



wwPDB NMR Structure Validation Summary Report ⓘ

Sep 9, 2021 – 05:11 PM BST

PDB ID : 6YFY
Title : Solid-state NMR structure of the D-Arg4,L10-teixobactin - Lipid II complex
in lipid bilayers
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Deposited on : 2020-03-26

This is a wwPDB NMR 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/NMRValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
RCI	:	v_1n_11_5_13_A (Berjanski et al., 2005)
PANAV	:	Wang et al. (2010)
ShiftChecker	:	2.23.1
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

SOLID-STATE NMR

The overall completeness of chemical shifts assignment is 12%.

There are no overall percentile quality scores available for this entry.

The sequence quality summary graphics cannot be shown.

2 Ensemble composition and analysis

This entry contains 26 models. Model 1 is the overall representative, medoid model (most similar to other models).

The following residues are included in the computation of the global validation metrics.

Well-defined (core) protein residues			
Well-defined core	Residue range (total)	Backbone RMSD (Å)	Medoid model
1	A:2-A:3, A:6-A:7, A:9-A:11, B:2-B:3, B:6-B:7, B:9-B:11, E:2-E:3, E:6-E:7, E:9-E:11, F:2-F:3, F:6-F:7 (25)	0.99	1

Ill-defined regions of proteins are excluded from the global statistics.

Ligands and non-protein polymers are included in the analysis.

The models can be grouped into 5 clusters and 3 single-model clusters were found.

Cluster number	Models
1	1, 14, 17, 18, 22, 23
2	2, 8, 9, 11, 24, 26
3	5, 10, 12, 16, 20, 25
4	3, 4, 19
5	15, 21
Single-model clusters	6; 7; 13

3 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 1460 atoms, of which 756 are hydrogens and 0 are deuteriums.

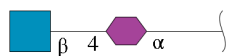
- Molecule 1 is a protein called D-Arg4,Leu10-Teixobactin.

Mol	Chain	Residues	Atoms					Trace
1	A	11	Total	C	H	N	O	0
			187	59	100	14	14	
1	B	11	Total	C	H	N	O	0
			187	59	100	14	14	
1	E	11	Total	C	H	N	O	0
			187	59	100	14	14	
1	F	11	Total	C	H	N	O	0
			187	59	100	14	14	

- Molecule 2 is a protein (with D amino acids) called Lipid II.

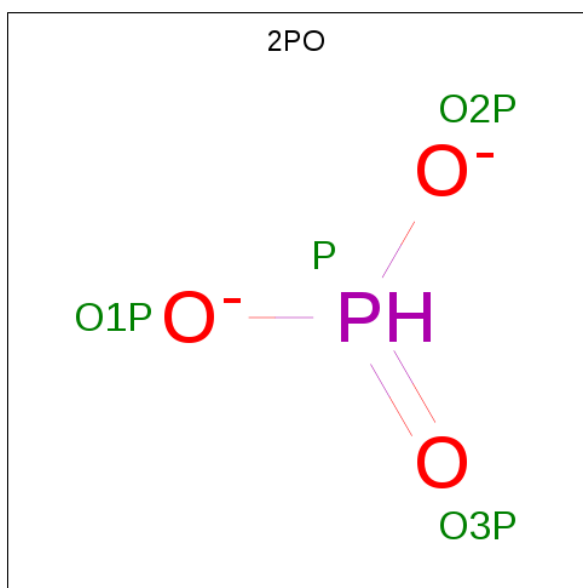
Mol	Chain	Residues	Atoms					Trace
2	C	5	Total	C	H	N	O	0
			67	20	34	6	7	
2	D	5	Total	C	H	N	O	0
			67	20	34	6	7	
2	G	5	Total	C	H	N	O	0
			67	20	34	6	7	
2	H	5	Total	C	H	N	O	0
			67	20	34	6	7	

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid.



