NAME

PDBCORE − Extracts part of a PDB structure surrounding core residues

SYNOPSIS

pdbcore [**−d?** (?:0˜3)] [**−h**] [**−i** *filename*] [**−near** number] [**−o** *filename*] [**−q**] [**−resid** *listfile*]

DESCRIPTION

This program extracts part of a structure from a given PDB file based on a specified distance between the core region and the surrounding atoms of the given PDB file.

OPTIONS

Command line option specifications are processed from left to right and may be specified more than once. If conflicting options are specified, later specifications override earlier ones.

−d? (?:0˜3)   Turn on debug printing. The printing level can be controlled by a given number. The larger the number, the more information will be printed when the program is running.

−h
−−help   Print full PDBCORE documentation via perldoc. Cannot be used with other options.

−i *filename*   Input PDB file.

−near number   number is in Angstroms. Atoms within number distance of core residue atoms will be extracted. Default is 12.0.

−o *filename*   Output PDB file. The default is newONIOMFile.gjf.

−q   Run in quiet mode and do not print progress messages.

−resid *listfile*   File containing the list of core residues. The distance between surrounding atoms and these core residues will be used to set up the optimization flags. The file format is [Residue Name] "Residue ID", eg:

[GLU] "345"

[ASP] "233"

[GLY] "344"

Information for each core residue needs to be on a separate line.

Please note that Residue ID is a string, which can contain both the residue number and chain name, for example "A 345" (residue 345 in chain A) may also be used as Residue ID.

EXAMPLES

pdbcore
Called without any parameters, PDBCORE will display usage information. If **−h** or **−−help** is passed then the full PDBCORE documentation is displayed via perldoc.

pdbcore −resid listfile −near 14 −i foo.pdb −o foosmall.pdb
PDBCORE takes all the residues which have at least one atom within 14 Angstroms of any atom in the core region and saves to foosmall.pdb.

NOTES

When running PDBCORE, there may be some warning signs that some atoms or residues cannot be recognized. Therefore, atom types or partial charges cannot be assigned. These warnings usually do not affect the output PDB file. Please check the output PDB file.

VERSION

1.0

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