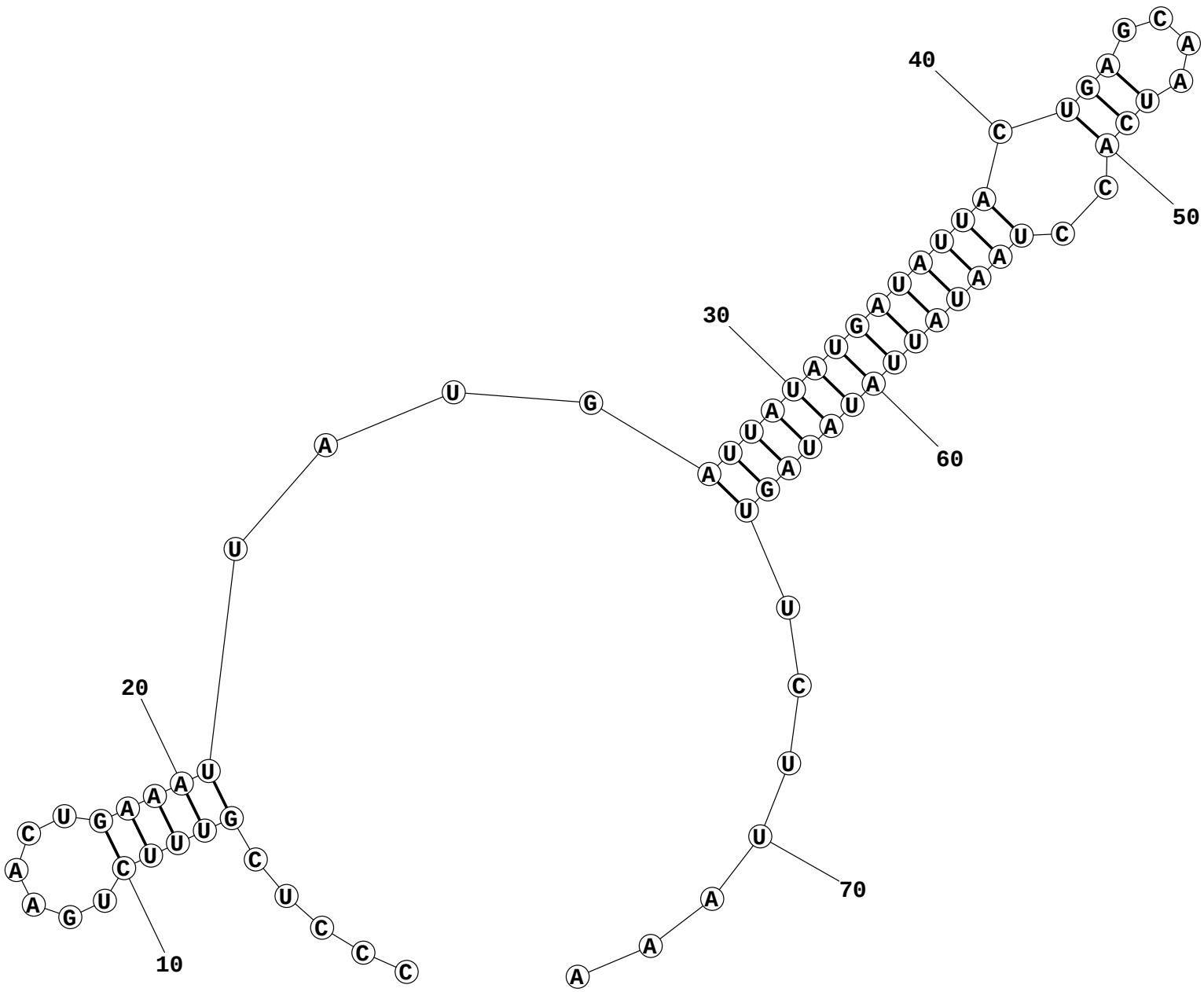

ENERGY = -13.8 P_simplex_TH_48_Paa_48