Full wwPDB X-ray Structure Validation Report (i)

Oct 5, 2023 – 06:28 AM EDT

PDB ID	:	6URH
Title	:	Crystal structure of broadly neutralizing antibody AR3X in complex with Hepatitis C virus envelope glycoprotein E2 ectodomain
Authors	:	Flyak, A.I.; Bjorkman, P.J.
Deposited on	:	2019-10-23
Resolution	:	2.20 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 (i) 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 (i)) 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 2.20 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 9 unique types of molecules in this entry. The entry contains 5124 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 HCV envelope glycoprotein E2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	161	1255	801	219	221	14	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	646	ILE	-	expression tag	UNP A0A2P0NE21
C	647	GLY	-	expression tag	UNP A0A2P0NE21

- Molecule 2 is a protein called AR3X Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	242	1819	1140	311	356	12	0	0	0

- Molecule 3 is a protein called AR3X Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	L	213	1623	1012	277	330	4	2	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
			Total	C	N	O			
4	A	2	28	16	2	10	0	0	0

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

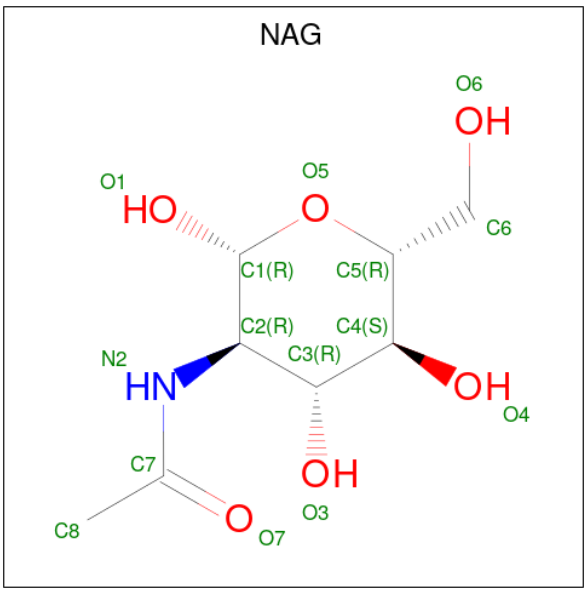
- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

- Molecule 7 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose-(1-6)-[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
			Total	C	N	O			
7	E	7	83	46	2	35	0	0	0

- Molecule 8 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
9	C	40	40	40	0	0
			Total	O		
9	H	91	91	91	0	0
			Total	O		
9	L	71	71	71	0	0

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	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	64.73Å 69.23Å 176.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.49 – 2.20	Depositor
% Data completeness (in resolution range)	99.2 (54.49-2.20)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.186 , 0.233	Depositor
Wilson B-factor (Å^2)	44.4	Xtriage
Anisotropy	0.172	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	5124	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (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)

17 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	$\#\|Z\| > 2$
4	NAG	A	1	1,4	14,14,15	0.33	0	17,19,21	1.05	1 (5%)
4	NAG	A	2	4	14,14,15	0.39	0	17,19,21	0.76	0
5	NAG	B	1	1,5	14,14,15	0.28	0	17,19,21	0.96	1 (5%)
5	NAG	B	2	5	14,14,15	0.30	0	17,19,21	2.11	3 (17%)
5	BMA	B	3	5	11,11,12	0.41	0	15,15,17	2.18	4 (26%)
5	MAN	B	4	5	11,11,12	1.62	2 (18%)	15,15,17	1.42	2 (13%)
6	NAG	D	1	1,6	14,14,15	0.27	0	17,19,21	0.71	0
6	NAG	D	2	6	14,14,15	0.40	0	17,19,21	0.63	0
6	BMA	D	3	6	11,11,12	0.32	0	15,15,17	0.80	1 (6%)
6	MAN	D	4	6	11,11,12	1.11	1 (9%)	15,15,17	1.06	1 (6%)
7	NAG	E	1	1,7	14,14,15	0.35	0	17,19,21	0.93	1 (5%)
7	NAG	E	2	7	14,14,15	0.43	0	17,19,21	0.88	0
7	BMA	E	3	7	11,11,12	0.35	0	15,15,17	0.84	0
7	MAN	E	4	7	11,11,12	0.89	0	15,15,17	1.38	1 (6%)
7	MAN	E	5	7	11,11,12	1.12	1 (9%)	15,15,17	0.97	0
7	MAN	E	6	7	11,11,12	0.88	0	15,15,17	1.05	1 (6%)
7	MAN	E	7	7	11,11,12	0.82	0	15,15,17	1.05	2 (13%)

