

## BCH 258 lecture notes Mon. Sept 15, 2008

### Motions

- Assignment: WrkSht8-motions2008

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 2<sup>nd</sup> 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

HBAllo-KiNG.kin paradigm allostery, subunits as domains

2dn2H-Deoxy-KiNG.kin, 2dn2.omap.gz,

2dn1H-OXY-KiNG.kin, 2dn1.omap.gz

follow alpha1 Heme Deoxy-Oxy change out to alpha1/alpha2 interface (salt-links)

(B-factors vs map density)

Davis\_Backrub\_kinSup.kin smooth backrub with two-state alternate conformations

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.)

COORDINATES FROM FILE: 2DN1HABCD.PDB

HEADER OXYGEN STORAGE/TRANSPORT 25-APR-06 2DN1  
TITLE 1.25A RESOLUTION CRYSTAL STRUCTURE OF HUMAN HEMOGLOBIN IN  
TITLE 2 THE OXY FORM  
KEYWDS HUMAN HEMOGLOBIN, HIGH RESOLUTION CRYSTAL STRUCTURE, OXYGEN  
KEYWDS 2 TRANSPORT  
EXPDTA X-RAY DIFFRACTION  
AUTHOR S.-Y.PARK,T.YOKOYAMA,N.SHIBAYAMA,Y.SHIRO,J.R.TAME  
REMARK 2 RESOLUTION. 1.25 ANGSTROMS.

COORDINATES FROM FILE: 2DN2H.PDB

HEADER OXYGEN STORAGE/TRANSPORT 25-APR-06 2DN2  
TITLE 1.25A RESOLUTION CRYSTAL STRUCTURE OF HUMAN HEMOGLOBIN IN  
TITLE 2 THE DEOXY FORM  
KEYWDS HUMAN HEMOGLOBIN, HIGH RESOLUTION CRYSTAL STRUCTURE, OXYGEN  
KEYWDS 2 TRANSPORT  
EXPDTA X-RAY DIFFRACTION  
AUTHOR S.-Y.PARK,T.YOKOYAMA,N.SHIBAYAMA,Y.SHIRO,J.R.TAME  
REMARK 2 RESOLUTION. 1.25 ANGSTROMS.