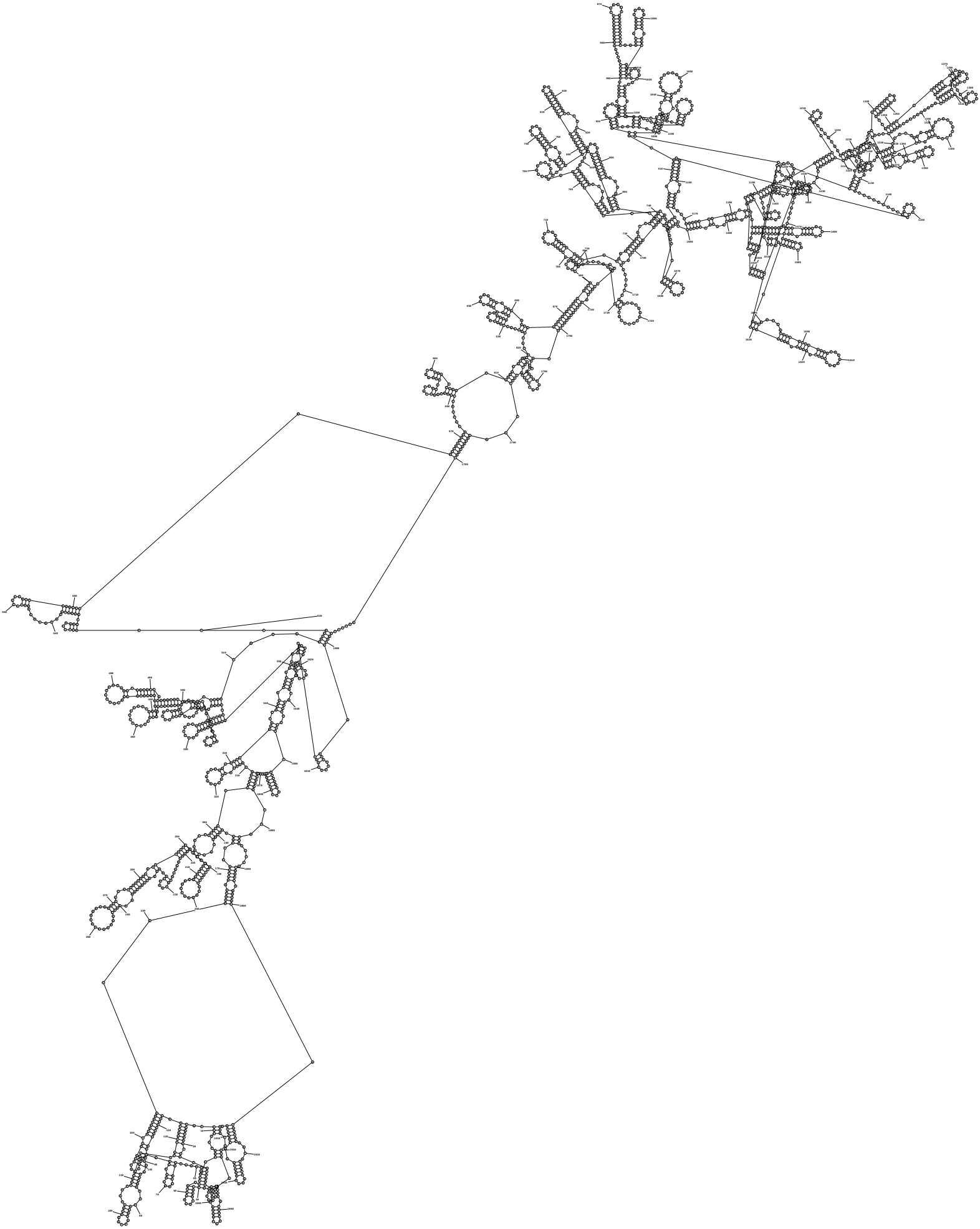

ENERGY = -332.1 gap