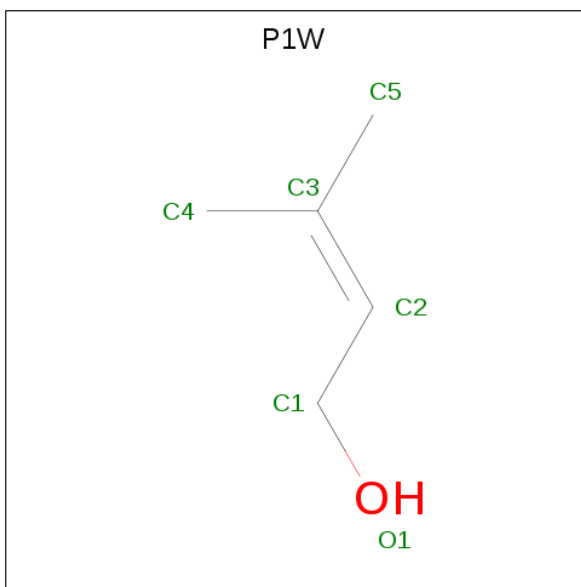
Mol	Chain	Residues	Atoms					Trace
3	I	2	Total	C	H	N	O	0
			63	19	30	2	12	
3	J	2	Total	C	H	N	O	0
			63	19	30	2	12	
3	K	2	Total	C	H	N	O	0
			63	19	30	2	12	
3	L	2	Total	C	H	N	O	0
			63	19	30	2	12	

- Molecule 4 is PHOSPHONATE (three-letter code: 2PO) (formula: HO_3P).



Mol	Chain	Residues	Atoms		
4	I	1	Total	O	P
			4	3	1
4	I	1	Total	O	P
			4	3	1
4	J	1	Total	O	P
			4	3	1
4	J	1	Total	O	P
			4	3	1
4	K	1	Total	O	P
			4	3	1
4	K	1	Total	O	P
			4	3	1
4	L	1	Total	O	P
			4	3	1
4	L	1	Total	O	P
			4	3	1

- Molecule 5 is 3-methylbut-2-en-1-ol (three-letter code: P1W) (formula: $\text{C}_5\text{H}_{10}\text{O}$).



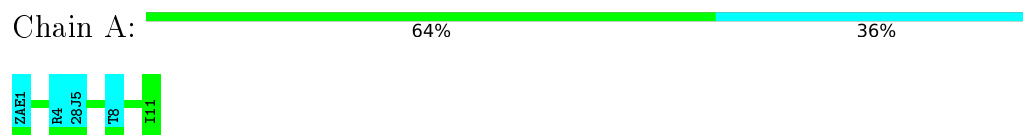
Mol	Chain	Residues	Atoms		
5	I	1	Total	C	H
			13	5	8
5	I	1	Total	C	H
			13	5	8
5	I	1	Total	C	H
			14	5	9
5	J	1	Total	C	H
			13	5	8
5	J	1	Total	C	H
			14	5	9
5	J	1	Total	C	H
			13	5	8
5	K	1	Total	C	H
			13	5	8
5	K	1	Total	C	H
			13	5	8
5	K	1	Total	C	H
			14	5	9
5	L	1	Total	C	H
			13	5	8
5	L	1	Total	C	H
			13	5	8
5	L	1	Total	C	H
			14	5	9

4 Residue-property plots [i](#)

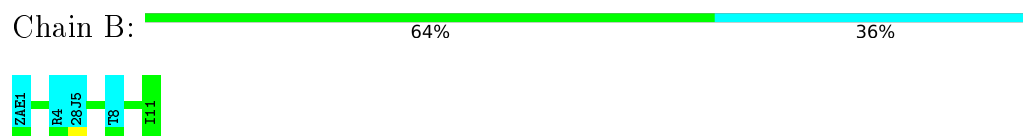
4.1 Average score per residue in the NMR ensemble

These plots are provided for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic is the same as shown in the summary in section 1 of this report. The second graphic shows the sequence where residues are colour-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 outliers are shown as green connectors. Residues which are classified as ill-defined in the NMR ensemble, are shown in cyan with an underline colour-coded according to the previous scheme. Residues which were present in the experimental sample, but not modelled in the final structure are shown in grey.

