Supporting Information: File 1 of 2

Structural and Energetic Determinants of Thermal Stability, and Hierarchical Unfolding Pathways of Hyperthermophilic Proteins, Sac7d and Sso7d

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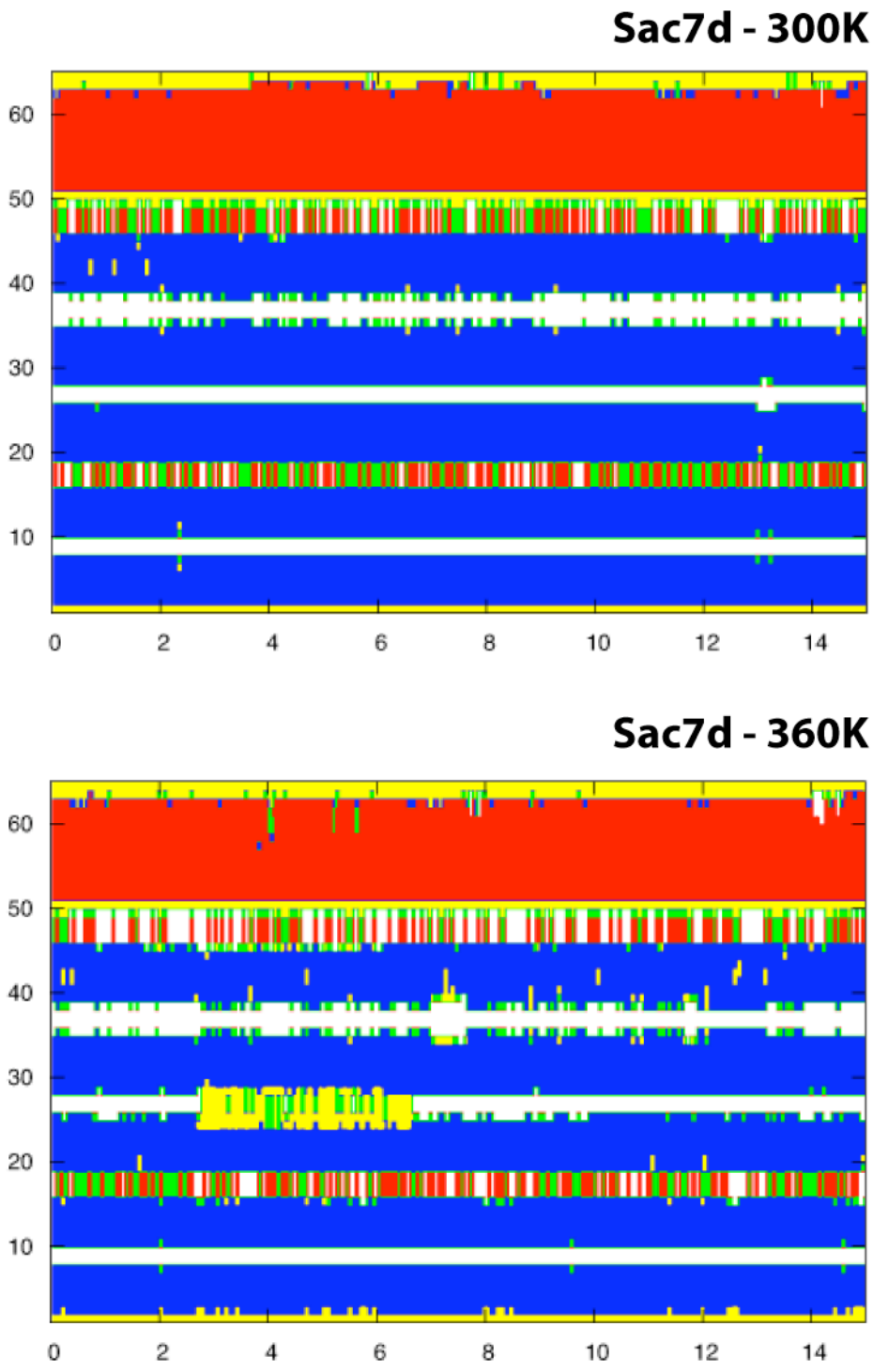

Figure S1: The evolution of the secondary structure of Sac7d with respect to time obtained at 300 and 360 K. β-sheets, α-helices, coils, turns, 3-10 helices are given in blue, red, yellow, white, and green respectively.

