$$k_{\mathrm{eff}} = \exp\left(2.1\Big(-0.068 \mathrm{Bound\ bases\ in\ body} - 5.9\exp\left(-2.9\left(1 - 0.045 \mathrm{Total\ bases\ bound}\right)^2 - 0.081(0.12 \mathrm{Bound\ bases\ in\ transition\ area\ body} - 0.52 \mathrm{Free\ bases\ in\ toe} - 1)^2\Big) + 1.6\Big) - 10.76\Big)$$

$$k_{\text{eff}} = \exp\left(2.1\Big(0.053\text{ddG} + 3.2\tanh(0.2\text{Free bases in toe} - 0.39) - 1.5\Big) - 10.76\right)$$