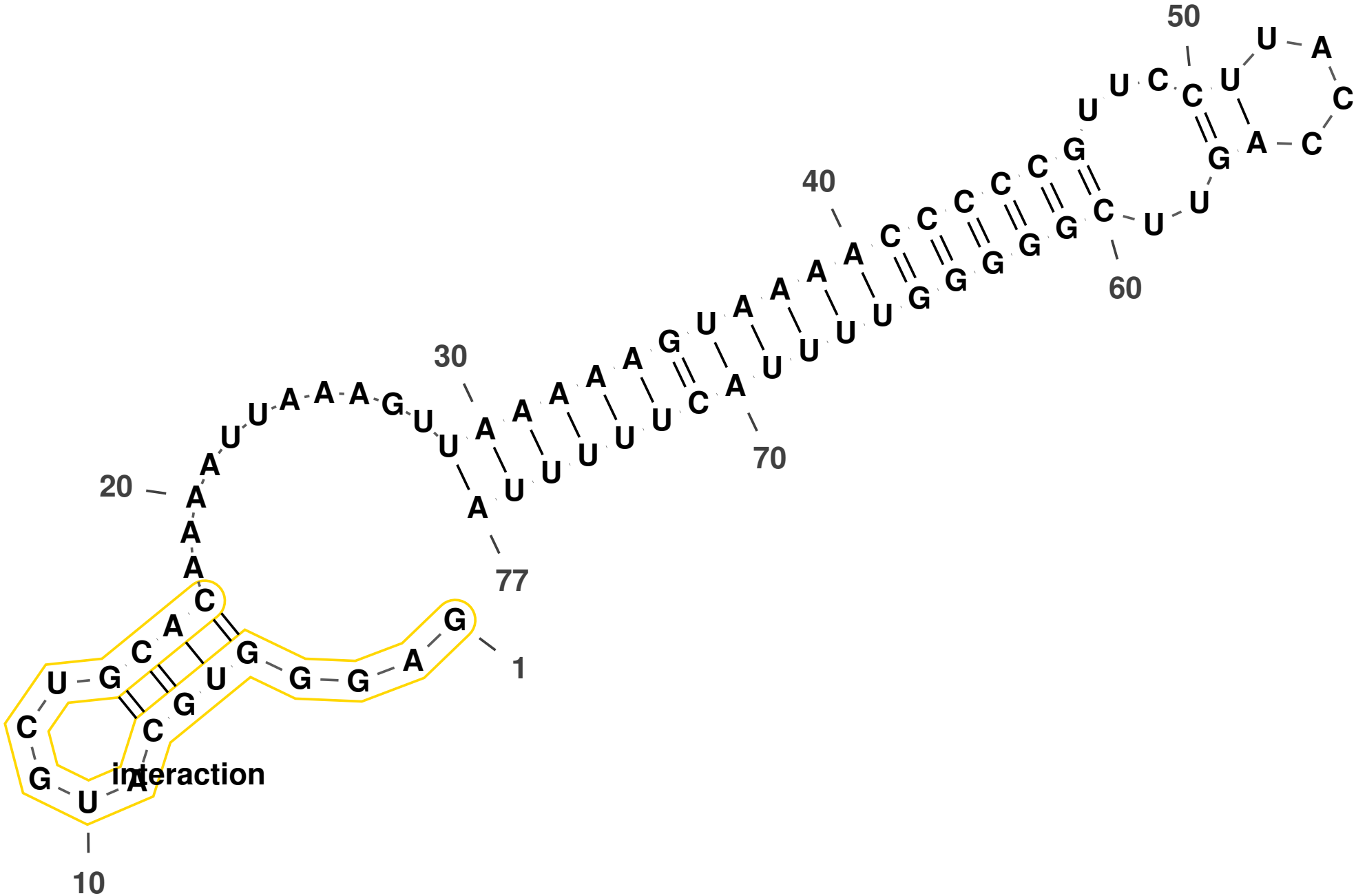

[initially -31.30] 12 (E=-31.30 kcal/mol)