中央研究院
應用科學研究中心

Molecular graphics and analytics for biomolecule-drug interactions

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- **MolProbility**
  validate macromolecule

- **Chimera**
  molecular graphics

- **Ligplot and ligplot+**
  biomolecule-drug interactions

Basic Linux Commands

- **clear**
- **pwd** print working directory
- **ls** list
- **mkdir** make directory
- **cd** change directory
- **mv** move
- **rm** remove file
- **rmdir** remove directory
- **man** manual

- **cat**
- **more**
- **vi**
- **exit**

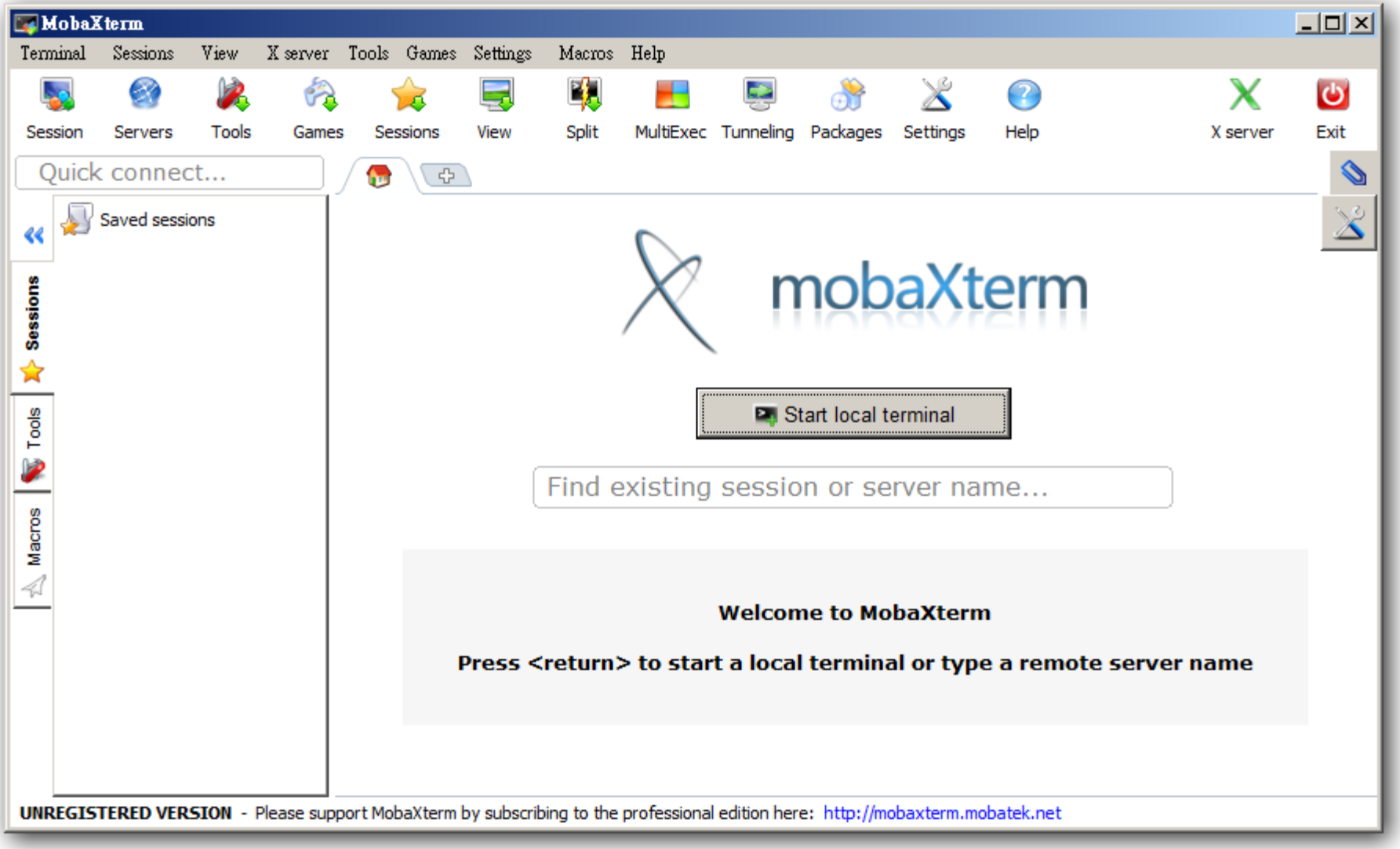
Use SSH/SCP clients to connect to a remote computer, and/or to transfer files between computers.

SSH/SCP client for windows:

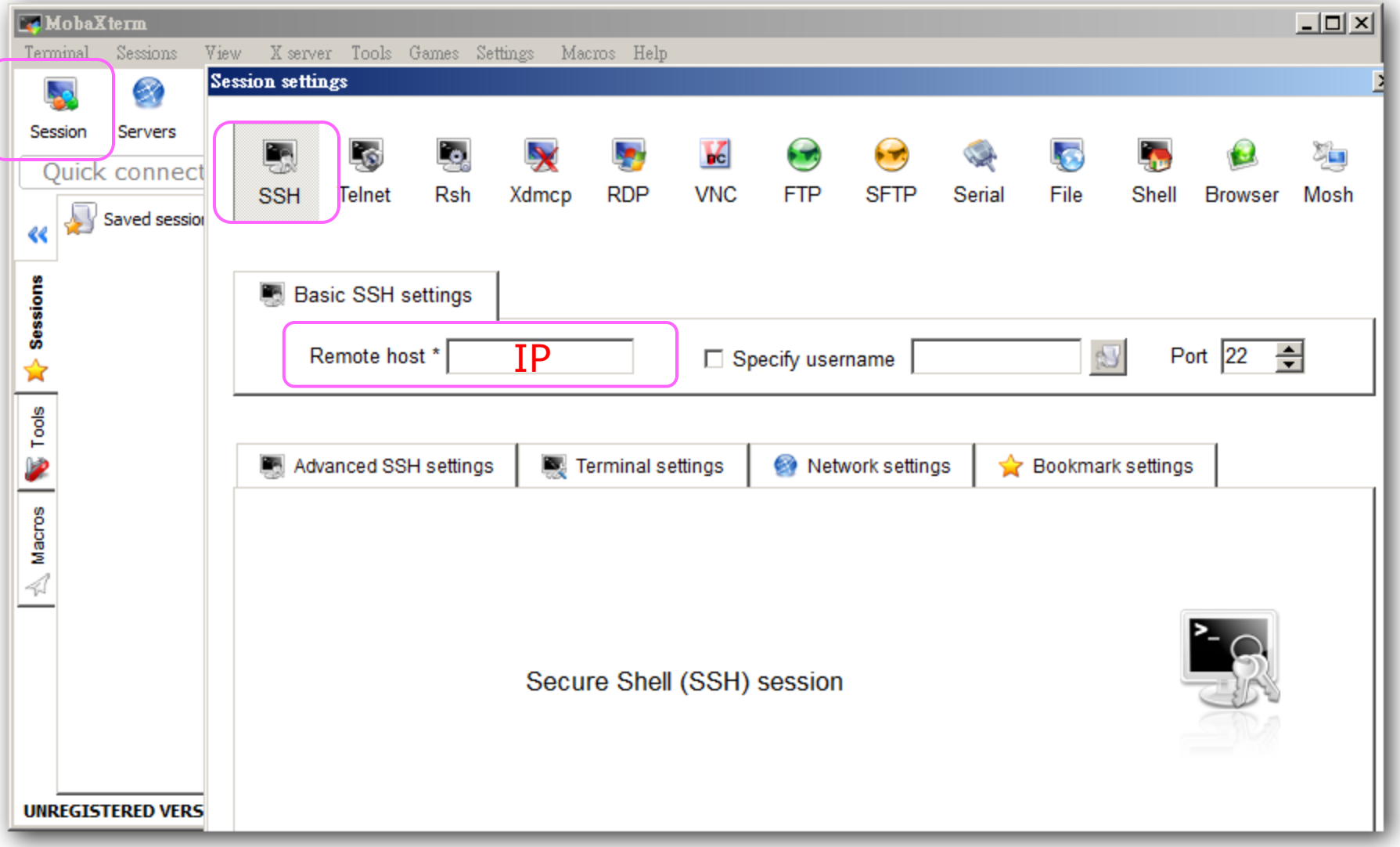
- putty https://www.putty.org/
  - Xming https://sourceforge.net/projects/xming/ (X Server)
- WinSCP https://winscp.net/eng/download.php

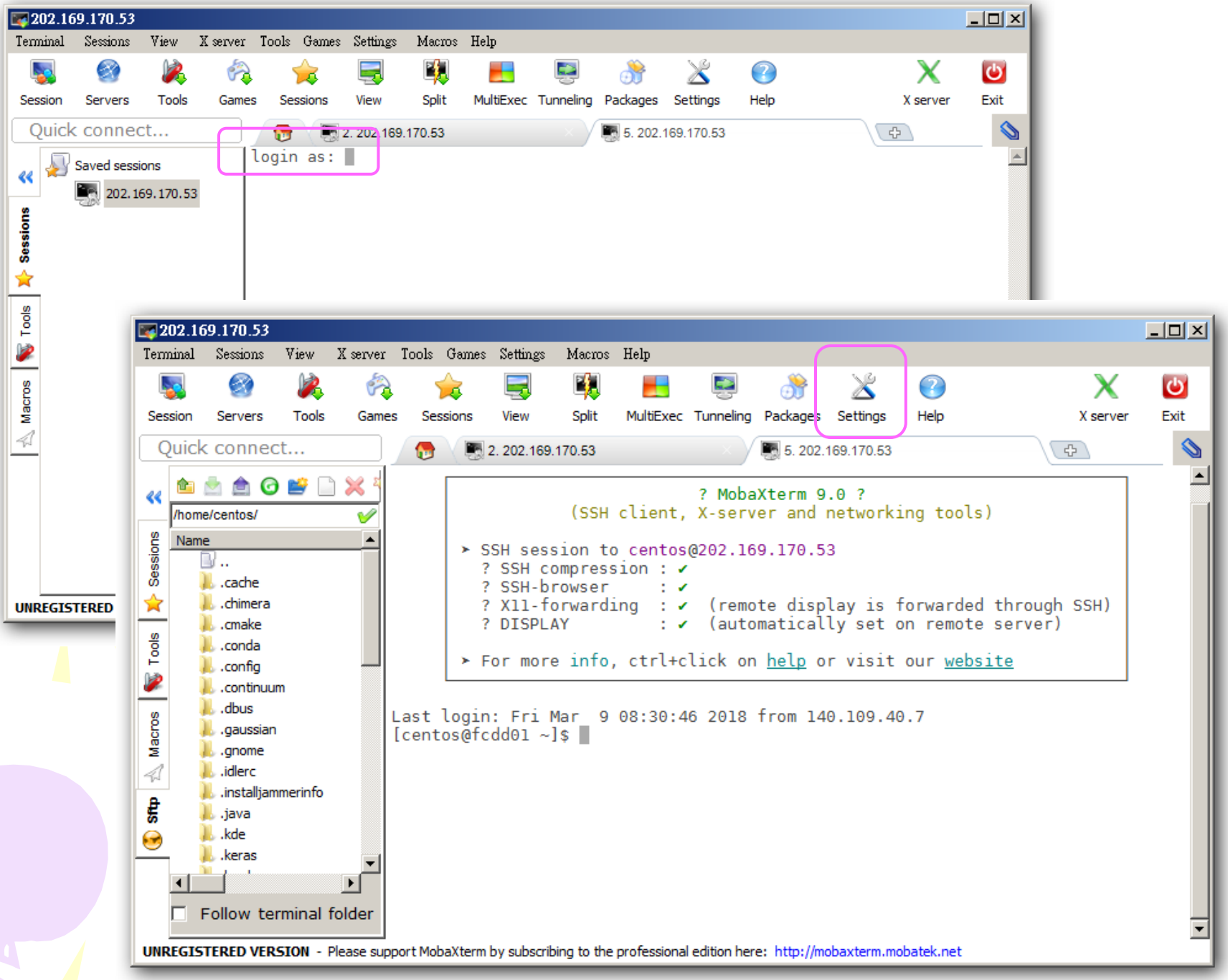
- MobaXterm http://mobaxterm.mobatek.net/download.html

Launching mobaXterm



Choose **Session** → **SSH**




202.169.170.53
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
2. 202.169.170.53
5. 202.169.170.53
Saved sessions
202.169.170.53
login as:
Sessions
Tools
Macros
UNREGISTERED
202.169.170.53
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
2. 202.169.170.53
5. 202.169.170.53
/home/centos/
Name
..
.cache
.chimera
.cmake
.conda
.config
.continuum
.dbus
.gaussian
.gnome
.idlerc
.installjammerinfo
.java
.kde
.keras
Follow terminal folder
? MobaXterm 9.0 ?
(SSH client, X-server and networking tools)
➤ SSH session to centos@202.169.170.53
? SSH compression : ✔
? SSH-browser : ✔
? X11-forwarding : ✔ (remote display is forwarded through SSH)
? DISPLAY : ✔ (automatically set on remote server)
➤ For more info, ctrl+click on help or visit our website
Last login: Fri Mar 9 08:30:46 2018 from 140.109.40.7
[centos@fcdd01 ~]$
Sessions
Tools
Macros
Sftp
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: http://mobaxterm.mobatek.net

Display Xterm in Mac

Create a file "config" under "~/.ssh/"
$ vi config

```
-----------------------------------
Host username
Hostname 123.123.123.123
User=login_id
ForwardX11 yes
-----------------------------------
```

Then, login with the following comment:
$ ssh –Y *username@ip_address*

MolProbility

- all-atom structure validation for macromolecular crystallography

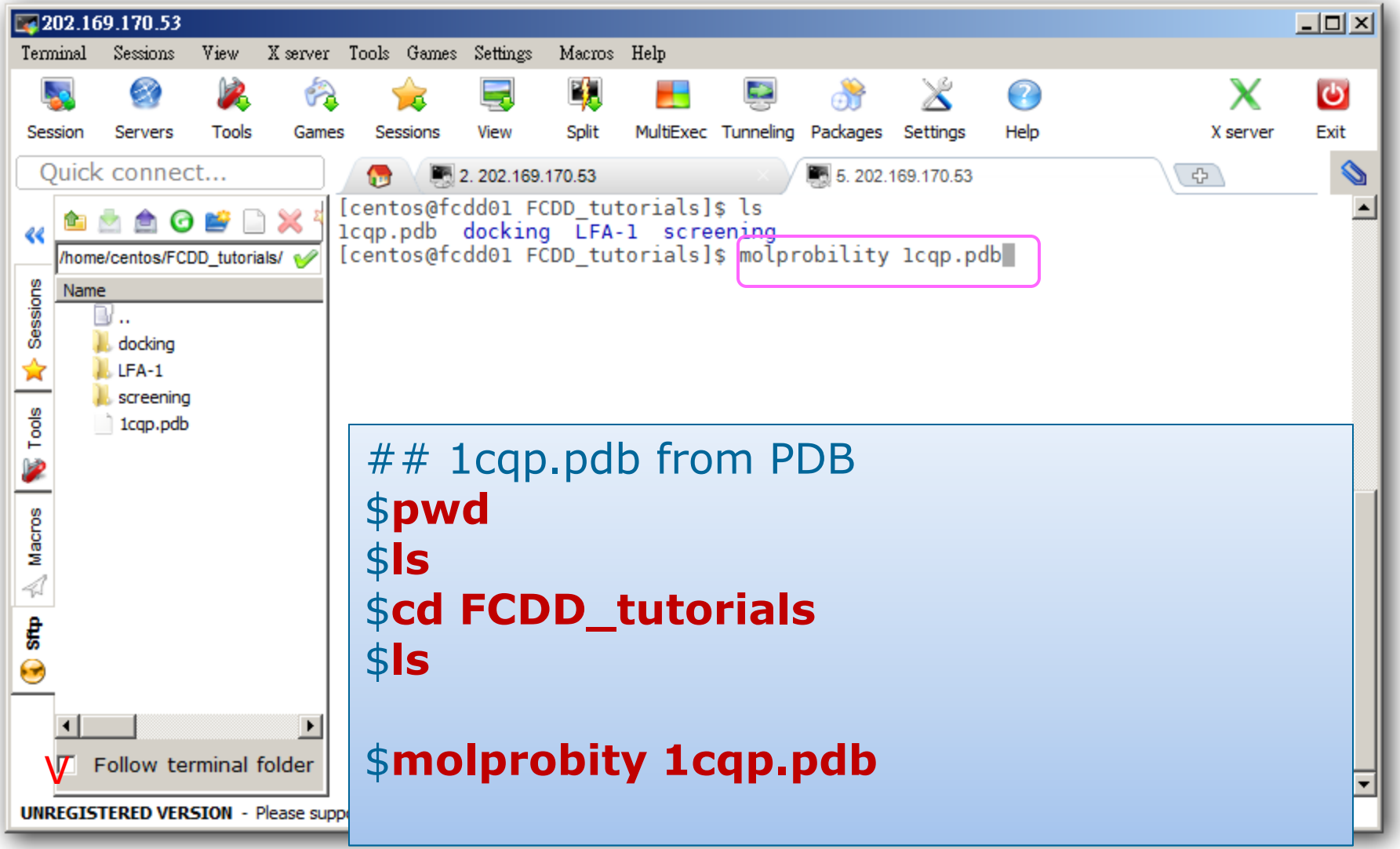
- Server

  http://molprobity.biochem.duke.edu/

- Standalone program

  https://github.com/rlabduke/MolProbity

  A standalone version was installed.



1cqp.pdb from PDB

$**pwd**

$**ls**

$**cd FCDD_tutorials**

$**ls**

$**molprobity 1cqp.pdb**

MolProbity: structure validation

Web service for all-atom contact, conformation, & geometry analysis of x-ray or NMR models, with automated correction of Asn/Gln/His flips. As a structure user, you can evaluate reliability of the parts you care about.

Uploaded PDB file as 1cqp.pdb

Your file from http://www.pdb.org/ was uploaded as 1cqp.pdb.

- This compound is identified as **CRYSTAL STRUCTURE ANALYSIS OF THE COMPLEX LFA-1 (CD11A) I-DO LOVASTATIN AT 2.6 A RESOLUTION**
- This structure was solved by X-RAY DIFFRACTION.
- This structure was solved at 2.60 Å resolution.
- 2 chain(s) is/are present [1 unique chain(s)]
- A total of 364 residues are present.
- Protein mainchain and sidechains are present.
- No explicit hydrogen atoms are included.
- 90 hetero group(s) is/are present.
- Refinement was carried out in X-PLOR 3.851.
- R = 0.190; Rfree = 0.257
- 0 PDBv2.3 atoms were found. Proceeding assuming PDBv3 formatted file.

Continue >

Main page

Duke Biochemistry
Duke University School of Medicine

Main page
About hydrogens
Evaluate X-ray
Evaluate NMR
Fix up structure
Work with kins

View & download files
Lab notebook
Feedback & bugs
Site map

Save session
Log out

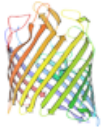
You are using 0% of your 200 Mb of disk space.

SUGGESTED TOOLS (ALL TOOLS)

Due to the parameter adjustments to hydrogen bondlengths and van der Waals radii, the current default behavior for MolProbity is to remove hydrogens, if they are present, before analysis. Please re-add hydrogens using the "Add hydrogens" option below, where you will have the option to choose either the default electron-cloud position hydrogens (i.e. for crystal structures) or nuclear-position hydrogens (i.e. for neutron-diffraction structures or for NMR structures).

Currently working on: **1cqp.pdb**

Add hydrogens


Make simple kinemages


Edit PDB file


Downgrade file to PDBv2.3 format (for download only)


Fill gaps in protein backbone with JiffiLoop (beta test)


Analyze geometry without all-atom contacts

Job is running...

- ✓ Do bond length and angle geometry analysis (`mp_geo`)
- ✓ Do Ramachandran analysis and make plots (`ramalyze`) - preview kinemage | PDF
- ✓ Do rotamer analysis (`rotalyze`)
- ✓ Do Cβ deviation analysis and make kins (`cbetadev`) - preview
- ✓ Do cis-peptide analysis (`omegalyze`)
- ✓ Do CaBLAM analysis (`cablam_validate`)
- ✓ Create multi-criterion chart - preview
- ♻ Create multi-criterion kinemage

Your job has been running for 14 seconds.
If this page doesn't update after 5 seconds, click here.
If needed, you can abort this job.

Analysis output: geometry for 1cqp.pdb

Summary statistics

Protein Geometry	Poor rotamers	13	4.01%	Goal: <0.3%
	Favored rotamers	287	88.58%	Goal: >98%
	Ramachandran outliers	4	1.11%	Goal: <0.05%
	Ramachandran favored	333	92.50%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 2998	0.00%	Goal: 0%
	Bad angles:	2 / 4040	0.05%	Goal: <0.1%
Peptide Omegas	Cis Prolines:	2 / 8	25.00%	Expected: ≤1 per chain, or ≤5%
Low-resolution Criteria	CaBLAM outliers	7	1.96%	Goal: <1.0%
	CA Geometry outliers	5	1.40%	Goal: <0.5%

In the two column results, the left column gives the raw count, right column gives the percentage.

Multi-criterion visualizations

Multi-criterion kinemage

View in KiNG | Download (276 Kb)

Multi-criterion chart

View (492 Kb)

Single-criterion visualizations

- **Ramachandran plot kinemage** (428 Kb): View in KiNG | Download
- **Ramachandran plot PDF** (1.7 Mb): View
- **Cβ deviation scatter plot** (27 Kb): View in KiNG | Download

Continue >

Viewing 1cqp-multi.table

MOLPROBITY

Duke Biochemistry
Duke University School of Medicine

When finished, you should close this window.

Hint: Use File | Save As... to save a copy of this page.

Protein Geometry	Poor rotamers	13	4.01%	Goal: <0.3%
	Favored rotamers	287	88.58%	Goal: >98%
	Ramachandran outliers	4	1.11%	Goal: <0.05%
	Ramachandran favored	333	92.50%	Goal: >98%
	Cβ deviations >0.25Å	0	0.00%	Goal: 0
	Bad bonds:	0 / 2998	0.00%	Goal: 0%
	Bad angles:	2 / 4040	0.05%	Goal: <0.1%
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	CA Geometry outliers	5	1.40%	Goal: <0.5%

In the two column results, the left column gives the raw count, right column gives the percentage.

#	Alt	Res	High B	Ramachandran	Rotamer	Cβ deviation	CaBLAM	Bond lengths	Bond angles	Cis Peptides
			Avg: 46.35	Outliers: 4 of 360	Poor rotamers: 13 of 324	Outliers: 0 of 348	Outliers: 32 of 357	Outliers: 0 of 364	Outliers: 2 of 364	Non-Trans: 2 of 362
A 128		GLY	60.46	-	-					
A 129		ASN	46.54	Favored (54.86%) General / -121.9,134.7	Favored (66.4%) *m* chi angles: 280.1,34					
A 130		VAL	29.02	Favored (55.92%) Ile or Val / -120.7,118.3	Favored (22.8%) chi angles: 186.4					
A 131		ASP	21.27	Favored (16.45%) General / -101.7,105.5	Favored (20%) *m* chi angles: 272.2,0					
A 132		LEU	28.68	Favored (51.28%) General / -106.1,125.7	Favored (3.8%) chi angles: 194.3,14					
A 133		VAL	19.95	Favored (68.36%) Ile or Val / -111.0,126.4	Favored (57.9%) chi angles: 180.2					
A 134		PHE	18.58	Favored (32.04%) General / -92.7,119.4	Favored (47.8%) *m* chi angles: 287.8,11					
A 135		LEU	22.33	Favored (5.06%) General / -106.5,94.3	Favored (16.9%) chi angles: 183.9,4					
A 136		PHE	17.83	Favored (39.59%) General / -100.2,136.8	Favored (2.1%) *p* chi angles: 65.8,115					
A 160		LYS	25.81	Favored (79.35%) General / -64.6,-47.3	Favored (33.1%) *tptt* chi angles: 195.4,62.2,178.2,171.3	0.03Å	Favored (84.242%)	-	-	-
A 161		LEU	20.69	Allowed (1.99%) General / -88.2,24.0	Favored (40.5%) *mt* chi angles: 307,183.1	0.03Å	Favored (15.108%)	-	-	-
A 162		SER	26.32	Favored (41.72%) General / -74.8,146.7	Favored (81.8%) *p* chi angles: 62	0.02Å	Favored (14.202%)	-	-	-
A 163		ASN	32.93	Favored (10.51%) General / 66.7,16.9	Favored (70.8%) *m-40* chi angles: 304.7,305.1	0.04Å	Favored (11.937%)	-	-	-
A 164		THR	20.9	Allowed (1.11%) General / -98.0,-164.2	Favored (52%) *p* chi angles: 65.4	0.04Å	Favored (15.536%)	-	-	-
A 165		SER	52.41	Favored (59.19%) General / -86.2,-5.4	Favored (61.7%) *m* chi angles: 293.8	0.12Å	Favored (5.28%)	-	-	-
A 166		TYR	32.36	Favored (36.65%) General / -79.2,135.0	Favored (97.7%) *m-80* chi angles: 294.7,90.7	0.03Å	Favored (28.022%)	-	-	-
A 167		GLN	28.69	Favored (47.95%) General / -118.1,141.9	OUTLIER (0.3%) chi angles: 237.3,190.7,5.5	0.14Å	Favored (68.792%) beta sheet	-	-	-
A 168		PHE	27.08	Favored (29.71%) General / -123.7,159.3	Favored (90.8%) *m-80* chi angles: 300.7,96.5	0.04Å	Favored (50.652%) beta sheet	-	-	-
A 169		ALA	20.6	Favored (28.01%) General / -151.4,148.4	-	0.07Å	Favored (48.127%) beta sheet	-	-	-
A 170		ALA	13.79	Favored (37.59%) General / -130.7,126.9	-	0.04Å	Favored (59.952%) beta sheet	-	-	-
A 171		VAL	15.27	Favored (71.92%) Ile or Val / -124.0,126.1	Favored (85%) *t* chi angles: 177.6	0.03Å	Favored (65.002%) beta sheet	-	-	-
A 172		GLN	21.83	Favored (34.77%) General / -97.9,138.7	Favored (53.8%) *tt0* chi angles: 191.1,183,357.8	0.07Å	Favored (61.427%) beta sheet	-	-	-
A 173		PHE	23.89	Favored (49.02%) General / -135.5,147.9	Favored (8.4%) *p90* chi angles: 84.2,280.3	0.07Å	Favored (17.706%) beta sheet	-	-	-
A 174		SER	20.81	OUTLIER (0.03)%) General / -156.4,-101.2	OUTLIER (0.2%) chi angles: 216.4	0.12Å	CaBLAM Disfavored (1.167%)	-	-	-
A 175		THR	27.91	Favored (10.02%) General / -89.9,-44.3	Favored (52.1%) *m* chi angles: 294.8	0.11Å	CA Geom Outlier (0.469%)	-	-	-
A 176		SER	46.66	Allowed (1.9%) General / -109.8,-171.7	Favored (3.5%) *t* chi angles: 197.9	0.06Å	CaBLAM Disfavored (2.547%)	-	-	-

$molprobity 1cqp.pdb

```
real    0m0.095s
user    0m0.056s
sys     0m0.040s
^time to make suitename kin


running mp_geo bond geometry

real    0m12.269s
user    0m11.976s
sys     0m0.293s
^time to run mp_geo for bond geometry


running clashscore
...in ecloud mode

real    0m5.345s
user    0m5.006s
sys     0m0.472s
^time for clashscore


[centos@fcdd01 FCDD_examples]$
```

$ls
$cd molprobity_1cqp
$ls

```
[centos@fcdd01 molprobity_1cqp]$ ls
1cqp.cablam     1cqp.geom          1cqp.rama.kin       1cqp.suitename_midpoint
1cqp.cbdev      1cqp.geom.sorted   1cqp.rama.pdf       1cqp.suitestring
1cqp.cbdev.kin  1cqp.omega         1cqp.rota           1cqp.trim.pdb
1cqp.clash      1cqp.pucker        1cqp.suitename      thumbnail.kin
1cqp.FH.pdb     1cqp.rama          1cqp.suitename.kin
[centos@fcdd01 molprobity_1cqp]$
```

```
[centos@fcdd01 molprobity_1cqp]$ ls
1cqp.cablam      1cqp.geom          1cqp.rama.kin        1cqp.suitename_midpoint
1cqp.cbdev       1cqp.geom.sorted   1cqp.rama.pdf        1cqp.suitestring
1cqp.cbdev.kin   1cqp.omega         1cqp.rota            1cqp.trim.pdb
1cqp.clash       1cqp.pucker        1cqp.suitename       thumbnail.kin
1cqp.FH.pdb      1cqp.rama          1cqp.suitename.kin
[centos@fcdd01 molprobity_1cqp]$
```

$cd molprobity_1cqp
$ls

$vi 1cqp.rama

$grep "SUMMARY:" 1cqp.rama

$grep "OUTLIER" 1cqp.rama

$grep "OUTLIER" 1cqp.rota

Vi Editor

Window motions

<ctrl>d	Scroll down (half a screen)
<ctrl>u	Scroll up (half a screen)
<ctrl>f	Page forward
<ctrl>b	Page backward
/string	Search forward
?string	Search backward
<ctrl>l	Redraw screen
<ctrl>g	Display current line number and file information

File management commands

:w *name*	Write edit buffer to file *name*
:wq	Write to file and quit
:q!	Quit without saving changes
ZZ	Same as :wq

Input commands (end with Esc)

a	Append after cursor
i	Insert before cursor
o	Open line below
O	Open line above
:r *file*	Insert *file* after current line

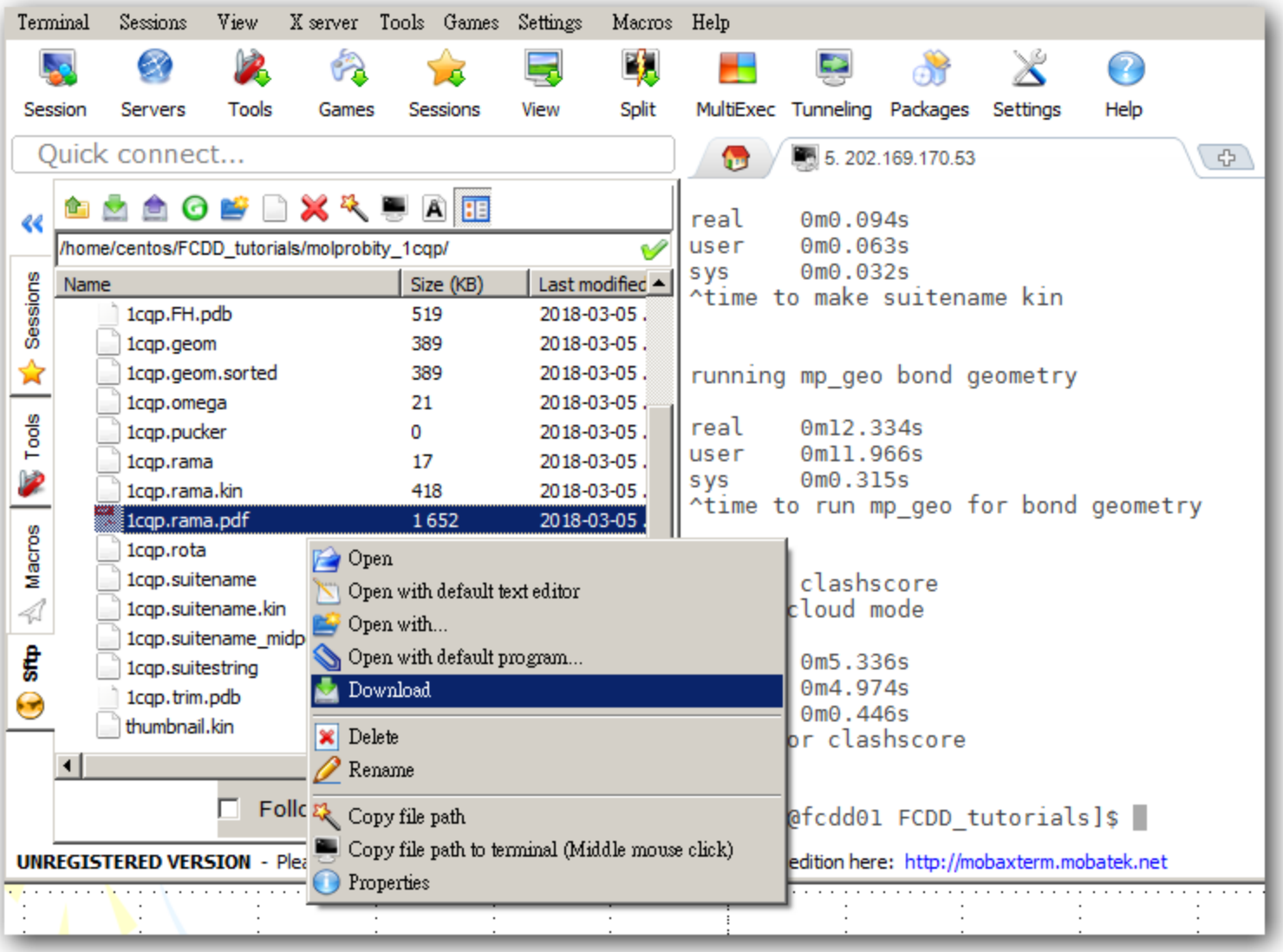
Any of these commands leaves vi in input mode until you press **Esc**. Pressing the **RETURN** key will not take you out of input mode.

Deletion commands

dd or *n*dd	Delete *n* lines to general buffer
dw	Delete word to general buffer
d*n*w	Delete *n* words
d)	Delete to end of sentence
db	Delete previous word
D	Delete to end of line
x	Delete character

http://www.atmos.albany.edu/daes/atmclasses/atm350/vi_cheat_sheet.pdf

download 1cqp.rama.pdf to local computer



Protein Backbone Structures and Ramachandran Plot

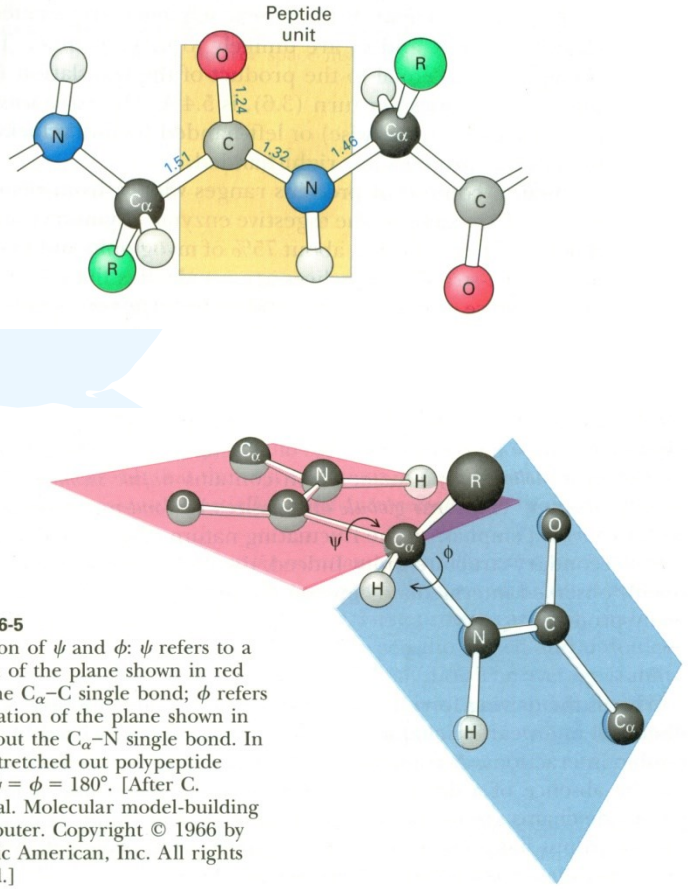


Figure 16-5
Definition of ψ and ϕ: ψ refers to a rotation of the plane shown in red about the C_α–C single bond; ϕ refers to a rotation of the plane shown in blue about the C_α–N single bond. In a fully stretched out polypeptide chain, $\psi = \phi = 180°$. [After C. Levinthal. Molecular model-building by computer. Copyright © 1966 by Scientific American, Inc. All rights reserved.]

