

In the name of LORD who made the word

Structural Bioinformatics
VMD

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For this homework assignment, we focused on studying a specific gene, **Gene Name:** APOL1. Utilizing the Protein Data Bank (PDB), we analyzed the corresponding protein structure with the PDB **ID** 7l6k. The detailed information about the protein and its structure can be accessed through the provided link:
<https://www.rcsb.org/structure/7l6k>.

Part 1: In order to analyze the composition of the molecule, we employ a systematic approach. Firstly, we create a comprehensive list that contains the symbol of each amino acid present. This list serves as a reference for our subsequent calculations.

Once the list is established, we proceed to iterate over each amino acid symbol within the list. During this iterative process, we carefully calculate the percentage of each amino acid in the molecule. This enables us to gain valuable insights into the relative abundance and distribution of the various amino acids.

To facilitate our analysis, we utilize the following code:

Code:

```
set amino_acids {ALA ARG ASN ASP CYS GLN GLU GLY HIS ILE LEU
                 LYS MET PHE PRO SER THR TRP TYR VAL}

puts "Amino acid names: [[atomselect 0 "alpha" frame 0] get {resname}]"

foreach amino_acid $amino_acids {
    set sel [atomselect 0 "alpha and resname $amino_acid" frame 0]
    set count [$sel num]
    $sel delete
    puts "Number of $amino_acid residues: $count"
}
```

Upon execution of the code, we obtain the following insightful results:

Result:

```
Amino acid names: GLY SER ASP PRO GLU SER SER ILE PHE ILE GLU ASP ALA
ILE LYS TYR PHE LYS GLU LYS VAL SER THR GLN ASN LEU LEU LEU LEU LEU
THR ASP ASN GLU ALA TRP ASN GLY PHE VAL ALA ALA ALA GLU LEU PRO ARG
ASN GLU ALA ASP GLU LEU ARG LYS ALA LEU ASP ASN LEU ALA ARG GLN MET
ILE MET LYS ASP LYS ASN TRP HIS ASP LYS GLY GLN GLN TYR ARG ASN TRP
PHE LEU LYS GLU PHE PRO ARG LEU LYS SER GLU LEU GLU ASP ASN ILE ARG
ARG LEU ARG ALA LEU ALA ASP GLY VAL GLN LYS VAL HIS LYS GLY THR
```

```
Number of ALA residues: 10
Number of ARG residues: 8
Number of ASN residues: 8
Number of ASP residues: 9
```

```

Number of CYS residues: 0
Number of GLN residues: 5
Number of GLU residues: 10
Number of GLY residues: 5
Number of HIS residues: 2
Number of ILE residues: 5
Number of LEU residues: 14
Number of LYS residues: 11
Number of MET residues: 2
Number of PHE residues: 5
Number of PRO residues: 3
Number of SER residues: 5
Number of THR residues: 3
Number of TRP residues: 3
Number of TYR residues: 2
Number of VAL residues: 4

```

Part 2: I have developed a procedure to address this task, which requires obtaining the ID of a PDB file loaded in VMD as input. Within the code, I begin by iterating through each frame of the molecule. Within this iteration, I further iterate through the secondary structure elements of the current frame, calculating their respective percentages.

```

proc struct_cal {id} {
    set secondary_structures {C T G B E H};
    set total_frames [molinfo $id get numframes];
    puts "H or G: Representing an alpha-helix."
    puts "E or B: Representing a beta-strand."
    puts "C: Representing a coil or loop region."
    puts "T: Representing a turn or bend region."

    for {set frame 0} {$frame < $total_frames} {incr frame} {
        puts "Frame: $frame";
        set selection [atomselect $id "alpha" frame $frame];
        set total_residues [$selection num];
        puts "Secondary structure: [$selection get {structure}]";

        foreach secondary_struct $secondary_structures {
            set ss_selection [atomselect $id "alpha and structure
            $secondary_struct" frame $frame];
            set count [expr [$ss_selection num] * 100];
            set proportion [expr {double($count) / $total_residues}];
            puts "Percentage of $secondary_struct: $proportion";
        }

        puts "=====";
    }
}

