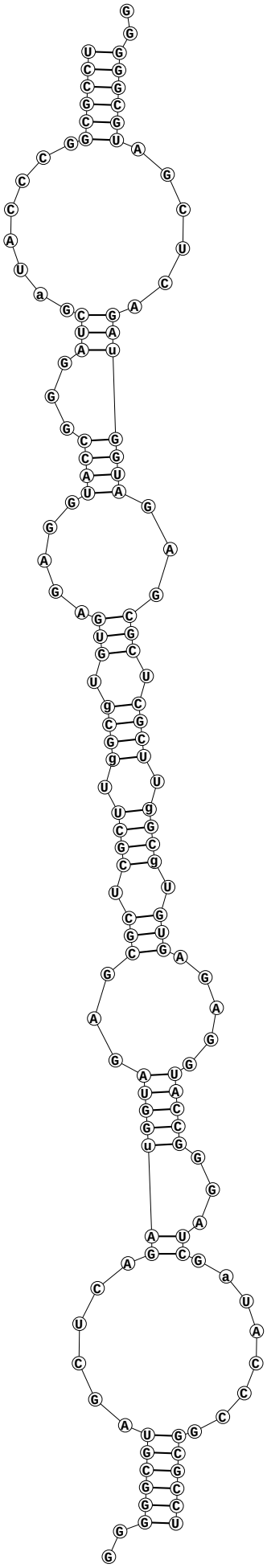

ENERGY = -47.2 a;exitmd5’w4p1t1_md5...