

## BCH 258 lecture notes Fri. Aug 28, 2009

Graphics: restrictions on mainchain conformation, continued:

Mage: ala\_dipept\_geom\_dotball5.1.kin

Mage: idealpolyala12.kin, appendstuff2.kin

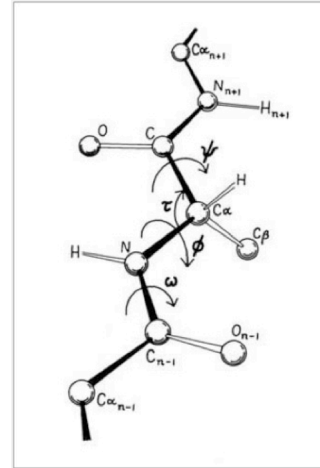
Ramachandran plot regions

Handouts:

Amino-Acids diagram

Homework: Worksheet 3: Handedness & Amino Acid Roles

Kinimage file – c1Basics-2-5-QKiNG.kin



Amino Acid Roles: introduce homework...  
occurrence vs secondary structure

Geometry of polypeptide backbone: in class...

ala\_dipep\_geom\_dotball5.1.kin, revisited,

now lead in to idealpolyala12.kin and secondary structure

rotatable-bond Ala dipeptide (~like c1Basics)

Rama regions - show  $\beta$  better than 180, 180

general data contours - show helix good; go off edge; 0,0 dire

Gly data, contours - show  $C_{\beta}$  clash in  $L3_{10}$ ,  $L\beta$ ; not in  $\beta$

Polypeptide: amino acids condense to residues, forming peptide bond

peptide bond (C--N) and C--O are partial double bonds, so planar & shorter  
entire  $C_{\alpha}$ --- $C_{\alpha}$  peptide unit is planar and trans

Sidechains have  $\chi_1$ ,  $\chi_2$ , etc. dihedrals ( $\chi_4$  max, for Lys & Arg)

for bonds between tetrahedral carbons, staggered >> eclipsed

overall, a few well-defined sidechain conformations are good: rotamers

[only 2 good ( 4 more OK) for Leu;

13 for Met with 3  $\chi$  angles and no branches]

RNA has one  $\chi$  from ribose to base, but the ribose has limited flexibility and there are 7 degrees of freedom along the backbone between the attachment of one base to the attachment of the next.  
suitefitroc\_...kin