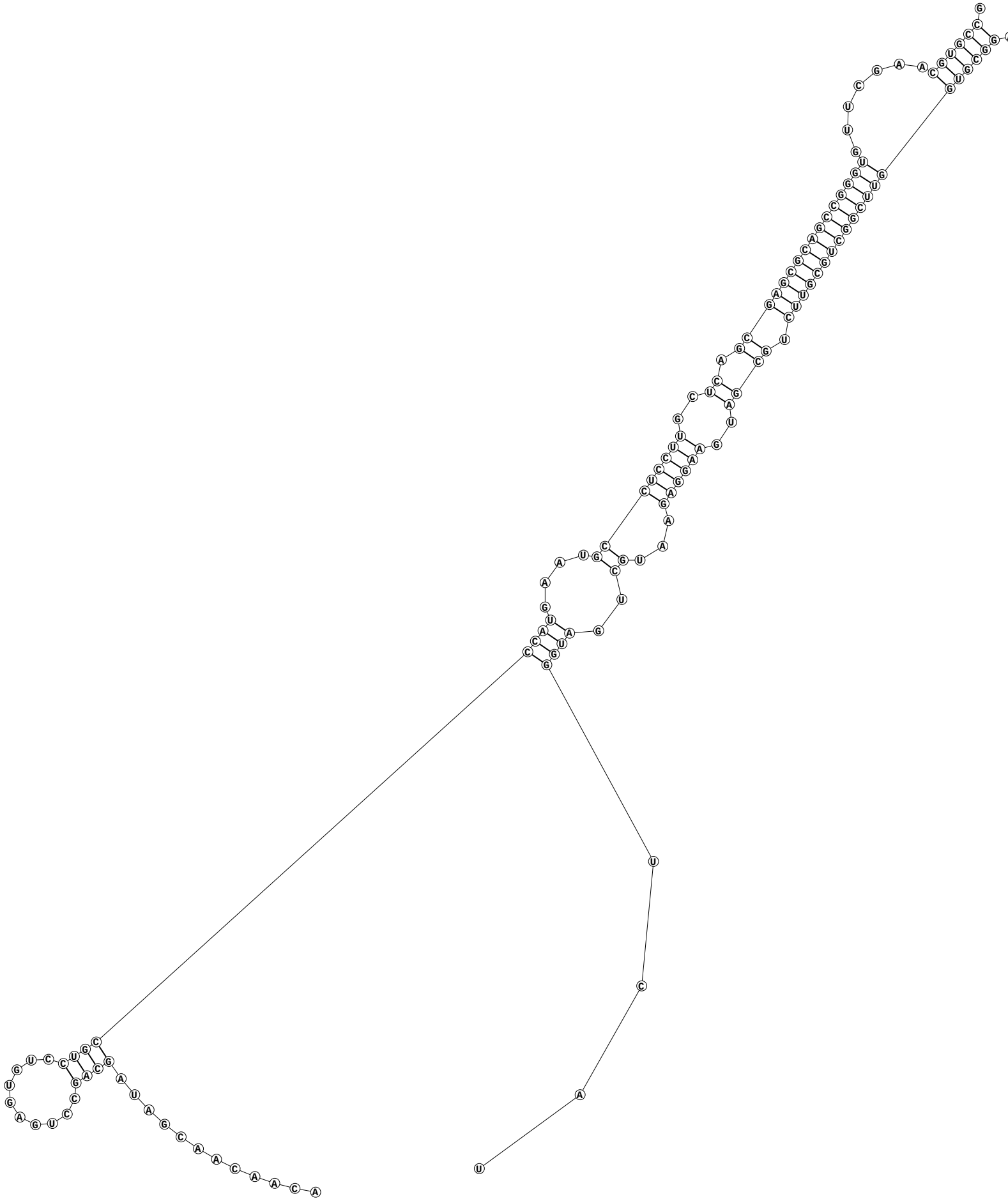

ENERGY = -48.3 xylS_ 6963