

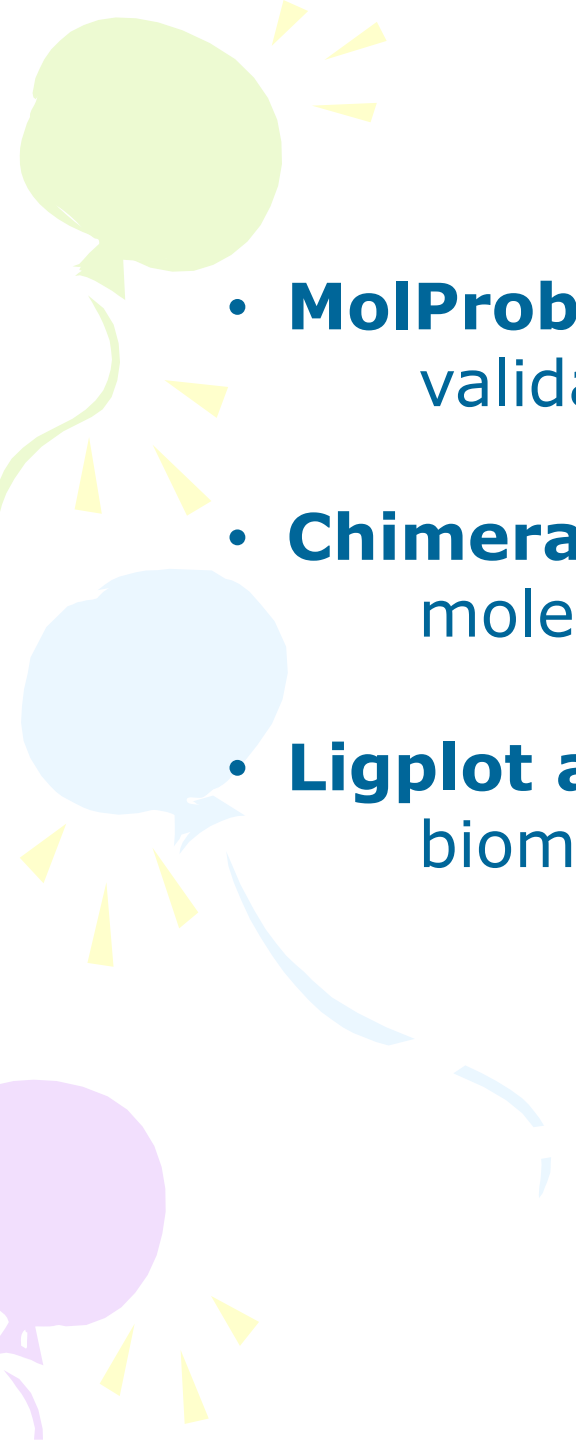


# Molecular graphics and analytics for biomolecule-drug interactions

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**Supervisor: Jung-Hsin Lin (林榮信)**


Research Center for Applied Sciences, Academia Sinica

- 
- **MolProbability**  
validate macromolecule
  - **Chimera**  
molecular graphics
  - **Ligplot and ligplot+**  
biomolecule-drug interactions



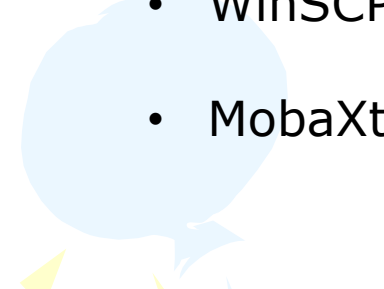

# Basic Linux Commands

- **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**

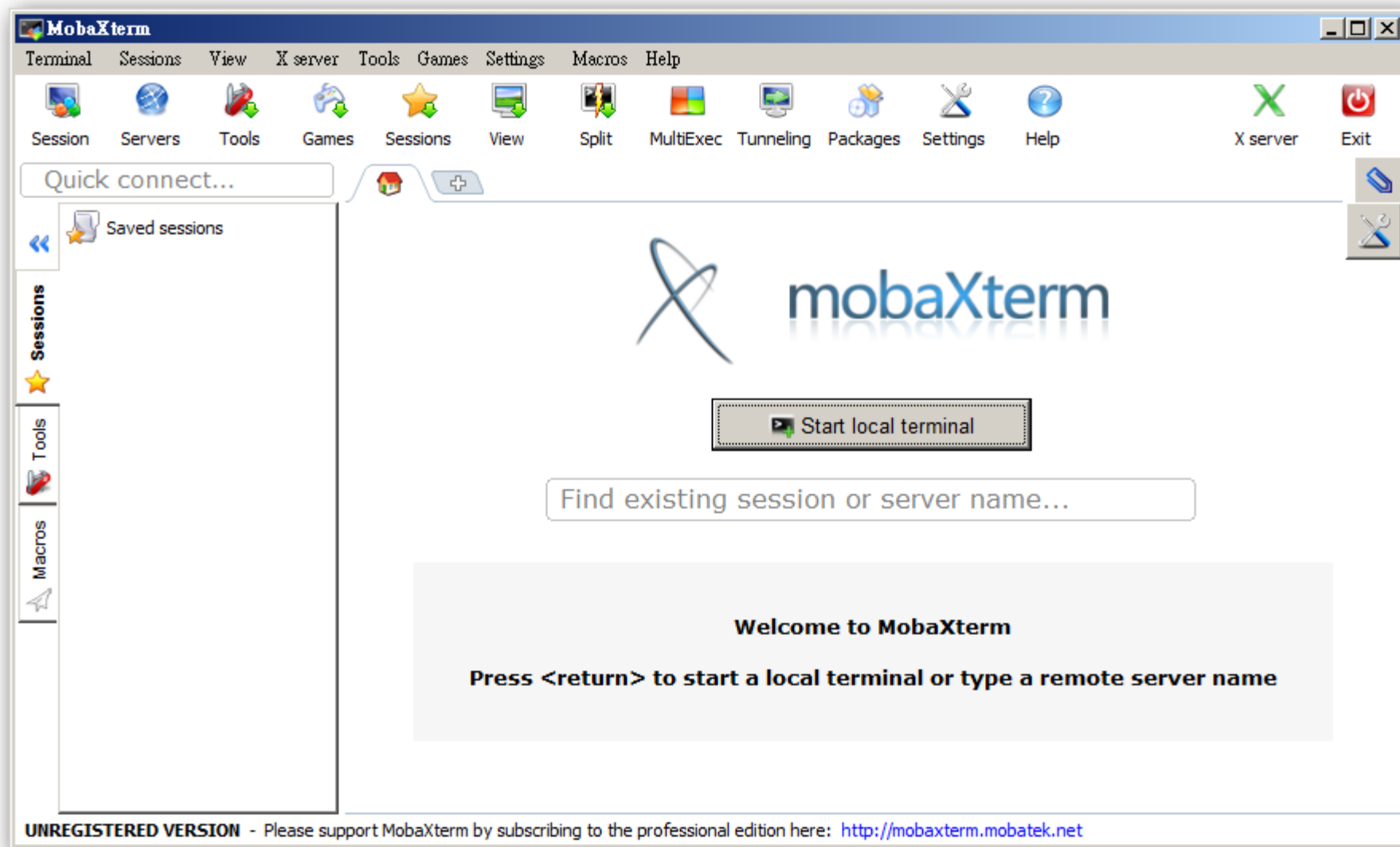


Use SSH/SCP clients to connect to a remote computer, and/or to transfer files between computers.

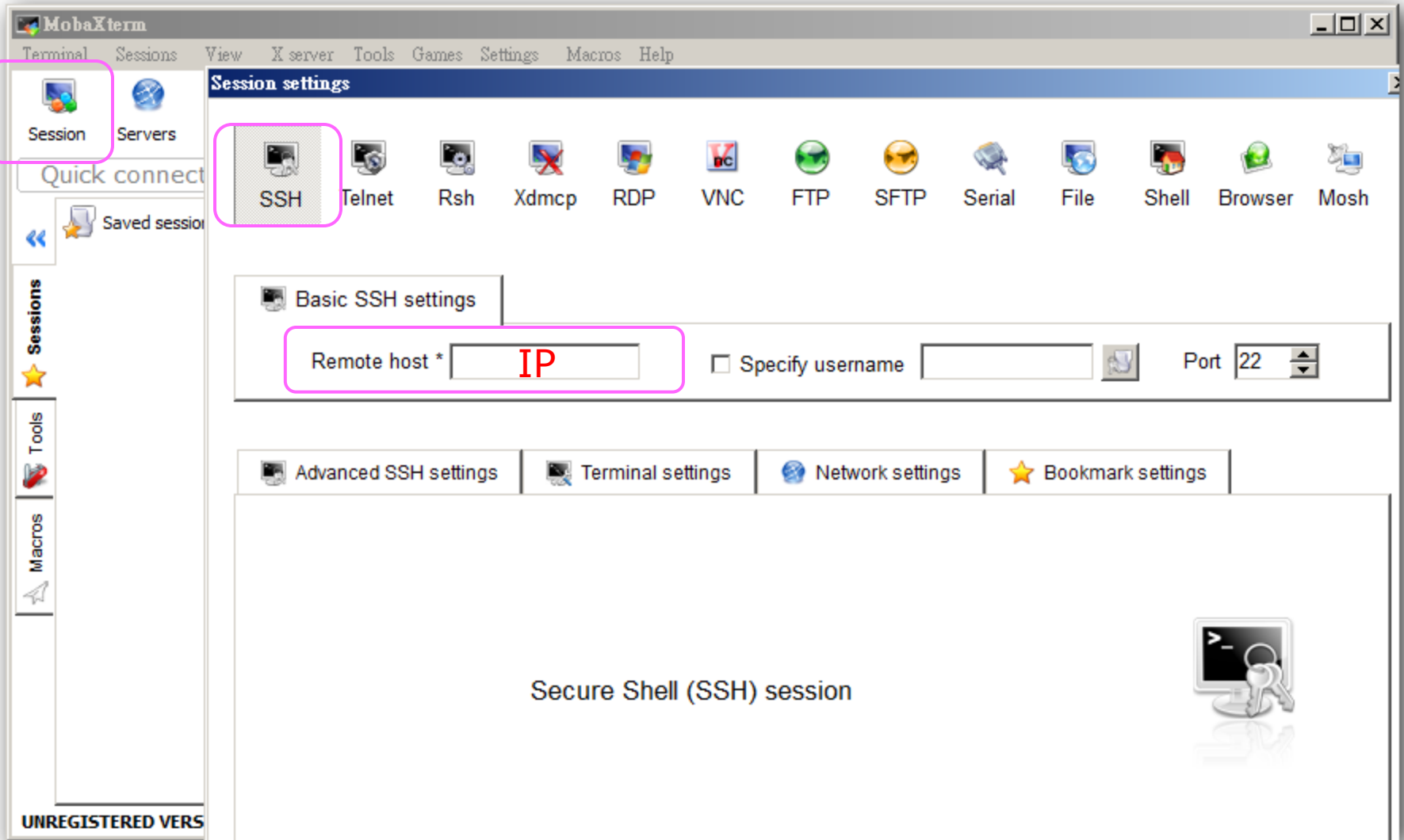
SSH/SCP client for windows:

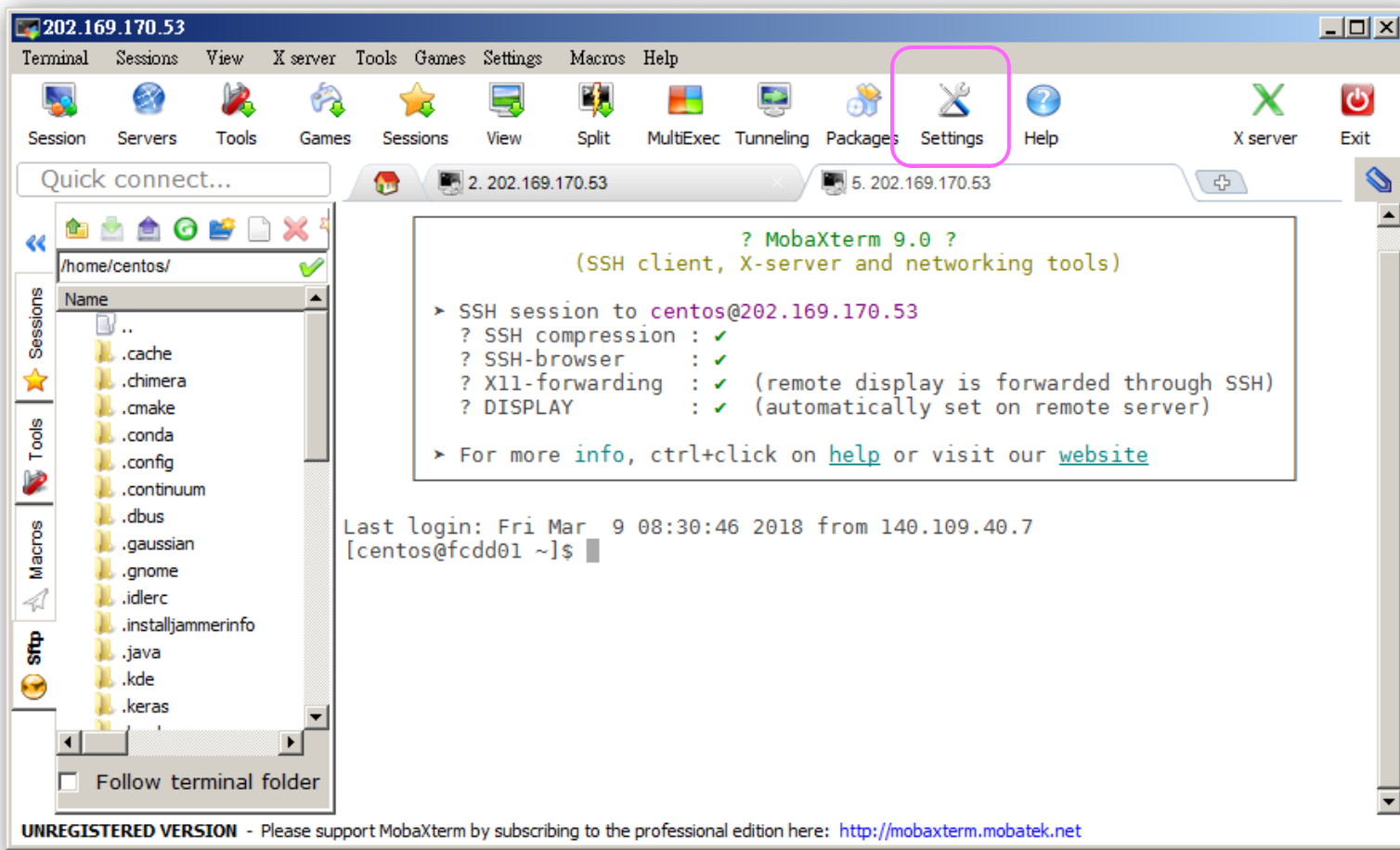
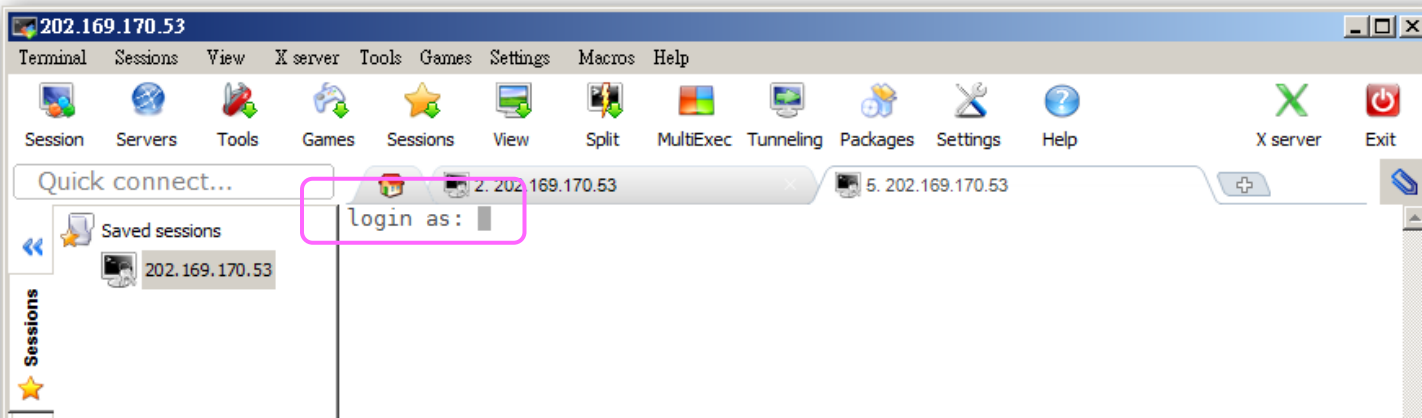
- putty <https://www.putty.org/>
    - Xming <https://sourceforge.net/projects/xming/> (X Server)
  - WinSCP <https://winscp.net/eng/download.php>
  - MobaXterm <http://mobaxterm.mobatek.net/download.html>
- 
- 

# Launching mobaXterm



Choose **Session** → **SSH**





## 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:

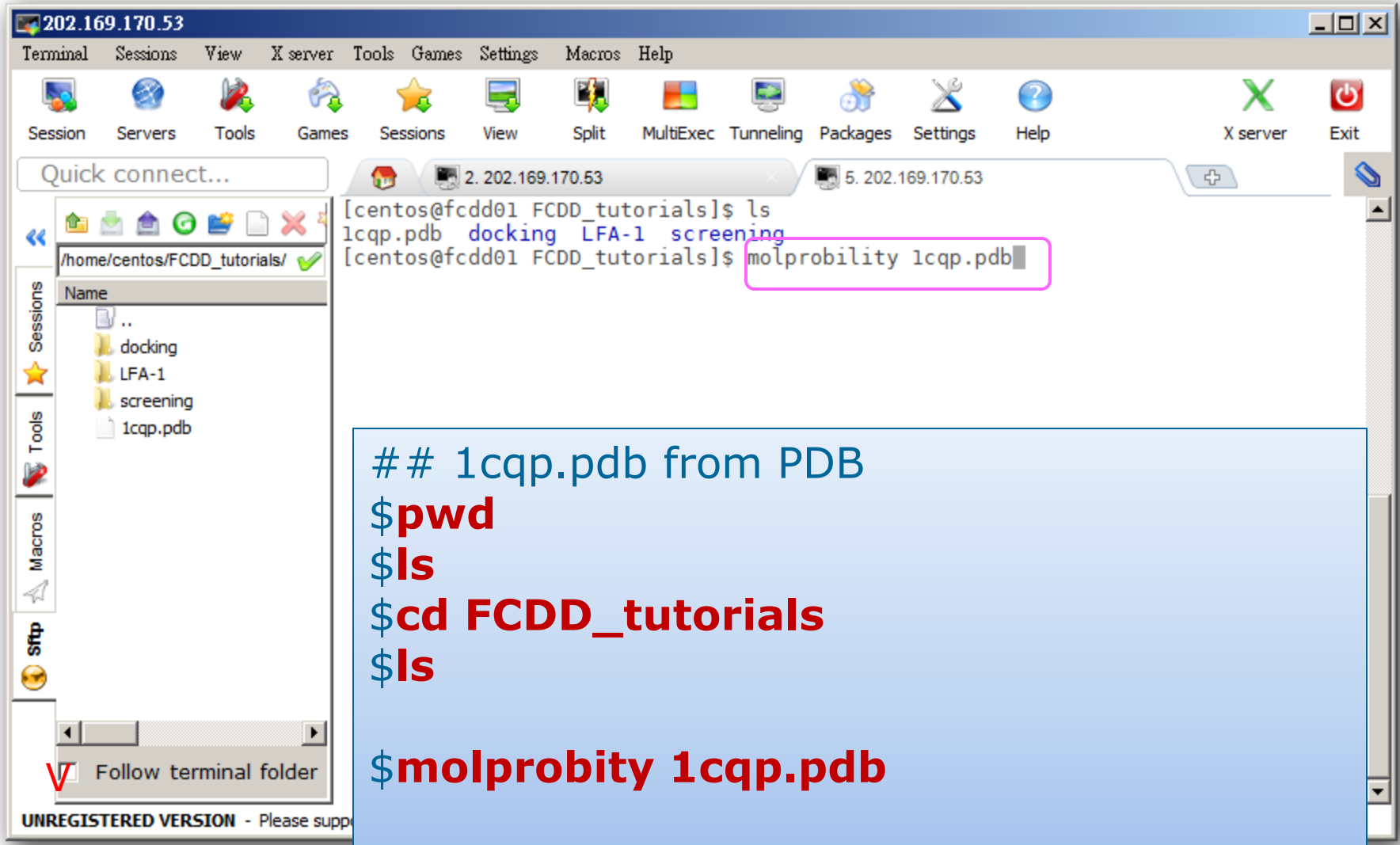
```
$ ssh -Y username@ip_address
```





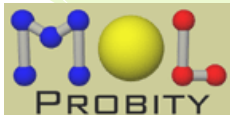
# MolProbability

- all-atom structure validation for macromolecular crystallography
  - Server  
<http://molprobability.biochem.duke.edu/>
  - Standalone program  
<https://github.com/r1abduke/MolProbability>  
A standalone version was installed.
- 
- 



# 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.



## Main page



Duke Biochemistry  
Duke University School of Medicine

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

FILE UPLOAD/RETRIEVAL (MORE OPTIONS)

PDB/NDB code:

type:

No file selected.

type:

### Molprobity sites:

[Duke \(US\)](#) | [Manchester \(UK\)](#) | [Beta \(Recent developments; Unstable\)](#)

Legacy version 4.02 has been retired. Please contact us through the 'Feedback & bugs' link if this affects your MolProbity use.

### Usage Guidelines:

These web services are provided for analysis of individual structures, not batch runs.

### 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.

## Walkthroughs, tutorials, and usage FAQs:

**Evaluate X-ray structure:** Typical steps for a published X-ray crystal structure or one still undergoing refinement.

**Evaluate NMR structure:** Typical steps for a published NMR ensemble or one still undergoing refinement.

**Fix up structure:** Rebuild the model to remove outliers as part of the refinement cycle.

**Work with kinemages:** Create and view interactive 3-D graphics from your web browser.

**Guide to Reduce options:** Learn about adding hydrogens to a structure for all-atom contact analysis.

**Guide to validation options:** Choose validations appropriate to a structure.

## Citations, science, and technical FAQs:

**Cite MolProbity:** Chen et al. (2010) MolProbity: all-atom structure validation for macromolecular crystallography. *Acta Crystallographica D*66:12-21.

and/or

Davis et al. (2007) MolProbity: all-atom contacts and structure validation for proteins and nucleic acids. *Nucleic Acids Research* 35:W375-W383.

**Cite KiNG:** Chen et al. (2009) KiNG (Kinemage, Next Generation): A versatile interactive molecular and scientific visualization program. *Protein Science* 18:2403-2409.

**Cite CCTBX:** Grosse-Kunstleve et al. (2002) The Computational Crystallography Toolbox: crystallographic algorithms in a reusable software framework. *J. Appl. Cryst.* 35:126-136.

**About hydrogens:** Why have the hydrogen bond lengths changed?

**Installing Java:** how to make kinemage graphics work in your

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 Å 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

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.

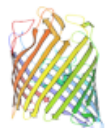
### SUGGESTED TOOLS (ALL TOOLS)

Due to the parameter adjustments to hydrogen bond lengths 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



- ✓ Do bond length and angle geometry analysis (`mp_geo`)
- ✓ Do Ramachandran analysis and make plots (`ramalyze`) - [preview kinemage](#) | [PDF](#)
- ✓ Do rotamer analysis (`rotalyze`)
- ✓ Do C $\beta$  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](#).

## 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%
	C $\beta$ 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: $\leq 1$ per chain, or $\leq 5\%$
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](#)
- [C \$\beta\$  deviation scatter plot \(27 Kb\)](#): [View in KiNG](#) | [Download](#)

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%
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.

