Relaxed Energy Contour Plot for Man(β1-2)Man(βOMe)
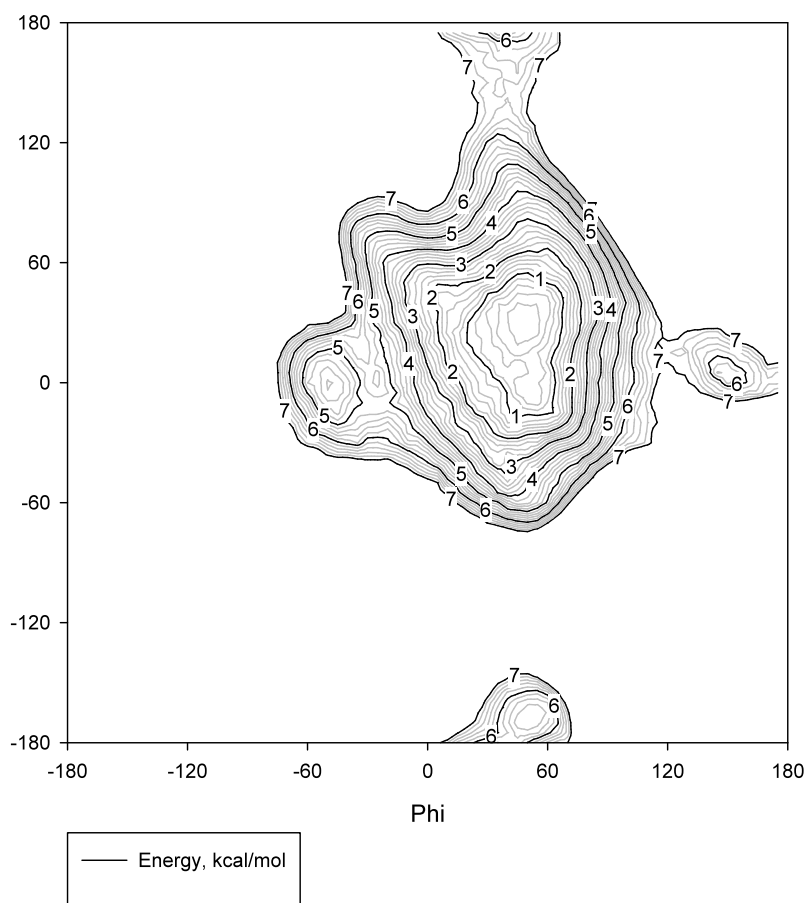

FIGURE S2. Relaxed potential energy contour plot for the Man(β1-2)Man(βOMe) disaccharide. Energy contours are labeled every 1 kcal/mol up to 7 kcal/mol above the global minimum of ~ 50°, 30°. The plot was generated by restraining the dihedral angles to within ±0.5° with a large force constant, then carrying out 30 ps of molecular dynamics at 300 K with the GLYCAM06g force field to relax the rest of the molecule; this was repeated after incrementing the ϕ and ψ dihedral angles in 5° steps. The resulting data were smoothed and plotted with SigmaPlot 11.0 for Windows.