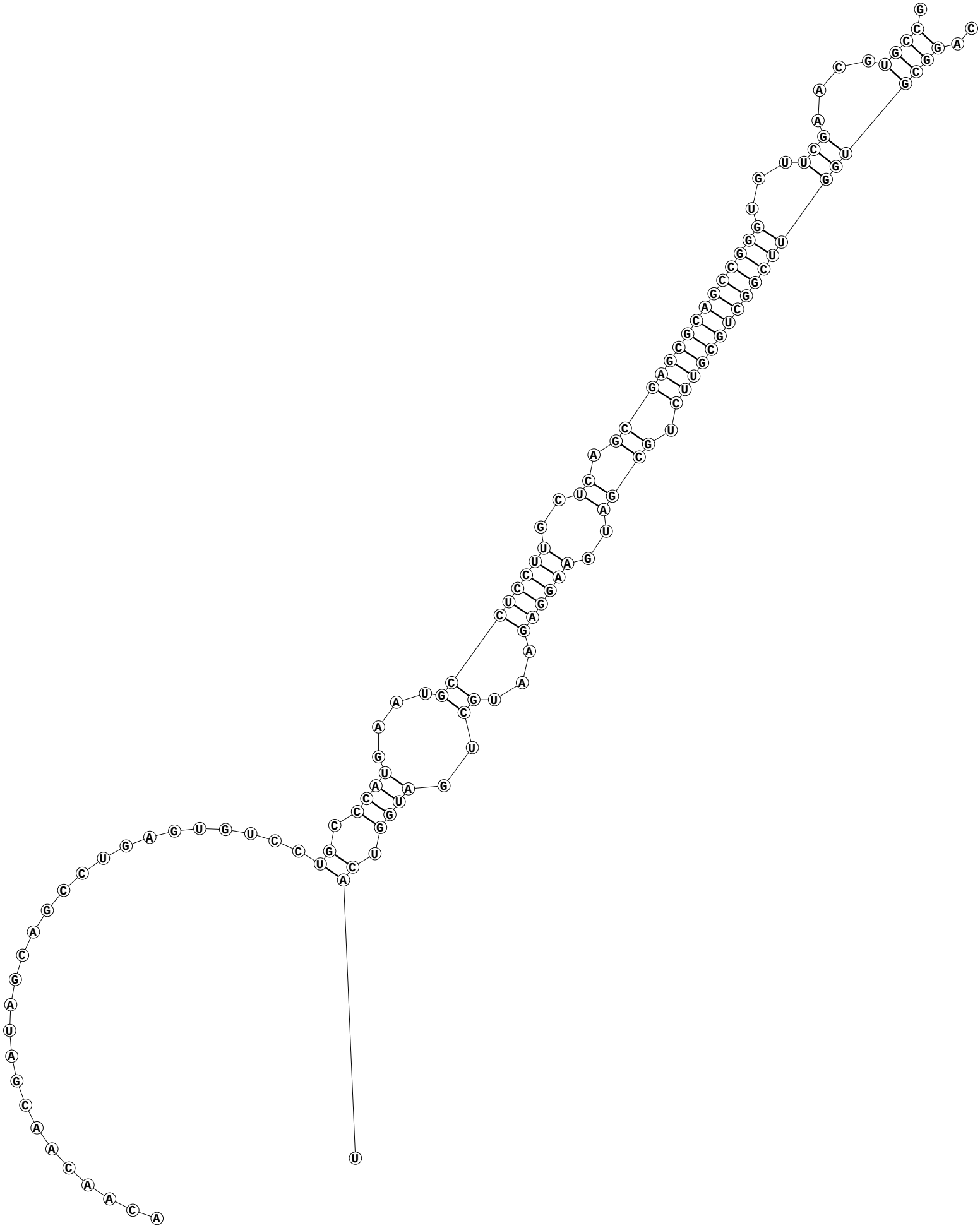

ENERGY = -45.2 xylS_ 6963