

BCH 258 lecture notes Fri. Sept 10, 2010

- Assignment: [WrkSht6-H-bonds2009.pdf](#)
- Suggested exploration: on line version of: Anatomy and Taxonomy of Protein Structure link on Kinemage Home page in Gallery section to "HTML version"

In class: N-caps: [Top5200_Ncaps_i+3_phipsiSubset.kin](#)

Tight turns : in loops, or connect $\uparrow\downarrow\beta$; change chain direction {kendrew: -tightturns...}

4-residue square corner; CO(1) may H-bond to NH(4)

central peptide perpendicular to approx. plane of turn

Type I ("common" turn): central CO on side opposite C β (2)&(3); any sidechain

Type II ("Gly" turn): central CO on same side as C β (2)&(3); res. 3 should be Gly

Turns non-planar, handed: actually need type I' (mirror of I) to match

The β -sheet twist and work well for a β -hairpin; Gly-Gly or Gly-Asp best

Non-repetitive structure (NOT random!) or "coil": α , β , L α , conf's in various orders

Lots of sc-mc H-bonds

~2 types: links between secondary str's, or compact, convoluted loops

Water – a few internal; at active site may mimic substrate

\leq one layer well-ordered on outside, esp. around polar groups

crystal or domain contacts often through 1 layer of ordered water

How things fit together: 2v2p helix contacts: [2v2pFH-multi.kin.gz](#) & [2v2p.omap.gz](#)

Hydrogens: [all-atom contacts](#), [H-bonds](#), & [waters](#)

1) Hydrogen atoms : half of atoms; make most intra- & inter-molecular contacts,

both H-bonds and van der Waals

Just edge "decoration" on 1D, but central to 3D

Imagine (visualize) polypeptide chain white with red O, blue N, add H's as green

e.g. [c2Motifs.kin](#) [kin5](#) RNase with H (& H-bonds)

fuzz on the outside of the sticks, but are what makes contacts!

Hydrogens are usually omitted (for very good but not adequate reasons)

make images fuzzy and calculations slow | so only used for H-bonds

not seen well by x-ray data |

Can be handled now, and give big payoffs

We'll usually show either all or none, but other programs may add just polars, for H-bonds

(Note: many of our kinemages specify a "lens" zone to control amount of detail for some particular group, e.g. the Hydrogens. This can be toggled by the "e" key or from the menu: Display/"Lens at center")

2) All-atom contacts : using std. vdW radii, see which atoms touch (or within 0.5Å)

to directly visualize the non-covalent 3D interactions

[howdotwork3KiNG.kin](#) : overview sticks; vdW; dots; \rightarrow closeup,

small probe generating dots

3 terms: vdW, clashes, H-bonds; color-coding by gap or by atom

[1mjHdot-KiNG.kin](#) : good packing, at Leu, at Arg

H atoms interdigitate; even methyls fit staggered

H-bonds on Arg: significant overlap, but favorable

H-bonds to waters at interface; water really part of structure

(technique also finds occasional mistakes:

impossible overlap at Lys 74,

His flips (in active site!)

(Note: All-atom contact analysis empowers evaluation of proposed mutations: to be continued...)

3) Hydrogen bonds : much weaker than covalent, but very significant to 3D structure

close, oriented interaction of H donor and H acceptor , e.g. (mc) NH --- OC

H donors: -NH, -NH₂, -NH₃, water, -OH, (-SH) ...

H acceptors: O, N, water, (S)

obligate donors: mc & other NH, Lys, Arg, ...

obligate acceptors: mc & other CO, COO⁻, PO₄⁼

ambiguous: -OH, water, His, ...

distance: N & O < 3.5Å approx;

H & O < 2.5Å (i.e. < vdW touch) good H-bond has H & O ~ 2Å

angles: N → H vector should point at O position (good ± 30°) N—H—O angle 180° ± 30

C—O—H angle OK ± 90° : N—H --- O (not: H --- O—C)
C (N)

electrostatic dipoles: H partial +, O⁻, so attractive

some bonding, or orbital-sharing, character: H partly “shared”

overlap of H & acceptor vdW directly shows H-bonding

e.g. c2Motifs.kin kin5 for RNase mc H-bonds

Coloring Book

In the Protein Structure Coloring Book (class hand-out), pick one α/β protein and one All-β protein to color, using any system that interests you and that makes sense relative to the 3D structure; hand in those two. [Note that the coloring book includes All-α and Small Irregular proteins as well.]

Graphics: Coloring Book Slides (shown in class) [slide_archive/ribbons_etc/]

- | | |
|-----------------------------|-------------------------------------------|
| 11.GammaCrystallinJane.jpg | barrel fold |
| 12.GammaCrystallinCyrus.jpg | sheet sandwich |
| 13.GammaCrystallinTom.jpg | evolution, gene duplications |
| 21.RubiscoJSRic.jpg | sec. str. |
| 22.BPTISSluminated.jpg | β sidedness, SS |
| 31.SODpastel.jpg | depth |
| 32.TIMpastel.jpg | depth and sec. str. |
| 41.IggVLcolorBkice.jpg | simple topol.: connections: GK vs hairpin |
| 43.CAPgreekKeyPair.jpg | simple: GK pair |
| 45.CPAspider_Duncan.jpg | complex: sec. str., sided, ~H-bonds, etc. |