Full wwPDB X-ray Structure Validation Report (i)

Oct 4, 2023 – 11:06 PM EDT

PDB ID	:	6V47
Title	:	The crystal structure of hemagglutinin from A/duck/Memphis/546/1974 (H11N9)
Authors	:	Yang, H.; Stevens, J.
Deposited on	:	2019-11-27
Resolution	:	2.80 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 2.80 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 3 unique types of molecules in this entry. The entry contains 11712 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	321	2513	1588	430	482	13	0	0	0
1	C	321	2513	1588	430	482	13	0	0	0
1	E	321	2513	1588	430	482	13	0	0	0

- Molecule 2 is a protein called Hemagglutinin HA2 chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	167	1363	839	244	275	5	0	0	0
2	D	167	1363	839	244	275	5	0	0	0
2	F	167	1363	839	244	275	5	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	SER	-	expression tag	UNP A2V851
B	176	GLY	-	expression tag	UNP A2V851
B	177	ARG	-	expression tag	UNP A2V851
B	178	LEU	-	expression tag	UNP A2V851
B	179	VAL	-	expression tag	UNP A2V851
B	180	PRO	-	expression tag	UNP A2V851
B	181	ARG	-	expression tag	UNP A2V851
D	175	SER	-	expression tag	UNP A2V851
D	176	GLY	-	expression tag	UNP A2V851
D	177	ARG	-	expression tag	UNP A2V851
D	178	LEU	-	expression tag	UNP A2V851
D	179	VAL	-	expression tag	UNP A2V851

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	180	PRO	-	expression tag	UNP A2V851
D	181	ARG	-	expression tag	UNP A2V851
F	175	SER	-	expression tag	UNP A2V851
F	176	GLY	-	expression tag	UNP A2V851
F	177	ARG	-	expression tag	UNP A2V851
F	178	LEU	-	expression tag	UNP A2V851
F	179	VAL	-	expression tag	UNP A2V851
F	180	PRO	-	expression tag	UNP A2V851
F	181	ARG	-	expression tag	UNP A2V851

- 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
			Total	C	N	O			
3	G	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	H	2	28	16	2	10	0	0	0
			Total	C	N	O			
3	I	2	28	16	2	10	0	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	80.12Å 121.15Å 217.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.21 – 2.80	Depositor
% Data completeness (in resolution range)	89.3 (49.21-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	4.38 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.234 , 0.278	Depositor
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.163	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11712	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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)

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	1,3	14,14,15	1.07	1 (7%)	17,19,21	2.44	4 (23%)
3	NAG	G	2	3	14,14,15	1.15	1 (7%)	17,19,21	1.79	7 (41%)
3	NAG	H	1	1,3	14,14,15	0.68	0	17,19,21	1.39	1 (5%)
3	NAG	H	2	3	14,14,15	1.08	0	17,19,21	2.51	5 (29%)
3	NAG	I	1	1,3	14,14,15	2.33	6 (42%)	17,19,21	2.53	7 (41%)
3	NAG	I	2	3	14,14,15	1.54	3 (21%)	17,19,21	2.21	5 (29%)

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

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C4-C5	5.07	1.63	1.53
3	I	1	NAG	C1-C2	3.28	1.57	1.52
3	I	2	NAG	C3-C2	3.23	1.59	1.52
3	I	1	NAG	O4-C4	3.04	1.50	1.43
3	I	1	NAG	C6-C5	2.67	1.60	1.51
3	I	1	NAG	O3-C3	2.50	1.48	1.43
3	G	2	NAG	C1-C2	2.43	1.56	1.52
3	I	2	NAG	O4-C4	2.38	1.48	1.43
3	I	1	NAG	C4-C3	2.35	1.58	1.52
3	G	1	NAG	C4-C5	2.22	1.57	1.53
3	I	2	NAG	C1-C2	2.15	1.55	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	C1-O5-C5	7.27	122.05	112.19
3	H	2	NAG	O5-C5-C6	5.71	116.16	107.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	1	NAG	C1-O5-C5	5.51	119.66	112.19
3	H	2	NAG	C4-C3-C2	4.57	117.72	111.02
3	I	2	NAG	O5-C5-C6	4.55	114.34	107.20
3	I	1	NAG	O4-C4-C5	4.27	119.90	109.30
3	H	2	NAG	C2-N2-C7	4.19	128.87	122.90
3	I	1	NAG	C6-C5-C4	4.18	122.80	113.00
3	I	2	NAG	C2-N2-C7	3.74	128.24	122.90
3	I	2	NAG	O3-C3-C2	3.55	116.82	109.47
3	H	2	NAG	C3-C4-C5	3.49	116.47	110.24
3	I	2	NAG	C3-C4-C5	-3.41	104.16	110.24
3	I	2	NAG	O4-C4-C5	3.37	117.66	109.30
3	G	1	NAG	O5-C1-C2	3.15	116.26	111.29
3	G	2	NAG	O4-C4-C5	3.11	117.01	109.30
3	G	2	NAG	O3-C3-C2	3.05	115.78	109.47
3	I	1	NAG	O6-C6-C5	2.93	121.35	111.29
3	G	1	NAG	C6-C5-C4	2.90	119.80	113.00
3	G	2	NAG	O5-C5-C6	2.87	111.70	107.20
3	G	1	NAG	C1-C2-N2	-2.81	105.69	110.49
3	H	2	NAG	C6-C5-C4	-2.76	106.55	113.00
3	I	1	NAG	C1-C2-N2	2.66	115.03	110.49
3	I	1	NAG	O3-C3-C4	2.57	116.28	110.35
3	G	2	NAG	O5-C5-C4	-2.47	104.81	110.83
3	I	1	NAG	C4-C3-C2	-2.47	107.40	111.02
3	G	2	NAG	C2-N2-C7	2.35	126.26	122.90
3	H	1	NAG	O5-C5-C6	2.25	110.74	107.20
3	G	2	NAG	C3-C4-C5	-2.18	106.35	110.24
3	G	2	NAG	O5-C1-C2	2.06	114.54	111.29