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	A	1	1,4	-	4/6/23/26	0/1/1/1
4	NAG	A	2	4	-	4/6/23/26	0/1/1/1
5	NAG	B	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	B	2	5	-	0/6/23/26	0/1/1/1
5	BMA	B	3	5	-	2/2/19/22	0/1/1/1
5	MAN	B	4	5	-	1/2/19/22	0/1/1/1
6	NAG	D	1	1,6	-	0/6/23/26	0/1/1/1
6	NAG	D	2	6	-	2/6/23/26	0/1/1/1
6	BMA	D	3	6	-	1/2/19/22	0/1/1/1
6	MAN	D	4	6	-	0/2/19/22	0/1/1/1
7	NAG	E	1	1,7	-	2/6/23/26	0/1/1/1
7	NAG	E	2	7	-	0/6/23/26	0/1/1/1
7	BMA	E	3	7	-	0/2/19/22	0/1/1/1
7	MAN	E	4	7	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MAN	E	5	7	-	2/2/19/22	0/1/1/1
7	MAN	E	6	7	-	0/2/19/22	0/1/1/1
7	MAN	E	7	7	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	4	MAN	C1-C2	3.97	1.61	1.52
5	B	4	MAN	C2-C3	2.93	1.56	1.52
6	D	4	MAN	C2-C3	2.27	1.55	1.52
7	E	5	MAN	C2-C3	2.07	1.55	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	2	NAG	O3-C3-C2	-7.54	93.87	109.47
5	B	3	BMA	C1-O5-C5	-6.99	102.73	112.19
7	E	4	MAN	C1-O5-C5	3.97	117.57	112.19
5	B	4	MAN	C1-C2-C3	3.31	113.74	109.67
5	B	3	BMA	C1-C2-C3	-2.92	106.08	109.67
7	E	1	NAG	C1-O5-C5	2.84	116.05	112.19
5	B	4	MAN	C1-O5-C5	2.82	116.01	112.19
7	E	6	MAN	C1-O5-C5	2.77	115.94	112.19
5	B	2	NAG	C3-C4-C5	2.51	114.71	110.24
5	B	2	NAG	C6-C5-C4	-2.40	107.39	113.00
7	E	7	MAN	O2-C2-C3	-2.38	105.36	110.14
7	E	7	MAN	C1-O5-C5	2.35	115.38	112.19
5	B	3	BMA	O4-C4-C3	-2.29	105.05	110.35
5	B	1	NAG	C1-O5-C5	2.21	115.18	112.19
6	D	3	BMA	O5-C1-C2	-2.12	107.49	110.77
6	D	4	MAN	C1-O5-C5	2.10	115.04	112.19
5	B	3	BMA	O5-C5-C6	2.09	110.49	107.20
4	A	1	NAG	C2-N2-C7	2.01	125.76	122.90

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2	NAG	C8-C7-N2-C2
4	A	2	NAG	O7-C7-N2-C2
5	B	3	BMA	O5-C5-C6-O6

