Full wwPDB X-ray Structure Validation Report ⓘ

Oct 5, 2023 – 04:05 AM EDT

PDB ID	:	6VFR
Title	:	Crystal structure of human protocadherin 18 EC1-EC4
Authors	:	Harrison, O.J.; Brasch, J.; Shapiro, L.
Deposited on	:	2020-01-06
Resolution	:	2.79 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 ⓘ 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 ⓘ) 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 2.79 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 10 unique types of molecules in this entry. The entry contains 13535 atoms, of which 6487 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 Protocadherin-18.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	428	Total	C	H	N	O	S	0	1	0
			6596	2117	3222	571	678	8			
1	B	428	Total	C	H	N	O	S	0	0	0
			6562	2113	3194	570	677	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q9HCL0
A	432	HIS	-	expression tag	UNP Q9HCL0
A	433	HIS	-	expression tag	UNP Q9HCL0
A	434	HIS	-	expression tag	UNP Q9HCL0
A	435	HIS	-	expression tag	UNP Q9HCL0
A	436	HIS	-	expression tag	UNP Q9HCL0
B	431	HIS	-	expression tag	UNP Q9HCL0
B	432	HIS	-	expression tag	UNP Q9HCL0
B	433	HIS	-	expression tag	UNP Q9HCL0
B	434	HIS	-	expression tag	UNP Q9HCL0
B	435	HIS	-	expression tag	UNP Q9HCL0
B	436	HIS	-	expression tag	UNP Q9HCL0

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-4)-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
2	C	4	Total	C	N	O	0	0	0
			49	28	2	19			

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	D	2	Total C N O 24 14 1 9	0	0	0

- Molecule 4 is an oligosaccharide called 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
4	E	3	Total C H N O 61 22 23 2 14	0	0	0

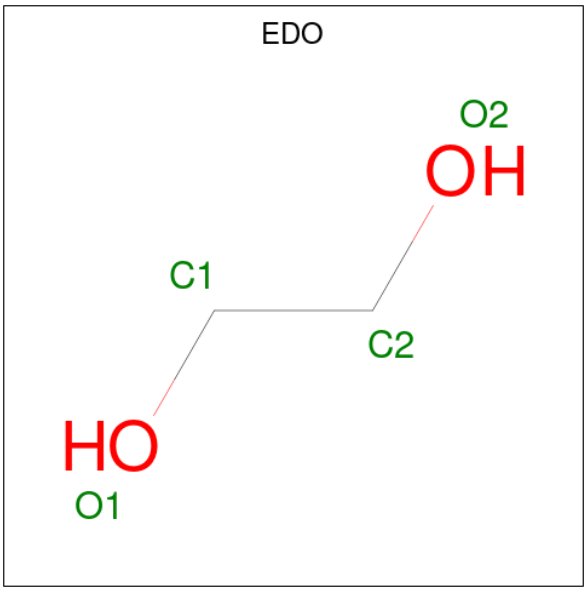
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-L-fucopyranose-(1-6)]2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
5	F	6	Total C N O 71 40 2 29	0	0	0

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	9	Total Ca 9 9	0	0
6	B	9	Total Ca 9 9	0	0

