

PyMOL软件使用示例

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PyMOL简介

- PyMOL (Python molecule)
- 主要功能：创作高品质的小分子或是生物大分子（特别是蛋白质）的三维结构图像。
- 网站：<http://www.pymol.org/>

PyMOL 功能

- 读取多种文件格式(.pdb, .xyz, .mol2...)
- 读取电子密度图 (.ccp4 或xplor格式)
- 可拓展的界面程序/python语言
- 将screen 存为图片文件(.png格式)
- 会话保存/session save
- 结构比对
- 测量：距离、角度、二面角
- 立体效果
- 光线追踪/ray
- 探测静电力学
- 动画制作
-
- **没有undo功能**

PyMOL界面

The image shows a screenshot of the PyMOL GUI with several components labeled:

- External GUI window**: The top window containing the menu bar (File, Edit, Build, Movie), a toolbar (Reset, Zoom, Draw, Ray, Rock, Unpick, Deselect, Get View, Stop, Play, MClear, Builder), and a command line area.
- command line: Ctrl-C/X/V**: A yellow callout pointing to the command line area in the External GUI window.
- Viewer window**: The main window displaying a 3D ribbon model of a protein structure.
- Object list**: A yellow callout pointing to the object list panel on the right side of the Viewer window.
- Mouse Mode**: A yellow callout pointing to the Mouse Mode panel at the bottom right of the Viewer window.
- Movie player**: A yellow callout pointing to the Movie player controls at the bottom of the Viewer window.
- command line**: A yellow callout pointing to the command line area at the bottom left of the Viewer window.

The command line in the External GUI window shows the following text:

```
TITLE RECOMBINANT SPERM WHALE MYOGLOBIN L89W MUTANT (MET)
COMPND MOL_ID: 1;
COMPND 2 MOLECULE: PROTEIN (MYOGLOBIN);
COMPND 3 CHAIN: A;
COMPND 4 ENGINEERED: YES;
COMPND 5 MUTATION:
ObjectMolecule: Read
ObjectMolecule: Read
Symmetry: Found 6 sy
CmdLoad: "C:/Users/A
```

The object list panel shows the following text:

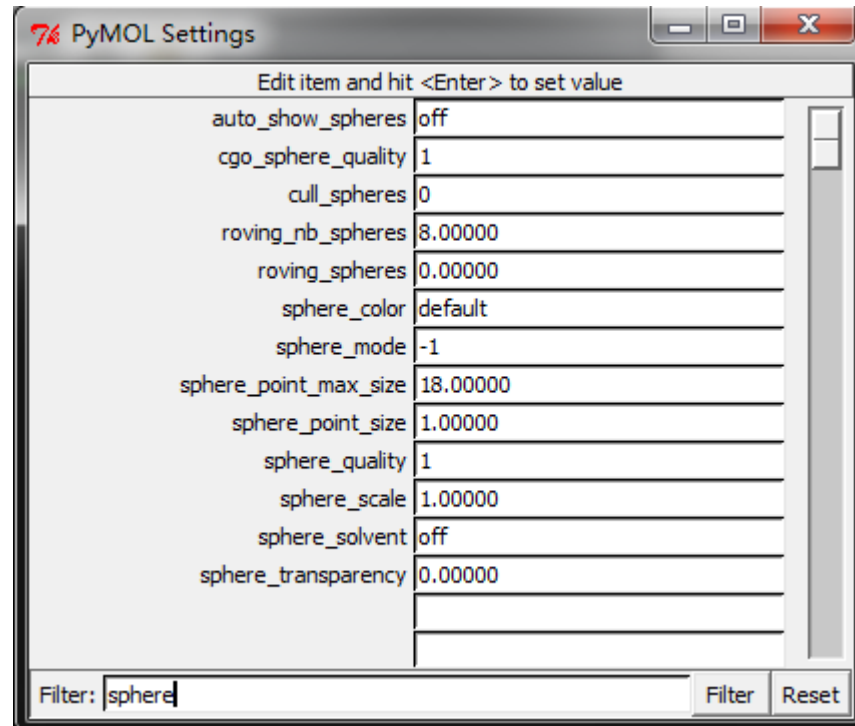
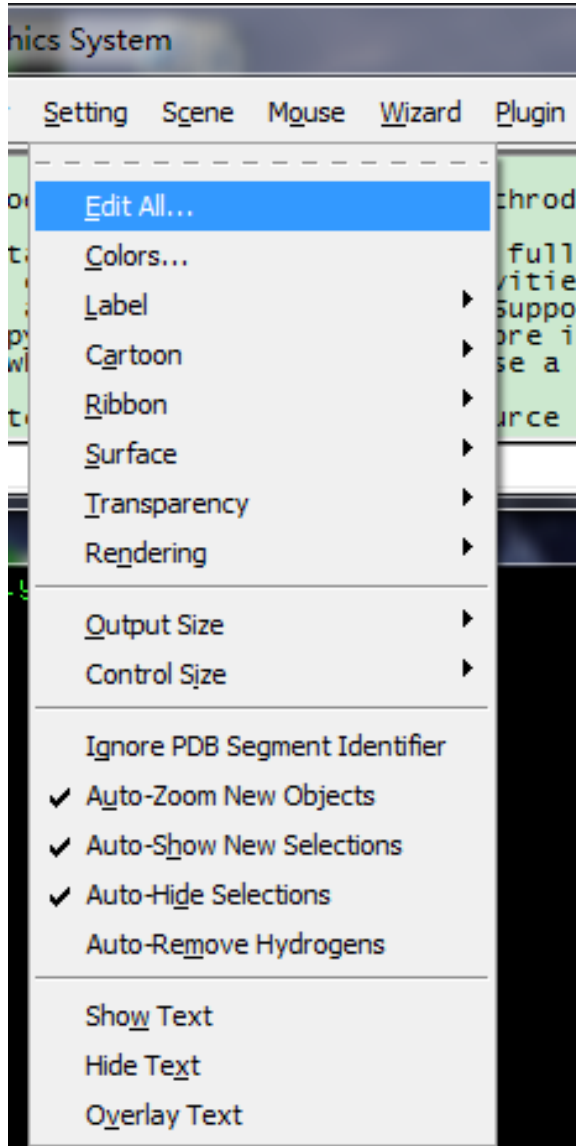
```
all
1CH3
```

The Mouse Mode panel shows the following text:

```
Mouse Mode 3-Button Viewing
Buttons L M R Wheel
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip MovS
Ctrl +/- PkAt PK1 MvSZ
CtSh Sele Drag Clip MovZ
SnglClk +/-
DblClk Menu
Selecting Res
Frame [ 1/
```