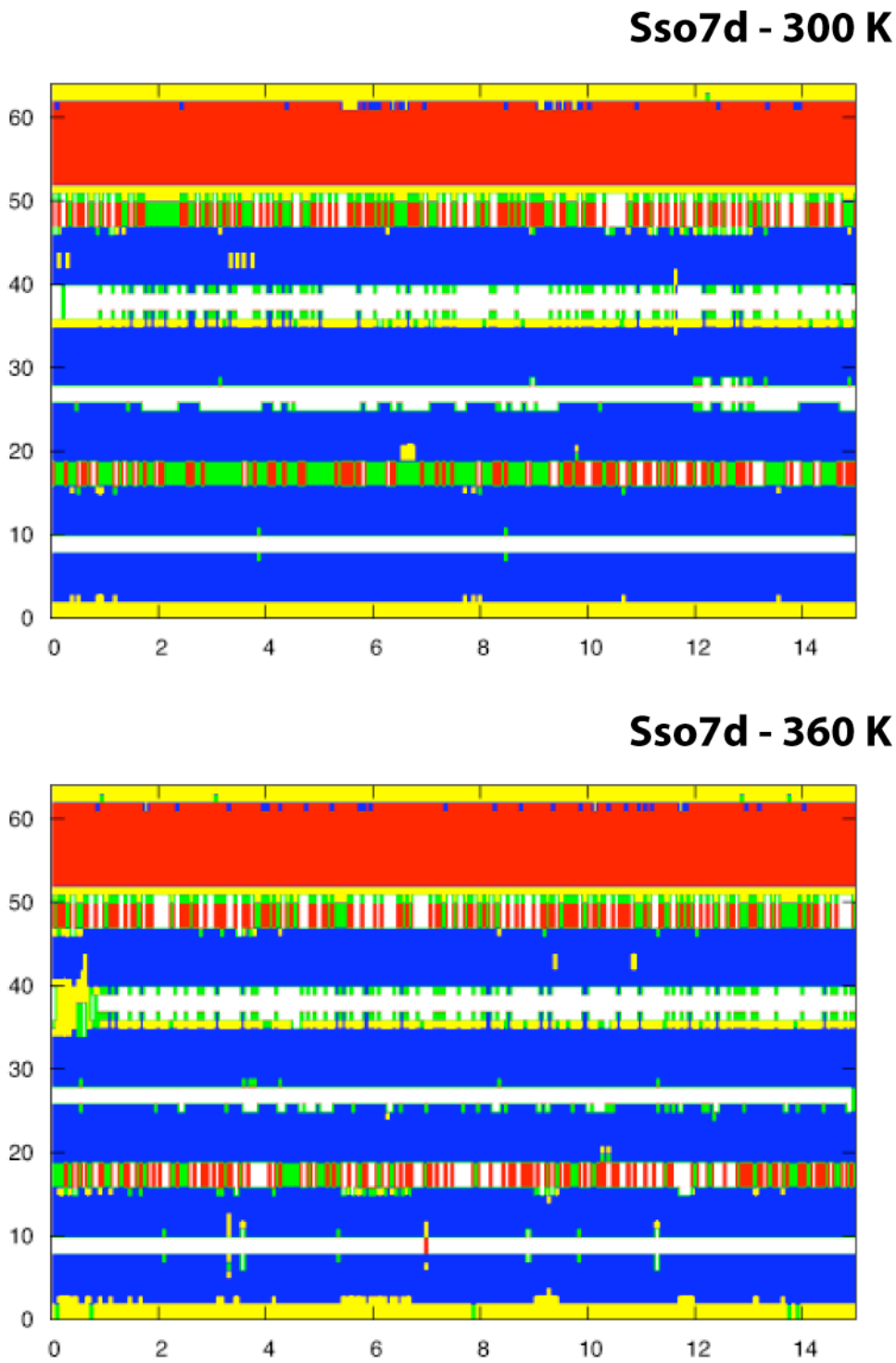

Figure S2: The evolution of the secondary structure of Sso7d with respect to time obtained at 300 and 360 K. β-sheets, α-helices, coils, turns, 3-10 helices are given in blue, red, yellow, white, and green respectively.

