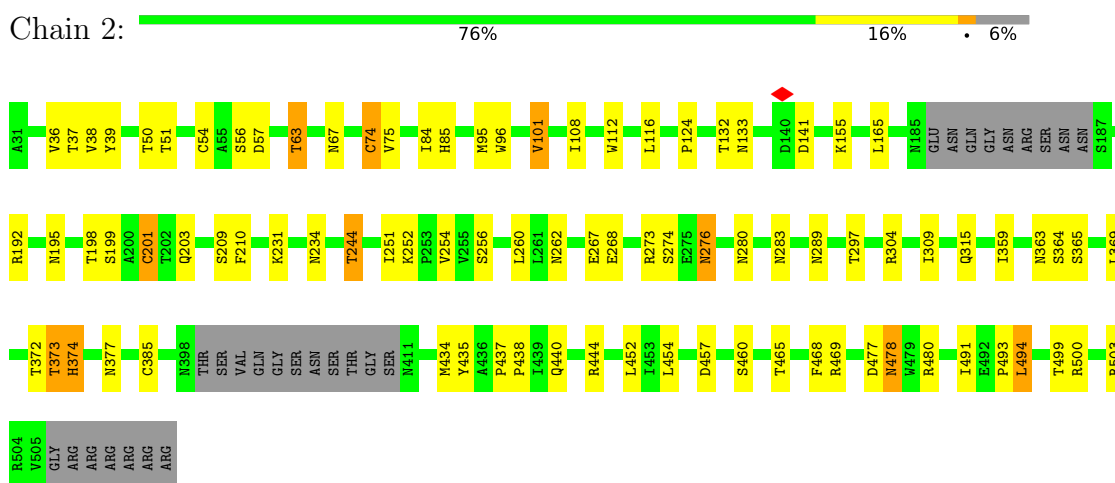


| Mol | Chain | Residues | Atoms |   |   |   | AltConf |
|-----|-------|----------|-------|---|---|---|---------|
| 16  | 2     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | A     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | B     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | G     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | K     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | Q     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |
| 16  | Q     | 1        | Total | C | N | O | 0       |
|     |       |          | 14    | 8 | 1 | 5 |         |

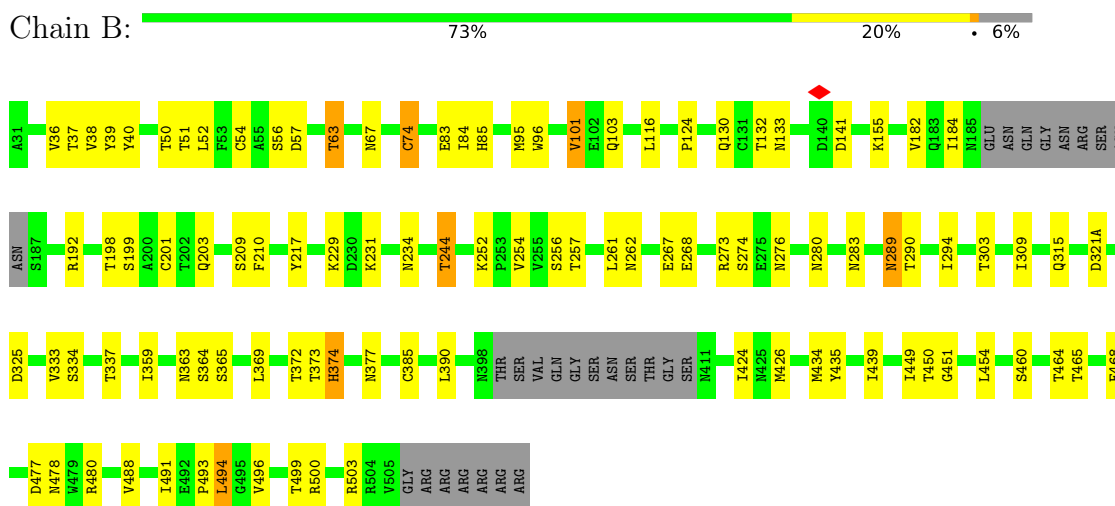
### 3 Residue-property plots

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

- Molecule 1: BG505 gp120

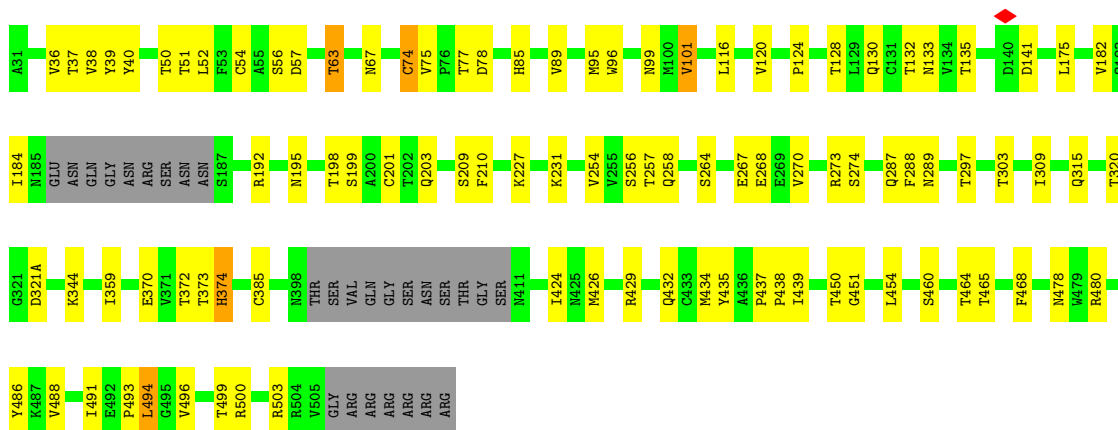


- Molecule 1: BG505 gp120

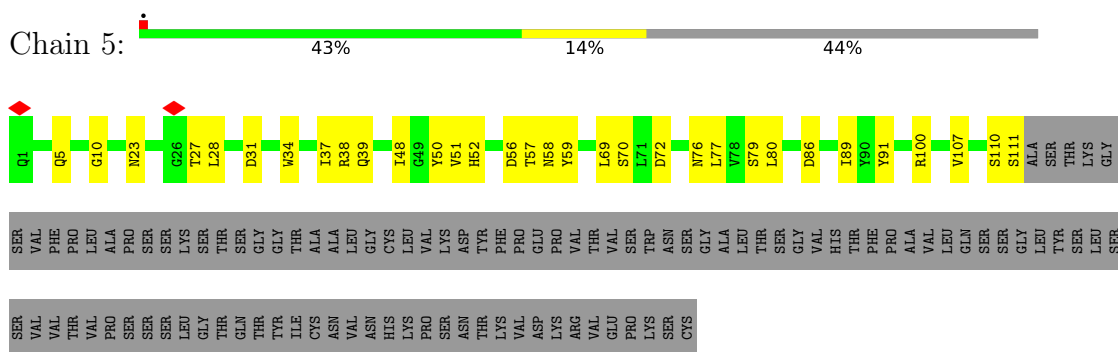


- Molecule 1: BG505 gp120

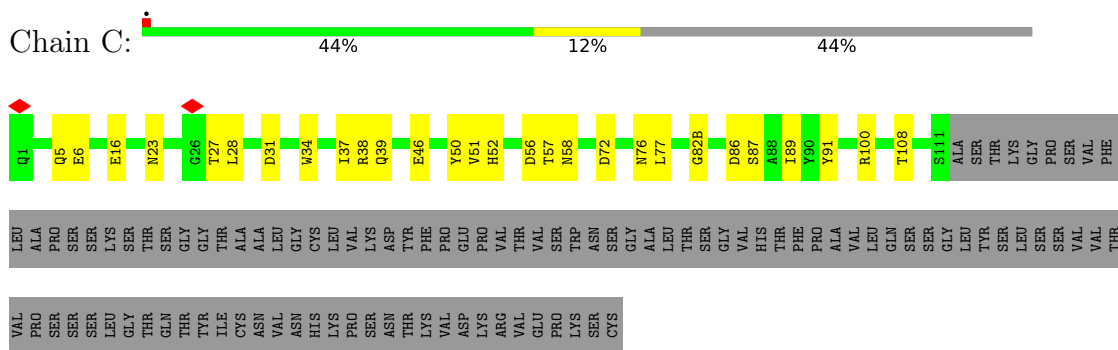




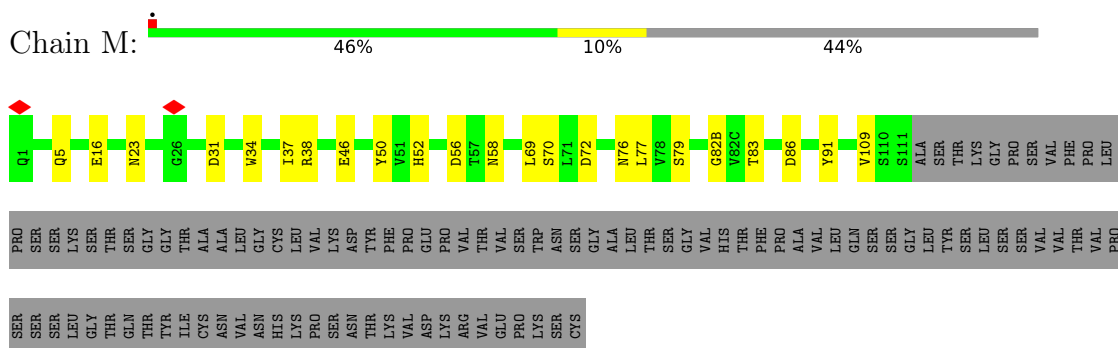
- Molecule 2: PGT122 Heavy



- Molecule 2: PGT122 Heavy

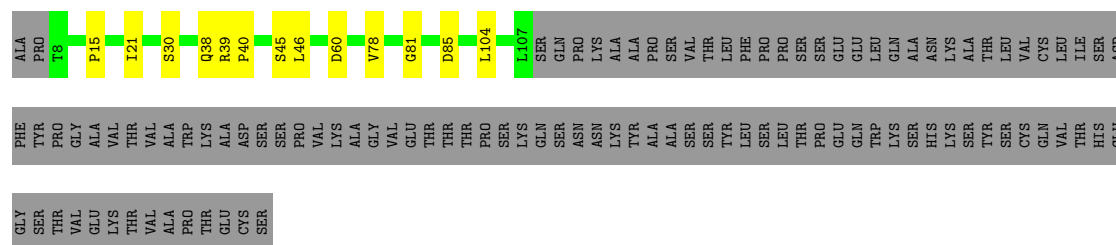


- Molecule 2: PGT122 Heavy



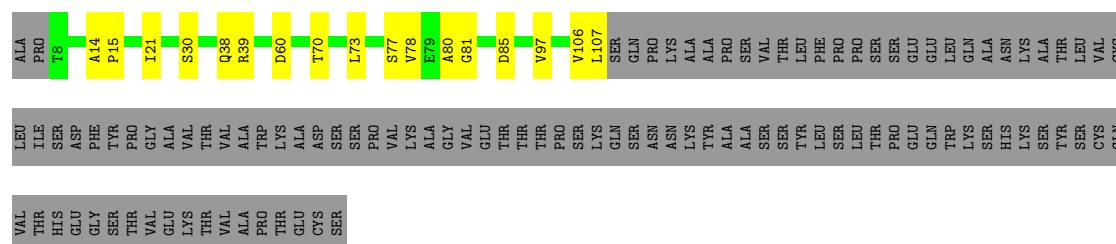
- Molecule 3: PGT122 Light

Chain 6:  43% 6% 51%



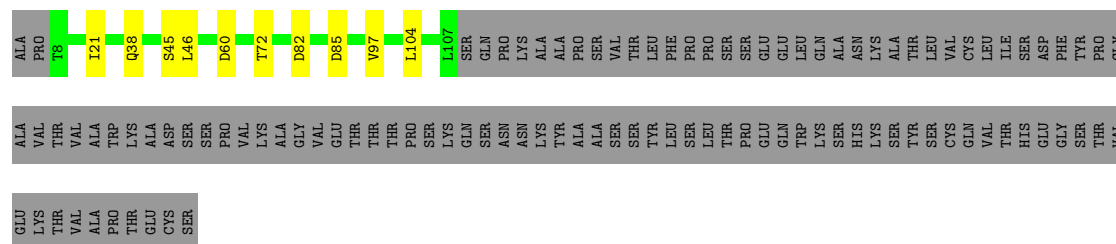
- Molecule 3: PGT122 Light

Chain D:  41% 8% 51%



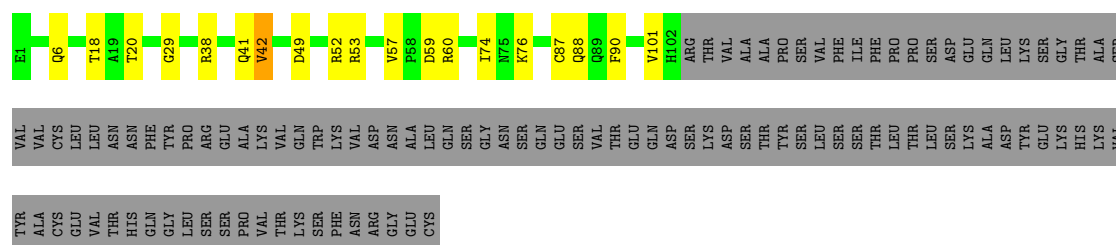
- Molecule 3: PGT122 Light

Chain N:  45% 5% 51%



- Molecule 4: VRC03 Light

Chain 7:  40% 9% 51%



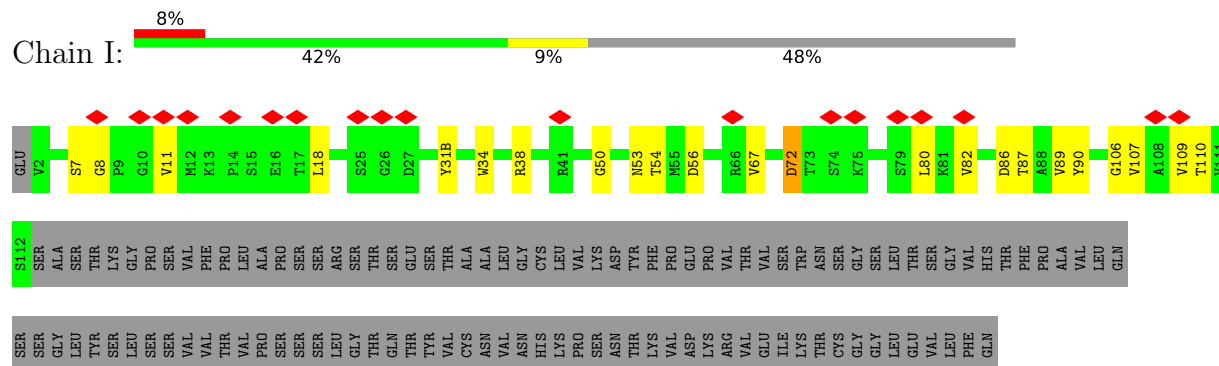
- Molecule 4: VRC03 Light



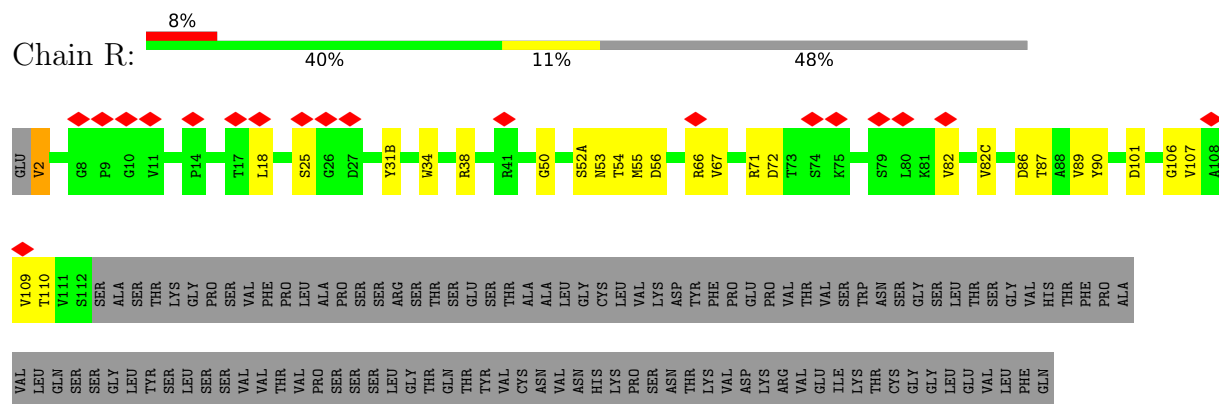


PRO ALA VAL LEU GLN SER SER GLY TYR SER LEU VAL THR VAL THR PRO SER SER SER SER VAL THR VAL THR PRO SER SER SER SER LEU GLY THR GLN THR TYR VAL CYS ASN VAL VAL HIS TYR LYS PHE TYR PRO PRO SER ASN THR THR VAL ASP LYS ARG VAL VAL ILE GLU ILE THR CYS THR CYS GLY GLY LEU VAL LEU PHE GLN

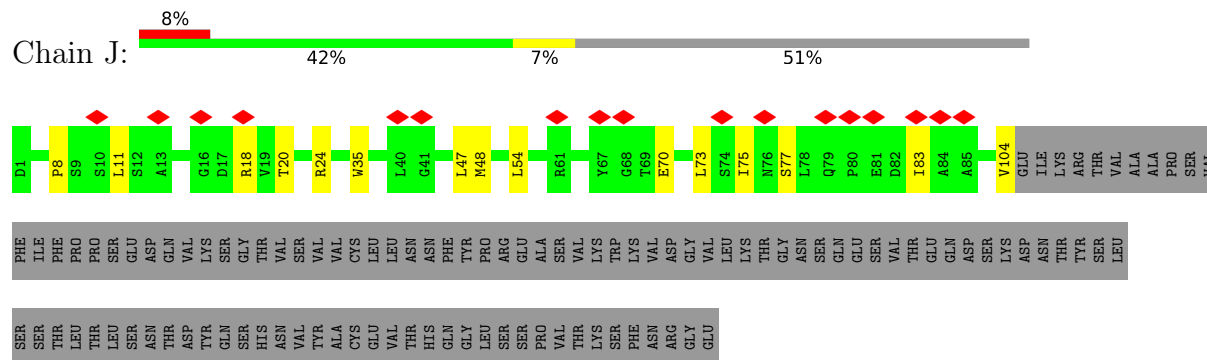
• Molecule 7: 0PV-a.01 Heavy



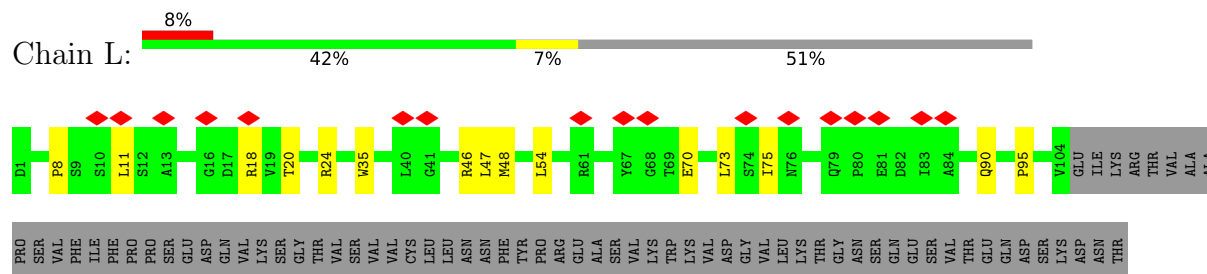
• Molecule 7: 0PV-a.01 Heavy



• Molecule 8: 0PV-a.01 Light

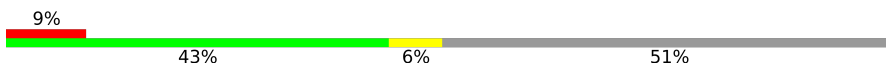


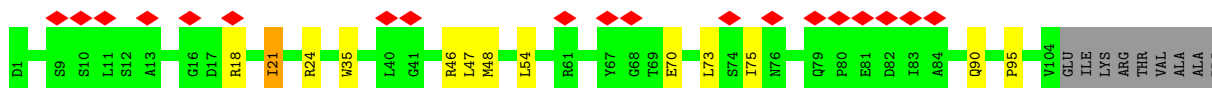
• Molecule 8: 0PV-a.01 Light



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

• Molecule 8: 0PV-a.01 Light

Chain S: 



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

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

• Molecule 9: 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 T: 



• Molecule 9: 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 V: 

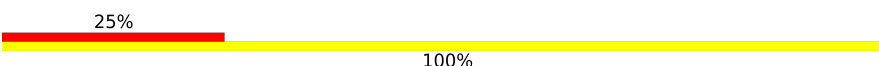


• Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain i: 



• Molecule 9: 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 j: 



• Molecule 9: 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 l:  25% 25% 50%



- Molecule 9: 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 y:  75% 25%



- Molecule 9: 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 z:  50% 100%



- Molecule 9: 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 1:  25% 25% 50%

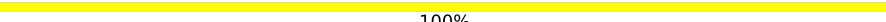


- Molecule 9: alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain JA:  75% 25%



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

Chain U:  100%



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

Chain Z:  50% 50%



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

Chain b:  100%



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

Chain c:  100%



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

Chain f:  100%



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

Chain h:  50% 50%



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

Chain k:  100%



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

Chain p:  100%



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

Chain r:  100%

MAG1  
MAG2

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

Chain s:  100%

MAG1  
MAG2

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

Chain v:  100%

MAG1  
MAG2

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

Chain x:  50%  50%

MAG1  
MAG2

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

Chain 0:  100%

MAG1  
MAG2

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

Chain AA:  50%  50%

MAG1  
MAG2

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

Chain CA:  100%

MAG1  
MAG2

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

Chain DA:  100%

MAG1  
MAG2

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

Chain GA:  100%

MAG1  
MAG2

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

Chain IA:  50% 50%

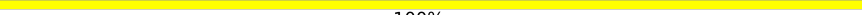
MAG1  
MAG2

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

Chain W:  20% 80%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain e:  100%

MAG1  
MAG2  
BMA3  
MAN4  
MAN5

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

Chain m:  20% 80%



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

Chain u: 100%



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

Chain 3: 20% 80%



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

Chain FA: 100%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain X: 100%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain d: 100%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain n: 67% 33%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain t:  100%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain 4:  33% 33% 33%



- Molecule 12: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain EA:  100%



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

Chain Y:  50% 75% 25%



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

Chain o:  25% 75% 25%



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

Chain 9:  25% 75% 25%



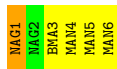
- Molecule 14: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain a: 17% 67% 17%



- Molecule 14: 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

Chain q: 17% 67% 17%



- Molecule 14: 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

Chain BA: 17% 67% 17%



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain g: 100%



- Molecule 15: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain w: 100%



- Molecule 15:  $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-2)- $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-3)-[ $\alpha$ -D-mannopyranose-(1-6)] $\alpha$ -D-mannopyranose-(1-6)] $\beta$ -D-mannopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain HA:  100%

MAG1  
MAG2  
BKA3  
MAN4  
MAN5  
MAN6  
MAN7  
MAN8  
MAN9

## 4 Experimental information

| Property                             | Value                                   | Source    |
|--------------------------------------|-----------------------------------------|-----------|
| EM reconstruction method             | SINGLE PARTICLE                         | Depositor |
| Imposed symmetry                     | POINT, C3                               | Depositor |
| Number of particles used             | 55345                                   | Depositor |
| Resolution determination method      | FSC 0.143 CUT-OFF                       | Depositor |
| CTF correction method                | PHASE FLIPPING AND AMPLITUDE CORRECTION | Depositor |
| Microscope                           | FEI TITAN KRIOS                         | Depositor |
| Voltage (kV)                         | 300                                     | Depositor |
| Electron dose ( $e^-/\text{\AA}^2$ ) | 70.49                                   | Depositor |
| Minimum defocus (nm)                 | Not provided                            |           |
| Maximum defocus (nm)                 | Not provided                            |           |
| Magnification                        | Not provided                            |           |
| Image detector                       | GATAN K2 SUMMIT (4k x 4k)               | Depositor |
| Maximum map value                    | 3.230                                   | Depositor |
| Minimum map value                    | -1.878                                  | Depositor |
| Average map value                    | 0.006                                   | Depositor |
| Map value standard deviation         | 0.138                                   | Depositor |
| Recommended contour level            | 0.45                                    | Depositor |
| Map size (Å)                         | 377.78403, 377.78403, 377.78403         | wwPDB     |
| Map dimensions                       | 352, 352, 352                           | wwPDB     |
| Map angles (°)                       | 90.0, 90.0, 90.0                        | wwPDB     |
| Pixel spacing (Å)                    | 1.07325, 1.07325, 1.07325               | Depositor |

## 5 Model quality [i](#)

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

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

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

| Mol | Chain | Bond lengths |             | Bond angles |                 |
|-----|-------|--------------|-------------|-------------|-----------------|
|     |       | RMSZ         | $\# Z  > 5$ | RMSZ        | $\# Z  > 5$     |
| 1   | 2     | 0.73         | 0/3638      | 0.92        | 3/4939 (0.1%)   |
| 1   | B     | 0.73         | 0/3638      | 0.92        | 3/4939 (0.1%)   |
| 1   | K     | 0.73         | 0/3638      | 0.92        | 6/4939 (0.1%)   |
| 2   | 5     | 0.46         | 0/1076      | 0.76        | 0/1465          |
| 2   | C     | 0.46         | 0/1076      | 0.75        | 0/1465          |
| 2   | M     | 0.46         | 0/1076      | 0.74        | 0/1465          |
| 3   | 6     | 0.54         | 0/826       | 0.80        | 2/1130 (0.2%)   |
| 3   | D     | 0.54         | 0/826       | 0.79        | 2/1130 (0.2%)   |
| 3   | N     | 0.53         | 0/826       | 0.79        | 2/1130 (0.2%)   |
| 4   | 7     | 0.56         | 0/820       | 0.91        | 2/1107 (0.2%)   |
| 4   | E     | 0.56         | 0/820       | 0.90        | 2/1107 (0.2%)   |
| 4   | O     | 0.55         | 0/820       | 0.89        | 2/1107 (0.2%)   |
| 5   | 8     | 0.63         | 0/1056      | 0.92        | 5/1439 (0.3%)   |
| 5   | F     | 0.63         | 0/1056      | 0.89        | 5/1439 (0.3%)   |
| 5   | P     | 0.63         | 0/1056      | 0.87        | 3/1439 (0.2%)   |
| 6   | A     | 0.65         | 0/1052      | 0.89        | 3/1427 (0.2%)   |
| 6   | G     | 0.64         | 0/1052      | 0.91        | 3/1427 (0.2%)   |
| 6   | Q     | 0.63         | 0/1052      | 0.90        | 3/1427 (0.2%)   |
| 7   | H     | 0.35         | 0/982       | 0.69        | 0/1341          |
| 7   | I     | 0.34         | 0/982       | 0.66        | 0/1341          |
| 7   | R     | 0.35         | 0/982       | 0.68        | 0/1341          |
| 8   | J     | 0.30         | 0/819       | 0.69        | 0/1109          |
| 8   | L     | 0.29         | 0/819       | 0.67        | 0/1109          |
| 8   | S     | 0.30         | 0/819       | 0.67        | 0/1109          |
| All | All   | 0.60         | 0/30807     | 0.85        | 46/41871 (0.1%) |

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 |
|-----|-------|---------------------|---------------------|
| 1   | 2     | 0                   | 3                   |
| 1   | B     | 0                   | 2                   |
| 1   | K     | 0                   | 2                   |
| 4   | 7     | 0                   | 1                   |
| 4   | E     | 0                   | 1                   |
| 4   | O     | 0                   | 1                   |
| 6   | A     | 0                   | 1                   |
| 6   | G     | 0                   | 1                   |
| 6   | Q     | 0                   | 1                   |
| All | All   | 0                   | 13                  |

There are no bond length outliers.

All (46) bond angle outliers are listed below:

| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 5   | 8     | 48     | ILE  | CA-C-N   | -7.52 | 113.60      | 121.35   |
| 5   | 8     | 48     | ILE  | C-N-CA   | -7.52 | 113.60      | 121.35   |
| 4   | 7     | 49     | ASP  | CA-C-N   | 7.37  | 135.61      | 121.54   |
| 4   | 7     | 49     | ASP  | C-N-CA   | 7.37  | 135.61      | 121.54   |
| 4   | E     | 49     | ASP  | CA-C-N   | 7.28  | 135.45      | 121.54   |
| 4   | E     | 49     | ASP  | C-N-CA   | 7.28  | 135.45      | 121.54   |
| 4   | O     | 49     | ASP  | CA-C-N   | 7.28  | 135.44      | 121.54   |
| 4   | O     | 49     | ASP  | C-N-CA   | 7.28  | 135.44      | 121.54   |
| 6   | A     | 570    | VAL  | N-CA-C   | -6.71 | 106.69      | 113.47   |
| 6   | G     | 570    | VAL  | N-CA-C   | -6.68 | 106.72      | 113.47   |
| 3   | 6     | 60     | ASP  | CA-C-N   | 6.12  | 134.06      | 123.91   |
| 3   | 6     | 60     | ASP  | C-N-CA   | 6.12  | 134.06      | 123.91   |
| 3   | N     | 60     | ASP  | CA-C-N   | 6.08  | 134.00      | 123.91   |
| 3   | N     | 60     | ASP  | C-N-CA   | 6.08  | 134.00      | 123.91   |
| 3   | D     | 60     | ASP  | CA-C-N   | 6.04  | 133.94      | 123.91   |
| 3   | D     | 60     | ASP  | C-N-CA   | 6.04  | 133.94      | 123.91   |
| 1   | K     | 101    | VAL  | N-CA-C   | -6.00 | 105.83      | 113.22   |
| 6   | Q     | 570    | VAL  | N-CA-C   | -5.96 | 107.45      | 113.47   |
| 5   | F     | 100(D) | PHE  | N-CA-C   | 5.95  | 122.96      | 109.81   |
| 1   | 2     | 101    | VAL  | N-CA-C   | -5.92 | 104.96      | 113.07   |
| 6   | A     | 601    | LYS  | CA-C-N   | 5.87  | 132.74      | 121.54   |
| 6   | A     | 601    | LYS  | C-N-CA   | 5.87  | 132.74      | 121.54   |
| 1   | K     | 54     | CYS  | CA-CB-SG | 5.68  | 127.47      | 114.40   |
| 1   | B     | 124    | PRO  | CA-N-CD  | -5.68 | 104.05      | 112.00   |
| 1   | B     | 101    | VAL  | N-CA-C   | -5.61 | 105.38      | 113.07   |
| 6   | Q     | 601    | LYS  | CA-C-N   | 5.57  | 132.18      | 121.54   |
| 6   | Q     | 601    | LYS  | C-N-CA   | 5.57  | 132.18      | 121.54   |
| 1   | K     | 494    | LEU  | CA-CB-CG | 5.48  | 135.47      | 116.30   |

*Continued on next page...*

*Continued from previous page...*

| Mol | Chain | Res    | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|--------|------|----------|-------|-------------|----------|
| 6   | G     | 601    | LYS  | CA-C-N   | 5.46  | 131.97      | 121.54   |
| 6   | G     | 601    | LYS  | C-N-CA   | 5.46  | 131.97      | 121.54   |
| 1   | 2     | 494    | LEU  | CA-CB-CG | 5.43  | 135.30      | 116.30   |
| 1   | B     | 494    | LEU  | CA-CB-CG | 5.37  | 135.09      | 116.30   |
| 1   | 2     | 124    | PRO  | CA-N-CD  | -5.24 | 104.67      | 112.00   |
| 5   | 8     | 100(D) | PHE  | N-CA-C   | 5.21  | 121.31      | 109.81   |
| 5   | P     | 100(D) | PHE  | N-CA-C   | 5.16  | 121.22      | 109.81   |
| 5   | 8     | 41     | PRO  | CA-C-N   | 5.16  | 131.39      | 121.54   |
| 5   | 8     | 41     | PRO  | C-N-CA   | 5.16  | 131.39      | 121.54   |
| 5   | F     | 48     | ILE  | CA-C-N   | -5.15 | 112.76      | 121.47   |
| 5   | F     | 48     | ILE  | C-N-CA   | -5.15 | 112.76      | 121.47   |
| 1   | K     | 124    | PRO  | CA-N-CD  | -5.12 | 104.83      | 112.00   |
| 5   | P     | 41     | PRO  | CA-C-N   | 5.05  | 131.18      | 121.54   |
| 5   | P     | 41     | PRO  | C-N-CA   | 5.05  | 131.18      | 121.54   |
| 5   | F     | 41     | PRO  | CA-C-N   | 5.02  | 131.13      | 121.54   |
| 5   | F     | 41     | PRO  | C-N-CA   | 5.02  | 131.13      | 121.54   |
| 1   | K     | 99     | ASN  | CA-C-N   | 5.01  | 131.11      | 121.54   |
| 1   | K     | 99     | ASN  | C-N-CA   | 5.01  | 131.11      | 121.54   |

There are no chirality outliers.

All (13) planarity outliers are listed below:

| Mol | Chain | Res | Type | Group   |
|-----|-------|-----|------|---------|
| 1   | 2     | 201 | CYS  | Peptide |
| 1   | 2     | 373 | THR  | Peptide |
| 1   | 2     | 74  | CYS  | Peptide |
| 4   | 7     | 88  | GLN  | Peptide |
| 6   | A     | 517 | ALA  | Peptide |
| 1   | B     | 201 | CYS  | Peptide |
| 1   | B     | 74  | CYS  | Peptide |
| 4   | E     | 88  | GLN  | Peptide |
| 6   | G     | 517 | ALA  | Peptide |
| 1   | K     | 201 | CYS  | Peptide |
| 1   | K     | 74  | CYS  | Peptide |
| 4   | O     | 88  | GLN  | Peptide |
| 6   | Q     | 517 | ALA  | Peptide |

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 1   | 2     | 3564  | 0        | 3489     | 48      | 0            |
| 1   | B     | 3564  | 0        | 3489     | 53      | 0            |
| 1   | K     | 3564  | 0        | 3489     | 52      | 0            |
| 2   | 5     | 1047  | 0        | 1026     | 22      | 0            |
| 2   | C     | 1047  | 0        | 1026     | 20      | 0            |
| 2   | M     | 1047  | 0        | 1026     | 15      | 0            |
| 3   | 6     | 805   | 0        | 761      | 7       | 0            |
| 3   | D     | 805   | 0        | 761      | 11      | 0            |
| 3   | N     | 805   | 0        | 761      | 4       | 0            |
| 4   | 7     | 802   | 0        | 780      | 11      | 0            |
| 4   | E     | 802   | 0        | 780      | 15      | 0            |
| 4   | O     | 802   | 0        | 780      | 13      | 0            |
| 5   | 8     | 1023  | 0        | 971      | 15      | 0            |
| 5   | F     | 1023  | 0        | 971      | 13      | 0            |
| 5   | P     | 1023  | 0        | 971      | 18      | 0            |
| 6   | A     | 1034  | 0        | 1013     | 9       | 0            |
| 6   | G     | 1034  | 0        | 1013     | 16      | 0            |
| 6   | Q     | 1034  | 0        | 1013     | 13      | 0            |
| 7   | H     | 957   | 0        | 925      | 16      | 0            |
| 7   | I     | 957   | 0        | 925      | 13      | 0            |
| 7   | R     | 957   | 0        | 925      | 18      | 0            |
| 8   | J     | 802   | 0        | 769      | 9       | 0            |
| 8   | L     | 802   | 0        | 769      | 9       | 0            |
| 8   | S     | 802   | 0        | 769      | 9       | 0            |
| 9   | 1     | 50    | 0        | 43       | 2       | 0            |
| 9   | JA    | 50    | 0        | 43       | 1       | 0            |
| 9   | T     | 50    | 0        | 43       | 0       | 0            |
| 9   | V     | 50    | 0        | 43       | 2       | 0            |
| 9   | i     | 50    | 0        | 43       | 1       | 0            |
| 9   | j     | 50    | 0        | 43       | 0       | 0            |
| 9   | l     | 50    | 0        | 43       | 2       | 0            |
| 9   | y     | 50    | 0        | 43       | 1       | 0            |
| 9   | z     | 50    | 0        | 43       | 0       | 0            |
| 10  | 0     | 28    | 0        | 25       | 0       | 0            |
| 10  | AA    | 28    | 0        | 25       | 0       | 0            |
| 10  | CA    | 28    | 0        | 25       | 0       | 0            |
| 10  | DA    | 28    | 0        | 25       | 0       | 0            |
| 10  | GA    | 28    | 0        | 25       | 0       | 0            |
| 10  | IA    | 28    | 0        | 25       | 1       | 0            |
| 10  | U     | 28    | 0        | 25       | 0       | 0            |
| 10  | Z     | 28    | 0        | 25       | 0       | 0            |

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| Mol | Chain | Non-H | H(model) | H(added) | Clashes | Symm-Clashes |
|-----|-------|-------|----------|----------|---------|--------------|
| 10  | b     | 28    | 0        | 25       | 0       | 0            |
| 10  | c     | 28    | 0        | 25       | 0       | 0            |
| 10  | f     | 28    | 0        | 25       | 0       | 0            |
| 10  | h     | 28    | 0        | 25       | 1       | 0            |
| 10  | k     | 28    | 0        | 25       | 0       | 0            |
| 10  | p     | 28    | 0        | 25       | 0       | 0            |
| 10  | r     | 28    | 0        | 25       | 0       | 0            |
| 10  | s     | 28    | 0        | 25       | 0       | 0            |
| 10  | v     | 28    | 0        | 25       | 0       | 0            |
| 10  | x     | 28    | 0        | 25       | 1       | 0            |
| 11  | 3     | 61    | 0        | 52       | 0       | 0            |
| 11  | FA    | 61    | 0        | 52       | 0       | 0            |
| 11  | W     | 61    | 0        | 52       | 0       | 0            |
| 11  | e     | 61    | 0        | 52       | 0       | 0            |
| 11  | m     | 61    | 0        | 52       | 0       | 0            |
| 11  | u     | 61    | 0        | 52       | 0       | 0            |
| 12  | 4     | 39    | 0        | 34       | 1       | 0            |
| 12  | EA    | 39    | 0        | 34       | 0       | 0            |
| 12  | X     | 39    | 0        | 34       | 0       | 0            |
| 12  | d     | 39    | 0        | 34       | 0       | 0            |
| 12  | n     | 39    | 0        | 34       | 1       | 0            |
| 12  | t     | 39    | 0        | 34       | 0       | 0            |
| 13  | 9     | 50    | 0        | 43       | 1       | 0            |
| 13  | Y     | 50    | 0        | 43       | 1       | 0            |
| 13  | o     | 50    | 0        | 43       | 1       | 0            |
| 14  | BA    | 72    | 0        | 61       | 1       | 0            |
| 14  | a     | 72    | 0        | 61       | 1       | 0            |
| 14  | q     | 72    | 0        | 61       | 1       | 0            |
| 15  | HA    | 105   | 0        | 88       | 0       | 0            |
| 15  | g     | 105   | 0        | 88       | 0       | 0            |
| 15  | w     | 105   | 0        | 88       | 0       | 0            |
| 16  | 2     | 14    | 0        | 13       | 0       | 0            |
| 16  | A     | 28    | 0        | 26       | 0       | 0            |
| 16  | B     | 14    | 0        | 13       | 0       | 0            |
| 16  | G     | 28    | 0        | 26       | 0       | 0            |
| 16  | K     | 14    | 0        | 13       | 0       | 0            |
| 16  | Q     | 28    | 0        | 26       | 0       | 0            |
| All | All   | 32463 | 0        | 31248    | 403     | 0            |

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

All (403) 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) |
|-----------------|-------------------|--------------------------|-------------------|
| 7:H:90:TYR:O    | 7:H:106:GLY:HA2   | 1.72                     | 0.88              |
| 7:I:90:TYR:O    | 7:I:106:GLY:HA2   | 1.74                     | 0.86              |
| 7:R:90:TYR:O    | 7:R:106:GLY:HA2   | 1.77                     | 0.85              |
| 8:S:18:ARG:HA   | 8:S:75:ILE:O      | 1.77                     | 0.85              |
| 8:J:18:ARG:HA   | 8:J:75:ILE:O      | 1.80                     | 0.81              |
| 8:L:18:ARG:HA   | 8:L:75:ILE:O      | 1.81                     | 0.80              |
| 8:J:83:ILE:HA   | 8:J:104:VAL:O     | 1.88                     | 0.74              |
| 2:5:37:ILE:O    | 2:5:91:TYR:HB2    | 1.95                     | 0.66              |
| 4:O:18:THR:HA   | 4:O:74:ILE:O      | 1.97                     | 0.64              |
| 2:5:28:LEU:HA   | 2:5:76:ASN:HD21   | 1.61                     | 0.64              |
| 2:C:28:LEU:HA   | 2:C:76:ASN:HD21   | 1.64                     | 0.62              |
| 2:C:37:ILE:O    | 2:C:91:TYR:HB2    | 2.00                     | 0.61              |
| 2:M:37:ILE:O    | 2:M:91:TYR:HB2    | 2.00                     | 0.61              |
| 4:7:18:THR:HA   | 4:7:74:ILE:O      | 2.02                     | 0.59              |
| 8:J:8:PRO:HG2   | 8:J:11:LEU:HD21   | 1.85                     | 0.59              |
| 14:BA:1:NAG:H62 | 10:IA:1:NAG:H81   | 1.84                     | 0.59              |
| 14:a:1:NAG:H62  | 10:h:1:NAG:H81    | 1.84                     | 0.58              |
| 6:Q:605:CYS:SG  | 6:Q:606:THR:N     | 2.76                     | 0.58              |
| 5:P:50:TRP:HZ3  | 5:P:52:LYS:HG3    | 1.69                     | 0.58              |
| 2:C:5:GLN:HB3   | 2:C:23:ASN:HB2    | 1.86                     | 0.58              |
| 4:O:60:ARG:NH1  | 4:O:76:LYS:O      | 2.37                     | 0.58              |
| 4:7:60:ARG:NH1  | 4:7:76:LYS:O      | 2.37                     | 0.58              |
| 2:M:5:GLN:HB3   | 2:M:23:ASN:HB2    | 1.86                     | 0.58              |
| 5:8:6:GLN:HE22  | 5:8:91:PHE:HA     | 1.69                     | 0.58              |
| 1:B:309:ILE:HB  | 1:B:315:GLN:HB2   | 1.85                     | 0.58              |
| 4:E:60:ARG:NH1  | 4:E:76:LYS:O      | 2.36                     | 0.57              |
| 14:q:1:NAG:H62  | 10:x:1:NAG:H81    | 1.84                     | 0.57              |
| 1:K:460:SER:O   | 5:P:61:ARG:NH2    | 2.38                     | 0.57              |
| 1:2:309:ILE:HB  | 1:2:315:GLN:HB2   | 1.85                     | 0.57              |
| 2:5:5:GLN:HB3   | 2:5:23:ASN:HB2    | 1.86                     | 0.57              |
| 1:B:460:SER:O   | 5:F:61:ARG:NH2    | 2.37                     | 0.57              |
| 1:K:309:ILE:HB  | 1:K:315:GLN:HB2   | 1.87                     | 0.57              |
| 1:2:460:SER:O   | 5:8:61:ARG:NH2    | 2.37                     | 0.57              |
| 2:5:23:ASN:HA   | 2:5:77:LEU:HD22   | 1.87                     | 0.57              |
| 6:G:620:SER:O   | 6:G:624:ASP:HB2   | 2.04                     | 0.57              |
| 6:A:606:THR:OG1 | 6:A:607:ASN:N     | 2.38                     | 0.56              |
| 4:E:18:THR:HA   | 4:E:74:ILE:O      | 2.05                     | 0.56              |
| 8:L:48:MET:HB3  | 8:L:54:LEU:HD13   | 1.87                     | 0.56              |
| 4:O:29:GLY:HA3  | 9:JA:2:NAG:H3     | 1.88                     | 0.56              |
| 6:A:605:CYS:SG  | 6:A:606:THR:N     | 2.78                     | 0.56              |
| 2:C:23:ASN:HA   | 2:C:77:LEU:HD22   | 1.88                     | 0.56              |
| 1:B:85:HIS:HB3  | 7:I:31(B):TYR:HE2 | 1.70                     | 0.56              |

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| Atom-1           | Atom-2             | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|--------------------|--------------------------|-------------------|
| 5:F:6:GLN:HE22   | 5:F:91:PHE:HA      | 1.70                     | 0.56              |
| 6:G:605:CYS:SG   | 6:G:606:THR:N      | 2.78                     | 0.56              |
| 5:8:62:GLN:HG2   | 5:8:63:LEU:HD12    | 1.86                     | 0.56              |
| 8:J:48:MET:HB3   | 8:J:54:LEU:HD13    | 1.88                     | 0.56              |
| 2:M:23:ASN:HA    | 2:M:77:LEU:HD22    | 1.88                     | 0.55              |
| 2:C:52:HIS:HB3   | 2:C:56:ASP:HB3     | 1.87                     | 0.55              |
| 4:E:53:ARG:HE    | 4:E:57:VAL:HG23    | 1.72                     | 0.55              |
| 2:5:52:HIS:HB3   | 2:5:56:ASP:HB3     | 1.88                     | 0.55              |
| 1:B:101:VAL:HG11 | 1:B:480:ARG:HE     | 1.72                     | 0.55              |
| 8:S:48:MET:HB3   | 8:S:54:LEU:HD13    | 1.88                     | 0.55              |
| 7:H:18:LEU:HB3   | 7:H:82:VAL:HB      | 1.88                     | 0.55              |
| 1:2:198:THR:OG1  | 1:2:199:SER:N      | 2.40                     | 0.55              |
| 5:8:37:VAL:HG12  | 5:8:47:TRP:HA      | 1.87                     | 0.55              |
| 4:E:52:ARG:NH2   | 4:E:53:ARG:O       | 2.39                     | 0.55              |
| 1:2:132:THR:OG1  | 1:2:133:ASN:N      | 2.41                     | 0.54              |
| 3:D:39:ARG:NH1   | 3:D:81:GLY:O       | 2.40                     | 0.54              |
| 2:M:52:HIS:HB3   | 2:M:56:ASP:HB3     | 1.89                     | 0.54              |
| 5:P:37:VAL:HG12  | 5:P:47:TRP:HA      | 1.89                     | 0.54              |
| 7:H:16:GLU:H     | 7:H:82(C):VAL:HG12 | 1.72                     | 0.54              |
| 1:2:503:ARG:NH2  | 6:A:653:GLN:OE1    | 2.41                     | 0.54              |
| 1:B:499:THR:OG1  | 1:B:500:ARG:N      | 2.41                     | 0.54              |
| 1:B:491:ILE:HG22 | 1:B:493:PRO:HD3    | 1.90                     | 0.54              |
| 3:D:80:ALA:HA    | 3:D:106:VAL:HG11   | 1.89                     | 0.54              |
| 7:H:67:VAL:HG12  | 7:H:82:VAL:HG22    | 1.88                     | 0.54              |
| 1:K:499:THR:OG1  | 1:K:500:ARG:N      | 2.40                     | 0.54              |
| 1:B:465:THR:O    | 5:F:61:ARG:NH1     | 2.41                     | 0.54              |
| 7:R:89:VAL:HA    | 7:R:107:VAL:O      | 2.07                     | 0.54              |
| 2:5:31:ASP:OD1   | 2:5:31:ASP:N       | 2.40                     | 0.53              |
| 4:7:29:GLY:HA3   | 9:i:2:NAG:H3       | 1.90                     | 0.53              |
| 1:K:198:THR:OG1  | 1:K:199:SER:N      | 2.41                     | 0.53              |
| 2:5:72:ASP:O     | 2:5:76:ASN:N       | 2.41                     | 0.53              |
| 1:K:56:SER:OG    | 1:K:57:ASP:N       | 2.41                     | 0.53              |
| 4:7:53:ARG:HE    | 4:7:57:VAL:HG23    | 1.72                     | 0.53              |
| 6:Q:620:SER:O    | 6:Q:624:ASP:HB2    | 2.09                     | 0.53              |
| 3:6:39:ARG:NH1   | 3:6:81:GLY:O       | 2.42                     | 0.53              |
| 1:B:424:ILE:HD12 | 1:B:426:MET:HB2    | 1.90                     | 0.53              |
| 2:C:72:ASP:O     | 2:C:76:ASN:N       | 2.42                     | 0.53              |
| 5:P:16:SER:OG    | 5:P:17:SER:N       | 2.40                     | 0.53              |
| 1:2:85:HIS:HB3   | 7:H:31(B):TYR:HE2  | 1.73                     | 0.52              |
| 1:K:503:ARG:NH2  | 6:Q:653:GLN:OE1    | 2.42                     | 0.52              |
| 5:P:89:GLU:HB3   | 5:P:108:VAL:HG12   | 1.91                     | 0.52              |

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| Atom-1           | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-----------------|--------------------------|-------------------|
| 1:2:283:ASN:ND2  | 1:2:477:ASP:OD2 | 2.42                     | 0.52              |
| 4:E:29:GLY:HA3   | 9:y:2:NAG:H3    | 1.90                     | 0.52              |
| 5:F:37:VAL:HG12  | 5:F:47:TRP:HA   | 1.90                     | 0.52              |
| 7:H:54:THR:OG1   | 7:H:55:MET:N    | 2.40                     | 0.52              |
| 4:O:53:ARG:HE    | 4:O:57:VAL:HG23 | 1.74                     | 0.52              |
| 1:2:465:THR:O    | 5:8:61:ARG:NH1  | 2.41                     | 0.52              |
| 1:B:132:THR:OG1  | 1:B:133:ASN:N   | 2.42                     | 0.52              |
| 2:M:72:ASP:O     | 2:M:76:ASN:N    | 2.41                     | 0.52              |
| 8:J:20:THR:HA    | 8:J:73:LEU:O    | 2.08                     | 0.52              |
| 7:R:38:ARG:NH2   | 7:R:86:ASP:OD1  | 2.43                     | 0.52              |
| 1:B:503:ARG:NH2  | 6:G:653:GLN:OE1 | 2.43                     | 0.52              |
| 1:2:364:SER:OG   | 1:2:365:SER:N   | 2.42                     | 0.52              |
| 6:G:606:THR:OG1  | 6:G:607:ASN:N   | 2.38                     | 0.52              |
| 2:C:38:ARG:NH1   | 2:C:86:ASP:OD1  | 2.43                     | 0.52              |
| 1:B:56:SER:OG    | 1:B:57:ASP:N    | 2.41                     | 0.52              |
| 1:K:101:VAL:HG11 | 1:K:480:ARG:HE  | 1.74                     | 0.52              |
| 1:K:132:THR:OG1  | 1:K:133:ASN:N   | 2.42                     | 0.52              |
| 1:K:465:THR:O    | 5:P:61:ARG:NH1  | 2.42                     | 0.52              |
| 2:C:100:ARG:NH2  | 3:D:30:SER:OG   | 2.43                     | 0.52              |
| 1:B:50:THR:OG1   | 1:B:51:THR:N    | 2.42                     | 0.52              |
| 6:Q:606:THR:OG1  | 6:Q:607:ASN:N   | 2.38                     | 0.52              |
| 1:2:56:SER:OG    | 1:2:57:ASP:N    | 2.42                     | 0.51              |
| 1:B:364:SER:OG   | 1:B:365:SER:N   | 2.42                     | 0.51              |
| 4:7:6:GLN:NE2    | 4:7:87:CYS:SG   | 2.78                     | 0.51              |
| 1:2:50:THR:OG1   | 1:2:51:THR:N    | 2.44                     | 0.51              |
| 1:B:198:THR:OG1  | 1:B:199:SER:N   | 2.41                     | 0.51              |
| 1:K:50:THR:OG1   | 1:K:51:THR:N    | 2.43                     | 0.51              |
| 6:Q:569:THR:OG1  | 6:Q:570:VAL:N   | 2.43                     | 0.51              |
| 1:2:209:SER:OG   | 1:2:210:PHE:N   | 2.44                     | 0.51              |
| 1:2:491:ILE:HG22 | 1:2:493:PRO:HD3 | 1.92                     | 0.51              |
| 1:B:373:THR:OG1  | 1:B:374:HIS:N   | 2.43                     | 0.51              |
| 7:I:87:THR:HG23  | 7:I:110:THR:HA  | 1.93                     | 0.51              |
| 1:K:209:SER:OG   | 1:K:210:PHE:N   | 2.44                     | 0.51              |
| 4:O:52:ARG:NH2   | 4:O:53:ARG:O    | 2.39                     | 0.51              |
| 2:5:38:ARG:NH1   | 2:5:86:ASP:OD1  | 2.43                     | 0.51              |
| 2:5:51:VAL:HG23  | 2:5:57:THR:HG23 | 1.93                     | 0.51              |
| 3:6:45:SER:OG    | 3:6:46:LEU:N    | 2.44                     | 0.51              |
| 7:I:34:TRP:O     | 7:I:50:GLY:HA2  | 2.11                     | 0.51              |
| 7:I:67:VAL:HG12  | 7:I:82:VAL:HG22 | 1.92                     | 0.51              |
| 6:G:569:THR:OG1  | 6:G:570:VAL:N   | 2.44                     | 0.50              |
| 5:P:52:LYS:O     | 5:P:55:GLY:HA2  | 2.12                     | 0.50              |

