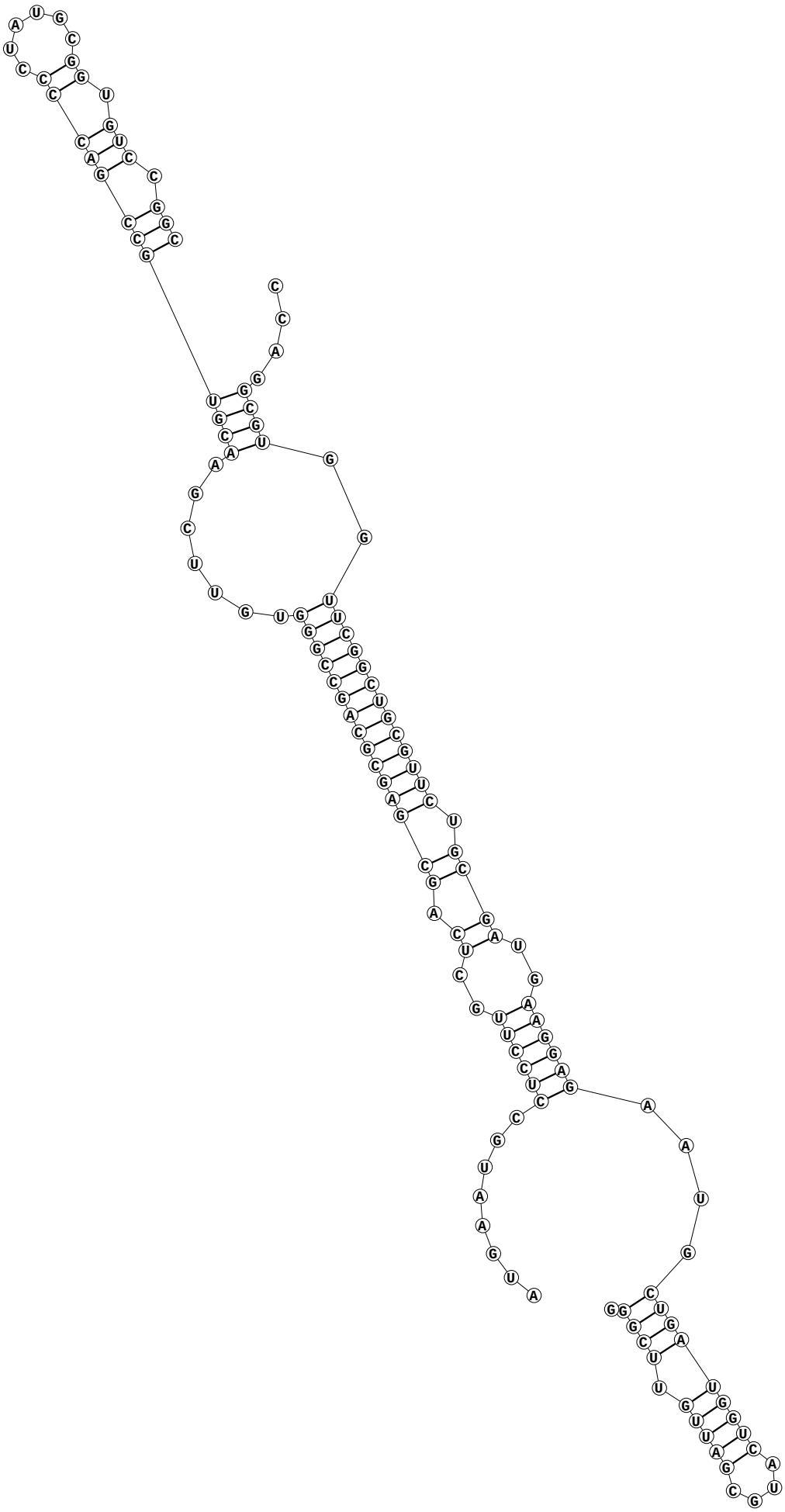

ENERGY = -54.6 xylS_ 6963