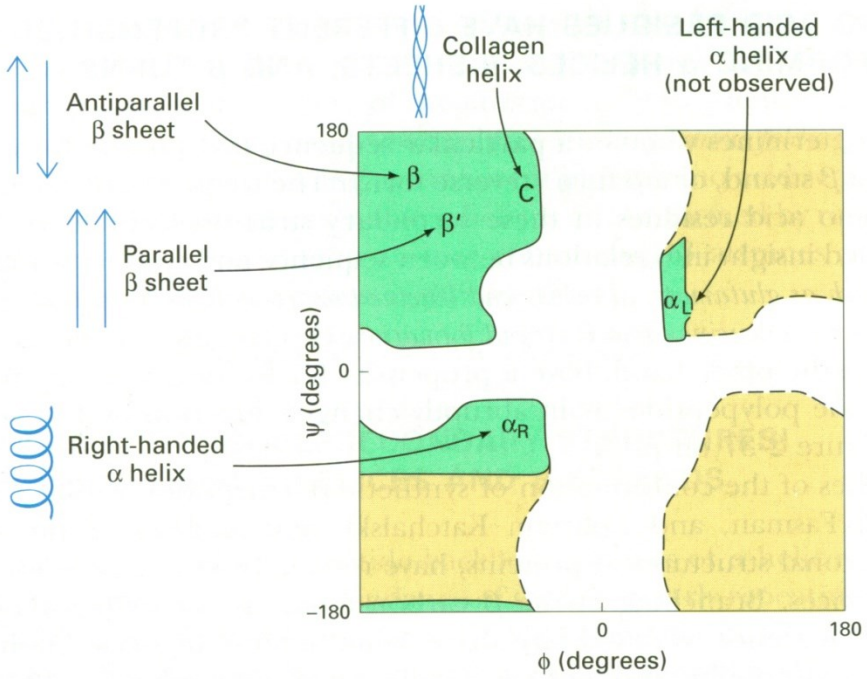
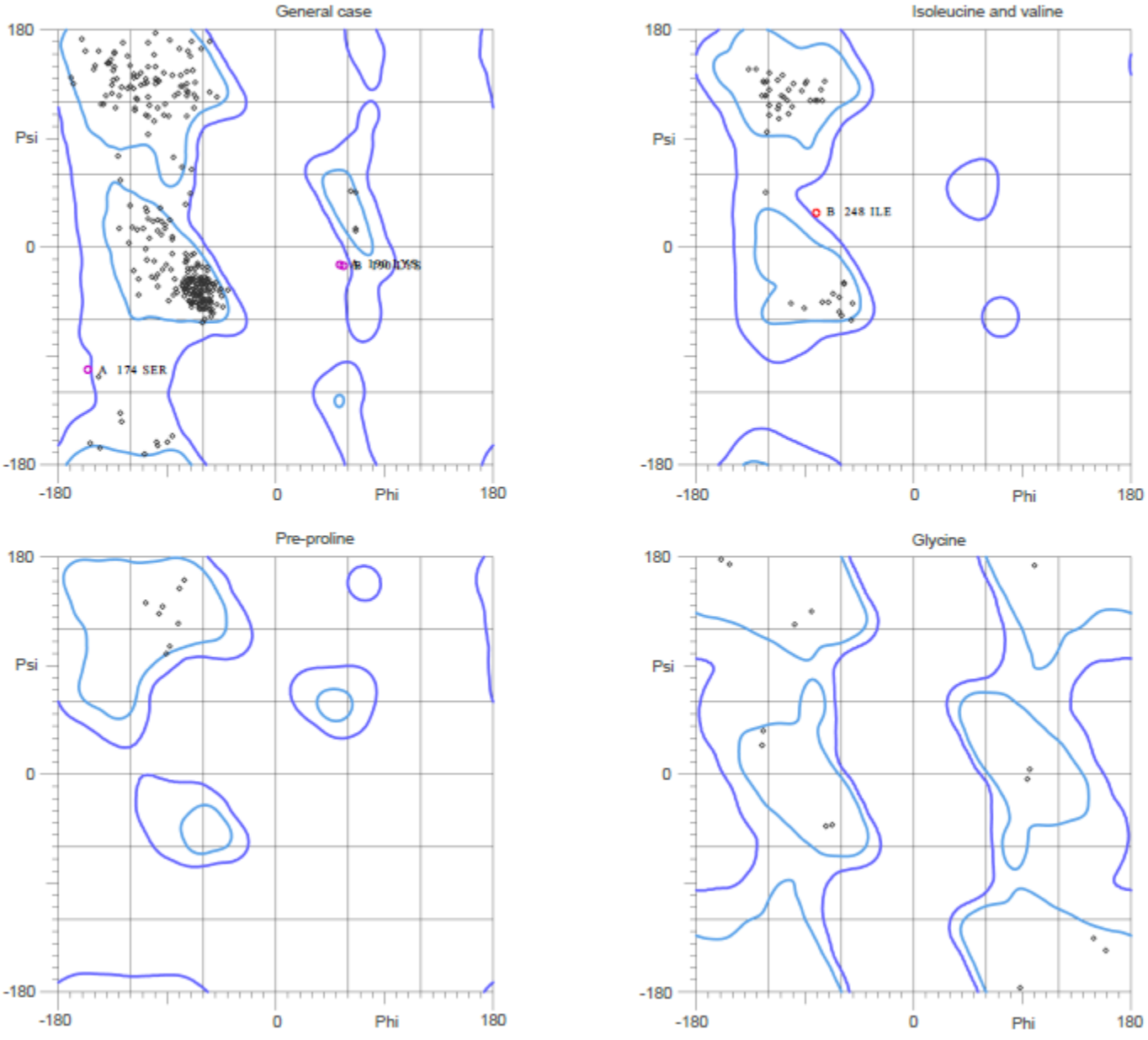
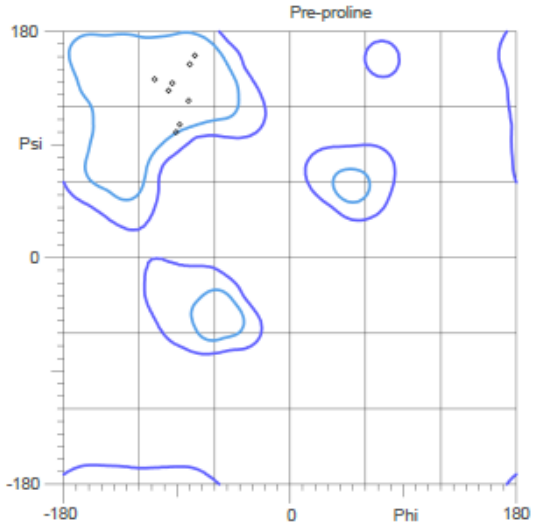


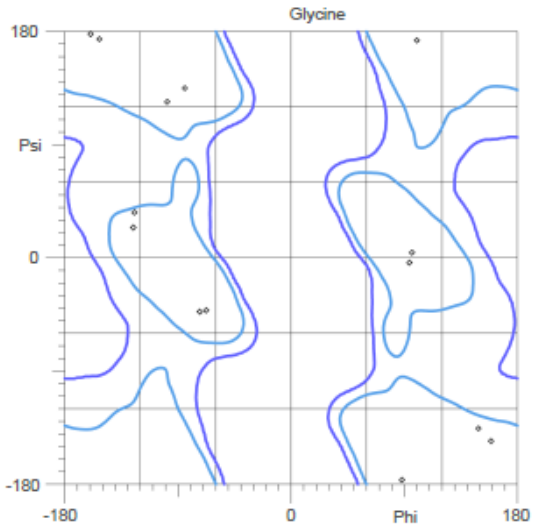
Figure 16-6
Ramachandran plot showing allowed values of ϕ and ψ for L-alanine residues (green regions). Additional conformations are accessible to glycine (yellow regions) because it has a very small side chain.

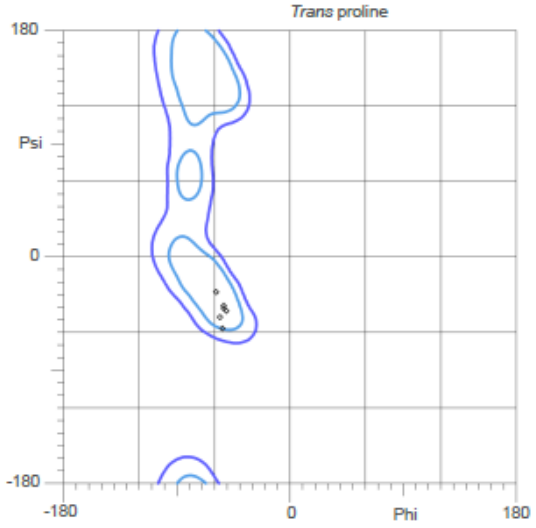
MolProbity Ramachandran analysis

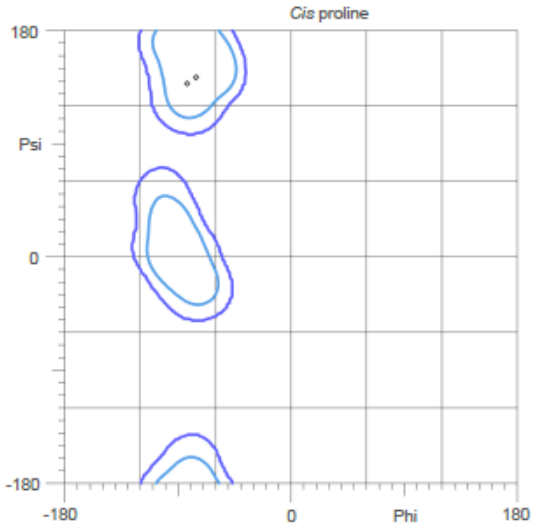
1cqp.FH.pdb, model 1











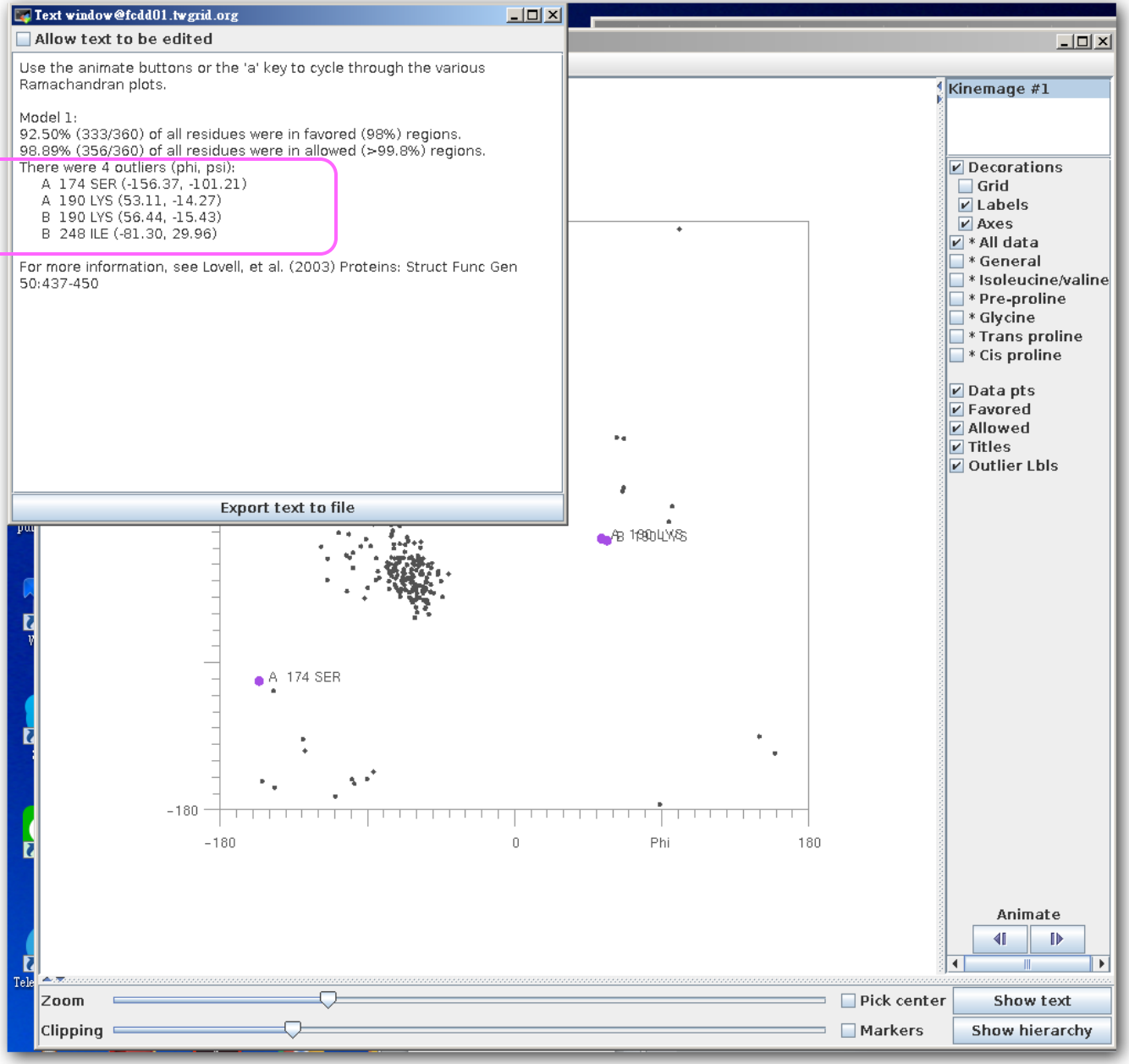
92.5% (333/360) of all residues were in favored (98%) regions.
98.9% (356/360) of all residues were in allowed (>99.8%) regions.

There were 4 outliers (phi, psi):
A 174 SER (-156.4, -101.2)
A 190 LYS (53.1, -14.3)
B 190 LYS (56.4, -15.4)
B 248 ILE (-81.3, 30.0)

http://kinemage.biochem.duke.edu

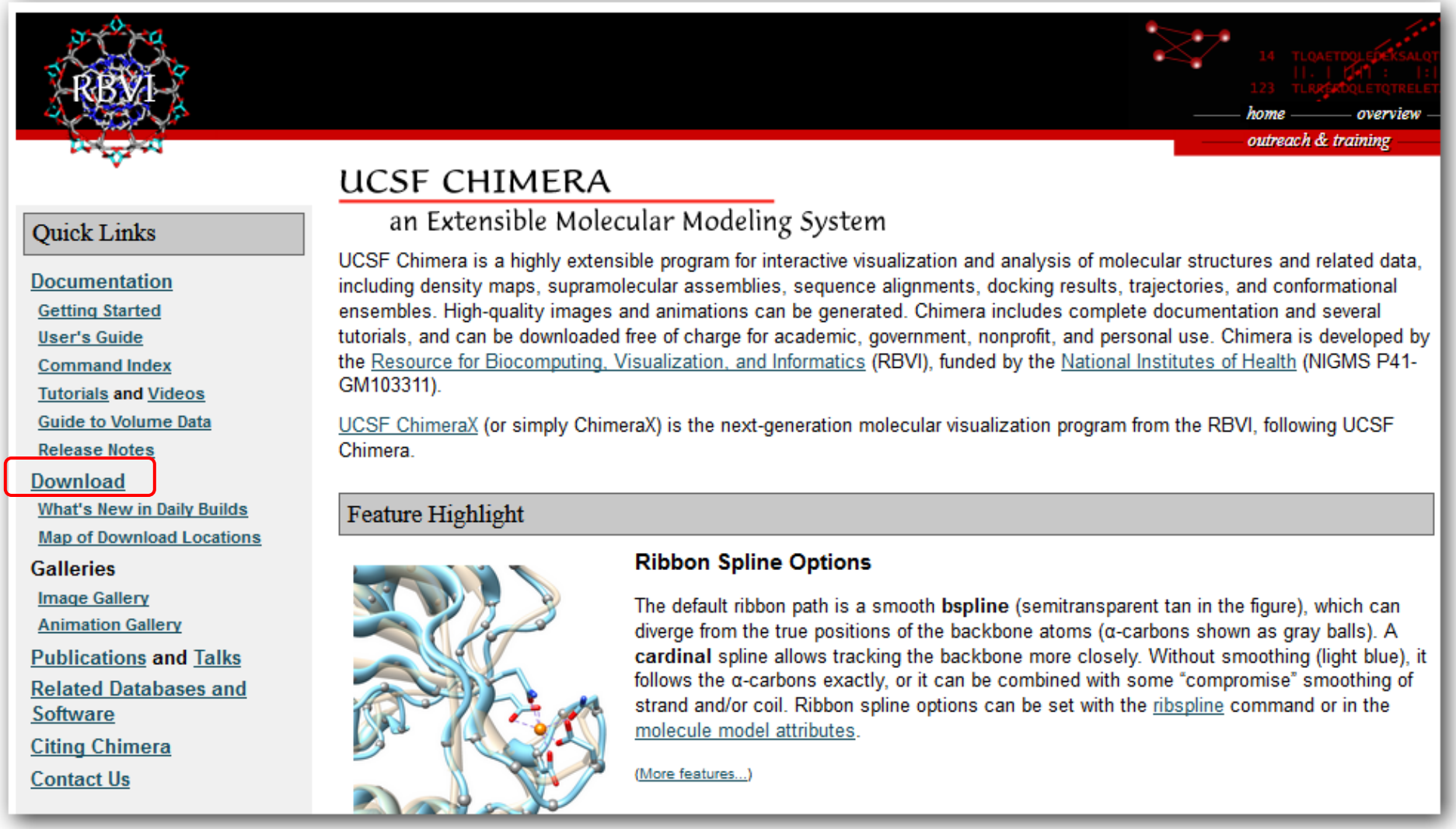
Lovell, Davis, et al. Proteins 50:437 (2003)

$king 1cqp.rama.kin

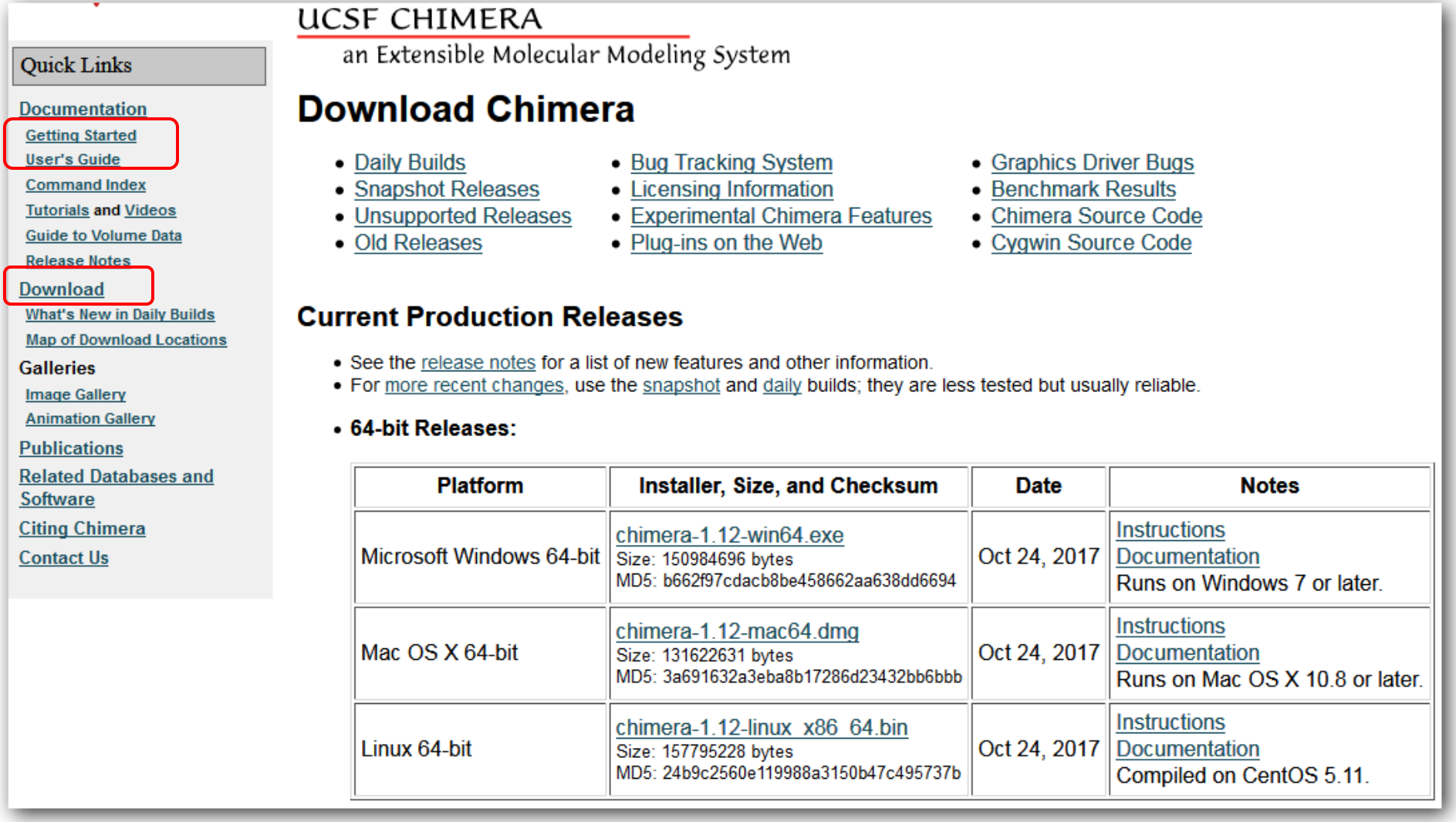


UCSF CHIMERA

https://www.cgl.ucsf.edu/chimera/



https://www.cgl.ucsf.edu/chimera/download.html



UCSF CHIMERA

an Extensible Molecular Modeling System

Quick Links

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- Licensing Information
- Experimental Chimera Features
- Plug-ins on the Web
- Graphics Driver Bugs
- Benchmark Results
- Chimera Source Code
- Cygwin Source Code

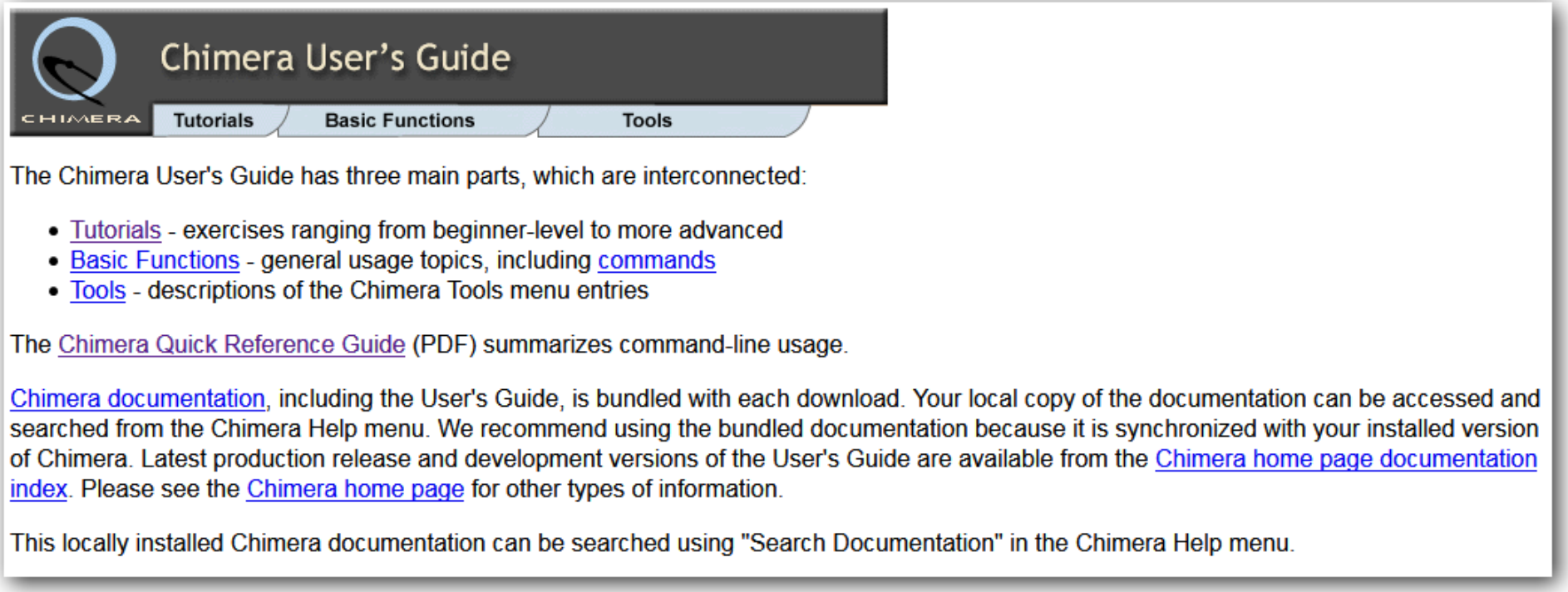
Current Production Releases

- See the release notes for a list of new features and other information.
- For more recent changes, use the snapshot and daily builds; they are less tested but usually reliable.

- **64-bit Releases:**

Platform	Installer, Size, and Checksum	Date	Notes
Microsoft Windows 64-bit	chimera-1.12-win64.exe Size: 150984696 bytes MD5: b662f97cdacb8be458662aa638dd6694	Oct 24, 2017	Instructions Documentation Runs on Windows 7 or later.
Mac OS X 64-bit	chimera-1.12-mac64.dmg Size: 131622631 bytes MD5: 3a691632a3eba8b17286d23432bb6bbb	Oct 24, 2017	Instructions Documentation Runs on Mac OS X 10.8 or later.
Linux 64-bit	chimera-1.12-linux_x86_64.bin Size: 157795228 bytes MD5: 24b9c2560e119988a3150b47c495737b	Oct 24, 2017	Instructions Documentation Compiled on CentOS 5.11.

https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/



Chimera User's Guide

CHIMERA | Tutorials | Basic Functions | Tools

The Chimera User's Guide has three main parts, which are interconnected:

- Tutorials - exercises ranging from beginner-level to more advanced
- Basic Functions - general usage topics, including commands
- Tools - descriptions of the Chimera Tools menu entries

The Chimera Quick Reference Guide (PDF) summarizes command-line usage.

Chimera documentation, including the User's Guide, is bundled with each download. Your local copy of the documentation can be accessed and searched from the Chimera Help menu. We recommend using the bundled documentation because it is synchronized with your installed version of Chimera. Latest production release and development versions of the User's Guide are available from the Chimera home page documentation index. Please see the Chimera home page for other types of information.

This locally installed Chimera documentation can be searched using "Search Documentation" in the Chimera Help menu.

Chimera User's Guide

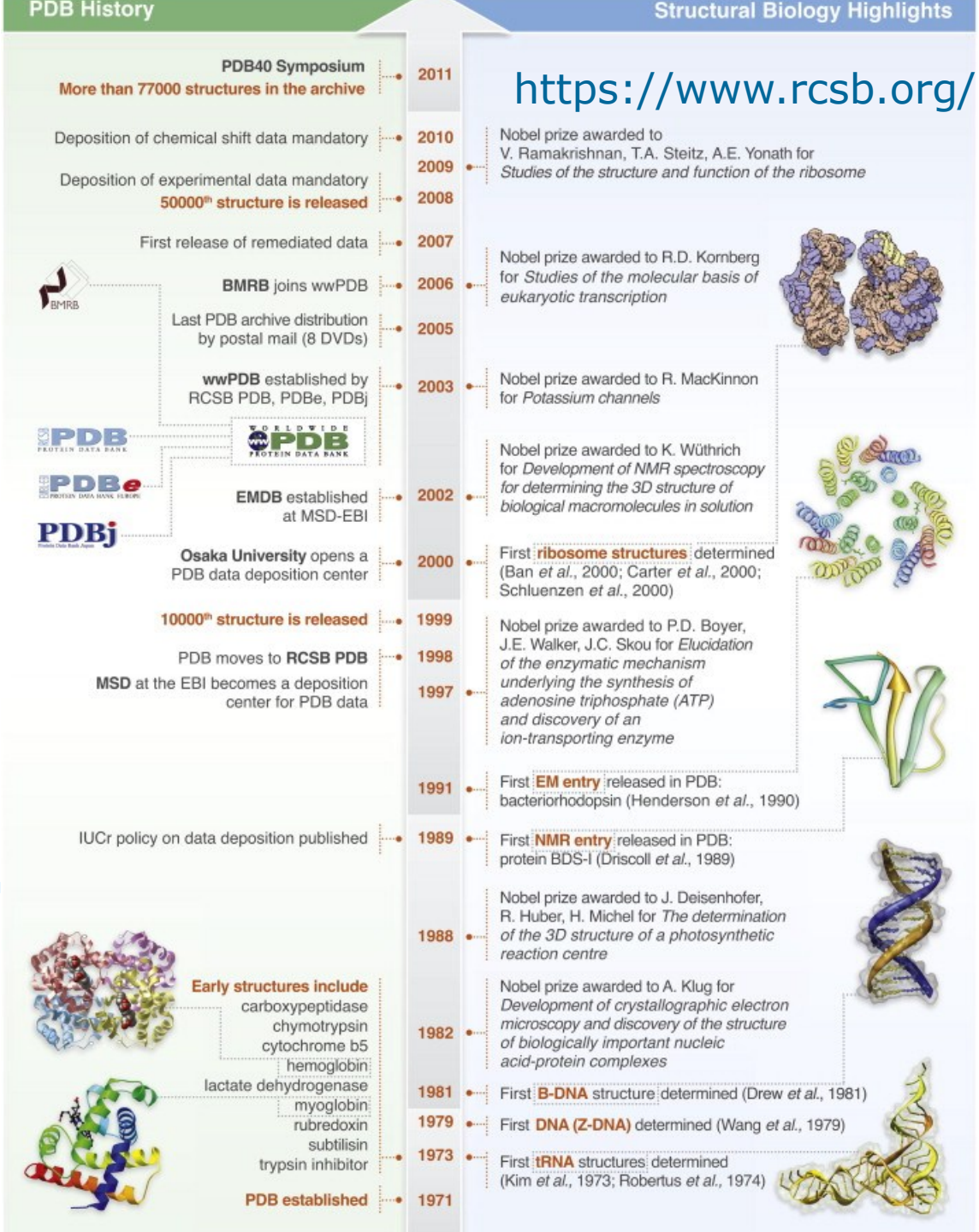
CHIMERA | Tutorials | Basic Functions | Tools

Tutorials Index

More tutorials are available at the Chimera web site.

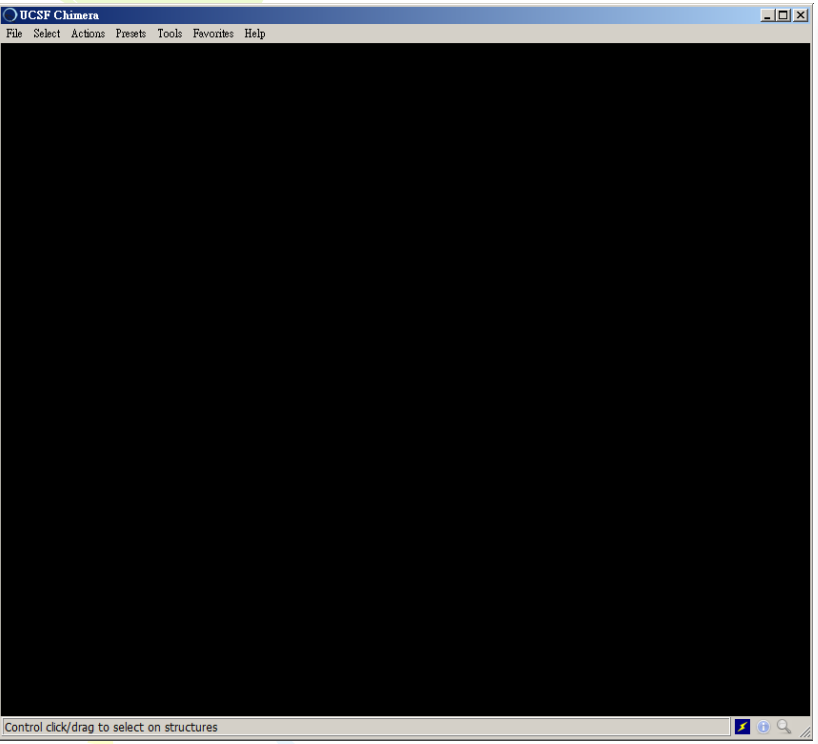
https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/tutorials/framepdbintro.html

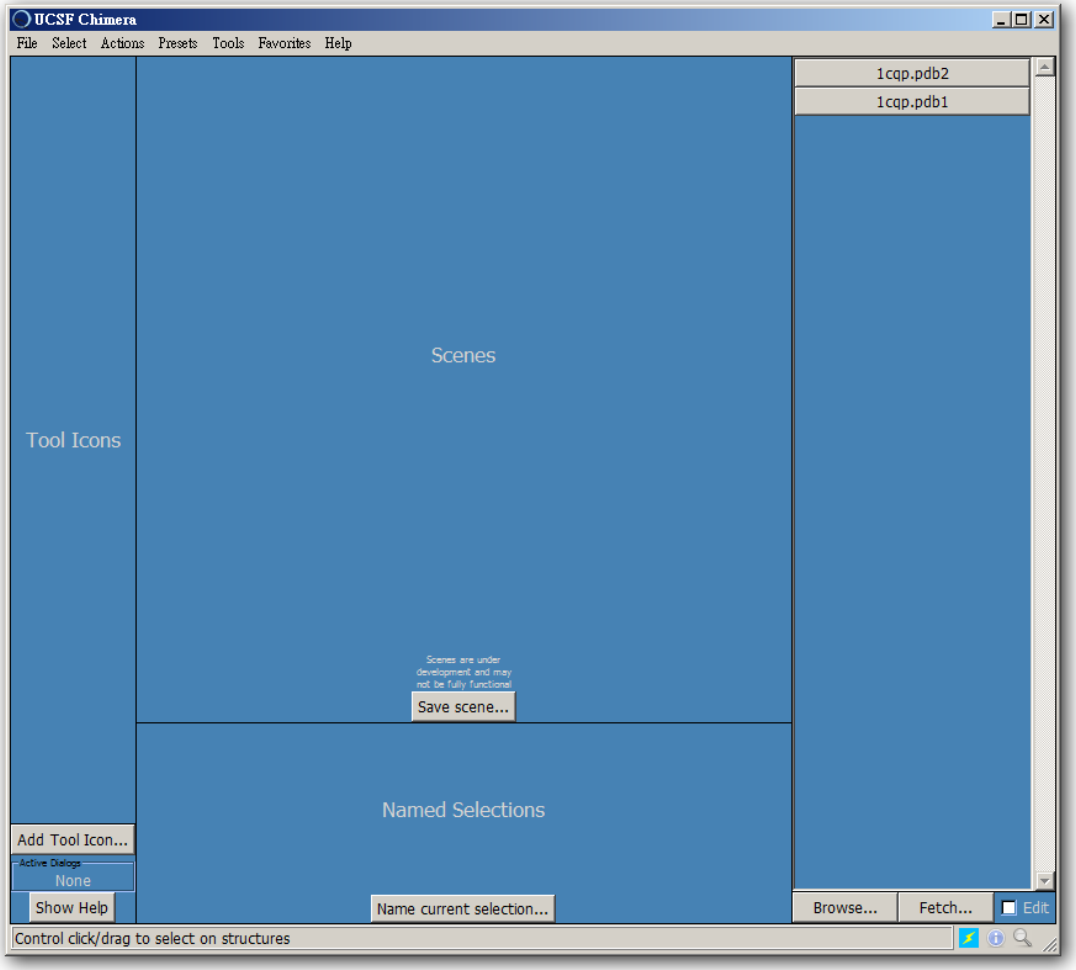
Protein Data Bank Format: Coordinate Section				
Record Type	**Columns**	**Data**	**Justification**	**Data Type**
ATOM	1-4	"ATOM"		character
	7-11[#]	Atom serial number	right	integer
	13-16	Atom name	left[*]	character
	17	Alternate location indicator		character
	18-20[§]	Residue name	right	character
	22	Chain identifier		character
	23-26	Residue sequence number	right	integer
	27	Code for insertions of residues		character
	31-38	X orthogonal Å coordinate	right	real (8.3)
	39-46	Y orthogonal Å coordinate	right	real (8.3)
	47-54	Z orthogonal Å coordinate	right	real (8.3)
	55-60	Occupancy	right	real (6.2)
	61-66	Temperature factor	right	real (6.2)
	73-76	Segment identifier[¶]	left	character
	77-78	Element symbol	right	character
79-80	Charge		character	
HETATM	1-6	"HETATM"		character
	7-80	same as ATOM records		

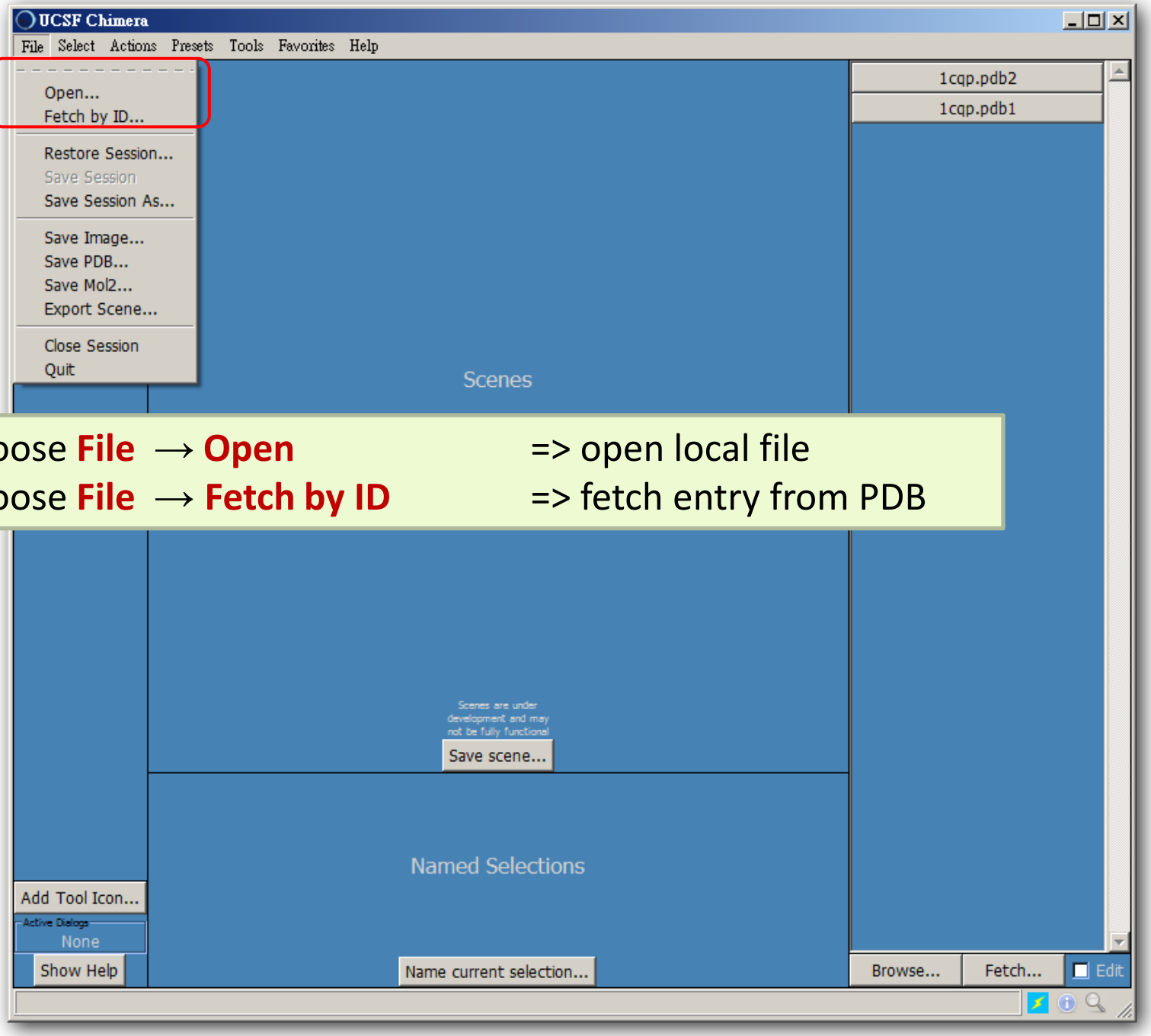


https://www.rcsb.org/pages/aboutus

Launching Chimera

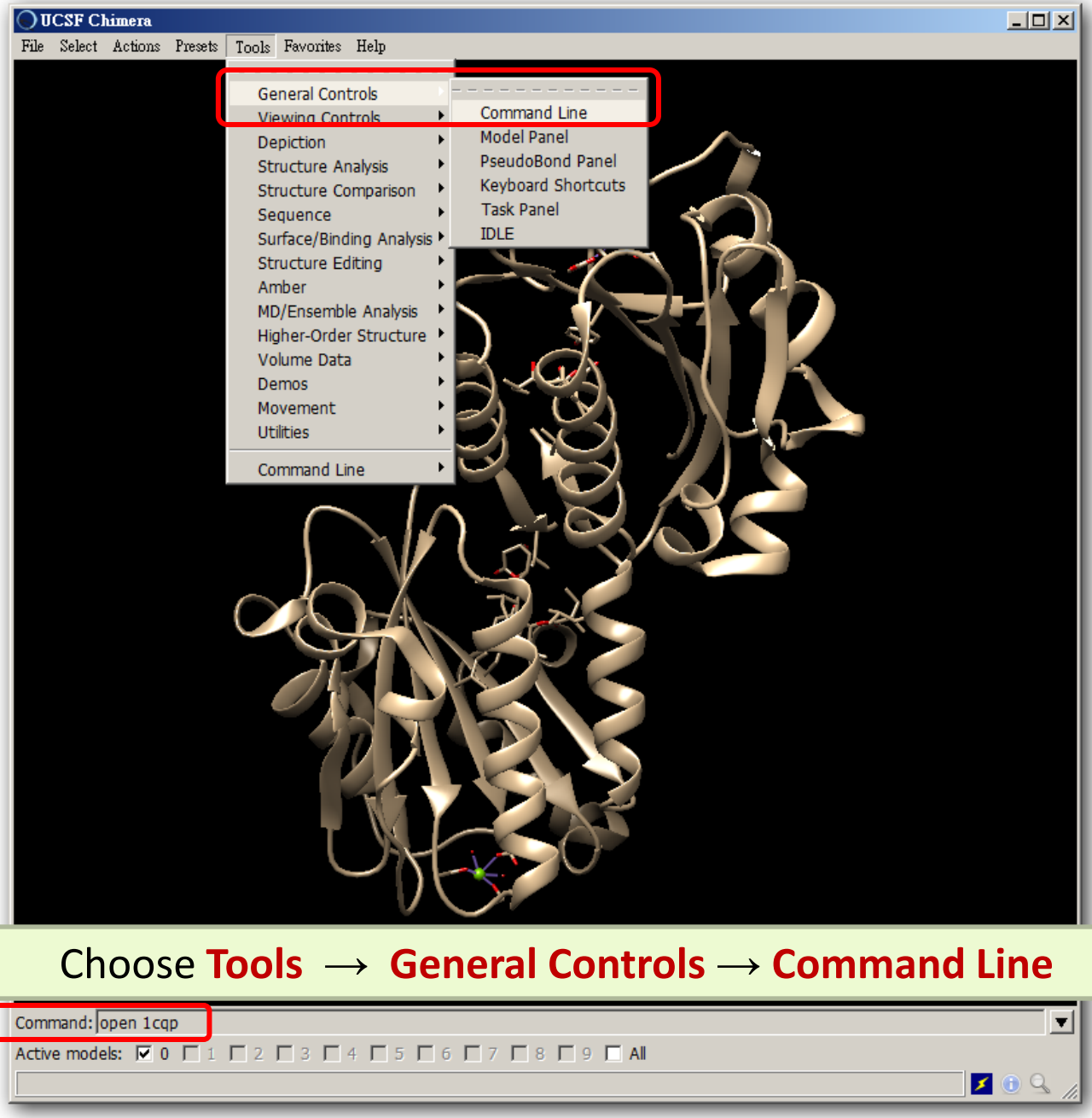






Choose **File** → **Open** => open local file

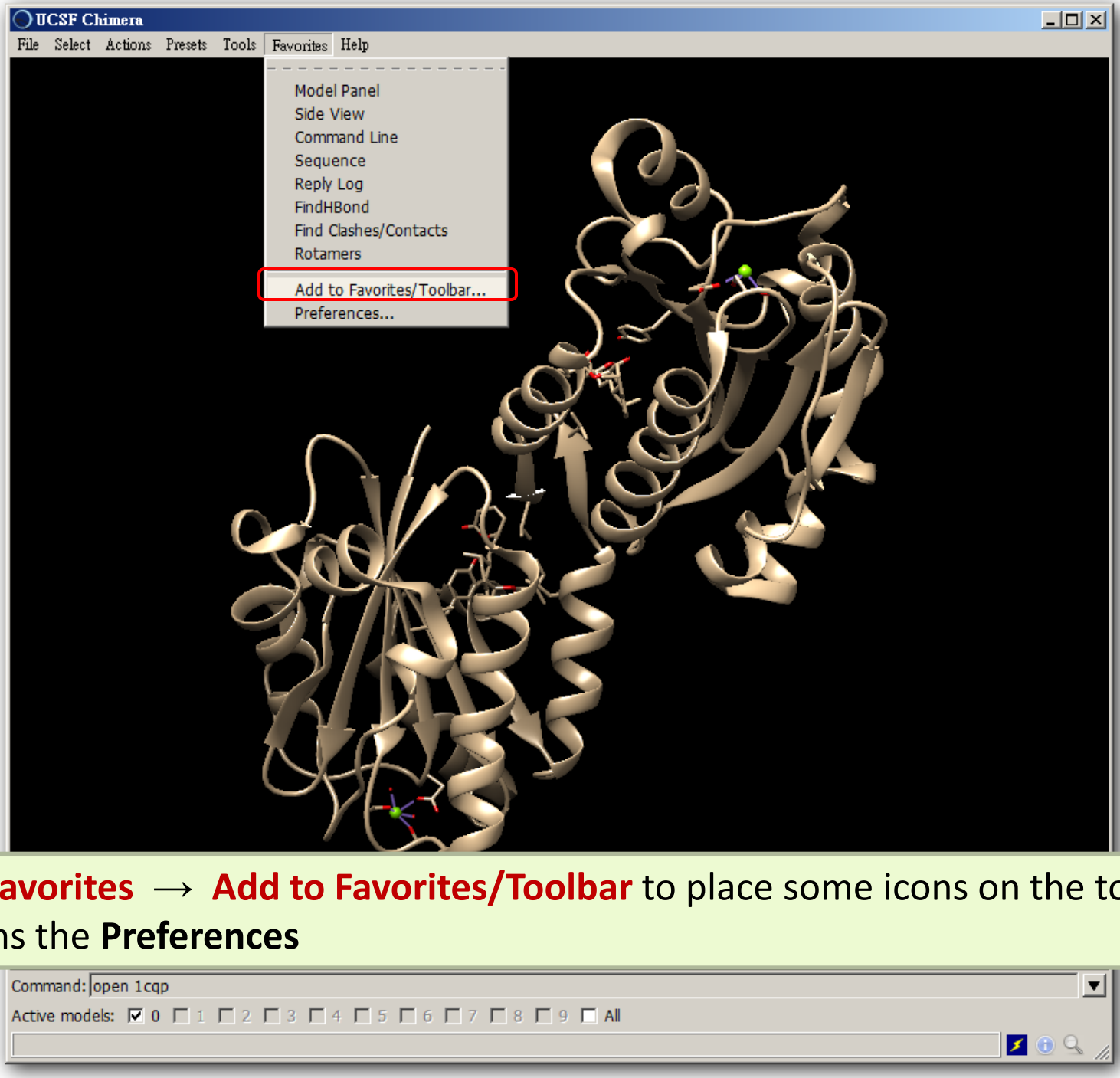
Choose **File** → **Fetch by ID** => fetch entry from PDB



