Supporting information

Unveiling the role of histidine and tyrosine residues on the conformation of the avian prion hexarepeat domain

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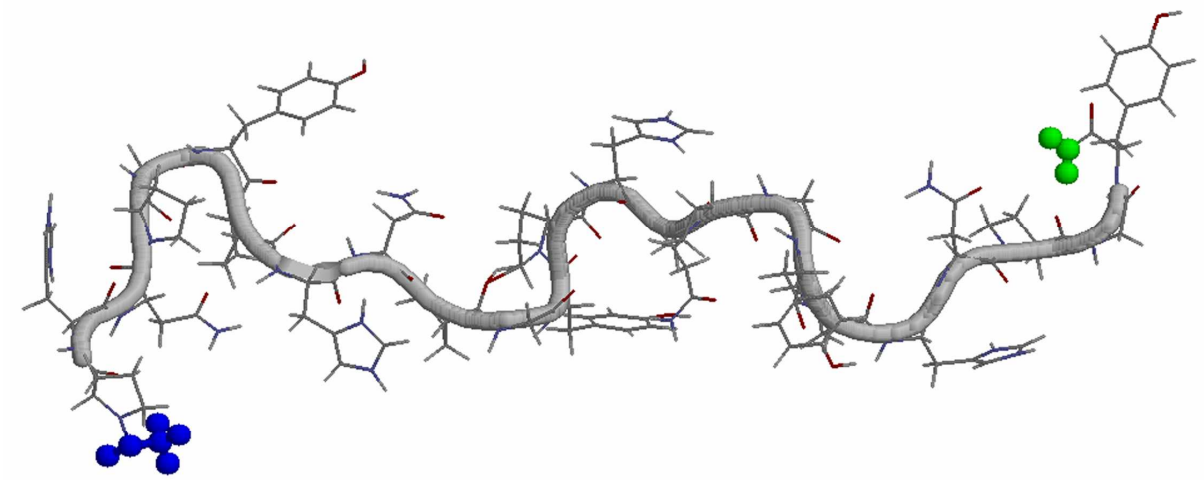
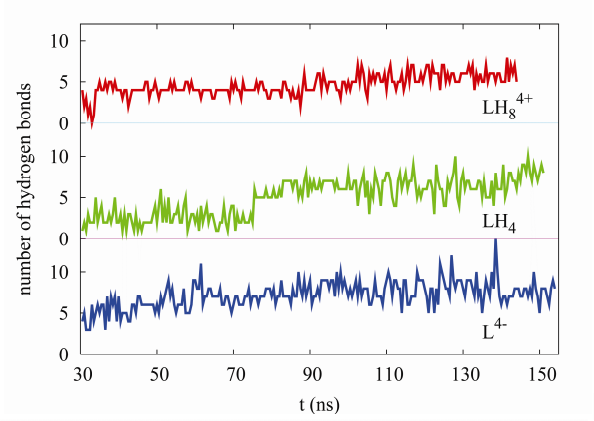
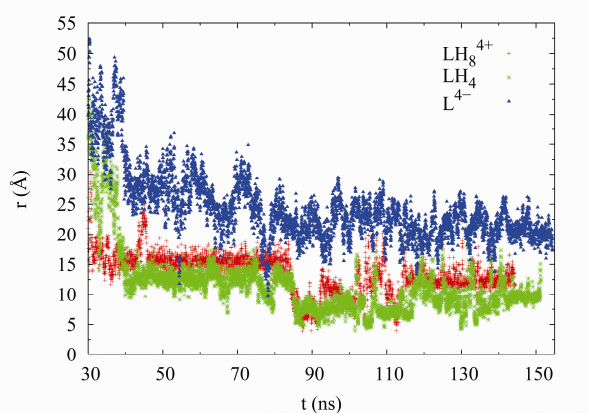


Figure 1: Starting configuration of TetraHexaPY, where the N-terminal Acetyl and the C-terminal amide are shown in blue and in green respectively.



