wwPDB X-ray Structure Validation Summary Report (i)

Oct 4, 2023 – 11:26 PM EDT

PDB ID	:	6VHQ
Title	:	Crystal structure of Bacillus subtilis levansucrase (D86A/E342A) in complex with oligosaccharides
Authors	:	Diaz-Vilchis, A.; Raga-Carbajal, E.; Rojas-Trejo, S.; Olvera, C.; Rudino-Pinera, E.
Deposited on	:	2020-01-10
Resolution	:	2.05 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 2.05 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 6 unique types of molecules in this entry. The entry contains 7871 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 Glycoside hydrolase family 68 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	440	3528	2222	588	707	11	0	6	0
1	B	440	3569	2248	598	712	11	0	11	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	ALA	ASP	engineered mutation	UNP A0PFL2
A	342	ALA	GLU	engineered mutation	UNP A0PFL2
A	474	THR	-	expression tag	UNP A0PFL2
A	475	ASP	-	expression tag	UNP A0PFL2
A	476	PRO	-	expression tag	UNP A0PFL2
A	477	ASN	-	expression tag	UNP A0PFL2
A	478	SER	-	expression tag	UNP A0PFL2
A	479	SER	-	expression tag	UNP A0PFL2
A	480	SER	-	expression tag	UNP A0PFL2
A	481	VAL	-	expression tag	UNP A0PFL2
A	482	ASP	-	expression tag	UNP A0PFL2
A	483	LYS	-	expression tag	UNP A0PFL2
A	484	LEU	-	expression tag	UNP A0PFL2
A	485	ALA	-	expression tag	UNP A0PFL2
A	486	ALA	-	expression tag	UNP A0PFL2
A	487	ALA	-	expression tag	UNP A0PFL2
A	488	LEU	-	expression tag	UNP A0PFL2
A	489	GLU	-	expression tag	UNP A0PFL2
A	490	HIS	-	expression tag	UNP A0PFL2
A	491	HIS	-	expression tag	UNP A0PFL2
A	492	HIS	-	expression tag	UNP A0PFL2
A	493	HIS	-	expression tag	UNP A0PFL2
A	494	HIS	-	expression tag	UNP A0PFL2
A	495	HIS	-	expression tag	UNP A0PFL2
B	86	ALA	ASP	engineered mutation	UNP A0PFL2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	342	ALA	GLU	engineered mutation	UNP A0PFL2
B	474	THR	-	expression tag	UNP A0PFL2
B	475	ASP	-	expression tag	UNP A0PFL2
B	476	PRO	-	expression tag	UNP A0PFL2
B	477	ASN	-	expression tag	UNP A0PFL2
B	478	SER	-	expression tag	UNP A0PFL2
B	479	SER	-	expression tag	UNP A0PFL2
B	480	SER	-	expression tag	UNP A0PFL2
B	481	VAL	-	expression tag	UNP A0PFL2
B	482	ASP	-	expression tag	UNP A0PFL2
B	483	LYS	-	expression tag	UNP A0PFL2
B	484	LEU	-	expression tag	UNP A0PFL2
B	485	ALA	-	expression tag	UNP A0PFL2
B	486	ALA	-	expression tag	UNP A0PFL2
B	487	ALA	-	expression tag	UNP A0PFL2
B	488	LEU	-	expression tag	UNP A0PFL2
B	489	GLU	-	expression tag	UNP A0PFL2
B	490	HIS	-	expression tag	UNP A0PFL2
B	491	HIS	-	expression tag	UNP A0PFL2
B	492	HIS	-	expression tag	UNP A0PFL2
B	493	HIS	-	expression tag	UNP A0PFL2
B	494	HIS	-	expression tag	UNP A0PFL2
B	495	HIS	-	expression tag	UNP A0PFL2

- Molecule 2 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	C	6	67	36	31	0	0	0
2	D	6	67	36	31	0	0	0
2	E	6	67	36	31	0	0	0

- Molecule 3 is an oligosaccharide called beta-D-fructofuranose-(2-6)-beta-D-fructofuranose.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
3	F	2	22	12	10	0	0	0

