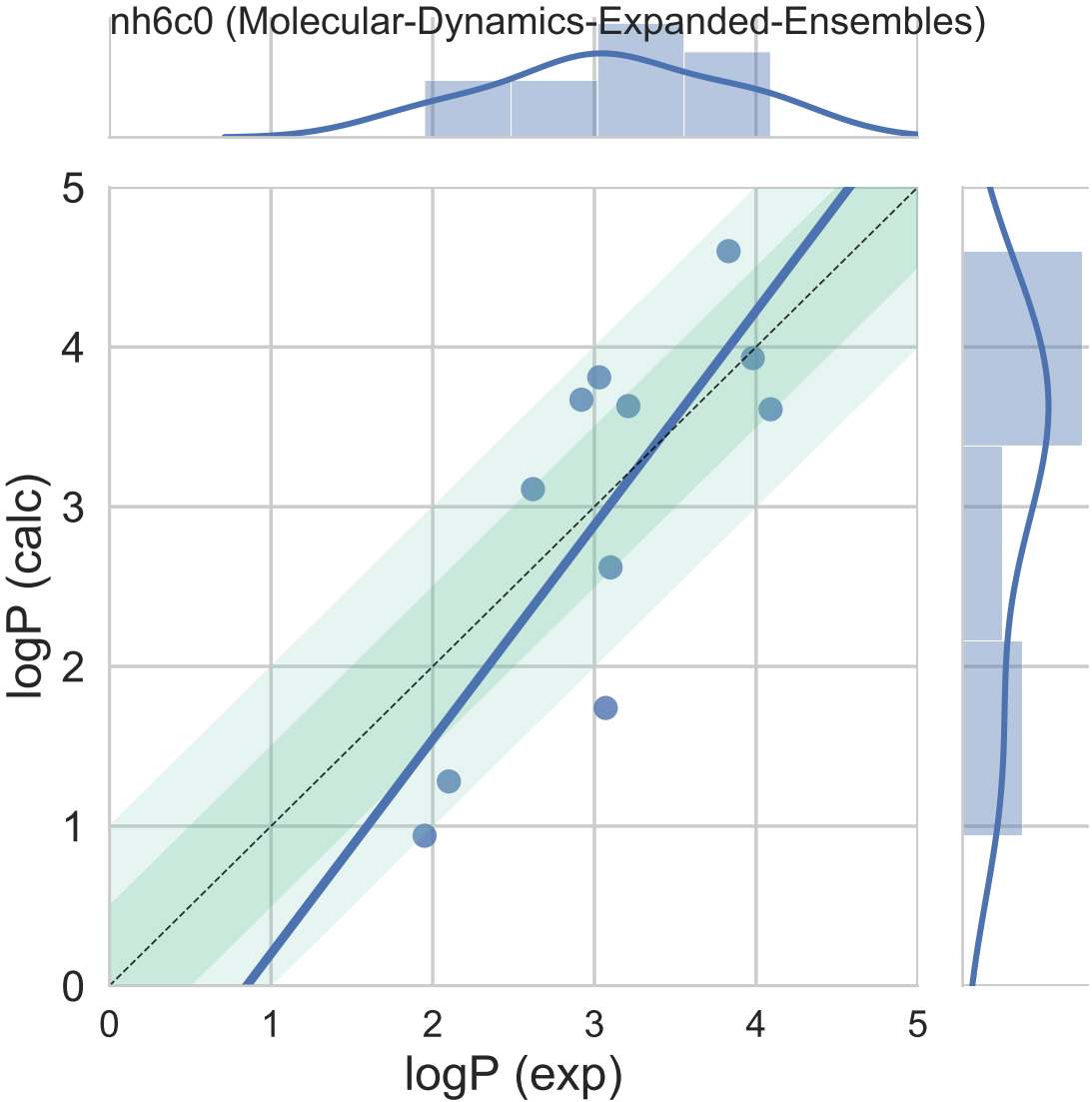
nh6c0 (Molecular-Dynamics-Expanded-Ensembles)
logP (calc)
logP (exp)
0
1
2
3
4
5