Motions

- Assignment: WrkSht8—motions2009

Handout pages: motions [p.11--15]

NMR & x-ray: movements vs. multiple conformations vs errors or lack of information
but NMR sometimes directly measures motion: line width, ring flips

[p.11] time scales (nmr can now do faster)
- fluctuations vs transitions
- folding & allostery in 2nd half of semester

[p.12] individual residues; xray low B vs multiple conformations vs disappear
- nmr: ring flips; NH exchange

[p.13] loop motions—Staph. nuclease; protease sensitivity, ends not seen
- HEW lysozyme: calc. vs. B’s (vs evolution)
- TIM: order-disorder; entropy → specific but not too tight
  (get some with any induced fit)

[p.14] domains (very common for catalysis or binding)
- hexoKinase: specificity; exclude water; line up site
- hinge motion: approx. rigid, but some bending

Graphics: (B&T kinemages on main website under Kinemages/Kins List)

(c15 k2) [p.15] IgG flex
(c8 k4) allostery: Trp repressor with Trp, DNA: 3 state
(c6 k7) [p.14] hexoK hinge
(c6 k8) more unusual & dramatic: CDK2/cyclin
(c6 k9) calmodulin
(c6 k5) Gro EL/ES v1, slice; negative cooperativity
(c6 k6) EL subunit: bow

70S_anim.kin RNA also does it! : ribosome binds tRNA

70S_anim.kin: coords real-space fit into cryo EM 12.3Å map EfgG GTP state of 70S
1P6G is 30S part, 1P85 50S part (incl. 5S)
1P6G 11.5Å initiation-like state
1P87 is 30S part, 1P86 50S (+5S, +tRNA)
(P only for RNA, Calpha for prot.)

Davis_Backrub_kinSup.kin smooth backrub with two-state alternate conformations

HBAllo-KiNG.kin paradigm allostery, subunits as domains
(intro to molecular machines...