

Probability \geq **99%**

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

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

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

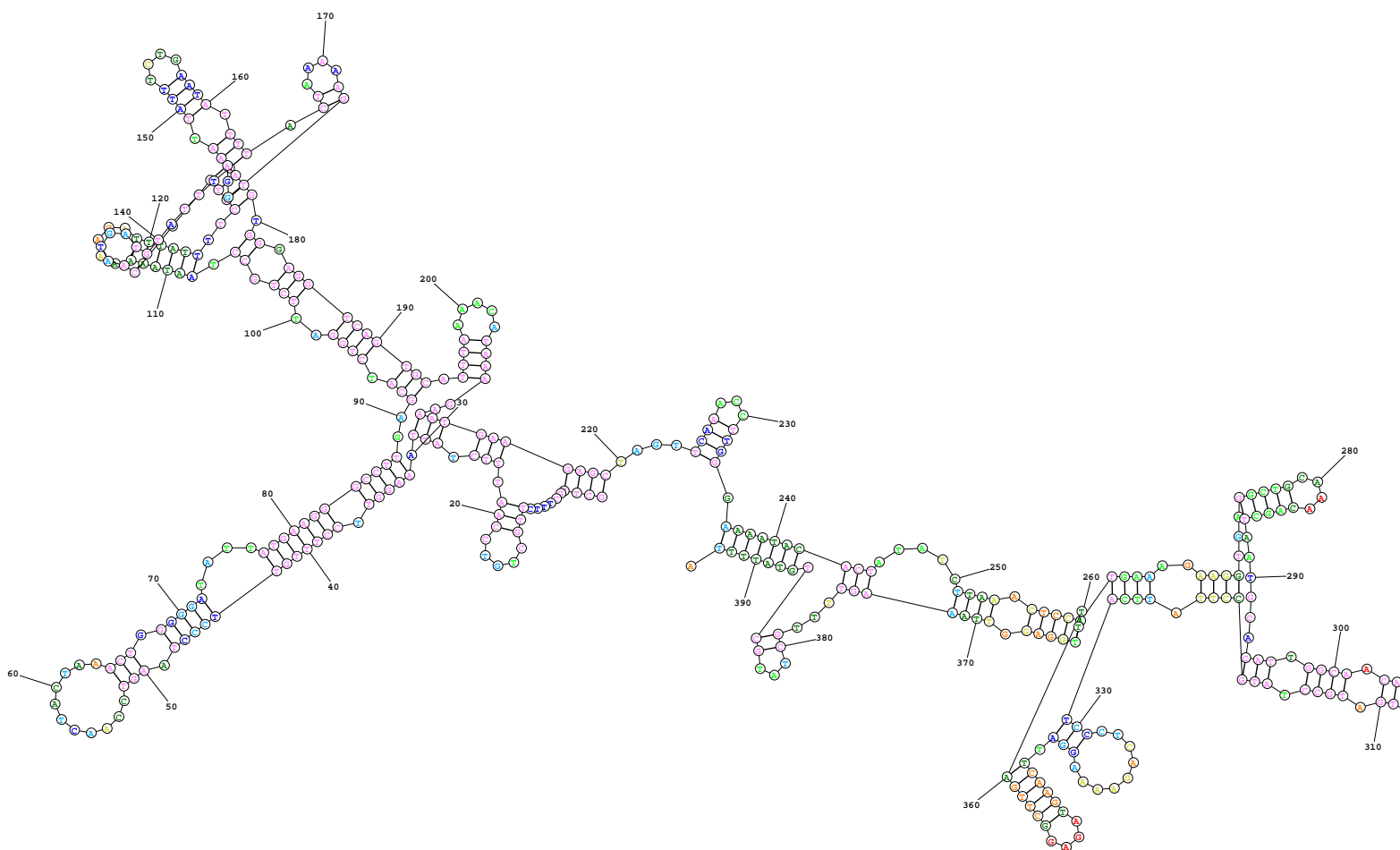
80% $>$ **Probability** \geq **70%**

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

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

50% $>$ **Probability**

ENERGY = **-47.2** ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

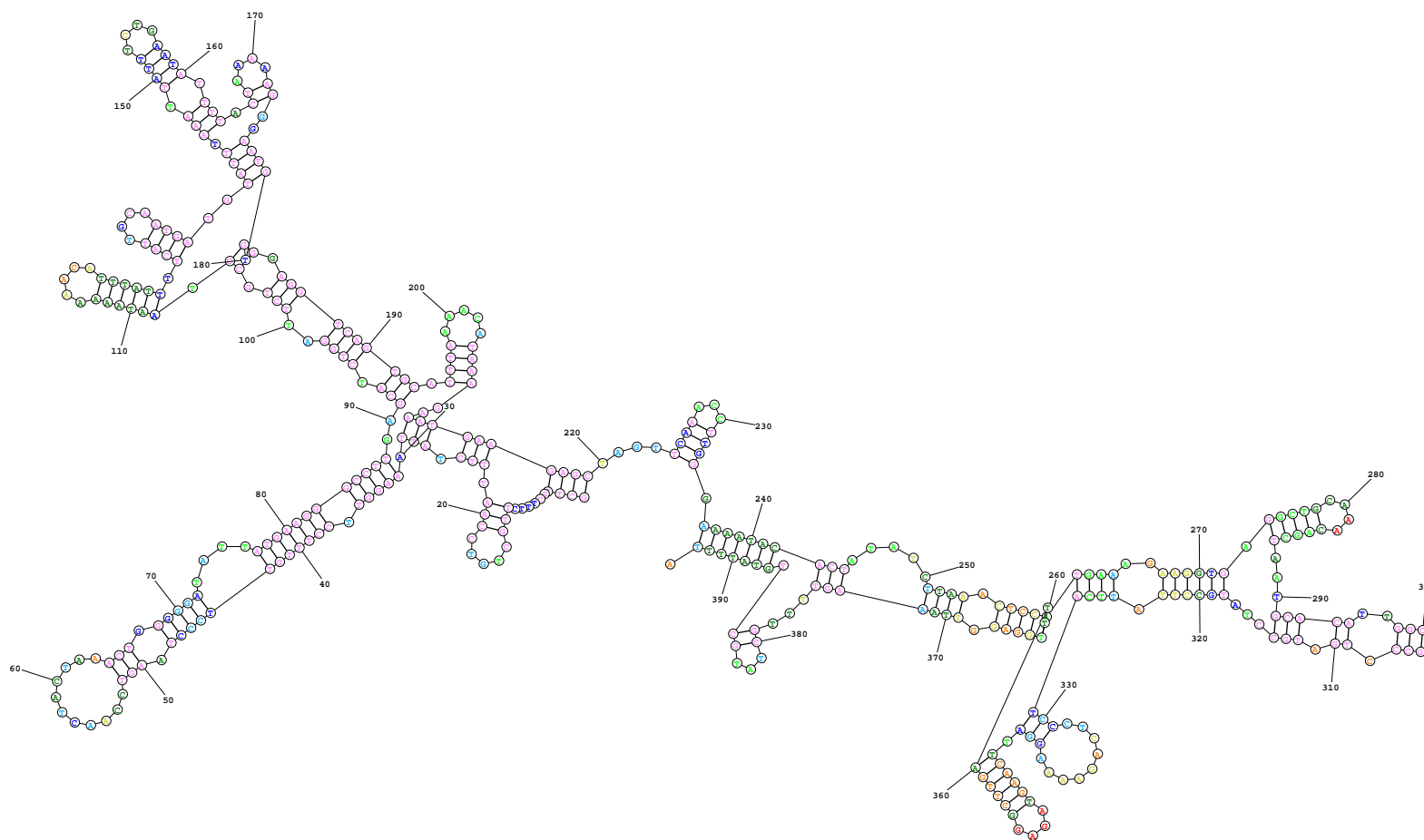
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -47.1 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

