

## NAME

ModifyPDBFiles.pl - Modify data in PDBFile(s)

## SYNOPSIS

ModifyPDBFiles.pl PDBFile(s)...

ModifyPDBFiles.pl [-a, --AtomNumberStart *number*] [-c, --ChainIDStart *character*] [--ChainIDRenameEmpty *yes | no*] [-h, --help] [-k, --KeepOldRecords *yes | no*] [-m, --mode *RenumberAtoms | RenumberResidues | RenumberWaters | RenameChainIDs*] [--ModifyHeader *yes | no*] [-o, --overwrite] [--ResidueNumberMode *Sequential | PerChain*] [--ResidueNumberStart *number*] [--ResidueNumberHetatmMode *automatic | specify*] [--ResidueNumberStarHetatm *number*] [-r, --root *rootname*] [--WaterResidueNames *Automatic | "ResidueName, [ResidueName,...]"*] [--WaterResidueStart *number*] [-w, --WorkingDir *dirname*] PDBFile(s)...

## DESCRIPTION

Modify data in *PDBFile(s)*: renumber atoms, residues, and water residues or assign new chain IDs. Multiple PDBFile names are separated by spaces. The valid file extension is *.pdb*. All other file name extensions are ignored during the wild card expansion. All the PDB files in a current directory can be specified either by *\*.pdb* or the current directory name.

## OPTIONS

-a, --AtomNumberStart *number*

Starting atom number to use during *RenumberAtoms* value of -m, --mode option. Default: 1. Valid values: positive integers.

-c, --ChainIDStart *character*

A single character to use for starting IDs for chains during *RenameChainIDs* value of -m, --mode option. Default: A. Valid values: A to Z.

--ChainIDRenameEmpty *Yes | No*

Specify whether to rename empty chain IDs during *RenameChainIDs* -m, --mode value. By default, ATOM and HETATM records with no chain IDs are left unchanged. Possible values: *yes | no*. Default: *No*.

-h, --help

Print this help message.

-k, --KeepOldRecords *yes | no*

Specify whether to transfer old non ATOM and HETATM records from input PDBFile(s) to new PDBFile(s). By default, except for the HEADER record, all records other than ATOM/HETATM are dropped during the generation of new PDB files. Possible values: *yes | no*. Default: *no*.

-m, --mode *RenumberAtoms | RenumberResidues | RenumberWaters | RenameChainIDs*

Specify how to modify *PDBFile(s)*. Possible values: *RenumberAtoms | RenumberResidues | RenumberWaters | RenameChainIDs*. Default: *RenumberResidues*.

For *RenumberAtoms* mode, residue number in ATOM and HETATM records are reassigned sequentially starting using value of -a, --AtomNumberStart option.

For *RenumberResidues* mode, serial number in ATOM and HETATM records are reassigned either sequentially or starting from specified values for ATOM and HETATM records in each chain.

For *RenumberWaters* mode, residue number for waters are reassigned starting from a specific value.

For *RenameChainIDs* mode, all the chain IDs are reassigned starting from a specific chain ID.

During the generation of new PDB files, unnecessary CONECT records are dropped.

--ModifyHeader *yes | no*

Specify whether to modify HEADER record during the generation of new PDB files. Possible values: *yes | no*. Default: *yes*. By default, Classification data is replaced by *Data modified using MayaChemTools* before writing out HEADER record.

-o, --overwrite

Overwrite existing files

--ResidueNumberMode *Sequential | PerChain*

Specify how to renumber residues: renumber residues sequentially across all the chains or start from the beginning for each chain. Possible values: *Sequential | PerChain*. Default: *PerChain*.

--ResidueNumberStart *number*

Starting residue number to use for ATOM records in chains. Default: 1. Valid values positive integers.

For *Sequential* value of --ResidueNumberMode option, residue numbers are assigned sequentially across all the chains starting from the specified value.

For *PerChain* value of --ResidueNumberMode option, residue numbers are starting again from the specified value for each chain.

HETATM residues within the chains are numbered using this value as well

--ResidueNumberHetatmMode *automatic | specify*

Specify how to start residue number for HETATM records: use the next sequential residue number after the last residue

number from ATOM records or start from a specific residue number. Possible values: *automatic* / *specify*. Default: *automatic*

For *automatic*, residue number after highest residue number of ATOM records is used as the starting residue number for HETATM records.

