

Conformation of polyalanine and polyglycine dications in the gas phase: Insight from ion mobility spectrometry and replica-exchange molecular dynamics

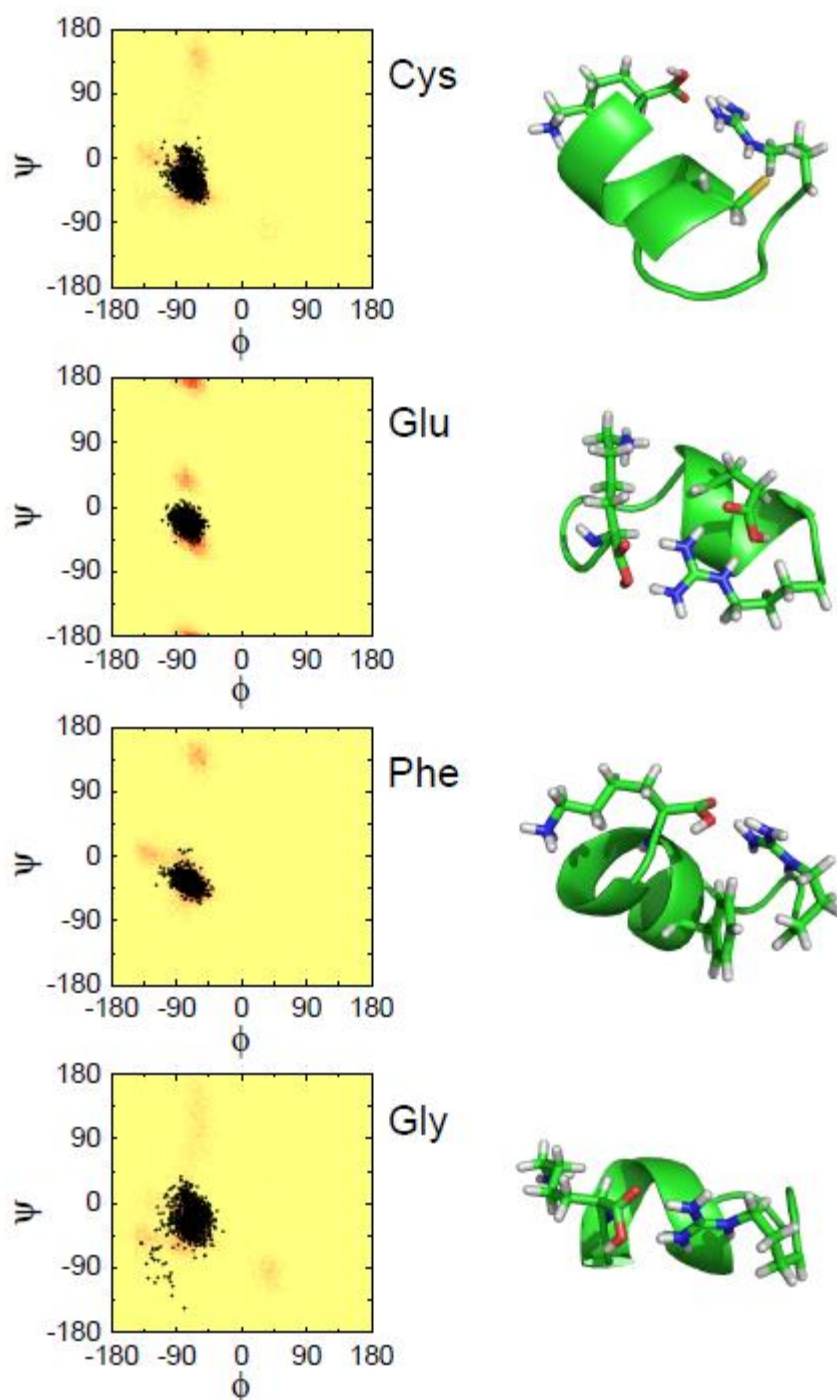
(Supporting Information)

