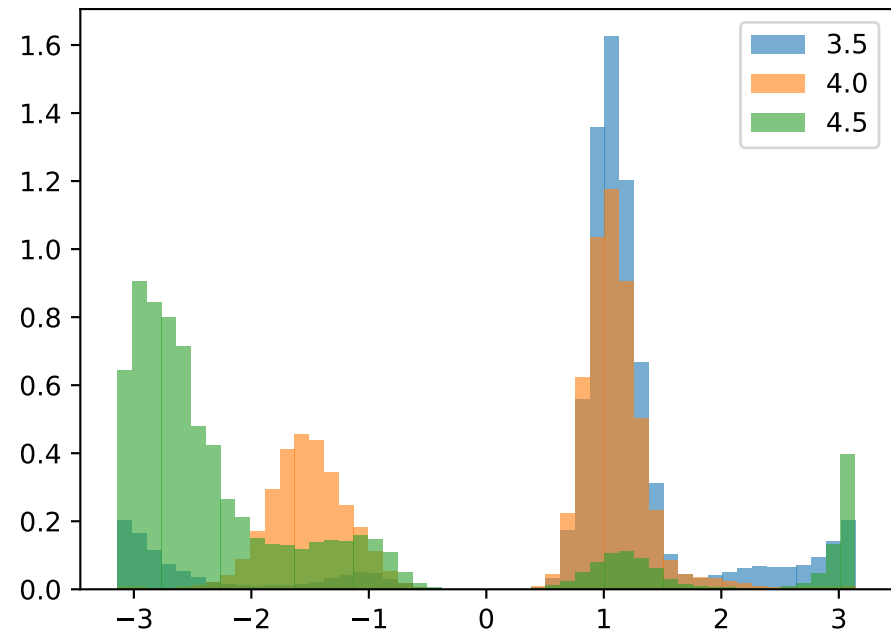


protonation state 1

obs. chi



obs. eRMSD

