Intermediate PyMOL

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115 PUBLICATIONS **8,883** CITATIONS

SEE PROFILE

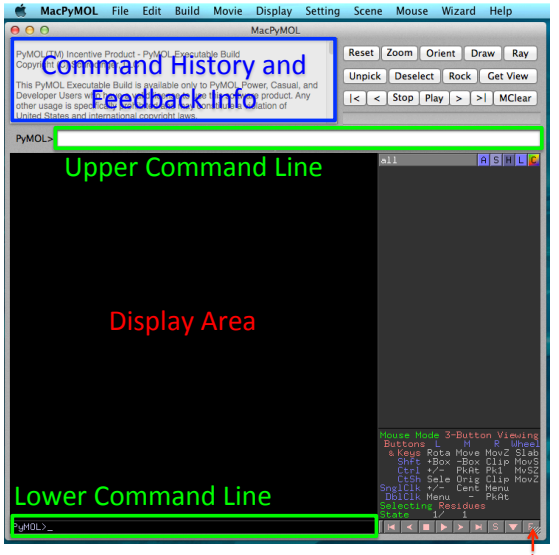
PyMOL: Intermediate

Using the command line
Keeping a command log
Commands, Selections and Settings
Defining default settings
Writing and executing simple scripts

The PyMOL Interface: Command Line (CL)

Use **up and down arrow** to scroll through command history

<ESC> toggles display of feedback text in the display area (useful when working in full-screen mode)



General Command Syntax

command parameter1[, parameter2[, parameter3]]

parameter1 is always required

square brackets denote optional Parameters

<TAB>
In the empty command line list of all commands recognized by the current version of PyMOL

c<TAB>
list of all commands that start with c

command ? (e.g. show ?)
Usage: show [representation [, selection]]

help command (e.g. help show)
DESCRIPTION
"show" turns on representations for objects and selections.
... With no arguments, "show" alone turns on lines for all bonds and nonbonded for all atoms in all molecular objects.

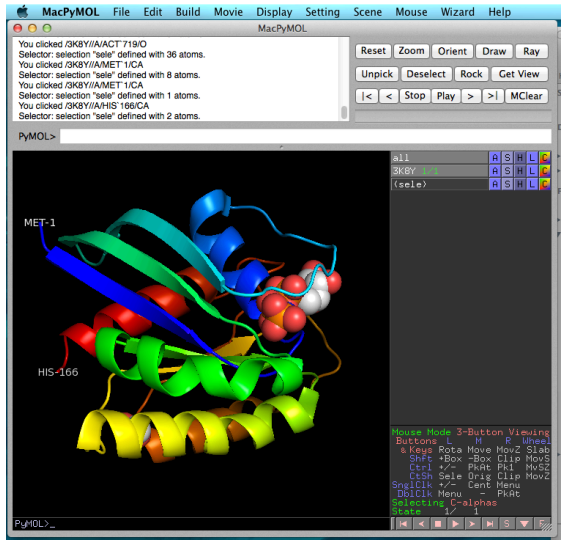
Combining Different Representations: GUI

open file 3K8Y.pdb with PyMOL

Object Menu:
3K8Y: Hide: everything
3K8Y: Show: cartoon
3K8Y: C: spectrum: rainbow */CA
3K8Y: Show: organic : spheres
select these by left click,
sele: C: by element : CHNOS
select C-alpha atoms at either end of the protein chain
sele: L: residues

rotate so that both ends of the chain are clearly visible

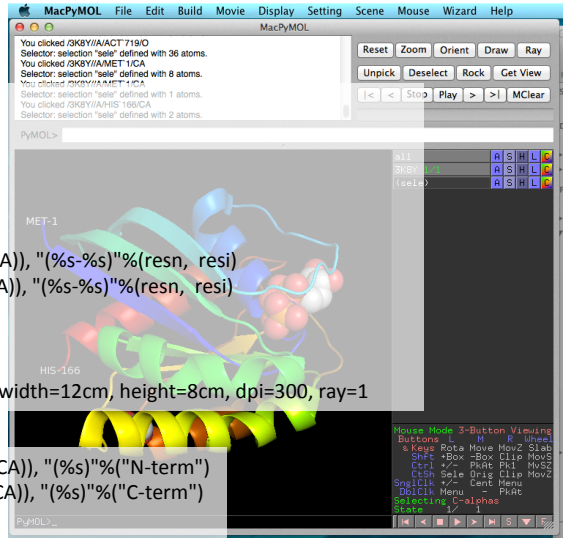
For printing:
Display: Background: white
click on the "ray" button
File: save image: png: fig1a.png



Combining Different Representations:

Command-line script to do the same:

```
load ~/pymol/pdb/3K8Y.pdb
hide all
show cartoon
util.chainbow polymer
show spheres, organic
util.cbaw organic
label (first (polymer and name CA)), "(%s-%s)"%(resn,  resi)
label (last (polymer and name CA)), "(%s-%s)"%(resn,  resi)
#rotate so that both ends of the
#chain are clearly visible
bg_color white
png ~/pymol/figures/fig1b.png, width=12cm, height=8cm, dpi=300, ray=1
```




```
label (first (polymer and name CA)), "(%s)"%("N-term")
label (last (polymer and name CA)), "(%s)"%("C-term")
set label_size, 30
set label_position,(-1.5,1,1)
```

DEMO, play along

Two Types of Scripts:

PyMOL scripts (extension .pml)**:**

Use only PyMOL commands

Commands are either in PyMOL syntax:
cartoon type, (selection)
or PyMOL API syntax:
cmd.cartoon(string type, string selection)

Can either be copy-pasted into the command line (whole or in segments) or by
@ path/scriptname.pml
and are executed immediately

This course deals only with .pml scripts

Python scripts (extension .py)

Use the **Python programming language** and can access functionalities of Python libraries (NumPy, SciPy, ChemPy, cctbx, OpenBabel …) and interact with external command-line driven programs, e.g. APBS, Caver, etc..

Always contain at least this line near top:
from pymol import cmd
additional similar lines indicate other dependencies, e.g.
from cctbx import sgtbx, uctbx
Commands only in the pymol API syntax:
cmd.cartoon(string type, string selection)

PlugIns are installed through the **PlugIn manager** or are imported by
run path/scriptname.pml
They introduce new commands defined by **cmd.extend**("cmd_name", python_function) that can be accessed through the command line or in some cases from the GUI.

PyMOL command line

More than 300 different commands in PyMOL
Scripts and PlugIns further expand the repertoire
More than ~~700~~ **1400** different setting variables modify the effects of these commands

Only a fraction of these can be accessed through the GUI

Use of the command line allows:
- much better **control of atom selections**
- access to **all commands** and their **parameters**
- **keeping a log** of applied commands and parameters
- **command sequences can be prepared as a text file** (script) and copied to the command line or called by other scripts
- adaptation and **re-use of scripts**
- automation

Nobody knows all these commands by heart

Always keep the PyMOL Wiki at hand!

http://pymolwiki.org/index.php/Main_Page

Google PyMOL and <command> to find things

The PyMOL Interface:

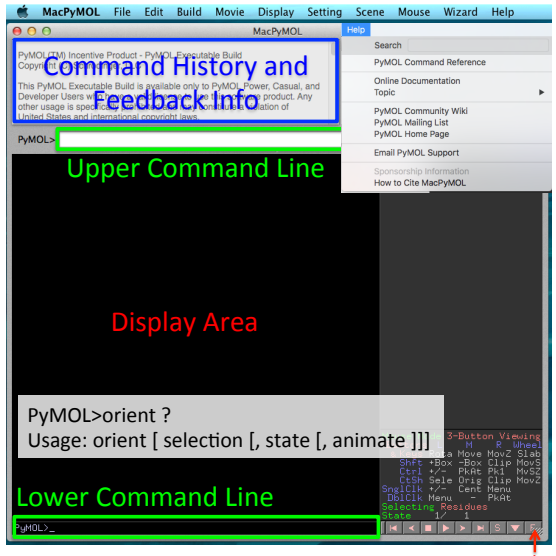
Enter **<TAB> in empty CL** for a list of all commands

<TAB> in non-empty CL: autocompletiton
e.g. “ori”<TAB> orient, origin

help <command> lists full information on that command

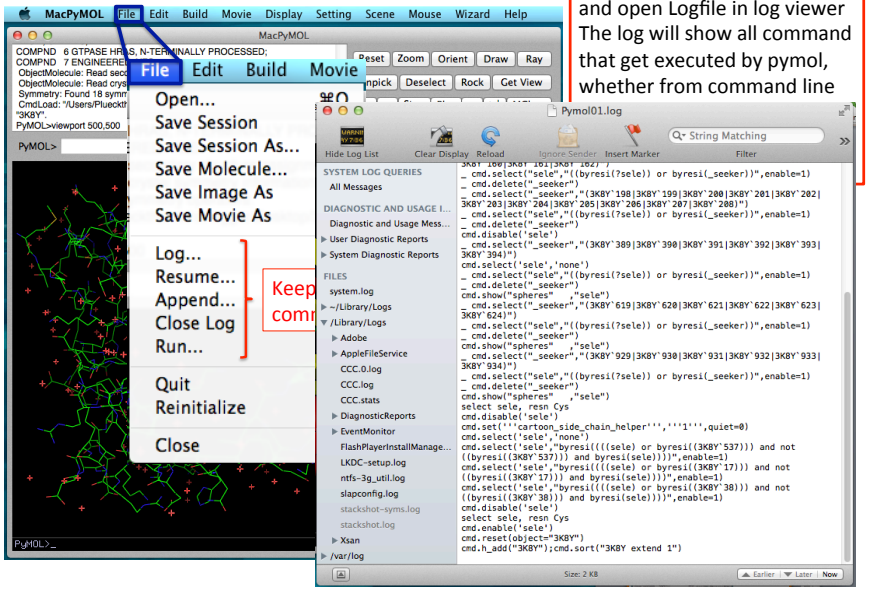
<command> ? to get a list of parameters

<ESC> toggles display of feedback text in the display area (useful when working in full-screen mode)