#	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 333										
A 128	GLY	60.46	-	-	A 160	LYS 25.81	Favored (79.35%) General / -64.6,-47.3	Favored (33.1%) <i>tp</i> chi angles: 195.4,62.2,178.2,171.3	0.03Å	Favored (84.242%)	-	-	-	
A 129	ASN	46.54	Favored (54.86%) General / -121.9,134.7	Favored (66.4%) <i>n</i> chi angles: 280.1,34	A 161	LEU 20.69	Allowed (1.99%) General / -88.2,24.0	Favored (40.5%) <i>mt</i> chi angles: 307,183.1	0.03Å	Favored (15.108%)	-	-	-	
A 130	VAL	29.02	Favored (55.92%) Ile or Val / -120.7,118.3	Favored (22.8%) chi angles: 186.4	A 162	SER 26.32	Favored (41.72%) General / -74.8,146.7	Favored (81.8%) <i>p</i> chi angles: 62	0.02Å	Favored (14.202%)	-	-	-	
A 131	ASP	21.27	Favored (16.45%) General / -101.7,105.5	Favored (20%) <i>m</i> chi angles: 272.2,0	A 163	ASN 32.93	Favored (10.51%) General / 66.7,16.9	Favored (70.8%) <i>m-40</i> chi angles: 304.7,305.1	0.04Å	Favored (11.937%)	-	-	-	
A 132	LEU	28.68	Favored (51.28%) General / -106.1,125.7	Favored (3.8%) chi angles: 194.3,14	A 164	THR 20.9	Allowed (1.11%) General / -98.0,-164.2	Favored (52%) <i>p</i> chi angles: 65.4	0.04Å	Favored (15.536%)	-	-	-	
A 133	VAL	19.95	Favored (68.36%) Ile or Val / -111.0,126.4	Favored (57.9%) chi angles: 180.2	A 165	SER 52.41	Favored (59.19%) General / -86.2,-5.4	Favored (61.7%) <i>m</i> chi angles: 293.8	0.12Å	Favored (5.28%)	-	-	-	
A 134	PHE	18.58	Favored (32.04%) General / -92.7,119.4	Favored (47.8%) <i>n</i> chi angles: 287.8,11	A 166	TYR 32.36	Favored (36.65%) General / -79.2,135.0	Favored (97.7%) <i>m-80</i> chi angles: 294.7,90.7	0.03Å	Favored (28.022%)	-	-	-	
A 135	LEU	22.33	Favored (5.06%) General / -106.5,94.3	Favored (16.9%) chi angles: 183.9,45	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 136	PHE	17.83	Favored (39.59%) General / -100.2,136.8	Favored (2.1%) <i>p</i> chi angles: 65.8,115	#	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 168	PHE	27.08	Favored (29.71%) General / -123.7,159.3	Favored (90.8%) <i>m-80</i> 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%) <i>t</i> 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%) <i>tt0</i> 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%) <i>p90</i> 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%) <i>m</i> 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%) <i>t</i> 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 suitefilename 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
lcqp.cablam      lcqp.geom        lcqp.rama.kin    lcqp.suitefilename_midpoint
lcqp.cbdev       lcqp.geom.sorted lcqp.rama.pdf    lcqp.suitestring
lcqp.cbdev.kin  lcqp.omega       lcqp.rota        lcqp.trim.pdb
lcqp.clash       lcqp.pucker      lcqp.suitefilename
lcqp.FH.pdb     lcqp.rama        lcqp.suitefilename.kin
lcqp.thumbail.kin
[centos@fcdd01 molprobity_1cqp]$
```



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

---

## Input commands (end with Esc)

---

a	Append after cursor
i	Insert before cursor
o	Open line below
O	Open line above
:r <i>file</i>	Insert <i>file</i> 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.

---

## File management commands

---

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

---

## Deletion commands

---

dd or <i>n</i> dd	Delete <i>n</i> lines to general buffer
dw	Delete word to general buffer
<i>n</i> rw	Delete <i>n</i> 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](http://www.atmos.albany.edu/daes/atmclasses/atm350/vi_cheat_sheet.pdf)

# ## download 1cqp.rama.pdf to local computer

The screenshot shows a terminal window with a file browser interface. The file browser displays a directory listing for `/home/centos/FCDD_tutorials/molprobity_1cqp/`. The file `1cqp.rama.pdf` is selected, and a context menu is open with the `Download` option highlighted.

Name	Size (KB)	Last modified
1cqp.FH.pdb	519	2018-03-05 .
1cqp.geom	389	2018-03-05 .
1cqp.geom.sorted	389	2018-03-05 .
1cqp.omega	21	2018-03-05 .
1cqp.pucker	0	2018-03-05 .
1cqp.rama	17	2018-03-05 .
1cqp.rama.kin	418	2018-03-05 .
1cqp.rama.pdf	1 652	2018-03-05 .
1cqp.rota		
1cqp.suitename		
1cqp.suitename.kin		
1cqp.suitename_midp		
1cqp.suitestring		
1cqp.trim.pdb		
thumbnail.kin		

```
real    0m0.094s
user    0m0.063s
sys     0m0.032s
^time to make suite name kin

running mp_geo bond geometry

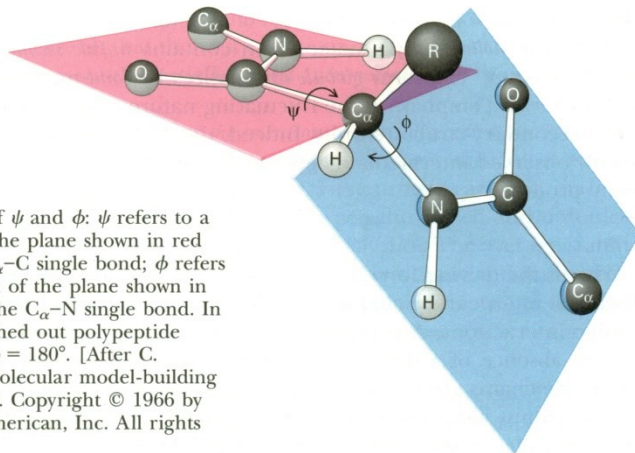
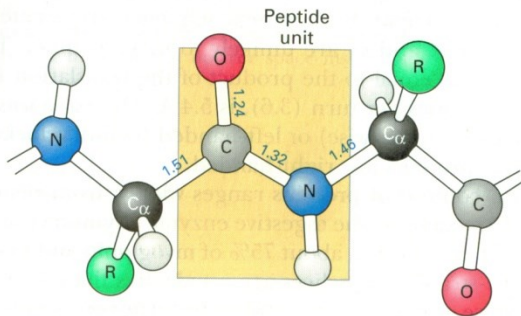
real    0m12.334s
user    0m11.966s
sys     0m0.315s
^time to run mp_geo for bond geometry

clashscore
cloud mode

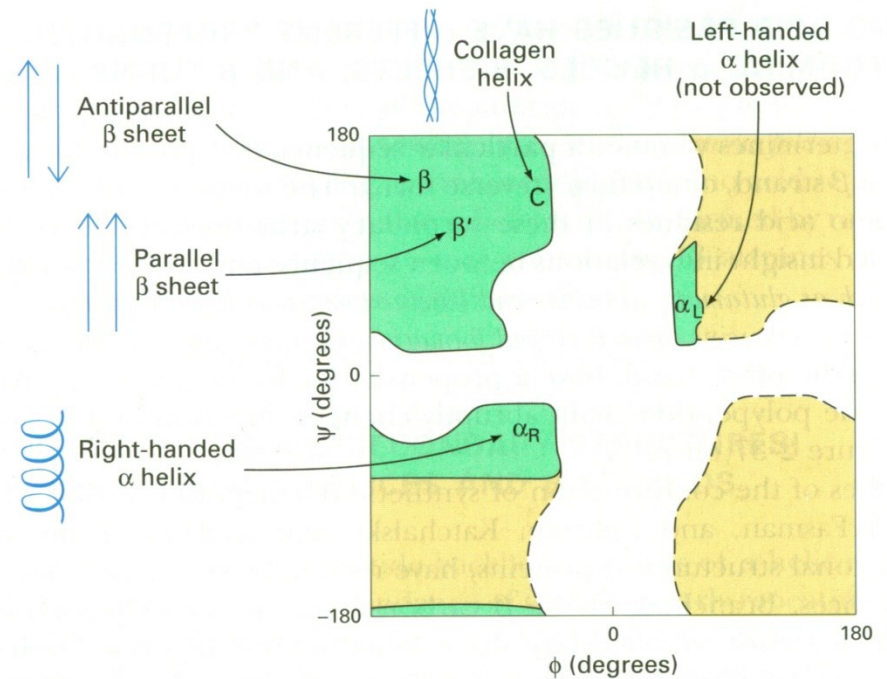
0m5.336s
0m4.974s
0m0.446s
or clashscore