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is BROMIDE ION (three-letter code: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total Br 6 6	0	0
5	B	3	Total Br 3 3	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	290	Total O 290 290	0	0
6	B	250	Total O 250 250	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 21 1	Depositor
Cell constants a, b, c, α, β, γ	69.31Å 78.67Å 78.73Å 90.00° 93.94° 90.00°	Depositor
Resolution (Å)	35.20 – 2.05	Depositor
% Data completeness (in resolution range)	99.2 (35.20-2.05)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 2.05Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.167 , 0.235	Depositor
Wilson B-factor (Å^2)	25.1	Xtriage
Anisotropy	0.030	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	7871	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% 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)

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	$\#\|Z\| > 2$
2	FRU	C	1	2	11,12,12	4.57	7 (63%)	10,18,18	1.80	2 (20%)
2	FRU	C	2	2	11,11,12	4.42	8 (72%)	15,15,18	1.17	2 (13%)
2	FRU	C	3	2	11,11,12	4.28	8 (72%)	15,15,18	2.53	8 (53%)
2	FRU	C	4	2	11,11,12	4.45	8 (72%)	15,15,18	1.25	2 (13%)
2	FRU	C	5	2	11,11,12	4.29	8 (72%)	15,15,18	1.84	4 (26%)
2	FRU	C	6	2	11,11,12	4.12	8 (72%)	15,15,18	1.32	2 (13%)
2	FRU	D	1	2	11,12,12	4.64	7 (63%)	10,18,18	4.92	1 (10%)
2	FRU	D	2	2	11,11,12	4.51	8 (72%)	15,15,18	1.31	1 (6%)
2	FRU	D	3	2	11,11,12	4.51	8 (72%)	15,15,18	1.16	1 (6%)
2	FRU	D	4	2	11,11,12	4.09	8 (72%)	15,15,18	2.20	5 (33%)
2	FRU	D	5	2	11,11,12	4.32	8 (72%)	15,15,18	1.70	2 (13%)
2	FRU	D	6	2	11,11,12	4.50	8 (72%)	15,15,18	0.95	1 (6%)
2	FRU	E	1	2	11,12,12	4.47	7 (63%)	10,18,18	3.62	2 (20%)
2	FRU	E	2	2	11,11,12	4.50	8 (72%)	15,15,18	1.48	3 (20%)
2	FRU	E	3	2	11,11,12	4.52	8 (72%)	15,15,18	1.74	4 (26%)
2	FRU	E	4	2	11,11,12	4.50	8 (72%)	15,15,18	2.72	3 (20%)
2	FRU	E	5	2	11,11,12	4.74	7 (63%)	15,15,18	1.48	3 (20%)
2	FRU	E	6	2	11,11,12	4.26	8 (72%)	15,15,18	1.82	6 (40%)
3	FRU	F	1	3	11,12,12	4.36	7 (63%)	10,18,18	1.10	1 (10%)
3	FRU	F	2	3	10,10,12	5.18	8 (80%)	12,14,18	1.89	2 (16%)

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	FRU	C	1	2	-	3/5/24/24	0/1/1/1
2	FRU	C	2	2	-	1/4/20/24	0/1/1/1
2	FRU	C	3	2	-	1/4/20/24	0/1/1/1
2	FRU	C	4	2	-	1/4/20/24	0/1/1/1
2	FRU	C	5	2	-	2/4/20/24	0/1/1/1
2	FRU	C	6	2	-	0/4/20/24	0/1/1/1
2	FRU	D	1	2	-	3/5/24/24	0/1/1/1
2	FRU	D	2	2	-	2/4/20/24	0/1/1/1
2	FRU	D	3	2	-	2/4/20/24	0/1/1/1
2	FRU	D	4	2	-	0/4/20/24	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FRU	D	5	2	-	2/4/20/24	0/1/1/1
2	FRU	D	6	2	-	0/4/20/24	0/1/1/1
2	FRU	E	1	2	-	3/5/24/24	0/1/1/1
2	FRU	E	2	2	-	2/4/20/24	0/1/1/1
2	FRU	E	3	2	-	4/4/20/24	0/1/1/1
2	FRU	E	4	2	-	4/4/20/24	0/1/1/1
2	FRU	E	5	2	-	3/4/20/24	0/1/1/1
2	FRU	E	6	2	-	0/4/20/24	0/1/1/1
3	FRU	F	1	3	-	0/5/24/24	0/1/1/1
3	FRU	F	2	3	-	2/2/18/24	0/1/1/1