- Molecule 1: D-Arg4,Leu10-Teixobactin



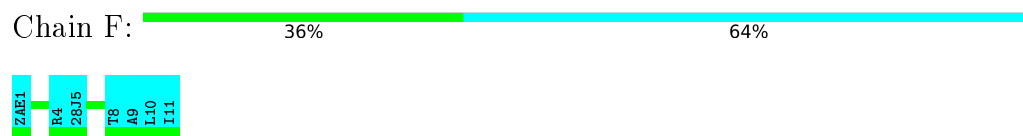
- Molecule 1: D-Arg4,Leu10-Teixobactin



- Molecule 1: D-Arg4,Leu10-Teixobactin



- Molecule 1: D-Arg4,Leu10-Teixobactin



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain J:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain K:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain L:  50% 50%

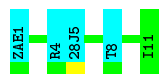


4.2 Residue scores for the representative (medoid) model from the NMR ensemble

The representative model is number 1. Colouring as in section 4.1 above.

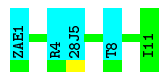
- Molecule 1: D-Arg4,Leu10-Teixobactin

Chain A:  64% 36%



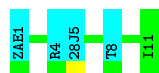
- Molecule 1: D-Arg4,Leu10-Teixobactin

Chain B:  64% 36%



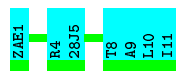
- Molecule 1: D-Arg4,Leu10-Teixobactin

Chain E:  64% 36%



- Molecule 1: D-Arg4,Leu10-Teixobactin

Chain F:  36% 64%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain I:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain J:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain K:  50% 50%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-N-acetyl-alpha-muramic acid

Chain L:  50% 50%



5 Refinement protocol and experimental data overview

The models were refined using the following method: *torsion angle dynamics*.

Of the 26 calculated structures, 26 were deposited, based on the following criterion: *all calculated structures submitted*.

The following table shows the software used for structure solution, optimisation and refinement.

Software name	Classification	Version
CNS	refinement	
HADDOCK	structure calculation	

The following table shows chemical shift validation statistics as aggregates over all chemical shift files. Detailed validation can be found in section 7 of this report.

Chemical shift file(s)	working_cs.cif
Number of chemical shift lists	2
Total number of shifts	70
Number of shifts mapped to atoms	51
Number of unparsed shifts	0
Number of shifts with mapping errors	19
Number of shifts with mapping warnings	0
Assignment completeness (well-defined parts)	12%

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

6 Model quality [i](#)

6.1 Standard geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.2 Too-close contacts [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3 Torsion angles [i](#)

6.3.1 Protein backbone [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.2 Protein sidechains [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.3.3 RNA [i](#)

MolProbity failed to run properly - this section will have to be empty.

