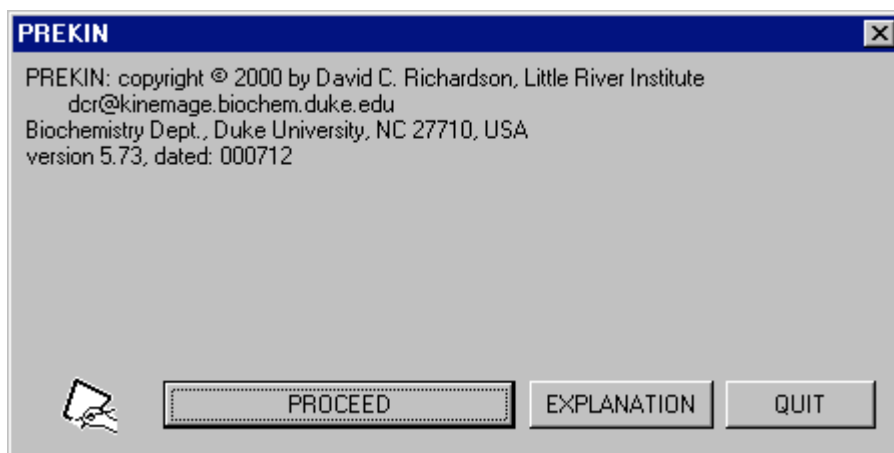
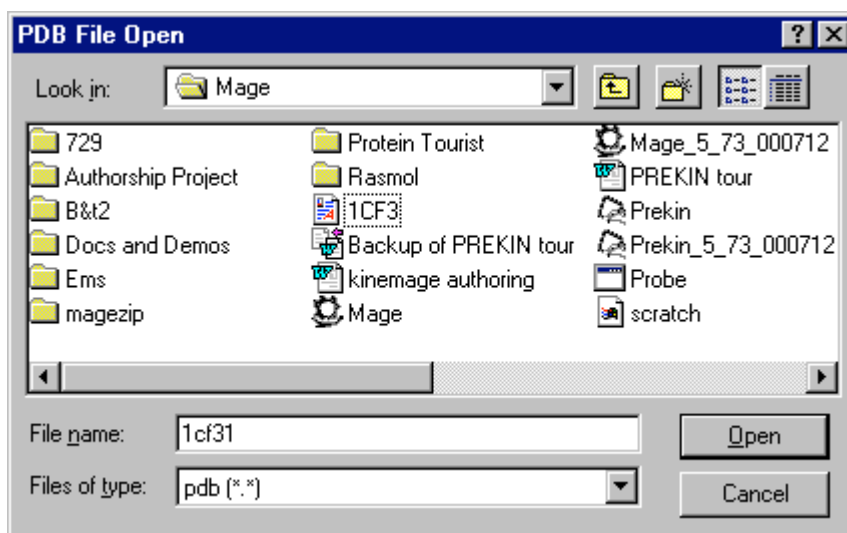


A quick tour through PREKIN (shown for the PC)

Double clicking on the PREKIN icon will open the following dialog box.

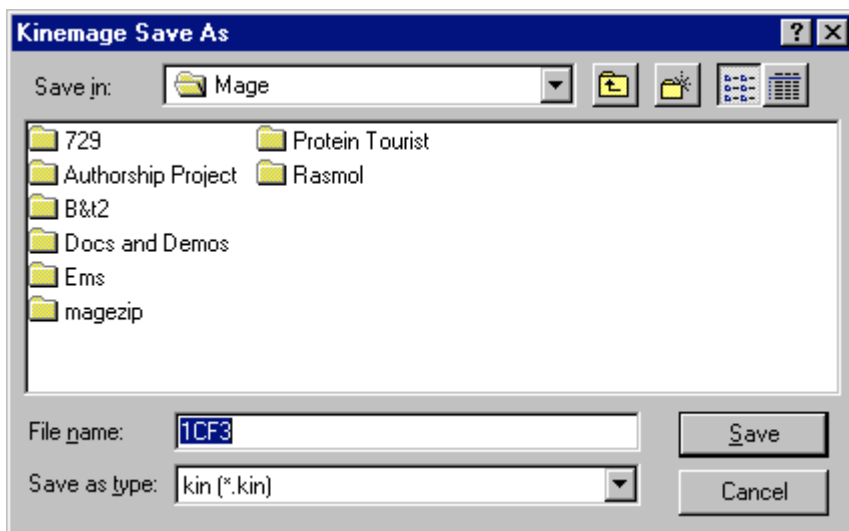


The dialog box reminds you that Professor David Richardson wrote (and maintains) this program, and, very importantly, that this is Version 5.73 of PREKIN, which was completed on July 12, 2000. If you want to report any bugs or make any suggestions about PREKIN, please state the version of your software, operating system, and hardware platform. Click PROCEED to proceed!



