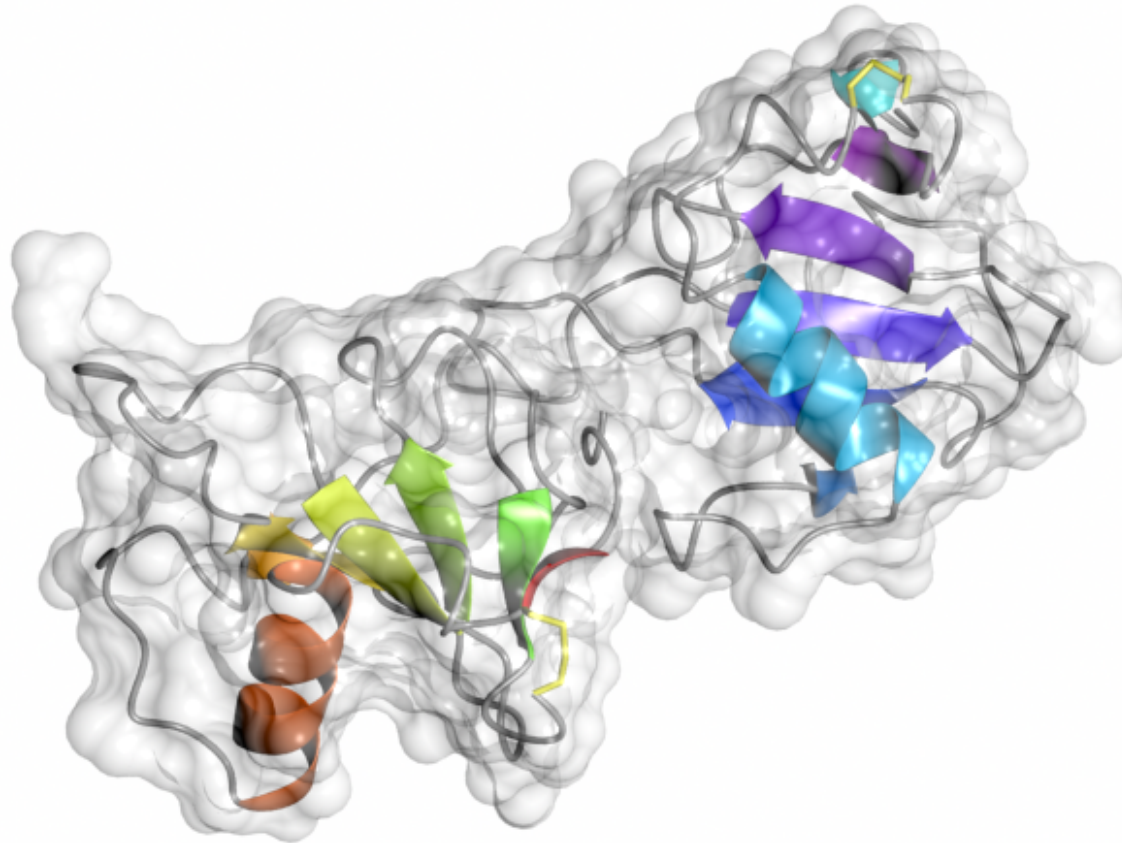# CCP4MG

CCP4 Molecular Graphics Program

Stuart McNicholas and Liz Potterton, University of York

Introduction

- CCP4MG is a molecular graphics program funded by CCP4.

- Its primary focus is the visualization and analysis of macromolecular structure.

- It produces high quality rendered images and movies.

- Version 2 is now available.

Displaying Molecules (styles)

- CCP4MG can display molecules in many different ways:

  - Bonds, cylinders, ball and stick, spheres
  - CA traces
  - Thermal ellipsoids
  - Ribbons, worms, etc.
  - Base pair "sticks", base blocks
  - Lipid cartoons
  - Surfaces

Displaying Molecules (colouring)

- Molecules can be coloured by various methods:
  - Atom type
  - Chain, model
  - Main/side chain
  - Rainbow through model
  - Atom/residue properties
  - Electrostatic potential (currently surfaces only)
- All of the colouring methods can be customized.

Atom Selections

- CCP4MG can use the various styles/colours with all atoms in a coordinate file or a subset of the atoms.

- There are quickly accessible menu items for common selections, e.g.:

  - All atoms

  - CA trace

  - Main chain/side chains

  - All peptide/nucleic acid/solvent/metals, etc.

Display Table

⊟ Crystals			
	Xtl parameters ▾	Crystal conte.. ▾	Symmetry off ▾
⊟ toxd			
	/ / / ▾	Blend through.. ▾	Ribbons ▾
	Disulphide br.. ▾	yellow ▾	Cylinders ▾
	Solvent ▾	Atom type ▾	Ball and stick ▾
	Solute ▾	Atom type ▾	Ball and stick ▾
⊟ rnase			
	A/ or B/ ▾	Blend through.. ▾	Ribbons ▾
	Disulphide br.. ▾	yellow ▾	Cylinders ▾
	Solvent ▾	Atom type ▾	Ball and stick ▾
	Solute ▾	Atom type ▾	Cylinders ▾
	All non-solvent ▾	Same as other ▾	white ▾
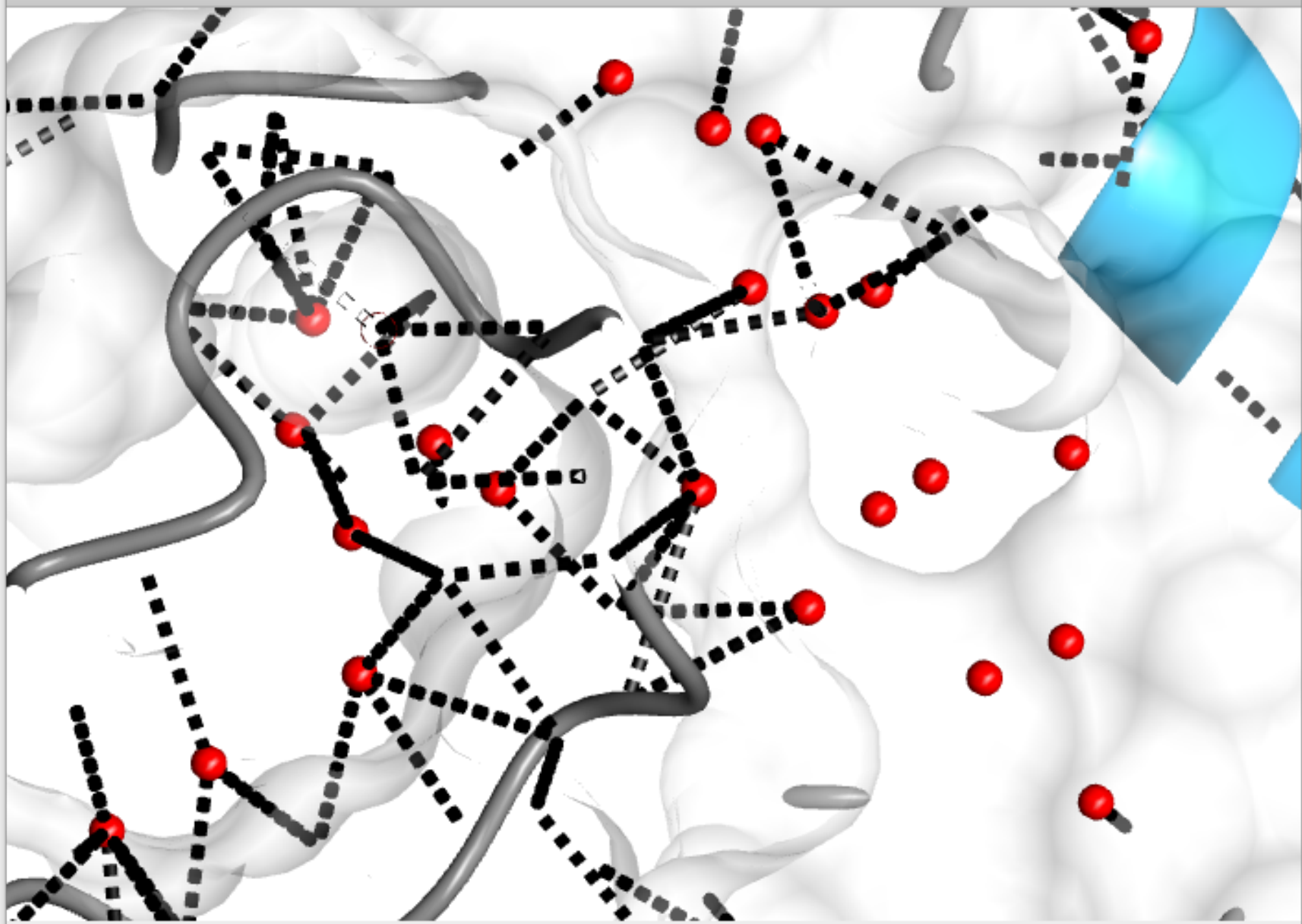
Atom Selections

- More complicated selections may be made using the "Selection browser":