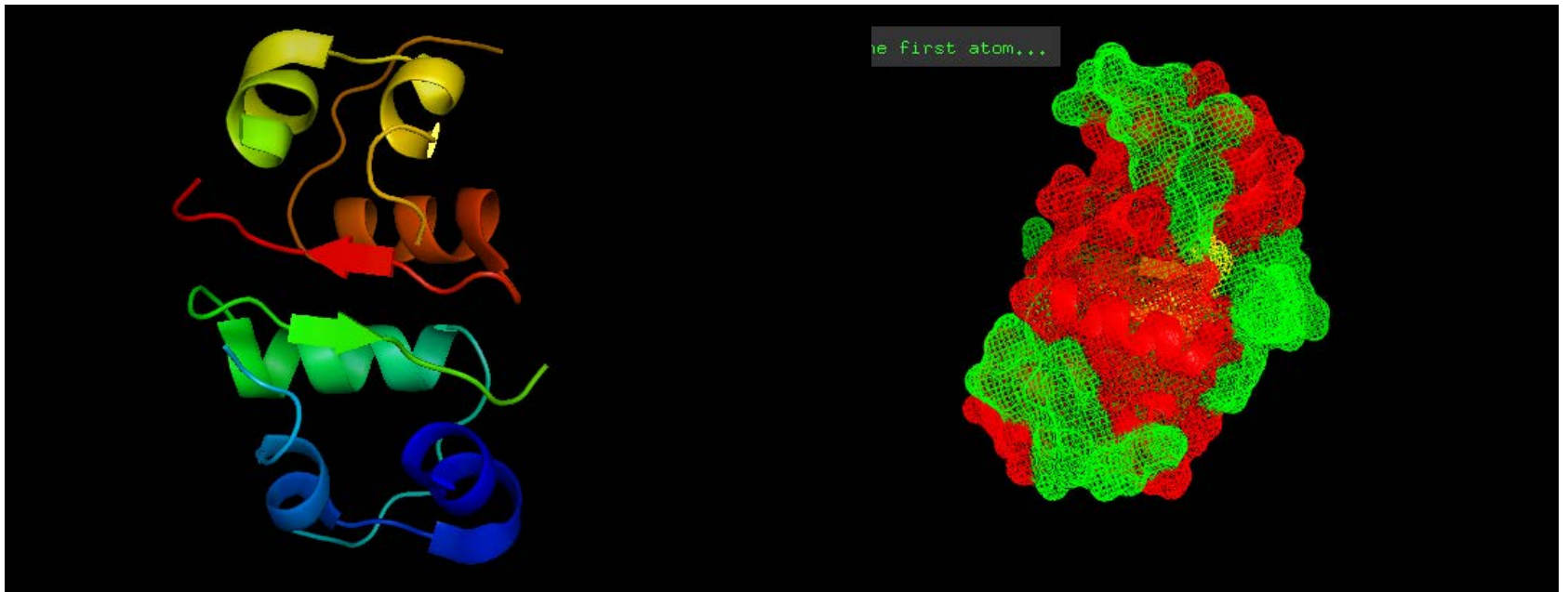
Settings

PyMol has over 600 settings!
Everything from ray tracing fog, to perspective viewing, stereo rendering, colors, textures, memory settings and **many** more!



实例演示

以胰岛素(PDB:4INS)为例



1. Load the PDB file

- File > Open > 4INS.pdb

- load ../4INS.pdb

- Display>sequence or 单击右下角“s”按钮 #显示序列 (4条链, 2 ZN)

2. show/hide different representation

- Show > as>cartoon

- hide everything, all

- show cartoon, all

- 鼠标L/M/R键示例

3. Color the helix, sheet, and loop

- color > by ss > Helix Sheet Loop

- color > by chain > chainbows #用于观察链的走向

- color red , ss h

- color yellow, ss s

- color green, ss ""

4. Color chain A and B

- color blue, chain A

- ⑩color red, chain B

5. Create a surface display for chain A and chain B

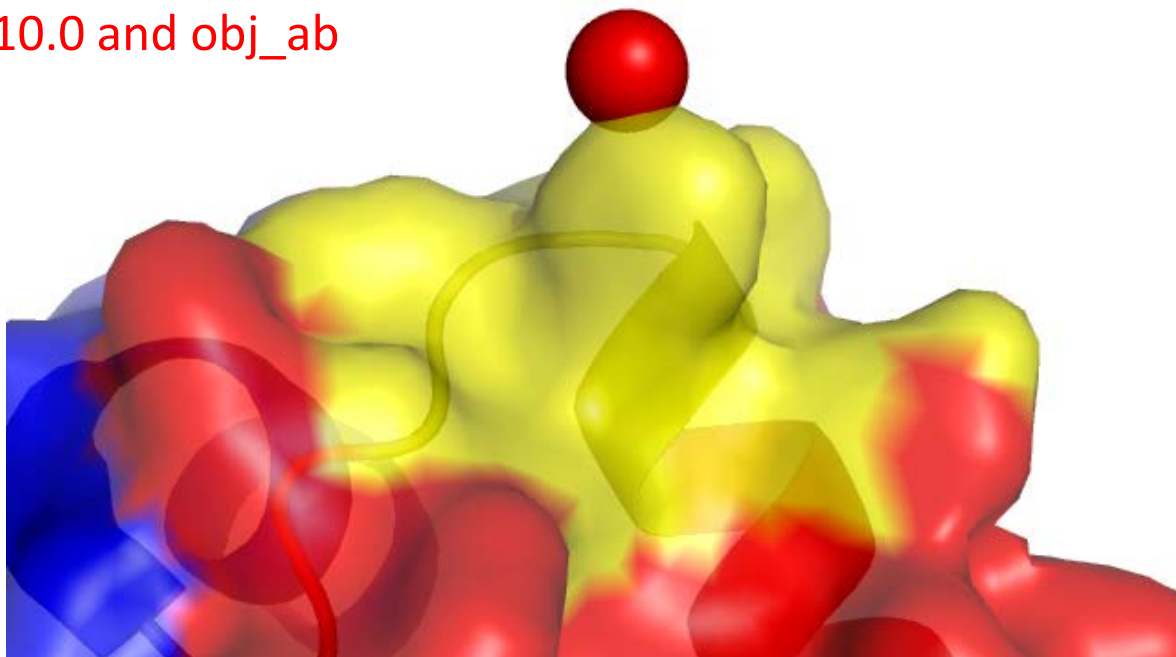
- create obj_ab, chain A or chain B
- show surface, obj_ab