There are no chirality outliers.

All (5) torsion outliers are listed below:

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

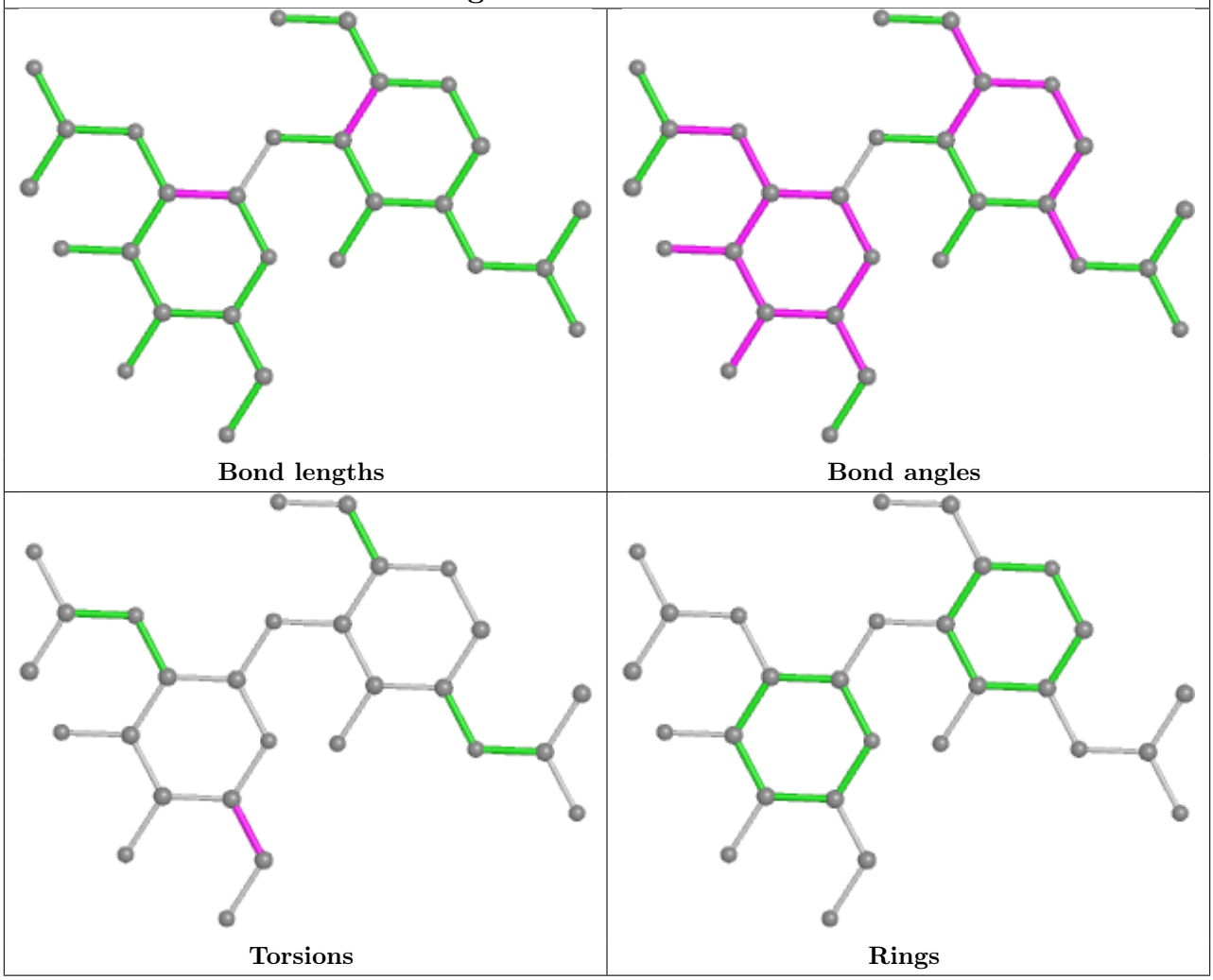
There are no ring outliers.

