



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 02:10 AM EDT

PDB ID : 6VU6  
Title : Sialic acid binding region of Streptococcus Sanguinis SK1 adhesin bound to 3'sLn  
Authors : Stubbs, H.E.; Iverson, T.M.  
Deposited on : 2020-02-14  
Resolution : 2.10 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](mailto: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)  
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 2.10 Å.

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

MolProbity and EDS failed to run properly - the sequence quality summary graphics cannot be shown.

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6792 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Adhesin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	A	409	3136	1947	545	644	0	0	0
1	E	409	3147	1953	549	645	0	1	0

- Molecule 2 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-3)-beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	3	46	25	2	19	0	0	0
2	C	3	46	25	2	19	0	0	0
2	D	3	46	25	2	19	0	0	0
2	F	3	46	25	2	19	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
3	A	4	4	4	0	0
3	E	4	4	4	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	174	174	174	0	0

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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	E	143	Total 143	O 143	0	0

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

### 3 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.21Å 269.86Å 47.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.10 – 2.10	Depositor
% Data completeness (in resolution range)	87.4 (35.10-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.51 (at 2.08Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.225 , 0.248	Depositor
Wilson B-factor (Å <sup>2</sup> )	32.0	Xtrriage
Anisotropy	0.450	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6792	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.72% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical 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.

## 4 Model quality [i](#)

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

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

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### 4.3 Torsion angles [i](#)

#### 4.3.1 Protein backbone [i](#)

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#### 4.3.2 Protein sidechains [i](#)

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

#### 4.3.3 RNA [i](#)

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

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

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

### 4.5 Carbohydrates [i](#)

12 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
2	NAG	B	1	2	15,15,15	0.58	0	21,21,21	0.77	1 (4%)
2	GAL	B	2	2	11,11,12	1.40	1 (9%)	15,15,17	1.65	2 (13%)
2	SIA	B	3	2	20,20,21	2.98	2 (10%)	24,28,31	1.68	3 (12%)
2	NAG	C	1	2	15,15,15	0.20	0	21,21,21	0.39	0
2	GAL	C	2	2	11,11,12	1.02	1 (9%)	15,15,17	0.98	2 (13%)
2	SIA	C	3	2	20,20,21	2.52	2 (10%)	24,28,31	1.81	5 (20%)
2	NAG	D	1	2	15,15,15	0.32	0	21,21,21	0.51	0
2	GAL	D	2	2	11,11,12	0.72	0	15,15,17	0.92	1 (6%)
2	SIA	D	3	2	20,20,21	2.43	4 (20%)	24,28,31	1.78	8 (33%)
2	NAG	F	1	2	15,15,15	0.30	0	21,21,21	0.56	0
2	GAL	F	2	2	11,11,12	0.90	0	15,15,17	1.48	3 (20%)
2	SIA	F	3	2	20,20,21	2.59	3 (15%)	24,28,31	1.56	3 (12%)

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	NAG	B	1	2	-	4/6/26/26	0/1/1/1
2	GAL	B	2	2	-	1/2/19/22	0/1/1/1
2	SIA	B	3	2	-	2/18/34/38	0/1/1/1
2	NAG	C	1	2	-	2/6/26/26	0/1/1/1
2	GAL	C	2	2	-	2/2/19/22	0/1/1/1
2	SIA	C	3	2	-	3/18/34/38	0/1/1/1
2	NAG	D	1	2	-	2/6/26/26	0/1/1/1
2	GAL	D	2	2	-	2/2/19/22	0/1/1/1
2	SIA	D	3	2	-	8/18/34/38	0/1/1/1
2	NAG	F	1	2	-	0/6/26/26	0/1/1/1
2	GAL	F	2	2	-	1/2/19/22	0/1/1/1
2	SIA	F	3	2	-	3/18/34/38	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3	SIA	C2-C1	12.45	1.63	1.52
2	F	3	SIA	C2-C1	10.12	1.61	1.52
2	C	3	SIA	C2-C1	9.94	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	SIA	C2-C1	8.93	1.60	1.52
2	B	2	GAL	O5-C1	-3.68	1.37	1.43
2	D	3	SIA	C7-C6	3.64	1.57	1.53
2	F	3	SIA	O6-C2	3.25	1.48	1.43
2	D	3	SIA	O6-C2	3.16	1.48	1.43
2	C	3	SIA	O6-C2	3.12	1.47	1.43
2	B	3	SIA	O6-C2	3.09	1.47	1.43
2	D	3	SIA	C8-C7	2.64	1.58	1.53
2	C	2	GAL	O5-C1	-2.31	1.40	1.43
2	F	3	SIA	O1A-C1	2.08	1.28	1.22

