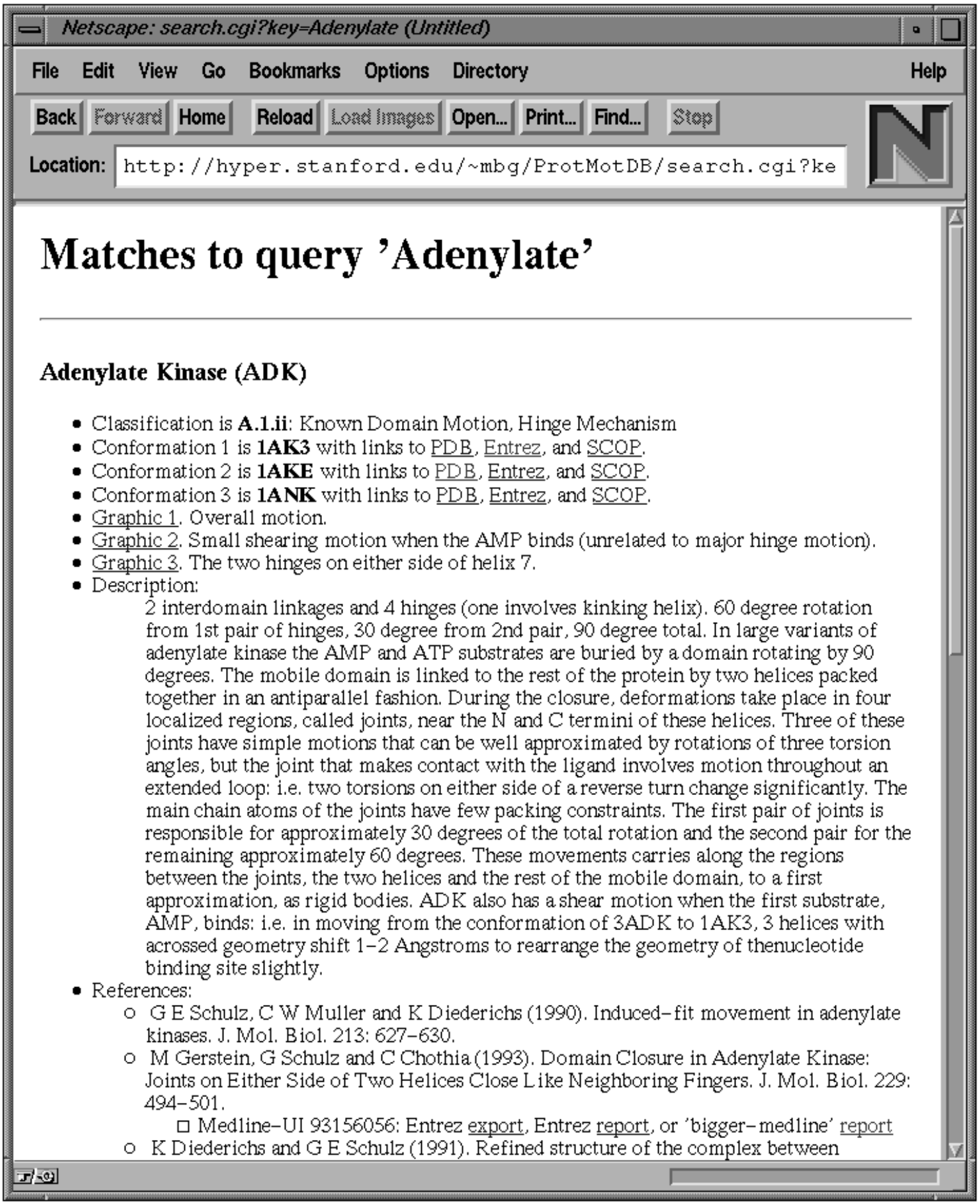

Matches to query 'Adenylate'

Adenylate Kinase (ADK)

- Classification is **A.1.ii**: Known Domain Motion, Hinge Mechanism
- Conformation 1 is **1AK3** with links to PDB, Entrez, and SCOP.
- Conformation 2 is **1AKE** with links to PDB, Entrez, and SCOP.
- Conformation 3 is **1ANK** with links to PDB, Entrez, and SCOP.
- Graphic 1. Overall motion.
- Graphic 2. Small shearing motion when the AMP binds (unrelated to major hinge motion).
- Graphic 3. The two hinges on either side of helix 7.
- Description:

  2 interdomain linkages and 4 hinges (one involves kinking helix). 60 degree rotation from 1st pair of hinges, 30 degree from 2nd pair, 90 degree total. In large variants of adenylate kinase the AMP and ATP substrates are buried by a domain rotating by 90 degrees. The mobile domain is linked to the rest of the protein by two helices packed together in an antiparallel fashion. During the closure, deformations take place in four localized regions, called joints, near the N and C termini of these helices. Three of these joints have simple motions that can be well approximated by rotations of three torsion angles, but the joint that makes contact with the ligand involves motion throughout an extended loop: i.e. two torsions on either side of a reverse turn change significantly. The main chain atoms of the joints have few packing constraints. The first pair of joints is responsible for approximately 30 degrees of the total rotation and the second pair for the remaining approximately 60 degrees. These movements carries along the regions between the joints, the two helices and the rest of the mobile domain, to a first approximation, as rigid bodies. ADK also has a shear motion when the first substrate, AMP, binds: i.e. in moving from the conformation of 3ADK to 1AK3, 3 helices with acrossed geometry shift 1–2 Angstroms to rearrange the geometry of thenucleotide binding site slightly.
- References:
  - G E Schulz, C W Muller and K Diederichs (1990). Induced-fit movement in adenylate kinases. J. Mol. Biol. 213: 627–630.
  - M Gerstein, G Schulz and C Chothia (1993). Domain Closure in Adenylate Kinase: Joints on Either Side of Two Helices Close Like Neighboring Fingers. J. Mol. Biol. 229: 494–501.
    - Medline-UI 93156056: Entrez export, Entrez report, or 'bigger-medline' report
  - K Diederichs and G E Schulz (1991). Refined structure of the complex between