The worst 5 of 155 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	5	FRU	C4-C3	-11.10	1.22	1.53
3	F	2	FRU	C4-C3	-10.50	1.24	1.53
2	E	3	FRU	C4-C3	-10.36	1.25	1.53
2	E	2	FRU	C4-C3	-10.25	1.25	1.53
2	C	5	FRU	C4-C3	-10.25	1.25	1.53

The worst 5 of 55 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1	FRU	O6-C6-C5	15.07	162.99	111.29
2	E	1	FRU	O6-C6-C5	11.05	149.22	111.29
2	E	4	FRU	O6-C6-C5	9.27	143.10	111.29
2	C	3	FRU	O5-C2-C1	6.37	122.98	109.21
3	F	2	FRU	C6-C5-C4	-5.60	109.81	115.70

There are no chirality outliers.

5 of 35 torsion outliers are listed below:

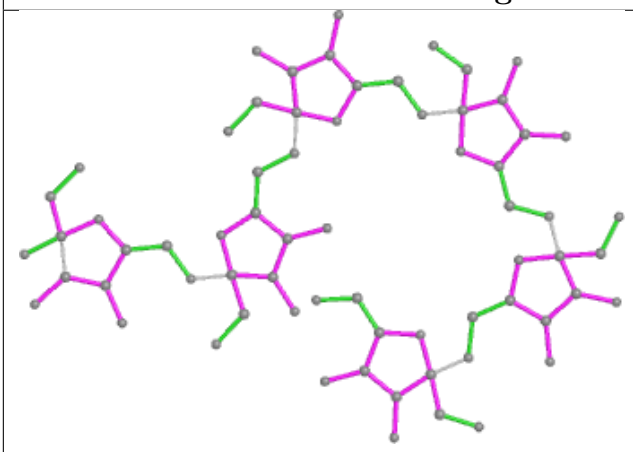
Mol	Chain	Res	Type	Atoms
2	C	1	FRU	O1-C1-C2-C3
2	C	1	FRU	O1-C1-C2-O2
2	D	1	FRU	O1-C1-C2-C3
2	E	1	FRU	O1-C1-C2-C3
2	E	1	FRU	O1-C1-C2-O2

There are no ring outliers.

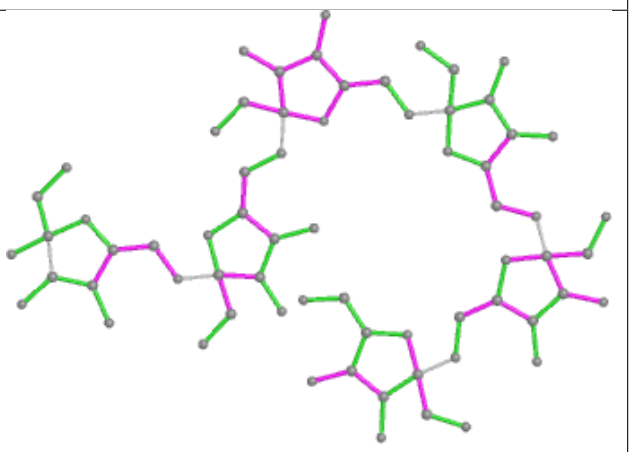
No monomer is involved in short contacts.

