Supplementary information to Local symmetry determines the phases of linear chains : a simple model for the self-assembly of peptides

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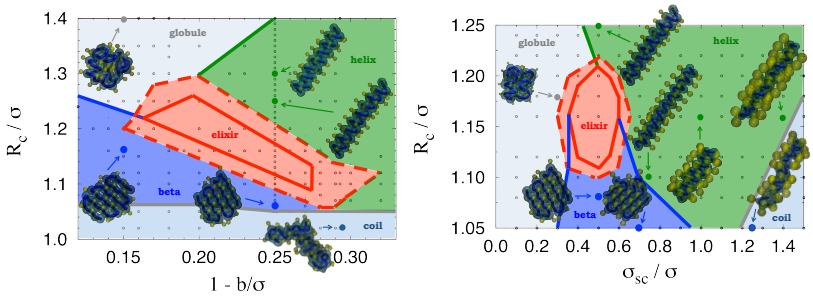
I. SUPPLEMENTARY FIGURES AND TABLES



(a) (b)

FIG. S1: The ground state phase diagram along the additional two planes. (a) R_c/σ-$(1-b/\sigma)$; (b) R_c/σ-σ_{sc}/σ. Here $N = 40$. In all cases, the third non-varying variable has been set to the center of the elixir phase $1 - b/\sigma = 0.25$; $\sigma_{sc}/\sigma = 0.25$; $R_c/\sigma = 1.167$.

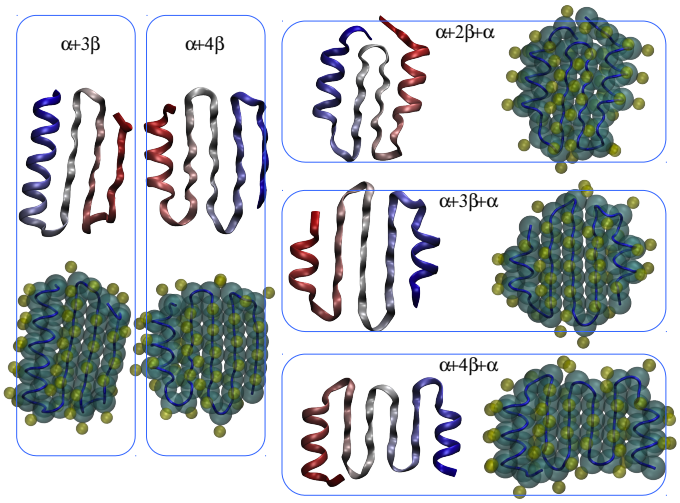


FIG. S2: Gallery of 5 different folds obtained in the elixir phase of a chain of $N = 56$.

Helix radius	(2.314 ± 0.06) Å
Helix pitch	≈ 5.5 Å
Helix angle	$\varphi_{i,i+1} = (100.10 \pm 2.56)$ deg
β angle $(i, i+2)$	122.5 ± 9.9 deg

TABLE S1: Helix and β parameters determined by a statistical analysis of the conformations present in structures deposited in the PDB database . This analysis includes proteins with a wide range of lengths and topologies of the folded states. In addition to the helix radius and pitch, the angle between $(i, i+2)$ residues in a β strand is also displayed

II. MOVIE DESCRIPTION

The following movies are available

- (Movie1) Annealing trajectory ending into a α helix structure. Here $b/\sigma = 0.75$, $\sigma_{sc}/\sigma = 0.833$, $R_c/\sigma = 1.167$.