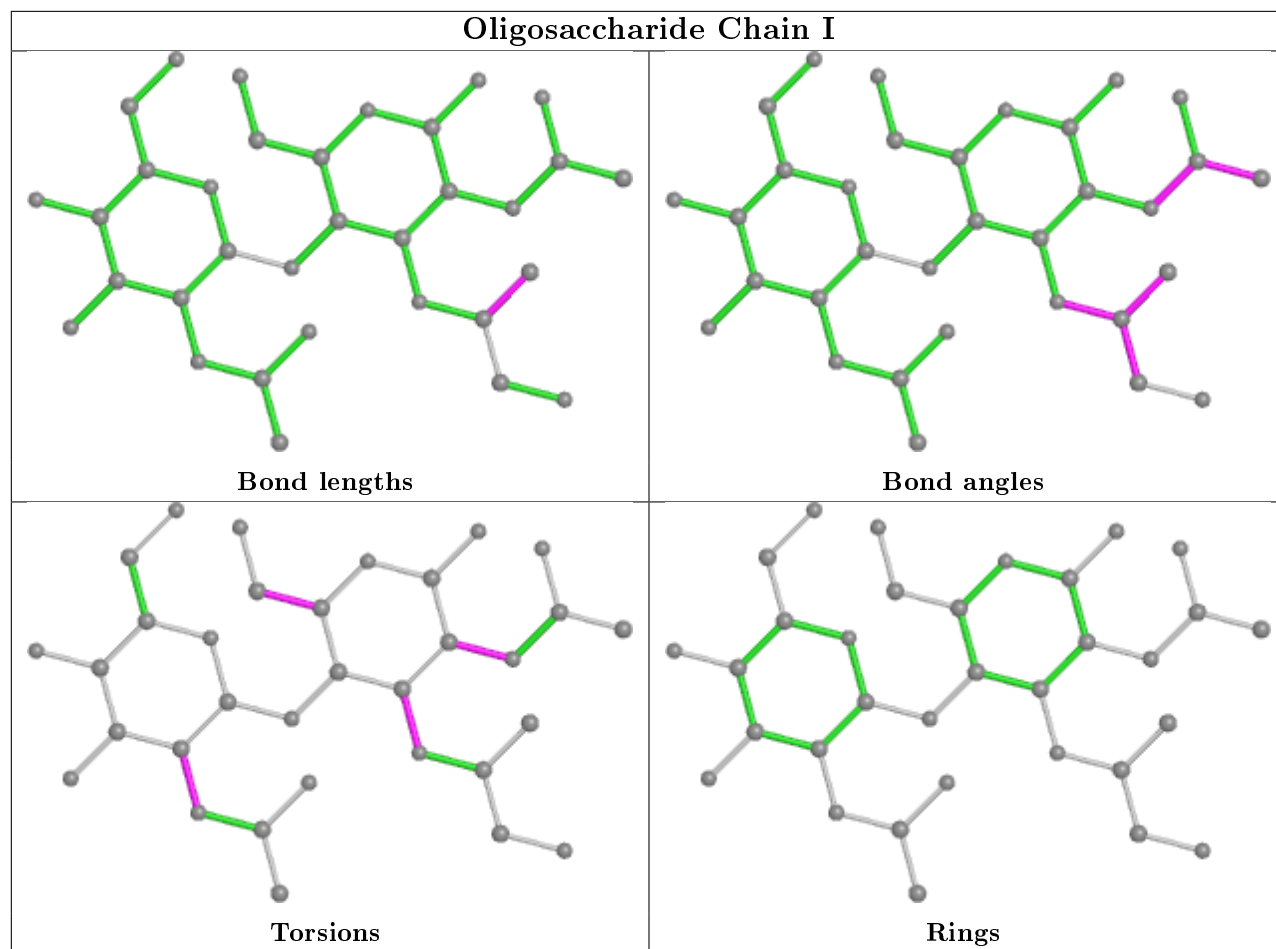
6.4 Non-standard residues in protein, DNA, RNA chains [i](#)

