

Type of file: figure

Label: proteins 71 684 figures

Filename: Structural_Analysis_Proteins_71_2_684_2009_PROTEINS_FIGURES.pdf

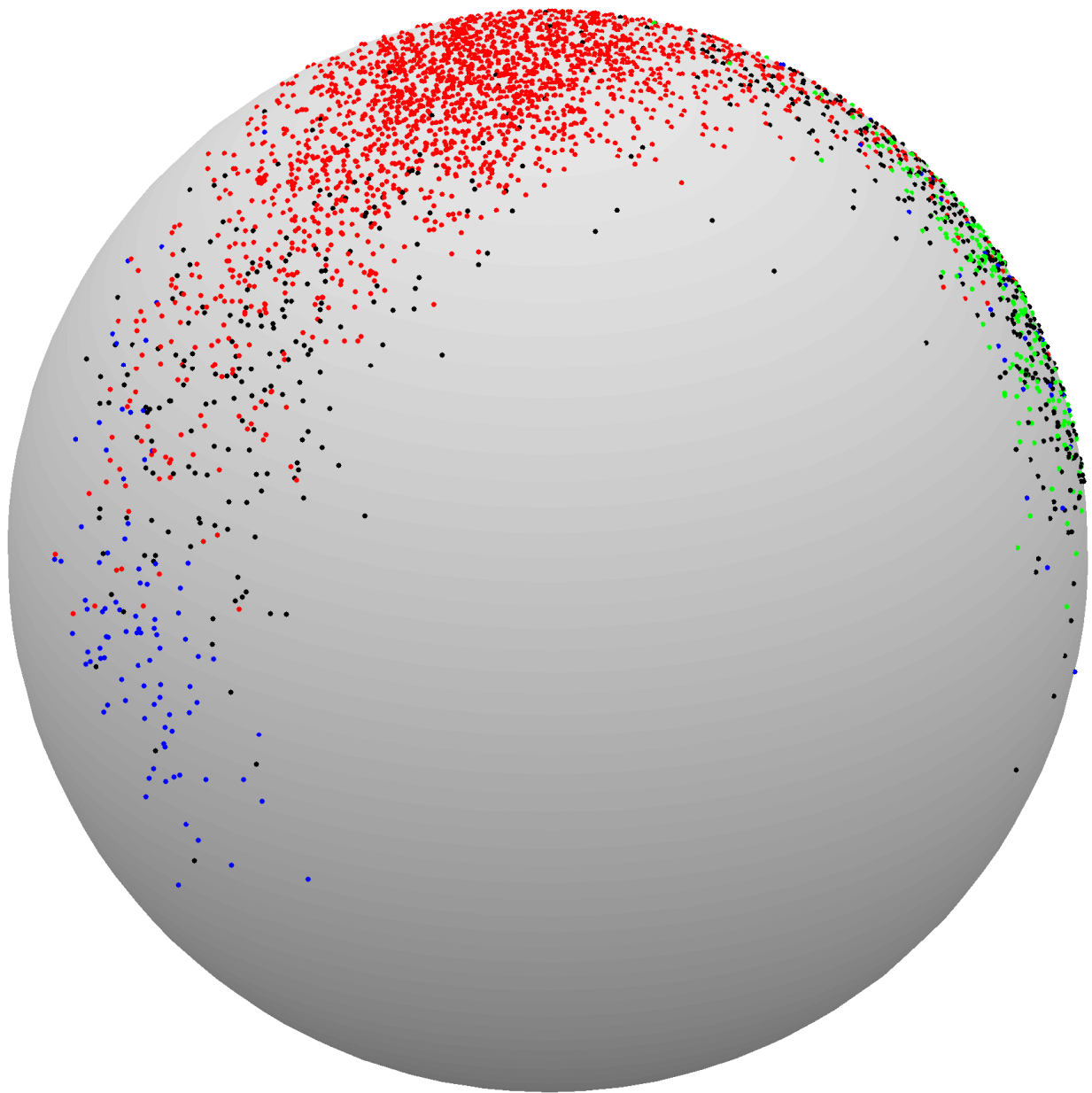


Figure S1. Rotated spherical plot for Gly9 from ff03 simulations, displaying the additional third conformation. Red dots indicate natively hydrogen bonded conformations, green dots indicate non-natively hydrogen bonded conformations (other than solvent exposed), blue dots indicate conformations hydrogen bonded to solvent, and black dots indicate not hydrogen bonded conformations.

