NAME

PyMOLMutateAminoAcids.py - Mutate amino acids

SYNOPSIS

PyMOLMutateAminoAcids.py [--mutations <Spec1,Spec2,...>] [--overwrite] [-w <dir>] -i <infile> -o <outfile>

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

DESCRIPTION

Mutate amino acids in macromolecules. The mutations are performed using protein mutagenesis wizard available in PyMOL.

The supported input and output file format is: PDB (.pdb)

OPTIONS

-m, --mutations <Spec1,Spec2,...> [default: None]

Comma delimited list of specifications for mutating amino acid residues in proteins.

The format of mutation specification is as follows:

```
<ChainID>:<ResName><ResNum><ResName>,...
```

A chain ID in the first specification of a mutation is required. It may be skipped in subsequent specifications. The most recent chain ID is used for the missing chain ID. The first reside name corresponds to the residue to be mutated. The second residue name represents the new residue. The residue number corresponds to the first residue name and must be present in the current chain.

Examples:

```
E:LEU49CYS, E:SER53TYR
E:LEU49CYS, SER53TYR
E:LEU49CYS, SER53TYR, I:TYR7SER, ILE11VAL
```

The residue names must be valid amino acid names. No validation is performed before mutating residues via protein mutagenesis wizard available in PyMOL.

-e, --examples

Print examples.

-h, --help

Print this help message.

-i, --infile <infile>

Input file name.

-o, --outfile <outfile>

Output file name.

--overwrite

Overwrite existing files.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To mutate a single residue in a specific chain and write a PDB file, type:

```
% PyMOLMutateAminoAcids.py -m "I:TYR7SER" -i Sample3.pdb
  -o Sample3Out.pdb
```

To mutate multiple residues in a single chain and write a PDB file, type:

```
% PyMOLMutateAminoAcids.py -m "I:TYR7SER, ILE11VAL" -i Sample3.pdb
  -o Sample3Out.pdb
```

To mutate multiple residues across multiple chains and write a PDB file, type:

```
% PyMOLMutateAminoAcids.py -m "E:LEU49CYS,SER53TYR,I:TYR7SER,ILE11VAL"
  -i Sample3.pdb -o Sample3Out.pdb
```

AUTHOR

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SEE ALSO

DownloadPDBFiles.pl, PyMOLMutateNucleicAcids.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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