Pymol简述

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内容

1. 背景
2. Python和它的脚本们
3. Pymol实例-1faw

背景：若说pymol必说python

* Python, 是一种面向对象、解释型计算机程序设计语言。因为它你才能看到pymol。
* 安装pymol之必须先安装python。
* 众多的科研软件都需要Python在后台默默地支持。

pymol

* PyMOL是一个开源软件，由使用者赞助的分子三维结构显示软件。由Warren Lyford DeLano编写，并且由DeLano Scientific LLC将它商业化。DeLano Scientific LLC是一个私人的软件公司，它致力于创造让普遍的科学与教育社群都能取得的好用软件工具。当然他1.7版本是收费的。

脚本

* Pymol本身功能很简单，应用操作也不如swiss pdbview直接，功能也有一定差距，唯一可圈点的时它的作图十分漂亮并且有众多的参与者提供的脚本和插件，他正在越来越完善。

Python和它的脚本们：PyMOLWiki社区

Structural Biology

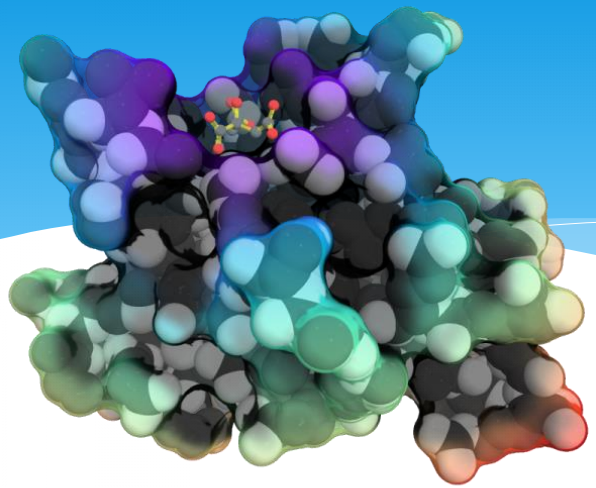
- AAindex
- AngleBetweenHelices
- AutoMultiFit
- Average b
- BbPlane
- BiologicalUnit
- BiologicalUnit/Quat
- Bondpack
- Cart to frac
- Ccp4 contact
- Ccp4 ncont
- Ccp4 pisa
- Centroid
- ColorByRMSD
- Color By Mutations
- Color by conservation
- Colorblindfriendly
- Colorbydisplacement

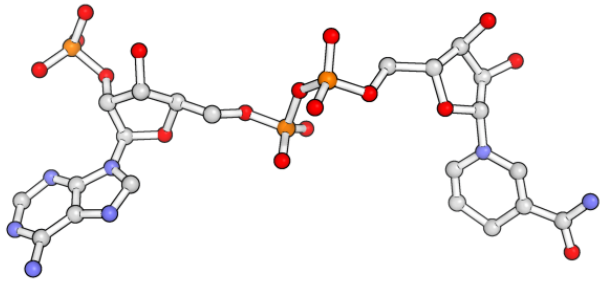
Objects and Selections

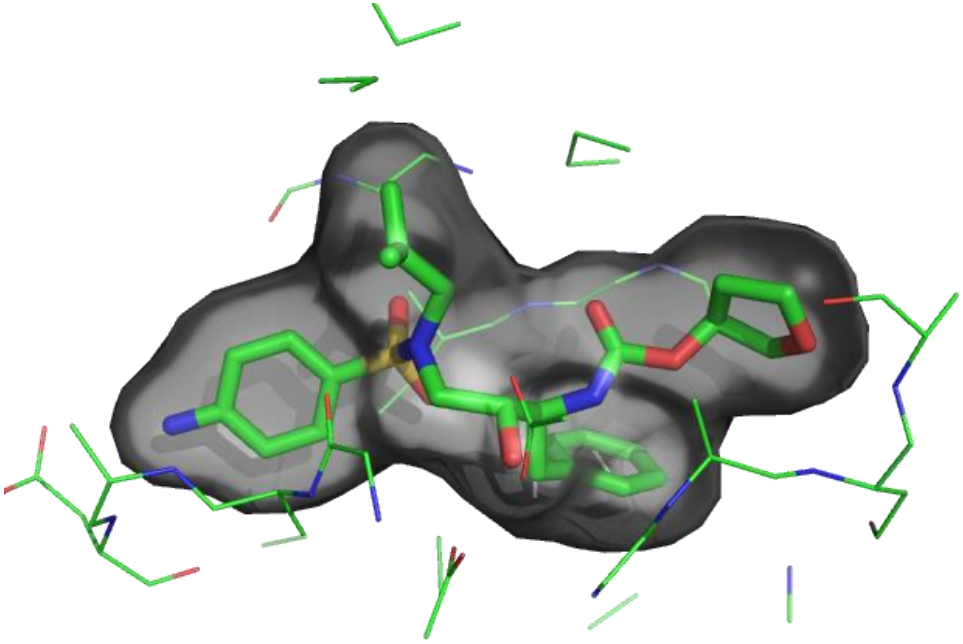
- AlphaToAll
- Cluster Count
- CollapseSel
- Color Objects
- ConnectedCloud
- Count molecules in selection
- DistancesRH
- Expand To Surface
- FindObjectsNearby
- FindSurfaceResidues
- Find buried waters
- Findseq
- Flatten obj
- GetNamesInSel
- Get Coordinates I
- Get Coordinates II
- Get raw distances
- Grepsel

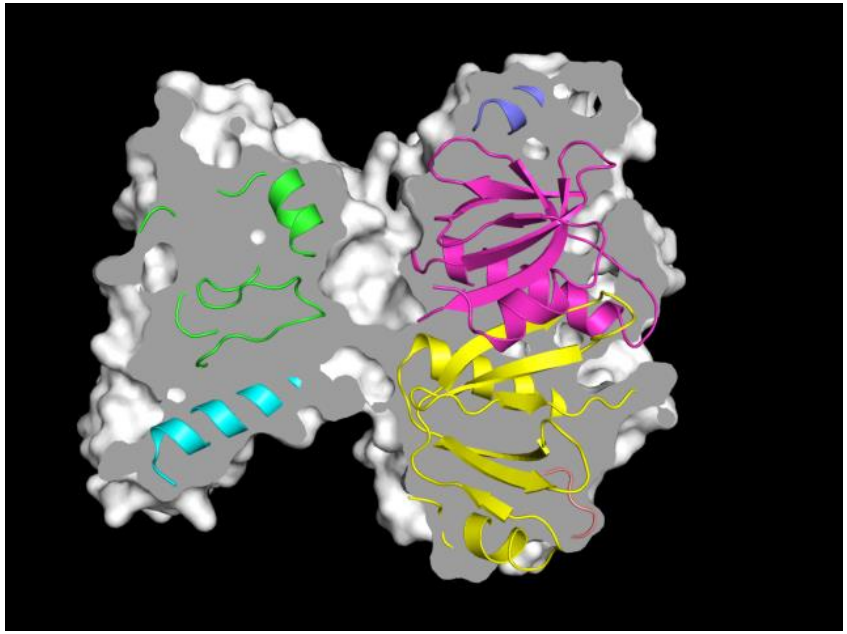
Math/Geometry/CGO

- Axes
- BbPlane
- BiologicalUnit
- BiologicalUnit/Quat
- Bounding Box
- CGO Text
- Cart to frac
- Center of mass
- CgoCircle
- Cgo arrow
- Cgo grid
- Contact Surface
- Cubes
- Distancetoatom
- DrawBoundingBox
- Dump2CGO
- Ellipsoid
- Mark center









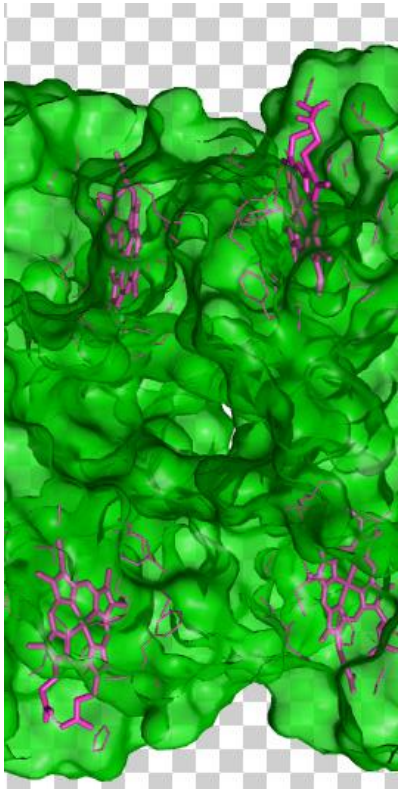
```
PyMOL(TM) Molecular Graphics System, Version 1.5.0.3.
Copyright (c) Schrodinger, LLC.
All Rights Reserved.

   Created by Warren L. DeLano, Ph.D.

   PyMOL is user-supported open-source software.  Although some versions
   are freely available, PyMOL is not in the public domain.

   If PyMOL is helpful in your work or study, then please volunteer
   support for our ongoing efforts to create open and affordable scientific
   software by purchasing a PyMOL Maintenance and/or Support subscription.

   More information can be found at "http://www.pymol.org".

   Enter "help" for a list of commands.
   Enter "help <command-name>" for information on a specific command.

Hit ESC anytime to toggle between text and graphics.

Detected OpenGL version 2.0 or greater. Shaders available.
Detected GLSL version 1.20.
Adjusting settings to improve performance for Intel cards.
OpenGL quad-buffer stereo 3D detected and enabled.
Error: set_startup_path failed
parser: matching commands:
 GetBoxHelp          gradient            recolor
 aaindex2b           group               redo
 abort               h_add               reference
 accept              h_fill              refresh
 alias               h_fix               refresh_wizard
 align               help                reinitialize
 alignto             hide                remove
 alter               id_atom             remove_picked
 alter_state         identify            rename
 angle               if                  replace
 as                  import              replace_wizard
 assert              index               reset
 attach              indicate            resibox
 autobox             intra_fit           resume
 backward            intra_rms           return
 bg_color            intra_rms_cur       rewind
 bond                invert              rms
 break               isodot              rms_cur
 button              isolevel            rock
 cache               isomesh             rotate
 capture             isosurface          run
 cartoon             iterate             save
 cd                  iterate_state       scene
 cealign             label               scene_order
 center              load                sculpt_activate
 check               load_embedded       sculpt_deactivate
 class               load_png            sculpt_iterate
 clean               load_traj           sculpt_purge
 clip                log                 select
 cls                 log_close           set
 color               log_open            set_bond
```

