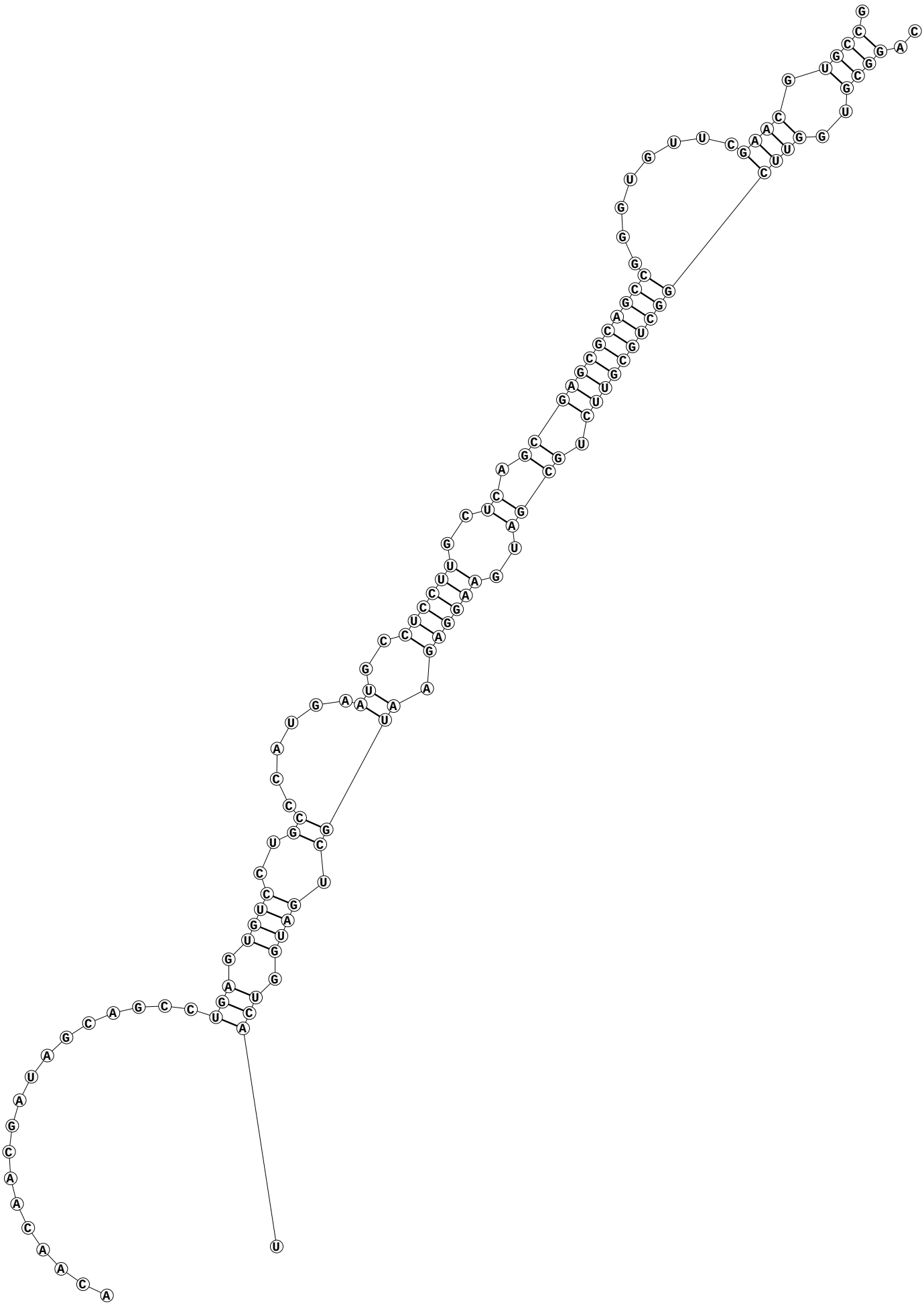

ENERGY = -44.5 xylS_ 6963