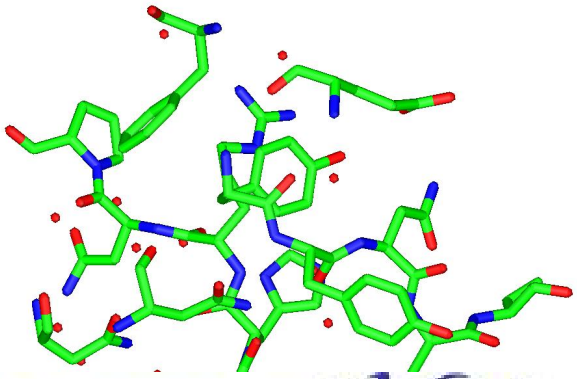
CCP4 Molecular Graphics Project

Stuart McNicholas



THE UNIVERSITY of York

CCP4

Aims:

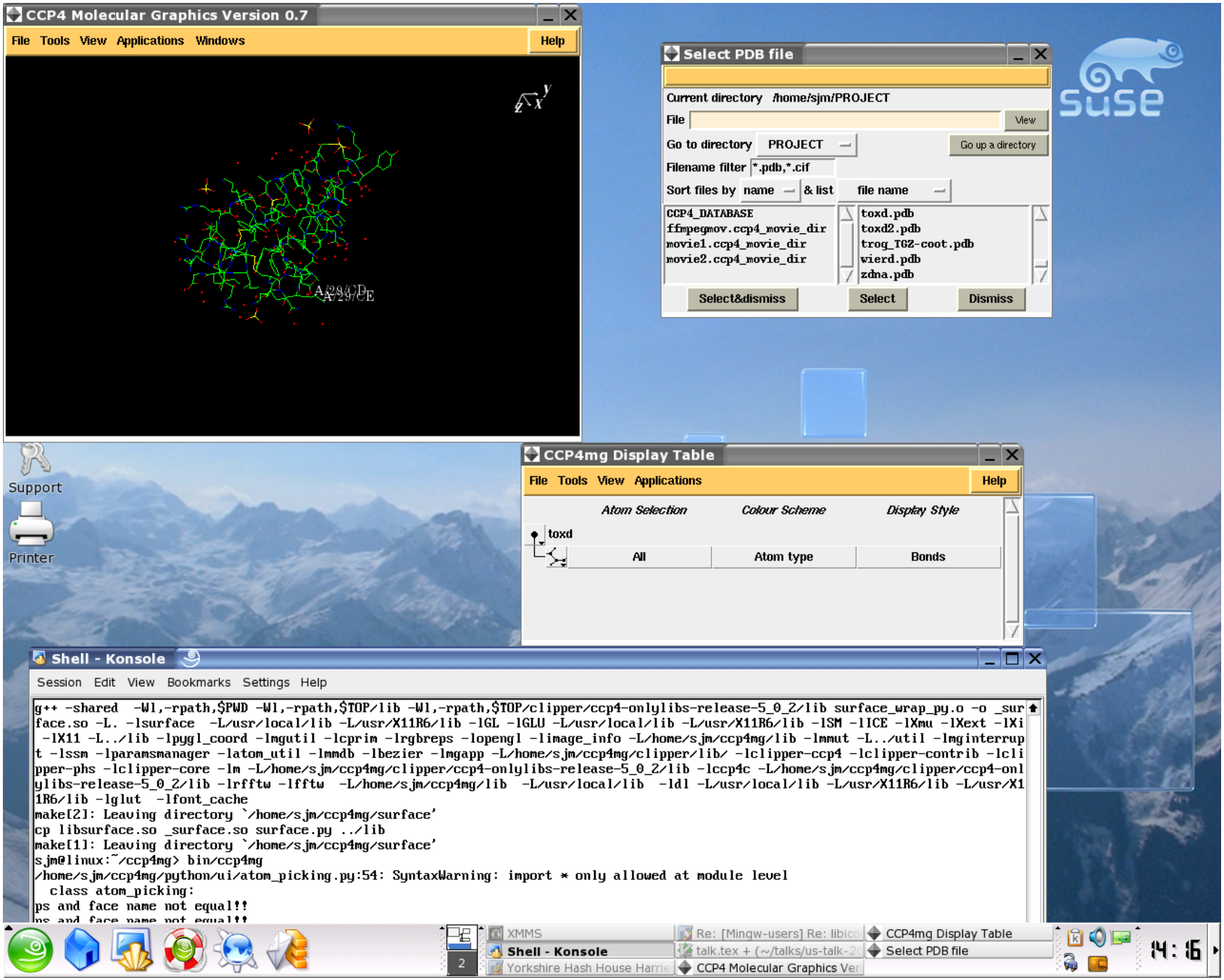
- Molecular structure viewer.
- Electron density viewer.
- Model building/refinement program.
- Picture/movie creator.

General Design:

- High level stuff done in Python.
- Lower level stuff in C/C++.
- Python/C++ communication done via SWIG wrappers.
- Uses MMDB (Eugene Krissenel).
- Uses Clipper (Kevin Cowtan).
- Tcl/Tk GUI.

GUI Considerations:

- GUI with same look and feel as CCP4i.
- Context sensitive menus in graphics window.


CCP4 Molecular Graphics Version 0.7
File Tools View Applications Windows Help
Select PDB file
Current directory /home/sjm/PROJECT
File View
Go to directory PROJECT
Go up a directory
Filename filter *.pdb,*.cif
Sort files by name & list file name
CCP4_DATABASE
ffmpegmov.ccp4_movie_dir
movie1.ccp4_movie_dir
movie2.ccp4_movie_dir
toxd.pdb
toxd2.pdb
trog_TG2-coot.pdb
wierd.pdb
zdna.pdb
Select&dismiss
Select
Dismiss
suse
Support
Printer
CCP4mg Display Table
File Tools View Applications Help
Atom Selection
Colour Scheme
Display Style
toxd
All
Atom type
Bonds
Shell - Konsole
Session Edit View Bookmarks Settings Help
g++ -shared -Wl,-rpath,$PWD -Wl,-rpath,$TOP/lib -Wl,-rpath,$TOP/clipper/ccp4-onlylibs-release-5_0_2/lib surface_wrap_py.o -o _surface.so -L. -lsurface -L/usr/local/lib -L/usr/X11R6/lib -lGL -lGLU -L/usr/local/lib -L/usr/X11R6/lib -lSM -lICE -lXmu -lXext -lX11 -L../lib -lpygl_coord -lmgutil -lcprim -lrgbreps -lopengl -limage_info -L/home/sjm/ccp4mg/lib -lmmut -L../util -lmginterrupt -lssm -lparamsmanager -latom_util -lmmdb -lbezier -lmgapp -L/home/sjm/ccp4mg/clipper/lib/ -lclipper-ccp4 -lclipper-contrib -lclipper-phs -lclipper-core -lm -L/home/sjm/ccp4mg/clipper/ccp4-onlylibs-release-5_0_2/lib -lccp4c -L/home/sjm/ccp4mg/clipper/ccp4-onlylibs-release-5_0_2/lib -lrfftw -lfftw -L/home/sjm/ccp4mg/lib -L/usr/local/lib -ldl -L/usr/local/lib -L/usr/X11R6/lib -L/usr/X11R6/lib -lglut -lfont_cache
make[2]: Leaving directory `/home/sjm/ccp4mg/surface'
cp libsurface.so _surface.so surface.py ../lib
make[1]: Leaving directory `/home/sjm/ccp4mg/surface'
sjm@linux:~/ccp4mg> bin/ccp4mg
/home/sjm/ccp4mg/python/ui/atom_picking.py:54: SyntaxWarning: import * only allowed at module level
class atom_picking:
ps and face name not equal!!
XMMS
Shell - Konsole
Yorkshire Hash House Harrie
Re: [Mingw-users] Re: libico
talk.tex + (~/talks/us-talk-2
CCP4 Molecular Graphics Ver
CCP4mg Display Table
Select PDB file
14:16

Old Prerequisites:

- Tcl/Tk, with BLT and Itcl.
- Python 2.2 or later with working thread support.
- OpenGL (or Mesa).

New Prerequisites:

- OpenGL (or Mesa).

Some basic features:

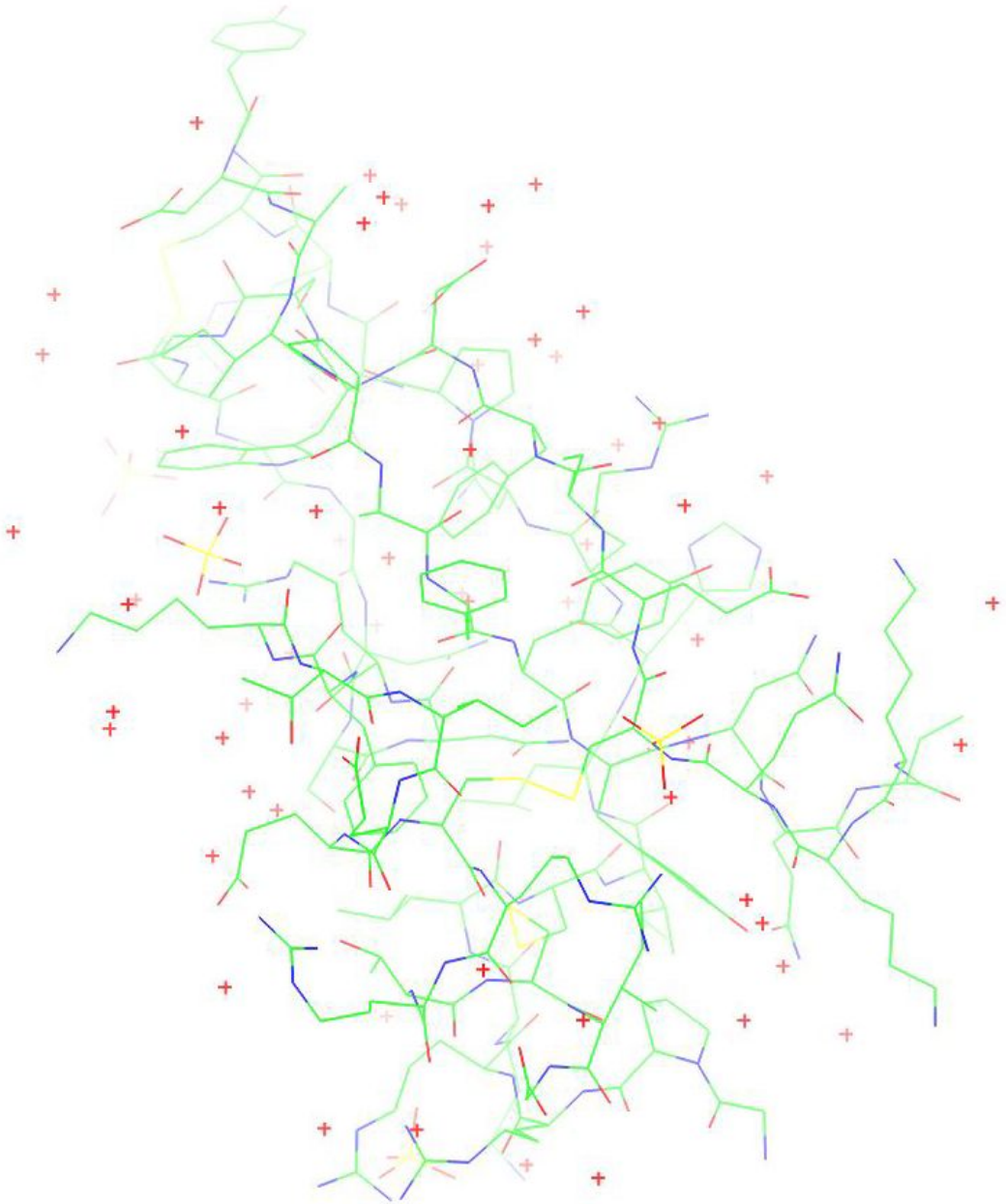
- View PDB/mmCIF files.
- Download and view PDB/mmCIF over web (and save locally).
- Convert MTZ files to electron density isosurfaces.
- Display all map files supported by CCP4 as electron density isosurfaces.