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

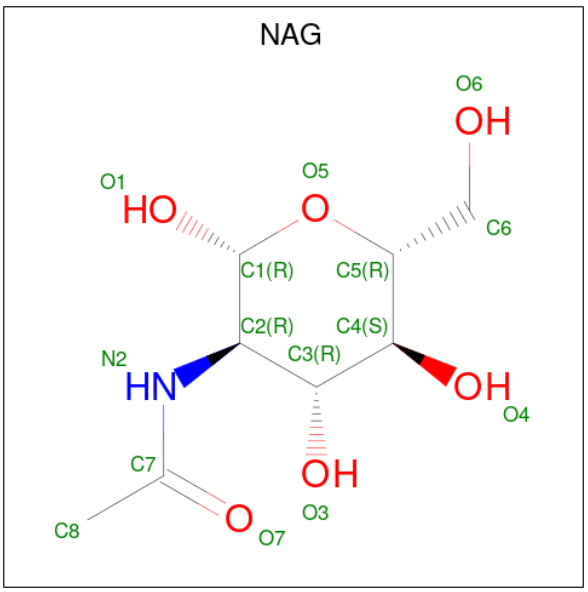


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	A	1	Total C H O 10 2 6 2	0	0
7	B	1	Total C H O 10 2 6 2	0	0
7	B	1	Total C H O 10 2 6 2	0	0
7	B	1	Total C H O 10 2 6 2	0	0

- Molecule 8 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Na 1 1	0	0
8	B	1	Total Na 1 1	0	0

- Molecule 9 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	26	Total	O	0	0
			26	26		
10	B	18	Total	O	0	0
			18	18		

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, α, β, γ	126.96Å 176.94Å 71.87Å 90.00° 101.42° 90.00°	Depositor
Resolution (Å)	19.90 – 2.79	Depositor
% Data completeness (in resolution range)	98.7 (19.90-2.79)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.00 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.236 , 0.272	Depositor
Wilson B-factor (Å^2)	63.7	Xtriage
Anisotropy	0.822	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13535	wwPDB-VP
Average B, all atoms (Å^2)	121.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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

15 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	$\#\|Z\|>2$
2	NAG	C	1	2,1	14,14,15	0.20	0	17,19,21	0.42	0
2	NAG	C	2	2	14,14,15	0.37	0	17,19,21	0.47	0
2	BMA	C	3	2	11,11,12	0.77	0	15,15,17	0.80	0
2	FUC	C	4	2	10,10,11	0.69	0	14,14,16	0.83	0
3	NAG	D	1	1,3	14,14,15	0.38	0	17,19,21	0.36	0
3	FUC	D	2	3	10,10,11	0.87	0	14,14,16	1.27	2 (14%)
4	NAG	E	1	1,4	14,14,15	0.40	0	17,19,21	0.56	0
4	NAG	E	2	4	14,14,15	0.52	0	17,19,21	0.42	0
4	FUC	E	3	4	10,10,11	1.01	1 (10%)	14,14,16	0.99	1 (7%)
5	NAG	F	1	5,1	14,14,15	0.45	0	17,19,21	0.83	0
5	NAG	F	2	5	14,14,15	0.26	0	17,19,21	0.55	0
5	BMA	F	3	5	11,11,12	0.64	0	15,15,17	0.72	0
5	MAN	F	4	5	11,11,12	0.69	0	15,15,17	1.09	2 (13%)
5	MAN	F	5	5	11,11,12	0.77	1 (9%)	15,15,17	1.10	2 (13%)
5	FUC	F	6	5	10,10,11	0.85	0	14,14,16	0.98	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
2	NAG	C	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	0/6/23/26	0/1/1/1
2	BMA	C	3	2	-	0/2/19/22	0/1/1/1
2	FUC	C	4	2	-	-	0/1/1/1
3	NAG	D	1	1,3	-	1/6/23/26	0/1/1/1
3	FUC	D	2	3	-	-	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NAG	E	2	4	-	2/6/23/26	0/1/1/1
4	FUC	E	3	4	-	-	0/1/1/1
5	NAG	F	1	5,1	-	3/6/23/26	0/1/1/1
5	NAG	F	2	5	-	4/6/23/26	0/1/1/1
5	BMA	F	3	5	-	2/2/19/22	0/1/1/1
5	MAN	F	4	5	-	0/2/19/22	0/1/1/1
5	MAN	F	5	5	-	0/2/19/22	0/1/1/1
5	FUC	F	6	5	-	-	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	3	FUC	C1-C2	2.30	1.57	1.52
5	F	5	MAN	C1-C2	2.26	1.57	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2	FUC	C1-O5-C5	2.84	119.22	112.78
5	F	4	MAN	C1-O5-C5	2.82	116.02	112.19
3	D	2	FUC	O5-C5-C4	2.81	114.56	109.52
5	F	5	MAN	C1-O5-C5	2.46	115.52	112.19
4	E	3	FUC	O2-C2-C1	2.37	114.00	109.15
5	F	5	MAN	O2-C2-C3	-2.16	105.80	110.14
5	F	4	MAN	O2-C2-C3	-2.11	105.92	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

