

BCH 258 lecture notes Fri. Sept 11, 2009

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...)