wwPDB X-ray Structure Validation Summary Report (i)

Oct 2, 2023 – 03:13 PM EDT

PDB ID	:	6NRQ
Title	:	Crystal structure of Dpr10 IG1 bound to DIP-alpha IG1
Authors	:	Cheng, S.; Park, Y.J.; Kurleto, J.D.; Ozkan, E.
Deposited on	:	2019-01-24
Resolution	:	1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 1.80 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 7 unique types of molecules in this entry. The entry contains 3999 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 Defective proboscis extension response 10, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			899	569	163	164	3			
1	C	108	Total	C	N	O	S	0	0	0
			894	566	162	163	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	48	GLY	-	expression tag	UNP Q9VT83
A	49	SER	-	expression tag	UNP Q9VT83
A	155	HIS	-	expression tag	UNP Q9VT83
A	156	HIS	-	expression tag	UNP Q9VT83
A	157	HIS	-	expression tag	UNP Q9VT83
A	158	HIS	-	expression tag	UNP Q9VT83
A	159	HIS	-	expression tag	UNP Q9VT83
A	160	HIS	-	expression tag	UNP Q9VT83
C	48	GLY	-	expression tag	UNP Q9VT83
C	49	SER	-	expression tag	UNP Q9VT83
C	155	HIS	-	expression tag	UNP Q9VT83
C	156	HIS	-	expression tag	UNP Q9VT83
C	157	HIS	-	expression tag	UNP Q9VT83
C	158	HIS	-	expression tag	UNP Q9VT83
C	159	HIS	-	expression tag	UNP Q9VT83
C	160	HIS	-	expression tag	UNP Q9VT83

- Molecule 2 is a protein called Dpr-interacting protein alpha, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	104	Total	C	N	O	S	0	0	0
			812	511	145	152	4			
2	D	105	Total	C	N	O	S	0	0	0
			816	512	147	153	4			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	37	SER	-	expression tag	UNP Q9W4R3
B	38	ARG	-	expression tag	UNP Q9W4R3
B	144	HIS	-	expression tag	UNP Q9W4R3
B	145	HIS	-	expression tag	UNP Q9W4R3
B	146	HIS	-	expression tag	UNP Q9W4R3
B	147	HIS	-	expression tag	UNP Q9W4R3
B	148	HIS	-	expression tag	UNP Q9W4R3
B	149	HIS	-	expression tag	UNP Q9W4R3
D	37	SER	-	expression tag	UNP Q9W4R3
D	38	ARG	-	expression tag	UNP Q9W4R3
D	144	HIS	-	expression tag	UNP Q9W4R3
D	145	HIS	-	expression tag	UNP Q9W4R3
D	146	HIS	-	expression tag	UNP Q9W4R3
D	147	HIS	-	expression tag	UNP Q9W4R3
D	148	HIS	-	expression tag	UNP Q9W4R3
D	149	HIS	-	expression tag	UNP Q9W4R3

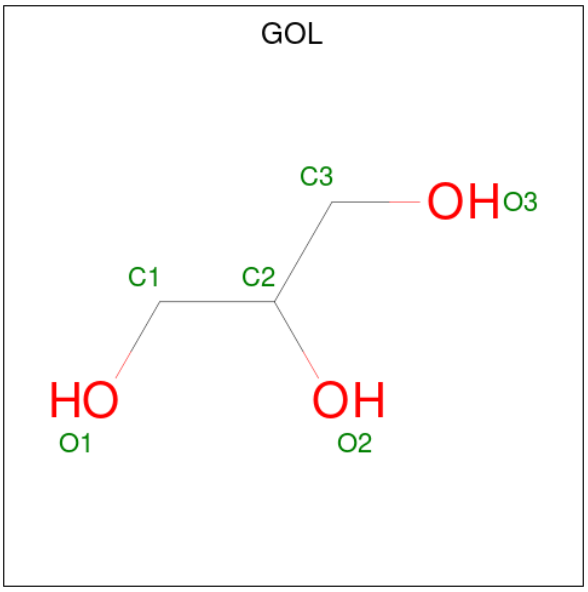
- Molecule 3 is an oligosaccharide called alpha-L-fucopyranose-(1-3)-[2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)][alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	E	4	Total	C	N	O	0	0	0
			48	28	2	18			
3	H	4	Total	C	N	O	0	0	0
			48	28	2	18			