  - Neighbourhoods of various atoms

  - Atom types, residue types

  - Residue ranges

  - Secondary structure elements

  - Individual atoms

  - Logical and/or/not of all the above

Selection Browser
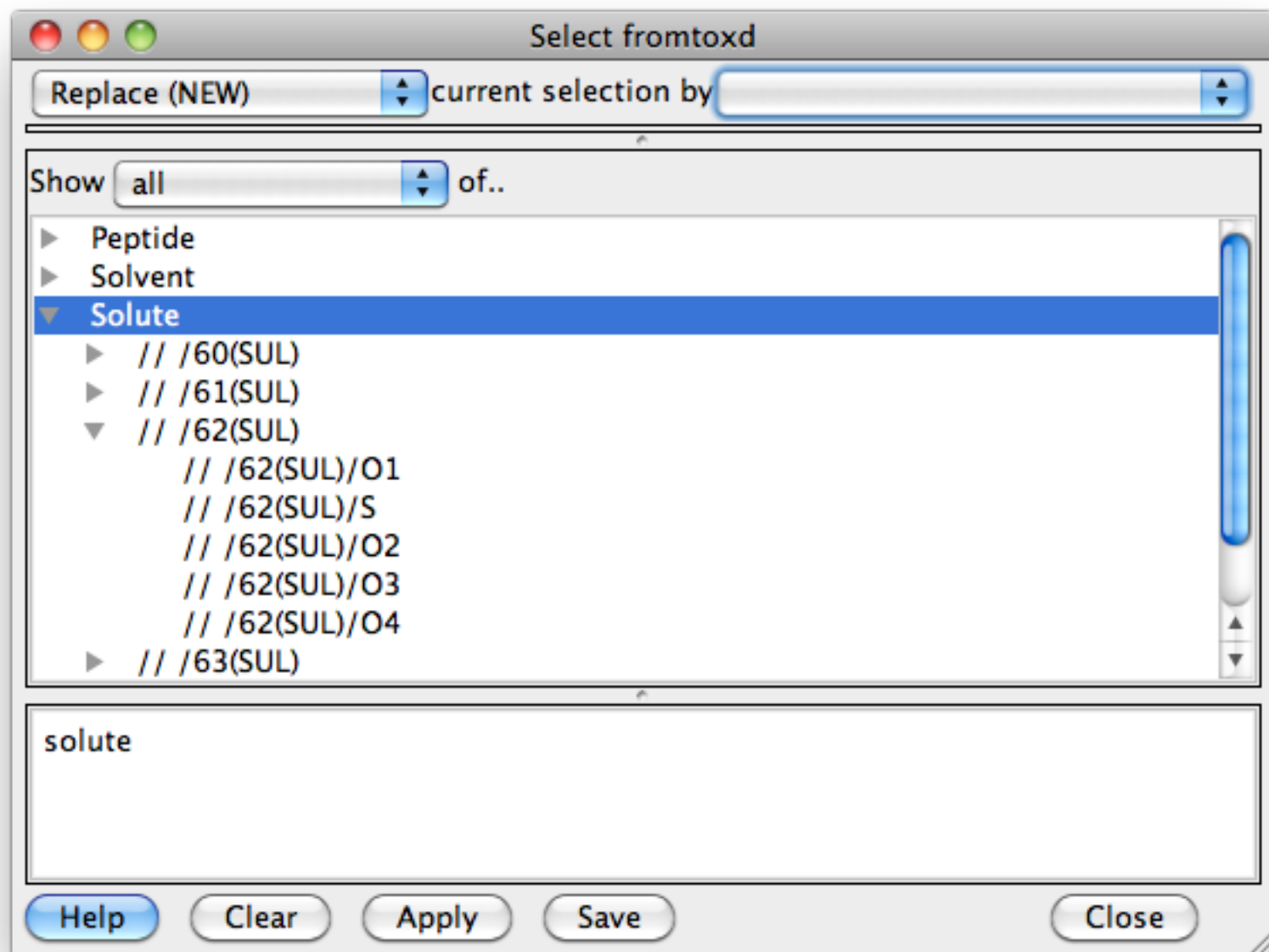