



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 06:53 AM EDT

PDB ID : 6V49  
Title : The crystal structure of hemagglutinin from A/wedge-tailed shearwater/Western Australia/2576/1979 (H15N9)  
Authors : Yang, H.; Stevens, J.  
Deposited on : 2019-11-27  
Resolution : 2.50 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 2.50 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.

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	B	301	X	-	-	-
4	NAG	D	301	X	-	-	-
4	NAG	F	301	X	-	-	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11781 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 Hemagglutinin HA1 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	329	2516	1566	446	490	14	0	0	0
1	C	329	2516	1566	446	490	14	0	0	0
1	E	329	2516	1566	446	490	14	0	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q20ND8
A	132	SER	THR	conflict	UNP Q20ND8
A	133	SER	VAL	conflict	UNP Q20ND8
C	0	GLY	-	expression tag	UNP Q20ND8
C	132	SER	THR	conflict	UNP Q20ND8
C	133	SER	VAL	conflict	UNP Q20ND8
E	0	GLY	-	expression tag	UNP Q20ND8
E	132	SER	THR	conflict	UNP Q20ND8
E	133	SER	VAL	conflict	UNP Q20ND8

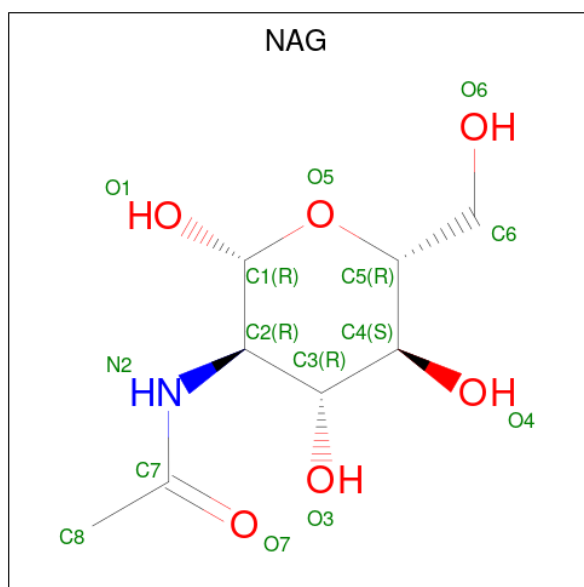
- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	167	1369	843	245	275	6	0	0	0
2	D	167	1369	843	245	275	6	0	0	0
2	F	167	1369	843	245	275	6	0	0	0

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	H	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		

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

### 3 Data and refinement statistics i

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.67Å 101.38Å 163.27Å 90.00° 90.74° 90.00°	Depositor
Resolution (Å)	44.09 – 2.50	Depositor
% Data completeness (in resolution range)	99.4 (44.09-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.230 , 0.265	Depositor
Wilson B-factor (Å <sup>2</sup> )	54.3	Xtrriage
Anisotropy	0.316	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for -h,-k,l	Xtrriage
Total number of atoms	11781	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	70.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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](#)

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

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

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

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

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

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

#### 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](#)

6 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
3	NAG	G	1	3,1	14,14,15	0.55	0	17,19,21	2.44	9 (52%)
3	NAG	G	2	3	14,14,15	1.56	3 (21%)	17,19,21	2.57	7 (41%)
3	NAG	H	1	3,1	14,14,15	0.90	1 (7%)	17,19,21	2.78	8 (47%)
3	NAG	H	2	3	14,14,15	1.23	1 (7%)	17,19,21	2.36	9 (52%)
3	NAG	I	1	3,1	14,14,15	0.67	0	17,19,21	1.94	4 (23%)
3	NAG	I	2	3	14,14,15	0.65	0	17,19,21	1.70	4 (23%)

