Electronic Supplementary Information

Microscopic understanding of the conformational features of a protein–DNA complex†

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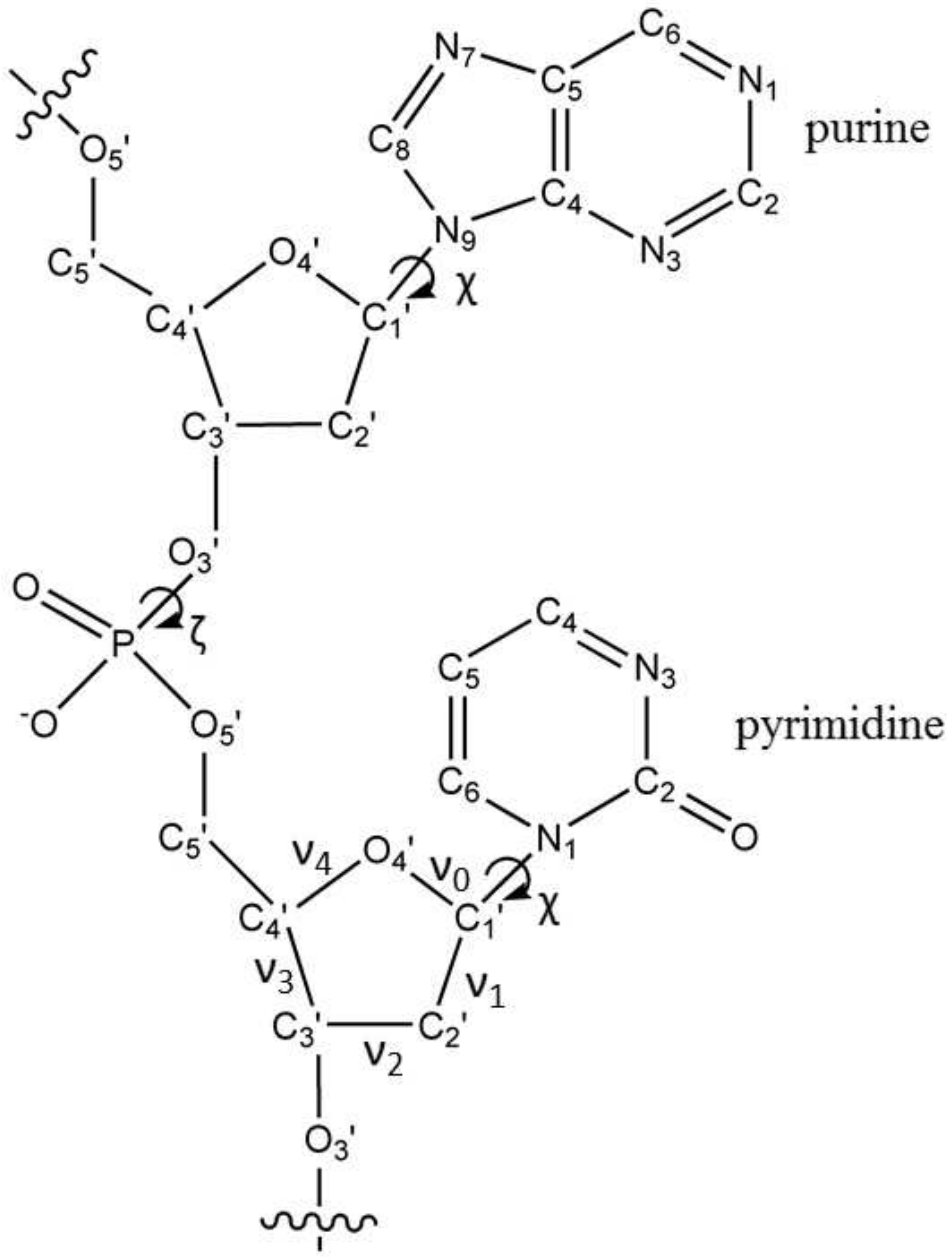

Fig. SI-1 Schematic representation of purine and pyrimidine nucleotides with IUPAC nomenclature of the individual atoms. The five endocyclic torsional angles (ν_i with i = 0 to 4) of the sugar moiety are C4′–O4′–C1′–C2′; O4′–C1′–C2′–C3′; C1′–C2′–C3′–C4′; C2′–C3′–C4′–O4′; and C3′–C4′–O4′–C1′, respectively, while the glycosidic torsion angles (χ) are O4′–C1′–N9–C4 (purine) and O4′–C1′–N1–C2 (pyrimidine). The angle ζ associated with the backbone phosphate group of the nucleotide is C3′–O3′–P–O5′.