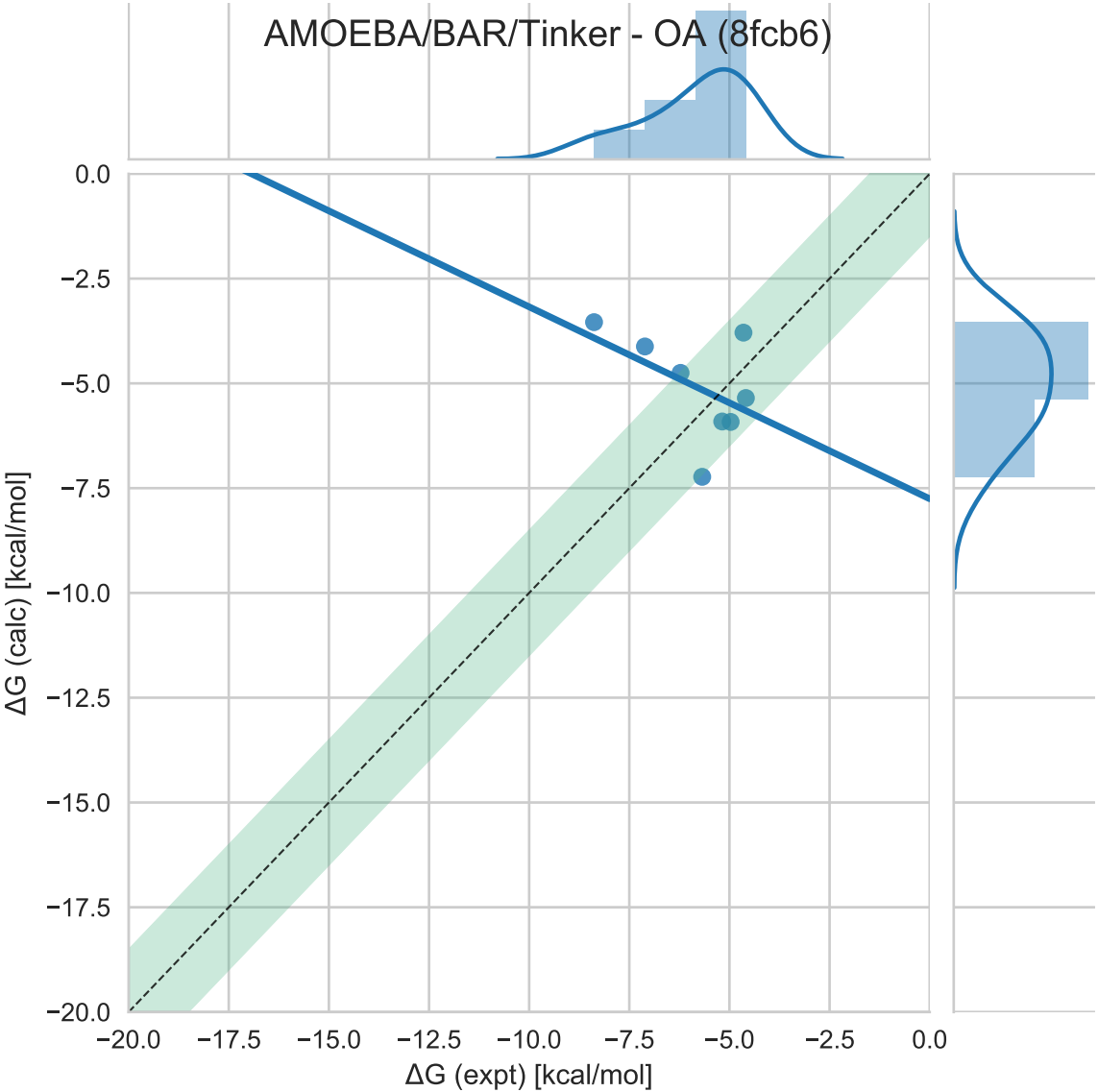
AMOEBA/BAR/Tinker - OA (8fcb6)
0.0
−2.5
−5.0
−7.5
−10.0
−12.5
−15.0
−17.5
−20.0
ΔG (calc) [kcal/mol]
−20.0
−17.5
−15.0
−12.5
−10.0
−7.5
−5.0
−2.5
0.0
ΔG (expt) [kcal/mol]