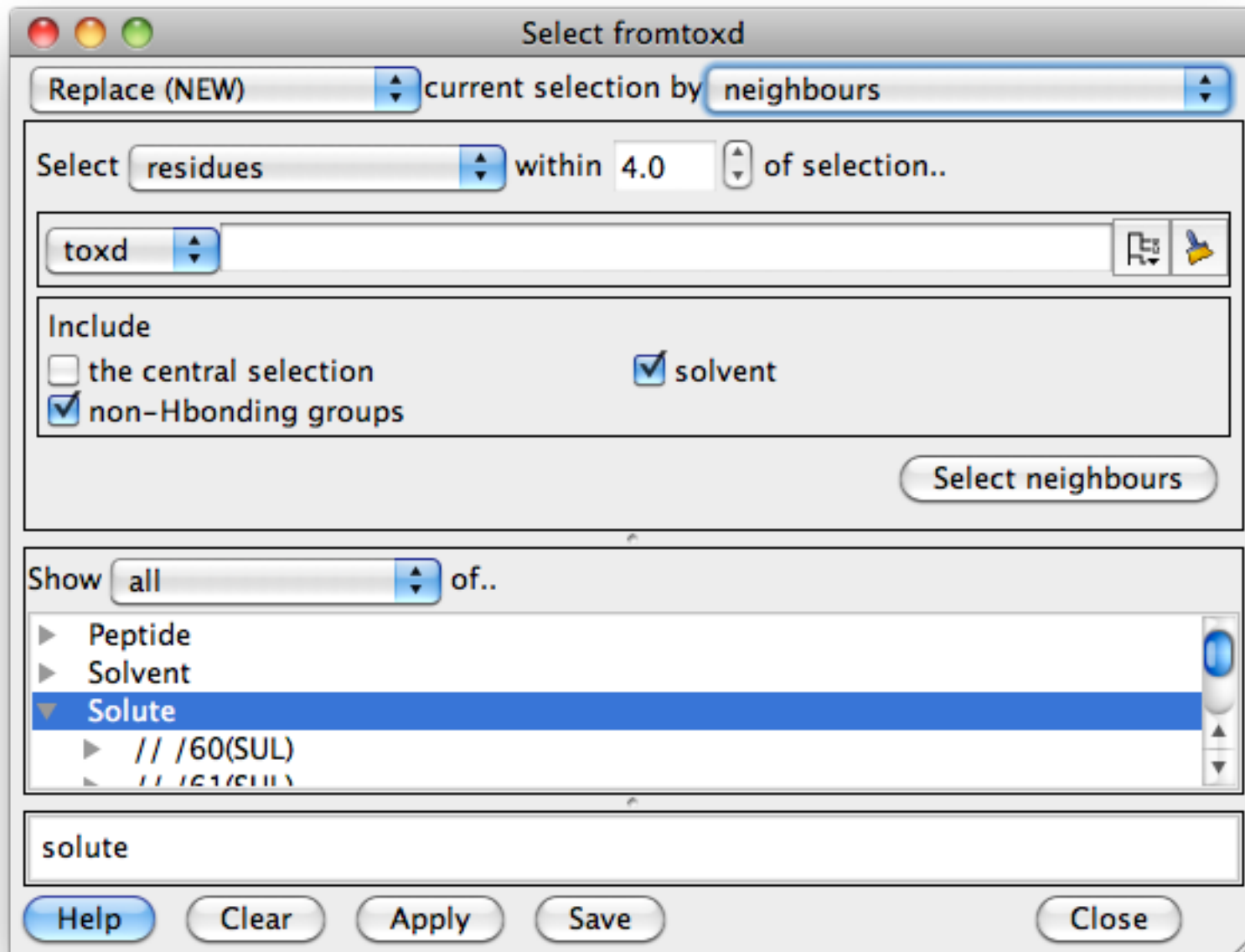
Selection Browser
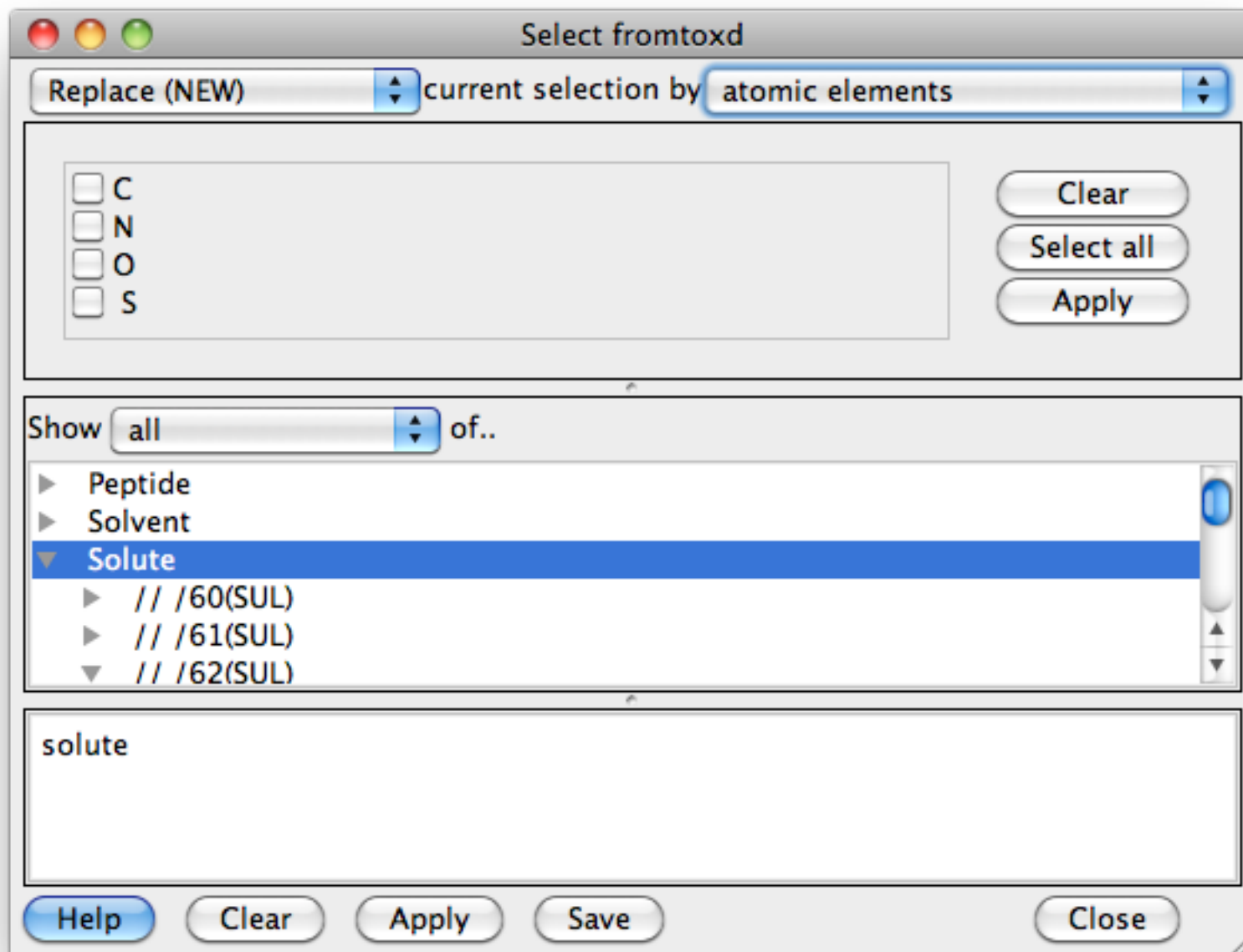
Selection Browser
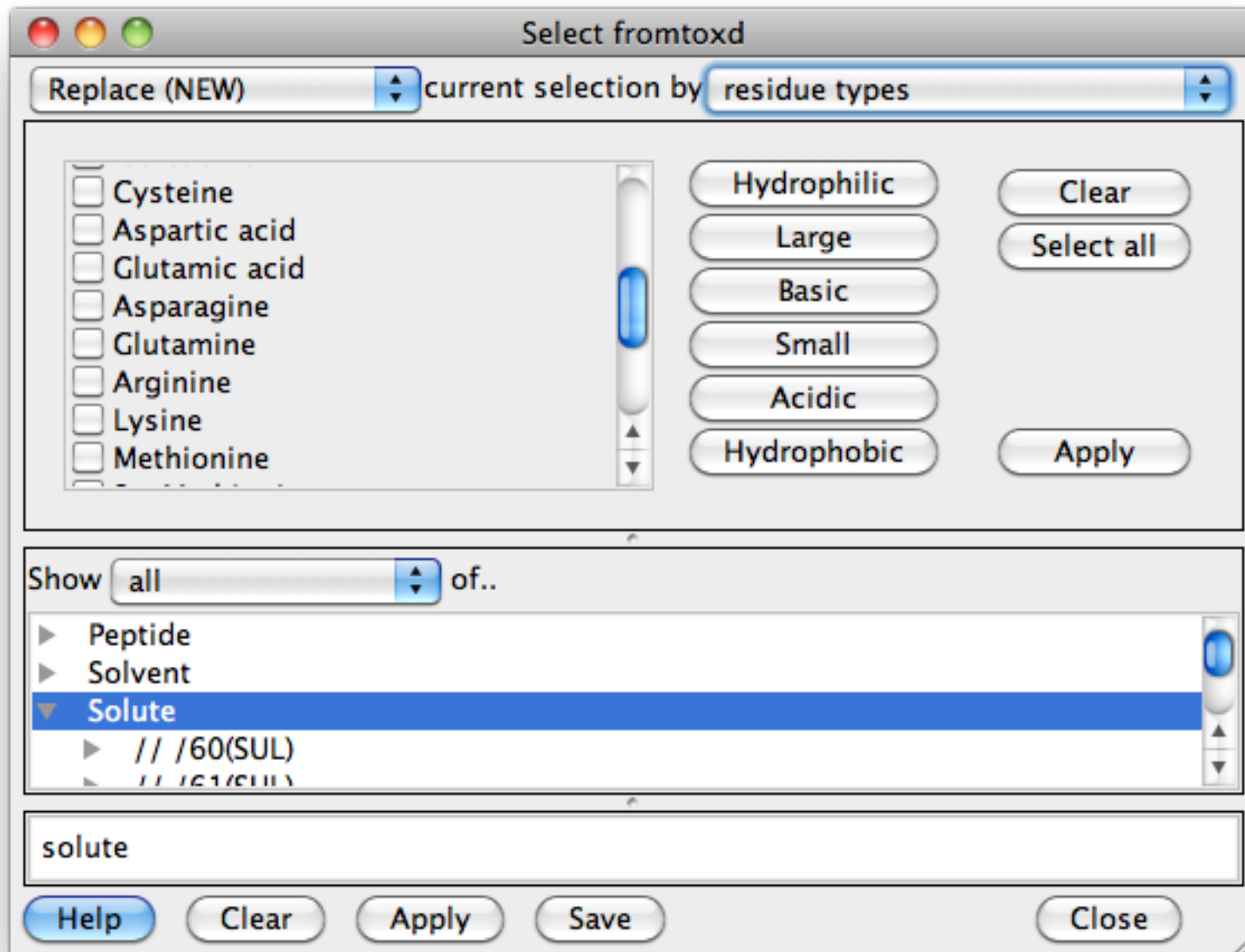
Selection Browser
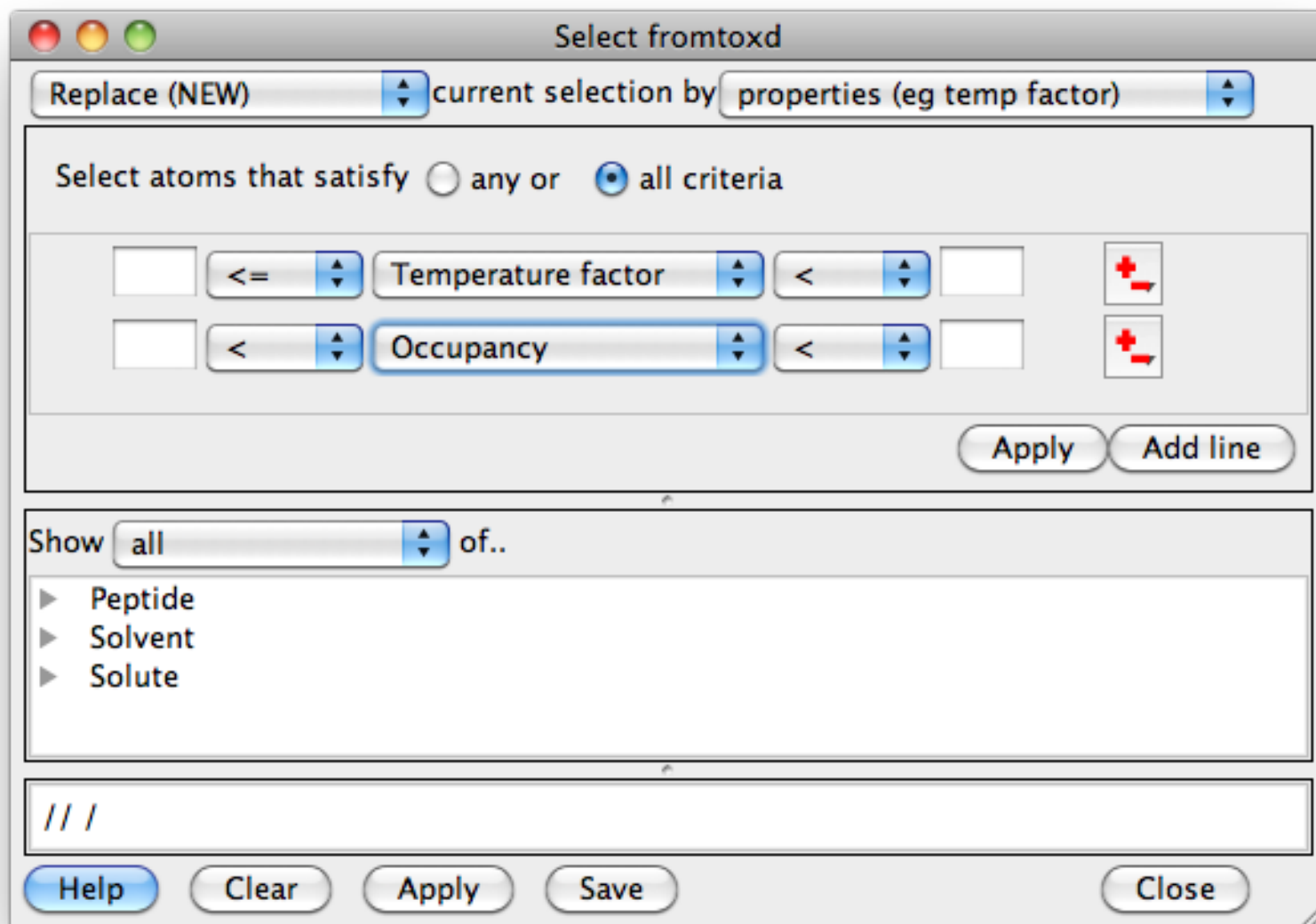
Selection Browser

