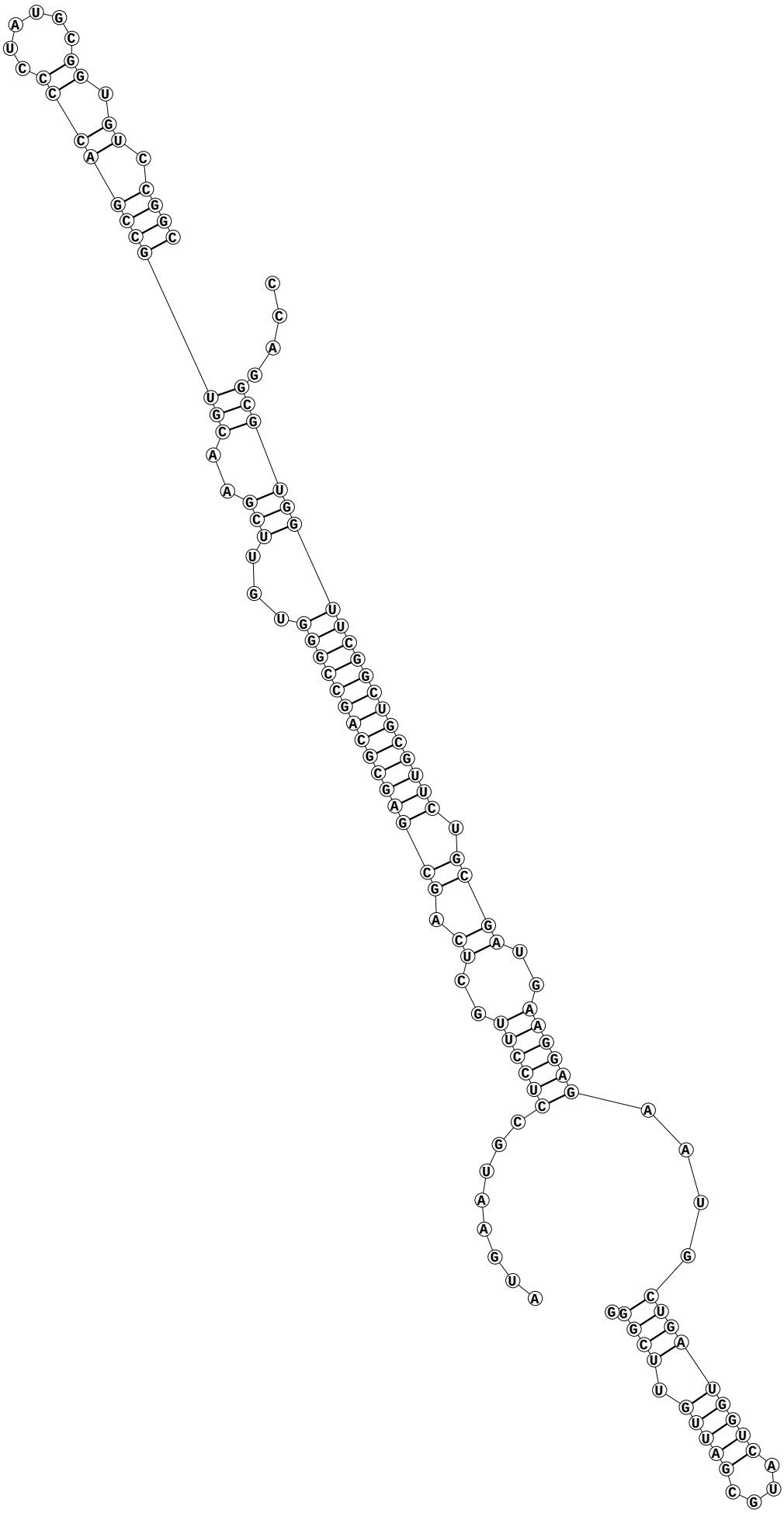

ENERGY = -53.6 xylS_ 6963