

NAME

PyMOLAlignChains.py - Align chains

SYNOPSIS

```
PyMOLAlignChains.py [--alignMethod <align, cealign, super>] [--alignMode <FirstChain or Complex>] [
--alignRefFile <filename>] [--outSuffix <text>] [--overwrite] [-w <dir>] -i <infile1,infile2,infile3...>
```

```
PyMOLAlignChains.py -h | --help | -e | --examples
```

DESCRIPTION

Align chains in input files to a reference file and write out aligned files.

The supported input and output file format are: PDB (.pdb), CIF(.cif)

The names of the aligned output files are automatically generated from the names of input as shown below:

```
<InfileRoot><OutSuffux>.pdb
Default: <InfileRoot>_Aligned.pdb
```

OPTIONS

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

Alignment methodology to use for aligning input files to a reference file.

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

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

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

--alignRefFile <filename> [default: FirstInputFile]

Reference input file name. The default is to use the first input file name specified using '-i, --infiles' option.

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infiles <infile1,infile2,...>

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

--outSuffix <text> [default: _Aligned]

Suffix to append to input file root for generating name of output file.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To align first chain in all input files to the first chain in first input file and write out aligned output files, type:

```
% PyMOLAlignChains.py -i "Sample3.pdb,Sample4.pdb,Sample5.pdb"
```

To align first chain in all input files to the first chain in specific reference file and write out aligned output files, type:

```
% PyMOLAlignChains.py --alignRefFile Sample5.pdb
```

```
-i "Sample3.pdb,Sample4.pdb,Sample5.pdb"
```

To align first chain in all input files to the first chain in first input file using a specific alignment method and write out aligned output files with specific suffix in names, type:

```
% PyMOLAlignChains.py --alignMethod cealign --outSuffix "_aligned"
-i "Sample3.pdb,Sample4.pdb,Sample5.pdb"
```

To align all chains in each input files to all chains in first input file and write out aligned output files, type:

```
% PyMOLAlignChains.py --alignMode Complex
-i "Sample3.pdb,Sample4.pdb,Sample5.pdb"
```

AUTHOR

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SEE ALSO

PyMOLCalculateRMSD.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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