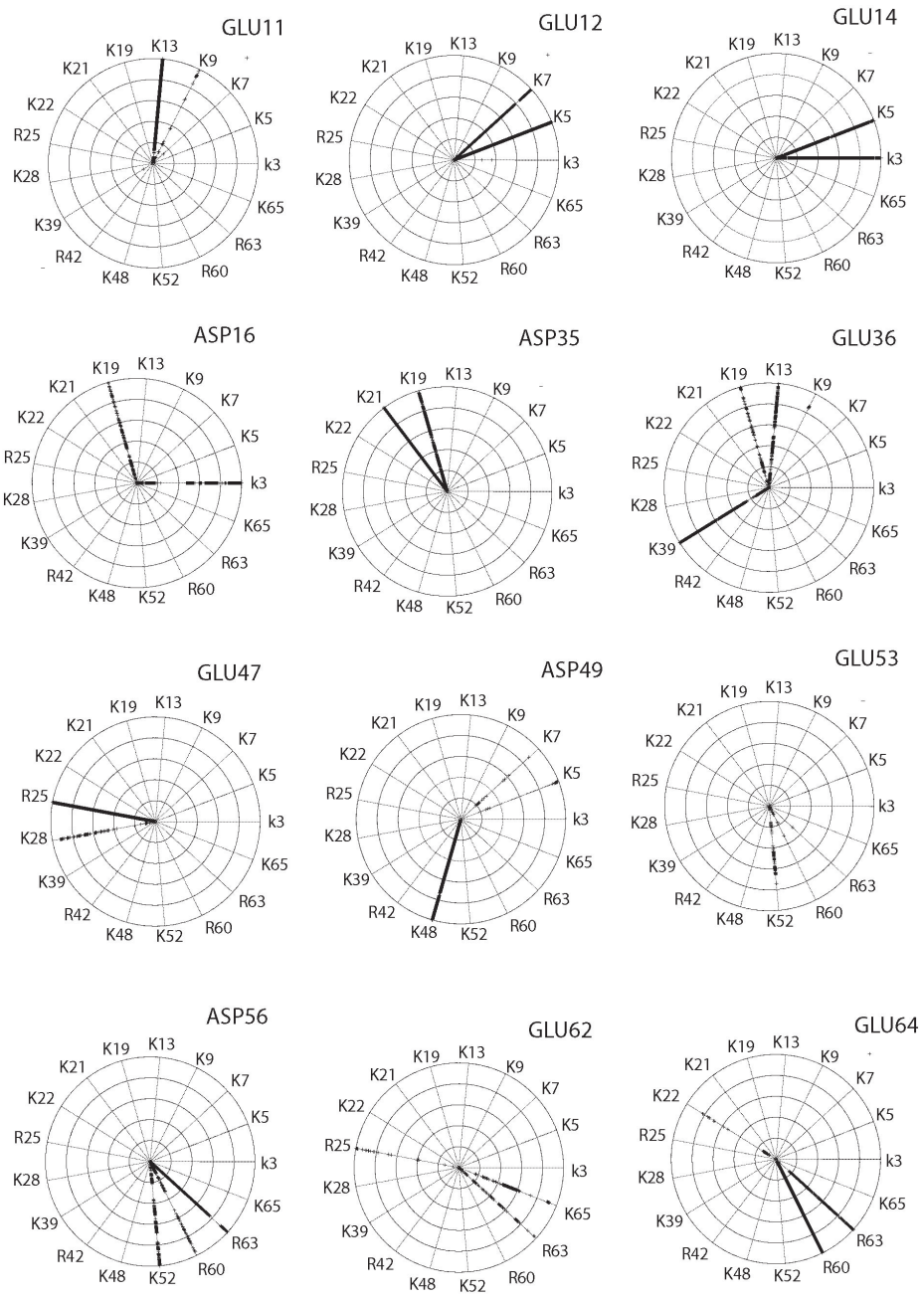

Figure S3: Plots showing the salt bridge networks of Sac7d at 300 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.

