

**Probability  $\geq$  99%**

**99% > Probability  $\geq$  95%**

**95% > Probability  $\geq$  90%**

**90% > Probability  $\geq$  80%**

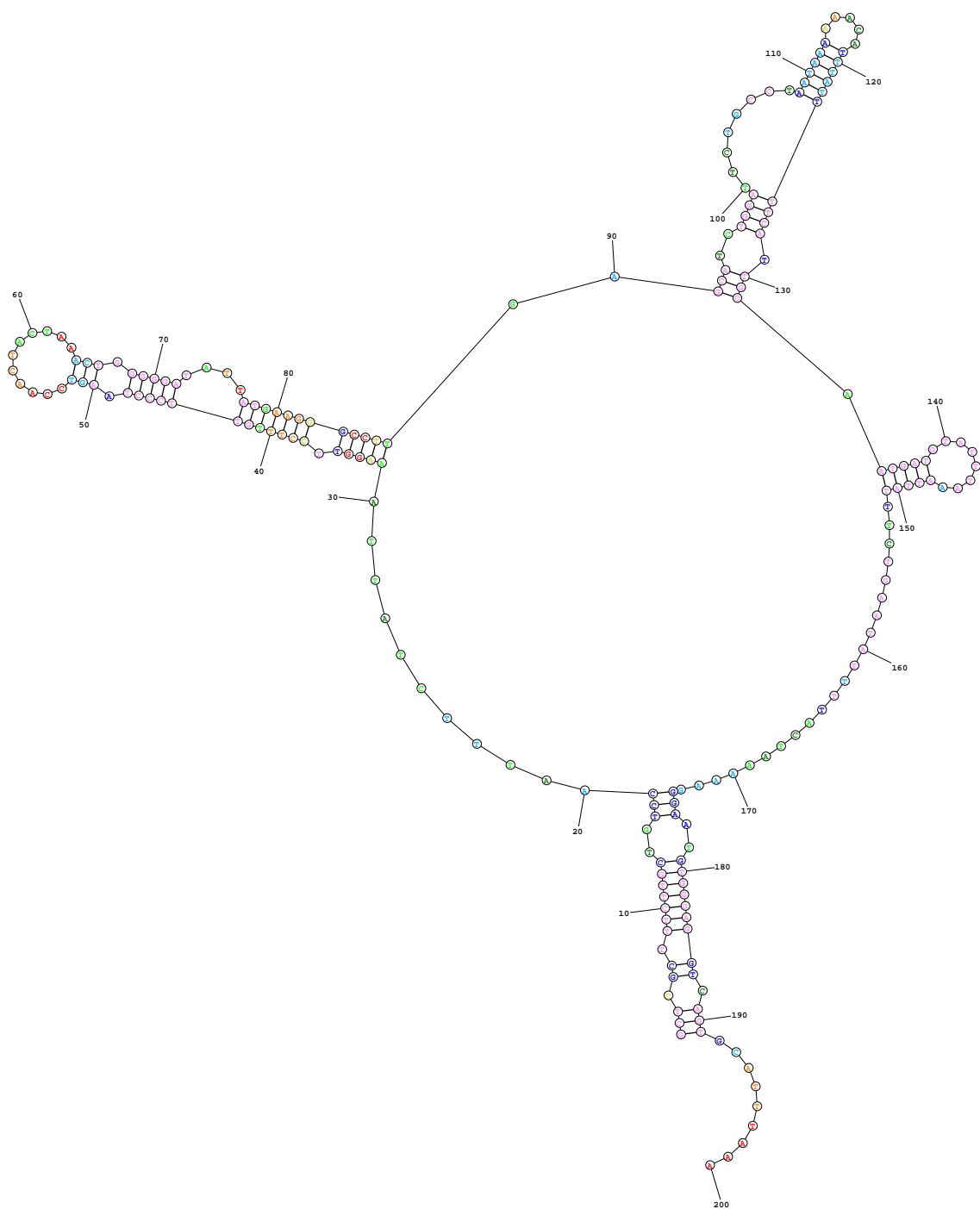
**80% > Probability  $\geq$  70%**

**70% > Probability  $\geq$  60%**

**60% > Probability  $\geq$  50%**

**50% > Probability**

**ENERGY = -37.1 kJ/mol**



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

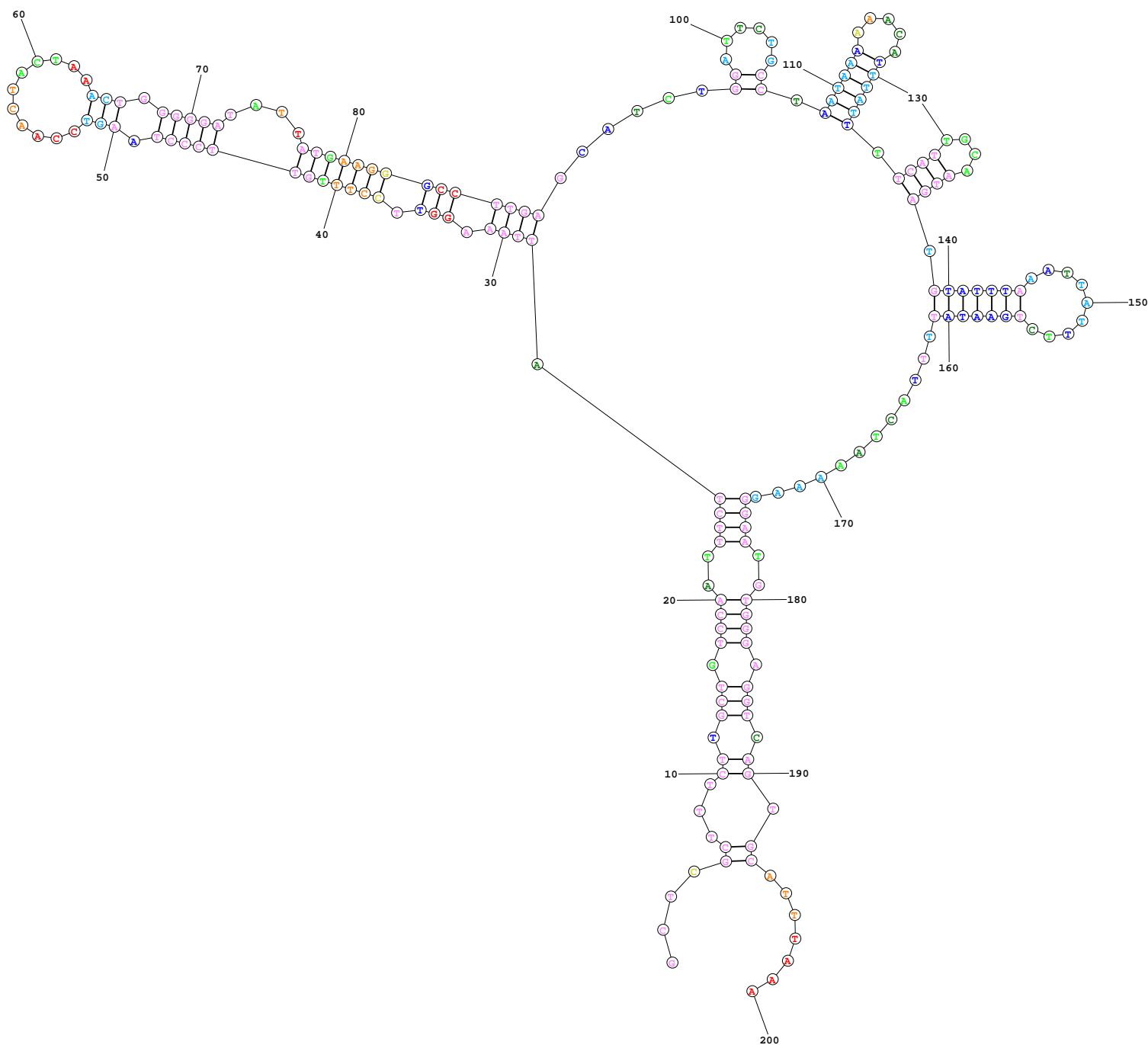
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -35.9 ,†-pA**



