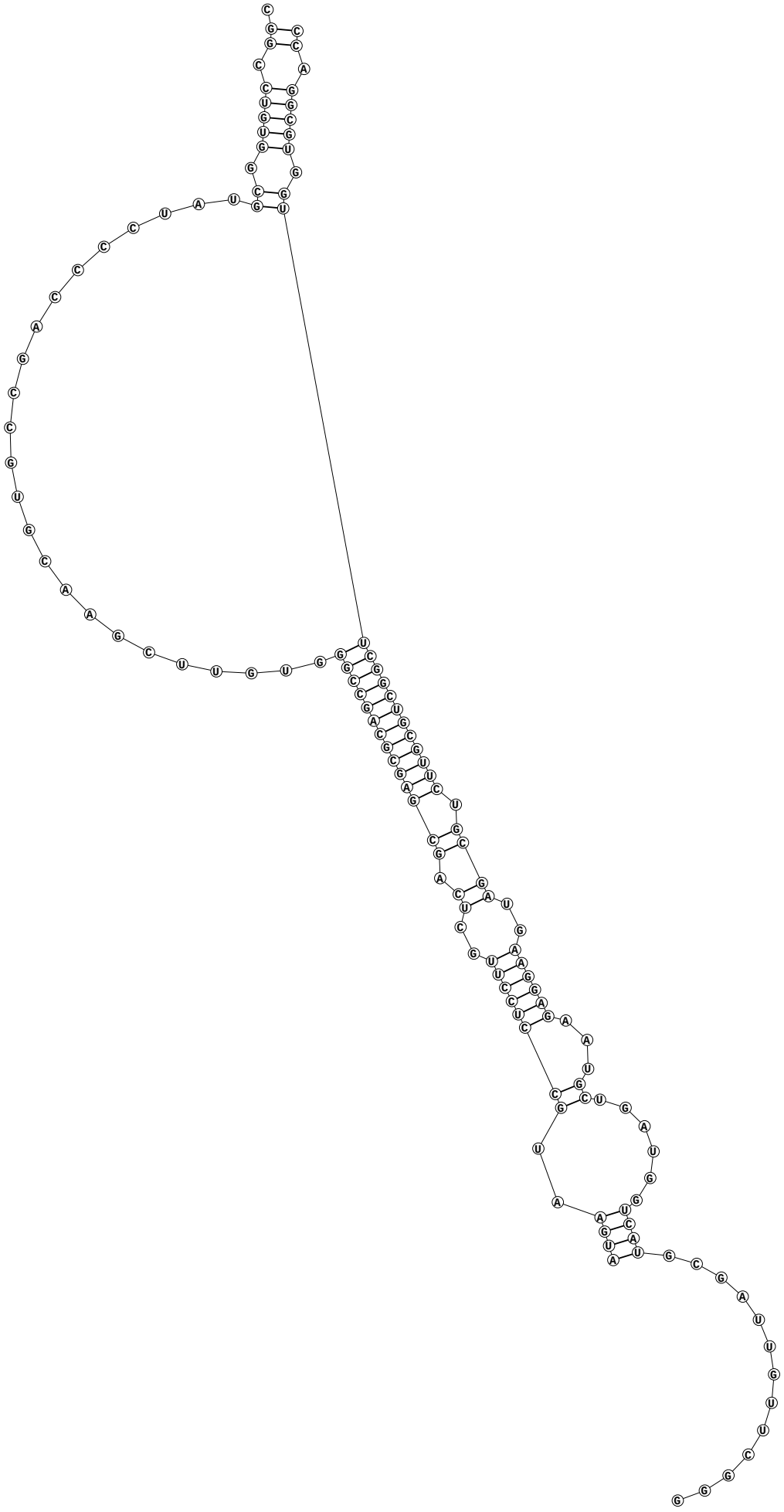

ENERGY = -41.2 xylS_ 6963