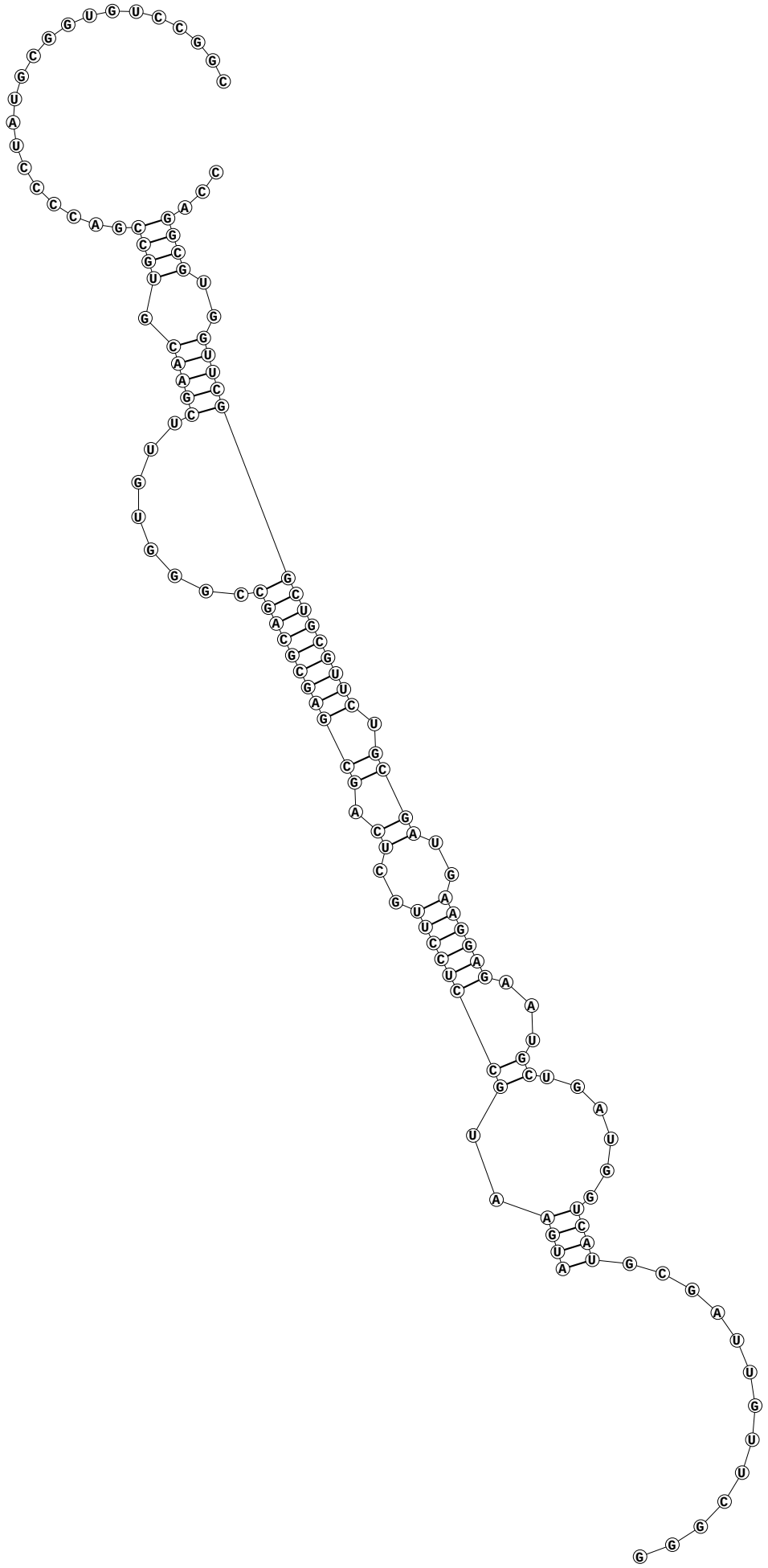

ENERGY = -40.4 xylS_ 6963