wwPDB X-ray Structure Validation Summary Report (i)

Sep 28, 2024 – 06:06 AM EDT

PDB ID	:	1SLB
Title	:	X-RAY CRYSTALLOGRAPHY REVEALS CROSSLINKING OF MAMMALIAN LECTIN (GALECTIN-1) BY BIANTENNARY COMPLEX TYPE SACCHARIDES
Authors	:	Bourne, Y.; Cambillau, C.
Deposited on	:	1994-03-12
Resolution	:	2.30 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:

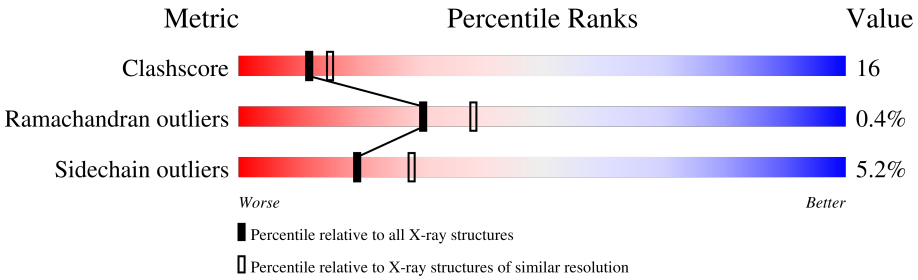
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.30 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	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	134	68% 29% .
1	B	134	68% 30% .
1	C	134	66% 32% .
1	D	134	66% 31% .
2	E	8	38% 50% 12%
3	F	7	57% 43%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MAN	F	1	X	-	-	-

2 Entry composition (i)

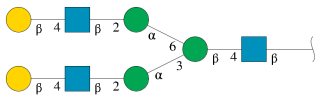
There are 4 unique types of molecules in this entry. The entry contains 4677 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 BOVINE GALECTIN-1.

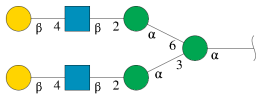
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1027	649	178	195	5			
1	B	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			
1	C	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			
1	D	134	Total	C	N	O	S	0	0	0
			1028	649	178	195	6			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	8	Total	C	N	O	0	0	0
			98	54	3	41			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	7	Total	C	N	O	0	0	0
			84	46	2	36			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	83	Total	O	0	0
			83	83		
4	C	90	Total	O	0	0
			90	90		
4	D	78	Total	O	0	0
			78	78		

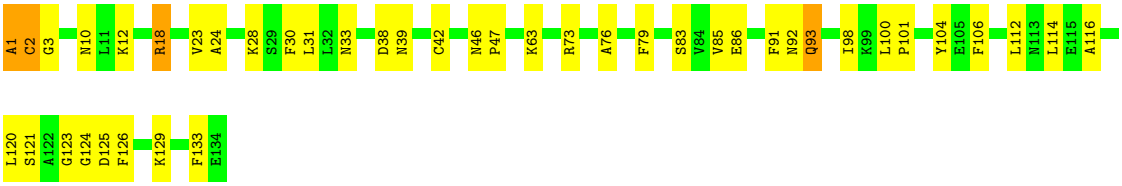
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: BOVINE GALECTIN-1

Chain A:



• Molecule 1: BOVINE GALECTIN-1

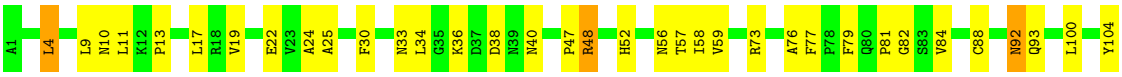
Chain B:

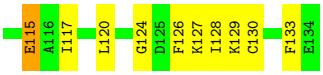
• Molecule 1: BOVINE GALECTIN-1

Chain C:

• Molecule 1: BOVINE GALECTIN-1

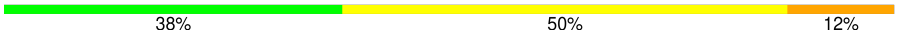
Chain D:

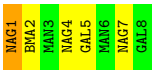




• Molecule 2: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:





• Molecule 3: beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[beta-D-galactopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-2)-alpha-D-mannopyranose-(1-6)]alpha-D-mannopyranose

Chain F:

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.80Å 41.60Å 110.00Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.177 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4677	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.60	2/1048 (0.2%)	0.93	6/1417 (0.4%)
1	B	0.41	0/1049	0.68	1/1418 (0.1%)
1	C	0.36	0/1049	0.61	0/1418
1	D	0.39	0/1049	0.65	0/1418
All	All	0.45	2/4195 (0.0%)	0.73	7/5671 (0.1%)

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	A	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	CYS	C-N	-9.86	1.15	1.33
1	A	2	CYS	C-O	-8.42	1.07	1.23

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	CYS	O-C-N	-14.79	98.06	123.20
1	A	1	ALA	O-C-N	10.30	139.18	122.70
1	A	2	CYS	N-CA-CB	-7.79	96.58	110.60
1	A	1	ALA	CA-C-N	-7.18	101.39	117.20
1	A	2	CYS	CA-C-N	6.67	129.53	116.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	GLY	Mainchain

5.2 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	1027	0	997	33	0
1	B	1028	0	1001	31	0
1	C	1028	0	1001	30	0
1	D	1028	0	1001	37	0
2	E	98	0	84	1	0
3	F	84	0	72	1	0
4	A	133	0	0	4	0
4	B	83	0	0	3	0
4	C	90	0	0	4	0
4	D	78	0	0	4	0
All	All	4677	0	4156	132	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 16.

The worst 5 of 132 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:A:1:ALA:HB1	1:A:123:GLY:HA3	1.09	1.09
1:A:1:ALA:CB	1:A:123:GLY:HA3	2.02	0.83
1:A:30:PHE:HB2	1:A:126:PHE:HB2	1.62	0.80
1:C:30:PHE:HB2	1:C:126:PHE:HB2	1.65	0.79
1:C:92:ASN:HB3	1:C:95:ASP:O	1.83	0.79

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
1	B	132/134 (98%)	126 (96%)	6 (4%)	0	100	100
1	C	132/134 (98%)	125 (95%)	7 (5%)	0	100	100
1	D	132/134 (98%)	123 (93%)	7 (5%)	2 (2%)	8	8
All	All	528/536 (98%)	500 (95%)	26 (5%)	2 (0%)	30	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	4	LEU
1	D	82	GLY

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	109/110 (99%)	105 (96%)	4 (4%)	29	43
1	B	110/110 (100%)	104 (94%)	6 (6%)	18	26
1	C	110/110 (100%)	102 (93%)	8 (7%)	11	16
1	D	110/110 (100%)	105 (96%)	5 (4%)	23	34
All	All	439/440 (100%)	416 (95%)	23 (5%)	19	28

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	95	ASP
1	C	133	PHE
1	C	113	ASN
1	D	48	ARG
1	B	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	40	ASN
1	D	80	GLN
1	D	113	ASN
1	D	56	ASN
1	B	113	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

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	E	1	2	15,15,15	0.55	0	21,21,21	1.03	1 (4%)
2	BMA	E	2	2	11,11,12	0.63	0	15,15,17	1.23	2 (13%)
2	MAN	E	3	2	11,11,12	0.44	0	15,15,17	0.55	0
2	NAG	E	4	2	14,14,15	0.55	0	17,19,21	0.75	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	E	5	2	11,11,12	0.38	0	15,15,17	0.73	1 (6%)
2	MAN	E	6	2	11,11,12	0.71	0	15,15,17	0.91	0
2	NAG	E	7	2	14,14,15	0.65	0	17,19,21	0.71	0
2	GAL	E	8	2	11,11,12	0.38	0	15,15,17	0.54	0
3	MAN	F	1	3	12,12,12	0.35	0	17,17,17	0.63	0
3	MAN	F	2	3	11,11,12	0.64	0	15,15,17	0.44	0
3	NAG	F	3	3	14,14,15	0.46	0	17,19,21	0.76	1 (5%)
3	GAL	F	4	3	11,11,12	0.29	0	15,15,17	0.82	1 (6%)
3	MAN	F	5	3	11,11,12	0.33	0	15,15,17	0.64	0
3	NAG	F	6	3	14,14,15	0.47	0	17,19,21	0.65	0
3	GAL	F	7	3	11,11,12	0.41	0	15,15,17	0.46	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	E	1	2	-	0/6/26/26	0/1/1/1
2	BMA	E	2	2	-	0/2/19/22	0/1/1/1
2	MAN	E	3	2	-	0/2/19/22	0/1/1/1
2	NAG	E	4	2	-	0/6/23/26	0/1/1/1
2	GAL	E	5	2	-	0/2/19/22	0/1/1/1
2	MAN	E	6	2	-	2/2/19/22	0/1/1/1
2	NAG	E	7	2	-	1/6/23/26	0/1/1/1
2	GAL	E	8	2	-	2/2/19/22	0/1/1/1
3	MAN	F	1	3	1/1/5/5	2/2/22/22	0/1/1/1
3	MAN	F	2	3	-	0/2/19/22	0/1/1/1
3	NAG	F	3	3	-	0/6/23/26	0/1/1/1
3	GAL	F	4	3	-	0/2/19/22	0/1/1/1
3	MAN	F	5	3	-	1/2/19/22	0/1/1/1
3	NAG	F	6	3	-	2/6/23/26	0/1/1/1
3	GAL	F	7	3	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	2	BMA	C3-C4-C5	3.34	116.29	110.23
2	E	1	NAG	O5-C1-C2	2.82	112.35	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	5	GAL	C1-C2-C3	2.33	113.04	109.64
2	E	4	NAG	C2-N2-C7	-2.29	119.84	122.90
2	E	2	BMA	C6-C5-C4	-2.22	107.56	113.02