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	SIA	O6-C2-C3	-5.05	103.51	110.46
2	C	3	SIA	O6-C2-C3	-4.72	103.96	110.46
2	F	3	SIA	O6-C2-C3	-4.35	104.47	110.46
2	F	2	GAL	C1-O5-C5	3.77	117.30	112.19
2	B	2	GAL	O5-C5-C6	-3.75	101.33	107.20
2	D	3	SIA	O6-C2-C3	-3.58	105.54	110.46
2	B	2	GAL	C1-O5-C5	3.54	116.99	112.19
2	D	3	SIA	C4-C5-N5	-3.43	103.59	110.38
2	C	3	SIA	O1A-C1-C2	-3.15	115.13	122.57
2	C	3	SIA	C5-N5-C10	2.75	129.86	123.18
2	C	3	SIA	C4-C5-N5	-2.67	105.10	110.38
2	D	3	SIA	O8-C8-C7	2.66	115.56	109.10
2	B	1	NAG	C1-O5-C5	2.63	118.62	113.66
2	F	3	SIA	O9-C9-C8	-2.63	105.35	111.07
2	B	3	SIA	O6-C2-C1	2.52	112.64	107.70
2	D	3	SIA	O1A-C1-C2	-2.52	116.62	122.57
2	D	3	SIA	C5-N5-C10	2.42	129.07	123.18
2	F	3	SIA	C4-C3-C2	2.41	114.13	109.81
2	C	2	GAL	O2-C2-C3	-2.38	105.37	110.14
2	D	3	SIA	C6-O6-C2	2.38	116.42	111.34
2	D	3	SIA	O6-C2-C1	2.28	112.16	107.70
2	C	3	SIA	C6-O6-C2	2.21	116.07	111.34
2	D	3	SIA	O7-C7-C8	2.20	114.12	108.81
2	D	2	GAL	C1-O5-C5	2.19	115.16	112.19
2	B	3	SIA	C4-C3-C2	2.16	113.68	109.81
2	F	2	GAL	O5-C5-C6	-2.14	103.84	107.20
2	F	2	GAL	C1-C2-C3	2.07	112.20	109.67
2	C	2	GAL	C1-C2-C3	2.02	112.15	109.67



There are no chirality outliers.

