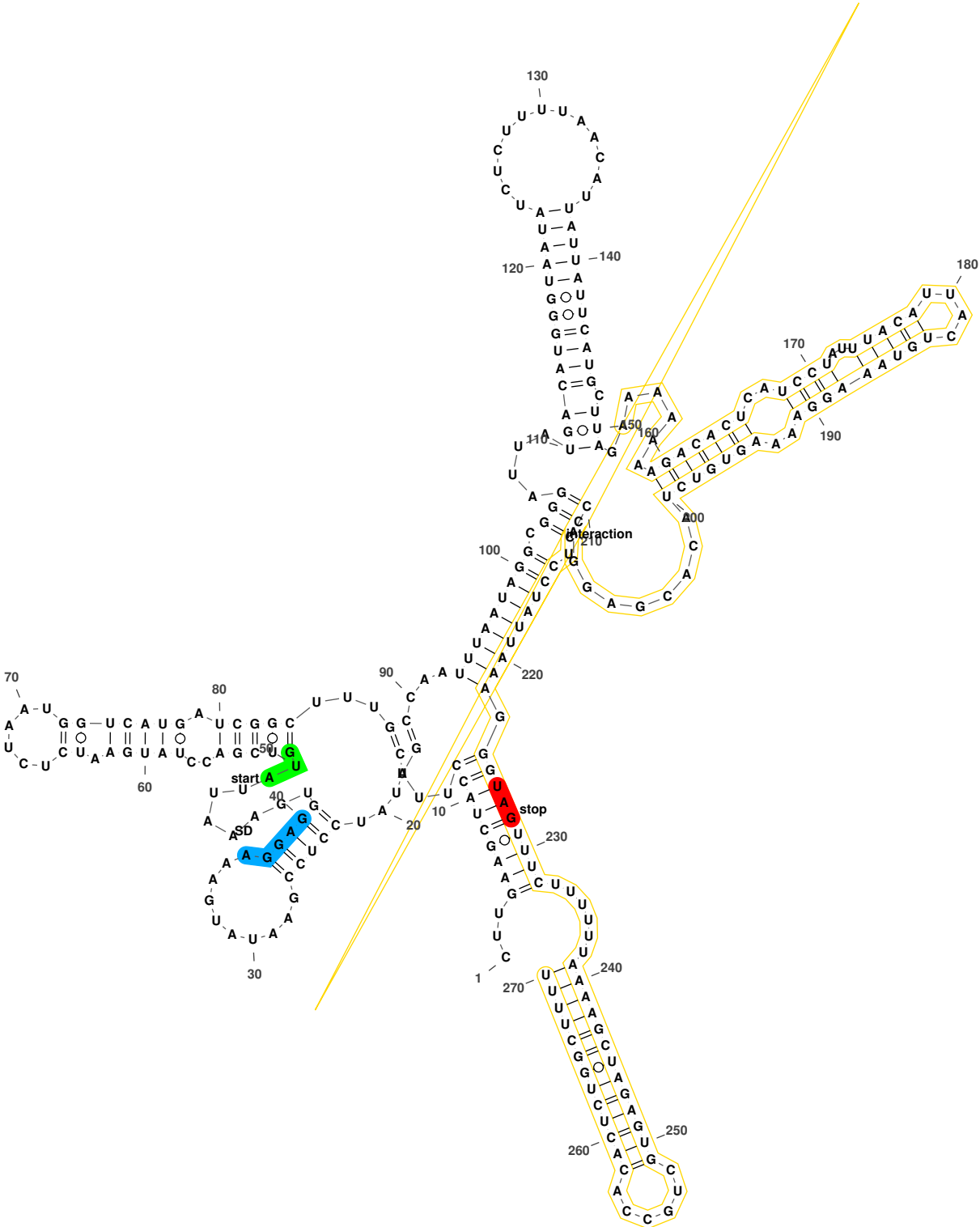

[initially -89.70] 2 (E=-78.03 kcal/mol)