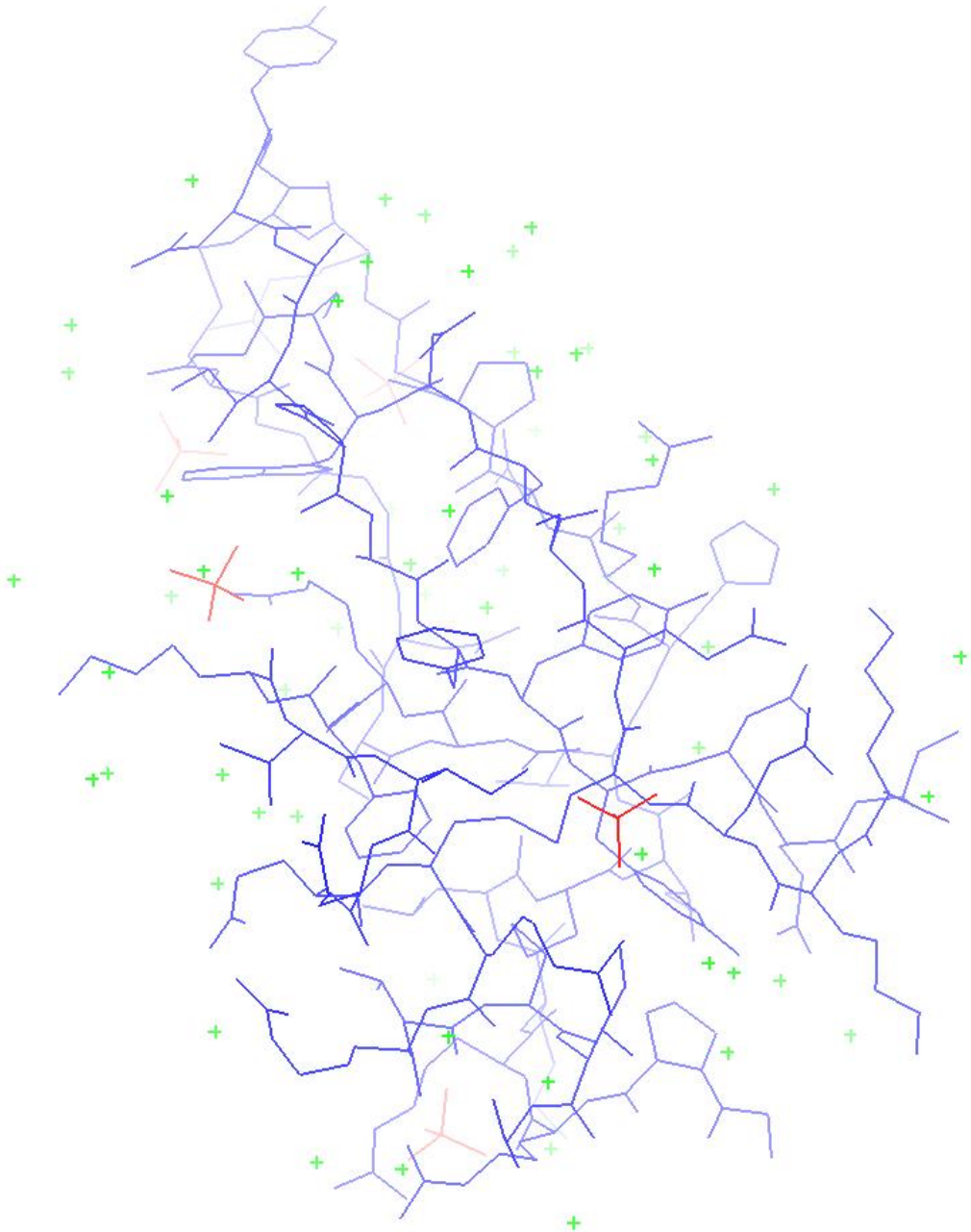
Model display features:

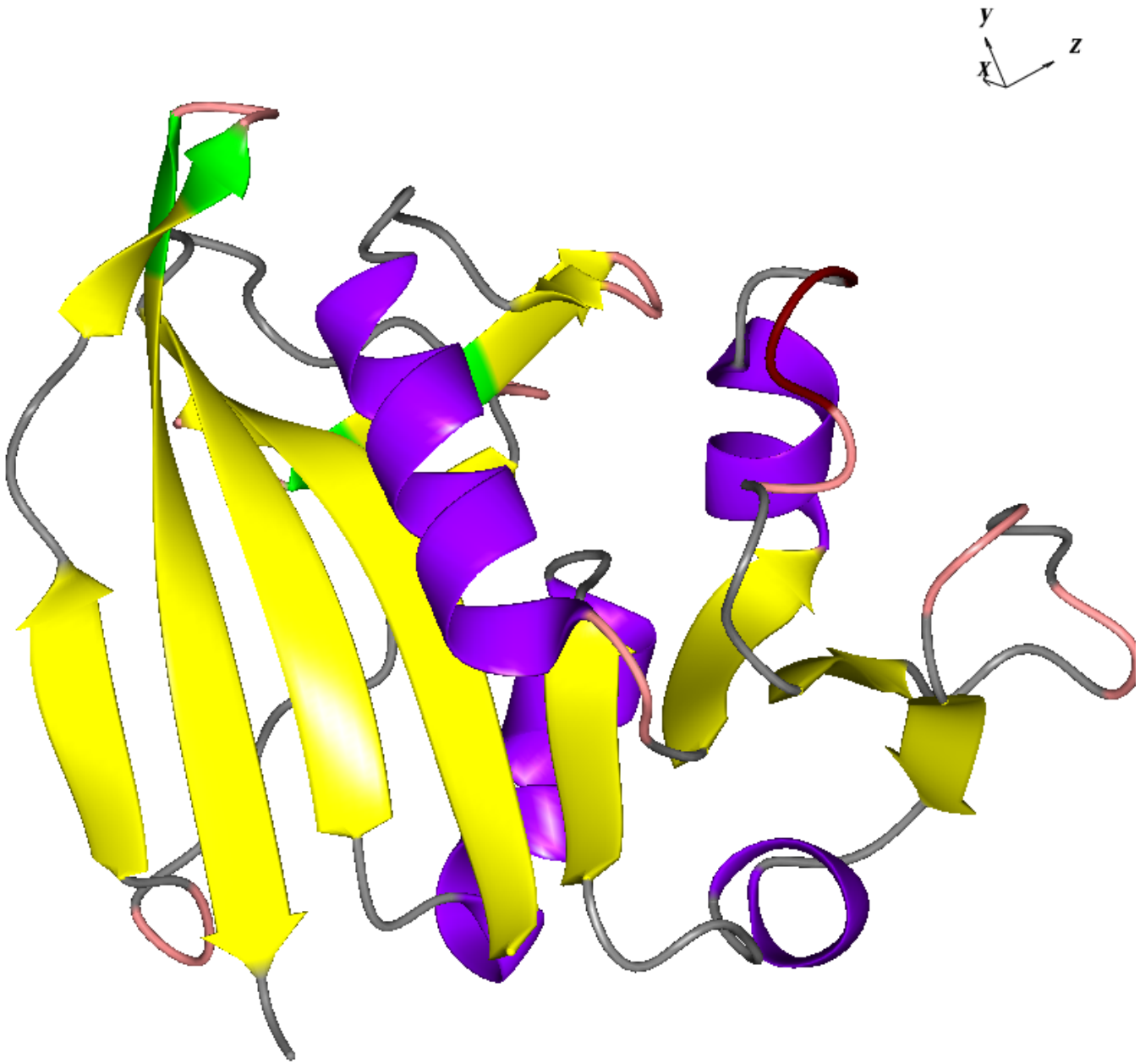
- Colour by variety of criteria
  - By atom, residue, chain, etc.
  - By atom/residue property.
  - By user defined criteria.
- Draw in various styles, stick, lines, ribbons, etc.

Model display features:

- Define many different atom selections
  - All
  - Chains
  - Residue types
  - Atom types
  - Lots more

