User Manual for view

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1 STARTING THE APP

Within the ereg directory tree, file "src/avp/avp.app/Contents/MacOS/avp" is the viewing app executable. The app takes no command line arguments. In directory "test/car", the script file "zzview" starts the viewing app. Use of the script enables replacement of the lengthy relative path name "../../src/avp/avp.app/Contents/MacOS/avp" with the easily typed script name.

2 USER INTERFACE

The user interface contains a 2×2 array of 4 text boxes. A structure contained in a pdb format file is selected for display by entering into a text box the name of the file, excluding the .pdb suffix. Path names are relative to the directory from which the app is executed. The directory "test/car" is the directory to which program generated structures are written.

Below each test box is a row of 6 buttons labeled r, d, h, m, lab r, and lab a. Button r will read and display the molecule specified in the test box. As an intermediate step in rendering the molecule, the app creates a ".obj" file and a ".mtl" file in the directory containing the ".pdb" file. Button d will delete a previously read molecule, including the previously created ".obj" and ".mtl" files. Button h toggles on and off display of the molecule. The button label is colored red when display is on. Turning off the display does not delete the molecule or change the connectivity to mouse and keyboard input. Button m toggles on and off connectivity to mouse and keyboard input. The button label is colored red when translation and rotation of the molecule is connected to the mouse and keyboard. Button lab r will toggle display of residue labels. The button label is colored red when display is on. Button lab a will toggle display of atom labels. The button label is colored red when display is on.

The quit button in the top row quits the app. Also in the top row, the buttons labeled 1, 2, and 4 enable user control of the number of frames in which molecules are displayed. The active number of frames is highlighted in red. Button 1 displays all of the 4 possible molecules superposed in a single frame. Button 2 displays molecules in 2 side by side frames. Button 4 displays each of the 4 possible molecules in a separate quadrant frame.

3 MOUSE AND KEYBOARD CONTROL

Molecule translation and rotation is controlled by input from the mouse and keyboard. For rotation about the x-axis, press the left mouse button and drag vertically. For rotation about the y-axis, press the left mouse button and drag horizontally. For rotation about the z-axis, press the right mouse button and drag horizontally. Translation is controlled by mouse motion with the space key pressed.

From the keyboard, rotation can also be controlled by pressing the a, d, w, x, z, and e keys. Translation can be controlled using these same keys with the space key pressed.

4 STANDARD PDB AND EREG FORMAT

For structures generated by the ereg program, consistency with the pdb format for proteins, and with the ereg format for nuncleic acids, is guaranteed. Because of deviations from these formats, the viewing app, as currently implemented, will often fail when attempting to read a ".pdb" file generated by other sources. Common problems include missing atoms, use of non-standard atom names, or use of residue names not included in the ereg dataset. For a non-conforming file "MOL.pdb", visualization using the viewing app becomes possible if geometry regularization succeeds in reading the ".pdb" file. Enter the file "MOL.pdb" into directory "test/exp". From directory "src/str", run command "greg test MOL" to regularize geometry. In directory "test/car", use the viewing app to display the regularized structure file "MOL.00.pdb".