For *specify*, value of option --ResidueNumberStartHetatm is used as the starting residue number for HETATM records.

This option along with --ResidueNumberStartHetatm only applies to HETATM records outside the chains.

--ResidueNumberStartHetatm *number*

Starting residue number to use for HETATM records. Default: 6000. Valid values positive integers.

-r, --root *rootname*

New PDB and sequence file name is generated using the root: <Root><Mode>.<Ext>. Default new file name: <PDBFileName><Mode>.pdb. This option is ignored for multiple input files.

--WaterResidueNames *Automatic* / "*ResidueName,[ResidueName,...]*"

Identification of water residues during *RenumberWaters* value of -m, --mode option. Possible values: *Automatic* / "*ResidueName,[ResidueName,...]*". Default: *Automatic* which corresponds to "HOH,WAT,H2O". You can also specify a different comma delimited list of residue names to use for water.

--WaterResidueStart *number*

Starting water residue number to use during *RenumberWaters* -m, --mode value. Default: 8000. Valid values: positive integers.

-w, --WorkingDir *dirname*

Location of working directory. Default: current directory.

## EXAMPLES

To renumber ATOM and HETATM residues starting from 1 for each chain with continuation to HETATM residues outside TER records in Sample2.pdb and generate Sample2RenumberResidues.pdb file, type:

```
% ModifyPDBFiles.pl Sample1.pdb
```

To renumber ATOM and HETATM residues sequentially across all chains starting from 1 with continuation to HETATM residues outside TER records in Sample2.pdb and generate Sample2RenumberResidues.pdb file, type:

```
% ModifyPDBFiles.pl --ResidueNumberMode Sequential -o Sample1.pdb
```

To renumber ATOM and HETATM residues sequentially across all chains starting from 1 and HETATM residues outside TER records starting from 6000 in Sample2.pdb and generate Sample2RenumberResidues.pdb file, type:

```
% ModifyPDBFiles.pl --ResidueNumberMode Sequential
--ResidueNumberHetatmMode Specify -o Sample1.pdb
```

To renumber ATOM and HETATM residues sequentially across all chains starting from 100 for ATOM/HETATM residues with in TER records and starting from 999 for HETATM residues outside TER records in Sample2.pdb and generate Sample2RenumberResidues.pdb file, type:

```
% ModifyPDBFiles.pl --ResidueNumberMode Sequential
--ResidueNumberHetatmMode Specify --ResidueNumberStart 100
--ResidueNumberStartHetatm 999 -o Sample2.pdb
```

To renumber ATOM and HETATM residues from 100 for each chain and starting from 999 for HETATM residues outside TER records in Sample2.pdb and generate Sample2RenumberResidues.pdb file, type:

```
% ModifyPDBFiles.pl --ResidueNumberMode PerChain
--ResidueNumberHetatmMode Specify --ResidueNumberStart 100
--ResidueNumberStartHetatm 999 -o Sample2.pdb
```

To renumber ATOM serial numbers sequentially starting from 100 in Sample1.pdb file and generate Sample1RenumberAtoms.pdb file, type:

```
% ModifyPDBFiles.pl -m RenumberAtoms --AtomNumberStart 100
-o Sample1.pdb
```

To renumber water residues identified by "HOH,WAT" starting from residue number 1000 in Sample2.pdb file and generate Sample2RenumberWaters.pdb file, type:

```
% ModifyPDBFiles.pl -m RenumberWaters --WaterResidueNames "HOH,WAT"
-o --WaterResidueStart 950 Sample2.pdb
```

To rename all chain IDs starting from A in Sample1.pdb file and generate Sample1RenameChainIDs.pdb file, type:

```
% ModifyPDBFiles.pl -m RenameChainIDs -o Sample1.pdb
```

To rename all chain IDs starting from B without assigning any chain IDs to ATOM/HETATOM with no chain IDs in Sample2.pdb file and generate Sample2RenameChainIDs.pdb file, type:

```
% ModifyPDBFiles.pl 1 -m RenameChainIDs -c B --ChainIDRenameEmpty No  
-o Sample2.pdb
```

#### AUTHOR

Manish Sud <msud@san.rr.com>

#### SEE ALSO

ExtractFromPDBFiles.pl, InfoPDBFiles.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.