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
3	NAG	G	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	H	2	3	-	0/6/23/26	0/1/1/1
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	2	NAG	C1-C2	3.80	1.58	1.52
3	G	2	NAG	O5-C1	2.51	1.47	1.43
3	H	1	NAG	O7-C7	2.30	1.28	1.23
3	G	2	NAG	C2-N2	2.24	1.50	1.46
3	H	2	NAG	O4-C4	2.02	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1	NAG	C1-O5-C5	-6.13	103.89	112.19
3	G	1	NAG	C1-O5-C5	-6.07	103.97	112.19
3	G	2	NAG	C1-O5-C5	5.66	119.86	112.19
3	G	2	NAG	O5-C1-C2	5.60	120.13	111.29
3	H	1	NAG	C2-N2-C7	-4.81	116.05	122.90
3	H	2	NAG	O4-C4-C5	4.59	120.70	109.30
3	H	1	NAG	C3-C4-C5	-4.57	102.09	110.24
3	I	2	NAG	O5-C1-C2	3.98	117.58	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	NAG	C2-N2-C7	3.89	128.44	122.90
3	H	2	NAG	C3-C4-C5	-3.88	103.31	110.24
3	I	1	NAG	O4-C4-C5	3.53	118.07	109.30
3	H	1	NAG	O5-C5-C6	3.49	112.67	107.20
3	I	1	NAG	O3-C3-C4	-3.34	102.62	110.35
3	I	2	NAG	O5-C5-C4	-3.30	102.79	110.83
3	G	1	NAG	C2-N2-C7	-3.09	118.50	122.90
3	G	1	NAG	C1-C2-N2	2.99	115.60	110.49
3	H	2	NAG	O5-C5-C6	2.98	111.87	107.20
3	H	1	NAG	O5-C1-C2	-2.78	106.91	111.29
3	I	1	NAG	C1-C2-N2	2.76	115.20	110.49
3	G	1	NAG	O3-C3-C2	-2.69	103.89	109.47
3	G	1	NAG	C6-C5-C4	2.68	119.27	113.00
3	H	2	NAG	O6-C6-C5	-2.63	102.28	111.29
3	H	1	NAG	C6-C5-C4	2.63	119.15	113.00
3	G	1	NAG	C8-C7-N2	2.58	120.46	116.10
3	I	1	NAG	O5-C5-C4	-2.56	104.61	110.83
3	H	2	NAG	C8-C7-N2	-2.55	111.78	116.10
3	H	2	NAG	O7-C7-N2	2.44	126.44	121.95
3	H	2	NAG	O3-C3-C2	2.39	114.40	109.47
3	I	2	NAG	O4-C4-C5	2.38	115.20	109.30
3	G	2	NAG	C1-C2-N2	2.25	114.33	110.49
3	G	1	NAG	O5-C5-C4	-2.25	105.36	110.83
3	G	1	NAG	O5-C5-C6	2.25	110.72	107.20
3	H	1	NAG	C8-C7-N2	-2.22	112.34	116.10
3	G	2	NAG	O7-C7-C8	-2.21	117.95	122.06
3	G	2	NAG	C3-C4-C5	-2.17	106.36	110.24
3	H	2	NAG	C2-N2-C7	2.10	125.90	122.90
3	I	2	NAG	C1-O5-C5	2.07	114.99	112.19
3	G	1	NAG	O4-C4-C5	2.06	114.40	109.30
3	G	2	NAG	C8-C7-N2	2.05	119.58	116.10
3	H	1	NAG	O4-C4-C5	2.05	114.39	109.30
3	H	2	NAG	C6-C5-C4	2.01	117.72	113.00