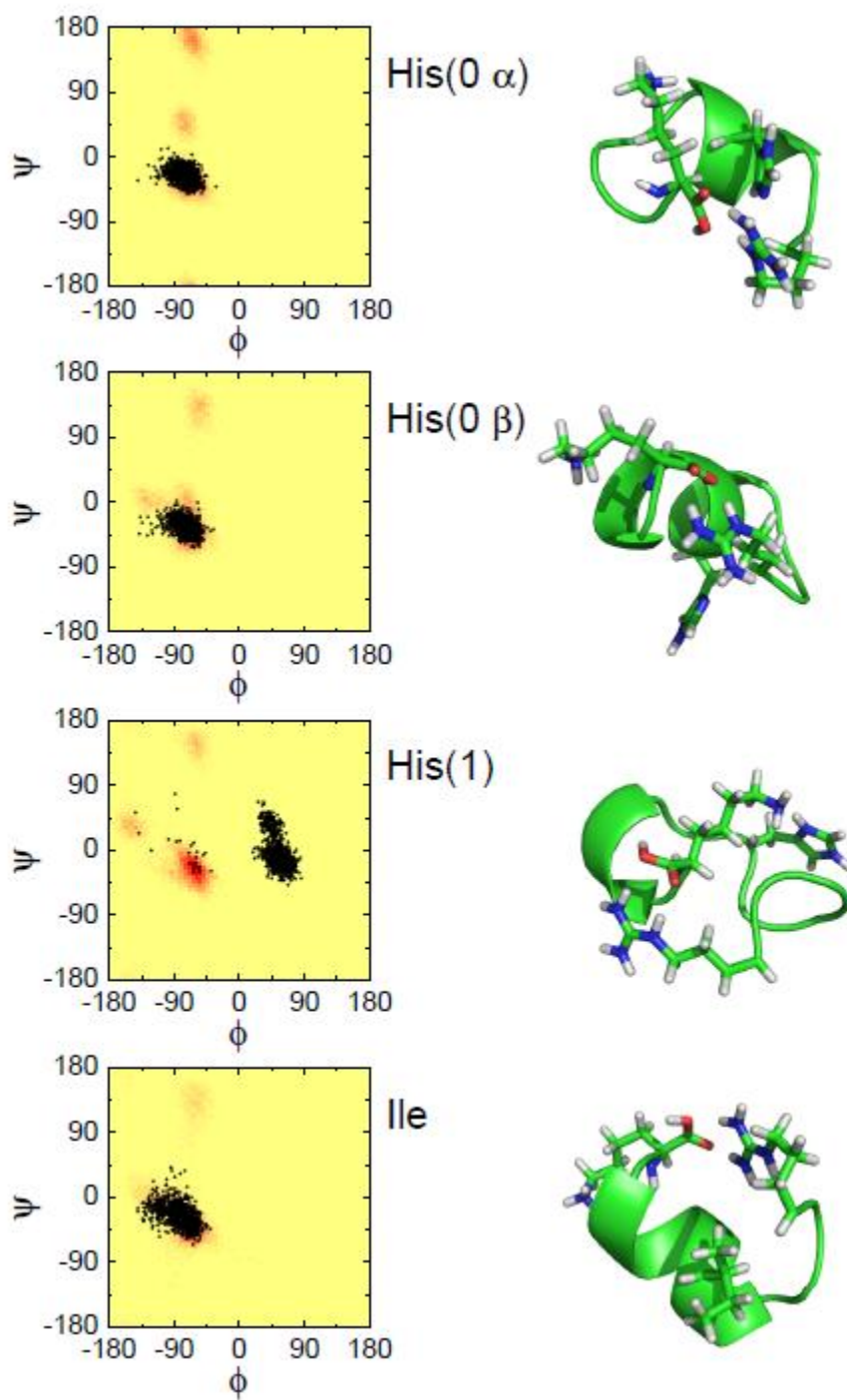
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Valéria Lepère^{a,d}, Rodolphe Antoine^a, Jérôme Lemoine^b, and Philippe Dugourd^a.*