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| Atom-1            | Atom-2          | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|-----------------|--------------------------|-------------------|
| 6:Q:652:GLN:HG3   | 6:Q:655:LYS:HE2 | 1.93                     | 0.50              |
| 1:2:101:VAL:HG11  | 1:2:480:ARG:HE  | 1.76                     | 0.50              |
| 7:R:87:THR:HA     | 7:R:109:VAL:O   | 2.10                     | 0.50              |
| 1:K:203:GLN:HA    | 1:K:435:TYR:HB3 | 1.93                     | 0.50              |
| 1:2:499:THR:OG1   | 1:2:500:ARG:N   | 2.41                     | 0.50              |
| 1:2:297:THR:HB    | 1:2:444:ARG:HG3 | 1.93                     | 0.50              |
| 1:B:209:SER:OG    | 1:B:210:PHE:N   | 2.44                     | 0.50              |
| 1:2:63:THR:OG1    | 1:2:67:ASN:ND2  | 2.44                     | 0.50              |
| 1:K:256:SER:O     | 1:K:478:ASN:ND2 | 2.45                     | 0.50              |
| 2:C:51:VAL:HG23   | 2:C:57:THR:HG23 | 1.93                     | 0.50              |
| 6:G:617:ARG:NH1   | 6:G:634:GLU:OE2 | 2.45                     | 0.50              |
| 2:M:38:ARG:NH1    | 2:M:86:ASP:OD1  | 2.43                     | 0.50              |
| 1:2:39:TYR:O      | 1:2:494:LEU:HA  | 2.11                     | 0.49              |
| 6:A:652:GLN:HG3   | 6:A:655:LYS:HE2 | 1.93                     | 0.49              |
| 2:C:58:ASN:ND2    | 9:l:2:NAG:O7    | 2.44                     | 0.49              |
| 5:F:76(E):ASP:OD1 | 5:F:76(E):ASP:N | 2.44                     | 0.49              |
| 3:N:38:GLN:HB3    | 3:N:85:ASP:O    | 2.11                     | 0.49              |
| 5:P:2:VAL:HG11    | 5:P:94:ARG:HH21 | 1.77                     | 0.49              |
| 6:Q:617:ARG:NH1   | 6:Q:634:GLU:OE2 | 2.45                     | 0.49              |
| 4:7:52:ARG:NH2    | 4:7:53:ARG:O    | 2.40                     | 0.49              |
| 1:K:373:THR:OG1   | 1:K:374:HIS:N   | 2.45                     | 0.49              |
| 1:2:359:ILE:HD12  | 1:2:468:PHE:HE2 | 1.77                     | 0.49              |
| 7:I:38:ARG:NH2    | 7:I:86:ASP:OD1  | 2.43                     | 0.49              |
| 1:B:192:ARG:NH2   | 13:o:1:NAG:O6   | 2.46                     | 0.49              |
| 1:B:203:GLN:HA    | 1:B:435:TYR:HB3 | 1.95                     | 0.49              |
| 7:H:87:THR:HG23   | 7:H:110:THR:HA  | 1.94                     | 0.49              |
| 2:M:56:ASP:OD1    | 9:1:3:BMA:O2    | 2.31                     | 0.49              |
| 8:J:35:TRP:HB3    | 8:J:47:LEU:HD13 | 1.94                     | 0.49              |
| 8:L:35:TRP:HB3    | 8:L:47:LEU:HD13 | 1.95                     | 0.49              |
| 2:5:56:ASP:OD1    | 9:V:3:BMA:O2    | 2.30                     | 0.49              |
| 1:K:268:GLU:O     | 1:K:289:ASN:ND2 | 2.42                     | 0.49              |
| 2:5:100:ARG:NH2   | 3:6:30:SER:OG   | 2.45                     | 0.49              |
| 1:B:256:SER:O     | 1:B:478:ASN:ND2 | 2.45                     | 0.49              |
| 2:C:56:ASP:OD1    | 9:l:3:BMA:O2    | 2.30                     | 0.49              |
| 1:2:195:ASN:OD1   | 1:2:195:ASN:N   | 2.40                     | 0.49              |
| 7:I:56:ASP:OD1    | 7:I:56:ASP:N    | 2.46                     | 0.49              |
| 8:L:24:ARG:HG2    | 8:L:70:GLU:HG2  | 1.94                     | 0.49              |
| 8:S:35:TRP:HB3    | 8:S:47:LEU:HD13 | 1.95                     | 0.49              |
| 2:5:27:THR:OG1    | 2:5:28:LEU:N    | 2.45                     | 0.48              |
| 2:5:58:ASN:ND2    | 9:V:2:NAG:O7    | 2.45                     | 0.48              |
| 1:B:63:THR:OG1    | 1:B:67:ASN:ND2  | 2.46                     | 0.48              |

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| Atom-1           | Atom-2            | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|-------------------|--------------------------|-------------------|
| 1:2:268:GLU:O    | 1:2:289:ASN:ND2   | 2.44                     | 0.48              |
| 4:7:53:ARG:NH2   | 4:7:57:VAL:O      | 2.46                     | 0.48              |
| 8:S:21:ILE:HG23  | 8:S:73:LEU:HB3    | 1.94                     | 0.48              |
| 7:H:38:ARG:NH2   | 7:H:86:ASP:OD2    | 2.45                     | 0.48              |
| 1:K:491:ILE:HG22 | 1:K:493:PRO:HD3   | 1.94                     | 0.48              |
| 2:C:27:THR:OG1   | 2:C:28:LEU:N      | 2.47                     | 0.48              |
| 6:G:652:GLN:HG3  | 6:G:655:LYS:HE2   | 1.94                     | 0.48              |
| 7:R:87:THR:HG23  | 7:R:110:THR:HA    | 1.95                     | 0.48              |
| 8:S:24:ARG:HG2   | 8:S:70:GLU:HG2    | 1.94                     | 0.48              |
| 5:8:89:GLU:HB3   | 5:8:108:VAL:HG12  | 1.96                     | 0.48              |
| 7:I:72:ASP:OD2   | 7:I:72:ASP:N      | 2.42                     | 0.48              |
| 8:J:24:ARG:HG2   | 8:J:70:GLU:HG2    | 1.94                     | 0.48              |
| 5:P:6:GLN:HE22   | 5:P:91:PHE:HA     | 1.78                     | 0.48              |
| 1:B:234:ASN:OD1  | 1:B:234:ASN:N     | 2.40                     | 0.48              |
| 6:G:632:ASP:O    | 6:G:636:SER:OG    | 2.31                     | 0.48              |
| 1:2:192:ARG:NH2  | 13:Y:1:NAG:O6     | 2.47                     | 0.48              |
| 7:R:53:ASN:OD1   | 7:R:53:ASN:N      | 2.44                     | 0.48              |
| 4:E:6:GLN:NE2    | 4:E:87:CYS:SG     | 2.77                     | 0.48              |
| 1:K:85:HIS:HB3   | 7:R:31(B):TYR:HE2 | 1.79                     | 0.48              |
| 2:M:46:GLU:HG2   | 3:N:97:VAL:HG22   | 1.96                     | 0.48              |
| 1:K:192:ARG:NH2  | 13:9:1:NAG:O6     | 2.47                     | 0.48              |
| 6:A:620:SER:O    | 6:A:624:ASP:HB2   | 2.14                     | 0.47              |
| 1:B:359:ILE:HD12 | 1:B:468:PHE:HE2   | 1.79                     | 0.47              |
| 1:K:63:THR:OG1   | 1:K:67:ASN:ND2    | 2.47                     | 0.47              |
| 7:R:34:TRP:O     | 7:R:50:GLY:HA2    | 2.14                     | 0.47              |
| 1:2:457:ASP:OD2  | 1:2:469:ARG:NH1   | 2.47                     | 0.47              |
| 1:K:450:THR:OG1  | 1:K:451:GLY:N     | 2.47                     | 0.47              |
| 4:O:53:ARG:NH2   | 4:O:57:VAL:O      | 2.46                     | 0.47              |
| 1:B:40:TYR:HB3   | 6:G:602:LEU:HD12  | 1.95                     | 0.47              |
| 7:I:18:LEU:HB3   | 7:I:82:VAL:HB     | 1.96                     | 0.47              |
| 1:K:256:SER:OG   | 1:K:258:GLN:O     | 2.32                     | 0.47              |
| 1:K:454:LEU:HD23 | 1:K:468:PHE:HB3   | 1.96                     | 0.47              |
| 7:I:53:ASN:OD1   | 7:I:53:ASN:N      | 2.46                     | 0.47              |
| 1:K:40:TYR:HB3   | 6:Q:602:LEU:HD12  | 1.95                     | 0.47              |
| 1:K:141:ASP:OD1  | 1:K:141:ASP:N     | 2.43                     | 0.47              |
| 6:G:626:MET:HE2  | 6:G:626:MET:HB3   | 1.79                     | 0.47              |
| 7:H:53:ASN:OD1   | 7:H:53:ASN:N      | 2.46                     | 0.47              |
| 2:5:110:SER:OG   | 2:5:111:SER:N     | 2.48                     | 0.47              |
| 2:M:58:ASN:ND2   | 9:1:2:NAG:O7      | 2.47                     | 0.47              |
| 2:5:59:TYR:OH    | 2:5:69:LEU:N      | 2.44                     | 0.47              |
| 3:D:15:PRO:HA    | 3:D:78:VAL:HG13   | 1.96                     | 0.47              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 5:P:38:ARG:NH2   | 5:P:86:ASP:OD1   | 2.47                     | 0.47              |
| 1:B:363:ASN:OD1  | 1:B:363:ASN:N    | 2.40                     | 0.47              |
| 1:K:270:VAL:HG13 | 1:K:288:PHE:HB3  | 1.97                     | 0.47              |
| 4:E:53:ARG:NH2   | 4:E:57:VAL:O     | 2.48                     | 0.47              |
| 1:K:359:ILE:HD12 | 1:K:468:PHE:HE2  | 1.80                     | 0.47              |
| 7:H:89:VAL:HA    | 7:H:107:VAL:O    | 2.14                     | 0.46              |
| 2:M:31:ASP:OD1   | 2:M:31:ASP:N     | 2.41                     | 0.46              |
| 5:P:62:GLN:HG2   | 5:P:63:LEU:HD12  | 1.97                     | 0.46              |
| 5:8:48:ILE:HG23  | 5:8:63:LEU:HD22  | 1.97                     | 0.46              |
| 5:P:7:SER:OG     | 5:P:8:GLY:N      | 2.49                     | 0.46              |
| 8:L:20:THR:HA    | 8:L:73:LEU:O     | 2.15                     | 0.46              |
| 4:O:6:GLN:NE2    | 4:O:87:CYS:SG    | 2.77                     | 0.46              |
| 1:2:256:SER:O    | 1:2:478:ASN:ND2  | 2.49                     | 0.46              |
| 1:2:363:ASN:OD1  | 1:2:363:ASN:N    | 2.40                     | 0.46              |
| 7:H:101:ASP:OD2  | 8:L:46:ARG:NH1   | 2.49                     | 0.46              |
| 5:8:52:LYS:O     | 5:8:55:GLY:HA2   | 2.15                     | 0.46              |
| 1:B:83:GLU:OE2   | 1:B:229:LYS:NZ   | 2.45                     | 0.46              |
| 3:D:38:GLN:HB3   | 3:D:85:ASP:O     | 2.16                     | 0.46              |
| 1:K:424:ILE:HD12 | 1:K:426:MET:HB2  | 1.96                     | 0.46              |
| 7:R:54:THR:OG1   | 7:R:55:MET:N     | 2.40                     | 0.46              |
| 1:B:496:VAL:HG11 | 6:G:642:ILE:HG21 | 1.97                     | 0.46              |
| 1:K:39:TYR:O     | 1:K:494:LEU:HA   | 2.16                     | 0.46              |
| 2:C:31:ASP:OD1   | 2:C:31:ASP:N     | 2.40                     | 0.46              |
| 5:8:7:SER:OG     | 5:8:8:GLY:N      | 2.48                     | 0.45              |
| 7:I:89:VAL:HA    | 7:I:107:VAL:O    | 2.15                     | 0.45              |
| 5:F:7:SER:OG     | 5:F:8:GLY:N      | 2.49                     | 0.45              |
| 1:K:464:THR:O    | 1:K:464:THR:OG1  | 2.34                     | 0.45              |
| 3:N:45:SER:OG    | 3:N:46:LEU:N     | 2.47                     | 0.45              |
| 5:P:38:ARG:HD2   | 5:P:48:ILE:HD11  | 1.98                     | 0.45              |
| 6:A:569:THR:OG1  | 6:A:570:VAL:N    | 2.45                     | 0.45              |
| 7:H:34:TRP:O     | 7:H:50:GLY:HA2   | 2.16                     | 0.45              |
| 2:M:34:TRP:O     | 2:M:50:TYR:HA    | 2.17                     | 0.45              |
| 2:5:34:TRP:O     | 2:5:50:TYR:HA    | 2.16                     | 0.45              |
| 3:6:38:GLN:HB3   | 3:6:85:ASP:O     | 2.16                     | 0.45              |
| 1:B:210:PHE:HB3  | 1:B:377:ASN:HD21 | 1.81                     | 0.45              |
| 1:B:268:GLU:O    | 1:B:289:ASN:ND2  | 2.44                     | 0.45              |
| 3:D:77:SER:O     | 3:D:77:SER:OG    | 2.33                     | 0.45              |
| 5:F:98:CYS:SG    | 5:F:100(A):CYS:N | 2.89                     | 0.45              |
| 6:A:632:ASP:O    | 6:A:636:SER:OG   | 2.29                     | 0.45              |
| 5:F:87:THR:HG22  | 5:F:111:VAL:H    | 1.81                     | 0.45              |
| 1:B:84:ILE:HG13  | 1:B:244:THR:HG23 | 1.99                     | 0.45              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:2:203:GLN:HA   | 1:2:435:TYR:HB3  | 1.99                     | 0.45              |
| 1:K:96:TRP:NE1   | 1:K:274:SER:O    | 2.50                     | 0.45              |
| 7:R:52(A):SER:O  | 7:R:71:ARG:NH2   | 2.49                     | 0.45              |
| 8:S:35:TRP:O     | 8:S:47:LEU:N     | 2.49                     | 0.45              |
| 1:2:234:ASN:OD1  | 1:2:234:ASN:N    | 2.40                     | 0.45              |
| 4:E:21:LEU:HB2   | 4:E:72:LEU:HB3   | 1.99                     | 0.45              |
| 1:K:303:THR:OG1  | 1:K:321(A):ASP:N | 2.47                     | 0.45              |
| 1:B:184:ILE:HD12 | 1:B:184:ILE:HA   | 1.87                     | 0.44              |
| 1:B:334:SER:OG   | 1:B:337:THR:OG1  | 2.31                     | 0.44              |
| 4:E:59:ASP:OD1   | 4:E:59:ASP:N     | 2.50                     | 0.44              |
| 1:K:496:VAL:HG11 | 6:Q:642:ILE:HG21 | 1.99                     | 0.44              |
| 1:2:373:THR:OG1  | 1:2:385:CYS:N    | 2.50                     | 0.44              |
| 1:2:280:ASN:OD1  | 1:2:280:ASN:N    | 2.46                     | 0.44              |
| 1:B:280:ASN:OD1  | 1:B:280:ASN:N    | 2.44                     | 0.44              |
| 1:K:373:THR:OG1  | 1:K:385:CYS:N    | 2.50                     | 0.44              |
| 8:L:90:GLN:NE2   | 8:L:95:PRO:O     | 2.51                     | 0.44              |
| 2:M:70:SER:OG    | 2:M:79:SER:OG    | 2.35                     | 0.44              |
| 5:P:98:CYS:SG    | 5:P:100(A):CYS:N | 2.90                     | 0.44              |
| 6:A:626:MET:HE2  | 6:A:626:MET:HB3  | 1.82                     | 0.44              |
| 1:B:454:LEU:HD23 | 1:B:468:PHE:HB3  | 1.98                     | 0.44              |
| 7:R:18:LEU:HB3   | 7:R:82:VAL:HB    | 1.98                     | 0.44              |
| 2:C:34:TRP:O     | 2:C:50:TYR:HA    | 2.17                     | 0.44              |
| 2:C:5:GLN:NE2    | 2:C:6:GLU:O      | 2.50                     | 0.44              |
| 4:E:85:TYR:O     | 4:E:97:SER:OG    | 2.34                     | 0.44              |
| 5:F:89:GLU:HB3   | 5:F:108:VAL:HG22 | 1.99                     | 0.44              |
| 1:K:184:ILE:HD12 | 1:K:184:ILE:HA   | 1.89                     | 0.44              |
| 7:R:67:VAL:HG12  | 7:R:82:VAL:HG22  | 1.99                     | 0.44              |
| 7:R:72:ASP:OD2   | 7:R:72:ASP:N     | 2.49                     | 0.44              |
| 3:D:21:ILE:HG23  | 3:D:73:LEU:HB3   | 2.00                     | 0.44              |
| 7:R:66:ARG:HH11  | 7:R:82(C):VAL:HA | 1.83                     | 0.44              |
| 8:S:24:ARG:NE    | 8:S:70:GLU:OE2   | 2.51                     | 0.44              |
| 2:5:10:GLY:HA2   | 2:5:107:VAL:HG22 | 2.00                     | 0.43              |
| 1:B:283:ASN:ND2  | 1:B:477:ASP:OD2  | 2.41                     | 0.43              |
| 4:O:21:LEU:HB2   | 4:O:72:LEU:HB3   | 1.99                     | 0.43              |
| 7:R:56:ASP:OD1   | 7:R:56:ASP:N     | 2.43                     | 0.43              |
| 1:B:116:LEU:HD11 | 1:B:434:MET:HE3  | 2.00                     | 0.43              |
| 1:K:270:VAL:HG21 | 1:K:344:LYS:HB3  | 1.99                     | 0.43              |
| 5:P:48:ILE:HG23  | 5:P:63:LEU:HD22  | 1.99                     | 0.43              |
| 5:P:52:LYS:O     | 5:P:55:GLY:CA    | 2.66                     | 0.43              |
| 7:R:101:ASP:OD2  | 8:S:46:ARG:NH1   | 2.50                     | 0.43              |
| 1:2:37:THR:HG22  | 6:A:605:CYS:HA   | 2.01                     | 0.43              |

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| Atom-1            | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|-------------------|------------------|--------------------------|-------------------|
| 7:I:87:THR:HA     | 7:I:109:VAL:O    | 2.19                     | 0.43              |
| 4:O:11:LEU:HD12   | 4:O:11:LEU:HA    | 1.85                     | 0.43              |
| 3:6:39:ARG:HA     | 3:6:40:PRO:HD3   | 1.91                     | 0.43              |
| 1:B:96:TRP:NE1    | 1:B:274:SER:O    | 2.51                     | 0.43              |
| 1:2:84:ILE:HG13   | 1:2:244:THR:HG23 | 1.99                     | 0.43              |
| 1:2:231:LYS:HG3   | 1:2:267:GLU:HB2  | 2.01                     | 0.43              |
| 2:C:46:GLU:HG2    | 3:D:97:VAL:HG22  | 1.99                     | 0.43              |
| 3:6:15:PRO:HA     | 3:6:78:VAL:HG13  | 2.01                     | 0.43              |
| 7:H:72:ASP:OD2    | 7:H:72:ASP:N     | 2.51                     | 0.43              |
| 1:K:95:MET:HE1    | 1:K:273:ARG:HD3  | 2.01                     | 0.43              |
| 6:Q:632:ASP:O     | 6:Q:636:SER:OG   | 2.31                     | 0.43              |
| 7:H:2:VAL:HA      | 7:H:25:SER:O     | 2.19                     | 0.43              |
| 1:K:195:ASN:OD1   | 1:K:195:ASN:N    | 2.40                     | 0.43              |
| 4:O:85:TYR:O      | 4:O:97:SER:OG    | 2.35                     | 0.43              |
| 1:B:231:LYS:HG3   | 1:B:267:GLU:HB2  | 2.01                     | 0.43              |
| 1:K:135:THR:O     | 1:K:135:THR:OG1  | 2.34                     | 0.43              |
| 1:K:175:LEU:O     | 1:K:320:THR:OG1  | 2.35                     | 0.43              |
| 1:2:95:MET:HE1    | 1:2:273:ARG:HD3  | 2.01                     | 0.43              |
| 1:2:141:ASP:OD1   | 1:2:141:ASP:N    | 2.45                     | 0.43              |
| 1:B:95:MET:HE1    | 1:B:273:ARG:HD3  | 2.01                     | 0.43              |
| 8:L:24:ARG:NE     | 8:L:70:GLU:OE2   | 2.51                     | 0.43              |
| 5:P:82(C):LEU:HB3 | 5:P:111:VAL:HG11 | 2.01                     | 0.43              |
| 1:2:155:LYS:HA    | 1:2:155:LYS:HD2  | 1.91                     | 0.42              |
| 1:2:252:LYS:HD2   | 1:2:262:ASN:HB3  | 2.00                     | 0.42              |
| 1:2:454:LEU:HD23  | 1:2:468:PHE:HB3  | 2.00                     | 0.42              |
| 1:B:103:GLN:HE21  | 1:B:217:TYR:HE1  | 1.66                     | 0.42              |
| 4:E:38:ARG:NH2    | 4:E:41:GLN:OE1   | 2.48                     | 0.42              |
| 5:F:52:LYS:O      | 5:F:55:GLY:CA    | 2.67                     | 0.42              |
| 1:B:252:LYS:HD2   | 1:B:262:ASN:HB3  | 2.01                     | 0.42              |
| 4:E:21:LEU:O      | 4:E:71:PHE:HA    | 2.19                     | 0.42              |
| 1:K:231:LYS:HG3   | 1:K:267:GLU:HB2  | 2.00                     | 0.42              |
| 1:2:96:TRP:NE1    | 1:2:274:SER:O    | 2.52                     | 0.42              |
| 1:2:289:ASN:OD1   | 1:2:289:ASN:N    | 2.45                     | 0.42              |
| 4:7:59:ASP:OD1    | 4:7:59:ASP:N     | 2.48                     | 0.42              |
| 5:8:98:CYS:SG     | 5:8:100(A):CYS:N | 2.92                     | 0.42              |
| 1:B:373:THR:OG1   | 1:B:385:CYS:N    | 2.52                     | 0.42              |
| 7:H:56:ASP:OD1    | 7:H:56:ASP:N     | 2.42                     | 0.42              |
| 7:R:2:VAL:HA      | 7:R:25:SER:O     | 2.19                     | 0.42              |
| 5:8:52:LYS:O      | 5:8:55:GLY:CA    | 2.67                     | 0.42              |
| 1:B:141:ASP:OD1   | 1:B:141:ASP:N    | 2.43                     | 0.42              |
| 7:H:52(A):SER:O   | 7:H:71:ARG:NH2   | 2.52                     | 0.42              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 1:K:116:LEU:HD11 | 1:K:434:MET:HE3  | 2.00                     | 0.42              |
| 2:M:69:LEU:HD23  | 2:M:69:LEU:HA    | 1.92                     | 0.42              |
| 1:K:52:LEU:HD21  | 1:K:488:VAL:HG11 | 2.00                     | 0.42              |
| 2:5:39:GLN:HB3   | 2:5:89:ILE:HG13  | 2.01                     | 0.42              |
| 4:E:20:THR:HG22  | 4:E:73:THR:HG22  | 2.01                     | 0.42              |
| 5:F:52:LYS:O     | 5:F:55:GLY:HA2   | 2.18                     | 0.42              |
| 2:M:16:GLU:O     | 2:M:82(B):GLY:N  | 2.48                     | 0.42              |
| 2:5:51:VAL:HB    | 2:5:69:LEU:HD13  | 2.00                     | 0.42              |
| 5:P:87:THR:HG22  | 5:P:111:VAL:H    | 1.85                     | 0.42              |
| 6:G:536:THR:O    | 6:G:536:THR:OG1  | 2.35                     | 0.42              |
| 1:B:39:TYR:O     | 1:B:494:LEU:HA   | 2.20                     | 0.42              |
| 2:C:16:GLU:O     | 2:C:82(B):GLY:N  | 2.49                     | 0.42              |
| 8:J:77:SER:O     | 8:J:77:SER:OG    | 2.38                     | 0.42              |
| 6:Q:577:GLN:HA   | 6:Q:580:VAL:HG22 | 2.02                     | 0.42              |
| 1:B:303:THR:OG1  | 1:B:321(A):ASP:N | 2.49                     | 0.41              |
| 4:E:32:MET:HE2   | 4:E:87:CYS:HB2   | 2.02                     | 0.41              |
| 6:G:637:ASN:OD1  | 6:G:637:ASN:N    | 2.50                     | 0.41              |
| 1:2:116:LEU:HD11 | 1:2:434:MET:HE3  | 2.01                     | 0.41              |
| 4:7:42:VAL:HG23  | 5:8:103:TRP:HB2  | 2.01                     | 0.41              |
| 1:B:325:ASP:OD1  | 3:D:30:SER:N     | 2.44                     | 0.41              |
| 2:C:39:GLN:HB3   | 2:C:89:ILE:HG13  | 2.03                     | 0.41              |
| 5:F:48:ILE:HG23  | 5:F:63:LEU:HD22  | 2.01                     | 0.41              |
| 1:K:52:LEU:HD13  | 1:K:52:LEU:HA    | 1.96                     | 0.41              |
| 1:K:437:PRO:HA   | 1:K:438:PRO:HD3  | 1.91                     | 0.41              |
| 4:O:38:ARG:NH2   | 4:O:41:GLN:OE1   | 2.48                     | 0.41              |
| 8:S:90:GLN:NE2   | 8:S:95:PRO:O     | 2.53                     | 0.41              |
| 1:B:333:VAL:HG21 | 1:B:390:LEU:HD21 | 2.01                     | 0.41              |
| 7:I:7:SER:OG     | 7:I:8:GLY:N      | 2.53                     | 0.41              |
| 8:J:24:ARG:NE    | 8:J:70:GLU:OE2   | 2.53                     | 0.41              |
| 1:K:37:THR:HG22  | 6:Q:605:CYS:HA   | 2.03                     | 0.41              |
| 2:5:48:ILE:HG21  | 2:5:80:LEU:HD11  | 2.02                     | 0.41              |
| 3:6:21:ILE:HG21  | 3:6:104:LEU:HD21 | 2.03                     | 0.41              |
| 1:K:429:ARG:NE   | 1:K:432:GLN:OE1  | 2.54                     | 0.41              |
| 1:2:437:PRO:HA   | 1:2:438:PRO:HD3  | 1.91                     | 0.41              |
| 1:B:130:GLN:HG3  | 12:n:1:NAG:H82   | 2.03                     | 0.41              |
| 4:E:11:LEU:HD12  | 4:E:11:LEU:HA    | 1.85                     | 0.41              |
| 5:F:40:ILE:HB    | 5:F:43:LYS:HB2   | 2.03                     | 0.41              |
| 1:K:227:LYS:HD3  | 1:K:486:TYR:HE1  | 1.85                     | 0.41              |
| 1:2:304:ARG:N    | 1:2:440:GLN:OE1  | 2.53                     | 0.41              |
| 4:7:20:THR:O     | 4:7:20:THR:OG1   | 2.35                     | 0.41              |
| 1:B:52:LEU:HD11  | 1:B:488:VAL:HG11 | 2.02                     | 0.41              |

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| Atom-1           | Atom-2           | Interatomic distance (Å) | Clash overlap (Å) |
|------------------|------------------|--------------------------|-------------------|
| 2:C:27:THR:OG1   | 2:C:31:ASP:OD2   | 2.37                     | 0.41              |
| 2:C:87:SER:HA    | 2:C:108:THR:HA   | 2.03                     | 0.41              |
| 3:D:38:GLN:HB3   | 3:D:85:ASP:HB2   | 2.03                     | 0.41              |
| 3:N:21:ILE:HG21  | 3:N:104:LEU:HD21 | 2.03                     | 0.41              |
| 1:2:108:ILE:O    | 1:2:112:TRP:HB2  | 2.21                     | 0.41              |
| 2:5:27:THR:OG1   | 2:5:31:ASP:OD2   | 2.38                     | 0.41              |
| 4:7:38:ARG:NH2   | 4:7:41:GLN:OE1   | 2.49                     | 0.41              |
| 1:B:37:THR:HG22  | 6:G:605:CYS:HA   | 2.02                     | 0.41              |
| 1:B:289:ASN:OD1  | 1:B:289:ASN:N    | 2.43                     | 0.41              |
| 1:B:450:THR:OG1  | 1:B:451:GLY:N    | 2.54                     | 0.41              |
| 6:G:577:GLN:HA   | 6:G:580:VAL:HG22 | 2.03                     | 0.41              |
| 6:G:638:TYR:HB3  | 6:G:641:ILE:HD11 | 2.03                     | 0.41              |
| 1:K:264:SER:O    | 1:K:287:GLN:NE2  | 2.54                     | 0.41              |
| 2:M:72:ASP:HB3   | 2:M:77:LEU:H     | 1.85                     | 0.41              |
| 8:L:8:PRO:HG2    | 8:L:11:LEU:HD11  | 2.02                     | 0.41              |
| 7:R:66:ARG:NH1   | 7:R:86:ASP:OD2   | 2.54                     | 0.41              |
| 1:2:165:LEU:HD13 | 1:K:128:THR:HG22 | 2.03                     | 0.40              |
| 5:8:38:ARG:HD2   | 5:8:48:ILE:HD11  | 2.02                     | 0.40              |
| 1:B:155:LYS:HA   | 1:B:155:LYS:HD2  | 1.88                     | 0.40              |
| 3:D:14:ALA:HA    | 3:D:107:LEU:HB2  | 2.02                     | 0.40              |
| 1:2:210:PHE:HB3  | 1:2:377:ASN:HD21 | 1.86                     | 0.40              |
| 1:2:457:ASP:OD1  | 5:8:58:SER:OG    | 2.33                     | 0.40              |
| 5:8:40:ILE:HB    | 5:8:43:LYS:HB2   | 2.03                     | 0.40              |
| 1:B:464:THR:O    | 1:B:464:THR:OG1  | 2.35                     | 0.40              |
| 4:O:20:THR:O     | 4:O:20:THR:OG1   | 2.35                     | 0.40              |
| 6:Q:626:MET:HE2  | 6:Q:626:MET:HB3  | 1.79                     | 0.40              |
| 2:5:70:SER:OG    | 2:5:79:SER:OG    | 2.36                     | 0.40              |
| 1:2:276:ASN:OD1  | 1:2:276:ASN:N    | 2.54                     | 0.40              |
| 1:K:77:THR:OG1   | 1:K:78:ASP:N     | 2.55                     | 0.40              |
| 4:O:59:ASP:N     | 4:O:59:ASP:OD1   | 2.50                     | 0.40              |
| 1:2:373:THR:OG1  | 1:2:374:HIS:N    | 2.55                     | 0.40              |
| 1:K:130:GLN:HG3  | 12:4:1:NAG:H82   | 2.03                     | 0.40              |
| 1:K:373:THR:OG1  | 1:K:374:HIS:O    | 2.35                     | 0.40              |

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

| Mol | Chain | Analysed        | Favoured   | Allowed   | Outliers | Percentiles |     |
|-----|-------|-----------------|------------|-----------|----------|-------------|-----|
| 1   | 2     | 447/480 (93%)   | 406 (91%)  | 41 (9%)   | 0        | 100         | 100 |
| 1   | B     | 447/480 (93%)   | 405 (91%)  | 42 (9%)   | 0        | 100         | 100 |
| 1   | K     | 447/480 (93%)   | 405 (91%)  | 42 (9%)   | 0        | 100         | 100 |
| 2   | 5     | 130/235 (55%)   | 117 (90%)  | 13 (10%)  | 0        | 100         | 100 |
| 2   | C     | 130/235 (55%)   | 117 (90%)  | 13 (10%)  | 0        | 100         | 100 |
| 2   | M     | 130/235 (55%)   | 115 (88%)  | 15 (12%)  | 0        | 100         | 100 |
| 3   | 6     | 103/213 (48%)   | 92 (89%)   | 11 (11%)  | 0        | 100         | 100 |
| 3   | D     | 103/213 (48%)   | 91 (88%)   | 12 (12%)  | 0        | 100         | 100 |
| 3   | N     | 103/213 (48%)   | 92 (89%)   | 11 (11%)  | 0        | 100         | 100 |
| 4   | 7     | 100/209 (48%)   | 89 (89%)   | 11 (11%)  | 0        | 100         | 100 |
| 4   | E     | 100/209 (48%)   | 90 (90%)   | 10 (10%)  | 0        | 100         | 100 |
| 4   | O     | 100/209 (48%)   | 89 (89%)   | 11 (11%)  | 0        | 100         | 100 |
| 5   | 8     | 126/233 (54%)   | 112 (89%)  | 14 (11%)  | 0        | 100         | 100 |
| 5   | F     | 126/233 (54%)   | 112 (89%)  | 14 (11%)  | 0        | 100         | 100 |
| 5   | P     | 126/233 (54%)   | 112 (89%)  | 14 (11%)  | 0        | 100         | 100 |
| 6   | A     | 128/153 (84%)   | 118 (92%)  | 10 (8%)   | 0        | 100         | 100 |
| 6   | G     | 128/153 (84%)   | 117 (91%)  | 11 (9%)   | 0        | 100         | 100 |
| 6   | Q     | 128/153 (84%)   | 118 (92%)  | 10 (8%)   | 0        | 100         | 100 |
| 7   | H     | 120/235 (51%)   | 110 (92%)  | 10 (8%)   | 0        | 100         | 100 |
| 7   | I     | 120/235 (51%)   | 110 (92%)  | 10 (8%)   | 0        | 100         | 100 |
| 7   | R     | 120/235 (51%)   | 107 (89%)  | 13 (11%)  | 0        | 100         | 100 |
| 8   | J     | 102/213 (48%)   | 94 (92%)   | 8 (8%)    | 0        | 100         | 100 |
| 8   | L     | 102/213 (48%)   | 94 (92%)   | 8 (8%)    | 0        | 100         | 100 |
| 8   | S     | 102/213 (48%)   | 95 (93%)   | 7 (7%)    | 0        | 100         | 100 |
| All | All   | 3768/5913 (64%) | 3407 (90%) | 361 (10%) | 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   | 2     | 405/428 (95%) | 388 (96%)  | 17 (4%)  | 26          | 48  |
| 1   | B     | 405/428 (95%) | 386 (95%)  | 19 (5%)  | 23          | 46  |
| 1   | K     | 405/428 (95%) | 390 (96%)  | 15 (4%)  | 30          | 51  |
| 2   | 5     | 116/205 (57%) | 116 (100%) | 0        | 100         | 100 |
| 2   | C     | 116/205 (57%) | 116 (100%) | 0        | 100         | 100 |
| 2   | M     | 116/205 (57%) | 114 (98%)  | 2 (2%)   | 53          | 67  |
| 3   | 6     | 88/181 (49%)  | 88 (100%)  | 0        | 100         | 100 |
| 3   | D     | 88/181 (49%)  | 87 (99%)   | 1 (1%)   | 65          | 74  |
| 3   | N     | 88/181 (49%)  | 86 (98%)   | 2 (2%)   | 44          | 64  |
| 4   | 7     | 86/182 (47%)  | 83 (96%)   | 3 (4%)   | 32          | 54  |
| 4   | E     | 86/182 (47%)  | 83 (96%)   | 3 (4%)   | 32          | 54  |
| 4   | O     | 86/182 (47%)  | 83 (96%)   | 3 (4%)   | 32          | 54  |
| 5   | 8     | 108/199 (54%) | 104 (96%)  | 4 (4%)   | 30          | 51  |
| 5   | F     | 108/199 (54%) | 107 (99%)  | 1 (1%)   | 70          | 76  |
| 5   | P     | 108/199 (54%) | 105 (97%)  | 3 (3%)   | 38          | 59  |
| 6   | A     | 110/129 (85%) | 108 (98%)  | 2 (2%)   | 51          | 67  |
| 6   | G     | 110/129 (85%) | 108 (98%)  | 2 (2%)   | 51          | 67  |
| 6   | Q     | 110/129 (85%) | 108 (98%)  | 2 (2%)   | 51          | 67  |
| 7   | H     | 107/207 (52%) | 107 (100%) | 0        | 100         | 100 |
| 7   | I     | 107/207 (52%) | 103 (96%)  | 4 (4%)   | 30          | 51  |
| 7   | R     | 107/207 (52%) | 106 (99%)  | 1 (1%)   | 70          | 76  |
| 8   | J     | 90/190 (47%)  | 90 (100%)  | 0        | 100         | 100 |
| 8   | L     | 90/190 (47%)  | 90 (100%)  | 0        | 100         | 100 |
| 8   | S     | 90/190 (47%)  | 89 (99%)   | 1 (1%)   | 65          | 74  |

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| Mol | Chain | Analysed        | Rotameric  | Outliers | Percentiles |
|-----|-------|-----------------|------------|----------|-------------|
| All | All   | 3330/5163 (64%) | 3245 (97%) | 85 (3%)  | 41 60       |

All (85) residues with a non-rotameric sidechain are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 36  | VAL  |
| 1   | 2     | 38  | VAL  |
| 1   | 2     | 54  | CYS  |
| 1   | 2     | 63  | THR  |
| 1   | 2     | 74  | CYS  |
| 1   | 2     | 75  | VAL  |
| 1   | 2     | 201 | CYS  |
| 1   | 2     | 244 | THR  |
| 1   | 2     | 251 | ILE  |
| 1   | 2     | 254 | VAL  |
| 1   | 2     | 260 | LEU  |
| 1   | 2     | 276 | ASN  |
| 1   | 2     | 369 | LEU  |
| 1   | 2     | 372 | THR  |
| 1   | 2     | 374 | HIS  |
| 1   | 2     | 452 | LEU  |
| 1   | 2     | 478 | ASN  |
| 4   | 7     | 42  | VAL  |
| 4   | 7     | 90  | PHE  |
| 4   | 7     | 101 | VAL  |
| 5   | 8     | 37  | VAL  |
| 5   | 8     | 67  | VAL  |
| 5   | 8     | 87  | THR  |
| 5   | 8     | 108 | VAL  |
| 6   | A     | 518 | VAL  |
| 6   | A     | 608 | VAL  |
| 1   | B     | 36  | VAL  |
| 1   | B     | 38  | VAL  |
| 1   | B     | 54  | CYS  |
| 1   | B     | 63  | THR  |
| 1   | B     | 74  | CYS  |
| 1   | B     | 182 | VAL  |
| 1   | B     | 244 | THR  |
| 1   | B     | 254 | VAL  |
| 1   | B     | 257 | THR  |
| 1   | B     | 261 | LEU  |
| 1   | B     | 276 | ASN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | B     | 289 | ASN  |
| 1   | B     | 290 | THR  |
| 1   | B     | 294 | ILE  |
| 1   | B     | 369 | LEU  |
| 1   | B     | 372 | THR  |
| 1   | B     | 374 | HIS  |
| 1   | B     | 439 | ILE  |
| 1   | B     | 449 | ILE  |
| 3   | D     | 70  | THR  |
| 4   | E     | 42  | VAL  |
| 4   | E     | 90  | PHE  |
| 4   | E     | 101 | VAL  |
| 5   | F     | 5   | VAL  |
| 6   | G     | 608 | VAL  |
| 6   | G     | 641 | ILE  |
| 7   | I     | 11  | VAL  |
| 7   | I     | 54  | THR  |
| 7   | I     | 72  | ASP  |
| 7   | I     | 80  | LEU  |
| 1   | K     | 36  | VAL  |
| 1   | K     | 38  | VAL  |
| 1   | K     | 63  | THR  |
| 1   | K     | 74  | CYS  |
| 1   | K     | 75  | VAL  |
| 1   | K     | 89  | VAL  |
| 1   | K     | 120 | VAL  |
| 1   | K     | 182 | VAL  |
| 1   | K     | 254 | VAL  |
| 1   | K     | 257 | THR  |
| 1   | K     | 297 | THR  |
| 1   | K     | 370 | GLU  |
| 1   | K     | 372 | THR  |
| 1   | K     | 374 | HIS  |
| 1   | K     | 439 | ILE  |
| 2   | M     | 83  | THR  |
| 2   | M     | 109 | VAL  |
| 3   | N     | 72  | THR  |
| 3   | N     | 82  | ASP  |
| 4   | O     | 42  | VAL  |
| 4   | O     | 90  | PHE  |
| 4   | O     | 101 | VAL  |
| 5   | P     | 37  | VAL  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | P     | 51  | ILE  |
| 5   | P     | 108 | VAL  |
| 6   | Q     | 518 | VAL  |
| 6   | Q     | 608 | VAL  |
| 7   | R     | 2   | VAL  |
| 8   | S     | 21  | ILE  |

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 1   | 2     | 33  | ASN  |
| 1   | 2     | 67  | ASN  |
| 1   | 2     | 82  | GLN  |
| 1   | 2     | 94  | ASN  |
| 1   | 2     | 216 | HIS  |
| 1   | 2     | 279 | ASN  |
| 1   | 2     | 302 | ASN  |
| 1   | 2     | 348 | GLN  |
| 1   | 2     | 425 | ASN  |
| 1   | 2     | 462 | ASN  |
| 1   | 2     | 478 | ASN  |
| 2   | 5     | 23  | ASN  |
| 4   | 7     | 75  | ASN  |
| 5   | 8     | 6   | GLN  |
| 5   | 8     | 64  | GLN  |
| 6   | A     | 640 | GLN  |
| 6   | A     | 652 | GLN  |
| 1   | B     | 33  | ASN  |
| 1   | B     | 66  | HIS  |
| 1   | B     | 67  | ASN  |
| 1   | B     | 82  | GLN  |
| 1   | B     | 94  | ASN  |
| 1   | B     | 99  | ASN  |
| 1   | B     | 103 | GLN  |
| 1   | B     | 216 | HIS  |
| 1   | B     | 279 | ASN  |
| 1   | B     | 348 | GLN  |
| 1   | B     | 462 | ASN  |
| 1   | B     | 478 | ASN  |
| 2   | C     | 23  | ASN  |
| 4   | E     | 75  | ASN  |
| 5   | F     | 6   | GLN  |

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| Mol | Chain | Res | Type |
|-----|-------|-----|------|
| 5   | F     | 64  | GLN  |
| 5   | F     | 101 | GLN  |
| 6   | G     | 652 | GLN  |
| 7   | H     | 3   | GLN  |
| 7   | H     | 76  | ASN  |
| 7   | I     | 3   | GLN  |
| 8   | J     | 49  | HIS  |
| 8   | J     | 79  | GLN  |
| 1   | K     | 67  | ASN  |
| 1   | K     | 82  | GLN  |
| 1   | K     | 94  | ASN  |
| 1   | K     | 216 | HIS  |
| 1   | K     | 348 | GLN  |
| 1   | K     | 462 | ASN  |
| 1   | K     | 478 | ASN  |
| 8   | L     | 38  | GLN  |
| 8   | L     | 49  | HIS  |
| 8   | L     | 79  | GLN  |
| 2   | M     | 23  | ASN  |
| 4   | O     | 75  | ASN  |
| 5   | P     | 6   | GLN  |
| 5   | P     | 64  | GLN  |
| 5   | P     | 101 | GLN  |
| 6   | Q     | 652 | GLN  |
| 7   | R     | 3   | GLN  |
| 7   | R     | 76  | ASN  |
| 8   | S     | 49  | HIS  |
| 8   | S     | 79  | GLN  |