Pymol脚本和插件

* 在脚本库中有181个脚本涉及7个大方面。脚本运行非常简单。并且每一个脚本都有教程，简单易学。
* 还有一些第三方写成的插件，针对具体应用。

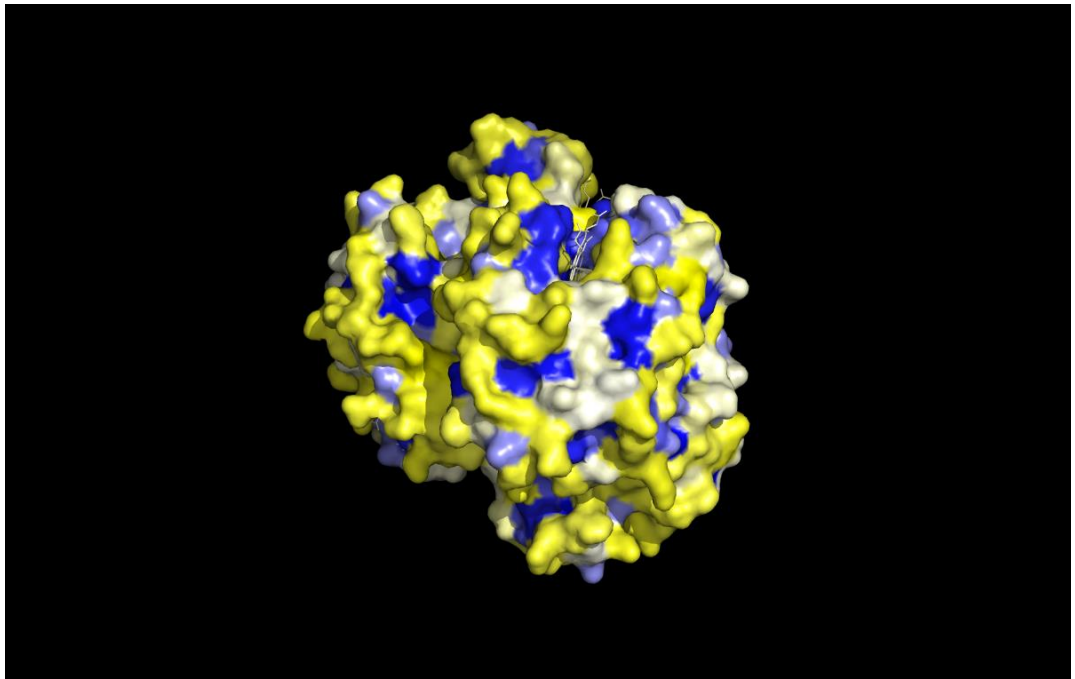
1faw suface脚本演示

```
# grey surface
set surface_color, grey

# cavity mode
set surface_mode, 3

# layered transparency mode
set transparency_mode, 1

# surface transparency
set transparency, 0.5

# oblique and contrast define the
# look of the surface transparency:
# if the normal vector is
set ray_transparency_oblique
set ray_transparency_oblique_power, 8
set ray_transparency_contrast, 7

# fetch a protein, with a
# small molecule in a nice
# hidden pocket
fetch 1faw, async=0

hide

# show the small molecule as surface
show surface, org

# arrange the view
orient org

# zoom back a little
zoom org, 1

# show the small molecule inside as sticks
show sticks, org

# show some nearby sidechains
show lines, poly within 5 of org

# enable frame caching for playback
```

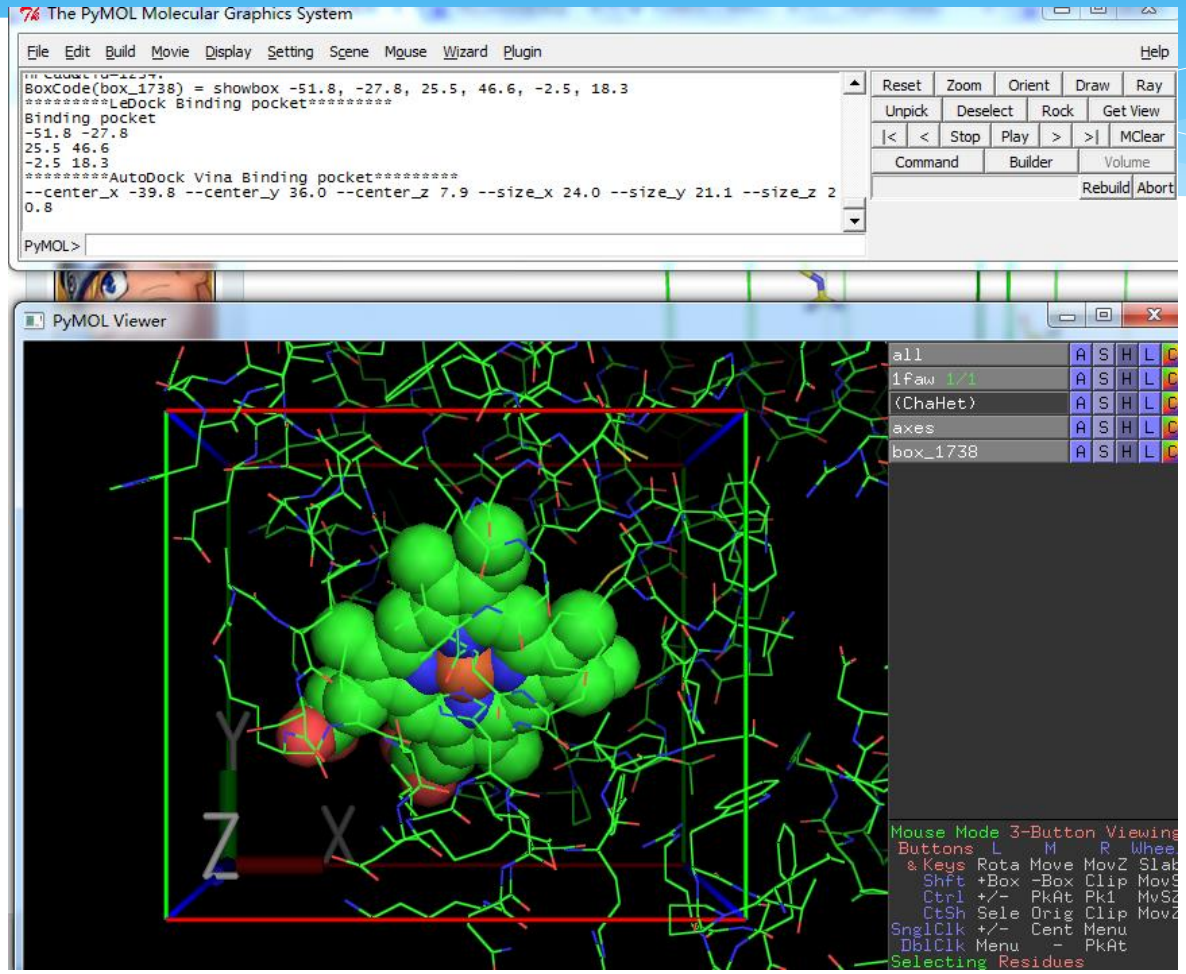


Aaindex实例

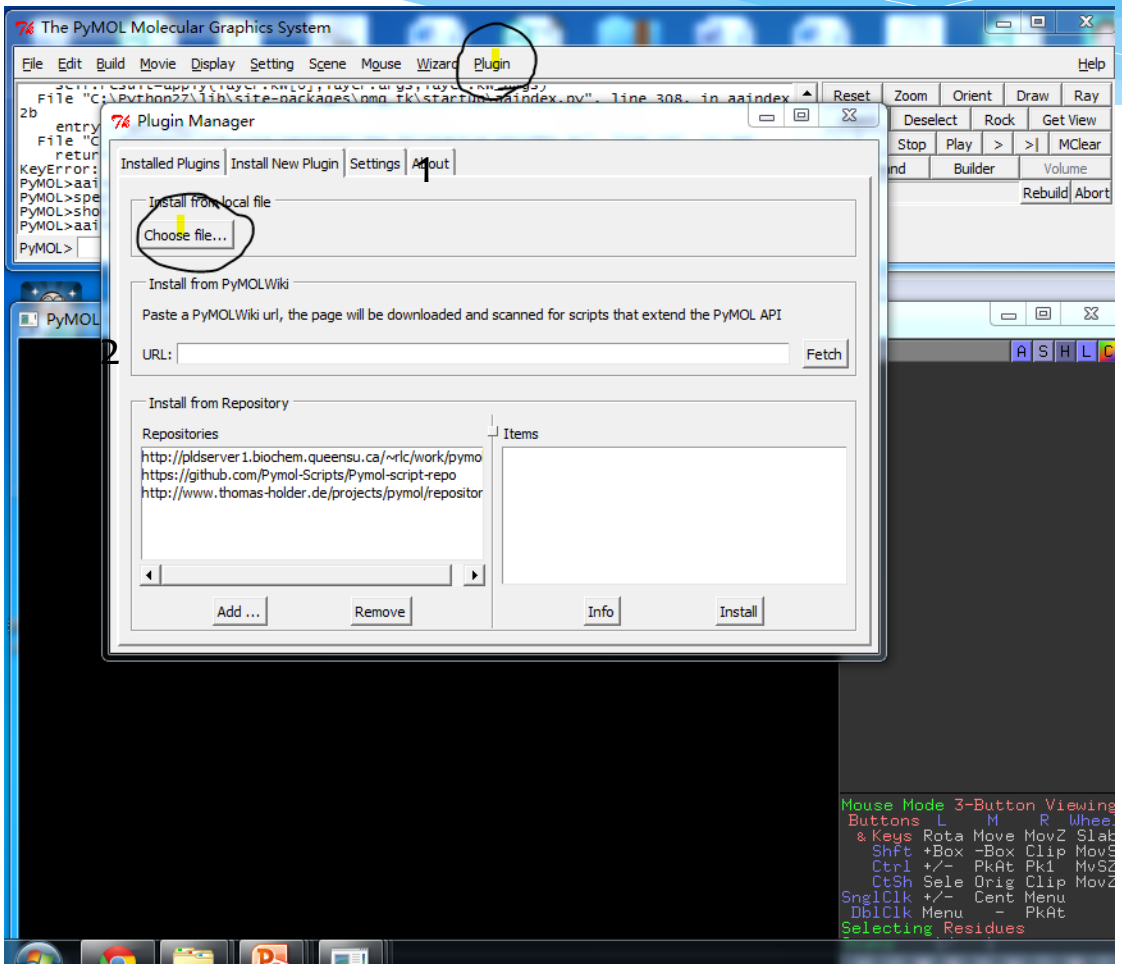
Pymol>aaindex
aaindex2b KYTJ820101 spectrum b, yellow_white_blue show surface



