Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Electronic Supporting Information

Are stabilizing osmolytes preferentially excluded from the protein surface? FTIR and MD studies.

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MD simulations – Preferential interaction coefficients for other osmolytes solutions

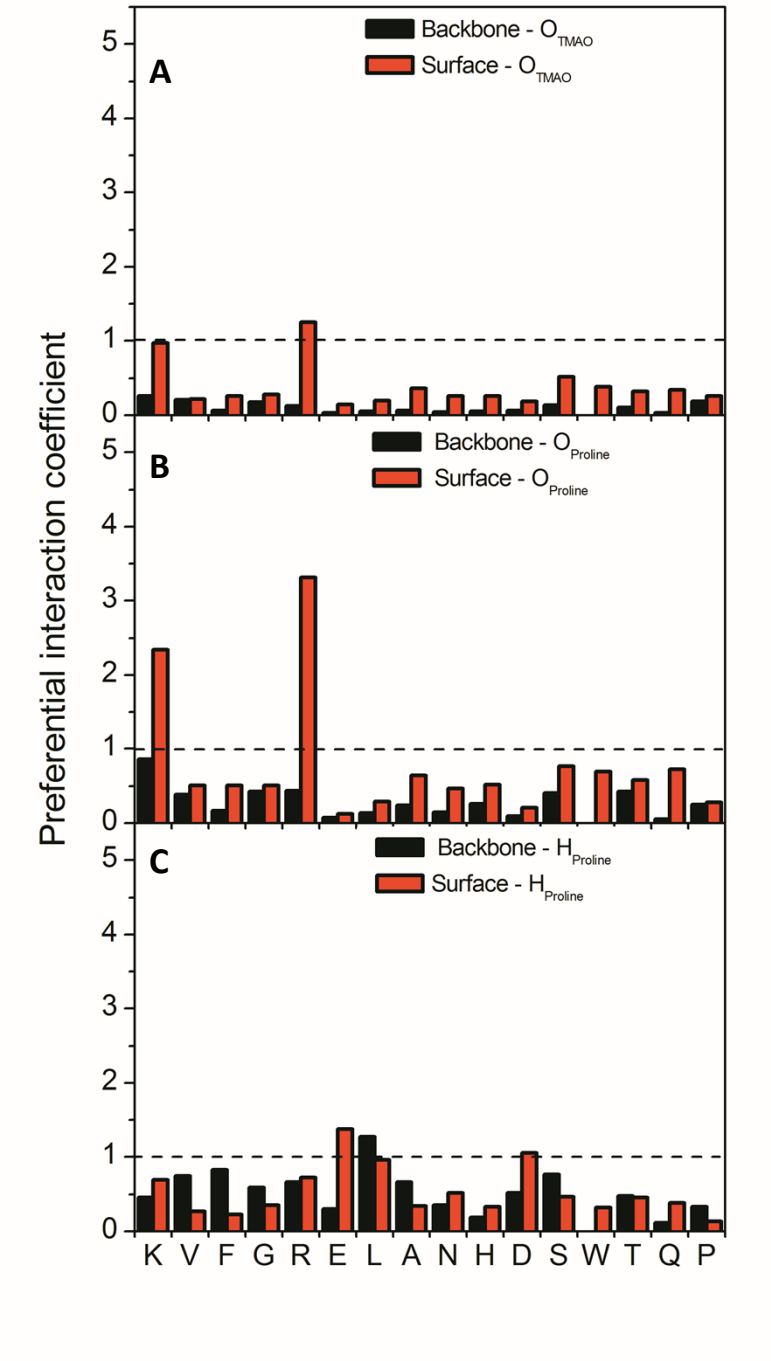

Figure S1. Preferential interaction coefficients calculated on the basis of interatomic distances obtained for individual amino acid residues at the surface of Lysozyme from molecular dynamics simulations for 2 M osmolyte solution: (A) Lysozyme – TMAO oxygen, (B) Lysozyme – Proline carboxylic oxygens, (C) Lysozyme – Proline amine protons. For each amino acid the coefficient was computed separately for the backbone and for the side chain surface – Equation (3)