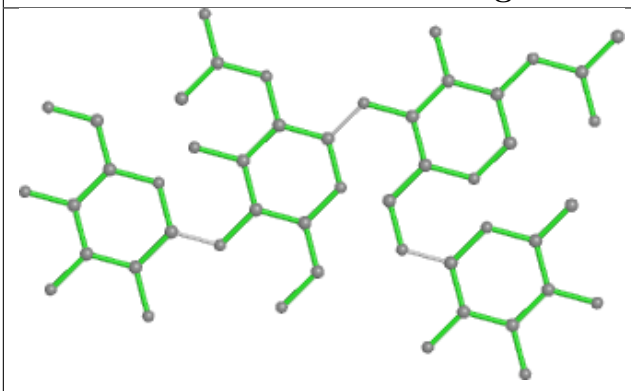
Mol	Chain	Res	Type	Atoms
5	F	1	NAG	C3-C2-N2-C7
4	E	1	NAG	C4-C5-C6-O6
4	E	2	NAG	O5-C5-C6-O6
4	E	2	NAG	C4-C5-C6-O6
5	F	2	NAG	C8-C7-N2-C2
5	F	2	NAG	O7-C7-N2-C2
4	E	1	NAG	O5-C5-C6-O6
5	F	2	NAG	O5-C5-C6-O6
5	F	1	NAG	C4-C5-C6-O6
5	F	3	BMA	C4-C5-C6-O6
3	D	1	NAG	O5-C5-C6-O6
5	F	1	NAG	O5-C5-C6-O6
5	F	3	BMA	O5-C5-C6-O6
5	F	2	NAG	C4-C5-C6-O6

There are no ring outliers.

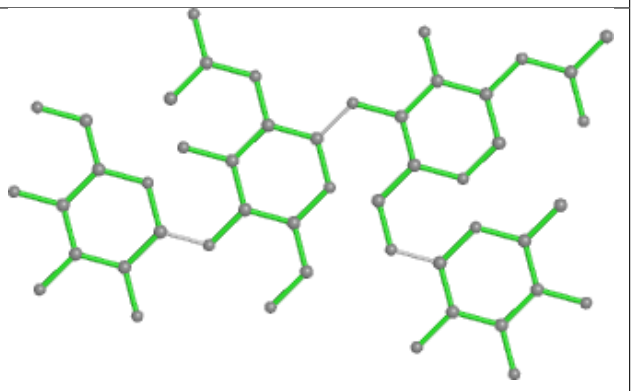
No monomer is involved in short contacts.