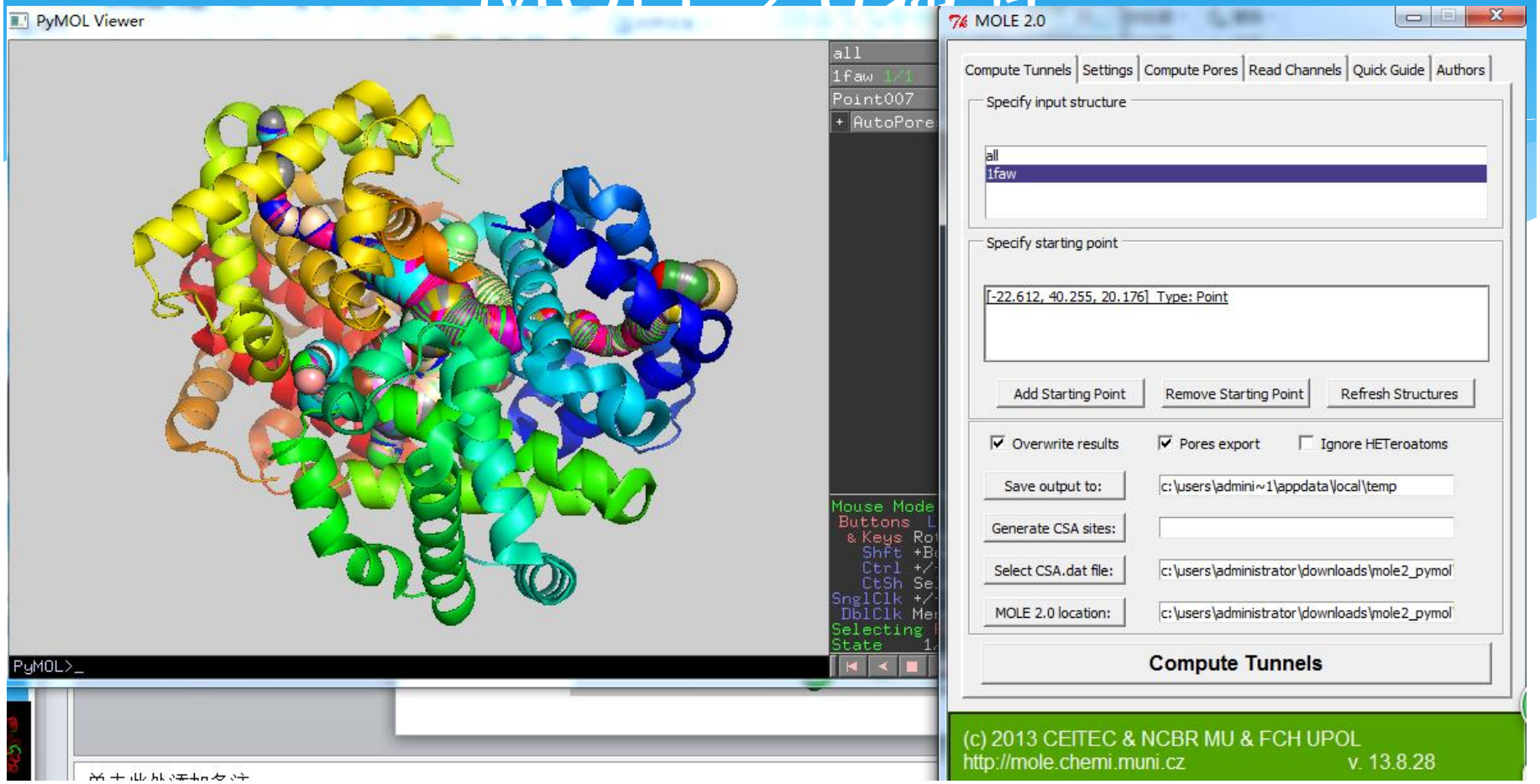
GETBOX


The PyMOL Molecular Graphics System
File Edit Build Movie Display Setting Scene Mouse Wizard Plugin
Help
BoxCode(box_1738) = showbox -51.8, -27.8, 25.5, 46.6, -2.5, 18.3
*********LeDock Binding pocket*********
Binding pocket
-51.8 -27.8
25.5 46.6
-2.5 18.3
*********AutoDock Vina Binding pocket*********
--center_x -39.8 --center_y 36.0 --center_z 7.9 --size_x 24.0 --size_y 21.1 --size_z 2
0.8
PyMOL>
Reset Zoom Orient Draw Ray
Unpick Deselect Rock Get View
Stop Play MClear
Command Builder Volume
Rebuild Abort
PyMOL Viewer
all
1faw 1/1
(ChaHet)
axes
box_1738
Y
Z
X
Mouse Mode 3-Button Viewing
Buttons L M R Whee
& Keys Rota Move MovZ Slab
Shft +Box -Box Clip
Ctrl +/- PkAt Pk1
CtSh Sele Orig Clip
SnglClk +/- Cent Menu
DblClk Menu - PkAt
Selecting Residues

