STRUCTURAL BIOLOGY COMMUNICATIONS

Volume 71 (2015)

Supporting information for article:

Structures of exoglucanase from Clostridium cellulovorans: cellotetraose binding and cleavage

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Table S1 The distances between calcium ion and coordination residues in ExgS and CelF enzyme.

ExgS (4xwm)			CelF (4jjj)		
Residue	atom	Distance (Å)	Residue	atom	Distance (Å)
Q178	C=O	2.4	R180	C=O	2.4
	Oe1	2.6	W1	O	2.5
E183	Oe1	3.0	E185	Oe1	2.4
	Oe2	2.5		Oe2	2.6
D397	Od2	2.4	D408	Od2	2.3
W1	O	2.6	E560	Oe1	2.4
W2	O	2.5	W2	O	2.3

Table S2 The interaction residues found in ExgS-dockerin and ExgS-cohesin complex model.

ExgS		dockerin	
residue	atom	atom	residue
K239	nz	c=o	N40
K239	nz	c=o	L41
S325	c=o	nz	K55
A338	c=o	nz	K55
K346	n	c=o	Y59
Y418	oh	c=o	G12
S420	c=o	n	Y5
K422	nz	od2	D7
K422	c=o	n	V14
D423	od2	c=o	M60
S505	og	c=o	D10
S505	og	n	G12
ExgS		Cohesin	
N343	c=o	nd2	N81
K346	nz	og	S85
E350	oe2	og1	T83
E350	oe2	nz	K125
A425	c=o	od2	D126
K427	n	od2	D126
S428	n	od2	D126
T466	c=o	n	Y52
S468	og	og1	T123

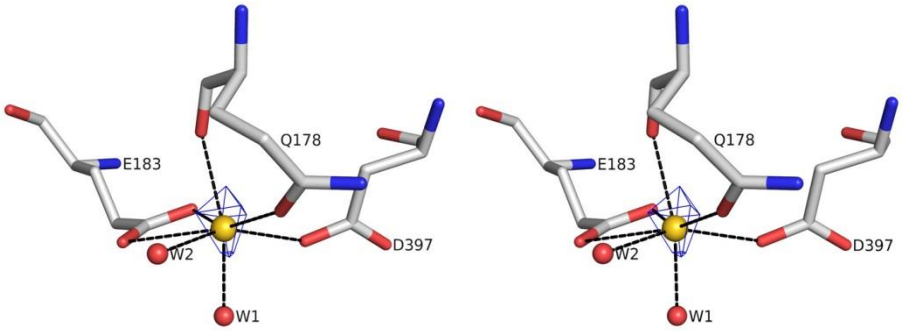

Figure S1 Electron density map contoured at 4 σ around the Ca^{2+} binding site. The calcium ion is coordinated with seven ligands: the backbone carbonyl oxygen atom of Gln178, the side chain oxygen of Glu183 and Asp397, and two water molecules.

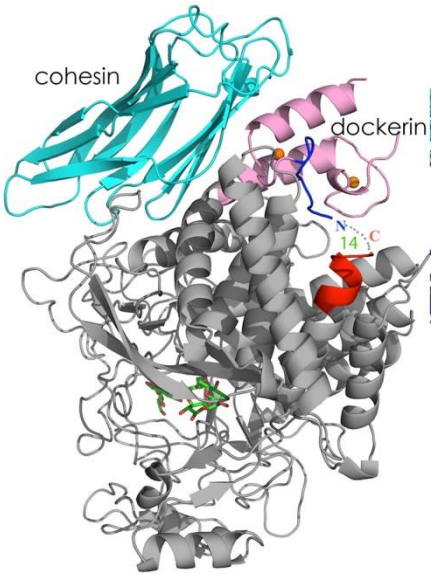

Figure S2 The dockerin-cohesin model structure docked with the ExgS is shown in the Cα ribbon drawing. The ExgS is indicated in grey with a red C-terminus tail, the dockerin is in pink with blue N-terminus, and the cohesin is shown in cyan. The distance between the C-terminus of ExgS and the N-terminus of dockerin is 14 Å. The protein-protein interactions between ExgS and dockerin-cohesin (2vn5.pdb) are listed in Table 2. The substrate oligosaccharide is shown in sticks in green and red. The two orange balls are calcium ions in the dockerin structure.