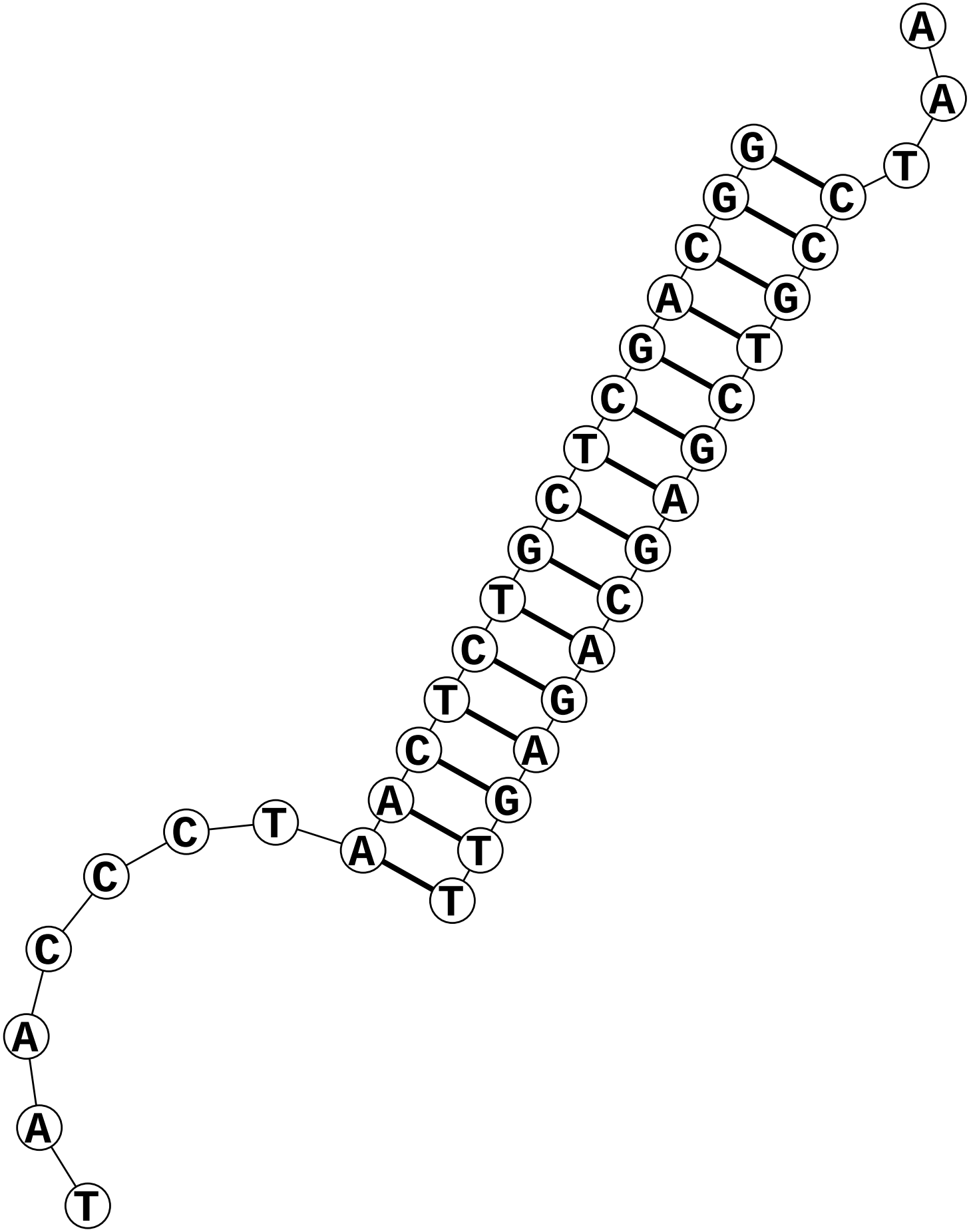

ENERGY = -21.4 probe2_ TS