用于分子对接，获取配体文件盒子的坐标值。

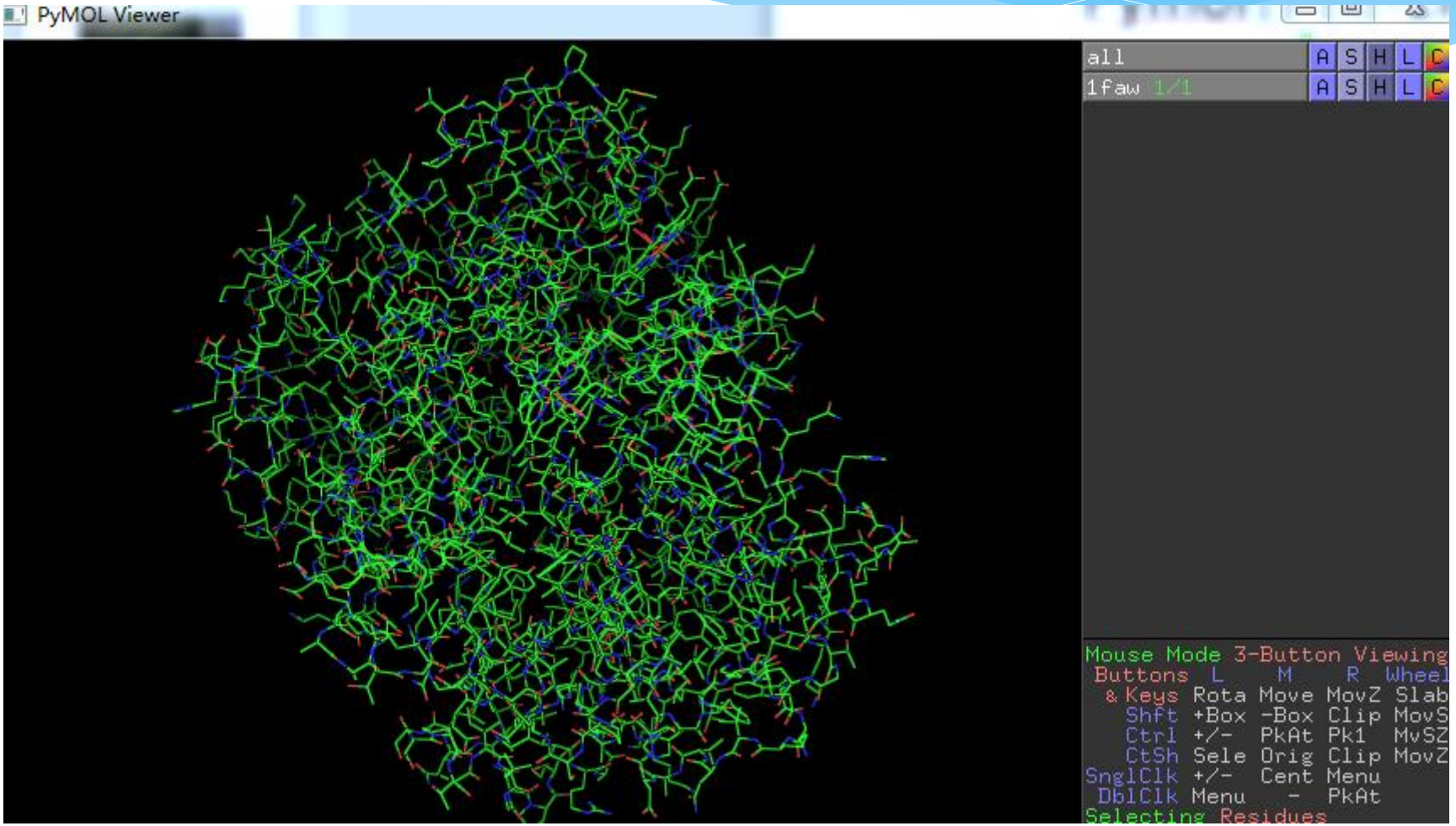


MOLE 2.0插件

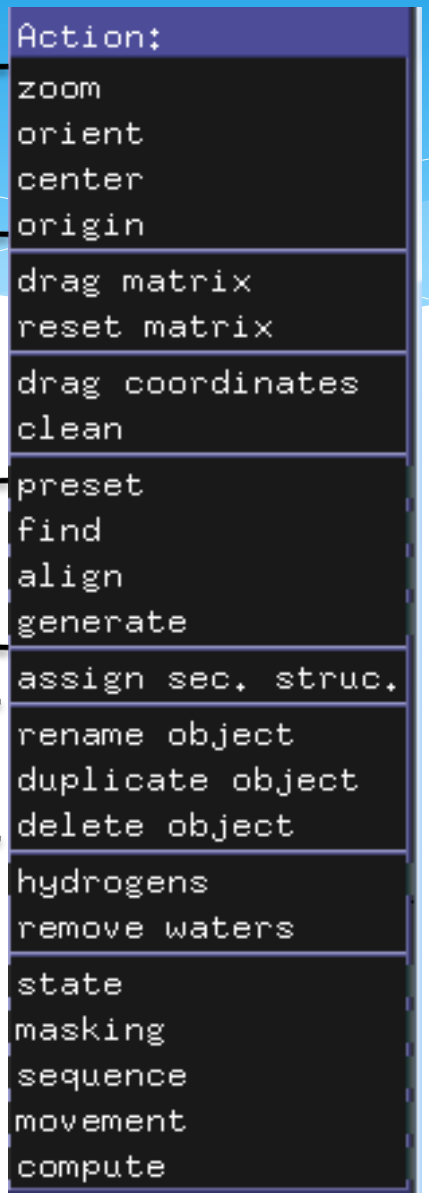


* MOLE2.0 不仅计算通道的理化性质，也可以计算亲水性，疏水性，极性，电荷，和可变性。

Pymol作图-1faw



Pymol主要操作界面



导航工具

分析工具

Object工具

All指所有的对象，3ODU指刚才打开的文件，(sele)是选择的对象

A:代表对这个对象的各种action，

S：显示这个对象的某种样式，

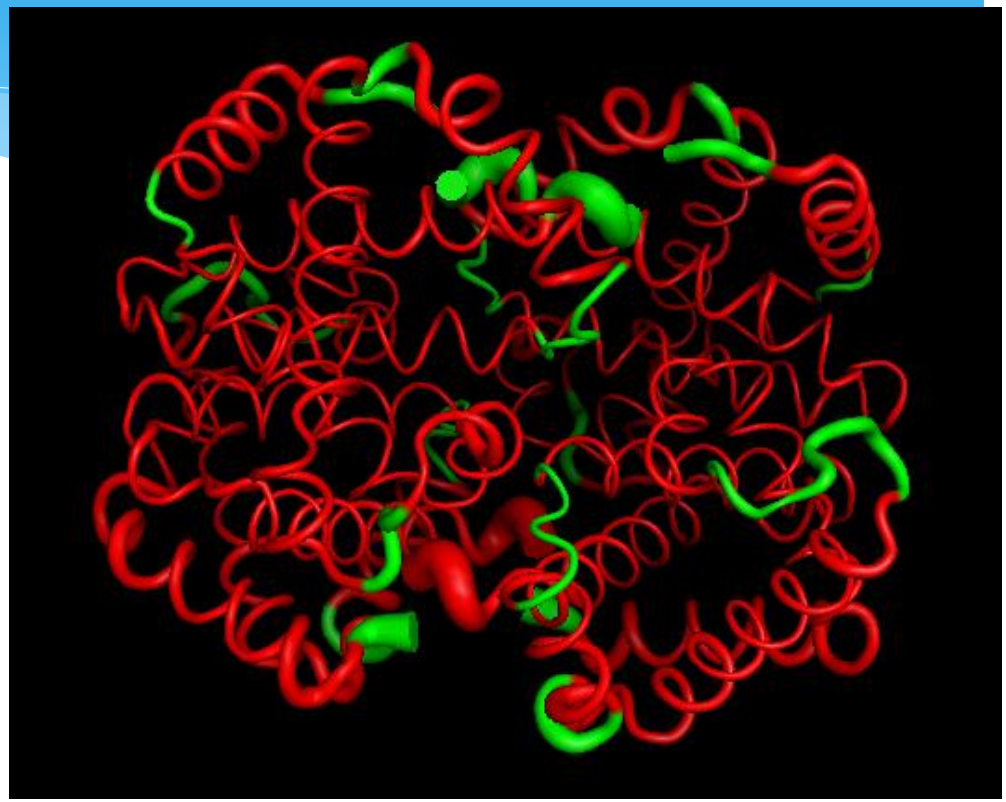
H：隐藏某种样式，

L：显示某种label，

C：显示的颜色

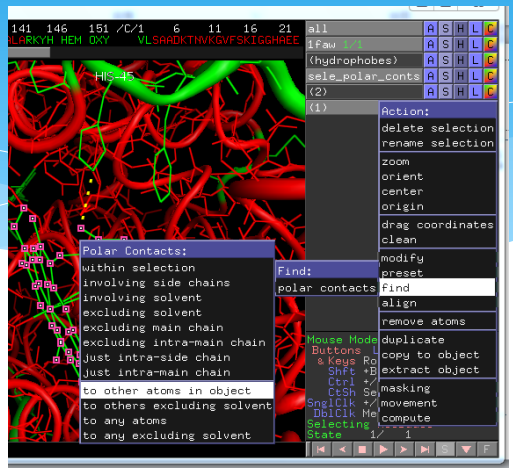
Pymol> color red, ss h
color yellow, ss s
color green, ss l+
其中“ss”代表secondary structure，“h”代表Helix，“s”代表Beta sheet，l+""代表Loop和所以其他结构。select helix, ss h
select sheet, ss s
select loop, ss l+
此命令是选择相应二级结构
选择残基
select resi 1-5 #选择1-5号残基
select resi 13 #选择13号残基
select resn tyr #选择所有的tyr残基

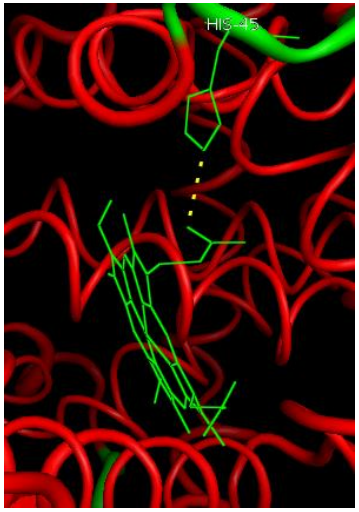
* PyMOL>cartoon putty
* hide line



* 选中相应display –sequence 找到HEM，选中重命名为1，获得相应的氢键。选中相应残基为2。

* PyMOL>hide line
* show line, （1 + 2）
* show label, 2



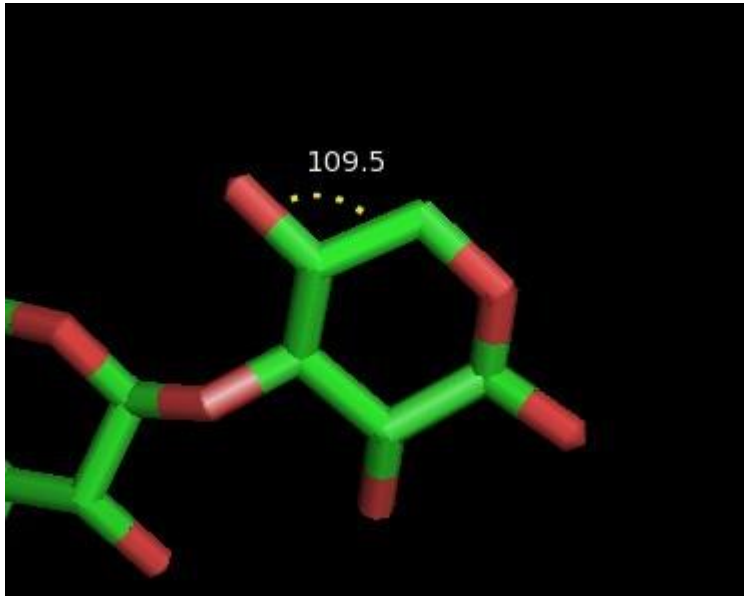


计算二面角，氢键距离

* 第一步，点击菜单栏上面的wizard 里面measurement。
* 第二步，在右边蓝色的 measurement mode 中选择Angles（点击distance，会出现不同的模式的选择，选择angles就是键角，选择dihedral就是二面角，还有其他一些选项）。
* 注 显示2位有效数字。在命令行中输入