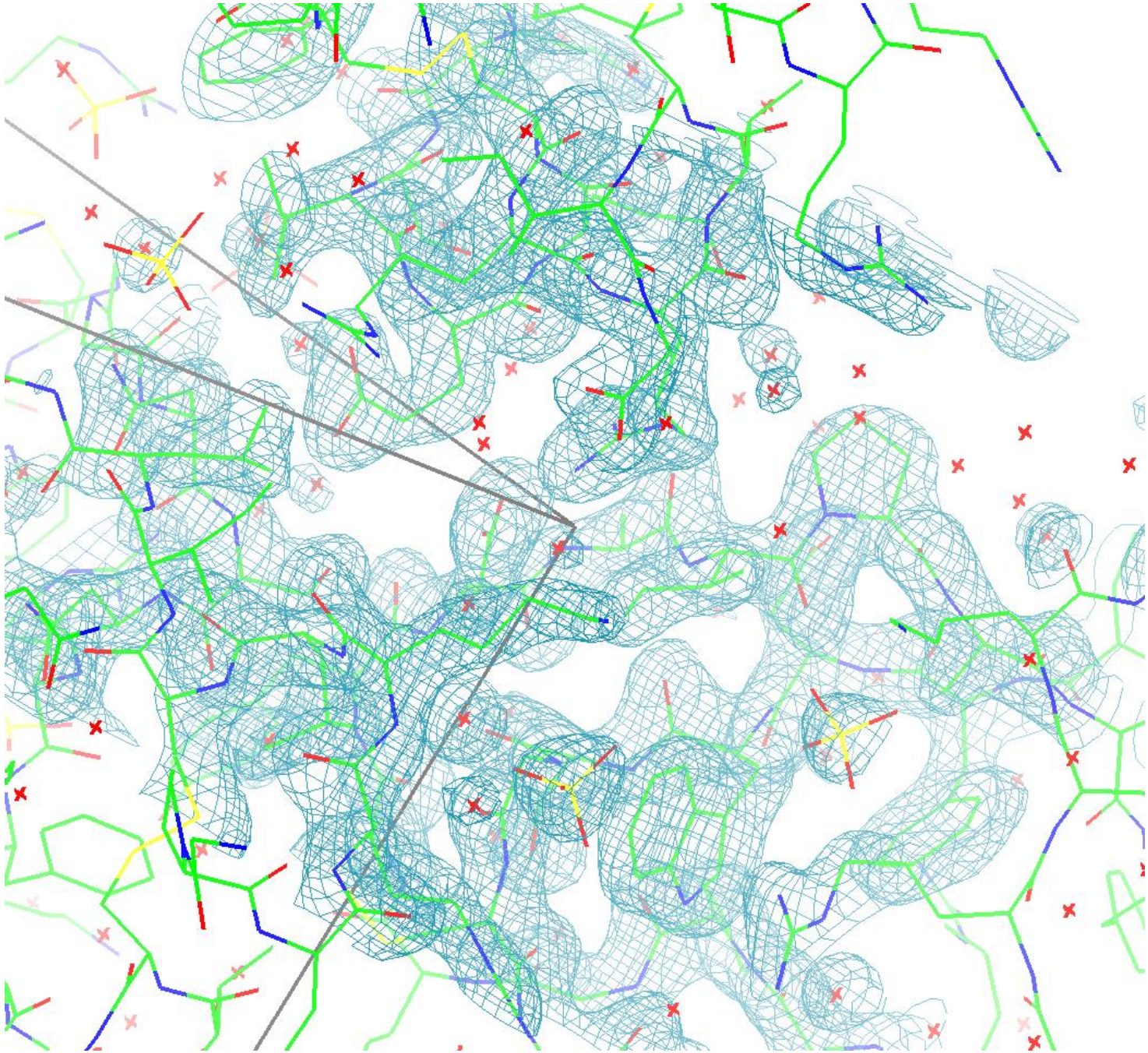


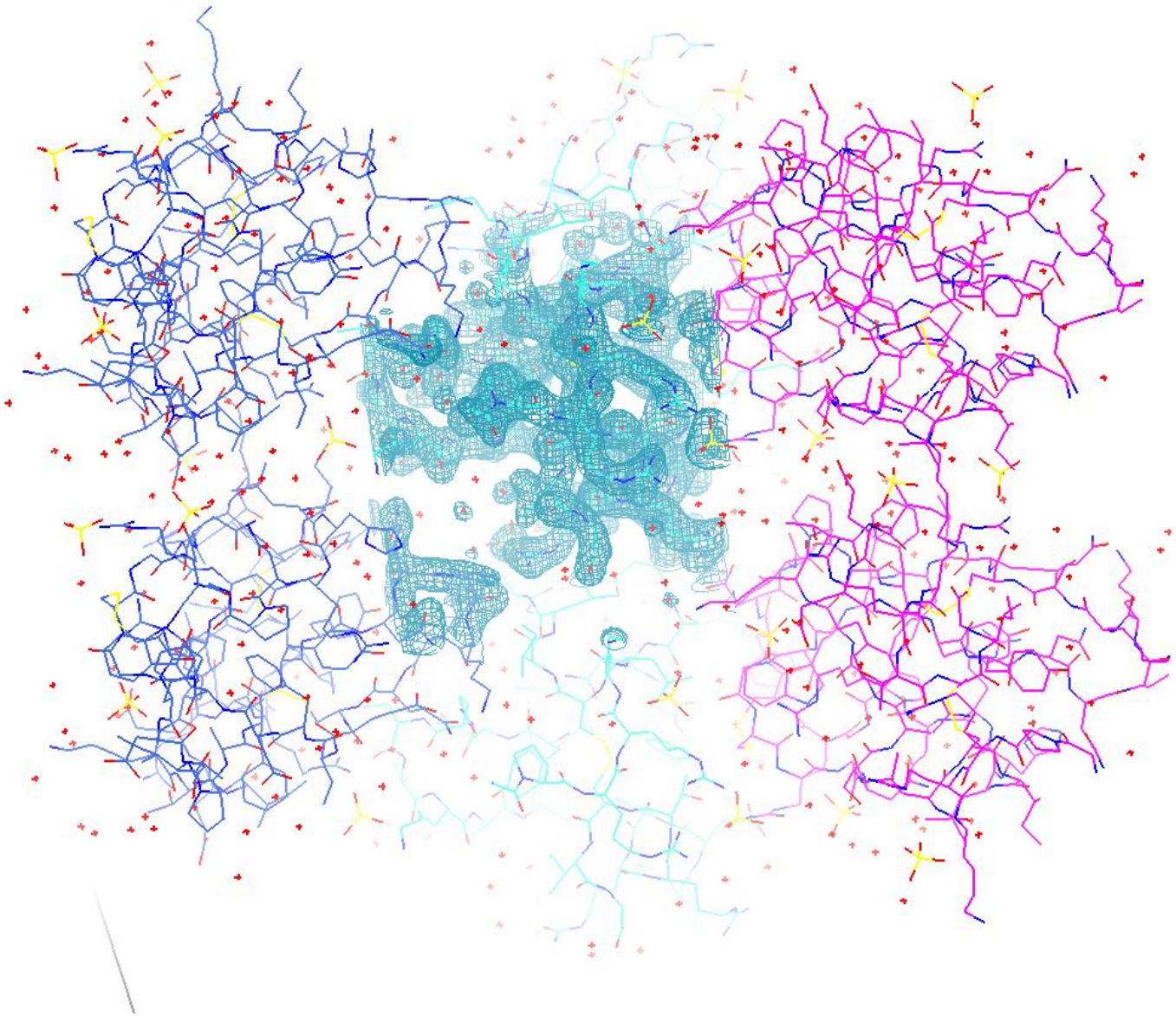


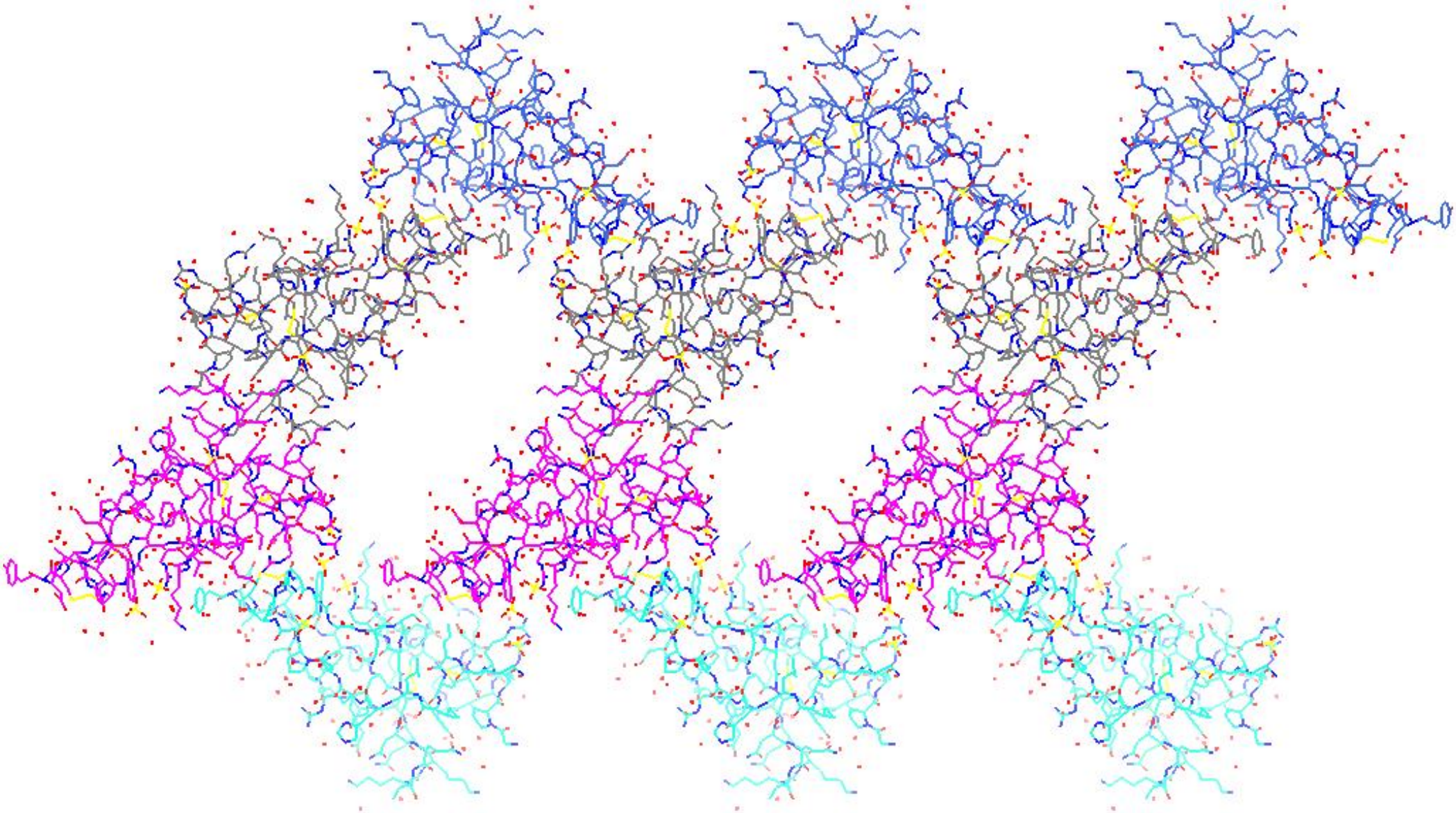

y
z
x

Map display features:

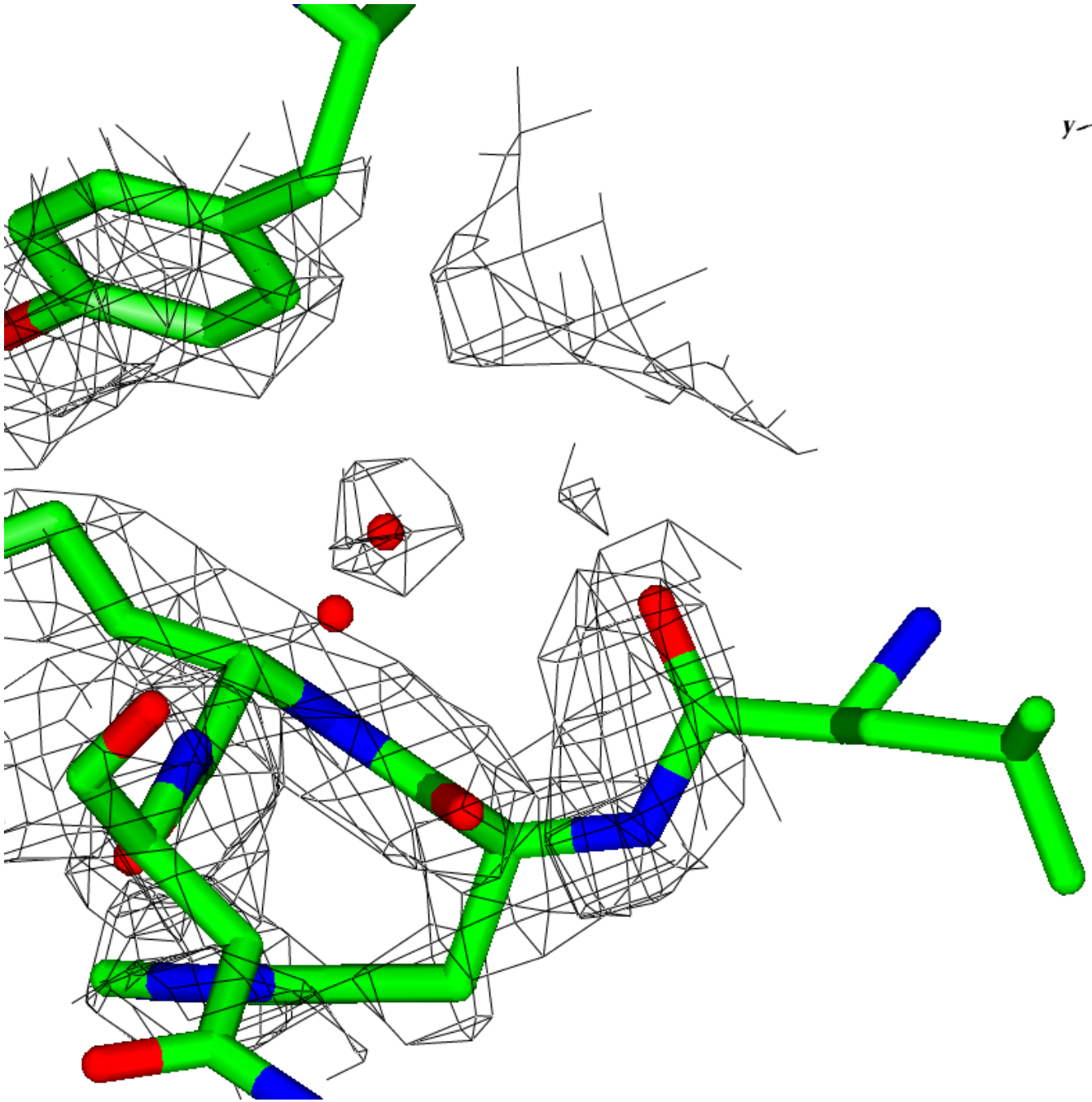
- Display electron density as wireframe, cylinders or solid.
- Vary quality of fft calculation on map load.
- Apply symmetry from mtz file to molecule drawing.
- Colour molecules by symmetry transformation.
- Clip to point or atom selection.
- Show unit cell.





