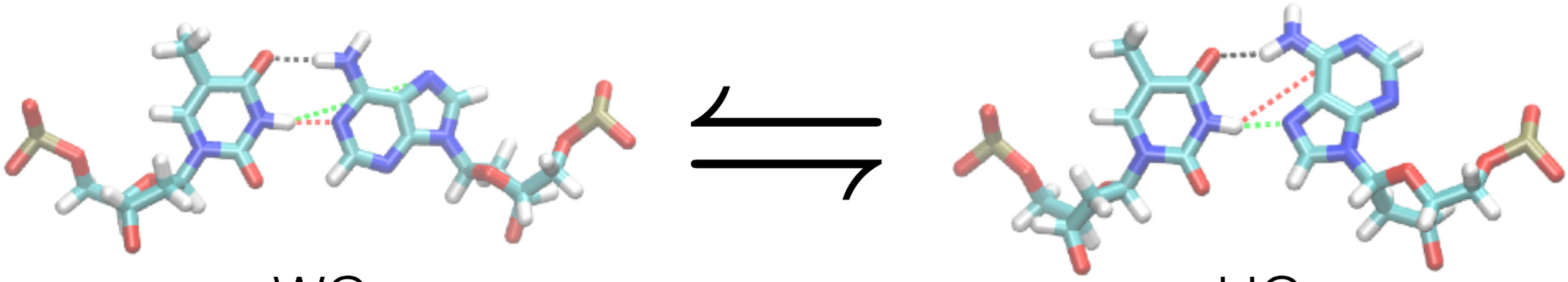
Rates and Free Energies



WC ⇌ HG

	expt*	TIS	TIS / expt
$k_{WC \to HG}$ (s^{-1})	14.2 ± 1.03	742	~52
$k_{HG \to WC}$ (s^{-1})	3670 ± 200	$1.6 \cdot 10^5$	~43
ΔG ($k_B T$)	5.5	5.4	
	at 26.0°C	at 300K	

*Nikolova et. al. Nature **470**, 498 (2011).

$$\frac{\Delta G}{k_{\mathrm{B}} T} = -\ln\left(\frac{k_{\mathrm{WC}\to\mathrm{HG}}}{k_{\mathrm{HG}\to\mathrm{WC}}}\right)$$

Conclusions

- ***Background:*** Hoogsteen base pairs are significant, and may play a role in biology
- ***Mechanisms:*** We see both the "inside" and "outside" mechanism, although there might be more preference for "outside"
- ***Rates and Free Energies:*** We overestimate the rates, but in a consistent manner. The free energy difference between the states is in very good agreement.
- ***Interesting remaining questions:***
  - Motions correlated with each of the mechanisms?
  - Role of specific sequence?
  - Paths based on leaving via minor groove?