@fcdd01 FCDD_tutorials]$
edition here: http://mobaxterm.mobatek.net
```

# Protein Backbone Structures and Ramachandran Plot



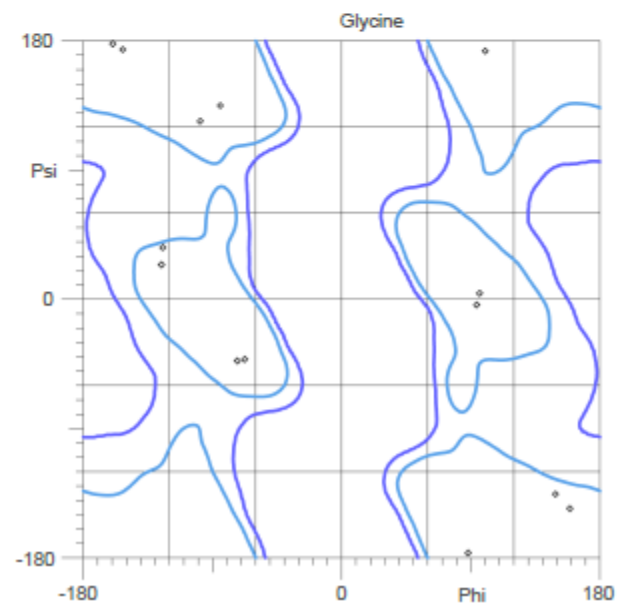
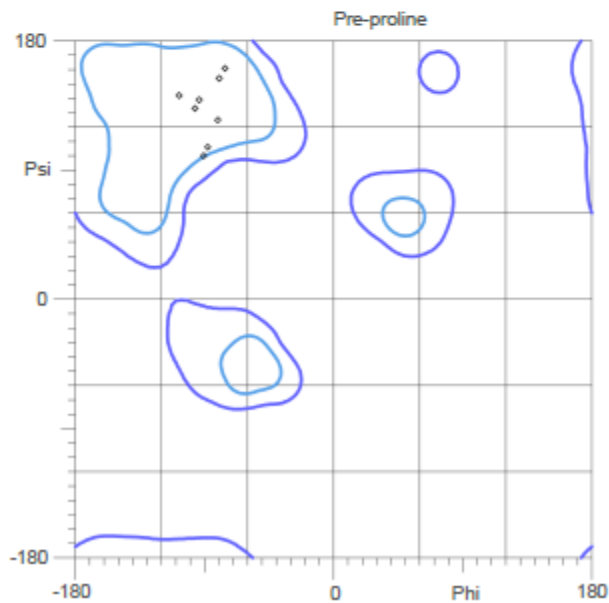
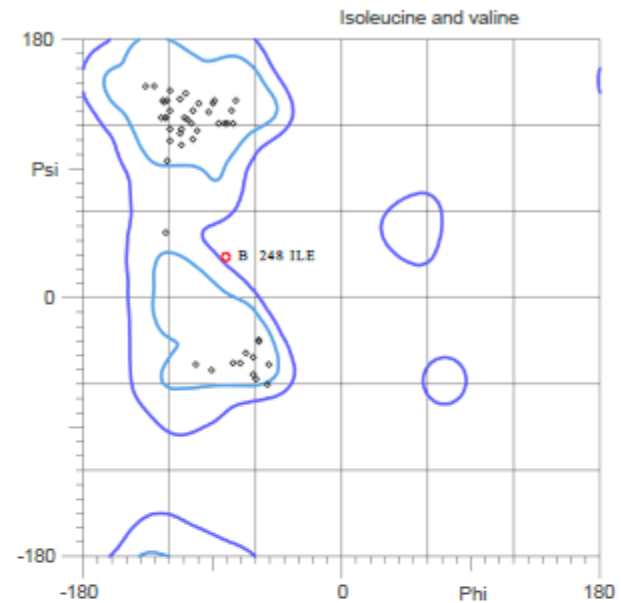
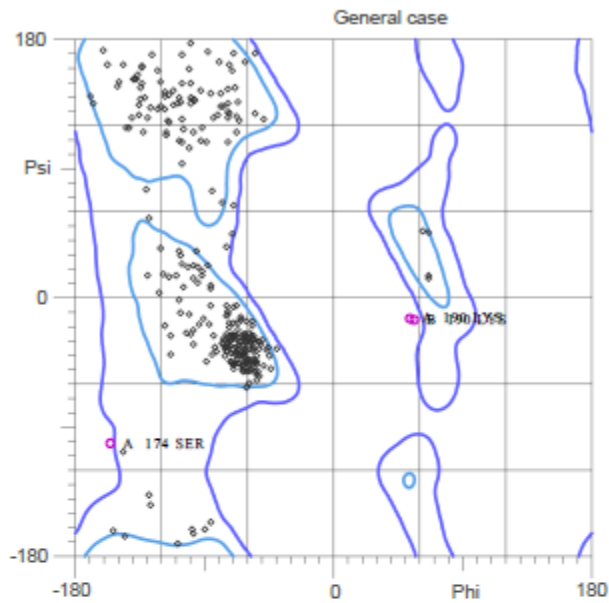
**Figure 16-5**  
 Definition of  $\psi$  and  $\phi$ :  $\psi$  refers to a rotation of the plane shown in red about the  $C_{\alpha}$ -C single bond;  $\phi$  refers to a rotation of the plane shown in blue about the  $C_{\alpha}$ -N single bond. In a fully stretched out polypeptide chain,  $\psi =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

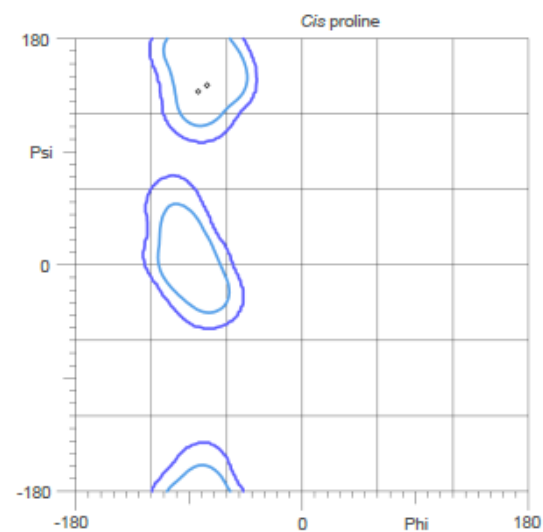
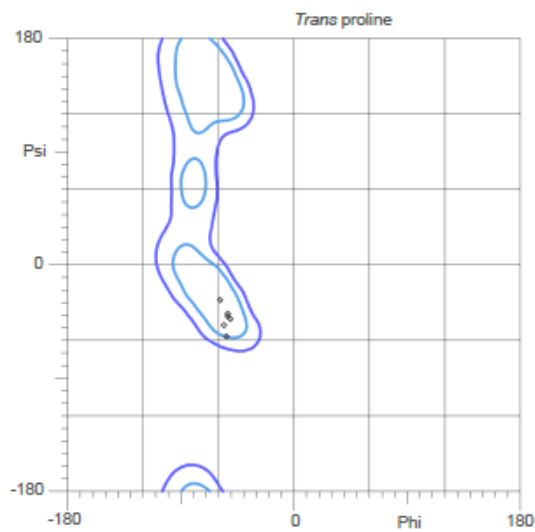
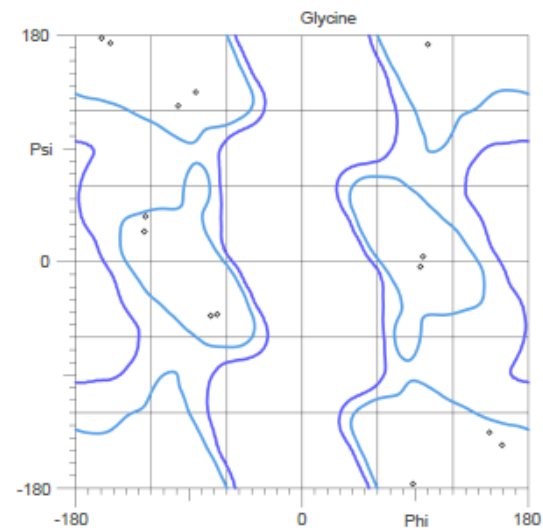
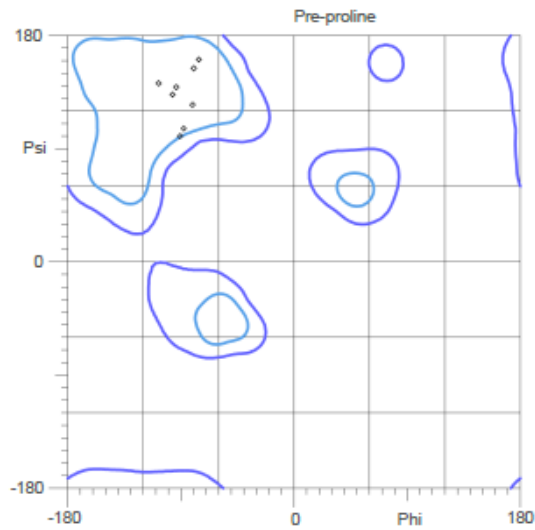


**Figure 16-6**  
 Ramachandran plot showing allowed values of  $\phi$  and  $\psi$  for L-alanine residues (green regions). Additional conformations are accessible to glycine (yellow regions) because it has a very small side chain.

# MolProbity Ramachandran analysis

1cqp.FH.pdb, model 1



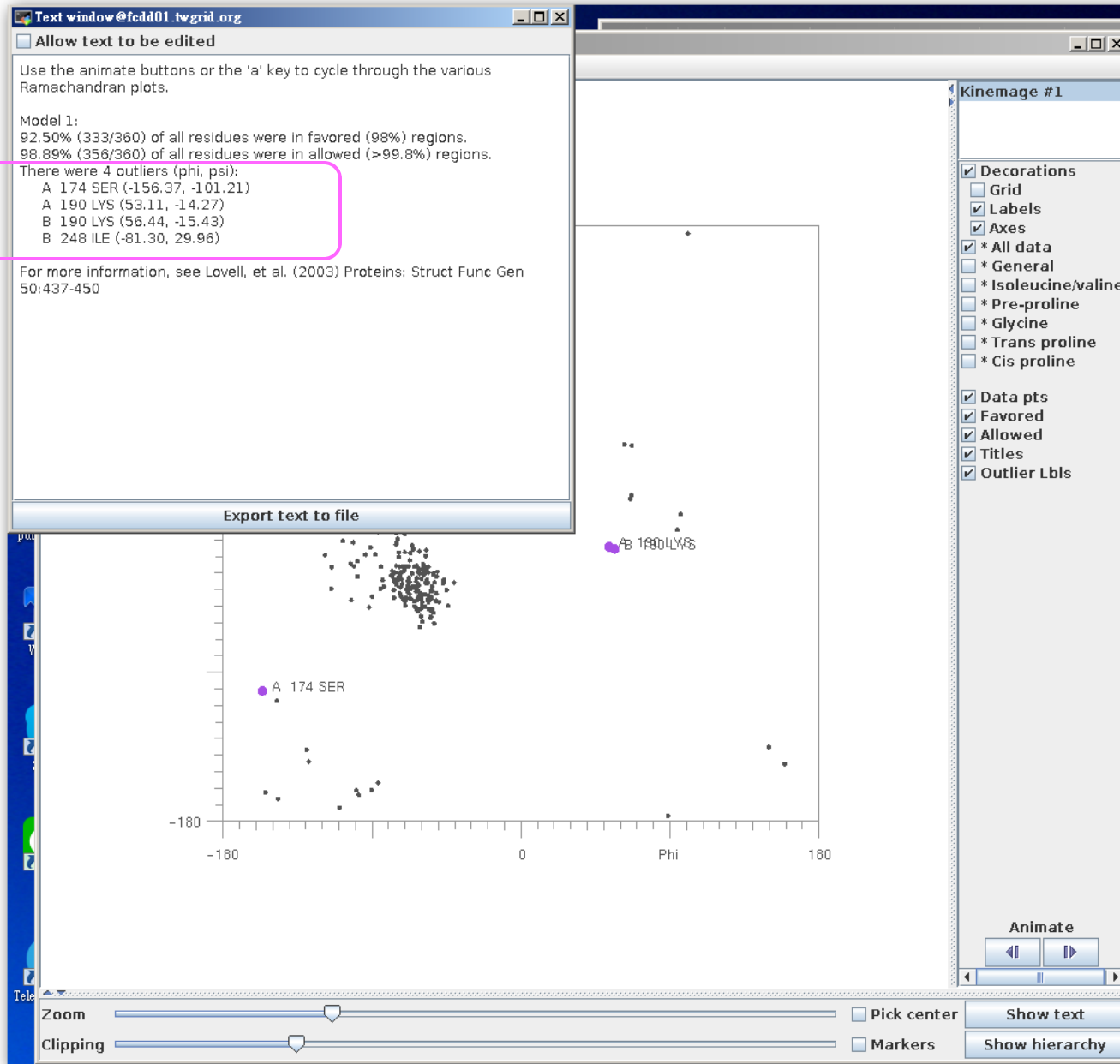


92.5% (333/360) of all residues were in favored (98%) regions.  
 98.9% (356/360) of all residues were in allowed (>99.8%) regions.

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)

# \$king 1cqp.rama.kin



# UCSF CHIMERA

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



## UCSF CHIMERA

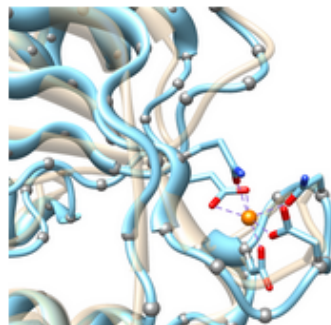
### an Extensible Molecular Modeling System

UCSF Chimera is a highly extensible program for interactive visualization and analysis of molecular structures and related data, including density maps, supramolecular assemblies, sequence alignments, docking results, trajectories, and conformational ensembles. High-quality images and animations can be generated. Chimera includes complete documentation and several tutorials, and can be downloaded free of charge for academic, government, nonprofit, and personal use. Chimera is developed by the [Resource for Biocomputing, Visualization, and Informatics](#) (RBVI), funded by the [National Institutes of Health](#) (NIGMS P41-GM103311).

[UCSF ChimeraX](#) (or simply ChimeraX) is the next-generation molecular visualization program from the RBVI, following UCSF Chimera.

### Feature Highlight

#### Ribbon Spline Options



The default ribbon path is a smooth **bspline** (semitransparent tan in the figure), which can diverge from the true positions of the backbone atoms ( $\alpha$ -carbons shown as gray balls). A **cardinal** spline allows tracking the backbone more closely. Without smoothing (light blue), it follows the  $\alpha$ -carbons exactly, or it can be combined with some "compromise" smoothing of strand and/or coil. Ribbon spline options can be set with the [ribspline](#) command or in the [molecule model attributes](#).

[\(More features...\)](#)

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## UCSF CHIMERA

an Extensible Molecular Modeling System

### Download Chimera

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- [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	<a href="#">chimera-1.12-win64.exe</a> Size: 150984696 bytes MD5: b662f97cdacb8be458662aa638dd6694	Oct 24, 2017	<a href="#">Instructions</a> <a href="#">Documentation</a> Runs on Windows 7 or later.
Mac OS X 64-bit	<a href="#">chimera-1.12-mac64.dmg</a> Size: 131622631 bytes MD5: 3a691632a3eba8b17286d23432bb6bbb	Oct 24, 2017	<a href="#">Instructions</a> <a href="#">Documentation</a> Runs on Mac OS X 10.8 or later.
Linux 64-bit	<a href="#">chimera-1.12-linux_x86_64.bin</a> Size: 157795228 bytes MD5: 24b9c2560e119988a3150b47c495737b	Oct 24, 2017	<a href="#">Instructions</a> <a href="#">Documentation</a> Compiled on CentOS 5.11.





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.



## Tutorials

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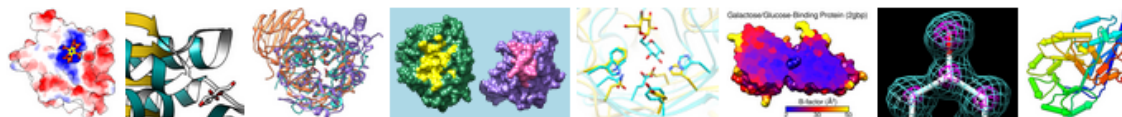
[Trajectories/Ensemble](#)

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## Tutorials Index







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2. [Getting Started - Command Version](#)
  - [Part 1](#) - Manipulation, Selection, and Chains
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4. [Structure Analysis and Comparison](#)
  - [Background and Setup](#)
  - [Distances, H-bonds, Contacts](#)
  - [Angles, Rotamers, Clashes](#)
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  - [Part 1](#) - Collagen Peptide
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11. [ViewDock](#)

[More tutorials](#) are available at the Chimera web site.

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		

	<b>PDB40 Symposium</b> More than 77000 structures in the archive	2011
	Deposition of chemical shift data mandatory	2010
	Deposition of experimental data mandatory 50000 <sup>th</sup> structure is released	2009
	First release of remediated data	2008
	<b>BMRB</b> joins wwPDB	2006
	Last PDB archive distribution by postal mail (8 DVDs)	2005
	<b>wwPDB</b> established by RCSB PDB, PDBe, PDBj	2003
  	 <b>EMDB</b> established at MSD-EBI	2002
	<b>Osaka University</b> opens a PDB data deposition center	2000
	10000 <sup>th</sup> structure is released	1999
	PDB moves to <b>RCSB PDB</b>	1998
	<b>MSD</b> at the EBI becomes a deposition center for PDB data	1997
	IUCr policy on data deposition published	1989
	<b>Early structures include</b> carboxypeptidase chymotrypsin cytochrome b5 hemoglobin lactate dehydrogenase myoglobin rubredoxin subtilisin trypsin inhibitor	
	<b>PDB established</b>	1971

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

Nobel prize awarded to V. Ramakrishnan, T.A. Steitz, A.E. Yonath for *Studies of the structure and function of the ribosome*



Nobel prize awarded to R.D. Kornberg for *Studies of the molecular basis of eukaryotic transcription*

Nobel prize awarded to R. MacKinnon for *Potassium channels*

Nobel prize awarded to K. Wüthrich for *Development of NMR spectroscopy for determining the 3D structure of biological macromolecules in solution*



First **ribosome structures** determined (Ban *et al.*, 2000; Carter *et al.*, 2000; Schluenzen *et al.*, 2000)

Nobel prize awarded to P.D. Boyer, J.E. Walker, J.C. Skou for *Elucidation of the enzymatic mechanism underlying the synthesis of adenosine triphosphate (ATP) and discovery of an ion-transporting enzyme*



1991 First **EM entry** released in PDB: bacteriorhodopsin (Henderson *et al.*, 1990)

1989 First **NMR entry** released in PDB: protein BDS-I (Driscoll *et al.*, 1989)

1988 Nobel prize awarded to J. Deisenhofer, R. Huber, H. Michel for *The determination of the 3D structure of a photosynthetic reaction centre*

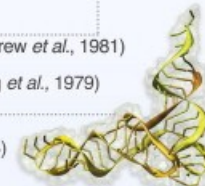


1982 Nobel prize awarded to A. Klug for *Development of crystallographic electron microscopy and discovery of the structure of biologically important nucleic acid-protein complexes*

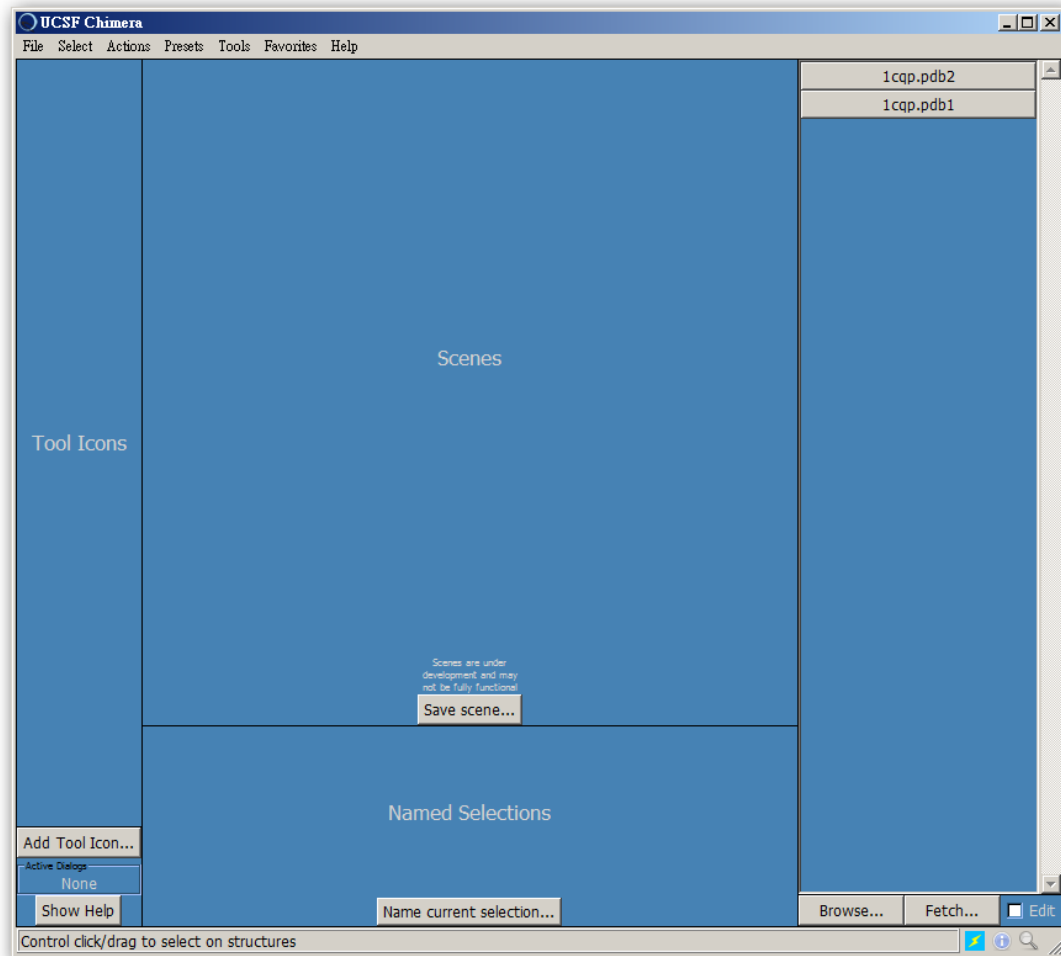
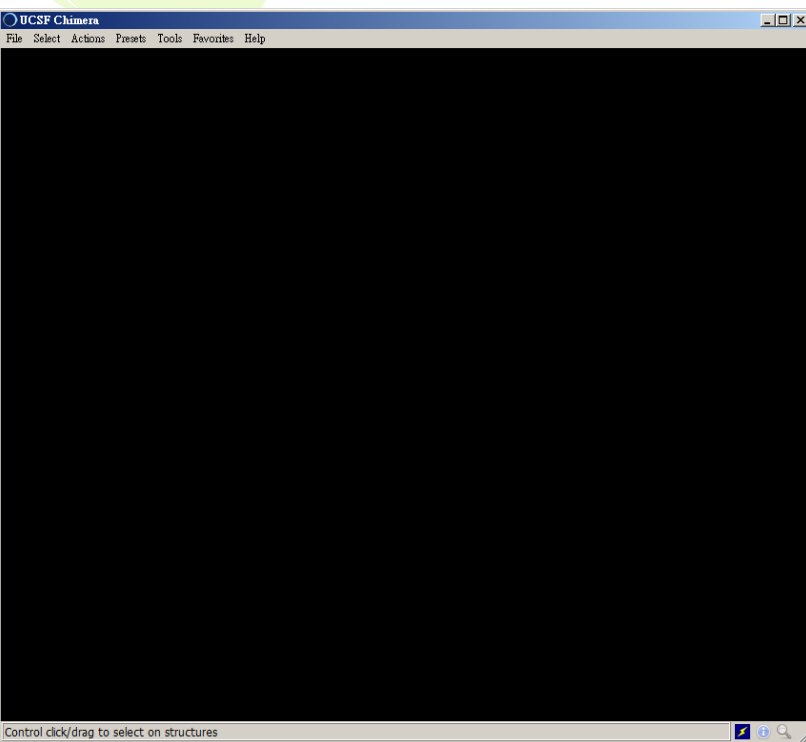
1981 First **B-DNA** structure determined (Drew *et al.*, 1981)

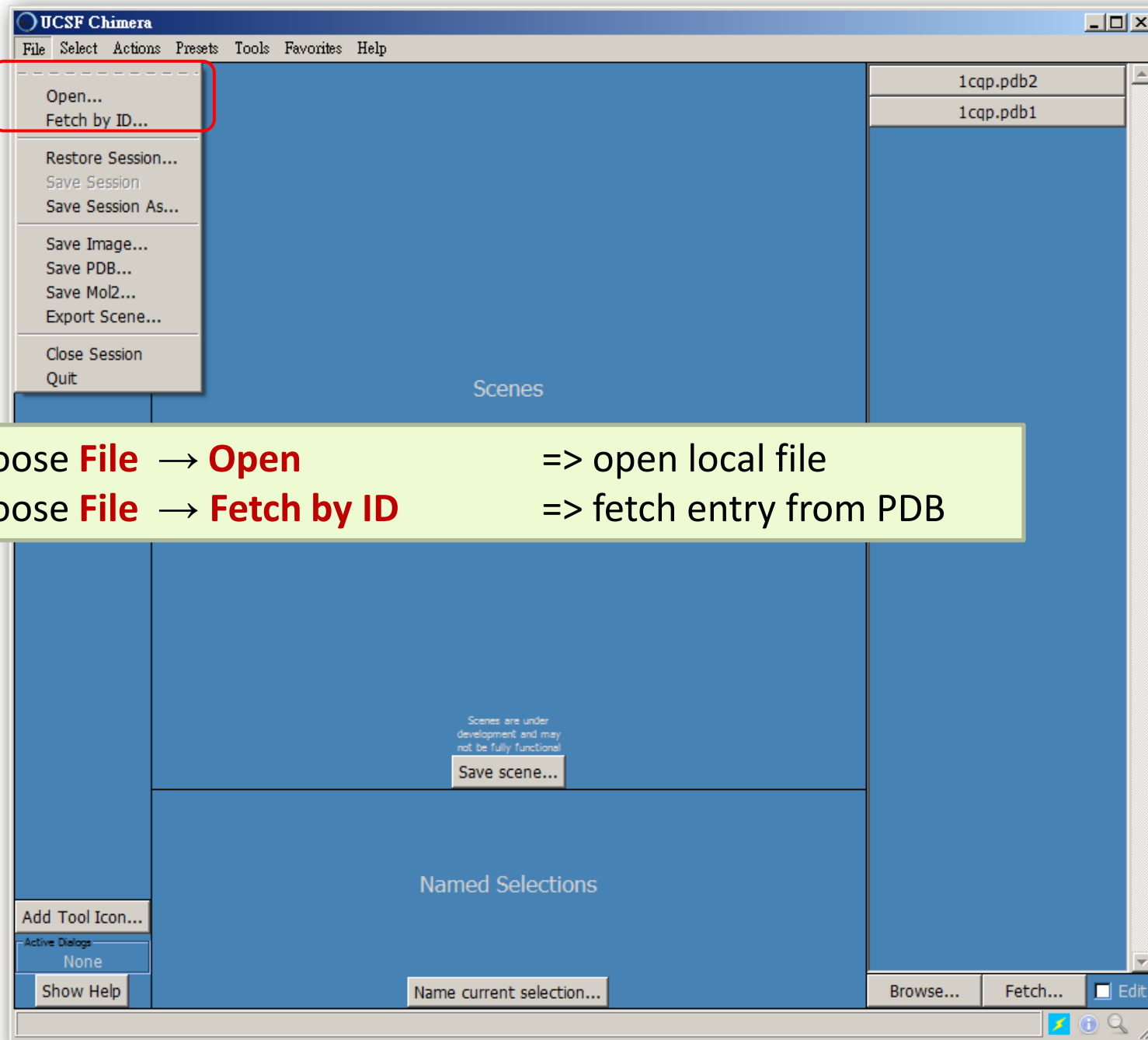
1979 First **DNA (Z-DNA)** determined (Wang *et al.*, 1979)

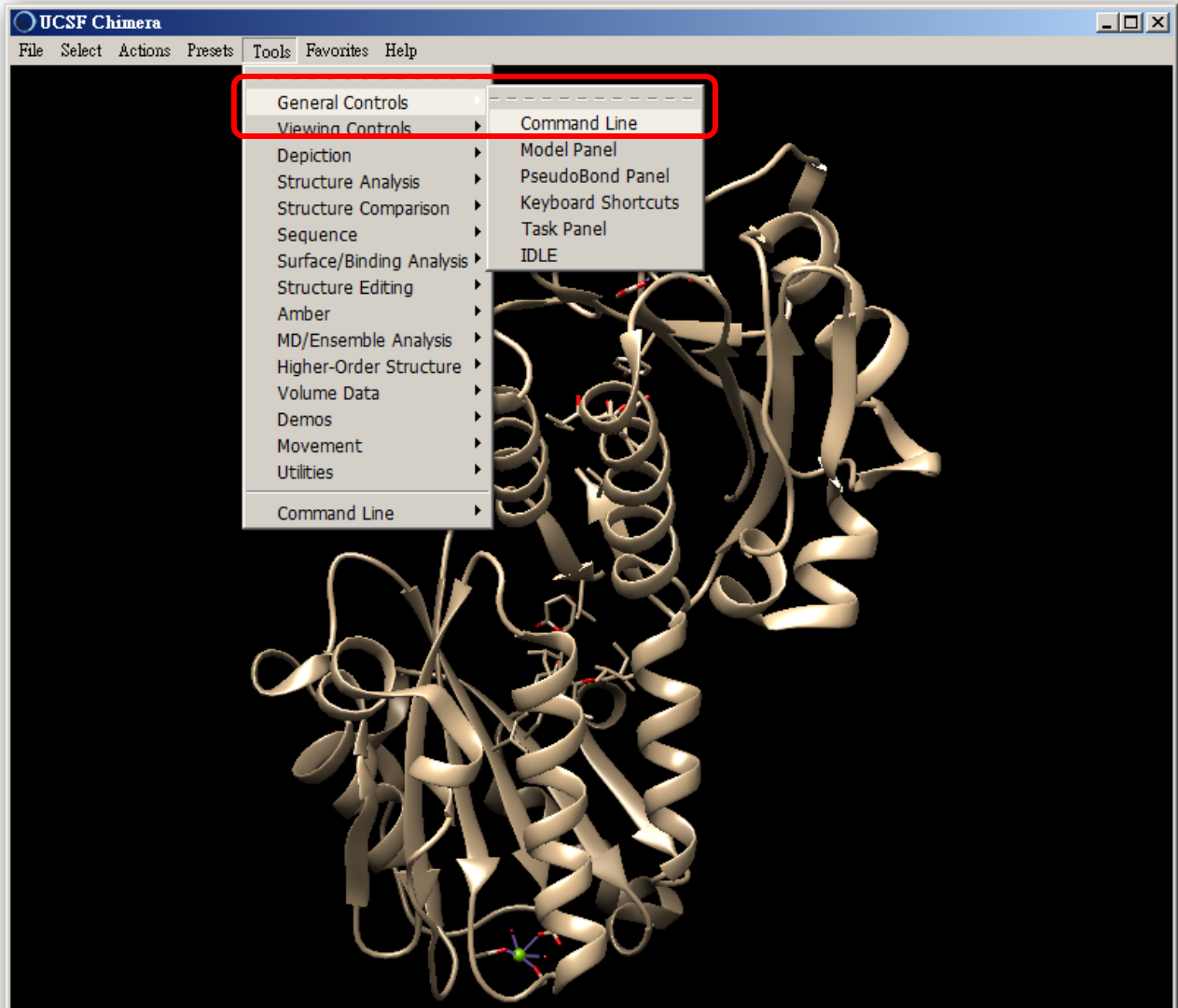
1973 First **tRNA** structures determined (Kim *et al.*, 1973; Robertus *et al.*, 1974)



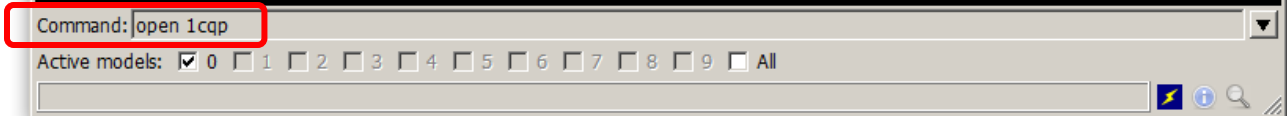
# Launching Chimera







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



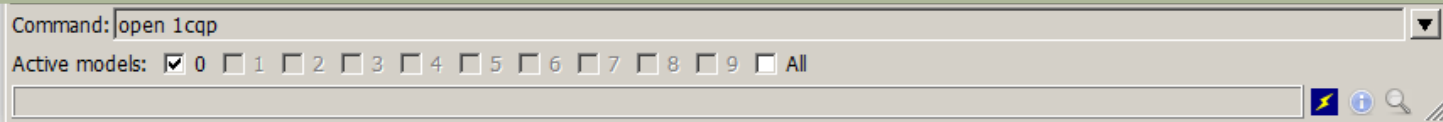
Command: **open 1cqp**

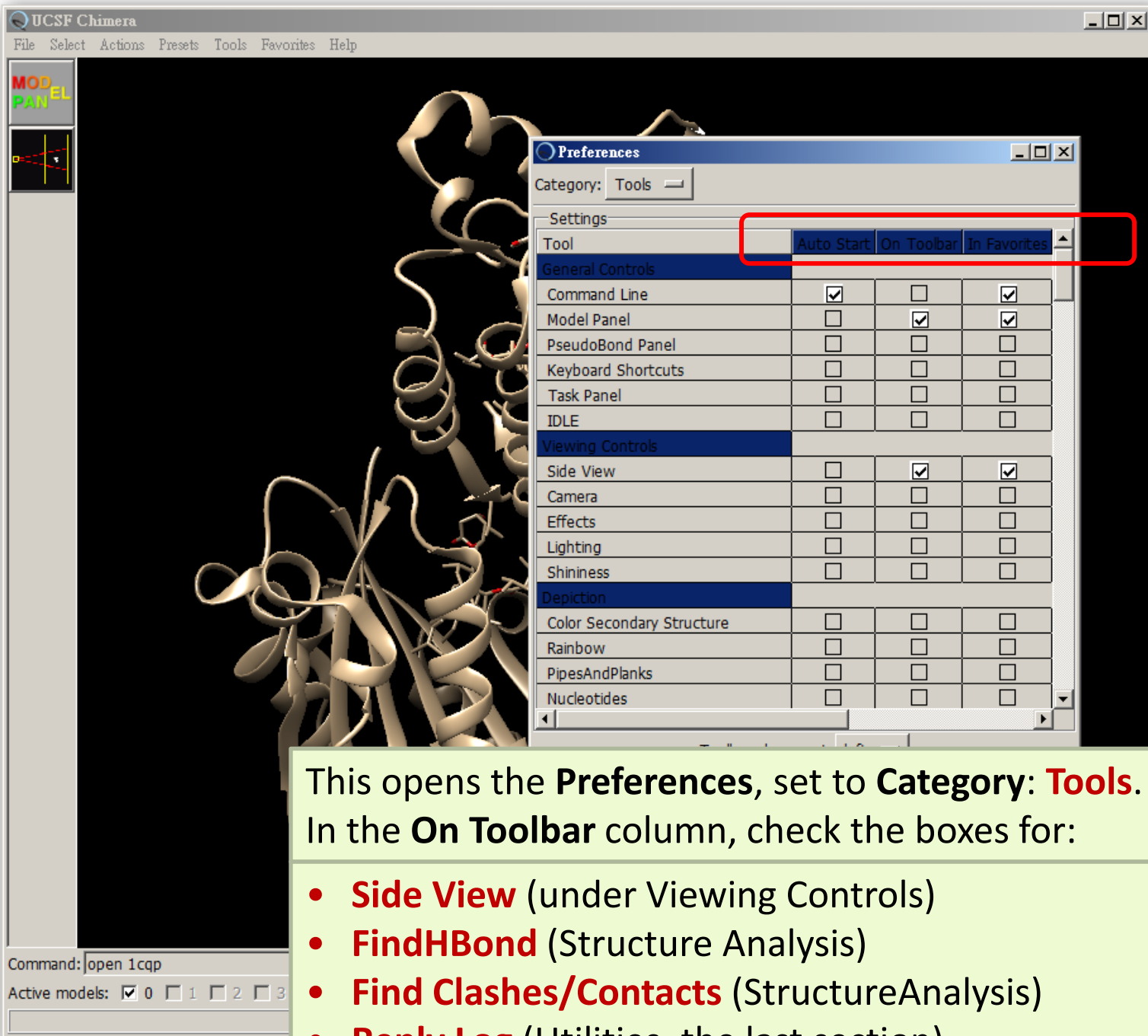
fetch the entry with ID **1cqp** from the Protein Data Bank (**PDB**)





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.



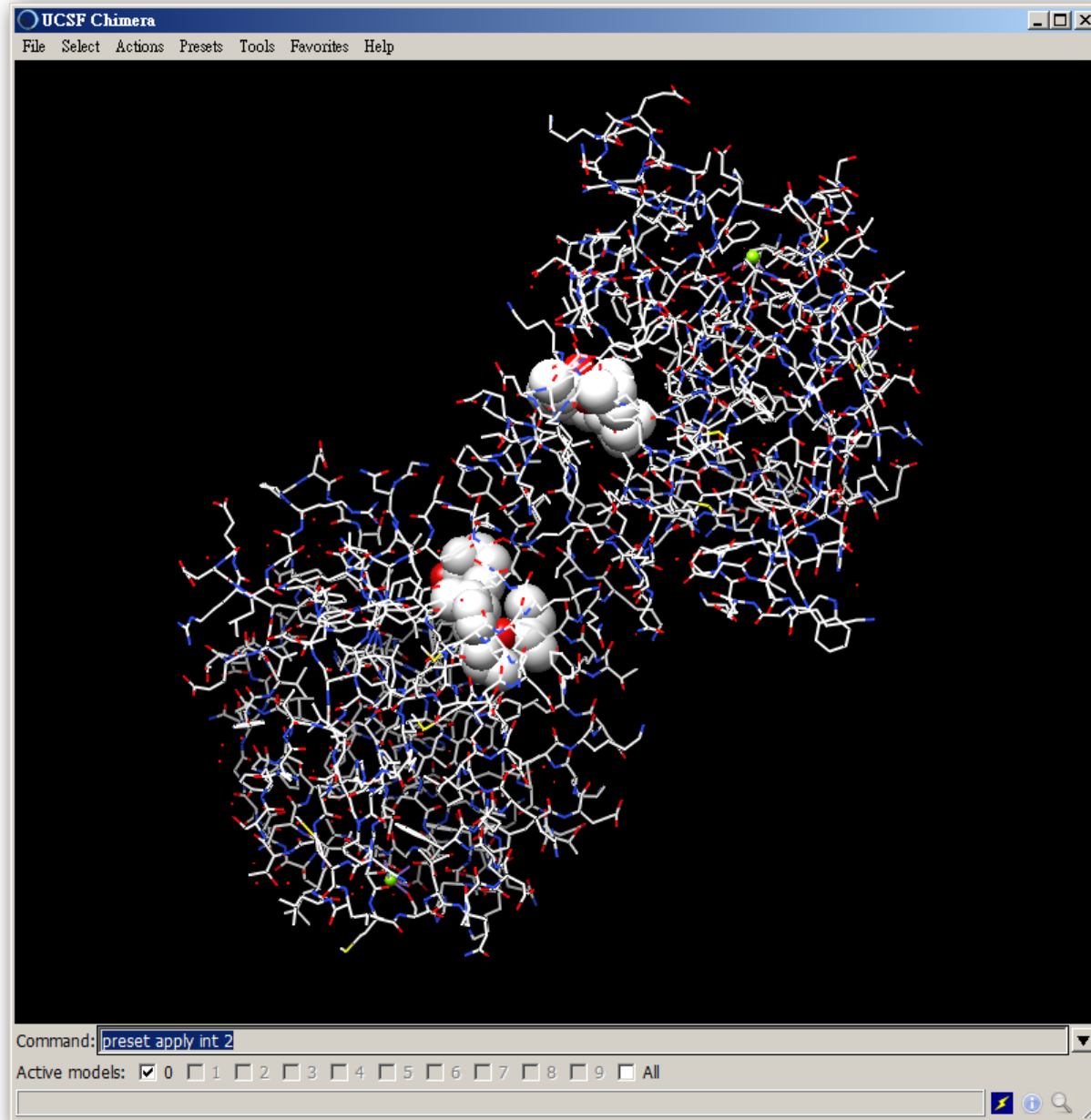
The Chimera User's Guide has three main parts, which are interconnected:

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- [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.



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 (silhouette, rounded ribbon, sticks)
  - 2 (silhouette, 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...



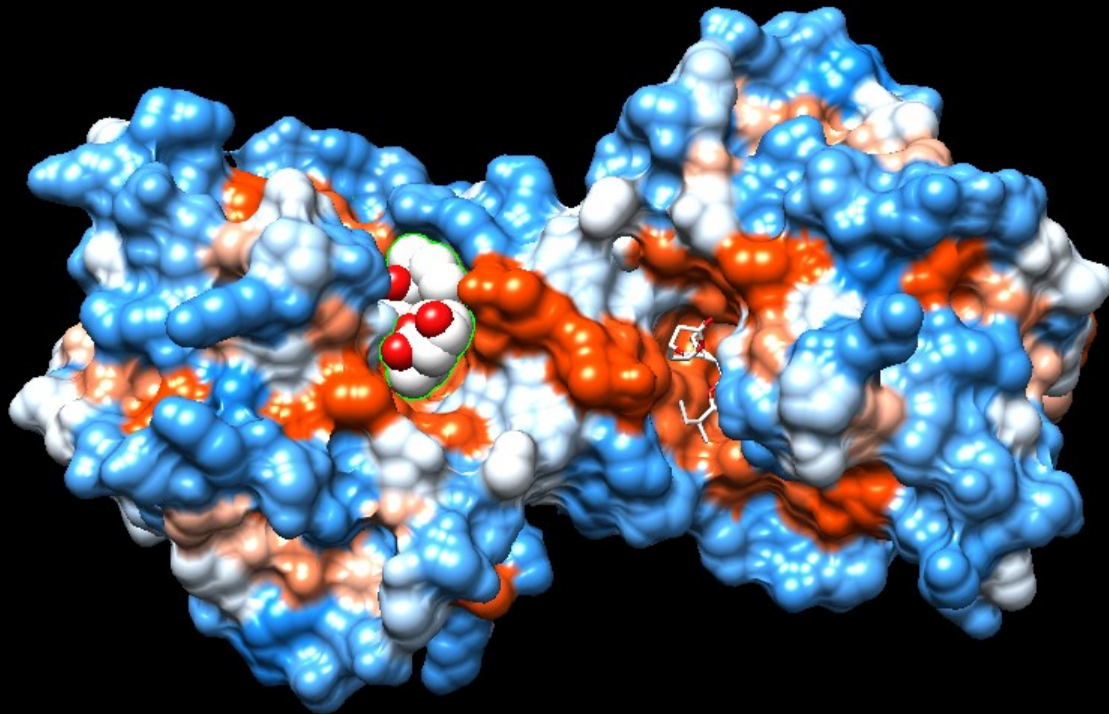