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	F	1	MAN	C1

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	6	MAN	O5-C5-C6-O6
3	F	1	MAN	C4-C5-C6-O6
2	E	8	GAL	C4-C5-C6-O6
3	F	6	NAG	C4-C5-C6-O6
3	F	1	MAN	O5-C5-C6-O6

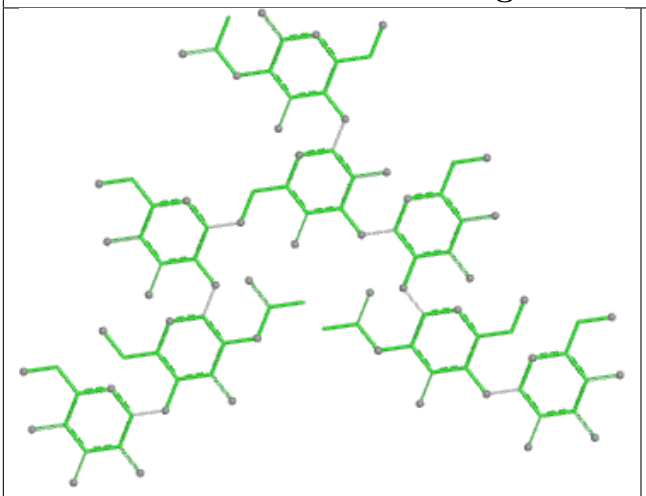
There are no ring outliers.

3 monomers are involved in 2 short contacts:

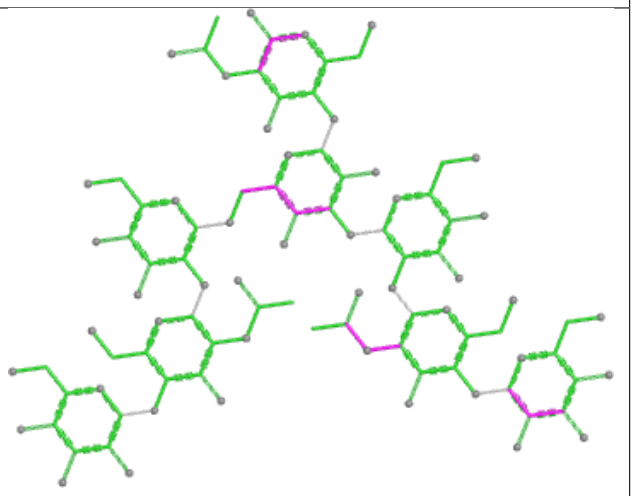
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0
2	E	7	NAG	1	0
3	F	1	MAN	1	0