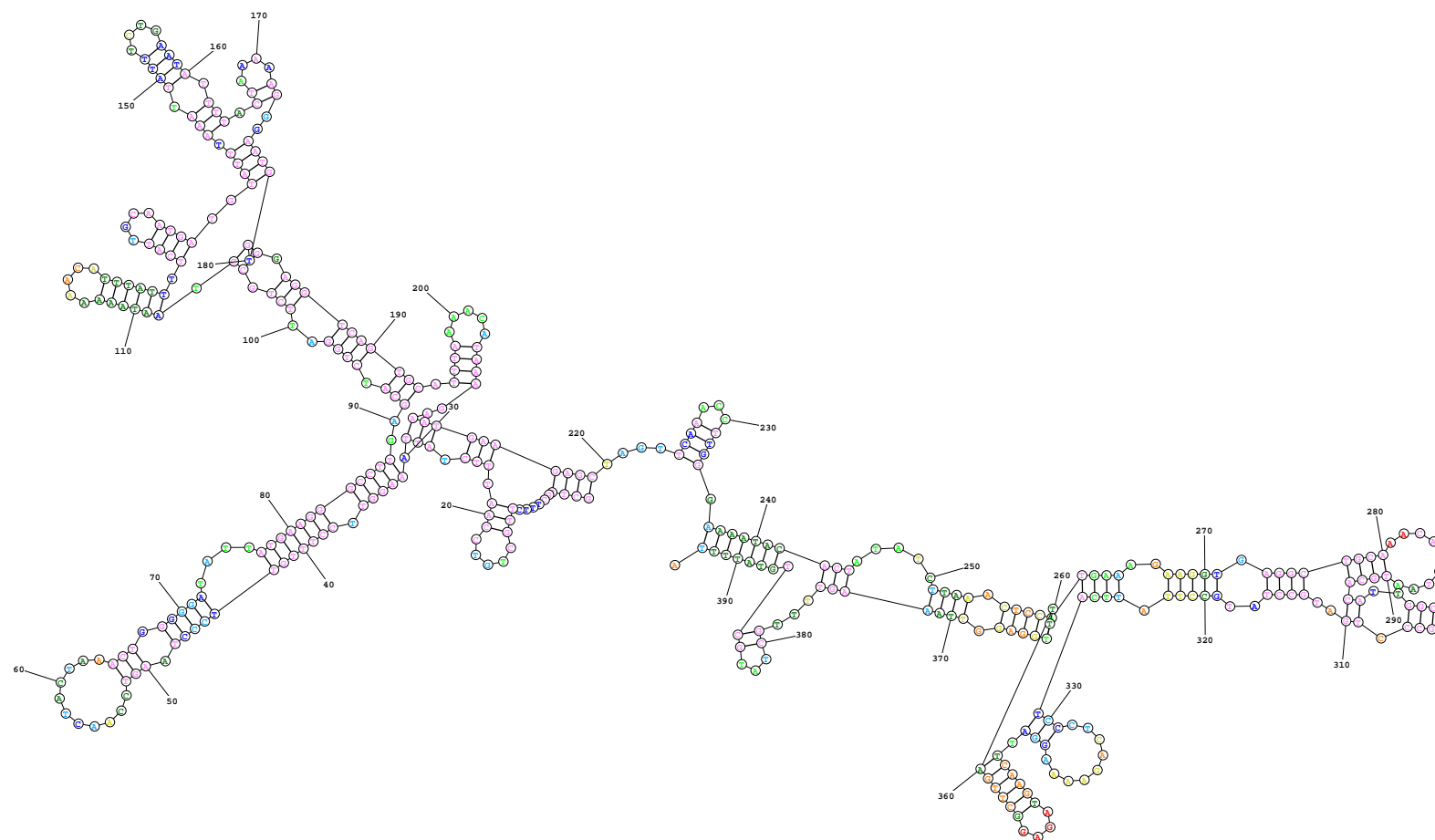
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -47.0 ,†-pA



Probability \geq 99%

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

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

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

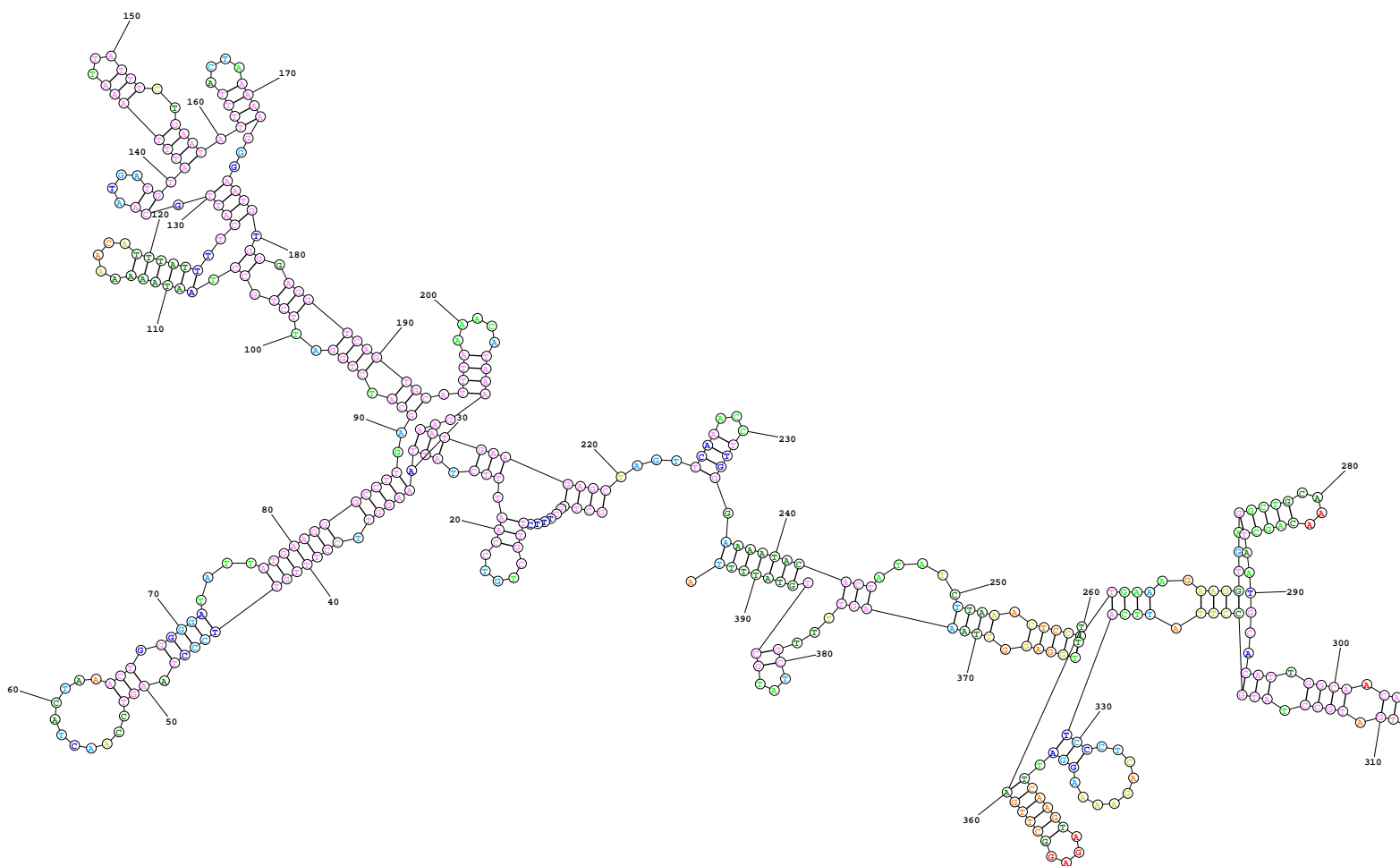
80% $>$ **Probability** \geq 70%

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

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

50% $>$ **Probability**

ENERGY = -46.6 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

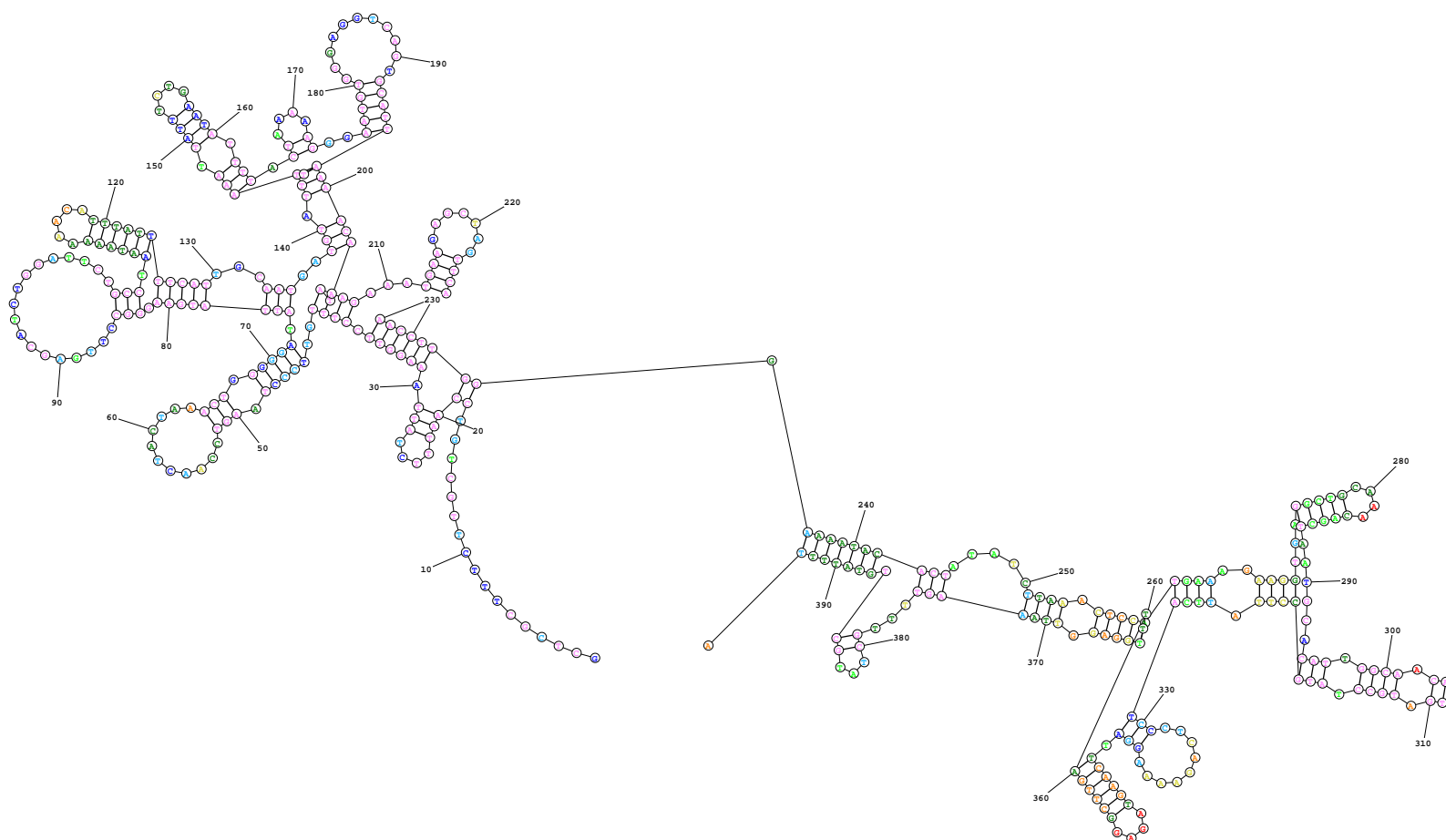
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -46.6 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

