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Poster 6

NMR studies on N-terminal domain of DNA2

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Saccharomyces cerevisiae Dna2 protein has biochemical activities: DNA-dependent ATPase, DNA helicase and DNA nuclease and is essential for cell viability. Especially, Pro^{504} is determined as an important residue in ATPase, helicase, and nuclease activity. We have determined the three-dimensional solution structure of N-terminal domain (Val^{501}-Phe^{508}), using two-dimensional ^{1}H-NMR data and dynamical simulated annealing calculations. On the basis of a total of 44 experimental restraints including NOEs, $^3J_{\alpha\beta}$ and $^3J_{\alpha N}$ coupling constants, we calculated 50 structures with the program CNS. The 23 lowest energy structures were selected out of 50 final simulated-annealing structures. The average structure $(\overline{<SA>})_k$ was calculated from the geometrical average from 23 $(<SA>)_k$ structure coordinates and subjected to restraint energy minimization (REM) to correct covalent bonds and angle distortions. The atomic rmsds of the final 23 structures for the individual residues were calculated with respect to the average structure. The mean RMSDs for the 23 structures were 0.042 nm for backbone atoms and 0.316 nm for all heavy atoms, respectively. The Ramachandran plot indicates that the φ,Ψ angles of the 23 final structures are properly distributed in energetically acceptable regions. Solution structure of nuclease activity domain of Dna2 showed a single unique turn spanning residues of Pro^{503} - Phe^{506}.