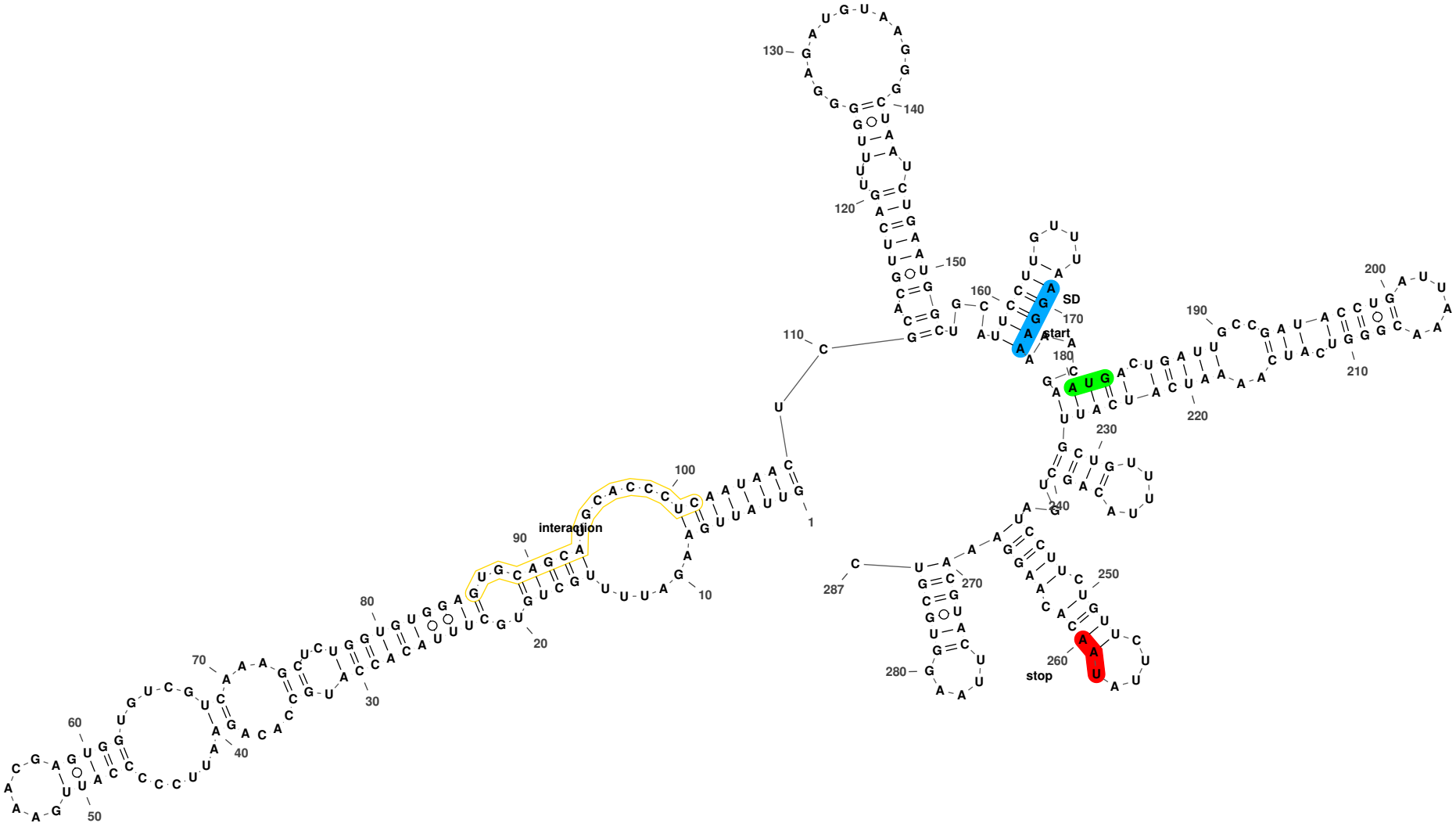

[initially -88.60] 21 (E=-89.40 kcal/mol)