



wwPDB NMR Structure Validation Summary Report ⓘ

Dec 20, 2023 – 09:52 AM EST

PDB ID : 1BP8
Title : 4:2:1 mithramycin:Mg⁺⁺:d(ACCCGGGT)₂ complex
Authors : Keniry, M.A.; Owen, E.A.; Shafer, R.H.
Deposited on : 1998-08-13

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
wwPDB-RCI : v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV : Wang et al. (2010)
wwPDB-ShiftChecker : v1.2
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

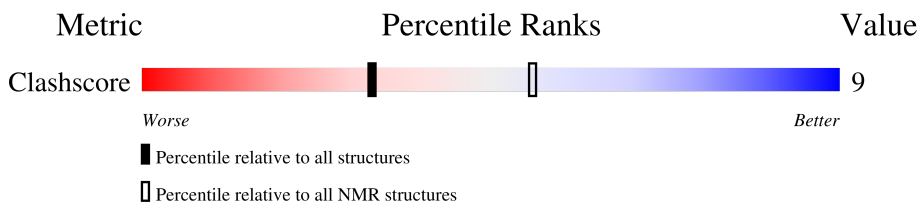
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLUTION NMR



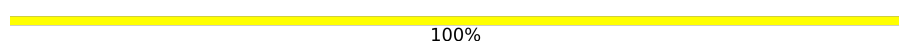
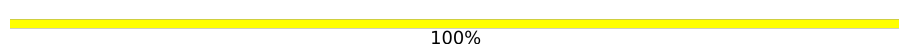
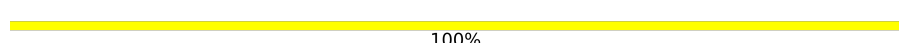
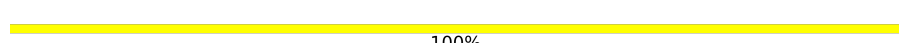
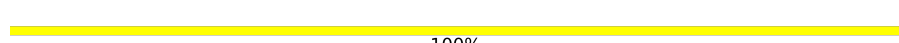

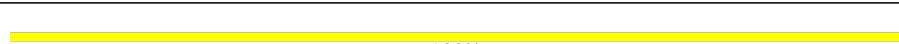
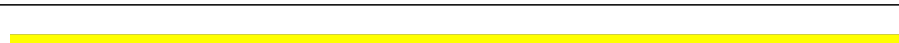
The overall completeness of chemical shifts assignment was not calculated.

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 (#Entries) | NMR archive (#Entries) |
|------------|-----------------------------|---------------------------|
| Clashscore | 158937 | 12864 |

The table below summarises the geometric issues observed across the polymeric chains and their fit to the experimental data. The red, orange, yellow and green segments indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A cyan segment indicates the fraction of residues that are not part of the well-defined cores, and a grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

| Mol | Chain | Length | Quality of chain |
|-----|-------|--------|--|
| 1 | A | 8 |  50% 38% 12% |
| 1 | B | 8 |  25% 62% 12% |
| 2 | C | 2 |  100% |
| 2 | E | 2 |  100% |
| 2 | H | 2 |  100% |
| 2 | I | 2 |  100% |
| 3 | D | 3 |  100% |
| 3 | F | 3 |  67% 33% |
| 3 | G | 3 |  100% |
| 3 | J | 3 |  100% |

2 Ensemble composition and analysis

This entry contains 1 models. Identification of well-defined residues and clustering analysis are not possible.

3 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 1109 atoms, of which 481 are hydrogens and 0 are deuteriums.

- Molecule 1 is a DNA chain called 5'-D(*AP*CP*CP*CP*GP*GP*GP*T)-3'.

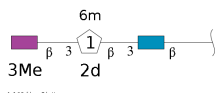
| Mol | Chain | Residues | Atoms | | | | | Trace | |
|-----|-------|----------|-------|----|----|----|----|-------|---|
| | | | Total | C | H | N | O | | P |
| 1 | A | 8 | 252 | 77 | 91 | 31 | 46 | 7 | 0 |
| 1 | B | 8 | 252 | 77 | 91 | 31 | 46 | 7 | 0 |

- Molecule 2 is an oligosaccharide called beta-D-Olivopyranose-(1-3)-beta-D-Olivopyranose.



| Mol | Chain | Residues | Atoms | | | | Trace |
|-----|-------|----------|-------|----|----|---|-------|
| | | | Total | C | H | O | |
| 2 | C | 2 | 40 | 12 | 21 | 7 | 0 |
| 2 | E | 2 | 40 | 12 | 21 | 7 | 0 |
| 2 | H | 2 | 40 | 12 | 21 | 7 | 0 |
| 2 | I | 2 | 39 | 12 | 20 | 7 | 0 |

- Molecule 3 is an oligosaccharide called 2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose-(1-3)-2,6-dideoxy-beta-D-galactopyranose-(1-3)-beta-D-Olivopyranose.



| Mol | Chain | Residues | Atoms | | | | Trace |
|-----|-------|----------|-------|----|----|----|-------|
| | | | Total | C | H | O | |
| 3 | D | 3 | 62 | 19 | 33 | 10 | 0 |
| 3 | F | 3 | 62 | 19 | 33 | 10 | 0 |
| 3 | G | 3 | 62 | 19 | 33 | 10 | 0 |

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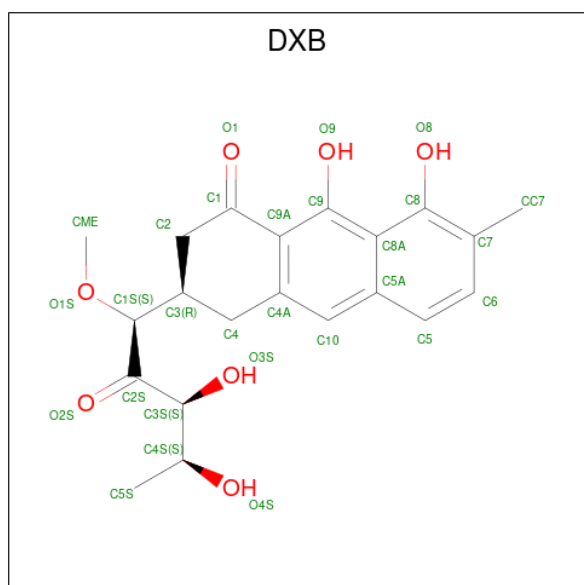
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| Mol | Chain | Residues | Atoms | | | | Trace |
|-----|-------|----------|-------|----|----|----|-------|
| | | | Total | C | H | O | |
| 3 | J | 3 | 62 | 19 | 33 | 10 | 0 |

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

| Mol | Chain | Residues | Atoms | |
|-----|-------|----------|-------|----|
| | | | Total | Mg |
| 4 | A | 2 | 2 | 2 |

- Molecule 5 is 1,2-HYDRO-1-OXY-3,4-HYDRO-3-(1-METHOXY-2-OXY-3,4-DIHYDRO XYPENTYL)-8,9-DIHYDROXY-7-METHYL-ANTHRACENE (three-letter code: DXB) (formula: C₂₁H₂₄O₇).



| Mol | Chain | Residues | Atoms | | | |
|-----|-------|----------|-------|----|----|---|
| | | | Total | C | H | O |
| 5 | A | 1 | 49 | 21 | 21 | 7 |
| 5 | A | 1 | 49 | 21 | 21 | 7 |
| 5 | B | 1 | 49 | 21 | 21 | 7 |
| 5 | B | 1 | 49 | 21 | 21 | 7 |

4 Residue-property plots

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: 5'-D(*AP*CP*CP*CP*GP*GP*GP*T)-3'

Chain A:  50% 38% 12%

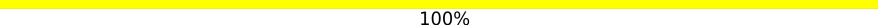


- Molecule 1: 5'-D(*AP*CP*CP*CP*GP*GP*GP*T)-3'