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

**80% > Probability >= 70%**

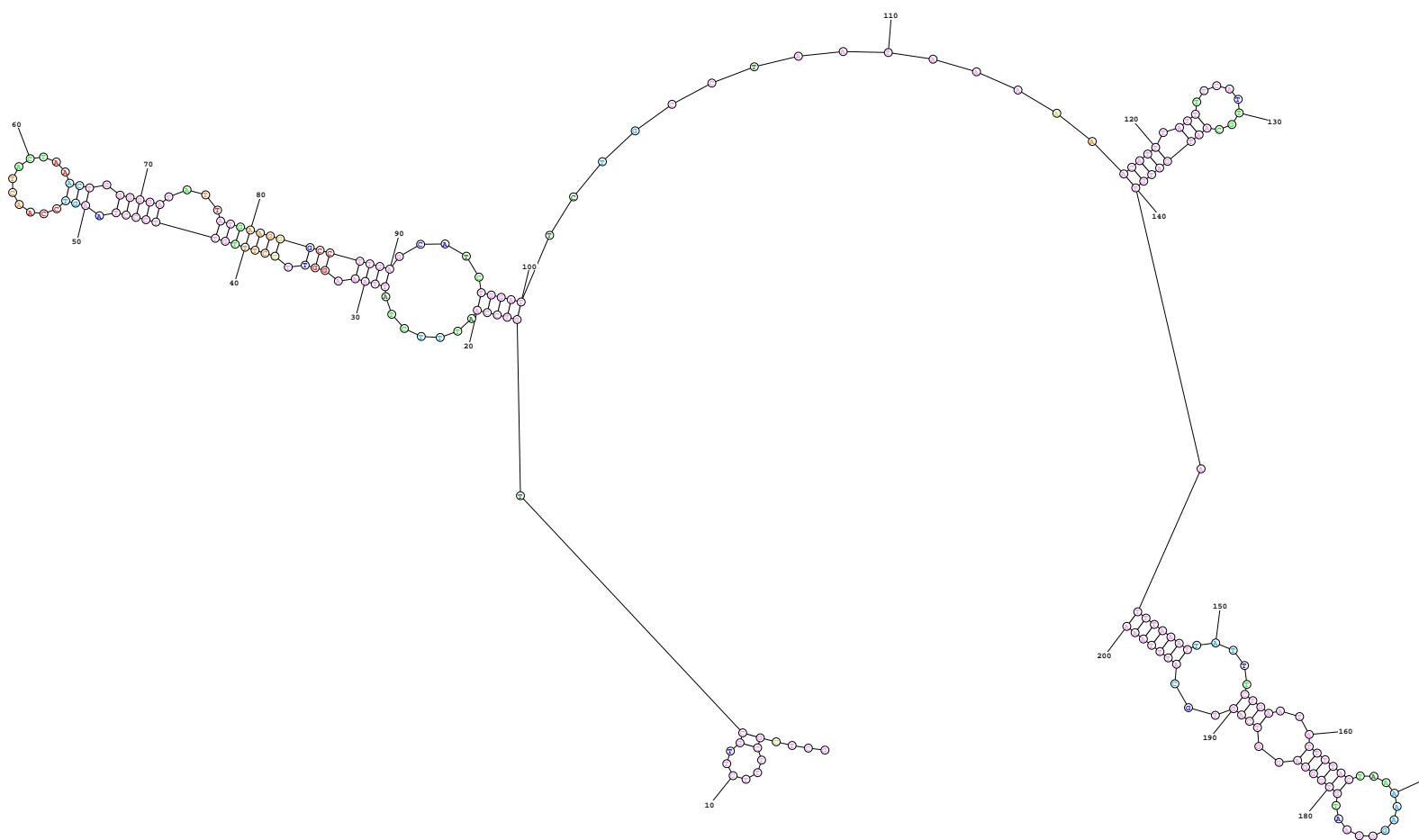
**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -35.9 ,†-pA**





**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

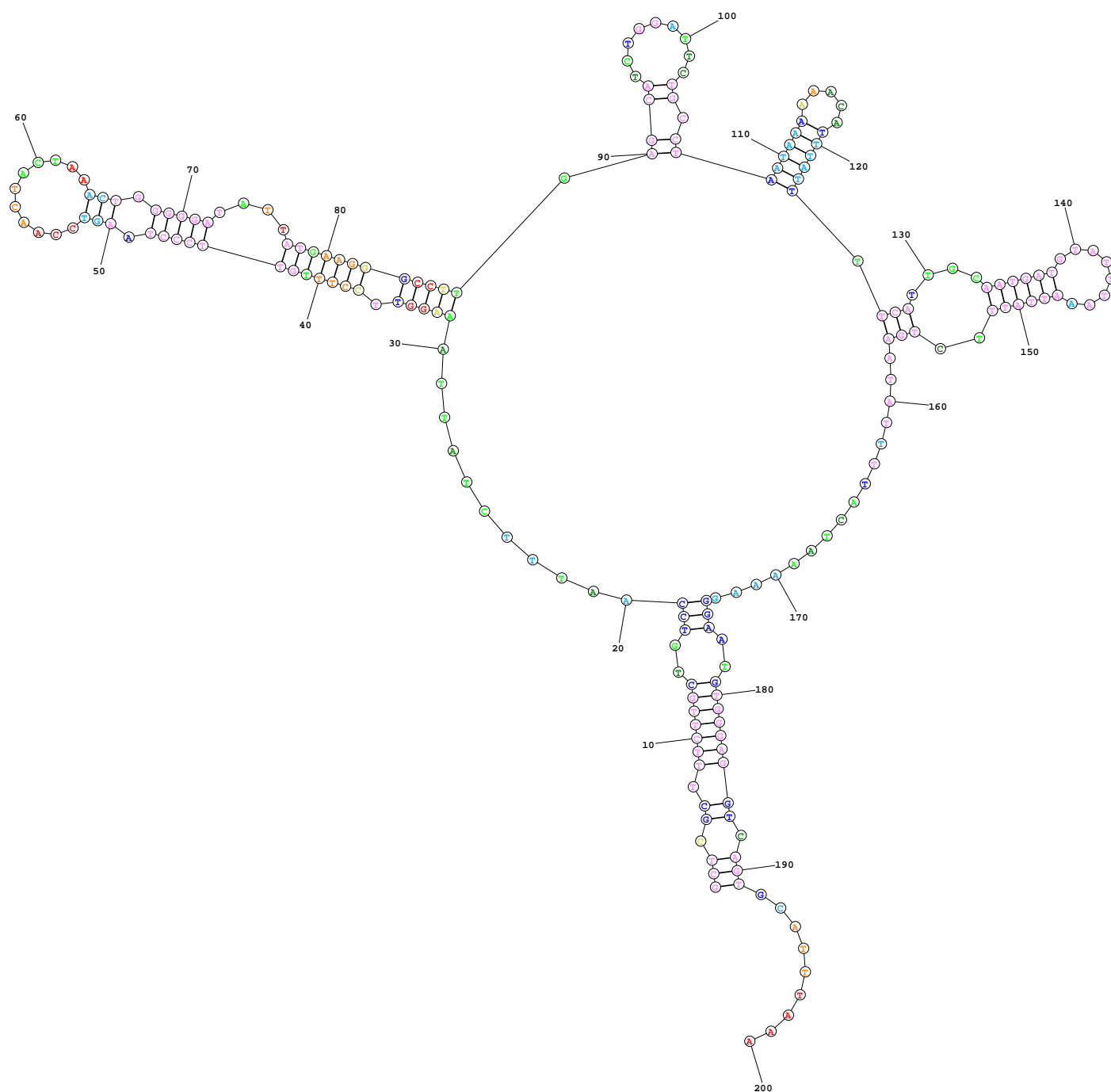
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -35.8 ,†-pA**