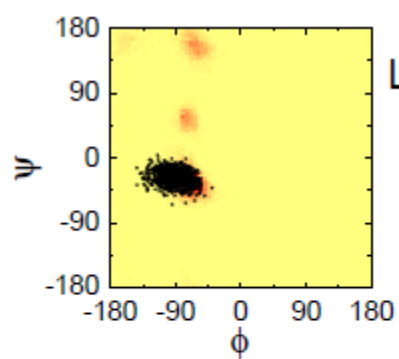
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France.

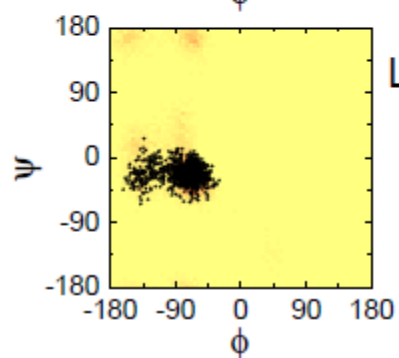
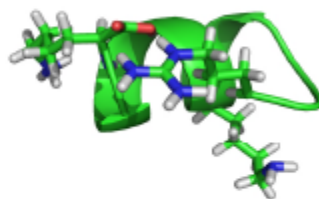
Ramachandran plots for $[\text{Arg}-(\text{Ala})_4\text{-X}-(\text{Ala})_4\text{-Lys}+2\text{H}]^{2+}$ extracted from samples of 1000 structures obtained from the 300 K REMD trajectories. The (ϕ, ψ) angles for the central residue are plotted as black dots and superimposed over a density plot of the backbone dihedral angles for all residues. The most stable structures are displayed next to the plots. In the case where several conformers are found to coexist, the most stable one is labeled (a), and the others (b), (c), etc. For $\text{X} = \text{His}$, Lys, and Arg the different protonation schemes are denoted as follows: (1) if the central residue is protonated and the terminal Lys is neutral, and (0) in the other case. For $\text{X} = \text{His}$, the two possible neutral tautomers are further labeled α and β .



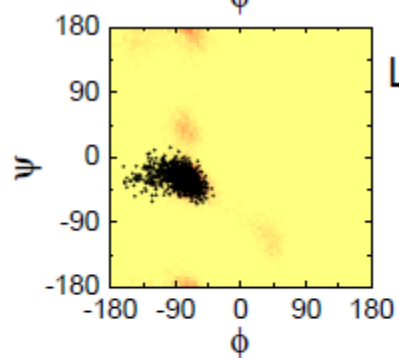
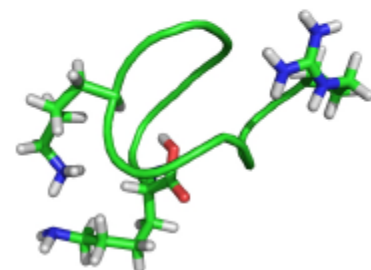




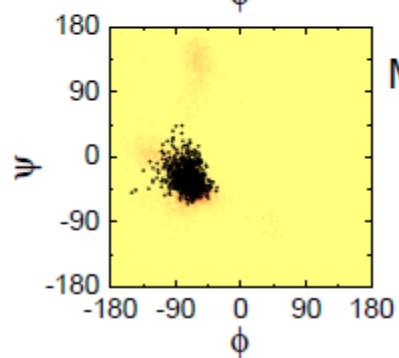
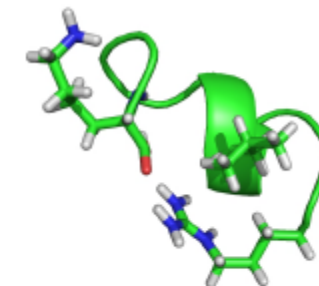
Lys(0)