Select a PDB file and input the file name. Many programs use PDB files, so they may have a variety of icons. Here I have selected 1CF3.pdb, which is one of the PDB files for glucose oxidase. Click the open button to proceed.

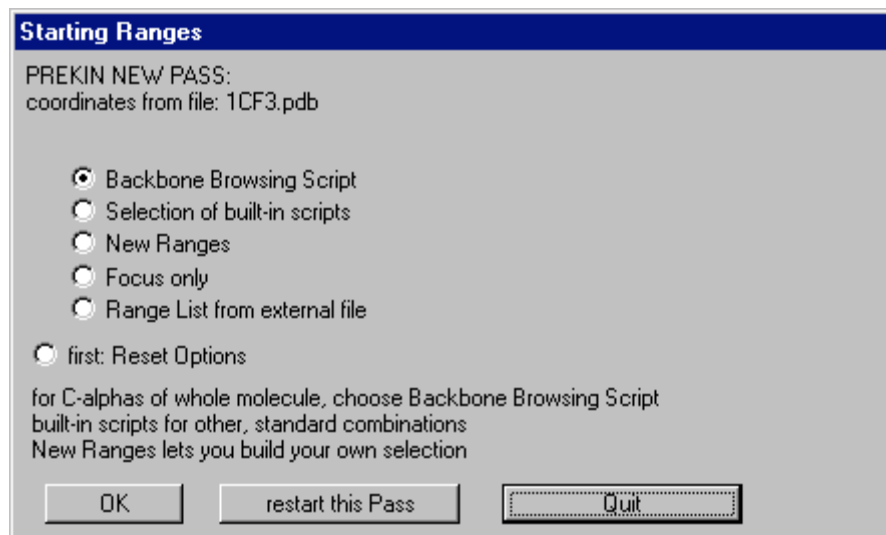
NOTE: If you started this session by dragging the icon for your PDB file onto the PREKIN icon, you will bypass both dialog boxes on this page.



This dialog box asks where you want to save the kinemage file when you have completed it. The default name is the same as the PDB name, with the exception of the extension. It is a good idea to give the file a descriptive name. For example, I might want to call this *Glox.kin*, since it is a file of glucose oxidase.

Warning: PREKIN should automatically include the *.kin* extension, but the PC version sometimes doesn't. Also, always look at the top of the dialog box and make sure this folder is where you want the kinemage to go.

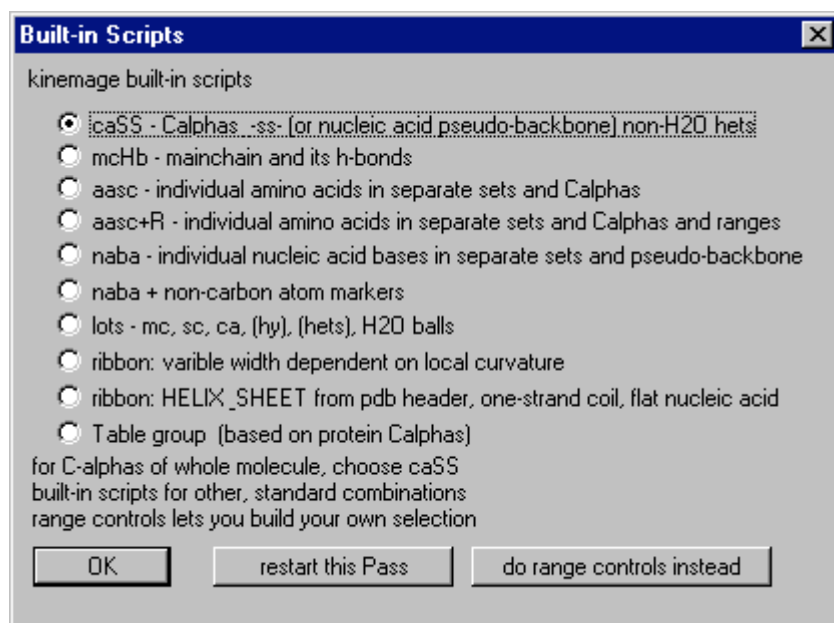
Click save to proceed.



The *Starting Ranges* dialog box is where you begin to make selections about what kind of information you want to extract from the PDB file you opened.

