

$$\Delta E(t) = \sum_k \beta_k \Delta F_k(t)$$

$\Delta E(t)$ Change in antigen-antibody interaction energy (Coulomb + LJ) at pulling frame t relative to frame 0

$\Delta F_k(t)$ Change in pairwise contact frequency for residue pair k at frame t relative to frame 0

β_k Elastic net regression coefficient for pair k (sparse, L1/L2 regularized)

10 replicas \times 50 subsampled frames | Leave-2-replicas-out CV (45 folds) | Test $R^2 = 0.959$