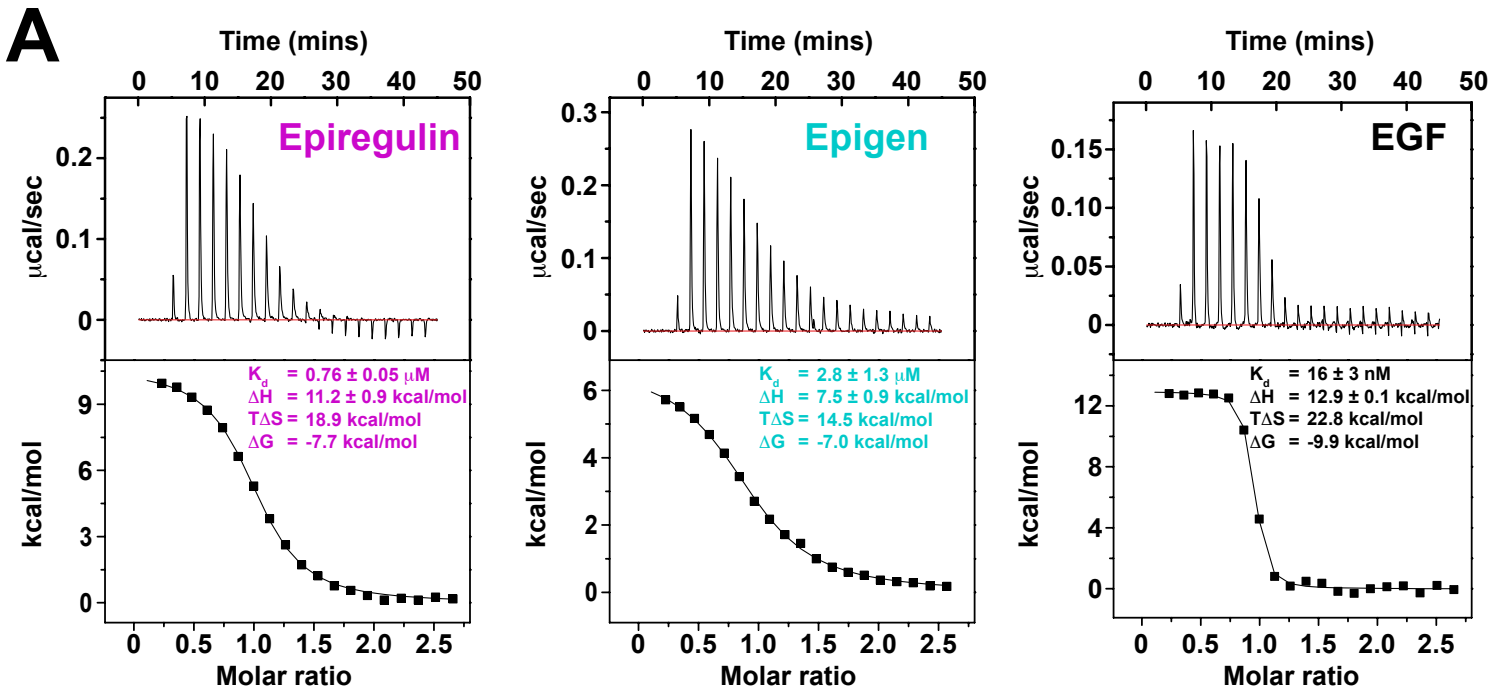
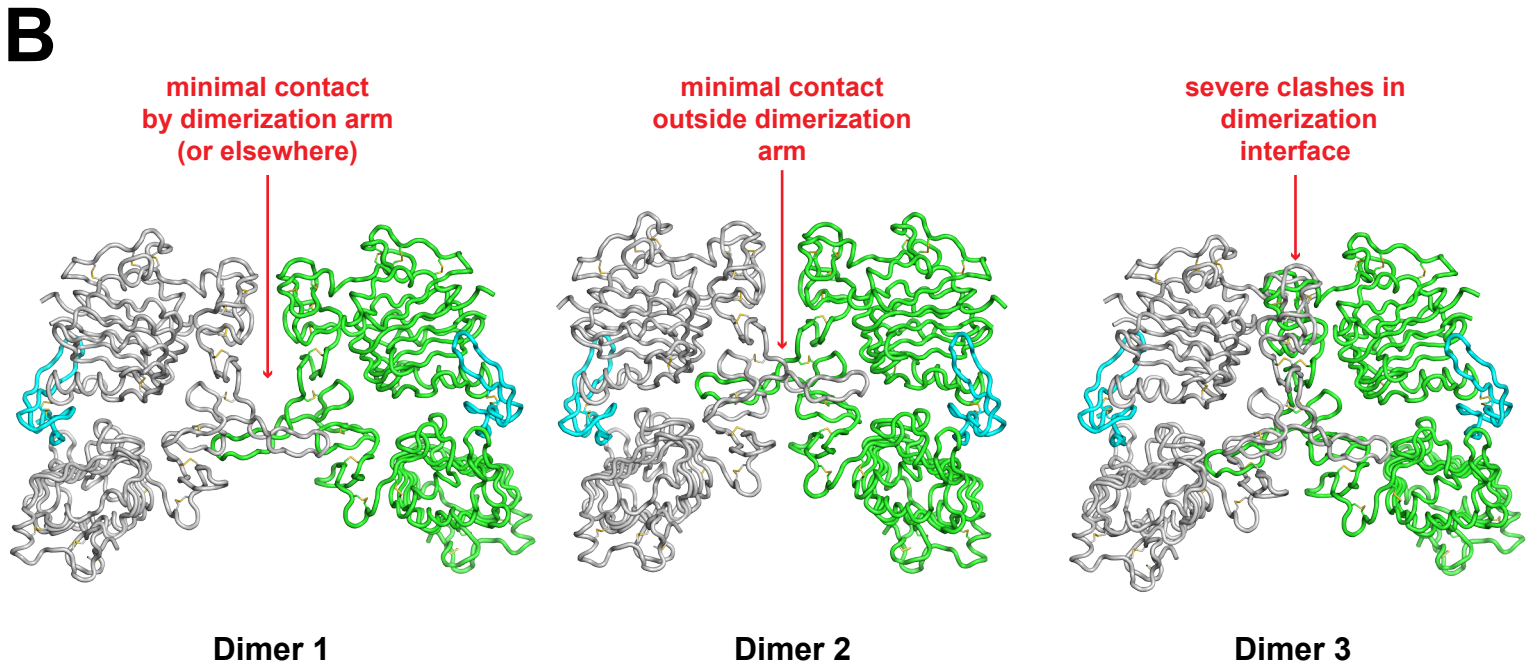

A
Time (mins)
Epiregulin
μcal/sec
kcal/mol
Molar ratio
K_d = 0.76 ± 0.05 μM
ΔH = 11.2 ± 0.9 kcal/mol
TΔS = 18.9 kcal/mol
ΔG = -7.7 kcal/mol
Epigen
K_d = 2.8 ± 1.3 μM
ΔH = 7.5 ± 0.9 kcal/mol
TΔS = 14.5 kcal/mol
ΔG = -7.0 kcal/mol
EGF
K_d = 16 ± 3 nM
ΔH = 12.9 ± 0.1 kcal/mol
TΔS = 22.8 kcal/mol
ΔG = -9.9 kcal/mol


B
minimal contact by dimerization arm (or elsewhere)
minimal contact outside dimerization arm
severe clashes in dimerization interface
Dimer 1
Dimer 2
Dimer 3