Command: preset apply int 2

Active models:  0  1  2  3  4  5  6  7  8  9  All

The image shows the UCSF Chimera software interface. The main window displays a protein structure with two chains: one in red and one in blue. Both chains are shown as ribbons, with a stick model of a small molecule bound to the protein. A 'Presets' menu is open, showing various rendering options. The command line at the bottom shows 'preset apply int 2' and the 'Active models' section has '0' selected.



Choose **Presets** → **Interactive 3**  
Use mouse to click and select one ligand  
Choose **Actions** → **Atoms/Bonds 3** → **sphere**

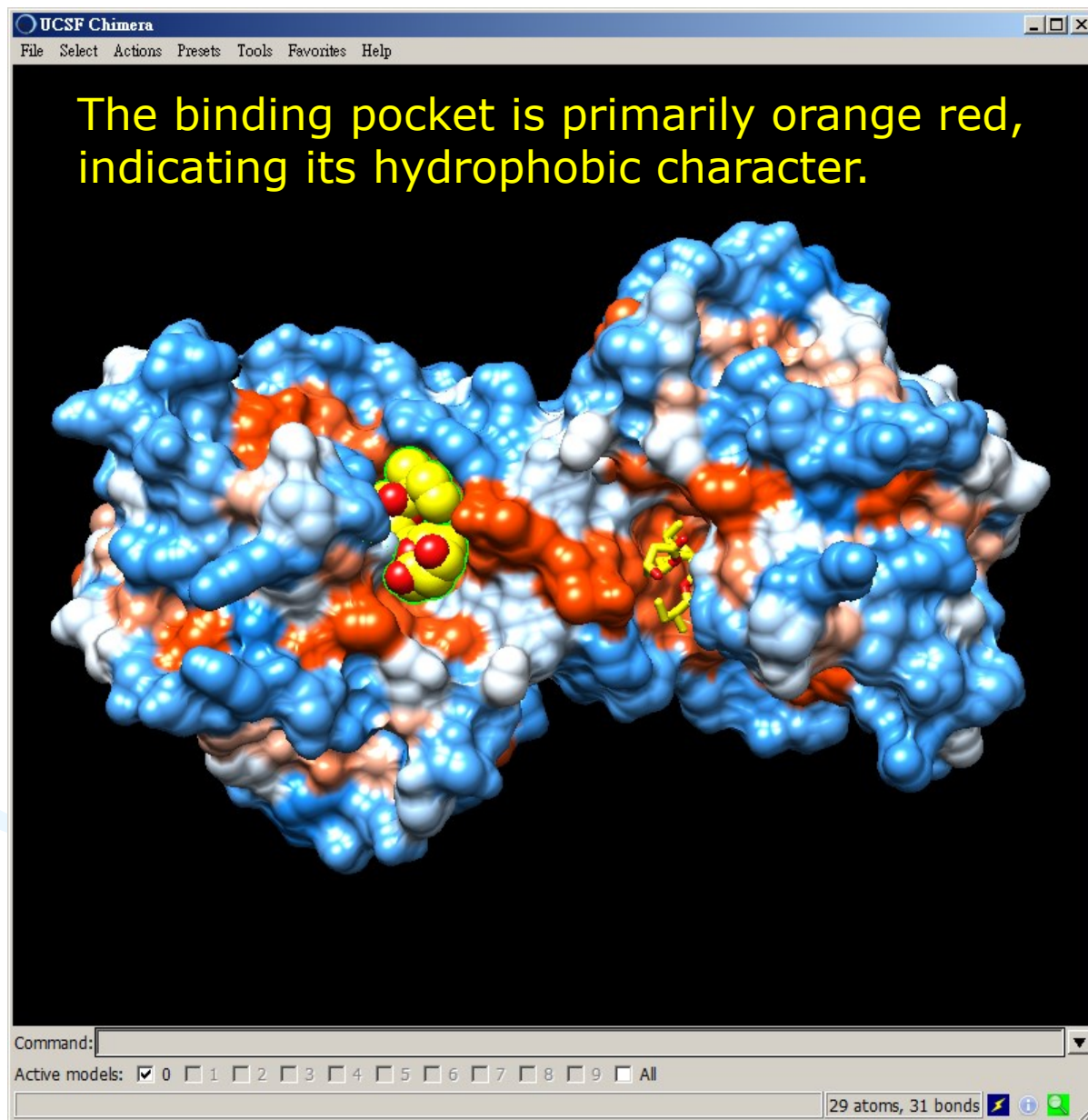


“hydrophobicity surface” preset:  
from **dodger blue** for the  
most **hydrophilic**, to **white**, to  
**orange red** for the most  
**hydrophobic**.

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

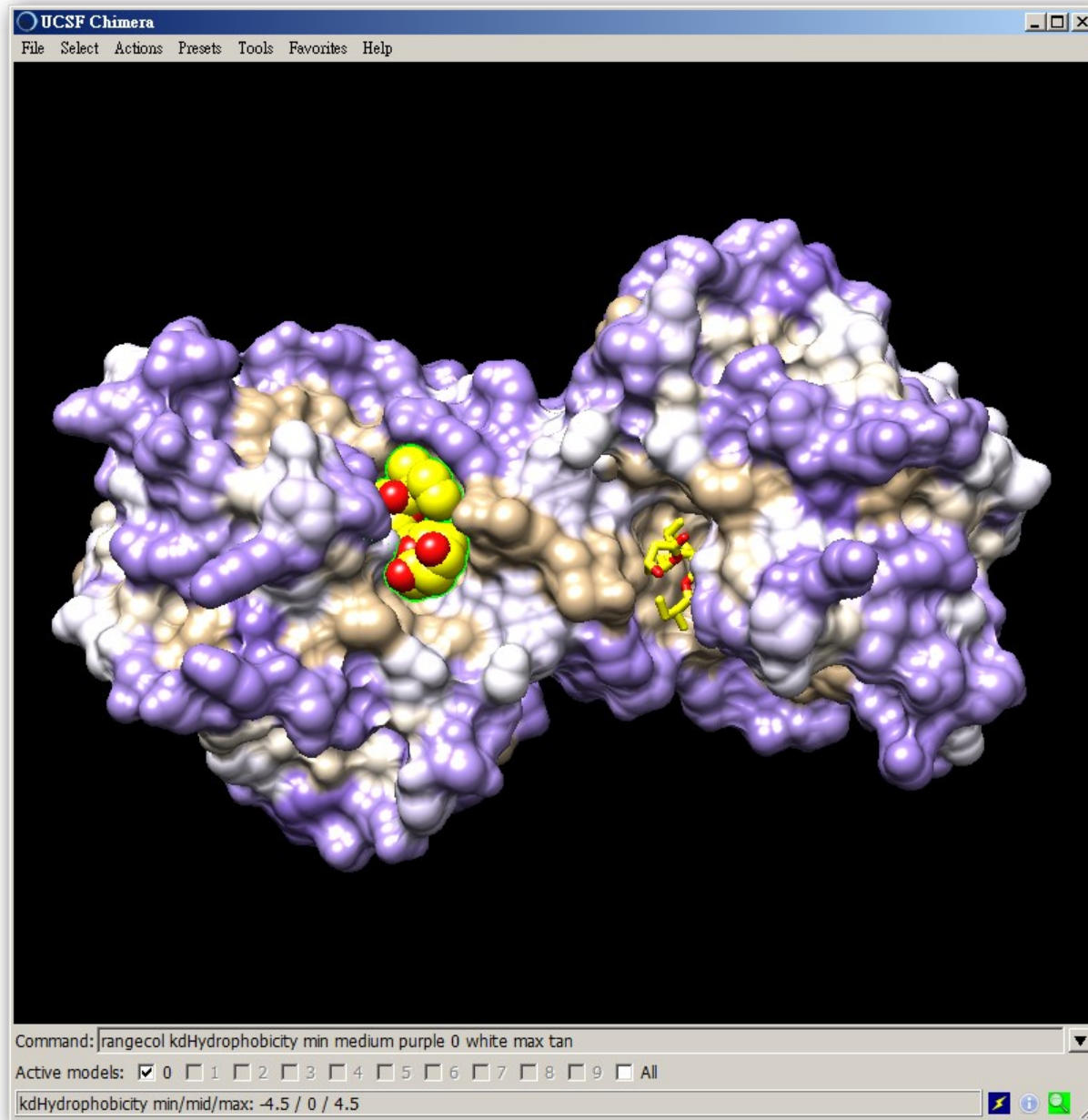
Command:  
**preset apply int 3 ; select :311.A ; rep sphere :311.A**

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



Command:

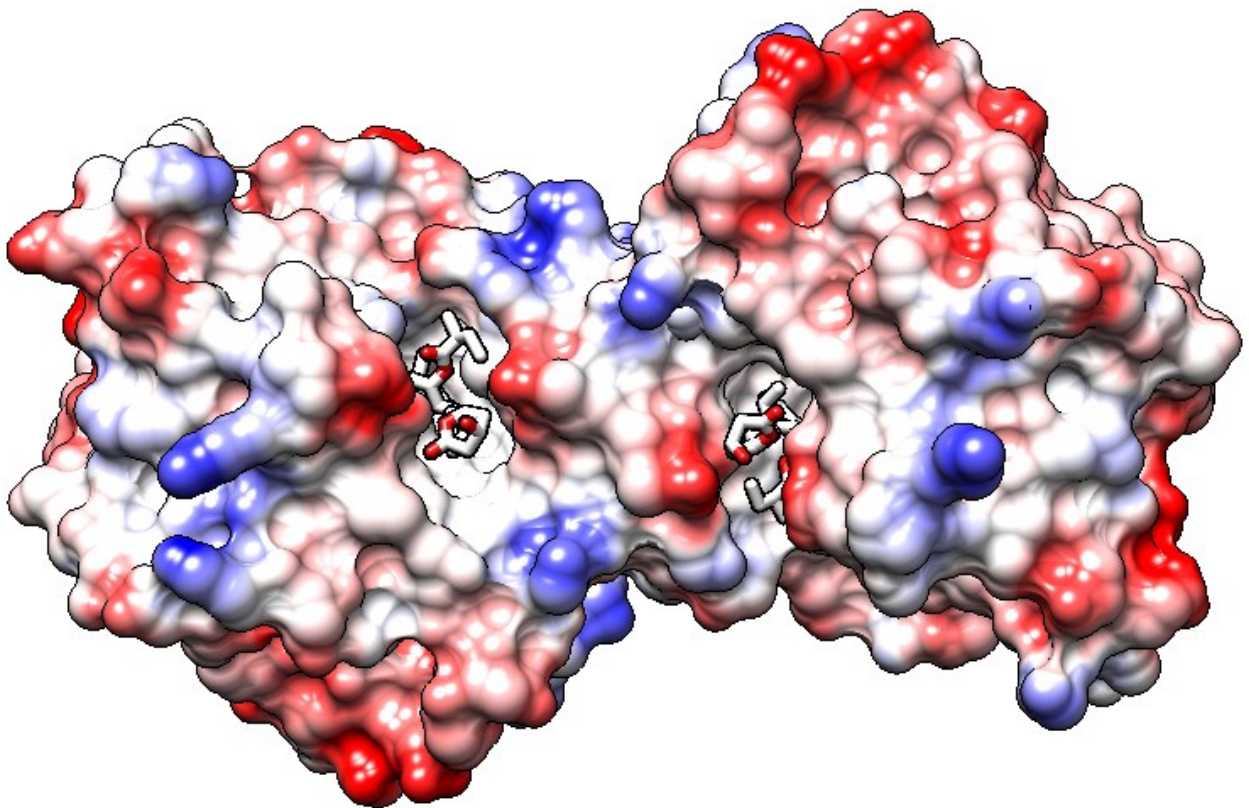
**setattr m stickScale 2 ; color yellow ligand & C**



Command:

**rangecol kdHydrophobicity min medium purple 0 white max tan**

Choose **Presets** → **Publication 1**  
Choose **Tools** → **Surface/Binding Analysis** → **Coulombic Surface Coloring**



**Coulombic Surface Coloring**

Surfaces to color by ESP:  
MSMS main surface of 1cqp.pdb (#0)

Number of colors/values: 3

-10 0 10 kcal/(mol/e)

Distance-dependent dielectric: true

Dielectric constant: 4.0

Distance from surface: 1.4

Implicit Histidine Protonation  
*Assumed histidine protonation for structures without explicit hydrogens*

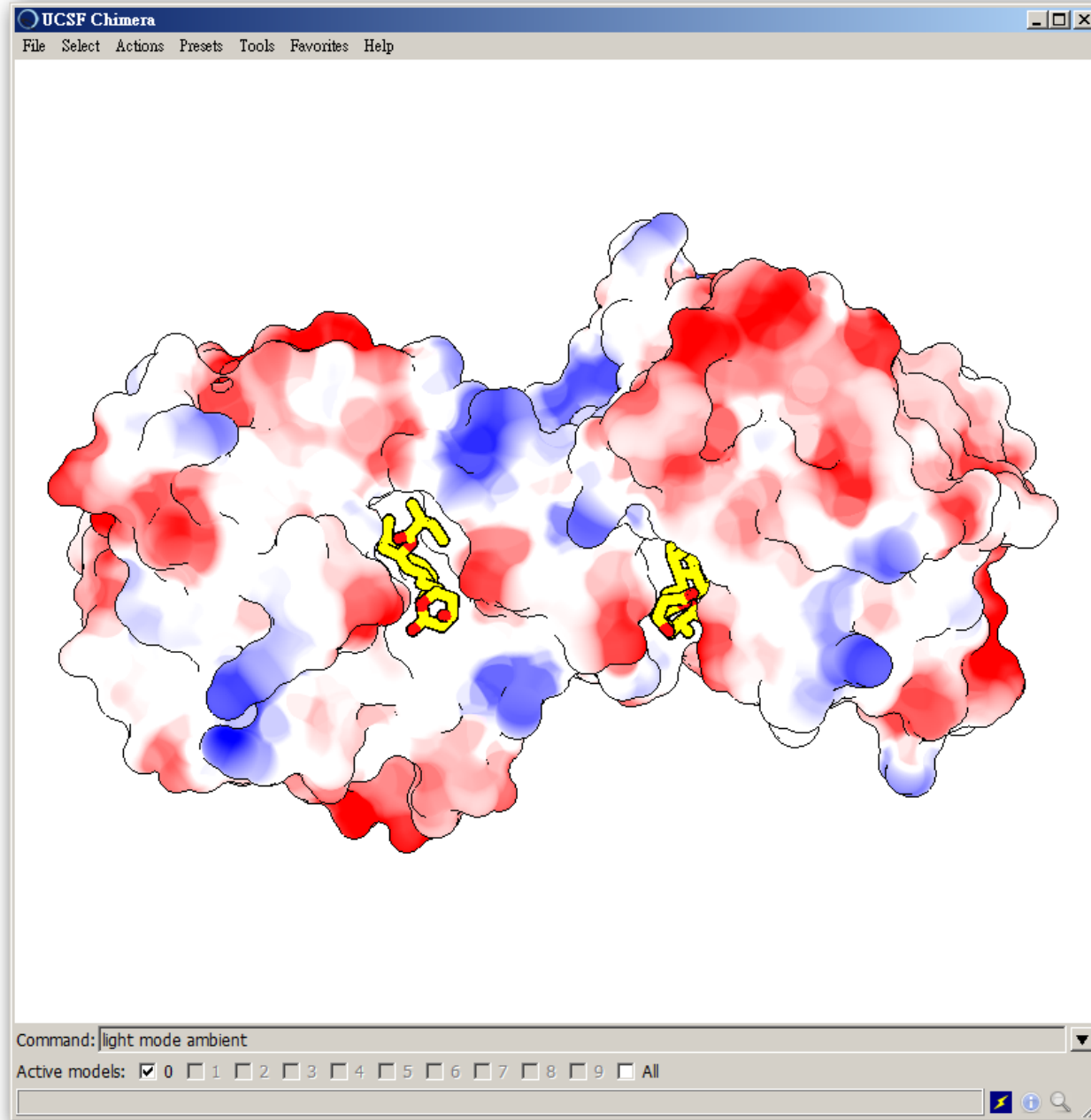
Residue name-based  
HID/HIE/HIP = delta/epsilon/both  
HIS = estimated from H-bonds

Specified individually...

Compute grid...

Create corresponding color key

OK Apply Close Help



Command: **light mode ambient**

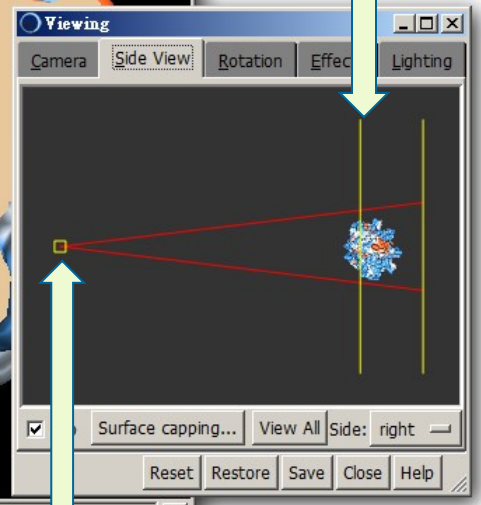
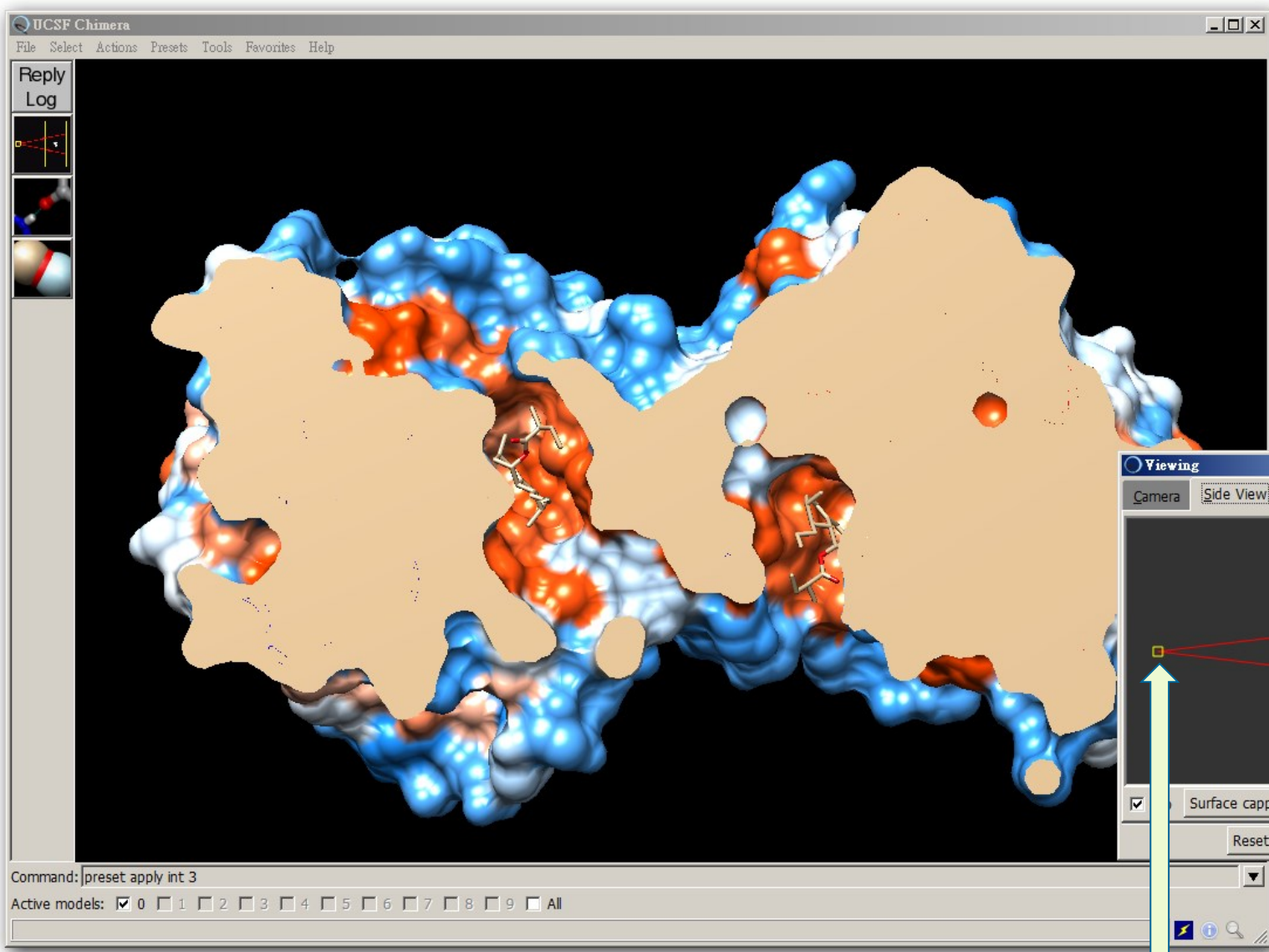
## Side View

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

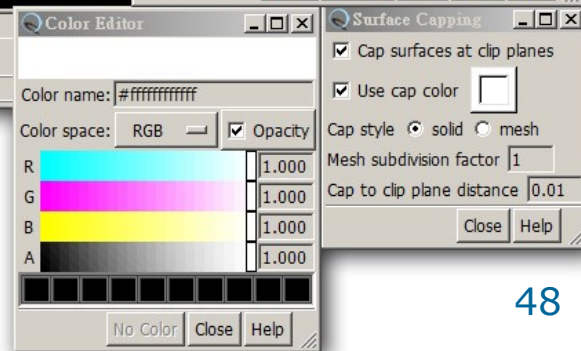
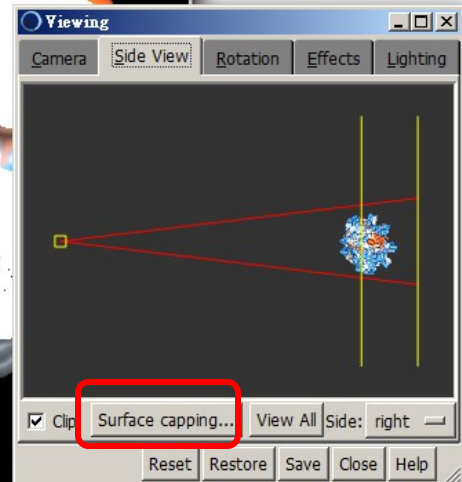
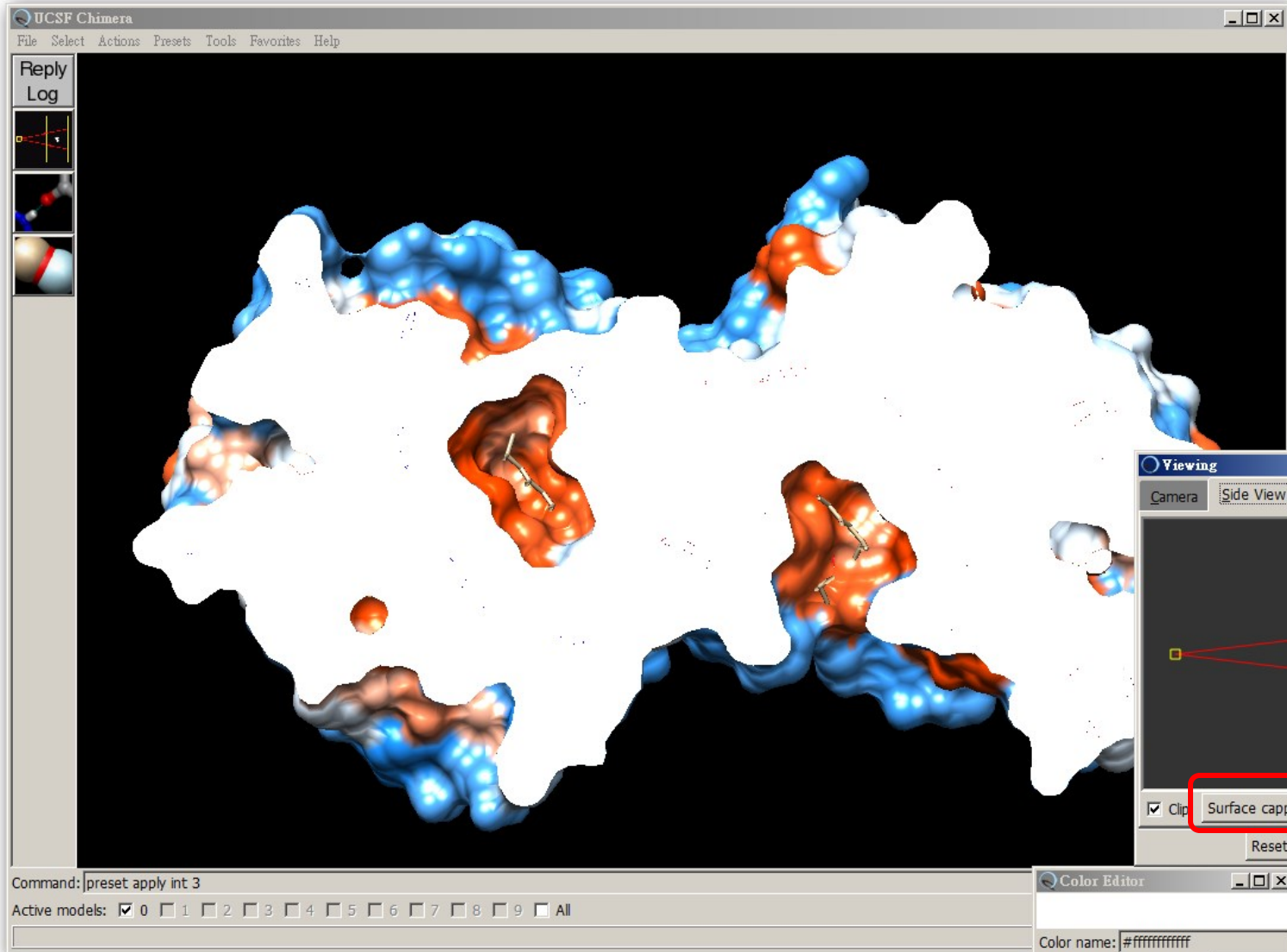
Choose **Tools** → **Viewing Controls** → **Side View**

The image shows a screenshot of the UCSF Chimera software interface. The main window displays a protein structure rendered as a blue and orange surface model. A yellow box highlights the navigation path: **Choose Tools** → **Viewing Controls** → **Side View**. The **Viewing** panel is open, showing the **Side View** camera mode. The **Command** line at the bottom contains the text: `Command: preset apply int 3`. The **Active models** section shows a list of models from 0 to 9, with model 0 selected.

adjust the clip plane



scale





## Atom Specification Symbols

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

## Specification Symbols

Symbol	Function	Usage
#	model number	# <i>model</i> (integer)
#.	submodel number	#. <i>submodel</i> (integer)
:	residue	: <i>residue</i> (name or number)
::	residue name	:: <i>residue</i>
::.	chain ID	::. <i>chain</i>
@	atom name	@ <i>atom</i>
@.	alternate location ID	@. <i>alt_loc</i>
-	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< <i>zone</i> or zr< <i>zone</i> specifies all residues within <i>zone</i> angstroms, za< <i>zone</i> specifies all atoms (rather than entire residues)

## 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/CI'  
- or -  
:26-28.a,33.a & with CA/CI'  
- 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

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

&	intersection	intersection of specified sets
	union	union of specified sets
~	negation	negation of specified set

0  
solvent & Ng+ z<3 | solvent & N3+ z<3  
- solvent residues within 3 angstroms of guanidinium nitrogens or sp3-hybridized, formally positive nitrogens

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

# Coloring by B-Factor

The image shows the UCSF Chimera software interface. The main window displays a protein structure colored by B-factor, with a color scale ranging from 2 (blue) to 50 (yellow). The protein is shown as a ribbon structure. A color key is visible at the bottom of the main window, showing a gradient from blue to yellow with labels 2, 30, and 50. The '2D Labels/Color Key' dialog box is open on the right, showing settings for the color key. The dialog box has tabs for 'Labels', 'Arrows', and 'Color Key'. The 'Color Key' tab is selected. The 'Number of colors/labels' is set to 3. The 'Colors' section shows three color swatches: blue (value 2), red (value 30), and yellow (value 50). The 'Label positions' are set to 'right/bottom'. The 'Label color' is set to white. The 'Label justification' is set to 'decimal point'. The 'Numeric label separation' is set to 'proportional to value'. The 'Font size' is set to 24. The 'Font style' is set to 'normal'. The 'Font typeface' is set to 'sans serif'. The 'Border color' is set to 'No'. The 'Border width' is set to 3. The 'Show tick marks' is set to 'false'. The 'Tick length' is set to 10. The 'Tick thickness' is set to 4. The 'Use mouse for key placement' checkbox is checked. The 'Grab middle of key to reposition' checkbox is checked. The 'Delete', 'Close', and 'Help' buttons are visible at the bottom of the dialog box.

UCSF Chimera  
File Select Actions Presets Tools Favorites Help

Reply  
Log

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

Grab middle of key to reposition

Delete Close Help

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

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Reply Log

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:

Label positions:

Label color:

Label justification:

Numeric label separation:

Label offset:

Font size:

Font style:

Font typeface:

Border color:

Border width:

Show tick marks:

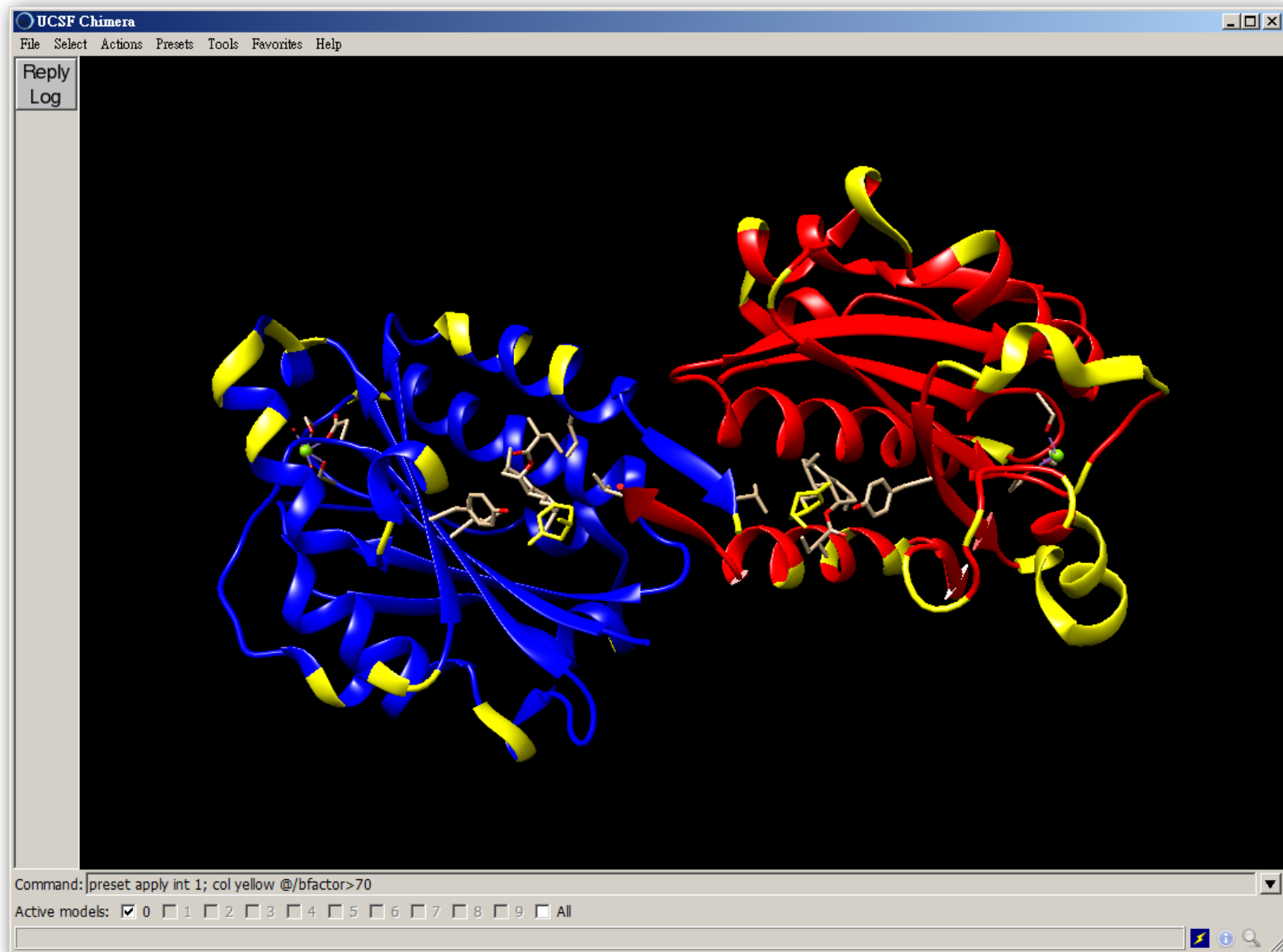
Tick length:

Tick thickness:

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.

The screenshot shows the UCSF Chimera interface. The main window displays a protein structure (white sticks) with an electron density map (gray mesh) overlaid. A callout box points to the Volume Viewer dialog, which is open in the bottom right corner. The dialog shows the volume name '2fma.omap #1' and a step number '2'. The eye icon is highlighted with a red box. Below the dialog, the command line shows 'Command: open edsID:2fma' and the active models list includes '0', '1', '2', '3', '4', '5', '6', '7', '8', '9', and 'All'.

Command: **show :168-170**

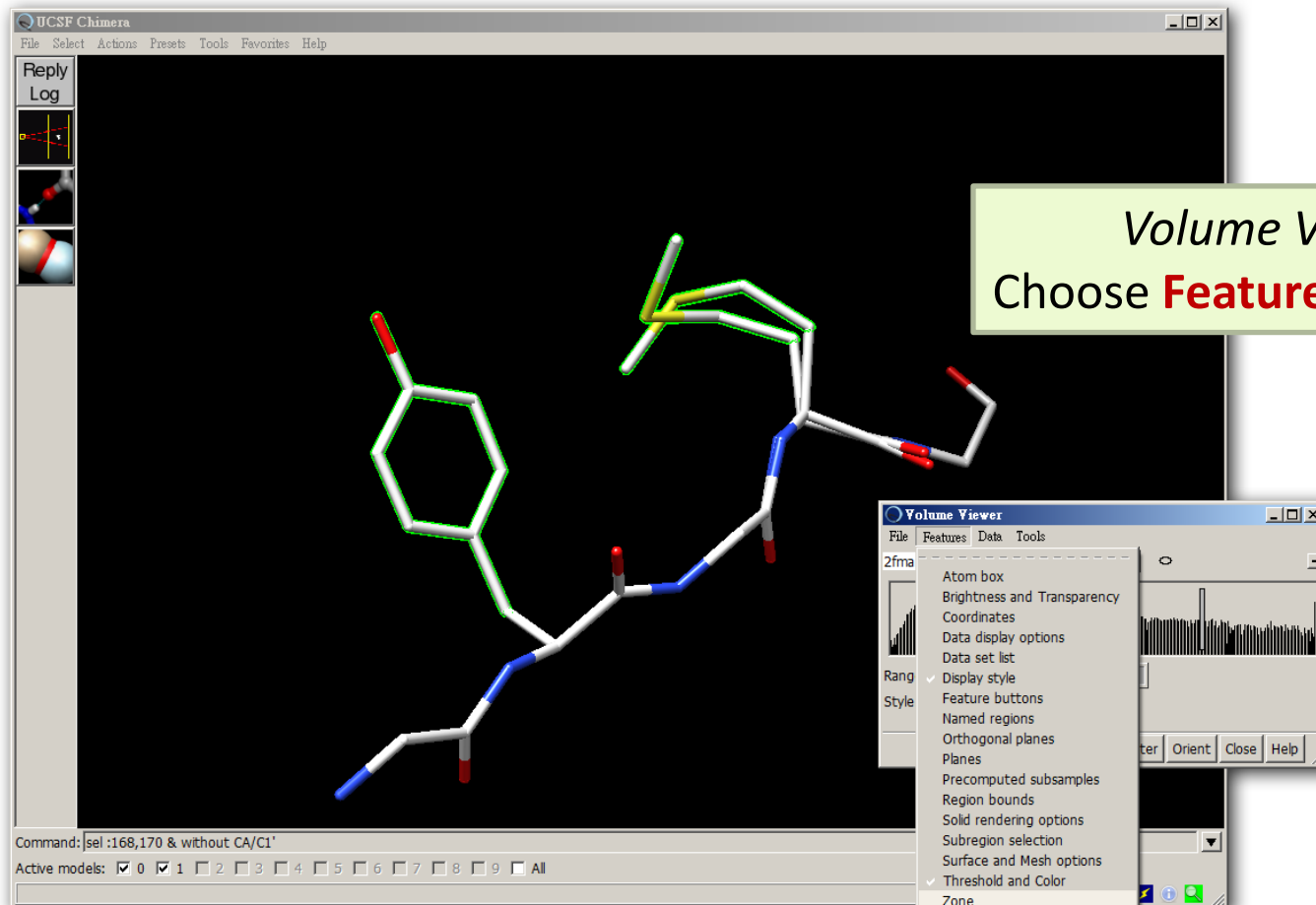
**focus**

**disp :167,171@n,ca,c,o**

**rep stick**

**setattr m stickScale 0.5**

**sel :168,170 & without CA/C1'**



The image shows a screenshot of the UCSF Chimera software interface. The main window displays a 3D molecular model of a protein-ligand complex. The protein backbone is shown in a stick representation, colored by atom type (carbon in white, oxygen in red, nitrogen in blue). A ligand molecule is bound to the protein, with its atoms colored in green and yellow. The Volume Viewer dialog box is open in the bottom right corner, showing a density map of the ligand. The dialog box has a menu bar (File, Features, Data, Tools) and a title bar (Volume Viewer). Below the menu bar, it shows the file name '2fma.omap #1' and the step number '1'. A histogram of the density map is displayed. The 'Range' is set to '-1.15 - 5' and the 'Level' is '3.35'. The 'Color' is set to a gray square. The 'Style' is set to 'mesh'. The 'Zone' button is highlighted with a red box and a green arrow pointing to it. The 'Zone' button is labeled 'Zone near selected atoms.' and has 'No Zone' and 'Mask' buttons next to it. The 'Center', 'Orient', 'Close', and 'Help' buttons are at the bottom of the dialog box. The command line at the bottom of the Chimera window shows the command: 'sel :168,170 & without CA/C1'. The status bar shows 'Active models: 0 1 2 3 4 5 6 7 8 9 All' and 'Done reading 2fma.omap'.

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Reply Log

Volume Viewer

