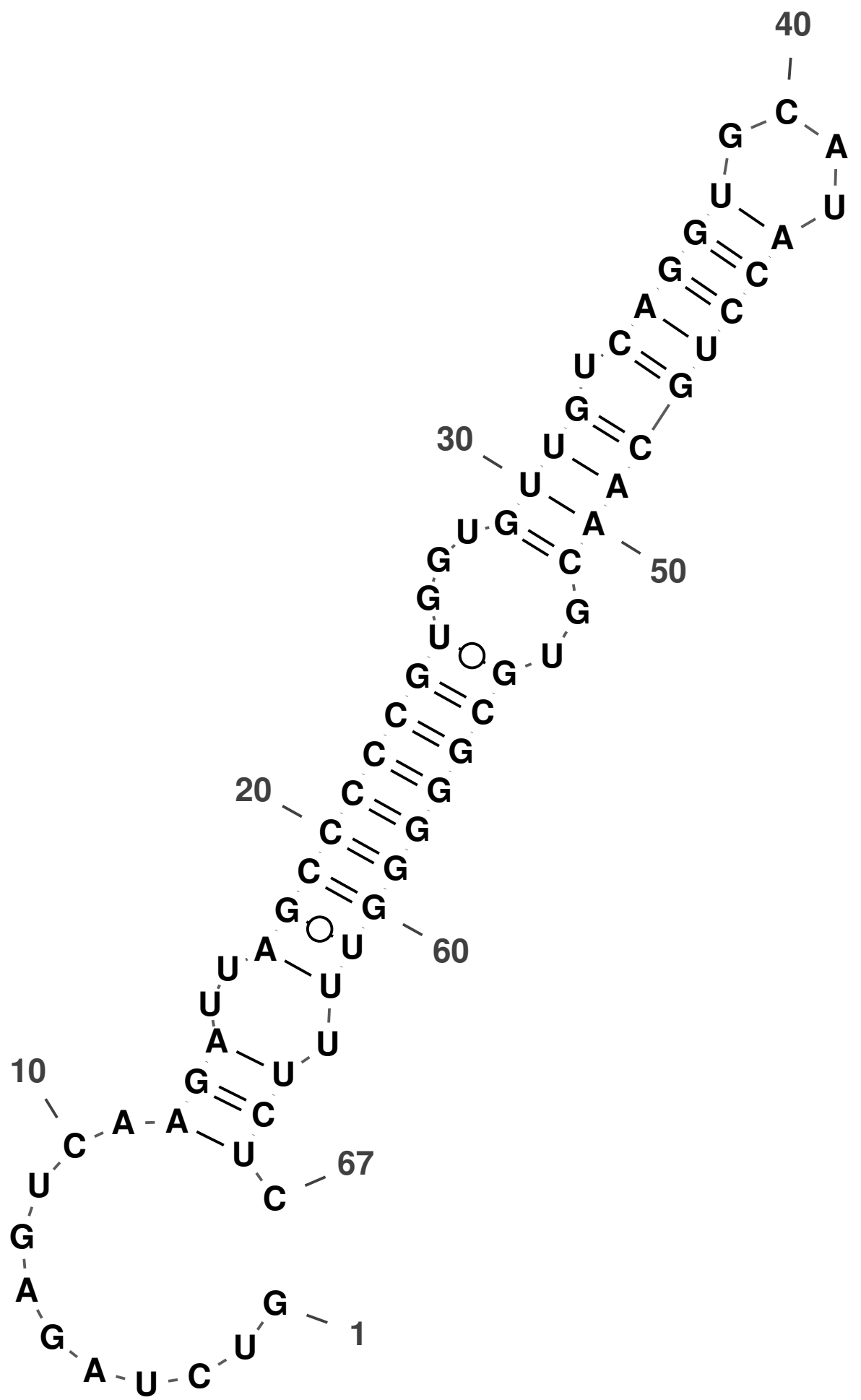


[initially -29.00] 639 (E=-29.00 kcal/mol)