Keep a Log

Pymol Tricks
After opening Pymol, save log and open Logfile in log viewer
The log will show all command that get executed by pymol, whether from command line



Example

DEMO, play along

load filename [, object]
hide [representation [, selection]]
show [representation [, selection]]

Command:	Effect:
load ~/pymol/pdb/3K8Y.pdb	loads structure 3K8Y.pdb from folder pdb
	4K8Y is shown in “lines” representation
hide	nothing displayed
show cartoon, 3K8Y	4K8Y is shown in cartoon representation
show spheres, organic	ligands GNP and ACT are shown as spheres
hide spheres, resn ACT	ligand ACT is no longer visible
show surface, polymer	protein is shown in surface representation
#now use the mouse to orient the molecule into a pleasing view	

color color [, selection]
png filename [, width [, height [, dpi [, ray]]]]
save filename [, selection [, state [, format]]]

Command:	Effect:
color white, polymer	the color of the protein is changed to white
png ~/pymol/figures/fig1a.png	save image to folder “figures”
hide surface, polymer	the surface is no longer shown, we can see that the cartoon representation also changed color, although it was not visible.
png ~/pymol/figures/fig1b.png	save image to folder “figures” size and resolution are as in the display window
save ~/pymol/fig1a.pse	save the PyMOL session to pymol folder

Advanced Coloring: util.cba

color atoms by atom type: Oxygen red, nitrogen blue, sulfur yellow, hydrogen white, … the color of the carbon atom can be varied

util.cbax selection
util.cnc selection

util.cba colors atoms by atom type, carbon atoms by the color defined by the last letter in the command

util.cnc colors atoms by atom type, but does not alter the color of the carbon atoms

command	carbon color
util.cba**g**	green
util.cba**c**	cyan
util.cba**m**	light magenta
util.cba**y**	yellow
util.cba**s**	salmon
util.cba**w**	white/grey
util.cba**b**	slate
util.cba**o**	bright orange
util.cba**p**	purple
util.cba**k**	pink

util.chainbow object

colors each chain in the object in a rainbow of colors, from Nterm:blue to Cterm: red

util.cbc [object]

colors each chain in a different color

util.cbss("object", "helixcolor", "sheetcolor", "coilcolor")

colors object by secondary structure, if the secondary structure of the object is poorly defined, use command **dss selection** to re-assign secondary structure

Defining your own colors

The color names used by pymol are documented here:
http://www.pymolwiki.org/index.php/Color_Values

You can list the colors used in a selection by this command:

iterate all, print color

You can define your own color names and associated colors by their RGB values

set_color dblue, [0.05 , 0.19 , 0.57] values between 0 and 1
set_color dblue, [13 ,48 , 146] values between 0 and 255

(Or: select menu settings/color, enter a new color name in the name field and adjust the colors with the sliders. This can also be used to adjust the colors used for different elements. However, if you write a script, you can reproduce your color scheme across different PyMol sessions)

Read the PyMOL wiki on the "spectrum" command to see how you can generate and apply color gradients

Write the Command Sequence to a Text File

On the Mac, TextWrangler is a good free text editor
http://www.barebones.com/products/textwrangler/

```
load ~/pymol/pdb/3K8Y.pdb
hide all
show cartoon, 3K8Y
show spheres, resn GNP
show surface, polymer
color white, polymer
bg_color white
ray
png ~/pymol/figures/fig1c.png
hide surface, polymer
ray
png ~/pymol/figures/fig1d.png
save ~/pymol/fig1b.pse
```

Save as plain text file as
~/pymol/pml_scripts/MyScript1.pml

Running your script

Re-initialize or restart PyMOL and type:

@~/pymol/pml_scripts/MyScript1.pml

Were the two figures and the PyMOL file saved to your pymol folder?

Congratulations!
You've successfully generated and executed a functioning PyMOL script.

Setting the File Path

To keep PyMOL-related data together, we have placed the "pymol" data folder in the home directory, and within this folder, subfolders called "pdb", "figures", "movies" and "pml_scripts".

Find the file path to your home directory (~/)

- this is where saved files are stored by default
- this is where PyMOL is looking for files to load

On my MacBook, this would be /Users/ahonegger
Under Windows, this would be something like …

To set the PyMOL default path to the pymol folder, type in the command line:

cd ~/pymol

.pymolrc

If a PyMOL command file named "pymolrc" (visible) or ".pymolrc" (invisible) exists in your home directory, PyMOL will excute this file on start-up.

This is a convenient way to have Pymol always open with your preferred settings, e.g. default path, viewport size, background color, parameters modifying the representation, illumination etc.

Files ending on **.pml** or without suffix will be parsed as **PyMOL command files**.

Files ending on **.py** (or .pym) will be parsed as **python command files**.

If neither extension is used, PyMOL will judge based on the content of the file.

Now we only need to specify the local path:

```
load pdb/3K8Y.pdb
hide all
show cartoon, 3K8Y
show spheres, resn GNP
show surface, polymer
color white, polymer
bg_color white
ray
png figures/fig1c.png
hide surface, polymer
ray
png figures/fig1d.png
save fig1b.pse
```

Delete all instances of ~/pymol/ from the script file and run the script in PyMOL

reinitialize
@pml_scripts/MyScript1.pml

Selections

Greatly expand on the selection capabilities of the GUI

explicit selections:

select (expression)
produces a **temporary selection object** named "**sele**"

select sele, (expression)
produces a **temporary selection object** named "**sele**"

select name, (expression)
produces a **named selection object** for further use

implicit selections:

color red, (expression)
colors the residues specified by the expression red without creating a selection object

show cartoon, (expression)
displays the specified residues as cartoon, no selection object

Single word selectors

Single-Word Selector	Abbrev. Selector	Description
all	*	All atoms currently loaded into PyMOL
none		No atoms (empty selection)
hydro	h.	All hydrogen atoms currently loaded into PyMOL
hetatm	het	All atoms loaded from Protein Data Bank HETATM records
polymer	pol.	All atoms on the polymer (not het). Protein, DNA or RNA
visible	v.	All atoms in enabled objects with at least one visible representation
enabled		All atoms in enabled objects
backbone	bb.	Polymer backbone atoms
sidechain	sc.	Polymer non-backbone atoms
donors	don.	All potential hydrogen bond donors
acceptors	acc.	All potential hydrogen bond acceptors
solvent	sol.	All water molecules
organic	org.	All atoms in non-polymer organic compounds (e.g. ligands, buffers).
inorganic	ino.	All non-polymer inorganic atoms/ions.
bonded		All atoms making at least one bond
metals		All metal atoms/cations
guide		All protein CA and nucleic acid C4*/C4'
present	pr.	All atoms with defined coordinates in the current state (used e.g in creating movies)

Propery Selectors: Selecting Atoms, Residues, Chains

One word Selector	Abbrev. Selector	Description
element	e.	**chemical element**, e.g. C, N, O, H, …, Ca, Fe, Mg
name	n.	**atom name**, eg. select mainchain, n. N+CA+C+O
resn	r.	**residue name**, e.g. select neg, r. Glu+Asp
resi	i.	**residue number** e.g. select domain1, i. 33-126 if you have a negative residue number, a "\" is needed, e.g. select Ntag, i. \-5+\-4+\-3+\-2+\-1
alt	alt	**alternative conformation**, e.g. "", a, b, c
chain	c.	**chain identifier**
ss	ss	**secondary structure**, e.g. select allSTR, h+s+l+""
id	id	**atom number**
b	b	**b-factor value**, e.g. select fuzzy, b > 10
q	q	**occupancy**, e.g. select lowOccupancy, q < 0.5

Selection Macros

Shorthand for selecting specific parts of a protein or nucleic acid chain
Instead of
select name, pept1 and segi a1 and chain b and resi 142 and name ca
you can type
select name, /pept1/lig/b/142/ca
also for wildcards, ranges, multiple selections
select name, /pept1//b/142-163/n+ca+c+o
select name, /pept1//A/L* selects Leu and Lys

If you click on an atom in PyMol, the feedback window shows the selection in this form:

You clicked /3K8Y//A/GLU`3/CA
Selector: selection "sele" defined with 9 atoms.

