Utilities menu

• Batch File Settings...: Dialog to limit the quality (resolution, refinement) and type of files which will be considered during a batch process.
Data bases can also be selected (Feature not available on all versions.): 'Boberg Files' are the files listed by Boberg, J., Salakoski, T., & Vihinen, M. (1992) Proteins 14, 265-276, 'Stickle Files' are the ones listed by Stickle, D.F., Presta, L.G., Dill, K.A., & Rose, G.D. (1992) J.Mol.Biol. 226, 1143-1159 and 'Swindells Files' are the ones listed by Swindells, M.B., MacArthur, M.W., &Thornton, J. (1995) Nature Struct.Biol. 2, 596-603. Thus if the option 'Boberg Files' has been selected, only the files belonging to this group and located in the 'Batch Fldr' will be considered in statistics.
• StdW Settings... (Standard Window Settings):
Profiles:Energy Maximum & Profiles:Auto Scaling: Used to scale 'Top Profile' curves which can be requested from atom info windows.
Histograms:Ordinate Maximum & Histograms:Sampling Width: Used to display the histograms produced by Batch/Stat/Atom Prms. Changes in the values of ordinate maximum and sampling width can be made dynamically using the keyboard shortcuts âŒ˜◆, âŒ˜⊘, âŒ˜≠ and âŒ˜¬.
• Steric Settings...:
Nearest Atom Range (Å): Used in Utilities/Look For/Nearest Atoms.
Steric Threshold (kcal): Under this threshold steric conflicts are neglected.
Clash Profile Interpolation (points): Used for the Clash Profile procedure in atom info windows.
Show Clash Between Atoms During Torsion : Clash forecast and display during torsion when a torsion atom has been selected.
• EDmap Settings...: Feature not available on all versions.
Higher/Lower Threshold:
Show ED map frame.
• Atom Parameters Analysis...: Operate structural statistics on .FIT files (up to 104 files) located in the 'Batch Fldr' or on the current structure. Statistics can be done on Bond Length Spread or Bond Angle Spread or Torsion Angle Spread, SS-Bond Angle Spread or H-Bond Angle Spread. However, if a structure is already in memory, the Current structure can be analyzed and statistics will be done with standard deviations. If the Batch button is selected, the results are displayed in a series of stat windows which can be saved on disk. Clicking on one of the bottom marks of a stat window gives the length and angle information. Displaying histograms is possible by clicking on a stat window with the OptionKey down: histogram parameters can be set through the Utilities/StdW Settings menu. Clicking OK in the dialog with the OptionKey down will display all stat windows in the histogram mode.
RamPlot (Ramachandran Plot) of the Current structure or of all Batch files (files located in the Batch Fldr) can also be done; plots including all residues or only/except the selected residues can be done (a multiple selection is possible). Clicking on a point gives phi, psi and name of the corresponding residue (which is shortly highlighted in the current structure). Clicking with the OptionKey down: shows the energy profile of the corresponding residue; move the mouse to see the energy profile changing with psi. 3 cases for the energy profile: Pro, Gly and all the rest. Clicking with the ControlKey down: shows the energy map of the concerned residue; move the mouse to see the local energy; click the mouse to stop.
• Sequence Analysis...: Feature not available on all versions. Operate motif and sequence statistics on .FIT files (up to 104 files) located in the 'Batch Fldr' or on the current structure.
• Select...: Limit display to 1 or More portions of structure in memory. Possibility to select chains. Type highlights only blocks of the selected type. It is also possible to show/hide the differents elements of a structure and to select blocks on the basis of their main chain state, of the Ramachandran region they occupy or of their class (hydrophobic, hydrophillic, positively or negatively charged). Pen settings for the class-based selection are predetermined: yellow (hydrophobic), green (hydrophillic), red (positively charged) and blue (negatively charged)
Subsequent analysis of the structure in memory will only be limited to selected portion(s).
• Write...: Write all data that are available (highlighted): Sequence & Composition, Coordinates, Charges, Occupation & B-Factors, Bond Lengths, Bond Angles, Torsion Angles, H-bonds, I- Bonds, SS-Bonds, Secondary Structures, Steric Conflicts .
Many of these data can only be written if they have been previously looked for (Utilities/Look For).
For Secondary Structures, structural information concerning each residue is given:
region (region of Ramachandran plot): pack (helix region), packG (symetrical of helix region), extd (sheet region), extdG (symetrical of sheet region), out (none of the preceeding);
state : alpha, 310, strand, turn, coil;
phi : phi angle in degree.

psi : psi angle in degree.
chi1 : chi1 angle in degree.
OBded: indicates to what atom(s) main chain oxygen is H-bonded (Bded= bonded).
NBded: indicates to what atom(s) main chain nitrogen is H-bonded.
SCBded: indicates to what atom(s) side chain atoms are H-bonded.

If the OptionKey was down when the Write button was selected, results are written to disk. This is highly recommended when resquests concern H-bonds or secondary structure of big structures.

• Look For:
* Sec-Struct: Determine the secondary structure class of each residue (alpha, 310, strand, turn, coil).
* H-Bonds: Look for H-bonds. 'FoldIt (light)' calculates the missing protons implicated in H-bonds.
* I-Bonds: Look for ionic bonds.

If Sec-Struct/H-Bond/I-Bond menu items have been chosen with the OptionKey down, results will be made automatically visible on the image window.

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* SS-Bonds: Look for SS-bonds (this is automatically done each time a PDB structure is loaded into memory).
* All Sec-Bds: Look for all secondary bonds (H-bonds & I-bonds).
* Steric Conflicts: Determine which atoms are collided with energies above 'Steric Threshold'.
* Near Atoms/Near Residues (item enabled if 1 atom or 1 residue has been selected): Mark and list all atoms or all residues located at a distance < Near Atom Range to the first selected atom or the selected residue; the atoms linked by 3 or less covalent bonds to the selected atom are ignored.

• Overlap:
* Structural: Overlap 2 structures having same length. If called with ControlKey down, identical residues on both structures will be selected.
* Sequential: Feature not available on all versions.

• Tools: Only for development purposes (not available in all versions).

• .PDB=>.FIT...: Transform all '.PDB', '.pdb' or '.ent' files (up to 400!) located in the 'Batch Fldr' into .FIT files, and store them on disk in that same 'Batch Fldr'. As FoldIt is able to work in background, the computer can still be used for other purposes during the .PDB=>.FIT operation. Moreover, if full CPU power is requested for another process for a given period of time, this operation can be paused/reactivated using the File/Pause menu.