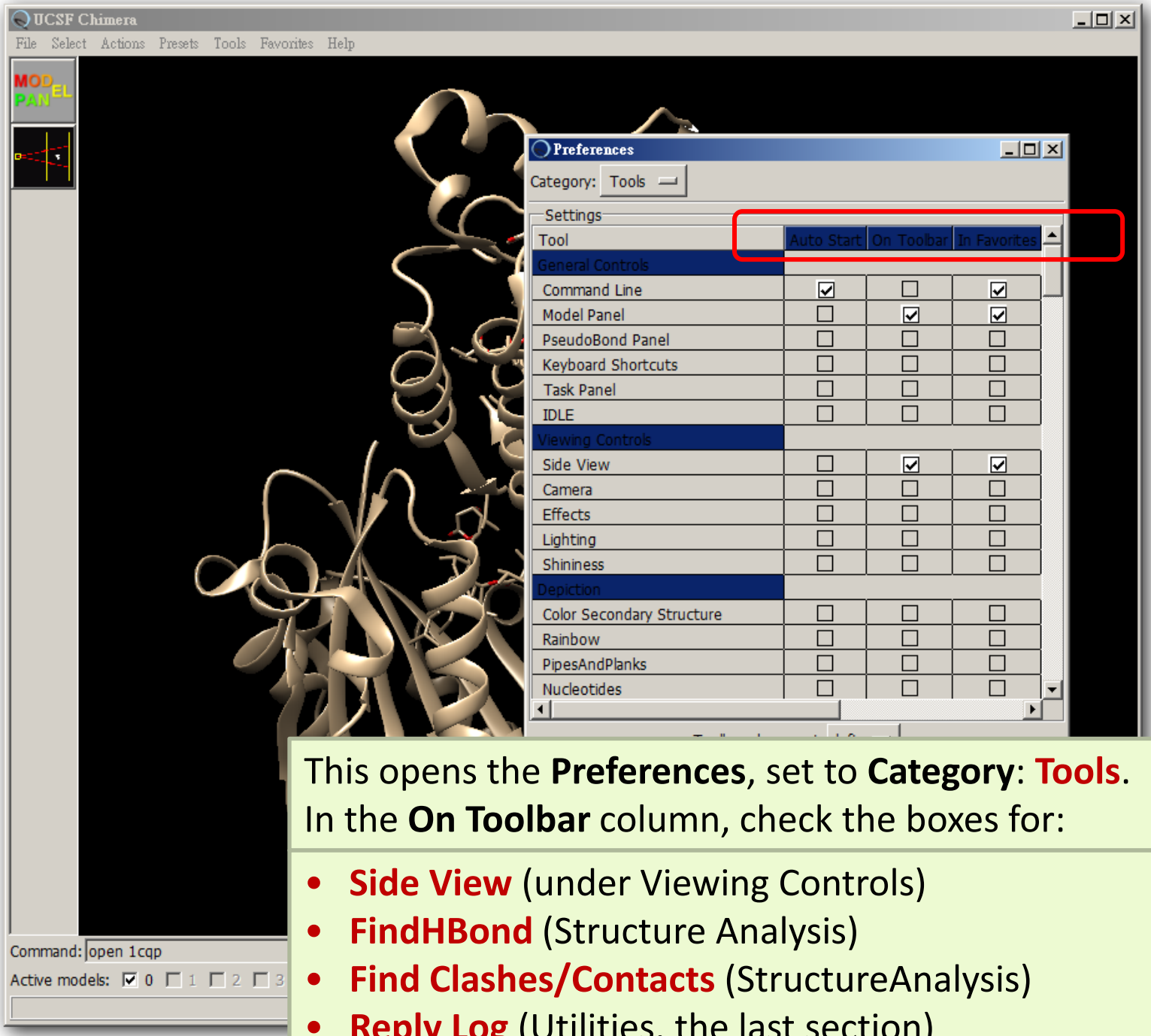
Choose **Tools** → **General Controls** → **Command Line**

Command: **open 1cqp**

fetch the entry with ID **1cqp** from the Protein Data Bank (**PDB**)



Choose **Favorites** → **Add to Favorites/Toolbar** to place some icons on the toolbar. This opens the **Preferences**



Auto Start

On Toolbar

In favorites

This opens the **Preferences**, set to **Category**: **Tools**.
In the **On Toolbar** column, check the boxes for:

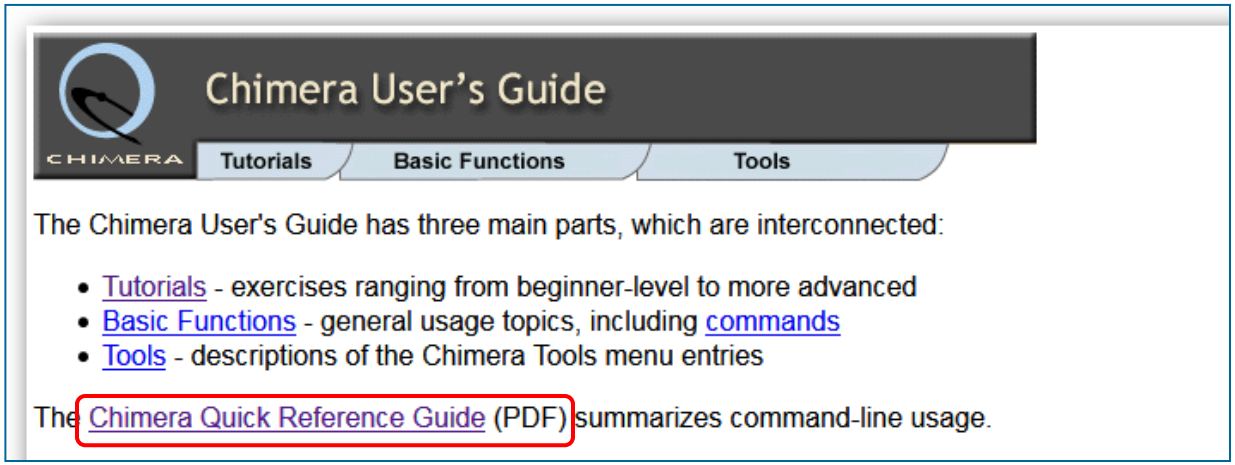
- **Side View** (under Viewing Controls)
- **FindHBond** (Structure Analysis)
- **Find Clashes/Contacts** (StructureAnalysis)
- **Reply Log** (Utilities, the last section)

Default Mouse Button Assignments

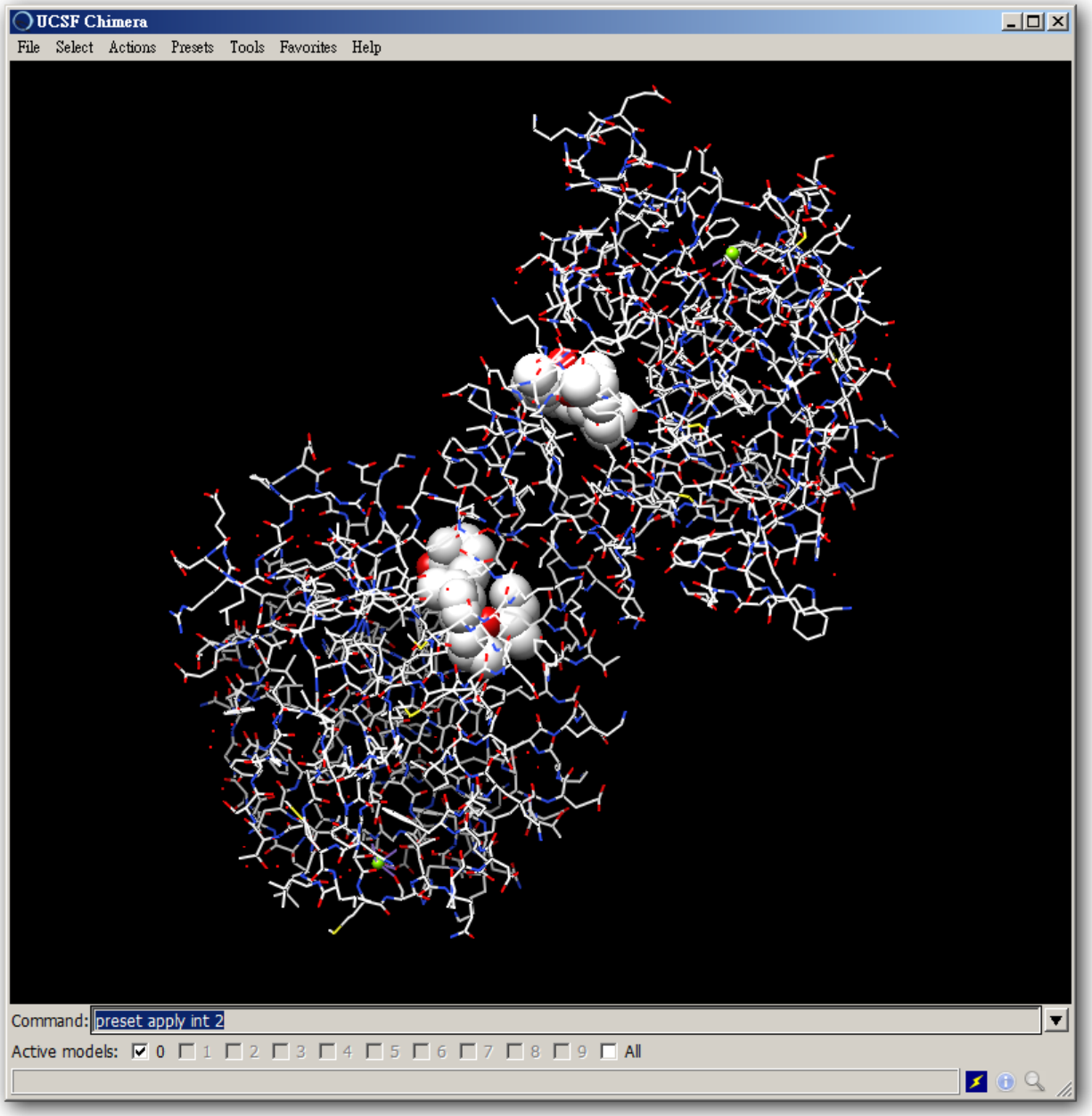
Mouse button	Modifier	Action
Btn1 (left button)		Rotation
Btn2 (middle button)		XY Translation
Btn3 (right button)		Scaling
Btn1	Ctrl	Picking (selection)
Btn1	Ctrl-Shift	Addition to (removal from) selection

The arrow keys can be used to broaden (↑), narrow (↓), or invert (→) a selection.

You can interact with Chimera using menus and/or commands. The basic features of Chimera are available either way, but not all command functions are available in menus or graphical interfaces, and not all menu or graphical interface functions are available in commands.



Command: **modelcol white**



Command: **preset apply int 2**

- A ***preset*** is a predefined combination of display settings. Choosing an entry in the **Presets** menu applies its settings and is much easier than adjusting the many settings individually. Presets are provided for a handful of usage scenarios; of course, many more combinations of settings are possible. See also: the **preset** command, the **New Molecules** preferences
- **Interactive** presets are meant for interactive manipulation and analysis. They may change what items (atoms, ribbons, surfaces) are displayed and how they are colored. The background color is set to black.
- The **ribbons** preset shows most peptide and nucleic acid chains as ribbons, plus atomic detail (excluding hydrogens on carbon atoms) for residues within 3.5 Å of a ligand residue or metal ion. Atomic detail is also used for chains that are very short. Nucleic acids may be shown with special sugar and base representations (as produced by **Nucleotides**), with the level of abstraction dependent on size.
- The **all atoms** preset displays all atoms and bonds as wires with heteroatom colorcoding. Carbons are shown in the model colors so that models will be distinguishable from one another.
- The **hydrophobicity surface** preset shows amino acid hydrophobicity in the Kyte-Doolittle scale with colors ranging from dodger blue for the most hydrophilic to white at 0.0 to to orange red for the most hydrophobic (different color-codings can be applied with **rangecolor** or **Render by Attribute**). Surfaces of nonpeptides will be colored to match the underlying atoms instead.
- **Publication** presets are intended for generating images for presentation and publication. They do not change what items are displayed or their colors, but may change their styles, and the background color is set to white. For example, choosing a preset with **rounded ribbon** or **licorice** will not turn on ribbon display, but will adjust any currently displayed ribbon segments; similarly, only the currently displayed atoms and bonds will be shown as **sticks**. Publication presets may decrease interactive performance because finer divisions are used to depict curved objects (molecular surfaces, ribbons, *etc.*). Individual display parameters are discussed in more detail in the tips on preparing images.

Usage:
preset apply *type number*

Usage:
preset list [*type* **]**

Preset with the keyword **apply** applies a predefined combination of display settings. It has the same effect as choosing the corresponding entry from the Presets menu. Currently presets cannot be user-defined, but Chimera includes several presets grouped by *type*:

- interactive - for interactive manipulation and analysis; may change what items (atoms, ribbons, surfaces) are displayed and how they are colored, and make the background black:
  - **1** (ribbons)
  - **2** (all atoms)
  - **3** (hydrophobicity surface)
- publication - for generating presentation and publication images; do not change what items are displayed or their colors, but may change their styles and make the background white:
  - **1** (sihouette, rounded ribbon, sticks)
  - **2** (sihouette, licorice, sticks)
  - **3** (depth-cued, rounded ribbon, sticks)
  - **4** (depth-cued, licorice, sticks)

  Publication presets may decrease interactive performance because finer divisions are used to depict curved objects (molecular surfaces, ribbons, *etc.*). Individual display parameters are discussed in more detail in the tips on preparing images.

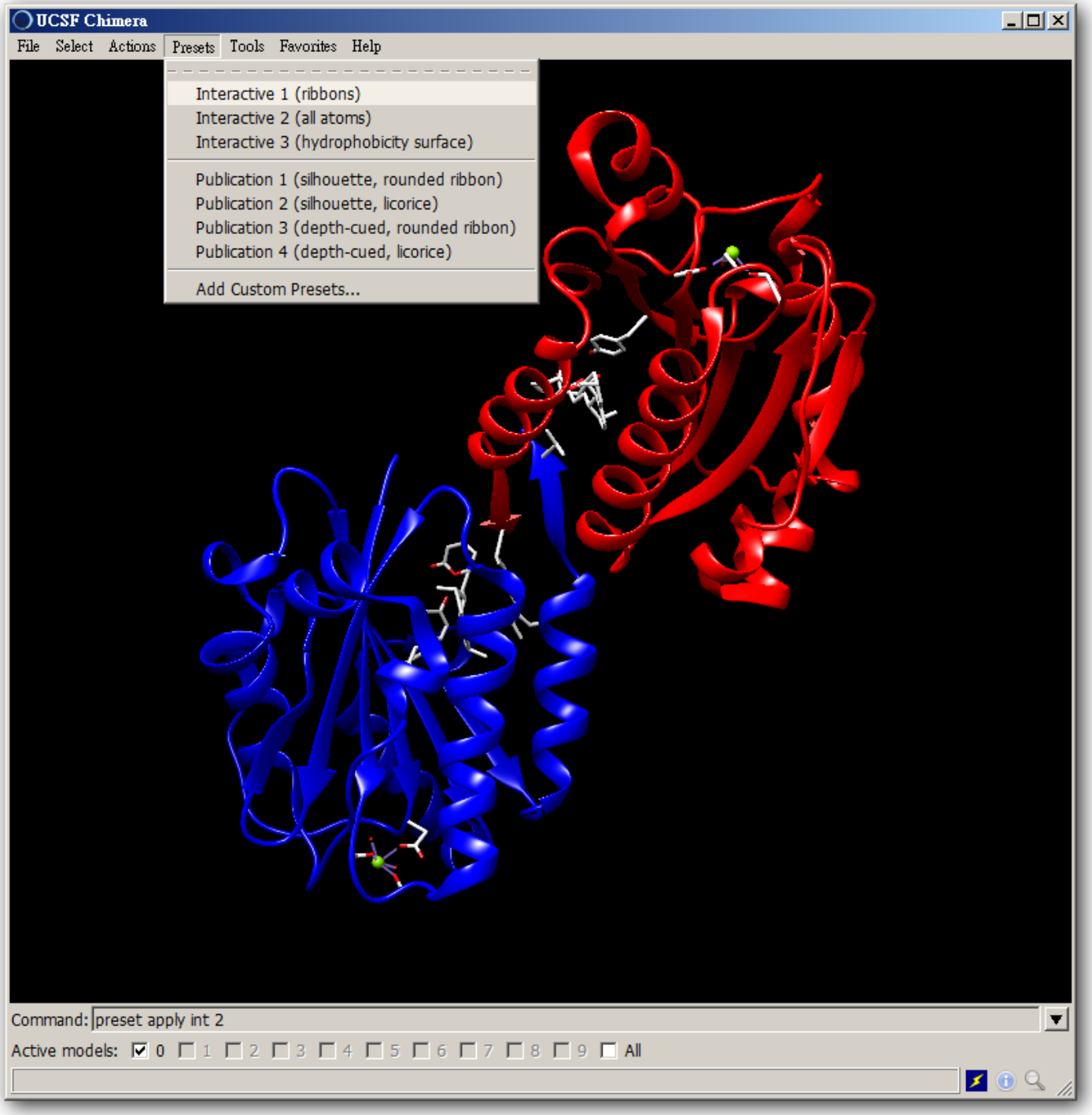
The *type* can be truncated to a unique string. The *number* is the ID number of the specific preset to be applied.

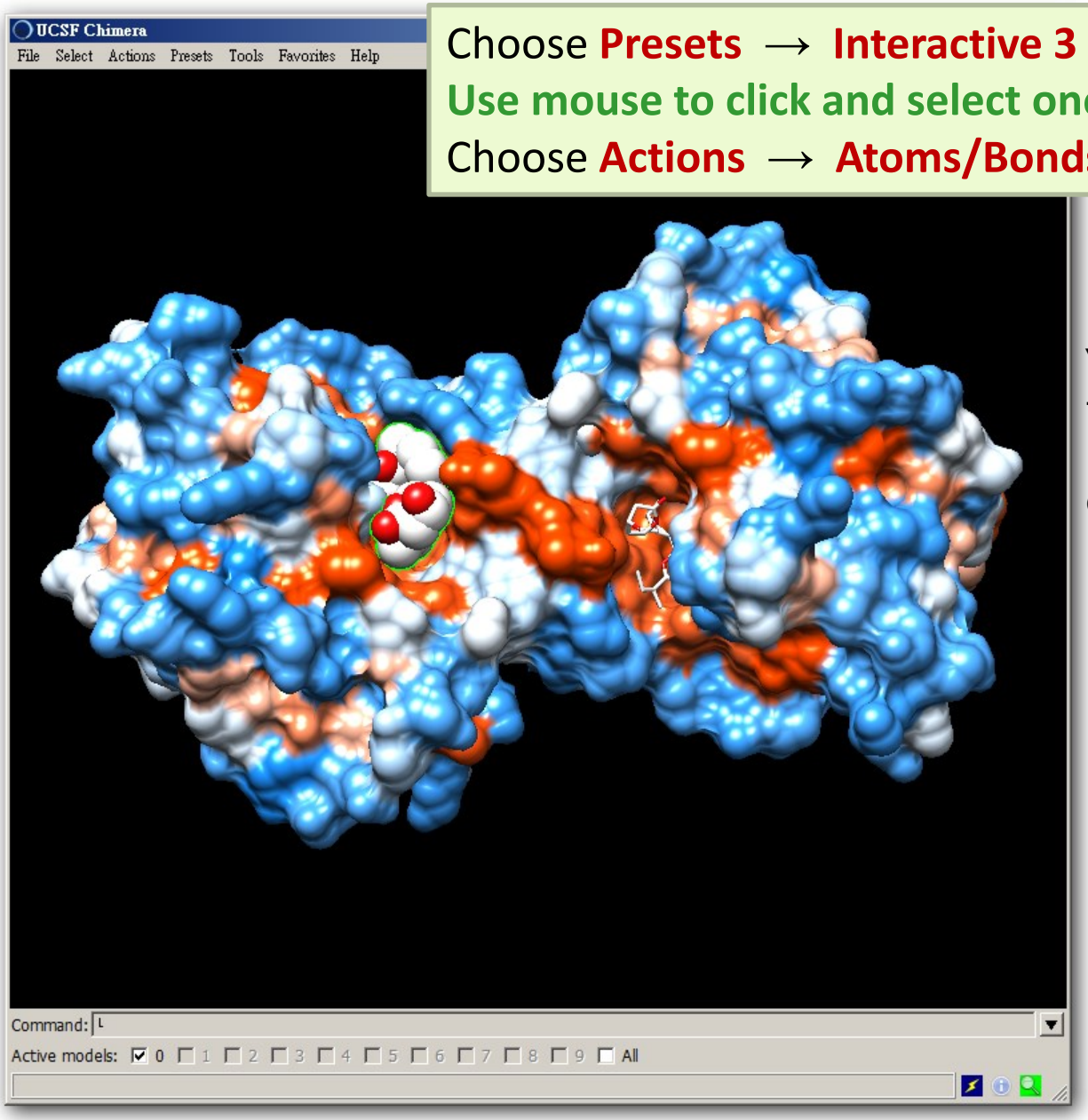
Preset with the keyword **list** sends a list of presets of the specified *type* (all types, if not specified) to the Reply Log.

Examples:

preset apply int 1
- apply the ribbons **interactive** preset

preset list pub
- list all **publication** presets in the **Reply Log**


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Interactive 1 (ribbons)
Interactive 2 (all atoms)
Interactive 3 (hydrophobicity surface)
Publication 1 (silhouette, rounded ribbon)
Publication 2 (silhouette, licorice)
Publication 3 (depth-cued, rounded ribbon)
Publication 4 (depth-cued, licorice)
Add Custom Presets...
Command: preset apply int 2
Active models: 0 1 2 3 4 5 6 7 8 9 All



Choose **Presets** → **Interactive 3**

Use mouse to click and select one ligand

Choose **Actions** → **Atoms/Bonds 3** → **sphere**

"*hydrophobicity surface*" preset: from **dodger blue** for the most hydrophilic, to **white**, to **orange red** for the most hydrophobic.

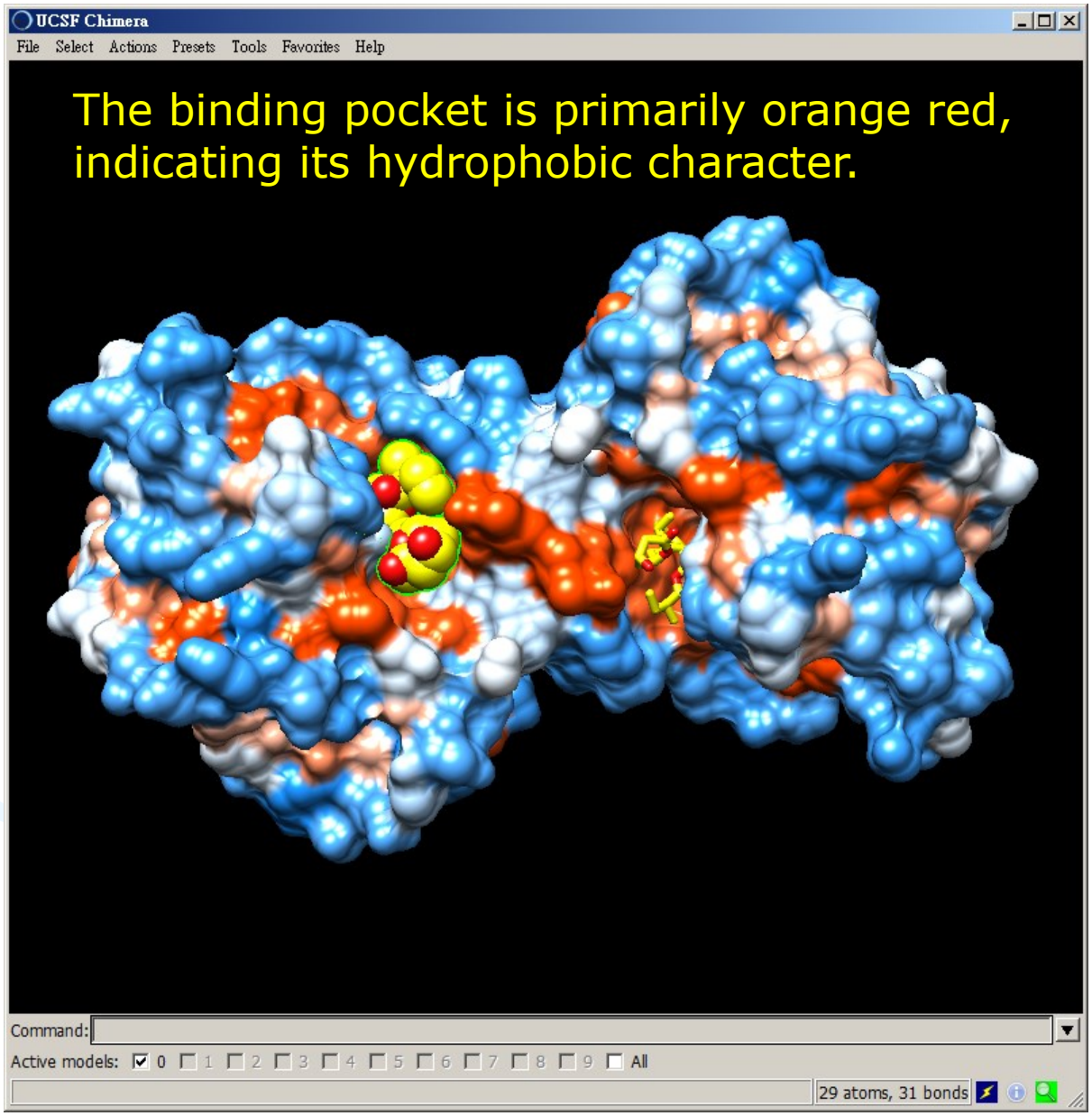
Command:

preset apply int 3
select :311.A
rep sphere :311.A

Command:

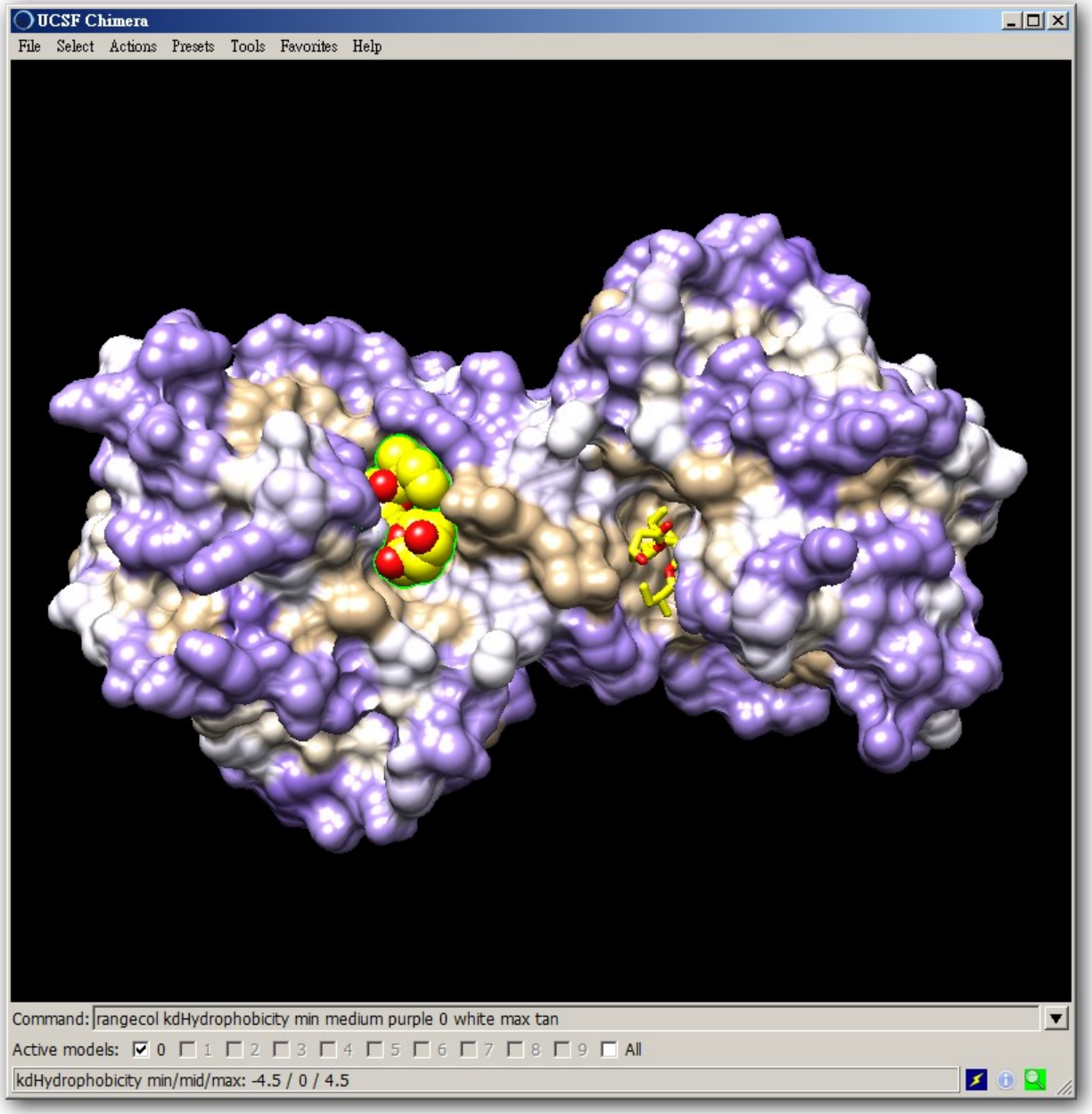
preset apply int 3 ; select :311.A ; rep sphere :311.A

"hydrophobicity surface" preset: from **dodger blue** for the most hydrophilic, to **white**, to **orange red** for the most hydrophobic.



