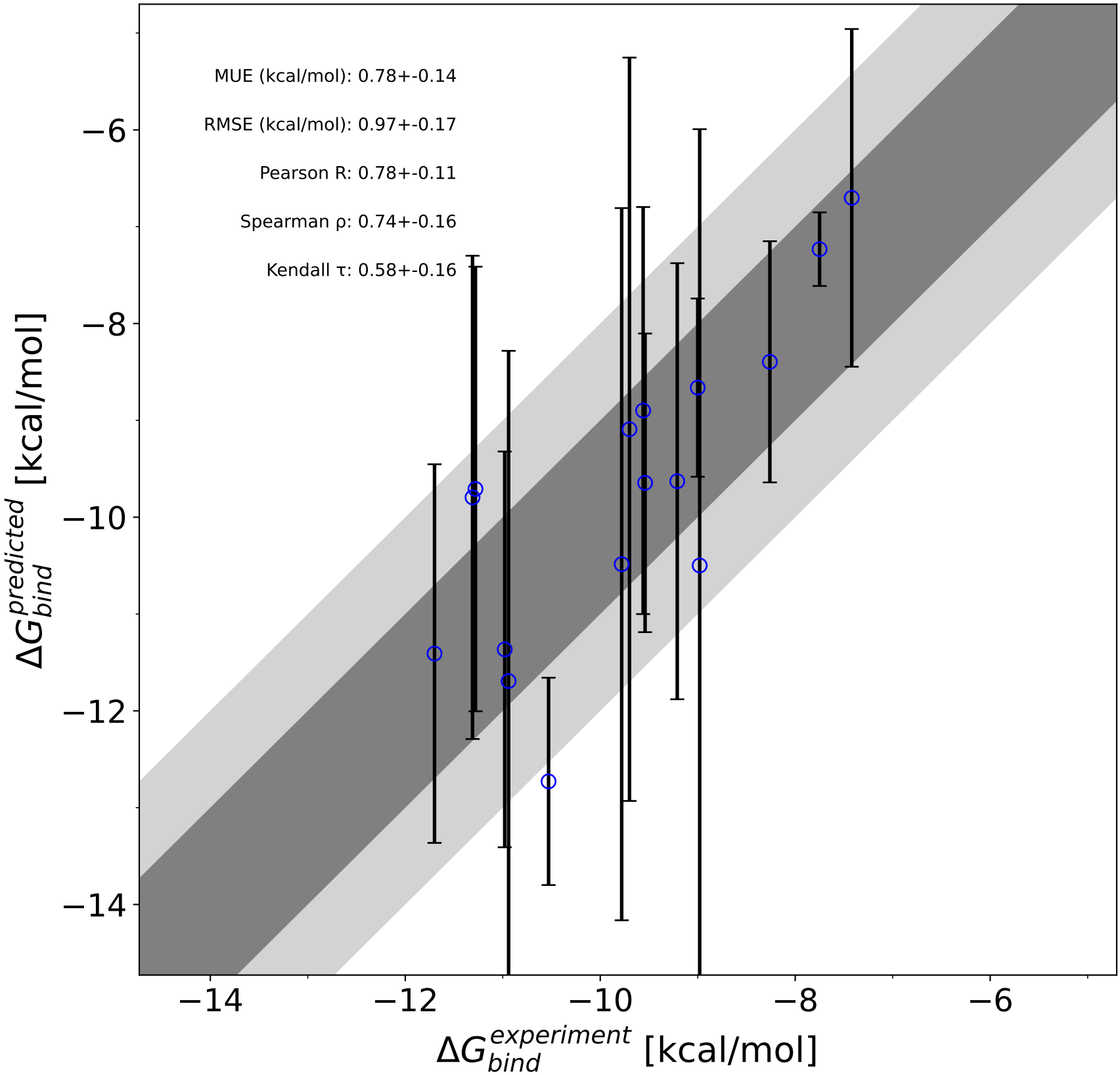
MUE (kcal/mol): 0.78+-0.14
RMSE (kcal/mol): 0.97+-0.17
Pearson R: 0.78+-0.11
Spearman ρ: 0.74+-0.16
Kendall τ: 0.58+-0.16
−6
−8
−10
−12
−14
−14
−12
−10
−8
−6
$\Delta G_{bind}^{predicted}$ [kcal/mol]
$\Delta G_{bind}^{experiment}$ [kcal/mol]