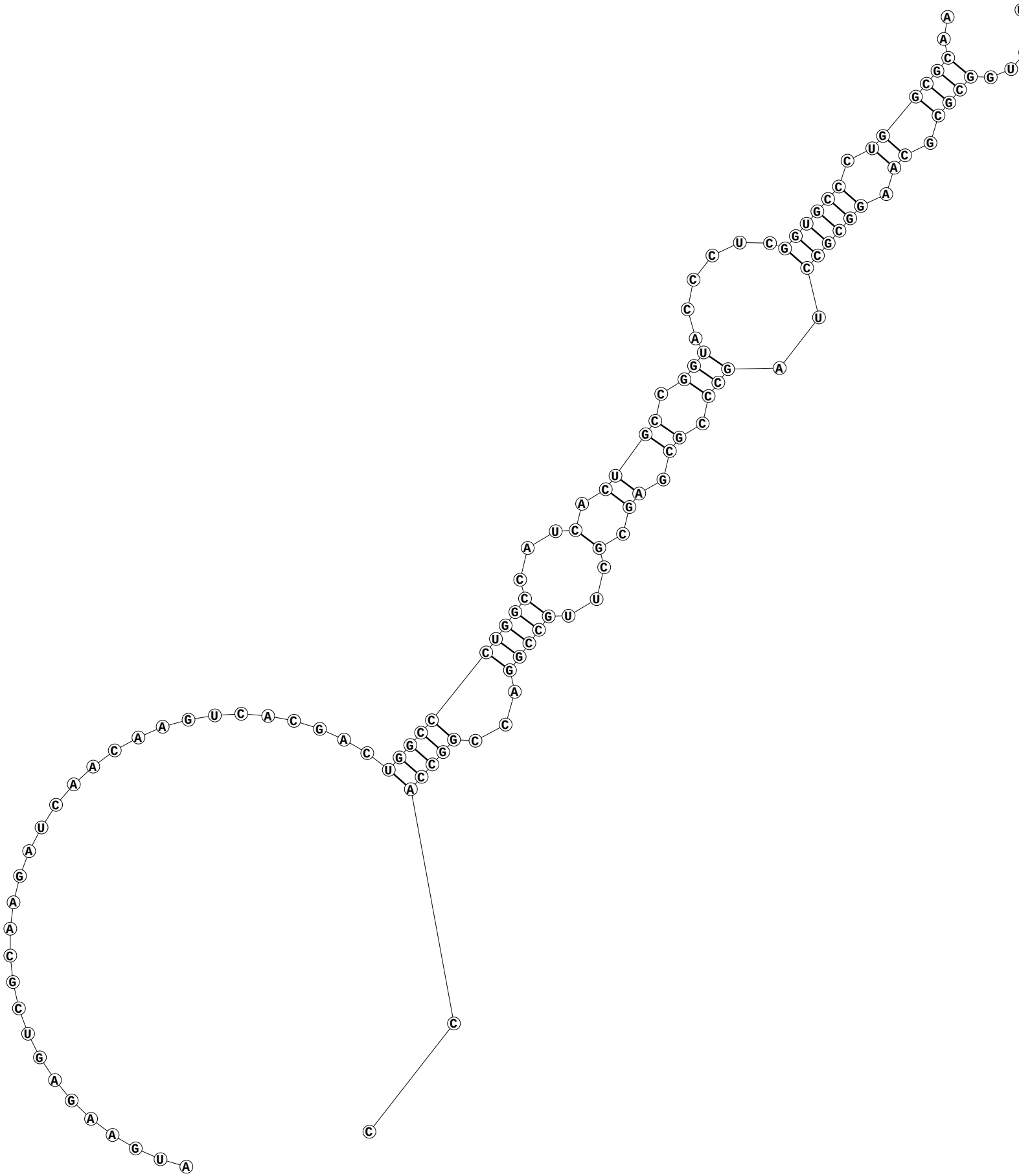

ENERGY = -42.2 OprE_ 12514