# WORLDWIDE PDB

PROTEIN DATA BANK

# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 4, 2023 – 07:07 PM EDT

|  |  |  |
|---|---|---|
| PDB ID | : | 6ORF |
| Title | : | Crystal structure of SpGH29 |
| Authors | : | Pluvinage, B.; Boraston, A.B. |
| Deposited on | : | 2019-04-30 |
| Resolution | : | 1.70 Å(reported) |

This is a wwPDB X-ray 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/XrayValidationReportHelp
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:

|  |  |  |
|---|---|---|
| MolProbity | : | FAILED |
| Mogul | : | 1.8.5 (274361), CSD as541be (2020) |
| Xtriage (Phenix) | : | 1.13 |
| EDS | : | FAILED |
| Percentile statistics | : | 20191225.v01 (using entries in the PDB archive December 25th 2019) |
| Ideal geometry (proteins) | : | Engh & Huber (2001) |
| Ideal geometry (DNA, RNA) | : | Parkinson et al. (1996) |
| Validation Pipeline (wwPDB-VP) | : | 2.35.1 |

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.70 Å.

There are no overall percentile quality scores available for this entry.

ENTRY-COMPOSITION INFOmissingINFO

SEQUENCE-PLOTS INFOmissingINFO

# 2 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

| Property | Value | Source |
|---|---|---|
| Space group | P 1 21 1 | Depositor |
| Cell constants<br>a, b, c, $\alpha$, $\beta$, $\gamma$ | 69.99Å    98.98Å    79.09Å<br>90.00°    97.57°     90.00° | Depositor |
| Resolution (Å) | 49.54   –   1.70 | Depositor |
| % Data completeness<br>(in resolution range) | 96.6 (49.54-1.70) | Depositor |
| $R_{merge}$ | 0.07 | Depositor |
| $R_{sym}$ | (Not available) | Depositor |
| $< I/\sigma(I) >$ [1] | 3.63 (at 1.70Å) | Xtriage |
| Refinement program | REFMAC 5.8.0238 | Depositor |
| R, $R_{free}$ | 0.174   ,   0.210 | Depositor |
| Wilson B-factor (Å$^2$) | 16.3 | Xtriage |
| Anisotropy | 0.041 | Xtriage |
| L-test for twinning[2] | $< |L| > = 0.46, < L^2 > = 0.29$ | Xtriage |
| Estimated twinning fraction | No twinning to report. | Xtriage |
| Total number of atoms | 8453 | wwPDB-VP |
| Average B, all atoms (Å$^2$) | 18.0 | wwPDB-VP |

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

# 3 Model quality ⓘ

## 3.1 Standard geometry ⓘ

MolProbity failed to run properly - this section is therefore empty.

## 3.2 Too-close contacts ⓘ

MolProbity failed to run properly - this section is therefore empty.

## 3.3 Torsion angles ⓘ

### 3.3.1 Protein backbone ⓘ

MolProbity failed to run properly - this section is therefore empty.

### 3.3.2 Protein sidechains ⓘ

MolProbity failed to run properly - this section is therefore empty.