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

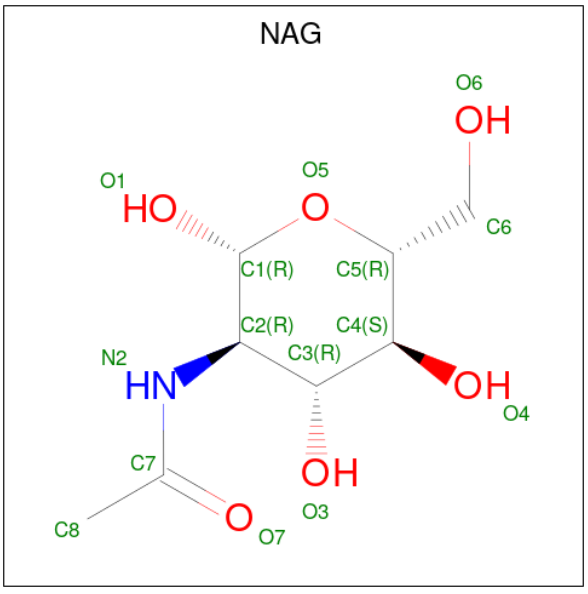
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	F	6	Total	C	N	O	0	0	0
			70	40	2	28			
4	G	6	Total	C	N	O	0	0	0
			70	40	2	28			

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0

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



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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	85	Total O 85 85	0	0
7	B	78	Total O 78 78	0	0
7	C	88	Total O 88 88	0	0
7	D	45	Total O 45 45	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 1	Depositor
Cell constants a, b, c, α, β, γ	51.01Å 53.55Å 56.69Å 119.68° 103.77° 92.88°	Depositor
Resolution (Å)	48.55 – 1.80	Depositor
% Data completeness (in resolution range)	87.2 (48.55-1.80)	Depositor
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.79Å)	Xtriage
Refinement program	PHENIX dev_3112	Depositor
R, R_{free}	0.174 , 0.205	Depositor
Wilson B-factor (Å^2)	29.9	Xtriage
Anisotropy	0.338	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3999	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.54% 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

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

20 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	E	1	1,3	14,14,15	0.35	0	17,19,21	0.57	0
3	FUC	E	2	3	10,10,11	0.82	0	14,14,16	0.85	0
3	NAG	E	3	3	14,14,15	0.57	0	17,19,21	0.44	0
3	FUC	E	4	3	10,10,11	1.14	1 (10%)	14,14,16	1.90	3 (21%)
4	NAG	F	1	1,4	14,14,15	0.65	0	17,19,21	0.76	1 (5%)
4	NAG	F	2	4	14,14,15	0.24	0	17,19,21	0.52	0
4	BMA	F	3	4	11,11,12	1.28	2 (18%)	15,15,17	1.01	1 (6%)
4	MAN	F	4	4	11,11,12	1.25	1 (9%)	15,15,17	1.88	3 (20%)
4	FUC	F	5	4	10,10,11	0.86	1 (10%)	14,14,16	0.71	0
4	FUC	F	6	4	10,10,11	1.35	1 (10%)	14,14,16	0.95	1 (7%)
4	NAG	G	1	2,4	14,14,15	0.15	0	17,19,21	0.58	0
4	NAG	G	2	4	14,14,15	0.34	0	17,19,21	0.51	0
4	BMA	G	3	4	11,11,12	0.68	0	15,15,17	0.87	0
4	MAN	G	4	4	11,11,12	0.85	0	15,15,17	1.10	1 (6%)
4	FUC	G	5	4	10,10,11	0.72	0	14,14,16	1.08	1 (7%)
4	FUC	G	6	4	10,10,11	0.91	0	14,14,16	0.86	0
3	NAG	H	1	1,3	14,14,15	0.43	0	17,19,21	0.50	0
3	FUC	H	2	3	10,10,11	0.57	0	14,14,16	0.90	0
3	NAG	H	3	3	14,14,15	0.35	0	17,19,21	0.43	0
3	FUC	H	4	3	10,10,11	0.75	0	14,14,16	1.15	2 (14%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MAN	G	4	4	-	0/2/19/22	0/1/1/1
4	FUC	G	5	4	-	-	0/1/1/1
4	FUC	G	6	4	-	-	0/1/1/1
3	NAG	H	1	1,3	-	0/6/23/26	0/1/1/1
3	FUC	H	2	3	-	-	0/1/1/1
3	NAG	H	3	3	-	0/6/23/26	0/1/1/1
3	FUC	H	4	3	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	4	MAN	C1-C2	3.87	1.61	1.52
4	F	6	FUC	C2-C3	3.18	1.57	1.52
3	E	4	FUC	C1-C2	2.72	1.58	1.52
4	F	3	BMA	O5-C5	2.29	1.48	1.43
4	F	5	FUC	O5-C1	-2.09	1.40	1.43

