

NAME

DownloadPDBFiles.pl - Download PDB files for PDB ID(s)

SYNOPSIS

DownloadPDBFiles.pl PDBID(s) or PDBIDsTextFile

DownloadPDBFiles.pl [-c, --colmode *colnum* | *collabel*] [-d, --dataLocationURL *PDB URL*] [-h, --help] [-d, --dataLocationURL *PDB URL*] [-e, --EDSMap *yes* | *no*] [--EDSMapLocationURL *EDS Map URL*] [-m, --mode <IDsOnCmdLine | IDsInFile>] [--PDBIDsCol *number* | *string*] [-w, --WorkingDir *dirname*] PDBID(s) or PDBIDsTextFile

DESCRIPTION

Download PDB files corresponding to PDB IDs specified in a column in a CSV/TSV text file or on the command line as space delimited parameters.

OPTIONS

-c, --colmode *colnum* | *collabel*

Specify how columns are identified in a *TextFile* containing PDB IDs: using column number or column label. Possible values: *colnum* or *collabel*. Default value: *colnum*.

-d, --dataLocationURL *PDB URL*

Specify location of PDB URL where data files are available for download. Default value: <http://www.rcsb.org/pdb/files/>.

-e, --EDSMap *yes* | *no*

Download Electron Density Map (EDS) in CCP4 format. Possible values: *Yes* or *No*. Default value: *no*.

--EDSMapLocationURL *EDS Map URL*

Specify location of EDS Map URL where data files are available for download. Default value: <http://www.ebi.ac.uk/pdbe/coordinates/files/>.

-h, --help

Print this help message.

--indelim *comma* | *semicolon*

Input delimiter for CSV *TextFile* containing PDB IDs. Possible values: *comma* or *semicolon*. Default value: *comma*. For TSV files, this option is ignored and *tab* is used as a delimiter.

-m, --mode <IDsOnCmdLine | IDsInFile>

Indicate how PDB IDs are specified: PDB IDs are either present as space delimited command line parameters or in a specific column in a CSV/TSV text file. Possible values: *IDsOnCmdLine* or *IDsInFile*. Default: *IDsOnCmdLine*.

-p, --PDBIDsCol *number* | *string*

Column used to identify PDB ID(s) in a text file. Default value: First column containing text string PDB_ID or <PDBID>.

For *colnum* value of -c, --colmode option, input value is a column number. Example: *1*.

For *collabel* value of -c, --colmode option, input value is a column label. Example: *PDB_ID*.

This option is ignored during *IDsOnCmdLine* value of m, --mode option.

-w, --WorkingDir *dirname*

Location of working directory. Default: current directory.

EXAMPLES

To retrieve a PDB files for PDB ID 2HYY and generate a local 2HYY.pdb file, type:

```
% DownloadPDBFiles.pl 2HYY
```

To retrieve PDB files for multiple PDB IDs 2HYY and 1KV2 and generate corresponding local PDB files, type:

```
% DownloadPDBFiles.pl 2HYY 1KV2
```

To download PDB files for PDB IDs present in column name PDB_ID or PDBID in SamplePDBIDs.csv file and generate corresponding PDB files, type

```
% DownloadPDBFiles.pl -m IDsInFile SamplePDBIDs.csv
```

To download PDB files for PDB IDs present in a specific column name in SamplePDBIDs.csv file and generate corresponding PDB files, type

```
% DownloadPDBFiles.pl -m IDsInFile -c collabel -p PDB_ID SamplePDBIDs.csv
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

[ExtractFromPDBFiles.pl](#), [InfoPDBFiles.pl](#), [ModifyPDBFiles.pl](#)

COPYRIGHT

Copyright (C) 2018 Manish Sud. All rights reserved.

This file is part of MayaChemTools.

MayaChemTools is free software; you can redistribute it and/or modify it under the terms of the GNU Lesser General Public License as published by the Free Software Foundation; either version 3 of the License, or (at your option) any later version.