Selection Macros

You need only the relevant part of the chain
e.g.
show spheres, CYS/CA
shows the Calpha atoms of all cysteins as spheres,
show spheres, CYS/
shows all atoms in Cystein residues as spheres

beginning with a slash:
/object-name/segi-identifier/chain-identifier/resi-identifier/name-identifier
/object-name/segi-identifier/chain-identifier/resi-identifier
/object-name/segi-identifier/chain-identifier
/object-name/segi-identifier
/object-name

or not beginning with a slash:
resi-identifier/name-identifier
chain-identifier/resi-identifier/name-identifier
segi-identifier/chain-identifier/resi-identifier/name-identifier
object-name/segi-identifier/chain-identifier/resi-identifier/name-identifier

Selection-Algebra

Selections can be combined by logical operators:

not s1	!s1	all atoms except those in selection s1
s1 and s2	s1 & s2	intersection, atoms that are both in s1 and in s2
s1 or s2	s1 | s2	union, atoms that are either part of s1 or s2

Expansion of selections

byres s1	br. s1	expands sel. from atoms to residues
bymolecule s1	bm. s1	expands sel. to molecule
bychain s1	bc. s1	expands sel. to chain
byobject s1	bo. s1	expands sel. to object
bycell s1		expands sel. to unit cell
neighbor s1	nbr. s1	directly bonded to s1, excl. s1
bound_to s1	bto. s1	directly bonded to s1, incl. s1
first, last		first or last atom in selection

Selection: Distance operators

select s3, s1 within 5.0 of s2
all atoms in s1 that are no farther than 5.0 Å from atoms in s2

select s3, s1 near_to 5.0 of s2 ((s1 within 5.0 of s2) and not s2))
all atoms in s1 that are no farther than 5.0 Å from a atoms in s2, excludes s2

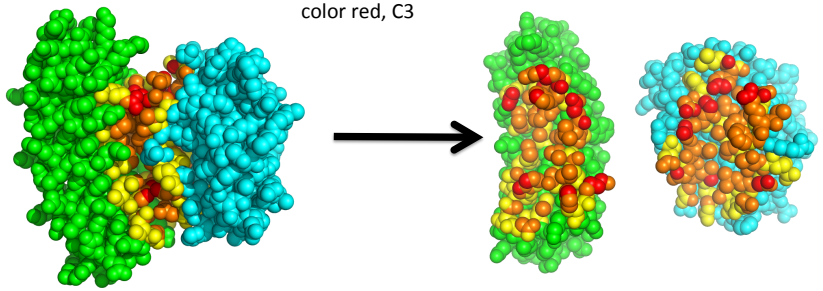
select s3, s1 beyond 5.0 of s2 ((s1 and not (s1 within 5.0 of s2))
all atoms in s1 that are farther than 5.0 Å away from atoms in s2

select s3, s2 around 5.0 ((all within 5.0 of s2) and not s2))
all atoms within 5.0 Å of s2, excluding s2

select s3, s2 expand 5.0 (all within 5.0 of s2)
all atoms in s2 or within 5.0 Å of s2

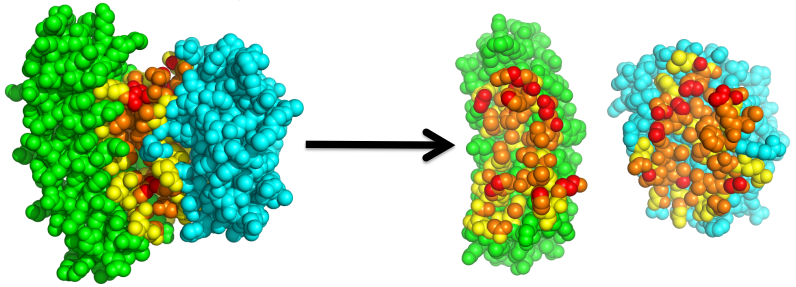
Example: Determine Contact Residues

```
# load complex and separate its components
load pdb/S4K5B_B-C.pdb, Cplx
extract darp, Cplx and chain B
extract lig, Cplx and chain C
delete Cplx

color green, darp
color cyan, lig
select C3, (darp within 3.6 of lig) or (lig within 3.6 of darp)
select C2, (darp within 5.0 of lig) or (lig within 5.0 of darp)
select C1, br. C2
color yellow, C1
color orange, C2
color red, C3
```



Listing Contact Residues

```
select C3, (darp within 3.6 of lig) or (lig within 3.6 of darp)
select C2, (darp within 5.0 of lig) or (lig within 5.0 of darp)
select C1, br. C2
```



list contact atoms

```
list=[]
iterate (C2),list.append((chain,resi,resn,name))
print list
```

list contact residues

```
list=[]
iterate (C1 and name CA),list.append((chain,resi,resn))
print list
```

Setting the Orientation of a Molecule in a Script

get_view [output [, quiet]]
set_view view

Open fig1a.pse, rotate structure into a nice orientation and type:

get_view

from the feedback window, copy-paste this to your script:

```
### cut below here and paste into script ###
set_view (\
     0.2857,   -0.0944,    0.9536,\
     0.0625,    0.9948,    0.0797,\
    -0.9562,    0.0368,    0.2902,\
     0.0000,    0.0000, -128.3235,\
   -16.5101,   63.8420,  -76.8616,\
   103.0045, 153.6425,  -20.0000 )
### cut above here and paste into script ###
```

Rotation Matrix

Origin in Camera Space

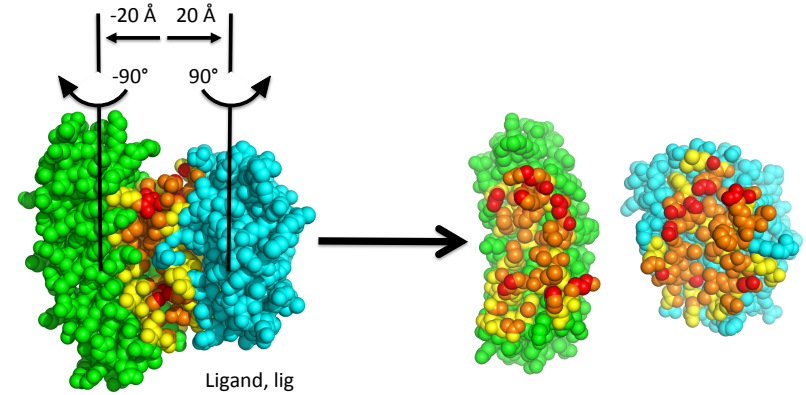
Origin in Coordinate Space

Back & Front Clipping Planes, Perspective

Defined Transformations

reset [object]
turn axis, angle
move axis, distance
orient object-or-selection [, state]
center [selection [, state [, origin [, animate]]]]
zoom [selection [,buffer [, state [, complete]]]]
clip mode, distance [, selection [, state]]
origin selection [, object [,position, [, state]]]
translate vector [,selection [,state [,camera [,object]]]]
rotate axis, angle [,selection [,state [,camera [,object [,origin]]]]]

Example: Looking at a Binding Interface



rotate y, -90, darp
translate [-20,0,0], darp
rotate y, 90, lig
translate [20,0,0], lig

Measuring Distances

distance [name [, selection1 [, selection2 [, cutoff [, mode]]]]]

name	string: name of the distance object to create
selection1	string: first atom selection
selection2	string: second atom selection
cutoff	float: longest distance to show
mode	0: all interatomic distances
	1: only bond distances
	2: only show polar contact distances
	3: like mode=0, but use distance_exclusion setting
	4: distance between centroids (*new in 1.8.2*)

Simple H-bond detection:

dist name, sele1, sele2, mode=2

dependent on parameters:

```
set h_bond_cutoff_center, 3.6
set h_bond_cutoff_edge, 3.2
```

More sophisticated H-Bond detection

load target.pdb,prot
load docked_ligs.sdf,lig

 # add hydrogens to protein

h_add prot

select don, (elem n,o **and** (neighbor hydro))
select acc, (elem o **or** (elem n **and not** (neighbor hydro)))
dist HBA, (lig **and** acc),(prot **and** don), 3.2
dist HBD, (lig **and** don),(prot **and** acc), 3.2
delete don
delete acc
hide (hydro)

hide labels,HBA
hide labels,HBD

Get information

get	get_extent	get_title
get_angle	get_position	get_type
get_area	get_property	get_version
get_bond	get_property_list	get_view
get_chains	get_renderer	get_viewport
get_dihedral	get_sasa_relative	
get_distance	get_symmetry	

get_angle [atom1 [, atom2 [, atom3 [, state [, quiet]]]]]

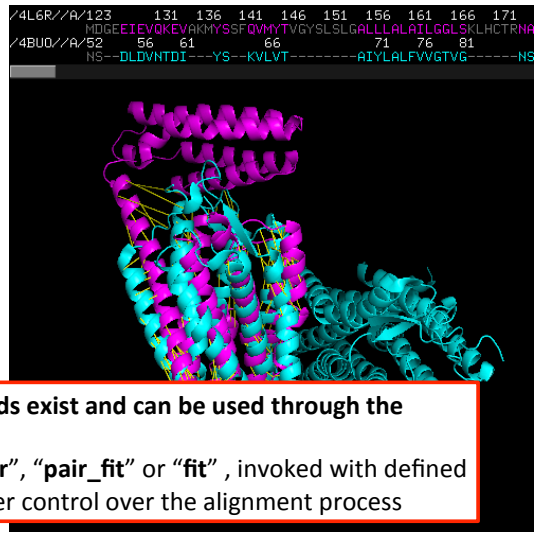
get_dihedral [atom1 [, atom2 [, atom3 [, atom4 [, state [, quiet]]]]]]
also: **phi_psi [selection [, quiet]]** to get main chain torsion angles

get_area [selection [, state [, load_b [, quiet]]]] to get the surface area of an selection

get_sasa_relative [selection [, state [, vis [, var]]]] to get per-residue relative accessibility

If align does not give reasonable results

In this alignment of the glucagon receptor (4L6R) to the rat neuro-tensin receptor 1 (4BUO) the sequence similarity was too low for a good sequence alignment, resulting in a bad residue pairing for the structural alignment



Other alignment methods exist and can be used through the command line:
"**cealign**", "**align**", "**super**", "**pair_fit**" or "**fit**" , invoked with defined atom selections for better control over the alignment process

Least Squares Superposition of two Structures

PyMOL offers several different commands for sequence-based and sequence independent structural alignments:

fit, intra_fit, pair_fit, super, align, cealign, rms, rms_cur, intra_rms, intra_rms_cur, extra_fit.py, super_all.py, align_all.py, tmalign.py

They differ in how they determine the atom pairs included in the fit, and how they treat outliers (parts of the molecule that do not fit well).

