## Comparison of average reduced $\chi^2$ of Bcl-x<sub>L</sub> - PUMA replicates [2M04] replicate 1 (CHARMM22\* + TIP3P) replicate 2 (CHARMM22\* + TIP3P) replicate 3 (CHARMM22\* + TIPS3P) 6 replicate 3 (a99SB-disp) 5 Average reduced $\chi^2$ 3 2 1 0 Ċα Сβ Ν Н

Atom type