No monomer is involved in short contacts.

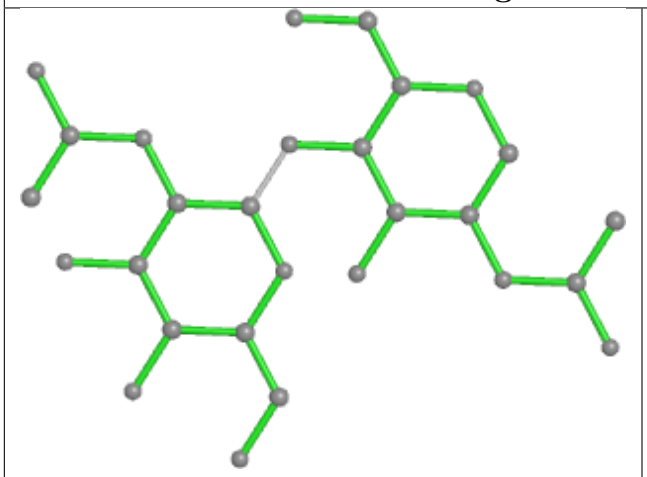
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

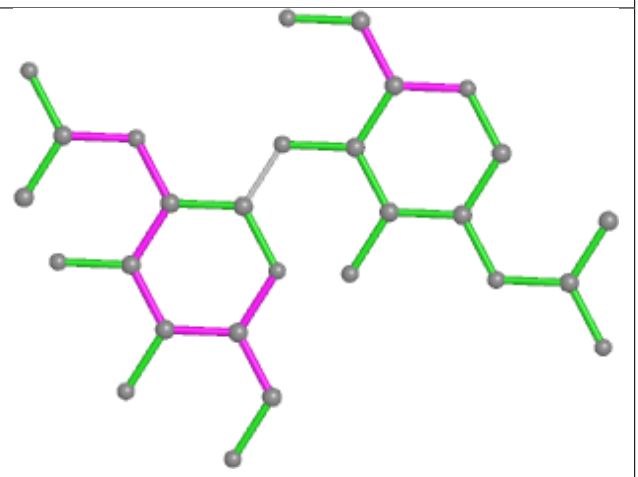
Oligosaccharide Chain G



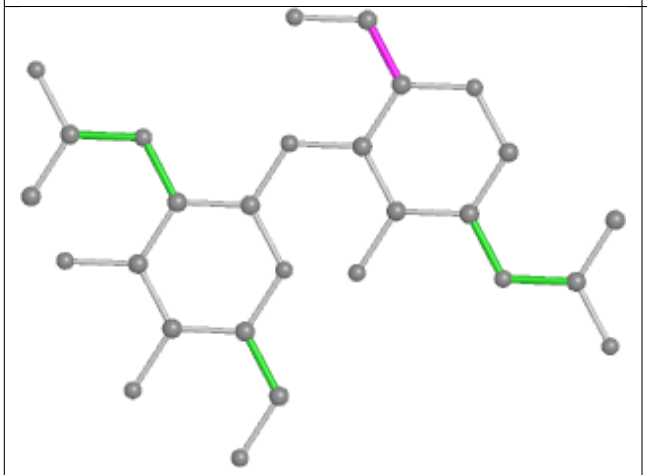
Oligosaccharide Chain H



