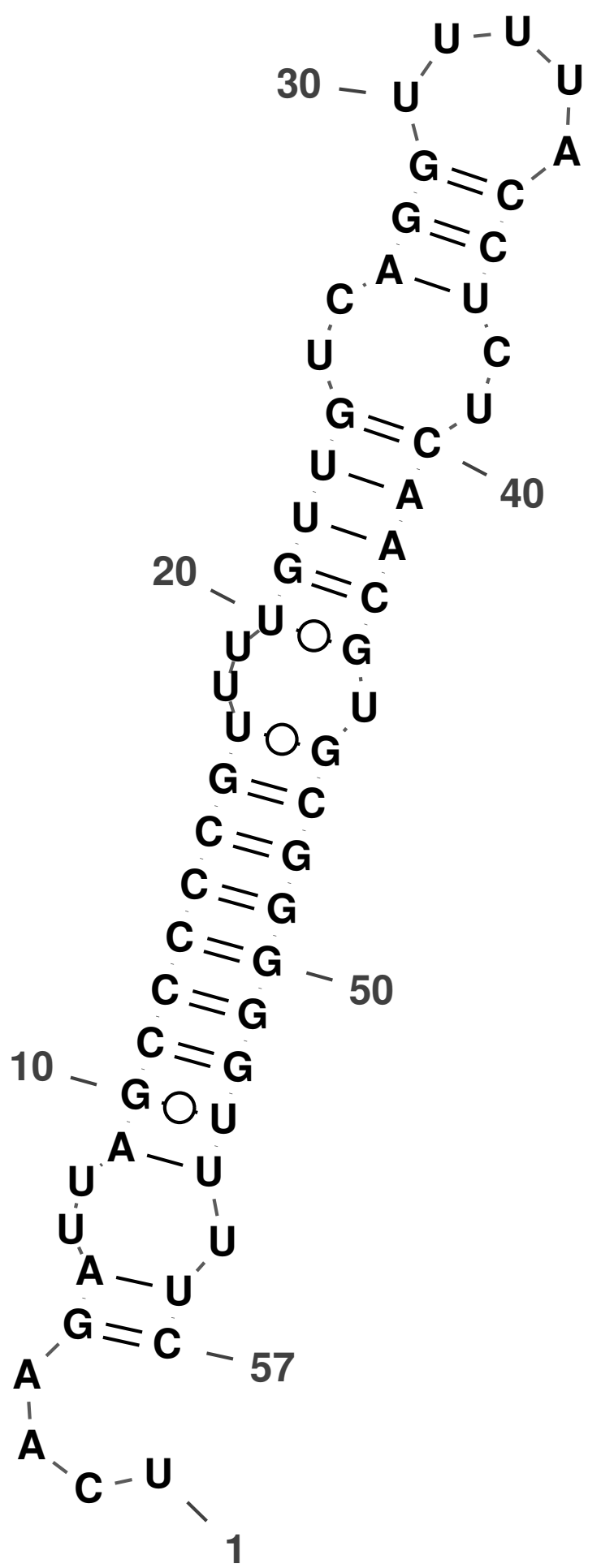

tially -25.60] 791 (E=-25.60 kcal/m