Figure S1: Water Surface Accessible Area for AA3 plotted against the Ramachandran angles $\Phi$ and $\Psi$, $nm^2$
Figure S2: Relative ‘local’ density of sodium cations (top) and anions (bottom) in the first (left) and second solvation shell of the whole tripeptide plotted against the molar concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - $F^-$; green dashed line (□) - $Cl^-$; black dotted line (♦) - $Br^-$; purple dash-dotted line (•) - $I^-$. 
Figure S3: Relative 'local' density of sodium cations (top) and anions (bottom) in the first (left) and second solvation shell of the tripeptide amino terminus plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - $F^-$; green dashed line (□) - $Cl^-$; black dotted line (◊) - $Br^-$; purple dash-dotted line (●) - $I^-$. 
Figure S4: Relative 'local' density of sodium cations (top) and anions (bottom) in the first (left) and second solvation shell of the tripeptide carboxyl terminus group plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - $F^-$; green dashed line (□) - $Cl^-$; black dotted line (◊) - $Br^-$; purple dash-dotted line (●) - $I^-$. 
Figure S5: Relative 'local' density of sodium cations (top) and anions (bottom) in the first (left) and second solvation shell of the tripeptide backbone groups plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - F⁻; green dashed line (□) - Cl⁻; black dotted line (♦) - Br⁻; purple dash-dotted line (•) - I⁻.
Figure S6: Relative 'local' density of sodium cations (top) and anions (bottom) in the first (left) and second solvation shell of the tripeptide side groups plotted against the concentration of ions. The concentrations are 0.20, 0.50, 1.00 and 2.00 M. Different lines correspond to different anions: blue solid line (○) - F⁻; green dashed line (□) - Cl⁻; black dotted line (♦) - Br⁻; purple dash-dotted line (●) - I⁻.
Figure S7: Depth (left side) and position (right side) of the PMF minima between the carboxyl terminus, $F^-$ anions (top) and $Na^+$ cations (bottom) in $NaF$ solution. The data are shown as functions of salt concentration. Different lines correspond to different PMFs: tripeptide group - water oxygen PMF corresponds to the solid blue line (thick, ◦); tripeptide group - ion PMF corresponds to the green dashed line (□); ion - water PMF corresponds to the black dotted line (♦), ion - ion PMF corresponds to the purple dash-dotted line (●) - $I^-$ and ion - counterion PMF corresponds to the red solid line (thin, crosses). The values for the minima depths are shown in $k_BT$ units and the minima positions are shown in Angstroems.
Figure S8: The same data as on the Fig. 7 for the second side chain group and NaF solution.
Figure S9: The same data as on the Fig. 7 for the **second side chain group** and NaCl solution.
Figure S10: The same data as on the Fig. 7 for the second side chain group and NaBr solution.
Figure S11: The same data as on the Fig. 7 for the second side chain group and NaI solution.
Figure S12: The same data as on the Fig. 7 for the first backbone group and NaF solution.
Figure S13: The same data as on the Fig. 7 for the first backbone group and NaCl solution.
Figure S14: The same data as on the Fig. 7 for the first backbone group and NaBr solution.
Figure S15: The same data as on the Fig. 7 for the first backbone group and NaI solution.