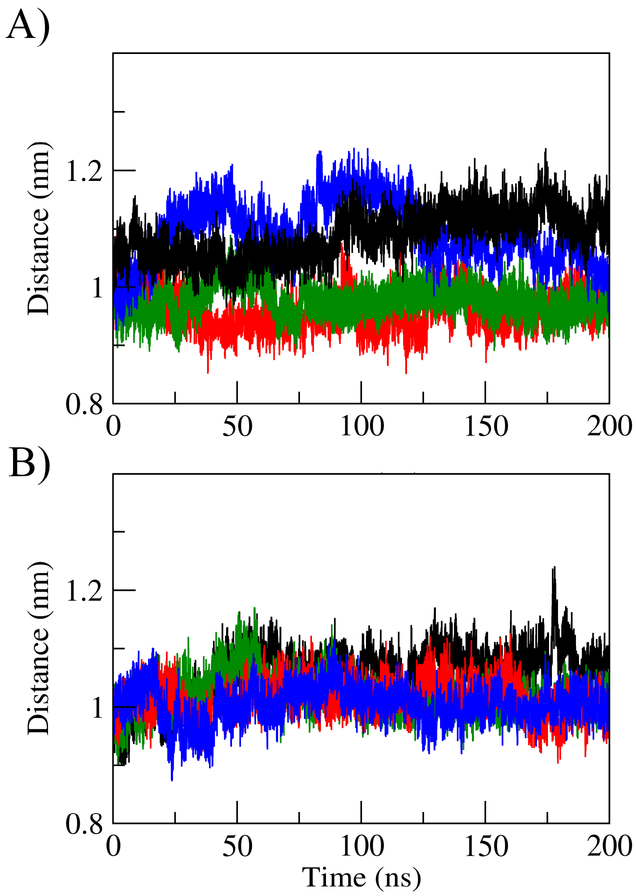

Fig. S7. Structural 'oscillation' observed for (A) chain A, and (B) chain B of Fel d 1 in four different simulations. The distance between each original chain in the native Fel d 1 (half chains of the crystallographic protein) is shown. The oscillation may indicate an opening-closing behavior. (calcium-free system in black, calcium-bound system in red, minimally glycosylated system in blue, fully glycosylated system in green; distances measured for the centers of mass in each structure).