Full wwPDB X-ray Structure Validation Report (i)

Dec 18, 2023 – 08:51 am GMT

PDB ID	:	3ZZV
Title	:	BambL complexed with Htype2 tetrasaccharide
Authors	:	Audfray, A.; Claudinon, J.; Abounit, S.; Ruvoen-Clouet, N.; Larson, G.; Wimmerova, M.; LePendu, J.; Romer, W.; Varrot, A.; Imberty, A.
Deposited on	:	2011-09-05
Resolution	:	1.68 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:

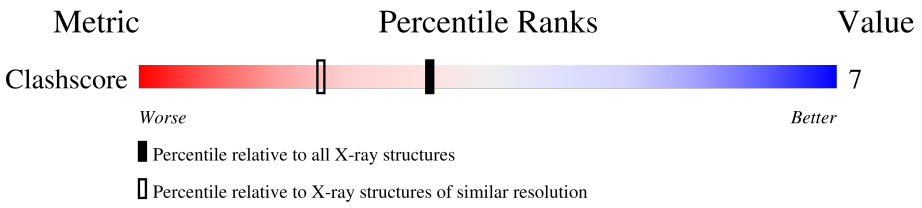
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.68 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	7310 (1.70-1.66)

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GAL	F	2	X	-	-	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 2392 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.

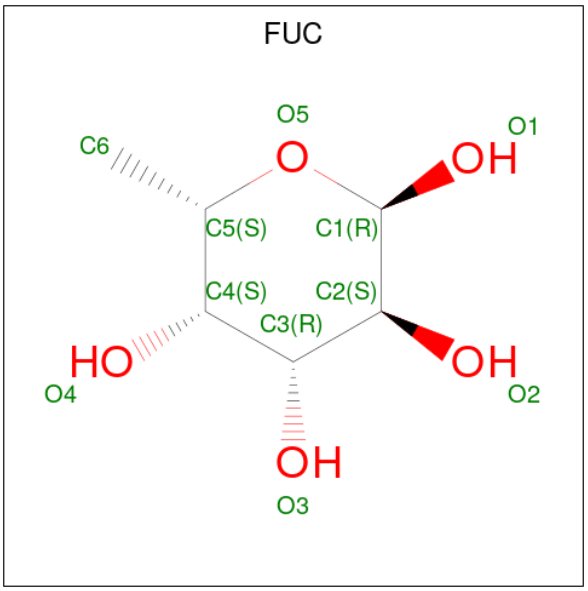
- Molecule 1 is a protein called BAMBL LECTIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	87	665	413	116	132	4	0	1	0
1	B	87	661	410	115	132	4	0	0	0
1	C	87	667	413	116	134	4	0	1	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	36	20	1	15	0	0	0
2	E	3	36	20	1	15	0	0	0
2	F	3	36	20	1	15	0	0	0
2	G	3	36	20	1	15	0	0	0
2	H	3	36	20	1	15	0	0	0

- Molecule 3 is alpha-L-fucopyranose (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	11	6	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	106	106	106	0	0
			Total	O		
4	B	58	58	58	0	0
			Total	O		
4	C	44	44	44	0	0

SEQUENCE-PLOTS INFOmissingINFO

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	35.74Å 47.77Å 74.60Å 90.00° 100.81° 90.00°	Depositor
Resolution (Å)	73.28 – 1.68	Depositor
% Data completeness (in resolution range)	96.7 (73.28-1.68)	Depositor
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 1.68Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.211 , 0.271	Depositor
Wilson B-factor (Å^2)	20.7	Xtriage
Anisotropy	0.263	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	2392	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.04% 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)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, FUC, GAL

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 $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.93	1/687 (0.1%)	0.89	0/940
1	B	0.74	0/680	0.83	0/929
1	C	0.75	0/686	0.85	1/937 (0.1%)
All	All	0.81	1/2053 (0.0%)	0.85	1/2806 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	35	TYR	CD1-CE1	-5.32	1.31	1.39

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	ARG	NE-CZ-NH1	5.20	122.90	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	39	PHE	Peptide