Chain B:  25% 62% 12%



- Molecule 2: beta-D-Olivopyranose-(1-3)-beta-D-Olivopyranose

Chain C:  100%



- Molecule 2: beta-D-Olivopyranose-(1-3)-beta-D-Olivopyranose

Chain E:  100%

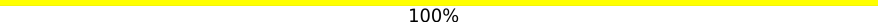


- Molecule 2: beta-D-Olivopyranose-(1-3)-beta-D-Olivopyranose

Chain H:  100%




- Molecule 2: beta-D-Olivopyranose-(1-3)-beta-D-Olivopyranose

Chain I:  100%

DDA1
DDL2
MDA3

- Molecule 3: 2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose-(1-3)-2,6-dideoxy-beta-D-galactopyranose-(1-3)-beta-D-Olivopyranose

Chain D:  100%DDA1
DDL2
MDA3

- Molecule 3: 2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose-(1-3)-2,6-dideoxy-beta-D-galactopyranose-(1-3)-beta-D-Olivopyranose

Chain F:  67% 33%DDA1
DDL2
MDA3

- Molecule 3: 2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose-(1-3)-2,6-dideoxy-beta-D-galactopyranose-(1-3)-beta-D-Olivopyranose

Chain G:  100%DDA1
DDL2
MDA3

- Molecule 3: 2,6-dideoxy-3-C-methyl-beta-D-ribo-hexopyranose-(1-3)-2,6-dideoxy-beta-D-galactopyranose-(1-3)-beta-D-Olivopyranose

Chain J:  100%DDA1
DDL2
MDA3

5 Refinement protocol and experimental data overview

The models were refined using the following method: *FULL RELAXATION MATRIX ANALYSIS AND RESTRAINED MOLECULAR DYNAMICS*.

Of the 7 calculated structures, 1 were deposited, based on the following criterion: ?.

The following table shows the software used for structure solution, optimisation and refinement.

| Software name | Classification | Version |
|---------------|--------------------|---------|
| CHARMM | refinement | 23.2 |
| VNMR | structure solution | |
| MARDIGRAS | structure solution | |
| CORMA CHARMM | structure solution | CHARMM |

No chemical shift data was provided.

6 Model quality i

6.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: DXB, MG, DDL, MDA, DDA

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 (average) root-mean-square of all Z scores of the bond lengths (or angles).

| Mol | Chain | Bond lengths | | Bond angles | |
|-----|-------|--------------|-----------------|-------------|-----------------|
| | | RMSZ | #Z>5 | RMSZ | #Z>5 |
| 1 | A | 4.51 | 29/180 (16.1%) | 3.33 | 45/276 (16.3%) |
| 1 | B | 3.66 | 27/180 (15.0%) | 3.30 | 46/276 (16.7%) |
| All | All | 4.11 | 56/360 (15.6%) | 3.31 | 91/552 (16.5%) |

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 | Planarity |
|-----|-------|-----------|-----------|
| 1 | A | 0 | 2 |
| 1 | B | 0 | 2 |
| All | All | 0 | 4 |

5 of 56 bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|--------|-------------|----------|
| 1 | A | 1 | DA | O5'-C5' | -25.70 | 0.78 | 1.42 |
| 1 | A | 8 | DT | C3'-O3' | -18.22 | 1.20 | 1.44 |
| 1 | A | 8 | DT | C3'-C2' | -15.07 | 1.34 | 1.52 |
| 1 | A | 3 | DC | N1-C6 | -14.01 | 1.28 | 1.37 |
| 1 | B | 3 | DC | N1-C6 | -12.38 | 1.29 | 1.37 |

5 of 91 angle outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|-------|-------------|----------|
| 1 | A | 2 | DC | N1-C2-O2 | 14.18 | 127.41 | 118.90 |
| 1 | B | 2 | DC | N1-C2-O2 | 13.88 | 127.23 | 118.90 |
| 1 | A | 1 | DA | C5-C6-N1 | 9.72 | 122.56 | 117.70 |
| 1 | B | 1 | DA | C5-C6-N1 | 9.71 | 122.55 | 117.70 |

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| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 1 | A | 8 | DT | C4'-C3'-C2' | 9.19 | 111.37 | 103.10 |

There are no chirality outliers.

All planar outliers are listed below.

| Mol | Chain | Res | Type | Group |
|-----|-------|-----|------|-----------|
| 1 | A | 3 | DC | Sidechain |
| 1 | A | 6 | DG | Sidechain |
| 1 | B | 3 | DC | Sidechain |
| 1 | B | 6 | DG | Sidechain |

6.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in each 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 averaged over the ensemble.

| Mol | Chain | Non-H | H(model) | H(added) | Clashes |
|-----|-------|-------|----------|----------|---------|
| 1 | A | 161 | 91 | 86 | 7 |
| 1 | B | 161 | 91 | 86 | 3 |
| 3 | F | 29 | 33 | 31 | 1 |
| All | All | 628 | 481 | 455 | 10 |

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 9.

5 of 10 clashes are listed below, sorted by their clash magnitude.

| Atom-1 | Atom-2 | Clash(Å) | Distance(Å) |
|--------------|---------------|----------|-------------|
| 1:A:1:DA:O5' | 1:A:1:DA:H5' | 1.10 | 1.41 |
| 1:A:1:DA:O5' | 1:A:1:DA:C4' | 1.07 | 2.02 |
| 1:A:1:DA:O5' | 1:A:1:DA:C5' | 1.07 | 0.78 |
| 1:A:1:DA:O5' | 1:A:1:DA:H5'' | 1.02 | 1.41 |
| 1:A:1:DA:C5' | 1:A:1:DA:HO5' | 0.61 | 1.32 |

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

There are no protein molecules in this entry.

6.3.2 Protein sidechains [i](#)

There are no protein molecules in this entry.

6.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

6.5 Carbohydrates [i](#)

20 monosaccharides are modelled in this entry.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|------|---------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | DDA | C | 1 | 2,5 | 10,10,10 | 1.77 | 3 (30%) |
| 2 | DDA | C | 2 | 2 | 9,9,10 | 1.64 | 3 (33%) |
| 3 | DDA | D | 1 | 5,3 | 10,10,10 | 1.18 | 1 (10%) |
| 3 | DDL | D | 2 | 3 | 9,9,10 | 1.04 | 1 (11%) |
| 3 | MDA | D | 3 | 3 | 10,10,11 | 1.05 | 1 (10%) |
| 2 | DDA | E | 1 | 2,5 | 10,10,10 | 1.51 | 2 (20%) |
| 2 | DDA | E | 2 | 2 | 9,9,10 | 2.87 | 6 (66%) |
| 3 | DDA | F | 1 | 5,3 | 10,10,10 | 1.11 | 0 (0%) |
| 3 | DDL | F | 2 | 3 | 9,9,10 | 0.88 | 0 (0%) |
| 3 | MDA | F | 3 | 3 | 10,10,11 | 0.95 | 1 (10%) |
| 3 | DDA | G | 1 | 5,3 | 10,10,10 | 1.07 | 0 (0%) |
| 3 | DDL | G | 2 | 3 | 9,9,10 | 1.12 | 0 (0%) |
| 3 | MDA | G | 3 | 3 | 10,10,11 | 0.86 | 1 (10%) |
| 2 | DDA | H | 1 | 2,5 | 10,10,10 | 1.73 | 3 (30%) |
| 2 | DDA | H | 2 | 2 | 9,9,10 | 2.23 | 6 (66%) |