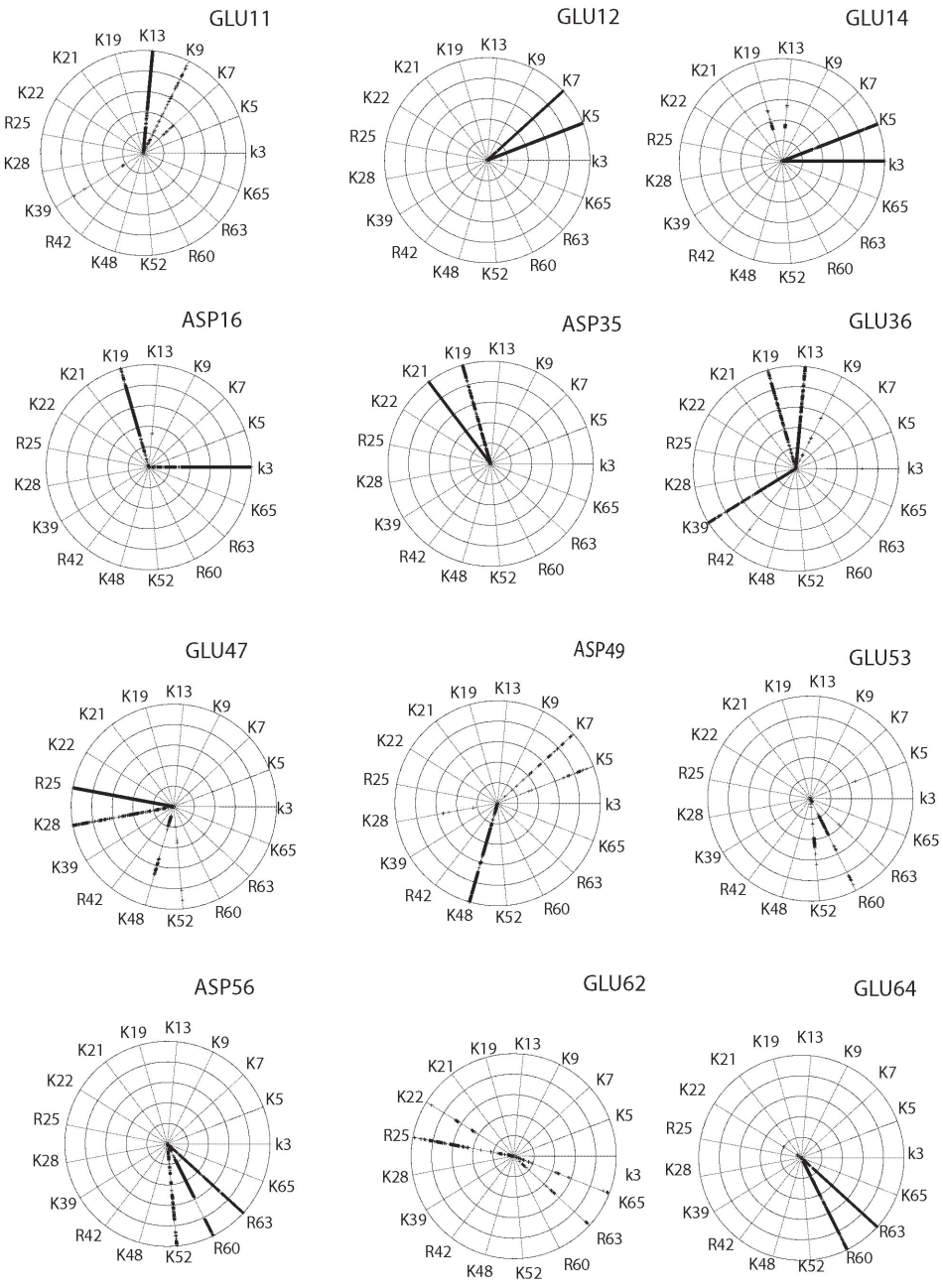

Figure S4: Plots showing the salt bridge networks of Sac7d at 360 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.