Each method will return an rmsd value (root mean squares deviation)
However, the values you get depend on the method used!

rmsd values are meaningless
if you do not indicate exactly what method and what parameters you used!!!

fit mobile, target [, mobile_state [, target_state [, quiet [, matchmaker [, cutoff [, cycles [, object]]]]]]]

Fit superimposes the model in the first selection on to the model in the second selection. Only matching atoms in both selections will be used for the fit.

- mobile = string: atom selection
- target = string: atom selection
- mobile_state = integer: object state {default=0, all states)
- target_state = integer: object state {default=0, all states)
- matchmaker = integer: how to match atom pairs {default: 0}
- -1: assume that atoms are stored in the identical order
- 0/1: match based on all atom identifiers (segi,chain,resn,resi,name,alt)
- 2: match based on ID
- 3: match based on rank
- 4: match based on index (same as -1 ?)
- cutoff = float: outlier rejection cutoff (only if cycles>0) {default: 2.0}
- cycles = integer: number of cycles in outlier rejection refinement {default: 0}
- object = string: name of alignment object to create {default: None}

Fit, Rms, Rms_Cur are finicky and only work when all atom identifiers match: segi, chain, resn, name, alt. If they don't, you'll need to use the alter command to change the identifiers to make them match -- typically that means clearing out the SEGI field, renaming chains, and sometimes renumbering.

pair_fit (selection), (selection), [(selection), (selection) [...]]

Pair_Fit fits **a set of atom pairs between two models**. Each atom in each pair must be specified individually, which can be tedious to enter manually. Script files are recommended when using this command. So long as the atoms are stored in PyMOL with the same order internally, you can provide just two selections. Otherwise, you may need to specify each pair of atoms separately, two by two, as additional arguments to pair_fit.

Useful if you want to fit, e.g. the ring systems of ligands.

Examples:
 # superimpose protA residues 10-25 and 33-46 to protB residues 22-37 and 41-54:
pair_fit protA///10-25+33-46/CA, protB///22-37+41-54/CA

 # superimpose ligA atoms C1, C2, and C4 to ligB atoms C8, C4, and C10, respectively:
pair_fit ligA////C1, ligB////C8, ligA////C2, ligB////C4, ligA////C3, ligB////C10

intra_fit (selection),state

intra_fit fits **all states of an object** (e.g. NMR) to an atom selection in the specified state. It returns the rms values to python as an array.

extra_fit [selection [, reference [, method]]]

extra_fit aligns **multiple objects** to one reference object. It can use any of PyMOL's pairwise alignment methods (align, super, cealign, fit...). More precisely it can use any function which takes arguments mobile and target, so it will for example also work with tmalign.
Additional keyword arguments are passed to the used method, so you can for example adjust outlier cutoff or create an alignment object.

rms, rms_cur, intra_rms, Intra_rms_cur
compute a RMS fit between two atom selections, but **do not transform the models after performing the fit.**

align mobile, target [, cutoff [, cycles [, gap [, extend [, max_gap [, object [, matrix [, mobile_state [, target_state [, quiet [, max_skip [, transform [, reset]]]]]]]]]]]]

align performs a **sequence alignment followed by a structural superposition**, and then carries out zero or more cycles of refinement in order to reject structural outliers found during the fit. align does a good job on proteins with decent sequence similarity (identity >30%). For comparing proteins with lower sequence identity, the super and cealign commands perform better.

cealign target, mobile [, target_state [, mobile_state [, quiet [, guide [, d0 [, d1 [, window [, gap_max [, transform [, object]]]]]]]]]]

cealign aligns two proteins using the CE algorithm. It is **very robust for proteins with little to no sequence similarity** (twilight zone). For proteins with decent structural similarity, the super command is preferred and with decent sequence similarity, the align command is preferred, because these commands are much faster than cealign.

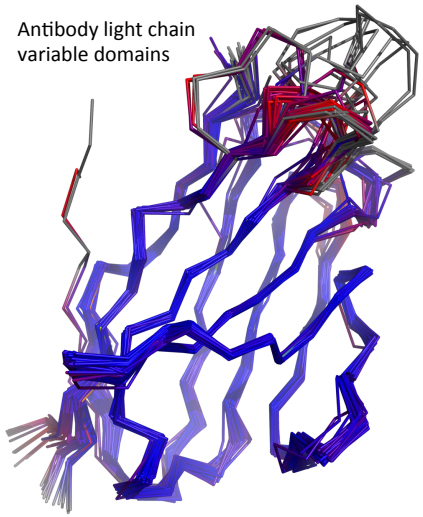
super mobile, target [, cutoff [, cycles [, gap [, extend [, max_gap [, object [, matrix [, mobile_state [, target_state [, quiet [, max_skip [, transform [, reset [, seq [, radius [, scale [, base [, coord [, expect [, window [, ante]]]]]]]]]]]]]]]]]]]]]]

super aligns two selections. It does a **sequence-independent** (unlike align) **structure-based dynamic programming alignment** followed by a series of refinement cycles intended to improve the fit by eliminating pairing with high relative variability (just like align). super is more robust than align for proteins with low sequence similarity.

Python Scripts offer additional Functionalities:

run py_scripts/colorbyrmsd.py

colorbyrmsd 4d3c, 2x7l
colorbyrmsd 4ht1, 2x7l
colorbyrmsd 5ds8, 2x7l
colorbyrmsd 5dtf, 2x7l
colorbyrmsd 5dub, 2x7l
colorbyrmsd 4ma3, 2x7l
colorbyrmsd 4o4y, 2x7l
colorbyrmsd 4jo3, 2x7l
colorbyrmsd 4jo4, 2x7l
colorbyrmsd 4o51, 2x7l
colorbyrmsd 4hbc, 2x7l
colorbyrmsd 5i8o, 2x7l
colorbyrmsd 4jo1, 2x7l
…
hide all
show ribbon



PyMOL Settings

Style and quality of PyMOL representations are controlled by more than ~~600~~ 1400 different settings …

General Syntax for Settings

set name [, value [, selection [, state [, updates [, log [, quiet]]]]]]

"set" is a command

the command "set" assigns a value to named variable

dependent on the setting, one or more additional parameters are required
for boolean variables (on/off or 0/1), no parameter means "on"
some settings are global (default), others can be applied to a selection.

set<TAB>
parser: matching commands:

set	set_dihedral	set_property
set_atom_property	set_geometry	set_symmetry
set_bond	set_key	set_title
set_color	set_name	set_view

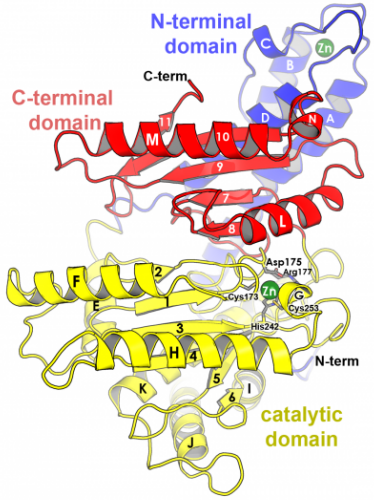
set <TAB>
list of all settings set by "set" recognized by the current version of PyMOL

set ?
Usage: set name [, value [, selection [, state [, updates [, log [, quiet]]]]]]

Settings define the Style of the Figure

```
set antialias = 1

set ambient=0.3
set direct=1.0

set ray_trace_mode=1

set stick_radius = 0.2
set cartoon_tube_radius, 0.2
set cartoon_fancy_helices=1
set cartoon_cylindrical_helices=0
set cartoon_flat_sheets = 1.0
set cartoon_smooth_loops = 0
set cartoon_highlight_color =grey50

bg_color white

set_color maarine=  [0.3, 0.8, 1.0]
set_color graay=[0.8,0.8,0.8]
set_color greeen=[0.0,0.5,0.0]
```

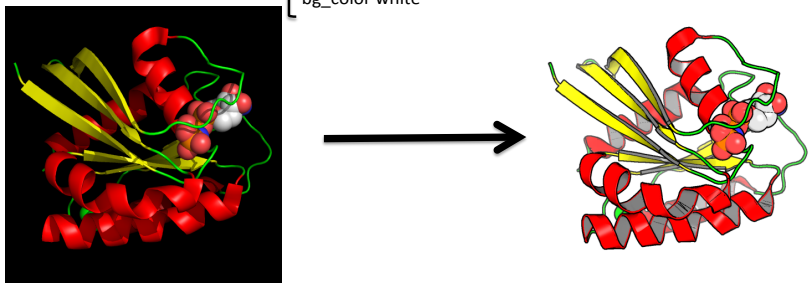
copy



PLoS_script1.pml

paste

```
set antialias = 1
set ambient=0.3
set direct=1.0

set ray_trace_mode=1

set stick_radius = 0.2
set cartoon_tube_radius, 0.2
set cartoon_fancy_helices=1
set cartoon_cylindrical_helices=0
set cartoon_flat_sheets = 1.0
set cartoon_smooth_loops = 0
set cartoon_highlight_color =grey50

bg_color white
```