File Features Data Tools

2fma.omap #1 45 40 33 step 1

Range -1.15 - 5 Level 3.35 Color

Style  surface  mesh  solid

Zone near selected atoms. No Zone Mask

Center Orient Close Help

Command: sel :168,170 & without CA/C1

Active models:  0  1  2  3  4  5  6  7  8  9  All

Done reading 2fma.omap

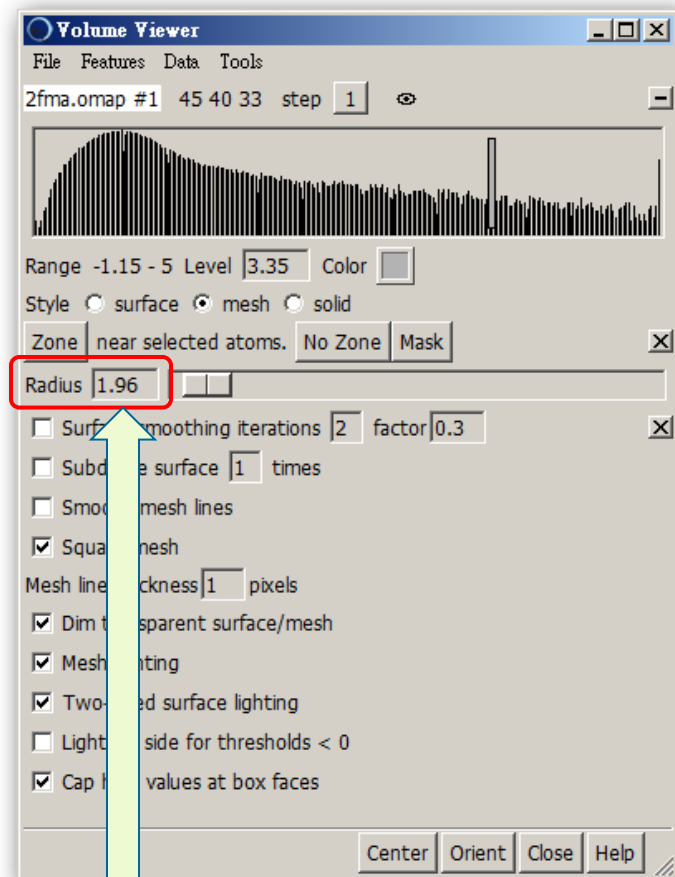
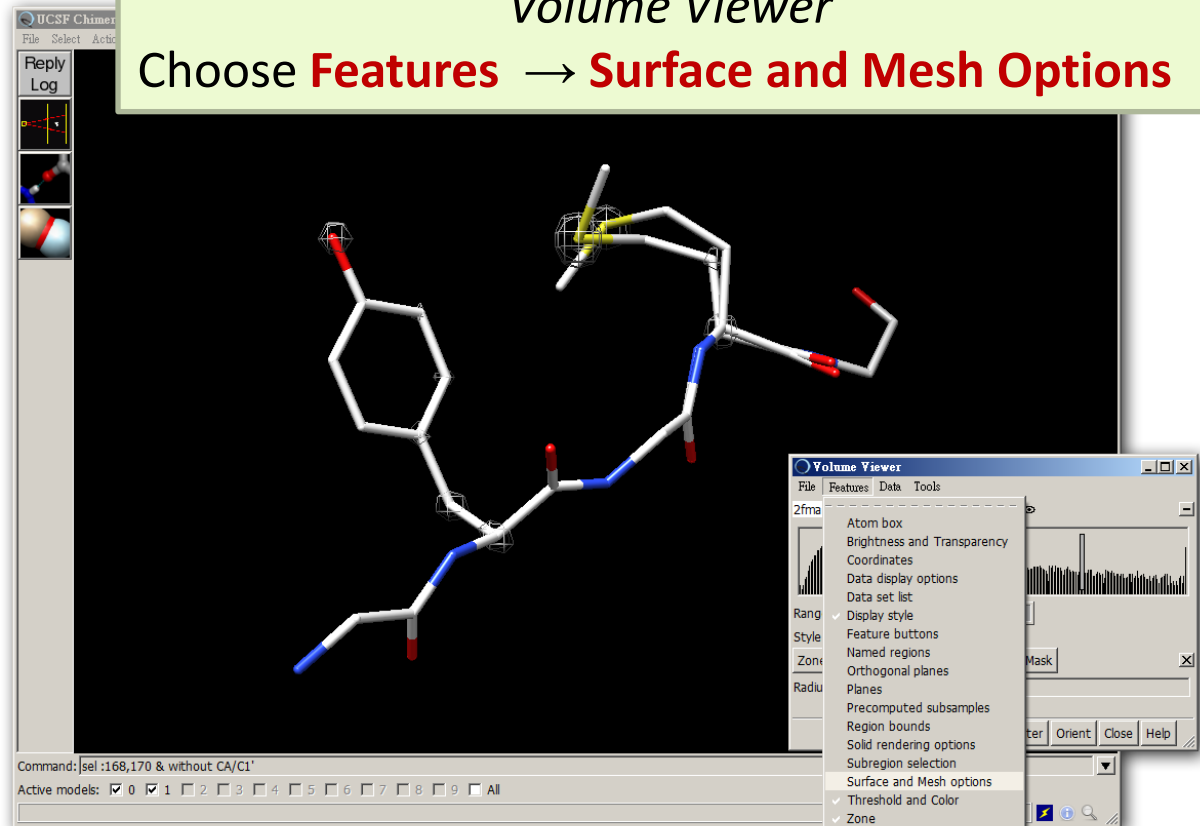
Click on **Zone**

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.

The screenshot displays the UCSF Chimera interface. The main window shows a molecular model with a volume map overlaid. The Volume Viewer dialog is open, showing a histogram of the volume map. The Level field is set to 2.06, and the Color well is set to a magenta color. The Color Editor dialog is also open, showing the color well and the RGB values (1.0, 0.0, 1.0, 0.6). The Command line at the bottom shows the command: `sel :168,170 & without CA/C1'`

**Level** 2.06,  
**Color (RGBA)** 1.0 0.0 1.0 0.6

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

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

The screenshot shows the UCSF Chimera interface. The main window displays a molecular model with a cyan surface and a purple mesh. The Volume Viewer panel is open, showing a histogram with a red arrow pointing to a peak. The Color Editor panel is also open, showing the color settings for the selected volume.

Volume Viewer settings:

- Range: -1.15 - 5
- Level: 0.42
- Color: [selected]
- Style:  surface  mesh  solid
- Zone: near selected atoms. No Zone Mask
- Radius: 1.96
- Surface smoothing iterations: 2 factor: 0.3
- Subdivide surface: 1 times
- Smooth mesh lines
- Square mesh
- Mesh line thickness: 1 pixels
- Dim transparent surface/mesh
- Mesh lighting
- Two-sided surface lighting
- Light flip side for thresholds < 0
- Cap high values at box faces

Color Editor settings:

- Color name: #5c29ffffff
- Color space: RGB [selected] Opacity [checked]
- R: 0.360
- G: 1.000
- B: 1.000
- A: 0.400

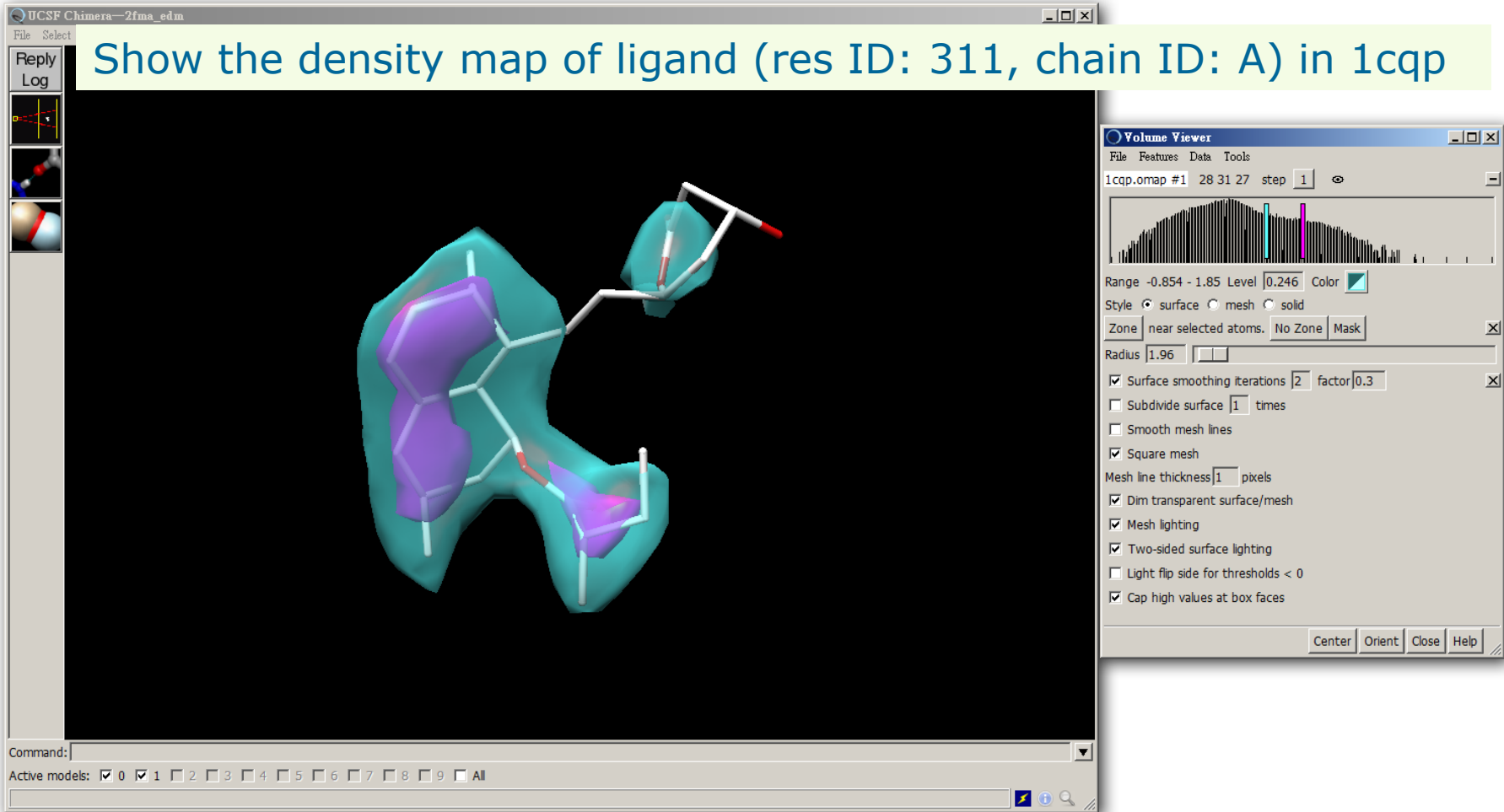
**Level 0.426,**  
**Color (RGBA) 0.36 1.0 1.0 0.4**  
**Style surface**  
turned **on Surface smoothing iterations 2 factor 0.3**

UCSF Chimera—2fma\_edm

File Select

Reply Log

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



Volume Viewer

File Features Data Tools

1cqp.omap #1 28 31 27 step 1

Range -0.854 - 1.85 Level 0.246 Color

Style  surface  mesh  solid

Zone near selected atoms. No Zone Mask

Radius 1.96

Surface smoothing iterations 2 factor 0.3

Subdivide surface 1 times

Smooth mesh lines

Square mesh

Mesh line thickness 1 pixels

Dim transparent surface/mesh

Mesh lighting

Two-sided surface lighting

Light flip side for thresholds < 0

Cap high values at box faces

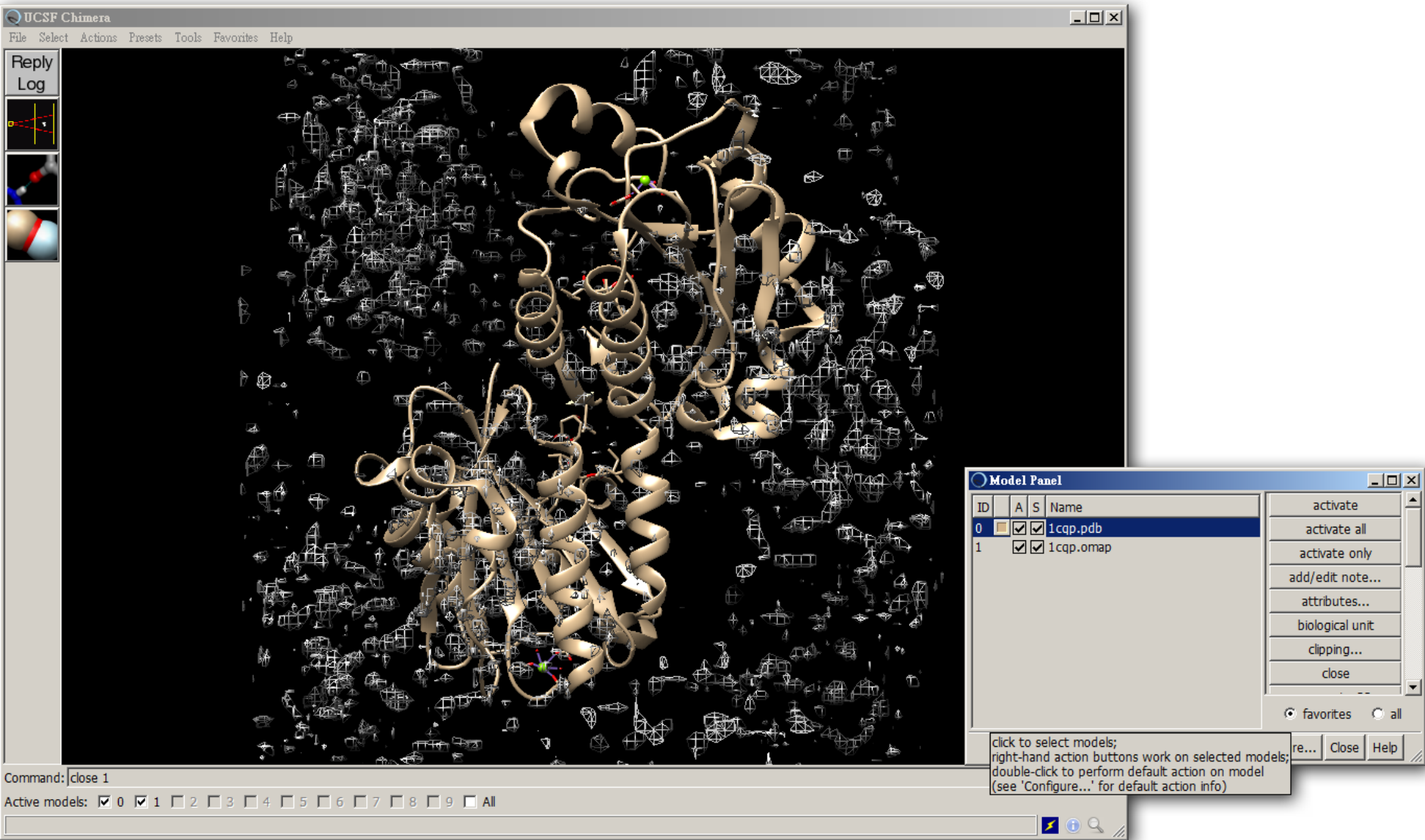
Center Orient Close Help

Command:

Active models:  0  1  2  3  4  5  6  7  8  9  All

**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**



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:  angstroms  
 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

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

The screenshot shows the UCSF Chimera interface. The main window displays a protein structure in a tan ribbon representation with a yellow and green ligand molecule. A red box highlights the 'Find Clashes/Contacts' icon in the left-hand toolbar. The 'Find Clashes/Contacts' dialog box is open on the right, showing various settings for finding contacts between atoms. The 'Default' dropdown is set to 'contact', and the 'Draw pseudobonds' checkbox is checked. The 'Frequency of Checking' is set to 'when OK/Apply clicked'.

UCSF Chimera  
File Select Actions Presets Tools Favorites Help

Reply Log

Click on Find steric clashes or atomic contacts icon

Find Clashes/Contacts

Atoms to Check  
Designate currently selected atoms for checking  
58 atoms designated  
 themselves  
 all other atoms  
Check designated atoms against:  
 other atoms in same model  
 second set of designated atoms  
Designate selection as second set  
No second set

Clash/Contact Parameters  
Find atoms with VDW overlap  $\geq$  -0.4 angstroms  
Subtract 0.0 from overlap for potentially H-bonding pairs  
Default clash / contact criteria  
Ignore contacts of pairs 4 or fewer bonds apart  
 Include intra-residue contacts  
 Include intra-molecule contacts

Treatment of Clash/Contact Atoms  
 Select  
 Color (red) (and color all other atoms Mo)  
 Draw pseudobonds of color (yellow) and width 2.0  
 If endpoint atom hidden, show endpoint residue  
 Assign 'overlap' attribute  
 Write information to file  
 Write information to reply log

Frequency of Checking  
 when OK/Apply clicked  
Check...  after relative motions (until dialog closed)  
 continuously (until dialog closed)

Command:   
Active models:  0  1  2  3  4  5  6  7  8  9  All

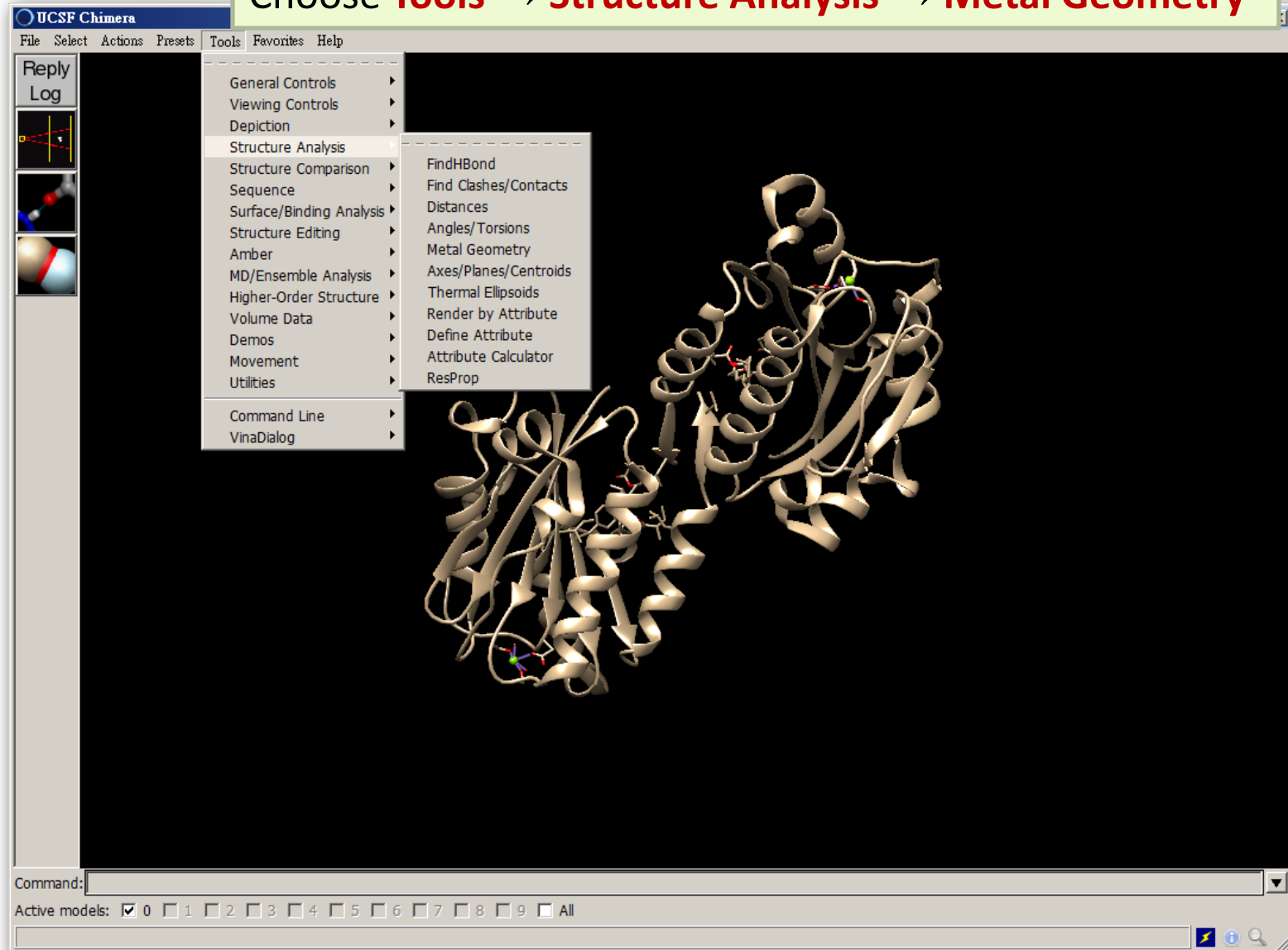
OK Apply Close Help

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

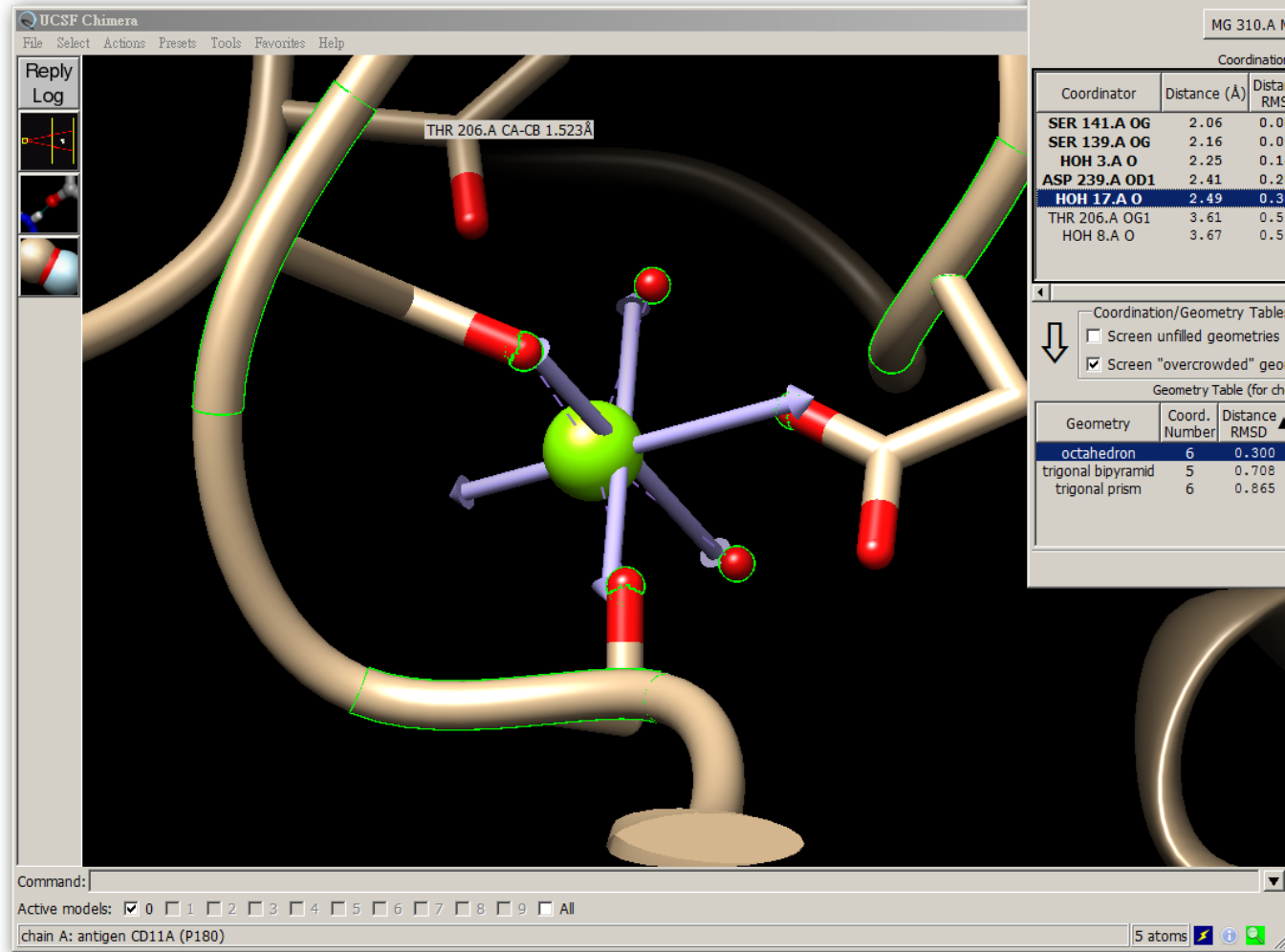


# Metal Geometry

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



# Metal Geometry



Metal Geometry

MG 310.A MG

Metal transparency:  opaque  transparent

Coordination Table

Coordinator	Distance (Å)	Distance RMSD	Best Geometry
SER 141.A OG	2.06	0.000	N/A
SER 139.A OG	2.16	0.095	octahedron
HOH 3.A O	2.25	0.140	trigonal prism
ASP 239.A OD1	2.41	0.281	octahedron
HOH 17.A O	2.49	0.300	octahedron
THR 206.A OG1	3.61	0.516	trigonal prism, square face-tri
HOH 8.A O	3.67	0.569	bicapped square antipris

Coordination Table Atoms

Add atoms selected in graphics window

Remove atoms selected in graphics window

Alt loc: N/A

Create/Update metal-complex pseudobonds

Display options...

Coordination/Geometry Tables

Screen unfilled geometries

Screen "overcrowded" geometries Show parameters

Geometry Table (for chosen coordination)

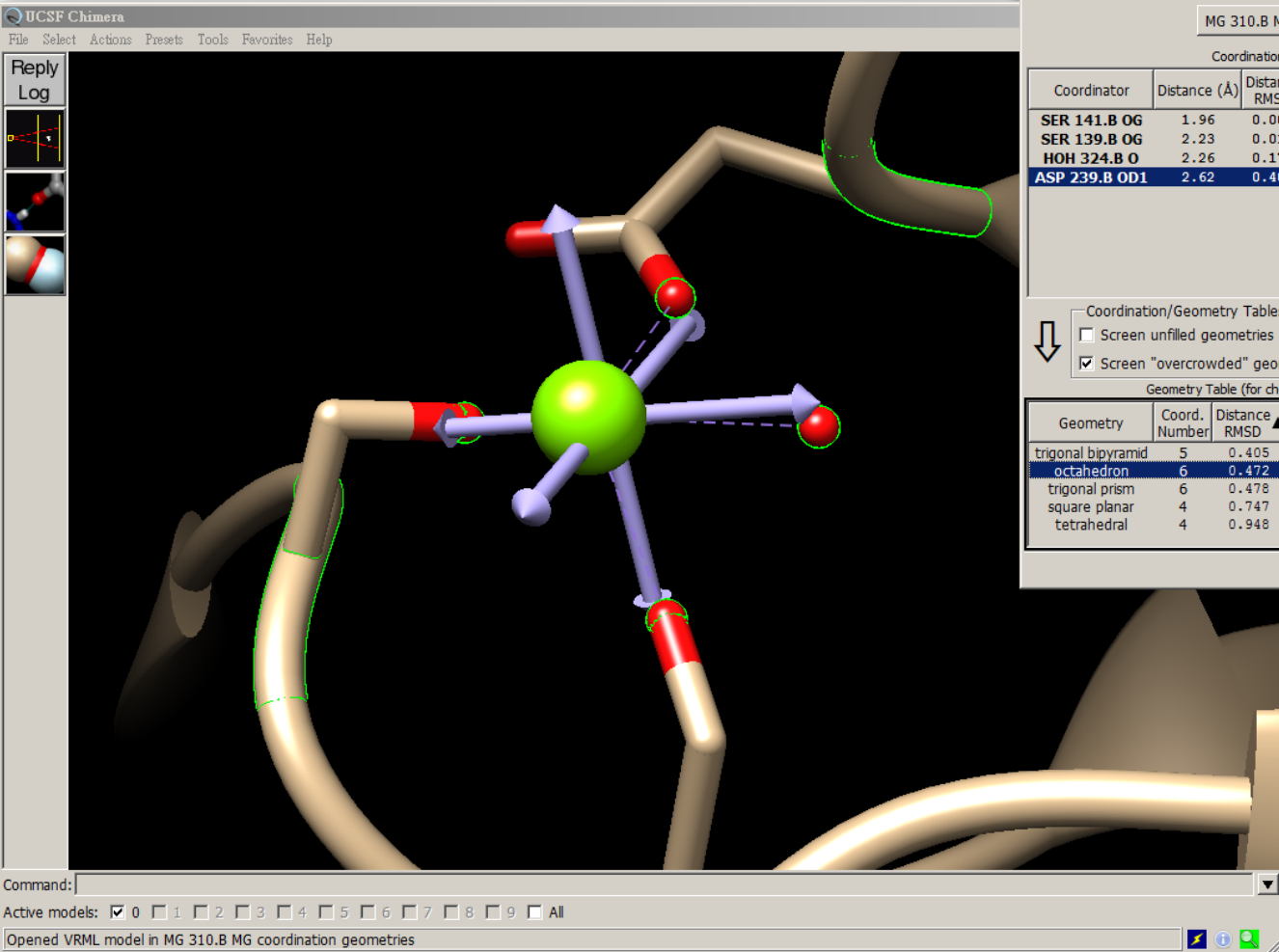
Geometry	Coord. Number	Distance RMSD
octahedron	6	0.300
trigonal bipyramid	5	0.708
trigonal prism	6	0.865

Depict idealized geometry

Add water oxygens at unfilled sites at a distance of 2.273 Å

Close Help

# Metal Geometry



**Metal Geometry**

MG 310.B MG

Metal transparency:  transparent

Coordination Table

Coordinator	Distance (Å)	Distance RMSD	Best Geometry
SER 141.B OG	1.96	0.000	N/A
SER 139.B OG	2.23	0.010	octahedron
HOH 324.B O	2.26	0.176	trigonal prism
ASP 239.B OD1	2.62	0.405	trigonal bipyramid

Coordination Table Atoms  
Add atoms selected in graphics window  
Remove atoms selected in graphics window  
Alt loc: N/A

Create/Update metal-complex pseudobonds  
Display options...

Coordination/Geometry Tables  
 Screen unfilled geometries  
 Screen "overcrowded" geometries Show parameters

Geometry Table (for chosen coordination)

Geometry	Coord. Number	Distance RMSD ▲
trigonal bipyramid	5	0.405
octahedron	6	0.472
trigonal prism	6	0.478
square planar	4	0.747
tetrahedral	4	0.948

Depict idealized geometry  
Add water oxygens at unfilled sites at a distance of 2.267 Å

Close Help

# Match Maker

Open 1cqp.pdb1 and 1cqp.pdb2

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

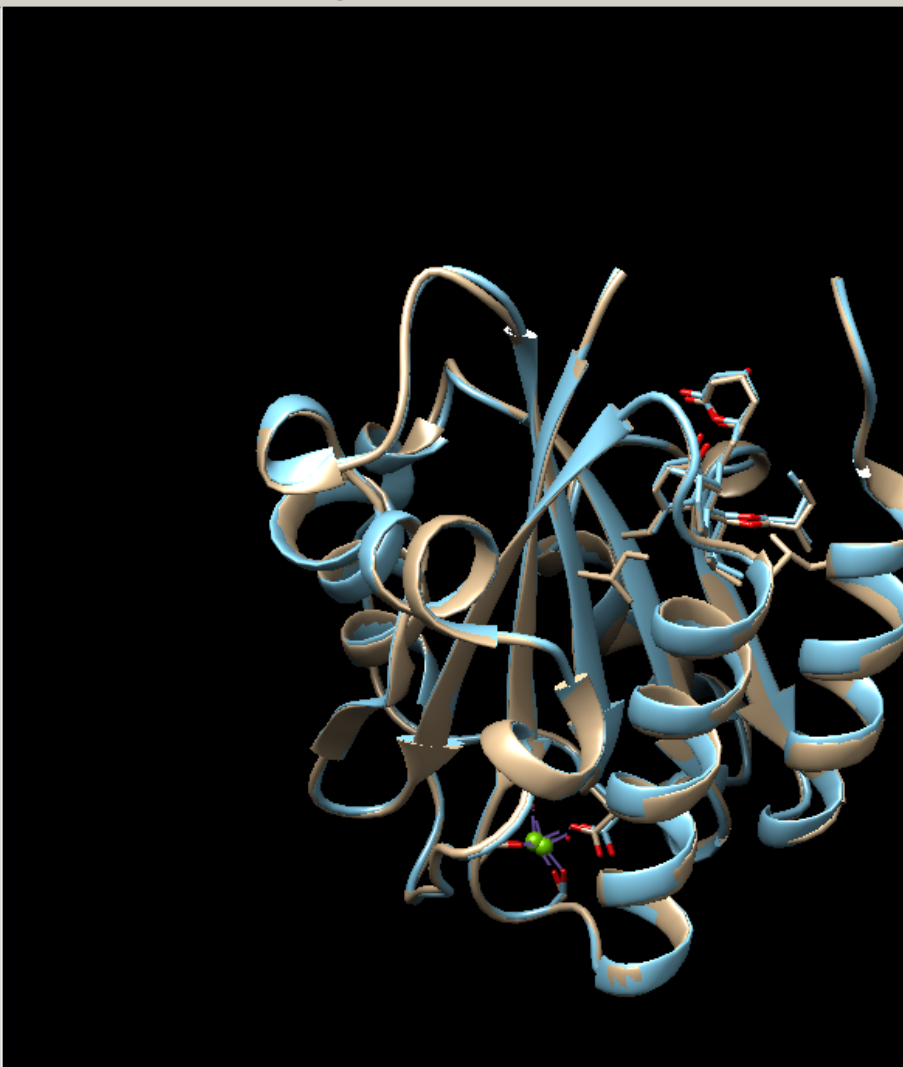
The screenshot displays the MatchMaker software interface. The main window shows two protein structures: a tan one on the left and a light blue one on the right. A menu is open, showing the path: **Tools** → **Structure Comparison** → **MatchMaker**. The **MatchMaker** dialog box is open, with the following settings:

- Reference structure:** 1cqp.pdb1 (#0), 1cqp.pdb2 (#1)
- Structure(s) to match:** 1cqp.pdb1 (#0), 1cqp.pdb2 (#1)
- Further restrict matching to current selection
- Further restrict matching to current selection
- Chain pairing:**
  - Best-aligning pair of chains between reference and match structure
  - Specific chain in reference structure with best-aligning chain in match structure
  - Specific chain(s) in reference structure with specific chain(s) in match structure
- Alignment algorithm:** Needleman-Wunsch
- Matrix:** BLOSUM-62
- Gap opening penalty:** 12
- Gap extension penalty:** 1
- Include secondary structure score (30%) **Show parameters**
- Compute secondary structure assignments