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

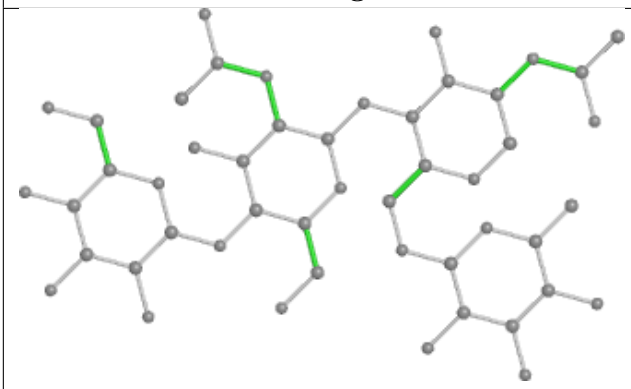
Oligosaccharide Chain C



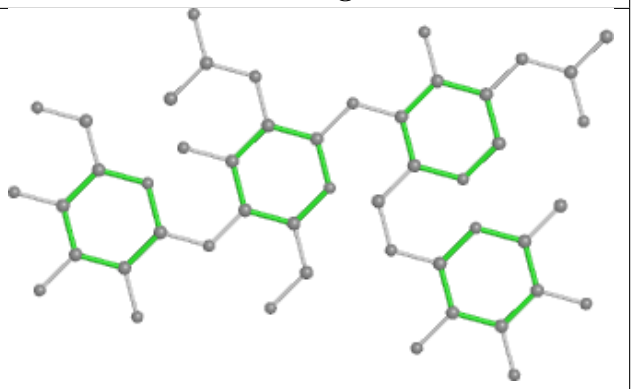
Bond lengths



Bond angles

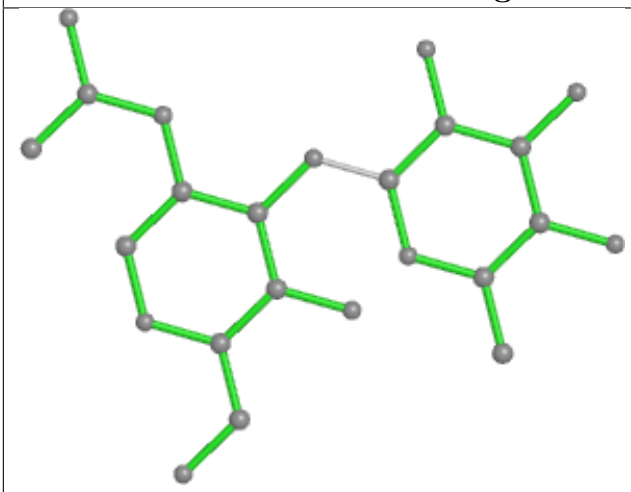


Torsions

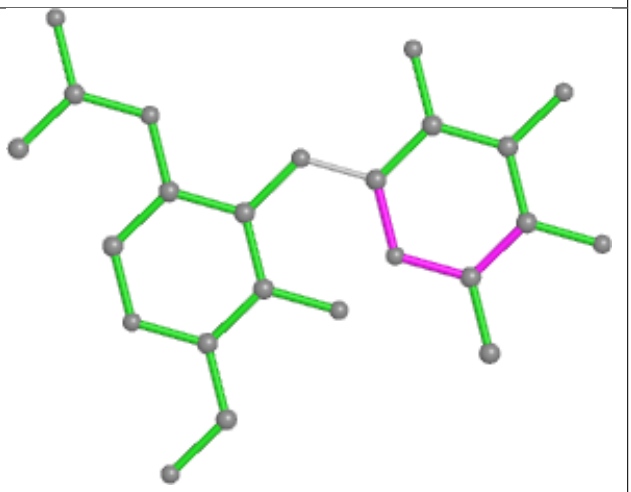


Rings

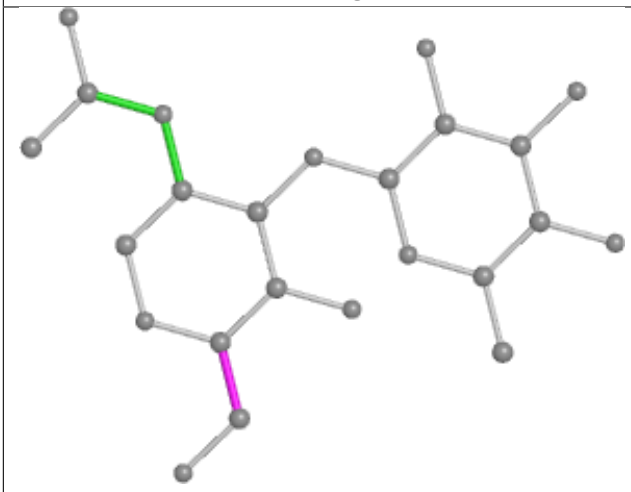
Oligosaccharide Chain D



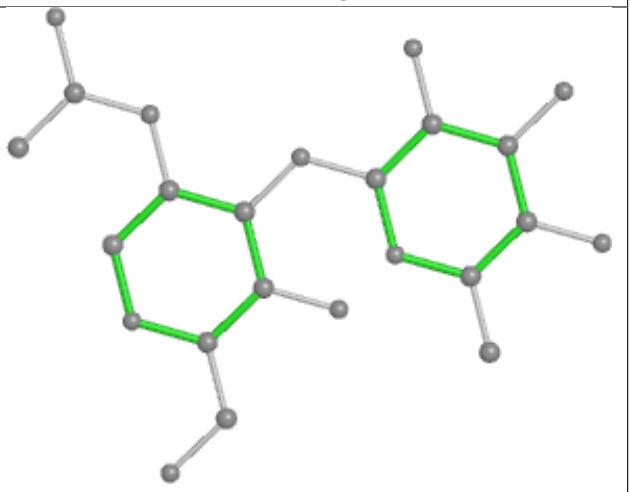
Bond lengths



Bond angles

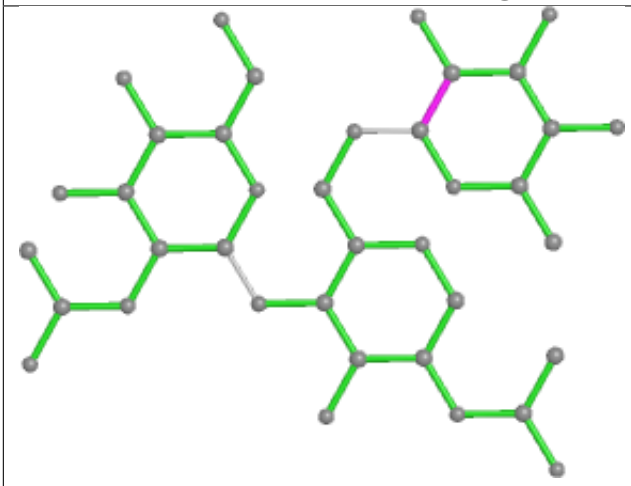


Torsions

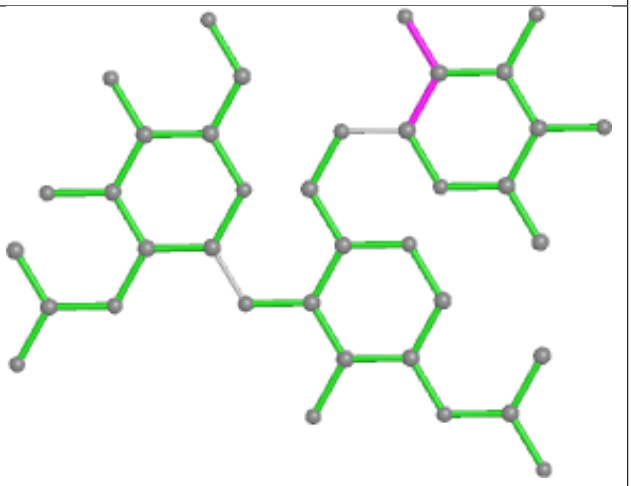


Rings