### 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 ⓘ

177 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 | $\# Z  > 2$ |
| 10  | NAG  | 0     | 1   | 10,1 | 14,14,15     | 0.55 | 0           | 17,19,21    | 1.63 | 2 (11%)     |
| 10  | NAG  | 0     | 2   | 10   | 14,14,15     | 1.04 | 2 (14%)     | 17,19,21    | 0.53 | 0           |
| 9   | NAG  | 1     | 1   | 9,1  | 14,14,15     | 0.43 | 0           | 17,19,21    | 0.79 | 0           |
| 9   | NAG  | 1     | 2   | 9    | 14,14,15     | 0.74 | 1 (7%)      | 17,19,21    | 1.16 | 2 (11%)     |
| 9   | BMA  | 1     | 3   | 9    | 11,11,12     | 2.16 | 3 (27%)     | 15,15,17    | 2.18 | 3 (20%)     |
| 9   | MAN  | 1     | 4   | 9    | 11,11,12     | 1.36 | 2 (18%)     | 15,15,17    | 2.02 | 2 (13%)     |
| 11  | NAG  | 3     | 1   | 11,1 | 14,14,15     | 0.45 | 0           | 17,19,21    | 0.81 | 0           |
| 11  | NAG  | 3     | 2   | 11   | 14,14,15     | 0.34 | 0           | 17,19,21    | 0.91 | 1 (5%)      |
| 11  | BMA  | 3     | 3   | 11   | 11,11,12     | 1.46 | 2 (18%)     | 15,15,17    | 1.14 | 0           |
| 11  | MAN  | 3     | 4   | 11   | 11,11,12     | 1.45 | 2 (18%)     | 15,15,17    | 1.41 | 3 (20%)     |
| 11  | MAN  | 3     | 5   | 11   | 11,11,12     | 1.19 | 2 (18%)     | 15,15,17    | 1.27 | 1 (6%)      |
| 12  | NAG  | 4     | 1   | 12,1 | 14,14,15     | 0.88 | 1 (7%)      | 17,19,21    | 1.59 | 2 (11%)     |
| 12  | NAG  | 4     | 2   | 12   | 14,14,15     | 0.68 | 0           | 17,19,21    | 0.71 | 0           |
| 12  | BMA  | 4     | 3   | 12   | 11,11,12     | 1.34 | 1 (9%)      | 15,15,17    | 1.22 | 2 (13%)     |
| 13  | NAG  | 9     | 1   | 13,1 | 14,14,15     | 0.31 | 0           | 17,19,21    | 0.96 | 1 (5%)      |
| 13  | NAG  | 9     | 2   | 13   | 14,14,15     | 0.38 | 0           | 17,19,21    | 0.85 | 1 (5%)      |
| 13  | BMA  | 9     | 3   | 13   | 11,11,12     | 1.18 | 2 (18%)     | 15,15,17    | 1.74 | 1 (6%)      |
| 13  | MAN  | 9     | 4   | 13   | 11,11,12     | 1.32 | 1 (9%)      | 15,15,17    | 1.85 | 2 (13%)     |
| 10  | NAG  | AA    | 1   | 10,1 | 14,14,15     | 0.64 | 0           | 17,19,21    | 0.81 | 0           |
| 10  | NAG  | AA    | 2   | 10   | 14,14,15     | 0.84 | 1 (7%)      | 17,19,21    | 0.62 | 1 (5%)      |
| 14  | NAG  | BA    | 1   | 14,1 | 14,14,15     | 0.46 | 0           | 17,19,21    | 0.75 | 1 (5%)      |
| 14  | NAG  | BA    | 2   | 14   | 14,14,15     | 0.42 | 0           | 17,19,21    | 0.69 | 0           |
| 14  | BMA  | BA    | 3   | 14   | 11,11,12     | 1.06 | 0           | 15,15,17    | 1.31 | 2 (13%)     |
| 14  | MAN  | BA    | 4   | 14   | 11,11,12     | 0.94 | 1 (9%)      | 15,15,17    | 1.66 | 1 (6%)      |
| 14  | MAN  | BA    | 5   | 14   | 11,11,12     | 1.00 | 0           | 15,15,17    | 1.33 | 2 (13%)     |
| 14  | MAN  | BA    | 6   | 14   | 11,11,12     | 1.09 | 1 (9%)      | 15,15,17    | 1.35 | 2 (13%)     |
| 10  | NAG  | CA    | 1   | 10,1 | 14,14,15     | 0.56 | 0           | 17,19,21    | 0.86 | 1 (5%)      |
| 10  | NAG  | CA    | 2   | 10   | 14,14,15     | 0.74 | 1 (7%)      | 17,19,21    | 0.68 | 1 (5%)      |
| 10  | NAG  | DA    | 1   | 10,1 | 14,14,15     | 0.42 | 0           | 17,19,21    | 0.91 | 1 (5%)      |
| 10  | NAG  | DA    | 2   | 10   | 14,14,15     | 0.78 | 1 (7%)      | 17,19,21    | 0.82 | 1 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 12  | NAG  | EA    | 1   | 12,1 | 14,14,15     | 0.77 | 0        | 17,19,21    | 0.91 | 1 (5%)   |
| 12  | NAG  | EA    | 2   | 12   | 14,14,15     | 0.54 | 0        | 17,19,21    | 1.14 | 1 (5%)   |
| 12  | BMA  | EA    | 3   | 12   | 11,11,12     | 1.59 | 3 (27%)  | 15,15,17    | 1.61 | 2 (13%)  |
| 11  | NAG  | FA    | 1   | 11,1 | 14,14,15     | 0.27 | 0        | 17,19,21    | 1.13 | 1 (5%)   |
| 11  | NAG  | FA    | 2   | 11   | 14,14,15     | 0.39 | 0        | 17,19,21    | 1.34 | 2 (11%)  |
| 11  | BMA  | FA    | 3   | 11   | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 1.85 | 3 (20%)  |
| 11  | MAN  | FA    | 4   | 11   | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 1.19 | 1 (6%)   |
| 11  | MAN  | FA    | 5   | 11   | 11,11,12     | 1.00 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 10  | NAG  | GA    | 1   | 10,1 | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.88 | 1 (5%)   |
| 10  | NAG  | GA    | 2   | 10   | 14,14,15     | 0.85 | 1 (7%)   | 17,19,21    | 0.68 | 1 (5%)   |
| 15  | NAG  | HA    | 1   | 15,1 | 14,14,15     | 0.78 | 1 (7%)   | 17,19,21    | 0.90 | 1 (5%)   |
| 15  | NAG  | HA    | 2   | 15   | 14,14,15     | 0.38 | 0        | 17,19,21    | 1.76 | 3 (17%)  |
| 15  | BMA  | HA    | 3   | 15   | 11,11,12     | 2.01 | 6 (54%)  | 15,15,17    | 2.07 | 3 (20%)  |
| 15  | MAN  | HA    | 4   | 15   | 11,11,12     | 0.82 | 0        | 15,15,17    | 1.78 | 1 (6%)   |
| 15  | MAN  | HA    | 5   | 15   | 11,11,12     | 1.32 | 1 (9%)   | 15,15,17    | 2.20 | 2 (13%)  |
| 15  | MAN  | HA    | 6   | 15   | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.22 | 2 (13%)  |
| 15  | MAN  | HA    | 7   | 15   | 11,11,12     | 1.49 | 2 (18%)  | 15,15,17    | 1.74 | 3 (20%)  |
| 15  | MAN  | HA    | 8   | 15   | 11,11,12     | 1.30 | 1 (9%)   | 15,15,17    | 1.14 | 1 (6%)   |
| 15  | MAN  | HA    | 9   | 15   | 11,11,12     | 1.04 | 1 (9%)   | 15,15,17    | 1.57 | 2 (13%)  |
| 10  | NAG  | IA    | 1   | 10,1 | 14,14,15     | 0.48 | 0        | 17,19,21    | 1.60 | 3 (17%)  |
| 10  | NAG  | IA    | 2   | 10   | 14,14,15     | 0.60 | 0        | 17,19,21    | 1.24 | 1 (5%)   |
| 9   | NAG  | JA    | 1   | 9,1  | 14,14,15     | 0.95 | 1 (7%)   | 17,19,21    | 1.50 | 3 (17%)  |
| 9   | NAG  | JA    | 2   | 9    | 14,14,15     | 0.74 | 1 (7%)   | 17,19,21    | 1.04 | 1 (5%)   |
| 9   | BMA  | JA    | 3   | 9    | 11,11,12     | 1.72 | 3 (27%)  | 15,15,17    | 1.84 | 2 (13%)  |
| 9   | MAN  | JA    | 4   | 9    | 11,11,12     | 2.11 | 5 (45%)  | 15,15,17    | 2.44 | 5 (33%)  |
| 9   | NAG  | T     | 1   | 9,1  | 14,14,15     | 0.64 | 0        | 17,19,21    | 1.01 | 1 (5%)   |
| 9   | NAG  | T     | 2   | 9    | 14,14,15     | 0.84 | 1 (7%)   | 17,19,21    | 0.72 | 0        |
| 9   | BMA  | T     | 3   | 9    | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.00 | 1 (6%)   |
| 9   | MAN  | T     | 4   | 9    | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 1.69 | 2 (13%)  |
| 10  | NAG  | U     | 1   | 10,1 | 14,14,15     | 0.53 | 0        | 17,19,21    | 1.63 | 2 (11%)  |
| 10  | NAG  | U     | 2   | 10   | 14,14,15     | 1.03 | 2 (14%)  | 17,19,21    | 0.54 | 0        |
| 9   | NAG  | V     | 1   | 9,1  | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.77 | 0        |
| 9   | NAG  | V     | 2   | 9    | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 1.16 | 2 (11%)  |
| 9   | BMA  | V     | 3   | 9    | 11,11,12     | 2.13 | 3 (27%)  | 15,15,17    | 2.16 | 3 (20%)  |
| 9   | MAN  | V     | 4   | 9    | 11,11,12     | 1.36 | 2 (18%)  | 15,15,17    | 2.00 | 2 (13%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 11  | NAG  | W     | 1   | 11,1 | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.78 | 0        |
| 11  | NAG  | W     | 2   | 11   | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.87 | 1 (5%)   |
| 11  | BMA  | W     | 3   | 11   | 11,11,12     | 1.43 | 2 (18%)  | 15,15,17    | 1.14 | 0        |
| 11  | MAN  | W     | 4   | 11   | 11,11,12     | 1.45 | 2 (18%)  | 15,15,17    | 1.39 | 3 (20%)  |
| 11  | MAN  | W     | 5   | 11   | 11,11,12     | 1.20 | 2 (18%)  | 15,15,17    | 1.27 | 1 (6%)   |
| 12  | NAG  | X     | 1   | 12,1 | 14,14,15     | 0.90 | 1 (7%)   | 17,19,21    | 1.58 | 3 (17%)  |
| 12  | NAG  | X     | 2   | 12   | 14,14,15     | 0.70 | 0        | 17,19,21    | 0.73 | 1 (5%)   |
| 12  | BMA  | X     | 3   | 12   | 11,11,12     | 1.36 | 1 (9%)   | 15,15,17    | 1.22 | 2 (13%)  |
| 13  | NAG  | Y     | 1   | 13,1 | 14,14,15     | 0.32 | 0        | 17,19,21    | 0.87 | 1 (5%)   |
| 13  | NAG  | Y     | 2   | 13   | 14,14,15     | 0.37 | 0        | 17,19,21    | 0.87 | 1 (5%)   |
| 13  | BMA  | Y     | 3   | 13   | 11,11,12     | 1.18 | 2 (18%)  | 15,15,17    | 1.72 | 1 (6%)   |
| 13  | MAN  | Y     | 4   | 13   | 11,11,12     | 1.34 | 1 (9%)   | 15,15,17    | 1.86 | 2 (13%)  |
| 10  | NAG  | Z     | 1   | 10,1 | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.81 | 0        |
| 10  | NAG  | Z     | 2   | 10   | 14,14,15     | 0.83 | 1 (7%)   | 17,19,21    | 0.62 | 1 (5%)   |
| 14  | NAG  | a     | 1   | 14,1 | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.84 | 1 (5%)   |
| 14  | NAG  | a     | 2   | 14   | 14,14,15     | 0.39 | 0        | 17,19,21    | 0.71 | 0        |
| 14  | BMA  | a     | 3   | 14   | 11,11,12     | 1.03 | 0        | 15,15,17    | 1.26 | 2 (13%)  |
| 14  | MAN  | a     | 4   | 14   | 11,11,12     | 0.96 | 1 (9%)   | 15,15,17    | 1.65 | 1 (6%)   |
| 14  | MAN  | a     | 5   | 14   | 11,11,12     | 1.00 | 0        | 15,15,17    | 1.33 | 2 (13%)  |
| 14  | MAN  | a     | 6   | 14   | 11,11,12     | 1.08 | 1 (9%)   | 15,15,17    | 1.34 | 2 (13%)  |
| 10  | NAG  | b     | 1   | 10,1 | 14,14,15     | 0.49 | 0        | 17,19,21    | 0.87 | 1 (5%)   |
| 10  | NAG  | b     | 2   | 10   | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 0.69 | 1 (5%)   |
| 10  | NAG  | c     | 1   | 10,1 | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.92 | 1 (5%)   |
| 10  | NAG  | c     | 2   | 10   | 14,14,15     | 0.82 | 1 (7%)   | 17,19,21    | 0.83 | 1 (5%)   |
| 12  | NAG  | d     | 1   | 12,1 | 14,14,15     | 0.73 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 12  | NAG  | d     | 2   | 12   | 14,14,15     | 0.55 | 0        | 17,19,21    | 1.19 | 1 (5%)   |
| 12  | BMA  | d     | 3   | 12   | 11,11,12     | 1.58 | 2 (18%)  | 15,15,17    | 1.68 | 2 (13%)  |
| 11  | NAG  | e     | 1   | 11,1 | 14,14,15     | 0.28 | 0        | 17,19,21    | 1.13 | 1 (5%)   |
| 11  | NAG  | e     | 2   | 11   | 14,14,15     | 0.36 | 0        | 17,19,21    | 1.34 | 2 (11%)  |
| 11  | BMA  | e     | 3   | 11   | 11,11,12     | 0.99 | 1 (9%)   | 15,15,17    | 1.83 | 3 (20%)  |
| 11  | MAN  | e     | 4   | 11   | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 1.21 | 1 (6%)   |
| 11  | MAN  | e     | 5   | 11   | 11,11,12     | 0.98 | 1 (9%)   | 15,15,17    | 1.44 | 2 (13%)  |
| 10  | NAG  | f     | 1   | 10,1 | 14,14,15     | 0.35 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 10  | NAG  | f     | 2   | 10   | 14,14,15     | 0.82 | 1 (7%)   | 17,19,21    | 0.68 | 1 (5%)   |
| 15  | NAG  | g     | 1   | 15,1 | 14,14,15     | 0.78 | 1 (7%)   | 17,19,21    | 0.88 | 0        |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 15  | NAG  | g     | 2   | 15   | 14,14,15     | 0.44 | 0        | 17,19,21    | 1.75 | 3 (17%)  |
| 15  | BMA  | g     | 3   | 15   | 11,11,12     | 1.99 | 5 (45%)  | 15,15,17    | 2.07 | 4 (26%)  |
| 15  | MAN  | g     | 4   | 15   | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.81 | 1 (6%)   |
| 15  | MAN  | g     | 5   | 15   | 11,11,12     | 1.29 | 1 (9%)   | 15,15,17    | 2.18 | 2 (13%)  |
| 15  | MAN  | g     | 6   | 15   | 11,11,12     | 1.12 | 1 (9%)   | 15,15,17    | 1.21 | 2 (13%)  |
| 15  | MAN  | g     | 7   | 15   | 11,11,12     | 1.47 | 2 (18%)  | 15,15,17    | 1.74 | 4 (26%)  |
| 15  | MAN  | g     | 8   | 15   | 11,11,12     | 1.28 | 1 (9%)   | 15,15,17    | 1.16 | 1 (6%)   |
| 15  | MAN  | g     | 9   | 15   | 11,11,12     | 1.04 | 1 (9%)   | 15,15,17    | 1.59 | 2 (13%)  |
| 10  | NAG  | h     | 1   | 10,1 | 14,14,15     | 0.46 | 0        | 17,19,21    | 1.60 | 3 (17%)  |
| 10  | NAG  | h     | 2   | 10   | 14,14,15     | 0.60 | 0        | 17,19,21    | 1.17 | 1 (5%)   |
| 9   | NAG  | i     | 1   | 9,1  | 14,14,15     | 1.84 | 1 (7%)   | 17,19,21    | 2.49 | 3 (17%)  |
| 9   | NAG  | i     | 2   | 9    | 14,14,15     | 0.38 | 0        | 17,19,21    | 1.33 | 1 (5%)   |
| 9   | BMA  | i     | 3   | 9    | 11,11,12     | 1.89 | 5 (45%)  | 15,15,17    | 1.99 | 3 (20%)  |
| 9   | MAN  | i     | 4   | 9    | 11,11,12     | 2.12 | 5 (45%)  | 15,15,17    | 2.49 | 5 (33%)  |
| 9   | NAG  | j     | 1   | 9,1  | 14,14,15     | 0.63 | 0        | 17,19,21    | 1.04 | 1 (5%)   |
| 9   | NAG  | j     | 2   | 9    | 14,14,15     | 0.84 | 1 (7%)   | 17,19,21    | 0.72 | 0        |
| 9   | BMA  | j     | 3   | 9    | 11,11,12     | 1.16 | 1 (9%)   | 15,15,17    | 1.00 | 2 (13%)  |
| 9   | MAN  | j     | 4   | 9    | 11,11,12     | 1.14 | 1 (9%)   | 15,15,17    | 1.66 | 2 (13%)  |
| 10  | NAG  | k     | 1   | 10,1 | 14,14,15     | 0.54 | 0        | 17,19,21    | 1.62 | 2 (11%)  |
| 10  | NAG  | k     | 2   | 10   | 14,14,15     | 1.02 | 2 (14%)  | 17,19,21    | 0.54 | 0        |
| 9   | NAG  | l     | 1   | 9,1  | 14,14,15     | 0.41 | 0        | 17,19,21    | 0.77 | 0        |
| 9   | NAG  | l     | 2   | 9    | 14,14,15     | 0.71 | 1 (7%)   | 17,19,21    | 1.18 | 2 (11%)  |
| 9   | BMA  | l     | 3   | 9    | 11,11,12     | 2.17 | 3 (27%)  | 15,15,17    | 2.17 | 4 (26%)  |
| 9   | MAN  | l     | 4   | 9    | 11,11,12     | 1.40 | 2 (18%)  | 15,15,17    | 2.03 | 2 (13%)  |
| 11  | NAG  | m     | 1   | 11,1 | 14,14,15     | 0.47 | 0        | 17,19,21    | 0.80 | 0        |
| 11  | NAG  | m     | 2   | 11   | 14,14,15     | 0.34 | 0        | 17,19,21    | 0.91 | 1 (5%)   |
| 11  | BMA  | m     | 3   | 11   | 11,11,12     | 1.46 | 2 (18%)  | 15,15,17    | 1.12 | 0        |
| 11  | MAN  | m     | 4   | 11   | 11,11,12     | 1.45 | 2 (18%)  | 15,15,17    | 1.41 | 3 (20%)  |
| 11  | MAN  | m     | 5   | 11   | 11,11,12     | 1.18 | 2 (18%)  | 15,15,17    | 1.25 | 1 (6%)   |
| 12  | NAG  | n     | 1   | 12,1 | 14,14,15     | 0.91 | 1 (7%)   | 17,19,21    | 1.59 | 3 (17%)  |
| 12  | NAG  | n     | 2   | 12   | 14,14,15     | 0.70 | 0        | 17,19,21    | 0.72 | 1 (5%)   |
| 12  | BMA  | n     | 3   | 12   | 11,11,12     | 1.36 | 1 (9%)   | 15,15,17    | 1.24 | 2 (13%)  |
| 13  | NAG  | o     | 1   | 13,1 | 14,14,15     | 0.31 | 0        | 17,19,21    | 0.94 | 1 (5%)   |
| 13  | NAG  | o     | 2   | 13   | 14,14,15     | 0.38 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 13  | BMA  | o     | 3   | 13   | 11,11,12     | 1.14 | 1 (9%)   | 15,15,17    | 1.73 | 1 (6%)   |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 13  | MAN  | o     | 4   | 13   | 11,11,12     | 1.32 | 1 (9%)   | 15,15,17    | 1.86 | 2 (13%)  |
| 10  | NAG  | p     | 1   | 10,1 | 14,14,15     | 0.61 | 0        | 17,19,21    | 0.82 | 1 (5%)   |
| 10  | NAG  | p     | 2   | 10   | 14,14,15     | 0.84 | 1 (7%)   | 17,19,21    | 0.61 | 0        |
| 14  | NAG  | q     | 1   | 14,1 | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.82 | 1 (5%)   |
| 14  | NAG  | q     | 2   | 14   | 14,14,15     | 0.40 | 0        | 17,19,21    | 0.72 | 0        |
| 14  | BMA  | q     | 3   | 14   | 11,11,12     | 1.04 | 0        | 15,15,17    | 1.25 | 2 (13%)  |
| 14  | MAN  | q     | 4   | 14   | 11,11,12     | 0.93 | 1 (9%)   | 15,15,17    | 1.62 | 1 (6%)   |
| 14  | MAN  | q     | 5   | 14   | 11,11,12     | 1.00 | 0        | 15,15,17    | 1.35 | 2 (13%)  |
| 14  | MAN  | q     | 6   | 14   | 11,11,12     | 1.08 | 1 (9%)   | 15,15,17    | 1.35 | 2 (13%)  |
| 10  | NAG  | r     | 1   | 10,1 | 14,14,15     | 0.50 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 10  | NAG  | r     | 2   | 10   | 14,14,15     | 0.72 | 1 (7%)   | 17,19,21    | 0.69 | 1 (5%)   |
| 10  | NAG  | s     | 1   | 10,1 | 14,14,15     | 0.44 | 0        | 17,19,21    | 0.92 | 1 (5%)   |
| 10  | NAG  | s     | 2   | 10   | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 0.84 | 1 (5%)   |
| 12  | NAG  | t     | 1   | 12,1 | 14,14,15     | 0.71 | 0        | 17,19,21    | 0.85 | 1 (5%)   |
| 12  | NAG  | t     | 2   | 12   | 14,14,15     | 0.54 | 0        | 17,19,21    | 1.14 | 1 (5%)   |
| 12  | BMA  | t     | 3   | 12   | 11,11,12     | 1.56 | 2 (18%)  | 15,15,17    | 1.68 | 2 (13%)  |
| 11  | NAG  | u     | 1   | 11,1 | 14,14,15     | 0.27 | 0        | 17,19,21    | 1.10 | 1 (5%)   |
| 11  | NAG  | u     | 2   | 11   | 14,14,15     | 0.39 | 0        | 17,19,21    | 1.31 | 2 (11%)  |
| 11  | BMA  | u     | 3   | 11   | 11,11,12     | 0.98 | 1 (9%)   | 15,15,17    | 1.83 | 3 (20%)  |
| 11  | MAN  | u     | 4   | 11   | 11,11,12     | 1.18 | 1 (9%)   | 15,15,17    | 1.19 | 1 (6%)   |
| 11  | MAN  | u     | 5   | 11   | 11,11,12     | 0.98 | 1 (9%)   | 15,15,17    | 1.43 | 2 (13%)  |
| 10  | NAG  | v     | 1   | 10,1 | 14,14,15     | 0.36 | 0        | 17,19,21    | 0.89 | 1 (5%)   |
| 10  | NAG  | v     | 2   | 10   | 14,14,15     | 0.85 | 1 (7%)   | 17,19,21    | 0.67 | 0        |
| 15  | NAG  | w     | 1   | 15,1 | 14,14,15     | 0.83 | 1 (7%)   | 17,19,21    | 0.91 | 1 (5%)   |
| 15  | NAG  | w     | 2   | 15   | 14,14,15     | 0.42 | 0        | 17,19,21    | 1.79 | 3 (17%)  |
| 15  | BMA  | w     | 3   | 15   | 11,11,12     | 2.00 | 5 (45%)  | 15,15,17    | 2.07 | 3 (20%)  |
| 15  | MAN  | w     | 4   | 15   | 11,11,12     | 0.87 | 1 (9%)   | 15,15,17    | 1.82 | 1 (6%)   |
| 15  | MAN  | w     | 5   | 15   | 11,11,12     | 1.25 | 1 (9%)   | 15,15,17    | 2.17 | 2 (13%)  |
| 15  | MAN  | w     | 6   | 15   | 11,11,12     | 1.15 | 1 (9%)   | 15,15,17    | 1.22 | 2 (13%)  |
| 15  | MAN  | w     | 7   | 15   | 11,11,12     | 1.51 | 2 (18%)  | 15,15,17    | 1.81 | 4 (26%)  |
| 15  | MAN  | w     | 8   | 15   | 11,11,12     | 1.30 | 2 (18%)  | 15,15,17    | 1.15 | 1 (6%)   |
| 15  | MAN  | w     | 9   | 15   | 11,11,12     | 1.07 | 0        | 15,15,17    | 1.55 | 2 (13%)  |
| 10  | NAG  | x     | 1   | 10,1 | 14,14,15     | 0.43 | 0        | 17,19,21    | 1.60 | 3 (17%)  |
| 10  | NAG  | x     | 2   | 10   | 14,14,15     | 0.58 | 0        | 17,19,21    | 1.20 | 1 (5%)   |
| 9   | NAG  | y     | 1   | 9,1  | 14,14,15     | 1.84 | 1 (7%)   | 17,19,21    | 2.42 | 3 (17%)  |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 9   | NAG  | y     | 2   | 9    | 14,14,15     | 0.38 | 0        | 17,19,21    | 1.38 | 1 (5%)   |
| 9   | BMA  | y     | 3   | 9    | 11,11,12     | 1.82 | 4 (36%)  | 15,15,17    | 1.97 | 3 (20%)  |
| 9   | MAN  | y     | 4   | 9    | 11,11,12     | 2.21 | 5 (45%)  | 15,15,17    | 2.48 | 5 (33%)  |
| 9   | NAG  | z     | 1   | 9,1  | 14,14,15     | 0.63 | 0        | 17,19,21    | 1.01 | 1 (5%)   |
| 9   | NAG  | z     | 2   | 9    | 14,14,15     | 0.86 | 1 (7%)   | 17,19,21    | 0.73 | 0        |
| 9   | BMA  | z     | 3   | 9    | 11,11,12     | 1.17 | 1 (9%)   | 15,15,17    | 0.98 | 1 (6%)   |
| 9   | MAN  | z     | 4   | 9    | 11,11,12     | 1.18 | 1 (9%)   | 15,15,17    | 1.69 | 2 (13%)  |

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   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 10  | NAG  | 0     | 1   | 10,1 | -       | 3/6/23/26 | 0/1/1/1 |
| 10  | NAG  | 0     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | 1     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | 1     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | 1     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | 1     | 4   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | NAG  | 3     | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | 3     | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | 3     | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | 3     | 4   | 11   | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | MAN  | 3     | 5   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | NAG  | 4     | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | 4     | 2   | 12   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | BMA  | 4     | 3   | 12   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | NAG  | 9     | 1   | 13,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 13  | NAG  | 9     | 2   | 13   | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | 9     | 3   | 13   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | MAN  | 9     | 4   | 13   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | AA    | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | AA    | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | BA    | 1   | 14,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | BA    | 2   | 14   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | BMA  | BA    | 3   | 14   | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | BA    | 4   | 14   | -       | 0/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 14  | MAN  | BA    | 5   | 14   | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | BA    | 6   | 14   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | CA    | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | CA    | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | DA    | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | DA    | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | EA    | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | EA    | 2   | 12   | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | EA    | 3   | 12   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | NAG  | FA    | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | FA    | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | FA    | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | FA    | 4   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | FA    | 5   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | GA    | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | GA    | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | HA    | 1   | 15,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | HA    | 2   | 15   | -       | 4/6/23/26 | 0/1/1/1 |
| 15  | BMA  | HA    | 3   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 4   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 5   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 6   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 7   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 8   | 15   | -       | 2/2/19/22 | 0/1/1/1 |
| 15  | MAN  | HA    | 9   | 15   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | IA    | 1   | 10,1 | -       | 3/6/23/26 | 0/1/1/1 |
| 10  | NAG  | IA    | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | JA    | 1   | 9,1  | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | JA    | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | JA    | 3   | 9    | -       | 1/2/19/22 | 1/1/1/1 |
| 9   | MAN  | JA    | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | T     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | T     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | T     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | T     | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | U     | 1   | 10,1 | -       | 3/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 10  | NAG  | U     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | V     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | V     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | V     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | V     | 4   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | NAG  | W     | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | W     | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | W     | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | W     | 4   | 11   | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | MAN  | W     | 5   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | NAG  | X     | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | X     | 2   | 12   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | BMA  | X     | 3   | 12   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | NAG  | Y     | 1   | 13,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 13  | NAG  | Y     | 2   | 13   | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | Y     | 3   | 13   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | MAN  | Y     | 4   | 13   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | Z     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | Z     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | a     | 1   | 14,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | a     | 2   | 14   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | BMA  | a     | 3   | 14   | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | a     | 4   | 14   | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | a     | 5   | 14   | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | a     | 6   | 14   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | b     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | b     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | c     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | c     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | d     | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | d     | 2   | 12   | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | d     | 3   | 12   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | NAG  | e     | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | e     | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | e     | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | e     | 4   | 11   | -       | 2/2/19/22 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 11  | MAN  | e     | 5   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | f     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | f     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | g     | 1   | 15,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | g     | 2   | 15   | -       | 4/6/23/26 | 0/1/1/1 |
| 15  | BMA  | g     | 3   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 4   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 5   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 6   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 7   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 8   | 15   | -       | 2/2/19/22 | 0/1/1/1 |
| 15  | MAN  | g     | 9   | 15   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | h     | 1   | 10,1 | -       | 4/6/23/26 | 0/1/1/1 |
| 10  | NAG  | h     | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | i     | 1   | 9,1  | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | i     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | i     | 3   | 9    | -       | 1/2/19/22 | 1/1/1/1 |
| 9   | MAN  | i     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | j     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | j     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | j     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | j     | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | k     | 1   | 10,1 | -       | 3/6/23/26 | 0/1/1/1 |
| 10  | NAG  | k     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | NAG  | l     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | l     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | l     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | l     | 4   | 9    | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | NAG  | m     | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | m     | 2   | 11   | -       | 1/6/23/26 | 0/1/1/1 |
| 11  | BMA  | m     | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | m     | 4   | 11   | -       | 1/2/19/22 | 0/1/1/1 |
| 11  | MAN  | m     | 5   | 11   | -       | 0/2/19/22 | 0/1/1/1 |
| 12  | NAG  | n     | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | n     | 2   | 12   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | BMA  | n     | 3   | 12   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | NAG  | o     | 1   | 13,1 | -       | 2/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 13  | NAG  | o     | 2   | 13   | -       | 0/6/23/26 | 0/1/1/1 |
| 13  | BMA  | o     | 3   | 13   | -       | 0/2/19/22 | 0/1/1/1 |
| 13  | MAN  | o     | 4   | 13   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | p     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | p     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | q     | 1   | 14,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | NAG  | q     | 2   | 14   | -       | 2/6/23/26 | 0/1/1/1 |
| 14  | BMA  | q     | 3   | 14   | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | q     | 4   | 14   | -       | 0/2/19/22 | 0/1/1/1 |
| 14  | MAN  | q     | 5   | 14   | -       | 2/2/19/22 | 0/1/1/1 |
| 14  | MAN  | q     | 6   | 14   | -       | 1/2/19/22 | 0/1/1/1 |
| 10  | NAG  | r     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | r     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | s     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | s     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | t     | 1   | 12,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 12  | NAG  | t     | 2   | 12   | -       | 0/6/23/26 | 0/1/1/1 |
| 12  | BMA  | t     | 3   | 12   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | NAG  | u     | 1   | 11,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 11  | NAG  | u     | 2   | 11   | -       | 0/6/23/26 | 0/1/1/1 |
| 11  | BMA  | u     | 3   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | u     | 4   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 11  | MAN  | u     | 5   | 11   | -       | 2/2/19/22 | 0/1/1/1 |
| 10  | NAG  | v     | 1   | 10,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 10  | NAG  | v     | 2   | 10   | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | w     | 1   | 15,1 | -       | 2/6/23/26 | 0/1/1/1 |
| 15  | NAG  | w     | 2   | 15   | -       | 4/6/23/26 | 0/1/1/1 |
| 15  | BMA  | w     | 3   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 4   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 5   | 15   | -       | 1/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 6   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 7   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 8   | 15   | -       | 2/2/19/22 | 0/1/1/1 |
| 15  | MAN  | w     | 9   | 15   | -       | 0/2/19/22 | 0/1/1/1 |
| 10  | NAG  | x     | 1   | 10,1 | -       | 4/6/23/26 | 0/1/1/1 |
| 10  | NAG  | x     | 2   | 10   | -       | 0/6/23/26 | 0/1/1/1 |
| 9   | NAG  | y     | 1   | 9,1  | -       | 0/6/23/26 | 0/1/1/1 |

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| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 9   | NAG  | y     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | y     | 3   | 9    | -       | 1/2/19/22 | 1/1/1/1 |
| 9   | MAN  | y     | 4   | 9    | -       | 0/2/19/22 | 0/1/1/1 |
| 9   | NAG  | z     | 1   | 9,1  | -       | 1/6/23/26 | 0/1/1/1 |
| 9   | NAG  | z     | 2   | 9    | -       | 2/6/23/26 | 0/1/1/1 |
| 9   | BMA  | z     | 3   | 9    | -       | 2/2/19/22 | 0/1/1/1 |
| 9   | MAN  | z     | 4   | 9    | -       | 2/2/19/22 | 0/1/1/1 |

All (169) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | i     | 1   | NAG  | O5-C1 | 6.78  | 1.55        | 1.43     |
| 9   | y     | 1   | NAG  | O5-C1 | 6.77  | 1.55        | 1.43     |
| 9   | y     | 4   | MAN  | C1-C2 | 5.39  | 1.65        | 1.52     |
| 9   | i     | 4   | MAN  | C1-C2 | 4.86  | 1.63        | 1.52     |
| 9   | JA    | 4   | MAN  | C1-C2 | 4.77  | 1.63        | 1.52     |
| 9   | l     | 3   | BMA  | O5-C5 | 4.62  | 1.52        | 1.43     |
| 9   | 1     | 3   | BMA  | O5-C5 | 4.56  | 1.52        | 1.43     |
| 9   | V     | 3   | BMA  | O5-C5 | 4.46  | 1.52        | 1.43     |
| 9   | 1     | 3   | BMA  | C2-C3 | -4.16 | 1.46        | 1.52     |
| 9   | l     | 3   | BMA  | C2-C3 | -4.14 | 1.46        | 1.52     |
| 9   | V     | 3   | BMA  | C2-C3 | -4.08 | 1.46        | 1.52     |
| 11  | 3     | 4   | MAN  | C1-C2 | 3.59  | 1.60        | 1.52     |
| 11  | m     | 4   | MAN  | C1-C2 | 3.59  | 1.60        | 1.52     |
| 11  | W     | 4   | MAN  | C1-C2 | 3.57  | 1.60        | 1.52     |
| 15  | HA    | 3   | BMA  | O3-C3 | -3.53 | 1.34        | 1.43     |
| 15  | w     | 3   | BMA  | O3-C3 | -3.52 | 1.34        | 1.43     |
| 9   | i     | 3   | BMA  | C4-C3 | 3.50  | 1.61        | 1.52     |
| 15  | HA    | 5   | MAN  | O5-C5 | 3.50  | 1.50        | 1.43     |
| 15  | g     | 3   | BMA  | O3-C3 | -3.49 | 1.34        | 1.43     |
| 9   | l     | 4   | MAN  | O5-C1 | 3.37  | 1.49        | 1.43     |
| 15  | g     | 5   | MAN  | O5-C5 | 3.37  | 1.50        | 1.43     |
| 9   | y     | 3   | BMA  | C4-C3 | 3.33  | 1.61        | 1.52     |
| 9   | 1     | 4   | MAN  | O5-C1 | 3.32  | 1.49        | 1.43     |
| 15  | w     | 5   | MAN  | O5-C5 | 3.31  | 1.49        | 1.43     |
| 12  | t     | 3   | BMA  | C1-C2 | 3.30  | 1.60        | 1.52     |
| 12  | EA    | 3   | BMA  | C1-C2 | 3.30  | 1.60        | 1.52     |
| 12  | d     | 3   | BMA  | C1-C2 | 3.27  | 1.60        | 1.52     |
| 9   | JA    | 3   | BMA  | C4-C3 | 3.27  | 1.60        | 1.52     |
| 9   | V     | 4   | MAN  | O5-C1 | 3.25  | 1.49        | 1.43     |
| 13  | Y     | 4   | MAN  | C1-C2 | 3.17  | 1.59        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 13  | o     | 4   | MAN  | C1-C2 | 3.16  | 1.59        | 1.52     |
| 13  | 9     | 4   | MAN  | C1-C2 | 3.09  | 1.59        | 1.52     |
| 12  | n     | 1   | NAG  | C1-C2 | 3.02  | 1.56        | 1.52     |
| 10  | 0     | 2   | NAG  | O5-C1 | 2.95  | 1.48        | 1.43     |
| 10  | U     | 2   | NAG  | O5-C1 | 2.93  | 1.48        | 1.43     |
| 12  | X     | 1   | NAG  | C1-C2 | 2.93  | 1.56        | 1.52     |
| 12  | n     | 3   | BMA  | C1-C2 | 2.93  | 1.59        | 1.52     |
| 12  | X     | 3   | BMA  | C1-C2 | 2.91  | 1.59        | 1.52     |
| 9   | z     | 4   | MAN  | C1-C2 | 2.91  | 1.59        | 1.52     |
| 12  | 4     | 1   | NAG  | C1-C2 | 2.89  | 1.56        | 1.52     |
| 9   | T     | 4   | MAN  | C1-C2 | 2.87  | 1.59        | 1.52     |
| 11  | 3     | 3   | BMA  | C1-C2 | 2.87  | 1.59        | 1.52     |
| 11  | m     | 3   | BMA  | C1-C2 | 2.85  | 1.59        | 1.52     |
| 12  | 4     | 3   | BMA  | C1-C2 | 2.84  | 1.59        | 1.52     |
| 10  | k     | 2   | NAG  | O5-C1 | 2.84  | 1.48        | 1.43     |
| 10  | v     | 2   | NAG  | O5-C1 | 2.83  | 1.48        | 1.43     |
| 9   | y     | 3   | BMA  | O5-C1 | 2.82  | 1.48        | 1.43     |
| 10  | GA    | 2   | NAG  | O5-C1 | 2.80  | 1.48        | 1.43     |
| 9   | j     | 4   | MAN  | C1-C2 | 2.80  | 1.58        | 1.52     |
| 9   | JA    | 4   | MAN  | O5-C1 | 2.80  | 1.48        | 1.43     |
| 9   | i     | 4   | MAN  | C2-C3 | 2.79  | 1.56        | 1.52     |
| 11  | W     | 3   | BMA  | C1-C2 | 2.79  | 1.58        | 1.52     |
| 15  | w     | 1   | NAG  | C1-C2 | -2.78 | 1.48        | 1.52     |
| 15  | w     | 7   | MAN  | O5-C5 | 2.78  | 1.48        | 1.43     |
| 9   | i     | 3   | BMA  | O5-C1 | 2.75  | 1.48        | 1.43     |
| 9   | JA    | 3   | BMA  | O5-C1 | 2.74  | 1.48        | 1.43     |
| 10  | f     | 2   | NAG  | O5-C1 | 2.74  | 1.48        | 1.43     |
| 11  | W     | 5   | MAN  | O5-C5 | 2.69  | 1.48        | 1.43     |
| 9   | JA    | 1   | NAG  | C1-C2 | -2.67 | 1.48        | 1.52     |
| 15  | w     | 7   | MAN  | O3-C3 | -2.66 | 1.36        | 1.43     |
| 9   | y     | 4   | MAN  | C2-C3 | 2.66  | 1.56        | 1.52     |
| 11  | 3     | 5   | MAN  | O5-C5 | 2.63  | 1.48        | 1.43     |
| 9   | y     | 4   | MAN  | O5-C1 | 2.62  | 1.48        | 1.43     |
| 15  | HA    | 7   | MAN  | O3-C3 | -2.62 | 1.36        | 1.43     |
| 15  | HA    | 1   | NAG  | C1-C2 | -2.61 | 1.48        | 1.52     |
| 15  | g     | 1   | NAG  | C1-C2 | -2.61 | 1.48        | 1.52     |
| 15  | HA    | 7   | MAN  | O5-C5 | 2.59  | 1.48        | 1.43     |
| 15  | HA    | 8   | MAN  | C4-C3 | 2.59  | 1.59        | 1.52     |
| 15  | g     | 7   | MAN  | O3-C3 | -2.59 | 1.36        | 1.43     |
| 14  | a     | 4   | MAN  | O5-C5 | 2.58  | 1.48        | 1.43     |
| 11  | m     | 5   | MAN  | O5-C5 | 2.57  | 1.48        | 1.43     |
| 9   | l     | 4   | MAN  | O5-C5 | 2.56  | 1.48        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 9   | JA    | 4   | MAN  | C2-C3 | 2.56  | 1.56        | 1.52     |
| 15  | w     | 8   | MAN  | C4-C3 | 2.56  | 1.59        | 1.52     |
| 13  | 9     | 3   | BMA  | O5-C5 | 2.56  | 1.48        | 1.43     |
| 15  | g     | 3   | BMA  | O2-C2 | -2.55 | 1.38        | 1.43     |
| 9   | i     | 4   | MAN  | O5-C1 | 2.55  | 1.48        | 1.43     |
| 15  | HA    | 3   | BMA  | O2-C2 | -2.53 | 1.38        | 1.43     |
| 14  | BA    | 4   | MAN  | O5-C5 | 2.52  | 1.48        | 1.43     |
| 15  | g     | 7   | MAN  | O5-C5 | 2.51  | 1.48        | 1.43     |
| 15  | w     | 3   | BMA  | O2-C2 | -2.50 | 1.38        | 1.43     |
| 14  | BA    | 6   | MAN  | O5-C5 | 2.50  | 1.48        | 1.43     |
| 15  | g     | 8   | MAN  | C4-C3 | 2.50  | 1.58        | 1.52     |
| 13  | Y     | 3   | BMA  | O5-C5 | 2.48  | 1.48        | 1.43     |
| 13  | o     | 3   | BMA  | O5-C5 | 2.46  | 1.48        | 1.43     |
| 9   | 1     | 4   | MAN  | O5-C5 | 2.46  | 1.48        | 1.43     |
| 11  | 3     | 3   | BMA  | C2-C3 | 2.45  | 1.56        | 1.52     |
| 9   | V     | 4   | MAN  | O5-C5 | 2.45  | 1.48        | 1.43     |
| 15  | HA    | 3   | BMA  | O4-C4 | -2.45 | 1.36        | 1.43     |
| 9   | JA    | 2   | NAG  | O5-C1 | 2.44  | 1.47        | 1.43     |
| 15  | g     | 3   | BMA  | O4-C4 | -2.43 | 1.36        | 1.43     |
| 10  | AA    | 2   | NAG  | O5-C1 | 2.43  | 1.47        | 1.43     |
| 9   | z     | 2   | NAG  | C1-C2 | 2.43  | 1.55        | 1.52     |
| 14  | q     | 4   | MAN  | O5-C5 | 2.42  | 1.48        | 1.43     |
| 10  | p     | 2   | NAG  | O5-C1 | 2.42  | 1.47        | 1.43     |
| 15  | w     | 3   | BMA  | O4-C4 | -2.41 | 1.37        | 1.43     |
| 11  | m     | 3   | BMA  | C2-C3 | 2.41  | 1.56        | 1.52     |
| 10  | Z     | 2   | NAG  | O5-C1 | 2.41  | 1.47        | 1.43     |
| 9   | V     | 2   | NAG  | O5-C1 | 2.40  | 1.47        | 1.43     |
| 9   | 1     | 2   | NAG  | O5-C1 | 2.40  | 1.47        | 1.43     |
| 15  | w     | 6   | MAN  | O5-C5 | 2.39  | 1.48        | 1.43     |
| 9   | j     | 2   | NAG  | C1-C2 | 2.39  | 1.55        | 1.52     |
| 14  | a     | 6   | MAN  | O5-C5 | 2.38  | 1.48        | 1.43     |
| 9   | y     | 3   | BMA  | O5-C5 | 2.38  | 1.48        | 1.43     |
| 9   | i     | 3   | BMA  | C4-C5 | 2.38  | 1.58        | 1.53     |
| 9   | l     | 2   | NAG  | O5-C1 | 2.37  | 1.47        | 1.43     |
| 12  | EA    | 3   | BMA  | O5-C1 | 2.37  | 1.47        | 1.43     |
| 12  | d     | 3   | BMA  | O5-C1 | 2.37  | 1.47        | 1.43     |
| 9   | T     | 2   | NAG  | C1-C2 | 2.36  | 1.55        | 1.52     |
| 11  | W     | 3   | BMA  | C2-C3 | 2.36  | 1.56        | 1.52     |
| 9   | i     | 3   | BMA  | O5-C5 | 2.36  | 1.48        | 1.43     |
| 9   | l     | 3   | BMA  | C4-C5 | 2.36  | 1.58        | 1.53     |
| 14  | q     | 6   | MAN  | O5-C5 | 2.36  | 1.48        | 1.43     |
| 11  | u     | 4   | MAN  | C2-C3 | 2.35  | 1.56        | 1.52     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 10  | 0     | 2   | NAG  | C1-C2 | 2.34  | 1.55        | 1.52     |
| 15  | HA    | 6   | MAN  | O5-C5 | 2.33  | 1.48        | 1.43     |
| 10  | k     | 2   | NAG  | C1-C2 | 2.33  | 1.55        | 1.52     |
| 11  | FA    | 4   | MAN  | C2-C3 | 2.33  | 1.56        | 1.52     |
| 11  | FA    | 3   | BMA  | O5-C5 | 2.33  | 1.48        | 1.43     |
| 10  | U     | 2   | NAG  | C1-C2 | 2.33  | 1.55        | 1.52     |
| 11  | e     | 4   | MAN  | C2-C3 | 2.33  | 1.56        | 1.52     |
| 12  | t     | 3   | BMA  | O5-C1 | 2.32  | 1.47        | 1.43     |
| 10  | CA    | 2   | NAG  | O5-C1 | 2.31  | 1.47        | 1.43     |
| 9   | V     | 3   | BMA  | C4-C5 | 2.31  | 1.58        | 1.53     |
| 9   | l     | 3   | BMA  | C4-C5 | 2.31  | 1.58        | 1.53     |
| 9   | i     | 4   | MAN  | C4-C3 | 2.31  | 1.58        | 1.52     |
| 9   | JA    | 4   | MAN  | C4-C3 | 2.30  | 1.58        | 1.52     |
| 11  | e     | 3   | BMA  | O5-C5 | 2.30  | 1.47        | 1.43     |
| 9   | y     | 4   | MAN  | C4-C3 | 2.29  | 1.58        | 1.52     |
| 11  | u     | 3   | BMA  | O5-C5 | 2.29  | 1.47        | 1.43     |
| 10  | r     | 2   | NAG  | O5-C1 | 2.27  | 1.47        | 1.43     |
| 11  | 3     | 5   | MAN  | C2-C3 | 2.27  | 1.56        | 1.52     |
| 11  | m     | 5   | MAN  | C2-C3 | 2.26  | 1.56        | 1.52     |
| 11  | W     | 5   | MAN  | C2-C3 | 2.24  | 1.55        | 1.52     |
| 10  | b     | 2   | NAG  | O5-C1 | 2.24  | 1.47        | 1.43     |
| 15  | w     | 4   | MAN  | O2-C2 | -2.23 | 1.38        | 1.43     |
| 10  | c     | 2   | NAG  | O5-C1 | 2.23  | 1.47        | 1.43     |
| 15  | g     | 3   | BMA  | C6-C5 | -2.22 | 1.44        | 1.51     |
| 15  | w     | 3   | BMA  | C6-C5 | -2.21 | 1.44        | 1.51     |
| 15  | g     | 6   | MAN  | O5-C5 | 2.20  | 1.47        | 1.43     |
| 15  | HA    | 3   | BMA  | C6-C5 | -2.19 | 1.44        | 1.51     |
| 11  | FA    | 5   | MAN  | O5-C5 | 2.17  | 1.47        | 1.43     |
| 15  | g     | 9   | MAN  | O5-C5 | 2.17  | 1.47        | 1.43     |
| 15  | HA    | 9   | MAN  | O5-C5 | 2.16  | 1.47        | 1.43     |
| 11  | 3     | 4   | MAN  | O5-C5 | 2.15  | 1.47        | 1.43     |
| 9   | i     | 3   | BMA  | O3-C3 | 2.15  | 1.48        | 1.43     |
| 13  | Y     | 3   | BMA  | C1-C2 | 2.14  | 1.57        | 1.52     |
| 9   | j     | 3   | BMA  | C2-C3 | 2.14  | 1.55        | 1.52     |
| 11  | m     | 4   | MAN  | O5-C5 | 2.14  | 1.47        | 1.43     |
| 9   | y     | 3   | BMA  | C4-C5 | 2.14  | 1.57        | 1.53     |
| 9   | z     | 3   | BMA  | C2-C3 | 2.13  | 1.55        | 1.52     |
| 10  | DA    | 2   | NAG  | O5-C1 | 2.13  | 1.47        | 1.43     |
| 9   | JA    | 4   | MAN  | O5-C5 | 2.12  | 1.47        | 1.43     |
| 11  | W     | 4   | MAN  | O5-C5 | 2.12  | 1.47        | 1.43     |
| 9   | i     | 4   | MAN  | O5-C5 | 2.11  | 1.47        | 1.43     |
| 11  | u     | 5   | MAN  | O5-C5 | 2.10  | 1.47        | 1.43     |

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| Mol | Chain | Res | Type | Atoms | Z     | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|-------|-------------|----------|
| 15  | g     | 3   | BMA  | C2-C3 | -2.10 | 1.49        | 1.52     |
| 10  | s     | 2   | NAG  | O5-C1 | 2.10  | 1.47        | 1.43     |
| 15  | HA    | 3   | BMA  | O6-C6 | -2.09 | 1.33        | 1.42     |
| 9   | JA    | 3   | BMA  | O5-C5 | 2.09  | 1.47        | 1.43     |
| 15  | g     | 4   | MAN  | O2-C2 | -2.08 | 1.39        | 1.43     |
| 11  | e     | 5   | MAN  | O5-C5 | 2.06  | 1.47        | 1.43     |
| 15  | w     | 3   | BMA  | C2-C3 | -2.06 | 1.49        | 1.52     |
| 15  | HA    | 3   | BMA  | C2-C3 | -2.06 | 1.49        | 1.52     |
| 9   | T     | 3   | BMA  | C2-C3 | 2.04  | 1.55        | 1.52     |
| 9   | y     | 4   | MAN  | O5-C5 | 2.03  | 1.47        | 1.43     |
| 15  | w     | 8   | MAN  | O5-C5 | 2.03  | 1.47        | 1.43     |
| 12  | EA    | 3   | BMA  | O5-C5 | 2.01  | 1.47        | 1.43     |
| 13  | 9     | 3   | BMA  | C1-C2 | 2.01  | 1.57        | 1.52     |