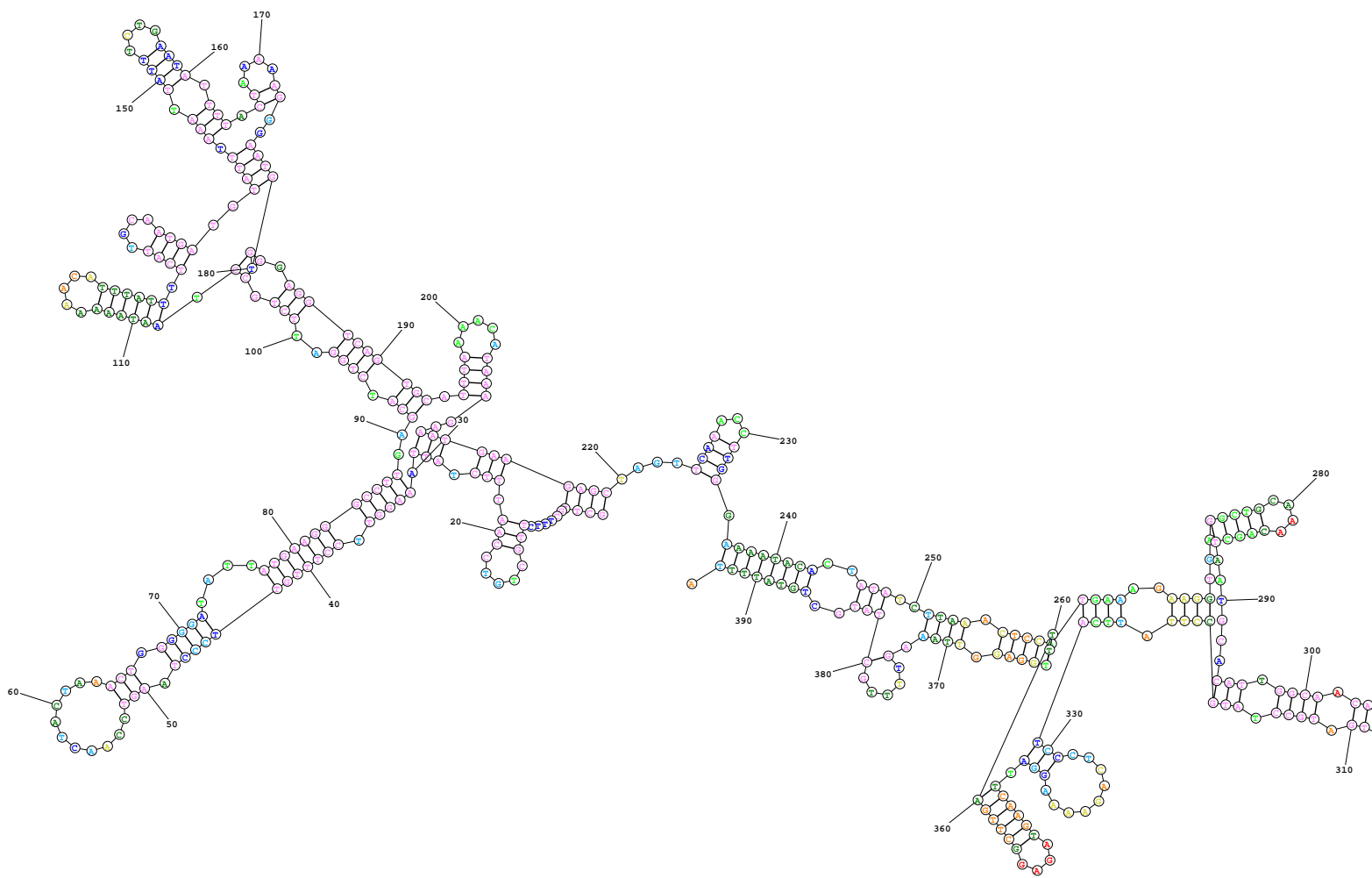
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.9 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

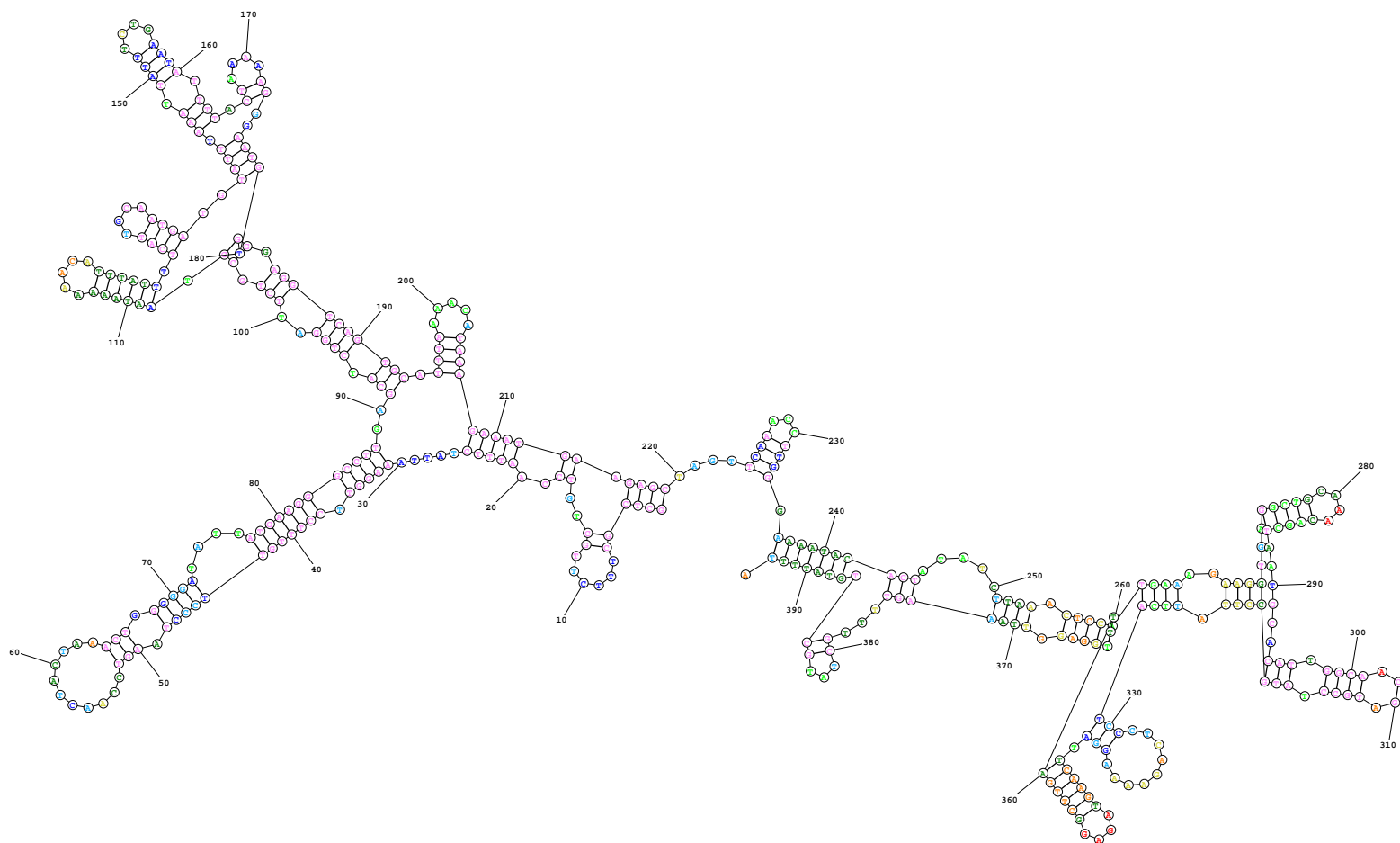
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.9 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

