

## NAME

ExtractFromPDBFiles.pl - Extract specific data from PDBFile(s)

## SYNOPSIS

ExtractFromPDBFiles.pl PDBFile(s)...

```
ExtractFromPDBFiles.pl [-c, --chains First | All | "ChainID, [ChainID,...]"] [<--CombineChains> yes | no] [-d,
--distance number] [--DistanceMode Atom | Hetatm | Residue | XYZ] [--DistanceOrigin "AtomNumber,
AtomName" | "HetatmNumber, HetAtmName" | "ResidueName, ResidueNumber, [ChainID]" | "X,Y,Z">] [-h,
--help] [-k, --KeepOldRecords yes | no] [-m, --mode Chains | Sequences | Atoms | CAlphas | Distance |
NonWater | NonHydrogens] [--ModifyHeader yes | no] [--NonStandardKeep yes | no] [
--NonStandardCode character] [-o, --overwrite] [-r, --root rootname] [--SequenceLength number] [
--SequenceRecords Atom | SeqRes] [--SequenceIDPrefix FileName | HeaderRecord | Automatic] [
--WaterResidueNames Automatic | "ResidueName, [ResidueName,...]"] [-w, --WorkingDir dirname]
PDBFile(s)...
```

## DESCRIPTION

Extract specific data from *PDBFile(s)* and generate appropriate PDB or sequence file(s). 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.

During *Chains* and *Sequences* values of *-m, --mode* option, all ATOM/HETAM records for chains after the first model in PDB files containing data for multiple models are ignored.

## OPTIONS

*-c, --chains First | All | ChainID,[ChainID,...]*

Specify which chains to extract from *PDBFile(s)* during *Chains | Sequences* value of *-m, --mode* option: first chain, all chains, or a specific list of comma delimited chain IDs. Possible values: *First | All | ChainID,[ChainID,...]*. Default: *First*. Examples:

```
A
A,B
All
```

*--CombineChains yes | no*

Specify whether to concatenate all the chains before generating sequence file(s). Possible values: *yes | no*. Default: *no*

*-d, --distance number*

Specify distance used to extract ATOM and HETATM records during *Distance* value of *-m, --mode* option. Default: *10.0* angstroms.

*--DistanceMode Atom | Hetatm | Residue | XYZ*

Specify how to extract ATOM and HETATM records from *PDBFile(s)* during *Distance* value of *-m, --mode* option: extract all the records within a certain distance specified by *-d, --distance* from an atom or hetroatom record, a residue, or any arbitrary point. Possible values: *Atom | Hetatm | Residue | XYZ*. Default: *XYZ*

During *Residue* value of *--distancemode*, distance of ATOM/HETATM records is calculated from all the atoms in the residue and the records are selected as long as any atom of the residue lies with in the distace specified using *-d, --distance* option.

*--DistanceOrigin "AtomNumber,AtomName" | "HetatmNumber,HetAtmName" | "ResidueName,ResidueNumber[,ChainID]" | "X,Y,Z"*

This value is *--distancemode* specific. In general, it identifies a point used to select other ATOM/HETATMS with in a specific distance from this point.

For *Atom* value of *--distancemode*, this option corresponds to an atom specification. Format: *AtomNumber,AtomName*. Example:

```
455,CA
```

For *Hetatm* value of *--distancemode*, this option corresponds to a hetatm specification. Format: *HetatmNumber,HetAtmName*. Example:

```
5295,C1
```

For *Residue* value of *--distancemode*, this option corresponds to a residue specification. Format:

*ResidueNumber, ResidueName[, ChainID]*. Example:

```
78 ,MSE
977 ,RET ,A
978 ,RET ,B
```

For *XYZ* value of `--distancemode`, this option corresponds to a coordinate of an arbitrary point.  
Format: *X,Y,X*. Example:

```
10.044 ,19.261 , -4.292
```

`-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) during *Chains* / *Atoms* / *HetAtoms* / *CAAlphas* / *Distance* / *NonWater* / *NonHydrogens* value of `-m --mode` option. By default, except for the HEADER record, all other unnecessary non ATOM/HETATM records are dropped during the generation of new PDB files. Possible values: *yes* / *no*. Default: *no*.

`-m, --mode Chains / Sequences / Atoms / CAAlphas / Distance / NonWater / NonHydrogens`

Specify what to extract from *PDBFile(s)*: *Chains* - retrieve records for specified chains; *Sequences* - generate sequence files for specific chains; *Atoms* - extract atom records; *CAAlphas* - extract records for alpha carbon atoms corresponding to amino acids; *Distance* - extract records with in a certain distance from a specific position; *NonWater* - extract records corresponding to residues other than water; *NonHydrogens* - extract non-hydrogen records.

Possible values: *Chains, Sequences Atoms, CAAlphas, Distance*. Default value: *NonWater*

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

For *Chains* mode, data for appropriate chains specified by `--c --chains` option is extracted from *PDBFile(s)* and placed into new PDB file(s).

For *Sequences* mode, residues names using various sequence related options are extracted for chains specified by `--c --chains` option from *PDBFile(s)* and FASTA sequence file(s) are generated.

For *Distance* mode, all ATOM and HETATM records with in a distance specified by `-d --distance` option from a specific atom, residue or a point indicated by `--distancemode` are extracted and placed into new PDB file(s).

