

Set up	
Set working directory	cd C:\Users\...
Load pdb file from pdb website	fetch 1ubq
Load pdb file from local disk	load 1ubq.pdb

Log files	
new log file	log_open file_name.pml
save and quit log file	log_close
comment	#
record the view coordinate	get_view
run a log as a script	@file_name.pml
resume log file = run then edit at the end	
append log file = edit at the end without running	

Selection	
select selection_name, selection_expression	select carbon_beta, n. cb
select selection_name= (selection expression)	select carbon_beta = (n; cb)
logical operator: and (/), not, or. lorder of precedence --> use ()	

Selection - single word		
All atoms	all	*
No atoms	none	none
All hydrogen atoms	hydro	h.
All atoms from HETATM record	het	hetatm

Property selector identifiers		
Atom by chemical symbol ex: Oxygen = O	symbol	e.
Atom/nucleic acid by code ex: C α = ca, C β = cb	name	n
Aa/nucleic acid by code ex: Asparagine = asp / adenosine = a	resn	r
residue identifier (1-9999)	resi	i
PDB chain identifier (check in PDB file if letter or number ID)	chain	c
Secondary structure: α helix = 'H', β strand = "S", Loop = 'L'	ss	ss
carbon α : first carbon bond to the side chain carbon β : second carbon bond to the side chain		

selection macros	
/object-name/seg1-identifier/chain-identifier/resi-identifier/name-identifier	
start by "/": start from the top of the hierarchie (object-name)	
end by "": start from the bottom of the hierarchie (name-id)	
// :skip one level of hierarchie	
ex: select lys, /helix_alpha///lys	
select all the residue of lysine from the object "helix_alpha"	

Display	
show the selection as this display type	show_as lines, selection_name cmd.show_as("lines", "selection_name")
add this display type of the selection	show lines, selection_name cmd.show("lines", "selection_name")
hide this display type of the selection	hide lines, selection_name cmd.hide("lines", "selection_name")
color the selection	coloc color_name, selection_name
zoom on the selection	zoom selection_name
Show (S button) - Hide (H button) - Color (C button) display type: lines, ribbon, cartoon, stick, label, nonbonded, mainchain, sidechain	

Structure modification	
adds hydrogens in the appropriate places	h_add

get information	
count the number of atome of the selection	count_atoms selection_name

selection algebra		
Selects atoms that are not included in s1	not s1	! s1
Selects atoms included in both s1 and s2	s1 and s2	s1 & s2
Selects atoms included in either s1 or s2	s1 or s2	s1 s2



selection algebra (cont)

Selects atoms in s1 whose identifiers name, resi, resn, chain and segi all match atoms in s2

```
s1 in s2 s1
in
s2
```

Selects atoms in s1 whose identifiers name and resi match atoms in s2

```
s1 like s1
s2 l.
s2
```

Selects all atoms whose van der Waals radii are separated from the van der Waals radii of s1 by a minimum of X Angstroms.

```
s1 gap s1
X gap
X
```

Selects atoms with centers within X Angstroms of the center of any atom in s1

```
s1 s1
around a.
X X
```

Expands s1 by all atoms within X Angstroms of the center of any atom in s1

```
s1 s1
expand e.
X X
```

Selects atoms in s1 that are within X Angstroms of the s2

```
s1 s1
within w.
X of s2 X of
s2
```

Expands selection to complete residues

```
byres s1 br.
s1
```

Expands selection to complete objects

```
byobject bo.
s1 s1
```

Selects atoms directly bonded to s1

```
neighbor nbr.
s1 s1
```



By **leilaP**

cheatography.com/leilap/

Not published yet.

Last updated 20th April, 2017.

Page 2 of 2.

Sponsored by **ApolloPad.com**

Everyone has a novel in them. Finish Yours!

<https://apollopad.com>