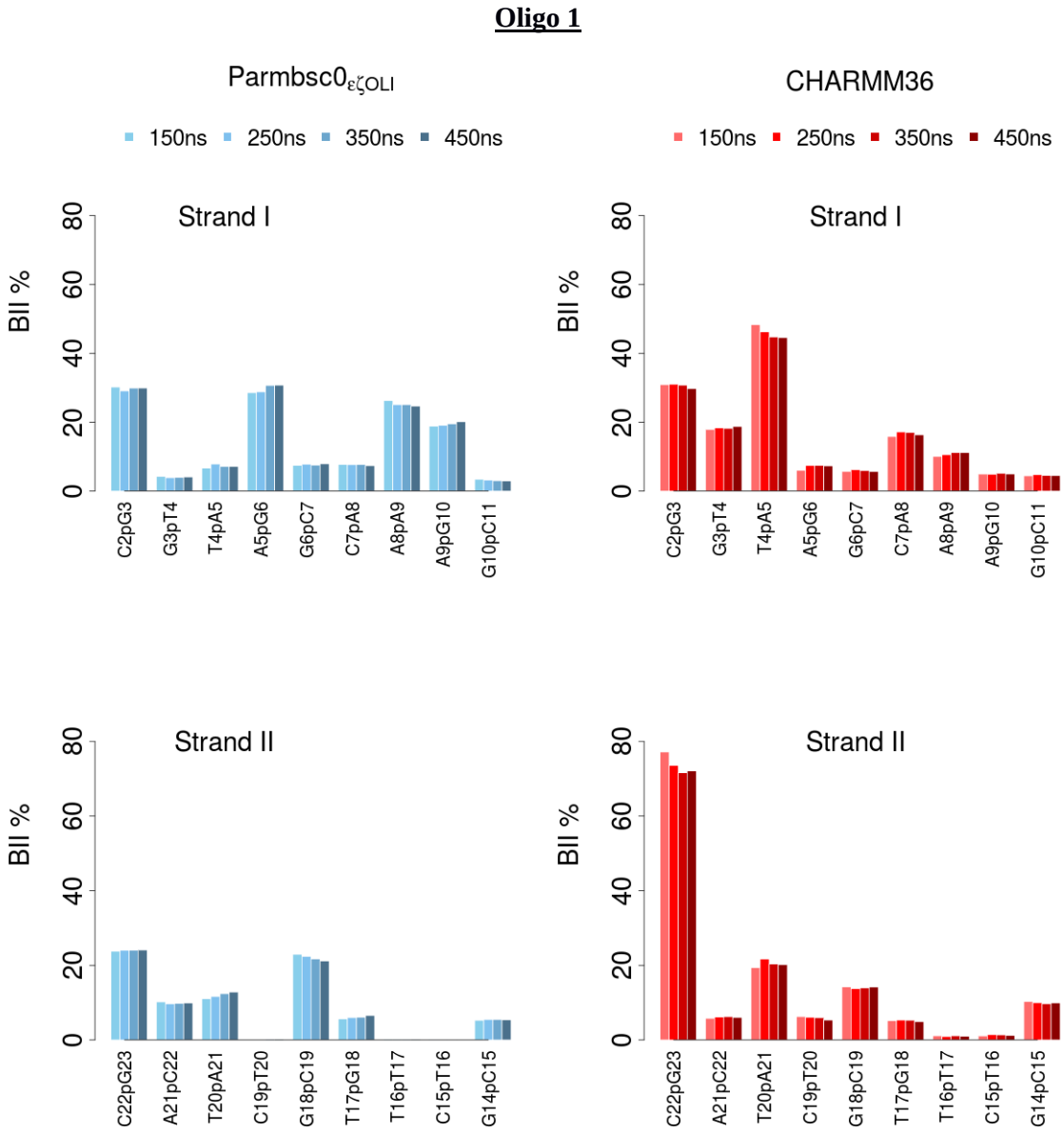
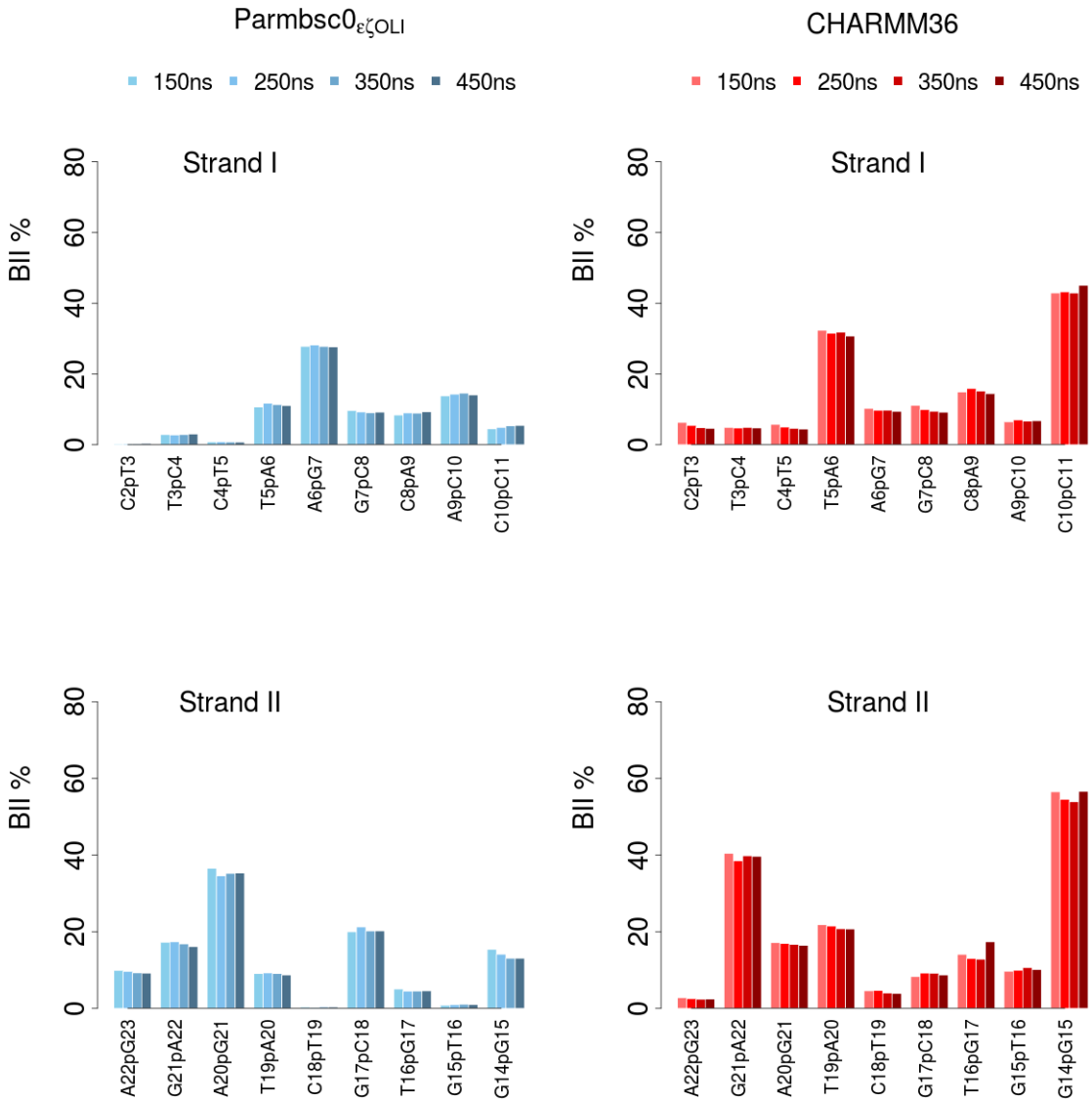
S2 Fig. Convergence of BII percentages in 450ns and 1μs MD simulations.



Cumulative BII percentages (BII%) of the dinucleotide steps were extracted from trajectories carried out with either Parmbsc0$_{\varepsilon\zeta OLI}$ (left, blue) or CHARMM36 (right, red) force fields. BII% were calculated for increasing length of MDs. The BII% were clearly not stabilized during the first 50ns, which are not considered in this analysis. To help identification of the facing steps, sequence in Strand 1 is shown from 5' to 3', while sequence in Strand 2 is shown from 3' to 5'.

