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Ramachandran Plot in Python

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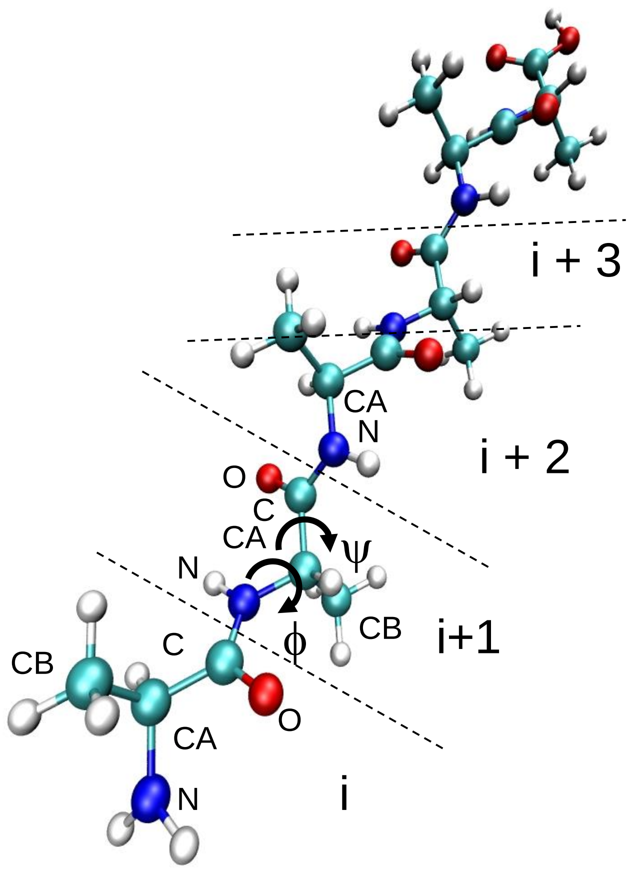
Ramachandra Plot

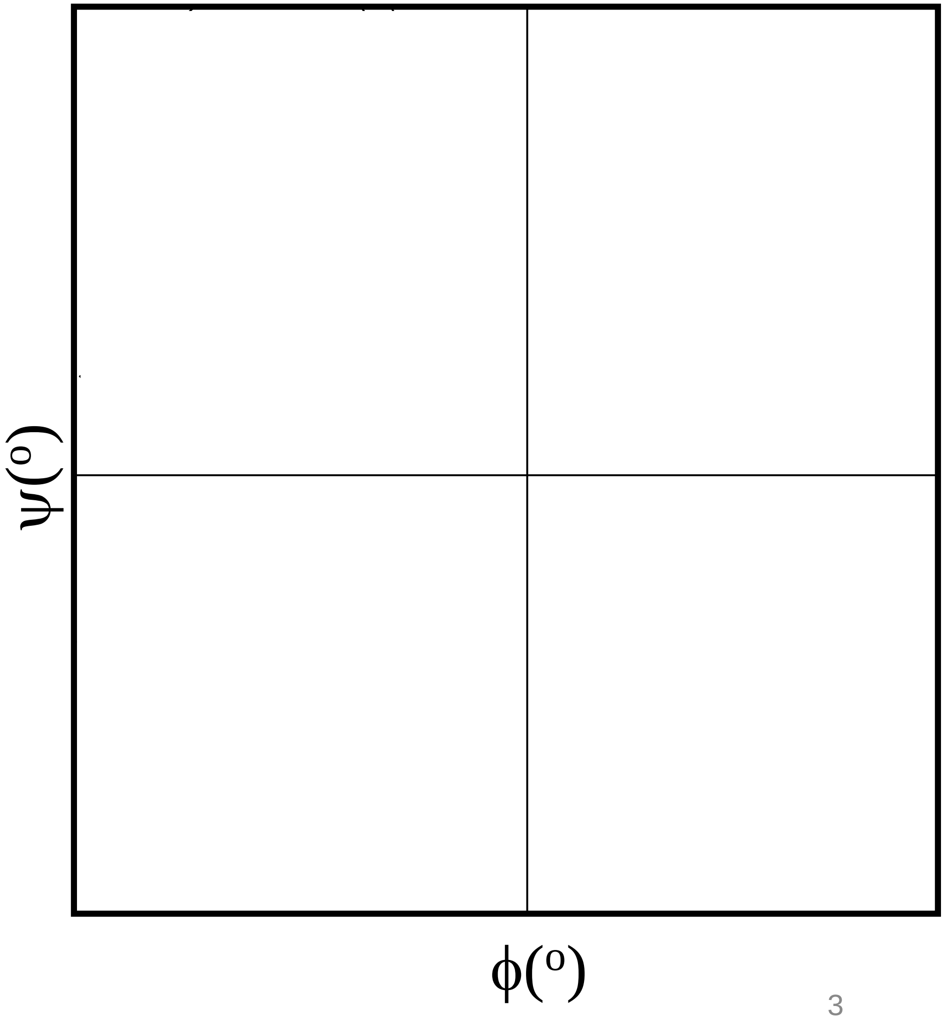
In the 1960s, G. N. Ramachandran, C. Ramakrishnan, and V. Sasisekharan (1963) proposed a methodology to evaluate stereochemical quality of protein models. The basic idea is to investigate the allowed regions for a two-dimensional plot of main-chain torsion angles. These torsion angles, referred to as phi and psi are illustrated in the figure on the right.



