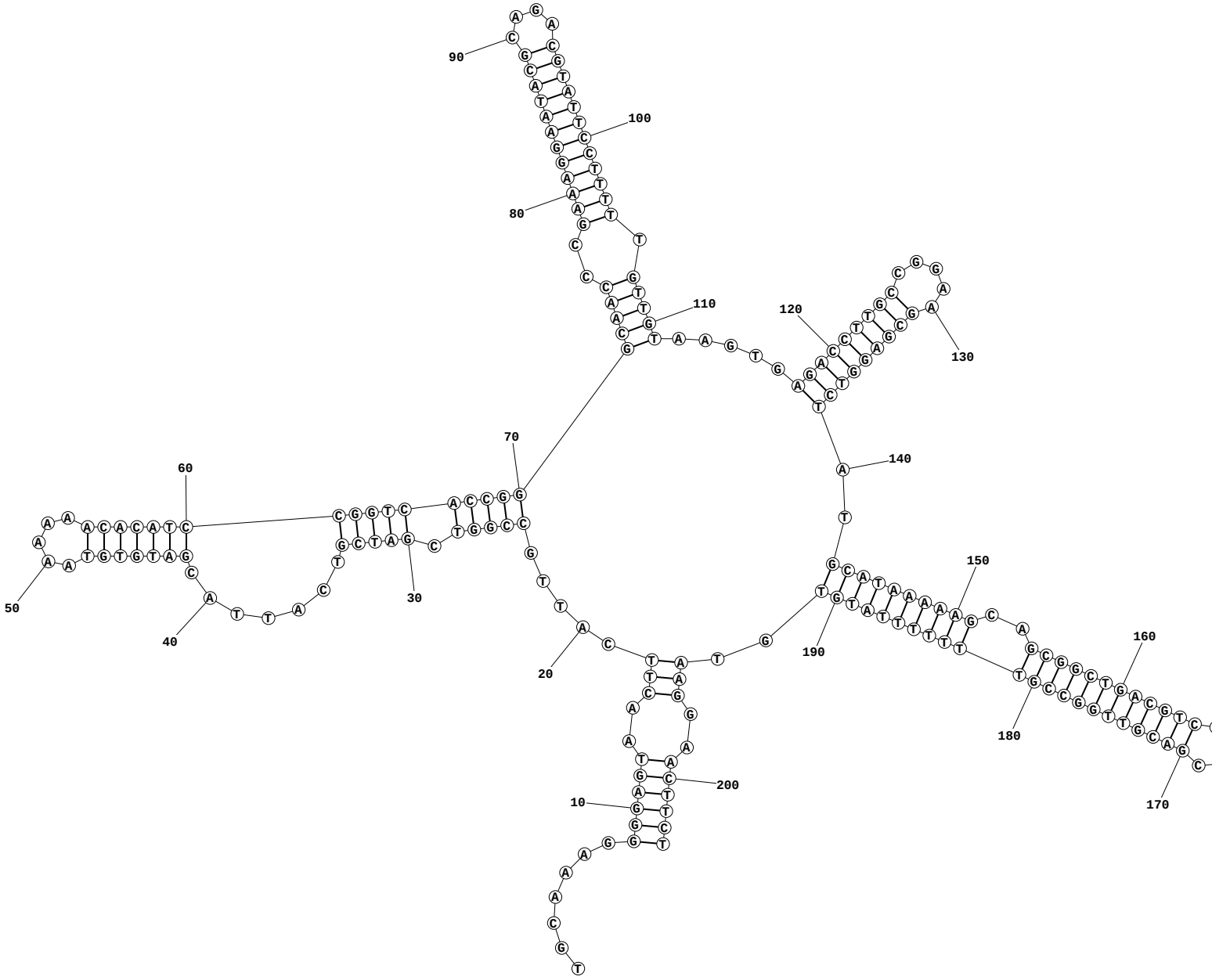

ENERGY = -84.3 DDD rev comp