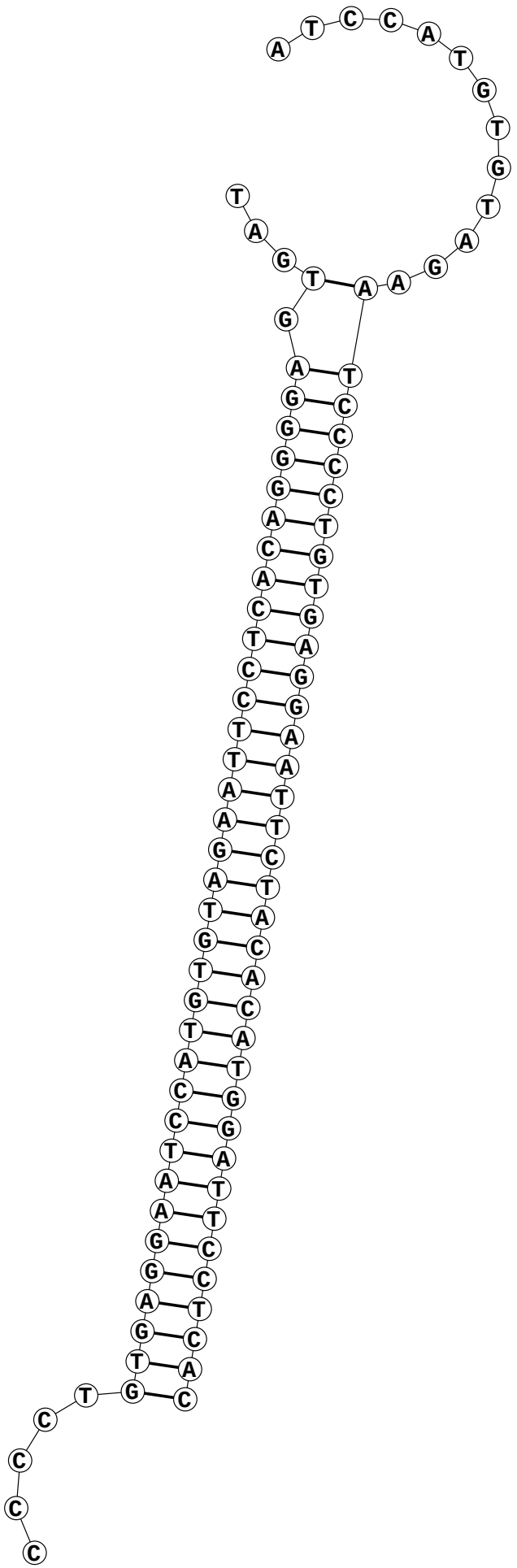

ENERGY = -54.2 H1_ H2