i is for residue number.

Ramachandra Plot

Here we describe a program written in Python to generate Ramachandran plots. Information to generate plots is based on the atomic coordinates of a protein structure in the PDB format. In the Ramachandran plot, the x-axis is for phi (ϕ) angle and y-axis is for psi (ψ). Both axis range from -180º to +180º, as shown in the plot on the right.



Protein Data Bank

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Below we have a typical line for atomic coordinates in a Protein Data Bank (PDB) file. Each field brings a specific information related to the atoms in the structure. These lines starts either with “ATOM ” or “HETATM” strings. Additional information for each field is given red.

```
ATOM      1  N   MET A   1     101.710 112.330  93.759  1.00 48.54           N
```

Columns ranging from 57 to 60 for occupancy, they are assigned to *line[56:60]* variable

Columns ranging from 32 to 53 for atomic coordinates, they are assigned to *line[30:38], line[38:46], line[46:54]* variables

Columns ranging from 23 to 26 for residue/ligand number, they are assigned to *line[22:26]* variable

Colum 22 for chain identification, it is assigned to *line[21:22]* variable

Columns ranging from 18 to 20 for residue or ligand name, they are assigned to *line[17:20]* variable

Columns ranging from 14 to 15 for atom name, they are assigned to *line[13:15]* variable

Columns ranging from 7 to 11 for atom order, they are assigned to *line[6:11]* variable

Columns ranging from 1 to 6 for “*ATOM *“ or “*HETATM” strings*, they are assigned to *line[0:6]* variable

Last fields are indicated below.

```
ATOM      1  N   MET A   1     101.710 112.330  93.759  1.00 48.54           N
```

Columns ranging from 62 to 65 for B-values, they are assigned to *line[61:65]* variable

Colunan 77-77 for chemical element, it is assigned to *line[76:77]* vairable

Besides the fields indicated beforehand, we have a field for segment identification, columns ranging from 73 to 76, which are assigned to *line[72:76]* variable. In addition, we have a field for atomic charge, columns ranging from 79 to 80), which are assigned to *line[78:80]* variable.

Ramachandran Plot

Program: *rama_plot.py*

Abstract
Program to generate two-dimensional plot of protein srtuctures. This program reads a file in the Protein Data Bank (PDB) (Berman, Westbrook, Feng *et al*. 2000; Berman, Battistuz, Bhat *et al*. 2002; Westbrook *et al*., 2003) format and generates the Ramachandran plot for the structure.

Program: *bfactor_plot.py (main program)*

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In the main program we call *read_PDB*() function, which reads a PDB file and returns a list with all lines that starts with “ATOM “. To calculate torsion angles, we call *calc_torsion()* function, which returns two arrays with torsion angles for each residue in the structure, and finally call *plot_2_arrays()* function. Below we have the main program.

```
# Main function
def main():
    # Call function to read PDB
    my_list_of_atoms = read_PDB()

    # Call function to calculate torsion angles
    phi,psi = calc_torsion(my_list_of_atoms)

    # Call function to plot torsion angles
    plot_2_arrays(phi,psi,"Phi(deg)","Psi(deg)")

# Main program
main()
```

Function: *read_PDB()*

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```
def read_PDB():
    """Function to read a PDB file"""
    # Import library
    import sys
    # Set up empty list
    my_atoms = []
    # Call read_file_name() function
    input_file_name = read_file_name()
    # Try to open PDB file
    try:
        # Open PDB file
        my_fo = open(input_file_name,"r")
    except IOError:
        print("Error! I can't find file ",input_file_name)
        sys.exit("Finishing program execution!")
    # Looping through PDB file content
    for line in my_fo:
        if line[0:6] == "ATOM  " or line[0:6] == "HETATM":
            my_atoms.append(line)
    # Close file
    my_fo.close()
    # Return list
    return my_atoms
```

Initially, we set up an empty list, named *my_atoms.* Then we call *read_file_name()* function, which reads the input file name. At this point, we open this file, and assigns its content to a file object, named *my_fo.*
After we have for loop, which loops through *my_fo* and assigns all coordinate lines to *my_atoms* list. Then, we close the file and return *my_atoms* list..

Function: *read_file_name()*

This funciton is quite simple, it only reads the input file name and returns it, as shown below.