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	4	MAN	C1-O5-C5	4.95	118.90	112.19
3	E	4	FUC	O5-C1-C2	4.02	116.98	110.77
3	E	4	FUC	C1-O5-C5	3.64	121.04	112.78
4	F	4	MAN	C1-C2-C3	3.60	114.09	109.67
3	E	4	FUC	C1-C2-C3	3.39	113.83	109.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

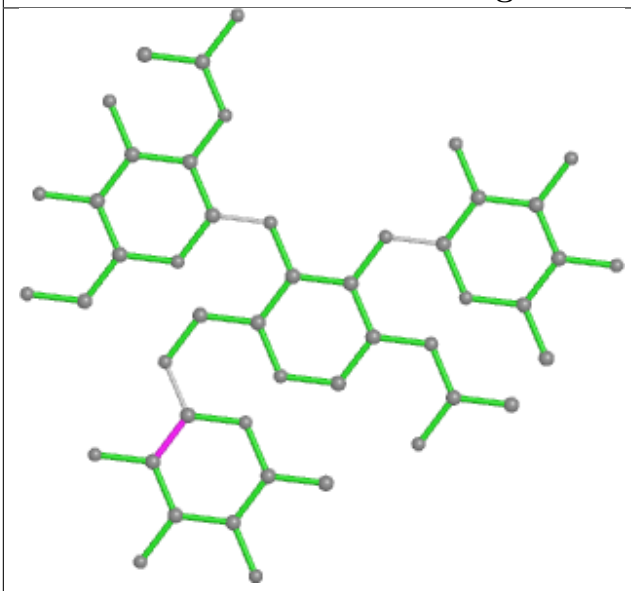
Mol	Chain	Res	Type	Atoms
3	E	1	NAG	O5-C5-C6-O6
4	F	4	MAN	C4-C5-C6-O6
3	E	1	NAG	C4-C5-C6-O6
4	F	4	MAN	O5-C5-C6-O6
4	G	3	BMA	O5-C5-C6-O6

There are no ring outliers.

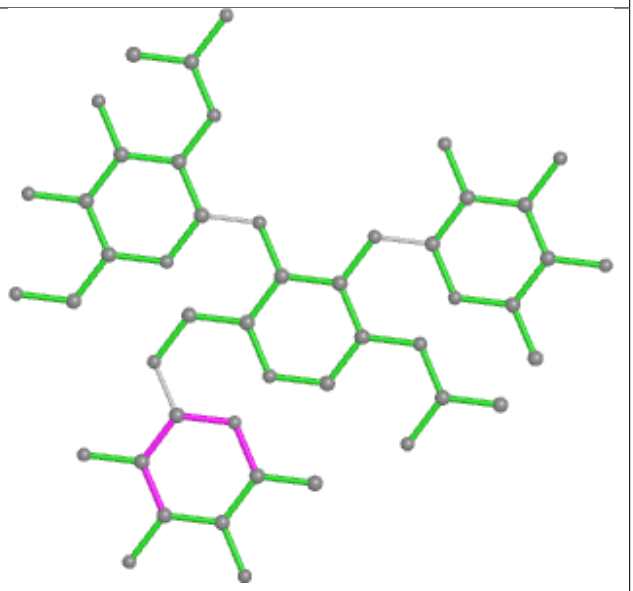
No monomer is involved in short contacts.

