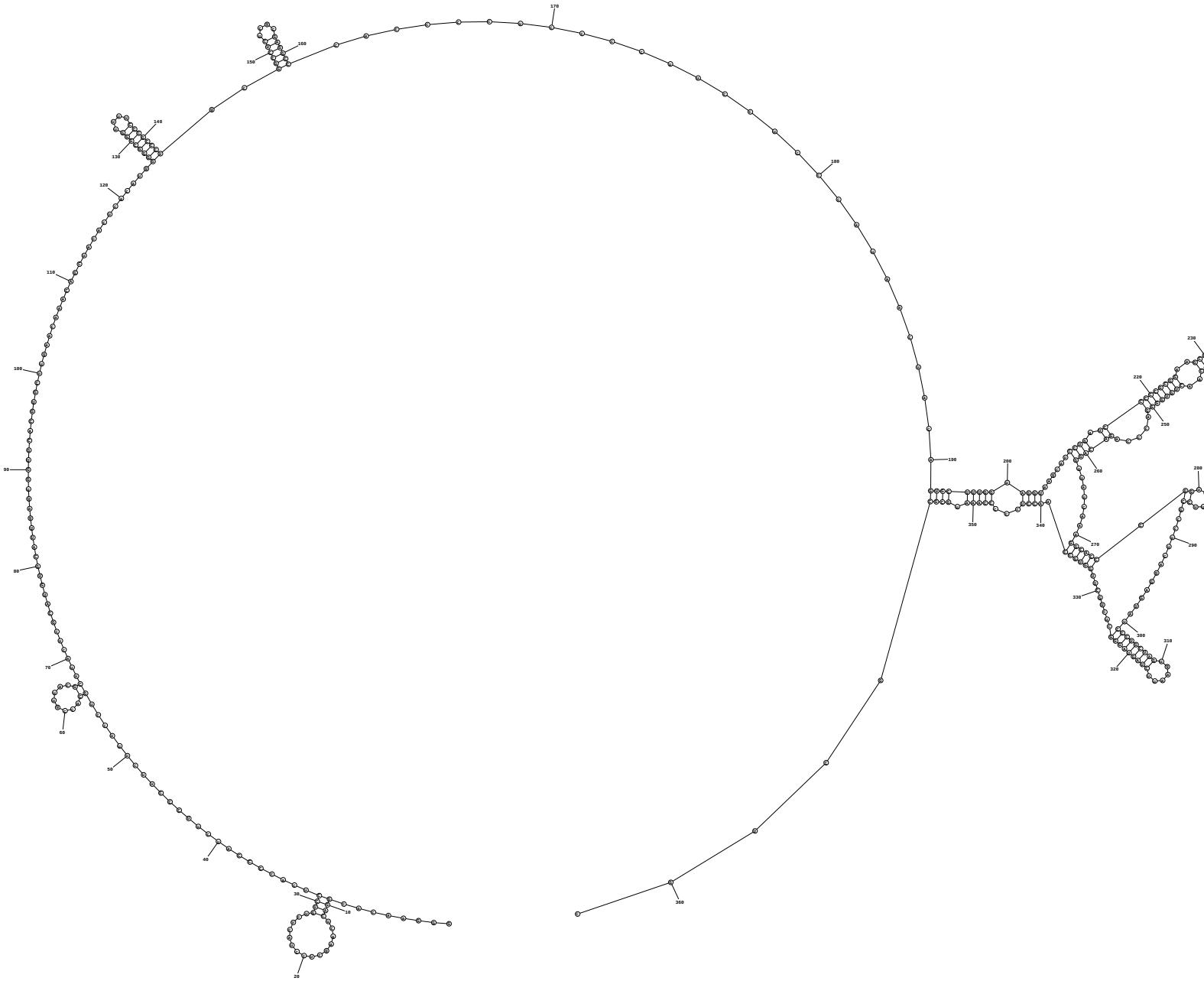

ENERGY = -112.1 rep.SFP.dot.s1.e361...