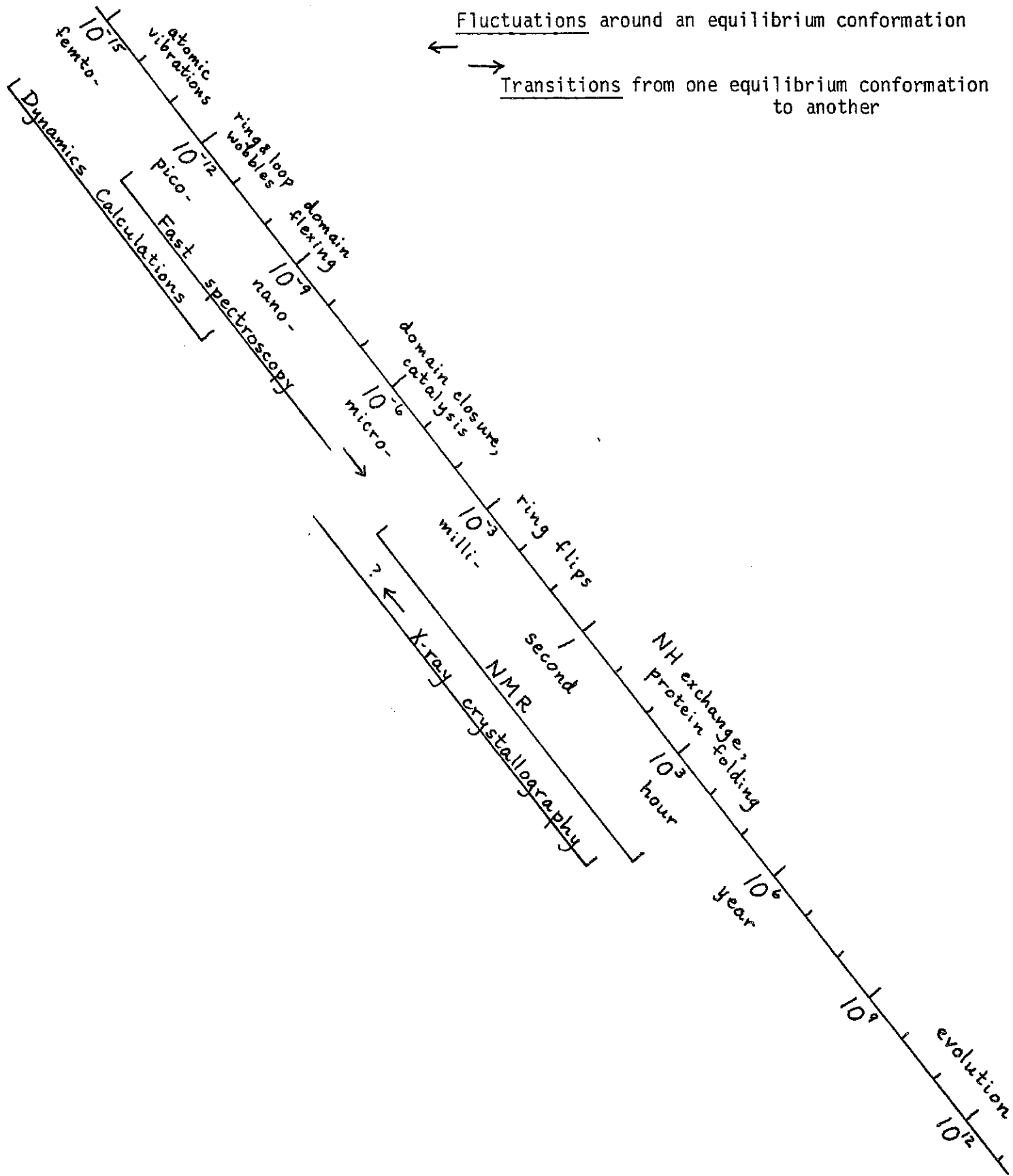
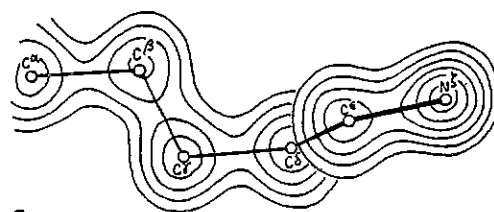