```

Result:

H or G: Representing an alpha-helix.
E or B: Representing a beta-strand.
C : Representing a coil or loop region.
T : Representing a turn or bend region.

frame: 0

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 1

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 2

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 3

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C

Number of C portion: 18.42105263157895

Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 4

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 5

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 6

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 7

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T

T T T C
Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 8
secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C
Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 9
secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C
Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 10
secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C H T
T T T C
Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 11
secondary : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H

H H H H H H H H H H H H H C C C T T T T T T T T T C H
 H H H C C C C C H H H H H H H H H H H H H H H H H H H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 12

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 13

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 14

secondary : C C C C C H H H H H H H H H H H H H H H C C H H
 H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
 H H H H H H H H H H H H H C C C T T T T T T T T T T C H
 H H H C C C C C H T
 T T T C

Number of C portion: 18.42105263157895
 Number of T portion: 12.280701754385966
 Number of G portion: 0.0
 Number of B portion: 0.0
 Number of E portion: 0.0
 Number of H portion: 69.29824561403508

frame: 15

secondery : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C C H H H H H H H H H H H H H H H H H H H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 16

secondery : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C C H H H H H H H H H H H H H H H H H H H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 17

secondery : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C C H H H H H H H H H H H H H H H H H H H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

frame: 18

secondery : C C C C C H H H H H H H H H H H H H H H C C H H
H H H H H H H C H H H H H H H H H H H C C C H H H H H H H
H H H H H H H H H H H H H H C C C T T T T T T T T T T C H
H H H C C C C C C H H H H H H H H H H H H H H H H H H H T
T T T C

Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

```

frame: 19
secondary : C C C C C H H H H H H H H H H H H H C C H H
            H H H H H H H C H H H H H H H H H H C C C H H H H H H
            H H H H H H H H H H H H H C C C T T T T T T T T T C H
            H H H C C C C C H H H H H H H H H H H H H H H H H H T
            T T T C
Number of C portion: 18.42105263157895
Number of T portion: 12.280701754385966
Number of G portion: 0.0
Number of B portion: 0.0
Number of E portion: 0.0
Number of H portion: 69.29824561403508

```

Part 3: We begin by calculating the ϕ and ψ angles for proteins and save the results in a file named `phi_psi.txt`. Next, in our Python code, we generate a Ramachandran chart to visualize the data: **Code:**

```

tcl

set se1 [atomselect top "protein and alpha"]
set se2 [$se1 get {phi psi}]
set file_txt [open phi_psi.txt w]
puts $file_txt $se2
close $file_txt

python

from matplotlib import pyplot as plt
import matplotlib.image as mpimg

with open('phi_psi.txt') as f:
    input_string = f.read()

angle = list(map(lambda s: s.replace("{", "").strip().split(' '), input_string.sp

background_image = mpimg.imread('ram.jpg')
plt.imshow(background_image, extent=[-180, 180, -180, 180])

for i in angle:
    plt.plot(float(i[0]), float(i[1]), 'co', alpha=0.7)
plt.xlim(-180, 180)
plt.ylim(-180, 180)

plt.xlabel('$\phi$')
plt.ylabel('$\psi$')

plt.title('Ramachandran')
plt.legend()

plt.show()