- Show pairwise alignment(s)
- Matching:**
  - Iterate by pruning long atom pairs until no pair exceeds: 2.0 angstroms
- After superposition, compute structure-based multiple sequence alignment
- Buttons:** Save settings, Reset to defaults, OK, Apply, Cancel, Help

UCSF Chimera

File Select Actions Presets Tools Favorites Help

Reply Log



MatchMaker

Reference structure: 1cqp.pdb1 (#0)  
1cqp.pdb2 (#1)

Structure(s) to match: 1cqp.pdb1 (#0)  
1cqp.pdb2 (#1)

Further restrict matching to current selection

Further restrict matching to current selection

Chain pairing

- Best-aligning pair of chains between reference and match structure
- Specific chain in reference structure with best-aligning chain in match structure
- Specific chain(s) in reference structure with specific chain(s) in match structure

Alignment algorithm: Needleman-Wunsch Matrix: BLOSUM-62

Gap opening penalty 12 Gap extension penalty 1

Include secondary structure score (30%) Show parameters

Compute secondary structure assignments

Show pairwise alignment(s)

Matching

Iterate by pruning long atom pairs until no pair exceeds: 2.0 angstroms

After superposition, compute structure-based multiple sequence alignment

Save settings Reset to defaults

OK Apply Cancel Help

Command:

Active models:  0  1  2  3  4  5  6  7  8  9  All

Previous message also written to reply log

Command: **mm #0 #1**

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

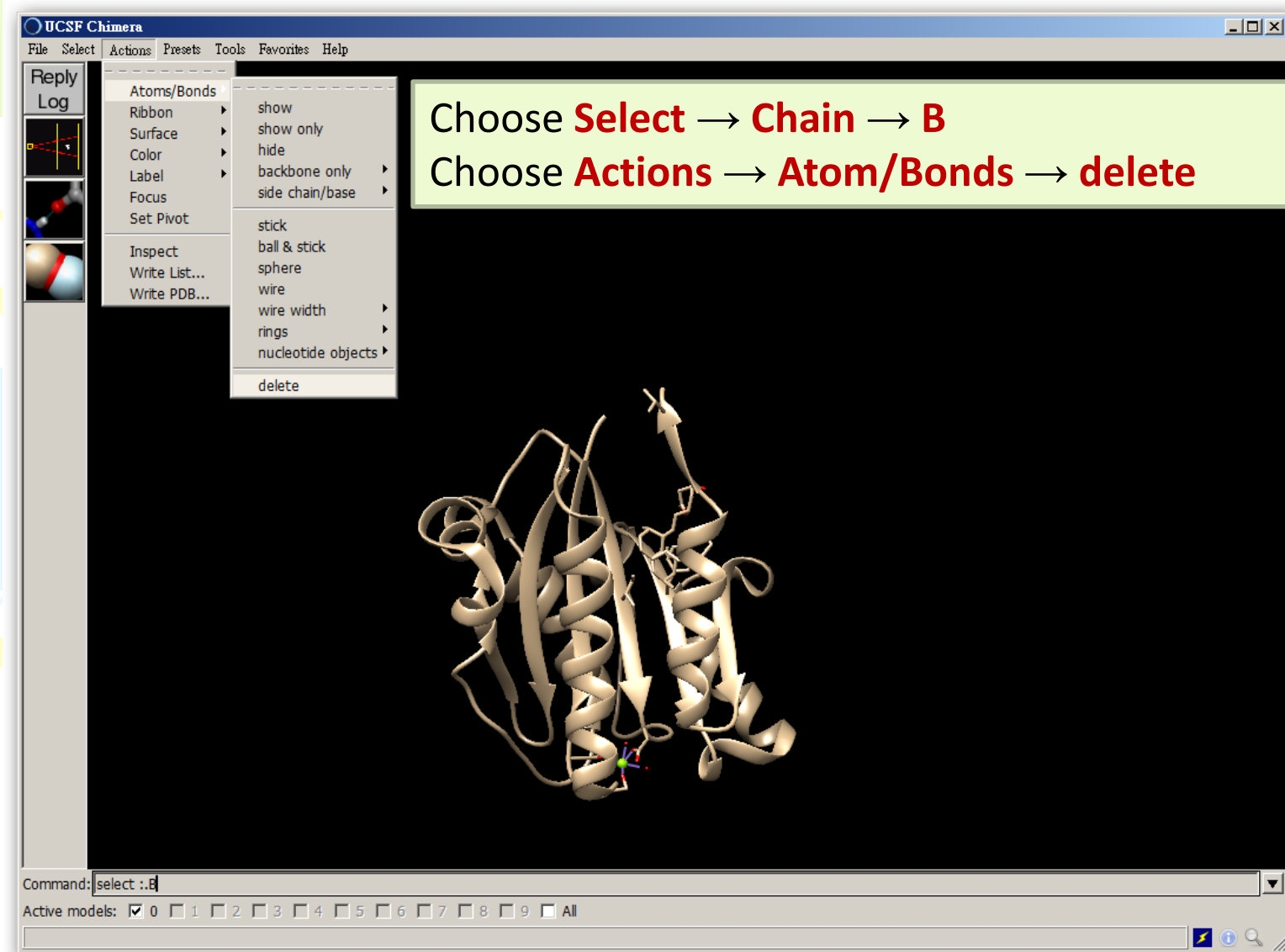
The screenshot displays the UCSF Chimera interface. The main window shows a 3D ribbon representation of a protein structure. A dialog box titled "Create Alignment from Superposition" is open, showing the selection of two chains: "1cqp.pdb1 (#0) chain A" and "1cqp.pdb2 (#1) chain B". Below the dialog, the "Match of 1cqp.pdb1, chain A and 1cqp.pdb2, chain B" window shows a sequence alignment. The alignment is as follows:

	1	11	21	31	41	
<b>RMSD: ca</b>						
<b>1cqp.pdb1, chain A</b>	128	G N V D L V F L F D	G S M S L Q P D E F	Q K I L D F M K D V	M K K L S N T S Y Q	F A A V Q F S T S Y
<b>1cqp.pdb2, chain B</b>	128	G N V D L V F L F D	G S M S L Q P D E F	Q K I L D F M K D V	M K K L S N T S Y Q	F A A V Q F S T S Y
	51	61	71	81	91	
<b>RMSD: ca</b>						
<b>1cqp.pdb1, chain A</b>	178	K T E F D F S D Y V	K W K D P D A L L K	H V K H M L L L T N	T F G A I N Y V A T	E V F R E E L G A R
<b>1cqp.pdb2, chain B</b>	178	K T E F D F S D Y V	K W K D P D A L L K	H V K H M L L L T N	T F G A I N Y V A T	E V F R E E L G A R
	101	111	121	131	141	
<b>RMSD: ca</b>						
<b>1cqp.pdb1, chain A</b>	228	P D A T K V L I I I	T D G E A T D S G N	I D A A K D I I R Y	I I G I G K H F Q T	K E S Q E T L H K F
<b>1cqp.pdb2, chain B</b>	228	P D A T K V L I I I	T D G E A T D S G N	I D A A K D I I R Y	I I G I G K H F Q T	K E S Q E T L H K F
	151	161	171	181		

At the bottom of the alignment window, it states: "1cqp.pdb2, chain B (#2 of 2; 182 non-gap residues)" and "1cqp.pdb2, chain B associated with #1 (1cqp.pdb2 1cqp.pdb2, chain B)".

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

# Delete Selected Structure



Command: **delete** **..B**

# Save Selected Structure

The image shows the UCSF Chimera software interface. The main window displays a protein structure (1CQP) with a specific region highlighted in green. A dialog box titled "Save 1cqp.pdb1 as PDB File" is open, showing the file name "803.AwH" and the file type "PDB [.pdb]". The "Save selected atoms only" checkbox is checked and highlighted with a red box. The command bar at the bottom shows the command "select :311.A".

Command: `select :311.A`

Active models:  0  1  2  3  4  5  6  7  8  9  All

Command: **select :311.A**



# Save Selected Structure

The screenshot displays the UCSF Chimera interface. The main window shows a protein structure (1CQP) in a ribbon representation, with a selected region highlighted in green. A dialog box titled "Save 1cqp.pdb1 as PDB File" is open, showing the folder path "C:\Users\elfin\Downloads\FDCC2018\1CQP". The file name is "1cqp\_proteinH.pdb". The file type is "PDB [.pdb]". The "Save models:" section is empty. The "Use untransformed coordinates" checkbox is checked. The "Keep dialog up after Save" checkbox is unchecked. The "Save" button is highlighted.

UCSF Chimera  
File Select Actions Presets Tools Favorites Help

Reply  
Log

Command: select protein

Active models:  0  1  2  3  4  5  6  7  8  9  All

Wrote 1cqp.pdb1 to C:\Users\elfin\Downloads\FDCC2018\1CQP\1cqp\_proteinH.pdb

Save 1cqp.pdb1 as PDB File  
Folder: C:\Users\elfin\Downloads\FDCC2018\1CQP

1CQP\	1cqp.pdb
test\	1cqp_proteinH.pdb

File name: 1cqp\_proteinH.pdb

Add .pdb suffix if none given

File type: PDB [.pdb] New folder...

Save models:

- Save displayed atoms only
- Save selected atoms only
- Use untransformed coordinates

Keep dialog up after Save

Save Close Help

Command: **select protein**

# Add Hydrogen

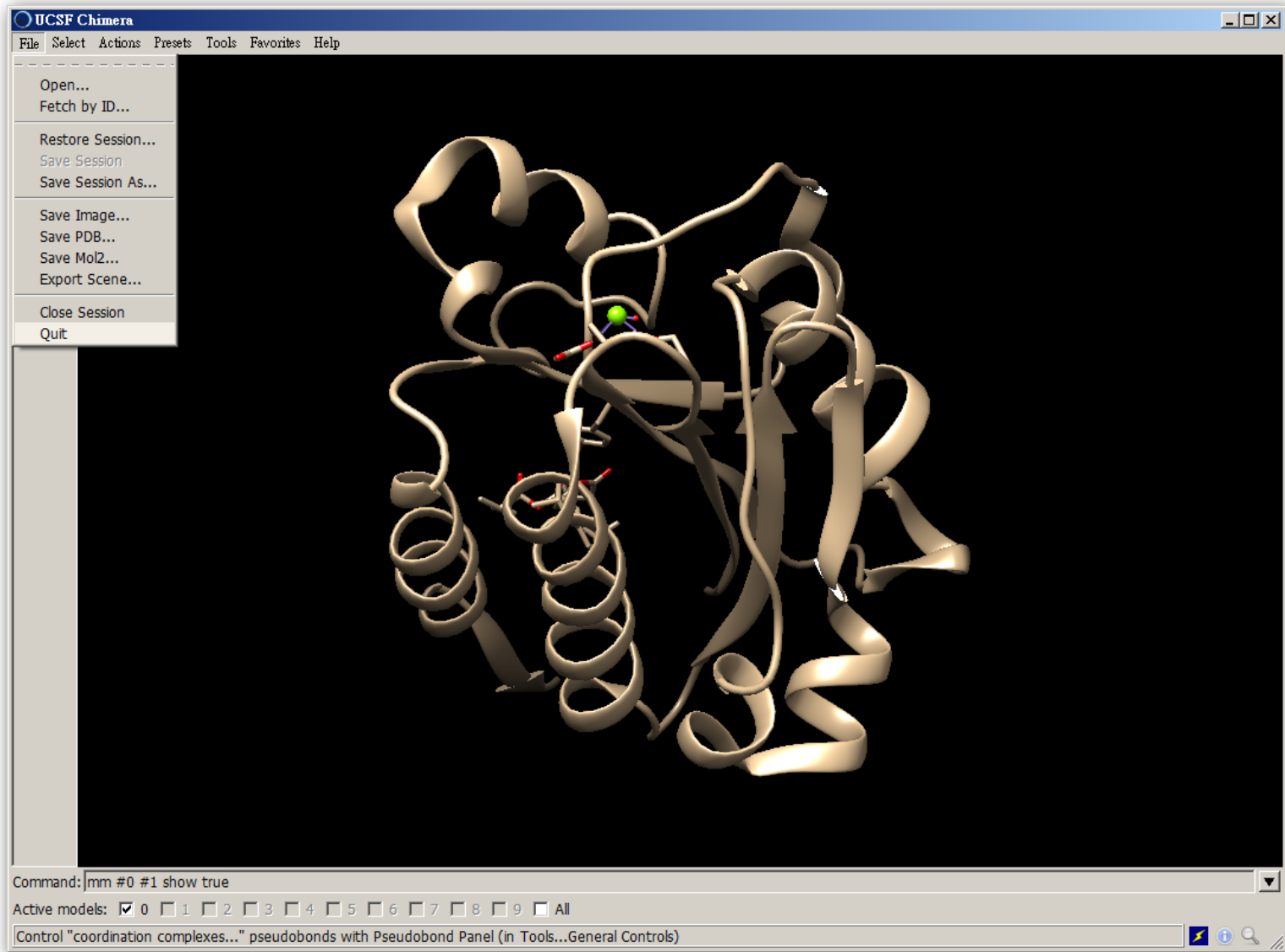
Choose **Tools** → **Structure Editing** → **AddH**

The image shows the UCSF Chimera software interface. The main window displays a protein structure in a ribbon representation. The 'Tools' menu is open, and the 'Structure Editing' sub-menu is selected, showing the 'AddH' option. A dialog box titled 'Add Hydrogens' is open, showing the file '1cqp.pdb1 (#0)' selected. The dialog has several options:

- Consider each model in isolation from all others
- Method:
  - steric only
  - also consider H-bonds (slower)
- Protonation states for: histidine
- Residue-name-based (HIS/HID/HIE/HIP = unspecified/delta/epsilon/both)
- Specified individually...
- Unspecified (determined by method)

The 'Add Hydrogens' dialog box has 'OK', 'Close', and 'Help' buttons at the bottom right. The main window has a 'Command:' field at the bottom left and a status bar at the bottom showing 'Active models: 0 1 2 3 4 5 6 7 8 9 All'.

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](#)  
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## Structure Comparison

[MatchMaker](#)  
[Match -> Align](#)  
[Morph Conformations](#)  
[RR Distance Maps](#)  
[Ensemble Cluster](#)  
[Ensemble Match](#)  
[Tile Structures](#)  
[Minrms Plot](#)

## Sequence

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[PDB/UniProt Info](#)  
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[Match -> Align](#)  
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[Find Clashes/Contacts](#)  
[Electrostatic Surface Coloring](#)  
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[Surfnct](#)  
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[Add Charge](#)  
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[PDB2PQR](#)  
[Rotamers](#)  
[Adjust Torsions](#)  
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[Minimize Structure](#)  
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## Amber

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## 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

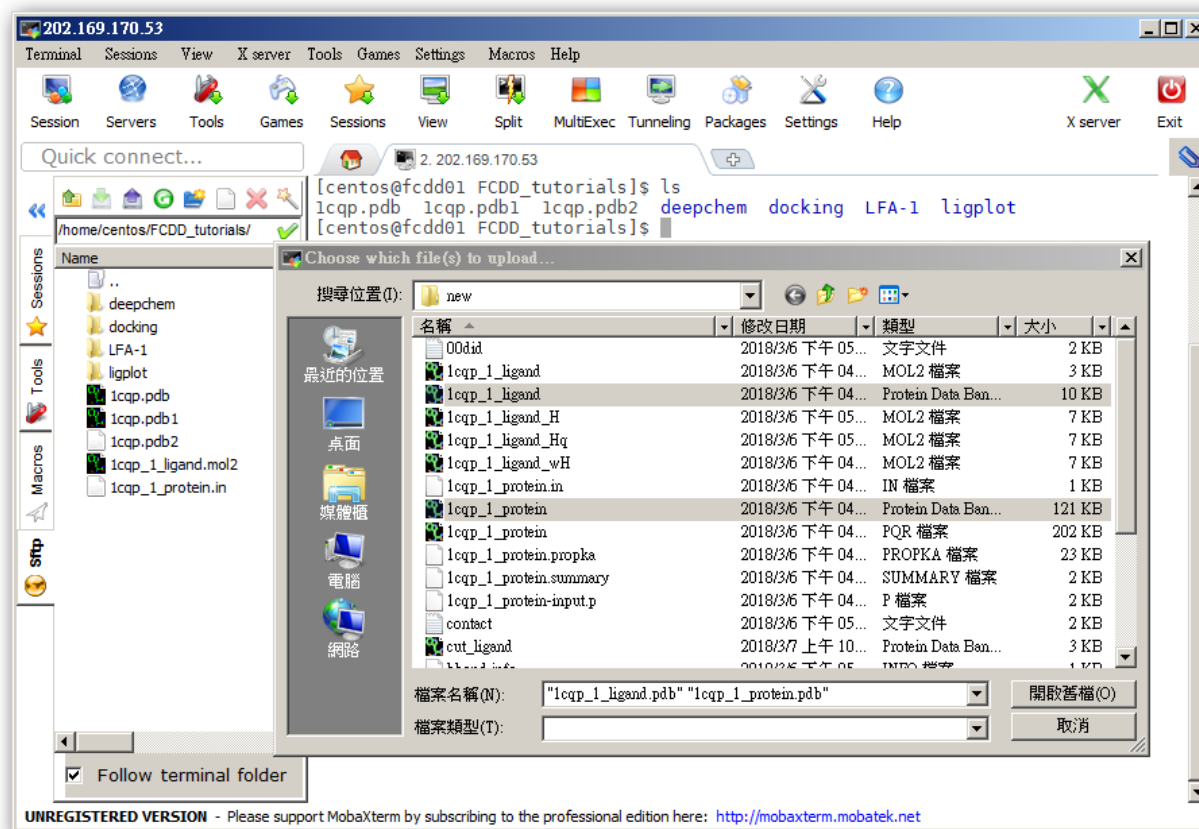
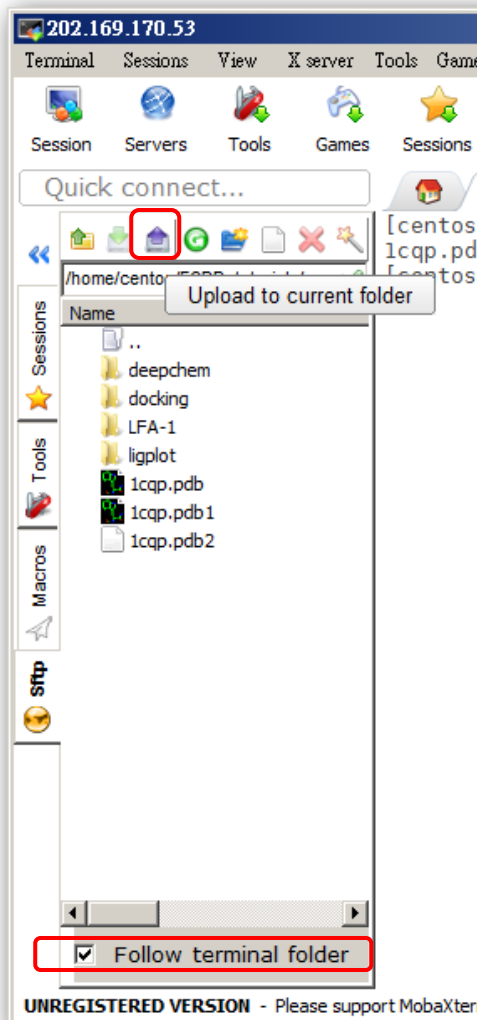
While the command line can be used for many things, the ultimate control of chimera is through Python scripts.

<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](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<sup>+</sup>

<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

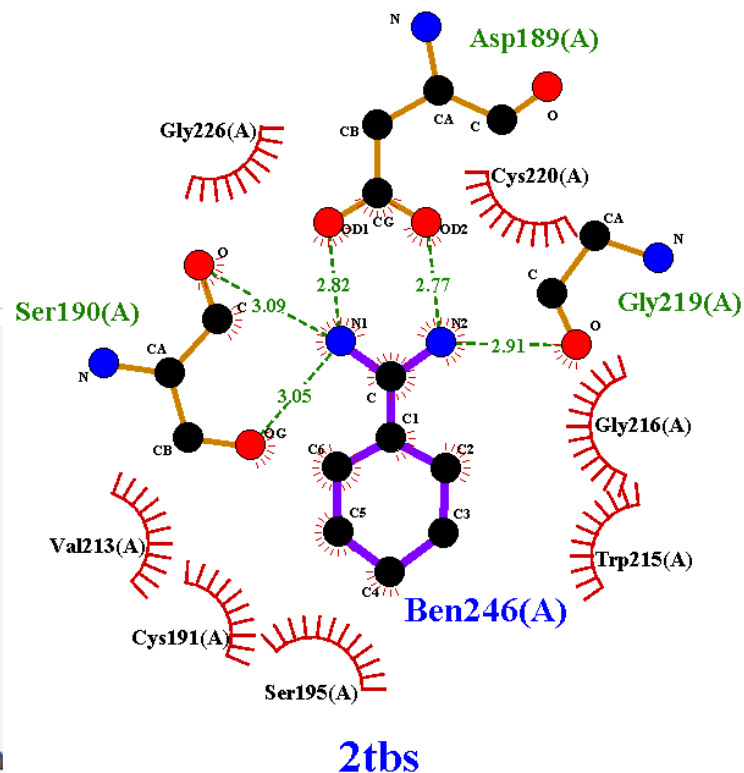
*Protein Engineering, Design and Selection*, Volume 8, Issue 2, 1 February 1995, Pages 127–134, <https://doi.org/10.1093/protein/8.2.127>

**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<sup>+</sup>

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

## LigPlot<sup>+</sup>: Multiple Ligand–Protein Interaction Diagrams for Drug Discovery

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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

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 openURL

E-mail: [roman@ebi.ac.uk](mailto:roman@ebi.ac.uk)

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

 RIS Citation

**LigPlot<sup>+</sup>** 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>

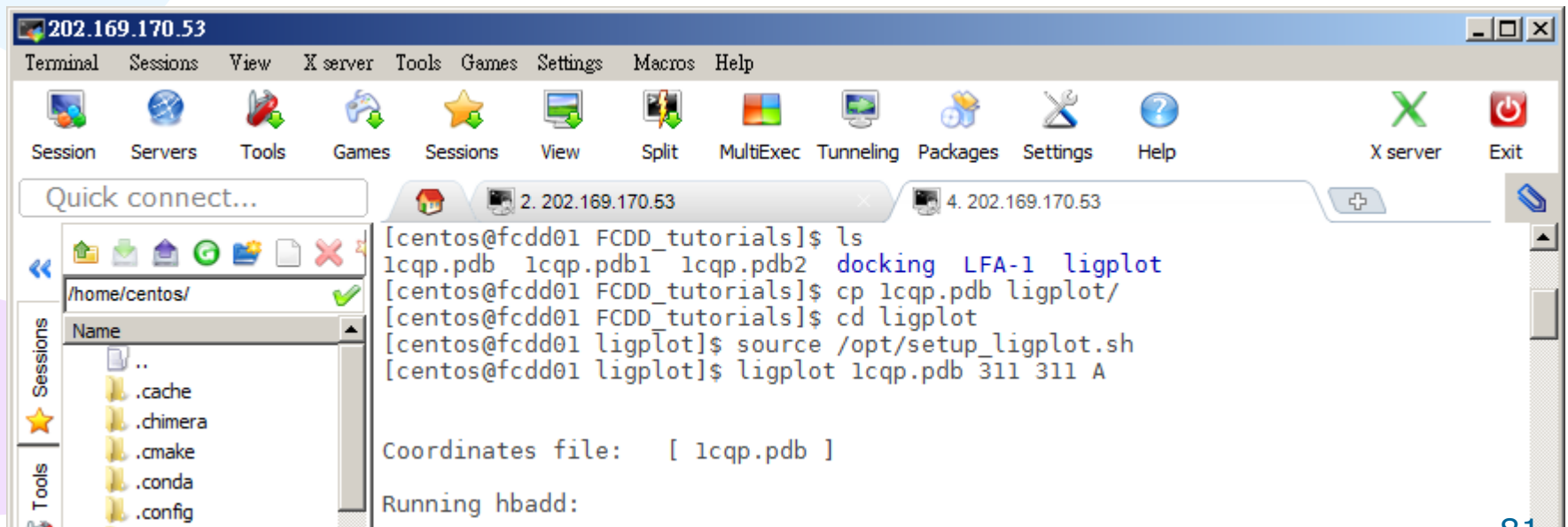


