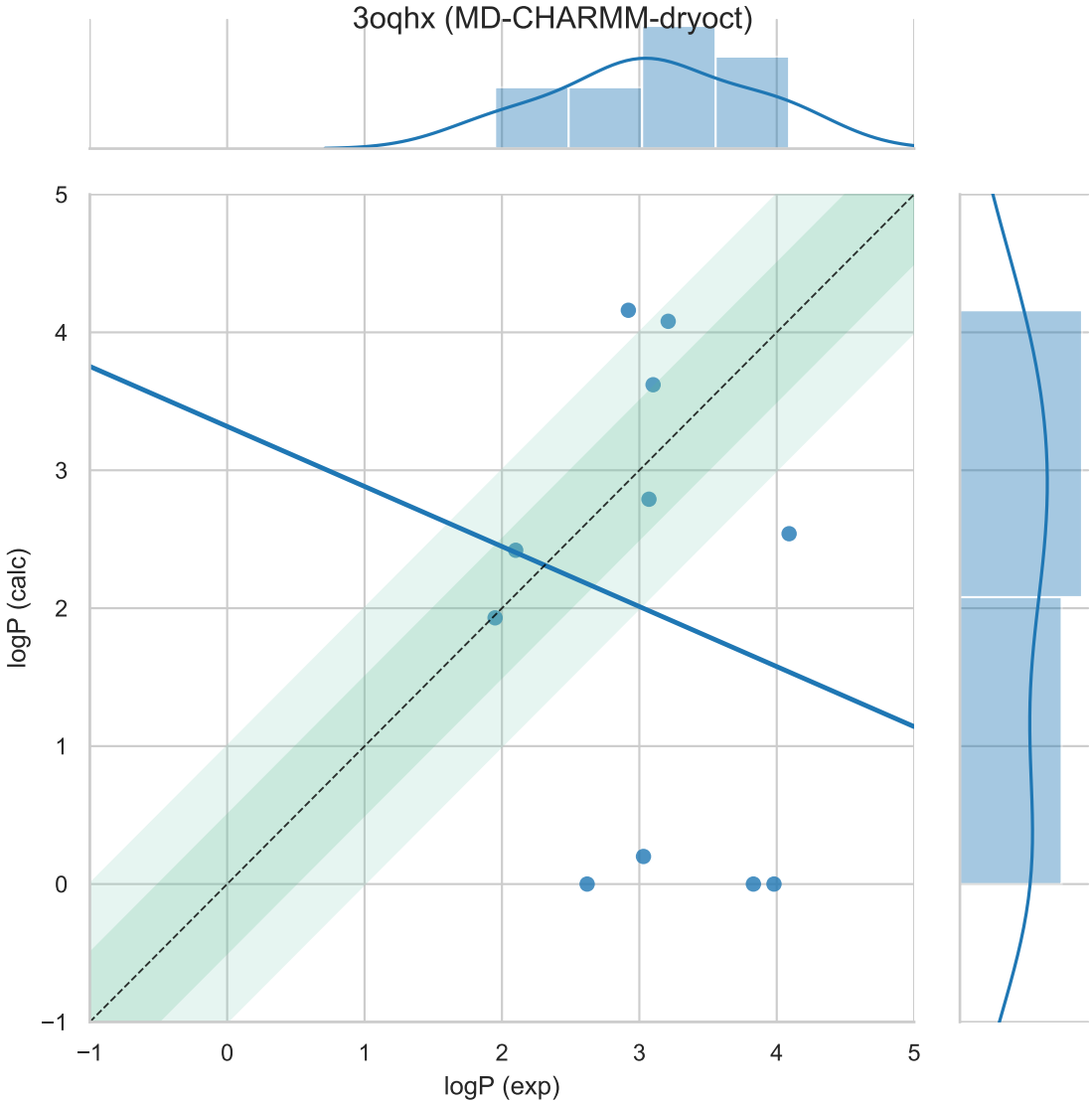
3oqhx (MD-CHARMM-dryoct)
logP (calc)
logP (exp)
5
4
3
2
1
0
−1
−1
0
1
2
3
4
5