[a]



[b]

Figure 2: Time evolution of hydrogen bonds number [a] and of the end-to-end distance relative to the C_α carbons [b]. Both of them are useful to check the equilibration of the starting configuration of the peptide, initially with an elongated structure and thus having few hydrogen bonds. This starting configuration is clearly lost during the run.

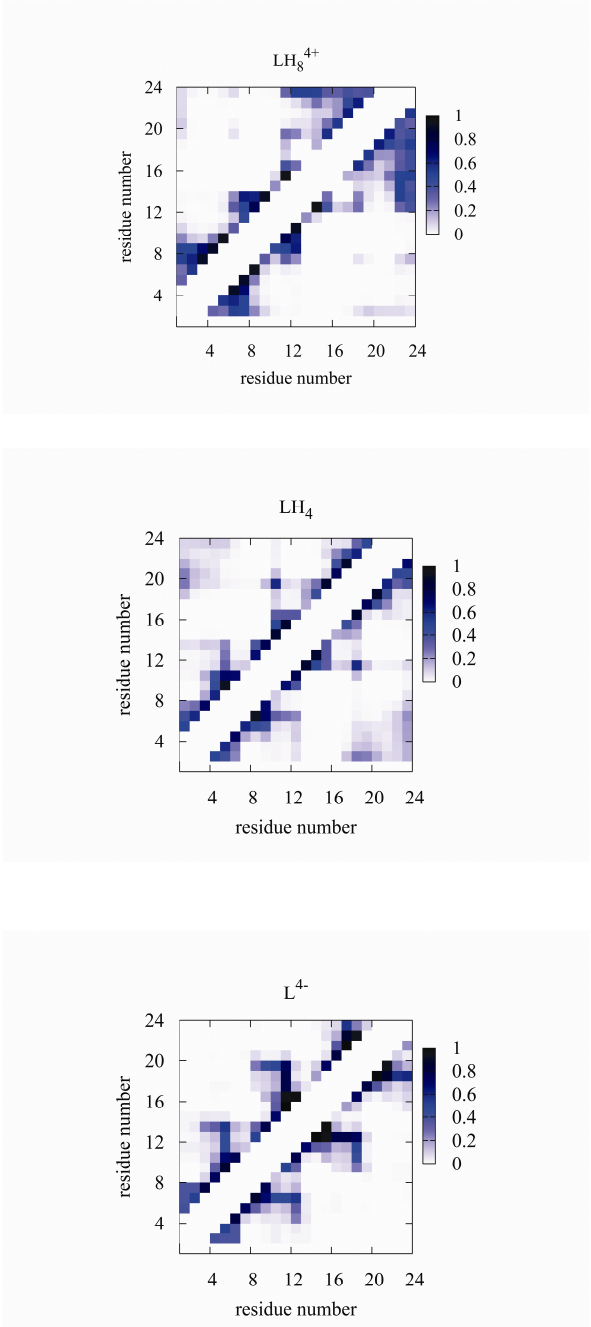


Figure 3: Contact maps of TetraHexaPY as a function of pH. It is worth to note a more compact structure at neutral pH (LH_4), underlined from the N- and C-terminal contacts and that the L^{4-} state shows the most expanded structure. The relative occurrence of the contacts is shown with a color code ranging from white to black.

Table 1: Average G values and relative standard deviations, σ_G, of the ideal secondary structures, involving at least NR residues. Each structure was built by extracting ϕ and ψ angles from a gaussian distribution, centered on the ideal ϕ and ψ values, with a gaussian half-height amplitude of 15 degree (see reference [38]).

Structure	$\langle G \rangle$	σ_G	Number of residues
α helix	-.04	0.02	>3
3_{10} helix	-.07	0.01	>3
β Turn I	-.07	0.01	2,3
β Sheets	+.00	0.01	≥2
PPII	+.10	0.03	>3
π helix	-.01	0.02	>3