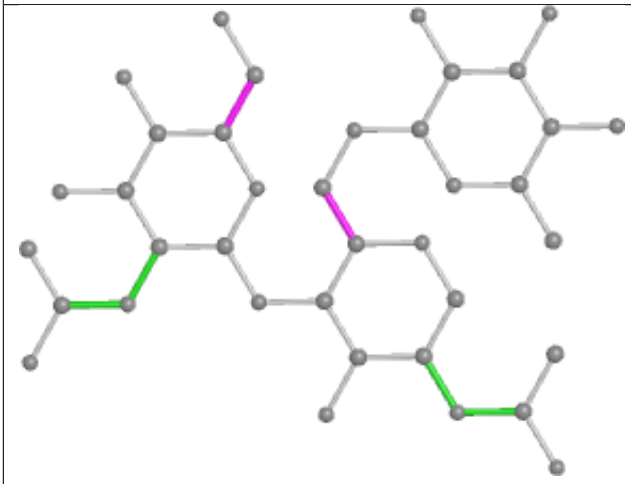
Oligosaccharide Chain E



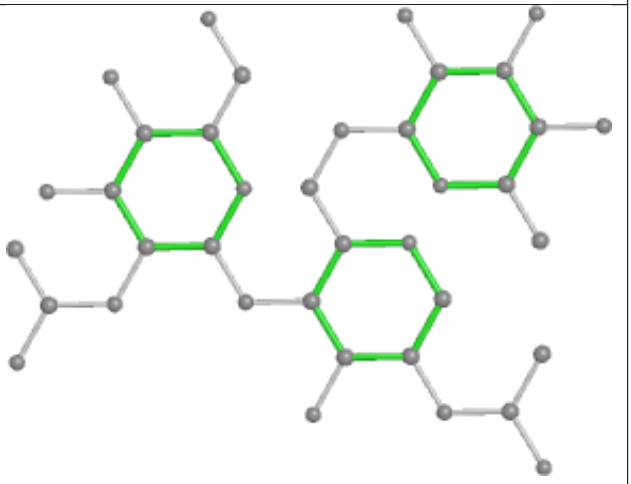
Bond lengths



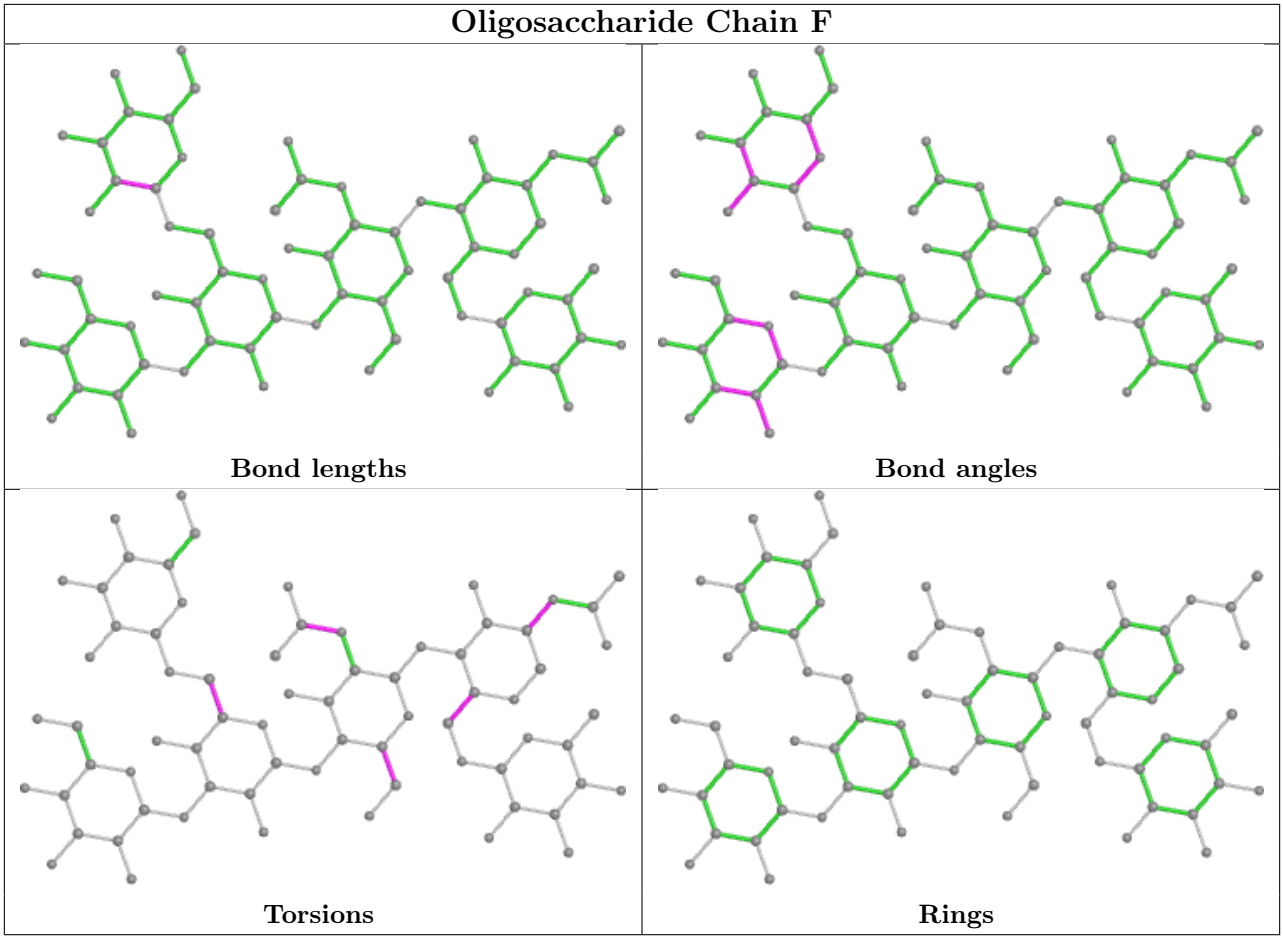
Bond angles



Torsions



Rings



4.6 Ligand geometry (i)

Of 30 ligands modelled in this entry, 20 are monoatomic - leaving 10 for Mogul analysis.

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	$\#\|Z\| > 2$
7	EDO	A	522	-	3,3,3	0.47	0	2,2,2	0.27	0
7	EDO	A	520	-	3,3,3	0.42	0	2,2,2	0.31	0
7	EDO	A	523	-	3,3,3	0.40	0	2,2,2	0.24	0
7	EDO	B	518	-	3,3,3	0.41	0	2,2,2	0.28	0