Picture Wizard

- The picture wizard is an automatic way of generating complex scenes with multiple selections, colouring, styles, etc.

- Representations are organised into various "styles"

- The picture wizard is shown at the top of the file browser window when a coordinate file is loaded, or can be accessed from the display table.

Display Table

	Solute	Atom type	Ball and stick

rnase

- ✓ Visible
- Centre on
- Picture wizard..
- Copy picture style from..
- Add model display object
- Add display object ▶
- File save/restore ▶
- List data
- Structure definition ▶
- Transform coordinates ▶
- Generate symmetry mates..
- Animation ▶
- Clone ▶
- Delete

	Blend through..	Ribbons
	yellow	Cylinders
	Atom type	Ball and stick
	Atom type	Cylinders
	Same as other	electrostatic
	All peptide	purple

cyan   1.86

Open file(s)

ribbons
- broken ribbons
- broken ribbons neighbours
- **colour blend thru chain**
- colour chains
- cylinder ranges

Picture wizard

- ● Automatic picture setup
- ○ Open picture wizard choices

Look in: 🏠 /Users/stuart

Computer
stuart

1orb.png	apple.tar.gz	clip-surf2.png.
1orb.png.pkl	apple2.tar.gz	clip-surf3.png
1pmp.pdb	apps	clip-surf3.png.
1pmp.png	bigshadow.png	clip.png
1pmp.png.pkl	bigshadow.png.pkl	clip.png.pkl
1yiv.pdb	ccp4-6.0.2-F6.tar.gz	contours.png
8dfr.ccp4mg	ccp4mg_tutorial	contours.png.p
8dfr.pdb	ccp4mg-F6.tar.gz	contours2.png
8dfr.png	ccp4mg-rel2B-i386	contours2.png.
8dfr.png.pkl	ccp4mg-rel2B-ppc	cwibble.txt
200-left.png	Centos 4.4.ovf	Desktop
200-right.png	Centos 4.4.vmdk	Documents
200.png	clip-surf1.png	Downloads
200.png.pkl	clip-surf1.png.pkl	eden-dots.png
ALL_BIG_PHOTOS.tar.gz	clip-surf2.png	eden-dots.png

File name: [   ] Open

Files of type: All files (*.pdb *.cif *.ent *.map *.mtz *.vector *.ppm *.xbm *.bmp ▼)   Cancel

Picture wizard: rnase

☑ Delete any existing display object

side chain spheres
▶ interfaces
▼ ligand binding site
  site
  site and broken ribbons
  site and ribbons
  surface around ligand

Creates three display objects by selecting the neighbourhood of the ligand(s):
1) close side chains or main chains shown as cylinders
2) main chain within a larger radius shown as worms

Ligand 1 [   ]
Ligand 2 [   ]
Ligand 3 [   ]

☐ Label binding site residues

(Help)   (Create picture)   (Cancel)

CCP4MG version 2.0.0

Display Table

8dfr

	/ / /	Blend through..	Ribbons
	//191(NDP) or..	Atom type	Cylinders
	Solvent	Atom type	Ball and stick
	Metals	Atom type	Spheres
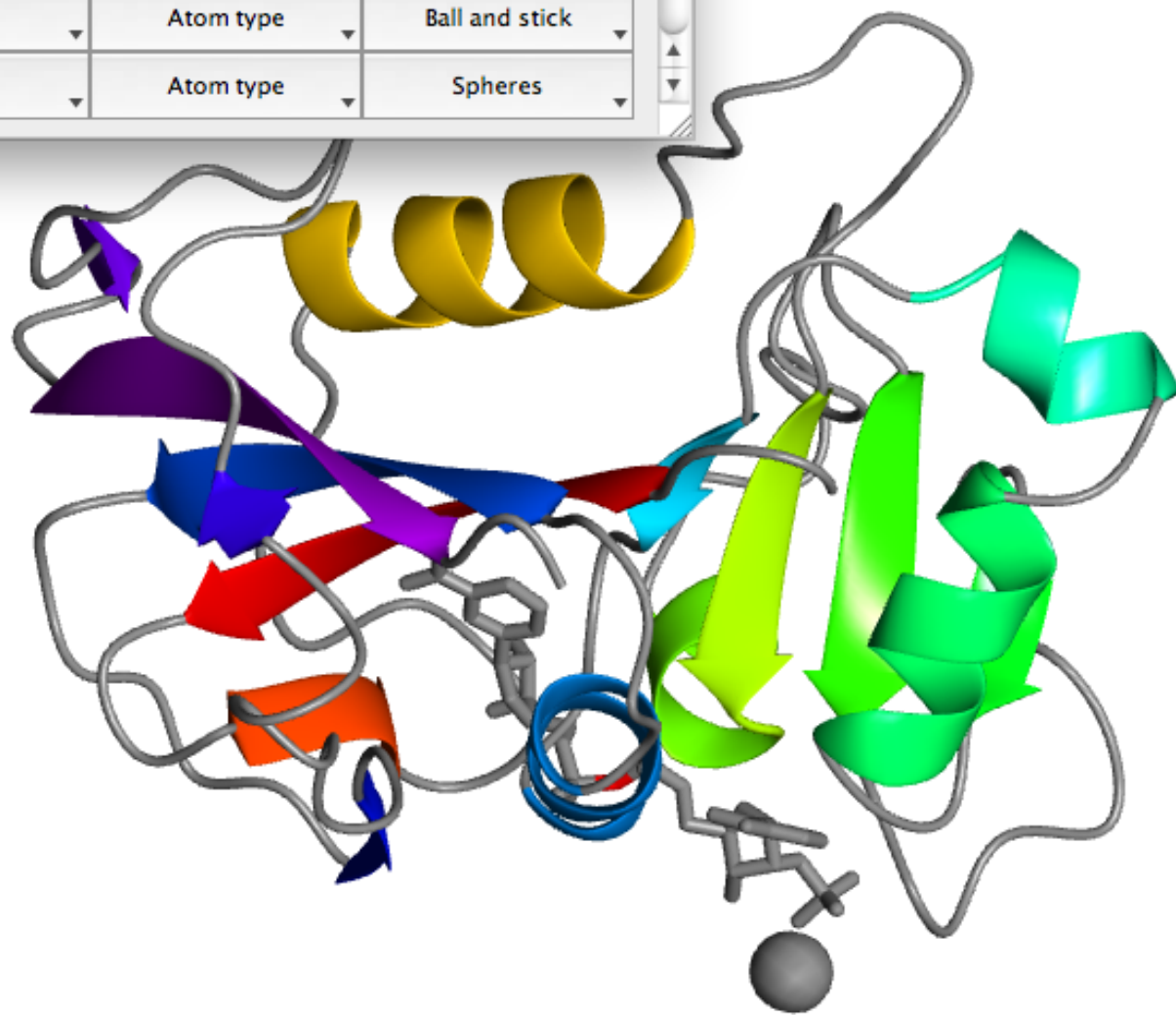
Molecular Symmetry

- Symmetry mates of a molecule can be displayed using data from pdb file, mtz file or by specifying by hand.

- The user may choose:

  - Continuous crystal, symmetry mates generated within certain radius of screen centre.

  - Unit cell, with optional extensions along crystal axes.

  - Generate specific mates from symmetry operations.

Electron Density

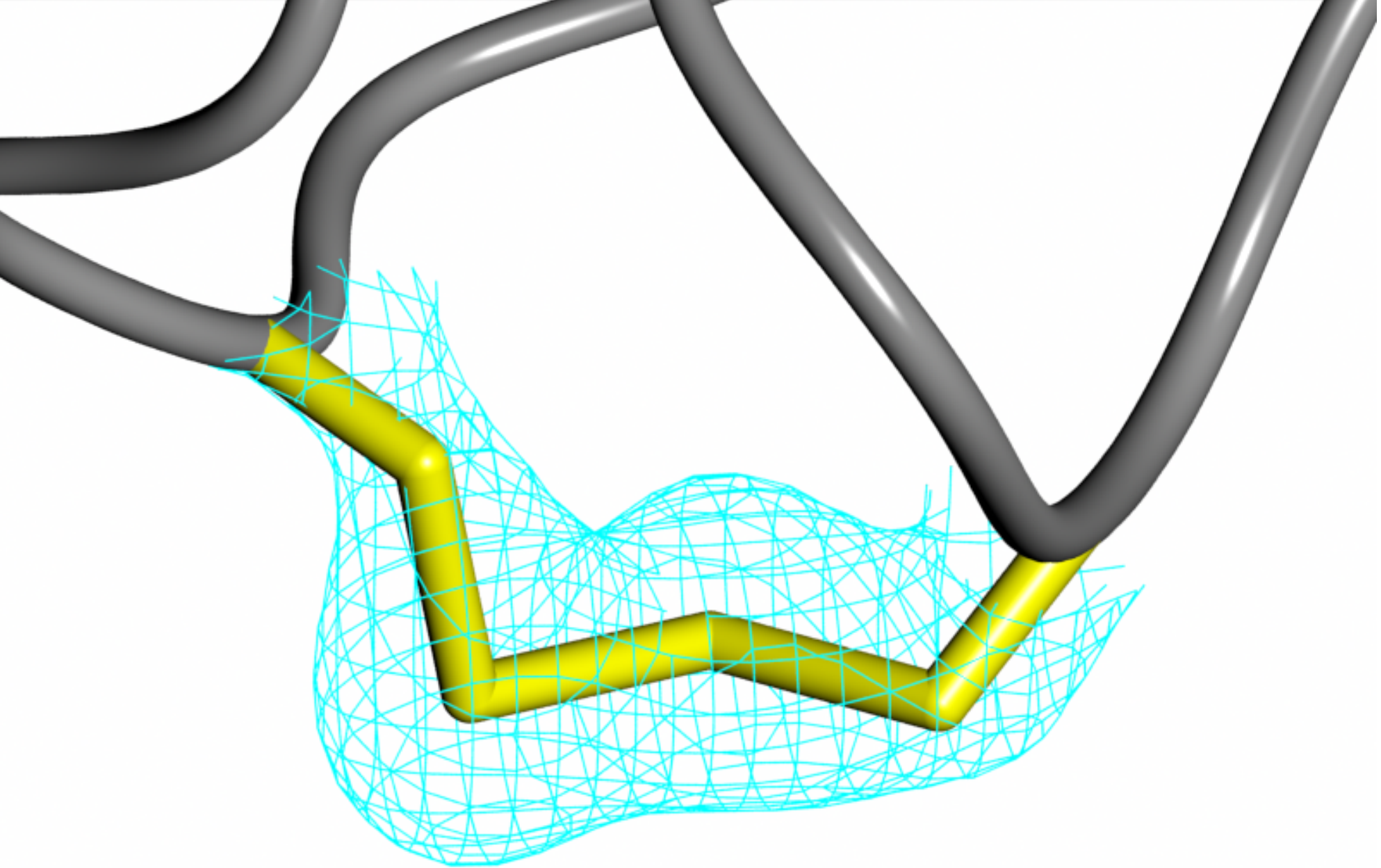- Electron density maps can be read/created from any CCP4 supported file format.

- Density can be represented as chickenwire lines, chickenwire cylinders, solid surface or dots.