Oligo 2



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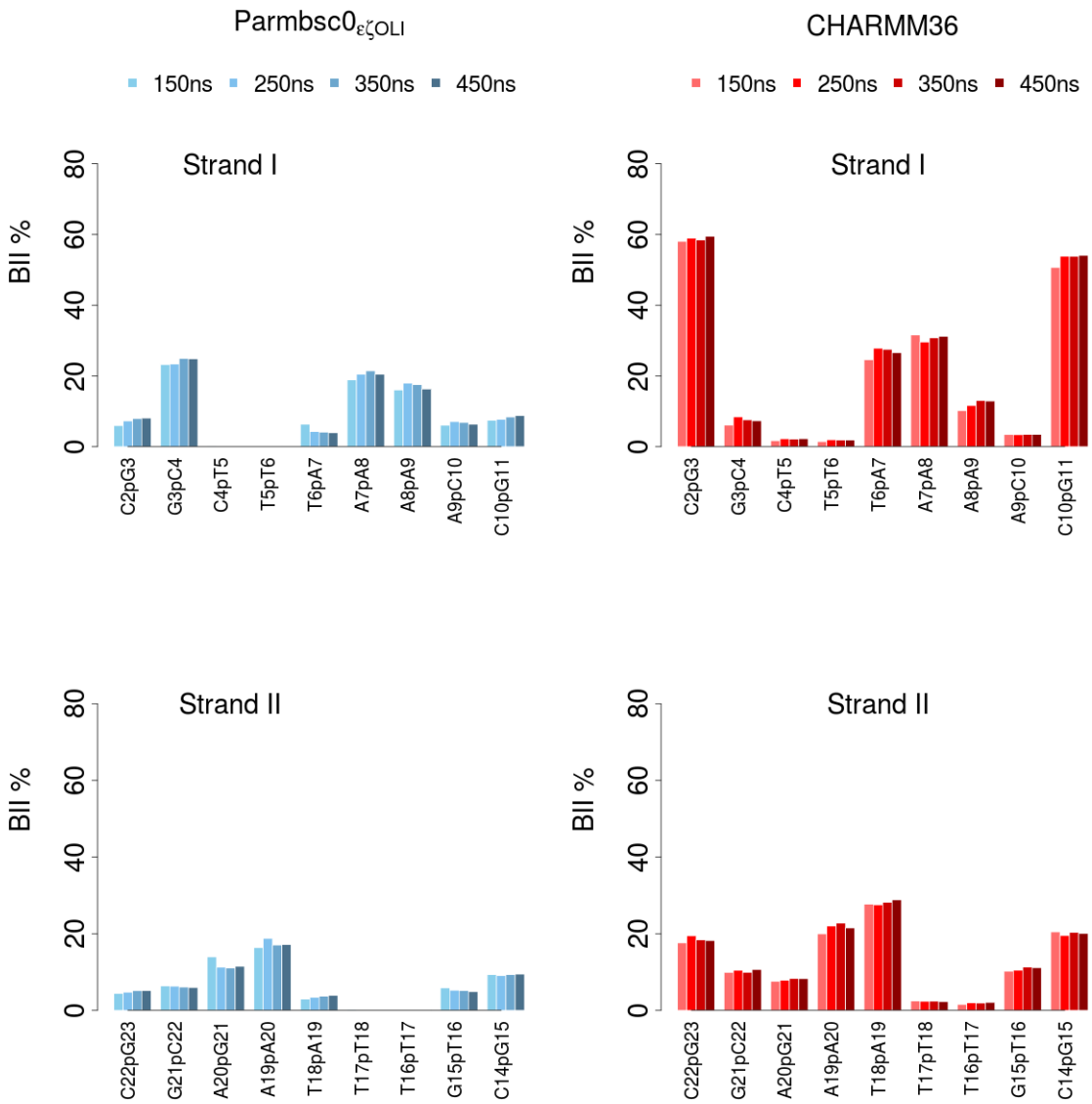
Oligo 3



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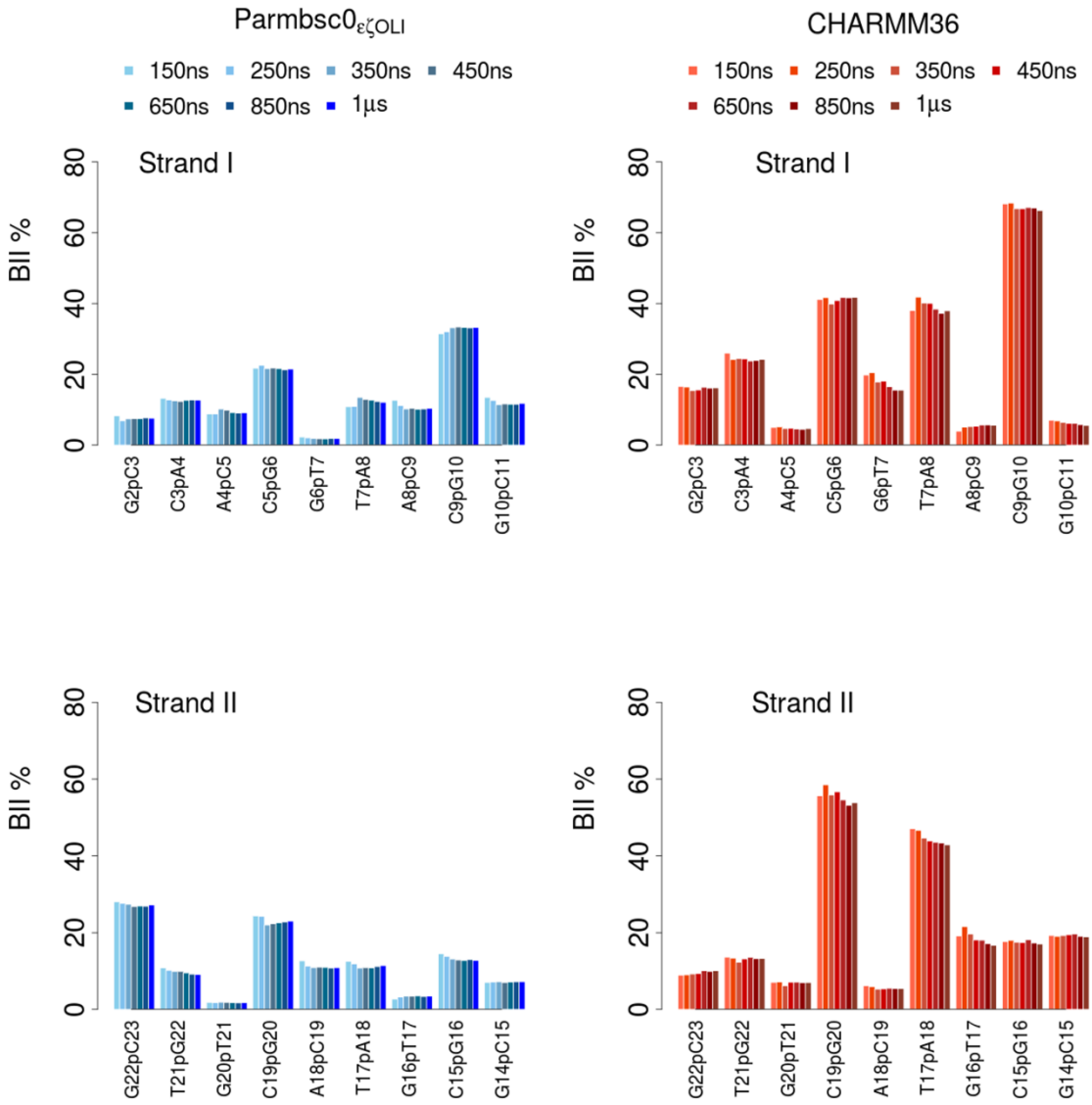
Oligo 4



Cumulative BII percentages (BII%) of the dinucleotide steps were extracted from trajectories carried out with either Parmbsc0$_{\varepsilon\zeta OLI}$ (left, blue) or CHARMM36 (right, red) force fields. BII% were calculated for increasing length of MDs. The BII% were clearly not stabilized during the first 50ns, which are not considered in this analysis. To help identification of the facing steps, sequence in Strand 1 is shown from 5' to 3', while sequence in Strand 2 is shown from 3' to 5'.

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