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Figure 7. (See Chapter 2.) The native-state conformation of the bovine pancreatic trypsin inhibitor (BPTI). The figure was produced with the program RasMol 2.7.1 [126] from the PDB entry 1bpi. There are three disulfide bonds in this protein: Cys5–Cys55 shown in red, Cys14–Cys38 shown in black, and Cys30–Cys51 shown in blue. The corresponding Cys residues are in the ball-and-stick representation and are labeled. The two helices (residues 2–7 and 47–56) are shown in green.

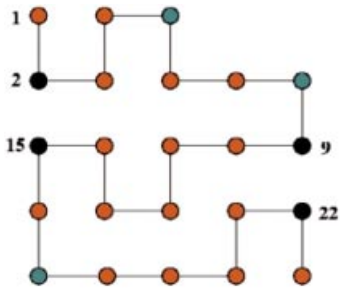


Figure 8. (See Chapter 2.) (a) The ground-state conformation of the two-dimensional model sequence with $M = 23$ beads and four covalent (S) sites. The red, green, and black circles represent, respectively, the hydrophobic (H), polar (P), and S sites.

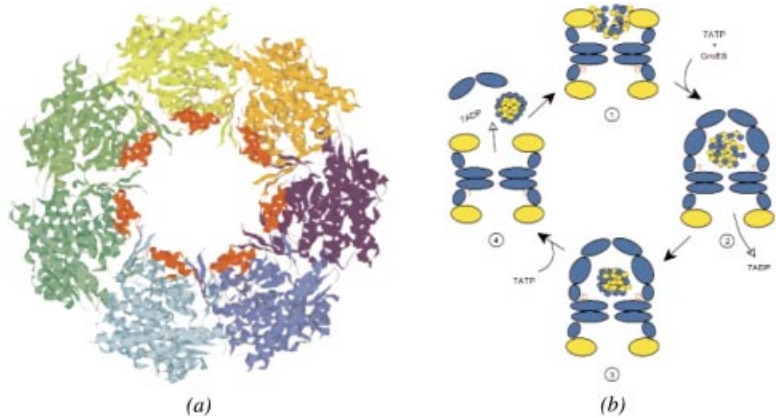
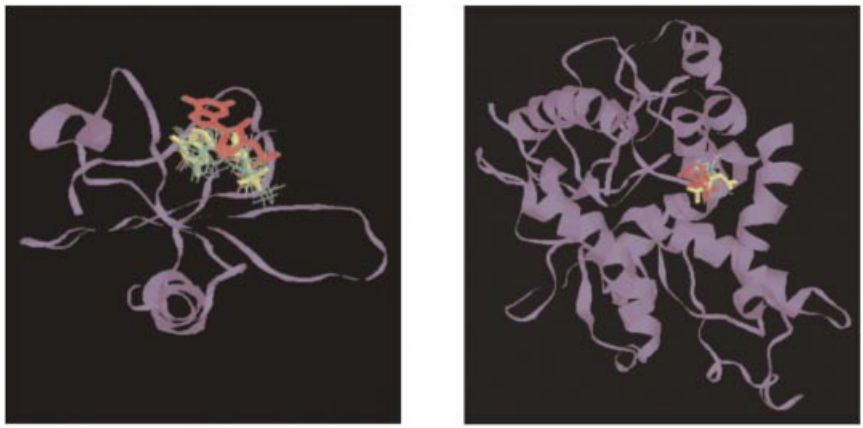


Figure 9. (See Chapter 2.) (a) Rasmol [126] view of one of the two rings of GroEL, from the PDB file 1oel. The seven chains are indicated by different colors. The amino acid residues forming the binding site of the apical domain of each chain (199–204, helix H: 229–244 and helix I: 256–268) are shown in red. The most exposed hydrophobic amino acids that are facing the cavity and are implicated in the binding of the substrate as indicated by mutagenesis experiments [112, 127] are: Tyr199, Tyr203, Phe204, Leu234, Leu237, Leu259, Val263, and Val264. (b) A schematic sketch of the hemicycle in the GroEL–GroES-mediated folding of proteins. In step 1 the substrate protein is captured into the GroEL cavity. The ATPs and GroES are added in step 2, which results in doubling the volume, in which the substrate protein is confined. The hydrolysis of ATP in the *cis*-ring occurs in a quantified fashion (step 3). After binding ATP to the *trans*-ring, GroES and the substrate protein are released that completes the cycle (step 4).



(a) (b)

Figure 4. (See Chapter 4.) For the predicted protein structure of 2sarA (2cmd_) generated by GeneComp using a template provided by the Fischer Database [34], the red-colored ligand represents the superposition of the ligand bound to the native receptor. The highest-scored match is colored in yellow.

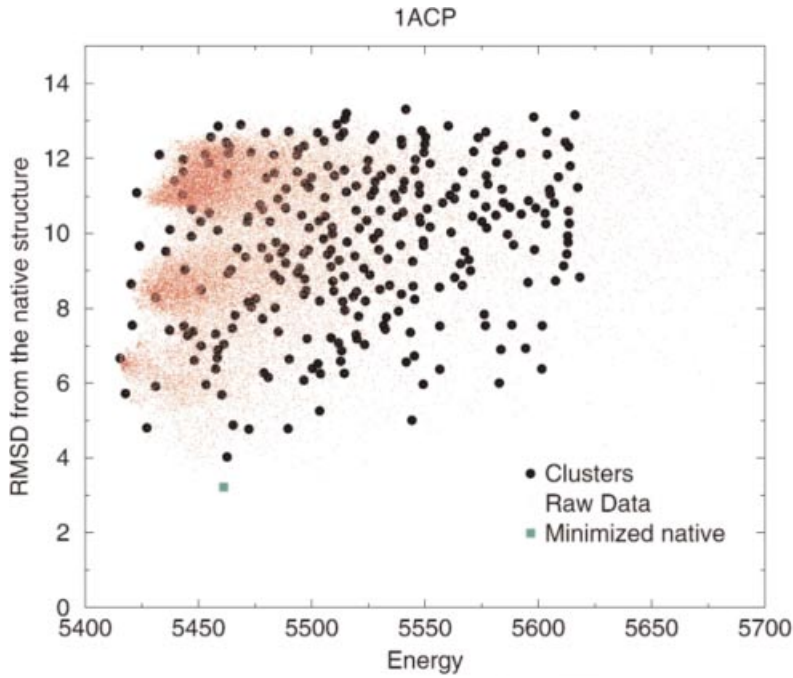


Figure 7. (See Chapter 6.) Comparison of raw data and clustered results (red dots: raw simulation data, black circles: cluster representatives, green square: locally minimized native structure).