```
$ cd ~/FCDD_tutorials
$ mkdir ligplot
$ copy 1cqp.pdb ligplot
$ cd ligplot
$ source /opt/setup_ligplot.sh
$ ligplot 1cqp.pdb 311 311 A
```

**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



The screenshot shows a terminal window titled "202.169.170.53" with a menu bar (Terminal, Sessions, View, X server, Tools, Games, Settings, Macros, Help) and a toolbar. The terminal output is as follows:

```
[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
```

Below the terminal output, the following text is displayed:

```
Coordinates file: [ 1cqp.pdb ]
Running hbadd:
```

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

```

[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]
*** Warning. Invalid element identifier in CIF file [C14]
*** Warning. Invalid element identifier in CIF file [C14]
Plotting hydrophobic contacts ...
Printing residue names ...

Writing out the drw file...

Program complete

.....
[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]$

```

UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <http://mobaxterm.mobatek.net>

**\$ls**

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

The screenshot shows a MobaXterm terminal window with the following content:

```
[centos@fcdd01 ligplot]$ ls
lcqp.hhb      hbadd.log    hhb.log      ligplot.gif  ligplot.prm  nnb.log
lcqp.nnb      hbadd.map    ligplot.bonds ligplot.hhb  ligplot.ps   ranseed.dat
lcqp.pdb      hbadd.sum    ligplot.drw   ligplot.nnb  ligplot.rcm  WhatIdid
hbadd.bonds   hbplus.rc    ligplot.frm   ligplot.pdb  ligplot.sum

[centos@fcdd01 ligplot]$ cat ligplot.sum
lcqp
```

Interacting residues			Hydrogen bonds			Non-bonded contacts
	M-M	S-S	M-S			
Residues: [803 311 A] -> [ILE 309 B]	0	0	0		1	
Residues: [803 311 A] -> [VAL 308 B]	0	0	0		2	
Residues: [803 311 A] -> [LEU 302 A]	0	0	0		3	
Residues: [803 311 A] -> [LEU 298 A]	0	0	0		2	
Residues: [803 311 A] -> [TYR 257 A]	0	1	0		1	
Residues: [803 311 A] -> [ILE 235 A]	0	0	0		5	
Residues: [803 311 A] -> [LEU 132 A]	0	0	0		2	

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**\$ more ligplot.hhb**  
**\$ more ligplot.nnb**

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

[centos@fcdd01 ligplot]\$ more ligplot.hhb  
ligplot.hhb output:

Donor	Acceptor	Distance
TYR A 257 OH	803 A 311 O1	2.42

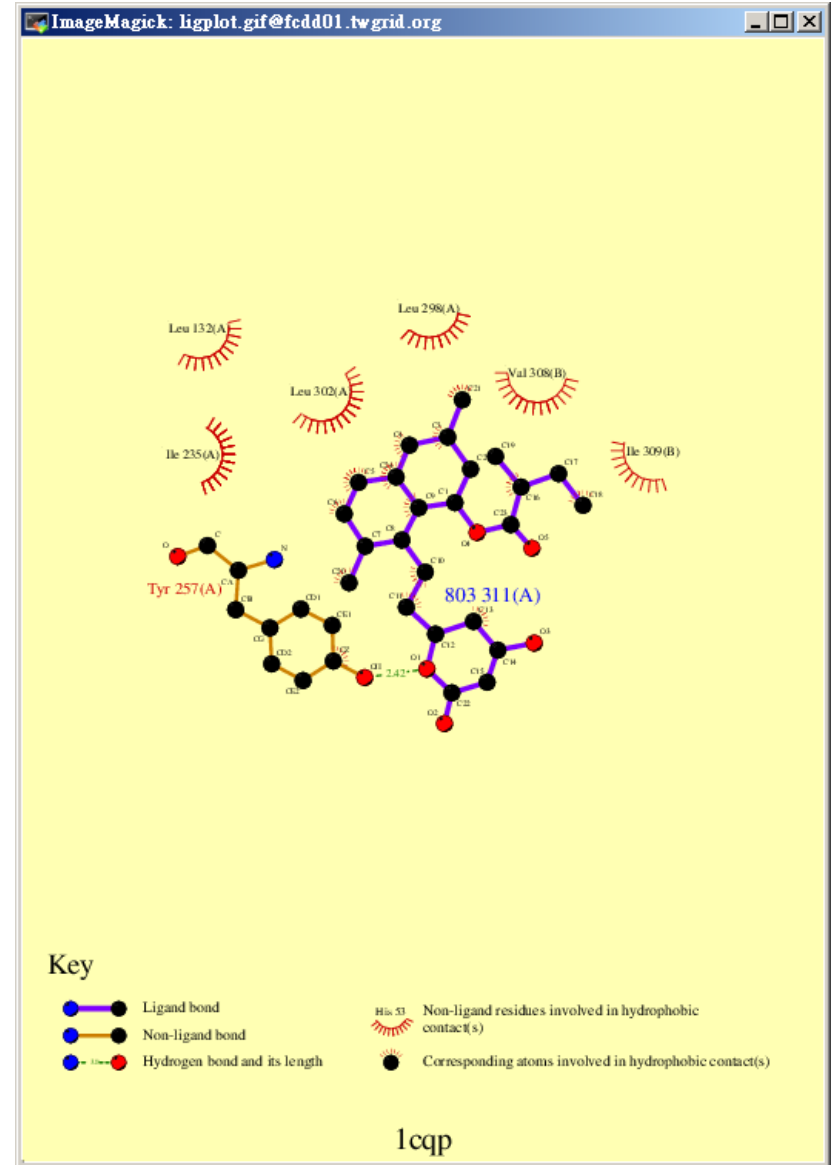
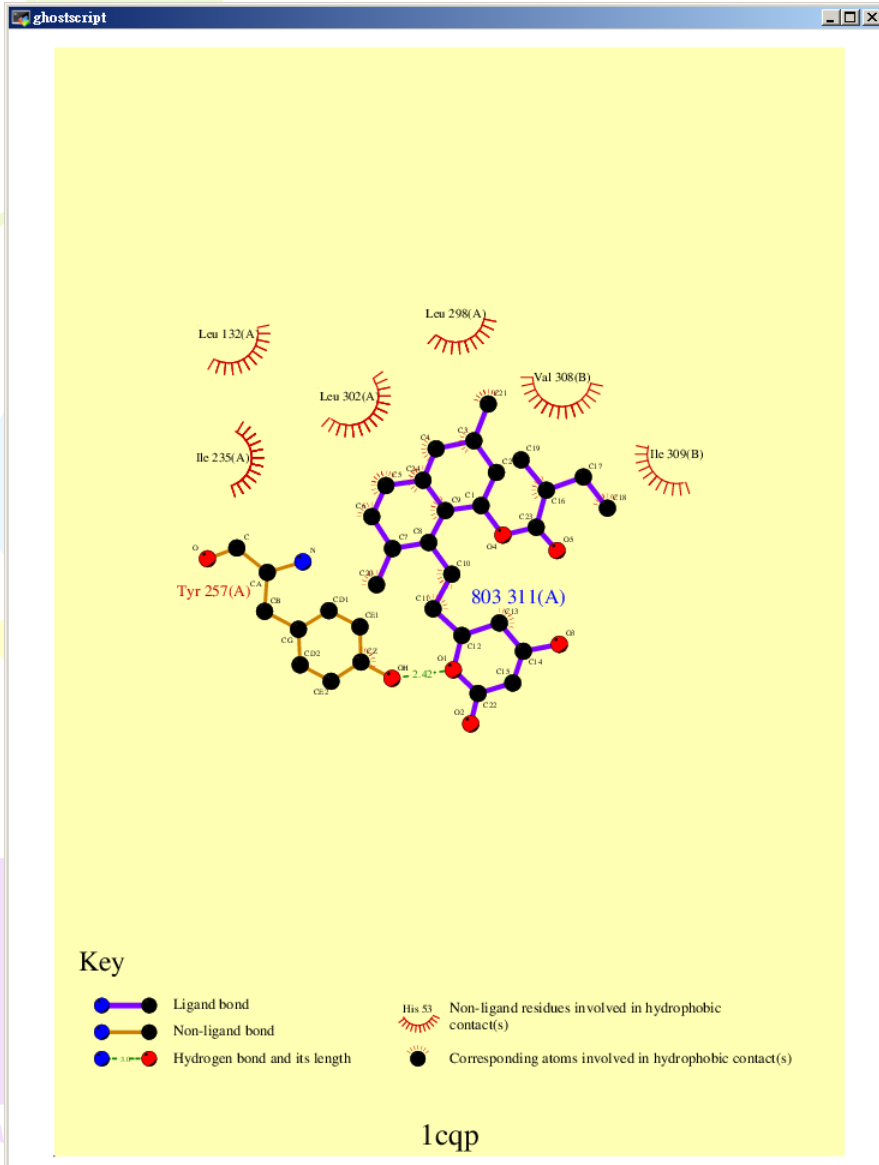
[centos@fcdd01 ligplot]\$ more ligplot.nnb  
ligplot.nnb output:

Atom 1	Atom 2	Distance
803 A 311 C13	ILE B 309 C	3.79
803 A 311 C18	VAL B 308 CG1	3.31
803 A 311 C11	VAL B 308 CG1	3.74
803 A 311 C16	LEU A 302 CD1	3.76
803 A 311 C5	LEU A 302 CD1	3.71
803 A 311 C24	LEU A 302 CD1	3.74
803 A 311 C21	LEU A 298 CD2	3.68
803 A 311 C21	LEU A 298 CG	3.89
803 A 311 C10	TYR A 257 CZ	3.87
803 A 311 C9	ILE A 235 CD1	3.88
803 A 311 C5	ILE A 235 CD1	3.88
803 A 311 C24	ILE A 235 CD1	3.38
803 A 311 C4	ILE A 235 CD1	3.26
803 A 311 C3	ILE A 235 CD1	3.68
803 A 311 C20	LEU A 132 CD1	3.63
803 A 311 C6	LEU A 132 CD1	3.67

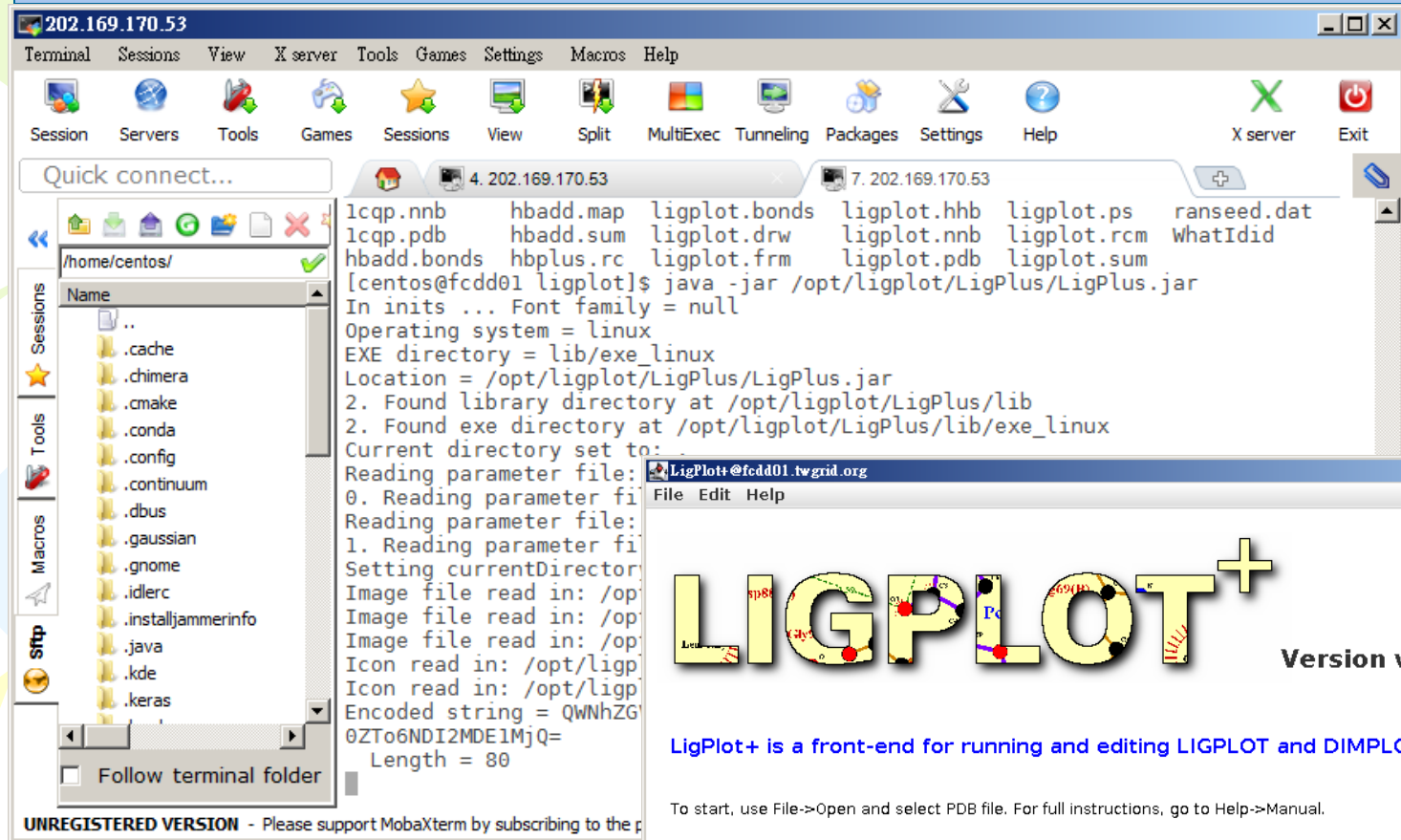
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the professional edition here: <http://mobaxterm.mobatek.net>

\$ghostscript ligplot.ps

\$convert ligplot.ps ligplot.gif  
\$display



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



```
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... 4. 202.169.170.53 7. 202.169.170.53
/home/centos/
Name
..
.cache
.chimera
.cmake
.conda
.config
.continuum
.dbus
.gaussian
.gnome
.idlrc
.installjammerinfo
.java
.kde
.keras
Follow terminal folder
UNREGISTERED VERSION - Please support MobaXterm by subscribing to the p

1cqp.nnb hbadb.map ligplot.bonds ligplot.hhb ligplot.ps ranseed.dat
1cqp.pdb hbadb.sum ligplot.drw ligplot.nnb ligplot.rcm WhatIdid
hbadb.bonds hbplus.rc ligplot.frm ligplot.pdb ligplot.sum
[centos@fcdd01 ligplot]$ java -jar /opt/ligplot/LigPlus/LigPlus.jar
In inits ... Font family = null
Operating system = linux
EXE directory = lib/exe_linux
Location = /opt/ligplot/LigPlus/LigPlus.jar
2. Found library directory at /opt/ligplot/LigPlus/lib
2. Found exe directory at /opt/ligplot/LigPlus/lib/exe_linux
Current directory set to:
Reading parameter file:
0. Reading parameter fi
Reading parameter fi
1. Reading parameter fi
Setting currentDirector
Image file read in: /op
Image file read in: /op
Image file read in: /op
Icon read in: /opt/ligp
Icon read in: /opt/ligp
Encoded string = QWNhZG
0ZTo6NDI2MDE1MjQ=
Length = 80