**Probability  $\geq$  99%**

**99% > Probability  $\geq$  95%**

**95% > Probability  $\geq$  90%**

**90% > Probability  $\geq$  80%**

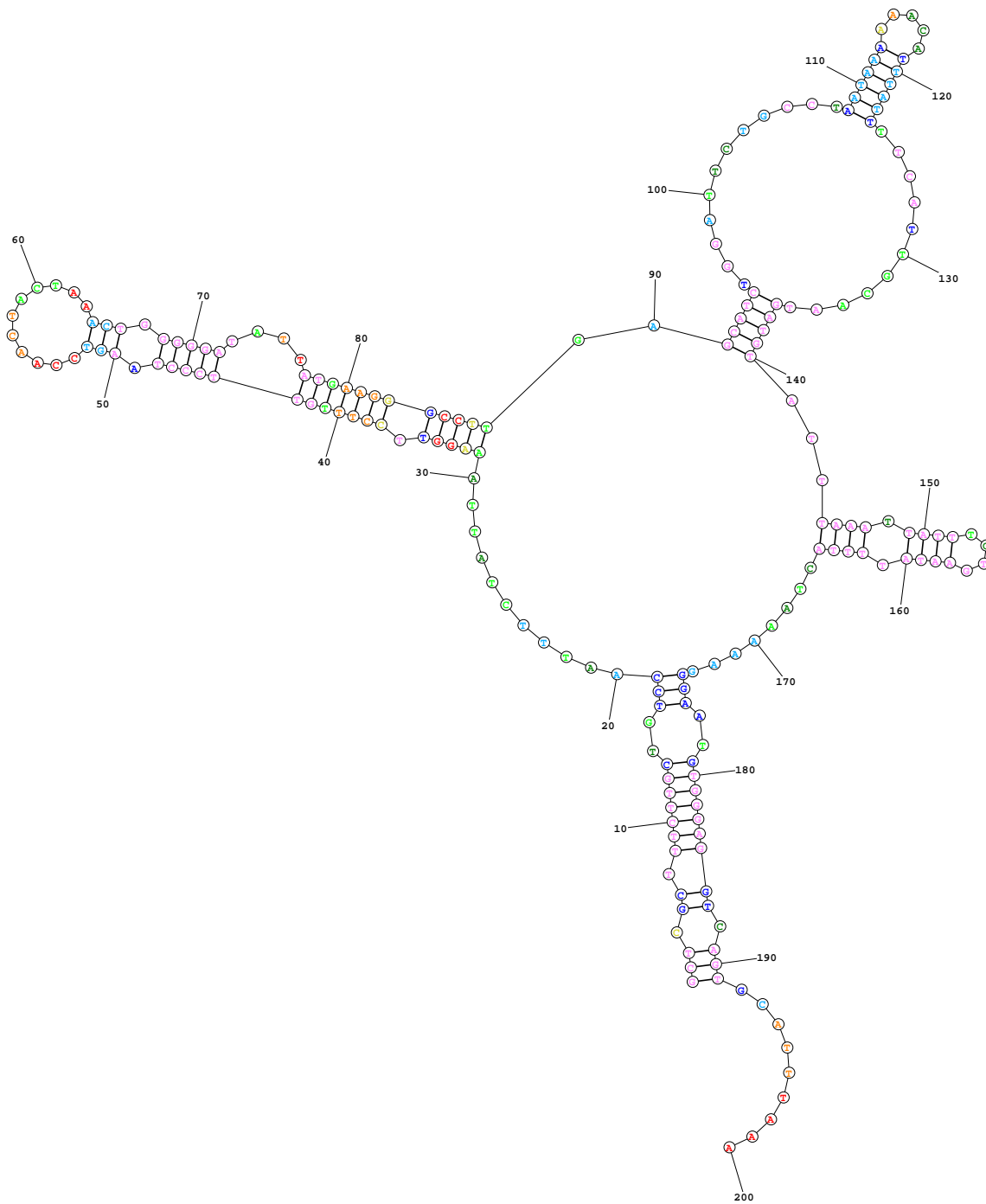
**80% > Probability  $\geq$  70%**

**70% > Probability  $\geq$  60%**

**60% > Probability  $\geq$  50%**

**50% > Probability**

**ENERGY = -35.6 ,†-pA**



**Probability  $\geq$  99%**

**99% > Probability  $\geq$  95%**

**95% > Probability  $\geq$  90%**

**90% > Probability  $\geq$  80%**

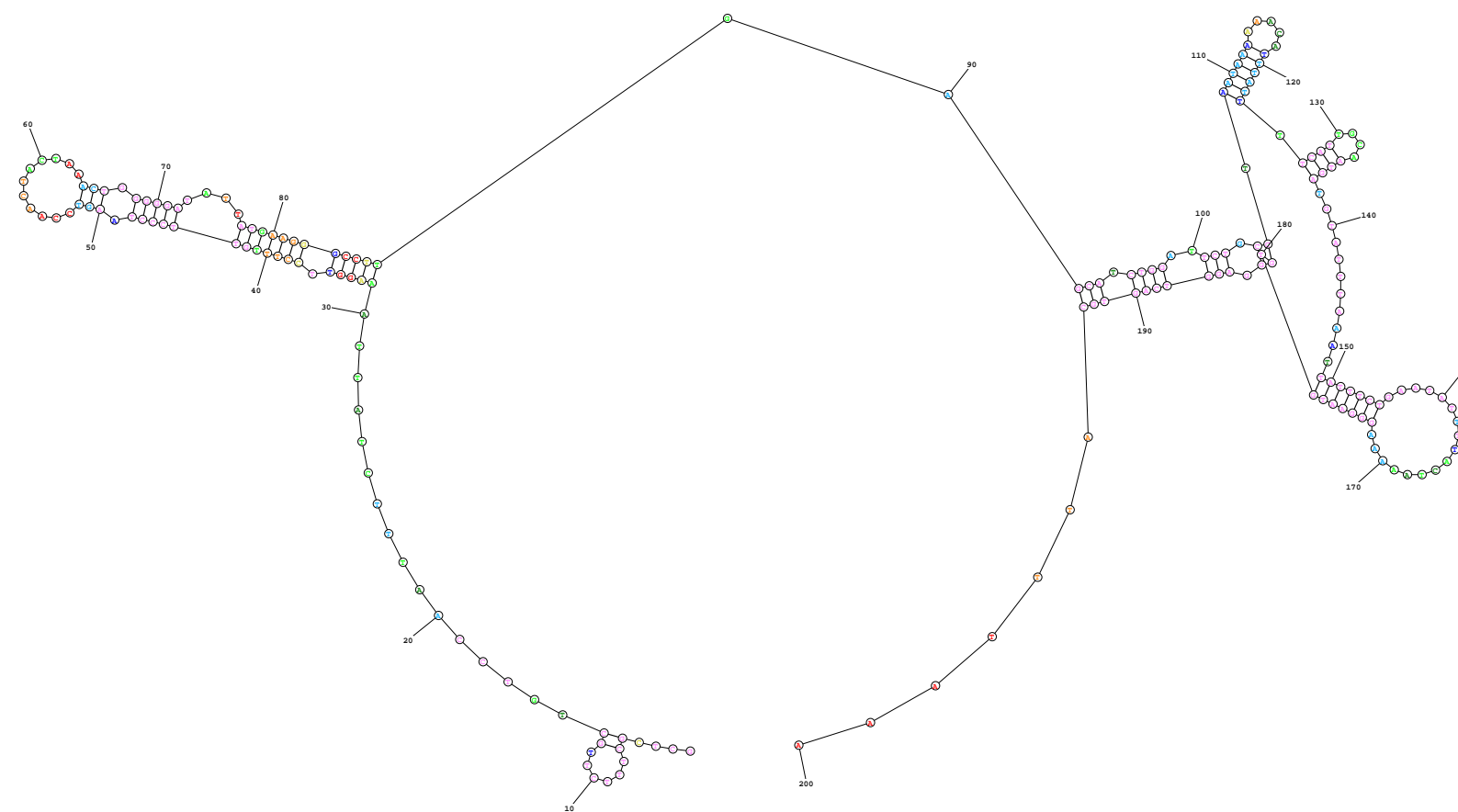
**80% > Probability  $\geq$  70%**

**70% > Probability  $\geq$  60%**

**60% > Probability  $\geq$  50%**

**50% > Probability**

**ENERGY = -35.6 kJ/mol**



**Probability**  $\geq$  99%

99%  $>$  **Probability**  $\geq$  95%

95%  $>$  **Probability**  $\geq$  90%