9	NAG	B	508	1	14,14,15	0.81	1 (7%)	17,19,21	0.67	0
7	EDO	B	520	-	3,3,3	0.50	0	2,2,2	0.21	0
9	NAG	B	501	1	14,14,15	0.27	0	17,19,21	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	A	521	-	3,3,3	0.45	0	2,2,2	0.27	0
7	EDO	B	519	-	3,3,3	0.46	0	2,2,2	0.31	0
7	EDO	A	519	-	3,3,3	0.45	0	2,2,2	0.34	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
7	EDO	A	522	-	-	1/1/1/1	-
7	EDO	A	520	-	-	0/1/1/1	-
7	EDO	A	523	-	-	1/1/1/1	-
7	EDO	B	518	-	-	0/1/1/1	-
9	NAG	B	508	1	-	4/6/23/26	0/1/1/1
7	EDO	B	520	-	-	1/1/1/1	-
9	NAG	B	501	1	-	4/6/23/26	0/1/1/1
7	EDO	A	521	-	-	0/1/1/1	-
7	EDO	B	519	-	-	0/1/1/1	-
7	EDO	A	519	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	508	NAG	C1-C2	2.11	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	501	NAG	C4-C5-C6-O6
9	B	501	NAG	O5-C5-C6-O6
9	B	508	NAG	C8-C7-N2-C2
9	B	508	NAG	O7-C7-N2-C2
7	A	523	EDO	O1-C1-C2-O2
9	B	501	NAG	C1-C2-N2-C7
7	A	522	EDO	O1-C1-C2-O2
7	B	520	EDO	O1-C1-C2-O2
9	B	508	NAG	C4-C5-C6-O6
9	B	508	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
9	B	501	NAG	C3-C2-N2-C7

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.