Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2023 – 03:40 PM EDT

PDB ID	:	6NS9
Title	:	Crystal structure of the IVR-165 (H3N2) influenza virus hemagglutinin apo form
Authors	:	Wu, N.C.; Wilson, I.A.
Deposited on	:	2019-01-24
Resolution	:	1.95 Å(reported)

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 1.95 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 ⓘ

There are 7 unique types of molecules in this entry. The entry contains 4582 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
1	A	317	Total 2531	C 1594	N 445	O 480	S 12	0	8	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	9	PRO	-	expression tag	UNP L0HR89
A	10	GLY	-	expression tag	UNP L0HR89

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	173	Total 1444	C 906	N 254	O 277	S 7	0	8	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	4	Total 50	C 28	N 2	O 20	0	0	0

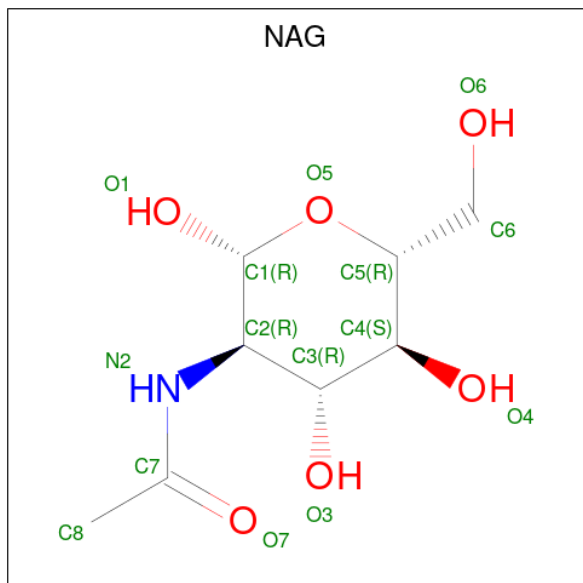- Molecule 4 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	2	Total 28	C 16	N 2	O 10	0	0	0
4	F	2	Total 28	C 16	N 2	O 10	0	0	0

- Molecule 5 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	E	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

NAG

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	206	Total	O	0	0
			206	206		
7	B	200	Total	O	0	0
			200	200		

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	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	100.40Å 100.40Å 382.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 1.95	Depositor
% Data completeness (in resolution range)	100.0 (50.00-1.95)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$<I/\sigma(I)>$ [1]	2.08 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.167 , 0.193	Depositor
Wilson B-factor (Å^2)	31.0	Xtriage
Anisotropy	0.014	Xtriage
L-test for twinning[2]	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4582	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.82% 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.

4 Model quality ⓘ

4.1 Standard geometry ⓘ

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

4.2 Too-close contacts ⓘ

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

4.3 Torsion angles ⓘ

4.3.1 Protein backbone ⓘ

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

4.3.2 Protein sidechains ⓘ

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

4.3.3 RNA ⓘ

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

4.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

4.5 Carbohydrates ⓘ

11 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	C	1	1,3	14,14,15	0.54	0	17,19,21	1.19	2 (11%)
3	NAG	C	2	3	14,14,15	0.36	0	17,19,21	0.83	1 (5%)
3	BMA	C	3	3	11,11,12	0.37	0	15,15,17	0.76	0
3	MAN	C	4	3	11,11,12	0.33	0	15,15,17	0.88	1 (6%)
4	NAG	D	1	4,1	14,14,15	0.34	0	17,19,21	0.90	0
4	NAG	D	2	4	14,14,15	0.48	0	17,19,21	1.34	2 (11%)
5	NAG	E	1	5,1	14,14,15	0.54	0	17,19,21	1.13	2 (11%)
5	NAG	E	2	5	14,14,15	0.38	0	17,19,21	0.77	0
5	BMA	E	3	5	11,11,12	0.40	0	15,15,17	0.91	1 (6%)
4	NAG	F	1	4,1	14,14,15	0.53	0	17,19,21	0.87	0
4	NAG	F	2	4	14,14,15	0.30	0	17,19,21	0.64	0