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

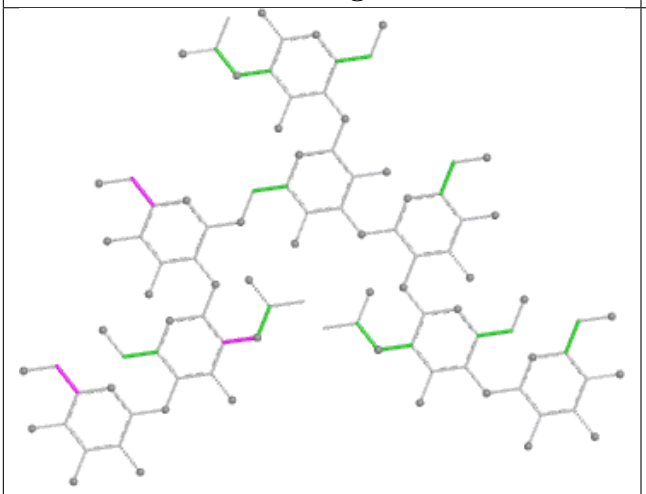
Oligosaccharide Chain E



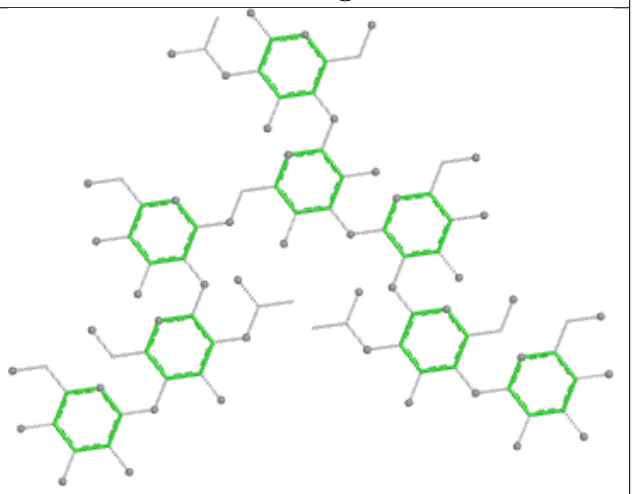
Bond lengths



Bond angles

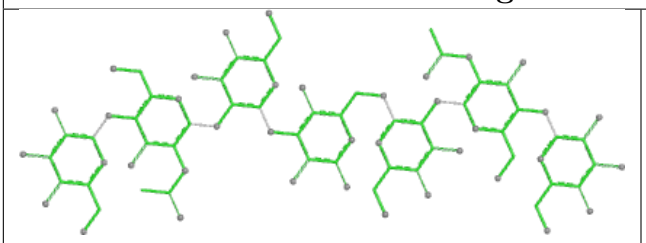


Torsions

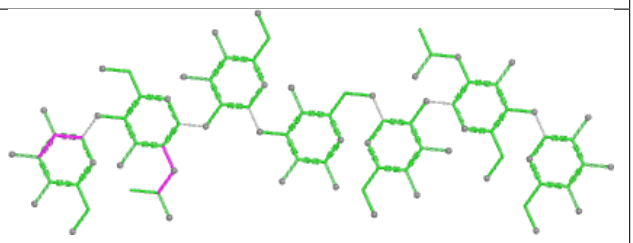


Rings

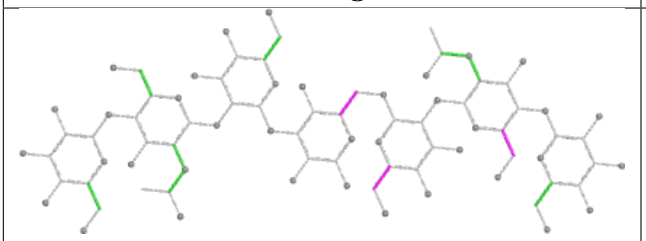
Oligosaccharide Chain F



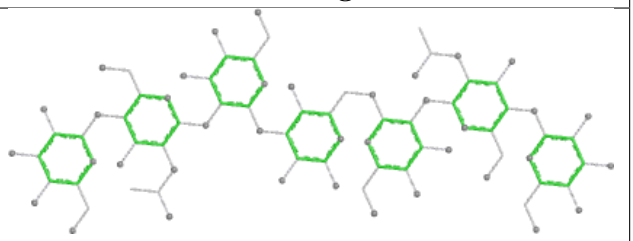
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	2:CYS	C	3:GLY	N	1.15

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.