PyMOL

Download PDB from rcsb.org, or get PDB from File > Get PDB...

High B-factor value → high mobility; more freedom to move

> hide all
> show cartoon [, selection]

model	1ubq	m.
chain	C	c.
segi	S	s.
resn	ALA	r.
resi	100-200	i.
name	CA	n.
alt	A	
index	123	idx.
id	123	
rank	123	
pepseq	ACDEF	ps.
label	"Hello"	

[A] [S] [H] [L] [C]
action show hide label color

Load two structures into the same editor/view

[A] > Center in the object

> align 1b41, 1acj

> orient 1acj

> hide all
> show cartoon

> color green, 1acj (selection) > color orange, 1b41

> select humantriad, 1b41 and resi (number) 203+334+447 ~ active site

> select raytriad, 1acj and resi 200+440+327 ~ active site

> select tacrine, 1acj and resn (name) THA
(THA: code used in the PDB for the molecule on site)

> show sticks, humantriad > show sticks, raytriad
> color red, humantriad > color white, raytriad

fasciculin-II inhibitor is the chain B of the 1b41 structure

> select fasciculin, 1b41 and chain B
> show cartoon, fasciculin
> color cyan, fasciculin

Calculating distances by hand Cα (CA) atom of Pro31 and CA atom of His447

ATOM 4420 CA PRO B 31 114.590 113.66 -126.288 1.00 43.16 C
ATOM 3390 CA HIS A 447 117.582 93.303 -133.707 1.00 43.80 C

$$\sqrt{(x_2-x_1)^2+(y_2-y_1)^2+(z_2-z_1)^2} \approx 16\ \text{Å}$$

> select toxinPro31, 1B41 and chain B and resi 31
> show sticks, toxinPro31
> color magenta, toxinPro31

> label fasciculin and resi 31, name ~ label atom name
> label fasciculin and resi 31 and name CA, resn ~ residue name on CA

> label toxinPro31, name

Wizard > Measurement (Distances)
select CA of Pro31, then select CA of His447

> Done → 16.4 Å

> select tryptophans, resname TRP and chain A
> color yellow, tryptophans
> show sticks, tryptophans

> select chain A and resi 5-13

Wizard > Mutagenesis > Protein   pick a residue → mutate to xxx → Apply → Done

> select hydrophobic, (resn ala+gly+val+ile+leu +phe+met+pro)

> fetch 2bv6

EXPDTA X-RAY DIFFRACTION

> hide everything
> show cartoon
> util.chainbow → like coloring by chain > chainbows ~ chain + rainbow

Biological relevant assembly   multimeric proteins → rearrangement of the individual polypeptide chain

> fetch 2bv6, type=pdb1 → access to two different states = biological assembly
> split_states 2bv6 → splits to component monomers → different objects
> delete 2bv6 → delete original monomer

Select residues at the interface of the 2 polymers

> set_name sele, interface
> show ribbon, (all &! interface)   &! = and not