90%  $>$  **Probability**  $\geq$  80%

80%  $>$  **Probability**  $\geq$  70%

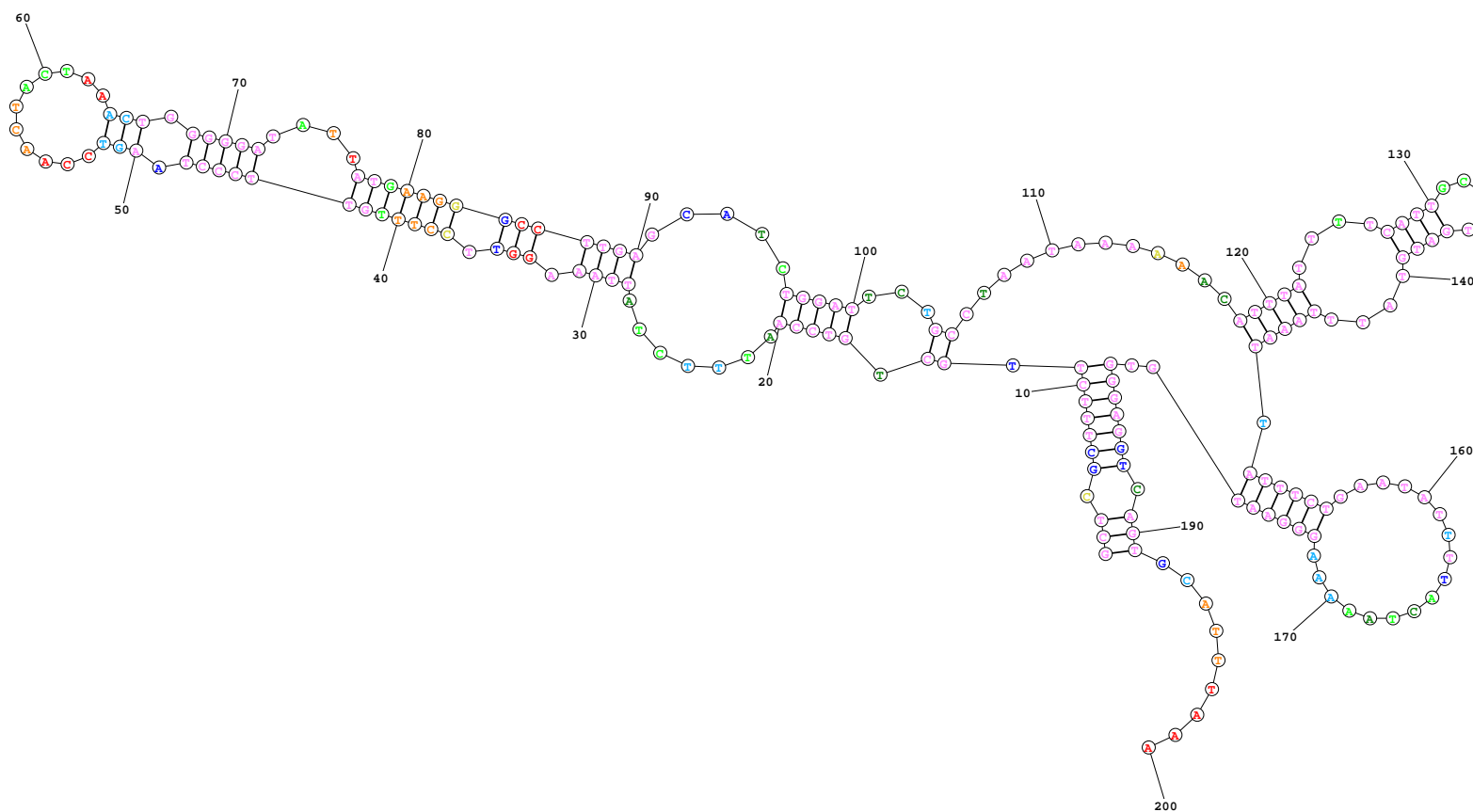
70%  $>$  **Probability**  $\geq$  60%

60%  $>$  **Probability**  $\geq$  50%

50%  $>$  **Probability**

**ENERGY** = -35.6  $\mu$ t-pA





**Probability**  $\geq$  99%

99% > **Probability**  $\geq$  95%

95% > **Probability**  $\geq$  90%

90% > **Probability**  $\geq$  80%

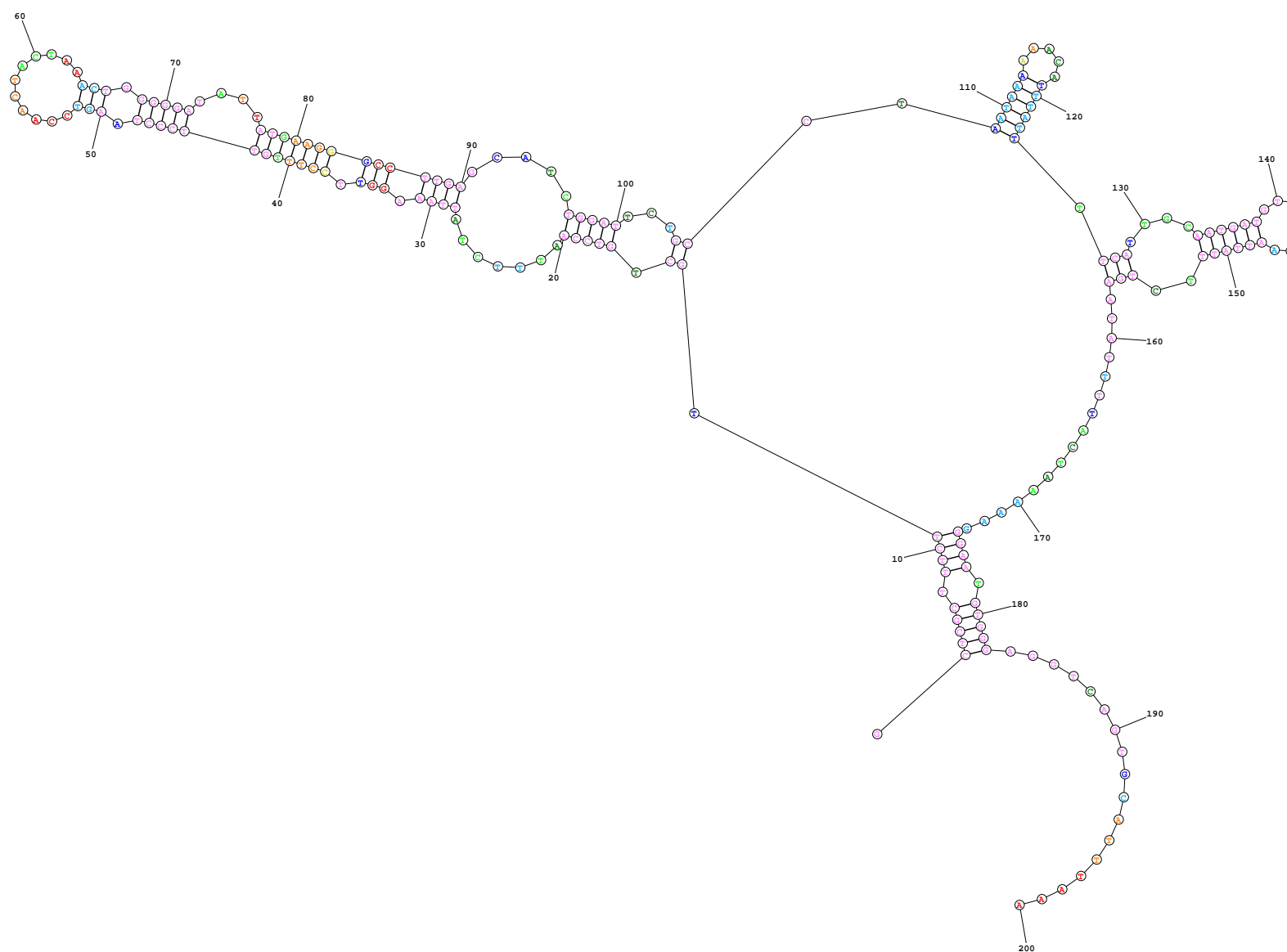
80% > **Probability**  $\geq$  70%

70% > **Probability**  $\geq$  60%

60% > **Probability**  $\geq$  50%

50% > **Probability**

**ENERGY** = -35.5  $\mu$ †-pA



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

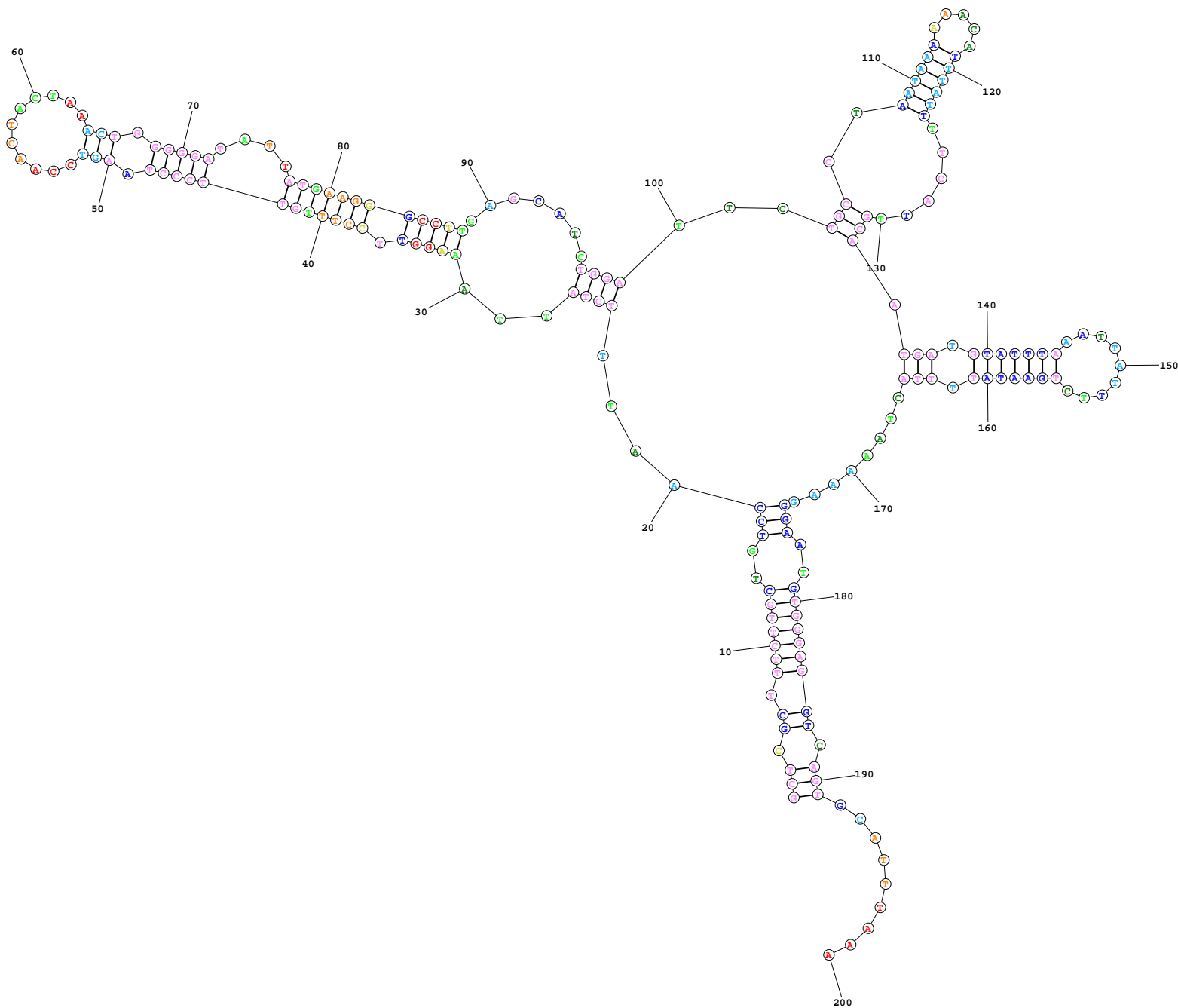
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -35.3 ,†-pA**



