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Supporting information for article:

Crystal structures of the GH6 *Orpinomyces* sp. Y102 CelC7 enzyme with exo and endo activity and its complex with cellobiose

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Table S1. The validation data of cellobiose structures.

Name	Chain	Q*[1]	Phi	Theta	Anomer	D/L*[2]	Conformation	RSCC	<Bfactor>	Diagnostic
CBI	A	0.569	358.974	7.2438	beta	D	$^4C_1$	0.80	30.0052	Ok
CBI	B	0.569	1.84473	7.2986	beta	D	$^4C_1$	0.83	29.1552	Ok
CBI	C	0.568	0.103757	7.26776	beta	D	$^4C_1$	0.73	31.4704	Ok
CBI	D	0.569	359.022	7.06488	beta	D	$^4C_1$	0.71	45.1161	Ok

We have validated the cellobiose structures with Privateer.

[*1]Q is the total puckering amplitude, measured in Angstroms.

[*2]Whenever N is displayed in the D/L column, it means that Privateer has been unable to determine the handedness based solely on the structure.

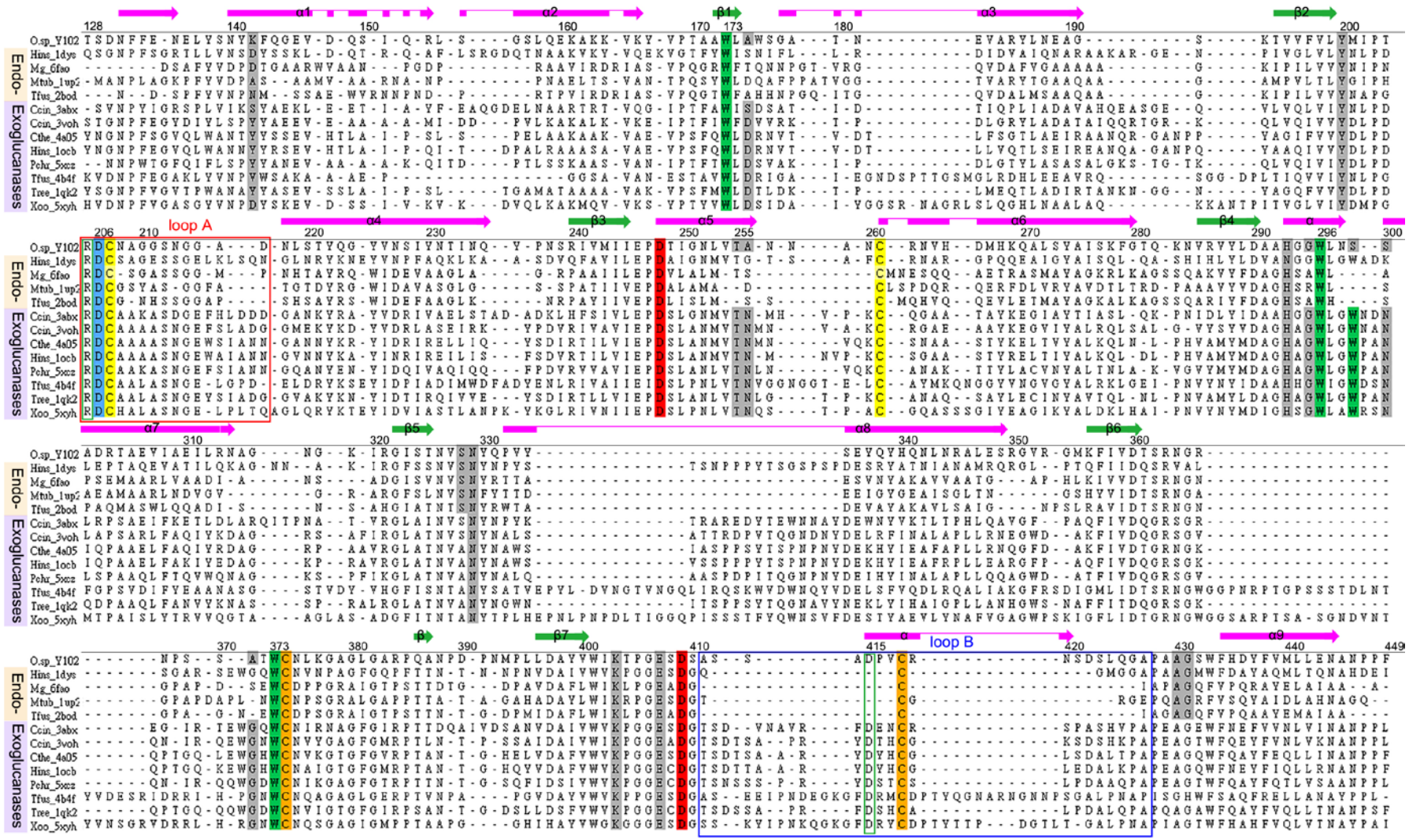

Figure S1. Amino acid structure-sequence alignment analysis for the catalytic domain of *Orp* CelC7 with the determined structures of GH6 endo- and exo-enzymes from *Cthe*, *Ccin*, *Tree*, *Hins*, *Mtub*, *Tfus*, *Pchr*, Mg and O.sp_Y102 (*Orp* CelC7), the pdb code is presented. There are nine alpha helixes and seven beta strands. The disulfide bond forming cysteine residues are marked in yellow and orange, respectively. The proposed key residues, D248 and D409 are marked in red. The amino acids involved in substrate binding either in endo- or exo-enzymes are colored grey. The tryptophan in green is stacked with substrate, while residue D206 in blue is conserved in all enzymes. Loop A and loop B are in red and blue boxes, respectively.