



FIG. 3: Puckering free energy landscape (already corrected with the results from the umbrella sampling phase) of  $\beta$ -D-Glc using the standard 45a4 parameter set. Upper panel: the  $(\theta, \phi)$  plane is shown, with isolines drawn every 10 kJ/mol starting from the absolute minimum. Lower panel: projection of the free energy profile onto the  $\phi = 0$  plane. Darker colors correspond to lower energies.