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

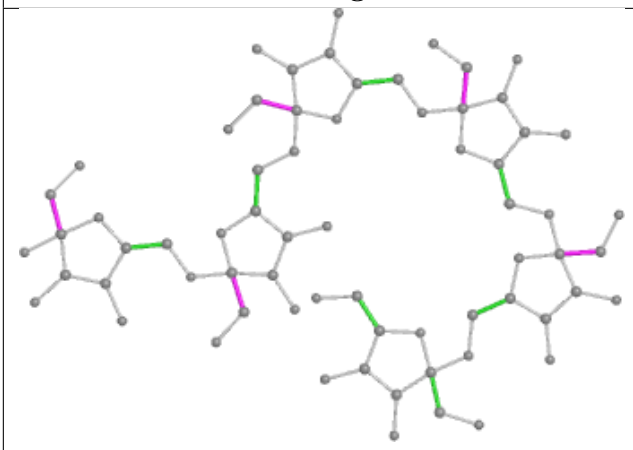
Oligosaccharide Chain C



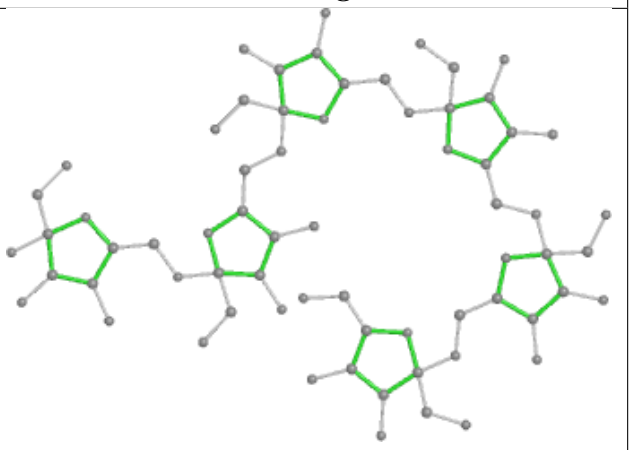
Bond lengths



Bond angles

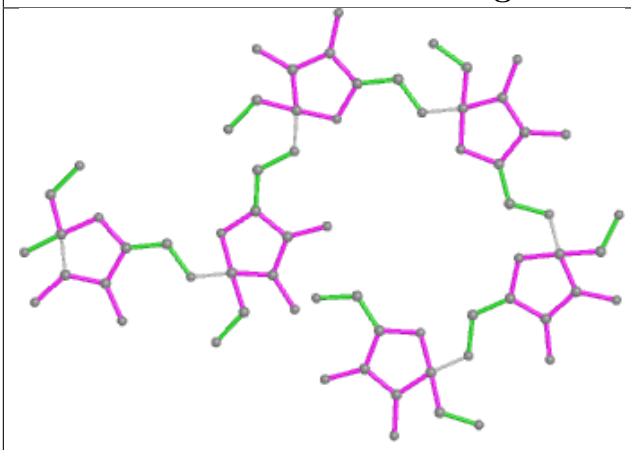


Torsions