For *NonWater* mode, non water ATOM and HETATM record lines, identified using value of `--WaterResidueNames`, are extracted and written to new PDB file(s).

For *NonHydrogens* mode, ATOM and HETATOM record lines containing element symbol other than *H* are extracted and written to new PDB file(s).

For all other options, appropriate ATOM and HETATM records are extracted to generate new PDB file(s).

`--ModifyHeader yes / no`

Specify whether to modify HEADER record during the generation of new PDB files for `-m, --mode` values of *Chains* / *Atoms* / *CAAlphas* / *Distance*. Possible values: *yes* / *no*. Default: *yes*. By default, Classification data is replaced by *Data extracted using MayaChemTools* before writing out HEADER record.

`--NonStandardKeep yes / no`

Specify whether to include and convert non-standard three letter residue codes into a code specified using `--nonstandardcode` option and include them into sequence file(s) generated during *Sequences* value of `-m, --mode` option. Possible values: *yes* / *no*. Default: *yes*

A warning is also printed about the presence of non-standard residues. Any residue other than standard 20 amino acids and 5 nucleic acid is considered non-standard; additionally, HETATM residues in chains also tagged as non-standard.

`--NonStandardCode character`

A single character code to use for non-standard residues. Default: *X*. Possible values: *?, -, or X*

`-o, --overwrite`

Overwrite existing files

`-r, --root rootname`

New PDB and sequence file name is generated using the root: `<Root><Mode>.<Ext>`. Default new file name: `<PDBFileName>Chain<ChainID>.pdb` for *Chains* mode;  
`<PDBFileName>SequenceChain<ChainID>.fasta` for *Sequences* mode;

<PDBFileName>DistanceBy<DistanceMode>.pdb for *Distance* -m, --mode  
 <PDBFileName><Mode>.pdb for *Atoms* | *CAAlphas* | *NonWater* | *NonHydrogens* -m, --mode values. This  
 option is ignored for multiple input files.

--SequenceLength *number*

Maximum sequence length per line in sequence file(s). Default: 80

--SequenceRecords *Atom* | *SeqRes*

Specify which records to use for extracting residue names from *PDBFiles(s)* during *Sequences* value of  
 -m, --mode option: use ATOM records to compile a list of residues in a chain or parse SEQRES record  
 to get a list of residues. Possible values: *Atom* | *SeqRes*. Default: *Atom*.

--SequenceIDPrefix *FileName* | *HeaderRecord* | *Automatic*

Specify how to generate a prefix for sequence IDs during *Sequences* value of -m, --mode option: use  
 input file name prefix; retrieve PDB ID from HEADER record; or automatically decide the method for  
 generating the prefix. The chain IDs are also appended to the prefix. Possible values: *FileName* |  
*HeaderRecord* | *Automatic*. Default: *Automatic*

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

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

-w, --WorkingDir *dirname*

Location of working directory. Default: current directory

## EXAMPLES

To extract non-water records from Sample2.pdb file and generate Sample2NonWater.pdb file, type:

```
% ExtractFromPDBFiles.pl Sample2.pdb
```

To extract non-water records from Sample2.pdb file using HOH or WAT residue name for water along with all  
 old non-coordinate records and generate Sample2NewNonWater.pdb file, type:

```
% ExtractFromPDBFiles.pl -m NonWater --WaterResidueNames "HOH,WAT"  

  -KeepOldRecords Yes -r Sample2New -o Sample2.pdb
```

To extract non-hydrogens records from Sample2.pdb file and generate Sample2NonHydrogen.pdb file, type:

```
% ExtractFromPDBFiles.pl -m NonHydrogens Sample2.pdb
```

To extract data for first chain in Sample2.pdb and generate Sample2ChainA.pdb, type file, type:

```
% ExtractFromPDBFiles.pl -m chains -o Sample2.pdb
```

To extract data for both chains in Sample2.pdb and generate Sample2ChainA.pdb and Sample2ChainB.pdb,  
 type:

```
% ExtractFromPDBFiles.pl -m chains -c All -o Sample2.pdb
```

To extract data for alpha carbons in Sample2.pdb and generate Sample2CAAlphas.pdb, type:

```
% ExtractFromPDBFiles.pl -m CAAlphas -o Sample2.pdb
```

To extract data for all ATOM and HETATM records with in 10 angstrom of an atom specified by atom serial  
 number and name "1,N" in Sample2.pdb file and generate Sample2DistanceByAtom.pdb, type:

```
% ExtractFromPDBFiles.pl -m Distance --DistanceMode Atom  

  --DistanceOrigin "1,N" -k No --distance 10 -o Sample2.pdb
```

To extract data for all ATOM and HETATM records with in 25 angstrom of an arbitrary point "0,0,0" in  
 Sample2.pdb file and generate Sample2DistanceByXYZ.pdb, type:

```
% ExtractFromPDBFiles.pl -m Distance --DistanceMode XYZ  

  --DistanceOrigin "0,0,0" -k No --distance 25 -o Sample2.pdb
```

AUTHOR

Manish Sud <msud@san.rr.com>

SEE ALSO

InfoPDBFiles.pl, ModifyPDBFiles.pl

COPYRIGHT

Copyright (C) 2004-2008 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.