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|------|--------------|------|---------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | DDA | I | 1 | 2,5 | 10,10,10 | 1.54 | 2 (20%) |
| 2 | DDA | I | 2 | 2 | 9,9,10 | 1.47 | 2 (22%) |
| 3 | DDA | J | 1 | 5,3 | 10,10,10 | 1.15 | 0 (0%) |
| 3 | DDL | J | 2 | 3 | 9,9,10 | 1.02 | 0 (0%) |
| 3 | MDA | J | 3 | 3 | 10,10,11 | 0.91 | 0 (0%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|------|-------------|------|---------|
| | | | | | Counts | RMSZ | #Z>2 |
| 2 | DDA | C | 1 | 2,5 | 12,14,14 | 2.34 | 4 (33%) |
| 2 | DDA | C | 2 | 2 | 12,12,14 | 1.47 | 1 (8%) |
| 3 | DDA | D | 1 | 5,3 | 12,14,14 | 1.27 | 1 (8%) |
| 3 | DDL | D | 2 | 3 | 12,12,14 | 2.01 | 4 (33%) |
| 3 | MDA | D | 3 | 3 | 13,15,17 | 1.31 | 3 (23%) |
| 2 | DDA | E | 1 | 2,5 | 12,14,14 | 2.11 | 4 (33%) |
| 2 | DDA | E | 2 | 2 | 12,12,14 | 1.39 | 1 (8%) |
| 3 | DDA | F | 1 | 5,3 | 12,14,14 | 1.24 | 1 (8%) |
| 3 | DDL | F | 2 | 3 | 12,12,14 | 2.45 | 5 (41%) |
| 3 | MDA | F | 3 | 3 | 13,15,17 | 1.65 | 3 (23%) |
| 3 | DDA | G | 1 | 5,3 | 12,14,14 | 1.47 | 3 (25%) |
| 3 | DDL | G | 2 | 3 | 12,12,14 | 2.24 | 3 (25%) |
| 3 | MDA | G | 3 | 3 | 13,15,17 | 1.59 | 4 (30%) |
| 2 | DDA | H | 1 | 2,5 | 12,14,14 | 2.26 | 2 (16%) |
| 2 | DDA | H | 2 | 2 | 12,12,14 | 1.44 | 2 (16%) |
| 2 | DDA | I | 1 | 2,5 | 12,14,14 | 2.37 | 3 (25%) |
| 2 | DDA | I | 2 | 2 | 12,12,14 | 1.24 | 1 (8%) |
| 3 | DDA | J | 1 | 5,3 | 12,14,14 | 1.26 | 2 (16%) |
| 3 | DDL | J | 2 | 3 | 12,12,14 | 2.37 | 5 (41%) |
| 3 | MDA | J | 3 | 3 | 13,15,17 | 1.59 | 4 (30%) |

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 |
|-----|------|-------|-----|------|---------|----------|---------|
| 2 | DDA | C | 1 | 2,5 | - | - | 0,1,1,1 |
| 2 | DDA | C | 2 | 2 | - | - | 0,1,1,1 |
| 3 | DDA | D | 1 | 5,3 | - | - | 0,1,1,1 |
| 3 | DDL | D | 2 | 3 | - | - | 0,1,1,1 |
| 3 | MDA | D | 3 | 3 | - | - | 0,1,1,1 |
| 2 | DDA | E | 1 | 2,5 | - | - | 0,1,1,1 |
| 2 | DDA | E | 2 | 2 | - | - | 0,1,1,1 |
| 3 | DDA | F | 1 | 5,3 | - | - | 0,1,1,1 |
| 3 | DDL | F | 2 | 3 | - | - | 0,1,1,1 |
| 3 | MDA | F | 3 | 3 | - | - | 0,1,1,1 |
| 3 | DDA | G | 1 | 5,3 | - | - | 0,1,1,1 |
| 3 | DDL | G | 2 | 3 | - | - | 0,1,1,1 |
| 3 | MDA | G | 3 | 3 | - | - | 0,1,1,1 |
| 2 | DDA | H | 1 | 2,5 | - | - | 0,1,1,1 |
| 2 | DDA | H | 2 | 2 | - | - | 0,1,1,1 |
| 2 | DDA | I | 1 | 2,5 | - | - | 0,1,1,1 |
| 2 | DDA | I | 2 | 2 | - | - | 0,1,1,1 |
| 3 | DDA | J | 1 | 5,3 | - | - | 0,1,1,1 |
| 3 | DDL | J | 2 | 3 | - | - | 0,1,1,1 |
| 3 | MDA | J | 3 | 3 | - | - | 0,1,1,1 |

5 of 32 bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|-------|------|-------------|----------|
| 2 | E | 2 | DDA | O5-C1 | 4.49 | 1.33 | 1.44 |
| 2 | E | 2 | DDA | O5-C5 | 4.23 | 1.34 | 1.43 |
| 2 | H | 2 | DDA | O5-C1 | 4.10 | 1.34 | 1.44 |
| 2 | E | 2 | DDA | C2-C3 | 3.72 | 1.46 | 1.52 |
| 2 | H | 1 | DDA | O5-C1 | 3.62 | 1.37 | 1.44 |

5 of 56 angle outliers are listed below. They are sorted according to the Z-score.

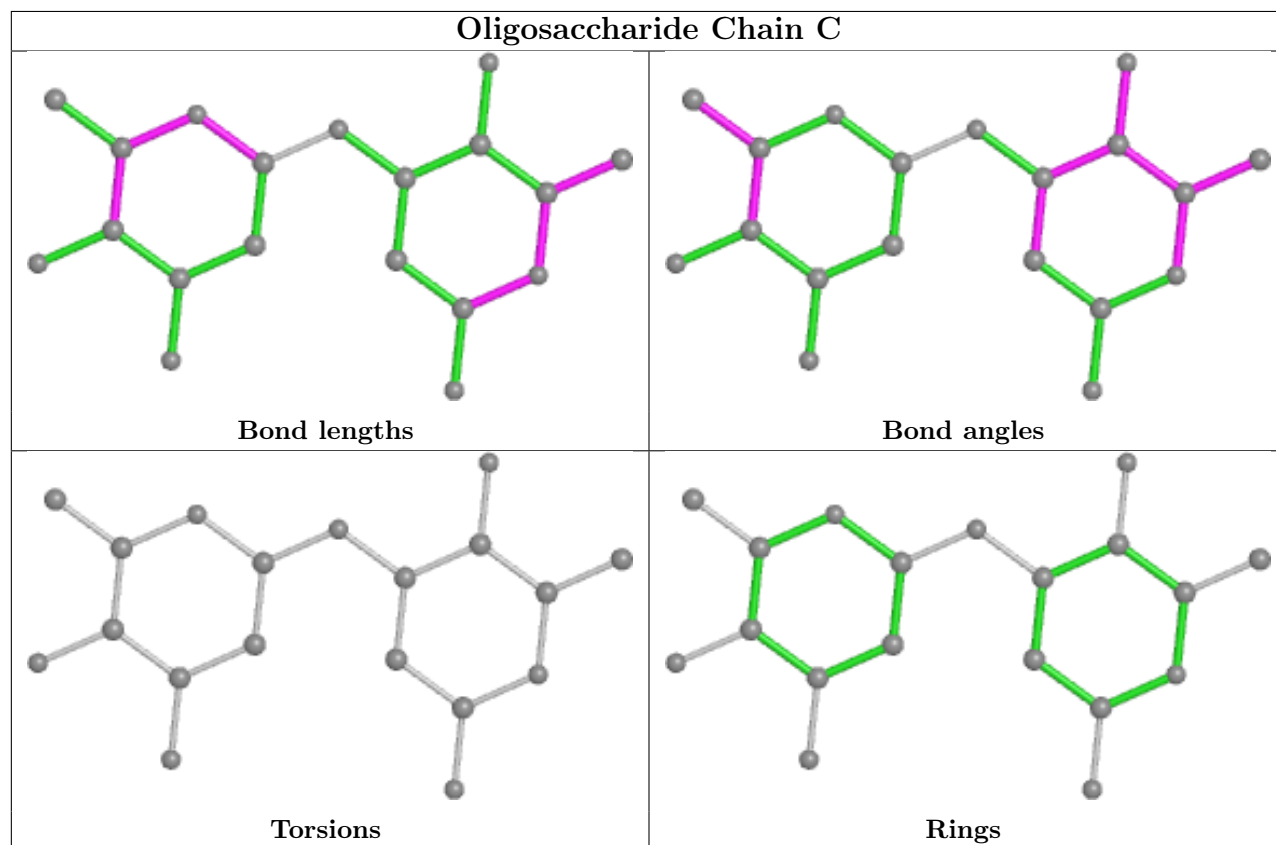
| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|----------|------|-------------|----------|
| 2 | C | 1 | DDA | O5-C5-C4 | 5.72 | 99.26 | 109.52 |
| 2 | H | 1 | DDA | O5-C5-C4 | 5.63 | 99.42 | 109.52 |
| 3 | J | 2 | DDL | C2-C3-C4 | 5.51 | 104.82 | 111.16 |
| 2 | I | 1 | DDA | O5-C5-C4 | 5.38 | 99.87 | 109.52 |
| 3 | G | 2 | DDL | C2-C3-C4 | 5.37 | 104.99 | 111.16 |