4.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	665	0	606	10	0
1	B	661	0	600	5	0
1	C	667	0	604	17	0
2	D	36	0	33	0	0
2	E	36	0	33	0	0
2	F	36	0	33	0	0
2	G	36	0	33	0	0
2	H	36	0	33	1	0
3	B	11	0	12	0	0
4	A	106	0	0	2	0
4	B	58	0	0	1	0
4	C	44	0	0	1	0
All	All	2392	0	1987	29	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (29) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:GLN:HE22	1:C:46:VAL:H	1.21	0.88
1:C:54:GLY:HA3	1:C:55:SER:HB3	1.66	0.76
1:C:54:GLY:HA3	1:C:55:SER:CB	2.17	0.74
1:C:54:GLY:CA	1:C:55:SER:HB3	2.19	0.73
1:C:2:GLN:HE22	1:C:46:VAL:N	1.91	0.68
1:C:2:GLN:NE2	1:C:45:ASN:HA	2.15	0.62
1:C:22:ASN:ND2	1:C:44:ASP:OD2	2.34	0.60
1:A:23:LYS:HD2	4:A:2035:HOH:O	2.05	0.56
1:B:70:THR:HG23	1:B:81:ARG:HD3	1.86	0.56
1:A:81:ARG:NH2	4:A:2082:HOH:O	2.39	0.55
1:A:32:SER:OG	1:A:33:ASN:N	2.44	0.51
1:C:54:GLY:CA	1:C:55:SER:CB	2.85	0.49
1:C:53[A]:SER:O	1:C:55:SER:HB3	2.14	0.47
1:A:11:THR:N	1:A:12:PRO:HA	2.29	0.47
1:A:12:PRO:HG3	1:C:51:TRP:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:PHE:CD1	1:C:40:ASN:HA	2.50	0.47
1:A:2:GLN:HG2	1:C:45:ASN:HD21	1.80	0.46
1:C:53[A]:SER:C	1:C:55:SER:HB3	2.36	0.45
1:C:2:GLN:HE21	1:C:45:ASN:HA	1.81	0.45
1:A:26:GLU:HB2	1:A:39:PHE:HB3	2.00	0.44
1:B:40:ASN:ND2	4:B:2028:HOH:O	2.43	0.44
1:C:58:HIS:HA	1:C:74:TRP:O	2.18	0.44
1:A:43:GLY:HA2	1:A:65:SER:OG	2.18	0.43
1:C:53[B]:SER:C	1:C:55:SER:HB3	2.38	0.43
1:A:64:THR:HG21	1:B:1:MET:HB3	2.02	0.42
4:C:2035:HOH:O	2:H:1:NAG:H62	2.20	0.41
1:C:71:GLU:HB2	1:C:84:TYR:HB3	2.03	0.40
1:B:52:LEU:HD23	1:B:57:VAL:HA	2.03	0.40
1:A:51:TRP:CZ2	1:B:12:PRO:HG3	2.57	0.40

There are no symmetry-related clashes.

4.3 Torsion angles (i)

4.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

4.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

4.3.3 RNA (i)

There are no RNA molecules in this entry.

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)

15 monosaccharides are modelled in this entry.