All (273) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 9   | i     | 1   | NAG  | C1-O5-C5 | 9.11 | 124.39      | 112.19   |
| 9   | y     | 1   | NAG  | C1-O5-C5 | 8.89 | 124.10      | 112.19   |
| 15  | g     | 5   | MAN  | C1-O5-C5 | 7.56 | 122.32      | 112.19   |
| 15  | HA    | 5   | MAN  | C1-O5-C5 | 7.53 | 122.28      | 112.19   |
| 15  | w     | 5   | MAN  | C1-O5-C5 | 7.50 | 122.23      | 112.19   |
| 9   | l     | 4   | MAN  | C1-O5-C5 | 7.16 | 121.78      | 112.19   |
| 9   | 1     | 4   | MAN  | C1-O5-C5 | 7.10 | 121.71      | 112.19   |
| 9   | V     | 4   | MAN  | C1-O5-C5 | 7.02 | 121.59      | 112.19   |
| 9   | 1     | 3   | BMA  | C1-O5-C5 | 6.95 | 121.50      | 112.19   |
| 9   | l     | 3   | BMA  | C1-O5-C5 | 6.86 | 121.38      | 112.19   |
| 9   | V     | 3   | BMA  | C1-O5-C5 | 6.86 | 121.38      | 112.19   |
| 9   | i     | 4   | MAN  | C1-O5-C5 | 6.67 | 121.12      | 112.19   |
| 9   | JA    | 4   | MAN  | C1-O5-C5 | 6.47 | 120.86      | 112.19   |
| 15  | w     | 4   | MAN  | C1-O5-C5 | 6.46 | 120.84      | 112.19   |
| 9   | y     | 4   | MAN  | C1-O5-C5 | 6.34 | 120.69      | 112.19   |
| 15  | g     | 4   | MAN  | C1-O5-C5 | 6.34 | 120.68      | 112.19   |
| 15  | HA    | 4   | MAN  | C1-O5-C5 | 6.32 | 120.65      | 112.19   |
| 15  | w     | 3   | BMA  | C1-O5-C5 | 6.28 | 120.61      | 112.19   |
| 13  | 9     | 3   | BMA  | C1-O5-C5 | 6.28 | 120.61      | 112.19   |
| 15  | g     | 3   | BMA  | C1-O5-C5 | 6.27 | 120.58      | 112.19   |
| 13  | Y     | 3   | BMA  | C1-O5-C5 | 6.25 | 120.56      | 112.19   |
| 13  | o     | 3   | BMA  | C1-O5-C5 | 6.24 | 120.55      | 112.19   |
| 15  | HA    | 3   | BMA  | C1-O5-C5 | 6.21 | 120.52      | 112.19   |
| 13  | 9     | 4   | MAN  | C1-O5-C5 | 6.01 | 120.25      | 112.19   |
| 13  | o     | 4   | MAN  | C1-O5-C5 | 6.01 | 120.24      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 13  | Y     | 4   | MAN  | C1-O5-C5 | 6.00 | 120.23      | 112.19   |
| 9   | i     | 3   | BMA  | C1-O5-C5 | 5.93 | 120.13      | 112.19   |
| 9   | y     | 3   | BMA  | C1-O5-C5 | 5.90 | 120.09      | 112.19   |
| 14  | BA    | 4   | MAN  | C1-O5-C5 | 5.64 | 119.75      | 112.19   |
| 11  | FA    | 3   | BMA  | C1-O5-C5 | 5.58 | 119.66      | 112.19   |
| 9   | JA    | 3   | BMA  | C1-O5-C5 | 5.56 | 119.63      | 112.19   |
| 14  | a     | 4   | MAN  | C1-O5-C5 | 5.54 | 119.61      | 112.19   |
| 11  | e     | 3   | BMA  | C1-O5-C5 | 5.53 | 119.60      | 112.19   |
| 11  | u     | 3   | BMA  | C1-O5-C5 | 5.49 | 119.55      | 112.19   |
| 14  | q     | 4   | MAN  | C1-O5-C5 | 5.46 | 119.50      | 112.19   |
| 9   | z     | 4   | MAN  | C1-O5-C5 | 5.03 | 118.93      | 112.19   |
| 9   | T     | 4   | MAN  | C1-O5-C5 | 5.03 | 118.93      | 112.19   |
| 9   | j     | 4   | MAN  | C1-O5-C5 | 4.93 | 118.79      | 112.19   |
| 15  | g     | 9   | MAN  | C1-O5-C5 | 4.88 | 118.73      | 112.19   |
| 10  | IA    | 2   | NAG  | C1-O5-C5 | 4.87 | 118.71      | 112.19   |
| 15  | HA    | 9   | MAN  | C1-O5-C5 | 4.81 | 118.63      | 112.19   |
| 9   | y     | 2   | NAG  | C1-O5-C5 | 4.77 | 118.58      | 112.19   |
| 10  | 0     | 1   | NAG  | C2-N2-C7 | 4.76 | 129.27      | 122.90   |
| 10  | k     | 1   | NAG  | C2-N2-C7 | 4.75 | 129.26      | 122.90   |
| 10  | U     | 1   | NAG  | C2-N2-C7 | 4.73 | 129.24      | 122.90   |
| 10  | x     | 2   | NAG  | C1-O5-C5 | 4.72 | 118.52      | 112.19   |
| 10  | IA    | 1   | NAG  | C2-N2-C7 | 4.65 | 129.13      | 122.90   |
| 10  | x     | 1   | NAG  | C2-N2-C7 | 4.64 | 129.12      | 122.90   |
| 10  | h     | 1   | NAG  | C2-N2-C7 | 4.62 | 129.10      | 122.90   |
| 11  | u     | 5   | MAN  | C1-O5-C5 | 4.58 | 118.33      | 112.19   |
| 10  | h     | 2   | NAG  | C1-O5-C5 | 4.57 | 118.31      | 112.19   |
| 11  | e     | 5   | MAN  | C1-O5-C5 | 4.54 | 118.28      | 112.19   |
| 15  | w     | 9   | MAN  | C1-O5-C5 | 4.53 | 118.26      | 112.19   |
| 11  | FA    | 5   | MAN  | C1-O5-C5 | 4.53 | 118.25      | 112.19   |
| 11  | e     | 2   | NAG  | C1-O5-C5 | 4.49 | 118.20      | 112.19   |
| 9   | i     | 2   | NAG  | C1-O5-C5 | 4.48 | 118.19      | 112.19   |
| 12  | t     | 3   | BMA  | C1-O5-C5 | 4.46 | 118.17      | 112.19   |
| 12  | d     | 2   | NAG  | C1-O5-C5 | 4.44 | 118.14      | 112.19   |
| 11  | FA    | 2   | NAG  | C1-O5-C5 | 4.44 | 118.13      | 112.19   |
| 15  | g     | 2   | NAG  | C2-N2-C7 | 4.42 | 128.83      | 122.90   |
| 12  | X     | 1   | NAG  | C2-N2-C7 | 4.42 | 128.83      | 122.90   |
| 12  | d     | 3   | BMA  | C1-O5-C5 | 4.42 | 118.11      | 112.19   |
| 12  | n     | 1   | NAG  | C2-N2-C7 | 4.42 | 128.82      | 122.90   |
| 15  | w     | 2   | NAG  | C2-N2-C7 | 4.42 | 128.82      | 122.90   |
| 15  | HA    | 2   | NAG  | C2-N2-C7 | 4.41 | 128.80      | 122.90   |
| 12  | 4     | 1   | NAG  | C2-N2-C7 | 4.40 | 128.79      | 122.90   |
| 14  | q     | 5   | MAN  | C1-O5-C5 | 4.29 | 117.94      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 14  | BA    | 6   | MAN  | C1-O5-C5 | 4.25  | 117.89      | 112.19   |
| 12  | EA    | 2   | NAG  | C1-O5-C5 | 4.24  | 117.87      | 112.19   |
| 11  | u     | 2   | NAG  | C1-O5-C5 | 4.24  | 117.87      | 112.19   |
| 12  | t     | 2   | NAG  | C1-O5-C5 | 4.24  | 117.87      | 112.19   |
| 15  | w     | 7   | MAN  | C1-O5-C5 | 4.23  | 117.86      | 112.19   |
| 12  | EA    | 3   | BMA  | C1-O5-C5 | 4.23  | 117.85      | 112.19   |
| 14  | q     | 6   | MAN  | C1-O5-C5 | 4.20  | 117.82      | 112.19   |
| 14  | BA    | 5   | MAN  | C1-O5-C5 | 4.18  | 117.79      | 112.19   |
| 14  | a     | 5   | MAN  | C1-O5-C5 | 4.17  | 117.77      | 112.19   |
| 14  | a     | 6   | MAN  | C1-O5-C5 | 4.16  | 117.76      | 112.19   |
| 15  | w     | 2   | NAG  | C1-O5-C5 | 4.16  | 117.76      | 112.19   |
| 15  | HA    | 2   | NAG  | C1-O5-C5 | 4.10  | 117.68      | 112.19   |
| 15  | g     | 2   | NAG  | C1-O5-C5 | 4.04  | 117.61      | 112.19   |
| 9   | JA    | 1   | NAG  | C1-O5-C5 | 4.04  | 117.61      | 112.19   |
| 15  | g     | 7   | MAN  | C1-O5-C5 | 3.98  | 117.51      | 112.19   |
| 15  | HA    | 7   | MAN  | C1-O5-C5 | 3.96  | 117.49      | 112.19   |
| 11  | W     | 5   | MAN  | C1-O5-C5 | 3.94  | 117.46      | 112.19   |
| 11  | 3     | 5   | MAN  | C1-O5-C5 | 3.93  | 117.45      | 112.19   |
| 11  | m     | 5   | MAN  | C1-O5-C5 | 3.87  | 117.38      | 112.19   |
| 11  | FA    | 1   | NAG  | C1-O5-C5 | 3.86  | 117.36      | 112.19   |
| 9   | y     | 4   | MAN  | O2-C2-C3 | -3.85 | 102.19      | 110.15   |
| 11  | e     | 1   | NAG  | C1-O5-C5 | 3.84  | 117.34      | 112.19   |
| 12  | d     | 3   | BMA  | O2-C2-C3 | -3.83 | 102.21      | 110.15   |
| 14  | BA    | 3   | BMA  | C1-O5-C5 | 3.81  | 117.29      | 112.19   |
| 12  | t     | 3   | BMA  | O2-C2-C3 | -3.81 | 102.26      | 110.15   |
| 9   | i     | 4   | MAN  | O2-C2-C3 | -3.70 | 102.48      | 110.15   |
| 9   | y     | 4   | MAN  | C1-C2-C3 | 3.70  | 115.03      | 109.64   |
| 11  | u     | 1   | NAG  | C1-O5-C5 | 3.70  | 117.14      | 112.19   |
| 9   | j     | 1   | NAG  | C1-O5-C5 | 3.70  | 117.14      | 112.19   |
| 9   | z     | 1   | NAG  | C1-O5-C5 | 3.64  | 117.07      | 112.19   |
| 12  | EA    | 3   | BMA  | O2-C2-C3 | -3.63 | 102.63      | 110.15   |
| 9   | l     | 2   | NAG  | C1-O5-C5 | 3.60  | 117.01      | 112.19   |
| 14  | q     | 3   | BMA  | C1-O5-C5 | 3.59  | 117.00      | 112.19   |
| 9   | JA    | 4   | MAN  | O2-C2-C3 | -3.57 | 102.76      | 110.15   |
| 11  | 3     | 4   | MAN  | C1-O5-C5 | 3.56  | 116.95      | 112.19   |
| 11  | e     | 4   | MAN  | C1-O5-C5 | 3.56  | 116.95      | 112.19   |
| 14  | a     | 3   | BMA  | C1-O5-C5 | 3.55  | 116.95      | 112.19   |
| 9   | T     | 1   | NAG  | C1-O5-C5 | 3.55  | 116.94      | 112.19   |
| 9   | l     | 2   | NAG  | C1-O5-C5 | 3.53  | 116.92      | 112.19   |
| 9   | V     | 2   | NAG  | C1-O5-C5 | 3.52  | 116.91      | 112.19   |
| 15  | w     | 9   | MAN  | O2-C2-C3 | -3.50 | 102.91      | 110.15   |
| 11  | m     | 4   | MAN  | C1-O5-C5 | 3.49  | 116.86      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | u     | 4   | MAN  | C1-O5-C5 | 3.49  | 116.86      | 112.19   |
| 9   | JA    | 4   | MAN  | C1-C2-C3 | 3.46  | 114.68      | 109.64   |
| 11  | FA    | 4   | MAN  | C1-O5-C5 | 3.43  | 116.78      | 112.19   |
| 11  | W     | 4   | MAN  | C1-O5-C5 | 3.41  | 116.76      | 112.19   |
| 15  | w     | 7   | MAN  | C1-C2-C3 | -3.40 | 104.69      | 109.64   |
| 15  | HA    | 7   | MAN  | C1-C2-C3 | -3.30 | 104.84      | 109.64   |
| 15  | HA    | 6   | MAN  | C1-O5-C5 | 3.29  | 116.60      | 112.19   |
| 15  | w     | 6   | MAN  | C1-O5-C5 | 3.28  | 116.58      | 112.19   |
| 9   | i     | 4   | MAN  | C1-C2-C3 | 3.28  | 114.42      | 109.64   |
| 15  | g     | 7   | MAN  | C1-C2-C3 | -3.24 | 104.92      | 109.64   |
| 12  | 4     | 1   | NAG  | C1-O5-C5 | 3.23  | 116.51      | 112.19   |
| 15  | g     | 6   | MAN  | C1-O5-C5 | 3.20  | 116.48      | 112.19   |
| 11  | 3     | 2   | NAG  | C1-O5-C5 | 3.18  | 116.45      | 112.19   |
| 9   | i     | 4   | MAN  | C2-C3-C4 | 3.17  | 116.44      | 110.86   |
| 11  | m     | 2   | NAG  | C1-O5-C5 | 3.17  | 116.44      | 112.19   |
| 15  | HA    | 3   | BMA  | O2-C2-C3 | -3.16 | 103.61      | 110.15   |
| 15  | g     | 9   | MAN  | O2-C2-C3 | -3.15 | 103.63      | 110.15   |
| 15  | w     | 2   | NAG  | C1-C2-N2 | 3.14  | 115.38      | 110.43   |
| 15  | HA    | 9   | MAN  | O2-C2-C3 | -3.12 | 103.68      | 110.15   |
| 15  | g     | 8   | MAN  | C1-O5-C5 | 3.12  | 116.36      | 112.19   |
| 9   | i     | 3   | BMA  | C1-C2-C3 | -3.11 | 105.12      | 109.64   |
| 10  | s     | 2   | NAG  | C1-O5-C5 | 3.08  | 116.32      | 112.19   |
| 13  | 9     | 1   | NAG  | C1-O5-C5 | 3.08  | 116.32      | 112.19   |
| 9   | JA    | 4   | MAN  | C2-C3-C4 | 3.07  | 116.26      | 110.86   |
| 12  | n     | 1   | NAG  | C1-O5-C5 | 3.07  | 116.30      | 112.19   |
| 9   | y     | 3   | BMA  | C1-C2-C3 | -3.06 | 105.19      | 109.64   |
| 15  | w     | 3   | BMA  | O2-C2-C3 | -3.06 | 103.82      | 110.15   |
| 10  | c     | 2   | NAG  | C1-O5-C5 | 3.05  | 116.27      | 112.19   |
| 15  | g     | 3   | BMA  | O2-C2-C3 | -3.04 | 103.85      | 110.15   |
| 15  | w     | 8   | MAN  | C1-O5-C5 | 3.01  | 116.22      | 112.19   |
| 12  | X     | 1   | NAG  | C1-O5-C5 | 3.01  | 116.22      | 112.19   |
| 11  | W     | 2   | NAG  | C1-O5-C5 | 3.00  | 116.21      | 112.19   |
| 9   | JA    | 2   | NAG  | C1-O5-C5 | 3.00  | 116.20      | 112.19   |
| 13  | o     | 1   | NAG  | C1-O5-C5 | 2.99  | 116.19      | 112.19   |
| 10  | DA    | 2   | NAG  | C1-O5-C5 | 2.99  | 116.19      | 112.19   |
| 15  | HA    | 8   | MAN  | C1-O5-C5 | 2.96  | 116.15      | 112.19   |
| 15  | HA    | 2   | NAG  | C1-C2-N2 | 2.93  | 115.06      | 110.43   |
| 15  | g     | 2   | NAG  | C1-C2-N2 | 2.92  | 115.04      | 110.43   |
| 10  | x     | 1   | NAG  | C1-O5-C5 | 2.91  | 116.09      | 112.19   |
| 9   | y     | 1   | NAG  | O4-C4-C5 | -2.91 | 102.16      | 109.32   |
| 12  | n     | 3   | BMA  | C1-O5-C5 | 2.90  | 116.08      | 112.19   |
| 11  | m     | 4   | MAN  | O2-C2-C3 | -2.90 | 104.14      | 110.15   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | i     | 1   | NAG  | O4-C4-C5 | -2.88 | 102.23      | 109.32   |
| 10  | IA    | 1   | NAG  | C1-O5-C5 | 2.88  | 116.04      | 112.19   |
| 11  | W     | 4   | MAN  | O2-C2-C3 | -2.87 | 104.21      | 110.15   |
| 11  | 3     | 4   | MAN  | O2-C2-C3 | -2.86 | 104.22      | 110.15   |
| 10  | b     | 1   | NAG  | C1-O5-C5 | 2.85  | 116.01      | 112.19   |
| 10  | h     | 1   | NAG  | C1-O5-C5 | 2.85  | 116.01      | 112.19   |
| 12  | 4     | 3   | BMA  | C1-O5-C5 | 2.84  | 116.00      | 112.19   |
| 12  | X     | 3   | BMA  | C1-O5-C5 | 2.84  | 116.00      | 112.19   |
| 9   | y     | 4   | MAN  | C2-C3-C4 | 2.84  | 115.85      | 110.86   |
| 9   | l     | 3   | BMA  | O3-C3-C4 | 2.82  | 117.03      | 110.38   |
| 9   | 1     | 3   | BMA  | O3-C3-C4 | 2.80  | 116.98      | 110.38   |
| 9   | V     | 3   | BMA  | O3-C3-C4 | 2.79  | 116.96      | 110.38   |
| 10  | CA    | 1   | NAG  | C1-O5-C5 | 2.78  | 115.91      | 112.19   |
| 10  | r     | 1   | NAG  | C1-O5-C5 | 2.76  | 115.88      | 112.19   |
| 13  | Y     | 1   | NAG  | C1-O5-C5 | 2.74  | 115.86      | 112.19   |
| 9   | l     | 4   | MAN  | O2-C2-C3 | -2.68 | 104.61      | 110.15   |
| 15  | HA    | 5   | MAN  | O2-C2-C3 | -2.68 | 104.61      | 110.15   |
| 9   | 1     | 4   | MAN  | O2-C2-C3 | -2.66 | 104.64      | 110.15   |
| 10  | c     | 1   | NAG  | C1-O5-C5 | 2.65  | 115.73      | 112.19   |
| 10  | U     | 1   | NAG  | C4-C3-C2 | 2.65  | 114.90      | 111.02   |
| 9   | V     | 4   | MAN  | O2-C2-C3 | -2.64 | 104.68      | 110.15   |
| 10  | DA    | 1   | NAG  | C1-O5-C5 | 2.64  | 115.72      | 112.19   |
| 14  | a     | 1   | NAG  | C1-O5-C5 | 2.64  | 115.72      | 112.19   |
| 10  | 0     | 1   | NAG  | C4-C3-C2 | 2.63  | 114.87      | 111.02   |
| 10  | s     | 1   | NAG  | C1-O5-C5 | 2.61  | 115.69      | 112.19   |
| 15  | w     | 6   | MAN  | O2-C2-C3 | -2.59 | 104.78      | 110.15   |
| 15  | g     | 6   | MAN  | O2-C2-C3 | -2.59 | 104.78      | 110.15   |
| 14  | q     | 1   | NAG  | C1-O5-C5 | 2.58  | 115.64      | 112.19   |
| 10  | k     | 1   | NAG  | C4-C3-C2 | 2.56  | 114.78      | 111.02   |
| 10  | x     | 1   | NAG  | C1-C2-N2 | 2.55  | 114.46      | 110.43   |
| 15  | HA    | 6   | MAN  | O2-C2-C3 | -2.53 | 104.91      | 110.15   |
| 10  | h     | 1   | NAG  | C1-C2-N2 | 2.50  | 114.38      | 110.43   |
| 15  | g     | 5   | MAN  | O2-C2-C3 | -2.50 | 104.97      | 110.15   |
| 13  | o     | 2   | NAG  | C1-O5-C5 | 2.50  | 115.53      | 112.19   |
| 15  | w     | 5   | MAN  | O2-C2-C3 | -2.47 | 105.03      | 110.15   |
| 13  | Y     | 2   | NAG  | C1-O5-C5 | 2.45  | 115.48      | 112.19   |
| 9   | JA    | 3   | BMA  | C1-C2-C3 | -2.45 | 106.08      | 109.64   |
| 10  | IA    | 1   | NAG  | C1-C2-N2 | 2.45  | 114.30      | 110.43   |
| 12  | EA    | 1   | NAG  | C1-O5-C5 | 2.45  | 115.47      | 112.19   |
| 9   | z     | 4   | MAN  | O2-C2-C3 | -2.44 | 105.10      | 110.15   |
| 14  | q     | 3   | BMA  | O2-C2-C3 | -2.43 | 105.11      | 110.15   |
| 11  | e     | 5   | MAN  | O2-C2-C3 | -2.42 | 105.14      | 110.15   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 11  | FA    | 5   | MAN  | O2-C2-C3 | -2.41 | 105.16      | 110.15   |
| 14  | a     | 3   | BMA  | O2-C2-C3 | -2.41 | 105.17      | 110.15   |
| 14  | BA    | 3   | BMA  | O2-C2-C3 | -2.41 | 105.17      | 110.15   |
| 9   | JA    | 1   | NAG  | C3-C4-C5 | 2.41  | 114.59      | 110.23   |
| 13  | 9     | 2   | NAG  | C1-O5-C5 | 2.41  | 115.41      | 112.19   |
| 9   | l     | 2   | NAG  | O4-C4-C3 | 2.40  | 116.02      | 110.38   |
| 11  | u     | 5   | MAN  | O2-C2-C3 | -2.39 | 105.19      | 110.15   |
| 9   | T     | 4   | MAN  | O2-C2-C3 | -2.39 | 105.19      | 110.15   |
| 13  | o     | 4   | MAN  | O2-C2-C3 | -2.39 | 105.20      | 110.15   |
| 13  | 9     | 4   | MAN  | O2-C2-C3 | -2.38 | 105.22      | 110.15   |
| 10  | b     | 2   | NAG  | C1-O5-C5 | 2.38  | 115.37      | 112.19   |
| 9   | V     | 2   | NAG  | O4-C4-C3 | 2.37  | 115.97      | 110.38   |
| 9   | j     | 4   | MAN  | O2-C2-C3 | -2.36 | 105.27      | 110.15   |
| 10  | r     | 2   | NAG  | C1-O5-C5 | 2.36  | 115.34      | 112.19   |
| 9   | i     | 1   | NAG  | C3-C4-C5 | 2.34  | 114.48      | 110.23   |
| 9   | 1     | 2   | NAG  | O4-C4-C3 | 2.34  | 115.89      | 110.38   |
| 10  | CA    | 2   | NAG  | C1-O5-C5 | 2.33  | 115.31      | 112.19   |
| 13  | Y     | 4   | MAN  | O2-C2-C3 | -2.31 | 105.37      | 110.15   |
| 9   | JA    | 1   | NAG  | O5-C5-C6 | -2.30 | 103.19      | 107.66   |
| 15  | HA    | 7   | MAN  | C3-C4-C5 | -2.29 | 106.08      | 110.23   |
| 9   | T     | 3   | BMA  | C1-O5-C5 | 2.27  | 115.23      | 112.19   |
| 15  | w     | 7   | MAN  | C3-C4-C5 | -2.27 | 106.12      | 110.23   |
| 10  | f     | 1   | NAG  | C1-O5-C5 | 2.26  | 115.22      | 112.19   |
| 14  | BA    | 1   | NAG  | C1-O5-C5 | 2.25  | 115.21      | 112.19   |
| 15  | g     | 7   | MAN  | C3-C4-C5 | -2.24 | 106.18      | 110.23   |
| 10  | GA    | 1   | NAG  | C1-O5-C5 | 2.23  | 115.18      | 112.19   |
| 10  | v     | 1   | NAG  | C1-O5-C5 | 2.22  | 115.17      | 112.19   |
| 9   | j     | 3   | BMA  | C1-O5-C5 | 2.20  | 115.14      | 112.19   |
| 9   | y     | 4   | MAN  | O2-C2-C1 | 2.19  | 114.24      | 109.22   |
| 14  | a     | 5   | MAN  | O2-C2-C3 | -2.17 | 105.65      | 110.15   |
| 9   | 1     | 3   | BMA  | C3-C4-C5 | -2.17 | 106.30      | 110.23   |
| 11  | FA    | 2   | NAG  | O4-C4-C3 | 2.16  | 115.48      | 110.38   |
| 11  | FA    | 3   | BMA  | C1-C2-C3 | 2.16  | 112.79      | 109.64   |
| 11  | u     | 2   | NAG  | O4-C4-C3 | 2.16  | 115.46      | 110.38   |
| 9   | JA    | 4   | MAN  | O2-C2-C1 | 2.15  | 114.15      | 109.22   |
| 9   | i     | 4   | MAN  | O2-C2-C1 | 2.15  | 114.15      | 109.22   |
| 9   | z     | 3   | BMA  | C1-O5-C5 | 2.15  | 115.06      | 112.19   |
| 15  | g     | 7   | MAN  | O2-C2-C3 | -2.14 | 105.71      | 110.15   |
| 14  | a     | 6   | MAN  | O2-C2-C3 | -2.13 | 105.74      | 110.15   |
| 14  | q     | 5   | MAN  | O2-C2-C3 | -2.13 | 105.74      | 110.15   |
| 14  | q     | 6   | MAN  | O2-C2-C3 | -2.13 | 105.75      | 110.15   |
| 12  | d     | 1   | NAG  | C1-O5-C5 | 2.12  | 115.03      | 112.19   |

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| Mol | Chain | Res | Type | Atoms    | Z     | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 9   | V     | 3   | BMA  | C3-C4-C5 | -2.11 | 106.41      | 110.23   |
| 11  | u     | 3   | BMA  | O2-C2-C3 | -2.10 | 105.80      | 110.15   |
| 9   | y     | 1   | NAG  | C3-C4-C5 | 2.10  | 114.04      | 110.23   |
| 11  | W     | 4   | MAN  | C1-C2-C3 | 2.10  | 112.70      | 109.64   |
| 11  | FA    | 3   | BMA  | O2-C2-C3 | -2.09 | 105.81      | 110.15   |
| 11  | m     | 4   | MAN  | C1-C2-C3 | 2.09  | 112.69      | 109.64   |
| 15  | HA    | 3   | BMA  | C3-C4-C5 | -2.09 | 106.44      | 110.23   |
| 12  | X     | 2   | NAG  | C1-O5-C5 | 2.09  | 114.98      | 112.19   |
| 14  | BA    | 5   | MAN  | O2-C2-C3 | -2.08 | 105.83      | 110.15   |
| 14  | BA    | 6   | MAN  | O2-C2-C3 | -2.08 | 105.84      | 110.15   |
| 15  | w     | 1   | NAG  | C1-O5-C5 | 2.08  | 114.97      | 112.19   |
| 11  | 3     | 4   | MAN  | C1-C2-C3 | 2.08  | 112.67      | 109.64   |
| 15  | HA    | 1   | NAG  | C1-O5-C5 | 2.08  | 114.97      | 112.19   |
| 11  | u     | 3   | BMA  | C1-C2-C3 | 2.08  | 112.67      | 109.64   |
| 10  | Z     | 2   | NAG  | C1-O5-C5 | 2.07  | 114.96      | 112.19   |
| 9   | l     | 3   | BMA  | C3-C4-C5 | -2.07 | 106.49      | 110.23   |
| 12  | X     | 3   | BMA  | O2-C2-C3 | -2.06 | 105.88      | 110.15   |
| 10  | AA    | 2   | NAG  | C1-O5-C5 | 2.06  | 114.95      | 112.19   |
| 12  | X     | 1   | NAG  | C4-C3-C2 | 2.06  | 114.03      | 111.02   |
| 12  | n     | 1   | NAG  | C4-C3-C2 | 2.05  | 114.03      | 111.02   |
| 11  | e     | 3   | BMA  | O2-C2-C3 | -2.05 | 105.90      | 110.15   |
| 9   | l     | 3   | BMA  | C1-C2-C3 | -2.05 | 106.66      | 109.64   |
| 10  | f     | 2   | NAG  | C1-O5-C5 | 2.05  | 114.94      | 112.19   |
| 11  | e     | 3   | BMA  | C1-C2-C3 | 2.05  | 112.63      | 109.64   |
| 15  | g     | 3   | BMA  | O6-C6-C5 | -2.04 | 104.40      | 111.33   |
| 10  | p     | 1   | NAG  | C4-C3-C2 | 2.04  | 114.00      | 111.02   |
| 12  | 4     | 3   | BMA  | O2-C2-C3 | -2.03 | 105.94      | 110.15   |
| 12  | n     | 3   | BMA  | O2-C2-C3 | -2.03 | 105.94      | 110.15   |
| 11  | e     | 2   | NAG  | O4-C4-C3 | 2.03  | 115.15      | 110.38   |
| 9   | y     | 3   | BMA  | O5-C1-C2 | 2.02  | 115.61      | 110.79   |
| 9   | j     | 3   | BMA  | C2-C3-C4 | 2.02  | 114.42      | 110.86   |
| 10  | GA    | 2   | NAG  | C1-O5-C5 | 2.02  | 114.89      | 112.19   |
| 9   | i     | 3   | BMA  | O5-C1-C2 | 2.02  | 115.60      | 110.79   |
| 15  | w     | 3   | BMA  | O6-C6-C5 | -2.01 | 104.47      | 111.33   |
| 12  | n     | 2   | NAG  | C1-O5-C5 | 2.01  | 114.88      | 112.19   |
| 15  | w     | 7   | MAN  | O6-C6-C5 | -2.00 | 104.51      | 111.33   |
| 15  | g     | 3   | BMA  | C3-C4-C5 | -2.00 | 106.60      | 110.23   |
| 12  | t     | 1   | NAG  | C1-O5-C5 | 2.00  | 114.87      | 112.19   |

There are no chirality outliers.

All (258) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 15  | w     | 1   | NAG  | C4-C5-C6-O6 |
| 12  | EA    | 3   | BMA  | C4-C5-C6-O6 |
| 15  | g     | 1   | NAG  | C4-C5-C6-O6 |
| 15  | HA    | 1   | NAG  | C4-C5-C6-O6 |
| 9   | y     | 2   | NAG  | O5-C5-C6-O6 |
| 13  | Y     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 2   | NAG  | O5-C5-C6-O6 |
| 12  | d     | 3   | BMA  | C4-C5-C6-O6 |
| 12  | t     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | JA    | 2   | NAG  | O5-C5-C6-O6 |
| 10  | DA    | 1   | NAG  | O5-C5-C6-O6 |
| 11  | e     | 1   | NAG  | O5-C5-C6-O6 |
| 14  | BA    | 5   | MAN  | O5-C5-C6-O6 |
| 15  | g     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | k     | 2   | NAG  | O5-C5-C6-O6 |
| 14  | q     | 5   | MAN  | O5-C5-C6-O6 |
| 15  | w     | 1   | NAG  | O5-C5-C6-O6 |
| 15  | HA    | 1   | NAG  | O5-C5-C6-O6 |
| 9   | l     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | b     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | r     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | 0     | 2   | NAG  | O5-C5-C6-O6 |
| 11  | u     | 5   | MAN  | O5-C5-C6-O6 |
| 9   | T     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | T     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | j     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | j     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | z     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | z     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | l     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | JA    | 1   | NAG  | O5-C5-C6-O6 |
| 10  | Z     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | c     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | s     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | AA    | 1   | NAG  | O5-C5-C6-O6 |
| 11  | u     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | u     | 3   | BMA  | O5-C5-C6-O6 |
| 11  | FA    | 1   | NAG  | O5-C5-C6-O6 |
| 12  | EA    | 3   | BMA  | O5-C5-C6-O6 |
| 13  | o     | 1   | NAG  | O5-C5-C6-O6 |
| 13  | 9     | 1   | NAG  | O5-C5-C6-O6 |
| 14  | a     | 5   | MAN  | O5-C5-C6-O6 |
| 9   | V     | 3   | BMA  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 10  | p     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | CA    | 1   | NAG  | O5-C5-C6-O6 |
| 9   | y     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | U     | 2   | NAG  | C4-C5-C6-O6 |
| 11  | u     | 1   | NAG  | C4-C5-C6-O6 |
| 11  | FA    | 1   | NAG  | C4-C5-C6-O6 |
| 9   | l     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | l     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | h     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | e     | 3   | BMA  | O5-C5-C6-O6 |
| 9   | l     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | k     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | 0     | 2   | NAG  | C4-C5-C6-O6 |
| 11  | e     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | U     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | GA    | 1   | NAG  | O5-C5-C6-O6 |
| 11  | e     | 5   | MAN  | O5-C5-C6-O6 |
| 11  | FA    | 3   | BMA  | O5-C5-C6-O6 |
| 11  | FA    | 5   | MAN  | O5-C5-C6-O6 |
| 15  | g     | 8   | MAN  | O5-C5-C6-O6 |
| 10  | Z     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | V     | 3   | BMA  | O5-C5-C6-O6 |
| 13  | Y     | 4   | MAN  | O5-C5-C6-O6 |
| 13  | o     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | z     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | l     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | JA    | 2   | NAG  | C4-C5-C6-O6 |
| 10  | Z     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | AA    | 1   | NAG  | C4-C5-C6-O6 |
| 12  | n     | 2   | NAG  | C4-C5-C6-O6 |
| 12  | 4     | 2   | NAG  | C4-C5-C6-O6 |
| 13  | 9     | 4   | MAN  | C4-C5-C6-O6 |
| 13  | 9     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | T     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | j     | 2   | NAG  | C4-C5-C6-O6 |
| 12  | X     | 2   | NAG  | C4-C5-C6-O6 |
| 14  | BA    | 5   | MAN  | C4-C5-C6-O6 |
| 12  | n     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | p     | 2   | NAG  | C4-C5-C6-O6 |
| 13  | Y     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 13  | o     | 4   | MAN  | C4-C5-C6-O6 |
| 9   | T     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | j     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | z     | 4   | MAN  | O5-C5-C6-O6 |
| 10  | f     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | v     | 1   | NAG  | O5-C5-C6-O6 |
| 12  | X     | 2   | NAG  | O5-C5-C6-O6 |
| 12  | d     | 3   | BMA  | O5-C5-C6-O6 |
| 12  | 4     | 2   | NAG  | O5-C5-C6-O6 |
| 14  | BA    | 2   | NAG  | O5-C5-C6-O6 |
| 10  | p     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | AA    | 2   | NAG  | C4-C5-C6-O6 |
| 12  | t     | 3   | BMA  | O5-C5-C6-O6 |
| 14  | a     | 2   | NAG  | O5-C5-C6-O6 |
| 14  | q     | 2   | NAG  | O5-C5-C6-O6 |
| 11  | e     | 3   | BMA  | C4-C5-C6-O6 |
| 11  | FA    | 3   | BMA  | C4-C5-C6-O6 |
| 12  | d     | 1   | NAG  | C4-C5-C6-O6 |
| 13  | Y     | 4   | MAN  | C4-C5-C6-O6 |
| 10  | s     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | DA    | 1   | NAG  | C4-C5-C6-O6 |
| 14  | q     | 5   | MAN  | C4-C5-C6-O6 |
| 9   | l     | 2   | NAG  | C4-C5-C6-O6 |
| 11  | e     | 5   | MAN  | C4-C5-C6-O6 |
| 11  | FA    | 5   | MAN  | C4-C5-C6-O6 |
| 15  | g     | 8   | MAN  | C4-C5-C6-O6 |
| 15  | HA    | 8   | MAN  | O5-C5-C6-O6 |
| 9   | T     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | j     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | z     | 3   | BMA  | C4-C5-C6-O6 |
| 9   | 1     | 2   | NAG  | C4-C5-C6-O6 |
| 10  | b     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | r     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | CA    | 1   | NAG  | C4-C5-C6-O6 |
| 11  | m     | 1   | NAG  | C4-C5-C6-O6 |
| 11  | 3     | 1   | NAG  | C4-C5-C6-O6 |
| 14  | a     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | JA    | 1   | NAG  | C4-C5-C6-O6 |
| 10  | c     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | s     | 1   | NAG  | C4-C5-C6-O6 |
| 12  | t     | 1   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 13  | 9     | 1   | NAG  | C4-C5-C6-O6 |
| 14  | a     | 5   | MAN  | C4-C5-C6-O6 |
| 15  | HA    | 8   | MAN  | C4-C5-C6-O6 |
| 9   | z     | 4   | MAN  | C4-C5-C6-O6 |
| 11  | u     | 5   | MAN  | C4-C5-C6-O6 |
| 15  | w     | 8   | MAN  | O5-C5-C6-O6 |
| 13  | o     | 1   | NAG  | C4-C5-C6-O6 |
| 14  | q     | 2   | NAG  | C4-C5-C6-O6 |
| 14  | BA    | 2   | NAG  | C4-C5-C6-O6 |
| 11  | W     | 3   | BMA  | O5-C5-C6-O6 |
| 10  | DA    | 2   | NAG  | O5-C5-C6-O6 |
| 9   | T     | 4   | MAN  | C4-C5-C6-O6 |
| 9   | j     | 4   | MAN  | C4-C5-C6-O6 |
| 10  | f     | 2   | NAG  | C4-C5-C6-O6 |
| 11  | u     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | c     | 2   | NAG  | O5-C5-C6-O6 |
| 15  | w     | 2   | NAG  | O5-C5-C6-O6 |
| 15  | HA    | 2   | NAG  | O5-C5-C6-O6 |
| 11  | m     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | 3     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | GA    | 1   | NAG  | C4-C5-C6-O6 |
| 15  | w     | 8   | MAN  | C4-C5-C6-O6 |
| 9   | l     | 4   | MAN  | O5-C5-C6-O6 |
| 15  | g     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | h     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | v     | 1   | NAG  | C4-C5-C6-O6 |
| 11  | W     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | l     | 4   | MAN  | O5-C5-C6-O6 |
| 10  | f     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | Z     | 2   | NAG  | O5-C5-C6-O6 |
| 11  | 3     | 3   | BMA  | O5-C5-C6-O6 |
| 15  | g     | 2   | NAG  | C4-C5-C6-O6 |
| 15  | w     | 2   | NAG  | C4-C5-C6-O6 |
| 15  | HA    | 2   | NAG  | C4-C5-C6-O6 |
| 10  | x     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | e     | 4   | MAN  | O5-C5-C6-O6 |
| 11  | m     | 3   | BMA  | O5-C5-C6-O6 |
| 11  | W     | 3   | BMA  | C4-C5-C6-O6 |
| 10  | p     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | GA    | 2   | NAG  | C4-C5-C6-O6 |
| 12  | EA    | 1   | NAG  | C4-C5-C6-O6 |
| 9   | V     | 4   | MAN  | O5-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 10  | AA    | 2   | NAG  | O5-C5-C6-O6 |
| 11  | u     | 4   | MAN  | O5-C5-C6-O6 |
| 11  | FA    | 4   | MAN  | O5-C5-C6-O6 |
| 10  | v     | 2   | NAG  | C4-C5-C6-O6 |
| 15  | g     | 9   | MAN  | O5-C5-C6-O6 |
| 11  | 3     | 3   | BMA  | C4-C5-C6-O6 |
| 11  | m     | 3   | BMA  | C4-C5-C6-O6 |
| 12  | d     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | f     | 2   | NAG  | O5-C5-C6-O6 |
| 11  | W     | 1   | NAG  | O5-C5-C6-O6 |
| 12  | t     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | i     | 3   | BMA  | O5-C5-C6-O6 |
| 15  | HA    | 9   | MAN  | O5-C5-C6-O6 |
| 10  | GA    | 2   | NAG  | O5-C5-C6-O6 |
| 10  | v     | 2   | NAG  | O5-C5-C6-O6 |
| 9   | y     | 3   | BMA  | O5-C5-C6-O6 |
| 15  | HA    | 3   | BMA  | O5-C5-C6-O6 |
| 15  | g     | 3   | BMA  | O5-C5-C6-O6 |
| 15  | w     | 3   | BMA  | O5-C5-C6-O6 |
| 15  | w     | 5   | MAN  | O5-C5-C6-O6 |
| 10  | CA    | 2   | NAG  | C4-C5-C6-O6 |
| 12  | EA    | 1   | NAG  | O5-C5-C6-O6 |
| 15  | HA    | 5   | MAN  | O5-C5-C6-O6 |
| 11  | m     | 4   | MAN  | O5-C5-C6-O6 |
| 11  | W     | 4   | MAN  | O5-C5-C6-O6 |
| 15  | g     | 5   | MAN  | O5-C5-C6-O6 |
| 10  | r     | 2   | NAG  | C4-C5-C6-O6 |
| 9   | JA    | 3   | BMA  | O5-C5-C6-O6 |
| 10  | U     | 1   | NAG  | O5-C5-C6-O6 |
| 11  | 3     | 4   | MAN  | O5-C5-C6-O6 |
| 9   | l     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | 1     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | V     | 1   | NAG  | O5-C5-C6-O6 |
| 14  | q     | 1   | NAG  | C4-C5-C6-O6 |
| 14  | BA    | 6   | MAN  | C4-C5-C6-O6 |
| 10  | b     | 2   | NAG  | C4-C5-C6-O6 |
| 14  | a     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | IA    | 1   | NAG  | O5-C5-C6-O6 |
| 10  | CA    | 2   | NAG  | O5-C5-C6-O6 |
| 10  | x     | 1   | NAG  | C4-C5-C6-O6 |
| 11  | e     | 4   | MAN  | C4-C5-C6-O6 |
| 14  | a     | 6   | MAN  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 11  | u     | 4   | MAN  | C4-C5-C6-O6 |
| 11  | FA    | 4   | MAN  | C4-C5-C6-O6 |
| 10  | r     | 2   | NAG  | O5-C5-C6-O6 |
| 14  | BA    | 1   | NAG  | C4-C5-C6-O6 |
| 9   | z     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | k     | 1   | NAG  | O5-C5-C6-O6 |
| 9   | j     | 1   | NAG  | C4-C5-C6-O6 |
| 9   | T     | 1   | NAG  | C4-C5-C6-O6 |
| 10  | IA    | 1   | NAG  | C3-C2-N2-C7 |
| 15  | g     | 2   | NAG  | C3-C2-N2-C7 |
| 15  | w     | 2   | NAG  | C3-C2-N2-C7 |
| 15  | HA    | 2   | NAG  | C3-C2-N2-C7 |
| 10  | 0     | 1   | NAG  | O5-C5-C6-O6 |
| 14  | q     | 1   | NAG  | O5-C5-C6-O6 |
| 15  | g     | 9   | MAN  | C4-C5-C6-O6 |
| 14  | q     | 6   | MAN  | C4-C5-C6-O6 |
| 10  | s     | 2   | NAG  | C4-C5-C6-O6 |
| 14  | a     | 1   | NAG  | O5-C5-C6-O6 |
| 10  | b     | 2   | NAG  | O5-C5-C6-O6 |
| 10  | U     | 1   | NAG  | C1-C2-N2-C7 |
| 10  | h     | 1   | NAG  | C1-C2-N2-C7 |
| 10  | k     | 1   | NAG  | C1-C2-N2-C7 |
| 10  | x     | 1   | NAG  | C1-C2-N2-C7 |
| 10  | 0     | 1   | NAG  | C1-C2-N2-C7 |
| 10  | IA    | 1   | NAG  | C1-C2-N2-C7 |
| 12  | X     | 1   | NAG  | C1-C2-N2-C7 |
| 12  | n     | 1   | NAG  | C1-C2-N2-C7 |
| 12  | 4     | 1   | NAG  | C1-C2-N2-C7 |
| 15  | g     | 2   | NAG  | C1-C2-N2-C7 |
| 15  | w     | 2   | NAG  | C1-C2-N2-C7 |
| 15  | HA    | 2   | NAG  | C1-C2-N2-C7 |
| 14  | BA    | 6   | MAN  | O5-C5-C6-O6 |
| 10  | U     | 1   | NAG  | C3-C2-N2-C7 |
| 10  | h     | 1   | NAG  | C3-C2-N2-C7 |
| 10  | k     | 1   | NAG  | C3-C2-N2-C7 |
| 10  | x     | 1   | NAG  | C3-C2-N2-C7 |
| 10  | 0     | 1   | NAG  | C3-C2-N2-C7 |
| 12  | X     | 1   | NAG  | C3-C2-N2-C7 |
| 12  | n     | 1   | NAG  | C3-C2-N2-C7 |
| 12  | 4     | 1   | NAG  | C3-C2-N2-C7 |
| 15  | HA    | 9   | MAN  | C4-C5-C6-O6 |
| 11  | m     | 2   | NAG  | C4-C5-C6-O6 |

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| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 15  | w     | 4   | MAN  | C4-C5-C6-O6 |
| 10  | DA    | 2   | NAG  | C4-C5-C6-O6 |
| 10  | c     | 2   | NAG  | C4-C5-C6-O6 |
| 14  | a     | 6   | MAN  | O5-C5-C6-O6 |
| 14  | BA    | 1   | NAG  | O5-C5-C6-O6 |

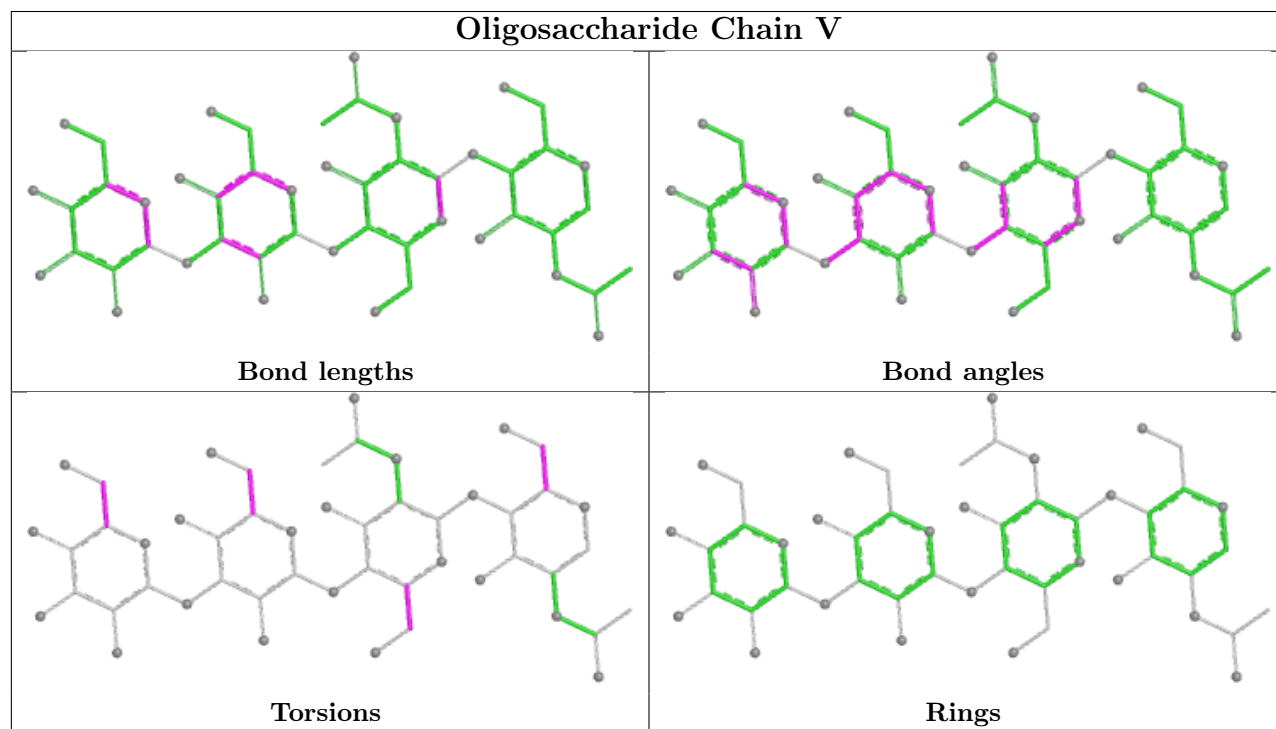
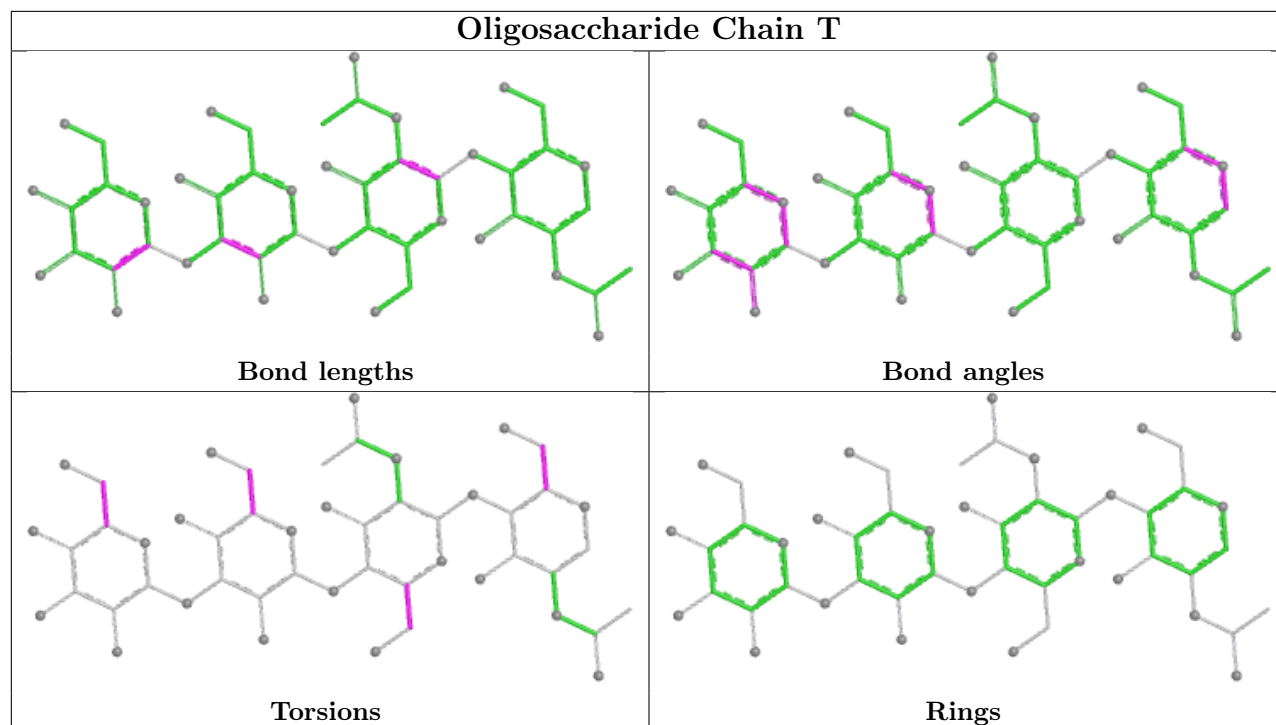
All (3) ring outliers are listed below:

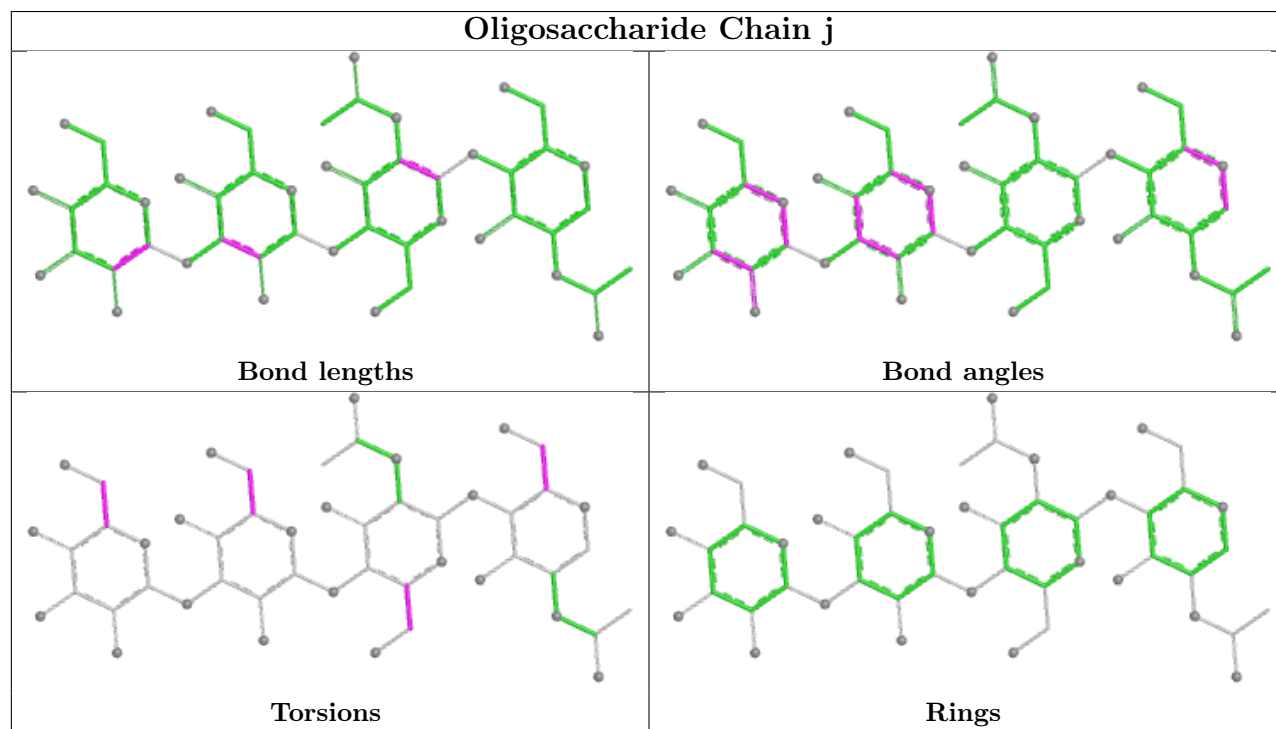
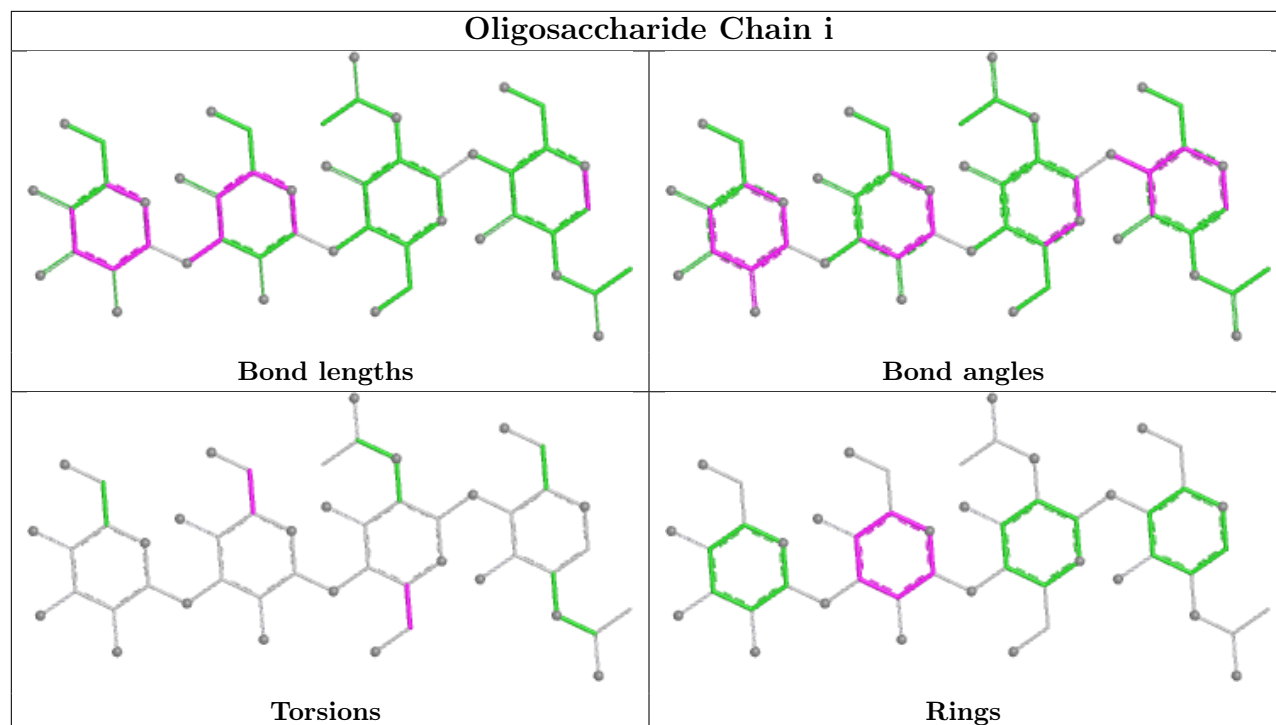
| Mol | Chain | Res | Type | Atoms             |
|-----|-------|-----|------|-------------------|
| 9   | i     | 3   | BMA  | C1-C2-C3-C4-C5-O5 |
| 9   | y     | 3   | BMA  | C1-C2-C3-C4-C5-O5 |
| 9   | JA    | 3   | BMA  | C1-C2-C3-C4-C5-O5 |