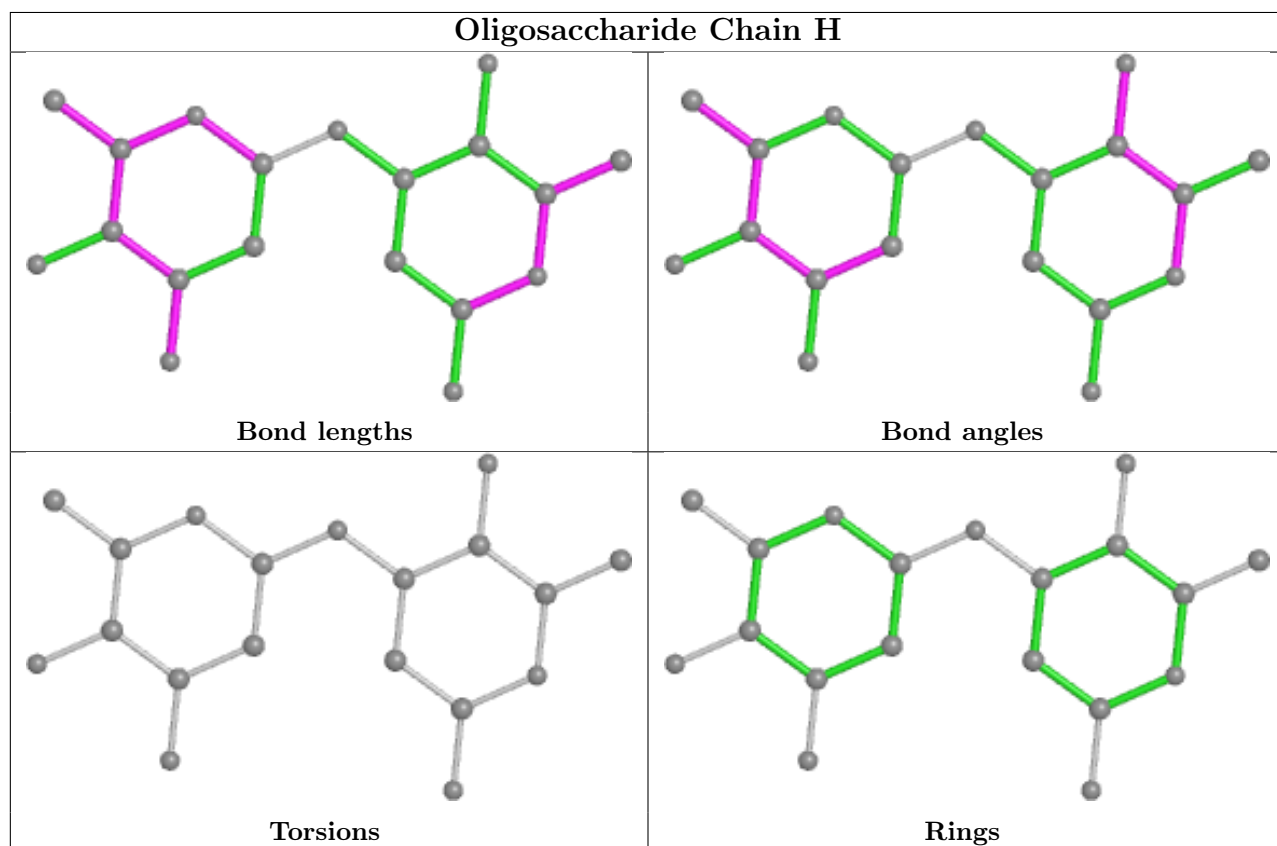
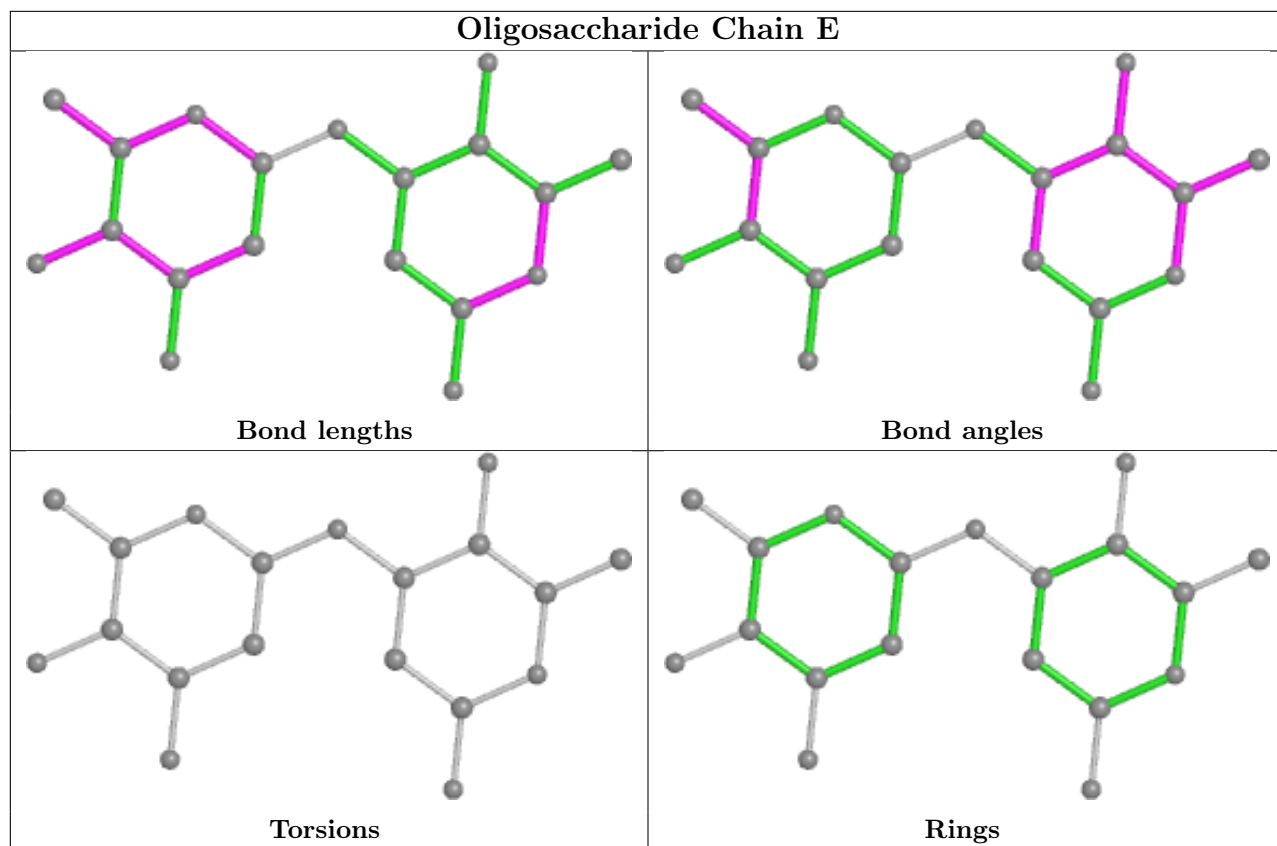
There are no chirality outliers.

