

# BCH 258 lecture notes Fri. Sep 3, 2010

Graphics: restrictions on mainchain conformation, continued:

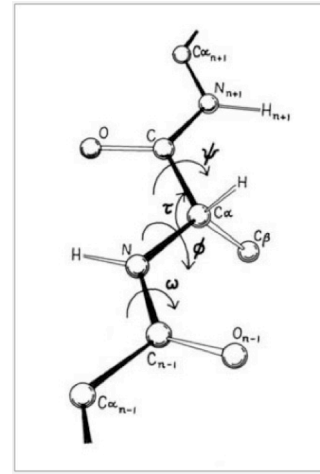
Mage: ala\_dipept\_geom\_dotball5.1.kin  
 Mage: idealpolyala12.kin, appendstuff2.kin  
 Ramachandran plot regions

Handouts:

Amino-Acids diagram

Homework: Worksheet 3: Handedness & Amino Acid Roles

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



Amino Acid Roles: introduce homework... [hypertext in KiNG text window]  
 occurrence vs secondary structure (sidechains in homework, backbone in class)

Geometry of polypeptide backbone: in class...

ala\_dipept\_geom\_dotball5.1.kin, revisited, (howdotwork3KiNG.kin?)

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<sub>10</sub>, 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]

Geometry of RNA backbone: in class...

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\_080323all.kin