**Probability  $\geq$  99%**

**99% > Probability  $\geq$  95%**

**95% > Probability  $\geq$  90%**

**90% > Probability  $\geq$  80%**

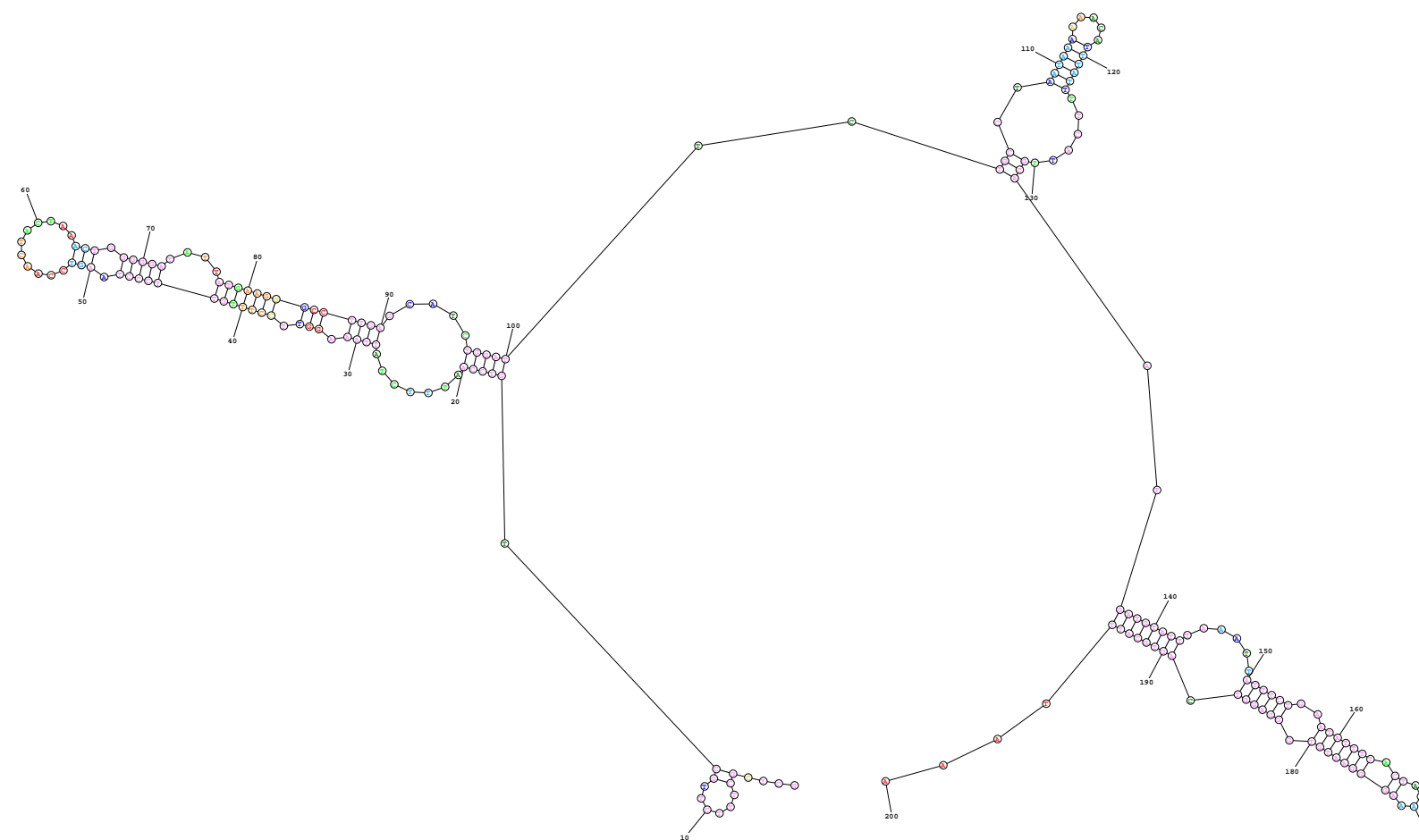
**80% > Probability  $\geq$  70%**

**70% > Probability  $\geq$  60%**

**60% > Probability  $\geq$  50%**

**50% > Probability**

**ENERGY = -35.1 kJ/mol**



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

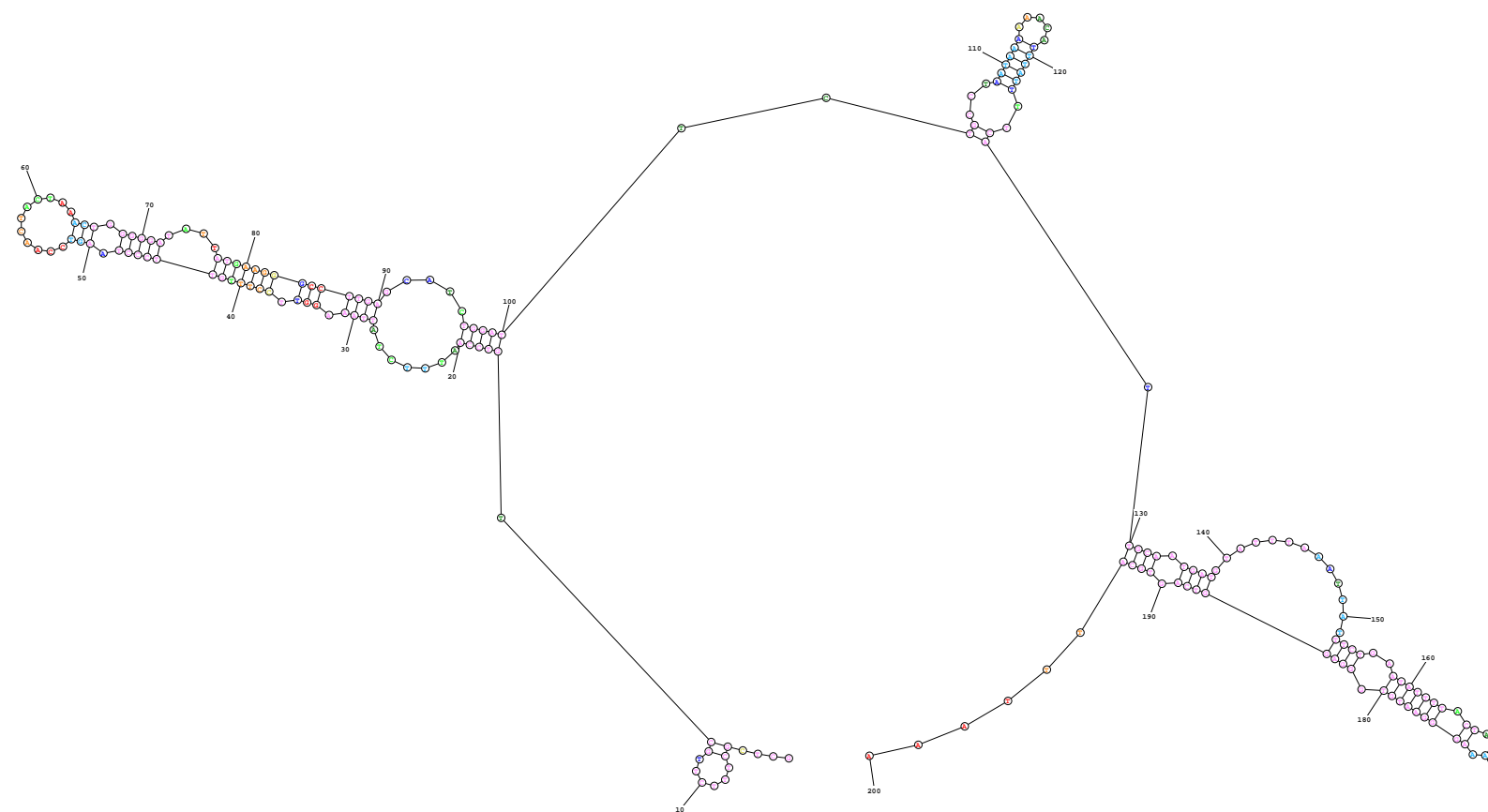
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -35.1 ,†-pA**



