The phi angle is the dihedral angle formed between the Cα-N bonds through interactions between 2 conjoining amino acids. The psi angle is the dihedral angle formed between the Cα-C bond through interactions of the N-C-Ca-N atoms between 2 conjoining amino acids.

To acquire dihedral angles from your PDB file, you can use biopython. For this example, the PDB file for protein 4N6N was used. You can download the PDB file for your protein of interest on the RCSB PDB website: https://www.rcsb.org/structure/4N6N

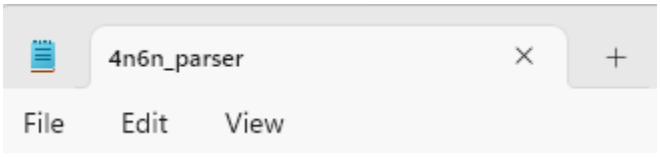
You will need Biopython to access PDBParser to extract the necessary data from your PDB file. For the pdb_file_path, you can replace the example file with the path to your own PDB file. PDBParser module source found here: https://warwick.ac.uk/fac/sci/moac/people/students/peter_cock/python/ramachandran/calculate/#BioPython (Note: this code was edited to include a file path)

```python
import Bio.PDB
from Bio.PDB import PDBParser

#PDB file reader

def main():
    pdb_file_path = r"C:\Users\Tania\Documents\Bioinformatics\Protein Bioinformatics\4n6n.pdb"
    parser = PDBParser
    structure = parser.get_structure('protein', pdb_file_path)

for model in Bio.PDB.PDBParser().get_structure("4N6N", r"C:\Users\Tania\Documents\Bioinformatics\Protein Bioinformatics\4n6n.pdb") :
    for chain in model :
        polypeptides = Bio.PDB.PPBuilder().build_peptides(chain)
        for poly_index, poly in enumerate(polypeptides) :
            print ("Model %s Chain %s" % (str(model.id), str(chain.id))),
            print ("(part %i of %i)" % (poly_index+1, len(polypeptides))),
            print ("length %i" % (len(poly))),
            print ("from %s%i" % (poly[0].resname, poly[0].id[1])),
            print ("to %s%i" % (poly[-1].resname, poly[-1].id[1]))
            phi_psi = poly.get_phi_psi_list()
            for res_index, residue in enumerate(poly) :
                res_name = "%s%i" % (residue.resname, residue.id[1])
                print (res_name, phi_psi[res_index])
```

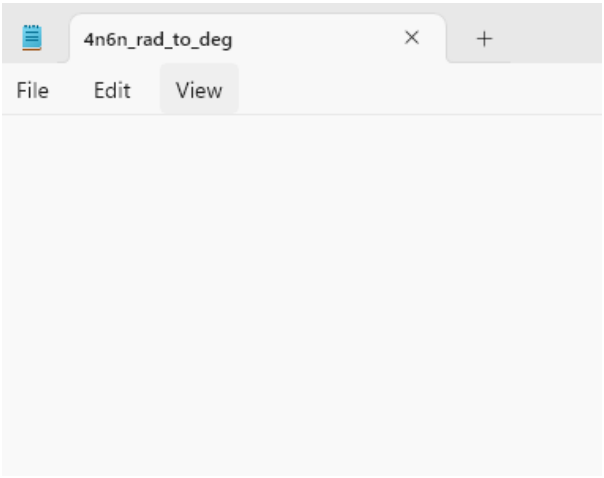
After inputting your PDB file into this program, you will then receive an output in the program's terminal. You can then copy and paste the output onto a notepad file:

```
Model 0 Chain A
(part 1 of 3)
length 121
from GLY26
to THR146
GLY26 (None, 1.0759131600635423)
GLY27 (2.8422732602553893, 2.9856141150538598)
LYS28 (-1.9517648336615823, -0.6906251709242297)
HIS29 (-1.9302022284973064, 2.2007684160610483)
TRP30 (-2.0732327665778563, 2.650215320451784)
VAL31 (-2.4162259146490466, 2.395793416914984)
VAL32 (-2.1330254415311902, 2.1731421536833757)
ILE33 (-2.0407257577051925, 2.2581105674424204)
VAL34 (-2.3061751528296757, 2.153831893010605)
ALA35 (-1.7729260469564396, 2.1494923222449174)
GLY36 (-1.6199425540794166, -0.03903658630951815)
SER37 (-2.1145335192433343, 3.015055398716476)
ASN38 (-2.527169761807301, 3.1260876121695396)
GLY39 (1.5942406541362533, 2.5917420370869575)
TRP40 (-1.0654963052734547, -0.6762101666031828)
TYR41 (-1.2977216694369518, -0.1639781628660284)
ASN42 (-1.737149536985012, 0.2872948825757097)
TYR43 (-0.5586304277469437, -0.9048439666303671)
ARG44 (-0.9044543516813437, -0.6351005050579855)
HIS45 (-1.226539914117705, -0.6952058629868663)
GLN46 (-1.3281735185430106, -0.5627384897993521)
```

