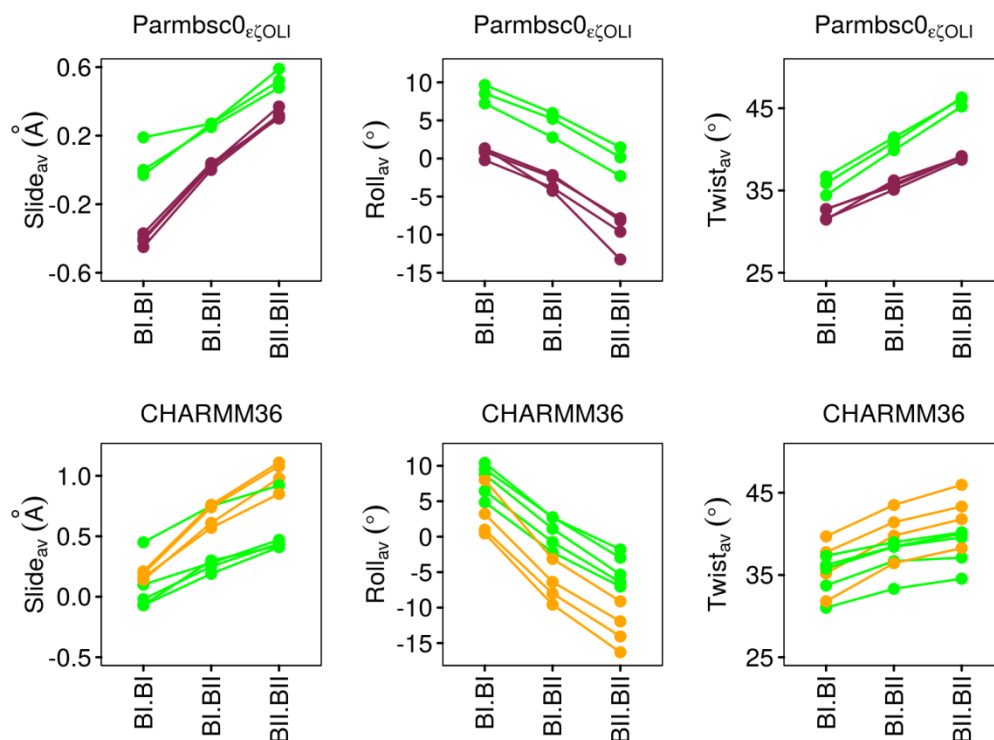


S9 Fig. Slide, Roll and Twist values associated to conformational combinations of facing phosphate linkages in representative BII-rich steps, generated by Parmbsc0_{εζ}OLI and CHARMM36.



The values of Slide, Roll and Twist were calculated for representative BII-rich steps, CpG•CpG of Oligos 1, 3 and 4 (green), GpC•GpC of Oligos 1, 2, 3 and 4 (violet) and TpA•TpA of Oligos 1, 3 and 4 (orange) according to the BI•BI, BI•BII|BII•BI and BII•BII combinations of their facing phosphate groups. The data were extracted from C-MDs (top panels) and P-MDs (bottom panels), and averaged along the MD for each backbone state. For clarity, the standard deviations were omitted.

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Akli Ben Imeddourene, Ahmad Elbahnsi, Marc Guérault, Christophe Oguey, Nicolas Foloppe, and Brigitte Hartmann