

Table 3. Binding free energy from the MM/PBSA approximation

Free energy terms	(kcal/mol)
G_{LP}	-1624.5 ± 38
G_P	-1474.3 ± 31
G_L	-788.3 ± 5
ΔE_{LP}	-728.8 ± 41
ΔG_{LP}	-90.7 ± 20
Orientation	+4.5
Translation	+3.4
G_{bind}	-82.8 ± 20