The output of the PDBParser will come out as radians. Save this file as a .txt input file. You will need this input for interpretation by the next module. See the input .txt file example:



For the next step, create a .txt output. This file will receive data output. Copy the path of this file, then replace the “output_file_path” of the next 2 coding packages with this file.



Based on what you’ve titled your .txt files, they should look like this:

```
input_file_path = r"C:\Users\Tania\Documents\4n6n_parser.txt" #replace your input file path with where you saved the radian coordinates data in your PC
output_file_path = r"C:\Users\Tania\Documents\4n6n_rad_to_deg.txt" #replace your output file path with a .txt document in which you want to save your degree conversions in your PC
convert_rads_to_degs(input_file_path, output_file_path)
```

Add your files to the “radians-to-degrees-converter” below:

```
import numpy as np
import re

#Radiants to degrees coordinate converter

def convert_rads_to_degs(input_file_path, output_file_path):
    with open(input_file_path, 'r') as input_file:
        lines = input_file.readlines()

    convert_coords = []

    for line in lines:
        parts = line.strip().split(' ')
        residue_name = parts[0]
        radian_coords = parts[1:]

        converted_coords = []
        for coord in radian_coords:
            if coord.lower() == 'none':
                converted_coords.append('None')
            else:
                real_coord = re.sub(r'[^-.\d]+', '', coord)
                try:
                    converted_coords.append(str(np.degrees(float(real_coord))))
                except ValueError:
                    converted_coords.append('None')

        converted_line = ' '.join([residue_name] + converted_coords)

        convert_coords.append(converted_line)

    with open(output_file_path, 'w') as output_file:
        output_file.write('\n'.join(convert_coords))

input_file_path = r"C:\Users\Tania\Documents\4n6n_parser.txt" #replace your input file path with where you saved the radian coordinates data in your PC
output_file_path = r"C:\Users\Tania\Documents\4n6n_rad_to_deg.txt" #replace your output file path with a .txt document in which you want to save your degree conversions in your PC
convert_rads_to_degs(input_file_path, output_file_path)

```

After inputting your file from the previous program, you will receive an output file like this:

```
GLY26 None 61.64528319422437
GLY27 162.85026203552243 171.06308804727234
LYS28 -111.82788757086182 -39.569907519459456
HIS29 -110.5924412996418 126.09474192598925
TRP30 -118.78748747314252 151.84615266279823
VAL31 -138.43954725952744 137.26885137445504
VAL32 -122.21335539376615 124.51187368802755
ILE33 -116.92497306014457 129.38020518834213
VAL34 -132.13410307507803 123.40547725018033
ALA35 -101.58117987941681 123.15683816040809
GLY36 -92.81587140239368 -2.23663164213356
SER37 -121.1538462915881 172.74994934458772
ASN38 -144.79616146463988 179.11162656544394
GLY39 91.3432610101829 148.49588031172115
TRP40 -61.048441378951715 -38.743988610200624
TYR41 -74.3539746414087 -9.395256664532267
ASN42 -99.5313368523463 16.46078424729474
TYR43 -32.00716581748775 -51.84374040579633
ARG44 -51.821417113582086 -36.38857850644956
HIS45 -70.27556048328294 -39.83236184189761
GLN46 -76.09873707355509 -32.242540435068605
ALA47 -64.55256967509463 -43.637017993739626
ASP48 -52.90422089706059 -53.286917505464686
ALA49 -62.29690318312271 -40.562195939988115
CYS50 -64.37234077218275 -44.15034263085482
```