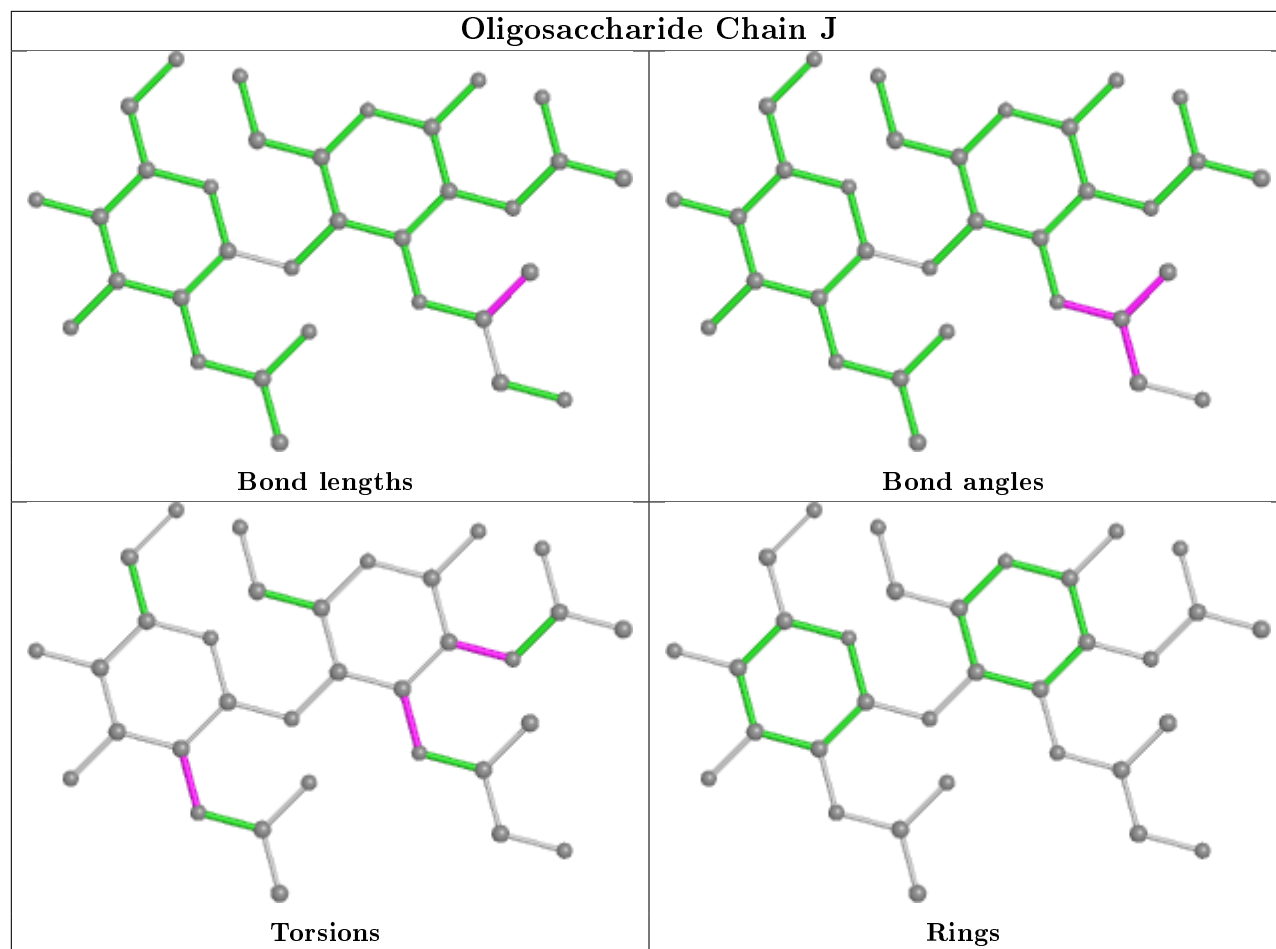
MolProbity failed to run properly - this section will have to be empty.

