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Supplemental Information

Structure and Ligand-Binding Properties of the O Antigen ABC Transporter Carbohydrate-Binding Domain

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Figure S1, related to Figures 1 and 2

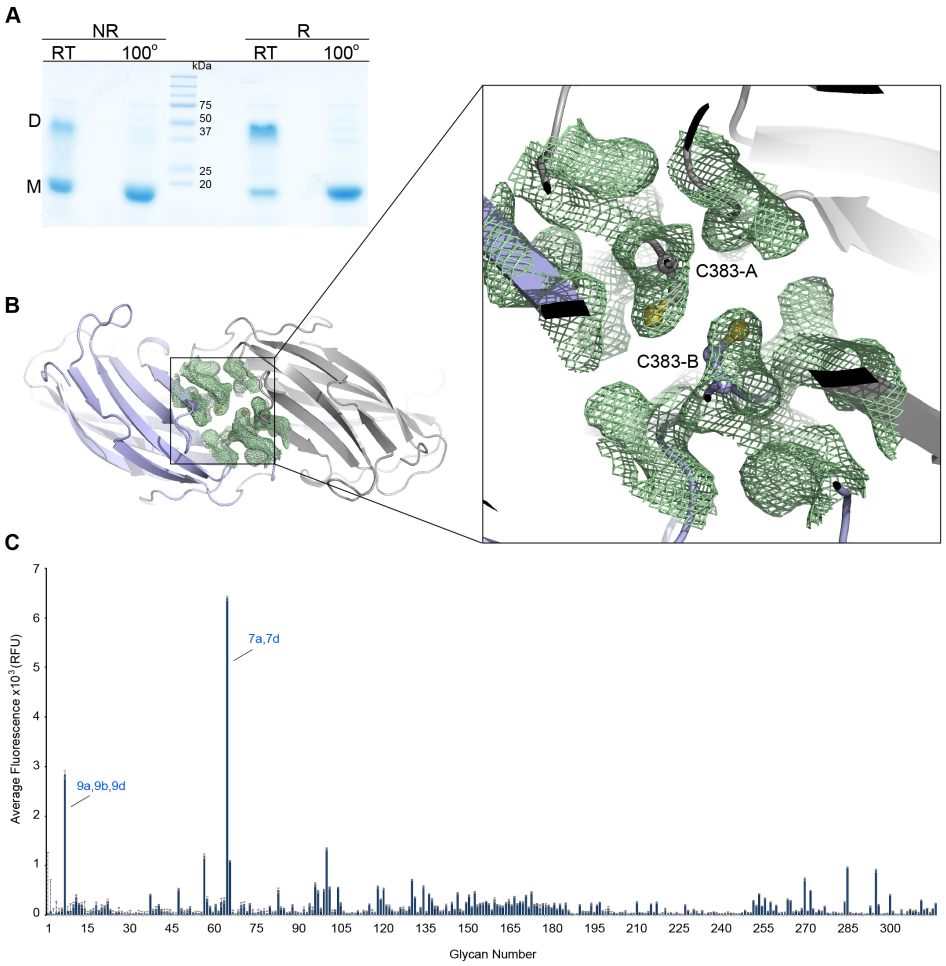

Figure S1: The *Aquifex aeolicus* Wzt carbohydrate-binding domain forms a stable dimer.
(A) SDS-PAGE analysis of purified AaCBD. The protein was analyzed under non-reducing (NR) and reducing (R) conditions. Prior to electrophoresis, the sample was incubated either at room temperature or 100°C for 10 min. CBD monomers (M) and dimers (D) are indicated.
(B) Cysteine 383 at the CBD dimer interface is not oxidized. Shown is the SigmaA-weighted 2FoFc electron density contoured at 1.2σ for residues at the dimer interface. The density does not suggest disulfide bond formation between Cys383 in chains A and B. We cannot exclude that an existing disulfide bond was reduced during data collection.
(C) Microbial Glycan Array binding assay. The data shown were obtained under identical conditions to those presented in Figure 2 but at a lower AaCBD concentration of 5µg/mL.

Table S1, related to STAR Methods

	Wzt-CBD long (235-395)	**Wzt-CBD short (245-395)**
Data collection		
Space group	$P4_12_12$	$P6_3$
Cell dimensions		
a, *b*, *c* (Å)	107.50, 107.50, 327.33	128.35, 128.35, 45.16
α, β, γ (°)	90, 90, 90	90, 90, 120
Resolution (Å)	24.86-3.55 (3.80-3.55)*	28.64-2.65 (2.78-2.65)*
R_{merge} R_{pim} $CC_{1/2}$^	0.43(2.27) 0.12(0.72) 0.989(0.632)	0.20(1.14) 0.06(0.36) 0.988(0.731)
Mean *I* / s*I*	7.3(1.5)	6.9(1.5)
Completeness (%)	99.7(100.0)	99.8 (100.0)
Redundancy	14.5(10.3)	9.2 (9.5)
Refinement		
Resolution (Å)		28.64-2.65
No. reflections		
Total		12535
R_{free}		614
R_{work} / R_{free} (%)		18.0/23.9
No. atoms		
Chain A Chain B Glycerol		1202 1170 28
B-factors (Å^2)		
Chain A Chain B Glycerol		67.6 77.1 89
R.m.s deviations		
Bond lengths (Å)		0.009
Bond angles (°)		1.07

* Values in parentheses refer to the highest-resolution shell.

^ Correlation between intensities from random half-data sets (Karplus and Diederichs, 2012).