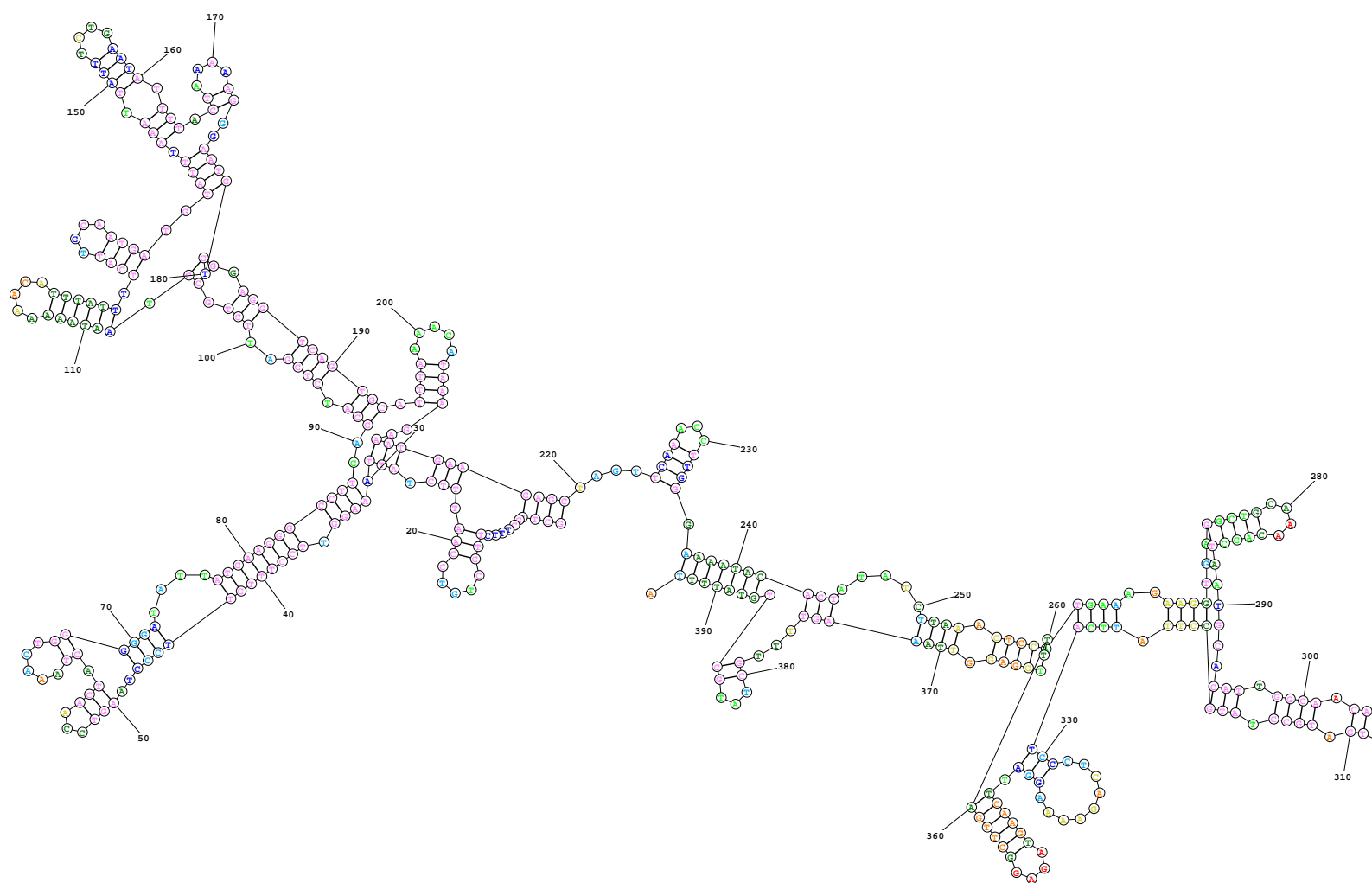
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.9 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

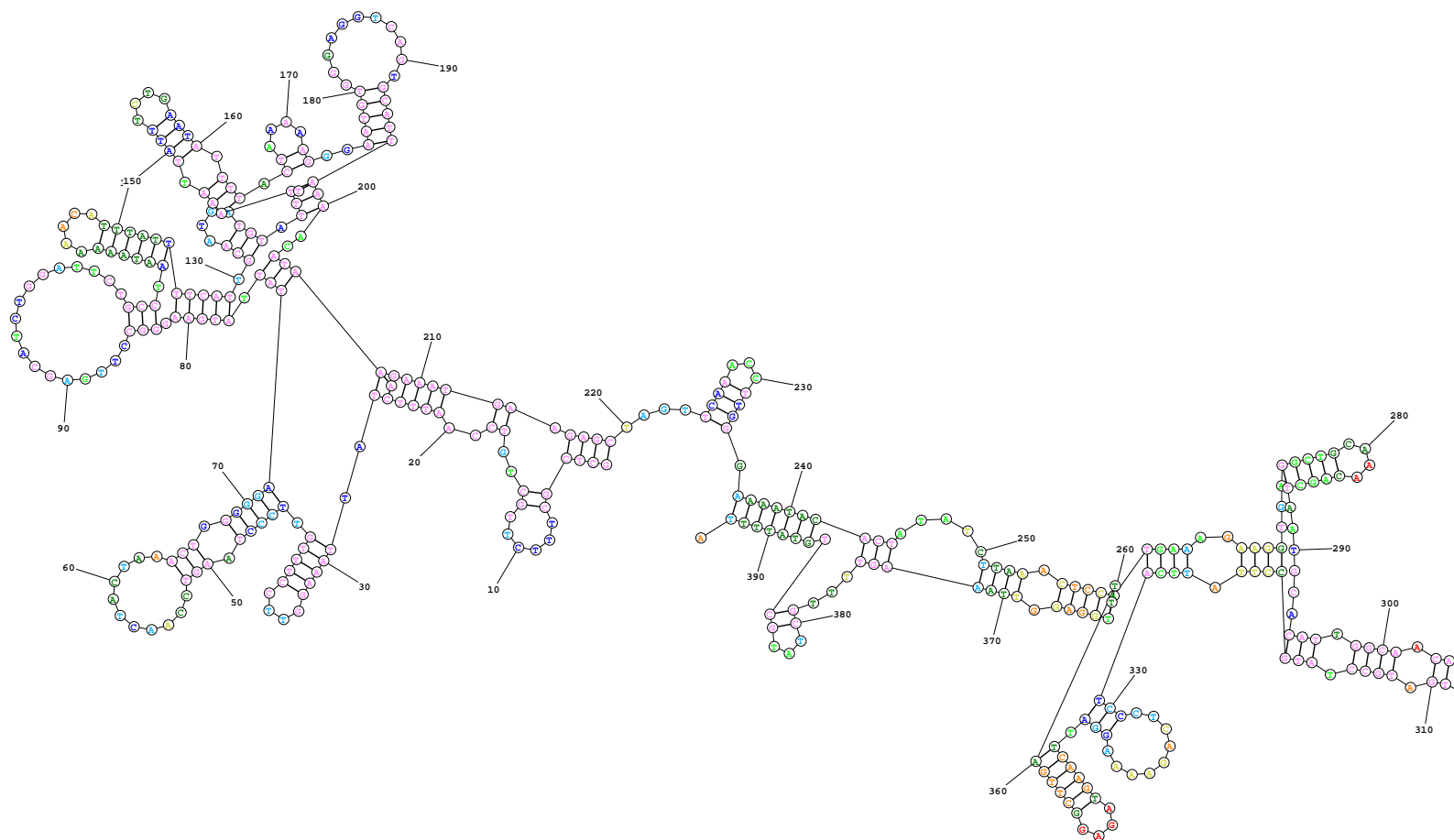
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.9 kcal/mol