LigPlot+ @fcdd01.twgrid.org
File Edit Help
LIGPLOT+
Version v.1.3.5
LigPlot+ is a front-end for running and editing LIGPLOT and DIMPLOT schematic diagram
To start, use File->Open and select PDB file. For full instructions, go to Help->Manual.
For academic use only
© Roman Laskowski 2009
```

# LIGPLOT+

Version v.1.3.5

LigPlot+ is a front-end for running and editing LIGPLOT and DIMPLOT schematic diagram

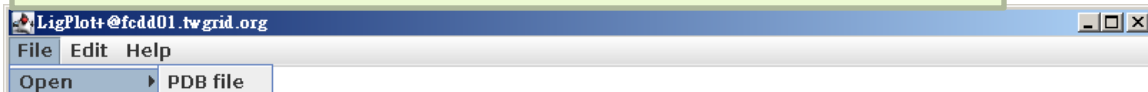
To start, use File->Open and select PDB file. For full instructions, go to Help->Manual.

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Choose **File** → **Open** → **PDB file**



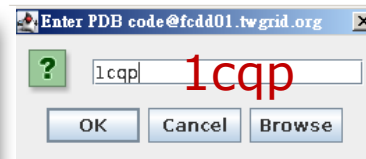
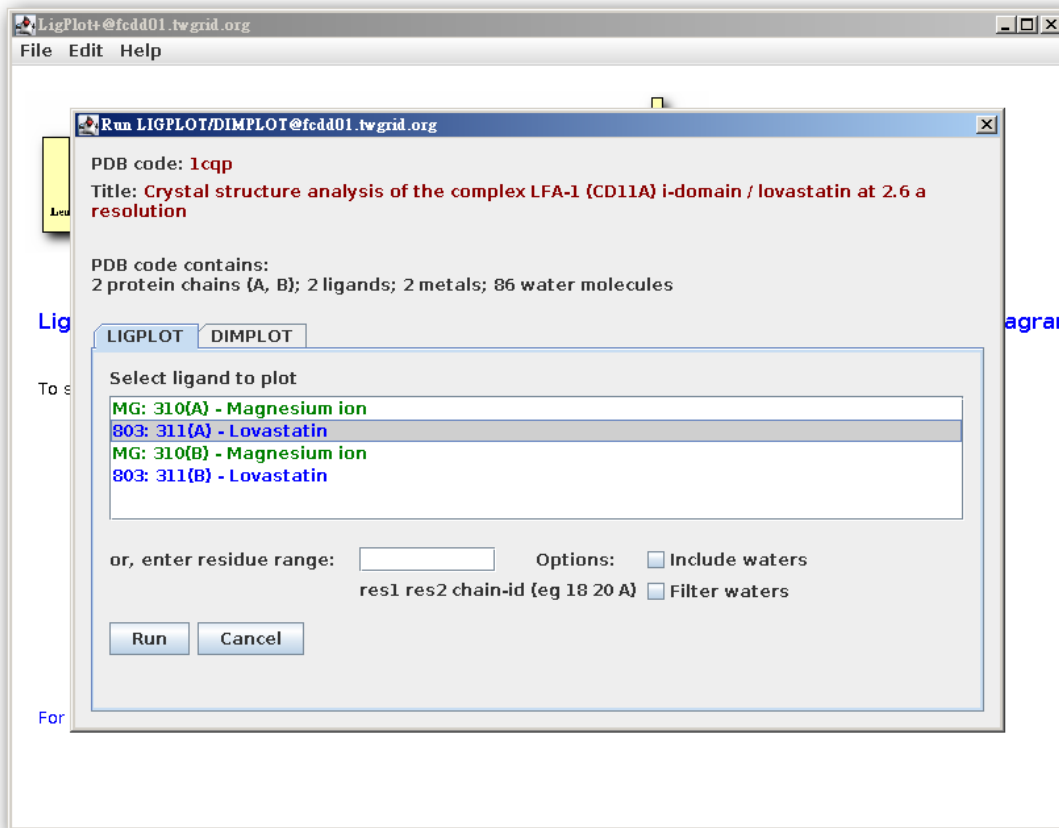
# G P L O T +



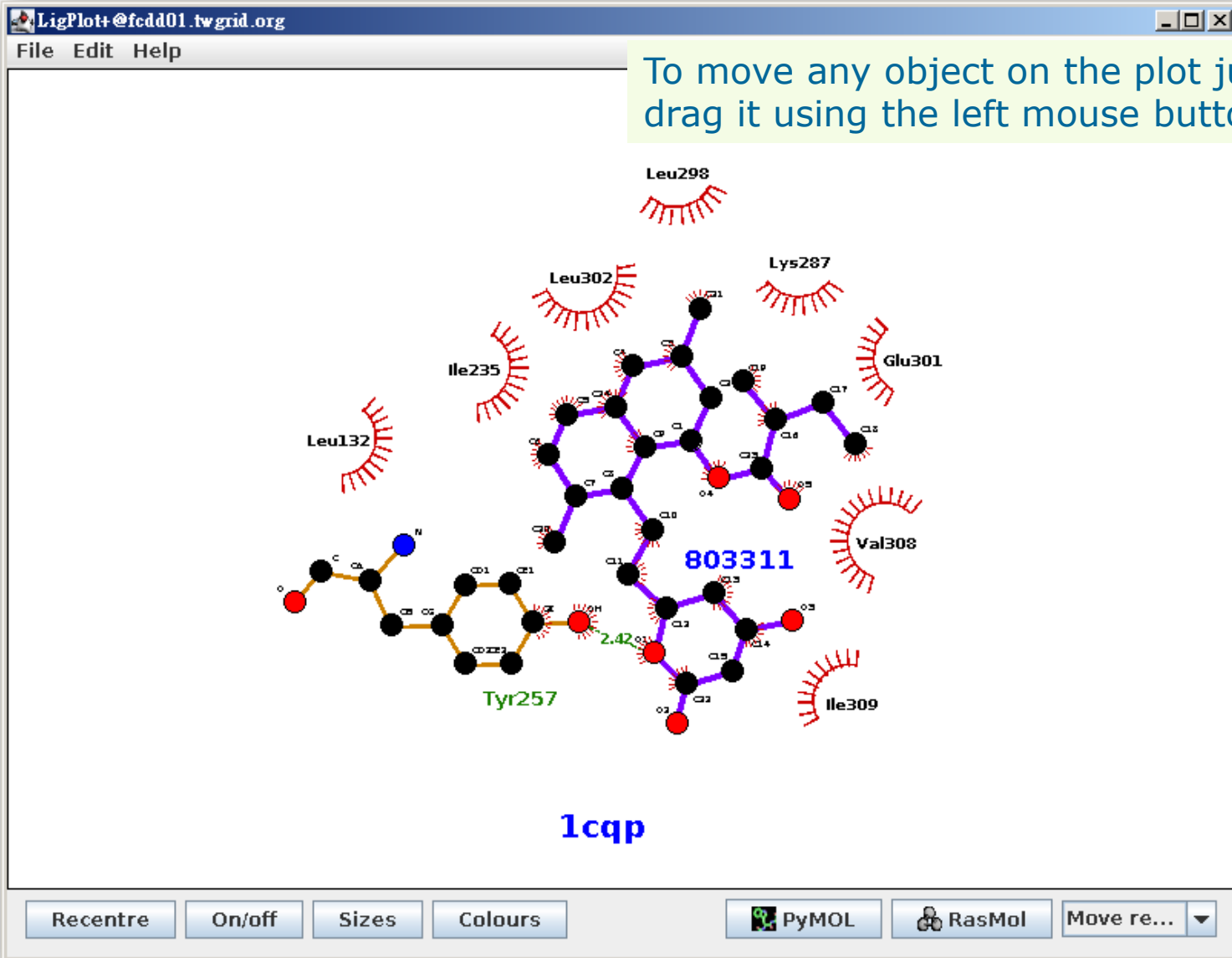
LigPlot+ is a front-end for running and editing LIGPLOT

To start, use File->Open and select PDB file. For full instructions, go to Help->M

LigPlot+ is a front-end for running and editing LIGPLOT and DIMPLOT schematic diagram

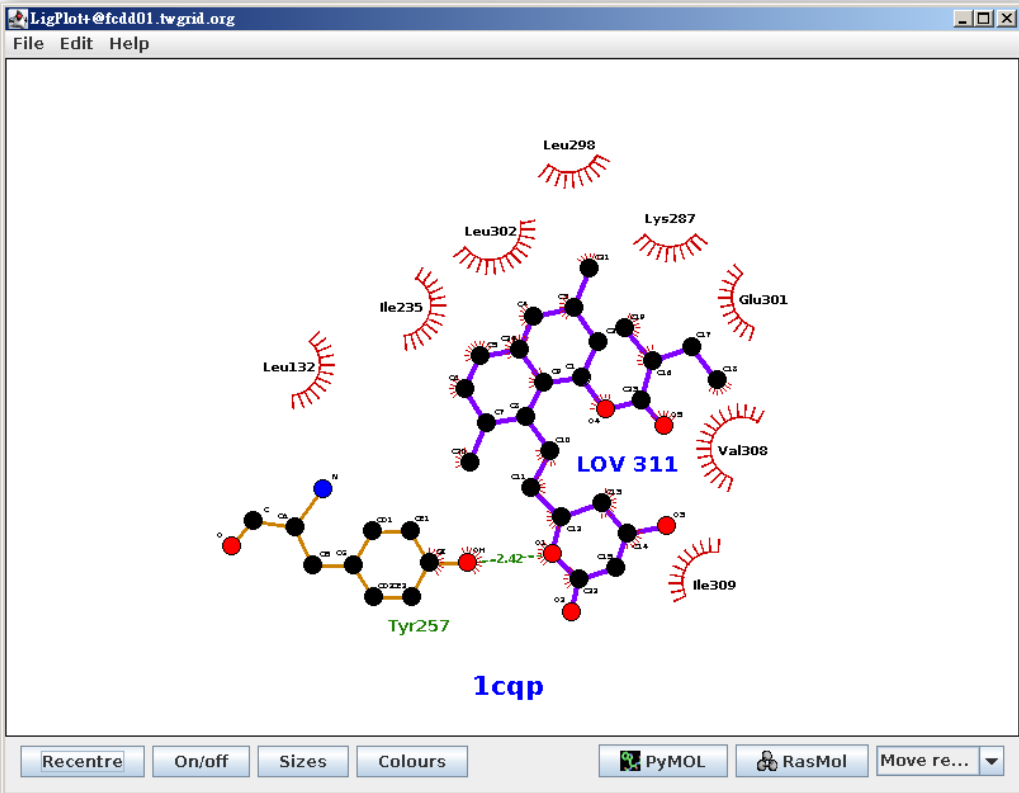
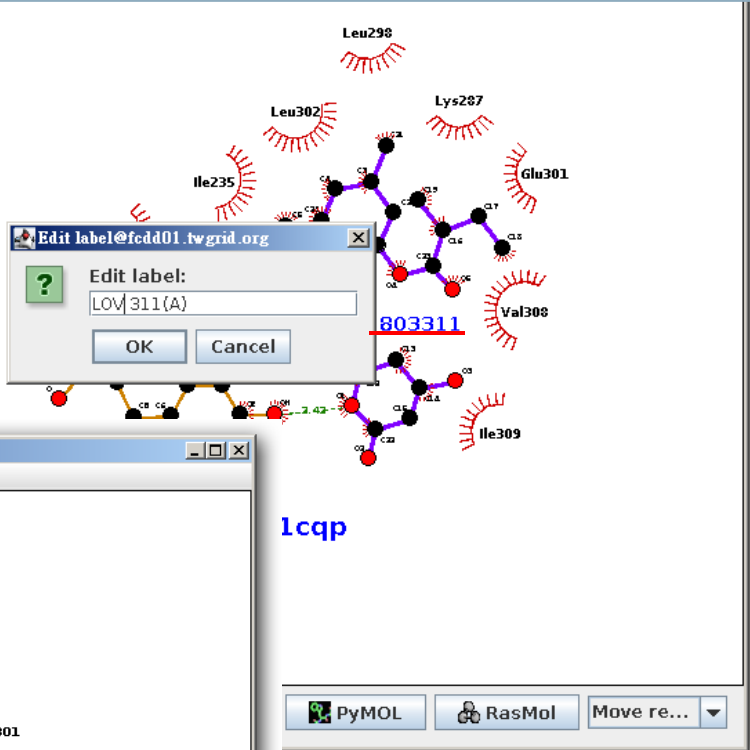


© Roman Laskowski 2009



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.

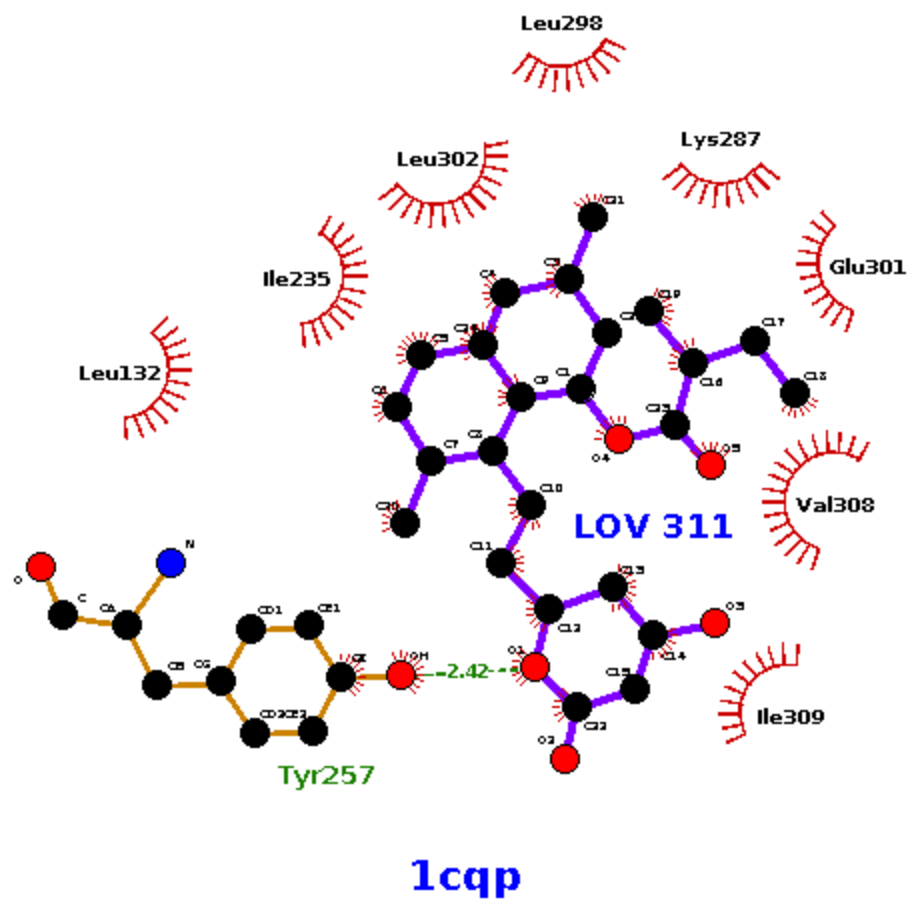
To edit the text label on the plot, you can select the text item by right-clicking on it.



1cqp

- Open
- Close
- Save
- Add
- Delete
- Import
- Write PS file
- Print Screen
- Exit

Choose **File** → **Write PS file**



## Change on/off parameter

On/off parameter selection@fcdd01.twgrid.org

<b>Labels</b>	<b>Atoms</b>
<input checked="" type="checkbox"/> Plot title	<input checked="" type="checkbox"/> Ligand atoms
<input checked="" type="checkbox"/> Ligand residue names	<input checked="" type="checkbox"/> Non-ligand atoms
<input checked="" type="checkbox"/> Non-ligand residue names	<input checked="" type="checkbox"/> Water atoms
<input checked="" type="checkbox"/> Hydrophobic residue names	<input checked="" type="checkbox"/> Atom edges
<input checked="" type="checkbox"/> Water names	<b>Bonds</b>
<input checked="" type="checkbox"/> Ligand atom names	<input checked="" type="checkbox"/> Hydrogen bonds
<input checked="" type="checkbox"/> Non-ligand atom names	<input type="checkbox"/> Hydrophobic interactions
<input checked="" type="checkbox"/> Hydrogen bond labels	<input type="checkbox"/> Double/triple bonds
<input type="checkbox"/> Show blank labels as hyphens	
<b>Misc</b>	<input type="checkbox"/> Highlight equivalent side chains
<input checked="" type="checkbox"/> Show inactive plots	<input checked="" type="checkbox"/> Highlight equivalent hydrophobics
<input checked="" type="checkbox"/> Circle equivalent side chains	
<input type="checkbox"/> Show chain identifiers	

OK Cancel Set as default

Recentre

On/off

Sizes

Colours

PyMOL

RasMol

Move re... ▼

LigPlot+@fcdd01.twgrid.org

File Edit Help

## Change size definitions

Size definitions@fcdd01.twgrid.org

<b>Label sizes</b>		<b>Atom and residue sizes</b>	
Plot title	<input type="text" value="1.000"/>	Ligand atom radius	<input type="text" value="0.330"/>
Ligand residue names	<input type="text" value="0.800"/>	Non-ligand atom radius	<input type="text" value="0.330"/>
Non-ligand residue names	<input type="text" value="0.630"/>	Water atom radius	<input type="text" value="0.400"/>
Hydrophobic residue names	<input type="text" value="0.500"/>	Hydrophobic residue radius	<input type="text" value="1.150"/>
Water names	<input type="text" value="0.500"/>	Schematic residue radius	<input type="text" value="0.800"/>
Ligand atom names	<input type="text" value="0.310"/>	<b>Bond widths</b>	
Non-ligand atom names	<input type="text" value="0.310"/>	Ligand bond width	<input type="text" value="0.190"/>
Hydrogen bond labels	<input type="text" value="0.440"/>	Non-ligand bond width	<input type="text" value="0.130"/>
<b>Note:</b> all sizes are in "Ångströms" (ie relative to original coords)		Hydrogen bond width	<input type="text" value="0.070"/>
		External bond width	<input type="text" value="0.070"/>
		Hydrophobic "bond" width	<input type="text" value="0.070"/>

1cqp

Recentre

On/off

Sizes

Colours

PyMOL

RasMol

Move re... ▾

LigPlot+@fcdd01.twgrid.org

File Edit Help

Change colors

Colour selection@fcdd01.twgrid.org

Background Labels Atoms Bonds

Blue	Plot title
Blue	Ligand residue names
Olive green	Non-ligand residue names
Black	Hydrophobic residue names
Blue	Hydrophobic residue names {2}
Purple	Water names
Black	Ligand atom names
Black	Non-ligand atom names
Olive green	H-bond labels

OK Cancel Save as default

1cqp

Recentre

On/off

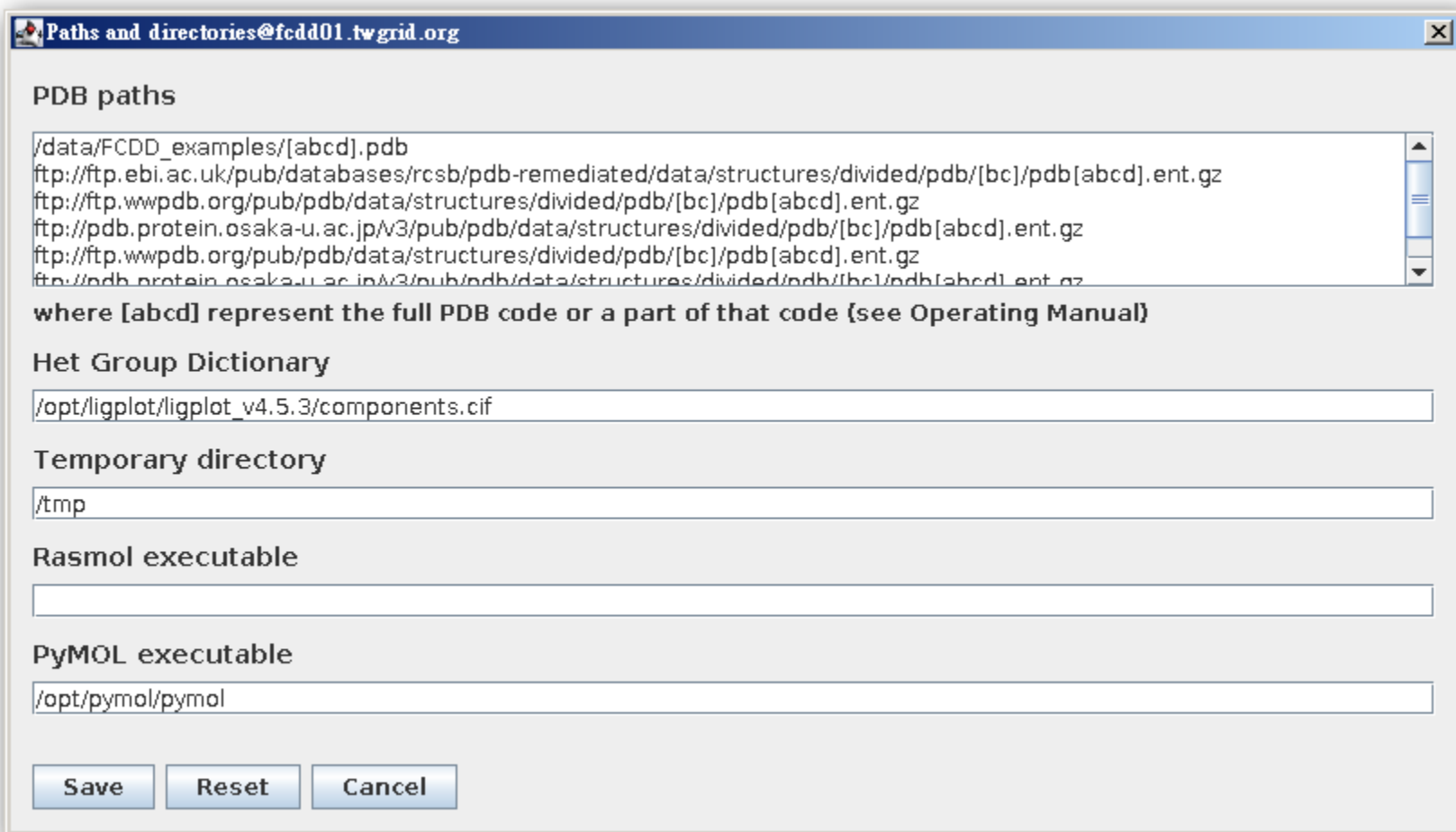
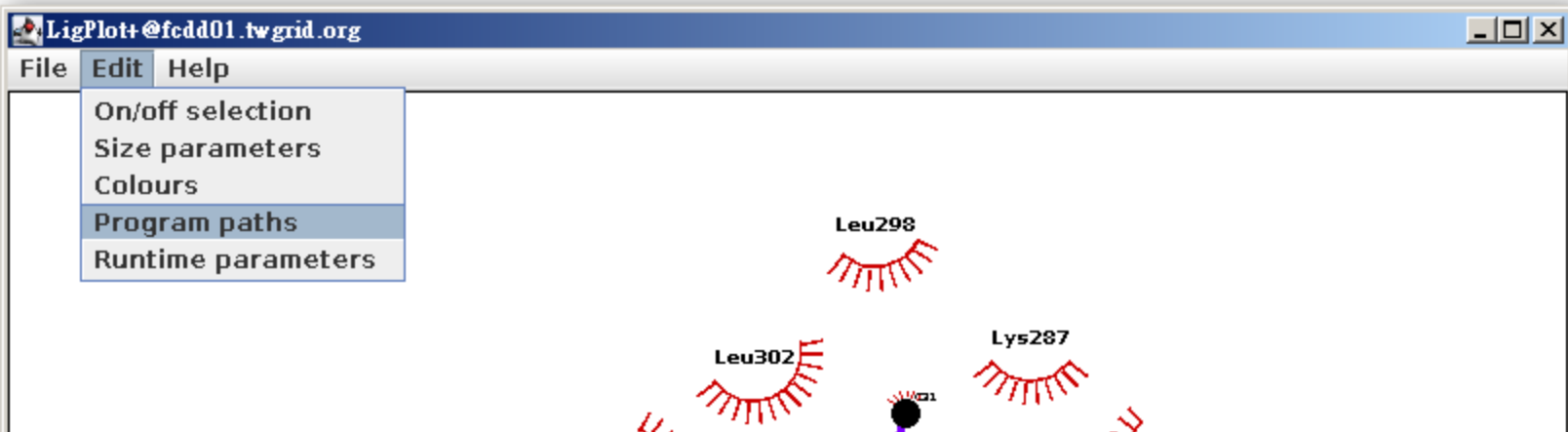
Sizes

Colours

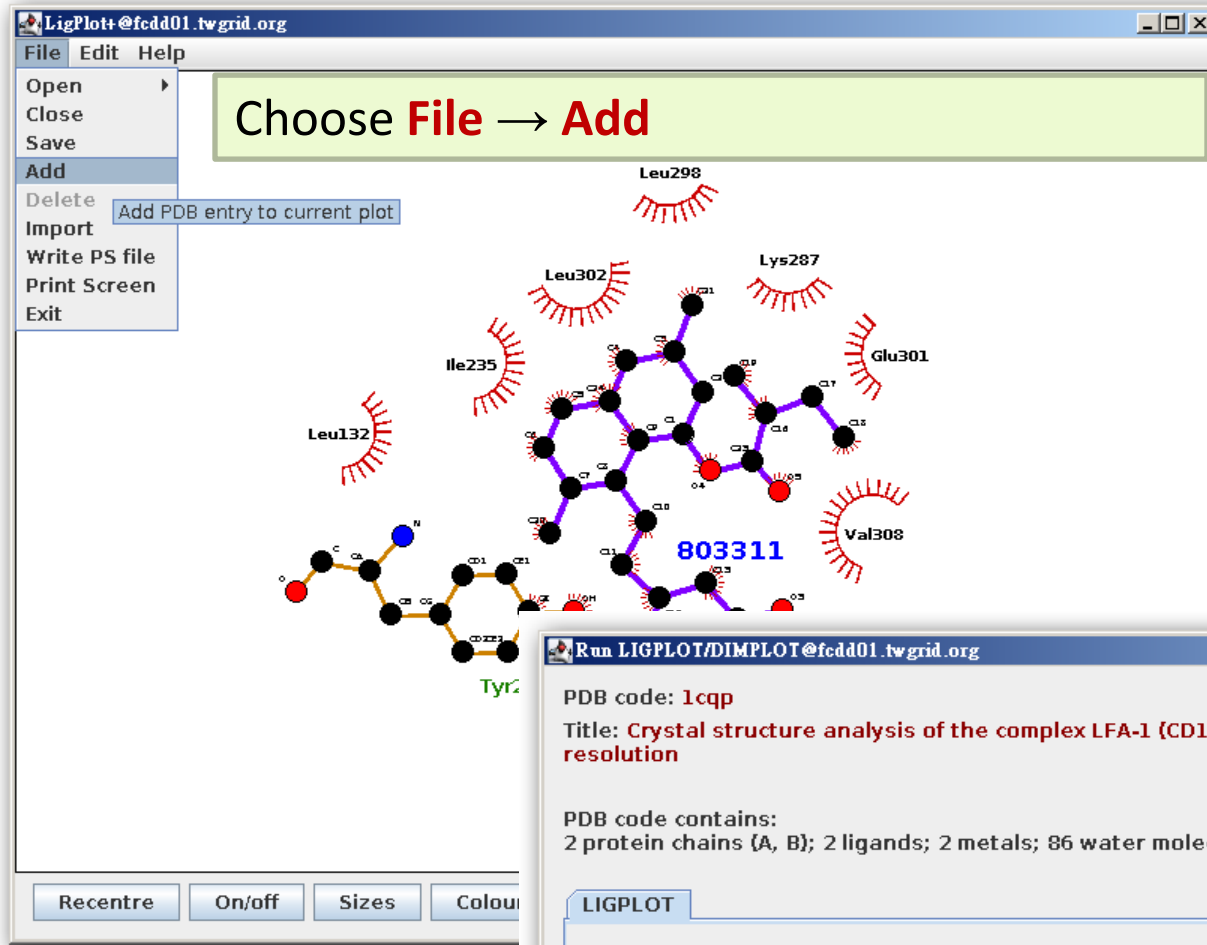
PyMOL

RasMol

Move re... ▼







## Multiple plots

Run LIGPLOT/DIMPLOT@fcdd01.twgrid.org

PDB code: 1cqp  
Title: Crystal structure analysis of the complex LFA-1 (CD11A) i-domain / lovastatin at 2.6 a resolution

PDB code contains:  
2 protein chains (A, B); 2 ligands; 2 metals; 86 water molecules

**LIGPLOT**

Select ligand to plot

- MG: 310(A) - Magnesium ion
- 803: 311(A) - Lovastatin
- MG: 310(B) - Magnesium ion
- 803: 311(B) - Lovastatin

or, enter residue range:  Options:  Include waters  
res1 res2 chain-id (eg 18 20 A)  Filter waters  
 Force fit on ligands

Run Cancel

