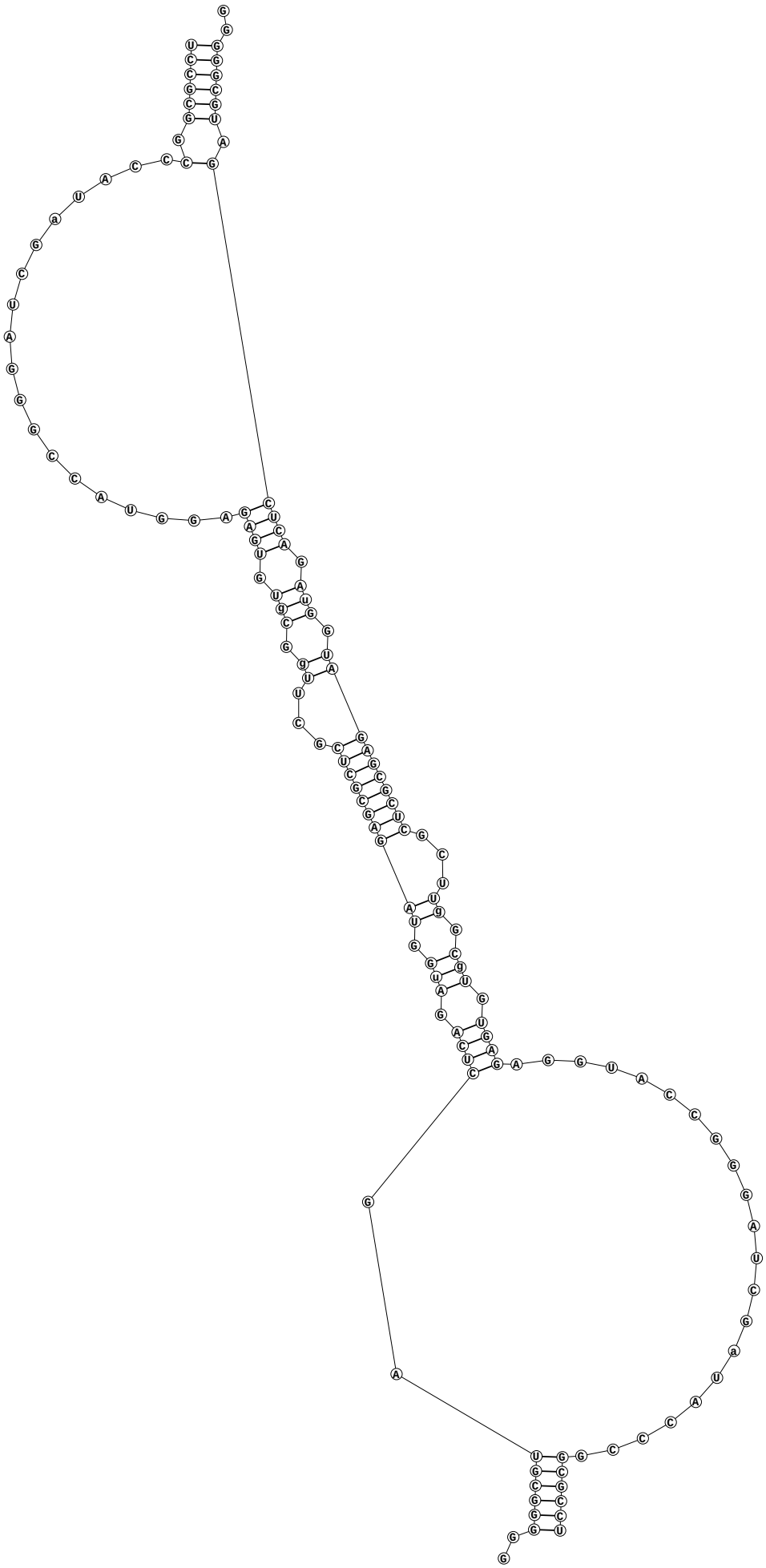

ENERGY = -46.6 ’.exitmd5’w4p1t1_md5...