set label_distance_digits, 2

* 第三步，依次点你的分子上的原子，三个原子出来键角（如果是二面角则是点击四个原子），效果如下图



选中一原子半径的原子

* Pymol>select 5A, sele expand 5

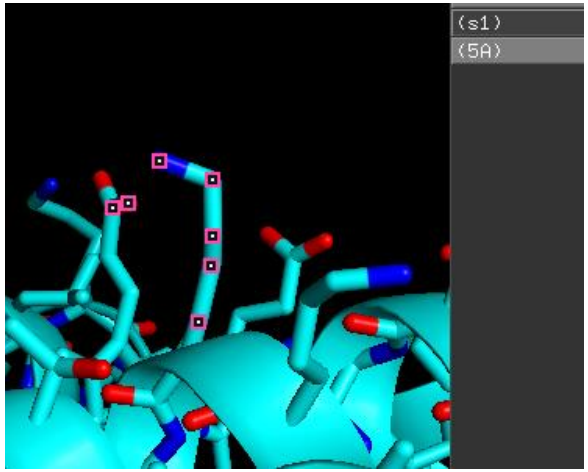
#显示选中原子5A以内的原子

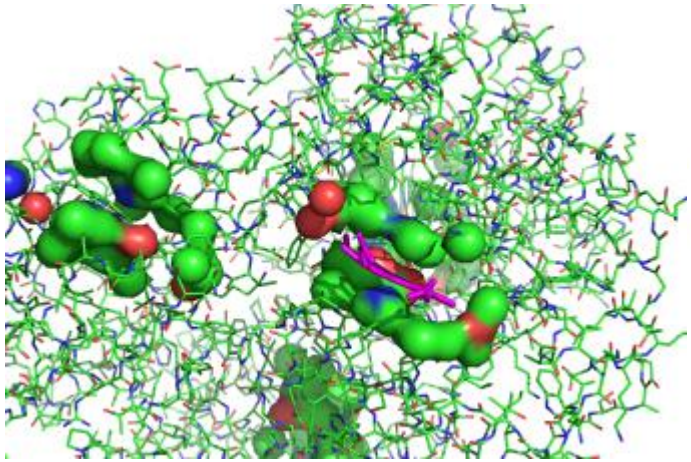
* select HEM, resn HEM around 4

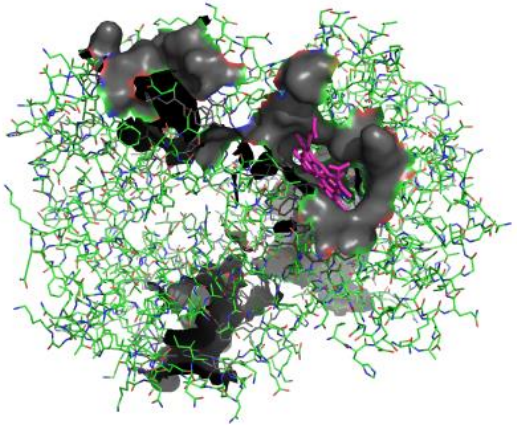
#选择离HEMA范围内的原子

* select HEMress,byres HEM

#选择离HEM4A范围内的氨基酸残基



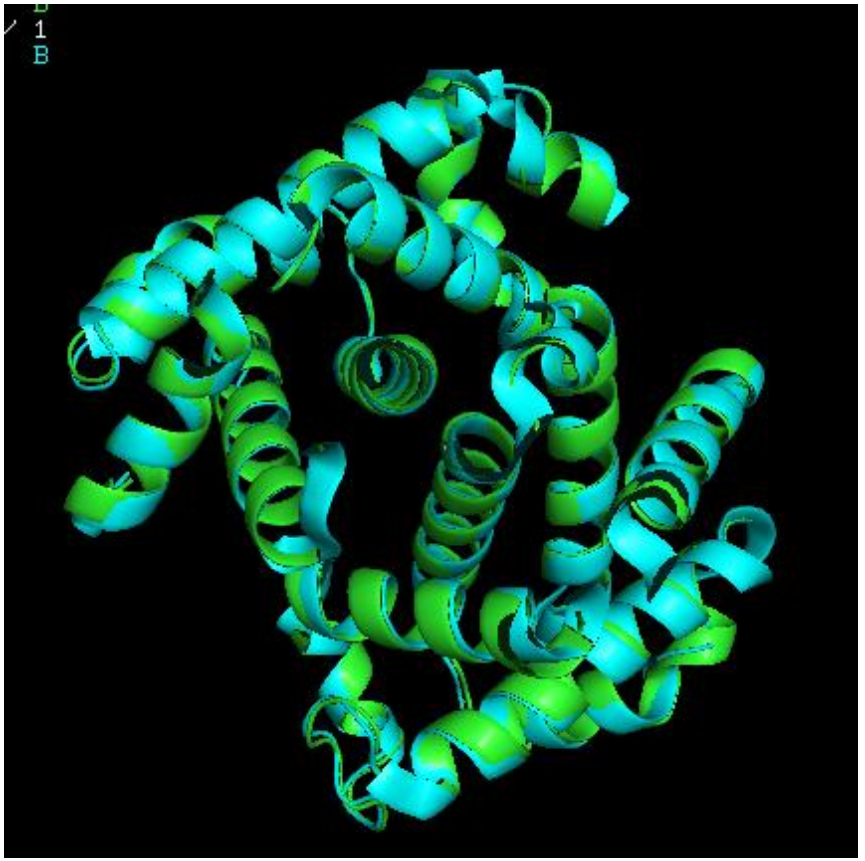




叠合1faw与1a4f

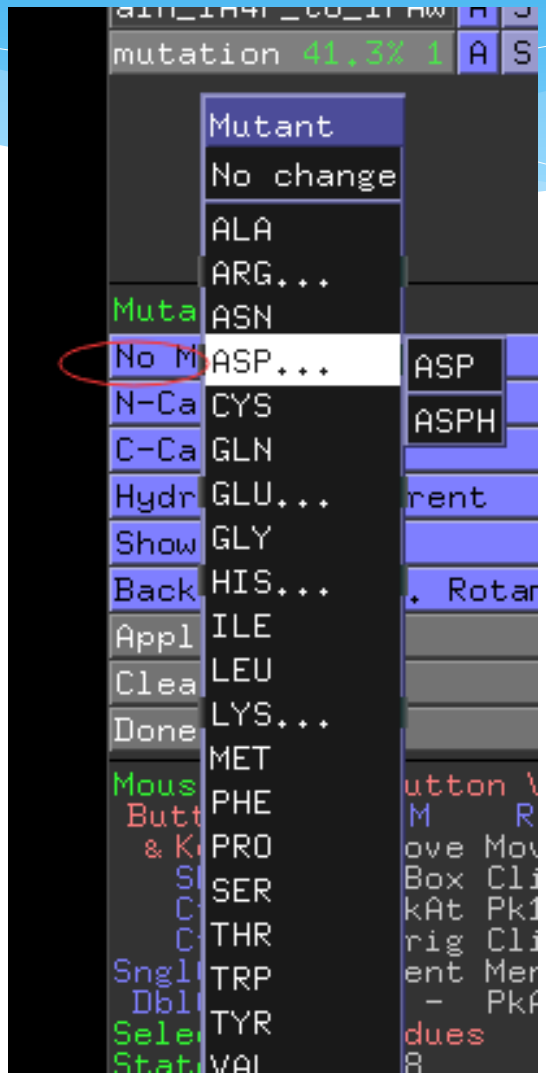
Action –align
-to molecule
Align –enable
this

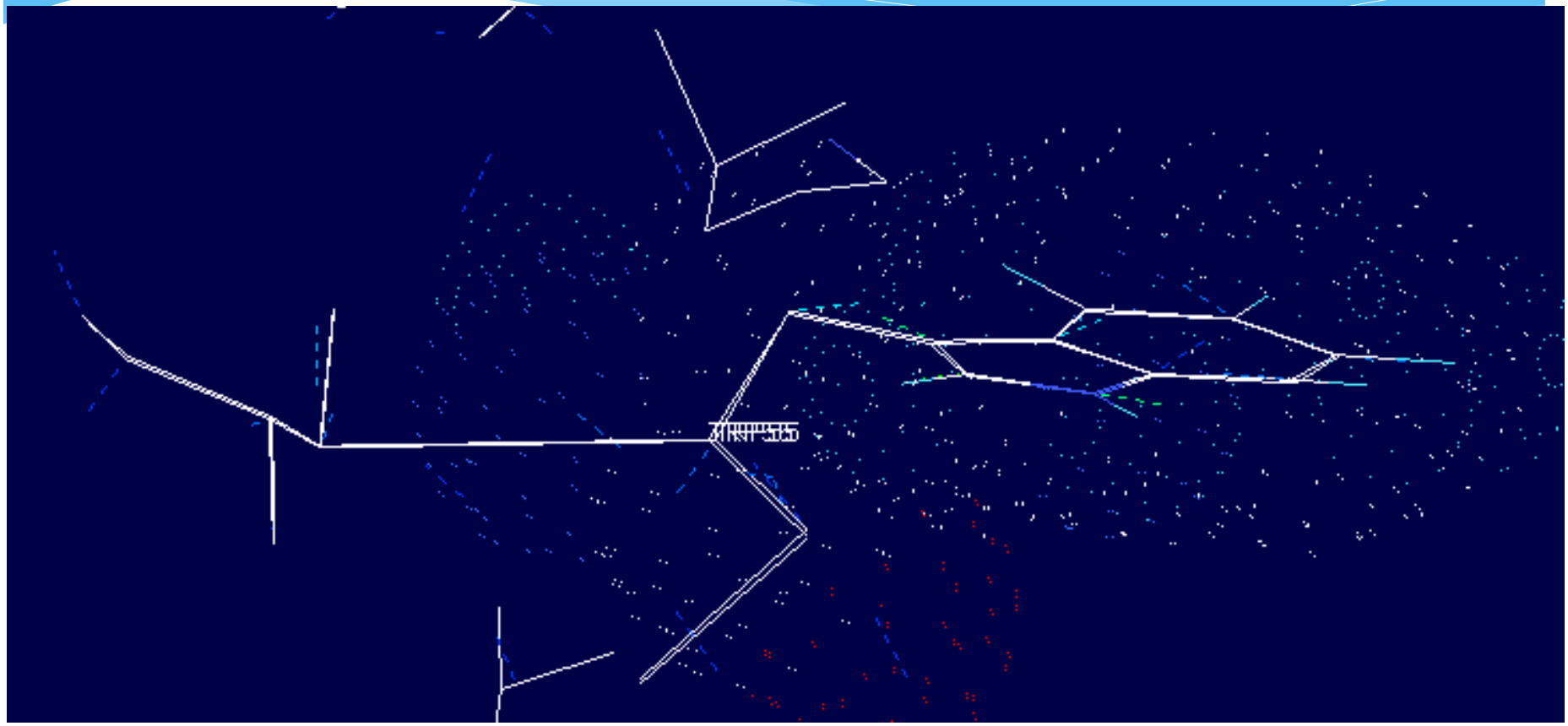
Match: read scoring matrix.
Match: assigning 287 x 574 pairwise scores.
MatchAlign: aligning residues (287 vs 574)...
ExecutiveAlign: 287 atoms aligned.
ExecutiveRMS: 11 atoms rejected during cycle 1 (RMS=0.48).
ExecutiveRMS: 10 atoms rejected during cycle 2 (RMS=0.36).
Executive: RMS = 0.325 (266 to 266 atoms)