```

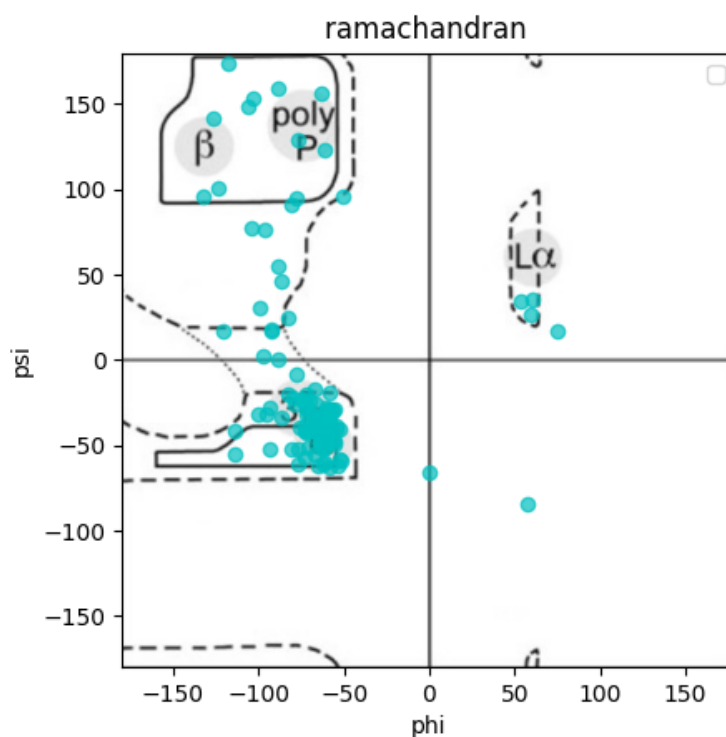



Figure 1: result of part 3 : Ramachandran chart

Part 4: In this section, we will develop a robust procedure that effectively compares each pair of frames and accurately calculates their Root Mean Square Deviation (RMSD) to each other. The RMSD metric provides valuable insights into the structural similarity or dissimilarity between frames.

Code:

```
proc cal_rmsd { id } {
    set total_frames [molinfo $id get numframes];
    for {set frame1 0} {$frame1 < $total_frames} {incr frame1} {
        for {set frame2 [expr $frame1 + 1]} {$frame2 < $total_frames}
            {incr frame2} {
                puts "Analyzing Frame $frame1 versus Frame $frame2";
                set rmsd [measure rmsd [atomselect $id all frame $frame1]
                    [atomselect $id all frame $frame2]];
                puts "RMSD: $rmsd";
            }
        }
    }
}
```

Result:

```
frame 0 : frame 1
result : 4.871898174285889
frame 0 : frame 2
result : 4.044975280761719
```

frame 0 : frame 3
result : 4.650674343109131
frame 0 : frame 4
result : 5.882270336151123
frame 0 : frame 5
result : 4.953680515289307
frame 0 : frame 6
result : 4.740062236785889
frame 0 : frame 7
result : 4.1517333984375
frame 0 : frame 8
result : 4.4630632400512695
frame 0 : frame 9
result : 5.9443440437316895
frame 0 : frame 10
result : 3.5653045177459717
frame 0 : frame 11
result : 3.6274757385253906
frame 0 : frame 12
result : 5.179007530212402
frame 0 : frame 13
result : 6.628292560577393
frame 0 : frame 14
result : 6.2243733406066895
frame 0 : frame 15
result : 3.7709567546844482
frame 0 : frame 16
result : 4.438200950622559
frame 0 : frame 17
result : 4.0528740882873535
frame 0 : frame 18
result : 5.35756778717041
frame 0 : frame 19
result : 6.636552810668945
frame 1 : frame 2
result : 3.968817949295044
frame 1 : frame 3
result : 4.941702365875244
frame 1 : frame 4
result : 5.3175554275512695
frame 1 : frame 5
result : 4.088255882263184
frame 1 : frame 6
result : 4.6155524253845215
frame 1 : frame 7
result : 4.561079025268555
frame 1 : frame 8
result : 4.830169200897217
frame 1 : frame 9
result : 4.208715915679932

```

frame 1 : frame 10
result : 4.5770158767700195
frame 1 : frame 11
result : 4.485307693481445
frame 1 : frame 12
result : 4.50715446472168
frame 1 : frame 13
result : 5.624903202056885
frame 1 : frame 14
result : 5.422607898712158
frame 1 : frame 15
result : 5.403294086456299
frame 1 : frame 16
result : 4.435463905334473
frame 1 : frame 17
result : 5.0816264152526855
frame 1 : frame 18
result : 4.5703229904174805
frame 1 : frame 19
result : 5.940220832824707
frame 2 : frame 3
result : 4.335323333740234
frame 2 : frame 4
result : 5.825480937957764
frame 2 : frame 5
result : 3.861464023590088
frame 2 : frame 6
result : 4.1796770095825195
frame 2 : frame 7
result : 4.448683738708496
frame 2 : frame 8
result : 4.900425434112549
frame 2 : frame 9
result : 5.3165082931518555
frame 2 : frame 10
result : 4.304056167602539
frame 2 : frame 11
result : 4.189539432525635
frame 2 : frame 12
result : 4.909340858459473
frame 2 : frame 13
result : 6.3749494552612305
frame 2 : frame 14
result : 6.023650169372559
frame 2 : frame 15
result : 4.620950222015381
frame 2 : frame 16
result : 4.71707820892334
frame 2 : frame 17
result : 4.136999607086182

