SUPPORTING INFORMATION

Induction of Rare Conformation of Oligosaccharide by Binding to Calcium-dependent Bacterial Lectin: X-ray Crystallography and Modelling Study

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Table S1. X-ray data collection and processing of LecB structures

Data set	**$LecB_{PAO1}$- Le^x**	**$LecB_{PA14}$- Le^x**
PDB code	6R35	5A70
Data Collection		
Beamline	PROXIMA1 (SOLEIL)	BM30A (ESRF)
Wavelength (Å)	0.9792	0.9802
Detector	Pilatus 6M	ADSC Q315 CCD
Resolution (Å)[a]	47.82-1.84 (1.80-1.80)	44.94-1.60 (1.63-1.60)
Space Group	$P2_1$	$P2_1$
a, b, c (Å)	52.60, 72.48, 62.06	53.0, 63.3, 63.9
α, β, γ (°)	90.0,114.6 ,90.0	90.0, 91.2, 90.0
Total observations	203335	161897
Unique reflections	39320	53856
Multiplicity[a]	5.2 (5.0)	3.0 (2.3)
Mean $I/\sigma(I)$[a]	13.7 (3.1)	17.5 (2.5)
Completeness (%)[a]	99.9 (99.6)	96.8 (74.7)
R_{merge}[a,b]	0.076 (0.533)	0.041 (0.330)
$CC_{½}$[a,c]	1.0 (0.9)	1.0 (0.8)
Refinement		
Reflections: working/free[d]	39301/2004	50981/2857
R_{work}/ R_{free}[e]	0.132/0.176	0.136/0.171
Ramachandran plot: allowed/favoured/outliers (%)[f]	100/97.8/0	100/97.5/0
R.m.s. bond deviations (Å)	0.0172	0.0170
R.m.s. angle deviations (°)	1.869	1.700
Mean *B*-factors: protein/ligand[f]**/ /water (Å²)**	19/36/31	13/20/27

[a] Values for the outer resolution shell are given in parentheses.
[b] $R_{merge} = \sum_{hkl} \sum_i |I_i(hkl) - \langle I(hkl)\rangle| / \sum_{hkl} \sum_i I_i(hkl)$.
[c] $CC_{½}$ is the correlation coefficient between symmetry-related intensities taken from random halves of the dataset.
[d] The data set was split into "working" and "free" sets consisting of 95 and 5% of the data, respectively. The free set was not used for refinement.
[e] The R-factors R_{work} and R_{free} are calculated as follows: $R = \sum(|F_{obs} - F_{calc}|)/\sum|F_{obs}|$, where F_{obs} and F_{calc} are the observed and calculated structure factor amplitudes, respectively
[f] refers to ligands bound in the active site and potential surface binding sites