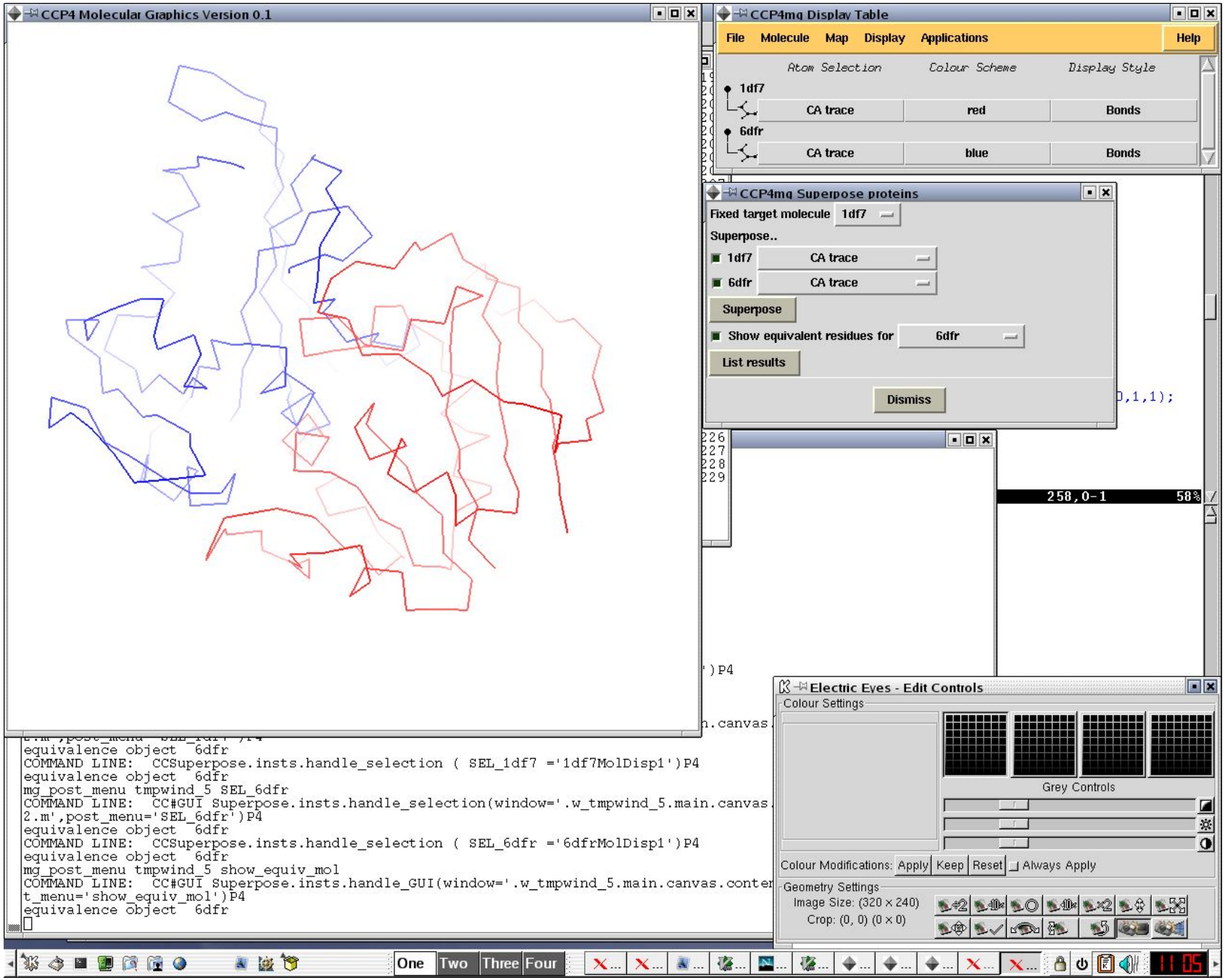


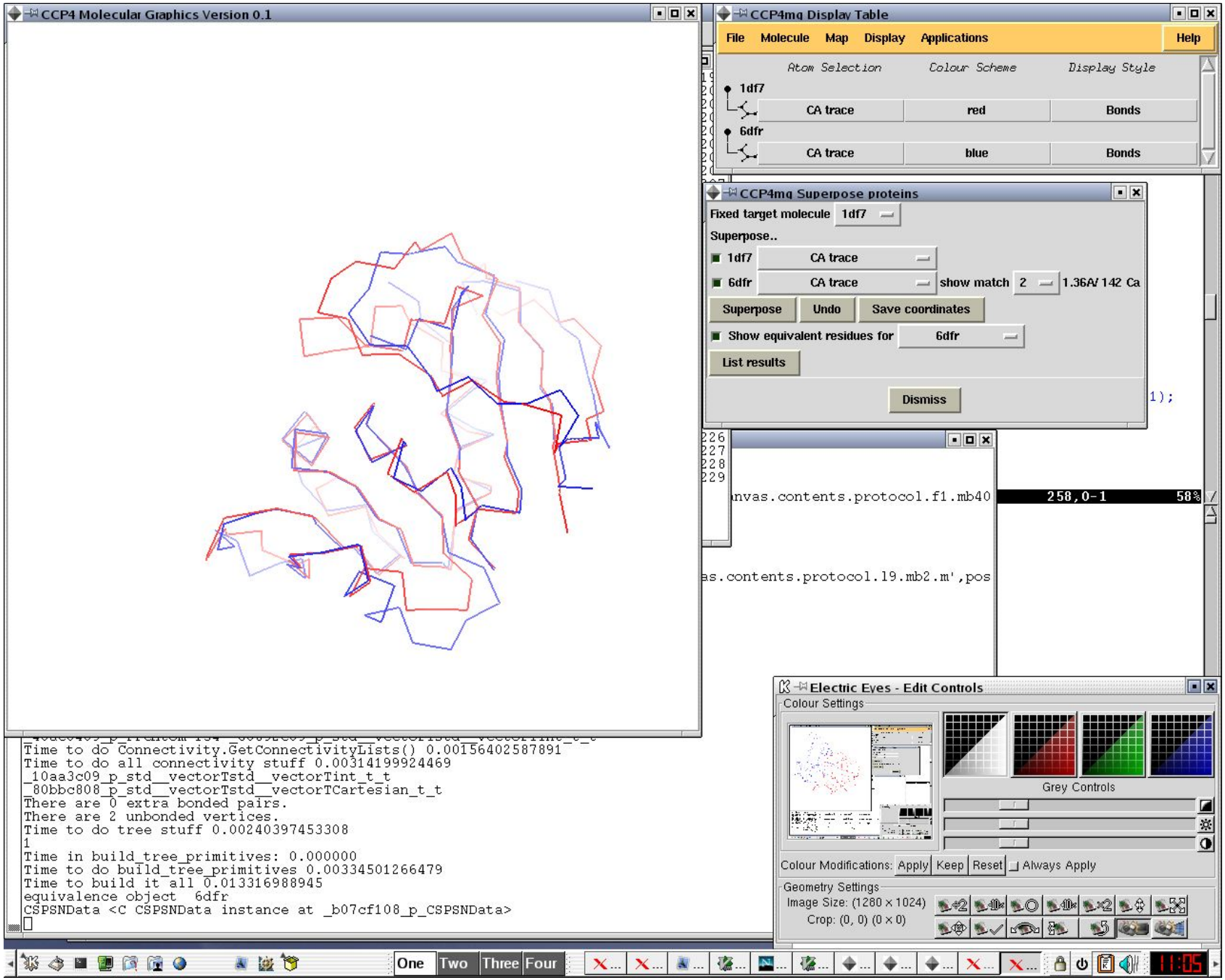

z
x
y


z
y
x

Superposition of proteins

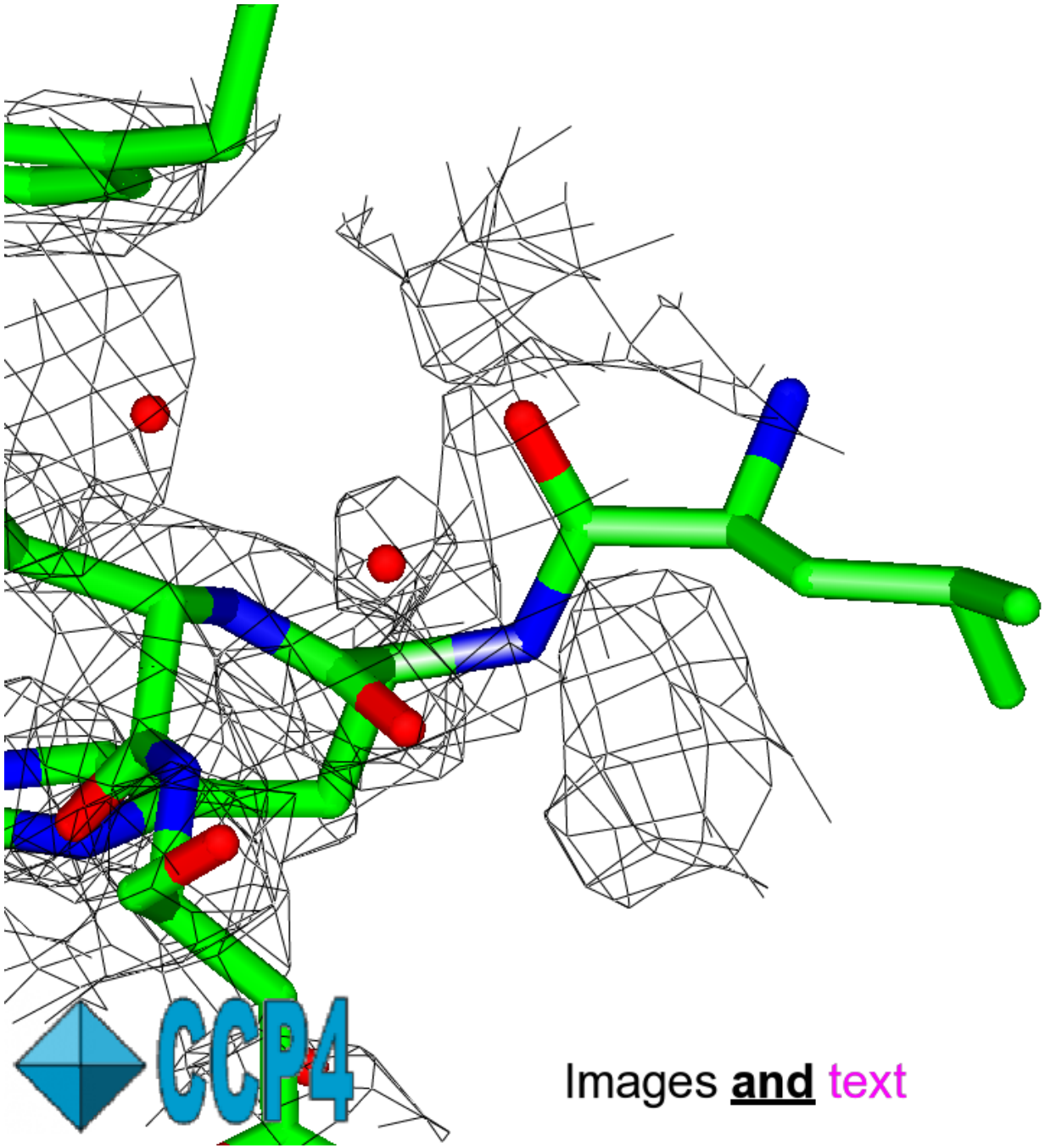
- Graph theory structure analysis.
- Whole molecule or selection.
- Two or more molecules.