- **Backbone Browsing Script** - The top radio button will generate a tracing of the protein by connecting the alpha carbons of the amino acid backbone. It will also include any disulfide bonds and any nonpeptide or 'het' groups such as metals or sugars. Clicking this button and the OK button will make a kinemage and immediately open MAGE to view it. On the PC, a MAGE executable named MAGE.exe (case-insensitive) has to be in the same directory as the saved file for this to work reliably.
- **Selection of Built-In Scripts** - The second radio button will open a new dialog box of several possible scripts which illustrate the entire macromolecule in a variety of ways. More on this dialog box later.
- **New Ranges** - The third radio button will open a new dialog box which allows you to generate a kinemage of only the pieces of the structure that you deliberately select.
- **Focus Only** - The fourth radio button will allow you to generate a kinemage focussed within a radius around an individual amino acid or XYZ coordinate. As in the ricin tutorial, this is very useful for illustrating active sites, metal binding sites, coenzymes, or any feature in which you want to remove the clutter of the rest of the structure.
- **Range List and Reset Options** are research features you don't need to worry about.

Let's begin with the selection of built-in scripts. The dialog box is below.



- **CaSS** - This is essentially the same as the backbone browsing script, except it doesn't throw you into MAGE when it is finished. You can build on the initial backbone.
- **McHb** - This feature will give you the complete polypeptide backbone and will draw in hydrogen bonds between the properly positioned peptide oxygens and nitrogens.
- **Aasc** - This generates an alpha carbon backbone plus all of the amino acid sidechains colored by type, i.e. 20 different buttons and 7 colors!

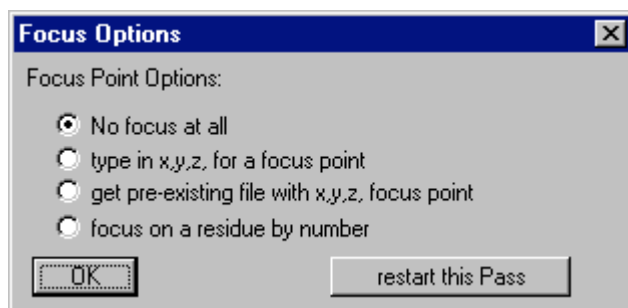
- **Naba** - This button and the one below it are intended for DNA and RNA structures; they give a simplified backbone and color-coded bases. They might be interesting to try on the DNA portion of protein:DNA complexes.
- **Lots** - This script displays literally everything in the PDB file. Using this script and zooming in on a particular sidechain or feature is a good way of examining its molecular neighborhood.
- **Ribbon** - This script displays the backbone as a thin golden ribbon. The picture on the official kinemage homepage was made using this feature.
- **Ribbon HELIX_SHEET** - This script generates a kinemage with the helices, beta strands, and loops (as defined in the PDB file header) shown as color-coded spirals, arrows, and ropes. You definitely should use this feature for one of your kinemages.
- **Table group** - This is a new feature used for research purposes.

If you had selected “new ranges” in the *Starting Ranges* dialog box, you would see the following large box.

Without going into the role of each box, this screen allows you to build one or more individual pieces of your structure, such as stretches of mainchain and sidechains from residues 34 to 55 and 102 to 111 plus a ligand (het). It is also sometimes helpful to check the ‘at’ box to put small colored balls on noncarbon atoms, particularly when

illustrating bonds with them. One of the most useful features of this dialog box is the ability to make rotatable amino acid residues of either the original residue or a mutation using the 'ro' box. The tutorial gives an example of making a rotatable glutamate residue in the active site of ricin. Notice that the radio button 'OK accepts and comes back for more' is checked. This is used for making multiple pieces, but when you are finished check the button below it before hitting OK.

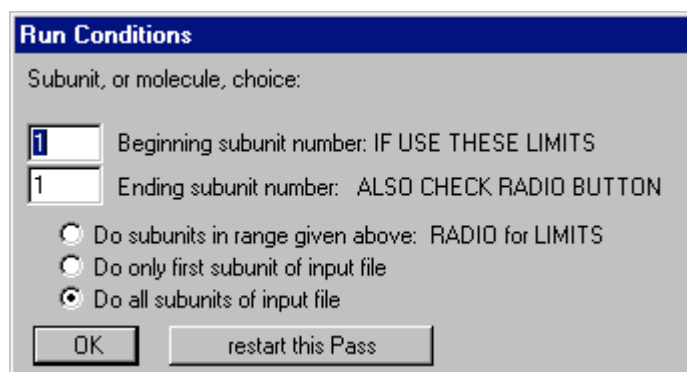
When you leave *New Ranges*, the next dialog box you see is the *Focus Options* box. This allows you to select a focus around a particular residue or XYZ