```

```

frame 2 : frame 18
result : 5.058647632598877
frame 2 : frame 19
result : 6.454563617706299
frame 3 : frame 4
result : 4.285496711730957
frame 3 : frame 5
result : 3.6444549560546875
frame 3 : frame 6
result : 4.245429515838623
frame 3 : frame 7
result : 4.276737213134766
frame 3 : frame 8
result : 4.1074981689453125
frame 3 : frame 9
result : 4.787784099578857
frame 3 : frame 10
result : 4.696900367736816
frame 3 : frame 11
result : 4.40242338180542
frame 3 : frame 12
result : 4.113626956939697
frame 3 : frame 13
result : 5.898701190948486
frame 3 : frame 14
result : 5.5118536949157715
frame 3 : frame 15
result : 4.230776309967041
frame 3 : frame 16
result : 4.179084300994873
frame 3 : frame 17
result : 4.192858695983887
frame 3 : frame 18
result : 4.270309925079346
frame 3 : frame 19
result : 5.256998062133789
frame 4 : frame 5
result : 5.103140354156494
frame 4 : frame 6
result : 4.237977504730225
frame 4 : frame 7
result : 4.776193618774414
frame 4 : frame 8
result : 4.979176044464111
frame 4 : frame 9
result : 4.451472282409668
frame 4 : frame 10
result : 5.400258541107178
frame 4 : frame 11
result : 5.494015693664551

```

```

frame 4 : frame 12
result : 4.453736782073975
frame 4 : frame 13
result : 5.727537155151367
frame 4 : frame 14
result : 5.1992411613464355
frame 4 : frame 15
result : 5.066088676452637
frame 4 : frame 16
result : 4.771238327026367
frame 4 : frame 17
result : 5.727817535400391
frame 4 : frame 18
result : 5.141618728637695
frame 4 : frame 19
result : 3.873225688934326
frame 5 : frame 6
result : 4.268548488616943
frame 5 : frame 7
result : 3.995980978012085
frame 5 : frame 8
result : 4.199228286743164
frame 5 : frame 9
result : 4.828934669494629
frame 5 : frame 10
result : 4.5621657371521
frame 5 : frame 11
result : 4.194313049316406
frame 5 : frame 12
result : 4.509161472320557
frame 5 : frame 13
result : 5.659115314483643
frame 5 : frame 14
result : 5.737384796142578
frame 5 : frame 15
result : 4.945915699005127
frame 5 : frame 16
result : 4.3587870597839355
frame 5 : frame 17
result : 4.202098369598389
frame 5 : frame 18
result : 4.6066508293151855
frame 5 : frame 19
result : 5.752995014190674
frame 6 : frame 7
result : 4.314727306365967
frame 6 : frame 8
result : 4.929575443267822
frame 6 : frame 9
result : 4.878720760345459

