PYMOL NOTES

Contents

1. General Manipulation

category

create protein, polymer

create ligand, organic

create solvent, solvent

create ions, resn NA+K+CL+CA+MG+ZN+MN+FE+CU+CO+NI

highlight binding site

select binding_site, protein within 5 of ligand

show sticks, binding_site

color orange, binding_site

define docking box

change wd

create protein, polymer

create ligand, organic

create solvent, solvent

create ions, resn NA+K+CL+CA+MG+ZN+MN+FE+CU+CO+NI

select ligand_selection, resn UNK

run shaded_box.py

draw_shaded_box()

Show surface of binding pocket

show surface, binding_site

set transparency, 0.5, binding_site

2. Ligand Observation

waters near the ligand

create waters_near_ligand_obj, solvent within 4 of ligand

show lines, waters_near_ligand_obj

color blue, waters_near_ligand_obj

Ions in Binding Site

select ions_near_ligand, ions within 5 of ligand

show spheres, ions_near_ligand

color yellow, ions_near_ligand

Metal Coordination (if present)

Elements: Zn, Mg, Ca, etc.

select zn, resn ZN

create zn_obj, zn

distance metal_coord, zn_obj, ligand_obj within 2.5

set dash_color, white, metal_coord

set dash_width, 3

Hydrogen Bonds

distance hbonds_lig_prot, ligand, protein, 3.2, mode=2

distance hbonds_lig_solvent, ligand, solvent, 3.2, mode=2

Salt Bridges / Ionic Interactions

Detect charged groups in protein near charged groups in ligand (e.g., acidic/basic residues near ligand ions):

select charged_prot_near_lig, (protein and (resn ARG+LYS+HIS+ASP+GLU)) within 4 of ligand

 show sticks, charged_prot_near_lig

PI / PI

select arom_prot_near_lig, (protein and resn PHE+TYR+TRP+HIS) within 5 of ligand

 show sticks, arom_prot_near_lig

Label interacting residues

label binding_site and name CA, "%s`%s" % (resn, resi)

Orient the view:

orient ligand

zoom ligand, 10

3. Protein Observation

Dynamic Factors

Blue: low B-factor (rigid)

White: intermediate

Red: high B-factor (flexible)

color blue, polymer and b < 20

color white, polymer and b >= 20 and b < 40

color red, polymer and b >= 40

Protein / Protein Rx

fetch 1H4G, async=0

select interfaceA, byres (chain A within 4 of chain B)

select interfaceB, byres (chain B within 4 of chain A)

show cartoon, chain A+B

show sticks, interfaceA

show sticks, interfaceB

color red, interfaceA

color blue, interfaceB

distance contacts, chain A within 4 of chain B, chain B within 4 of chain A

label interfaceA, resn + resi

label interfaceB, resn + resi

Superimpose Proteins

super ptn_1, ptn_2   # ptn_1 will be pushed to the position of ptn_2 and align on it (ptn_2 is the ref.)

Fast sequence

print(cmd.get_fastastr("protein"))

hiding H

hide (hydro)

4. Images and Videos

ray tracing for final images

ray 1600,1200

png binding_site_view.png, dpi=300

Scenes

scene 001, store

video

mset 1 x 600   # 20 sec (30 frame/sec)

mview store, 1

mview store, 200

mview store, 300

mview store, 400

mplay

mstop

frame 1

label size

set label_size, 14

5. Dashes

dash color

set dash_color, red   # Strong visual, good for highlighting

set dash_color, blue

set dash_color, green

set dash_color, yellow

set dash_color, orange

set dash_color, cyan

set dash_color, magenta

set dash_color, white

set dash_color, black

set dash_color, grey50   # Soft neutral tone

dash width

set dash_width, 4   # Default is 2; 4 is bolder, good for visibility

dash gab

set dash_gap, 0.4   # Default is 0.3; 0.4–0.5 for better separation

dash length

set dash_length, 0.3   # Default is 0.2; 0.3–0.4 for better visibility

6. Labels

label color

set label_color, white   # Common options: white, black, red, yellow, etc.