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	GAL	F	2	2	1/1/4/5	-	-

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	F	2	GAL	C1

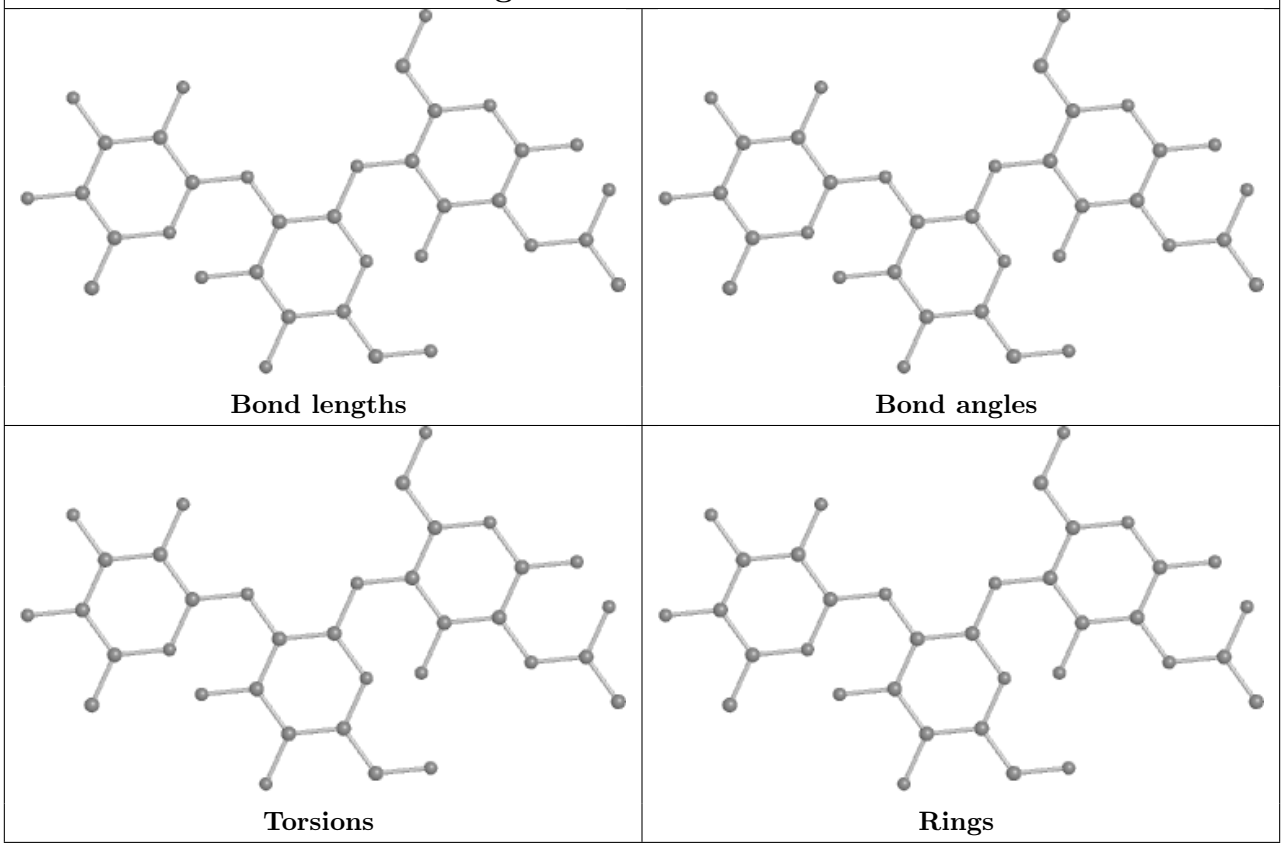
There are no torsion outliers.

There are no ring outliers.

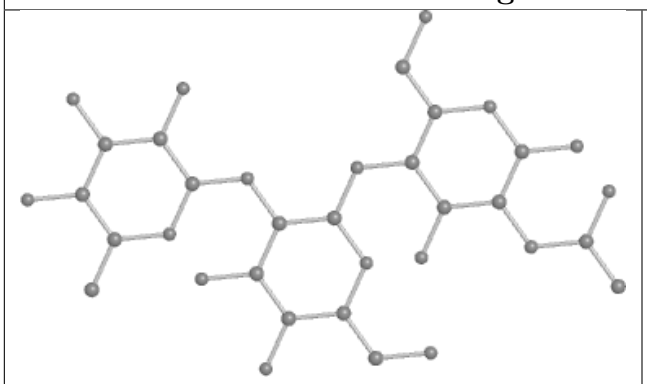
No monomer is involved in short contacts.