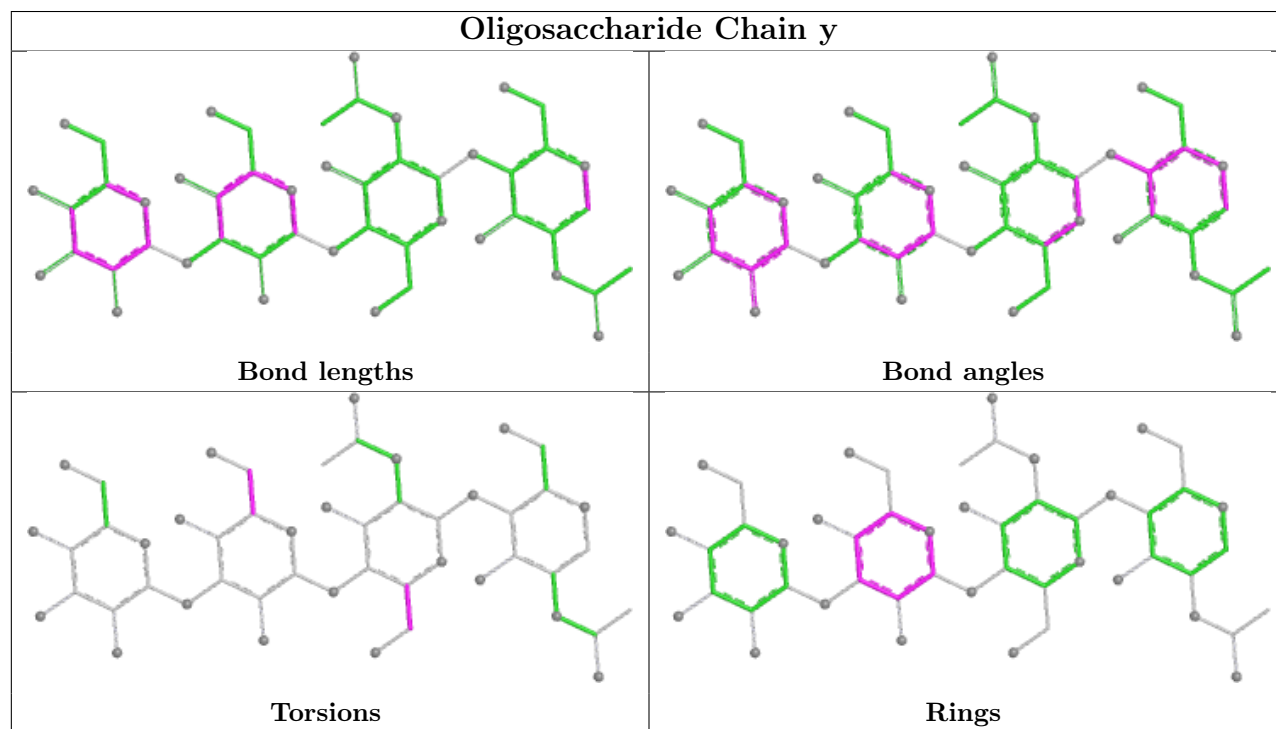
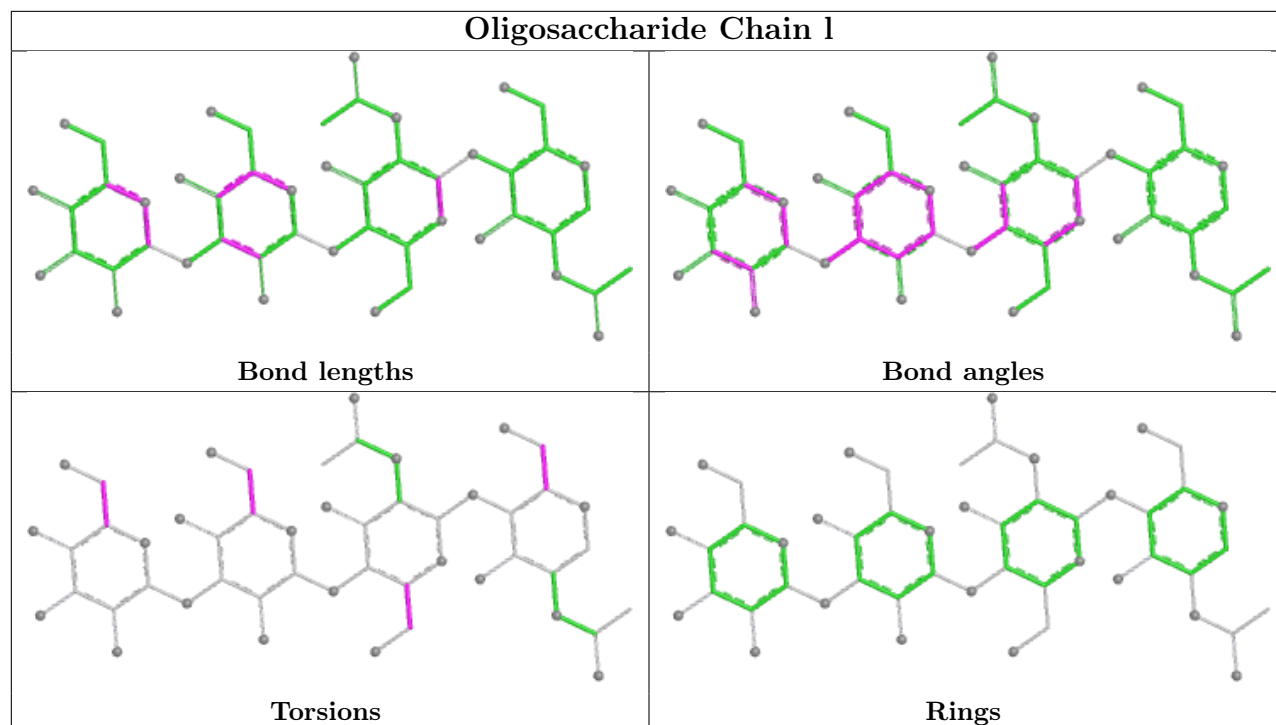
20 monomers are involved in 17 short contacts:

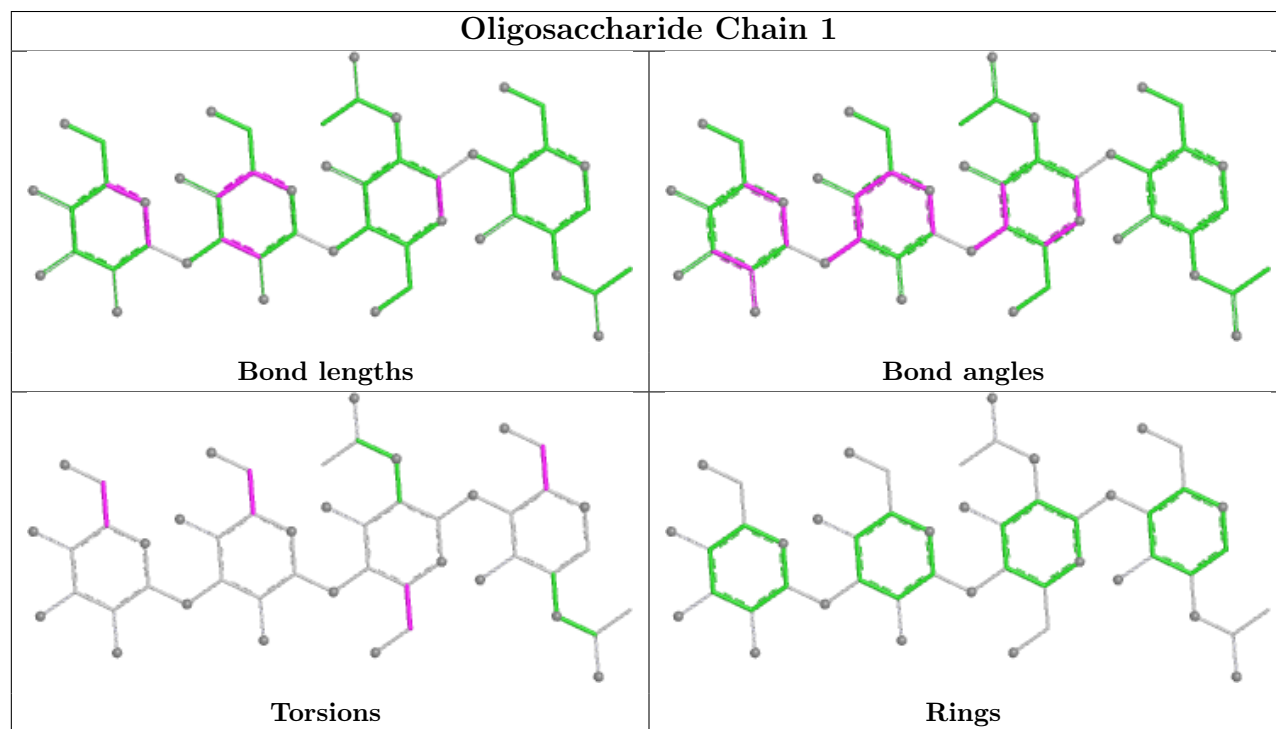
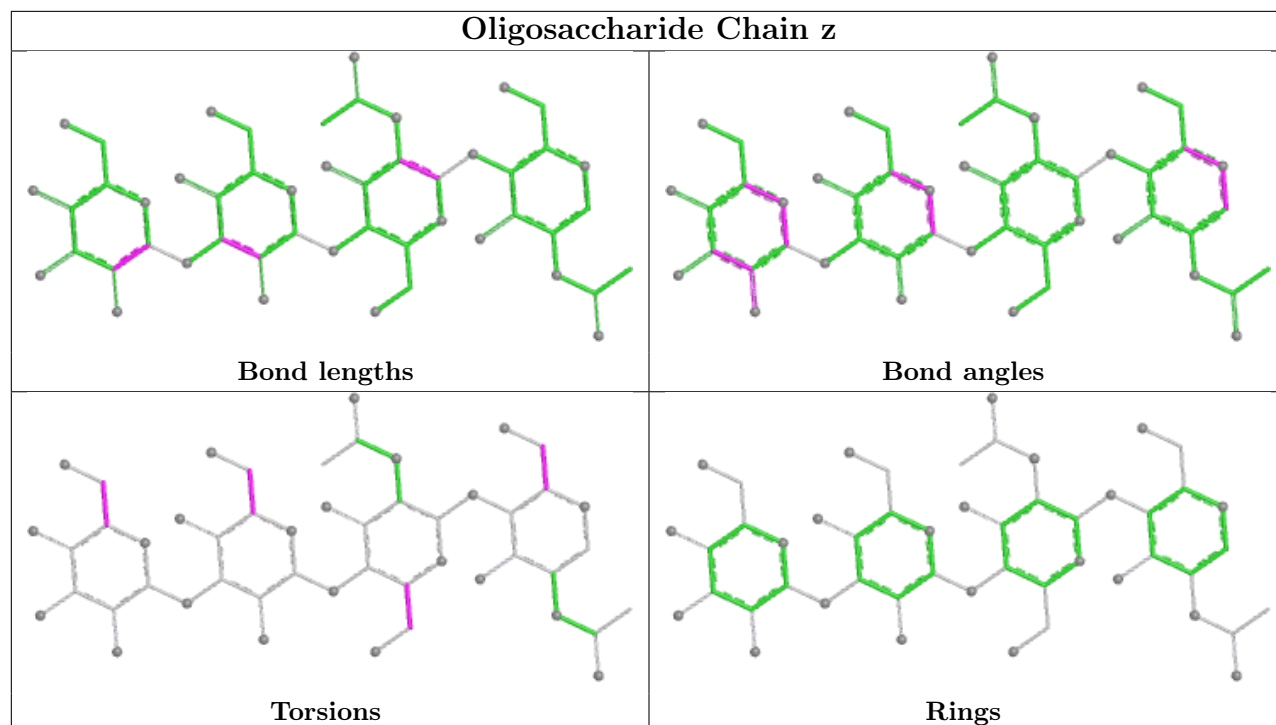
| Mol | Chain | Res | Type | Clashes | Symm-Clashes |
|-----|-------|-----|------|---------|--------------|
| 9   | y     | 2   | NAG  | 1       | 0            |
| 13  | Y     | 1   | NAG  | 1       | 0            |
| 9   | V     | 2   | NAG  | 1       | 0            |
| 9   | i     | 2   | NAG  | 1       | 0            |
| 9   | 1     | 2   | NAG  | 1       | 0            |
| 13  | 9     | 1   | NAG  | 1       | 0            |
| 10  | x     | 1   | NAG  | 1       | 0            |
| 9   | 1     | 3   | BMA  | 1       | 0            |
| 10  | IA    | 1   | NAG  | 1       | 0            |
| 10  | h     | 1   | NAG  | 1       | 0            |
| 9   | V     | 3   | BMA  | 1       | 0            |
| 9   | l     | 3   | BMA  | 1       | 0            |
| 14  | a     | 1   | NAG  | 1       | 0            |
| 13  | o     | 1   | NAG  | 1       | 0            |
| 12  | 4     | 1   | NAG  | 1       | 0            |
| 9   | JA    | 2   | NAG  | 1       | 0            |
| 14  | q     | 1   | NAG  | 1       | 0            |
| 12  | n     | 1   | NAG  | 1       | 0            |
| 14  | BA    | 1   | NAG  | 1       | 0            |
| 9   | l     | 2   | NAG  | 1       | 0            |

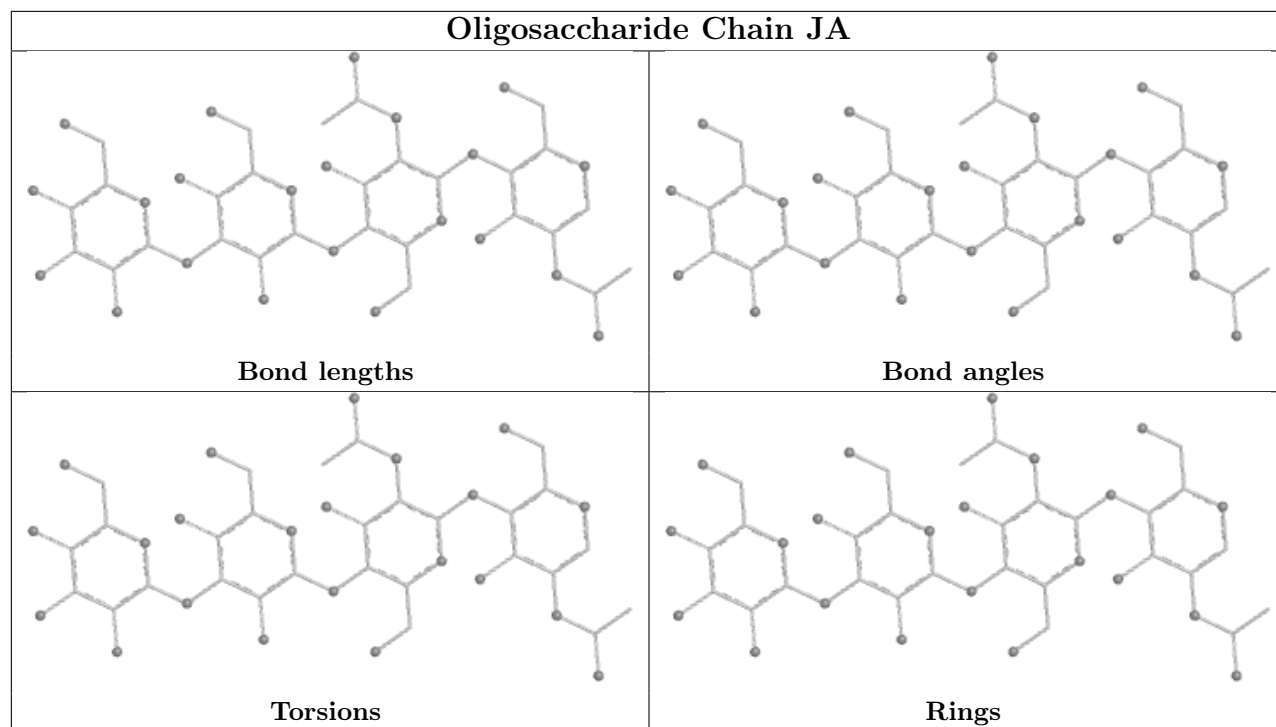
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.

