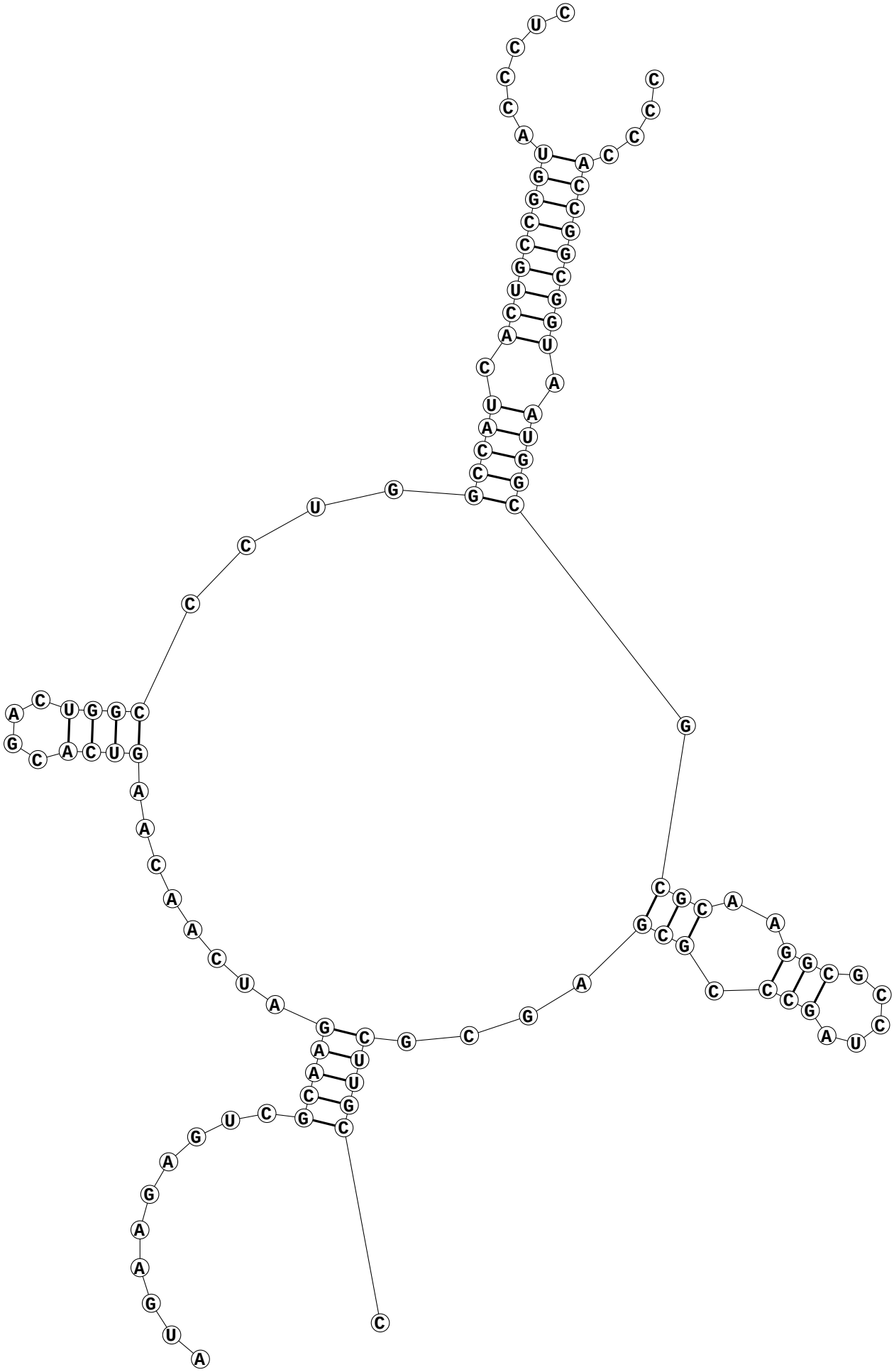

ENERGY = -40.8 OprE_ 12514