Time Scale of Protein Motions

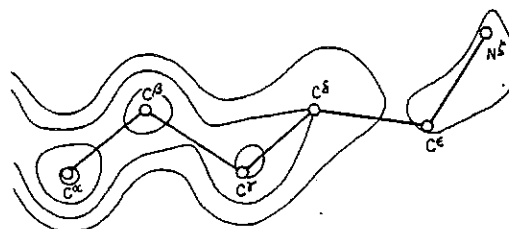


Motions

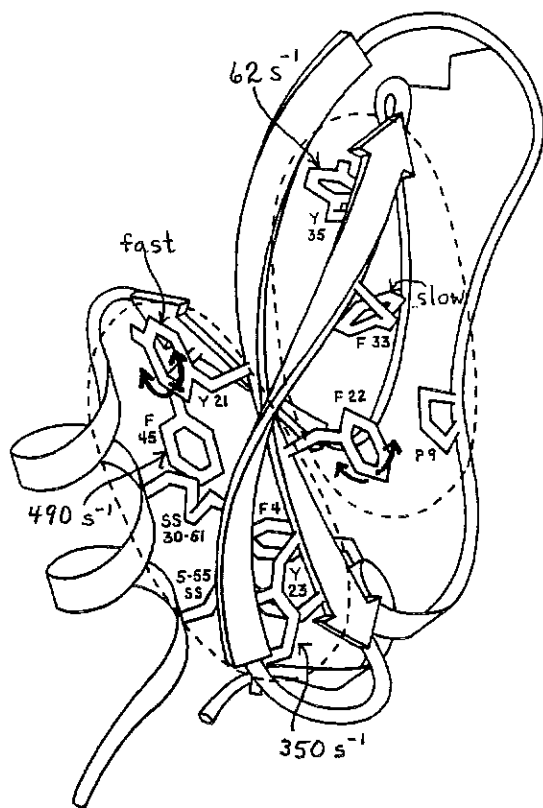
Two lysine side chains from the refined rubredoxin structure: a) has a well-defined position but b) is disordered beyond C β and presumably moves fairly freely in the solvent.



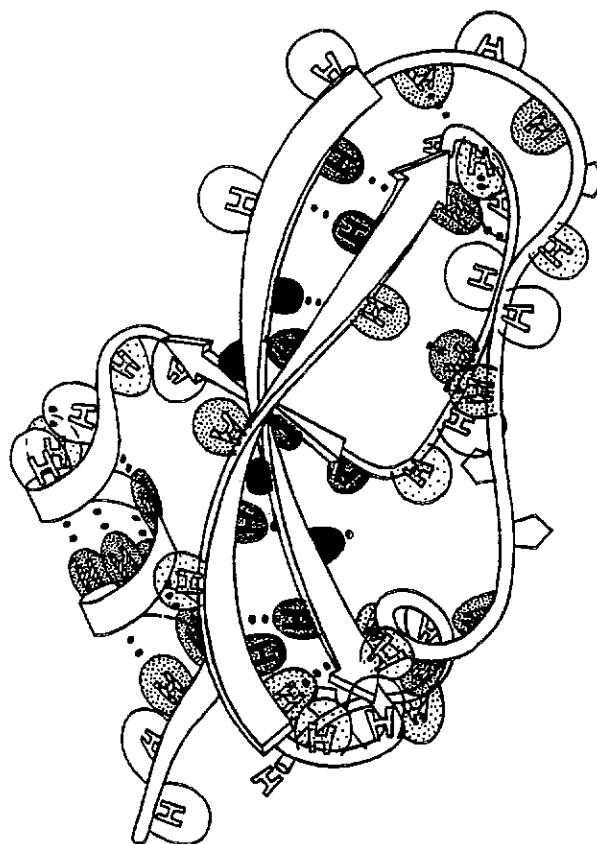
a



b

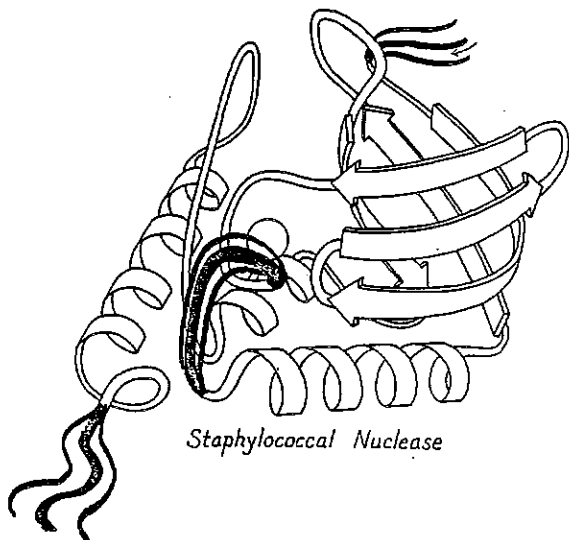


NMR measures rapid flip-over rates even for tightly-packed internal side chains (PTI, at 40°C.)



