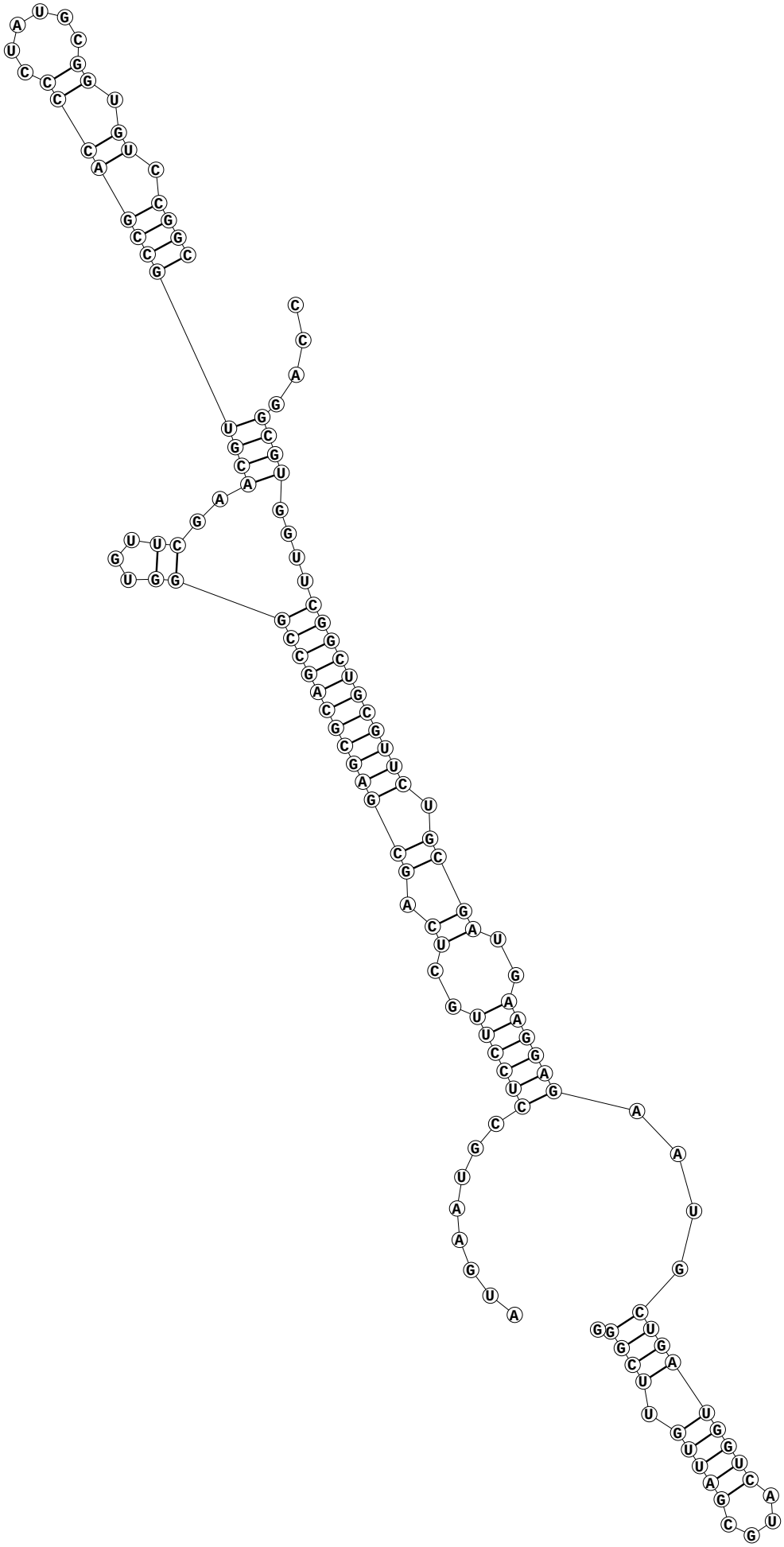

ENERGY = -52.6 xylS_ 6963