CCP4 Molecular Graphics Version 0.1
CCP4mg Display Table
File
Molecule
Map
Display
Applications
Help
Atom Selection
Colour Scheme
Display Style
1df7
CA trace
red
Bonds
6dfr
CA trace
blue
Bonds
CCP4mg Superpose proteins
Fixed target molecule
1df7
Superpose..
1df7
CA trace
6dfr
CA trace
Superpose
Show equivalent residues for
6dfr
List results
Dismiss
258,0-1
58%
Electric Eyes - Edit Controls
Colour Settings
Grey Controls
Colour Modifications:
Apply
Keep
Reset
Always Apply
Geometry Settings
Image Size: (320 x 240)
Crop: (0, 0) (0 x 0)
equivalence object 6dfr
COMMAND LINE: CCSuperpose.insts.handle_selection (SEL_1df7 ='1df7MolDisp1')P4
equivalence object 6dfr
mg_post_menu tmpwind_5 SEL_6dfr
COMMAND LINE: CC#GUI Superpose.insts.handle_selection(window='.w_tmpwind_5.main.canvas.
2.m',post_menu='SEL_6dfr')P4
equivalence object 6dfr
COMMAND LINE: CCSuperpose.insts.handle_selection (SEL_6dfr ='6dfrMolDisp1')P4
equivalence object 6dfr
mg_post_menu tmpwind_5 show_equiv_mol
COMMAND LINE: CC#GUI Superpose.insts.handle_GUI(window='.w_tmpwind_5.main.canvas.conter
t_menu='show_equiv_mol')P4
equivalence object 6dfr
One
Two
Three
Four
11:05


CCP4 Molecular Graphics Version 0.1
CCP4mg Display Table
File
Molecule
Map
Display
Applications
Help
Atom Selection
Colour Scheme
Display Style
1df7
CA trace
red
Bonds
6dfr
CA trace
blue
Bonds
CCP4mg Superpose proteins
Fixed target molecule
1df7
Superpose..
1df7
CA trace
6dfr
CA trace
show match
2
1.36A/ 142 Ca
Superpose
Undo
Save coordinates
Show equivalent residues for
6dfr
List results
Dismiss
1);
226
227
228
229
nvas.contents.protocol.f1.mb40
258,0-1
58%
as.contents.protocol.19.mb2.m',pos
Electric Eyes - Edit Controls
Colour Settings
Grey Controls
Colour Modifications:
Apply
Keep
Reset
Always Apply
Geometry Settings
Image Size: (1280 x 1024)
Crop: (0, 0) (0 x 0)
Time to do Connectivity.GetConnectivityLists() 0.00156402587891
Time to do all connectivity stuff 0.00314199924469
_10aa3c09_p_std__vectorTstd__vectorTint_t_t
_80bbc808_p_std__vectorTstd__vectorTCartesian_t_t
There are 0 extra bonded pairs.
There are 2 unbonded vertices.
Time to do tree stuff 0.00240397453308
1
Time in build_tree_primitives: 0.000000
Time to do build_tree_primitives 0.00334501266479
Time to build it all 0.013316988945
equivalence object 6dfr
CSPSNData <C CSPSNData instance at _b07cf108_p_CSPSNData>
One
Two
Three
Four
11:05

Some more display features:

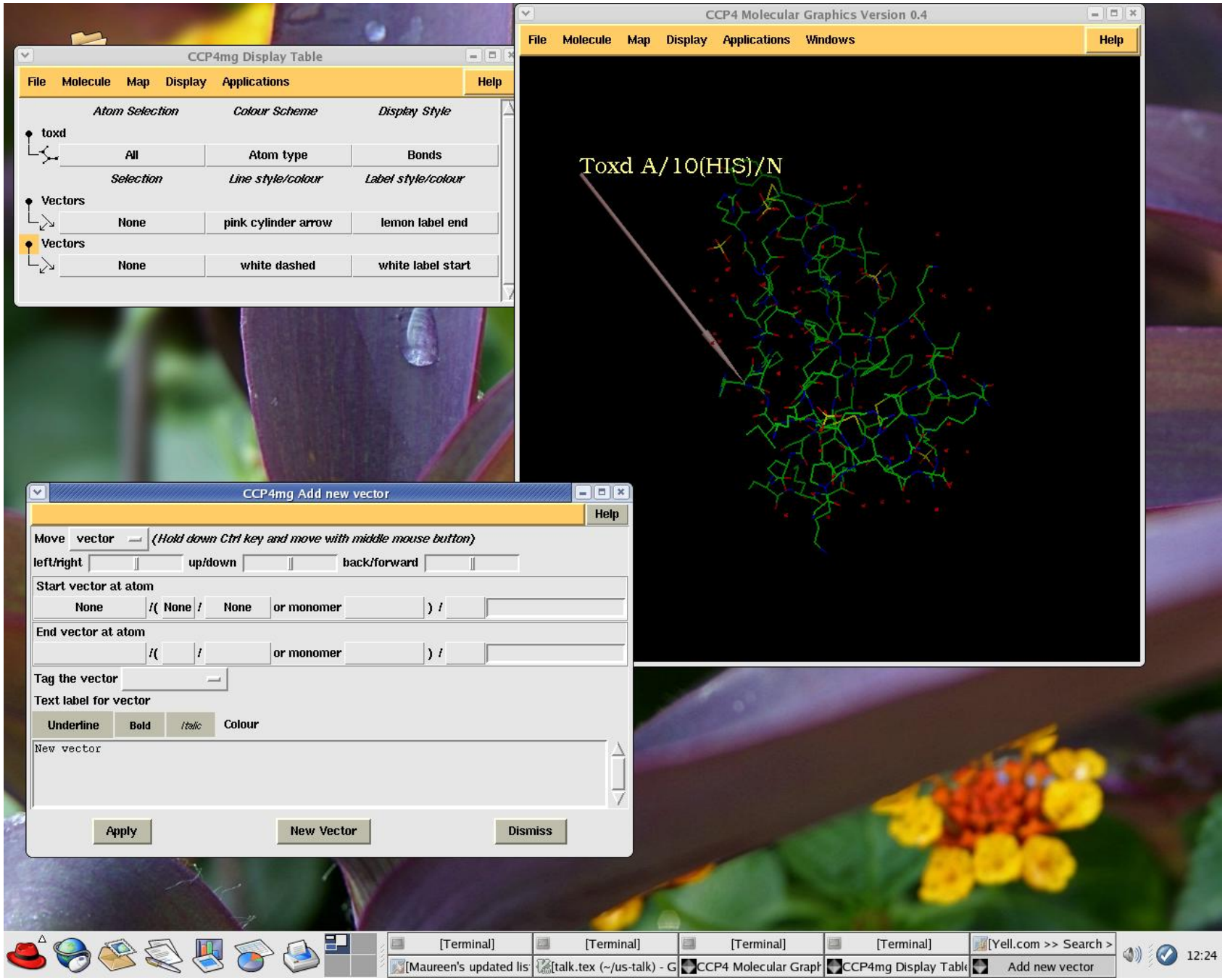
- Overlay arbitrary text and images
  - Text with any system font, inc anti-aliased TrueType and PostScript.
  - Text at any size (for scalable and vector fonts).
  - Sub- and super-scripting.
  - Text any colour or combination of colours.
  - Scale/position images.



Images **and** text

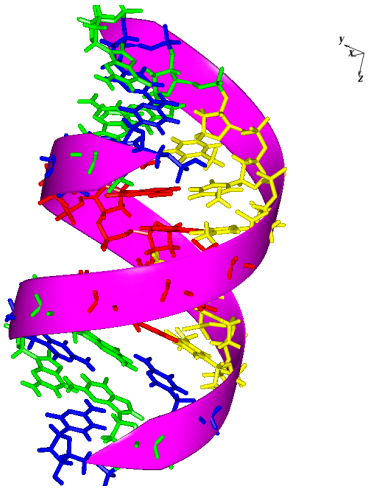
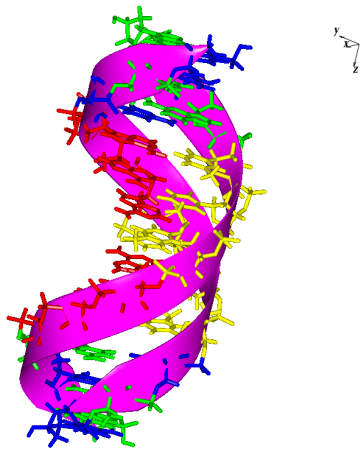
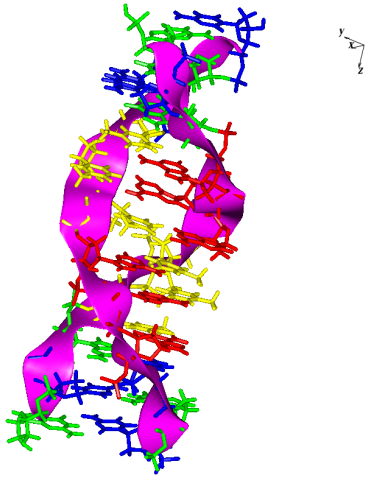
"Vectors":

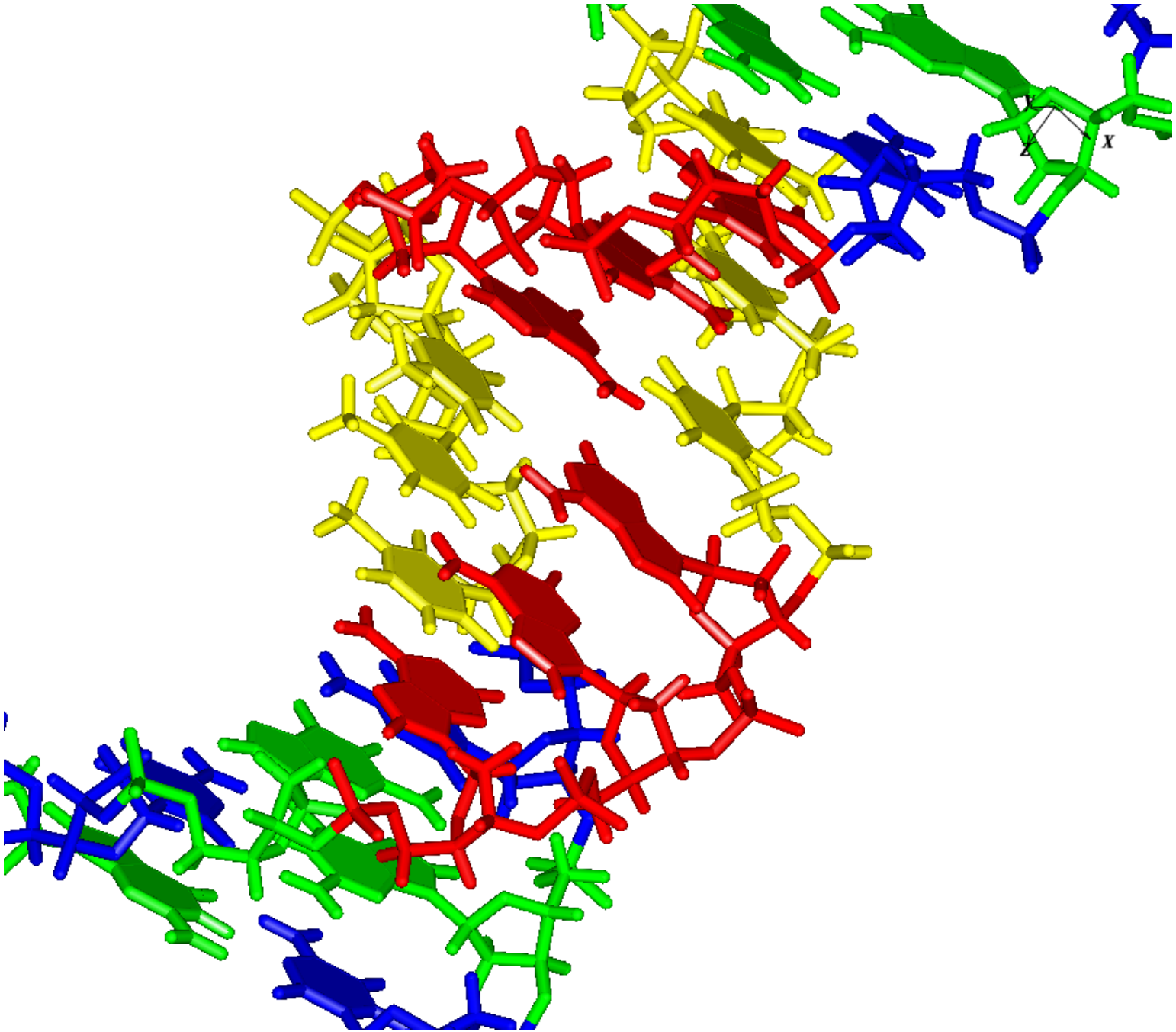
- Display TLS refinement vectors.
- Display vector between two arbitrary points/atoms.


