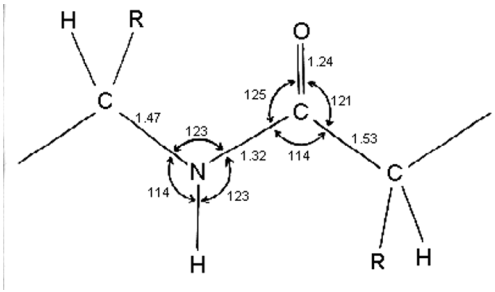
Problem set 6

Due December 1, 2026

1. Using the standard bond length and angles of the peptide backbone shown in the picture below (bond lengths in ångströms, bond angles in degrees),



   and the values of the backbone ϕ and ψ angles of Table 3.2 of the handout pages, determine the $C^{\alpha} \cdots C^{\alpha}$ distance per periodic unit for the following periodic structures:

   (a) α-helix,

   (b) 3_{10}-helix,

   (c) parallel β-strand,

   (d) antiparallel β-strand.

   The structures can be built with `molden` or `avogadro`; it is also acceptable to use `pymol`, which has standard geometry built in, to build the structures. The above software also enable us to measure the distances.

2. Search the Protein Data Bank (PDB; `https://www.rcsb.org/`) for representative structures containing α and β structures and compare your results with the average length per periodic unit calculated from the structures. You can use the 1IGD $\alpha + \beta$ protein for a start. The secondary structure is identified in a PDB entry with the HELIX and SHEET records. You can use `rasmol`, `pymol` or other software to calculate the distances.