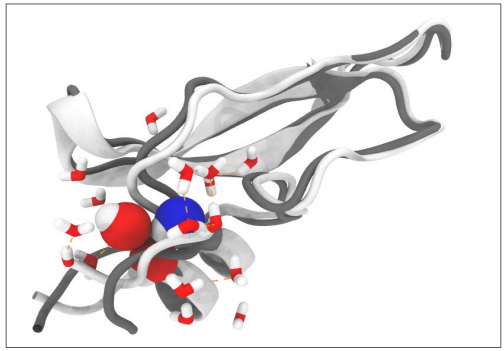
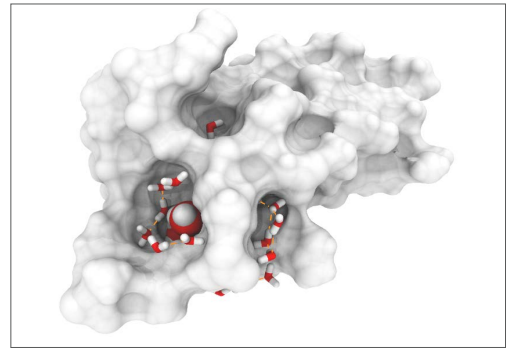
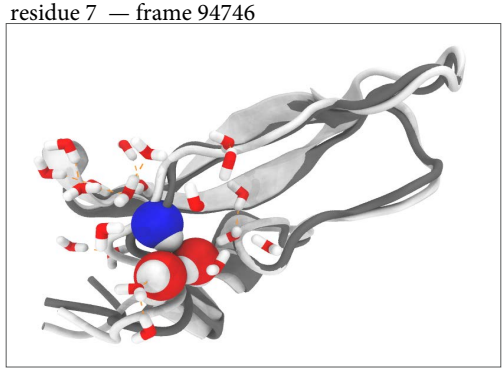
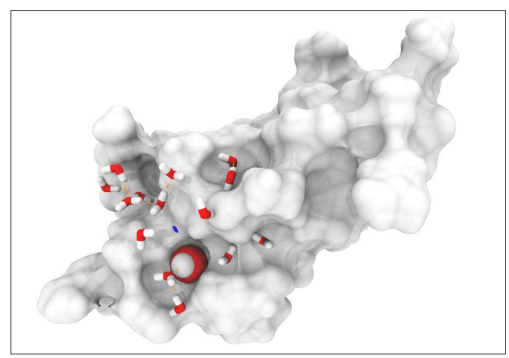
residue 5 — frame 649203



