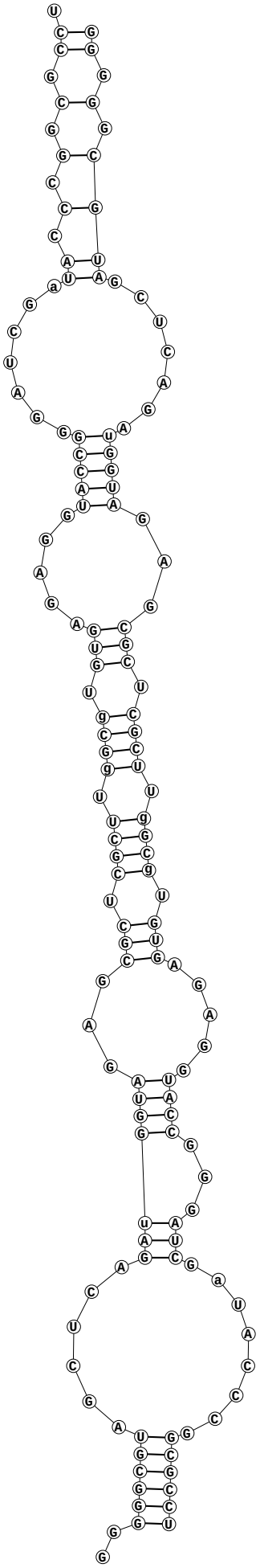

ENERGY = -46.6 a;exitmd5’w4p1t1_md5...