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

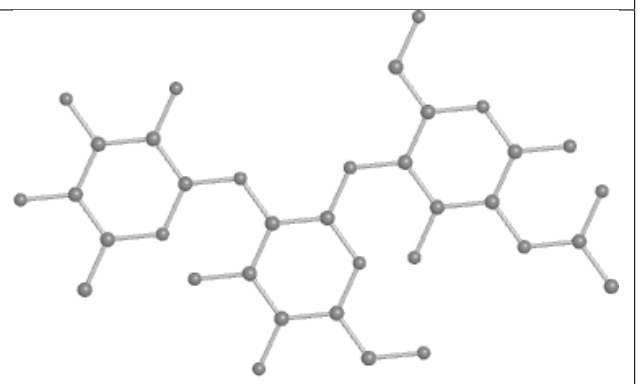
Oligosaccharide Chain D



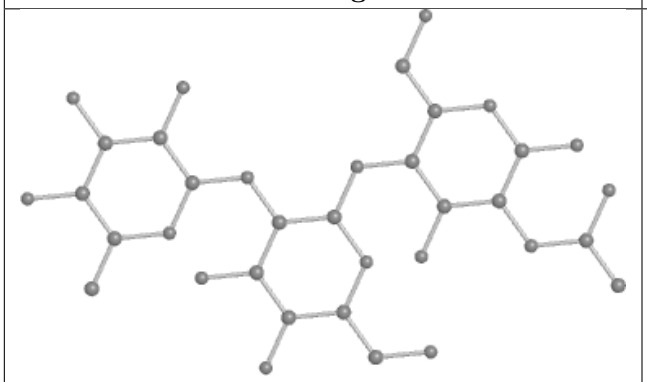
Oligosaccharide Chain E



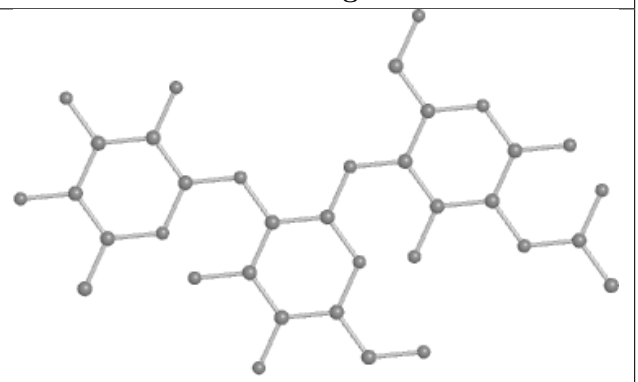
Bond lengths



Bond angles

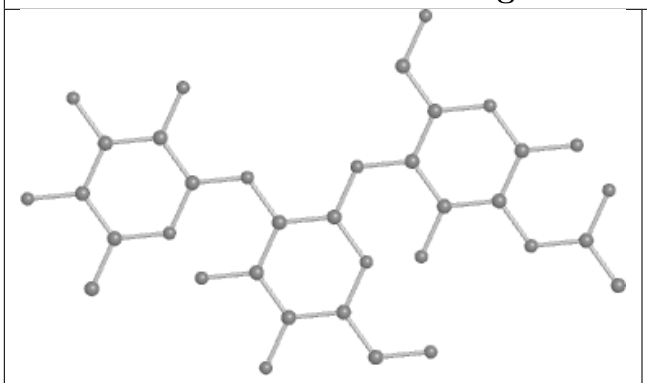


Torsions

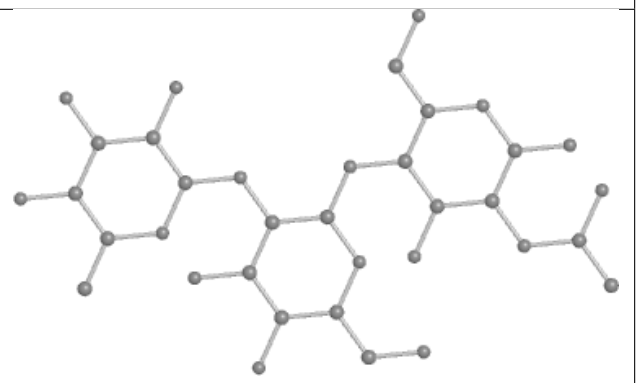


Rings