Command:

setattr m stickScale 2 ; color yellow ligand & C

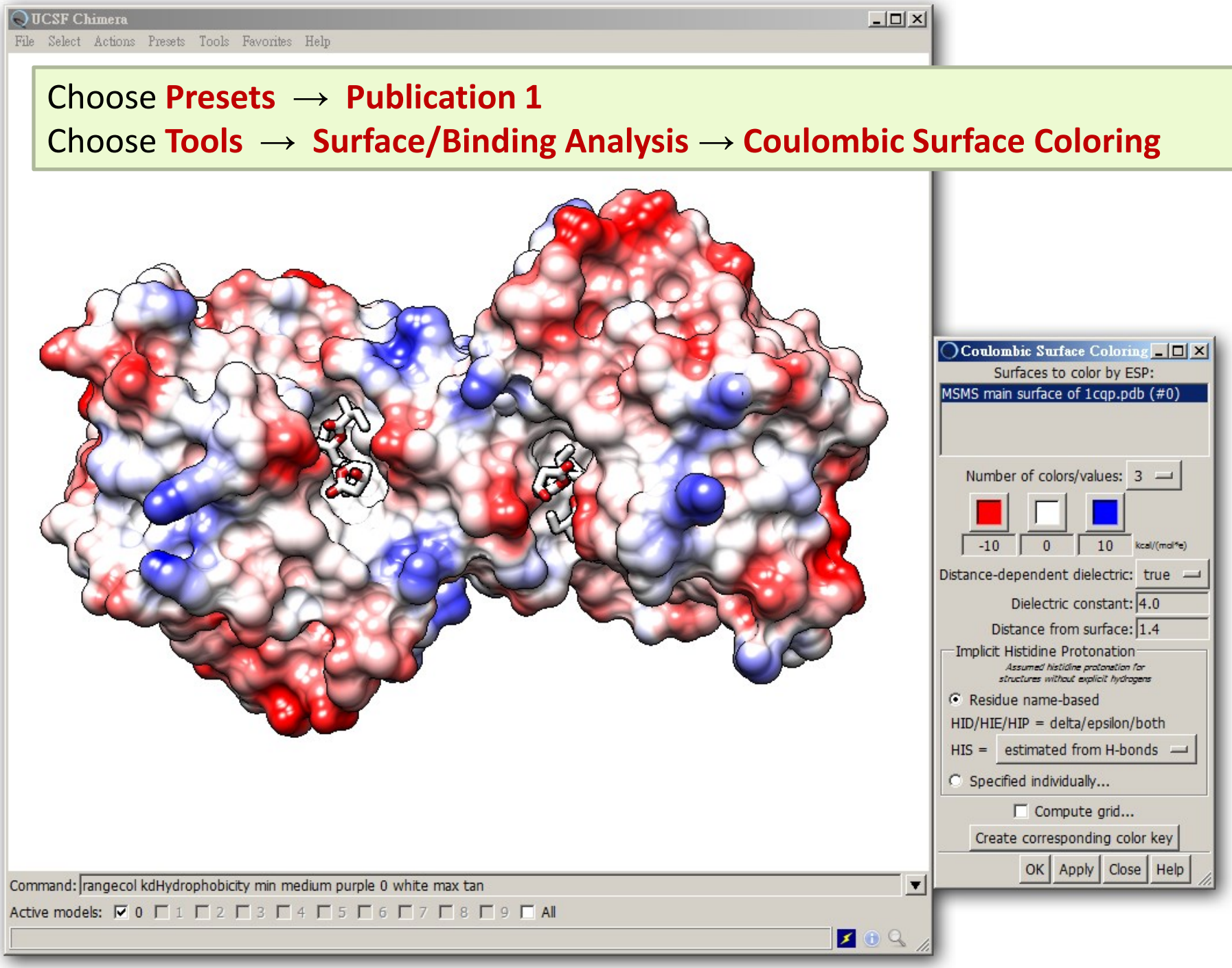


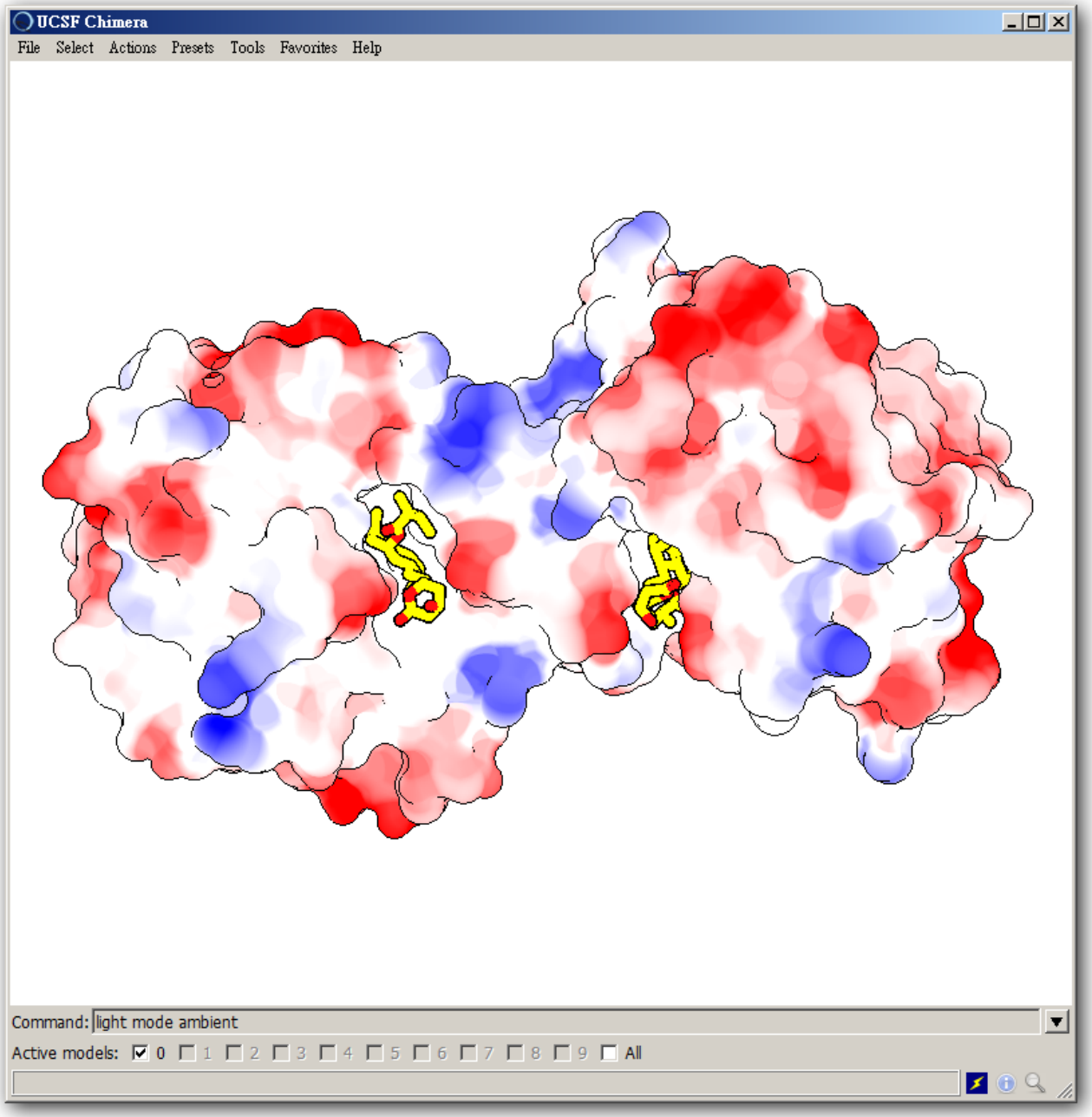
Command:

rangecol kdHydrophobicity min medium purple 0 white max tan

Choose **Presets** → **Publication 1**

Choose **Tools** → **Surface/Binding Analysis** → **Coulombic Surface Coloring**

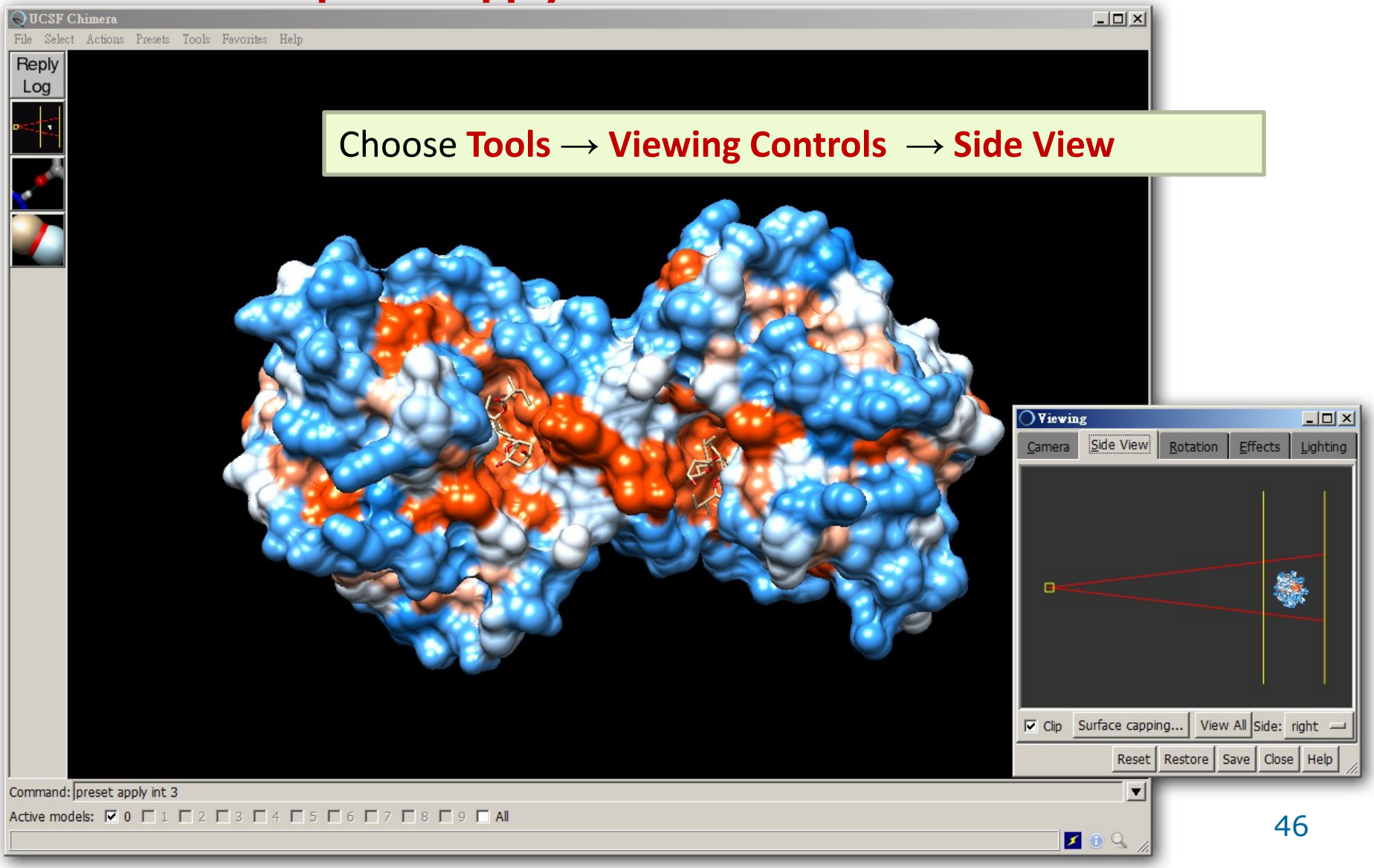




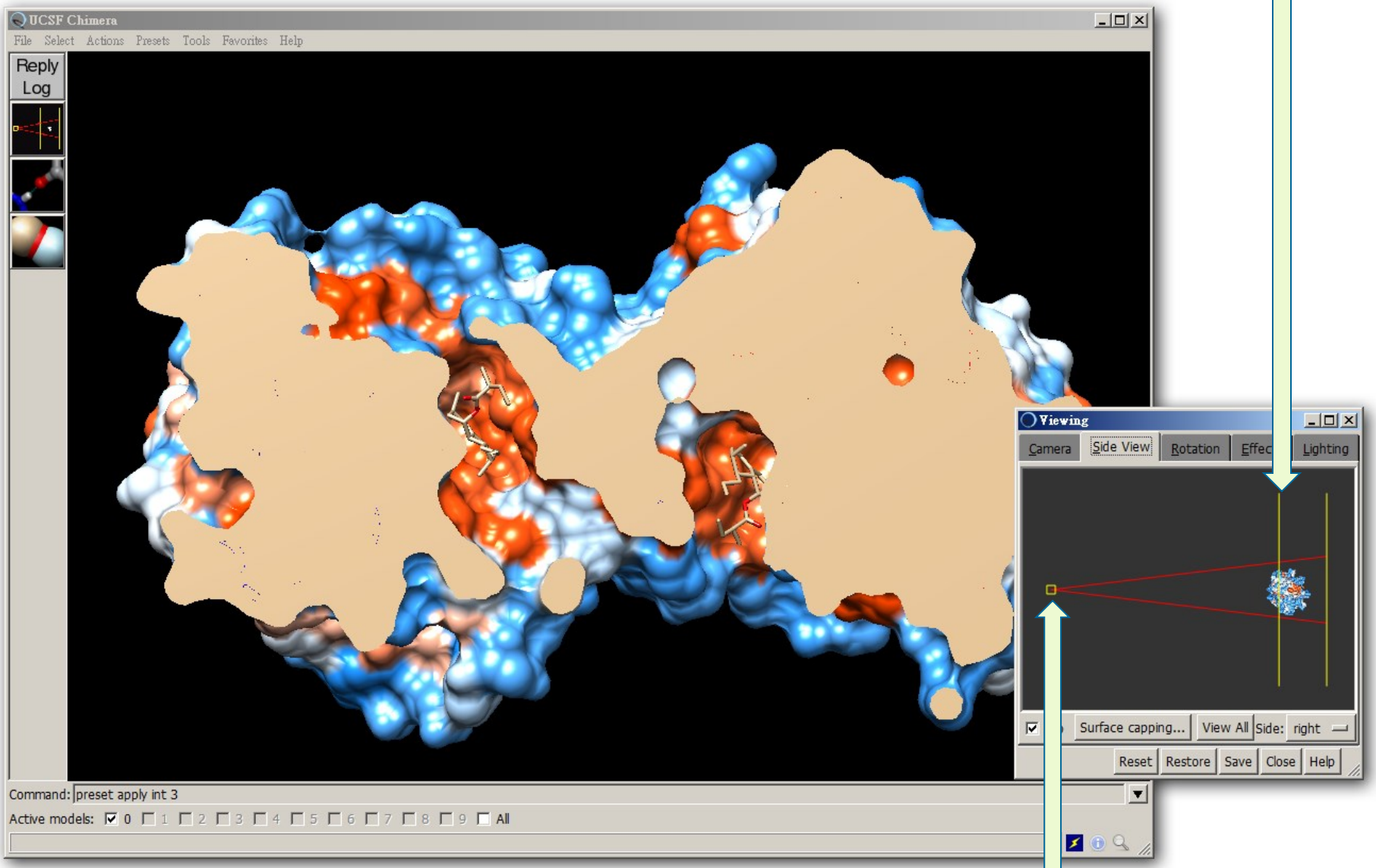
Command: **light mode ambient**

Side View

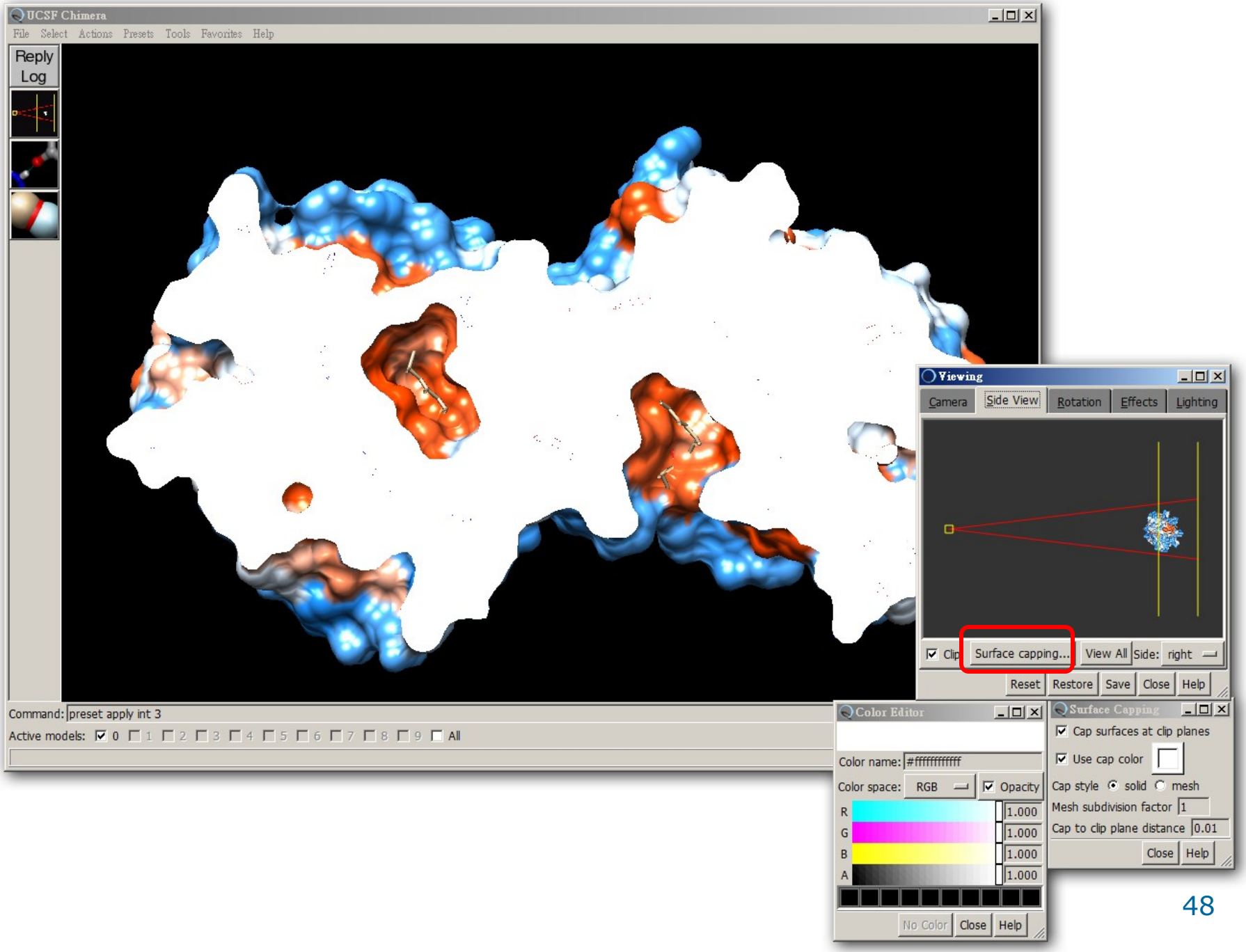
Command: **close all; open 1cqp**
preset apply int 3



adjust the clip plane



scale


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Reply Log
Viewing
Camera Side View Rotation Effects Lighting
Surface capping...
View All
Side: right
Reset Restore Save Close Help
Color Editor
Color name: #ffffffffffff
Color space: RGB
Opacity
R 1.000
G 1.000
B 1.000
A 1.000
No Color Close Help
Surface Capping
Cap surfaces at clip planes
Use cap color
Cap style solid mesh
Mesh subdivision factor 1
Cap to clip plane distance 0.01
Close Help
Command: preset apply int 3
Active models: 0 1 2 3 4 5 6 7 8 9 All

Atom Specification Symbols		
Symbol	**Meaning**	**Usage**
#	model	*#model* (model ID number)
:	residue	*:residue* (residue name or number)
:.	chain	*:.chain* (chain ID)
@	atom	*@atom* (atom name)
=	partial wildcard	matches partial atom or residue name, *e.g.*, @C= specifies all atoms with names beginning with C
?	single-character wildcard	matches single character in atom or residue name, *e.g.*, :G?? specifies all residues with three-letter names beginning with G

Specification Symbols

Symbol	Function	Usage
#	model number	# *model* (integer)
#.	submodel number	#. *submodel* (integer)
:	residue	: *residue* (name or number)
::	residue name	:: *residue*
:.	chain ID	:. *chain*
@	atom name	@*atom*
@.	alternate location ID	@. *alt_loc*
–	range	specifies a range of models, submodels, or residues
,	name separator	separates models or residues, ranges of models or residues, or names of atoms
*	whole wildcard	matches whole atom or residue names, *e.g.*,:*@CA specifies the alpha-carbons of all residues
=	partial wildcard	matches partial atom or residue names, *e.g.*, @C= specifies all atoms with names beginning with C
?	single-char wildcard	used for atom and residue names only, *e.g.*, :G?? selects all residues with three-letter names beginning with G
;	command separator	separates multiple commands on a single line
z<	zone specifier	z<*zone* or zr<*zone* specifies all residues within *zone* angstroms, za<*zone* specifies all atoms (rather than entire residues)
&	intersection	intersection of specified sets
|	union	union of specified sets
~	negation	negation of specified set

Specification Examples

#
- all models

#0
- model 0

#3:45-83,90-98
- residues 45-83 and 90-98 in model 3

:lys,arg
- lysine and arginine residues

:12,14@ca
- alpha-carbons in residues 12 and 14

:12:14@ca
- all atoms in residue 12 and the alpha-carbon in residue 14

:.A@n,ca,c,o
- atoms named N, CA, C, and O in chain A

:50.B,.D
- residue 50 in chain B and all residues in chain D

:12-15,26-28.a,45.b
- residues 12-15 in all chains (except het/water), 26-28 in chain A, and 45 in chain B

#0.1-3,5
- submodels 1-3 of model 0 and all of model 5

#0.1-3,.5
- submodels 1-3 of model 0 and submodel 5 of all models

ligand
- any/all residues automatically classified as ligand

:.A & protein
- chain A residues classified as protein

:26-28.a,33.a & side chain/base.with CA/C1'
- or -
:26-28.a,33.a & with CA/C1'
- sidechain + CA of residues 26-28 and 33 in chain A

S | Fe
- all sulfur and iron atoms

@ca/!label and color!=green and color!=red
- atoms named CA which are not labeled, and are not green or red

@/bfactor>=20 and bfactor<=40
- atoms with B-factor values ranging from 20 to 40

:asn & helix

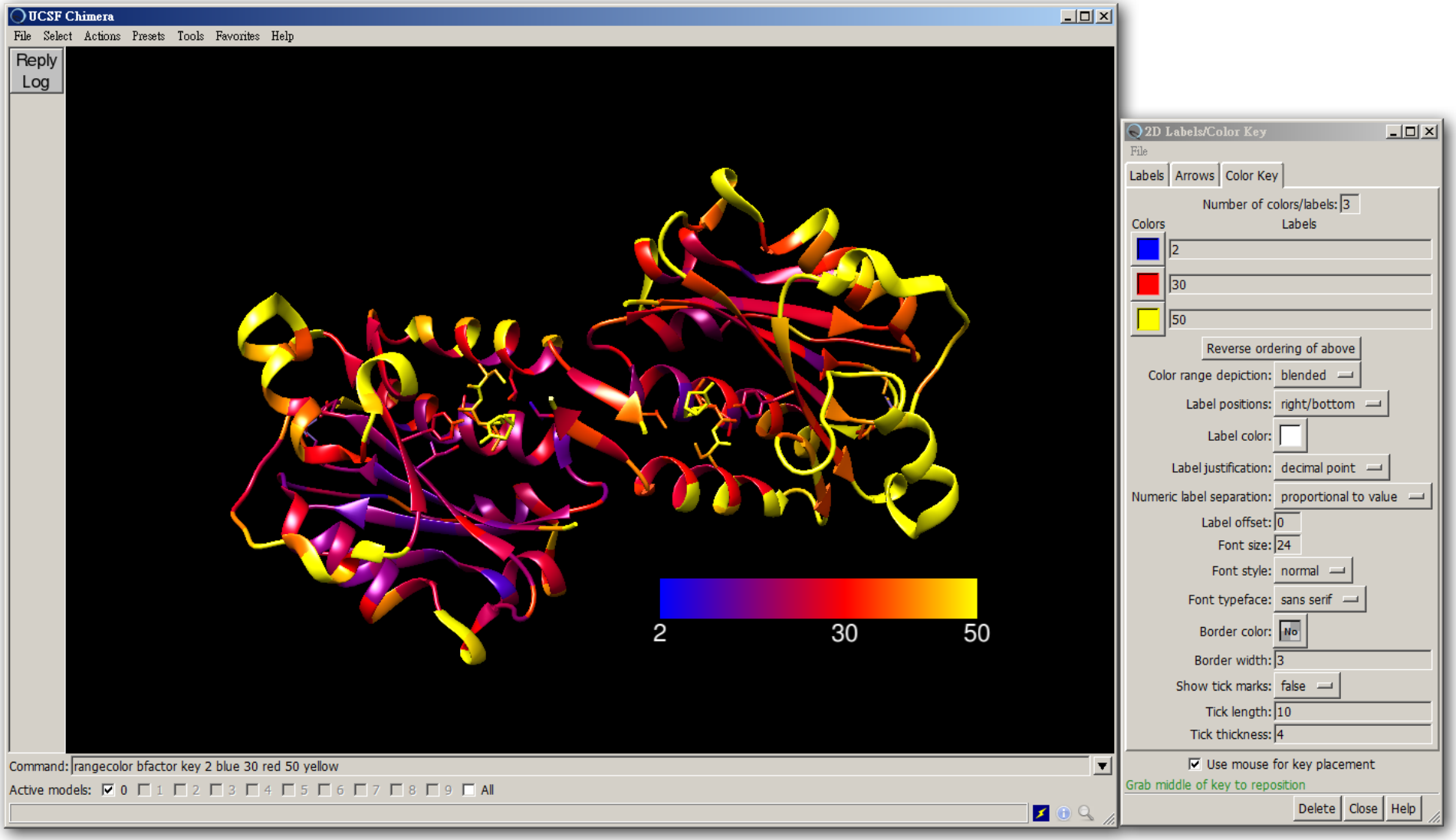
0

solvent & Ng+ z<3 | solvent & N3+ z<3
- solvent residues within 3 angstroms of guanidinium nitrogens or *sp*3-hybridized, formally positive nitrogens

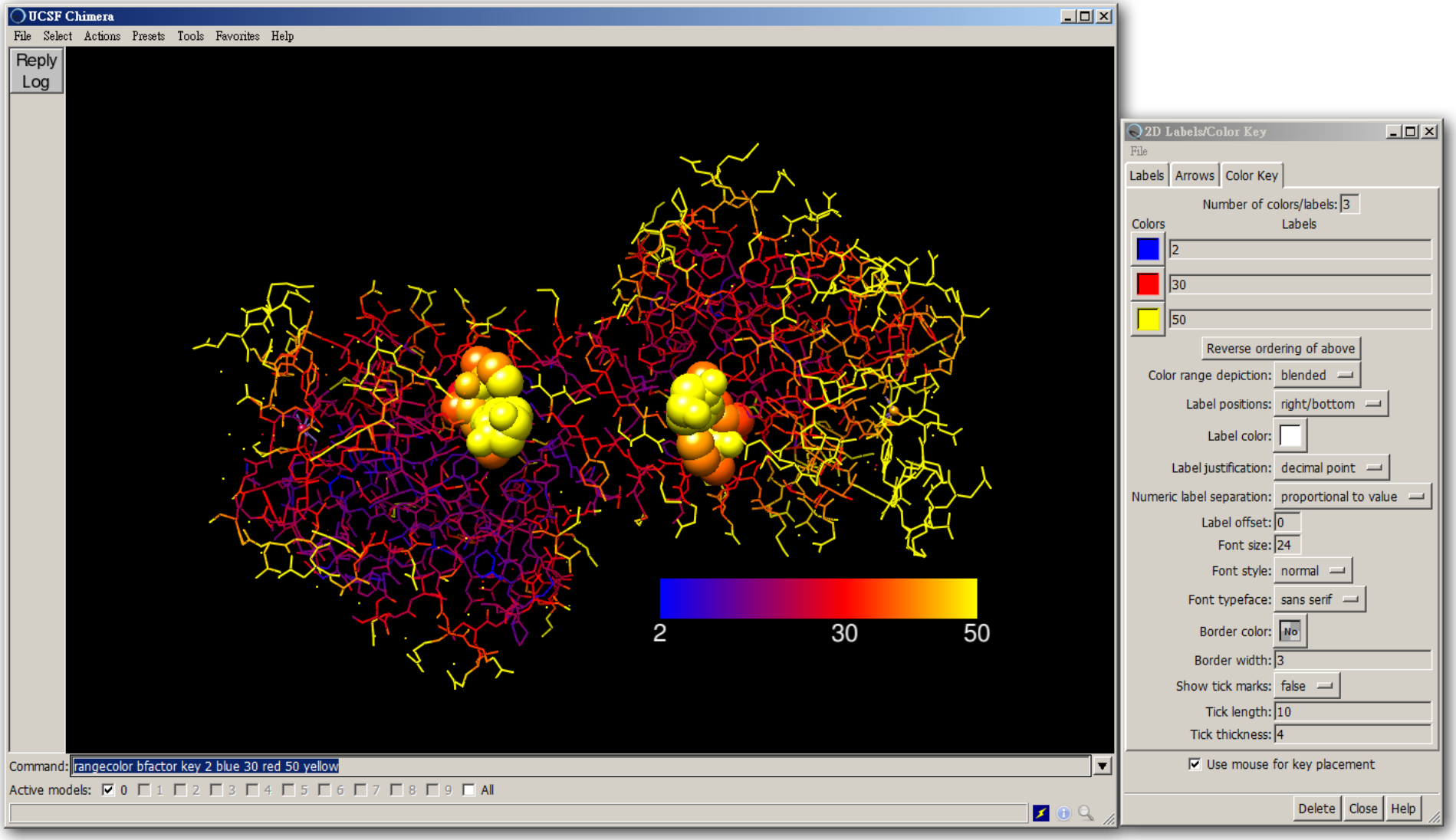
@/bfactor>50 & ~ solvent & ~ ions
- atoms with B-factor values over 50, excluding solvent and ions

https://www.cgl.ucsf.edu/chimera/current/docs/UsersGuide/quickref.pdf

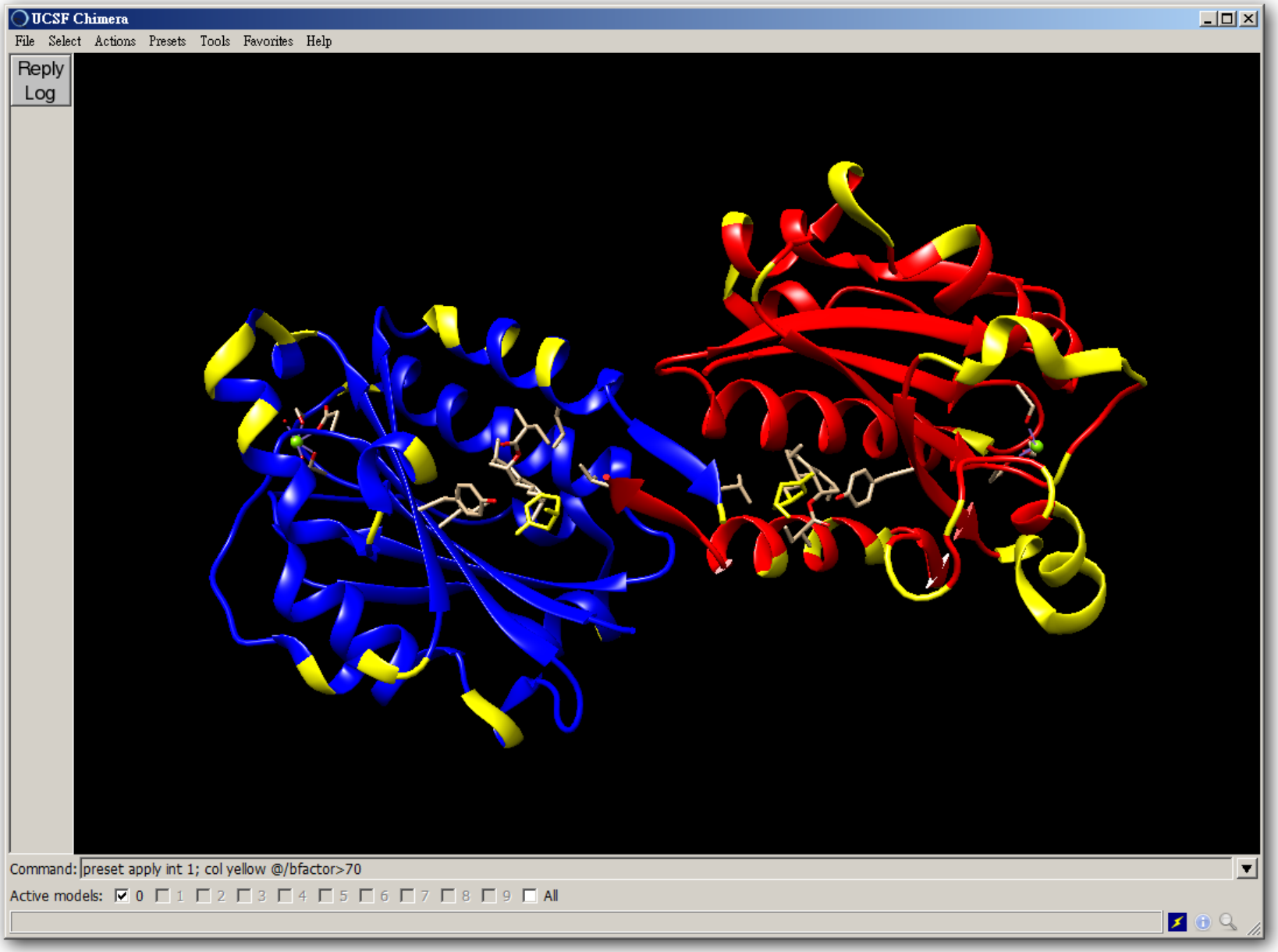
Coloring by B-Factor



Command: **rangecolor bfactor key 2 blue 30 red 50 yellow**


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Reply Log
2
30
50
Command: rangecolor bfactor key 2 blue 30 red 50 yellow
Active models: 0 1 2 3 4 5 6 7 8 9 All
2D Labels/Color Key
File
Labels Arrows Color Key
Number of colors/labels: 3
Colors
Labels
2
30
50
Reverse ordering of above
Color range depiction: blended
Label positions: right/bottom
Label color:
Label justification: decimal point
Numeric label separation: proportional to value
Label offset: 0
Font size: 24
Font style: normal
Font typeface: sans serif
Border color: No
Border width: 3
Show tick marks: false
Tick length: 10
Tick thickness: 4
Use mouse for key placement
Delete Close Help

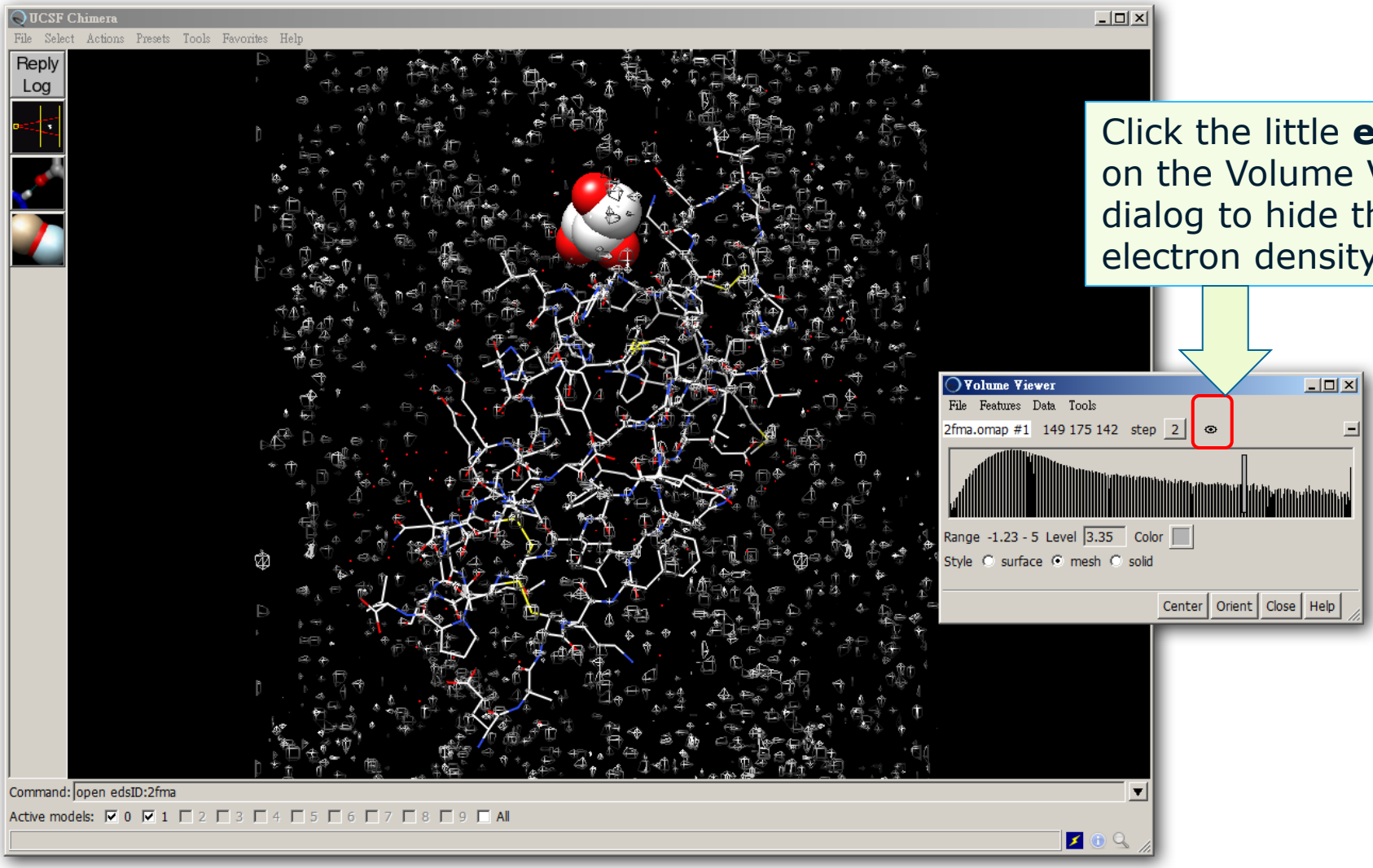
Command: **preset apply int 1; col yellow @/bfactor>70**



Electron Density Map

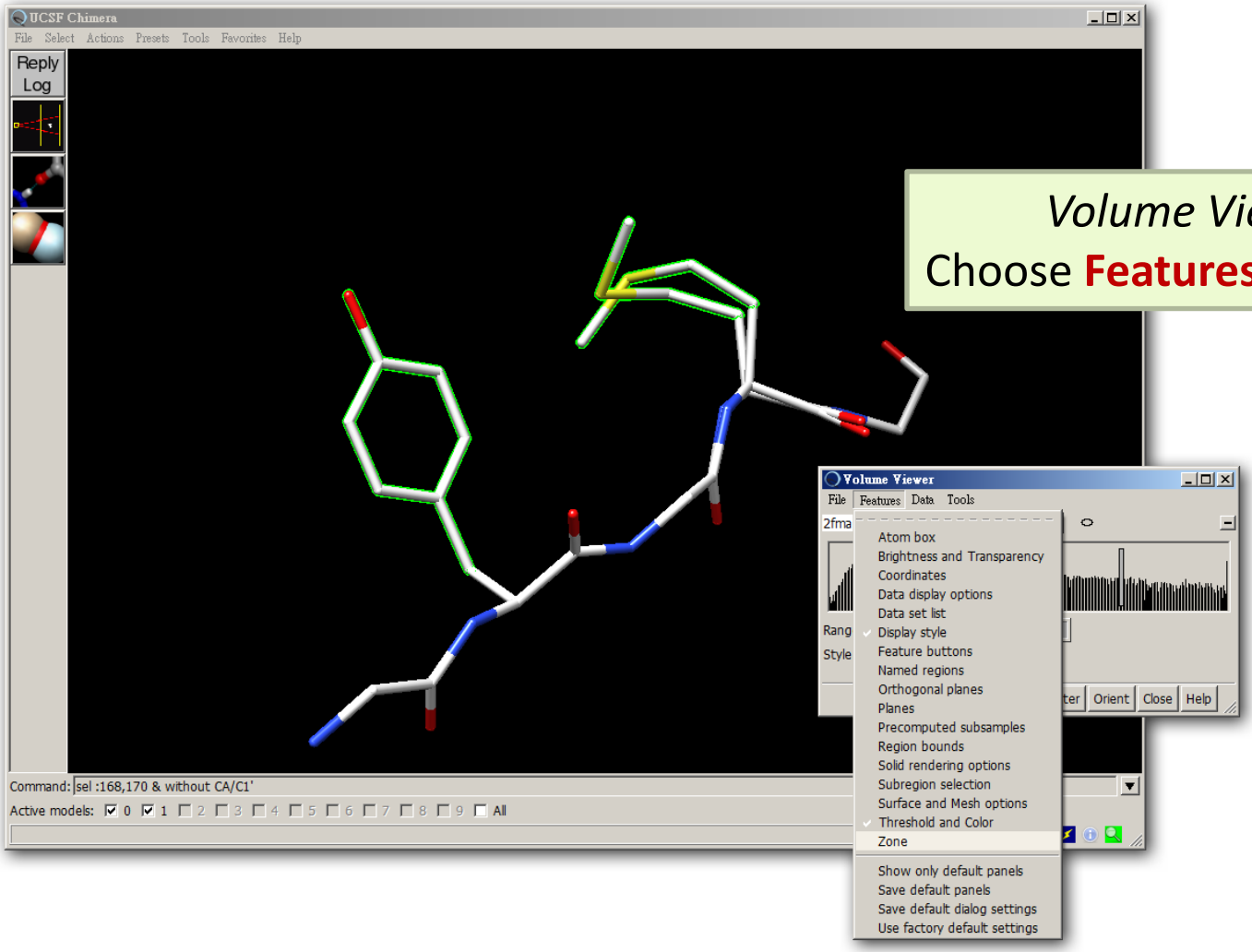
Command: **close session**
open 2fma; modelcol white; preset apply int 2;
open edsID:2fma

Fetch the density map for 2fma from the **Electron Density Server**

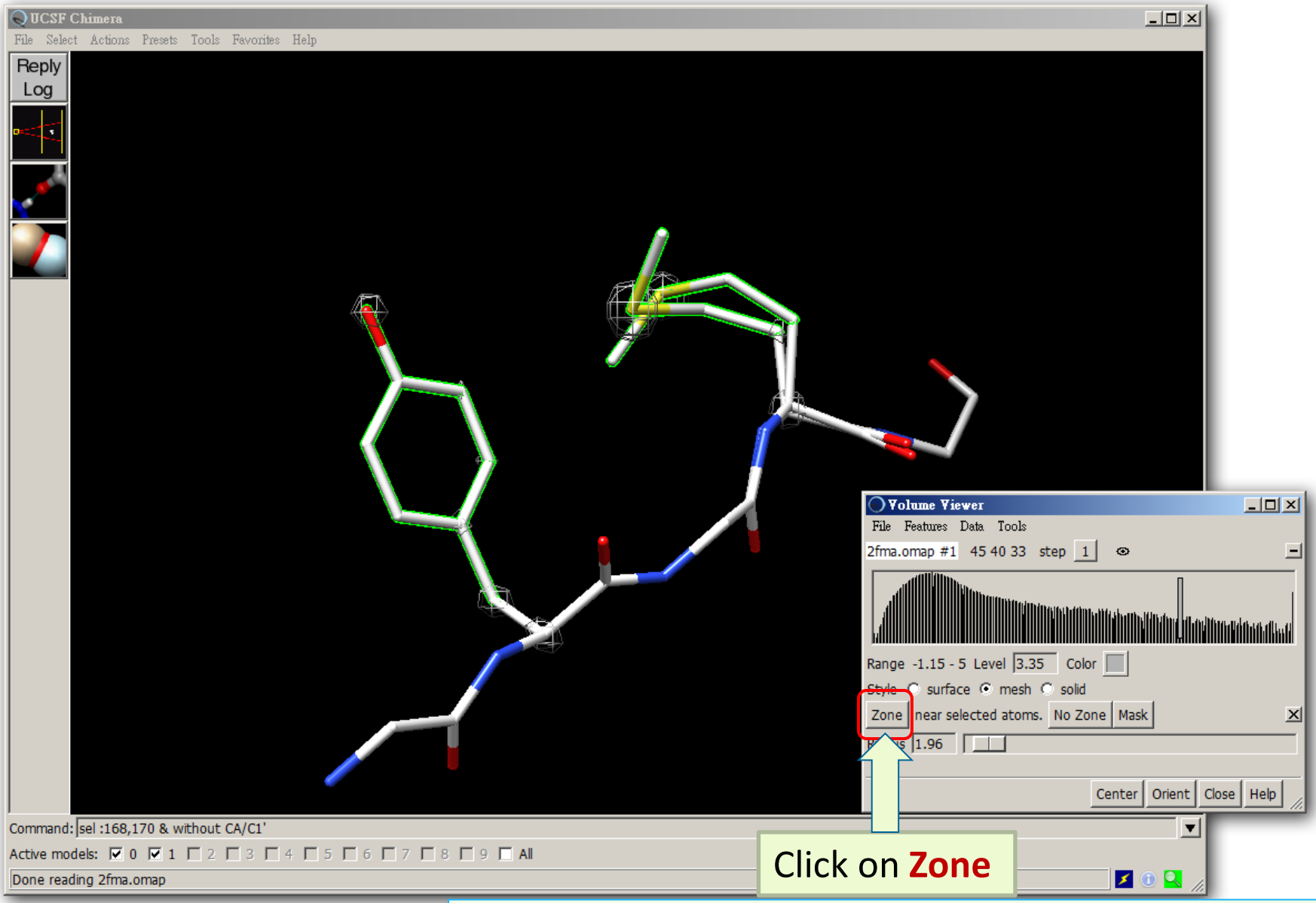


Click the little **eye icon** on the Volume Viewer dialog to hide the electron density for now.