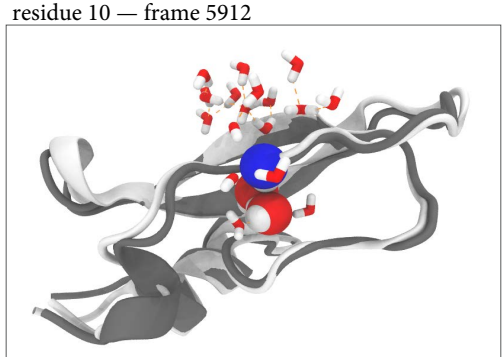


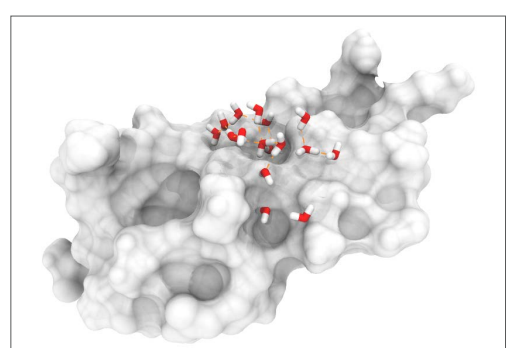
residue 7 — frame 94746



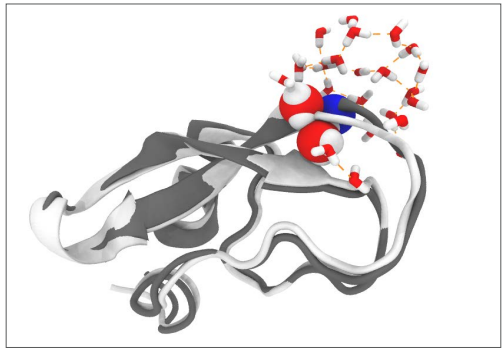


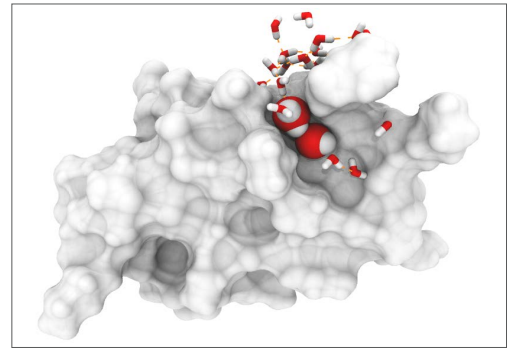
residue 10 — frame 5912



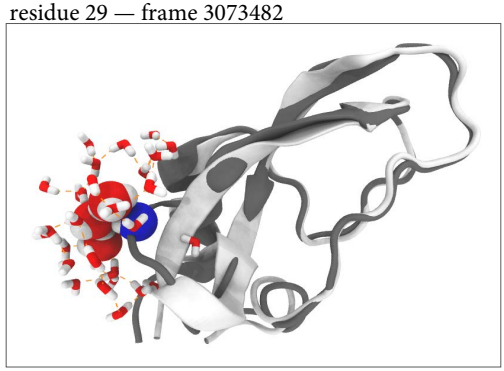


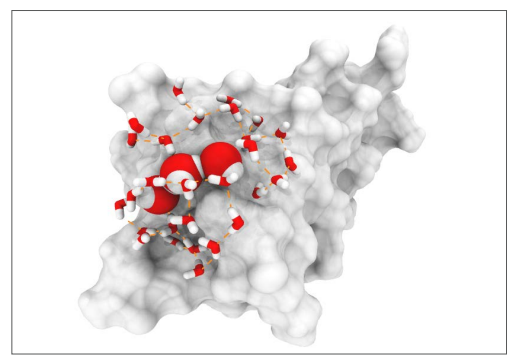
residue 18 — frame 64345



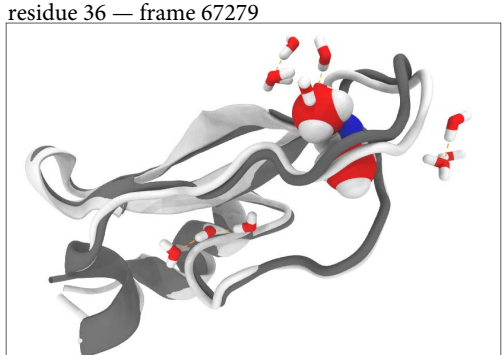


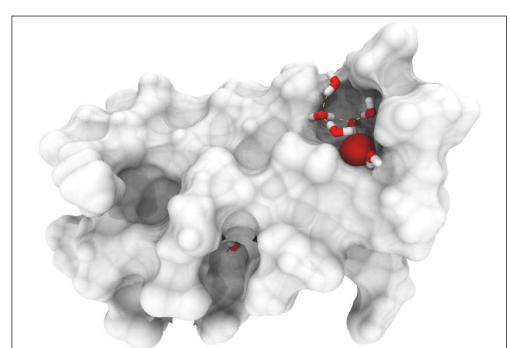
residue 29 — frame 3073482



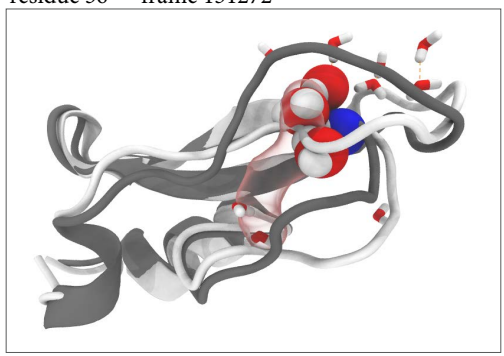


