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 s are identified using polymer selection operator available in PyMOL.

-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 marcomolecules 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 marcomolecules in input file, type:

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

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SEE ALSO

DownloadPDBFiles.pl, PyMOLSplitChainsAndLigands.py, PyMOLVisualizeMacromolecules.py

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