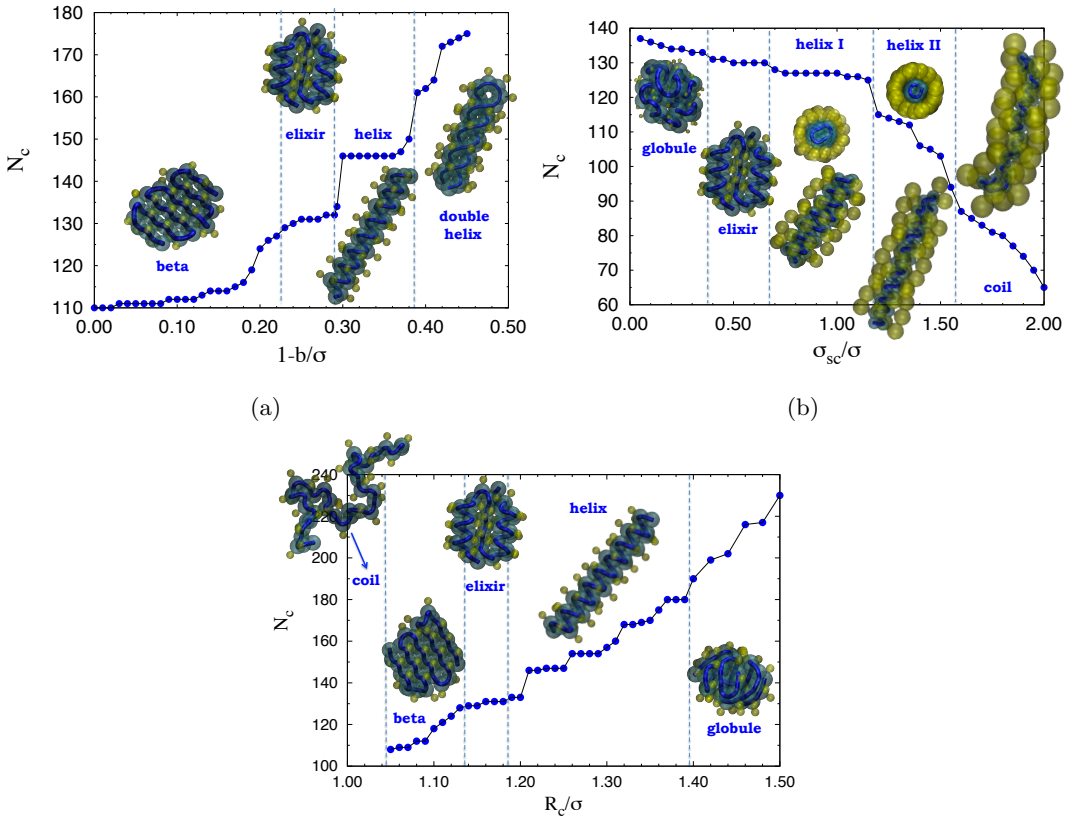


FIG. S3: (a) Number of ground state contacts N_c as a function of $1 - b/\sigma$; (b) Number of ground state contacts N_c as a function of σ_{sc}/σ; (c) Number of ground state contacts N_c as a function of R_c/σ for a chain of length 40. The vertical lines indicate transitions to the phases housing conformations shown in the snapshots, and are consistent with the transitions in the phase diagrams in Figure 6 of the main text. In all cases, the remaining two parameters have been set to the center of the elixir phase: $1 - b/\sigma = 0.25$, $\sigma_{sc}/\sigma = 0.5$, and $R_c/\sigma = 1.167$.

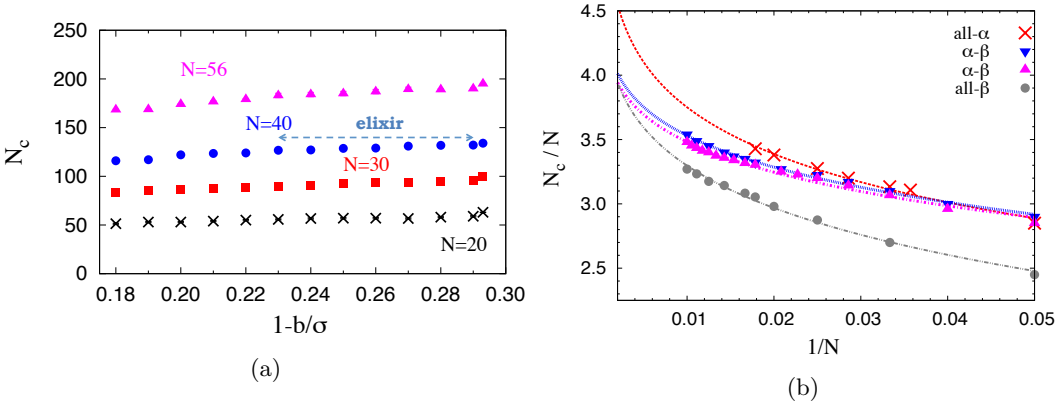
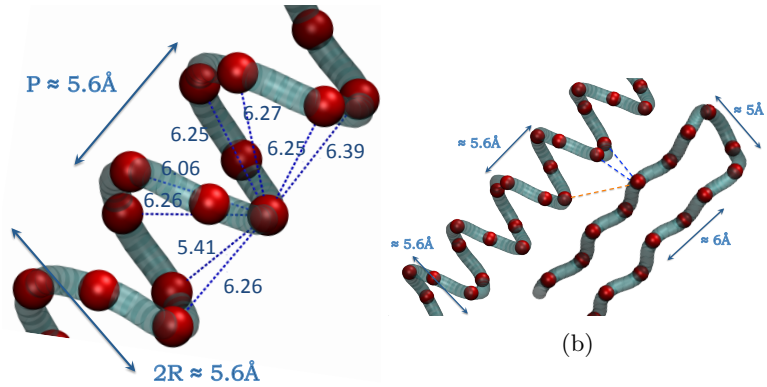