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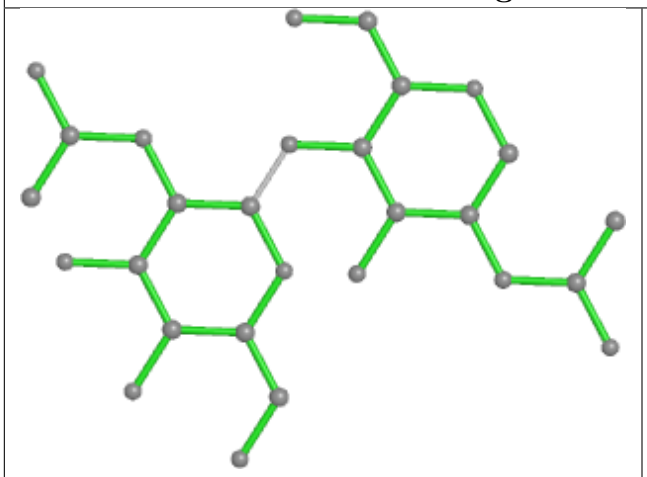
Mol	Chain	Res	Type	Atoms
5	B	3	BMA	C4-C5-C6-O6
6	D	2	NAG	O5-C5-C6-O6
5	B	1	NAG	C8-C7-N2-C2
5	B	1	NAG	O7-C7-N2-C2
5	B	4	MAN	O5-C5-C6-O6
6	D	3	BMA	O5-C5-C6-O6
4	A	1	NAG	C4-C5-C6-O6
4	A	2	NAG	C4-C5-C6-O6
7	E	5	MAN	C4-C5-C6-O6
4	A	1	NAG	O5-C5-C6-O6
7	E	5	MAN	O5-C5-C6-O6
4	A	2	NAG	O5-C5-C6-O6
7	E	1	NAG	C8-C7-N2-C2
7	E	1	NAG	O7-C7-N2-C2
6	D	2	NAG	C4-C5-C6-O6
4	A	1	NAG	C1-C2-N2-C7
4	A	1	NAG	C3-C2-N2-C7

There are no ring outliers.

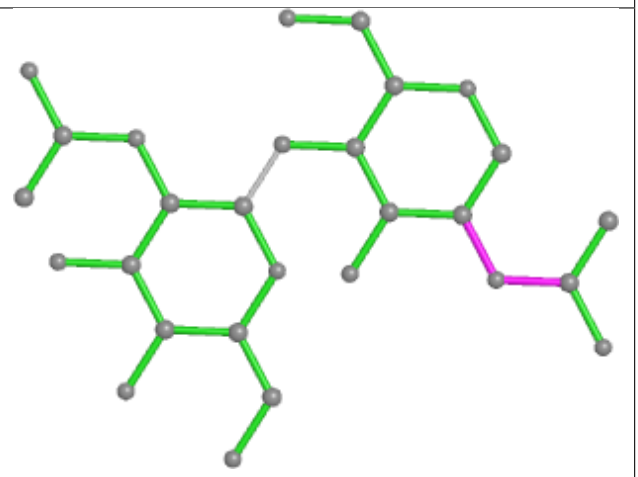
No monomer is involved in short contacts.

