NAME

PyMOLCalculateRMSD.py - Calculate RMSD between macromolecules

SYNOPSIS

PyMOLCalculateRMSD.py [--alignMethod <align, cealign, super>] [--alignMode <FirstChain or Complex>] [--mode <OneToOne, AllToAll, FirstToAll>] [--outMatrix <yes or no>] [--overwrite] [-w <dir>] -p <probefile1,probefile2,probefile3...> -r <reffile1,reffile2,reffile3...> -o <outfile>

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

DESCRIPTION

Calculate Root Mean Square Distance (RMSD) between a set of similar macromolecules in reference and probe input files. The probe and reference files are spatially aligned before the the calculation of RMSD values.

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

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

OPTIONS

-a, --alignMethod <align, cealign, super> [default: super]

Alignment methodology to use for aligning probe input files to reference files.

--alignMode <FirstChain or Complex> [default: FirstChain]

Portion of probe and reference files to use for spatial alignment of probe files against reference files. Possible values: FirstChain or Complex.

The FirstChain mode allows alignment of the first chain in probe files to the first chain in reference files along with moving the rest of the complex to coordinate space of the reference files. The complete complex in probe files is aligned to the complete complex in reference files for the Complex mode.

-e, --examples

Print examples.

-h, --help

Print this help message.

-m, --mode <OneToOne, AllToAll, FirstToAll> [default: OneToOne]

Specify how reference and probe input files are handled during the calculation of RMSD between reference and probe files. Possible values: OneToOne, AllToAll and AllToFirst. For OneToOne mode, the number of reference input files must be equal to the number of probe input files. The RMSD is calculated for each pair of reference and probe file and written to the output file. For AllToAll mode, the RMSD is calculated for each reference input file against all probe input files. For FirstToAll mode, however, the RMSD is only calculated for the first reference input file against all probe files.

-p, --probefiles <probefile1,probefile2,probelfile3...>

A comma delimited list of probe input files. The wildcards are also allowed in file names.

-r, --reffiles <reffile1,reffile2,reffile3...>

A comma delimited list of reference input files. The wildcards are also allowed in file names.

-o, --outfile <outfile>

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

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

Output file in a matrix format during 'AllToAll' value for '-m, --mode' option.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To calculate RMSD between pair of macromolecules in reference and probe files using only first chain in each file and write out a CSV file containing calculated RMSD values along with IDs, type:

```
% PyMOLCalculateRMSD.py  -r "Sample3.pdb,Sample4.pdb,Sample5.pdb"
  -p "Sample3.pdb,Sample4.pdb,Sample5.pdb" -o SampleOut.csv
```

To calculate RMSD between all macromolecules in reference and probe files using complete complex and write out a CSV matrix file, type:

```
% PyMOLCalculateRMSD.py  -m AllToAll --alignMode Complex
   --outMatrix Yes -r "Sample3.pdb,Sample4.pdb,Sample5.pdb"
  -p "Sample3.pdb,Sample4.pdb" -o SampleOut.csv
```

To calculate RMSD between macromolecule in first reference against all probe files using only first chain in each file and write out a TSV file containing calculated RMSD values along with IDs, type:

```
% PyMOLCalculateRMSD.py  -m FirstToAll
  -r "Sample3.pdb,Sample4.pdb,Sample5.pdb"
  -p "Sample3.pdb,Sample4.pdb,Sample5.pdb" -o SampleOut.tsv
```

To calculate RMSD between pair of macromolecules in reference and probe files using only first chain in each file along with a specific alignment method and write out a CSV file containing calculated RMSD values, type:

```
% PyMOLCalculateRMSD.py  --alignMethod align
  -r "Sample3.pdb,Sample4.pdb,Sample5.pdb"
  -p "Sample3.pdb,Sample4.pdb,Sample5.pdb" -o SampleOut.csv
```

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SEE ALSO

PyMOLAlignChains.py, PyMOLSplitChainsAndLigands.py, PyMOLVisualizeMacromolecules.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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