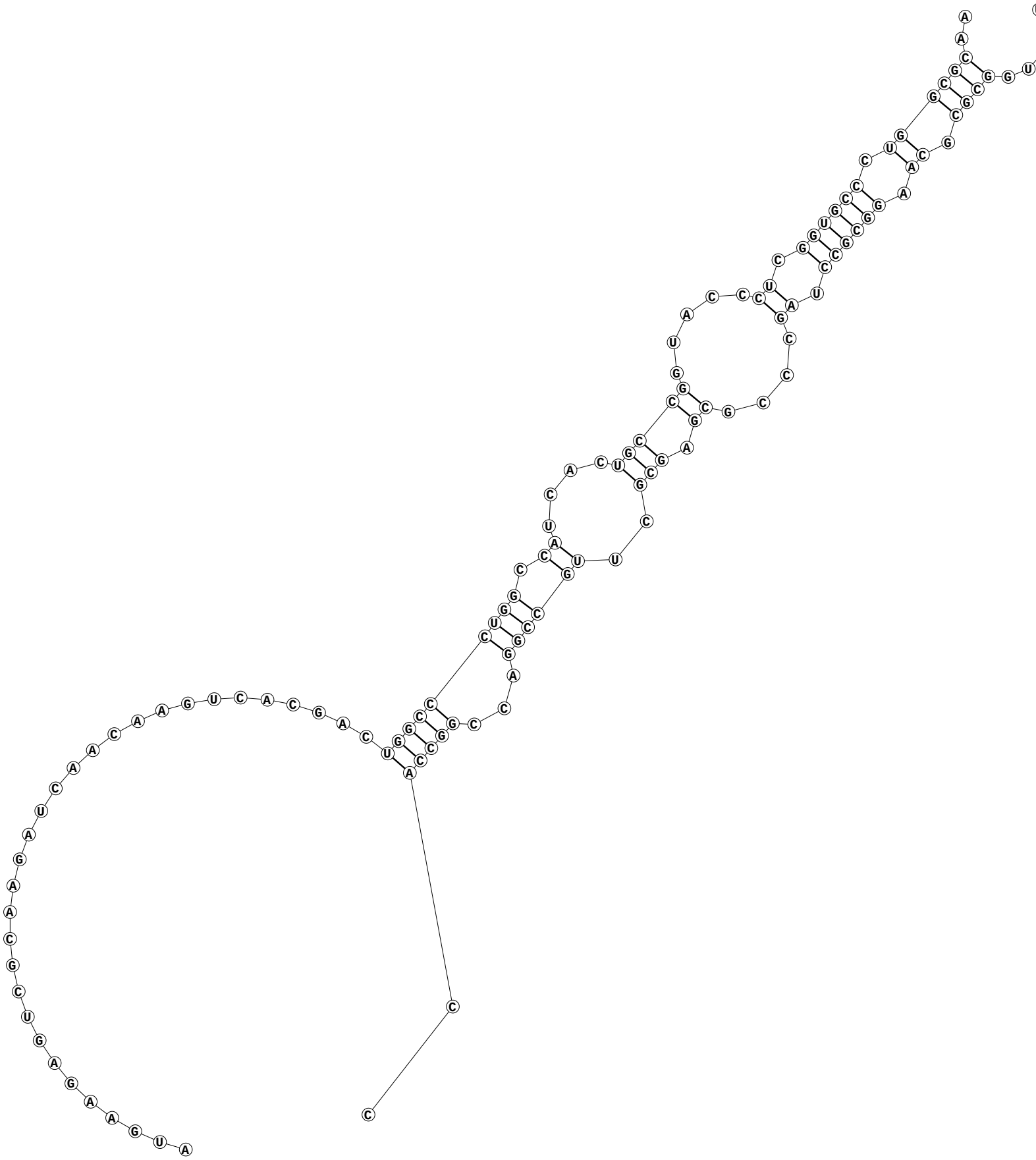

ENERGY = -41.3 OprE_ 12514