Structures of active-site mutant of plant 1,3-β-glucanase in complex with oligosaccharide products of hydrolysis

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Supplementary Material

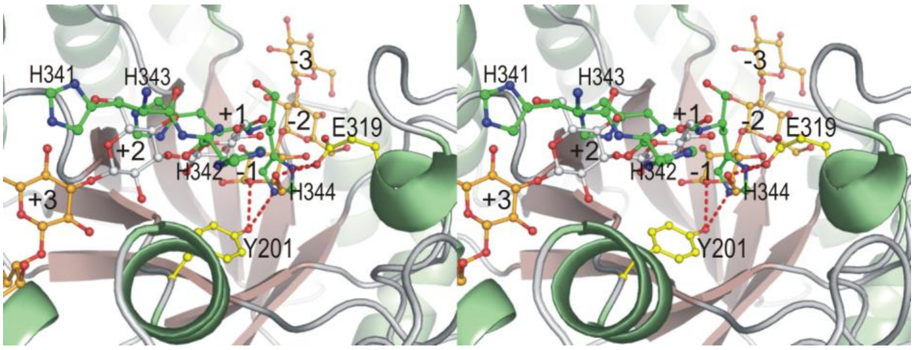

Figure S1 Superposition of the binding sites of native GLUB20-2 (PDB code 3ur8) and of the present E259A mutant structure 7G, shown in stereo. The space occupied in the mutant structure by the trisaccharide and tetrasaccharide products (orange, included in the atomic coordinate set; gray, omitted from the coordinate set because of disorder, and only tentatively placed in this figure) is taken in the native structure by a fragment of the His-tag (green) from an adjacent protein molecule. Hydrogen bonds with the strictly conserved residues (Tyr201, Glu319) formed by His344 (native structure) and by the glucose unit −1 (E259A mutant) are marked by dashed lines.

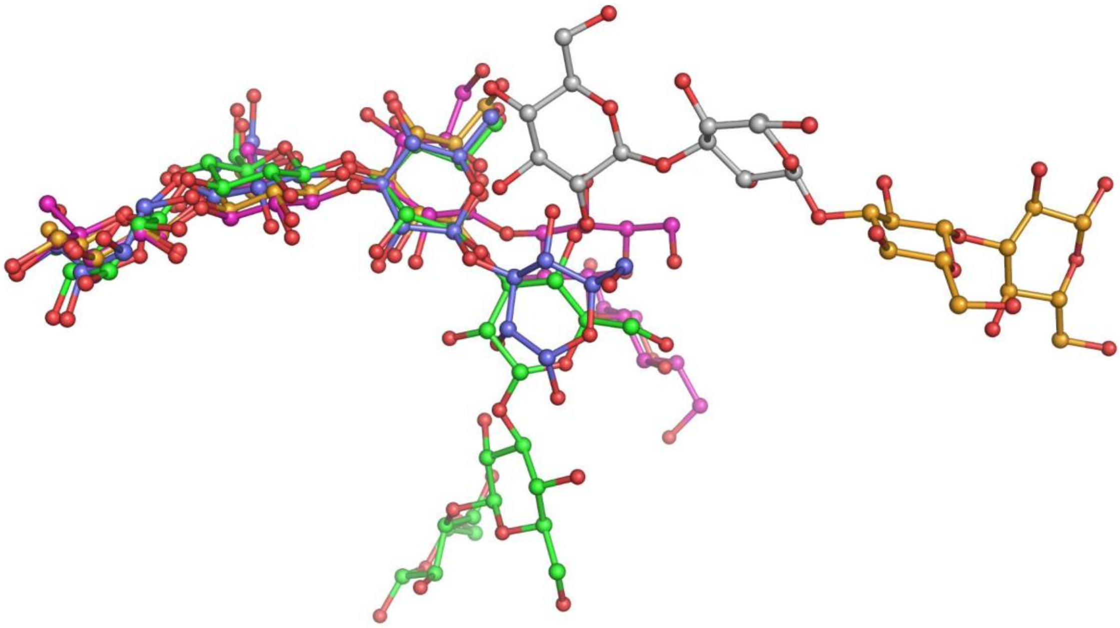

Figure S2 Atomic models of (1→3)-β-glucans superposed on the trisaccharide present in the 7G complex. Color code for the 7G complex: orange - the glucose units included in the coordinate set; gray - two modeled glucose units absent in the coordinate set due to disorder. Color code for the superposed oligosaccharides: green - hexasaccharide observed in family 6 Carbohydrate Binding Modules (PDB code 1gui), magenta - pentasaccharide observed in transglycosylase Gas2p (2w62), blue - tetrasaccharide observed in laminaripentaose-producing β-1,3-glucanase (3gd9).