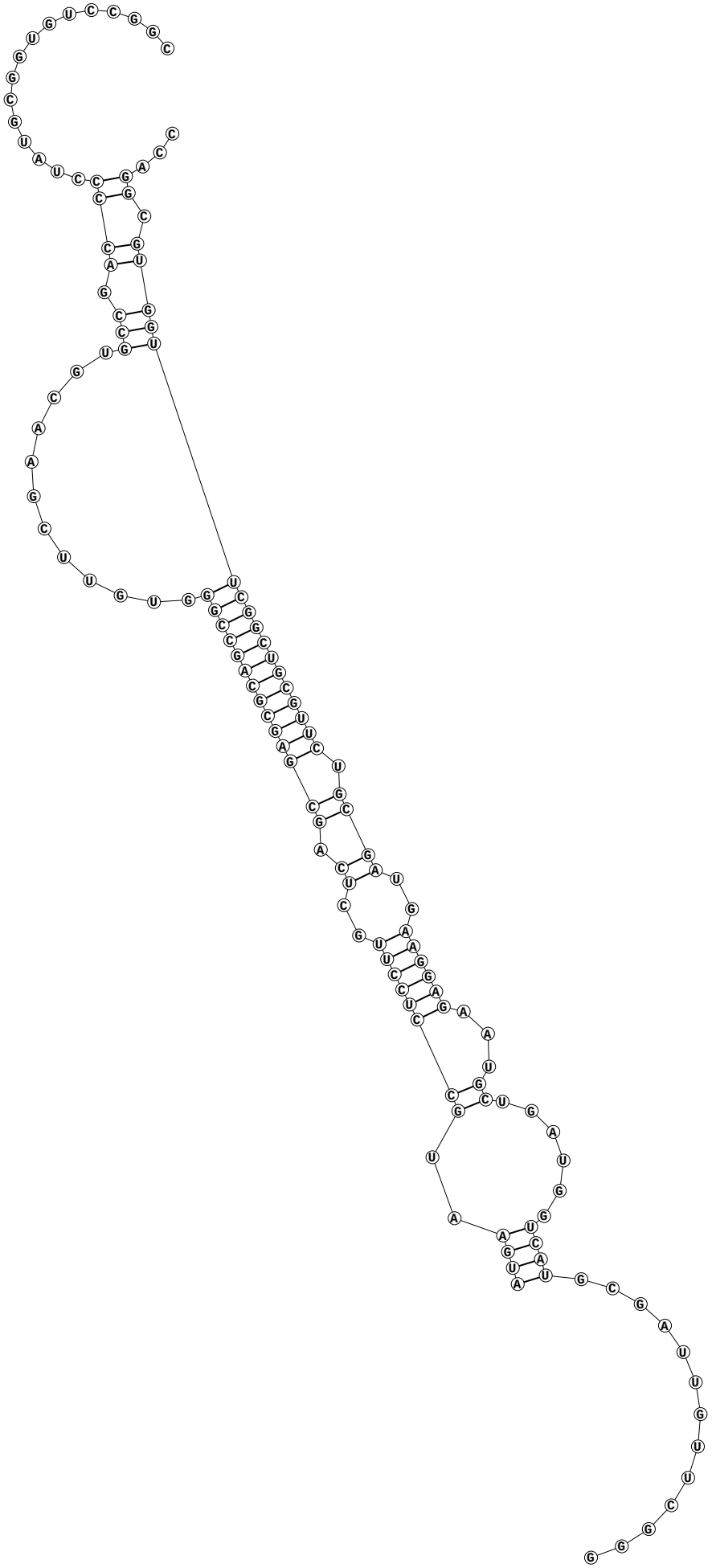

ENERGY = -40.8 xylS_ 6963