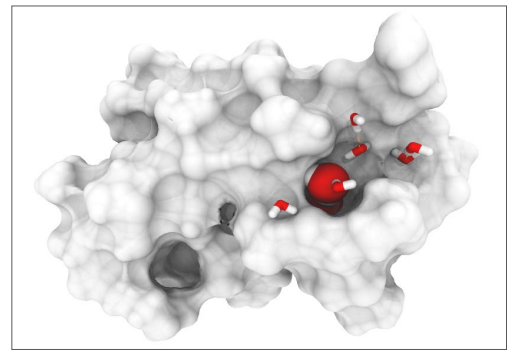
residue 36 — frame 67279



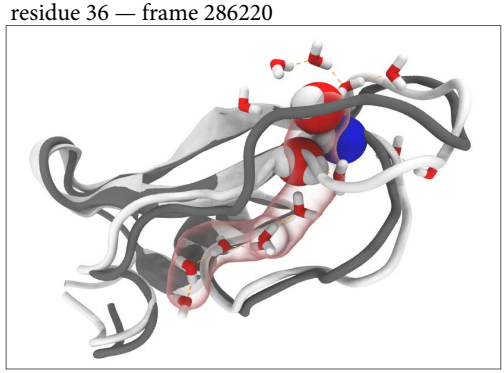


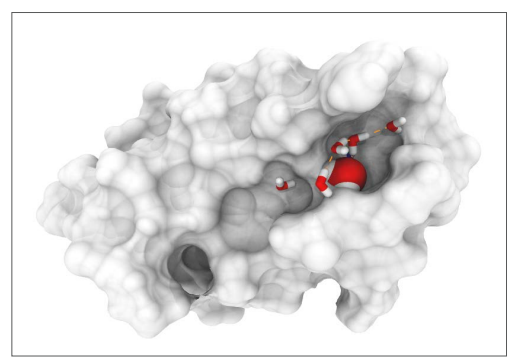
residue 36 — frame 151272



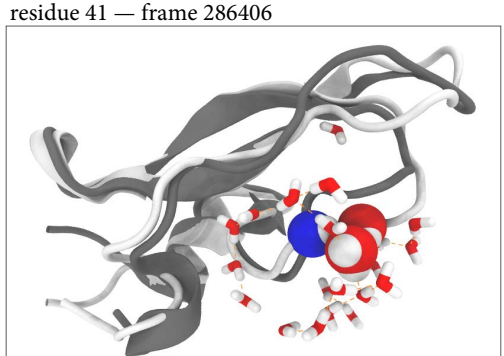


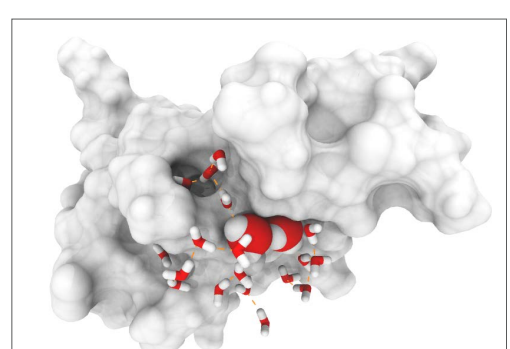
residue 36 — frame 286220





residue 41 — frame 286406





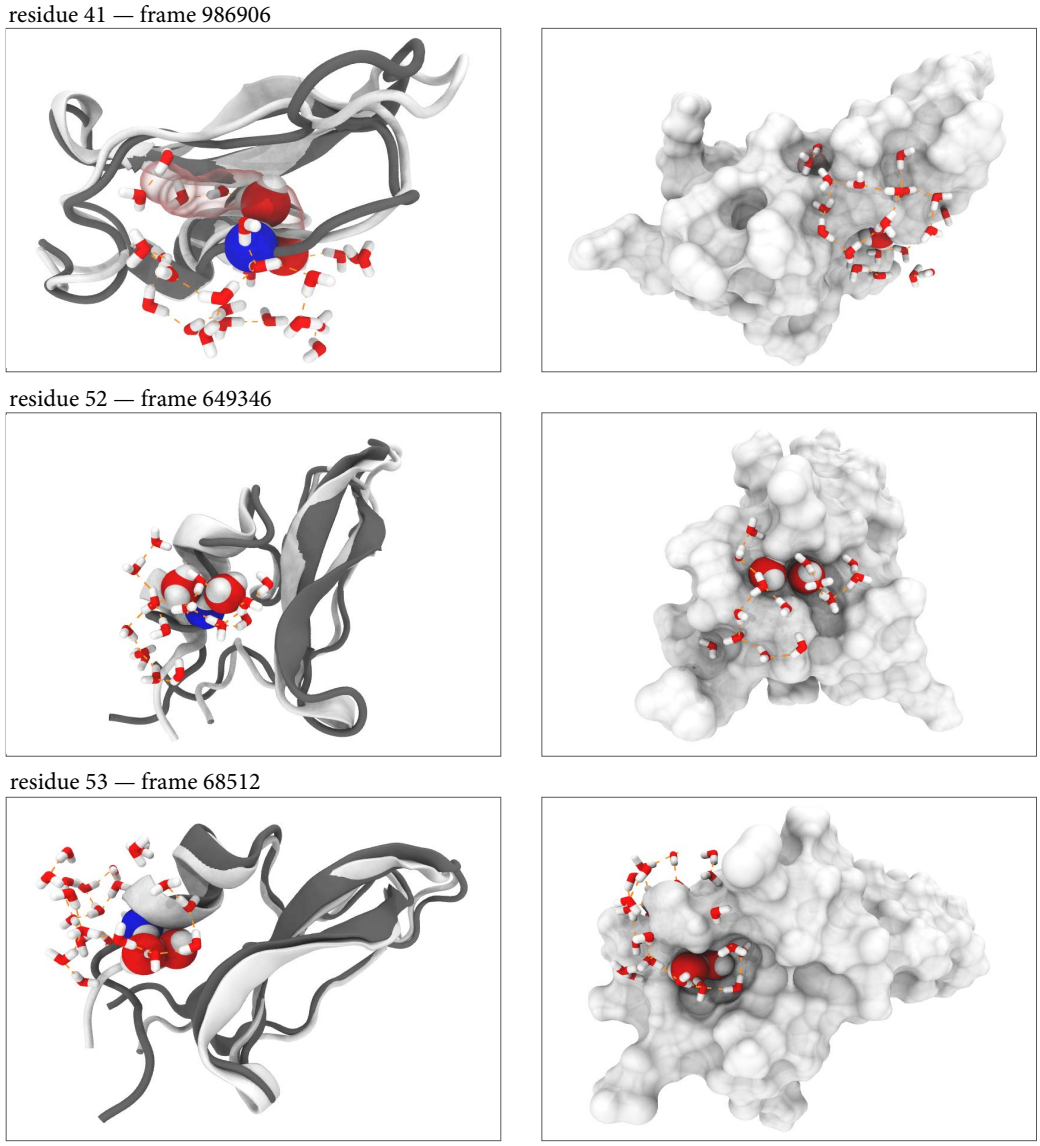


Figure S6. Snapshots of O states for 9 selected amides with the NH group and the 2 (or 3) primary waters in space-filling and other waters within a 7-Å sphere (and in tunnels or pores) in stick representation. To the left, the backbone conformation is shown for the selected O-state frame (dark gray) and for the first C-state frame in the trajectory (light gray). To the right, the molecular surface (1.4 Å probe radius, standard vdW radii) is shown. For Gly36 and Lys41, several snapshots (with and without water tunnels) are shown. Click on a structure to activate the interactive mode!