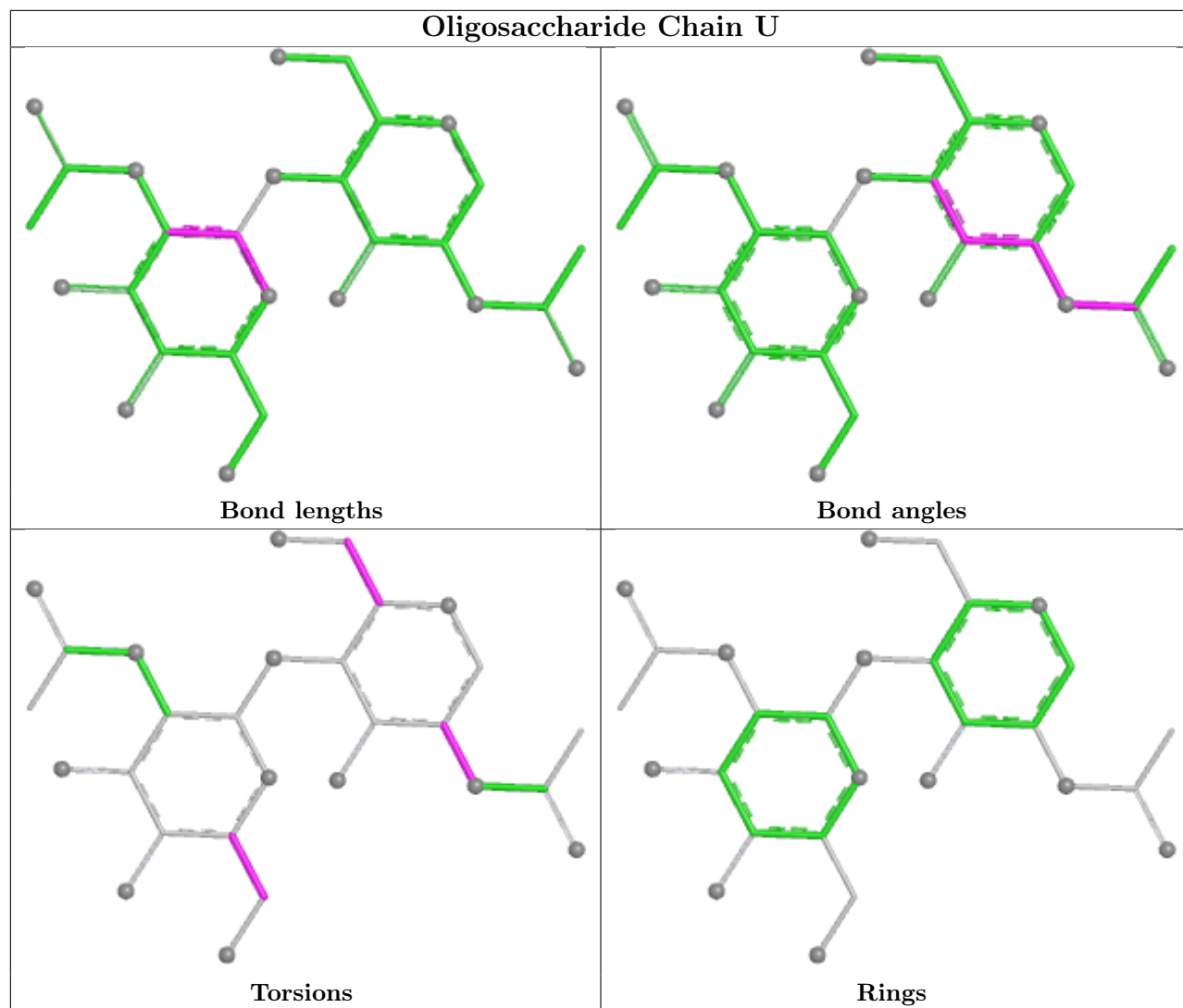


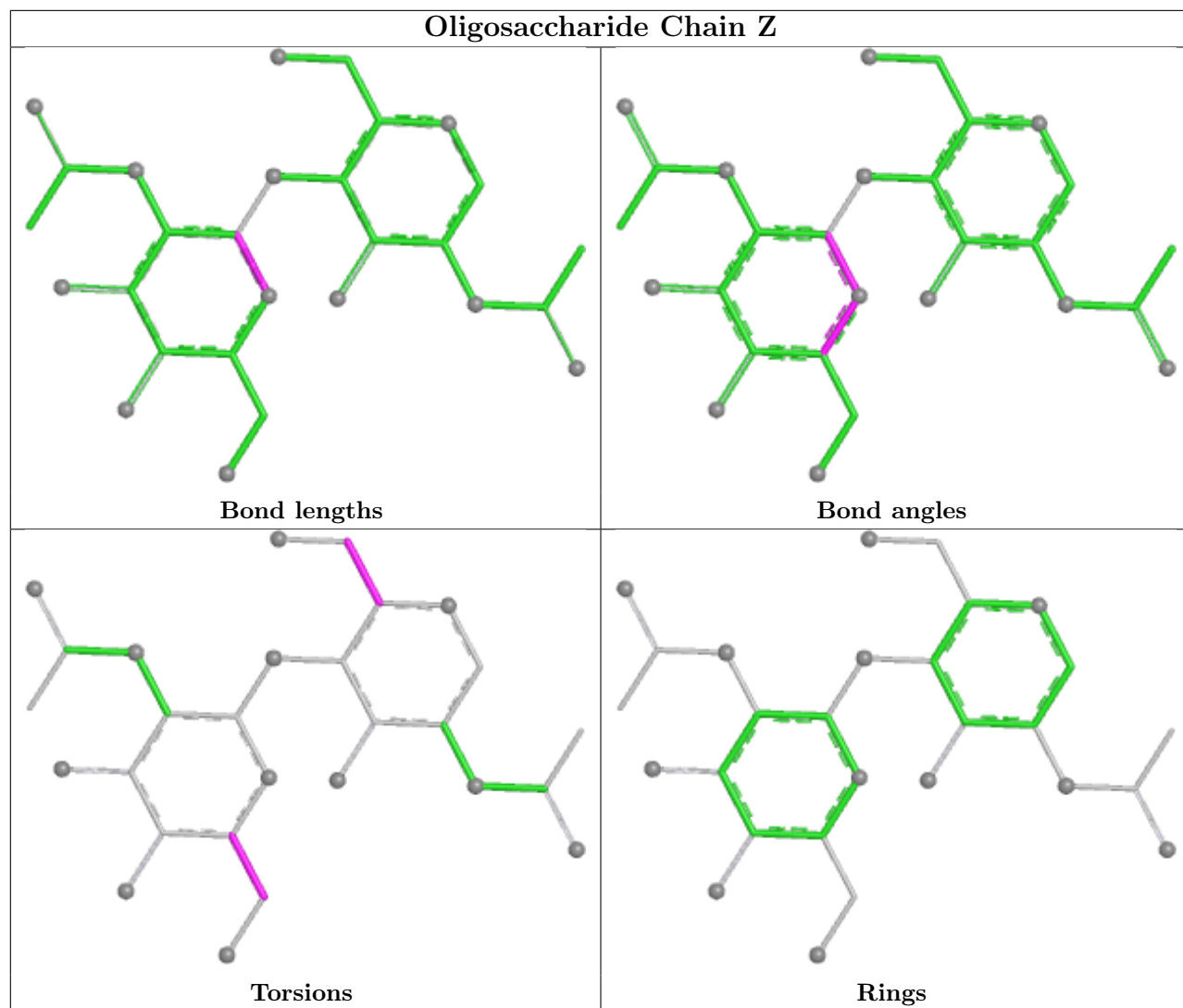


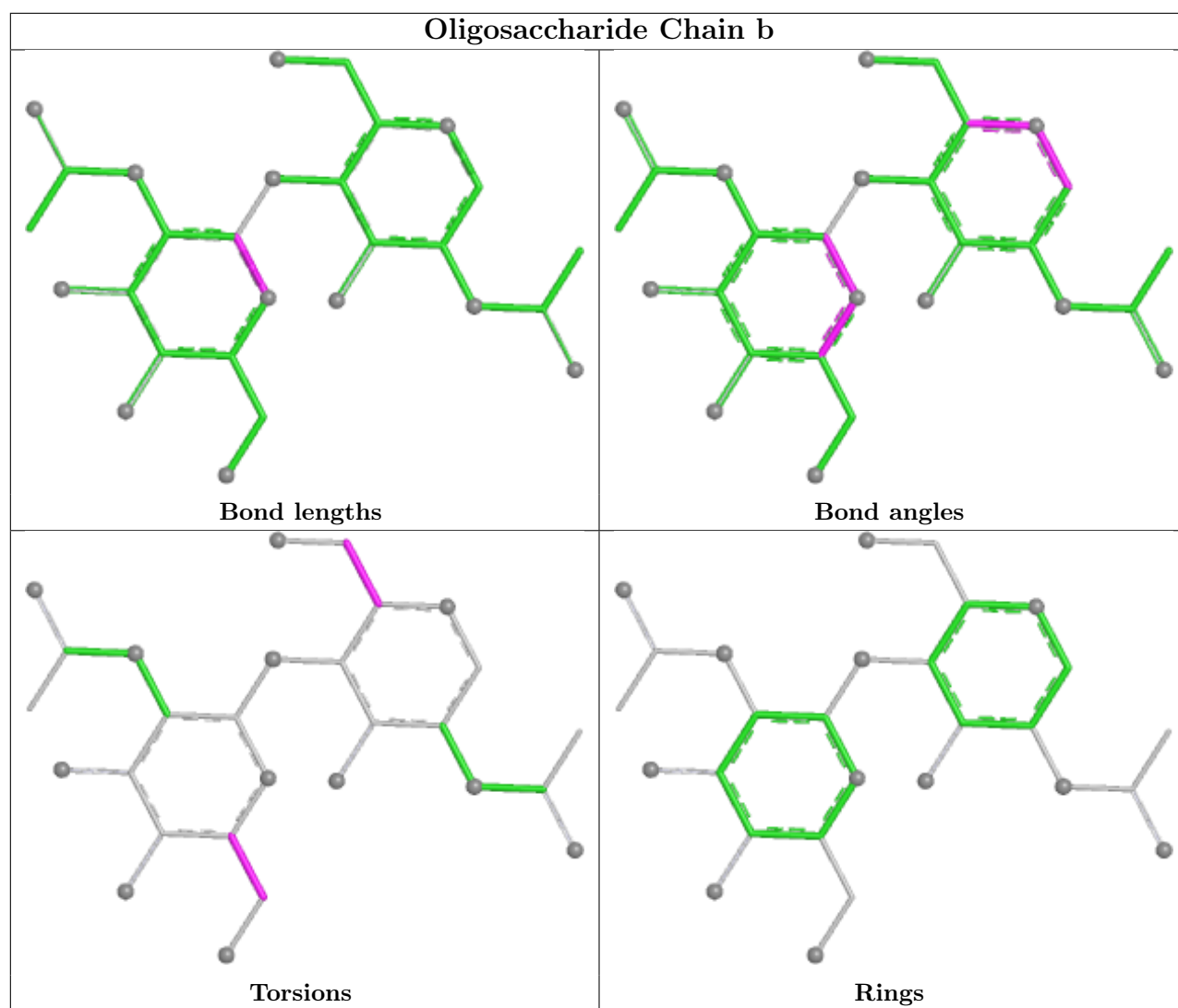


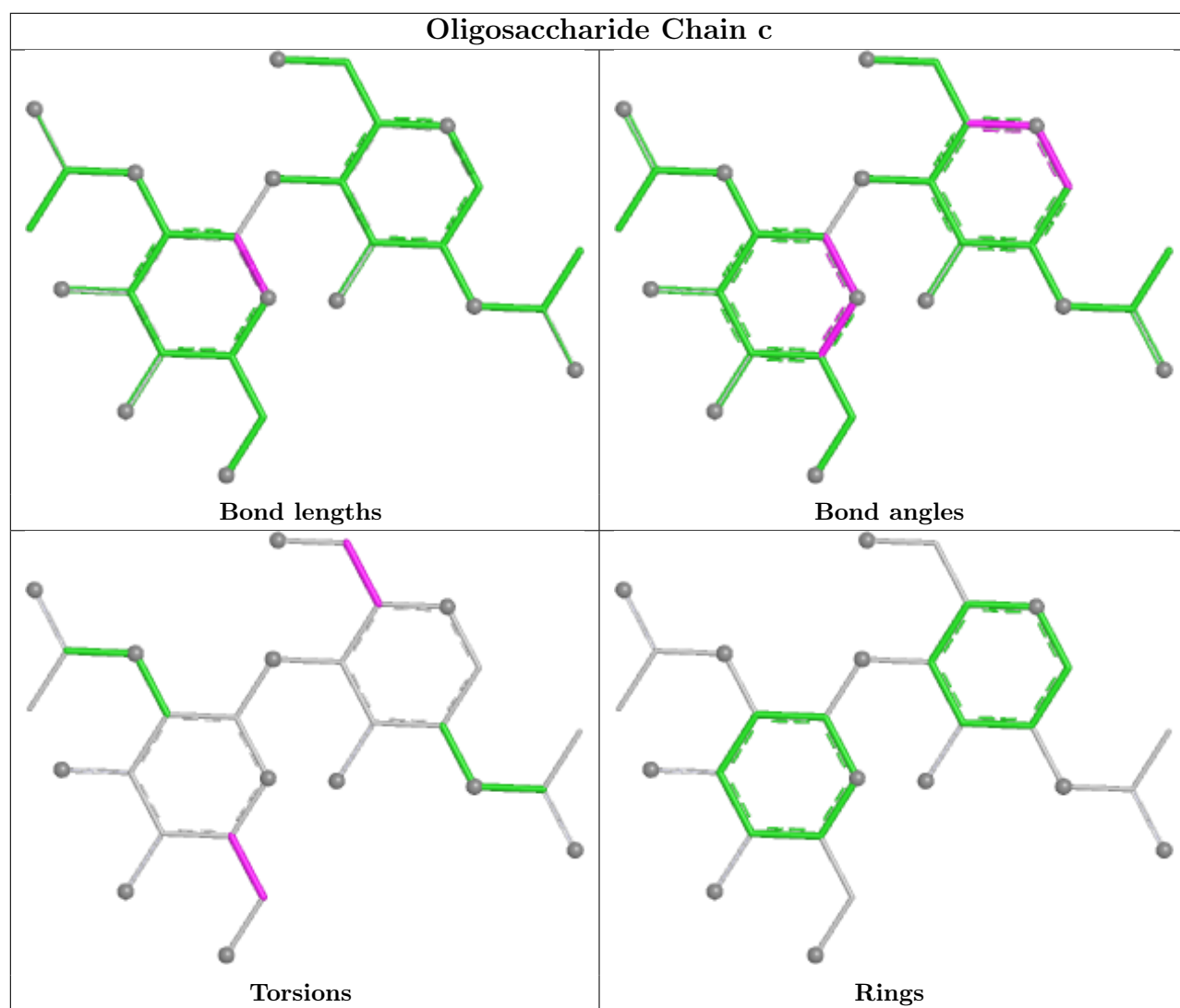


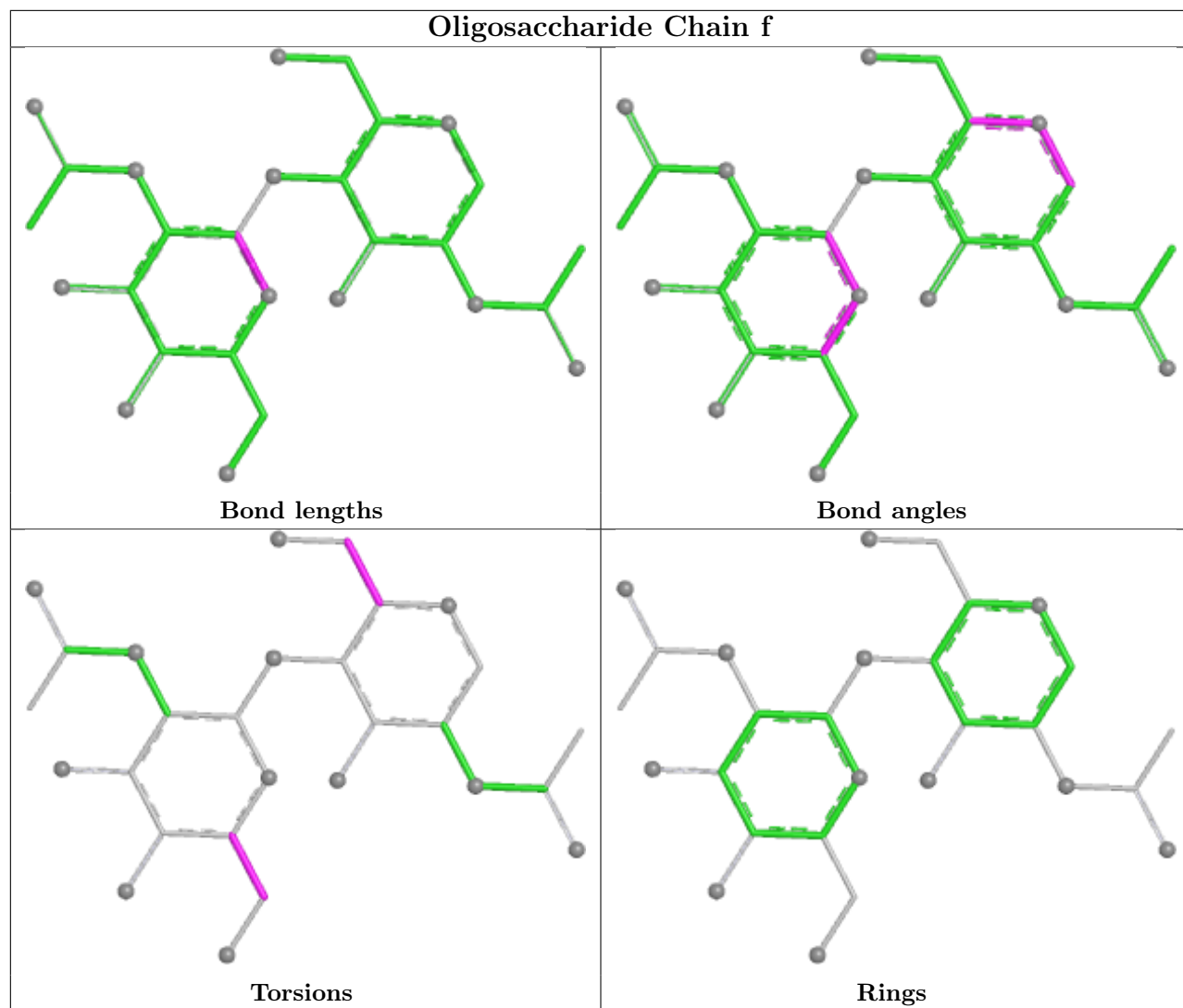


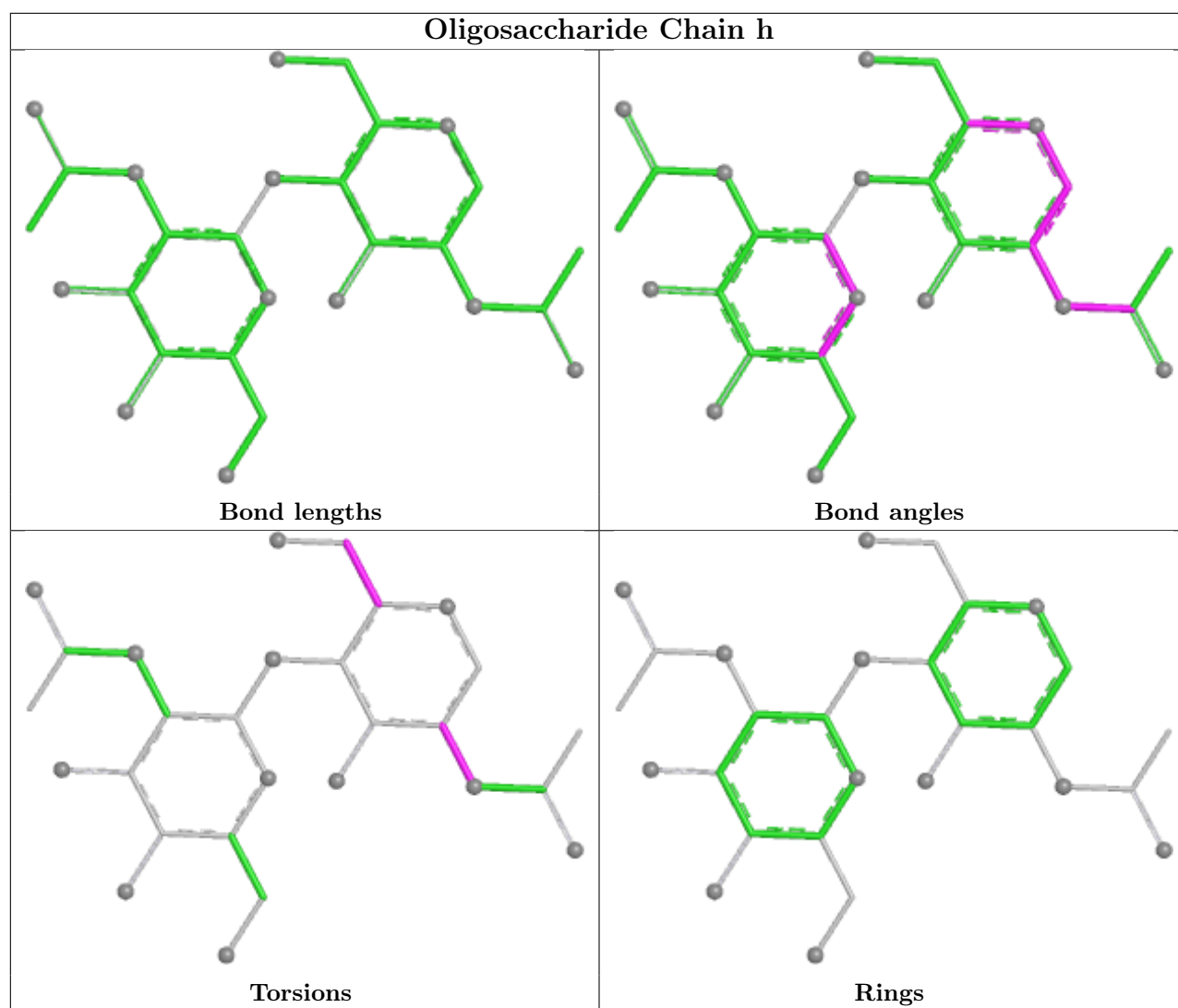


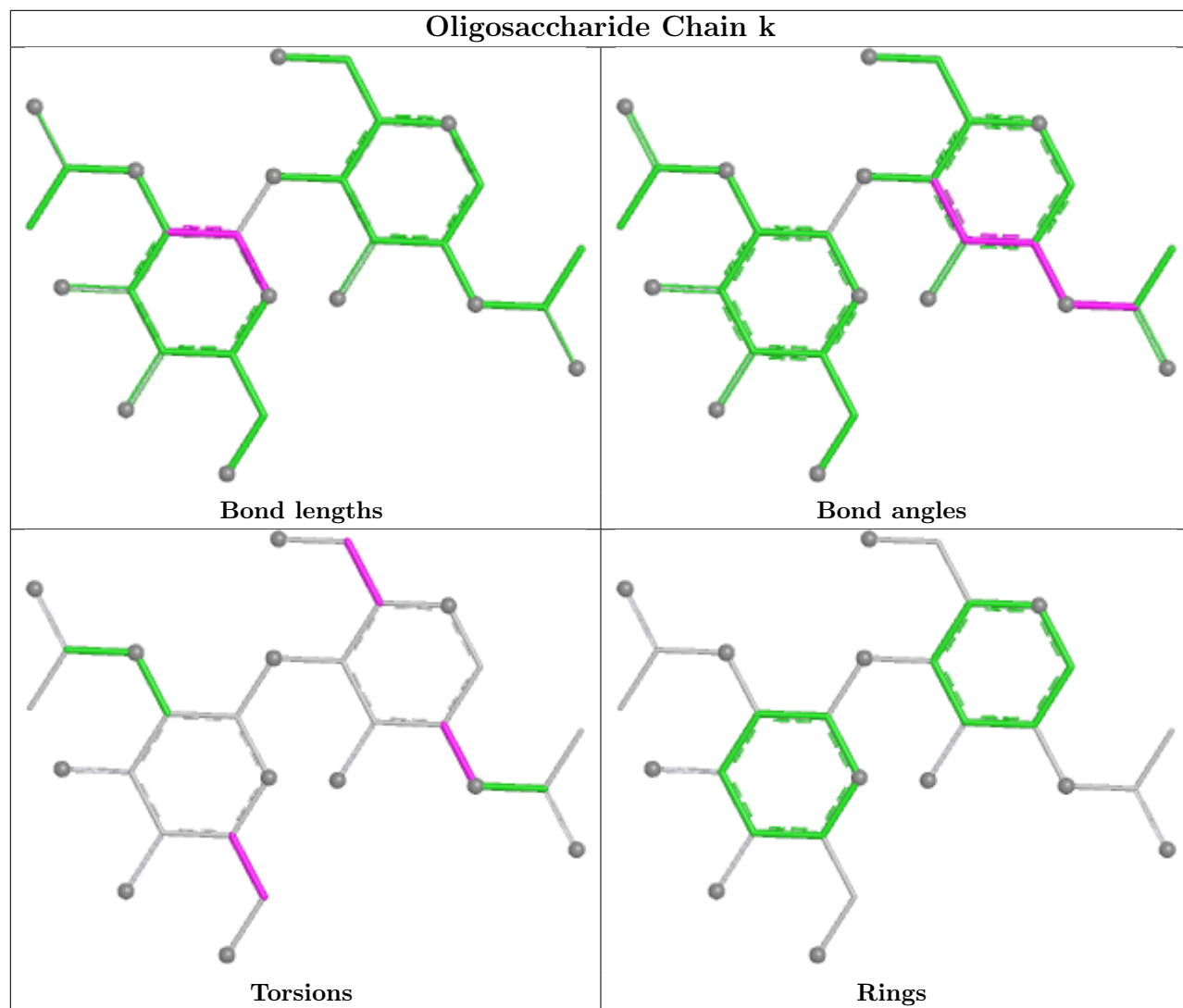


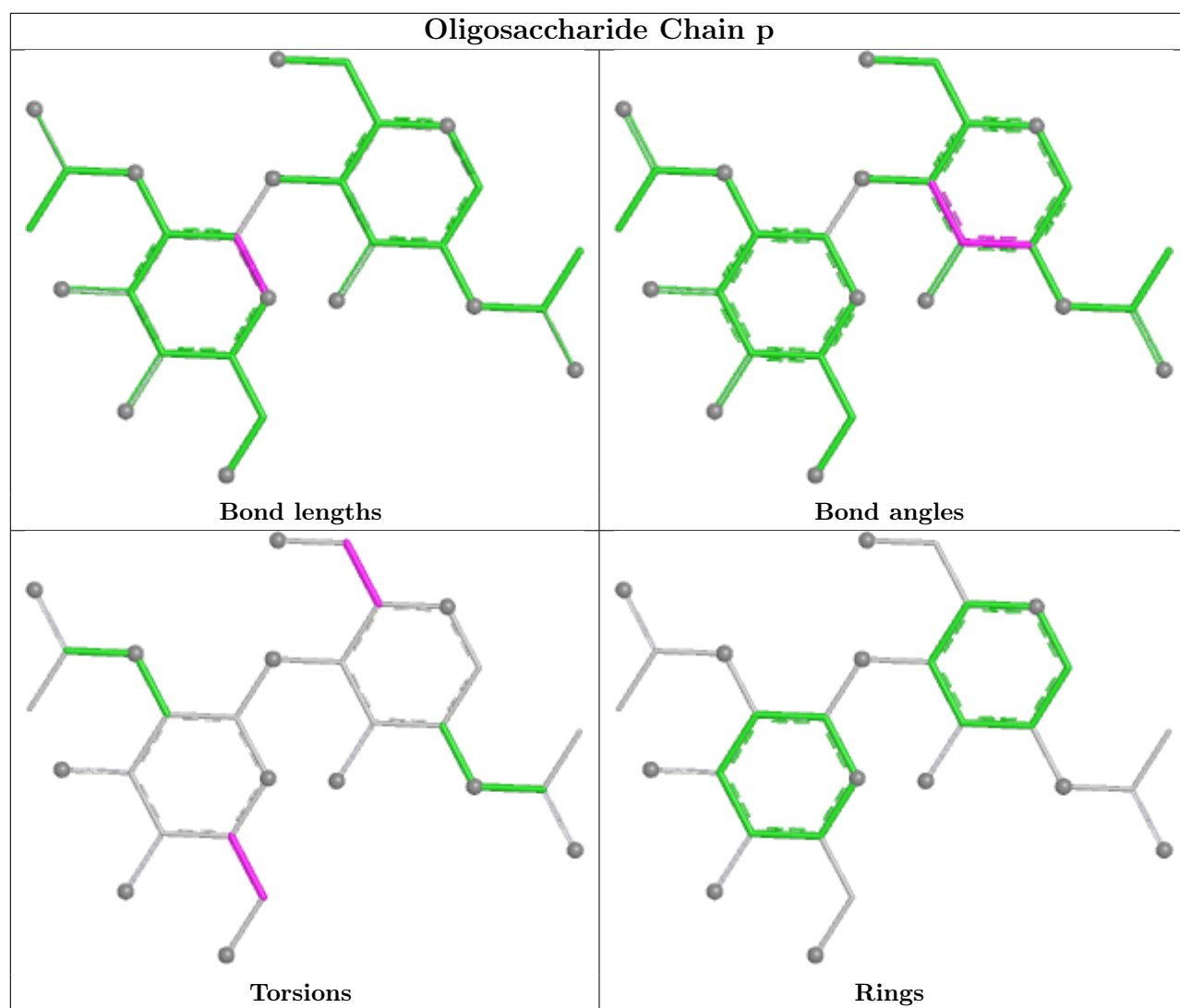


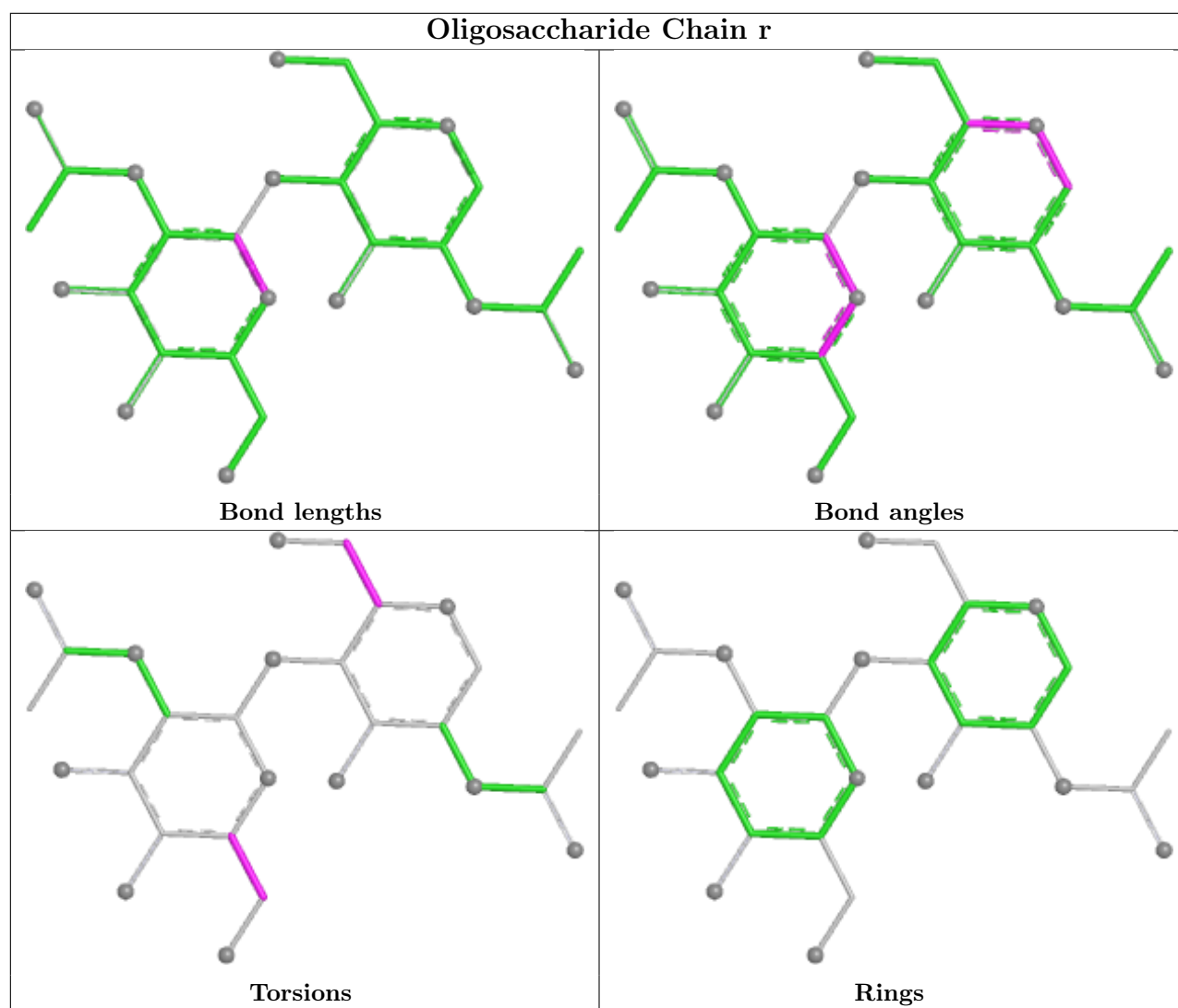


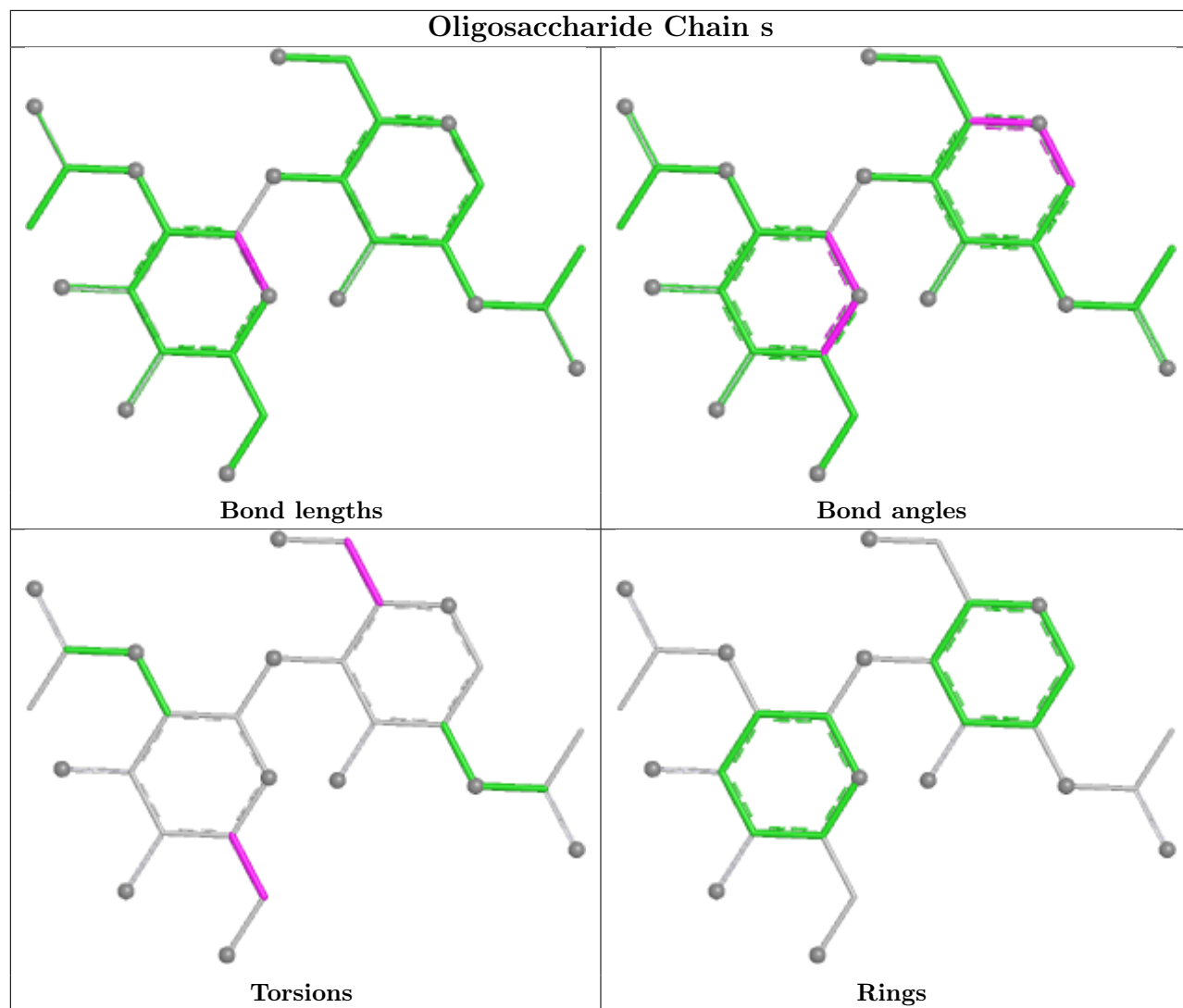


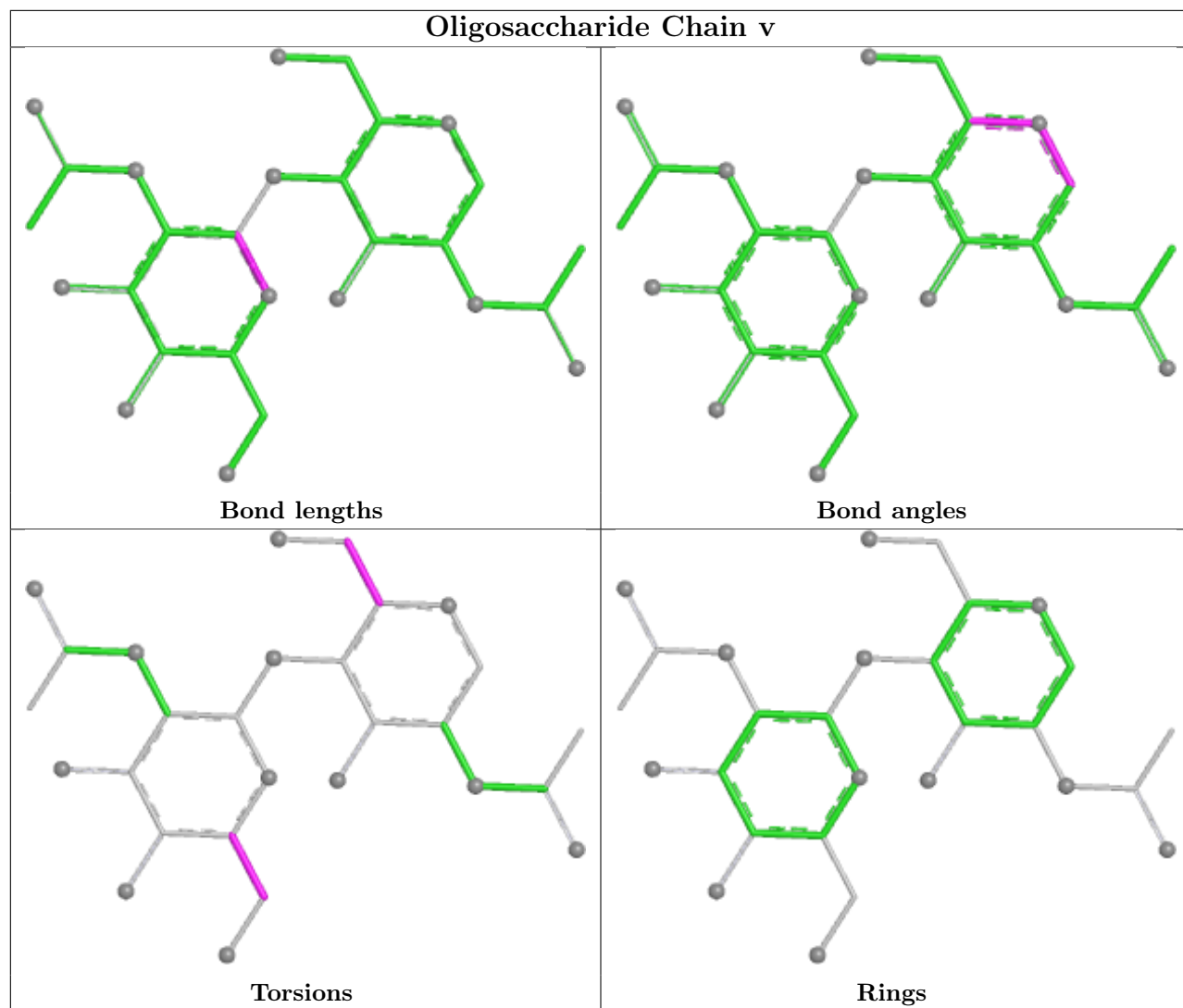


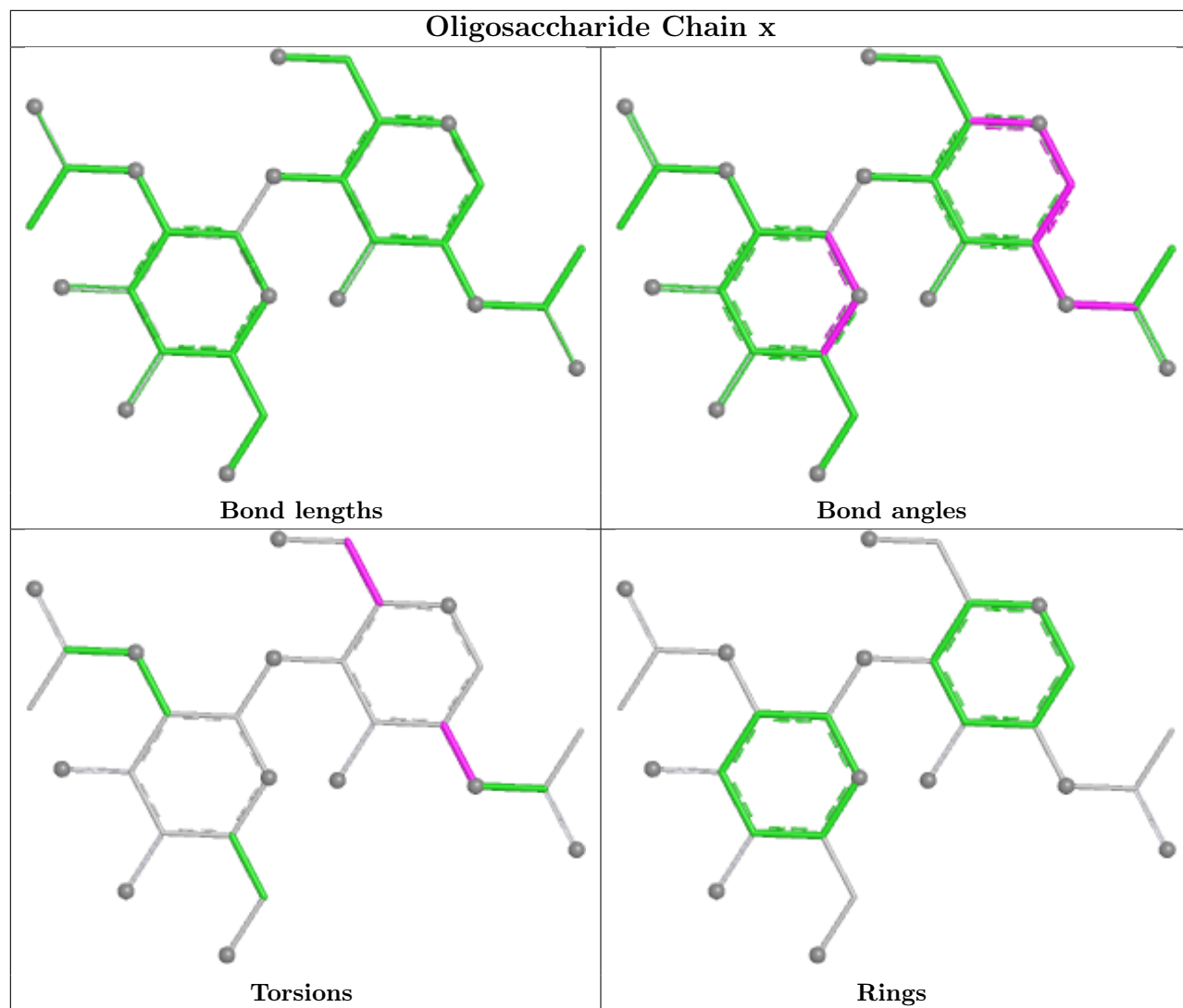


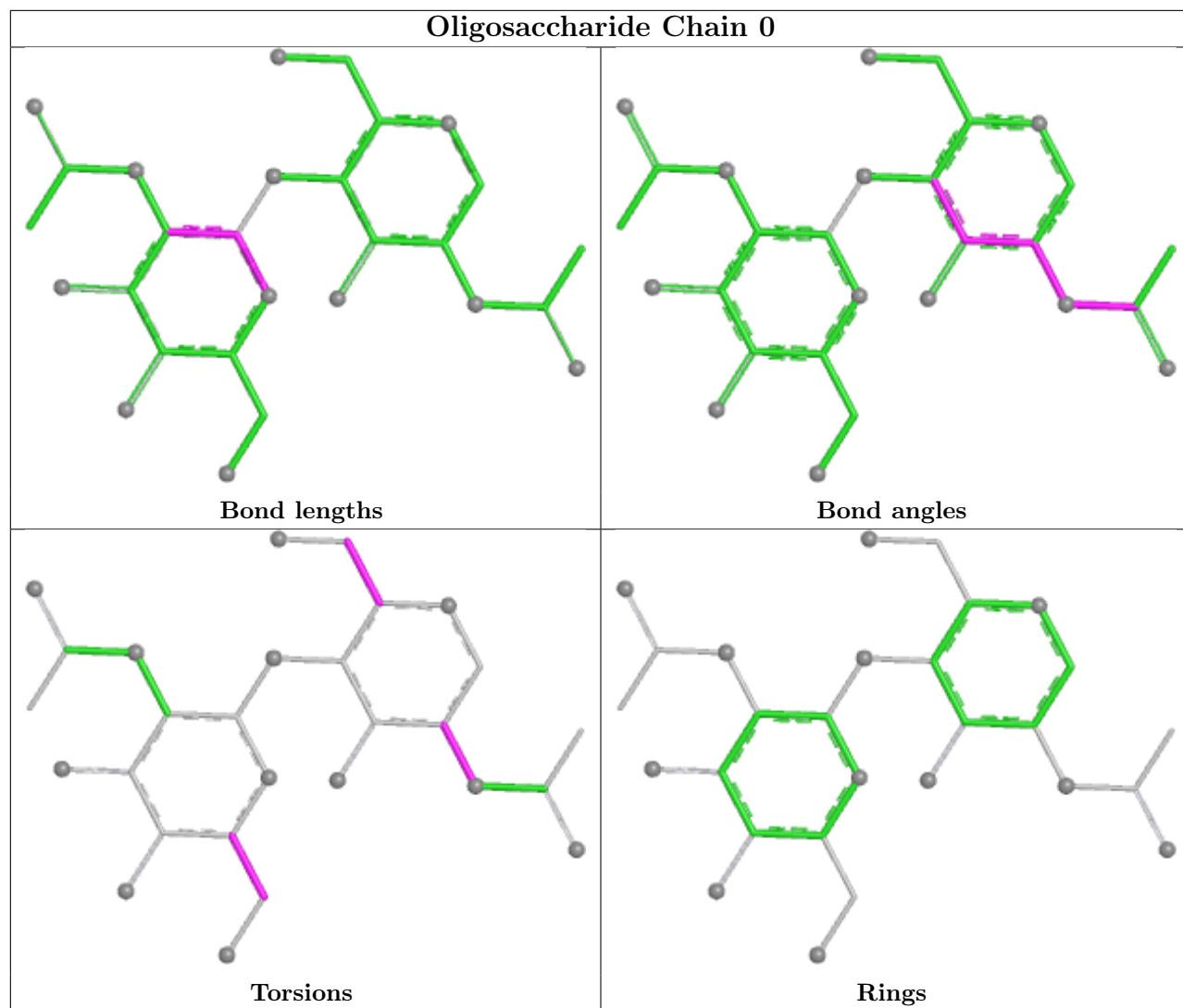


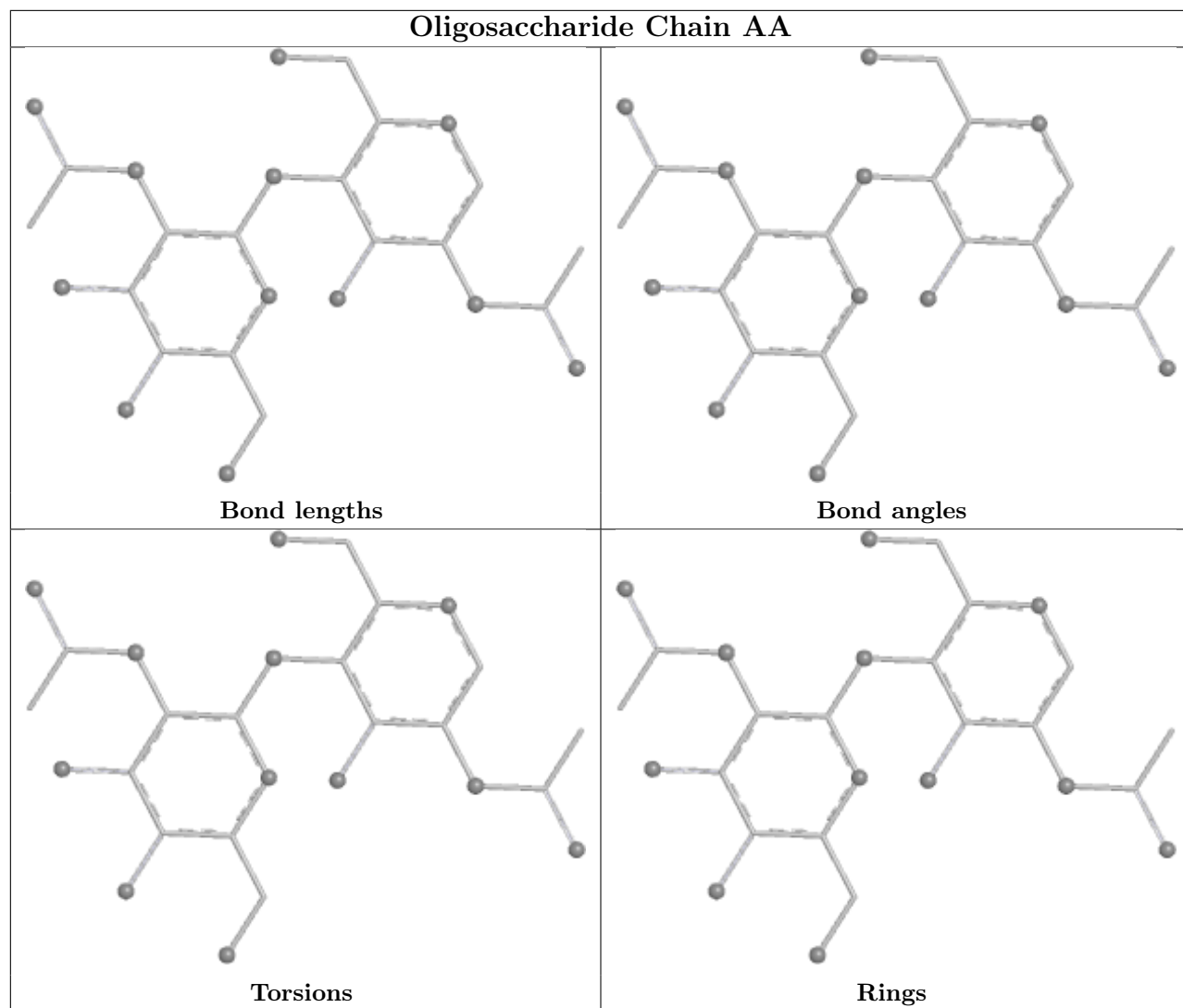


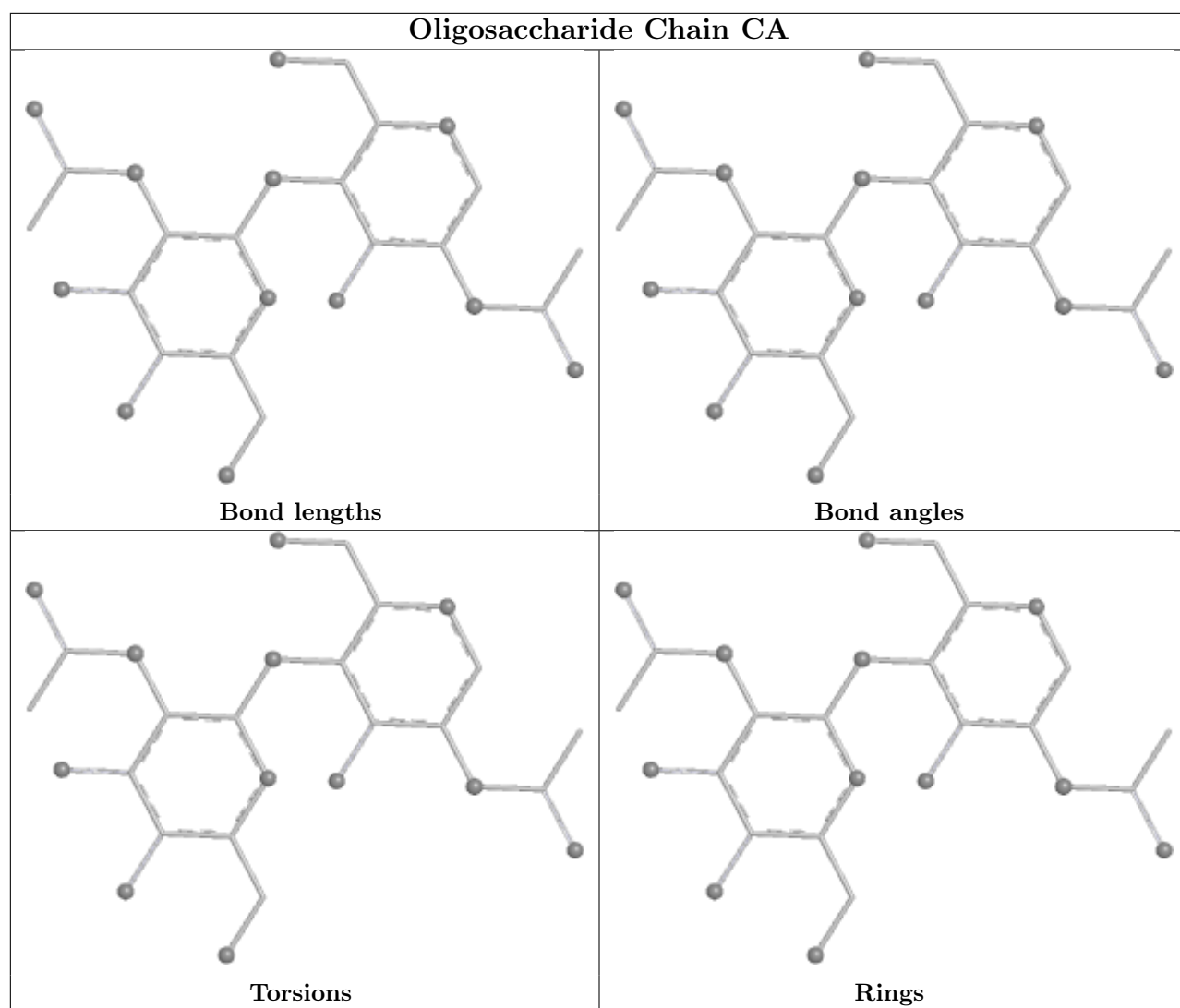


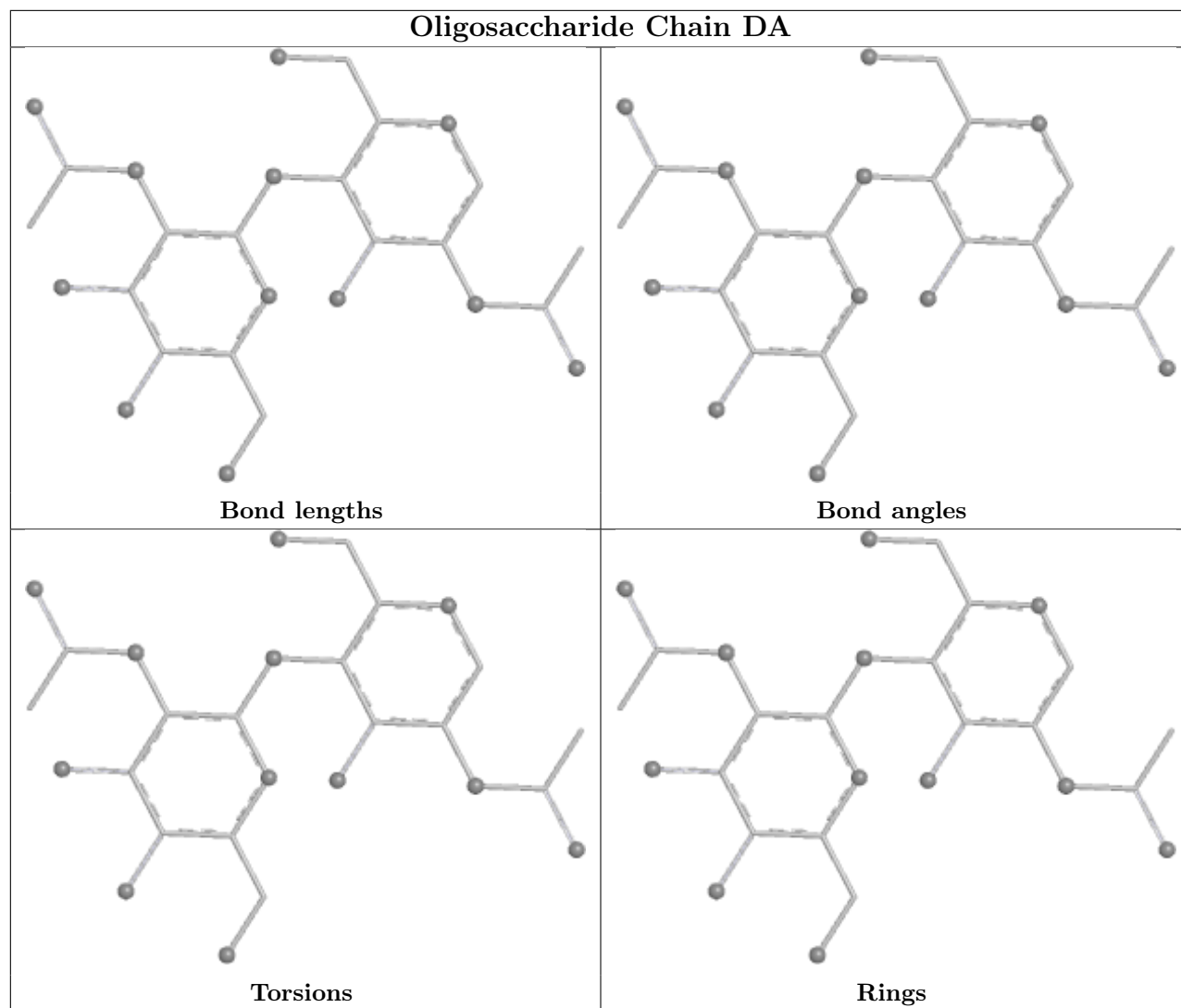


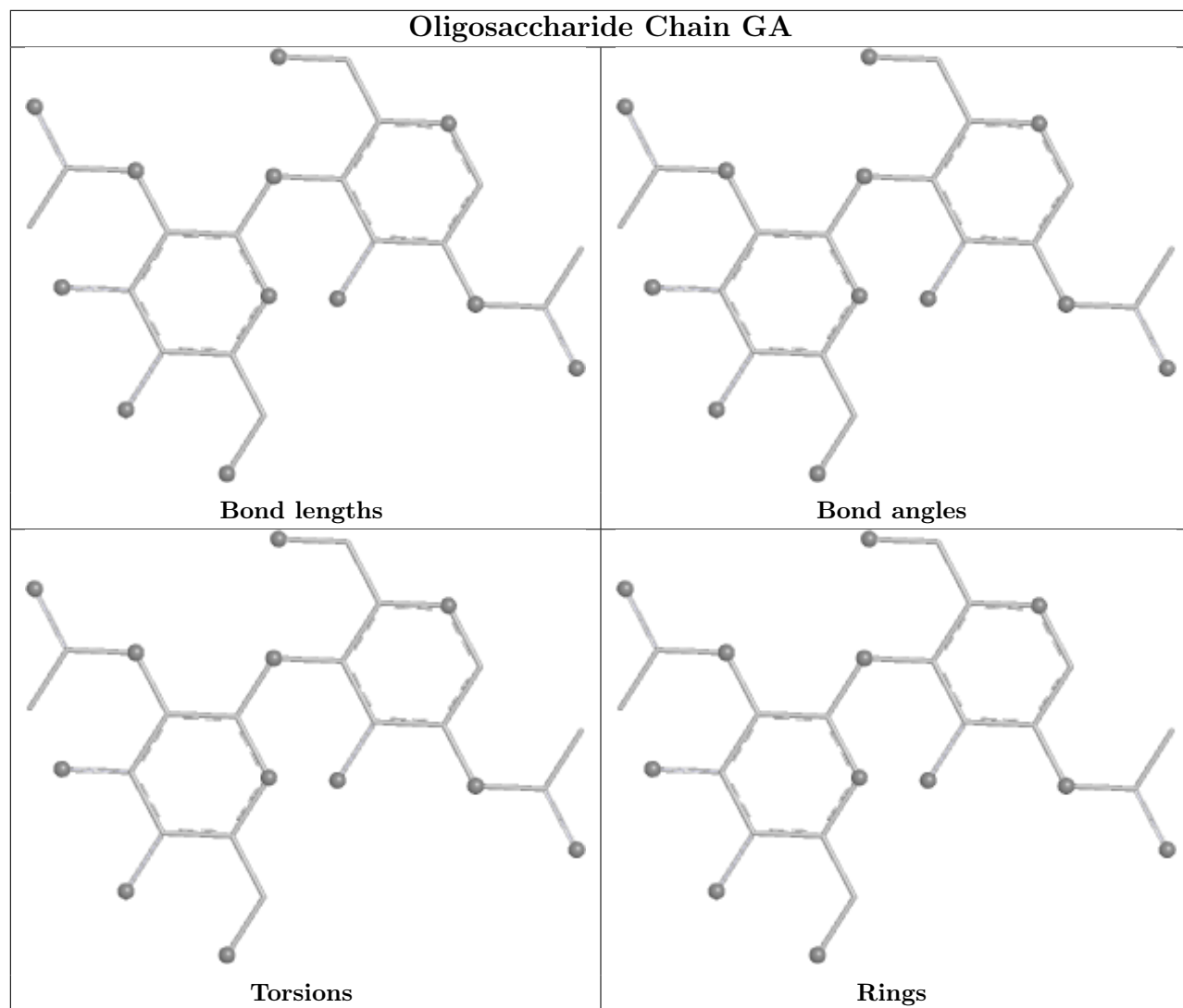


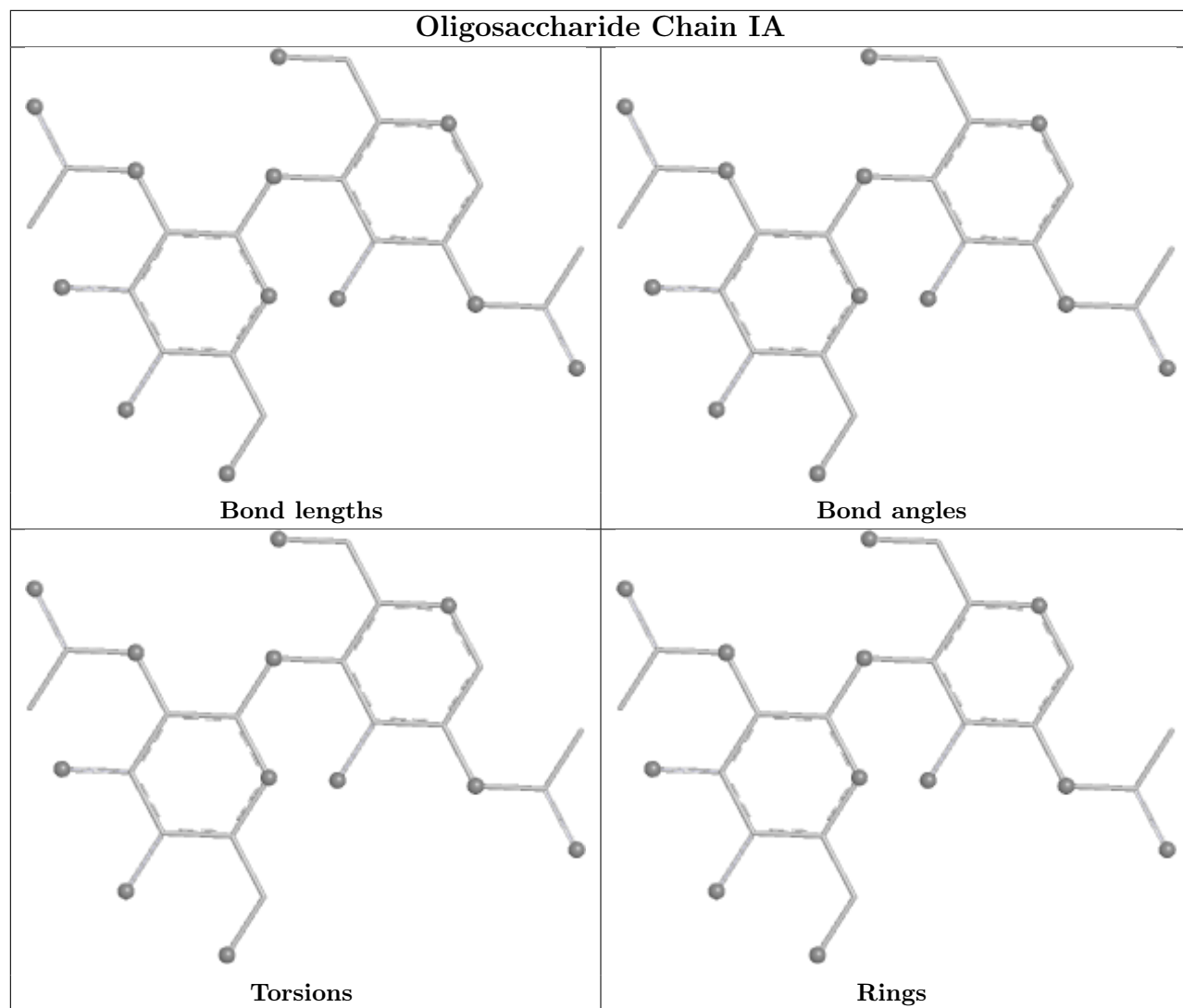


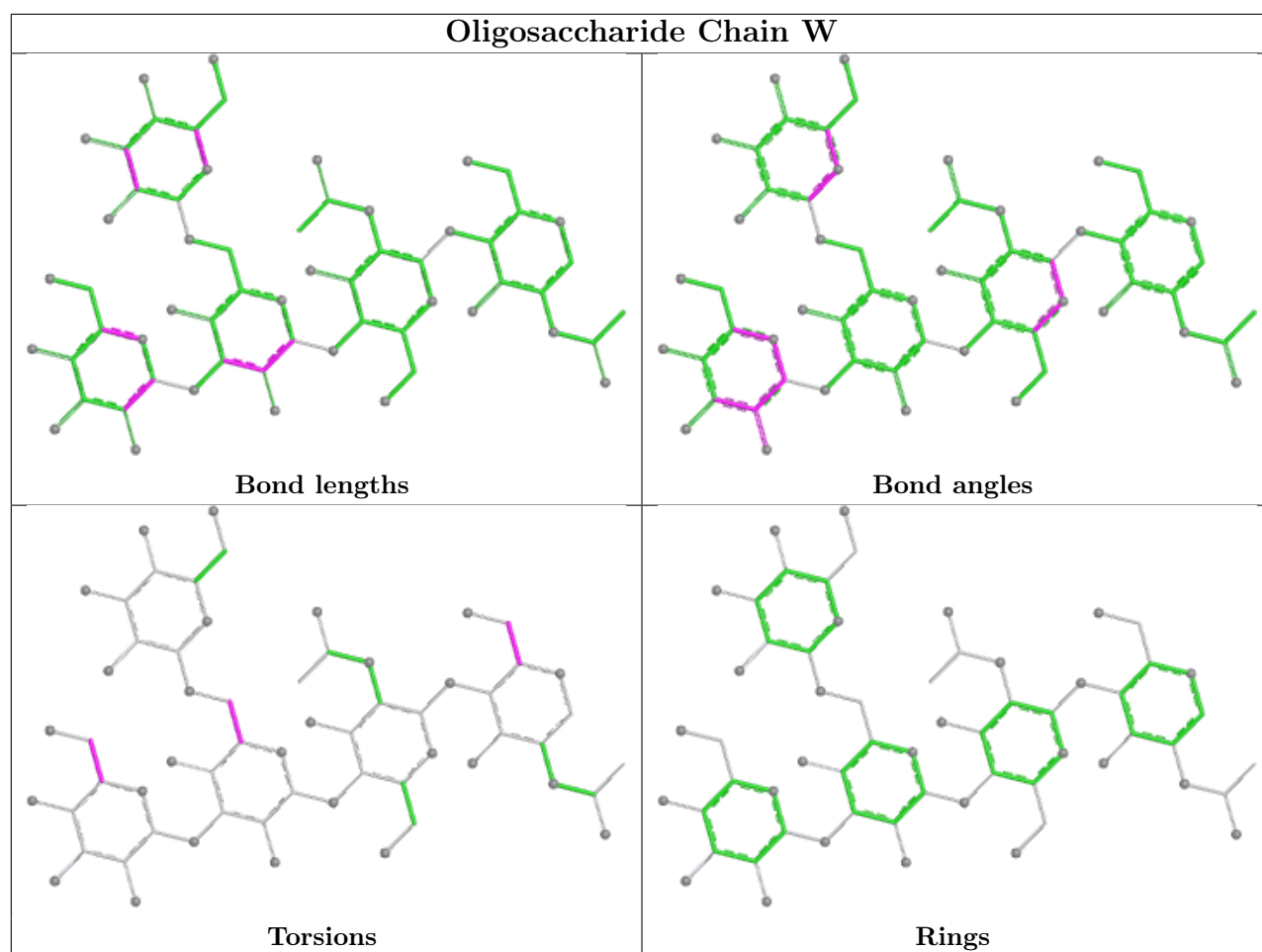


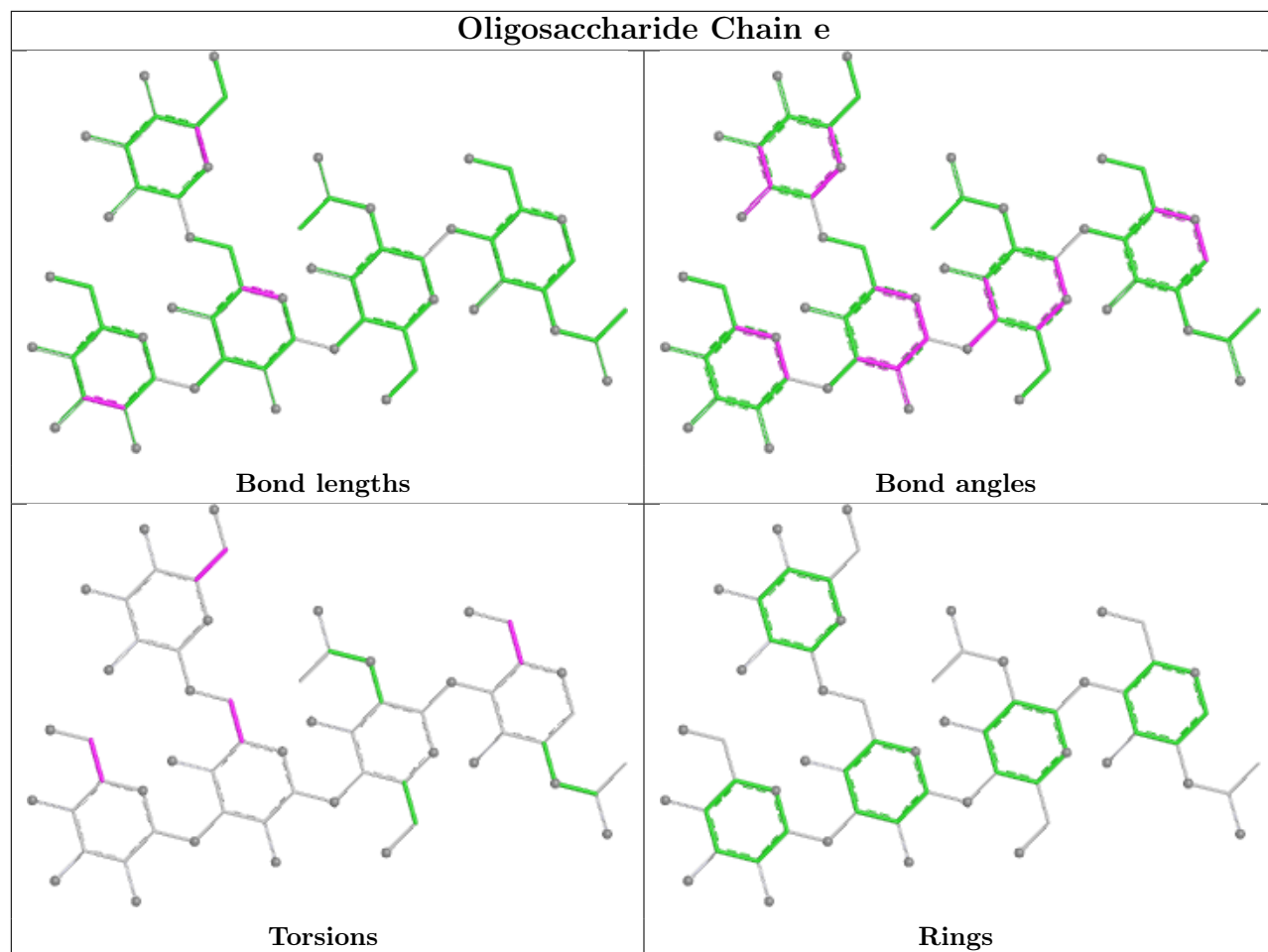


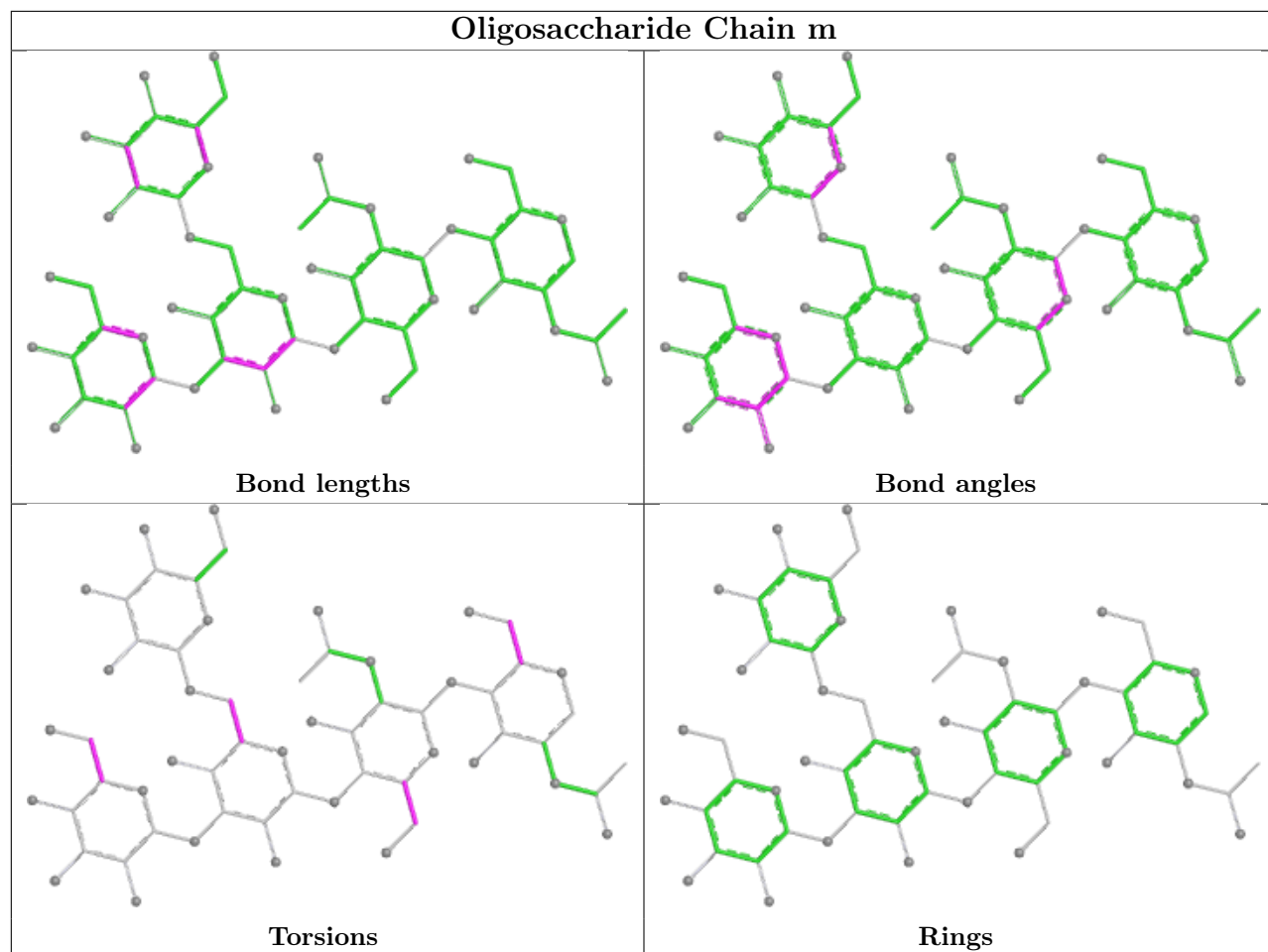