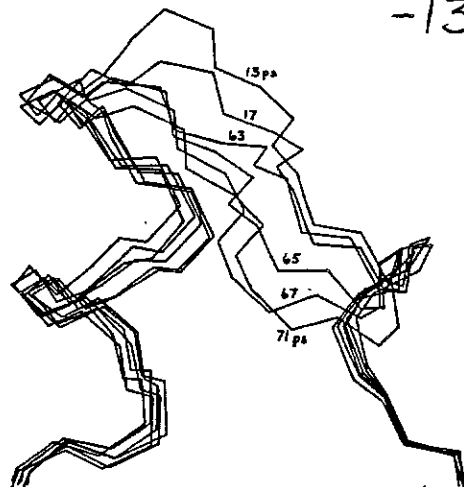
Rates of hydrogen exchange for NH protons in trypsin inhibitor, from NMR
At 36°C., white are too fast to measure and black too slow; others have half-times from 10 min. to 2 months.

~~1-24~~ KLHKEPATL IKA IGDGVKLMYGGPMTFRLLVDTPET ~~57-64~~ YGPEASFTKKMVENAKKIEVE
~~101-108~~ FNKGQRTOKYGRGLAYIYADGKHYNEALVRQGLAKVAVVYKPNHTEQHLRKSEAQAKKEKLNINSE ~~111-118~~

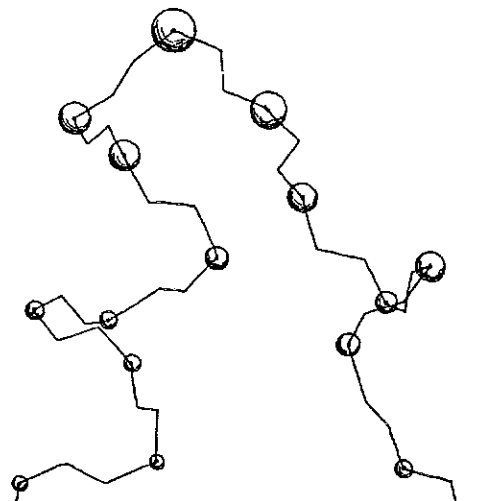


Staphylococcal Nuclease

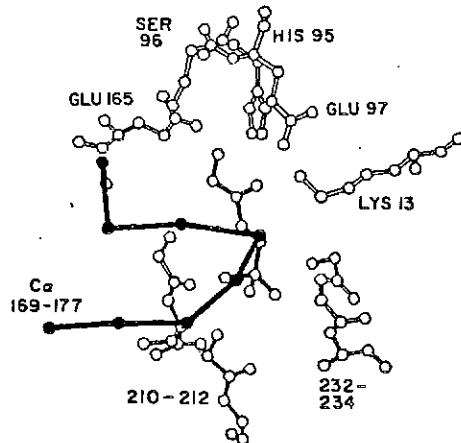
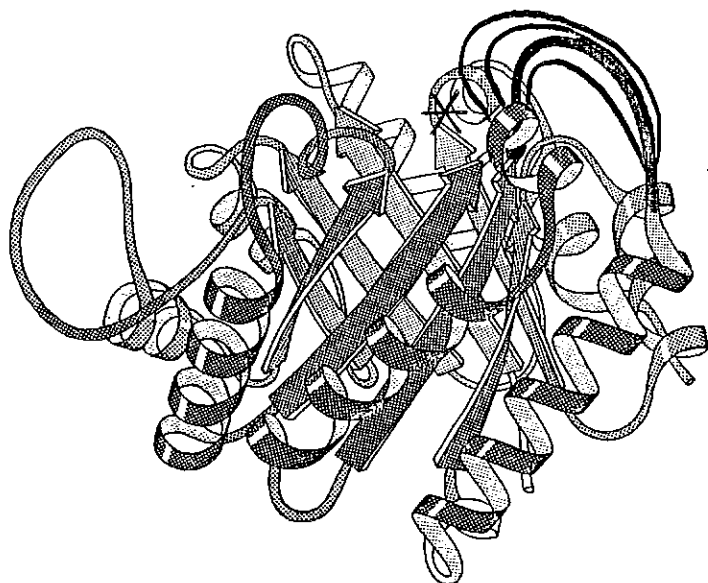
Motion of external loops: Above are shown the locations of highly mobile regions in the sequence and in the 3-D structure of Staph. nuclease. Arrows show sites of rapid trypsin cleavage.



