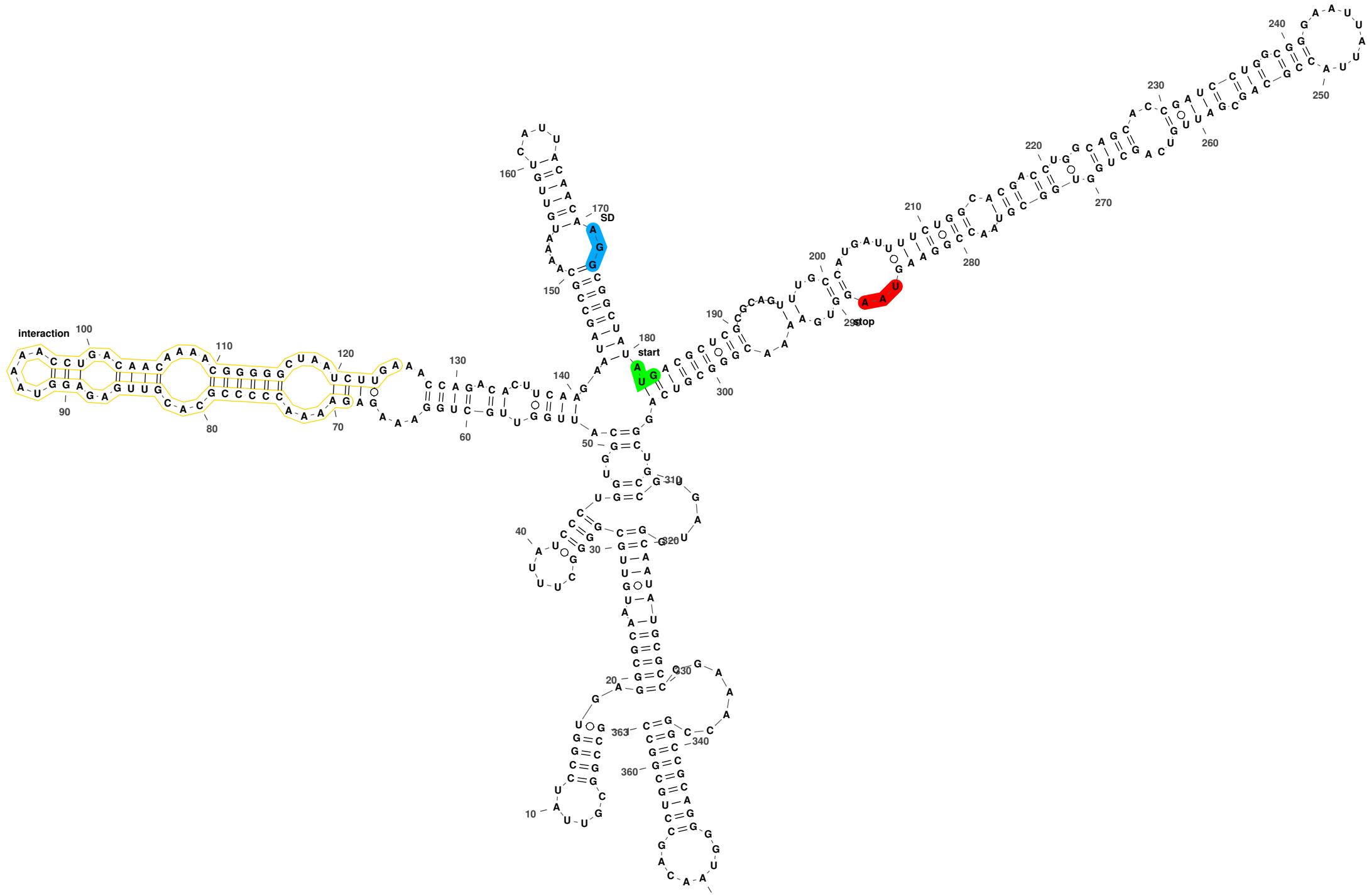

[initially -157.70] 570 (E=-155.43 kcal/mol)