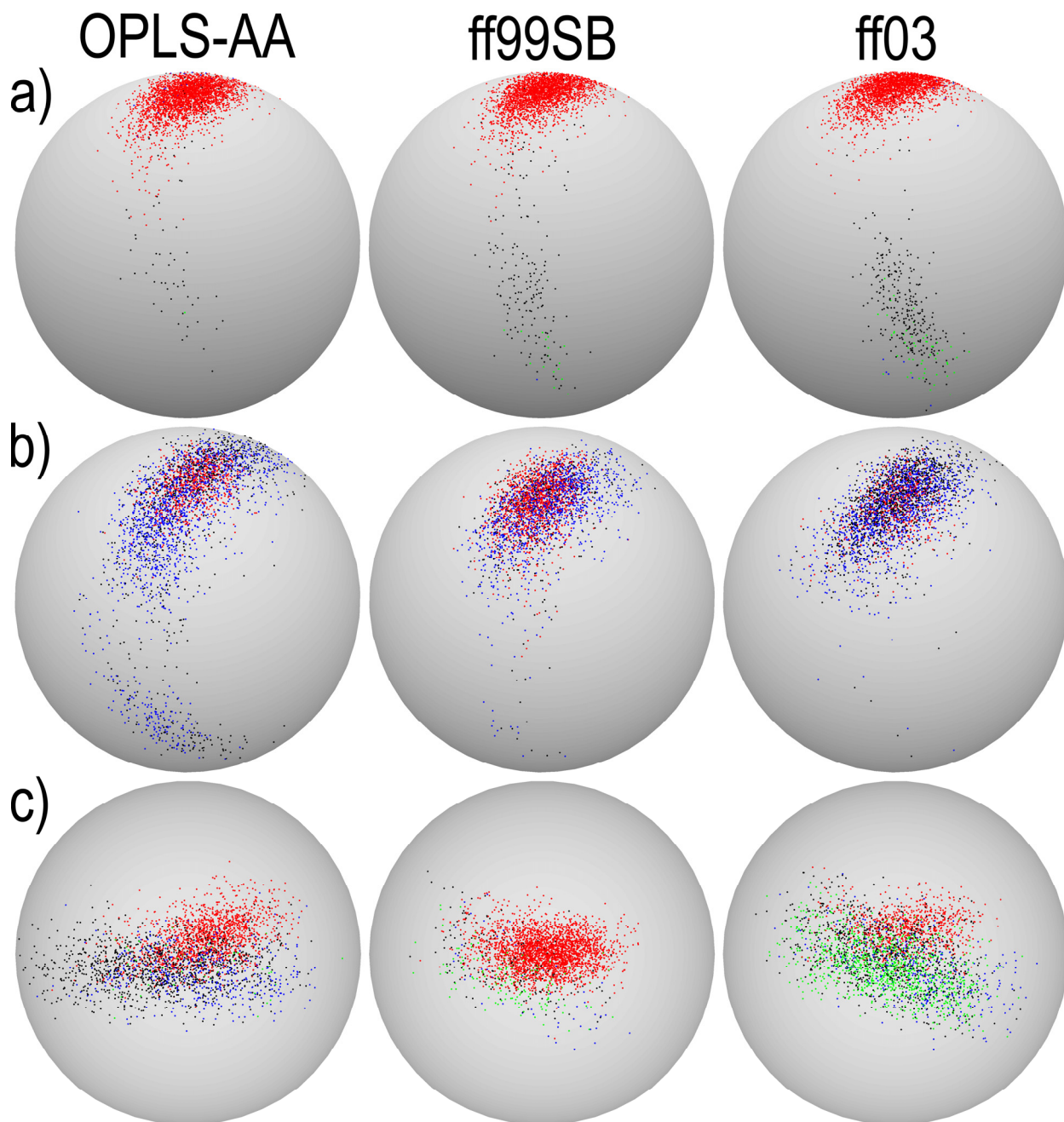


Figure S2. Spherical plots for remaining primary outliers. Red dots indicate natively hydrogen bonded conformations, green dots indicate non-natively hydrogen bonded conformations (other than solvent exposed), blue dots indicate conformations hydrogen bonded to solvent and black dots indicate not hydrogen bonded conformations. To reduce the amount of data and display equal numbers of conformations for each set of simulations every 23rd conformation was selected from the OPLS-AA simulations, every 11th from the ff99SB simulations, and every 10th from the ff03 simulations. a) A20; b) D40; c) E56.