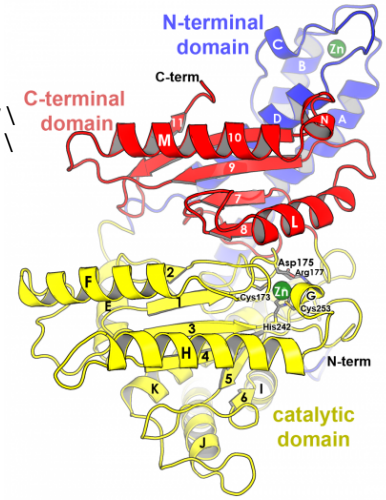


These commands define what's shown

```
load csos3_18o_nobreak.pdb, csos3
hide all
show cartoon
show sticks, (resid 173 or resid 175 or resid 177 \
      or resid 242 or resid 253) and not (name n \
      or name c or name o)
show spheres,  elem ZN
```

and how it's colored

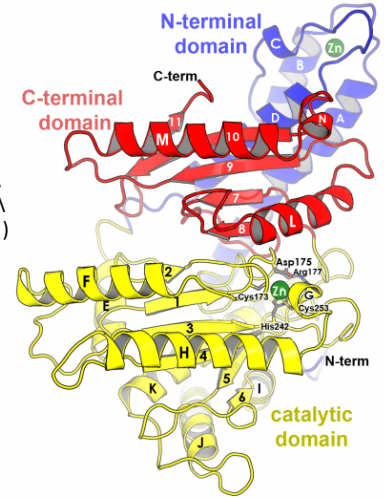
```
color gray50, elem C
color greeen, elem ZN
color blue, resid 38:147 and name ca
color yellow, resid 148:397 and name ca
color red, resid 398:514 and name ca
```



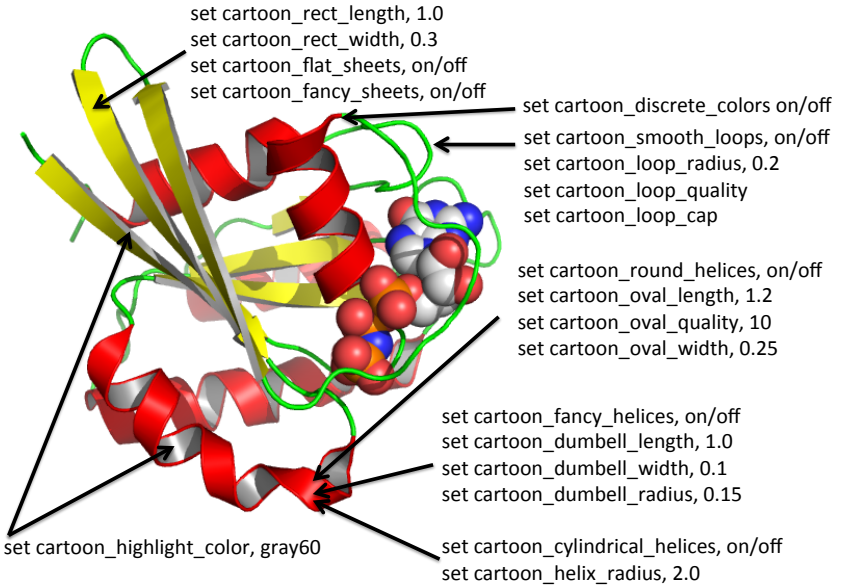
Carbonic anhydrase, CsoS3,
from Halothiobacillus neapolitanus.
(PDB ID 2G13)

These commands define the orientation

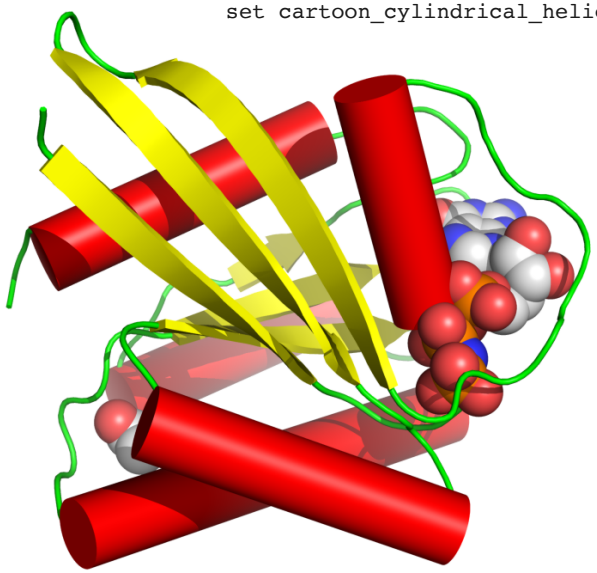
```
set_view (\
    0.091340274,   -0.606698275,    0.789650559,\
   -0.991202235,   -0.131515890,    0.013612081,\
    0.095602803,   -0.783963323,   -0.613382638,\
    0.001799395,    0.001679182, -246.492980957,\
   12.976243019,   41.245639801,   62.928291321,\
  187.538497925,  249.492980957,    0.000000000 )
turn y, 3.5


# and generate the figure
viewport 1200,1500
ray
png csos3-left.png

# labels were added in a generic graphics program
# e.g. Photoshop, Illustrator ...
```



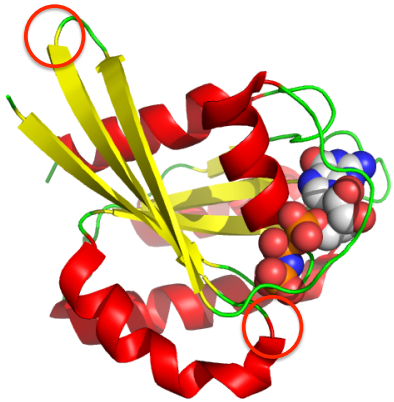
Settings: Cartoon representation



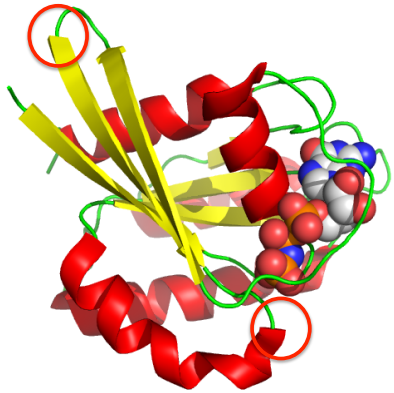
```
set cartoon_cylindrical_helices, on
```



Settings: cartoon_discrete_colors



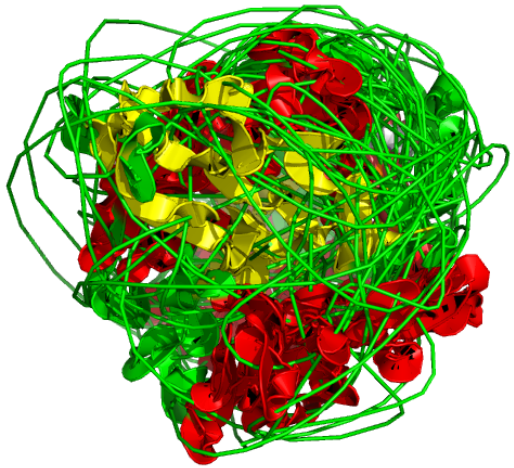
set cartoon_discrete_colors , off



set cartoon_discrete_colors , on

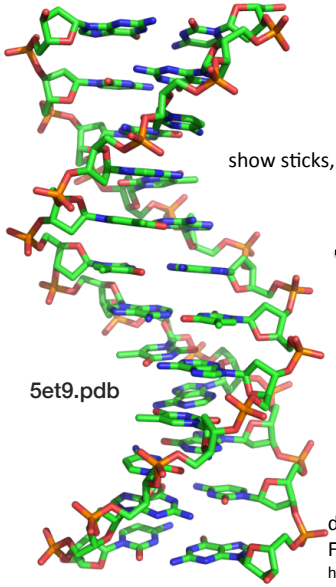
Stops secondary structure colors from bleeding into the coil areas

When things going haywire



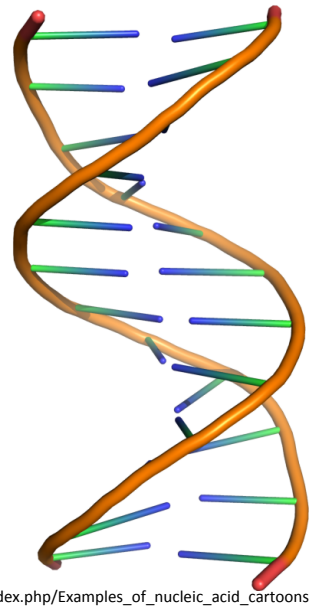
"set cartoon_trace, 1" seems to confuse PyMOL if the structure contains more than just Calpha atoms