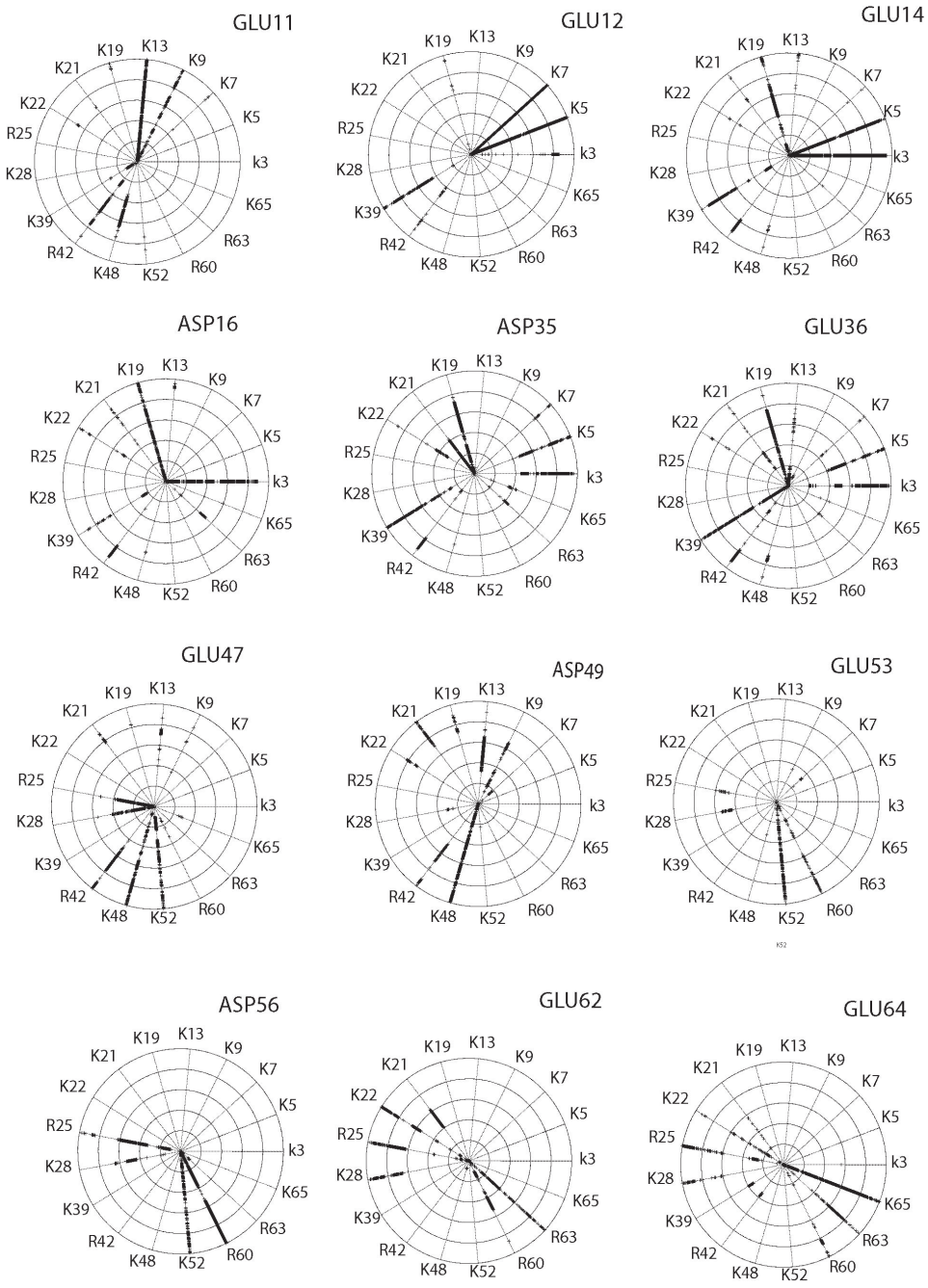

Figure S5: Plots showing the salt bridge networks of Sac7d at 500 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.

