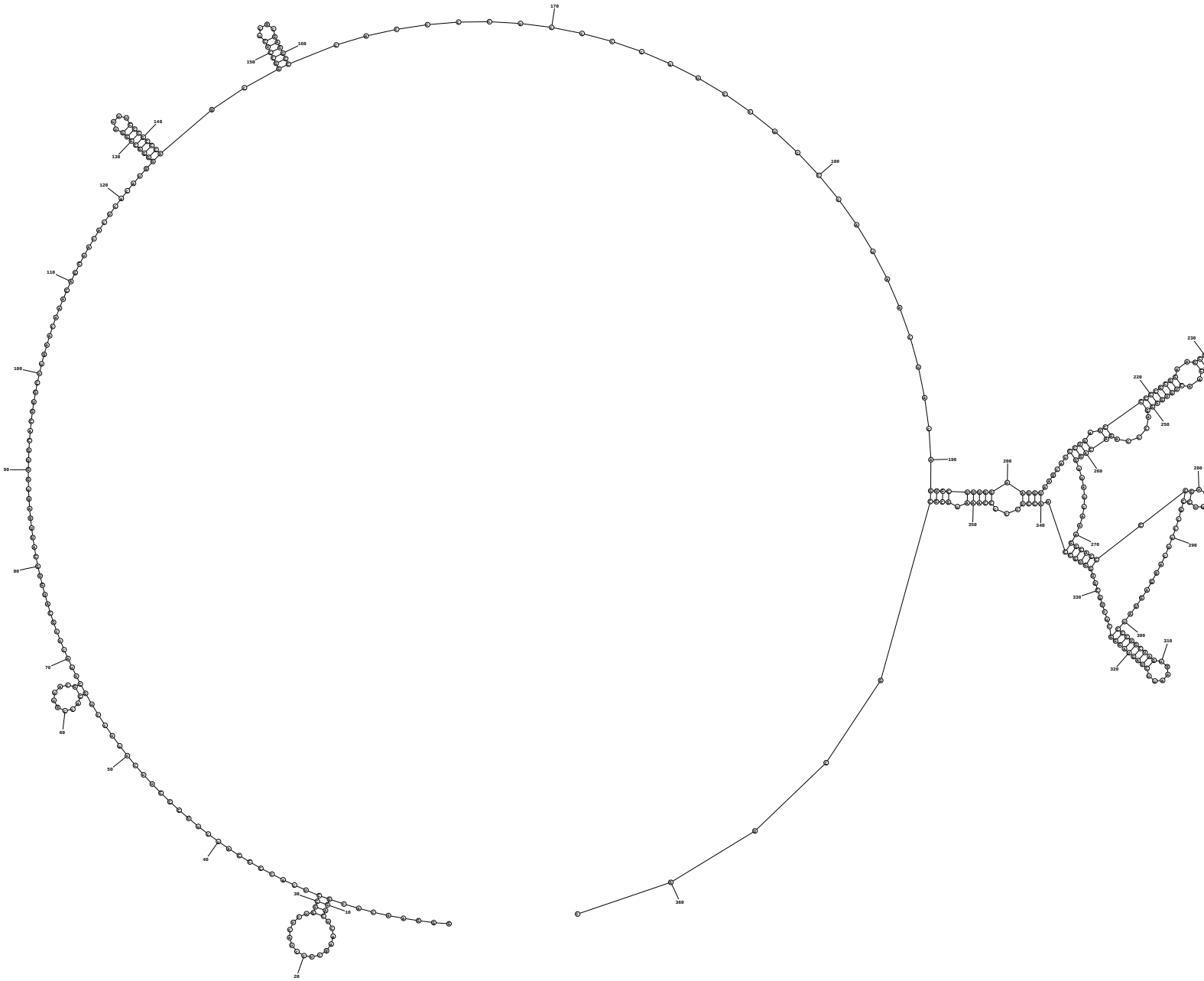

ENERGY = -111.3 rep.SFP.dot.s1.e361...