Han Li Lab PyMol Guide

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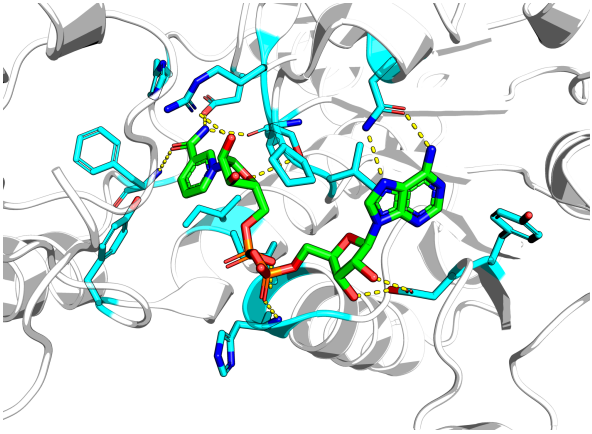
Selection Shortcuts

```
sel <variable_name>, <object>          # selection template
remove solv                            # remove solvent
remove inorg                           # remove ions
remove not chain <chain>               # remove other chains
sel <ligand>, org                      # select all ligands
sel <protein>, poly                    # select all protein atoms
sel <target>, rep sticks               # select by representation
sel <residue>, resi <residue number>   # select residue by number
sel <residue>, resn <residue name>     # select object by residue name
sel <atom>, name <atom name>           # select atom by atom name
reset                                  # reset camera origin

# Examples
# selects residues 23, 54, 55, 56, 57, 99
sel target_residues, resi 23+54-57+99

# selects ligand with 3-letter code NAD from chain A
sel target_ligand, resn NAD and chain A
```

Displaying Binding Pocket Interactions



```
# all residues with any atom
    around 3.5 angstrom
sel pocket, br. org around 3.5
show sticks, pocket
color cyan, pocket
util.cnc
dist hbonds, org, poly, mode=2
hide labels
```

Alignment

```
# 1 to 1 alignment
fetch 1j49; fetch 4e5n
remove solv; remove not chain A; remove inorg
align 1j49, 4e5n  # fits 1j49 onto 4e5n
reset

# multiple to 1 alignment
fetch 1j49; fetch 4e5n; fetch 6ih4
remove solv; remove not chain A; remove inorg
alignto 4e5n  # align all to 4e5n
reset
```

Ligand Transfer

```
fetch 1qi1; fetch 1qi6          # 1qi1 gapn with nadp, 1qi6 apo gapn
remove not chain A
remove solv
remove inorg
align 1qi1, 1qi6                # align binding pockets
extract nadp, resn NAP
sel 1qi6_nadp, 1qi6 + nadp
save 1qi6_nadp.pdb, 1qi6_nadp   # or save with File -> Export Molecule
# type pwd to see the default directory the file is saved to
```

Mutagenesis

Follow instructions from the PyMol website
https://pymolwiki.org/index.php/Mutagenesis

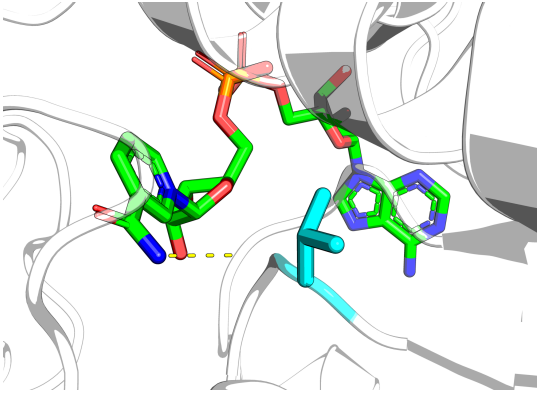
1. Wizard → Mutagenesis → Protein
2. Select target residue by clicking
3. Select mutation residue in Mutagenesis box
4. Examine rotamers with arrows on bottom right
5. Apply to save

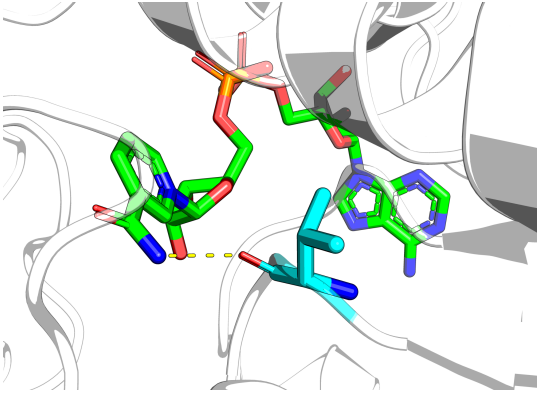
General Settings

```
bg white                          # change background color
set ray_opaque_background, 1      # make background solid
set ray_shadow, 0                 # turn off shadows
set antialias, 2                  # smooth edges
set cartoon_fancy_helices, 1      # adds ridges to helix edges
util.cnc                          # colors oxygen and nitrogen atoms
ray <width>                       # ray and scale resolution

# Recommended settings
set ray_trace_mode, 3             # optional neon colors and outline
color white, poly
color green, org
color cyan, poly and rep sticks
```