```
def read_file_name():
    """Function to read file name"""

    # Read input file name
    my_file = input("Type input file name => ")

    # Return input file name
    return my_file
```

Function: *calc_torsion()*

```
def calc_torsion(list_of_atoms_in):
    """Function to calculate torsion angles"""
    # Import library
    import numpy as np
    # We have the number of rows and number of columns equal to 3
    # matrix = [[0]*column for i in range(row)]
    columns = 3
    rows = 9999
    co    = np.array([[0]*columns]*rows,float)
    n    = np.array([[0]*columns]*rows,float)
    ca   = np.array([[0]*columns]*rows,float)
    # Set up counts
    count_res = 0
    former_res = -9999
    new_res = -9998
    found_co = 0
    found_n = 0
    found_ca = 0
```

This function has more than 50 lines, so we divide the presentation in several slides.
These lines set up arrays and counts.

Function: *calc_torsion()*

```
# Looping through list_of_atoms_in
for line in list_of_atoms_in:
    if line[0:6] == "ATOM  " and line[13:15] == "C ":
        co[count_res,0] = float(line[30:38])
        co[count_res,1] = float(line[38:46])
        co[count_res,2] = float(line[46:54])
        new_res = int(line[22:26])
        found_co = 1
    elif line[0:6] == "ATOM  " and line[13:15] == "N ":
        n[count_res,0] = float(line[30:38])
        n[count_res,1] = float(line[38:46])
        n[count_res,2] = float(line[46:54])
        new_res = int(line[22:26])
        found_n = 1
    elif line[0:6] == "ATOM  " and line[13:15] == "CA":
        ca[count_res,0] = float(line[30:38])
        ca[count_res,1] = float(line[38:46])
        ca[count_res,2] = float(line[46:54])
        found_ca =1
        new_res = int(line[22:26])
    complete_mc = found_co*found_n*found_ca
    if former_res != new_res and complete_mc:
        former_res = new_res
        count_res += 1
        found_co = 0
        found_n = 0
        found_ca = 0
```

In this for loop, we select main-chain and side-chain atoms.

Function: *calc_torsion()*

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```
# Set up arrays for phi and psi angles
phi = np.zeros(count_res-1)
psi = np.zeros(count_res-1)

# Looping through phi psi atoms in each residue
for i in range(count_res-1):
    # Calls torsion function
    phi[i] = torsion(co[i],n[i+1],ca[i+1],co[i+1])
    psi[i] = torsion(n[i+1],ca[i+1],co[i+1],n[i+2])

# Show torsion angles
print("Atomic coordinates for atoms N, CA and C\n")
print("Residue\tN[  x\t   y        z\t ]     CA[   x\t   y        z\t ]      C[  x\t   y        z\t ]")
for i in range(count_res-1):
    print(i+1,"\t",n[i],"\t",ca[i],"\t",co[i])

# Return arrays
return phi,psi
```

The atomic coordinates are then used to calculate torsion angles. We call the *torsion()* function to carry out phi and psi calculation.
This function returns phi and psi arrays.

```python
def torsion(p1,p2,p3,p4):
    """Function to calculate torsion angle for atoms a,b,c, and d"""
    # Equation from http://www.stem2.org/je/proteina.pdf
    # Import libraries
    import numpy as np
    import math
    # Get coordinates for vectors q1, q2 and q3
    q1 = np.subtract(p2,p1) # b - a
    q2 = np.subtract(p3,p2) # c - b
    q3 = np.subtract(p4,p3) # d - c
    # Calculate cross vectors
    q1_x_q2 = np.cross(q1,q2)
    q2_x_q3 = np.cross(q2,q3)
    n1 = q1_x_q2/np.sqrt(np.dot(q1_x_q2,q1_x_q2))
    n2 = q2_x_q3/np.sqrt(np.dot(q2_x_q3,q2_x_q3))
    # Calculate unit vectors
    u1 = n2
    u3 = q2/(np.sqrt(np.dot(q2,q2)))
    u2 = np.cross(u3,u1)
    # Calculate cosine and sine
    cos_theta = np.dot(n1,u1)
    sin_theta = np.dot(n1,u2)
    # Calculate torsion angle
    theta = -math.atan2(sin_theta,cos_theta)    # it is different from atan2 from fortran
    theta_deg = np.degrees(theta)
    # Show results
    print("theta (rad) = ",theta)
    print("theta (deg) = ",theta_deg)
    # Return torsion angle in degrees
    return theta_deg
```

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This function calculates torsion angles, based on the coordinates of four points. It returns angle as a float. Details about torsion angle equation are given here.

