Supplemental Figure 1
Electrostatic potential maps of the molecular surface of molecules A (upper panels) and B (lower panels). Positive (blue) and negative (red) potentials are mapped on the van der Waals surfaces in the range $-5 \, k_BT$ (red) to $+5 \, k_BT$ (blue), where $k_B$ is Boltzmann’s constant and $T$ is the absolute temperature. These molecules are viewed from the same orientation as in Fig. 2a.
Supplemental Figure 2
Electron density map of the N-terminal "loose belt" region. For molecules A (cyan), B (pink), and D (yellow), the loose belt regions (Cys44 – Tyr58) are shown in rod model while the rest is presented as ribbon model. $2|F_o|-|F_c|$ electron density maps of loose belt regions contoured at the 1.0 $\sigma$ level are overlaid with the rod models.