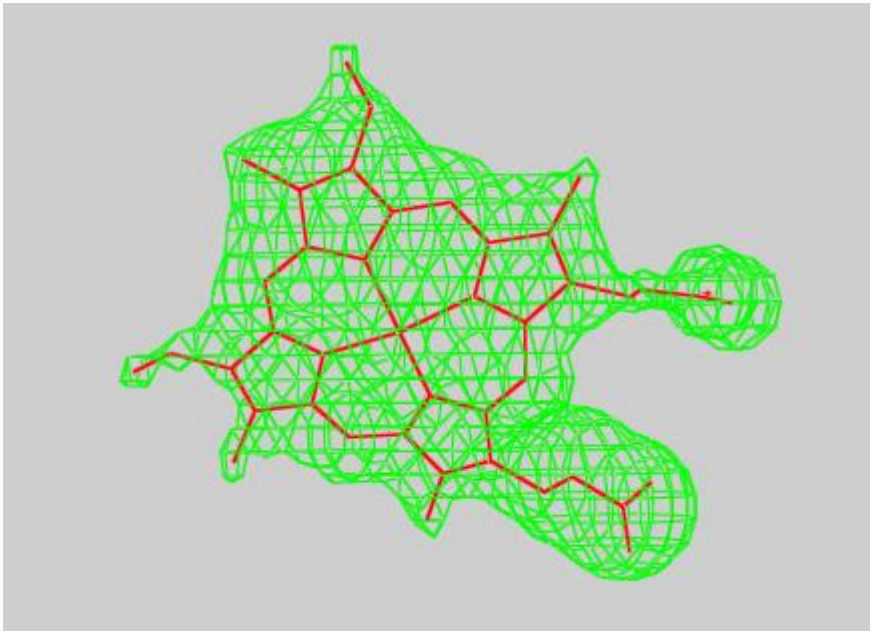
突变

* Wizard-mutagenesis
* Pymol的突变存在问题是无法进行优化。



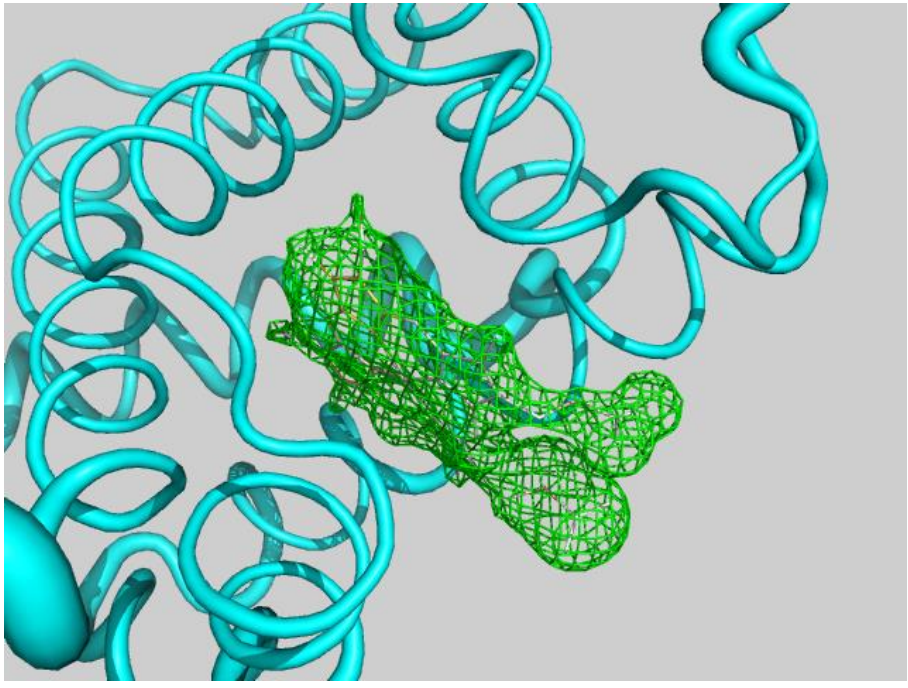


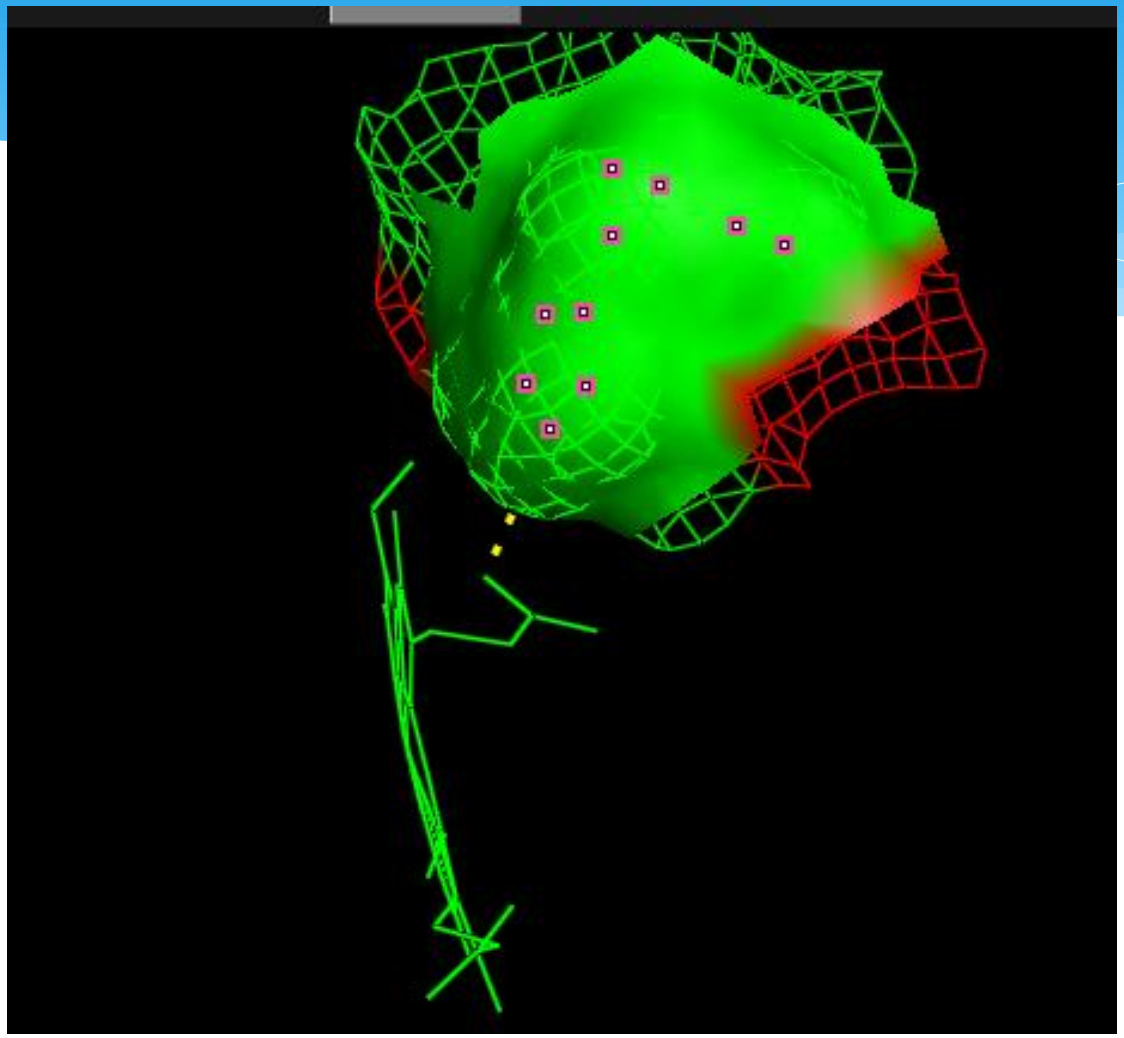
mesh分子表面显示



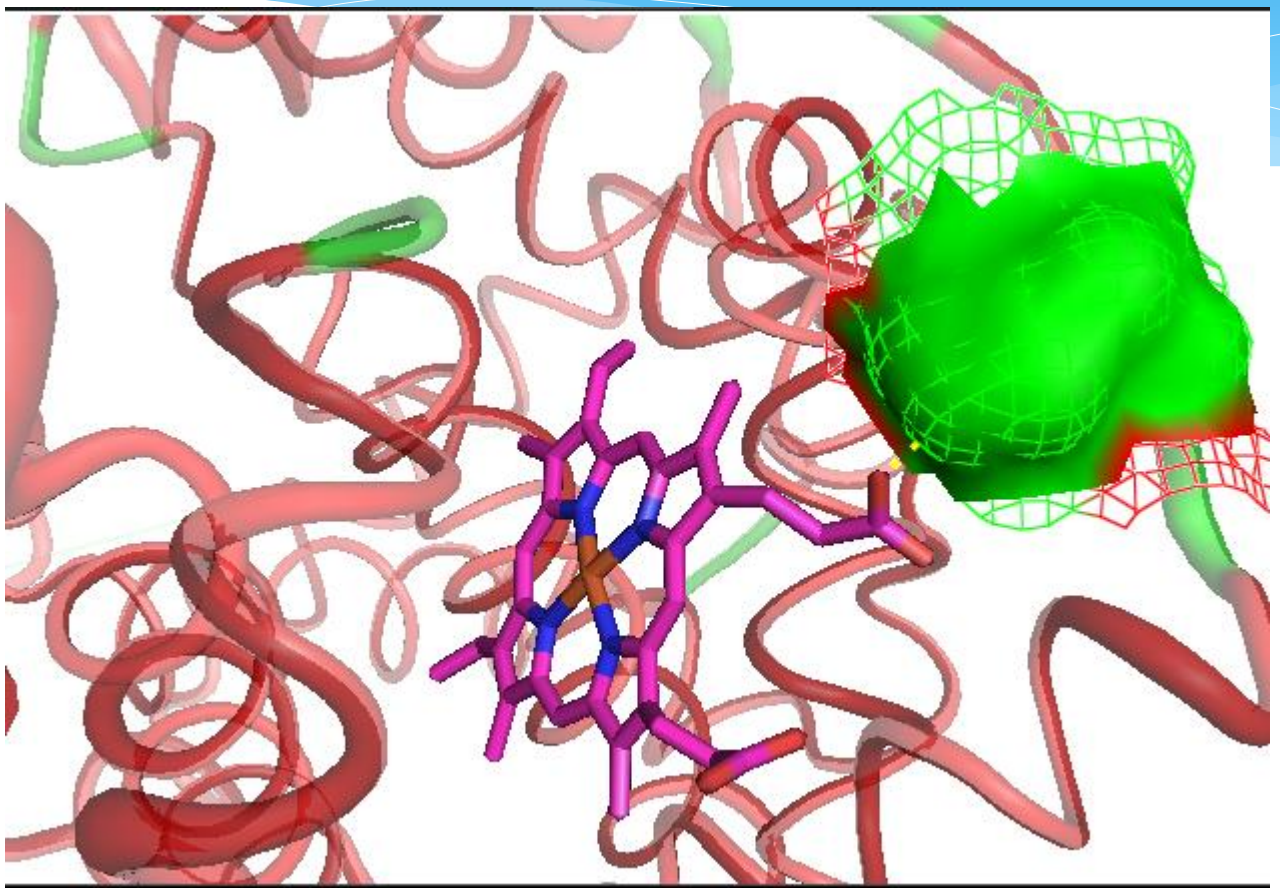
1、打开复合物pdb文件，选中配体分子。
2、创建单独的object，命令如下：
create ligand, sele
3、保存ligand 为pdb格式。
4、用文本编辑器打开ligand.pdb修改HETATM为ATOM （ATOM后面保留两个空格，否则会出现白色的分子骨架，且配体不在原来的位置的问题）。最后保存。
5、在pymol中打开ligand.pdb，在对应的ligand的S中选择 mesh。