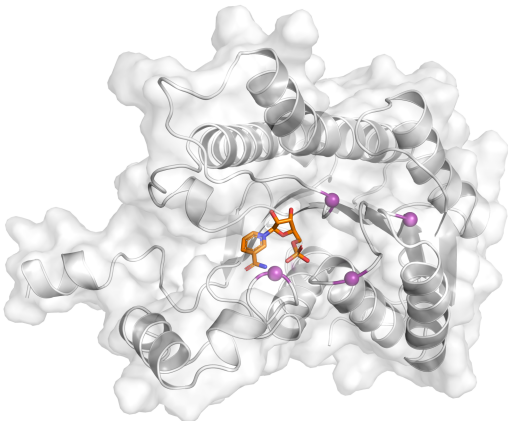
Showing Backbone Atoms





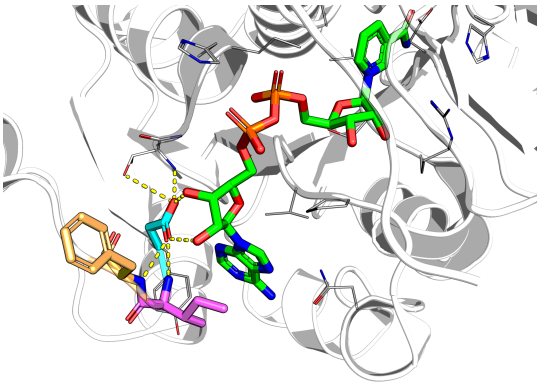
```
fetch 1j49
[...]  # clean up
dist hbonds, org, resi 234, mode=2
hide labels
set cartoon_side_chain_helper, 0, resi 234
```

Glucose Dehydrogenase



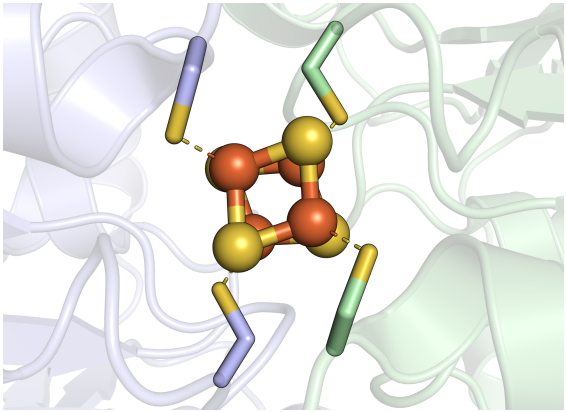
```
load gludh_80_nmn.pdb
bg white
set ray_opaque_background, 1
set cartoon_fancy_helices, 1
set ray_shadow, 0
color white, poly
color orange, org
show cart
show surf
set transparency, 0.7
sel mutations, i. 93+39+195+17 and
    name ca
show spheres, mutations
color deeppurple, rep spheres
set sphere_scale, 0.5
util.cnc org
```

Lactate Dehydrogenase



```
fetch 1j49
bg white; color white, poly
remove chain A; remove inorg;
    remove solv
set ray_opaque_background, 1
set ray_trace_mode, 3
set cartoon_transparency, 0.3
color green, org
show lines, br. org around 3.5
color silver, rep lines
sel spec_loop, resi 176-178
show sticks, spec_loop
color cyan, resi 176
color violet, resi 177
color lightorange, resi 178
dist hbonds, resi 176, all, mode=2
hide labels; show lines, resi 154
set cartoon_side_chain_helper, 0,
    resi 154+177+178
util.cnc
```

Nitrogenase Iron Protein



```
fetch 6nzj
bg white
color lightblue, chain A
color palegreen, chain B
util.cnc
remove resn SO4; remove solv
set ray_opaque_background, 1
# outline with regular colors
set ray_trace_mode, 1
set cartoon_transparency, 0.7
show sticks, inorg
set sphere_scale, 0.4
set cartoon_transparency, 0.5
show sticks, br. inorg around 3.5
hide sticks, resi 96
```

Rotation Movies

Common options under Movie → Program

GluDH

```
movie.add_roll(16.0, axis='y', start=1)
File -> Export Movie
```

https://youtu.be/eaRJjZ0OLRs