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C8-C7-N2-C2

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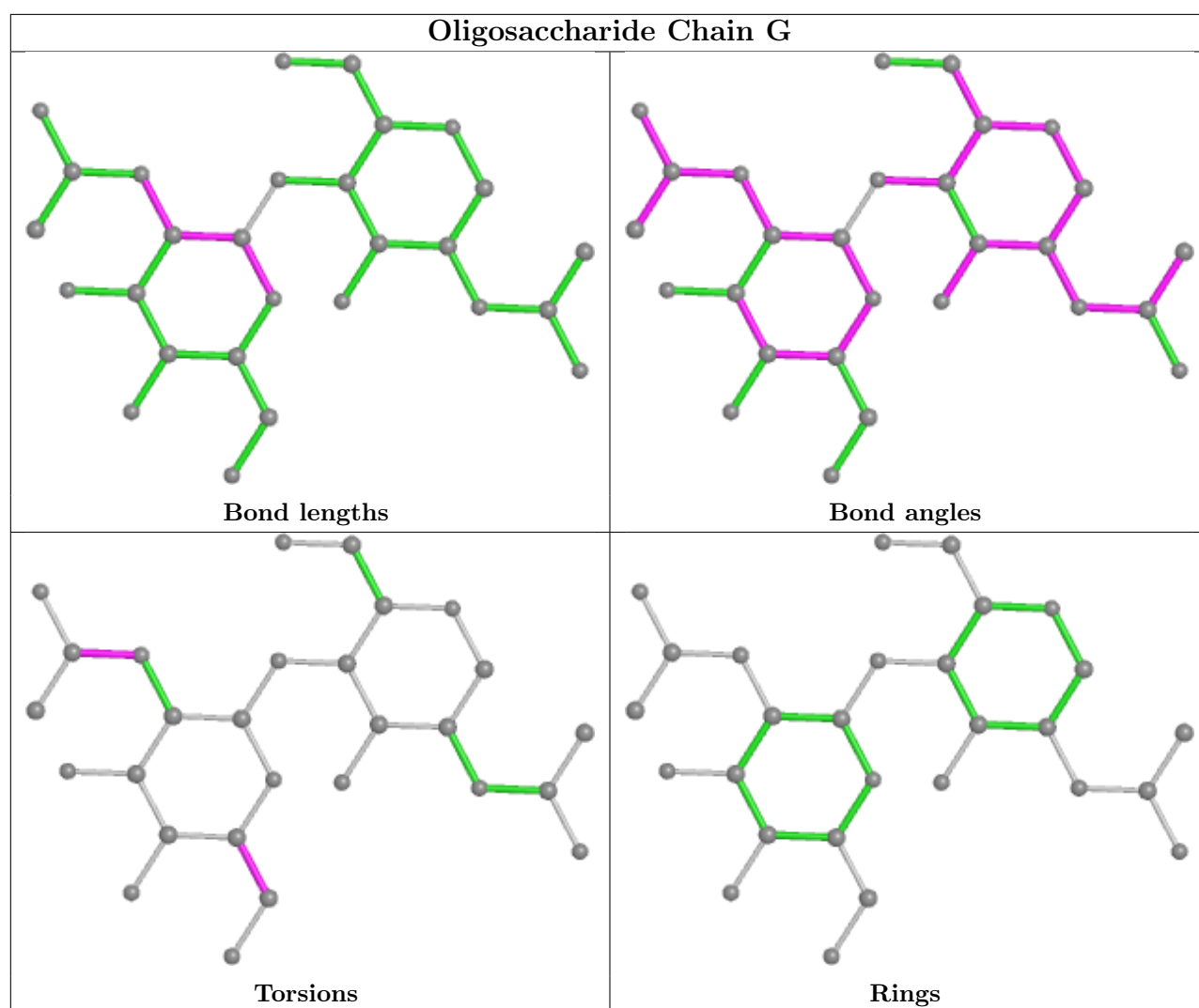
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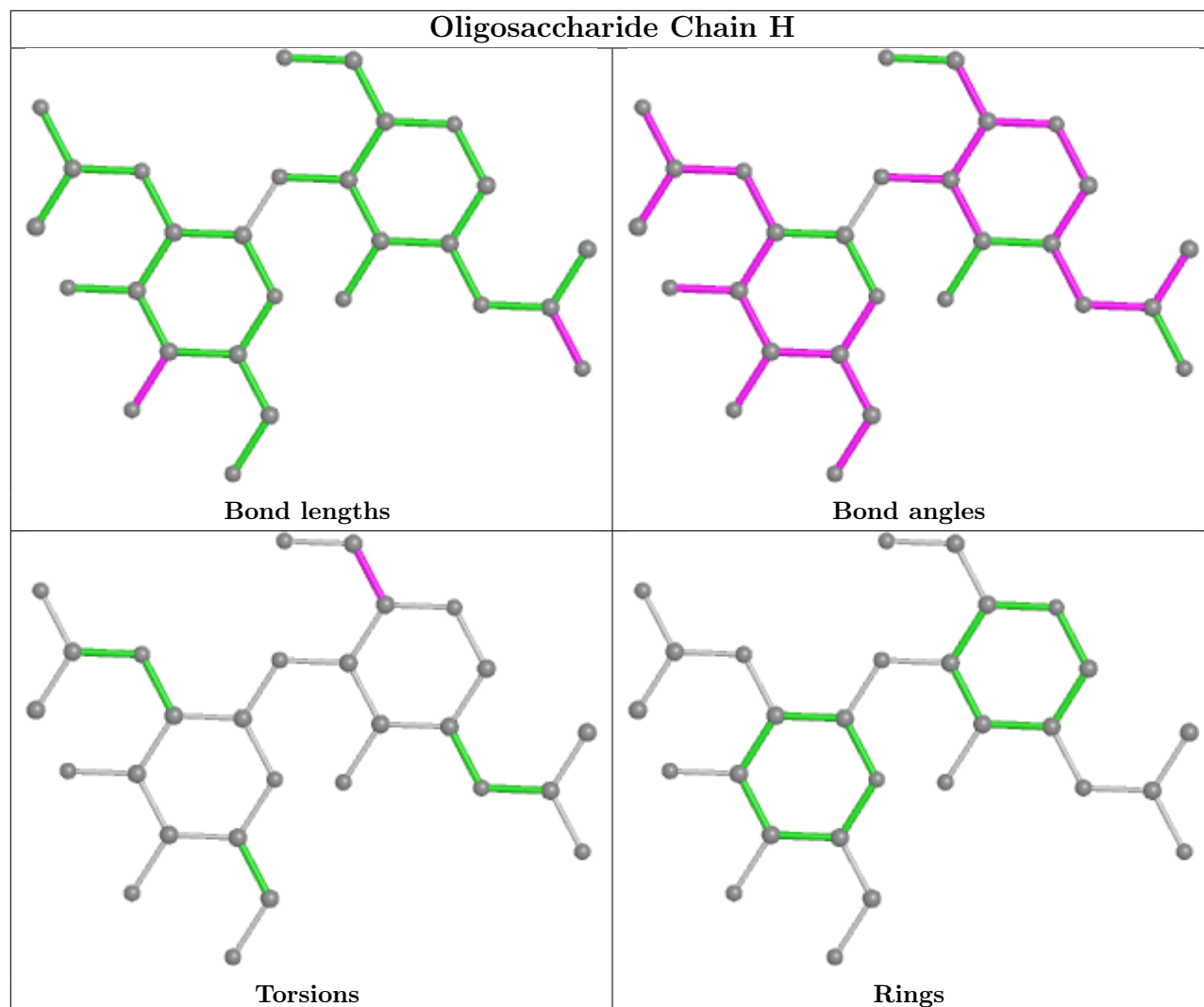
Mol	Chain	Res	Type	Atoms
3	I	1	NAG	O5-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	G	2	NAG	O7-C7-N2-C2
3	H	1	NAG	C4-C5-C6-O6

