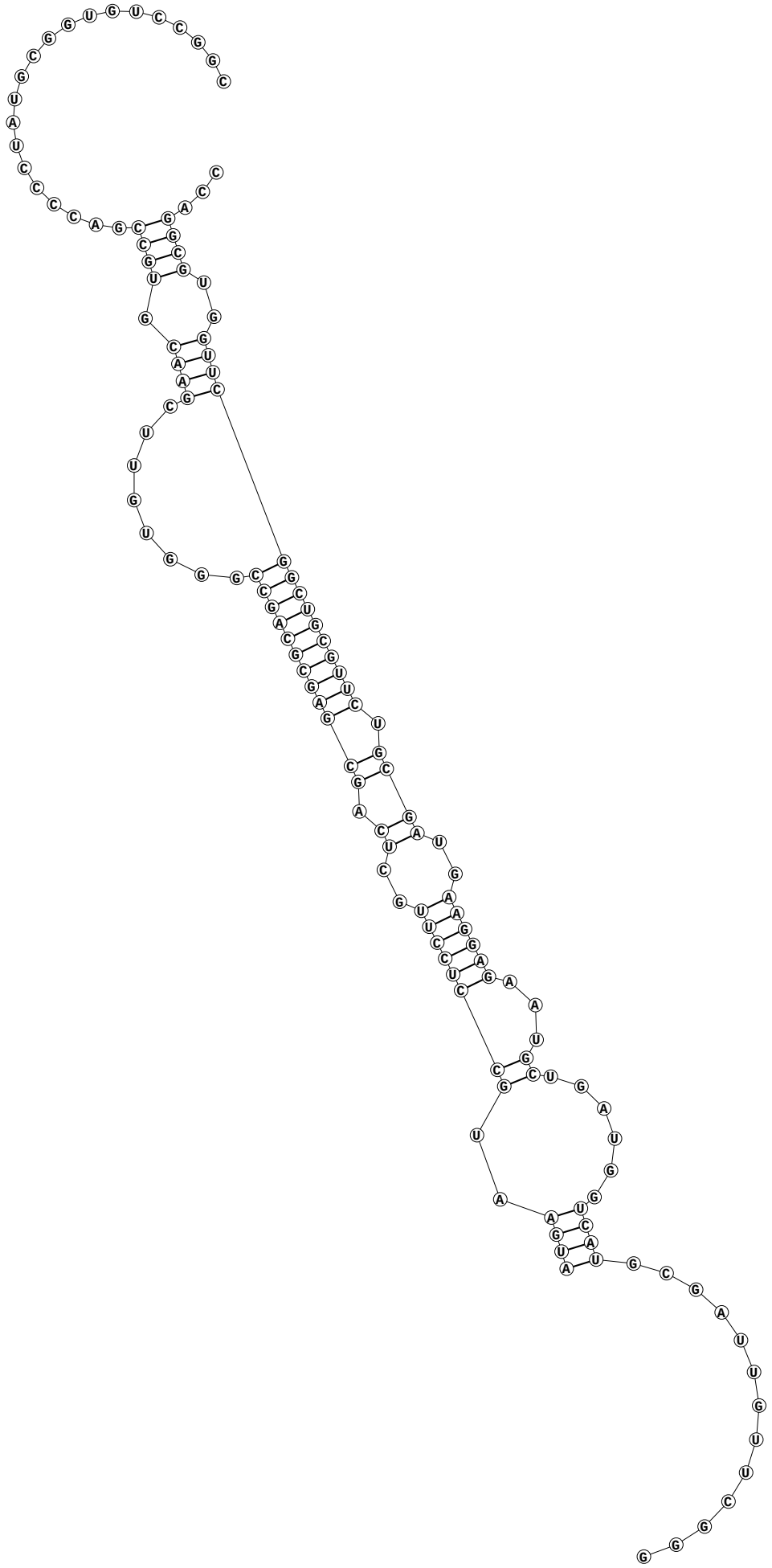

ENERGY = -41.3 xylS_ 6963