

Activities: Cooting

- Coot is:
 - an application (and libraries) for (protein) crystallography
 - clipper-based
 - mmdb-based
 - Where do you draw the line between GUI simplicity and flexibility?
 - a test-bed for experimental interfaces
 - * some successful:
 - dragged refinement
 - Undo/Redo
 - * some not
 - edit phi/psi puller [Withdrawn]
 - Auto C α building [Withdrawn]

March 2003: To Finish/To Do:

- C α building: Completely re-written (skeleton-based baton)
- C α \rightarrow mainchain cleanup/rewrite: Completely re-written
- Side-chain (rotamer) fitting Works nicely now
- Delete Atoms, merge fragments (fffear/ffjoin) Done, redundant
- To Finish: “refinement”
 - Bonds, angles, torsions & planes, non-bonded
 - on the fly with fragment-drag Works nicely
 - Dictionary...? Sorted

- To Finish: Ligand-finding:
 - Given Coordinates for a search ligand and a map:
 - * Using Rigid body refinement
 - * Using Refinement (as above) with map target
- Find Waters
 - Similar to ligands
 - (No Refinement, but Rigid Body needed?)
- TODO: Torsion angle refinement
- TODO: Validation markup
- TODO: High Resolution Map Fitting

What I did that I didn't say I'd do:

- CCP4i interface
- pepflip
- phosphodiester linkage
- ϕ/ψ editing
- mutations (and autofitting thereof)
- Refmac interface
- Sequence View (now with Sec. Struc. markup)
- Add Terminal Residue
- Residue Property Editor
- Alt Conf support
- User Manual

User Testing or Usability Testing?

- Recently I've put users in front of Coot
- Big Surprise! No one read the manual *at all!*
- Another Surprise! No-one reads the console
 - Users *really* want an “intuitive” tool
- So I was building the wrong tool
- Result:
 - Downplay console,
 - emphasize tooltips, help buttons
 - feedback via pop-ups, on-screen labels

To Do

- Do Coot Feature Requests
 - mostly “interface issues”
 - and carbohydrate linkages?
- CHART