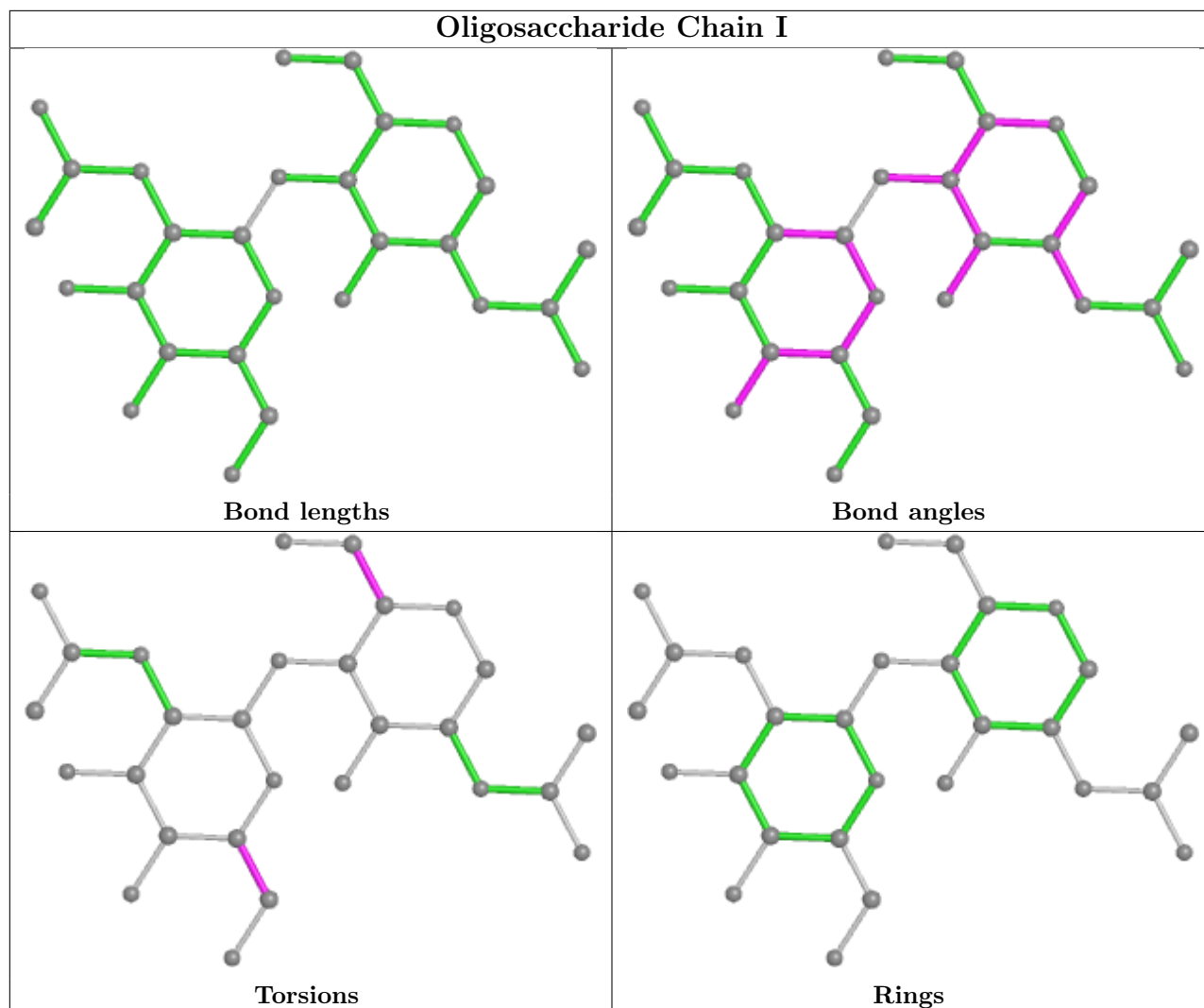
There are no ring outliers.