Nucleic Acid Cartoons



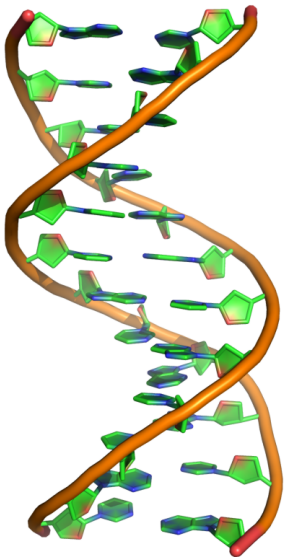
show sticks, 5et9

5et9.pdb

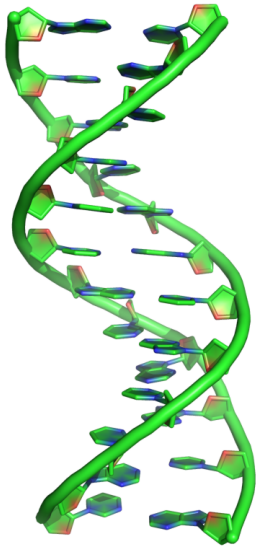


default cartoon view
For other options, see:
http://www.pymolwiki.org/index.php/Examples_of_nucleic_acid_cartoons

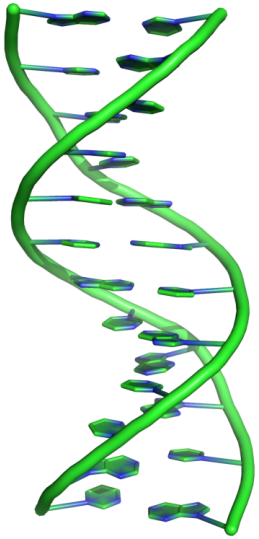
Nucleic Acid Cartoons



set cartoon_ring_mode, 3



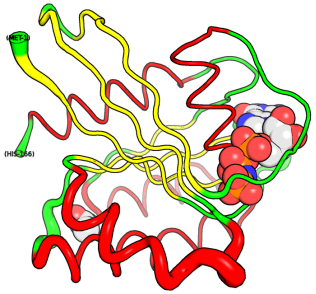
set cartoon_nucleic_acid_mode, 3



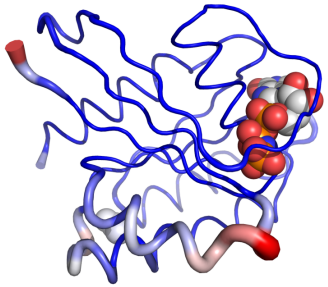
set cartoon_ring_finder,2

cartoon putty

Show which parts of the structure are more flexible in the crystal (b-factor)

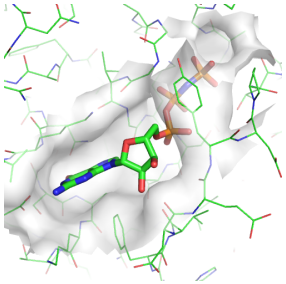


show cartoon
cartoon putty
unset cartoon_smooth_loops
unset cartoon_flat_sheets



spectrum b, blue_white_red, minimum=20, maximum=40
as cartoon
cartoon putty

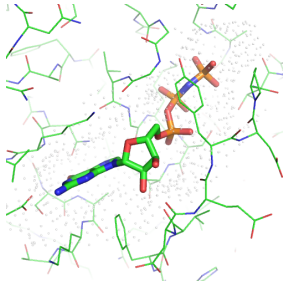
Surface Settings



set surface_type, 0

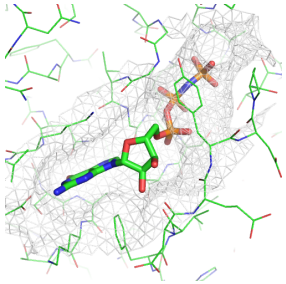
smooth surface, made transparent by

set transparency, 0.5



set surface_type, 1

dot surface

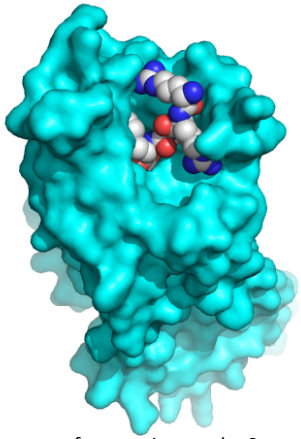


set surface_type, 2

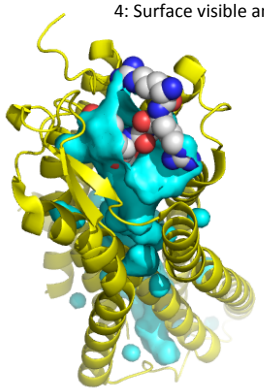
mesh surface

Surface settings

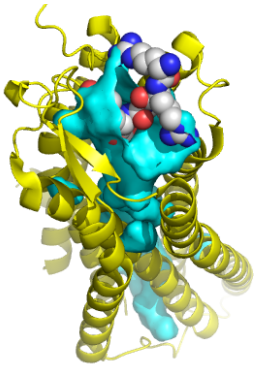
set surface_mode, **int**
0: Default mode, surfacing with respect to flags.
1: Surface everything, including HET and hydrogens
2: Surface only heavy atoms
3: Surface only visible
4: Surface visible and heavy



set surface_cavity_mode, 0

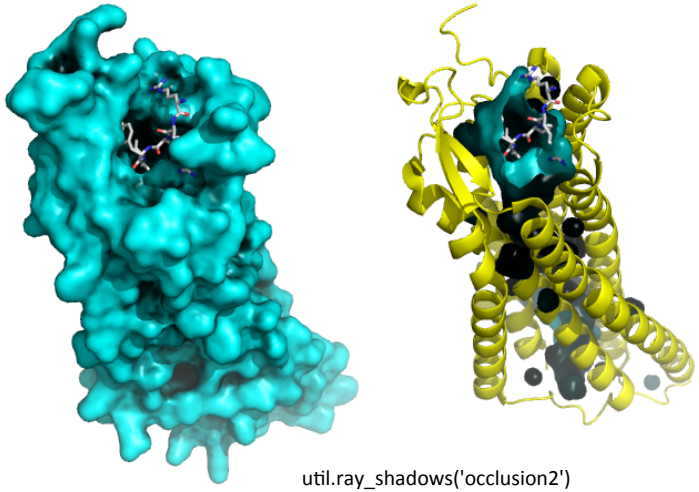


set surface_cavity_mode, 1



set surface_cavity_mode, 2
set surface_cavity_radius, -3
set surface_cavity_cutoff, 7

Shading the Surface



util.ray_shadows('occlusion2')

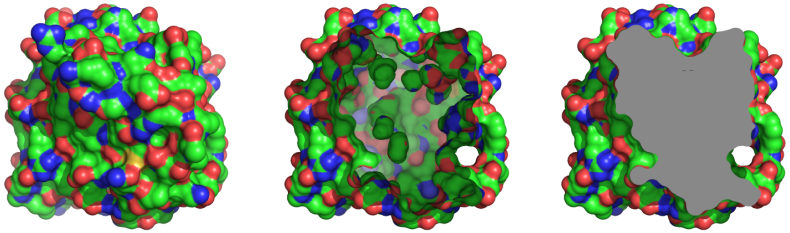
highlights pockets and cavities by depth-dependent shadowing

Showing a solid clipping plane

Pymol Tricks

Normally, if the near clipping plane cuts a surface, the surface is shown as an open shell.

By turning interior lighting off and assigning a fixed color to the interior, in the ray-traced image, the cut appears closed by the clipping plane.

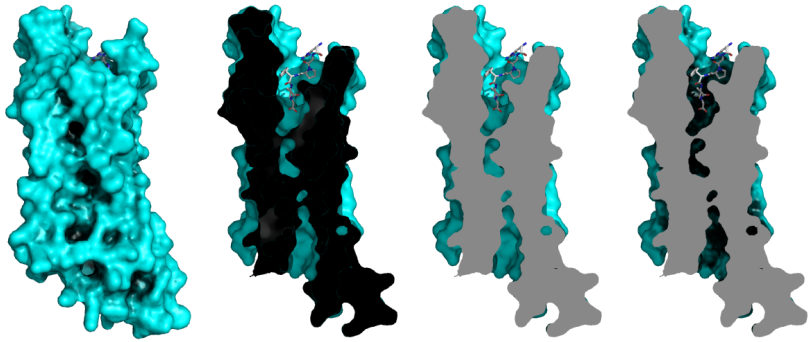


hide all
show surface

clip near, -20

set two_sided_lighting, off
set ray_interior_color, grey70

Solid Clipping Plane



clip near, -30

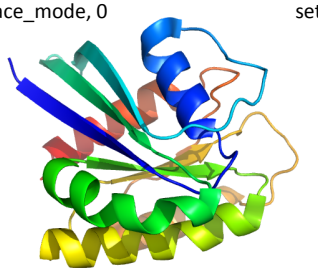
set two_sided_lighting, off
set ray_interior_color, grey70

util.ray_shadows('occlusion2')

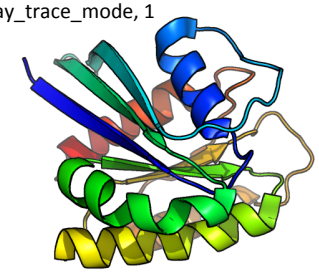
util.ray_shadows('occlusion2')