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	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
3	MAN	C	4	3	-	0/2/19/22	0/1/1/1
4	NAG	D	1	4,1	-	2/6/23/26	0/1/1/1
4	NAG	D	2	4	-	0/6/23/26	0/1/1/1
5	NAG	E	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	E	2	5	-	2/6/23/26	0/1/1/1
5	BMA	E	3	5	-	0/2/19/22	0/1/1/1
4	NAG	F	1	4,1	-	0/6/23/26	0/1/1/1
4	NAG	F	2	4	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	NAG	C4-C3-C2	3.40	116.01	111.02
3	C	2	NAG	C1-O5-C5	2.78	115.96	112.19
3	C	1	NAG	C1-C2-N2	-2.52	106.18	110.49
5	E	1	NAG	C4-C3-C2	2.47	114.64	111.02
3	C	1	NAG	C1-O5-C5	2.41	115.46	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	2	NAG	O5-C5-C6	2.35	110.89	107.20
3	C	4	MAN	C1-O5-C5	2.33	115.34	112.19
5	E	1	NAG	C2-N2-C7	2.20	126.03	122.90
5	E	3	BMA	O5-C5-C6	2.18	110.63	107.20

There are no chirality outliers.

All (8) torsion outliers are listed below:

| Mol	Chain	Res	Type	Atoms
5	E	2	NAG	C4-C5-C6-O6
5	E	2	NAG	O5-C5-C6-O6
4	D	1	NAG	O5-C5-C6-O6
4	F	2	NAG	C4-C5-C6-O6
4	D	1	NAG	C4-C5-C6-O6
4	F	2	NAG	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-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.