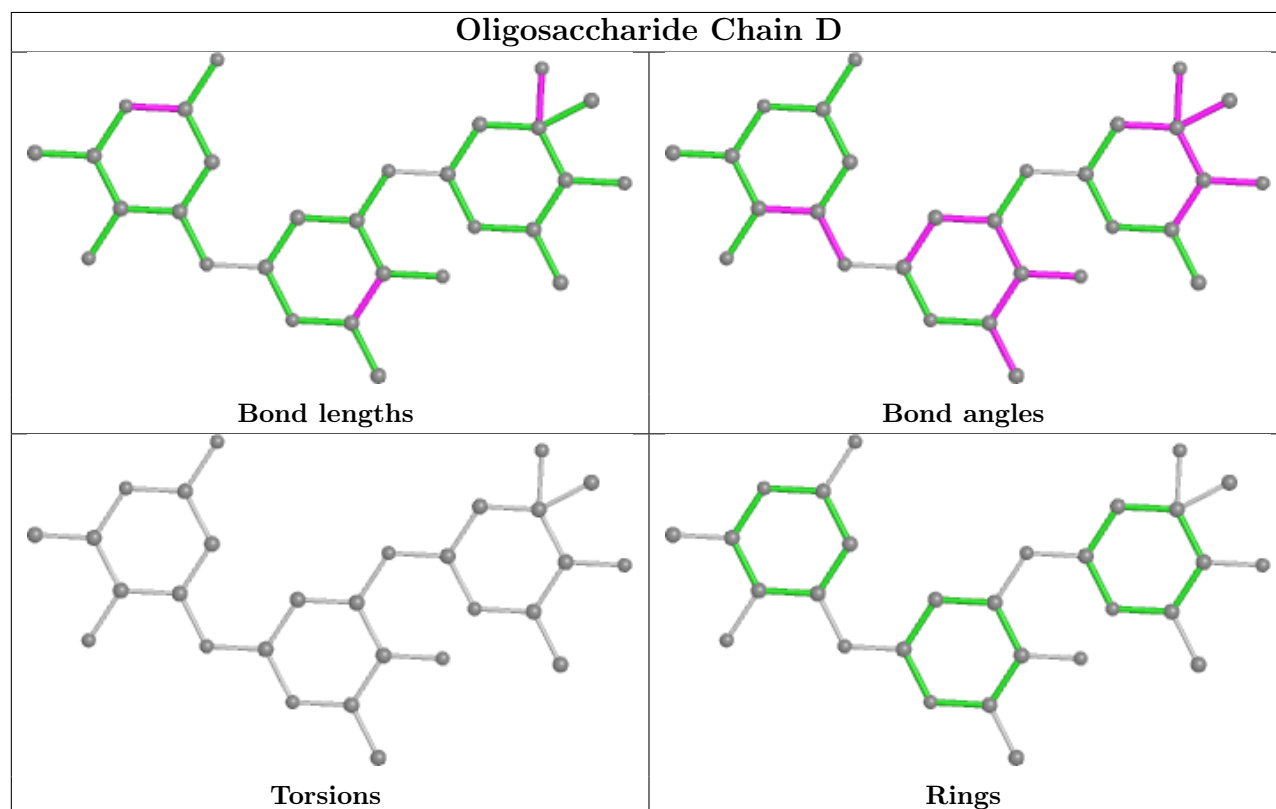
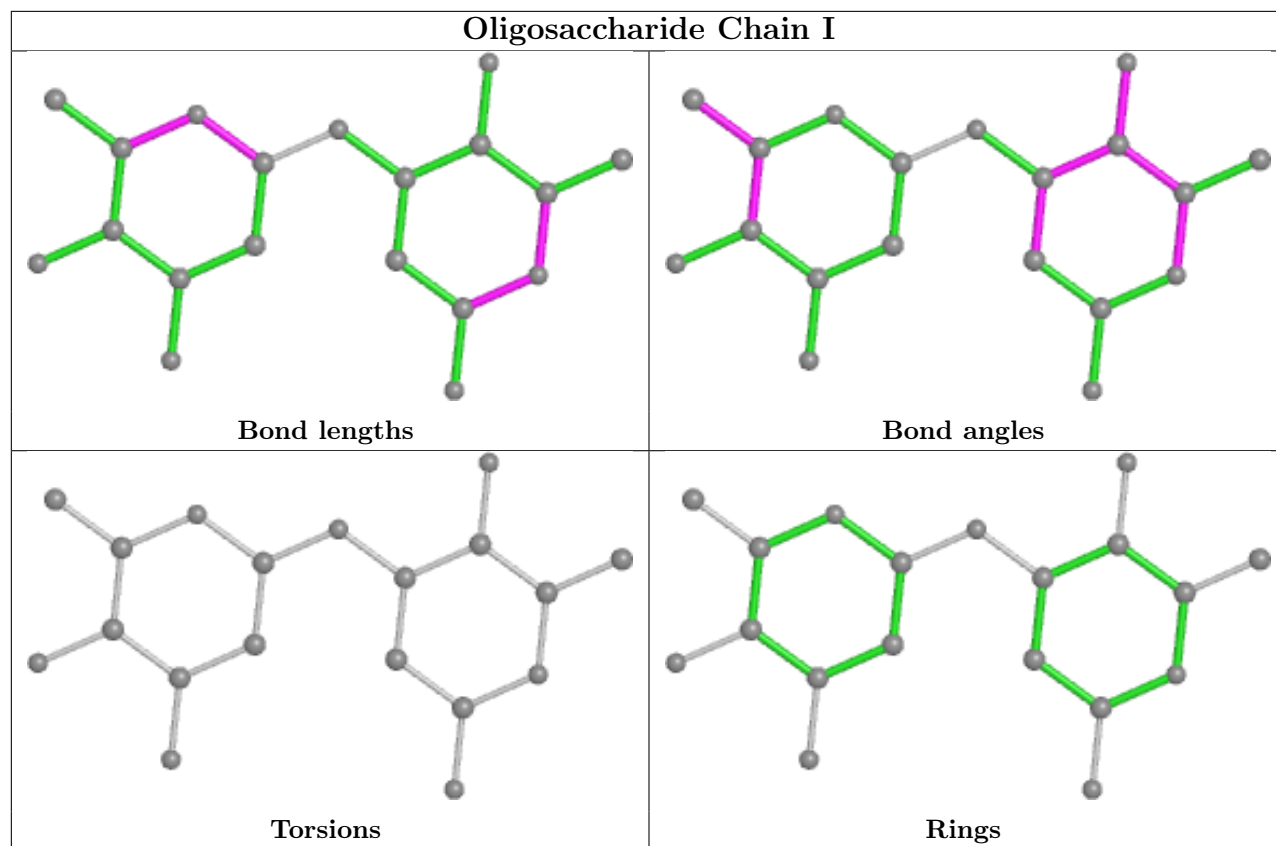
There are no torsion outliers.