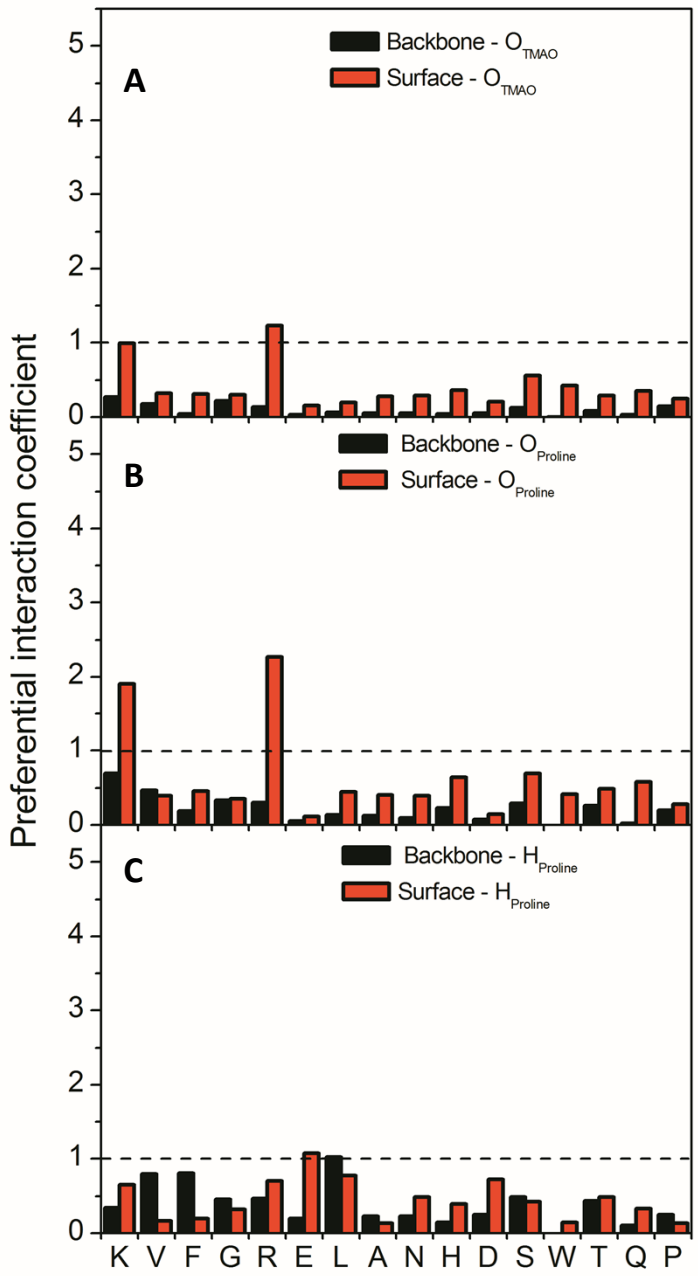

Figure S2. Preferential interaction coefficients calculated on the basis of interatomic distances obtained for individual amino acid residues at the surface of Lysozyme from molecular dynamics simulations for 3 M osmolyte solution: (A) Lysozyme – TMAO oxygen, (B) Lysozyme – Proline carboxylic oxygens, (C) Lysozyme – Proline amine protons. For each amino acid the coefficient was computed separately for the backbone and for the side chain surface – Equation (3)