FIG. S4: (a) The number of ground state contacts N_c as a function of $1 - b/\sigma$ for different chain lengths ($N = 20, 30, 40, 56$). Each point is the average over $5 - 10$ independent runs, with errors bars of the order of the size of each point. For $N = 40$ the range of the elixir phase is highlighted; Lines represent a simple fit of the form $N_c/N = c_1/(c_2 + 1/N))$, with c_1 and c_2 being fitting parameters; (b) The number of ground state contacts per bead N_c/N for large N, showing that it tends to a value of ≈ 4. Note that the all-β conformations tend to extrapolate to the same value, whereas the all-α conformations approach a slightly higher value of ≈ 4.5.



(a) (b)

FIG. S5: Non-compatibility of the α-β configurations outside the elixir phase. (a) Single model helix outside, but close to, the elixir phase at $1 - b/\sigma = 0.29$, $R_c/\sigma = 1.16$, $\sigma_{sc}/\sigma = 0.5$; (b) Same helix combined with a β hairpin from within the elixir phase, underscoring the incompatibility between these two structures as a helix-hairpin combination. The helix and hairpin structures occur at the elixir-helix transition of Figure 9 of the main text, the hairpin being inside the elixir phase at the left of the transition line and the helix being outside at the right of the transition line. While the two contacts highlighted in blue are within 6 ≈ Å, the bond highlighted in orange is outside this characteristic length and hence it cannot make an energetically favorable contact.

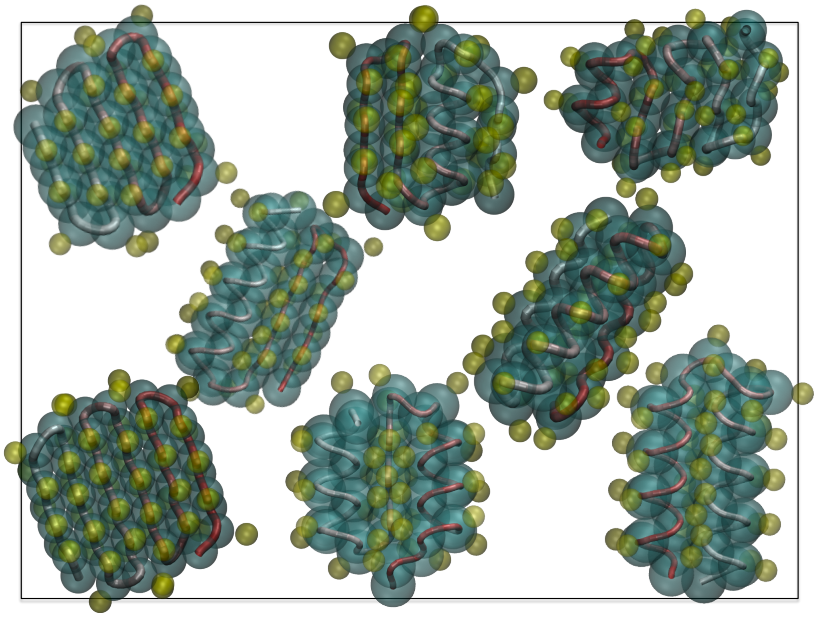


FIG. S6: A gallery of representative ground state structures found in the elixir phase and in the extended region surrounding it. All helices have radii (2.4 ± 0.1) Åand pitches (5.5 ± 0.5) Åmatching those of protein helices within error bars. Likewise, all strands have distances between C_α^i and $C_\alpha^{i+2} \approx 6$ Å, as in proteins.

- (Movie2) Annealing trajectory ending into a β sheet. Here $b/\sigma = 0.85$, $\sigma_{sc}/\sigma = 0.667$,$R_c/\sigma = 1.167$.
- (Movie3) Annealing trajectory ending into an elixir structure. Here $b/\sigma = 0.75$, $\sigma_{sc}/\sigma = 0.667$,$R_c/\sigma = 1.167$.