NAME

PyMOLCalculatePhiPsiAngles.py - Calculate phi and psi torsion angles

SYNOPSIS

PyMOLCalculatePhiPsiAngles.py [--chainIDs <First, All or ID1,ID2...>] [--outMode <SingleFile or MultipleFies>] [--outChainID <yes or no>] [--outCategory <yes or no>] [--overwrite] [--precision <number>] [-w <dir>] -i <infile> -o <outfile>

PyMOLCalculatePhiPsiAngles.py -h | --help | -e | --examples

DESCRIPTION

Calculate phi and psi torsion angels for amino acid residues present in macromolecules.

The phi and psi angles are categorized into the following groups corresponding to four types of Ramachandran plots:

```
General: All residues except glycine, proline, or pre-proline
Glycine: Only glycine residues
Proline: Only proline residues
Pre-Proline: Only residues before proline not including glycine or
    proline
```

The supported input file format are: PDB (.pdb), mmCIF (.cif)

The supported output file formats are: CSV (.csv), TSV (.tsv, .txt)

OPTIONS

-c, --chainIDs <First, All or ID1,ID2...> [default: All]

List of chain IDs to use for calculating phi and psi angles for residues in chains. Possible values: First, All, or a comma delimited list of chain IDs. The default is to use all chain IDs in input file.

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

-o, --outfile <outfile>

Output file name for writing out calculated values. Supported text file extensions: csv, tsv or txt.

In addition to the specified outfile containing phi and psi angles for all residues, a set of additional output files is generated for 'MultipleFiles' value of '--outMode' option. The names of these output files are automatically generated from the the name of the specified output file as shown below:

```
General: <OutfileRoot>_General.<OutfileExt>
Glycine: <OutfileRoot>_Glycine.<OutfileExt>
Proline: <OutfileRoot>_Proline.<OutfileExt>
Pre-Proline: <OutfileRoot>_PreProline.<OutfileExt>
```

--outMode <SingleFile or MultipleFiles> [default: SingleFile]

A single output file containing phi and psi angles for all residues or multiple output files corresponding to different categories of angles.

The phi and psi angles are categorized into the following groups corresponding to four types of Ramachandran plots:

```
General: All residues except glycine, proline, or pre-proline
Glycine: Only glycine residues
Proline: Only proline residues
Pre-Proline: Only residues before proline not including glycine or
    proline
```

The output files contain the following information:

```
ChainID ResNum ResName Phi Psi Category
```

--outChainID <yes or no> [default: yes]

Write chain IDs to output file.

--outCategory <yes or no> [default: yes]

Write phi and psi category to output file.

--overwrite

Overwrite existing files.

-p, --precision <number> [default: 2]

Floating point precision for writing the calculated phi and psi angles.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To calculate phi and psi angles for all residues across all chains in input file and write out a single CSV file containing calculated values along with chain IDs, residue names and numbers, and category of angles corresponding to Ramachandran plots, type:

```
% PyMOLCalculatePhiPsiAngles.py -i Sample3.pdb -o Sample3Out.csv
```

To calculate phi and psi angles for all residues across all chains in input file and write out a multiple CSV files corresponding to categories of angles for Ramachandran plots along with other relevant information, type:

```
% PyMOLCalculatePhiPsiAngles.py --outMode MultipleFiles -i Sample3.pdb
  -o Sample3Out.csv
```

To calculate phi and psi angles for all residues in a specific chain in input file and write out a single TSV file containing calculated values along with other relevant information, type:

```
% PyMOLCalculatePhiPsiAngles.py -c E  -i Sample3.pdb -o Sample3Out.csv
```

To calculate phi and psi angles for all residues in a specific chain in input file and write out a multiple TSV files containing calculated values at a specific precision along with other relevant information, type:

```
% PyMOLCalculatePhiPsiAngles.py --outMode MultipleFiles --chainIDs I
  -i Sample3.pdb -o Sample3Out.csv
```

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SEE ALSO

DownloadPDBFiles.pl, PyMOLCalculateRMSD.py, PyMOLCalculateProperties.py, PyMOLGenerateRamachandranPlots.py

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The functionality available in this script is implemented using PyMOL, a molecular visualization system on an open source foundation originally developed by Warren DeLano.

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