Ray_trace_mode

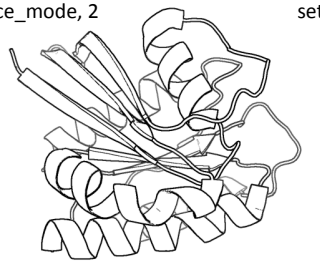
set ray_trace_mode, 0



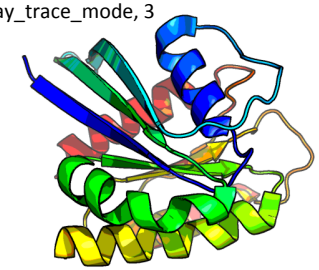
set ray_trace_mode, 1



set ray_trace_mode, 2



set ray_trace_mode, 3



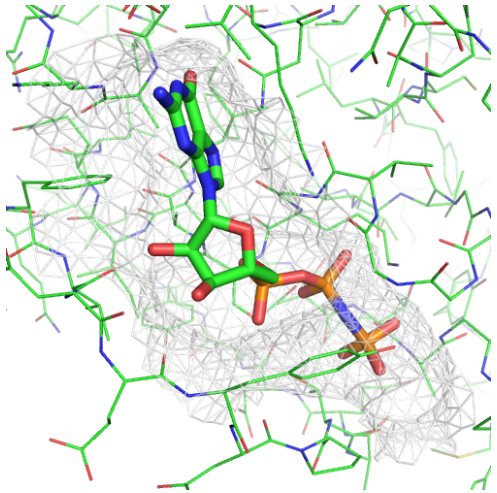
set ray_trace_gain, 0.0 - sets thickness of outline, set ray_trace_disco_factor, 1 to clean up

Examples from the PyMOL Gallery

adapted to 3K8Y

http://www.pymolwiki.org/index.php/Gallery

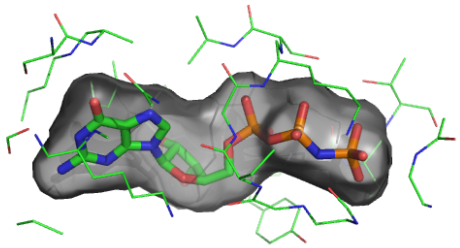
Binding Pocket



@pml_scripts/AHo_BindingPocket.pml

```
#load your molecule, extract prot, lig
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
hide all
show lines, prot
show surface, prot within 8 of lig
show sticks, lig
#coloring, prot & lig in default color
bg_color white
set surface_color, white
#orientation (correct as needed)
orient lig
# special settings for this representation
set surface_carve_cutoff, 4.5
set surface_carve_selection, lig
set surface_carve_normal_cutoff, -0.1
set two_sided_lighting
set transparency, 0.5
set surface_type, 2
unset ray_shadows
#render image and save
ray
png figures/BindingPocket.png
save examples/AHo_BindingPocket.pse
```

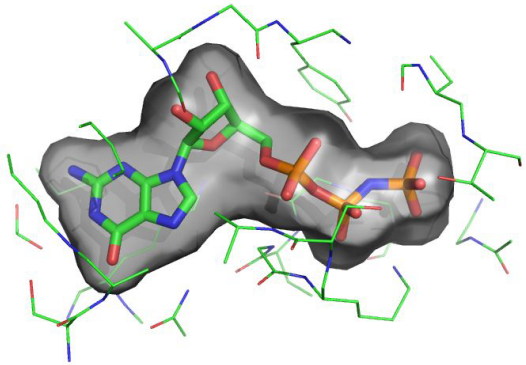
Ray-Normal-Based Transparency



@pml_scripts/AHo_RayNormal.pml

```
#load your molecule, extract prot, lig
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
hide all
show surface, lig
show sticks, lig
show lines, prot within 5 of lig
#coloring
bg_color white
set surface_color, grey
# set the view (correct as needed)
orient lig
# special settings for this representation
set surface_mode, 3
set transparency_mode, 1
set transparency, 0.5
set ray_transparency_oblique
set ray_transparency_oblique_power, 8
set ray_transparency_contrast, 7
#render image and save
ray
png figures/RayNormal.png
save examples/AHo_RayNormal.pse
```

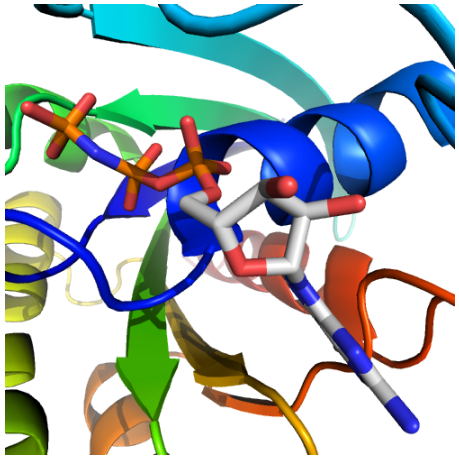
Make a Movie



```
#continued from last slide

# animate
set cache_frames, 1
set ray_trace_frames, 1
mset 1x120
movie.roll 1, 120, 1, x
mplay

save movie as:
as image sequence
or Quicktime movie
```

Get Quicktime Pro 7 from:
http://www.id.uzh.ch/dl/sw/angebote/grafik/QuickTimePro.html

Cool Perspective

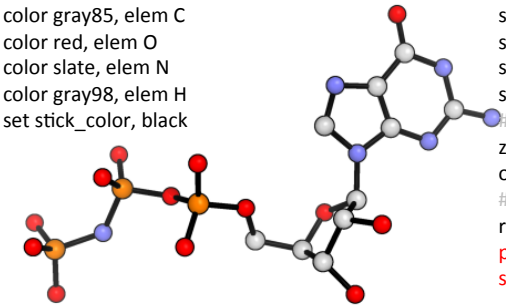


@pml_scripts/AHo_CoolPerspective.pml

```
#load your molecule, extract protein and ligand
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
hide all
show cartoon, prot
show sticks, lig
#coloring
bg_color white
spectrum count, rainbow, prot, byres=1
util.cbaw lig
#correct orientation and zoom factor as needed
zoom lig
# special settings for this representation
set field_of_view, 60
#render image and save
ray
png figures/CoolPerspective.png
save examples/AHo_CoolPerspective.pse
```

Stylized Ball-and-Stick

```
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
hide everything
show sticks, Lig
show spheres, Lig
#coloring
color gray85, elem C
color red, elem O
color slate, elem N
color gray98, elem H
set stick_color, black
# special settings
set stick_radius, .07
set sphere_scale, .18
set sphere_scale, .13, elem H
set bg_rgb=[1, 1, 1]
set stick_quality, 50
set sphere_quality, 4
set ray_trace_mode, 1
set ray_texture, 2
set antialias, 3
set ambient, 0.5
set spec_count, 5
set shininess, 50
set specular, 1
set reflect, .1
set dash_gap, 0
set dash_color, black
set dash_gap, .15
set dash_length, .05
set dash_round_ends, 0
set dash_radius, .05
#orientation
zoom lig
orient lig
#render image and save
ray
png figures/Ball-and-Sticks.png
save examples/AHo_Ball-and-Sticks.pse
```

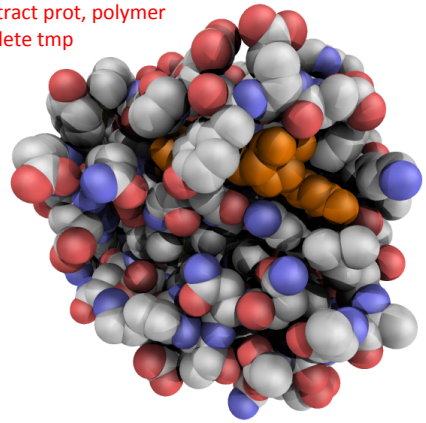


@pml_scripts/AHo_Ball-and-Sticks.pml

QuteMol Style

http://qutemol.sourceforge.net

```
#load your molecule, extract prot, lig
load 3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
```

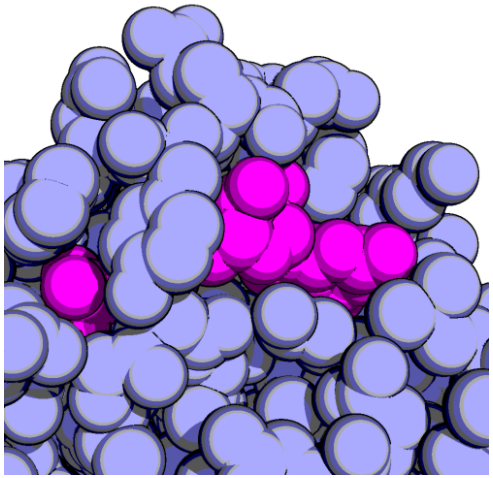


@pml_scripts/AHo_QuteMol.pml

```
# representation
hide all
as spheres
#coloring
bg_color white
set_color oxygen, [1.0,0.4,0.4]
set_color nitrogen, [0.5,0.5,1.0]
util.cbaw
color orange, resn GNP
# special settings for this representation
set light_count, 8
set spec_count, 1
set shininess, 10
set specular, 0.25
set ambient, 0
set direct, 0
set reflect, 1.5
set ray_shadow_decay_factor, 0.1
set ray_shadow_decay_range, 2
unset depth_cue
set field_of_view, 60
#render image and save
ray
png figures/QuteMol.png
save examples/AHo_QuteMol.pse
```

Goodsell-like Representation

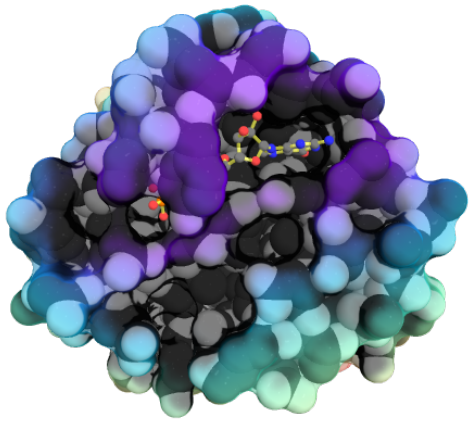
http://www.rcsb.org/pdb/101/motm.do?momID=184



