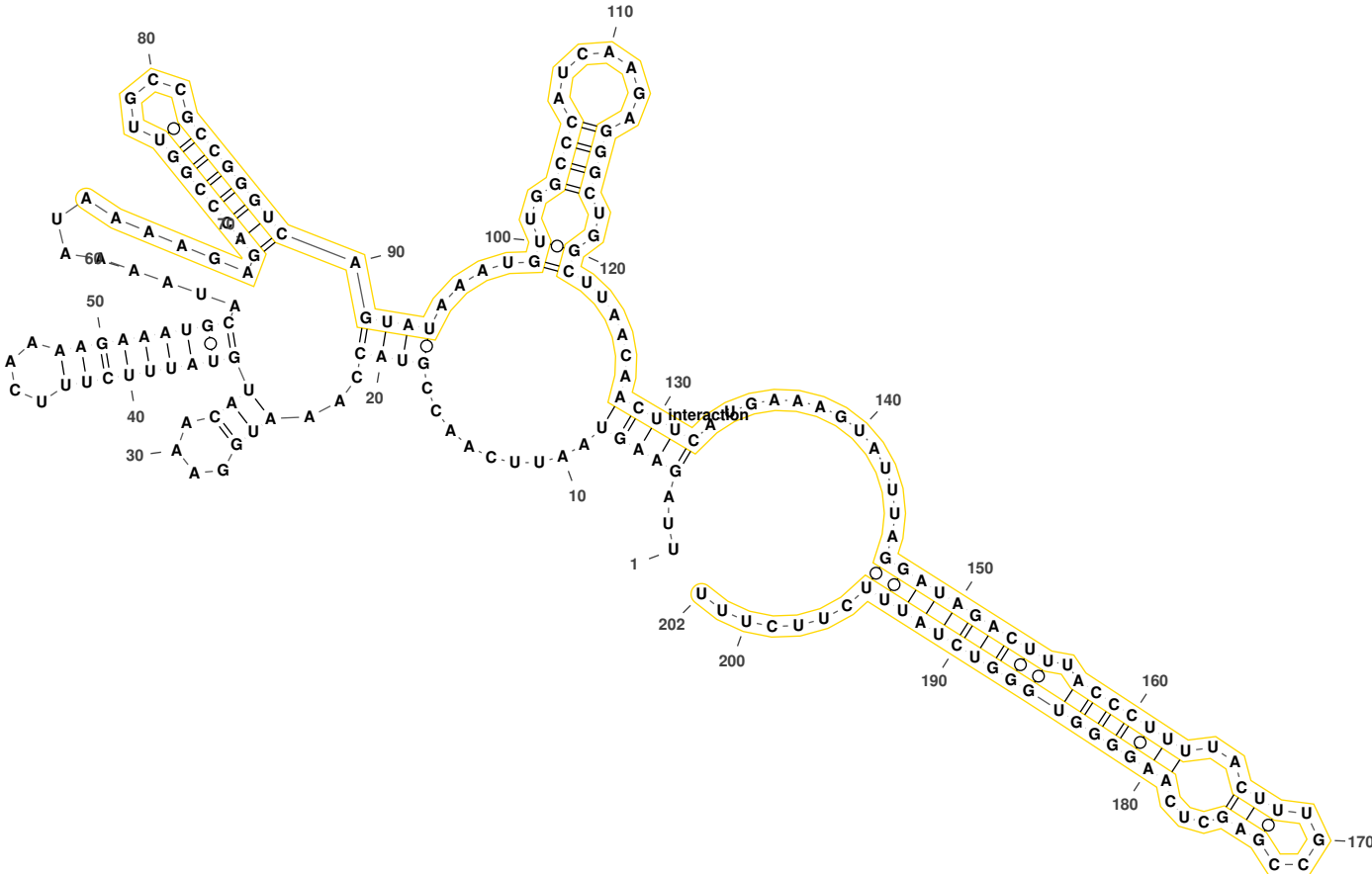

[initially -64.10] 7 (E=-57.28 kcal/mol)