Command: **show :168-170**
focus
disp :167,171@n,ca,c,o
rep stick
setattr m stickScale 0.5
sel :168,170 & without CA/C1'



Volume Viewer
Choose **Features** → **Zone**

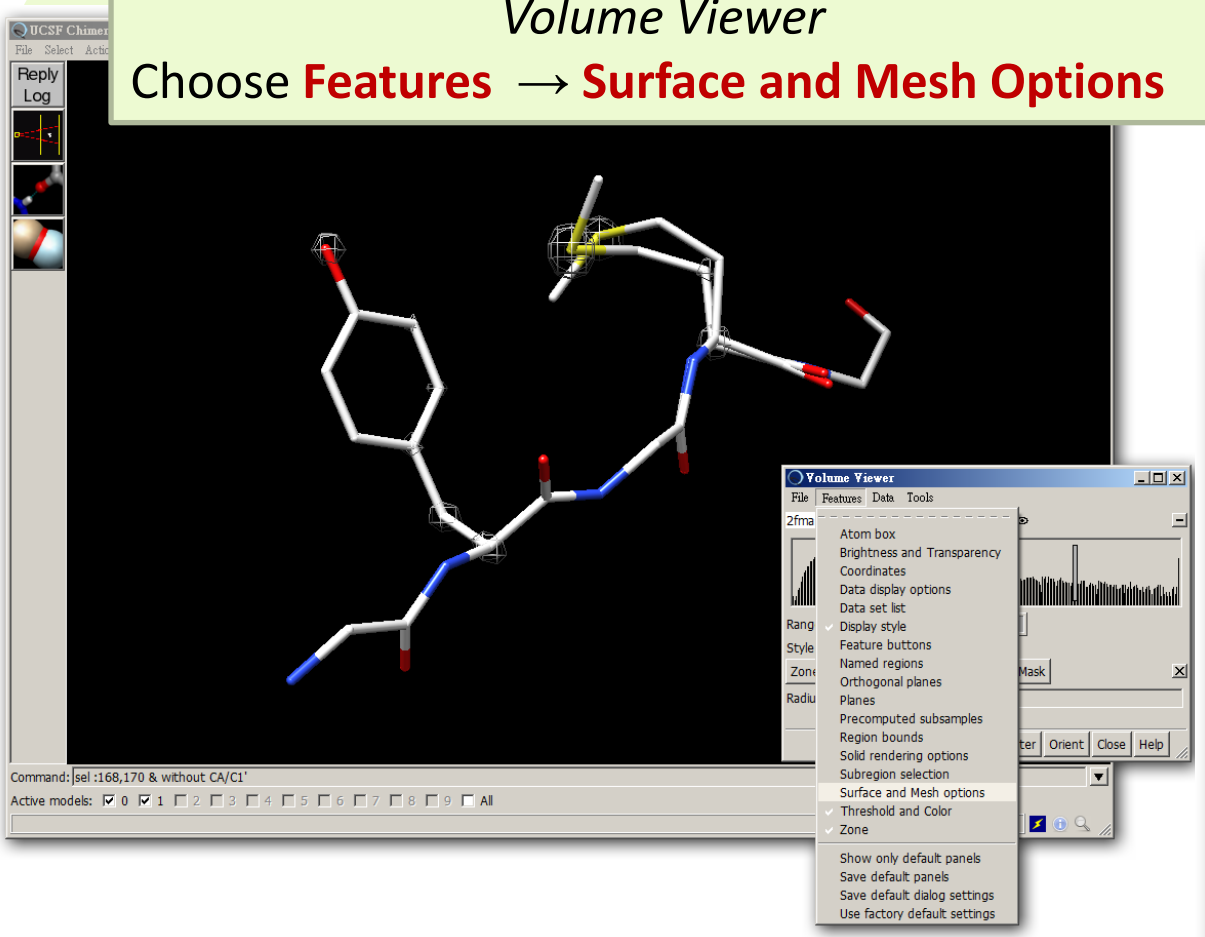


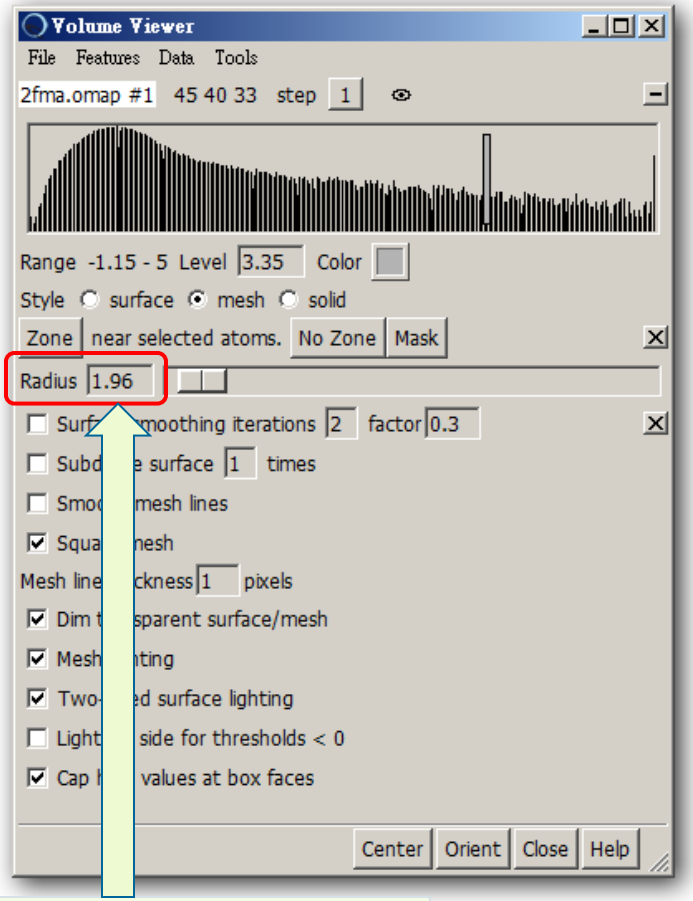
Click on **Zone**

This limits the density display to a zone near the selected atoms. After this, the selection can be cleared.

Volume Viewer

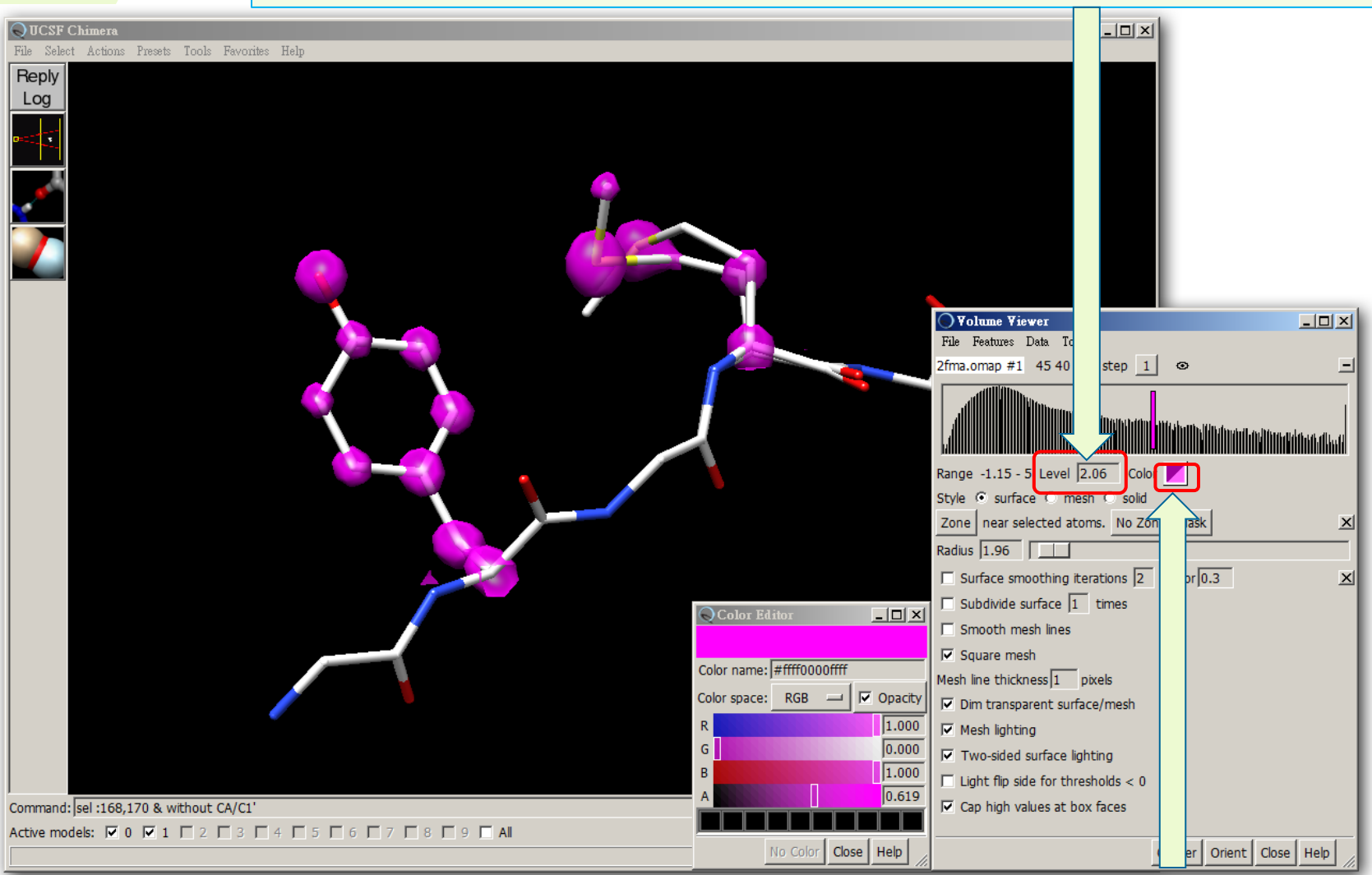
Choose **Features** → **Surface and Mesh Options**





Set the zone **Radius** to be 1.96 Å

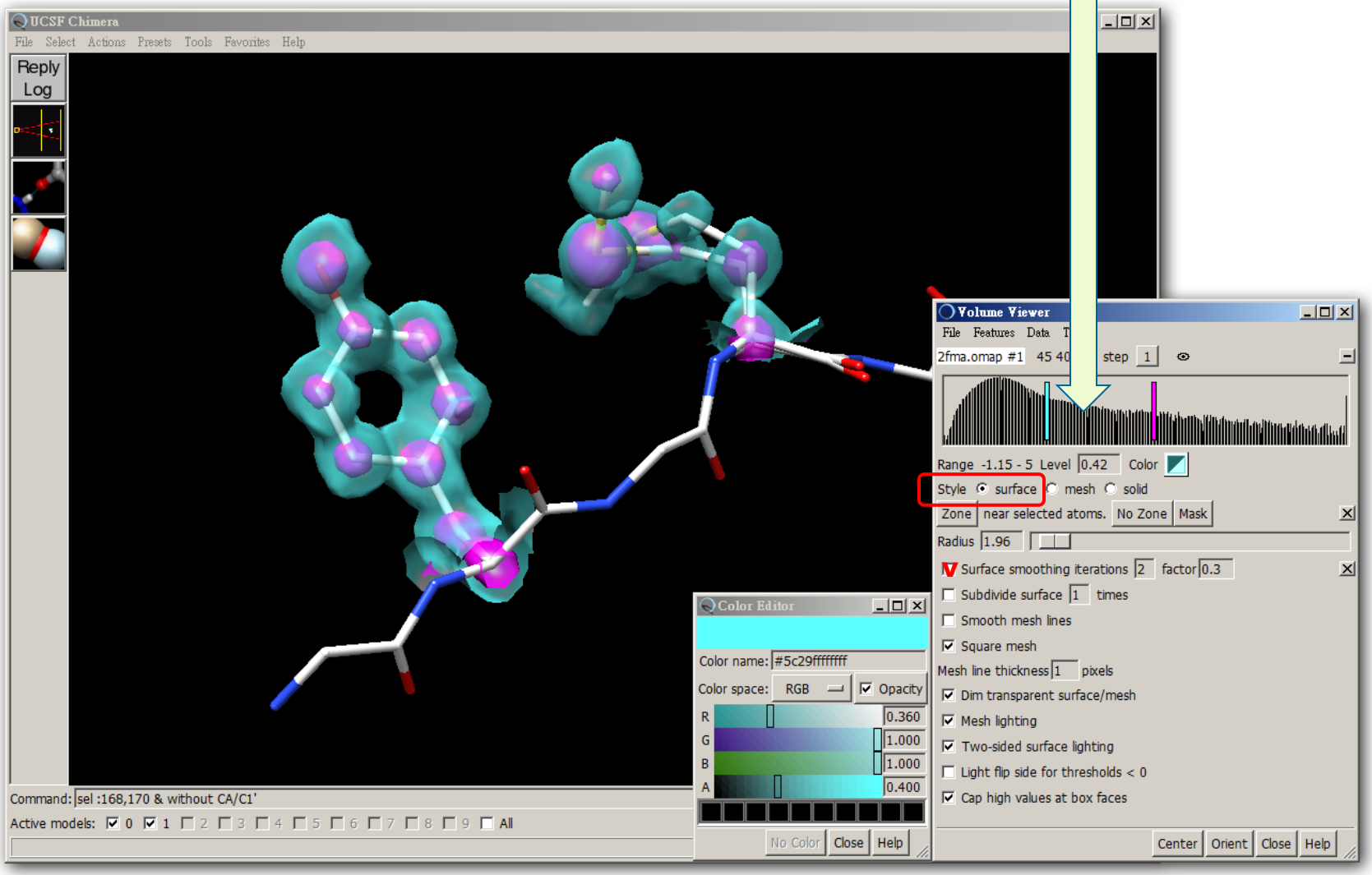
To change the level, drag the threshold to the left or right with the mouse or type a different value into the **Level** field below the histogram; to see more density, move the threshold to the left.



To modify the color, click on **color well**

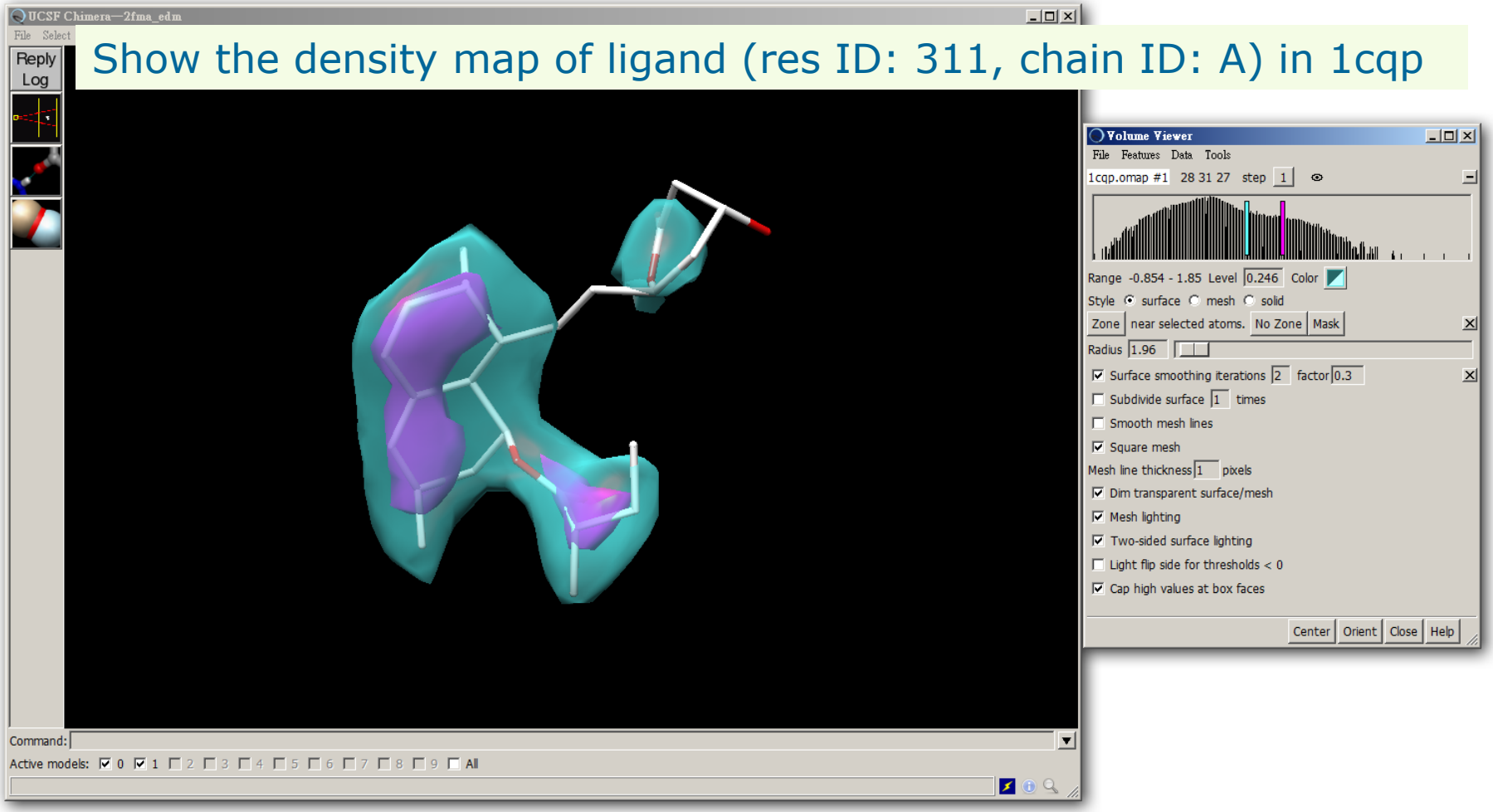
Level 2.06,
Color (RGBA) 1.0 0.0 1.0 0.6

To add another contour level, **Ctrl-click** on the histogram.



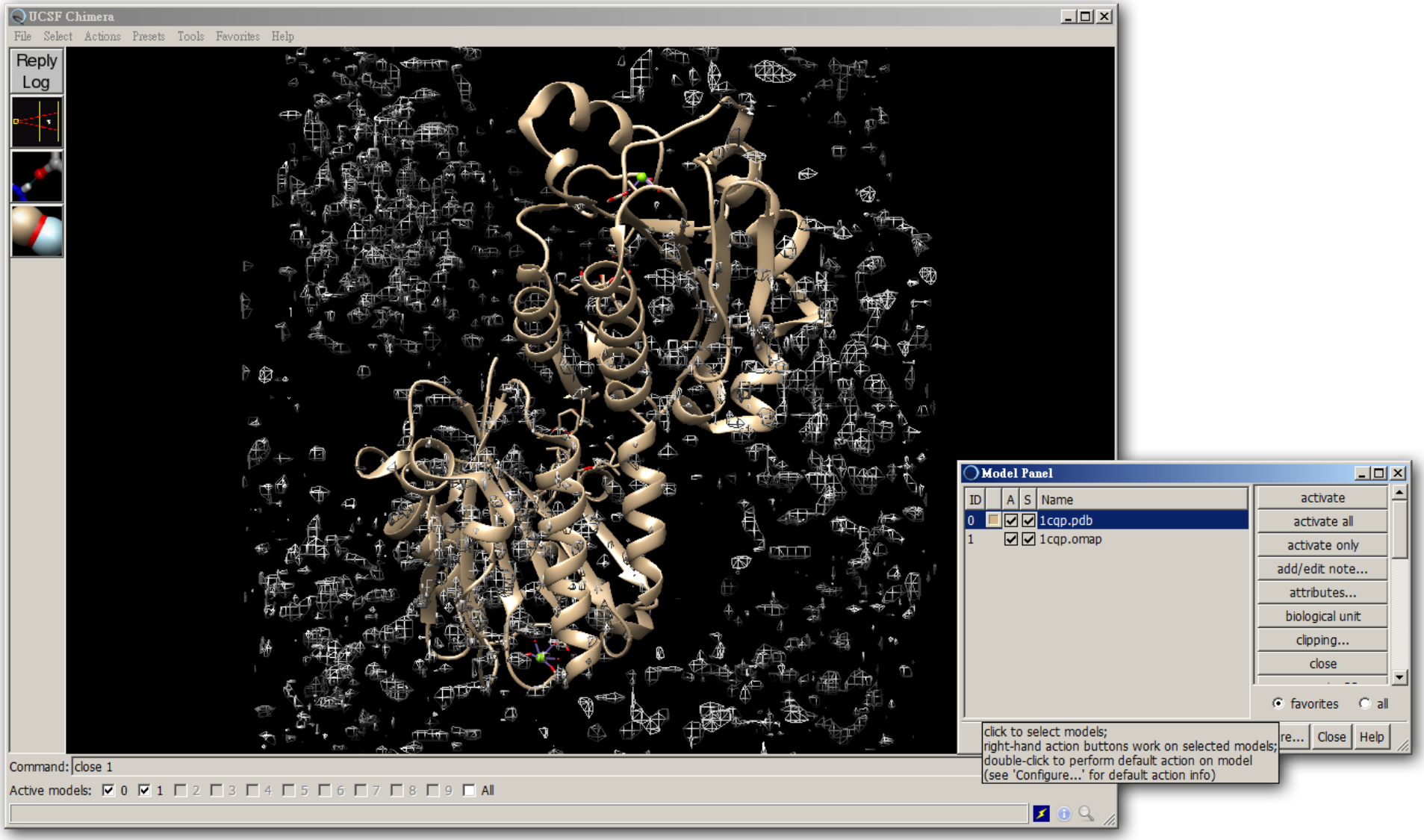
Level 0.426,
Color (RGBA) 0.36 1.0 1.0 0.4
Style surface
turned on **Surface smoothing iterations 2 factor 0.3**

Show the density map of ligand (res ID: 311, chain ID: A) in 1cqp



Command: **close all; open 1cqp**
modelcol white; preset apply int 2;
open edsID:1cqp
show :311.A; focus;
disp :311.A
rep stick; setattr m stickScale 0.5
sel :311.A

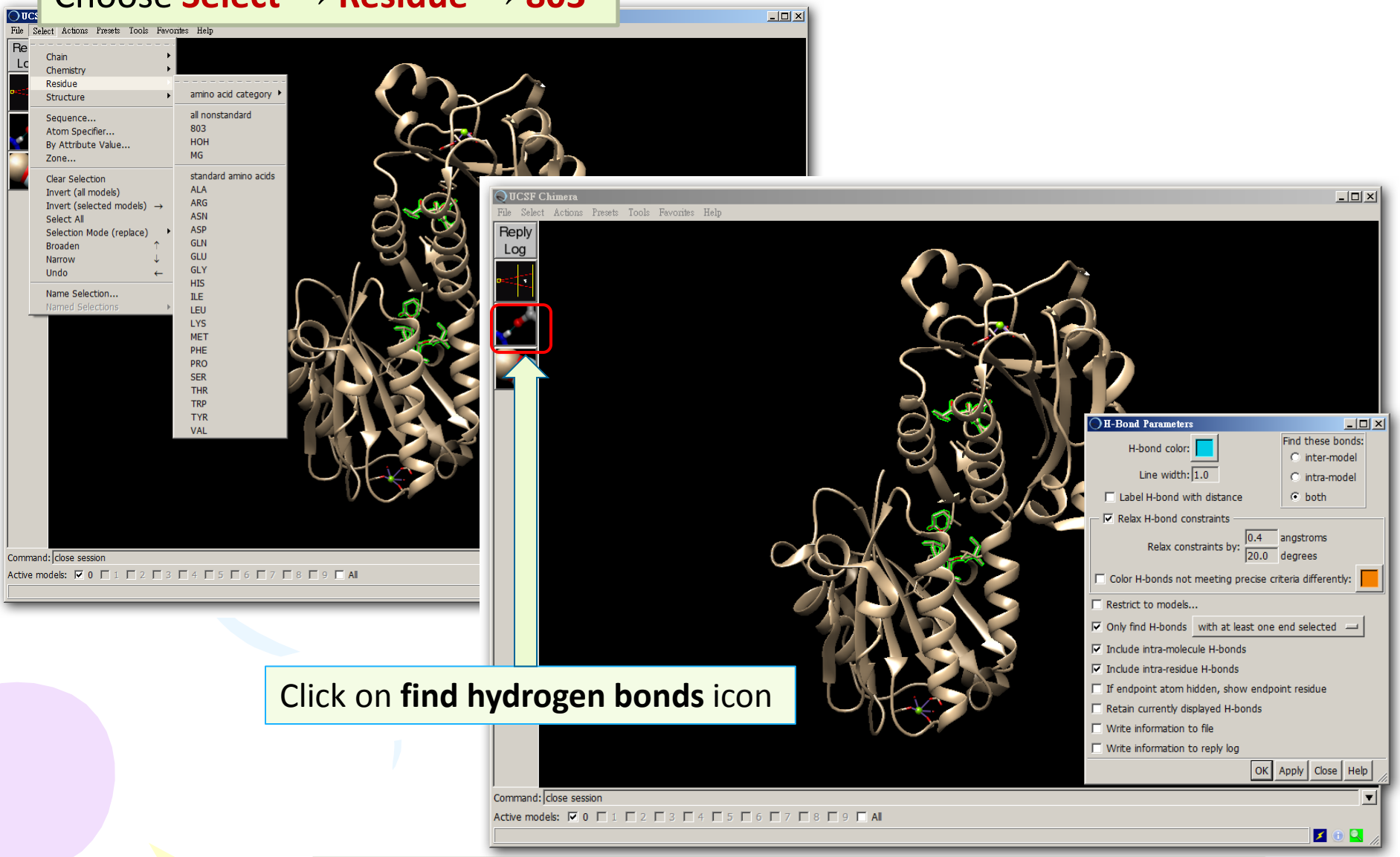
Each file of atomic coordinates opened in Chimera becomes a ***model*** with an associated model ID number. Surfaces and other types of models also have ID numbers.



Command: **close 1**

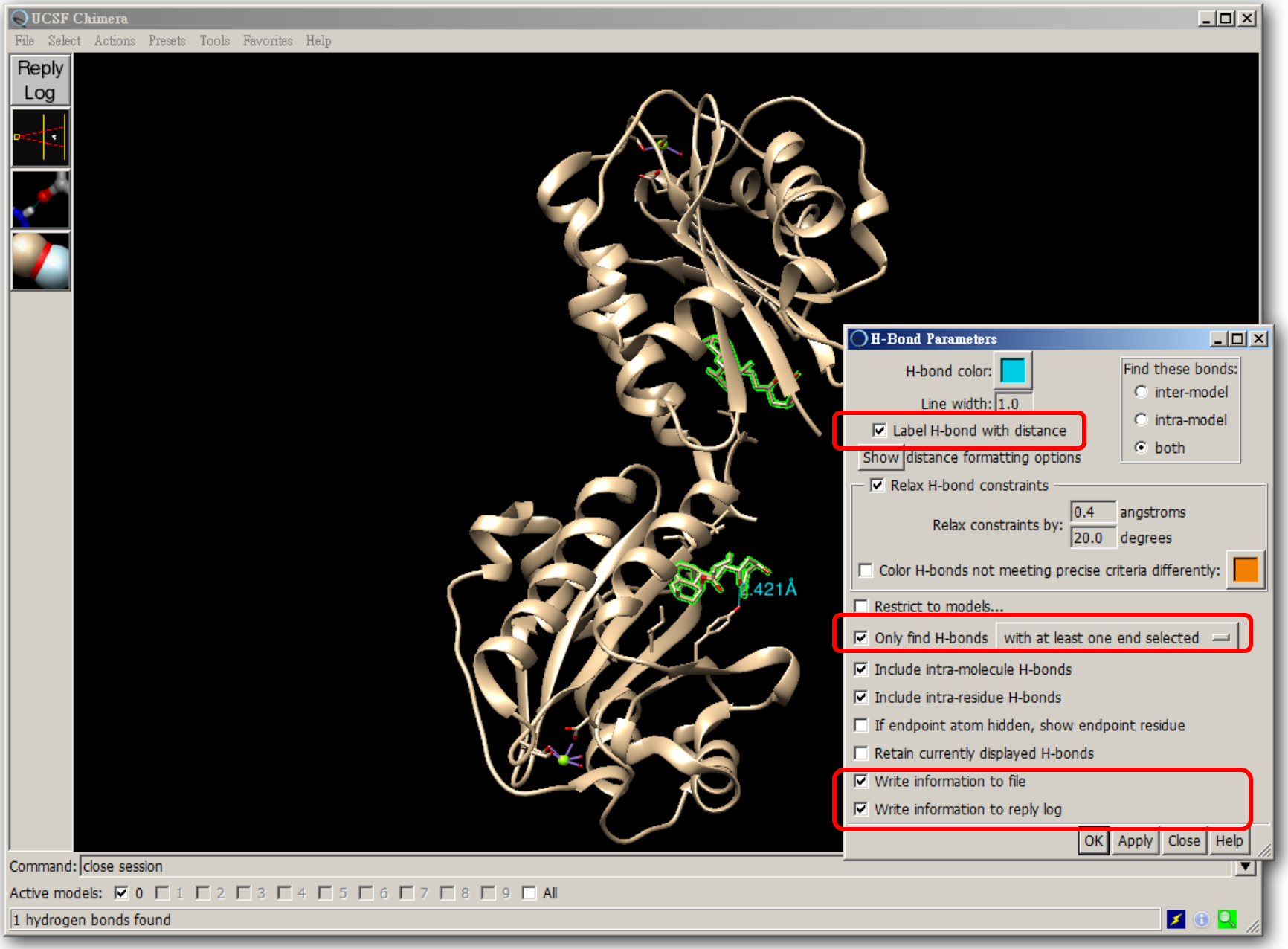
Find H-bond between ligand and protein

Choose **Select** → **Residue** → **803**

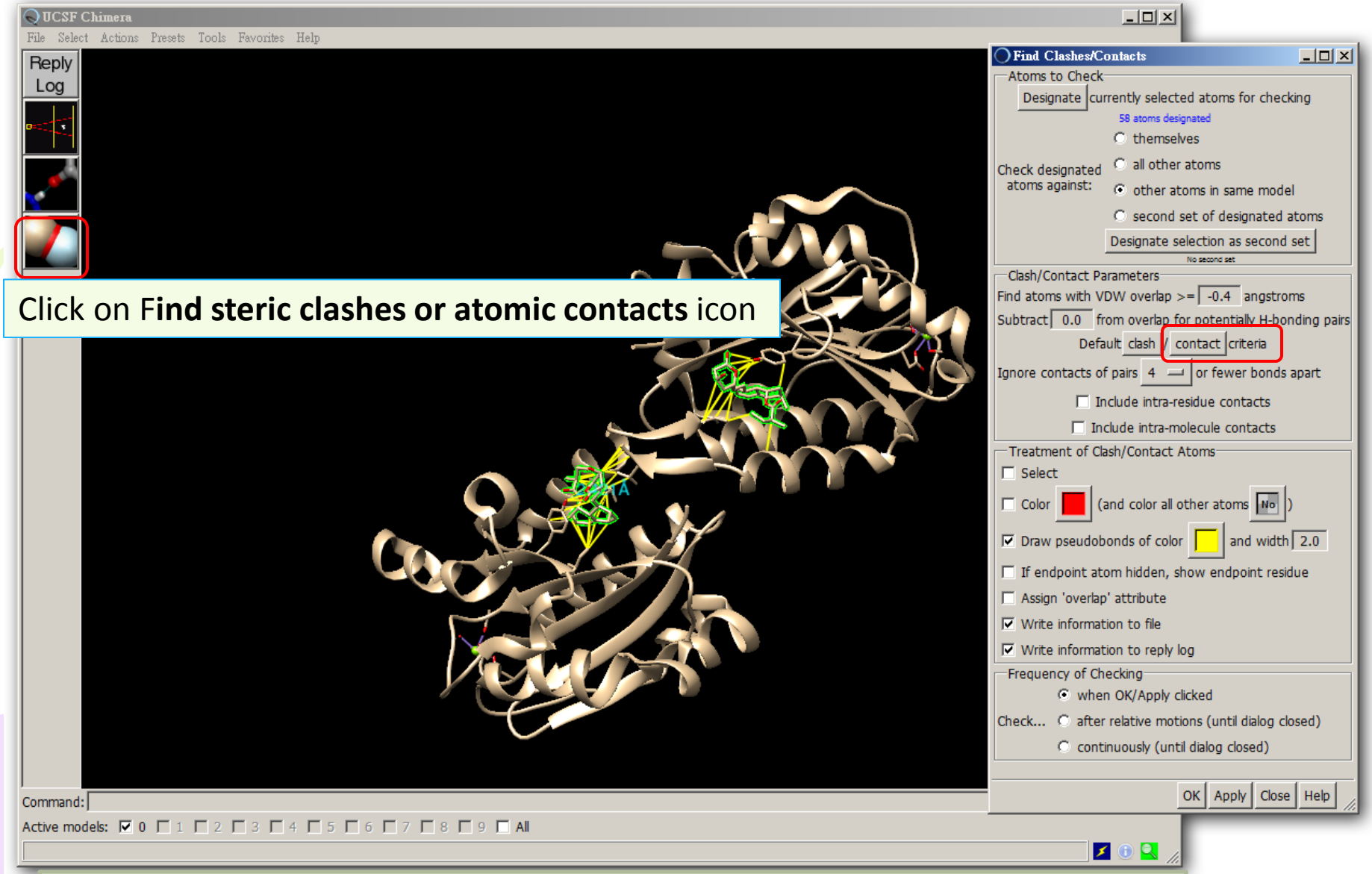


Click on **find hydrogen bonds** icon

Choose **Tools** → **Structure Analysis** → **FindHBond**


UCSF Chimera
File Select Actions Presets Tools Favorites Help
Reply Log
H-Bond Parameters
H-bond color:
Line width: 1.0
Label H-bond with distance
Show distance formatting options
Find these bonds:
inter-model
intra-model
both
Relax H-bond constraints
Relax constraints by: 0.4 angstroms
20.0 degrees
Color H-bonds not meeting precise criteria differently:
Restrict to models...
Only find H-bonds with at least one end selected
Include intra-molecule H-bonds
Include intra-residue H-bonds
If endpoint atom hidden, show endpoint residue
Retain currently displayed H-bonds
Write information to file
Write information to reply log
OK Apply Close Help
3.421Å
Command: close session
Active models: 0 1 2 3 4 5 6 7 8 9 All
1 hydrogen bonds found

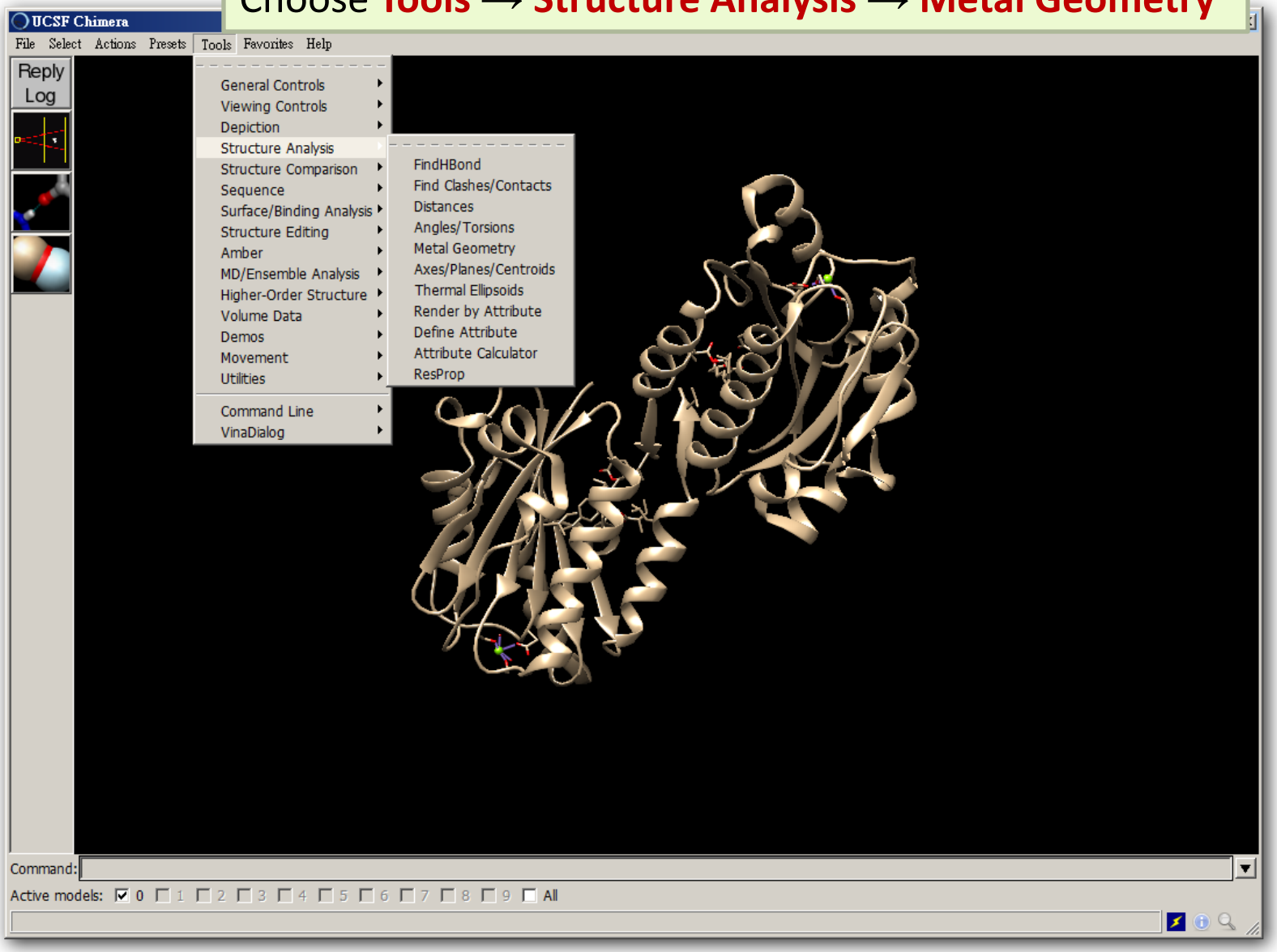
Find contacts between ligand and protein