- By default a 10Å cube of density is drawn, this size may be changed.

- The density can be clipped to a set of atoms.
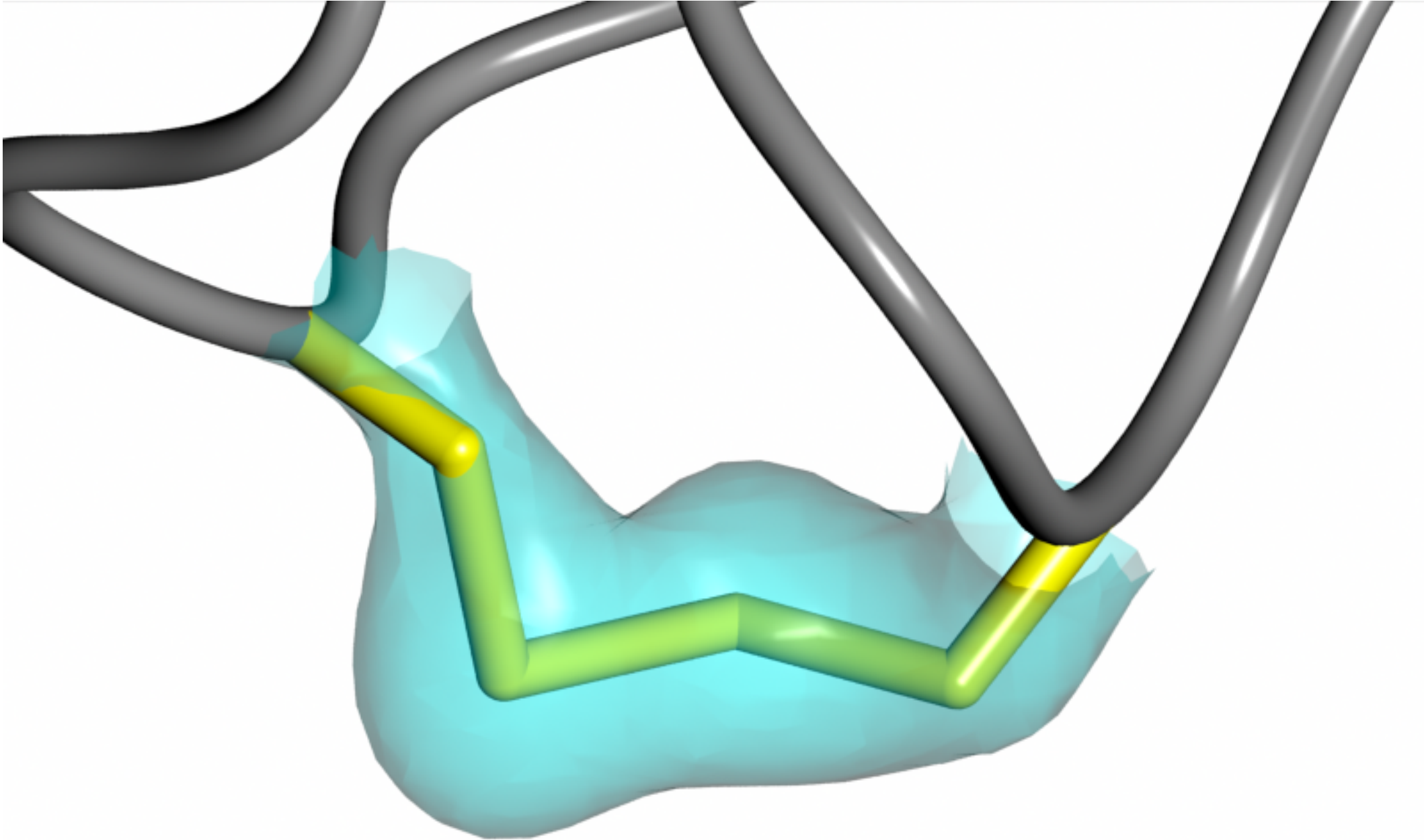
Vectors

- "Vectors" can be drawn between pairs of atoms and arbitrary points in 3D space.

- The vector may be a line, dashed line, cylinder, arrow, etc.

- Vectors can have text labels.

- Vectors can be read/saved in cif format.

Geometry

- In "geometry mode" double clicking on atoms allows one to measure distances, angles and dihedral angles.

- A table displaying this information is displayed. The table is interactive, so that one may delete atoms from the current selected set.

Other Display Details

- All objects
  - May be visible/invisible
  - "Flash"
  - Be transparent with arbitrary opacity
- One can have multiple views (e.g. side-by-side stereo)
- Depth-cueing fog, clipping, background colour and lighting are all user definable
- Lots of stuff is highly customizable

Preferences Model drawing style

- ▼ Model display
    - **Model drawing style**
    - Hbond/contact drawing style
    - Atom label style
    - Pick atom label style
- ▶ Model colours
- ▶ Model analysis
- ▶ Surfaces
- ▶ Maps
- ▼ Display
    - Render quality
    - Fonts
    - Animation and flashing
- ▶ Images and movies
- ▶ Behaviour
- ▶ Tools
- ▶ Plugins preferences

Bond width	2
Fat bond width	4
Thin bond width	1
Dashed bonds	☐
Dash length for dashed bonds	0.30
Cylinder thickness (Angstrom)	0.20
Ball cylinder thickness	0.10
Ball radius = VDW radii x	0.20
Sphere radius = VDW radii x	0.80
Nucleic base stick thickness (A)	0.40
Base block thickness	0.20

[Apply] [Reset defaults] [Help] [Close]

Images and Text

- Text may be added to the scene in multiple ways:

  - Annotations to models

  - Atom labels and labels creates by clicking on atoms

  - "Legends". Text objects in 2D window coordinates.

- All text objects can use any system font/style/size.

- Annotations and Legends can display text with multiple FoNTS/styles/sizes/colours.

*Lege*nd
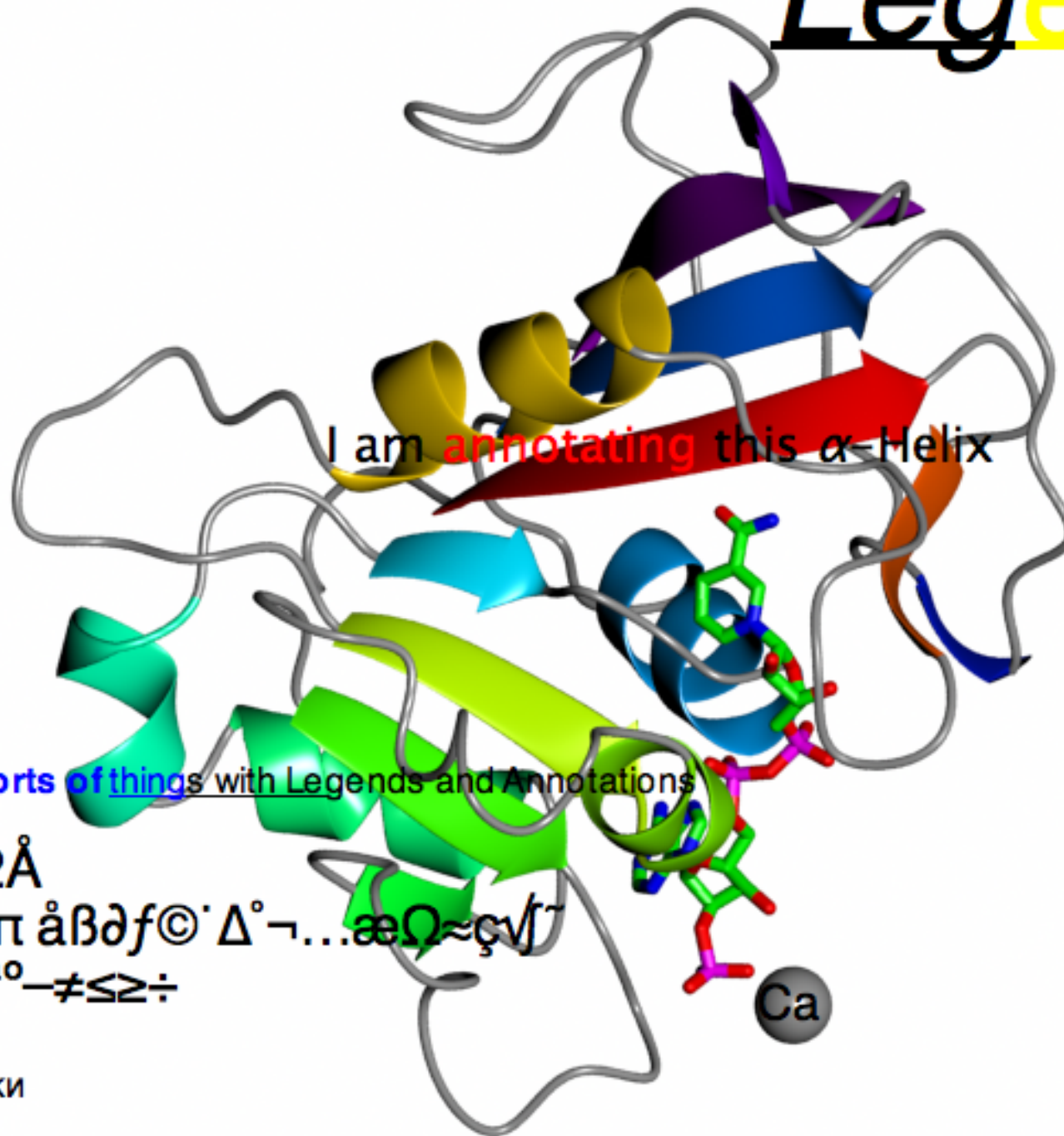
I am annotating this α-Helix

You *can do* **all sorts of** things with Legends and Annotations

Legend 2.2Å
œ∑® †¥ø π åߌƒ©˙∆˚¬…æΩ≈ç√ʃ˜
¡™£¢∞§¶•ªº–≠≤≥÷
⁄€‡°·—±
вот это по-русски
Ελληναζ
český

PISA

The EBI website defines PISA:

PISA is an interactive tool for the exploration of macromolecular (protein, DNA/RNA and ligand) interfaces, prediction of probable quaternary structures (assemblies), database searches of structurally similar interfaces and assemblies, as well as searches on various assembly and PDB entry parameters

E. Krissinel and K. Henrick (2007). *Inference of macromolecular assemblies from crystalline state*. J. Mol. Biol. **372**, 774--797.