Function: *plot_2_arrays()*

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```
def plot_2_arrays(x,y,x_label_in,y_label_in):
    """Function to plot two one-dimensional arrays"""
    # Import libraries
    import matplotlib.pyplot as plt
    import numpy as np
    # Generate plot
    plt.plot(x,y,".")
    plt.xlim(-180,180)      # Sets axis limits
    plt.ylim(-180,180)      # Sets axis limits
    plt.xticks(np.arange(-180.1,180.1,30))  # Sets ticks markers for x axis
    plt.yticks(np.arange(-180.1,180.1,30))  # Sets ticks makers for y axis
    plt.xlabel(x_label_in)    # Adds axis label
    plt.ylabel(y_label_in)    # Adds axis label
    plt.arrow(-180,0,360,0)   # Creates an arrow
    plt.arrow(0,-180,0,360)   # Creates an arrow
    # Show plot
    plt.show()

    # Create a file for plot
    fig = plt.gcf()                   # Creates a figure
    fig.set_size_inches(7.0, 7.0)     # Changes figure size
    fig.savefig('rama.png', dpi=300)  # Saves figures
```

This function plots two arrays, phi and psi.

Running *rama_plot.py*

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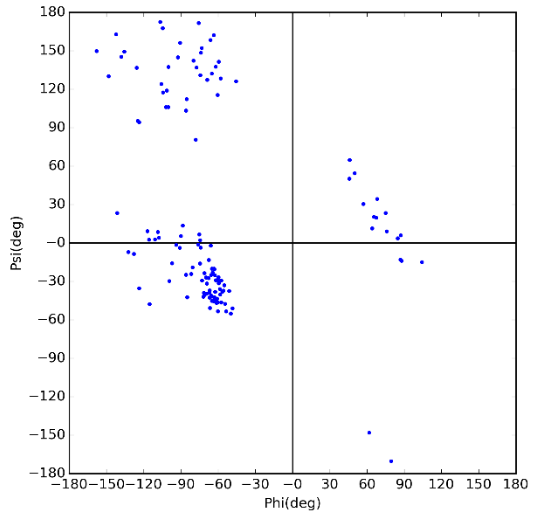
To run *rama_plot.py,* type *python rama_plot.py*, and then type the PDB file name, as shown below.

```
C:\Users\Walter>python rama_plot.py
Type input file name => 1kxy.pdb
C:\Users\Walter>
```

The plot is generated and shown on the screen, as we can see below.
To run this tutorial, you need the following files: *rama_plot.py and 1KXY.pdb.*
All files should be in the same folder.



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Colophon

This text was produced in a DELL Inspiron notebook with 6GB of memory, a 750 GB hard disk, and an Intel® Core® i5-3337U CPU @ 1.80 GHz running Windows 8.1. Text and layout were generated using PowerPoint 2013 and graphical figures were generated by *Visual Molecular Dynamics (VMD)(http://www.ks.uiuc.edu/Research/vmd/)*. This tutorial uses Arial font.

Author

I graduated in Physics (BSc in Physics) at University of Sao Paulo (USP) in 1990. I completed a Master Degree in Applied Physics also at USP (1992), working under supervision of Prof. Yvonne P. Mascarenhas, the founder of crystallography in Brazil.
My dissertation was about X-ray crystallography applied to organometallics compounds (De Azevedo Jr. *et al.*,1995).
During my PhD I worked under supervision of Prof. Sung-Hou Kim (University of California, Berkeley. Department of Chemistry), on a split PhD program with a fellowship from Brazilian Research Council (CNPq)(1993-1996). My PhD was about the crystallographic structure of CDK2 (Cyclin-Dependent Kinase 2) (De Azevedo Jr. *et al.*,1996). In 1996, I returned to Brazil. In April 1997, I finished my PhD and moved to Sao Jose do Rio Preto (SP, Brazil) (UNESP) and worked there from 1997 to 2005. In 1997, I started the Laboratory of Biomolecular Systems-Department of Physics-UNESP - São Paulo State University. In 2005, I moved to Porto Alegre/RS (Brazil), where I am now. My current position is coordinator of the Laboratory of Computational Systems Biology at Pontifical Catholic University of Rio Grande do Sul (PUCRS). My research interests are focused on application of computer simulations to analyze protein-ligand interactions. I'm also interested in the development of biological inspired computing and machine learning algorithms. We apply these algorithms to molecular docking simulations, protein-ligand interactions and other scientific and technological problems. I published over 160 scientific papers about protein structures and computer simulation methods applied to the study of biological systems (H-index: 36). These publications have over 4000 citations. I am editor for the following journals: