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 statring 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 defailt, 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 begining 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 with in 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 --ResidueNumberStarHetatm 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,H20". 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 l -m RenameChainIDs -c B --ChainIDRenameEmpty No
  -o Sample2.pdb
```

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SEE ALSO

ExtractFromPDBFiles.pl, InfoPDBFiles.pl

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