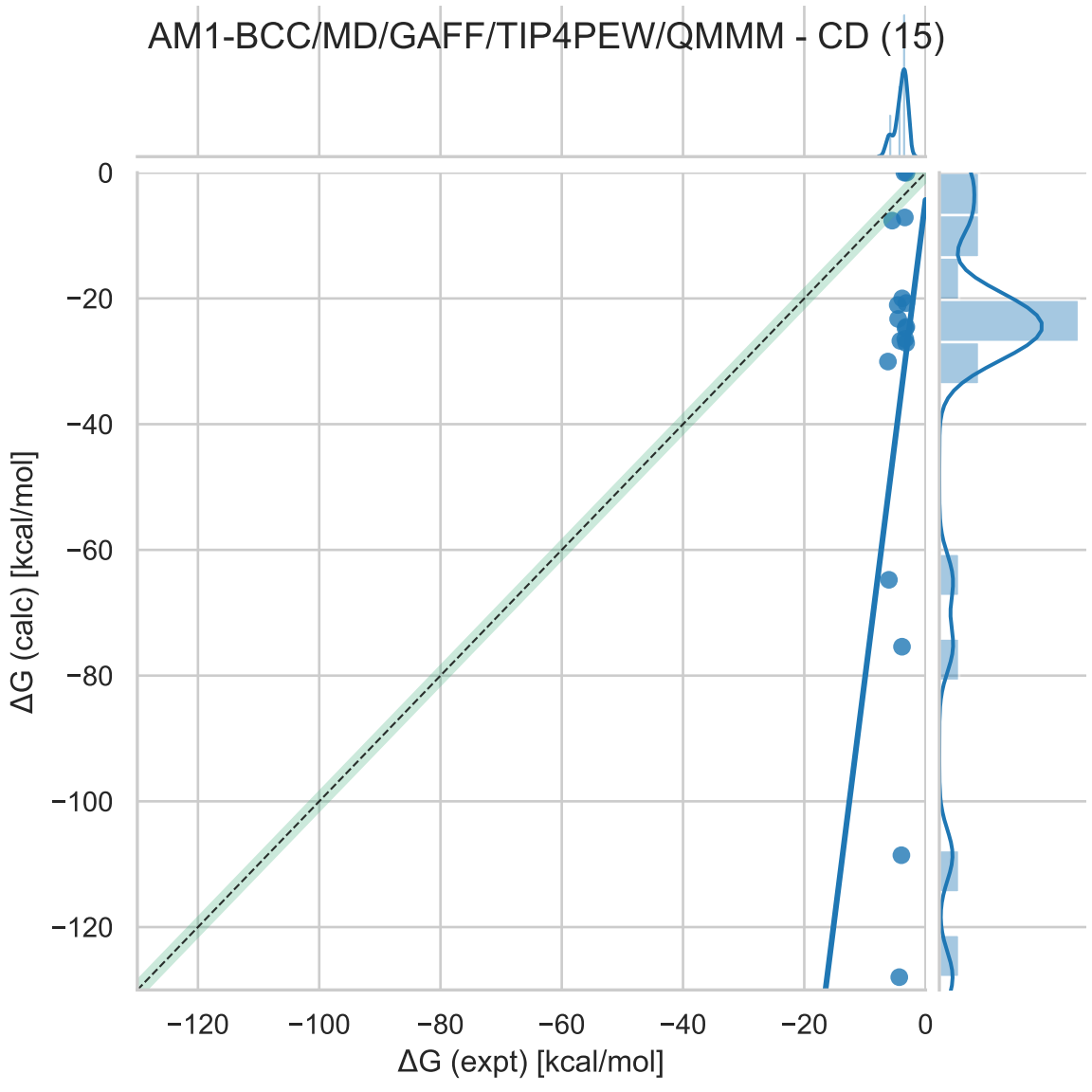
AM1-BCC/MD/GAFF/TIP4PEW/QMMM - CD (15)
0
−20
−40
−60
−80
−100
−120
ΔG (calc) [kcal/mol]
−120
−100
−80
−60
−40
−20
0
ΔG (expt) [kcal/mol]