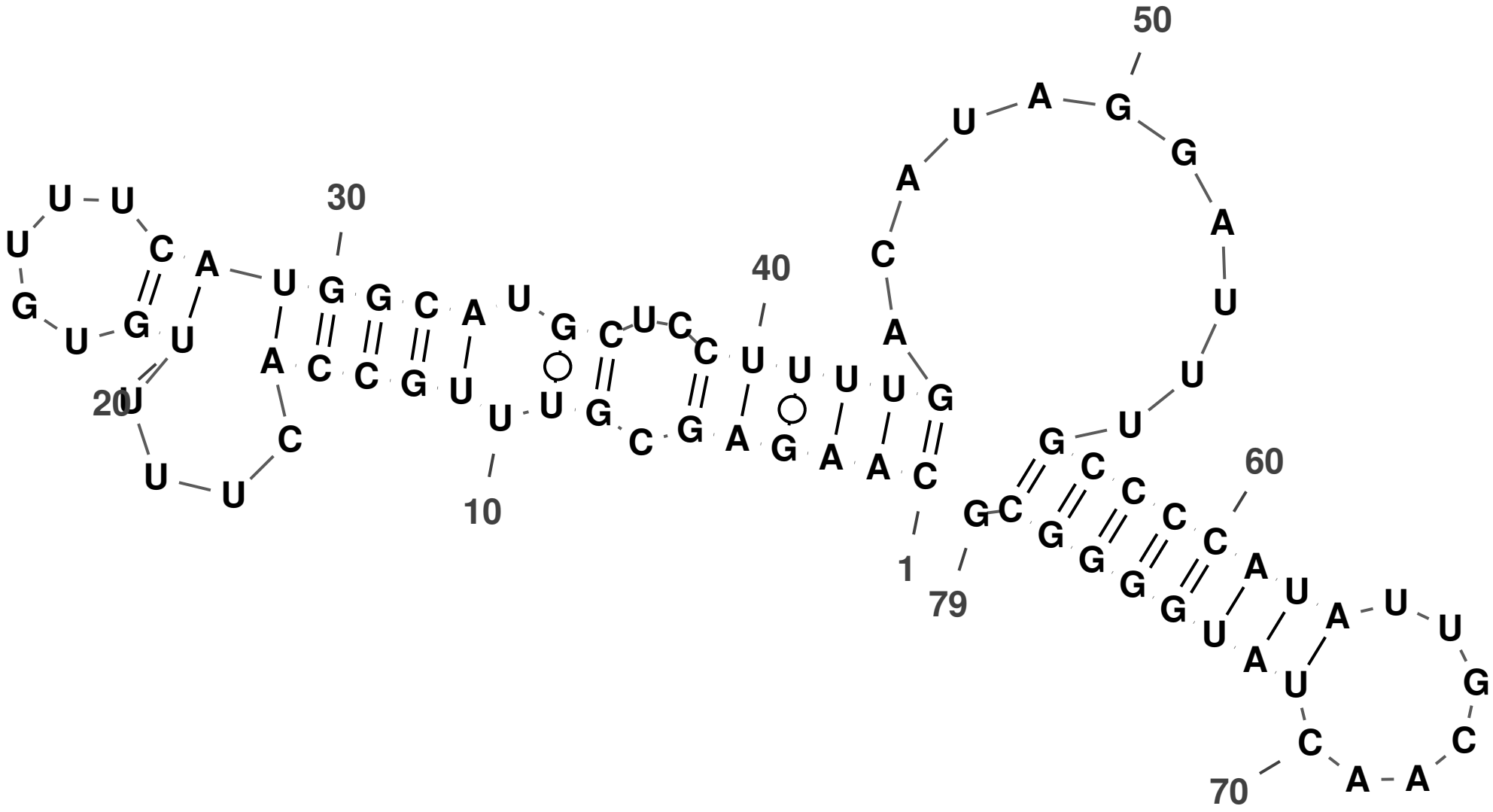

[initially -25.20] 69 (E=-25.20 kcal/mol)