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

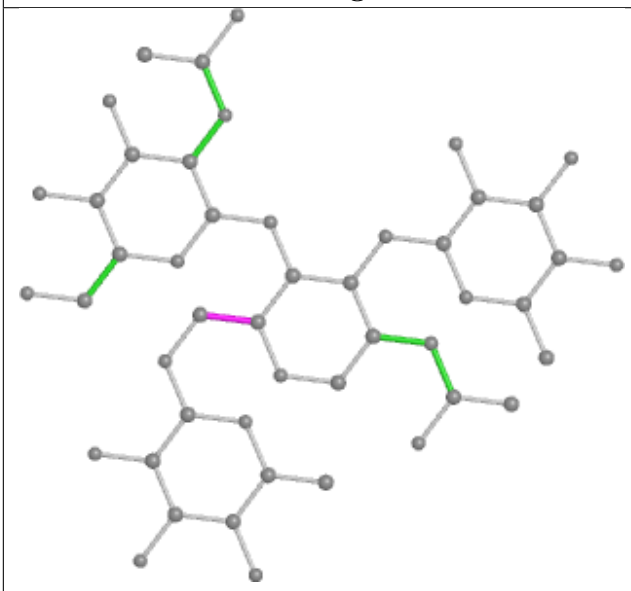
Oligosaccharide Chain E



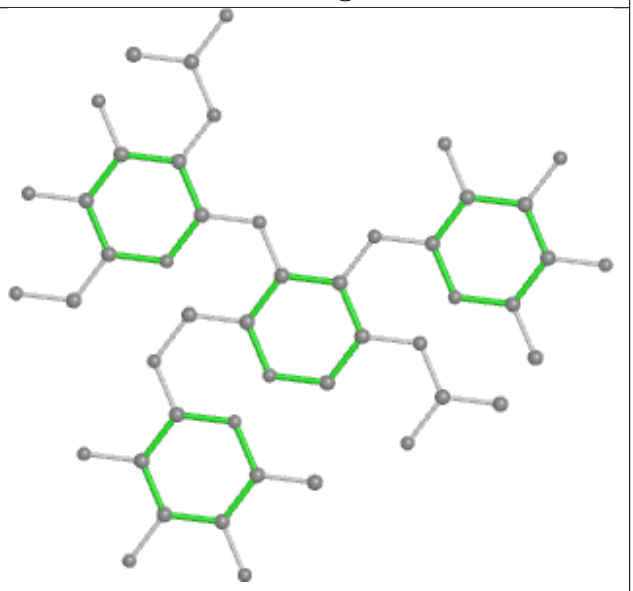
Bond lengths



Bond angles

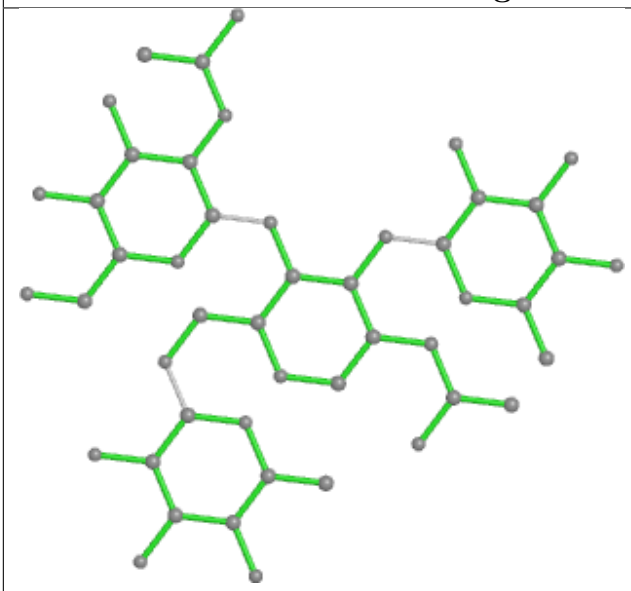


Torsions

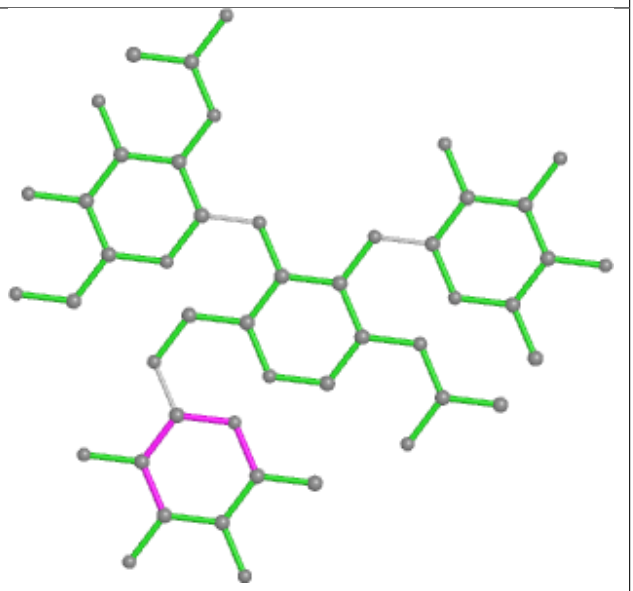


Rings

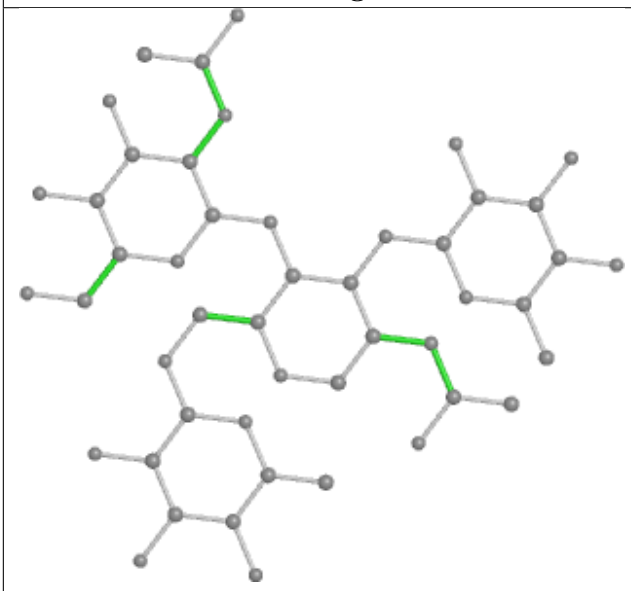
Oligosaccharide Chain H



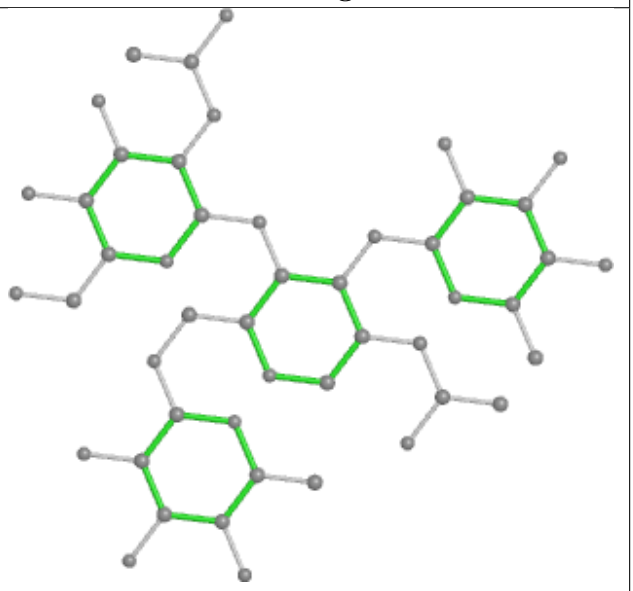
Bond lengths