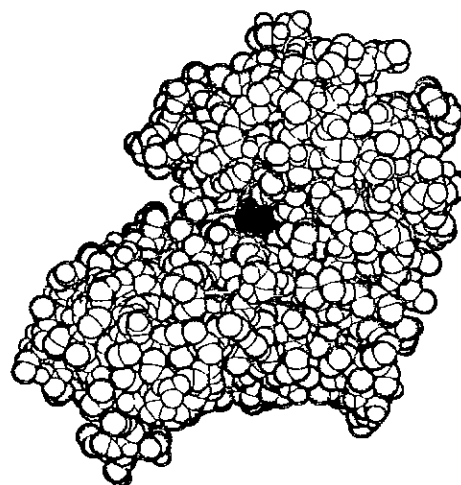
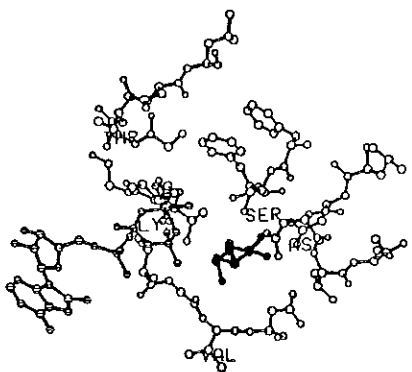
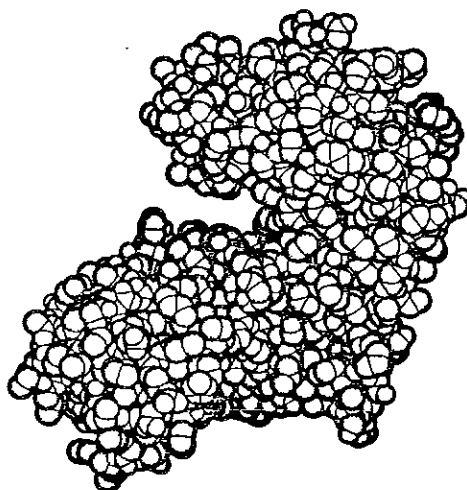
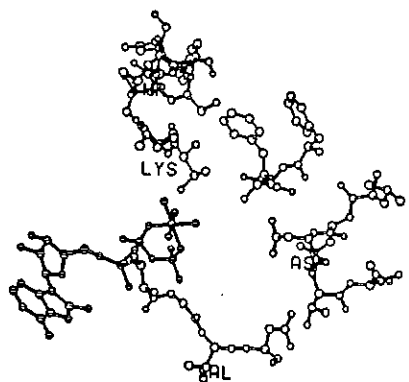
Lysozyme 94-109: dynamics run



Lysozyme 94-109: Crystal B values

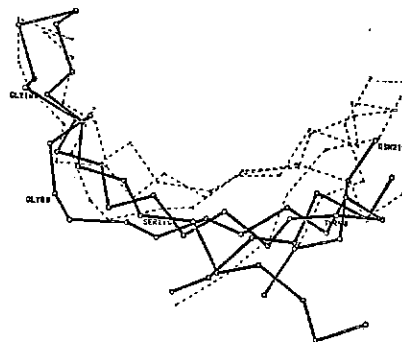
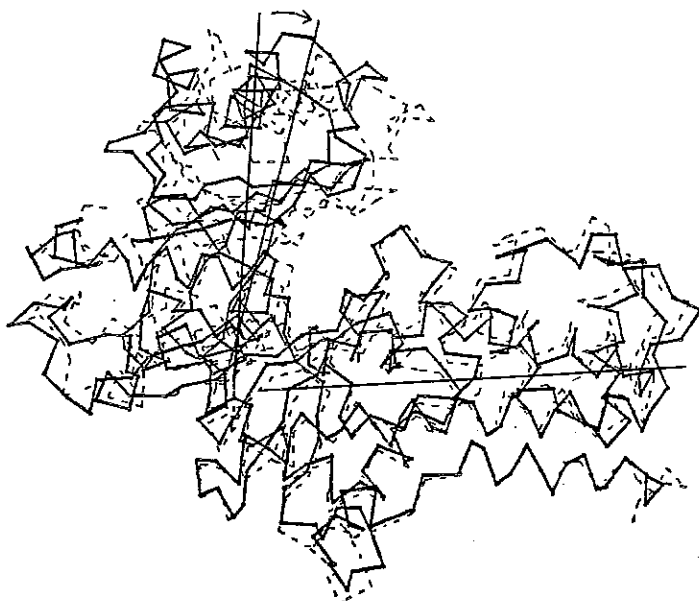