CCP4mg Display Table
File Molecule Map Display Applications Help
Atom Selection Colour Scheme Display Style
toxd
All Atom type Bonds
Selection Line style/colour Label style/colour
Vectors
None pink cylinder arrow lemon label end
Vectors
None white dashed white label start
CCP4 Molecular Graphics Version 0.4
File Molecule Map Display Applications Windows Help
Toxd A/10(HIS)/N
CCP4mg Add new vector
Help
Move vector (Hold down Ctrl key and move with middle mouse button)
left/right up/down back/forward
Start vector at atom
None /(None / None or monomer) /
End vector at atom
/(/ or monomer) /
Tag the vector
Text label for vector
Underline Bold Italic Colour
New vector
Apply New Vector Dismiss
[Terminal] [Terminal] [Terminal] [Terminal] [Yell.com >> Search >
[Maureen's updated lis [talk.tex (~/us-talk) - G CCP4 Molecular Graph CCP4mg Display Table Add new vector
12:24

Nucleic acids display:

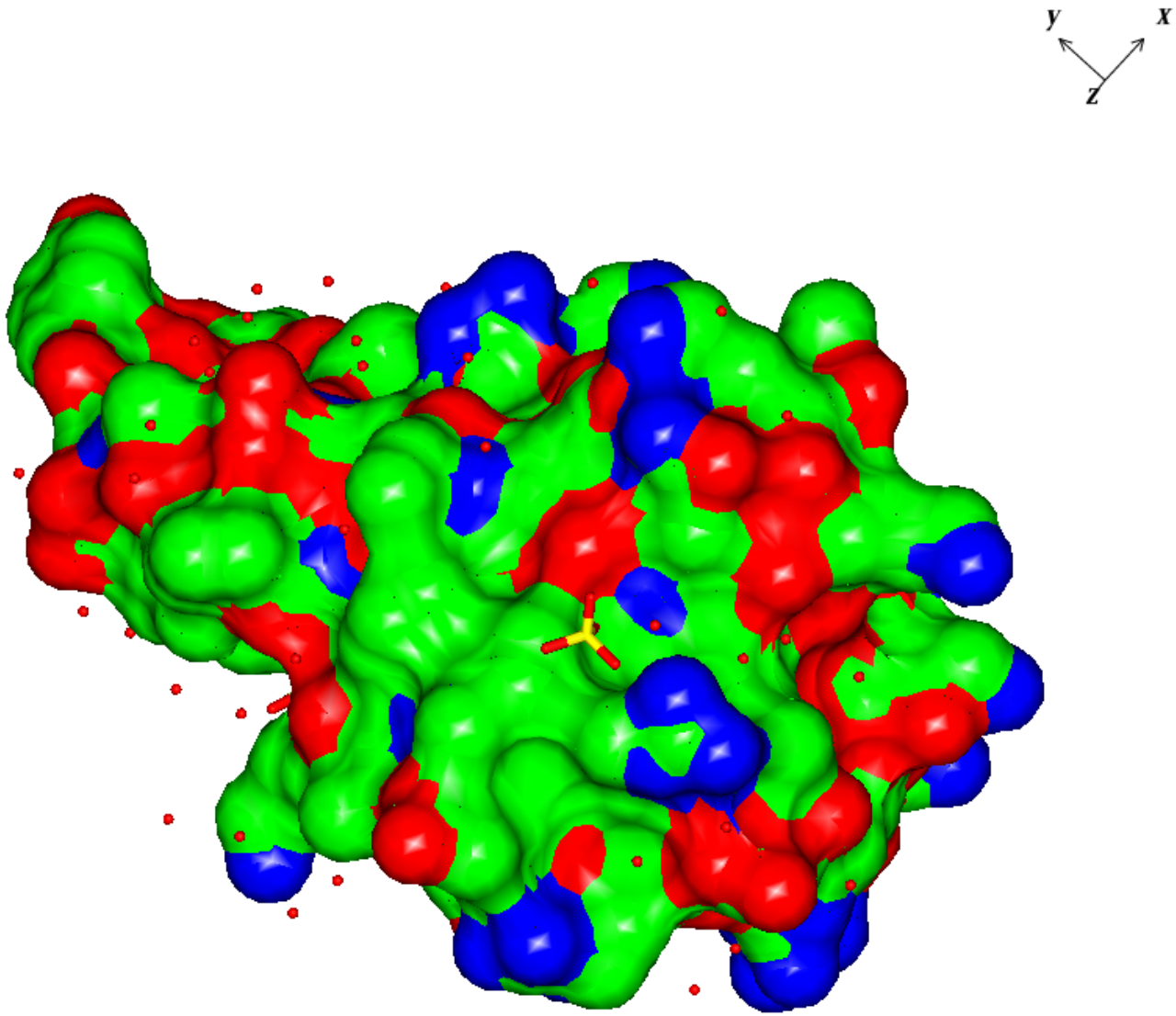
- Display nucleic acids just as any other molecule.
- Display as ribbons through phosphate.
- Display as base-pair ”blocks”.