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

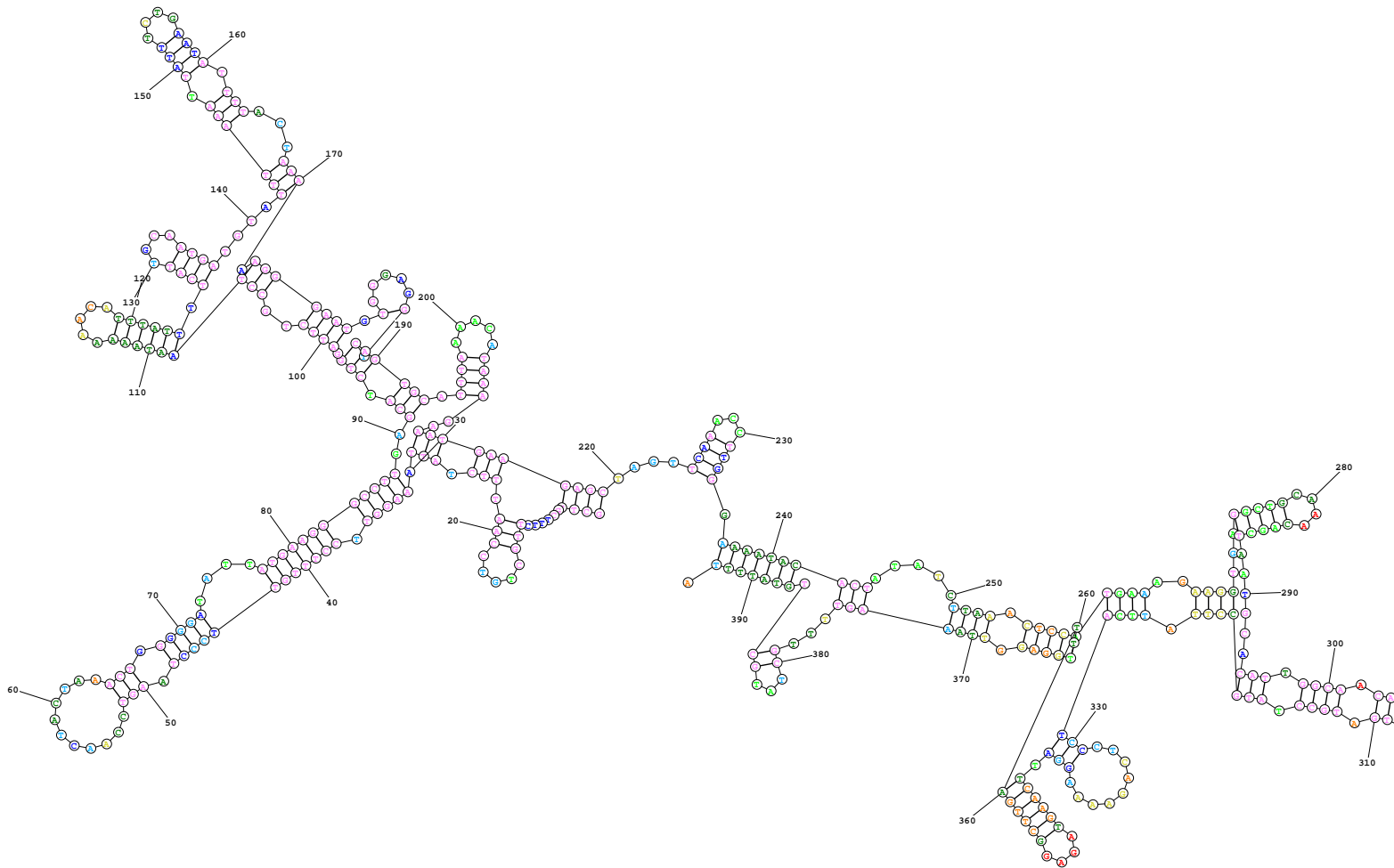
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.7 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

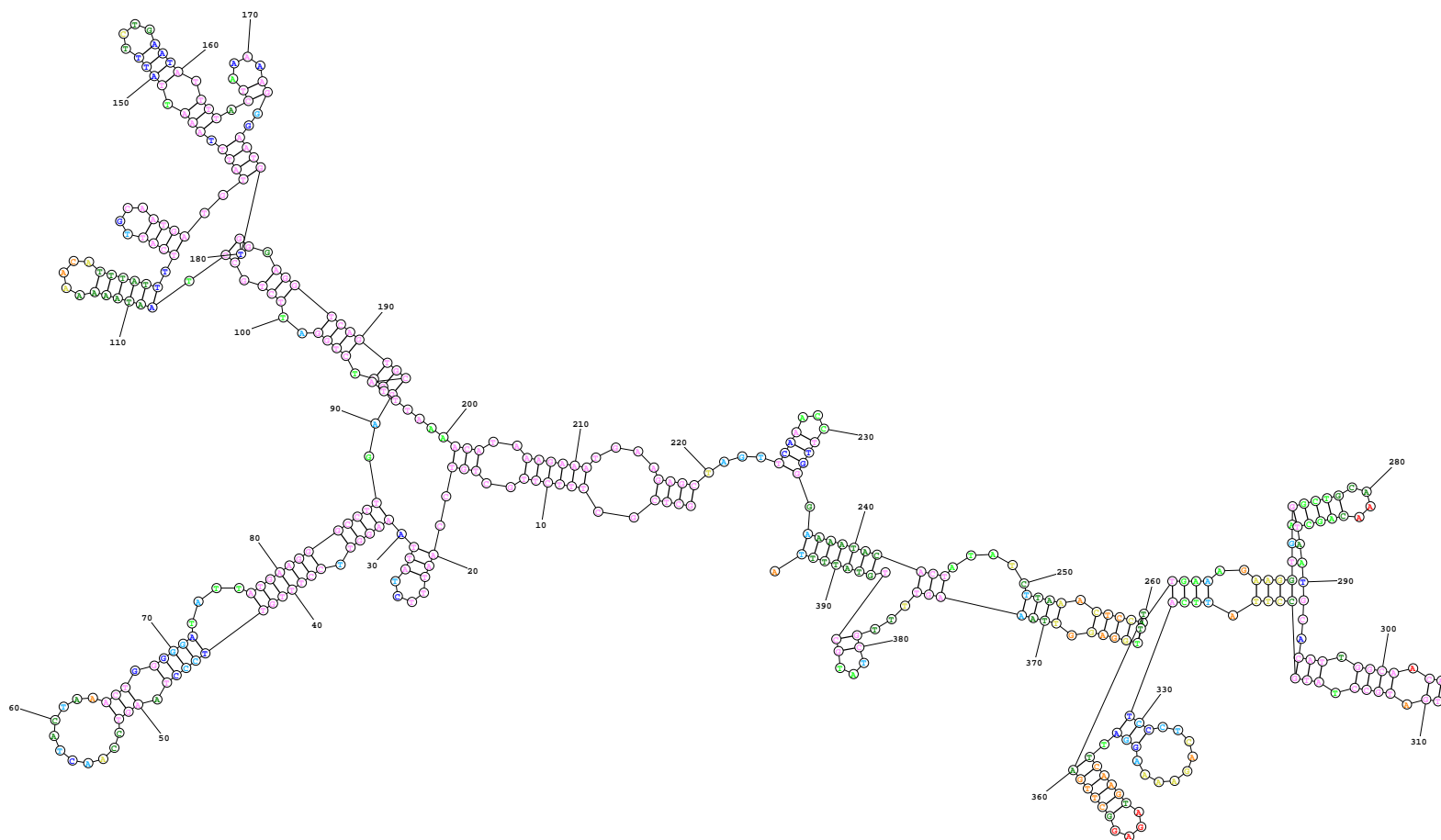
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.7 kcal/mol



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

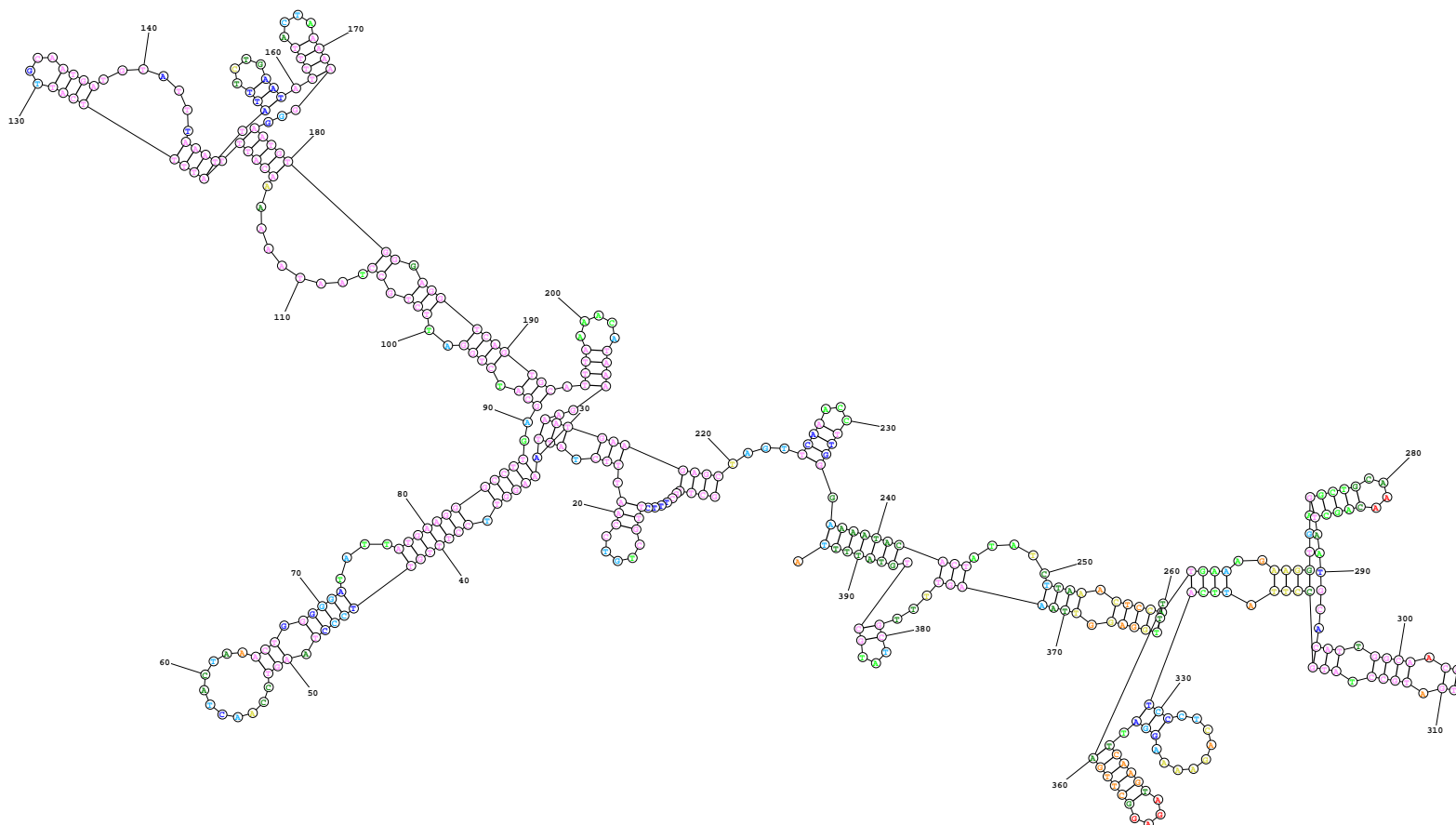
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.6 kcal/mol