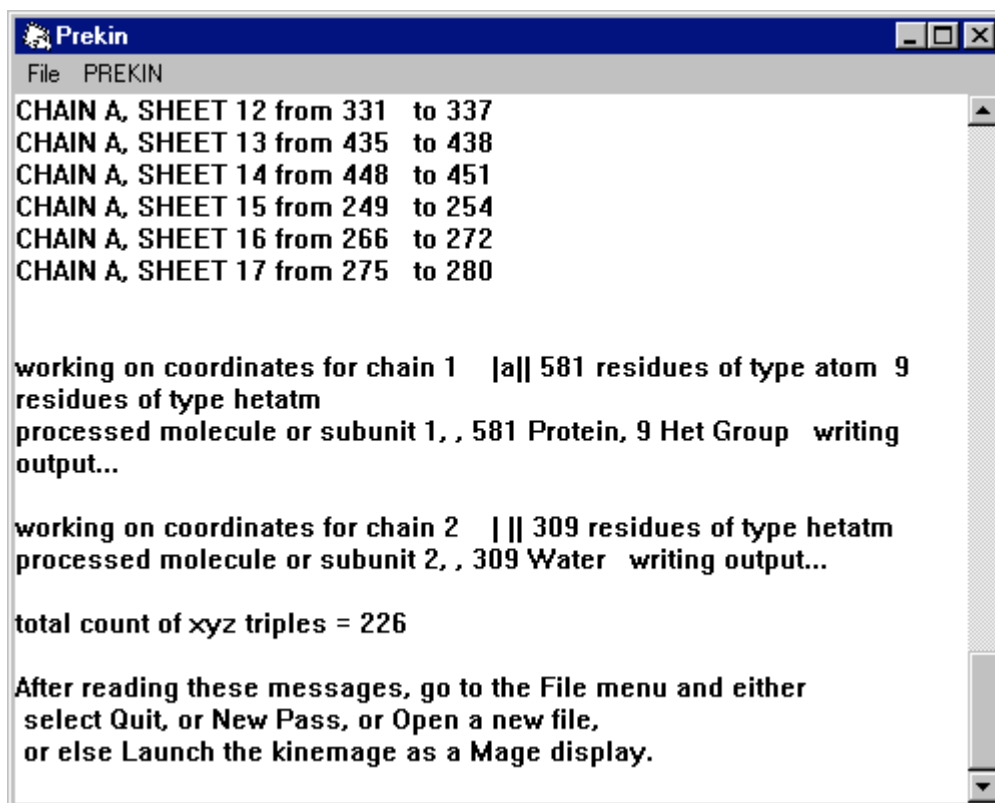
coordinate.* If you select one of those, you will get a dialog for choosing what features you want to show within what radii of the focus. The default in *Focus Options* is no focus at all. Note: This is the same box you would get if you checked the "focus only" button in the *Starting Ranges* dialog box.

*You can find such an XYZ point in MAGE by activating the XYZ point tool under the Tools menu, then clicking on the desired point in a kinemage you have already made. Write down the numbers that appear on the top of the MAGE screen so you can use them as the PREKIN focus (or use "Save Special ... XYZ point" in Mage and then the "pre-existing file" focus option).

The final dialog box is the *Run Conditions* box, which allows you to select the subunit (chain; or model for nmr structures) that you want to use. The default is to do all the subunits of the input file.



However, there will be times when you want to select only one or just some of the subunits. If you want to select only subunit 3, for example, put a 3 in both boxes and also click the top radio button, then OK. This is a very important box, so be sure it says what you want it to say!



```
Prekin
File PREKIN
CHAIN A, SHEET 12 from 331 to 337
CHAIN A, SHEET 13 from 435 to 438
CHAIN A, SHEET 14 from 448 to 451
CHAIN A, SHEET 15 from 249 to 254
CHAIN A, SHEET 16 from 266 to 272
CHAIN A, SHEET 17 from 275 to 280

working on coordinates for chain 1 |a|| 581 residues of type atom 9
residues of type hetatm
processed molecule or subunit 1, , 581 Protein, 9 Het Group writing
output...

working on coordinates for chain 2 | || 309 residues of type hetatm
processed molecule or subunit 2, , 309 Water writing output...

total count of xyz triples = 226

After reading these messages, go to the File menu and either
select Quit, or New Pass, or Open a new file,
or else Launch the kinemage as a Mage display.
```

The last thing you will see when you have completed a sequence in PREKIN is the following window:

The important portion of this screen is the section at the very bottom. If you have completed this kinemage, open the file menu and select quit. If you haven't finished this kinemage, and want to add more components in another "pass" through the menus, open the file menu and select "new pass". If you want to see the kinemage you have just made, and this is usually a good idea, open the file menu and select "launch MAGE". On the PC, this will only work properly if your kinemage and MAGE are in the same folder on your hard drive, so it is a good practice to designate a folder named kinemage to keep your authoring materials together. Otherwise, open the kinemage from inside Mage.

This was a whirlwind tour through the most commonly used PREKIN features. We are considering ways to improve the PREKIN interface to make it more user friendly by looking for suggestions of new features, bug reports, and any other comments that would help us improve this software. Please send PREKIN comments via email to Dr. David Richardson (dcr@kinemage.biochem.duke.edu) with an email copy to Robert.Bateman@usm.edu.