Supplementary data

Figure 1. Structural alignment of LytC modules

(*a*) Structural alignment of Cellosyl (1jfxa) and the CM of LytC (lytc0). (*b*) Structural alignment of the CBM of LytC (1lcxa and 2lcxa) with the two fragments of the CBM of Cpl-1 (1cpxa and 2cpxa) used as templates. JOY does not recognize the strands forming the β-hairpin of *p1* (Ala^{35}-His^{37} and Gly^{40}-Tyr^{42}). Blue, β-strand; red, α-helix; brown, 3_{10} helix; upper case, solvent inaccessible; lower case, solvent accessible; bold, hydrogen bond to main chain amide; underlined, hydrogen bond to main chain carboxyl; tilde, hydrogen bond to other side chain; italic, positive ϕ. Numbers correspond to residue numbers including the signal peptide. In contrast with Figure 1, which displays sequence alignments, the JOY output shows the structural superposition of the template and the final model generated with COMPARER.

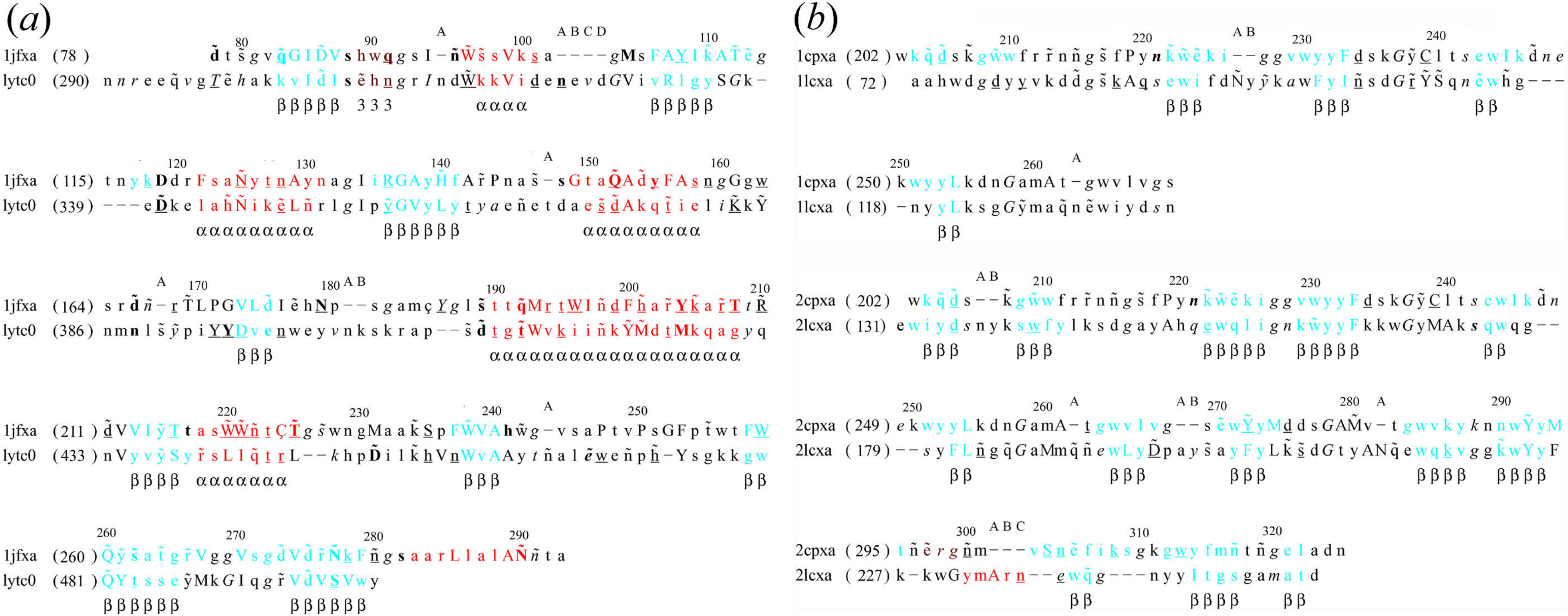

Figure 1 Supplementary data