Probability \geq 99%

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

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

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

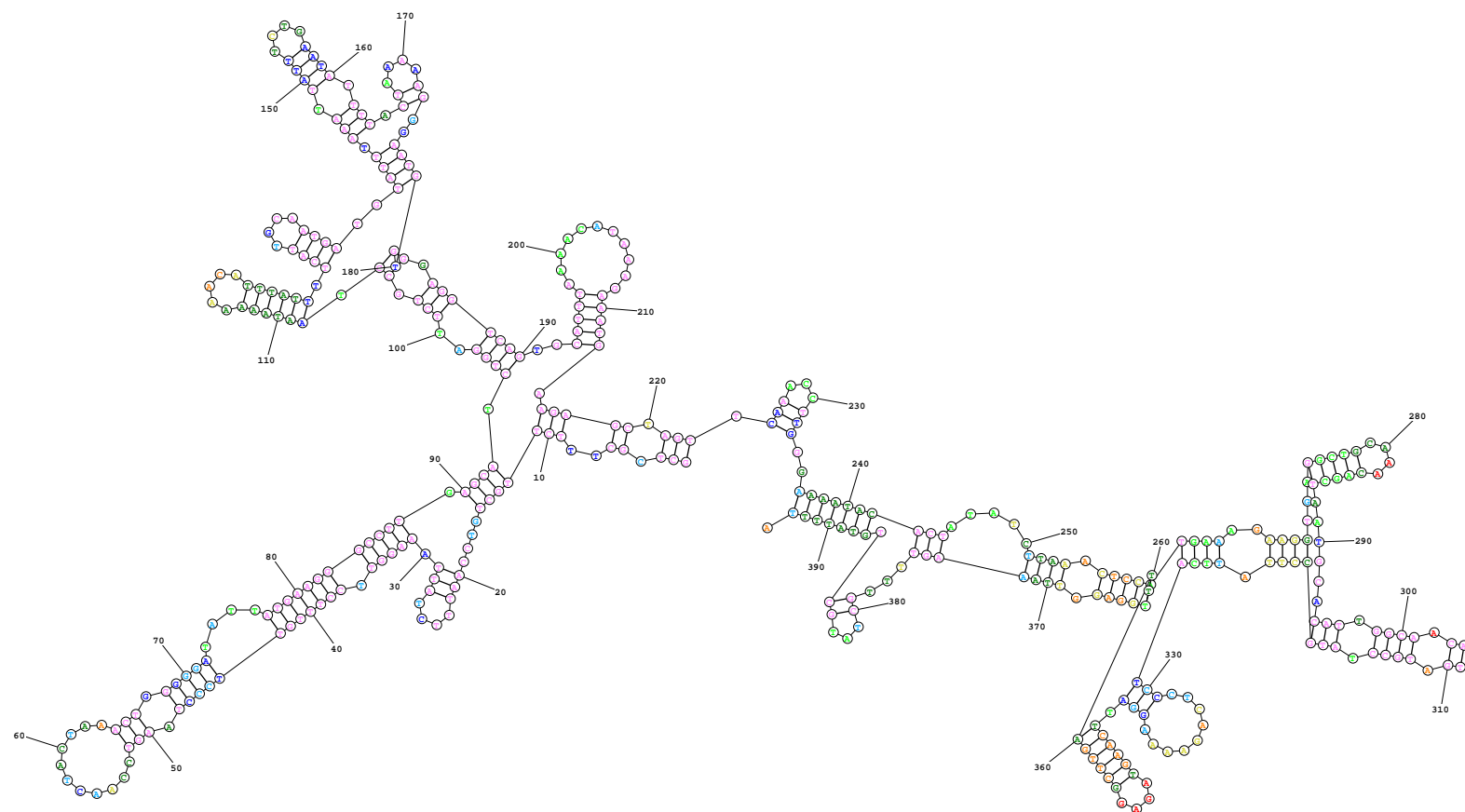
80% $>$ **Probability** \geq 70%

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

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

50% $>$ **Probability**

ENERGY = -45.6 kcal/mol



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

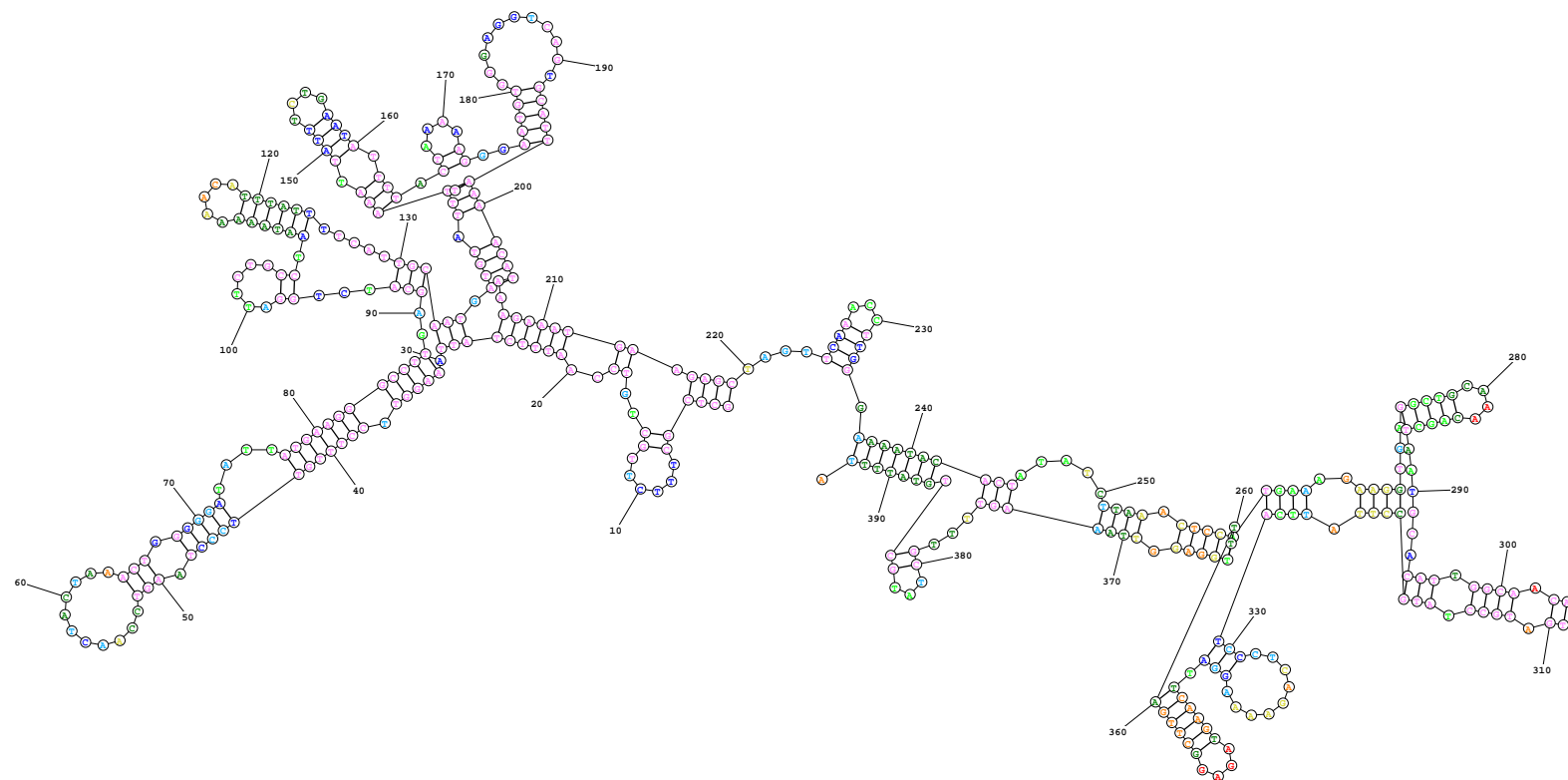
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.5 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