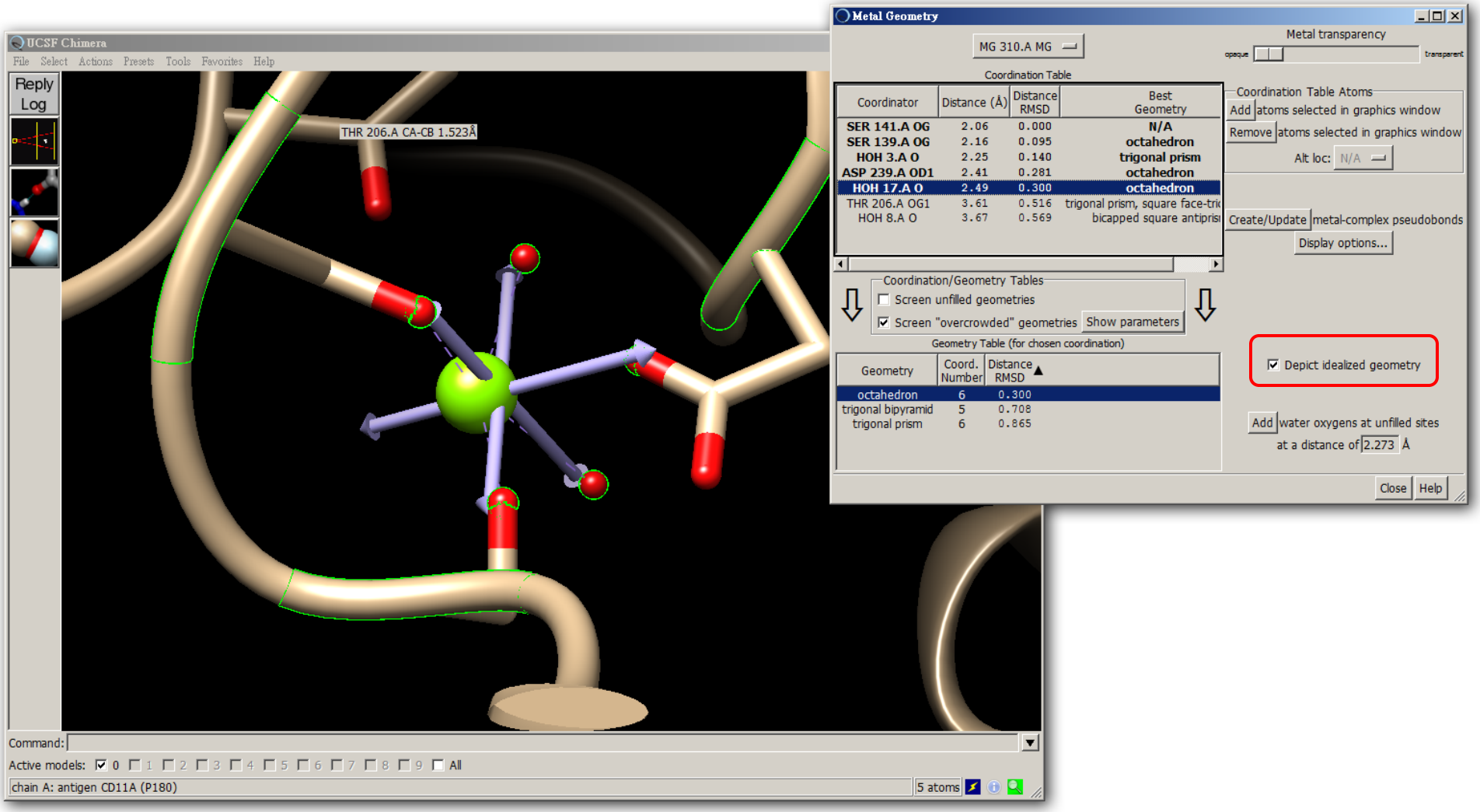
Choose **Tools** → **Structure Analysis** → **Find Clashes/Contacts**

Metal Geometry

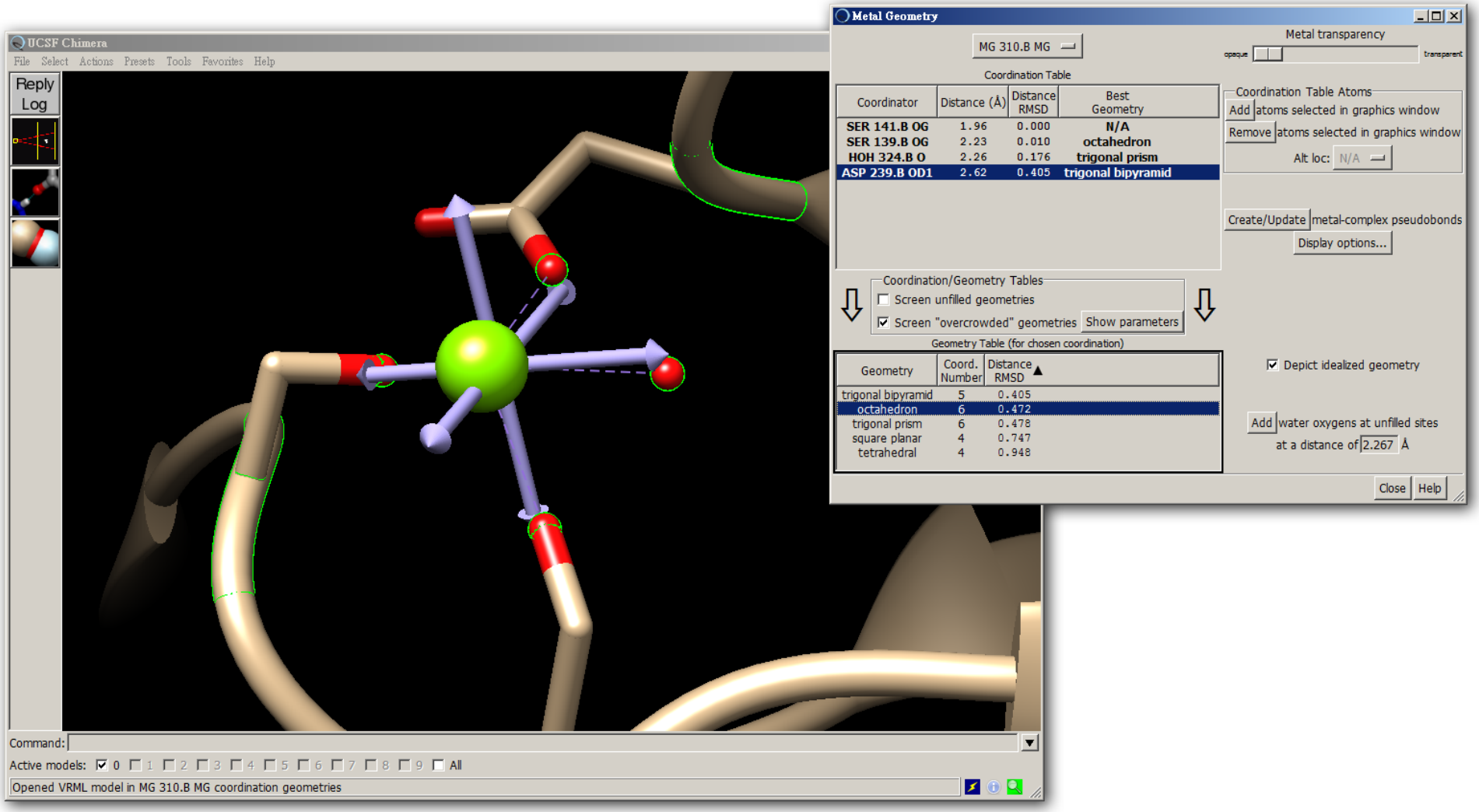
Choose **Tools** → **Structure Analysis** → **Metal Geometry**



Metal Geometry



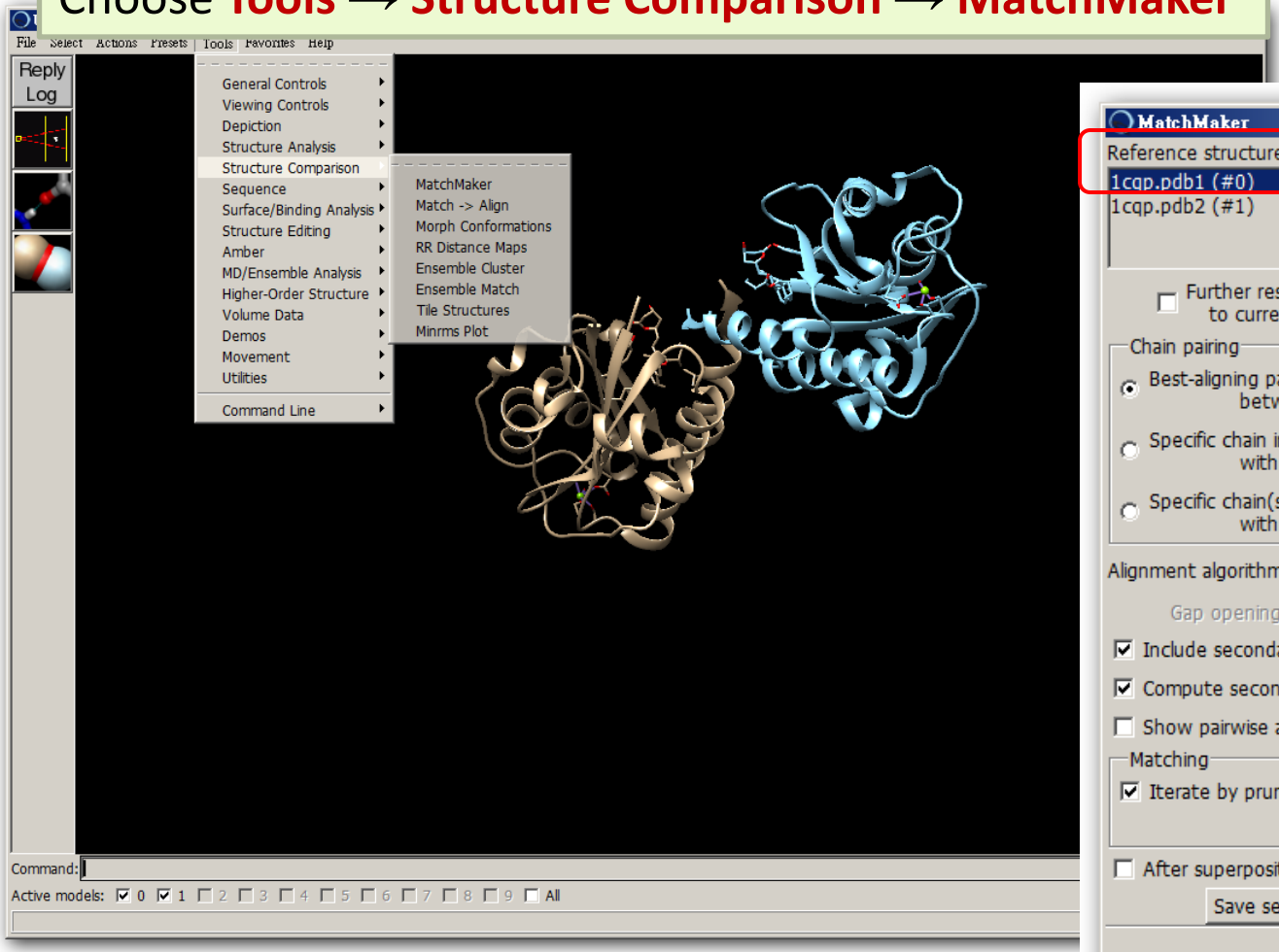
Metal Geometry

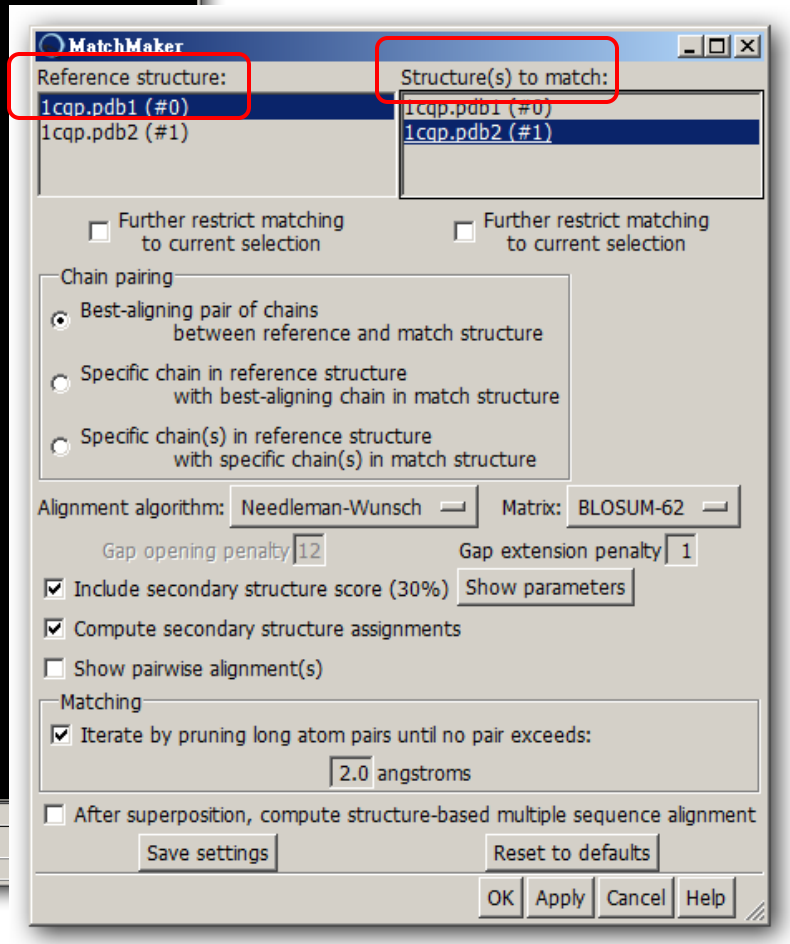


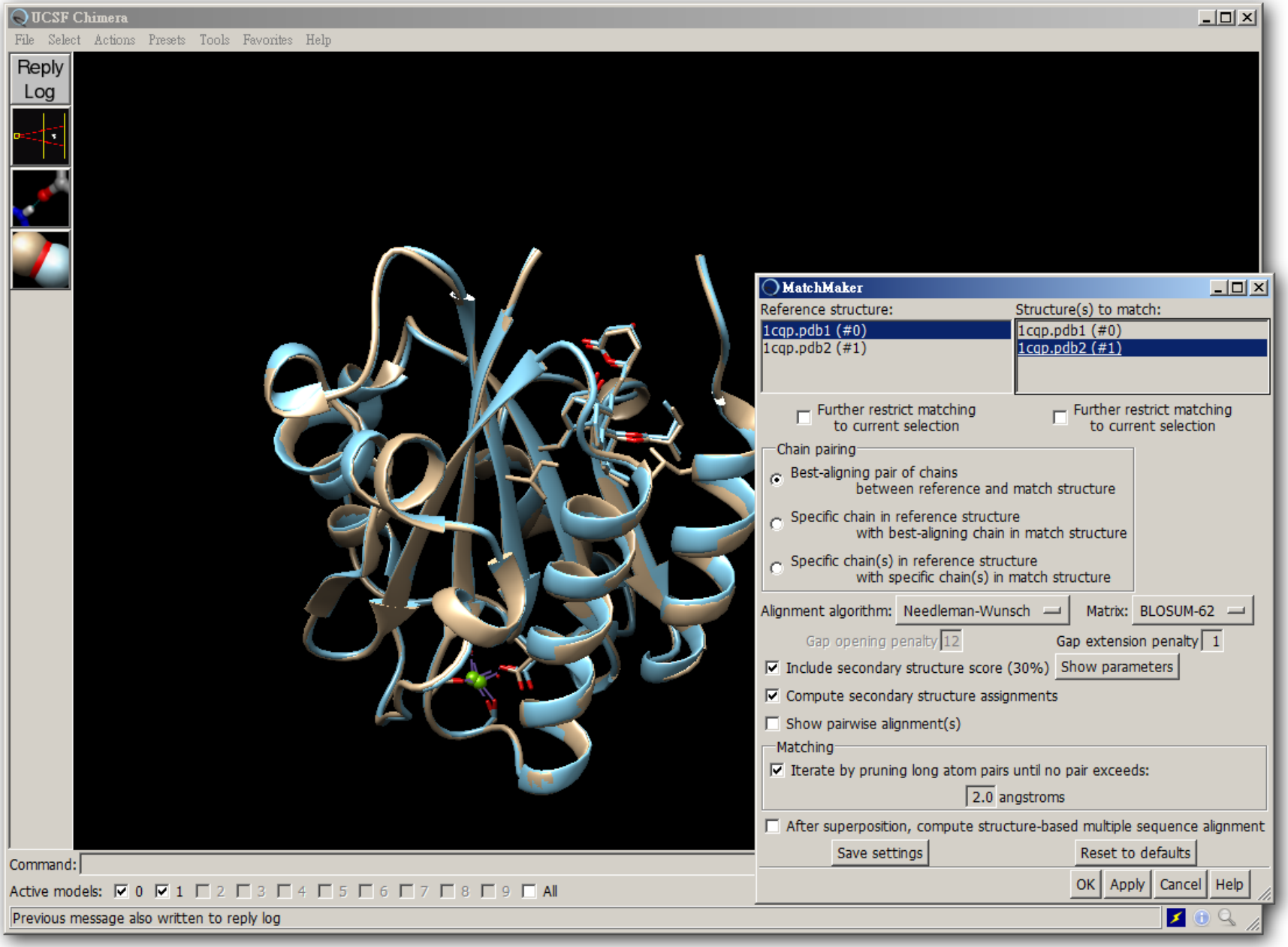
Match Maker

Open 1cqp.pdb1 and 1cqp.pdb2

Choose **Tools** → **Structure Comparison** → **MatchMaker**





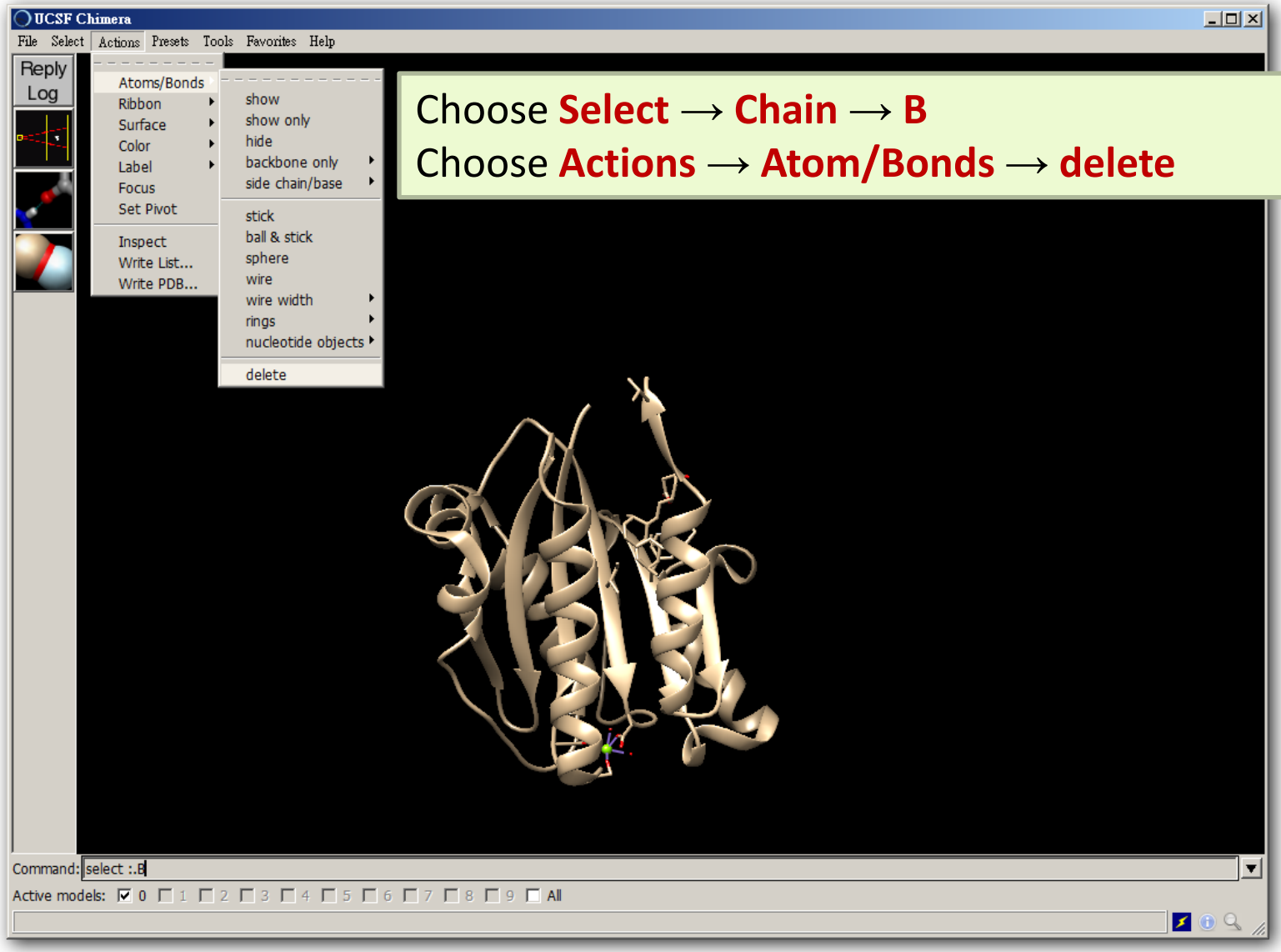


Command: **mm #0 #1**

Choose **Tools** → **Structure Comparison** → **Match Align**

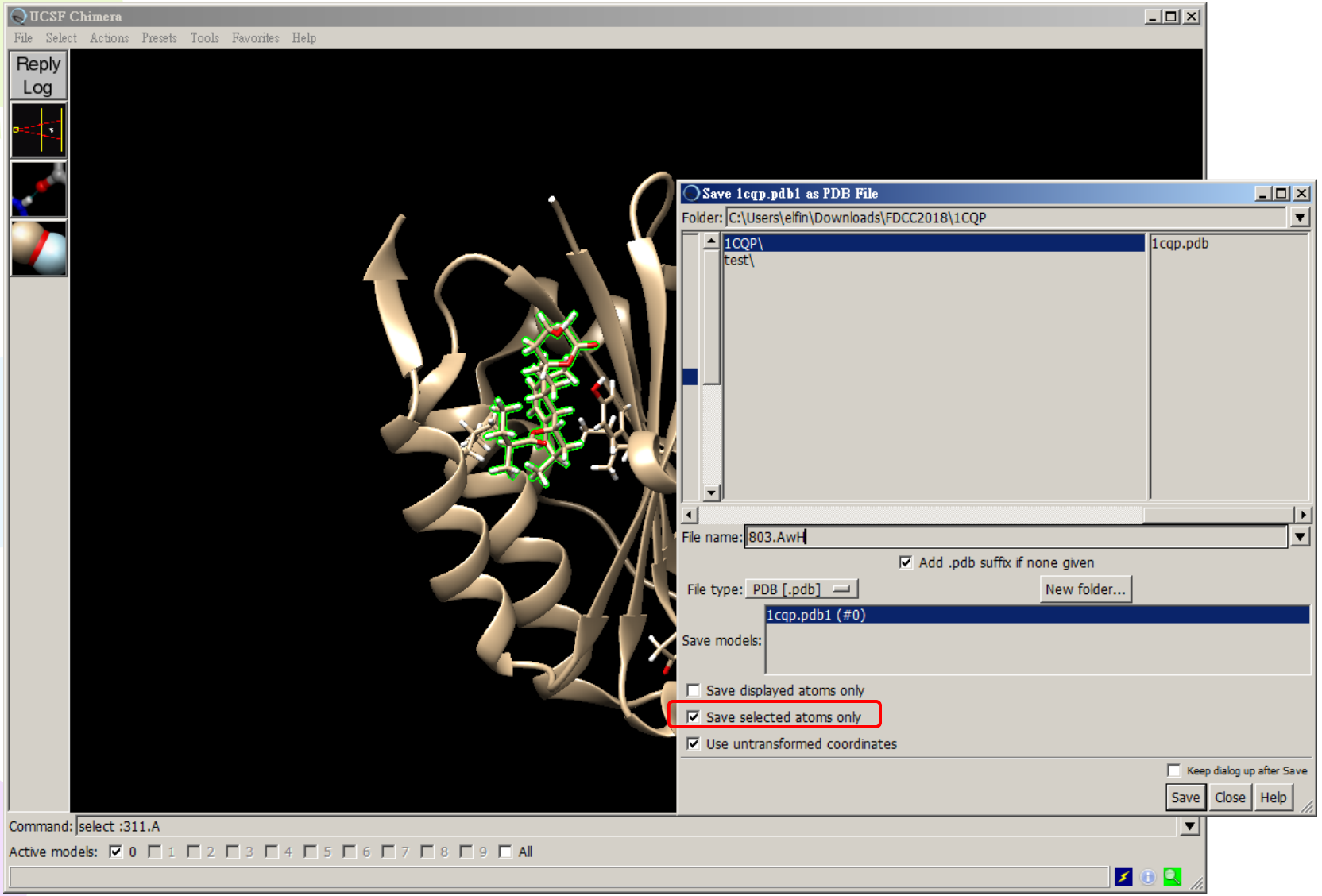
Command: **mm #0 #1 show true**

Delete Selected Structure



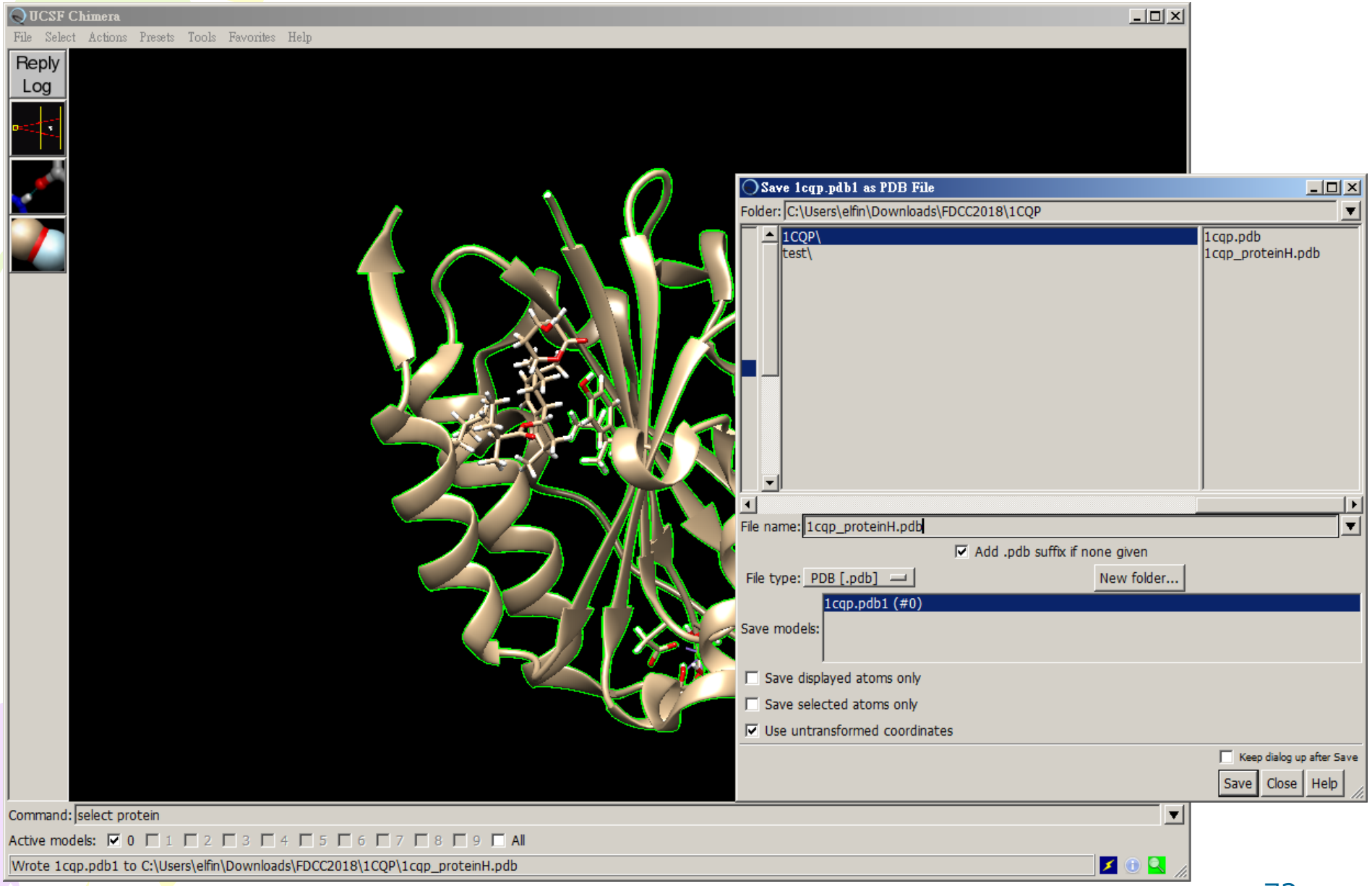
Command: **delete :.B**

Save Selected Structure



Command: **select :311.A**

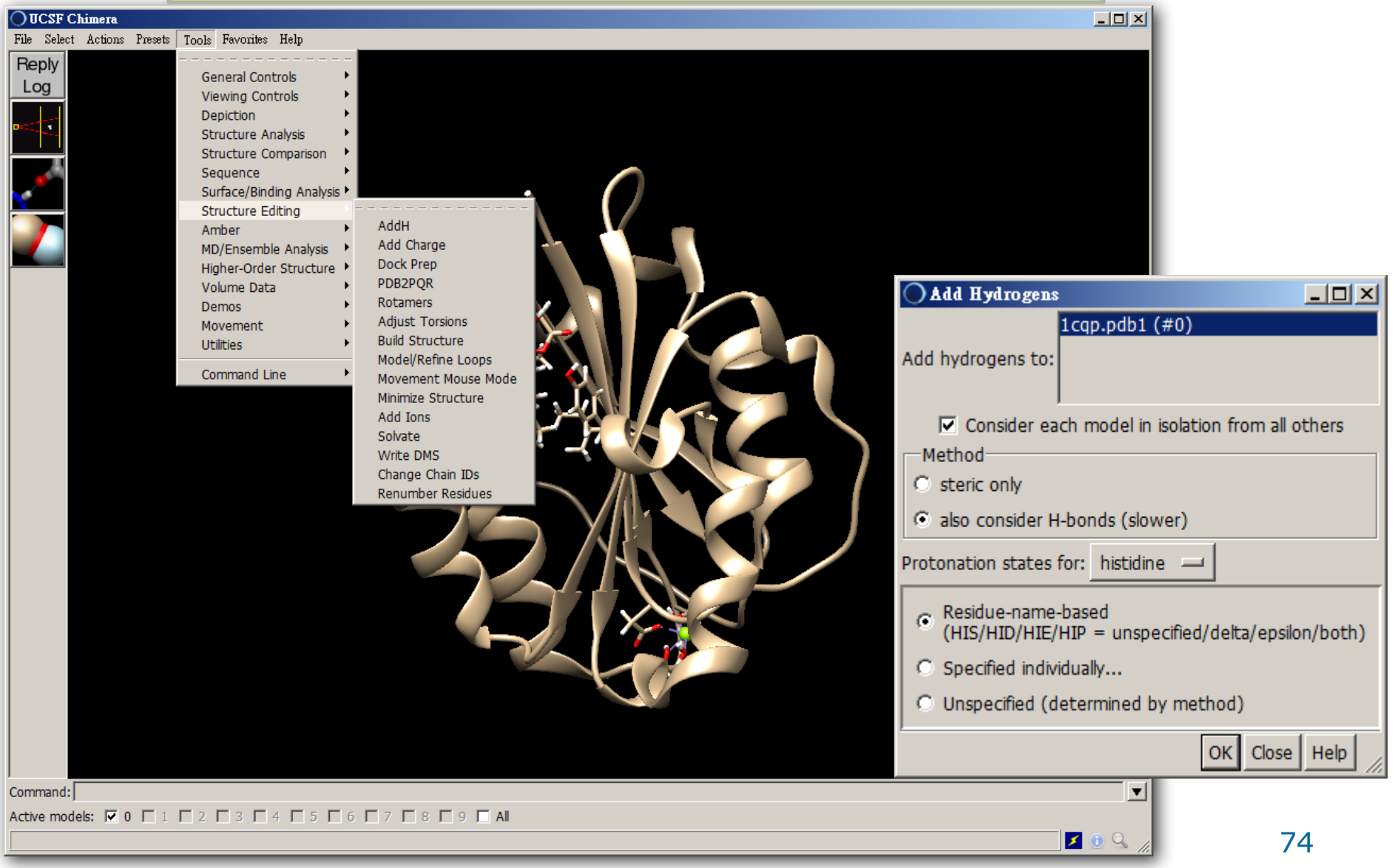
Save Selected Structure



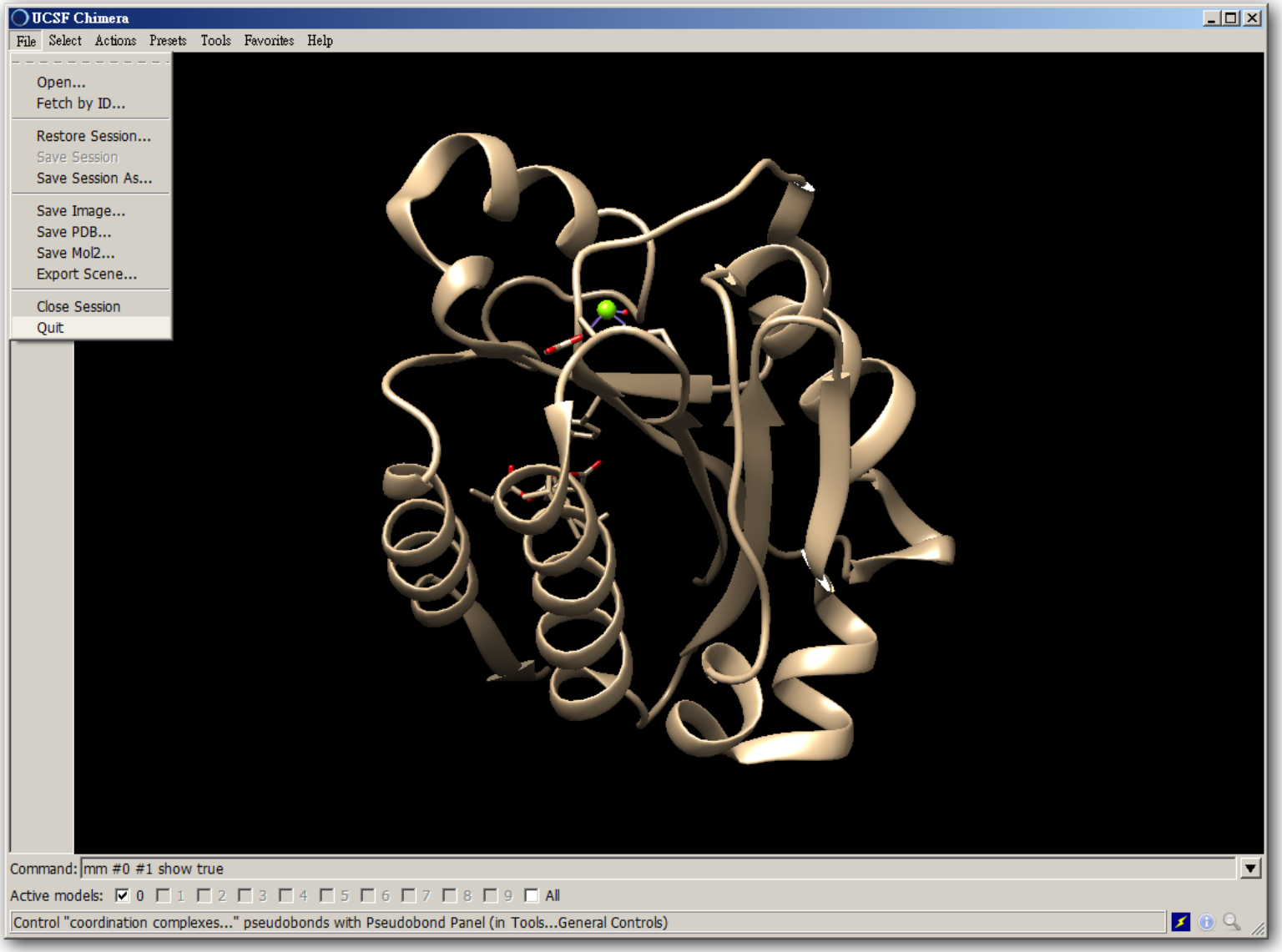
Command: **select protein**

Add Hydrogen

Choose **Tools** → **Structure Editing** → **AddH**



Choose **Files** → **Quit**



Command: **stop**

More than molecular graphics

General Controls
Command Line
Model Panel
PseudoBond Panel
Keyboard Shortcuts
Task Panel
IDLE

Viewing Controls
Side View
Camera
Effects
Lighting
Shininess

Depiction
Color Secondary Structure
Rainbow
PipesAndPlanks
Nucleotides
Render by Attribute
2D Labels
Color Actions
Ribbon Style Editor
Surface Capping
Per-Model Clipping
Color Zone
PseudoBond Reader
Color Key

Structure Analysis
FindHBond
Find Clashes/Contacts
Distances
Angles/Torsions
Metal Geometry
Axes/Planes/Centroids
Thermal Ellipsoids
Render by Attribute
Define Attribute
Attribute Calculator
ResProp

Structure Comparison
MatchMaker
Match -> Align
Morph Conformations
RR Distance Maps
Ensemble Cluster
Ensemble Match
Tile Structures
Minrms Plot

Sequence
Sequence
PDB/UniProt Info
Multalign Viewer
Match -> Align
Blast Protein
Align Chain Sequences

Surface/Binding Analysis
FindHBond
Find Clashes/Contacts
Electrostatic Surface Coloring
Coulombic Surface Coloring
APBS
Surface Capping
Surface Zone
ViewDock
Dock Prep
AutoDock Vina
Measure Volume and Area
Area/Volume from Web
Measure and Color Blobs
Intersurf
Surfnet
DelPhiController

Structure Editing
AddH
Add Charge
Dock Prep
PDB2PQR
Rotamers
Adjust Torsions
Build Structure
Model/Refine Loops
Movement Mouse Mode
Minimize Structure
Add Ions
Solvate
Write DMS
Change Chain IDs
Renumber Residues

Amber
Add Ions
Solvate
Write Prmtop

MD/Ensemble Analysis
MD Movie
Ensemble Cluster
Ensemble Match
Tile Structures
Molecular Dynamics Simulation

Higher-Order Structure
Multiscale Models
Unit Cell
Crystal Contacts
Small-Angle X-Ray Profile
Scale Bar
Icosahedron Surface
Flatten Icosahedron
Cage Builder

Volume Data
Volume Viewer
Fit in Map
Surface Color
Color Zone
Morph Map
Volume Tracer
Volume Filter
Hide Dust
Segment Map
Fit to Segments
MultiFit
Volume Eraser
Measure Volume and Area
Measure and Color Blobs
Volume Mean, SD, RMS
Values at Atom Positions
Volume Series
Volume Menu on Menubar

Demos
Demo Editor

Movement
Rotation
Undo Move
Redo Move
Movement Mouse Mode
Constrained Move
Transform Coordinates

Utilities
Reply Log
2D Labels
Notepad
Movie Recorder
Color Key
Animation
Structure Diagram
Browser Configuration
Benchmark
Color Editor
Palette Editor
ReadStdin
RESTServer

Chimera Command Line Scripts

Hbond.com

```
## find hydrogen bond between ligand and protein
open 1cqp.pdb
select ligand
hbonds selRestrict cross showDist true saveFile 1cqp_Hbondinfo.txt
~sel
color  byelement ligand
copy file 1cqp_Hbond.png png width 400 height 300
#stop
```

$**chimera Hbond.com**

Command: **open Hbond.com**

Chimera Python Scripts

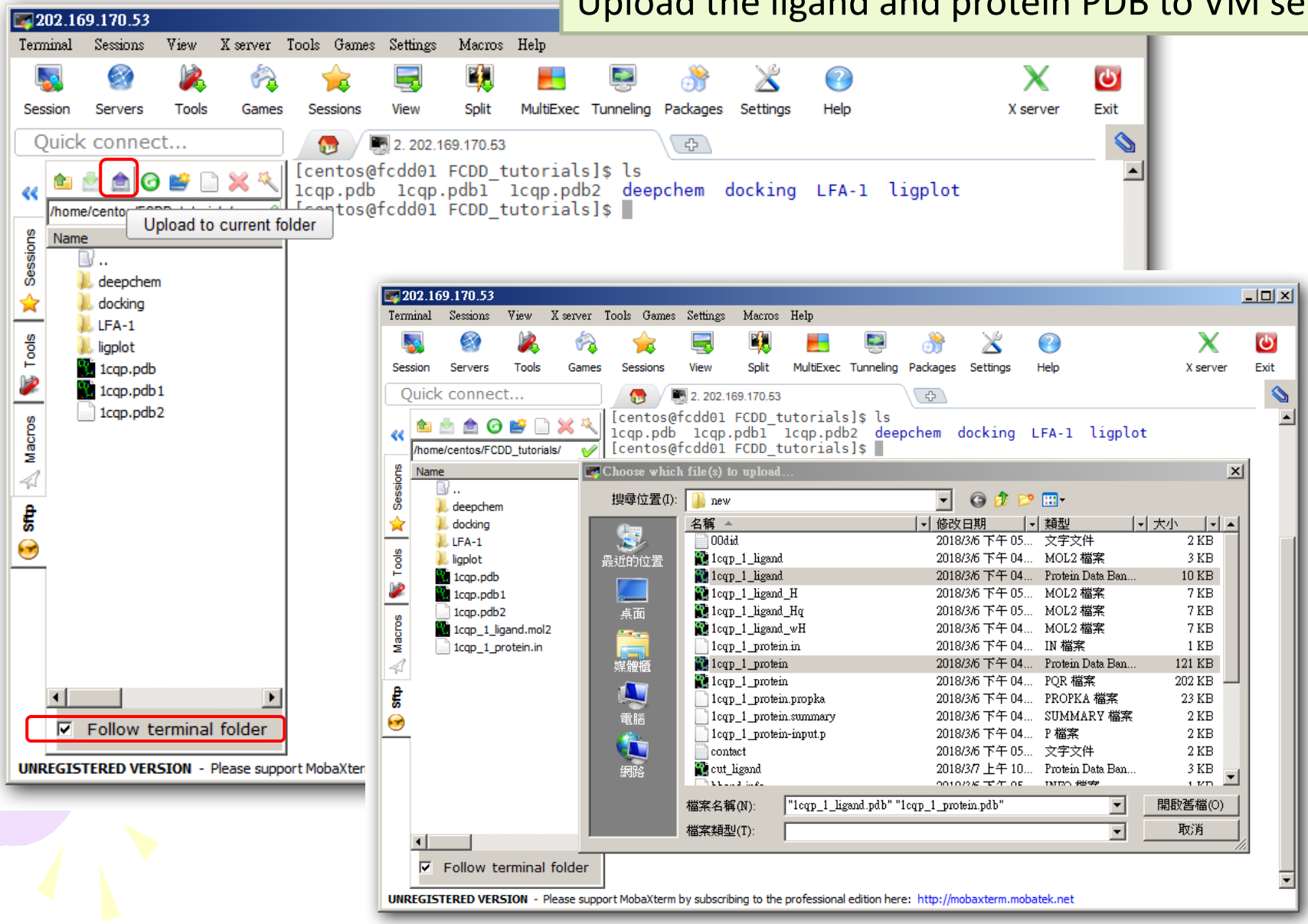
While the command line can be used for many things, the ultimate control of chimera is through Python scripts.

https://www.cgl.ucsf.edu/chimera/current/docs/ProgrammersGuide/index.html

http://www.cgl.ucsf.edu/Outreach/Workshops/UCSF-Fall-2005/09-ScriptDemo/Scripting_Tutorial.html

```
$cd ~/FCDD_tutorials
$ls
```

Upload the ligand and protein PDB to VM server.



