

BCH 258 lecture notes Wed. Aug 26, 2009

ala-dipeptide Lesson

Graphics: restrictions on mainchain conformation:

KiNG: c1Basics kinemage 1 (B&T chapt. 1 Basics, c1Basics.kin

Mage: ala_dipept_geom_dotball5.1.kin

In class work: "sticks" brass Kendrew model parts:

ala-dipeptide,

Points: planar peptides, tetrahedral C α s, handed sidechain attachment.

DO NOT BEND THE BRASS

C α is tetrahedral, handed: L amino acid = biological

"CORN crib" mnemonic for L vs D

Gly not handed, since R = H; special properties

R

H

CO

N

dihedral angles define conformation:

atom distance angle dihedral

measured around central bond of 4 atoms; + = CW, - = CCW

ω is dihedral for peptide; always $\sim 180^\circ$ unless cis ($\sim 0^\circ$),

cis happens $\sim 5-10\%$ of the time for X-Pro; very rarely otherwise

ϕ (phi) & ψ (psi) dihedrals describe backbone conformation

[chain direction named N-term to C-term, as synthesized,
so ϕ (N--C α bond) listed first, then ψ (C α --C bond)]

ϕ, ψ plot (or "Ramachandran plot") of 2 parameters (see handout sheets)

atom bumps leave 3 regions for non-Gly: α , β , L α

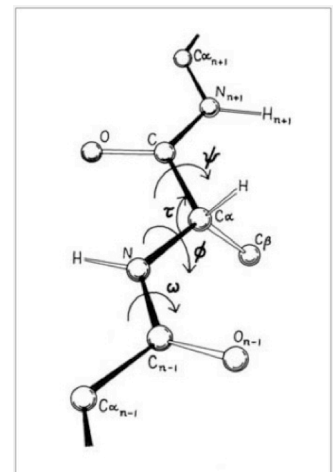
[note handedness inverts through center of plot]

(there are also a few allowed but disfavored regions)

helix and sheet are repeating versions of 2 best conformations

Gly ϕ, ψ plot symmetric; allows both L α , L β ; less constraints

Pro: closed ring makes $\phi \sim -70^\circ$; only ψ varies; so no L α



ala_dipep_geom_dotball5.1.kin

rotatable-bond Ala dipeptide (\sim like c1Basics)

Rama regions - show β better than $180, 180$

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

Gly data, contours - show C β clash in L 3_{10} , L β ; not in β

Homework: Worksheet 2: Dihedrals & Handedness

Kinimage file - c1Basics-1n6-KiNG.kin

PDB file -- 4FXN.pdb