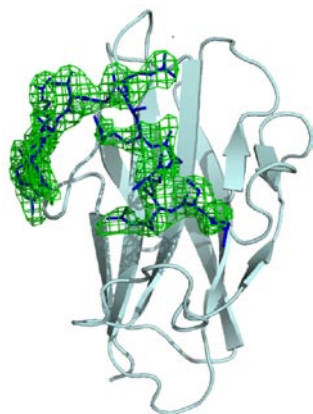


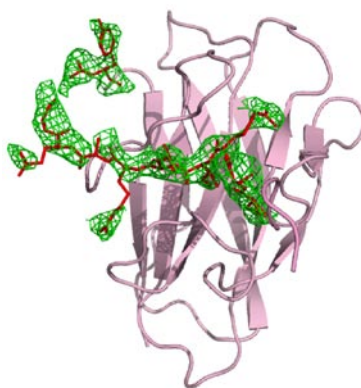
Supplemental Figure 1

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 $-5 \text{ k}_\text{B}T$ (red) to $+5 \text{ k}_\text{B}T$ (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.

Molecule A



Molecule B



Molecule D



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 1.0σ level are overlaid with the rod models.