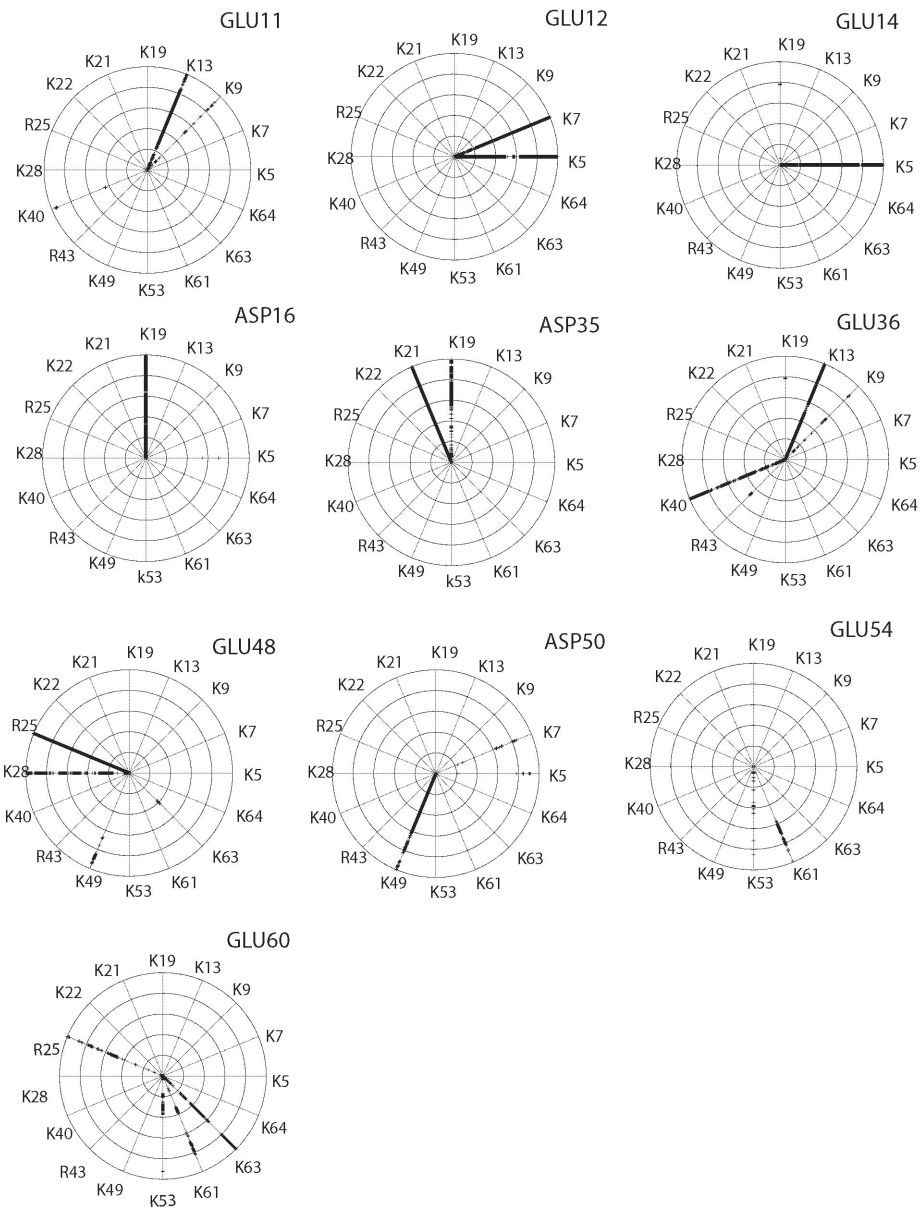

Figure S6: Plots showing the salt bridge networks of Sso7d at 300 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.

