Protein folding

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- protein = fundamental building block of life
  - created by "ribosome" from DNA
  - immediately fold from chain into 3D shape
    - ↳ fast (< 1 second), reliable (consistent ~)
  - misfolding cause of several diseases (mad cow, some cancers, ...)
  - want to design synthetic protein drugs

- fixed-angle chain (can't change angles between incident bars) roughly model protein backbone
  - can no longer straighten chain
  - closest analog: flatten into plane
- deciding flattenability is NP-hard [Soss & Toussaint 2000]
- flat-state connected = can fold between any two flat states
  - nonacute chains are [Aloupis et al. 2002, 2002]
  - OPEN: all chains?
  - OPEN: all trees?

(- OPEN: locked equilateral obtuse chain?)

- "producible" fixed-angle chains [Demaine, Langerman, O'Rourke 2003]
  - are flat-state connected
  - have a flat state
  - have a canonical state similar to helix
- energy minimization dictates protein folding
  - even in simple models, finding optimal folding is NP-hard [Crescenzi et al. 1998; Berger & Leighton 1998]
  - OPEN: design proteins whose opt. folding has desired properties
    - known: unique optimum [Aichholzer et al. 2003]