```

frame 6 : frame 10
result : 3.94209361076355
frame 6 : frame 11
result : 4.446964263916016
frame 6 : frame 12
result : 4.094987869262695
frame 6 : frame 13
result : 6.408860206604004
frame 6 : frame 14
result : 5.938652038574219
frame 6 : frame 15
result : 4.400593280792236
frame 6 : frame 16
result : 4.348577976226807
frame 6 : frame 17
result : 4.510675430297852
frame 6 : frame 18
result : 4.537966728210449
frame 6 : frame 19
result : 5.5725860595703125
frame 7 : frame 8
result : 3.7893753051757812
frame 7 : frame 9
result : 4.565632343292236
frame 7 : frame 10
result : 3.940666437149048
frame 7 : frame 11
result : 3.3908298015594482
frame 7 : frame 12
result : 3.729754686355591
frame 7 : frame 13
result : 6.005640983581543
frame 7 : frame 14
result : 5.557159900665283
frame 7 : frame 15
result : 3.567365884780884
frame 7 : frame 16
result : 3.567272901535034
frame 7 : frame 17
result : 4.344783306121826
frame 7 : frame 18
result : 4.462493896484375
frame 7 : frame 19
result : 5.4912428855896
frame 8 : frame 9
result : 5.461273670196533
frame 8 : frame 10
result : 4.021915912628174
frame 8 : frame 11
result : 3.5024149417877197

```

frame 8 : frame 12
result : 4.696935176849365
frame 8 : frame 13
result : 5.577124118804932
frame 8 : frame 14
result : 5.08076286315918
frame 8 : frame 15
result : 4.2954912185668945
frame 8 : frame 16
result : 3.2466771602630615
frame 8 : frame 17
result : 4.313701629638672
frame 8 : frame 18
result : 4.122776031494141
frame 8 : frame 19
result : 5.159609317779541
frame 9 : frame 10
result : 5.417654514312744
frame 9 : frame 11
result : 5.187352657318115
frame 9 : frame 12
result : 3.016108274459839
frame 9 : frame 13
result : 6.026569843292236
frame 9 : frame 14
result : 5.494571208953857
frame 9 : frame 15
result : 5.2087225914001465
frame 9 : frame 16
result : 4.4334282875061035
frame 9 : frame 17
result : 5.8470587730407715
frame 9 : frame 18
result : 5.466747283935547
frame 9 : frame 19
result : 4.8923163414001465
frame 10 : frame 11
result : 3.2304131984710693
frame 10 : frame 12
result : 4.519182205200195
frame 10 : frame 13
result : 6.037379264831543
frame 10 : frame 14
result : 5.521186828613281
frame 10 : frame 15
result : 3.818498134613037
frame 10 : frame 16
result : 3.8310060501098633
frame 10 : frame 17
result : 3.5762393474578857

```

frame 10 : frame 18
result : 4.495012283325195
frame 10 : frame 19
result : 5.644600868225098
frame 11 : frame 12
result : 4.072977542877197
frame 11 : frame 13
result : 5.786230087280273
frame 11 : frame 14
result : 5.278048515319824
frame 11 : frame 15
result : 3.649400234222412
frame 11 : frame 16
result : 2.8713486194610596
frame 11 : frame 17
result : 3.7031569480895996
frame 11 : frame 18
result : 4.4038615226745605
frame 11 : frame 19
result : 5.847635746002197
frame 12 : frame 13
result : 5.93612813949585
frame 12 : frame 14
result : 5.3070902824401855
frame 12 : frame 15
result : 4.156188011169434
frame 12 : frame 16
result : 3.4400064945220947
frame 12 : frame 17
result : 5.0320820808410645
frame 12 : frame 18
result : 4.883937835693359
frame 12 : frame 19
result : 4.670203685760498
frame 13 : frame 14
result : 3.4389467239379883
frame 13 : frame 15
result : 6.089236736297607
frame 13 : frame 16
result : 5.500631809234619
frame 13 : frame 17
result : 6.611961364746094
frame 13 : frame 18
result : 6.165401458740234
frame 13 : frame 19
result : 5.500183582305908
frame 14 : frame 15
result : 5.607179641723633
frame 14 : frame 16
result : 5.008121967315674


```

frame 14 : frame 17
result : 6.060944080352783
frame 14 : frame 18
result : 5.568432807922363
frame 14 : frame 19
result : 5.247612476348877
frame 15 : frame 16
result : 3.977944850921631
frame 15 : frame 17
result : 3.7890114784240723
frame 15 : frame 18
result : 4.672051429748535
frame 15 : frame 19
result : 5.712950229644775
frame 16 : frame 17
result : 4.6188812255859375
frame 16 : frame 18
result : 4.223783016204834
frame 16 : frame 19
result : 4.848609447479248
frame 17 : frame 18
result : 4.117199420928955
frame 17 : frame 19
result : 6.435068130493164
frame 18 : frame 19
result : 5.9046430587768555

```

Part 5: In this section, we will develop a procedure to calculate and print various values, including dihedral angles (phi, psi, omega), amino acid names and numbers, and the radius of gyration. We will focus on atoms that form hydrogen bonds with a maximum distance of 3.4 Å between them, allowing for a tolerance of up to 10 degrees in their angles.

