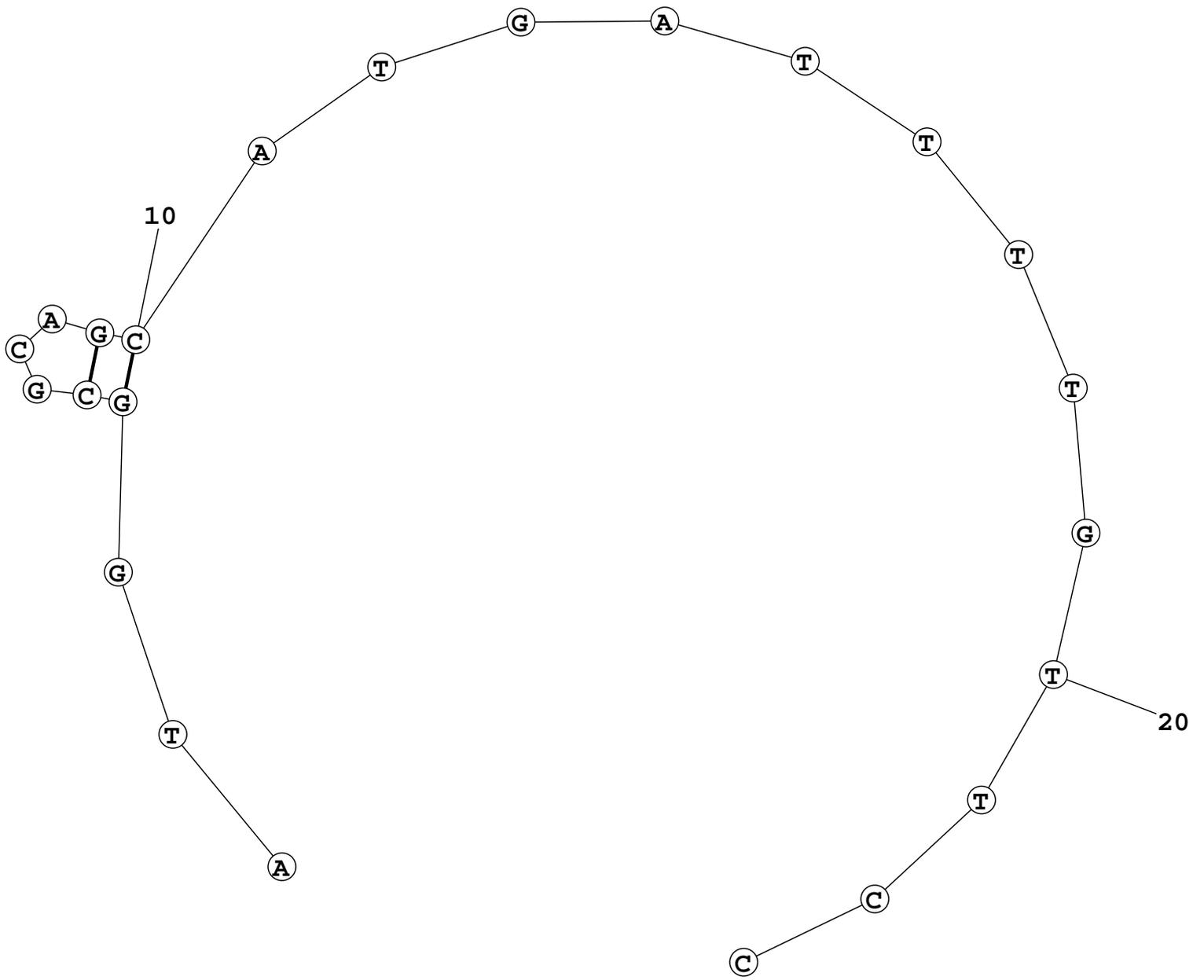ENERGY = -3.0  rev

ENERGY = -2.9  rev