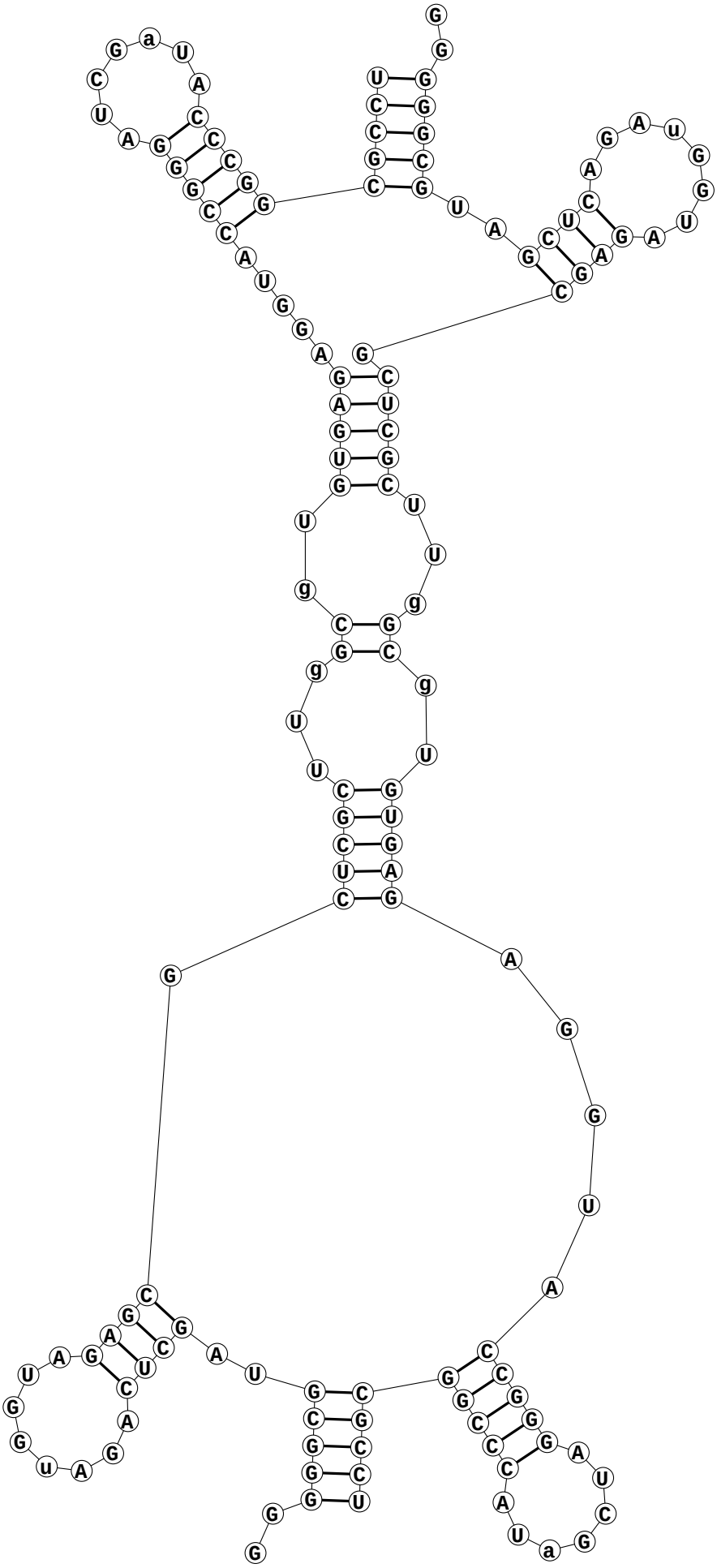

ENERGY = -57.9 ’.exitmd5’w4p1t1_md5...