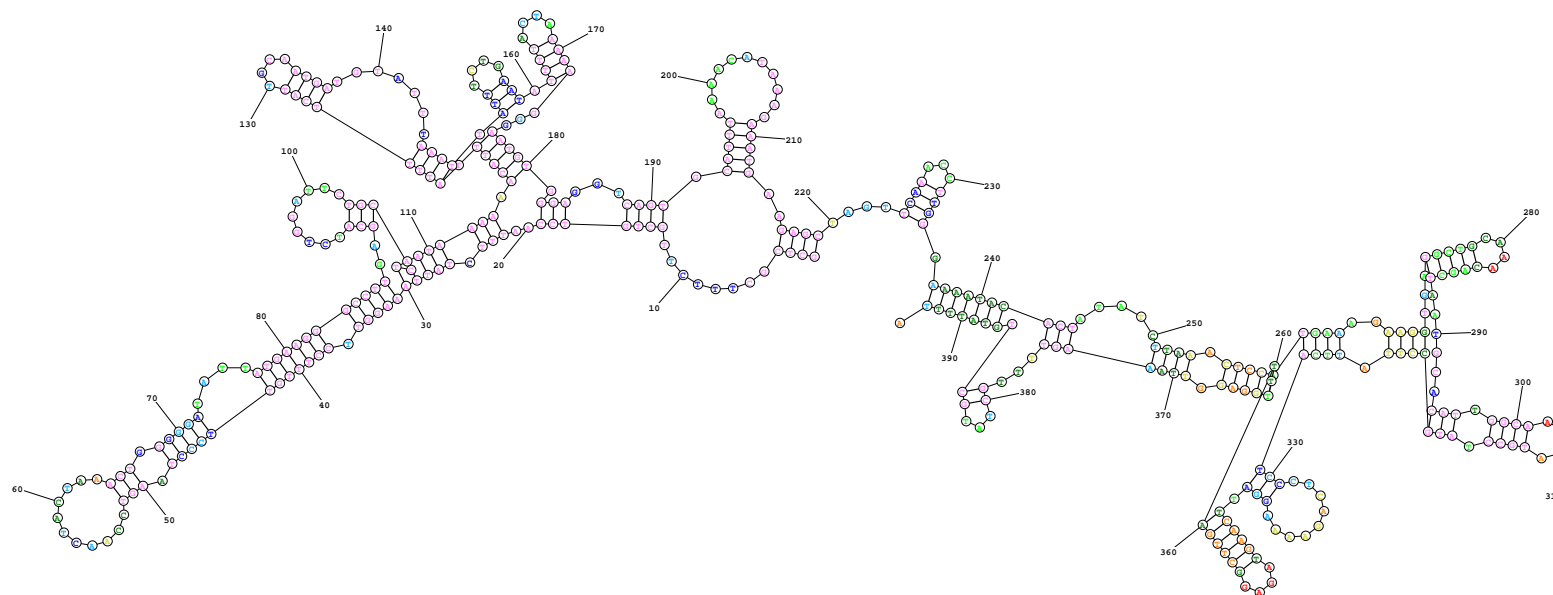
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.5 kJ/mol



Probability >= **99%**

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

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

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

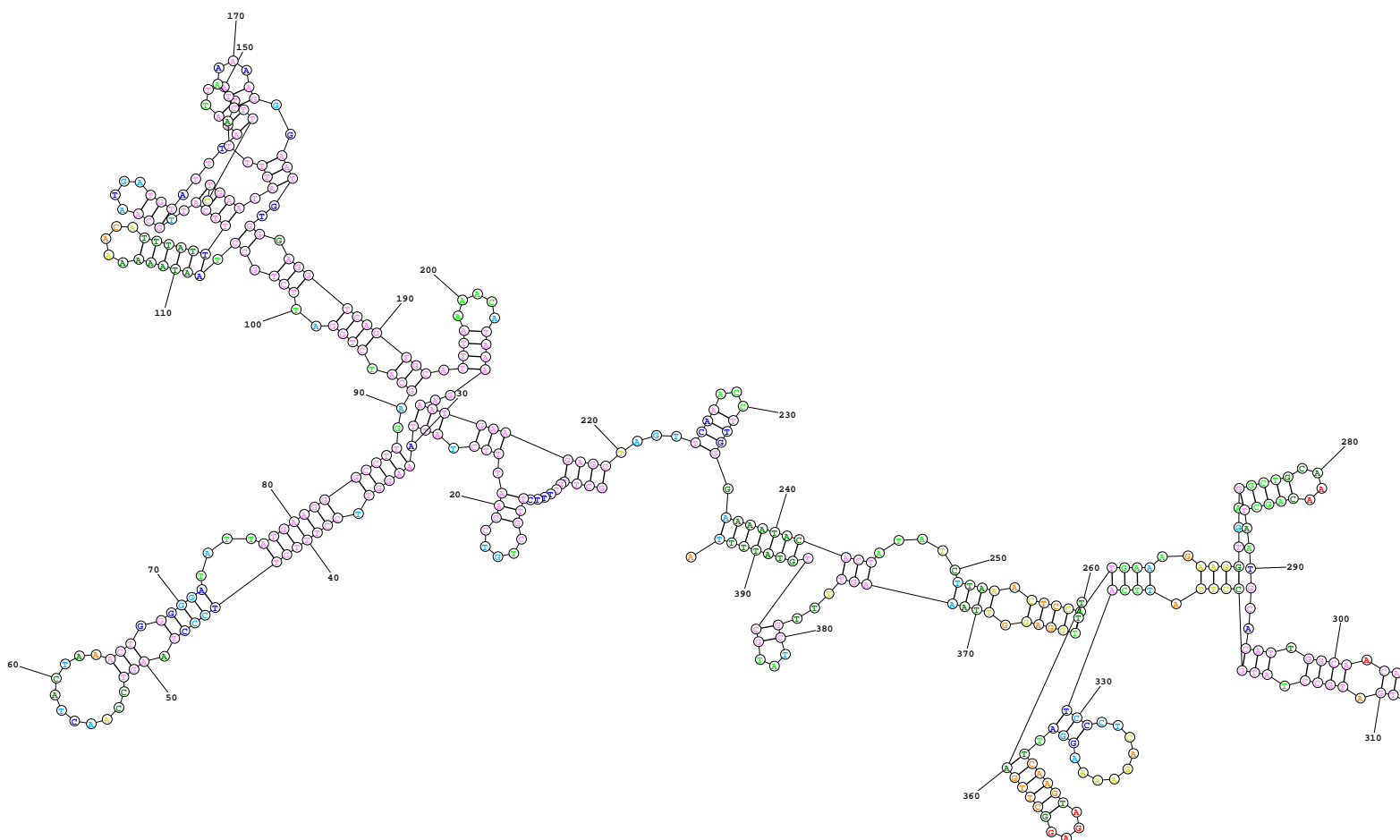
80% > **Probability** >= **70%**

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

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

50% > **Probability**

ENERGY = **-45.4** ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

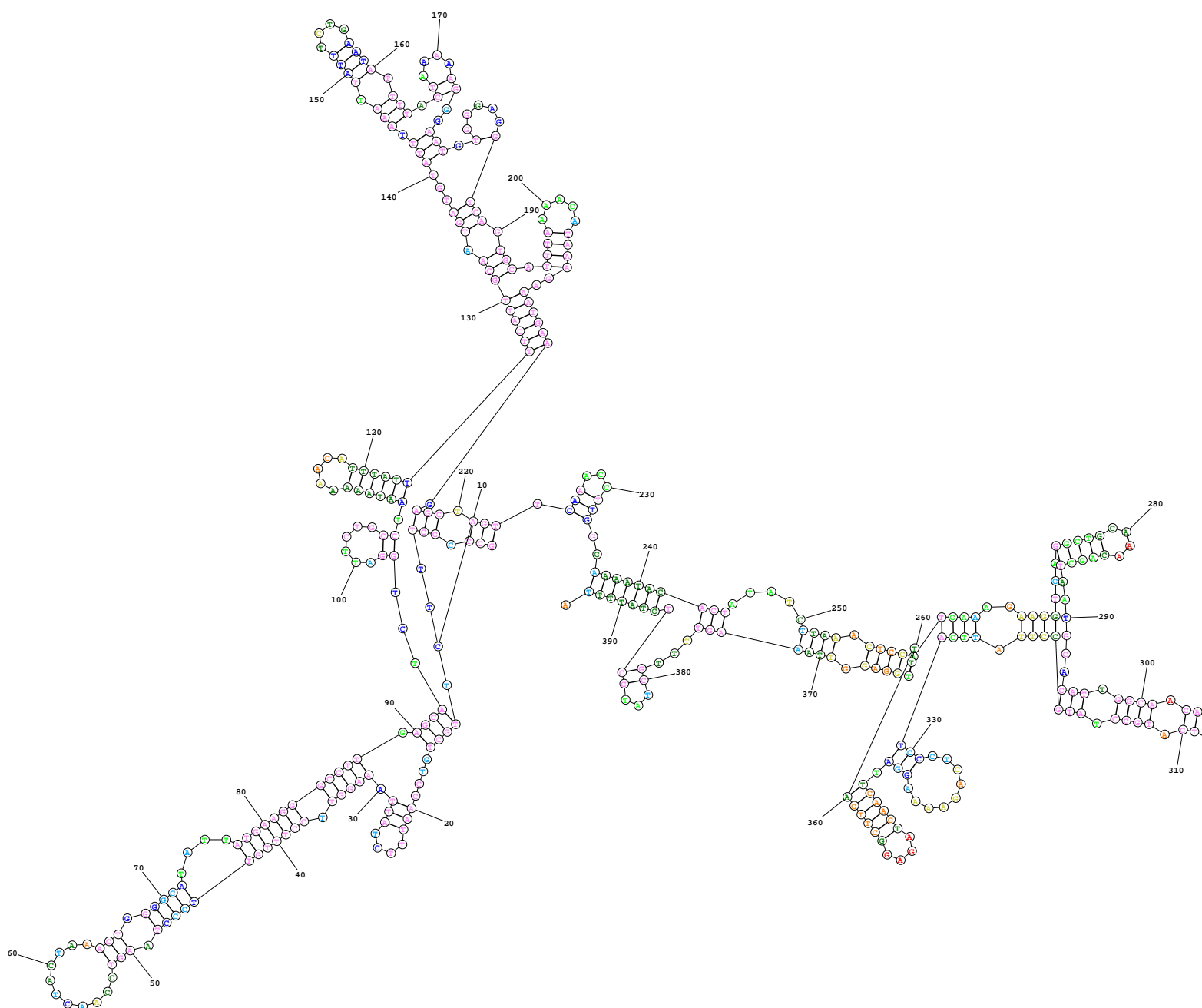
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.4 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

