

BCH 258 lecture notes Wed. Sept 10, 2008

How things fit together: 2v2p.pdb: helix contacts; brass models: alpha--3-10--tightturns

Hydrogens: all-atom contacts, H-bonds, & waters

• Assignment: WrkSht6-H-bonds2008.pdf

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; → 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