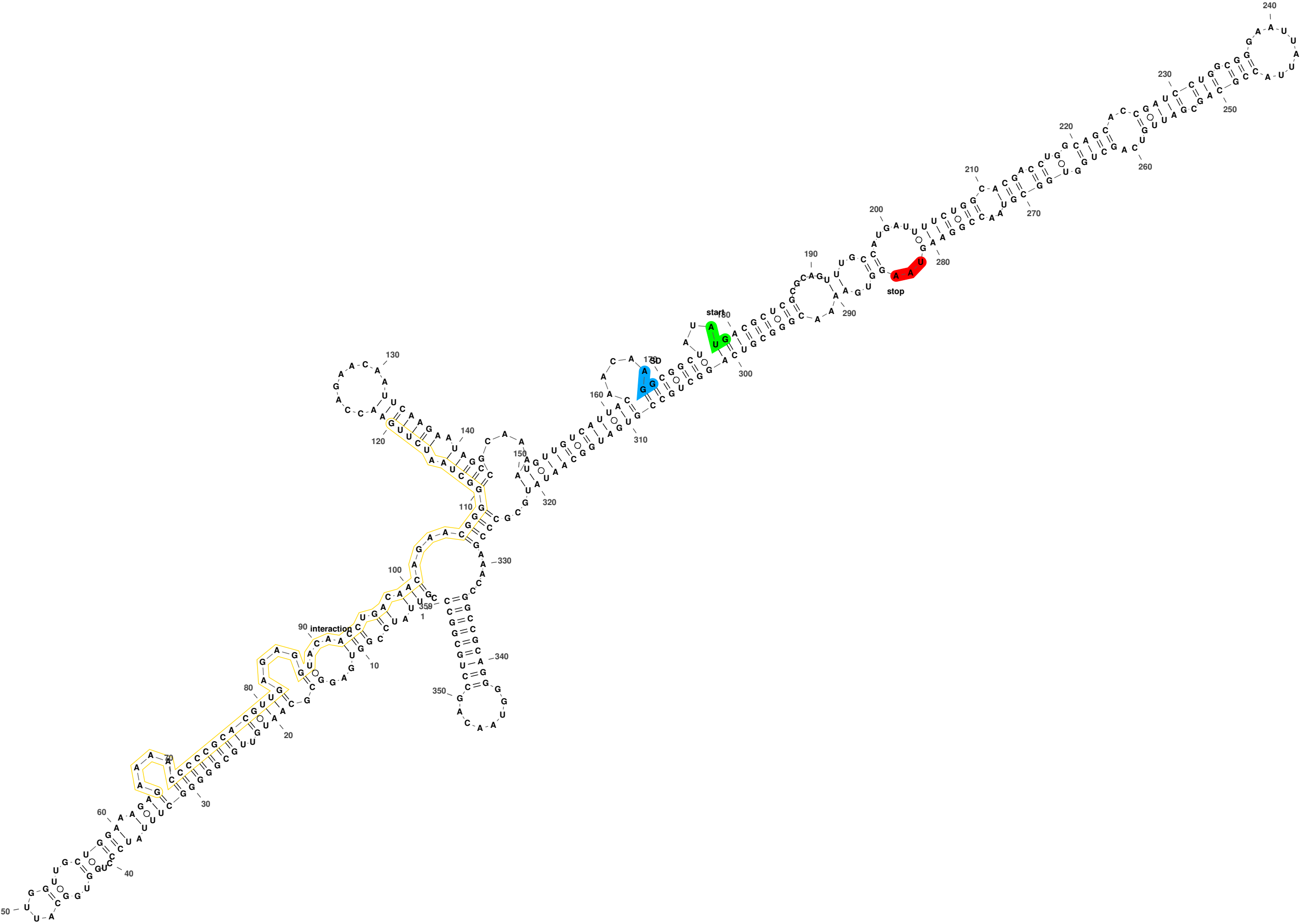

[initially -156.20] 364 (E=-154.58 kcal/mol)