6、对mesh着色，命令：
set mesh_color, green
7、在ligand的最后选择颜色。





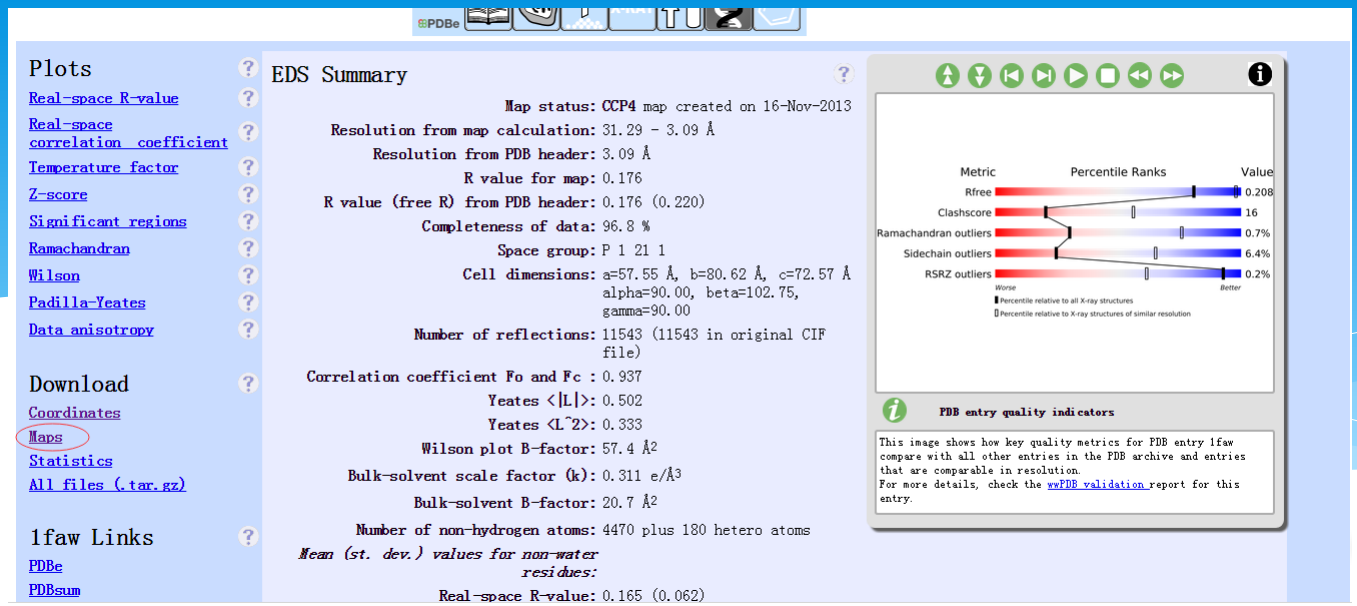
经过后续调节背景，选择透明度，宽度，ray的到最终图。

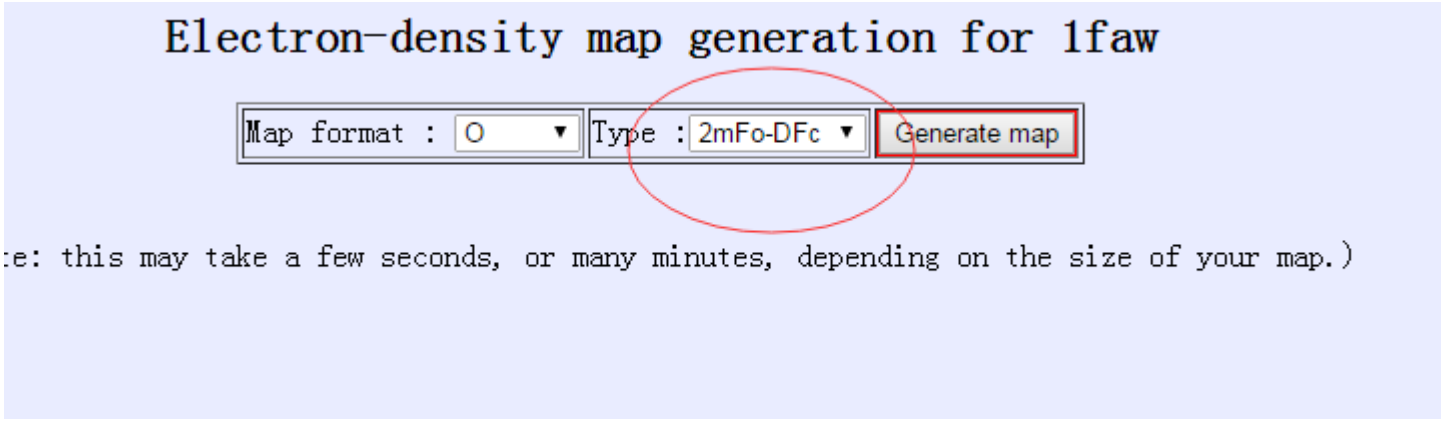


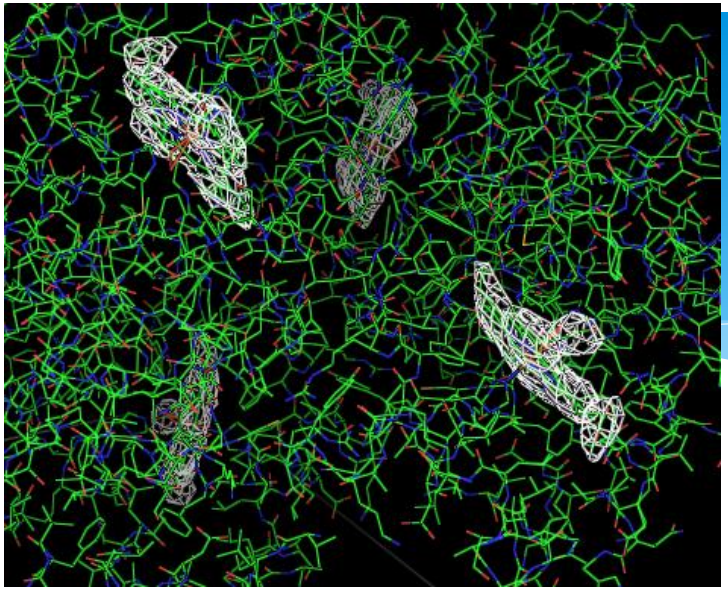
输入ray 1200,760就生成1200*760分辨率的图片。

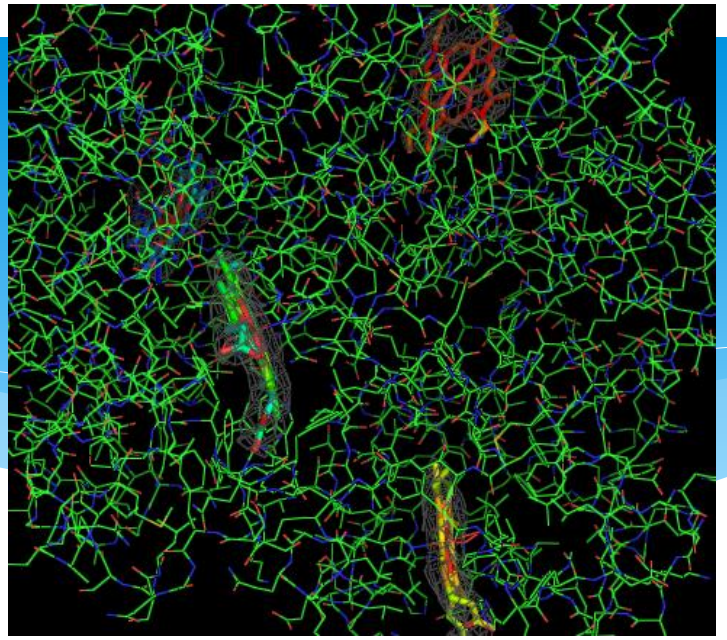
显示配体的电子密度

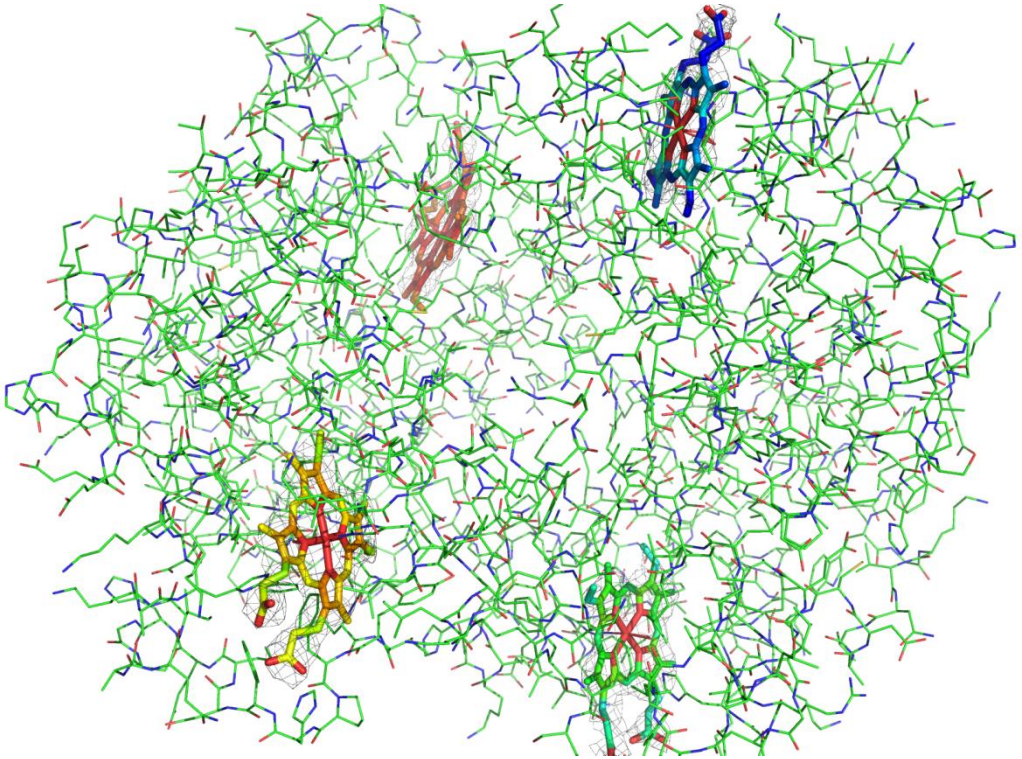
* 1. 进入http://eds.bmc.uu.se/eds/这个网址中（ElectronDensity server），输入所需要的PDB号（1faw.pdb），submitted，选择左侧download-Maps，弹出对话框后选择：Map format为CCP4。Type为2mFo-DFc，然后Generate map，下载完生成的压缩文件后解压，修改生成的文件名1faw.map.ccp4
* 2. 首先用pymol打开pdb文件，然后file-open 1faw.map.ccp4文件。分别加载完1faw.pdb和1faw.map.ccp4后，依次点击1faw.map文件的Action-mesh-@level 1.0（2.0，3.0根据自己的需要进行选择）。
* 3. select ligand, resn lig #本例子中选择显示的是配体的电子密度(lig为配体名，本例中以lig代替)。
* 4 . isomesh map, 1faw.map, 1.0, ligand, carve=1.6
* 5. 此时配体的电子密度已经显示出来，剩下的只是修改受体的显示方式及整体的可视化效果，比如：
* set mesh_radius, 0.01 #set radius to 0.01
* color grey30, map # sets map to 30% gray
* bg_color white #sets background to white
* set ray_trace_fog, 0 #turns off raytrace fog–optional
* set depth_cue, 0 # turns off depth cueing–optional
* set ray_shadows, off #turns off ray-tracing shadows

