

BCH 258 lecture notes Fri. Aug 29, 2008

Graphics: restrictions on mainchain conformation:

Mage: ala_dipept_geom_dotball5.1.kin
Mage: idealpolyala12.kin, appendstuff2.kin
Ramachandran plot regions

Handouts:

-0- Amino-Acids diagram
-1- Dihedral angle definition and original Ramachandran Plot
-2- F4.Rama.g.G.P.pP-v1.pdf

Homework: Worksheet 3: Dihedrals & Handedness

Kinimage file – c1Basics-B-KiNG.kin

PDB file -- 4FXN.pdb

Polypeptide: entire $C\alpha$ --- $C\alpha$ peptide unit is planar and trans

$C\alpha$ is tetrahedral, "CORN crib" mnemonic for L aa

dihedral angles define conformation:

atom	distance	angle	dihedral
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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 ~ 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-- $C\alpha$ bond) listed first,
then ψ ($C\alpha$ --C bond)]

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

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

[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 $L\alpha$, $L\beta$; less constraints

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

HowDotsWork3.kin

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 $C\beta$ clash in $L3_{10}$, $L\beta$; not in β

...and if there were time...

Sidechains have χ_1, χ_2 , etc. dihedrals (χ_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 χ angles and no branches]

RNA has one χ 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