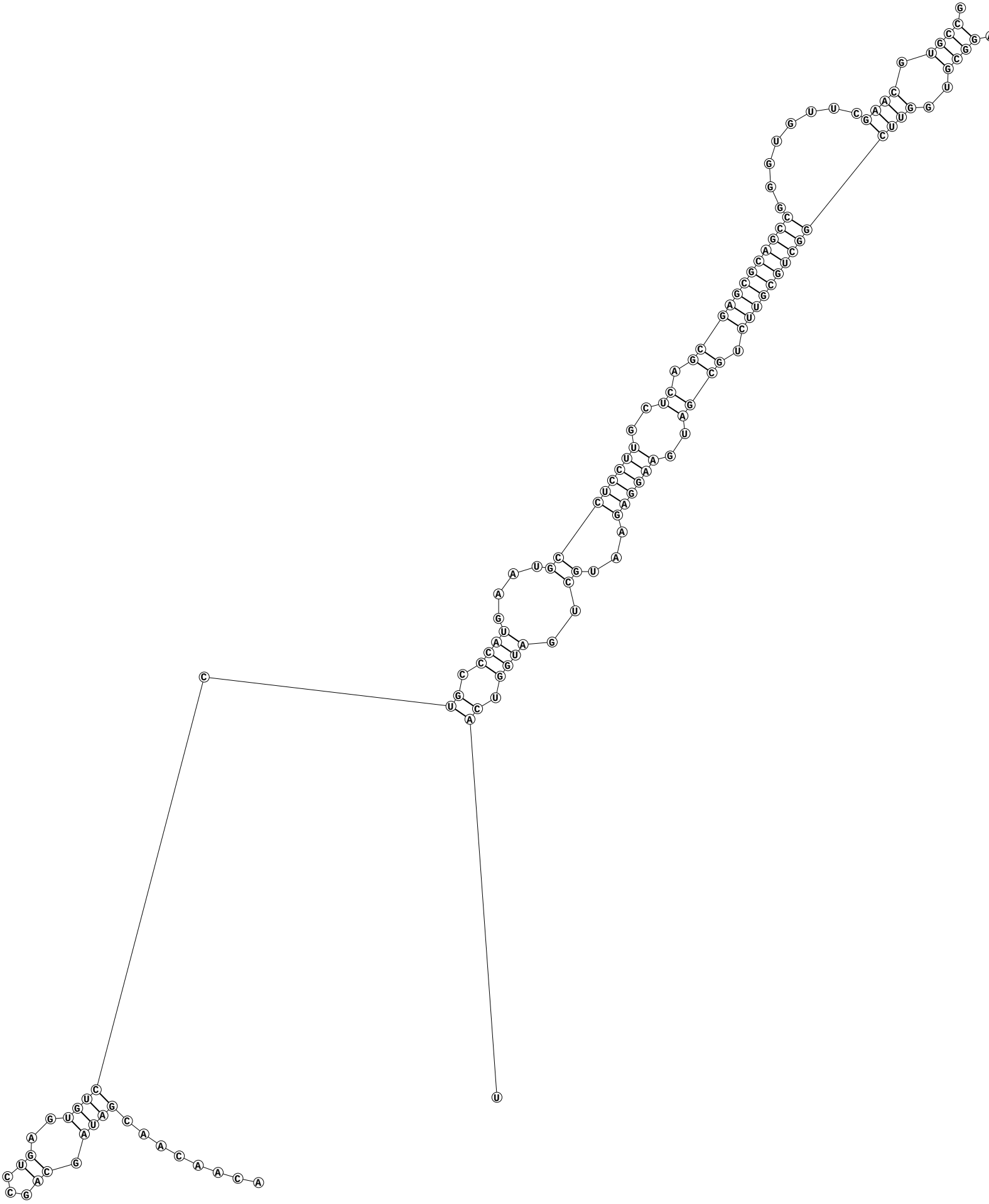

ENERGY = -47.5 xylS_ 6963