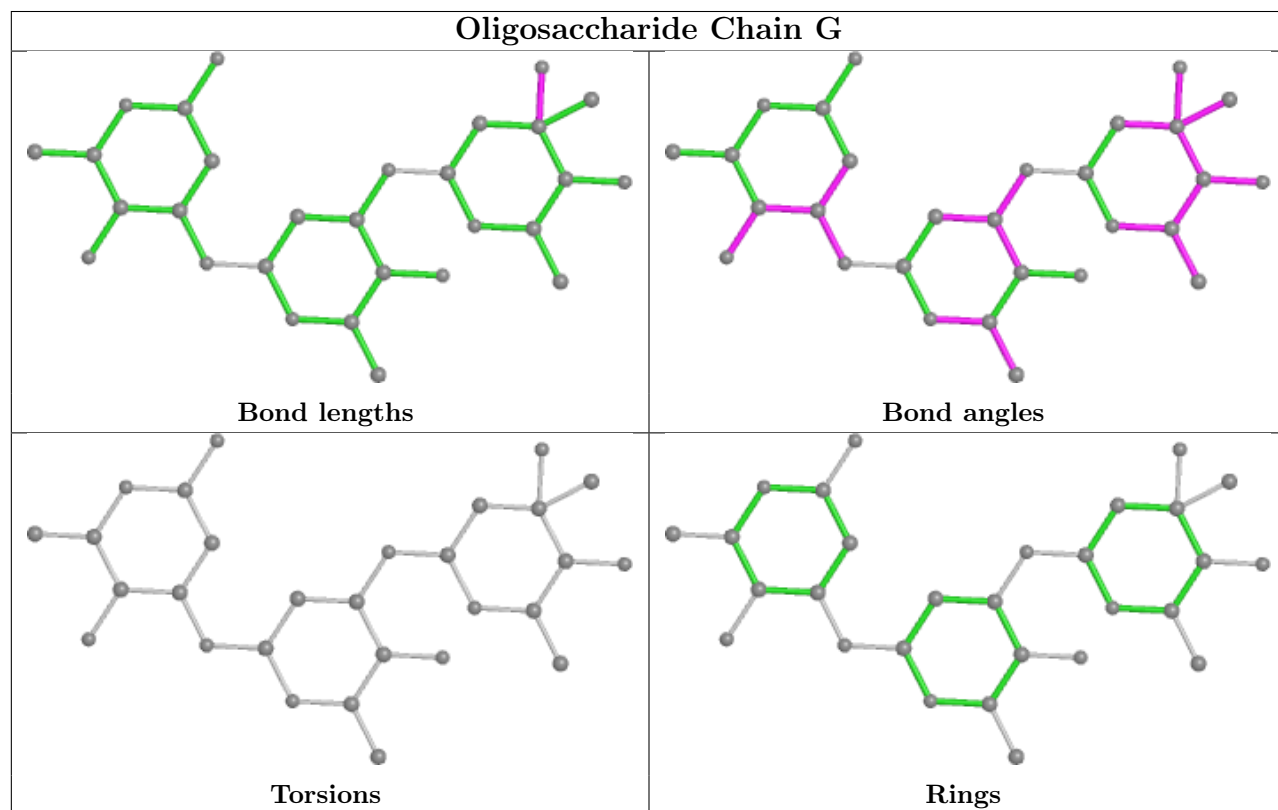
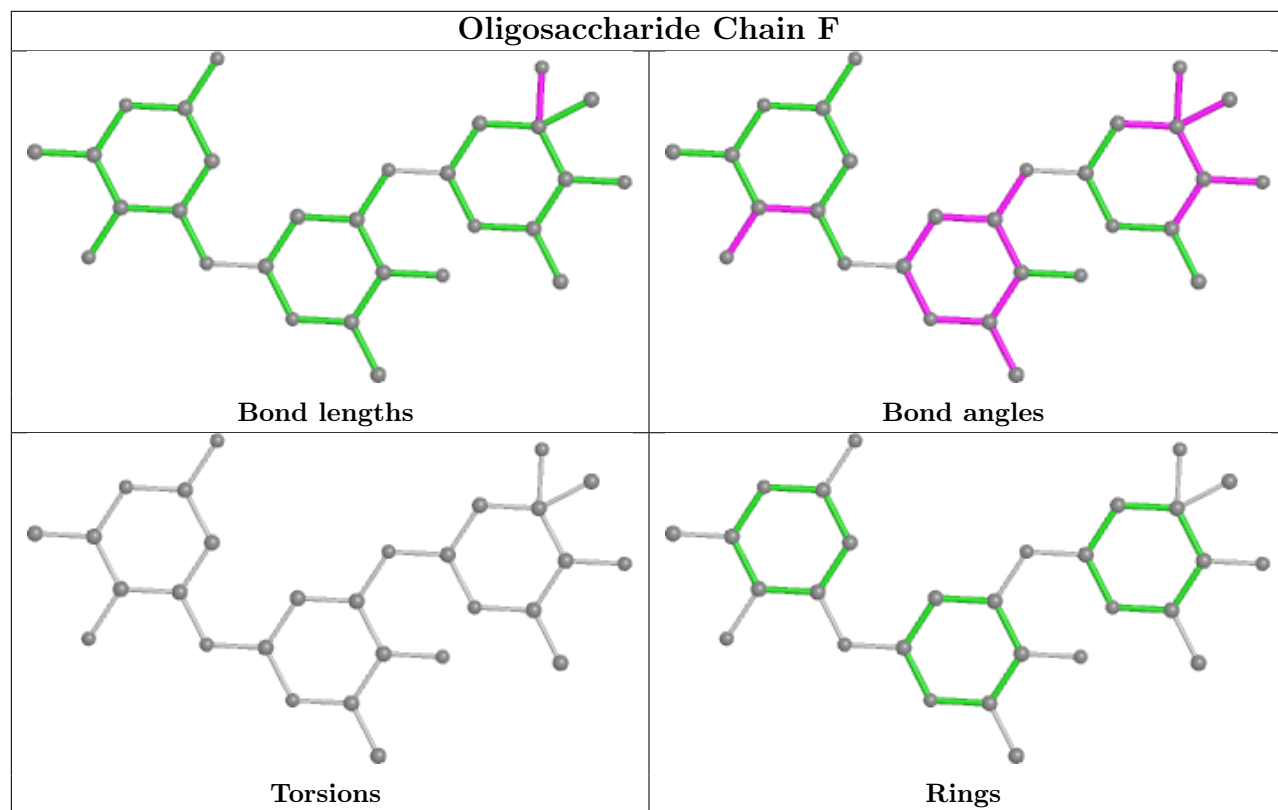
There are no ring outliers.