Triose phosphate isomerase has a loop (with highly conserved sequence) that is quite disordered in the apoenzyme x-ray structure(left). In the x-ray structure of an intermediate-analog complex, the loop has moved down into a well-ordered conformation covering the active site (see detailed figure on right). It is thought that the entropy of loop disorder partly balances enthalpy of substrate binding, allowing high specificity along with easy release of product.

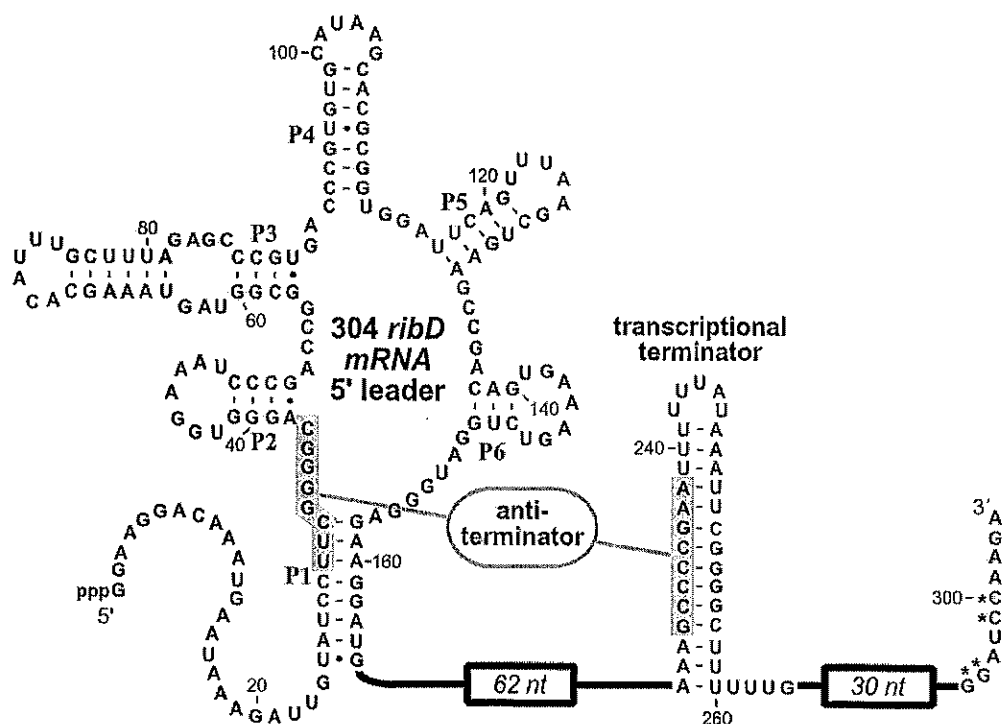


Domain motions important in catalysis: Hexokinase normally has the "jaws" of its two domains in an open position (top figures), even with ATP bound. But when glucose (the substrate, shown in black) binds the jaws clamp shut around it, ensuring specificity and excluding water from the active site. That prevents the enzyme from wasting energy as an unproductive ATPase.

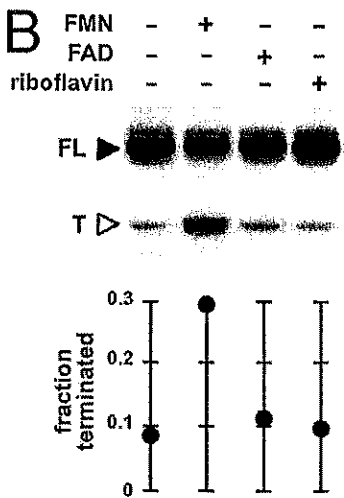
To the first approximation, the domain motion is a rigid-body hinge of about 12° (left). A closer look, however, shows many internal readjustments, including a bending of the beta sheet as shown below.



A



B



C