Bond angles

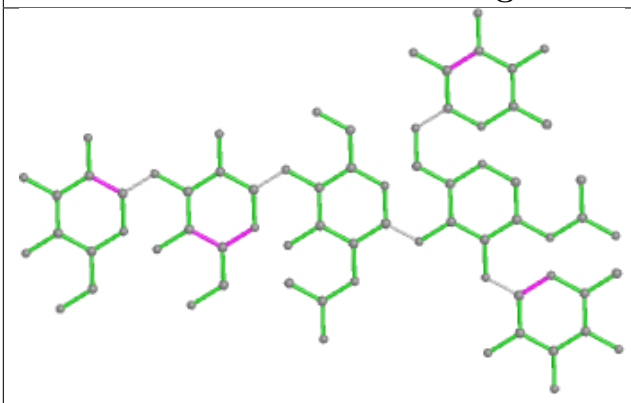


Torsions

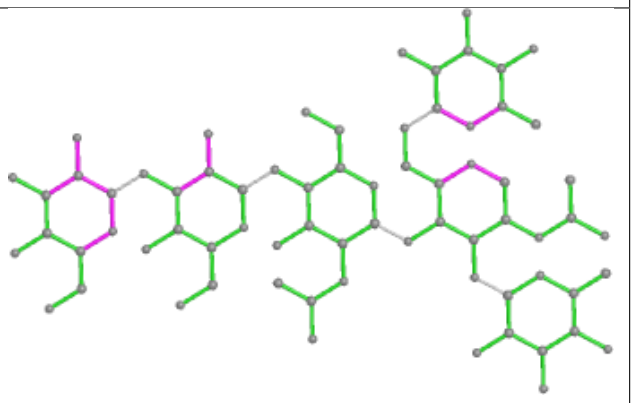


Rings

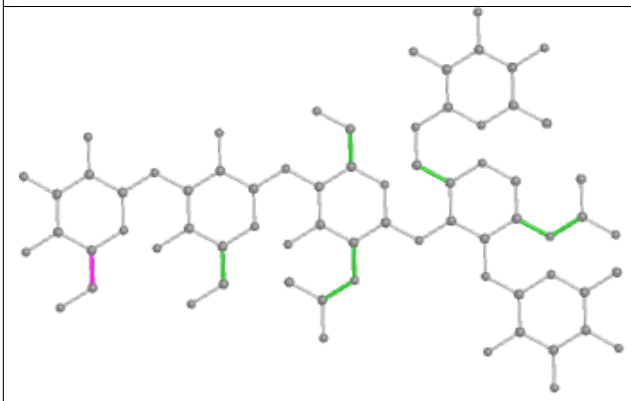
Oligosaccharide Chain F



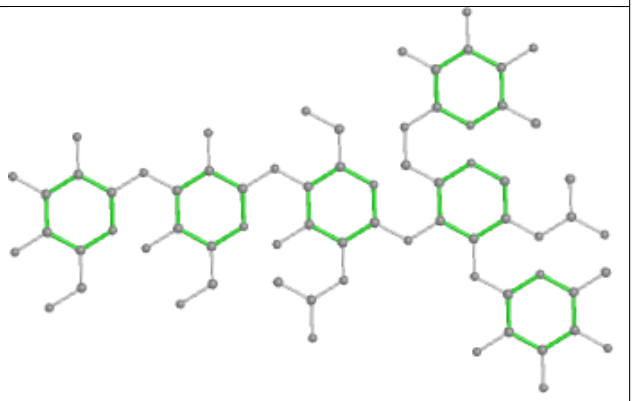
Bond lengths



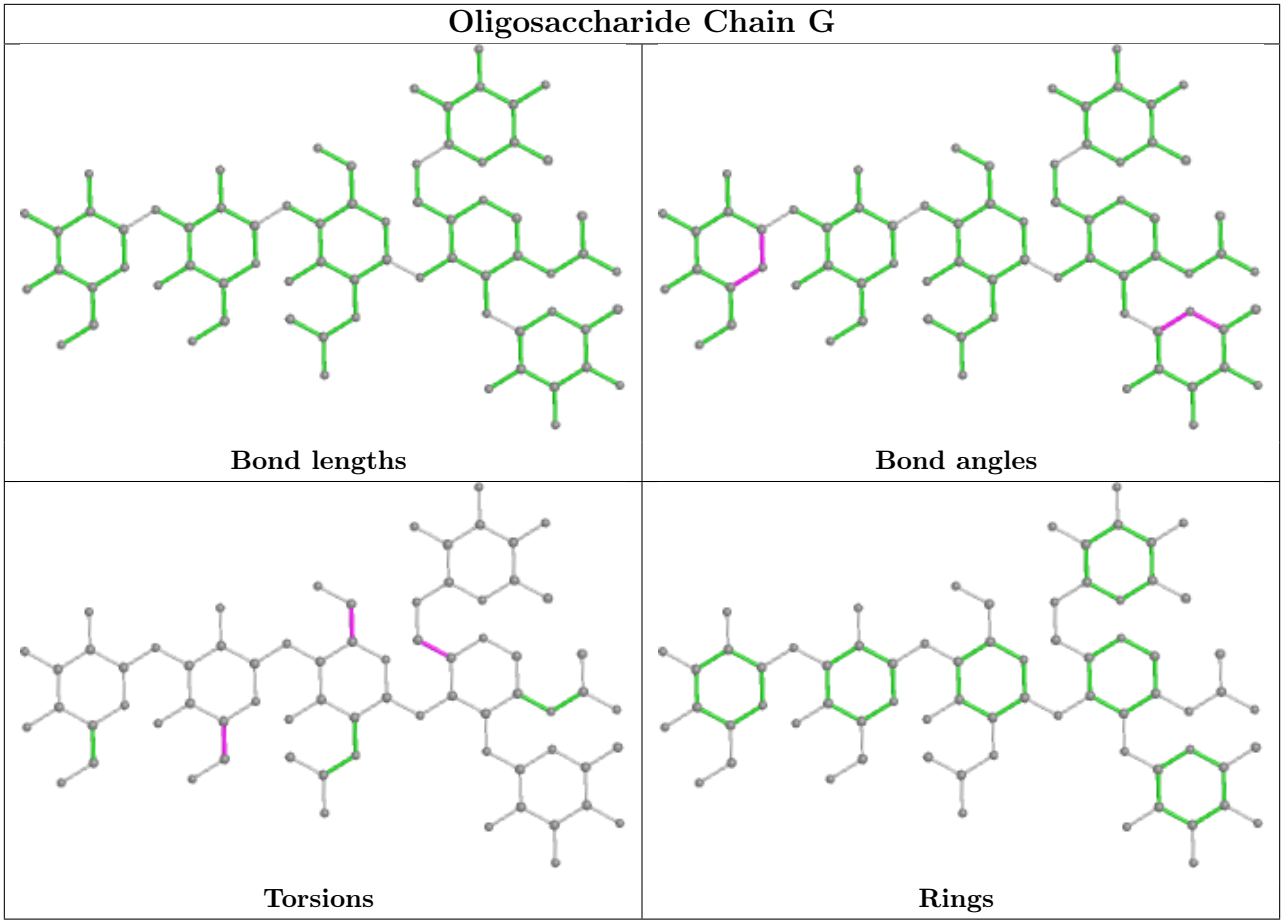
Bond angles



Torsions



Rings



4.6 Ligand geometry (i)

5 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	$\#\|Z\| > 2$
5	GOL	C	906	-	5,5,5	0.87	0	5,5,5	0.97	0
5	GOL	B	907	-	5,5,5	0.75	0	5,5,5	1.12	1 (20%)
6	NAG	D	901	2	14,14,15	0.78	1 (7%)	17,19,21	0.73	1 (5%)
5	GOL	A	911	-	5,5,5	0.99	0	5,5,5	0.80	0
6	NAG	C	905	1	14,14,15	0.28	0	17,19,21	0.50	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
5	GOL	C	906	-	-	4/4/4/4	-
5	GOL	B	907	-	-	0/4/4/4	-
6	NAG	D	901	2	-	2/6/23/26	0/1/1/1
5	GOL	A	911	-	-	2/4/4/4	-
6	NAG	C	905	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	901	NAG	O5-C1	2.36	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	901	NAG	C1-O5-C5	2.54	115.64	112.19
5	B	907	GOL	C3-C2-C1	-2.09	103.58	111.70

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	906	GOL	O1-C1-C2-C3
5	C	906	GOL	C1-C2-C3-O3
6	D	901	NAG	O5-C5-C6-O6
6	D	901	NAG	C4-C5-C6-O6
5	A	911	GOL	C1-C2-C3-O3

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.