LigPlot and LigPlot+

https://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/

LIGPLOT: a program to generate schematic diagrams of protein-ligand interactions

Andrew C. Wallace ✉, Roman A. Laskowski, Janet M. Thornton

Protein Engineering, Design and Selection, Volume 8, Issue 2, 1 February 1995, Pages 127–134, https://doi.org/10.1093/protein/8.2.127

Published: 01 February 1995 **Article history** ▾

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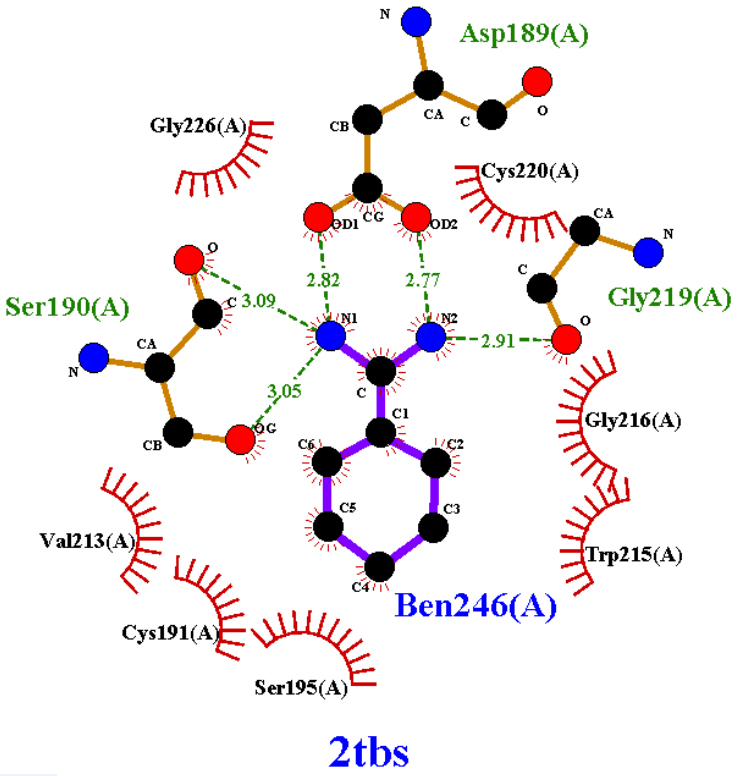
Abstract

The LIGPLOT program automatically generates schematic 2-D representations of protein-ligand complexes from standard Protein Data Bank file input The output is a colour, or black-and-white, PostScript file giving a simple and informative representation of the intermolecular interactions and their strengths, including hydrogen bonds, hydrophobic interactions and atom accessibilities. The program is completely general for an ligand and can also be used to show other types of interaction in proteins and nucleic acids. It was designed to facilitate the rapid inspection of many enzyme complexes, but has found many other applications



LigPlot and LigPlot+

https://www.ebi.ac.uk/thornton-srv/software/LigPlus/

LigPlot+: Multiple Ligand–Protein Interaction Diagrams for Drug Discovery

Roman A. Laskowski*† and Mark B. Swindells‡
European Bioinformatics Institute, Wellcome Trust Genome Campus, Hinxton, Cambridge CB10 1SD, United Kingdom
Ebisu, 12 High Street Easton on the Hill near Stamford, PE9 3LR, United Kingdom

J. Chem. Inf. Model., **2011**, *51* (10), pp 2778–2786
DOI: 10.1021/ci200227u
Publication Date (Web): September 15, 2011

E-mail: roman@ebi.ac.uk.

Cite this: *J. Chem. Inf. Model. 51, 10, 2778-2786*
RIS Citation GO

LigPlot+ is a successor to the original **LIGPLOT** program. It is run from an intuitive java interface which allows on-screen editing of the plots via mouse click-and-drag operations.

1. Superposition of related diagrams
2. Improved DIMPLOT program
3. Links to PyMOL and RasMol

https://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/manual/

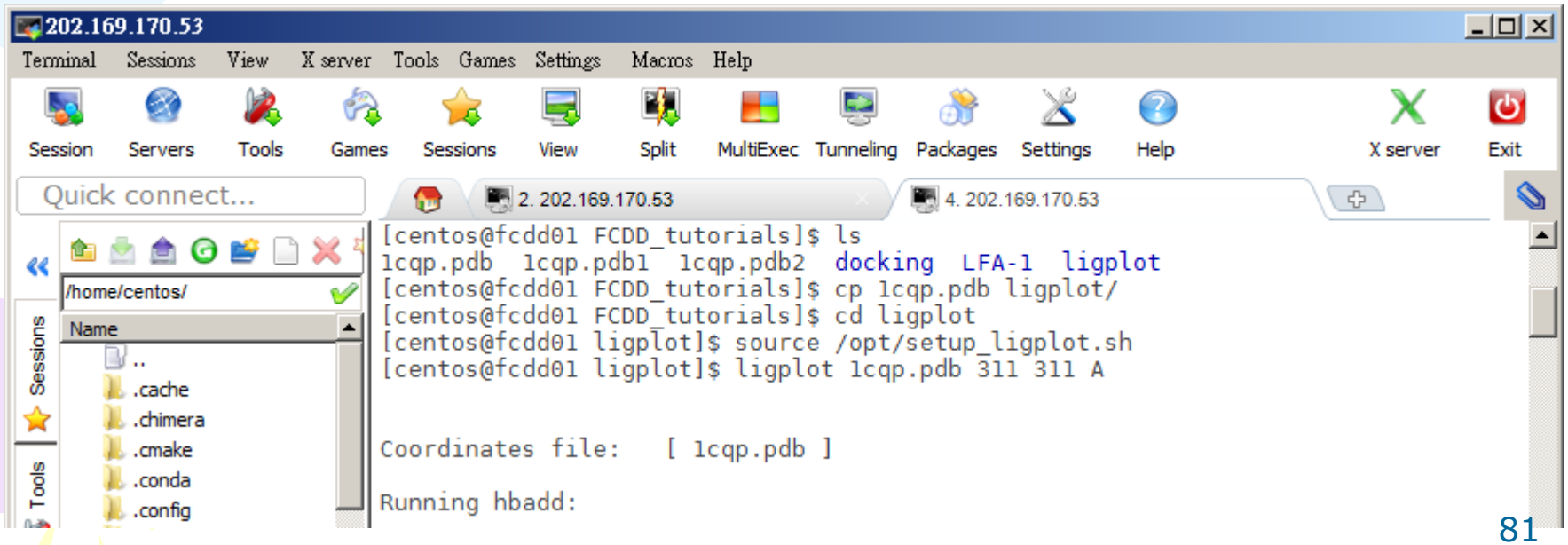
https://www.ebi.ac.uk/thornton-srv/software/LigPlus/manual2/manual.html

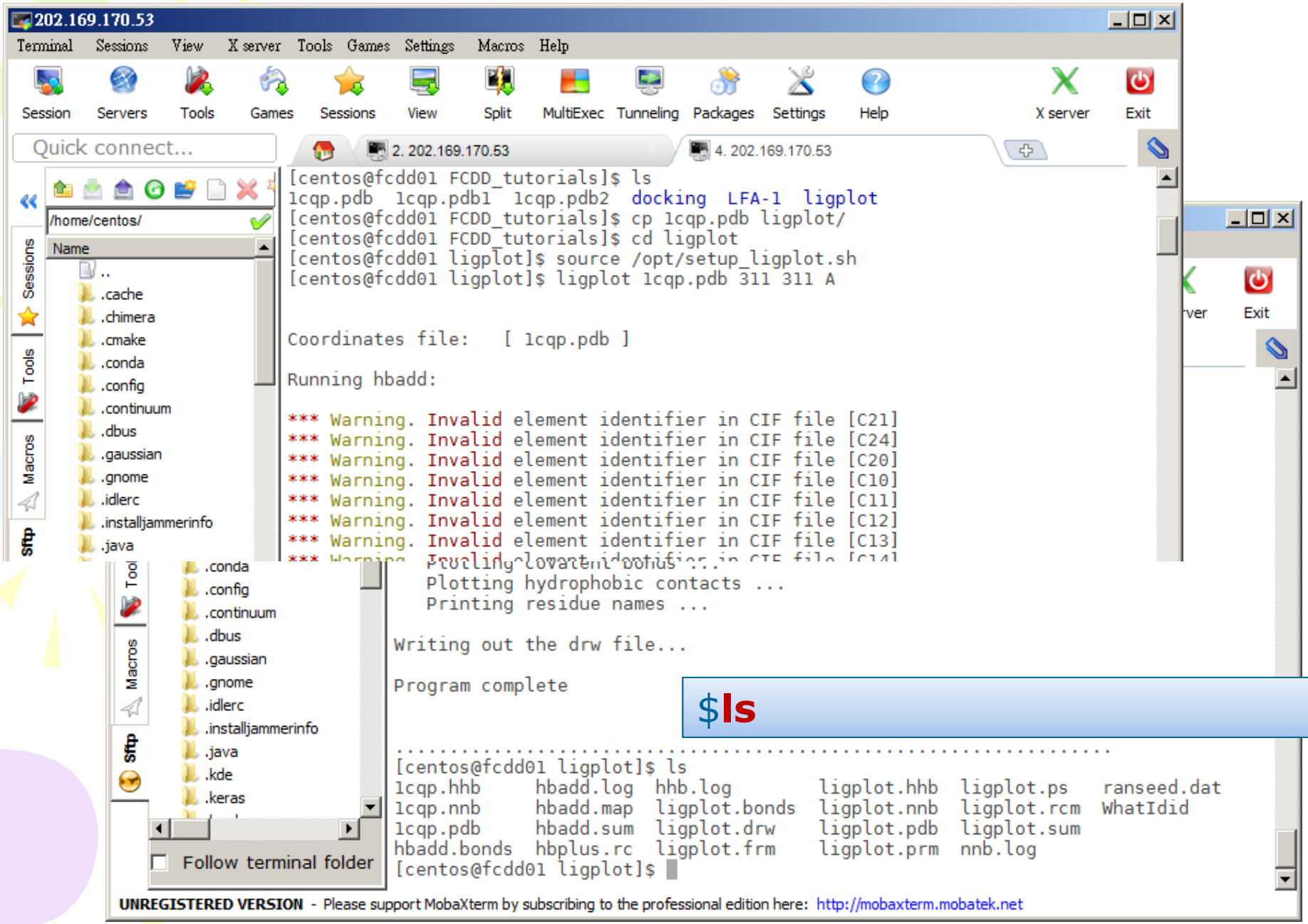
https://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/manual/

```
$cd ~/FCDD_tutorials
$mkdir ligplot
$copy 1cqp.pdb ligplot
$cd ligplot
$source /opt/setup_ligplot.sh
$ligplot 1cqp.pdb 311 311 A
```

ligplot *filename* [residue1] [residue2] [chain_id] [-w] [-m]

[-w] indicates that the ligand is a single water molecule or group of water molecules
[-m] indicates that the ligand is a single metal ion




202.169.170.53
Terminal Sessions View X server Tools Games Settings Macros Help
Session Servers Tools Games Sessions View Split MultiExec Tunneling Packages Settings Help X server Exit
Quick connect...
2. 202.169.170.53
4. 202.169.170.53
/home/centos/
Name
.cache
.chimera
.cmake
.conda
.config
.continuum
.dbus
.gaussian
.gnome
.idlerc
.installjammerinfo
.java
.kde
.keras
Sessions
Tools
Macros
Sftp
[centos@fcdd01 FCDD_tutorials]$ ls
1cqp.pdb 1cqp.pdb1 1cqp.pdb2 docking LFA-1 ligplot
[centos@fcdd01 FCDD_tutorials]$ cp 1cqp.pdb ligplot/
[centos@fcdd01 FCDD_tutorials]$ cd ligplot
[centos@fcdd01 ligplot]$ source /opt/setup_ligplot.sh
[centos@fcdd01 ligplot]$ ligplot 1cqp.pdb 311 311 A
Coordinates file: [1cqp.pdb]
Running hbadd:
*** Warning. Invalid element identifier in CIF file [C21]
*** Warning. Invalid element identifier in CIF file [C24]
*** Warning. Invalid element identifier in CIF file [C20]
*** Warning. Invalid element identifier in CIF file [C10]
*** Warning. Invalid element identifier in CIF file [C11]
*** Warning. Invalid element identifier in CIF file [C12]
*** Warning. Invalid element identifier in CIF file [C13]
Plotting hydrophobic contacts ...
Printing residue names ...
Writing out the drw file...
Program complete
$ls
[centos@fcdd01 ligplot]$ ls
1cqp.hhb hbadd.log hhb.log ligplot.hhb ligplot.ps ranseed.dat
1cqp.nnb hbadd.map ligplot.bonds ligplot.nnb ligplot.rcm WhatIdid
1cqp.pdb hbadd.sum ligplot.drw ligplot.pdb ligplot.sum
hbadd.bonds hbplus.rc ligplot.frm ligplot.prm nnb.log
[centos@fcdd01 ligplot]$
Follow terminal folder
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: http://mobaxterm.mobatek.net

The input files to LIGPLOT are:

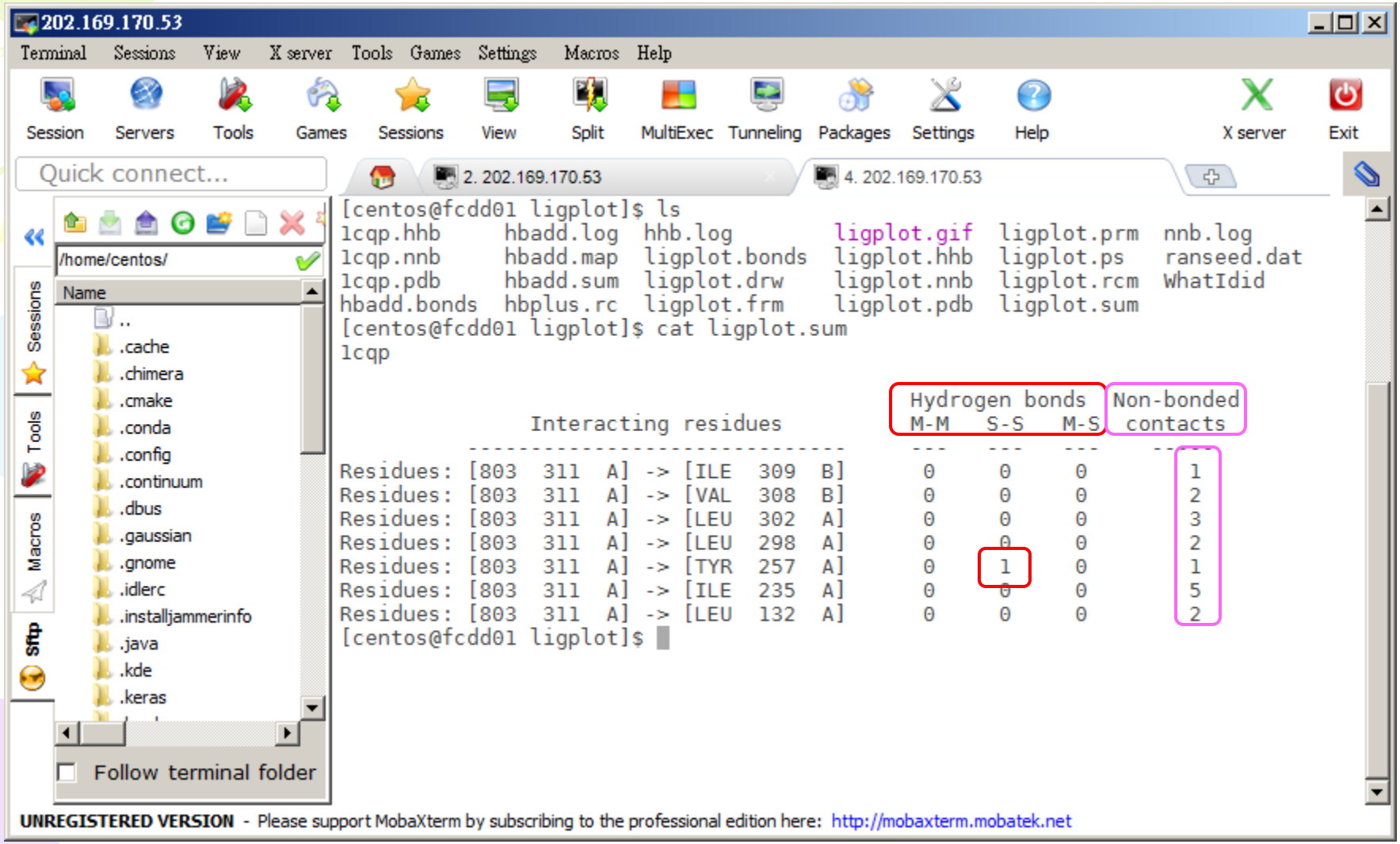
- **filename.pdb** - Input PDB file holding the coordinates of the protein and ligand.
- filename.hhb - List of hydrogen-bonds in the structure. This can either be generated by the **HBPLUS** program, or supplied by any other program in the format specified.
- filename.nnb - List of nonbonded contacts in the structure. Again, this can either be generated by the **HBPLUS** program, or supplied by any other program in the format specified.
- **ligplot.prm** - Parameter file containing parameters governing the final appearance of the plot. It is automatically created when you first run LIGPLOT. It can then be edited using any text-based editor to alter the parameters controlling the appearance of the plot - eg colours, text sizes, etc.

https://www.ebi.ac.uk/thornton-srv/software/LIGPLOT/manual/man5.html

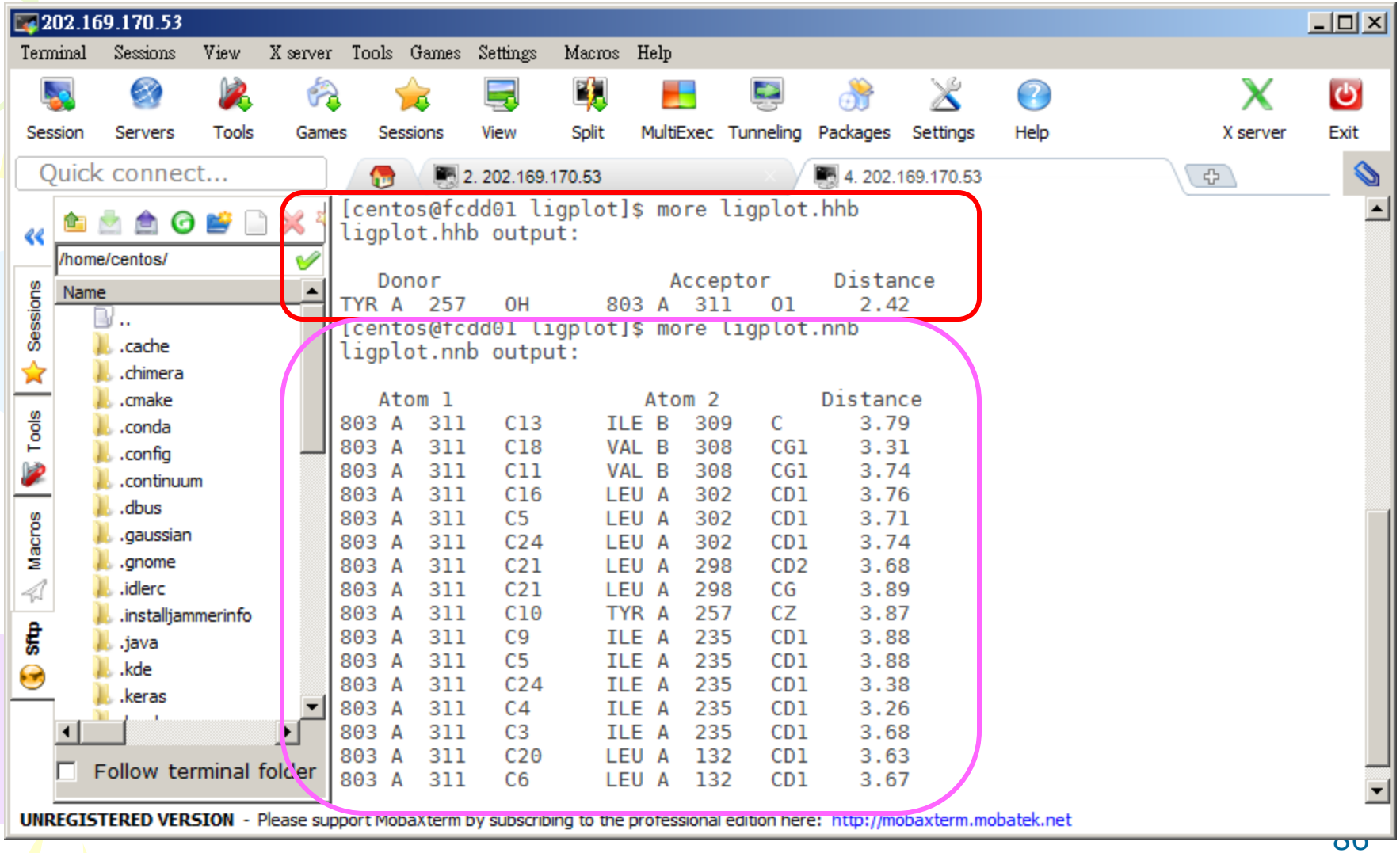
The output files produced by LIGPLOT are:

- **ligplot.ps** - Colour or black-and-white PostScript showing the plotted LIGPLOT diagram. This can be viewed using any PostScript viewer, or plotted on any PostScript printer.
- ligplot.pdb - Output file, in PDB format, of the final flattened molecules (ligand and interacting protein residues) as shown in the plot. This file can be loaded into any standard molecular graphics package, and appears as a very flat molecule(!).
- **ligplot.hhb** - Output file, in LIGPLOT format, of just those hydrogen bonds in the original *filename*.hhb file that were used by LIGPLOT in producing the final picture.
- **ligplot.nnb** - Output file, in LIGPLOT format, of just those hydrophobic contacts in the original *filename*.nnb file that were used by LIGPLOT in producing the final.
- ligplot.bonds - Output file listing of bonds and bond-types in the final LIGPLOT picture.
- ligplot.frm - Output file, in PDB format, of the molecules shown in the plot, prior to flattening. You can view this file using any molecular graphics program (*eg* Rasmol) to see only those residues that interact with the ligand.
- ligplot.rcm - Output file listing all the residues on the plot, together with the *x*-*y* coordinates of their centres of mass. The file provides a useful starting point if positional restraints on the residues of the plot are required.
- ligplot.drw - File for input to the Java-based LIGPLOT editor, LigEd.