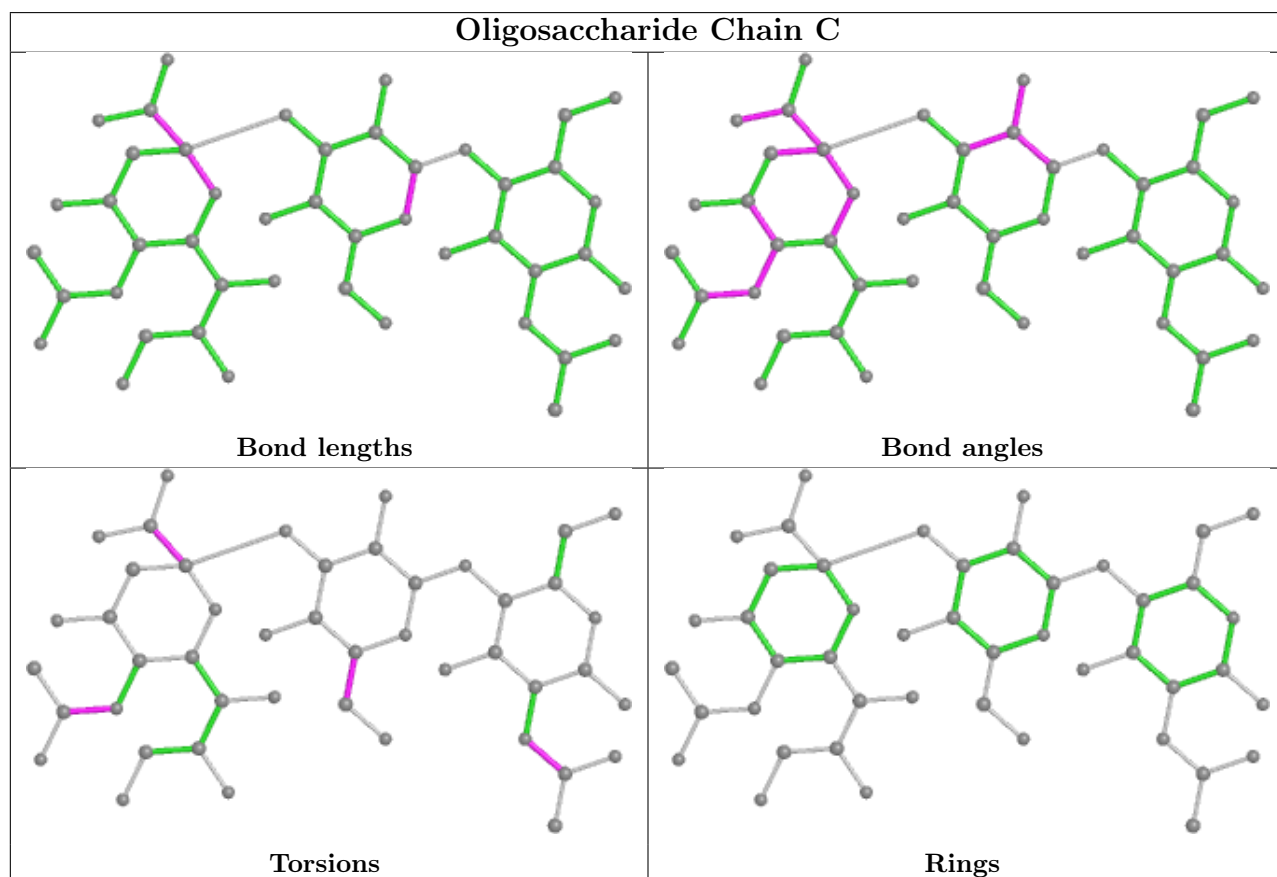
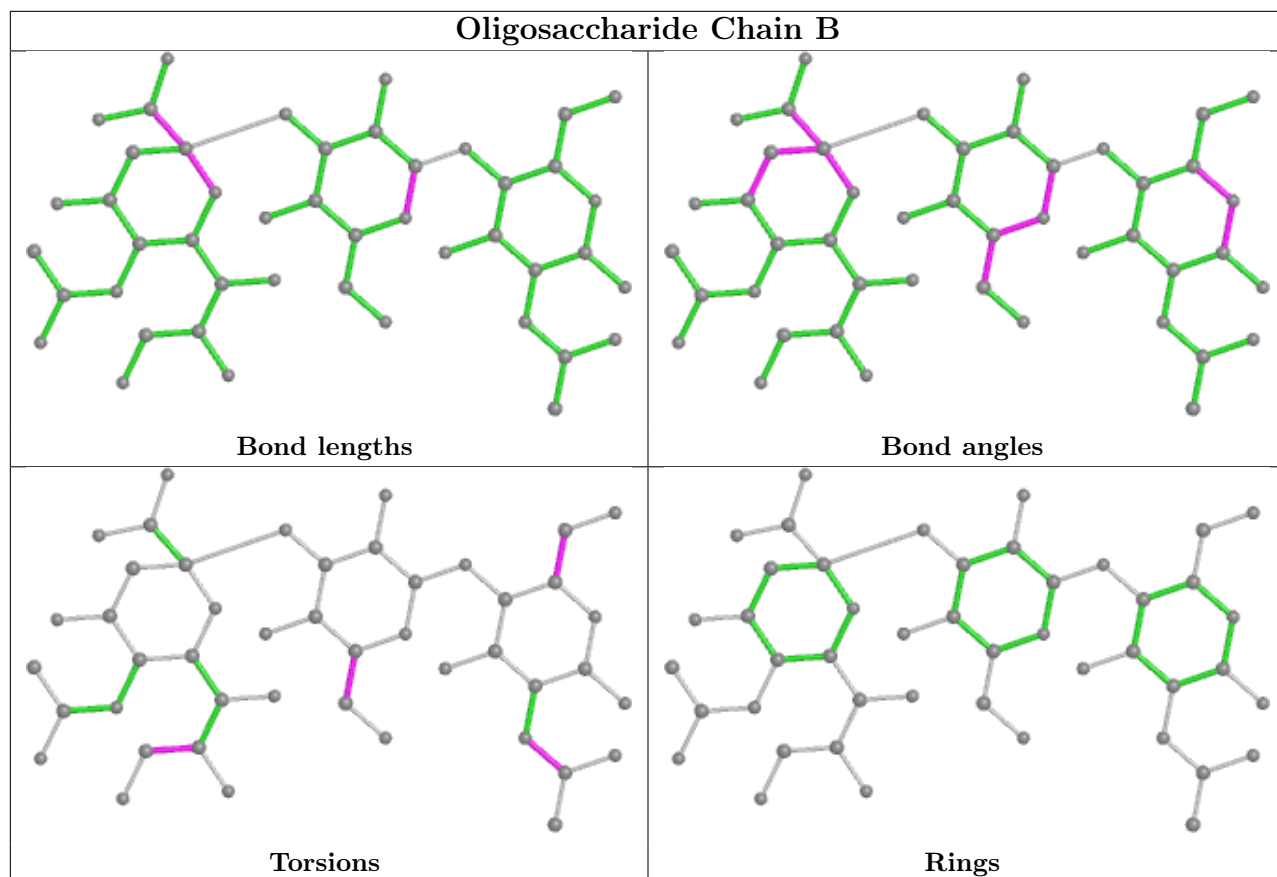
All (30) torsion outliers are listed below:

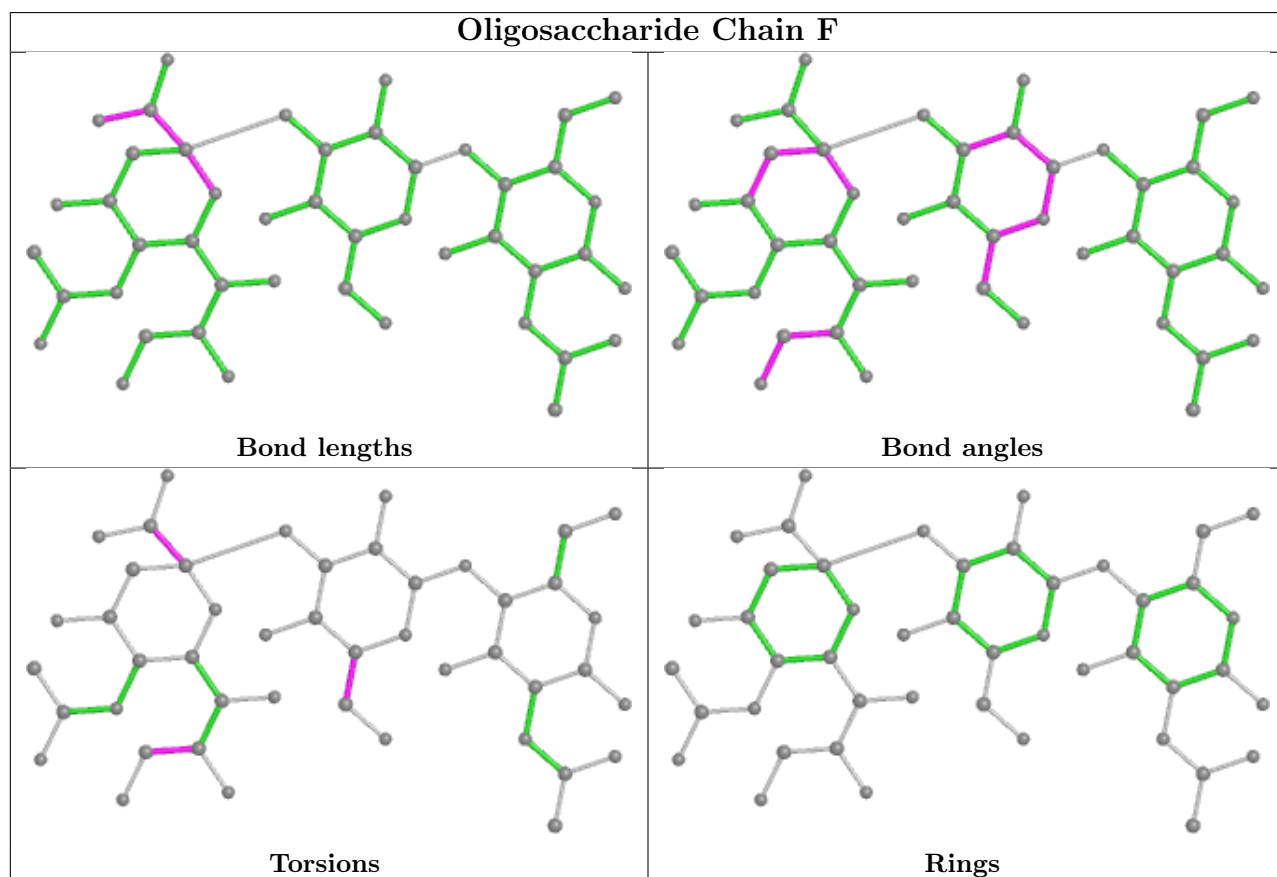
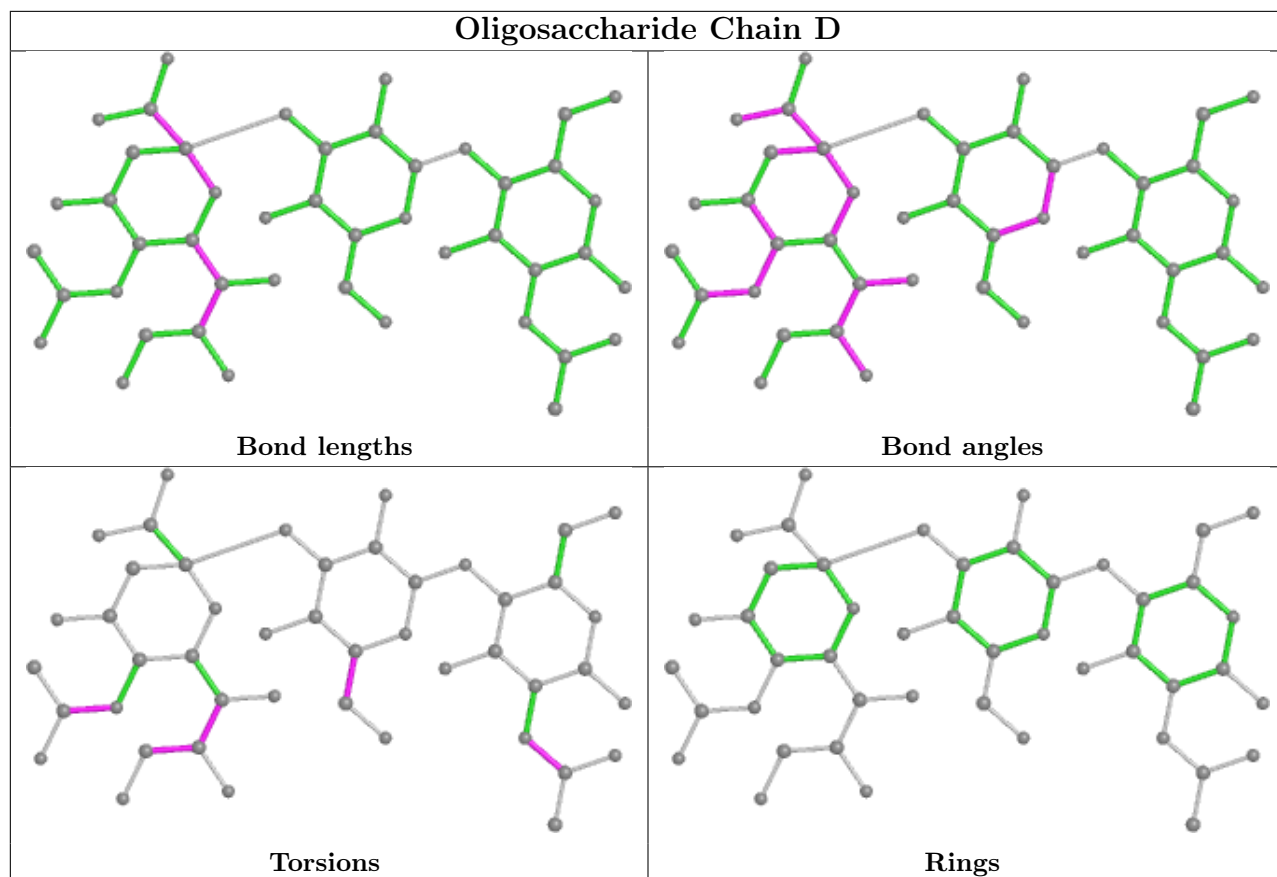
Mol	Chain	Res	Type	Atoms
2	B	3	SIA	O8-C8-C9-O9
2	D	3	SIA	C6-C7-C8-C9
2	D	3	SIA	O7-C7-C8-C9
2	D	3	SIA	O7-C7-C8-O8
2	D	2	GAL	O5-C5-C6-O6
2	D	3	SIA	O8-C8-C9-O9
2	B	3	SIA	C7-C8-C9-O9
2	B	1	NAG	C4-C5-C6-O6
2	D	2	GAL	C4-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
2	C	2	GAL	C4-C5-C6-O6
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	3	SIA	C11-C10-N5-C5
2	C	3	SIA	O10-C10-N5-C5
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	3	SIA	C11-C10-N5-C5
2	D	3	SIA	O10-C10-N5-C5
2	C	2	GAL	O5-C5-C6-O6
2	F	3	SIA	C7-C8-C9-O9
2	D	3	SIA	C6-C7-C8-O8
2	D	3	SIA	C7-C8-C9-O9
2	B	2	GAL	O5-C5-C6-O6
2	F	3	SIA	O8-C8-C9-O9
2	C	3	SIA	O1A-C1-C2-O6
2	F	3	SIA	O1A-C1-C2-O6
2	F	2	GAL	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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





## 4.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 4.7 Other polymers

There are no such residues in this entry.

## 4.8 Polymer linkage issues

There are no chain breaks in this entry.

## 5 Fit of model and data

### 5.1 Protein, DNA and RNA chains

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

### 5.2 Non-standard residues in protein, DNA, RNA chains

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

### 5.3 Carbohydrates

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

### 5.4 Ligands

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

### 5.5 Other polymers

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