

NAME

PyMOLInfoMacromolecules.py - List information about macromolecules

SYNOPSIS

```
PyMOLInfoMacromolecules.py [--all] [--boundingBox] [--chains] [--countResidues] [--header] [--inorganics] [--ligands] [
--pocketLigands] [--pocketDistanceCutoff <number>] [--pocketSolvents] [--pocketInorganics] [--solvents] [-w <dir>] -i
<infile1,infile2,infile3...>
```

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

DESCRIPTION

List information regarding ID, classification, experimental technique, chains, solvents, inorganics, ligands, and ligand binding pockets in macromolecules present including proteins and nucleic acids.

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

OPTIONS

-a, --all

All available information.

-b, --boundingBox

Min and max coordinates for bounding box along with its size.

-c, --chains

Number of chains and their IDs. This is also default behavior. --countResidues Number of residues across chains. The chain residues are identified using polymer selection operator available in PyMOL. In addition, the non-standard amino acid residues are listed.

-e, --examples

Print examples.

-h, --help

Print this help message. --header Header information including experimental technique information along with any available resolution. This is also default behavior.

-i, --infiles <infile1,infile2,infile3...>

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

--inorganics

Inorganic residues across chains. The inorganic residues are identified using inorganic selection operator available in PyMOL.

-l, --ligands

Ligands across chains. This is also default behavior. The ligands residues are identified using organic selection operator available in PyMOL.

-p, --pocketLigands

Chain residues in ligand pockets.

--pocketDistanceCutoff <number> [default: 5.0]

Distance in Angstroms for identifying pocket residues around ligands.

--pocketSolvents

Solvent residues in ligand pockets. The solvent residues are identified using solvent selection operator available in PyMOL.

--pocketInorganics

Inorganic residues in ligand pockets. The inorganic residues are identified using Inorganic selection operator available in PyMOL.

-s, --solvents

Solvent residues across chains. The solvent residues are identified using solvent selection operator available in PyMOL.

-w, --workingdir <dir>

Location of working directory which defaults to the current directory.

EXAMPLES

To list header, chains, and ligand information for macromolecules in input file, type:

```
% PyMOLInfoMacromolecules.py -i Sample3.pdb
```

To list all available information for macromolecules in input files, type:

```
% PyMOLInfoMacromolecules.py -a -i "Sample3.pdb,Sample4.pdb"
```

To list pockets residues information along with other default information for macromolecules in input file, type:

```
% PyMOLInfoMacromolecules.py -p --pocketDistanceCutoff 4.5  
--pocketSolvents --pocketInorganics -i Sample3.pdb
```

To list chain residues information along with other default information for macromolecules in input file, type:

```
% PyMOLInfoMacromolecules.py -c --countResidues --solvents  
--inorganics -i "Sample3.pdb,Sample4.pdb"
```

AUTHOR

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SEE ALSO

DownloadPDBFiles.pl, 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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