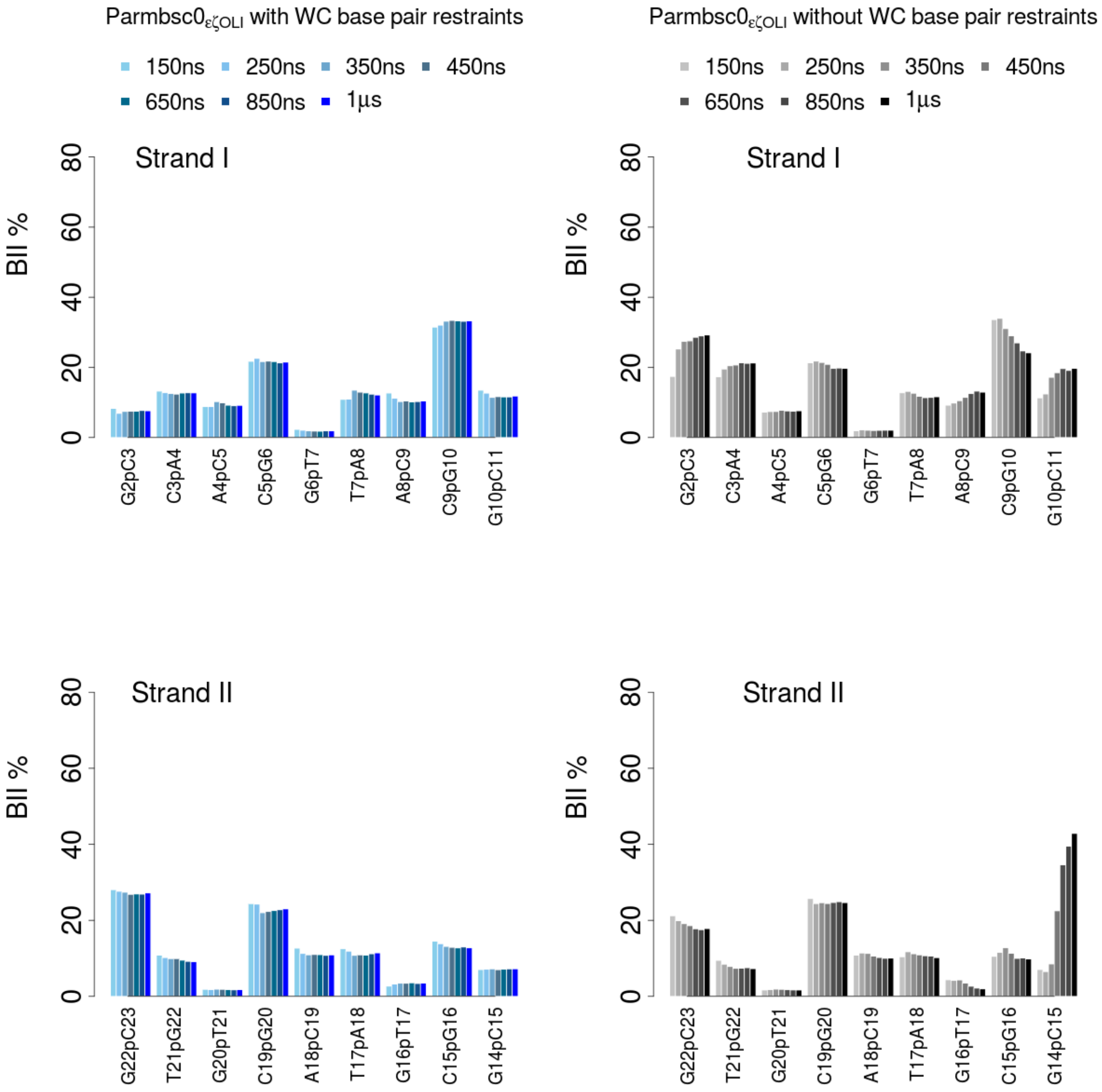
S4 Fig. Convergence of BII percentages in 1µs P-MD simulations of Oligo 4, with or without restraints on the pairing of the first and last base pairs.



Cumulative BII percentages (BII%) of the dinucleotide steps were extracted from trajectories carried out with Parmbsc0$_{\varepsilon\zeta OLI}$ with (left, blue) or without (right, grey red) restraining the Watson-Crick pairing of the first and last base pairs. BII% were calculated for increasing length of MDs. The first 50ns 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’. The convergence issues illustrated here with the unrestrained P-MD of Oligo 4 also occur with the three other Oligos and with the corresponding unrestrained C-MDs.

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