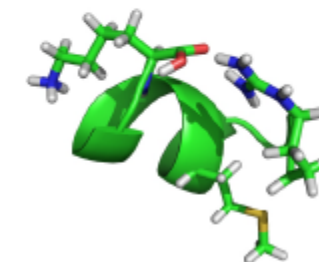
Lys(1)

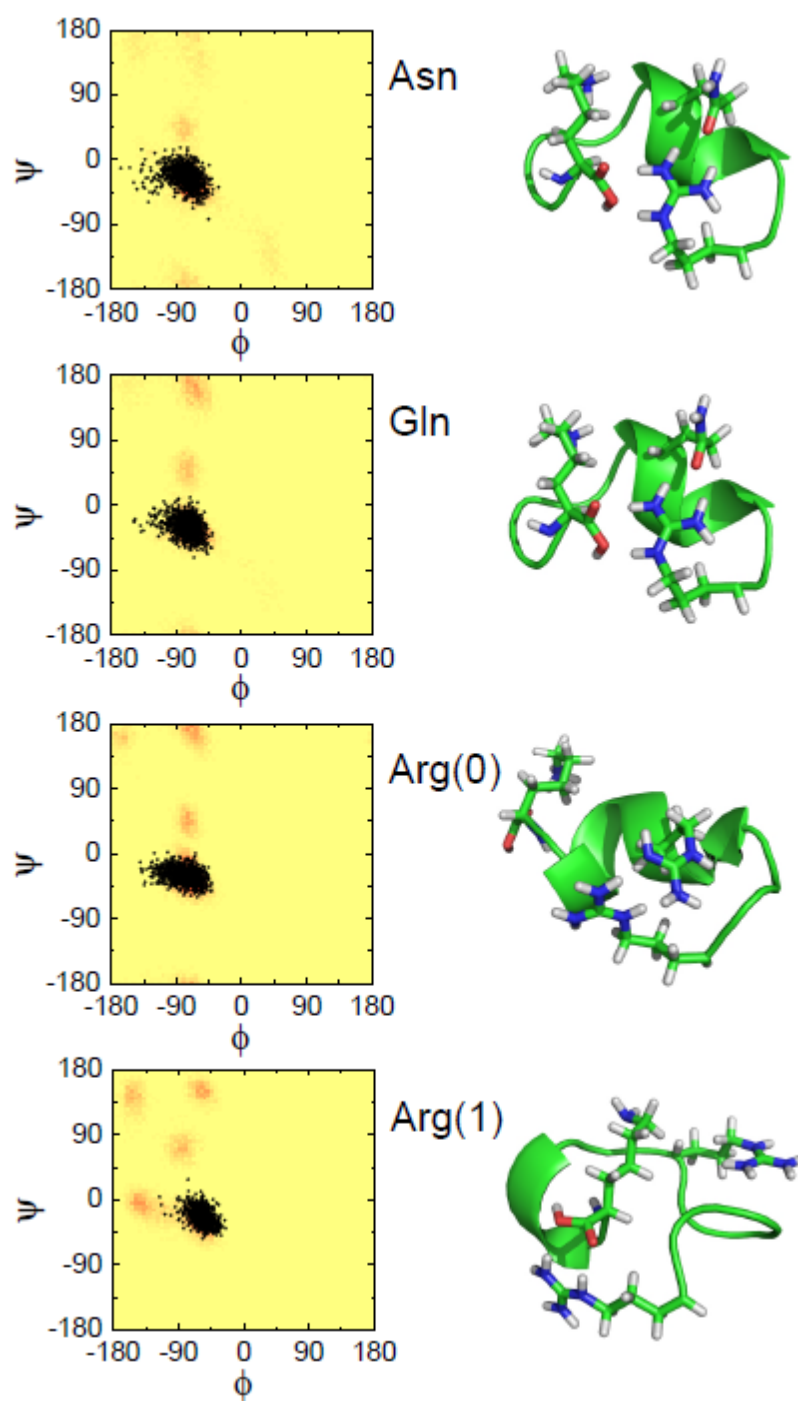


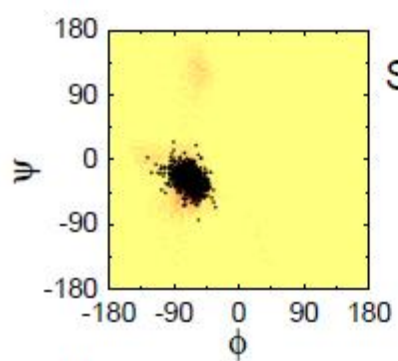
Leu



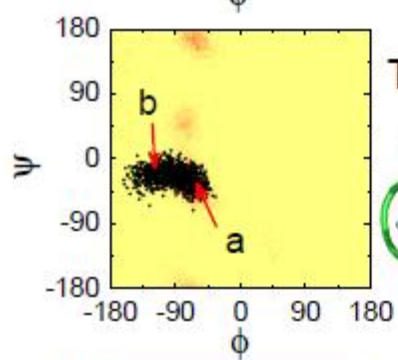
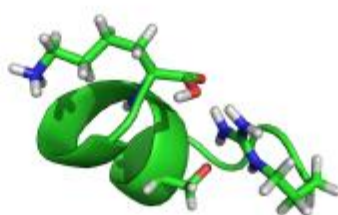
Met



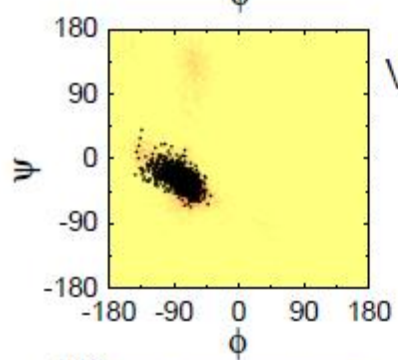
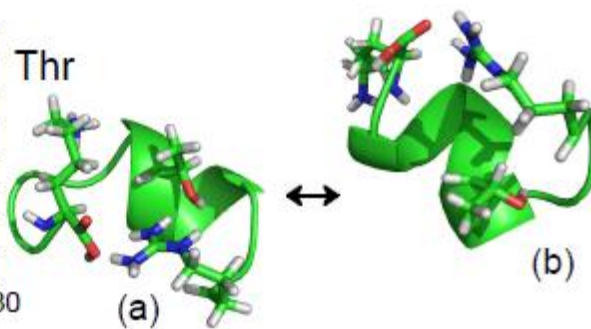




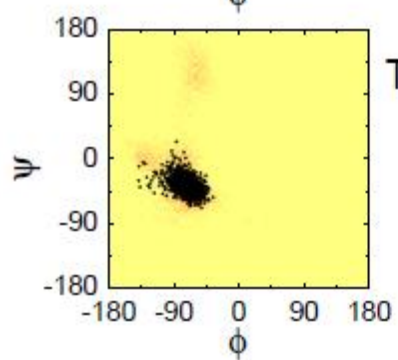
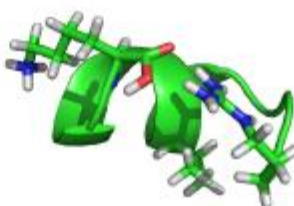
Ser



Thr



Val



Tyr



Ramachandran plots for $[\text{Arg}-(\text{Gly})_4\text{-X}-(\text{Gly})_4\text{-Lys}+2\text{H}]^{2+}$ extracted from samples of 1000 structures obtained from the 300 K REMD trajectories. The (ϕ, ψ) angles for the central residue are plotted as black dots and superimposed over a density plot of the backbone dihedral angles for all residues. The most stable structures are displayed next to the corresponding plots. In the case where several conformers are found to coexist, the most stable one is labeled (a), and the others (b), (c), etc. For X = His, Lys, and Arg the different protonation schemes are denoted as follows: (1) if the central residue is protonated and the terminal Lys is neutral, and (0) in the other case. For X = His, the two possible neutral tautomers are further labeled α and β .

