



**S6 Fig. Average mass-weighted fluctuations of C $\alpha$  atoms.** B-factors were calculated as function of enzyme amino acid residues along 100ns MD simulation of  $\Delta N_{123}$ -GBD-CD2 in complex with sucrose (yellow line) or the free-ligand MD simulation (black line). The bottom strip represents the secondary structures of X-ray  $\Delta N_{123}$ -GBD-CD2 for reference: helix (blue), sheet (orange) and coil (grey). The strips in the background of the B-factors lines highlight structural motifs surrounding the active site, represented using the same color code as Fig 3B in the main text. The highlighted regions are loop 2127-2138, helix-loop-helix motif corresponding to region 2324-2368 and its adjacent loop 2592-2605, then the 2290-2300 and 2757-2780  $\beta$ -hairpin motifs in green, light blue, red, magenta and forest green, respectively.