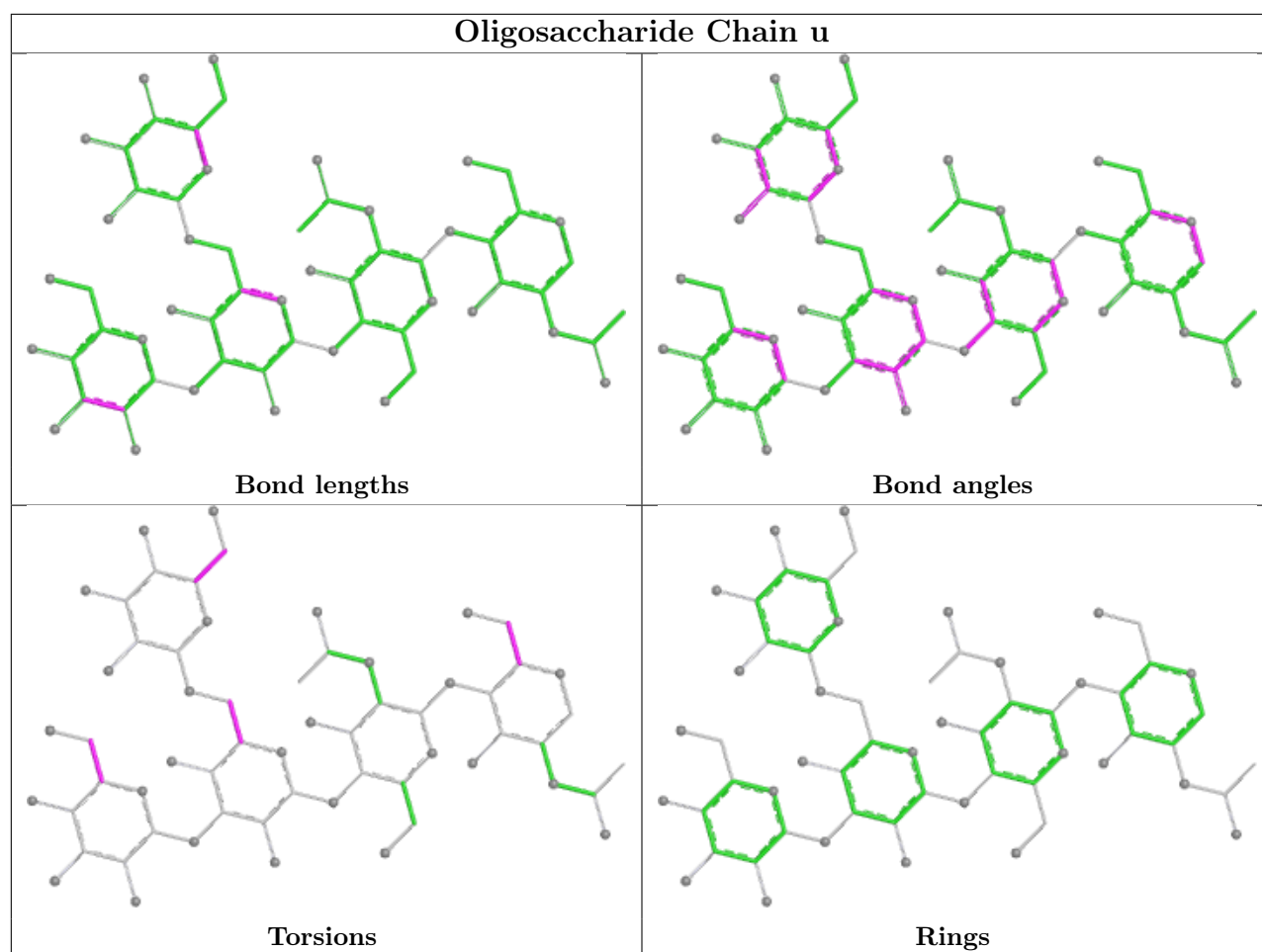


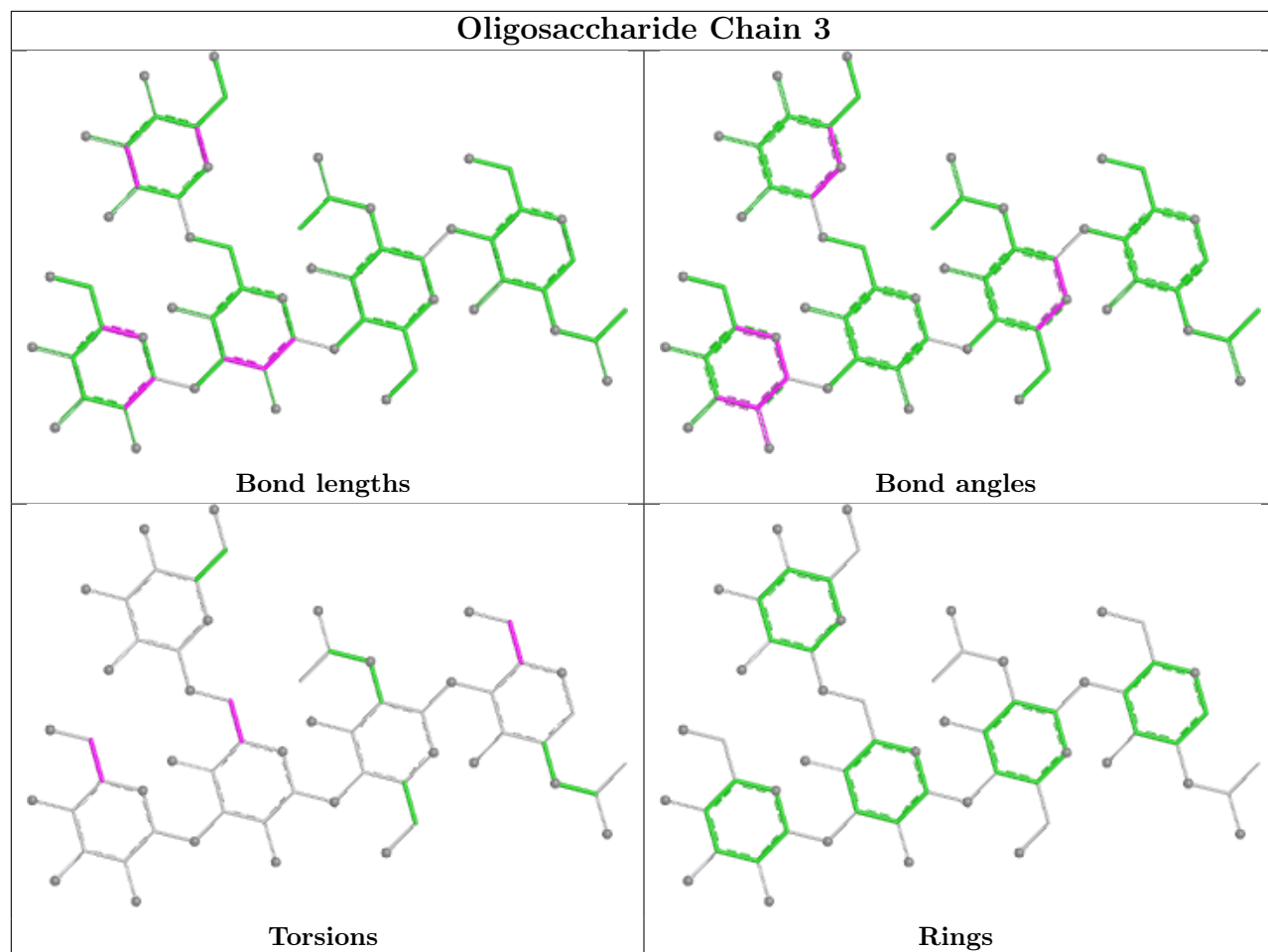




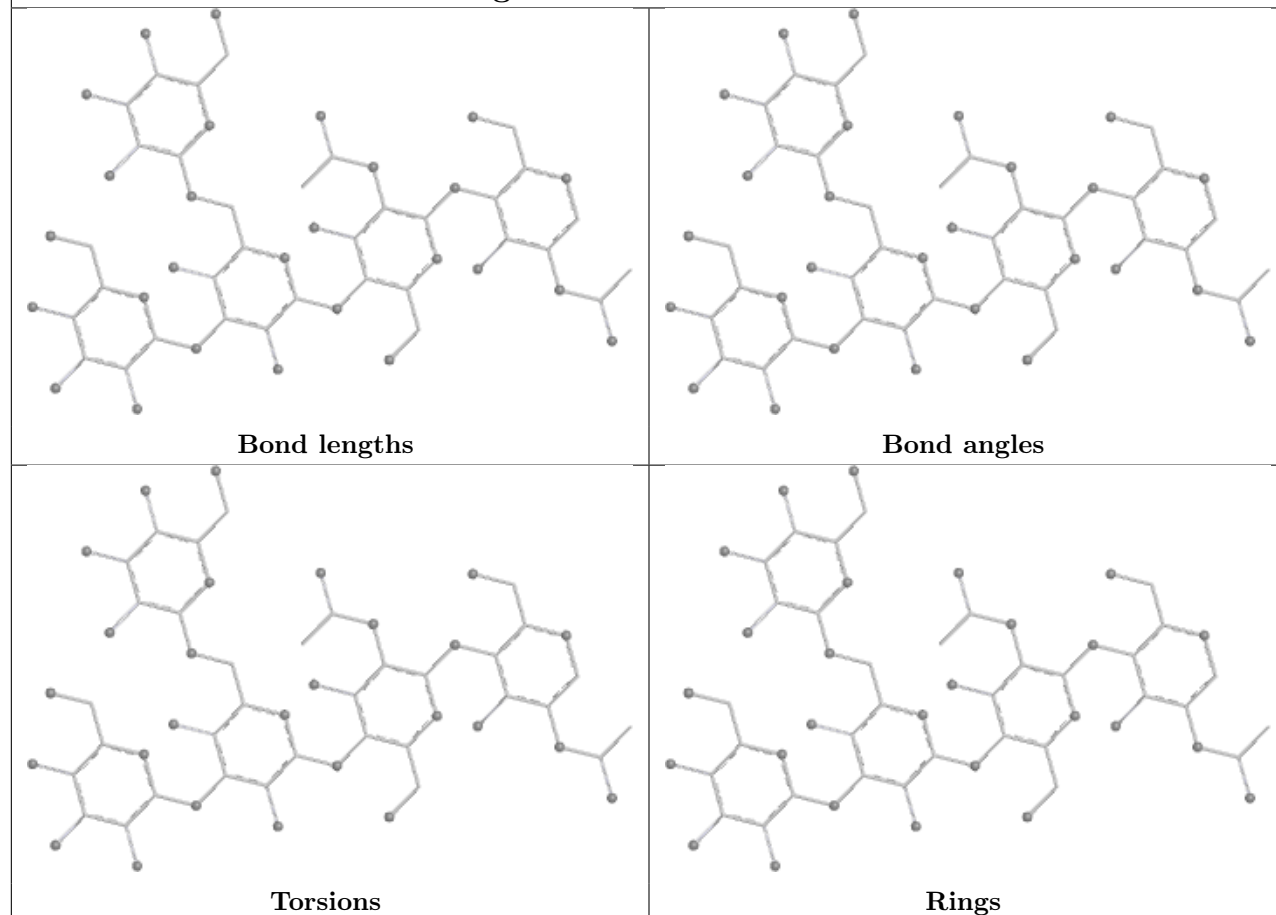




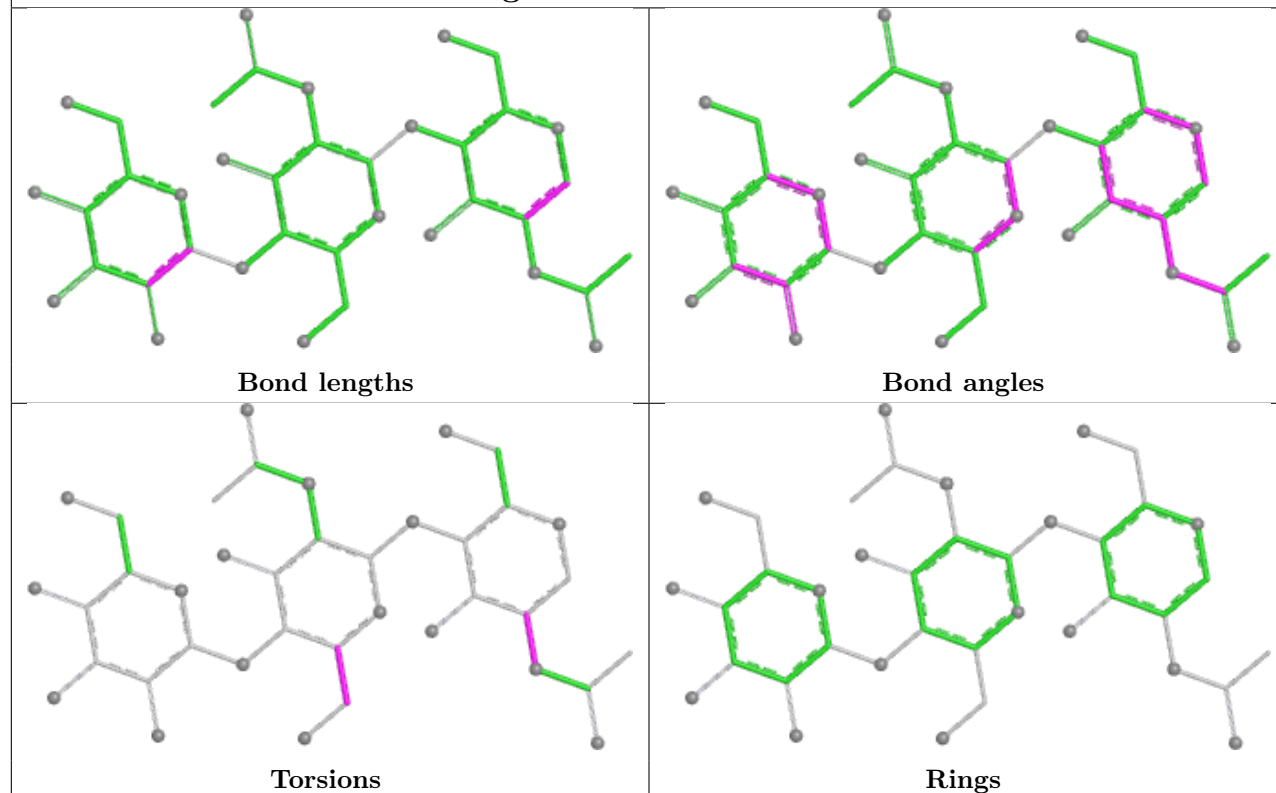


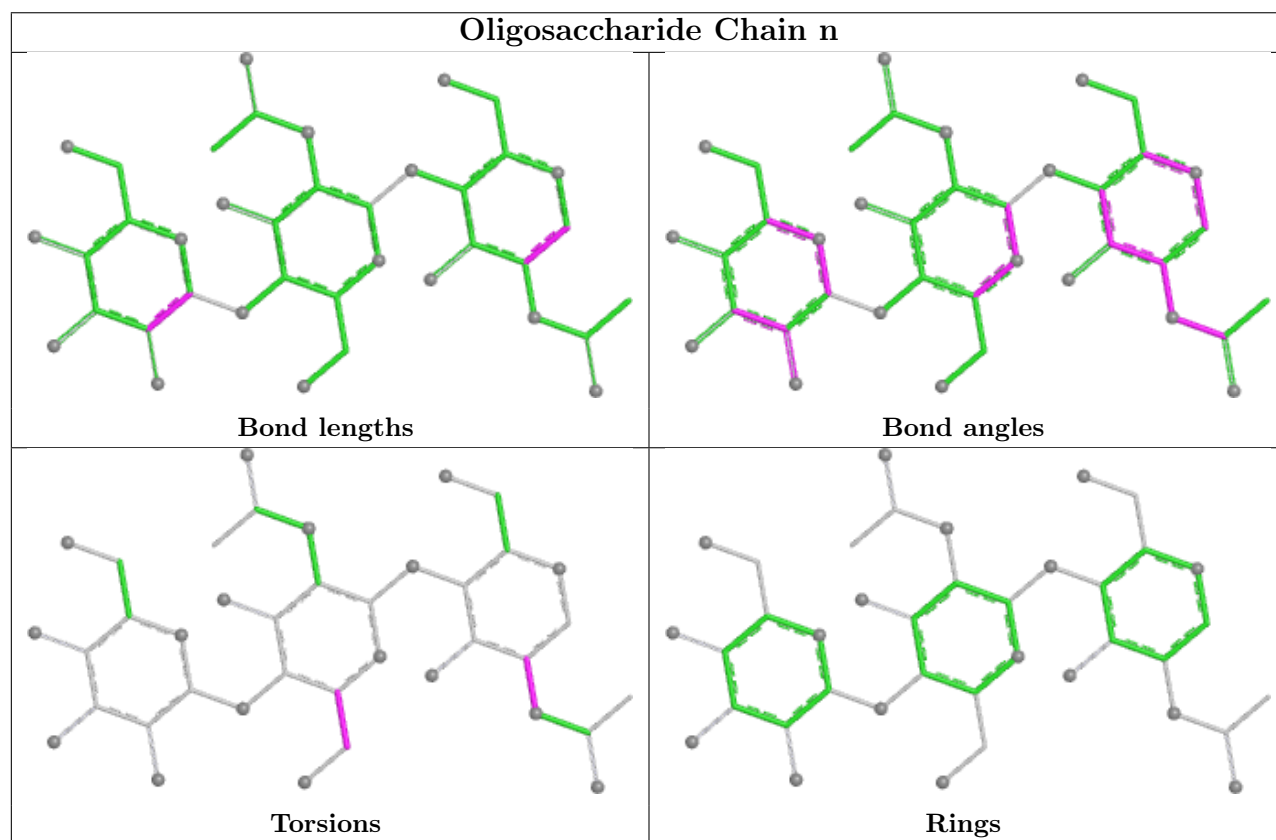
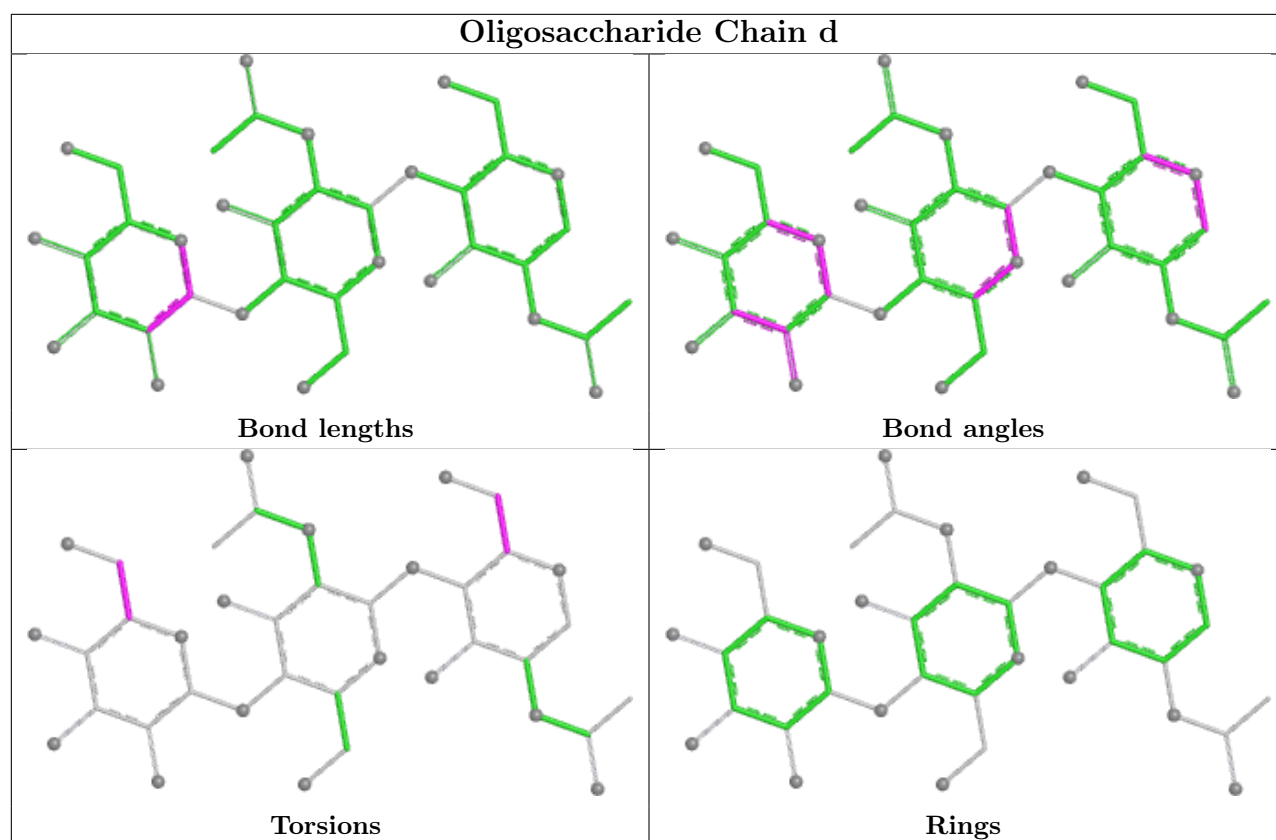


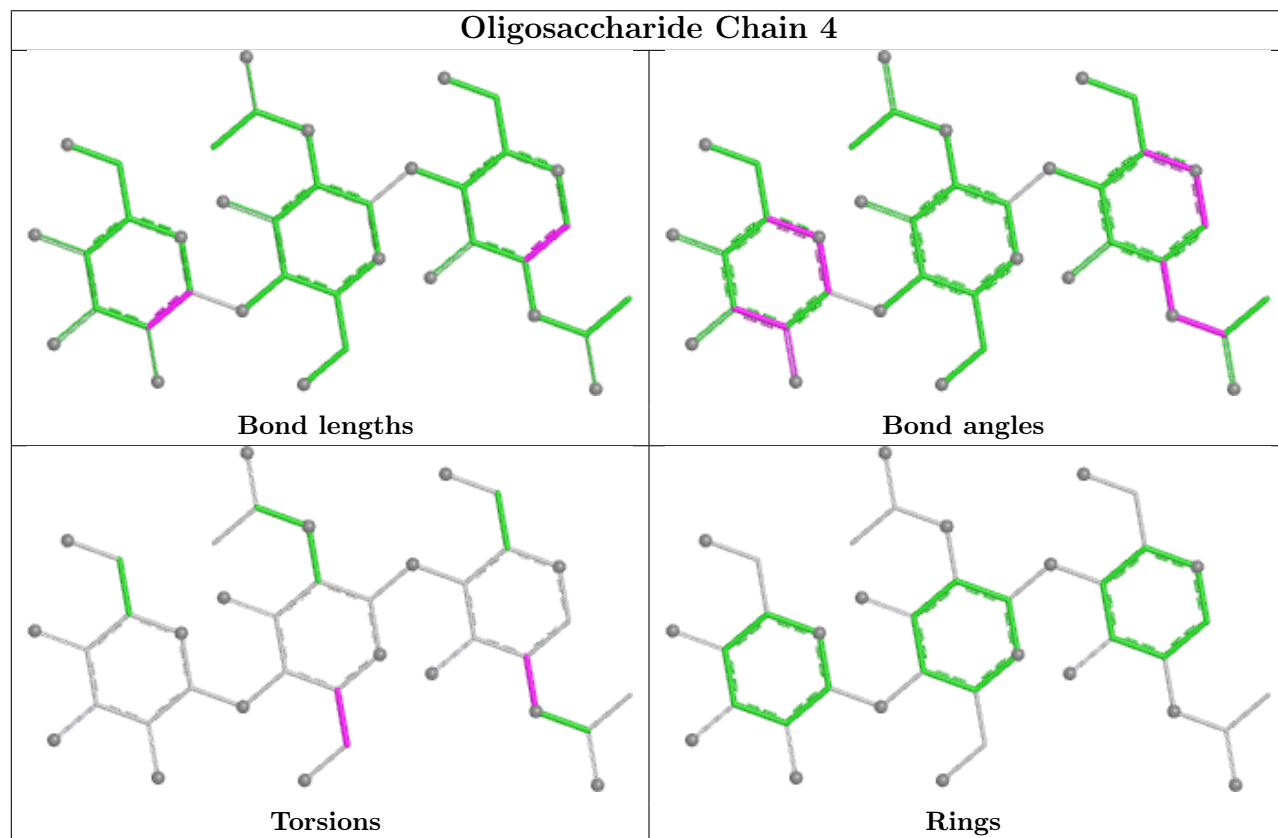
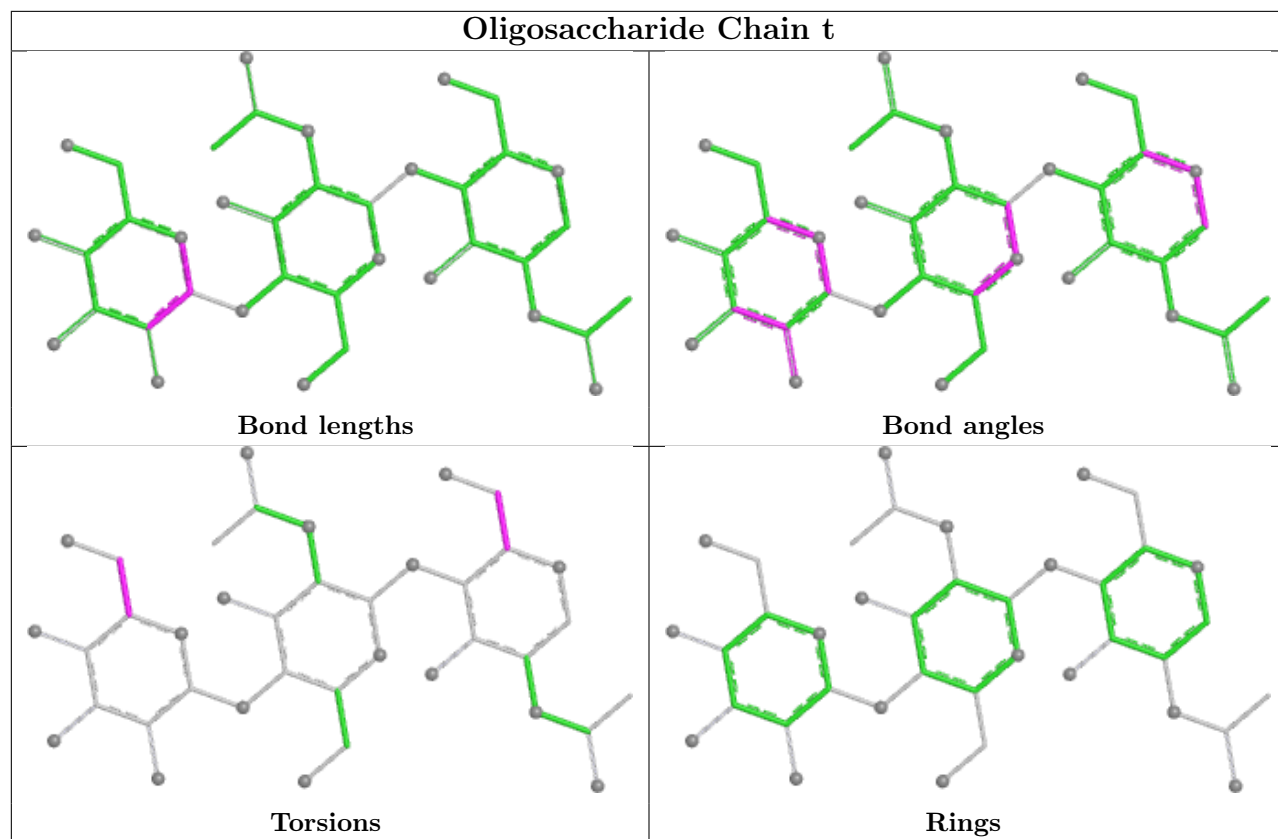
## Oligosaccharide Chain FA

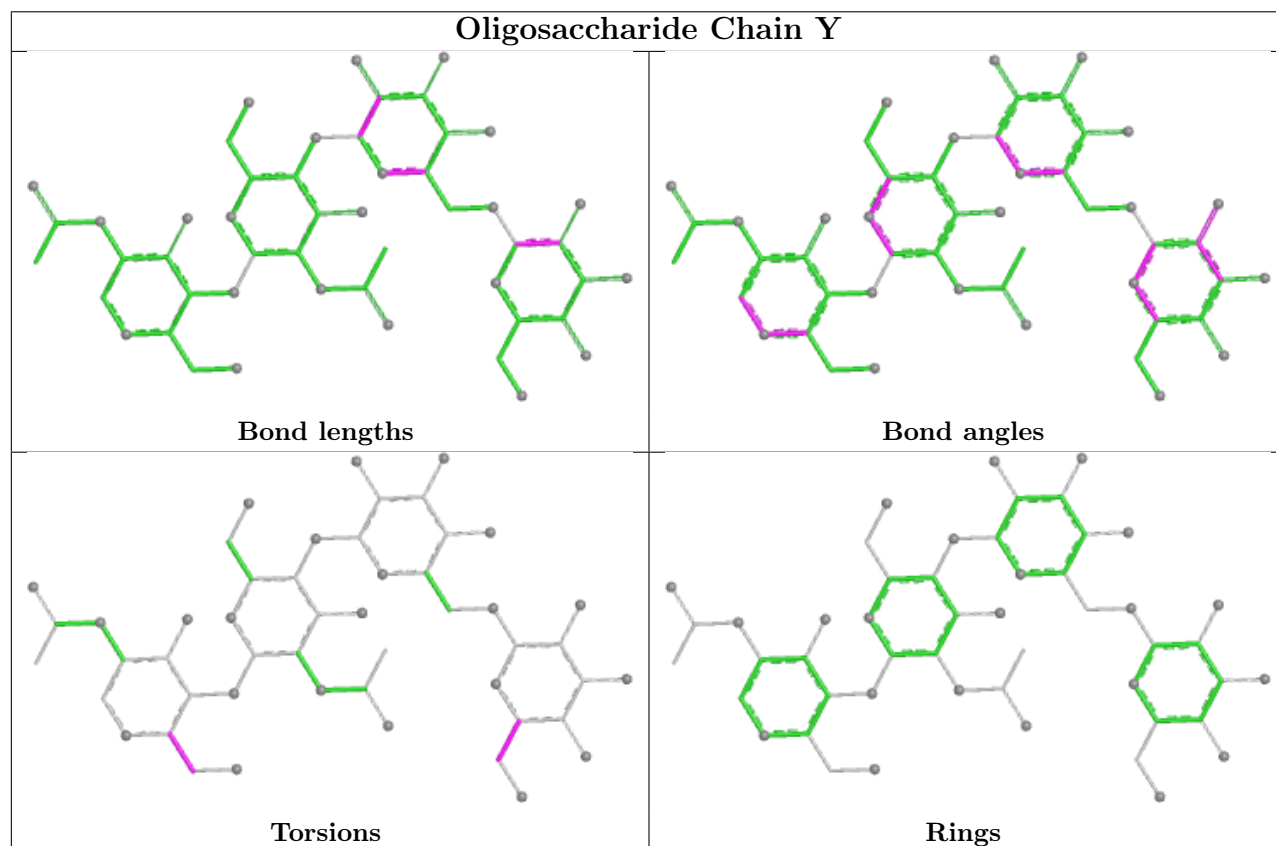
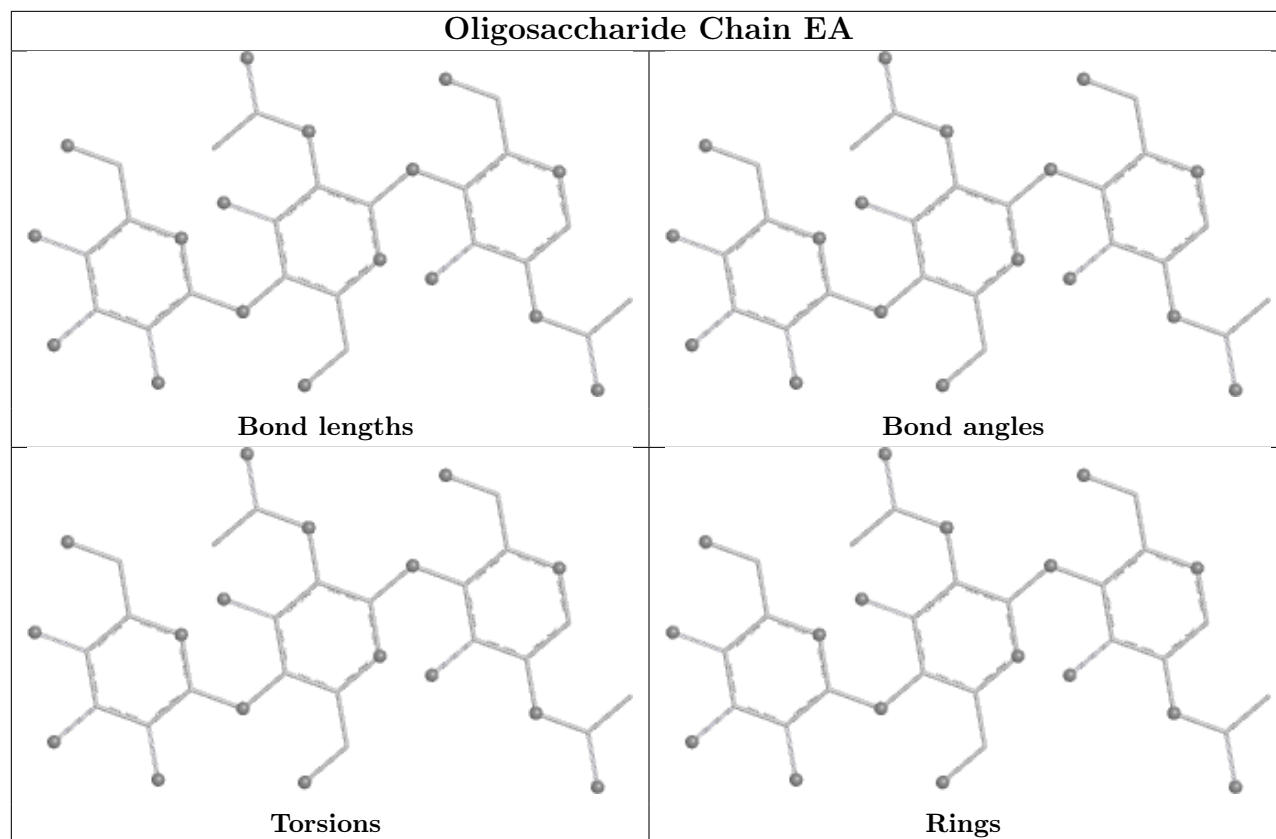


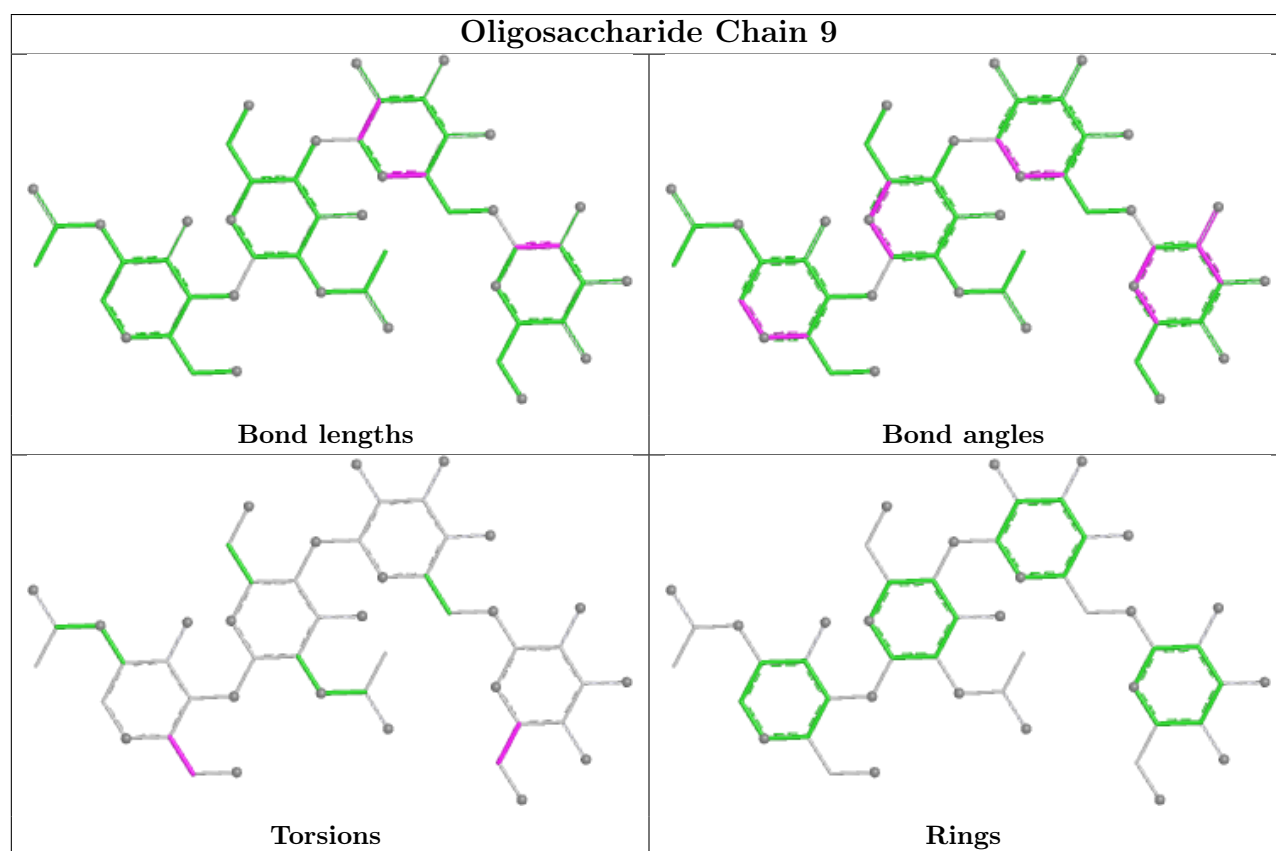
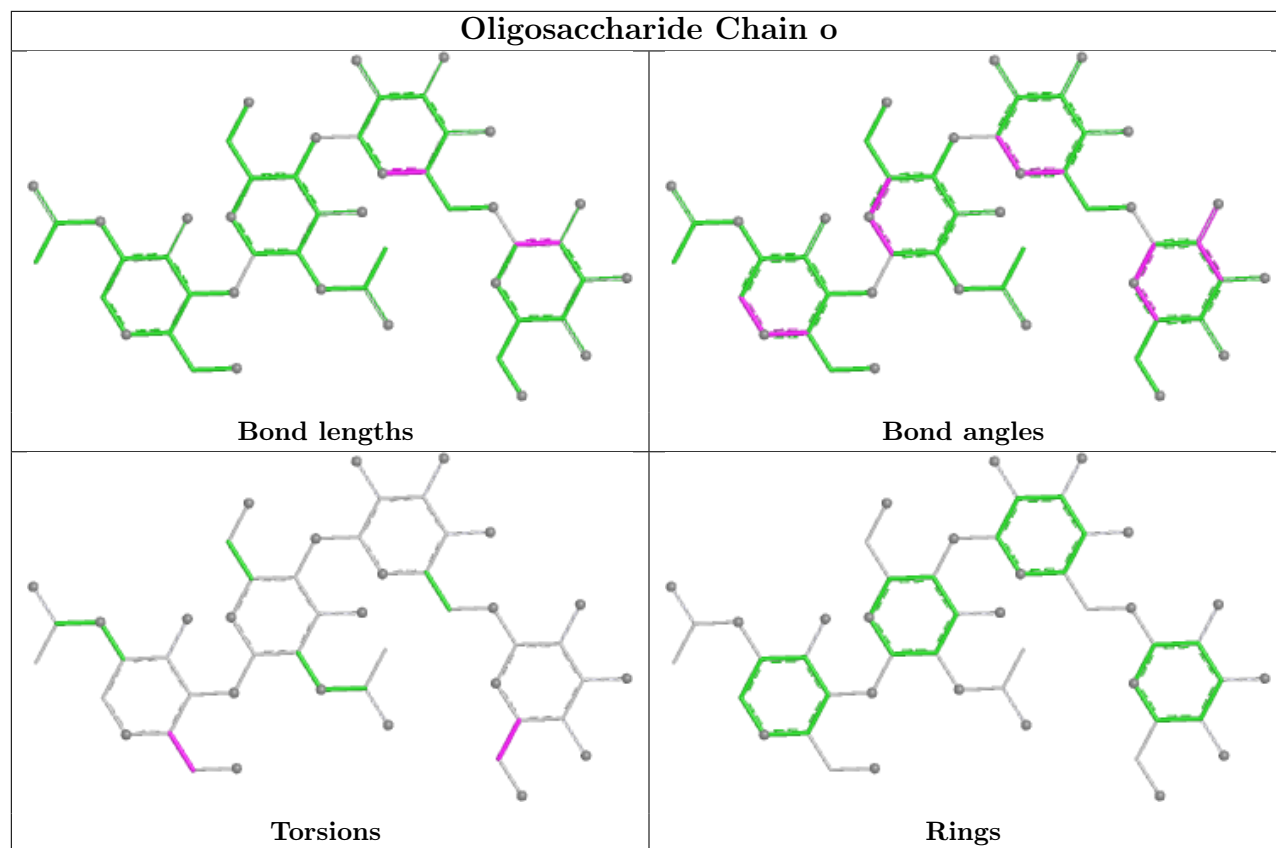
## Oligosaccharide Chain X

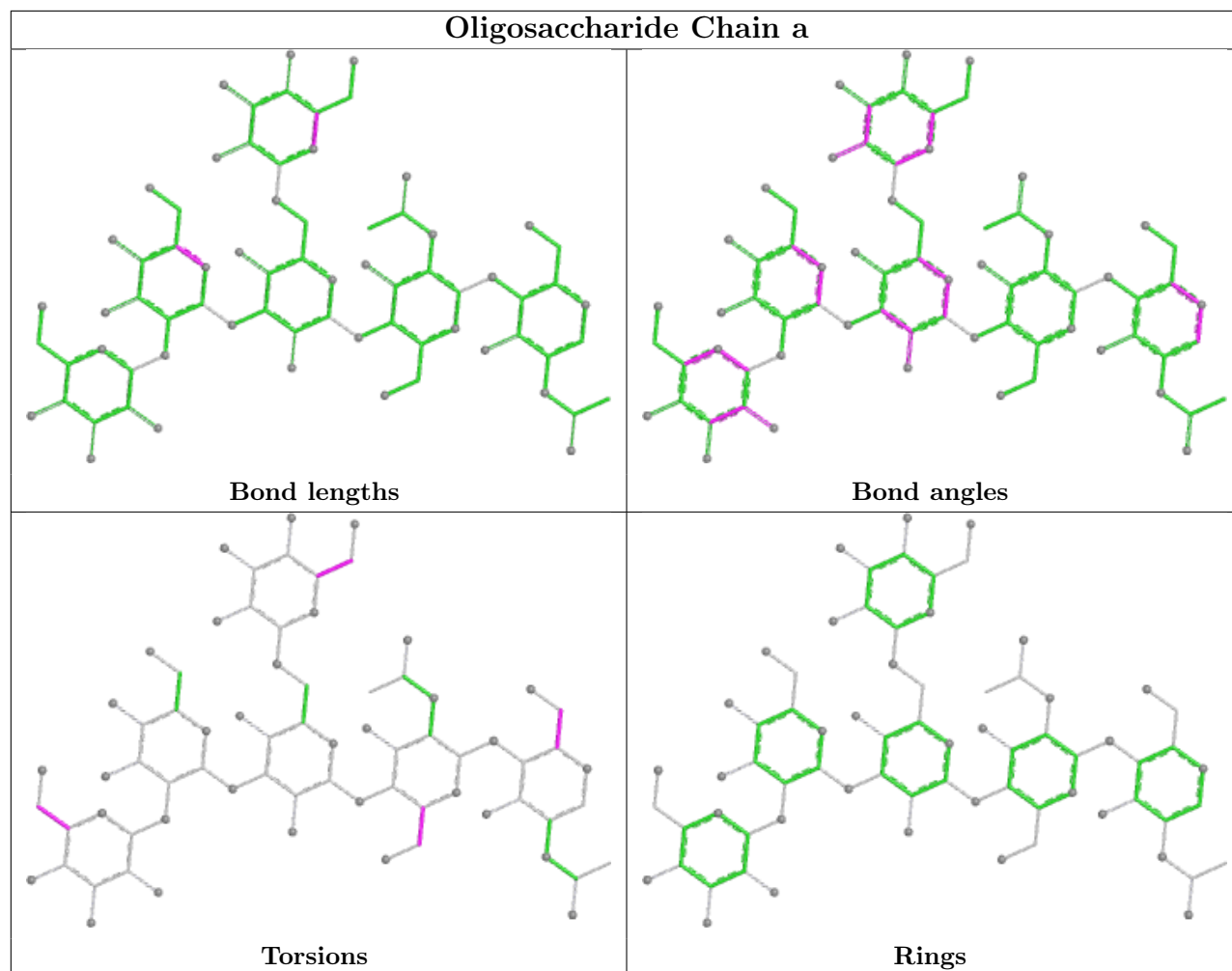


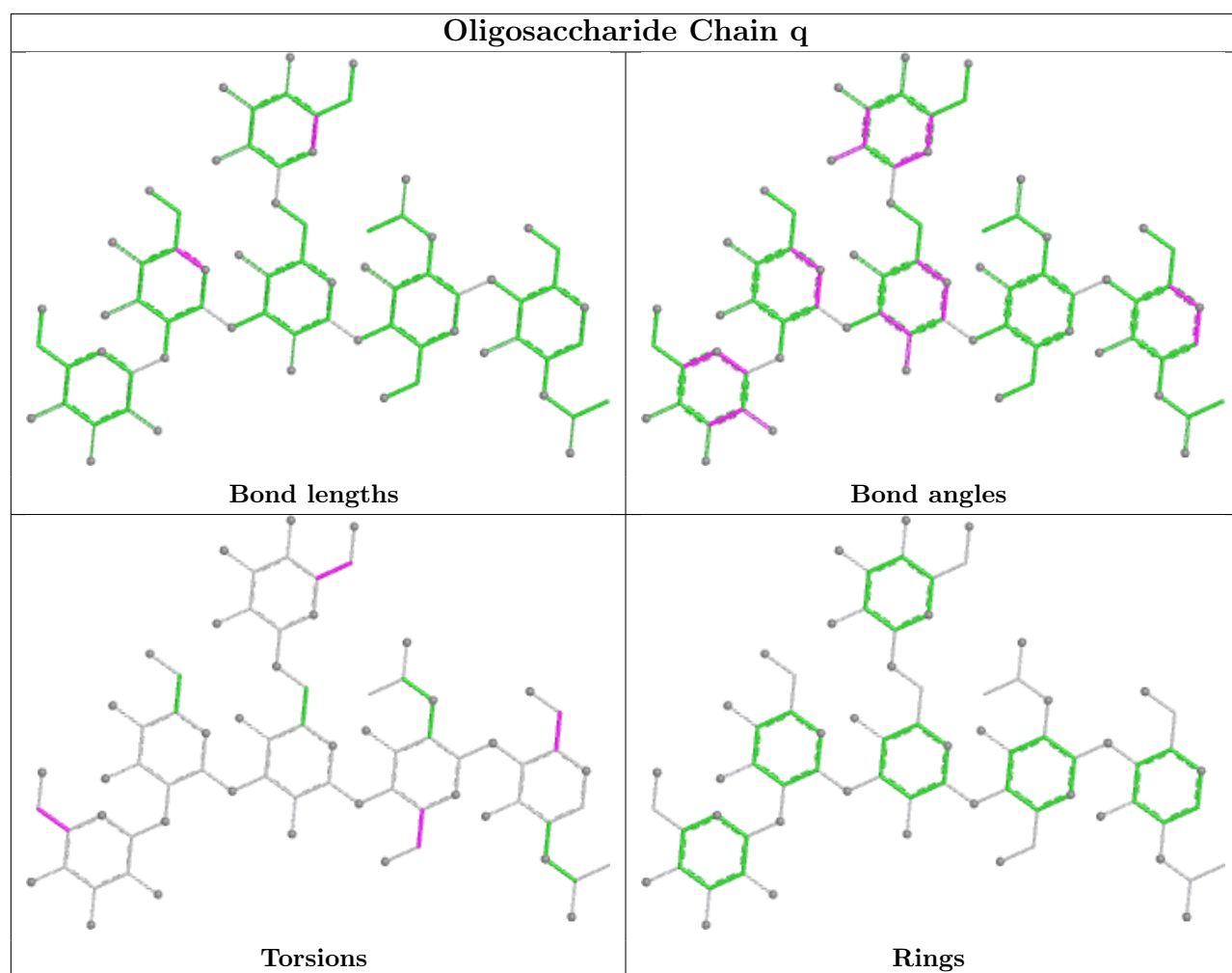


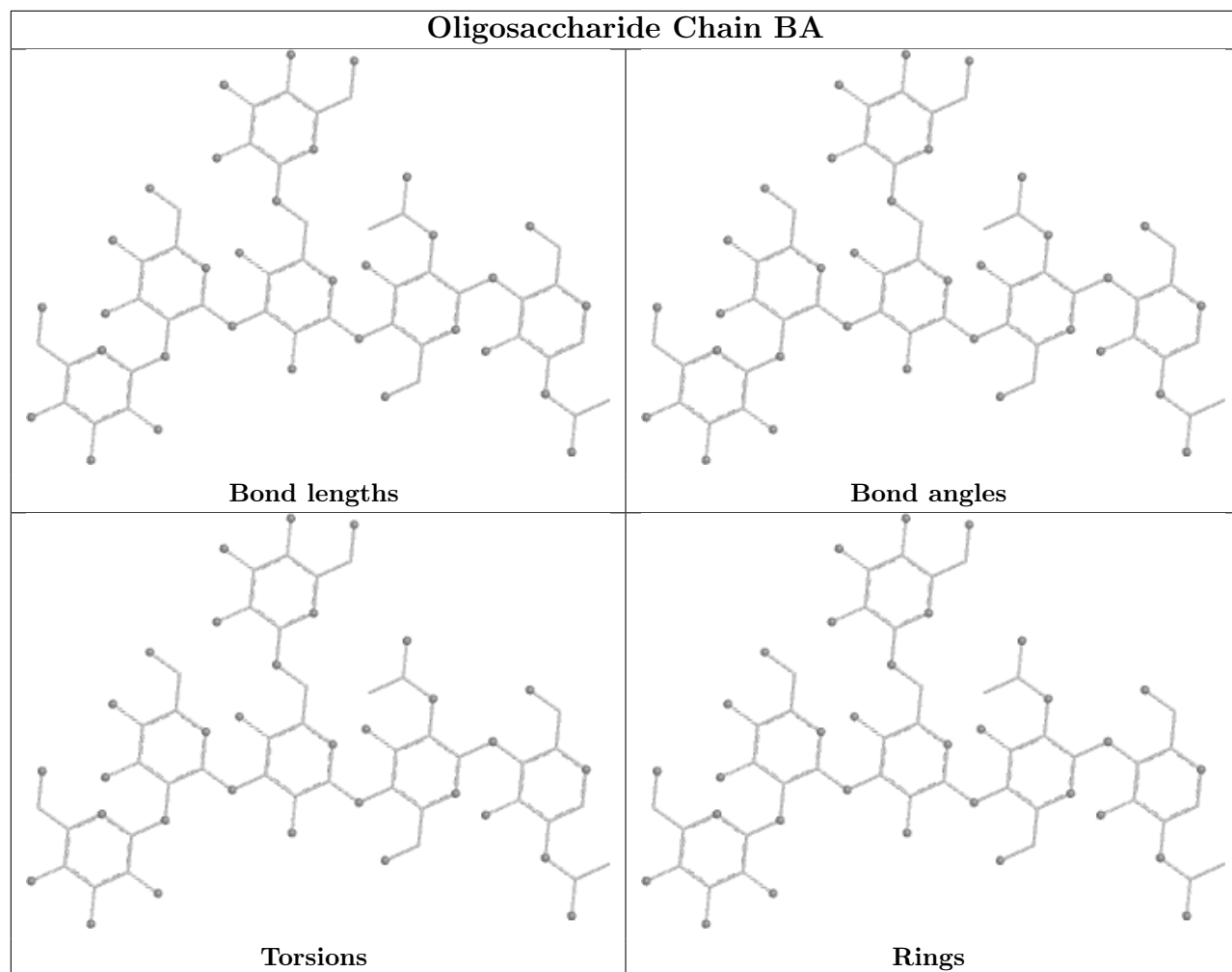


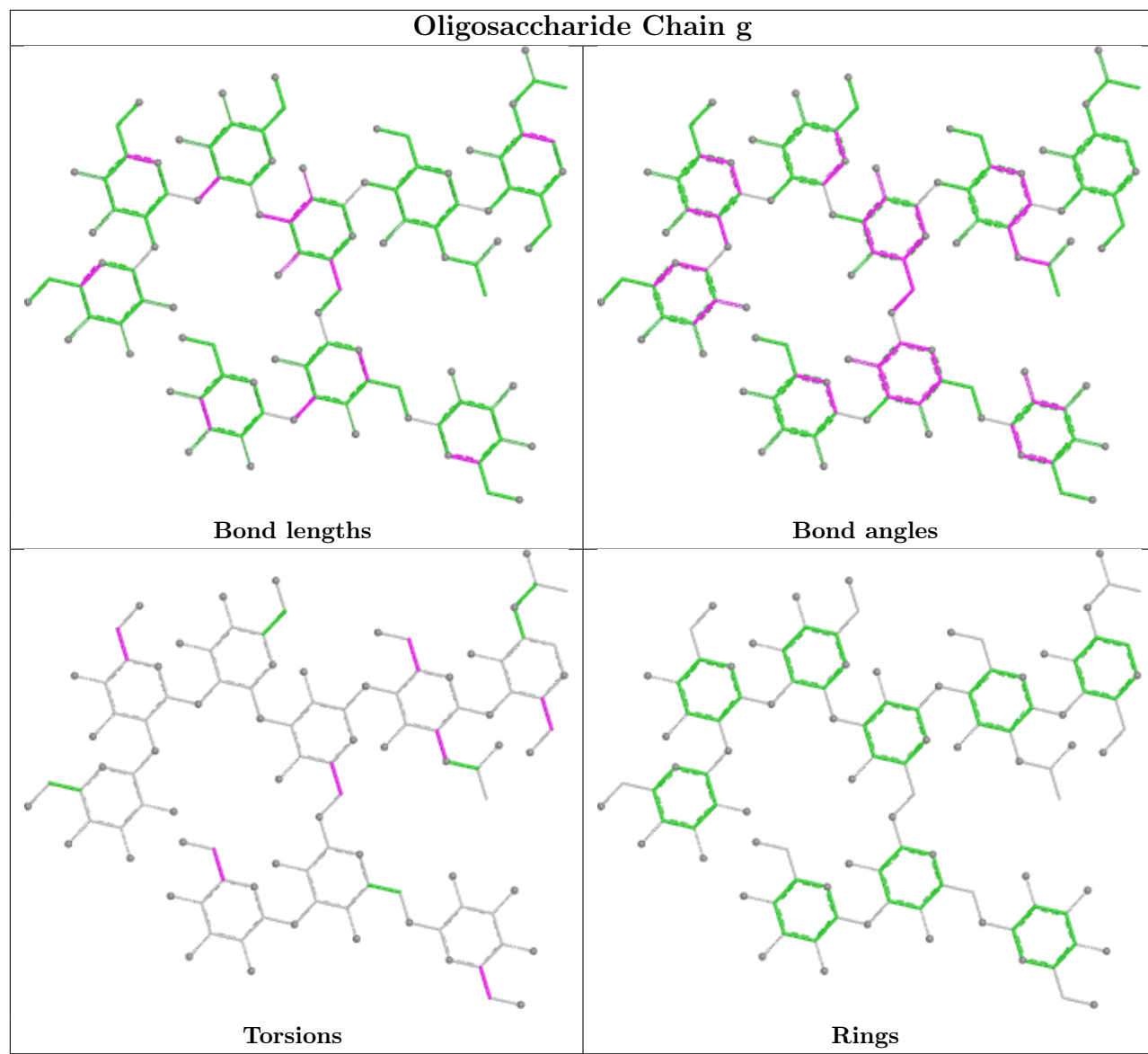


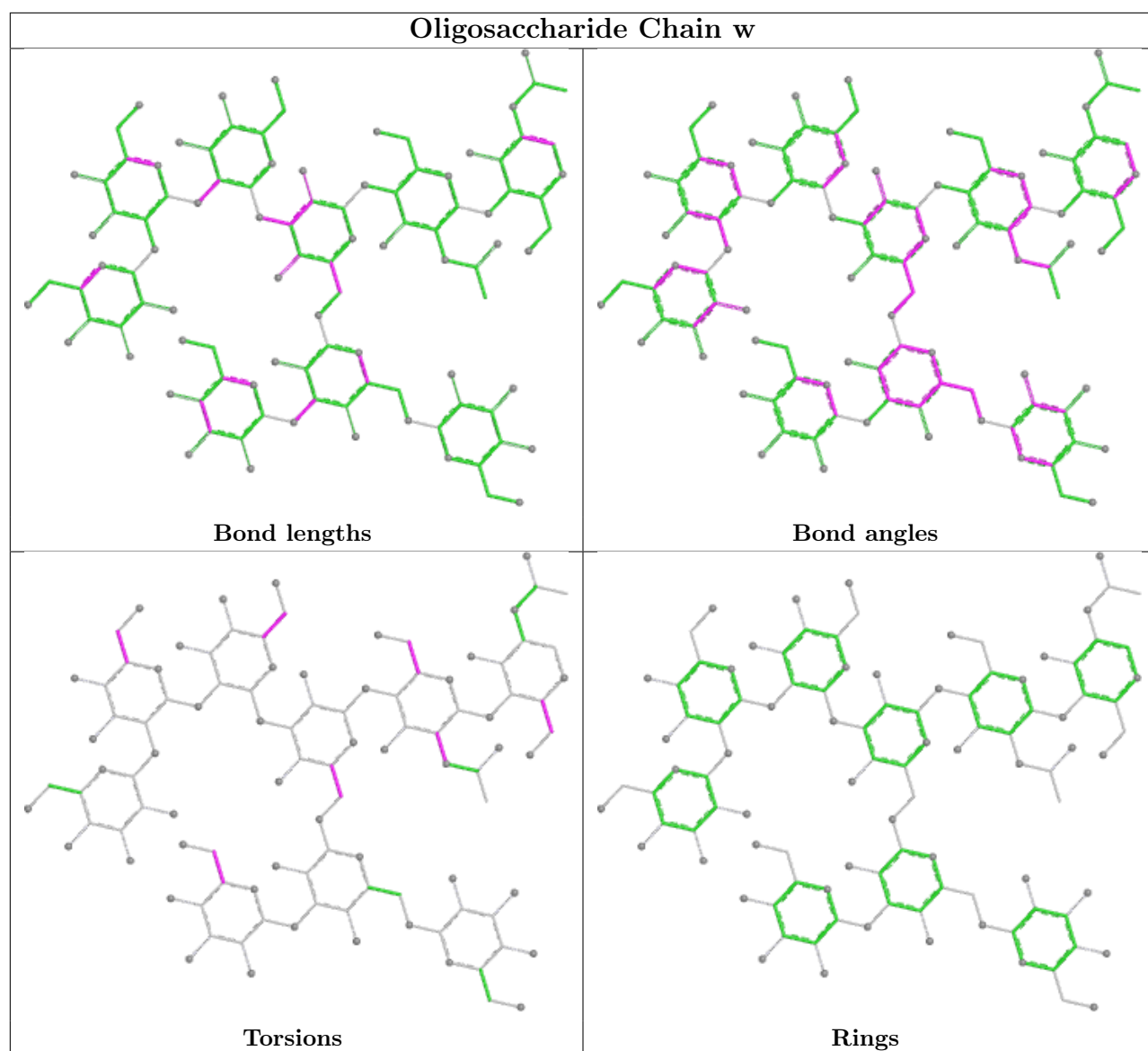


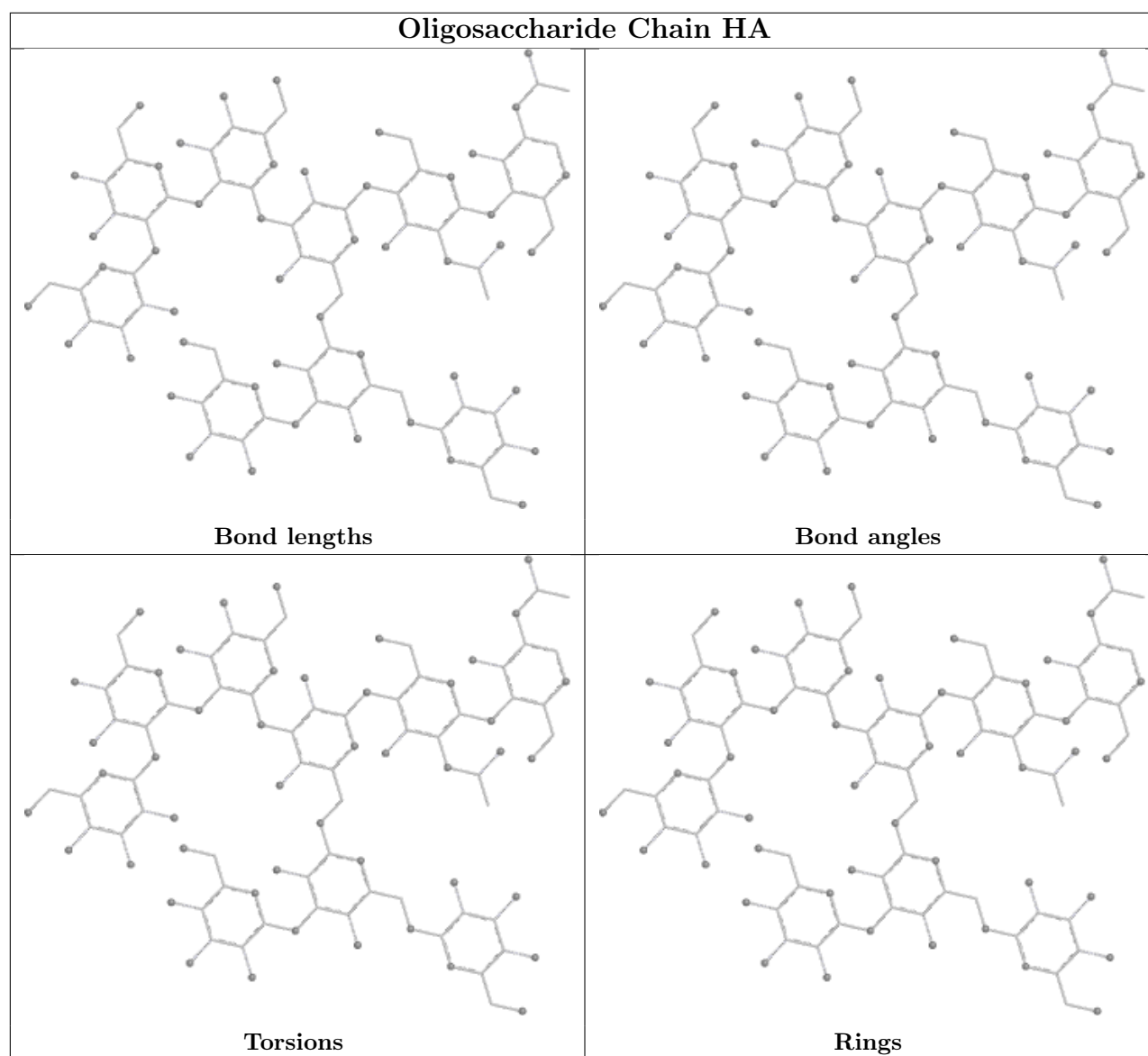




**Oligosaccharide Chain BA**







## 5.6 Ligand geometry [i](#)

9 ligands are modelled in this entry.