E. Krissinel and K. Henrick (2005). *Detection of Protein Assemblies in Crystals*. In: M.R. Berthold *et.al.* (Eds.): CompLife 2005, LNBI 3695, pp. 163--174. Springer-Verlag Berlin Heidelberg.

E. Krissinel (2009). *Crystal contacts as nature's docking solutions*. J. Comp. Chem., in press; published on-line 6 May 2009; DOI 10.1002/jcc.21303}

PISA

- PISA identifies the chemical monomers and the interfaces between the monomers including the monomers generated by applying symmetry to the input file coordinates.

- By evaluating the strength of interaction between the neighbouring monomers in a crystal, PISA predicts what would be the most stable multimer and therefore the most likely biological form of the structure.

PISA

- There is a command line version of PISA to which CCP4MG has an interface.

- One can simply ask PISA to analyse a structure

- Interfaces and assemblies may be visualized from the results.

Pisa structure analysis 1an4

Analyse model   1an4

| monomers | interfaces | assemblies |

## Id	Monomer1	Monomer2	Symmetry operation	Sym.Id	Area	DeltaG	Nhb	Nsb	Nds
1 1	D	C	X,Y,Z	1_555	954.6	-14.0	57	0	0
2 2	B	A	X,Y,Z	1_555	762.6	-11.4	1	2	0
3 3	C	B	X,Y,Z	1_555	443.2	-8.5	6	0	0
4 4	C	A	X,Y,Z	1_555	385.5	-1.3	5	0	0
5 5	D	A	X,Y,Z	1_555	364.4	-4.8	7	0	0
6 6	D	B	X,Y,Z	1_555	319.9	1.3	4	0	0

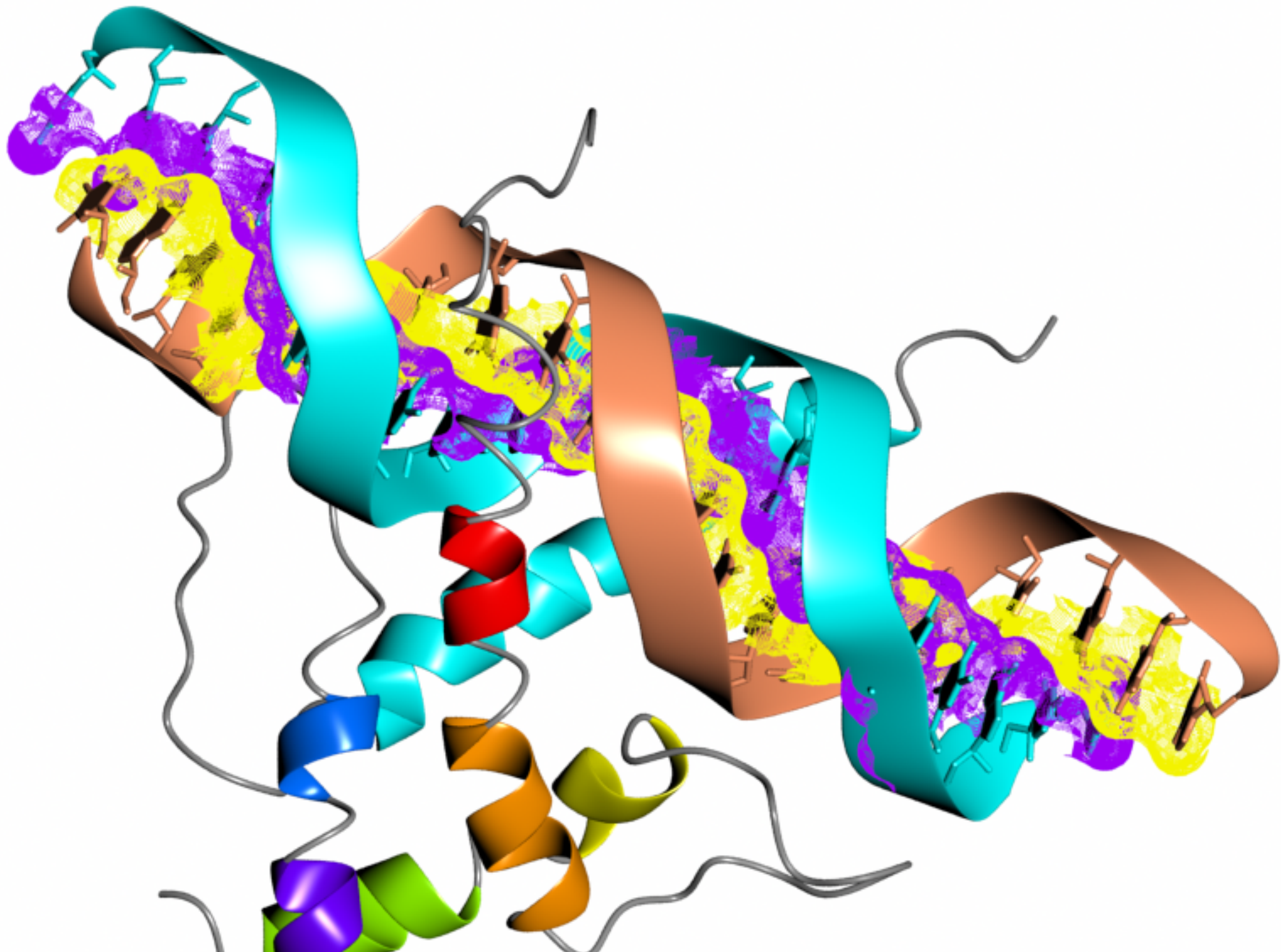PISA data files in /Users/stuart/.CCP4MG2/pisa_data/pisa_1an4

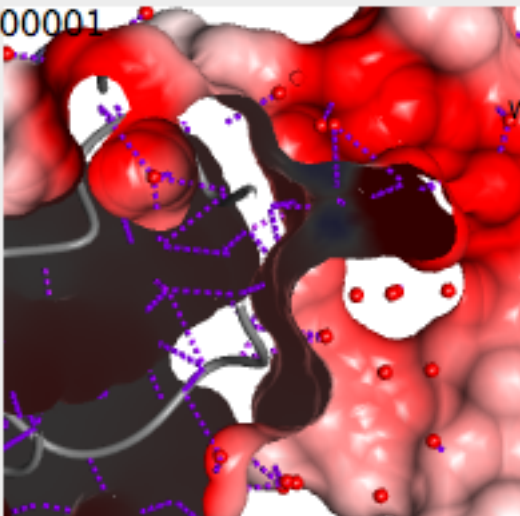| Help | Analyse structure | Show | Clear display | Close |

Structure Superposition

- CCP4MG has three methods of structure superposition:

    - SSM. This is the default method. It is the simplest to use and usually gives excellent results. The method attempts to match secondary structure elements in different coordinate sets.

    - Close Residues.This method is useful for performing locally optimised superposition after a global superposition by SSM

    - User-defined. This is the most flexible: the user can specify in many ways the atoms to superpose.

Movies

- Movies are creates by defining a series of "key frames" and then (optionally) interpolating between them.

- Key frames may also define simple transformations (rock, roll, etc.)

- Movies can be created either as animated gifs or as MPEG streams.

Rendering

- CCP4MG has two methods of producing final images:

  - Screenshot. A simple dump of the screen pixels is performed.

