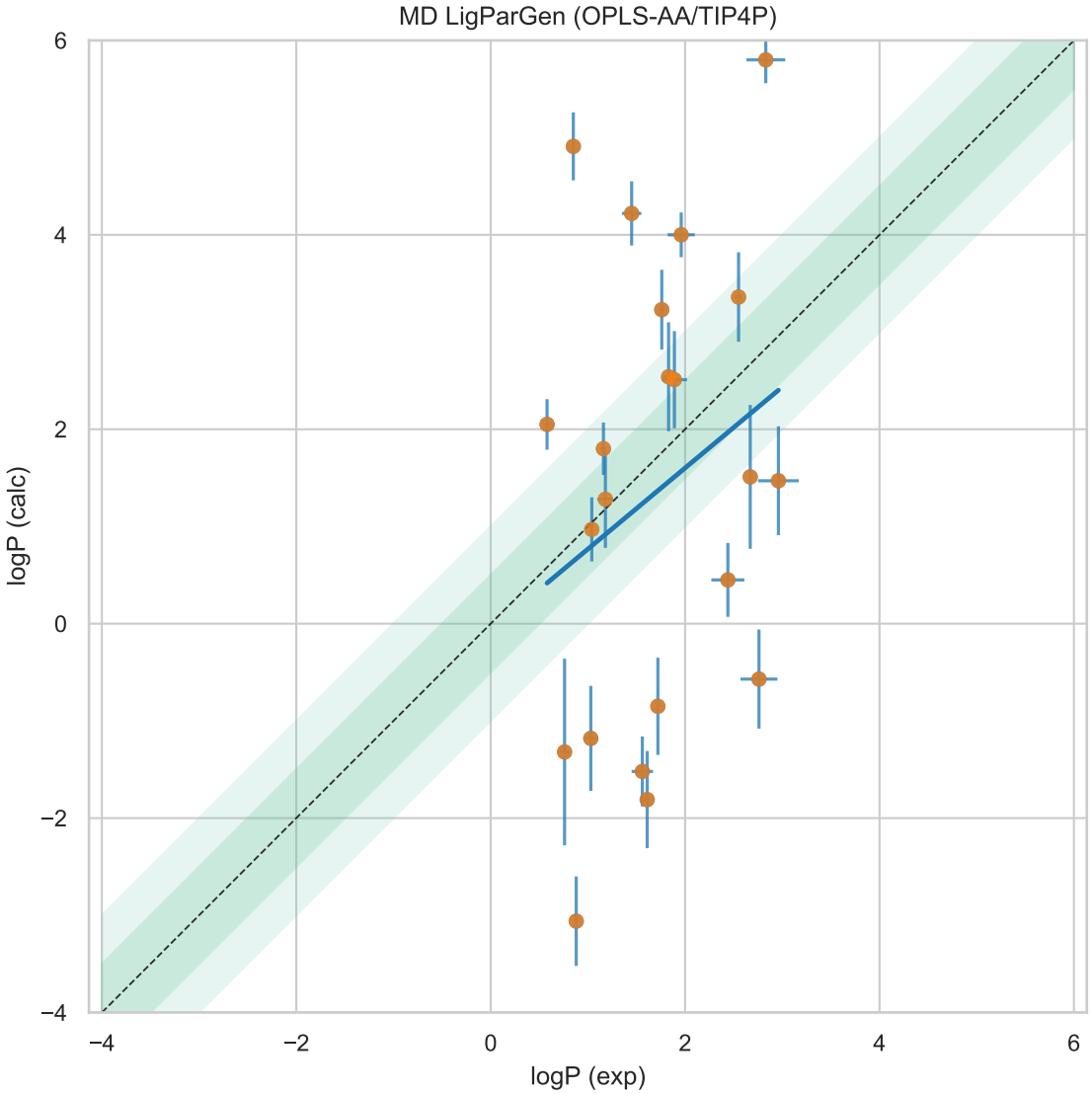
MD LigParGen (OPLS-AA/TIP4P)
logP (calc)
logP (exp)
6
4
2
0
−2
−4
−4
−2
0
2
4
6