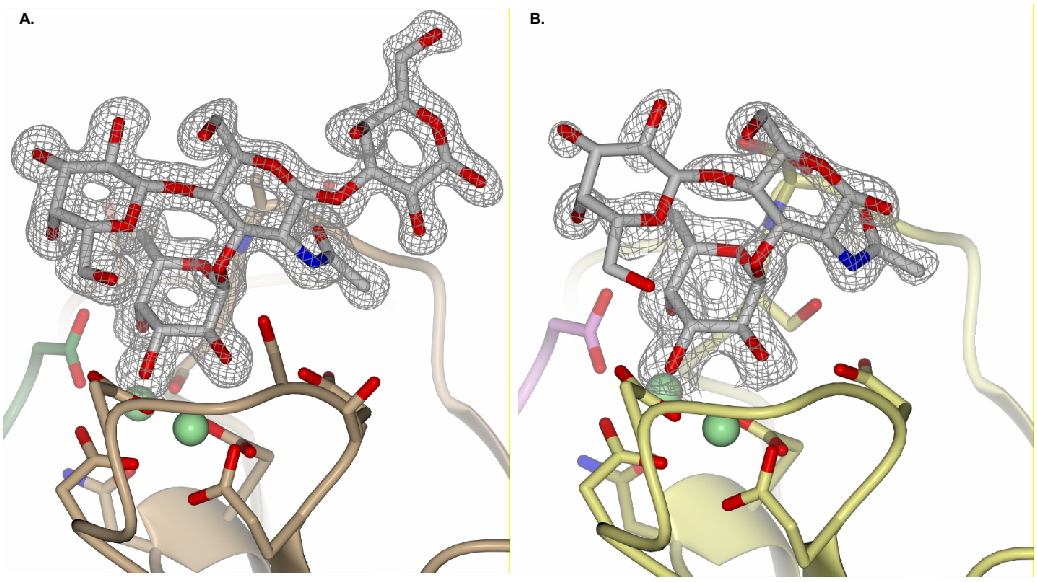

Figure S1. Electron density map for Le^x in complex with two LecB variants, **A.** $LecB_{PA14}$ and **B.** $LecB_{PAO1}$. The electron density is displayed at 1σ. Figure was prepared with CCP4MG.

Table S2. Φ, Ψ torsion angles (°) for the two glycosidic linkages of Le^x trisaccharide core in the crystal structures of $LecB_{PA14}/Le^x$ and $LecB_{PAO1}/Le^x$ complexes.

	$LecB_{PA14}/Le^x$				$LecB_{PAO1}/Le^x$			
	*α*Fuc1-3GlcNAc		*β*Gal1-4GlcNAc		*α*Fuc1-3GlcNAc		*β*Gal1-4GlcNAc	
Chain	Φ O5-C1-O1-C3	Ψ C1-O1-C3-C4	Φ O5-C1-O1-C4	Ψ C1-O1-C4-C5	Φ O5-C1-O1-C3	Ψ C1-O1-C3-C4	Φ O5-C1-O1-C4	Ψ C1-O1-C4-C5
A	-69.6	136.9	-72.6	-103.8	-86.1	146.6	-67.6	-107.8
B	-76.8	140.7	-68.1	-108.7	-87.4	148.1	-58.4	-110.9
C	-70.9	139.2	-72.2	-107.4	-83.8	150.7	-63.0	-104.3
D	-71.4	138.4	-68.3	-107.7	-70.5	138.9	-73.3	-107.8

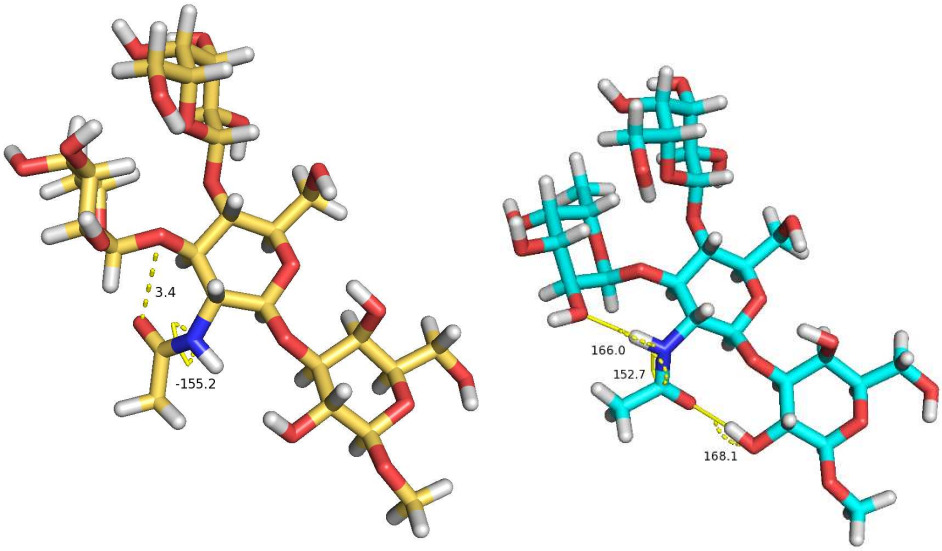

Figure S2. Optimised structures of Le^x from rotational profile at QM/COSMO level. **A.** Barrier at -96°, **B.** Barrier at 96°. Colour coding: red – oxygen, blue – nitrogen, white hydrogen, yellow/cyan – carbon. Distances are in Å, dihedral angles in degrees. Figure prepared with PyMol, version 1.8.

