NAME

PyMOLInfoMacromolecules.py - List information about macromolecules

SYNOPSIS

PyMOLInfoMacromolecules.py [--all] [--boundingBox] [--centroid] [--chains] [--countResidues] [--header] [--inorganics] [--interfaceResidues] [--interfaceResiduesChains <ChainID1,ChainD2,...>] [--interfaceResiduesMethod <text>] [--interfaceResiduesCutoff <number>] [--ligands] [--pocketLigands] [--pocketDistanceCutoff <number>] [--pocketSolvents] [--pocketInorganics] [--phiPsi] [--phiPsiMode <All or Categories>] [--phiPsiPrecision <number>] [--surfaceResidues] [--surfaceResiduesCutoff <number>] [--surfaceResiduesIDs <yes or no>] [--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. --centroid Centroid of atomic coordinates. It corresponds to the mean of all 3D coordinates in input file. --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.

--interfaceResidues

Interface residues between specified pairs of chains.

--interfaceResiduesChains <ChainID1,Chain1D2,...> [default: Auto]

Pairwise comma delimited list of chain IDs for the identification of interface residues. Each chain ID may contain mutiple chain IDs delimited by a plus sign. For example: A+B,C+D chain pair specifies interface between chain complexes A+B and C+D.

The interface residues are identified between first two chains in input files by default.

--interfaceResiduesMethod <text> [default: BySASAChange]

Methodology for the identification of interface residues between a pair of chains in an input file. The interface residues may be identified by change in solvent accessible surface area (SASA) for a residue between a chain and chains complex, distance between heavy atoms in two chains, or distance between CAlpha atoms. Possible values: BySASAChange, ByHeavyAtomsDistance, or ByCAlphaAtomsDistance.

--interfaceResiduesCutoff <number> [default: auto]

Cutoff value used by different methodologies during identification of interface residues between a pair

of chains. The default values are shown below:

```
BySASAChange: 1.0; Units: Angstrom**2 [ Ref 141 ]
ByHeavyAtomsDistance: 5.0; Units: Angstrom [ Ref 142 ]
ByCAlphaAtomsDistance: 8.0; Units: Angstrom [ Ref 143 ]
```

-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.

--phiPsi

Phi and psi torsion angles across chains in macromolecules containing amino acids.

--phiPsiMode <All or Categories> [default: Categories]

List all phi and psi torsion angles for residues as a single group or split them into the following categories corresponding to four types of Ramachandran plots:

```
General: All residues except glycine, proline, or pre-proline
Glycine: Only glycine residues
Proline: Only proline residues
Pre-Proline: Only residues before proline not including glycine
    or proline
```

--phiPsiPrecision <number> [default: 2]

Precision for listing phi and psi torsion angles.

-s, --solvents

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

--surfaceResidues

Surface and buried residues in chains.

--surfaceResiduesCutoff <number> [default: 2.5]

Solvenet Accessible Surface Area (SASA) cutoff value in Angstroms**2 for surface and buried resiudes in chains. The residues with SASA less than the cutoff value correspond to burried residues.

--surfaceResiduesIDs <yes or no> [default: No]

List residue IDs for surface and buried residues during listing of the distribution of these residues for '--surfaceResidues' option.

-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"
```

To list interface residues between first two chains by SASA change for marcomolecules in input file, type:

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

To list interface residues between chains E and I by heay atoms distance for marcomolecules in input file, type:

```
% PyMOLInfoMacromolecules.py  --interfaceResidues
--interfaceResiduesChains E,I  --interfaceResiduesMethod
ByHeavyAtomsDistance --interfaceResiduesCutoff  5 -i Sample3.pdb
```

To list interface residues between two sets of chains by SASA change for marcomolecules in input file, type:

```
% PyMOLInfoMacromolecules.py  --interfaceResidues
--interfaceResiduesChains "A+B,C+D" -i Sample8.pdb
```

AUTHOR

Manish Sud(msud@san.rr.com)

SEE ALSO

DownloadPDBFiles.pl, PyMOLSplitChainsAndLigands.py, PyMOLVisualizeMacromolecules.py

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