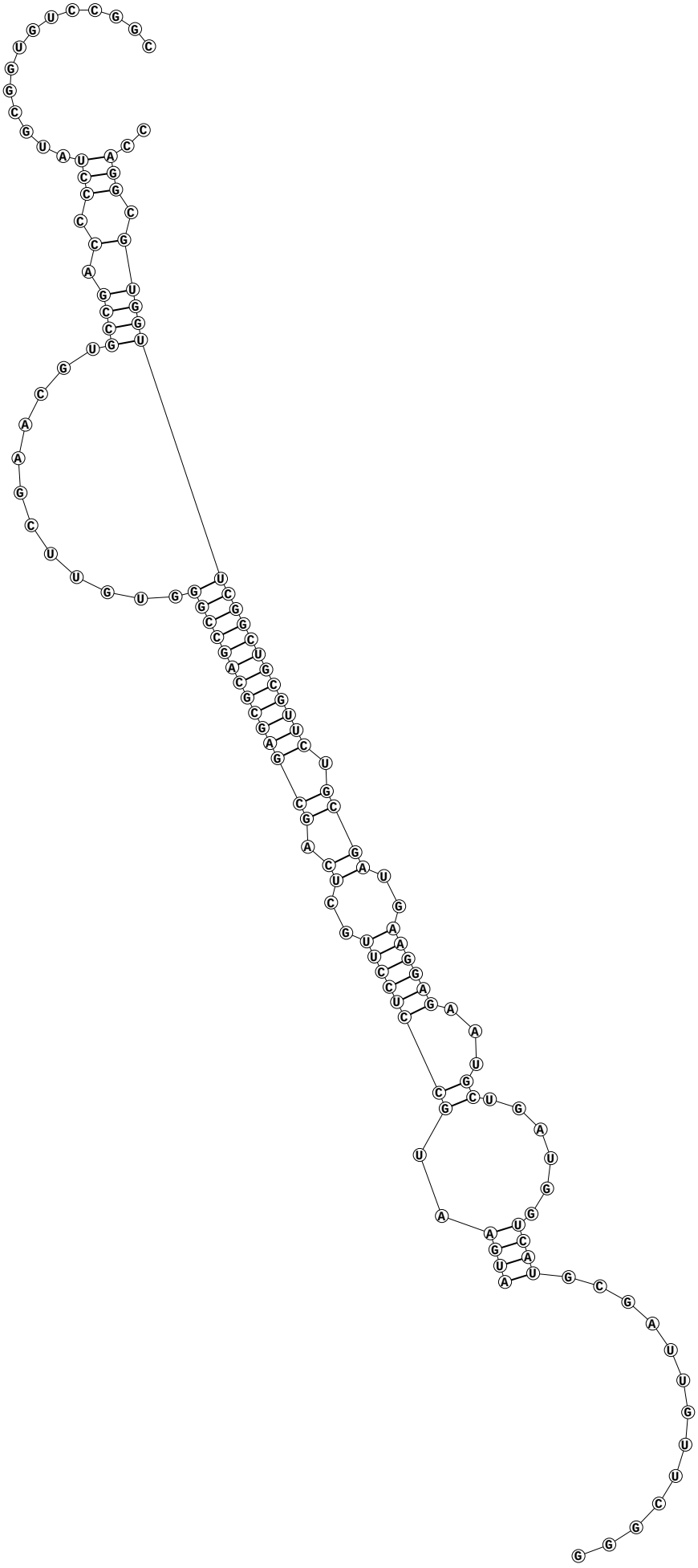

ENERGY = -41.8 xylS_ 6963