  - Rendering. This uses a Renderman compatible renderer "Pixie". The images are of much higher quality than the simple screen dump. This method is preferred for publication images. The images may be rendered at any size and effects such as ray-traced shadows and proper transparency are possible.
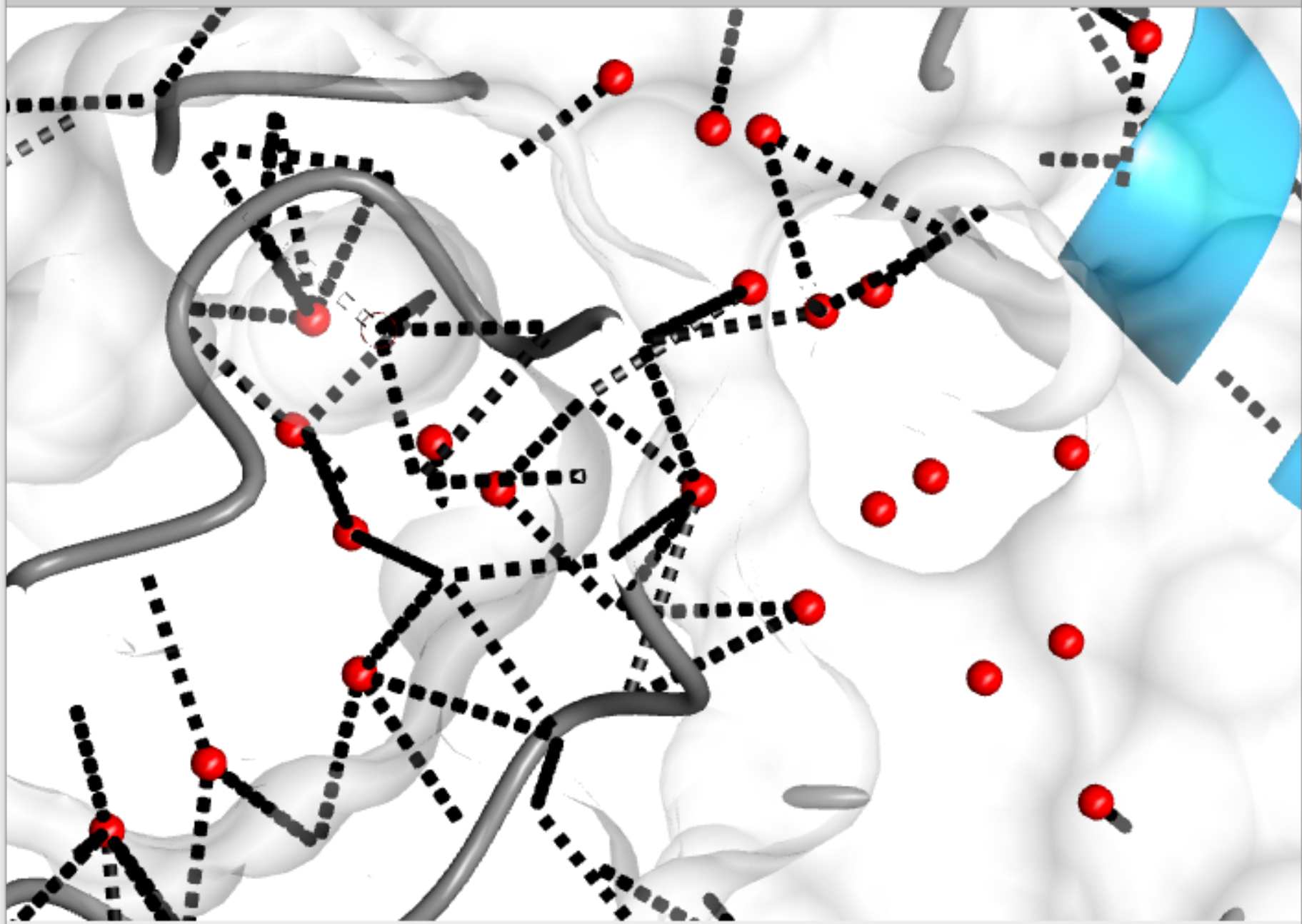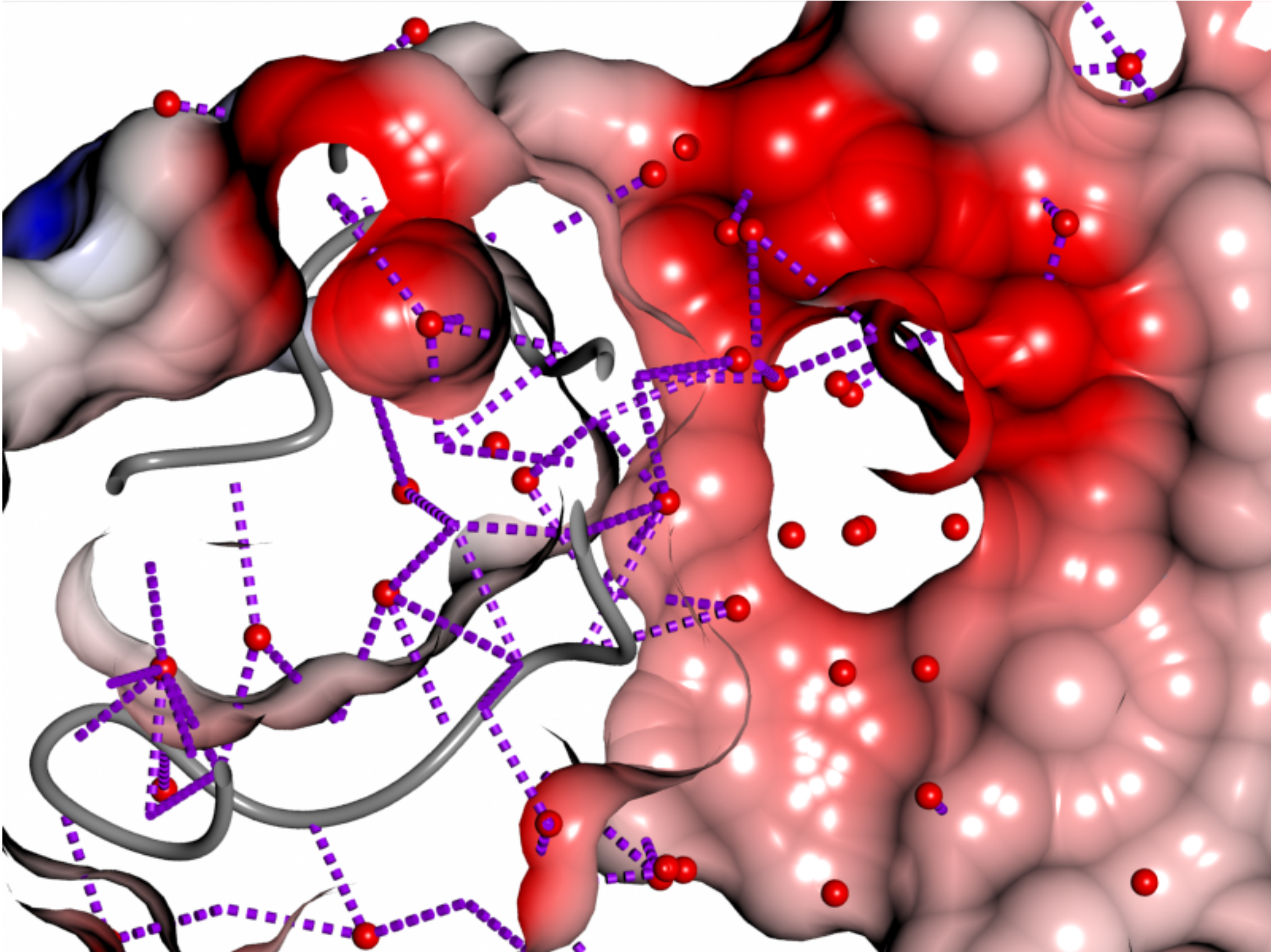
Model display
  Model drawing style
  Hbond/contact drawing style
  Atom label style
  Pick atom label style
▶ Model colours
▶ Model analysis
▼ Surfaces
  Surface drawing style
  Electrostatic potential
▶ Maps
▶ Display
▶ Images and movies
▶ Behaviour
▶ Tools
▶ Plugins preferences

