Compute Dihedrals with VMD

Dihedrals

The angle between two planes ABC and BCD is called a dihedral as shown in Fig. 1.

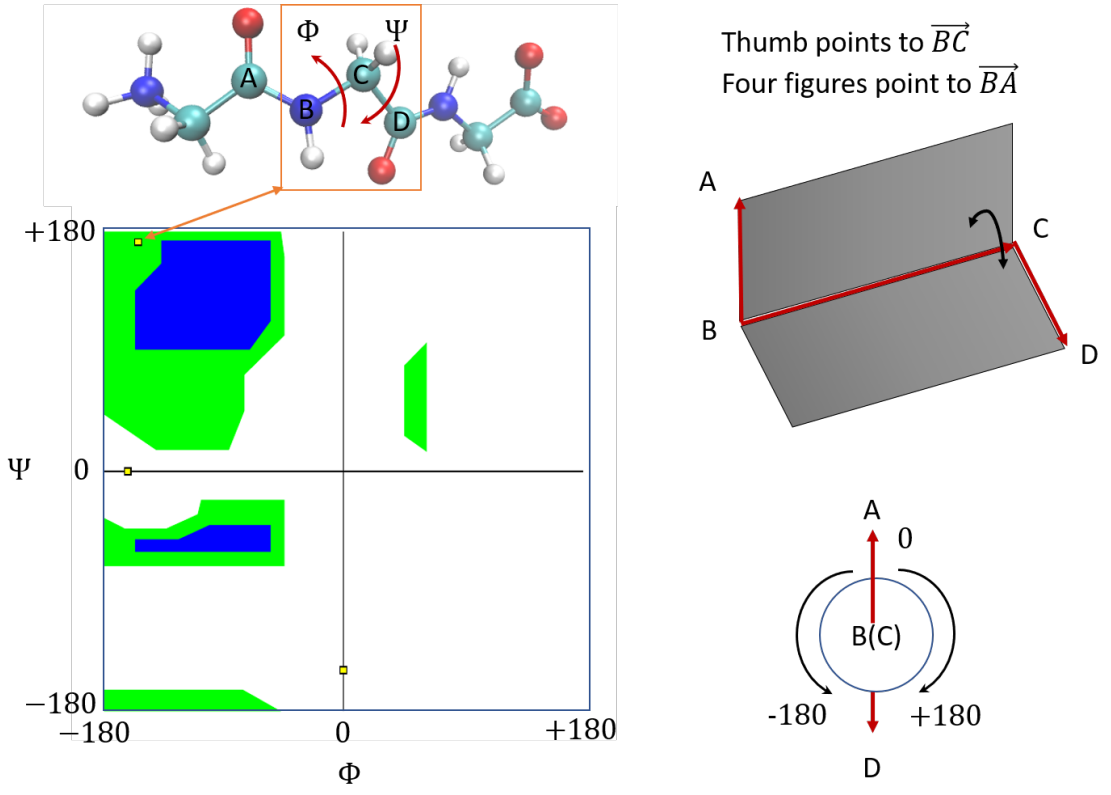

Figure 1: The dihedrals of protein backbones and Ramachandran plot.

Code to compute dihedrals with VMD

```
set wrkDir "/home/kuangz/WRK/FY22/dLE"
set outfile [open "dihedral.dat" w]
cd $wrkDir
# load molecule
# mol delete all
mol new test.pdb type pdb waitfor all
# mol new com.psf type psf waitfor all
# mol addfile min.coor type pdb waitfor all
# mol addfile tmp.dcd type dcd waitfor all
set SEL [atomselect top "backbone and (not (name O))"]
set SELindx [$SEL get index]
# index for first C in VMD list, starting with 0
set strtID [lsearch $SELindx 17]
# index for last C in VMD list
set endID [lsearch $SELindx 92]
for {set i $strtID} {$i < $endID} {incr i} {
   set j [expr $i + 3]
   set atom4 [lrange $SELindx $i $j]
   set phi [measure dihed $atom4]
   incr i
   set j [expr $i + 3]
   set atom4 [lrange $SELindx $i $j]
```

```
    set psi [measure dihed $atom4]
    puts $outfile "$phi $psi"
    incr i
}
close $outfile
exit
```