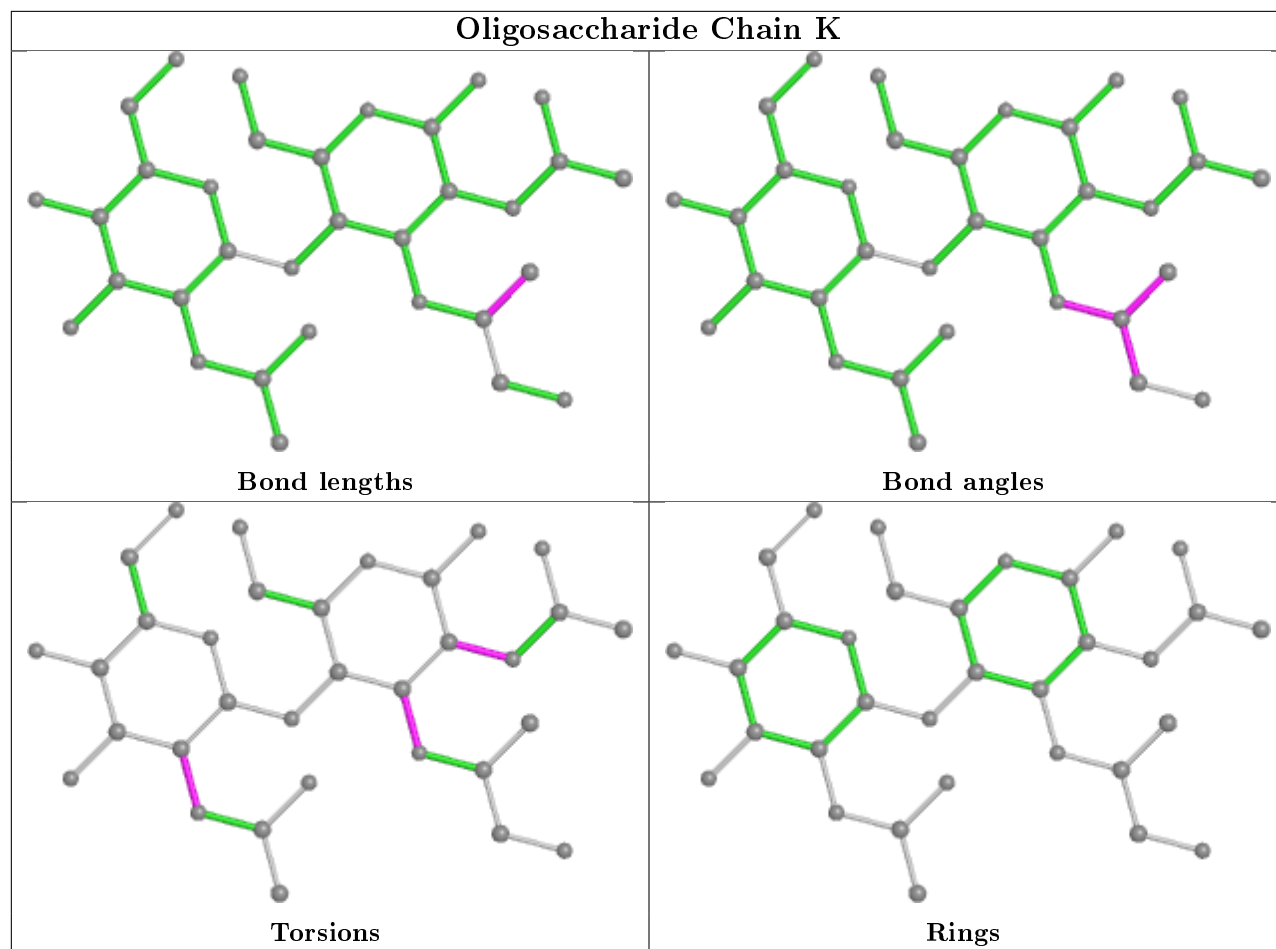
6.5 Carbohydrates [i](#)