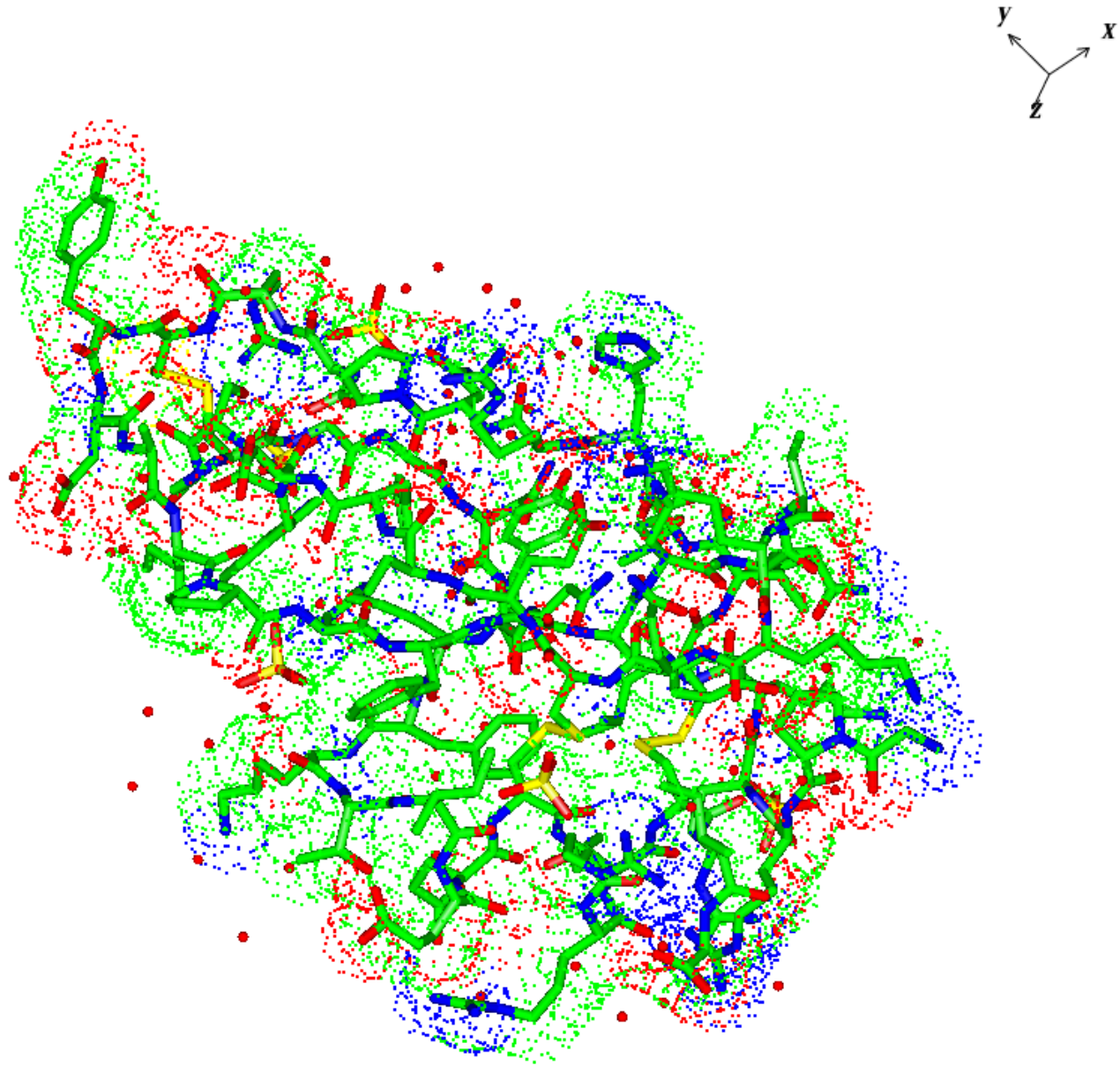




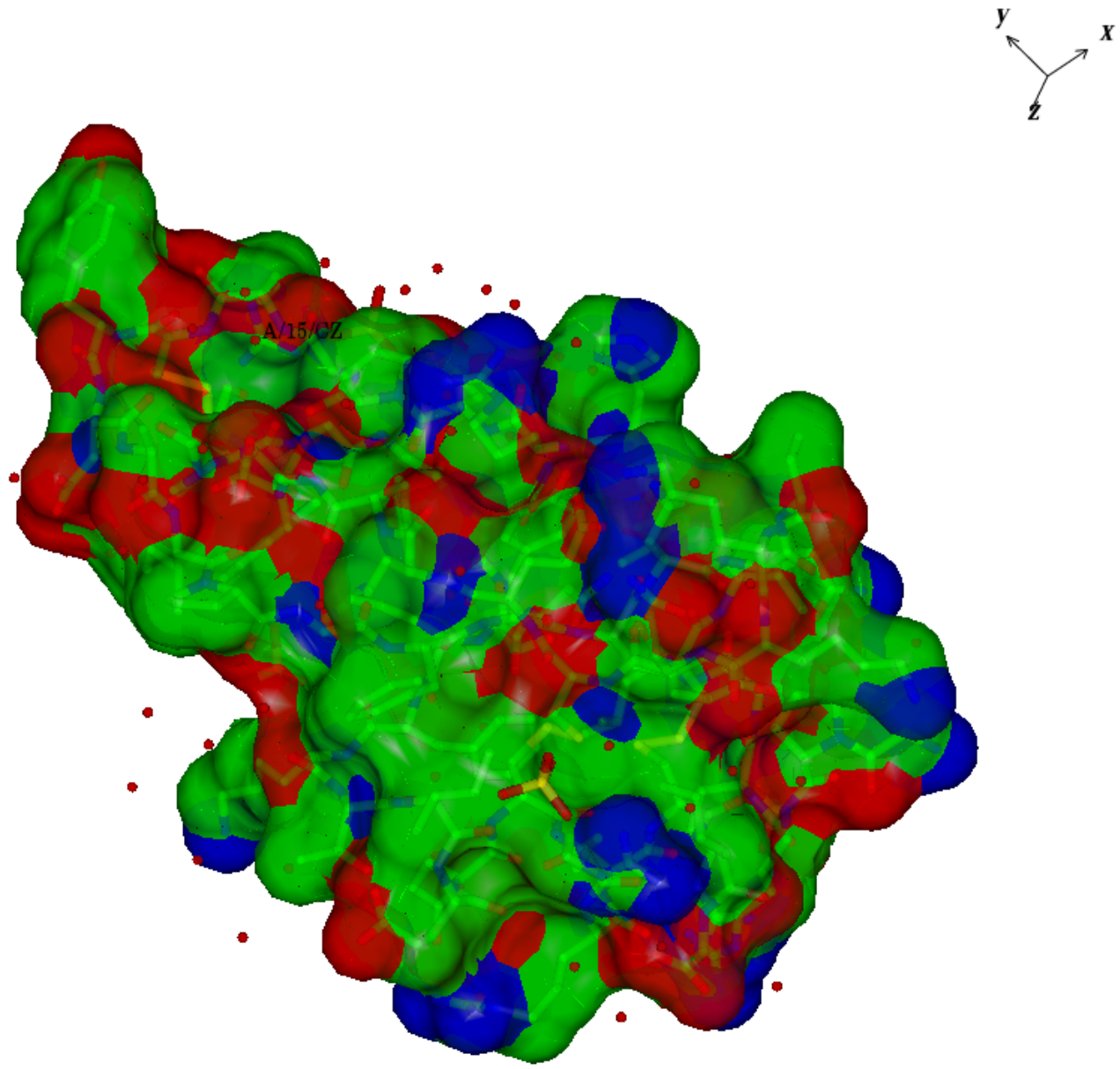

Y
Z
X

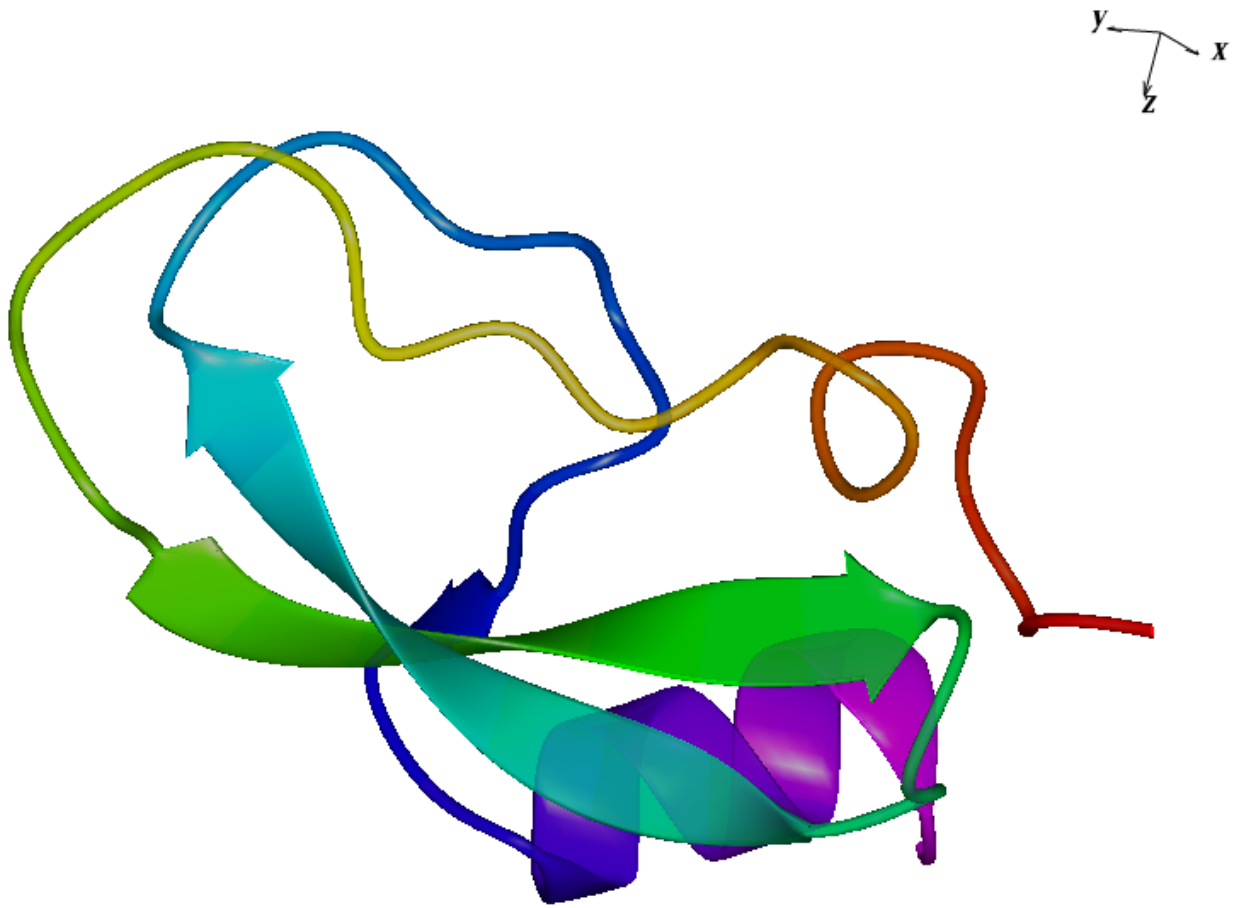
Surfaces:

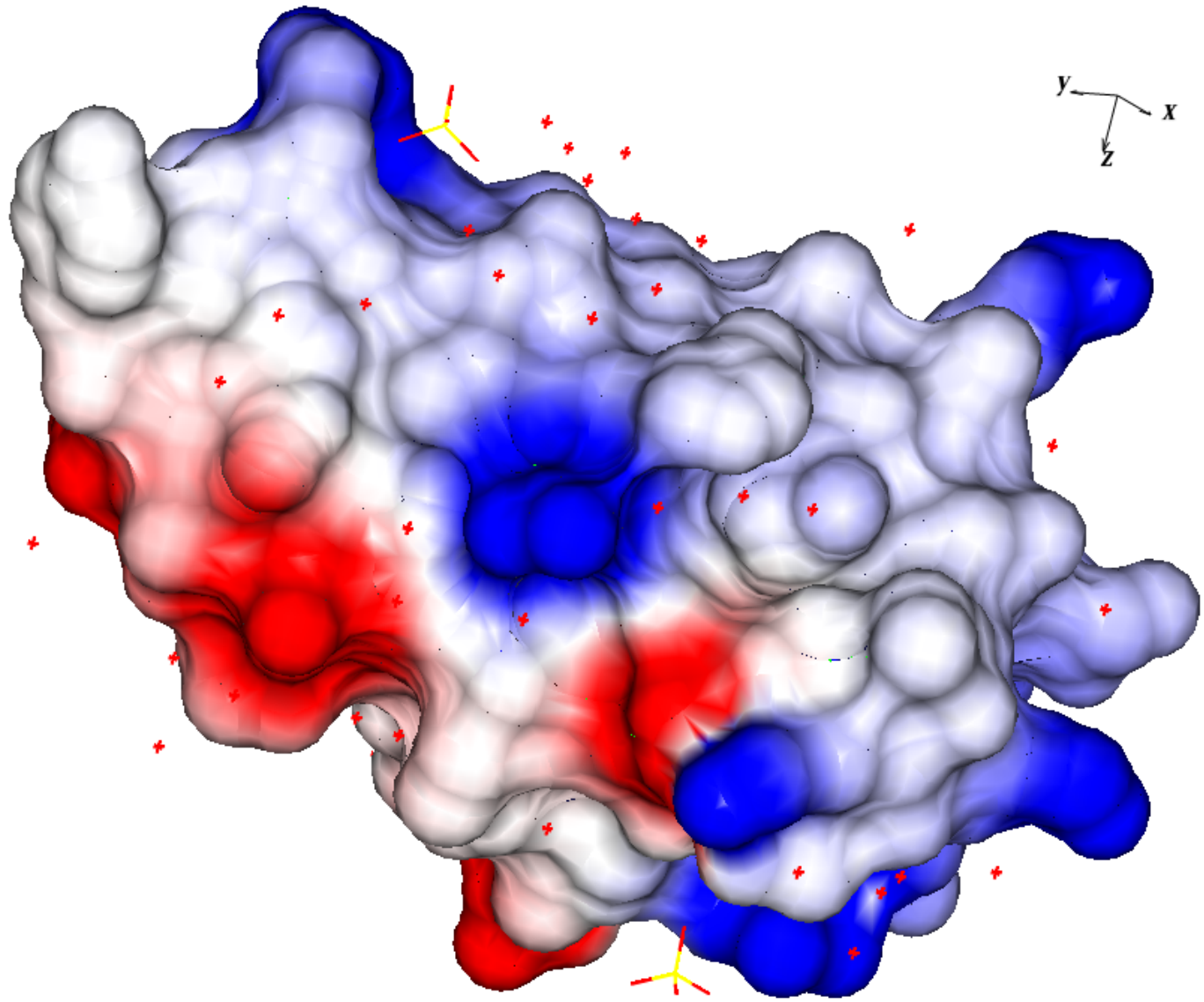
- Display molecular surfaces.
- Display electrostatic potential on surface
- (Work by Martin Noble and Jan Gruber).