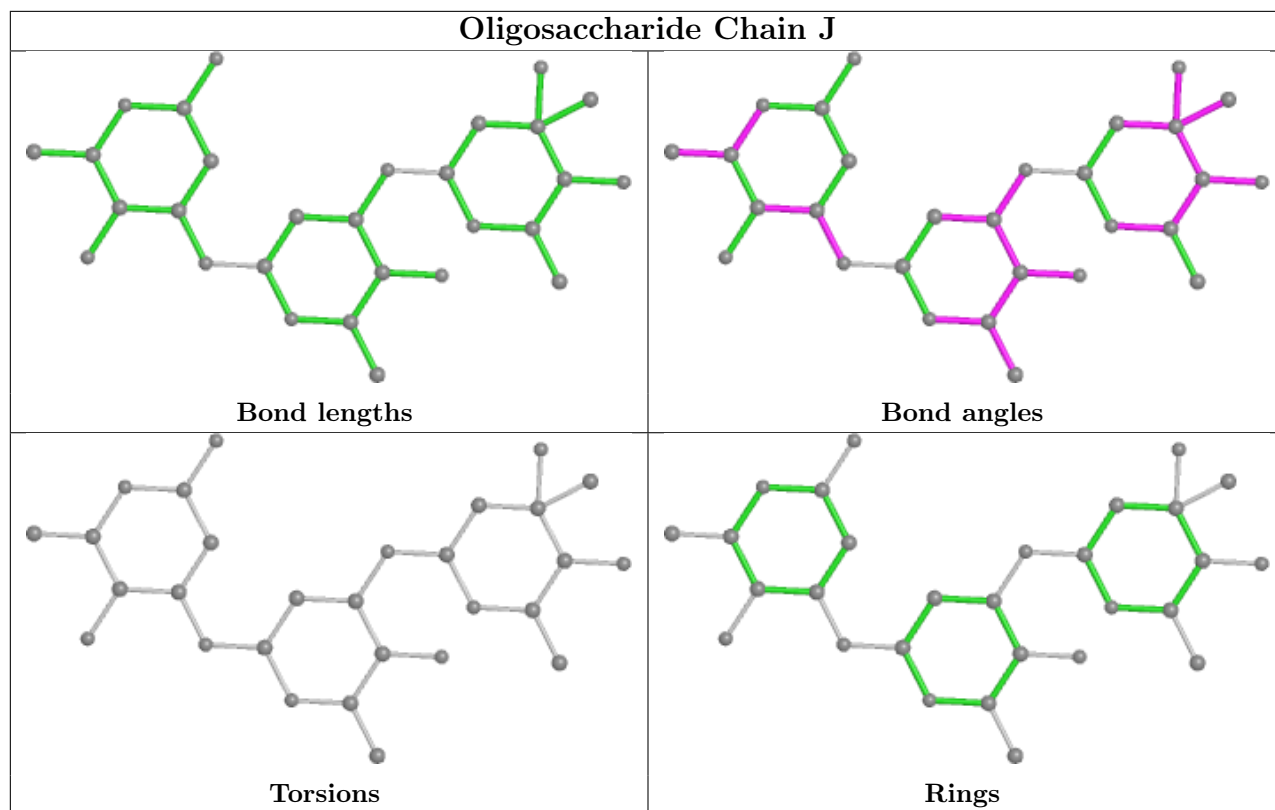
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











6.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds for which Mogul statistics could be retrieved, the number of bonds that are observed in the model and the number of bonds 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 is the number of standard deviations the observed value is removed from the expected value. A bond length with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond lengths.

| Mol | Type | Chain | Res | Link | Bond lengths | | |
|-----|------|-------|-----|-------|--------------|------|---------|
| | | | | | Counts | RMSZ | #Z>2 |
| 5 | DXB | B | 20 | 2,3,4 | 29,30,30 | 1.17 | 1 (3%) |
| 5 | DXB | B | 19 | 2,3,4 | 29,30,30 | 1.14 | 1 (3%) |
| 5 | DXB | A | 22 | 2,3,4 | 29,30,30 | 4.08 | 8 (27%) |
| 5 | DXB | A | 21 | 2,3,4 | 29,30,30 | 1.11 | 2 (6%) |

In the following table, the Counts columns list the number of angles for which Mogul statistics could be retrieved, the number of angles that are observed in the model and the number of 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 angle is the number of standard

deviations the observed value is removed from the expected value. A bond angle with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the average root-mean-square of all Z scores of the bond angles.

| Mol | Type | Chain | Res | Link | Bond angles | | |
|-----|------|-------|-----|-------|-------------|------|---------|
| | | | | | Counts | RMSZ | #Z>2 |
| 5 | DXB | B | 20 | 2,3,4 | 37,45,45 | 1.45 | 8 (21%) |
| 5 | DXB | B | 19 | 2,3,4 | 37,45,45 | 1.53 | 6 (16%) |
| 5 | DXB | A | 22 | 2,3,4 | 37,45,45 | 1.74 | 9 (24%) |
| 5 | DXB | A | 21 | 2,3,4 | 37,45,45 | 1.36 | 3 (8%) |

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

| Mol | Type | Chain | Res | Link | Chirals | Torsions | Rings |
|-----|------|-------|-----|-------|---------|------------|---------|
| 5 | DXB | B | 20 | 2,3,4 | - | 0,18,30,30 | 0,3,3,3 |
| 5 | DXB | B | 19 | 2,3,4 | - | 0,18,30,30 | 0,3,3,3 |
| 5 | DXB | A | 22 | 2,3,4 | - | 0,18,30,30 | 0,3,3,3 |
| 5 | DXB | A | 21 | 2,3,4 | - | 0,18,30,30 | 0,3,3,3 |

5 of 12 bond outliers are listed below. They are sorted according to the Z-score.

| Mol | Chain | Res | Type | Atoms | Z | Observed(Å) | Ideal(Å) |
|-----|-------|-----|------|---------|-------|-------------|----------|
| 5 | A | 22 | DXB | O4S-C4S | 14.35 | 1.04 | 1.43 |
| 5 | A | 22 | DXB | C5S-C4S | 11.75 | 1.17 | 1.51 |
| 5 | A | 22 | DXB | O2S-C2S | 8.52 | 1.07 | 1.21 |
| 5 | A | 22 | DXB | O3S-C3S | 4.43 | 1.33 | 1.42 |
| 5 | B | 19 | DXB | C2-C1 | 3.87 | 1.56 | 1.50 |

5 of 26 angle outliers are listed below. They are sorted according to the Z-score.

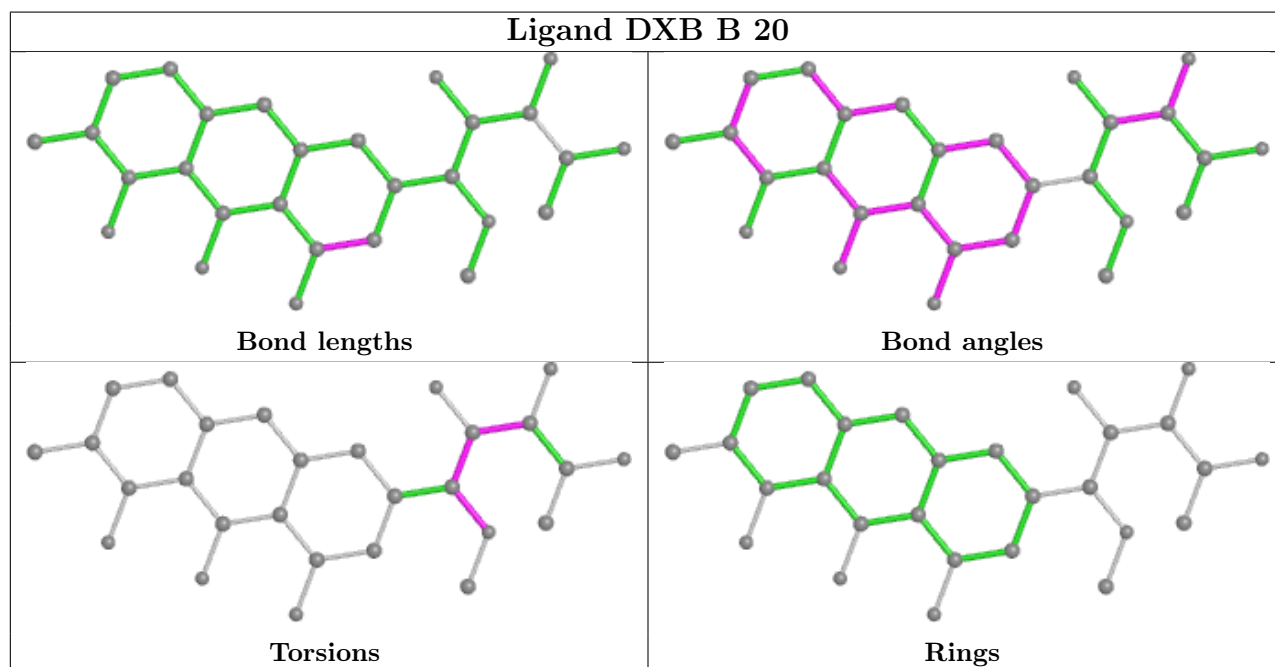
| Mol | Chain | Res | Type | Atoms | Z | Observed(°) | Ideal(°) |
|-----|-------|-----|------|-------------|------|-------------|----------|
| 5 | B | 19 | DXB | C9-C9A-C1 | 4.45 | 121.12 | 119.50 |
| 5 | A | 22 | DXB | C9-C9A-C1 | 4.22 | 121.04 | 119.50 |
| 5 | A | 22 | DXB | O4S-C4S-C5S | 4.20 | 97.30 | 109.74 |
| 5 | A | 22 | DXB | C5-C5A-C10 | 3.44 | 115.94 | 122.02 |
| 5 | A | 21 | DXB | C3-C2-C1 | 3.21 | 105.97 | 113.37 |

