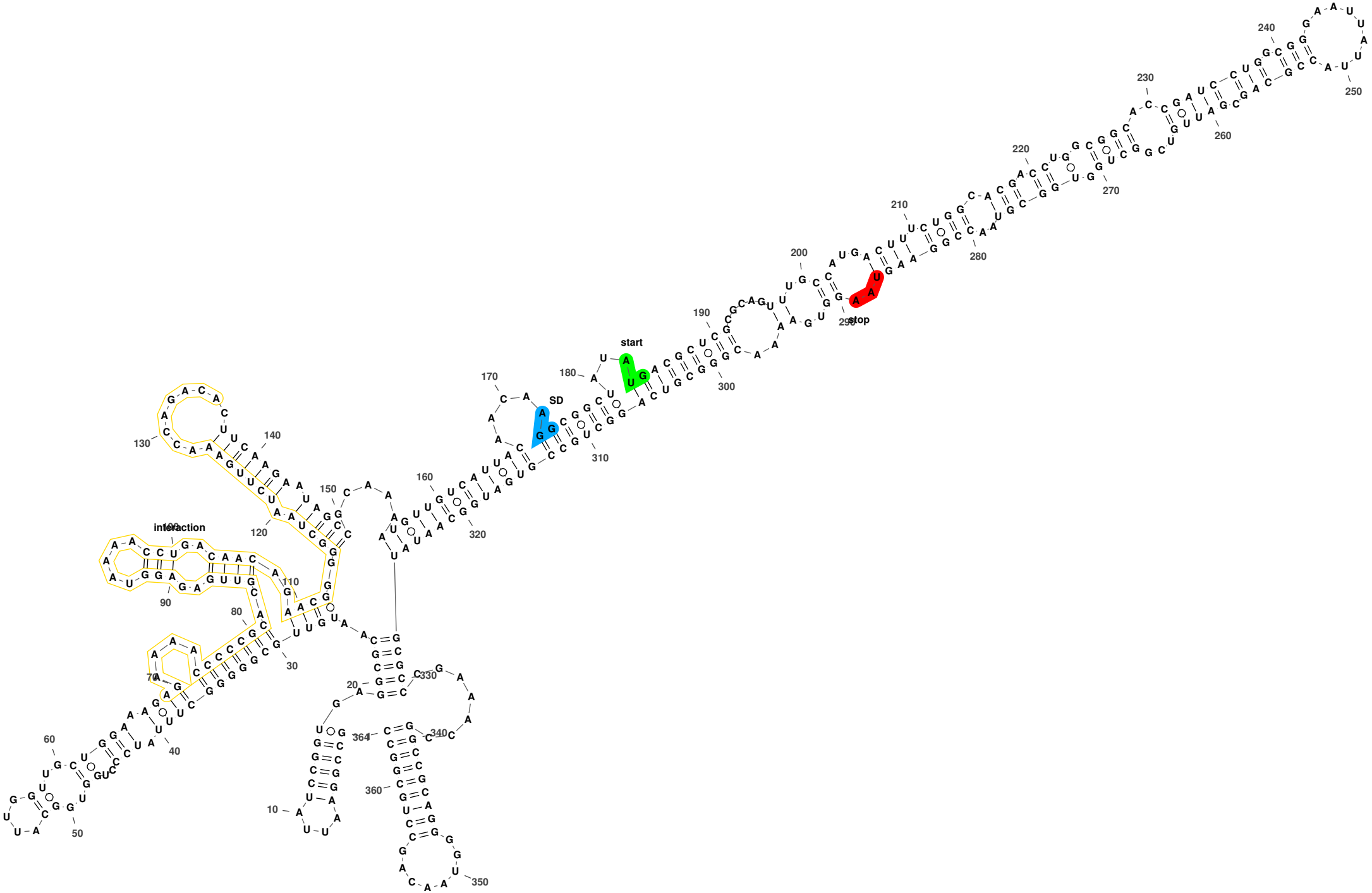

[initially -164.70] 564 (E=-158.75 kcal/mol)