Oligosaccharide Chain C

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain D

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain F

Bond lengths

Bond angles

Torsions

Rings

Oligosaccharide Chain E

Bond lengths

Bond angles

Torsions

Rings
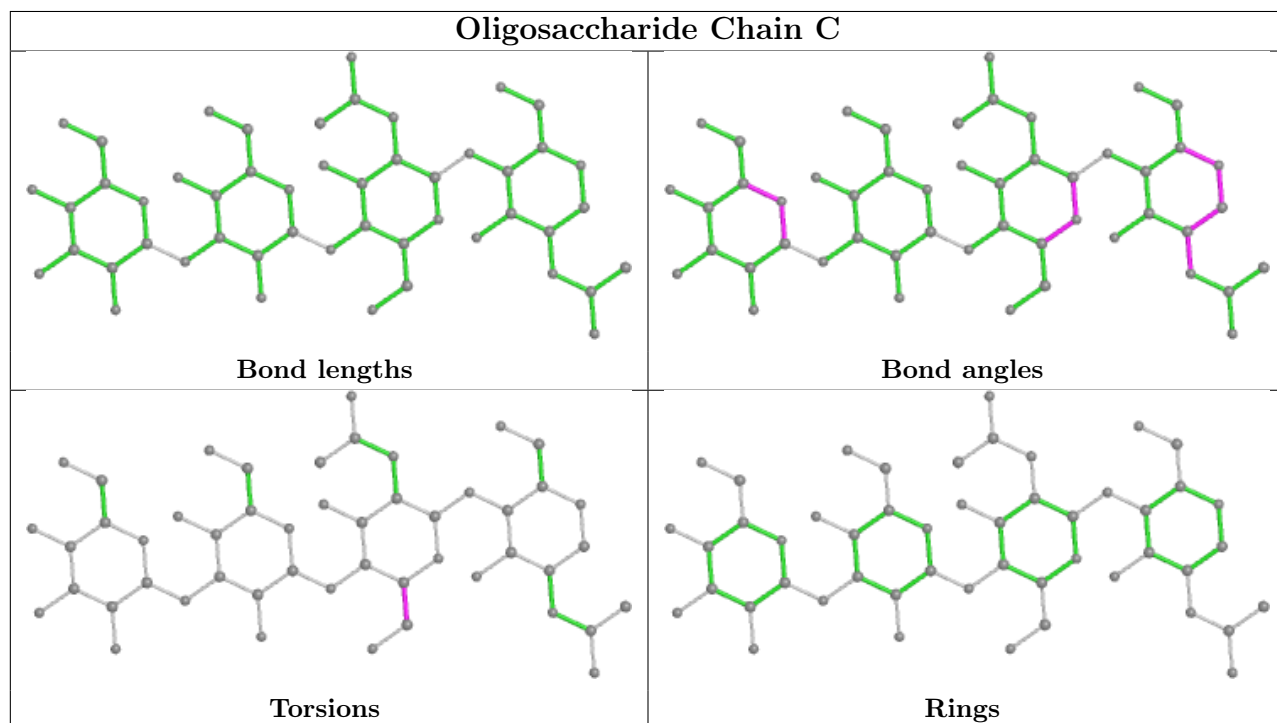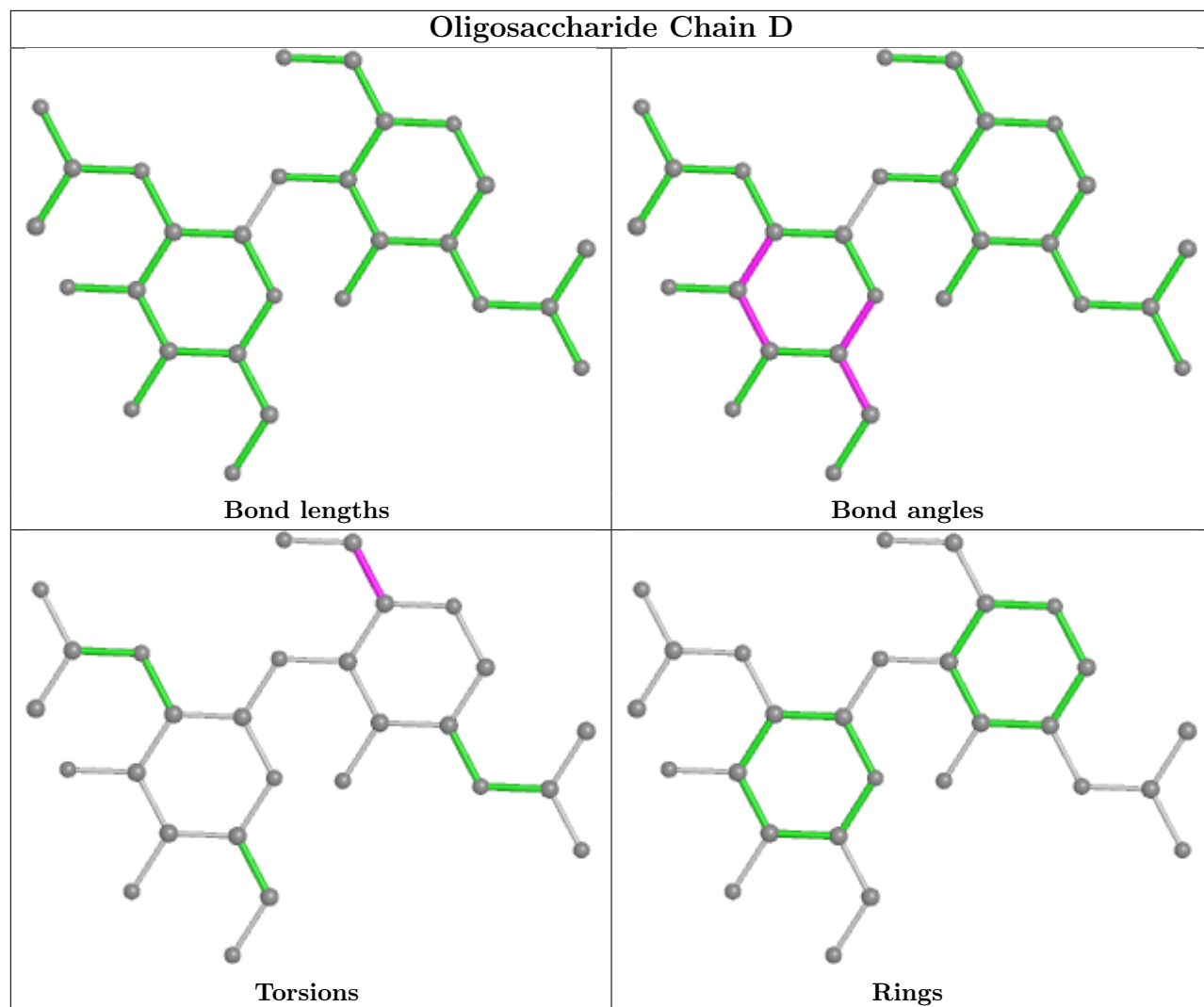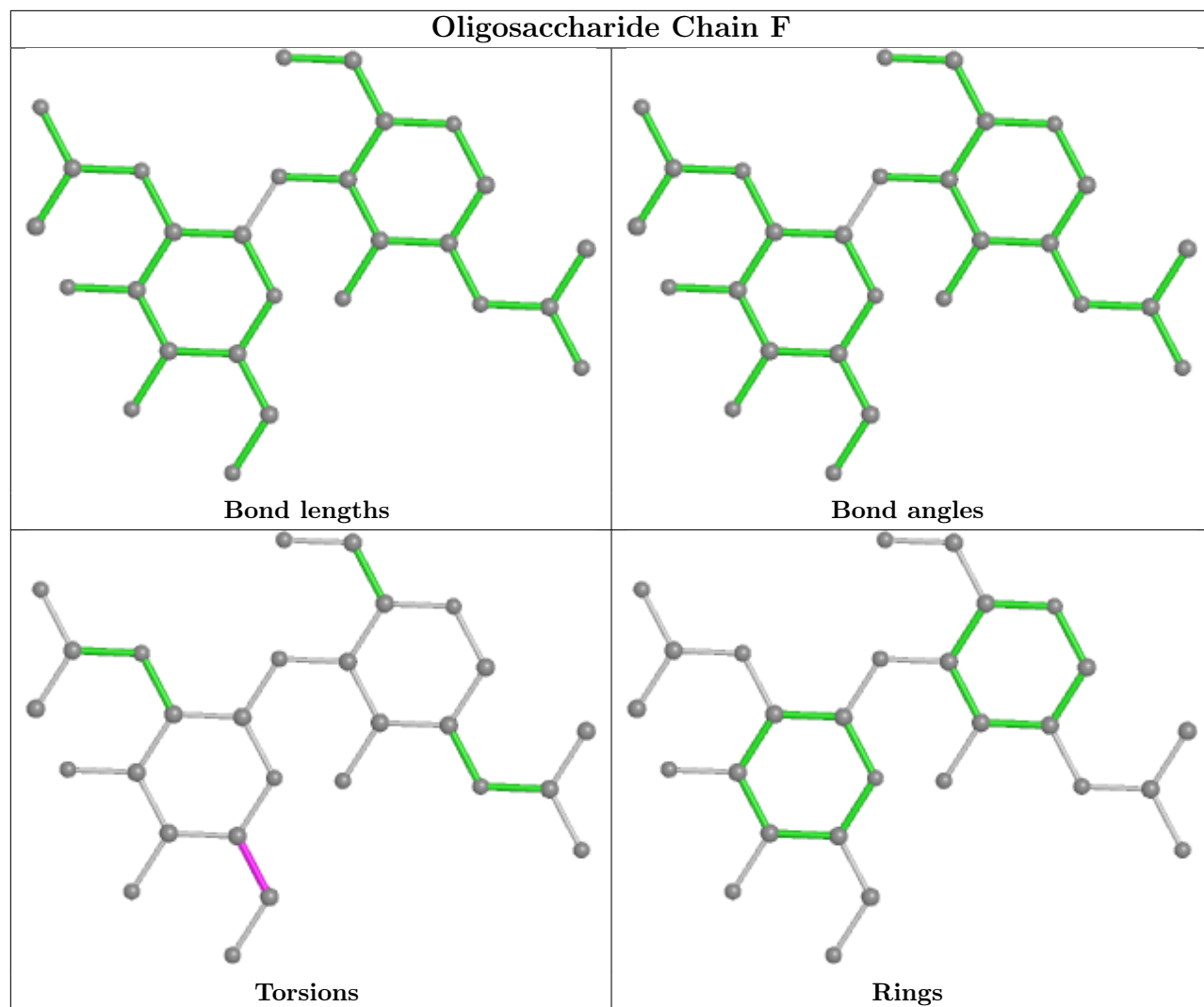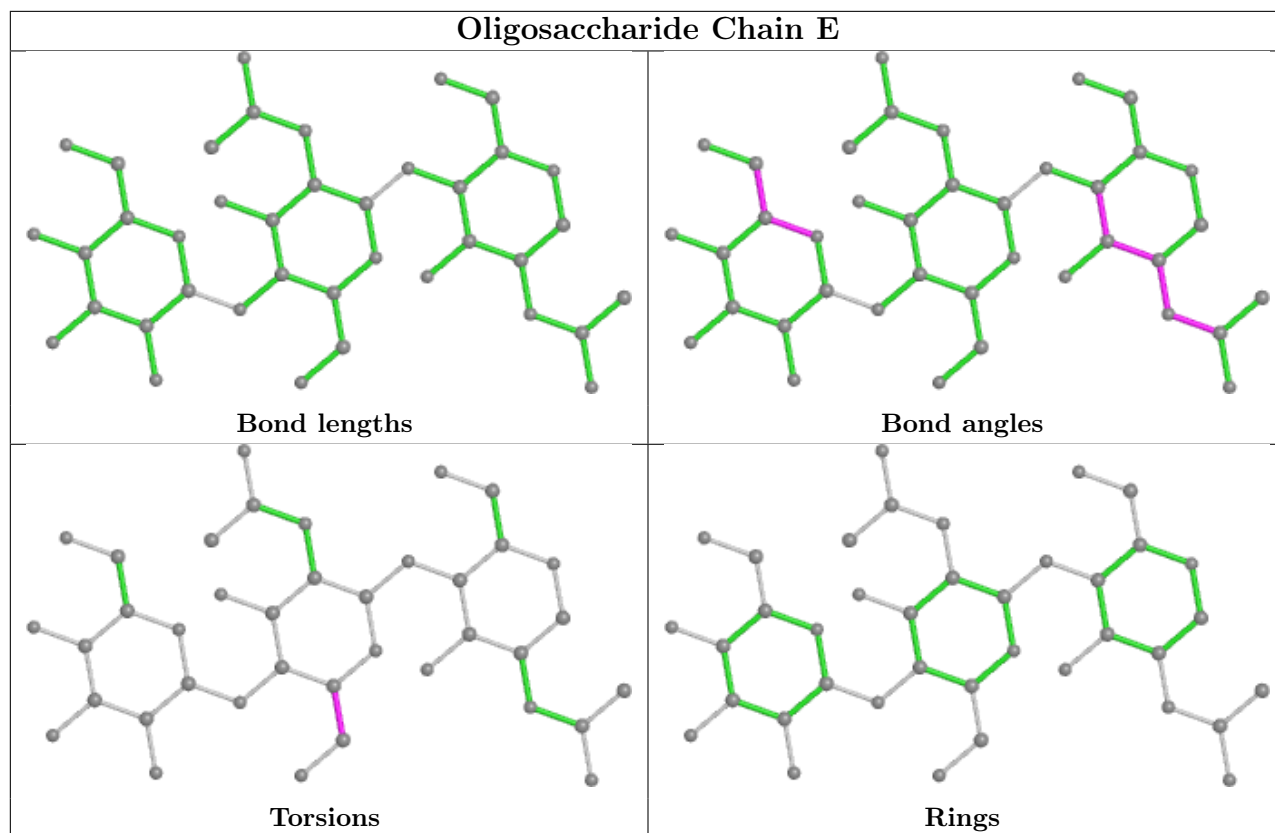
4.6 Ligand geometry ⓘ

4 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	$\#|Z| > 2$
6	NAG	B	201	2	14,14,15	0.59	0	17,19,21	0.95	0
6	NAG	A	414	1	14,14,15	0.37	0	17,19,21	0.89	1 (5%)
6	NAG	A	413	1	14,14,15	0.39	0	17,19,21	0.93	0
6	NAG	A	401	1	14,14,15	0.66	0	17,19,21	1.45	2 (11%)

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.

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	B	201	2	-	2/6/23/26	0/1/1/1
6	NAG	A	414	1	-	0/6/23/26	0/1/1/1
6	NAG	A	413	1	-	0/6/23/26	0/1/1/1
6	NAG	A	401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	401	NAG	C1-O5-C5	3.86	117.42	112.19
6	A	401	NAG	C1-C2-N2	2.58	114.89	110.49
6	A	414	NAG	O5-C1-C2	-2.09	107.99	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	201	NAG	C4-C5-C6-O6
6	B	201	NAG	O5-C5-C6-O6
6	A	401	NAG	C4-C5-C6-O6
6	A	401	NAG	O5-C5-C6-O6

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.