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

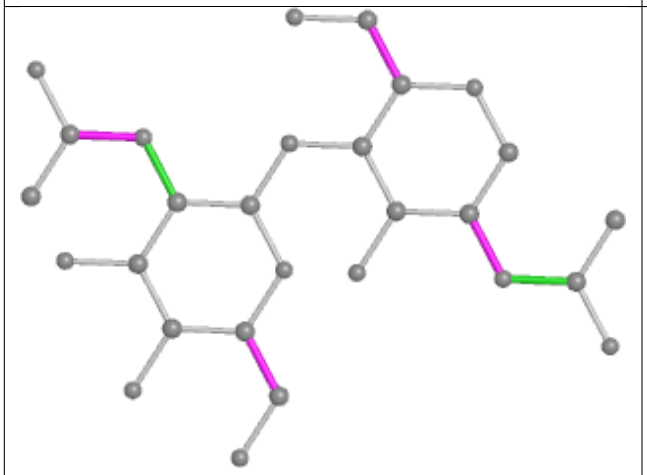
Oligosaccharide Chain A



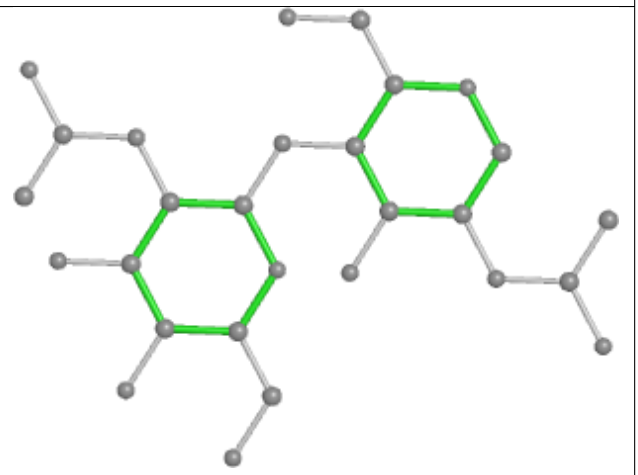
Bond lengths



Bond angles