@pml_scripts/AHo_GoodsellLike.pml

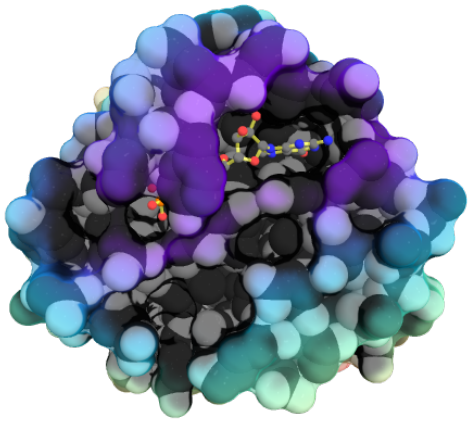
```
#load your molecule, extract prot, lig
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
as spheres
#coloring
bg_color white
color lightblue, prot
color magenta, lig
# set the view (correct as needed)
orient all within 8 of lig
# special settings for this representation
unset specular
set ray_trace_gain, 0
set ray_trace_mode, 3
set ray_trace_color, black
unset depth_cue
# render image and save
ray
png figures/GoodsellLike.png
save examples/AHo_GoodsellLike.pse
```

Complex Stylized Protein



```
...
# representation
hide all
preset.ball_and_stick("lig")
show spheres, prot
set sphere_scale, 0.99, prot
show surface, prot
# coloring
bg_color white
set_bond stick_color, 0xffff44, lig
set_bond stick_transparency, 0.35, lig
color grey, lig and e. C
ramp_new pRamp, lig, selection=prot, \
      range=[5,30], color=rainbow
set surface_color, pRamp, prot
color white, prot
color grey30, prot and e. C
disable pRamp

# continued on next slide
```

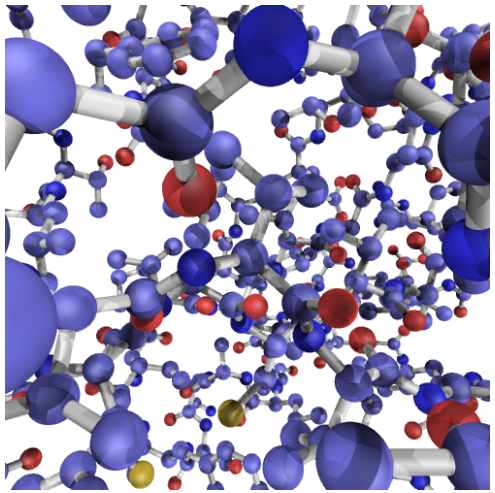
Complex Stylized Protein



@pml_scripts/AHo_StylizedProtein.pml

```
# special settings for this representation
set ray_transparency_contrast, 0.20
set ray_transparency_oblique, 1.0
set ray_transparency_oblique_power, 20
set surface_quality, 2
set light_count, 5
set ambient_occlusion_mode, 1
set ambient_occlusion_scale, 50
set ambient, 0.40
set transparency, 0.50
set spec_power, 1200
set spec_reflect, 0.20
set ray_opaque_background, 0
set ray_shadow, 0
set field_of_view, 50
# orientation
zoom complete=1
# render image and save
ray
png figures/StylizedProtein.png
save examples/AHo_StylizedProtein.pse
```

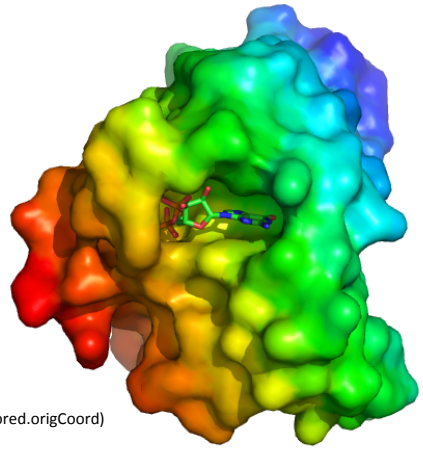
Ball-and-Stick



@pml_scripts/AHo_Ball_and_Stick2.pml

```
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
hide all
show spheres
show sticks
#coloring
bg_color white
util.cbab
set stick_ball_color, atomic
set_bond stick_color, white, all, all
# special settings for this representation
set stick_radius, 0.4, (all)
set sphere_scale, 0.3, (all)
set_bond stick_radius, -0.14, all, all
set light_count, 8
set spec_count, 1
set shininess, 10
set specular, 0.25
set ambient, 0
set direct, 0
set reflect, 1.5
set ray_shadow_decay_factor, 0.1
set ray_shadow_decay_range, 2
unset depth_cue
set field_of_view, 60
# render and save
ray
png figures/Ball_and_Stick2.png
save examples/AHo_Ball_and_Stick2.pse
```

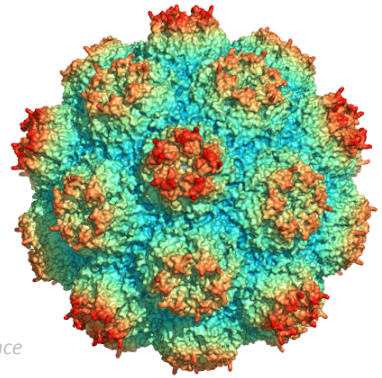
Color by Distance from Origin



@pml_scripts/AHo_ColorDist.pml

```
diff_len = lambda x,y : math.sqrt((x[0]-y[0])*(x[0]-y[0]) + (x[1]-y[1])*(x[1]-y[1]) + (x[2]-y[2])*(x[2]-y[2]))
#load your molecule, extract prot, lig
load pdb/3K8Y.pdb, tmp
extract lig, resn GNP
extract prot, polymer
delete tmp
#representation
as surface, prot
as stick, lig
# create the pseudoatom at the origin
pseudoatom pOrig, pos=(0,0,0), label=origin
# these are special PyMOL variables that will hold the
# coordinates of the atoms and the  pseudoatom
stored.origCoord = []
stored.distCoord = []
# copy the coordinates into those special variables
iterate_state 1, pOrig, stored.origCoord.append((x,y,z))
iterate_state 1, prot, stored.distCoord.append((x,y,z))
# extend origCoord to be the same length as the other
stored.origCoord *= len(stored.distCoord)
# calculate the distances
newB = map(lambda x,y: diff_len(x,y), stored.distCoord, stored.origCoord)
# put them into the b-factor of the protein
alter prot, b=newB.pop(0)
# color by rainbow_rev or any other palette listed in "help spectrum"
spectrum b, rainbow_rev, prot
bg_color white
...
```

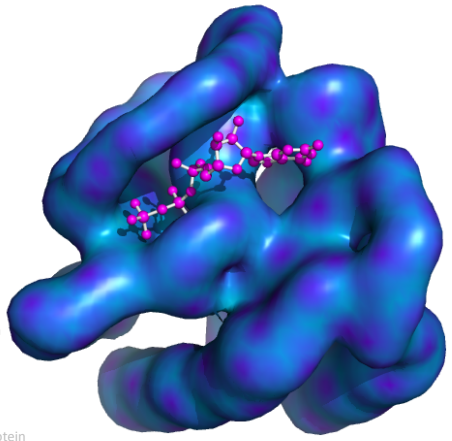
Virus Capsid



```
...
# create a pseudoatom at the origin-- we will
# measure the distance from this point
pseudoatom pOrig, pos=(0,0,0), label=origin
# load and build the capsid
load pdb/2xpj.pdb1.gz
split_states 2xpj
delete 2xpj
# show all 60 subunits it as a surface
# this will take a few minutes to calculate
as surface
# create a new color ramp, measuring the distance
# from pOrig to 1hug, colored as rainbow
ramp_new proximityRamp, pOrig, selection=(2xpj*), range=[110,160], color=rainbow
# set the surface color to the ramp coloring
set surface_color, proximityRamp, (2xpj*)
# some older PyMOLs need this recoloring/rebuilding
recolor
bg_color white
disable proximityRamp
# render image and save
...
```

@pml_scripts/AHo_VirusCapsid.pml

Smooth Pseudo-Surface with Ligand



```
...

# Ligand as ball and stick
bg_color white
hide lines
show sticks, lig
show spheres, lig
color magenta, lig
set_bond stick_radius, 0.13, lig
set sphere_scale, 0.26, lig
set_bond stick_radius, 0.13, lig
set_bond stick_color, white, lig
set sphere_scale, 0.26, lig

#protein pseudo-surface
# set the B-factors nice and high for smoothness
alter all, b=10
alter all, q=1
# 3.5 A map resolution
set gaussian_resolution, 8
# new gaussian map w/resolution=0.5 Ang on just the main chain
map_new map, gaussian, 1, n. C+O+N+CA, 5
# create a surface from the map
isosurface surf, map, 1.5
# color the protein by number
spectrum count, rainbow, prot
# now color the map based on the b-factors of the underlying protein
cmd.ramp_new("ramp", "prot", [0,10,10], "rainbow")
# set the surface color
cmd.set("surface_color", "ramp", "surf")
# hide the ramp and lines
disable ramp
...
```

#pml_scripts//AHo_SmoothSurfwLig.pml