A) Elastic Net Regression Fit

$R^2 = 0.9981$
RMSE = 8.0 kJ/mol
52/549 non-zero β
$\alpha = 12.92$, $\ell_1 = 0.50$

Predicted ΔE (kJ/mol)

Actual ΔE (kJ/mol)
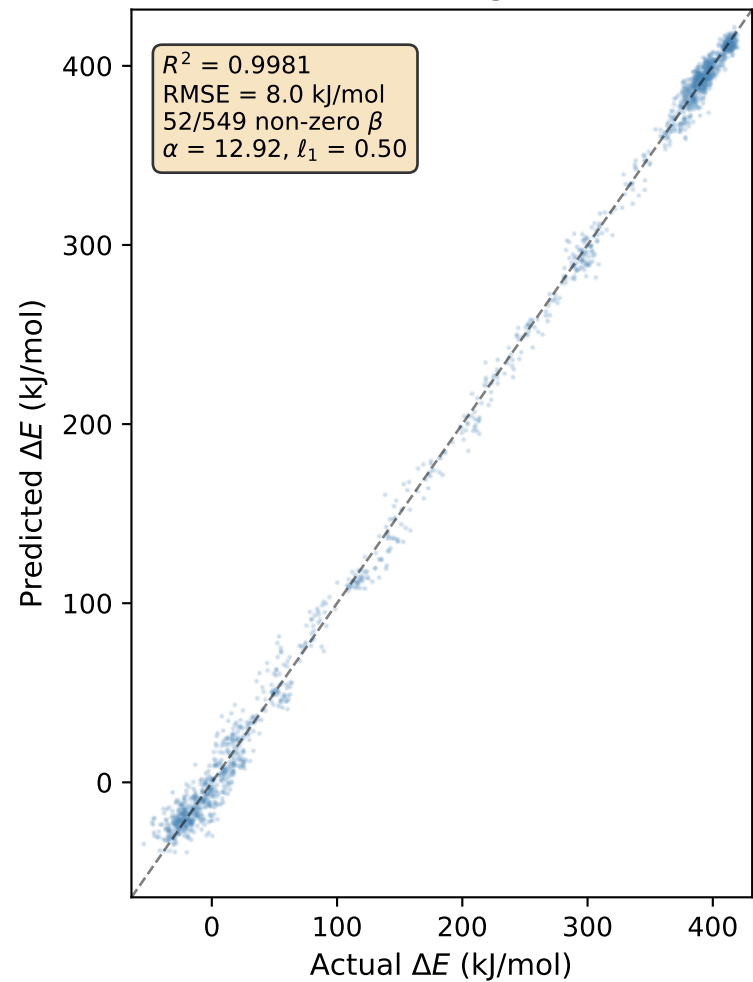
$$\Delta E(t) = \sum_k \beta_k \cdot \Delta F_k(t)$$

B) Top Contact Contributions

K84–Y227
Q160–Y406
F157–Y406
F123–F287
V150–Y405
Y172–R249
E151–Y405
F157–Y404
Q160–Y227
Y172–D245
R70–D245
F123–Y406
F153–Y406
E303–L306
R70–N248

Favorable ($\beta < 0$)
Unfavorable ($\beta > 0$)

$|\beta_k \times \bar{F}_k|$
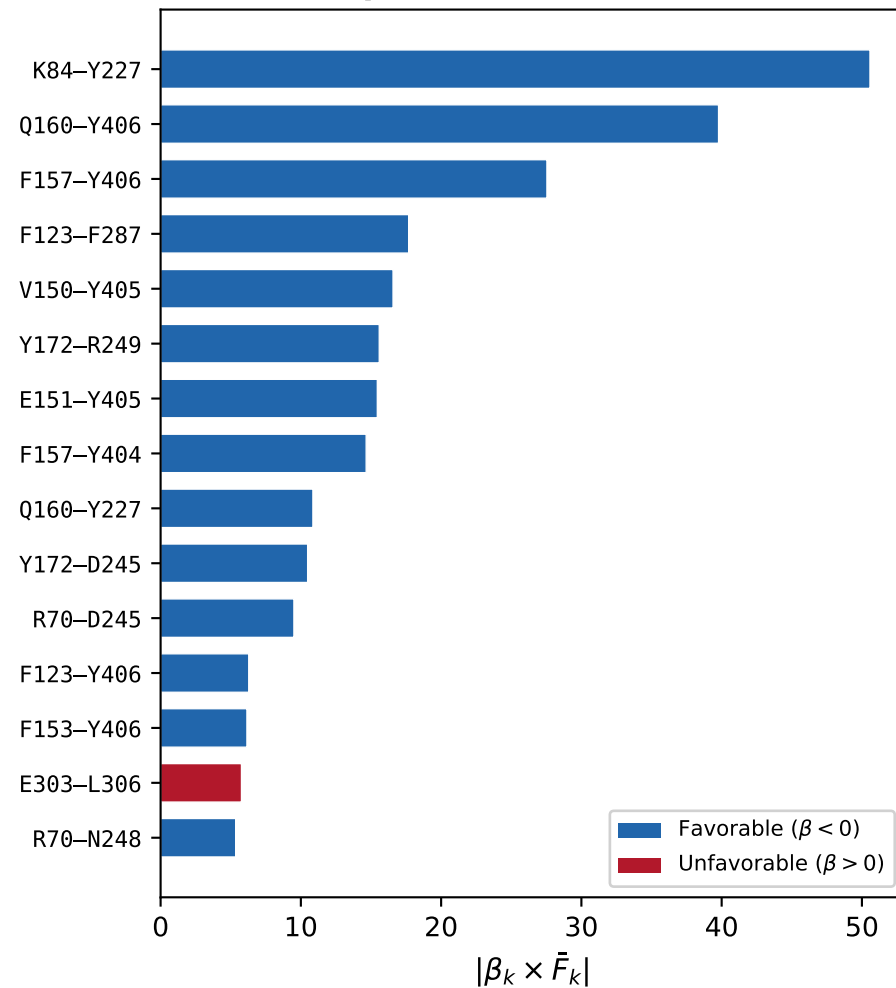
C) Antibody Residue Ranking

Y406
Y227
Y405
Y404
D245
F287
R249
A246
N248
L306
T330
E401
F244
S247
N288
Y334
H225
S262
A255
G357
Q222
K378

70th pct

Hot (high leverage)
Warm (favorable)
Warm (unfavorable)

NetFavorability $\left(\sum |\beta_k \times \bar{F}_k|\right)$