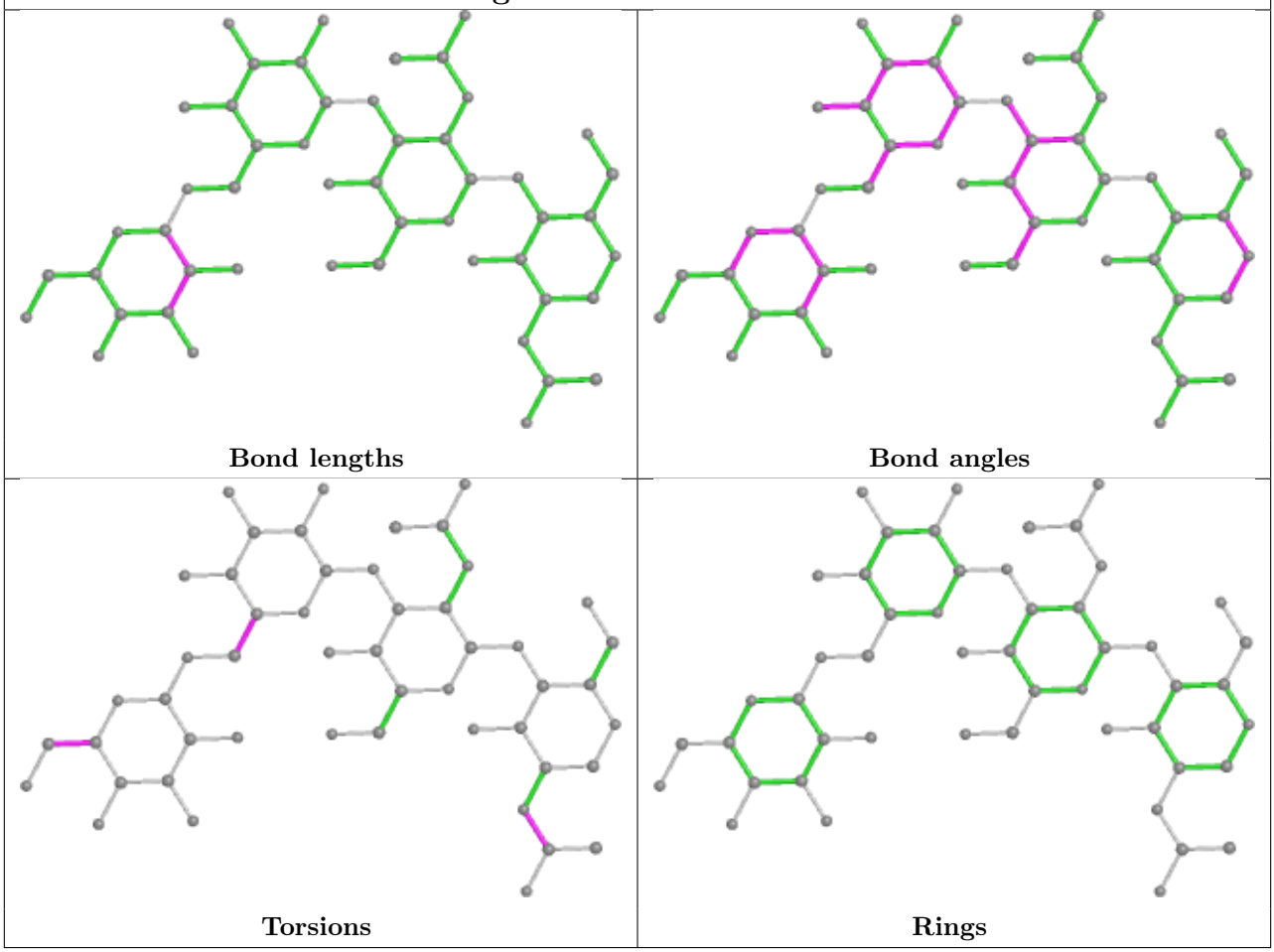


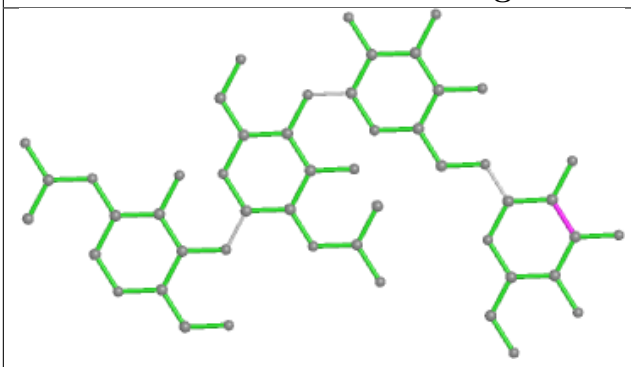
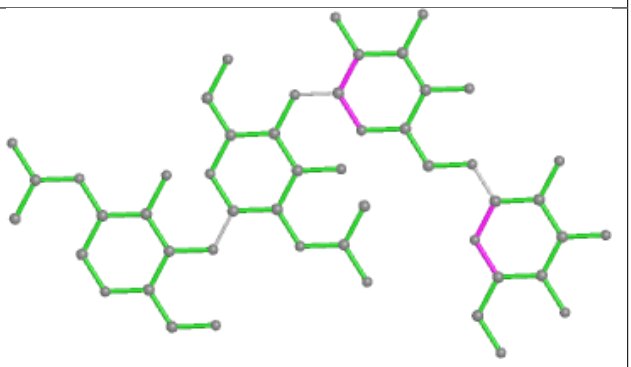
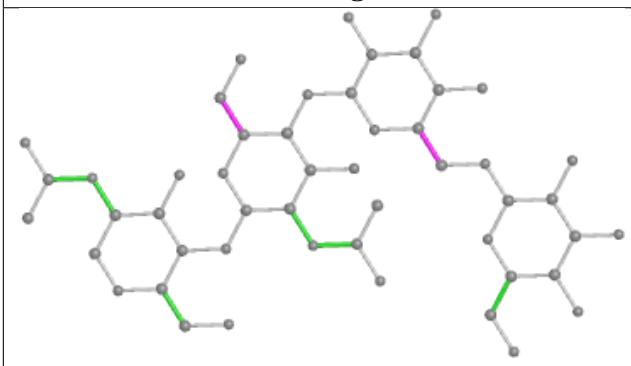
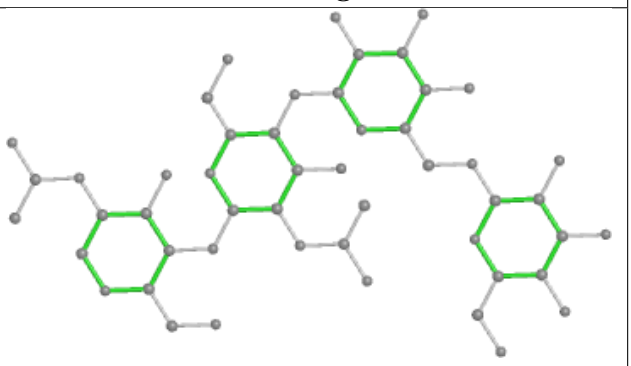
Torsions



