

BCH 258 lecture notes Mon. Sept 20, 2010

- Assignment: Coloring Book due Wed Sept. 22

Allosteric Machinery: Hemoglobin THE example

2dn2H-Deoxymod-KiNG.kin, 2dn2.omap.gz,
2dn1H-OXYmod-KiNG.kin, 2dn1.omap.gz
follow alpha1 Heme Deoxy-Oxy change out to alpha1/alpha2 interface (salt-links)
(B-factors vs map density)

Perutz (1970) "Stereochemistry of cooperative effects in haemoglobin", Nature 228: 726

Baldwin & Chothia (1979) "Haemoglobin. The structural changes related to ligand binding and its allosteric mechanism", J. Mol. Biol. 129: 175.

Dickerson & Geis (1983) "Hemoglobin: Structure, Function, and Pathology", Benjamin/Cummings Publ., Menlo Park, CA

S.-Y.Park,T.Yokoyama,N.Shibayama,Y.Shiro,J.R.Tame (2006)

"1.25 Resolution Crystal Structures of Human Haemoglobin in the Oxy, Deoxy, and Carbonmonoxy Forms" J. Mol. Biol. 360: 690

coordinates from file: 2dn1Habcd.pdb

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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.
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coordinates from file: 2dn2H.pdb

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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.
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