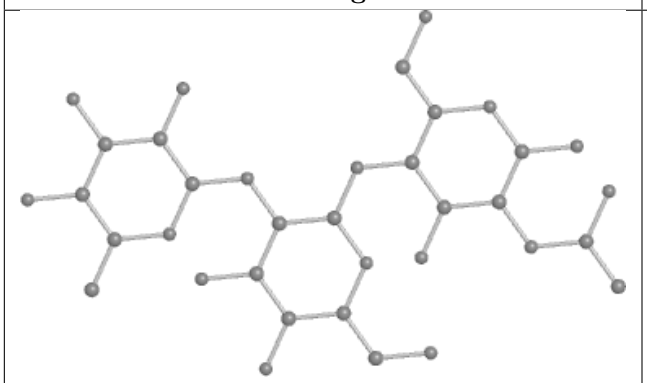
Oligosaccharide Chain F



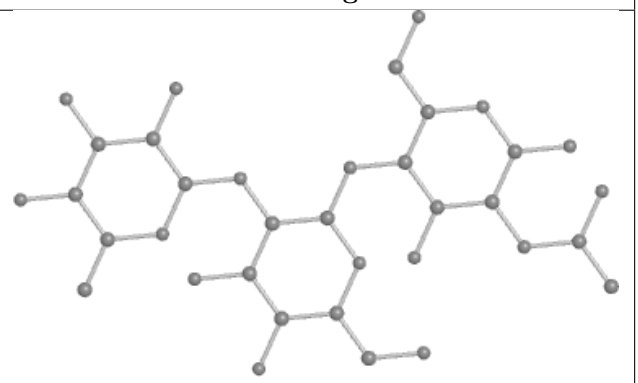
Bond lengths



Bond angles

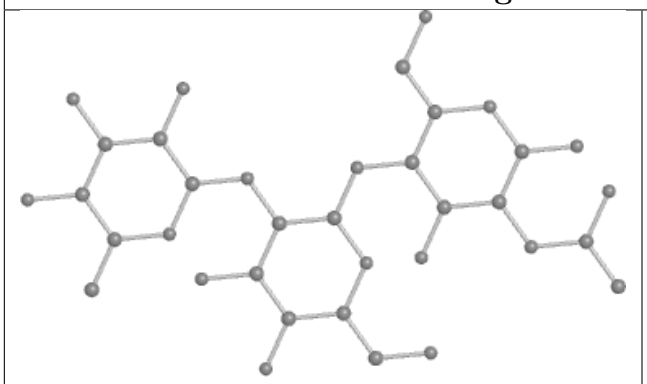


Torsions

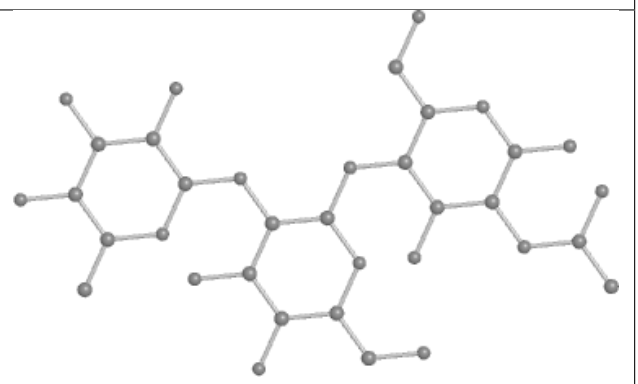


Rings

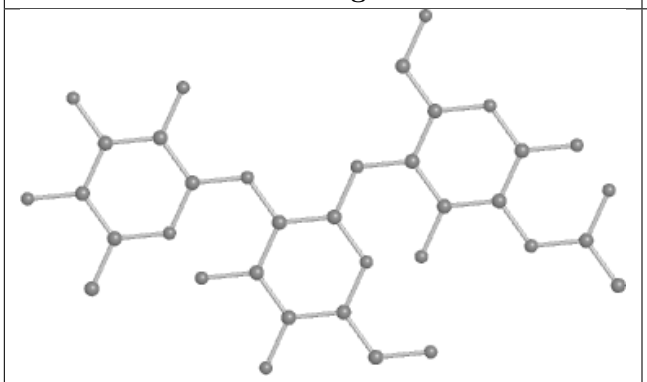
Oligosaccharide Chain G



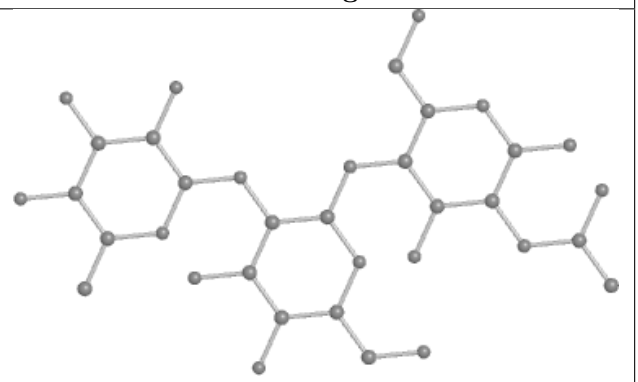
Bond lengths



Bond angles