**Probability**  $\geq$  99%

99%  $>$  **Probability**  $\geq$  95%

95%  $>$  **Probability**  $\geq$  90%

90%  $>$  **Probability**  $\geq$  80%

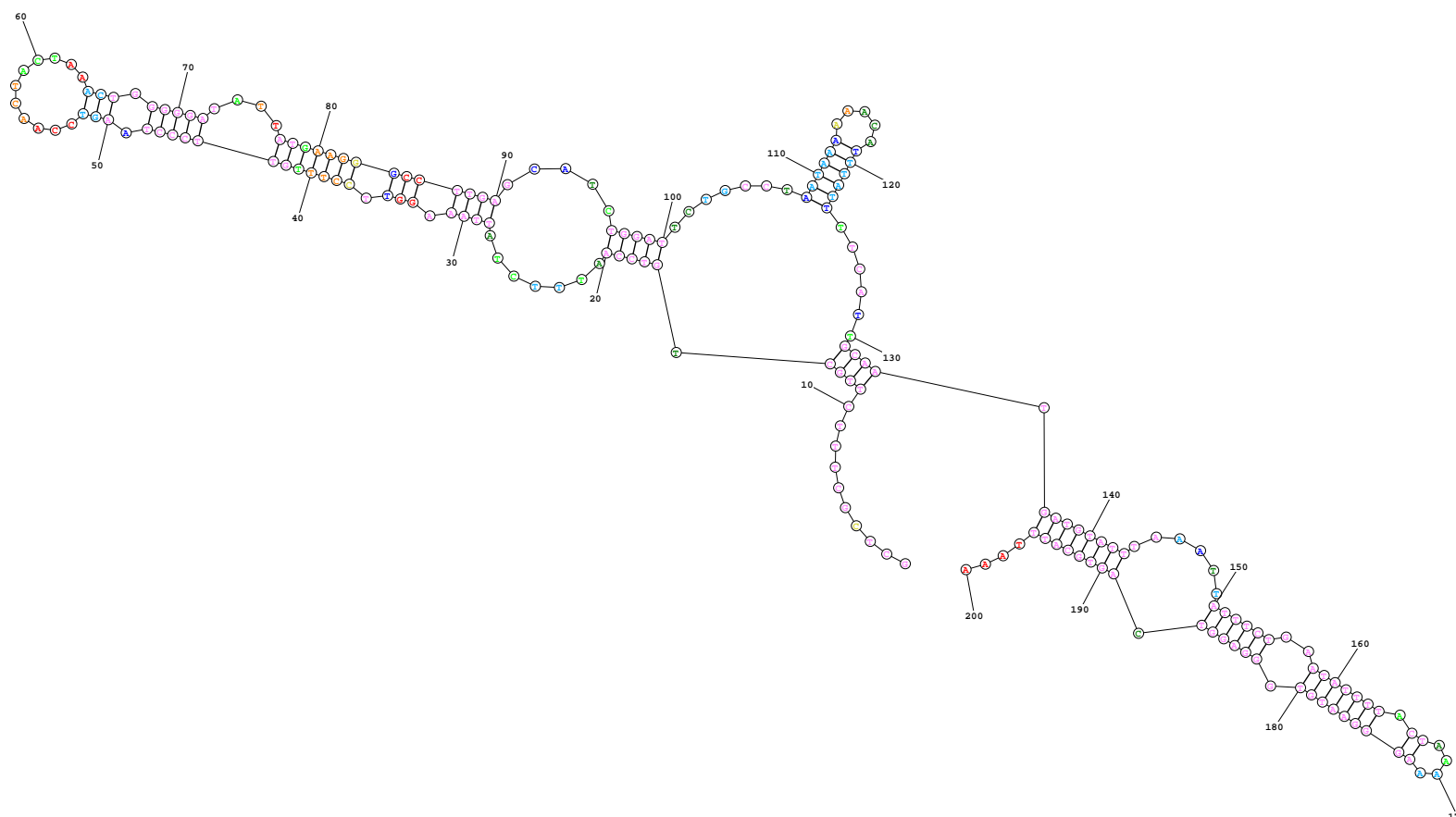
80%  $>$  **Probability**  $\geq$  70%

70%  $>$  **Probability**  $\geq$  60%

60%  $>$  **Probability**  $\geq$  50%

50%  $>$  **Probability**

**ENERGY** = -35.0  $\mu$ t-pA



**Probability**  $\geq$  **99%**

**99%**  $>$  **Probability**  $\geq$  **95%**

**95%**  $>$  **Probability**  $\geq$  **90%**

**90%**  $>$  **Probability**  $\geq$  **80%**

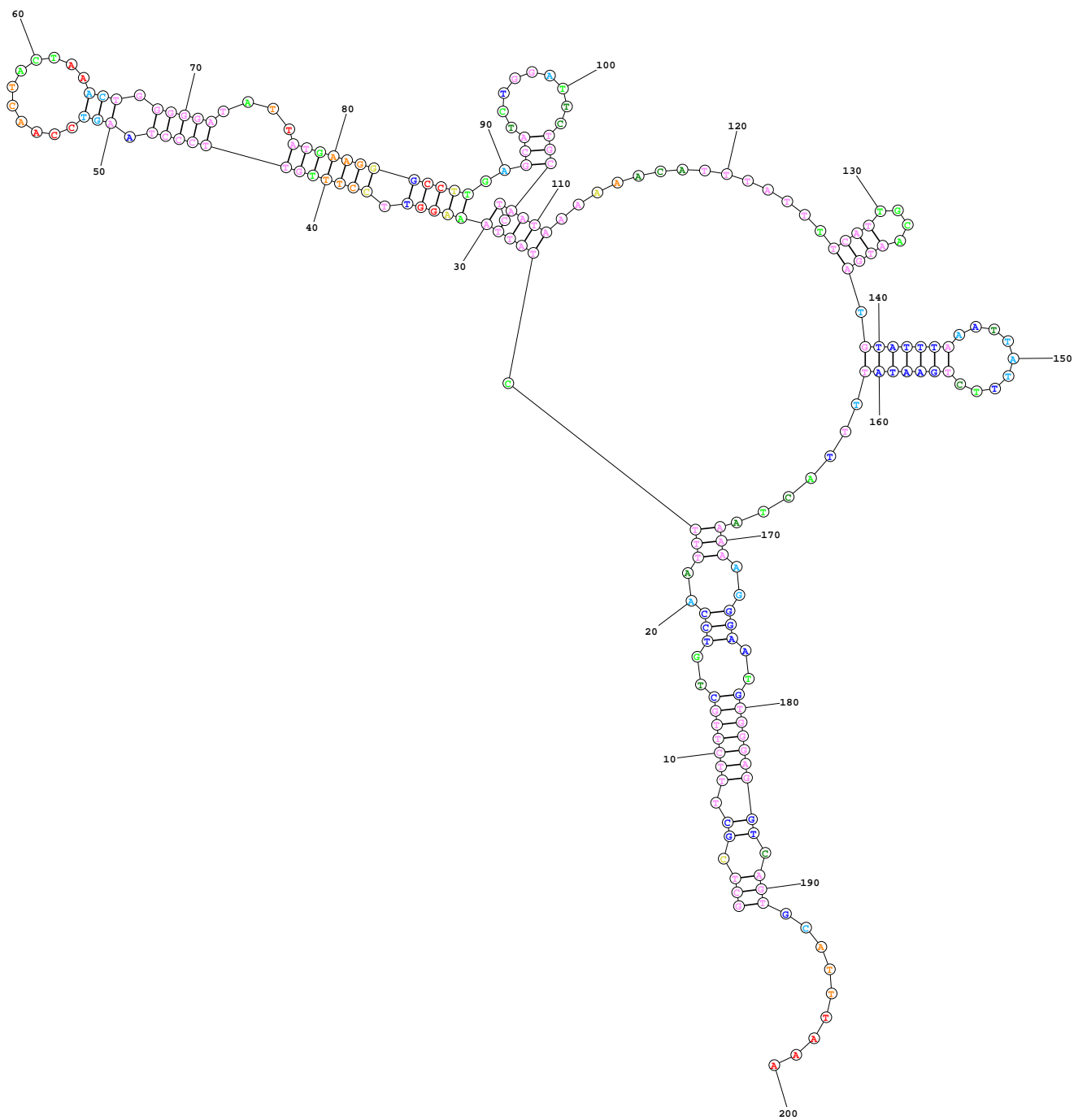
**80%**  $>$  **Probability**  $\geq$  **70%**