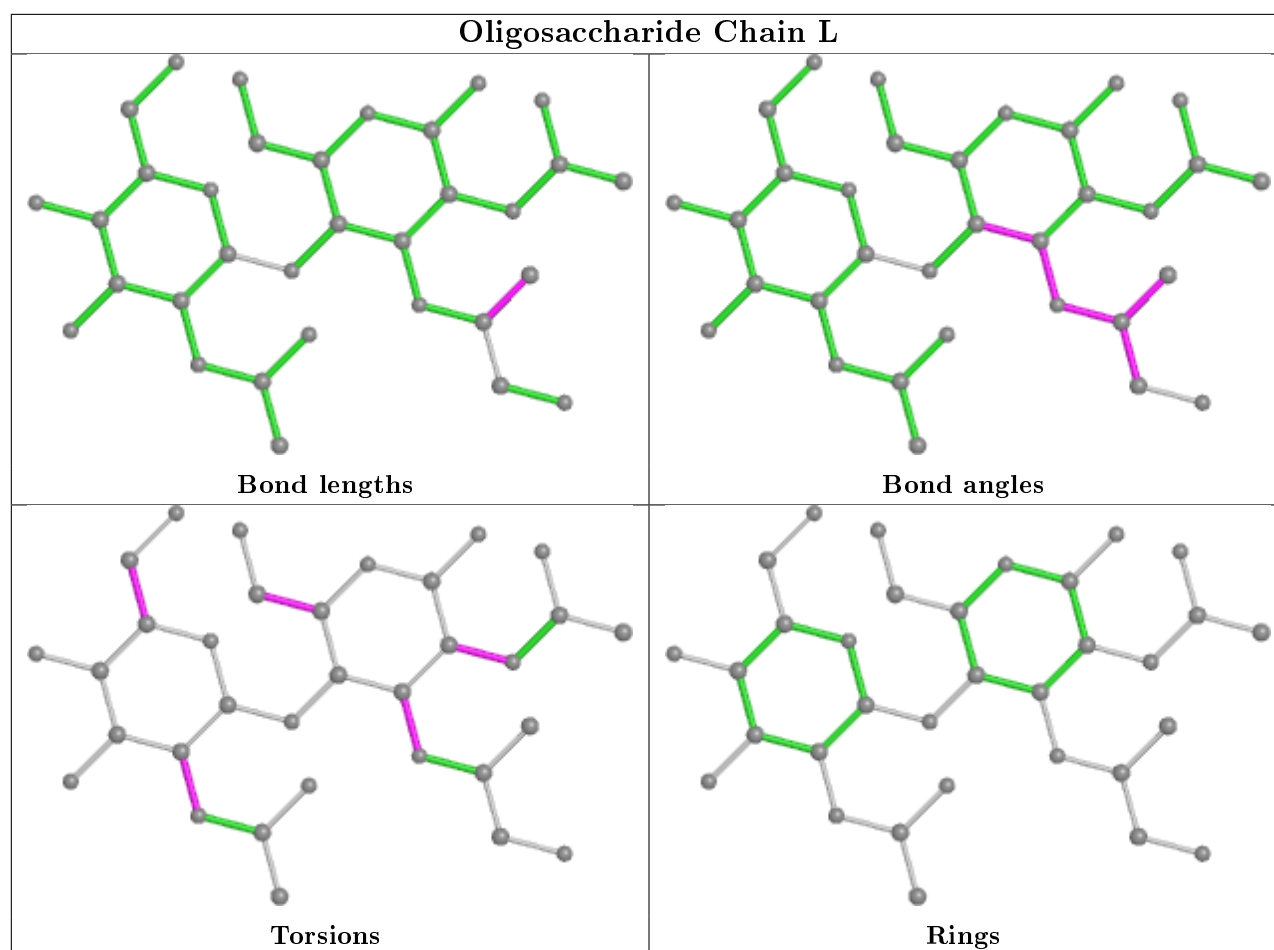
MolProbity failed to run properly - this section will have to be empty.

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









6.6 Ligand geometry [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.7 Other polymers [i](#)

MolProbity failed to run properly - this section will have to be empty.

6.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	3-G	1
2	16-C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
3	G	2:DGL	C	3:LYS	N	2.92
16	C	2:DGL	C	3:LYS	N	2.77

7 Chemical shift validation

The completeness of assignment taking into account all chemical shift lists is 12% for the well-defined parts and 11% for the entire structure.

7.1 Chemical shift list 1

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_1*

7.1.1 Bookkeeping

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	39
Number of shifts mapped to atoms	39
Number of unparsed shifts	0
Number of shifts with mapping errors	0
Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	1

7.1.2 Chemical shift referencing

No chemical shift referencing corrections were calculated (not enough data).

7.1.3 Completeness of resonance assignments

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 10%, i.e. 39 atoms were assigned a chemical shift out of a possible 381. 1 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	24/165 (15%)	6/66 (9%)	12/66 (18%)	6/33 (18%)
Sidechain	15/216 (7%)	0/125 (0%)	15/87 (17%)	0/4 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	39/381 (10%)	6/191 (3%)	27/153 (18%)	6/37 (16%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.1.4 Statistically unusual chemical shifts [i](#)