6. Find and Color the active site residue

- ⑩select zn, resn ZN and obj_ab
- ⑩showspheres, zn
- ⑩alter zn, vdw=1.3
- ⑩rebuild
- select active, zn around 10.0 and obj_ab
- color yellow, active
- set transparency=0.25
- zoom active
- orient active

7. Rendering and output

- bg_color white
- ray
- File > Save Image



8. Display the side-chain of active site residues

⑩ hide surface

- select sidechain, not (name c+n+o)
- show sticks, (active and sidechain)
- color blue, name n*
- color red, name o*
- color white, name c*

9. Display and measure distances

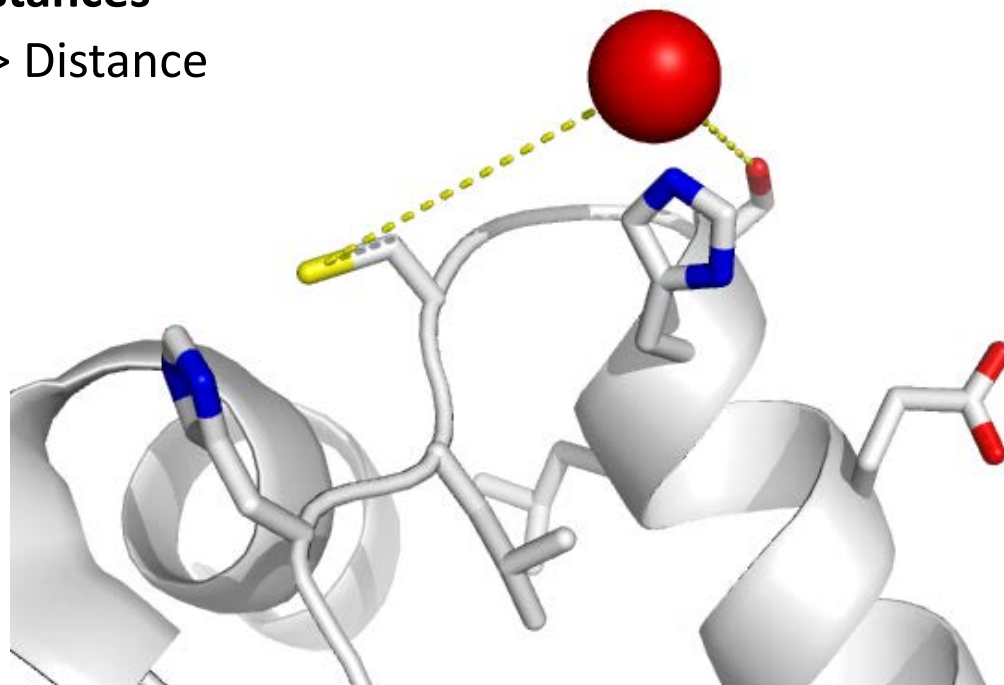
Wizard -> Measurement -> Distance

- hide labels
- ray

File > Save Image

10. Other commands

- File> save session as
- diabale
- enable
- delete sidechain



注意事项:

- ⑩ GUI窗口命令行可以识别全角字符，Viewer窗口不可
- ⑩ 涉及A、B链的情况需要命令符，界面上的工具按钮无法识别单条链。
- ⑩ 命令符的大小写、空格非常严格
- ⑩ 逻辑操作子or 和and的使用
- ⑩ 选择表达的名字可以由字母[A/a—Z/z]，数字[0—9]已经下划线[_]组成，但是要避免使用：

!@#\$%^&*()' "[] { } \ | ~ ` < > ? /

THANK YOU!