Code:

```

proc hydrogen_show { id } {

    set hbonds [measure hbonds 20 3.4 [atomselect $id all]];
    set hbond_atoms {};
    set donor_index [lindex $hbonds 0];
    set acceptor_index [lindex $hbonds 1];

    lappend hbond_atoms [concat $donor_index $acceptor_index] ;

    set unique_hbond_atoms [lsort -unique [lindex $hbond_atoms 0]];

    set hyd_atoms [atomselect $id "index $unique_hbond_atoms"];
    puts "{resid resname phi psi structure} :
\n [ $hyd_atoms get {resid resname phi psi structure}];
    set min_resid [lindex [lsort -unique -real
[[atomselect $id all] get resid]] 0];

```

```

set hyd_atoms_res [$hyd_atoms get resid];
set omega_list {}
foreach i $hyd_atoms_res {
    if {$i > $min_resid} {

        set sel_resi_min [atomselect $id "resid [expr $i-1] and name CA"];
        set sel_C [atomselect $id "resid $i and name C"];
        set sel_N [atomselect $id "resid $i and name N"];
        set sel_resi_plus [atomselect $id "resid $i and name CA"];
        lappend omega_list [measure dihedral [$sel_resi_min get index]
        [$sel_C get index] [$sel_N get index] [$sel_resi_plus get index]];

    } else {
        lappend omega_list "OUT OF RANGE";
    }

}
puts "\nOMEGA : \n$omega_list";
puts "\nRadius of gyration [measure rgyr $hyd_atoms]" ;
}

```

Result:

```

{resid resname phi psi structure} :
{75 PHE -74.63381958007812 -23.3912296295166 H} {76 LYS
-95.77405548095703 -32.14047622680664 H} {76 LYS
-95.77405548095703 -32.14047622680664 H} {77 GLU
-93.66175079345703 -51.799560546875 H} {79 VAL
-106.42286682128906 148.68817138671875 C} {79 VAL
-106.42286682128906 148.68817138671875 C} {80 SER
-88.40367126464844 159.2229766845703 C} {80 SER
-88.40367126464844 159.2229766845703 C} {80 SER
-88.40367126464844 159.2229766845703 C} {81 THR
-54.043697357177734 -61.76611328125 H} {81 THR
-54.043697357177734 -61.76611328125 H} {82 GLN
-58.65222930908203 -34.35117721557617 H} {84 LEU
-72.50909423828125 -31.33561134338379 H} {84 LEU
-72.50909423828125 -31.33561134338379 H} {85 LEU
-60.991146087646484 -31.68219566345215 H} {85 LEU
-60.991146087646484 -31.68219566345215 H} {86 LEU
-61.835514068603516 -32.04574203491211 H} {86 LEU
-61.835514068603516 -32.04574203491211 H} {88 LEU
-70.07576751708984 -23.81214714050293 H} {89 THR
-62.36330795288086 -35.258079528808594 H} {113 LYS
-71.80187225341797 -41.92543029785156 H} {115 LEU
-72.69270324707031 -23.819318771362305 H} {125 LYS
-113.53621673583984 -41.25303268432617 C}

```

OMEGA :

```

-147.76174926757812 -139.7421875 -139.7421875

```

-140.9047393798828 -144.43211364746094
-144.43211364746094 -145.5150604248047 -145.5150604248047
-145.5150604248047 -155.26109313964844
-155.26109313964844 -153.88555908203125
-149.62771606445312 -149.62771606445312
-156.00828552246094 -156.00828552246094
-155.03668212890625 -155.03668212890625
-148.65994262695312 -150.6446533203125
-151.58103942871094 -154.14187622070312
-141.9339599609375

Radius of gyration 7.107532978057861

2023/6/8