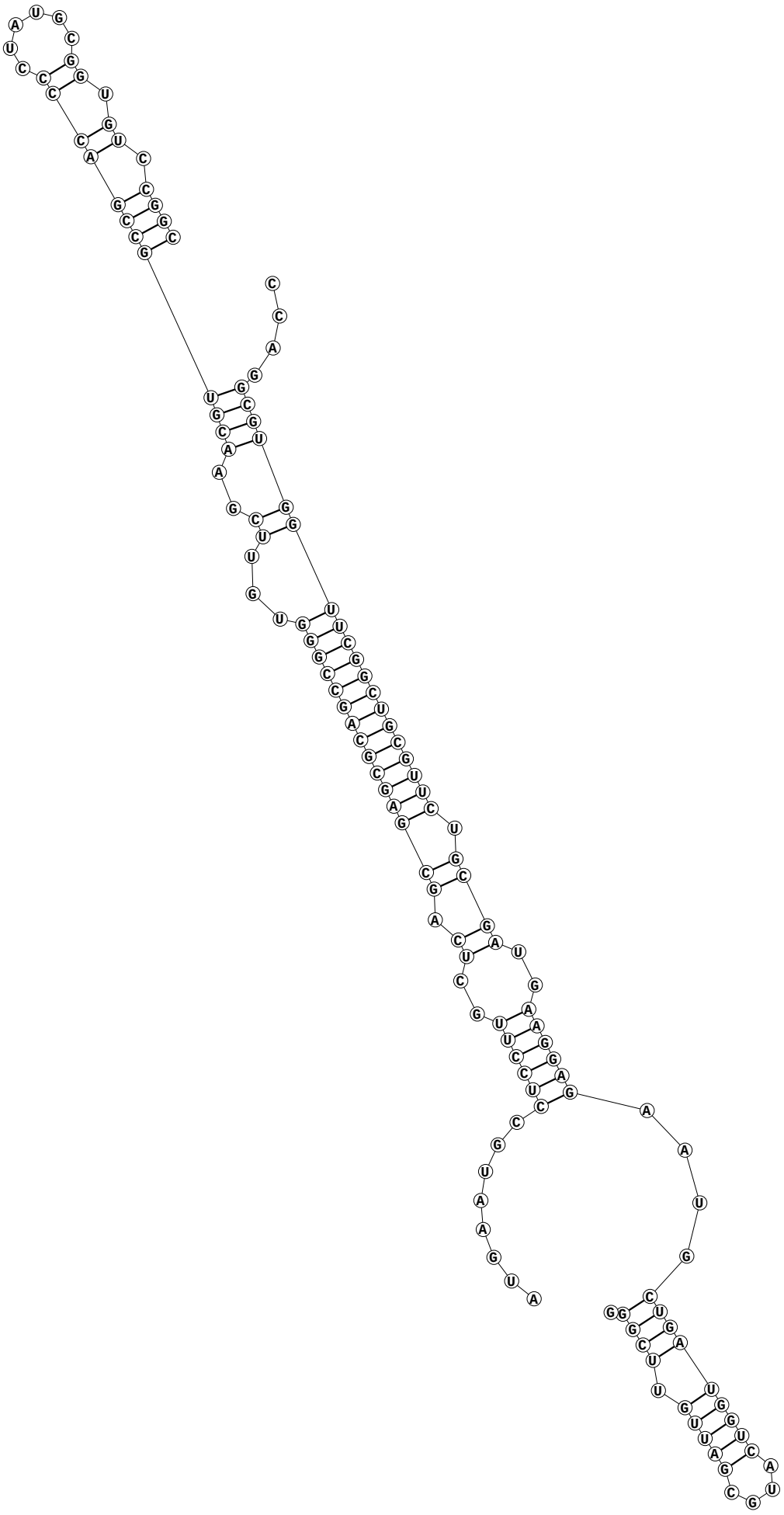

ENERGY = -54.4 xylS_ 6963