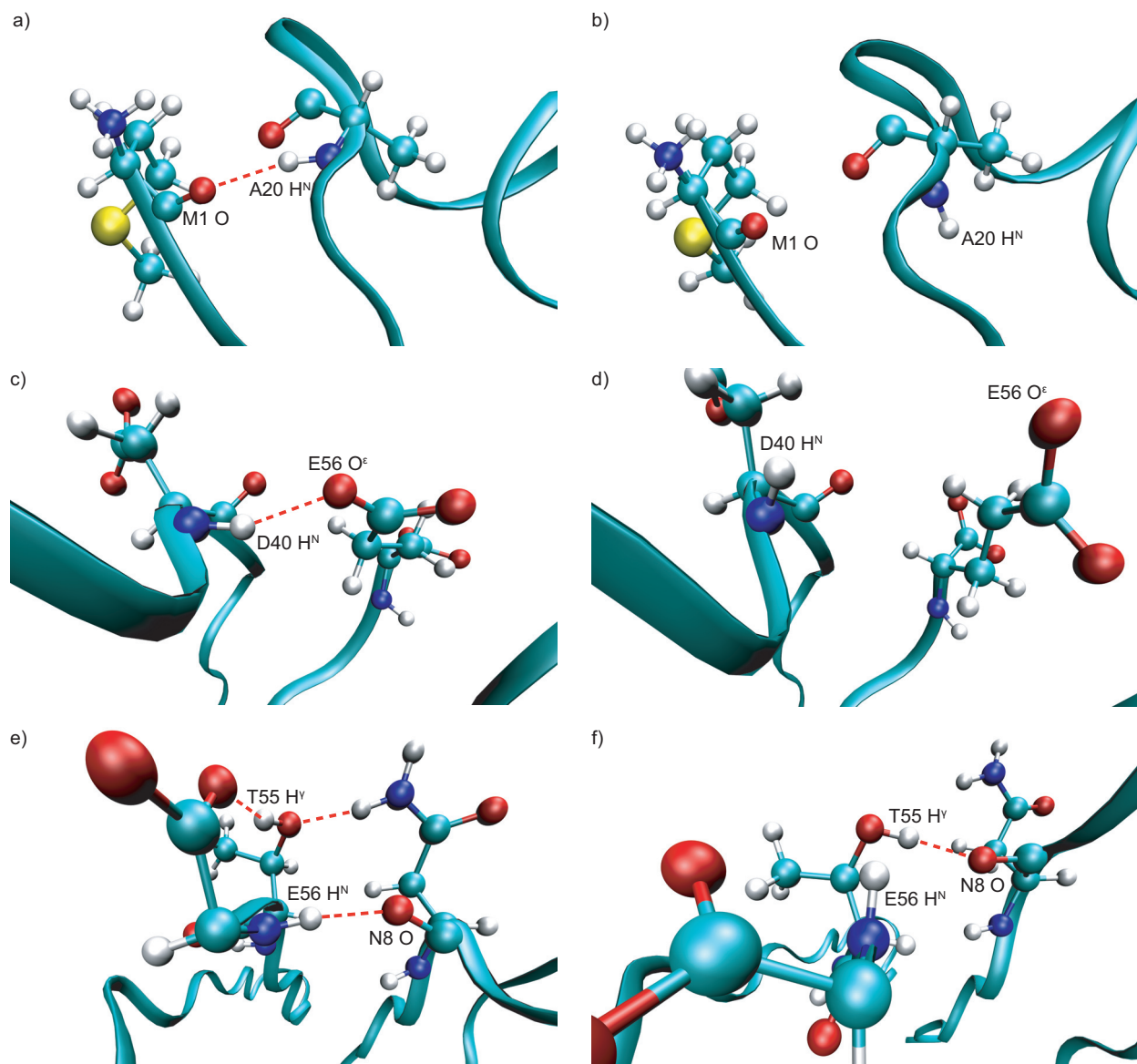


Figure S3. Structures representative of two conformations for remaining primary outliers. Red dashed lines indicate hydrogen bonds. Left column (a, c, e): native conformations; right column (b, d, f): non-native conformations.