y
x
z


y
x
z

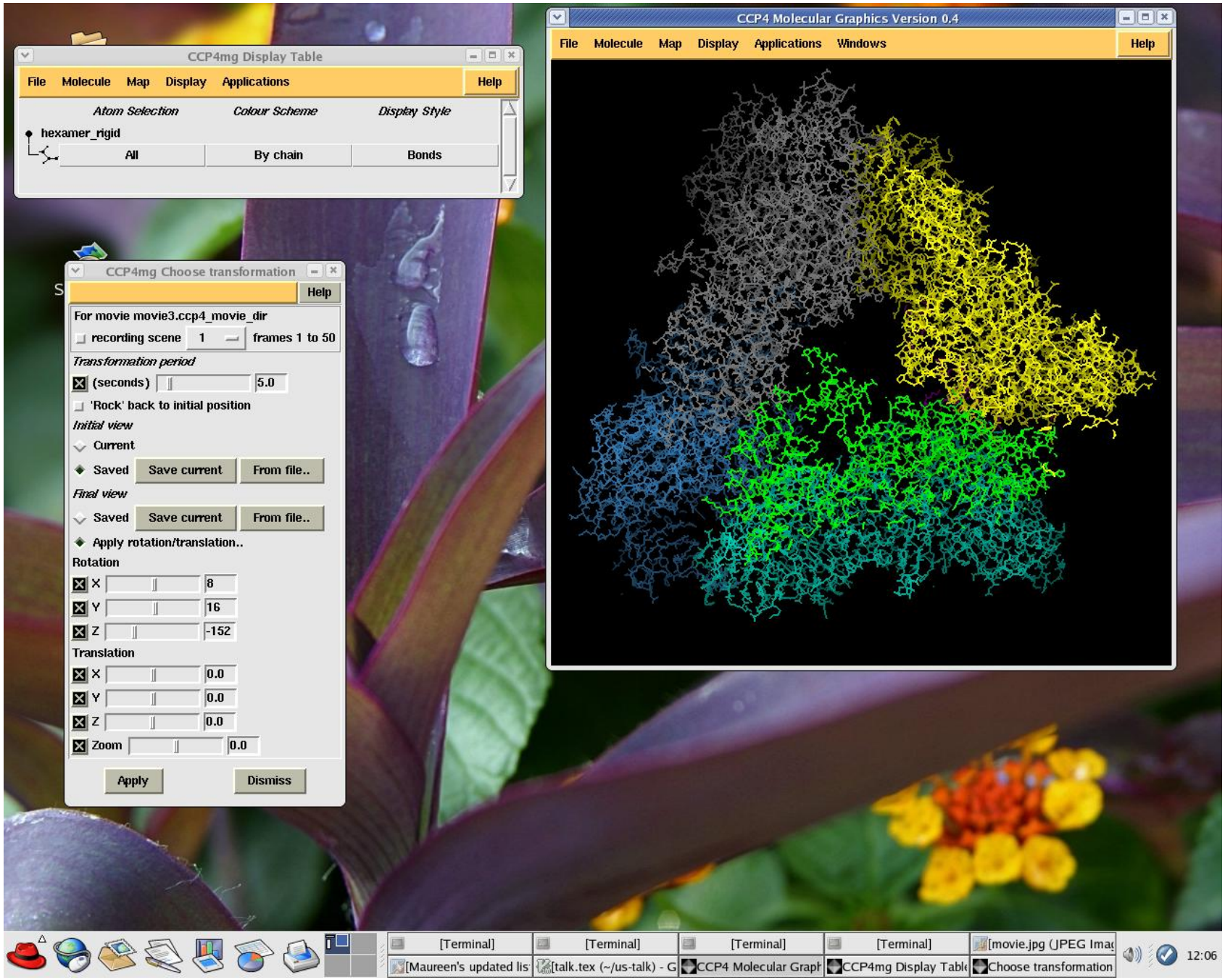

y
x
z
A/15/CZ

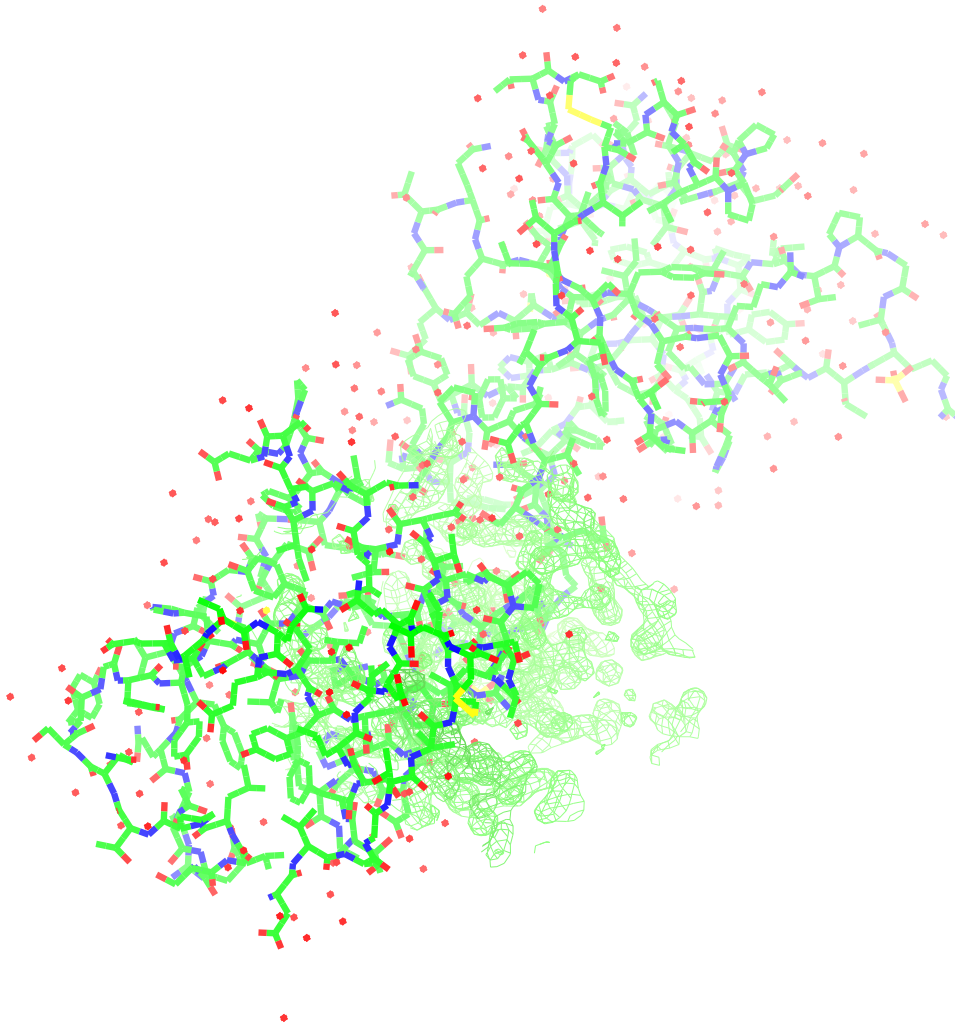

y
x
z

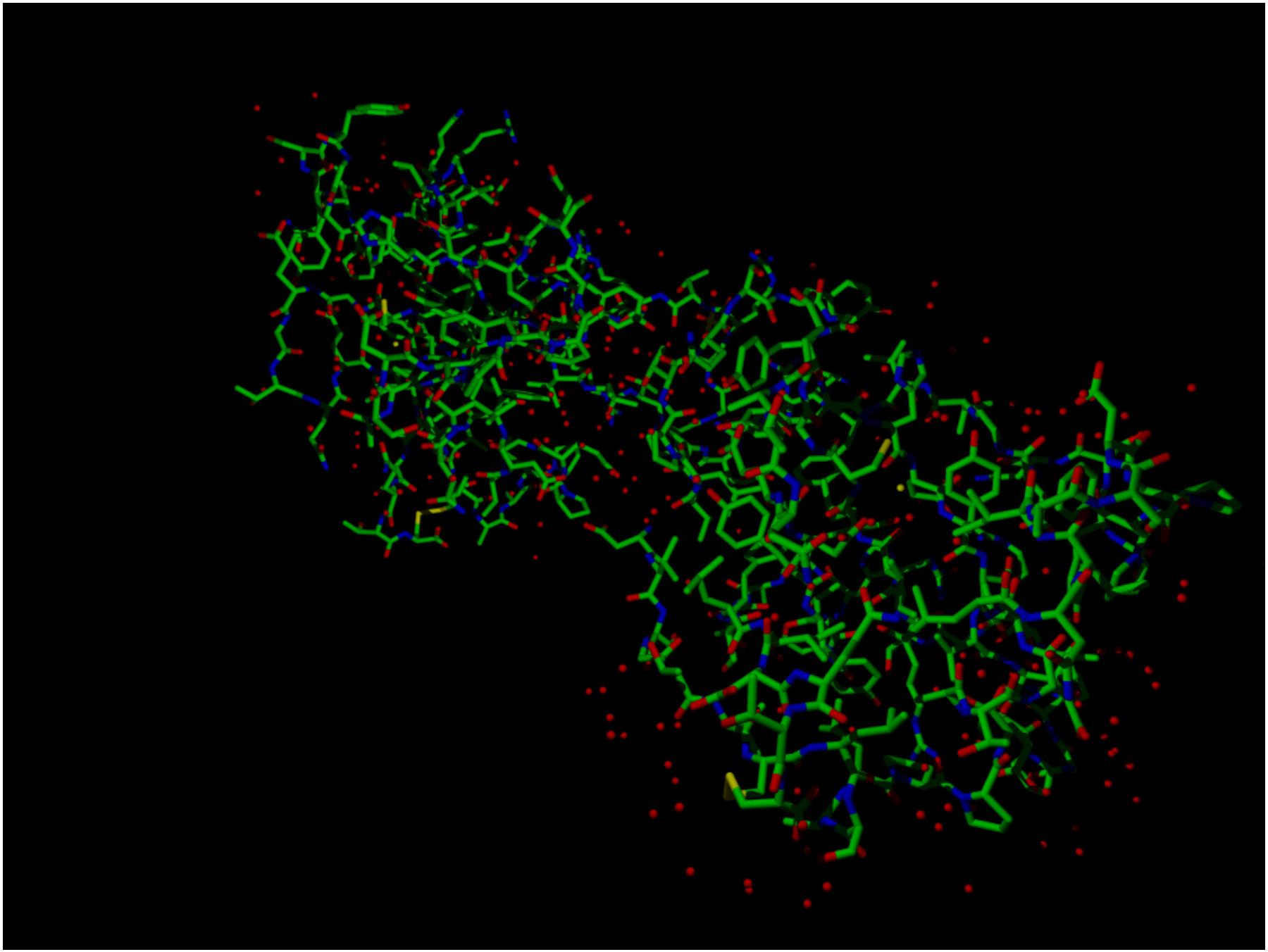

y
x
z

Output:

- Output screenshots, jpeg, png, tiff, etc.
- Output series of screenshots for making movie.
- Export postscript.
- Export Povray scene description.


CCP4mg Display Table
File Molecule Map Display Applications Help
Atom Selection Colour Scheme Display Style
hexamer_rigid
All By chain Bonds
CCP4mg Choose transformation
Help
For movie movie3.ccp4_movie_dir
recording scene 1 frames 1 to 50
Transformation period
(seconds) 5.0
'Rock' back to initial position
Initial view
Current
Saved Save current From file..
Final view
Saved Save current From file..
Apply rotation/translation..
Rotation
X 8
Y 16
Z -152
Translation
X 0.0
Y 0.0
Z 0.0
Zoom 0.0
Apply Dismiss
CCP4 Molecular Graphics Version 0.4
File Molecule Map Display Applications Windows Help
[Terminal] [Terminal] [Terminal] [Terminal] [movie.jpg (JPEG Ima
[Maureen's updated lis [talk.tex (~/us-talk) - G CCP4 Molecular Graph CCP4mg Display Table Choose transformation
12:06





Portability:

- Linux: SuSE 8.x, 9.x, Red Hat 7.x, 8.x, 9, Fedora 1,2,3.
- Apple Mac OS X 10.2, 10.3 (10.4?).
- Windows 2000, XP (using MinGW compiler).
- Compaq Tru64 Unix v5.0.
- Irix 6.4.
- Solaris 8.

Current version at `http://www.ysbl.york.ac.uk/~ccp4mg/`

To Do:

- Incorporate parts of Paul Emsley's Coot.
- Fix some speed problems, most notably start up time on OS X.
- Fix bugs.

Acknowledgements:

- Liz Potterton
- Martin Noble, Jan Gruber (surfaces)
- Paul Emsley, Kevin Cowtan (maps)
- Eugene Krissinel (mmdb coordinate library, structure superposition)
- CCP4 staff
-