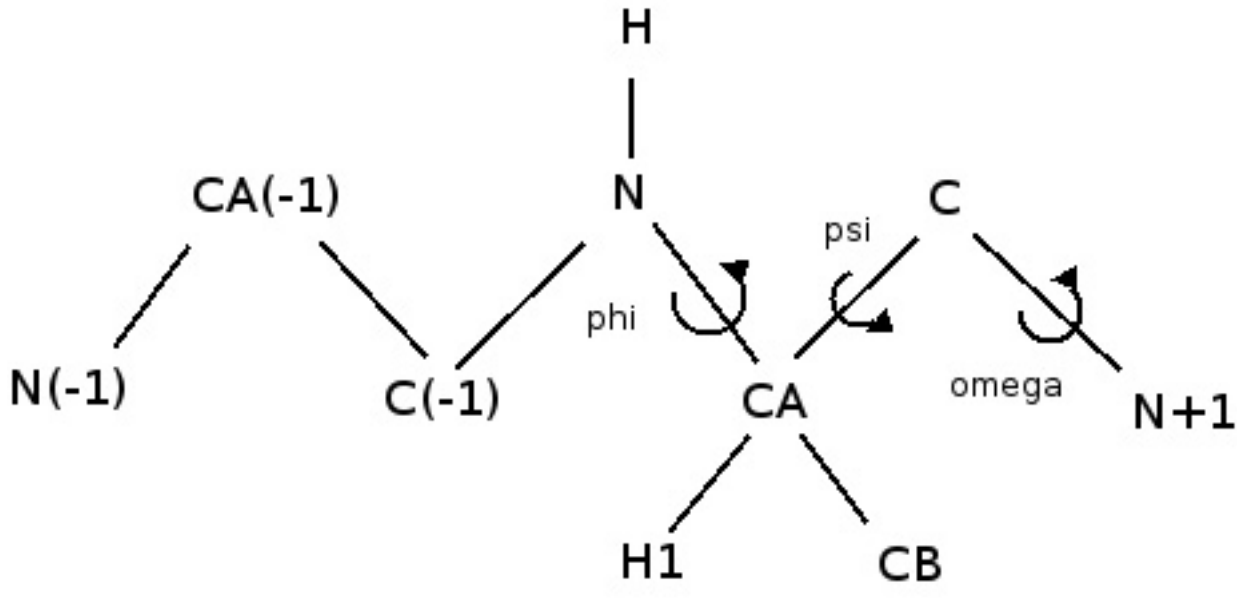
20.181 Notes by Mike Yee - October 25, 2006

Dihedrals



Protein backbone

Where CA is the alpha carbon, C(-1) is the C before the current carbon, etc.

Structure of data files for protein backbone:

Angle	First atom	Second	Third	Fourth
φ	C_{-1}	N	CA	C
ψ	N	CA	C	N_{+1}
ω	CA	C	N_{+1}	CA_{+1}

Now we want to add other stuff.

Atom	First atom	Second	Third	Fourth	Dihedral angle
Amide hydrgeon (NH)	CA_{-1}	C	N	NH	dih_{NH}
Alpha carbon hydrogen (H_1)	C_{-1}	N	CA	H_1	dih_{H1}
First carbon on R-group (CB)	C_{-1}	N	CA	CB	dih_{CB}

Cool. But do we always need to calculate stuff from the inputs? Not for the so-called "improper dihedrals", such as the C-CA-N-NH dihedral, or the C-CA-N-NH dihedral, because these are always the same. The "proper" dihedrals (N, CA, C) must be calculated from inputs, but the "improper" dihedrals can be taken from a table.

Build order

N terminus to C terminus, with increasing *i*

- Within the residue, calculate proper dihedrals, take improper dihedrals from a table