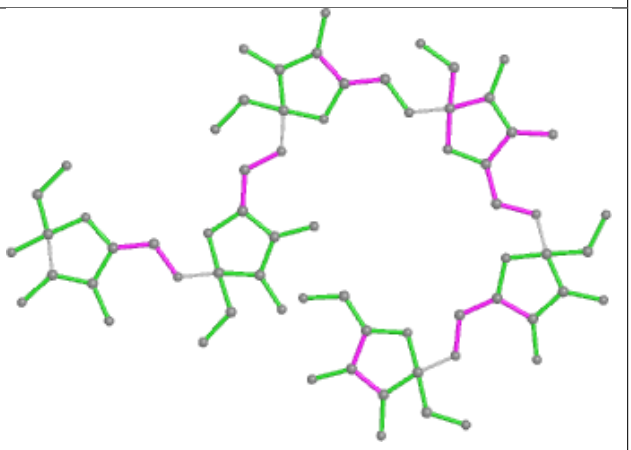


Rings

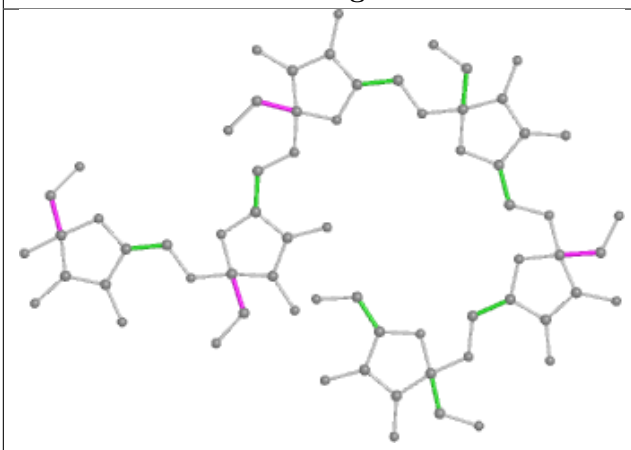
Oligosaccharide Chain D



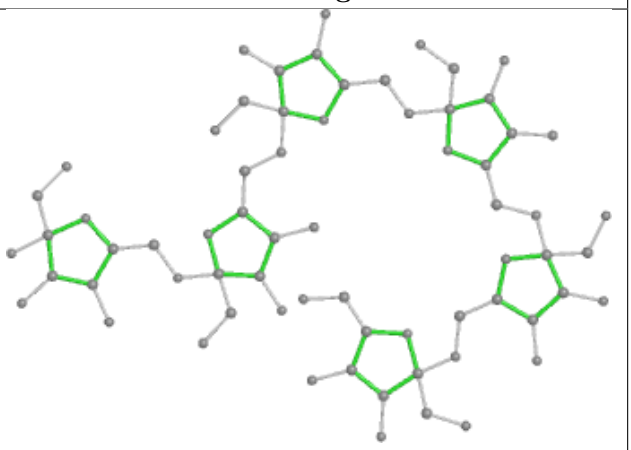
Bond lengths



Bond angles

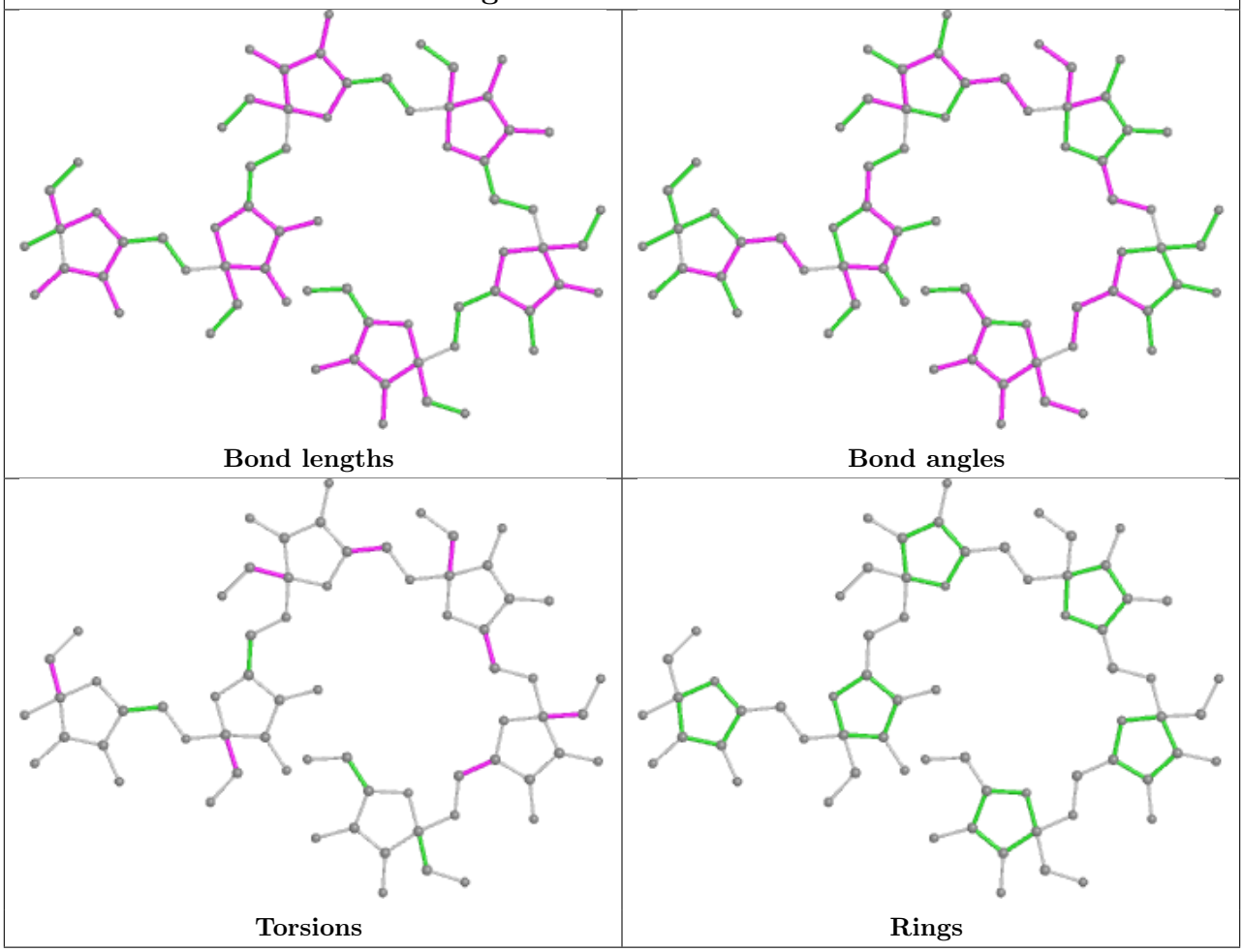


