What Does 'FoldIt (light)' do?

'FoldIt (light)' is an interactive application to analyze and display the coordinate files of the Protein Data Bank (PDB) not exceeding 1600 residues, 400 bases, 30 hetero-residues and 1000 water molecules. FoldIt can read NMR-resolved structures (maximum of 10 models per file).

'FoldIt (light)' has two main windows:

• a color image window to display the protein structure

• a report window to record the results of all operations requested by the user.

The protein structure can be manipulated easily in real time with the mouse, zoomed or observed in stereo. Structure movement can also occur stepwise for a more precise control. Animations can be created.

Steric conflicts, disulfide bonds, hydrogen and ionic interactions can be located and displayed in the protein structure. These interactions are also reported in the report window.

Atoms and residues can be tagged individually (or globally) and structural information can then be extracted.

Portions of a structure can be read into memory or displayed.

Two structures can be read at the same time in memory and can be overlapped automatically.   The second structure can be manipulated independently of the first.

Bonds can be rotated and atomic parameters can be changed.

The sequential folding of a protein can be simulated.

It is possible to create a protein de novo from the menu or by entering the sequence from the keyboard. Structures can then be manipulated locally or forced into helices.

The application can process structures in the batch mode to extract a number of structural features: Ramachandran plots, SS-bond plots, H-bond plots. Statistics on atomic parameters are displayed as histograms. The application can work in the background.

'FoldIt (light)' does not support printing but can save the content of its report window, image window and histograms in TEXT or PICT formats. These files can then be manipulated by other specialized applications and printed.

This application has been originally written as a platform to improve protein folding prediction methods (hence the name 'FoldIt') but many general features have been added (like display and analysis functions). The program portions related to prediction methods are also the sole desactivated feature of this released version (hence the adjective '(light)').

Balloon Help is supported as well as an in-line help. A printable User Manual is provided.