Table S3. Nonbonded parameters for Ca^{2+}, K^+, Cl^- ions in different MD setups

	1	2	3	4
Setup	12-6 IOD	12-6-4	ECCR	ECCR2
Ca^{2+}				
charge (e)	2.0	2.0	1.5	1.5
σ (GROMACS, Å)			2.5376	2.6656
$R_{min}/2$ (AMBER, Å)	1.6080	1.6420	1.4236	1.4954
ε (GROMACS, kJ/mol)			0.5072	0.5072
ε (AMBER, kcal/mol)	0.0830	0.1019	0.1212	0.1212
Cl^-				
charge (e)	-1.00	-1.00	-0.75	-0.75
σ (GROMACS, Å)			3.7824	4.1000
$R_{min}/2$ (AMBER, Å)	2.1620	2.1500	2.1219	2.3001
ε (GROMACS, kJ/mol)			0.4184	0.4928
ε (AMBER, kcal/mol)	0.5315	0.5215	0.1000	0.1178
K^+				
charge (e)	1.00	1.00	0.75	n.d
σ (GROMACS, Å)			3.154	n.d
$R_{min}/2$ (AMBER, Å)	1.7450	1.7580	1.7694	n.d
ε (GROMACS, kJ/mol)			0.4187	n.d
ε (AMBER, kcal/mol)	0.1702	0.1800	0.1001	n.d

Table S4. Partial charges on the Ca^{2+}-coordinating carboxylates in different MD setups

		Setups 1-3	Setup 4
ASP	OD1	-0.8014	-0.6011
	CG	0.7994	0.5996
GLU	OE1	-0.8188	-0.6141
	CD	0.8054	0.6041
G114*	O	-0.7855	-0.5891
	C	0.7231	0.5423

* C-term of B-chain residue

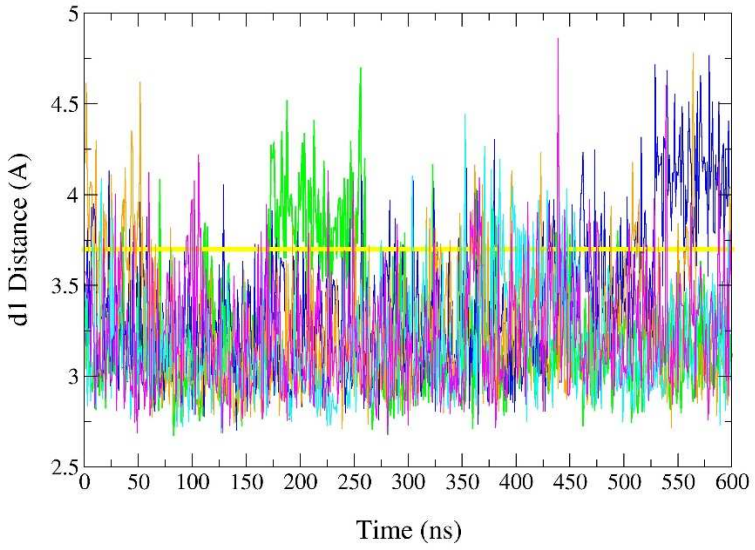

Figure S3. Evolution of the **d1** distance in the tested MD protocols and comparison with the $LecB_{PA14}/Le^x$ crystal structure (chain A) determined here - yellow, MD colour coding: black – Setup 1; red – Setup 2; green – Setup 3; blue – Setup 4, orange – Setup 5, cyan – Setup 6, magenta – Setup 7.