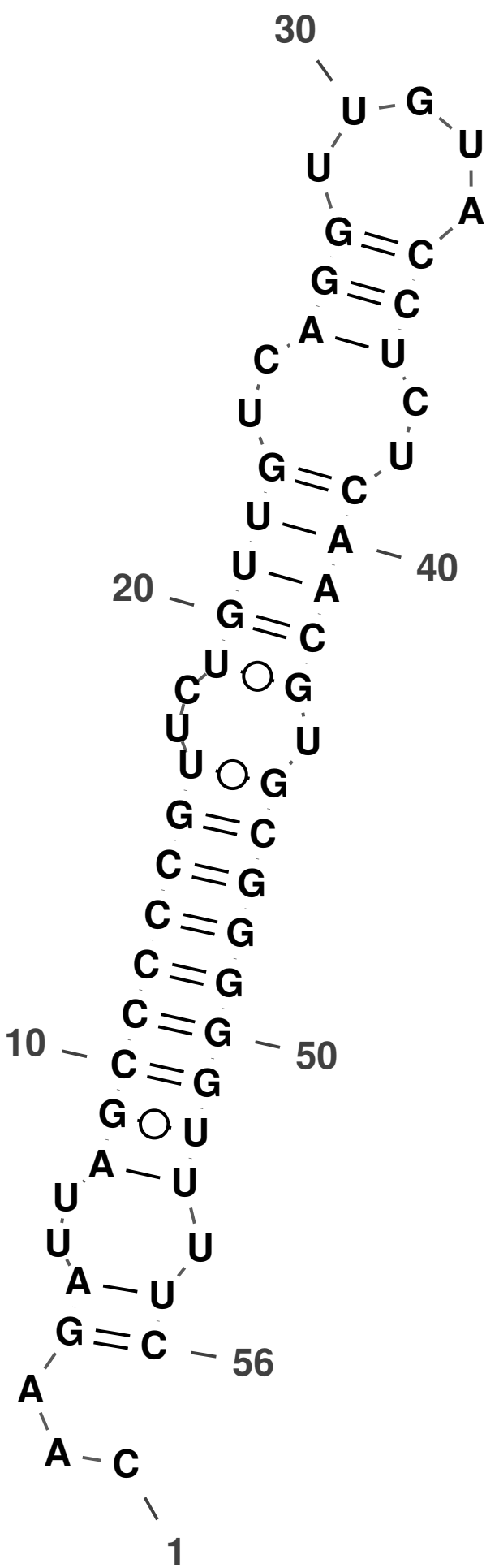

ally -25.10] 388 (E=-25.10 kcal