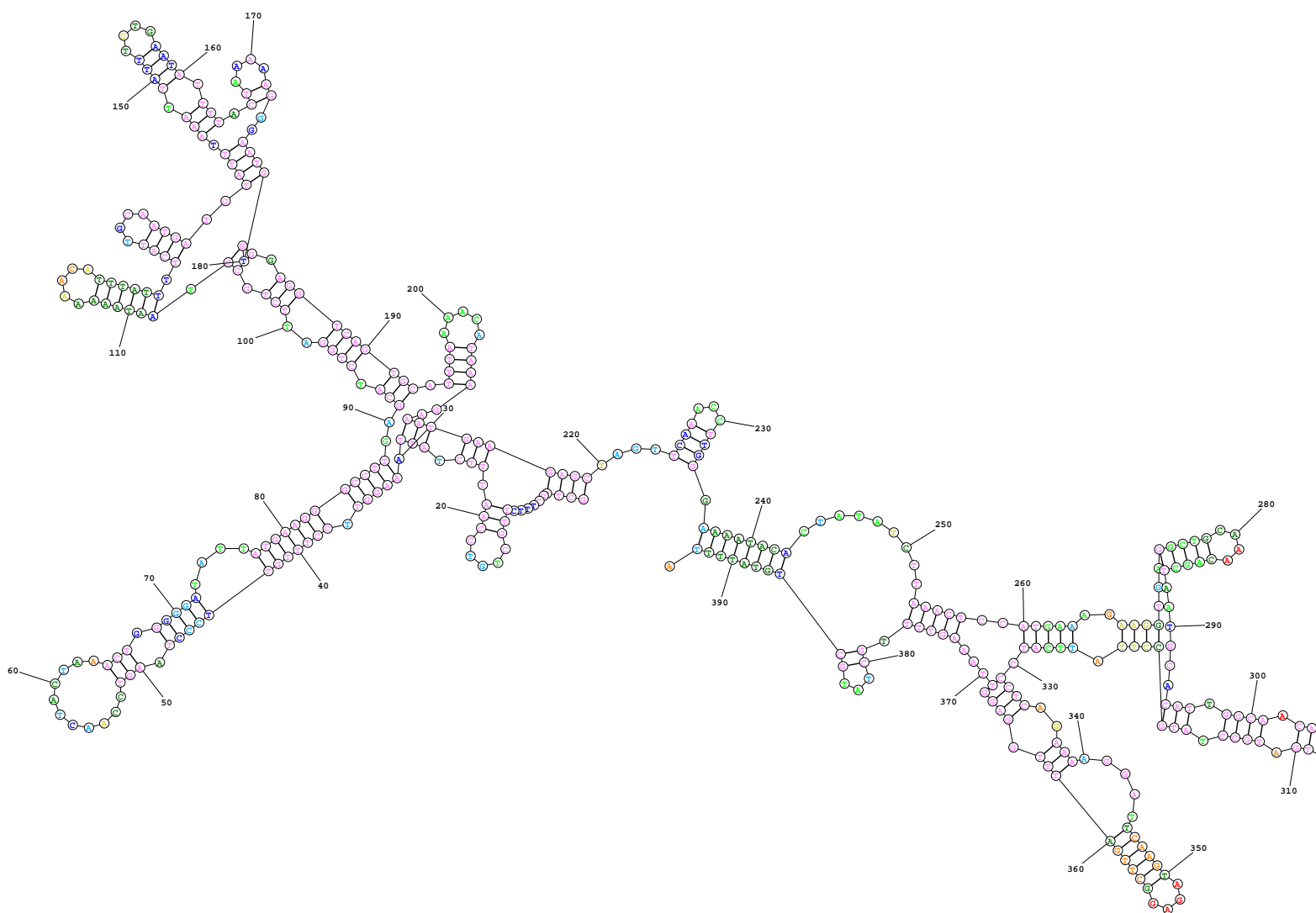
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.4 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

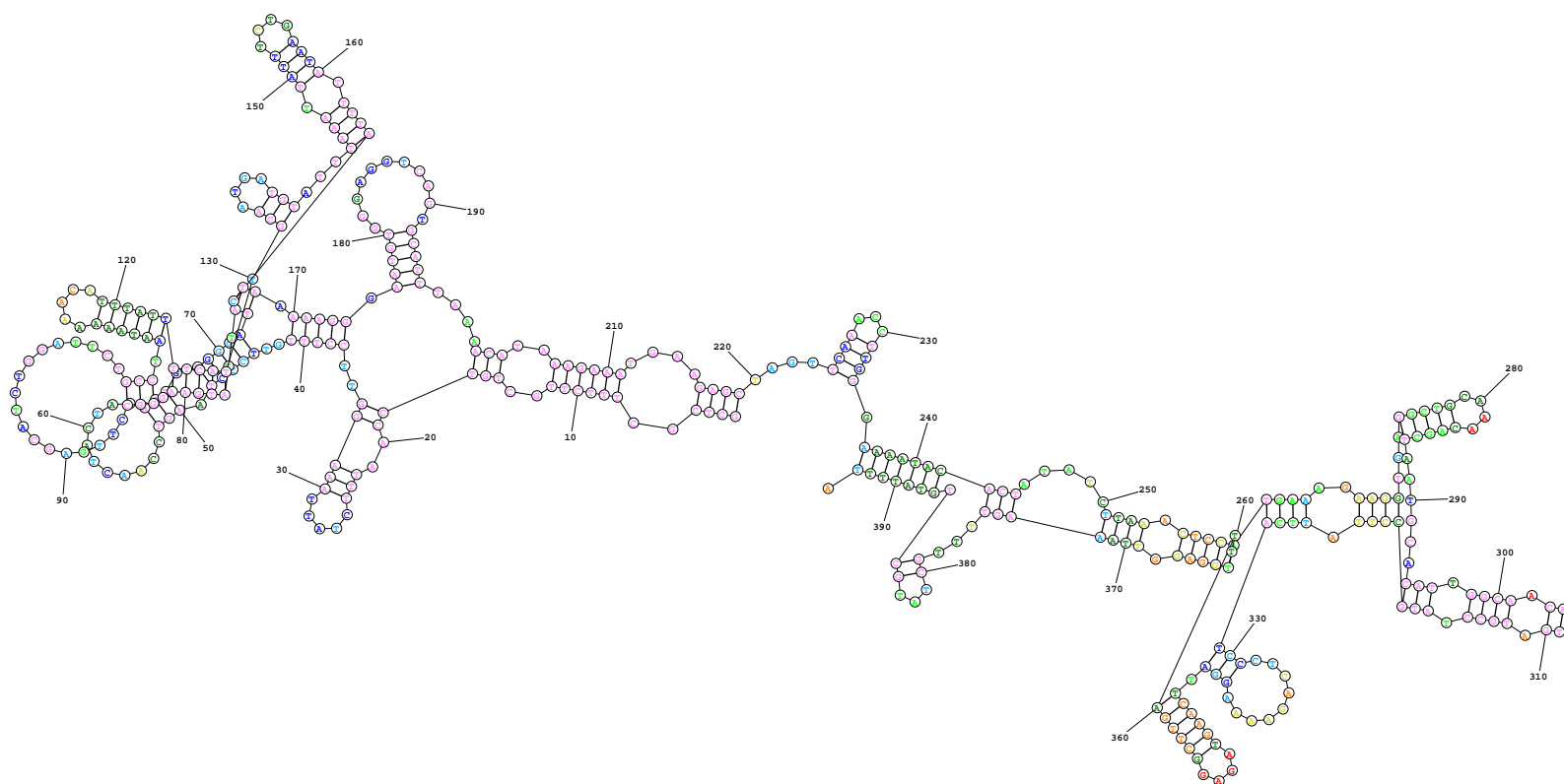
80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.3 ,†-pA



Probability >= 99%

99% > Probability >= 95%

95% > Probability >= 90%

90% > Probability >= 80%

80% > Probability >= 70%

70% > Probability >= 60%

60% > Probability >= 50%

50% > Probability

ENERGY = -45.2 ,†-pA