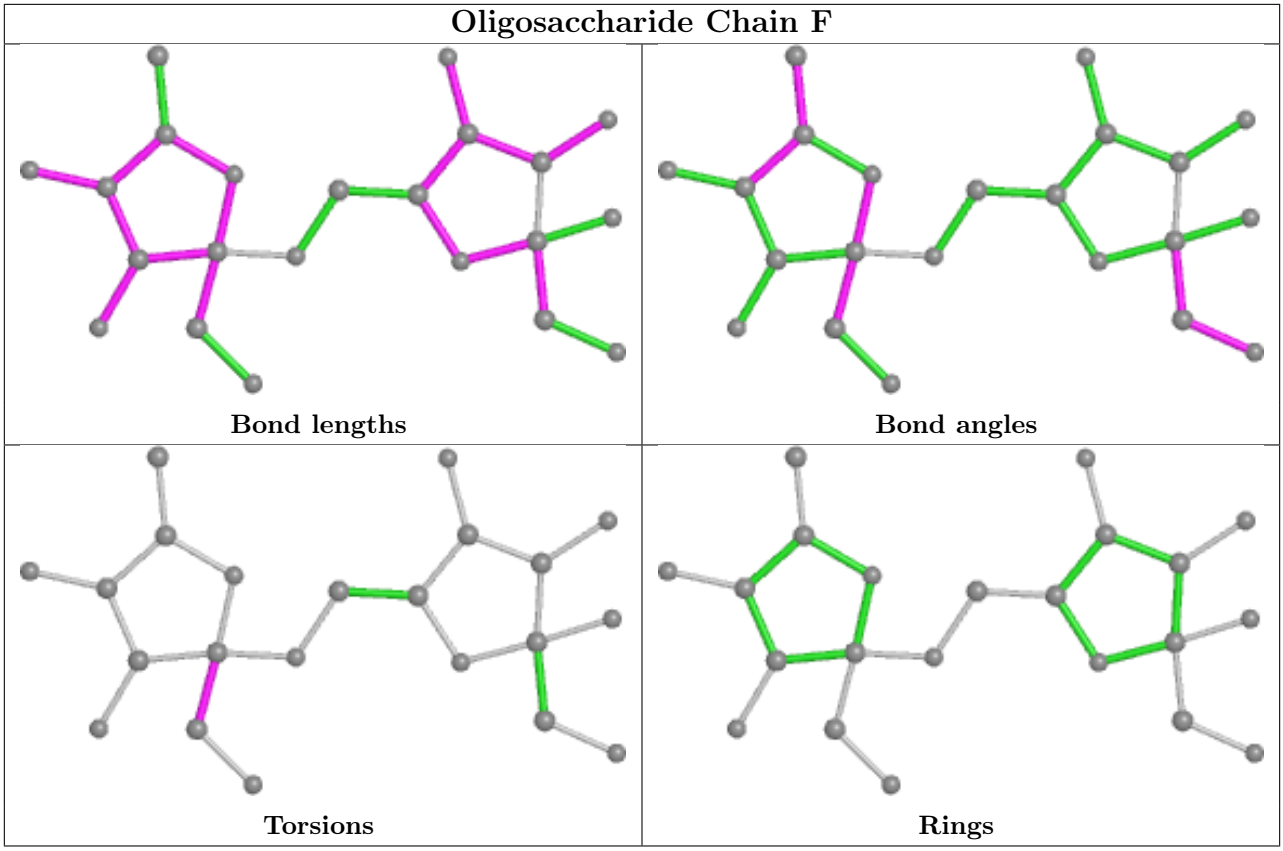
Torsions



Rings

Oligosaccharide Chain E





4.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 11 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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.