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 [i](#)

3 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
4	NAG	F	301	2	14,14,15	0.98	1 (7%)	17,19,21	1.90	6 (35%)
4	NAG	B	301	2	14,14,15	1.32	1 (7%)	17,19,21	2.51	10 (58%)
4	NAG	D	301	2	14,14,15	1.25	2 (14%)	17,19,21	1.83	4 (23%)

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
4	NAG	F	301	2	1/1/5/7	3/6/23/26	0/1/1/1
4	NAG	B	301	2	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	D	301	2	1/1/5/7	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	301	NAG	C1-C2	4.21	1.58	1.52
4	D	301	NAG	C1-C2	3.28	1.57	1.52
4	F	301	NAG	C1-C2	2.55	1.56	1.52
4	D	301	NAG	C3-C2	2.31	1.57	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	301	NAG	C4-C3-C2	4.41	117.48	111.02
4	B	301	NAG	C1-O5-C5	4.25	117.96	112.19
4	B	301	NAG	C1-C2-N2	4.18	117.64	110.49
4	F	301	NAG	C4-C3-C2	3.79	116.58	111.02
4	B	301	NAG	O5-C1-C2	3.72	117.17	111.29
4	F	301	NAG	O3-C3-C4	-3.47	102.33	110.35
4	B	301	NAG	O4-C4-C5	3.28	117.44	109.30
4	D	301	NAG	O3-C3-C4	-3.05	103.30	110.35
4	B	301	NAG	O6-C6-C5	-2.99	101.04	111.29
4	F	301	NAG	C6-C5-C4	2.80	119.57	113.00
4	B	301	NAG	O4-C4-C3	-2.76	103.96	110.35
4	F	301	NAG	O4-C4-C5	2.49	115.47	109.30
4	D	301	NAG	C1-C2-N2	2.48	114.72	110.49
4	B	301	NAG	C6-C5-C4	2.45	118.74	113.00
4	F	301	NAG	C2-N2-C7	-2.42	119.46	122.90
4	B	301	NAG	O5-C5-C6	-2.42	103.42	107.20
4	D	301	NAG	O4-C4-C3	-2.37	104.88	110.35
4	B	301	NAG	C3-C4-C5	-2.30	106.14	110.24
4	B	301	NAG	O3-C3-C4	-2.02	105.68	110.35
4	F	301	NAG	O5-C5-C4	-2.00	105.96	110.83

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	301	NAG	C1
4	D	301	NAG	C1
4	F	301	NAG	C1

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	301	NAG	O5-C5-C6-O6
4	D	301	NAG	C8-C7-N2-C2
4	B	301	NAG	C4-C5-C6-O6
4	D	301	NAG	O7-C7-N2-C2
4	F	301	NAG	C8-C7-N2-C2
4	F	301	NAG	O7-C7-N2-C2
4	F	301	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

#### 4.7 Other polymers [i](#)

There are no such residues in this entry.

#### 4.8 Polymer linkage issues [i](#)

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.