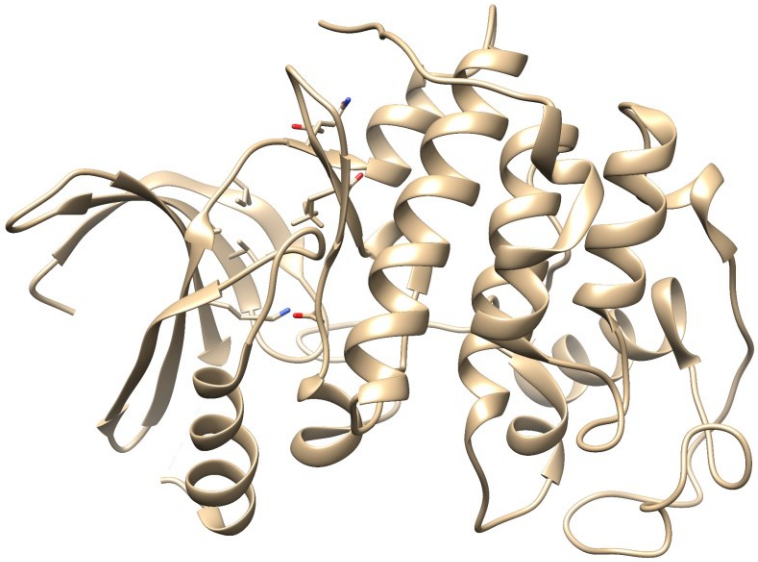
Selected proteins:

7kjs and 2w05



What is the resolution and how many chains are there?

Resolution: 2.19 Å for 7kjs

Resolution: 1.90 Å for 2W05

Both PDB IDs have 2 chains

Specify ligand binding site and protein residues in contact with ligand?

Using command:

```
[atomselect 0 "protein and name CA and same residue as within 5 of resname FRT"] writepdb "bindingsite-7kjs.pdb"

[atomselect 1 "protein and name CA and same residue as within 5 of resname WG1"] writepdb "bindingsite-2w05.pdb"


set center1 [atomselect 0 "protein and name CA and same residue as within 5 of resname FRT"]

set center2 [atomselect 1 "protein and name CA and same residue as within 5 of resname WG1"]

set masscenter1 [measure center $center1]

set masscenter2 [measure center $center2]


puts $masscenter1

puts $masscenter2
```

Result files:

bindingsite-7kjs.pdb

bindingsite-2w05.pdb

Create a separate PDB file that contain “only” CDK2 and ligand and use REDUCE to add hydrogen atoms to protein and ligand

Using command:

[atomselect 0 "protein and not water"] writepdb "protein1_2w05_clean.pdb"

[atomselect 1 "protein and not water"] writepdb "protein2_7kjs_clean.pdb"

[atomselect 0 "resname FRT"] writepdb "ligand1_2w05_clean.pdb"

[atomselect 1 "resname WG1"] writepdb "ligand2_7kjs_clean.pdb"

Result files:

protein1_2w05_clean.pdb

protein2_7kjs_clean.pdb

ligand1_2w05_clean.pdb

ligand2_7kjs_clean.pdb

Aligne two CDK2 structure from c alpha atoms of common ligand binding residues and after alignment report the carbon alpha RMSD values for all protein residues and union of ligand binding residues

Using command:

```
mol load pdb bindingsite1.pdb
mol load pdb bindingsite2.pdb

set com1 [atomselect 2 "index 1 to 15"]
set com2 [atomselect 3 "index 1 to 15"]
set align1 [measure fit $com1 $com2]
set rmsd1 [measure rmsd $com1 $com2]

puts $align1
puts $rmsd1
```

Result:

```
1.3731051683425903 29.28715705871582 8.521210670471191
35.77804946899414 22.87290009155273 -8.706850051879883 1.3731051683425903 29.28715705871582 8.521210670471191
```

35.77804946899414 22.87290000915273 -8.706850051879883

{0.0768376439809799 2 0.12285700440406799 -0.9894453883171082 40.85408020019531} {0.8803139328956604 -0.4742970764636993 0.009470490738749504 35.464359283447266} {-0.4681275188922882 -0.871750235557556 2 -0.14459659159183502 18.95899200439453} {0.0 0.0 0.0 1.0}

41.37579345703125

{0.0768376439809799 2 0.12285700440406799 -0.9894453883171082 40.85408020019531} {0.8803139328956604 -0.4742970764636993 0.009470490738749504 35.464359283447266} {-0.4681275188922882 -0.871750235557556 2 -0.14459659159183502 18.95899200439453} {0.0 0.0 0.0 1.0}

41.37579345703125