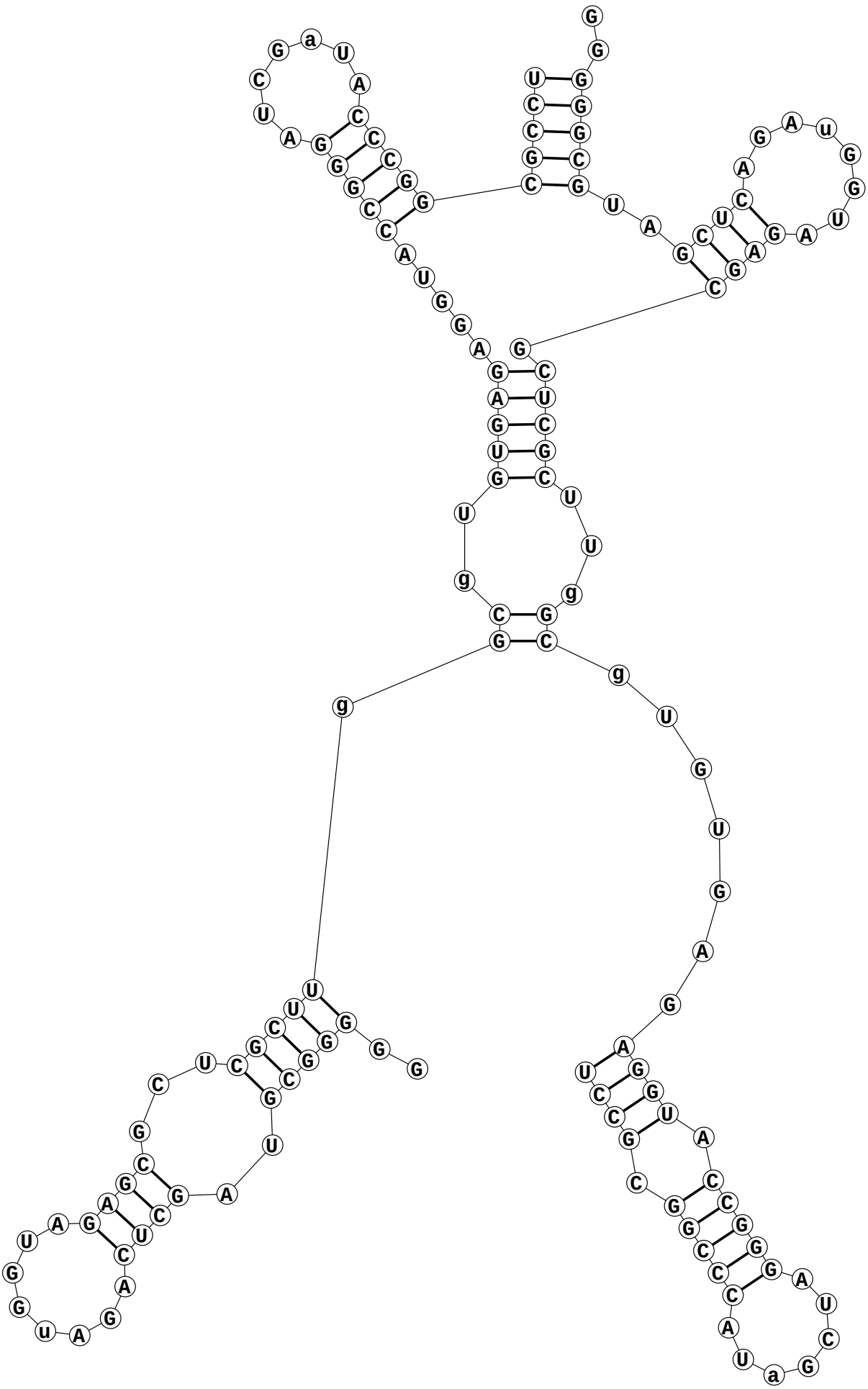

ENERGY = -57.0 ’.exitmd5’w4p1t1_md5...