

To Start

This application works well on Macintosh computers running under System 7. If you use a machine equipped with a 68030 CPU (+68881/82 coprocessor) or with a full 68040 CPU (not a 68LC040!), use the 'FoldIt (light) FPU' version. Otherwise (e.g. on all other Macs and on PowerMacs), use the 'FoldIt (light) FAT' version.

A 256-color monitor is recommended (although 'FoldIt (light)' runs on any monitor (B&W, gray levels, thousands-color... monitors). Using a higher color resolution slows down motion by about 10% with hardly any color benefit. Monitors having a vertical resolution higher than 400 ppi (portable, 13" ...) are recommended to display dialogs correctly. This means that 12" monitors will cut off some dialogs (in fact a single one).

The application manual, 'FoldIt User Manual', is a stand alone document. It can be printed.

Put the 'FoldIt Prefs' folder (delivered with this application) into the 'System Folder' (not into the Preferences Folder!). If you don't do this, some features will not be available.

The application requires a memory partition of 879KB for the FPU version and 1.98MB for the FAT version. This has been kept to a minimum and there is no advantage in increasing partition size. However, to read a structure or to create additional utility windows, FoldIt makes use of the extra memory available on your Mac (dynamic memory allocation). For instance, about 3.3 KB are necessary to read one residue and 4.3 KB to read one base: this means that, for a typical 200-residue protein, 660 KB of extra RAM is necessary. If you want to do some animations, you may be prompted to close some other applications.

Conventions

- Rotation atom: Atom around which the whole structure is rotated.
 - Torsion atom: Atom separating the stationary part of a structure from its mobile part. Torsion angle sign convention is that of IUPAC-IUB (JMB, 1970): clockwise is positive.
- Rotation concerns only the display (no coordinate change) while torsion concerns a structural modification to part of the structure (coordinate change).
- Two atoms are covalently interacting when the shortest covalent pathway between them is <4 bonds.

In the following:

main menus are underlined

menu items are in bold

dialog items are in italics

Abbreviations

- MC = main chain.
 - SC = side chain.
 - CA = carbon alpha (the first carbon of a residue main chain atoms — the second is C).
 - H-bond (Hbd) = hydrogen bond.
 - I-bond (Ibd) = ionic bond.
 - SS-bond (SSbd) = disulfide bond.
 - Sec-bond = secondary bond (H-bond, I-bond).
 - bded = -bonded (applies to hydrogen bonds -H-bonds-, ionic bonds, .
 - bdLen = bond length (distance to the previous atom in the chain).
 - bdAng = bond angle of an atom (angle formed by this atom, its previous neighbor and its previous-previous neighbor).
 - trAng = torsion angle of an atom (angle formed by the preceding neighbor of this atom, this atom, its previous neighbor and its previous-previous neighbor).
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- Water: the letter 'w' marks water atoms (wO, wH1, wH2).
 - Block: a 'block' designates a residue, a base, a hetero-residue or a water molecule.