set label_color, black

set label_color, red

set label_color, yellow

set label_color, cyan

set label_color, green

Label size

set label_size, 18   # (default = 14) Good for presentations; try 12–24 based on need

Label font

set label_font_id, 7   # Common fonts:

5: Sans, 6: Sans Bold, 7: Serif, 8: Serif Bold, 9: Fixed Width (monospace)

Label transparency

set label_transparency, 0.3   # 0 = opaque, 1 = fully transparent

7. colorblind-friendly Commands

```
bg_color white
set antialias=1
set orthoscopic=1
set gamma=1.15
set cartoon_fancy_helices, 1
set cartoon_fancy_sheets, 1
set_color wred, [0.788,0.000,0.140]
set_color wblue, [0.31,0.506,0.686]
set_color wgold, [0.855,0.647,0.125]
set_color wgreen, [0.134,0.545,0.134]
set_color wgray, [0.800,0.800,0.800]
set_color wrose, [0.65,0.47,0.55]
set_color wpurple, [0.37,0.31,0.62]
set_color mpurple, [0.75,0.57,0.80]
set_color mpgrey, [0.73,0.68,0.82]
set ray_shadows, 0
set ray_trace_fog, 1
```

8. Reference Values

INTERACTION TYPE	DISTANCE RANGE (Å)	ANGLE CRITERIA (°)	NOTES
HYDROGEN BOND	2.5 – 3.5 Å (ideal ~2.8)	>120° (donor-H-acceptor)	H-bond is directional; angle close to 180° is ideal
SALT BRIDGE (IONIC)	≤ 4.0 Å	—	Between oppositely charged groups (e.g., Lys–Asp)
Π–Π STACKING	3.3 – 4.0 Å	Parallel or T-shaped	Between aromatic rings (e.g., Phe–Phe or ligand ring)
CATION–Π	3.5 – 6.0 Å	—	Between a positive charge (e.g., Lys+) and aromatic ring
VAN DER WAALS	3.0 – 4.0 Å	—	Close but not overlapping atoms; weak individually
HYDROPHOBIC CONTACT	≤ 4.0 Å	—	Nonpolar groups (e.g., Val–Leu, methyl–phenyl)
METAL COORDINATION	1.8 – 2.5 Å (strong)	~90°–180°	For Zn, Mg, Fe, Ca, etc. Usually involves O or N
HALOGEN BOND	3.0 – 3.5 Å	~160°–180°	Between halogen (Br, Cl, I) and O/N; highly directional
WATER BRIDGE	H-bonds through water	Same as H-bonds	Bridging ligand and protein via water molecule
CH–Π INTERACTION	~2.5 – 3.0 Å	—	Between C-H and aromatic system; often overlooked

FEATURE	TYPICAL RANGE	NOTES
CA–CA (ADJACENT RESIDUES)	~3.8 Å	Peptide bond spacing
C=O TO N (H-BOND IN HELIX/SHEET)	~2.8 Å	Backbone H-bonds
H-BOND IN A-HELIX	i → i+4	C=O of residue *i* bonds to N-H of *i+4*
B-SHEET SPACING (BETWEEN STRANDS)	~4.5 – 5.0 Å	Between aligned residues across strands

When validating interactions or modeling:

- **H-bonds**: Check donor–acceptor distance and angle
- **Salt bridges**: Charged groups <4.0 Å apart
- **π–π**: Parallel rings within ~3.5–4 Å
- **Cation–π**: Aromatic ring within 6 Å of positive group
- **Metal ions**: Coordinating atoms within ~2 Å (depends on metal)
- **Hydrophobic contacts**: Any nonpolar groups within 4 Å
- **Angles**: Especially for hydrogen bonds and halogen bonds