Example: Antibodies bind to regions of the HIV envelope and neutralize the virus. What do these regions look like?

*PNAS (2014), Nature Structural Biology (2015)*
Distribution of Structures

**Maximum Likelihood**
(pick most probable)

**Bayesian**
(average over all conformations)

\[
\min \left( \frac{1}{Z} \int \right)
\]

*Global Minimum Energy Conformation*

*Probability ↔ Energy using Boltzmann distribution*
Distribution of Structures

**Maximum Likelihood**
(pick most probable)

**Bayesian**
(weighted average over all conformations)

\[
\min \left( \int \frac{1}{Z} \prod \right)
\]

Global Minimum Energy Conformation

Proability $\leftrightarrow$ Energy using Boltzmann distribution

\[
K = \frac{[EL]}{[E][L]} \approx \frac{P(B)}{P(U)} \approx K^* = \frac{\sum_{b \in B} e^{-E_b/RT}}{\sum_{f \in F} e^{-E_f/RT} \sum_{l \in L} e^{-E_l/RT}}
\]
For more information see:

Algorithms in Structural Molecular Biology

BRUCE R. DONALD

MIT Press (2011)