### 3.3.3 RNA ⓘ

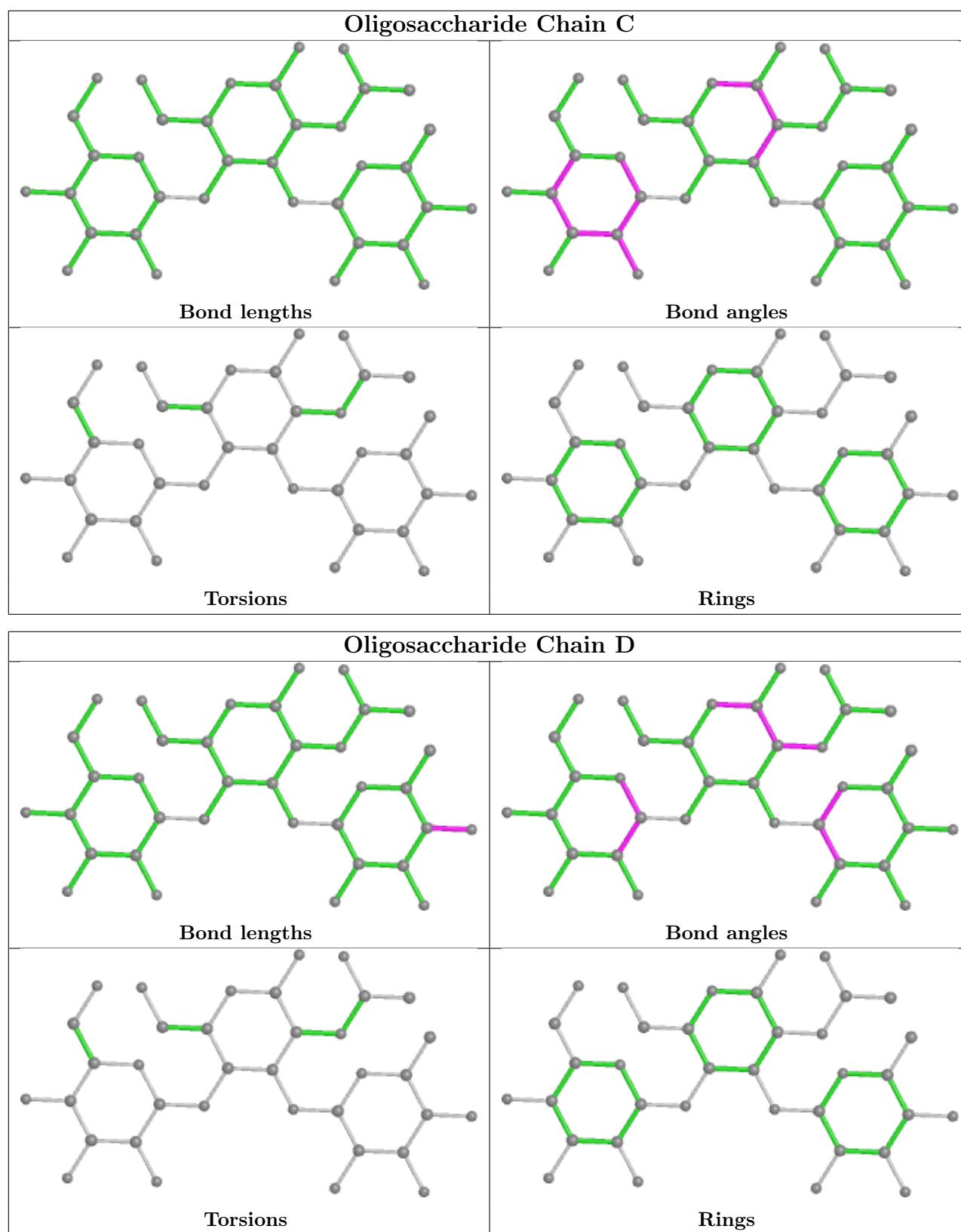MolProbity failed to run properly - this section is therefore empty.

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

validation-pack failed to run properly - this section is therefore empty.

## 3.5 Carbohydrates ⓘ

validation-pack failed to run properly - this section is therefore empty.

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 C**

Bond lengths

Bond angles

Torsions

Rings

**Oligosaccharide Chain D**

Bond lengths

Bond angles

Torsions

Rings

## 3.6   Ligand geometry ⓘ

validation-pack failed to run properly - this section is therefore empty.

## 3.7   Other polymers ⓘ

validation-pack failed to run properly - this section is therefore empty.

## 3.8   Polymer linkage issues ⓘ

There are no chain breaks in this entry.

# 4 Fit of model and data ⓘ

## 4.1 Protein, DNA and RNA chains ⓘ

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

## 4.3 Carbohydrates ⓘ

EDS failed to run properly - this section is therefore empty.

## 4.4 Ligands ⓘ

EDS failed to run properly - this section is therefore empty.

## 4.5 Other polymers ⓘ

EDS failed to run properly - this section is therefore empty.