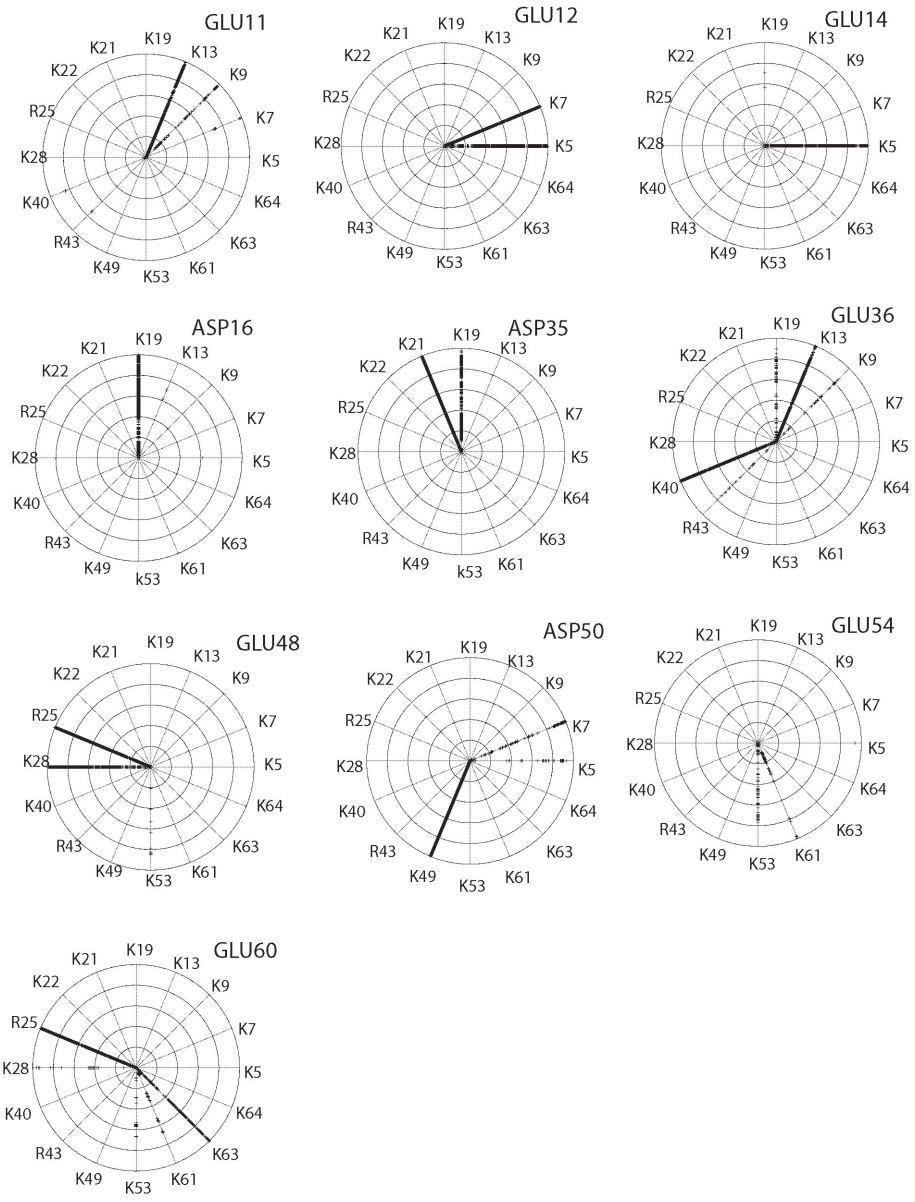

Figure S7: Plots showing the salt bridge networks of Sso7d at 360 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.