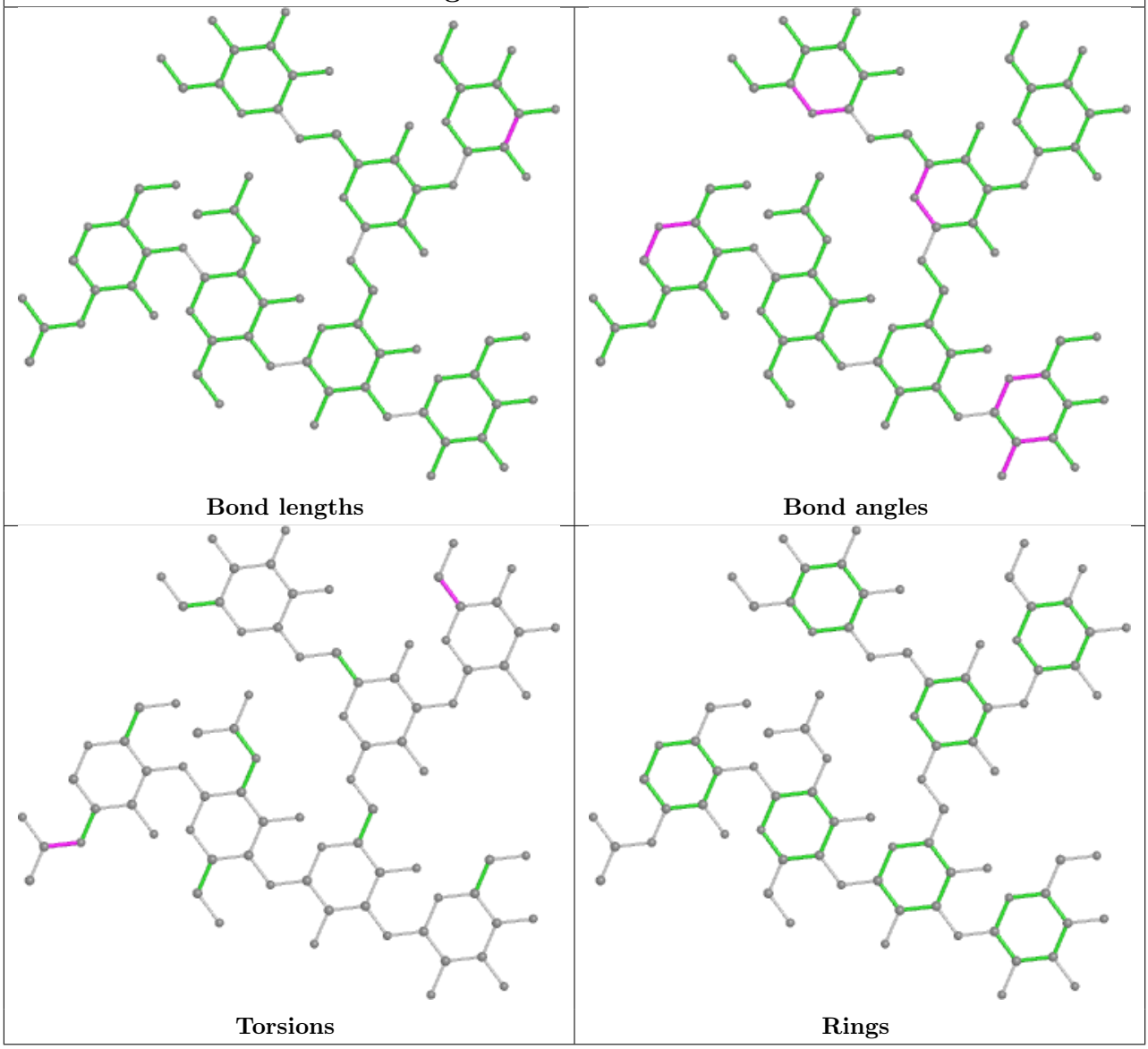
Rings

Oligosaccharide Chain B



Oligosaccharide Chain D	
 Bond lengths	 Bond angles
 Torsions	 Rings

Oligosaccharide Chain E



4.6 Ligand geometry (i)

1 ligand is 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	$\#\|Z\| > 2$
8	NAG	C	4318	1	14,14,15	1.44	3 (21%)	17,19,21	3.48	7 (41%)

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
8	NAG	C	4318	1	-	2/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	4318	NAG	C2-N2	-2.69	1.41	1.46
8	C	4318	NAG	C3-C2	-2.43	1.47	1.52
8	C	4318	NAG	O5-C1	-2.01	1.40	1.43

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	C	4318	NAG	C2-N2-C7	-7.86	111.71	122.90
8	C	4318	NAG	O5-C5-C6	6.10	116.77	107.20
8	C	4318	NAG	C3-C4-C5	-5.45	100.52	110.24
8	C	4318	NAG	C1-C2-N2	-5.20	101.60	110.49
8	C	4318	NAG	C1-O5-C5	-4.85	105.62	112.19
8	C	4318	NAG	O7-C7-C8	2.77	127.20	122.06
8	C	4318	NAG	O4-C4-C3	-2.04	105.64	110.35

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	4318	NAG	C8-C7-N2-C2
8	C	4318	NAG	O7-C7-N2-C2

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 (i)

5.1 Protein, DNA and RNA chains (i)

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

5.2 Non-standard residues in protein, DNA, RNA chains (i)

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

5.3 Carbohydrates (i)

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

5.4 Ligands (i)

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

5.5 Other polymers (i)

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