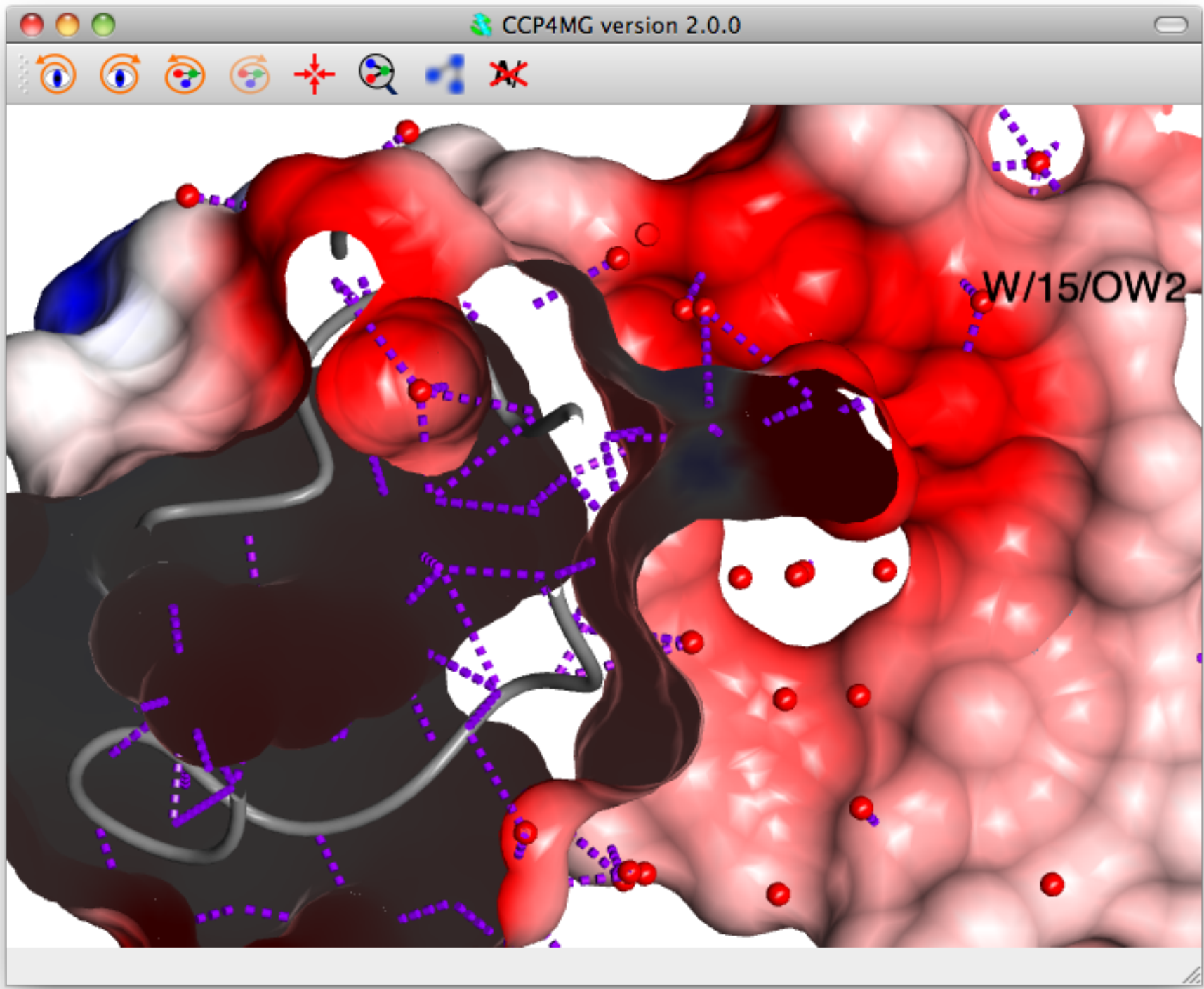Surface probe radius(0-3)   1.50

Cutoff distance for context atoms   6.00

Resolution in degrees(2-80)   30.00

Blend colour borders   ☐

Maximum dot separation(0.005-0.5)   0.10

Dot size(1.0-3.0)   1.00

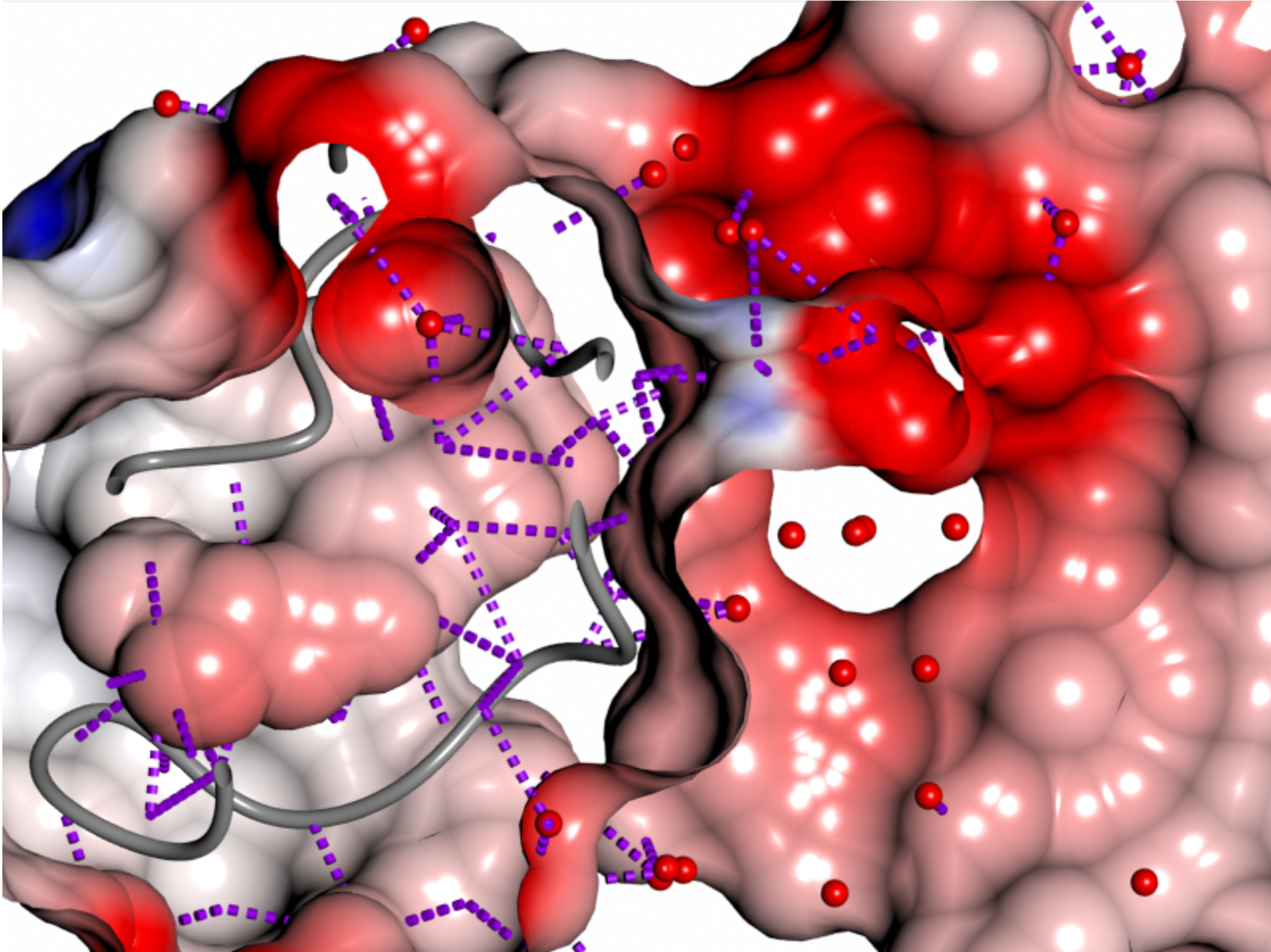Mesh line width   1.00

Draw both sides of surface   ☑

Apply   Reset defaults   Help   Close

Render

Output image size

○ Display window size x [1.00 ▲▼]

◉ Width (in pixels) [800 ▲▼] height [600 ▲▼]

☐ Keep graphics window aspect

☑ Scale font sizes

☑ Scale image sizes

☐ Transparent background
☐ Stereo image

◉ Shear stereo with separation [0.10 ▲▼]
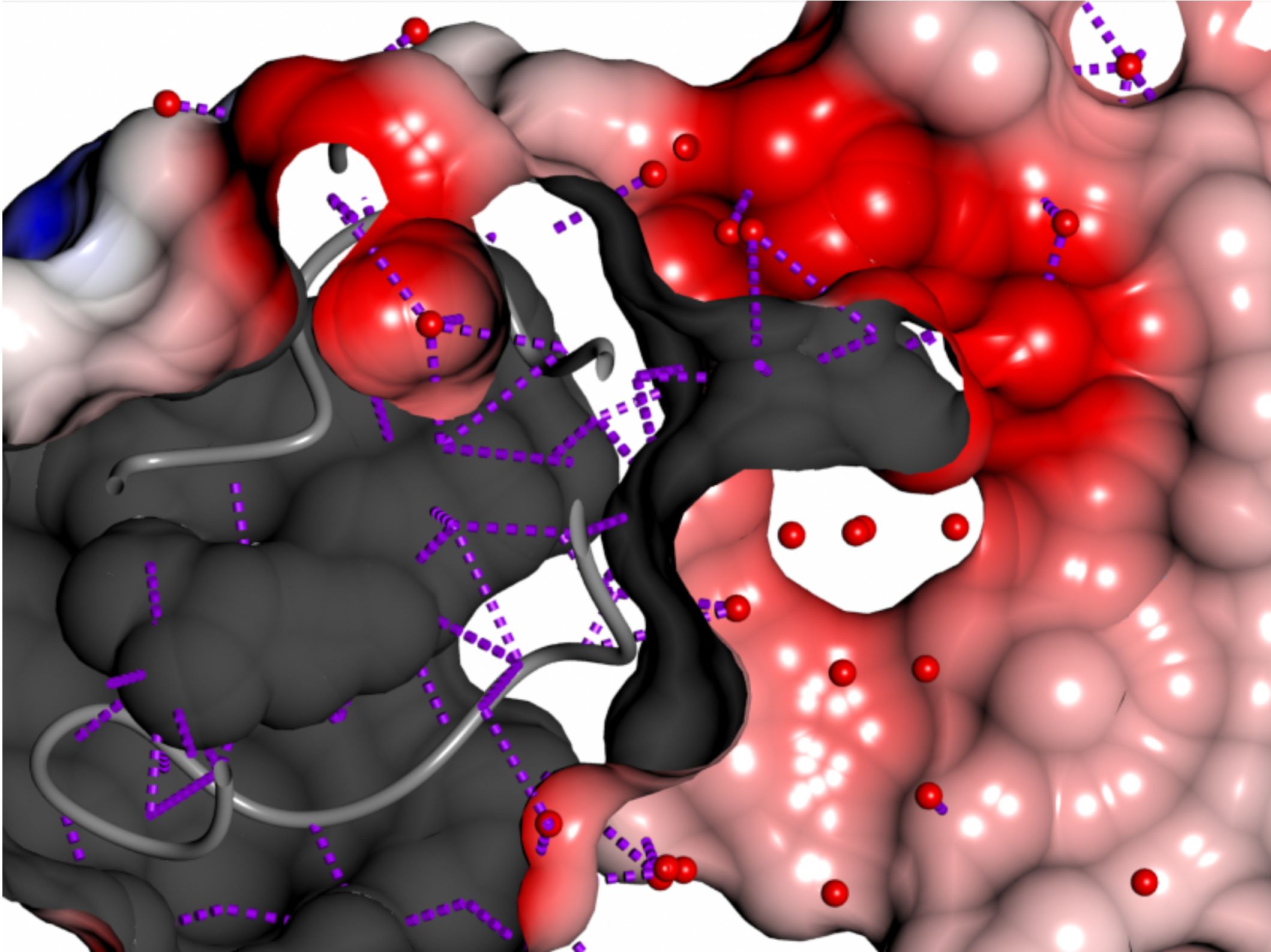
○ Rotation stereo with angle [6.00 ▲▼]

☑ Save status file
☑ View output

☐ Ray-traced shadows

💡 Edit lighting

☐ Save renderer input file (.rib)

☑ Ultra-smooth ribbons

☑ Colour inside of clipped surfaces black

(Help)   (Cancel) (Render)

Documentation

- Lots of user documentation is provided with the CCP4MG. The program contains a built in browser to view the documentation.

- The documentation is also available online at http://www.ysbl.york.ac.uk/~ccp4mg/

- CCP4MG also has help buttons on most GUIs to take the user to the correct position in the documentation.

CCP4MG version 2

- Version 2.0.1 of CCP4MG is now available from http://www.ysbl.york.ac.uk/~ccp4mg/

- This version is a considerable rewrite from version 1 using a modern GUI (and much other stuff!) toolkit Qt (http://qt.nokia.com/)

- CCP4MG should now be much faster, more stable, prettier and easier to develop.

- Available of Microsoft Windows, Apple Mac and Linux.

Online updates

- CCP4MG can be patched online via the menu item Tools->Check for updates

- Program can be configured to check for updates at startup (disabled by default).

- Currently not reliable on Microsoft Windows.

Acknowledgements

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- Eugene Krissenel
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