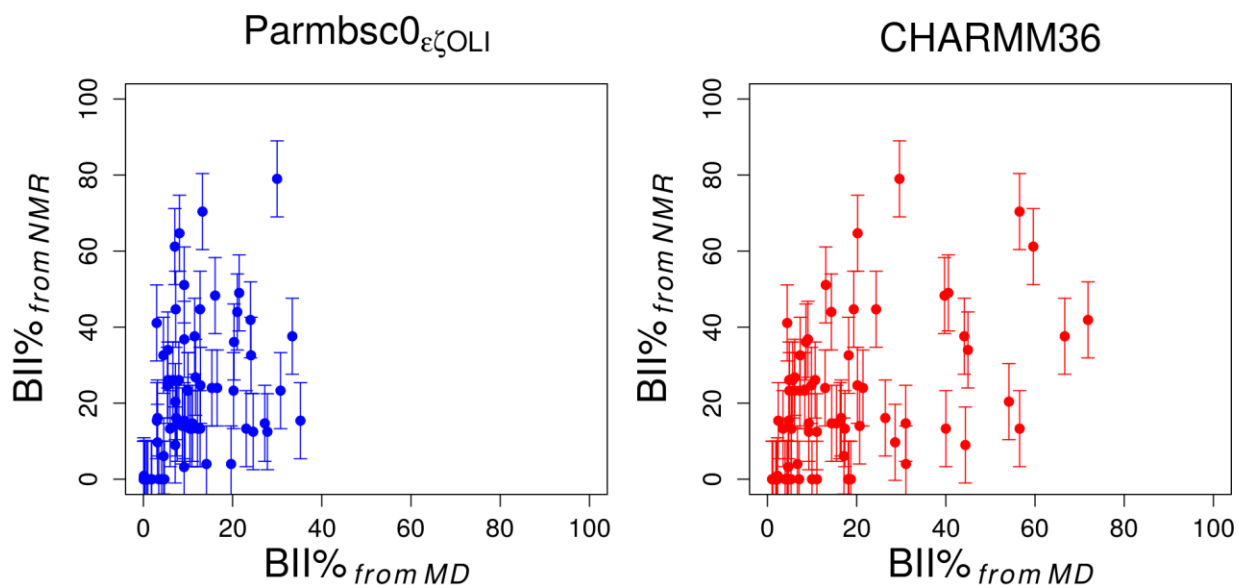


**S7 Fig.** Comparison between simulated and experimental BII percentages.



BII percentages were extracted from MDs ( $BII\%_{from\ MD}$ ) with Parmbsc0<sub>εζOLI</sub> (left panels, blue points) or CHARMM36 (right panels, red points) and compared with the corresponding values inferred from  $\delta$ Ps ( $BII\%_{from\ NMR}$ ). The vertical bars represent the error on  $BII\%_{from\ NMR}$ . The correlation coefficients are given in Table 2 (text section “Sequence-dependent BII propensities from simulations versus NMR.”).

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