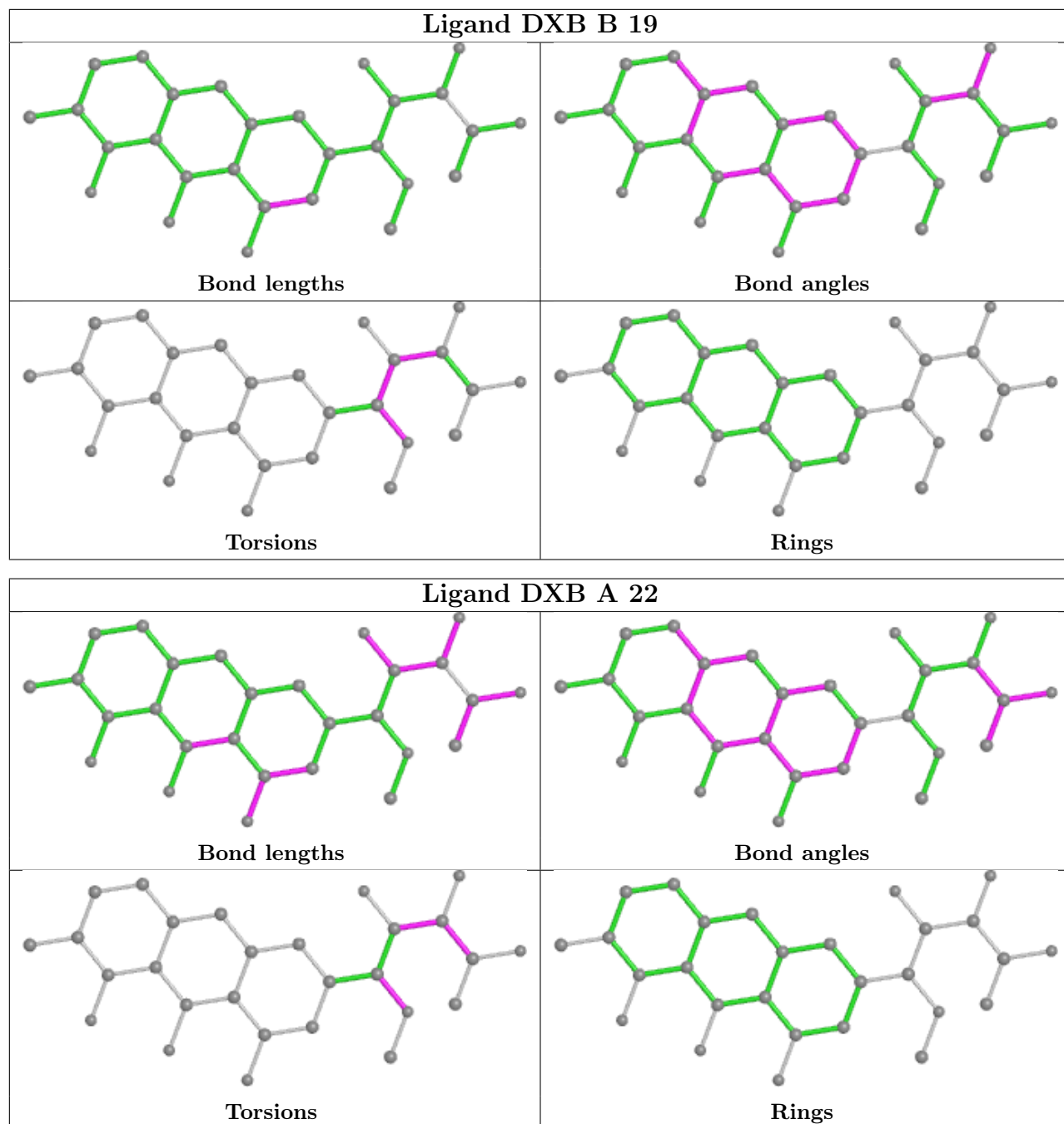
There are no chirality outliers.

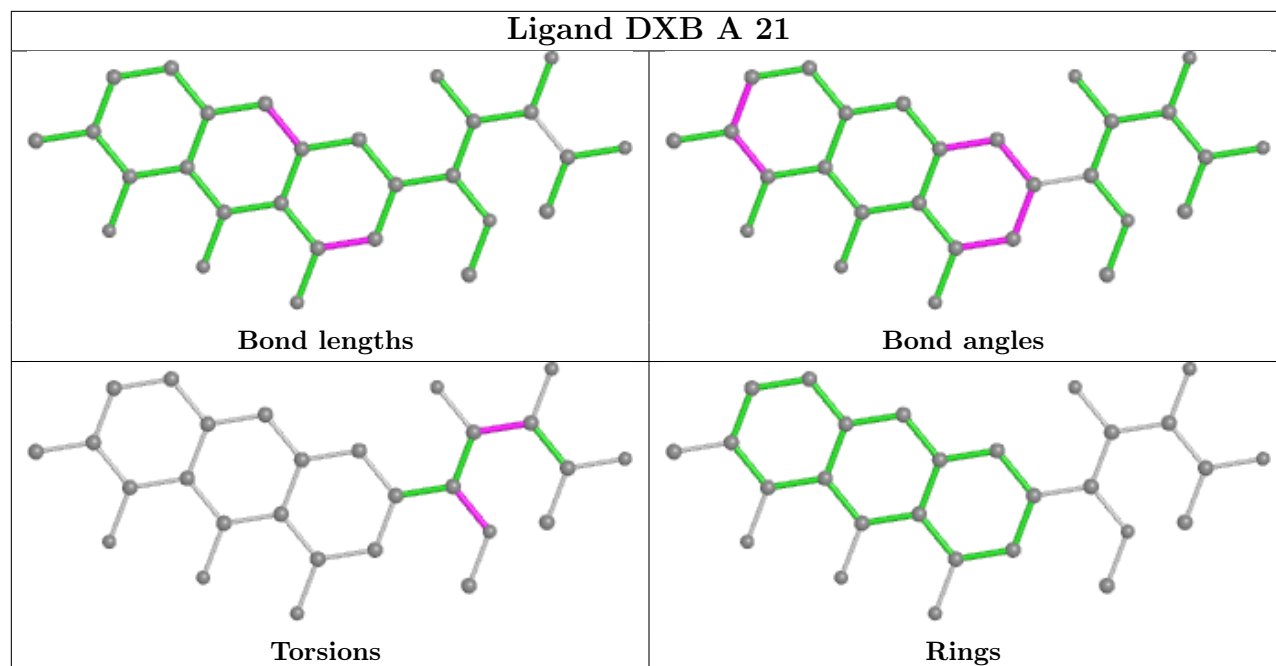
There are no torsion outliers.

There are no ring outliers.

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







6.7 Other polymers [\(i\)](#)

There are no such molecules in this entry.

6.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

7 Chemical shift validation

No chemical shift data were provided