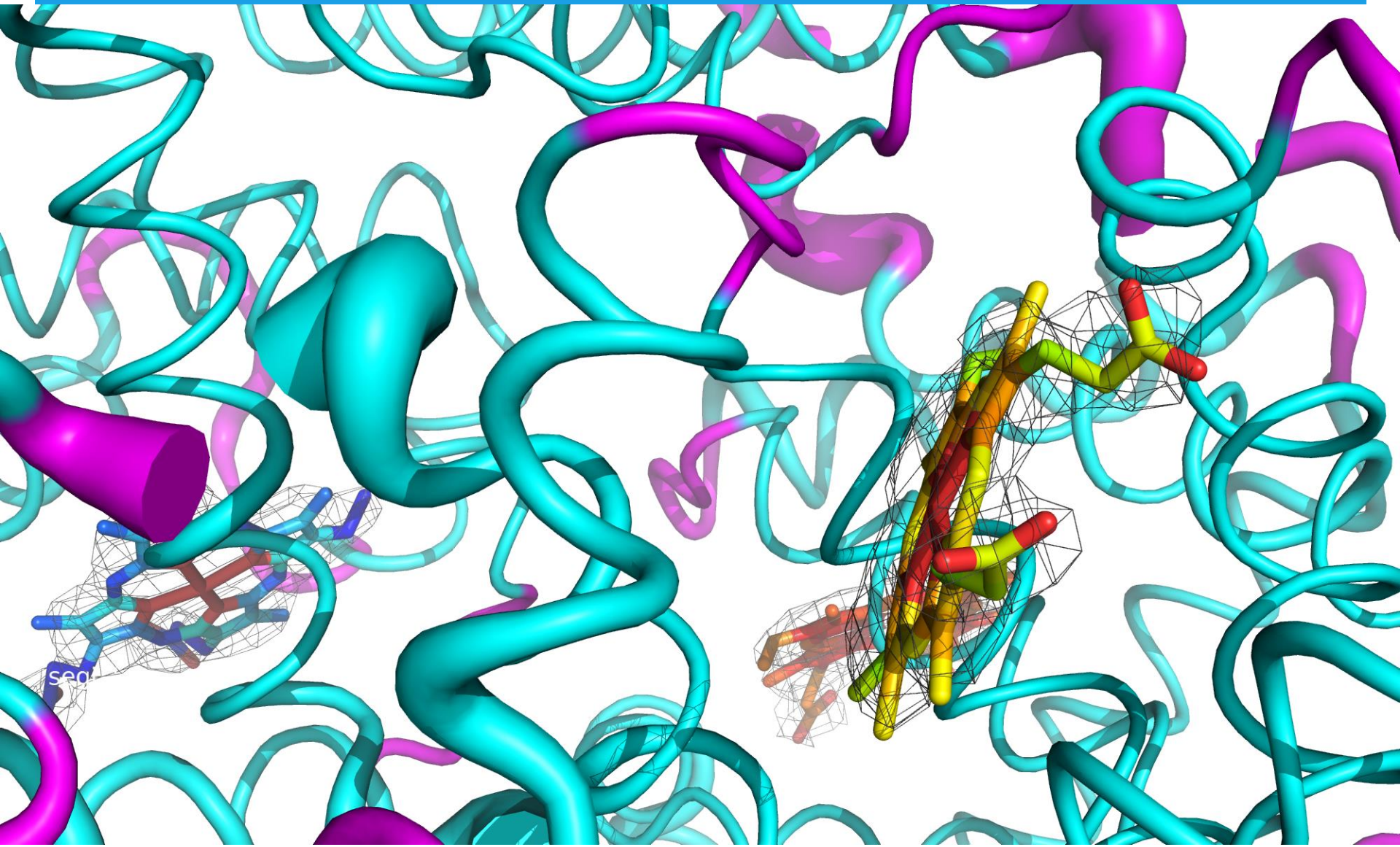

PDBe
Plots
Real-space R-value
Real-space correlation coefficient
Temperature factor
Z-score
Significant regions
Ramachandran
Wilson
Padilla-Yeates
Data anisotropy
Download
Coordinates
Maps
Statistics
All files (.tar.gz)
1faw Links
PDBe
PDBsum
EDS Summary
Map status: CCP4 map created on 16-Nov-2013
Resolution from map calculation: 31.29 - 3.09 Å
Resolution from PDB header: 3.09 Å
R value for map: 0.176
R value (free R) from PDB header: 0.176 (0.220)
Completeness of data: 96.8 %
Space group: P 1 21 1
Cell dimensions: a=57.55 Å, b=80.62 Å, c=72.57 Å alpha=90.00, beta=102.75, gamma=90.00
Number of reflections: 11543 (11543 in original CIF file)
Correlation coefficient Fo and Fc : 0.937
Yeates <|L|>: 0.502
Yeates <L^2>: 0.333
Wilson plot B-factor: 57.4 Å2
Bulk-solvent scale factor (k): 0.311 e/Å3
Bulk-solvent B-factor: 20.7 Å2
Number of non-hydrogen atoms: 4470 plus 180 hetero atoms
Mean (st. dev.) values for non-water residues:
Real-space R-value: 0.165 (0.062)
Metric
Percentile Ranks
Value
Rfree
0.208
Clashscore
16
Ramachandran outliers
0.7%
Sidechain outliers
6.4%
RSRZ outliers
0.2%
Worse
Better
Percentile relative to all X-ray structures
Percentile relative to X-ray structures of similar resolution
PDB entry quality indicators
This image shows how key quality metrics for PDB entry 1faw compare with all other entries in the PDB archive and entries that are comparable in resolution.
For more details, check the wwPDB validation report for this entry.

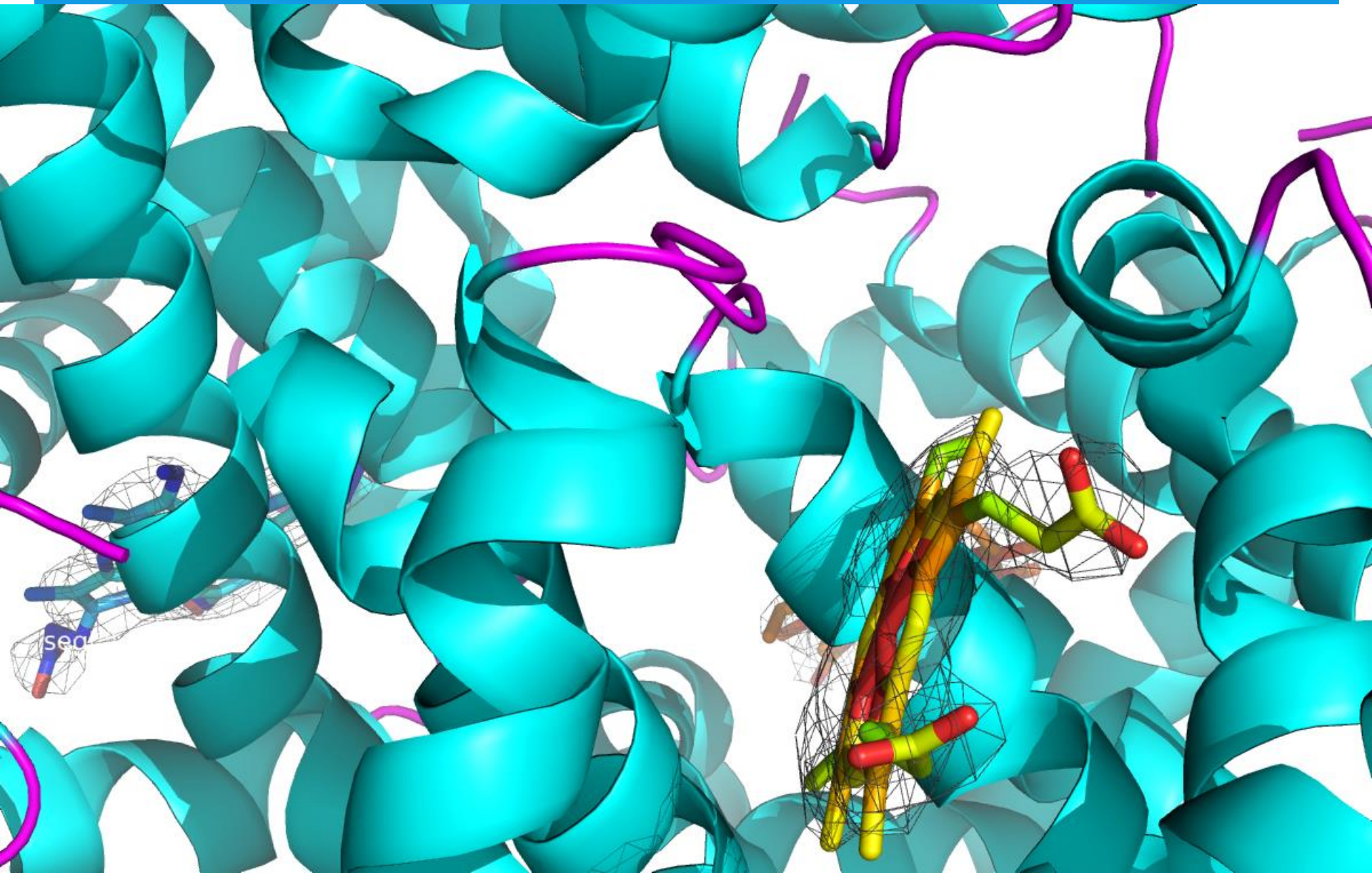

Electron-density map generation for 1faw
Map format : O
Type : 2mFo-DFc
Generate map
e: this may take a few seconds, or many minutes, depending on the size of your map.)

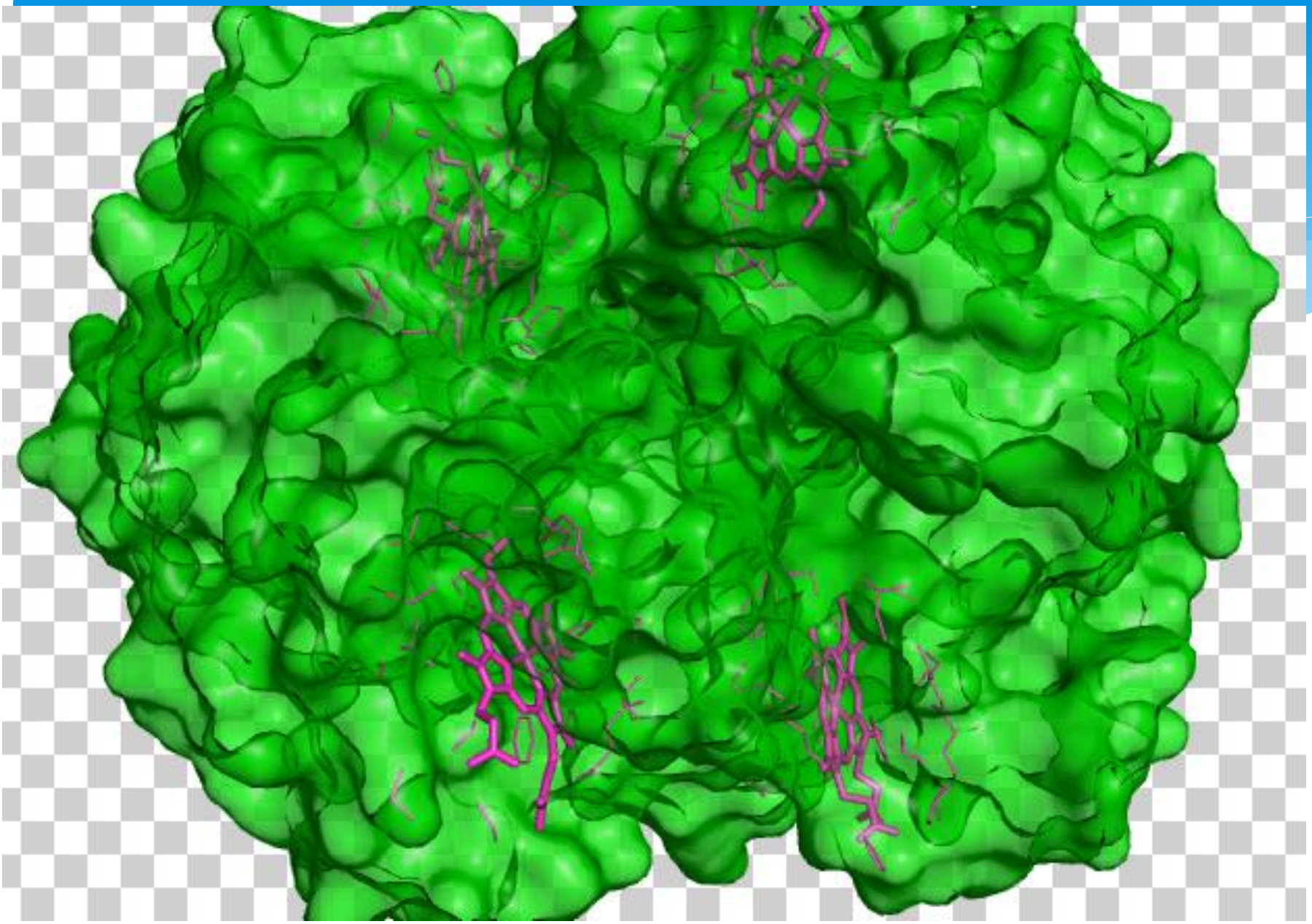












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3、pymowiki，http://www.pymolwiki.org/index.php/Main_Page

* 谢谢！！！