$cat ligplot.sum

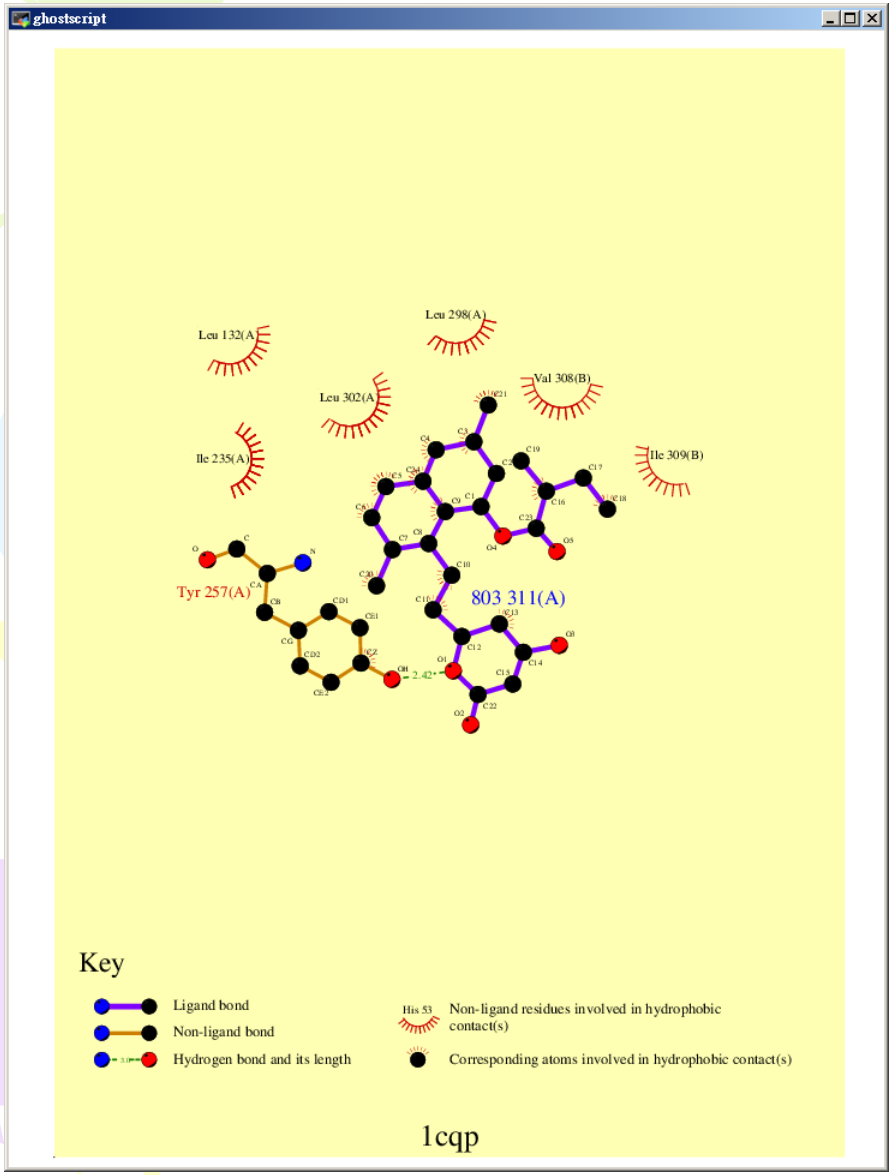


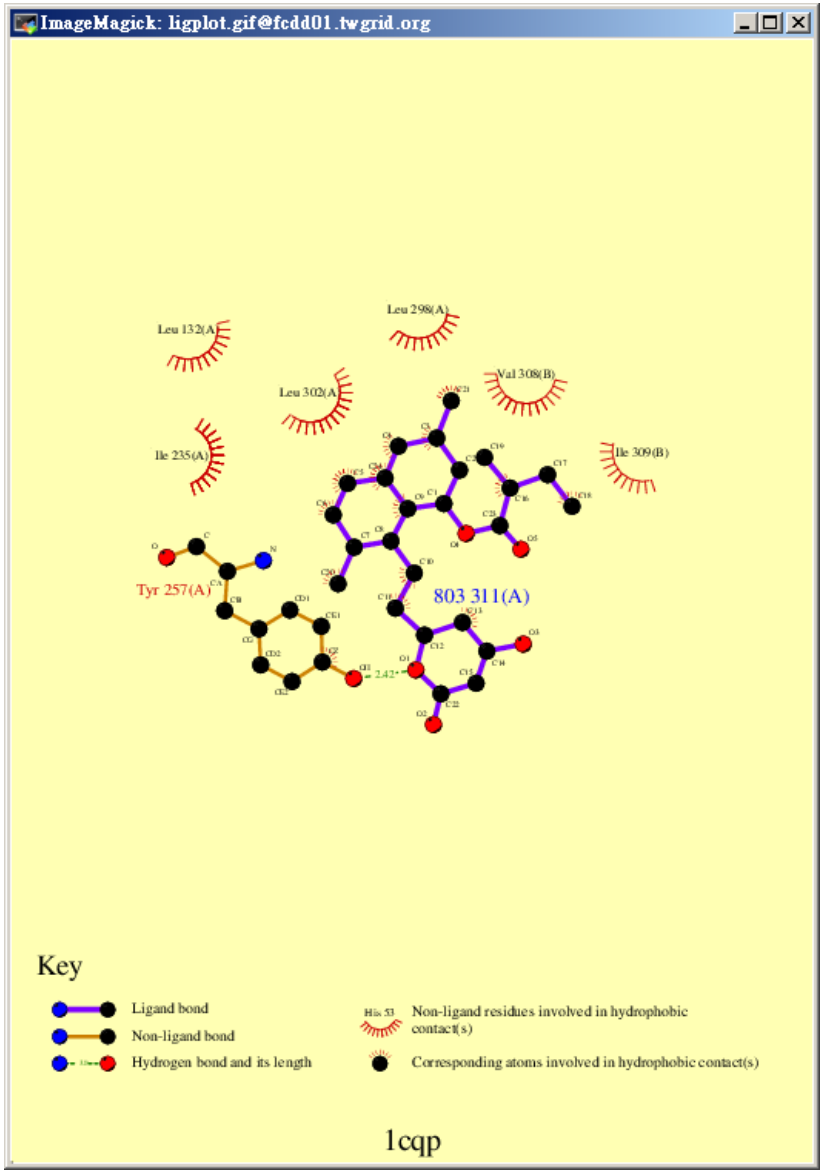
$more ligplot.hhb
$more ligplot.nnb



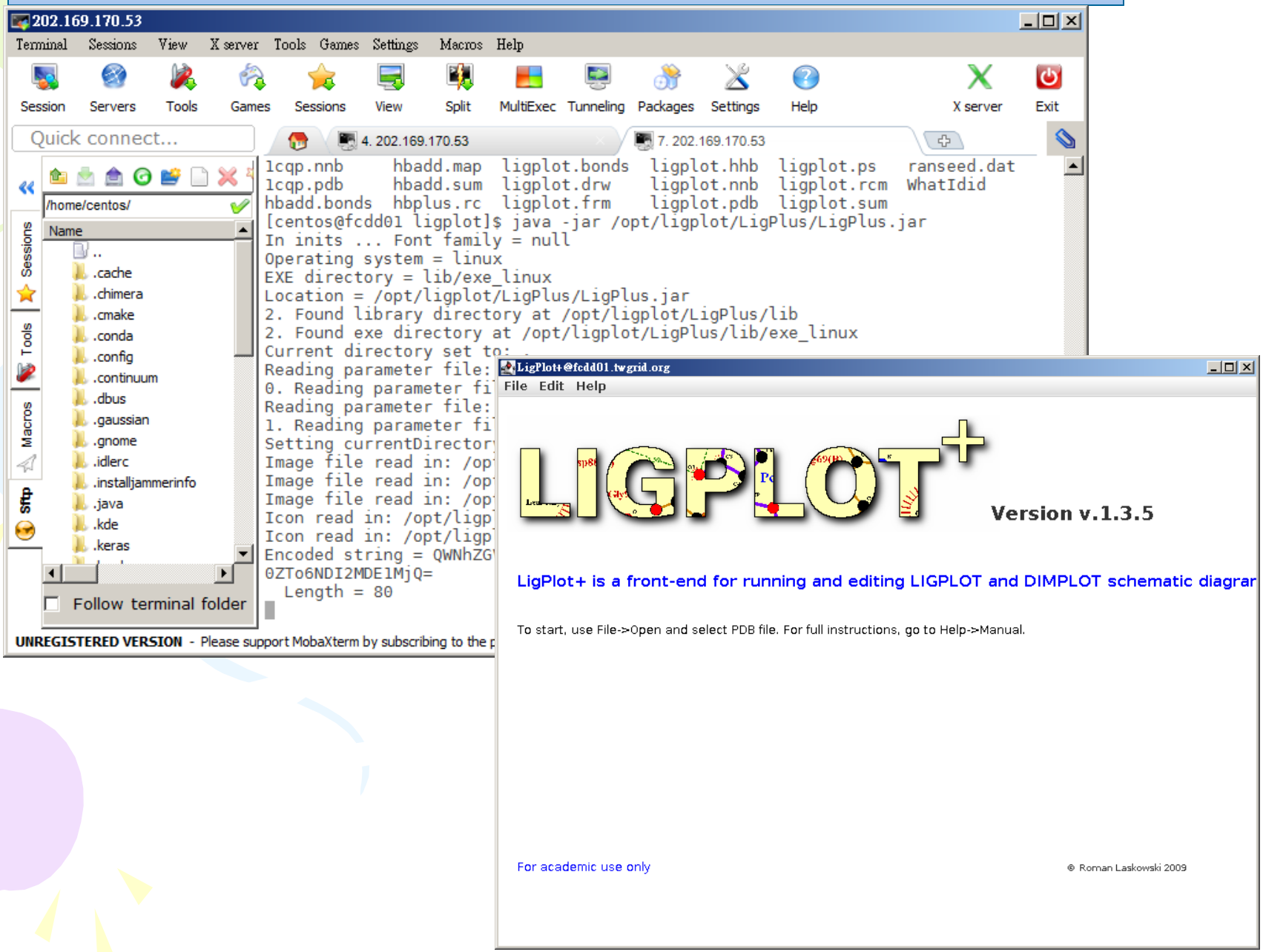
$ghostscript ligplot.ps

$convert ligplot.ps ligplot.gif
$display

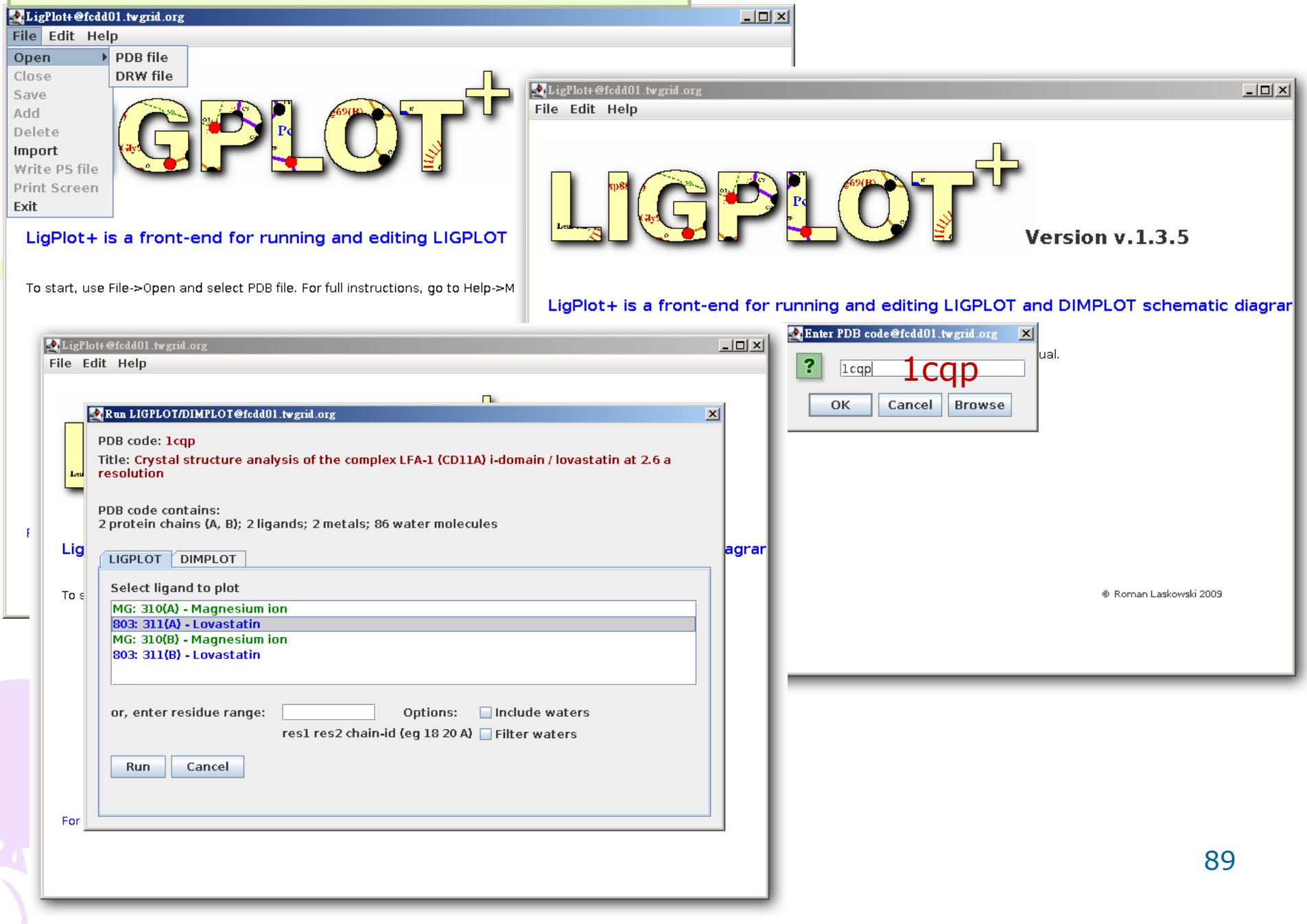


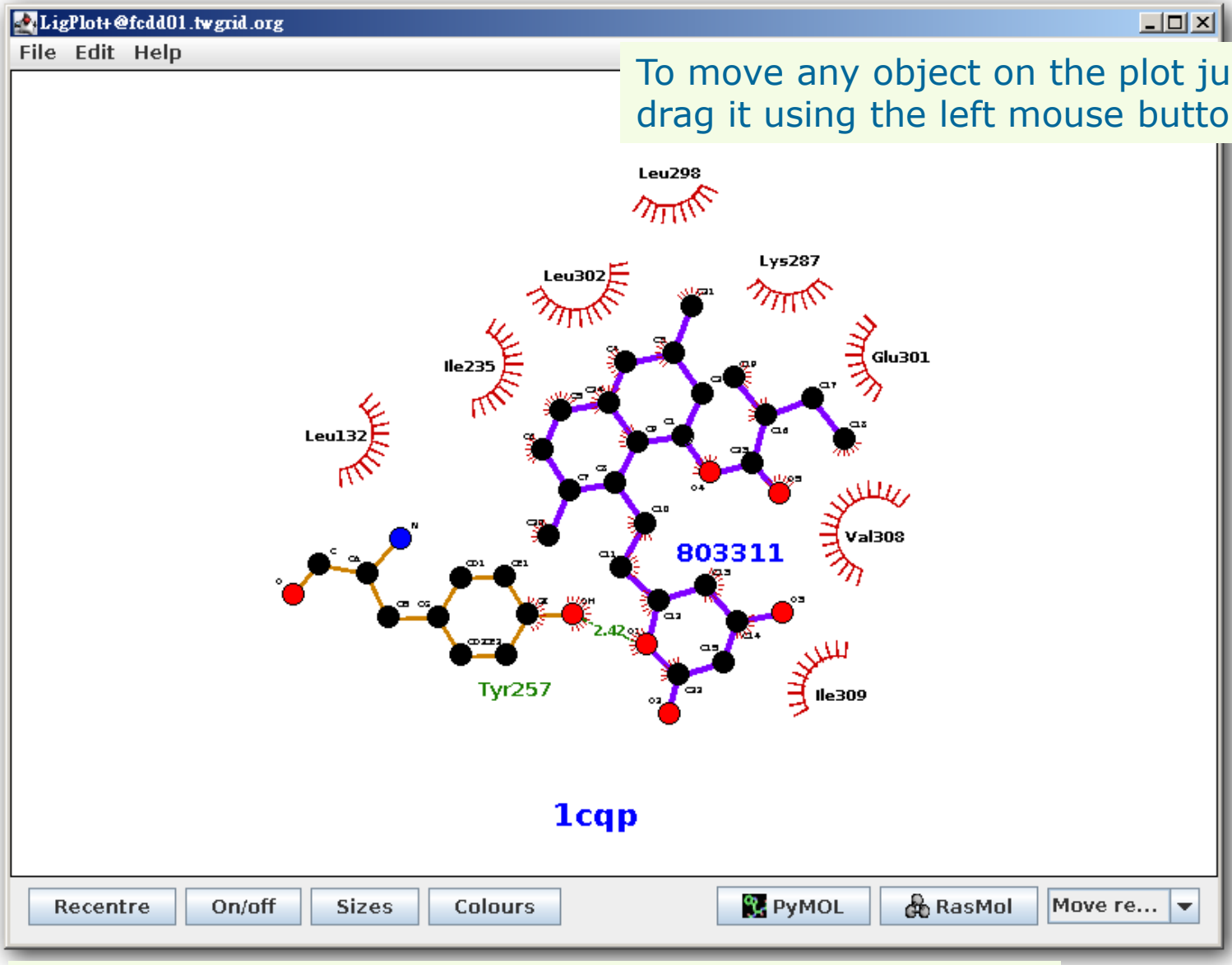


$java -jar /opt/ligplot/LigPlus/LigPlus.jar



Choose File → Open → PDB file

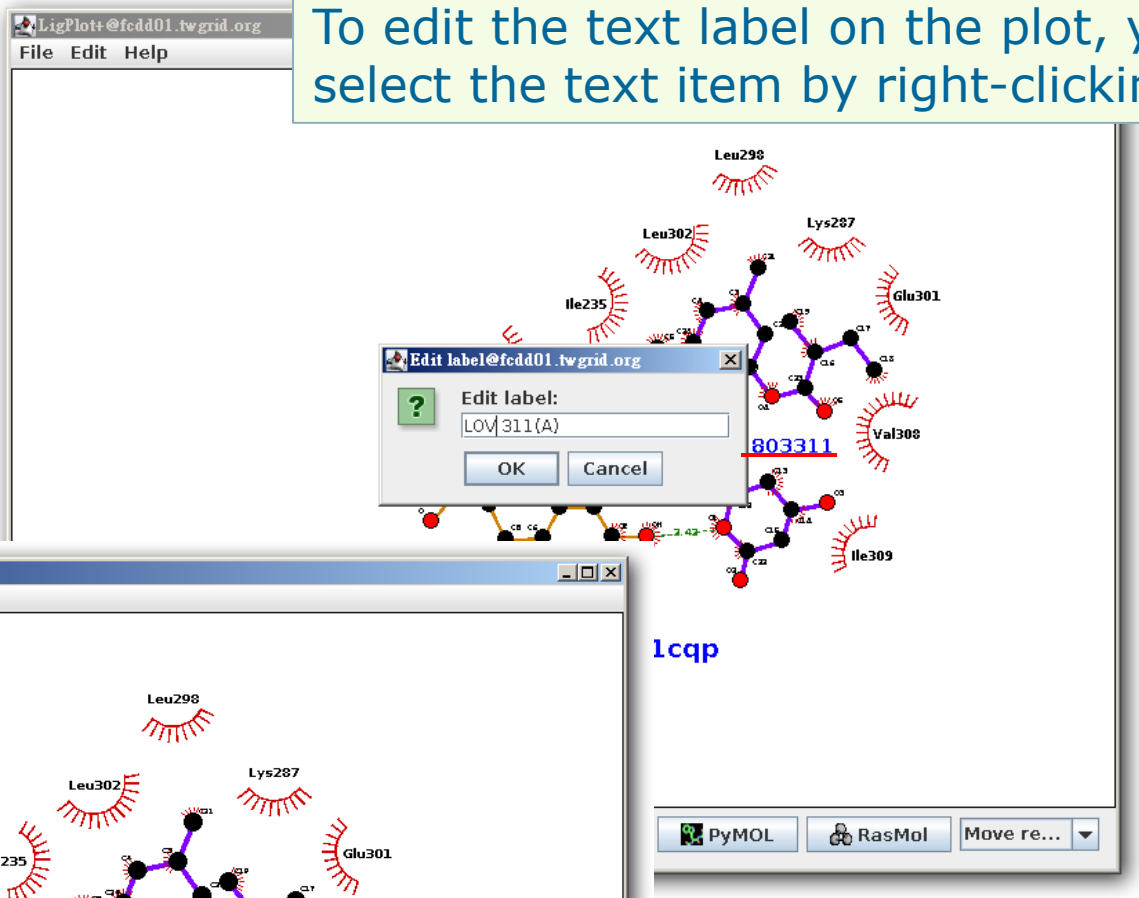


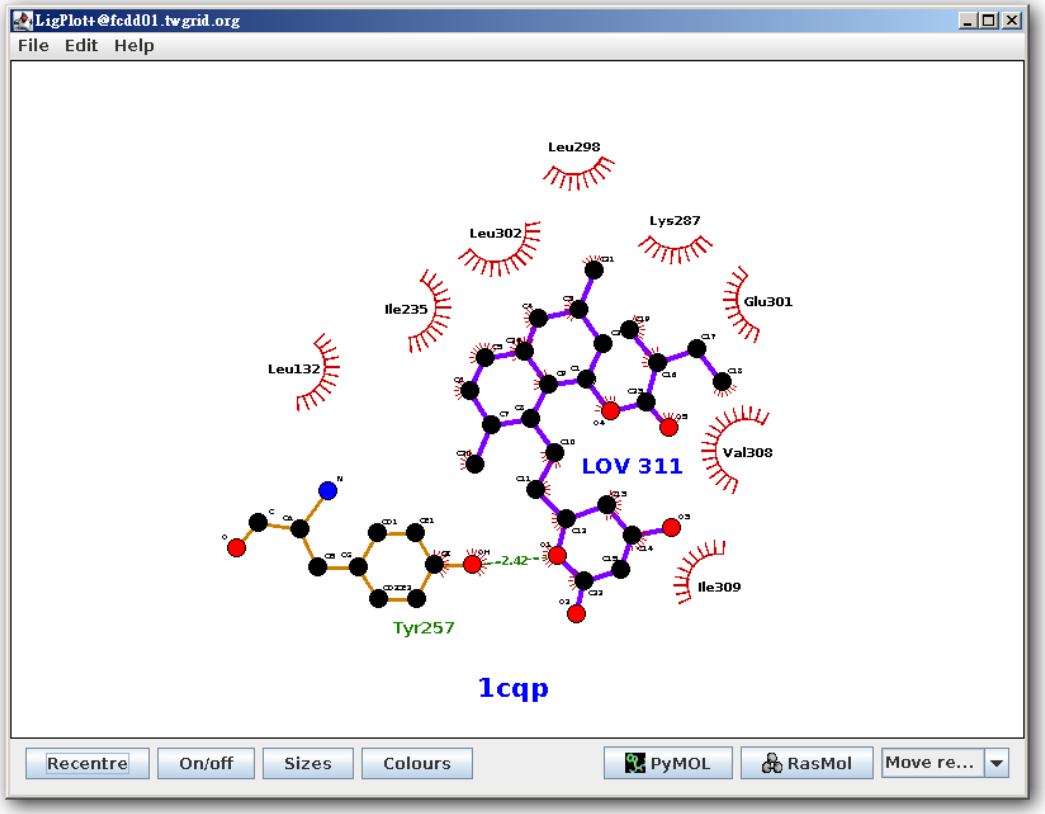


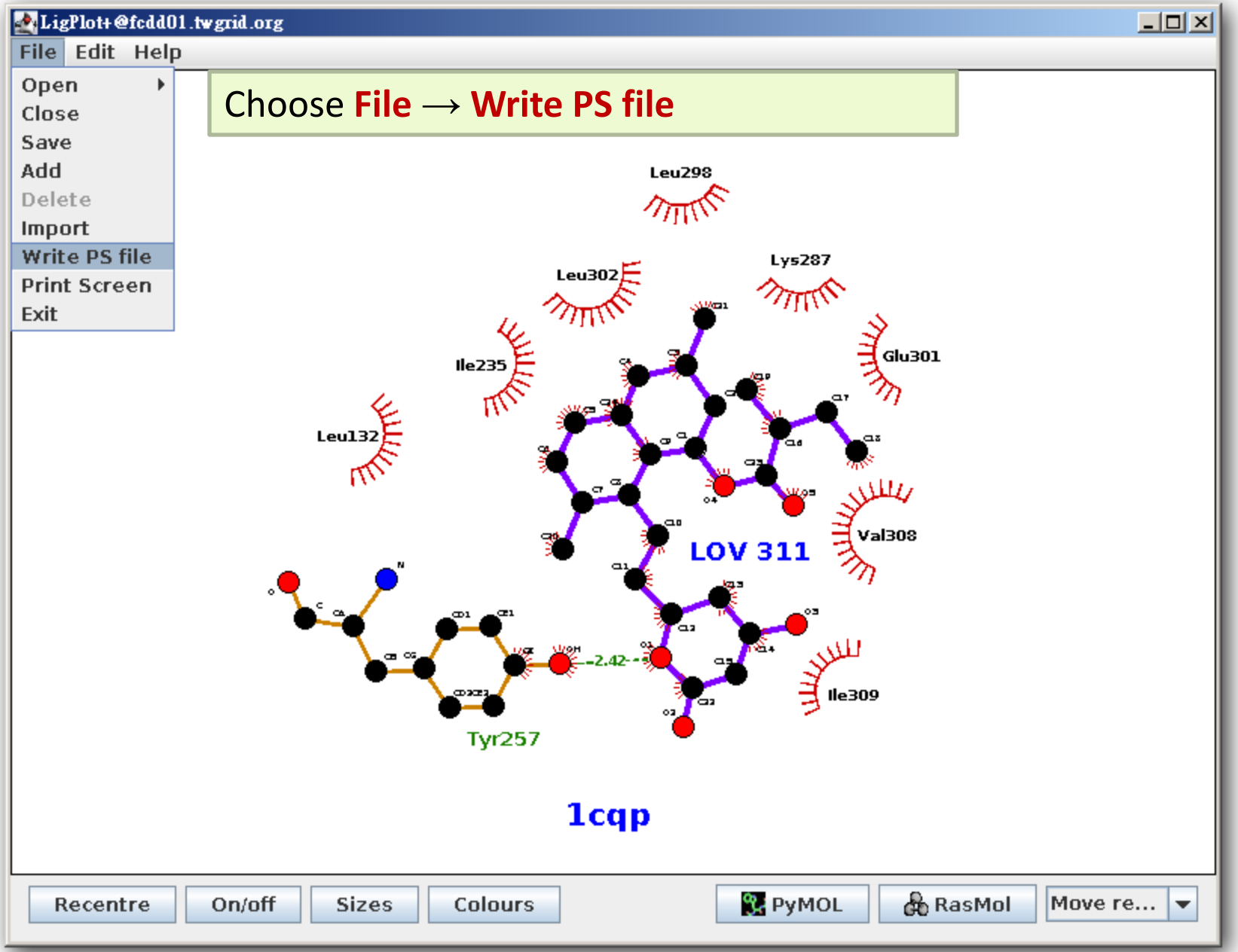
To move any object on the plot just click and drag it using the left mouse button.

Use the **left** mouse button to click-and-drag on any blank area of the plot to pan around the plot.
Use the **right** mouse button to click-and-drag on any blank area of the plot to zoom in and out of the plot.

To edit the text label on the plot, you can select the text item by right-clicking on it.






LigPlot+@fcdd01.twgrid.org
File
Edit
Help
Open
Close
Save
Add
Delete
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Write PS file
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Choose File → Write PS file
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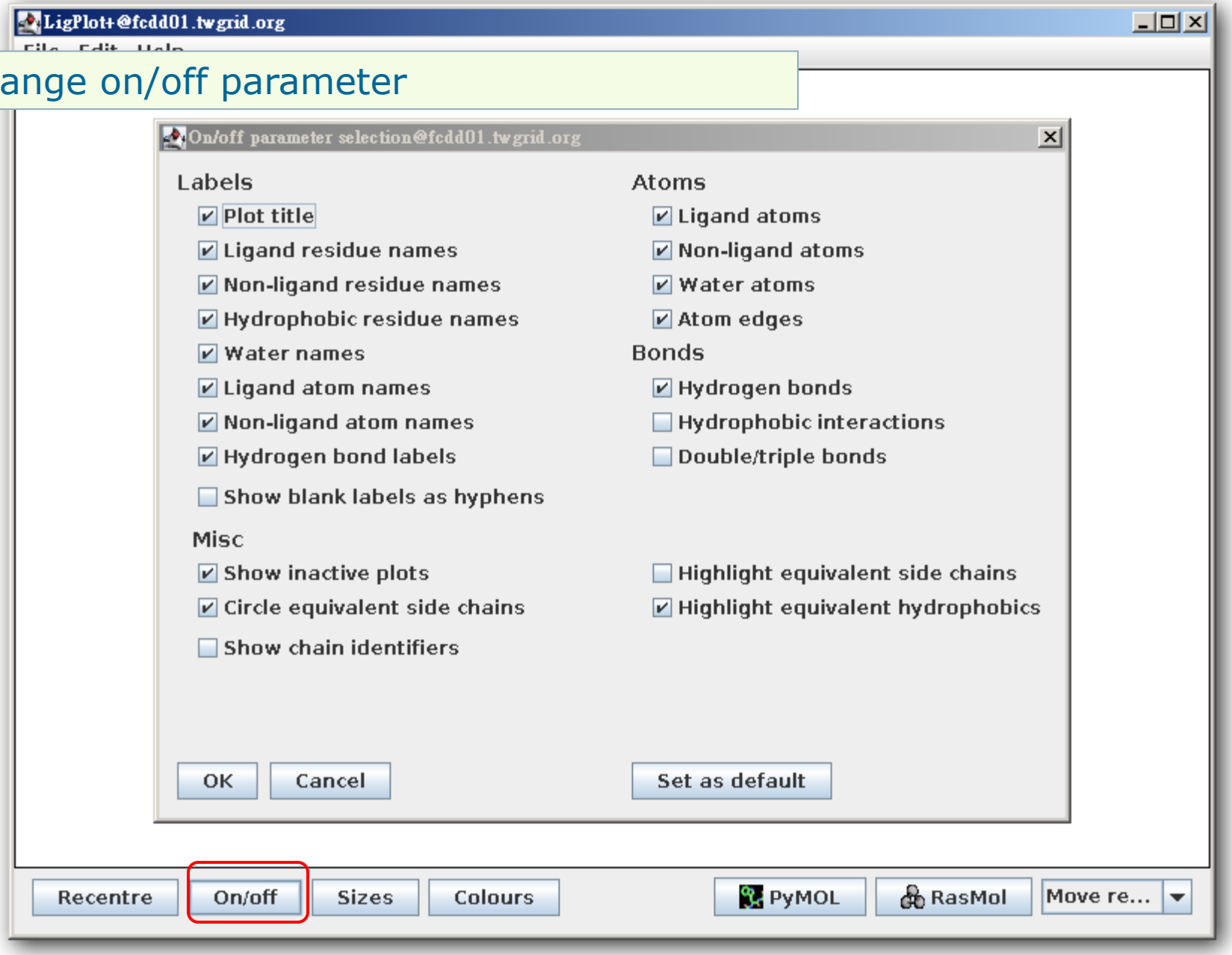
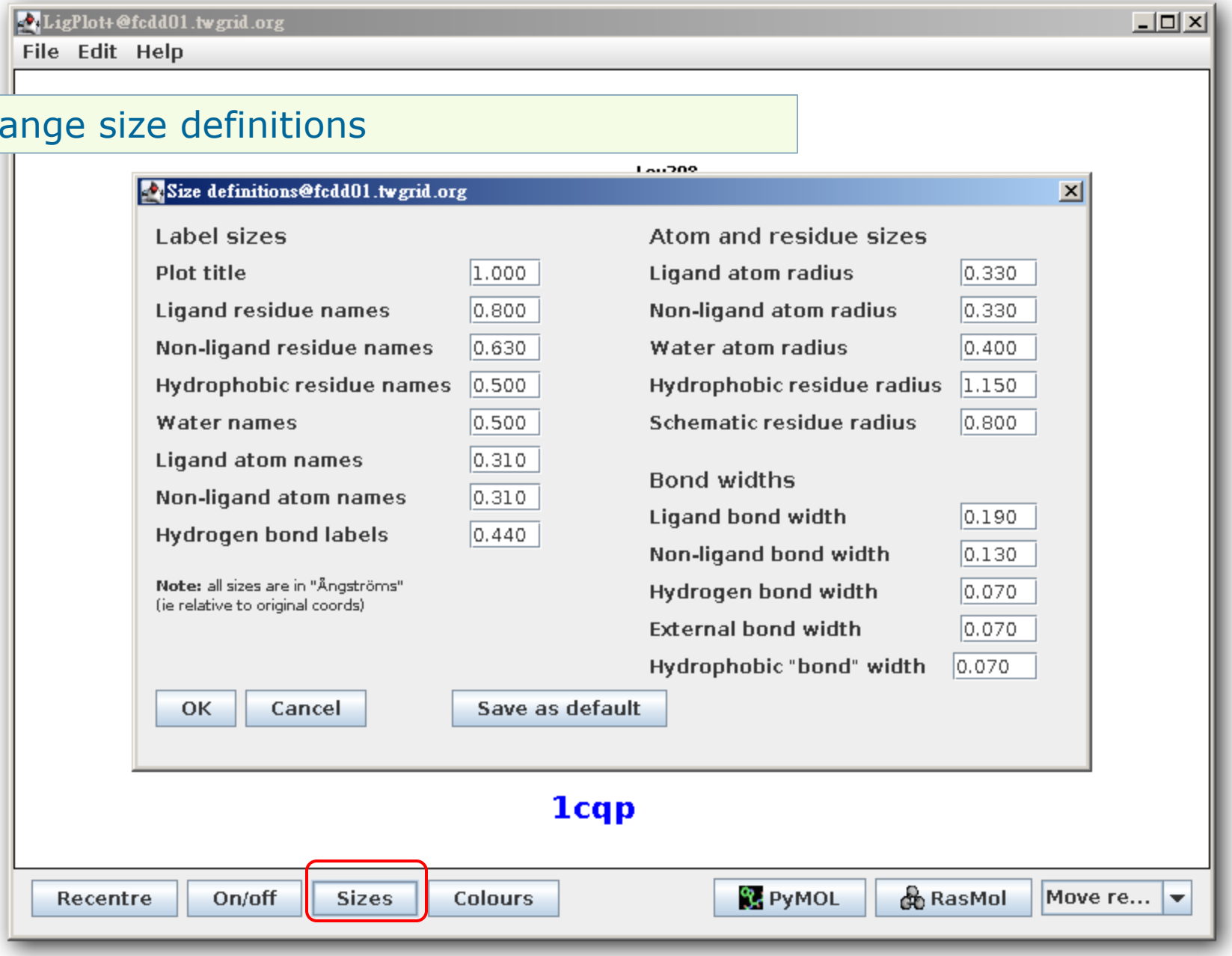
Change on/off parameter

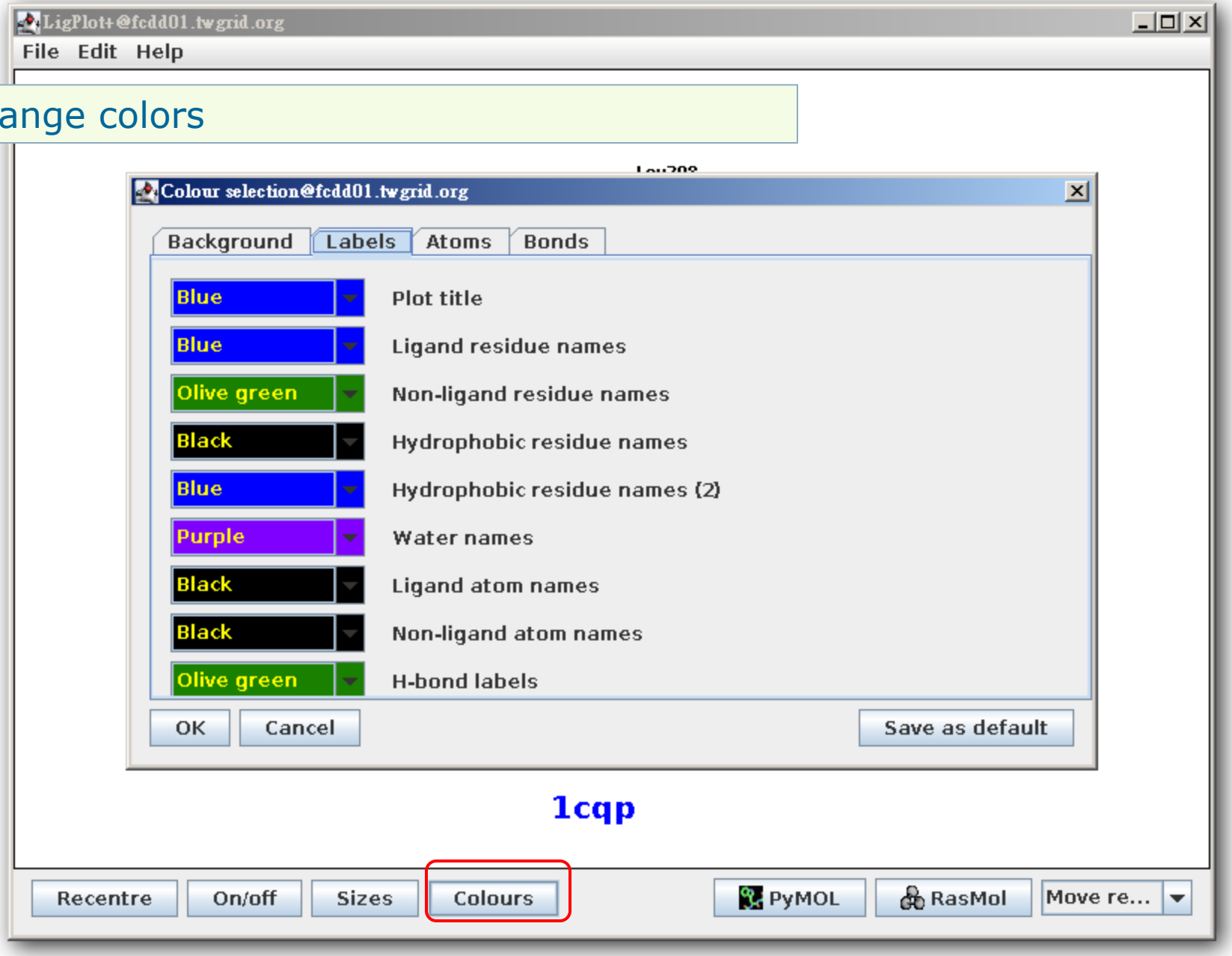


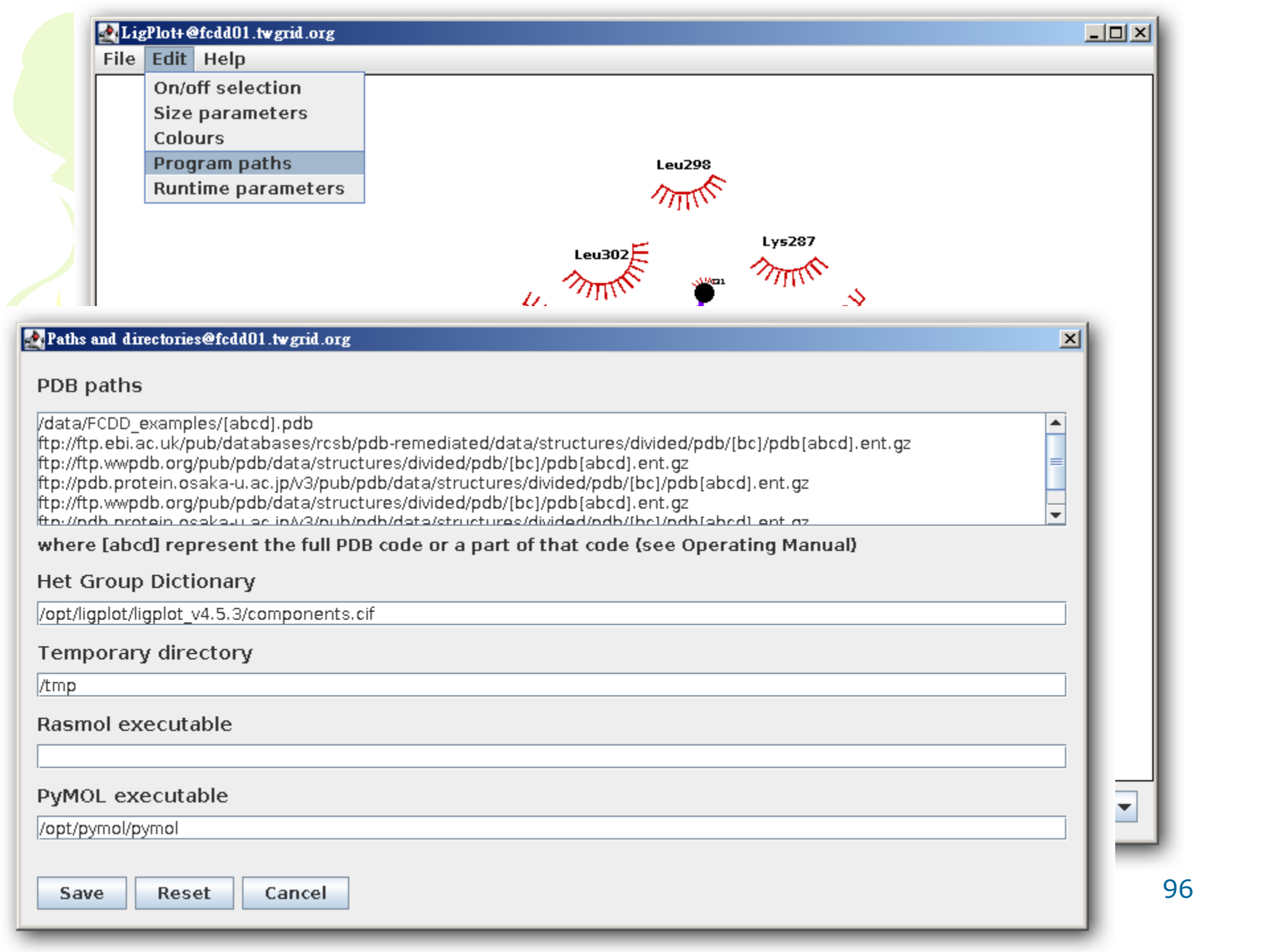
ligplot.prm

Change size definitions



Change colors




LigPlot+@fcdd01.twgrid.org
File
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Paths and directories@fcdd01.twgrid.org
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where [abcd] represent the full PDB code or a part of that code (see Operating Manual)
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PyMOL executable
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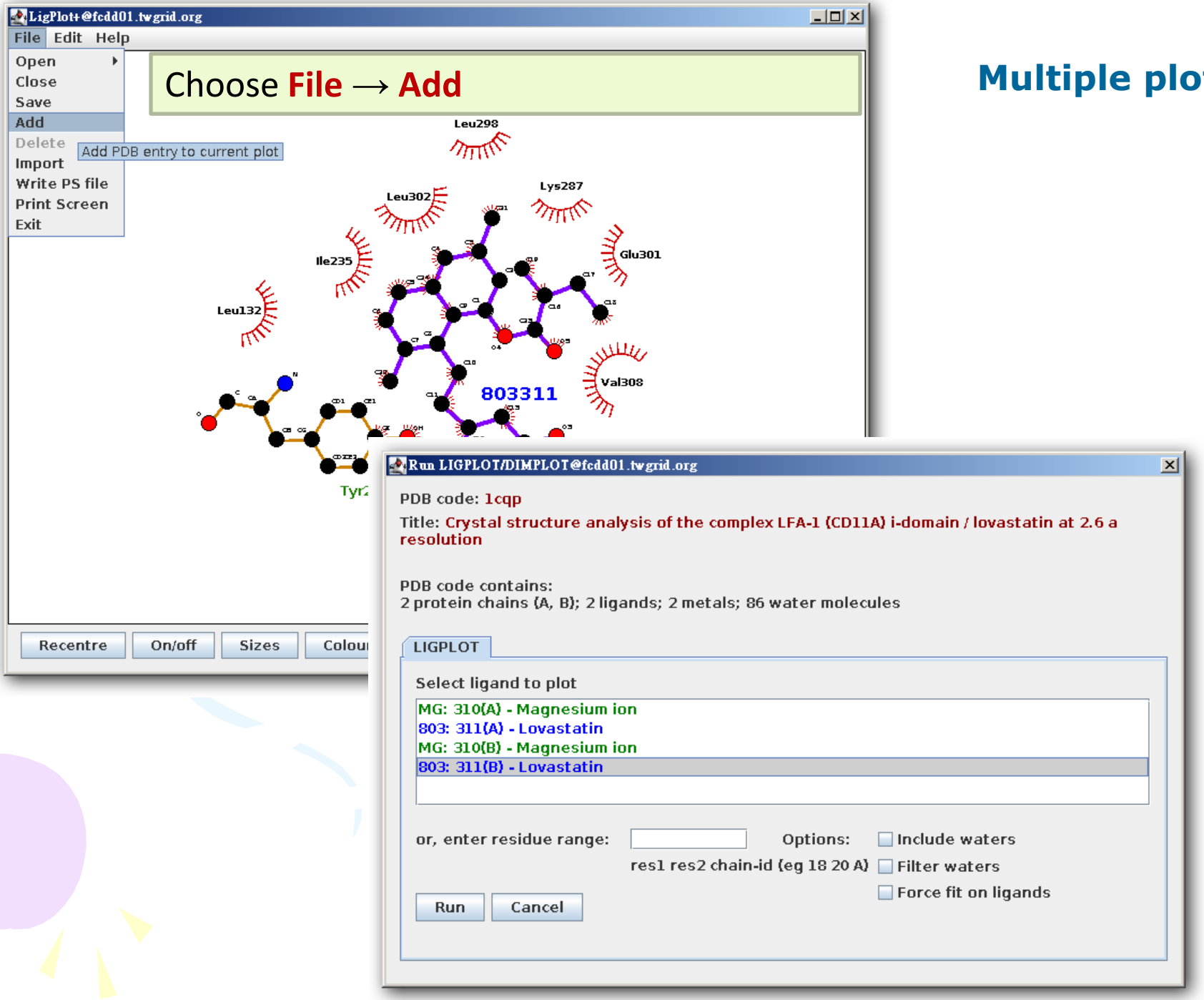
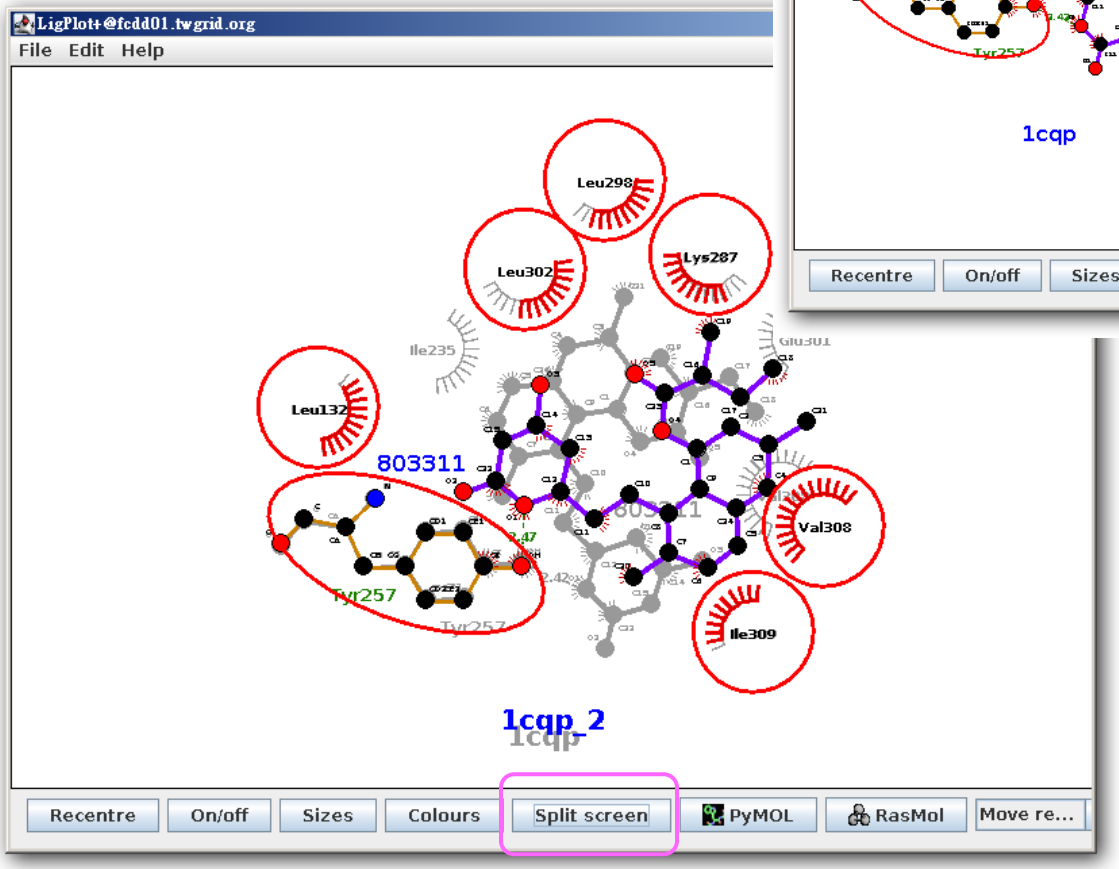
Save
Reset
Cancel

Multiple plots

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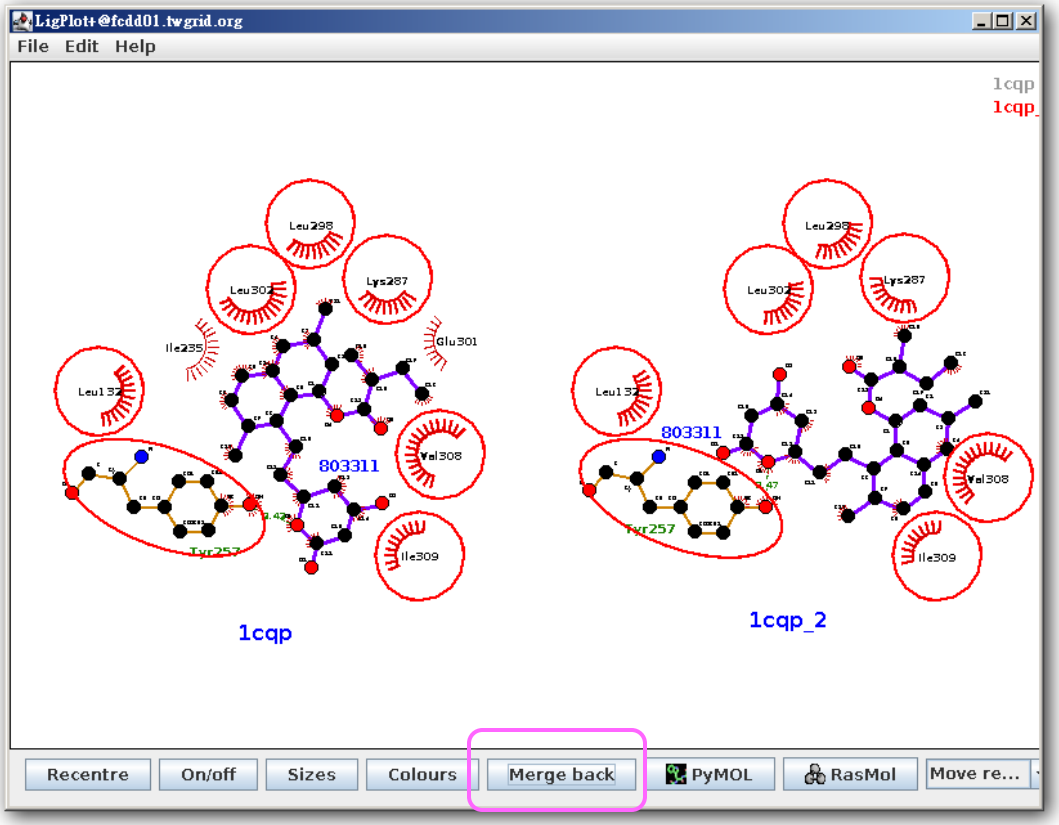
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Merge back
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