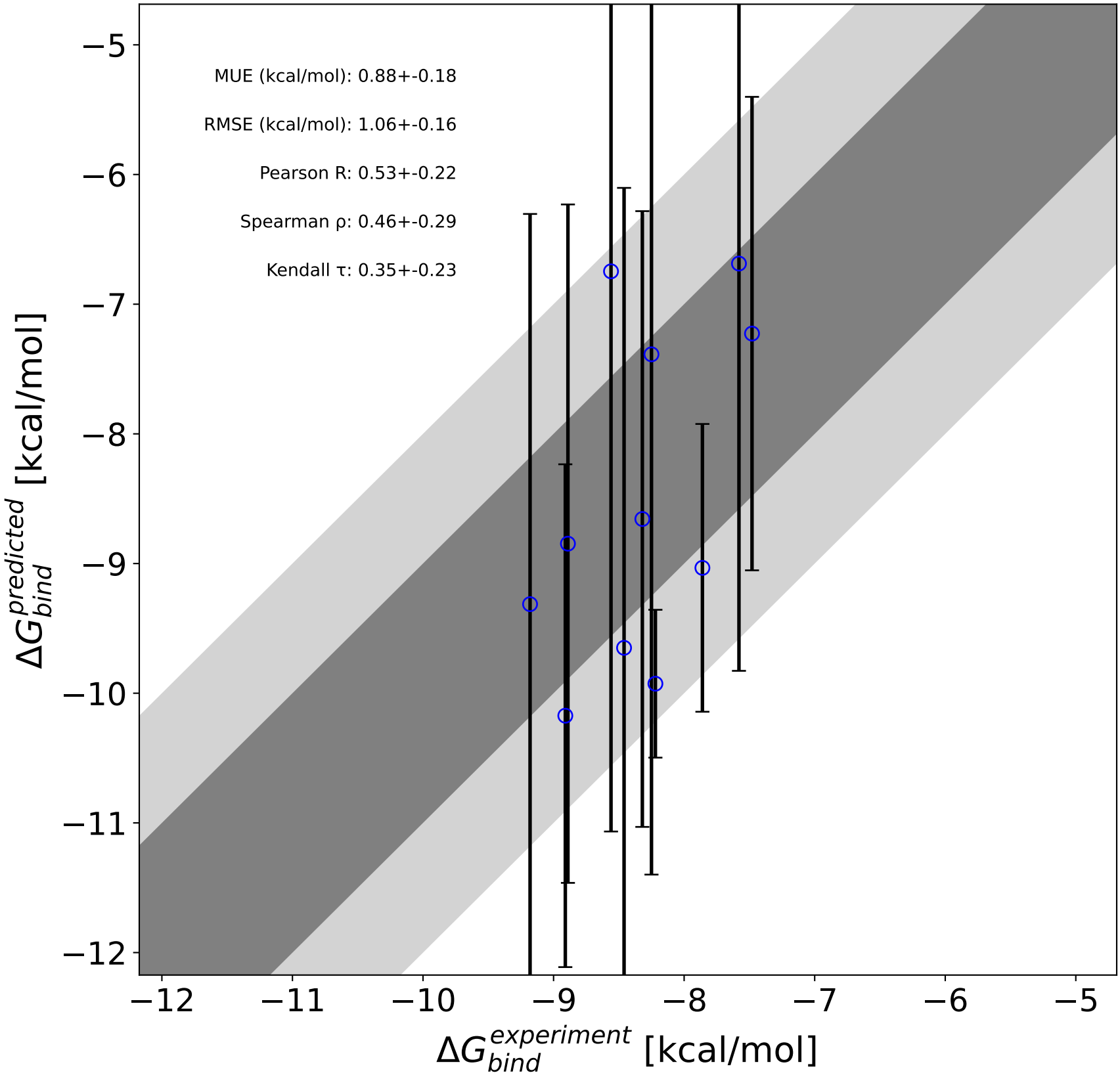
MUE (kcal/mol): 0.88+-0.18
RMSE (kcal/mol): 1.06+-0.16
Pearson R: 0.53+-0.22
Spearman ρ: 0.46+-0.29
Kendall τ: 0.35+-0.23
−5
−6
−7
−8
−9
−10
−11
−12
−12
−11
−10
−9
−8
−7
−6
−5
$\Delta G_{bind}^{predicted}$ [kcal/mol]
$\Delta G_{bind}^{experiment}$ [kcal/mol]