

DIHEDRAL(TORSION ANGLES)

Introduction :

A dihedral angle is formed by three consecutive bonds in a molecule and defined by the angle created between the two outer bonds. The backbone of a protein has three different torsion angles.

These angles are called ϕ (phi) which involves the backbone atoms C-N-C α -C, and ψ (psi) which involves the backbone atoms N-C α -C-N, (ω) omega C α -C-N-C α .

API's :

- **MTA.Dihedral.calculateAngle**

INPUT: X,Y,Z Co-ordinates of 4 atoms.

OUTPUT: Dihedral angle between these atoms.

DESCRIPTION: Using Vector of Vector of X,Y,Z co-ordinates of four atoms, this will compute dihedral angle.

- **MTA.DihedralBackbone.phiAngle**

INPUT: PDB file.

OUTPUT: DATAFRAME containing the phi angles.

DESCRIPTION: **PHI** (ϕ) angle is between "C-N-C α -C" backbone atoms. It will extract X,Y,Z co-ordinates of these atoms inside residues or chain and pass it to **calculateAngle** to calculate angle.

- **MTA.DihedralBackbone.psiAngle**

INPUT: PDB file

OUTPUT: DATAFRAME containing psi angles.

DESCRIPTION: **PSI** (ψ) angle is between "N-C α -C-N" backbone atoms. It will extract X,Y,Z co-ordinates of these atoms inside residues or chain and pass it to **calculateAngle** to calculate angle.

- **MTA.DihedralBackbone.omegaAngle**

INPUT: PDB file.

OUTPUT: DATAFRAME containing omega angles.

DESCRIPTION: **OMEGA** (ω) angle is between "C α -C-N-C α " atoms. It will extract X,Y,Z co-ordinates of these atoms inside residues or chain and pass it to **calculateAngle** to calculate angle.

- **MTA.DihedralSpecifiedSet.getAngle**

INPUT: PDB file and 4 ATOMS as specified set.

OUTPUT: DATAFRAME containing dihedral angle between all set of these atoms.

DESCRIPTION: It will extract X,Y,Z co-ordinates of these specified 4 atoms inside residues or chain and pass it to **calculateAngle** to calculate angle.

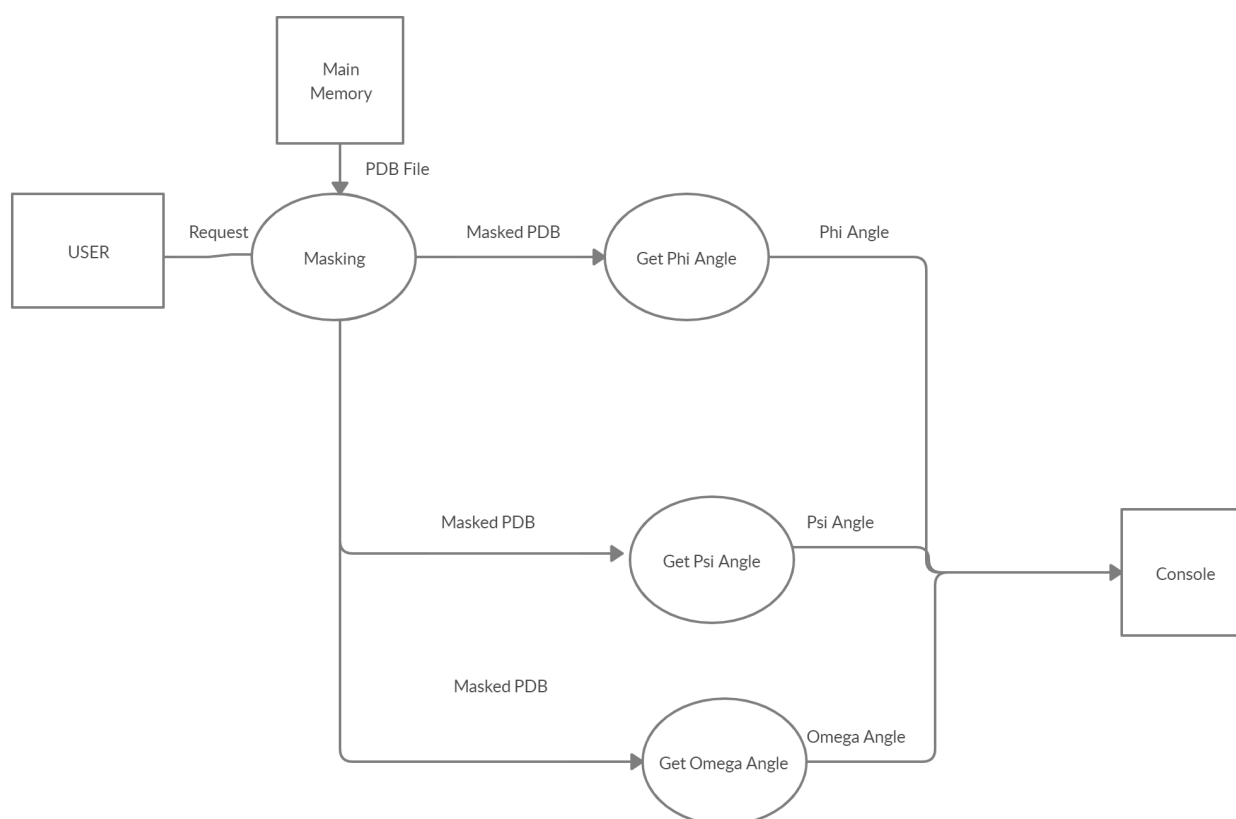
Output Format :- DATAFRAME containing dihedral angles.

Atom	Res.	Res.No.	Atom	Res.	Res.No.	Atom	Res.	Res.No.	Atom	Res.	Res.No.	Dihedral Angle
N	ALA	1	CA	ALA	1	C	ALA	1	N	PHE	2	X ANGLE (PSI)
CA	ALA	1	C	ALA	1	N	PHE	2	CA	PHE	2	Y ANGLE (OME)
C	ALA	1	N	PHE	2	CA	PHE	2	C	PHE	2	Z ANGLE (PHI)

Dependencies :-

- Masking Module
- Breeze Library for Vector Mathematics.

Data Flow Diagram :-



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