

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

$\Delta E(t)$  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

$\beta_k$  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  $R^2 = 0.959$