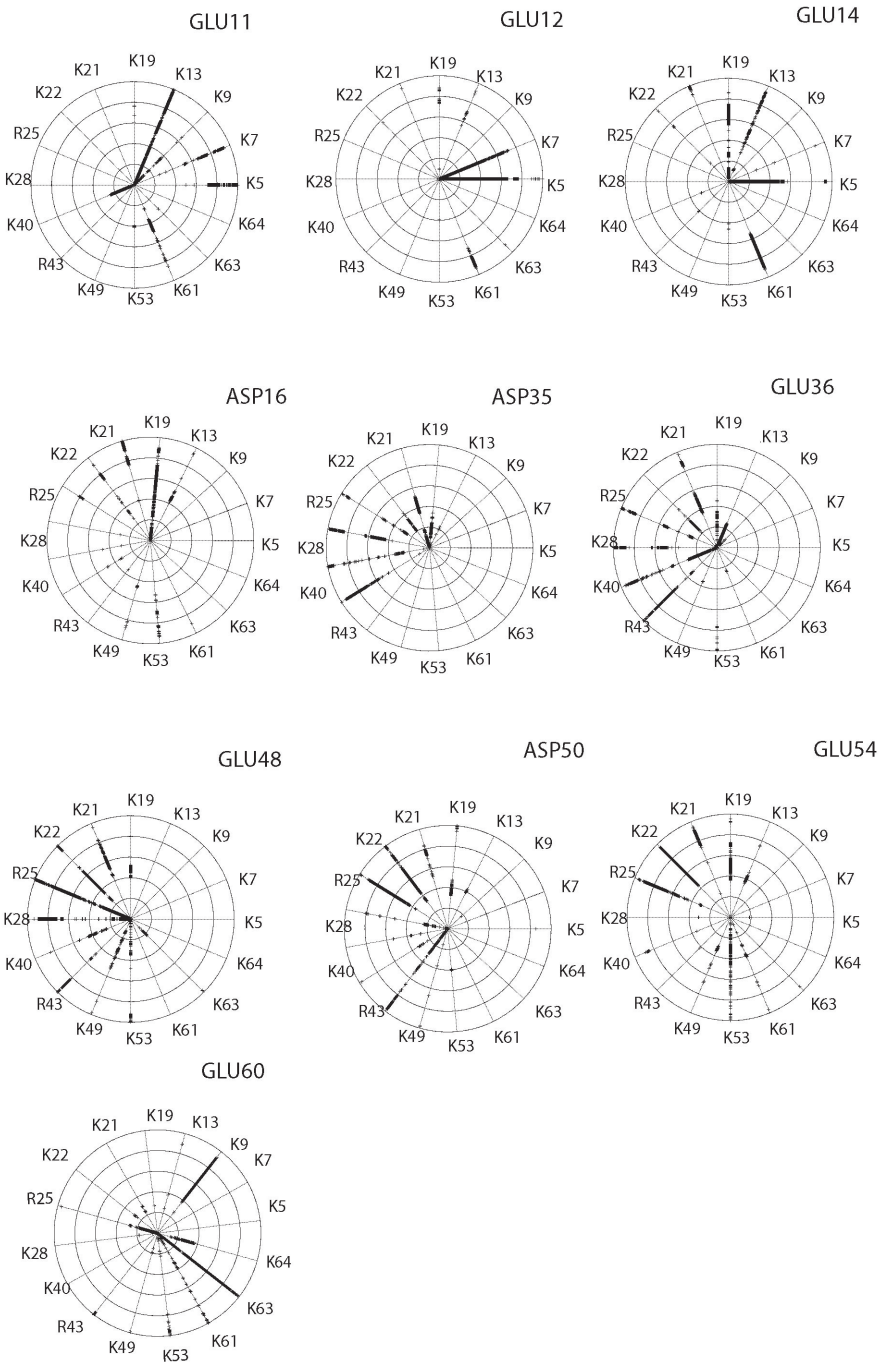

Figure S8: Plots showing the salt bridge networks of Sso7d at 500 K. In each of the circular plots, the center represents t = 0, and the outermost circle represents t = 15 ns. Each plot gives information on the existence/nonexistence of salt bridge interaction between each of the negative residue and all other positive residues present in the protein. Presence of a data point along the spokes indicates salt bridging interaction (less than 6 Å) between the corresponding positive and negative residue pairs.