**70%**  $>$  **Probability**  $\geq$  **60%**

**60%**  $>$  **Probability**  $\geq$  **50%**

**50%**  $>$  **Probability**

**ENERGY** = **-34.5** ,†-pA



**Probability**  $\geq$  99%

99%  $>$  **Probability**  $\geq$  95%

95%  $>$  **Probability**  $\geq$  90%

90%  $>$  **Probability**  $\geq$  80%

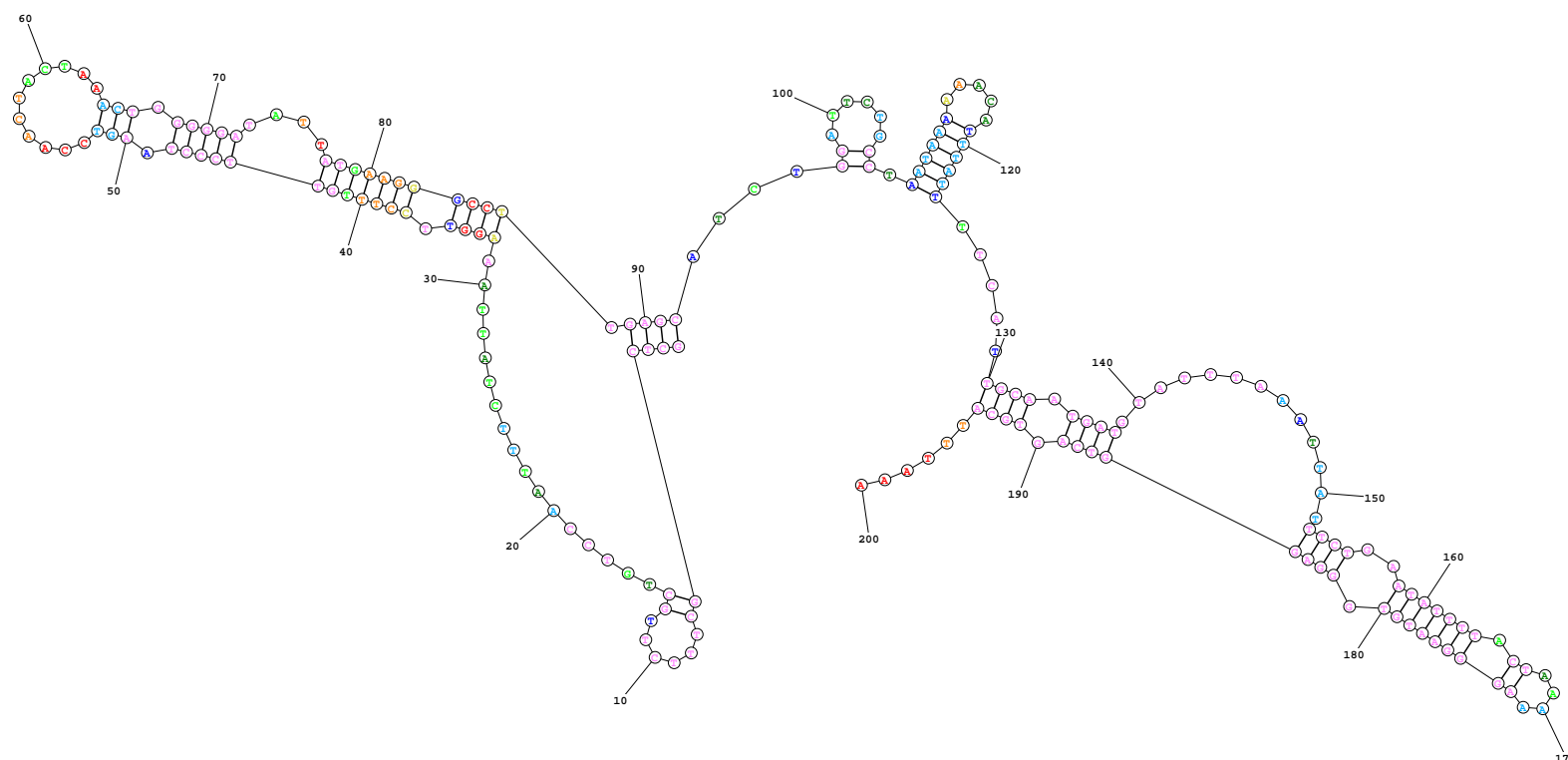
80%  $>$  **Probability**  $\geq$  70%

70%  $>$  **Probability**  $\geq$  60%

60%  $>$  **Probability**  $\geq$  50%

50%  $>$  **Probability**

**ENERGY** = -34.2 kJ/mol



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

**80% > Probability >= 70%**

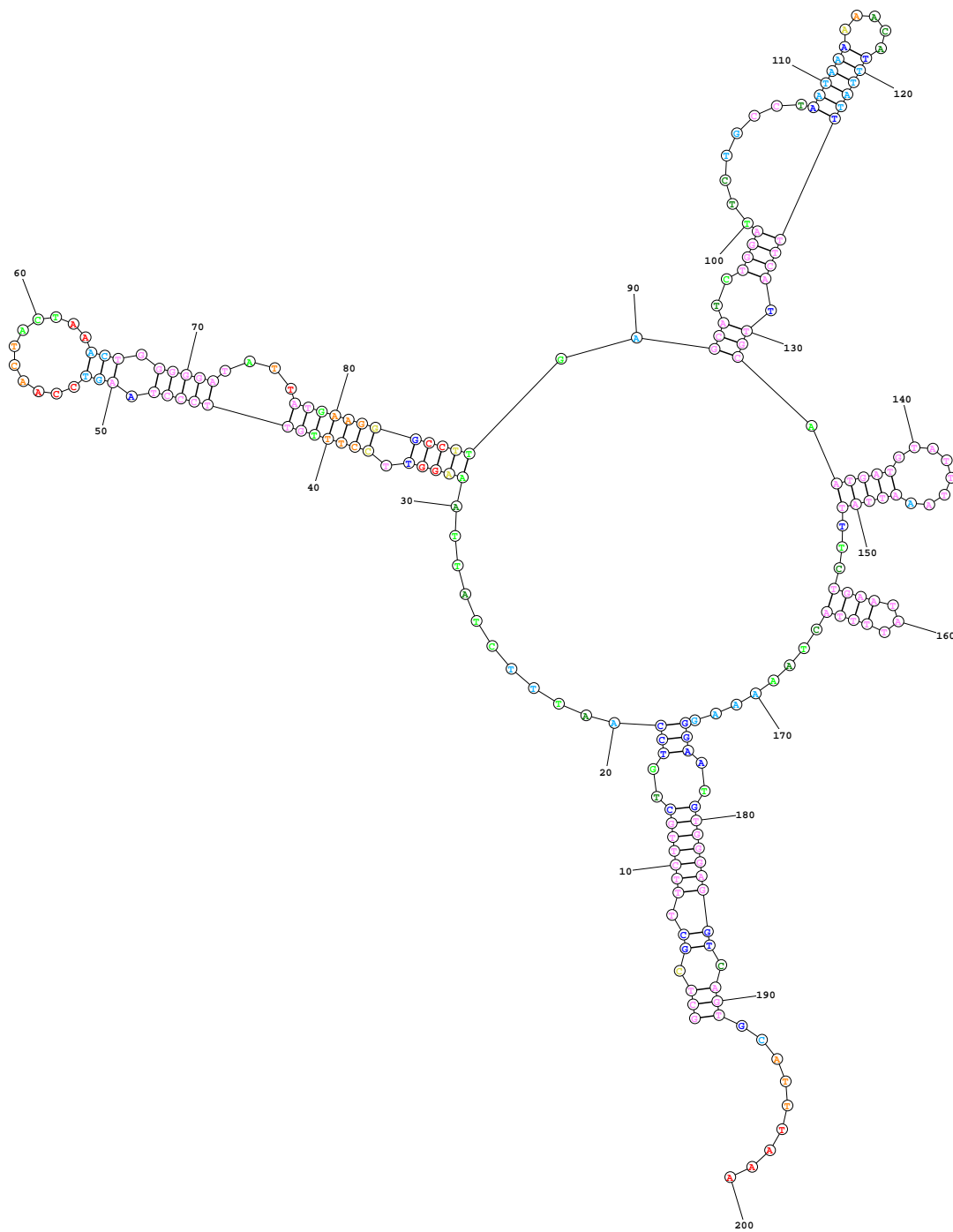
**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -34.2 ,†-pA**