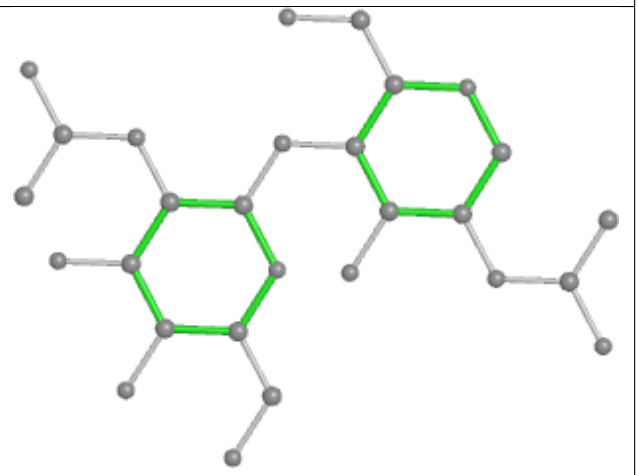
Bond lengths



Bond angles

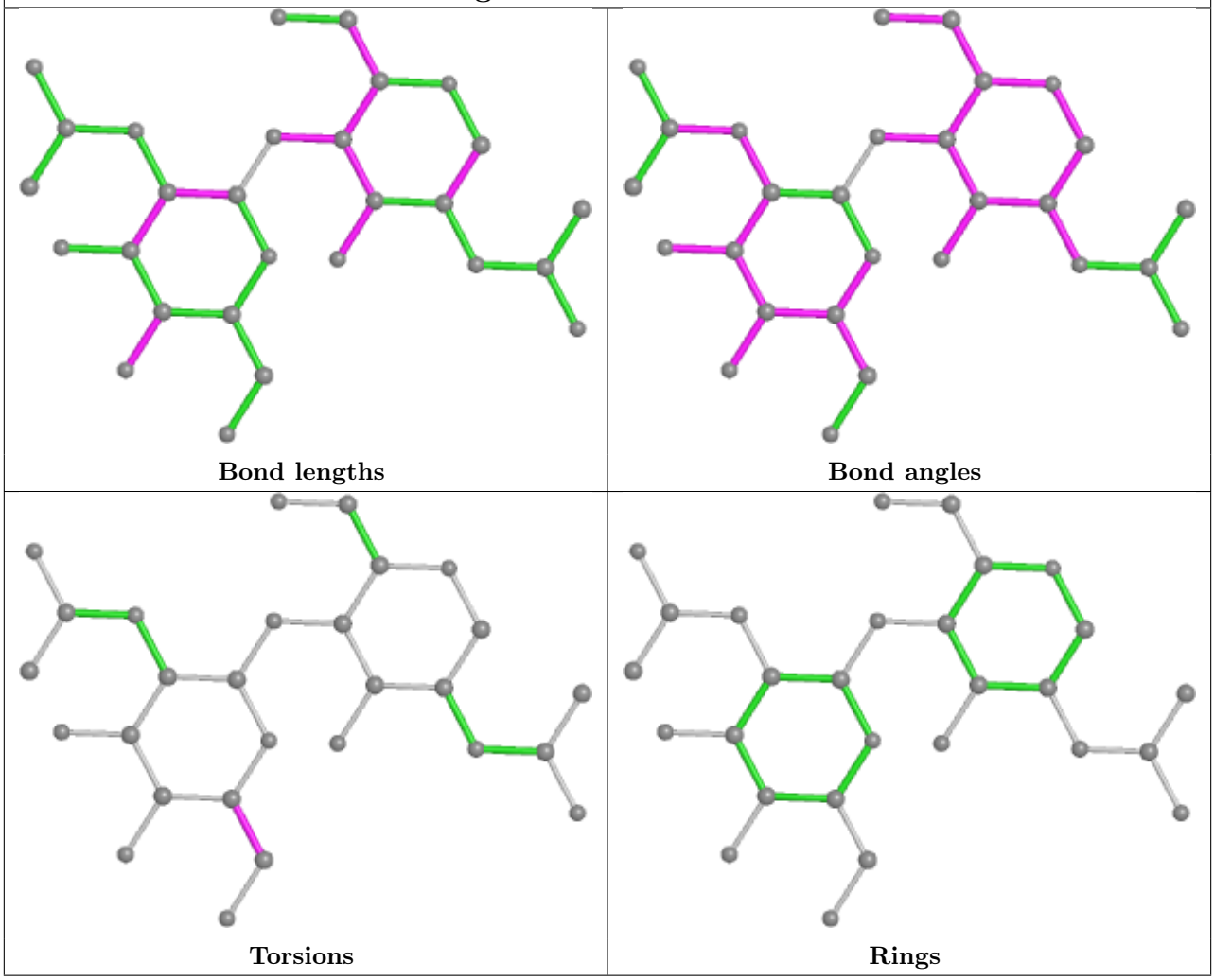


Torsions



Rings

Oligosaccharide Chain I



4.6 Ligand geometry (i)

There are no ligands in this entry.

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.