

The role of dipole interactions in the formation of secondary and super-secondary structures of proteins

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Table S1: System Sizes

| System | Box Size (X x Y x Z) | Water Molecules |
|--------------|----------------------|-----------------|
| Helix | 7 x 6 x 4 | 1625 |
| Capped Helix | 7.5 x 6 x 4 | 1722 |
| Helix Bundle | 13.5 x 10 x 4 | 5036 |
| Sheet Bundle | 9 x 7.5 x 4 | 2572 |

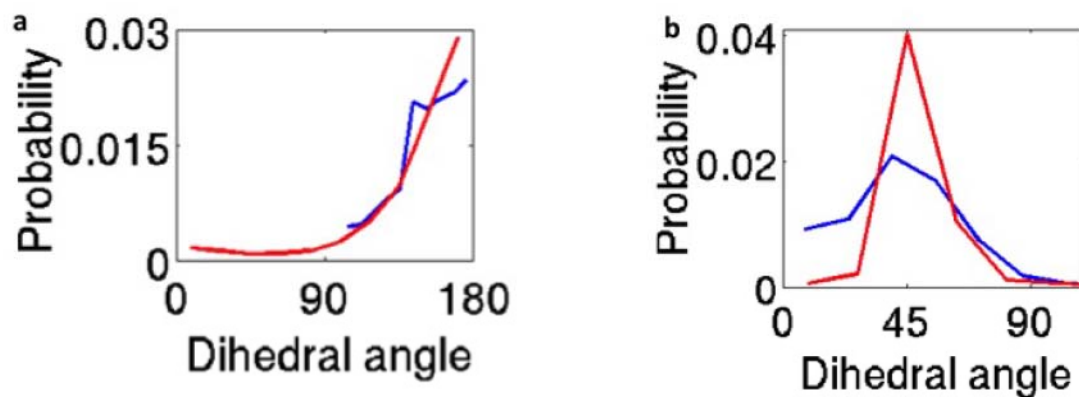


Figure S1: (a) Probability distribution of alpha dihedral angles for β -strand regions of 6898 non-redundant proteins from the Protein Data Bank (red) in comparison with the folded CG ensemble of β -sheets from Figure S2 (blue). (b) Probability distribution of alpha dihedral angles for α -helical regions of 6898 non-redundant proteins from the Protein Data Bank (red) in comparison with the folded CG ensemble of α -helices from Figure 2 (blue).

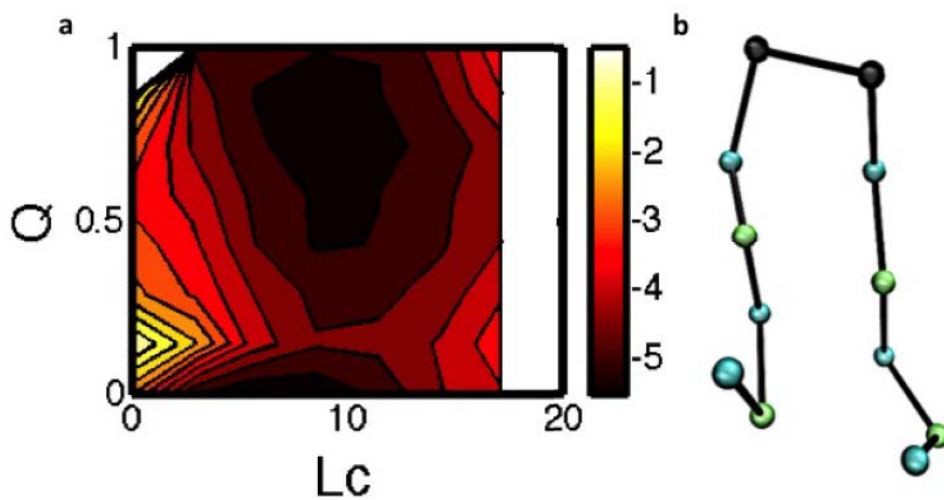


Figure S2: (a) Potential of mean force of a β -sheet system as a function of the fraction of sheet contacts (Q) and end-to-end distance (L_c) at 300K. Each contour level marks a kT unit. (b) Representative CG β -sheet conformation of the folded ensemble, only backbone beads are shown (green for polar and cyan for hydrophobic residues).

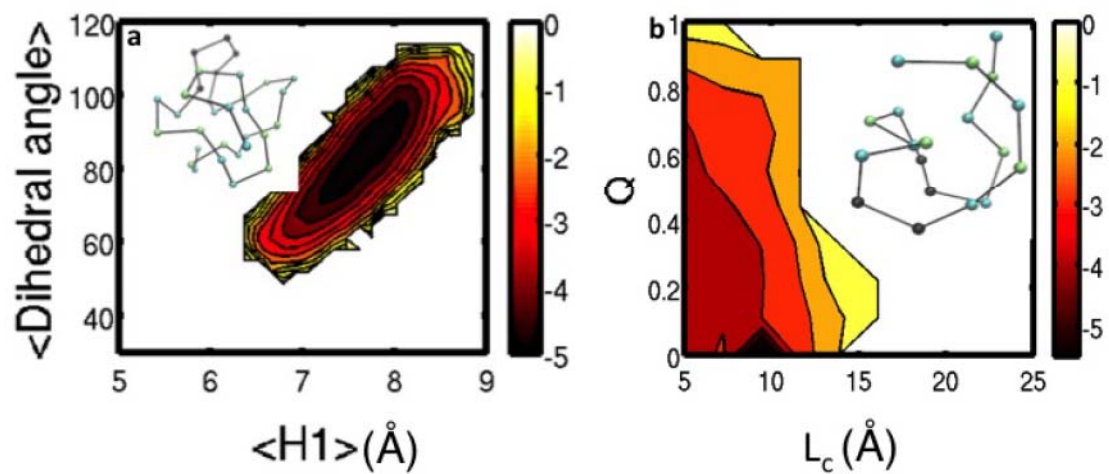


Figure S3: (a) Potential of mean force of a helix bundle sequence without backbone dipoles, as a function of average α dihedral angle and H1 parameter. Inset is a representative structure of the coil like conformation seen.(b) Potential of mean force plot of a sheet bundle sequence without backbone dipoles, as a function of sheet contacts (Q) and end-to-end distance (L_c). Inset is a representative structure of the coil like conformation seen.