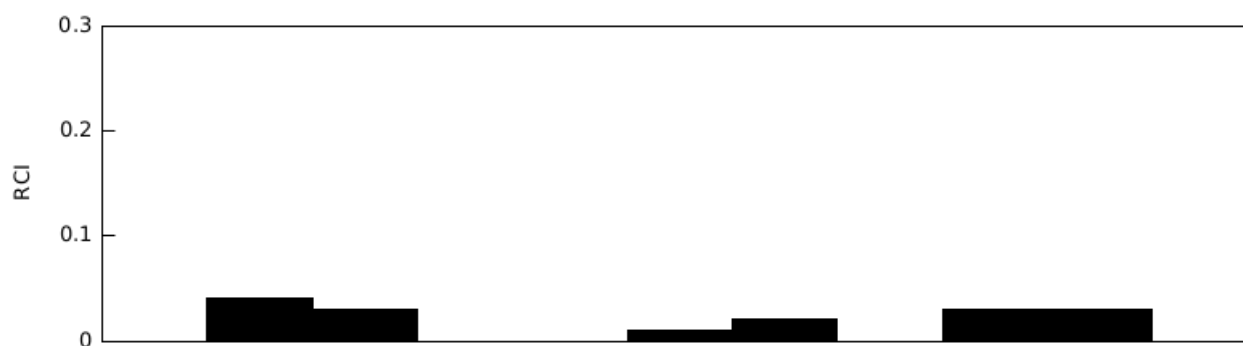
The following table lists the statistically unusual chemical shifts. These are statistical measures, and large deviations from the mean do not necessarily imply incorrect assignments. Molecules containing paramagnetic centres or hemes are expected to give rise to anomalous chemical shifts.

Mol	Chain	Res	Type	Atom	Shift, <i>ppm</i>	Expected range, <i>ppm</i>	Z-score
1	A	7	SER	H	11.57	11.23 – 5.33	5.6

7.1.5 Random Coil Index (RCI) plots [i](#)

The image below reports *random coil index* values for the protein chains in the structure. The height of each bar gives a probability of a given residue to be disordered, as predicted from the available chemical shifts and the amino acid sequence. A value above 0.2 is an indication of significant predicted disorder. The colour of the bar shows whether the residue is in the well-defined core (black) or in the ill-defined residue ranges (cyan), as described in section 2 on ensemble composition.

Random coil index (RCI) for chain A:



7.2 Chemical shift list 2

File name: working_cs.cif

Chemical shift list name: *assigned_chemical_shifts_2*

7.2.1 Bookkeeping [i](#)

The following table shows the results of parsing the chemical shift list and reports the number of nuclei with statistically unusual chemical shifts.

Total number of shifts	31
Number of shifts mapped to atoms	12
Number of unparsed shifts	0
Number of shifts with mapping errors	19

Number of shifts with mapping warnings	0
Number of shift outliers (ShiftChecker)	0

The following assigned chemical shifts were not mapped to the molecules present in the coordinate file.

- Residue not found in structure. First 5 (of 19) occurrences are reported below.

Chain	Res	Type	Atom	Shift Data		
				Value	Uncertainty	Ambiguity
C	11	MUB	C1	97.91	0.3	1
C	11	MUB	C2	56.52	0.3	1
C	11	MUB	C3	81.47	0.3	1
C	11	MUB	C4	73.24	0.3	1
C	11	MUB	C5	76.11	0.3	1

7.2.2 Chemical shift referencing [i](#)

No chemical shift referencing corrections were calculated (not enough data).

7.2.3 Completeness of resonance assignments [i](#)

The following table shows the completeness of the chemical shift assignments for the well-defined regions of the structure. The overall completeness is 2%, i.e. 8 atoms were assigned a chemical shift out of a possible 381. 0 out of 3 assigned methyl groups (LEU and VAL) were assigned stereospecifically.

	Total	¹ H	¹³ C	¹⁵ N
Backbone	3/165 (2%)	0/66 (0%)	3/66 (5%)	0/33 (0%)
Sidechain	5/216 (2%)	0/125 (0%)	5/87 (6%)	0/4 (0%)
Aromatic	0/0 (—%)	0/0 (—%)	0/0 (—%)	0/0 (—%)
Overall	8/381 (2%)	0/191 (0%)	8/153 (5%)	0/37 (0%)

Note: This is a solid-state NMR structure, where hydrogen atoms are typically not assigned a chemical shift value, which may lead to lower completeness of assignment measure.

7.2.4 Statistically unusual chemical shifts [i](#)

There are no statistically unusual chemical shifts.

7.2.5 Random Coil Index (RCI) plots

No *random coil index* (RCI) plot could be generated from the current chemical shift list (assigned_chemical_shifts_2). RCI is only applicable to proteins.