



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 4, 2023 – 07:07 PM EDT

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

This is a Full wwPDB X-ray Structure Validation 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>.

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)
Xtrriage (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

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

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

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

Xtrriage'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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

3 Model quality [i](#)

3.1 Standard geometry [i](#)

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3.2 Too-close contacts [i](#)

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3.3 Torsion angles [i](#)

3.3.1 Protein backbone [i](#)

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3.3.2 Protein sidechains [i](#)

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3.3.3 RNA [i](#)

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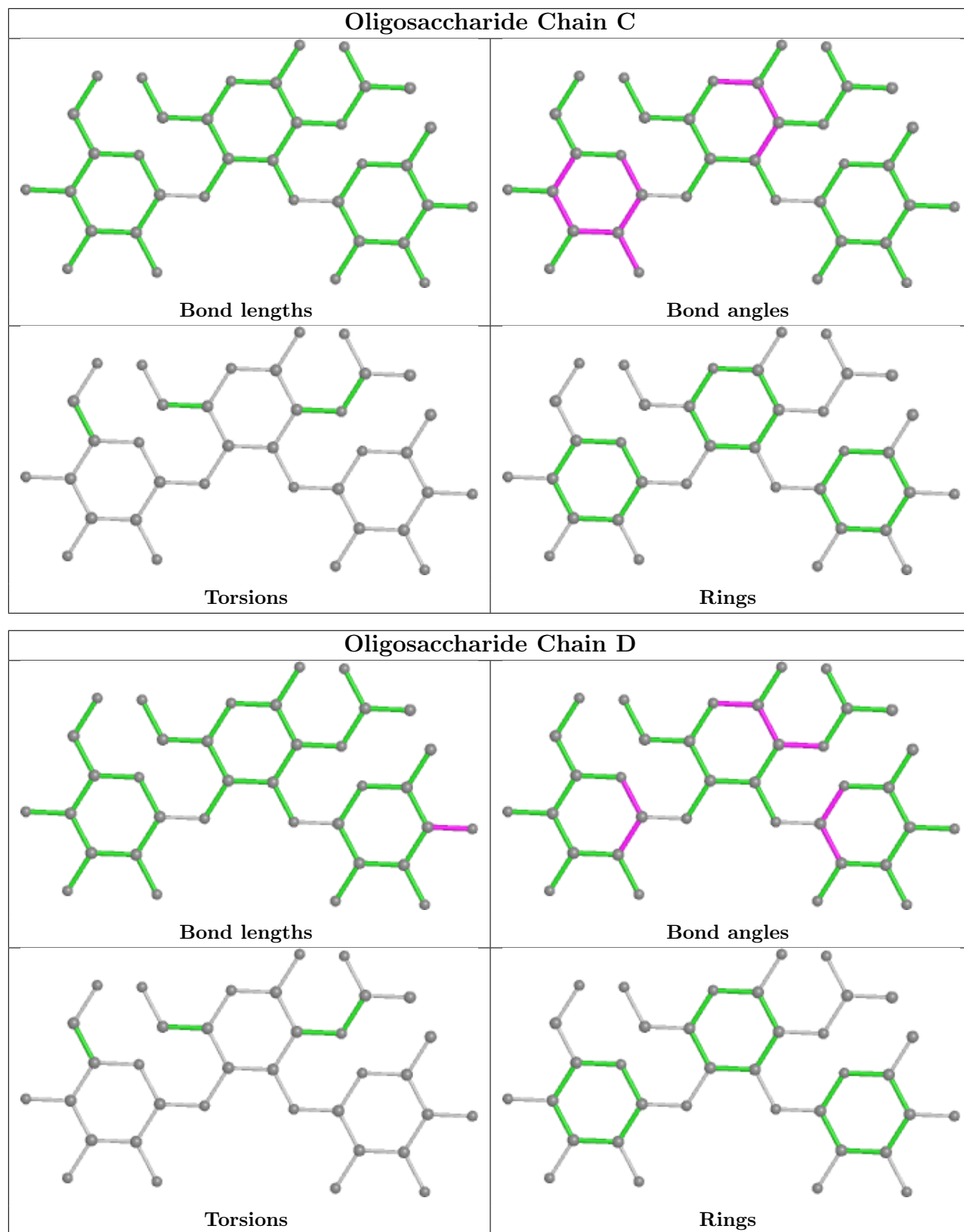
3.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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3.5 Carbohydrates [i](#)

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



3.6 Ligand geometry [i](#)

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3.7 Other polymers [i](#)

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3.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

4 Fit of model and data [i](#)

4.1 Protein, DNA and RNA chains [i](#)

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

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

4.3 Carbohydrates [i](#)

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

4.4 Ligands [i](#)

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

4.5 Other polymers [i](#)

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