**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

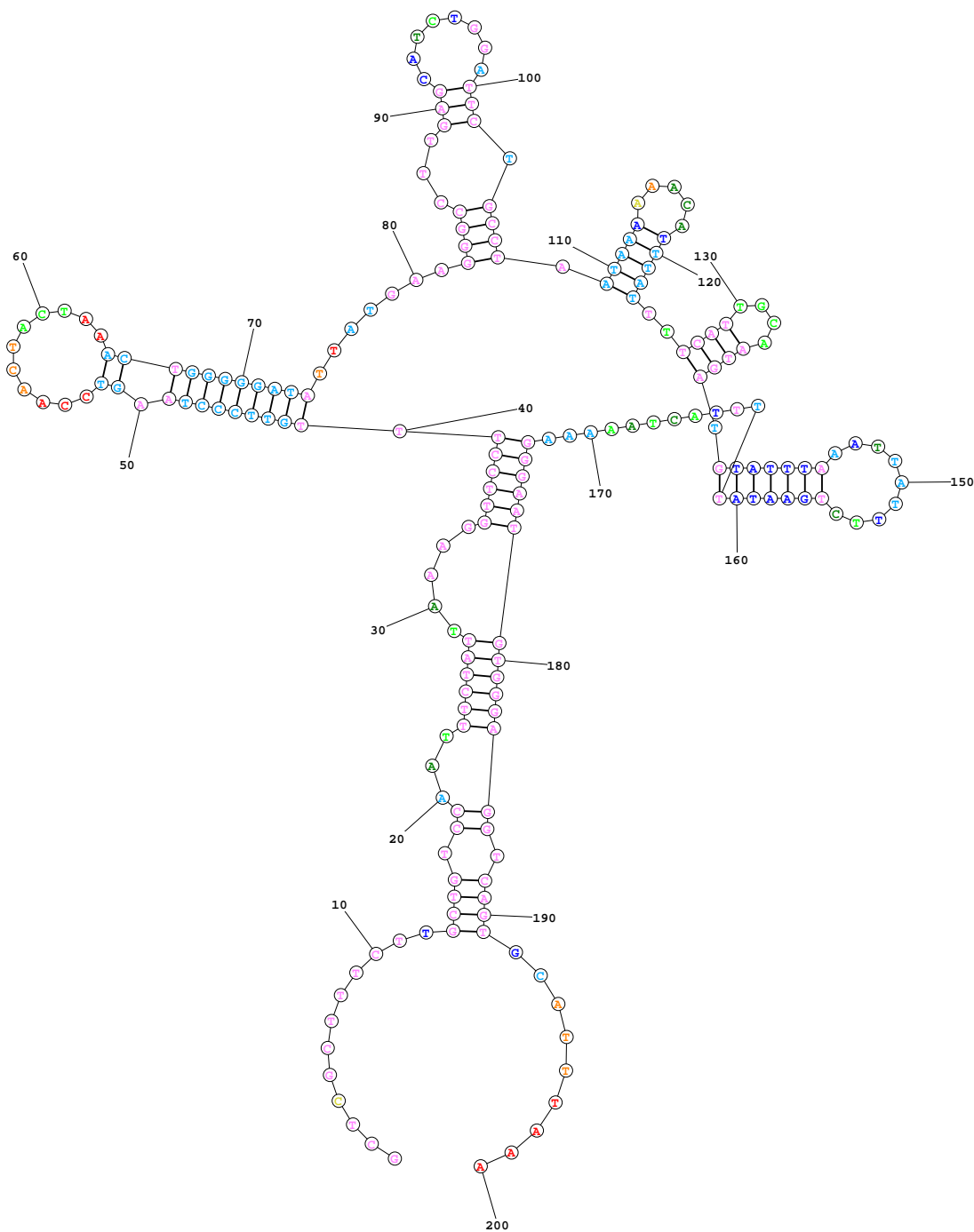
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -34.0 kJ/mol**



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

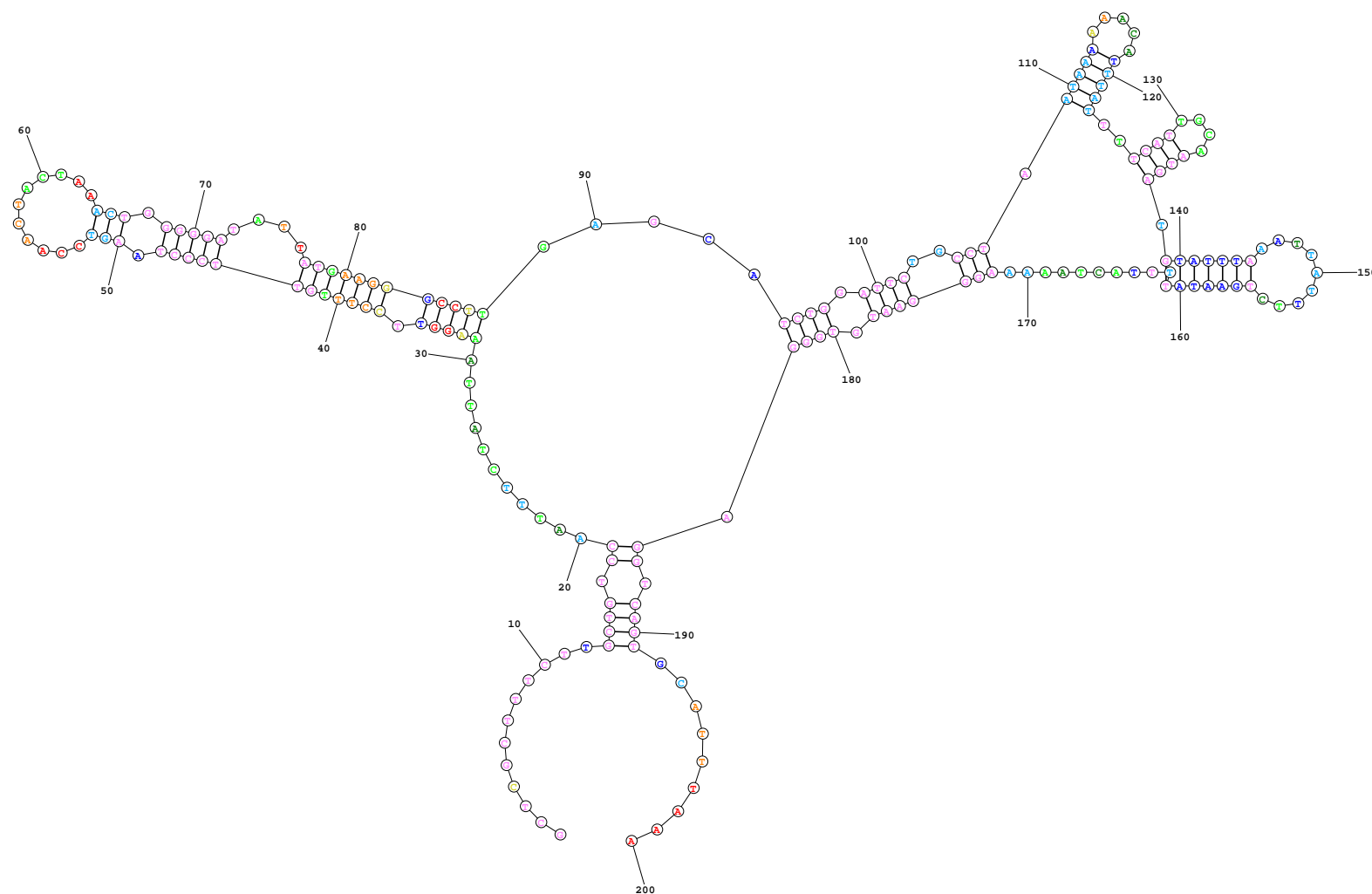
**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -33.9 ,†-pA**



**Probability >= 99%**

**99% > Probability >= 95%**

**95% > Probability >= 90%**

**90% > Probability >= 80%**

**80% > Probability >= 70%**

**70% > Probability >= 60%**

**60% > Probability >= 50%**

**50% > Probability**

**ENERGY = -33.7 ,†-pA**