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

| Mol | Type | Chain | Res | Link | Bond lengths |      |             | Bond angles |      |             |
|-----|------|-------|-----|------|--------------|------|-------------|-------------|------|-------------|
|     |      |       |     |      | Counts       | RMSZ | $\# Z  > 2$ | Counts      | RMSZ | $\# Z  > 2$ |
| 16  | NAG  | G     | 701 | 6    | 14,14,15     | 0.85 | 2 (14%)     | 17,19,21    | 0.87 | 1 (5%)      |

| Mol | Type | Chain | Res | Link | Bond lengths |      |          | Bond angles |      |          |
|-----|------|-------|-----|------|--------------|------|----------|-------------|------|----------|
|     |      |       |     |      | Counts       | RMSZ | # Z  > 2 | Counts      | RMSZ | # Z  > 2 |
| 16  | NAG  | B     | 635 | 1    | 14,14,15     | 0.78 | 1 (7%)   | 17,19,21    | 0.86 | 1 (5%)   |
| 16  | NAG  | 2     | 635 | 1    | 14,14,15     | 0.76 | 1 (7%)   | 17,19,21    | 0.86 | 1 (5%)   |
| 16  | NAG  | G     | 702 | 6    | 14,14,15     | 0.57 | 0        | 17,19,21    | 0.99 | 1 (5%)   |
| 16  | NAG  | A     | 702 | 6    | 14,14,15     | 0.54 | 0        | 17,19,21    | 0.98 | 1 (5%)   |
| 16  | NAG  | Q     | 701 | 6    | 14,14,15     | 0.79 | 1 (7%)   | 17,19,21    | 0.85 | 1 (5%)   |
| 16  | NAG  | K     | 635 | 1    | 14,14,15     | 0.76 | 1 (7%)   | 17,19,21    | 0.90 | 1 (5%)   |
| 16  | NAG  | A     | 701 | 6    | 14,14,15     | 0.82 | 1 (7%)   | 17,19,21    | 0.87 | 1 (5%)   |
| 16  | NAG  | Q     | 702 | 6    | 14,14,15     | 0.56 | 0        | 17,19,21    | 0.97 | 1 (5%)   |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions  | Rings   |
|-----|------|-------|-----|------|---------|-----------|---------|
| 16  | NAG  | G     | 701 | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 16  | NAG  | B     | 635 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 16  | NAG  | 2     | 635 | 1    | -       | 0/6/23/26 | 0/1/1/1 |
| 16  | NAG  | G     | 702 | 6    | -       | 3/6/23/26 | 0/1/1/1 |
| 16  | NAG  | A     | 702 | 6    | -       | 3/6/23/26 | 0/1/1/1 |
| 16  | NAG  | Q     | 701 | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 16  | NAG  | K     | 635 | 1    | -       | 1/6/23/26 | 0/1/1/1 |
| 16  | NAG  | A     | 701 | 6    | -       | 2/6/23/26 | 0/1/1/1 |
| 16  | NAG  | Q     | 702 | 6    | -       | 3/6/23/26 | 0/1/1/1 |

All (7) bond length outliers are listed below:

| Mol | Chain | Res | Type | Atoms | Z    | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 16  | B     | 635 | NAG  | O5-C1 | 2.66 | 1.48        | 1.43     |
| 16  | K     | 635 | NAG  | O5-C1 | 2.59 | 1.48        | 1.43     |
| 16  | 2     | 635 | NAG  | O5-C1 | 2.58 | 1.48        | 1.43     |
| 16  | G     | 701 | NAG  | O5-C1 | 2.09 | 1.47        | 1.43     |
| 16  | G     | 701 | NAG  | C1-C2 | 2.06 | 1.55        | 1.52     |
| 16  | A     | 701 | NAG  | O5-C1 | 2.03 | 1.47        | 1.43     |
| 16  | Q     | 701 | NAG  | O5-C1 | 2.03 | 1.47        | 1.43     |

All (9) bond angle outliers are listed below:

| Mol | Chain | Res | Type | Atoms    | Z    | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 16  | G     | 702 | NAG  | C1-O5-C5 | 3.75 | 117.22      | 112.19   |
| 16  | A     | 702 | NAG  | C1-O5-C5 | 3.66 | 117.08      | 112.19   |
| 16  | Q     | 702 | NAG  | C1-O5-C5 | 3.63 | 117.06      | 112.19   |
| 16  | K     | 635 | NAG  | C1-O5-C5 | 3.42 | 116.78      | 112.19   |
| 16  | 2     | 635 | NAG  | C1-O5-C5 | 3.21 | 116.49      | 112.19   |
| 16  | B     | 635 | NAG  | C1-O5-C5 | 3.20 | 116.47      | 112.19   |
| 16  | G     | 701 | NAG  | C1-O5-C5 | 2.86 | 116.02      | 112.19   |
| 16  | A     | 701 | NAG  | C1-O5-C5 | 2.83 | 115.97      | 112.19   |
| 16  | Q     | 701 | NAG  | C1-O5-C5 | 2.79 | 115.93      | 112.19   |

There are no chirality outliers.

All (17) torsion outliers are listed below:

| Mol | Chain | Res | Type | Atoms       |
|-----|-------|-----|------|-------------|
| 16  | G     | 702 | NAG  | O5-C5-C6-O6 |
| 16  | A     | 702 | NAG  | O5-C5-C6-O6 |
| 16  | Q     | 702 | NAG  | O5-C5-C6-O6 |
| 16  | A     | 702 | NAG  | C4-C5-C6-O6 |
| 16  | Q     | 702 | NAG  | C4-C5-C6-O6 |
| 16  | G     | 702 | NAG  | C4-C5-C6-O6 |
| 16  | Q     | 701 | NAG  | O5-C5-C6-O6 |
| 16  | A     | 701 | NAG  | O5-C5-C6-O6 |
| 16  | G     | 701 | NAG  | O5-C5-C6-O6 |
| 16  | Q     | 701 | NAG  | C4-C5-C6-O6 |
| 16  | A     | 701 | NAG  | C4-C5-C6-O6 |
| 16  | G     | 701 | NAG  | C4-C5-C6-O6 |
| 16  | A     | 702 | NAG  | C1-C2-N2-C7 |
| 16  | G     | 702 | NAG  | C1-C2-N2-C7 |
| 16  | Q     | 702 | NAG  | C1-C2-N2-C7 |
| 16  | B     | 635 | NAG  | O5-C5-C6-O6 |
| 16  | K     | 635 | NAG  | O5-C5-C6-O6 |

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

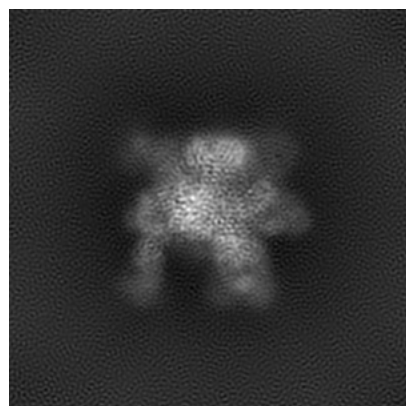
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20189. These allow visual inspection of the internal detail of the map and identification of artifacts.

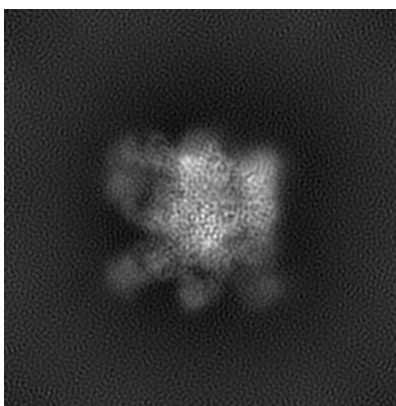
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

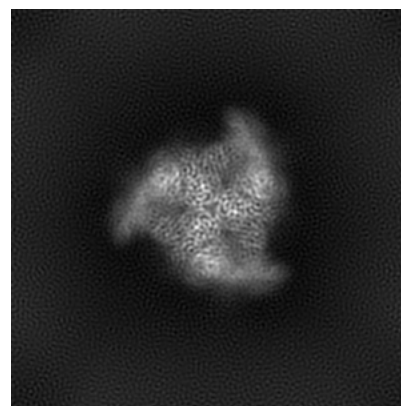
#### 6.1.1 Primary map



X

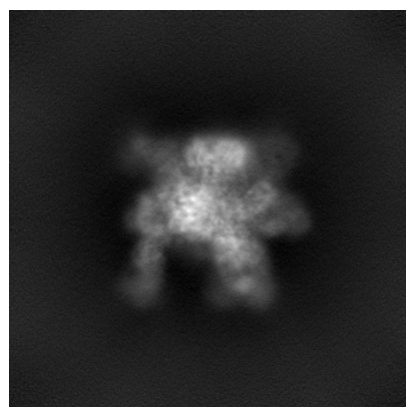


Y

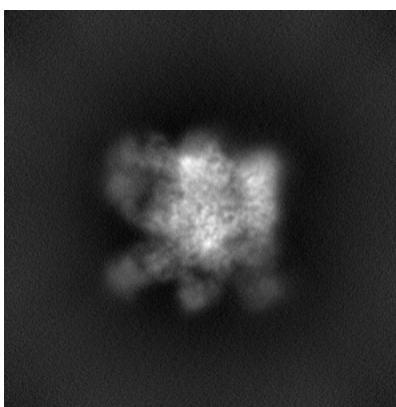


Z

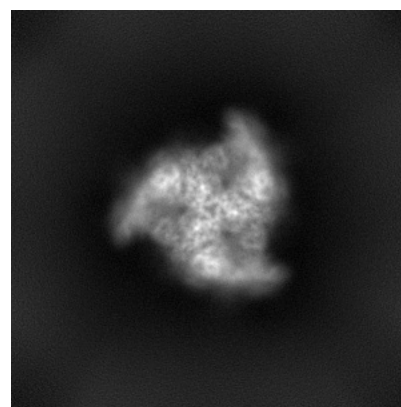
#### 6.1.2 Raw map



X



Y

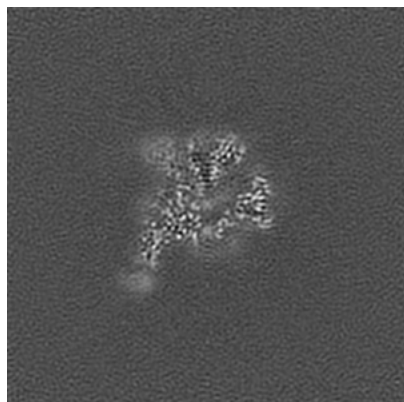


Z

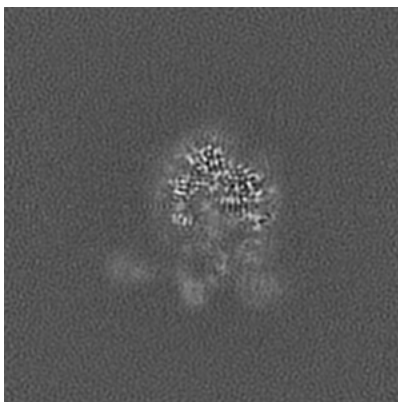
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

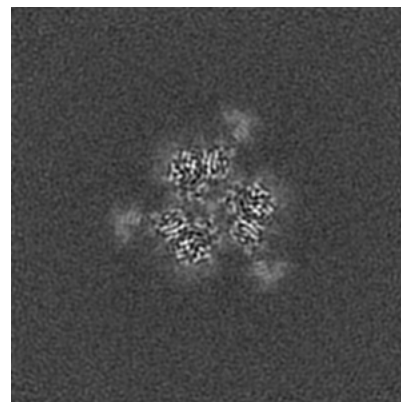
### 6.2.1 Primary map



X Index: 176

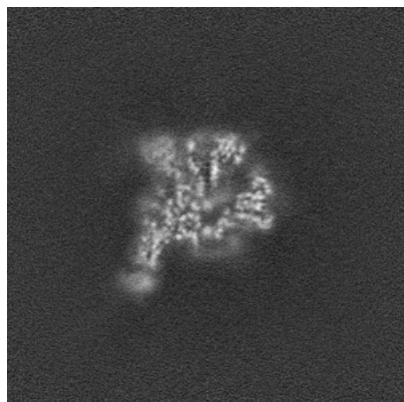


Y Index: 176

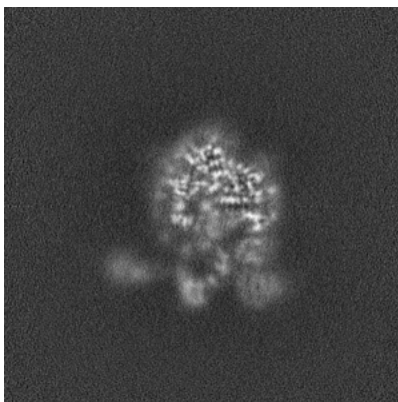


Z Index: 176

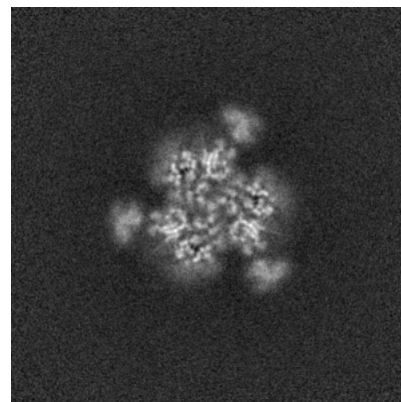
### 6.2.2 Raw map



X Index: 176



Y Index: 176

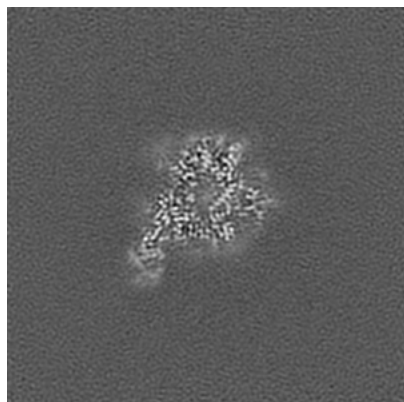


Z Index: 176

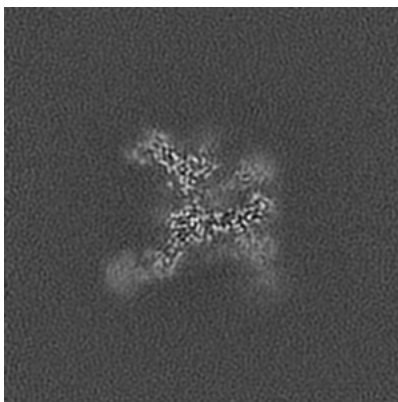
The images above show central slices of the map in three orthogonal directions.

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

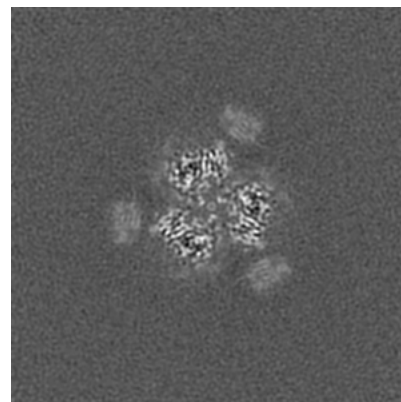
### 6.3.1 Primary map



X Index: 168

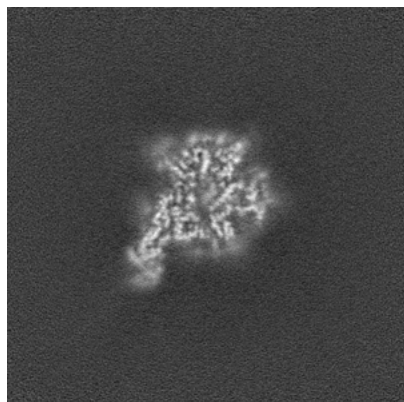


Y Index: 193

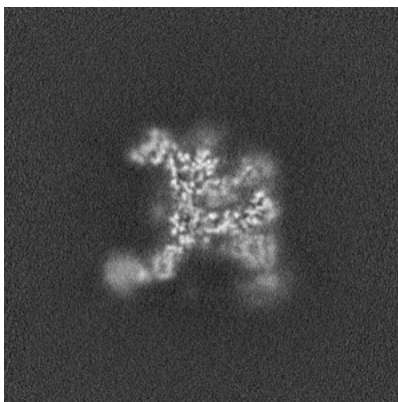


Z Index: 174

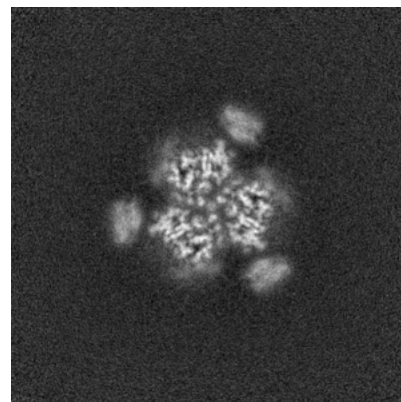
### 6.3.2 Raw map



X Index: 169



Y Index: 189

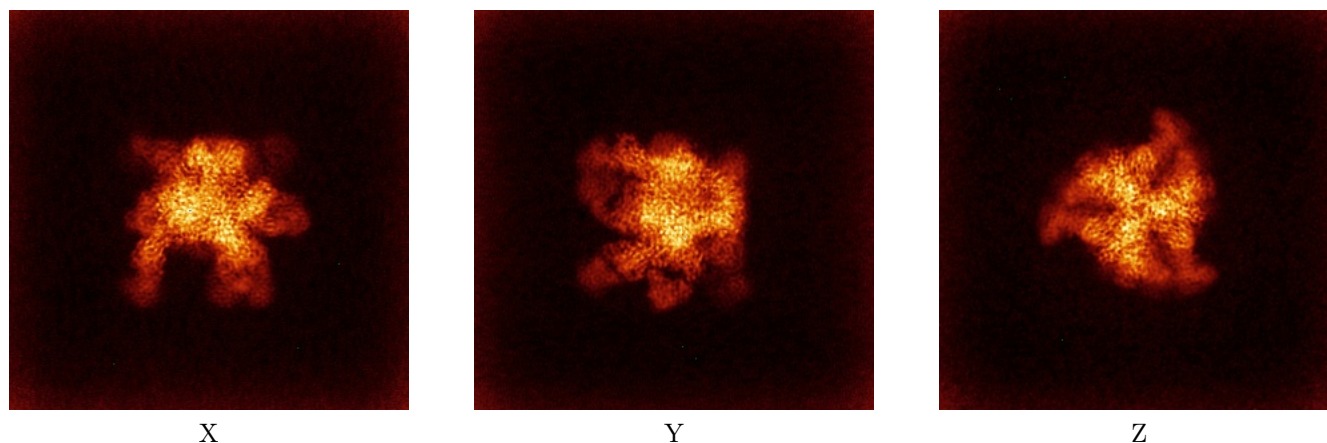


Z Index: 174

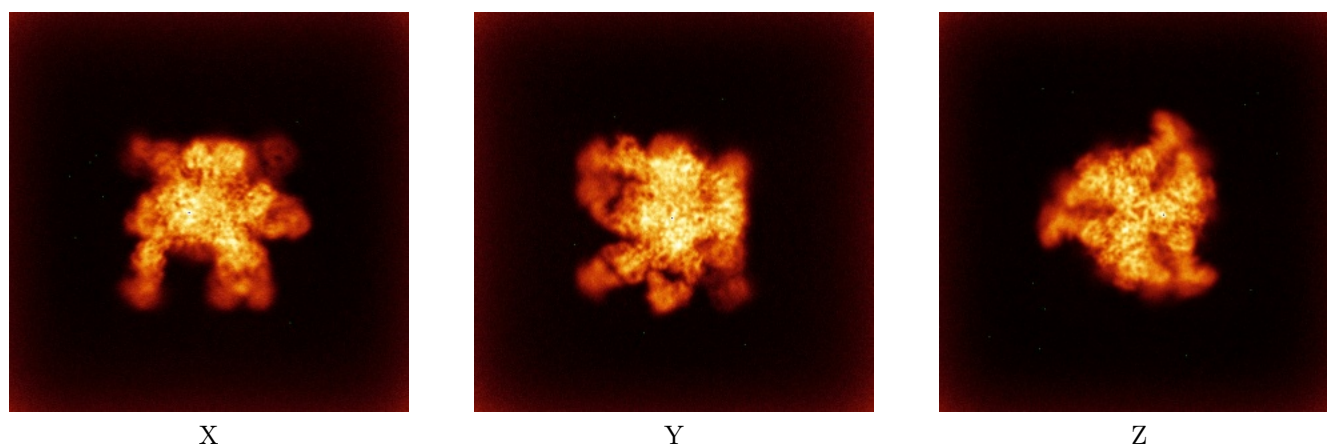
The images above show the largest variance slices of the map in three orthogonal directions.

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

### 6.4.1 Primary map



### 6.4.2 Raw map



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](#)

This section was not generated.

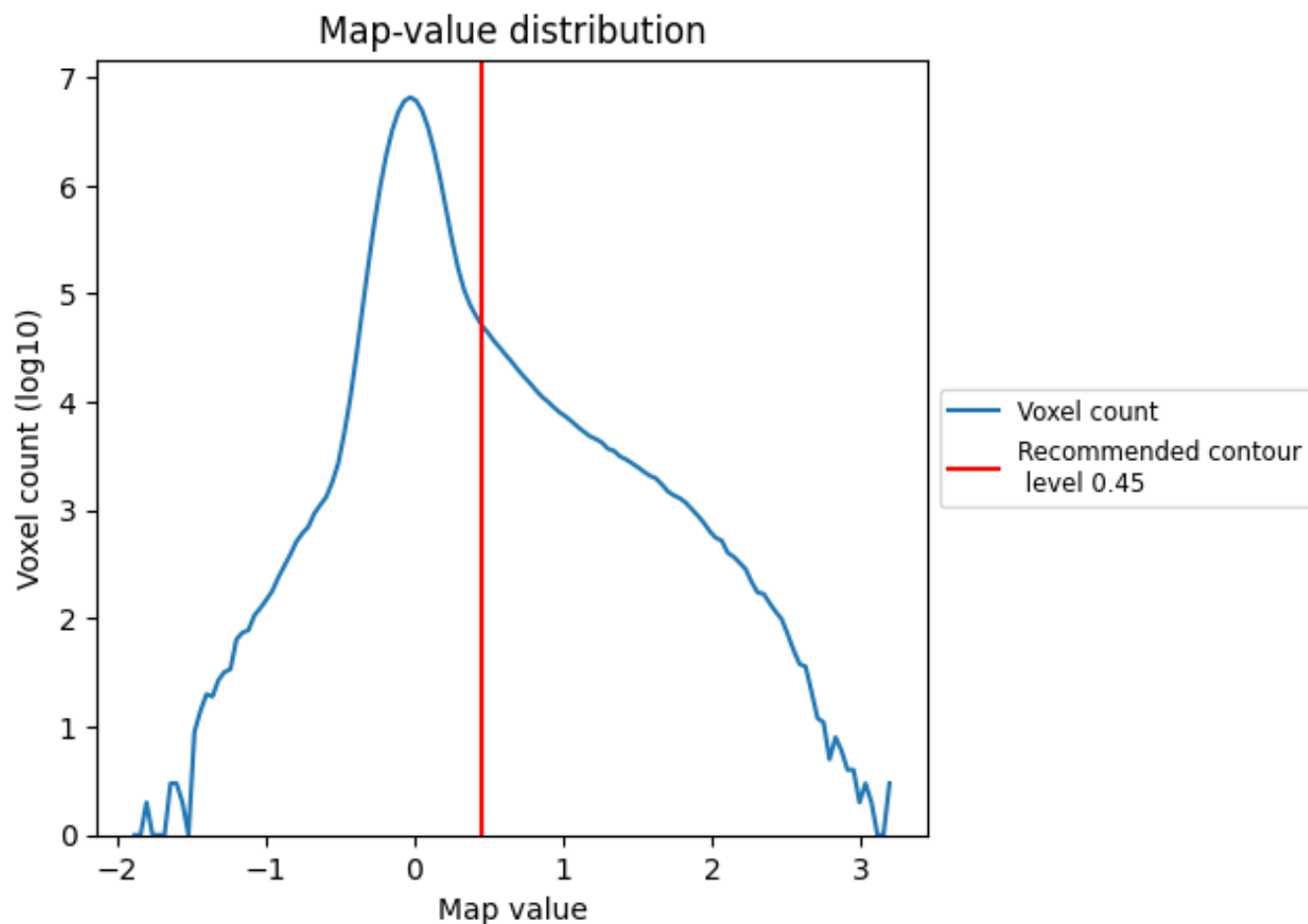
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

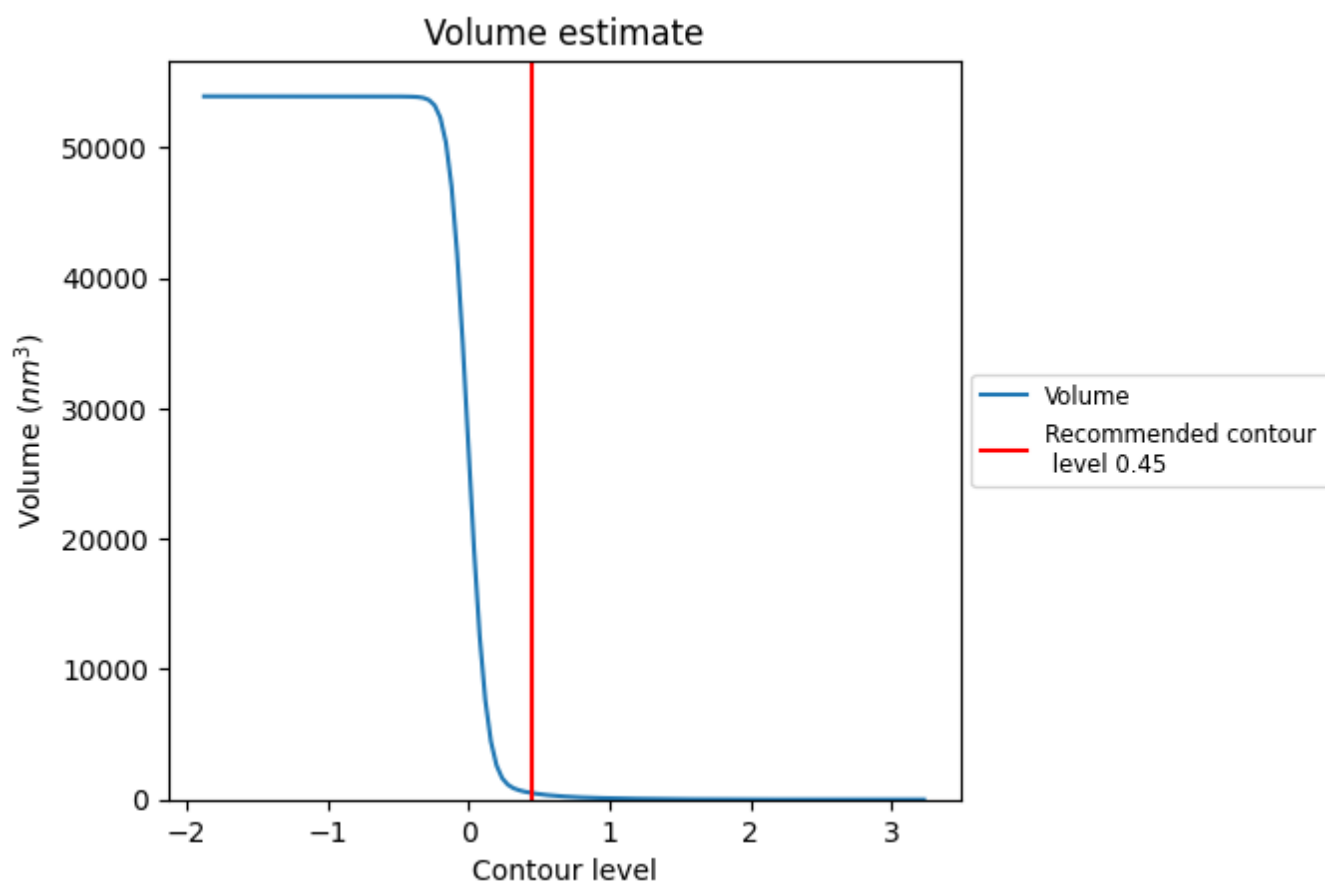
This section contains the results of statistical analysis of the map.

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



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

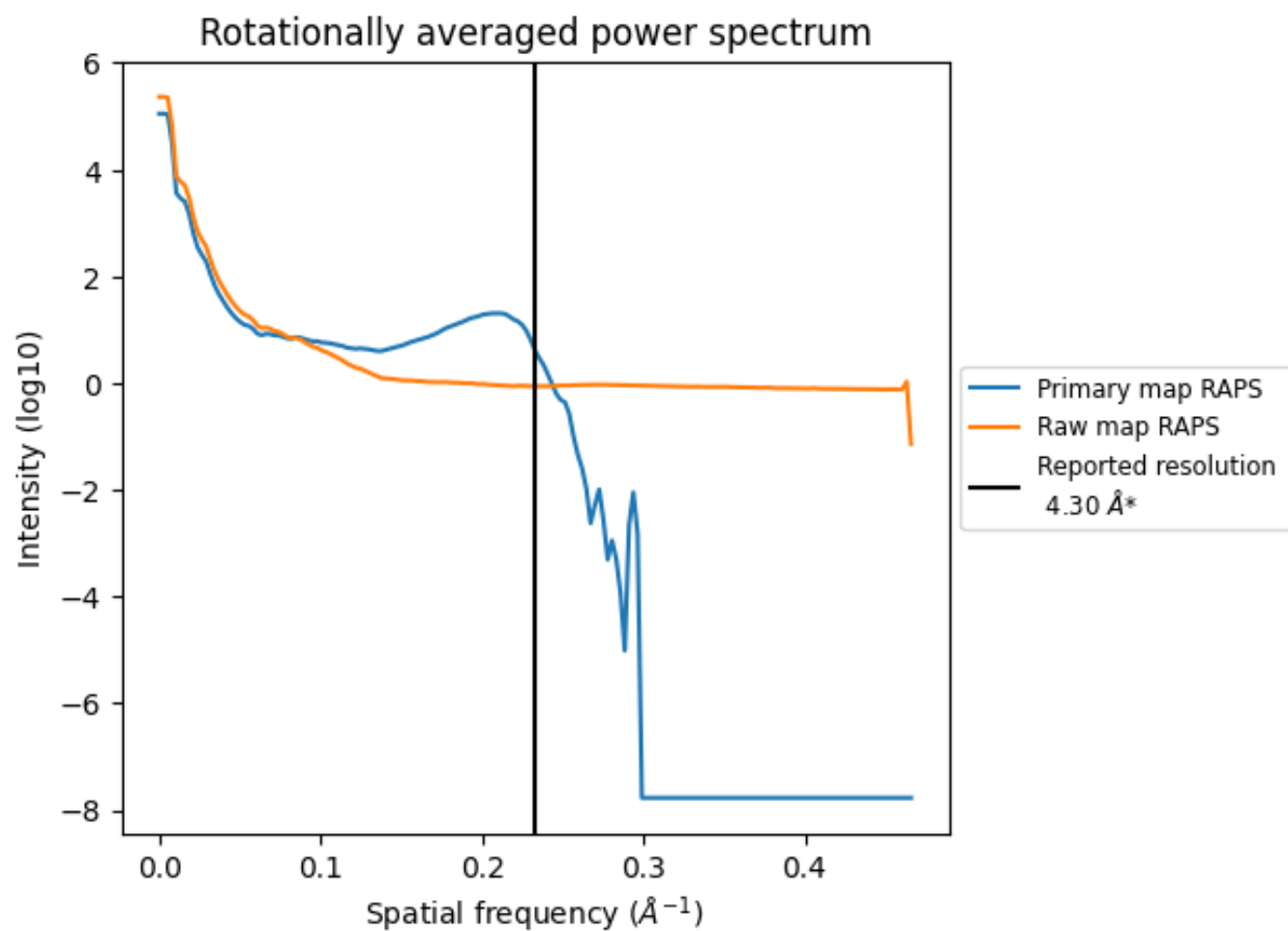
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 497 nm<sup>3</sup>; this corresponds to an approximate mass of 449 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 ⓘ

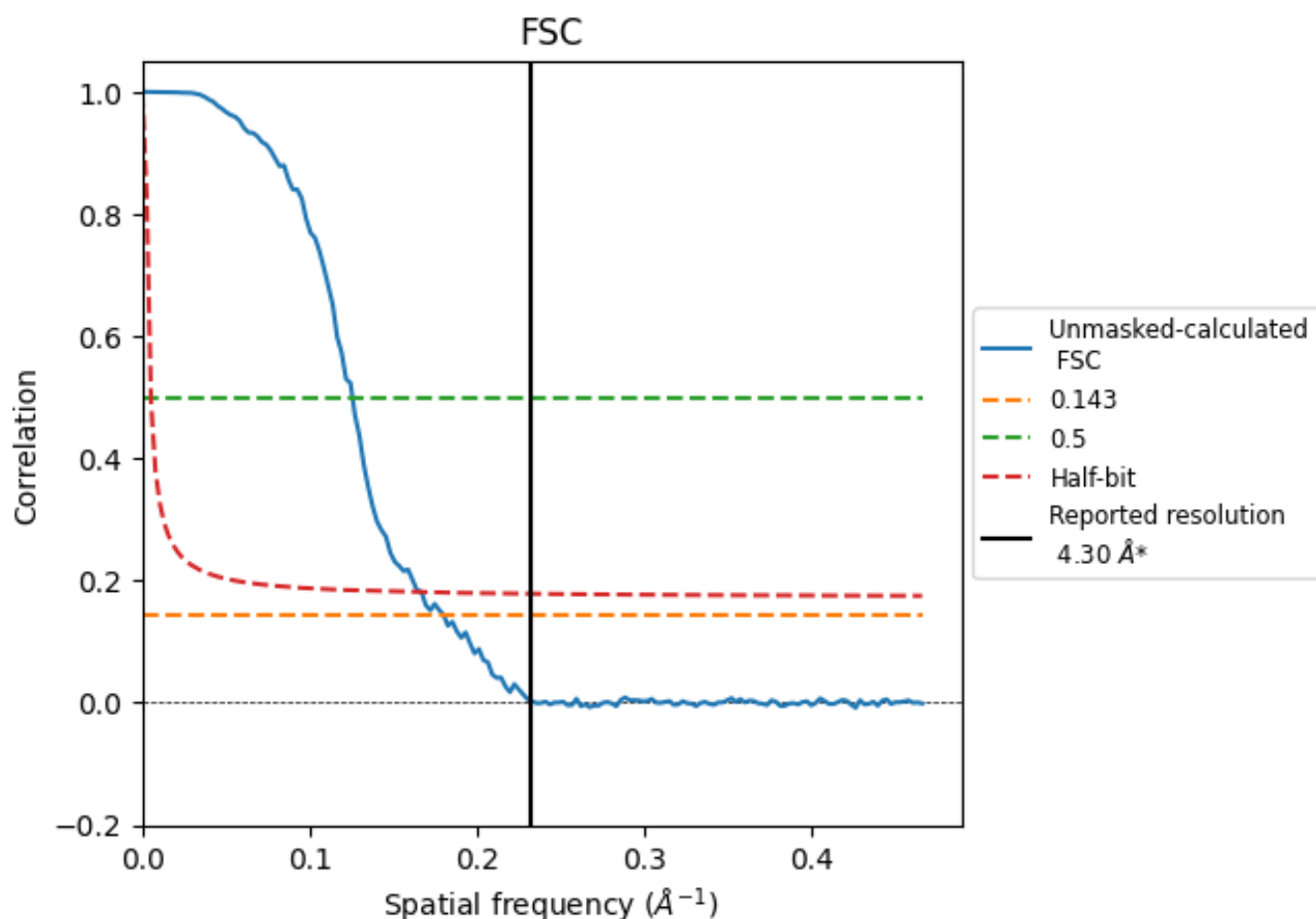


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 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 0.233  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

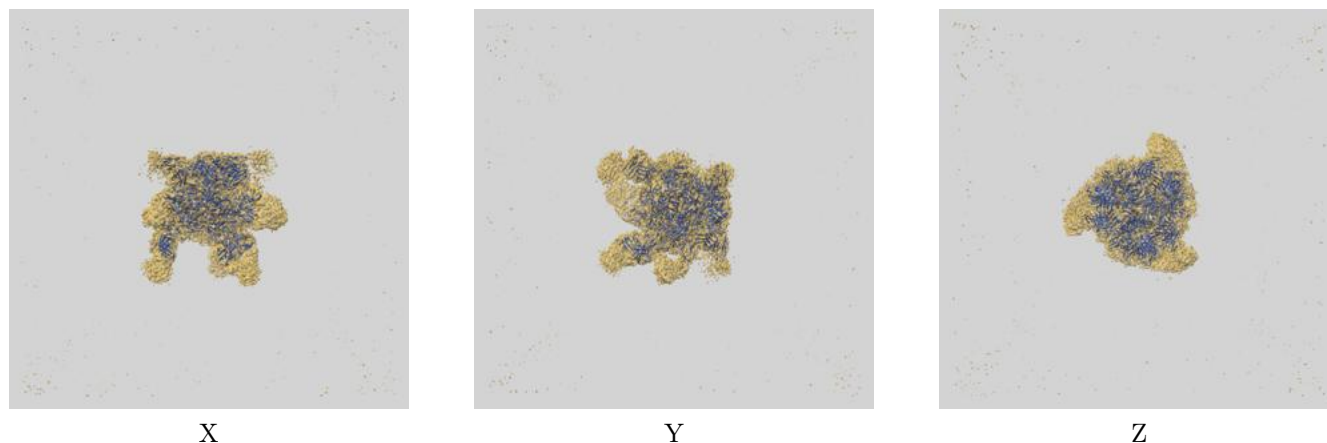
| Resolution estimate (Å)   | Estimation criterion (FSC cut-off) |      |          |
|---------------------------|------------------------------------|------|----------|
|                           | 0.143                              | 0.5  | Half-bit |
| Reported by author        | 4.30                               | -    | -        |
| Author-provided FSC curve | -                                  | -    | -        |
| Unmasked-calculated*      | 5.55                               | 7.96 | 6.00     |

\*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 5.55 differs from the reported value 4.3 by more than 10 %

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

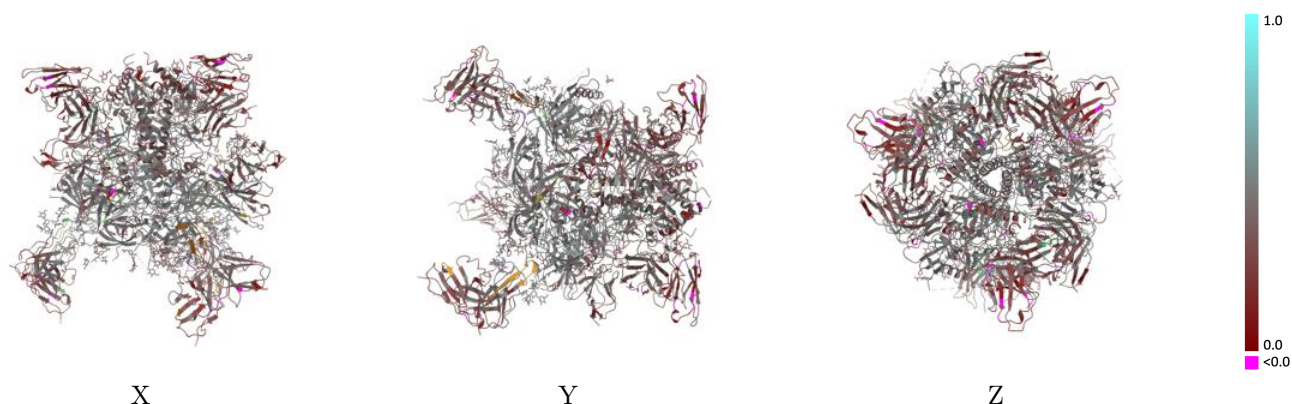
This section contains information regarding the fit between EMDB map EMD-20189 and PDB model 6OSY. Per-residue inclusion information can be found in section [3](#) on page [14](#).

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



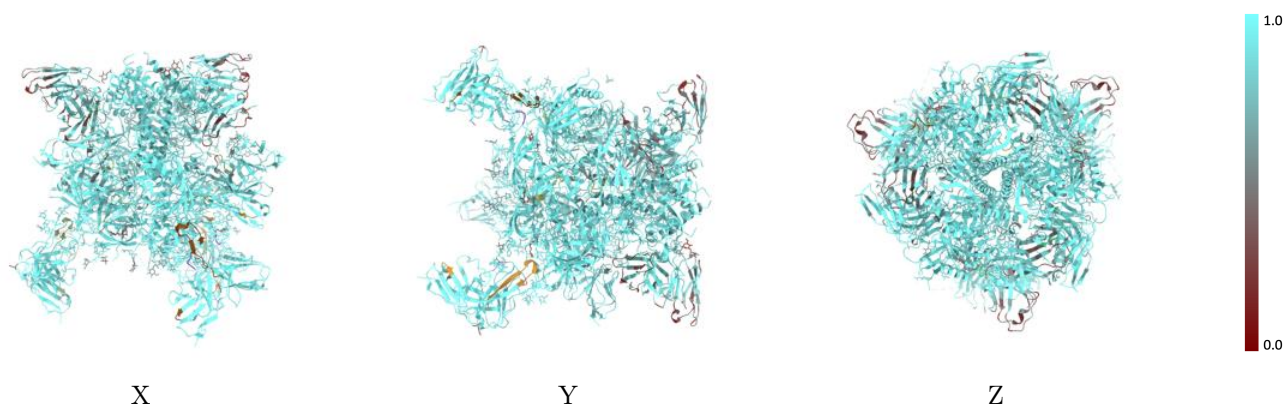
The images above show the 3D surface view of the map at the recommended contour level 0.45 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



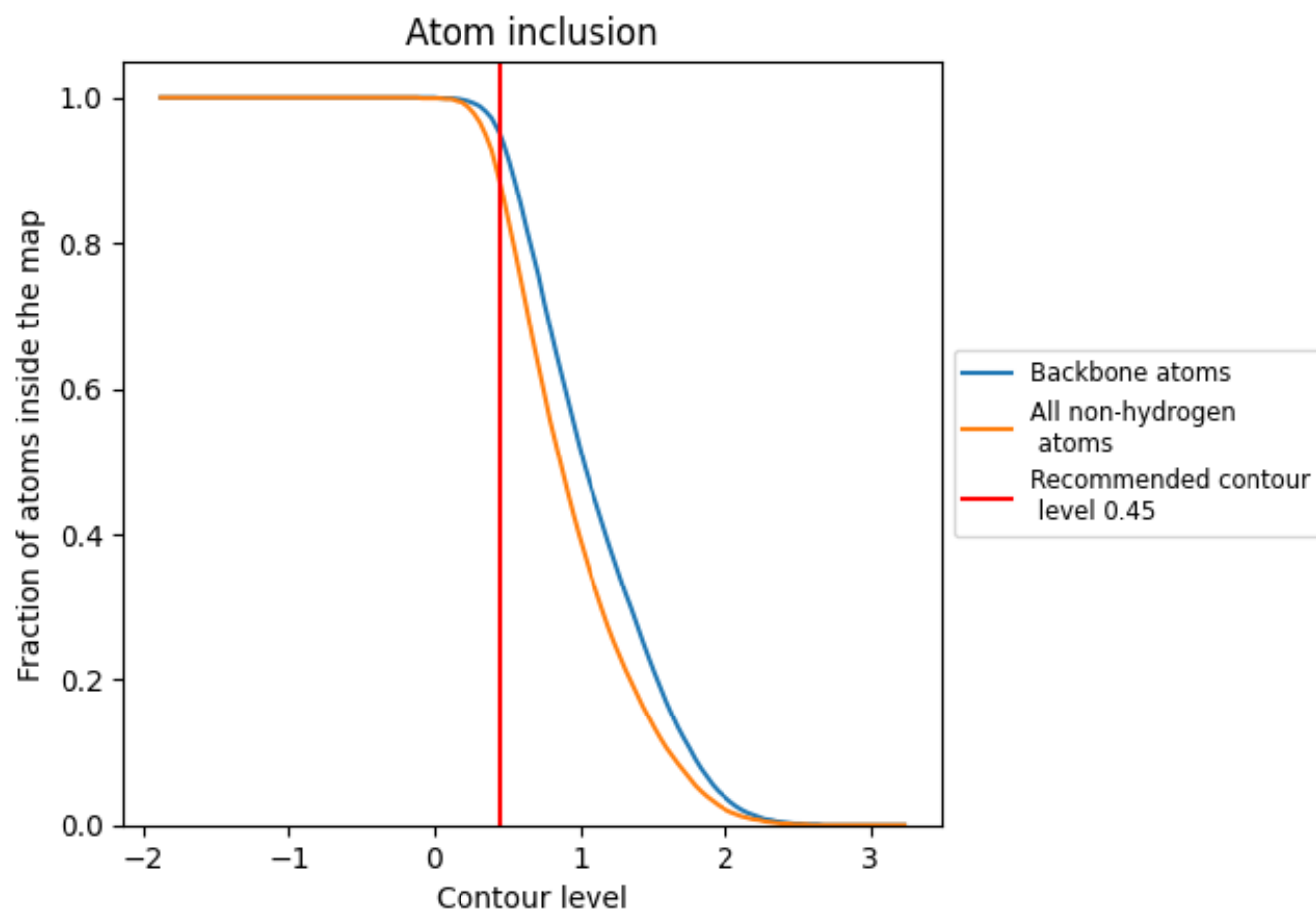
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.45).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.45) and Q-score for the entire model and for each chain.

| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| All   |  0.8870   |  0.3960   |
| 0     |  0.8930   |  0.3550   |
| 1     |  0.9200   |  0.4370   |
| 2     |  0.9450   |  0.4520   |
| 3     |  0.7870   |  0.4140   |
| 4     |  0.6670   |  0.3220   |
| 5     |  0.9300   |  0.3550   |
| 6     |  0.9210   |  0.3910   |
| 7     |  0.9080   |  0.3680   |
| 8     |  0.8800   |  0.4030   |
| 9     |  0.5000   |  0.3690   |
| A     |  0.9300   |  0.3840   |
| AA    |  0.7860   |  0.4360   |
| B     |  0.9450   |  0.4500   |
| BA    |  0.9030  |  0.4680  |
| C     |  0.9260 |  0.3540 |
| CA    |  0.9290 |  0.4820 |
| D     |  0.9250 |  0.3870 |
| DA    |  0.9640 |  0.4880 |
| E     |  0.9210 |  0.3710 |
| EA    |  0.9230 |  0.4770 |
| F     |  0.8780 |  0.4030 |
| FA    |  0.9340 |  0.4720 |
| G     |  0.9280 |  0.3870 |
| GA    |  0.8570 |  0.4010 |
| H     |  0.7320 |  0.3520 |
| HA    |  0.9240 |  0.4610 |
| I     |  0.7280 |  0.3480 |
| IA    |  0.8210 |  0.4050 |
| J     |  0.7150 |  0.2720 |
| JA    |  0.8000 |  0.3830 |
| K     |  0.9430 |  0.4510 |
| L     |  0.7100 |  0.2750 |
| M     |  0.9250 |  0.3540 |
| N     |  0.9300 |  0.3870 |



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| Chain | Atom inclusion                                                                             | Q-score                                                                                    |
|-------|--------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------|
| O     |  0.9130   |  0.3690   |
| P     |  0.8890   |  0.4010   |
| Q     |  0.9290   |  0.3880   |
| R     |  0.7240   |  0.3460   |
| S     |  0.7060   |  0.2720   |
| T     |  0.5600   |  0.3390   |
| U     |  0.8930   |  0.3720   |
| V     |  0.9400   |  0.4420   |
| W     |  0.7870   |  0.4150   |
| X     |  0.6670   |  0.3290   |
| Y     |  0.4800   |  0.3750   |
| Z     |  0.8210   |  0.4360   |
| a     |  0.9310   |  0.4730   |
| b     |  0.9290   |  0.4860   |
| c     |  0.9640   |  0.4690   |
| d     |  0.9230   |  0.4680   |
| e     |  0.9180   |  0.4650   |
| f     |  0.8570   |  0.3960   |
| g     |  0.9330   |  0.4620   |
| h     |  0.8210  |  0.4060  |
| i     |  0.8200 |  0.3790 |
| j     |  0.5800 |  0.3610 |
| k     |  0.8930 |  0.3640 |
| l     |  0.9400 |  0.4370 |
| m     |  0.7700 |  0.4170 |
| n     |  0.6670 |  0.3220 |
| o     |  0.5000 |  0.3850 |
| p     |  0.7860 |  0.4430 |
| q     |  0.9310 |  0.4710 |
| r     |  0.9290 |  0.4820 |
| s     |  0.9640 |  0.4730 |
| t     |  0.9490 |  0.4750 |
| u     |  0.9180 |  0.4650 |
| v     |  0.8570 |  0.4080 |
| w     |  0.9240 |  0.4590 |
| x     |  0.8210 |  0.4120 |
| y     |  0.8400 |  0.3750 |
| z     |  0.5400 |  0.3530 |