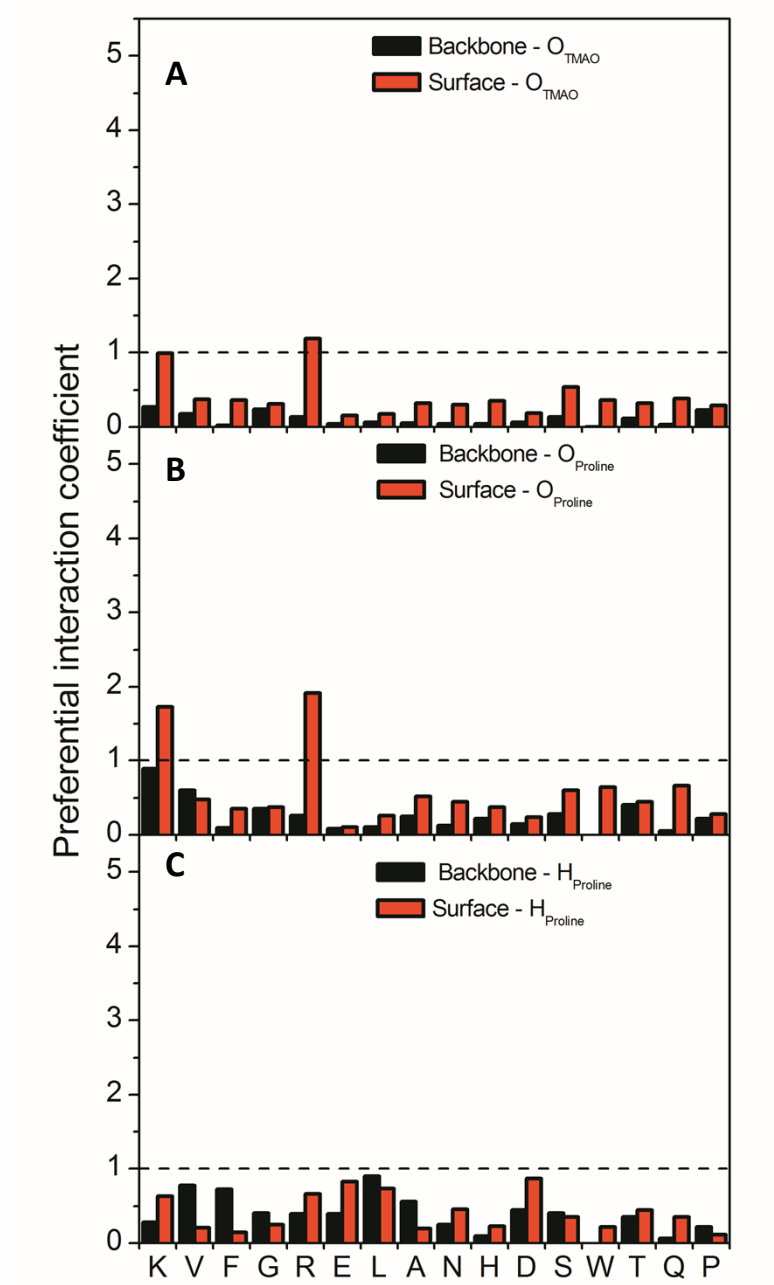

Figure S3. Preferential interaction coefficients calculated on the basis of interatomic distances obtained for individual amino acid residues at the surface of Lysozyme from molecular dynamics simulations for 4 M osmolyte solution: (A) Lysozyme – TMAO oxygen, (B) Lysozyme – Proline carboxylic oxygens, (C) Lysozyme – Proline amine protons. For each amino acid the coefficient was computed separately for the backbone and for the side chain surface – Equation (3)

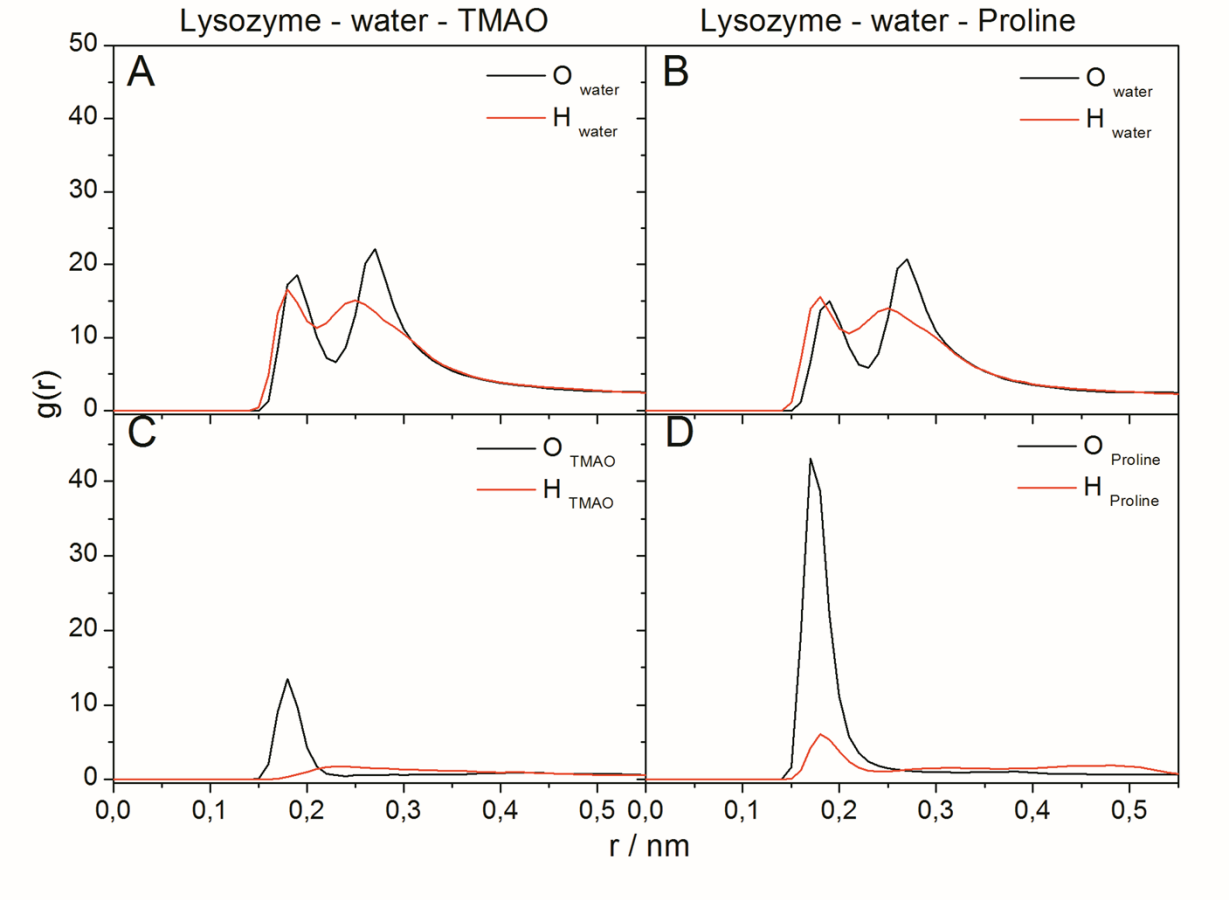

Figure S4. Radial distribution functions for the water molecules with respect to the surface of Lysozyme, in the 1 M TMAO (**A**) and 1 M Proline (**B**) systems. Radial distribution functions for TMAO and Proline atoms with respect to the surface of the protein, in the 1 M TMAO (**C**) and 1 M Proline (**D**) systems.