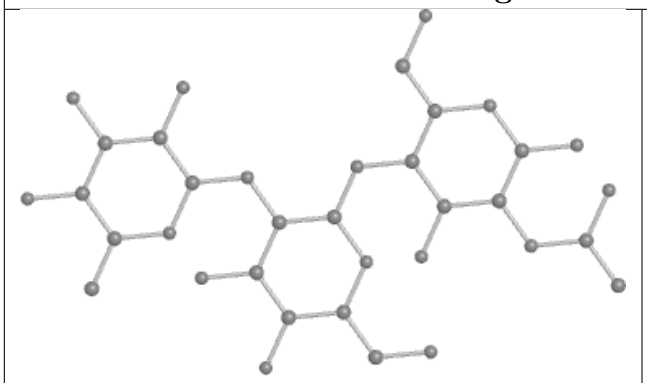


Torsions

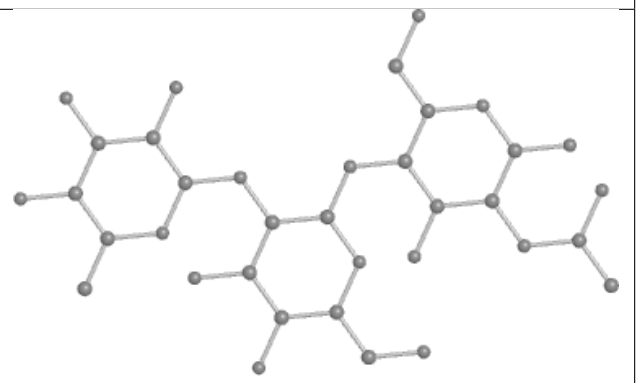


Rings

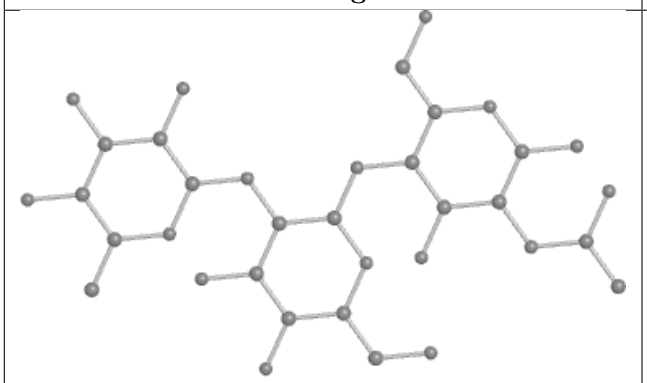
Oligosaccharide Chain H



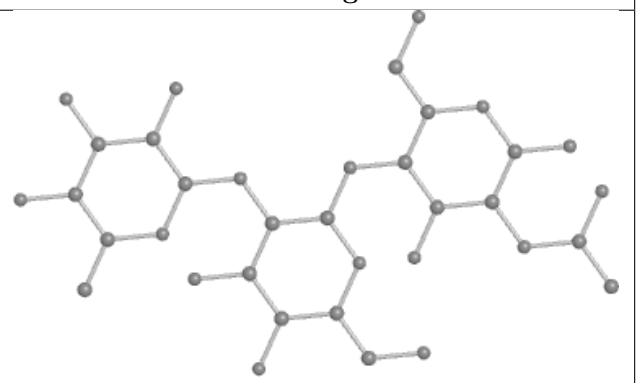
Bond lengths



Bond angles



Torsions



Rings

4.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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.